

DEVELOPING ANTIANGIOGENIC COMPOUNDS:
COMPUTATIONAL STUDIES OF CURCUMIN BASED DRUGS
AND METHIONINE AMINOPEPTIDASE TYPE II INHIBITORS

by

TEDMAN J. EHLERS

(Under the direction of Joel Phillip Bowen)

ABSTRACT

Angiogenesis has been identified as a crucial process in the growth and spread of cancers. There are many regulators of angiogenesis and their role is not yet fully understood. It has been shown that small molecule binding of the enzyme methionine aminopeptidase type II (MetAP2) results in the inhibition of endothelial cell proliferation. From a drug design prospective, this enzyme is an attractive target. Fumagillin and ovalicin, known natural products, bind with an IC_{50} in low nanomolar concentrations. Crystal structures of the bound complexes provide 3-dimensional coordinates for advanced computational studies.

Semi-synthetic fumagillin derivatives, e.g. TNP-470, have been shown to have better drug properties, but have yet to make it through clinical trials successfully. Previous work within our lab has resulted in the preparation of novel multicyclic analogs of fumagillin. With the early development of drug analogs, it is important to verify the feasibility of molecular binding, as well as provide a rationale for subsequent modification to produce more effective binding. With the information that can be obtained from a proper model, potential drugs can be examined *in silico*.

Additional work has led to the discovery of aromatic enones and dienones that show a remarkable ability to inhibit endothelial cell proliferation. These compounds are related to the natural product curcumin, which has been shown to inhibit angiogenesis *in vivo*. With a growing experimental data set, computational tools examining possible structure-activity relationships have been used to examine and accelerate the optimization of these compounds.

INDEX WORDS: Computer-aided drug design, angiogenesis, curcumin, fumagillin, methionine aminopeptidase, molecular mechanics

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of the
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DOCTOR OF PHILOSOPHY

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DEDICATION

To my parents,

Jim and Jeannie Ehlers,

Who provided endless patience and support throughout the past years.

My gratitude and love extends beyond that which I can describe with words.

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I would like to thank my friends for always keeping me in good spirits. My graduate experience would not have been the same without all of you. Thanks go to Karl, Jen, Pat and Phil for their friendships which have extended beyond our time here in the lab. I would also like to thank Richard Hubbard for the daily mental sparring which has taught me much more than just vocabulary.

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CHAPTER 1

INTRODUCTION

1.1 CHALLENGE OF TREATING CANCER

Cancer is a complex disease state, existing in a diverse collection of forms. Cancerous cells divide very rapidly, having lost their ability to undergo controlled division and lost internal mechanisms for self-destruction (apoptosis). It is a leading killer in the United States, second only to heart disease. Chemotherapy research has historically concentrated on cytotoxic agents, which target any rapidly dividing cell;¹ however, the side effects of these therapies often leave much to be desired. Alternatives to the direct attack of unstable cells are being pursued as more information about the bio-molecular basis of cancer is revealed. One such promising alternative targets the vascular system. Common to all types of cancer is the necessity of obtaining a blood supply. In 1972, Judah Folkman published a monumental hypothesis in which he stated that the inhibition of angiogenesis could be used to control the growth and spread of cancers.² This radical approach to cancer treatment required decades of study before gaining acceptance, but the idea has now exploded into a huge field of research. Antiangiogenic therapy is beginning to be realized as the first angiogenesis inhibitor, Avastin (bevacizumab), was approved by the U.S. Food and Drug Administration in 2004. There are currently over 20 other compounds in current clinical trials that target angiogenesis and may soon be available for widespread use.

1.2 ANGIOGENESIS AND CANCER

The vascular system, comprised of nearly 100,000 miles of capillary blood vessels, is responsible for delivering oxygen and nutrients to every cell in the body, as well as removing

metabolic waste products from them. The inner lining of blood vessels is made up of endothelial cells. These cells form a barrier between tissues and the circulating blood supply. Endothelial cells are genetically stable and generally proliferate slowly. They do have the unique ability; however, to increase proliferation and spur the formation of new blood capillaries from the preexisting vasculature. This process is known as *angiogenesis*. This normal bodily process is complex and under the strict regulation of numerous angiogenic promoters and inhibitors (see Table 1.1). The process begins with the degradation of the basement membrane structure by activated matrix metallo-proteinases (MMPs). A stimulus then directs the outward migration of endothelial cells. Rapid endothelial cell proliferation ensues, followed by the formation of a lumen. A last stage is the formation of the extracellular matrix. This angiogenic process is crucial to the developing embryo, but remains relatively inactive in the adult body. In adults, tissues are fully developed, and the need for new blood vessels is limited to healing responses to injury and processes associated with the menstrual cycle.^{3,4}

Table 1.1: Selected examples of positive and negative regulators of angiogenesis

Angiogenesis regulators	
Positive regulation	Negative regulation
Angiogenin	Angiostatin
Angiopoietin-1	Endostatin
Epidermal growth factor	
Fibroblast growth factors (a & b)	Genistein
Hepatocyte growth factor	Interferon alpha
Interleukin 8	
Platelet-derived EC growth factor	Metallo-proteinase inhibitors
Scatter factor	
Tumor necrosis factor alpha	Thrombospondin-1
Vascular endothelial growth factor	Vasostatin

The pathological conversion of benign tumors to a malignant state involves passing a critical point of signal transduction. Tumors send out signals to nearby endothelial cells calling for them to exit quiescence and become angiogenic. The balance between endogenous angiogenic promoters and inhibitors is disrupted, and the *angiogenic switch* is said to be

turned on. Newly recruited blood supplies feed diseased tissue with oxygen and nutrients, allowing it to thrive as well as provide a means to spread to other locations in the body (metastasize). It has been shown that tumors will remain dormant and grow only to a 1-2 mm diameter if they do not acquire new blood supplies.⁵ The original postulation of Judah Folkman was that the inhibition of angiogenesis would limit tumor growth and the probability of metastases.^{2,6} A drug-like compound capable of restoring the natural balance of angiogenic regulators has the potential to be a minimally toxic, non-competing tool which could complement current cytotoxic treatments. This is the major goal which antiangiogenic therapy seeks to achieve.

1.3 DRUG DISCOVERY AND COMPUTATIONAL CHEMISTRY

The drug discovery process is a long and expensive endeavor. DiMasi recently published a latest report on current pharmaceutical company investments toward bringing new drugs to market. The results show that it takes an average of \$802 million and around 12 years to bring a drug from the discovery stage to market.⁷ With increasing computer power becoming available at lower and lower costs, there has been a large focus toward developing computational techniques to aid in the ever complex and multi-step discovery process. The computational chemist in a drug discovery setting plays a interactive role, acquiring and providing information among many scientists in various fields. The importance of computational chemistry was once questioned, but the proven advantages associated with using computer-assisted drug design methods have led to the formation of CADD groups within every major pharmaceutical company.

Two main research avenues face the computational chemist who is involved with drug discovery. The first, and most common situation, is in which knowledge of the drug target can only be inferred by the analysis of varied biological activities of compounds with similar structure. By analyzing the biological data, structural features are selected or modified in order to increase potency while reducing unwanted side effects. The second avenue is one in

which the 3-dimensional structure of the drug target is known from x-ray crystallography or any other experimental technique. In this case, the chemist must attempt to rationally design drugs that complement the known active site. The work described within this dissertation involves both of the above mentioned cases. The studies on aromatic enone and dienone analogs of curcumin follow the first case (ligand-based drug design), while the studies on fumagillin derived MetAP2 inhibitors follow the second case (structure-based drug design).

CHAPTER 2

CURCUMIN ANALOGS AS ANTIANGIOGENIC DRUGS

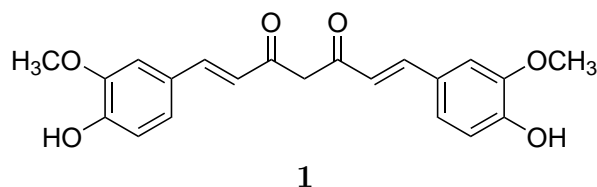


Figure 2.1: Structure of the natural product curcumin

2.1 CURCUMIN INTRODUCTION

Curcumin (**1**) is a carotenoid that is obtained from the rhizome of *Curcuma longa* and is regularly used as a flavoring and coloring agent in curries. This small molecular weight compound possesses a range of interesting biological activities including antibacterial,^{8,9} anti-carcinogenic,^{10,11} antioxidant,^{12,13} antiprotozoan,¹⁴ antitumoral¹⁵ and antiviral.¹⁶ Curcumin has been found to be a potent inhibitor of angiogenesis *in vitro* and *in vivo*.¹⁷ The exact mechanism by which its antiangiogenic activity is accomplished is yet to be fully understood. Curcumin has recently been found to be an irreversible inhibitor of aminopeptidase N (CD13), which may be the source of its angiogenic activity.¹⁸ To date, no 3-dimensional coordinates of this interaction are known.

2.1.1 STRUCTURAL ANALYSIS

Curcumin is often presented in the form shown in Figure 2.1 which may be misleading. It has been shown to exist almost entirely in the keto-enol form in the solid state (Figure 2.2).¹⁹ *Ab initio* calculations performed at the HF/6-31G* level support the experimental data

by reproducing the C2–O3 bond lengthening and the C1–C2 bond shortening. The overall structure is generally planar as opposed to the diketo form. The aromatic ring centroids are in plane with the C7–O8 bond. The diketo form is bent at C1 to 107° as one would expect from a system containing an sp^3 hybridized carbon.

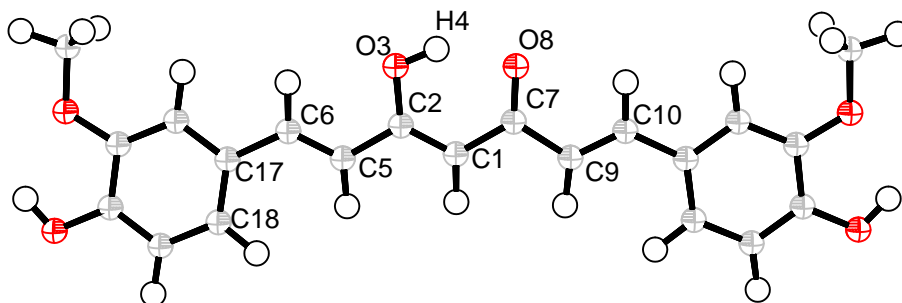


Figure 2.2: Crystal structure of curcumin showing keto–enol bridge

Co-planarity plays a role in curcumin’s known antioxidant activity and may be required for achieving antiangiogenic activity. A recent publication demonstrates that curcumin can undergo a sequential proton loss electron transfer (SPLET) mechanism of radical trapping to yield its antioxidant activity²⁰(Figure 2.3). Initial proton abstraction occurs at the more acidic keto–enol moiety. Calculations at the B3LYP/6-311+G** level^{21,22} show the anionic keto–enol to be planar. After the subsequent electron transfer step, the optimized geometry of the neutral doublet contains a slightly out of plane keto–enol moiety. A phenolic hydrogen is the target of the second proton abstraction. The radical anion product reorganizes, returning the keto–enol region to planarity. This is evidence for charge migration from the phenolic oxygen to the keto–enol bridge.

2.2 ENONE AND DIENONE RATIONALE

The structure of curcumin shown in Figure 2.4 is comprised of two substituted aromatic rings (A,C) tethered with a conjugated β -diketone (B), which is known to exist in a keto–enol form. Shortening the tether to one composed of a simple enone or dienone allows straightforward

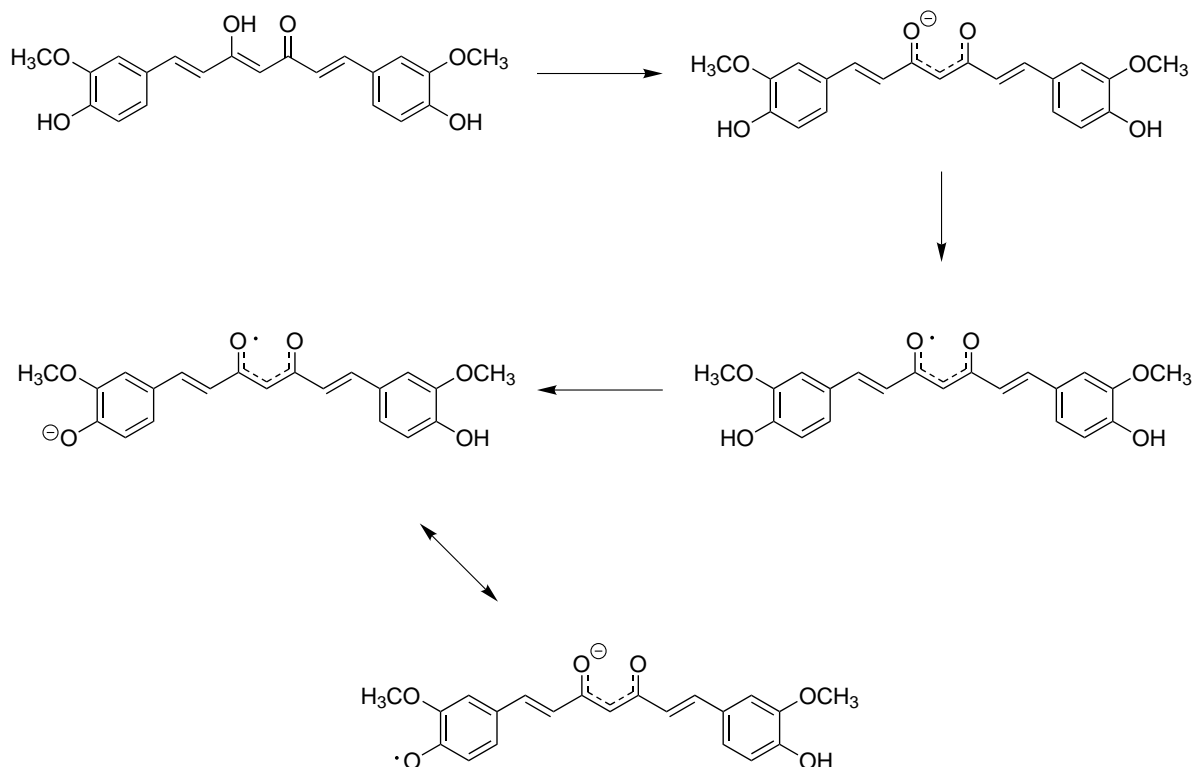


Figure 2.3: Sequential proton loss electron transfer process

access to various substituted aromatic systems via organic synthesis. The β -diketone moiety, as described above, is believed to be important for curcumin's antioxidant activity.^{23,24} The α, β -unsaturated carbonyl, however, suggests an electrophilic role. Conceivably a nucleophilic attack could occur through a 1,2 or 1,4 (Michael) addition. Pursuing the potential Michael acceptor role has led toward the development of analogs that replace the β -diketone region (B) with a single conjugated ketone (Figure 2.4).

2.3 DEVELOPMENT OF PHARMACOPHORE

A common situation in pharmaceutical design is the lack of known structural data of a receptor. It is the job of the medicinal chemist to derive an accurate model of the receptor based on data obtained from biological assays and structure-activity relationships.

A preliminary and simple three-dimensional pharmacophore has been developed based on the association of three main functional groups. The exploration of two substituted aromatic regions linked together by either an enone or dienone tether has yielded an impressive series of bio-active compounds.

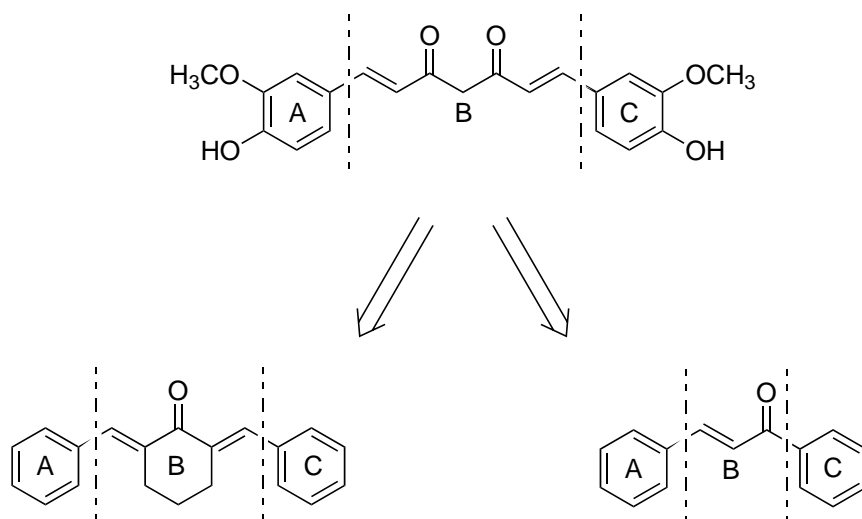


Figure 2.4: Simple 3-D pharmacophore explored

The three dimensional spacings between functional groups of the proposed pharmacophore are shown in Figure 2.5. Points of interest include the carbonyl donor oxygen and the head on and 60° off hydrogen bond donating sites. The aromatic centroids are also as crucial regions to calculate geometric spacing. The distance between aromatic units is found to be $7.57 \text{ \AA} \pm 0.25$ for the enone series and $10.10 \text{ \AA} \pm 0.25$ for the dienone series. Conformational flexibility allows for two main pharmacophore geometries. One of these presents the enone in an *s-trans* conformation. This conformation is analogous to related flavonoid structures which are known for their beneficial effects resulting from various anticancer, antiinflammatory, antioxidant, and antiviral activities.²⁵ Added ring systems provide rigidity which, in the case of tetralone and chromanone derivatives, force the pharmacophore to adopt an *s-cis* conformation.

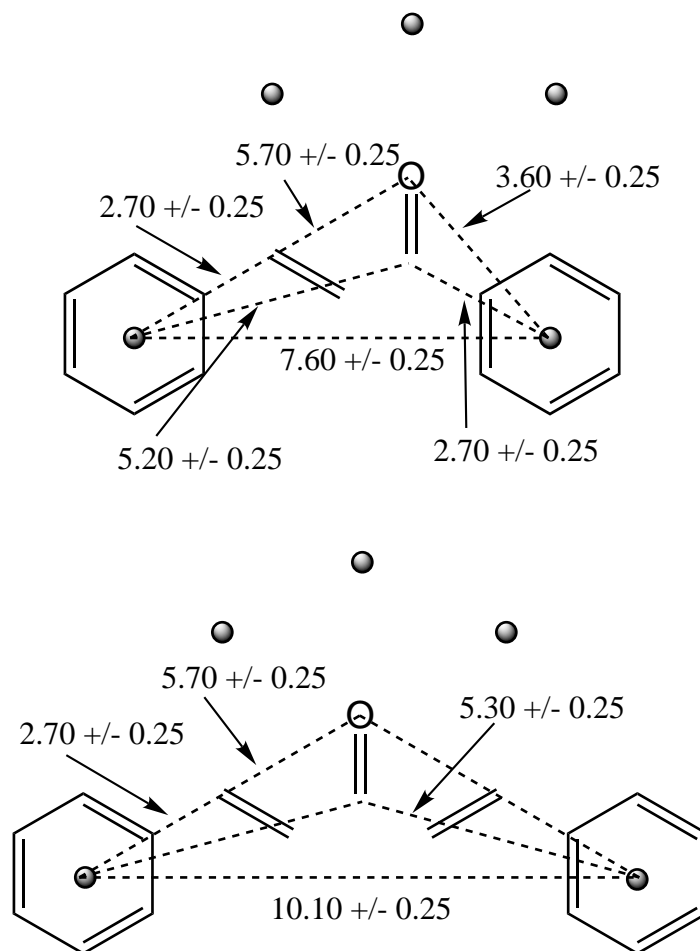


Figure 2.5: Distances between pharmacophoric regions

2.3.1 ELECTROPHILIC SITES

α,β -Unsaturated carbonyl compounds can undergo nucleophilic addition at either the carbonyl carbon (carbonyl addition) or at the β -carbon (Michael addition). Figure 2.6 shows a lowest occupied molecular orbital (LUMO) map projected onto a bond density surface according to an AM1 calculation implemented in Spartan02.²⁶ The darker regions indicated with an arrow are the more reactive sites in which the LUMO values are the greatest (see Section 2.6.1). The importance of the α,β -unsaturation has been a major discovery within the study.

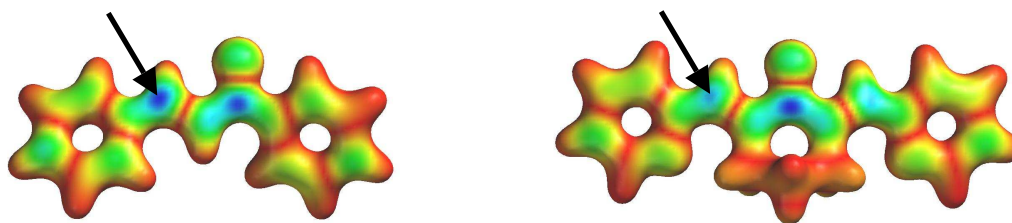


Figure 2.6: LUMO projection onto bond density showing electrophilic character

Choosing appropriate compounds to synthesize for biological testing is a difficult job for the medicinal chemist. Though it is important for pharmacophore verification to synthesize inactive compounds, any tool which allows for a synthetic chemist to forgo synthesizing unnecessary compounds is invaluable. The Topliss tree shown in Figure 2.7 shows a scheme in which analogs of a lead compound should be selected for synthesis with the goal of maximizing the potential of finding the most active compounds within a series. The scheme is based on a Hansch analysis where substituents affect activities based on hydrophobic, electronic, and steric contributions.²⁷ In retrospect, this type of scheme was loosely followed in the choosing of analogs that were synthesized in this group. Planning stages incorporated the utilization of the synthetic scheme combined with the more utilitarian approach of making use of available chemicals and chemicals that are commercially available.

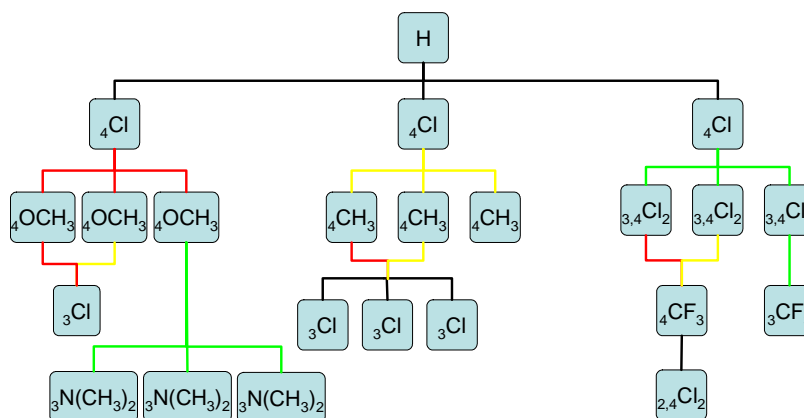


Figure 2.7: Topliss scheme for the design of more active compounds

2.4 CONFORMATIONAL ANALYSIS

As mentioned previously in Section 2.3, pharmacophore mapping must not overlook conformational flexibility in the procedure of aligning the active molecules.

The aromatic enones and dienones are highly conjugated molecules, but they do possess flexibility. Crystal structure data, as well as results from *ab initio* calculations, show the aromatic regions to be bent out of plane. This appears to be due to 1-4 hydrogen interactions, as in *s-cis* butadiene which has a dihedral angle of 18° . Microwave determination of geometries shows that the rings are indeed planar as one would expect. This would be consistent with a low energy barrier for phenyl rotations that could not be resolved. The isomerization from an *s-cis* to an *s-trans* conformation is not rapidly achieved at room temperatures. Calculations have been performed on various enone and dienone compounds exploring rotational energy barriers. Results are presented in Figure 2.8. Compounds with 2,6-substituted aromatics have more significant rotational barriers, but maintain the same general potential energy surface shape.

Perhaps a more important torsion is the rotation of the aromatic ring at C3. Figure 2.10 shows that planarity is difficult to achieve in compounds which contain 2,6-disubstitution

and a tetralone ring system. This bending out of plane interrupts the π -system overlap and creates a more favorable Michael acceptor. The π -system in compound **49** is nearly orthogonal at C3 and yet the compound is as active as curcumin, supporting the possible importance of a Michael acceptor.

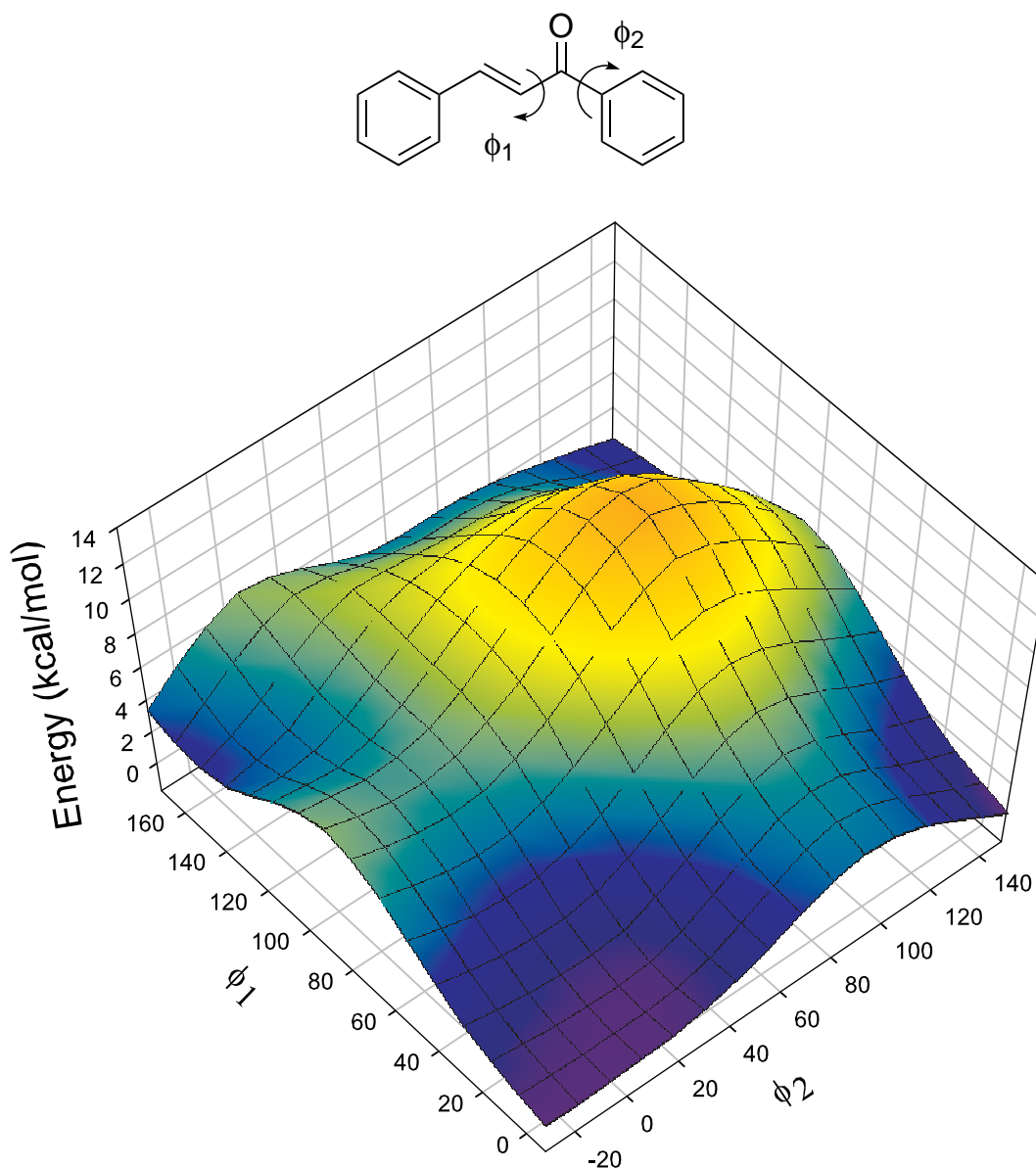


Figure 2.8: Potential energy surface for rotatable bonds in chalcone

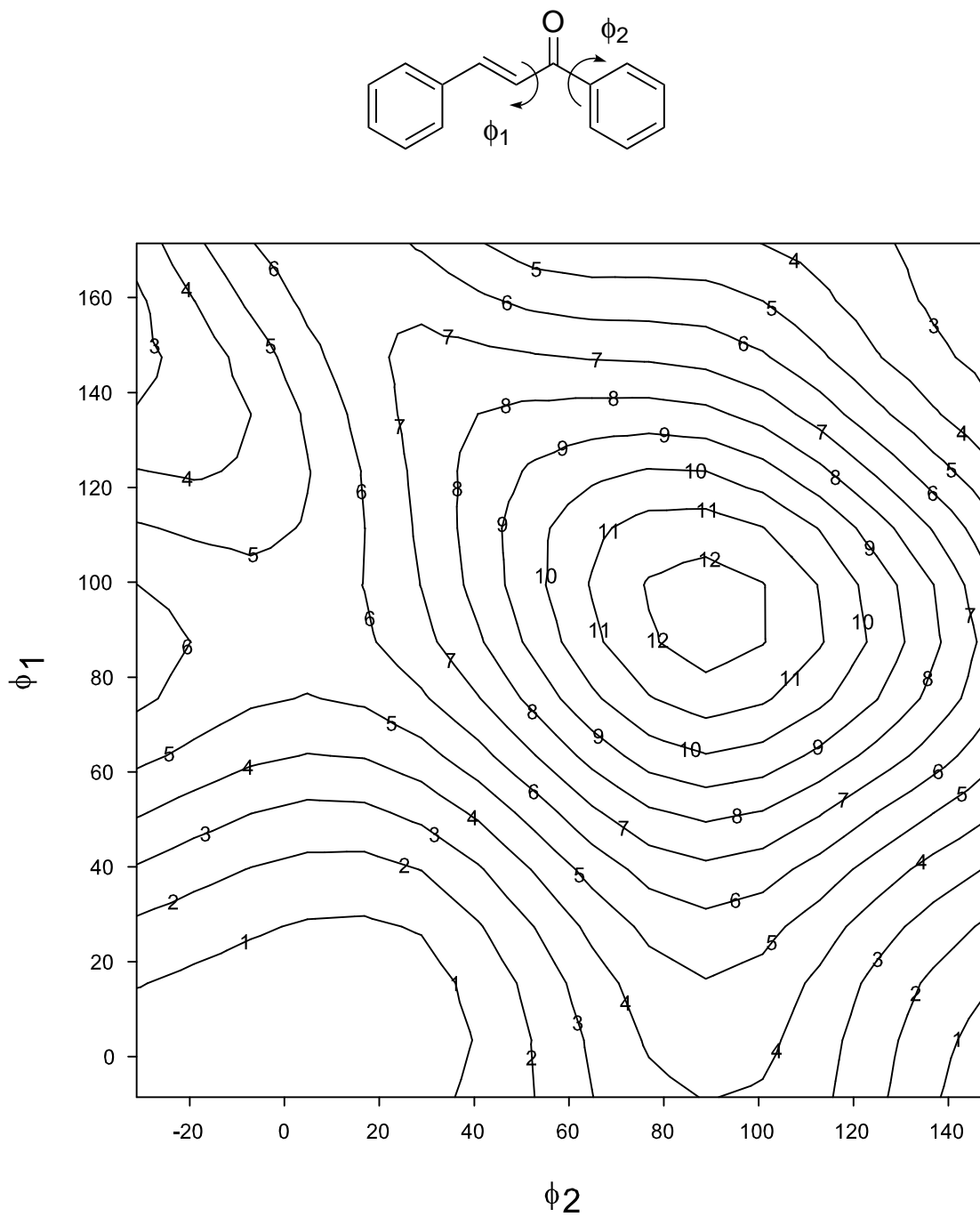
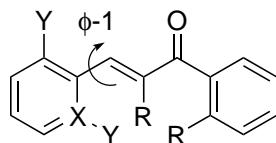


Figure 2.9: Topographical map of torsional barriers in chalcone (energy values shown are kcal/mol)



Torsion Curves for Phi-1

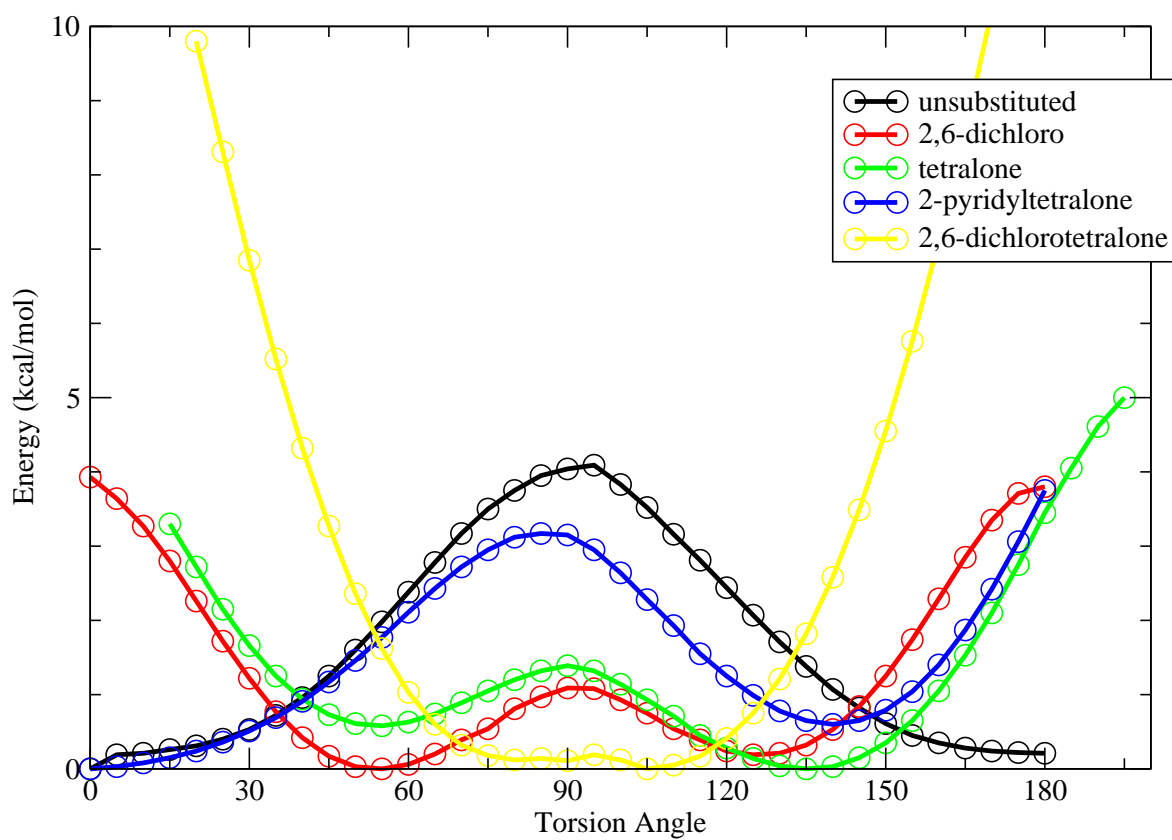


Figure 2.10: Rotational barriers for the aromatic ring at C3 computed with MM3

2.5 BIOLOGICAL TESTING

The development of any specific pharmaceutical compound is dependent upon the utilization of a reliable assay. The choice of an *in vitro* or *in vivo* assay should reflect the stage at which the study is. The pursuit of these enone and dienone analogs of curcumin has resulted in a large number of compounds to be screened. The unknown specific targets of these compounds also necessitates the use of an *in vitro* assay. *in vitro* assays are less expensive and more time efficient when compared to *in vivo* assays (e.g. the hamster cheek pouch assay or the corneal micropocket assay).^{28,29}

2.5.1 SVR PROLIFERATION AS ANGIOGENIC PROBE

An immortalized endothelial cell proliferation assay has been developed by Jack Arbiser et al.³⁰ at Emory University. The cell line, designated SVR, is transfected with the simian virus 40 and then further transfected with an additional retrovirus which encodes for activated H-ras. This assay is a proven method in which its results has been shown to coincide with *in vivo* antiangiogenic activity.¹⁷ This assay is the primary screen for antiangiogenic activity in the studies outlined herein.

2.5.2 RESULTS

Constraining the enone moiety into the *s-trans* configuration was achieved by introducing an additional ring as in the tetralones. Compound **24** maintains decent activity; however **23**, **34**, and **60** each perform poorly. This might indicate the need for some degree of conformational flexibility at the aromatic ketone connection.

Electron donating groups in the *ortho* and *para* positions have been previously reported to increase antioxidant activity of chalcones.³¹ This is consistent with observations that can be made of our enones. Methyl, halogen, and methoxy groups each could induce strong inhibition when placed in the *ortho*, *para* positions.

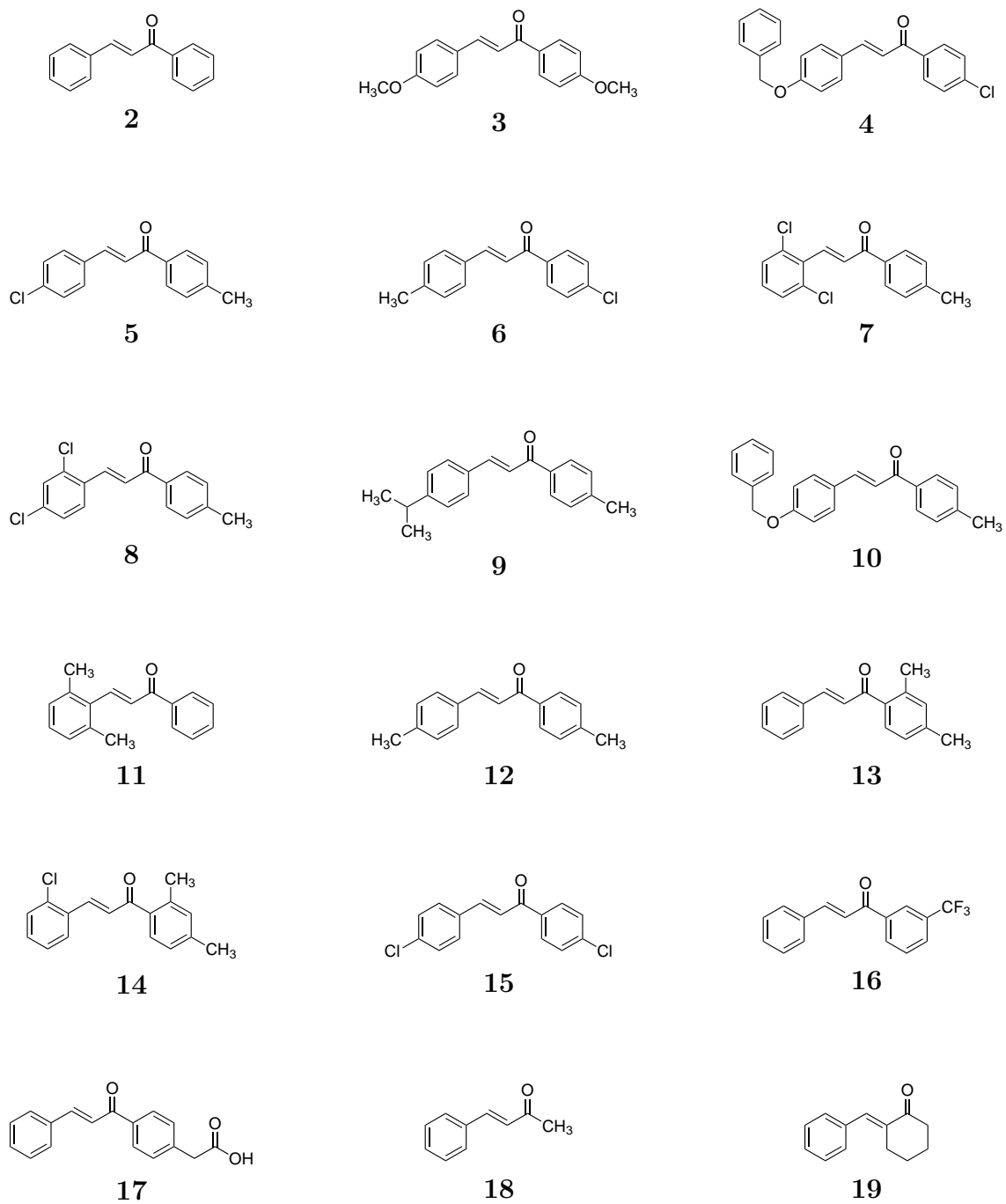


Figure 2.11: Enone structures 1

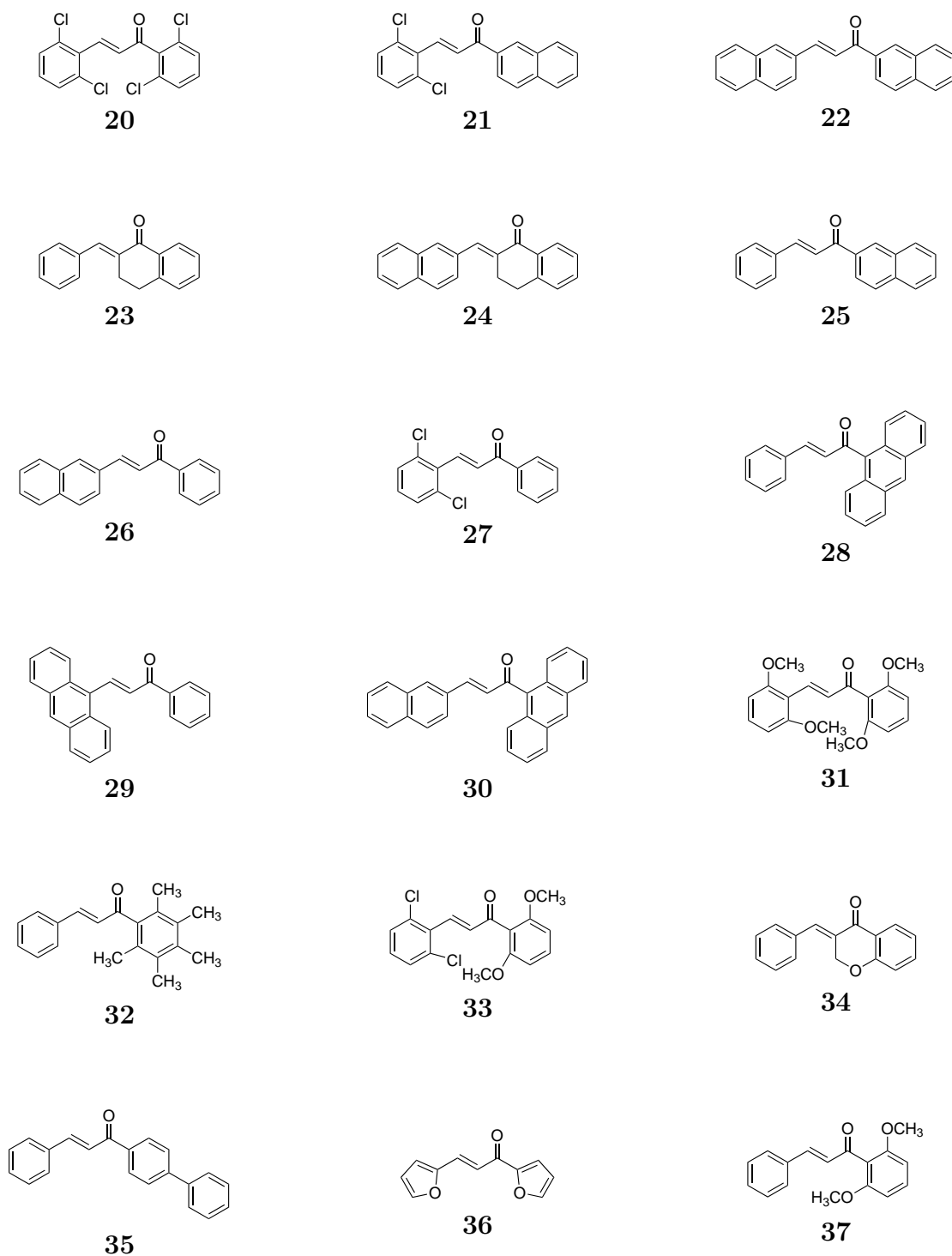


Figure 2.12: Enone structures 2

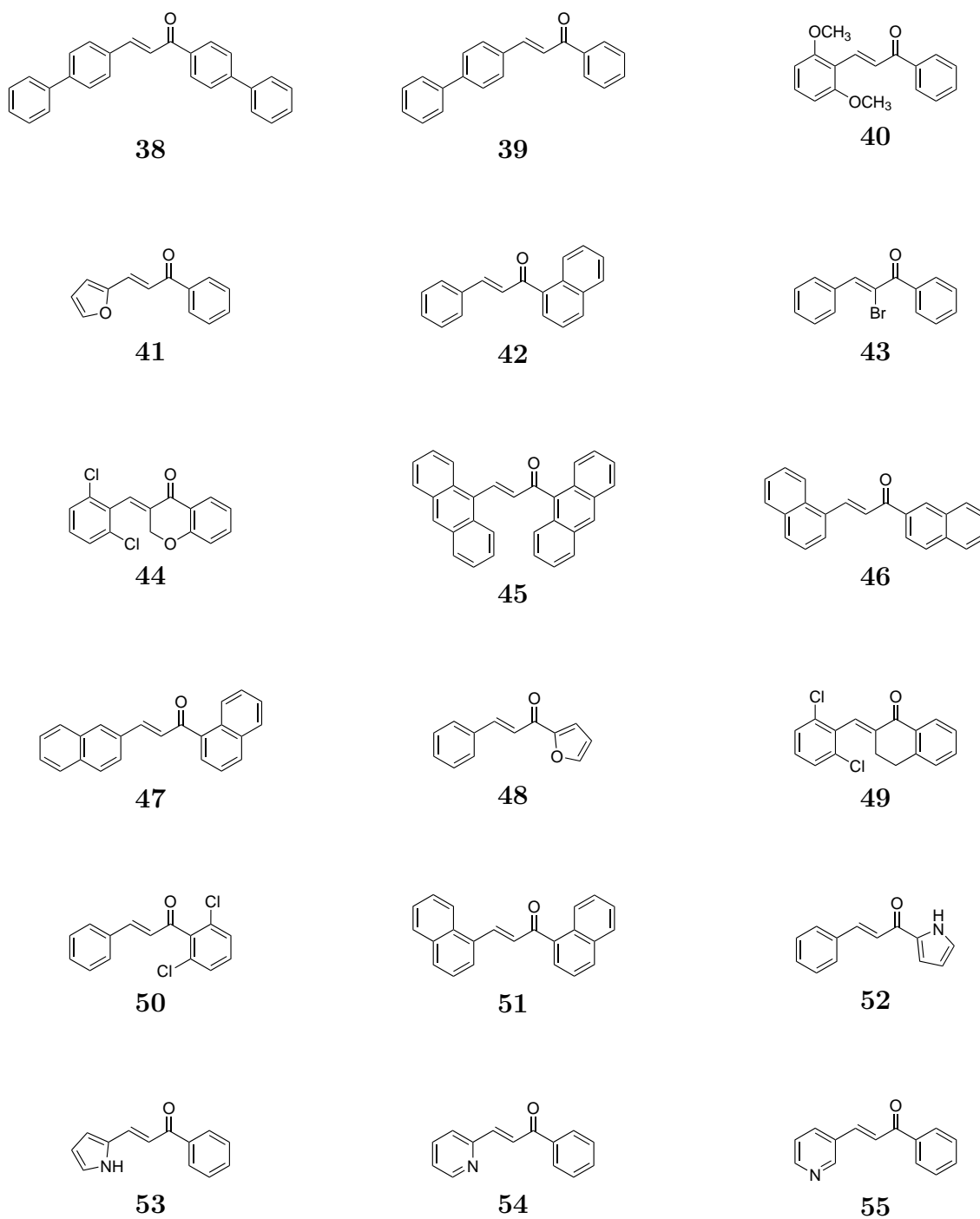


Figure 2.13: Enone structures 3

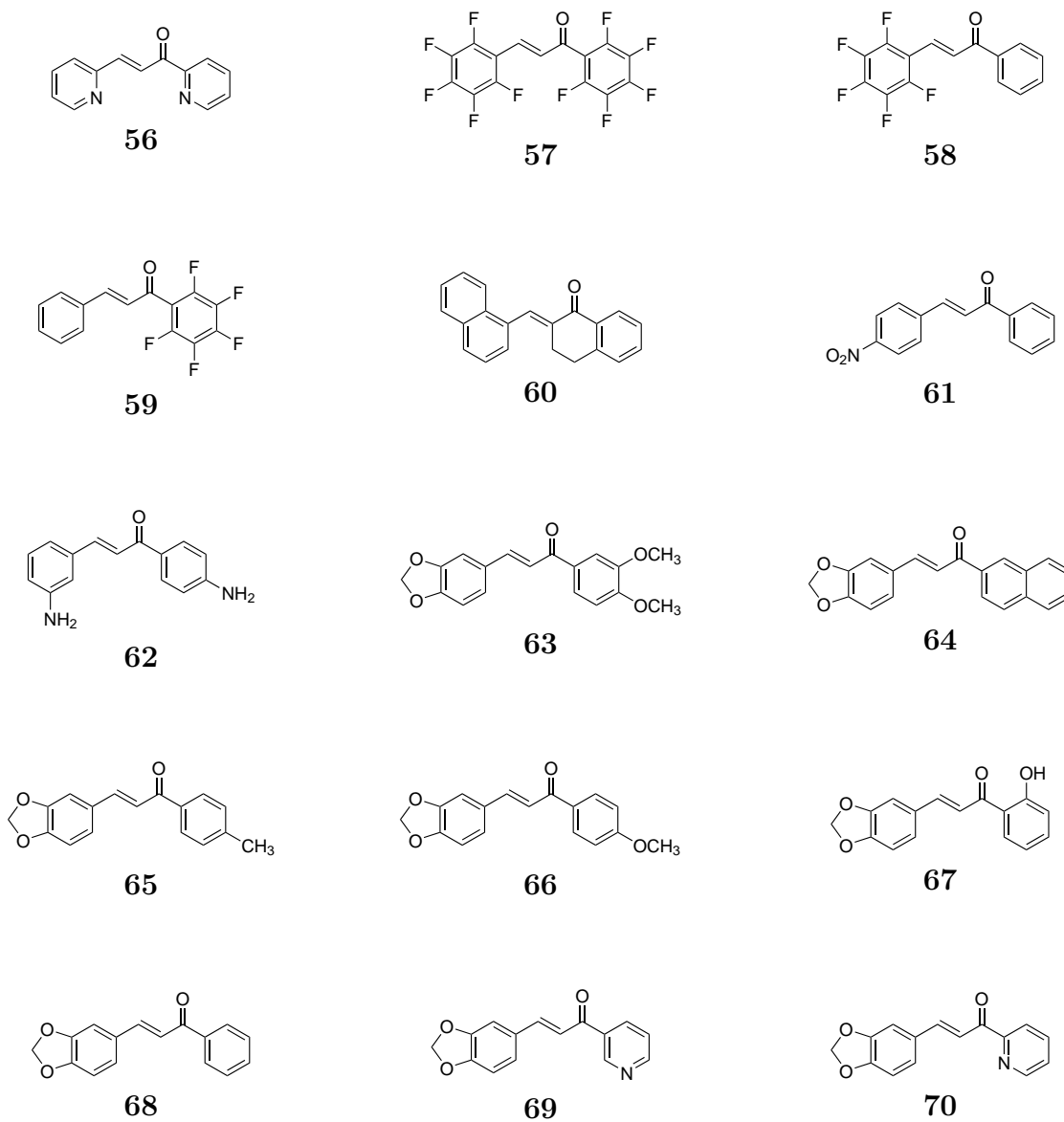


Figure 2.14: Enone structures 4

Table 2.1: Enone properties 1

Cpd	Name	% SVR cell growth inhibition		
		1 $\mu\text{g/mL}$	3 $\mu\text{g/mL}$	6 $\mu\text{g/mL}$
1	Curcumin	41.5	37.8	56.2
2	1,3-Diphenylpropenone	71.6	92.8	94.4
3	1,3-Di(4-methoxyphenyl)propenone	29.1	63.4	85.2
4	3-(4-Benzyloxyphenyl)-1-(4-chlorophenyl)propenone	25.6	4.4	62.9
5	3-(4-Chlorophenyl)-1-p-tolylpropenone	22.3	24.5	46.5
6	1-(4-Chlorophenyl)-3-p-tolylpropenone	29.9	40.2	58.5
7	3-(2,6-Dichlorophenyl)-1-p-tolylpropenone	73.7	98.2	98.1
8	3-(2,4-Dichlorophenyl)-1-p-tolylpropenone	19.9	10.4	84.7
9	3-(4-Isopropylphenyl)-1-p-tolylpropenone	19.5	14.2	59.2
10	3-(4-Benzyloxyphenyl)-1-p-tolylpropenone	18.4	5.1	17.0
11	3-(2,6-Dimethylphenyl)-1-phenylpropenone	47.7	57.9	89.6
12	1,3-Di-p-tolylpropenone	36.3	67.3	89.5
13	1-(2,4-Dimethylphenyl)-3-phenylpropenone	41.7	80.4	87.3
14	3-(2-Chlorophenyl)-1-(2,4-dimethylphenyl)propenone	29.6	25.3	73.4
15	1,3-Di(4-chlorophenyl)propenone	13.8	11.7	31.1
16	Phenyl-1-(3-trifluoromethylphenyl)propenone	42.3	87.4	96.9
17	1-(4-carboxymethylphenyl)-3-phenylpropenone	13.7	3.8	29.7
18	4-Phenylbut-3-en-2-one	41.9	69.0	64.0
19	2-Benzylidenecyclohexanone	23.0	29.5	72.4
20	1,3-Bis(2,6-dichloro-phenyl)propenone	48.3	75.3	93.7
21	3-(2,6-Dichlorophenyl)-1-naphthalen-2-ylpropenone	12.2	35.3	96.8
22	1,3-Dinaphthalen-2-ylpropenone	–	13.2	20.3
23	2-Benzylidene-3,4-dihydro-2H-naphthalen-1-one	5.7	11.4	40.8
24	2-Naphthalen-2-ylmethylene-3,4-dihydro-2H-naphthalen-1-one	84.7	84.9	78.8
25	1-Naphthalen-2-yl-3-phenylpropenone	0.0	78.7	88.6
26	3-Naphthalen-2-yl-1-phenylpropenone	0.0	75.4	66.2
27	3-(2,6-Dichlorophenyl)-1-phenylpropenone	4.6	61.0	94.0
28	1-Anthracen-9-yl-3-phenylpropenone	25.5	46.4	69.0
29	3-Anthracen-9-yl-1-phenylpropenone	54.6	53.5	71.3
30	1-Anthracen-9-yl-3-naphthalen-2-ylpropenone	52.5	57.3	48.1
31	1,3-Bis(2,6-dimethoxyphenyl)propenone	36.2	49.2	39.2
32	1-Pentamethylphenyl-3-phenylpropenone	12.6	0.0	5.3
33	3-(2,6-Dichlorophenyl)-1-(2,6-dimethoxyphenyl)propenone	23.2	43.7	52.3
34	3-Benzylidenechroman-4-one	12.3	23.8	54.3
35	1-Biphenyl-4-yl-3-phenylpropenone	10.4	34.7	0.0
36	1,3-Difuran-2-ylpropenone	7.7	8.1	12.0
37	1-(2,6-Dimethoxyphenyl)-3-phenylpropenone	25.8	39.8	63.5

Table 2.2: Enone properties 2

Cpd	Name	% SVR cell growth inhibition		
		1 $\mu\text{g/mL}$	3 $\mu\text{g/mL}$	6 $\mu\text{g/mL}$
38	1,3-Bis-biphenyl-4-ylpropenone	19.2	0.0	0.0
39	3-Biphenyl-4-yl-1-phenylpropenone	24.9	12.9	41.4
40	3-(2,6-Dimethoxyphenyl)-1-phenylpropenone	31.8	56.4	60.8
41	3-Furan-2-yl-1-phenylpropenone	9.8	1.0	0.0
42	1-Naphthalen-1-yl-3-phenylpropenone	10.9	33.2	68.2
43	2-Bromo-1,3-diphenylpropenone	57.2	75.7	79.8
44	3-(2,6-Dichlorobenzylidene)chroman-4-one	5.4	3.6	12.5
45	1,3-Dianthracen-9-ylpropenone	0.0	0.0	4.7
46	3-Naphthalen-1-yl-1-naphthalen-2-ylpropenone	0.0	24.9	50.3
47	3-Naphthalen-2-yl-1-naphthalen-1-ylpropenone	0.0	22.4	52.0
48	1-Furan-2-yl-3-phenylpropenone	28.2	57.7	90.2
49	2-(2,6-Dichlorobenzylidene)-3,4-dihydro-2H-naphthalen-1-one	32.8	37.0	53.7
50	1-(2,6-Dichlorophenyl)-3-phenylpropenone	2.2	51.1	88.7
51	1,3-Dinaphthalen-1-ylpropenone	12.0	55.5	60.3
52	3-Phenyl-1-(1H-pyrrol-2-yl)propenone	8.3	11.4	19.4
53	1-Phenyl-3-(1H-pyrrol-2-yl)propenone	19.0	21.5	0.4
54	1-Phenyl-3-pyridin-2-ylpropenone	40.7	89.1	96.9
55	1-Phenyl-3-pyridin-3-ylpropenone	30.3	31.7	83.2
56	1,3-Dipyridin-2-ylpropenone	0.0	53.4	85.2
57	1,3-Bispentafluorophenylpropenone	31.1	88.6	88.6
58	3-Pentafluorophenyl-1-phenylpropenone	0.0	0.0	0.0
59	1-Pentafluorophenyl-3-phenylpropenone	6.6	55.6	88.7
60	2-Naphthalen-1-ylmethylene-3,4-dihydro-2H-naphthalen-1-one	18.7	15.9	23.6
61	3-(4-Nitro-phenyl)-1-phenylpropenone	47.6	70.3	84.5
62	1-(4-Aminophenyl)-3-(3-aminophenyl)propenone	43.5	38.1	69.1
63	3-Benzo[1,3]dioxol-5-yl-1-(3,4-dimethoxyphenyl)propenone	1.9	24.2	48.1
64	3-Benzo[1,3]dioxol-5-yl-1-naphthalen-2-ylpropenone	5.7	1.4	11.9
65	3-Benzo[1,3]dioxol-5-yl-1-p-tolylpropenone	21.3	0.0	0.0
66	3-Benzo[1,3]dioxol-5-yl-1-(4-methoxyphenyl)propenone	1.0	14.4	45.5
67	3-Benzo[1,3]dioxol-5-yl-1-(2-hydroxyphenyl)propenone	36.5	12.7	24.5
68	3-Benzo[1,3]dioxol-5-yl-1-phenylpropenone	31.0	34.3	80.8
69	3-Benzo[1,3]dioxol-5-yl-1-pyridin-3-ylpropenone	33.0	32.5	68.9
70	3-Benzo[1,3]dioxol-5-yl-1-pyridin-2-ylpropenone	28.3	44.1	78.4

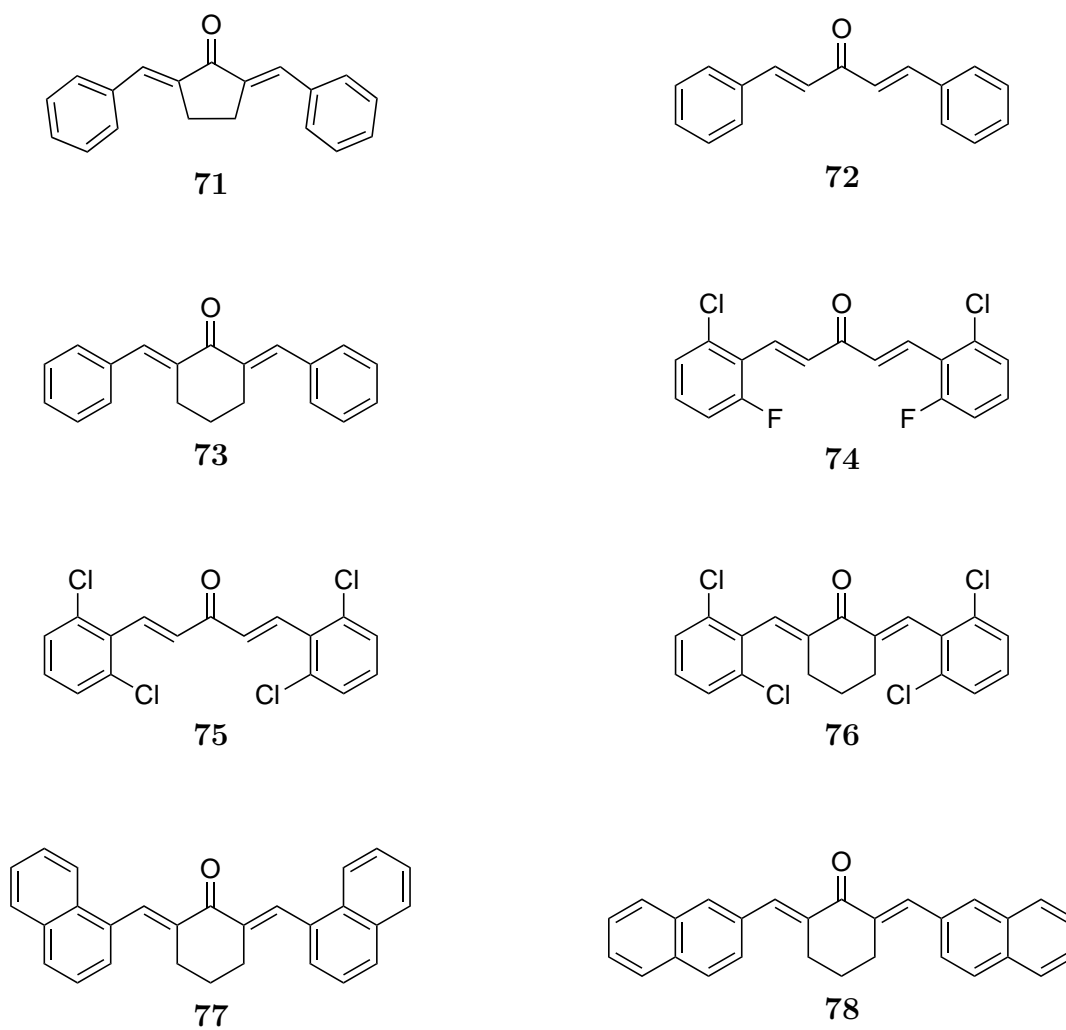


Figure 2.15: Dienone structures for compounds related to curcumin

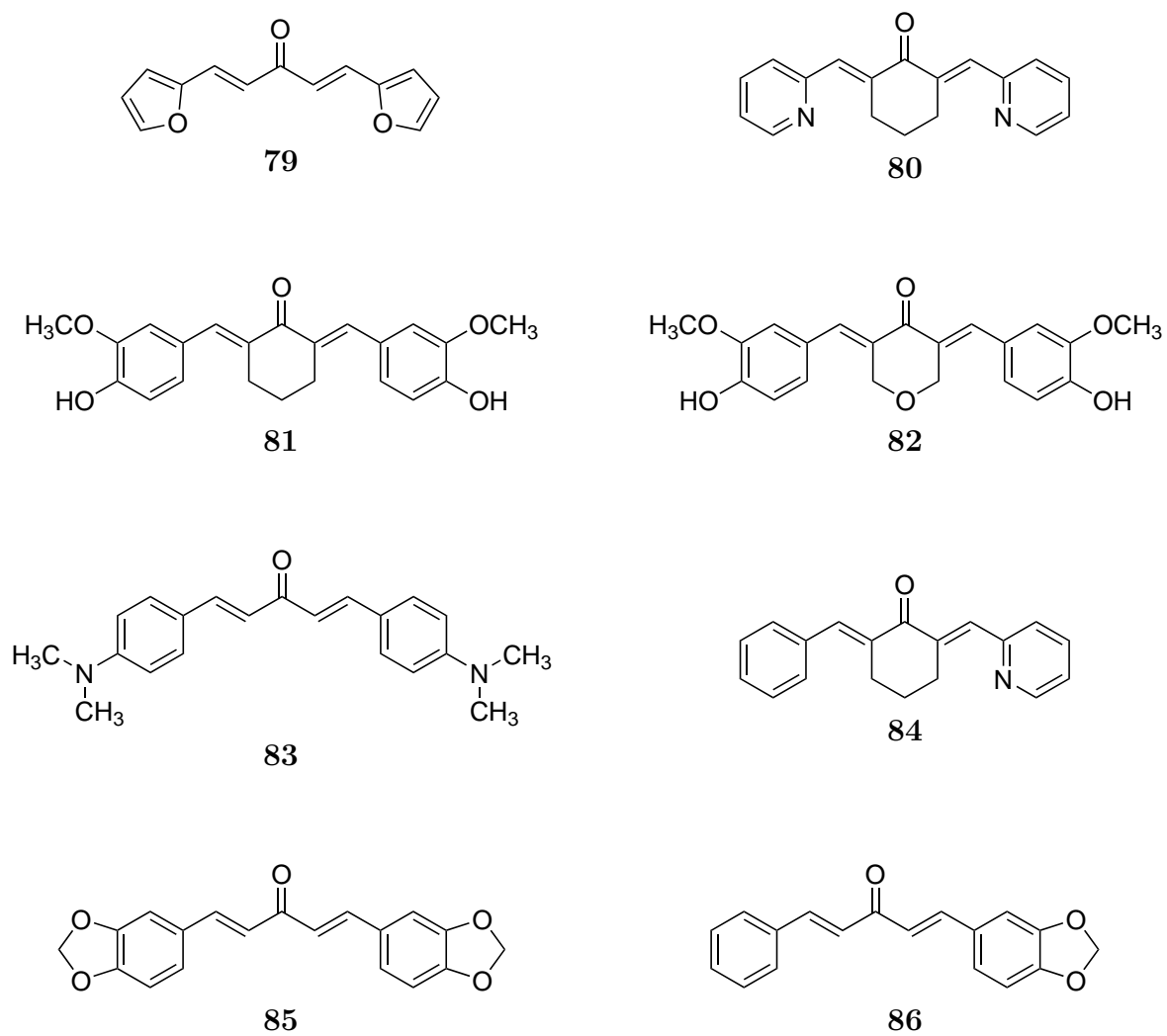


Figure 2.16: Dienone structures for compounds related to curcumin, cont.

Table 2.3: Dienone properties

Cpd	Name	% SVR cell growth inhibition		
		1 $\mu\text{g}/\text{mL}$	3 $\mu\text{g}/\text{mL}$	6 $\mu\text{g}/\text{mL}$
71	2,5-Dibenzylidenecyclopentanone	19.6	23.8	38.6
72	1,5-Diphenylpenta-1,4-dien-3-one	86.1	96.6	97.7
73	2,6-Dibenzylidenecyclohexanone	49.9	94.4	97.7
74	1,5-Bis(2-chloro-6-fluorophenyl)penta-1,4-dien-3-one	57.0	70.6	86.6
75	1,5-Bis(2,6-dichlorophenyl)penta-1,4-dien-3-one	60.7	87.1	90.4
76	2,6-Bis(2,6-dichlorobenzylidene)cyclohexanone	8.4	29.8	27.1
77	2,6-Di(naphthalen-1-ylmethylene)cyclohexanone	15.9	5.2	11.4
78	2,6-Di(naphthalen-2-ylmethylene)cyclohexanone	15.0	25.7	15.2
79	1,5-Difuran-2-ylpenta-1,4-dien-3-one	0.0	9.3	56.5
80	2,6-Di(pyridin-2-ylmethylene)cyclohexanone	88.3	92.9	96.7
81	2,6-Di(4-hydroxy-3-methoxybenzylidene)cyclohexanone	61.4	90.1	96.0
82	3,5-Di(4-hydroxy-3-methoxybenzylidene)tetrahydropyran-4-one	51.2	60.3	96.3
83	1,5-Bis(4-dimethylaminophenyl)penta-1,4-dien-3-one	34.0	41.3	49.2
84	2-Benzylidene-6-pyridin-2-ylmethylenecyclohexanone	24.5	39.2	59.6
85	1,5-Bisbenzo[1,3]dioxol-5-ylpenta-1,4-dien-3-one	0.0	12.4	17.1
86	1-Benzo[1,3]dioxol-5-yl-5-phenylpenta-1,4-dien-3-one	21.5	18.5	56.1

2.5.3 RESULTS

Compound **80**, which contains 2-pyridyl aromatic rings and a central cyclohexanone ring, is the most effective dienone, as the data in Table 2.3 shows. Endothelial cell proliferation is almost entirely ceased at concentrations as low as 1 $\mu\text{g}/\text{mL}$. Other dienones based on the central cyclohexanone or cyclopentanone ring with halogen substituted, or larger aromatic rings did not share in this remarkable activity. Aromatic substitutions involving the methoxyphenol system found in curcumin provided compounds **81** and **82**, which were stronger inhibitors than curcumin itself. Eliminating the central cycloalkanone ring to give a parent dibenzalacetone resulted in no loss of activity.

2.5.4 DOSE RESPONSE

To be certain that the compounds tested in the SVR assay were showing dose-dependent behavior, a series of dose response curves were generated for select enones and dienones (Figures 2.17 and 2.18). As can be seen from the figures, effectiveness does appear to show expected sigmoidal dose-dependency. The figures show regressions based on a variable slope four parameter logistic equation (2.1) where min and max are plateau regions. It should be noted that the potency of compounds **24** and **75** are greater than the other compound shown even though their efficacies do not reach the same levels. Potency refers to the dose required to achieve a desired effect. Efficacy refers to the maximum response that the drug is capable of achieving (at any dose).

$$Y = \text{minimum} + \frac{(\text{max} - \text{min})}{1 + 10^{(\log \text{EC}_{50} - x) \cdot \text{HillSlope}}} \quad (2.1)$$

2.6 STRUCTURE–ACTIVITY RELATIONSHIPS

Structure–activity models are continuously refined as new data becomes available. The following subsections include data calculated in order to extract some relationship which corresponds to the measured activities of our compounds

2.6.1 HOMO–LUMO GAPS

Reactivity of compounds can be estimated, in part, by examining the energy gap between the highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO). Frontier molecular orbital theory (FMO) states that transition states between reacting molecules involves overlap interactions between the HOMO and LUMO. The energy of the HOMO is related to a potential attack by an electrophile. The LUMO energy is directly related to the likelihood of being attacked by a nucleophile. The HOMO–LUMO gap, therefore, should be a measure of stability in terms of resisting chemical reaction.³²

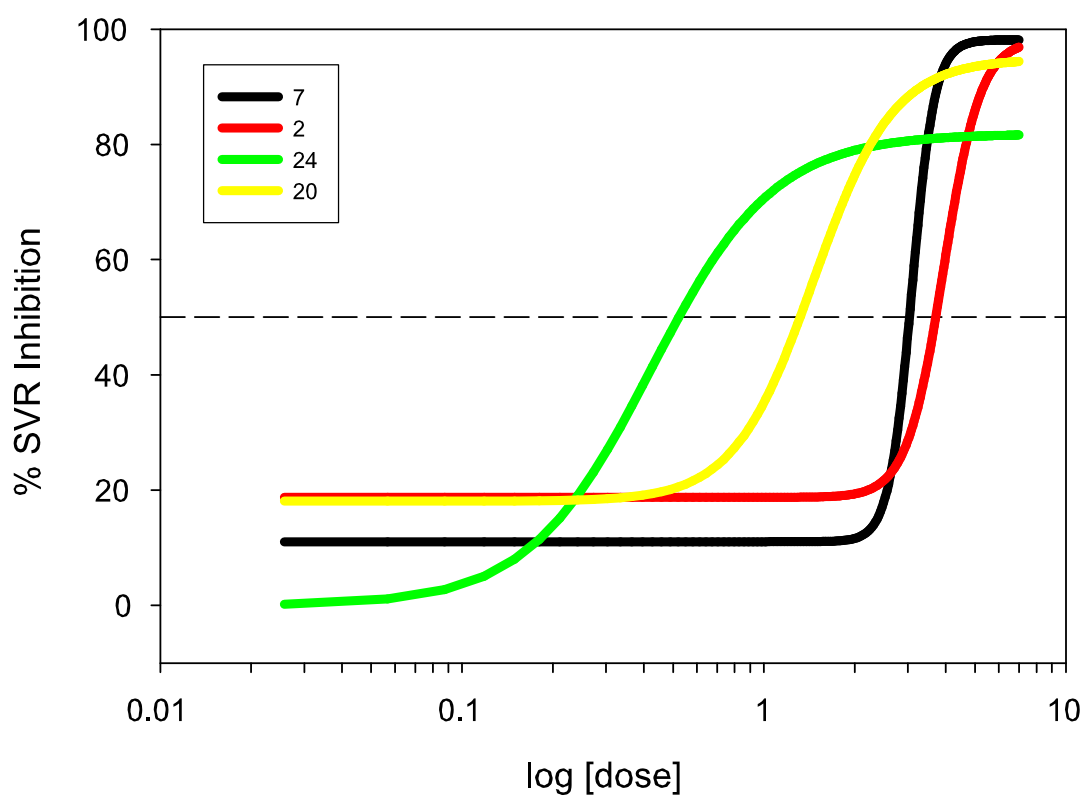


Figure 2.17: Dose response curves for selected enones

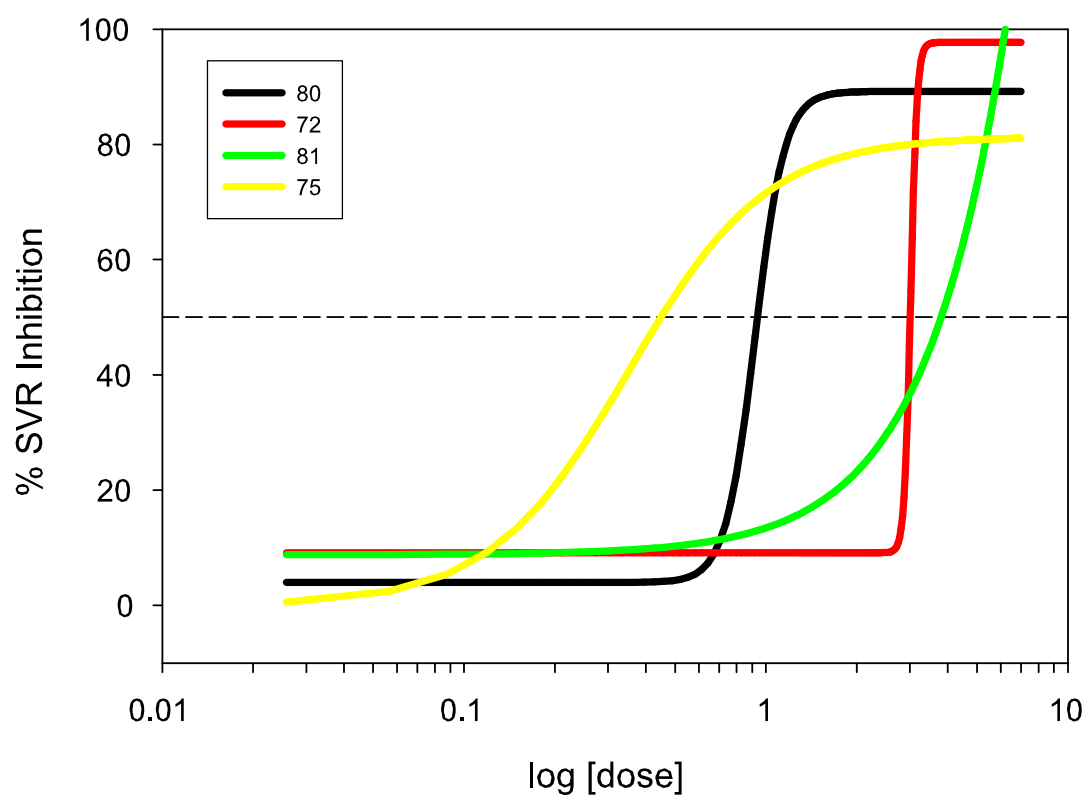


Figure 2.18: Dose response curves for selected dienones

Calculating these electronic energies requires a semi-empirical or *ab initio* level of theory. The enones and dienones in this study are within the realm of normal atomic configurations. This allows us to use the less computationally expensive semi-empirical method, AM1,³³ to calculate these energies. Results of these calculations are presented in table 2.4. Though there is no completely universal trend immediately evident, larger HOMO–LUMO gaps do appear to coincide with higher activity. This would mean that compounds with higher stability, or lower likelihood of chemical reactivity, are performing at greater levels.

2.6.2 LOGP CALCULATIONS

For a drug to be clinically useful, it needs to be not only capable of binding to a target, but also be able to reach the target. Drugs must be capable of moving through cell membranes. Since cell membranes are hydrophobic, the drug must be lipophilic enough to pass through the membrane, but not so lipophilic that it remains in the membrane indefinitely. The partition coefficient, logP, is an experimental value that can be measured directly³⁴ which is based on the equation (2.2). Current methods for calculating these values are becoming increasingly accurate.^{35,36,37,38,39,40} Among the most accurate programs to calculate these values is the KowWIN program developed by the Environmental Protection Agency and the Moriguchi logP method (mlogP). These programs utilize a fragment constant method to predict the logP value. Structures are divided into atoms or larger functional groups, and coefficient values for these fragments are added to give the final estimated logP value.

$$\log P_{oct/wat} = \frac{K_{oct}}{K_{wat}} \quad (2.2)$$

Effective drugs not only must be active against a target, they also need to have appropriate ADME (Absorption, Distribution, Metabolism, and Excretion) properties that make it suitable for drug use. The study of ADME properties is an entire field of research in itself. The medicinal chemist can follow some basic rules that were developed by Lipinski *ex post facto*. The “Rule of Five” resulted from the structural analysis of current drugs on the

Table 2.4: HOMO, LUMO, and gap energies for enones

cpd	HOMO(eV)	LUMO(eV)	ΔE	cpd	HOMO(eV)	LUMO(eV)	ΔE
2	-9.29	-0.71	8.58	37	-9.10	-0.49	8.61
3	-8.83	-0.64	8.19	38	-8.90	-0.87	8.03
4	-8.94	-0.83	8.11	39	-8.91	-0.83	8.08
5	-9.29	-0.88	8.41	40	-8.88	-0.45	8.43
6	-9.16	-0.84	8.32	41	-9.03	-0.79	8.24
7	-9.58	-0.65	8.93	42	-8.82	-0.79	8.03
8	-9.45	-0.95	8.50	43	-9.46	-0.51	8.95
9	-9.10	-0.67	8.43	44	-9.30	-0.63	8.67
10	-8.86	-0.67	8.19	45	-8.21	-1.06	7.15
11	-9.29	-0.55	8.74	46	-8.73	-0.87	7.86
12	-9.07	-0.68	8.39	47	-8.79	-0.92	7.87
13	-9.26	-0.66	8.60	48	-9.27	-0.81	8.46
14	-9.38	-0.74	8.64	49	-9.60	-0.49	9.11
15	-9.38	-1.03	8.35	50	-9.33	-0.67	8.66
16	-9.44	-0.98	8.46	51	-8.74	-0.89	7.85
17	-9.32	-0.82	8.50	52	-8.97	-0.66	8.31
18	-9.30	-0.63	8.67	53	-8.61	-0.60	8.01
19	-9.28	-0.32	8.96	54	-9.49	-0.81	8.68
20	-9.76	-0.66	9.10	55	-9.54	-0.95	8.59
21	-8.90	-0.75	8.15	56	-9.44	-0.86	8.58
22	-8.80	-0.92	7.88	57	-10.22	-1.94	8.28
23	-9.28	-0.59	8.69	58	-9.98	-1.65	8.33
24	-8.76	-0.71	8.05	59	-9.55	-1.44	8.11
25	-8.88	-0.78	8.10	60	-8.70	-0.65	8.05
26	-8.79	-0.87	7.92	61	-10.08	-1.60	8.48
27	-9.75	-0.67	9.08	62	-8.64	-0.52	8.12
28	-8.25	-1.07	7.18	63	-8.90	-0.84	8.06
29	-8.19	-1.12	7.07	64	-8.91	-0.88	8.03
30	-8.25	-1.08	7.17	65	-8.94	-0.82	8.12
31	-8.69	-0.25	8.44	66	-8.94	-0.81	8.13
32	-8.95	-0.58	8.37	67	-9.02	-0.96	8.06
33	-9.29	-0.44	8.85	68	-8.95	-0.84	8.11
34	-9.29	-0.66	8.63	69	-9.04	-1.01	8.03
35	-9.12	-0.77	8.35	70	-8.88	-0.90	7.98
36	-9.04	-0.91	8.13				

market. The rule of 5 states that drugs tend toward having poor absorptions or permeations if the following are true:³⁷ There are more than 5 H-bond donors, the molecular weight is over 500, the ClogP (a commercially available logP calculator) value is over 5 (or mlogP^{35,36} of over 4.15) or there are more than 10 H-bond acceptors. Compounds in classes that are known substrates for biological transporters are exceptions to this rule.

By analysis of the results presented in Table 2.5, one can see that most of the compounds have logP values that are elevated into the hydrophobic realm of poor absorption. Solubilities of these compounds has always been a concern. It is known that curcumin possesses potent *in vivo* activity even though it has poor bio-availability.⁴¹ Therefore these studies have not been overly concerned with addressing this issue at this early stage in the development process.

2.6.3 COP9 SIGNALOSOME AS POTENTIAL TARGET

With the molecular mechanism of action for these compounds still unknown, it was decided to perform a more specific assay. The COP9 signalosome is a new protein complex recently garnered from human red blood cells. The eight polypeptide complex is known to be involved in signal transduction pathways and possesses kinase activity that specifically phosphorylates transcriptional regulating factors. Inhibition of the signalosome results in the accumulation of the tumor suppressing gene p53.⁴² The interest in this signalosome as a potential target is due to the fact that curcumin (**1**) is a potent inhibitor with a K_{i50} of 11 μM .⁴³ A small collection of enones and dienones (Figures 2.19 and 2.20) were tested for their ability to inhibit the COP9 signalosome-associated kinase activity via an assay developed in the Dubiel laboratory.⁴⁴ Experimental concentrations were decided upon based on known activity of curcumin. The K_{i50} values were determined graphically from non-linear curve fits.

2.7 RESULTS

The results of the COP9 inhibition assay are presented in Table 2.6. The activity for curcumin is given as a reference. The compound with the most potent activity is enone **94**. This

Table 2.5: Calculated partition coefficients for enones based ClogP and KOWWIN methods

Cmpd	mlogP	KowWIN	Cmpd	mlogP	KowWIN	Cmpd	mlogP	KowWIN
71	3.99	5.00	15	4.79	4.95	43	4.13	4.05
72	3.91	4.02	16	4.64	4.62	44	4.42	5.29
73	4.22	5.49	17	3.27	3.09	45	6.51	8.36
74	5.68	5.71	18	2.37	2.04	46	5.25	6.01
75	5.90	6.60	19	2.82	3.45	47	5.25	6.01
76	6.16	8.07	20	5.53	6.24	48	2.05	2.78
77	5.54	7.85	21	5.56	6.12	49	5.26	6.25
78	5.54	7.85	22	5.25	6.01	50	4.79	4.95
79	0.87	2.76	23	4.25	4.96	51	5.25	6.01
80	2.04	3.12	24	5.03	6.13	52	2.05	2.54
81	2.42	4.18	25	4.57	4.83	53	2.05	2.54
82	1.43	2.44	26	4.57	4.83	54	2.23	2.47
83	3.65	4.38	27	4.79	4.95	55	2.23	2.47
84	3.11	4.31	28	5.25	6.01	56	1.13	1.28
85	2.56	4.15	29	5.25	6.01	57	5.76	5.66
86	2.98	4.08	30	5.93	7.19	58	5.18	4.66
2	3.76	3.66	31	2.22	3.98	59	5.18	4.66
3	3.07	3.82	32	4.95	6.39	60	5.03	6.13
4	5.04	6.09	33	3.81	5.11	61	3.60	3.48
5	4.52	4.85	34	3.40	4.00	62	2.58	1.82
6	4.52	4.85	35	4.95	5.42	63	2.00	3.36
7	5.03	5.49	36	0.66	2.15	64	3.64	4.90
8	5.03	5.49	37	3.07	3.82	65	3.09	4.27
9	4.72	5.66	38	6.00	7.19	66	2.55	3.80
10	4.77	5.99	39	4.95	5.42	67	2.82	4.02
11	4.25	4.75	40	3.07	3.82	68	2.84	3.72
12	4.25	4.75	41	2.05	3.03	69	1.79	2.53
13	4.25	4.75	42	4.57	4.83	70	1.79	2.53
14	4.76	5.40						

compound possesses a 9-anthryl group on C1 and a 2-naphthyl on C3 of the enone linker. A second compound, **95**, with this same functionality gives an inhibition constant that is consistent with the prior, suggesting that this large aromatic group positively affects inhibition. However, when the anthryl group was on carbon three of the enone, only weak activity was found. Compound **98** gives a K_{i50} value near that of curcumin. The 2-methoxy and 6-methoxy substituents may cause the aromatic ring to rotate into a similar orientation as the anthryl derivatives. Aromatic substitution on C3 of the enone effectively stops all kinase inhibition. This is most strikingly evident in compound **99**. The addition of a 2,6-dichloro substitution renders one of the most potent inhibitors ineffective. This is not to say the the 3-position is unimportant. The second most potent inhibitor (**105**) contains a small heterocycle at this position. Interestingly, this enone was one of the worst performers in the SVR assay (**41** in Table 2.2). This suggests that the COP9 signalosome is not present or is not required for SVR cell growth. It should be noted that the dienone compounds tested did not show any activity at all; however, they each did contain 2,6-dihalogen substitutions. From the resulting hits in this COP9 assay, the next generation compounds should expand upon structures **94**, **95**, and **105**. Testing should most certainly include variations of the 9-anthryl substituent on the ketone end with a furan or similar small aromatic at the ene end of a propenone linker.

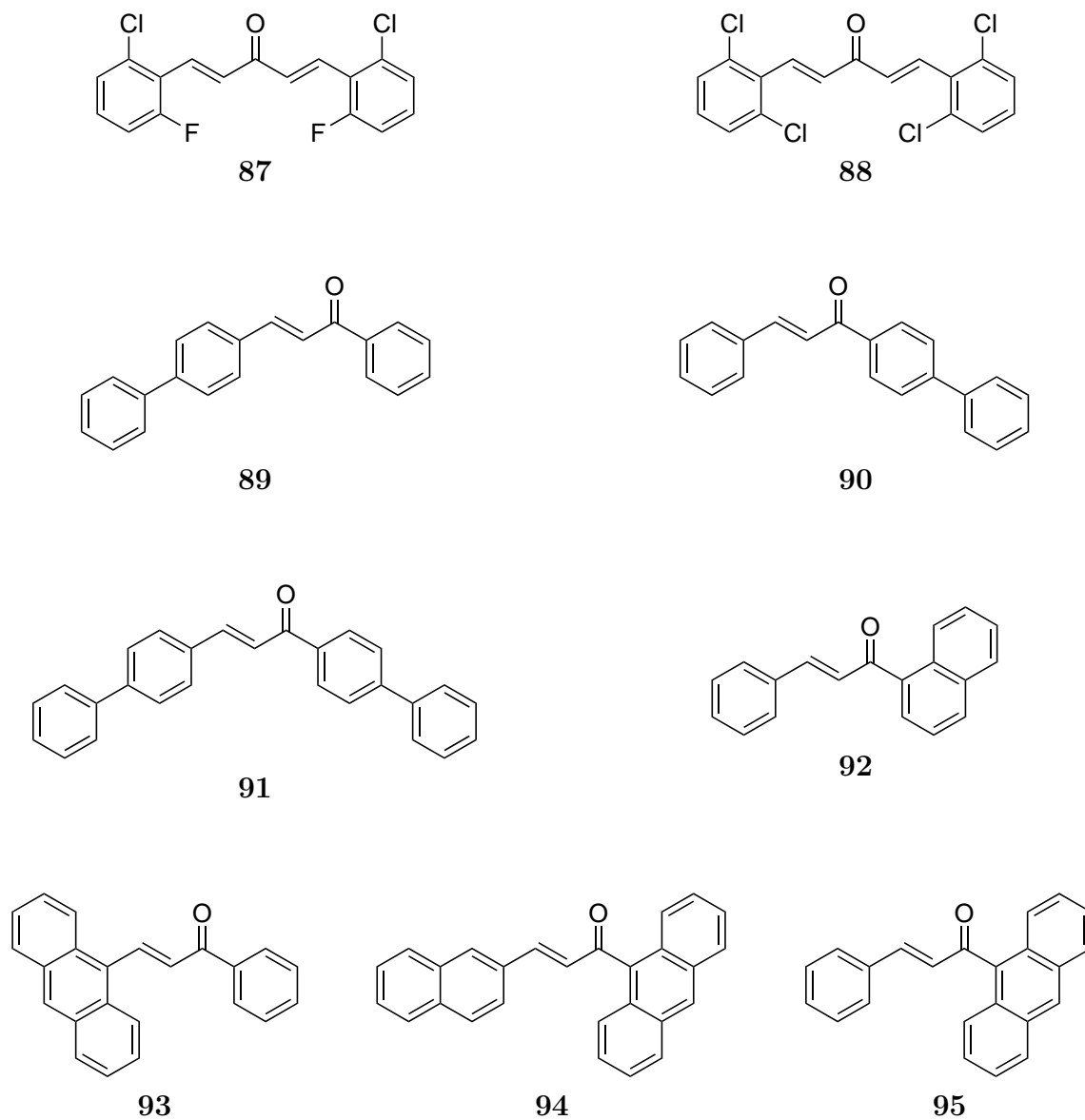


Figure 2.19: Compounds tested for COP9 signalosome activity

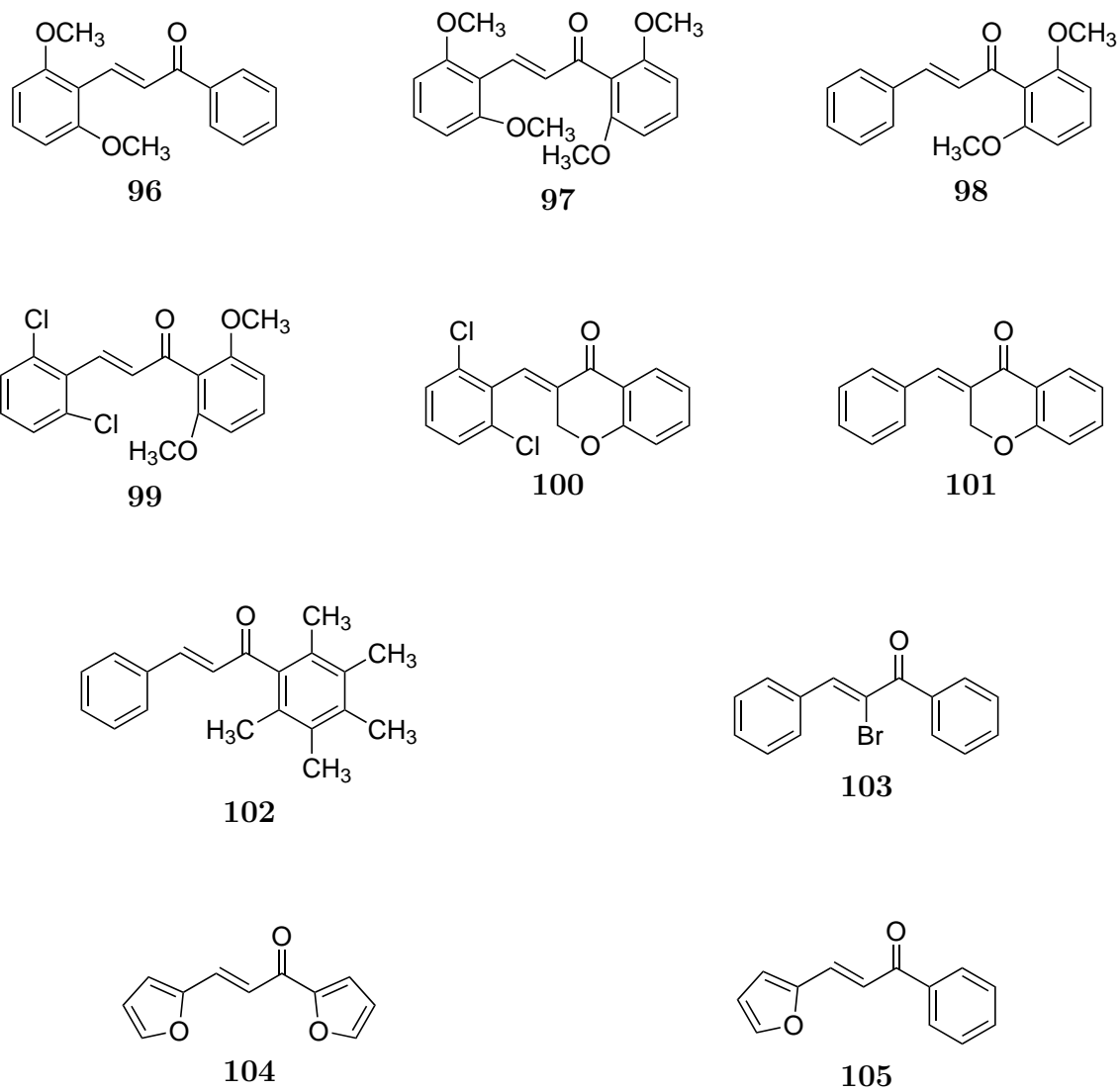


Figure 2.20: Compounds tested for COP9 signalosome activity, cont.

Table 2.6: Inhibition of COP9 signalosome-associated kinase activity

compound	% Activity at 3.7 μ g/mL	% Activity at 18.5 μ g/mL	Inhibition ($K_{i50\%}$)
87	94.8	88.7	none
88	101.2	98.8	none
89	90.4	96.2	none
90	95.8	93.1	none
91	101.9	99.6	none
92	87.0	74.0	weak
93	85.1	72.1	weak
94	47.3	2.7	approx. 3 μ M
95	78.0	28.4	approx. 12 μ M
96	86.4	82.5	none
97	96.1	96.1	none
98	75.5	29.9	approx. 12 μ M
99	94.2	85.3	none
100	65.6	79.8	weak
101	75.5	58.1	approx. 30 μ M
102	115.0	84.2	none
103	84.8	89.1	none
104	73.8	67.5	weak
105	64.2	28.3	approx. 10 μ M
1	50.0	11.7	approx. 10 μ M

CHAPTER 3

METHIONINE AMINOPEPTIDASE TYPE II INHIBITORS

Fumagillin (**106**) is a natural product isolated from *Aspergillus fumigatus*. It was originally identified by Eble and Hanson in 1951, and was found to be a powerful antibiotic.⁴⁵ The sesquiterpene-like structure, easily attained from fumagillol, consists of a functionalized *cis*-diol, two epoxides, and a total of six contiguous stereocenters. There was little interest in this compound until the discovery that fumagillin and related compounds (Figure 3.1) are highly potent inhibitors of angiogenesis.⁴⁶ The mechanism of action of these compounds has been identified by way of crystallography to be a nucleophilic attack on the *spiro*-epoxide by a histidine of the methionine aminopeptidase type-2 enzyme.^{47,48}

The semi-synthetic derivative TNP-470 (**108**) has been shown to be a more potent inhibitor than fumagillin⁴⁶ and does not induce drug resistance,⁴⁹ confirming the potential of creating a more effective drug. Previous synthetic work within our lab has resulted in novel multicyclic analogs of fumagillin. With the early development of novel analogs, it is important to verify the feasibility of molecular binding as well as provide a rationale for subsequent modification to produce more effective binding. With the crystal structure of the bound complex in hand, the rational design of fumagillin analogs was undertaken.

3.1 METHIONINE AMINOPEPTIDASE TYPE II INTRODUCTION

Methionine aminopeptidase (MetAP) is the enzyme which removes the N-terminal methionine residue from newly synthesized proteins. The removal of this translation initiator is often crucial to the stability and function of the protein. There are two forms of methionine aminopeptidase (type I and type II). The crystal structures of both forms have been solved

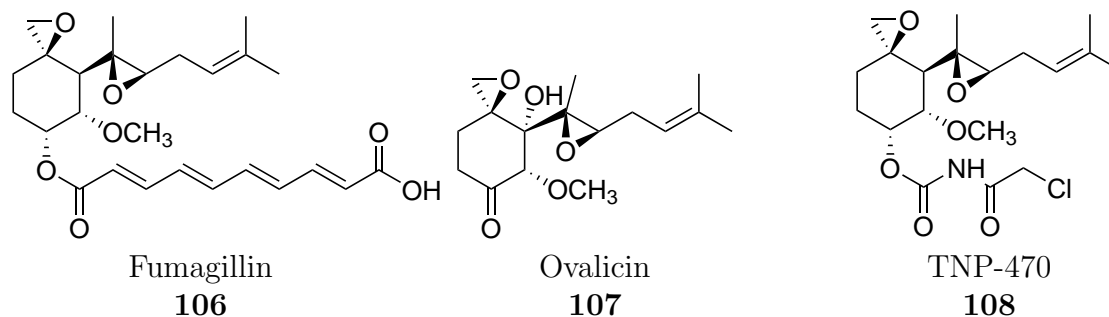


Figure 3.1: Structures of known inhibitors fumagillin, ovalicin, and TNP-470

and deposited in the protein data bank which is currently housed by the Research Collaboratory for Structural Bioinformatics (RCSB).⁵⁰ Prior to publication, the x-ray data was kindly provided by Clardy at Cornell University. The crystal structures of MetAP2 show an active site pocket which is located at the center of a large β -sheet with two small β -sheets capping the top and bottom. The active site contains two metal cofactors reported as being Co^{2+} . Early studies came to the conclusion that the metals are Fe^{2+} .^{51,52} More recent studies have shown that the physiological metal is likely to be Mn^{2+} .⁵³ The active site is strictly conserved throughout the isoforms of the methionine aminopeptidases.⁵⁴

Though the strong correlation between tight binding of MetAP2 and increased antiangiogenic activity exists,⁵⁵ the exact means of endothelial cell growth inhibition remains unclear.⁵⁶ This study was undertaken with the hope that devising a more tightly binding structure containing a multicyclic core will produce a compound with potent antiangiogenic activity while avoiding the known toxicity problems with compound such as fumagillin and TNP-470.

3.2 CRYSTAL STRUCTURE PREPARATION

All calculations were performed using the SYBYL7.0 collection of programs.⁵⁷ Crystal structures (1bn5, 1boa) were retrieved from the RCSB protein data bank and analyzed. The side

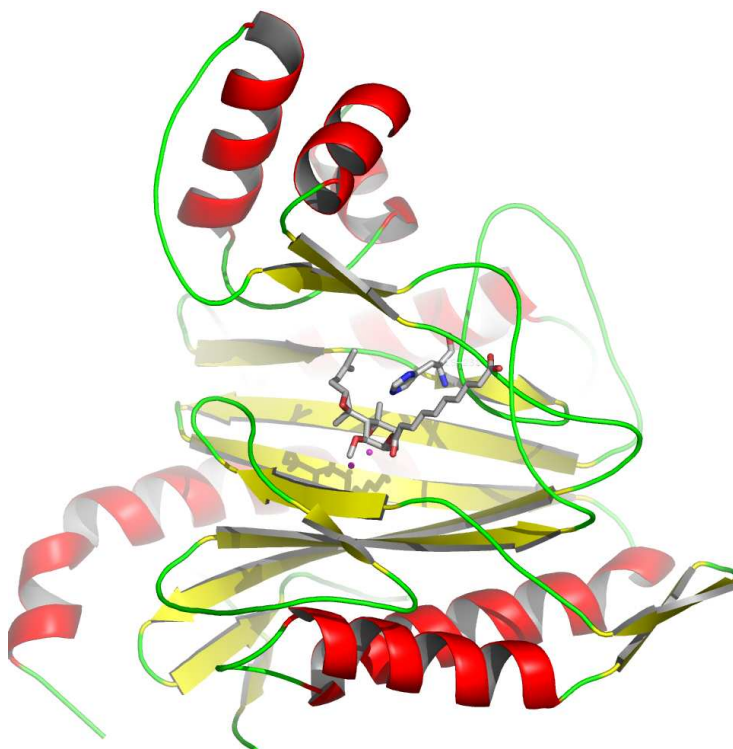
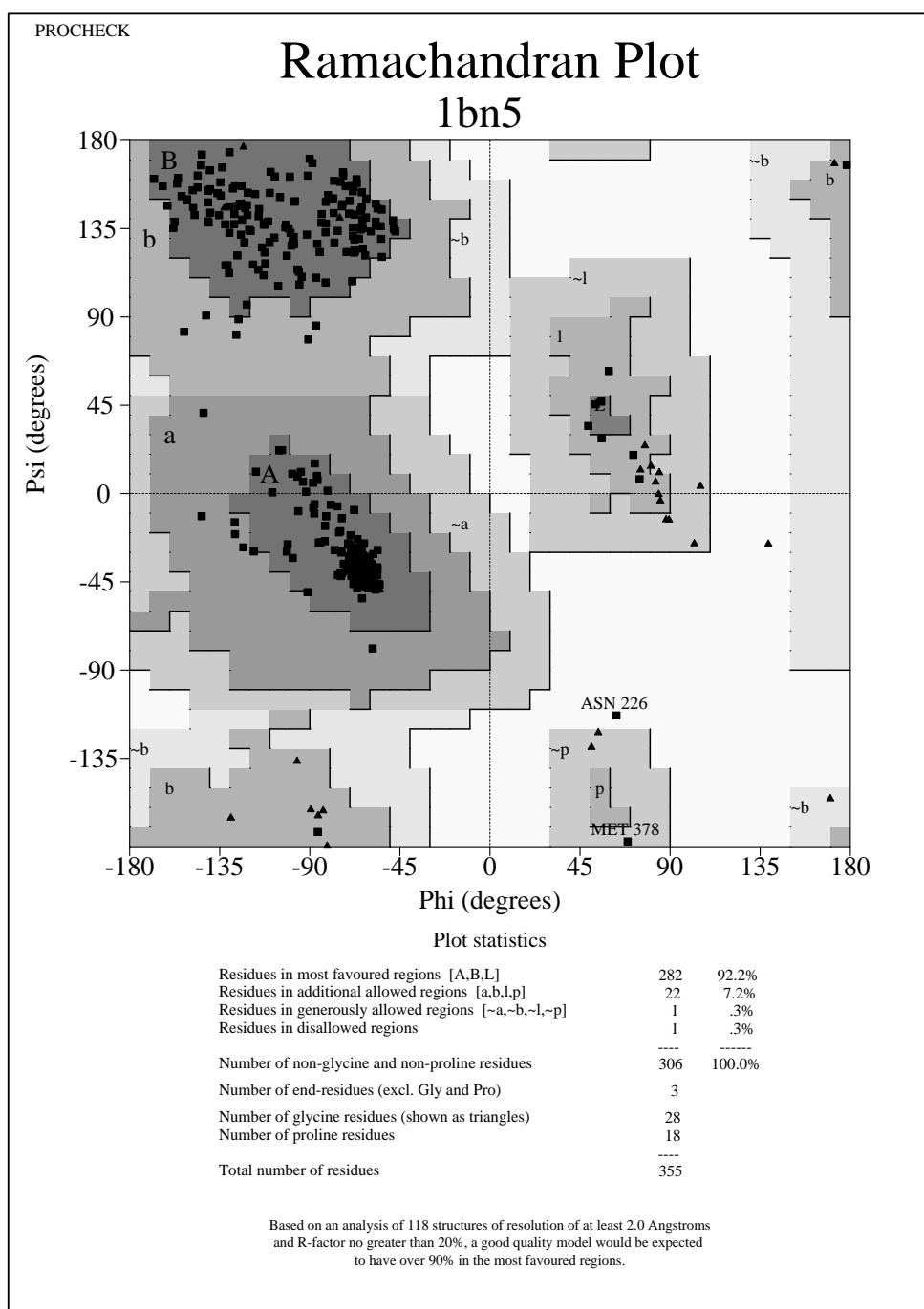


Figure 3.2: Ribbon structure of MetAP2 showing bound fumagillin and His231

chain conformations are often misaligned in the published crystal structures. Tools such as a Ramachandran plot can be used to locate abnormal peptide linkages, or other unlikely bond angles. Figure 3.3 shows the Ramachandran plot for MetAP2 (1bn5) as computed with PROCHECK.⁵⁸ The Asn226 amide substituent was fixed via the BIOPOLYMER menu.

Crystallographic waters were removed. Disorder within the crystal structure required four residues to be repaired. The side-chains of Lys110, Asp114, Asn126, and Glu136 were inserted and placed in the lowest energy rotamer conformation. Termini were blocked using charged groups and all hydrogens were added. Charges were loaded from the Amber99 charge set and the charges of the metal cofactors was fixed at 2^+ .^{59,60} Gasteiger charges were applied to each ligand.⁶¹ Hydrogen relaxation was achieved by fixing all non-hydrogen atoms and subjecting all hydrogens to 1000 steps of Powell minimization using the TriposFF. Full



1bn5_01.ps

Figure 3.3: Ramachandran plot for MetAP2

minimizations were performed for a minimum of 10,000 steps. Conformational changes in the protein backbone were quantified with a root mean square deviation value. An overlay of resulting backbone structures is shown in Figure 3.4.

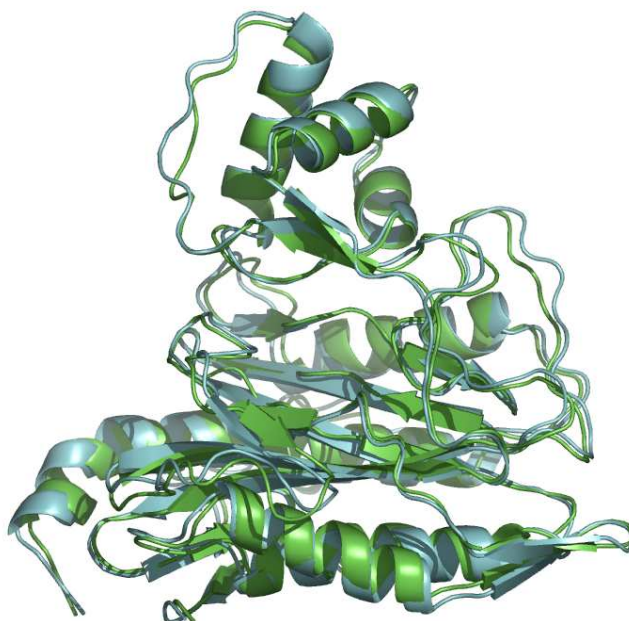


Figure 3.4: Backbone conformations as a result of minimization run

The residues around the bound conformations of either fumagillin (**106**) are labeled in Figure 3.5.

3.3 MULTICYCLIC FUMAGILLIN MIMICS

The multicyclic fumagillin analogs are shown in Figure 3.7. The ultimate analog targets are shown in Figure 3.8.

The rationale behind the multicyclic core is that there is a substantial active site pocket in which the additional ring can extend (Figure 3.9). It is the hope that this steric bulk will allow for more finely tuned Van der Waals interactions.

Active site pocket overlays are shown in Figure 3.10 for our synthesized compound (**109**) as well as the compound fitted with eventual sidearm substituent.

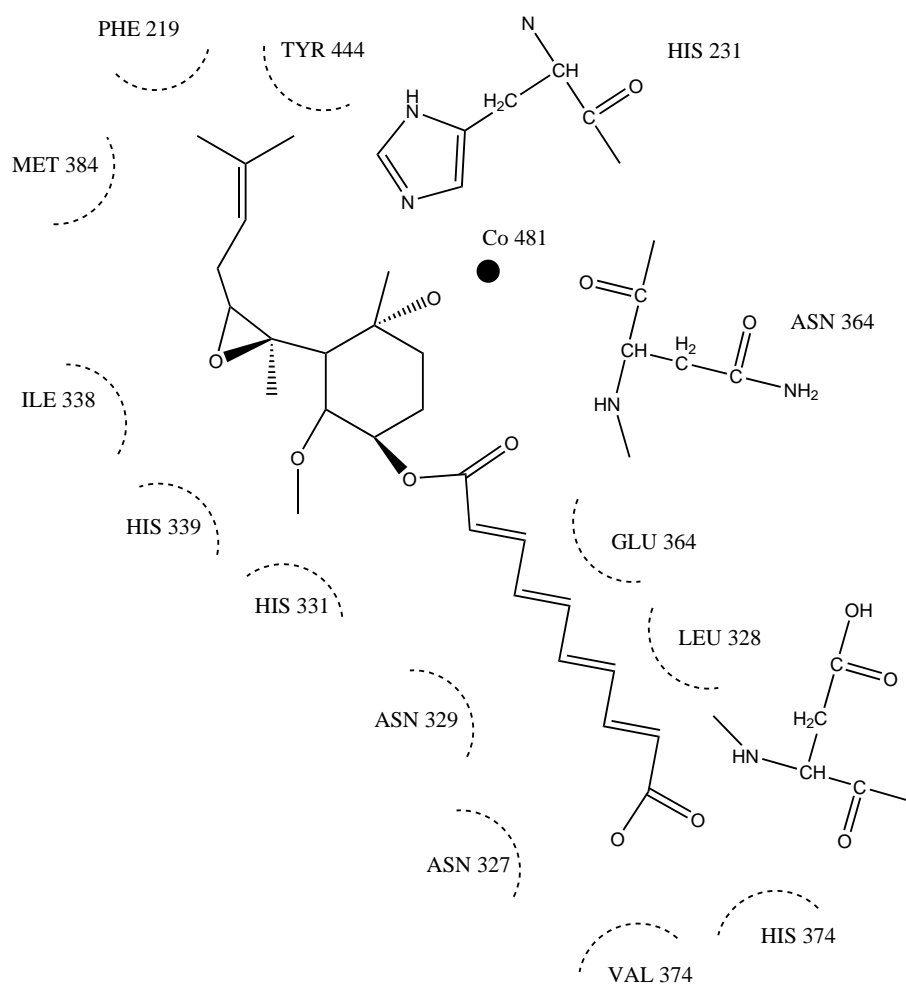


Figure 3.5: Residues surrounding bound fumagillin

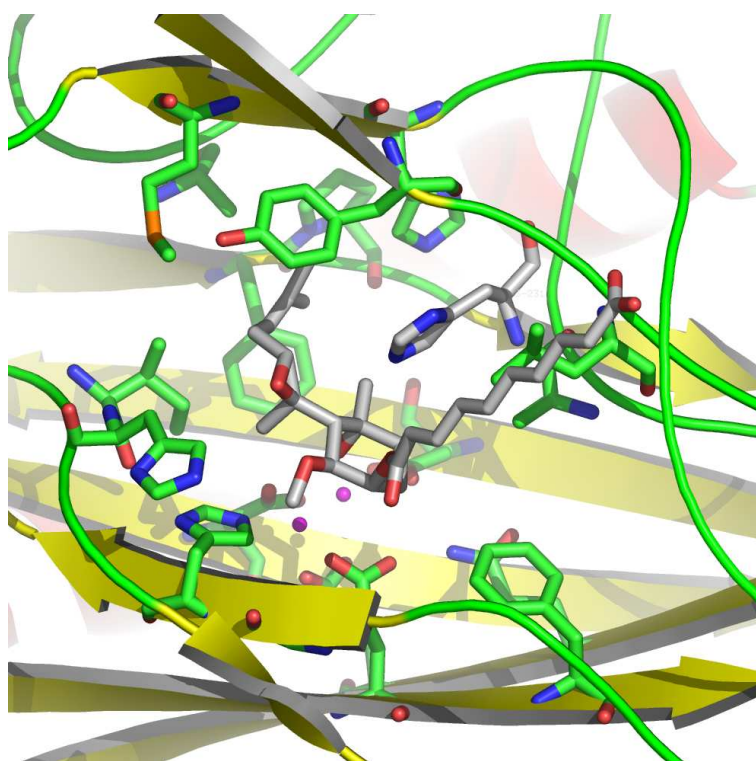


Figure 3.6: Bound conformation of fumagillin in the active site

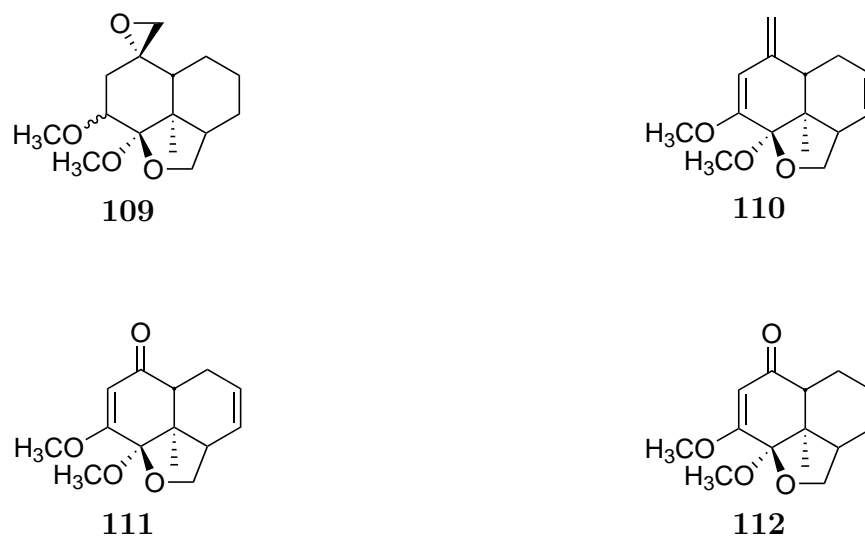


Figure 3.7: Tricyclic fumagillin analogs

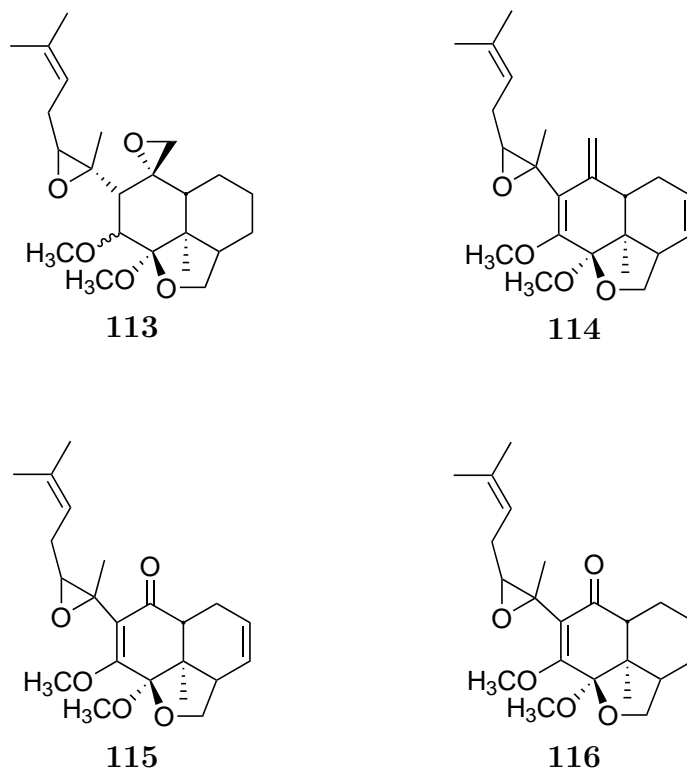


Figure 3.8: Ultimate fumagillin analog targets

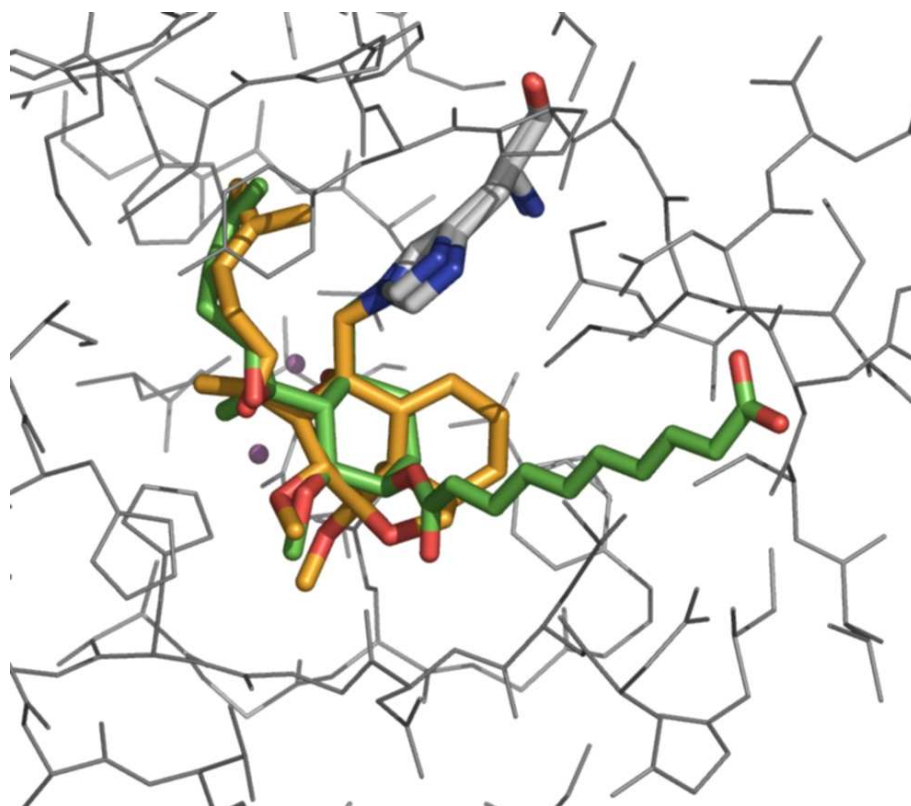


Figure 3.9: Additional ring is accommodated by active site

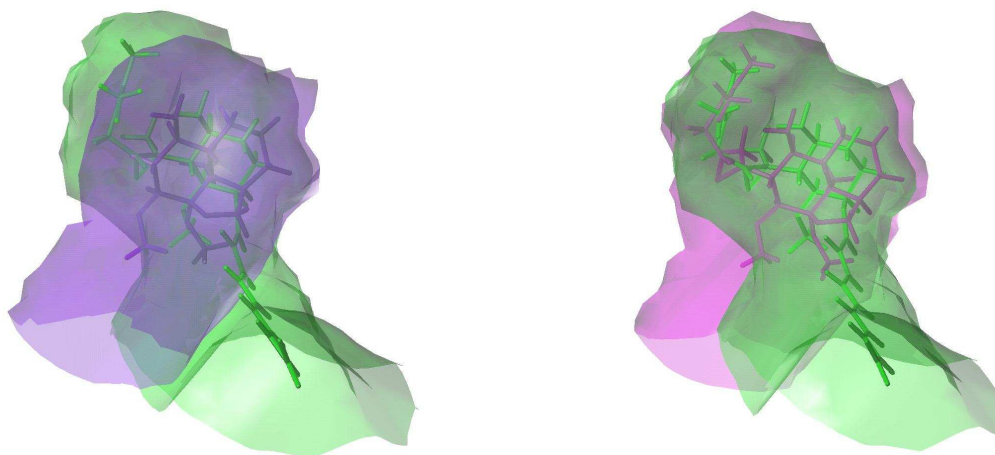


Figure 3.10: Active site pocket for fumagillin overlayed with **109** and corresponding target

The SVR endothelial cell proliferation assay results are presented in Table 3.1. Interestingly the enone containing analogs were the least active. Further studies would require an assay which directly measures MetAP2 binding.

Table 3.1: Activity of fumagillin analogs

compound	% SVR cell growth inhibition			
	1 $\mu\text{g}/\text{mL}$	3 $\mu\text{g}/\text{mL}$	6 $\mu\text{g}/\text{mL}$	9 $\mu\text{g}/\text{mL}$
109	–	10.4	50.6	29.9
110	9.9	15.7	65.8	–
111	11.6	10.9	8.4	–
112	12.6	1.8	0.0	–

3.3.1 SYNTHETIC PRECURSORS–DECALIN DIONES

Decalin ring systems can be found in numerous biologically important molecules. The importance of synthesizing this system to achieve various steroids and terpenoids has led to numerous means of preparation.⁶² One such method of synthesizing a *trans*-fused decalin dione system is an intermolecular Diels–Alder reaction. The resulting adduct is a *cis*-decalin

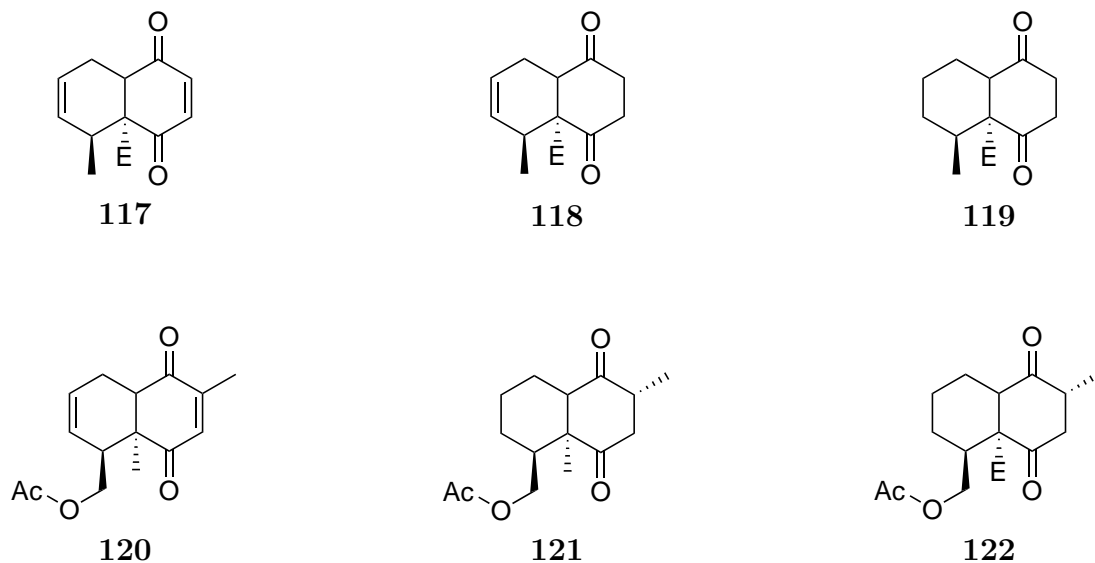


Figure 3.11: Decalin-1,4-diones used for *cis/trans* ratio calculations (E=–COOCH₃)

dione, but a base promoted thermodynamic isomerization will usually yield the *trans*-decalin dione. The amount of isomerization is dependent upon the difference in energy of the two systems. Conformational populations can be calculated by utilizing a Boltzmann distribution (equation (3.1)). A series of substituted decalin-1,4-dione compounds has been previously synthesized, and the isomerization results characterized via NMR.⁶³ The use of these compounds as intermediates in the synthesis of multicyclic fumagillin analogs has led to a desire to predict epimerization ratios. Figure 3.12 shows a synthetic scheme to prepare fumagillin analogs with a *trans*-decalin core. Rapid and accurate prediction of *cis/trans* ratios through the use of stochastic searching and molecular mechanics would provide foresight into expected yields, and perhaps alter the synthetic plan.

Decalin-1,4-dione has been studied by x-ray crystallography⁶⁴ and the calculated bond distances and bond angles for compounds **117–122** are in agreement.

$$P_i = \frac{100 \cdot e^{\frac{-\Delta E_i}{kT}}}{\sum_{i=1}^n e^{\frac{-\Delta E_i}{kT}}} \quad (3.1)$$

where:

P = Population

ΔE = energy difference from global minimum

k = Boltzmann Constant

T = Temperature

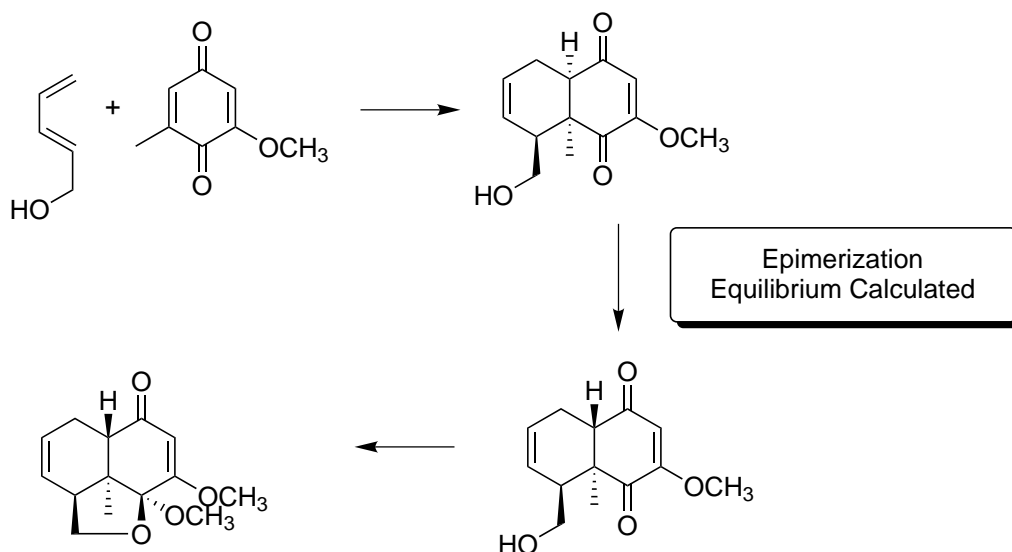
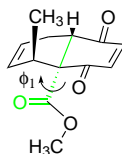


Figure 3.12: Synthetic approach to fumagillin analogs showing base promoted epimerization

3.3.2 RESULTS

Equilibrated epimerizations were carried out under basic conditions and analyzed by ^1H NMR. The olefins in compound **117** make for a conformationally rigid ring system. Only two low energy conformations exist within 3 kcal/mol for each *cis* and *trans* isomer (Table 3.2). The Boltzmann populations were calculated from MM3 free energy values at 298 K. As expected, the *trans* ring juncture conformations dominate the population. The *trans*

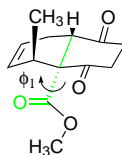
Table 3.2: MM3 Energies and Populations for Low Energy Conformations of **117**

Conf	ϕ_1	E_{steric}	ΔG	rel ΔG	% ^a
<i>trans</i> 1	227.1	18.12	143.547	0.000	50.5
<i>trans</i> 2	18.3	18.20	143.570	0.023	48.6
<i>cis</i> 1	230.1	20.90	146.513	2.966	0.3
<i>cis</i> 2	336.8	21.06	146.207	2.660	0.6

cis:trans = 1 : 99^b

^aPopulations calculated at 298K from equation (3.1)

^bExperimental *cis:trans* = 7 : 93

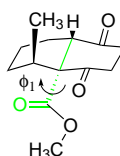
Table 3.3: MM3 Energies and Populations for Low Energy Conformations of **118**

conf	ring B	ϕ_1	E_{steric}	ΔG	rel ΔG	% ^a
<i>trans</i> 1	twist	232.3	26.307	163.451	0.278	31.0
<i>trans</i> 2	chair	19.6	26.442	164.003	0.830	12.9
<i>trans</i> 3	twist	20.1	26.510	163.173	0.000	48.3
<i>trans</i> 4	chair	222.0	26.635	164.356	1.183	7.3
<i>cis</i> 1	twist	232.8	29.125	166.613	3.440	0.2
<i>cis</i> 2	twist	21.6	29.461	166.802	3.629	0.1
<i>cis</i> 3	twist	335.2	30.391	167.329	4.156	0.1
<i>cis</i> 4	chair	342.0	30.790	168.135	4.962	0.1

cis:trans = 1 : 99^b

^aPopulations calculated at 316K from equation (3.1)

^bExperimental *cis:trans* = 6 : 94

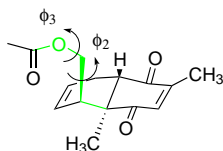
Table 3.4: MM3 Energies and Populations for Low Energy Conformations of **119**

conf	ring B	ϕ_1	E_{steric}	ΔG	rel ΔG	% ^a
<i>trans</i> 1	twist	12.7	29.667	178.315	0.000	34.3
<i>trans</i> 2	chair	13.4	29.785	178.981	0.666	12.7
<i>trans</i> 3	twist	225.1	30.214	178.566	0.251	23.6
<i>trans</i> 4	chair	214.0	30.461	179.781	1.466	3.9
<i>cis</i> 1	chair	340.5	30.803	179.758	1.443	4.0
<i>cis</i> 2	twist	230.3	31.432	180.512	2.197	1.3
<i>cis</i> 3	twist	18.7	31.520	180.450	2.135	1.4
<i>cis</i> 4	chair	142.1	31.754	179.963	1.648	3.0
<i>cis</i> 5	twist	134.3	31.870	179.641	1.326	4.8
<i>cis</i> 7	twist	291.8	30.842	179.217	0.902	9.0
<i>cis</i> 8	chair	236.2	32.830	181.113	2.798	0.5
<i>cis</i> 9	twist	262.1	33.074	180.401	2.086	1.5

cis:trans = 25.5 : 74.5^b

^aPopulations calculated at 338K from equation (3.1)

^bExperimental *cis:trans* = 30 : 70

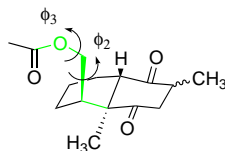
Table 3.5: MM3 Energies and Populations for Low Energy Conformations of **120**

conf	ϕ_2	ϕ_3	E_{steric}	ΔG	rel ΔG	% ^a
<i>trans</i> 1	187.6	182.3	17.962	171.153	0.000	53.7
<i>trans</i> 2	181.5	76.7	18.333	172.242	1.089	9.5
<i>trans</i> 4	67.1	179.7	18.916	172.153	1.000	10.9
<i>trans</i> 5	188.0	251.0	19.160	172.147	0.994	11.0
<i>trans</i> 6	65.9	99.9	19.710	173.662	2.509	1.0
<i>trans</i> 7	296.7	175.3	19.841	172.848	1.695	3.6
<i>trans</i> 8	287.1	282.2	20.027	173.782	2.629	0.8
<i>trans</i> 9	275.9	284.4	20.150	173.409	2.256	1.5
<i>trans</i> 12	295.1	121.3	20.383	173.611	2.458	1.1
<i>cis</i> 1	187.6	179.5	19.326	173.196	2.043	2.1
<i>cis</i> 2	185.5	78.2	19.617	173.807	2.654	0.8
<i>cis</i> 3	292.0	14.8	19.685	173.416	2.263	1.5
<i>cis</i> 5	196.1	78.3	19.870	173.644	2.491	1.0
<i>cis</i> 6	195.5	178.2	20.406	173.365	2.212	1.6

cis:trans = 7 : 93^b

^aPopulations calculated at 316K from equation (3.1)

^bExperimental *cis:trans* = 8 : 92

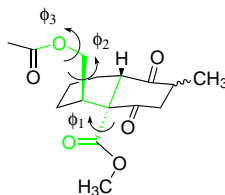
Table 3.6: MM3 Energies and Populations for Low Energy Conformations of **121**

conf	ring B	ϕ_2	ϕ_3	E_{steric}	ΔG	rel ΔG	% ^a
<i>trans</i> R1	chair	186.9	185.1	30.911	214.058	1.166	3.2
<i>trans</i> R2	twist	185.5	183.7	31.315	214.444	1.552	1.7
<i>trans</i> R3	chair	177.5	76.5	31.785	215.621	2.729	0.3
<i>trans</i> R4	twist	60.9	180.5	31.921	214.921	2.029	0.8
<i>trans</i> R5	twist	293.6	171.9	31.926	214.802	1.910	1.0
<i>trans</i> R6	chair	56.3	177.1	32.008	215.230	2.338	0.5
<i>trans</i> R8	twist	179.4	77.9	32.310	215.746	2.854	0.2
<i>trans</i> S1	twist	185.2	184.0	30.169	213.047	0.155	16.1
<i>trans</i> S3	twist	58.9	179.9	30.830	213.561	0.669	7.1
<i>trans</i> S4	twist	293.9	172.0	31.081	213.622	0.730	6.5
<i>trans</i> S5	twist	178.3	77.4	31.127	214.338	1.446	2.1
<i>trans</i> S6	twist	292.4	280.5	31.465	214.854	1.962	0.9
<i>cis</i> R1	chair	192.7	78.7	29.666	213.115	0.223	14.5
<i>cis</i> R2	chair	191.9	177.8	30.164	212.892	0.000	20.6
<i>cis</i> R3	chair	287.6	282.6	30.479	214.130	1.238	2.9
<i>cis</i> R4	chair	286.0	180.7	30.744	213.603	0.711	6.7
<i>cis</i> R5	chair	197.0	246.9	31.649	213.983	1.091	3.6
<i>cis</i> R6	twist	187.1	180.2	31.789	215.041	2.149	0.7
<i>cis</i> R9	chair	70.7	183.2	32.796	215.500	2.608	0.3
<i>cis</i> S1	twist	195.2	78.7	31.049	214.020	1.128	3.4
<i>cis</i> S2	twist	195.0	178.2	31.629	213.796	0.904	4.9
<i>cis</i> S3	twist	290.8	282.5	32.295	215.438	2.546	0.4
<i>cis</i> S4	twist	289.6	181.8	32.592	214.910	2.018	0.8
<i>cis</i> S6	twist	199.9	247.2	32.960	214.928	2.036	0.8

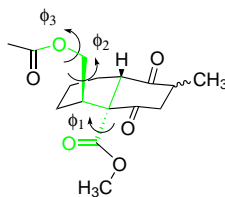
cis:trans = 59.6 : 40.1^b

^aPopulations calculated at 316K from equation (3.1)

^bExperimental *cis:trans* = 26 : 74

Table 3.7: MM3 Energies and Populations for Low Energy Conformations of **122**

conf	ring B	ϕ_1	ϕ_2	ϕ_3	E_{steric}	ΔG	rel ΔG	%
<i>trans</i> R1	chair	13.5	185.6	184.5	31.631	220.604	0.264	11.5
<i>trans</i> R2	chair	213.8	187.7	184.5	32.259	221.347	1.015	3.8
<i>trans</i> R3	chair	11.9	177.1	77.3	32.454	220.368	1.794	1.2
<i>trans</i> R4	chair	10.2	56.1	177.4	32.947	222.181	1.623	1.5
<i>trans</i> R5	chair	215.0	60.9	178.1	33.491	222.830	2.284	0.6
<i>trans</i> R6	twist	11.3	184.7	183.5	33.636	222.328	1.983	0.9
<i>trans</i> R7	chair	17.1	301.0	175.4	33.815	223.088	2.187	0.7
<i>trans</i> R11	chair	12.9	279.5	283.0	34.143	222.094	2.971	0.2
<i>trans</i> R13	twist	220.7	186.4	183.1	34.192	222.876	2.518	0.4
<i>trans</i> R15	chair	216.2	306.4	175.0	34.262	223.611	2.793	0.3
<i>trans</i> R17	twist	8.9	58.7	180.0	34.458	223.458	2.939	0.2
<i>trans</i> S1	twist	11.3	184.6	183.8	31.926	220.407	0.000	17.1
<i>trans</i> S2	twist	221.8	186.5	183.4	32.700	221.171	0.743	5.7
<i>trans</i> S3	twist	9.7	177.4	77.7	32.846	221.752	1.264	2.6
<i>trans</i> S4	twist	8.9	56.8	179.1	32.872	223.150	0.696	6.1
<i>trans</i> S5	twist	223.3	297.0	172.8	33.170	221.929	1.330	2.4
<i>trans</i> S6	twist	227.1	62.2	181.4	33.275	223.560	1.108	3.3
<i>trans</i> S7	twist	16.9	293.5	279.0	33.369	222.483	1.897	1.0
<i>trans</i> S8	chair	13.7	185.9	184.4	33.442	222.449	2.114	0.7
<i>trans</i> S10	twist	223.5	296.4	278.5	33.801	222.962	2.479	0.4
<i>trans</i> S11	twist	222.8	181.0	79.8	33.875	222.738	2.207	0.6
<i>trans</i> S12	chair	213.0	187.9	184.4	34.131	223.275	2.943	0.2

Table 3.8: MM3 Energies and Populations for Low Energy Conformations of **122**, cont.

conf	ring B	ϕ_1	ϕ_2	ϕ_3	E_{steric}	ΔG	rel ΔG	% ^a
<i>cis</i> R1	chair	339.9	186.6	78.7	32.205	219.862	1.188	2.9
<i>cis</i> R2	chair	338.9	278.0	183.4	32.967	221.862	1.481	1.9
<i>cis</i> R3	chair	132.4	294.9	179.8	33.552	222.561	1.960	0.9
<i>cis</i> R4	chair	3.9	294.4	282.8	33.656	222.950	1.935	1.0
<i>cis</i> R5	twist	229.4	187.1	180.1	33.871	221.109	2.680	0.3
<i>cis</i> R6	twist	18.4	186.3	179.7	33.906	222.525	2.242	0.6
<i>cis</i> R7	chair	234.8	203.0	180.6	34.043	222.757	2.193	0.7
<i>cis</i> R9	chair	341.3	63.2	187.5	34.332	223.373	2.784	0.3
<i>cis</i> S1	twist	335.8	189.0	79.1	32.330	219.452	0.785	5.3
<i>cis</i> S2	twist	333.4	189.0	177.2	32.550	220.640	0.291	11.1
<i>cis</i> S3	twist	331.9	285.4	282.6	32.630	220.019	1.622	1.5
<i>cis</i> S4	twist	134.9	194.0	78.7	32.824	221.405	0.896	4.5
<i>cis</i> S5	twist	334.1	281.2	184.6	33.100	221.496	1.013	3.8
<i>cis</i> S6	twist	132.0	295.7	180.5	33.896	222.478	1.898	1.0
<i>cis</i> S7	twist	138.5	282.9	280.8	33.982	222.586	2.199	0.6
<i>cis</i> S8	twist	332.4	193.2	246.3	34.055	222.235	1.332	2.4

cis:trans = 38.6 : 61.4^b

^aPopulations calculated at 338K from equation (3.1)

^bExperimental *cis:trans* = 28 : 72

conformers account for 99% which is in agreement with the NMR data. The NMR data shows the *trans* conformation exists in about 96%. A stochastic search implemented in MM3 reveals that compound **118** has four low energy *trans* conformers and three low energy *cis* conformers. NMR analysis of compound **118** indicates that the *trans* isomer should exist as 94%. The calculated percent is in similar agreement to compound **117**, with a predicted 99% *trans* isomer (Table 3.3).

The fully saturated decalin-1,4-dione ring system of compound **119** gives eight low energy *cis* conformers (Table 3.4). The dione ring exists as a chair or twist boat conformation. The twist boat conformations are the most significant for the *cis* structure. Two low energy *trans* ring orientations with 2 substituent rotamers each were found. The dione ring exists as either a chair or twist boat. Again, the twist boat gives the predominant conformations. From the twelve conformers, MM3 accurately predicts that the *trans* conformers are more stable with a population of 74%. The NMR population for the *trans* structure of **3** is 70%.

Structure **120** contains a flexible acetate ester substituent, however, the decalin ring system is held rigidly by the two olefins. Due to the side chain flexibility, there are fourteen conformations within 3 kcal/mol. The results of the MM3 Boltzmann distribution at 316 K are in excellent agreement with a *trans* population of 93% compared to the experimental 92% (Table 3.5). Initial calculations on compound **121** suggested that the *cis* conformations were 95% predominant. This was counter to the NMR data which shows the *cis* conformations accounting for only 26%. It was realized that under basic conditions, carbon 2 will also epimerize providing a more complex mixture of structures. The diastereomers (2-R and 2-S) were included in the following calculations. The inclusion of these structures brought the *cis* population down to 60%. Unfortunately, the incorrect ring juncture is still predicted. The lowest energy conformation is from the *cis* structure, where both rings adopt a chair conformation and the methyl at carbon 2 is equatorial. Carbon 2 of compound **122** undergoes epimerization as with compound **121**. The *cis* and *trans* low energy conformations of **122**

(2-R and 2-S) were found. A Boltzmann population at 338 K results in a 61% *trans* ratio which is in agreement with the NMR derived ratio of 72% *trans*.

All of the molecular mechanics calculations were carried out with MM3(2000) force field as implemented in Sybyl7.0.⁵⁷ The generation of conformers was accomplished with the stochastic search option within MM3. Limits were set at 500 pushes with kick sizes of 3.0 Å. Boltzmann populations were calculated based on free energy values (ΔG) from MM3 full geometry optimizations. A vibrational frequency analysis was performed on each structure to ensure valid conformations. In cases where restricted internal rotations were encountered, vibrational entropies were applied by hand.

3.4 DIRECTIONS

It has been shown that the multicyclic fumagillin analogs are synthetically accessible and should be easily accepted into the binding pocket of MetAP2. The report⁶⁵ of a cinnamic acid ester analog with 1000-fold increase in endothelial proliferation compared to TNP-470 provides a connection to the work previously described in Chapter 2. Combining SVR inhibiting enones with this novel multicyclic fumagillin core would be an interesting and worthy pursuit.

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APPENDIX A

MM3 COORDINATES FROM DECALIN DIONE CALCULATIONS

117c1

C(1)	-0.70001	2.58055	-0.15950	(2)
C(2)	-0.63017	1.98478	-1.35566	(2)
C(3)	-0.34821	0.51718	-1.56889	(1)
C(4)	0.23963	-0.13848	-0.26852	(1)
C(5)	-0.53179	0.34162	0.99969	(1)
C(6)	-0.46632	1.86736	1.14298	(1)
C(7)	-1.94516	-0.21707	1.04599	(3)
C(8)	-2.04522	-1.67787	0.77990	(2)
C(9)	-1.05248	-2.34242	0.16900	(2)
C(10)	0.15499	-1.67199	-0.37475	(3)
O(11)	-2.92461	0.43763	1.34860	(81)
O(12)	1.01876	-2.32636	-0.93186	(81)
C(13)	-1.62395	-0.13768	-2.13505	(1)
C(14)	1.71657	0.20458	-0.13171	(3)
O(15)	2.39324	0.77682	-0.96419	(78)
O(16)	2.22251	-0.21395	1.05785	(75)
C(17)	3.61978	0.05368	1.27374	(1)
H(18)	-0.89771	3.66498	-0.10556	(5)
H(19)	-0.79574	2.59108	-2.26312	(5)
H(20)	0.42355	0.44101	-2.36832	(5)
H(21)	-0.03650	-0.08701	1.90124	(5)
H(22)	0.53333	2.16712	1.52758	(5)
H(23)	-1.20263	2.21477	1.89929	(5)
H(24)	-2.95697	-2.19837	1.11455	(5)
H(25)	-1.13586	-3.42923	0.00364	(5)
H(26)	-1.48030	-1.21769	-2.35626	(5)
H(27)	-2.49309	-0.04380	-1.45015	(5)
H(28)	-1.92659	0.33809	-3.09504	(5)
H(29)	4.23927	-0.45337	0.50887	(5)
H(30)	3.81813	1.14281	1.25394	(5)
H(31)	3.91404	-0.33264	2.26789	(5)

117t1

C(1)	-1.76900	1.89992	1.07076	(2)
C(2)	-2.51319	1.05164	0.34797	(2)
C(3)	-2.02616	-0.29375	-0.14265	(1)
C(4)	-0.46904	-0.31233	-0.15814	(1)
C(5)	0.02656	0.15099	1.24439	(1)
C(6)	-0.34704	1.62158	1.47947	(1)
C(7)	1.51019	-0.10449	1.47943	(3)
C(8)	2.05488	-1.37456	0.93287	(2)
C(9)	1.36869	-2.12123	0.05653	(2)
C(10)	0.05888	-1.71445	-0.50216	(3)
O(11)	2.21686	0.65185	2.11972	(81)
O(12)	-0.54404	-2.46449	-1.24920	(81)
C(13)	-2.68003	-1.38351	0.73499	(1)
C(14)	0.05324	0.58453	-1.27252	(3)
O(15)	-0.61454	1.04723	-2.17724	(78)
O(16)	1.38666	0.81288	-1.16171	(75)
C(17)	1.96758	1.65349	-2.17463	(1)
H(18)	-2.19393	2.87269	1.37242	(5)
H(19)	-3.54676	1.33276	0.08227	(5)
H(20)	-2.39516	-0.43268	-1.18390	(5)
H(21)	-0.49795	-0.45570	2.01518	(5)
H(22)	0.32801	2.29637	0.90921	(5)
H(23)	-0.22277	1.87206	2.55506	(5)
H(24)	3.04889	-1.69342	1.28653	(5)
H(25)	1.79264	-3.07093	-0.30942	(5)
H(26)	-2.37049	-2.40964	0.44285	(5)
H(27)	-2.44262	-1.26434	1.81406	(5)
H(28)	-3.78966	-1.35382	0.64926	(5)
H(29)	3.04957	1.76822	-1.97390	(5)
H(30)	1.84828	1.19928	-3.17727	(5)
H(31)	1.50532	2.65950	-2.16195	(5)

117c2

C(1)	2.57643	1.56019	-0.37715	(2)
C(2)	1.50067	2.31550	-0.62551	(2)
C(3)	0.10326	1.76276	-0.79156	(1)
C(4)	-0.02885	0.33576	-0.16153	(1)
C(5)	1.15954	-0.52079	-0.69067	(1)
C(6)	2.51792	0.06622	-0.22831	(1)
C(7)	1.04540	-1.95641	-0.18465	(3)
C(8)	0.55081	-2.12801	1.21115	(2)
C(9)	0.11898	-1.08758	1.94224	(2)
C(10)	0.01082	0.27863	1.36953	(3)
O(11)	1.38385	-2.91510	-0.85401	(81)
O(12)	-0.05786	1.25211	2.09438	(81)
C(13)	-0.92624	2.79534	-0.29915	(1)
C(14)	-1.34213	-0.27859	-0.62303	(3)
O(15)	-1.47481	-1.00731	-1.58674	(78)
O(16)	-2.38270	0.08216	0.17136	(75)
C(17)	-3.66671	-0.45722	-0.19139	(1)
H(18)	3.56306	2.03914	-0.25454	(5)
H(19)	1.62571	3.40691	-0.72906	(5)
H(20)	-0.05299	1.65744	-1.89048	(5)
H(21)	1.13504	-0.52907	-1.79927	(5)
H(22)	3.33738	-0.39372	-0.82326	(5)
H(23)	2.71540	-0.18952	0.83514	(5)
H(24)	0.59388	-3.14080	1.64338	(5)
H(25)	-0.18597	-1.22370	2.99237	(5)
H(26)	-1.97155	2.44229	-0.42983	(5)
H(27)	-0.79506	3.06190	0.77078	(5)
H(28)	-0.84750	3.74618	-0.87297	(5)
H(29)	-4.42801	-0.09558	0.52541	(5)
H(30)	-3.96030	-0.12303	-1.20529	(5)
H(31)	-3.65254	-1.56363	-0.15166	(5)

117t2

C(1)	-0.54996	-2.61907	0.75035	(2)
C(2)	-1.47131	-2.18222	-0.11783	(2)
C(3)	-1.27536	-0.97855	-1.01091	(1)
C(4)	-0.20933	-0.02968	-0.37638	(1)
C(5)	1.06709	-0.86279	-0.08459	(1)
C(6)	0.78234	-1.95307	0.96330	(1)
C(7)	2.26247	-0.00212	0.31303	(3)
C(8)	2.38731	1.31933	-0.35558	(2)
C(9)	1.41505	1.82104	-1.12951	(2)
C(10)	0.10955	1.14707	-1.31076	(3)
O(11)	3.11054	-0.38115	1.10006	(81)
O(12)	-0.68750	1.56665	-2.13056	(81)
C(13)	-0.92592	-1.49668	-2.42375	(1)
C(14)	-0.73821	0.63755	0.88644	(3)
O(15)	-0.10665	0.81646	1.90925	(78)
O(16)	-2.02262	1.05396	0.74174	(75)
C(17)	-2.60391	1.70725	1.88467	(1)
H(18)	-0.76887	-3.50356	1.37310	(5)
H(19)	-2.42741	-2.72512	-0.21253	(5)
H(20)	-2.24778	-0.44279	-1.08151	(5)
H(21)	1.36988	-1.37117	-1.02653	(5)
H(22)	0.80545	-1.53128	1.99068	(5)
H(23)	1.58207	-2.72516	0.92009	(5)
H(24)	3.33095	1.87059	-0.21235	(5)
H(25)	1.55595	2.78728	-1.64116	(5)
H(26)	-0.02160	-2.14262	-2.43146	(5)
H(27)	-0.74744	-0.67455	-3.14903	(5)
H(28)	-1.75618	-2.10960	-2.84157	(5)
H(29)	-2.62174	1.02716	2.75823	(5)
H(30)	-3.64633	1.99300	1.64833	(5)
H(31)	-2.04247	2.62724	2.13827	(5)

118c1

C(1)	0.68083	2.62569	-0.11852	(2)
C(2)	0.57966	2.17669	1.13746	(2)
C(3)	0.31843	0.73830	1.51185	(1)
C(4)	-0.24781	-0.06665	0.29519	(1)
C(5)	0.53989	0.25893	-1.01582	(1)
C(6)	0.49844	1.75991	-1.33324	(1)
C(7)	1.94182	-0.33777	-0.99065	(3)
C(8)	2.02288	-1.82215	-0.64679	(1)
C(9)	0.63783	-2.43049	-0.37563	(1)
C(10)	-0.17185	-1.58126	0.59195	(3)
O(11)	2.93166	0.30005	-1.27498	(7)
O(12)	-0.72520	-2.07117	1.55286	(7)
C(13)	1.61140	0.17404	2.13555	(1)
C(14)	-1.72453	0.23888	0.09443	(3)
O(15)	-2.40969	0.94194	0.81207	(78)
O(16)	-2.21912	-0.38150	-1.00842	(75)
C(17)	-3.61631	-0.16491	-1.27470	(1)
H(18)	0.86680	3.69901	-0.29552	(5)
H(19)	0.70859	2.88818	1.97139	(5)
H(20)	-0.45254	0.73632	2.31558	(5)
H(21)	0.04012	-0.25144	-1.86994	(5)
H(22)	-0.48247	2.01605	-1.79144	(5)
H(23)	1.26700	2.01387	-2.09456	(5)
H(24)	2.66912	-1.95603	0.24639	(5)
H(25)	2.51418	-2.36937	-1.47886	(5)
H(26)	0.75718	-3.45483	0.02733	(5)
H(27)	0.07564	-2.53587	-1.32843	(5)
H(28)	2.47959	0.24029	1.44644	(5)
H(29)	1.50650	-0.88857	2.44372	(5)
H(30)	1.89358	0.73866	3.05268	(5)
H(31)	-3.82133	0.90990	-1.44403	(5)
H(32)	-4.23781	-0.53695	-0.43731	(5)
H(33)	-3.90171	-0.71883	-2.18897	(5)

118c3

C(1)	-2.42729	-1.79374	-0.32831	(2)
C(2)	-1.29224	-2.45989	-0.56579	(2)
C(3)	0.04814	-1.79040	-0.76743	(1)
C(4)	0.06647	-0.34513	-0.15981	(1)
C(5)	-1.19412	0.39604	-0.69799	(1)
C(6)	-2.49890	-0.29668	-0.22770	(1)
C(7)	-1.22803	1.86004	-0.24620	(3)
C(8)	-0.38949	2.22445	0.97154	(1)
C(9)	-0.30740	1.08190	1.99030	(1)
C(10)	0.02823	-0.27663	1.37531	(3)
O(11)	-1.91355	2.68251	-0.81345	(7)
O(12)	0.20913	-1.24242	2.08334	(7)
C(13)	1.17581	-2.72122	-0.28709	(1)
C(14)	1.32491	0.35218	-0.65308	(3)
O(15)	1.39905	1.03552	-1.65564	(78)
O(16)	2.38549	0.13155	0.16506	(75)
C(17)	3.62372	0.75039	-0.22818	(1)
H(18)	-3.36678	-2.35303	-0.17891	(5)
H(19)	-1.32079	-3.56084	-0.63204	(5)
H(20)	0.17193	-1.68878	-1.87095	(5)
H(21)	-1.17218	0.37819	-1.80819	(5)
H(22)	-3.35133	0.06915	-0.84144	(5)
H(23)	-2.72742	-0.02537	0.82522	(5)
H(24)	0.63186	2.51265	0.64286	(5)
H(25)	-0.81541	3.12237	1.46157	(5)
H(26)	0.45048	1.33114	2.76272	(5)
H(27)	-1.27943	0.99846	2.52255	(5)
H(28)	2.18223	-2.27590	-0.44004	(5)
H(29)	1.08958	-2.99027	0.78669	(5)
H(30)	1.17302	-3.68007	-0.85296	(5)
H(31)	4.40730	0.49613	0.51039	(5)
H(32)	3.94972	0.38023	-1.21943	(5)
H(33)	3.51960	1.85232	-0.25627	(5)

118c2

C(1)	0.36340	-2.64850	-0.18683	(2)
C(2)	-0.03611	-2.02626	-1.30112	(2)
C(3)	-0.15097	-0.52873	-1.44205	(1)
C(4)	-0.23550	0.15799	-0.03274	(1)
C(5)	0.83799	-0.41806	0.93904	(1)
C(6)	0.70339	-1.94156	1.09477	(1)
C(7)	2.24197	0.04946	0.57335	(3)
C(8)	2.41442	1.55591	0.40637	(1)
C(9)	1.09232	2.31222	0.61354	(1)
C(10)	-0.03762	1.68423	-0.18640	(3)
O(11)	3.18132	-0.70864	0.47130	(7)
O(12)	-0.73225	2.34968	-0.92426	(7)
C(13)	1.00860	-0.05025	-2.34008	(1)
C(14)	-1.61639	0.00228	0.59743	(3)
O(15)	-1.82762	-0.13438	1.78659	(78)
O(16)	-2.61502	0.05471	-0.32024	(75)
C(17)	-3.95268	-0.06831	-0.19583	(1)
H(18)	0.41931	-3.75071	-0.17478	(5)
H(19)	-0.27806	-2.62822	-2.19407	(5)
H(20)	-1.09014	-0.31852	-1.99994	(5)
H(21)	0.66289	0.01264	1.95134	(5)
H(22)	-0.09652	-2.17263	1.83206	(5)
H(23)	1.63662	-2.36897	1.52020	(5)
H(24)	3.17417	1.92595	1.12680	(5)
H(25)	2.80874	1.76757	-0.61013	(5)
H(26)	0.82007	2.31940	1.69072	(5)
H(27)	1.22291	3.37184	0.32051	(5)
H(28)	1.00060	1.05048	-2.49334	(5)
H(29)	2.00421	-0.32522	-1.93282	(5)
H(30)	0.94586	-0.50760	-3.35323	(5)
H(31)	-4.08878	-1.04239	0.70433	(5)
H(32)	-4.17884	0.75580	0.89980	(5)
H(33)	-4.67204	-0.01318	-0.64301	(5)

118c4

C(1)	-2.47198	1.71841	0.50157	(2)
C(2)	-1.34512	2.41675	0.67180	(2)
C(3)	0.03453	1.80331	0.73243	(1)
C(4)	0.06682	0.34679	0.15424	(1)
C(5)	-1.15445	-0.43577	0.74476	(1)
C(6)	-2.49542	0.22607	0.33798	(1)
C(7)	-1.15109	-1.88762	0.26175	(3)
C(8)	-1.04249	-2.10695	-1.24238	(1)
C(9)	0.01266	-1.19862	-1.91398	(1)
C(10)	-0.02425	0.22324	-1.37240	(3)
O(11)	-1.30512	-2.81432	1.02713	(7)
O(12)	-0.12391	1.17556	-2.11344	(7)
C(13)	1.04995	2.78036	0.11063	(1)
C(14)	1.36080	-0.31444	0.60568	(3)
O(15)	1.46642	-1.08557	1.53912	(78)
O(16)	2.41786	0.05292	-0.16275	(75)
C(17)	3.68657	-0.52418	0.19528	(1)
H(18)	-3.43979	2.24628	0.45184	(5)
H(19)	-1.41130	3.51216	0.78784	(5)
H(20)	0.28311	1.73274	1.81716	(5)
H(21)	-1.08430	-0.42705	1.85093	(5)
H(22)	-3.31533	-0.19795	0.95854	(5)
H(23)	-2.74738	0.00032	-0.71964	(5)
H(24)	-0.80264	-3.16744	-1.45289	(5)
H(25)	-2.03605	-1.91912	-1.70404	(5)
H(26)	1.02433	-1.62720	-1.75109	(5)
H(27)	-0.14629	-1.19429	-3.00951	(5)
H(28)	2.09274	2.40340	0.17120	(5)
H(29)	0.83810	3.00399	-0.95628	(5)
H(30)	1.04623	3.75752	0.64421	(5)
H(31)	3.65213	-1.62790	0.11442	(5)
H(32)	4.46369	-0.15118	-0.49833	(5)
H(33)	3.97338	-0.23329	1.22436	(5)

118t1

C(1)	1.88382	-1.48314	1.52930	(2)
C(2)	2.58438	-0.82843	0.59352	(2)
C(3)	2.02610	0.28535	-0.26258	(1)
C(4)	0.46576	0.24219	-0.24647	(1)
C(5)	-0.00641	0.14215	1.23870	(1)
C(6)	0.44114	-1.19416	1.84602	(1)
C(7)	-1.50744	0.37202	1.41322	(3)
C(8)	-2.12652	1.49427	0.58938	(1)
C(9)	-1.06625	2.35146	-0.10672	(1)
C(10)	-0.10062	1.50854	-0.92234	(3)
O(11)	-2.17502	-0.28233	2.18407	(7)
O(12)	0.25154	1.84930	-2.03110	(7)
C(13)	2.62624	1.62119	0.22414	(1)
C(14)	-0.03540	-0.93297	-1.07323	(3)
O(15)	0.65353	-1.65551	-1.76778	(78)
O(16)	-1.37774	-1.09457	-0.96079	(75)
C(17)	-1.94479	-2.18660	-1.70566	(1)
H(18)	2.36375	-2.30242	2.09165	(5)
H(19)	3.63690	-1.10886	0.41598	(5)
H(20)	2.37604	0.12213	-1.30691	(5)
H(21)	0.48810	0.95349	1.81674	(5)
H(22)	-0.18448	-2.03087	1.46681	(5)
H(23)	0.31118	-1.16514	2.95037	(5)
H(24)	-2.80968	1.05701	-0.17025	(5)
H(25)	-2.75138	2.13481	1.24587	(5)
H(26)	-1.56197	3.09633	-0.75932	(5)
H(27)	-0.49366	2.93018	0.65046	(5)
H(28)	2.27988	2.48495	-0.38385	(5)
H(29)	2.37449	1.84130	1.28406	(5)
H(30)	3.73727	1.61210	0.15413	(5)
H(31)	-3.03679	-2.21687	-1.53017	(5)
H(32)	-1.77274	-2.05242	-2.79112	(5)
H(33)	-1.51497	-3.15191	-1.37503	(5)

118t3

C(1)	0.57910	-2.67410	-0.59911	(2)
C(2)	1.46898	-2.19624	0.27926	(2)
C(3)	1.25897	-0.93610	1.08522	(1)
C(4)	0.21371	-0.01534	0.37072	(1)
C(5)	-1.05517	-0.85749	0.06268	(1)
C(6)	-0.73103	-2.00492	-0.91174	(1)
C(7)	-2.23399	-0.02323	-0.44701	(3)
C(8)	-2.33145	1.40668	0.06115	(1)
C(9)	-1.59056	1.58134	1.38690	(1)
C(10)	-0.12658	1.18874	1.27633	(3)
O(11)	-3.06541	-0.47987	-1.20107	(7)
O(12)	0.72570	1.77391	1.90971	(7)
C(13)	0.86540	-1.34871	2.52039	(1)
C(14)	0.78602	0.59956	-0.90043	(3)
O(15)	0.17615	0.76382	-1.93842	(78)
O(16)	2.07943	0.98174	-0.74717	(75)
C(17)	2.69863	1.58432	-1.89793	(1)
H(18)	0.81028	-3.59867	-1.15564	(5)
H(19)	2.41084	-2.74586	0.44852	(5)
H(20)	2.23463	-0.40537	1.14772	(5)
H(21)	-1.40270	-1.31321	1.01606	(5)
H(22)	-0.69608	-1.63534	-1.95891	(5)
H(23)	-1.54179	-2.76556	-0.87032	(5)
H(24)	-1.90976	2.09931	-0.69918	(5)
H(25)	-3.39664	1.68640	0.18900	(5)
H(26)	-1.67270	2.63409	1.72242	(5)
H(27)	-2.07492	0.96012	2.17199	(5)
H(28)	0.69563	-0.47218	3.18211	(5)
H(29)	-0.05795	-1.96662	2.54926	(5)
H(30)	1.66852	-1.95362	2.99847	(5)
H(31)	3.74487	1.84676	-1.65163	(5)
H(32)	2.71106	0.87874	-2.75111	(5)
H(33)	2.16860	2.51222	-2.18772	(5)

118t2

C(1)	0.87443	2.54536	0.71774	(2)
C(2)	1.66881	2.02498	-0.21211	(2)
C(3)	1.31063	0.85829	-1.09808	(1)
C(4)	0.20946	0.01518	-0.38310	(1)
C(5)	-0.96337	0.97793	-0.01103	(1)
C(6)	-0.50411	2.02147	1.01929	(1)
C(7)	-2.22135	0.23765	0.43447	(3)
C(8)	-2.68937	-0.87595	-0.48295	(1)
C(9)	-1.54661	-1.86038	-0.79092	(1)
C(10)	-0.29458	-1.14077	-1.26642	(3)
O(11)	-2.86406	0.57136	1.40573	(7)
O(12)	0.31078	-1.52464	-2.24327	(7)
C(13)	0.91534	1.43575	-2.47589	(1)
C(14)	0.76651	-0.68580	0.84944	(3)
O(15)	0.18832	-0.80936	1.91107	(78)
O(16)	1.99819	-1.21030	0.62433	(75)
C(17)	2.59889	-1.90350	1.73308	(1)
H(18)	1.22595	3.39527	1.32776	(5)
H(19)	2.68586	2.46745	-0.36681	(5)
H(20)	2.21661	0.22961	-1.24477	(5)
H(21)	-1.26045	1.52462	-0.93221	(5)
H(22)	-0.50311	1.59641	2.04537	(5)
H(23)	-1.22094	2.87207	1.02911	(5)
H(24)	-3.06254	-0.43010	-1.43056	(5)
H(25)	-3.54079	-1.41847	-0.02875	(5)
H(26)	-1.88076	-2.58784	-1.55585	(5)
H(27)	-1.30685	-2.45122	0.11931	(5)
H(28)	0.08759	2.17430	-2.41062	(5)
H(29)	0.59849	0.65285	-3.19662	(5)
H(30)	1.77366	1.96570	-2.94716	(5)
H(31)	1.98184	-2.77254	2.03298	(5)
H(32)	2.73072	-1.22276	2.59630	(5)
H(33)	3.59619	-2.27569	1.43139	(5)

118t4

C(1)	1.77873	1.61593	-1.44612	(2)
C(2)	2.52212	0.92257	-0.57212	(2)
C(3)	2.03259	-0.29824	0.17667	(1)
C(4)	0.47663	-0.27675	0.22458	(1)
C(5)	-0.03547	-0.10568	-1.24615	(1)
C(6)	0.35204	1.27653	-1.78688	(1)
C(7)	-1.52203	-0.40197	-1.39833	(3)
C(8)	-1.98128	-1.72683	-0.82387	(1)
C(9)	-1.56152	-1.86515	0.65074	(1)
C(10)	-0.08647	-1.55921	0.87133	(3)
O(11)	-2.27552	0.32704	-2.00515	(7)
O(12)	0.58576	-2.26057	1.59575	(7)
C(13)	2.66020	-1.53854	-0.49812	(1)
C(14)	0.00907	0.85647	1.13136	(3)
O(15)	0.69054	1.41655	1.96864	(78)
O(16)	-1.28973	1.18287	0.91320	(75)
C(17)	-1.81476	2.25244	1.71899	(1)
H(18)	2.20954	2.50576	-1.93651	(5)
H(19)	3.55890	1.24379	-0.37268	(5)
H(20)	2.42344	-0.24427	1.21772	(5)
H(21)	0.47391	-0.86585	-1.87704	(5)
H(22)	-0.31126	2.06699	-1.37514	(5)
H(23)	0.22701	1.29338	-2.89200	(5)
H(24)	-3.07995	-1.82776	-0.91372	(5)
H(25)	-1.53403	-2.55304	-1.41798	(5)
H(26)	-2.17559	-1.18580	1.27992	(5)
H(27)	-1.78719	-2.89188	0.99954	(5)
H(28)	2.34526	-2.49240	-0.02499	(5)
H(29)	2.41100	-1.61218	-1.57851	(5)
H(30)	3.77123	-1.50894	-0.43224	(5)
H(31)	-1.25190	3.18938	1.54229	(5)
H(32)	-2.87210	2.42787	1.44439	(5)
H(33)	-1.77584	1.98933	2.79373	(5)

119c1

C(1)	2.54210	-1.68361	0.78876	(1)
C(2)	1.35434	-2.47059	0.22660	(1)
C(3)	0.01446	-1.81508	0.60084	(1)
C(4)	-0.07585	-0.32854	0.12025	(1)
C(5)	1.15658	0.44670	0.70732	(1)
C(6)	2.49093	-0.23022	0.32127	(1)
C(7)	1.17190	1.90208	0.23835	(3)
C(8)	1.05477	2.13404	-1.25995	(1)
C(9)	-0.08585	1.30595	-1.88817	(1)
C(10)	-0.06628	-0.13644	-1.40522	(3)
O(11)	1.33731	2.82058	1.01109	(7)
O(12)	-0.05800	-1.05674	-2.19218	(7)
C(13)	-1.14469	-2.71582	0.14036	(1)
C(14)	-1.35916	0.28486	0.65997	(3)
O(15)	-1.44040	0.98079	1.65300	(78)
O(16)	-2.43652	-0.02539	-0.10632	(75)
C(17)	-3.69625	0.51574	0.33109	(1)
H(18)	2.52607	-1.72114	1.90239	(5)
H(19)	3.49874	-2.15501	0.46487	(5)
H(20)	1.45014	-2.55557	-0.87849	(5)
H(21)	1.38909	-3.51133	0.62429	(5)
H(22)	-0.03004	-1.79565	1.71538	(5)
H(23)	1.08669	0.44331	1.81353	(5)
H(24)	3.34038	0.33268	0.76828	(5)
H(25)	2.63488	-0.19839	-0.78023	(5)
H(26)	0.89105	3.20922	-1.46786	(5)
H(27)	2.01855	1.86567	-1.74403	(5)
H(28)	-1.06301	1.76816	-1.63280	(5)
H(29)	-0.00536	1.34114	-2.99168	(5)
H(30)	-2.12521	-2.37406	0.53626	(5)
H(31)	-1.23264	-2.77488	-0.96501	(5)
H(32)	-1.01295	-3.75869	0.50597	(5)
H(33)	-3.66724	1.62255	0.33522	(5)
H(34)	-4.49171	0.19369	-0.36723	(5)
H(35)	-3.95284	0.14452	1.34215	(5)

119c2

C(1)	1.34156	-2.44090	0.31708	(1)
C(2)	0.47845	-2.35438	-0.94608	(1)
C(3)	0.28512	-0.90670	-1.43381	(1)
C(4)	-0.27778	0.00769	-0.30241	(1)
C(5)	0.56878	-0.10896	1.01307	(1)
C(6)	0.75603	-1.57093	1.43082	(1)
C(7)	1.88134	0.66773	0.93674	(3)
C(8)	1.78720	2.10360	0.43178	(1)
C(9)	0.34313	2.50808	0.10575	(1)
C(10)	-0.32242	1.47522	-0.78606	(3)
O(11)	2.93735	0.20371	1.30732	(7)
O(12)	-0.85920	1.79127	-1.82609	(7)
C(13)	1.58929	-0.39027	-2.06644	(1)
C(14)	-1.73363	-0.33619	-0.01428	(3)
O(15)	-2.41687	-1.12384	-0.63984	(78)
O(16)	-2.21574	0.36418	1.04545	(75)
C(17)	-3.59338	0.12208	1.38241	(1)
H(18)	2.38532	-2.12878	0.09189	(5)
H(19)	1.39940	-3.50014	0.65966	(5)
H(20)	-0.51243	-2.81771	-0.73762	(5)
H(21)	0.93664	-2.96829	-1.75528	(5)
H(22)	-0.46549	-0.93203	-2.25824	(5)
H(23)	0.00833	0.38231	1.84007	(5)
H(24)	-0.22999	-1.99119	1.73026	(5)
H(25)	1.39846	-1.63310	2.33668	(5)
H(26)	2.41706	2.21042	-0.47717	(5)
H(27)	2.20619	2.79430	1.19347	(5)
H(28)	0.33755	3.49904	-0.38775	(5)
H(29)	-0.24338	2.62225	1.04227	(5)
H(30)	2.43391	-0.35715	-1.34803	(5)
H(31)	1.47691	0.63119	-2.49014	(5)
H(32)	1.91331	-1.04293	-2.90771	(5)
H(33)	-4.25736	0.39382	0.53910	(5)
H(34)	-3.86900	0.74605	2.25355	(5)
H(35)	-3.74991	-0.93963	1.65481	(5)

119c3

C(1)	0.93635	2.60378	0.14739	(1)
C(2)	-0.20412	2.18852	1.08335	(1)
C(3)	-0.19935	0.67916	1.37678	(1)
C(4)	-0.26184	-0.14298	0.04732	(1)
C(5)	0.85885	0.29243	-0.95196	(1)
C(6)	0.87893	1.81197	-1.16037	(1)
C(7)	2.22511	-0.28321	-0.58765	(3)
C(8)	2.27134	-1.78354	-0.31877	(1)
C(9)	0.88481	-2.43189	-0.44400	(1)
C(10)	-0.14506	-1.65389	0.35486	(3)
O(11)	3.23350	0.38797	-0.56613	(7)
O(12)	-0.82263	-2.19412	1.20275	(7)
C(13)	0.98916	0.31689	2.28420	(1)
C(14)	-1.62158	-0.00269	-0.63156	(3)
O(15)	-1.79967	0.06941	-1.83171	(78)
O(16)	-2.64552	0.01513	0.25969	(75)
C(17)	-3.96702	0.12512	-0.29943	(1)
H(18)	0.86302	3.69441	-0.07145	(5)
H(19)	1.91909	2.45229	0.64618	(5)
H(20)	-0.13485	2.76088	2.03687	(5)
H(21)	-1.17695	2.47463	0.62126	(5)
H(22)	-1.11228	0.45555	1.97501	(5)
H(23)	0.63146	-0.15626	-1.94583	(5)
H(24)	-0.03645	2.11535	-1.71514	(5)
H(25)	1.73235	2.09905	-1.81335	(5)
H(26)	2.97752	-2.26821	-1.02547	(5)
H(27)	2.67105	-1.95600	0.70336	(5)
H(28)	0.57344	-2.47346	-1.50939	(5)
H(29)	0.93131	-3.48028	-0.09164	(5)
H(30)	0.98903	-0.75800	2.56758	(5)
H(31)	1.97236	0.53214	1.81860	(5)
H(32)	0.95631	0.89159	3.23677	(5)
H(33)	-4.70926	0.12937	0.52108	(5)
H(34)	-4.07490	1.06913	-0.86788	(5)
H(35)	-4.18653	-0.73614	-0.95967	(5)

119c4

C(1)	2.48269	-0.67086	-1.67301	(1)
C(2)	2.64957	0.56858	-0.78660	(1)
C(3)	1.30745	1.28174	-0.55545	(1)
C(4)	0.22798	0.33551	0.06106	(1)
C(5)	0.08243	-0.91718	-0.87810	(1)
C(6)	1.44115	-1.62258	-1.08360	(1)
C(7)	-0.93820	-1.89926	-0.30800	(3)
C(8)	-0.70731	-2.35576	1.12323	(1)
C(9)	-0.43153	-1.16840	2.07195	(1)
C(10)	0.55618	-0.17396	1.47612	(3)
O(11)	-1.85965	-2.32132	-0.97159	(7)
O(12)	1.52995	0.18247	2.10150	(7)
C(13)	1.52656	2.57892	0.24117	(1)
C(14)	-1.08606	1.09984	0.14599	(3)
O(15)	-1.52916	1.63286	1.14506	(78)
O(16)	-1.72750	1.14084	-1.04954	(75)
C(17)	-2.98812	1.83385	-1.06432	(1)
H(18)	2.17060	-0.36124	-2.69705	(5)
H(19)	3.46022	-1.19547	-1.78042	(5)
H(20)	3.10687	0.27488	0.18396	(5)
H(21)	3.36867	1.26898	-1.27117	(5)
H(22)	0.93396	1.59018	-1.56017	(5)
H(23)	-0.27288	-0.59016	-1.87493	(5)
H(24)	1.31165	-2.49631	-1.76035	(5)
H(25)	1.82066	-2.02247	-0.11888	(5)
H(26)	-1.58289	-2.92689	1.48790	(5)
H(27)	0.15367	-3.05785	1.14564	(5)
H(28)	-1.38682	-0.65083	2.30105	(5)
H(29)	-0.05003	-1.55031	3.03856	(5)
H(30)	0.58416	3.15459	0.37020	(5)
H(31)	1.94445	2.39713	1.25379	(5)
H(32)	2.23940	3.25546	-0.28126	(5)
H(33)	-3.41355	1.79204	-2.08482	(5)
H(34)	-3.70655	1.35568	-0.37066	(5)
H(35)	-2.85401	2.89785	-0.78897	(5)

119c5

C(1)	-2.54975	0.79957	-1.49358	(1)
C(2)	-2.66909	-0.50660	-0.69949	(1)
C(3)	-1.31519	-1.22794	-0.60294	(1)
C(4)	-0.22336	-0.32441	0.05672	(1)
C(5)	-0.10719	0.97807	-0.80062	(1)
C(6)	-1.46709	1.70564	-0.90414	(1)
C(7)	0.95248	1.93923	-0.25477	(3)
C(8)	1.37475	1.75191	1.19382	(1)
C(9)	0.21977	1.27302	2.07669	(1)
C(10)	-0.53596	0.07177	1.51177	(3)
O(11)	1.43113	2.81219	-0.94543	(7)
O(12)	-1.36245	-0.50049	2.18746	(7)
C(13)	-1.48774	-2.60153	0.06698	(1)
C(14)	1.09338	-1.08332	0.06313	(3)
O(15)	1.62751	-1.56081	1.04571	(78)
O(16)	1.62882	-1.17878	-1.18082	(75)
C(17)	2.88190	-1.87954	-1.27396	(1)
H(18)	-2.30452	0.56914	-2.55610	(5)
H(19)	-3.52920	1.33146	-1.49957	(5)
H(20)	-3.06851	-0.29173	0.31647	(5)
H(21)	-3.41484	-1.16948	-1.19628	(5)
H(22)	-0.98573	-1.43123	-1.64884	(5)
H(23)	0.19928	0.70474	-1.83208	(5)
H(24)	-1.36239	2.61322	-1.53930	(5)
H(25)	-1.78850	2.05999	0.09888	(5)
H(26)	2.21703	1.02931	1.24049	(5)
H(27)	1.77005	2.70712	1.59292	(5)
H(28)	0.60794	1.02051	3.08563	(5)
H(29)	-0.49983	2.10829	2.21912	(5)
H(30)	-0.52740	-3.15799	0.13387	(5)
H(31)	-1.90311	-2.53272	1.09425	(5)
H(32)	-2.18539	-3.24538	-0.51409	(5)
H(33)	3.65998	-1.37315	-0.67054	(5)
H(34)	2.77079	-2.92828	-0.93680	(5)
H(35)	3.21503	-1.88926	-2.32898	(5)

119c8

C(1)	2.49311	1.46671	1.21300	(1)
C(2)	2.85017	0.21003	0.41905	(1)
C(3)	1.74434	-0.85478	0.50896	(1)
C(4)	0.35010	-0.33672	0.04279	(1)
C(5)	0.02667	1.01320	0.79880	(1)
C(6)	1.17650	2.03975	0.69976	(1)
C(7)	-1.25320	1.66860	0.28293	(3)
C(8)	-1.34703	1.87448	-1.21905	(1)
C(9)	-0.96797	0.60733	-2.01367	(1)
C(10)	0.28051	-0.08194	-1.47777	(3)
O(11)	-2.11654	2.06390	1.03571	(7)
O(12)	1.16488	-0.40597	-2.23851	(7)
C(13)	2.24640	-2.12692	-0.20926	(1)
C(14)	-0.70384	-1.37715	0.42569	(3)
O(15)	-0.48003	-2.46979	0.90946	(78)
O(16)	-1.96770	-0.93588	0.20925	(75)
C(17)	-3.02578	-1.83650	0.58162	(1)
H(18)	2.40661	1.22285	2.29667	(5)
H(19)	3.30455	2.22443	1.11462	(5)
H(20)	3.03714	0.48323	-0.64380	(5)
H(21)	3.80697	-0.20805	0.80961	(5)
H(22)	1.64395	-1.11467	1.58915	(5)
H(23)	-0.12167	0.77690	1.87206	(5)
H(24)	0.91731	2.95141	1.28290	(5)
H(25)	1.31079	2.36493	-0.35449	(5)
H(26)	-2.37078	2.19261	-1.49622	(5)
H(27)	-0.67356	2.70897	-1.51080	(5)
H(28)	-1.81638	-0.10826	-2.01626	(5)
H(29)	-0.81237	0.88324	-3.07503	(5)
H(30)	1.45791	-2.89592	-0.34593	(5)
H(31)	2.66571	-1.91383	-1.21550	(5)
H(32)	3.06443	-2.61238	0.36915	(5)
H(33)	-2.99137	-2.05522	1.66644	(5)
H(34)	-4.00032	-1.36380	0.35575	(5)
H(35)	-2.95833	-2.78040	0.00687	(5)

119c7

C(1)	-2.55041	-1.72940	-0.63544	(1)
C(2)	-1.31153	-2.49287	-0.15574	(1)
C(3)	-0.01674	-1.80811	-0.62315	(1)
C(4)	0.07215	-0.32771	-0.11957	(1)
C(5)	-1.18919	0.42212	-0.65064	(1)
C(6)	-2.49476	-0.26694	-0.19370	(1)
C(7)	-1.21762	1.89402	-0.22247	(3)
C(8)	-0.30284	2.29648	0.92298	(1)
C(9)	-0.20410	1.19805	1.98435	(1)
C(10)	0.11702	-0.18132	1.41293	(3)
O(11)	-1.94904	2.69693	-0.75982	(7)
O(12)	0.36122	-1.10641	-2.15581	(7)
C(13)	1.19535	-2.68822	-0.27384	(1)
C(14)	1.32470	0.30570	-0.70557	(3)
O(15)	1.37095	0.93306	-1.74563	(78)
O(16)	2.41501	0.10292	0.07787	(75)
C(17)	3.64898	0.66706	-0.40180	(1)
H(18)	-2.61472	-1.78133	-1.74687	(5)
H(19)	-3.47288	-2.21265	-0.23824	(5)
H(20)	-1.32817	-2.57621	0.95362	(5)
H(21)	-1.35164	-3.53483	-0.54952	(5)
H(22)	-0.05856	-1.76872	-1.73723	(5)
H(23)	-1.17203	0.40396	-1.76133	(5)
H(24)	-3.37360	0.27437	-0.60929	(5)
H(25)	-2.58672	-0.21210	0.91265	(5)
H(26)	0.70680	2.53595	0.52650	(5)
H(27)	-0.87674	3.22833	1.39117	(5)
H(28)	0.56904	1.47510	2.73138	(5)
H(29)	-1.16684	1.13718	2.53674	(5)
H(30)	2.14163	-2.28561	-0.69556	(5)
H(31)	1.34228	-2.80959	0.81983	(5)
H(32)	1.08096	-3.71246	-0.69406	(5)
H(33)	4.45843	0.43202	0.31490	(5)
H(34)	3.92147	0.23615	-1.38461	(5)
H(35)	3.57009	1.76829	-0.48529	(5)

119c9

C(1)	-2.80613	-1.17116	0.86536	(1)
C(2)	-2.85834	0.17874	0.14621	(1)
C(3)	-1.63302	1.03644	0.49469	(1)
C(4)	-0.29836	0.34415	0.07344	(1)
C(5)	-0.25772	-1.07945	0.73727	(1)
C(6)	-1.53135	-1.92165	0.48803	(1)
C(7)	0.96818	-1.88470	0.31002	(3)
C(8)	1.40022	-1.78213	-1.14769	(1)
C(9)	0.38976	-1.05869	-2.04054	(1)
C(10)	-0.13619	0.24905	-1.46102	(3)
O(11)	1.56438	-2.59166	1.09306	(7)
O(12)	-0.42687	1.16492	-2.19852	(7)
C(13)	-1.83643	2.45406	-0.07348	(1)
C(14)	0.86710	1.15812	0.62779	(3)
O(15)	0.79569	1.95724	1.54169	(78)
O(16)	2.03545	0.87683	-0.00135	(75)
C(17)	3.19376	1.58346	0.47691	(1)
H(18)	-2.83950	-1.01375	1.96802	(5)
H(19)	-3.70065	-1.78072	0.59984	(5)
H(20)	-2.91433	0.01913	-0.95451	(5)
H(21)	-3.79110	0.71363	0.43994	(5)
H(22)	-1.61759	1.13691	1.60515	(5)
H(23)	-0.18008	-0.92953	1.83456	(5)
H(24)	-1.47418	-2.86572	1.07458	(5)
H(25)	-1.59555	-2.22566	-0.57662	(5)
H(26)	2.38163	-1.26503	-1.20057	(5)
H(27)	1.57318	-2.80338	-1.54721	(5)
H(28)	0.86129	-0.85735	-3.02344	(5)
H(29)	-0.46875	-1.72884	-2.25698	(5)
H(30)	-0.92738	3.08694	0.01652	(5)
H(31)	-2.13141	2.44556	-1.14461	(5)
H(32)	-2.64959	2.98728	0.46847	(5)
H(33)	4.08019	1.25994	-0.10080	(5)
H(34)	3.07119	2.67527	0.34007	(5)
H(35)	3.37763	1.35839	1.54532	(5)

119t1

C(1)	-0.16867	2.88810	-0.63906	(1)
C(2)	-1.48307	2.18295	-0.28154	(1)
C(3)	-1.29819	1.10755	0.80388	(1)
C(4)	-0.23632	0.05769	0.34550	(1)
C(5)	1.10081	0.78520	0.02448	(1)
C(6)	0.91483	1.88063	-1.03444	(1)
C(7)	2.21922	-0.18795	-0.35646	(3)
C(8)	2.21012	-1.53829	0.34589	(1)
C(9)	1.41746	-1.48923	1.65306	(1)
C(10)	-0.00922	-1.00106	1.44758	(3)
O(11)	3.08538	0.09985	-1.15351	(7)
O(12)	-0.91196	-1.40508	2.14892	(7)
C(13)	-0.97064	1.76490	2.15750	(1)
C(14)	-0.74341	-0.73121	-0.85483	(3)
O(15)	-0.10477	-0.98389	-1.85703	(78)
O(16)	-2.02150	-1.15545	-0.68138	(75)
C(17)	-2.58305	-1.92279	-1.76163	(1)
H(18)	-0.34128	3.60278	-1.47697	(5)
H(19)	0.18277	3.49830	0.22332	(5)
H(20)	-2.23256	2.93574	0.05504	(5)
H(21)	-1.90687	1.71610	-1.20026	(5)
H(22)	-2.27834	0.59448	0.93550	(5)
H(23)	1.45226	1.28404	0.95473	(5)
H(24)	0.65196	1.42685	-2.01404	(5)
H(25)	1.87266	2.42574	-1.18893	(5)
H(26)	1.77142	-2.30391	-0.33009	(5)
H(27)	3.25134	-1.85850	0.55294	(5)
H(28)	1.40534	-2.49563	2.11682	(5)
H(29)	1.92928	-0.81560	2.37507	(5)
H(30)	-0.90769	1.02189	2.98166	(5)
H(31)	-0.00994	2.32094	2.15085	(5)
H(32)	-1.75960	2.49281	2.45145	(5)
H(33)	-3.62077	-2.20717	-1.50394	(5)
H(34)	-2.60965	-1.32619	-2.69398	(5)
H(35)	-2.00158	-2.85030	-1.92759	(5)

119t3

C(1)	2.19114	1.74508	-1.00402	(1)
C(2)	2.58668	0.98511	0.26955	(1)
C(3)	1.96167	-0.42266	0.35669	(1)
C(4)	0.41490	-0.35243	0.18205	(1)
C(5)	0.08948	0.36038	-1.16882	(1)
C(6)	0.67055	1.77555	-1.19073	(1)
C(7)	-1.39782	0.32357	-1.51296	(3)
C(8)	-2.10565	-1.00850	-1.29246	(1)
C(9)	-1.12387	-2.13522	-0.95574	(1)
C(10)	-0.19236	-1.77307	0.19155	(3)
O(11)	-1.98594	1.28222	-1.96365	(7)
O(12)	0.09835	-2.58536	1.04322	(7)
C(13)	2.64832	-1.37203	-0.64203	(1)
C(14)	-0.21003	0.35426	1.38002	(3)
O(15)	0.35242	0.59630	2.43075	(78)
O(16)	-1.50660	0.68484	1.16049	(75)
C(17)	-2.17834	1.35699	2.24033	(1)
H(18)	2.58573	2.78661	-0.95836	(5)
H(19)	2.66735	1.26896	-1.89111	(5)
H(20)	3.69682	0.90808	0.32789	(5)
H(21)	2.27989	1.58816	1.15381	(5)
H(22)	2.18117	-0.82522	1.37296	(5)
H(23)	0.58516	-0.20490	-1.98809	(5)
H(24)	0.20640	2.39398	-0.39203	(5)
H(25)	0.43492	2.27251	-2.15797	(5)
H(26)	-2.84556	-0.90090	-0.47056	(5)
H(27)	-2.68175	-1.27656	-2.20250	(5)
H(28)	-1.68941	-3.05394	-0.70479	(5)
H(29)	-0.51369	-2.38082	-1.85232	(5)
H(30)	2.25803	-2.41047	-0.56953	(5)
H(31)	2.52840	-1.05193	-1.69833	(5)
H(32)	3.74278	-1.43376	-0.44953	(5)
H(33)	-3.22001	1.57637	1.93870	(5)
H(34)	-2.20757	0.71693	3.14326	(5)
H(35)	-1.67814	2.31595	2.47715	(5)

119t2

C(1)	0.77795	-2.76766	-0.69912	(1)
C(2)	1.90328	-1.82551	-0.24635	(1)
C(3)	1.45411	-0.85332	0.86249	(1)
C(4)	0.23638	-0.02205	0.36080	(1)
C(5)	-0.91757	-1.00559	-0.01944	(1)
C(6)	-0.48132	-1.99381	-1.10581	(1)
C(7)	-2.20477	-0.26597	-0.37122	(3)
C(8)	-2.68790	0.73075	0.66674	(1)
C(9)	-1.56806	1.70689	1.07657	(1)
C(10)	-0.27061	0.98461	1.41021	(3)
O(11)	-2.85513	-0.51693	-1.36213	(7)
O(12)	0.35789	1.26366	2.40771	(7)
C(13)	1.20658	-1.63306	2.16840	(1)
C(14)	0.63877	0.85772	-0.81544	(3)
O(15)	0.00979	0.99442	-1.84599	(78)
O(16)	1.79658	1.52552	-0.57536	(75)
C(17)	2.24963	2.39797	-1.62636	(1)
H(18)	1.12993	-3.38800	-1.55583	(5)
H(19)	0.52981	-3.48131	0.11871	(5)
H(20)	2.77318	-2.42573	0.10690	(5)
H(21)	2.26817	-1.24714	-1.12589	(5)
H(22)	2.30167	-0.15968	1.06692	(5)
H(23)	-1.17043	-1.60178	0.88413	(5)
H(24)	-0.29057	-1.46125	-2.06169	(5)
H(25)	-1.30127	-2.71815	-1.30962	(5)
H(26)	-3.55814	1.29718	0.28280	(5)
H(27)	-3.03968	0.17349	1.56225	(5)
H(28)	-1.38238	2.42719	0.25071	(5)
H(29)	-1.90174	2.30878	1.94400	(5)
H(30)	0.94795	-0.96933	3.02022	(5)
H(31)	0.39025	-2.38018	2.08463	(5)
H(32)	2.11762	-2.19279	2.47751	(5)
H(33)	1.50663	3.19529	-1.82167	(5)
H(34)	3.19753	2.87745	-1.31695	(5)
H(35)	2.43857	1.82695	-2.55596	(5)

119t4

C(1)	2.10202	1.60807	-1.31094	(1)
C(2)	2.53224	1.07226	0.06323	(1)
C(3)	1.97808	-0.33720	0.36429	(1)
C(4)	0.42932	-0.33595	0.23104	(1)
C(5)	0.06338	0.11923	-1.22222	(1)
C(6)	0.58262	1.53125	-1.50102	(1)
C(7)	-1.41830	-0.05336	-1.53298	(3)
C(8)	-1.97402	-1.44098	-1.27521	(1)
C(9)	-1.64568	-1.92312	0.15116	(1)
C(10)	-0.18106	-1.72298	0.51934	(3)
O(11)	-2.09191	0.82242	-2.02992	(7)
O(12)	0.43613	-2.59693	1.08832	(7)
C(13)	2.69965	-1.37299	-0.52002	(1)
C(14)	-0.17053	0.56586	1.30786	(3)
O(15)	0.35360	0.83412	2.37204	(78)
O(16)	-1.39231	1.04211	0.96131	(75)
C(17)	-2.02918	1.90587	1.91912	(1)
H(18)	2.60810	1.02965	-2.11679	(5)
H(19)	2.44191	2.66350	-1.42566	(5)
H(20)	2.19373	1.78628	0.84774	(5)
H(21)	3.64478	1.06048	0.12615	(5)
H(22)	2.23908	-0.58456	1.41950	(5)
H(23)	0.57644	-0.56368	-1.93345	(5)
H(24)	0.08690	2.26585	-0.83061	(5)
H(25)	0.33131	1.83183	-2.54250	(5)
H(26)	-1.53582	-2.14596	-2.01480	(5)
H(27)	-3.06952	-1.45441	-1.43374	(5)
H(28)	-1.91304	-2.99379	0.24496	(5)
H(29)	-2.28345	-1.38328	0.88360	(5)
H(30)	2.56016	-1.19336	-1.60633	(5)
H(31)	2.36685	-2.41344	-0.32089	(5)
H(32)	3.79734	-1.35788	-0.33632	(5)
H(33)	-2.20492	1.37177	2.87289	(5)
H(34)	-3.00850	2.23059	1.51958	(5)
H(35)	-1.41459	2.80826	2.10308	(5)

120c1

C(1)	0.66850	-2.31586	-1.61845	(2)
C(2)	-0.30185	-2.16488	-0.70894	(2)
C(3)	-0.22596	-1.23669	0.48033	(1)
C(4)	1.25895	-0.81144	0.76604	(1)
C(5)	2.00223	-0.44771	-0.54625	(1)
C(6)	1.99576	-1.61246	-1.54978	(1)
C(7)	1.48761	0.85429	-1.14479	(3)
C(8)	1.34754	1.99694	-0.19298	(2)
C(9)	1.30622	1.75553	1.12847	(2)
C(10)	1.29934	0.38820	1.72179	(3)
O(11)	1.30493	0.24834	2.93143	(81)
O(12)	1.26289	0.99557	-2.33234	(81)
C(13)	1.26937	3.38191	-0.77839	(1)
C(14)	1.98311	-2.00403	1.43178	(1)
C(15)	-1.22162	-0.08030	0.26331	(1)
O(16)	-2.55918	-0.61901	0.19252	(75)
C(17)	-3.55449	0.28795	0.01348	(3)
O(18)	-3.35622	1.48311	-0.07518	(78)
C(19)	-4.88990	-0.37308	-0.05622	(1)
H(20)	0.52256	-3.02307	-2.45317	(5)
H(21)	-1.23756	-2.73796	-0.82994	(5)
H(22)	-0.57957	-1.80916	1.36874	(5)
H(23)	3.07003	-0.24694	-0.29127	(5)
H(24)	2.77342	-2.35653	-1.27090	(5)
H(25)	2.27871	-1.25116	-2.56171	(5)
H(26)	1.22736	2.59544	1.83790	(5)
H(27)	0.37369	3.49289	-1.42552	(5)
H(28)	2.16529	3.60624	-1.39511	(5)
H(29)	1.20614	4.16375	0.00720	(5)
H(30)	1.52587	-2.27654	2.40658	(5)
H(31)	3.05215	-1.77585	1.62995	(5)
H(32)	1.95646	-2.92199	0.80999	(5)
H(33)	-0.99278	0.46335	-0.67284	(5)
H(34)	-1.16857	0.63545	1.10652	(5)
H(35)	-4.92946	-1.09439	-0.89895	(5)
H(36)	-5.69651	0.36904	-0.20384	(5)
H(37)	-5.10378	-0.93001	0.87981	(5)

120c3

C(1)	-2.80341	0.66748	-1.63102	(2)
C(2)	-1.69574	1.41654	-1.68757	(2)
C(3)	-0.60611	1.42578	-0.64039	(1)
C(4)	-1.12422	0.79958	0.70674	(1)
C(5)	-1.94394	-0.49334	0.44831	(1)
C(6)	-3.14187	-0.23875	-0.48031	(1)
C(7)	-1.05897	-1.63809	-0.02572	(3)
C(8)	0.19165	-1.86064	0.76007	(2)
C(9)	0.65102	-0.88426	1.56100	(2)
C(10)	0.03870	0.47168	1.65225	(3)
O(11)	0.46781	1.28182	2.45389	(81)
O(12)	-1.36411	-2.37710	-0.94306	(81)
C(13)	0.87633	-3.19358	0.61450	(1)
C(14)	-2.04248	1.83671	1.39345	(1)
C(15)	0.65131	0.79557	-1.27329	(1)
O(16)	1.79638	1.06148	-0.43782	(75)
C(17)	2.95025	0.43357	-0.78201	(3)
O(18)	3.04147	-0.31640	-1.73289	(78)
C(19)	4.05998	0.78353	0.15125	(1)
H(20)	-3.54559	0.73574	-2.44515	(5)
H(21)	-1.54456	2.07154	-2.56368	(5)
H(22)	-0.36604	2.49533	-0.43865	(5)
H(23)	-2.36085	-0.83577	1.42534	(5)
H(24)	-3.97576	0.21989	0.09456	(5)
H(25)	-3.54103	-1.20050	-0.86798	(5)
H(26)	1.55877	-1.05035	2.16366	(5)
H(27)	1.77335	-3.27444	1.26353	(5)
H(28)	0.19418	-4.02566	0.88944	(5)
H(29)	1.21163	-3.35879	-0.43127	(5)
H(30)	-2.47514	1.44092	2.33704	(5)
H(31)	-1.49512	2.76704	1.65531	(5)
H(32)	-2.89210	2.14780	0.75210	(5)
H(33)	0.51630	-0.28943	-1.43107	(5)
H(34)	0.83327	1.24759	-2.26975	(5)
H(35)	4.99724	0.26861	-0.13068	(5)
H(36)	4.25305	1.87650	0.14250	(5)
H(37)	3.80769	0.49023	1.19163	(5)

120c2

C(1)	-0.37476	-2.80024	0.41805	(2)
C(2)	0.71011	-2.05309	0.18089	(2)
C(3)	0.68471	-0.67316	-0.43288	(1)
C(4)	-0.68548	-0.40537	-1.15277	(1)
C(5)	-1.88040	-0.88856	-0.28906	(1)
C(6)	-1.77286	-2.38326	0.05439	(1)
C(7)	-2.08349	-0.00956	0.93731	(3)
C(8)	-2.08328	1.46304	0.68681	(2)
C(9)	-1.54296	1.93929	-0.44773	(2)
C(10)	-0.85056	1.08950	-1.45772	(3)
O(11)	-0.42384	1.58842	-2.48338	(81)
O(12)	-2.30108	-0.45737	2.04754	(81)
C(13)	-2.71077	2.34550	1.73301	(1)
C(14)	-0.69048	-1.18855	-2.48591	(1)
C(15)	1.07908	0.34733	0.65679	(1)
O(16)	2.40712	0.07900	1.16086	(75)
C(17)	3.45086	0.48204	0.38930	(3)
O(18)	3.31379	1.06285	-0.66850	(78)
C(19)	4.75837	0.12292	0.01103	(1)
H(20)	-0.25469	-3.80145	0.86680	(5)
H(21)	1.70103	-2.45039	0.46173	(5)
H(22)	1.47179	-0.65147	-1.21976	(5)
H(23)	-2.81135	-0.76262	-0.89160	(5)
H(24)	-2.10713	-2.99509	-0.81173	(5)
H(25)	-2.46566	-2.63895	0.88460	(5)
H(26)	-1.56001	3.02228	-0.65226	(5)
H(27)	-2.69699	3.41580	1.43857	(5)
H(28)	-3.77111	2.06555	1.90806	(5)
H(29)	-2.17259	2.26374	2.70098	(5)
H(30)	-1.65092	-1.06520	-3.03044	(5)
H(31)	0.11431	-0.84796	-3.17143	(5)
H(32)	-0.53536	-2.27738	-2.34308	(5)
H(33)	1.02981	1.38618	0.27896	(5)
H(34)	0.37853	0.29017	1.51041	(5)
H(35)	5.60519	0.45292	0.38082	(5)
H(36)	4.86620	0.60025	2.00730	(5)
H(37)	4.84107	-0.97548	1.14809	(5)

120c5

C(1)	0.10821	-2.58851	-0.29810	(2)
C(2)	-0.99267	-1.83450	-0.39047	(2)
C(3)	-1.04894	-0.37252	-0.00741	(1)
C(4)	0.36957	0.26336	0.05117	(1)
C(5)	1.28926	-0.67467	0.87786	(1)
C(6)	1.42536	-2.06219	0.19716	(1)
C(7)	2.67673	-0.06499	1.03662	(3)
C(8)	3.26399	0.58721	-0.17579	(2)
C(9)	2.49709	0.80010	-1.26153	(2)
C(10)	1.03539	0.50063	-1.30508	(3)
O(11)	0.44371	0.47780	-2.36624	(81)
O(12)	3.29962	-0.13986	2.07964	(81)
C(13)	4.72709	0.94079	-0.12771	(1)
C(14)	0.25206	1.62743	0.79115	(1)
C(15)	-2.04975	0.35505	-0.93143	(1)
O(16)	-3.40404	-0.05965	-0.64299	(75)
C(17)	-3.99271	0.49022	0.45195	(3)
O(18)	-3.44417	1.30615	1.16514	(78)
C(19)	-5.37509	-0.03444	0.64881	(1)
H(20)	0.07376	-3.64685	-0.60899	(5)
H(21)	-1.92720	-2.29811	-0.75069	(5)
H(22)	-1.45990	-0.34958	1.02722	(5)
H(23)	0.84428	-0.81192	1.88526	(5)
H(24)	1.85881	-2.78465	0.92326	(5)
H(25)	2.12960	-2.01373	-0.66120	(5)
H(26)	2.93665	1.23383	-2.17439	(5)
H(27)	5.07739	1.39707	-1.07720	(5)
H(28)	4.93647	1.66949	0.68373	(5)
H(29)	5.35031	0.03974	0.05423	(5)
H(30)	1.23789	2.10754	0.95971	(5)
H(31)	-0.35412	2.36133	0.22171	(5)
H(32)	-0.22178	1.51652	1.78937	(5)
H(33)	-1.97023	1.45428	-0.84138	(5)
H(34)	-1.84585	0.11824	-1.99254	(5)
H(35)	-5.85052	0.41521	1.54041	(5)
H(36)	-6.01268	0.19289	-0.23087	(5)
H(37)	-5.36284	-1.13586	0.78594	(5)

120c6

C(1)	-0.24500	2.21839	-1.31548	(2)
C(2)	0.86286	1.65788	-0.81798	(2)
C(3)	0.86199	0.60961	0.27262	(1)
C(4)	-0.52770	-0.07713	0.40649	(1)
C(5)	-1.61404	1.03042	0.46105	(1)
C(6)	-1.62780	1.86265	-0.84831	(1)
C(7)	-2.99406	0.41939	0.67151	(3)
C(8)	-3.30575	-0.81551	-0.11482	(2)
C(9)	-2.32598	-1.44805	-0.78743	(2)
C(10)	-0.89217	-1.03738	-0.72667	(3)
O(11)	-0.09211	-1.47515	-1.52977	(81)
O(12)	-3.82050	0.92792	1.40624	(81)
C(13)	-4.74116	-1.27012	-0.14429	(1)
C(14)	-0.54780	-0.86440	1.74881	(1)
C(15)	2.04870	-0.35107	0.06337	(1)
O(16)	3.27338	0.36898	0.32238	(75)
C(17)	4.42127	-0.34996	0.21878	(3)
O(18)	4.44270	-1.53084	-0.06483	(78)
C(19)	5.62057	0.49271	0.49611	(1)
H(20)	-0.16343	2.96849	-2.12087	(5)
H(21)	1.84358	1.98109	-1.20734	(5)
H(22)	1.05188	1.15928	1.22379	(5)
H(23)	-1.39082	1.70592	1.31283	(5)
H(24)	-2.20996	2.79573	-0.68252	(5)
H(25)	-2.14190	1.30849	-1.66299	(5)
H(26)	-2.55844	-2.32817	-1.40868	(5)
H(27)	-4.87872	-2.17708	-0.76954	(5)
H(28)	-5.10423	-1.51632	0.87592	(5)
H(29)	-5.40212	-0.48029	-0.55986	(5)
H(30)	-1.54376	-1.29805	1.97413	(5)
H(31)	0.16355	-1.71551	1.74506	(5)
H(32)	-0.28069	-0.21783	2.61129	(5)
H(33)	1.97999	-1.21034	0.75703	(5)
H(34)	2.06603	-0.74468	-0.97074	(5)
H(35)	6.55245	-0.09654	0.40922	(5)
H(36)	5.68222	1.33885	-0.21965	(5)
H(37)	5.57702	0.91572	1.52141	(5)

120t2

C(1)	-0.20161	2.77628	-0.20758	(2)
C(2)	-1.18558	1.89842	-0.44042	(2)
C(3)	-1.00627	0.39706	-0.40680	(1)
C(4)	0.49483	0.02881	-0.61355	(1)
C(5)	1.35321	0.86962	0.36505	(1)
C(6)	1.21974	2.37328	0.07544	(1)
C(7)	2.81294	0.43216	0.37175	(3)
C(8)	3.07115	-1.03772	0.38719	(2)
C(9)	2.08360	-1.89261	0.07417	(2)
C(10)	0.73330	-1.46784	-0.38423	(3)
O(11)	-0.11547	-2.30421	-0.63472	(81)
O(12)	3.73214	1.22838	0.42240	(81)
C(13)	4.45157	-1.49279	0.78189	(1)
C(14)	0.89187	0.33646	-2.08564	(1)
C(15)	-1.61994	-0.11656	0.91793	(1)
O(16)	-3.01849	0.23585	1.01520	(75)
C(17)	-3.89293	-0.50098	0.28080	(3)
O(18)	-3.55647	-1.43456	-0.41927	(78)
C(19)	-5.29310	-0.01642	0.45392	(1)
H(20)	-0.41501	3.85798	-0.25675	(5)
H(21)	-2.20070	2.27362	-0.65722	(5)
H(22)	-1.57917	-0.02895	-1.26025	(5)
H(23)	0.97884	0.68996	1.39847	(5)
H(24)	1.85037	2.66372	-0.79252	(5)
H(25)	1.59218	2.95299	0.94885	(5)
H(26)	2.26539	-2.97921	0.11104	(5)
H(27)	4.53756	-2.59950	0.79823	(5)
H(28)	5.21680	-1.11443	0.07156	(5)
H(29)	4.71811	-1.12725	1.79616	(5)
H(30)	1.97379	0.16333	-2.26603	(5)
H(31)	0.34103	-0.31394	-2.79811	(5)
H(32)	0.67639	1.38243	-2.38365	(5)
H(33)	-1.50313	-1.20971	1.03526	(5)
H(34)	-1.09901	0.33721	1.78239	(5)
H(35)	-6.00188	-0.61877	-0.14438	(5)
H(36)	-5.60371	-0.07837	1.51774	(5)
H(37)	-5.38644	1.04183	0.13219	(5)

120t1

C(1)	0.20456	2.77885	-0.08976	(2)
C(2)	1.07542	2.01229	0.57935	(2)
C(3)	0.85069	0.54662	0.87741	(1)
C(4)	-0.67051	0.21336	0.82554	(1)
C(5)	-1.24790	0.75283	-0.50678	(1)
C(6)	-1.12595	2.28321	-0.58788	(1)
C(7)	-2.68203	0.29324	-0.73782	(3)
C(8)	-2.97958	-1.13952	-0.44328	(2)
C(9)	-2.12388	-1.86041	0.30010	(2)
C(10)	-0.90637	-1.29650	0.94322	(3)
O(11)	-0.17366	-2.01557	1.59827	(81)
O(12)	-3.53761	1.02828	-1.19500	(81)
C(13)	-4.24253	-1.71673	-1.02654	(1)
C(14)	-1.37840	0.88327	2.03758	(1)
C(15)	1.72271	-0.26622	-0.10535	(1)
O(16)	3.11301	0.00932	0.17086	(75)
C(17)	4.01311	-0.59746	-0.64569	(3)
O(18)	3.69259	-1.33116	-1.55911	(78)
C(19)	5.41368	-0.24452	-0.27280	(1)
H(20)	0.44044	3.84240	-0.26653	(5)
H(21)	2.02728	2.45196	0.92403	(5)
H(22)	1.21108	0.34875	1.91256	(5)
H(23)	-0.65256	0.32101	-1.34332	(5)
H(24)	-1.93018	2.77279	0.00286	(5)
H(25)	-1.26110	2.60975	-1.64273	(5)
H(26)	-2.32931	-2.92554	0.49605	(5)
H(27)	-4.35980	-2.79386	-0.78465	(5)
H(28)	-4.24956	-1.62558	-2.13336	(5)
H(29)	-5.14045	-1.19279	-0.63600	(5)
H(30)	-1.02664	0.45415	2.99995	(5)
H(31)	-2.47859	0.73614	2.00523	(5)
H(32)	-1.19877	1.97572	2.09638	(5)
H(33)	1.48798	0.00819	-1.15228	(5)
H(34)	1.54056	-1.35150	0.00645	(5)
H(35)	5.57554	0.85154	-0.34005	(5)
H(36)	6.14256	-0.73896	-0.94170	(5)
H(37)	5.63593	-0.55891	0.76827	(5)

120t4

C(1)	0.49955	-2.66886	0.96538	(2)
C(2)	1.15337	-2.42431	-0.17770	(2)
C(3)	0.84262	-1.26488	-1.09654	(1)
C(4)	-0.59685	-0.72377	-0.83279	(1)
C(5)	-0.79682	-0.51535	0.68918	(1)
C(6)	-0.65357	-1.83764	1.45908	(1)
C(7)	-2.11773	0.17580	1.00061	(3)
C(8)	-2.46244	1.35559	0.15373	(2)
C(9)	-1.83027	1.54240	-1.01696	(2)
C(10)	-0.84649	0.58458	-1.59118	(3)
O(11)	-0.32994	0.81526	-2.66946	(81)
O(12)	-2.83272	-0.16210	1.92564	(81)
C(13)	-3.50854	2.30262	0.67997	(1)
C(14)	-1.62381	-1.76452	-1.36622	(1)
C(15)	1.99807	-0.24368	-0.98847	(1)
O(16)	2.15830	0.20647	0.37126	(75)
C(17)	3.15218	1.10486	0.59266	(3)
O(18)	3.88003	1.52128	-0.28599	(78)
C(19)	3.22101	1.49764	2.03000	(1)
H(20)	0.78503	-3.54106	1.57854	(5)
H(21)	1.98289	-3.08940	-0.47487	(5)
H(22)	0.85715	-1.66475	-2.13707	(5)
H(23)	-0.00835	0.17744	1.05598	(5)
H(24)	-1.58388	-2.44073	1.38088	(5)
H(25)	-0.50461	-1.62058	2.54001	(5)
H(26)	-2.06471	2.42657	-1.63213	(5)
H(27)	-3.66940	3.16600	0.00089	(5)
H(28)	-4.48746	1.79214	0.79999	(5)
H(29)	-3.21470	2.71259	1.66942	(5)
H(30)	-2.66928	-1.46871	-1.13717	(5)
H(31)	-1.55759	-1.87121	-2.46998	(5)
H(32)	-1.47286	-2.77807	-0.94260	(5)
H(33)	2.93922	-0.72314	-1.32770	(5)
H(34)	1.82495	0.62290	-1.65309	(5)
H(35)	4.03292	2.22733	2.20732	(5)
H(36)	2.26666	1.95998	2.35818	(5)
H(37)	3.40922	0.61213	2.67226	(5)

120t5

C(1)	0.76031	-2.26499	-0.79941	(2)
C(2)	1.44155	-1.15364	-1.10608	(2)
C(3)	0.91621	0.24666	-0.88215	(1)
C(4)	-0.64085	0.22755	-0.80721	(1)
C(5)	-1.07206	-0.85258	0.21655	(1)
C(6)	-0.63398	-2.25535	-0.23449	(1)
C(7)	-2.56649	-0.80174	0.50904	(3)
C(8)	-3.16154	0.55148	0.71448	(2)
C(9)	-2.48749	1.64456	0.32044	(2)
C(10)	-1.18928	1.60125	-0.40500	(3)
O(11)	-0.63439	2.63727	-0.72416	(81)
O(12)	-3.24246	-1.80658	0.63096	(81)
C(13)	-4.50809	0.61903	1.38581	(1)
C(14)	-1.21300	-0.09823	-2.21638	(1)
C(15)	1.61189	0.82861	0.37006	(1)
O(16)	3.03219	0.96997	0.11400	(75)
C(17)	3.87553	0.11917	0.75775	(3)
O(18)	3.50247	-0.73884	1.53228	(78)
C(19)	5.29687	0.37967	0.38657	(1)
H(20)	1.21527	-3.25171	-0.99264	(5)
H(21)	2.45634	-1.24550	-1.52995	(5)
H(22)	1.20970	0.86360	-1.76188	(5)
H(23)	-0.56604	-0.63544	1.18469	(5)
H(24)	-1.33013	-2.65572	-1.00294	(5)
H(25)	-0.67814	-2.95311	0.63083	(5)
H(26)	-2.91482	2.64558	0.49505	(5)
H(27)	-4.85186	1.66507	1.52757	(5)
H(28)	-5.28249	0.09749	0.78449	(5)
H(29)	-4.47869	0.14374	2.38913	(5)
H(30)	-2.31910	-0.19511	-2.19974	(5)
H(31)	-0.97335	0.70420	-2.94625	(5)
H(32)	-0.81140	-1.03999	-2.64175	(5)
H(33)	1.21717	1.83347	0.60783	(5)
H(34)	1.41761	0.20815	1.26364	(5)
H(35)	5.98102	-0.31271	0.91166	(5)
H(36)	5.44928	0.24925	-0.70517	(5)
H(37)	5.59018	1.41709	0.65062	(5)

120t7

C(1)	0.98807	3.06092	0.51046	(2)
C(2)	-0.12884	2.89712	-0.21116	(2)
C(3)	-0.62885	1.55132	-0.69239	(1)
C(4)	0.57073	0.55406	-0.78702	(1)
C(5)	1.30543	0.55320	0.57618	(1)
C(6)	1.91173	1.93229	0.88231	(1)
C(7)	2.34535	-0.55424	0.66949	(3)
C(8)	1.90418	-1.90681	0.21940	(2)
C(9)	0.84154	-2.01898	-0.59417	(2)
C(10)	0.10807	-0.85826	-1.16902	(3)
O(11)	-0.76444	-1.04420	-1.99852	(81)
O(12)	3.45070	-0.38083	1.14743	(81)
C(13)	2.68250	-3.09333	0.72339	(1)
C(14)	1.52947	1.02267	-1.91976	(1)
C(15)	-1.77918	1.16252	0.26569	(1)
O(16)	-2.41709	-0.05298	-0.16896	(75)
C(17)	-3.38161	-0.55145	0.64625	(3)
O(18)	-3.71302	-0.01946	1.68647	(78)
C(19)	-3.95836	-1.81305	0.09810	(1)
H(20)	1.28648	4.07519	0.82722	(5)
H(21)	-0.74472	3.77899	-0.45939	(5)
H(22)	-1.05139	1.69039	-1.71325	(5)
H(23)	0.56026	0.32840	1.37220	(5)
H(24)	2.87159	2.06733	0.33831	(5)
H(25)	2.14830	2.00046	1.96716	(5)
H(26)	0.50132	-3.01663	-0.91680	(5)
H(27)	2.25400	-4.05429	0.36925	(5)
H(28)	3.73747	-3.05671	0.37851	(5)
H(29)	2.68812	-3.12473	1.83352	(5)
H(30)	2.43419	0.38150	-1.98210	(5)
H(31)	1.03599	0.97679	-2.91392	(5)
H(32)	1.88124	2.06615	-1.79396	(5)
H(33)	-1.40530	1.04779	1.30096	(5)
H(34)	-2.53499	1.97454	0.28090	(5)
H(35)	-4.74492	-2.21574	0.76312	(5)
H(36)	-4.40968	-1.63932	-0.90096	(5)
H(37)	-3.17281	-2.58950	-0.01305	(5)

120t6

C(1)	1.28862	0.96998	2.01319	(2)
C(2)	1.69158	-0.27792	1.74092	(2)
C(3)	0.94129	-1.23183	0.84048	(1)
C(4)	-0.55054	-0.79356	0.70282	(1)
C(5)	-0.61233	0.71738	0.36649	(1)
C(6)	0.01239	1.56642	1.48482	(1)
C(7)	-2.02903	1.17304	0.04235	(3)
C(8)	-2.81712	0.29071	-0.86782	(2)
C(9)	-2.42297	-0.97711	-1.07261	(2)
C(10)	-1.27544	-1.61365	-0.37030	(3)
O(11)	-0.99186	-2.77582	-0.59729	(81)
O(12)	-2.48605	2.22733	0.44311	(81)
C(13)	-4.02616	0.89055	-1.53613	(1)
C(14)	-1.27549	-1.06736	2.05272	(1)
C(15)	1.73709	-1.40477	-0.47551	(1)
O(16)	1.91234	-0.14879	-1.17115	(75)
C(17)	3.10792	0.48497	-1.03521	(3)
O(18)	4.03773	0.03614	-0.39538	(78)
C(19)	3.11914	1.78441	-1.76791	(1)
H(20)	1.89708	1.60234	2.68247	(5)
H(21)	2.63952	-0.64193	2.17395	(5)
H(22)	0.94367	-2.22260	1.35174	(5)
H(23)	-0.02566	0.89468	-0.56116	(5)
H(24)	-0.69861	1.68814	2.33034	(5)
H(25)	0.22522	2.58742	1.09755	(5)
H(26)	-2.98929	-1.62261	-1.76382	(5)
H(27)	-4.52426	0.17214	-2.22041	(5)
H(28)	-4.78179	1.20864	-0.78705	(5)
H(29)	-3.74870	1.78092	-2.13918	(5)
H(30)	-2.32436	-0.70305	2.03995	(5)
H(31)	-1.31873	-2.15449	2.27709	(5)
H(32)	-0.77568	-0.58731	2.91828	(5)
H(33)	2.71407	-1.88261	-0.26676	(5)
H(34)	1.21998	-2.10345	-1.15786	(5)
H(35)	4.09697	2.29148	-1.66883	(5)
H(36)	2.92024	1.63052	-2.84890	(5)
H(37)	2.33822	2.46630	-1.37089	(5)

120t8

C(1)	0.61733	3.10116	0.19405	(2)
C(2)	-0.60330	2.62697	-0.08704	(2)
C(3)	-0.93182	1.15674	-0.23870	(1)
C(4)	0.36878	0.36448	-0.59367	(1)
C(5)	1.46709	0.73771	0.43423	(1)
C(6)	1.83223	2.22752	0.34762	(1)
C(7)	2.69796	-0.14950	0.31171	(3)
C(8)	2.44167	-1.61543	0.20747	(2)
C(9)	1.23032	-2.04786	-0.17831	(2)
C(10)	0.12461	-1.14985	-0.61042	(3)
O(11)	-0.89845	-1.62845	-1.06470	(81)
O(12)	3.83226	0.28720	0.36720	(81)
C(13)	3.57284	-2.54468	0.56036	(1)
C(14)	0.81922	0.75723	-2.03038	(1)
C(15)	-1.65560	0.74001	1.06751	(1)
O(16)	-2.33742	-0.52629	0.95237	(75)
C(17)	-3.52816	-0.52107	0.29581	(3)
O(18)	-4.02575	0.48206	-0.17454	(78)
C(19)	-4.12915	-1.88560	0.24307	(1)
H(20)	0.77026	4.19059	0.28272	(5)
H(21)	-1.44049	3.33692	-0.20582	(5)
H(22)	-1.63982	1.06385	-1.09203	(5)
H(23)	1.06696	0.55019	1.45590	(5)
H(24)	2.51621	2.41596	-0.50793	(5)
H(25)	2.38091	2.52902	1.26719	(5)
H(26)	1.02968	-3.12997	-0.24146	(5)
H(27)	3.27309	-3.61145	0.49234	(5)
H(28)	4.43700	-2.40175	-0.12231	(5)
H(29)	3.92600	-2.36758	1.59830	(5)
H(30)	1.78162	0.27567	-2.30474	(5)
H(31)	0.07437	0.43889	-2.79056	(5)
H(32)	0.95400	1.84944	-2.16328	(5)
H(33)	-0.94095	0.67417	1.90820	(5)
H(34)	-2.38599	1.51764	1.36921	(5)
H(35)	-5.10632	-1.87197	-0.27469	(5)
H(36)	-3.46593	-2.59143	-0.29857	(5)
H(37)	-4.28936	-2.28597	1.26577	(5)

120t9

C(1)	0.44697	3.06446	0.13687	(2)
C(2)	-0.73994	2.49299	-0.10177	(2)
C(3)	-0.96247	1.00149	-0.22720	(1)
C(4)	0.38486	0.28753	-0.56967	(1)
C(5)	1.47297	0.77972	0.41993	(1)
C(6)	1.72716	2.28747	0.27249	(1)
C(7)	2.76595	-0.01569	0.29830	(3)
C(8)	2.62554	-1.49865	0.21965	(2)
C(9)	1.44014	-2.03543	-0.11210	(2)
C(10)	0.24643	-1.23876	-0.50706	(3)
O(11)	-0.76958	-1.80817	-0.86118	(81)
O(12)	3.86368	0.50870	0.32945	(81)
C(13)	3.84213	-2.32708	0.53847	(1)
C(14)	0.78403	0.64560	-2.03003	(1)
C(15)	-1.65604	0.53638	1.08283	(1)
O(16)	-2.45938	-0.64645	0.88617	(75)
C(17)	-3.65306	-0.47592	0.25807	(3)
O(18)	-4.06638	0.60666	-0.10576	(78)
C(19)	-4.36961	-1.77276	0.08580	(1)
H(20)	0.51838	4.16378	0.20319	(5)
H(21)	-1.63144	3.13559	-0.20911	(5)
H(22)	-1.65951	0.84968	-1.08113	(5)
H(23)	1.10830	0.60308	1.45697	(5)
H(24)	2.36632	2.49552	-0.61261	(5)
H(25)	2.28245	2.65875	1.16212	(5)
H(26)	1.32709	-3.13128	-0.15109	(5)
H(27)	3.62999	-3.41574	0.49110	(5)
H(28)	4.66592	-2.12140	-0.17735	(5)
H(29)	4.21728	-2.10903	1.56079	(5)
H(30)	1.77757	0.22884	-2.29916	(5)
H(31)	0.05624	0.23449	-2.76172	(5)
H(32)	0.82947	1.73813	-2.21297	(5)
H(33)	-0.90992	0.32547	1.87044	(5)
H(34)	-2.29704	1.34128	1.49504	(5)
H(35)	-5.35181	-1.62477	-0.40067	(5)
H(36)	-3.77810	-2.46981	-0.54374	(5)
H(37)	-4.54331	-2.26219	1.06659	(5)

120t12

C(1)	1.40933	2.90689	0.70733	(2)
C(2)	0.24849	3.02147	0.04769	(2)
C(3)	-0.52286	1.84068	-0.50483	(1)
C(4)	0.46515	0.65963	-0.76745	(1)
C(5)	1.24815	0.38867	0.54031	(1)
C(6)	2.11694	1.59648	0.92683	(1)
C(7)	2.06086	-0.89571	0.46748	(3)
C(8)	1.34349	-2.09250	-0.06207	(2)
C(9)	0.24586	-1.92450	-0.81759	(2)
C(10)	-0.26948	-0.59671	-1.25030	(3)
O(11)	-1.18928	-0.53249	-2.04616	(81)
O(12)	3.20276	-0.97787	0.87888	(81)
C(13)	1.89378	-3.44677	0.29914	(1)
C(14)	1.44111	1.05941	-1.91208	(1)
C(15)	-1.66939	1.58544	0.50262	(1)
O(16)	-2.58711	0.57289	0.02585	(75)
C(17)	-2.76310	-0.53307	0.79808	(3)
O(18)	-2.17356	-0.72353	1.84242	(78)
C(19)	-3.75940	-1.46538	0.19437	(1)
H(20)	1.91170	3.81431	1.08467	(5)
H(21)	-0.19769	4.02179	-0.08989	(5)
H(22)	-0.96863	2.14931	-1.47739	(5)
H(23)	0.51218	0.22827	1.35966	(5)
H(24)	3.06120	1.60252	0.34043	(5)
H(25)	2.40780	1.51637	1.99756	(5)
H(26)	-0.29748	-2.80487	-1.19813	(5)
H(27)	1.26920	-4.27165	-0.10328	(5)
H(28)	2.91930	-3.58361	-0.10436	(5)
H(29)	1.94119	-3.57726	1.40102	(5)
H(30)	2.20413	0.27279	-2.09259	(5)
H(31)	0.90195	1.20798	-2.87188	(5)
H(32)	1.99002	2.00160	-1.71411	(5)
H(33)	-1.27123	1.34729	1.50510	(5)
H(34)	-2.25186	2.52035	0.63137	(5)
H(35)	-3.92572	-2.34609	0.84229	(5)
H(36)	-4.73596	-0.95922	0.04716	(5)
H(37)	-3.41264	-1.83092	-0.79448	(5)

121cR1

C(1)	0.16987	-2.45927	1.00138	(1)
C(2)	1.04359	-1.24784	1.34155	(1)
C(3)	1.05818	-0.21698	0.19780	(1)
C(4)	-0.37405	0.25799	-0.18120	(1)
C(5)	-1.25918	-0.99406	-0.50008	(1)
C(6)	-1.25095	-2.01274	0.66178	(1)
C(7)	-2.69476	-0.58303	-0.82211	(3)
C(8)	-3.39563	0.29787	0.20923	(1)
C(9)	-2.50577	1.50279	0.60481	(1)
C(10)	-1.07344	1.08591	0.90342	(3)
O(11)	-0.53573	1.41398	1.93660	(7)
O(12)	-3.24740	-0.96153	-1.83150	(7)
C(13)	-0.27693	1.10601	-1.48133	(1)
C(14)	2.03657	0.92251	0.54031	(1)
O(15)	3.39492	0.43201	0.58765	(75)
C(16)	4.02134	0.24410	-0.60407	(3)
O(17)	3.50294	0.48388	-1.67602	(78)
C(18)	5.40411	-0.28267	-0.41534	(1)
C(19)	-4.76003	0.78533	-0.28201	(1)
H(20)	0.60851	-3.01091	0.13823	(5)
H(21)	0.15130	-3.16863	1.86089	(5)
H(22)	0.67871	-0.77886	2.28230	(5)
H(23)	2.08080	-1.59859	1.54913	(5)
H(24)	1.46024	-0.74485	-0.69721	(5)
H(25)	-0.84078	-1.49806	-1.39577	(5)
H(26)	-1.86489	-2.89964	0.38880	(5)
H(27)	-1.71661	-1.57007	1.56830	(5)
H(28)	-3.56508	-0.32438	1.11728	(5)
H(29)	-2.50323	2.25592	-0.21102	(5)
H(30)	-2.94169	2.00755	1.48845	(5)
H(31)	-1.26939	1.30004	-1.93727	(5)
H(32)	0.18154	2.10000	-1.30008	(5)
H(33)	0.33150	0.60059	-2.26079	(5)
H(34)	1.96826	1.75707	-0.18147	(5)
H(35)	1.80133	1.35591	1.52982	(5)
H(36)	5.91083	-0.43366	-1.38673	(5)
H(37)	6.01665	0.42206	0.18482	(5)
H(38)	5.38554	-1.25688	0.11634	(5)
H(39)	-5.26582	1.41250	0.48293	(5)
H(40)	-4.67212	1.39864	-1.20416	(5)
H(41)	-5.44290	-0.06153	-0.50808	(5)

121cR2

C(1)	0.16722	2.63576	0.80695	(1)
C(2)	-0.91357	1.55892	0.94696	(1)
C(3)	-0.88676	0.56843	-0.23213	(1)
C(4)	0.50690	-0.10369	-0.39828	(1)
C(5)	1.59965	1.01175	-0.51744	(1)
C(6)	1.54702	1.99388	0.67428	(1)
C(7)	2.99531	0.40076	-0.62856	(3)
C(8)	3.38930	-0.59321	0.46132	(1)
C(9)	2.28478	-1.66107	0.66320	(1)
C(10)	0.89702	-1.04347	0.74902	(3)
O(11)	0.15914	-1.30392	1.67206	(7)
O(12)	3.74965	0.71190	-1.52392	(7)
C(13)	0.50619	-0.90547	-1.73076	(1)
C(14)	-2.06005	-0.41827	-0.11550	(1)
O(15)	-3.29575	0.31595	-0.24884	(75)
C(16)	-4.43523	-0.42282	-0.21550	(3)
O(17)	-4.44087	-1.63120	-0.09225	(78)
C(18)	-5.64734	0.43640	-0.34936	(1)
C(19)	4.73093	-1.26736	0.16802	(1)
H(20)	-0.04244	3.26686	-0.08720	(5)
H(21)	0.14584	3.31369	1.69141	(5)
H(22)	-0.77863	1.01914	1.91048	(5)
H(23)	-1.90951	2.05534	1.00484	(5)
H(24)	-1.06435	1.16738	-1.15635	(5)
H(25)	1.40716	1.59138	-1.44386	(5)
H(26)	2.31583	2.78728	0.54206	(5)
H(27)	1.79266	1.46746	1.62143	(5)
H(28)	3.49857	-0.01989	1.40990	(5)
H(29)	2.30695	-2.39174	-0.17250	(5)
H(30)	2.49593	-2.23926	1.58339	(5)
H(31)	1.52338	-1.22861	-2.03308	(5)
H(32)	-0.10570	-1.82870	-1.66308	(5)
H(33)	0.10507	-0.30549	-2.57479	(5)
H(34)	-2.00581	-1.18193	-0.91419	(5)
H(35)	-2.04581	-0.94202	0.85867	(5)
H(36)	-6.57233	-0.16916	-0.32020	(5)
H(37)	-5.69763	1.17868	0.47438	(5)
H(38)	-5.63232	0.99298	-1.30961	(5)
H(39)	5.01320	-1.97655	0.97529	(5)
H(40)	4.70491	-1.84357	-0.78148	(5)
H(41)	5.55493	-0.52643	0.08647	(5)

121cR3

C(1)	0.25214	-2.85069	0.65385	(1)
C(2)	-0.72857	-2.29208	-0.38276	(1)
C(3)	-1.07173	-0.81652	-0.10373	(1)
C(4)	0.20538	0.07393	-0.06184	(1)
C(5)	1.19906	-0.51872	0.99452	(1)
C(6)	1.52131	-2.00219	0.70478	(1)
C(7)	2.49144	0.29447	1.04515	(3)
C(8)	3.21613	0.50057	-0.28316	(1)
C(9)	2.23784	0.99107	-1.38079	(1)
C(10)	0.94670	0.18636	-1.40047	(3)
O(11)	0.55105	-0.32289	-2.42454	(7)
O(12)	2.92219	0.72865	2.09084	(7)
C(13)	-0.19351	1.49702	0.41606	(1)
C(14)	-2.16862	-0.35516	-1.08526	(1)
O(15)	-2.84725	0.83056	-0.61929	(75)
C(16)	-3.77372	0.66576	0.36189	(3)
O(17)	-4.05503	-0.41453	0.84052	(78)
C(18)	-4.38425	1.96781	0.75843	(1)
C(19)	4.39365	1.46851	-0.15221	(1)
H(20)	-0.22994	-2.86657	1.65844	(5)
H(21)	0.50929	-3.90611	0.40427	(5)
H(22)	-0.30243	-2.40827	-1.40363	(5)
H(23)	-1.65885	-2.90599	-0.36128	(5)
H(24)	-1.51287	-0.79518	0.91922	(5)
H(25)	0.72140	-0.46252	1.99445	(5)
H(26)	2.20333	-2.39892	1.48932	(5)
H(27)	2.05888	-2.10023	-0.26263	(5)
H(28)	3.62371	-0.48789	-0.59522	(5)
H(29)	1.99697	2.06325	-1.22292	(5)
H(30)	2.73346	0.92977	-2.36883	(5)
H(31)	0.68491	2.11937	0.68288	(5)
H(32)	-0.74434	2.05770	-0.36725	(5)
H(33)	-0.83791	1.46496	1.31987	(5)
H(34)	-1.74685	-0.14275	-2.08347	(5)
H(35)	-2.91127	-1.16113	-1.24765	(5)
H(36)	-5.13808	1.82997	1.55584	(5)
H(37)	-3.60983	2.66741	1.13652	(5)
H(38)	-4.88513	2.44894	-0.10737	(5)
H(39)	4.92125	1.59835	-1.12128	(5)
H(40)	4.06497	2.47615	0.18076	(5)
H(41)	5.14673	1.10437	0.57913	(5)

121cR4

C(1)	0.86164	3.02231	-0.30243	(1)
C(2)	-0.40409	2.47160	0.36337	(1)
C(3)	-0.84399	1.13742	-0.26850	(1)
C(4)	0.28689	0.06813	-0.20448	(1)
C(5)	1.57362	0.65328	-0.87968	(1)
C(6)	1.99205	1.99674	-0.24036	(1)
C(7)	2.73072	-0.34164	-0.80439	(3)
C(8)	3.07615	-0.87780	0.58328	(1)
C(9)	1.80608	-1.37088	1.32257	(1)
C(10)	0.65843	-0.37780	1.21573	(3)
O(11)	0.09082	0.02117	2.20732	(7)
O(12)	3.34996	-0.66341	-1.79460	(7)
C(13)	-0.15140	-1.17548	-1.02561	(1)
C(14)	-2.19578	0.70640	0.32990	(1)
O(15)	-2.84346	-0.22366	-0.56147	(75)
C(16)	-4.06036	-0.68116	-0.16774	(3)
O(17)	-4.59785	-0.33698	0.86571	(78)
C(18)	-4.62901	-1.64118	-1.15785	(1)
C(19)	4.12176	-1.99314	0.52535	(1)
H(20)	0.64653	3.28044	-1.36496	(5)
H(21)	1.17584	3.96628	0.20009	(5)
H(22)	-0.23112	2.34904	1.45528	(5)
H(23)	-1.21874	3.22545	0.25966	(5)
H(24)	-1.02929	1.35455	-1.34699	(5)
H(25)	1.35279	0.83939	-1.95101	(5)
H(26)	2.88850	2.39854	-0.76282	(5)
H(27)	2.28389	1.84656	0.82113	(5)
H(28)	3.51304	-0.03431	1.16490	(5)
H(29)	1.48188	-2.34890	0.90927	(5)
H(30)	2.04779	-1.55224	2.38759	(5)
H(31)	0.68550	-1.87829	-1.21492	(5)
H(32)	-0.93569	-1.76127	-0.50275	(5)
H(33)	-0.55259	-0.89391	-2.02210	(5)
H(34)	-2.07098	0.25298	1.32982	(5)
H(35)	-2.84747	1.59508	0.45090	(5)
H(36)	-5.61866	-2.01253	-0.83255	(5)
H(37)	-4.75312	-1.15802	-2.14941	(5)
H(38)	-3.95962	-2.51721	-1.28682	(5)
H(39)	4.37531	-2.36414	1.54141	(5)
H(40)	3.76365	-2.86480	-0.06305	(5)
H(41)	5.07013	-1.64499	0.06279	(5)

121cR5

C(1)	-0.23863	2.28524	1.09671	(1)
C(2)	-1.19820	1.10988	0.88644	(1)
C(3)	-0.93208	0.38255	-0.44471	(1)
C(4)	0.54159	-0.10742	-0.55840	(1)
C(5)	1.50437	1.10383	-0.31640	(1)
C(6)	1.21085	1.80987	1.02580	(1)
C(7)	2.96515	0.66000	-0.36310	(3)
C(8)	3.35165	-0.49572	0.55623	(1)
C(9)	2.36555	-1.68029	0.39921	(1)
C(10)	0.91301	-1.22773	0.42070	(3)
O(11)	0.11288	-1.75029	1.16299	(7)
O(12)	3.77007	1.21566	-1.07783	(7)
C(13)	0.77836	-0.60892	-2.01184	(1)
C(14)	-1.98739	-0.71603	-0.66588	(1)
O(15)	-3.27138	-0.09835	-0.93569	(75)
C(16)	-4.25710	-0.25467	-0.01189	(3)
O(17)	-4.11770	-0.87676	1.02187	(78)
C(18)	-5.51062	0.43580	-0.43375	(1)
C(19)	4.78766	-0.96610	0.31744	(1)
H(20)	-0.41883	3.06338	0.31968	(5)
H(21)	-0.43457	2.76461	2.08370	(5)
H(22)	-1.11035	0.40050	1.73926	(5)
H(23)	-2.24285	1.49615	0.90673	(5)
H(24)	-1.07951	1.13530	-1.25459	(5)
H(25)	1.34716	1.84223	-1.12963	(5)
H(26)	1.89464	2.67855	1.15171	(5)
H(27)	1.40796	1.12316	1.87674	(5)
H(28)	3.28695	-0.12334	1.60384	(5)
H(29)	2.56544	-2.21551	-0.55290	(5)
H(30)	2.54163	-2.41511	1.20834	(5)
H(31)	1.85320	-0.76425	-2.23791	(5)
H(32)	0.27727	-1.57934	-2.20751	(5)
H(33)	0.40174	0.11407	-2.76594	(5)
H(34)	-1.72805	-1.33231	-1.54631	(5)
H(35)	-2.03914	-1.41021	0.19101	(5)
H(36)	-6.31072	0.30824	0.31907	(5)
H(37)	-5.33573	1.52389	-0.56656	(5)
H(38)	-5.87983	0.02927	-1.39833	(5)
H(39)	5.06117	-1.79694	1.00243	(5)
H(40)	4.93480	-1.33386	-0.72051	(5)
H(41)	5.52213	-0.15037	0.48990	(5)

121cR9

C(1)	0.57559	-2.78741	-1.06078	(1)
C(2)	-0.76365	-2.08024	-0.81750	(1)
C(3)	-0.75107	-1.30706	0.51261	(1)
C(4)	0.39922	-0.26020	0.57401	(1)
C(5)	1.75213	-1.01912	0.34401	(1)
C(6)	1.73829	-1.79594	-0.99354	(1)
C(7)	2.93727	-0.05520	0.38167	(3)
C(8)	2.86071	1.15512	-0.54662	(1)
C(9)	1.48880	1.86698	-0.42090	(1)
C(10)	0.33396	0.87705	-0.45527	(3)
O(11)	-0.54188	0.98748	-1.28234	(7)
O(12)	3.89205	-0.26021	1.09851	(7)
C(13)	0.42582	0.34489	2.00395	(1)
C(14)	-2.15878	-0.80240	0.86805	(1)
O(15)	-2.67971	0.06923	-0.15218	(75)
C(16)	-3.89261	0.62682	0.09471	(3)
O(17)	-4.52869	0.41306	1.10688	(78)
C(18)	-4.31941	1.51660	-1.02366	(1)
C(19)	3.99760	2.14726	-0.29446	(1)
H(20)	0.72178	-3.58625	-0.29755	(5)
H(21)	0.56325	-3.29273	-2.05416	(5)
H(22)	-0.98703	-1.39923	-1.66765	(5)
H(23)	-1.57866	-2.84055	-0.80401	(5)
H(24)	-0.51079	-2.06505	1.29688	(5)
H(25)	1.88758	-1.75380	1.16439	(5)
H(26)	2.69949	-2.34207	-1.11974	(5)
H(27)	1.66023	-1.09125	-1.84902	(5)
H(28)	2.96433	0.77866	-1.58986	(5)
H(29)	1.44600	2.45080	0.52184	(5)
H(30)	1.37918	2.60145	-1.24191	(5)
H(31)	1.35382	0.91634	2.20968	(5)
H(32)	-0.41807	1.04634	2.17175	(5)
H(33)	0.36394	-0.44010	2.78703	(5)
H(34)	-2.83820	-1.67196	0.98041	(5)
H(35)	-2.14684	-0.28161	1.84433	(5)
H(36)	-5.31406	1.95811	-0.82651	(5)
H(37)	-3.59720	2.34799	-1.16327	(5)
H(38)	-4.37775	0.95192	-1.97741	(5)
H(39)	3.93882	3.01514	-0.98556	(5)
H(40)	3.97276	2.54920	0.74095	(5)
H(41)	4.99388	1.67966	-0.44734	(5)

121cR6

C(1)	-0.06966	-2.03945	-1.78841	(1)
C(2)	-0.76216	-2.30765	-0.44745	(1)
C(3)	-0.49050	-1.20405	0.59368	(1)
C(4)	1.04590	-0.96808	0.78272	(1)
C(5)	1.77752	-0.75459	-0.57618	(1)
C(6)	1.43684	-1.84950	-1.59817	(1)
C(7)	1.57348	0.65040	-1.14456	(3)
C(8)	1.75238	1.81863	-0.17258	(1)
C(9)	2.20145	1.32682	1.21137	(1)
C(10)	1.28661	0.22848	1.72238	(3)
O(11)	0.79993	0.27765	2.83107	(7)
O(12)	1.34205	0.84402	-2.31806	(7)
C(13)	1.65590	-2.21401	1.48363	(1)
C(14)	-1.27456	0.07088	0.24753	(1)
O(15)	-2.68751	-0.22368	0.26015	(75)
C(16)	-3.51209	0.81507	-0.03340	(3)
O(17)	-3.10822	1.93124	-0.29137	(78)
C(18)	-4.94512	0.40273	0.00454	(1)
C(19)	2.74070	2.85664	-0.72917	(1)
H(20)	-0.25481	-2.89187	-2.48255	(5)
H(21)	-0.51149	-1.14141	-2.27444	(5)
H(22)	-1.85804	-2.41928	-0.61163	(5)
H(23)	-0.42083	-3.29035	-0.05086	(5)
H(24)	-0.89306	-1.56492	1.56949	(5)
H(25)	2.87371	-0.83120	-0.38429	(5)
H(26)	1.88280	-2.81400	-1.27176	(5)
H(27)	1.91385	-1.62332	-2.57716	(5)
H(28)	0.75984	2.31264	-0.06199	(5)
H(29)	3.24431	0.94687	1.16688	(5)
H(30)	2.20685	2.17408	1.92381	(5)
H(31)	2.73675	-2.07106	1.69717	(5)
H(32)	1.16398	-2.42288	2.45730	(5)
H(33)	1.57083	-3.13938	0.88051	(5)
H(34)	-1.06706	0.86506	0.99044	(5)
H(35)	-0.98387	0.45365	-0.74784	(5)
H(36)	-5.61215	1.25117	-0.23708	(5)
H(37)	-5.14197	-0.40741	-0.72826	(5)
H(38)	-5.22078	0.02615	1.01164	(5)
H(39)	2.87023	3.71041	-0.03032	(5)
H(40)	3.74499	2.41393	-0.90099	(5)
H(41)	2.39414	3.27907	-1.69643	(5)

121cS1

C(1)	0.09001	2.15603	-1.50210	(1)
C(2)	0.94698	0.89280	-1.62090	(1)
C(3)	1.04468	0.15696	-0.27341	(1)
C(4)	-0.36897	-0.25959	0.24618	(1)
C(5)	-1.25586	1.01351	0.33797	(1)
C(6)	-1.30611	1.80736	-0.99040	(1)
C(7)	-2.68407	0.71229	0.79862	(3)
C(8)	-3.26020	-0.65961	0.44715	(1)
C(9)	-2.55794	-1.27171	-0.77095	(1)
C(10)	-1.04151	-1.33020	-0.62976	(3)
O(11)	-0.41116	-2.19939	-1.18869	(7)
O(12)	-3.33704	1.54371	1.39085	(7)
C(13)	-0.19388	-0.82881	1.68640	(1)
C(14)	2.07005	-0.98720	-0.39236	(1)
O(15)	3.40733	-0.45763	-0.53151	(75)
C(16)	4.01608	-0.02134	0.60299	(3)
O(17)	3.49851	-0.07257	1.70063	(78)
C(18)	5.37877	0.51456	0.31824	(1)
C(19)	-4.77358	-0.58320	0.20554	(1)
H(20)	0.57699	2.87763	-0.80640	(5)
H(21)	0.01772	2.66274	-2.49219	(5)
H(22)	0.51743	0.21858	-2.39604	(5)
H(23)	1.96424	1.17751	-1.97566	(5)
H(24)	1.44805	0.88908	0.46306	(5)
H(25)	-0.80531	1.68290	1.10284	(5)
H(26)	-1.88904	2.74423	-0.84632	(5)
H(27)	-1.84168	1.22520	-1.76896	(5)
H(28)	-3.09352	-1.33022	1.32094	(5)
H(29)	-2.94363	-2.29804	-0.93467	(5)
H(30)	-2.81847	-0.69905	-1.68601	(5)
H(31)	-1.15923	-0.96055	2.21377	(5)
H(32)	0.29576	-1.82424	1.68872	(5)
H(33)	0.42129	-0.15928	2.32397	(5)
H(34)	2.03120	-1.67374	0.47308	(5)
H(35)	1.86216	-1.60448	-1.28607	(5)
H(36)	6.02335	-0.26666	-0.13591	(5)
H(37)	5.32664	1.36798	-0.38962	(5)
H(38)	5.87107	0.86810	1.24334	(5)
H(39)	-5.19604	-1.57877	-0.04856	(5)
H(40)	-5.31822	-0.22250	1.10419	(5)
H(41)	-5.02124	0.10372	-0.63181	(5)

121cS2

C(1)	-0.23037	2.52538	-0.97574	(1)
C(2)	0.83268	1.43007	-1.09817	(1)
C(3)	0.87369	0.55009	0.16337	(1)
C(4)	-0.50743	-0.13688	0.41474	(1)
C(5)	-1.59666	0.96755	0.51062	(1)
C(6)	-1.60443	1.91065	-0.71733	(1)
C(7)	-3.00240	0.39929	0.71881	(3)
C(8)	-3.29433	-0.98297	0.13405	(1)
C(9)	-2.34750	-1.31854	-1.02454	(1)
C(10)	-0.87360	-1.16788	-0.66645	(3)
O(11)	-0.03982	-1.84879	-1.21998	(7)
O(12)	-3.85297	1.03681	1.30057	(7)
C(13)	-0.43194	-0.86196	1.79219	(1)
C(14)	2.08399	-0.39620	0.09075	(1)
O(15)	3.28720	0.39238	0.21184	(75)
C(16)	4.45704	-0.29814	0.20571	(3)
O(17)	4.51484	-1.50789	0.11331	(78)
C(18)	5.63074	0.61473	0.32629	(1)
C(19)	-4.75487	-1.09756	-0.32251	(1)
H(20)	0.03543	3.21657	-0.14300	(5)
H(21)	-0.25587	3.13818	-1.90638	(5)
H(22)	0.26550	0.80407	-1.99566	(5)
H(23)	1.82542	1.90739	-1.26592	(5)
H(24)	1.05483	1.23020	1.02876	(5)
H(25)	-1.36596	1.59110	1.40165	(5)
H(26)	-2.34744	2.72422	-0.56136	(5)
H(27)	-1.93132	1.36178	-1.62490	(5)
H(28)	-3.13613	-1.73219	0.94319	(5)
H(29)	-2.53252	-2.36066	-1.35427	(5)
H(30)	-2.57857	-0.67669	-1.90076	(5)
H(31)	-1.42462	-1.19403	2.15512	(5)
H(32)	0.20117	-1.77225	1.75334	(5)
H(33)	-0.01394	-0.20450	2.58360	(5)
H(34)	2.05307	-1.13644	0.91215	(5)
H(35)	2.10227	-0.94527	-0.86959	(5)
H(36)	6.58063	0.04831	0.31940	(5)
H(37)	5.65660	1.33737	-0.51584	(5)
H(38)	5.58429	1.19431	1.27181	(5)
H(39)	-4.97132	-2.10138	-0.74641	(5)
H(40)	-5.46440	-0.94364	0.51842	(5)
H(41)	-4.99978	-0.34880	-1.10592	(5)

121cS4

C(1)	-0.91098	2.97019	0.13699	(1)
C(2)	0.33520	2.38882	-0.53842	(1)
C(3)	0.82285	1.12430	0.19195	(1)
C(4)	-0.28770	0.02149	0.18096	(1)
C(5)	-1.55580	0.60923	0.86263	(1)
C(6)	-2.02672	1.92902	0.20273	(1)
C(7)	-2.72325	-0.37954	0.89806	(3)
C(8)	-2.80948	-1.40417	-0.23365	(1)
C(9)	-2.07125	-0.92702	-1.48925	(1)
C(10)	-0.63550	-0.47962	-1.23230	(3)
O(11)	0.17714	-0.51293	-2.12866	(7)
O(12)	-3.55736	-0.32864	1.77555	(7)
C(13)	0.20974	-1.18277	1.03294	(1)
C(14)	2.20897	0.72944	-0.34880	(1)
O(15)	2.84902	-0.18296	0.56563	(75)
C(16)	4.10223	-0.58576	0.23016	(3)
O(17)	4.67856	-0.20458	-0.76882	(78)
C(18)	4.65715	-1.53724	1.23619	(1)
C(19)	-4.26876	-1.73893	-0.57095	(1)
H(20)	-0.65520	3.31050	1.16694	(5)
H(21)	-1.26184	3.86978	-0.41974	(5)
H(22)	0.11723	2.15909	-1.60557	(5)
H(23)	1.13617	3.16382	-0.53854	(5)
H(24)	0.97982	1.41933	1.25645	(5)
H(25)	-1.29614	0.84090	1.91838	(5)
H(26)	-2.88647	2.34737	0.77201	(5)
H(27)	-2.40022	1.73579	-0.82442	(5)
H(28)	-2.32580	-2.34265	0.12115	(5)
H(29)	-2.06234	-1.74601	-2.23690	(5)
H(30)	-2.63193	-0.09222	-1.96068	(5)
H(31)	-0.59559	-1.90524	1.26872	(5)
H(32)	0.99758	-1.76298	0.50939	(5)
H(33)	0.62666	-0.85550	2.00881	(5)
H(34)	2.14694	0.28318	-1.35658	(5)
H(35)	2.83807	1.63824	-0.43781	(5)
H(36)	5.67697	-1.86322	0.95899	(5)
H(37)	4.70899	-1.06489	2.23931	(5)
H(38)	4.01854	-2.44148	1.31772	(5)
H(39)	-4.33613	-2.48342	-1.39279	(5)
H(40)	-4.80575	-2.17176	0.30004	(5)
H(41)	-4.83227	-0.83793	-0.89497	(5)

121cS3

C(1)	-0.35300	2.86726	0.27612	(1)
C(2)	0.61602	2.21108	-0.71250	(1)
C(3)	1.04602	0.81552	-0.22469	(1)
C(4)	-0.19885	-0.12188	-0.08062	(1)
C(5)	-1.18783	0.54239	0.91909	(1)
C(6)	-1.57728	1.98221	0.50169	(1)
C(7)	-2.45998	-0.28111	1.13150	(3)
C(8)	-2.94296	-1.14020	-0.03754	(1)
C(9)	-2.42021	-0.61759	-1.38026	(1)
C(10)	-0.91011	-0.40401	-1.41639	(3)
O(11)	-0.31935	-0.44753	-2.47185	(7)
O(12)	-3.07049	-0.22810	2.17687	(7)
C(13)	0.27575	-1.47223	0.53084	(1)
C(14)	2.20621	0.31099	-1.10644	(1)
O(15)	2.89956	-0.80671	-0.51182	(75)
C(16)	3.77244	-0.52895	0.49281	(3)
O(17)	3.99362	0.59588	0.89405	(78)
C(18)	4.40816	-1.77107	1.02047	(1)
C(19)	-4.47465	-1.23307	-0.06401	(1)
H(20)	0.16466	3.04517	1.24691	(5)
H(21)	-0.66965	3.86537	-0.10573	(5)
H(22)	0.14389	2.14077	-1.71811	(5)
H(23)	1.50923	2.86790	-0.82674	(5)
H(24)	1.45982	0.96075	0.79966	(5)
H(25)	-0.67842	0.60997	1.90481	(5)
H(26)	-2.22143	2.43902	1.28569	(5)
H(27)	-2.18509	1.96463	-0.42677	(5)
H(28)	-2.54907	-2.17098	0.11402	(5)
H(29)	-2.69958	-1.33290	-2.18027	(5)
H(30)	-2.92771	0.33654	-1.63616	(5)
H(31)	-0.56385	-2.11170	0.86593	(5)
H(32)	0.84981	-2.07890	-0.19956	(5)
H(33)	0.92197	-1.31892	1.42075	(5)
H(34)	1.85273	0.01037	-2.10731	(5)
H(35)	2.93090	1.12805	-1.29387	(5)
H(36)	5.11816	-1.54149	1.83675	(5)
H(37)	3.64157	-2.46772	1.41934	(5)
H(38)	4.96589	-2.29988	0.21968	(5)
H(39)	-4.83008	-1.85678	-0.91188	(5)
H(40)	-4.87727	-1.69226	0.86408	(5)
H(41)	-4.94476	-0.23212	-0.17095	(5)

121cS6

C(1)	-0.17332	-2.24388	-1.09251	(1)
C(2)	-1.11982	-1.04991	-0.94326	(1)
C(3)	-0.92796	-0.34572	0.41124	(1)
C(4)	0.54151	0.16402	0.57829	(1)
C(5)	1.50983	-1.03694	0.38969	(1)
C(6)	1.27815	-1.79644	-0.93888	(1)
C(7)	2.98284	-0.63400	0.48968	(3)
C(8)	3.35520	0.78058	0.04465	(1)
C(9)	2.31868	1.35958	-0.92633	(1)
C(10)	0.89482	1.30938	-0.38606	(3)
O(11)	0.09302	2.15979	-0.70104	(7)
O(12)	3.81915	-1.41872	0.88104	(7)
C(13)	0.70119	0.67991	2.04065	(1)
C(14)	-2.02325	0.72039	0.59967	(1)
O(15)	-3.28319	0.06210	0.88667	(75)
C(16)	-4.27101	0.14746	-0.04424	(3)
O(17)	-4.15168	0.73614	-1.09986	(78)
C(18)	-5.49898	-0.57417	0.40002	(1)
C(19)	4.75374	0.81611	-0.58605	(1)
H(20)	-0.41384	-3.01371	-0.32351	(5)
H(21)	-0.32049	-2.72558	-2.08680	(5)
H(22)	-0.95156	-0.32960	-1.77568	(5)
H(23)	-2.16835	-1.41204	-1.04247	(5)
H(24)	-1.09116	-1.11393	1.20319	(5)
H(25)	1.31639	-1.75632	1.21497	(5)
H(26)	1.94411	-2.68680	-0.98389	(5)
H(27)	1.55373	-1.15858	-1.80415	(5)
H(28)	3.37985	1.42407	0.95386	(5)
H(29)	2.58115	2.41263	-1.15173	(5)
H(30)	2.36327	0.82108	-1.89626	(5)
H(31)	1.75895	0.86636	2.31318	(5)
H(32)	0.16765	1.63754	2.21058	(5)
H(33)	0.31090	-0.04911	2.78192	(5)
H(34)	-1.79066	1.37382	1.46036	(5)
H(35)	-2.10171	1.38088	-0.28187	(5)
H(36)	-6.30081	-0.50439	-0.35851	(5)
H(37)	-5.28361	-1.64933	0.57270	(5)
H(38)	-5.88648	-0.14714	1.34843	(5)
H(39)	5.02901	1.84301	-0.90840	(5)
H(40)	5.53757	0.48164	0.12671	(5)
H(41)	4.81664	0.16124	-1.48133	(5)

121tR1

C(1)	-0.56371	-2.60159	-0.33720	(1)
C(2)	-1.13203	-1.92778	0.92144	(1)
C(3)	-0.85542	-0.40797	0.97239	(1)
C(4)	0.66974	-0.12625	0.82821	(1)
C(5)	1.17964	-0.77084	-0.49902	(1)
C(6)	0.92093	-2.27960	-0.54134	(1)
C(7)	2.63936	-0.41286	-0.73856	(3)
C(8)	2.92267	1.08006	-0.82398	(1)
C(9)	2.40351	1.78967	0.44771	(1)
C(10)	0.98555	1.38047	0.83152	(3)
O(11)	0.19469	2.20591	1.23166	(7)
O(12)	3.49899	-1.25069	-0.89877	(7)
C(13)	1.41925	-0.73590	2.04948	(1)
C(14)	-1.72932	0.31027	-0.07339	(1)
O(15)	-3.11953	0.10603	0.25837	(75)
C(16)	-4.02224	0.58968	-0.63408	(3)
O(17)	-3.70414	1.15561	-1.66068	(78)
C(18)	-5.42238	0.33241	-0.18849	(1)
C(19)	4.40589	1.38086	-1.04138	(1)
H(20)	-0.70141	-3.70550	-0.26596	(5)
H(21)	-1.14064	-2.27550	-1.23211	(5)
H(22)	-2.22834	-2.11727	0.97550	(5)
H(23)	-0.70911	-2.42139	1.82430	(5)
H(24)	-1.17388	-0.04011	1.97577	(5)
H(25)	0.61811	-0.31549	-1.34462	(5)
H(26)	1.52597	-2.80038	0.23094	(5)
H(27)	1.24912	-2.69009	-1.52243	(5)
H(28)	2.35751	1.47348	-1.69988	(5)
H(29)	3.08153	1.56921	1.30012	(5)
H(30)	2.44523	2.86622	0.29751	(5)
H(31)	2.51676	-0.58651	1.98350	(5)
H(32)	1.09055	-0.26512	3.00054	(5)
H(33)	1.26484	-1.82567	2.16630	(5)
H(34)	-1.52423	1.39612	-0.09295	(5)
H(35)	-1.52618	-0.07819	-1.08855	(5)
H(36)	-6.15351	0.72536	-0.91938	(5)
H(37)	-5.60553	-0.75616	-0.07201	(5)
H(38)	-5.62072	0.81828	0.78960	(5)
H(39)	4.59062	2.47370	-1.11783	(5)
H(40)	5.03222	0.99924	-0.20696	(5)
H(41)	4.78479	0.92234	-1.97990	(5)

121tR3

C(1)	0.45910	-2.69499	0.17879	(1)
C(2)	1.27827	-1.77944	-0.74208	(1)
C(3)	1.02042	-0.27687	-0.48499	(1)
C(4)	-0.50296	0.03908	-0.59886	(1)
C(5)	-1.29541	-0.88329	0.38250	(1)
C(6)	-1.03650	-2.36879	0.11767	(1)
C(7)	-2.77654	-0.53086	0.36746	(3)
C(8)	-3.09385	0.90907	0.74565	(1)
C(9)	-2.29858	1.88160	-0.15591	(1)
C(10)	-0.82498	1.51145	-0.28514	(3)
O(11)	0.02821	2.36967	-0.24474	(7)
O(12)	-3.63844	-1.34640	0.12518	(7)
C(13)	-0.96348	-0.21361	-2.06488	(1)
C(14)	1.65285	0.13882	0.86068	(1)
O(15)	3.04775	-0.23247	0.92778	(75)
C(16)	3.92857	0.53719	0.23544	(3)
O(17)	3.60231	1.51525	-0.40633	(78)
C(18)	5.32348	0.02665	0.37403	(1)
C(19)	-4.59065	1.21366	0.67767	(1)
H(20)	0.62322	-3.75982	-0.10718	(5)
H(21)	0.82014	-2.59492	1.22755	(5)
H(22)	2.36099	-2.00929	-0.62060	(5)
H(23)	1.05068	-2.02836	-1.80215	(5)
H(24)	1.53819	0.29153	-1.29112	(5)
H(25)	-0.94951	-0.66832	1.41766	(5)
H(26)	-1.44360	-2.66488	-0.87253	(5)
H(27)	-1.57351	-2.98521	0.87289	(5)
H(28)	-2.75845	1.05449	1.79822	(5)
H(29)	-2.75231	1.90676	-1.16982	(5)
H(30)	-2.38915	2.90955	0.24622	(5)
H(31)	-2.04958	-0.03242	-2.20064	(5)
H(32)	-0.43746	0.45987	-2.77475	(5)
H(33)	-0.78053	-1.24766	-2.41473	(5)
H(34)	1.55355	1.22204	1.05404	(5)
H(35)	1.13550	-0.35881	1.70104	(5)
H(36)	6.03772	0.65566	-0.18932	(5)
H(37)	5.63778	0.02059	1.43855	(5)
H(38)	5.40333	-1.01127	-0.01128	(5)
H(39)	-4.80425	2.26327	0.97259	(5)
H(40)	-4.99572	1.07121	-0.34694	(5)
H(41)	-5.17439	0.56049	1.36121	(5)

121tR2

C(1)	-0.49626	2.64858	0.26635	(1)
C(2)	-1.03681	1.93497	-0.98145	(1)
C(3)	-0.78656	0.41157	-0.96880	(1)
C(4)	0.72618	0.10270	-0.73196	(1)
C(5)	1.21304	0.81414	0.56132	(1)
C(6)	0.98207	2.32605	0.51014	(1)
C(7)	2.66130	0.43683	0.84567	(3)
C(8)	2.94376	-1.06281	0.96809	(1)
C(9)	1.68998	-1.89938	0.64035	(1)
C(10)	0.95979	-1.41537	-0.60488	(3)
O(11)	0.56338	-2.19346	-1.44494	(7)
O(12)	3.53538	1.26481	0.97842	(7)
C(13)	1.53683	0.58934	-1.96524	(1)
C(14)	-1.70551	-0.28542	0.04668	(1)
O(15)	-3.08171	-0.05247	-0.32110	(75)
C(16)	-4.01566	-0.54530	0.53322	(3)
O(17)	-3.73339	-1.14225	1.55270	(78)
C(18)	-5.39915	-0.25610	0.05648	(1)
C(19)	4.13512	-1.48214	0.08920	(1)
H(20)	-0.62672	3.75003	0.15509	(5)
H(21)	-1.09452	2.35240	1.15785	(5)
H(22)	-2.12672	2.14150	-1.08142	(5)
H(23)	-0.56969	2.38360	-1.88679	(5)
H(24)	-1.06013	0.01788	-1.97569	(5)
H(25)	0.62268	0.43032	1.42242	(5)
H(26)	1.60485	2.79219	-0.28245	(5)
H(27)	1.30133	2.78867	1.47074	(5)
H(28)	3.22044	-1.25880	2.02999	(5)
H(29)	1.97066	-2.96383	0.52608	(5)
H(30)	0.98451	-1.86438	1.49910	(5)
H(31)	2.61908	0.36884	-1.86287	(5)
H(32)	1.19924	0.09152	-2.89898	(5)
H(33)	1.45509	1.67937	-2.14226	(5)
H(34)	-1.51584	-1.37632	0.05568	(5)
H(35)	-1.52037	0.09463	1.06883	(5)
H(36)	-6.15563	-0.65696	0.75663	(5)
H(37)	-5.56378	0.83768	-0.03646	(5)
H(38)	-5.57714	-0.71366	-0.93902	(5)
H(39)	4.38807	-2.55426	0.23284	(5)
H(40)	3.92447	-1.33786	-0.99089	(5)
H(41)	5.05030	-0.90023	0.32954	(5)

121tR4

C(1)	0.76614	-2.66633	0.52092	(1)
C(2)	0.95801	-2.41404	-0.98181	(1)
C(3)	0.70811	-0.95383	-1.41963	(1)
C(4)	-0.65484	-0.42113	-0.86970	(1)
C(5)	-0.77099	-0.67362	0.66021	(1)
C(6)	-0.58779	-2.14905	1.01823	(1)
C(7)	-2.07193	-0.08017	1.18370	(3)
C(8)	-2.27008	1.41425	0.91570	(1)
C(9)	-1.14016	1.98046	0.02999	(1)
C(10)	-0.81139	1.08452	-1.15609	(3)
O(11)	-0.66952	1.53996	-2.26983	(7)
O(12)	-2.89279	-0.73731	1.78486	(7)
C(13)	-1.80148	-1.15469	-1.62176	(1)
C(14)	1.92386	-0.05920	-1.12536	(1)
O(15)	2.13097	0.09110	0.29072	(75)
C(16)	3.17617	0.87325	0.66500	(3)
O(17)	3.90917	1.42795	-0.12893	(78)
C(18)	3.29302	0.95338	2.14992	(1)
C(19)	-3.65108	1.69385	0.29757	(1)
H(20)	0.84850	-3.75828	0.72984	(5)
H(21)	1.58639	-2.18037	1.09517	(5)
H(22)	1.98582	-2.72424	-1.28024	(5)
H(23)	0.27178	-3.08779	-1.54394	(5)
H(24)	0.62070	-0.97201	-2.53258	(5)
H(25)	0.03674	-0.11812	1.18178	(5)
H(26)	-1.40771	-2.76333	0.58979	(5)
H(27)	-0.64330	-2.27894	2.12219	(5)
H(28)	-2.22790	1.93308	1.90139	(5)
H(29)	-1.41449	2.99270	-0.32340	(5)
H(30)	-0.21955	2.11359	0.63904	(5)
H(31)	-2.80298	-0.82546	-1.27701	(5)
H(32)	-1.76492	-0.96113	-2.71485	(5)
H(33)	-1.77082	-2.25484	-1.49661	(5)
H(34)	2.82864	-0.50414	-1.58658	(5)
H(35)	1.78591	0.93683	-1.58938	(5)
H(36)	4.14600	1.58971	2.45088	(5)
H(37)	2.37100	1.38261	2.59476	(5)
H(38)	3.44541	-0.05486	2.58842	(5)
H(39)	-3.82539	2.78344	0.16926	(5)
H(40)	-3.75985	1.22526	-0.70270	(5)
H(41)	-4.47457	1.30875	0.93592	(5)

121tR5

C(1)	-0.70580	3.07470	-0.56612	(1)
C(2)	0.03599	2.85404	0.76124	(1)
C(3)	0.56339	1.41223	0.92822	(1)
C(4)	-0.60210	0.38394	0.74286	(1)
C(5)	-1.28352	0.61590	-0.63588	(1)
C(6)	-1.81916	2.04247	-0.78068	(1)
C(7)	-2.33940	-0.45398	-0.88164	(3)
C(8)	-1.83941	-1.90023	-0.82907	(1)
C(9)	-0.36762	-1.96557	-0.36543	(1)
C(10)	-0.09897	-1.07046	0.83554	(3)
O(11)	0.45261	-1.49601	1.82736	(7)
O(12)	-3.49657	-0.18460	-1.11712	(7)
C(13)	-1.62710	0.57293	1.89524	(1)
C(14)	1.76212	1.19888	-0.01202	(1)
O(15)	2.42093	-0.04310	0.30576	(75)
C(16)	3.39385	-0.44559	-0.55120	(3)
O(17)	3.70853	0.18329	-1.54124	(78)
C(18)	3.99983	-1.73767	-0.11772	(1)
C(19)	-2.74034	-2.76832	0.06614	(1)
H(20)	-1.13758	4.10215	-0.58846	(5)
H(21)	0.01686	3.02234	-1.41210	(5)
H(22)	0.88209	3.57542	0.83581	(5)
H(23)	-0.64202	3.10922	1.60607	(5)
H(24)	0.94588	1.31610	1.97118	(5)
H(25)	-0.52468	0.47888	-1.43698	(5)
H(26)	-2.64720	2.22686	-0.06418	(5)
H(27)	-2.25124	2.18053	-1.79704	(5)
H(28)	-1.89393	-2.30697	-1.86540	(5)
H(29)	-0.09465	-3.01178	-0.13028	(5)
H(30)	0.30214	-1.65885	-1.19755	(5)
H(31)	-2.45494	-0.16361	1.83521	(5)
H(32)	-1.15363	0.43714	2.89077	(5)
H(33)	-2.10047	1.57355	1.90705	(5)
H(34)	1.43927	1.20134	-1.06937	(5)
H(35)	2.48774	2.02772	0.11296	(5)
H(36)	4.79400	-2.06147	-0.81595	(5)
H(37)	4.44890	-1.64377	0.89294	(5)
H(38)	3.23215	-2.53850	-0.07667	(5)
H(39)	-2.41406	-3.83018	0.06323	(5)
H(40)	-2.72880	-2.42451	1.12159	(5)
H(41)	-3.79722	-2.75487	-0.27561	(5)

121tR8

C(1)	0.36299	-2.76135	0.13104	(1)
C(2)	1.18842	-1.83679	-0.77477	(1)
C(3)	0.96567	-0.33737	-0.48093	(1)
C(4)	-0.55743	0.01198	-0.52707	(1)
C(5)	-1.34701	-0.92999	0.42506	(1)
C(6)	-1.12731	-2.40713	0.09217	(1)
C(7)	-2.81726	-0.53165	0.44709	(3)
C(8)	-3.10427	0.92068	0.83657	(1)
C(9)	-1.79876	1.72449	1.00611	(1)
C(10)	-0.79763	1.47754	-0.11424	(3)
O(11)	-0.20981	2.39482	-0.64461	(7)
O(12)	-3.70694	-1.31189	0.18845	(7)
C(13)	-1.06103	-0.14060	-1.98942	(1)
C(14)	1.63290	0.06912	0.84590	(1)
O(15)	3.03526	-0.27930	0.86015	(75)
C(16)	3.88097	0.53329	0.17335	(3)
O(17)	3.51761	1.53090	-0.41631	(78)
C(18)	5.28785	0.04272	0.24718	(1)
C(19)	-4.04515	1.59749	-0.17557	(1)
H(20)	0.50556	-3.82119	-0.18358	(5)
H(21)	0.73621	-2.69301	1.17819	(5)
H(22)	2.26838	-2.08963	-0.67504	(5)
H(23)	0.93614	-2.05136	-1.83750	(5)
H(24)	1.46485	0.23727	-1.29444	(5)
H(25)	-0.97607	-0.77976	1.46282	(5)
H(26)	-1.54706	-2.65196	-0.90645	(5)
H(27)	-1.67164	-3.04383	0.82497	(5)
H(28)	-3.62549	0.89905	1.82168	(5)
H(29)	-2.03169	2.80421	1.07577	(5)
H(30)	-1.31960	1.45686	1.97310	(5)
H(31)	-2.13396	0.12275	-2.08797	(5)
H(32)	-0.50671	0.52503	-2.68464	(5)
H(33)	-0.95403	-1.16915	-2.38544	(5)
H(34)	1.51392	1.15143	1.04464	(5)
H(35)	1.15016	-0.44689	1.69608	(5)
H(36)	5.97316	0.70695	-0.31168	(5)
H(37)	5.63599	-0.00110	1.30023	(5)
H(38)	5.37268	-0.97701	-0.18300	(5)
H(39)	-4.31413	2.62641	0.14546	(5)
H(40)	-3.58277	1.67936	-1.18116	(5)
H(41)	-4.99719	1.03726	-0.29258	(5)

121tR6

C(1)	-0.87802	-2.44981	-1.03538	(1)
C(2)	-1.13879	-2.50750	0.47656	(1)
C(3)	-0.86461	-1.17558	1.21346	(1)
C(4)	0.56078	-0.63522	0.87911	(1)
C(5)	0.76185	-0.56146	-0.66895	(1)
C(6)	0.51992	-1.90950	-1.35135	(1)
C(7)	2.12212	0.03481	-0.99986	(3)
C(8)	2.34895	1.43755	-0.45473	(1)
C(9)	2.11248	1.45576	1.07307	(1)
C(10)	0.82919	0.74861	1.49691	(3)
O(11)	0.13250	1.21635	2.36946	(7)
O(12)	2.93776	-0.53895	-1.68689	(7)
C(13)	1.60904	-1.60860	1.49778	(1)
C(14)	-2.04467	-0.20471	1.00792	(1)
O(15)	-2.08846	0.29744	-0.33976	(75)
C(16)	-3.12899	1.11594	-0.64327	(3)
O(17)	-3.99249	1.41887	0.15549	(78)
C(18)	-3.06405	1.57722	-2.06040	(1)
C(19)	3.73948	1.97659	-0.79155	(1)
H(20)	-1.64606	-1.81377	-1.52943	(5)
H(21)	-0.99300	-3.46832	-1.47377	(5)
H(22)	-0.51125	-3.31429	-0.91773	(5)
H(23)	-2.19100	-2.82736	0.65601	(5)
H(24)	-0.86674	-1.41599	2.30385	(5)
H(25)	0.02474	0.15558	-1.08761	(5)
H(26)	1.28716	-2.64905	-1.03804	(5)
H(27)	0.62517	-1.79792	-2.45372	(5)
H(28)	1.59433	2.10314	-0.93339	(5)
H(29)	2.09163	2.50512	1.42689	(5)
H(30)	2.97131	0.97423	1.58833	(5)
H(31)	2.65103	-1.31489	1.25507	(5)
H(32)	1.49500	-2.65463	1.15318	(5)
H(33)	1.53595	-1.63043	2.60611	(5)
H(34)	-1.98799	0.64238	1.71602	(5)
H(35)	-2.99279	-0.73218	1.23632	(5)
H(36)	-3.91317	2.24242	-2.30448	(5)
H(37)	-3.09290	0.71401	-2.75765	(5)
H(38)	-2.12431	2.13685	-2.24979	(5)
H(39)	3.90778	2.02195	-1.88892	(5)
H(40)	4.54420	1.34641	-0.35626	(5)
H(41)	3.88043	3.00664	-0.39987	(5)

121tS1

C(1)	-0.49319	2.58347	0.50963	(1)
C(2)	-1.09949	2.02481	-0.78461	(1)
C(3)	-0.84809	0.51312	-0.96270	(1)
C(4)	0.67665	0.18985	-0.86661	(1)
C(5)	1.25368	0.74700	0.46352	(1)
C(6)	0.99729	2.24950	0.62405	(1)
C(7)	2.73172	0.39338	0.61154	(3)
C(8)	3.11871	-1.04674	0.26708	(1)
C(9)	1.87203	-1.92587	0.07900	(1)
C(10)	0.90925	-1.33082	-0.93799	(3)
O(11)	0.35706	-2.02431	-1.76410	(7)
O(12)	3.55068	1.19294	1.00852	(7)
C(13)	1.40571	0.82045	-2.08670	(1)
C(14)	-1.69772	-0.29925	0.02863	(1)
O(15)	-3.09490	-0.02817	-0.21216	(75)
C(16)	-3.96992	-0.61289	0.64661	(3)
O(17)	-3.62114	-1.31862	1.57163	(78)
C(18)	-5.38139	-0.27351	0.30373	(1)
C(19)	4.04825	-1.64345	1.33497	(1)
H(20)	-0.63410	3.68873	0.54395	(5)
H(21)	-1.03713	2.17271	1.39023	(5)
H(22)	-2.19308	2.23527	-0.80158	(5)
H(23)	-0.67991	2.58040	-1.65311	(5)
H(24)	-1.19100	0.23515	-1.98682	(5)
H(25)	0.73543	0.23948	1.30837	(5)
H(26)	1.56859	2.82384	-0.13606	(5)
H(27)	1.36743	2.59171	1.61635	(5)
H(28)	3.67490	-1.01939	-0.69838	(5)
H(29)	2.17820	-2.93864	-0.24782	(5)
H(30)	1.34560	-2.05525	1.04922	(5)
H(31)	2.48745	0.57318	-2.09662	(5)
H(32)	0.98857	0.45007	-3.04720	(5)
H(33)	1.33574	1.92534	-2.11581	(5)
H(34)	-1.51577	-1.38373	-0.09892	(5)
H(35)	-1.43882	-0.03960	1.07212	(5)
H(36)	-6.08964	-0.74960	1.00722	(5)
H(37)	-5.54413	0.82376	0.34375	(5)
H(38)	-5.63235	-0.61843	-0.72102	(5)
H(39)	4.33593	-2.68731	1.08660	(5)
H(40)	4.99028	-1.06290	1.43346	(5)
H(41)	3.56367	-1.66267	2.33446	(5)

121tS3

C(1)	-0.73660	-2.32905	-1.39867	(1)
C(2)	-1.06095	-2.61308	0.07387	(1)
C(3)	-0.84165	-1.40539	1.00987	(1)
C(4)	0.57763	-0.78071	0.81167	(1)
C(5)	0.85772	-0.49734	-0.69072	(1)
C(6)	0.66750	-1.74063	-1.56404	(1)
C(7)	2.22954	0.14426	-0.87712	(3)
C(8)	2.56635	1.29507	0.07444	(1)
C(9)	1.33676	1.71089	0.89969	(1)
C(10)	0.71323	0.52350	1.61839	(3)
O(11)	0.35644	0.60191	2.77357	(7)
O(12)	2.99615	-0.20668	-1.74690	(7)
C(13)	1.63337	-1.77735	1.37118	(1)
C(14)	-2.01300	-0.41087	0.92509	(1)
O(15)	-2.03957	0.25802	-0.34869	(75)
C(16)	-3.03810	1.15979	-0.53314	(3)
O(17)	-3.87566	1.40650	0.31122	(78)
C(18)	-2.96238	1.78827	-1.88385	(1)
C(19)	3.13984	2.49823	-0.69023	(1)
H(20)	-0.81888	-3.27164	-1.98820	(5)
H(21)	-1.48970	-1.63075	-1.82720	(5)
H(22)	-2.11337	-2.96910	0.15918	(5)
H(23)	-0.43157	-3.46502	0.41859	(5)
H(24)	-0.87397	-1.80852	2.05057	(5)
H(25)	0.13043	0.26152	-1.05192	(5)
H(26)	1.42895	-2.51057	-1.31666	(5)
H(27)	0.82432	-1.47827	-2.63424	(5)
H(28)	3.34910	0.92651	0.77703	(5)
H(29)	1.63011	2.48088	1.63936	(5)
H(30)	0.57518	2.18282	0.24219	(5)
H(31)	2.66654	-1.38194	1.28429	(5)
H(32)	1.46698	-1.98755	2.44907	(5)
H(33)	1.62433	-2.75658	0.85323	(5)
H(34)	-2.96793	-0.95254	1.07971	(5)
H(35)	-1.93877	0.33914	1.73617	(5)
H(36)	-3.77775	2.52075	-2.03117	(5)
H(37)	-1.99640	2.31859	-2.01769	(5)
H(38)	-3.04270	1.02022	-2.68116	(5)
H(39)	3.39126	3.33443	-0.00347	(5)
H(40)	4.07163	2.23511	-1.23491	(5)
H(41)	2.41722	2.88967	-1.43775	(5)

121tS5

C(1)	-0.36403	2.70438	0.25085	(1)
C(2)	-1.23852	1.85160	-0.67684	(1)
C(3)	-1.01109	0.33671	-0.49223	(1)
C(4)	0.50202	-0.01887	-0.65730	(1)
C(5)	1.36349	0.85268	0.29817	(1)
C(6)	1.11872	2.35245	0.10107	(1)
C(7)	2.84285	0.48989	0.19003	(3)
C(8)	3.17071	-1.00473	0.16922	(1)
C(9)	1.93611	-1.84650	0.52910	(1)
C(10)	0.74406	-1.50967	-0.35503	(3)
O(11)	0.02875	-2.37906	-0.80296	(7)
O(12)	3.71369	1.33139	0.15712	(7)
C(13)	0.91675	0.22034	-2.13694	(1)
C(14)	-1.59839	-0.14621	0.84798	(1)
O(15)	-2.98624	0.23205	0.98514	(75)
C(16)	-3.89908	-0.50400	0.29796	(3)
O(17)	-3.60508	-1.45963	-0.39143	(78)
C(18)	-5.28330	0.01124	0.50765	(1)
C(19)	4.34267	-1.33046	1.10762	(1)
H(20)	-0.51866	3.78506	0.02540	(5)
H(21)	-0.67938	2.55712	1.30870	(5)
H(22)	-2.31055	2.10209	-0.50931	(5)
H(23)	-1.03374	2.13623	-1.73327	(5)
H(24)	-1.56728	-0.18199	-1.30634	(5)
H(25)	1.07161	0.61475	1.34598	(5)
H(26)	1.48145	2.67698	-0.89753	(5)
H(27)	1.70374	2.93241	0.84950	(5)
H(28)	3.47872	-1.26352	-0.87016	(5)
H(29)	2.17933	-2.92230	0.43014	(5)
H(30)	1.65982	-1.68429	1.59330	(5)
H(31)	1.97089	-0.07054	-2.32505	(5)
H(32)	0.29513	-0.37776	-2.83667	(5)
H(33)	0.82178	1.27767	-2.45259	(5)
H(34)	-1.49710	-1.24174	0.96640	(5)
H(35)	-1.04445	0.29782	1.69536	(5)
H(36)	-6.02344	-0.59068	-0.05186	(5)
H(37)	-5.55787	-0.02069	1.58265	(5)
H(38)	-5.36821	1.06356	0.16486	(5)
H(39)	4.58689	-2.41407	1.09250	(5)
H(40)	5.26698	-0.78642	0.81810	(5)
H(41)	4.11226	-1.05787	2.15966	(5)

121tS4

C(1)	0.76064	-2.94673	-0.93283	(1)
C(2)	-0.05904	-2.95719	0.36573	(1)
C(3)	-0.60783	-1.56365	0.73804	(1)
C(4)	0.55946	-0.52431	0.81918	(1)
C(5)	1.33726	-0.51028	-0.52595	(1)
C(6)	1.87634	-1.89646	-0.89650	(1)
C(7)	2.42667	0.55836	-0.51924	(3)
C(8)	2.00485	1.94489	-0.02646	(1)
C(9)	0.48620	2.00861	0.21731	(1)
C(10)	0.03158	0.88753	1.13857	(3)
O(11)	-0.66129	1.11021	2.10784	(7)
O(12)	3.55044	0.33969	-0.91514	(7)
C(13)	1.50727	-0.91362	1.98819	(1)
C(14)	-1.73428	-1.18938	-0.24195	(1)
O(15)	-2.42509	-0.01285	0.22212	(75)
C(16)	-3.33378	0.52785	-0.62924	(3)
O(17)	-3.57001	0.06810	-1.72812	(78)
C(18)	-3.97839	1.73695	-0.04009	(1)
C(19)	2.44559	3.04159	-1.00887	(1)
H(20)	1.20102	-3.95591	-1.10676	(5)
H(21)	0.09008	-2.74688	-1.79928	(5)
H(22)	-0.90129	-3.68001	0.26581	(5)
H(23)	0.57031	-3.35141	1.19454	(5)
H(24)	-1.06836	-1.64643	1.75010	(5)
H(25)	0.63390	-0.21313	-1.33563	(5)
H(26)	2.66424	-2.21200	-0.18009	(5)
H(27)	2.36457	-1.85569	-1.89591	(5)
H(28)	2.52107	2.12109	0.94550	(5)
H(29)	0.22160	2.98773	0.66090	(5)
H(30)	-0.06338	1.94262	-0.74577	(5)
H(31)	2.31728	-0.16705	2.12643	(5)
H(32)	0.96228	-0.97205	2.95428	(5)
H(33)	2.00463	-1.89261	1.84703	(5)
H(34)	-1.33248	-1.01915	-1.25769	(5)
H(35)	-2.46138	-2.02349	-0.31112	(5)
H(36)	-4.72129	2.17268	-0.73386	(5)
H(37)	-4.49976	1.48476	0.90674	(5)
H(38)	-3.22097	2.51673	0.18493	(5)
H(39)	2.14807	4.05069	-0.65211	(5)
H(40)	3.54832	3.05697	-1.14253	(5)
H(41)	1.99123	2.89789	-2.01239	(5)

121tS6

C(1)	-0.57921	-3.04179	0.68381	(1)
C(2)	0.56522	-2.72347	-0.28906	(1)
C(3)	0.92573	-1.22285	-0.31935	(1)
C(4)	-0.34396	-0.36833	-0.64684	(1)
C(5)	-1.46665	-0.68638	0.37947	(1)
C(6)	-1.81585	-2.17835	0.41184	(1)
C(7)	-2.68995	0.19617	0.14801	(3)
C(8)	-2.41476	1.69051	-0.03765	(1)
C(9)	-0.93188	2.01666	0.21793	(1)
C(10)	-0.02482	1.13838	-0.62932	(3)
O(11)	0.85675	1.61580	-1.30996	(7)
O(12)	-3.81747	-0.24666	0.15094	(7)
C(13)	-0.82116	-0.69930	-2.08885	(1)
C(14)	1.63007	-0.85121	1.00142	(1)
O(15)	2.23812	0.45679	0.95137	(75)
C(16)	3.43807	0.54839	0.31837	(3)
O(17)	4.00913	-0.40609	-0.16958	(78)
C(18)	3.94916	1.95003	0.31637	(1)
C(19)	-3.32319	2.53948	0.86562	(1)
H(20)	-0.84987	-4.12029	0.60518	(5)
H(21)	-0.23730	-2.88233	1.73169	(5)
H(22)	1.46376	-3.32175	-0.01245	(5)
H(23)	0.28612	-3.06785	-1.30981	(5)
H(24)	1.65855	-1.07841	-1.14583	(5)
H(25)	-1.09894	-0.42222	1.39602	(5)
H(26)	-2.28671	-2.48906	-0.54488	(5)
H(27)	-2.57118	-2.37131	1.20625	(5)
H(28)	-2.64840	1.94021	-1.09846	(5)
H(29)	-0.74094	3.08267	-0.01146	(5)
H(30)	-0.68442	1.87824	1.29185	(5)
H(31)	-1.68245	-0.06765	-2.39183	(5)
H(32)	-0.01917	-0.52054	-2.83627	(5)
H(33)	-1.14359	-1.75057	-2.21764	(5)
H(34)	0.91550	-0.86261	1.84410	(5)
H(35)	2.39804	-1.60690	1.25952	(5)
H(36)	4.91894	2.02099	-0.21050	(5)
H(37)	3.23566	2.63392	-0.18781	(5)
H(38)	4.09599	2.31672	1.35376	(5)
H(39)	-3.13196	3.62527	0.72937	(5)
H(40)	-4.39877	2.36959	0.64565	(5)
H(41)	-3.16307	2.30733	1.94014	(5)

122cR1

C(1)	-0.28810	-2.95460	0.51682	(1)
C(2)	-1.14926	-2.10872	-0.42506	(1)
C(3)	-1.09768	-0.61345	-0.06226	(1)
C(4)	0.37048	-0.06082	-0.05130	(1)
C(5)	1.23327	-0.96154	0.90234	(1)
C(6)	1.15370	-2.45321	0.51159	(1)
C(7)	2.69656	-0.51459	0.91454	(3)
C(8)	3.38107	-0.38312	-0.44433	(1)
C(9)	2.50695	0.43113	-1.42849	(1)
C(10)	1.05970	-0.03669	-1.42385	(3)
O(11)	3.29143	-0.33181	1.95438	(7)
O(12)	0.49949	-0.34492	-2.45189	(7)
C(13)	4.77295	0.24187	-0.32937	(1)
C(14)	0.35867	1.36202	0.49058	(3)
C(15)	-2.07955	0.16658	-0.95641	(1)
O(16)	-3.43007	-0.31832	-0.78401	(75)
C(17)	-4.09745	0.10489	0.32202	(3)
O(18)	-3.62160	0.86971	1.13683	(78)
C(19)	-5.46573	-0.48504	0.39170	(1)
O(20)	0.61468	1.67802	1.63607	(78)
O(21)	0.03527	2.27179	-0.46403	(75)
C(22)	-0.01452	3.64336	-0.03206	(1)
H(23)	-0.70078	-2.90767	1.55085	(5)
H(24)	-0.32088	-4.02426	0.20524	(5)
H(25)	-0.81564	-2.26370	-1.47515	(5)
H(26)	-2.19941	-2.47764	-0.37429	(5)
H(27)	-1.46756	-0.52713	0.98472	(5)
H(28)	0.83813	-0.86675	1.93366	(5)
H(29)	1.76057	-3.06032	1.21962	(5)
H(30)	1.58902	-2.61335	-0.49809	(5)
H(31)	3.50378	-1.41136	-0.85491	(5)
H(32)	2.54577	1.50784	-1.16001	(5)
H(33)	2.92587	0.35050	-2.44992	(5)
H(34)	5.26482	0.32147	-1.32235	(5)
H(35)	4.73148	1.26566	0.10008	(5)
H(36)	5.44469	-0.36394	0.31586	(5)
H(37)	-2.05295	1.25169	-0.74950	(5)
H(38)	-1.81320	0.05056	-2.02301	(5)
H(39)	-5.41559	-1.59329	0.42871	(5)
H(40)	-6.00589	-0.13761	1.29208	(5)
H(41)	-6.06443	-0.20001	-0.49844	(5)
H(42)	-0.29345	4.28407	-0.89896	(5)
H(43)	-0.77537	3.77744	0.76108	(5)
H(44)	0.97499	3.97386	0.33880	(5)

122cR2

C(1)	-1.05746	-3.17627	-0.79336	(1)
C(2)	0.19796	-2.80538	0.00262	(1)
C(3)	0.69033	-1.38954	-0.34500	(1)
C(4)	-0.41752	-0.30832	-0.09868	(1)
C(5)	-1.69116	-0.71772	-0.91944	(1)
C(6)	-2.16165	-2.14620	-0.56577	(1)
C(7)	-2.83687	0.26950	-0.68823	(3)
C(8)	-3.22186	0.53920	0.76514	(1)
C(9)	-1.97078	0.84197	1.62561	(1)
C(10)	-0.84705	-0.15091	1.36871	(3)
O(11)	-3.43897	0.76494	-1.61586	(7)
O(12)	-0.32633	-0.75545	2.27961	(7)
C(13)	-4.23824	1.67626	0.88920	(1)
C(14)	0.08224	1.04313	-0.58601	(3)
C(15)	2.04003	-1.12357	0.34993	(1)
O(16)	2.80907	-0.20010	-0.44904	(75)
C(17)	4.06036	0.07736	0.00161	(3)
O(18)	4.51979	-0.39618	1.02141	(78)
C(19)	4.77635	1.01542	-0.91123	(1)
O(20)	-0.16864	1.53503	-1.66875	(78)
O(21)	0.84336	1.67220	0.34603	(75)
C(22)	1.33281	2.97551	-0.01791	(1)
H(23)	-0.81287	-3.23117	-1.87919	(5)
H(24)	-1.41320	-4.18890	-0.49275	(5)
H(25)	-0.00748	-2.89158	1.09232	(5)
H(26)	0.99586	-3.54999	-0.22473	(5)
H(27)	0.89580	-1.39759	-1.44092	(5)
H(28)	-1.43895	-0.70511	-1.99865	(5)
H(29)	-3.04963	-2.41199	-1.18143	(5)
H(30)	-2.48619	-2.19563	0.49570	(5)
H(31)	-3.70004	-0.38683	1.15853	(5)
H(32)	-1.60943	1.86942	1.41000	(5)
H(33)	-2.24696	0.82930	2.69747	(5)
H(34)	-4.51877	1.85531	1.94918	(5)
H(35)	-3.83871	2.63245	0.48871	(5)
H(36)	-5.17770	1.45100	0.34036	(5)
H(37)	1.90000	-0.72448	1.37117	(5)
H(38)	2.60584	-2.07224	0.44143	(5)
H(39)	5.82573	1.15939	-0.59298	(5)
H(40)	4.78306	0.62999	-1.95161	(5)
H(41)	4.28380	2.01000	-0.91905	(5)
H(42)	1.98829	3.35543	0.78839	(5)
H(43)	1.92493	2.92957	-0.95195	(5)
H(44)	0.49241	3.68502	-0.14492	(5)

122cR3

C(1)	-1.09727	2.85390	1.55266	(1)
C(2)	0.20241	2.74649	0.74774	(1)
C(3)	0.72442	1.29978	0.69523	(1)
C(4)	-0.34248	0.31213	0.10865	(1)
C(5)	-1.66265	0.45480	0.95560	(1)
C(6)	-2.16113	1.91530	0.98543	(1)
C(7)	-2.74902	-0.46521	0.40320	(3)
C(8)	-3.09750	-0.28817	-1.07198	(1)
C(9)	-1.81926	-0.28524	-1.94823	(1)
C(10)	-0.70545	0.57527	-1.36395	(3)
O(11)	-3.31494	-1.26930	1.11104	(7)
O(12)	-0.14871	1.41031	-2.04119	(7)
C(13)	-4.07572	-1.35637	-1.56459	(1)
C(14)	0.18067	-1.11300	0.21704	(3)
C(15)	2.09393	1.27519	-0.00257	(1)
O(16)	2.71174	-0.01090	0.20018	(75)
C(17)	3.93352	-0.18398	-0.36665	(3)
O(18)	4.50879	0.68823	-0.98595	(78)
C(19)	4.45496	-1.56088	-0.12755	(1)
O(20)	0.54117	-1.80945	-0.71229	(78)
O(21)	0.20721	-1.54261	1.50492	(75)
C(22)	0.67556	-2.88732	1.70943	(1)
H(23)	-0.90163	2.59941	2.61981	(5)
H(24)	-1.46879	3.90463	1.53607	(5)
H(25)	0.03912	3.13946	-0.28000	(5)
H(26)	0.96943	3.40692	1.21485	(5)
H(27)	0.90450	0.99693	1.75288	(5)
H(28)	-1.45895	0.15483	2.00225	(5)
H(29)	-3.08522	1.98445	1.60136	(5)
H(30)	-2.43388	2.25584	-0.03618	(5)
H(31)	-3.59669	0.70163	-1.17862	(5)
H(32)	-1.45470	-1.32543	-2.07606	(5)
H(33)	-2.07383	0.07450	-2.96392	(5)
H(34)	-4.33150	-1.20862	-2.63560	(5)
H(35)	-3.65473	-2.37968	-1.46516	(5)
H(36)	-5.03125	-1.33217	-0.99804	(5)
H(37)	1.99967	1.48753	-1.08315	(5)
H(38)	2.74510	2.06021	0.43231	(5)
H(39)	5.46282	-1.68878	-0.56452	(5)
H(40)	4.52237	-1.77497	0.95935	(5)
H(41)	3.78532	-2.31983	-0.58356	(5)
H(42)	0.64562	-3.12179	2.79026	(5)
H(43)	0.02793	-3.61287	1.18026	(5)
H(44)	1.72091	-2.99594	1.36128	(5)

122cR4

C(1)	-0.58811	2.82420	1.55778	(1)
C(2)	0.44513	2.73548	0.43016	(1)
C(3)	0.92227	1.29054	0.19210	(1)
C(4)	-0.27451	0.32159	-0.10157	(1)
C(5)	-1.31701	0.44889	1.07229	(1)
C(6)	-1.77607	1.90882	1.26872	(1)
C(7)	-2.52255	-0.45397	0.81611	(3)
C(8)	-3.24840	-0.25252	-0.51142	(1)
C(9)	-2.24752	-0.24411	-1.69448	(1)
C(10)	-1.02165	0.61561	-1.41451	(3)
O(11)	-2.89156	-1.26304	1.63905	(7)
O(12)	-0.67539	1.47355	-2.19542	(7)
C(13)	-4.33192	-1.30790	-0.74105	(1)
C(14)	0.24182	-1.10961	-0.17494	(3)
C(15)	2.03870	1.30804	-0.86935	(1)
O(16)	2.74332	0.05215	-0.95629	(75)
C(17)	3.65692	-0.21359	0.01395	(3)
O(18)	3.87361	0.53000	0.94928	(78)
C(19)	4.35411	-1.51134	-0.23256	(1)
O(20)	0.43139	-1.74296	-1.19546	(78)
O(21)	0.45940	-1.63058	1.05974	(75)
C(22)	0.86547	-3.00976	1.10369	(1)
H(23)	-0.11637	2.53557	2.52523	(5)
H(24)	-0.93722	3.87657	1.67175	(5)
H(25)	0.01444	3.16075	-0.50332	(5)
H(26)	1.31605	3.38021	0.69225	(5)
H(27)	1.38014	0.95552	1.14997	(5)
H(28)	-0.84205	0.12670	2.01972	(5)
H(29)	-2.50291	1.96504	2.10933	(5)
H(30)	-2.30584	2.27753	0.36457	(5)
H(31)	-3.74821	0.74184	-0.46906	(5)
H(32)	-1.92762	-1.28290	-1.91820	(5)
H(33)	-2.75993	0.12087	-2.60547	(5)
H(34)	-4.86096	-1.14269	-1.70393	(5)
H(35)	-3.90889	-2.33478	-0.77026	(5)
H(36)	-5.10293	-1.28718	0.05876	(5)
H(37)	1.63039	1.54324	-1.86827	(5)
H(38)	2.76346	2.11830	-0.65414	(5)
H(39)	4.77767	-1.91907	0.70510	(5)
H(40)	3.67012	-2.26934	-0.66122	(5)
H(41)	5.19208	-1.36788	-0.94796	(5)
H(42)	1.00661	-3.31311	2.15825	(5)
H(43)	0.08828	-3.66026	0.65793	(5)
H(44)	1.82394	-3.15680	0.57141	(5)

122cR5

C(1)	0.30083	-0.79766	2.54389	(1)
C(2)	0.54042	-1.79511	1.40564	(1)
C(3)	0.44187	-1.14420	0.01235	(1)
C(4)	-0.92471	-0.40611	-0.16300	(1)
C(5)	-1.20734	0.58500	1.01780	(1)
C(6)	-1.05272	-0.10519	2.37664	(1)
C(7)	-0.40196	1.87821	0.90547	(3)
C(8)	-0.42310	2.57814	-0.45599	(1)
C(9)	-1.31562	1.82360	-1.45721	(1)
C(10)	-0.94685	0.35157	-1.50921	(3)
O(11)	0.16937	2.36815	1.85507	(7)
O(12)	-0.67136	-0.19535	-2.55540	(7)
C(13)	-0.87378	4.04197	-0.31911	(1)
C(14)	-2.06348	-1.41177	-0.28321	(3)
C(15)	1.67004	-0.26274	-0.26048	(1)
O(16)	2.85785	-1.08292	-0.23359	(75)
C(17)	4.03033	-0.43505	-0.45835	(3)
O(18)	4.09875	0.75876	-0.67183	(78)
C(19)	5.19040	-1.37127	-0.40717	(1)
O(20)	-1.94136	-2.61890	-0.36331	(78)
O(21)	-3.27570	-0.79901	-0.30881	(75)
C(22)	-4.41474	-1.66765	-0.44247	(1)
H(23)	0.33024	-1.33142	3.52213	(5)
H(24)	1.11922	-0.04486	2.57539	(5)
H(25)	1.53574	-2.27745	1.53592	(5)
H(26)	-0.20422	-2.61881	1.48883	(5)
H(27)	0.48011	-1.96504	-0.74092	(5)
H(28)	-2.26802	0.91753	0.95668	(5)
H(29)	-1.85812	-0.86469	2.49078	(5)
H(30)	-1.20843	0.62581	3.20035	(5)
H(31)	0.62028	2.57293	-0.84672	(5)
H(32)	-2.38538	1.92888	-1.17884	(5)
H(33)	-1.20900	2.27407	-2.46267	(5)
H(34)	-0.88417	4.55789	-1.30287	(5)
H(35)	-1.89787	4.11636	0.10493	(5)
H(36)	-0.19686	4.62146	0.34429	(5)
H(37)	1.58815	0.21767	-1.25444	(5)
H(38)	1.75619	0.53840	0.49584	(5)
H(39)	6.14260	-0.83881	-0.58872	(5)
H(40)	5.25676	-1.86320	0.58564	(5)
H(41)	5.09028	-2.16595	-1.17563	(5)
H(42)	-5.33749	-1.05724	-0.45253	(5)
H(43)	-4.36600	-2.23562	-1.39165	(5)
H(44)	-4.47471	-2.37014	0.41125	(5)

122cR7

C(1)	0.11132	-2.87600	-1.13051	(1)
C(2)	1.14764	-2.15408	-0.26925	(1)
C(3)	1.05837	-0.62640	-0.42556	(1)
C(4)	-0.36097	-0.06074	-0.10809	(1)
C(5)	-1.44229	-0.87804	-0.91890	(1)
C(6)	-1.28742	-2.40489	-0.74848	(1)
C(7)	-2.86867	-0.48549	-0.53353	(3)
C(8)	-3.20438	-0.52243	0.95440	(1)
C(9)	-2.13533	0.21777	1.79407	(1)
C(10)	-0.70899	-0.13225	1.39161	(3)
O(11)	-3.69684	-0.21635	-1.37643	(7)
O(12)	0.10131	-0.44431	2.23512	(7)
C(13)	-4.59354	0.05062	1.24353	(1)
C(14)	-0.40610	1.39975	-0.56046	(3)
C(15)	2.21373	0.01140	0.37662	(1)
O(16)	3.44015	-0.18186	-0.36045	(75)
C(17)	4.56704	0.31294	0.21454	(3)
O(18)	4.57180	0.88335	1.28695	(78)
C(19)	5.76795	0.06293	-0.63443	(1)
O(20)	0.54000	2.04167	-0.97357	(78)
O(21)	-1.65476	1.92388	-0.49472	(75)
C(22)	-1.79552	3.28478	-0.93857	(1)
H(23)	0.30186	-2.67356	-2.20937	(5)
H(24)	0.19618	-3.97805	-0.98707	(5)
H(25)	1.00717	-2.44148	0.79706	(5)
H(26)	2.16543	-2.50522	-0.55762	(5)
H(27)	1.24855	-0.40757	-1.50220	(5)
H(28)	-1.30649	-0.64655	-1.99493	(5)
H(29)	-2.04040	-2.93134	-1.37632	(5)
H(30)	-1.49073	-2.69772	0.30400	(5)
H(31)	-3.20946	-1.59229	1.26461	(5)
H(32)	-2.28103	1.31522	1.72106	(5)
H(33)	-2.28508	-0.02981	2.86312	(5)
H(34)	-4.83337	0.00536	2.32737	(5)
H(35)	-4.67399	1.11433	0.93300	(5)
H(36)	-5.39052	-0.51311	0.71288	(5)
H(37)	2.04821	1.09216	0.53999	(5)
H(38)	2.30875	-0.46251	1.37232	(5)
H(39)	6.68307	0.46587	-0.16182	(5)
H(40)	5.91674	-1.02498	-0.79683	(5)
H(41)	5.65544	0.54397	-1.62843	(5)
H(42)	-2.85319	3.59238	-0.83396	(5)
H(43)	-1.17554	3.96458	-0.32269	(5)
H(44)	-1.51154	3.38127	-2.00434	(5)

122cR6

C(1)	-0.23057	0.43702	2.63020	(1)
C(2)	-0.32877	1.57167	1.60452	(1)
C(3)	-0.27393	1.05933	0.15467	(1)
C(4)	1.03755	0.23269	-0.07576	(1)
C(5)	1.19624	-0.90545	0.98225	(1)
C(6)	1.04634	-0.37736	2.41458	(1)
C(7)	0.30268	-2.10886	0.68912	(3)
C(8)	0.35599	-2.66208	-0.73723	(1)
C(9)	1.33368	-1.85310	-1.60936	(1)
C(10)	1.04269	-0.36723	-1.49994	(3)
O(11)	-0.36372	-2.64508	1.54735	(7)
O(12)	0.79662	0.30126	-2.48090	(7)
C(13)	0.72680	-4.15467	-0.73945	(1)
C(14)	2.27462	1.12663	-0.04285	(3)
C(15)	-1.56264	0.30909	-0.21346	(1)
O(16)	-2.68268	1.21322	-0.10261	(75)
C(17)	-3.89888	0.68998	-0.40613	(3)
O(18)	-4.05758	-0.46307	-0.75362	(78)
C(19)	-4.98276	1.70377	-0.25645	(1)
O(20)	3.34682	0.81912	0.44004	(78)
O(21)	2.06089	2.32684	-0.64001	(75)
C(22)	3.18441	3.22545	-0.67091	(1)
H(23)	-0.23351	0.86248	3.66060	(5)
H(24)	-1.12422	-0.22207	2.56404	(5)
H(25)	-1.26506	2.15032	1.77452	(5)
H(26)	0.50726	2.28821	1.77598	(5)
H(27)	-0.24504	1.95183	-0.51084	(5)
H(28)	2.23133	-1.30990	0.90571	(5)
H(29)	1.91972	0.26729	2.65813	(5)
H(30)	1.08523	-1.21860	3.14111	(5)
H(31)	-0.66528	-2.55759	-1.17019	(5)
H(32)	2.38299	-2.04967	-1.30457	(5)
H(33)	1.24823	-2.17856	-2.66383	(5)
H(34)	0.75955	-4.56385	-1.77171	(5)
H(35)	1.72410	-4.32868	-0.28207	(5)
H(36)	-0.00938	-4.76293	-0.17183	(5)
H(37)	-1.50534	-0.06820	-1.25271	(5)
H(38)	-1.72079	-0.55904	0.45119	(5)
H(39)	-5.97090	1.27242	-0.50278	(5)
H(40)	-5.02524	2.08488	0.78519	(5)
H(41)	-4.80921	2.56917	-0.92952	(5)
H(42)	2.88646	4.16199	-1.17913	(5)
H(43)	3.51224	3.47869	0.35589	(5)
H(44)	4.02759	2.78001	-1.23349	(5)

122cR9

C(1)	0.78600	-3.22156	0.65686	(1)
C(2)	-0.60062	-2.61204	0.41665	(1)
C(3)	-0.68862	-1.19228	0.99877	(1)
C(4)	0.39682	-0.23683	0.39229	(1)
C(5)	1.79836	-0.88134	0.68924	(1)
C(6)	1.88758	-2.31271	0.11015	(1)
C(7)	2.93758	-0.02629	0.12913	(3)
C(8)	2.84115	0.36385	-1.34484	(1)
C(9)	1.42957	0.90196	-1.68710	(1)
C(10)	0.33819	0.00340	-1.12567	(3)
O(11)	3.89167	0.27587	0.81246	(7)
O(12)	-0.48873	-0.49481	-1.85585	(7)
C(13)	3.90872	1.38615	-1.74043	(1)
C(14)	0.29476	1.11380	1.08135	(3)
C(15)	-2.13951	-0.68827	0.99664	(1)
O(16)	-2.61795	-0.49613	-0.34711	(75)
C(17)	-3.83253	0.09651	-0.47499	(3)
O(18)	-4.50659	0.44296	0.47389	(78)
C(19)	-4.20882	0.25954	-1.90896	(1)
O(20)	0.99518	1.48854	2.00103	(78)
O(21)	-0.68974	1.88226	0.54851	(75)
C(22)	-0.87313	3.17793	1.14644	(1)
H(23)	0.94145	-3.37974	1.74907	(5)
H(24)	0.84773	-4.22557	0.17677	(5)
H(25)	-0.82754	-2.60662	-0.67173	(5)
H(26)	-1.36920	-3.26445	0.89206	(5)
H(27)	-0.42655	-1.29432	2.07906	(5)
H(28)	1.93428	-0.95272	1.78695	(5)
H(29)	2.88161	-2.75175	0.34972	(5)
H(30)	1.81419	-2.28599	-0.99821	(5)
H(31)	3.01695	-0.55945	-1.94309	(5)
H(32)	1.31003	1.92834	-1.28210	(5)
H(33)	1.32142	0.98723	-2.78539	(5)
H(34)	3.83508	1.65337	-2.81627	(5)
H(35)	3.81242	2.32860	-1.16007	(5)
H(36)	4.93545	0.99523	-1.57452	(5)
H(37)	-2.78828	-1.42593	1.51088	(5)
H(38)	-2.21741	0.25325	1.57336	(5)
H(39)	-5.20531	0.72838	-2.01042	(5)
H(40)	-3.47316	0.90053	-2.43841	(5)
H(41)	-4.23787	-0.72317	-2.42403	(5)
H(42)	-1.13573	3.08188	2.21772	(5)
H(43)	0.04185	3.79204	1.03911	(5)
H(44)	-1.70248	3.70017	0.63300	(5)

122cS1

C(1)	-0.26377	-2.99884	0.27400	(1)
C(2)	-1.12456	-2.09368	-0.61184	(1)
C(3)	-1.09457	-0.63330	-0.12783	(1)
C(4)	0.37090	-0.07124	-0.08634	(1)
C(5)	1.21742	-1.00838	0.82944	(1)
C(6)	1.16940	-2.47573	0.34976	(1)
C(7)	2.68247	-0.56445	0.93734	(3)
C(8)	3.18721	0.42557	-0.10952	(1)
C(9)	2.57130	0.12220	-1.48291	(1)
C(10)	1.04896	0.00830	-1.46543	(3)
O(11)	3.40901	-1.01150	1.79825	(7)
O(12)	0.42822	-0.04429	-2.50401	(7)
C(13)	4.71605	0.42350	-0.20245	(1)
C(14)	0.33573	1.32372	0.52150	(3)
C(15)	-2.09513	0.20494	-0.94493	(1)
O(16)	-3.44428	-0.27510	-0.74942	(75)
C(17)	-4.06946	0.10233	0.39708	(3)
O(18)	-3.55780	0.82329	1.23000	(78)
C(19)	-5.44128	-0.47674	0.48567	(1)
O(20)	0.49683	1.57796	1.69938	(78)
O(21)	0.11537	2.28427	-0.41233	(75)
C(22)	0.04948	3.63483	0.07961	(1)
H(23)	-0.70031	-3.04633	1.29830	(5)
H(24)	-0.26898	-4.03929	-0.12565	(5)
H(25)	-0.77325	-2.15918	-1.66570	(5)
H(26)	-2.17080	-2.47686	-0.60616	(5)
H(27)	-1.45580	-0.63707	0.92563	(5)
H(28)	0.79081	-0.97978	1.85506	(5)
H(29)	1.75760	-3.11988	1.04053	(5)
H(30)	1.64887	-2.56593	-0.64892	(5)
H(31)	2.87366	1.44598	0.20695	(5)
H(32)	2.86531	0.91455	-2.20238	(5)
H(33)	2.99207	-0.82938	-1.87341	(5)
H(34)	5.07751	1.14662	-0.96451	(5)
H(35)	5.18837	0.70938	0.76177	(5)
H(36)	5.11100	-0.57605	-0.48389	(5)
H(37)	-2.04544	1.27741	-0.68216	(5)
H(38)	-1.86958	0.14183	-2.02515	(5)
H(39)	-5.94690	-0.16684	1.41919	(5)
H(40)	-6.06622	-0.14419	-0.36924	(5)
H(41)	-5.40259	-1.58595	0.46907	(5)
H(42)	-0.77597	3.74675	0.80904	(5)
H(43)	1.00759	3.92749	0.55104	(5)
H(44)	-0.14258	4.32058	-0.76713	(5)

122cS3

C(1)	-0.46403	3.21638	0.36615	(1)
C(2)	0.53598	2.62311	-0.63225	(1)
C(3)	0.94456	1.19628	-0.22903	(1)
C(4)	-0.30367	0.24934	-0.14349	(1)
C(5)	-1.28499	0.86342	0.90245	(1)
C(6)	-1.68348	2.30895	0.52635	(1)
C(7)	-2.55649	0.02350	1.07994	(3)
C(8)	-2.87352	-0.99608	-0.01173	(1)
C(9)	-2.48800	-0.45178	-1.39509	(1)
C(10)	-1.06139	0.08760	-1.47387	(3)
O(11)	-3.28831	0.19112	2.03134	(7)
O(12)	-0.58344	0.39743	-2.54290	(7)
C(13)	-4.34999	-1.40370	0.00406	(1)
C(14)	0.15365	-1.12223	0.32958	(3)
C(15)	2.09339	0.70370	-1.13145	(1)
O(16)	2.82750	-0.36932	-0.50257	(75)
C(17)	3.70887	-0.02202	0.47254	(3)
O(18)	3.92006	1.12763	0.80272	(78)
C(19)	4.36629	-1.22210	1.06644	(1)
O(20)	0.23471	-1.47176	1.49107	(78)
O(21)	0.45261	-1.94557	-0.70823	(75)
C(22)	0.88676	-3.27160	-0.35661	(1)
H(23)	0.03150	3.35227	1.35520	(5)
H(24)	-0.78463	4.22869	0.02744	(5)
H(25)	0.09944	2.63175	-1.65524	(5)
H(26)	1.43638	3.27913	-0.66983	(5)
H(27)	1.35510	1.27617	0.80309	(5)
H(28)	-0.77540	0.90084	1.88893	(5)
H(29)	-2.35328	2.73170	1.30789	(5)
H(30)	-2.26749	2.30867	-0.41928	(5)
H(31)	-2.27339	-1.91112	0.19386	(5)
H(32)	-2.61301	-1.25203	-2.15414	(5)
H(33)	-3.18896	0.36253	-1.67864	(5)
H(34)	-4.57464	-2.14654	-0.79094	(5)
H(35)	-4.63919	-1.86942	0.97049	(5)
H(36)	-5.02016	-0.53296	-0.16023	(5)
H(37)	1.17367	0.34507	-2.10438	(5)
H(38)	2.78758	1.53230	-1.37341	(5)
H(39)	3.62414	-1.84951	1.60339	(5)
H(40)	4.83730	-1.84767	0.28047	(5)
H(41)	5.15134	-0.93138	1.78918	(5)
H(42)	1.80688	-3.23496	0.25758	(5)
H(43)	0.09176	-3.81044	0.19421	(5)
H(44)	1.11109	-3.83703	-1.28073	(5)

122cS2

C(1)	-0.08745	-3.09003	-0.31707	(1)
C(2)	0.98675	-2.18077	0.28777	(1)
C(3)	0.93360	-0.76668	-0.31652	(1)
C(4)	-0.47524	-0.10672	-0.10750	(1)
C(5)	-1.54161	-1.04764	-0.74817	(1)
C(6)	-1.47580	-2.47286	-0.15576	(1)
C(7)	-2.97002	-0.50735	-0.59983	(3)
C(8)	-3.19404	0.58751	0.44051	(1)
C(9)	-2.32519	0.34243	1.68267	(1)
C(10)	-0.84798	0.11854	1.36843	(3)
O(11)	-3.88006	-0.95806	-1.26129	(7)
O(12)	-0.02953	0.09413	2.26086	(7)
C(13)	-4.66880	0.69869	0.83906	(1)
C(14)	-0.48810	1.23396	-0.82743	(3)
C(15)	2.12377	0.06904	0.18020	(1)
O(16)	3.34712	-0.55511	-0.26471	(75)
C(17)	4.49684	0.09884	0.04490	(3)
O(18)	4.52060	1.15105	0.65129	(78)
C(19)	5.69496	-0.63742	-0.45284	(1)
O(20)	-0.83520	1.40613	-1.97962	(78)
O(21)	-0.06730	2.24758	-0.02815	(75)
C(22)	-0.03558	3.55408	-0.63003	(1)
H(23)	0.12588	-3.25363	-1.39864	(5)
H(24)	-0.05704	-4.09174	0.17073	(5)
H(25)	0.85999	-2.13517	1.39227	(5)
H(26)	1.98635	-2.63824	0.10663	(5)
H(27)	1.07048	-0.88011	-1.41731	(5)
H(28)	-1.33379	-1.12901	-1.83660	(5)
H(29)	-2.22630	-3.12546	-0.65471	(5)
H(30)	-1.74648	-2.45035	0.92199	(5)
H(31)	-2.89835	1.55805	-0.01825	(5)
H(32)	-2.41984	1.20463	2.37519	(5)
H(33)	-2.70810	-0.54509	2.23100	(5)
H(34)	-4.82608	1.49780	1.59470	(5)
H(35)	-5.31372	0.94720	-0.03091	(5)
H(36)	-5.05025	-0.24828	1.27728	(5)
H(37)	2.07429	1.09403	-0.23372	(5)
H(38)	2.12771	0.14284	1.28370	(5)
H(39)	6.62837	-0.10214	-0.19714	(5)
H(40)	5.74833	-1.65201	-0.00584	(5)
H(41)	5.65716	-0.75235	-1.55622	(5)
H(42)	0.32772	4.28787	0.11407	(5)
H(43)	0.65359	3.57012	-1.49643	(5)
H(44)	-1.04910	3.86156	-0.95269	(5)

122cS4

C(1)	-0.15335	2.59802	-1.47516	(1)
C(2)	-1.03051	2.24018	-0.27048	(1)
C(3)	-1.06583	0.72152	-0.03278	(1)
C(4)	0.37160	0.13858	0.18168	(1)
C(5)	1.23336	0.50369	-1.06939	(1)
C(6)	1.25684	2.02954	-1.31308	(1)
C(7)	2.67041	-0.01905	-0.96616	(3)
C(8)	3.17549	-0.39717	0.42429	(1)
C(9)	2.59356	0.53691	1.49555	(1)
C(10)	1.07419	0.67834	1.43931	(3)
O(11)	3.37535	-0.10378	-1.94828	(7)
O(12)	0.47614	1.22248	2.34094	(7)
C(13)	4.70625	-0.38951	0.49124	(1)
C(14)	0.25608	-1.36955	0.33385	(3)
C(15)	-2.06088	0.37972	1.09175	(1)
O(16)	-3.41586	0.66090	0.67566	(75)
C(17)	-4.01050	-0.25235	-0.13719	(3)
O(18)	-3.46585	-1.27365	-0.50561	(78)
C(19)	-5.39514	0.16462	-0.50326	(1)
O(20)	0.38877	-1.98470	1.37440	(78)
O(21)	-0.03303	-1.97576	-0.84542	(75)
C(22)	-0.20353	-3.40306	-0.79499	(1)
H(23)	-0.61411	2.19469	-2.40635	(5)
H(24)	-0.10569	3.70511	-1.59506	(5)
H(25)	-0.65355	2.76636	0.63461	(5)
H(26)	-2.06270	2.62098	-0.44774	(5)
H(27)	-1.45623	0.26312	-0.96923	(5)
H(28)	0.77928	0.03515	-1.96787	(5)
H(29)	1.85093	2.25762	-2.22583	(5)
H(30)	1.76701	2.54333	-0.47003	(5)
H(31)	2.83868	-1.43776	0.63241	(5)
H(32)	2.88399	0.16931	2.50169	(5)
H(33)	3.04573	1.54639	1.38822	(5)
H(34)	5.06996	-0.66760	1.50349	(5)
H(35)	5.15442	-1.11424	-0.22179	(5)
H(36)	5.12417	0.61241	0.25498	(5)
H(37)	-1.97829	-0.67813	1.40508	(5)
H(38)	-1.85395	0.98376	1.99428	(5)
H(39)	-5.87588	-0.58063	-1.16407	(5)
H(40)	-6.02629	0.27686	0.40287	(5)
H(41)	-5.38567	1.13868	-1.03545	(5)
H(42)	-0.44376	-3.77613	-1.80851	(5)
H(43)	0.72757	-3.89713	-0.45612	(5)
H(44)	-1.03806	-3.67464	-0.11991	(5)

122cS5

C(1)	1.09248	3.20029	-0.63788	(1)
C(2)	-0.17246	2.80799	0.13303	(1)
C(3)	-0.67781	1.41833	-0.29196	(1)
C(4)	0.41838	0.31932	-0.06095	(1)
C(5)	1.67971	0.73313	-0.88017	(1)
C(6)	2.18109	2.13948	-0.48048	(1)
C(7)	2.83254	-0.26881	-0.73319	(3)
C(8)	2.75933	-1.24572	0.43826	(1)
C(9)	2.15708	-0.56768	1.67758	(1)
C(10)	0.83822	0.15477	1.41113	(3)
O(11)	3.77186	-0.26658	-1.49894	(7)
O(12)	0.18924	0.60084	2.33155	(7)
C(13)	4.13327	-1.83481	0.77243	(1)
C(14)	-0.10440	-1.01446	-0.57094	(3)
C(15)	-2.05016	1.13932	0.34858	(1)
O(16)	-2.77289	0.19780	-0.47205	(75)
C(17)	-4.04683	-0.07298	-0.08509	(3)
O(18)	-4.56145	0.41910	0.89897	(78)
C(19)	-4.71238	-1.02840	-1.01807	(1)
O(20)	0.06019	-1.44741	-1.69488	(78)
O(21)	-0.76919	-1.70336	0.39187	(75)
C(22)	-1.26929	-2.99716	0.00894	(1)
H(23)	0.84809	3.32599	-1.71800	(5)
H(24)	1.46699	4.18641	-0.27785	(5)
H(25)	0.02843	2.83396	1.22675	(5)
H(26)	-0.95926	3.57381	-0.05927	(5)
H(27)	-0.85359	1.47683	-1.39150	(5)
H(28)	1.40838	0.76669	-1.95699	(5)
H(29)	3.05781	2.42010	-1.10558	(5)
H(30)	2.53709	2.13163	0.57238	(5)
H(31)	2.10001	-2.09035	0.13566	(5)
H(32)	1.99810	-1.32627	2.47229	(5)
H(33)	2.88472	0.16665	2.08513	(5)
H(34)	4.07400	-2.54558	1.62424	(5)
H(35)	4.56138	-2.39602	-0.08564	(5)
H(36)	4.86351	-1.04572	1.05241	(5)
H(37)	-1.95093	0.75181	1.37851	(5)
H(38)	-2.63043	2.08205	0.40593	(5)
H(39)	-5.78610	-1.13917	-0.77691	(5)
H(40)	-4.63041	-0.68206	-2.06875	(5)
H(41)	-4.24432	-2.03267	-0.95210	(5)
H(42)	-1.85559	-3.42220	0.84539	(5)
H(43)	-1.93203	-2.92092	-0.87409	(5)
H(44)	-0.43215	-3.68668	-0.21367	(5)

122cS7

C(1)	0.39171	2.87316	-1.35496	(1)
C(2)	-0.58163	2.65643	-0.19021	(1)
C(3)	-0.96117	1.17266	-0.04632	(1)
C(4)	0.30917	0.28256	0.17363	(1)
C(5)	1.25977	0.49913	-1.04729	(1)
C(6)	1.63216	1.99065	-1.21061	(1)
C(7)	2.54032	-0.33744	-0.94810	(3)
C(8)	2.91756	-0.87200	0.43192	(1)
C(9)	2.53308	0.12367	1.53630	(1)
C(10)	1.09214	0.62436	1.45471	(3)
O(11)	3.22775	-0.54404	-1.92451	(7)
O(12)	0.62675	1.29238	2.35154	(7)
C(13)	4.41003	-1.20796	0.51935	(1)
C(14)	-0.11723	-1.17250	0.28179	(3)
C(15)	-2.06685	1.00727	1.01587	(1)
O(16)	-2.81969	-0.20737	0.80464	(75)
C(17)	-3.77127	-0.17602	-0.16609	(3)
O(18)	-3.99442	0.80222	-0.85058	(78)
C(19)	-4.49392	-1.47737	-0.26643	(1)
O(20)	-0.19852	-1.80591	1.31679	(78)
O(21)	-0.38762	-1.71466	-0.93289	(75)
C(22)	-0.74564	-3.10820	-0.93329	(1)
H(23)	-0.12047	2.64011	-2.31706	(5)
H(24)	0.69180	3.94544	-1.40461	(5)
H(25)	-0.13278	3.03975	0.75248	(5)
H(26)	-1.49777	3.26524	-0.37092	(5)
H(27)	-1.40112	0.87318	-1.02446	(5)
H(28)	0.73387	0.18741	-1.97416	(5)
H(29)	2.28133	2.12210	-2.10472	(5)
H(30)	2.22838	2.33383	-0.33790	(5)
H(31)	2.35449	-1.81941	0.59024	(5)
H(32)	2.69473	-0.34699	2.52859	(5)
H(33)	3.21303	1.00145	1.49178	(5)
H(34)	4.68034	-1.59823	1.52380	(5)
H(35)	4.70186	-1.98669	-0.21747	(5)
H(36)	5.04507	-0.31607	0.33076	(5)
H(37)	-1.64463	0.98083	2.03560	(5)
H(38)	-2.75541	1.87487	1.00563	(5)
H(39)	-5.36193	-1.40024	-0.94757	(5)
H(40)	-3.82313	-2.26897	-0.66046	(5)
H(41)	-4.86430	-1.80633	0.72604	(5)
H(42)	-1.00396	-3.41680	-1.96386	(5)
H(43)	0.10489	-3.72780	-0.58892	(5)
H(44)	-1.62468	-3.29241	-0.28661	(5)

122cS6

C(1)	-1.12396	-2.92814	-1.36841	(1)
C(2)	0.18112	-2.77734	-0.57951	(1)
C(3)	0.70954	0.70954	-1.33279	(1)
C(4)	-0.35162	-0.32051	-0.06851	(1)
C(5)	-1.65987	-0.48547	-0.91078	(1)
C(6)	-2.17974	-1.94011	-0.87329	(1)
C(7)	-2.77405	0.46472	-0.45875	(3)
C(8)	-2.66067	1.05481	0.94516	(1)
C(9)	-2.00936	0.05955	1.91640	(1)
C(10)	-0.70019	-0.54590	-1.41350	(3)
O(11)	-3.71209	0.71482	-1.18414	(7)
O(12)	-0.00830	-1.20565	2.15689	(7)
C(13)	-4.02543	1.50008	1.48183	(1)
C(14)	0.18340	1.09589	-0.20435	(3)
C(15)	2.10051	-1.27623	0.02482	(1)
O(16)	2.70772	0.00286	-0.24356	(75)
C(17)	3.95246	0.19191	0.26568	(3)
O(18)	4.55411	-0.66196	0.88552	(78)
C(19)	4.46306	1.56600	-0.03578	(1)
O(20)	0.53661	1.80879	0.71574	(78)
O(21)	0.21695	1.50078	-1.50002	(75)
C(22)	0.69963	2.83649	-1.72911	(1)
H(23)	-0.92839	-2.75402	-2.45172	(5)
H(24)	-1.50594	-3.97112	-1.27572	(5)
H(25)	0.02108	-3.09797	0.47382	(5)
H(26)	0.94108	-3.47252	-1.00575	(5)
H(27)	0.85992	-1.08925	-1.70467	(5)
H(28)	-1.43602	-0.24449	-1.97130	(5)
H(29)	-3.09217	-2.03212	-1.50345	(5)
H(30)	-2.48372	-2.21195	0.16037	(5)
H(31)	-2.01977	1.96247	0.87619	(5)
H(32)	-1.82254	0.56309	2.88782	(5)
H(33)	-2.72115	-0.76783	2.12547	(5)
H(34)	-3.93984	1.93061	2.50242	(5)
H(35)	-4.48638	2.28176	0.84074	(5)
H(36)	-4.74147	0.65266	1.54083	(5)
H(37)	2.04545	-1.45182	1.11429	(5)
H(38)	2.73992	-2.07462	-0.40332	(5)
H(39)	5.49172	1.69731	0.34663	(5)
H(40)	4.47612	1.74602	-1.12990	(5)
H(41)	3.81821	2.33290	0.43344	(5)
H(42)	0.67931	3.04873	-2.81474	(5)
H(43)	0.05528	3.57881	-1.21957	(5)
H(44)	1.74339	2.94285	-1.37594	(5)

122cS8

C(1)	0.47859	-2.81472	-0.60954	(1)
C(2)	1.40153	-1.75518	-0.00003	(1)
C(3)	1.04645	-0.34114	-0.49198	(1)
C(4)	-0.44634	0.02107	-0.16447	(1)
C(5)	-1.35552	-1.06774	-0.81362	(1)
C(6)	-0.98620	-2.48638	-0.32740	(1)
C(7)	-2.84756	-0.82028	-0.55636	(3)
C(8)	-3.20730	0.13760	0.57680	(1)
C(9)	-2.22689	-0.01484	1.74851	(1)
C(10)	-0.75907	0.08609	1.34098	(3)
O(11)	-3.69661	-1.38840	-1.20844	(7)
O(12)	0.10434	0.18668	2.18432	(7)
C(13)	-4.64632	-0.06912	1.05929	(1)
C(14)	-0.76101	1.37276	-0.79027	(3)
C(15)	2.08671	0.67619	0.00712	(1)
O(16)	3.36678	0.39966	-0.61616	(75)
C(17)	4.38254	-0.02374	0.18288	(3)
O(18)	4.27157	-0.18818	1.38107	(78)
C(19)	5.62865	-0.26012	-0.60277	(1)
O(20)	-1.19314	1.53932	-1.91420	(78)
O(21)	-0.51187	2.40184	0.05978	(75)
C(22)	-0.78256	3.71990	-0.45013	(1)
H(23)	0.64494	-2.86785	-1.71026	(5)
H(24)	0.72950	-3.81993	-0.19855	(5)
H(25)	1.34493	-1.80337	1.11030	(5)
H(26)	2.45278	-2.00301	-0.27191	(5)
H(27)	1.13159	-0.35477	-1.60362	(5)
H(28)	-1.20535	-1.04364	-1.91421	(5)
H(29)	-1.63342	-3.23960	-0.82923	(5)
H(30)	-1.18232	-2.57974	0.76253	(5)
H(31)	-3.13373	1.17560	0.18044	(5)
H(32)	-2.44276	0.75993	2.51325	(5)
H(33)	-2.39070	-0.99732	2.24139	(5)
H(34)	-4.90324	0.63143	1.88240	(5)
H(35)	-5.38326	0.10568	0.24635	(5)
H(36)	-4.80924	-1.09959	1.44125	(5)
H(37)	1.79620	1.70140	-0.28826	(5)
H(38)	2.15947	0.67854	1.10847	(5)
H(39)	6.45305	-0.60558	0.04853	(5)
H(40)	5.46227	-1.03191	-1.38304	(5)
H(41)	5.95893	0.67098	-1.10871	(5)
H(42)	-0.53861	4.46743	0.32821	(5)
H(43)	-0.15931	3.93171	-1.34039	(5)
H(44)	-1.85360	3.82754	-0.70930	(5)

122tR1

C(1)	-0.80249	-0.35419	-2.56189	(1)
C(2)	-1.18817	-1.33189	-1.44165	(1)
C(3)	-1.00042	-0.73059	-0.03336	(1)
C(4)	0.48742	-0.29333	0.13455	(1)
C(5)	0.82646	0.76294	-0.96646	(1)
C(6)	0.61643	0.19492	-2.37373	(1)
C(7)	2.21518	1.36502	-0.76943	(3)
C(8)	2.47708	1.96421	0.60728	(1)
C(9)	2.14867	0.93481	1.71286	(1)
C(10)	0.77758	0.30226	1.52395	(3)
O(11)	3.02263	1.43915	-1.66983	(7)
O(12)	0.00289	0.20432	2.45022	(7)
C(13)	3.91198	2.47182	0.75630	(1)
C(14)	1.41311	-1.50132	0.06492	(3)
C(15)	-2.03003	0.38551	0.21487	(1)
O(16)	-3.35629	-0.18274	0.15826	(75)
C(17)	-4.38558	0.69731	0.26420	(3)
O(18)	-4.22515	1.89457	0.39145	(78)
C(19)	-5.70522	0.00476	0.20157	(1)
O(20)	2.44764	-1.56588	-0.56912	(78)
O(21)	0.96777	-2.52496	0.83802	(75)
C(22)	1.78802	-3.70721	0.85080	(1)
H(23)	-0.87753	-0.86691	-3.54890	(5)
H(24)	-1.52855	0.48909	-2.59630	(5)
H(25)	-2.24314	-1.66074	-1.58133	(5)
H(26)	-0.57023	-2.25377	-1.53878	(5)
H(27)	-1.21849	-1.53177	0.70879	(5)
H(28)	0.12497	1.61729	-0.84923	(5)
H(29)	1.35058	-0.61264	-2.58015	(5)
H(30)	0.80173	0.98732	-3.13287	(5)
H(31)	1.78858	2.83291	0.72352	(5)
H(32)	2.91935	0.13447	1.72115	(5)
H(33)	2.20041	1.42699	2.70324	(5)
H(34)	4.08165	2.91895	1.75906	(5)
H(35)	4.65413	1.65468	0.63086	(5)
H(36)	4.15049	3.25758	0.00780	(5)
H(37)	-1.88160	0.84993	1.20728	(5)
H(38)	-1.93627	1.18819	-0.53925	(5)
H(39)	-6.53980	0.72559	0.28551	(5)
H(40)	-5.81906	-0.54106	-0.75822	(5)
H(41)	-5.80399	-0.73138	1.02644	(5)
H(42)	1.32142	-4.46583	1.50724	(5)
H(43)	1.87372	-4.13611	-0.16637	(5)
H(44)	2.79663	-3.48039	1.24724	(5)

122tR3

C(1)	-0.60647	-1.62122	2.22575	(1)
C(2)	-1.34375	-0.34584	1.79423	(1)
C(3)	-1.14625	-0.02128	0.29884	(1)
C(4)	0.38222	0.13484	0.01728	(1)
C(5)	1.11067	-1.19324	0.40810	(1)
C(6)	0.88475	-1.55241	1.87988	(1)
C(7)	2.58882	-1.16682	0.02552	(3)
C(8)	2.88148	-0.83610	-1.43354	(1)
C(9)	2.16189	0.46870	-1.84598	(1)
C(10)	0.69146	0.46083	-1.45470	(3)
O(11)	3.46436	-1.47418	0.80477	(7)
O(12)	-0.16659	0.76903	-2.25208	(7)
C(13)	4.38104	-0.73359	-1.71611	(1)
C(14)	0.94321	1.33045	0.77686	(3)
C(15)	-1.86241	-1.06532	-0.58130	(1)
O(16)	-3.25414	-1.19512	-0.21324	(75)
C(17)	-4.10100	-0.22069	-0.63848	(3)
O(18)	-3.74837	0.72192	-1.31823	(78)
C(19)	-5.49492	-0.46708	-0.16762	(1)
O(20)	1.96524	1.33704	1.43389	(78)
O(21)	0.17537	2.43825	0.61349	(75)
C(22)	0.63387	3.62743	1.28149	(1)
H(23)	-0.73021	-1.77359	3.32307	(5)
H(24)	-1.06521	-2.50909	1.73492	(5)
H(25)	-2.42804	-0.44404	2.02825	(5)
H(26)	-0.98075	0.50735	2.41188	(5)
H(27)	-1.63621	0.95814	0.10352	(5)
H(28)	0.67415	-2.01510	-0.19972	(5)
H(29)	1.37934	-0.80979	2.54148	(5)
H(30)	1.35500	-2.53541	2.10599	(5)
H(31)	2.46977	-1.67035	-2.04743	(5)
H(32)	2.66082	1.33984	-1.37016	(5)
H(33)	2.25791	0.61414	-2.93927	(5)
H(34)	4.57737	-0.50711	-2.78587	(5)
H(35)	4.86001	0.06984	-1.11666	(5)
H(36)	4.90952	-1.68321	-1.48482	(5)
H(37)	-1.78566	-0.82397	-1.65714	(5)
H(38)	-1.39520	-2.06004	-0.46860	(5)
H(39)	-6.18134	0.32692	-0.51624	(5)
H(40)	-5.87396	-1.43881	-0.54722	(5)
H(41)	-5.53730	-0.49390	0.94125	(5)
H(42)	-0.07298	4.45385	1.07769	(5)
H(43)	0.67568	3.47056	2.37674	(5)
H(44)	1.63240	3.92653	0.90815	(5)

122tR2

C(1)	-0.77233	1.48144	2.12190	(1)
C(2)	-1.22427	1.89355	0.71234	(1)
C(3)	-1.07805	0.76119	-0.32892	(1)
C(4)	0.39658	0.26158	-0.34462	(1)
C(5)	0.75967	-0.24417	1.09221	(1)
C(6)	0.64099	0.88730	2.11537	(1)
C(7)	2.10439	-0.96113	1.13592	(3)
C(8)	2.25661	-2.11093	0.14878	(1)
C(9)	1.92836	-1.63561	-1.28514	(1)
C(10)	0.61540	-0.86837	-1.37037	(3)
O(11)	2.95978	-0.68697	1.94911	(7)
O(12)	-0.17538	-1.09372	-2.26040	(7)
C(13)	3.65018	-2.73865	0.19955	(1)
C(14)	1.30969	1.38494	-0.83286	(3)
C(15)	-2.12591	-0.33549	-0.06868	(1)
O(16)	-3.44371	0.22317	-0.25981	(75)
C(17)	-4.48589	-0.59963	0.02642	(3)
O(18)	-4.34308	-1.73659	0.42922	(78)
C(19)	-5.79516	0.07302	-0.21508	(1)
O(20)	0.96812	2.30592	-1.54995	(78)
O(21)	2.58427	1.24329	-0.39172	(75)
C(22)	3.51336	2.26098	-0.80384	(1)
H(23)	-0.80387	2.36610	2.79943	(5)
H(24)	-1.48682	0.74065	2.54687	(5)
H(25)	-2.28081	2.24433	0.74965	(5)
H(26)	-0.62875	2.77813	0.39203	(5)
H(27)	-1.30765	1.19053	-1.33123	(5)
H(28)	0.01941	-1.02235	1.37837	(5)
H(29)	1.37871	1.68838	1.89426	(5)
H(30)	0.88016	0.50779	3.13368	(5)
H(31)	1.51451	-2.89104	0.43640	(5)
H(32)	2.75009	-0.99288	-1.66650	(5)
H(33)	1.88806	-2.51279	-1.95989	(5)
H(34)	3.73969	-3.58525	-0.51423	(5)
H(35)	4.44323	-2.00496	-0.05946	(5)
H(36)	3.88385	-3.14077	1.20864	(5)
H(37)	-1.99334	-1.18670	-0.76185	(5)
H(38)	-2.03870	-0.73295	0.95905	(5)
H(39)	-6.64038	-0.59977	0.02182	(5)
H(40)	-5.89376	0.98188	0.41448	(5)
H(41)	-5.89019	0.38170	-1.27704	(5)
H(42)	4.50932	2.03671	-0.37730	(5)
H(43)	3.60679	2.28322	-1.90682	(5)
H(44)	3.19516	3.25520	-0.43488	(5)

122tR4

C(1)	-0.93094	1.01836	2.43400	(1)
C(2)	-0.71661	2.11022	1.37684	(1)
C(3)	-0.63886	1.57057	-0.06667	(1)
C(4)	0.47692	0.47754	-0.15365	(1)
C(5)	0.20740	-0.64727	0.89972	(1)
C(6)	0.12185	-0.08894	2.32253	(1)
C(7)	1.20322	-1.79638	0.76998	(3)
C(8)	1.29530	-2.42256	-0.61644	(1)
C(9)	1.54636	-1.33252	-1.68333	(1)
C(10)	0.58624	-0.15867	-1.55115	(3)
O(11)	1.80969	-2.24004	1.72050	(7)
O(12)	0.01929	0.29229	-2.52159	(7)
C(13)	2.37081	-3.50705	-0.69373	(1)
C(14)	1.84677	1.11416	0.05658	(3)
C(15)	-2.03852	1.20531	-0.59597	(1)
O(16)	-2.56380	0.02931	0.04442	(75)
C(17)	-3.81917	-0.34238	-0.31723	(3)
O(18)	-4.48549	0.26765	-1.12919	(78)
C(19)	-4.25310	-1.57284	0.40587	(1)
O(20)	2.71467	0.70149	0.80012	(78)
O(21)	2.02078	2.21154	-0.72432	(75)
C(22)	3.29437	2.87124	-0.60810	(1)
H(23)	-0.89004	1.47086	3.45203	(5)
H(24)	-1.94954	0.58252	2.33264	(5)
H(25)	-1.52894	2.86885	1.45507	(5)
H(26)	0.22733	2.65319	1.61506	(5)
H(27)	-0.31579	2.42851	-0.70095	(5)
H(28)	-0.77477	-1.10923	0.67125	(5)
H(29)	1.10732	0.30943	2.64466	(5)
H(30)	-0.13408	-0.90520	3.03442	(5)
H(31)	0.30923	-2.89714	-0.82808	(5)
H(32)	2.58932	-0.95874	-1.59881	(5)
H(33)	1.45658	-1.77711	-2.69334	(5)
H(34)	2.41473	-3.96290	-1.70591	(5)
H(35)	3.38140	-3.10286	-0.47100	(5)
H(36)	2.17548	-4.33243	0.02400	(5)
H(37)	-2.72520	2.05816	-0.42078	(5)
H(38)	-2.01351	1.04840	-1.69047	(5)
H(39)	-5.27610	-1.87144	0.11027	(5)
H(40)	-3.57106	-2.42043	0.18539	(5)
H(41)	-4.24744	-1.40770	1.50350	(5)
H(42)	3.31307	3.74640	-1.28477	(5)
H(43)	3.45690	3.23082	0.42641	(5)
H(44)	4.11866	2.19032	-0.90099	(5)

122tR5

C(1)	0.89097	1.58454	-2.10577	(1)
C(2)	0.89486	2.39552	-0.80119	(1)
C(3)	0.82472	1.53546	0.48172	(1)
C(4)	-0.38917	0.55839	0.39844	(1)
C(5)	-0.27340	-0.30449	-0.90419	(1)
C(6)	-0.26716	0.58186	-2.15017	(1)
C(7)	-1.30804	-1.42177	-0.96000	(3)
C(8)	-1.31646	-2.35101	0.24614	(1)
C(9)	-1.45333	-1.53494	1.55134	(1)
C(10)	-0.48243	-0.36331	1.63125	(3)
O(11)	-2.01373	-1.60697	-1.92733	(7)
O(12)	0.11289	-0.12790	2.65960	(7)
C(13)	-2.41737	-3.40860	0.15651	(1)
C(14)	-1.68435	1.37124	0.44531	(3)
C(15)	2.20285	0.93239	0.81370	(1)
O(16)	2.62006	-0.02555	-0.17498	(75)
C(17)	3.84415	-0.58503	0.00811	(3)
O(18)	4.56798	-0.31002	0.94398	(78)
C(19)	4.16594	-1.55926	-1.07474	(1)
O(20)	-1.79963	2.48331	0.92395	(78)
O(21)	-2.73232	0.70726	-0.10242	(75)
C(22)	-3.99146	1.40251	-0.10432	(1)
H(23)	0.81799	2.27762	-2.97590	(5)
H(24)	1.85786	1.04660	-2.22331	(5)
H(25)	1.80000	3.04470	-0.77109	(5)
H(26)	0.02785	3.09487	-0.82300	(5)
H(27)	0.61718	2.24112	1.32058	(5)
H(28)	0.69715	-0.84028	-0.88055	(5)
H(29)	-1.22984	1.12944	-2.24119	(5)
H(30)	-0.16993	-0.04486	-3.06449	(5)
H(31)	-0.33308	-2.87519	0.26379	(5)
H(32)	-2.49162	-1.15239	1.64890	(5)
H(33)	-1.29317	-2.20567	2.41797	(5)
H(34)	-2.39997	-4.08739	1.03580	(5)
H(35)	-3.42837	-2.94980	0.11522	(5)
H(36)	-2.30284	-4.04621	-0.74621	(5)
H(37)	2.94997	1.75008	0.86935	(5)
H(38)	2.19265	0.45278	1.80990	(5)
H(39)	5.16267	-2.01338	-0.92183	(5)
H(40)	3.41672	-2.37781	-1.10361	(5)
H(41)	4.16441	-1.06090	-2.06657	(5)
H(42)	-3.91926	2.34313	-0.68386	(5)
H(43)	-4.75838	0.76201	-0.57947	(5)
H(44)	-4.31867	1.62404	0.92992	(5)

122tR7

C(1)	-0.26168	1.80878	-2.51602	(1)
C(2)	0.04790	2.51422	-1.18490	(1)
C(3)	0.61947	1.55137	-0.12153	(1)
C(4)	-0.42143	0.41139	0.12006	(1)
C(5)	-0.60956	-0.35998	-1.22406	(1)
C(6)	-1.14159	0.56626	-2.32459	(1)
C(7)	-1.44853	-1.62127	-1.05291	(3)
C(8)	-0.95728	-2.58214	0.02046	(1)
C(9)	-0.82904	-1.84295	1.36889	(1)
C(10)	-0.03190	-0.54965	1.26210	(3)
O(11)	-2.38512	-1.88178	-1.77602	(7)
O(12)	0.76080	-0.24465	2.12674	(7)
C(13)	-1.86113	-3.80736	0.16240	(1)
C(14)	-1.74209	0.98313	0.62635	(3)
C(15)	2.02785	1.11506	-0.56934	(1)
O(16)	2.62795	0.23869	0.40196	(75)
C(17)	3.83348	-0.29154	0.07243	(3)
O(18)	4.39489	-0.06145	-0.97953	(78)
C(19)	4.35300	-1.17532	1.15573	(1)
O(20)	-2.84875	0.64110	0.25902	(78)
O(21)	-1.55246	1.91956	1.59152	(75)
C(22)	-2.74564	2.49923	2.14929	(1)
H(23)	-0.76847	2.52181	-3.20709	(5)
H(24)	0.68704	1.51784	-3.02048	(5)
H(25)	0.76424	3.34885	-1.36407	(5)
H(26)	-0.89245	2.99237	-0.80296	(5)
H(27)	0.74745	2.12512	0.82412	(5)
H(28)	0.38685	-0.72605	-1.55262	(5)
H(29)	-2.17855	0.88876	-2.09179	(5)
H(30)	-1.19847	0.01243	-3.28826	(5)
H(31)	0.05553	-2.93159	-0.28587	(5)
H(32)	-1.84149	-1.60922	1.76364	(5)
H(33)	-0.35265	-2.51224	2.11162	(5)
H(34)	-1.47962	-4.50473	0.93853	(5)
H(35)	-2.89587	-3.52629	0.45317	(5)
H(36)	-1.92526	-4.38313	-0.78574	(5)
H(37)	1.99655	0.61139	-1.55227	(5)
H(38)	2.68661	2.01260	-0.68680	(5)
H(39)	5.33527	-1.60536	0.88496	(5)
H(40)	4.47574	-0.60890	2.10236	(5)
H(41)	3.65277	-2.01473	1.34906	(5)
H(42)	-2.46280	3.24537	2.91572	(5)
H(43)	-3.33444	3.01465	1.36597	(5)
H(44)	-3.36822	1.72334	2.63538	(5)

122tR6

C(1)	0.77003	-0.13821	2.62032	(1)
C(2)	1.09674	-1.22617	1.58872	(1)
C(3)	0.93889	-0.73763	0.13625	(1)
C(4)	-0.51654	-0.20134	-0.08095	(1)
C(5)	-0.80943	0.92951	0.94689	(1)
C(6)	-0.62613	0.44876	2.39017	(1)
C(7)	-2.18094	1.56097	0.70967	(3)
C(8)	-2.50660	1.95616	-0.73226	(1)
C(9)	-1.30693	1.72641	-1.66355	(1)
C(10)	-0.68092	0.34759	-1.51657	(3)
O(11)	-2.95713	1.78272	1.61372	(7)
O(12)	-0.25633	-0.25013	-2.48222	(7)
C(13)	-3.76123	1.22356	-1.24689	(1)
C(14)	-1.52637	-1.33672	0.03531	(3)
C(15)	2.02770	0.28222	-0.23063	(1)
O(16)	3.32269	-0.34273	-0.10106	(75)
C(17)	4.39424	0.46190	-0.32309	(3)
O(18)	4.29276	1.63837	-0.60760	(78)
C(19)	5.67776	-0.28251	-0.17047	(1)
O(20)	-2.55796	-1.30486	0.67632	(78)
O(21)	-1.15131	-2.42603	-0.68308	(75)
C(22)	-2.05404	-3.54608	-0.64604	(1)
H(23)	0.83313	-0.56440	3.64844	(5)
H(24)	1.53157	0.67257	2.57228	(5)
H(25)	2.13140	-1.60235	1.75755	(5)
H(26)	0.42541	-2.09886	1.76029	(5)
H(27)	1.09639	-1.61541	-0.53075	(5)
H(28)	-0.07450	1.74792	0.78465	(5)
H(29)	-1.39091	-0.31524	2.64583	(5)
H(30)	-0.78236	1.29646	3.09414	(5)
H(31)	-2.73256	3.04707	-0.72803	(5)
H(32)	-1.61521	1.89026	-2.71433	(5)
H(33)	-0.52580	2.49011	-1.45387	(5)
H(34)	-4.05882	1.58774	-2.25331	(5)
H(35)	-3.59893	0.12925	-1.33192	(5)
H(36)	-4.63276	1.37862	-0.57584	(5)
H(37)	1.89726	0.62875	-1.27415	(5)
H(38)	1.97430	1.17179	0.42385	(5)
H(39)	6.54688	0.37754	-0.34967	(5)
H(40)	5.77121	-0.70191	0.85299	(5)
H(41)	5.73318	-1.12518	-0.89081	(5)
H(42)	-1.64278	-4.36455	-1.26662	(5)
H(43)	-2.17022	-3.92202	0.38889	(5)
H(44)	-3.04384	-3.26575	-1.05551	(5)

122tR11

C(1)	0.13295	-2.27520	-2.12634	(1)
C(2)	-0.82638	-2.27133	-0.92792	(1)
C(3)	-1.09049	-0.84843	-0.39146	(1)
C(4)	0.27708	-0.22142	0.03877	(1)
C(5)	1.23031	-0.18300	-1.20165	(1)
C(6)	1.45595	-1.58035	-1.78788	(1)
C(7)	2.53583	0.54812	-0.90094	(3)
C(8)	2.37876	1.95565	-0.34041	(1)
C(9)	1.45334	1.93630	0.89591	(1)
C(10)	0.15050	1.19248	0.63648	(3)
O(11)	3.61928	0.07867	-1.17288	(7)
O(12)	-0.90694	1.66153	0.99362	(7)
C(13)	3.72322	2.59742	0.00491	(1)
C(14)	0.88618	-1.02149	1.18505	(3)
C(15)	-1.90784	-0.06485	-1.44536	(1)
O(16)	-2.65036	1.03122	-0.87160	(75)
C(17)	-3.78987	0.71479	-0.20103	(3)
O(18)	-4.21165	-0.41977	-0.10107	(78)
C(19)	-4.43758	1.92843	0.37588	(1)
O(20)	2.04376	-1.38289	1.26082	(78)
O(21)	-0.01998	-1.27087	2.16512	(75)
C(22)	0.46627	-2.01005	3.29995	(1)
H(23)	0.33081	-3.32436	-2.44677	(5)
H(24)	-0.34457	-1.76765	-2.99500	(5)
H(25)	-1.78807	-2.75481	-1.21615	(5)
H(26)	-0.40079	-2.90778	-0.11891	(5)
H(27)	-1.73142	-0.95474	0.51133	(5)
H(28)	0.74310	0.42695	-1.99202	(5)
H(29)	2.02928	-2.21270	-1.07711	(5)
H(30)	2.07377	-1.50813	-2.71074	(5)
H(31)	1.89309	2.57276	-1.13122	(5)
H(32)	1.97939	1.45879	1.75034	(5)
H(33)	1.23371	2.97565	1.20824	(5)
H(34)	3.59124	3.62793	0.39846	(5)
H(35)	4.27102	2.01780	0.77835	(5)
H(36)	4.38354	2.67387	-0.88542	(5)
H(37)	-1.25390	0.34239	-2.23614	(5)
H(38)	-2.61117	-0.74015	-1.97151	(5)
H(39)	-3.77125	2.41763	1.11664	(5)
H(40)	-4.66711	2.66946	-0.41774	(5)
H(41)	-5.38394	1.67157	0.88729	(5)
H(42)	-0.36054	-2.15395	4.02094	(5)
H(43)	0.83242	-3.00803	2.99030	(5)
H(44)	1.27758	-1.45584	3.81037	(5)

122tR13

C(1)	-0.73958	1.77668	1.95662	(1)
C(2)	-1.17527	2.00799	0.50207	(1)
C(3)	-1.03330	0.75518	-0.38997	(1)
C(4)	0.42270	0.19729	-0.29591	(1)
C(5)	0.75793	-0.09749	1.19962	(1)
C(6)	0.66958	1.17816	2.03652	(1)
C(7)	2.08181	-0.84024	1.35155	(3)
C(8)	2.22376	-2.12759	0.53551	(1)
C(9)	1.00707	-2.35208	-0.38227	(1)
C(10)	0.56294	-1.09927	-1.12407	(3)
O(11)	2.95375	-0.46509	2.10494	(7)
O(12)	0.25372	-1.14033	-2.29548	(7)
C(13)	3.53661	-2.15299	-0.26785	(1)
C(14)	1.39149	1.18884	-0.93459	(3)
C(15)	-2.11211	-0.28600	-0.05757	(1)
O(16)	-3.41390	0.28100	-0.31897	(75)
C(17)	-4.47620	-0.50612	-0.00784	(3)
O(18)	-4.36106	-1.61758	0.46829	(78)
C(19)	-5.76805	0.16949	-0.32325	(1)
O(20)	1.08289	2.08509	-1.69657	(78)
O(21)	2.67564	0.96129	-0.56696	(75)
C(22)	3.66004	1.85035	-1.12322	(1)
H(23)	-0.77042	2.74052	2.51578	(5)
H(24)	-1.46339	1.09866	2.46342	(5)
H(25)	-2.22743	2.37289	0.48348	(5)
H(26)	-0.56560	2.83803	0.07857	(5)
H(27)	-1.21527	1.06895	-1.44368	(5)
H(28)	-0.00862	-0.79490	1.60091	(5)
H(29)	1.41531	1.92458	1.68737	(5)
H(30)	0.91179	0.95646	3.09966	(5)
H(31)	2.26160	-2.96968	1.26505	(5)
H(32)	1.23033	-3.16011	-1.10506	(5)
H(33)	0.15113	-2.72023	0.22492	(5)
H(34)	3.69229	-3.13796	-0.75750	(5)
H(35)	3.54824	-1.38697	-1.07042	(5)
H(36)	4.42112	-1.97126	0.37898	(5)
H(37)	-1.98051	-1.19015	-0.68339	(5)
H(38)	-2.04728	-0.59812	1.00138	(5)
H(39)	-6.62961	-0.47441	-0.06583	(5)
H(40)	-5.86664	1.11747	0.24569	(5)
H(41)	-5.83267	0.41222	-1.40444	(5)
H(42)	3.46086	2.89605	-0.81881	(5)
H(43)	4.66029	1.56541	-0.74570	(5)
H(44)	3.67415	1.77805	-2.22793	(5)

122tR17

C(1)	0.88741	0.94498	-2.50947	(1)
C(2)	0.62624	2.05702	-1.48556	(1)
C(3)	0.55985	1.56094	-0.02813	(1)
C(4)	-0.48008	0.39255	0.10046	(1)
C(5)	-0.16940	-0.73035	-0.93252	(1)
C(6)	-0.12458	-0.19540	-2.36628	(1)
C(7)	-1.12188	-1.91399	-0.77256	(3)
C(8)	-1.30296	-2.44724	0.65034	(1)
C(9)	-0.38680	-1.71664	1.64478	(1)
C(10)	-0.45500	-0.20128	1.52741	(3)
O(11)	-1.66807	-2.44051	-1.71768	(7)
O(12)	-0.41822	0.50258	2.51376	(7)
C(13)	-2.77739	-2.37634	1.09358	(1)
C(14)	-1.89566	0.92949	-0.08724	(3)
C(15)	1.95745	1.28001	0.54913	(1)
O(16)	2.56635	0.13625	-0.07571	(75)
C(17)	3.80692	-0.19878	0.36392	(3)
O(18)	4.39105	0.41365	1.23516	(78)
C(19)	4.33622	-1.39380	-0.35498	(1)
O(20)	-2.74423	0.45296	-0.81458	(78)
O(21)	-2.12938	2.02855	0.67511	(75)
C(22)	-3.44868	2.59467	0.57597	(1)
H(23)	0.83281	1.36570	-3.54040	(5)
H(24)	1.92112	0.55060	-2.39214	(5)
H(25)	1.40850	2.84459	-1.58207	(5)
H(26)	-0.33831	2.55356	-1.74283	(5)
H(27)	0.17787	2.41933	0.57171	(5)
H(28)	0.83678	-1.14474	-0.71539	(5)
H(29)	-1.12784	0.16210	-2.68147	(5)
H(30)	0.15175	-1.01424	-3.06751	(5)
H(31)	-1.00660	-3.52106	0.63681	(5)
H(32)	-0.63780	-2.02633	2.67772	(5)
H(33)	0.66628	-2.03495	1.48043	(5)
H(34)	-2.92588	-2.85434	2.08530	(5)
H(35)	-3.13638	-1.32995	1.17958	(5)
H(36)	-3.44765	-2.89925	0.37857	(5)
H(37)	2.60179	2.17000	0.40032	(5)
H(38)	1.89169	1.11310	1.64186	(5)
H(39)	5.34735	-1.66188	0.00391	(5)
H(40)	3.67374	-2.27113	-0.20117	(5)
H(41)	4.39910	-1.20155	-1.44637	(5)
H(42)	-3.51618	3.47665	1.24057	(5)
H(43)	-3.65650	2.92587	-0.45990	(5)
H(44)	-4.21491	1.86194	0.89530	(5)

122tR15

C(1)	-0.21310	2.46201	-1.90242	(1)
C(2)	0.18830	2.82841	-0.46274	(1)
C(3)	0.73154	1.62408	0.34191	(1)
C(4)	-0.33702	0.48775	0.33763	(1)
C(5)	-0.56935	0.06858	-1.15041	(1)
C(6)	-1.13912	1.23951	-1.95619	(1)
C(7)	-1.38366	-1.21093	-1.27878	(3)
C(8)	-0.82856	-2.39951	-0.50902	(1)
C(9)	-0.67348	-2.03398	0.98200	(1)
C(10)	0.06106	-0.71874	1.21712	(3)
O(11)	-2.35279	-1.29701	-2.00066	(7)
O(12)	0.82175	-0.60505	2.15438	(7)
C(13)	-1.69234	-3.65098	-0.66921	(1)
C(14)	-1.61495	0.97757	1.01825	(3)
C(15)	2.12101	1.26177	-0.21881	(1)
O(16)	2.65412	0.09532	0.43435	(75)
C(17)	3.82894	-0.38341	-0.04885	(3)
O(18)	4.41425	0.11723	-0.98775	(78)
C(19)	4.28271	-1.58143	0.71494	(1)
O(20)	-1.67775	1.87525	1.83644	(78)
O(21)	-2.70683	0.27279	0.62916	(75)
C(22)	-3.95647	0.66262	1.22517	(1)
H(23)	-0.71627	3.33305	-2.38289	(5)
H(24)	0.69832	2.26267	-2.51000	(5)
H(25)	0.95185	3.63986	-0.48664	(5)
H(26)	-0.69432	3.26714	0.05369	(5)
H(27)	0.88318	1.95710	1.39413	(5)
H(28)	0.41716	-0.18610	-1.59377	(5)
H(29)	-2.14360	1.52061	-1.57337	(5)
H(30)	-1.27988	0.93807	-3.01807	(5)
H(31)	0.18215	-2.62000	-0.92300	(5)
H(32)	-1.67613	-1.97432	1.45750	(5)
H(33)	-0.13631	-2.85124	1.50248	(5)
H(34)	-1.26400	-4.51287	-0.11432	(5)
H(35)	-2.72346	-3.49352	-0.28676	(5)
H(36)	-1.77440	-3.96022	-1.73327	(5)
H(37)	2.07510	1.08560	-1.30891	(5)
H(38)	2.81353	2.11321	-0.05950	(5)
H(39)	5.23713	-1.97269	0.31609	(5)
H(40)	4.43489	-1.33219	1.78581	(5)
H(41)	3.52836	-2.39385	0.65796	(5)
H(42)	-4.19623	1.71547	0.98043	(5)
H(43)	-4.76468	0.02211	0.82429	(5)
H(44)	-3.92452	0.53160	2.32409	(5)

122tS1

C(1)	0.77551	0.21835	-2.59107	(1)
C(2)	1.16803	1.26346	-1.53931	(1)
C(3)	0.98643	0.74916	-0.09899	(1)
C(4)	-0.50056	0.31154	0.11712	(1)
C(5)	-0.87622	-0.77637	-0.92764	(1)
C(6)	-0.65160	-0.28972	-2.36654	(1)
C(7)	-2.29460	-1.32116	-0.73009	(3)
C(8)	-2.80778	-1.38691	0.70817	(1)
C(9)	-1.63662	-1.43346	1.69791	(1)
C(10)	-0.69902	-0.24489	1.54369	(3)
O(11)	-2.96159	-1.71847	-1.66072	(7)
O(12)	-0.10600	0.20926	2.49864	(7)
C(13)	-3.73945	-2.58685	0.91867	(1)
C(14)	-1.43107	1.51470	0.03079	(3)
C(15)	2.00796	-0.35273	0.22637	(1)
O(16)	3.34037	0.18845	0.09859	(75)
C(17)	4.35872	-0.69233	0.27802	(3)
O(18)	4.18308	-1.86862	0.52467	(78)
C(19)	5.68688	-0.02946	0.13137	(1)
O(20)	-2.46749	1.56485	-0.60132	(78)
O(21)	-0.97902	2.55981	0.77017	(75)
C(22)	-1.80045	3.74131	0.76003	(1)
H(23)	0.86014	0.66130	-3.61053	(5)
H(24)	1.48804	-0.63659	-2.56387	(5)
H(25)	2.22237	1.58225	-1.70443	(5)
H(26)	0.54817	2.17731	-1.68824	(5)
H(27)	1.21005	1.59626	0.58854	(5)
H(28)	-0.20453	-1.64912	-0.76857	(5)
H(29)	-1.37058	0.52054	-2.61372	(5)
H(30)	-0.85451	-1.11667	-3.08306	(5)
H(31)	-3.39492	-0.45956	0.90124	(5)
H(32)	-2.02670	-1.46096	2.73460	(5)
H(33)	-1.05794	-2.37171	1.55254	(5)
H(34)	-4.11187	-2.63418	1.96423	(5)
H(35)	-4.63313	-2.53662	0.26057	(5)
H(36)	-3.22409	-3.54827	0.70812	(5)
H(37)	1.86738	-0.72263	1.26004	(5)
H(38)	1.88851	-1.21730	-0.45229	(5)
H(39)	6.51240	-0.75115	0.27570	(5)
H(40)	5.79520	0.41758	-0.87883	(5)
H(41)	5.80715	0.78262	0.87845	(5)
H(42)	-1.89469	4.14454	-0.26683	(5)
H(43)	-2.80564	3.52365	1.17006	(5)
H(44)	-1.32941	4.51650	1.39355	(5)

122tS2

C(1)	0.70866	-1.26613	2.30020	(1)
C(2)	1.19074	-1.84300	0.96216	(1)
C(3)	1.04621	-0.85455	-0.21455	(1)
C(4)	-0.42569	-0.34146	-0.30723	(1)
C(5)	-0.82820	0.30277	1.05516	(1)
C(6)	-0.71698	-0.71515	2.19279	(1)
C(7)	-2.19050	0.99521	1.01215	(3)
C(8)	-2.49032	1.82957	-0.23554	(1)
C(9)	-1.22966	2.02009	-1.09121	(1)
C(10)	-0.55849	0.69998	-1.43958	(3)
O(11)	-2.97544	0.92807	1.93297	(7)
O(12)	-0.09413	0.50371	-2.54204	(7)
C(13)	-3.10021	3.18881	0.13980	(1)
C(14)	-1.34701	-1.48875	-0.71138	(3)
C(15)	2.08442	0.27394	-0.11396	(1)
O(16)	3.40943	-0.29480	-0.18795	(75)
C(17)	4.43886	0.57894	-0.04063	(3)
O(18)	4.27789	1.76764	0.15010	(78)
C(19)	5.75839	-0.10916	-0.14160	(1)
O(20)	-0.98766	-2.54371	-1.19821	(78)
O(21)	-2.65250	-1.20529	-0.48103	(75)
C(22)	-3.59400	-2.23403	-0.83338	(1)
H(23)	0.74812	-2.05586	3.08593	(5)
H(24)	1.39853	-0.45848	2.63477	(5)
H(25)	2.25091	-2.17038	1.05907	(5)
H(26)	0.61191	-2.76935	0.74622	(5)
H(27)	1.27741	-1.41151	-1.15171	(5)
H(28)	-0.10407	1.11657	1.27964	(5)
H(29)	-1.43069	-1.55180	2.03032	(5)
H(30)	-0.99470	-0.24165	3.16062	(5)
H(31)	-3.24205	1.27299	-0.84105	(5)
H(32)	-1.49348	2.55739	-2.02302	(5)
H(33)	-0.50137	2.66556	-0.55398	(5)
H(34)	-3.32188	3.79836	-0.76210	(5)
H(35)	-4.05559	3.07353	0.69489	(5)
H(36)	-2.41348	3.78279	0.77993	(5)
H(37)	1.95519	0.99514	-0.94409	(5)
H(38)	1.97057	0.83228	0.83376	(5)
H(39)	6.59303	0.60596	-0.01848	(5)
H(40)	5.85733	-0.88945	0.64163	(5)
H(41)	5.87201	-0.80151	-1.12990	(5)
H(42)	-3.39970	-3.15826	-0.25552	(5)
H(43)	-4.61694	-1.88640	-0.59479	(5)
H(44)	-3.54774	-2.45361	-1.91757	(5)

122tS4

C(1)	-0.84364	0.97641	2.50273	(1)
C(2)	-0.59801	2.10188	1.49120	(1)
C(3)	-0.54882	1.61797	0.02959	(1)
C(4)	0.51057	0.47140	-0.12580	(1)
C(5)	0.23797	-0.66928	0.89677	(1)
C(6)	0.17904	-0.15067	2.33903	(1)
C(7)	1.21928	-1.83549	0.74918	(3)
C(8)	1.68151	-2.15916	-0.67163	(1)
C(9)	0.68824	-1.60519	-1.70236	(1)
C(10)	0.48366	-0.10418	-1.55842	(3)
O(11)	1.57400	-2.49896	1.69928	(7)
O(12)	0.27820	0.59279	-2.52863	(7)
C(13)	1.87863	-3.66750	-0.86850	(1)
C(14)	1.91877	1.03136	0.04580	(3)
C(15)	-1.95609	1.32002	-0.51802	(1)
O(16)	-2.51787	0.13934	0.08169	(75)
C(17)	-3.76975	-0.20126	-0.32003	(3)
O(18)	-4.40255	0.43739	-1.13676	(78)
C(19)	-4.24498	-1.43784	0.36562	(1)
O(20)	2.78742	0.56052	0.75297	(78)
O(21)	2.12101	2.14112	-0.70998	(75)
C(22)	3.42978	2.73312	-0.62306	(1)
H(23)	-0.78683	1.38523	3.53833	(5)
H(24)	-1.87404	0.57335	2.38679	(5)
H(25)	-1.38234	2.88496	1.60563	(5)
H(26)	0.36754	2.59951	1.74216	(5)
H(27)	-0.19386	2.48822	-0.56982	(5)
H(28)	-0.75534	-1.11063	0.66971	(5)
H(29)	1.17910	0.21301	2.65845	(5)
H(30)	-0.08814	-0.98068	3.03052	(5)
H(31)	2.66592	-1.66068	-0.82875	(5)
H(32)	1.04993	-1.83020	-2.72504	(5)
H(33)	-0.29297	-2.11695	-1.59459	(5)
H(34)	2.21430	-3.90252	-1.90107	(5)
H(35)	2.64714	-4.07733	-0.17880	(5)
H(36)	0.93746	-4.23055	-0.69116	(5)
H(37)	-2.61761	2.18738	-0.31949	(5)
H(38)	-1.92160	1.19384	-1.61724	(5)
H(39)	-5.26544	-1.71057	0.03799	(5)
H(40)	-3.57339	-2.29356	0.14436	(5)
H(41)	-4.26434	-1.29571	1.46629	(5)
H(42)	3.64986	3.62339	-1.27877	(5)
H(43)	3.64546	3.05737	0.41341	(5)
H(44)	4.20618	2.01974	-0.96102	(5)

122tS3

C(1)	-0.55930	1.72413	-2.16521	(1)
C(2)	-1.31995	0.44296	-1.80431	(1)
C(3)	-1.13177	0.04144	-0.32928	(1)
C(4)	0.39466	-0.15035	-0.03211	(1)
C(5)	1.16237	1.15701	-0.37904	(1)
C(6)	0.92929	1.59541	-1.83182	(1)
C(7)	2.65637	1.07116	-0.04920	(3)
C(8)	3.04266	0.20885	1.15191	(1)
C(9)	1.86146	0.07670	2.12148	(1)
C(10)	0.62186	-0.50218	1.45426	(3)
O(11)	3.48622	1.68882	-0.68057	(7)
O(12)	-0.16558	-1.17460	2.08467	(7)
C(13)	4.27329	0.76958	1.87498	(1)
C(14)	0.94161	-1.34087	-0.80964	(3)
C(15)	-1.82503	1.04474	0.61233	(1)
O(16)	-3.21366	1.22784	0.25550	(75)
C(17)	-4.08293	0.25288	0.63111	(3)
O(18)	-3.75187	-0.73153	1.26059	(78)
C(19)	-5.47100	0.55588	0.17633	(1)
O(20)	1.95737	-1.34588	-1.47621	(78)
O(21)	0.15972	-2.44148	-0.66744	(75)
C(22)	0.60143	-3.62369	-1.35878	(1)
H(23)	-0.68371	1.94244	-3.25125	(5)
H(24)	-0.99425	2.59218	-1.62040	(5)
H(25)	-2.40176	0.57192	-2.03492	(5)
H(26)	-0.96801	-0.38457	-2.46224	(5)
H(27)	-1.64001	-0.93804	-0.18798	(5)
H(28)	0.76843	1.96756	0.27343	(5)
H(29)	1.39905	0.87097	-2.53116	(5)
H(30)	1.42429	2.57472	-2.01715	(5)
H(31)	3.30202	-0.80622	0.77216	(5)
H(32)	2.15203	-0.56643	2.97574	(5)
H(33)	1.61064	1.07307	2.54658	(5)
H(34)	4.55263	0.14256	2.74845	(5)
H(35)	5.16182	0.80819	1.20915	(5)
H(36)	4.09413	1.79922	2.25181	(5)
H(37)	-1.74911	0.73146	1.67063	(5)
H(38)	-1.33381	2.03317	0.56035	(5)
H(39)	-6.17561	-0.23887	0.48464	(5)
H(40)	-5.82687	1.51522	0.60651	(5)
H(41)	-5.51350	0.64116	-0.92958	(5)
H(42)	1.59796	-3.94115	-0.99540	(5)
H(43)	-0.11421	-4.44536	-1.16678	(5)
H(44)	0.64042	-3.44748	-2.45118	(5)

122tS5

C(1)	-0.40205	2.27600	-2.13620	(1)
C(2)	0.08243	2.77953	-0.76863	(1)
C(3)	0.67154	1.65860	0.11580	(1)
C(4)	-0.37255	0.50358	0.26889	(1)
C(5)	-0.74923	-0.02490	-1.15009	(1)
C(6)	-1.36588	1.09242	-1.99583	(1)
C(7)	-1.61198	-1.28604	-1.11259	(3)
C(8)	-1.19159	-2.36740	-0.11387	(1)
C(9)	0.16893	-2.03748	0.52161	(1)
C(10)	0.18227	-0.64714	1.13666	(3)
O(11)	-2.54806	-1.44824	-1.86485	(7)
O(12)	0.61685	-0.45598	2.25244	(7)
C(13)	-1.15812	-3.75267	-0.77810	(1)
C(14)	-1.58951	1.00244	1.04326	(3)
C(15)	2.03994	1.23872	-0.44725	(1)
O(16)	2.67964	0.31221	0.45197	(75)
C(17)	3.82881	-0.26001	0.01039	(3)
O(18)	4.30663	-0.03176	-1.08245	(78)
C(19)	4.40130	-1.18698	1.02899	(1)
O(20)	-1.63752	2.02193	1.70459	(78)
O(21)	-2.64556	0.15860	0.93485	(75)
C(22)	-3.83826	0.54593	1.63934	(1)
H(23)	-0.90434	3.10597	-2.68530	(5)
H(24)	0.47087	1.97475	-2.75868	(5)
H(25)	0.84045	3.58298	-0.91554	(5)
H(26)	-0.77054	3.26736	-0.24590	(5)
H(27)	0.86252	2.09242	1.12426	(5)
H(28)	0.18541	-0.33930	-1.66345	(5)
H(29)	-2.31856	1.43833	-1.53931	(5)
H(30)	-1.61869	0.71081	-3.01001	(5)
H(31)	-1.95751	-2.39207	0.69518	(5)
H(32)	0.40779	-2.78982	1.29790	(5)
H(33)	0.97382	-2.10900	-0.24099	(5)
H(34)	-0.85752	-4.54244	-0.05700	(5)
H(35)	-2.15276	-4.04222	-1.17933	(5)
H(36)	-0.43710	-3.78388	-1.62269	(5)
H(37)	1.93489	0.78509	-1.44965	(5)
H(38)	2.68658	2.13252	-0.55844	(5)
H(39)	5.33859	-1.64942	0.66745	(5)
H(40)	4.62676	-0.64670	1.97196	(5)
H(41)	3.68605	-2.00221	1.26588	(5)
H(42)	-3.64763	0.60952	2.72812	(5)
H(43)	-4.21495	1.51850	1.26774	(5)
H(44)	-4.62280	-0.21564	1.46998	(5)

122tS6

C(1)	0.71311	-1.58018	2.22999	(1)
C(2)	0.69955	-2.45637	0.96954	(1)
C(3)	0.66862	-1.66624	-0.35734	(1)
C(4)	-0.46546	-0.59020	-0.33794	(1)
C(5)	-0.33109	0.30823	0.93235	(1)
C(6)	-0.40730	-0.53559	2.20493	(1)
C(7)	-1.30459	1.48486	0.93320	(3)
C(8)	-1.42956	2.25866	-0.38209	(1)
C(9)	-0.37935	1.79402	-1.40371	(1)
C(10)	-0.39482	0.28633	-1.60661	(3)
O(11)	-1.90624	1.82423	1.92877	(7)
O(12)	-0.30327	-0.20105	-2.71263	(7)
C(13)	-1.32070	3.77322	-0.14472	(1)
C(14)	-1.82463	-1.28233	-0.40224	(3)
C(15)	2.06599	-1.15639	-0.74845	(1)
O(16)	2.54849	-0.17684	0.18827	(75)
C(17)	3.76567	0.36263	-0.07978	(3)
O(18)	4.42919	0.05651	-1.05000	(78)
C(19)	4.16106	1.35909	0.95742	(1)
O(20)	-2.00761	-2.46070	-0.64061	(78)
O(21)	-2.84856	-0.42394	-0.17223	(75)
C(22)	-4.16975	-0.99127	-0.21126	(1)
H(23)	1.69825	-1.07215	2.33041	(5)
H(24)	0.60426	-2.22380	3.13370	(5)
H(25)	-0.19210	-3.12239	1.01998	(5)
H(26)	1.58111	-3.13773	0.98142	(5)
H(27)	0.40625	-2.40266	-1.15339	(5)
H(28)	0.67134	0.78410	0.92412	(5)
H(29)	-1.39529	-1.04033	2.27386	(5)
H(30)	-0.31579	0.11423	3.10348	(5)
H(31)	-2.44040	2.04923	-0.80123	(5)
H(32)	0.63553	2.10445	-1.07338	(5)
H(33)	-0.55835	2.29965	-2.37251	(5)
H(34)	-0.34502	4.04675	0.31073	(5)
H(35)	-2.11918	4.14311	0.53334	(5)
H(36)	-1.41355	4.34168	-1.09463	(5)
H(37)	2.04241	-0.71940	-1.76559	(5)
H(38)	2.77201	-2.01069	-0.78404	(5)
H(39)	3.42520	2.18876	1.00693	(5)
H(40)	5.15323	1.79490	0.73664	(5)
H(41)	4.20933	0.88618	1.96044	(5)
H(42)	-4.38571	-1.41441	-1.21132	(5)
H(43)	-4.91165	-0.19681	-0.00487	(5)
H(44)	-4.28198	-1.77748	0.56021	(5)

122tS7

C(1)	0.42319	-1.98931	-2.43667	(1)
C(2)	-0.60207	-2.25836	-1.32675	(1)
C(3)	-1.01596	-0.97251	-0.58427	(1)
C(4)	0.26354	-0.30392	0.02719	(1)
C(5)	1.26542	0.02046	-1.11681	(1)
C(6)	1.64935	-1.24193	-1.90218	(1)
C(7)	2.49916	0.78686	-0.63155	(3)
C(8)	2.27170	1.81490	0.47686	(1)
C(9)	0.78605	2.19601	0.56528	(1)
C(10)	-0.08940	0.97836	0.81229	(3)
O(11)	3.59015	0.62792	-1.13475	(7)
O(12)	-1.00808	1.01937	1.60216	(7)
C(13)	3.13933	3.06345	0.27127	(1)
C(14)	0.90463	-1.20842	1.07543	(3)
C(15)	-1.83807	-0.08124	-1.53648	(1)
O(16)	-2.44792	1.03431	-0.85315	(75)
C(17)	-3.60405	0.78090	-0.18334	(3)
O(18)	-4.13143	-0.31286	-0.15423	(78)
C(19)	-4.12875	2.00701	0.48547	(1)
O(20)	2.09718	-1.39867	1.20931	(78)
O(21)	-0.01952	-1.78514	1.88583	(75)
C(22)	0.49559	-2.64306	2.91991	(1)
H(23)	0.74240	-2.95426	-2.89456	(5)
H(24)	-0.04818	-1.39904	-3.25459	(5)
H(25)	-1.50141	-2.75360	-1.75988	(5)
H(26)	-0.17179	-2.98880	-0.60418	(5)
H(27)	-1.69303	-1.27419	0.24536	(5)
H(28)	0.76358	0.70956	-1.83074	(5)
H(29)	2.24276	-1.92744	-1.25987	(5)
H(30)	2.30556	-0.97088	-2.75913	(5)
H(31)	2.57079	1.34146	1.44070	(5)
H(32)	0.63768	2.93009	1.38090	(5)
H(33)	0.46323	2.69663	-0.37304	(5)
H(34)	2.97523	3.81005	1.07735	(5)
H(35)	4.22300	2.81879	0.27421	(5)
H(36)	2.91351	3.56470	-0.69411	(5)
H(37)	-1.20621	0.32295	-2.34713	(5)
H(38)	-2.61919	-0.67795	-2.04772	(5)
H(39)	-5.05375	1.78879	1.05104	(5)
H(40)	-3.38516	2.42490	1.19481	(5)
H(41)	-4.36313	2.79282	-0.26280	(5)
H(42)	-0.34858	-3.04992	3.50812	(5)
H(43)	1.05338	-3.49343	2.48213	(5)
H(44)	1.15459	-2.07739	3.60665	(5)

122tS8

C(1)	-0.62709	0.53456	2.55912	(1)
C(2)	-0.98490	1.48344	1.40519	(1)
C(3)	-0.85422	0.81625	0.02022	(1)
C(4)	0.60574	0.29585	-0.15287	(1)
C(5)	0.90750	-0.73341	0.98342	(1)
C(6)	0.75703	-0.09712	2.36926	(1)
C(7)	2.25467	-1.42734	0.79159	(3)
C(8)	2.49483	-2.06268	-0.57348	(1)
C(9)	2.18264	-1.06015	-1.70818	(1)
C(10)	0.84201	-0.36636	-1.52151	(3)
O(11)	3.06235	-1.53623	1.68839	(7)
O(12)	0.05404	-0.27368	-2.43699	(7)
C(13)	1.65895	-3.35112	-0.73461	(1)
C(14)	1.59368	1.45551	-0.14331	(3)
C(15)	-1.94431	-0.25383	-0.16470	(1)
O(16)	-3.23799	0.38582	-0.11743	(75)
C(17)	-4.31328	-0.44235	-0.17265	(3)
O(18)	-4.21747	-1.65078	-0.24924	(78)
C(19)	-5.59390	0.32102	-0.12494	(1)
O(20)	2.64172	1.48842	0.47069	(78)
O(21)	1.18794	2.47230	-0.94665	(75)
C(22)	2.06771	3.60886	-1.01662	(1)
H(23)	-0.65503	1.09149	3.52440	(5)
H(24)	-1.39543	-0.26678	2.64310	(5)
H(25)	-2.01938	1.87059	1.54873	(5)
H(26)	-0.32020	2.37618	1.45316	(5)
H(27)	-1.04404	1.59671	-0.75119	(5)
H(28)	0.15290	-1.54619	0.91859	(5)
H(29)	1.53733	0.67697	2.52880	(5)
H(30)	0.91453	-0.86646	3.15784	(5)
H(31)	3.56739	-2.34229	-0.64047	(5)
H(32)	2.98303	-0.29004	-1.74967	(5)
H(33)	2.21011	-1.58090	-2.68436	(5)
H(34)	1.90761	-3.87996	-1.67939	(5)
H(35)	1.84643	-4.06384	0.09681	(5)
H(36)	0.56850	-3.14385	-0.75435	(5)
H(37)	-1.83491	-0.76929	-1.13677	(5)
H(38)	-1.88202	-1.02603	0.62371	(5)
H(39)	-6.46612	-0.35764	-0.16747	(5)
H(40)	-5.66560	0.91296	0.81131	(5)
H(41)	-5.66558	1.02512	-0.98002	(5)
H(42)	1.62894	4.36662	-1.69294	(5)
H(43)	2.19403	4.06914	-0.01756	(5)
H(44)	3.05585	3.31551	-1.42089	(5)

122tS10

C(1)	-0.36602	-2.39370	2.06953	(1)
C(2)	0.63102	-2.55054	0.91201	(1)
C(3)	1.08274	-1.20001	0.31264	(1)
C(4)	-0.17286	-0.37363	-0.12178	(1)
C(5)	-1.09540	-0.16893	1.12010	(1)
C(6)	-1.56050	-1.51796	1.67458	(1)
C(7)	-2.25040	0.79760	0.85977	(3)
C(8)	-1.90421	2.08026	0.09906	(1)
C(9)	-0.38357	2.22710	-0.07809	(1)
C(10)	0.22911	0.99213	-0.71848	(3)
O(11)	-3.36919	0.59091	1.27693	(7)
O(12)	0.99193	1.08164	-1.65641	(7)
C(13)	-2.49065	3.31585	0.79947	(1)
C(14)	-0.89430	-1.08192	-1.26555	(3)
C(15)	2.02291	-0.49824	1.31176	(1)
O(16)	2.62191	0.69073	0.75399	(75)
C(17)	3.70892	0.50987	-0.04288	(3)
O(18)	4.18973	-0.58074	-0.27676	(78)
C(19)	4.22411	1.80773	-0.56830	(1)
O(20)	-0.43325	-1.97808	-1.94628	(78)
O(21)	-2.13904	-0.58393	-1.47030	(75)
C(22)	-2.89262	-1.18757	-2.53643	(1)
H(23)	-0.72722	-3.39765	2.39242	(5)
H(24)	0.14723	-1.94904	2.95219	(5)
H(25)	1.51957	-3.12487	1.26175	(5)
H(26)	0.16334	-3.17974	0.12202	(5)
H(27)	1.68195	-1.42570	-0.59820	(5)
H(28)	-0.49847	0.31918	1.92071	(5)
H(29)	-2.18120	-2.04965	0.92116	(5)
H(30)	-2.20600	-1.36383	2.56770	(5)
H(31)	-2.36737	2.00530	-0.91175	(5)
H(32)	-0.16703	3.11588	-0.70165	(5)
H(33)	0.10057	2.40946	0.90508	(5)
H(34)	-2.24608	4.24958	0.24954	(5)
H(35)	-3.59799	3.26296	0.87119	(5)
H(36)	-2.09564	3.42665	1.83187	(5)
H(37)	1.48032	-0.20744	2.22894	(5)
H(38)	2.81587	-1.19297	1.65235	(5)
H(39)	5.08304	1.65134	-1.24720	(5)
H(40)	3.43796	2.35161	-1.13116	(5)
H(41)	4.56042	2.46194	0.26317	(5)
H(42)	-3.04867	-2.26675	-2.34433	(5)
H(43)	-3.88443	-0.70129	-2.59976	(5)
H(44)	-2.37798	-1.05058	-3.50710	(5)

122tS12

C(1)	0.56996	-1.39815	2.20798	(1)
C(2)	1.00214	-1.93065	0.83282	(1)
C(3)	0.92454	-0.86587	-0.28440	(1)
C(4)	-0.51881	-0.28519	-0.34290	(1)
C(5)	-0.85263	0.34124	1.05243	(1)
C(6)	-0.80541	-0.72254	2.15173	(1)
C(7)	-2.14889	1.14591	1.04408	(3)
C(8)	-2.26732	2.20749	-0.04255	(1)
C(9)	-1.94984	1.60719	-1.43155	(1)
C(10)	-0.67282	0.77876	-1.44712	(3)
O(11)	-3.01052	0.99994	1.88349	(7)
O(12)	0.13604	0.90546	-2.34033	(7)
C(13)	-1.34602	3.40957	0.25837	(1)
C(14)	-1.49407	-1.38720	-0.75362	(3)
C(15)	2.03351	0.18402	-0.09312	(1)
O(16)	3.31706	-0.46031	-0.24300	(75)
C(17)	4.40464	0.31927	-0.00951	(3)
O(18)	4.32709	1.48686	0.31613	(78)
C(19)	5.67330	-0.44125	-0.20205	(1)
O(20)	-1.20760	-2.36800	-1.41323	(78)
O(21)	-2.75522	-1.15167	-0.31378	(75)
C(22)	-3.73929	-2.14401	-0.65405	(1)
H(23)	0.54641	-2.23530	2.94370	(5)
H(24)	1.32603	-0.67412	2.58756	(5)
H(25)	2.03672	-2.33766	0.90144	(5)
H(26)	0.35792	-2.79970	0.56921	(5)
H(27)	1.13099	-1.37543	-1.25362	(5)
H(28)	-0.06234	1.08405	1.29200	(5)
H(29)	-1.58968	-1.49119	1.98244	(5)
H(30)	-1.02296	-0.26004	3.14016	(5)
H(31)	-3.31474	2.57590	-0.05273	(5)
H(32)	-2.79741	0.96898	-1.76155	(5)
H(33)	-1.87993	2.42153	-2.17809	(5)
H(34)	-1.51095	4.23716	-0.46413	(5)
H(35)	-1.53313	3.82107	1.27327	(5)
H(36)	-0.27092	3.13851	0.20295	(5)
H(37)	1.94942	0.99428	-0.84077	(5)
H(38)	1.96809	0.65241	0.90611	(5)
H(39)	6.55564	0.19680	-0.00831	(5)
H(40)	5.72080	-1.31015	0.48703	(5)
H(41)	5.74946	-0.82505	-1.24077	(5)
H(42)	-3.84510	-2.23075	-1.75272	(5)
H(43)	-3.46846	-3.12816	-0.22515	(5)
H(44)	-4.71808	-1.84240	-0.23551	(5)

122tS11

C(1)	0.55107	-1.63661	2.24291	(1)
C(2)	1.36489	-1.69645	0.94353	(1)
C(3)	1.22146	-0.42762	0.07571	(1)
C(4)	-0.28855	-0.13955	-0.20534	(1)
C(5)	-1.04886	-0.01919	1.15232	(1)
C(6)	-0.91958	-1.30835	1.96674	(1)
C(7)	-2.49960	0.43503	0.99068	(3)
C(8)	-2.75089	1.56250	-0.01343	(1)
C(9)	-1.43087	2.19809	-0.47356	(1)
C(10)	-0.44616	1.16946	-1.00944	(3)
O(11)	-3.39833	-0.03434	1.65436	(7)
O(12)	0.22301	1.39708	-1.99424	(7)
C(13)	-3.68937	2.62823	0.57292	(1)
C(14)	-0.86383	-1.23164	-1.10297	(3)
C(15)	1.96683	0.76068	0.71083	(1)
O(16)	3.36158	0.44648	0.92560	(75)
C(17)	4.18615	0.53299	-0.15131	(3)
O(18)	3.81245	0.88523	-1.25188	(78)
C(19)	5.58405	0.14877	0.20014	(1)
O(20)	-0.21301	-2.02934	-1.75046	(78)
O(21)	-2.21934	-1.22067	-1.12084	(75)
C(22)	-2.84783	-2.21828	-1.94467	(1)
H(23)	0.62453	-2.61202	2.77785	(5)
H(24)	0.98479	-0.87178	2.92617	(5)
H(25)	2.43709	-1.87753	1.18399	(5)
H(26)	1.03773	-2.58736	0.36135	(5)
H(27)	1.71571	-0.63502	-0.90016	(5)
H(28)	-0.56686	0.78639	1.74842	(5)
H(29)	-1.39768	-2.15375	1.42591	(5)
H(30)	-1.45482	-1.20567	2.93680	(5)
H(31)	-3.25269	1.11718	-0.90300	(5)
H(32)	-1.63813	2.95369	-1.25626	(5)
H(33)	-0.95894	2.74512	0.37119	(5)
H(34)	-3.87671	3.44879	-0.15213	(5)
H(35)	-4.67957	2.20296	0.84280	(5)
H(36)	-3.26396	3.08814	1.49036	(5)
H(37)	1.87669	1.67443	0.09314	(5)
H(38)	1.52787	1.01849	1.69172	(5)
H(39)	6.25198	0.22150	-0.67835	(5)
H(40)	5.98805	0.81146	0.99365	(5)
H(41)	5.62334	-0.89536	0.57476	(5)
H(42)	-2.55719	-2.09121	-3.00543	(5)
H(43)	-2.57899	-3.23623	-1.60206	(5)
H(44)	-3.94643	-2.10864	-1.87217	(5)

APPENDIX B

AM1 COORDINATES FROM HOMO-LUMO CALCULATIONS

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GEOMETRY

1	-3.0579549	6.4544297	-3.3264579
6	-1.8979375	6.7047278	-1.6178106
6	1.0508744	7.3524250	2.7009069
6	-0.4899623	4.6604286	-0.6749754
6	-1.8389768	9.0364766	-0.4010742
6	-0.3649635	9.3658611	1.7606235
6	0.9905102	5.0123908	1.4945440
1	-2.9547793	10.6229458	-1.1493612
1	-0.3169524	11.2105087	2.7170933
1	2.1265718	3.4396689	2.2429999
1	2.2223332	7.6090169	4.3990691
6	-0.5981257	2.2542276	-1.9917281
1	-1.3102680	2.3350020	-3.9597733
6	0.0635317	0.0131139	-0.9998681
1	0.7712662	-0.1747174	0.9472935
6	-0.0996552	-2.3415649	-2.4722411
6	0.2132803	-4.7272602	-1.0446145
6	0.8305912	-9.2838101	1.5574860
6	1.3465579	-6.8012795	-2.2384482
6	-0.6306618	-4.9569894	1.4515350
6	-0.3247685	-7.2321358	2.7434479
6	1.6644767	-9.0668561	-0.9336299
1	1.9677930	-6.6206807	-4.2174754
1	-1.5609398	-3.3515752	2.3920013
1	-0.9991075	-7.4079679	4.7016621
1	2.5652778	-10.6861104	-1.8755354
1	1.0771081	-11.0740427	2.5850666
8	-0.4451195	-2.3462329	-4.7907358

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GEOMETRY

1	-3.6060233	0.1493085	-4.4446094
6	-2.1893984	0.5899559	-2.9842544
6	1.4180313	1.7107147	0.7090817
6	-0.5957489	-1.3284161	-2.0827820
6	-2.0169175	3.0460673	-2.0588792
6	-0.2099921	3.6080407	-0.2074519
6	1.2109926	-0.7270356	-0.2319526
1	-3.2938591	4.5080874	-2.7949790
1	2.4961083	-2.2011045	0.4791151
1	2.8292756	2.1906769	2.1560160
6	-0.8560833	-3.8588899	-3.1022340
1	-1.9845107	-4.0093032	-4.8609909
6	0.1254271	-5.9676101	-2.0809682
1	1.2530450	-5.9373406	-0.3340501
6	-0.2329890	-8.4583207	-3.2591420
6	0.5468049	-10.6770687	-1.7396902
6	2.0239974	-14.9129987	1.0316435
6	1.5296808	-12.8020072	-2.9753644
6	0.2856039	-10.7005614	0.8916211
6	1.0161134	-12.8133030	2.2820537
6	2.2820410	-14.9153954	-1.5989189
1	1.6896449	-12.7896034	-5.0521908
1	-0.5236644	-9.0561693	1.8774345
1	0.7973816	-12.8262685	4.3501141
1	3.0636152	-16.5745868	-2.5793504
8	-1.1069524	-8.7162325	-5.4186949
17	2.9342714	-17.4850136	2.7242387
8	0.1631338	5.9595901	0.8468423
6	-1.5593379	7.8992924	0.0439708
1	-1.3293884	8.2052808	-2.0459958
1	-3.5472737	7.2858606	0.4630779
6	-0.9043063	10.2566575	1.4469544
6	0.2460188	14.7608633	3.9505356
6	-2.8354996	11.9402315	2.1043123
6	1.6014036	10.8315060	2.0573125
6	2.1709119	13.0786906	3.3102912
6	-2.2558733	14.1892122	3.3457009
1	-4.8117191	11.4891254	1.6427678
1	3.1114396	9.4900086	1.5586609
1	4.1437367	13.5215517	3.7924278
1	-3.7769318	15.5115644	3.8539345
1	0.6977818	16.5349426	4.9343917

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GEOMETRY

1	-2.7918002	6.4958260	-3.8958581
6	-1.7644408	6.7271900	-2.1003659
6	0.8595661	7.3165557	2.4483570
6	-0.4578316	4.6656267	-1.0625369
6	-1.7908663	9.0638545	-0.8934388
6	-0.4775763	9.3574481	1.3858909
6	0.8569782	4.9997375	1.2204393
1	-2.8345370	10.6471135	-1.7393335
1	1.9153179	3.4110284	2.0479169
1	1.8878061	7.5883243	4.2325218
6	-0.4930937	2.2669903	-2.3890575
1	-1.1464126	2.3479021	-4.3776114
6	0.1679298	0.0250941	-1.3963488
1	0.8266303	-0.1713040	0.5662834
6	0.0753155	-2.3163563	-2.8950864
6	0.2673690	-4.7185240	-1.4826976
6	0.6611274	-9.3166411	1.0754286
6	1.3138816	-6.8319833	-2.6823488
6	-0.6096027	-4.9367014	1.0082325
6	-0.4260480	-7.2146287	2.2955378
6	1.5313363	-9.1294859	-1.4171828
1	1.9601870	-6.6609633	-4.6558134
1	-1.4805776	-3.2999257	1.9542839
1	-1.1147388	-7.4099930	4.2450309
1	2.3694351	-10.7626655	-2.3863610
8	-0.1180316	-2.2924178	-5.2331531
8	0.7732623	-11.4820865	2.5205226
8	-0.3650148	11.5736859	2.7533165
6	1.8254511	-13.6547736	1.3329305
1	0.6862250	-14.2053542	-0.3563049
1	1.7033252	-15.1404516	2.8341666
1	3.8352846	-13.3058046	0.7911009
6	-1.6815469	13.6795486	1.7197445
1	-0.8947949	14.1951069	-0.1700004
1	-1.3211749	15.2196404	3.1250362
1	-3.7473395	13.2693873	1.5767586

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GEOMETRY

1	-3.0584297	7.6562302	-3.6906623
6	-1.9385682	7.8986550	-1.9534209
6	0.9140090	8.5251769	2.4442194
6	-0.5341042	5.8578398	-0.9987145
6	-1.9368277	10.2225788	-0.7238375
6	-0.5074391	10.5323131	1.4787413
6	0.8939973	6.2027512	1.2063883
1	-3.0512988	11.8056883	-1.4839904
1	2.0288973	4.6336138	1.9664784
1	2.0461897	8.7743917	4.1711000
6	-0.5896951	3.4628666	-2.3391348
1	-1.2344150	3.5583450	-4.3293066
6	0.0458052	1.2171622	-1.3423366
1	0.6881573	1.0152276	0.6260155
6	-0.0597312	-1.1282993	-2.8394652
6	0.1585827	-3.5253224	-1.4183054
6	0.6023670	-8.1289040	1.1803234
6	1.2900425	-5.6161962	-2.5849688
6	-0.7700807	-3.7592732	1.0468940
6	-0.5521125	-6.0447000	2.3321810
6	1.5218098	-7.8937756	-1.2897652
1	1.9824198	-5.4367760	-4.5407454
1	-1.7010736	-2.1444838	1.9710348
1	-1.2931946	-6.2164033	4.2672493
1	2.4253311	-9.5226055	-2.2139013
8	-0.2837455	-1.1067675	-5.1728512
17	-0.4946857	13.3669806	2.9856949
6	0.8176870	-10.5627267	2.5441895
1	2.5593112	-11.6052045	1.9586384
1	-0.8582059	-11.7789611	2.1088245
1	0.8890075	-10.2594217	4.6334337

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GEOMETRY

1	-3.0129999	5.2517931	-3.7350385
6	-1.8743064	5.5010580	-2.0117043
6	1.0189651	6.1537794	2.3377097
6	-0.4926353	3.4512878	-1.0432245
6	-1.8203392	7.8373429	-0.8091430
6	-0.3748044	8.1878070	1.3793939
6	0.9605217	3.8112919	1.1433769
1	-2.9173307	9.4246379	-1.5848987
1	2.0811772	2.2389063	1.9162977
1	2.1728498	6.4127593	4.0480331
6	-0.5991201	1.0408974	-2.3481554
1	-1.3222366	1.1106140	-4.3128662
6	0.0752185	-1.1957520	-1.3522936
1	0.7956887	-1.3741899	0.5908332
6	-0.0893288	-3.5528057	-2.8163182
6	0.2568285	-5.9339468	-1.3851821
6	0.9372423	-10.4693160	1.2177094
6	1.3987112	-8.0001514	-2.5832290
6	-0.5652144	-6.1659959	1.1173017
6	-0.2332611	-8.4281342	2.4222504
6	1.7541476	-10.2633543	-1.2876000
1	2.0019020	-7.8205057	-4.5688925
1	-1.5036056	-4.5673171	2.0631089
1	-0.8911354	-8.6036834	4.3871452
1	2.6625081	-11.8764150	-2.2353592
8	-0.4626368	-3.5736012	-5.1302045
6	-0.3325402	10.6661777	2.6762399
1	1.5794132	11.0596898	3.4849120
1	-1.7338451	10.6712903	4.2616551
1	-0.8319042	12.2304528	1.3475055
17	1.3620723	-13.2246168	2.8106368

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GEOMETRY

6	-2.1716587	7.7625671	-1.5174882
6	1.3055975	8.5551419	2.3780516
6	-0.3982430	5.8661163	-0.9443669
6	-2.2191418	10.0297988	-0.1613676
6	-0.4753124	10.4153028	1.7824250
6	1.3289431	6.3052014	1.0198292
1	-3.6208635	11.4982371	-0.6246792
1	2.7399146	4.8441980	1.4780127
1	2.6809762	8.8663012	3.9073434
6	-0.3111776	3.5157501	-2.3685409
1	-0.7991214	3.6507227	-4.3997777
6	0.3070457	1.2723378	-1.3593787
1	0.7866728	1.0585530	0.6545161
6	0.3941279	-1.0535747	-2.8909125
6	0.3687279	-3.4688315	-1.4862208
6	0.3582830	-8.1087863	1.0855334
6	1.5697040	-5.5828923	-2.5359454
6	-0.8566998	-3.6972608	0.8464762
6	-0.8633596	-6.0004701	2.1181814
6	1.5750666	-7.8789686	-1.2528495
1	2.4981949	-5.4062572	-4.3917328
1	-1.8435119	-2.0630039	1.6736961
1	-1.8370276	-6.1674819	3.9477613
1	2.5337213	-9.5264637	-2.0837246
8	0.5198605	-0.9966254	-5.2299327
17	-4.3328032	7.3553616	-3.8581076
17	-0.5228648	13.1672910	3.4302915
6	0.3343224	-10.5609089	2.4329056
1	2.0975330	-11.6562912	2.0401892
1	-1.3180620	-11.7156324	1.7897685
1	0.1711607	-10.2794317	4.5200438

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GEOMETRY

6	-1.7795081	6.4233416	-0.3407604
6	1.2856047	10.0515576	1.9494694
6	0.8190003	5.9354850	-0.0897173
6	-2.8327754	8.6836562	0.5357461
6	-1.2967803	10.4864862	1.6816792
6	2.3325753	7.7949071	1.0634287
1	-4.8716883	9.0365337	0.3179687
1	-2.1253614	12.2632816	2.3760983
1	2.4977270	11.4803567	2.8543085
6	1.9826888	3.6190950	-1.0290637
1	3.5169347	3.8953274	-2.4265757
6	1.3363541	1.2910650	-0.2726593
1	-0.1501468	0.9640625	1.1474831
6	2.5972088	-0.9838294	-1.2775419
6	1.2818756	-3.4150534	-0.8698774
6	-1.1157767	-8.0868928	-0.1168164
6	2.7105711	-5.6366392	-0.6789887
6	-1.3546805	-3.5487819	-0.7045412
6	-2.5411535	-5.8675532	-0.3343115
6	1.5207168	-7.9504734	-0.2924522
1	4.7834713	-5.5285126	-0.8483409
1	-2.5029538	-1.8230467	-0.8900328
1	-4.6146345	-5.9592958	-0.2110638
1	2.6575144	-9.6839605	-0.1309748
8	4.6636051	-0.8767791	-2.3762845
17	-3.7295414	4.2940694	-1.7559788
17	5.4883027	7.3181906	1.4173896
6	-2.3857569	-10.5514975	0.2607007
1	-1.1400208	-11.8926964	1.3148163
1	-2.8483781	-11.4144519	-1.6148735
1	-4.1849905	-10.3179518	1.3417663

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GEOMETRY

1	-4.5719011	-2.3420212	-5.0748950
6	-4.8124802	-1.3592810	-3.2568982
6	-5.4452008	1.1362348	1.3334837
6	-2.7147415	-0.2292855	-2.0876337
6	-7.1876074	-1.2540648	-2.1346802
6	-7.5309086	-0.0055028	0.1735587
6	-3.0650221	1.0262124	0.2197050
1	-8.8081304	-2.1584466	-3.0745098
1	-1.4526564	1.9497172	1.1546262
1	-5.6912852	2.1325330	3.1429463
6	-0.2641550	-0.3817949	-3.3125641
1	-0.3024201	-0.8858341	-5.3450091
6	1.9696655	0.0100888	-2.1718106
1	2.1159323	0.5062044	-0.1570243
6	4.3728156	-0.1810110	-3.5602255
6	6.7041433	-0.2357044	-2.0172155
6	11.1880800	-0.3074105	0.8179066
6	8.9300604	0.8017514	-3.0078370
6	6.7419490	-1.3296049	0.3900807
6	8.9680740	-1.3670579	1.7927458
6	11.1488826	0.7776982	-1.5950713
1	8.9030168	1.6249396	-4.9204697
1	5.0170730	-2.1884853	1.1747240
1	8.9842438	-2.2366053	3.6812266
1	12.8853826	1.6084482	-2.3808972
8	4.4603104	-0.2583422	-5.9020149
6	-10.0948109	0.1003153	1.3620297
1	-11.4699276	-0.9352996	0.1005327
6	-11.0005791	2.8089663	1.6114977
1	-9.7188169	3.9101001	2.8754231
1	-12.9442831	2.8445840	2.4319683
1	-11.0468786	3.7473880	-0.2771752
6	-10.0968362	-1.1997353	3.9174324
1	-8.7763990	-0.2302797	5.2476648
1	-9.4927579	-3.2111983	3.7211532
1	-12.0368905	-1.1544083	4.7461660
6	13.5578649	-0.3638124	2.3043025
1	14.7438781	1.3367742	1.8989893
1	14.6788815	-2.0861527	1.8009244
1	13.1544213	-0.4206170	4.3768438

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GEOMETRY

1	-3.9136633	1.3933545	-4.4999047
6	-2.4409006	1.8123666	-3.0898385
6	1.3081703	2.8780942	0.4761926
6	-0.8363832	-0.1266538	-2.2551507
6	-2.2091552	4.2624272	-2.1604677
6	-0.3311884	4.7964845	-0.3730684
6	1.0416136	0.4468852	-0.4676709
1	-3.4962086	5.7409744	-2.8434959
1	2.3355108	-1.0443154	0.1899585
1	2.7752805	3.3360743	1.8735957
6	-1.1579581	-2.6501009	-3.2765895
1	-2.3389930	-2.7790961	-5.0017909
6	-0.1724732	-4.7735721	-2.2926186
1	1.0065211	-4.7634880	-0.5794310
6	-0.5940545	-7.2581538	-3.4686185
6	0.1590403	-9.4932059	-1.9659490
6	1.5936529	-13.7948392	0.7881455
6	1.0211832	-11.6594017	-3.2214801
6	-0.0030544	-9.5013727	0.6736042
6	0.7056358	-11.6375046	2.0370420
6	1.7454731	-13.7863073	-1.8534926
1	1.1073242	-11.6604207	-5.3021821
1	-0.7161161	-7.8269470	1.6818106
1	0.5666040	-11.6319108	4.1115523
1	2.4338633	-15.4746431	-2.8529553
8	-1.4988839	-7.4863660	-5.6201261
6	2.3303104	-16.0703147	2.2401474
1	3.8786588	-17.1228815	1.2613753
1	0.6691072	-17.3665859	2.4326727
1	2.9928101	-15.5533647	4.1781837
8	0.1044042	7.1393264	0.6789339
6	-1.6153408	9.1040917	-0.0650915
1	-1.4523512	9.4088973	-2.1616679
1	-3.5968303	8.5195344	0.4208650
6	-0.8800954	11.4510324	1.3154887
6	0.4178951	15.9361184	3.7813557
6	-2.7613445	13.1755546	2.0115316
6	1.6498981	11.9760783	1.8676220
6	2.2931652	14.2135727	3.1021418
6	-2.1083008	15.4146473	3.2341721
1	-4.7561313	12.7644241	1.5948063
1	3.1207949	10.6035829	1.3372835
1	4.2849572	14.6166051	3.5389036
1	-3.5902724	16.7688491	3.7736978
1	0.9278054	17.7024708	4.7505072

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GEOMETRY

1	-2.9859699	6.4667078	-4.0218759
6	-1.8860512	6.7060090	-2.2719720
6	0.9093633	7.3332694	2.1447334
6	-0.5181121	4.6532407	-1.2905220
6	-1.8671411	9.0326041	-1.0492917
6	-0.4710964	9.3700153	1.1733950
6	0.8859182	5.0006282	0.9297342
1	-2.9530958	10.6222174	-1.8356990
1	1.9950795	3.4255106	1.7135759
1	2.0246816	7.5817652	3.8823221
6	-0.5867956	2.2520492	-2.6162842
1	-1.2509707	2.3368955	-4.6008757
6	0.0562049	0.0086386	-1.6167011
1	0.7185130	-0.1840828	0.3457651
6	-0.0673230	-2.3414570	-3.1003711
6	0.1861510	-4.7322171	-1.6726301
6	0.6962133	-9.3217634	0.9401684
6	1.3148874	-6.8207640	-2.8454103
6	-0.7063216	-4.9615635	0.8061788
6	-0.4554070	-7.2401767	2.0986710
6	1.5795927	-9.0913212	-1.5434553
1	1.9787333	-6.6455161	-4.8114135
1	-1.6339788	-3.3480658	1.7360909
1	-1.1680868	-7.4076309	4.0447308
1	2.4807626	-10.7183109	-2.4729565
8	-0.3350485	-2.3365685	-5.4297696
6	0.9462440	-11.7483105	2.3105458
1	2.6944460	-12.7745487	1.7160421
1	-0.7197536	-12.9833972	1.8910895
1	1.0291833	-11.4375533	4.3981762
6	-0.4674809	11.8373393	2.4916820
1	1.4196268	12.2249649	3.3590732
1	-1.9142806	11.8292800	4.0353276
1	-0.9286870	13.4121124	1.1619259

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GEOMETRY

6	-2.0533075	4.6504873	-0.5755927
6	1.1863317	7.8401425	2.1403378
6	0.4677117	3.9275494	-0.1521346
6	-2.9201716	6.9672690	0.3700398
6	-1.3163589	8.5474984	1.7261417
6	2.0971874	5.5478763	1.2012270
1	-4.8919092	7.5340556	0.0299929
1	-2.0197702	10.3577137	2.4680875
1	2.4545483	9.0943238	3.2098896
6	1.4957971	1.5589026	-1.1114564
1	3.3432707	1.7178543	-2.0851055
6	0.4035853	-0.7136271	-0.8433461
1	-1.4246453	-0.9458398	0.1252626
6	1.5739100	-3.0333541	-1.8391111
6	0.5385726	-5.4552817	-0.8961661
6	-1.3625240	-10.0833473	0.8028062
6	0.5868472	-7.5783941	-2.4781313
6	-0.4492474	-5.6698456	1.5484320
6	-1.3914201	-7.9804128	2.3926865
6	-0.3731487	-9.8803778	-1.6320748
1	1.4018339	-7.4054709	-4.3863223
1	-0.4625881	-4.0221903	2.8183884
1	-2.1572536	-8.1434907	4.3180251
1	-0.3401876	-11.5389235	-2.8844442
1	-2.1140264	-11.9026186	1.4724405
8	3.3141419	-2.9810927	-3.4091088
6	4.7691229	4.8266502	1.6350508
1	5.7243521	6.1799103	2.9457702
1	5.8269023	4.8185394	-0.1981251
1	4.8900676	2.8896587	2.4728548
6	-3.8373591	3.0413904	-2.0168876
1	-2.8234724	1.8521703	-3.4390698
1	-5.2607078	4.2274924	-3.0332244
1	-4.8760878	1.7547826	-0.6971322

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GEOMETRY

1	-3.3156966	-3.2160916	-8.1719734
6	-2.1240427	-1.5250837	-8.3934584
6	0.9066200	2.7472353	-8.9677631
6	-0.7632555	-0.5953854	-6.3117019
6	-1.9787352	-0.3174806	-10.7261562
6	-0.4639696	1.8214263	-11.0186526
6	0.7597393	1.5500407	-6.6269148
1	-3.0586931	-1.0546390	-12.3422783
1	-0.3482875	2.7710505	-12.8638199
1	1.8602998	2.2861684	-5.0236505
1	2.1100423	4.4270627	-9.1950686
6	-0.9629187	-1.8994510	-3.9041894
1	-1.6895063	-3.8613996	-3.9989069
6	-0.3676363	-0.9009721	-1.6479516
1	0.3462412	1.0426024	-1.4442596
6	-0.6202271	-2.3578204	0.7123116
6	-0.2617710	-0.9023106	3.0762150
6	0.3442680	1.9360973	7.5190576
6	1.0940241	-1.9206641	5.1216449
6	-1.3135719	1.5178498	3.2796764
6	-1.0238726	2.9241976	5.4807119
6	1.3963184	-0.4774064	7.3175484
1	-2.3993455	2.3070114	1.6888517
1	-1.8691027	4.8177796	5.6222773
1	2.4728734	-1.2626669	8.9154187
8	-1.0910361	-4.6529987	0.7142762
6	0.6456988	3.4184177	9.8734572
1	2.4774745	2.9668471	10.8233856
1	-0.9249609	2.9605638	11.2148010
1	0.5909338	5.4918361	9.4755855
6	2.1891506	-4.4942453	4.9890133
1	3.4793358	-4.8685068	6.6166472
1	3.2708149	-4.7493787	3.1906319
1	0.6327957	-5.9296856	5.0052340

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GEOMETRY

6	-2.6953481	8.2499302	-0.6329568
6	1.4290173	8.9652354	2.5688143
6	-0.8948129	6.3102301	-0.3768479
6	-2.4340392	10.5170951	0.7010923
6	-0.3716741	10.8709641	2.2978709
6	1.1663871	6.7076325	1.2450762
1	-3.8566358	12.0198912	0.4877136
1	-0.1681052	12.6573948	3.3419546
1	2.5992631	5.2120061	1.4508670
1	3.0598125	9.2450628	3.8275591
6	-1.1211103	3.9577838	-1.7819093
1	-1.9815962	4.0997131	-3.6850710
6	-0.3646009	1.7025731	-0.9002835
1	0.4770243	1.4782708	0.9901122
6	-0.6057256	-0.6262855	-2.4126527
6	-0.2065624	-3.0188959	-1.0175995
6	0.4772810	-7.5190024	1.7118615
6	1.1021896	-5.0501459	-2.1223850
6	-1.1738488	-3.2657223	1.4340513
6	-0.8455603	-5.4944294	2.7867032
6	1.4444028	-7.2749613	-0.7328034
1	-2.2242007	-1.6864045	2.2917207
1	-1.6247162	-5.6695793	4.7058128
1	2.4844197	-8.8619249	-1.5865202
8	-1.0947564	-0.5739916	-4.7025686
17	-5.2537833	7.8923079	-2.5461686
6	2.1059372	-4.8759403	-4.7303808
1	3.3996513	-6.4850916	-5.1681421
1	3.1578318	-3.0624904	-5.0032027
1	0.5006558	-4.8933930	-6.1109269
6	0.8190183	-9.9028720	3.1374142
1	2.6255907	-10.8556392	2.5980321
1	-0.7776894	-11.2252487	2.7149110
1	0.8462852	-9.5440728	5.2188418

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GEOMETRY

6	-2.2630113	7.3622767	0.7242488
6	2.9736071	7.9218839	0.5254625
6	-0.7326665	5.2334493	0.3035563
6	-1.1785742	9.7358705	1.0582561
6	1.4412316	10.0211225	0.9598525
6	1.8976053	5.5403716	0.2003696
6	-1.9273707	2.7858451	-0.0332793
6	-0.7644981	0.5441554	0.2369036
6	-2.1120828	-1.8532234	-0.1537443
6	-0.5552793	-4.1643386	0.2410293
6	2.3672279	-8.4649325	1.2520845
6	-0.3072403	-6.0658203	-1.5828714
6	0.6824867	-4.4360193	2.5671842
6	2.1268233	-6.5768871	3.0753453
6	1.1567148	-8.2074055	-1.0715296
8	-4.3744074	-1.9796910	-0.7246854
6	-1.6143162	-5.9087896	-4.1555238
9	-0.5544465	-7.4362699	-5.9752227
9	-4.1084641	-6.6149582	-4.1335994
9	-1.5967635	-3.5601907	-5.2556276
1	-4.3308300	7.1460837	0.7950375
1	3.1218844	3.8980836	-0.1595723
1	5.0386636	8.1432867	0.4347409
1	2.2944509	11.8988459	1.2185697
1	-2.3919359	11.3899818	1.3954651
1	1.2459197	0.3837173	0.7470292
1	-3.9611786	2.8340197	-0.5330511
1	0.4916858	-2.9424095	4.0044275
1	3.0763034	-6.7752040	4.9152549
1	3.5085221	-10.1588680	1.6422706
1	1.3499271	-9.6939862	-2.5183814

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GEOMETRY

1	-3.0818596	6.4433856	-3.3485443
6	-1.9131277	6.6962211	-1.6451355
6	1.0632536	7.3498386	2.6666479
6	-0.4870157	4.6595319	-0.7137027
6	-1.8717580	9.0293666	-0.4338545
6	-0.3803940	9.3527904	1.7258247
6	1.0031799	5.0179290	1.4481548
1	-3.0037386	10.6094302	-1.1748871
1	2.1557850	3.4522829	2.1887055
1	2.2441899	7.6097392	4.3591524
6	-0.5859288	2.2547221	-2.0332011
1	-1.2913025	2.3353855	-4.0035685
6	0.0773938	0.0153688	-1.0387600
1	0.7790590	-0.1717547	0.9105400
6	-0.0751324	-2.3381985	-2.5144383
6	0.2174954	-4.7258141	-1.0847899
6	0.7975621	-9.2777544	1.5140649
6	1.3487154	-6.8045275	-2.2723323
6	-0.6443760	-4.9534765	1.4048514
6	-0.3625176	-7.2235550	2.7074554
6	1.6539902	-9.0759817	-0.9784130
1	1.9837161	-6.6276763	-4.2484909
1	-1.5754237	-3.3455711	2.3421552
1	-1.0517023	-7.3957712	4.6621330
1	2.5538918	-10.6987713	-1.9178116
8	-0.3952447	-2.3429433	-4.8356372
17	1.1604677	-12.0425468	3.1045639
17	-0.3191775	12.1983505	3.2093177

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GEOMETRY

1	9.3729971	1.9135150	-4.0155088
6	9.3071397	1.3101290	-2.0253914
6	9.1576647	-0.2208777	3.0123467
6	6.9665132	0.7566466	-0.8965939
6	11.5380088	1.0960086	-0.6481221
6	11.4693592	0.3297586	1.8740007
6	6.9196271	-0.0100735	1.6401104
1	13.3588902	1.5336197	-1.5519670
1	13.2336240	0.1616239	2.9601391
1	5.1099318	-0.4492261	2.5650890
1	9.0957703	-0.8239848	5.0009459
6	4.6873854	1.0064257	-2.4035257
1	4.9706247	1.7592673	-4.3387830
6	2.3372206	0.4082788	-1.6504549
1	1.9304815	-0.3714832	0.2343024
6	0.1461548	0.7240436	-3.3332657
6	-2.3776186	0.4231231	-2.1597280
6	-7.1942447	-0.1702010	-0.0395348
6	-4.3506060	-0.6024931	-3.5949830
6	-2.8337537	1.1680189	0.3364335
6	-5.2282543	0.8777014	1.3879235
6	-6.7410039	-0.9112839	-2.5370472
1	-3.9932062	-1.1513059	-5.5717597
1	-1.3079952	2.0092810	1.4736949
1	-5.5848452	1.4478012	3.3609755
1	-8.2739012	-1.7341514	-3.6765209
8	0.3733608	1.1806956	-5.6210071
6	-9.7757436	-0.4246082	1.0482625
1	-10.6160162	1.5108536	1.3234822
1	-11.0399217	-1.5105403	-0.2687371
6	-9.7607511	-1.6976824	3.5772760
8	-11.0912331	-3.9020373	3.6352865
1	-11.0232341	-4.6241260	5.3221962
8	-8.7824237	-1.0127168	5.5804654

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GEOMETRY

1	-2.9620210	3.5362976	-2.9453170
6	-1.7666204	3.8104851	-1.2648714
6	1.2640205	4.5197155	2.9852904
6	-0.4156232	1.7538520	-0.2641324
6	-1.6069737	6.1847830	-0.1433771
6	-0.0920748	6.5453014	1.9847461
6	1.1060290	2.1386974	1.8711628
1	-2.6767856	7.7797925	-0.9393469
1	0.0334313	8.4225885	2.8680796
1	2.1939485	0.5587025	2.6730884
1	2.4645688	4.7987010	4.6592783
6	-0.6388444	-0.6927835	-1.4865417
1	-1.6032733	-0.6828350	-3.3469556
6	0.1965919	-2.8979284	-0.5474579
1	1.1522617	-3.0384648	1.2945151
6	-0.1206890	-5.2959448	-1.9179805
8	-1.2000193	-5.4466141	-3.9894964
6	0.9577043	-7.5679900	-0.6268127
1	3.0397335	-7.3202074	-0.3746693
1	0.6051138	-9.3106446	-1.7641456
1	0.0695227	-7.7955040	1.2749438

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GEOMETRY

6	-2.3065444	6.3523525	-0.4562192
6	2.3993188	7.6679938	1.5102103
6	-0.2829641	4.6436069	-0.7093364
6	-1.9915060	8.6706242	0.7678668
6	0.3645639	9.3191102	1.7473629
6	2.0754180	5.3442267	0.2919696
1	-3.5981723	9.9793846	0.9557641
1	0.6186690	11.1452510	2.7100598
1	4.2614104	8.1898001	2.2785849
6	-0.6726578	2.2587875	-2.0365649
1	-1.3880078	2.4356361	-3.9966552
6	-0.2690821	-0.0240976	-1.0165998
1	0.4221169	-0.2646428	0.9321524
6	-0.7250862	-2.3681942	-2.4472374
6	-0.2344483	-4.7368016	-1.0050275
6	0.6824926	-9.2069957	1.6936482
6	2.1618094	-5.8688286	-1.0407603
6	-2.1639165	-5.8836965	0.4045448
6	-1.7108751	-8.1120129	1.7519343
6	2.6234496	-8.0970199	0.3040406
1	-3.2408961	-8.9977917	2.8486046
1	4.5108887	-8.9709812	0.2591411
1	1.0413661	-10.9628882	2.7497848
8	-1.4550008	-2.4067700	-4.6625713
17	4.5526913	-4.5462179	-2.7254625
17	-5.0951804	-4.5787386	0.4980597
17	4.6232924	3.4063914	0.0233424
17	-5.2031460	5.6125122	-1.6306365

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GEOMETRY

1	-3.4429606	0.5238009	-5.3337422
6	-3.3205588	2.0842975	-3.9650433
6	-2.9899842	6.0603578	-0.5211375
6	-1.2985309	2.1682897	-2.2488847
6	-5.1677281	3.9577032	-3.9341549
6	-5.0068306	5.9491280	-2.2126687
6	-1.1452902	4.1796405	-0.5333343
1	-6.7534088	3.8701767	-5.2759511
1	-6.4644090	7.4304904	-2.1963633
1	0.4552865	4.2832472	0.7915050
1	-2.8487792	7.6359597	0.8271796
6	0.6235971	0.2062882	-2.3571748
1	1.2636940	-0.2716119	-4.2940652
6	1.6361864	-1.0513573	-0.3892709
6	3.5755431	-3.0103350	-0.9049535
8	4.9996942	-2.8759031	-2.7564873
6	3.6937797	-5.2290010	0.8657380
1	5.5714696	-6.1926683	0.6590585
1	2.1979980	-6.6047360	0.2474263
6	0.9646580	-0.5805133	2.2975028
6	3.2645704	-4.4923582	3.5912450
1	3.1498471	-6.2434172	4.7790956
6	0.8599660	-2.9730924	3.8663511
1	0.5680537	-2.4575544	5.9006918
1	-0.9151194	0.4026320	2.4146184
1	-0.7976616	-4.1485409	3.2640002
1	2.4154883	0.7363694	3.1253159
1	4.9114293	-3.3572924	4.2935038

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GEOMETRY

6	2.5807636	8.3829572	-2.2525358
6	-1.7872629	9.4828294	0.4795393
6	0.7384598	6.4869129	-1.9539271
6	2.2557396	10.7808657	-1.1952010
6	0.0698630	11.3208716	0.1688291
6	-1.4512121	7.0821582	-0.5740896
1	3.7211955	12.2375815	-1.4409303
1	-0.1913542	13.2088008	1.0016000
1	-3.5175180	9.9181357	1.5502274
6	1.1223755	4.0169223	-3.1174823
1	1.4068840	4.0426650	-5.1917308
6	1.1898996	1.8334748	-1.8370409
1	0.9576373	1.7593505	0.2302901
6	1.6101694	-0.6069692	-3.1172738
8	2.4242767	-0.7396077	-5.3093295
17	5.2664754	7.7796159	-3.9065417
17	-3.7885403	4.9111435	-0.1713048
6	1.0435334	-2.9057609	-1.6274957
1	-1.9422162	-1.2364643	0.6101249
6	-0.8102538	-2.9357698	0.2018213
6	1.9884546	-7.3187723	-0.8285198
6	-1.3248189	-5.1765499	1.5881398
6	2.4439596	-5.1383721	-2.1535659
6	0.0958004	-7.3917555	1.0770881
6	-3.2307359	-5.2492522	3.4823951
1	3.8833720	-5.0671427	-3.6569325
1	0.6955444	-11.3353211	2.0687528
1	3.0728859	-9.0486533	-1.2244032
6	-3.6875990	-7.4335118	4.8054707
1	-4.3257552	-3.5225945	3.8619569
1	-5.1595636	-7.4962850	6.2720491
6	-2.2658913	-9.6437872	4.2982427
1	-2.6672803	-11.3707818	5.3842836
6	-0.4172898	-9.6269341	2.4774939

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GEOMETRY

6	-3.7429440	-0.5447506	3.8235872
1	-0.0845063	1.2481663	4.1388900
6	-1.6706341	0.3439984	5.1383332
6	-5.6900317	-1.9017376	7.7570215
6	-1.5395204	0.1360234	7.8105703
6	-5.7803933	-1.6725972	5.1789844
6	-3.5676642	-1.0049801	9.1406576
6	0.5822025	1.0453587	9.1880660
1	-7.4285745	-2.3625676	4.1130545
1	-5.0105597	-2.1058889	12.8283467
1	-7.2598867	-2.7803320	8.8014174
6	0.6691593	0.8179873	11.7713045
1	2.1454767	1.9319261	8.1414662
1	2.3075956	1.5192247	12.8417741
6	-1.3550235	-0.3246824	13.0972535
1	-1.2410752	-0.4854636	15.1669277
6	-3.4278287	-1.2163103	11.8141305
6	-3.9491639	-0.3585541	1.0925832
1	-5.8867466	-0.5397107	0.3191814
6	-1.9991528	-0.0171264	-0.4973127
1	-0.0380618	0.1615013	0.1735333
6	-2.3690056	0.1585864	-3.2486387
6	-0.0658304	-0.0158090	-4.8274565
1	-1.5548685	2.4696377	-7.6893143
6	0.0603149	1.3080925	-7.0702292
6	4.1259006	-1.7185874	-5.5348533
6	2.2550868	1.1873404	-8.6105474
6	1.9952728	-1.5573589	-4.0663405
6	4.3157377	-0.3417808	-7.8348285
6	2.4328067	2.5569963	-10.9160712
1	1.8502849	-2.6443811	-2.2983276
1	8.0990698	-1.6534744	-8.7636027
1	5.7230621	-2.9198386	-4.9593768
6	4.5740870	2.4047105	-12.3736317
1	0.8212848	3.7338245	-11.5025466
1	4.7181800	3.4607266	-14.1584614
6	6.6324278	0.8806682	-11.5973828
1	8.3276089	0.7899271	-12.7978408
6	6.5098028	-0.4630609	-9.3804655
8	-4.4838897	0.4742963	-4.2098555

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GEOMETRY

6	-1.7696517	2.3968985	1.7177134
1	2.2507839	1.9395110	2.2392232
6	0.4016997	2.2268220	3.1513121
6	-4.2705797	3.0226975	5.5159027
6	0.3077115	2.4522492	5.8250463
6	-4.1333811	2.8210962	2.9373006
6	-2.0548532	2.8435895	7.0271720
6	2.5297862	2.2920884	7.3279292
1	-5.8460204	2.9753217	1.7665659
1	-3.9876214	3.3573657	10.6175865
1	-6.0964803	3.3327964	6.4608409
6	2.3905866	2.5064519	9.9102771
1	4.3561331	1.9951619	6.3791641
1	4.1066851	2.3839962	11.0775572
6	0.0303768	2.8904185	11.1096955
1	-0.0325732	3.0552930	13.1810560
6	-2.1444913	3.0561996	9.7028959
6	-1.7419932	2.2444765	-1.0257871
6	-2.9125254	3.6950801	-1.9865350
1	-0.4874421	0.5470392	-2.4514954
6	-0.6739120	0.7326682	-5.2435637
6	0.3334552	-1.3957898	-6.7436705
6	2.2045250	-5.3764760	-9.6699976
6	0.5692562	-1.1303289	-9.3681128
6	1.0375586	-3.6754282	-5.5827972
6	1.9714034	-5.6576893	-7.0620063
6	1.5040934	-3.1124607	-10.8252702
1	-0.0016183	0.6654126	-10.2561102
1	2.5248589	-7.4450112	-6.1554753
1	1.6871845	-2.8917505	-12.8835638
1	2.9438371	-6.9446232	-10.8184830
6	1.1097761	-1.5128024	-1.4100998
1	3.1476069	-0.9213226	-1.5340559
1	0.6653442	-1.8211664	0.6442083
6	0.7516534	-3.9885063	-2.8074754
1	2.1517451	-5.4062048	-2.0787001
8	-1.6338762	2.6047487	-6.2802887
1	-1.1890414	-4.7578222	-2.4079587

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GEOMETRY

1	-1.0382394	2.5630013	-7.1005658
6	-1.9973427	0.7502959	-6.7570061
6	-4.4629908	-3.8263642	-5.8859775
6	-2.5143895	-0.0084232	-4.2675003
6	-2.6837993	-0.7834287	-8.7818427
6	-3.9182504	-3.0737419	-8.3511597
6	-3.7623863	-2.3068426	-3.8512354
1	-2.2577318	-0.1825636	-10.7259907
1	-4.4661511	-4.2779252	-9.9540033
1	-4.2114529	-2.8976329	-1.9076265
1	-5.4499384	-5.6227903	-5.5410694
6	-1.8153460	1.6562437	-2.1951796
1	-2.2863765	3.6754165	-2.5063039
6	-0.6694599	0.9914034	-0.0202163
6	-0.1431564	2.9769536	1.8884471
6	1.5115771	2.2938358	4.0308462
6	4.6423218	1.1044174	8.1160890
6	1.7384361	3.9654105	6.0725391
6	2.8673533	0.0129381	4.0398052
6	4.4305915	-0.5658724	6.0914231
6	3.2957082	3.3710764	8.1089728
1	0.6718631	5.7547810	6.0354551
1	5.4948411	-2.3515739	6.1013760
1	3.4642100	4.6894311	9.7066597
1	5.8745976	0.6325379	9.7230692
8	-1.0578635	5.1282743	1.6958858
6	0.0920943	-1.6331098	0.6223879
1	0.1225957	-2.8390675	-1.1258612
6	2.6714309	-1.7505705	1.8641293
1	3.0483137	-3.7408781	2.4948477
1	-1.3611448	-2.4594802	1.9355174
1	4.1700851	-1.2457518	0.4440875

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GEOMETRY

1	8.4635907	3.5806463	-4.2115725
6	8.8518379	2.6388855	-2.3978059
6	9.8491018	0.2432628	2.1886067
6	6.9405079	1.2234768	-1.2169928
6	11.2251417	2.8616268	-1.2845396
6	11.7293567	1.6648491	1.0107118
6	7.4678212	0.0225349	1.0858209
1	12.7062772	3.9811535	-2.2199586
1	13.6066937	1.8390290	1.8854749
1	6.0016495	-1.1162517	2.0230156
1	10.2439853	-0.7106312	3.9929952
6	4.4861418	1.0335851	-2.4315683
1	4.4485544	1.5194857	-4.4683383
6	2.3309507	0.3551011	-1.2747647
1	2.2603402	-0.1359840	0.7456314
6	-0.0813715	0.2041458	-2.6517158
8	-0.1905379	0.2318547	-4.9933637
6	-2.3922978	-0.0317545	-1.0919645
1	-4.3266602	-2.2850534	-3.8786681
6	-4.4219081	-1.3957957	-1.9968165
6	-4.6902865	0.9433269	2.7471707
6	-6.6540950	-1.6646244	-0.5310403
6	-2.5445532	1.1599885	1.3082605
6	-6.7924255	-0.4830992	1.8712453
6	-8.7572291	-3.0834996	-1.4181471
1	-0.9303812	2.2836578	1.9867347
1	-9.1210860	0.1732592	5.1944778
1	-4.8223213	1.8732423	4.6026256
6	-10.8964037	-3.3098365	0.0330387
1	-8.6311914	-3.9894147	-3.2861471
1	-12.5272080	-4.4050871	-0.6470282
6	-11.0334703	-2.1318421	2.4320223
1	-12.7682062	-2.3405423	3.5591384
6	-9.0303253	-0.7496954	3.3334613

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GEOMETRY

6	-0.9177892	0.3350125	-2.9611770
1	-1.6408677	0.4620735	-4.9225019
6	-0.3800964	-1.9429835	-1.9776647
1	0.3319028	-2.1737325	-0.0367473
6	-0.6955819	-4.2824647	-3.4498780
6	-0.5149058	-6.6836931	-2.0258310
6	-0.1513960	-11.2715062	0.5695494
6	0.4791056	-8.8219803	-3.2307218
6	-1.3481977	-6.8635986	0.4780056
6	-1.1689221	-9.1541339	1.7666664
6	0.6707568	-11.1038141	-1.9294146
1	1.0918086	-8.6777953	-5.2154226
1	-2.1709740	-5.2055862	1.4273532
1	-1.8343375	-9.2901657	3.7311483
1	1.4623958	-12.7742477	-2.8800076
1	-0.0046841	-13.0743085	1.5945582
8	-1.0599308	-4.2640196	-5.7652694
6	-0.6554215	2.7263407	-1.6397619
1	1.9149185	1.3908591	1.2420163
6	0.8433646	3.0033538	0.4789605
6	-1.8162449	7.1666303	-1.4304419
6	1.0598724	5.3753079	1.7154724
6	-1.9898344	4.8616908	-2.5988441
6	-0.2881118	7.4845072	0.7574025
6	2.5991828	5.6872754	3.8967917
1	-3.1692452	4.6227452	-4.2961123
1	-1.1268313	11.4784228	1.2449449
1	-2.8537268	8.8121389	-2.1672668
6	2.7754209	7.9986294	5.0632132
1	3.6419935	4.0422420	4.6252853
1	3.9646282	8.2455927	6.7505074
6	1.4260974	10.1024748	4.1073814
1	1.5976141	11.9343745	5.0753464
6	-0.0719629	9.8543585	2.0024602

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GEOMETRY

1	0.9151895	-7.8033879	3.2751147
6	0.6997911	-5.8820821	4.0407056
1	-1.0605203	-4.3885708	0.7010223
6	-0.3809306	-4.0112532	2.6326885
6	1.3207105	-3.0263903	7.5550908
6	-0.6727281	-1.5068465	3.6258379
6	1.5676233	-5.3841393	6.5410580
6	0.1904847	-1.0159902	6.1360797
6	-1.7915952	0.4523953	2.2240075
1	2.4301583	-6.9335711	7.6255169
1	0.5974784	1.7785451	9.0954573
1	1.9762226	-2.6107995	9.4847671
6	-2.1027242	2.8711741	3.2770572
6	-3.2838531	4.8992827	1.9220615
6	-1.2111095	3.3504181	5.7804722
1	-0.7979970	6.1645832	8.7564814
6	-0.0818088	1.4032624	7.1640853
6	-3.5353980	7.2358371	2.9836629
1	-4.0124326	4.5107638	0.0102373
1	-4.4495328	8.7859243	1.9420633
6	-2.6253477	7.7139888	5.4729152
1	-2.8537364	9.6198529	6.2705305
6	-1.5030172	5.8304059	6.8286686
6	-2.6423578	-0.0346353	-0.4104896
6	-0.5944598	-0.4918608	-2.2409216
1	1.3260972	-0.5196927	-1.4417544
6	-1.0634066	-0.8268339	-4.7135040
1	-3.0471557	-0.7690318	-5.3862797
6	0.8219552	-1.2665780	-6.6574404
6	4.3366329	-2.1144616	-10.5379853
6	3.4029600	-1.5112487	-6.1068121
6	0.0263889	-1.4560229	-9.1853838
6	1.7728720	-1.8751962	-11.1072482
6	5.1448423	-1.9324996	-8.0366953
1	4.0689107	-1.3729598	-4.1414713
1	-1.9940204	-1.2696807	-9.6452321
1	1.1286071	-2.0181983	-13.0786795
1	7.1644194	-2.1211169	-7.5804927
1	5.7147771	-2.4457710	-12.0582115
8	-4.9019894	-0.0276142	-1.0169800

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GEOMETRY

6	-2.1366951	5.1744990	0.4992583
6	1.5602658	8.9236586	0.7897795
6	0.2569822	4.7015251	-0.5494412
6	-2.6783018	7.4794707	1.6741816
6	-0.8261114	9.3427654	1.8190402
6	2.0916796	6.6218016	-0.3903978
1	-4.5659554	7.8196355	2.4808290
1	-1.2497963	11.1549366	2.7477049
1	3.0218967	10.4002798	0.9039997
6	0.8651823	2.3366899	-1.8300095
1	1.4943016	2.5346347	-3.8171089
6	0.7456913	0.0543655	-0.7403171
1	0.1692420	-0.1926185	1.2447355
6	1.4056969	-2.2724145	-2.1267290
6	0.5755662	-4.6809040	-0.9739126
6	-0.9180876	-9.2857155	1.1419308
6	2.0149065	-6.8658661	-1.3835390
6	-1.6286006	-4.8214079	0.4819319
6	-2.3713550	-7.1204223	1.5312453
6	1.2737135	-9.1568004	-0.3167043
1	3.7258096	-6.7494282	-2.5645687
1	-2.7933372	-3.1235618	0.7824288
1	-4.1085530	-7.2248945	2.6676373
1	2.4157830	-10.8642313	-0.6345675
1	-1.5048460	-11.0953369	1.9806156
6	2.6179036	-2.2270822	-4.1306831
17	5.0196517	6.1655880	-1.6282911
17	-4.4726353	2.9708337	0.3409511

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GEOMETRY

6	1.0650346	-4.4048302	5.2836033
6	-1.3731490	-6.1073106	9.6510764
6	2.4759091	-5.3383884	7.3213769
6	-1.5751290	-4.3522586	5.4379833
6	-2.7861524	-5.2058846	7.6159101
6	1.2576896	-6.1742372	9.5013321
1	4.5513131	-5.4133645	7.1708379
1	-2.7040519	-3.6599843	3.8334102
1	-4.8614357	-5.1683146	7.7264700
1	2.3742650	-6.8950965	11.0995358
1	-2.3346263	-6.7707532	11.3708685
6	2.4087633	-3.5270491	2.9933601
6	1.1890906	-1.4890868	1.5409297
1	-0.3677127	-0.4832354	2.4885964
6	1.9406464	-0.8797420	-0.8022024
1	3.5166832	-1.9207616	-1.7076698
1	2.7568326	7.4886933	3.3069648
6	1.8848191	6.8954345	1.5150939
1	2.8192848	2.9748491	1.9787200
6	1.9130952	4.4217166	0.7870974
6	-0.3495030	8.0978458	-2.2832840
6	0.7834311	3.6335251	-1.5463621
6	0.7285977	8.7658310	-0.0392147
6	-0.3487021	5.5193743	-3.1131244
6	0.7868914	1.0956510	-2.3453173
1	0.7324922	10.7422844	0.6042756
1	-2.3077142	6.2927969	-6.6193370
1	-1.2417432	9.5178724	-3.5134193
6	-0.2896708	0.4194616	-4.6868237
6	-0.3130385	-2.1404363	-5.5732414
6	-1.4168939	2.3187426	-6.2357207
1	-3.3765365	3.0980471	-9.7710071
6	-1.4321195	4.8329273	-5.4220299
6	-1.3773140	-2.7526584	-7.8420638
1	0.5481985	-3.6116886	-4.3797335
1	-1.3879747	-4.7189811	-8.5178632
6	-2.4991151	-0.8521412	-9.3839662
1	-3.3415107	-1.4079973	-11.2010932
6	-2.5181235	1.6055212	-8.6043429
8	4.4701790	-4.4463739	2.3603740

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GEOMETRY

1	-1.4770782	-6.4270087	-9.1098063
6	-1.1835314	-6.8786926	-7.1015423
1	0.9026037	-3.4877330	-6.2990852
6	0.1071581	-5.2645926	-5.5596748
6	-1.8229177	-9.8257305	-3.6666570
6	0.5018214	-5.8509441	-2.9433679
6	-2.1716270	-9.1927375	-6.1412671
6	-0.4718113	-8.1825545	-1.9909197
6	1.7973131	-4.2132363	-1.3020927
1	-3.2075479	-10.4485584	-7.4337057
1	-0.8350311	-10.6273808	1.2682016
1	-2.5651125	-11.6093839	-2.8967285
6	2.1953953	-4.8710361	1.2404185
6	3.5585201	-3.2713693	2.9513051
6	1.2377501	-7.2179178	2.1687547
1	0.9087680	-9.6937070	5.4412024
6	-0.0878700	-8.8251170	0.5430007
6	3.9309996	-3.9636479	5.4074610
1	4.3057130	-1.4678652	2.2269665
1	4.9833271	-2.7347121	6.7136680
6	2.9668399	-6.3028190	6.3300338
1	3.3005980	-6.8050694	8.3193085
6	1.6619078	-7.8783645	4.7604955
6	2.7452531	-1.7474509	-2.2625420
6	1.4327968	0.4896033	-1.2501193
1	-0.0478204	0.0953388	0.1574088
6	2.0031186	2.8398327	-2.0249647
1	3.5078579	3.1006000	-3.4596494
6	0.7998598	5.1443075	-1.1493602
1	-1.4147508	3.4420541	1.8368995
6	-0.9025209	5.1893675	0.8293990
6	0.3530733	9.6902905	-1.6630435
6	-2.0351613	7.4881793	1.6256004
6	1.4253169	7.4503838	-2.3972573
6	-1.4062409	9.7692027	0.3669889
6	-3.7914657	7.5571355	3.6593993
1	2.7876783	7.3981622	-3.9690404
1	-2.0468257	13.8243833	0.1764618
1	0.8353786	11.4667930	-2.6310175
6	-4.8663792	9.8019069	4.3937022
1	-4.2682359	5.7787630	4.6263391
1	-6.2261668	9.8610482	5.9651184
6	-4.2381761	12.0781561	3.1348480
1	-5.1252380	13.8524623	3.7575211
6	-2.5466243	12.0654737	1.1661756
8	4.4890855	-1.5958150	-3.8148370

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GEOMETRY

6	-1.1678238	6.3952095	-2.0270194
6	1.5808878	7.6691096	2.2855908
6	0.0778741	4.4333710	-0.6884024
6	-1.0574215	8.9154187	-1.2324942
6	0.3198462	9.5269472	0.9241119
6	1.4569189	5.1418922	1.4879265
1	-2.0369717	10.4118053	-2.2817638
1	0.4099255	11.5067481	1.5569725
1	2.6576651	8.1954074	3.9797955
6	-0.1058571	1.8686879	-1.6316749
1	-0.5682283	1.7201772	-3.6725620
6	0.1713399	-0.2569405	-0.2700700
1	0.5966829	-0.2506936	1.7686801
6	-0.0894967	-2.7652092	-1.4271038
6	-0.2585207	-4.9057622	0.3878926
6	-0.6522963	-8.8840656	3.9101963
6	1.8859101	-5.8364143	1.6483680
6	-2.6000250	-6.0443728	0.9161234
6	-2.8048150	-8.0219165	2.6664544
6	1.6981665	-7.8172167	3.3985408
1	-4.6695739	-8.8548957	3.0479213
1	3.4120843	-8.4887118	4.3617751
1	-0.8071221	-10.4255276	5.2974477
8	-0.1750782	-3.1281015	-3.7399589
8	4.2424343	-4.7151778	1.3567920
8	-4.8102798	-5.0903968	-0.1338401
8	-2.4825957	5.6166693	-4.1405888
8	2.6607457	3.2078079	2.7497941
6	5.4255411	-5.2664082	-1.0064019
1	5.8584585	-7.3277816	-1.1355284
1	7.2041324	-4.1260494	-0.9503287
1	4.1951250	-4.6673612	-2.6149329
6	-5.3720591	-6.1143594	-2.5699970
1	-7.1552047	-5.1244529	-3.1233120
1	-5.6818726	-8.1968417	-2.4279399
1	-3.8120074	-5.6814482	-3.9271189
6	4.2806749	3.9071297	4.7815767
1	5.1164557	2.0584348	5.3856782
1	3.1672727	4.7693304	6.3539846
1	5.7876703	5.2284933	4.1213454
6	-3.7296322	7.5339033	-5.5577084
1	-2.3412775	8.9440896	-6.2920608
1	-5.2079589	8.4817994	-4.3862278
1	-4.6159643	6.4576737	-7.1499331

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GEOMETRY

1	-3.3753824	9.6454866	-2.9606290
6	-1.6350294	9.7130468	-1.8228025
6	2.7778633	9.8962000	1.0497720
6	-0.4017879	7.4525802	-1.1729672
6	-0.6744577	12.0306506	-1.0311928
6	1.5341221	12.1280458	0.4063707
6	1.8190095	7.5712997	0.2681614
1	-1.6585901	13.7884513	-1.5437951
1	2.2929647	13.9607352	1.0269055
1	2.8222803	5.8226483	0.7775742
1	4.5230799	9.9669029	2.1768622
6	-1.4614523	5.0705942	-2.0313934
1	-2.9029238	5.2205072	-3.5436909
6	-0.8448955	2.7798001	-1.1297151
1	0.5516918	2.5105565	0.3886438
6	-2.0146150	0.4491582	-2.1098157
6	-1.0869549	-1.9278956	-0.9247719
6	0.6474506	-6.3982217	1.2964713
6	0.9788077	-3.1998078	-1.9892863
6	-2.2843872	-2.8575996	1.2479310
6	-1.3872082	-5.0832728	2.3840956
6	1.8738453	-5.4238259	-0.8478673
8	-3.6439587	0.4610246	-3.7884065
6	2.1990570	-2.2240082	-4.3193511
1	4.1099226	-1.4357637	-3.8699678
1	1.0507306	-0.6994102	-5.2259453
1	2.4341422	-3.7821602	-5.7300829
6	-4.5006166	-1.5196238	2.3288125
1	-3.9772201	-0.5964567	4.1586559
1	-6.0731413	-2.8855536	2.6951411
1	-5.2304399	-0.0285060	1.0214871
6	-2.5908138	-6.0552468	4.7242401
1	-1.1479583	-6.9073487	6.0138282
1	-4.0186096	-7.5394764	4.2413257
1	-3.5681265	-4.5195834	5.7956778
6	1.4935500	-8.8328500	2.4070166
1	2.2970605	-10.1104034	0.9273331
1	-0.1153580	-9.8592400	3.3153914
1	2.9792282	-8.4854420	3.8713712
6	4.1050902	-6.7525767	-1.9089128
1	5.2908010	-7.5808060	-0.3665459
1	5.3366918	-5.4450364	-3.0202356
1	3.4765168	-8.3175724	-3.1856934

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GEOMETRY

1	-3.9366807	3.0009867	0.6428613
6	-2.7446011	4.7049350	0.5980016
6	0.2500321	9.0438909	0.4407123
6	-0.4026467	4.6411709	-0.6363206
6	-3.5769124	6.9266327	1.7418204
6	-2.0798750	9.0948976	1.6727917
6	1.0836592	6.8340259	-0.7225144
1	-5.4214531	6.9657538	2.6995660
1	-2.7376729	10.8438840	2.5829995
1	2.9147009	6.8007981	-1.7075034
1	1.4317173	10.7530933	0.3792980
6	0.4786751	2.3695308	-1.9168653
1	0.9241267	2.6254658	-3.9494212
6	0.8120825	0.0786406	-0.8695004
6	1.6486606	-2.0756310	-2.4538912
6	1.2076069	-4.5879536	-1.3545247
6	0.1928157	-9.3722051	0.6777104
6	1.9090353	-6.7799978	-2.6684322
6	0.0141497	-4.8363999	1.0064562
6	-0.5078096	-7.2321649	2.0298833
6	1.4084642	-9.1532526	-1.6589251
1	2.8509706	-6.5790097	-4.5160649
1	-1.4618012	-7.3733664	3.8687240
1	1.9634325	-10.8629794	-2.7011156
1	-0.2076299	-11.2573197	1.4614546
8	2.6058618	-1.7700400	-4.5688237
6	0.4920165	-0.4631676	1.8721285
1	2.4028966	-0.5342614	2.8041306
1	-0.7272612	0.9834499	2.8416423
8	-0.7865606	-2.7894066	2.4037220

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GEOMETRY

6	-6.8460960	-1.6339095	1.1289722
6	-9.6328764	2.6560823	-0.1560649
6	-5.7796059	0.1395770	-0.5358018
6	-9.2629590	-1.2720530	2.1377632
6	-10.6443729	0.8726194	1.4952290
6	-7.2216889	2.2849376	-1.1660203
1	-10.0700247	-2.6818674	3.4379189
1	-12.5432973	1.1598173	2.2932521
1	-10.7283497	4.3504290	-0.6634882
6	-3.2854929	-0.2016615	-1.6599304
1	-3.2507898	-0.2086415	-3.7528380
6	-1.1396249	-0.4306498	-0.3369132
1	-1.0866969	-0.4251347	1.7470548
6	1.3347775	-0.6922940	-1.5881902
6	3.5406762	0.0296371	-0.0127421
6	7.6775699	1.5040261	3.0009889
6	5.0120331	2.1494245	-0.6461700
6	4.2079002	-1.3403688	2.1637384
6	6.2687034	-0.6189962	3.6625623
6	7.0716317	2.8879040	0.8468490
1	6.7320036	-1.7270337	5.3582654
1	8.1715014	4.5656512	0.3057955
1	9.2844489	2.0860089	4.1862488
8	1.5842940	-1.4468051	-3.7878261
17	-5.2485095	-4.2977808	1.9479468
17	-6.0382317	4.4957428	-3.1738661
8	4.3064994	3.6869130	-2.6535331
8	2.7468509	-3.3523634	3.0088142
6	5.4511961	2.9868049	-4.9992440
1	7.5525360	3.1034276	-4.8490171
1	4.7120547	4.4265574	-6.3583804
1	4.8442926	1.0403795	-5.5523368
6	3.0403224	-5.5980494	1.5388009
1	1.6969474	-6.9607771	2.4360650
1	2.5170266	-5.2366994	-0.4754113
1	5.0253469	-6.3008542	1.6715089

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GEOMETRY

1	-2.8046396	10.3806129	-4.7689786
6	-1.9472865	10.6024131	-2.8866976
6	0.2378616	11.1786818	1.8738959
6	-0.6458812	8.5656915	-1.7876076
6	-2.1636781	12.8907955	-1.6066727
6	-1.0723246	13.1842152	0.7759203
6	0.4507131	8.8813670	0.6041207
1	-3.1946448	14.4714681	-2.4790709
1	-1.2414040	14.9947536	1.7825469
1	1.5021371	7.3146415	1.4789616
1	1.1094704	11.4077284	3.7472651
6	-0.4595625	6.2035528	-3.1738355
1	-0.7976224	6.3387835	-5.2361233
6	0.0523582	3.9420400	-2.1410311
1	0.3906472	3.7036147	-0.1023518
6	0.2123287	1.6329838	-3.6841651
6	0.2718748	-0.7926780	-2.2926767
6	0.4277244	-5.4459524	0.2581275
6	1.6277093	-2.8281720	-3.3056800
6	-1.0250213	-1.1051286	-0.0093879
6	-0.9497848	-3.4116230	1.2531228
6	1.7144041	-5.1302939	-2.0370121
1	2.6151251	-2.5875534	-5.1234686
1	-2.1352123	0.4652902	0.7847878
1	-1.9926719	-3.6481118	3.0370457
1	2.8038456	-6.7116205	-2.8362247
8	0.3268817	1.6973752	-6.0246437
6	0.5131437	-7.8632773	1.5919941
6	0.6759119	-12.4978739	4.1494849
6	0.3784124	-10.1429094	0.2472064
6	0.7302701	-7.9317194	4.2323145
6	0.8141556	-10.2382663	5.4991945
6	0.4565273	-12.4445728	1.5235104
1	0.1939097	-10.1092370	-1.8239492
1	0.8503207	-6.1535701	5.3035028
1	0.9912811	-10.2737920	7.5698159
1	0.3430897	-14.2231451	0.4537621
1	0.7396302	-14.3165119	5.1529973

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GEOMETRY

6	-1.9337757	0.0000000	2.2140193
1	-4.0249054	0.0000000	2.2889723
6	-0.7126379	0.0000000	-0.0139174
1	1.3682199	0.0000000	-0.1255739
6	-2.0885253	0.0000000	-2.4256627
8	-4.4293366	0.0000000	-2.5664369
6	-0.5578932	0.0000000	-4.7248064
6	-0.7159626	0.0000000	4.6322408
6	-1.6648993	0.0000000	7.0779771
1	-3.6395968	0.0000000	7.6416940
6	-1.2102203	0.0000000	-7.2630419
1	-3.1131484	0.0000000	-8.0418251
6	1.1207575	0.0000000	-8.6759147
1	1.2864508	0.0000000	-10.7219711
6	3.0554759	0.0000000	-6.9196298
1	5.1072352	0.0000000	-7.0165554
6	0.4796820	0.0000000	8.7585920
1	0.3973286	0.0000000	10.8096332
6	2.6118244	0.0000000	7.2498535
1	4.6363389	0.0000000	7.5923071
8	1.9415847	0.0000000	4.7101482
8	2.0860235	0.0000000	-4.4801417

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GEOMETRY

1	-3.1182137	6.4271063	-5.3265144
6	-2.0166110	6.6713233	-3.5783041
6	0.7700561	7.3049176	0.8455768
6	-0.6195472	4.6314038	-2.6114818
6	-2.0295745	8.9900848	-2.3428207
6	-0.6368611	9.3347198	-0.1132975
6	0.7790529	4.9826880	-0.3887609
1	-3.1498230	10.5656483	-3.1110321
1	1.9130329	3.4185328	0.3821982
1	1.8906508	7.5567069	2.5801134
6	-0.6533156	2.2381100	-3.9535605
1	-1.2883286	2.3310156	-5.9471401
6	-0.0106008	-0.0060115	-2.9558317
1	0.6217609	-0.2049597	-0.9840670
6	-0.0951460	-2.3490027	-4.4533196
6	0.1280230	-4.7459369	-3.0291956
6	0.5773590	-9.3488895	-0.4221142
6	1.2915628	-6.8268828	-4.1801148
6	-0.8300493	-4.9874241	-0.5763784
6	-0.6091783	-7.2687847	0.7145663
6	1.5240091	-9.1043693	-2.8851603
1	2.0102893	-6.6415529	-6.1260234
1	-1.7894677	-3.3807693	0.3334111
1	-1.3863536	-7.4492482	2.6353323
1	2.4612030	-10.7221416	-3.7966827
8	-0.3077166	-2.3345828	-6.7878615
6	0.8148510	-11.7402513	0.9399770
6	1.2668981	-16.3251222	3.5517726
6	0.4418747	-14.0429032	-0.3177156
6	1.4169139	-11.7602385	3.5206546
6	1.6440932	-14.0423670	4.8141571
6	0.6643491	-16.3197335	0.9860304
1	-0.0445482	-14.0465603	-2.3395462
1	1.7258427	-9.9637647	4.5213030
1	2.1235769	-14.0402367	6.8364762
1	0.3615123	-18.1165517	-0.0141362
1	1.4439754	-18.1243164	4.5766107
6	-0.6487897	11.7718287	1.1853201
6	-0.6722925	16.4455810	3.6766004
6	-0.7462683	11.8812750	3.8315816
6	-0.5629319	14.0305768	-0.1986404
6	-0.5715909	16.3515935	1.0444400
6	-0.7611361	14.2070796	5.0655293
1	-0.8272570	10.1199749	4.9342754
1	-0.4719998	13.9650752	-2.2752116
1	-0.4969043	18.1133473	-0.0565009
1	-0.8448255	14.2745743	7.1414231
1	-0.6815561	18.2794379	4.6540627

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GEOMETRY

1	-2.8941465	-0.2740462	-8.1176643
6	-0.8318436	-0.0045687	-8.0860155
6	4.3926425	0.6739261	-8.0182174
6	0.4784656	-0.1607732	-5.7815327
6	0.4597534	0.4967972	-10.3221044
6	3.0746748	0.8372687	-10.2937147
6	3.1069897	0.1793202	-5.7737666
1	-0.5848233	0.6234353	-12.1147466
1	4.0926166	1.2312214	-12.0623061
1	4.1674010	0.0457683	-3.9893550
1	6.4546764	0.9361236	-7.9900008
6	-0.9329259	-0.6855071	-3.4866417
1	-2.8860543	-1.3841321	-3.7724776
6	-0.0600203	-0.3632902	-1.1255745
1	1.8548083	0.3418447	-0.7079584
6	-1.6221431	-0.9199152	1.1044771
6	-0.6922624	0.1804424	3.5127330
6	1.0689677	2.3624971	8.0432675
6	1.6492766	-0.5220248	4.5542517
6	-2.1296695	2.0010727	4.8084373
6	-1.2618839	3.0883881	7.0630600
6	2.5271833	0.5495888	6.8111720
1	-2.4286352	4.5176650	8.0188928
1	4.3705033	-0.0385275	7.5687008
1	1.7628739	3.2210418	9.8059775
8	-3.5761728	-2.2062250	1.0165745
8	3.2605328	-2.1728669	3.2974339
8	-4.3473530	2.9231271	3.7490961
6	2.4727727	-4.7528096	3.4109240
1	2.4846800	-5.4305947	5.4086836
1	3.9255508	-5.7702262	2.2619097
1	0.5498571	-4.9751519	2.5663126
6	-6.5564994	1.5815262	4.5387009
1	-6.4587870	-0.4249308	3.8857448
1	-8.1306889	2.6148225	3.5794276
1	-6.7603061	1.6797129	6.6362989

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GEOMETRY

1	-3.9469641	2.2714414	-3.9195491
6	-2.4995476	2.6174333	-2.4654480
6	1.1599222	3.5083740	1.2154156
6	-0.8319705	0.6675711	-1.7835737
6	-2.3459947	4.9741868	-1.3144417
6	-0.5141132	5.4482458	0.5425897
6	1.0035397	1.1482823	0.0657134
1	-3.6785157	6.4777436	-1.8535753
1	2.3495860	-0.3429597	0.6048444
1	2.6210841	3.8616660	2.6531385
6	-1.0517494	-1.7682281	-3.0277265
1	-2.1397514	-1.7713813	-4.8174084
6	-0.0750267	-3.9463063	-2.1634775
1	1.0118000	-4.0517775	-0.3929105
6	-0.3836913	-6.3379642	-3.5507355
6	0.3376467	-8.6711866	-2.1856214
6	1.7102302	-13.1290302	0.2954573
6	1.3345724	-10.7065798	-3.5551276
6	0.0096893	-8.8911997	0.4296365
6	0.6913086	-11.1172823	1.6617284
6	2.0298501	-12.9222893	-2.3128749
1	1.5477091	-10.5359283	-5.6191732
1	-0.8109884	-7.3183823	1.5158209
1	0.4219045	-11.2863719	3.7156968
1	2.8218644	-14.5107218	-3.3946415
1	2.2546133	-14.8801583	1.2748840
8	-1.1711033	-6.4117910	-5.7574611
6	-0.3509333	7.9255026	1.7518938
6	-0.0384332	12.6762674	4.0721325
6	0.1348142	8.1207699	4.3499444
6	-0.6780404	10.1375149	0.3294550
6	-0.5186360	12.4970576	1.4867422
6	0.2860435	10.4845536	5.4996064
1	0.3813200	6.3961669	5.4854301
1	-1.0461154	10.0054791	-1.7130266
1	-0.7709822	14.2219771	0.3544806
1	0.6609530	10.6189488	7.5397533
1	0.0841052	14.5403563	4.9824085

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GEOMETRY

6	-2.4628385	5.0799644	-1.3527277
6	1.1434885	6.4166134	2.2501417
6	-0.6245299	3.2550672	-0.6559859
6	-2.5095150	7.4954111	-0.2764012
6	-0.6989560	8.1399688	1.5201866
6	1.1772123	3.9926834	1.1730135
1	-3.9483575	8.8847914	-0.8291077
1	-0.7280491	10.0380047	2.3717744
1	2.5537729	6.9682433	3.6692797
6	-0.6841662	0.7983277	-1.8665727
1	-1.6409650	0.7665538	-3.7337953
6	0.2365208	-1.3680515	-0.9152017
1	1.1918006	-1.4590160	0.9314148
6	0.0496609	-3.7627731	-2.3129050
6	0.5881294	-6.0973897	-0.8622242
6	1.6190146	-10.5575782	1.7777512
6	1.6381336	-8.1788540	-2.1179012
6	0.0375224	-6.2720880	1.7185134
6	0.5496139	-8.4988831	3.0296159
6	2.1614001	-10.3960422	-0.7967386
1	2.0297958	-8.0413062	-4.1581911
1	-0.8205766	-4.6593377	-2.7138622
1	0.1061007	-8.6306891	5.0556425
1	2.9936519	-12.0210935	-1.7895589
1	2.0278170	-12.3093874	2.8191484
8	-0.4958066	-3.8575086	-4.5917625
8	-4.1761427	4.2780081	-3.1472307
8	2.9487850	2.1934855	1.8196846
6	-6.0497677	6.0542886	-3.9048199
1	-7.2619103	6.6013563	-2.2659041
1	-7.1754757	4.9838821	-5.3422262
1	-5.1568674	7.7574002	-4.7744010
6	4.9585722	2.9965192	3.4191753
1	6.2073740	1.2903061	3.5178504
1	4.2233202	3.4902909	5.3353543
1	5.9922332	4.6288320	2.5712465

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GEOMETRY

1	-3.4065715	8.1549147	-3.2052038
6	-2.6243536	8.3441358	-1.2868931
6	-0.6329929	8.8360267	3.5673591
6	-1.4953321	6.2454789	-0.1154421
6	-2.7661027	10.6526496	-0.0331503
6	-1.7714360	10.9040412	2.3962326
6	-0.4946272	6.5189982	2.3233102
1	-3.6618056	12.2821252	-0.9627330
1	-1.8817142	12.7302720	3.3825615
1	0.4213490	4.9023951	3.2575401
1	0.1610831	9.0308094	5.4787615
6	-1.3852276	3.8646397	-1.4769299
1	-1.6686346	3.9960216	-3.5479288
6	-1.0005660	1.5905280	-0.4163504
1	-0.7302204	1.3467342	1.6321759
1	-0.9073312	-0.7401405	-1.9365858
8	-1.0618353	-0.7201728	-4.2728022
1	-3.6792725	-2.1228863	2.0625724
6	-2.2261752	-3.5269933	1.5626062
6	-0.6326789	-3.1091994	-0.4597558
6	-0.2389308	-7.5404634	2.4384106
6	1.2397584	-4.9387369	-1.1098874
6	-2.0386956	-5.7618435	3.0111354
6	1.4405866	-7.1644872	0.3772775
6	2.9247847	-4.6165946	-3.1813276
1	-3.3511856	-6.0474298	4.5977042
1	3.4510737	-10.7032871	0.9442236
1	-0.0683354	-9.2846008	3.5590791
6	4.7167937	-6.4118816	-3.7255554
1	2.7447382	-2.9099536	-4.3618762
1	6.0106904	-6.1561984	-5.3329029
6	4.9214108	-8.6220160	-2.2324804
1	6.3742102	-10.0316866	-2.7047645
6	3.3175462	-8.9911988	-0.2283802

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GEOMETRY

6	-0.3747999	3.0958103	-2.1172485
1	-0.7814122	3.1271057	-4.1695371
6	0.1243592	0.9090030	-0.9253990
1	0.5544646	0.8552460	1.1108210
6	0.1610474	-1.5204477	-2.2805078
6	0.2644027	-3.8283324	-0.7051661
6	0.5026776	-8.2491353	2.1788595
6	1.4929730	-5.9747382	-1.6527413
6	-0.8645252	-3.9179066	1.6850685
6	-0.7466663	-6.1255939	3.1173451
6	1.6206503	-8.1721938	-0.2070210
1	2.3420455	-5.9038456	-3.5525907
1	-1.8682525	-2.2557098	2.4316890
1	-1.6429948	-6.1906071	4.9915688
1	2.5969962	-9.8479201	-0.9546670
1	0.6003278	-9.9852934	3.3182470
8	0.1427936	-1.6404974	-4.6219182
6	-0.4331117	5.5217185	-0.9147775
6	-0.8882933	7.9333115	-1.8399885
1	-1.3146760	8.4575971	-3.7793632
6	-0.6863417	9.6425593	0.2730339
1	-0.9357825	11.6787207	0.1974045
6	-0.1223099	8.1832046	2.3642591
1	0.2109569	8.5604940	4.3548405
8	0.0454718	5.6474503	1.6977892

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GEOMETRY

1	3.4605032	6.5044618	-2.0079088
6	1.6925116	6.6697835	-0.9256982
6	-2.7944065	7.0837701	1.8111669
6	0.3661129	4.4807355	-0.2334170
6	0.7868101	9.0407979	-0.2291035
6	-1.4577338	9.2522323	1.1380958
6	-1.8886967	4.7043298	1.1343542
1	1.8447461	10.7489882	-0.7623991
1	-2.1718171	11.1267955	1.6823489
1	-2.9525794	2.9998779	1.6700484
1	-4.5677301	7.2450975	2.8838759
6	1.3359090	2.0336427	-1.0305436
1	1.7695811	1.9026858	-3.0772549
6	1.7683667	0.0066699	0.4291237
6	2.7616887	-2.3604278	-0.7237719
6	1.1567326	-4.6350353	-0.5244285
6	-1.7934635	-9.0055258	-0.2210347
6	2.2950272	-7.0232889	-0.6591266
6	-1.4681533	-4.4494660	-0.2509942
6	-2.9354960	-6.6314870	-0.1055545
6	0.8207683	-9.1993862	-0.4971780
1	4.3593385	-7.1550532	-0.9002889
1	-2.3757284	-2.5795918	-0.1564204
1	-4.9977847	-6.4780904	0.1041536
1	1.7231235	-11.0695797	-0.5926801
1	-2.9564373	-10.7245197	-0.0962207
8	4.8349740	-2.3893583	-1.7992161
35	1.3838333	-0.0990580	3.9400723

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GEOMETRY

6	-5.5854317	-2.4141878	-0.7552145
6	-8.4540414	1.3963717	1.4955294
6	-4.6591199	0.0752961	-0.7640851
6	-7.9032757	-2.9957898	0.3725650
6	-9.3261227	-1.0870858	1.4953946
6	-6.1345870	1.9712854	0.3682151
1	-8.6019198	-4.9558416	0.3681434
1	-11.1514900	-1.5427211	2.3826596
1	-9.5877788	2.9027115	2.3758296
6	-2.2791616	0.6898345	-2.0208183
1	-2.4562431	1.1544351	-4.0565487
6	0.0059781	0.7295299	-0.9161684
6	2.2844020	1.3477385	-2.4281729
6	4.7065211	0.7070682	-1.2329685
6	9.3132038	-0.6738680	0.9855892
6	6.9983116	1.2565524	-2.4461186
6	4.7658379	-0.5227761	1.1205149
6	7.0720921	-1.2277025	2.2376179
6	9.2834350	0.5745858	-1.3438409
1	6.9453993	2.2256926	-4.2898414
1	7.0638619	-2.2074425	4.0683669
1	11.0721578	1.0114066	-2.3067256
1	11.1289962	-1.2184311	1.8428198
8	2.1367703	2.3029563	-4.5600782
17	-3.8990032	-4.7724280	-2.1320667
17	-5.1239775	5.0193115	0.3771613
8	2.6102027	-1.1939903	2.4171872
6	0.4018811	0.2532304	1.8287872
1	0.5404703	2.1109933	2.8557520
1	-1.1673689	-0.9167349	2.6605144

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GEOMETRY

6	-2.4412689	0.0000000	2.2178766
1	-4.5289115	0.0000000	2.3723538
6	-1.3136516	0.0000000	-0.0496164
1	0.7583724	0.0000000	-0.2564249
6	-2.7707893	0.0000000	-2.4257823
8	-5.1077831	0.0000000	-2.4768806
1	-1.0881600	8.7392523	-5.1134852
6	-0.4992460	6.9099200	-5.9068578
1	-2.4532145	4.6863049	-3.1241144
6	-1.2406251	4.6941280	-4.8159821
6	1.8078952	4.6655279	-9.1545982
6	-0.4816936	2.3087088	-5.8526402
6	1.0531376	6.8976950	-8.1080307
6	1.0625408	2.3001237	-8.0669846
6	-1.2117819	0.0000000	-4.7660594
1	1.6200180	8.7168986	-8.9386701
1	3.0056026	0.0000000	-10.8358396
1	3.0017443	4.6244593	-10.8571406
6	-0.4816936	-2.3087088	-5.8526402
6	-1.2406251	-4.6941280	-4.8159821
6	1.0625408	-2.3001237	-8.0669846
1	3.0017443	-4.6244593	-10.8571406
6	1.8118611	0.0000000	-9.1309058
6	-0.4992460	-6.9099200	-5.9068578
1	-2.4532145	-4.6863049	-3.1241144
1	-1.0881600	-8.7392523	-5.1134852
6	1.0531376	-6.8976950	-8.1080307
1	1.6200180	-8.7168986	-8.9386701
6	1.8078952	-4.6655279	-9.1545982
1	-0.9647765	-8.7399384	4.9823158
6	-0.4777225	-6.9102410	5.8409072
1	-2.0950964	-4.6877255	2.8498713
6	-1.0963580	-4.6944356	4.6758358
6	1.4444646	-4.6637201	9.3278740
6	-0.4660329	-2.3081332	5.7924921
6	0.8155605	-6.8968287	8.2032925
6	0.8216594	-2.2988971	8.1641629
6	-1.0834800	0.0000000	4.6267237
1	1.2896233	-8.7153863	9.0914816
1	2.4436901	0.0000000	11.1335070
1	2.4416855	-4.6211218	11.1525029
6	-0.4660329	2.3081332	5.7924921
6	-1.0963580	4.6944356	4.6758358
6	0.8216594	2.2988971	8.1641629
1	2.4416855	4.6211218	11.1525029
6	1.4473321	0.0000000	9.3065835
6	-0.4777225	6.9102410	5.8409072
1	-2.0950964	4.6877255	2.8498713
1	-0.9647765	8.7399384	4.9823158
6	0.8155605	6.8968287	8.2032925
1	1.2896233	8.7153863	9.0914816
6	1.4444646	4.6637201	9.3278740

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GEOMETRY

6	-1.1031004	2.5521148	3.1607049
1	-3.9243355	5.4660040	3.5296638
6	-2.6261688	4.1729462	4.5219090
6	0.7409340	0.9477525	7.0331385
6	-2.5380533	4.2069479	7.2041015
6	0.6094785	0.9319345	4.4438194
6	-0.8365895	2.5737098	8.4783290
6	-4.1097361	5.8450983	8.6425477
1	1.8507776	-0.3161171	3.3345902
1	0.5763515	1.3387184	12.1356182
1	2.0728781	-0.2957638	8.0355834
6	-3.9853770	5.8447516	11.2343403
1	-5.4194878	7.1080369	7.6347328
1	-5.1974824	7.1097194	12.3534218
6	-2.2890116	4.2118074	12.5063077
1	-2.2245935	4.2464162	14.5841807
6	-0.7486483	2.6124359	11.1631374
6	-1.2483990	2.5434243	0.3669415
6	-0.7821751	0.1068810	-0.8914812
1	-0.7556706	-1.5739812	0.3353568
6	-0.4231750	-0.0581463	-3.3987325
1	-0.4678720	1.6733203	-4.5721572
1	-2.6015549	-4.5363227	-2.4249869
6	-1.2732008	-4.5872570	-4.0263075
6	0.0083531	-2.4233987	-4.7350303
6	0.6916413	-6.9976398	-7.3662430
6	1.7275480	-2.5055073	-6.8212699
6	-0.9337949	-6.8806959	-5.3486814
6	2.0575519	-4.8182079	-8.1405961
6	3.1447781	-0.3619415	-7.6115713
1	-1.9944072	-8.5615266	-4.7383988
1	3.9864564	-6.7282965	-11.2253964
1	0.9665593	-8.7723793	-8.4152813
6	4.7775899	-0.5144820	-9.6232254
1	2.9298197	1.4327304	-6.5819510
1	5.8657388	1.1512739	-10.2271647
6	5.0875739	-2.8174750	-10.9462975
1	6.4032952	-2.8929698	-12.5536056
6	3.7591485	-4.9228580	-10.2185532
8	-1.7736400	4.4889429	-0.8314931

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GEOMETRY

1	-2.5159353	5.8988950	-3.1670030
6	-1.5481230	5.9713748	-1.3270091
6	0.9100048	6.1680153	3.3292803
6	-0.4382825	3.7703558	-0.3386158
6	-1.4377067	8.2349173	0.0090424
6	-0.2086676	8.3387803	2.3398972
6	0.7974147	3.8958848	2.0024455
1	-2.3197521	9.9451137	-0.7773727
1	-0.1201844	10.1293254	3.3915357
1	1.6967056	2.1968033	2.7956812
1	1.8866305	6.2454027	5.1627910
6	-0.5949813	1.4435704	-1.7851747
1	-1.1481271	1.6670122	-3.7930962
6	-0.1476533	-0.8827726	-0.8704230
1	0.3804798	-1.2249856	1.1141143
6	-0.3523835	-3.1383545	-2.4761397
8	-0.9586810	-3.0559726	-4.7398238
6	0.2002096	-5.5674000	-1.2787267
6	0.1975186	-8.0172842	-2.2081162
1	-0.2478078	-8.6015291	-4.1286169
6	0.8994960	-9.6469407	-0.1381427
1	1.0776327	-11.6901517	-0.2241113
6	1.2883903	-8.0981612	1.9295947
1	1.8294028	-8.3965438	3.8883651
8	0.8744014	-5.5853550	1.2896244

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GEOMETRY

1	-1.9646487	4.9657237	1.3433263
6	-1.4876042	4.5875840	3.3337966
6	-1.8811281	2.2198166	4.3546316
6	0.1322574	6.1488514	7.3038195
6	-1.2721654	1.7398160	6.9381137
6	-0.4890716	6.5678564	4.8201209
6	-0.2360047	3.7303948	8.4111388
6	-1.6475580	-0.6588895	8.0953438
1	-0.2178722	8.4388224	3.9555209
1	1.2124574	4.8338851	12.0949078
1	0.9202915	7.6743498	8.4781896
6	-1.0101604	-1.0475453	10.5799403
1	-2.4890873	-2.1940976	6.9666684
1	-1.3090547	-2.9042717	11.4665977
6	0.0336825	0.9360817	12.0400252
1	0.5311615	0.5774503	14.0260871
6	0.4090378	3.2729104	10.9803799
6	-2.9483162	0.2007640	2.7260547
6	-1.6846769	-0.1182347	0.2657335
1	-0.0048507	1.0680286	-0.0505434
6	-2.5356603	-1.7620993	-1.4722586
1	-4.2505726	-2.8925491	-1.0630008
6	-1.3931309	-2.1931783	-3.9299559
1	2.2630004	-0.6036458	-3.0323162
6	1.0660849	-1.5083634	-4.4747181
6	-1.9032403	-3.8472943	-8.1854806
6	2.1220852	-1.9708782	-6.8980736
6	-2.8806099	-3.3910074	-5.8310063
6	0.6231748	-3.1501205	-8.7813557
6	4.6523701	-1.2778588	-7.4832373
1	-4.8352841	-3.9379551	-5.3732826
1	0.5058093	-4.5223549	-12.6536526
1	-3.0556301	-4.7640503	-9.6548442
6	5.6314738	-1.7410793	-9.8411888
1	5.8029808	-0.3663300	-6.0102135
1	7.5877339	-1.2071134	-10.2993909
6	4.1330227	-2.9167588	-11.7207772
1	4.9602632	-3.2679901	-13.5955748
6	1.6844327	-3.6070144	-11.2056560
8	-4.7749927	-1.1116553	3.3761309

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GEOMETRY

6	-2.2445321	5.7673781	-0.8645198
6	1.6125663	8.7094640	1.1984166
6	0.2470157	4.8491063	-0.9227367
6	-2.8061610	8.1121487	0.2162771
6	-0.8735662	9.5719652	1.2462984
6	2.1664749	6.3634333	0.1162723
1	-4.7682625	8.8034078	0.2474710
1	-1.3123050	11.4184550	2.0969367
1	3.1378939	9.8719161	2.0053490
6	0.8458332	2.4403389	-2.1295309
1	1.3441662	2.5835197	-4.1592122
6	0.8386722	0.1718781	-0.9867162
6	1.4716800	-2.1196325	-2.4775543
6	0.8016052	-4.5867164	-1.3568277
6	-0.4375303	-9.3119880	0.6558051
6	1.5939473	-6.8062639	-2.5663613
6	-0.6224020	-4.7416386	0.8778196
6	-1.2340624	-7.1154365	1.8690984
6	0.9788944	-9.1595439	-1.5627999
1	2.7047018	-6.6565955	-4.3230560
1	-2.3498514	-7.2410474	3.6189650
1	1.6082748	-10.8934970	-2.5201601
1	-0.9268375	-11.1698978	1.4512740
8	2.5074810	-1.9648238	-4.5741836
6	0.2722878	-0.2079071	1.7376160
1	2.1002863	-0.5679162	2.7614950
1	-0.5802490	1.5501634	2.5660181
6	-1.5103671	-2.4088207	2.1659847
1	-1.7038384	-2.7508766	4.2510675
1	-3.4415706	-1.9179171	1.4259729
17	-4.6393163	4.0395735	-2.1301368
17	5.2190708	5.3677707	0.0656580

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GEOMETRY

1	3.4657048	2.7652588	-6.6043157
6	1.9376204	1.3637275	-6.7725960
6	-1.9394248	-2.1781063	-7.2109452
6	0.5720631	0.6421590	-4.6120613
6	1.3751483	0.3107437	-9.1168157
6	-0.5637940	-1.4625168	-9.3415287
6	-1.3776673	-1.1357397	-4.8587672
1	2.4611893	0.8811179	-10.7952296
1	-1.0076881	-2.2904223	-11.1956600
1	-2.4836858	-1.7040442	-3.1914859
1	-3.4744966	-3.5694168	-7.3834849
6	1.2166888	1.7755561	-2.1972400
1	2.3772599	3.5163995	-2.2995838
6	0.5381691	0.8658879	0.0743270
1	-0.5880515	-0.8691385	0.2949317
6	1.2789343	2.1344525	2.4321902
6	0.3777207	0.8698289	4.7831139
6	-1.3073119	-1.4926218	9.2211798
6	-1.9674201	1.5018641	5.8439989
6	1.8641562	-0.9663429	5.9847812
6	1.0278058	-2.1470930	8.1968860
6	-2.8116213	0.3266993	8.0559408
1	2.2130347	-3.5824577	9.1258860
1	-4.6535596	0.8423177	8.8742628
1	-1.9663885	-2.4161801	10.9647573
8	2.5477640	4.0928815	2.5062470
17	-3.8303486	3.7160372	4.4534031
17	4.7181830	-1.7908719	4.7678082

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GEOMETRY

1	-3.6231492	5.5592200	-2.3965315
6	-2.1809393	5.8740426	-0.9311094
6	1.4856535	6.6887091	2.7654343
6	-0.4145812	3.9659738	-0.3955111
6	-2.1187788	8.1526182	0.3828742
6	-0.2867273	8.5648755	2.2342732
6	1.4249422	4.4016140	1.4614562
1	-3.5148149	9.6323790	-0.0446295
1	-0.2372829	10.3680133	3.2669918
1	2.8453673	2.9413522	1.8777239
1	2.9404720	7.0137696	4.2141548
6	-0.5338231	1.6099548	-1.8008836
1	-1.5517838	1.7010188	-3.6278791
6	0.4537366	-0.5969971	-1.0316131
1	1.4967438	-0.7675154	0.7582614
6	0.2439725	-2.9042451	-2.5794837
8	0.0120761	-2.8179280	-4.9109468
6	0.3360242	-5.3294628	-1.2575247
6	0.6268042	-7.7399263	-2.3660192
1	0.8331917	-8.0999535	-4.3781271
6	0.5959498	-9.5543374	-0.3710512
1	0.7834944	-11.5877711	-0.5611730
6	0.2739642	-8.2129631	1.9028354
1	0.1427763	-8.9133226	3.8369336
7	0.1337331	-5.6594691	1.3624050
1	-0.1670223	-4.2896493	2.5891392

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GEOMETRY

6	-0.0368809	0.5976261	2.9055773
1	1.2859104	1.2713985	4.3798501
6	0.7579288	-1.0752118	1.1695538
1	-0.4900490	-1.7882169	-0.3370237
6	3.3544988	-2.0745996	1.1670296
8	4.9707048	-1.3990769	2.7194218
1	4.9418550	-6.7779687	2.0469640
6	4.6786156	-6.3897191	0.0190256
6	3.9004672	-4.0302531	-0.7700350
6	4.8643354	-7.8779441	-4.2929707
6	3.6302636	-3.4952112	-3.3980741
6	5.1497065	-8.3308944	-1.7548156
6	4.1127141	-5.4524692	-5.1693726
6	2.9352386	-1.0657700	-4.3174088
1	5.7511505	-10.1983505	-1.0672302
1	4.2216814	-6.4844780	-9.1454945
1	5.2222690	-9.3757862	-5.6912599
6	2.7038992	-0.6259985	-6.8637791
1	2.5965589	0.4648528	-2.9478574
1	2.1675103	1.2561912	-7.5655325
6	3.1594006	-2.5876969	-8.6245538
1	2.9580161	-2.1912725	-10.6550249
6	3.8507905	-4.9460425	-7.7960924
1	-4.3253096	-1.9045912	1.8587358
6	-4.6331685	0.0717911	2.4348164
6	-2.5950843	1.6013899	3.0124753
6	-7.5783625	3.4413042	3.3289482
6	-3.0134101	4.1668681	3.7612540
6	-7.1328482	0.9931815	2.5969331
6	-5.5321838	5.0776667	3.9208163
6	-0.9993169	5.8555340	4.3264979
1	-8.7079976	-0.2818444	2.1313306
1	-7.9372548	8.2954048	4.7861548
1	-9.5181037	4.1788399	3.4682279
6	-1.4768810	8.3052604	5.0383921
1	0.9633411	5.1827612	4.1755616
1	0.0895098	9.6004065	5.4764546
6	-3.9902225	9.2010447	5.2150124
1	-4.3261742	11.1692400	5.7927806
6	-5.9731190	7.6226342	4.6647114

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GEOMETRY

6	-0.2349149	2.8986252	-2.0568672
1	-0.5212662	2.9520003	-4.1314220
6	0.1343844	0.6700243	-0.8878916
1	0.4318082	0.5150272	1.1627360
6	0.1941282	-1.7184867	-2.3025469
6	0.2327428	-4.0649536	-0.7762882
6	0.3465407	-8.5436272	2.0230936
6	1.6056352	-6.1510484	-1.6551810
6	-1.1028742	-4.2436855	1.4993158
6	-1.0474382	-6.4802718	2.8895166
6	1.6712469	-8.3775075	-0.2495532
1	2.6155509	-6.0124446	-3.4705329
1	-2.2231345	-2.6292353	2.1805588
1	-2.1093643	-6.6177557	4.6708862
1	2.7606963	-10.0067352	-0.9418160
1	0.3936406	-10.3033976	3.1286766
8	0.2469608	-1.7906541	-4.6453176
6	-0.3114052	5.3301902	-0.8555412
6	-0.8296585	7.6780674	-2.0222154
1	-1.2445755	7.9611888	-4.0122886
6	-0.7058242	9.5760430	-0.1124988
1	-1.0096926	11.5888895	-0.3651595
6	-0.1139150	8.3532451	2.1739605
1	0.1493689	9.1427002	4.0594160
7	0.1165027	5.7890339	1.7203988
1	0.5548512	4.4847682	2.9765610

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GEOMETRY

1	-2.0505778	6.8254511	-3.7674435
6	-1.3786651	6.9821092	-1.8090846
6	0.3170859	7.1784234	3.0693014
6	-0.6480755	4.7904566	-0.4620512
6	-1.2266087	9.3311637	-0.6204458
6	-0.3656196	9.4522190	1.8655469
7	0.1924630	4.8978773	1.9667316
1	-1.7805411	11.0582577	-1.6355457
1	-0.2181389	11.2595206	2.8718127
1	1.0075135	7.1831566	5.0409108
6	-0.8271000	2.3540424	-1.7687271
1	-1.8338850	2.4151890	-3.6006872
6	0.1289417	0.1680533	-0.9123598
1	1.1686799	0.0313103	0.8873142
6	-0.1340344	-2.2004029	-2.3601968
6	0.2917772	-4.5780152	-0.9528230
6	1.1075960	-9.1284490	-1.6053049
6	1.1700306	-6.7064154	-2.2620500
6	-0.1956339	-4.7496912	1.6412735
6	0.2087816	-7.0219026	2.9109346
6	1.5866827	-8.9691341	-0.9813519
1	1.5141978	-6.5679747	-4.3110733
1	-0.9182362	-3.0994458	2.6828391
1	-0.1831457	-7.1504951	4.9481814
1	2.2864586	-10.6305713	-2.0158269
1	1.4333094	-10.9160055	2.6155734
8	-0.6532559	-2.2087267	-4.6460575

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GEOMETRY

1	-4.2280552	0.0000000	6.6494070
6	-2.1651853	0.0000000	6.8847824
6	2.9879486	0.0000000	7.2799332
6	-0.5687499	0.0000000	4.7384033
6	-1.0850285	0.0000000	9.2902981
6	1.5394892	0.0000000	9.5131863
7	1.9953070	0.0000000	4.9468425
1	-2.2921806	0.0000000	10.9822428
1	2.4671256	0.0000000	11.3678553
1	5.0752895	0.0000000	7.3638422
6	-1.7699682	0.0000000	2.2427144
1	-3.8612662	0.0000000	2.2846591
6	-0.5385165	0.0000000	0.0225811
1	1.5421975	0.0000000	-0.0877409
6	-1.9493468	0.0000000	-2.3742699
6	-0.4972639	0.0000000	-4.8079613
6	2.0173315	0.0000000	-9.3702212
6	-1.9025014	0.0000000	-7.0773533
7	2.0680873	0.0000000	-4.7827209
6	3.2661398	0.0000000	-7.0172463
6	-0.6150411	0.0000000	-9.3818985
1	-3.9813710	0.0000000	-6.9970757
1	5.3524072	0.0000000	-6.9161181
1	-1.6705338	0.0000000	-11.1723508
1	3.1072346	0.0000000	-11.1353244
8	-4.2934430	0.0000000	-2.4463725

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GEOMETRY

6	2.1103734	-6.5028647	-1.4225701
6	-1.2497252	-7.5950821	2.5539365
6	0.3745723	-4.6226035	-0.6412830
6	2.1938270	-8.8994092	-0.2332960
6	0.5051651	-9.4493162	1.7682020
6	-1.3038625	-5.1973991	1.3475328
6	0.3838409	-2.2137805	-1.9610264
1	1.0907403	-2.2986994	-3.9340251
6	-0.3241101	0.0153426	-0.9845929
1	-1.0362935	0.2159112	0.9618399
6	-0.2234015	2.3610262	-2.4970597
6	-0.3172954	4.7630206	-1.0748210
6	-0.5264271	9.3647545	1.5121043
6	-1.3510910	6.9043737	-2.2426475
6	0.6318970	4.9474716	1.3876306
6	0.5290487	7.2444484	2.6716508
6	-1.4644137	9.1930553	-0.9451380
1	-2.0596862	6.7555715	-4.1951942
1	1.4839420	3.2890425	2.3096555
1	1.2835113	7.3836141	4.6035897
1	-2.2875502	10.8651464	-1.8660581
1	-0.6129089	11.1728948	2.5350562
8	-0.1047025	2.3164805	-4.8354868
9	3.7370314	-6.0352234	-3.3326592
9	3.8750958	-10.6552470	-1.0037447
9	0.5703746	-11.7237930	2.9118322
9	-2.8773877	-8.0987382	4.4521730
9	-3.0305642	-3.4999980	2.1543992

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GEOMETRY

1	2.0180804	3.6957281	2.4706439
6	0.9167156	5.3094893	1.7590915
7	-1.8600110	9.4704347	-0.0588104
6	-0.5974253	5.0566352	-0.4035201
6	1.0255641	7.6366889	2.9908481
6	-0.3947809	9.6606243	2.0170053
6	-1.9442411	7.2204949	-1.2310605
1	2.1957721	7.8939042	4.6844509
1	-0.3631062	11.5354713	2.9353988
1	-3.1581590	7.1241706	-2.9291816
6	-0.8251855	2.7217852	-1.8127275
1	-1.7049628	2.8937228	-3.7064158
6	-0.0805071	0.4378612	-0.9917085
1	0.7980397	0.1557684	0.8726916
6	-0.3745160	-1.8437653	-2.5592466
6	0.0333067	-4.2954911	-1.2763461
6	0.8202636	-8.9738412	1.0479566
6	1.0502716	-6.3144533	-2.6550276
6	-0.6098949	-4.6411724	1.2659428
6	-0.2199849	-6.9767521	2.4193250
6	1.4534704	-8.6411940	-1.4890101
1	1.5119771	-6.0420045	-4.6669442
1	-1.4505087	-3.0796402	2.3529997
1	-0.7375740	-7.2440999	4.4145139
1	2.2625133	-10.2173280	-2.5763340
1	1.1337812	-10.8124803	1.9661681
8	-0.8988970	-1.7305566	-4.8407034

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GEOMETRY

6	-6.7462199	-1.8299814	-1.6368873
6	-7.4235143	1.4366026	2.5089497
6	-4.6404464	-0.4703402	-0.6996999
6	-9.1651655	-1.5904350	-0.5156743
6	-9.5064705	0.0510049	1.5704780
6	-5.0069782	1.1662196	1.3719327
6	-2.2170048	-0.8044254	-1.9483528
1	-2.3377485	-1.3876422	-3.9604711
6	0.0568494	-0.5180328	-0.8614730
1	0.2946768	0.0091383	1.1397109
6	2.4052810	-0.9066859	-2.3020129
6	4.7704378	-0.1776392	-0.9623201
6	9.3295366	1.2138159	1.5064920
6	6.4192742	1.5872512	-2.0808197
6	5.4063376	-1.2512823	1.3858779
6	7.6830896	-0.5712217	2.6292084
6	8.6953112	2.3017695	-0.8530588
8	2.4599066	-1.7417799	-4.4792711
9	5.8549198	2.6487851	-4.3275756
9	10.2516690	4.0067589	-1.9345696
9	11.4904858	1.8728794	2.6796834
9	8.2760846	-1.6217579	4.8754337
9	3.8763469	-2.9629499	2.4997640
9	-3.0831198	2.5469171	2.3228865
9	-6.4778128	-3.3985586	-3.6315977
9	-11.1395195	-2.9181023	-1.4322131
9	-11.7997642	0.2922708	2.6486015
9	-7.7264422	3.0174216	4.4869781

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GEOMETRY

1	-2.5689585	6.7154685	-3.6284642
6	-1.5273704	6.8660966	-1.8337940
6	1.1141679	7.2607376	2.7091980
6	-0.5539892	4.6749889	-0.6896571
6	-1.1905604	9.2190556	-0.7068925
6	0.1310593	9.4221073	1.5663349
6	0.7748193	4.8999709	1.5925952
1	-1.9670031	10.9212799	-1.6129963
1	0.3983523	11.2833648	2.4527879
1	1.5671403	3.2093919	2.5083870
1	2.1616313	7.4156581	4.4984044
6	-0.9502105	2.2564632	-1.9211476
1	-1.6258383	2.3543343	-3.9024804
6	-0.5794999	-0.0177877	-0.8495985
1	0.0496928	-0.2421957	1.1205836
6	-1.0216672	-2.3670467	-2.2517616
6	-0.2072801	-4.7252380	-0.9394471
6	1.3425264	-9.2624411	1.4764929
6	1.5320777	-6.3529867	-2.1257566
6	-1.1752499	-5.3704878	1.4510298
6	-0.4149189	-7.6364572	2.6689538
6	2.3251095	-8.6181329	-0.9258412
8	-1.9668164	-2.4563442	-4.3850518
9	-2.8588219	-3.8617262	2.6347119
9	-1.3642466	-8.2383574	4.9581642
9	2.0759440	-11.4140477	2.6243384
9	4.0045162	-10.1552204	-2.0742865
9	2.4953987	-5.7804476	-4.4148064

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GEOMETRY

6	1.9814429	0.8078559	-0.6990504
1	3.1506959	0.8667906	-2.4378508
6	1.2401463	-1.4542964	0.2048898
6	2.0279006	-3.7791264	-1.1496245
6	0.7750591	-6.1684174	-0.4306132
6	-1.5473461	-10.7398650	0.8409318
6	1.7086277	-8.4546817	-1.3876561
6	-1.3387919	-6.1781960	1.1736777
6	-2.4894839	-8.4749366	1.7985605
6	0.5534777	-10.7319867	-0.7518118
1	3.3630869	-8.4181154	-2.6538500
1	-4.1458730	-8.4864172	3.0543998
1	1.2964782	-12.5198362	-1.5073131
1	-2.4637232	-12.5374759	1.3439297
8	3.6697784	-3.7196424	-2.8234883
6	-0.3181992	-1.7918673	2.5156206
1	0.9568734	-2.3761253	4.1130092
1	-1.2204295	0.0491305	3.0703999
6	-2.3687079	-3.7620276	2.1666310
1	-3.3443307	-4.0864113	4.0222167
1	-3.8307900	-3.0361621	0.8050472
1	2.6244525	2.2395174	4.1488526
6	1.8789539	3.7464478	2.9217118
6	1.4184329	3.2679895	0.3972177
6	0.5262592	8.0847767	2.4753220
6	0.4635679	5.2399376	-1.1890255
6	1.4364381	6.1654654	3.9627033
6	0.0162754	7.6620963	-0.1282311
6	-0.0749158	4.8512438	-3.7939549
1	1.8369098	6.4808879	5.9783762
1	-1.2722151	11.4982341	-0.8424450
1	0.1772656	9.9763337	3.2660861
6	-0.9951894	6.7839709	-5.2614952
1	0.2514711	2.9699050	-4.6208002
1	-1.4057888	6.4762954	-7.2763431
6	-1.4312219	9.2003827	-4.2012675
1	-2.1683087	10.7190657	-5.4136862
6	-0.9382767	9.6292593	-1.6910767

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GEOMETRY

1	2.2923391	3.8417693	1.3566098
6	0.9741254	5.3610646	0.8256886
6	-2.3582478	9.1987812	-0.5738687
6	-0.7464831	4.9585878	-1.1365501
6	1.0389299	7.6933862	2.1259753
6	-0.6596769	9.6191350	1.3856650
6	-2.4108238	6.8975173	-1.8453837
1	-0.6535074	11.4532285	2.3642242
1	-3.7562830	6.5922463	-3.3992603
1	-3.6734969	10.7126000	-1.1278247
6	-0.8384843	2.5686509	-2.4931669
1	-1.6471315	2.6594285	-4.4216112
6	-0.0601385	0.3401522	-1.5642384
1	0.7446441	0.1568286	0.3454782
6	-0.2178217	-2.0065397	-3.0560523
6	-0.0306050	-4.4038098	-1.6451712
6	0.3539559	-9.0578587	0.9413261
6	0.8651428	-6.5662101	-2.8872167
6	-0.7635869	-4.5950676	0.8888572
6	-0.5929212	-6.8760457	2.1711444
6	1.0665625	-8.8576803	-1.6320016
1	1.4020845	-6.4244585	-4.8963291
1	-1.5179989	-2.9288319	1.8841894
1	-1.1872467	-6.9762204	4.1607279
1	1.7924263	-10.5204402	-2.6467935
8	-0.4611258	-1.9757936	-5.3896087
7	2.6453196	8.0324907	4.2013764
1	4.1659795	6.9233224	4.1895615
1	3.0480790	9.8323071	4.5768192
7	0.7027313	-11.3036745	2.2646914
1	-0.3301145	-11.4942480	3.8223427
1	0.8133770	-12.8546173	1.2104000

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GEOMETRY

1	-3.2663217	5.4408066	-3.4246058
6	-2.0160326	5.7464542	-1.7882100
6	1.1802625	6.5215386	2.3587988
6	-0.4373860	3.7829491	-0.9517859
6	-2.0276898	8.0753210	-0.5709167
6	-0.4236706	8.4560002	1.5094422
6	1.1590755	4.2005919	1.1219451
1	-3.2785153	9.6088089	-1.2301791
1	2.4293075	2.6882773	1.7785607
1	2.4436107	6.8403736	3.9876711
6	-0.4882286	1.3769721	-2.2794496
1	-1.1887421	1.4480960	-4.2513404
6	0.2148006	-0.8435093	-1.2759703
1	0.9139289	-1.0138479	0.6768003
6	0.1076264	-3.2117200	-2.7463854
6	0.3178684	-5.5892618	-1.2944099
6	0.7399678	-10.1419345	1.3526668
6	1.4282827	-7.7014049	-2.4433545
6	-0.6011433	-5.7785656	1.1791909
6	-0.3924817	-8.0515230	2.4933089
6	1.6485163	-9.9652288	-1.1154867
1	2.1104284	-7.5517187	-4.4051576
1	-1.5158136	-4.1443589	2.0844054
1	-1.1258468	-8.1959487	4.4331287
1	2.5316034	-11.6147805	-2.0216257
1	0.9091862	-11.9311779	2.3984854
8	-0.1105010	-3.2088017	-5.0785606
7	-0.4210183	10.9389224	2.8243278
8	0.9660437	11.2413710	4.5974552
8	-1.8071176	12.5772992	2.0812507

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GEOMETRY

1	1.2053370	5.5255687	1.5266996
6	0.0234923	6.8756159	0.4859532
6	-3.0236975	10.4548618	-2.2580301
6	-1.2751027	6.1788757	-1.7465538
6	-0.2529899	9.3425390	1.2702801
6	-1.7571868	11.1119750	-0.0745432
6	-2.7423396	7.9438088	-3.0703276
1	-3.7213500	7.3518900	-4.8095821
1	-4.1852419	11.8138344	-3.3083970
6	-1.1006621	3.6188477	-2.7263266
1	-1.6094936	3.3902453	-4.7448551
6	-0.4128877	1.5813880	-1.3780963
1	0.1026861	1.7001850	0.6338147
6	-0.2847269	-0.9508827	-2.5256973
6	-0.1003083	-3.1149474	-0.7660461
6	0.2936210	-7.2976808	2.4729647
6	-1.1606233	-3.0287581	1.6520237
6	1.1412840	-5.3055772	-1.5809025
6	1.3641121	-7.3893235	0.0247730
6	-0.9782649	-5.1013741	3.2554197
1	-2.1785184	-1.3318204	2.2942061
1	1.9272551	-5.3431707	-3.5083508
1	-1.8125001	-5.0548203	5.1591865
8	-0.2943596	-1.2666663	-4.8496312
8	-1.6803350	13.4301861	1.1543783
8	0.8006978	10.5212810	3.3725835
6	-0.0708578	13.1116923	3.3437631
1	1.6017698	14.3852850	3.1399236
1	-1.2221830	13.4560653	5.0807720
8	0.4548750	-9.1513748	4.2924434
8	2.6033637	-9.5958521	-0.6391670
6	0.8525357	-11.6805231	3.4560115
1	-0.4085515	-12.1552050	1.8351047
1	0.3693738	-12.8387287	5.1593775
1	2.8773571	-11.9443499	2.9182080
6	3.4850403	-9.7432009	-3.1769254
1	1.8888825	-9.5270921	-4.5406525
1	4.3110290	-11.6878293	-3.2923442
1	4.9694678	-8.2849674	-3.5314581

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GEOMETRY

1	-2.3844663	-0.6391025	-4.6187896
6	-1.1458355	-0.1715617	-6.2153275
6	2.0532149	1.0870889	-10.4348226
6	1.0172428	1.3729015	-5.9126230
6	-1.6296269	-1.0371702	-8.6223973
6	-0.0552002	-0.4243155	-10.7072118
6	2.5516942	1.9800995	-7.9856585
1	4.2163884	3.1965967	-7.6968210
1	3.2751512	1.5714715	-12.0383514
6	1.6866210	2.3792327	-3.4464835
1	2.9939466	4.0153626	-3.4661282
6	0.8716720	1.4666872	-1.2226431
1	-0.4195467	-0.1591515	-1.0908221
6	1.6460232	2.6089165	1.1941231
8	2.6815406	4.7091185	1.3078959
6	1.0821725	1.1372199	3.5050919
1	0.5394119	4.4732495	5.7773549
6	0.5349335	2.3902643	5.7255332
6	0.6131891	-2.9039035	5.6074665
6	-0.0293362	1.0242498	7.9657813
6	1.1318865	-1.5461080	3.4605987
6	0.0073864	-1.6556043	7.9087636
6	-0.6228001	2.2795172	10.2668768
1	1.6202995	-2.5230407	1.6898855
1	-0.5214189	-5.0980121	10.0921753
1	0.6606062	-4.9829592	5.5855496
6	-1.1566492	0.9150634	12.4084493
1	-0.6421432	4.3591685	10.2911308
1	-1.6159253	1.8791910	14.1920602
6	-1.1224305	-1.7602435	12.3506028
1	-1.5568970	-2.8110776	14.0913452
6	-0.5538620	-3.0198793	10.1539349
8	-3.6041494	-2.5671588	-9.4475035
8	-1.0058330	-1.5553527	-12.8767827
6	-3.2561254	-2.9225296	-12.1350650
1	-2.9483516	-4.9778985	-12.5103611
1	-4.9127765	-2.0903296	-13.1468273

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GEOMETRY

1	-4.1625690	6.5465559	-4.0341006
6	-2.8168844	7.0196944	-2.5177293
6	0.5847455	8.1215985	1.2518463
6	-1.1428532	5.1599239	-1.6468125
6	-2.8537920	9.4797830	-1.5214888
6	-1.1300274	9.9873170	0.3690811
6	0.6242195	5.7039294	0.2863606
1	-4.1805292	10.9139130	-2.2154846
1	1.9694397	4.2790143	0.9661075
6	-1.2479825	2.6617634	-2.7844793
1	-2.1742321	2.5642223	-4.6596344
6	-0.3504922	0.5363099	-1.7282421
1	0.5801866	0.5256731	0.1314904
6	-0.5385161	-1.9254684	-3.0162271
6	-0.1340724	-4.1969387	-1.4443404
6	0.6437570	-8.5612116	1.4176242
6	0.7993712	-6.3955388	-2.5833023
6	-0.7022281	-4.2117630	1.1440880
6	-0.3261677	-6.3720294	2.5828254
6	1.2068830	-8.5769172	-1.1687168
1	1.2033018	-6.3854592	-4.6275119
1	-1.4812860	-2.5079403	2.0512025
1	-0.7729448	-6.4084123	4.6108392
1	1.9525195	-10.2790608	-2.0939310
8	-0.9803679	-2.0927690	-5.3136498
8	0.9644238	-10.5967574	3.0117471
6	1.9074488	-12.8532994	1.8897791
1	0.5854073	-13.5533390	0.4005854
1	1.9908212	-14.2080707	3.5127935
1	3.8323492	-12.5348263	1.0841422
8	2.0961455	9.1573325	3.1396205
8	-0.7325905	12.2250482	1.6830726
6	1.3025246	11.7543330	3.4493527
1	2.9223365	13.0188670	2.9617127
1	0.5616557	12.0045229	5.4113797

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GEOMETRY

1	-3.6868594	6.0324970	-4.5392363
6	-2.4811631	6.4936900	-2.9058642
6	0.5686019	7.5642943	1.1617794
6	-0.9517304	4.6040910	-1.8520142
6	-2.5450628	8.9693603	-1.9513404
6	-0.9987027	9.4609990	0.0909497
6	0.6337265	5.1316659	0.2369727
1	-3.7573466	10.4271832	-2.7904747
1	1.8657296	3.6827726	1.0644300
6	-1.0159829	2.0932019	-2.9631962
1	-1.7918947	1.9875861	-4.9056996
6	-0.2467153	-0.0356241	-1.8150549
1	0.5296979	-0.0417473	0.1148430
6	-0.3780717	-2.5083711	-3.0871115
6	0.0250464	-4.7605522	-1.4812597
6	0.8155504	-9.0975292	1.4696837
6	1.1352676	-6.9171995	-2.5433388
6	-0.7114970	-4.7970499	1.0586857
6	-0.3227432	-6.9508613	2.5185291
6	1.5377759	-9.0623612	-1.0752969
1	1.6726219	-6.8969069	-4.5551897
1	-1.6271188	-3.1321010	1.9060287
1	-0.9169373	-6.9698171	4.5108989
1	2.4189130	-10.7446136	-1.9221016
8	-0.7703961	-2.7049057	-5.3901904
6	1.2647698	-11.3692661	3.0400330
1	3.1476222	-11.2208460	3.9936956
1	1.2586882	-13.1207373	1.8591882
1	-0.2178088	-11.5628535	4.5325165
8	-0.6671214	11.7080731	1.4067900
8	1.9180250	8.5889235	3.1742503
6	1.1732081	11.2114268	3.3689751
1	0.2534405	11.5147476	5.2458505
1	2.8684683	12.4228307	3.0232684

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GEOMETRY

1	4.7631745	4.0731070	-3.7983859
6	5.3330397	2.7791469	-2.2702197
6	6.6795159	-0.4971341	1.5305525
6	3.5773384	1.0298873	-1.3330427
6	7.8079060	2.9554459	-1.3275914
6	8.4393562	1.2922592	0.5798810
6	4.2481082	-0.6737195	0.6172012
1	9.1598254	4.3390451	-2.0741441
1	2.9075782	-2.0767477	1.3496770
6	1.0565242	0.9916033	-2.4216968
1	0.8693924	1.9152042	-4.2920296
6	-0.9939523	-0.0309266	-1.3285790
1	-0.9169871	-0.9701058	0.5258697
6	-3.4805879	0.0120118	-2.5772615
6	-5.7105270	-0.3945944	-0.9600742
6	-9.9056057	-1.1554566	2.2223377
6	-7.9814134	-1.4055381	-1.9177806
6	-5.6168905	0.2717240	1.6106174
6	-7.6796112	-0.0959504	3.1847873
6	-10.0721024	-1.8103047	-0.3052693
1	-3.8822780	1.1278771	2.3810002
1	-7.5727586	0.4445796	5.1877258
1	-11.8055907	-2.6310623	-1.1046603
1	-11.5344828	-1.4588516	3.4803181
8	-3.6789093	0.3474932	-4.8969999
8	-8.3714756	-2.1075001	-4.3722688
1	-6.9343085	-1.6160349	-5.4036130
8	10.7197804	1.0292271	1.8518561
8	7.8270476	-1.9214986	3.4207819
6	10.3875661	-0.9955654	3.6618574
1	10.6407200	-0.2081701	5.6053146
1	11.7206075	-2.5594511	3.1738388

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GEOMETRY

1	4.6667618	3.9572381	-4.0504604
6	5.1929480	2.6735487	-2.4981340
6	6.4270759	-0.5724066	1.3662154
6	3.3682294	1.0300918	-1.5031013
6	7.6832067	2.7561916	-1.5838629
6	8.2574641	1.1100179	0.3563075
6	3.9804391	-0.6567843	0.4807315
1	9.0894741	4.0578389	-2.3757672
1	2.5837818	-1.9773595	1.2598364
6	0.8363821	1.0841081	-2.5658186
1	0.6707589	1.9772578	-4.4530787
6	-1.2466134	0.1765242	-1.4342340
1	-1.1940733	-0.7196089	0.4423343
6	-3.7446586	0.3096801	-2.6544432
6	-5.9515815	-0.2901849	-1.0441646
6	-10.1807398	-1.4446109	1.9046394
6	-8.0702961	-1.4374742	-2.1429602
6	-5.9738420	0.2973439	1.5346673
6	-8.0863088	-0.2761583	2.9999486
6	-10.1713558	-2.0232344	-0.6669885
1	-8.0565565	-1.8562354	-4.1824703
1	-4.3357554	1.2365642	2.4073989
1	-8.0998480	0.1965363	5.0240040
1	-11.8254401	-2.9339831	-1.5360667
1	-11.8414473	-1.9030117	3.0683213
8	-4.0000307	0.8597660	-4.9186559
8	7.5277154	-2.0043570	3.2789166
8	10.5372693	0.7703666	1.6121115
6	10.1307917	-1.1937493	3.4723516
1	10.4421027	-0.3747500	5.3940032
1	11.3841461	-2.8291655	3.0084191

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GEOMETRY

1	-2.5917019	4.6696692	-4.9131062
6	-1.7994336	5.1616246	-3.0517487
6	0.2089440	6.3062276	1.6006224
6	-0.7096379	3.2577458	-1.5646877
6	-1.9319991	7.6894792	-2.2546091
6	-0.9114760	8.2176833	0.0873520
6	0.3377346	3.8223176	0.8313180
1	-2.7981290	9.1577651	-3.4346898
1	1.2196083	2.3599915	2.0092928
6	-0.6656850	0.6941488	-2.5473766
1	-0.9954561	0.5169641	-4.6081185
6	-0.2861376	-1.3993954	-1.1570002
1	0.0147211	-1.3126479	0.9001359
6	-0.2747344	-3.9120685	-2.3355223
6	0.3260208	-6.1636907	-0.7206396
6	1.4150933	-10.4059381	2.0997952
6	0.3769947	-8.5512712	-1.9130596
7	0.7973526	-5.8707505	1.7845024
6	1.3239112	-7.9523707	3.1331245
6	0.9306291	-10.6922640	-0.4716845
1	-0.0197512	-8.6887825	-3.9509863
1	1.6949655	-7.6360815	5.1642876
1	0.9806607	-12.5702780	-1.3608308
1	1.8576509	-12.0349307	3.3056090
8	-0.7399807	-4.2328600	-4.6116798
8	-0.7667476	10.5182408	1.3435543
8	1.0828815	7.3752763	3.8401150
6	0.4864095	10.0393806	3.7278579
1	-0.8524028	10.4987347	5.2955179
1	2.2896929	11.1380808	3.7726547

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GEOMETRY

1	-2.4775685	4.2431912	-5.0778745
6	-1.6652356	4.7913473	-3.2408204
6	0.4048713	6.0803148	1.3472806
6	-0.4039849	2.9694781	-1.7874271
6	-1.9442538	7.3064961	-2.4401230
6	-0.8902761	7.9081031	-0.1310739
6	0.6783876	3.6096638	0.5737859
1	-2.9430401	8.7104901	-3.5939529
1	1.7010518	2.2156573	1.7195371
6	-0.2168016	0.4111476	-2.7675789
1	-0.5508144	0.2077636	-4.8254738
6	0.2902920	-1.6546465	-1.3816217
1	0.6301186	-1.5623116	0.6680968
6	0.4452423	-4.1795589	-2.5379210
6	0.4988412	-6.3520254	-0.7879891
6	0.7600925	-10.5779762	2.2124475
6	1.7602326	-8.5915456	-1.5236652
6	-0.6883981	-6.3093334	1.5764121
6	-0.5625217	-8.4522917	3.1071094
7	1.9065862	-10.6640709	-0.0606830
1	2.6868588	-8.7012791	-3.3963137
1	-1.7273469	-4.6238840	2.2131937
1	-1.4762859	-8.4904233	4.9690143
1	0.9097219	-12.3109401	3.3687791
8	0.5582683	-4.4897730	-4.8587122
8	-0.8634022	10.2150627	1.1195522
8	1.2723438	7.2103305	3.5585672
6	0.4978026	9.8300525	3.4617700
1	-0.8160365	10.2056112	5.0723631
1	2.2252484	11.0453500	3.4433216