BHAGVAD P. SHRESTHA
Prediction of Hydrolysis Rate Constants for Esters and Hydration Equilibrium Constant for Aldehydes/Ketones and Quinazolines
(Under the Direction of LIONELL A. CARREIRA)

SPARC stands for **SPARC Performs Automated Reasoning** in **Chemistr**y. It analyzes an organic molecule like an expert chemist does. It calculates chemical reactivity and physical properties of organic compounds. For chemical reactivity parameters, it splits each organic molecule into its reaction center and a collection of perturbers. Then from the various interactions between the reaction center and the perturbers, it calculates the chemical reactivity of the molecule. For physical properties, intermolecular interactions are expressed as a summation of all the interacting forces between the molecules. Each of these interacting forces are then expressed in terms of a limited set of molecular-level descriptors that, in turn, are calculated from the molecular structure. It now calculates pKa, electron affinity, vapor pressure, activity coefficient, distribution coefficient, Henry's constant, etc. Our main goal is to extend the SPARC's capability to calculate hydrolysis rate constants of esters and hydration equilibrium constants of aldehydes/ketones and quinazolines.

INDEX WORDS: Base hydrolysis rate constant, Acid hydrolysis rate constant, General base hydrolysis constant, Hydration equilibrium constants of aldehydes and ketones, Hydration equilibrium constants of quinazolines

PREDICTION OF HYDROLYSIS RATE CONSTANTS FOR ESTERS AND HYDRATION EQUILIBRIUM CONSTANT FOR ALDEHYDES/KETONES AND QUINAZOLINES BY SPARC

by

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CHAPTER 1

INTRODUCTION

The main objective of this project is to extend the calculational ability of SPARC to the calculation of hydrolysis rate constants of ester compounds and hydration equilibrium constants of aldehydes/ketones and quinazolines. The SPARC calculator has been successful in calculating the pKa, electron affinity and various physical properties of organic compounds. [1] According to EPA, each year the number of organic compounds synthesized far exceeds their ability to evaluate the physical and chemical properties. Determining the physical and chemical reactivity properties of organic compounds experimentally is expensive and time consuming. Many times reactants half-lives cannot be determined within a reasonable time in the laboratory. As a result, alternative methods are needed, which is reliable, faster and determines the values of these physical and chemical properties within the experimental error. That alternative method is the SPARC calculator, which can accurately calculate the value of these properties inexpensively and within a reasonable time. In addition, the SPARC calculator can calculate values of physical and chemical properties of organic compounds at elevated temperatures and in many solvents. Esters, aldehydes/ketones and quinazolines have environmental, industrial and pharmaceutical importance. Understanding the hydrolysis rate constants and hydration equilibrium constants for these compounds will help us to assess and use them safely.

Esters

Esters are important carbonyl compounds. The general structure for esters is represented by R1C(=O)OR2, where R1 and R2 are substituents. These substituents can be substituted alkyl chains, phenyl groups or heteroatoms. They are used industrially to make flavors, soaps, herbicides, pesticides (phosphoesters in particular) and so on. The esters undergo hydrolysis through three different mechanisms. They are, namely, base, acid and general base-catalyzed ester hydrolyses.

Base Catalyzed Hydrolysis

The base-catalyzed or alkaline hydrolysis of esters generally takes place via a $B_{AC}2$ mechanism (figure 1). $B_{AC}2$ stands for base-catalyzed, acyl-oxygen fission and bimolecular reaction. It is similar to the S_N2 reaction and it occurs when the hydroxide ion attacks the carbonyl carbon of an ester to give the carboxylic acid and alcohol. In addition, alkaline hydrolysis of esters may also occur through other mechanisms, such as $B_{AC}1$ (base-catalyzed, acyl-oxygen fission, unimolecular), $B_{AL}1$ (base-catalyzed, alkyl-oxygen fission, unimolecular) and $B_{AL}2$ (base-catalyzed, alkyl-oxygen fission, bimolecular). However, $B_{AC}2$ is the most common mechanism for alkaline hydrolysis of esters and it usually masks all the other plausible mechanisms. [2, 3]

Acid Catalyzed Hydrolysis

The acid catalyzed hydrolysis of esters takes place via $A_{AC}2$ mechanism (figure 2). $A_{AC}2$ stands for acid-catalyzed, acyl-oxygen fission and bimolecular reaction. It is similar to the S_N2 reaction. It occurs when the positive hydrogen ion catalyzes the esters

Figure 1

$B_{AC}2$ mechanism: Base-catalyzed, Acyl-oxygen fission and Bimolecular reaction.

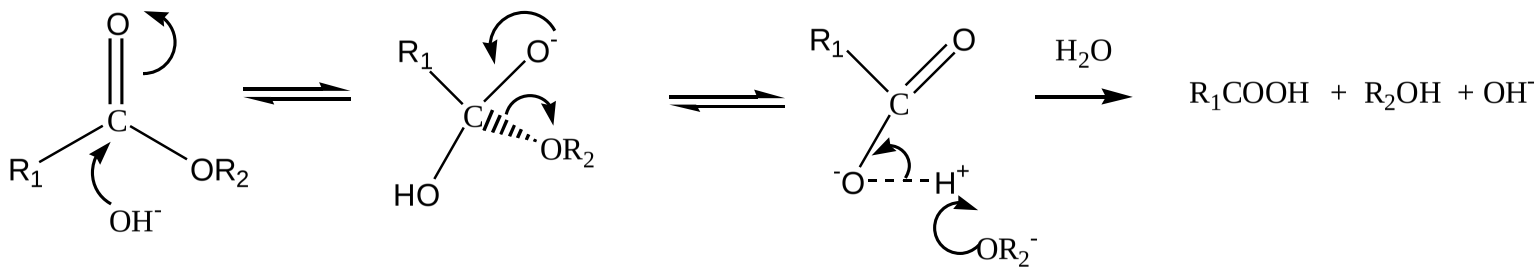
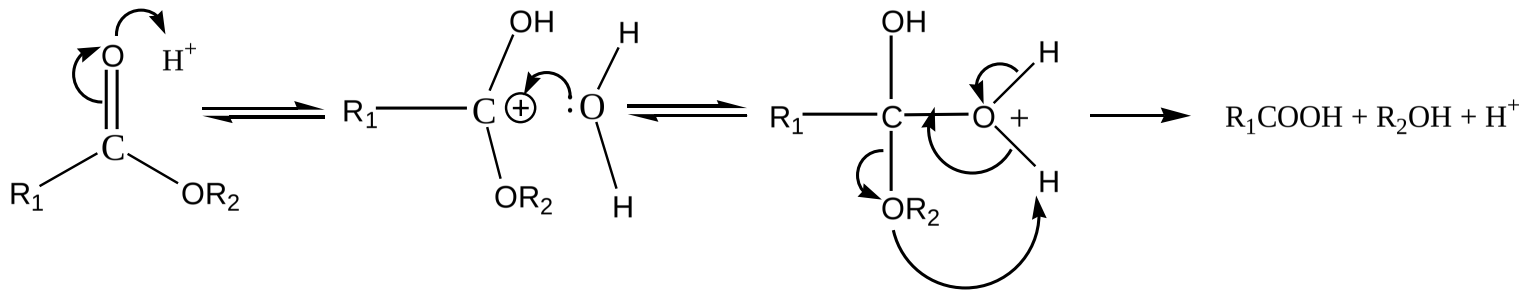

O
C
R1
OR2
OH-
R1
O-
C
OR2
HO
R1
O
C
-O
H+
OR2-
H2O
R1COOH + R2OH + OH-

Figure 2

$A_{AC}2$: Acid-catalyzed, acyl-oxygen fission and bimolecular reaction


O
H+
C
R1
OR2
OH
H
R1
C
O
OR2
H
OH
H
R1
C
O +
OR2
H
R1COOH + R2OH + H+

and the water molecule attacks the carbonyl carbon of the ester to give the carboxylic acid and alcohol. In addition, the acid-catalyzed hydrolysis of esters may also take place by other mechanisms, such as $A_{AC}1$ (acid-catalyzed, acyl-oxygen fission, unimolecular), $A_{AL}1$ (acid-catalyzed, alkyl-oxygen fission, unimolecular) and $A_{AL}2$ (acid-catalyzed, alkyl-oxygen fission, bimolecular). However, $A_{AC}2$ is the general mechanism for acid-catalyzed hydrolysis of esters and it usually masks all the other possible mechanisms. [2, 3]

General Base Catalyzed Hydrolysis

The general base-catalyzed hydrolysis of esters takes place via $B_{AC}2$ mechanism (figure 3). $B_{AC}2$ stands for base-catalyzed, acyl-oxygen fission, bimolecular reaction. It is similar to the S_N2 reaction. It occurs when the base (B:) abstracts the hydrogen atom from the water molecule releasing the hydroxide ion, which eventually attacks the carbonyl carbon of esters to give the carboxylic acid and alcohol. The base, B:, stands for any base, such as ammonia, acetate ion, imidazole and so on. In case of neutral hydrolysis, B: represents the water molecule. [2, 3]

Aldhehydes/Ketones

Aldehydes and ketones are important carbonyl compounds with the structures R1C(=O)H and R1C(=O)R2 respectively. R1 and R2 can either be alkyl chains, phenyl rings or heteroatoms. They are industrially used for making plastics, food additives and flavors. [4] The hydration of aldehydes/ketones takes place when a water molecule attacks the carbonyl carbon of the aldehydes/ketones and the released hydrogen ion of water molecule attacks the carbonyl oxygen to give the hydrated forms of aldehydes/ketones (figure 4). It is a nucleophilic reaction. The hydration of aldehydes/ketones may take place under a neutral,

Figure 3

$B_{AC}2$ mechanism (Base-catalyzed, Acyl-oxygen fission, Bimolecular reaction) for general base-catalyzed hydrolysis of esters. B: stands for any base and for neutral hydrolysis it represents the water molecule.

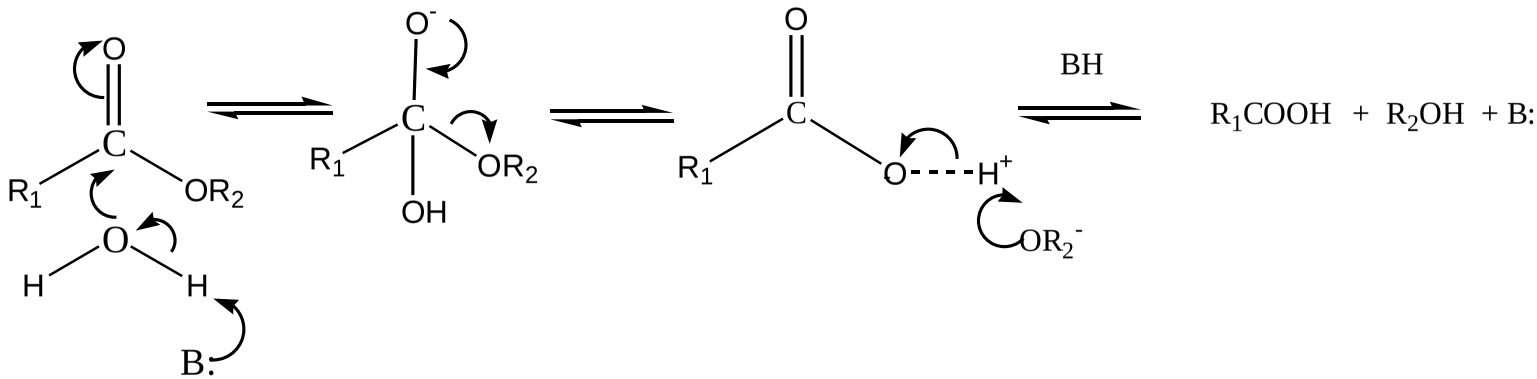
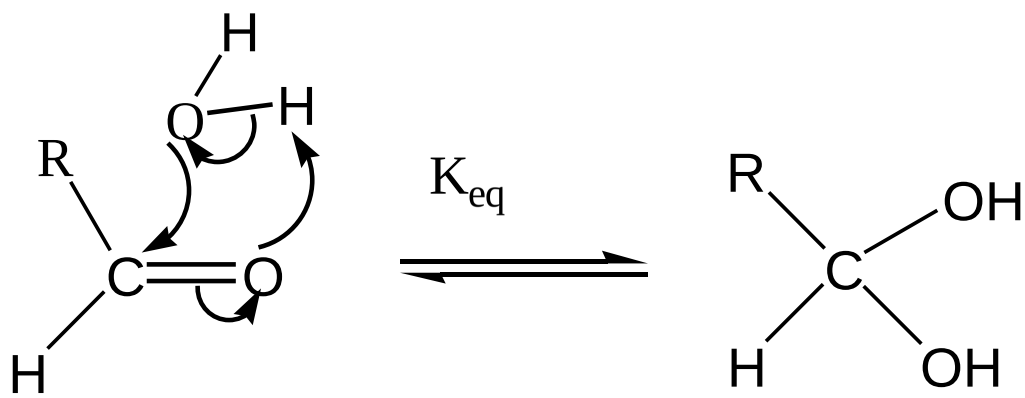

O
C
R1
OR2
O
H
H
B:
O-
C
R1
OR2
OH
O
C
R1
O
H+
OR2-
BH
R1COOH + R2OH + B:

Figure 4

Hydration of aldehydes and ketones under acidic, alkaline or neutral condition. Keq is the hydration equilibrium constant.


H
O
H
R
C
O
H
K_{eq}
R
OH
C
H
OH

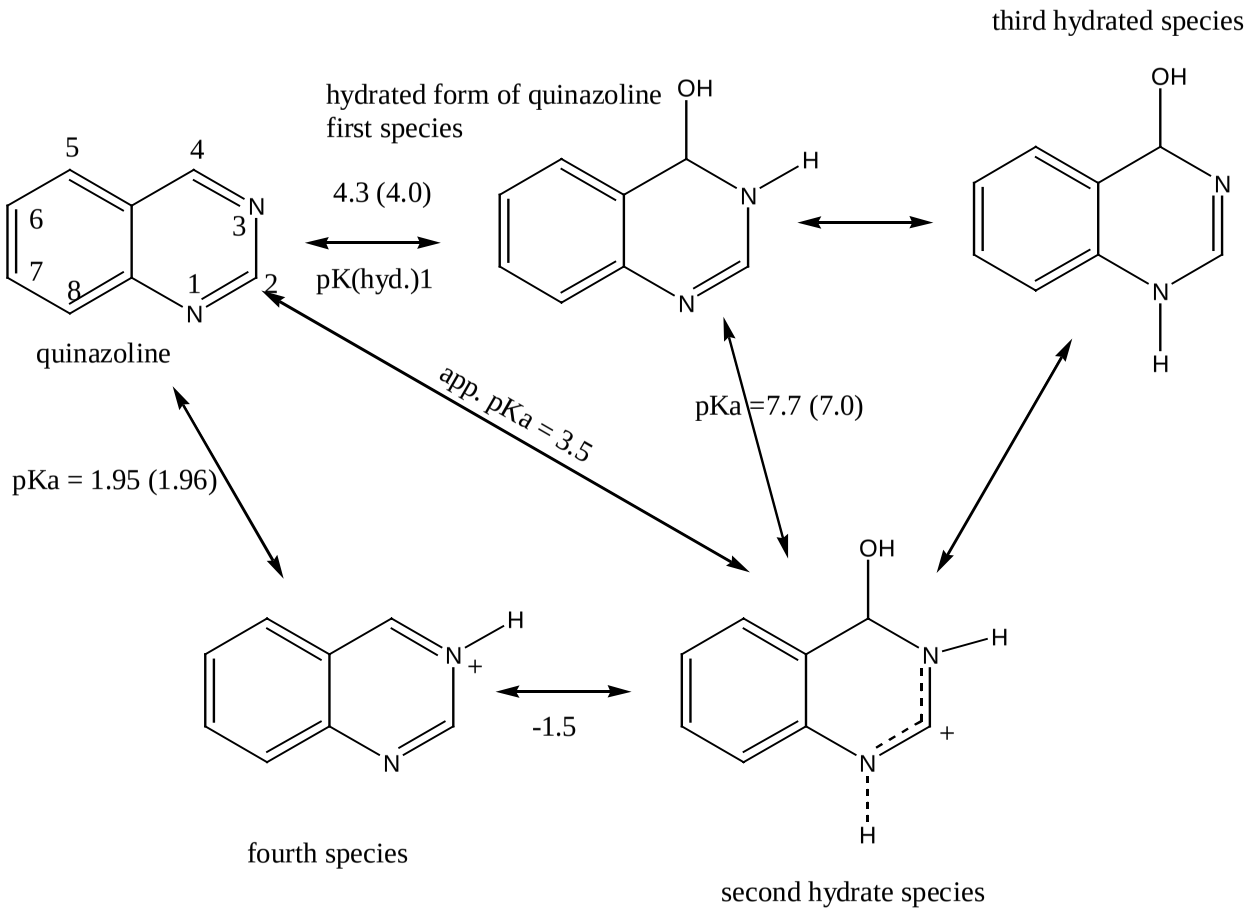
acidic or basic medium. [5, 6] Most of the aldehydes/ketones data we are reporting are hydrating under the basic condition.

Quinazolines

The quinazolines are also important organic compounds, which are used in the field of pharmaceutical research [7] and pesticide chemistry. The quinazolines have a basic structure of n(cc1cc2)cnc1cc2 and many different substituents can be added to 1, 2, 3, 4, 5, 6, 7 or 8 positions. The substituents can be an alkyl chains, phenyl rings or heteroatoms. The hydration of quinazolines takes place when the hydroxide ion of water molecule attacks the carbon at the fourth position and the remaining hydrogen ion attacks the nitrogen at the third position as shown in figure 5. The hydrated quinazolines can further transform into different tautomeric species. [8] However, we are currently interested in and concentrating on hydration of quinazolines into the first hydrated species as shown in the figure 5.

Figure 5

Hydration of quinazolines showing various hydrated species. However, we are currently interested only in hydration of quinazolines into its first hydrated species, displayed by pK(hyd.)1.


third hydrated species
hydrated form of quinazoline
first species
4.3 (4.0)
pK(hyd.)1
quinazoline
app. pKa = 3.5
pKa =7.7 (7.0)
pKa = 1.95 (1.96)
-1.5
fourth species
second hydrate species

CHAPTER 2

SPARC COMPUTATIONAL MODEL FOR HYDROLYSIS OF ESTERS

Hydrolysis Model

The hydrolysis computational model for hydrolysis of esters is categorized into three submodels, namely, reference rate, internal perturbation and external perturbation models. The reference rate model calculates the hydrolysis rate constant for the smallest ester compound, which excludes internal perturbation and steric effects. The internal perturbation model calculates the hydrolysis rate constant due to the internal perturbation interactions between the reaction center and the substituents. The internal perturbation interactions include resonance and electrostatic effects. Finally, the external perturbation model calculates the hydrolysis rate constant due to steric and solvent-reactants interactions. The external perturbation interactions include steric, solvation and field stabilization effects. The hydrolysis rate constant contributions from these three models are then added to give the total calculated hydrolysis rate constant.

Calculated Rate = Reference + Internal Perturbation + External Perturbation

Reference Rate Model

The reference rate is a hydrolysis rate constant for the smallest ester compound, which resembles the structure of reaction center (C(=O)O). It is methyl formate for the hydrolysis of esters. The reference rate does not show any internal perturbation interactions, such as resonance and electrostatic effects. Neither does it show steric

effects. However, it is dependent upon the temperature. As the temperature increases, the reference rate increases. The mathematical expression for the reference rate is given below.

$$\text{Reference} = \text{Pre-exp} + \text{Log}T_k + \text{Ref1} + \text{Ref2}/T_k$$

Where, Reference is the reference rate, Pre-exp is the logarithmic pre-exponential factor, T_k is the temperature in Kelvin, Ref1 is the entropic term and Ref2 is the enthalpic term.

Internal Perturbation Model

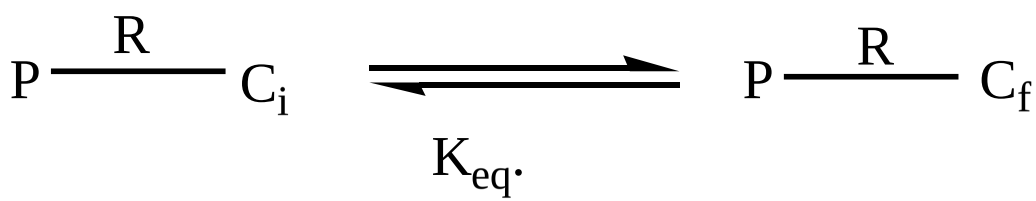
In the internal perturbation computational model for hydrolysis of esters, molecular structure is broken down into the reaction center (C), conductor (R) and perturber (P) (figure 6). The reaction center (C) is hooked to the perturber (P) via the conductor (R).[1, 10] The conductors are usually alkyl chains or phenyl rings. The perturbers are usually functional groups or heteroatoms attached to the conductor. Some molecules may not have the conductors, for example, the reaction center ('C(=O)O') of phenyl acetate is directly connected to the perturbers: the phenyl ring and the carbon atom. $K_{eq.}$ is a critical equilibrium constant, representing the equilibrium between the initial and transition states. The logarithm of the critical equilibrium ($\log K_{eq.}$) is a summation of various interactions between the reaction center and the perturber. The various interactions include electrostatic and resonance. Further, the electrostatic interaction embodies the direct field, the indirect field and sigma induction effects.

Electrostatic Effect

The electrostatic effect is a phenomenon of interaction of dipoles or charges of the perturber with the dipoles or charges of the reaction center. [1, 10] The types of electrostatic

Figure 6

$K_{(eq)c}$ is the critical equilibrium due to the unperturbed reaction center and δp is the change due to interaction between the reaction center and the perturber. δele and δres are changes due to electrostatic and resonance interactions between the reaction center and the perturbers and, of course, δele comprises changes due to sigma induction, direct and indirect field effects.



$$\log K_{(eq)} = \delta_p * \log K_{(eq)c}$$

$$\delta_p * \log K_{(eq)c} = \delta_{ele} * \log K_{(eq)c} + \delta_{res} * \log K_{(eq)c}$$

effects that can occur between the perturber and the reaction center are direct field, mesomeric field (also called pi-induction or indirect field) and sigma induction effects.

Direct Field Effect

The direct field effect occurs when the dipole of the perturber interacts with the dipole of the reaction center through space. [1, 10] Since the transition states for base and general base-catalyzed hydrolyses of esters are positively charged, the dipole will increase the hydrolysis rate constant for these reactions. In contrast, the transition state for acid hydrolysis of esters is positively charged and the dipoles will decrease the hydrolysis rate constant in this situation. The direct field effect due to the interaction between dipoles of the reaction center and the perturber is demonstrated in the following equation:

$$\delta_{field} * \log K_{(eq)c} = \rho_{field} \sigma_p = \rho_{field} \sum \sigma_{cs} F_s .$$

Where, ($\delta_{field} * \log K_{(eq)c}$) is the direct field effect due to the interaction between the field of the perturber and the reaction center. ρ_{field} is the susceptibility of the reaction center due to the field and is presumed to be independent of the perturber. [1, 10] σ_p is the field strength that the perturber exerts on the reaction center and has been previously calculated on ionization pKa. σ_p is further divided into σ_{cs} and F_s , which are conduction descriptor and field strength of the perturber. The conduction descriptor (σ_{cs}) accounts for the change that the conductor can bring about in the electrostatic interaction to the reaction center and is the length dependence on interaction. The field strength (F_s) is the dipole field parameter, which gauges the magnitude of the substituent dipole. [1, 9]

Mesomeric Field Effect (MF)

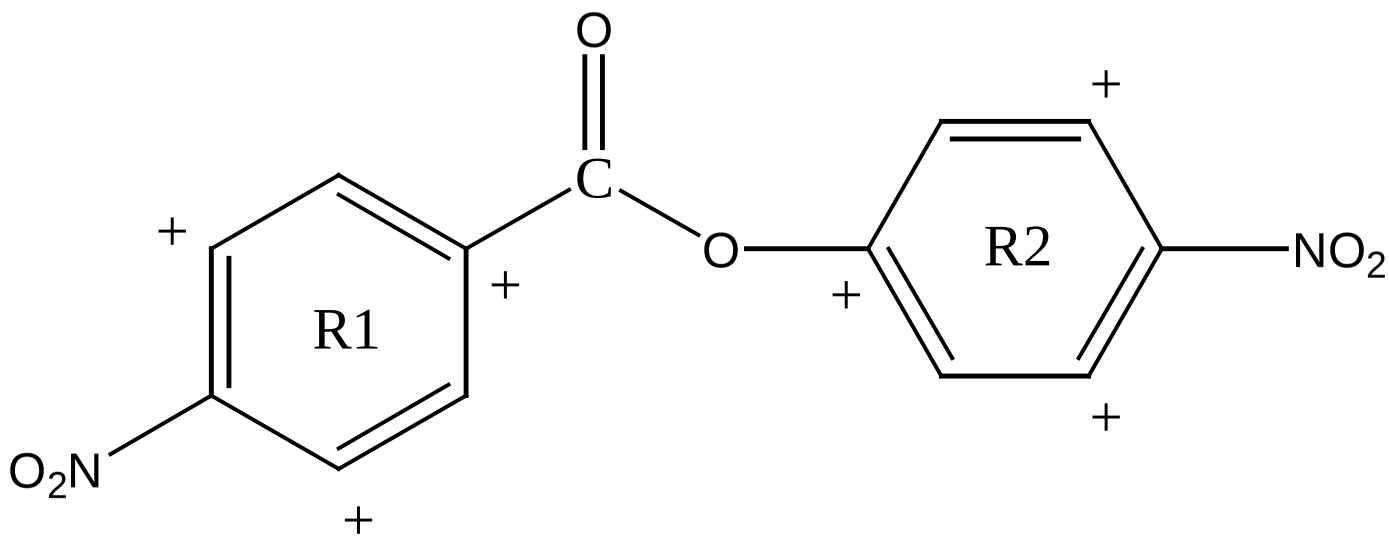
The mesomeric field is generated when an electron withdrawing or donating group puts (or removes) the charges on the conductor R (figure 7). An electron withdrawing group puts positive charges on the conductor, while an electron donating group puts the negative charges.[1, 9] Since the transition states of base and general base-catalyzed hydrolyses are negatively charged, the electron withdrawing groups will increase the hydrolysis rate constant because the induced positive charges on the conductor will stabilize negative charges or electrons that may exist in the reaction center. On the other hand, the induced negative charges have opposite effect. For acid hydrolysis of esters, the MF effect due to induced positive charges is smaller compared to the MF effect in base and general base-catalyzed hydrolyses because the transition state of acid hydrolysis is positively charged. However, the induced negative charges will have larger MF effect on acid hydrolysis than in base and general base-catalyzed hydrolyses for the same reason. Further, the MF effect due to interaction between either the electron withdrawing or donating group with the reaction center is shown in the following equation.

$$\delta_{MF} * \log K_{(eq)c} = \rho_{ele}\, MF\, q_R = \rho_{ele}\, MF\, \Sigma(q_{ik}/r_{kc})$$

Where, ($\delta_{MF} * \log K_{(eq)c}$) is the mesomeric field effect due to the interaction between the induced charges on the conductor and the reaction center. ρ_{ele} is the susceptibility of the reaction center, which is independent of the substituent. The MF is the mesomeric field constant that is characteristic of the substituents and it describes the ability of the substituent to induce the field in the pi-system. It has been previously calculated in

Figure 7

The figure 7 shows possible distribution of positive charges on the conductors R1 and R2.


O
C
O
R1
R2
O2N
NO2
+
+
+
+
+
+

ionization pKa. q_R describes the location and the relative charge distribution in conductor and it is further factored into q_{ik} and $r_{kc.}$ q_{ik} is the charge induced at atom k with a reference probe attached at atom I and is calculated using PMO theory.[1, 10] r_{kc} is the through cavity distance between the charge and the reaction center.[1, 10] The MF contribution also depends upon where the conductor is hooked to the reaction center. If it is hooked to the carbonyl carbon, the distance between the charge and the reaction center is smaller than if it is hooked to the oxygen. To illustrate, we have calculated the MF contribution for alkaline hydrolysis of ethyl p-nitrobenzoate to be 0.32 log-unit compared to 0.03 log-unit for alkaline hydrolysis of p-nitrophenyl acetate under the same conditions.

Sigma Induction Effect

The sigma induction occurs due to the difference in electronegativity between the reaction center and the substituents.[1, 10] For base and general base-catalyzed hydrolyses the reaction center has a large electronegativity and methyl substituents, for example, will move charge or electrons into the reaction center and decrease the hydrolysis rate constant. The acid reaction center, on the other hand, is found to be less electronegative and the perturbations are always quite small. The sigma induction is effective only up to two atoms away from the reaction center and beyond the second atom it is assumed to be negligible. The sigma induction due to electronegativity difference between the reaction center and the perturber is calculated using the following equation.

$$\delta_{sigma} * \log K_{(eq)c} = \rho_{ele} \Sigma (\chi_c - \chi_s).$$

Where, (δ_{sigma} * $logK_{(eq)c}$) is the sigma induction effect due to electronegativity difference between the reaction center and the perturber and ρ_{ele} is the susceptibility of the reaction center due to field. χ_c and χ_s are the electronegativity of the reaction center and the substituents respectively.[1] The χ_s terms were previously calibrated using ionization pKa.

Resonance Effect

Resonance is a phenomenon of pi-electrons moving in or out of the reaction center. It plays two important roles in ester hydrolysis. The major impact is that of resonance stabilization of the leaving group. Thus pi-network attached to the oxygen of the ester reaction center have a pronounced effect and greatly increase the hydrolysis rate. Pi-network attached to the carbonyl tends to destabilize the leaving group, but the effect is much smaller. The resonance effect is calculated from a following equation.

$$\delta_{res} * logK_{(eq)c} = \rho_{res} * (\Delta q)_c$$

Where (δ_{res} * $logK_{(eq)c}$) is the resonance effect due to interaction between the pi-network in the perturber and reaction center. ρ_{res} is the susceptibility of the reaction center to the resonance interactions. $(\Delta q)_c$ is the fraction loss of NBMO (nonbonding molecular orbital) charge from the surrogate reaction center calculated based on PMO theory. [1, 10]

External Perturbation Model

The external perturbation model describes the solvation, steric and temperature effects and their contributions to the hydrolysis rate constant.

Solvation Effect

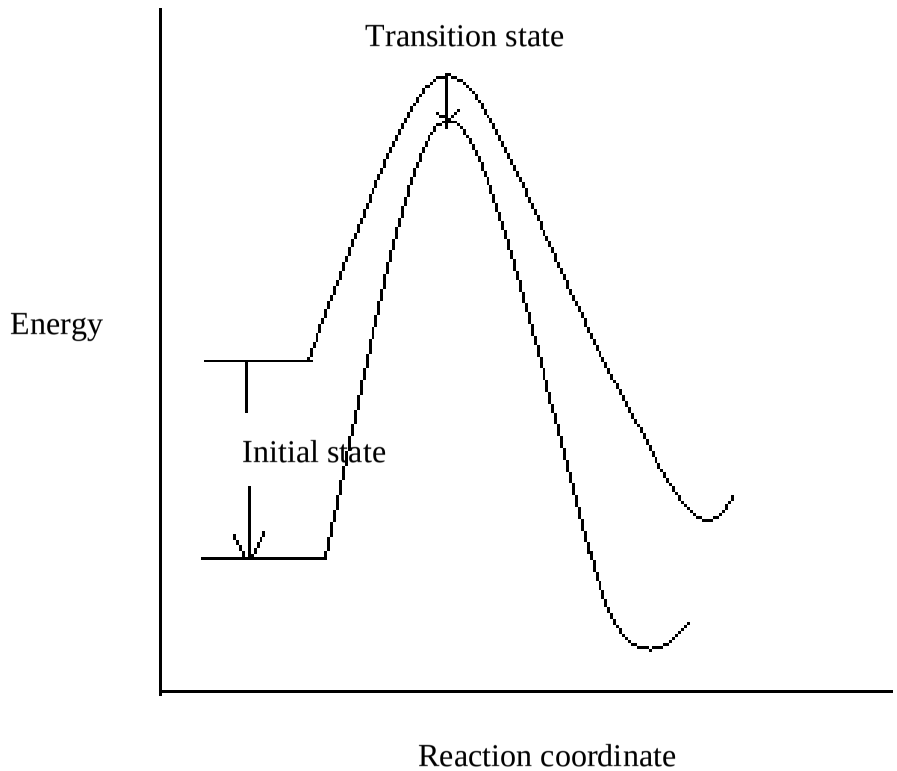
Solvation effect for ester hydrolysis includes hydrogen bonding and field stabilization effects. The hydrogen bonding gauges the hydrogen acceptor effect (alpha) and hydrogen donor effect (beta) of the esters, while the field stabilization describes the effect of dielectricity upon the hydrolysis rate constant.

Hydrogen Bonding

The hydrogen-bonding model for ester hydrolysis includes hydrogen acceptor effect (alpha) and hydrogen donor effect (beta). The alphas and betas describe the difference in solvation between the initial and transition states. If the transition state is more solvated or stabilized than the initial state, the hydrolysis rate constant increases. The negatively charged transition states of base and general base catalyzed hydrolysis are strongly solvated or stabilized by alphas, while the betas tend to destabilize it. Thus, the alphas are supposed to increase the hydrolysis rate constant and the betas decrease it. However, the alphas not only solvate the transition states, but also solvate the attacking hydroxide ion making the initial state more stabilized than the transition state (figure 8). Thus, the alphas decrease the hydrolysis rate constant. On the other hand, the betas interact with the alphas freeing up the hydroxide ions to react with the esters and it increases the hydrolysis rate constant. For acid-catalyzed hydrolysis both the alphas and betas stabilize the initial state more than the transition state. Therefore, they both decrease the hydrolysis rate constant. Further, the alpha and beta contributions to the hydrolysis rate constant from various mixed solvents depend on the amount of alphas and betas available in those solvents. To illustrate, pure water solvent has equal alpha and beta, while the mixed solvents have less alpha and more beta. Consequently, the alpha

Figure 8

The effect of alphas on initial and transition states. The alphas tremendously solvate the hydroxide ion and stabilize the initial state more than the transition state. As a result, the alphas decrease the hydrolysis rate constant during ester hydrolysis.


Transition state
Energy
Initial state
Reaction coordinate

contribution from pure water to hydrolysis rate constant in base and general base catalyzed hydrolysis should be lower or more negative than from the mixed solvents. The beta contribution, on the other hand, should be higher in mixed solvents than in pure water. The mathematical expressions for alpha and beta are given below.

$$\text{Alpha} = \left(C_A * \text{alpha} * \left(1 - \text{Fb6} * \text{Volume}\right) \right) \Big/ T_k$$

$$\text{Beta} = \left(B_A * \text{beta} \right) \Big/ T_k$$

Where, Alpha is the hydrogen acceptor effect of the esters, C_A is the data-fitted parameter for hydrogen donor effect, alpha is the hydrogen donating value of the solvent, Fb6 is the data-fitted parameter for the volume of alpha of the solvent, Volume is the volume of alpha of the solvent and T_k is the temperature in Kelvin. Further, Beta is the hydrogen donor effect of the ester, B_A is the data-fitted parameter for the hydrogen donor effect, beta is the hydrogen acceptor value of the solvent and T_k is the temperature in Kelvin.

Field Stabilization Effect

The field stabilization effect includes the dielectric constant term. The dielectric constant describes the solvation of initial and transition states of the reactants in the hydrolysis of esters. The dielectricity of the solvents solvates or stabilizes the initial state more than the transition state. Thus, it decreases the hydrolysis rate constant. Comparing dielectricity effect on hydrolysis rate constant in different mixed solvents, we observe dielectricity or field stabilization effect to be higher or less negative in pure water than in

other mixed aqueous solvents. The reason for this phenomenon is that the high dielectricity of pure water stabilizes the transition state more than by the mixed solvents, which have less dielectricity. The mathematical expression for the field stabilization effect is given below.

$$\text{Field stabilization} = C_{FS} * 1e^{6} \Big/ \left(T_k * \left(\text{Dielectric} + \text{Damp} \right) \right)$$

Where, C_{FS} is the data-fitted parameter for the field stabilization, T_k is the temperature in Kelvin and Damp is the adjustment factor.

Steric Effect

The normal trend for steric effect is that as the bulkiness of the substituents increases the steric effect increases. Thus, the steric effect always decreases the hydrolysis rate constant. Comparing the steric effect on hydrolysis rate constant in various solvents, we observe the trend of lesser steric effect in pure water than in other mixed solvents. The reason for this trend is that pure water solvates the substituents more and aligns the structure of the esters in suitable position for the attacking hydroxide ion or water molecule. On the other hand, the mixed aqueous solvents partially solvate the substituents and deform the structure of esters, which creates the hindrance to attack from the hydroxide ion or water molecule. Thus, the reaction does not proceed in normal rate and the hydrolysis rate constant decreases. The mathematical expression for steric effect is given below.

$$\text{Steric} = C_S * \text{Volume} \Big/ \left(T_k * \left(\text{Dielectric} + \text{Damp} \right) \right)$$

Where, C_S is the data-fitted parameter for the steric term, Volume is the steric volume of the substituents and Damp is the adjustment factor.

Temperature Effect

For temperature effect, we use the Arrhenius equation as shown below.

$$k = A\, e^{-(Ea/RT)} \quad \text{OR} \quad k = e^{-(\Delta G/RT)}$$

Where k is the hydrolysis rate constant, A is the pre-exponential factor or the frequency factor, E_a is the activation energy (the minimum energy required to form a product from the reactants), $\Delta G^{\neq}$ is the activation Gibbs energy, R is the gas constant (8.31451 JK^{-1} mol^{-1}) and T is the temperature in Kelvin. If we take a log of the above latter equation, we obtain $\log k = - \Delta G^{\neq} / 2.317(RT)$. The previous equation shows that the logarithmic rate constant increases as the temperature in Kelvin increases. The temperature effect is incorporated in field stabilization effect, alpha, beta and steric effect. To illustrate, we consider the temperature term in expression for steric effect above. According to the expression, as the temperature increases the steric effect decreases. The reason behind this trend is that as the temperature increases the reactants tend to mimic gas phase structure, which shows minimal or null steric effect for hydrolysis of esters.

CHAPTER 3

SPARC COMPUTATIONAL MODEL FOR HYDRATION EQUILIBRIA

Hydration Model

The computational model of hydration equilibria for aldehydes/ketones and quinazolines incorporates the pKa and Henry constant computational models. The pKa computational models are used to calculate the effects of resonance, mesomeric field, direct field, steric, etc. on the hydration reaction calculated. For detailed information on these effects, please, refer to reference 1. These various effects are perturbation terms. That is, appended molecular structures (the perturbers) perturb the reactivity of the reference compounds, which are formaldehyde and quinazoline for hydration of aldehydes/ketones and quinazolines, respectively. For the resonance contribution to the hydration equilibrium:

$$Res_{(hydration)} = (Res_{(ald/quin)} - Res_{(reference)}) * Zres.$$

Where, $Res_{(hydration)}$ is resonance contribution to the hydration equilibrium of aldehydes/ketones or quinazolines, $Res_{(ald/quin)}$ is the magnitude of NBMO (Non Bonding Molecular Orbit) delocalization out of the reaction center for aldehydes/ketones or quinazolines from the pKa resonance model, $Res_{(reference)}$ is this same resonance value for the reference compound (formaldehyde or quinazoline) and 'Zres' is a data fitted or trained parameter. The rest of the perturbation terms for hydration of aldehydes/ketones and quinazolines are calculated similarly. All the perturbations are assumed to be for gas phase hydration of the molecule. This was done to make the calculation in mixed solvent

system easier to do. On the other hand, the Henry constant model predicts the Henry constants for aldehydes/ketones, quinazolines and their hydrated forms.

The various free energies calculated in determining the hydration of a ketone/aldehyde are shown in figure 9. Here, $\Delta G_{hydration(g)}$ is the free energy for hydration of aldehydes/ketones in the gas phase, and its value is calculated by adding the perturbations as described earlier. $\Delta G_{transfer(o)}$ is the free energy of transfer of the hydrated form (the gem-diol). $\Delta G_{transfer(=o)}$ is the free energy of transfer of the aldehyde/ketone and $\Delta G_{hydration(l)}$ is the resultant free energy of hydration of aldehyde/ketone in solution. The resultant free energy ($\Delta G_{hydration(l)}$) is related to the hydration equilibrium constant by a following equation:

$$\triangle G_{hydration(l)} = -RT \ln K_{hydration(l)}$$

$$pK_{hydration(l)} = \triangle G_{hydration(l)} / (2.33 * RT).$$

Where R, T and $K_{hydration(l)}$ are gas constant, temperature in Kelvin and hydration equilibrium constant respectively. $pK_{hydration(l)}$ is the logarithmic hydration equilibrium constant. The hydration equilibrium constant for quinazolines is calculated similarly.

Figure 9

A thermodynamic Cycle involving various free energies, while determining the hydration equilibrium constant of a aldehyde/ketone.

P-C=O(g) ⟶ P-C$(OH)_2$ (g) $\triangle G_{hydration}$ (g) -----1.

P-C$(OH)_2$ (g) ⟶ P-C$(OH)_2$ (l) $\triangle G_{transfer}$ (O) -----2.

P-C=O(l) ⟶ P-C=O(g) $-\triangle G_{transfer}$ (=O) -----3.

P-C=O(l) ⟶ P-C$(OH)_2$ (l) $\triangle G_{hydration}$ (l) -----4.

CHAPTER 4

EXPERIMENTAL

Data Collection

For our calculational simulations, we have collected as many data as possible. The number of experimental measurements for hydrolysis of esters is reasonable. We have 653, 657, and 150 measurements for base, acid and general base-catalyzed ester hydrolysis. However, we have collected only 37-aldehydes/ketones and 28-quinazolines measurements for the hydration constants. We believe we have found all the measurements in the literatures for the hydration of these compounds.

Data File

After collecting the data, we convert these measurements into a format suitable for batch processing by the SPARC calculator. A sample data file is shown in figure 10. Four lines describe the molecule's conditions and the calculation type. The first line characterizes the reaction solvent specifying a list of volume fractions and a list of corresponding solvents that make up the reaction medium. The second line describes the experimental ester hydrolysis rate constant in log-unit and the temperature at which the hydrolysis took place. The third and the fourth lines give the molecular structure in SMILE notation and type of mechanism for the hydrolysis, respectively. For example, the 'a_rcor' in the fourth line means that the reaction mechanism for hydrolysis is acid-catalyzed.

Figure10

A data file for hydrolysis of esters.

```
[[1],[water]].  % 1
['-3.97/25'].
'CC(=O)OCC'.
a_rcor.

[[0.7,0.3],[acetone,water] % 377
['-4.83/25'].
'CCOC(=O)Cc1ccccc1'.
a_rcor.

[[0.25,0.75],[dioxane,water]].  % 499
['-4.46/25'].
'CC(=O)OCCl'.
a_rcor.

[[0.75,0.25],[ethanol,water]].  % 234
['-2.24/25'].
'CCOC(=O)Cc1c(I)cccc1'.
rcor. % base hydrolysis

[[0.33,0.67],[acetonitrile,water]].  % 314
['-1.25/25'].
'c1ccccc1C(=O)Oc2ccccc2'.
rcor.

[[1],[water]].  % 37
['-7.08/25'].
'CC(=O)Oc1cc(N(=O)=O)c(N(=O)=O)cc1'.
g_rcor. % general base hydrolysis
water. % catalyst

[[0.4,0.6],[ethanol,water]].  % 137
['-3.66/25'].
```

Training File

A training file is a modified version of the data file. The training file is used to train various reaction center susceptibility parameters, such as field, resonance and sigma to obtain a best least squares fit of the observed and calculated hydrolysis rate constants. A sample training file is shown in figure 11. The training file usually consists of three sections. The first section gives the number of hydrolysis rate constant calculations to be performed. The second section is a list of the various reaction center susceptibility parameters being trained. Finally, the last section consists of description of molecular structure, conditions and reaction type as in the data file.

Jacobian Least Squares Fit

We use a non-linear Jacobian Least Squares Fit method to extract training parameters, such as sigma, resonance, steric, alpha, beta, and so on, while determining the hydrolysis rate constant of esters. The Jacobian Least Squares Fit calculation involves the determination of $\Delta\phi$, J_{ij}, J, J^T and ΔC. $\Delta\phi$ is a vector representing the difference between the observed and calculated hydrolysis rate constants. J_{ij} is an element of the Jacobian matrix, i = 1, 2, 3,……m are the experimental data points and j = 1, 2, …..n are the parameters to be extracted. J is the Jacobian matrix of the J_{ij} elements and J^T is the transpose of Jacobian matrix J. ΔC is a correction factor for the parameter to be extracted, which is given an arbitrary guess. [9]

Figure 11

A sample training file

```
*First section

363.

*Second section

[
    [a_rcor,b2_factor,1,1],
    [a_rcor,b3_factor,1,1],
    [a_rcor,rcor_mf_adjust,1,1],
    [a_rcor,r_pi,1,1],
    [a_rcor_,pka_ro_minus,1,1],
%% [a_rcor,pka_ro_minus,1,1],
%  [a_rcor,pka_a_f,1,1],
%%  [a_rcor,pka_pe,1,1],
    [a_rcor,b5_factor,1,1],
    [a_rcor,reference_point2,1,1]
].

*Third section

['Acid Hydrolysis',[1],[water]].  % 1
25.
-3.97.
'CC(=O)OCC'.
a_rcor.

['Acid Hydrolysis',[1],[water]].  % 2
25.
-4.04.
'CCC(=O)OCC'.
a_rcor.
```

Determination of $\Delta\phi$

The $\Delta\phi$ vector is determined as follows. We make initial guesses of the parameters to be trained. Using these initial guesses and the models described above we calculate the hydrolysis rate constants for a large set of molecules. The $\Delta\phi$ vector is calculated for the m experimental data points as follows:

$$(\Delta\phi)_i = Rate_{i(observed)} - Rate_{i(calculated)} \quad 9$$

Where $Rate_{i(observed)}$ and $Rate_{i(calculated)}$ are the observed and calculated hydrolysis rate constants for the m experimental data points respectively.

Determination of J_{ij}

The J_{ij} represents the elements of Jacobian Matrix J, and it is denoted as:

$$J_{ij} = \frac{\delta Rate_i}{\delta C_j} \quad 9$$

Where, δ denotes partial derivative of the ith calculated hydrolysis rate constant with respect to the jth parameter. For example, if we extract two parameters Beta and Steric, the elements of Jacobian matrix will be as follows:

$$J_{i1} = \frac{\delta Rate_i}{\delta C_{Beta}}$$

$$J_{i2} = \frac{\delta Rate_i}{\delta C_{Steric}} \quad .$$

Since the above equations do not represent the exact analytical expressions for calculating the hydrolysis rate constant, the partial derivative of the hydrolysis rate

constant cannot be performed directly and a numerical solution must be chosen. For the numerical solution, for example, the C_{Beta} parameter is changed by 5 %, while C_{Steric} is kept unchanged or constant for every cycle. That is, $\delta C_{Beta} = 0.05 * C_{Beta}$. Then $(C_{Beta})_{modified}$ is calculated as follows: $(C_{Beta})_{modified} = C_{Beta} + \delta C_{Beta}$. Using the $(C_{Beta})_{modified}$ value, the new or modified hydrolysis rate constant ($Rate_{i(modified)}$) can be calculated. Then $\delta Rate_i$ is calculated as follows: $\delta Rate_i = Rate_i - Rate_{i(modified)}$. The matrix element J_{i1} is then calculated as the ratio of $\delta Rate_I / \delta C_{Beta}$. Similarly, the matrix element J_{i2} is calculated for C_{Steric} parameter provided that the C_{Beta} parameter is changed back to its original value and kept constant. [9]

For m experimental data points, the Jacobian matrix elements $J_{i1 \text{ and } J_{i2}}$ are calculated as follows [9] :

$$\begin{array}{l|l} J_{11} = \dfrac{\delta Rate_1}{\delta C_{Beta}} & J_{12} = \dfrac{\delta Rate_1}{\delta C_{Steric}} \\ J_{21} = \dfrac{\delta Rate_2}{\delta C_{Beta}} & J_{22} = \dfrac{\delta Rate_2}{\delta C_{Steric}} \\ J_{31} = \dfrac{\delta Rate_3}{\delta C_{Beta}} & J_{32} = \dfrac{\delta Rate_3}{\delta C_{Steric}} \\ \vdots & \vdots \\ J_{m1} = \dfrac{\delta Rate_m}{\delta C_{Beta}} & J_{m2} = \dfrac{\delta Rate_m}{\delta C_{Steric}} \end{array}$$

Determination of Jacobian matrix J and J^T

The Jacobian matrix J is defined as m * n elements [9], while J^T is simply a transposed matrix of J. The J^T matrix is formed by interchanging the rows and columns of the J

matrix. [9] Then ($J^T * J$) matrix is constructed as follows [9] :

$$J = \begin{vmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \\ J_{31} & J_{32} \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ J_{m1} & J_{m2} \end{vmatrix}$$

$$J^T * J = \underbrace{\begin{vmatrix} J_{11} & J_{21} & J_{31} & \cdot & \cdot & \cdot & J_{m1} \\ J_{12} & J_{22} & J_{32} & \cdot & \cdot & \cdot & J_{m2} \end{vmatrix}}_{J^T} \underbrace{\begin{vmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \\ J_{31} & J_{32} \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ J_{m1} & J_{m2} \end{vmatrix}}_{J} = \begin{vmatrix} \Sigma (J_{i1})^2 & \Sigma (J_{i1} * J_{i2}) \\ \Sigma (J_{i2} * J_{i1}) & \Sigma (J_{i2})^2 \end{vmatrix}$$

Next, an inverse matrix, $(J^T * J)^{-1}$, is formed. The $(J^T * J)^{-1}$ is formed in such a way so that the multiplication of ($J^T * J$) and $(J^T * J)^{-1}$ gives a unique matrix. [9]

$$(J^T * J)^{-1} = \begin{vmatrix} \Sigma (J_{i2})^2 & -\Sigma (J_{i1} * J_{i2}) \\ -\Sigma (J_{i2} * J_{i1}) & \Sigma (J_{i1})^2 \end{vmatrix}$$

Then $(J^T * \Delta\phi)$ matrix is formed as follows [9] :

$$(J^T * \Delta\phi_i) = \underbrace{\begin{vmatrix} J_{11} & J_{21} & J_{31} & \cdots & J_{m1} \\ J_{12} & J_{22} & J_{32} & \cdots & J_{m2} \end{vmatrix}}_{J^T} \underbrace{\begin{vmatrix} \Delta\phi_1 \\ \Delta\phi_2 \\ \Delta\phi_3 \\ \vdots \\ \Delta\phi_m \end{vmatrix}}_{\Delta\phi} = \begin{vmatrix} \Sigma (J_{i1} * \Delta\phi_i) \\ \Sigma (J_{i2} * \Delta\phi_i) \end{vmatrix}$$

Determination of ΔC

The ΔC vector is determined using an expression: $\Delta C = (J^T * J)^{-1} * (J^T * \Delta\phi)$. [9]

$$(\Delta C) = \underbrace{\begin{vmatrix} \Sigma (J_{i2})^2 & -\Sigma (J_{i1} * J_{i2}) \\ -\Sigma (J_{i2} * J_{i1}) & \Sigma (J_{i1})^2 \end{vmatrix}}_{(J^T * J)^{-1}} \underbrace{\begin{vmatrix} \Sigma (J_{i1} * \Delta\phi_i) \\ \Sigma (J_{i2} * \Delta\phi_i) \end{vmatrix}}_{(J^T * \Delta\phi_i)}$$

The multiplications generate the following elements of the ΔC matrix:

$$(\Delta C_{Beta}) = \Sigma (J_{i1} * \Delta\phi_i) * \Sigma (J_{i2})^2 - \Sigma (J_{i2} * \Delta\phi_i) * \Sigma (J_{i1} * J_{i2})$$

$$(\Delta C_{Steric}) = \Sigma (J_{i2} * \Delta\phi_i) * \Sigma (J_{i1})^2 - \Sigma (J_{i1} * \Delta\phi_i) * \Sigma (J_{i2} * J_i 1)$$

Where, ΔC_{Beta} and ΔC_{Steric} are corrections for arbitrary guesses $(C_{Beta})_{old}$ and $(C_{Steric})_{old}$ respectively. The new guesses for the parameters can then be calculated as follows:

$$(C_{Beta})_{new} = (C_{Beta})_{old} + (\Delta C_{Beta})$$

$$(C_{Steric})_{new} = (C_{Steric})_{old} + (\Delta C_{Steric})$$

Where $(C_{Beta})_{new}$ and $(C_{Steric})_{new}$ are new values for the parameters Beta and Steric respectively. Once the new values for the parameters are calculated, the convergence test is done to see if the newly calculated values are reasonable. The convergence test for Jacobian Least Squares Fit method requires that the difference between the old and new parameters be less than 0.1 % of the old value. [9] For example, if we were calculating the C_{Beta} parameter, the convergence test would have to satisfy following condition:

$$\left| (C_{Beta})_{new} - (C_{Beta})_{old} \right| < 0.001 * (C_{Beta})_{old}$$

If the above condition is met, the new value for C_{Beta} parameter gets accepted. Otherwise, the above cycle is repeated until the new value for C_{Beta} parameter is converged.

CHAPTER 5

RESULTS AND DISCUSSIONS FOR HYDROLYSIS

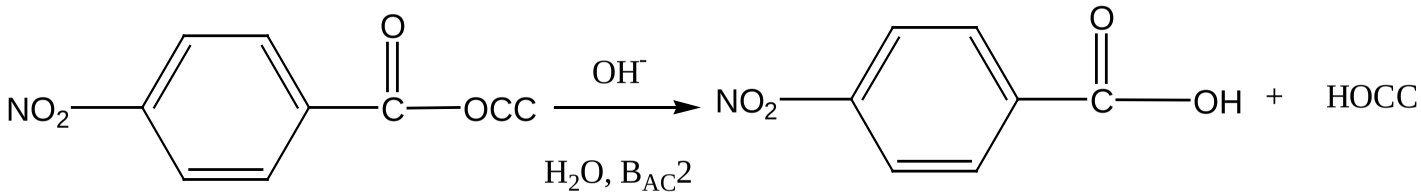
Tables 5-7 show observed versus calculated values for hydrolysis rate constants of esters in base, acid and general base catalyzed hydrolysis respectively. These sets represent 321, 416 and 50 unique esters in base, acid and general base catalyzed hydrolysis of esters respectively. Because several of the esters were measured under different conditions (solvent mixtures and temperatures) there were 653, 667 and 150 base, acid and general base catalyzed calculations performed. The RMS values obtained for these three mechanisms are 0.37, 0.37 and 0.35 log-units respectively. To show how the SPARC calculates each ester's hydrolysis rate constant, we have provided sample calculations for the hydrolysis rate constants for ethyl p-nitrobenzoate and p-nitrophenyl acetate. The calculations are described below.

Sample Calculation

Figures 12-14 show the sample calculations of hydrolysis rate constant for ethyl p-nitrobenzoate in base and acid catalyzed media and p-nitrophenyl acetate in general base medium at room temperatures. As described earlier in the SPARC computational model section, the hydrolysis rate constant is a summation of contributions from the reference rate, internal perturbations and external perturbations.

Figure 12

A sample calculation for determination of hydrolysis rate constant for alkaline hydrolysis of ethyl p-nitrobenzoate in water at 25C.



Reference Rate = Pre-exp + $LogT_k$ + Ref1 + Ref2 / T_k

= 3.357 + Log(298.15) + 2.283 + (-2134.6 / 298.15)

= <u>0.951</u>

$Rate_{(Internal\ Perturbation)}$ = Resonance + Sigma + Field + MF + r_pi

= -0.134 + (-0.905) + 0.319 + 0.647 + (-0.770)

= <u>-0.842</u>

$Rate_{(External\ Perturbation)}$ = Field Stabilization + Alpha + Beta + Steric

= -2.843 + (-1.559) + 5.311 + (-1.289)

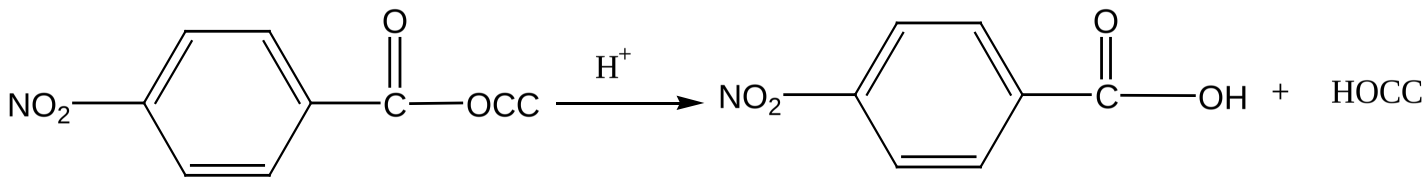
= <u>-0.382</u>

Calculated Rate = <u>-0.273</u>

Observed Rate = <u>-0.58</u>

Figure 13

A sample calculation for determination of hydrolysis rate constant for acid catalyzed hydrolysis of ethyl p-nitrobenzoate in 60% ethanol-water at 80C.



60% ethanol-water at 80C, $A_{AC}2$

Reference Rate = Pre-exp + $LogT_k$ + Ref1 + Ref2 / T_k

= 3.357 + Log(353.15) + 1.161 + (-2509.1 / 353.15)

= -0.041

$Rate_{(Internal\ Perturbation)}$ = Resonance + Sigma + Field + MF + r_pi

= -0.295 + (-0.154) + (-0.042) + 0.147 + (-0.977)

= -1.116

$Rate_{(External\ Perturbation)}$ = Field Stabilization + Alpha + Beta + Steric

= -0.297 + (-0.659) + (-0.792) + (-1.552)

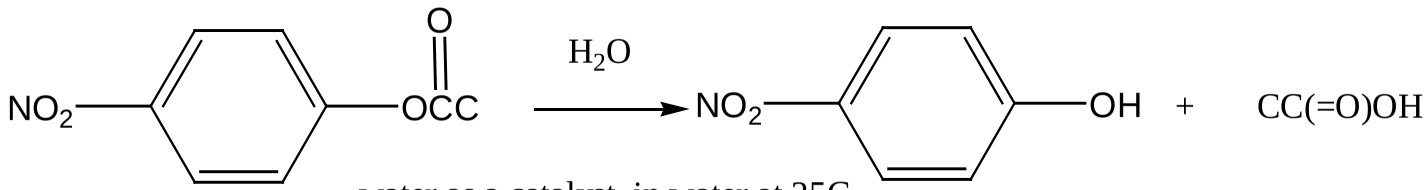
= -3.302

Calculated Rate = -4.459

Observed Rate = -4.54

Figure 14

A sample calculation for determination of hydrolysis rate constant for neutral hydrolysis of p-nitrophenyl acetate in water at 25C.



water as a catalyst, in water at 25C

Reference Rate = Pre-exp + $LogT_k$ + Ref1 + Ref2 / T_k

= 3.357 + Log(298.15) + 1.174 + (-4098.7 / 298.15)

= -9.096

$Rate_{(Internal\ Perturbation)}$ = Resonance + Sigma + Field + MF + r_pi

= 0.722 + (-1.865) + 0.346 + 0.513 + 0.904

= 0.622

$Rate_{(External\ Perturbation)}$ = Field Stabilization + Alpha + Beta + Steric + GBC effect

= -4.530 + (-0.736) + 7.173 + (-0.781) + (-0.769)

= 0.355

Calculated Rate = -8.118

Observed Rate = -7.81

Reference Rate

The reference rate is a summation of pre-exponential factor in log units, the log of temperature in Kelvin, the entropic (Ref1) and the enthalpic ($Ref2/T_k$) terms in log units. The reference rates for base and acid catalyzed hydrolysis of ethyl p-nitrobenzoate are 0.951 and -0.041 log-units (figures 12 and 13) respectively and –9.096 log-unit for general base catalyzed hydrolysis of p-nitrophenyl acetate (figure 14).

Internal Perturbations

The internal perturbations are summation of resonance, sigma, r_pi, direct field and indirect field (MF) interactions. The r_pi interaction term has not been described earlier. It is similar to sigma induction, except it involves the pi-electrons instead of sigma electrons. The internal perturbations for ethyl p-nitrobenzoate in base and acid catalyzed hydrolysis are –0.842 and –1.116 log-unit respectively, while 0.622 log-unit for p-nitrophenyl acetate in general base catalyzed hydrolysis. The analyses of various internal perturbation interactions, which contribute to the total internal perturbation, are described below.

Resonance Effect

The total forward resonance effects are -0.134 and –0.295 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid catalyzed media. That is, the resonance contributions are negative and decrease the hydrolysis rate constant because the phenyl ring attached to the alkyl side of the esters increases the activation energy. In contrast, the total forward resonance is 0.722 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. The huge positive contribution and resulting increase in

hydrolysis rate constant is due to stabilization of the leaving group by the phenyl ring and decreases the activation energy.

Sigma Induction

The total sigma induction is -0.905 and -0.154 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid catalyzed media respectively. Since the reaction center in the base catalyzed hydrolysis is more electronegative than in the acid catalyzed hydrolysis, we see more negative contribution from the ethyl group in the base than in the acid catalyzed hydrolysis. In addition, we observe –1.865 log-unit contribution from sigma for general base catalyzed hydrolysis of p-nitrophenyl acetate because the methyl substituent is attached directly to the highly electronegative reaction center. That is, the methyl substituent attached to the alkyl side does not encounter shielding from the oxygen atom and the sigma induction effect is enhanced more than if it is attached to the acyl side.

Direct Field

The direct field (F) is 0.319 and -0.042 log-units for base and acid catalyzed hydrolysis of ethyl p-nitrobenzoate respectively, while it is 0.346 log-unit for general base catalyzed hydrolysis of p-nitrophenyl acetate. Since the transition states of the base and general base catalyzed hydrolysis of esters are negative, the field always contributes positively to the internal perturbations. In contrast, the field contributes negatively to the internal perturbations for acid catalyzed hydrolysis because of the positive transition state that occurs during the hydrolysis reaction.

Pi-Induction (MF or Indirect Field)

The pi-induction or indirect field (MF) is 0.647 and 0.147 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid catalyzed media respectively and it is 0.513 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. The MF contributions are positive in all three catalyzed media and increase the hydrolysis rate constant because the induced positive charges on the phenyl ring stabilize the charged transition states. In addition, we see large positive values for the base and general base catalyzed hydrolysis because of the negative transition states that occur during the hydrolysis reactions for these mechanisms. The induced positive charges on the phenyl ring enhance the stabilization of the negative transition states more. In contrast, the small positive value for acid catalyzed hydrolysis is due to the positive transition state that occurs during the hydrolysis reaction and diminishing stabilization of it.

r_pi Effect

The r_pi effect is similar to the sigma induction, except it involves the pi-electrons instead of the sigma electrons. In addition, our SPARC computational model for r_pi divides the reaction center (C(=O)O) into e+ (carbonyl carbon) and e- (acyl oxygen) groups. If the substituent containing the pi-system is attached to the e+ group, the r_pi effect contributes negatively or lowers the hydrolysis rate constant. In contrast, if the pi-system is attached to the e- group, the r_pi increases the hydrolysis rate constant. That is exactly what we observe for hydrolysis of p-nitrobenzoate and p-nitrophenyl acetate. The r_pi effects are –0.770 and -0.977 log-units for base and acid catalyzed hydrolysis of ethyl p-nitrobenzoate and 0.904 log-unit for general base catalyzed hydrolysis of p-nitrophenyl acetate.

External Perturbations

The external perturbations are summation of Alpha, Beta, Field Stabilization, Steric and GBC interactions. The GBC effect applies only to the general base catalyzed hydrolysis of esters. The external perturbations for ethyl p-nitrobenzoate in base and acid catalyzed hydrolysis are –0.382 and –3.302 log-unit respectively, while 0.355 log-unit for p-nitrophenyl acetate in general base catalyzed hydrolysis. The analyses of various external perturbation interactions, which contribute to the total external perturbation, are described below.

Field Stabilization Effect

The field stabilization effects are –2.843 and –0.297 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid media respectively, while it is –4.530 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. The field stabilization effect involves the dielectric constant of the solvent and in general it raises the energy of the transition state more than the initial state. As a result, it lowers the hydrolysis rate constant. However, comparing the pure water solvent with the mixed aqueous-nonpolar solvents, we see that a higher dielectric constant increases the hydrolysis rate constant. For example, if we calculate the hydrolysis rate constants for base catalyzed hydrolysis of ethyl p-nitrobenzoate in aqueous-nonpolar mixed solvents, we will observe values more negative than –2.843 log-unit. Similar trends occur for acid and general base catalyzed hydrolysis of esters.

Alpha Effect (Hydrogen Acceptor Effect of Esters)

The Alpha effects are –1.559 and –0.659 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid media respectively, while it is –0.736 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. For base and general base catalyzed hydrolysis, the alphas of the solvent not only solvate the hydrogen acceptor site (β) of the ester, but also solvate the attacking hydroxide ions. This phenomenon stabilizes the initial state more than the transition state. As a result, we see negative contribution from Alpha to the external perturbations. For the acid catalyzed hydrolysis, the alphas of the solvent stabilize the initial state more than the positively charged transition state; therefore, we also see negative contribution from the Alpha to the external perturbations.

Beta Effect (Hydrogen Donor Effect of Esters)

The Beta effects are 5.311 and –0.792 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid media respectively, while it is 7.173 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. For base and general base catalyzed hydrolysis, the betas of the solvent interact less with the hydroxide ions. This phenomenon stabilizes the transition state more than the initial state. As a result, we see positive contribution from Beta to the external perturbations. For the acid catalyzed hydrolysis, the betas of the solvent also destabilize the transition state; therefore, we see negative contribution from the Beta to the external perturbations.

Steric Effect

The steric effects are –1.289 and –1.552 log-units for hydrolysis of ethyl p-nitrobenzoate in base and acid media respectively and it is -0.781 log-unit for hydrolysis of p-nitrophenyl acetate in general base catalyzed medium. The normal trend of steric effect is that bulkier the substituents lower the hydrolysis rate constants. Since both ethyl p-nitrobenzoate and p-nitrophenyl acetate have bulky phenyl rings, the steric effects display huge negative values.

GBC Effect

The GBC effect applies only to the general base catalyzed hydrolysis of esters. It is a product of data-fitted parameter, 'ro_g', and pKa of the catalyst. More basic catalysts have higher the hydrolysis rate constants. Since water is a weak base, we see –0.769 log-unit contribution from the GBC effect to the external perturbations.

Graphical Representation

Using a similar method described in the sample calculation, we have calculated the hydrolysis rate constants for 321, 416 and 50 unique esters in base, acid and general base catalyzed media in various solvents and at different temperatures. Because these measurements are often made in more than one solvent and/or at more than one temperature the total number of calculations for base, acid and general base catalyzed hydrolysis are 653, 667 and 150 respectively.

Base Hydrolysis

The figure 15 shows the graph of observed and calculated hydrolysis rate constants of 321 unique esters hydrolyzed in various solvents and different temperatures. The observed RMS and R^2 values for base catalyzed hydrolysis of esters are 0.37 log-unit and 0.936 respectively. In addition, the graphs for base catalyzed hydrolysis in pure water and individual mixed solvents have been constructed (figures 16-21). The mixed solvents are acetone-water, ethanol-water, methanol-water, dioxane-water and acetonitrile-water. All of the graphs show reasonable RMS and R^2 values, except for hydrolysis of esters in dioxane-water mixed solvents. The RMS and R^2 values for hydrolysis of esters in dioxane-water mixed solvents are 0.473 log-unit and 0.743 respectively. The values for the dioxane-water mixed solvents may be further off than the other sets because this set contains many measurements at very elevated temperatures. The observed values for hydrolysis rate constants in dioxane-water mixed solvents show 0.5 log-unit increase per every 10 C increase in temperature, but our SPARC calculation is showing only a 0.2- 0.3 log-unit increase of hydrolysis rate constant per every 10 C increase in temperature. Therefore, the difference in increase of hydrolysis rate constant per every 10 C increase in temperature between the observed and calculated hydrolysis rate constants adds up quickly in the calculated hydrolysis rate constant to give a significant error. This is probably due to the fact that we do not take into account the variation of effective dielectric constant as a function of temperature. In addition, SPARC was calculating the hydrolysis rate constants for pyridine esters in ethanol-water and methanol-water mixed solvents one log-unit slower than the observed hydrolysis rate constants. We believe that the reason SPARC is calculating the hydrolysis rate constants of pyridine esters one log-unit lower than the observed

Figure 15

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 321 unique esters in six different solvents and at varying temperatures.

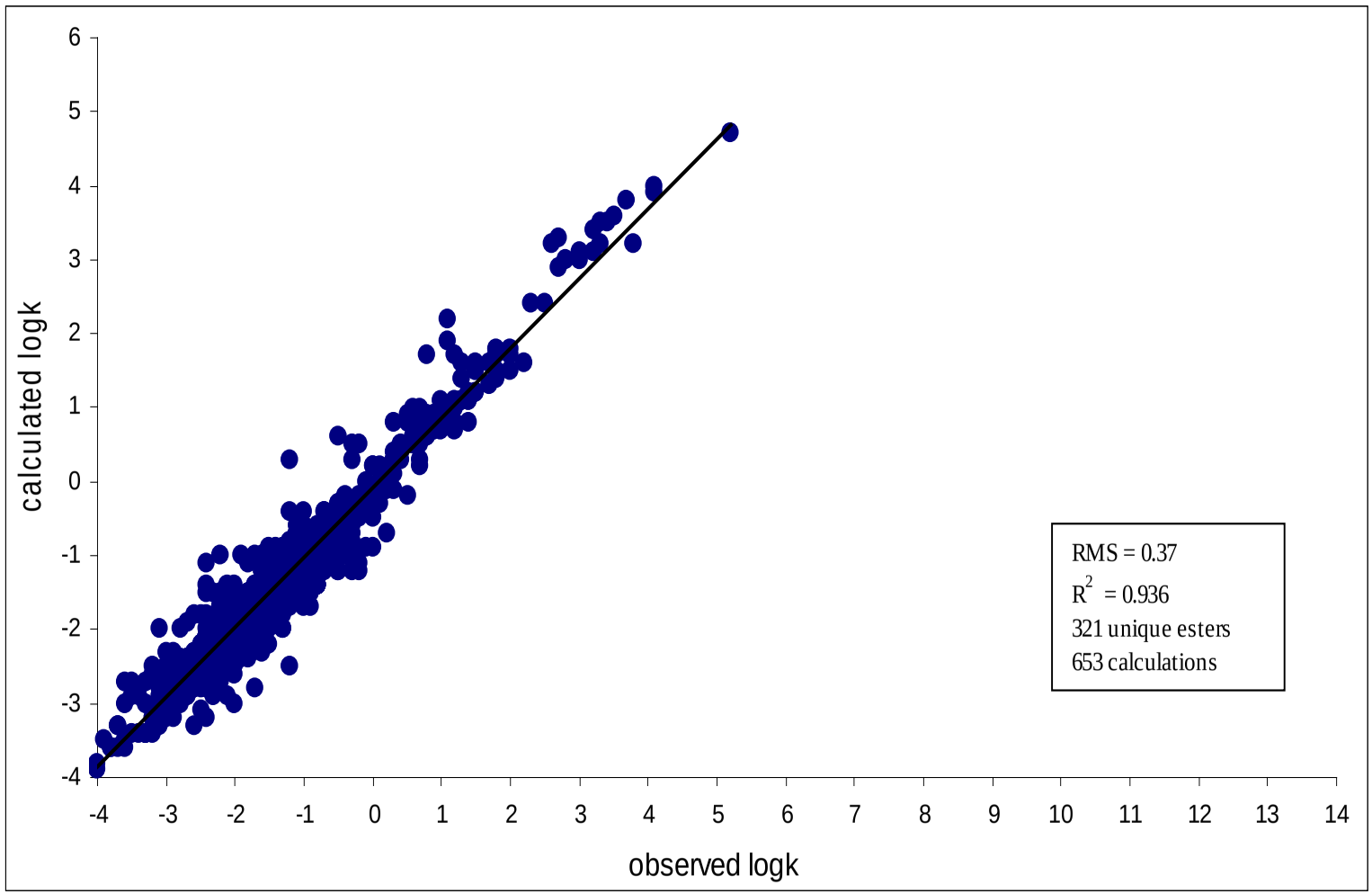

calculated logk
observed logk
6
5
4
3
2
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
RMS = 0.37
R2 = 0.936
321 unique esters
653 calculations

Figure 16

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 112 unique esters in water at various temperatures.

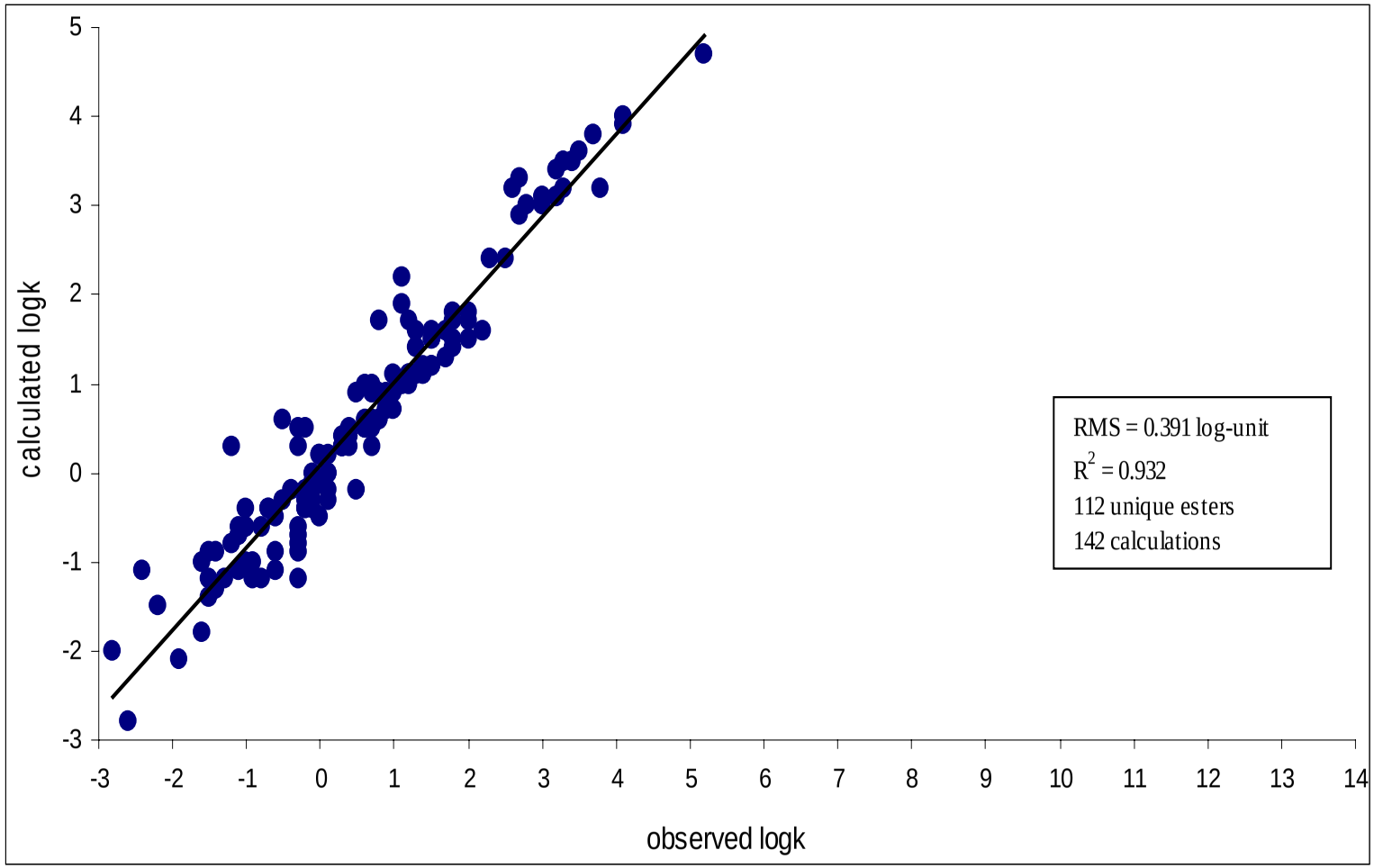

calculated logk
observed logk
5
4
3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
RMS = 0.391 log-unit
R2 = 0.932
112 unique esters
142 calculations

Figure17

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 100 unique esters in acetone-water mixed solvent at various temperatures.

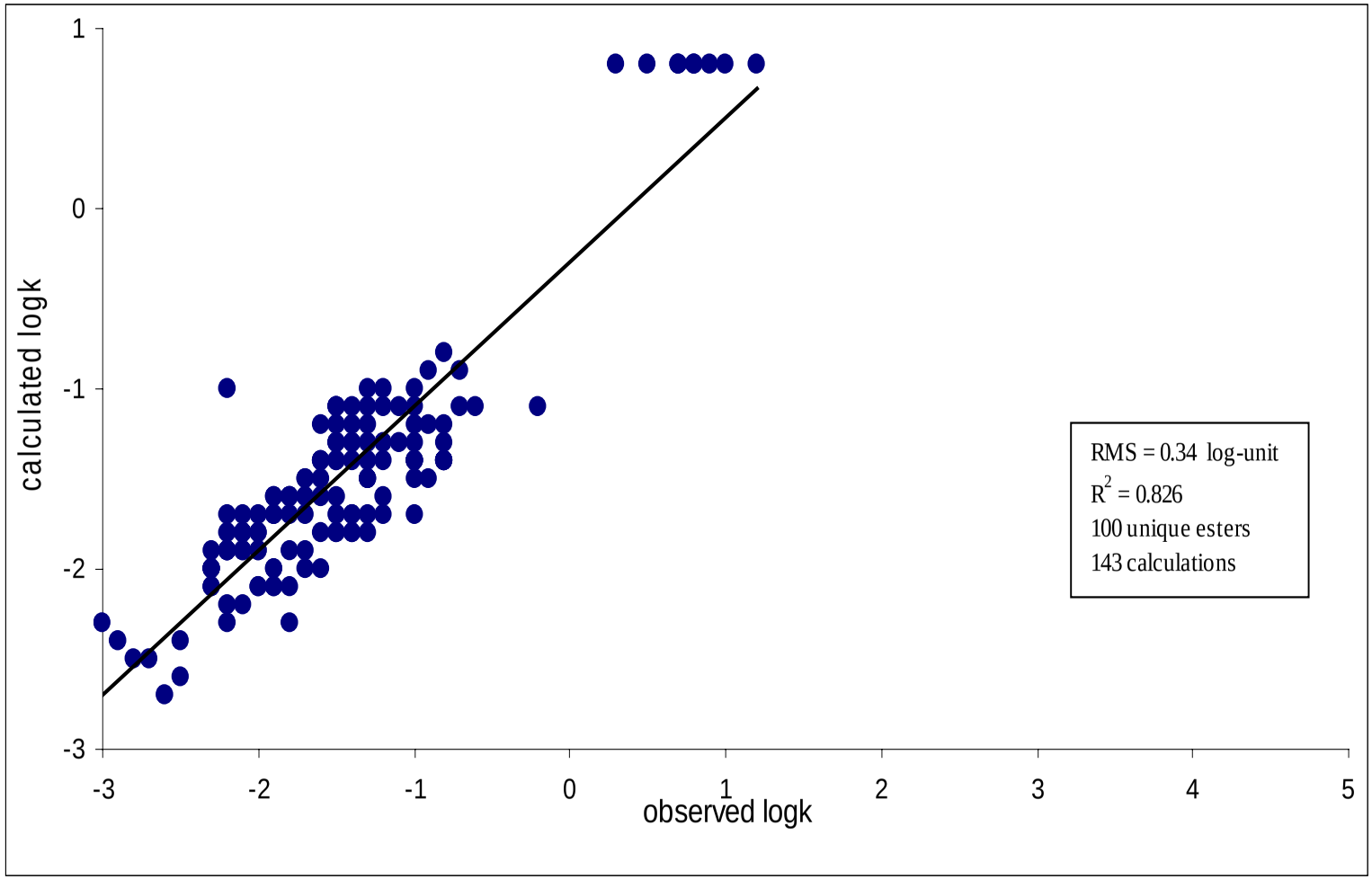

calculated logk
observed logk
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3
4
5
RMS = 0.34 log-unit
R2 = 0.826
100 unique esters
143 calculations

Figure 18

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 44 unique esters in ethanol-water mixed solvent at various temperature.

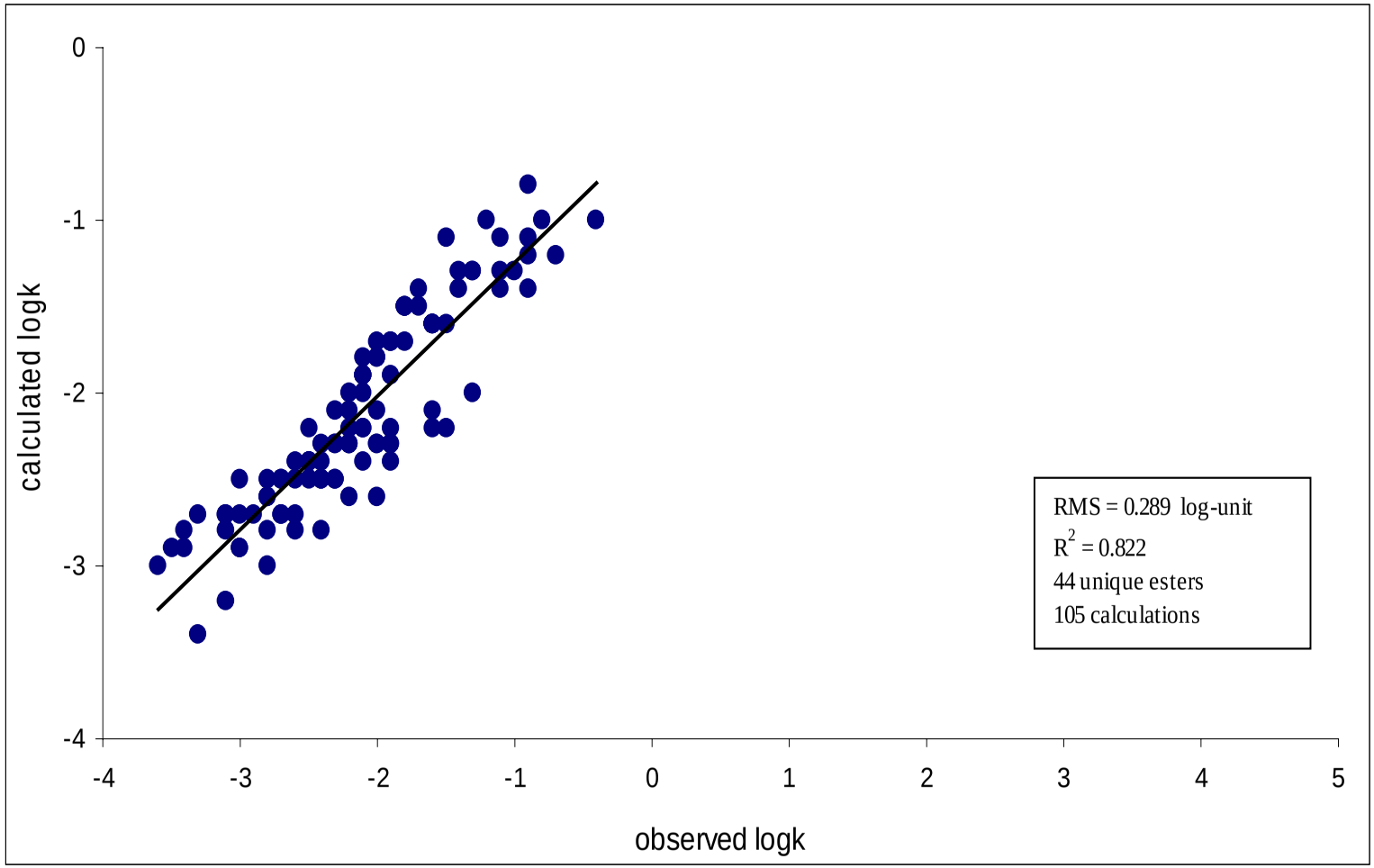

0
-1
-2
-3
-4
calculated logk
-4
-3
-2
-1
0
1
2
3
4
5
observed logk
RMS = 0.289 log-unit
R2 = 0.822
44 unique esters
105 calculations

Figure 19

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 69 unique esters in methanol-water mixed solvent at various temperatures.

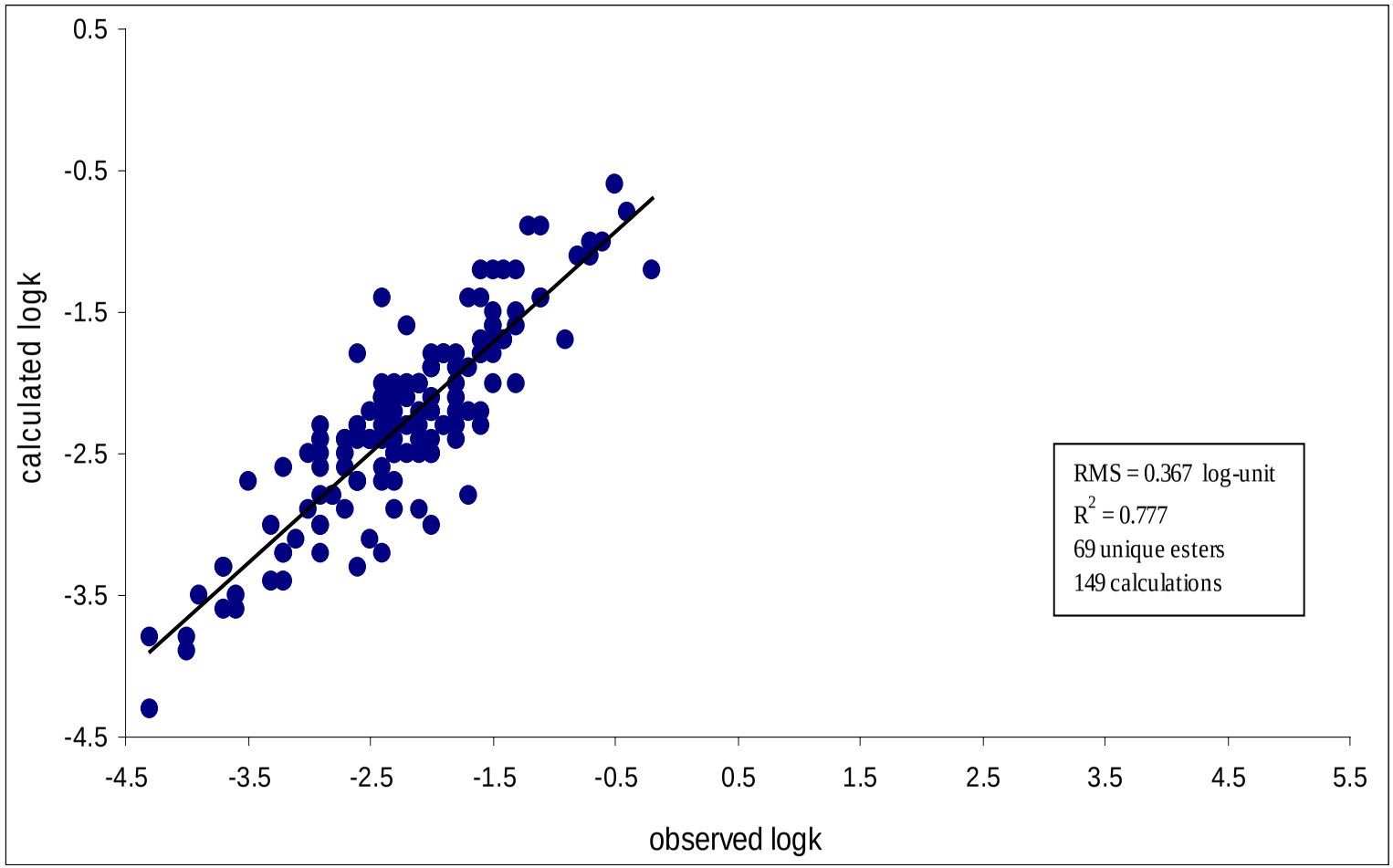

0.5
-0.5
-1.5
-2.5
-3.5
-4.5
calculated logk
-4.5
-3.5
-2.5
-1.5
-0.5
0.5
1.5
2.5
3.5
4.5
5.5
observed logk
RMS = 0.367 log-unit
R2 = 0.777
69 unique esters
149 calculations

Figure 20

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 57 unique esters in dioxane-water mixed solvent at various temperatures.

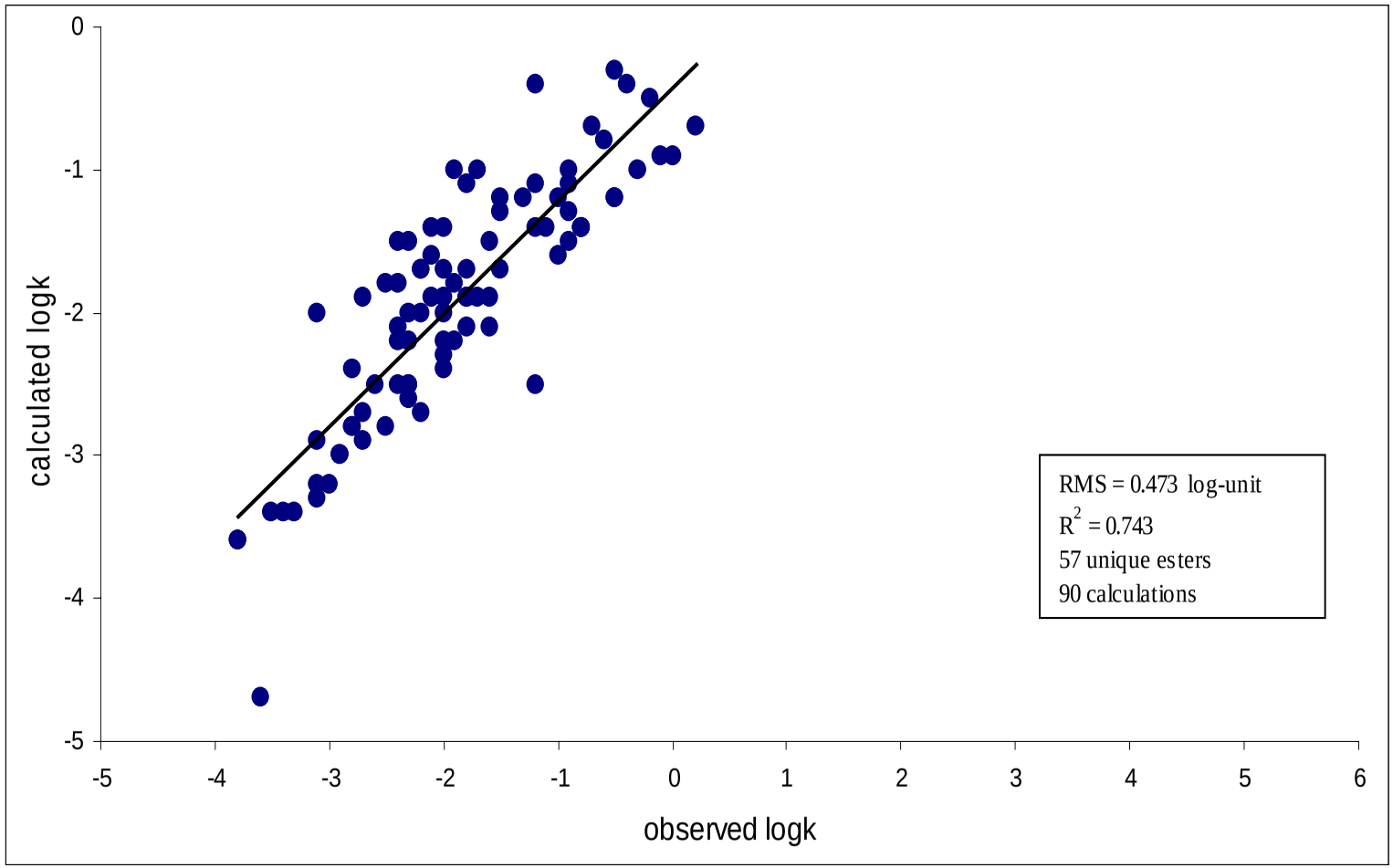
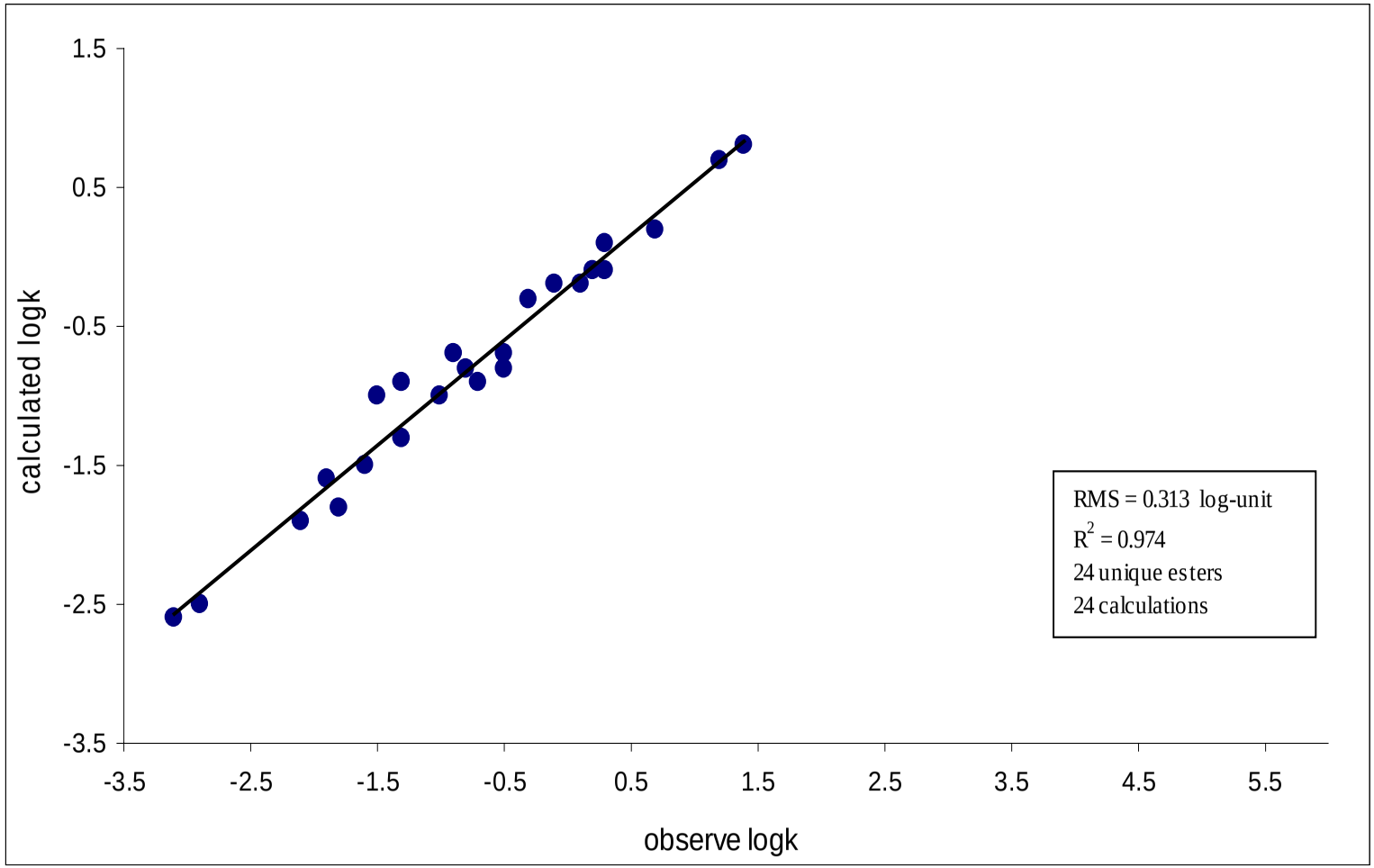

0
-1
-2
-3
-4
-5
calculated logk
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
observed logk
RMS = 0.473 log-unit
R2 = 0.743
57 unique esters
90 calculations

Figure 21

Observed vs calculated hydrolysis rate constants for alkaline hydrolysis of 24 unique esters in acetonitrile-water mixed solvent at 25C.


1.5
0.5
-0.5
-1.5
-2.5
-3.5
calculated logk
-3.5
-2.5
-1.5
-0.5
0.5
1.5
2.5
3.5
4.5
5.5
observe logk
RMS = 0.313 log-unit
R2 = 0.974
24 unique esters
24 calculations

calculations is that the pyridine esters were also undergoing general base catalysis in addition to the regular base catalyzed hydrolysis. If the pyridine esters were undergoing mixed hydrolysis reactions, this would result in faster observed hydrolysis rate constants. To overcome this one log-unit deficit for hydrolysis rate constants of pyridine esters, we have added one log-unit to the calculated hydrolysis rate constants in our SPARC model.

Acid Hydrolysis

The figure 22 shows the graph of observed and calculated hydrolysis rate constants of 416 unique esters hydrolyzed in various solvents and different temperatures. The calculated RMS and R^2 values for acid catalyzed hydrolysis of these esters are 0.359 log-unit and 0.893 respectively. In addition, the graphs for acid catalyzed hydrolysis in pure water and individual mixed solvents have been constructed (figures 23-27). The mixed solvents are acetone-water, ethanol-water, methanol-water and dioxane-water. All of the graphs show reasonable RMS and R^2 values.

General Base Catalyzed Hydrolysis

The figure 28 shows the graph of observed and calculated hydrolysis rate constants of 50 unique esters hydrolyzed in various solvents and different temperatures. The calculated RMS and R^2 values for general base catalyzed hydrolysis of esters are 0.371 log-unit and 0.96 respectively. In addition, the graphs for general base catalyzed hydrolysis in pure water and individual mixed solvents have been constructed (figures 29-32). The mixed solvents are acetone-water, ethanol-water and dioxane-water. All of the graphs show reasonable RMS and R^2 values, except for esters in dioxane-water mixed solvents. The RMS and R^2 values are 0.473 log-unit and 0.664 and the reason for

Figure 22

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 416 unique esters in five different solvents and at varying temperatures.

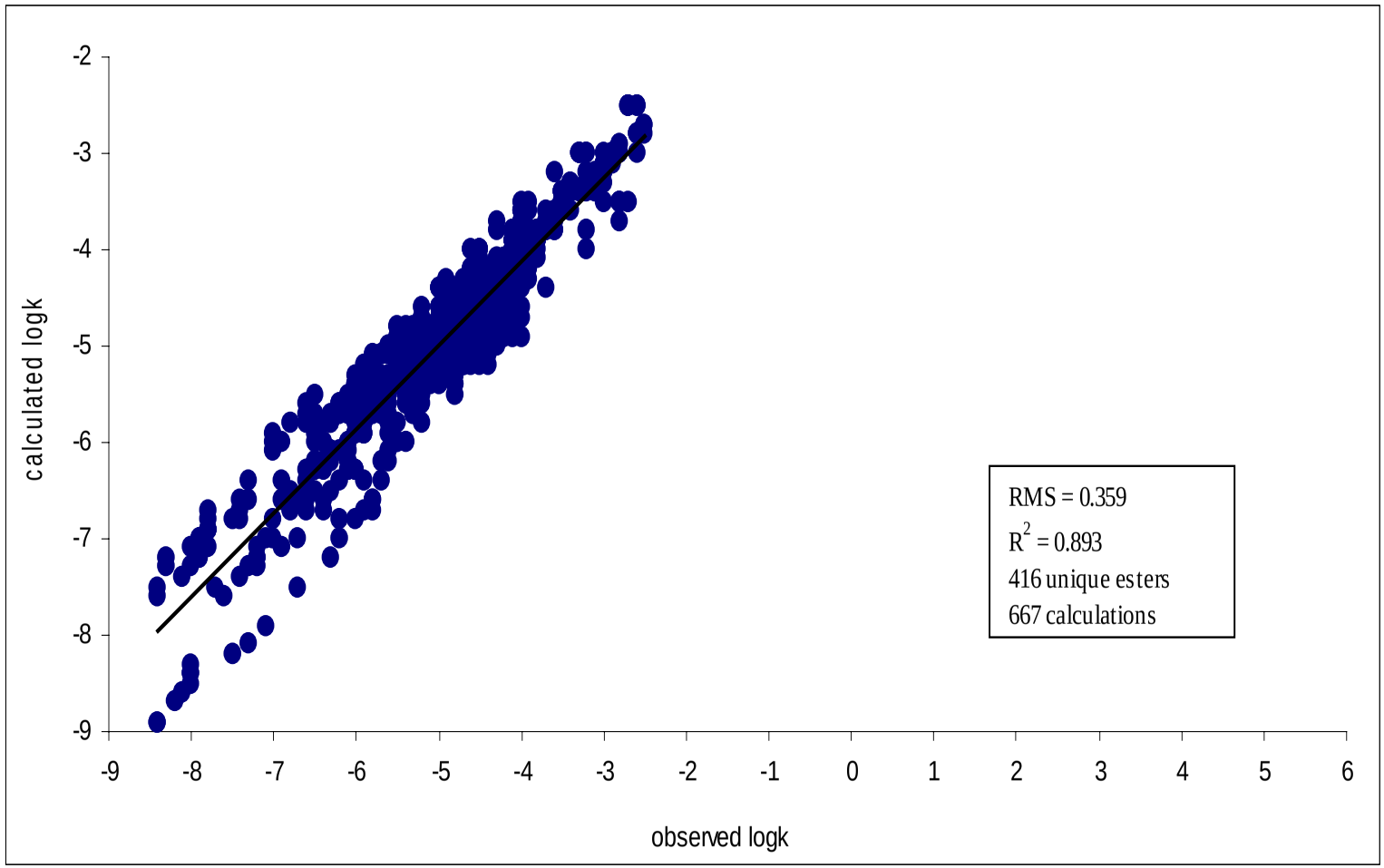

calculated logk
observed logk
-2
-3
-4
-5
-6
-7
-8
-9
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
RMS = 0.359
R2 = 0.893
416 unique esters
667 calculations

Figure 23

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 373 unique esters in pure water at varying temperatures.

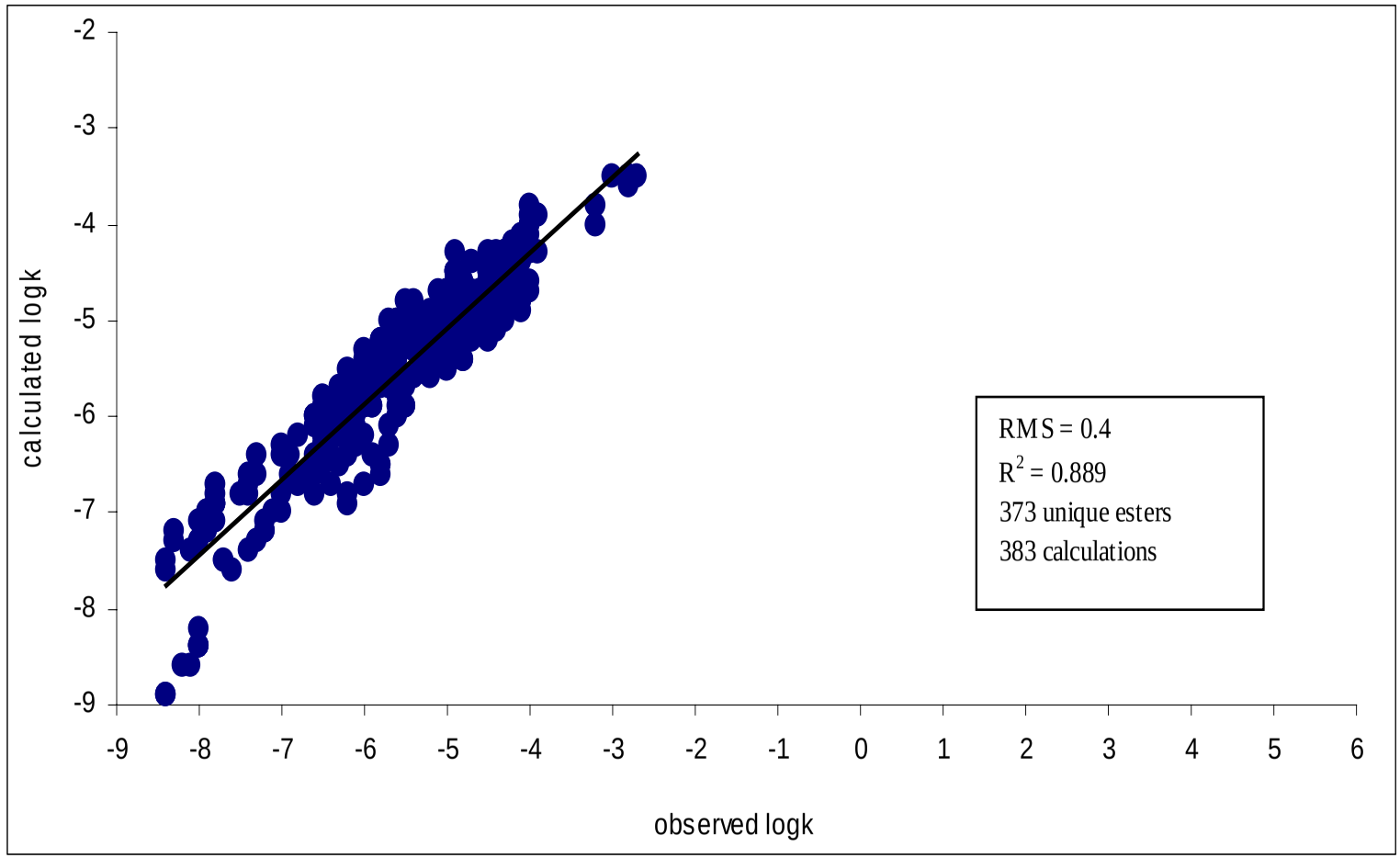

calculated logk
observed logk
-2
-3
-4
-5
-6
-7
-8
-9
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
RMS = 0.4
R2 = 0.889
373 unique esters
383 calculations

Figure 24

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 49 unique esters in acetone-water mixed solvent at varying temperatures.

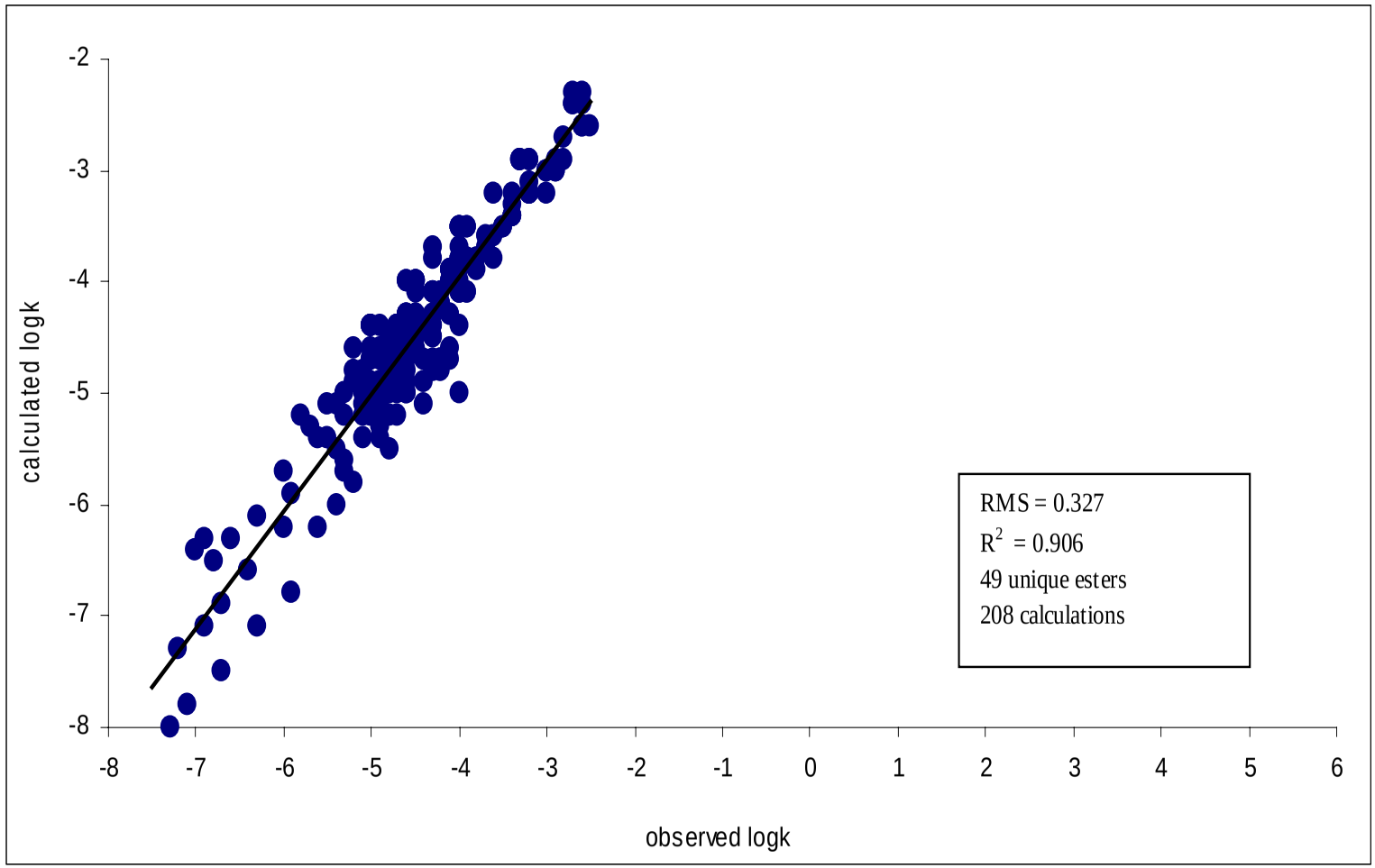

calculated logk
observed logk
-2
-3
-4
-5
-6
-7
-8
-8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
RMS = 0.327
R2 = 0.906
49 unique esters
208 calculations

Figure 25

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 9 unique esters in ethanol-water mixed solvents at varying temperatures.

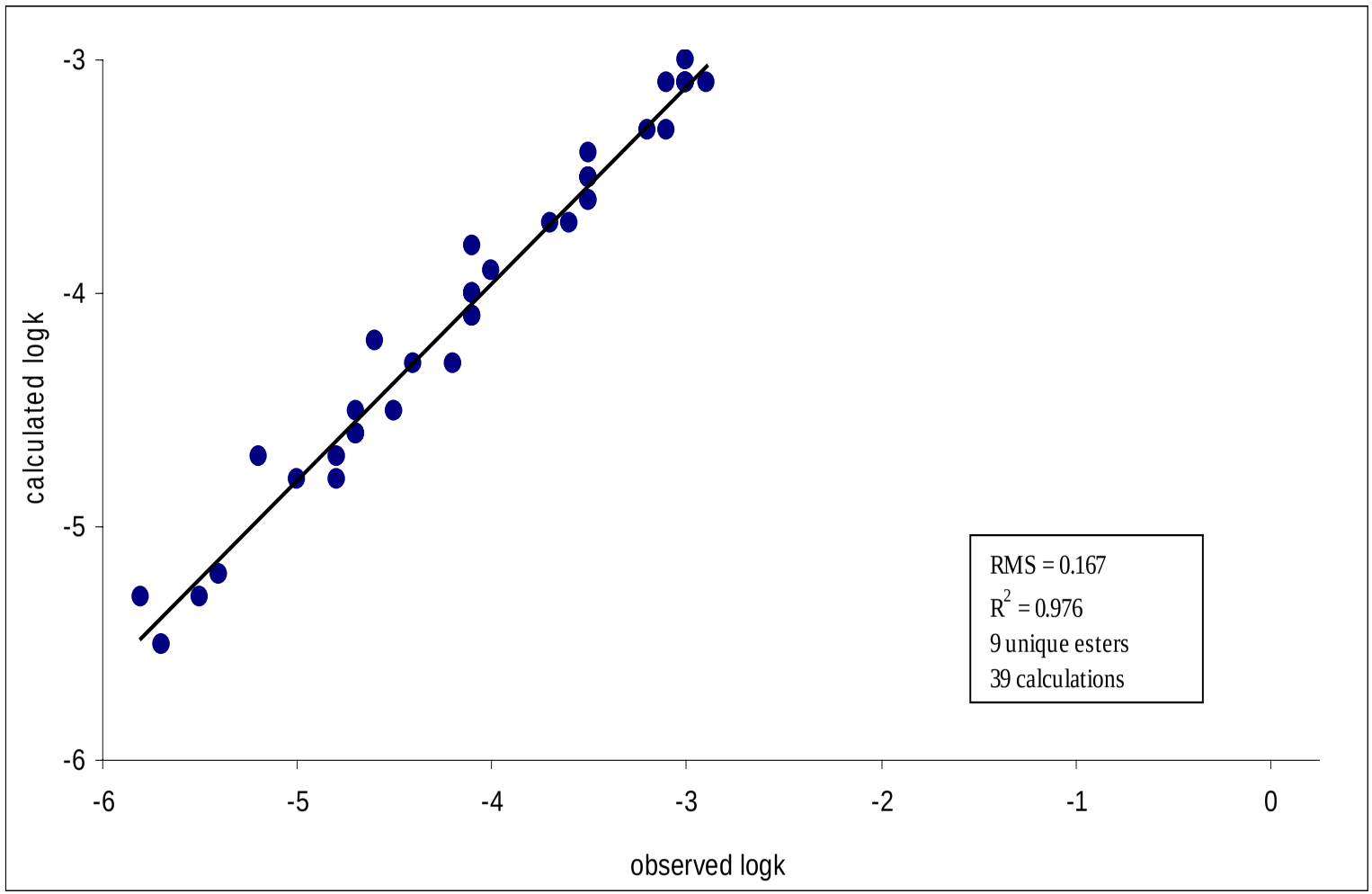

-3
-4
-5
-6
calculated logk
-6
-5
-4
-3
-2
-1
0
observed logk
RMS = 0.167
R2 = 0.976
9 unique esters
39 calculations

Figure 26

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 13 unique esters in methanol-water mixed solvent at varying temperatures.

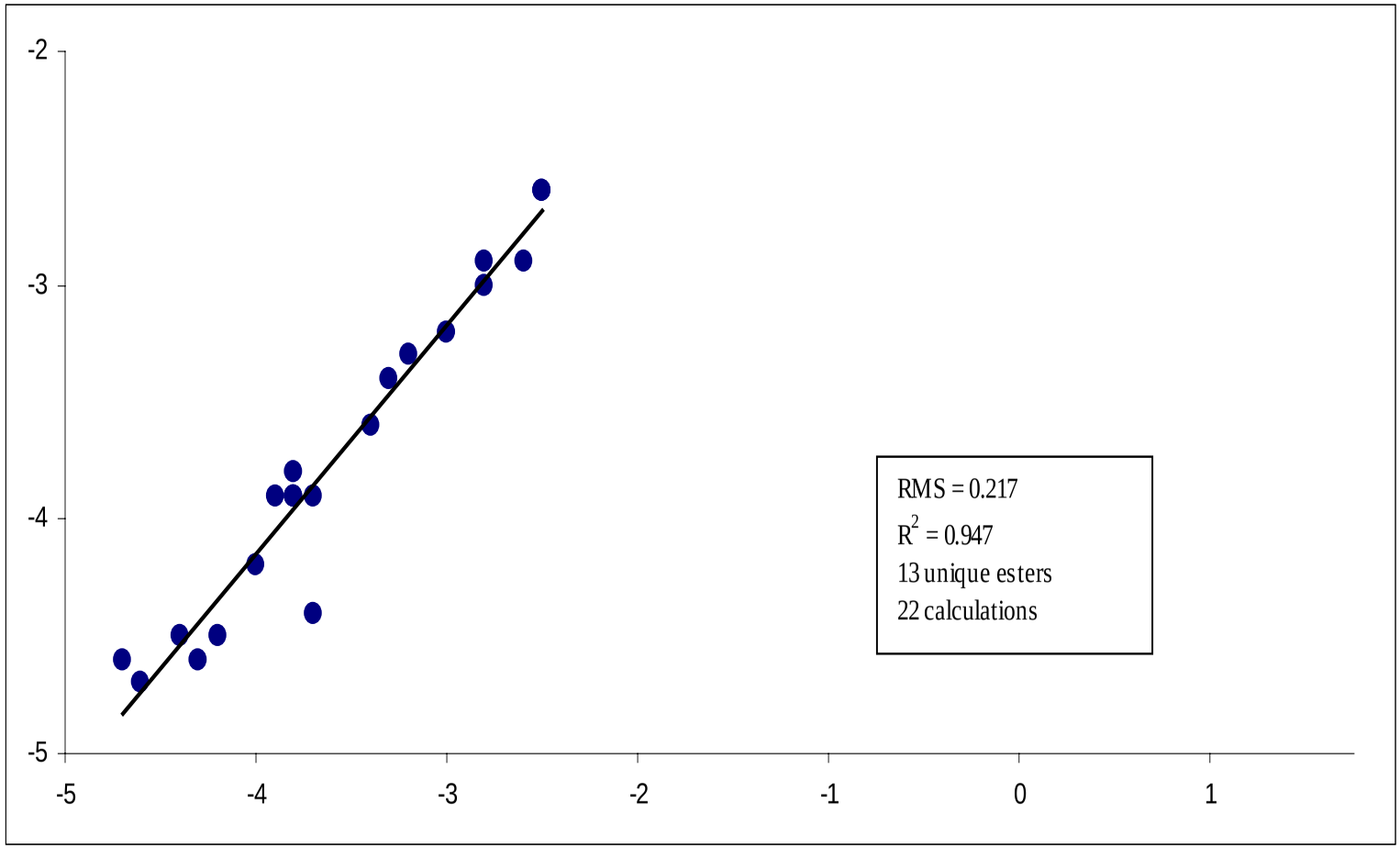

-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
RMS = 0.217
R2 = 0.947
13 unique esters
22 calculations

Figure 27

Observed vs calculated hydrolysis rate constants for acid catalyzed hydrolysis of 4 unique esters in dioxane-water mixed solvent at varying temperatures.

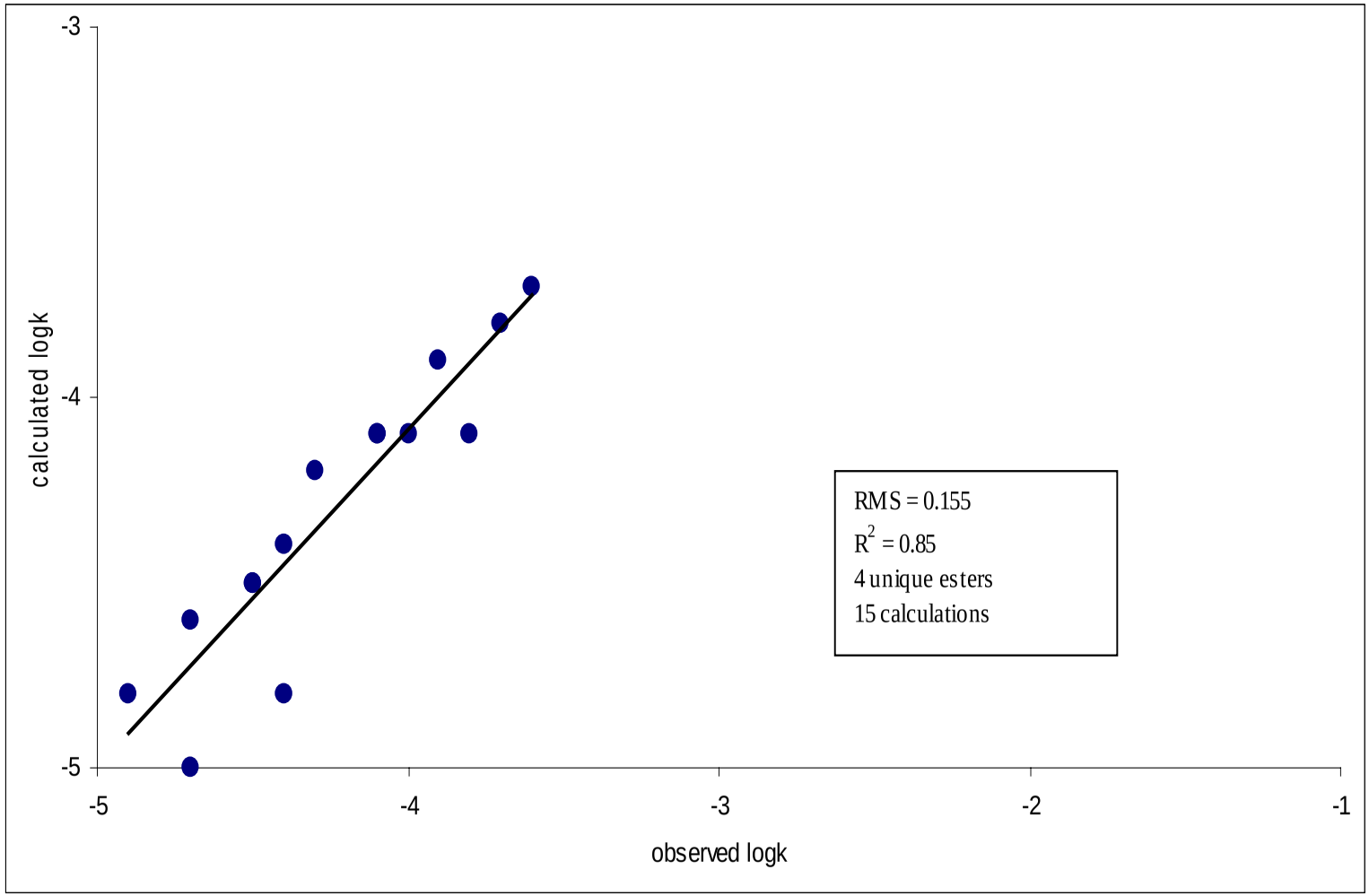

-3
-4
-5
calculated logk
-5
-4
-3
-2
-1
observed logk
RMS = 0.155
R2 = 0.85
4 unique esters
15 calculations

Figure 28

Observed vs calculated hydrolysis rate constants for general base catalyzed hydrolysis of 50 unique esters in various mixed solvents and at varying temperatures.

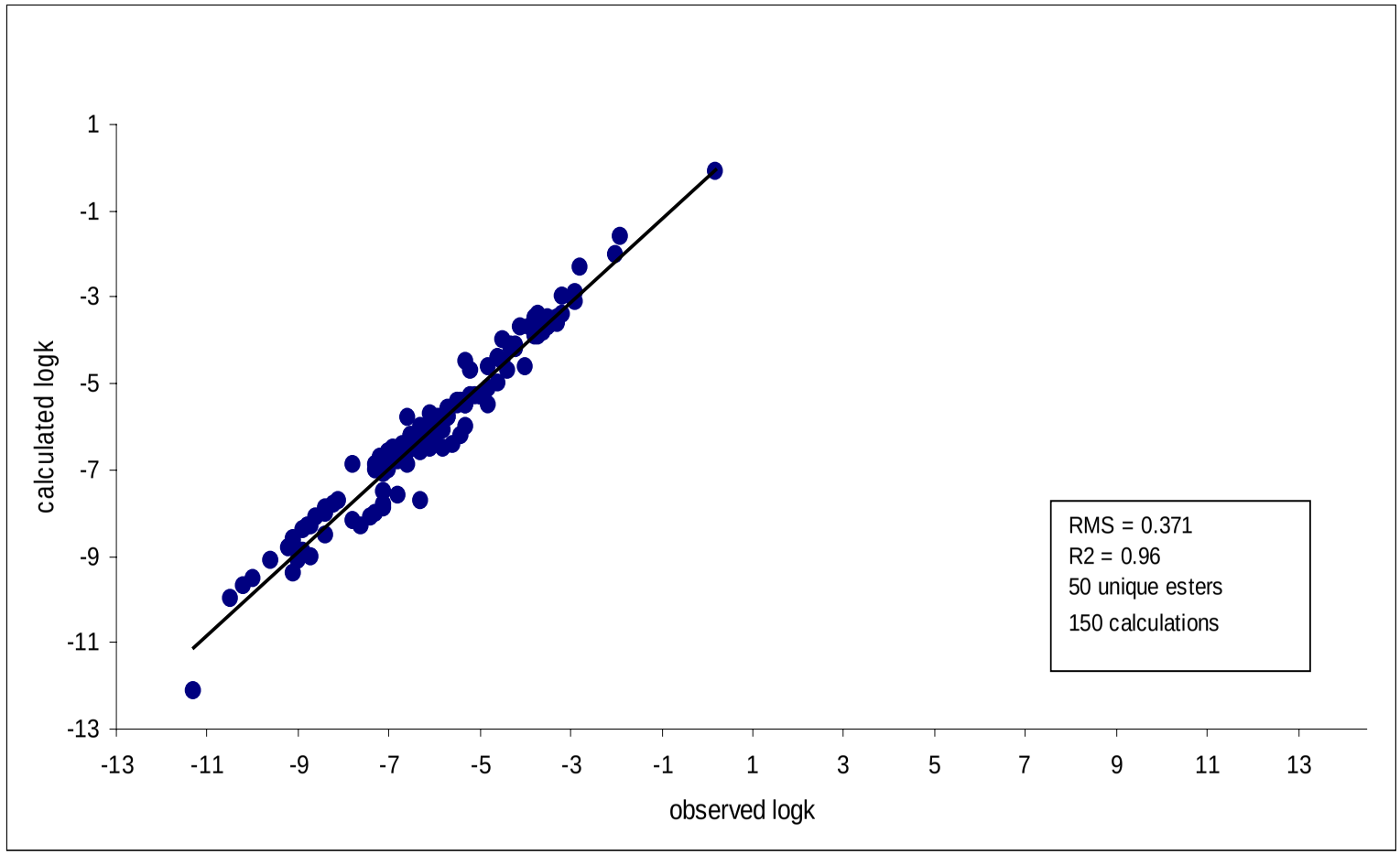

calculated logk
observed logk
1
-1
-3
-5
-7
-9
-11
-13
-13
-11
-9
-7
-5
-3
-1
1
3
5
7
9
11
13
RMS = 0.371
R2 = 0.96
50 unique esters
150 calculations

Figure 29

Observed vs calculated hydrolysis rate constants for general base catalyzed hydrolysis of 29 unique esters in water and at varying temperatures.

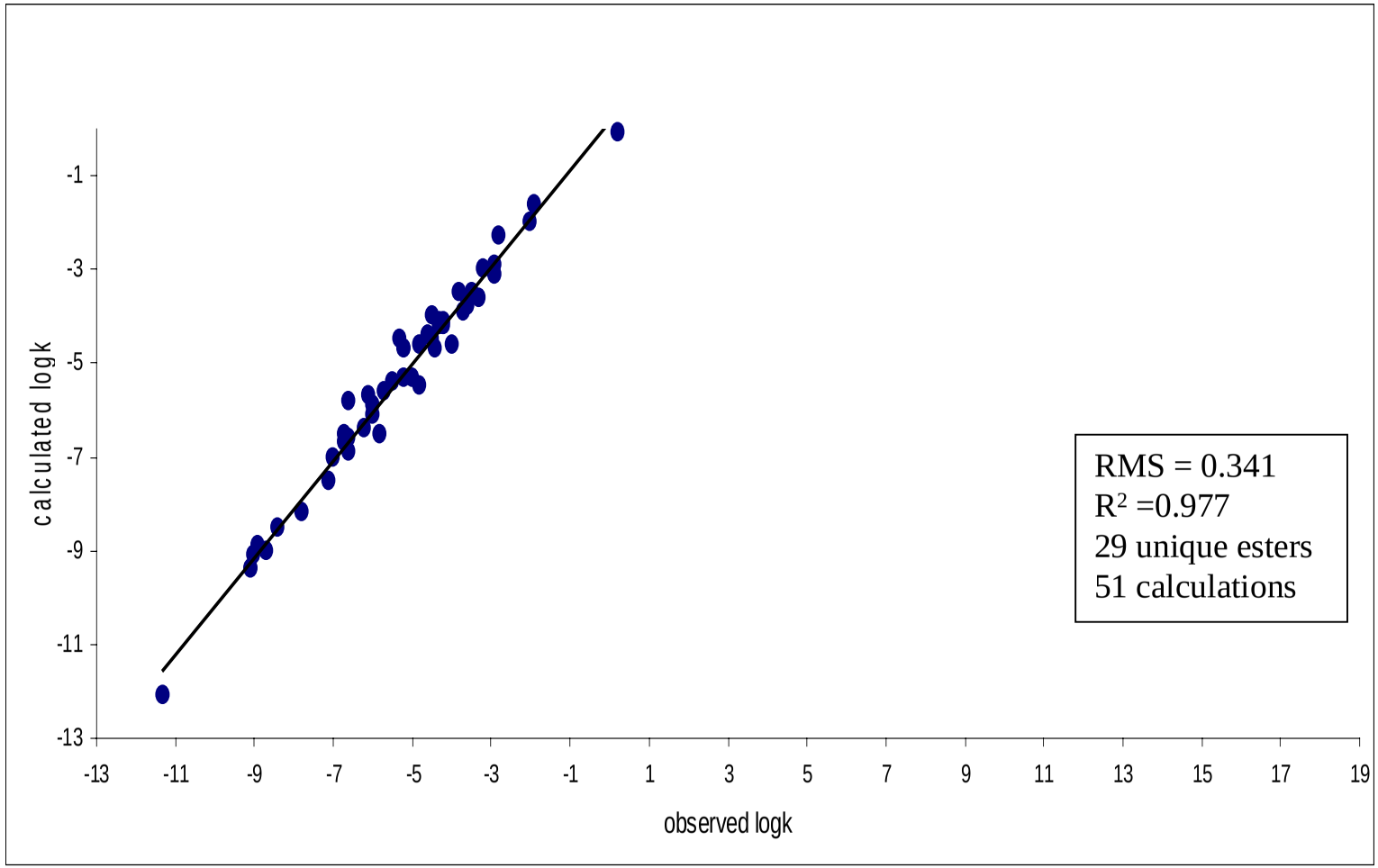

calculated logk
observed logk
-1
-3
-5
-7
-9
-11
-13
-13
-11
-9
-7
-5
-3
-1
1
3
5
7
9
11
13
15
17
19
RMS = 0.341
R2 =0.977
29 unique esters
51 calculations

Figure 30

Observed vs calculated hydrolysis rate constants for general base catalyzed hydrolysis of 19 unique esters in acetone-water mixed solvents and at varying temperatures.

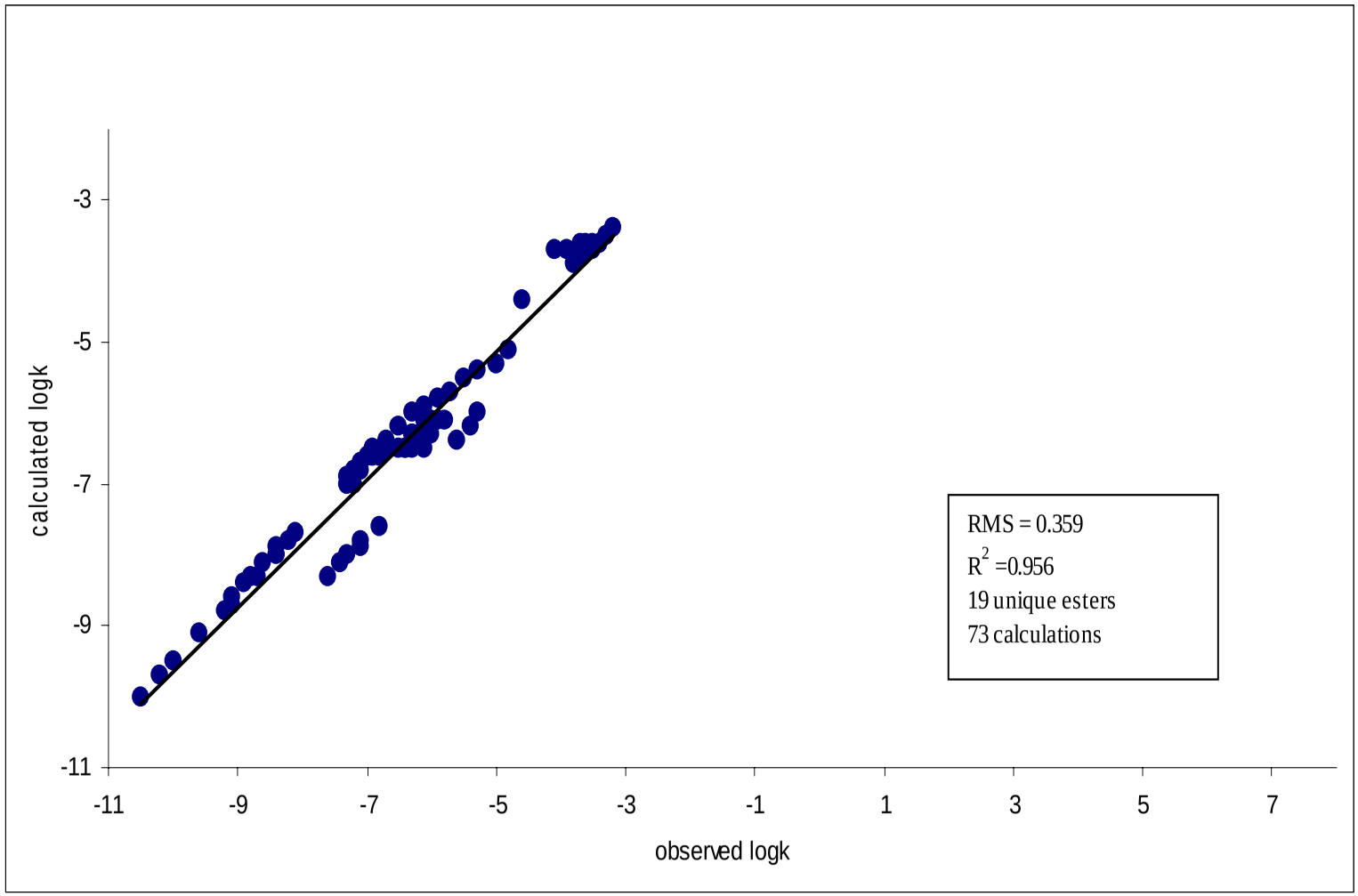

calculated logk
observed logk
-3
-5
-7
-9
-11
-11
-9
-7
-5
-3
-1
1
3
5
7
RMS = 0.359
R2 =0.956
19 unique esters
73 calculations

Figure31

Observed vs calculated hydrolysis rate constants for general base catalyzed hydrolysis of 2 unique esters in ethanol-water mixed solvents and at varying temperatures.

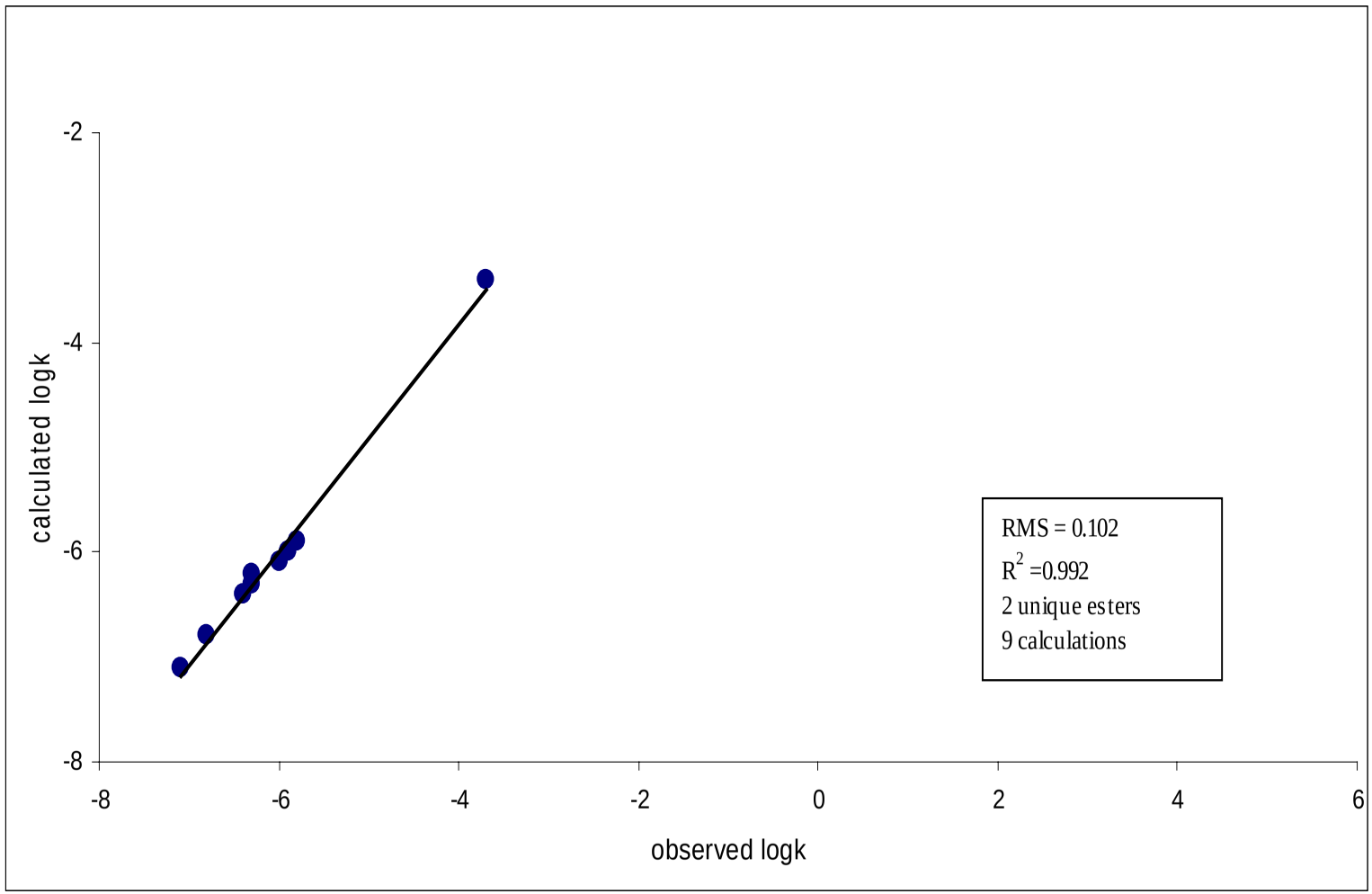
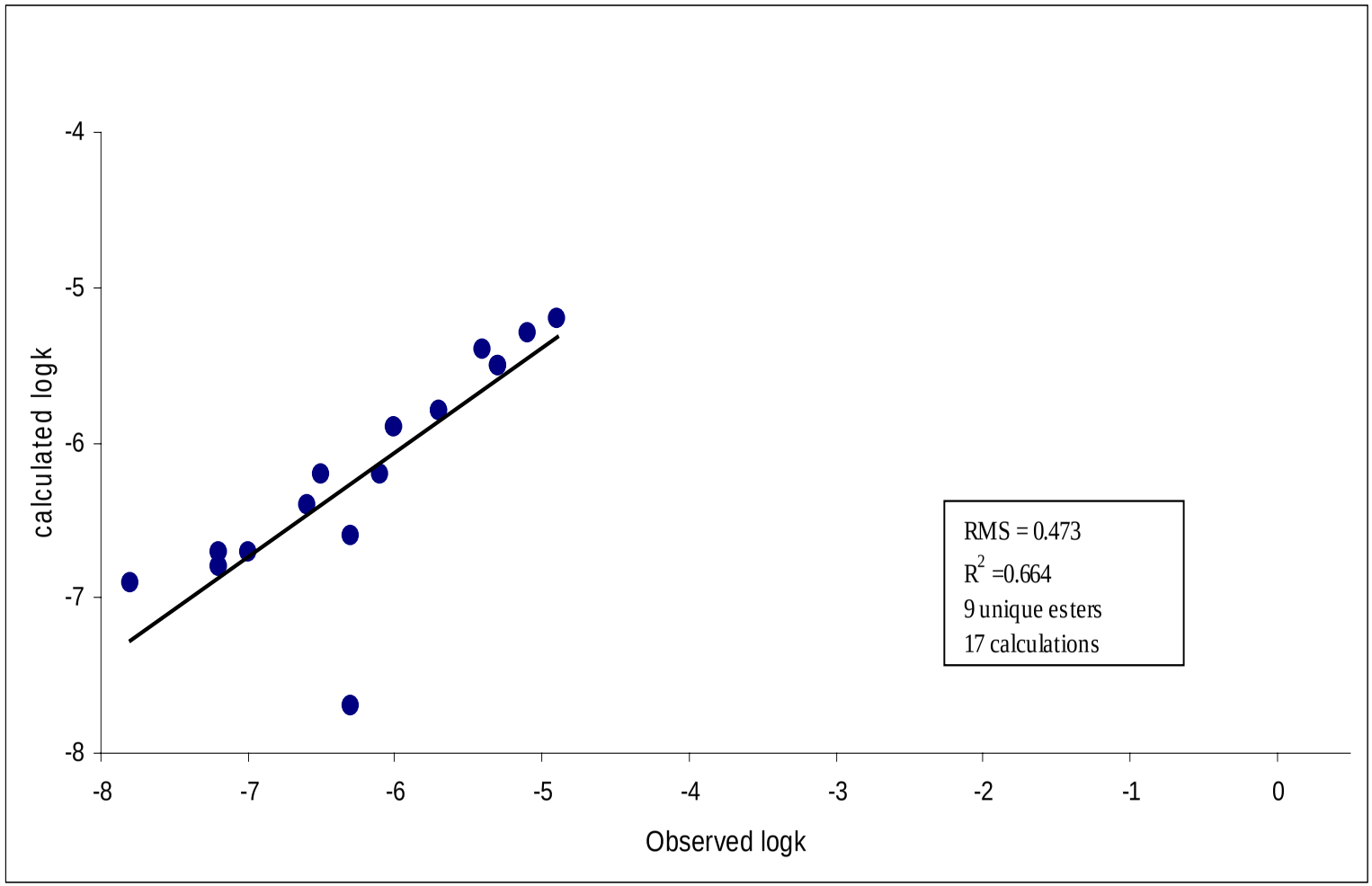

-2
-4
-6
-8
calculated logk
-8
-6
-4
-2
0
2
4
6
observed logk
RMS = 0.102
R2 =0.992
2 unique esters
9 calculations

Figure 32

Observed vs calculated hydrolysis rate constants for general base catalyzed hydrolysis of 9 unique esters in dioxane-water mixed solvents and at varying temperatures.


-4
-5
-6
-7
-8
calculated logk
-8
-7
-6
-5
-4
-3
-2
-1
0
Observed logk
RMS = 0.473
R2 =0.664
9 unique esters
17 calculations

these inconsistencies are due to the outlier trichloroethyl acetate, which shows huge field effect. If we remove this outlier, we obtain the RMS and R^2 values of 0.333 log-unit and 0.931 respectively.

Solvation Effect

Collecting data for different solvents in base, acid and general base catalyzed media, we have observed the trend of Alpha, the hydrogen bond donor strength of the solvent, to increase the activation energy and decrease the hydrolysis rate constant. In contrast, the Beta, the hydrogen bond acceptor strength of the solvent, to decrease the activation energy and increase the hydrolysis rate constant. These trends go contrary to what we originally expected of Alpha and Beta. The results are summarized in Table 1 for alkaline hydrolysis of esters. Water, with the largest alpha value lowers the hydrolysis rate constant the most and acetone with the smallest alpha value decreases it the least. Similarly, dioxane, with the largest beta value increases the hydrolysis rate constant the most and acetone with the smallest beta value increases it the least. Similar trends are observed in acid and general base catalyzed hydrolysis of esters (tables 2 and 3).

In addition, we have observed the Field Stabilization term, which depends on the dielectric constant of the medium. An increase in the dielectric constant stabilizes the complex and increases the rate. Table 1 shows the Field Stabilization increasing the alkaline hydrolysis rate constant with an increase in the dielectric constant or polarity of the solvents. Water, with a dielectric constant value of 78.54 increases the hydrolysis rate constant the most, while dioxane with a dielectric constant value of 2.2 increases it

Table 1

Alpha, Beta, Field Stabilization and Steric effects on determining hydrolysis rate constants for alkaline hydrolysis of ethyl acetate in six different solutions. The six solutions are pure water and the rest are 50% water and 50% listed solvents in the table.

Solvents	alpha of solvents	hydrogen acceptor effect of esters (Alpha)
acetone	0	-1.254
dioxane	0	-1.28
acetonitrile	0.1	-1.26
ethanol	0.25	-1.44
methanol	0.312	-1.54
water	0.384	-1.55
Solvents	beta of solvents	hydrogen donor effect of esters (Beta)
dioxane	0.88	6.513
acetone	0.466	5.54
ethanol	0.53	5.72
methanol	0.39	5.35
water	0.382	5.31
acetonitrile	0.27	4.91
Solvents	dielectric constant	Field Stabilization
water	78.54	-2.84
acetonitrile	35.94	-3.52
methanol	32.63	-3.58
ethanol	24.3	-3.76
acetone	20.7	-3.84
dioxane	2.2	-4.33

Table 2

Alpha, Beta, Field Stabilization and Steric effects on determining hydrolysis rate constants for acid-catalyzed hydrolysis of ethyl acetate in five different solutions at 25C. The five solutions are pure water and the rest are 50% water and 50% listed solvents in the table.

Solvents	alpha of solvents	hydrogen acceptor effect (Alpha)
acetone	0	-0.7
dioxane	0	-0.72
ethanol	0.25	-0.8
methanol	0.312	-0.87
water	0.384	-0.88
Solvents	beta of solvents	hydrogen donor effect (Beta)
dioxane	0.88	-1.02
ethanol	0.53	-0.91
acetone	0.466	-0.87
methanol	0.39	-0.84
water	0.382	-0.84
Solvents	dielectric constant	Field Stabilization
water	78.54	-0.21
methanol	32.63	-0.27
ethanol	24.3	-0.29
acetone	20.7	-0.29
dioxane	2.2	-0.33

Table 3

Alpha, Beta, Field Stabilization and Steric effects on determining hydrolysis rate constants for water-catalyzed hydrolysis of ethyl acetate in four different solvents at 25C. The four solvents are pure water and the rest are 50% water and 50% listed solvents in the table.

Solvents	alpha of solvents	hydrogen acceptor effect of esters (Alpha)
acetone	0	-0.6
dioxane	0	-0.61
ethanol	0.25	-0.68
water	0.384	-0.74
Solvents	beta of solvents	hydrogen donor effect of esters (Beta)
dioxane	0.88	8.8
ethanol	0.53	7.83
acetone	0.466	7.48
water	0.382	7.17
Solvents	dielectric constant	Field Stabilization
water	78.54	-4.53
ethanol	24.3	-6
acetone	20.7	-6.13
dioxane	2.2	-6.9

the least. Similar trends are observed in acid and general base catalyzed hydrolysis of esters (tables 2 and 3).

Temperature Effect

We use the Arrhenius equation for the temperature effect, as described earlier in the SPARC computational model. A general trend of temperature effect upon the hydrolysis rate constant is that as the temperature in Kelvin increases the logarithmic hydrolysis rate constant increases. The temperature effect is incorporated in field stabilization effect, alpha, beta and steric effect of the SPARC computational model. Our SPARC calculation shows 0.2 to 0.3, 0.3 to 0.4 and 0.3 and 0.4 log-units increase in hydrolysis rate constants per 10-degree Kelvin/ Celsius rise in temperature for base, acid and general base-catalyzed hydrolysis of esters respectively. Further, figures 33-35 show effect of temperature upon various esters in base, acid and general base catalyzed hydrolysis of esters respectively.

OUTLIERS

The outliers in the context of hydrolysis of esters are defined as esters, whose absolute difference in calculated and observed hydrolysis rate constant values exceeds 3RMS value. For example, we have observed seven outliers in our training set for the alkaline hydrolysis of esters. They are (1-methyl-1-vinyl)-propyl acetate, 2-fluorenyl benzoate, isopropenyl acetate at two different temperatures, methyl o-(tertiary)butylbenzoate, diphenylmethyl benzoate and methyl p-trifluoromethylbenzoate. We do not exactly know why (1-methyl-1-vinyl)-propyl acetate and isopropenyl acetate stand out as outliers because all the other compounds with carbon-carbon double bond

Figure 33

Temperature vs hydrolysis rate constants for alkaline hydrolysis of methyl benzoate in 80% methanol-water (circles), cyclopropyl acetate in pure water (triangles), and cyclohexyl acetate in 70% acetone-water (diamonds). In addition, the solid figures represent the observed values, while the empty figures represent the calculated values for the hydrolysis rate constants.

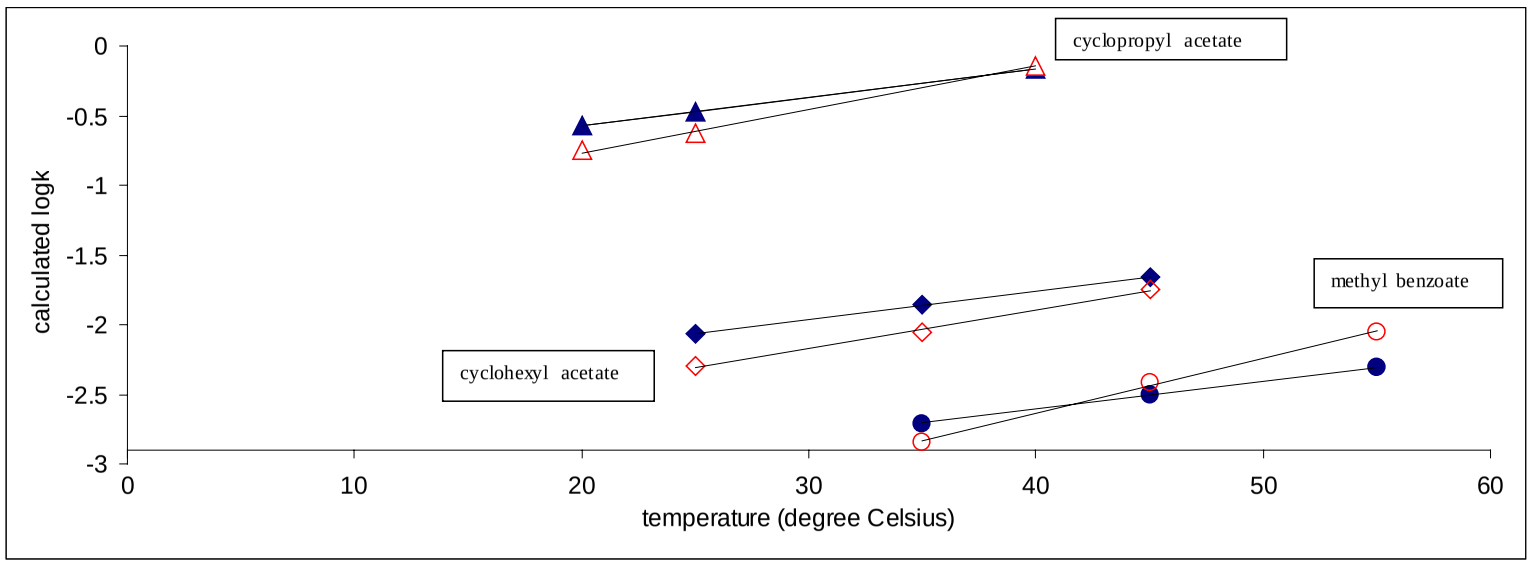

cyclopropyl acetate
methyl benzoate
cyclohexyl acetate
calculated logk
temperature (degree Celsius)
0
-0.5
-1
-1.5
-2
-2.5
-3
0
10
20
30
40
50
60

Figure 34

Temperature vs hydrolysis rate constants for acid-catalyzed hydrolysis of ethyl benzoate in 60% ethanol-water (diamonds) and ethyl isohexoate in 70% acetone-water (circles). In addition, the big figures represent the observed values, while the small figures represent the calculated values for the hydrolysis rate constants.

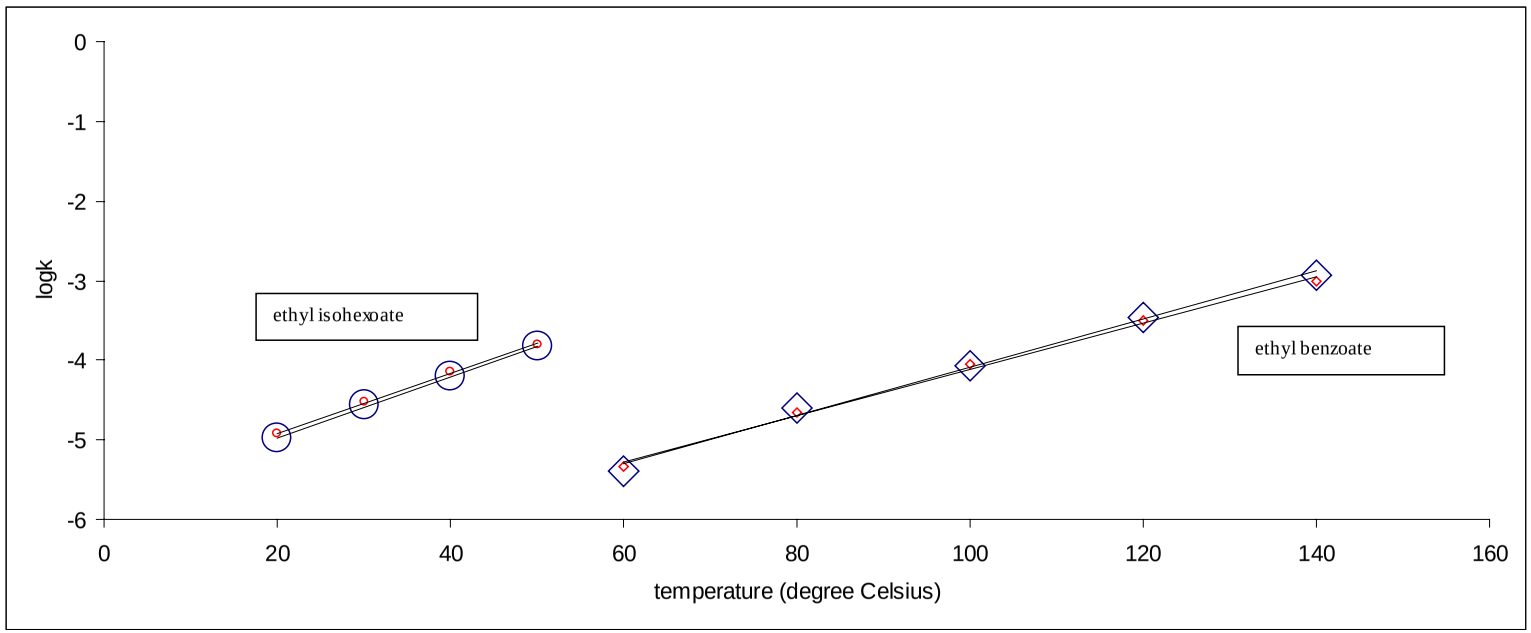
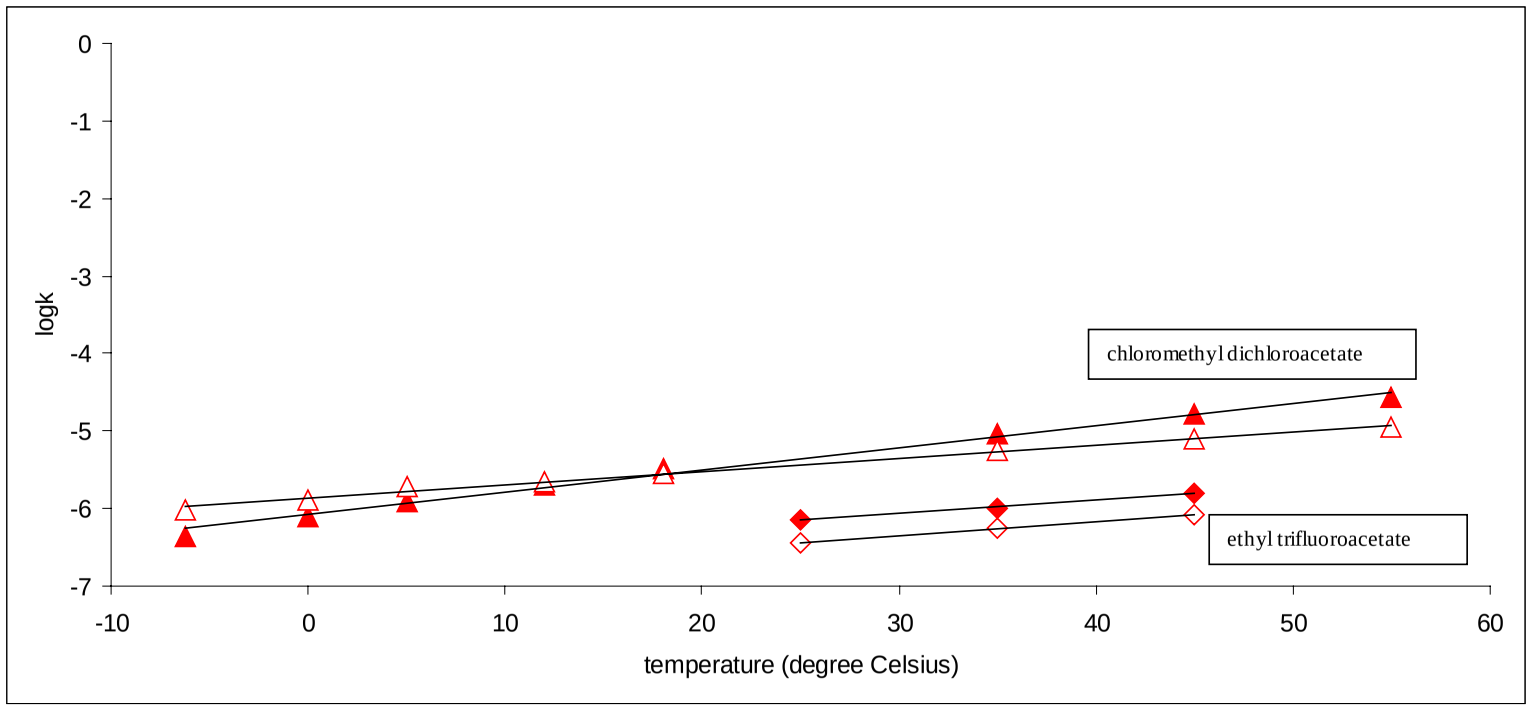

0
-1
-2
-3
-4
-5
-6
logk
ethyl isohexoate
ethyl benzoate
0
20
40
60
80
100
120
140
160
temperature (degree Celsius)

Figure 35

Temperature vs hydrolysis rate constants for neutral hydrolysis of chloromethyl dichloroacetate in 50% acetone-water (triangles) and ethyl trifluoroacetate in 70% acetone-water (diamonds). In addition, the solid figures represent the observed values, while the empty figures represent the calculated values for the hydrolysis rate constants.


0
-1
-2
-3
-4
-5
-6
-7
logk
-10
0
10
20
30
40
50
60
temperature (degree Celsius)
chloromethyl dichloroacetate
ethyl trifluoroacetate

and triple bond show consistent values for observed and calculated hydrolysis rate constants. 2-fluorenyl benzoate and diphenylmethyl benzoate, on the other hand, may be showing a steric effect problem. The former is showing smaller steric effect, while the latter is showing huge steric effect. Similarly bulky molecules seem to be well handled by our steric models and we have no explanation as to why these would show such large deviations. The methyl o-(tertiary)butylbenzoate is an outlier by virtue of its anomalous temperature behavior. Our calculation is showing a 0.2 to 0.3 log-unit increase in hydrolysis rate constant per 10 C increase in temperature; however, the literature data for this particular set is showing around a 0.6 log-unit increase per 10 C rise in temperature.[11] As a result, when the calculation is made at higher temperature, the difference in increase between the calculated and observed hydrolysis rate constants adds up quickly in the calculated hydrolysis rate constant to give a significant error. Again the bulk of the observed hydrolysis rates do not show such a steep slope and are more consistent with our calculated values.

Similarly, we have observed two outliers for acid catalyzed hydrolysis of esters. The major contribution to the rate differences is steric and our models do not reproduce the observed values. In addition, we have excluded the chloro-esters from Tim and Hinselwood's data set because they are showing a huge field effect. That is, the field effect due to the chlorine atoms is increasing the hydrolysis rate constants of chloro-esters. This trend contradicts our SPARC model based on R. W. Taft (Jr.) and Newman's theory, which states that the field has negligible effect on the hydrolysis rate constant of acid catalyzed hydrolysis of esters.[12, 13] We have calculated the hydrolysis

rate constants for these chloro-esters in table 4. The mono- and dichloro- esters are showing acceptable values, but the trichloro-esters differ by 1.5 to 2 log-unit.

Water catalyzed trichloroethyl acetate in 50% dioxane-water is the only outlier in our training set for general base hydrolysis of esters. It is an outlier because it shows small field effects. In addition, we have removed a data set by E.K. Euranto because the observed values for similar compounds did not make sense. To illustrate, the observed values for water-catalyzed chloromethyl acetate in 40% acetone, alphachloro-betatrichloroethyl acetate in 50% acetone-water and alphachloroethyl acetate in 50% acetone-water are –7.47, -8.4 and –4.96 log-units respectively.[3, 14] However, we believe that alphachloro-betatrichloroethyl acetate should have the largest positive hydrolysis rate constant value among the above esters and then chloromethyl acetate followed by alphachloroethyl acetate. Further, we have been selective while collecting data from Koehler and et al..[14] The reason for selecting the data, which fitted our training set, is that the authors specifically state that the undergoing reactions in the literature are nucleophilic.[14] However, we believe that the selected esters, which give good measurements, are undergoing the general base-catalyzed hydrolysis. The ones, which stand as outliers are definitely undergoing the nucleophilic reaction.

Table 4

Excluded chloro-esters from Tim and Hinselwood's data set. The observed and calculated hydrolysis rate constants are measured in 60% ethanol-water solvent.

Name	SMILES	Observed logk	Calculated logk	Difference	Temperature
Ethyl chloroacetate	ClCC(=O)OCC	-4.4	-4.87	0.47	24.86
		-3.87	-4.27	0.4	39.79
		-3.21	-3.55	0.34	60.04
		-2.65	-2.91	0.26	80.1
Ethyl dichloroacetate	ClC(Cl)C(=O)OCC	-4.67	-5.39	0.72	24.86
		-4.18	-4.78	0.6	39.79
		-3.57	-4.04	0.47	60.04
		-3.03	-3.38	0.35	80.1
Ethyl trichloroacetate	ClC(Cl)(Cl)C(=O)OCC	-4.08	-6.16	2.08	24.84
		-3.62	-5.53	1.91	39.97
		-3.11	-4.77	1.66	60.34
		-2.66	-4.11	1.45	80.15

CHAPTER 6

RESULT AND DISCUSSION FOR HYDRATION

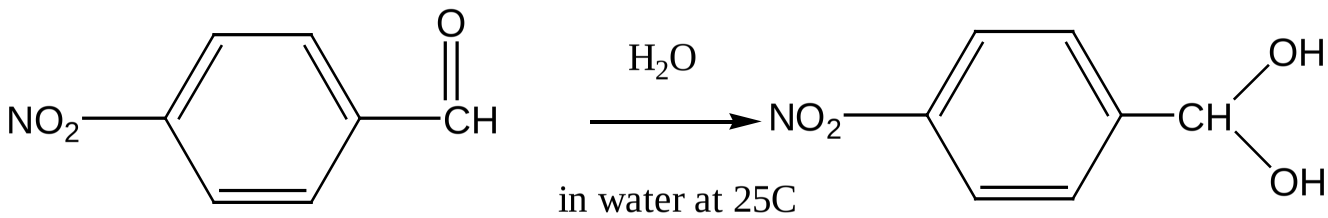
Tables 8 and 9 show observed versus calculated values for hydration equilibrium constants of aldehydes/ketones and quinazolines respectively. These sets represent 37 aldehydes and ketones and 27 quinazolines. The RMS values obtained are 0.356 and 0.43 pK(hyd)-units respectively. To show how the SPARC calculates each compound's hydration equilibrium constant, we have provided sample calculations for the hydration equilibrium constants for p-nitrobenzaldehyde and 5-nitroquinazoline. The calculations are described below.

Sample Calculation

Figures 36 and 37 show the sample calculations of hydration equilibrium constant for p-nitrobenzaldehyde and 5-nitroquinazoline in pure water and at room temperature. The hydration equilibrium constant is a summation of contributions from the Base, Henry difference and perturbations. The Base is a data-fitted parameter and it is calculated based on the observed pK(hyd) for the base compound and the calculated Henry difference of the base and its diol or hydrated form. The base compounds are formaldehyde and unsubstituted quinazoline for the hydration of aldehydes and quinazoline compounds respectively. The Henry difference is simply a difference of Henry constant values between the aldehydes/ketones or quinazolines and their respective hydrated forms. The perturbations represent various interactions, such as

Figure 36

A sample calculation for determination of hydration equilibrium constant of p-nitrobenzaldehyde in water at 25C.



Perturbations = Resonance + Field + MF + Total r_pi + Steric

= 0.5 + (-0.75) + (-0.5) + 2.6 + 1.42

= 3.27

Base = 2.97

Henry Difference = -(Henry constant of aldehyde/keotne - Henry constant of diol)

= -(-3.70 - (-9.20))

= -5.50

Calculated Hydration Constant = Base + Perturbations + Henry Difference

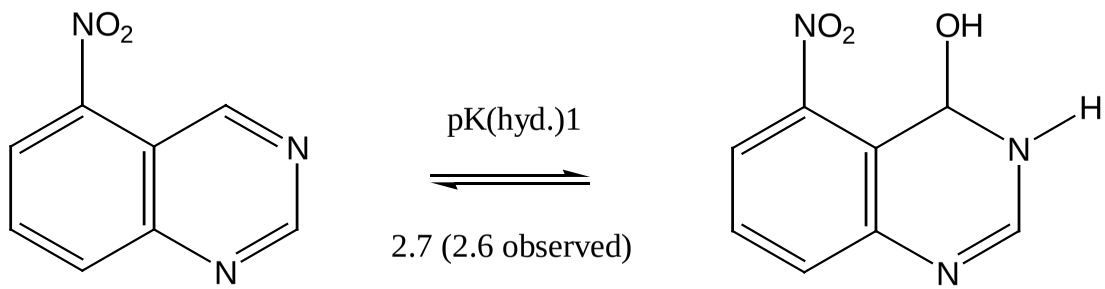
= 2.97 + 3.27 + (-5.5)

= 0.74

Observed Hydration Constant = 0.77

Figure 37

A sample calculation for determination of hydration equilibrium constant of 5-nitroquinazoline in water at 25C



Perturbations = Resonance + Field + MF + Total r_pi + Steric

= 0.01+ (- 1.22) + (- 0.31) + 0 + 0

= -1.53

Base = 6.98

Henry Difference = -(Henry constant of 5-nitroquinazoline -

Henry constant of hydrated 5-nitroquinazoline)

= -2.83

Calculated Hydration Constant = Base + Perturbations + Henry Difference

= 2.60

Observed Hydration Constant = 2.7

resonance, direct field, indirect field (MF), r_pi, steric, etc. between the substituents and the base compound. They are described below.

Perturbations

The perturbations are summation of interactions such as resonance, direct field, MF, r_pi, steric, and so on. The perturbations for p-nitrobenzaldehyde and 5-nitroquinazoline are 3.27 and -1.54 pK(hyd)-units respectively. The analyses of various interactions, which contribute to the total perturbation, are described below.

Resonance Effect

The total forward resonance effects are 0.5 and 0.01 pK(hyd)-units for hydration of p-nitrobenzaldehyde and 5-nitroquinazoline respectively. That is, the resonance is decreasing the hydration equilibrium constant of p-nitrobenzaldehyde because the pi-electrons from the phenyl ring can easily delocalize to the positive carbonyl carbon reaction center. This phenomenon increases the activation energy for hydration reaction and lowers the hydration equilibrium constant. Similar trend is observed for hydration of quinazolines and the pi-electrons are delocalized to the positive carbon reaction center at the 4^{th} position. Since the 5-nitroquinazoline shows a negligible resonance interaction with respect to the unsubstituted quinazoline, we observe minimal resonance contribution of 0.01 pK(hyd)-unit from it.

Direct Field

The direct fields are –0.75 and -1.22 pK(hyd)-units for hydration of p-nitrobenzaldehyde and 5-nitroquinazoline respectively. That is, the field is increasing the

hydration equilibrium constant for both aldehydes and quinazolines. The field creates a strong dipole between the field substituent and the positive reaction center resulting in increase reactivity of the reaction center. This phenomenon lowers the activation energy for hydration reaction and increases the hydration equilibrium constant.

Indirect Field (MF)

The indirect fields (MFs) are -0.5 and -0.31 pK(hyd)-units for hydration of p-nitrobenzaldehyde and 5-nitroquinazoline respectively. The MF is increasing the hydration equilibrium constant for both aldehydes/ketones and quinazolines. The induced positive charges generated by electron-withdrawing nitro group neutralizes any negative charges present in the reaction center. This phenomenon lowers the activation energy for hydration of aldehydes/ketones and quinazolines and increases the hydration equilibrium constant. In contrast, the electron-donating groups should decrease the hydration equilibrium constant.

r_pi Effect

The r_pi effects are 2.6 and 0 pK(hyd)-units for hydration of p-nitrobenzaldehyde and 5-nitroquinazoline respectively. The r_pi effect is decreasing the hydration equilibrium constant of p-nitrobenzaldehyde, while it is showing no effect for 5-nitroquinazoline. The r_pi effect induces negative charges to the positive carbonyl carbon reaction center of the p-nitrobenzaldehyde and reduces the reactivity of the reaction center. This phenomenon increases the activation energy for hydration reaction of p-nitrobenzaldehyde and lowers the hydration equilibrium constant. Similar trend is observed for hydration of quinazolines if the r_pi interaction should exist. However, 5-

nitroquinazoline shows negligible r_pi interaction with respect to the unsubstituted quinazoline.

Steric Effect

The steric effects are 1.42 and 0 pK(hyd)-units for hydration of p-nitrobenzaldehyde and 5-nitroquinazoline respectively. The rule of thumb is that the steric effect always decreases the hydration equilibrium constant. As a result, we see 1.42 pK(hyd)-unit decrease in hydration equilibrium constant from hydration of p-nitrobenzaldehyde because a bulky p-nitrophenyl substituent is attached to the base compound, formaldehyde. On the other hand, the nitro substituent has no effect upon the base compound, the unsubstituted quinazoline. In addition, the steric effects are most effective at 2^{nd} , 4^{th} and 5^{th} position of quinazoline for hydration of quinazolines.

Graphical Representation

Using a similar method described in the sample calculation, we have calculated the hydration equilibrium constants for 37 aldehydes/ketones and 27 quinazolines in water at room temperature. The figures 38 and 39 show the observed and calculated values of hydration equilibrium constants for aldehydes/ketones and quinazolines respectively. The R^2 and RMS values are 0.927 and 0.356 for aldehydes/ketones, while 0.74 and 0.43 for quinazolines. The higher R^2 and RMS value for quinazoline set is due to four trifluoro-quinazolines, which show larger difference between the observed and calculated values.

Figure 38

Observed vs calculated hydration equilibrium constants for hydration of 36 aldehydes/ketones in water at 25C.

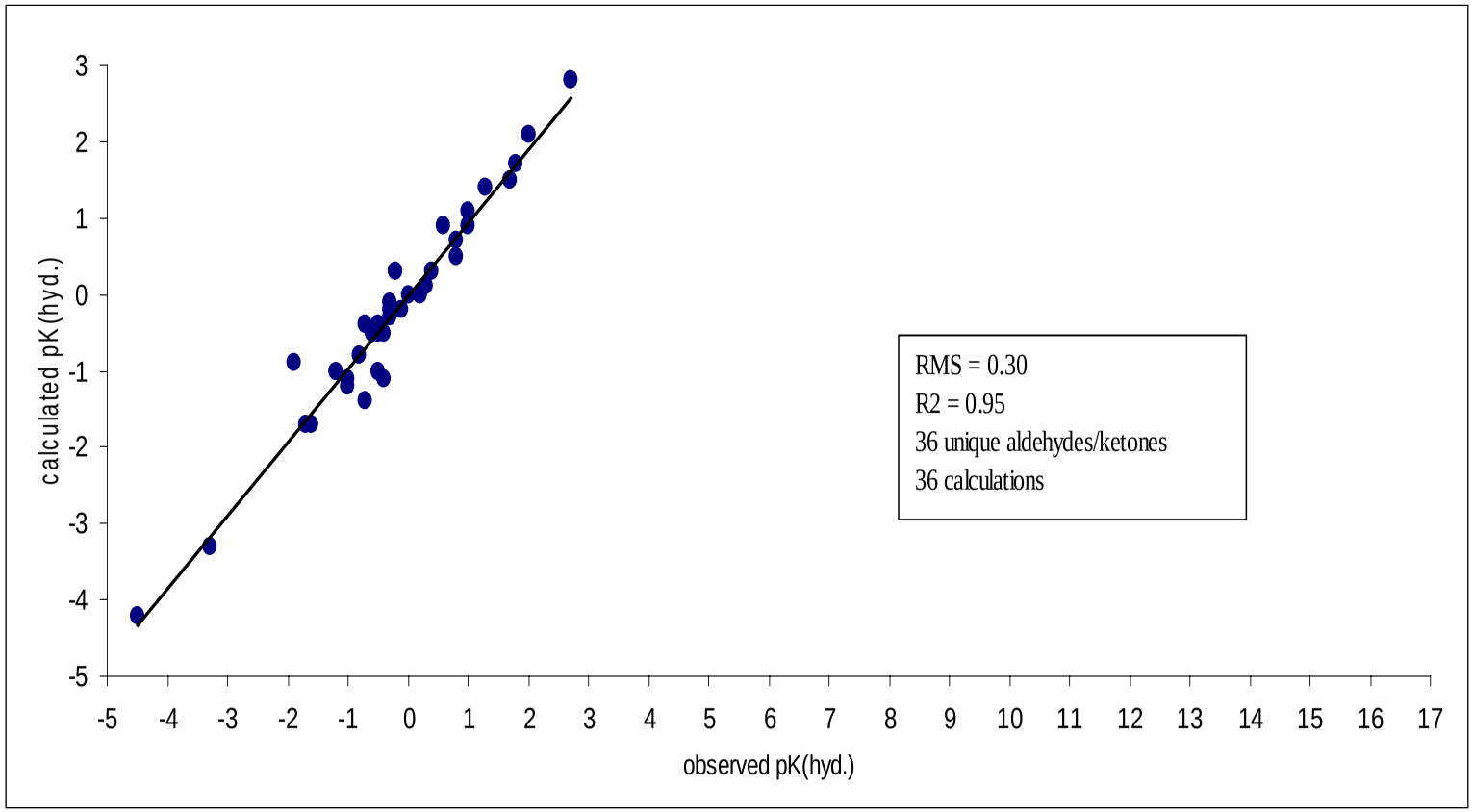
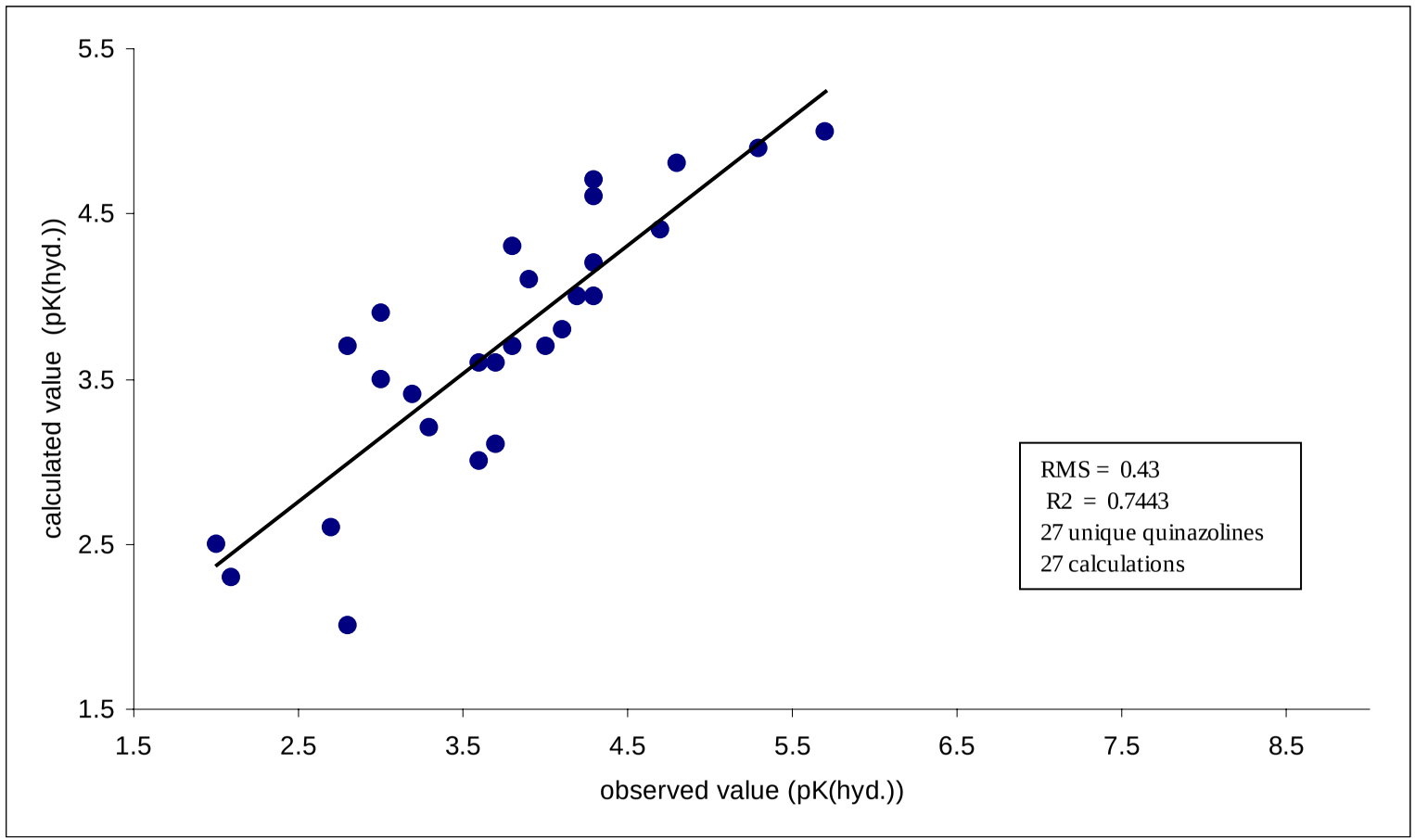

calculated pK(hyd.)
observed pK(hyd.)
RMS = 0.30
R2 = 0.95
36 unique aldehydes/ketones
36 calculations

Figure 39

Observed Vs calculated hydration equilibrium constant for 27 unique quinazolines in water at 25C.


5.5
4.5
3.5
2.5
1.5
calculated value (pK(hyd.))
1.5
2.5
3.5
4.5
5.5
6.5
7.5
8.5
observed value (pK(hyd.))
RMS = 0.43
R2 = 0.7443
27 unique quinazolines
27 calculations

Outliers

There were no outliers for hydration of aldehydes/ketones and quinazolines. For hydration of aldehydes/ketones, however, we have removed 1,2-cyclohexanedione and methyl glyoxal from M. R. Montoya and J. M. Rodriguez Mellado's data set. [16] 1,2-Cyclohexanedione's observed value is –2.06 pK(hyd) [15], but we believe that its observed value should be same as or close to the observed value of 3,4-hexanedione, which is –0.31 pK(hyd). [16] Similarly, we expect the observed value of methyl glyoxal, which observed value is -3.1 pK(hyd)-unit [15] , to be close to diacetyl's observed value, –0.28 pK(hyd.)-unit. [16] In addition, we have selected the observed values of 9-acridinium-CHO and 2, 3, and 4-pyridinium-aldehydes instead of the observed values of 9-acridine-CHO and 2, 3, and 4-pyridine-aldehydes [17, 18] because the values obtained under acidic condition fit better in our training set than the values obtained under the neutral condition.

CHAPTER 7

CONCLUSION

The SPARC calculator uses the chemical reactivity and physical interaction models to predict the chemical reactivity parameters and physical constants of organic compounds respectively. It has been successful in measuring the pKa, electron affinity and various physical constants, such as molecular polarizability, molecular volume, solute/solvent interaction, dispersion interaction, activity coefficient, vapor pressure, Henry's constant, unified retention index, and so on. Using the same SPARC chemical reactivity and physical interaction models, we have been successful in calculating the hydrolysis rate constant for esters in various solvents and at different temperatures. In addition, we have also successfully calculated the hydration equilibrium constants for aldehydes/ketones and quinazolines in water at room temperature.

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
1	Methyl formate	C(=O)OC	1.4	1.1	0.2	25	water	19
2	Ethyl formate	C(=O)OCC	1.4	1.1	0.3	25	water	19
3	Propyl formate	C(=O)OCCC	1.2	1.1	0.1	25	water	19
4	Butyl formate	C(=O)OCCCC	1.3	1.1	0.2	25	water	19
5	Methyl dichloroacetate	ClC(Cl)C(=O)OC	3.2	3.1	0.1	25	water	19
6	Ethyl difluoroacetate	FC(F)C(=O)OCC	3.7	3.8	-0.2	25	water	19
7	CS(=O)CC(=O)OCC	CS(=O)CC(=O)OCC	0.6	0.5	0.1	25	water	19
8	CS(=O)(=O)CC(=O)OCC	CS(=O)(=O)CC(=O)OCC	1.1	2.2	-1.1	25	water	19
9	Methyl acetate	CC(=O)OC	-0.7	-0.4	-0.3	25	water	20
10	Ethyl acetate	CC(=O)OCC	-1	-0.6	-0.4	25	water	11
11	Propyl acetate	CC(=O)OCCC	-1.1	-0.7	-0.4	25	water	11
12	Butyl acetate	CC(=O)OCCCC	-1.1	-0.7	-0.4	25	water	11
13	Isopropyl acetate	CC(=O)OC(C)C	-1.5	-0.9	-0.6	25	water	11
14	Cyclopropyl acetate	CC(=O)OC1CC1	-0.6	-0.5	-0.2	25	water	11
15	Cyclopentyl acetate	CC(=O)OC1CCCC1	-1.4	-0.9	-0.5	25	water	11
16	b-Methoxyethyl acetate	CC(=O)OCCOC	-0.7	-0.4	-0.3	25	water	11
17	b-Chloroethyl acetate	CC(=O)OCCCl	-0.4	-0.2	-0.2	25	water	11
18	Chloromethyl acetate	CC(=O)OCCl	1.8	1.8	0	25	water	11
19	Dichloromethyl acetate	CC(=O)OC(Cl)Cl	3.2	3.4	-0.2	25	water	11
20	Trichloromethyl acetate	CC(=O)OC(Cl)(Cl)Cl	4.1	3.9	0.2	25	water	11
21	Bromomethyl acetae	CC(=O)OCBr	2	1.7	0.3	25	water	11
22	Dimethyl-amino-ethyl acetate	CC(=O)OCCN(C)C	-1	-0.4	-0.6	25	water	11
23	Ethyl propionate	CCC(=O)OCC	-1	-1	0	25	water	11
24	Ethyl butyrate	CCCC(=O)OCC	-1.3	-1.2	-0.1	25	water	11
25	Ethyl sec-butyrate	CC(C)C(=O)OCC	-1.5	-1.4	-0.1	25	water	11
26	Ethyl neopentate	CC(C)(C)C(=O)OCC	-2.8	-2	-0.8	25	water	11
27	Ethyl fluoroacetate	FCC(=O)OCC	1.1	1.9	-0.8	25	water	11
28	Ethyl chloroacetate	ClCC(=O)OCC	1.5	1.5	0	25	water	11
29	Methyl chloroacetate	ClCC(=O)OC	1.8	1.6	0.1	25	water	11
30	Ethyl dichloroacetate	ClC(Cl)C(=O)OCC	2.8	3	-0.1	25	water	11
31	Ethyl trichloroacetate	ClC(Cl)(Cl)C(=O)OCC	3.4	3.5	-0.1	25	water	11
32	Isopropyl trichloroacetate	ClC(Cl)(Cl)C(=O)OC(C)C	2.6	3.2	-0.7	25	water	11
33	Ethyl bromoacetate	BrCC(=O)OCC	1.7	1.3	0.4	25	water	11
34	Methyl bromoacetate	BrCC(=O)OC	2	1.5	0.5	25	water	11
35	Ethyl dibromoacetate	BrC(Br)C(=O)OCC	2.3	2.4	-0.1	25	water	11
36	Ethyl bromopropionate	CC(Br)C(=O)OCC	1	0.8	0.2	25	water	11
37	Ethyl iodoacetate	ICC(=O)OCC	1.2	1.1	0.1	25	water	11

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
38	Ethyl methoxyacetate	COCC(=O)OCC	0.1	0.2	-0.1	25	water	11
39	Ethyl oxyacetate	OCC(=O)OCC	0	-0.1	0.1	25	water	11
40	CSCC(=O)OCC	CSCC(=O)OCC	0	0.2	-0.2	25	water	11
41	Ethyl aminoacetate	NCC(=O)OCC	-0.2	-0.3	0.1	25	water	11
42	CC(=O)OC(C)(CC)C=C	CC(=O)OC(C)(CC)C=C	-2.4	-1.1	-1.3	25	water	11
43	Vinyl acetate	CC(=O)OC=C	0.6	1	-0.3	25	water	11
44	C=CC(=O)OCC	C=CC(=O)OCC	-1.1	-0.7	-0.4	25	water	11
45	CC=CC(=O)OCC	CC=CC(=O)OCC	-1.9	-2.1	0.2	25	water	11
46	CC#CC(=O)OCC	CC#CC(=O)OCC	-0.3	-1.2	1	25	water	11
47	C#CC(=O)OCC	C#CC(=O)OCC	0.7	0.6	0.1	25	water	11
48	p-Nitrophenyl chloroacetate	ClCC(=O)Oc1ccc(N(=O)=O)cc1	3.8	3.2	0.6	25	water	11
49	Phenyl dichloroacetate	ClC(Cl)C(=O)Oc1ccccc1	4.1	4	0.1	25	water	11
50	Ethyl benzoate	CCOC(=O)c1ccccc1	-1.5	-1.3	-0.2	25	water	11
51	Ethyl p-aminobenzoate	CCOC(=O)c1ccc(N)cc1	-2.6	-2.8	0.2	25	water	11
52	Ethyl p-nitrobenzoate	CCOC(=O)c1ccc(N(=O)=O)cc1	-0.1	-0.3	0.2	25	water	11
53	Ethyl p-fluorobenzoate	CCOC(=O)c1ccc(F)cc1	-1.4	-1.3	-0.1	25	water	11
54	Ethyl m-aminobenzoate	CCOC(=O)c1cc(N)ccc1	-1.6	-1.8	0.1	25	water	11
55	Methyl benzoate	COC(=O)c1ccccc1	-1.1	-1.1	0	25	water	11
56	Isopropyl benzoate	CC(C)OC(=O)c1ccccc1	-2.2	-1.5	-0.7	25	water	11
57	p-Tolyl benzoate	Cc1ccc(OC(=O)c2ccccc2)cc1	-0.5	-0.3	-0.2	25	water	11
58	m-cyanophenyl benzoate	c1ccc(OC(=O)c2ccccc2)cc1C#N	0.3	0.4	-0.1	25	water	11
59	p-Nitrophenyl benzoate	O=N(=O)c1ccc(OC(=O)c2ccccc2)cc1	0.4	0.5	-0.1	25	water	11
60	2,4-dinitrophenyl benzoate	O=N(=O)c1ccc(OC(=O)c2ccccc2)c(N(=O)=O)c1	1.2	1.7	-0.5	25	water	11
61	Phenyl acetate	CC(=O)Oc1ccccc1	-0.3	0.5	-0.8	25	water	11
62	Phenyl propionate	CCC(=O)Oc1ccccc1	0.1	0	0.1	25	water	11
63	Phenyl butyrate	CCCC(=O)Oc1ccccc1	-0.1	-0.1	0	25	water	11
64	Phenyl sec-butyrate	CC(C)C(=O)Oc1ccccc1	-0.2	-0.4	0.2	25	water	11
65	Phenyl pentate	CCCCC(=O)Oc1ccccc1	-0.2	-0.2	0.1	25	water	11
66	Phenyl sec-pentate	CCC(C)C(=O)Oc1ccccc1	-0.6	-0.9	0.4	25	water	11
67	Phenyl neopentate	CC(C)(C)C(=O)Oc1ccccc1	-0.9	-1	0.1	25	water	11
68	Phenyl (t-butyl)acetate	CC(C)(C)CC(=O)Oc1ccccc1	-0.3	-0.9	0.6	25	water	11
69	p-Methoxyphenyl acetate	CC(=O)Oc1ccc(OC)cc1	0	0.2	-0.2	25	water	11
70	p-Methoxyphenyl propionate	CCC(=O)Oc1ccc(OC)cc1	-0.1	-0.2	0	25	water	11
71	p-Methoxyphenyl butyrate	CCCC(=O)Oc1ccc(OC)cc1	-0.1	-0.4	0.2	25	water	11
72	p-Methoxyphenyl sec-butyrate	CC(C)C(=O)Oc1ccc(OC)cc1	-0.3	-0.6	0.3	25	water	11
73	p-Methoxyphenyl pentate	CCCCC(=O)Oc1ccc(OC)cc1	-0.2	-0.4	0.3	25	water	11
74	p-Methoxyphenyl sec-pentate	CCC(C)C(=O)Oc1ccc(OC)cc1	-0.6	-1.1	0.6	25	water	11

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
75	p-Methoxyphenyl neopentate	CC(C)(C)C(=O)Oc1ccc(OC)cc1	-0.9	-1.2	0.3	25	water	11
76	o-Nitrophenyl acetate	CC(=O)Oc1cc(N(=O)=O)ccc1	1.3	1.1	0.2	25	water	20
77	p-Nitrophenyl acetate	CC(=O)Oc1ccc(N(=O)=O)cc1	1.5	1.2	0.3	25	water	20
78	p-Nitrophenyl propionate	CCC(=O)Oc1ccc(N(=O)=O)cc1	0.9	0.7	0.2	25	water	20
79	p-Nitrophenyl butyrate	CCCC(=O)Oc1ccc(N(=O)=O)cc1	0.8	0.5	0.2	25	water	20
80	p-Nitrophenyl sec-butyrate	CC(C)C(=O)Oc1ccc(N(=O)=O)cc1	0.7	0.3	0.4	25	water	20
81	p-Nitrophenyl pentate	CCCCC(=O)Oc1ccc(N(=O)=O)cc1	0.7	0.5	0.2	25	water	20
82	p-Nitrophenyl sec-pentate	CCC(C)C(=O)Oc1ccc(N(=O)=O)cc1	0.5	-0.2	0.7	25	water	20
83	p-Nitrophenyl neopentate	CC(C)(C)C(=O)Oc1ccc(N(=O)=O)cc1	0.1	-0.3	0.4	25	water	20
84	o-Fluorophenyl acetate	CC(=O)Oc1ccccc1F	0.9	0.9	0	25	water	20
85	o-Chlorophenyl acetate	CC(=O)Oc1ccccc1Cl	0.7	1	-0.2	25	water	20
86	o-Bromophenyl acetate	CC(=O)Oc1ccccc1Br	0.8	0.9	-0.1	25	water	20
87	o-Iodophenyl acetate	CC(=O)Oc1ccccc1I	0.7	0.9	-0.1	25	water	20
88	o-Methylphenyl acetate	CC(=O)Oc1ccccc1C	0.1	0	0.1	25	water	20
89	o-Ethylphenyl acetate	CC(=O)Oc1ccccc1CC	0.1	-0.2	0.3	25	water	20
90	o-Isopropylphenyl acetate	CC(=O)Oc1ccccc1C(C)C	0	-0.5	0.5	25	water	20
91	o-(t-Butyl)phenyl acetate	CC(=O)Oc1ccccc1C(C)(C)C	-0.3	-0.8	0.5	25	water	20
92	o-Methoxyphenyl acetate	CC(=O)Oc1ccccc1OC	0.3	0.3	0	25	water	20
93	o-Nitrophenyl acetate	CC(=O)Oc1ccccc1N(=O)=O	1.3	1.6	-0.3	25	water	20
94	o-Cyanophenyl acetate	CC(=O)Oc1ccccc1C#N	1.5	1.6	-0.1	25	water	20
95	m-Fluorophenyl acetate	CC(=O)Oc1cc(F)ccc1	0.9	0.7	0.2	25	water	20
96	m-Bromophenyl acetate	CC(=O)Oc1cc(Br)ccc1	0.9	0.8	0.1	25	water	20
97	m-Methylphenyl acetate	CC(=O)Oc1cc(C)ccc1	0.4	0.4	0	25	water	20
98	m-Ethylphenyl acetate	CC(=O)Oc1cc(CC)ccc1	0.4	0.4	0	25	water	20
99	m-Methoxyphenyl acetate	CC(=O)Oc1cc(OC)ccc1	0.6	0.5	0.1	25	water	20
100	m-Nitrophenyl acetate	CC(=O)Oc1cc(N(=O)=O)ccc1	1	1.1	-0.1	25	water	20
101	m-Cyanophenyl acetate	CC(=O)Oc1cc(C#N)ccc1	1.2	1	0.2	25	water	20
102	p-Fluorophenyl acetate	CC(=O)Oc1ccc(F)cc1	0.6	0.6	0	25	water	20
103	p-Chlorophenyl acetate	CC(=O)Oc1ccc(Cl)cc1	0.8	0.6	0.2	25	water	20
104	p-Bromophenyl acetate	CC(=O)Oc1ccc(Br)cc1	0.7	0.6	0.1	25	water	20
105	p-Ethylphenyl acetate	CC(=O)Oc1ccc(CC)cc1	0.3	0.3	0	25	water	20
106	p-(t-Butyl)phenyl acetate	CC(=O)Oc1ccc(C(C)(C)C)cc1	0.3	0.3	0	25	water	20
107	p-Cyanophenyl acetate	CC(=O)Oc1ccc(C#N)cc1	1.3	1.1	0.2	25	water	20
108	(p-Ethanal)phenyl acetate	CC(=O)Oc1ccc(C(=O)C)cc1	1	0.7	0.3	25	water	20
109	Isopropyl acetate	CC(=O)OC1CC1	-0.8	-0.6	-0.2	20	water	21
110	Cyclopropyl acetate	CC(=O)OC1CC1	-0.1	-0.2	0	40	water	21
111	Vinylic acetate	CC(=O)OC=C	-0.2	0.5	-0.8	0.2	water	21

TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE.

	Esters	SMILES	Observed logk	Calculated logk	Difference	Temperature	Solvents	References
112	Vinylic acetate	CC(=O)OC=C	0.5	0.9	-0.4	20	water	21
113	Isopropenyl acetate	CC(=O)OC(=C)C	-1.2	0.3	-1.5	0.2	water	21
114	Isopropenyl acetate	CC(=O)OC(=C)C	-0.5	0.6	-1.2	20	water	21
115	Cyclopentenyl acetate	CC(=O)OC1=CCCC1	-0.1	0	-0.1	0.2	water	21
116	Cyclopentenyl acetate	CC(=O)OC1=CCCC1	0.4	0.3	0.1	20	water	21
117	Cyclohexyl acetate	CC(=O)OC1CCCCC1	-0.8	-1.2	0.4	20	water	21
118	Cyclohexyl acetate	CC(=O)OC1CCCCC1	-0.3	-0.8	0.5	40	water	21
119	Cyclopentyl acetate	CC(=O)OC1CCCC1	-1.6	-1.1	-0.5	20	water	21
120	Cyclopentyl acetate	CC(=O)OC1CCCC1	-1	-0.7	-0.4	40	water	21
121	Butyl acetate	CC(=O)OCCCC	-1.2	-0.8	-0.4	20	water	21
122	Ethyl chloroacetate	ClCC(=O)OCC	1.3	1.4	-0.1	15	water	22
123	Ethyl chloroacetate	ClCC(=O)OCC	1.7	1.6	0.1	35	water	22
124	Ethyl dichloroacetate	ClC(Cl)C(=O)OCC	2.7	2.9	-0.2	15	water	22
125	Ethyl dichloroacetate	ClC(Cl)C(=O)OCC	3	3	0	35	water	22
126	Ethyl trichloroacetate	ClC(Cl)(Cl)C(=O)OCC	3.3	3.5	-0.2	15	water	22
127	Ethyl trichloroacetate	ClC(Cl)(Cl)C(=O)OCC	3.5	3.5	0	35	water	22
128	Ethyl bromoacetate	BrCC(=O)OCC	1.5	1.2	0.3	15	water	22
129	Ethyl bromoacetate	BrCC(=O)OCC	1.8	1.4	0.4	35	water	22
130	Ethyl iodoacetate	ICC(=O)OCC	1.1	1	0.1	15	water	22
131	Ethyl iodoacetate	ICC(=O)OCC	1.4	1.2	0.2	35	water	22
132	Ethyl dibromoacetate	BrC(Br)C(=O)OCC	2.5	2.4	0	35	water	22
133	Methyl chloroacetate	ClCC(=O)OC	1.5	1.5	0	15	water	22
134	Methyl chloroacetate	ClCC(=O)OC	2	1.8	0.2	35	water	22
135	Mehtyl bromoacetate	BrCC(=O)OC	1.8	1.3	0.4	15	water	22
136	Mehtyl bromoacetate	BrCC(=O)OC	2.2	1.6	0.5	35	water	22
137	Methyl dichloroacetate	ClC(Cl)C(=O)OC	3	3.1	-0.1	15	water	22
138	Methyl dichloroacetate	ClC(Cl)C(=O)OC	3.3	3.2	0.1	35	water	22
139	Ethyl trifluoroacetate	FC(F)(F)C(=O)OCC	5.2	4.7	0.5	15	water	22
140	Isopropyl trichloroacetate	ClC(Cl)(Cl)C(=O)OC(C)C	2.7	3.3	-0.6	35	water	22
141	Chloromethyl acetate	CC(=O)OCCl	0.8	1.7	-0.9	15	water	22
142	Ethyl 2-pyridine-carboxylate	n1ccccc1C(=O)OCC	-0.3	0.3	-0.5	25	water	19

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
1	Methyl formate	C(=O)OC	1.2	0.8	0.5	25	37% Acetone	23
2	Ethyl formate	C(=O)OCC	1	0.8	0.2	25	37% Acetone	23
3	Propyl formate	C(=O)OCCC	0.9	0.8	0.1	25	37% Acetone	23
4	Isopropyl formate	C(=O)OC(C)C	0.5	0.8	-0.2	25	37% Acetone	23
5	Butyl formate	C(=O)OCCCC	0.8	0.8	0.1	25	37% Acetone	23
6	sec-Butyl formate	C(=O)OC(C)CC	0.3	0.8	-0.5	25	37% Acetone	23
7	Isobutyl formate	C(=O)OCC(C)C	0.8	0.8	0	25	37% Acetone	23
8	Pentyl formate	C(=O)OCCCCC	0.7	0.8	0	25	37% Acetone	23
9	Isopentyl formate	C(=O)OCC(C)CC	0.7	0.8	-0.1	25	37% Acetone	23
10	Methyl acetate	CC(=O)OC	-0.8	-0.8	0	25	37% Acetone	23
11	Methyl propionate	CCC(=O)OC	-1	-1.3	0.3	25	37% Acetone	23
12	Methyl butyrate	CCCC(=O)OC	-1.3	-1.5	0.2	25	37% Acetone	23
13	Methyl isobutyrate	C(C)CC(=O)OC	-1.4	-1.5	0.1	25	37% Acetone	23
14	Ethyl acetate	CC(=O)OCC	-1.2	-1	-0.2	25	37% Acetone	23
15	propyl acetate	CC(=O)OCCC	-1.3	-1	-0.3	25	37% Acetone	23
16	Butyl acetate	CC(=O)OCCCC	-1.4	-1.1	-0.3	25	37% Acetone	23
17	sec-Butyl acetate	CC(=O)OC(C)CC	-2.2	-1.9	-0.3	25	37% Acetone	23
18	Isobutyl acetate	CC(=O)OCC(C)C	-1.5	-1.1	-0.4	25	37% Acetone	23
19	Pentyl acetate	CC(=O)OCCCCC	-1.5	-1.1	-0.4	25	37% Acetone	23
20	Isopentyl acetate	CC(=O)OCC(C)CC	-1.5	-1.6	0.2	25	37% Acetone	23
21	Hexyl acetate	CC(=O)OCCCCCC	-1.5	-1.1	-0.4	25	37% Acetone	23
22	Ethyl propionate	CCC(=O)OCC	-1.3	-1.5	0.2	25	37% Acetone	23
23	Ethyl butyrate	CCCC(=O)OCC	-1.7	-1.7	0	25	37% Acetone	23
24	Methyl acetate	CC(=O)OC	-1	-1.1	0.1	25	70% Acetone	24
25	Ethyl acetate	CC(=O)OCC	-1.3	-1.3	0	25	70% Acetone	24
26	propyl acetate	CC(=O)OCCC	-1.6	-1.4	-0.1	25	70% Acetone	24
27	Isopropyl acetate	CC(=O)OC(C)C	-2.2	-1.8	-0.4	25	70% Acetone	24
28	sec-Butyl acetate	CC(=O)OCC(C)C	-1.7	-1.5	-0.2	25	70% Acetone	24
29	Butyl acetate	CC(=O)OCCCC	-1.6	-1.5	-0.1	25	70% Acetone	24
30	sec-Butyl acetate	CC(=O)OC(C)CC	-2.5	-2.6	0.1	25	70% Acetone	24
31	t-Butyl acetate	CC(=O)OC(C)(C)C	-3.6	-2.7	-0.9	25	70% Acetone	24
32	Cyclohexyl acetate	CC(=O)OC1CCCCC1	-2.3	-2.1	-0.2	25	70% Acetone	24
33	Methyl propionate	CCC(=O)OC	-1.2	-1.7	0.5	25	70% Acetone	24
34	Ethyl propionate	CCC(=O)OCC	-1.7	-2	0.3	25	70% Acetone	24
35	Isopropyl propionate	CCC(=O)OC(C)C	-2.5	-2.4	-0.1	25	70% Acetone	24
36	Butyl propionate	CCC(=O)OCCCC	-2	-2.1	0.1	25	70% Acetone	24
37	Benzyl benzoate	c1ccccc1C(=O)OCc2ccccc2	-2.2	-1.9	-0.3	25	70% Acetone	24

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
38	p-Methylbenzyl benzoate	c1ccccc1C(=O)OCc2ccc(C)cc2	-2.3	-2	-0.3	25	70% Acetone	24
39	m-Methylbenzyl benzoate	c1ccccc1C(=O)OCc2cc(C)ccc2	-2.2	-2	-0.3	25	70% Acetone	24
40	p-Ethylbenzyl benzoate	c1ccccc1C(=O)OCc2ccc(CC)cc2	-2.3	-2	-0.3	25	70% Acetone	24
41	p-Isopropylbenzyl benzoate	c1ccccc1C(=O)OCc2ccc(C(C)C)cc2	-2.3	-2	-0.3	25	70% Acetone	24
42	p-(t-Butyl)benzyl benzoate	c1ccccc1C(=O)OCc2ccc(C(C)(C)C)cc2	-2.3	-2	-0.3	25	70% Acetone	24
43	p-Methoxylbenzyl benzoate	c1ccccc1C(=O)OCc2ccc(OC)cc2	-2.3	-2.1	-0.2	25	70% Acetone	24
44	p-Phenoxybenzyl benzoate	c1ccccc1C(=O)OCc2ccc(Oc3ccccc3)cc2	-2.1	-1.9	-0.2	25	70% Acetone	24
45	(p-Methiol)benzyl benzoate	c1ccccc1C(=O)OCc2ccc(CS)cc2	-2.1	-1.9	-0.2	25	70% Acetone	24
46	(m-Methiol)benzyl benzoate	c1ccccc1C(=O)OCc2cc(CS)ccc2	-2	-1.8	-0.2	25	70% Acetone	24
47	p-Phenylbenzyl benzoate	c1ccccc1C(=O)OCc2ccc(c3ccccc3)cc2	-2.1	-1.8	-0.3	25	70% Acetone	24
48	2-Naphthylcarbinyl benzoate	c1ccccc1C(=O)OCc3cc4ccccc4cc3	-2.1	-1.8	-0.3	25	70% Acetone	24
49	p-Fluorobenzyl benzoate	c1ccccc1C(=O)OCc2ccc(F)cc2	-2	-1.8	-0.2	25	70% Acetone	24
50	p-Chlorobenzyl benzoate	c1ccccc1C(=O)OCc2ccc(Cl)cc2	-1.9	-1.7	-0.2	25	70% Acetone	24
51	m-Chlorobenzyl benzoate	c1ccccc1C(=O)OCc2cc(Cl)ccc2	-1.8	-1.6	-0.2	25	70% Acetone	24
52	p-Bromobenzyl benzoate	c1ccccc1C(=O)OCc2ccc(Br)cc2	-1.9	-1.7	-0.2	25	70% Acetone	24
53	m-Bromobenzyl benzoate	c1ccccc1C(=O)OCc2cc(Br)ccc2	-1.8	-1.6	-0.2	25	70% Acetone	24
54	p-Nitrobenzyl benzoate	c1ccccc1C(=O)OCc2ccc(N(=O)=O)cc2	-1.4	-1.2	-0.2	25	70% Acetone	24
55	m-Nitrobenzyl benzoate	c1ccccc1C(=O)OCc2cc(N(=O)=O)ccc2	-1.5	-1.3	-0.2	25	70% Acetone	24
56	p-Cyanobenzyl benzoate	c1ccccc1C(=O)OCc2ccc(C#N)cc2	-1.5	-1.2	-0.2	25	70% Acetone	24
57	m-Cyanobenzyl benzoate	c1ccccc1C(=O)OCc2cc(C#N)ccc2	-1.5	-1.3	-0.2	25	70% Acetone	24
58	(p-S(=O)C)benzyl benzoate	c1ccccc1C(=O)OCc2ccc(S(=O)C)cc2	-1.6	-1.4	-0.2	25	70% Acetone	24
59	(p-S(=O)(=O)C)benzyl benzoate	c1ccccc1C(=O)OCc2ccc(S(=O)(=O)C)cc2	-1.4	-1.3	-0.1	25	70% Acetone	24
60	(m-S(=O)(=O)C)benzyl benzoate	c1ccccc1C(=O)OCc2cc(S(=O)(=O)C)ccc2	-1.5	-1.3	-0.2	25	70% Acetone	24
61	2-Fluorenylcarbinyl benzoate	c1c2Cc3cc(COC(=O)Cc4ccccc4)ccc3c2ccc1	-2.2	-1	-1.2	25	70% Acetone	24
62	1-Naphthylcarbinyl benzoate	c1ccccc1C(=O)OCc2c3ccccc3ccc2	-2.1	-1.9	-0.2	25	70% Acetone	24
63	2-Phenanthrylcabinyl benzoate	c1(COC(=O)c4ccccc4)cc2ccc3ccccc3c2cc1	-2	-1.8	-0.2	25	70% Acetone	24
64	3-Phenanthrylcarbinyl benzoate	c1cc2ccc3ccccc3c2cc1(COC(=O)c4ccccc4)	-2.1	-1.7	-0.4	25	70% Acetone	24
65	9-Phenanthrylcarbinyl benzoate	c1cc2cc(COC(=O)c4ccccc4)c3ccccc3c2cc1	-2	-1.9	-0.2	25	70% Acetone	24
66	9-Anthrylcarbinyl benzoate	c1ccc2c(COC(=O)c4ccccc4)c3ccccc3cc2c1	-2.2	-1.7	-0.5	25	70% Acetone	24
67	Ethyl phenylacetate	c1ccccc1CC(=O)OCC	-1.4	-1.4	0.1	25	60% Acetone	25
68	Ethyl o-fluorophenylacetate	Fc1ccccc1CC(=O)OCC	-1.5	-1.8	0.4	25	60% Acetone	25
69	Ethyl o-chlorophenylacetate	Clc1ccccc1CC(=O)OCC	-1.8	-1.9	0.1	25	60% Acetone	25
70	Ethyl o-bromophenylacetate	Brc1ccccc1CC(=O)OCC	-1.9	-2	0.1	25	60% Acetone	25
71	Ethyl o-iodophenylacetate	Ic1ccccc1CC(=O)OCC	-1.9	-2.1	0.1	25	60% Acetone	25
72	Ethyl m-iodophenylacetate	c1c(I)cccc1CC(=O)OCC	-1.1	-1.3	0.2	25	60% Acetone	25
73	Ethyl o-methylphenylacetate	Cc1ccccc1CC(=O)OCC	-2	-2.1	0.2	25	60% Acetone	25
74	Ethyl o-butylphenylacetate	CCCCc1ccccc1CC(=O)OCC	-2.8	-2.5	-0.4	25	60% Acetone	25

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
75	Ethyl 1,6-dichlorophenylacetate	Clc1cccc(Cl)c1CC(=O)OCC	-2.9	-2.4	-0.4	25	60% Acetone	25
76	Ethyl p-(t-butyl)phenylacetate	c1cc(C(C)(C)C)ccc1CC(=O)OCC	-1.7	-1.6	-0.1	25	60% Acetone	26
77	Ethyl p-dimethylaminophenylacetate	c1cc(N(C)C)ccc1CC(=O)OCC	-1.6	-1.9	0.3	25	60% Acetone	26
78	Ethyl o-nitrophenylacetate	O=N(=O)c1ccccc1CC(=O)OCC	-1.6	-2	0.4	25	60% Acetone	26
79	Ethyl p-aminophenylacetate	c1cc(N)ccc1CC(=O)OCC	-1.5	-1.9	0.3	25	60% Acetone	26
80	Ethyl m-methoxyphenylacetate	c1c(OC)cccc1CC(=O)OCC	-1.3	-1.5	0.2	25	60% Acetone	26
81	Ethyl (3,4-biphenyl)phenylacetate	c1c(c2ccccc2)c(c3ccccc3)ccc1CC(=O)OCC	-1.3	-1.4	0.1	25	60% Acetone	26
82	Ethyl (p-phenyl)phenylacetate	c1cc(c2ccccc2)ccc1CC(=O)OCC	-1.5	-1.4	-0.1	25	60% Acetone	26
83	Ethyl p-iodophenylacetate	c1cc(I)ccc1CC(=O)OCC	-1.2	-1.3	0.2	25	60% Acetone	26
84	Ethyl m-chlorophenylacetate	c1c(Cl)cccc1CC(=O)OCC	-1	-1.4	0.3	25	60% Acetone	26
85	Ethyl m-fluorophenylacetate	c1c(F)cccc1CC(=O)OCC	-1	-1.4	0.4	25	60% Acetone	26
86	Ethyl p-cyanophenylacetate	c1cc(C#N)ccc1CC(=O)OCC	-0.7	-1.1	0.4	25	60% Acetone	26
87	Ethyl p-nitrophenylacetate	c1cc(N(=O)=O)ccc1CC(=O)OCC	-0.6	-1.1	0.5	25	60% Acetone	26
88	Ethyl m-nitrophenylacetate	c1c(N(=O)=O)cccc1CC(=O)OCC	-0.8	-1.2	0.4	25	60% Acetone	26
89	Ethyl p-bromophenylacetate	c1cc(Br)ccc1CC(=O)OCC	-1	-1.4	0.4	25	60% Acetone	26
90	Ethyl p-chlorophenylacetate	c1cc(Cl)ccc1CC(=O)OCC	-1	-1.4	0.4	25	60% Acetone	26
91	Ethyl p-fluorophenylacetate	c1cc(F)ccc1CC(=O)OCC	-1.2	-1.4	0.2	25	60% Acetone	26
92	Ethyl p-methoxyphenylacetate	c1cc(OC)ccc1CC(=O)OCC	-1.4	-1.7	0.3	25	60% Acetone	26
93	Ethyl p-methylphenylacetate	c1cc(C)ccc1CC(=O)OCC	-1.6	-1.6	0	25	60% Acetone	26
94	Methyl phenylacetate	c1ccccc1CC(=O)OC	-0.9	-1.5	0.6	25	75% Acetone	27
95	Methyl 9-anthrylacetate	c1ccc2cc3ccccc3c(CC(=O)OC)c2c1	-1.8	-2.3	0.5	25	75% Acetone	27
96	Methyl 9-phenanthrylacetate	c1cc2cc(CC(=O)OC)c3ccccc3c2cc1	-1.4	-1.7	0.3	25	75% Acetone	27
97	Methyl 1-naphthylacetate	c1cc2c(CC(=O)OC)cccc2cc1	-1.3	-1.7	0.4	25	75% Acetone	27
98	Methyl p-methylbenzoate	c1cc(C)ccc1CC(=O)OC	-1	-1.7	0.7	25	75% Acetone	27
99	Methyl 2-naphthylacetate	c1cc2cc(CC(=O)OC)ccc2cc1	-0.8	-1.4	0.6	25	75% Acetone	27
100	Methyl 4-biphenylacetate	COC(=O)Cc1ccc(c2ccccc2)cc1	-0.8	-1.4	0.6	25	75% Acetone	27
101	Methyl 2-anthrylacetate	COC(=O)Cc1ccc2cc3ccccc3cc2c1	-0.8	-1.4	0.6	25	75% Acetone	27
102	Methyl 3-phenanthrylacetate	c1cc2ccc3ccccc3c2cc1CC(=O)OC	-0.8	-1.4	0.6	25	75% Acetone	27
103	Methyl 2-phenanthrylacetate	c1(CC(=O)OC)cc2ccc3ccccc3c2cc1	-0.8	-1.5	0.7	25	75% Acetone	27
104	Methyl acetate	CC(=O)OC	-1	-1.2	0.2	20	70% Acetone	24
105	Ethyl acetate	CC(=O)OCC	-1.5	-1.4	0	20	70% Acetone	24
106	Ethyl acetate	CC(=O)OCC	-1.3	-1.1	-0.2	35	70% Acetone	24
107	Ethyl acetate	CC(=O)OCC	-0.9	-0.9	0.1	44.7	70% Acetone	24
108	Propyl acetate	CC(=O)OCCC	-1.7	-1.5	-0.2	20	70% Acetone	24
109	Propyl acetate	CC(=O)OCCC	-1.3	-1.2	-0.1	35	70% Acetone	24
110	Propyl acetate	CC(=O)OCCC	-1	-1	0	44.7	70% Acetone	24
111	Isopropyl acetate	CC(=O)OC(C)C	-2.3	-1.9	-0.4	20	70% Acetone	24

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
112	Isopropyl acetate	CC(=O)OC(C)C	-1.9	-1.6	-0.3	35	70% Acetone	24
113	Isopropyl acetate	CC(=O)OC(C)C	-1.6	-1.4	-0.2	44.7	70% Acetone	24
114	Isobutyl acetate	CC(=O)OCC(C)C	-1.9	-1.6	-0.2	20	70% Acetone	24
115	Isobutyl acetate	CC(=O)OCC(C)C	-1.4	-1.3	-0.1	35	70% Acetone	24
116	Isobutyl acetate	CC(=O)OCC(C)C	-1.2	-1.1	-0.1	44.7	70% Acetone	24
117	n-Butyl acetate	CC(=O)OCCCC	-1.8	-1.6	-0.2	20	70% Acetone	24
118	n-Butyl acetate	CC(=O)OCCCC	-1.6	-1.3	-0.4	35	70% Acetone	24
119	n-Butyl acetate	CC(=O)OCCCC	-1.1	-1.1	0	44.7	70% Acetone	24
120	sec-Butyl acetate	CC(=O)OC(C)CC	-2.6	-2.7	0.1	20	70% Acetone	24
121	sec-Butyl acetate	CC(=O)OC(C)CC	-2.2	-2.3	0.2	35	70% Acetone	24
122	sec-Butyl acetate	CC(=O)OC(C)CC	-1.9	-2.2	0.3	44.7	70% Acetone	24
123	t-Butyl acetate	CC(=O)OC(C)(C)C	-3.2	-2.5	-0.7	35	70% Acetone	24
124	t-Butyl acetate	CC(=O)OC(C)(C)C	-3	-2.3	-0.7	44.7	70% Acetone	24
125	Cyclohexyl acetate	CC(=O)OC1CCCCC1	-2	-1.9	-0.2	35	70% Acetone	24
126	Cyclohexyl acetate	CC(=O)OC1CCCCC1	-1.8	-1.7	-0.1	44.7	70% Acetone	24
127	Methyl propionate	CCC(=O)OC	-1.3	-1.8	0.5	20	70% Acetone	24
128	Methyl propionate	CCC(=O)OC	-1	-1.5	0.6	35	70% Acetone	24
129	Methyl propionate	CCC(=O)OC	-0.8	-1.3	0.6	44.7	70% Acetone	24
130	Ethyl propionate	CCC(=O)OCC	-1.8	-2.1	0.3	20	70% Acetone	24
131	Ethyl propionate	CCC(=O)OCC	-1.4	-1.8	0.4	35	70% Acetone	24
132	Ethyl propionate	CCC(=O)OCC	-1.2	-1.6	0.4	44.7	70% Acetone	24
133	Isopropyl propionate	CCC(=O)OC(C)C	-2.7	-2.6	-0.1	20	70% Acetone	24
134	Isopropyl propionate	CCC(=O)OC(C)C	-2.2	-2.2	0	35	70% Acetone	24
135	Isopropyl propionate	CCC(=O)OC(C)C	-1.9	-2	0.1	44.7	70% Acetone	24
136	n-Butyl propionate	CCC(=O)OCCCC	-2.1	-2.2	0.1	20	70% Acetone	24
137	n-Butyl propionate	CCC(=O)OCCCC	-1.7	-1.9	0.2	35	70% Acetone	24
138	n-Butyl propionate	CCC(=O)OCCCC	-1.5	-1.7	0.3	44.7	70% Acetone	24
139	Ethyl picolinate	n1ccccc1C(=O)OCC	-0.7	-0.9	0.2	25	60% acetone	19
140	Ethyl isonicotinate	c1ncccc1C(=O)OCC	-0.2	-1.1	0.9	25	60% acetone	19
141	Ethyl nicotinate	c1cncccC(=O)OCC	-0.9	-1.2	0.3	25	60% acetone	19

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
1	Ethyl 1-naphthoate	c1ccc2ccccc2c1C(=O)OCC	-3.6	-3	-0.6	25	85% Ethanol	28
2	Ethyl 3-chloro-1-napthoate	c1c(Cl)cc2ccccc2c1C(=O)OCC	-2.7	-2.7	0	25	85% Ethanol	28
3	Ethyl 3-bromo-1-naphthoate	c1c(Br)cc2ccccc2c1C(=O)OCC	-2.7	-2.7	0	25	85% Ethanol	28
4	Ethyl 4-bromo-1-naphthoate	c1cc(Br)c2ccccc2c1C(=O)OCC	-3	-2.9	0	25	85% Ethanol	28
5	Ethyl 5-bromo-1-naphthoate	c1ccc2c(Br)cccc2c1C(=O)OCC	-3	-2.9	-0.1	25	85% Ethanol	28
6	Ethyl 4'-methoxy-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(OC)cc2)cc1	-3.5	-2.9	-0.5	25	91% Ethanol	29
7	Ethyl 4'-methyl-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(C)cc2)cc1	-3.4	-2.8	-0.5	25	91% Ethanol	29
8	Ethyl p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccccc2)cc1	-3.3	-2.7	-0.6	25	91% Ethanol	29
9	Ethyl 4'-chloro-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(Cl)cc2)cc1	-3.1	-2.7	-0.4	25	91% Ethanol	29
10	Ethyl 4'-bromo-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(Br)cc2)cc1	-3.1	-2.7	-0.4	25	91% Ethanol	29
11	Ethyl 3'-bromo-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2cc(Br)ccc2)cc1	-3	-2.7	-0.4	25	91% Ethanol	29
12	Ethyl 4'-nitro-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(N(=O)=O)cc2)cc1	-2.8	-2.5	-0.3	25	91% Ethanol	29
13	Ethyl benzoate	c1ccccc1C(=O)OCC	-3	-2.5	-0.5	25	75% Ethanol	30
14	Ethyl phenylacetate	CCOC(=O)Cc1ccccc1	-1.9	-1.7	-0.2	25	85% Ethanol	25
15	Ethyl o-iodophenyl acetate	CCOC(=O)Cc1c(I)cccc1	-2.3	-2.5	0.1	25	85% Ethanol	25
16	Ethyl p-iodophenylacetate	CCOC(=O)Cc1ccc(I)cc1	-1.5	-1.6	0.1	25	85% Ethanol	25
17	Ethyl p-nitrophenylacetate	CCOC(=O)Cc1ccc(N(=O)=O)cc1	-1	-1.3	0.3	25	85% Ethanol	25
18	Ethyl o-methylphenylacetate	CCOC(=O)Cc1c(C)cccc1	-2.4	-2.5	0	25	85% Ethanol	25
19	Ethyl p-methylphenylacetate	CCOC(=O)Cc1ccc(C)cc1	-2	-1.8	-0.2	25	85% Ethanol	25
20	Ethyl phenylacetate	CCOC(=O)Cc1ccccc1	-1.8	-1.6	-0.2	25	75% Ethanol	25
21	Ethyl o-iodophenylacetate	CCOC(=O)Cc1c(I)cccc1	-2.2	-2.3	0	25	75% Ethanol	25
22	Ethyl p-iodophenylacetate	CCOC(=O)Cc1ccc(I)cc1	-1.4	-1.4	0	25	75% Ethanol	25
23	Ethyl p-nitrophenylacetate	CCOC(=O)Cc1ccc(N(=O)=O)cc1	-0.9	-1.2	0.3	25	75% Ethanol	25
24	Ethyl o-methylphenylacetate	CCOC(=O)Cc1c(C)cccc1	-2.3	-2.3	0	25	75% Ethanol	25
25	Ethyl p-methylphenylacetate	CCOC(=O)Cc1ccc(C)cc1	-1.9	-1.7	-0.2	25	75% Ethanol	25
26	Ethyl phenylacetate	CCOC(=O)Cc1ccccc1	-1.7	-1.4	-0.3	25	65% Ethanol	25
27	Ethyl o-chlorophenylacetate	CCOC(=O)Cc1c(Cl)cccc1	-2.1	-1.8	-0.2	25	65% Ethanol	25
28	Ethyl o-chlorophenylacetate	CCOC(=O)Cc1ccc(Cl)cc1	-1.3	-1.3	0	25	65% Ethanol	25
29	Ethyl o-bromophenylacetate	CCOC(=O)Cc1c(Br)cccc1	-2.1	-2	-0.2	25	65% Ethanol	25
30	Ethyl o-iodophenylacetate	CCOC(=O)Cc1c(I)cccc1	-2.2	-2	-0.1	25	65% Ethanol	25
31	Ethyl p-iodophenylacetate	CCOC(=O)Cc1ccc(I)cc1	-1.3	-1.3	0	25	65% Ethanol	25
32	Ethyl o-nitrophenylacetate	CCOC(=O)Cc1c(N(=O)=O)cccc1	-1.9	-1.9	0	25	65% Ethanol	25
33	Ethyl m-nitrophenylacetate	CCOC(=O)Cc1cc(N(=O)=O)ccc1	-0.9	-1.1	0.2	25	65% Ethanol	25
34	Ethyl p-nitrophenylacetate	CCOC(=O)Cc1ccc(N(=O)=O)cc1	-0.8	-1	0.2	25	65% Ethanol	25
35	Ethyl o-methylphenylacetate	CCOC(=O)Cc1c(C)cccc1	-2.2	-2.1	-0.2	25	65% Ethanol	25
36	Ethyl p-methylphenylacetate	CCOC(=O)Cc1ccc(C)cc1	-1.8	-1.5	-0.2	25	65% Ethanol	25
37	Ethyl p-(t-butyl)phenylacetate	CCOC(=O)Cc1ccc(C(C)(C)C)cc1	-1.8	-1.5	-0.2	25	65% Ethanol	25

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
38	Ethyl phenylacetate	CCOC(=O)Cc1ccccc1	-2	-1.7	-0.3	25	90% Ethanol	25
39	Ethyl o-fluorophenylacetate	CCOC(=O)Cc1c(F)cccc1	-2.1	-2.2	0.1	25	90% Ethanol	25
40	Ethyl p-fluorophenylacetate	CCOC(=O)Cc1ccc(F)cc1	-1.8	-1.7	-0.1	25	90% Ethanol	25
41	Ethyl o-chlorophenylacetate	CCOC(=O)Cc1c(Cl)cccc1	-2.3	-2.3	-0.1	25	90% Ethanol	25
42	Ethyl m-chlorophenylacetate	CCOC(=O)Cc1cc(Cl)ccc1	-1.6	-1.6	0	25	90% Ethanol	25
43	Ethyl p-chlorophenylacetate	CCOC(=O)Cc1ccc(Cl)cc1	-1.6	-1.6	0	25	90% Ethanol	25
44	Ethyl o-bromophenylacetate	CCOC(=O)Cc1c(Br)cccc1	-2.4	-2.4	0.1	25	90% Ethanol	25
45	Ethyl p-bromophenylacetate	CCOC(=O)Cc1ccc(Br)cc1	-1.6	-1.6	0	25	90% Ethanol	25
46	Ethyl o-iodophenylacetate	CCOC(=O)Cc1c(I)cccc1	-2.4	-2.5	0.1	25	90% Ethanol	25
47	Ethyl m-iodophenylacetate	CCOC(=O)Cc1cc(I)ccc1	-1.6	-1.6	0	25	90% Ethanol	25
48	Ethyl p-iodophenylacetate	CCOC(=O)Cc1ccc(I)cc1	-1.6	-1.6	0	25	90% Ethanol	25
49	Ethyl o-nitrophenylacetate	CCOC(=O)Cc1c(N(=O)=O)cccc1	-2.1	-2.4	0.3	25	90% Ethanol	25
50	Ethyl m-nitrophenylacetate	CCOC(=O)Cc1cc(N(=O)=O)ccc1	-1.1	-1.4	0.3	25	90% Ethanol	25
51	Ethyl p-nitrophenylacetate	CCOC(=O)Cc1ccc(N(=O)=O)cc1	-1.1	-1.3	0.2	25	90% Ethanol	25
52	Ethyl o-methylphenylacetate	CCOC(=O)Cc1c(C)cccc1	-2.5	-2.5	0	25	90% Ethanol	25
53	Ethyl p-methylphenylacetate	CCOC(=O)Cc1ccc(C)cc1	-2.1	-1.9	-0.3	25	90% Ethanol	25
54	Ethyl o-(t-butyl)phenylacetate	CCOC(=O)Cc1c(C(C)(C)C)cccc1	-3.3	-3.4	0.1	25	90% Ethanol	25
55	Ethyl p-(t-butyl)phenylacetate	CCOC(=O)Cc1ccc(C(C)(C)C)cc1	-2.1	-1.9	-0.2	25	90% Ethanol	25
56	Ethyl o-methoxyphenylacetate	CCOC(=O)Cc1c(OC)cccc1	-2.8	-2.8	-0.1	25	90% Ethanol	25
57	Ethyl m-methoxyphenylacetate	CCOC(=O)Cc1cc(OC)ccc1	-2	-1.8	-0.2	25	90% Ethanol	25
58	Ethyl p-methoxyphenylacetate	CCOC(=O)Cc1ccc(OC)cc1	-2.1	-2	-0.1	25	90% Ethanol	25
59	Ethyl p-nitrophenylacetate	CCOC(=O)Cc1ccc(N)cc1	-2.3	-2.1	-0.2	25	90% Ethanol	25
60	Ethyl 1,6-dichlorophenylacetate	CCOC(=O)Cc1c(Cl)cccc1Cl	-3.4	-2.9	-0.5	25	90% Ethanol	25
61	Ethyl 3,4-dimethoxyphenylacetate	CCOC(=O)Cc1cc(OC)c(OC)cc1	-2	-2.1	0.1	25	90% Ethanol	25
62	Ethyl 1-naphthoate	c1ccc2ccccc2c1C(=O)OCC	-3.1	-2.8	-0.3	35	85% Ethanol	28
63	Ethyl 1-naphthoate	c1ccc2ccccc2c1C(=O)OCC	-2.8	-2.6	-0.1	45	85% Ethanol	28
64	Ethyl 1-naphthoate	c1ccc2ccccc2c1C(=O)OCC	-2.5	-2.4	0	55	85% Ethanol	28
65	Ethyl 1-naphthoate	c1ccc2ccccc2c1C(=O)OCC	-2.1	-2.3	0.2	65	85% Ethanol	28
66	Ethyl 3-chloro-1-naphthoate	c1c(Cl)cc2ccccc2c1C(=O)OCC	-2.7	-2.5	-0.1	35	85% Ethanol	28
67	Ethyl 3-chloro-1-naphthoate	c1c(Cl)cc2ccccc2c1C(=O)OCC	-2	-2.3	0.4	45	85% Ethanol	28
68	Ethyl 3-chloro-1-naphthoate	c1c(Cl)cc2ccccc2c1C(=O)OCC	-1.6	-2.2	0.6	55	85% Ethanol	28
69	Ethyl 4-chloro-1-naphthoate	c1cc(Cl)c2ccccc2c1C(=O)OCC	-2.6	-2.8	0.2	35	85% Ethanol	28
70	Ethyl 4-chloro-1-naphthoate	c1cc(Cl)c2ccccc2c1C(=O)OCC	-2.2	-2.6	0.4	45	85% Ethanol	28
71	Ethyl 4-chloro-1-naphthoate	c1cc(Cl)c2ccccc2c1C(=O)OCC	-1.9	-2.4	0.5	55	85% Ethanol	28
72	Ethyl 4-chloro-1-naphthoate	c1cc(Cl)c2ccccc2c1C(=O)OCC	-2.5	-2.2	-0.3	65	85% Ethanol	28
73	Ethyl 3-bromo-1-naphthoate	c1c(Br)cc2ccccc2c1C(=O)OCC	-2	-2.3	0.4	45	85% Ethanol	28
74	Ethyl 3-bromo-1-naphthoate	c1c(Br)cc2ccccc2c1C(=O)OCC	-1.3	-2	0.7	65	85% Ethanol	28

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
75	Ethyl 4-bromo-1-naphthoate	c1cc(Br)c2ccccc2c1C(=O)OCC	-2.6	-2.7	0.2	35	85% Ethanol	28
76	Ethyl 4-bromo-1-naphthoate	c1cc(Br)c2ccccc2c1C(=O)OCC	-1.9	-2.4	0.5	55	85% Ethanol	28
77	Ethyl 4-bromo-1-naphthoate	c1cc(Br)c2ccccc2c1C(=O)OCC	-1.5	-2.2	0.7	65	85% Ethanol	28
78	Ethyl 5-bromo-1-naphthoate	c1ccc2c(Br)cccc2c1C(=O)OCC	-2.3	-2.5	0.2	45	85% Ethanol	28
79	Ethyl 5-bromo-1-naphthoate	c1ccc2c(Br)cccc2c1C(=O)OCC	-1.9	-2.3	0.4	55	85% Ethanol	28
80	Ethyl 5-bromo-1-naphthoate	c1ccc2c(Br)cccc2c1C(=O)OCC	-1.6	-2.1	0.5	65	85% Ethanol	28
81	Ethyl 4-methyl-1-naphthoate	c1cc(C)c2ccccc2c1C(=O)OCC	-3.1	-3.2	0.1	45	85% Ethanol	28
82	Ethyl 4-methyl-1-naphthoate	c1cc(C)c2ccccc2c1C(=O)OCC	-2.8	-3	0.2	55	85% Ethanol	28
83	Ethyl 4-methyl-1-naphthoate	c1cc(C)c2ccccc2c1C(=O)OCC	-2.4	-2.8	0.4	65	85% Ethanol	28
84	Ethyl 4-methyl-1-naphthoate	c1cc(C)c2ccccc2c1C(=O)OCC	-2	-2.6	0.6	75	85% Ethanol	28
85	Ethyl 3-methyl-1-naphthoate	c1c(C)cc2ccccc2c1C(=O)OCC	-2.9	-2.7	-0.2	45	85% Ethanol	28
86	Ethyl 3-methyl-1-naphthoate	c1c(C)cc2ccccc2c1C(=O)OCC	-2.6	-2.5	0	55	85% Ethanol	28
87	Ethyl 3-methyl-1-naphthoate	c1c(C)cc2ccccc2c1C(=O)OCC	-2.2	-2.4	0.1	65	85% Ethanol	28
88	Ethyl 3-methyl-1-naphthoate	c1c(C)cc2ccccc2c1C(=O)OCC	-1.9	-2.2	0.3	75	85% Ethanol	28
89	Ethyl 4'-methoxy-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(OC)cc2)cc1	-2.8	-2.6	-0.2	40	91% Ethanol	29
90	Ethyl 4'-methyl-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(C)cc2)cc1	-2.7	-2.5	-0.2	40	91% Ethanol	29
91	Ethyl p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccccc2)cc1	-2.6	-2.4	-0.2	40	91% Ethanol	29
92	Ethyl 4'-chloro-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(Cl)cc2)cc1	-2.5	-2.4	-0.1	40	91% Ethanol	29
93	Ethyl 4'-bromo-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(Br)cc2)cc1	-2.5	-2.4	-0.1	40	91% Ethanol	29
94	Ethyl 3'-bromo-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2cc(Br)ccc2)cc1	-2.4	-2.4	-0.1	40	91% Ethanol	29
95	Ethyl 3'-nitro-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2cc(N(=O)=O)ccc2)cc1	-2.2	-2.3	0.1	40	91% Ethanol	29
96	Ethyl 4'-nitro-p-biphenyl carboxylate	CCOC(=O)c1ccc(c2ccc(N(=O)=O)cc2)cc1	-2.2	-2.2	0	40	91% Ethanol	29
97	Ethyl picolinate	n1ccccc1C(=O)OCC	-1.5	-1.1	-0.3	17	75% Ethanol	30
98	Ethyl nicotinate	c1ncccc1C(=O)OCC	-1.7	-1.5	-0.2	17	75% Ethanol	30
99	Ethyl isonicotinate	c1cncccC(=O)OCC	-0.9	-1.4	0.4	17	75% Ethanol	30
100	Ethyl picolinate	n1ccccc1C(=O)OCC	-1.2	-1	-0.2	25	75% Ethanol	30
101	Ethyl nicotinate	c1ncccc1C(=O)OCC	-1.4	-1.3	-0.1	25	75% Ethanol	30
102	Ethyl isonicotinate	c1cncccC(=O)OCC	-0.7	-1.2	0.5	25	75% Ethanol	30
103	Ethyl picolinate	n1ccccc1C(=O)OCC	-0.9	-0.8	0	35	75% Ethanol	30
104	Ethyl nicotinate	c1ncccc1C(=O)OCC	-1.1	-1.1	0	35	75% Ethanol	30
105	Ethyl isonicotinate	c1cncccC(=O)OCC	-0.4	-1	0.6	35	75% Ethanol	30

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
1	Methyl o-fluorobenzoate	Fc1ccccc1C(=O)OC	-2.6	-2.7	0.1	25	80% Methanol	31
2	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-1.6	-2.2	0.5	25	80% Methanol	31
3	Methyl m-chlorobenzoate	c1c(Cl)cccc1C(=O)OC	-2.4	-2.7	0.3	25	80% Methanol	31
4	Methyl benzoate	c1ccccc1C(=O)OC	-2.7	-2.2	-0.5	25	60% Methanol	31
5	Methyl p-bromobenzoate	c1cc(Br)ccc1C(=O)OC	-2.3	-2.2	0	25	60% Methanol	31
6	Methyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OC	-1.1	-1.4	0.2	25	60% Methanol	31
7	Methyl m-bromobenzoate	c1c(Br)cccc1C(=O)OC	-2	-2	0.1	25	60% Methanol	31
8	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-1.3	-1.6	0.3	25	60% Methanol	31
9	Mehtyl 9-anthrylacetate	c1ccc2cc3ccccc3c(CC(=O)OC)c2c1	-3.3	-2.9	-0.3	25	85% Methanol	27
10	Methyl 6-chryslacetate	c1c2ccccc2c3ccc4ccccc4c3c1CC(=O)OC	-2.9	-2.4	-0.5	25	85% Methanol	27
11	Mehtyl 9-phenanthrylacetate	c1cc2cc(CC(=O)OC)c3ccccc3c2cc1	-2.9	-2.4	-0.6	25	85% Methanol	27
12	Methyl 1-naphthylacetate	c1cc2cccc(CC(=O)OC)c2cc1	-2.9	-2.4	-0.6	25	85% Methanol	27
13	Methyl 1-pyrenylacetate	c(c(c(cc1(CC(=O)OC))ccc2)c2cc3)(c1ccc4)c34	-2.7	-2.3	-0.4	25	85% Methanol	27
14	Methyl p-methylphenylacetate	c1cc(C)ccc1CC(=O)OC	-2.6	-2.3	-0.3	25	85% Methanol	27
15	Methul 2-fluorenylacetate	c1c2Cc3cc(OC(=O)Cc4ccccc4)ccc3c2ccc1	-2.6	-1.7	-0.9	25	85% Methanol	27
16	Methyl phenylacetate	c1ccccc1CC(=O)OC	-2.5	-2.1	-0.4	25	85% Methanol	27
17	Methyl 2-naphthylacetate	COC(=O)Cc1ccc2ccccc2c1	-2.4	-2.1	-0.4	25	85% Methanol	27
18	Methyl 4-biphenylacetate	COC(=O)Cc1ccc(c2ccccc2)cc1	-2.4	-2.1	-0.3	25	85% Methanol	27
19	Methyl 2-anthrylacetate	COC(=O)Cc1ccc2cc3ccccc3cc2c1	-2.4	-2	-0.4	25	85% Methanol	27
20	Methyl 3-phenanthrylacetate	c1cc2ccc3ccccc3c2c(CC(=O)OC)c1	-2.4	-2.4	0	25	85% Methanol	27
21	Methyl 2-phenanthrylacetate	c1(CC(=O)OC)cc2ccc3ccccc3c2cc1	-2.4	-2.1	-0.3	25	85% Methanol	27
22	Methyl benzoate	COC(=O)c1ccccc1	-2.3	-2.1	-0.3	25	50% Methanol	33
23	Mehtyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OC	-1.9	-2.3	0.3	25	88% Methanol	34,35
24	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-2.1	-2.5	0.3	25	88% Methanol	34,35
25	Methyl m-bromobenzoate	c1c(Br)cccc1C(=O)OC	-2.9	-2.9	0.1	25	88% Methanol	34,35
26	Methyl p-bromobenzoate	c1cc(Br)ccc1C(=O)OC	-3.2	-3.1	0	25	88% Methanol	34,35
27	Methyl m-methoxybenzoate	c1c(OC)cccc1C(=O)OC	-3.6	-3.5	-0.1	25	88% Methanol	34,35
28	Methyl benzoate	c1ccccc1C(=O)OC	-3.7	-3.2	-0.5	25	88% Methanol	34,35
29	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-3.9	-3.5	-0.4	25	88% Methanol	34,35
30	Methyl m-dimethylaminobenzoate	c1c(N(C)C)cccc1C(=O)OC	-4	-3.7	-0.3	25	88% Methanol	34,35
31	Methyl p-methylbenzoate	c1cc(C)ccc1C(=O)OC	-4	-3.8	-0.2	25	88% Methanol	34,35
32	Methyl p-methoxybenzoate	c1cc(OC)ccc1C(=O)OC	-4.3	-4.3	-0.1	25	88% Methanol	34,35
33	Methyl benzoate	c1ccccc1C(=O)OC	-2.8	-2.7	-0.1	34.8	80% Methanol	31
34	Methyl benzoate	c1ccccc1C(=O)OC	-2.4	-2.5	0.1	44.8	80% Methanol	31
35	Methyl benzoate	c1ccccc1C(=O)OC	-2.3	-2.4	0.2	49.8	80% Methanol	31
36	Methyl benzoate	c1ccccc1C(=O)OC	-2	-2.3	0.3	55.2	80% Methanol	31
37	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-3.7	-3.5	-0.2	35	80% Methanol	31

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
38	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-3.3	-3.3	0.1	45	80% Methanol	31
39	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-2.9	-3.1	0.2	55	80% Methanol	31
40	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-2.3	-2.8	0.6	70.2	80% Methanol	31
41	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-3.6	-3.5	0	45	80% Methanol	31
42	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-3.2	-3.3	0.2	55	80% Methanol	31
43	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-2.5	-3	0.5	70.2	80% Methanol	31
44	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-2.1	-2.9	0.7	80.4	80% Methanol	31
45	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2.6	-3.1	0.5	71.6	80% Methanol	31
46	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2.4	-3	0.6	78.4	80% Methanol	31
47	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2	-2.8	0.8	89.9	80% Methanol	31
48	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-1.7	-2.6	0.9	100.2	80% Methanol	31
49	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-3.5	-2.4	-1.1	119.8	80% Methanol	31
50	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-3.2	-2.2	-0.9	129.8	80% Methanol	31
51	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-3	-2.2	-0.8	134	80% Methanol	31
52	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-1.8	-2.1	0.3	140	80% Methanol	31
53	Methyl o-fluorobenzoate	Fc1ccccc1C(=O)OC	-3	-2.9	-0.1	15.4	80% Methanol	31
54	Methyl o-fluorobenzoate	Fc1ccccc1C(=O)OC	-2.2	-2.5	0.3	35	80% Methanol	31
55	Methyl o-fluorobenzoate	Fc1ccccc1C(=O)OC	-1.8	-2.3	0.5	44.8	80% Methanol	31
56	Methyl o-chlorobenzoate	Clc1ccccc1C(=O)OC	-2.5	-2.4	-0.2	35	80% Methanol	31
57	Methyl o-chlorobenzoate	Clc1ccccc1C(=O)OC	-2.2	-2.2	0	44.8	80% Methanol	31
58	Methyl o-chlorobenzoate	Clc1ccccc1C(=O)OC	-2	-2.1	0.1	50	80% Methanol	31
59	Methyl o-chlorobenzoate	Clc1ccccc1C(=O)OC	-1.8	-2	0.2	55	80% Methanol	31
60	Methyl o-bromobenzoate	c1(Br)ccccc1C(=O)OC	-2.7	-2.5	-0.2	35	80% Methanol	31
61	Methyl o-bromobenzoate	c1(Br)ccccc1C(=O)OC	-2.3	-2.3	0	45	80% Methanol	31
62	Methyl o-bromobenzoate	c1(Br)ccccc1C(=O)OC	-2.1	-2.2	0.1	50	80% Methanol	31
63	Methyl o-bromobenzoate	c1(Br)ccccc1C(=O)OC	-2	-2.1	0.2	55	80% Methanol	31
64	Methyl o-iodobenzoate	c1(I)ccccc1C(=O)OC	-2.9	-2.5	-0.4	34.8	80% Methanol	31
65	Methyl o-iodobenzoate	c1(I)ccccc1C(=O)OC	-2.5	-2.3	-0.2	44.8	80% Methanol	31
66	Methyl o-iodobenzoate	c1(I)ccccc1C(=O)OC	-2.3	-2.2	-0.1	49	80% Methanol	31
67	Methyl o-iodobenzoate	c1(I)ccccc1C(=O)OC	-2.1	-2.1	0	54.9	80% Methanol	31
68	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-2.6	-2.6	0	4.6	80% Methanol	31
69	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-2.1	-2.4	0.3	15	80% Methanol	31
70	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-1.3	-2	0.7	34.5	80% Methanol	31
71	Methyl m-chlorobenzoate	c1c(Cl)cccc1C(=O)OC	-2.9	-2.9	0	15	80% Methanol	31
72	Methyl m-chlorobenzoate	c1c(Cl)cccc1C(=O)OC	-2	-2.5	0.4	34.5	80% Methanol	31
73	Methyl m-chlorobenzoate	c1c(Cl)cccc1C(=O)OC	-1.6	-2.3	0.6	45.2	80% Methanol	31
74	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-3.1	-3.1	-0.1	30.1	80% Methanol	31

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
75	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-2.7	-2.8	0.1	40.7	80% Methanol	31
76	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-2.3	-2.6	0.3	50	80% Methanol	31
77	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-2	-2.4	0.5	59.8	80% Methanol	31
78	Methyl 9-anthrylacetate	c1ccc2cc3ccccc3c(CC(=O)OC)c2c1	-2.9	-2.8	-0.1	32.5	85% Methanol	27
79	Methyl 9-phenanthrylacetate	c1cc2cc(CC(=O)OC)c3ccccc3c2cc1	-2.6	-2.2	-0.4	32.5	85% Methanol	27
80	Methyl 1-naphthylacetate	c1cc2cccc(CC(=O)OC)c2cc1	-2.6	-2.2	-0.4	32.5	85% Methanol	27
81	Methyl 6-chrysylacetate	c(c(c(cc1(CC(=O)OC))ccc2)c2cc3)(c1ccc4)c34	-2.4	-2.2	-0.2	32.5	85% Methanol	27
82	Methyl p-methylphenylacetate	c1cc(C)ccc1CC(=O)OC	-2.3	-2.2	-0.2	32.5	85% Methanol	27
83	2-Fluorenyl phenylacetate	c1c2Cc3cc(OC(=O)Cc4ccccc4)ccc3c2ccc1	-2.2	-1.6	-0.6	32.5	85% Methanol	27
84	Methyl phenylacetate	c1ccccc1CC(=O)OC	-2.2	-2	-0.2	32.5	85% Methanol	27
85	Methyl 2-naphthylacetate	COC(=O)Cc1ccc2ccccc2c1	-2.1	-1.9	-0.2	32.5	85% Methanol	27
86	Methyl p-biphenylacetate	COC(=O)Cc1ccc(c2ccccc2)cc1	-2.1	-1.9	-0.2	32.5	85% Methanol	27
87	Methyl 3-phenanthrylacetate	c1cc2ccc3ccccc3c2cc1(CC(=O)OC)	-2	-1.9	-0.2	32.5	85% Methanol	27
88	Methyl 2-phenanthrylacetate	c1(CC(=O)OC)cc2ccc3ccccc3c2cc1	-2.1	-1.9	-0.1	32.5	85% Methanol	27
89	Methyl phenylacetate	c1ccccc1CC(=O)OC	-2	-1.9	-0.1	40	85% Methanol	27
90	Methyl 2-naphthylacetate	COC(=O)Cc1ccc2ccccc2c1	-1.9	-1.8	-0.1	40	85% Methanol	27
91	Methyl p-biphenylacetate	COC(=O)Cc1ccc(c2ccccc2)cc1	-1.9	-1.8	-0.1	40	85% Methanol	27
92	Methyl 2-phenanthrylacetate	c1(CC(=O)OC)cc2ccc3ccccc3c2cc1	-1.8	-1.8	0	40	85% Methanol	27
93	Methyl 9-anthrylacetate	c1ccc2cc3ccccc3c(CC(=O)OC)c2c1	-2.3	-2.4	0.2	50	85% Methanol	27
94	Methyl 9-phenanthrylacetate	c1cc2cc(CC(=O)OC)c3ccccc3c2cc1	-2	-1.9	-0.1	50	85% Methanol	27
95	Methyl 1-naphthylacetate	c1cc2cccc(CC(=O)OC)c2cc1	-2	-1.9	-0.1	50	85% Methanol	27
96	Methyl 6-chrysylacetate	c(c(c(cc1(CC(=O)OC))ccc2)c2cc3)(c1ccc4)c34	-1.8	-1.9	0.1	50	85% Methanol	27
97	Methyl p-methylphenylacetate	c1cc(C)ccc1CC(=O)OC	-1.7	-1.8	0.1	50	85% Methanol	27
98	2-Fluorenyl phenylacetate	c1c2Cc3cc(OC(=O)Cc4ccccc4)ccc3c2ccc1	-1.6	-1.3	-0.3	50	85% Methanol	27
99	Methyl phenylacetate	c1ccccc1CC(=O)OC	-1.6	-1.7	0.1	50	85% Methanol	27
100	Methyl 2-naphthylacetate	COC(=O)Cc1ccc2ccccc2c1	-1.5	-1.6	0.1	50	85% Methanol	27
101	Methyl p-biphenylacetate	COC(=O)Cc1ccc(c2ccccc2)cc1	-1.5	-1.6	0.1	50	85% Methanol	27
102	Methyl 3-phenanthrylacetate	c1cc2ccc3ccccc3c2cc1(CC(=O)OC)	-1.5	-1.6	0.1	50	85% Methanol	27
103	Methyl 2-phenanthrylacetate	c1(CC(=O)OC)cc2ccc3ccccc3c2cc1	-1.5	-1.6	0.2	50	85% Methanol	27
104	Methyl 9-anthrylacetate	c1ccc2cc3ccccc3c(CC(=O)OC)c2c1	-1.9	-2.2	0.3	60.2	85% Methanol	27
105	Methyl 9-phenanthrylacetate	c1cc2cc(CC(=O)OC)c3ccccc3c2cc1	-1.6	-1.7	0.1	60.2	85% Methanol	27
106	Methyl 2-naphthylacetate	c1cc2cccc(CC(=O)OC)c2cc1	-1.6	-1.7	0.1	60.2	85% Methanol	27
107	Methyl 6-chrysylacetate	c(c(c(cc1(CC(=O)OC))ccc2)c2cc3)(c1ccc4)c34	-1.4	-1.7	0.3	60.2	85% Methanol	27
108	Methyl p-methylphenylacetate	c1cc(C)ccc1CC(=O)OC	-1.4	-1.6	0.3	60.2	85% Methanol	27
109	2-Fluorenyl phenylacetate	c1c2Cc3cc(OC(=O)Cc4ccccc4)ccc3c2ccc1	-1.3	-1.2	-0.1	60.2	85% Methanol	27
110	Methyl 3-phenanthrylacetate	c1cc2ccc3ccccc3c2cc1(CC(=O)OC)	-1.1	-1.4	0.3	60.2	85% Methanol	27
111	2-Carbomethoxyquinoline	c1cc2nc(C(=O)OC)ccc2cc1'	-0.5	-0.6	0.1	25	50% Methanol	33

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Difference	Temperature	Solvents	References
112	Methyl 2-nitropicolinate	n1c(N(=O)=O)cccc1C(=O)OC',	-0.6	-1	0.4	25	88% Methanol	32
113	Methyl 2-bromopicolinate	'n1c(Br)cccc1C(=O)OC',	-1.5	-1.5	0	25	88% Methanol	32
114	Methyl 2-methylpicolinates	'n1c(C)cccc1C(=O)OC',	-2.3	-2	-0.3	25	88% Methanol	32
115	Methyl 2-dimethylnitropicolinate	'n1c(N(C)C)cccc1C(=O)OC',	-2.9	-2.3	-0.6	25	88% Methanol	32
116	Methyl nicotinate	'c1ncccc1C(=O)OC',	-1.4	-1.2	-0.2	25	88% Methanol	19
117	Methyl picolinate	'c1cccnc1C(=O)OC',	-1.2	-0.9	-0.3	25	88% Methanol	19
118	Methyl isonicotinate	'c1cnccc1C(=O)OC',	-0.7	-1.1	0.4	25	88% Methanol	19
119	Methyl 5-nitropicolinate	'n1cc(N(=O)=O)ccc1C(=O)OC',	-0.4	-0.8	0.4	25	88% Methanol	32
120	Methyl 5-bromopicolinate	'n1cc(Br)ccc1C(=O)OC',	-1.5	-1.7	0.1	25	88% Methanol	32
121	Methyl picolinate	'n1ccccc1C(=O)OC',	-2	-1.8	-0.3	25	88% Methanol	32
122	Methyl 5-methylpicolinate	'n1cc(C)ccc1C(=O)OC',	-2.4	-2.3	-0.1	25	88% Methanol	32
123	Methyl 5-methoxylpicolinate	'n1cc(OC)ccc1C(=O)OC',	-2.8	-2.8	0	25	88% Methanol	32
124	Methyl 5-dimethylnitropicolinate	'n1cc(N(C)C)ccc1C(=O)OC',	-3.7	-3.3	-0.4	25	88% Methanol	32
125	Methyl 4-nitropicolinate	'n1ccc(N(=O)=O)cc1C(=O)OC',	-0.7	-1	0.3	25	88% Methanol	32
126	Methyl 4-bromopicolinate	n1ccc(Br)cc1C(=O)OC',	-1.3	-1.5	0.2	25	88% Methanol	32
127	Methyl 4-methylpicolinate	n1ccc(C)cc1C(=O)OC',	-2.2	-2	-0.2	25	88% Methanol	32
128	Methyl 4-methoxylpicolinate	n1ccc(OC)cc1C(=O)OC',	-2	-2.1	0.1	25	88% Methanol	32
129	Methyl 5-bromonicotinate	c1ncc(Br)cc1C(=O)OC',	-1.5	-1.8	0.4	25	88% Methanol	32
130	Methyl nicotinate	c1ncccc1C(=O)OC',	-2.3	-2.1	-0.2	25	88% Methanol	32
131	Methyl 5-methylnicotinate	c1ncc(C)cc1C(=O)OC',	-2.3	-2.3	0	25	88% Methanol	32
132	Methyl 5-methoxynicotinate	c1ncc(OC)cc1C(=O)OC',	-2.1	-2.4	0.2	25	88% Methanol	32
133	Methyl 5-dimethylnitronicotinate	c1ncc(N(C)C)cc1C(=O)OC',	-2.7	-2.6	-0.1	25	88% Methanol	32
134	Methyl 2-bromonicotinate	n1c(Br)ccc(C(=O)OC)c1',	-1.8	-2	0.2	25	88% Methanol	32
135	Methyl 2-methylnicotinate	'n1c(C)ccc(C(=O)OC)c1',	-2.6	-2.7	0.1	25	88% Methanol	32
136	Methyl 2-methoxynicotinate	n1c(OC)ccc(C(=O)OC)c1',	-3.2	-3.2	0	25	88% Methanol	32
137	Methyl 2-dimethylnitronicotinate	n1c(N(C)C)ccc(C(=O)OC)c1',	-4.3	-3.8	-0.6	25	88% Methanol	32
138	Methyl 2-nitroisonicotinate	n1c(N(=O)=O)cc(C(=O)OC)cc1',	0.2	-1.2	1	25	88% Methanol	32
139	Methyl 2-bromoisonicotinate	'n1c(Br)cc(C(=O)OC)cc1',	-0.9	-1.7	0.8	25	88% Methanol	32
140	Methyl isonicotinate	'n1ccc(C(=O)OC)cc1',	-1.5	-2	0.4	25	88% Methanol	32
141	Methyl 2-methylisonicotinate	'n1c(C)cc(C(=O)OC)cc1',	-1.7	-2.2	0.5	25	88% Methanol	32
142	Methyl 2-methoxyisonicotinate	n1c(OC)cc(C(=O)OC)cc1',	-1.8	-2.2	0.5	25	88% Methanol	32
143	Methyl 2-dimethylnitroisonicotinate	'n1c(N(C)C)cc(C(=O)OC)cc1',	-2.3	-2.5	0.2	25	88% Methanol	32
144	3-Carbomethoxyquinoline	'c1cc2ncc(C(=O)OC)cc2cc1',	-1.1	-0.9	-0.2	25	50% Methanol	33
145	4-Carbomethoxyquinoline	'c1cc2nccc(C(=O)OC)c2cc1',	-0.8	-1.1	0.3	25	50% Methanol	33
146	5-Carbomethoxyquinoline	'c1cc2ncccc2c(C(=O)OC)c1',	-1.7	-1.4	-0.3	25	50% Methanol	33
147	6-Carbomethoxyquinoline	'c1cc2ncccc2cc1(C(=O)OC)',	-1.6	-1.2	-0.4	25	50% Methanol	33
148	7-Carbomethoxyquinoline	'COC(=O)c1cc2ncccc2cc1',	-1.5	-1.2	-0.4	25	50% Methanol	33
149	8-Carbomethoxyquinoline	'c1c(C(=O)OC)c2ncccc2cc1',	-2.4	-1.4	-1	25	50% Methanol	33

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Diff.	Temperature	Solvents	References
1	Ethyl benzoate	c1ccccc1C(=O)OCC	-2.1	-1.6	-0.5	30	33% dioxane	19
2	p-Nitrobenzyl benzoate	c1ccccc1C(=O)OCc1ccc(N(=O)=O)cc1	-1.5	-1.2	-0.3	25	67% dioxane	38
3	p-Chlorobenzyl benzoate	c1ccccc1C(=O)OCc1ccc(Cl)cc1	-2	-1.4	-0.6	25	67% dioxane	38
4	p-Chlorobenzyl benzoate	c1ccccc1C(=O)OCc1ccc(Cl)cc1	-1.7	-1	-0.8	25	67% dioxane	38
5	Benzyl benzoate	c1ccccc1C(=O)OCc1ccccc1	-2.3	-1.5	-0.8	25	67% dioxane	38
6	p-Methoxybenzyl benzoate	c1ccccc1C(=O)OCc1ccc(OC)cc1	-2.4	-1.5	-0.9	25	67% dioxane	38
7	Methyl benzoate	c1ccccc1C(=O)OC	-1.6	-1.5	-0.2	25	33% dioxane	39
8	Methyl p-aminobenzoate	c1cc(N)ccc1C(=O)OC	-2.9	-3	0.1	25	33% dioxane	39
9	Methyl p-methylbenzoate	c1cc(C)ccc1C(=O)OC	-2	-2	0.1	25	33% dioxane	39
10	Methyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)OC	-1.2	-1.4	0.2	25	33% dioxane	39
11	Methyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OC	-0.2	-0.5	0.3	25	33% dioxane	39
12	Methyl acetate	CC(=O)OC	-0.5	-0.3	-0.2	35	40% dioxane	36
13	Methyl propionate	CCC(=O)OC	-0.6	-0.9	0.2	35	40% dioxane	36
14	Methyl isobutyrate	C(C)CC(=O)OC	-1.1	-1.1	0	35	40% dioxane	36
15	Methyl n-butyrate	CCCC(=O)OC	-0.9	-1.1	0.2	35	40% dioxane	36
16	Mehtyl n-pentate	CCCCC(=O)OC	-1	-1.2	0.2	35	40% dioxane	36
17	Methyl isopentate	C(C)CCC(=O)OC	-1.5	-1.2	-0.3	35	40% dioxane	36
18	Methyl sec-pentate	CCC(C)C(=O)OC	-1.6	-2.1	0.5	35	40% dioxane	36
19	Methyl neopentate	C(C)(C)CC(=O)OC	-2	-1.4	-0.6	35	40% dioxane	36
20	Methyl phenylacetate	c1ccc(CC(=O)OC)cc1	-0.4	-0.4	0.1	35	40% dioxane	36
21	Methyl benzoate	c1ccc(C(=O)OC)cc1	-1.5	-1.7	0.1	35	60% dioxane	37
22	Methyl p-methylbenzoate	Cc1ccc(C(=O)OC)cc1	-1.9	-2.2	0.3	35	60% dioxane	37
23	Methyl m-methylbenzoate	c1c(C)cc(C(=O)OC)cc1	-1.8	-1.9	0.1	35	60% dioxane	37
24	Methyl p-methoxybenzoate	COc1ccc(C(=O)OC)cc1	-2.2	-2.7	0.5	35	60% dioxane	37
25	Methyl p-aminobenzoate	Nc1ccc(C(=O)OC)cc1	-3	-3.2	0.2	35	60% dioxane	37
26	Methyl p-bromobenzoate	Brc1ccc(C(=O)OC)cc1	-1	-1.6	0.6	35	60% dioxane	37
27	Methyl m-iodobenzoate	c1c(I)cc(C(=O)OC)cc1	-0.9	-1.3	0.4	35	60% dioxane	37
28	Methyl m-chlorobenzoate	c1c(Cl)cc(C(=O)OC)cc1	-0.8	-1.4	0.6	35	60% dioxane	37
29	Methyl m-bromobenzoate	c1c(Br)cc(C(=O)OC)cc1	-0.8	-1.4	0.5	35	60% dioxane	37
30	Methyl m-nitrobenzoate	c1c(N(=O)=O)cc(C(=O)OC)cc1	0	-0.9	0.9	35	60% dioxane	37
31	Methyl p-nitrobenzoate	O=N(=O)c1ccc(C(=O)OC)cc1	0.2	-0.7	1	35	60% dioxane	37
32	Ethyl benzoate	c1ccc(C(=O)OCC)cc1	-2	-1.9	-0.1	35	60% dioxane	37
33	Propyl benzoate	c1ccc(C(=O)OCCC)cc1	-2.2	-2	-0.2	35	60% dioxane	37
34	Propyl p-chlorobenzoate	Clc1ccc(C(=O)OCCC)cc1	-1.6	-2	0.3	35	60% dioxane	37
35	Isopropyl benzoate	c1ccc(C(=O)OC(C)C)cc1	-2.8	-2.4	-0.4	35	60% dioxane	37
36	Isopropyl p-methoxybenzoate	COc1ccc(C(=O)OC(C)C)cc1	-3.4	-3.4	0	35	60% dioxane	37
37	Isopropyl p-nitrobenzoate	O=N(=O)c1ccc(C(=O)OC(C)C)cc1	-0.9	-1.5	0.6	35	60% dioxane	37

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Diff.	Temperature	Solvents	References
38	Butyl benzoate	c1ccc(C(=O)OCCCC)cc1	-2.3	-2.1	-0.3	35	60% dioxane	37
39	Butyl p-aminobenzoate	Nc1ccc(C(=O)OCCCC)cc1	-3.8	-3.6	-0.2	35	60% dioxane	37
40	Isobutyl benzoate	c1ccc(C(=O)OCC(C)C)cc1	-2.4	-2.1	-0.3	35	60% dioxane	37
41	Isobutyl p-aminobenzoate	Nc1ccc(C(=O)OCC(C)C)cc1	-3.8	-3.6	-0.2	35	60% dioxane	37
42	sec-Butyl benzoate	c1ccc(C(=O)OC(C)CC)cc1	-3.1	-3.2	0.1	35	60% dioxane	37
43	sec-Butyl m-methylbenzoate	c1c(C)cc(C(=O)OC(C)CC)cc1	-3.3	-3.4	0.1	35	60% dioxane	37
44	Isopentyl benzoate	c1ccc(C(=O)OCCC(C)C)cc1	-2.4	-1.8	-0.6	35	60% dioxane	37
45	Isopentyl p-chlorobenzoate	Clc1ccc(C(=O)OCCC(C)C)cc1	-1.8	-1.7	-0.1	35	60% dioxane	37
46	Benzyl benzoate	c1ccc(C(=O)OCc2ccccc2)cc1	-1.8	-1.1	-0.7	35	60% dioxane	37
47	Benzyl p-methylbenzoate	Cc1ccc(C(=O)OCc2ccccc2)cc1	-2.2	-1.7	-0.5	35	60% dioxane	37
48	1-Phenyl-ethyl benzoate	c1ccc(C(=O)OC(C)c2ccccc2)cc1	-2.1	-2.8	0.7	35	60% dioxane	37
49	1,1-Biphenyl-methyl benzoate	c1ccc(C(=O)OC(c2ccccc2)c3ccccc3)cc1	-3.6	-4.7	1.1	35	60% dioxane	37
50	Ethyl p-methoxybenzoate	COc1ccc(C(=O)OCC)cc1	-2.7	-2.9	0.3	35	60% dioxane	37
51	Ethyl p-fluorobenzoate	Fc1ccc(C(=O)OCC)cc1	-1.8	-1.9	0.2	35	60% dioxane	37
52	Ethyl m-nitrobenzoate	c1c(N(=O)=O)cccc1(C(=O)OCC)	-0.5	-1.2	0.7	35	60% dioxane	37
53	Ethyl p-nitrobenzoate	O=N(=O)c1ccc(C(=O)OCC)cc1	-0.3	-1	0.7	35	60% dioxane	37
54	Ethyl 3,4-dinitrobenzoate	c1c(N(=O)=O)cc(C(=O)OCC)cc1N(=O)=O	-1.2	-0.4	-0.8	35	60% dioxane	37
55	Ethyl p-aminobenzoate	Nc1ccc(C(=O)OCC)cc1	-3.5	-3.5	0	35	60% dioxane	37
56	Methyl benzoate	c1ccccc1C(=O)OC	-2.4	-2.4	0	10	60% dioxane	32
57	Methyl m-bromobenzoate	c1c(Br)cccc1C(=O)OC	-1.7	-2.1	0.4	10	60% dioxane	32
58	Methyl p-bromobenzoate	c1cc(Br)ccc1C(=O)OC	-1.8	-2.3	0.5	10	60% dioxane	32
59	Methyl p-methoxybenzoate	c1cc(OC)ccc1C(=O)OC	-3.1	-3.5	0.4	10	60% dioxane	32
60	Methyl m-methoxybenzoate	c1c(OC)cccc1C(=O)OC	-2.3	-2.7	0.4	10	60% dioxane	32
61	Methyl p-methylbenzoate	c1cc(C)ccc1C(=O)OC	-2.8	-3	0.2	10	60% dioxane	32
62	Methyl m-methylbenzoate	c1c(C)cccc1C(=O)OC	-2.6	-2.7	0	10	60% dioxane	32
63	Methyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OC	-0.5	-1.4	0.9	10	60% dioxane	32
64	Methyl m-nitrobenzoate	c1c(N(=O)=O)cccc1C(=O)OC	-0.8	-1.6	0.8	10	60% dioxane	32
65	Methyl p-trifluoromethylbenzoate	c1cc(C(F)(F)F)ccc1C(=O)OC	-1.2	-2.7	1.5	10	60% dioxane	32
66	Methyl benzoate	c1ccccc1C(=O)OC	-2.5	-2.2	-0.3	10	60% dioxane	31
67	Methyl benzoate	c1ccccc1C(=O)OC	-1.9	-1.9	-0.1	25	60% dioxane	31
68	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-2.8	-2.8	-0.1	25	60% dioxane	31
69	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-2.3	-2.5	0.1	40.2	60% dioxane	31
70	Methyl o-methylbenzoate	Cc1ccccc1C(=O)OC	-2	-2.3	0.3	50.4	60% dioxane	31
71	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-3.1	-2.9	-0.2	30	60% dioxane	31
72	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-2.7	-2.7	0	40	60% dioxane	31
73	Methyl o-ethylbenzoate	CCc1ccccc1C(=O)OC	-2.4	-2.5	0.1	50	60% dioxane	31
74	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2.9	-2.8	-0.1	40.9	60% dioxane	31

	TABLE 5: B740 ALKALINE HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Diff.	Temperature	Solvents	References
75	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2.5	-2.6	0.1	49.9	60% dioxane	31
76	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2.3	-2.4	0.1	60	60% dioxane	31
77	Methyl o-isopropylbenzoate	C(C)Cc1ccccc1C(=O)OC	-2	-2.3	0.3	70	60% dioxane	31
78	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-3.1	-1.7	-1.4	114.6	60% dioxane	31
79	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-2.7	-1.6	-1.1	124.1	60% dioxane	31
80	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-2.5	-1.5	-1	133.7	60% dioxane	31
81	Methyl o-(t-butyl)benzoate	C(C)(C)Cc1ccccc1C(=O)OC	-2.2	-1.4	-0.8	144.3	60% dioxane	31
82	Ethyl benzoate	c1ccccc1C(=O)OCC	-2	-1.7	-0.3	30	60% dioxane	19
83	Ethyl benzoate	c1ccccc1C(=O)OCC	-2.3	-2.2	-0.1	30	70% dioxane	19
84	Ethyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OCC	-1.2	-1.1	-0.2	30	60% dioxane	19
85	Ethyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)OCC	-1.3	-1.2	-0.1	30	70% dioxane	19
86	Benzyl benzoate	c1ccccc1C(=O)OCc2ccccc2	-1.9	-1	-0.9	30	50% dioxane	19
87	Benzyl benzoate	c1ccccc1C(=O)OCc2ccccc2	-2.1	-1.5	-0.6	30	70% dioxane	19
88	Methyl nicotinate	c1ncccc1C(=O)OC	-0.9	-1	0.1	10	65% dioxane	19
89	Methyl picolinate	n1ccccc1C(=O)OC	-0.7	-0.7	0	10	65% dioxane	19
90	Methyl isonicotinate	c1cnccc1C(=O)OC	-0.1	-0.9	0.8	10	65% dioxane	19

	TABLE 5: ALKALINE HYDROLYSIS OF ESTERS IN ACETONITRILE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE.							
			Observed	Calculated				
	Esters	SMILES	logk	logk	Diff.	Temperature	Solvents	References
1	p-Tolyl p-dimethylaminobenzoate	c1cc(N(C)C)ccc1C(=O)Oc2ccc(C)cc2	-3.1	-2.6	-0.5	25	33% Acetonitrile	40
2	p-Tolyl p-methylbenzoate	c1cc(C)ccc1C(=O)Oc2ccc(C)cc2	-1.9	-1.6	-0.2	25	33% Acetonitrile	40
3	p-Tolyl benzoate	c1ccccc1C(=O)Oc2ccc(C)cc2	-1.5	-1	-0.4	25	33% Acetonitrile	40
4	p-Tolyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)Oc2ccc(C)cc2	-1	-1	0	25	33% Acetonitrile	40
5	p-Tolyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)Oc2ccc(C)cc2	0.2	-0.1	0.2	25	33% Acetonitrile	40
6	Phenyl p-dimethylaminobenzoate	c1cc(N(C)C)ccc1C(=O)Oc2ccccc2	-2.9	-2.5	-0.5	25	33% Acetonitrile	40
7	Phenyl p-methylbenzoate	c1cc(C)ccc1C(=O)Oc2ccccc2	-1.6	-1.5	-0.2	25	33% Acetonitrile	40
8	Phenyl benzoate	c1ccccc1C(=O)Oc2ccccc2	-1.3	-0.9	-0.3	25	33% Acetonitrile	40
9	Phenyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)Oc2ccccc2	-0.8	-0.8	0.1	25	33% Acetonitrile	40
10	Phenyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)Oc2ccccc2	0.3	0.1	0.2	25	33% Acetonitrile	40
11	p-Chlorophenyl p-methylbenzoate	c1cc(C)ccc1C(=O)Oc2ccc(Cl)cc2	-1.3	-1.3	0	25	33% Acetonitrile	40
12	p-Chlorophenyl benzoate	c1ccccc1C(=O)Oc2ccc(Cl)cc2	-0.9	-0.8	-0.2	25	33% Acetonitrile	40
13	p-Chlorophenyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)Oc2ccc(Cl)cc2	-0.5	-0.7	0.2	25	33% Acetonitrile	40
14	p-Chlorophenyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)Oc2ccc(Cl)cc2	0.7	0.2	0.4	25	33% Acetonitrile	40
15	m-Nitrophenyl p-dimethylaminobenzoate	c1cc(N(C)C)ccc1C(=O)Oc2cc(N(=O)=O)ccc2	-2.1	-1.9	-0.2	25	33% Acetonitrile	40
16	m-Nitrophenyl p-methylbenzoate	c1cc(C)ccc1C(=O)Oc2cc(N(=O)=O)ccc2	-0.7	-0.9	0.1	25	33% Acetonitrile	40
17	m-Nitrophenyl benzoate	c1ccccc1C(=O)Oc2cc(N(=O)=O)ccc2	-0.3	-0.3	0	25	33% Acetonitrile	40
18	m-Nitrophenyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)Oc2cc(N(=O)=O)ccc2	0.1	-0.2	0.3	25	33% Acetonitrile	40
19	m-Nitrophenyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)Oc2cc(N(=O)=O)ccc2	1.2	0.7	0.5	25	33% Acetonitrile	40
20	p-Nitrophenyl p-dimethylaminobenzoate	c1cc(N(C)C)ccc1C(=O)Oc2ccc(N(=O)=O)cc2	-1.8	-1.8	-0.1	25	33% Acetonitrile	40
21	p-Nitrophenyl p-methylbenzoate	c1cc(C)ccc1C(=O)Oc2ccc(N(=O)=O)cc2	-0.5	-0.8	0.3	25	33% Acetonitrile	40
22	p-Nitrophenyl benzoate	c1ccccc1C(=O)Oc2ccc(N(=O)=O)cc2	-0.1	-0.2	0.1	25	33% Acetonitrile	40
23	p-Nitrophenyl p-chlorobenzoate	c1cc(Cl)ccc1C(=O)Oc2ccc(N(=O)=O)cc2	0.3	-0.1	0.4	25	33% Acetonitrile	40
24	p-Nitrophenyl p-nitrobenzoate	c1cc(N(=O)=O)ccc1C(=O)Oc2ccc(N(=O)=O)cc2	1.4	0.8	0.7	25	33% Acetonitrile	40

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
1	Ethyl acetate	'CC(=O)OCC',	-4	-3.9	-0.1	25	water	3, 12, 13, 41
2	Ethyl propionate	'CCC(=O)OCC',	-4	-4.3	0.2	25	water	3, 12, 13, 41
3	Ethyl cyclo-butyl carboxylate	'C1CCC1C(=O)OCC',	-4	-4.7	0.7	25	water	3, 12, 13, 41
4	Ethyl butyrate	'CCCC(=O)OCC',	-4.3	-4.4	0.1	25	water	3, 12, 13, 41
5	Ethyl pentate	'CCCCC(=O)OCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
6	Ethyl hexanoate	'CCCCCC(=O)OCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
7	Ethyl iso-hexanoate	'CC(C)CCC(=O)OCC',	-4.3	-4.4	0.1	25	water	3, 12, 13, 41
8	Ethyl (heptyl)acetate	'CCCCCCCCC(=O)OCC',	-4.3	-4.5	0.2	25	water	3, 12, 13, 41
9	Ethyl (t-butyl)propionate	'CC(C)(C)CCC(=O)OCC',	-4.3	-4.9	0.6	25	water	3, 12, 13, 41
10	Ethyl sec-butyrate	'CC(C)C(=O)OCC',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
11	Ethyl cyclopentate	'C1CCCC1C(=O)OCC',	-4.5	-5	0.5	25	water	3, 12, 13, 41
12	Ethyl cyclohexanoate	'C1CCCCC1C(=O)OCC',	-4.8	-5.1	0.3	25	water	3, 12, 13, 41
13	Ethyl iso-pentate	'CC(C)CC(=O)OCC',	-4.9	-4.6	-0.3	25	water	3, 12, 13, 41
14	Ethyl cyclohexyl-acetate	'C1CCCCC1CC(=O)OCC',	-4.9	-4.8	-0.1	25	water	3, 12, 13, 41
15	Ethyl sec-pentate	'CCC(C)C(=O)OCC',	-5.1	-5.1	0	25	water	3, 12, 13, 41
16	Ethyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCC',	-5	-5.1	0.1	25	water	3, 12, 13, 41
17	Ethyl neopentate	'CC(C)(C)C(=O)OCC',	-5.5	-5.2	-0.3	25	water	3, 12, 13, 41
18	Ethyl (t-butyl)acetate	'CC(C)(C)CC(=O)OCC',	-5.7	-5.4	-0.3	25	water	3, 12, 13, 41
19	Ethyl (t-butyl)-sec-butyrate	'CC(C)(C)CC(C)C(=O)OCC',	-5.8	-5.7	-0.1	25	water	3, 12, 13, 41
20	Ethyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCC',	-5.9	-5.9	-0.1	25	water	3, 12, 13, 41
21	Ethyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCC',	-6.1	-6.2	0.2	25	water	3, 12, 13, 41
22	Ethyl (2-isobutyl-4-methyl)pentate	'CC(C)CC(CC(C)C)C(=O)OCC',	-6.4	-6.7	0.2	25	water	3, 12, 13, 41
23	Ethyl (t-butyl)neopentate	'CC(C)(C)CC(C)(C)C(=O)OCC',	-6.5	-6.5	-0.1	25	water	3, 12, 13, 41
24	Ethyl (2-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCC',	-7.2	-7.1	0	25	water	3, 12, 13, 41
25	Ethyl (t-butyl)isopropionate	'CC(C)(C)C(C)C(=O)OCC',	-7.3	-6.6	-0.7	25	water	3, 12, 13, 41
26	Ethyl (t-butyl)t-butyrate	'CC(C)(C)C(C)(C)C(=O)OCC',	-7.9	-7.1	-0.8	25	water	3, 12, 13, 41
27	Ethyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCC',	-7.8	-6.8	-1	25	water	3, 12, 13, 41
28	(methyl) (neopentyl) (t-butyl)CC(=O)OCC	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCC',	-8	-8.4	0.4	25	water	3, 12, 13, 41
29	Isopropyl formate	'C(=O)OC(C)C',	-3	-3.5	0.5	25	water	3, 12, 13, 41
30	Isopropyl acetate	'CC(=O)OC(C)C',	-4.2	-4.2	-0.1	25	water	3, 12, 13, 41
31	Isopropyl propionate	'CCC(=O)OC(C)C',	-4.3	-4.5	0.3	25	water	3, 12, 13, 41
32	Isopropyl chloroacetate	'ClCC(=O)OC(C)C',	-4.4	-4.8	0.4	25	water	3, 12, 13, 41
33	Isopropyl butyrate	'CCCC(=O)OC(C)C',	-4.6	-4.7	0.1	25	water	3, 12, 13, 41
34	Isopropyl pentate	'CCCCC(=O)OC(C)C',	-4.6	-4.7	0.1	25	water	3, 12, 13, 41
35	Isopropyl hexanoate	'CCCCCC(=O)OC(C)C',	-4.6	-4.8	0.1	25	water	3, 12, 13, 41
36	Isopropyl iso-hexanoate	'CC(C)CCC(=O)OC(C)C',	-4.6	-4.7	0.1	25	water	3, 12, 13, 41
37	Isopropyl phenylacetate	'c1ccccc1CC(=O)OC(C)C',	-4.6	-4.8	0.2	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
38	Isopropyl phenylpropionate	'c1ccccc1CCC(=O)OC(C)C',	-4.6	-4.8	0.2	25	water	3, 12, 13, 41
39	Isopropyl phenylbutyrate	'c1ccccc1CCCC(=O)OC(C)C',	-4.7	-4.7	0	25	water	3, 12, 13, 41
40	Isopropyl isobutyrate	'CC(C)C(=O)OC(C)C',	-4.7	-4.9	0.2	25	water	3, 12, 13, 41
41	Isopropyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OC(C)C',	-5	-5.3	0.3	25	water	3, 12, 13, 41
42	Isopropyl isopentate	'CC(C)CC(=O)OC(C)C',	-5.1	-4.9	-0.3	25	water	3, 12, 13, 41
43	Isopropyl cyclohexylacetate	'C1CCCCC1CC(=O)OC(C)C',	-5.2	-5	-0.2	25	water	3, 12, 13, 41
44	Isopropyl (2-ethyl)propionate	'CC(CC)C(=O)OC(C)C',	-5.3	-5.4	0	25	water	3, 12, 13, 41
45	Isopropyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OC(C)C',	-5.4	-5.6	0.2	25	water	3, 12, 13, 41
46	Isopropyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OC(C)C',	-5.7	-6.1	0.4	25	water	3, 12, 13, 41
47	Isopropyl neopentate	'CC(C)(C)C(=O)OC(C)C',	-5.8	-5.4	-0.3	25	water	3, 12, 13, 41
48	Isopropyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OC(C)C',	-6	-6.7	0.7	25	water	3, 12, 13, 41
49	Isopropyl (2-ethyl)butyrate	'CCC(CC)C(=O)OC(C)C',	-6.2	-6.1	-0.1	25	water	3, 12, 13, 41
50	Isopropyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OC(C)C',	-6.2	-5.9	-0.3	25	water	3, 12, 13, 41
51	Isopropyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OC(C)C',	-6.3	-5.8	-0.5	25	water	3, 12, 13, 41
52	Isopropyl benzoate	'c1ccccc1C(=O)OC(C)C',	-6.8	-6.2	-0.6	25	water	3, 12, 13, 41
53	Isopropyl cyclobutyl-carboxylate	'C1CCC1C(=O)OC(C)C',	-4.3	-5	0.7	25	water	3, 12, 13, 41
54	Isopropyl methoxyacetate	'COCC(=O)OC(C)C',	-4.4	-4.9	0.5	25	water	3, 12, 13, 41
55	Isopropyl bromoacetate	'BrCC(=O)OC(C)C',	-4.5	-4.9	0.4	25	water	3, 12, 13, 41
56	Isopropyl thiolpropionate	'CSCC(=O)OC(C)C',	-4.6	-4.9	0.3	25	water	3, 12, 13, 41
57	Isopropyl iodoacetate	'ICC(=O)OC(C)C',	-4.6	-4.9	0.3	25	water	3, 12, 13, 41
58	CCCCCCCCC(=O)OC(C)C	'CCCCCCCCC(=O)OC(C)C',	-4.5	-4.8	0.2	25	water	3, 12, 13, 41
59	Isopropyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OC(C)C',	-4.6	-5.1	0.6	25	water	3, 12, 13, 41
60	Isopropyl phenoxy-acetate	'c1ccccc1OCC(=O)OC(C)C',	-4.5	-4.9	0.4	25	water	3, 12, 13, 41
61	Isopropyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OC(C)C',	-4.7	-5.2	0.5	25	water	3, 12, 13, 41
62	Isopropyl difluoroacetate	'FC(F)C(=O)OC(C)C',	-4.9	-5.1	0.2	25	water	3, 12, 13, 41
63	Isopropyl methoxypropionate	'COCCC(=O)OC(C)C',	-5	-4.8	-0.2	25	water	3, 12, 13, 41
64	Isopropyl chloropropionate	'ClCCC(=O)OC(C)C',	-5.1	-4.7	-0.4	25	water	3, 12, 13, 41
65	Isopropyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)C',	-5.4	-5.6	0.2	25	water	3, 12, 13, 41
66	Isopropyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OC(C)C',	-5.3	-5.3	0	25	water	3, 12, 13, 41
67	Isopropyl dichloracetate	'ClC(Cl)C(=O)OC(C)C',	-5.8	-5.2	-0.5	25	water	3, 12, 13, 41
68	Isopropyl neopentate	'CC(C)(C)C(=O)OC(C)C',	-5.9	-5.4	-0.5	25	water	3, 12, 13, 41
69	Isopropyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OC(C)C',	-6.1	-5.9	-0.1	25	water	3, 12, 13, 41
70	Isopropyl dibromoacetate	'BrC(Br)C(=O)OC(C)C',	-6.1	-5.6	-0.5	25	water	3, 12, 13, 41
71	Isopropyl (2-propyl)pentate	'CCCC(CCC)C(=O)OC(C)C',	-6.3	-6.5	0.2	25	water	3, 12, 13, 41
72	Isopropyl tribromoacetate	'BrC(Br)(Br)C(=O)OC(C)C',	-6.6	-6.4	-0.3	25	water	3, 12, 13, 41
73	Isopropyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OC(C)C',	-6.8	-6.7	-0.1	25	water	3, 12, 13, 41
74	Isopropyl (3-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OC(C)C',	-7.4	-7.4	0	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
75	Isopropyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OC(C)C',	-7.5	-6.8	-0.7	25	water	3, 12, 13, 41
76	Isopropyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OC(C)C',	-8.1	-7.4	-0.7	25	water	3, 12, 13, 41
77	Isopropyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OC(C)C',	-8	-7.1	-0.9	25	water	3, 12, 13, 41
78	(methyl) (neopentyl) (t-butyl)CC(=O)OC(C)C	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OC(C)C',	-8.2	-8.6	0.4	25	water	3, 12, 13, 41
79	n-Butyl formate	'C(=O)OCCCC',	-2.8	-3.5	0.7	25	water	3, 12, 13, 41
80	n-Butyl acetate	'CC(=O)OCCCC',	-4	-4	-0.1	25	water	3, 12, 13, 41
81	n-Butyl propionate	'CCC(=O)OCCCC',	-4.1	-4.3	0.2	25	water	3, 12, 13, 41
82	n-Butyl chloroacetate	'ClCC(=O)OCCCC',	-4.2	-4.6	0.4	25	water	3, 12, 13, 41
83	n-Butyl butyrate	'CCCC(=O)OCCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
84	n-Butyl pentate	'CCCCC(=O)OCCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
85	n-Butyl hexanoate	'CCCCCC(=O)OCCCC',	-4.4	-4.6	0.1	25	water	3, 12, 13, 41
86	n-Butyl iso-hexanoate	'CC(C)CCC(=O)OCCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
87	n-Butyl phenylacetate	'c1ccccc1CC(=O)OCCCC',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
88	n-Butyl phenylpropionate	'c1ccccc1CCC(=O)OCCCC',	-4.5	-4.6	0.2	25	water	3, 12, 13, 41
89	n-Butyl phenylbutyrate	'c1ccccc1CCCC(=O)OCCCC',	-4.5	-4.5	0	25	water	3, 12, 13, 41
90	n-Butyl isobutyrate	'CC(C)C(=O)OCCCC',	-4.5	-4.7	0.2	25	water	3, 12, 13, 41
91	n-Butyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCCCC',	-4.8	-5.1	0.3	25	water	3, 12, 13, 41
92	n-Butyl isopentate	'CC(C)CC(=O)OCCCC',	-5	-4.7	-0.3	25	water	3, 12, 13, 41
93	n-Butyl cyclohexylacetate	'C1CCCCC1CC(=O)OCCCC',	-5	-4.8	-0.2	25	water	3, 12, 13, 41
94	n-Butyl (2-ethyl)propionate	'CC(CC)C(=O)OCCCC',	-5.2	-5.2	0	25	water	3, 12, 13, 41
95	n-Butyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OCCCC',	-5.2	-5.4	0.2	25	water	3, 12, 13, 41
96	n-Butyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OCCCC',	-5.5	-5.9	0.4	25	water	3, 12, 13, 41
97	n-Butyl neopentate	'CC(C)(C)C(=O)OCCCC',	-5.6	-5.2	-0.3	25	water	3, 12, 13, 41
98	n-Butyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OCCCC',	-5.8	-6.5	0.7	25	water	3, 12, 13, 41
99	n-Butyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCCCC',	-6	-5.9	-0.1	25	water	3, 12, 13, 41
100	n-Butyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OCCCC',	-6	-5.7	-0.3	25	water	3, 12, 13, 41
101	n-Butyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCCC',	-6.1	-5.6	-0.5	25	water	3, 12, 13, 41
102	n-Butyl benzoate	'c1ccccc1C(=O)OCCCC',	-6.6	-6	-0.6	25	water	3, 12, 13, 41
103	n-Butyl cyclobutyl-carboxylate	'C1CCC1C(=O)OCCCC',	-4.1	-4.8	0.7	25	water	3, 12, 13, 41
104	n-Butyl methoxyacetate	'COCC(=O)OCCCC',	-4.2	-4.7	0.5	25	water	3, 12, 13, 41
105	n-Butyl bromoacetate	'BrCC(=O)OCCCC',	-4.3	-4.7	0.4	25	water	3, 12, 13, 41
106	n-Butyl thiolpropionate	'CSCC(=O)OCCCC',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41
107	n-Butyl iodoacetate	'ICC(=O)OCCCC',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41
108	CCCCCCCCC(=O)OCCCC	'CCCCCCCCC(=O)OCCCC',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
109	n-Butyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OCCCC',	-4.4	-5	0.6	25	water	3, 12, 13, 41
110	n-Butyl phenoxy-acetate	'c1ccccc1OCC(=O)OCCCC',	-4.4	-4.7	0.4	25	water	3, 12, 13, 41
111	n-Butyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCCCC',	-4.5	-5	0.5	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
112	n-Butyl difluoroacetate	'FC(F)C(=O)OCCCC',	-4.7	-4.9	0.2	25	water	3, 12, 13, 41
113	n-Butyl methoxypropionate	'COCCC(=O)OCCCC',	-4.8	-4.6	-0.2	25	water	3, 12, 13, 41
114	n-Butyl chloropropionate	'ClCCC(=O)OCCCC',	-4.9	-4.5	-0.4	25	water	3, 12, 13, 41
115	n-Butyl trifluoroacetate	'FC(F)(F)C(=O)OCCCC',	-5.2	-5.4	0.2	25	water	3, 12, 13, 41
116	n-Butyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCCCC',	-5.1	-5.1	0	25	water	3, 12, 13, 41
117	n-Butyl dichloracetate	'ClC(Cl)C(=O)OCCCC',	-5.6	-5	-0.5	25	water	3, 12, 13, 41
118	n-Butyl neopentate	'CC(C)(C)C(=O)OCCCC',	-5.8	-5.2	-0.5	25	water	3, 12, 13, 41
119	n-Butyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OCCCC',	-5.9	-5.7	-0.1	25	water	3, 12, 13, 41
120	n-Butyl dibromoacetate	'BrC(Br)C(=O)OCCCC',	-5.9	-5.4	-0.5	25	water	3, 12, 13, 41
121	n-Butyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCCCC',	-6.1	-6.3	0.2	25	water	3, 12, 13, 41
122	n-Butyl tribromoacetate	'BrC(Br)(Br)C(=O)OCCCC',	-6.5	-6.2	-0.3	25	water	3, 12, 13, 41
123	n-Butyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OCCCC',	-6.6	-6.5	-0.1	25	water	3, 12, 13, 41
124	n-Butyl (3-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCCCC',	-7.2	-7.2	0	25	water	3, 12, 13, 41
125	n-Butyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OCCCC',	-7.4	-6.7	-0.7	25	water	3, 12, 13, 41
126	n-Butyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OCCCC',	-7.9	-7.2	-0.7	25	water	3, 12, 13, 41
127	n-Butyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCCCC',	-7.8	-6.9	-0.9	25	water	3, 12, 13, 41
128	(methyl) (neopentyl) (t-butyl)CC(=O)OCCCC	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCCCC',	-8	-8.4	0.4	25	water	3, 12, 13, 41
129	Propyl formate	'C(=O)OCCC',	-2.8	-3.5	0.7	25	water	3, 12, 13, 41
130	Propyl acetate	'CC(=O)OCCC',	-4	-4	-0.1	25	water	3, 12, 13, 41
131	Propyl propionate	'CCC(=O)OCCC',	-4.1	-4.3	0.2	25	water	3, 12, 13, 41
132	Propyl chloroacetate	'ClCC(=O)OCCC',	-4.2	-4.6	0.4	25	water	3, 12, 13, 41
133	Propyl butyrate	'CCCC(=O)OCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
134	Propyl pentate	'CCCCC(=O)OCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
135	Propyl hexanoate	'CCCCCC(=O)OCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
136	Propyl iso-hexanoate	'CC(C)CCC(=O)OCCC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
137	Propyl phenylacetate	'c1ccccc1CC(=O)OCCC',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
138	Propyl phenylpropionate	'c1ccccc1CCC(=O)OCCC',	-4.5	-4.6	0.2	25	water	3, 12, 13, 41
139	Propyl phenylbutyrate	'c1ccccc1CCCC(=O)OCCC',	-4.5	-4.5	0	25	water	3, 12, 13, 41
140	Propyl isobutyrate	'CC(C)C(=O)OCCC',	-4.5	-4.7	0.2	25	water	3, 12, 13, 41
141	Propyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCCC',	-4.8	-5.1	0.3	25	water	3, 12, 13, 41
142	Propyl isopentate	'CC(C)CC(=O)OCCC',	-5	-4.7	-0.3	25	water	3, 12, 13, 41
143	Propyl cyclohexylacetate	'C1CCCCC1CC(=O)OCCC',	-5	-4.8	-0.2	25	water	3, 12, 13, 41
144	Propyl (2-ethyl)propionate	'CC(CC)C(=O)OCCC',	-5.2	-5.2	0	25	water	3, 12, 13, 41
145	Propyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OCCC',	-5.2	-5.4	0.2	25	water	3, 12, 13, 41
146	Propyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OCCC',	-5.5	-5.9	0.4	25	water	3, 12, 13, 41
147	Propyl neopentate	'CC(C)(C)C(=O)OCCC',	-5.6	-5.2	-0.3	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
148	Propyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OCCC',	-5.8	-6.5	0.7	25	water	3, 12, 13, 41
149	Propyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCCC',	-6	-5.9	-0.1	25	water	3, 12, 13, 41
150	Propyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OCCC',	-6	-5.7	-0.3	25	water	3, 12, 13, 41
151	Propyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCC',	-6.1	-5.6	-0.5	25	water	3, 12, 13, 41
152	Propyl benzoate	'c1ccccc1C(=O)OCCC',	-6.6	-6	-0.6	25	water	3, 12, 13, 41
153	Propyl cyclobutyl-carboxylate	'C1CCC1C(=O)OCCC',	-4.1	-4.8	0.7	25	water	3, 12, 13, 41
154	Propyl methoxyacetate	'COCC(=O)OCCC',	-4.2	-4.7	0.4	25	water	3, 12, 13, 41
155	Propyl bromoacetate	'BrCC(=O)OCCC',	-4.3	-4.7	0.4	25	water	3, 12, 13, 41
156	Propyl thiolpropionate	'CSCC(=O)OCCC',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41
157	Propyl iodoacetate	'ICC(=O)OCCC',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41
158	CCCCCCCCC(=O)OCCC	'CCCCCCCCC(=O)OCCC',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
159	Propyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OCCC',	-4.4	-4.9	0.6	25	water	3, 12, 13, 41
160	Propyl phenoxy-acetate	'c1ccccc1OCC(=O)OCCC',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41
161	Propyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCCC',	-4.5	-5	0.5	25	water	3, 12, 13, 41
162	Propyl difluoroacetate	'FC(F)C(=O)OCCC',	-4.7	-4.9	0.2	25	water	3, 12, 13, 41
163	Propyl methoxypropionate	'COCCC(=O)OCCC',	-4.8	-4.6	-0.2	25	water	3, 12, 13, 41
164	Propyl chloropropionate	'ClCCC(=O)OCCC',	-4.9	-4.5	-0.4	25	water	3, 12, 13, 41
165	Propyl trifluoroacetate	'FC(F)(F)C(=O)OCCC',	-5.2	-5.4	0.2	25	water	3, 12, 13, 41
166	Propyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCCC',	-5.1	-5.1	0	25	water	3, 12, 13, 41
167	Propyl dichloracetate	'ClC(Cl)C(=O)OCCC',	-5.6	-5	-0.6	25	water	3, 12, 13, 41
168	Propyl neopentate	'CC(C)(C)C(=O)OCCC',	-5.8	-5.2	-0.5	25	water	3, 12, 13, 41
169	Propyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OCCC',	-5.9	-5.7	-0.2	25	water	3, 12, 13, 41
170	Propyl dibromoacetate	'BrC(Br)C(=O)OCCC',	-5.9	-5.4	-0.5	25	water	3, 12, 13, 41
171	Propyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCCC',	-6.1	-6.3	0.2	25	water	3, 12, 13, 41
172	Propyl tribromoacetate	'BrC(Br)(Br)C(=O)OCCC',	-6.5	-6.2	-0.3	25	water	3, 12, 13, 41
173	Propyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OCCC',	-6.6	-6.5	-0.1	25	water	3, 12, 13, 41
174	Propyl (3-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCCC',	-7.2	-7.2	0	25	water	3, 12, 13, 41
175	Propyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OCCC',	-7.4	-6.6	-0.7	25	water	3, 12, 13, 41
176	Propyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OCCC',	-7.9	-7.2	-0.8	25	water	3, 12, 13, 41
177	Propyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCCC',	-7.8	-6.9	-1	25	water	3, 12, 13, 41
178	(methyl) (neopentyl) (t-butyl)CC(=O)OCCC	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCC',	-8	-8.4	0.3	25	water	3, 12, 13, 41
179	Methyl formate	'C(=O)OC',	-2.7	-3.5	0.8	25	water	3, 12, 13, 41
180	Methyl acetate	'CC(=O)OC',	-4	-3.8	-0.2	25	water	3, 12, 13, 41
181	Methyl propionate	'CCC(=O)OC',	-4	-4.1	0.1	25	water	3, 12, 13, 41
182	Methyl chloroacetate	'ClCC(=O)OC',	-4.2	-4.4	0.3	25	water	3, 12, 13, 41
183	Methyl butyrate	'CCCC(=O)OC',	-4.3	-4.3	0	25	water	3, 12, 13, 41
184	Methyl pentate	'CCCCC(=O)OC',	-4.3	-4.3	0	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
185	Methyl hexanoate	'CCCCCC(=O)OC',	-4.4	-4.4	0	25	water	3, 12, 13, 41
186	Methyl iso-hexanoate	'CC(C)CCC(=O)OC',	-4.3	-4.3	0	25	water	3, 12, 13, 41
187	Methyl phenylacetate	'c1ccccc1CC(=O)OC',	-4.3	-4.4	0.1	25	water	3, 12, 13, 41
188	Methyl phenylpropionate	'c1ccccc1CCC(=O)OC',	-4.4	-4.4	0	25	water	3, 12, 13, 41
189	Methyl phenylbutyrate	'c1ccccc1CCCC(=O)OC',	-4.4	-4.3	-0.2	25	water	3, 12, 13, 41
190	Methyl isobutyrate	'CC(C)C(=O)OC',	-4.4	-4.5	0.1	25	water	3, 12, 13, 41
191	Methyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OC',	-4.8	-4.9	0.2	25	water	3, 12, 13, 41
192	Methyl isopentate	'CC(C)CC(=O)OC',	-4.9	-4.5	-0.4	25	water	3, 12, 13, 41
193	Methyl cyclohexylacetate	'C1CCCCC1CC(=O)OC',	-4.9	-4.6	-0.3	25	water	3, 12, 13, 41
194	Methyl (2-ethyl)propionate	'CC(CC)C(=O)OC',	-5.1	-5	-0.1	25	water	3, 12, 13, 41
195	Methyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OC',	-5.2	-5.2	0	25	water	3, 12, 13, 41
196	Methyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OC',	-5.5	-5.7	0.3	25	water	3, 12, 13, 41
197	Methyl neopentate	'CC(C)(C)C(=O)OC',	-5.5	-5	-0.5	25	water	3, 12, 13, 41
198	Methyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OC',	-5.7	-6.3	0.6	25	water	3, 12, 13, 41
199	Methyl (2-ethyl)butyrate	'CCC(CC)C(=O)OC',	-5.9	-5.7	-0.2	25	water	3, 12, 13, 41
200	Methyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OC',	-5.9	-5.5	-0.4	25	water	3, 12, 13, 41
201	Methyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OC',	-6	-5.4	-0.6	25	water	3, 12, 13, 41
202	Methyl benzoate	'c1ccccc1C(=O)OC',	-6.5	-5.8	-0.7	25	water	3, 12, 13, 41
203	Methyl cyclobutyl-carboxylate	'C1CCC1C(=O)OC',	-4	-4.6	0.6	25	water	3, 12, 13, 41
204	Methyl methoxyacetate	'COCC(=O)OC',	-4.2	-4.5	0.3	25	water	3, 12, 13, 41
205	Methyl bromoacetate	'BrCC(=O)OC',	-4.2	-4.5	0.2	25	water	3, 12, 13, 41
206	Methyl thiolpropionate	'CSCC(=O)OC',	-4.3	-4.5	0.2	25	water	3, 12, 13, 41
207	Methyl iodoacetate	'ICC(=O)OC',	-4.3	-4.5	0.2	25	water	3, 12, 13, 41
208	CCCCCCCCC(=O)OC	'CCCCCCCCC(=O)OC',	-4.3	-4.4	0.1	25	water	3, 12, 13, 41
209	Methyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OC',	-4.3	-4.7	0.4	25	water	3, 12, 13, 41
210	Methyl phenoxy-acetate	'c1ccccc1OCC(=O)OC',	-4.3	-4.5	0.2	25	water	3, 12, 13, 41
211	Methyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCCC',	-4.5	-5	0.5	25	water	3, 12, 13, 41
212	Methyl difluoroacetate	'FC(F)C(=O)OC',	-4.6	-4.7	0.1	25	water	3, 12, 13, 41
213	Methyl methoxypropionate	'COCCC(=O)OC',	-4.7	-4.4	-0.4	25	water	3, 12, 13, 41
214	Methyl chloropropionate	'ClCCC(=O)OC',	-4.9	-4.3	-0.5	25	water	3, 12, 13, 41
215	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.1	-5.2	0.1	25	water	3, 12, 13, 41
216	Methyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OC',	-5.1	-4.9	-0.1	25	water	3, 12, 13, 41
217	Methyl dichloracetate	'ClC(Cl)C(=O)OC',	-5.5	-4.8	-0.7	25	water	3, 12, 13, 41
218	Methyl neopentate	'CC(C)(C)C(=O)OC',	-5.7	-5	-0.7	25	water	3, 12, 13, 41
219	Methyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OC',	-5.8	-5.5	-0.3	25	water	3, 12, 13, 41
220	Methyl dibromoacetate	'BrC(Br)C(=O)OC',	-5.8	-5.2	-0.6	25	water	3, 12, 13, 41
221	Methyl (2-propyl)pentate	'CCCC(CCC)C(=O)OC',	-6.1	-6.1	0	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
222	Methyl tribromoacetate	'BrC(Br)(Br)C(=O)OC',	-6.4	-6	-0.4	25	water	3, 12, 13, 41
223	Methyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OC',	-6.5	-6.3	-0.2	25	water	3, 12, 13, 41
224	Methyl (3-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OC',	-7.1	-7	-0.2	25	water	3, 12, 13, 41
225	Methyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OC',	-7.3	-6.4	-0.9	25	water	3, 12, 13, 41
226	Methyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OC',	-7.9	-7	-0.9	25	water	3, 12, 13, 41
227	Methyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OC',	-7.8	-6.7	-1.1	25	water	3, 12, 13, 41
228	(methyl) (neopentyl) (t-butyl)CC(=O)OC	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OC',	-8	-8.2	0.3	25	water	3, 12, 13, 41
229	Chloroethyl formate	'C(=O)OCCCl',	-2.8	-3.6	0.8	25	water	3, 12, 13, 41
230	Chloroethyl acetate	'CC(=O)OCCCl',	-4.1	-4.1	0	25	water	3, 12, 13, 41
231	Chloroethyl propionate	'CCC(=O)OCCCl',	-4.2	-4.5	0.3	25	water	3, 12, 13, 41
232	Chloroethyl chloroacetate	'ClCC(=O)OCCCl',	-4.3	-4.7	0.5	25	water	3, 12, 13, 41
233	Chloroethyl butyrate	'CCCC(=O)OCCCl',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
234	Chloroethyl pentate	'CCCCC(=O)OCCCl',	-4.5	-4.7	0.2	25	water	3, 12, 13, 41
235	Chloroethyl hexanoate	'CCCCCC(=O)OCCCl',	-4.5	-4.7	0.2	25	water	3, 12, 13, 41
236	Chloroethyl iso-hexanoate	'CC(C)CCC(=O)OCCCl',	-4.4	-4.6	0.2	25	water	3, 12, 13, 41
237	Chloroethyl phenylacetate	'c1ccccc1CC(=O)OCCCl',	-4.5	-4.7	0.3	25	water	3, 12, 13, 41
238	Chloroethyl phenylpropionate	'c1ccccc1CCC(=O)OCCCl',	-4.5	-4.7	0.2	25	water	3, 12, 13, 41
239	Chloroethyl phenylbutyrate	'c1ccccc1CCCC(=O)OCCCl',	-4.5	-4.6	0	25	water	3, 12, 13, 41
240	Chloroethyl isobutyrate	'CC(C)C(=O)OCCCl',	-4.6	-4.8	0.3	25	water	3, 12, 13, 41
241	Chloroethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCCCl',	-4.9	-5.3	0.4	25	water	3, 12, 13, 41
242	Chloroethyl isopentate	'CC(C)CC(=O)OCCCl',	-5	-4.8	-0.2	25	water	3, 12, 13, 41
243	Chloroethyl cyclohexylacetate	'C1CCCCC1CC(=O)OCCCl',	-5.1	-4.9	-0.1	25	water	3, 12, 13, 41
244	Chloroethyl (2-ethyl)propionate	'CC(CC)C(=O)OCCCl',	-5.2	-5.3	0.1	25	water	3, 12, 13, 41
245	Chloroethyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OCCCl',	-5.3	-5.5	0.2	25	water	3, 12, 13, 41
246	Chloroethyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OCCCl',	-5.6	-6	0.5	25	water	3, 12, 13, 41
247	Chloroethyl neopentate	'CC(C)(C)C(=O)OCCCl',	-5.6	-5.4	-0.3	25	water	3, 12, 13, 41
248	Chloroethyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OCCCl',	-5.8	-6.6	0.8	25	water	3, 12, 13, 41
249	Chloroethyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCCCl',	-6.1	-6	0	25	water	3, 12, 13, 41
250	Chloroethyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OCCCl',	-6.1	-5.8	-0.2	25	water	3, 12, 13, 41
251	Chloroethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCCl',	-6.1	-5.7	-0.4	25	water	3, 12, 13, 41
252	Chloroethyl benzoate	'c1ccccc1C(=O)OCCCl',	-6.6	-6.1	-0.5	25	water	3, 12, 13, 41
253	Chloroethyl cyclobutyl-carboxylate	'C1CCC1C(=O)OCCCl',	-4.1	-4.9	0.8	25	water	3, 12, 13, 41
254	Chloroethyl methoxyacetate	'COCC(=O)OCCCl',	-4.3	-4.8	0.5	25	water	3, 12, 13, 41
255	Chloroethyl bromoacetate	'BrCC(=O)OCCCl',	-4.3	-4.8	0.4	25	water	3, 12, 13, 41
256	Chloroethyl thiolpropionate	'CSCC(=O)OCCCl',	-4.4	-4.8	0.4	25	water	3, 12, 13, 41
257	Chloroethyl iodoacetate	'ICC(=O)OCCCl',	-4.4	-4.8	0.4	25	water	3, 12, 13, 41
258	CCCCCCCCC(=O)OCCCl	'CCCCCCCCC(=O)OCCCl',	-4.4	-4.7	0.3	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
259	Chloroethyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OCCCl',	-4.4	-5.1	0.6	25	water	3, 12, 13, 41
260	Chloroethyl phenoxy-acetate	'c1ccccc1OCC(=O)OCCCl',	-4.4	-4.8	0.4	25	water	3, 12, 13, 41
261	Chloroethyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCCCl',	-4.6	-5.1	0.6	25	water	3, 12, 13, 41
262	Chloroethyl difluoroacetate	'FC(F)C(=O)OCCCl',	-4.8	-5	0.3	25	water	3, 12, 13, 41
263	Chloroethyl methoxypropionate	'COCCC(=O)OCCCl',	-4.8	-4.7	-0.2	25	water	3, 12, 13, 41
264	Chloroethyl chloropropionate	'ClCCC(=O)OCCCl',	-5	-4.7	-0.3	25	water	3, 12, 13, 41
265	Chloroethyl trifluoroacetate	'FC(F)(F)C(=O)OCCCl',	-5.2	-5.5	0.3	25	water	3, 12, 13, 41
266	Chloroethyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCCCl',	-5.2	-5.3	0.1	25	water	3, 12, 13, 41
267	Chloroethyl dichloracetate	'ClC(Cl)C(=O)OCCCl',	-5.6	-5.1	-0.5	25	water	3, 12, 13, 41
268	Chloroethyl neopentate	'CC(C)(C)C(=O)OCCCl',	-5.8	-5.4	-0.5	25	water	3, 12, 13, 41
269	Chloroethyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OCCCl',	-5.9	-5.9	-0.1	25	water	3, 12, 13, 41
270	Chloroethyl dibromoacetate	'BrC(Br)C(=O)OCCCl',	-5.9	-5.5	-0.4	25	water	3, 12, 13, 41
271	Chloroethyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCCCl',	-6.2	-6.4	0.2	25	water	3, 12, 13, 41
272	Chloroethyl tribromoacetate	'BrC(Br)(Br)C(=O)OCCCl',	-6.5	-6.3	-0.2	25	water	3, 12, 13, 41
273	Chloroethyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OCCCl',	-6.7	-6.6	0	25	water	3, 12, 13, 41
274	Chloroethyl (3-neopentyl-4,4-dimethyl)pentate	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCCCl',	-7.3	-7.3	0	25	water	3, 12, 13, 41
275	Chloroethyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OCCCl',	-7.4	-6.8	-0.6	25	water	3, 12, 13, 41
276	Chloroethyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OCCCl',	-8	-7.3	-0.7	25	water	3, 12, 13, 41
277	Chloroethyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCCCl',	-7.9	-7	-0.9	25	water	3, 12, 13, 41
278	(methyl) (neopentyl) (t-butyl)CC(=O)OCCCl	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCCCl',	-8.1	-8.6	0.5	25	water	3, 12, 13, 41
279	Methoxymethyl formate	'C(=O)OCOC',	-3.2	-3.8	0.5	25	water	3, 12, 13, 41
280	Methoxymethyl acetate	'CC(=O)OCOC',	-4.5	-4.3	-0.2	25	water	3, 12, 13, 41
281	Methoxymethyl propionate	'CCC(=O)OCOC',	-4.5	-4.6	0.1	25	water	3, 12, 13, 41
282	Methoxymethyl chloroacetate	'ClCC(=O)OCOC',	-4.7	-4.9	0.2	25	water	3, 12, 13, 41
283	Methoxymethyl butyrate	'CCCC(=O)OCOC',	-4.8	-4.8	-0.1	25	water	3, 12, 13, 41
284	Methoxymethyl pentate	'CCCCC(=O)OCOC',	-4.9	-4.8	0	25	water	3, 12, 13, 41
285	Methoxymethyl hexanoate	'CCCCCC(=O)OCOC',	-4.9	-4.8	0	25	water	3, 12, 13, 41
286	Methoxymethyl iso-hexanoate	'CC(C)CCC(=O)OCOC',	-4.8	-4.8	0	25	water	3, 12, 13, 41
287	Methoxymethyl phenylacetate	'c1ccccc1CC(=O)OCOC',	-4.8	-4.9	0	25	water	3, 12, 13, 41
288	Methoxymethyl phenylpropionate	'c1ccccc1CCC(=O)OCOC',	-4.9	-4.9	0	25	water	3, 12, 13, 41
289	Methoxymethyl phenylbutyrate	'c1ccccc1CCCC(=O)OCOC',	-4.9	-4.7	-0.2	25	water	3, 12, 13, 41
290	Methoxymethyl isobutyrate	'CC(C)C(=O)OCOC',	-4.9	-5	0.1	25	water	3, 12, 13, 41
291	Methoxymethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCOC',	-5.3	-5.4	0.2	25	water	3, 12, 13, 41
292	Methoxymethyl isopentate	'CC(C)CC(=O)OCOC',	-5.4	-4.9	-0.5	25	water	3, 12, 13, 41
293	Methoxymethyl cyclohexylacetate	'C1CCCCC1CC(=O)OCOC',	-5.4	-5.1	-0.3	25	water	3, 12, 13, 41
294	Methoxymethyl (2-ethyl)propionate	'CC(CC)C(=O)OCOC',	-5.6	-5.5	-0.1	25	water	3, 12, 13, 41
295	Methoxymethyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OCOC',	-5.7	-5.7	0	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
296	Methoxymethyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OCOC',	-6	-6.2	0.2	25	water	3, 12, 13, 41
297	Methoxymethyl neopentate	'CC(C)(C)C(=O)OCOC',	-6	-5.5	-0.5	25	water	3, 12, 13, 41
298	Methoxymethyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OCOC',	-6.2	-6.8	0.6	25	water	3, 12, 13, 41
299	Methoxymethyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCOC',	-6.4	-6.2	-0.2	25	water	3, 12, 13, 41
300	Methoxymethyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OCOC',	-6.5	-6	-0.4	25	water	3, 12, 13, 41
301	Methoxymethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCOC',	-6.5	-5.9	-0.7	25	water	3, 12, 13, 41
302	Methoxymethyl benzoate	'c1ccccc1C(=O)OCOC',	-7	-6.3	-0.8	25	water	3, 12, 13, 41
303	Methoxymethyl cyclobutyl-carboxylate *	'C1CCC1C(=O)OCOC',	-4.5	-5.1	0.6	25	water	3, 12, 13, 41
304	Methoxymethyl methoxyacetate	'COCC(=O)OCOC',	-4.7	-5	0.3	25	water	3, 12, 13, 41
305	Methoxymethyl bromoacetate	'BrCC(=O)OCOC',	-4.7	-5	0.2	25	water	3, 12, 13, 41
306	Methoxymethyl thiolpropionate	'CSCC(=O)OCOC',	-4.8	-4.9	0.1	25	water	3, 12, 13, 41
307	Methoxymethyl iodoacetate	'ICC(=O)OCOC',	-4.8	-5	0.2	25	water	3, 12, 13, 41
308	CCCCCCCCC(=O)OCOC	'CCCCCCCCC(=O)OCOC',	-4.8	-4.9	0.1	25	water	3, 12, 13, 41
309	Methoxymethyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OCOC',	-4.8	-5.2	0.4	25	water	3, 12, 13, 41
310	Methoxymethyl phenoxy-acetate	'c1ccccc1OCC(=O)OCOC',	-4.8	-5	0.2	25	water	3, 12, 13, 41
311	Methoxymethyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCOC',	-5	-5.3	0.3	25	water	3, 12, 13, 41
312	Methoxymethyl difluoroacetate	'FC(F)C(=O)OCOC',	-5.1	-5.2	0	25	water	3, 12, 13, 41
313	Methoxymethyl methoxypropionate	'COCCC(=O)OCOC',	-5.2	-4.9	-0.4	25	water	3, 12, 13, 41
314	Methoxymethyl chloropropionate	'ClCCC(=O)OCOC',	-5.4	-4.8	-0.5	25	water	3, 12, 13, 41
315	Methoxymethyl trifluoroacetate	'FC(F)(F)C(=O)OCOC',	-5.6	-5.7	0.1	25	water	3, 12, 13, 41
316	Methoxymethyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCOC',	-5.6	-5.4	-0.1	25	water	3, 12, 13, 41
317	Methoxymethyl dichloracetate	'ClC(Cl)C(=O)OCOC',	-6	-5.3	-0.7	25	water	3, 12, 13, 41
318	Methoxymethyl neopentate	'CC(C)(C)C(=O)OCOC',	-6.2	-5.5	-0.7	25	water	3, 12, 13, 41
319	Methoxymethyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OCOC',	-6.3	-6	-0.3	25	water	3, 12, 13, 41
320	Methoxymethyl dibromoacetate	'BrC(Br)C(=O)OCOC',	-6.3	-5.7	-0.6	25	water	3, 12, 13, 41
321	Methoxymethyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCOC',	-6.6	-6.6	0	25	water	3, 12, 13, 41
322	Methoxymethyl tribromoacetate	'BrC(Br)(Br)C(=O)OCOC',	-6.9	-6.4	-0.5	25	water	3, 12, 13, 41
323	Methoxymethyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OCOC',	-7	-6.8	-0.2	25	water	3, 12, 13, 41
324	CC(C)(C)CC(CC(C)(C)C)C(=O)OCOC	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCOC',	-7.7	-7.5	-0.2	25	water	3, 12, 13, 41
325	Methoxymethyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OCOC',	-7.8	-6.9	-0.9	25	water	3, 12, 13, 41
326	Methoxymethyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OCOC',	-8.4	-7.5	-0.9	25	water	3, 12, 13, 41
327	Methoxymethyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCOC',	-8.3	-7.2	-1.1	25	water	3, 12, 13, 41
328	(methyl) (neopentyl) (t-butyl)CC(=O)OCOC	CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCOC',	-8.4	-8.9	0.4	25	water	3, 12, 13, 41
329	Chloromethyl formate	'C(=O)OCCl',	-3.2	-4	0.8	25	water	3, 12, 13, 41
330	Chloromethyl acetate	'CC(=O)OCCl',	-4.4	-4.4	0	25	water	3, 12, 13, 41
331	Chloromethyl propionate	'CCC(=O)OCCl',	-4.5	-4.8	0.3	25	water	3, 12, 13, 41
332	Chloromethyl chloroacetate	'ClCC(=O)OCCl',	-4.6	-5.1	0.4	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
333	Chloromethyl butyrate	'CCCC(=O)OCCl',	-4.8	-4.9	0.1	25	water	3, 12, 13, 41
334	Chloromethyl pentate	'CCCCC(=O)OCCl',	-4.8	-5	0.1	25	water	3, 12, 13, 41
335	Chloromethyl hexanoate	'CCCCCC(=O)OCCl',	-4.8	-5	0.2	25	water	3, 12, 13, 41
336	Chloromethyl iso-hexanoate	'CC(C)CCC(=O)OCCl',	-4.8	-4.9	0.1	25	water	3, 12, 13, 41
337	Chloromethyl phenylacetate	'c1ccccc1CC(=O)OCCl',	-4.8	-5.1	0.2	25	water	3, 12, 13, 41
338	Chloromethyl phenylpropionate	'c1ccccc1CCC(=O)OCCl',	-4.9	-5.1	0.2	25	water	3, 12, 13, 41
339	Chloromethyl phenylbutyrate	'c1ccccc1CCCC(=O)OCCl',	-4.9	-4.9	0	25	water	3, 12, 13, 41
340	Chloromethyl isobutyrate	'CC(C)C(=O)OCCl',	-4.9	-5.2	0.2	25	water	3, 12, 13, 41
341	Chloromethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCCl',	-5.2	-5.6	0.3	25	water	3, 12, 13, 41
342	Chloromethyl isopentate	'CC(C)CC(=O)OCCl',	-5.4	-5.1	-0.3	25	water	3, 12, 13, 41
343	Chloromethyl cyclohexylacetate	'C1CCCCC1CC(=O)OCCl',	-5.4	-5.3	-0.2	25	water	3, 12, 13, 41
344	Chloromethyl (2-ethyl)propionate	'CC(CC)C(=O)OCCl',	-5.6	-5.6	0	25	water	3, 12, 13, 41
345	Chloromethyl (2,2-methyl-phenyl)acetate	'c1ccccc1C(C)C(=O)OCCl',	-5.6	-5.8	0.2	25	water	3, 12, 13, 41
346	Chloromethyl (2,2-ethyl-phenyl)acetate	'c1ccccc1C(CC)C(=O)OCCl',	-5.9	-6.4	0.4	25	water	3, 12, 13, 41
347	Chloromethyl neopentate	'CC(C)(C)C(=O)OCCl',	-6	-5.7	-0.3	25	water	3, 12, 13, 41
348	Chloromethyl (2,2-diphenyl)acetate	'c1ccccc1C(c1ccccc1)C(=O)OCCl',	-6.2	-6.9	0.7	25	water	3, 12, 13, 41
349	Chloromethyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCCl',	-6.4	-6.4	-0.1	25	water	3, 12, 13, 41
350	Chloromethyl (3-phenyl)2-propenoate	'c1ccccc1C=CC(=O)OCCl',	-6.4	-6.2	-0.3	25	water	3, 12, 13, 41
351	Chloromethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCl',	-6.5	-6	-0.5	25	water	3, 12, 13, 41
352	Chloromethyl benzoate	'c1ccccc1C(=O)OCCl',	-7	-6.4	-0.6	25	water	3, 12, 13, 41
353	Chloromethyl cyclobutyl-carboxylate*	'C1CCC1C(=O)OCCl',	-4.5	-5.2	0.7	25	water	3, 12, 13, 41
354	Chloromethyl methoxyacetate	'COCC(=O)OCCl',	-4.6	-5.1	0.5	25	water	3, 12, 13, 41
355	Chloromethyl bromoacetate	'BrCC(=O)OCCl',	-4.7	-5.1	0.4	25	water	3, 12, 13, 41
356	Chloromethyl thiolpropionate	'CSCC(=O)OCCl',	-4.8	-5.1	0.3	25	water	3, 12, 13, 41
357	Chloromethyl iodoacetate	'ICC(=O)OCCl',	-4.8	-5.2	0.3	25	water	3, 12, 13, 41
358	CCCCCCCCC(=O)OCCl	'CCCCCCCCC(=O)OCCl',	-4.8	-5	0.2	25	water	3, 12, 13, 41
359	Chloromethyl (4,4-dimethyl)pentate	'CC(C)(C)CCC(=O)OCCl',	-4.8	-5.4	0.6	25	water	3, 12, 13, 41
360	Chloromethyl phenoxy-acetate	'c1ccccc1OCC(=O)OCCl',	-4.8	-5.1	0.4	25	water	3, 12, 13, 41
361	Chloromethyl cyclopentyl-carboxylate	'C1CCCC1C(=O)OCCl',	-5	-5.5	0.5	25	water	3, 12, 13, 41
362	Chloromethyl difluoroacetate	'FC(F)C(=O)OCCl',	-5.1	-5.3	0.2	25	water	3, 12, 13, 41
363	Chloromethyl methoxypropionate	'COCCC(=O)OCCl',	-5.2	-5	-0.2	25	water	3, 12, 13, 41
364	Chloromethyl chloropropionate	'ClCCC(=O)OCCl',	-5.3	-5	-0.4	25	water	3, 12, 13, 41
365	Chloromethyl trifluoroacetate	'FC(F)(F)C(=O)OCCl',	-5.6	-5.9	0.2	25	water	3, 12, 13, 41
366	Chloromethyl cycloheptyl-carboxylate	'C1CCCCCC1C(=O)OCCl',	-5.6	-5.6	0	25	water	3, 12, 13, 41
367	Chloromethyl dichloracetate	'ClC(Cl)C(=O)OCCl',	-6	-5.5	-0.5	25	water	3, 12, 13, 41
368	Chloromethyl neopentate	'CC(C)(C)C(=O)OCCl',	-6.2	-5.7	-0.5	25	water	3, 12, 13, 41
369	Chloromethyl (2-neopentyl)propionate	'CC(CC(C)(C)C)C(=O)OCCl',	-6.3	-6.2	-0.1	25	water	3, 12, 13, 41

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN WATER							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
370	Chloromethyl dibromoacetate	'BrC(Br)C(=O)OCCl',	-6.3	-5.9	-0.4	25	water	3, 12, 13, 41
371	Chloromethyl (2-propyl)pentate	'CCCC(CCC)C(=O)OCCl',	-6.6	-6.8	0.2	25	water	3, 12, 13, 41
372	Chloromethyl tribromoacetate	'BrC(Br)(Br)C(=O)OCCl',	-6.9	-6.6	-0.3	25	water	3, 12, 13, 41
373	Chloromethyl (3,3-methyl-neopentyl)acetate	'CC(C)(CC(C)(C)C)C(=O)OCCl',	-7	-7	0	25	water	3, 12, 13, 41
374	Chloromethyl (3-neopentyl-4,4-dimethyl)pentat	'CC(C)(C)CC(CC(C)(C)C)C(=O)OCCl',	-7.6	-7.6	0	25	water	3, 12, 13, 41
375	Chloromethyl (2-t-butyl)propionate	'CC(C(C)(C)C)C(=O)OCCl',	-7.8	-7.1	-0.7	25	water	3, 12, 13, 41
376	Chloromethyl (2,2-methyl-t-butyl)propionate	'CC(C)(C(C)(C)C)C(=O)OCCl',	-8.4	-7.6	-0.7	25	water	3, 12, 13, 41
377	Chloromethyl (2,2-diethyl)butyrate	'CCC(CC)(CC)C(=O)OCCl',	-8.3	-7.3	-0.9	25	water	3, 12, 13, 41
378	(methyl) (neopentyl) (t-butyl)CC(=O)OCCl	'CC(C)(C)CC(C)(C(C)(C)C)C(=O)OCCl',	-8.4	-8.9	0.4	25	water	3, 12, 13, 41
379	p-Nitrophenyl acetate	'c1cc(N(=O)=O)ccc1OC(=O)C',	-3.9	-3.9	0	30	water	42
380	p-Nitrophenyl propionate	'c1cc(N(=O)=O)ccc1OC(=O)CC',	-3.9	-4.3	0.4	30	water	42
381	p-Nitrophenyl butyrate	'c1cc(N(=O)=O)ccc1OC(=O)CCC',	-4.1	-4.4	0.3	30	water	42
382	p-Nitrophenyl isobutyrate	'c1cc(N(=O)=O)ccc1OC(=O)C(C)C',	-4.1	-4.6	0.5	30	water	42
383	p-Nitrophenyl 3,3-dimethylbutyrate	'c1cc(N(=O)=O)ccc1OC(=O)CC(C)(C)C',	-4.8	-5.4	0.5	30	water	42

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
1	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-7	-6.4	-0.6	25	60% acetone	43
2	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-6.9	-6.3	-0.5	25	60% acetone	43
3	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-4.9	-5.2	0.3	25	60% acetone	43
4	Ethyl iso-butyrate	'CC(C)C(=O)OCC',	-4.7	-4.9	0.3	25	60% acetone	43
5	Ethyl chloroacetate	'ClCC(=O)OCC',	-4.4	-4.7	0.3	25	60% acetone	43
6	Methyl acetate	'CC(=O)OC',	-4.3	-3.7	-0.6	25	60% acetone	43
7	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4.8	-5	0.2	25	70% acetone	44
8	Ethyl phenylpropionate	'CCOC(=O)CCc1ccccc1',	-4.9	-4.9	0.1	25	70% acetone	44
9	Ethyl phenylbutyrate	'CCOC(=O)CCCc1ccccc1',	-4.9	-4.6	-0.2	25	70% acetone	44
10	Ethyl phenylpentate	'CCOC(=O)CCCCc1ccccc1',	-4.8	-4.7	-0.2	25	70% acetone	44
11	Ethyl phenylisopropionate	'CCOC(=O)C(C)c1ccccc1',	-6.6	-6.3	-0.3	25	70% acetone	44
12	Ethyl (2-ethyl)phenylacetate	'CCOC(=O)C(CC)c1ccccc1',	-6.9	-7.1	0.2	25	70% acetone	44
13	Ethyl (2,2-diphenyl)acetate	'CCOC(=O)C(c1ccccc1)c2ccccc2',	-7.3	-8	0.7	25	70% acetone	44
14	Ethyl cyclohexylacetate	'CCOC(=O)CC1CCCCC1',	-5.3	-5.2	-0.1	25	70% acetone	44
15	Chloromethyl acetate	'CC(=O)OCCl',	-4.5	-4.4	-0.1	25	70% acetone	44
16	Chloromethyl acetate	'CC(=O)OCCl',	-4.6	-4.4	-0.2	25	70% acetone	44
17	Chloromethyl acetate	'CC(=O)OCCl',	-4.7	-4.4	-0.3	25	70% acetone	44
18	Chloromethyl propionate	'CCC(=O)OCCl',	-4.7	-4.9	0.1	25	70% acetone	44
19	Chloromethyl butyrate	'CCCC(=O)OCCl',	-5	-5.1	0.1	25	70% acetone	44
20	Ethyl acetate	'CC(=O)OCC',	-4.3	-3.8	-0.5	25	70% acetone	44
21	Ethyl propionate	'CCC(=O)OCC',	-4.4	-4.4	0	25	70% acetone	44
22	Ethyl butyrate	'CCCC(=O)OCC',	-4.7	-4.7	-0.1	25	70% acetone	44
23	Ethyl pentate	'CCCCC(=O)OCC',	-4.7	-4.8	0	25	70% acetone	44
24	Ethyl hexanoate	'CCCCCC(=O)OCC',	-4.8	-4.8	0	25	70% acetone	44
25	Ethyl heptanoate	'CCCCCCC(=O)OCC',	-4.8	-4.8	0	25	70% acetone	44
26	Ethyl octanoate	'CCCCCCCC(=O)OCC',	-4.8	-4.8	0	25	70% acetone	44
27	Ethyl isobutyrate	'CC(C)C(=O)OCC',	-4.9	-5	0.1	25	70% acetone	44
28	Ethyl isopentate	'CC(C)CC(=O)OCC',	-5.2	-4.9	-0.3	25	70% acetone	44
29	Ethyl hexanoate	'CC(C)CCC(=O)OCC',	-4.8	-4.7	-0.1	25	70% acetone	44
30	Ethyl sec-hexanoate	'CCCC(C)C(=O)OCC',	-5.4	-6	0.6	25	70% acetone	44
31	Ethyl neopentate	'CC(C)(C)C(=O)OCC',	-5.9	-5.9	0	25	70% acetone	44
32	Ethyl (2-ethyl)butyrate	'CCC(CC)C(=O)OCC',	-5.9	-6.8	0.9	25	70% acetone	44
33	Ethyl fluoroacetate	'FCC(=O)OCC',	-4.6	-4.7	0.1	25	70% acetone	45
34	Ethyl fluoroacetate	'FCC(=O)OCC',	-4.1	-4.3	0.2	35	70% acetone	45
35	Ethyl fluoroacetate	'FCC(=O)OCC',	-3.6	-3.8	0.2	50	70% acetone	45
36	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-4	-5	0.9	25	70% acetone	45
37	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-5.7	-5.3	-0.4	60	60% acetone	46

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
38	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-4.9	-4.7	-0.2	80.2	60% acetone	46
39	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-4.2	-4.2	-0.1	99.2	60% acetone	46
40	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3.6	-3.6	0	119.9	60% acetone	46
41	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3	-3.2	0.1	138.5	60% acetone	46
42	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-5	-4.7	-0.3	80.2	60% acetone	46
43	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-4.3	-4.1	-0.2	99.8	60% acetone	46
44	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-3.7	-3.6	-0.1	120.2	60% acetone	46
45	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-3.2	-3.2	0	138.9	60% acetone	46
46	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-4.8	-4.5	-0.2	80.3	60% acetone	46
47	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-4.1	-4	-0.1	100.05	60% acetone	46
48	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-3.5	-3.5	0	120.5	60% acetone	46
49	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-3	-3	0.1	138.9	60% acetone	46
50	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-4.7	-4.4	-0.2	80.3	60% acetone	46
51	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-4	-3.9	-0.1	100.2	60% acetone	46
52	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-3.4	-3.4	0	120.9	60% acetone	46
53	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-2.9	-2.9	0.1	139.3	60% acetone	46
54	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-4.7	-4.5	-0.2	80.3	60% acetone	46
55	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-4.1	-3.9	-0.1	99.85	60% acetone	46
56	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-3.4	-3.4	0	120.2	60% acetone	46
57	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-2.9	-3	0.1	139.4	60% acetone	46
58	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-5.5	-5.1	-0.3	60.05	60% acetone	46
59	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-4.7	-4.5	-0.2	80.2	60% acetone	46
60	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-4.1	-4	-0.1	100.15	60% acetone	46
61	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-3.5	-3.5	0	120.2	60% acetone	46
62	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-3	-3	0.1	139.2	60% acetone	46
63	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-5.3	-5	-0.4	60	60% acetone	46
64	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-4.6	-4.3	-0.2	80.2	60% acetone	46
65	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-4	-3.8	-0.2	99.4	60% acetone	46
66	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-3.4	-3.3	-0.1	120	60% acetone	46
67	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-2.8	-2.9	0	138.5	60% acetone	46
68	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-5.4	-5.1	-0.4	60	60% acetone	46
69	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-4.7	-4.4	-0.3	80.2	60% acetone	46
70	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-4.1	-3.9	-0.2	99.9	60% acetone	46
71	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-3.4	-3.4	-0.1	120.4	60% acetone	46
72	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-2.9	-3	0	139	60% acetone	46
73	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-5.8	-5.2	-0.6	80.3	60% acetone	46
74	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-5.2	-4.6	-0.5	99.85	60% acetone	46

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
75	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-4.5	-4.1	-0.4	120.7	60% acetone	46
76	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-4	-3.7	-0.3	139.2	60% acetone	46
77	Ethyl butyrate	'CCCC(=O)OCC',	-4.9	-4.9	-0.1	20	70% acetone	44, 47, 48
78	Ethyl butyrate	'CCCC(=O)OCC',	-4.5	-4.5	0	30	70% acetone	44, 47, 48
79	Ethyl butyrate	'CCCC(=O)OCC',	-4.2	-4.1	0	40	70% acetone	44, 47, 48
80	Ethyl butyrate	'CCCC(=O)OCC',	-3.8	-3.8	0	50	70% acetone	44, 47, 48
81	Ethyl pentate	'CCCCC(=O)OCC',	-4.9	-4.9	0	20	70% acetone	44, 47, 48
82	Ethyl pentate	'CCCCC(=O)OCC',	-4.6	-4.6	0	30	70% acetone	44, 47, 48
83	Ethyl pentate	'CCCCC(=O)OCC',	-4.2	-4.2	0.1	40	70% acetone	44, 47, 48
84	Ethyl pentate	'CCCCC(=O)OCC',	-3.8	-3.9	0.1	50	70% acetone	44, 47, 48
85	Ethyl isobutyrate	'CC(C)C(=O)OCC',	-5.1	-5.2	0.1	20	70% acetone	44, 47, 48
86	Ethyl isobutyrate	'CC(C)C(=O)OCC',	-4.7	-4.8	0.1	30	70% acetone	44, 47, 48
87	Ethyl isobutyrate	'CC(C)C(=O)OCC',	-4.3	-4.5	0.2	40	70% acetone	44, 47, 48
88	Ethyl isobutyrate	'CC(C)C(=O)OCC',	-3.9	-4.1	0.2	50	70% acetone	44, 47, 48
89	Ethyl sec-hexanoate	'CCCC(C)C(=O)OCC',	-5.6	-6.2	0.6	20	70% acetone	44, 47, 48
90	Ethyl sec-hexanoate	'CCCC(C)C(=O)OCC',	-5.2	-5.8	0.6	30	70% acetone	44, 47, 48
91	Ethyl sec-hexanoate	'CCCC(C)C(=O)OCC',	-4.8	-5.5	0.7	40	70% acetone	44, 47, 48
92	Ethyl sec-hexanoate	'CCCC(C)C(=O)OCC',	-4.4	-5.1	0.7	50	70% acetone	44, 47, 48
93	Ethyl iso-hexanoate	'CC(C)CCC(=O)OCC',	-5	-4.9	-0.1	20	70% acetone	44, 47, 48
94	Ethyl iso-hexanoate	'CC(C)CCC(=O)OCC',	-4.6	-4.5	-0.1	30	70% acetone	44, 47, 48
95	Ethyl iso-hexanoate	'CC(C)CCC(=O)OCC',	-4.2	-4.2	0	40	70% acetone	44, 47, 48
96	Ethyl iso-hexanoate	'CC(C)CCC(=O)OCC',	-3.8	-3.8	0	50	70% acetone	44, 47, 48
97	Ethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCC',	-5.3	-5.7	0.4	20	70% acetone	44, 47, 48
98	Ethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCC',	-4.9	-5.4	0.4	30	70% acetone	44, 47, 48
99	Ethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCC',	-4.6	-5	0.4	40	70% acetone	44, 47, 48
100	Ethyl cyclohexyl-carboxylate	'C1CCCCC1C(=O)OCC',	-4.2	-4.7	0.5	50	70% acetone	44, 47, 48
101	Ethyl acetate	'CCOC(=O)C',	-3.6	-3.2	-0.4	44.7	70% acetone	44
102	Ethyl propionate	'CCOC(=O)CC',	-3.7	-3.7	0.1	44.7	70% acetone	44
103	Ethyl butyrate	'CCOC(=O)CCC',	-4	-4	0	44.7	70% acetone	44
104	Ethyl pentate	'CCOC(=O)CCCC',	-4	-4.1	0.1	44.7	70% acetone	44
105	Ethyl hexanoate	'CCOC(=O)CCCCC',	-4	-4.1	0.1	44.7	70% acetone	44
106	Ethyl isobutyrate	'CCOC(=O)C(C)C',	-4.1	-4.3	0.2	44.7	70% acetone	44
107	Ethyl isopentate	'CCOC(=O)CC(C)C',	-4.5	-4.3	-0.2	44.7	70% acetone	44
108	Ethyl t-butyrate	'CCOC(=O)C(C)(C)C',	-4.9	-5.1	0.2	44.7	70% acetone	44
109	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4	-4.4	0.4	44.7	70% acetone	44
110	Ethyl acetate	'CCOC(=O)C',	-4	-3.5	-0.5	35	70% acetone	44
111	Ethyl propionate	'CCOC(=O)CC',	-4	-4.1	0	35	70% acetone	44

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
112	Ethyl butyrate	'CCOC(=O)CCC',	-4.3	-4.3	0	35	70% acetone	44
113	Ethyl pentate	'CCOC(=O)CCCC',	-4.3	-4.4	0	35	70% acetone	44
114	Ethyl hexanoate	'CCOC(=O)CCCCC',	-4.4	-4.4	0.1	35	70% acetone	44
115	Ethyl isobutyrate	'CCOC(=O)C(C)C',	-4.5	-4.6	0.2	35	70% acetone	44
116	Ethyl isopentate	'CCOC(=O)CC(C)C',	-4.8	-4.6	-0.2	35	70% acetone	44
117	Ethyl t-butyrate	'CCOC(=O)C(C)(C)C',	-5.4	-5.5	0	35	70% acetone	44
118	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4.1	-4.7	0.6	35	70% acetone	44
119	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-5	-5.2	0.2	20	70% acetone	44
120	Ethyl phenylpropionate	'CCOC(=O)CCc1ccccc1',	-5.1	-5.1	0	20	70% acetone	44
121	Ethyl phenylbutyrate	'CCOC(=O)CCCc1ccccc1',	-5.1	-4.8	-0.3	20	70% acetone	44
122	Ethyl phenylpentate	'CCOC(=O)CCCCc1ccccc1',	-5.1	-4.9	-0.2	20	70% acetone	44
123	Ethyl phenylisopropionate	'CCOC(=O)C(C)c1ccccc1',	-6.8	-6.5	-0.3	20	70% acetone	44
124	Ethyl 2-ethyl-2-phenylacetate	'CCOC(=O)C(CC)c1ccccc1',	-7.2	-7.3	0.1	20	70% acetone	44
125	Ethyl 2,2-diphenylacetate	'CCOC(=O)C(c1ccccc1)c2ccccc2',	-7.5	-8.2	0.7	20	70% acetone	44
126	Ethyl cyclohexyl-acetate	'CCOC(=O)CC1CCCCC1',	-5.5	-5.4	-0.1	20	70% acetone	44
127	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4.6	-4.8	0.2	30	70% acetone	44
128	Ethyl phenylpropionate	'CCOC(=O)CCc1ccccc1',	-4.7	-4.8	0.1	30	70% acetone	44
129	Ethyl phenylbutyrate	'CCOC(=O)CCCc1ccccc1',	-4.7	-4.5	-0.2	30	70% acetone	44
130	Ethyl phenylpentate	'CCOC(=O)CCCCc1ccccc1',	-4.6	-4.5	-0.2	30	70% acetone	44
131	Ethyl phenylisopropionate	'CCOC(=O)C(C)c1ccccc1',	-6.3	-6.1	-0.3	30	70% acetone	44
132	Ethyl 2-ethyl-2-phenylacetate	'CCOC(=O)C(CC)c1ccccc1',	-6.7	-6.9	0.2	30	70% acetone	44
133	Ethyl 2,2-diphenylacetate	'CCOC(=O)C(c1ccccc1)c2ccccc2',	-7.1	-7.8	0.8	30	70% acetone	44
134	Ethyl cyclohexyl-acetate	'CCOC(=O)CC1CCCCC1',	-5.1	-5	-0.1	30	70% acetone	44
135	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4.3	-4.5	0.2	40	70% acetone	44
136	Ethyl phenylpropionate	'CCOC(=O)CCc1ccccc1',	-4.3	-4.4	0.1	40	70% acetone	44
137	Ethyl phenylbutyrate	'CCOC(=O)CCCc1ccccc1',	-4.3	-4.1	-0.2	40	70% acetone	44
138	Ethyl phenylpentate	'CCOC(=O)CCCCc1ccccc1',	-4.3	-4.1	-0.1	40	70% acetone	44
139	Ethyl phenylisopropionate	'CCOC(=O)C(C)c1ccccc1',	-6	-5.7	-0.2	40	70% acetone	44
140	Ethyl 2-ethyl-2-phenylacetate	'CCOC(=O)C(CC)c1ccccc1',	-6.4	-6.6	0.2	40	70% acetone	44
141	Ethyl 2,2-diphenylacetate	'CCOC(=O)C(c1ccccc1)c2ccccc2',	-6.7	-7.5	0.8	40	70% acetone	44
142	Ethyl cyclohexyl-acetate	'CCOC(=O)CC1CCCCC1',	-4.7	-4.7	-0.1	40	70% acetone	44
143	Ethyl phenylacetate	'CCOC(=O)Cc1ccccc1',	-4.2	-4.2	0	50	70% acetone	44
144	Ethyl phenylpropionate	'CCOC(=O)CCc1ccccc1',	-3.9	-4.1	0.2	50	70% acetone	44
145	Ethyl phenylbutyrate	'CCOC(=O)CCCc1ccccc1',	-4	-3.8	-0.2	50	70% acetone	44
146	Ethyl phenylpentate	'CCOC(=O)CCCCc1ccccc1',	-3.9	-3.8	-0.1	50	70% acetone	44
147	Ethyl phenylisopropionate	'CCOC(=O)C(C)c1ccccc1',	-5.6	-5.4	-0.2	50	70% acetone	44
148	Ethyl 2-ethyl-2-phenylacetate	'CCOC(=O)C(CC)c1ccccc1',	-6	-6.2	0.2	50	70% acetone	44

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
149	Ethyl 2,2-diphenylacetate	'CCOC(=O)C(c1ccccc1)c2ccccc2',	-6.3	-7.1	0.8	50	70% acetone	44
150	Ethyl cyclohexyl-acetate	'CCOC(=O)CC1CCCCC1',	-4.3	-4.3	0	50	70% acetone	44
151	Benzyl acetate	'CC(=O)OCc1ccccc1',	-4.9	-4.4	-0.6	15	60% acetone	49
152	Benzyl acetate	'CC(=O)OCc1ccccc1',	-4.5	-4	-0.5	25	60% acetone	49
153	Benzyl acetate	'CC(=O)OCc1ccccc1',	-3.9	-3.5	-0.4	40	60% acetone	49
154	Benzyl acetate	'CC(=O)OCc1ccccc1',	-3.2	-2.9	-0.3	60	60% acetone	49
155	Benzyl acetate	'CC(=O)OCc1ccccc1',	-2.6	-2.3	-0.3	80	60% acetone	49
156	m-Methylbenzyl acetate	'CC(=O)OCc1cccc(C)c1',	-5	-4.4	-0.6	15	60% acetone	49
157	m-Methylbenzyl acetate	'CC(=O)OCc1cccc(C)c1',	-4.5	-4	-0.5	25	60% acetone	49
158	m-Methylbenzyl acetate	'CC(=O)OCc1cccc(C)c1',	-4	-3.5	-0.5	40	60% acetone	49
159	m-Methylbenzyl acetate	'CC(=O)OCc1cccc(C)c1',	-3.3	-2.9	-0.4	60	60% acetone	49
160	m-Methylbenzyl acetate	'CC(=O)OCc1cccc(C)c1',	-2.7	-2.3	-0.3	80	60% acetone	49
161	p-Methylbenzyl acetate	'CC(=O)OCc1ccc(C)cc1',	-4.5	-4	-0.5	25	60% acetone	49
162	p-Methylbenzyl acetate	'CC(=O)OCc1ccc(C)cc1',	-3.9	-3.5	-0.4	40	60% acetone	49
163	p-Methylbenzyl acetate	'CC(=O)OCc1ccc(C)cc1',	-3.2	-2.9	-0.3	60	60% acetone	49
164	p-Methylbenzyl acetate	'CC(=O)OCc1ccc(C)cc1',	-2.6	-2.4	-0.3	80	60% acetone	49
165	m-Nitrobenzyl acetate	'CC(=O)OCc1cccc(N(=O)=O)c1',	-5	-4.4	-0.6	15	60% acetone	49
166	m-Nitrobenzyl acetate	'CC(=O)OCc1cccc(N(=O)=O)c1',	-4.6	-4	-0.5	25	60% acetone	49
167	m-Nitrobenzyl acetate	'CC(=O)OCc1cccc(N(=O)=O)c1',	-4	-3.5	-0.5	40	60% acetone	49
168	m-Nitrobenzyl acetate	'CC(=O)OCc1cccc(N(=O)=O)c1',	-3.3	-2.9	-0.4	60	60% acetone	49
169	m-Nitrobenzyl acetate	'CC(=O)OCc1cccc(N(=O)=O)c1',	-2.7	-2.4	-0.4	80	60% acetone	49
170	p-Nitrobenzyl acetate	'CC(=O)OCc1ccc(N(=O)=O)cc1',	-5	-4.4	-0.6	15	60% acetone	49
171	p-Nitrobenzyl acetate	'CC(=O)OCc1ccc(N(=O)=O)cc1',	-4.6	-4	-0.5	25	60% acetone	49
172	p-Nitrobenzyl acetate	'CC(=O)OCc1ccc(N(=O)=O)cc1',	-4	-3.5	-0.4	40	60% acetone	49
173	p-Nitrobenzyl acetate	'CC(=O)OCc1ccc(N(=O)=O)cc1',	-3.3	-2.9	-0.4	60	60% acetone	49
174	p-Nitrobenzyl acetate	'CC(=O)OCc1ccc(N(=O)=O)cc1',	-2.7	-2.4	-0.3	80	60% acetone	49
175	Phenyl acetate	'CC(=O)Oc1ccccc1',	-5	-4.6	-0.3	15	60% acetone	49
176	Phenyl acetate	'CC(=O)Oc1ccccc1',	-4.6	-4.3	-0.3	25	60% acetone	49
177	Phenyl acetate	'CC(=O)Oc1ccccc1',	-3.9	-3.8	-0.2	40	60% acetone	49
178	Phenyl acetate	'CC(=O)Oc1ccccc1',	-3.2	-3.1	-0.1	60	60% acetone	49
179	Phenyl acetate	'CC(=O)Oc1ccccc1',	-2.6	-2.6	0	80	60% acetone	49
180	m-Methylphenyl acetate	'CC(=O)Oc1cccc(C)c1',	-5	-4.7	-0.3	15	60% acetone	49
181	m-Methylphenyl acetate	'CC(=O)Oc1cccc(C)c1',	-4.6	-4.3	-0.3	25	60% acetone	49
182	m-Methylphenyl acetate	'CC(=O)Oc1cccc(C)c1',	-4	-3.8	-0.2	40	60% acetone	49
183	m-Methylphenyl acetate	'CC(=O)Oc1cccc(C)c1',	-3.2	-3.2	-0.1	60	60% acetone	49
184	m-Methylphenyl acetate	'CC(=O)Oc1cccc(C)c1',	-2.6	-2.6	0	80	60% acetone	49
185	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-4.5	-4.3	-0.2	25	60% acetone	49

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
186	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-3.9	-3.8	-0.1	40	60% acetone	49
187	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-3.2	-3.2	0	60	60% acetone	49
188	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-2.5	-2.6	0.1	80	60% acetone	49
189	m-Nitrophenyl acetate	'CC(=O)Oc1cccc(N(=O)=O)c1',	-5.2	-4.8	-0.4	15	60% acetone	49
190	m-Nitrophenyl acetate	'CC(=O)Oc1cccc(N(=O)=O)c1',	-4.7	-4.4	-0.3	25	60% acetone	49
191	m-Nitrophenyl acetate	'CC(=O)Oc1cccc(N(=O)=O)c1',	-4.1	-3.9	-0.2	40	60% acetone	49
192	m-Nitrophenyl acetate	'CC(=O)Oc1cccc(N(=O)=O)c1',	-3.4	-3.2	-0.2	60	60% acetone	49
193	m-Nitrophenyl acetate	'CC(=O)Oc1cccc(N(=O)=O)c1',	-2.8	-2.7	-0.1	80	60% acetone	49
194	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.7	-5.2	0.5	35	35% acetone	50
195	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.8	-5.2	0.5	35	44% acetone	50
196	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.9	-5.3	0.4	35	51.5% acetone	50
197	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-5.1	-5.4	0.3	35	62% acetone	50
198	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-5.3	-5.6	0.3	35	82.5% acetone	50
199	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.3	-4.8	0.5	45	35% acetone	50
200	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.4	-4.9	0.4	45	42.5% acetone	50
201	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.6	-4.9	0.4	45	52% acetone	50
202	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.7	-5	0.3	45	62% acetone	50
203	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.9	-5.2	0.3	45	82% acetone	50
204	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.1	-4.6	0.6	55	35% acetone	50
205	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.2	-4.7	0.5	55	42.5% acetone	50
206	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.3	-4.7	0.4	55	52% acetone	50
207	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.2	-4.8	0.6	55	62% acetone	50
208	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-4.6	-5	0.4	55	81.5% aceton	50

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN METHANOL-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
1	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-4	-4.2	0.2	99.85	60% methanol	46
2	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3.4	-3.6	0.2	120.45	60% methanol	46
3	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3	-3.2	0.2	138.5	60% methanol	46
4	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-2.6	-2.9	0.3	153.9	60% methanol	46
5	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-3.8	-3.9	0.1	100.2	60% methanol	46
6	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-3.3	-3.4	0.1	121.2	60% methanol	46
7	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-2.8	-3	0.2	139.2	60% methanol	46
8	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-2.5	-2.6	0.2	153.9	60% methanol	46
9	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-3.8	-3.8	0	100.12	60% methanol	46
10	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-3.2	-3.3	0	120.75	60% methanol	46
11	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-2.8	-2.9	0.1	138.4	60% methanol	46
12	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-2.5	-2.6	0.1	153	60% methanol	46
13	Methyl benzoate	'c1ccccc1C(=O)OC',	-3.7	-3.9	0.1	100.8	80% methanol	31
14	Methyl o-methylbenzoate	'Cc1ccccc1C(=O)OC',	-4.4	-4.5	0	100.8	80% methanol	31
15	Methyl o-ethylbenzoate	'CCc1ccccc1C(=O)OC',	-4.7	-4.6	0	100.8	80% methanol	31
16	Methyl o-fluorobenzoate	'Fc1ccccc1C(=O)OC',	-3.7	-4.4	0.7	100.8	80% methanol	31
17	Methyl o-chlorobenzoate	'Clc1ccccc1C(=O)OC',	-4.2	-4.5	0.3	100.8	80% methanol	31
18	Methyl o-bromobenzoate	'Brc1ccccc1C(=O)OC',	-4.3	-4.6	0.3	100.8	80% methanol	31
19	Methyl o-iodobenzoate	'Ic1ccccc1C(=O)OC',	-4.6	-4.7	0.1	100.8	80% methanol	31
20	Methyl m-methylbenzoate	'c1c(C)cccc1C(=O)OC',	-3.8	-3.9	0	100.8	80% methanol	31
21	Methyl m-chlorobenzoate	'c1c(Cl)cccc1C(=O)OC',	-3.8	-3.9	0.1	100.8	80% methanol	31
22	Methyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OC',	-3.9	-3.9	0	100.8	80% methanol	31

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
1	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-5.7	-5.5	-0.2	60	60% ethanol	46
2	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-4.8	-4.8	0	80.2	60% ethanol	46
3	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-4.2	-4.3	0	99.4	60% ethanol	46
4	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3.6	-3.7	0.1	119.9	60% ethanol	46
5	Ethyl p-methoxybenzoate	'c1cc(OC)ccc1C(=O)OCC',	-3.1	-3.3	0.2	138.1	60% ethanol	46
6	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-5	-4.8	-0.2	80.2	60% ethanol	46
7	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-4.4	-4.3	-0.1	99.5	60% ethanol	46
8	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-3.7	-3.7	0	120	60% ethanol	46
9	Ethyl p-hydroxybenzoate	'c1cc(O)ccc1C(=O)OCC',	-3.2	-3.3	0.1	138.5	60% ethanol	46
10	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-5.5	-5.3	-0.2	60.05	60% ethanol	46
11	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-4.8	-4.7	-0.1	80.25	60% ethanol	46
12	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-4.1	-4.1	0	99.9	60% ethanol	46
13	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-3.5	-3.6	0.1	120.3	60% ethanol	46
14	Ethyl p-methylbenzoate	'c1cc(C)ccc1C(=O)OCC',	-3	-3.1	0.1	139.7	60% ethanol	46
15	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-5.4	-5.2	-0.2	60	60% ethanol	46
16	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-4.7	-4.5	-0.1	80.2	60% ethanol	46
17	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-4.1	-4	-0.1	99.6	60% ethanol	46
18	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-3.5	-3.5	0	120.2	60% ethanol	46
19	Ethyl benzoate	'c1ccccc1C(=O)OCC',	-2.9	-3.1	0.1	138.6	60% ethanol	46
20	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-4.7	-4.6	-0.1	80.3	60% ethanol	46
21	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-4.1	-4.1	0	100	60% ethanol	46
22	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-3.5	-3.5	0	120.6	60% ethanol	46
23	Ethyl p-chlorobenzoate	'c1cc(Cl)ccc1C(=O)OCC',	-3.1	-3.1	0	139.3	60% ethanol	46
24	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-4.7	-4.6	-0.1	80.2	60% ethanol	46
25	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-4.1	-4.1	0	100	60% ethanol	46
26	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-3.5	-3.6	0	120.2	60% ethanol	46
27	Ethyl p-bromobenzoate	'c1cc(Br)ccc1C(=O)OCC',	-3	-3.1	0.1	139.4	60% ethanol	46
28	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-4.5	-4.5	-0.1	80.2	60% ethanol	46
29	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-4	-3.9	0	98.9	60% ethanol	46
30	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-3.5	-3.4	-0.1	119.3	60% ethanol	46
31	Ethyl p-nitrobenzoate	'c1cc(N(=O)=O)ccc1C(=O)OCC',	-3	-3	0	138	60% ethanol	46
32	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-4.7	-4.6	-0.1	80.2	60% ethanol	46
33	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-4.1	-4	0	99.45	60% ethanol	46
34	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-3.5	-3.5	0	119.9	60% ethanol	46
35	Ethyl m-nitrobenzoate	'c1c(N(=O)=O)cccc1C(=O)OCC',	-3	-3.1	0	138.3	60% ethanol	46
36	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-5.8	-5.3	-0.5	80.3	60% ethanol	46
37	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-5.2	-4.7	-0.5	100	60% ethanol	46

	TABLE 6: ACID-CATALYZED HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
38	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-4.6	-4.2	-0.4	120.6	60% ethanol	46
39	Ethyl o-nitrobenzoate	'c1(N(=O)=O)ccccc1C(=O)OCC',	-4.1	-3.8	-0.3	138.9	60% ethanol	46

	TABLE 6:B817 ACID-CATALYZED HYDROLYSIS OF ESTERS IN DIOXANE-WATER MIXED SOLVENTS AND AT VARIOUS TEMPERATURE.							
			observed	calculated				
	Esters	SMILES string	logk	logk	Difference	Temperature	Solvents	References
1	Chloromethyl acetate	'CC(=O)OCCl',	-4.4	-4.4	0	25	10% dioxane	18
2	Chloromethyl acetate	'CC(=O)OCCl',	-4	-4.1	0	35	10% dioxane	18
3	Chloromethyl acetate	'CC(=O)OCCl',	-3.6	-3.7	0.1	45	10% dioxane	18
4	Chloromethyl acetate	'CC(=O)OCCl',	-4.5	-4.5	0	25	25% dioxane	18
5	Chloromethyl acetate	'CC(=O)OCCl',	-4.1	-4.1	0	35	25% dioxane	18
6	Chloromethyl acetate	'CC(=O)OCCl',	-3.7	-3.8	0.1	45	25% dioxane	18
7	Chloromethyl acetate	'CC(=O)OCCl',	-4.7	-4.6	0	25	50% dioxane	18
8	Chloromethyl acetate	'CC(=O)OCCl',	-4.3	-4.2	0	35	50% dioxane	18
9	Chloromethyl acetate	'CC(=O)OCCl',	-3.9	-3.9	0	45	50% dioxane	18
10	Chloromethyl acetate	'CC(=O)OCCl',	-4.9	-4.8	-0.1	25	75% dioxane	18
11	Chloromethyl acetate	'CC(=O)OCCl',	-4.5	-4.5	0	35	75% dioxane	18
12	Chloromethyl acetate	'CC(=O)OCCl',	-4.1	-4.1	0	45	75% dioxane	18
13	Methyl benzoate	'c1ccccc1C(=O)OC',	-3.8	-4.1	0.3	100	60% dioxane	17
14	Methyl o-methylbenzoate	'Cc1ccccc1C(=O)OC',	-4.4	-4.8	0.4	100	60% dioxane	17
15	Methyl o-ethylbenzoate	'CCc1ccccc1C(=O)OC',	-4.7	-5	0.3	100	60% dioxane	17

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES string	logk	logk	Difference	Catalysts	Temperature	Solvents	References
1	Ethyl acetate	'CC(=O)OCC',	-11.3	-12.1	0.7	water	25	water	3, 14
2	Vinyl acetate	'CC(=O)OC=C',	-8.7	-9	0.3	water	25	water	3, 14
3	Chloromethyl formate	'C(=O)OCCl',	-5.8	-6.5	0.7	water	25	water	3, 14, 51
4	Methyl chloroacetate	'ClCC(=O)OC',	-8.4	-8.5	0.1	water	25	water	3, 14
5	Methyl dichloroacetate	'ClC(Cl)C(=O)OC',	-6.6	-6.9	0.4	water	25	water	3, 14, 51
6	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-7	-7	-0.1	water	25	water	14
7	Chloroethyl dichloroacetate	'ClC(Cl)C(=O)OCCCl',	-6.2	-6.4	0.3	water	25	water	14
8	Methoxyethyl dichloroacetate	'ClC(Cl)C(=O)OCCOC',	-6.7	-6.7	0	water	25	water	14
9	Methyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OC',	-4.8	-5.5	0.7	water	25	water	3, 14
10	Methoxyethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCOC',	-5	-5.3	0.3	water	25	water	14
11	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-6	-5.9	-0.1	water	25	water	19
12	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-4.2	-4.1	-0.1	water	25	water	19
13	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-4.3	-4.2	-0.1	water	25	water	19
14	Isopropyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)C',	-4.2	-4.2	0	water	25	water	19
15	t-Butyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)(C)C',	-4.6	-4.4	-0.2	water	25	water	19
16	Chloromethyl chloroacetate	'ClCC(=O)OCCl',	-5.7	-5.6	-0.1	water	25	water	3, 14
17	Phenyl acetate	'CC(=O)Oc1ccccc1',	-9	-9.1	0.1	water	25	water	14
18	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-9.1	-9.4	0.3	water	25	water	19
19	p-Chlorophenyl acetate	'CC(=O)Oc1ccc(Cl)cc1',	-8.9	-8.9	0	water	25	water	19
20	p-Nitrophenyl acetate	'CC(=O)Oc1ccc(N(=O)=O)cc1',	-7.8	-8.2	0.4	water	25	water	19
21	3,4-Dinitrophenyl acetate	'CC(=O)Oc1cc(N(=O)=O)c(N(=O)=O)cc1',	-7.1	-7.5	0.4	water	25	water	19
22	2,4-Dinitrophenyl acetate	'CC(=O)Oc1c(N(=O)=O)cc(N(=O)=O)cc1',	-6.7	-6.5	-0.2	water	25	water	15, 51
23	2,6-Dinitrophenyl acetate	'CC(=O)Oc1c(N(=O)=O)cccc1(N(=O)=O)',	-6.6	-5.8	-0.8	water	25	water	19
24	p-Nitrophenyl chloroacetate	'ClCC(=O)Oc1ccc(N(=O)=O)cc1',	-5.2	-4.7	-0.5	water	25	water	15, 51
25	Phenyl dichloroacetate	'ClC(Cl)C(=O)Oc1ccccc1',	-4.5	-4	-0.5	water	25	water	15, 51
26	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-4.6	-4.4	-0.2	water	10	water	19
27	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-3.8	-3.5	-0.3	aniline	25	water	52
28	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-3.2	-3	-0.2	acetate	25	water	52
29	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-2	-2	0	imidazole	25	water	52
30	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-4.5	-4.5	0.1	formate	25	water	52
31	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-4.8	-4.6	-0.2	aniline	25	water	52
32	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-3.7	-3.9	0.2	pyridine	25	water	52
33	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-3.5	-3.5	0	picoline4	25	water	52
34	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-4.3	-4.1	-0.2	acetate	25	water	52
35	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-3.6	-3.7	0.1	succinate	25	water	52
36	Ethyl dichloroacetate	'ClC(Cl)C(=O)OCC',	-2.9	-3.1	0.2	imidazole	25	water	52
37	Ethyl chloroacetate	'ClCC(=O)OCC',	-6.1	-5.7	-0.4	acetate	25	water	52

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN WATER AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES string	logk	logk	Difference	Catalysts	Temperature	Solvents	References
38	Ethyl chloroacetate	'ClCC(=O)OCC',	-4.4	-4.7	0.2	imidazole	25	water	52
39	Ethyl trichloroacetate	'ClCC(=O)Oc1ccc(N(=O)=O)cc1',	-2.8	-2.3	-0.5	aniline	25	water	15
40	p-Nitrophenyl chloroacetate	'ClCC(=O)Oc1ccc(N(=O)=O)cc1',	-1.9	-1.6	-0.3	pyridine	25	water	15
41	p-Nitrophenyl chloroacetate	'ClC(Cl)C(=O)Oc1ccccc1',	0.2	-0.1	0.3	imidazole	25	water	15
43	2,6-dinitrophenyl acetate	'CC(=O)Oc1c(N(=O)=O)cccc1(N(=O)=O)',	-2.9	-2.9	0	acetate	25	water	53
44	2,4-dinitrophenyl acetate	'CC(=O)Oc1c(N(=O)=O)cc(N(=O)=O)cc1',	-3.3	-3.6	0.4	acetate	25	water	15, 53
45	2,3-dinitrophenyl acetate	'CC(=O)Oc1c(N(=O)=O)c(N(=O)=O)ccc1',	-3.6	-3.8	0.2	acetate	25	water	53
46	3,4-dinitrophenyl acetate	'CC(=O)Oc1cc(N(=O)=O)c(N(=O)=O)cc1',	-4	-4.6	0.6	acetate	25	water	53
47	p-Nitrophenyl acetate	'CC(=O)Oc1ccc(N(=O)=O)cc1',	-5.2	-5.3	0.1	acetate	25	water	53
48	o-Nitrophenyl acetate	'CC(=O)Oc1ccccc1(N(=O)=O)',	-5.3	-4.5	-0.8	acetate	25	water	53
49	m-Nitrophenyl acetate	'CC(=O)Oc1cc(N(=O)=O)ccc1',	-5.5	-5.4	0	acetate	25	water	53
50	p-Chlorophenyl acetate	'CC(=O)Oc1ccc(Cl)cc1',	-6	-6.1	0.1	acetate	25	water	53
51	p-Methylphenyl acetate	'CC(=O)Oc1ccc(C)cc1',	-6.6	-6.6	0	acetate	25	water	53

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES string	logk	logk	Difference	Catalysts	Temperature	Solvents	References
1	Chloromethyl chloroacetate	'ClCC(=O)OCCl',	-7.2	-7	-0.2	water	25	50% acetone-water	3, 14
2	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-5.3	-5.4	0.1	water	25	50% acetone-water	51
3	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.6	-6.4	0.8	water	25	70% acetone-water	14, 54
4	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-6.1	-6.5	0.3	water	25	70% acetone-water	54, 55
5	Propyl trifluoroacetate	'FC(F)(F)C(=O)OCCC',	-6.3	-6.5	0.2	water	25	70% acetone-water	54, 55
6	Butyl trifluoroacetate	'FC(F)(F)C(=O)OCCCC',	-6.4	-6.5	0.1	water	25	70% acetone-water	54, 55
7	Pentyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCC',	-6.4	-6.5	0	water	25	70% acetone-water	54, 55
8	Hexyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCCC',	-6.5	-6.5	0	water	25	70% acetone-water	54, 55
9	Isopropyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)C',	-7	-6.6	-0.4	water	25	70% acetone-water	56
10	sec-Butyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CC',	-7.2	-6.8	-0.4	water	25	70% acetone-water	56
11	sec-Pentyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCC',	-7.3	-6.9	-0.4	water	25	70% acetone-water	56
12	sec-Hexyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCCC',	-7.3	-7	-0.4	water	25	70% acetone-water	56
13	Phenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccccc1',	-3.5	-3.6	0	water	25	70% acetone-water	56
14	m-Methyl trifluoroacetate	'FC(F)(F)C(=O)Oc1cc(C)ccc1',	-3.7	-3.7	0	water	25	70% acetone-water	56
15	p-Methyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccc(C)cc1',	-3.8	-3.9	0.1	water	25	70% acetone-water	56
16	o-Methyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccccc1C',	-4.1	-3.7	-0.3	water	25	70% acetone-water	56
17	Ethyl pentafluoroacetate	'FC(F)(F)C(F)(F)C(=O)OCC',	-7.3	-8	0.7	water	25	70% acetone-water	54, 55
18	Ethyl heptafluoropropionate	'FC(F)(F)C(F)(F)C(F)(F)C(=O)OCC',	-7.6	-8.3	0.7	water	25	70% acetone-water	54, 55
19	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-6.3	-6	-0.3	water	-6.23	50% acetone-water	51
20	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-6.1	-5.9	-0.2	water	0	50% acetone-water	51
21	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-5.9	-5.8	-0.1	water	5	50% acetone-water	51
22	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-5.7	-5.7	0	water	12	50% acetone-water	51
23	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-5.5	-5.5	0.1	water	18	50% acetone-water	51
24	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-5	-5.3	0.2	water	35	50% acetone-water	51
25	Chloromethyl dichloroacetate	'ClC(Cl)C(=O)OCCl',	-4.8	-5.1	0.3	water	45	50% acetone-water	51
26	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-4.6	-4.4	-0.2	water	10	70% acetone-water	55
27	Isopropyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)C',	-6.7	-6.4	-0.3	water	35	70% acetone-water	56
28	Isopropyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)C',	-6.5	-6.2	-0.3	water	45	70% acetone-water	56
29	sec-Butyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CC',	-6.9	-6.6	-0.3	water	35	70% acetone-water	56
30	sec-Butyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CC',	-6.7	-6.5	-0.2	water	45	70% acetone-water	56
31	sec-Pentyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCC',	-7.1	-6.7	-0.4	water	35	70% acetone-water	56
32	sec-Pentyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCC',	-6.9	-6.5	-0.3	water	45	70% acetone-water	56
33	sec-Hexyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCCC',	-7.1	-6.8	-0.3	water	35	70% acetone-water	56
34	sec-Hexyl trifluoroacetate	'FC(F)(F)C(=O)OC(C)CCCC',	-6.8	-6.6	-0.3	water	45	70% acetone-water	56
35	Phenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccccc1',	-3.3	-3.5	0.1	water	35	70% acetone-water	56
36	Phenyl trifluoroacetat	'FC(F)(F)C(=O)Oc1ccccc1',	-3.2	-3.4	0.2	water	45	70% acetone-water	56
37	m-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1cc(C)ccc1',	-3.6	-3.6	0.1	water	35	70% acetone-water	56

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN ACETONE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES string	logk	logk	Difference	Catalysts	Temperature	Solvents	References
38	m-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1cc(C)ccc1',	-3.4	-3.6	0.1	water	45	70% acetone-water	56
39	p-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccc(C)cc1',	-3.7	-3.8	0.1	water	35	70% acetone-water	56
40	p-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccc(C)cc1',	-3.5	-3.7	0.2	water	45	70% acetone-water	56
41	o-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccccc1C',	-3.9	-3.7	-0.2	water	35	70% acetone-water	56
42	o-Methylphenyl trifluoroacetate	'FC(F)(F)C(=O)Oc1ccccc1C',	-3.7	-3.6	-0.2	water	45	70% acetone-water	56
43	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.4	-6.2	0.7	water	35	70% acetone-water	54, 55
44	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.3	-6	0.7	water	45	70% acetone-water	54, 55
45	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-6	-6.3	0.3	water	35	70% acetone-water	54, 55
46	Ethyl trifluoroacetate	'FC(F)(F)C(=O)OCC',	-5.8	-6.1	0.3	water	45	70% acetone-water	54, 55
47	Propyl trifluoroacetate	'FC(F)(F)C(=O)OCCC',	-6.1	-6.3	0.2	water	35	70% acetone-water	54, 55
48	Propyl trifluoroacetate	'FC(F)(F)C(=O)OCCC',	-5.9	-6.1	0.2	water	45	70% acetone-water	54, 55
49	Butyl trifluoroacetate	'FC(F)(F)C(=O)OCCCC',	-6.2	-6.3	0.1	water	35	70% acetone-water	54, 55
50	Butyl trifluoroacetate	'FC(F)(F)C(=O)OCCCC',	-6	-6.1	0.1	water	45	70% acetone-water	54, 55
51	Pentyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCC',	-6.3	-6.3	0	water	35	70% acetone-water	54, 55
52	Pentyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCC',	-6	-6.1	0.1	water	45	70% acetone-water	54, 55
53	Hexyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCCC',	-6.3	-6.3	0	water	35	70% acetone-water	54, 55
54	Hexyl trifluoroacetate	'FC(F)(F)C(=O)OCCCCCC',	-6.1	-6.1	0	water	45	70% acetone-water	54, 55
55	Ethyl pentafluoroacetate	'FC(F)(F)C(F)(F)C(=O)OCC',	-7.1	-7.8	0.7	water	35	70% acetone-water	54, 55
56	Ethyl pentafluoroacetate	'FC(F)(F)C(F)(F)C(=O)OCC',	-6.8	-7.6	0.8	water	45	70% acetone-water	54, 55
57	Ethyl heptafluoroacetate	'FC(F)(F)C(F)(F)C(F)(F)C(=O)OCC',	-7.4	-8.1	0.7	water	35	70% acetone-water	54, 55
58	Ethyl heptafluoroacetate	'FC(F)(F)C(F)(F)C(F)(F)C(=O)OCC',	-7.1	-7.9	0.8	water	45	70% acetone-water	54, 55
59	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.4	-8	-0.4	water	35	36% acetone-water	50
60	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.8	-8.3	-0.5	water	35	44% acetone-water	50
61	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-9.1	-8.7	-0.5	water	35	53% acetone-water	50
62	Ethyl dibromoacetate	BrC(Br)C(=O)OCC',	-10.5	-10	-0.5	water	35	83% acetone-water	50
63	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-9.6	-9.1	-0.5	water	35	63% acetone-water	50
64	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.2	-7.8	-0.4	water	45	36% acetone-water	50
65	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.6	-8.1	-0.5	water	45	44% acetone-water	50
66	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.9	-8.4	-0.5	water	45	53% acetone-water	50
67	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-9.2	-8.8	-0.4	water	45	63% acetone-water	50
68	Ethyl dibromoacetate	BrC(Br)C(=O)OCC',	-10.2	-9.7	-0.5	water	45	83% acetone-water	50
69	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.1	-7.7	-0.4	water	51	36% acetone-water	50
70	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.4	-7.9	-0.5	water	51	44% acetone-water	50
71	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-8.7	-8.3	-0.5	water	51	53% acetone-water	50
72	Ethyl dibromoacetate	'BrC(Br)C(=O)OCC',	-9.1	-8.6	-0.5	water	51	63% acetone-water	50
73	Ethyl dibromoacetate	BrC(Br)C(=O)OCC',	-10	-9.5	-0.5	water	51	83% acetone-water	50

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN ETHANOL-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES string	logk	logk	Difference	Catalysts	Temperature	Solvents	References
1	Ethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCC',	-6.3	-6.3	0	water	25	40% ethanol-water	52
2	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-5.8	-5.9	0.1	water	25	3% ethanol-water	52
3	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-5.9	-6	0.1	water	25	7 % ethanol-water	52
4	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-6	-6.1	0.1	water	25	12% ethanol-water	52
5	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-6.3	-6.2	0	water	25	22% ethanol-water	52
6	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-6.4	-6.4	0	water	25	32% ethanol-water	52
7	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-6.8	-6.8	0	water	25	52% ethanol-water	52
8	Ethyl difluoroacetate	'FC(F)C(=O)OCC',	-7.1	-7.1	0.1	water	25	72% ethanol-water	52
9	Ethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCC',	-3.7	-3.4	-0.2	acetate	25	40% ethanol-water	52

	TABLE 7: GENERAL BASE HYDROLYSIS OF ESTERS IN DIOXANE-WATER MIXED SOLVENTS AT VARIOUS TEMPERATURE								
			observed	calculated					
	Esters	SMILES	logk	logk	Difference	Catalysts	Temperature	Solvents	References
1	Mehtyl trichloroacetate	'ClC(Cl)C(=O)OCC(Cl)(Cl)Cl',	-6.3	-7.7	1.4	water	25	50% dioxane-water	3, 14
2	Trichloroethyl dichloroacetate	'ClC(Cl)(Cl)C(=O)OC',	-6.3	-6.6	0.3	water	25	50% dioxane-water	3, 14
3	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.3	-5.5	0.1	water	25	60% dioxane-water	3, 14
4	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.7	-5.8	0	water	10	70% dioxane-water	3, 14
5	Ethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCC',	-7	-6.7	-0.3	water	25	50% dioxane-water	14
6	Propyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCC',	-7.2	-6.7	-0.5	water	25	50% dioxane-water	14
7	Butyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCCC',	-7.2	-6.8	-0.4	water	25	50% dioxane-water	14
8	Isopropyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OC(C)C',	-7.8	-6.9	-1	water	25	50% dioxane-water	14
9	Chloroethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCCl',	-6.1	-6.2	0.1	water	25	50% dioxane-water	14
10	Methoxyethyl trichloroacetate	'ClC(Cl)(Cl)C(=O)OCCOC',	-6.6	-6.4	-0.1	water	25	50% dioxane-water	14
11	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.3	-5.5	0.1	water	25	60% dioxane-water	14
12	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.7	-5.8	0	water	25	70% dioxane-water	14
13	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-6.5	-6.2	-0.2	water	0	70% dioxane-water	57
14	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.4	-5.4	0.1	water	44.6	70% dioxane-water	57
15	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-6	-5.9	-0.1	water	0	60% dioxane-water	57
16	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-5.1	-5.3	0.2	water	34.8	60% dioxane-water	57
17	Methyl trifluoroacetate	'FC(F)(F)C(=O)OC',	-4.9	-5.2	0.3	water	44.6	60% dioxane-water	57

TABLE 8: HYDRATION OF ALDEHYDES/KETONES IN WATER AT ROOM TEMPERATURE						
			Observed	Calculated	Differenc	References
	Names of Compounds	SMILES string	pK(hyd.)	pK(hyd.)		
1	Formaldehyde	'OZ=C',	-3.3	-3.3	0	5,6
2	Ethanal	'OZ=CC',	-0.1	-0.2	0.1	5,6
3	Propanal	'OZ=CCC',	0.2	0	0.2	5,6
4	Isobutanal	'OZ=CC(C)C',	0.4	0.3	0.1	5,6
5	Butanal	'OZ=CCCC',	0.3	0.1	0.2	5,6
6	Pivaldehyde	'OZ=CC(C)(C)C',	0.6	0.9	-0.3	5,6
7	Chloroethanal	'ClCC=OZ',	-1.6	-1.7	0.1	5,6
8	Trichloroethanal	'ClC(Cl)(Cl)C=OZ',	-4.5	-4.2	-0.3	5,6
9	acetone	'CC(=OZ)C',	2.7	2.8	-0.1	5
10	Diacetyl	'OZ=C(C)C(=O)C',	-0.3	-0.3	0	5
11	Methyl chloroethanone	'ClCC(=OZ)C',	1	1.1	-0.1	5
12	Methyl dichloroethanone	'ClC(Cl)C(=OZ)C',	-0.5	-1	0.6	5
13	Chloromethyl chloroethanone	'ClCC(=OZ)CCl',	-1	-1.1	0.1	5
14	Methyl pyruvate	'OZ=C(C)C(=O)OC',	-0.5	-0.5	0	5
15	Me2CH2(C=O)COOH	'O=C(O)C(=OZ)C(C)C',	0	0	0	5
16	Benzaldehyde	'OZ=Cc1ccccc1',	2	2.1	-0.1	5
17	m-Chlorrobenzaldehyde	'OZ=Cc1cc(Cl)ccc1',	1.7	1.5	0.2	5
18	p-Chlorobenzaldehyde	'OZ=Cc1ccc(Cl)cc1',	1.8	1.7	0.1	5
19	m-Nitrobenzaldehyde	'OZ=Cc1cc(N(=O)=O)ccc1',	1	0.9	0.1	5
20	p-Nitrobenzaldehyde	'OZ=Cc1ccc(N(=O)=O)cc1',	0.8	0.7	0	5
21	3,5-Dinitrobenzaldehyde	'OZ=Cc1cc(N(=O)=O)cc(N(=O)=O)c1	-0.3	-0.1	-0.3	5
22	3-Nitro,4-chlorobenzaldehyde	'OZ=Cc1cc(N(=O)=O)c(Cl)cc1',	0.8	0.5	0.2	5
23	p-Trifluorobenzaldehyde	'OZ=Cc1ccc(C(F)(F)F)cc1',	1.3	1.4	-0.2	5
24	2-Chloro-isobutanal	'OZ=CC(Cl)(C)C',	-0.7	-0.4	-0.3	5
25	2-Dibromo-butanal	'OZ=CC(Br)(Br)CC',	-1	-1.2	0.2	5
26	2-Bromo-heptanal	'OZ=CC(Br)CCCCC',	-0.5	-0.4	-0.1	5
27	2-Chloro-butanal	'OZ=CC(Cl)CC',	-1.2	-1	-0.2	5
28	2-Chloro-heptanal	'OZ=CC(Cl)CCCCC',	-0.8	-0.8	0	5
29	2-Bromo-butanal	'OZ=CC(Br)CC',	-0.6	-0.5	0	5
30	3,4-hexanedione	'CCC(=OZ)C(=O)CC',	-0.3	-0.2	-0.1	5
31	acetylbenzoyl	'CC(=OZ)C(=O)c1ccccc1',	-0.2	0.3	-0.5	5
32	2-pyridine-aldehyde	'n1c(C=OZ)cccc1',	-1.9	-0.9	-0.9	17,18
33	3-pyridine-aldehyde	'n1cc(C=OZ)ccc1',	-0.7	-1.4	0.7	17,18
34	4-pyridine-aldehyde	'n1ccc(C=OZ)cc1',	-1.7	-1.7	0	17,18
35	Ethyl pyruvate	'CC(=OZ)C(=O)OCC',	-0.4	-0.5	0.1	17,18
36	9-acridine-aldehyde	'c1cc2nc3ccccc3c(C=OZ)c2cc1',	-0.4	-1.1	0.7	17,18

TABLE 9: HYDRATION OF QUINAZOLINES IN WATER AT ROOM TEMPERATURE						
			Observed	Calculated		
	Quinazolines	SMILES	value	value	Difference	References
1	Quinazoline (Unsubstituted)	'n(cc1cc2)cnc1cc2',	4.3	4	0.3	8
2	2-Methyl quinazoline	'n(cc1cc2)c(C)nc1cc2',	3.8	4.3	-0.5	8
3	2-Ethyl quinazoline	'n(cc1cc2)c(CC)nc1cc2',	3.9	4.1	-0.2	8
4	2-Isopropyl quinazoline	'n(cc1cc2)c(C(C)C)nc1cc2',	4.1	3.8	0.3	8
5	2-t-Butyl quinazoline	'n(cc1cc2)c(C(C)(C)C)nc1cc2',	4.2	4	0.2	8
6	5-Methyl quinazoline	'n(cc1c(C)c2)cnc1cc2',	4.3	4.7	-0.4	8
7	7-Methyl quinazoline	'n(cc1cc2)cnc1cc2C',	4.8	4.8	0	8
8	8-Methyl quinazoline	'n(cc1cc2)cnc1c(C)c2',	4.7	4.4	0.3	8
9	5-Methoxy quinazoline	'n(cc1c(OC)c2)cnc1cc2',	4.3	4.6	-0.2	8
10	6-Methoxy quinazoline	'n(cc1cc2(OC))cnc1cc2',	5.3	4.9	0.4	8
11	7-Methoxy quinazoline	'n(cc1cc2)cnc1cc2OC',	5.7	5	0.7	8
12	8-Methoxy quinazoline	'n(cc1cc2)cnc1c(OC)c2',	4.3	4.2	0.1	8
13	5-Chloro quinazoline	'n(cc1c(Cl)c2)cnc1cc2',	3.2	3.4	-0.2	8
14	6-Chloro quinazoline	'n(cc1cc2(Cl))cnc1cc2',	3.6	3.6	0	8
15	7-Chloro quinazoline	'n(cc1cc2)cnc1cc2Cl',	3.7	3.6	0.1	8
16	8-Chloro quinazoline	'n(cc1cc2)cnc1c(Cl)c2',	3.3	3.2	0	8
17	5-Fluoro quinazoline	'n(cc1c(F)c2)cnc1cc2',	3	3.5	-0.5	8
18	6-Fluoro quinazoline	'n(cc1cc2(F))cnc1cc2',	3.8	3.7	0.1	8
19	7-Fluoro quinazoline	'n(cc1cc2)cnc1cc2F',	4	3.7	0.3	8
20	5-Nitro quinazoline	'n(cc1c(N(=O)=O)c2)cnc1cc2',	2.7	2.6	0	8
21	6-Nitro quinazoline	'n(cc1cc2(N(=O)=O))cnc1cc2',	2.8	2	0.8	8
22	7-Nitro quinazoline	'n(cc1cc2)cnc1cc2N(=O)=O',	2.1	2.3	-0.2	8
23	8-Nitro quinazoline	'n(cc1cc2)cnc1c(N(=O)=O)c2',	2	2.5	-0.5	8
24	5-Trifluoro quinazoline	'n(cc1c(C(F)(F)F)c2)cnc1cc2',	3.7	3.1	0.6	8
25	6-Trifluoro quinazoline	'n(cc1cc2(C(F)(F)F))cnc1cc2',	2.8	3.7	-0.9	8
26	7-Trifluoro quinazoline	n(cc1cc2)cnc1cc2C(F)(F)F',	3	3.9	-0.9	8
27	8-Trifluoro quinazoline	'n(cc1cc2)cnc1c(C(F)(F)F)c2',	3.6	3	0.6	8

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