Supporting Information

Enhancing the Kinetics of Hydrazone Exchange Processes: An Experimental and Computational Study

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General Experimental: All chemicals, including Girard's reagent T (**R1**) were purchased from Sigma-Aldrich or Alfa Aesar and were used as received without further purification. ^{1}H and ^{13}C NMR spectra of synthesised compounds were recorded on a Bruker Avance 300 spectrometer (at 300 and 75 MHz respectively), Bruker Avance 400 spectrometer (at 400 MHz and 100 MHz, respectively), or a Bruker Avance III HD spectrometer (at 500 MHz and 125 MHz, respectively). High-resolution mass spectrometry was performed on a Waters LCT Premier mass spectrometer$^{\alpha}$ or an Agilent 6550 iFunnel Q-TOF LC/MS$^{\beta}$.

Synthetic Procedures:

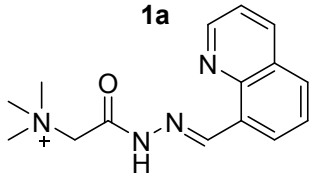
General Procedure for Preparation of Hydrazone Compounds (1a-1g): Aromatic aldehyde (1.00 eqv.) was dissolved in MeOH (2.5 mL) and stirred at rt. Girard's Reagent T (0.9 eqv) was dissolved in MeOH (2.5 mL), then added in one portion to the aldehyde solution. Reactions were judged complete by TLC (7:2 MeOH/2M H_4NCl), evaporated to dryness and the crude residue washed with dichloromethane (7 mL) and sonicated for 5 min. The final products were isolated by filtration and dried for 30 min under high vacuum.

Characterization of Hydrazones 1a-1g:

^{1}H AND ^{13}C NMR spectra of compounds **1a-1g** appear complex on account of *syn*/*anti* isomerization about the C-N amide bond that exhibits hindered rotation, consistent with previous literature reports.[1] The syn/anti ratio was typically in the range 50:50 to 30:70, with the *anti*-isomer being the preferred conformer in most cases.

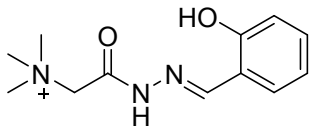
N,N,N-trimethyl-2-oxo-2-(2-(quinolin-8-ylmethylene)hydrazineyl)ethan-1-aminium (**1a**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.81 + 8.64 (1H, s, Ar-*H*C=N-, *anti* + *syn*), 8.75 + 8.68 (1H, d, Ar, *anti* + *syn*), 8.36 + 8.25 (1H, d, Ar, *anti* + *syn*), 8.10 (1H, d, Ar), 7.96 + 7.87 (1H, d, Ar, *anti* + *syn*), 7.55 (2H, m, Ar), 4.74 + 4.31 (1H, s, -C=N-N-CH_2-, *syn* + *anti*), 3.43 (9H, s, -N(Me)$_3$). ^{13}C NMR (101 MHz, D_2O) δ 160.91, 150.23, 149.58, 149.30, 147.38, 144.24, 131.94, 131.15, 128.40, 127.05, 126.55, 122.05, 121.87, 63.98, 62.90, 54.49, 54.40. HRMS$^+$ $C_{15}H_{19}N_4O^+$, Theoretical: 271.1559 Actual: 271.1556$^{\beta}$. mp. 159 °C.

1a



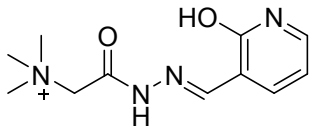
2-(2-(2-hydroxybenzylidene)hydrazineyl)-N,N,N-trimethyl-2-oxoethan-1-aminium (**1b**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.12 + 7.95 (1H, s, Ar-*H*C=N-, *anti* + *syn*), 7.35 (2H, m, Ar), 6.89 (2H, m, Ar) 4.54 + 4.12 (2H, s, -C=N-N-CH_2-, *syn* + *anti*), 3.30 + 3.28 ((9H, s, -N(Me)$_3$). ^{13}C NMR (101 MHz, D2O) δ 164.70, 160.08, 156.67, 155.87, 152.76, 148.08, 132.91, 132.53, 131.07, 129.93, 120.64, 120.47, 118.24, 117.48, 116.46, 116.33, 63.88, 62.58, 54.47. HRMS$^+$ $C_{12}H_{18}N_3O_2^+$, Theoretical: 236.1399, Actual: 236.1409.$^{\beta}$ mp. 206 °C.

1b



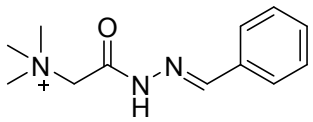
2-(2-((2-hydroxypyridin-3-yl)methylene)hydrazineyl)-N,N,N-trimethyl-2-oxoethan-1-aminium (**1c**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.35 + 8.10 (1H, s, Ar-*H*C=N-, *anti* + *syn*), 8.25 + 8.20 (1H, d, Ar, *anti* + *syn*) 7.71 + 7.65 (1H, d, Ar, *anti* + *syn*), 6.65 (1H, m, Ar), 4.74 + 4.26 (2H, s, -CH_2-N(Me)$_3$, *syn* + *anti*) 3.40 (9H, -CH$_2$-N(CH_3)$_3$. ^{13}C NMR (75 MHz, D2O) δ 165.59, 162.75, 162.70, 160.84, 147.22, 142.60, 141.24, 140.58, 138.26, 137.44, 122.79, 122.24, 108.96, 63.99, 62.82, 54.43, 54.32. HRMS$^+$ $C_{11}H_{17}N_4O_2^+$, Theoretical: 237.1232, Actual: 237.1345.$^{\beta}$ mp. 159 °C.

1c



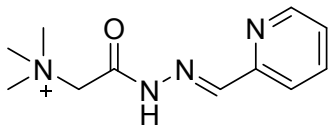
2-(2-benzylidenehydrazineyl)-N,N,N-trimethyl-2-oxoethan-1-aminium (**1d**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.18 + 7.95 (1H, s, Ar-*H*C=N-, *anti* + *syn*), 7.70 + 7.67 (2H, d, *anti* + *syn*), 7.43 (3H, m, Ar), 4.65 + 4.15 (2H, s, -C=N-N-C*H*$_2$-, *syn* + *anti*), 3.30 + 3.29 (9H, s, -N(Me)$_3$). ^{13}C NMR (101 MHz, D2O) δ 165.61, 160.81, 153.19, 148.32, 133.08, 132.47, 131.74, 131.06, 129.09, 128.99, 127.95, 127.44, 64.06, 62.88, 54.45. HRMS$^+$ $C_{12}H_{18}N_3O^+$, Theoretical: 220.1432, Actual: 220.1450.$^{\alpha}$ mp. 175 °C.

1d



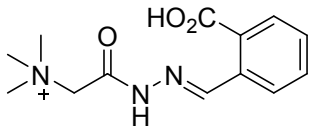
N,N,N-trimethyl-2-oxo-2-(2-(pyridin-2-ylmethylene)hydrazineyl)ethan-1-aminium (**1e**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.57 (1H, dd, Ar), 8.23 + 8.04 (1H, s, Ar-C*H*=N-N, *anti* + *syn*), 7.95 (2H, m, Ar) 7.51 (1H, dd, Ar), 4.29 (2H, s, -C=N-N-C*H*$_2$-, *anti*), 3.39 (9H, s, -N(Me)$_3$). ^{13}C NMR (101 MHz, D_2O) δ 166.11, 161.38, 150.80, 150.65, 150.60, 149.22, 149.11, 146.17, 138.39, 126.02, 125.63, 122.85, 122.55, 63.87, 62.85, 54.47, 54.34. HRMS$^+$ $C_{11}H_{17}N_4O^+$, Theoretical: 221.1402, Actual: 221.1393.$^{\alpha}$ mp. 190 °C.

1e



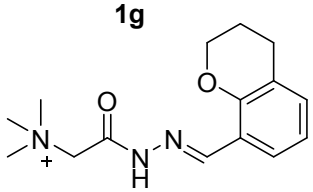
2-(2-(2-carboxybenzylidene)hydrazineyl)-N,N,N-trimethyl-2-oxoethan-1-aminium (**1f**) ^{1}H NMR (D_2O, 400 MHz, ppm) 8.34r + 8.28 (1H, s, br, Ar-HC=N-, *anti* + *syn*), 7.90-7.42 (4H, m, Ar), 4.66 + 4.13 (2H, s, -C=N-N-C*H*$_2$-, *syn* + *anti*), 3.38 + 3.28 (9H, s, -N(Me)$_3$). ^{13}C NMR (101 MHz, D2O) δ 171.26, 161.57, 146.74, 135.37, 133.19, 131.82, 131.07, 130.56, 129.38, 126.67, 63.94, 62.80, 54.33. HRMS$^+$ $C_{13}H_{18}N_3O_3^+$, Theoretical: 264.1348, Actual: 264.1355.$^{\beta}$ mp. 162 °C.

1f



2-(2-(chroman-8-ylmethylene)hydrazineyl)-N,N,N-trimethyl-2-oxoethan-1-aminium (**1g**) ^{1}H NMR (D_2O, 300 MHz, ppm) 8.48 + 8.21 (1H, s Ar-HC=N-, *anti* + *syn*), 7.64 (1H, d, Ar), 7.23 (1H, d, Ar), 6.94 (1H, dd, Ar), 4.67 + 4.21 (2H, s, -C*H*$_2$-N(Me)$_3$, *syn* + *anti*), 4.24 (2H, t, -OC*H*$_2$-), 2.77 (2H, t, -OCH$_2$-CH$_2$-C*H*$_2$-), 1.98 (2H, t, -OCH$_2$-C*H*$_2$-CH$_2$-). ^{13}C NMR (75 MHz, D2O) δ 165.28, 160.41, 153.99, 153.54, 148.98, 144.14, 133.58, 132.86, 124.62, 124.20, 120.48, 120.38, 119.87, 67.23, 64.06, 62.82, 54.41, 54.33, 24.05, 21.41, 21.34. HRMS$^+$ $C_{15}H_{22}N_3O_2^+$, Theoretical: 276.1721, Actual: 276.1712.$^{\beta}$ mp. 173 °C.

1g



^{1}H NMR Spectra:

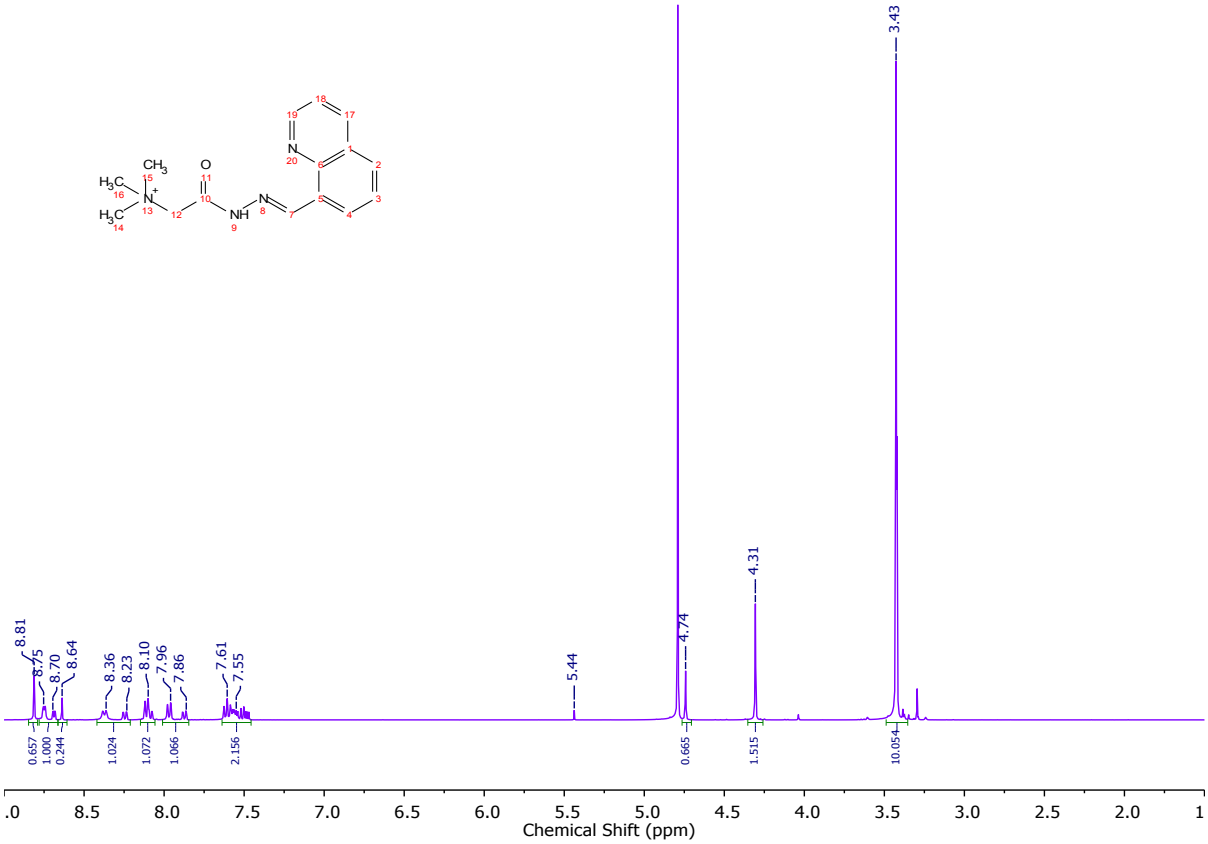


Figure S1A: ^{1}H NMR spectrum (400 MHz, D_2O) of **1a**

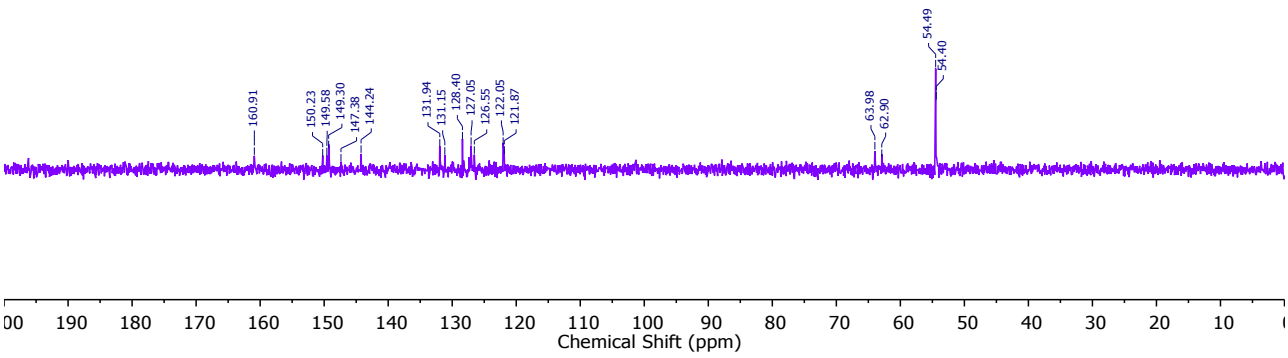


Figure S1B: ^{13}C NMR spectrum (400 MHz, D_2O) of **1a**

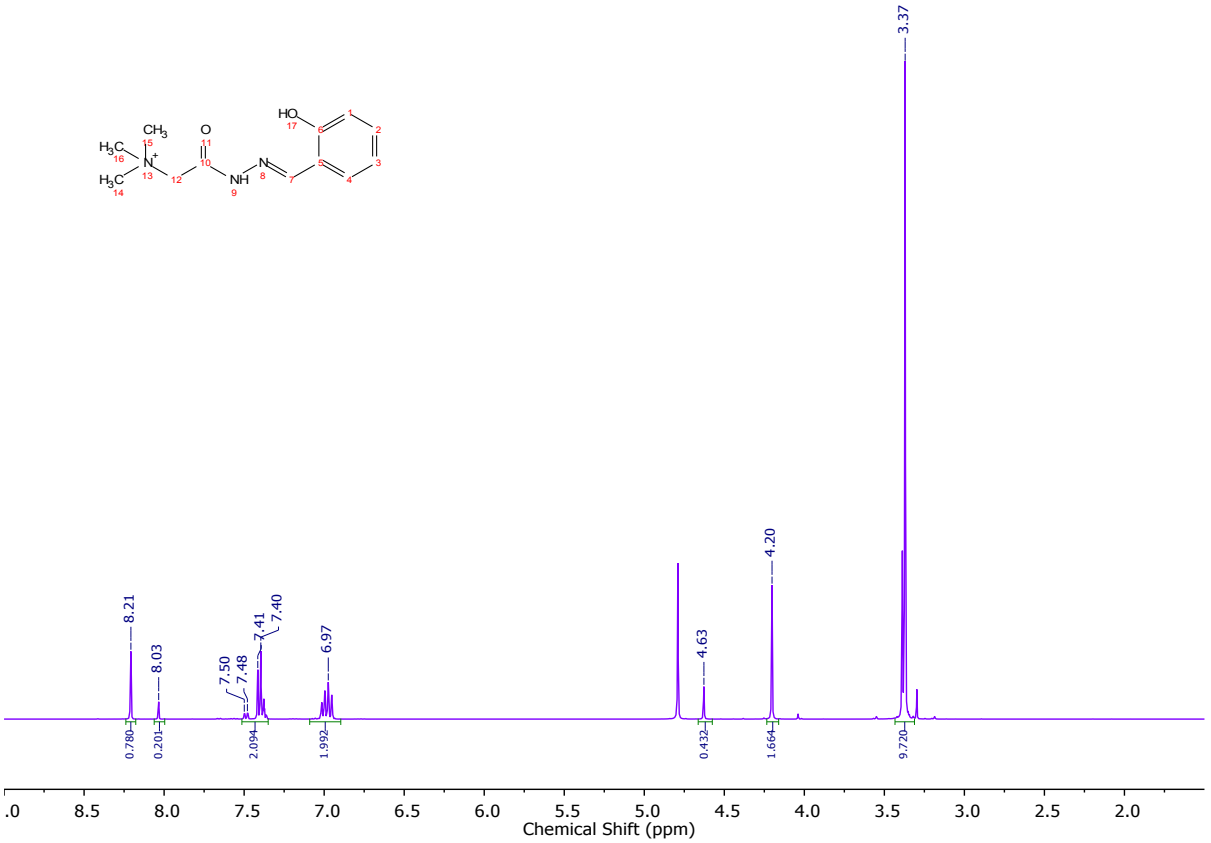


Figure S2A: ^{1}H NMR spectrum (400 MHz, D_2O) of **1b**

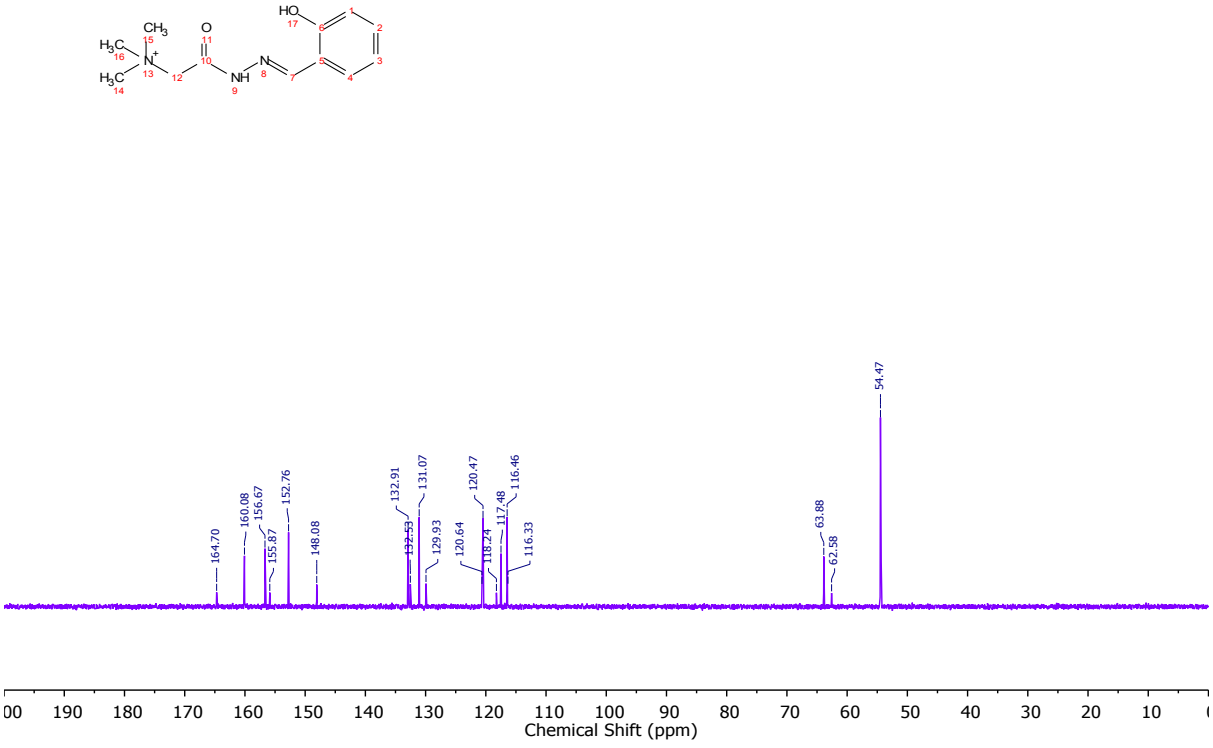


Figure S2B: ^{13}C NMR spectrum (400 MHz, D_2O) of **1b**

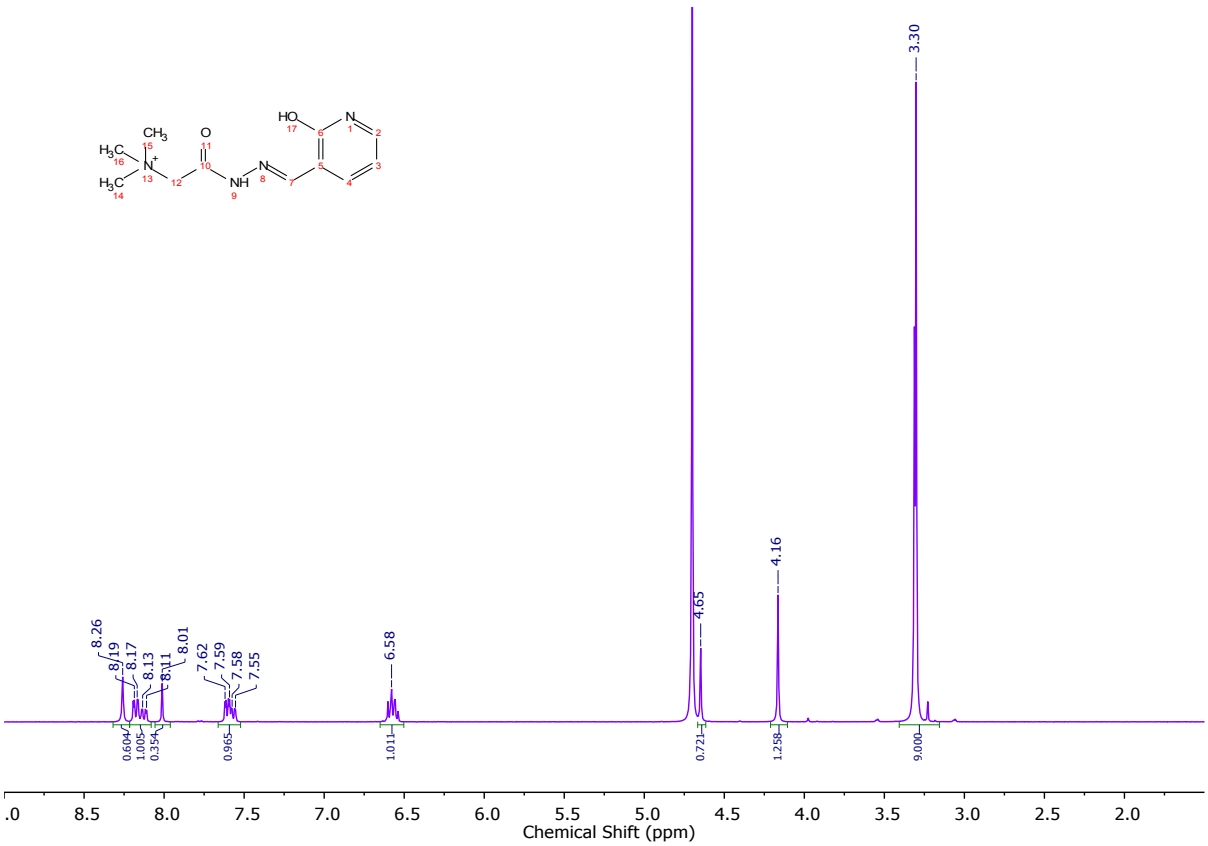


Figure S3A: ^{1}H NMR spectrum (300 MHz, D_2O) of **1c**

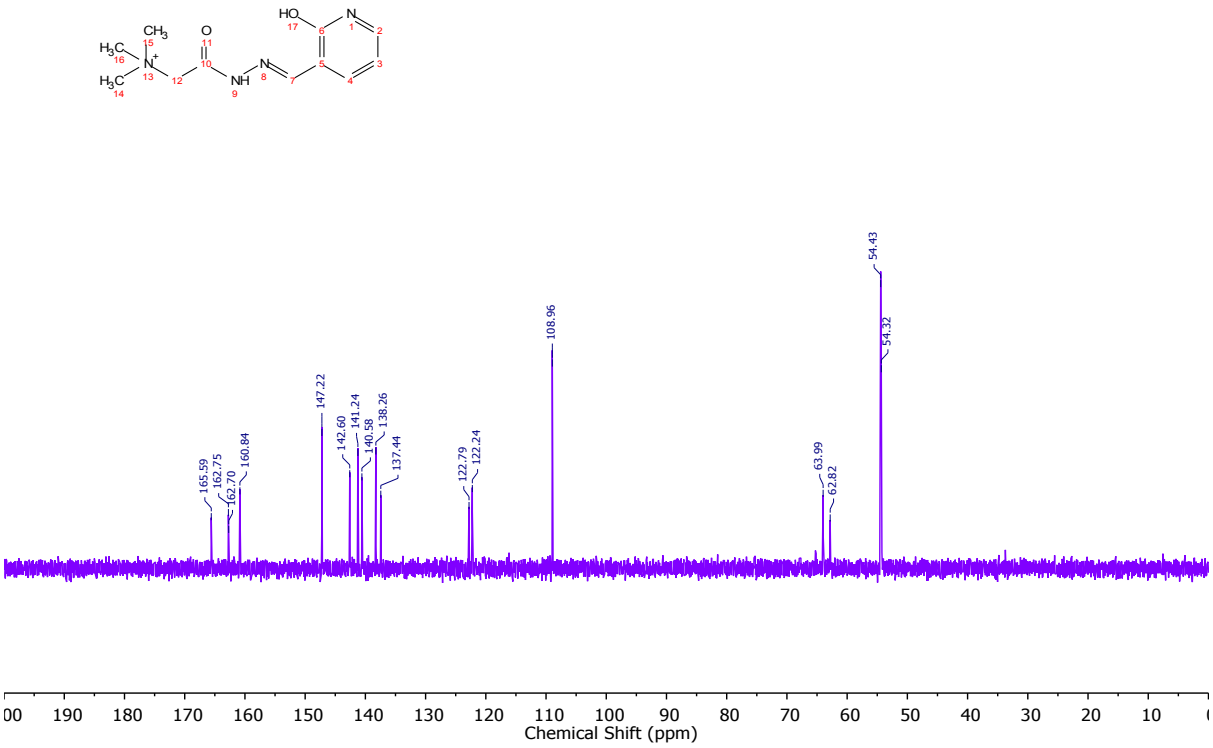


Figure S3B: ^{13}C NMR spectrum (300 MHz, D_2O) of **1c**

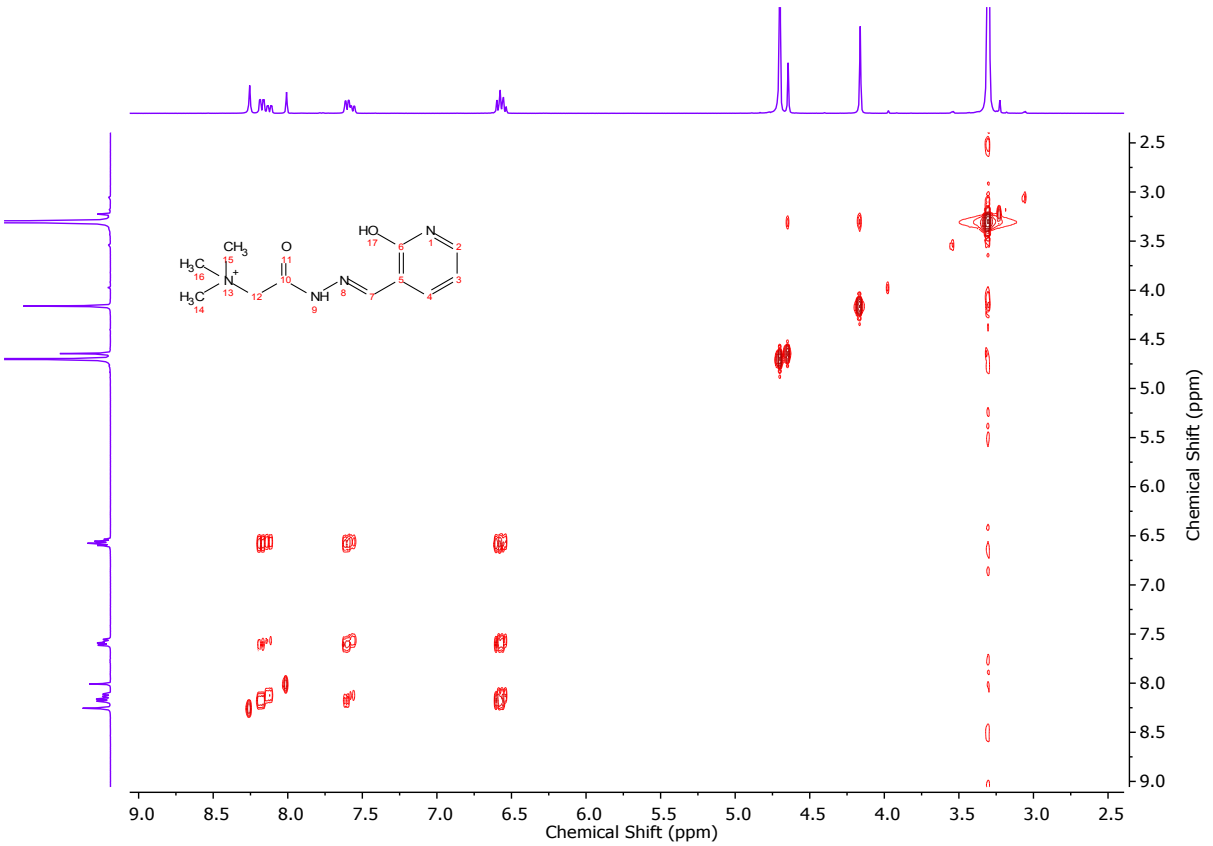


Figure S3C: COSY NMR spectrum (300 MHz, D_2O) of **1c**

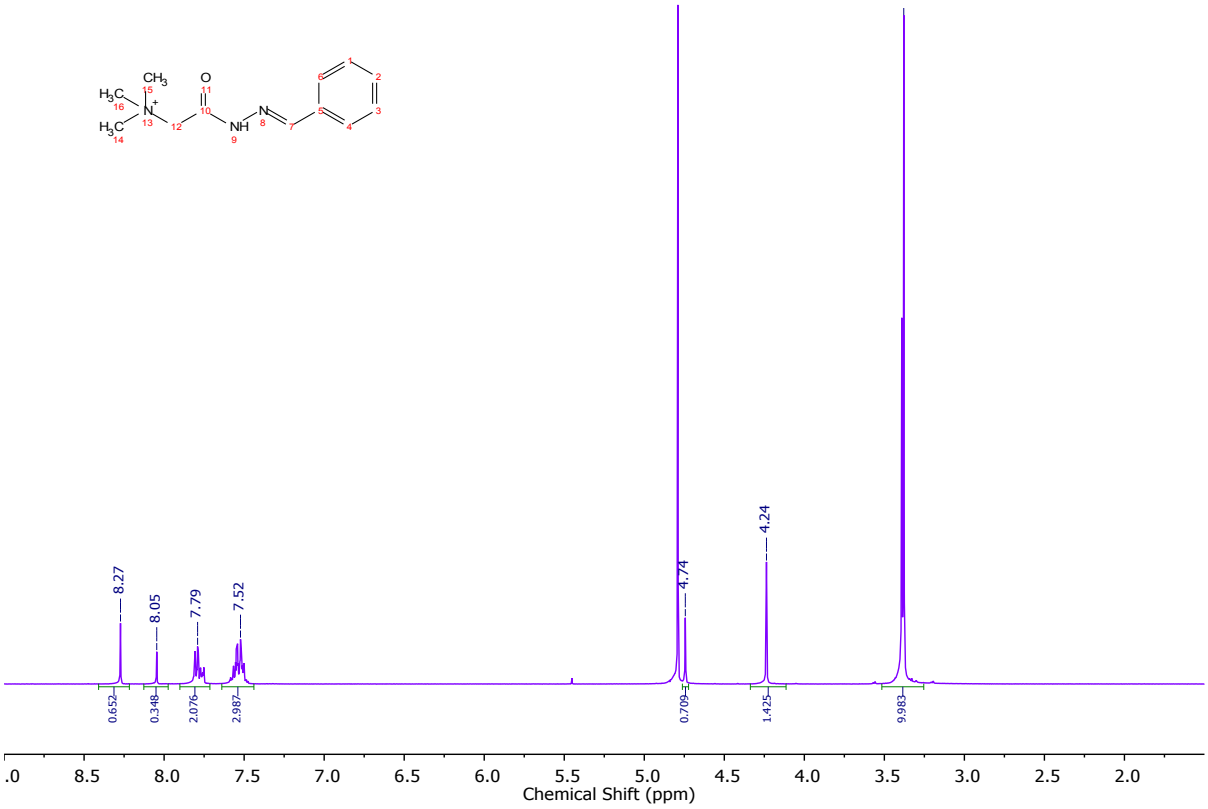


Figure S4A: ^1H NMR spectrum (400 MHz, D_2O) of **1d**

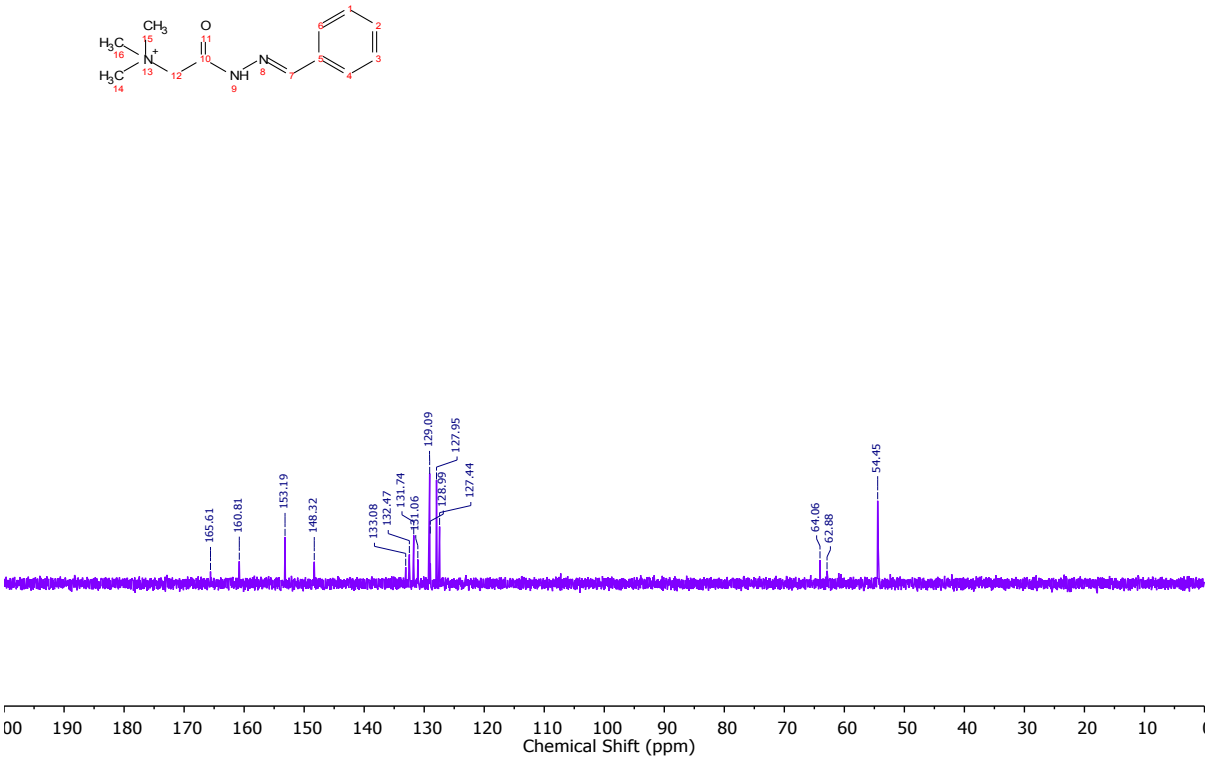


Figure S4B: ^{13}C NMR spectrum (400 MHz, D_2O) of **1d**

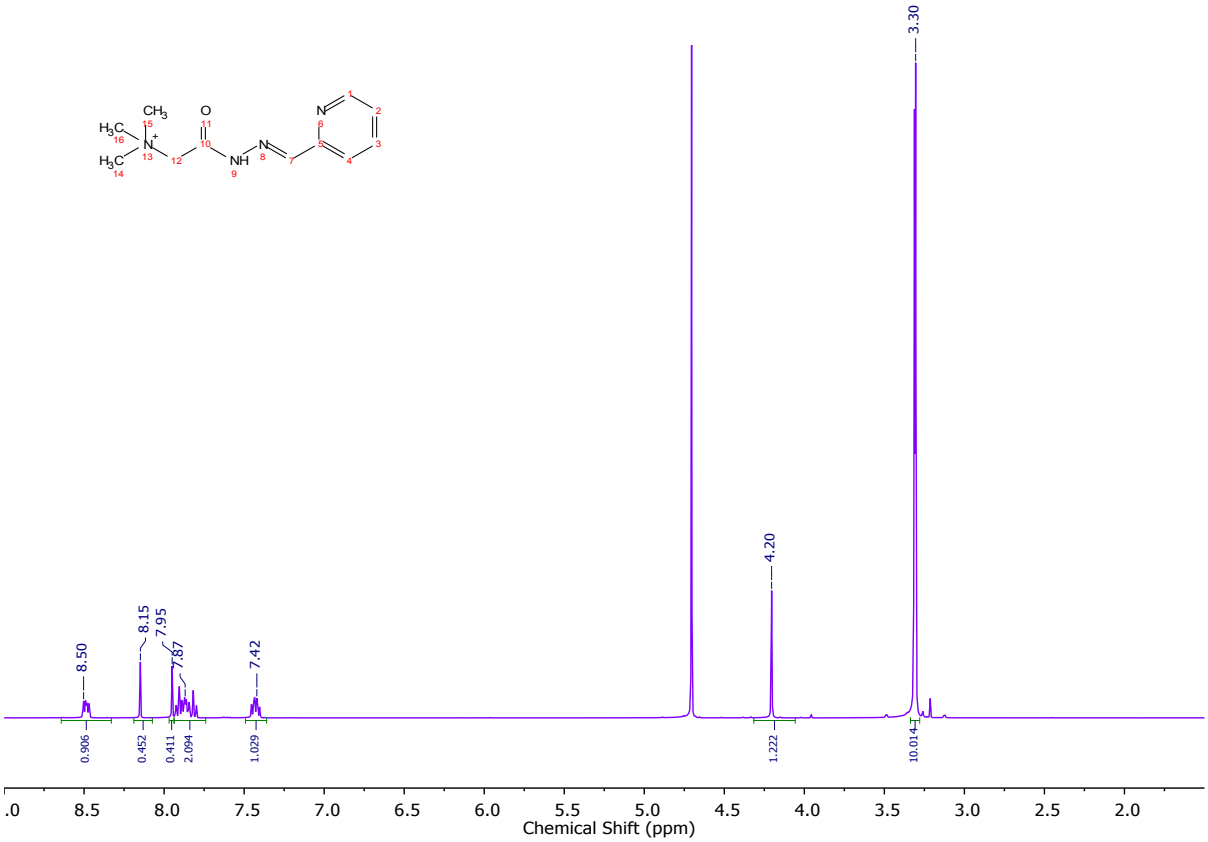


Figure S5A: ^{1}H NMR spectrum (400 MHz, D_2O) of **1e**

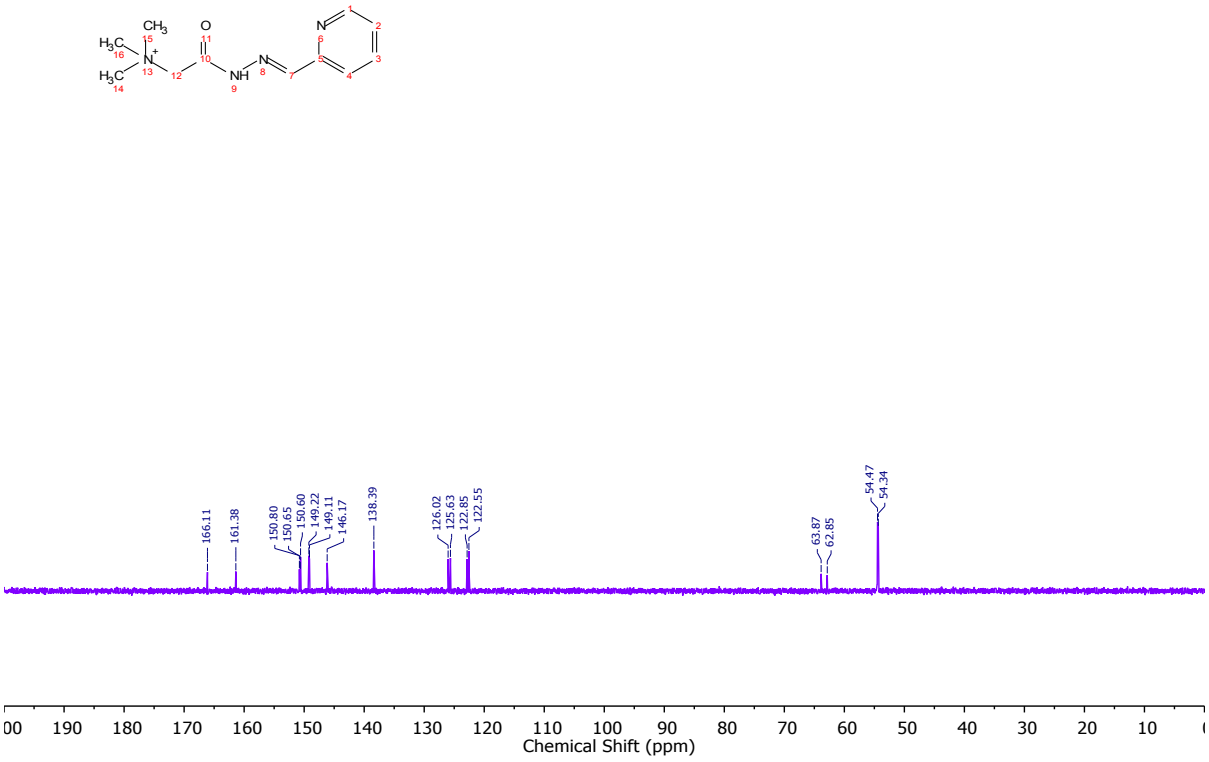


Figure S5B: ^{13}C NMR spectrum (400 MHz, D_2O) of **1e**

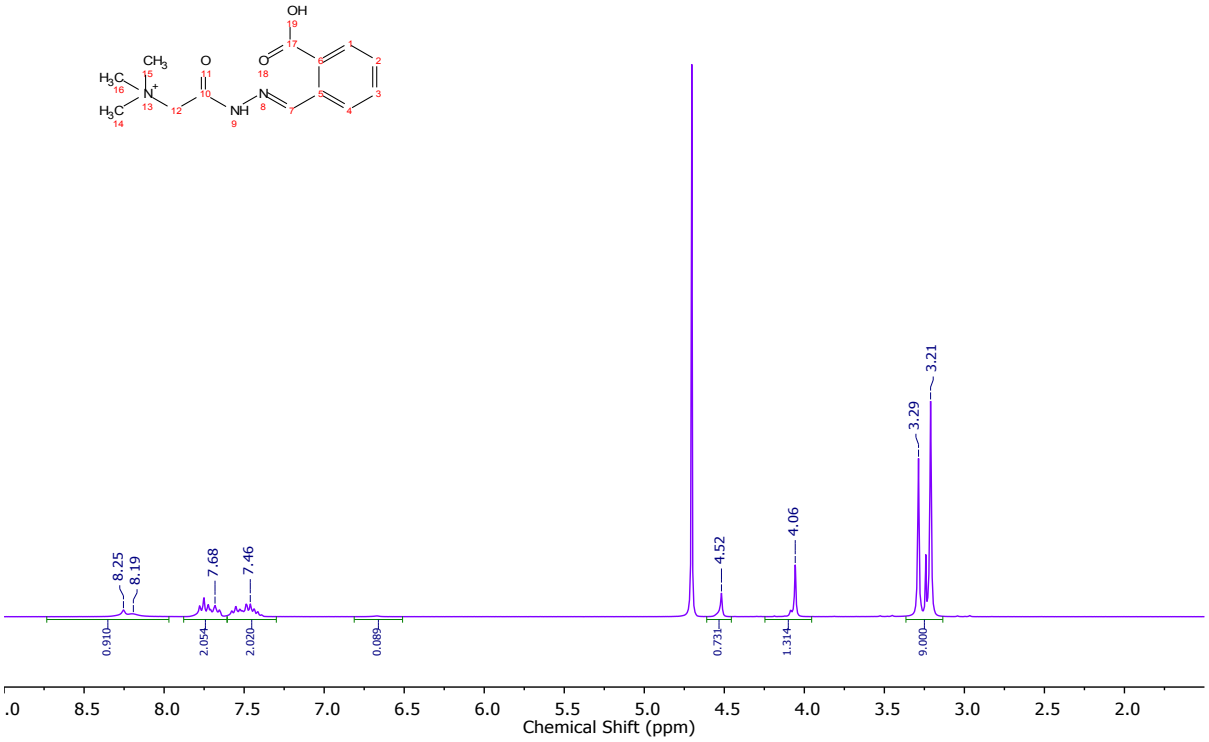


Figure S6A: ^{1}H NMR spectrum (300 MHz, D_2O) of **1f**

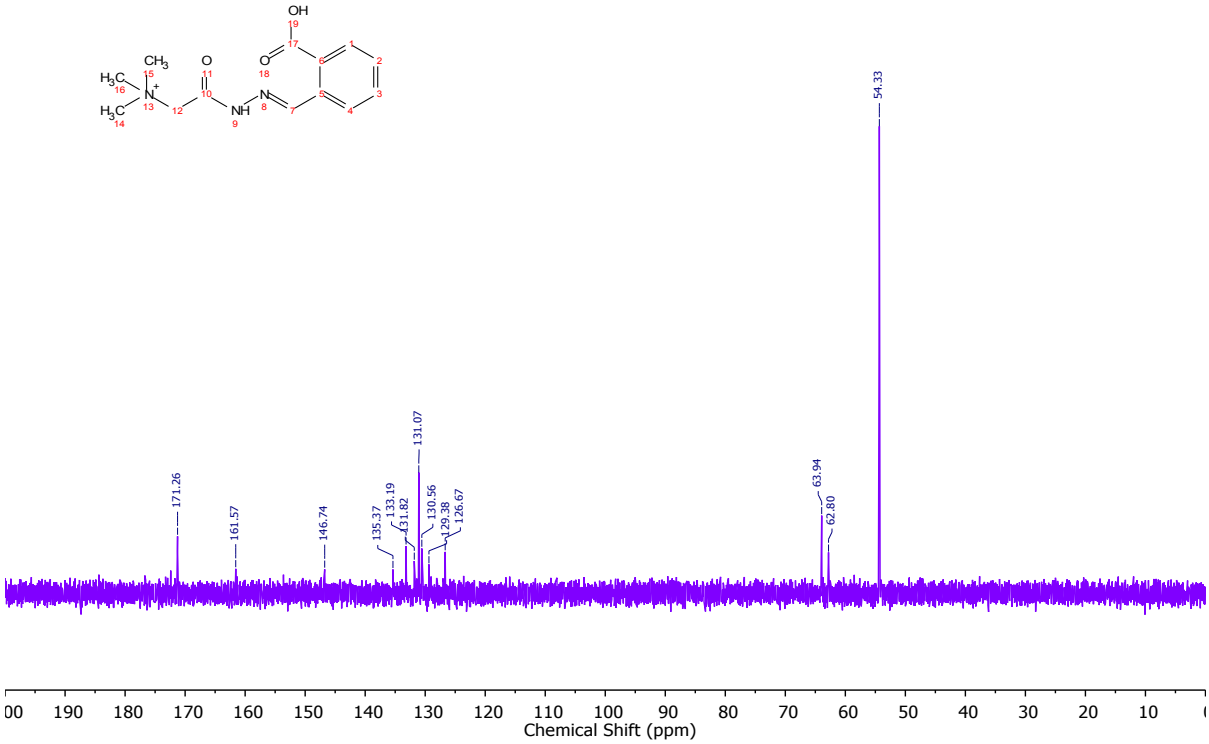


Figure S6B: ^{13}C NMR spectrum (300 MHz, D_2O) of **1f**

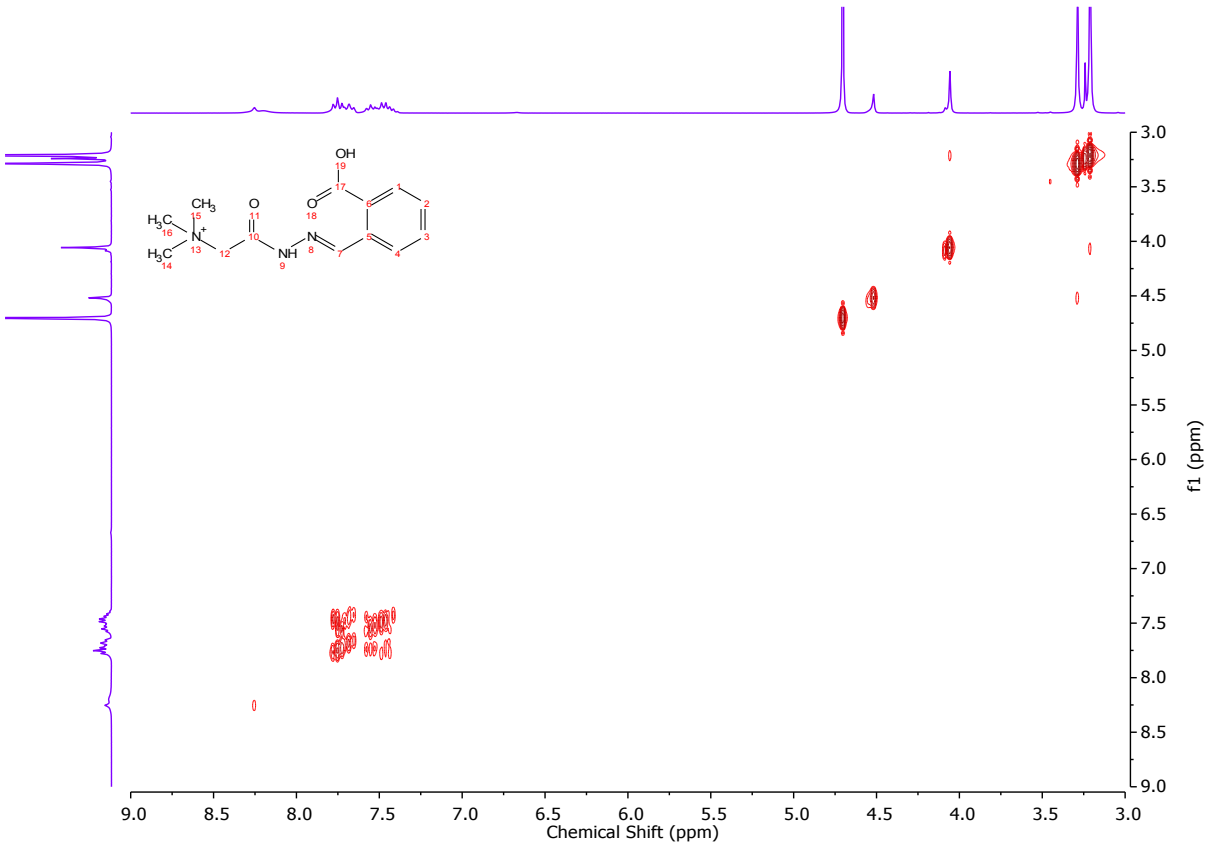


Figure S6C: COSY NMR spectrum (300 MHz, D_2O) of **1f**

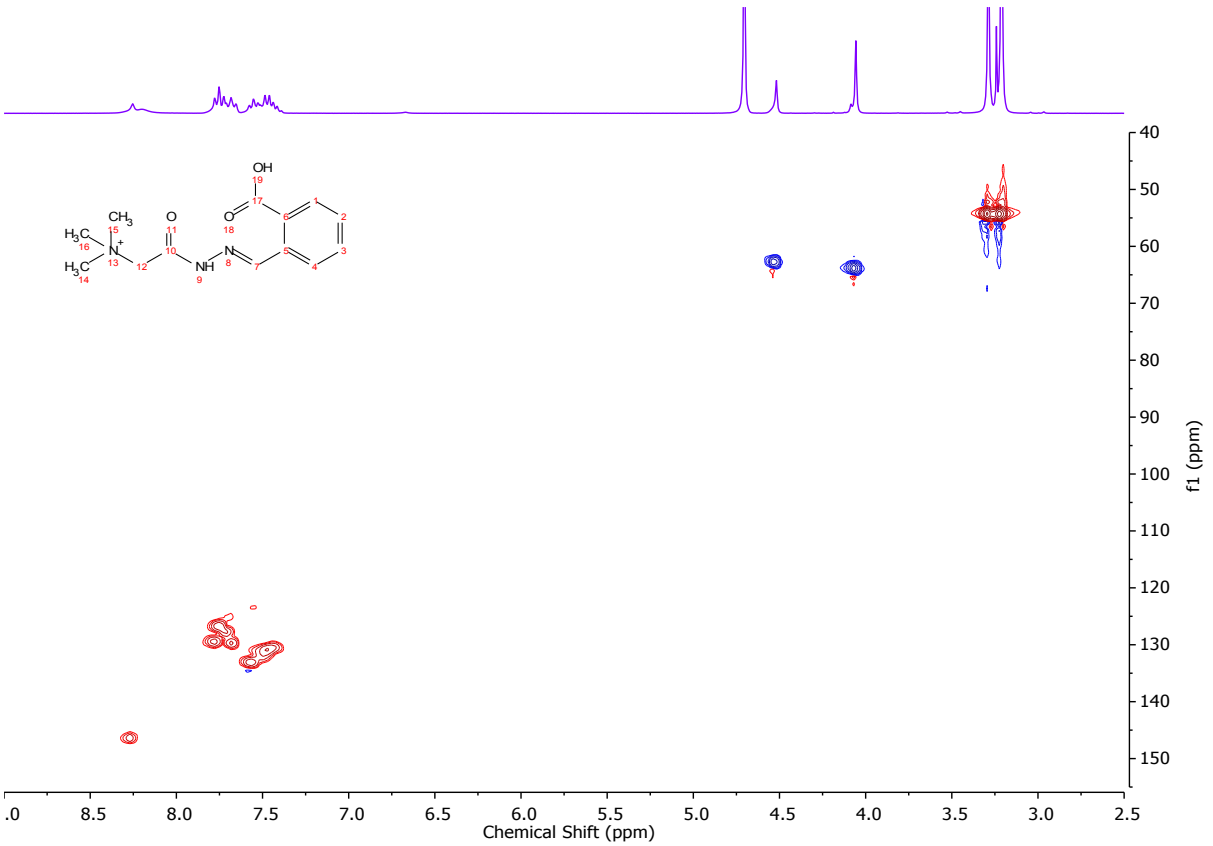


Figure S6D: HSQC NMR spectrum (300 MHz ^{1}H, 75 MHz ^{13}C, D_2O) of **1f**

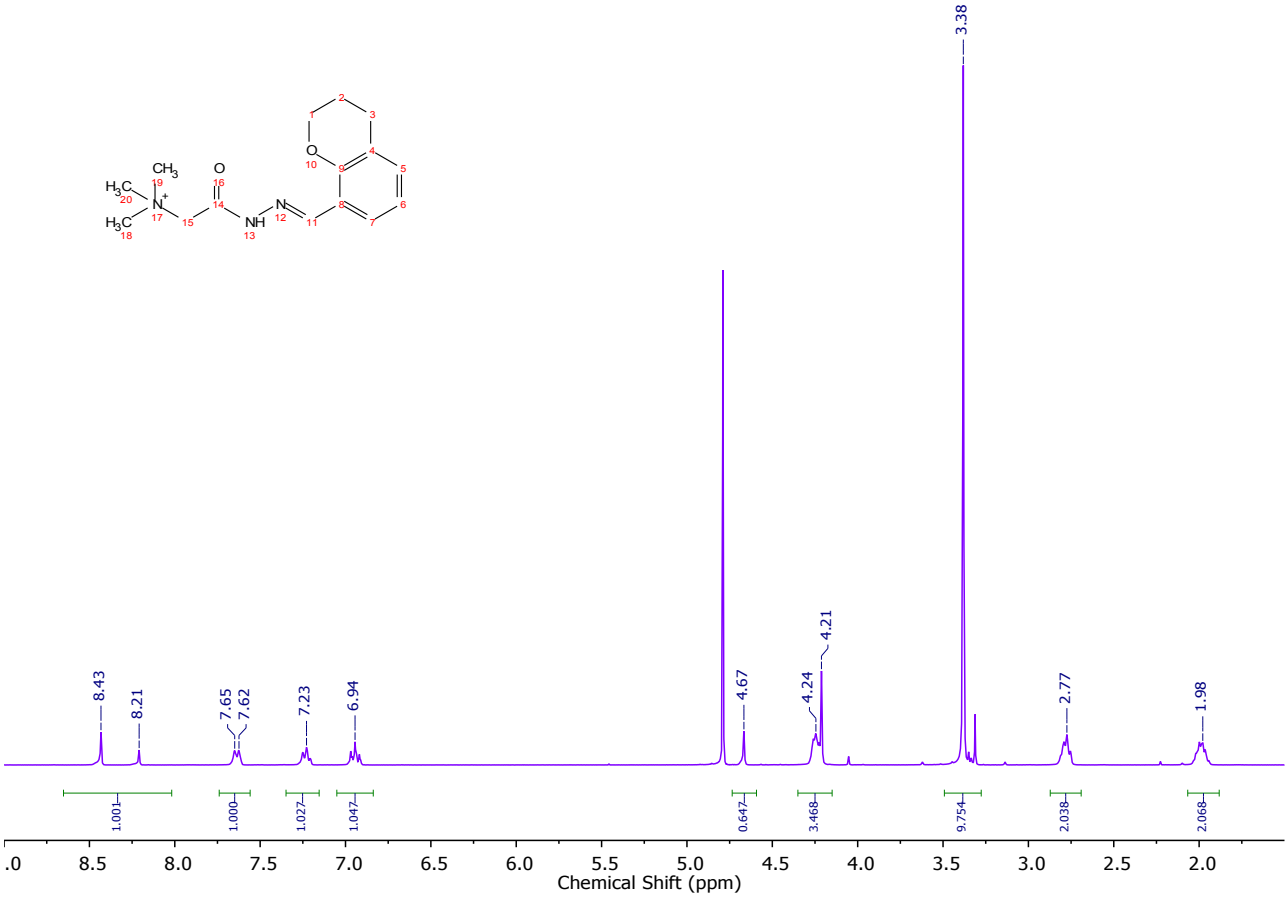


Figure S7A: ^{1}H NMR spectrum (300 MHz, D_2O) of **1g**

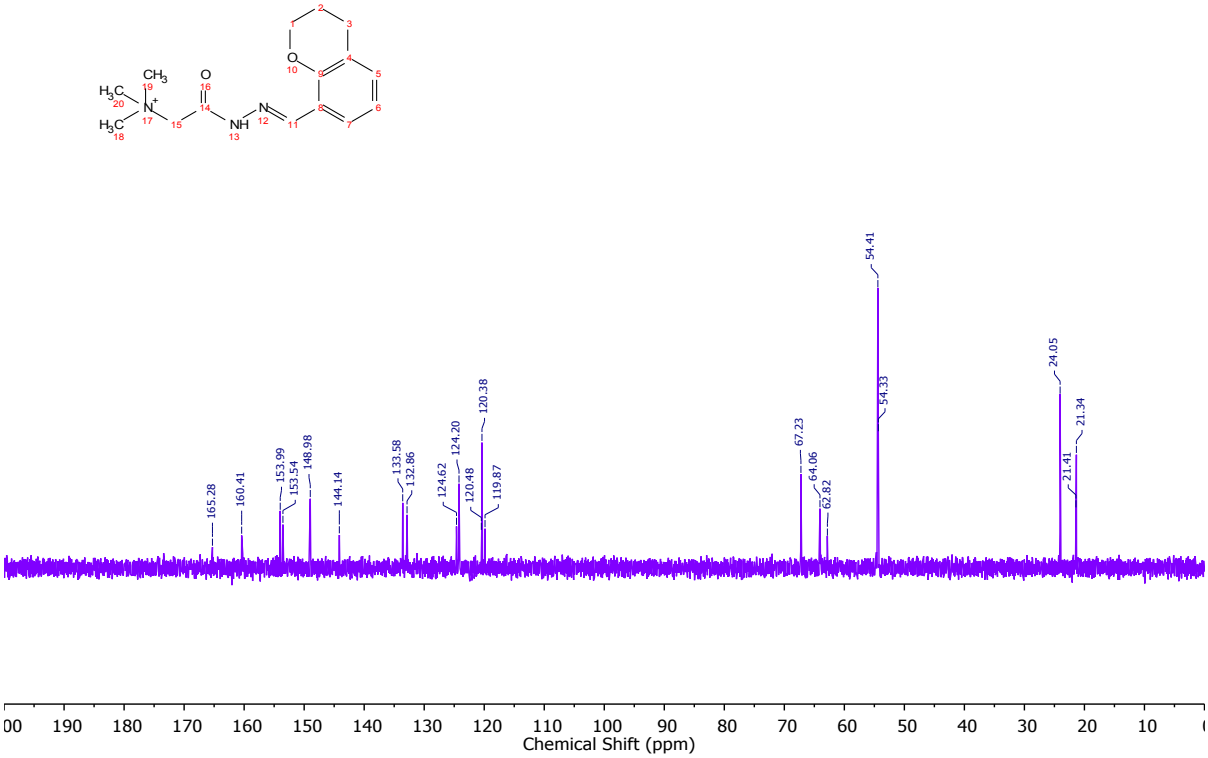


Figure S7B: ^{13}C NMR spectrum (300 MHz, D_2O) of **1g**

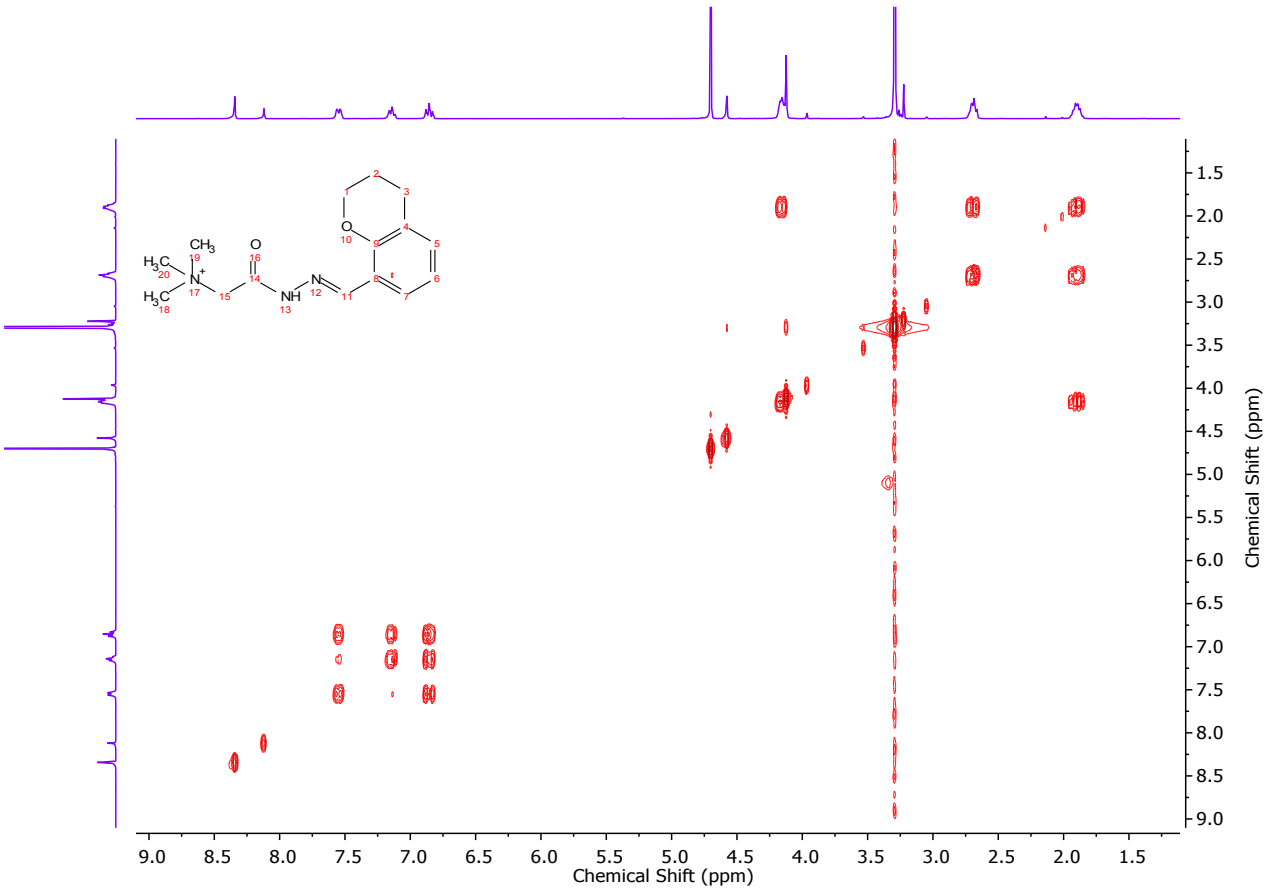
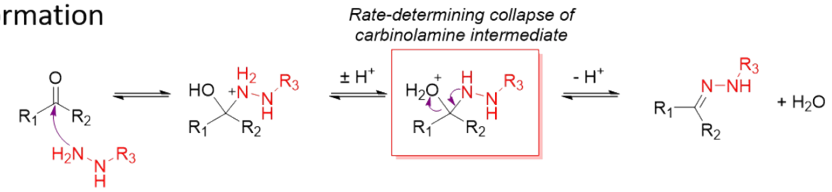


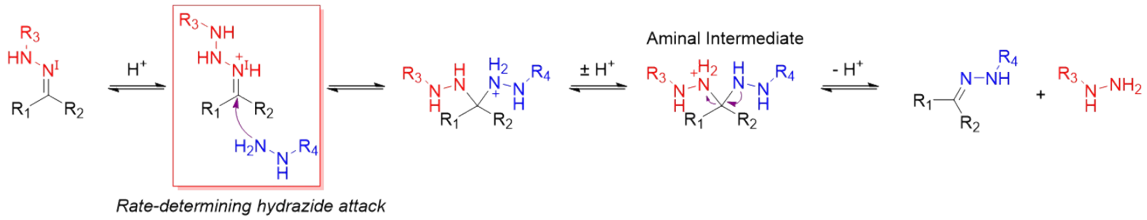
Figure S7C: COSY NMR spectrum (300 MHz, D_2O) of **1g**

Reaction Mechanisms:

A) Hydrazone Formation



B) Hydrazone Exchange



Scheme S8: Mechanisms of hydrazone formation (**A**) and hydrazone exchange (**B**). Computational studies reported herein suggest that the rate-determining step in hydrazone exchange is hydrazide attack, whereas in hydrazone formation the rate-limiting step is collapse of the tetrahedral intermediate.[2]

Kinetics Studies

Preparation of Kinetics Experiments:

Study 1 + Study 2: Hydrazones **1a**-**1g** were dissolved in 500 µL deuterated buffer solution (pD = 5.8-7.8), and hydrazide residue **3** (or **5** for **Study 2**) (5.0 eqv. dissolved in 500 µL buffer) was added, and solution mixed thoroughly by rapidly pipetting up and down 10 times. The sample was loaded into the NMR spectrometer to monitor the exchange kinetics over a minimum of 16 h at 25 ^{o}C. The kinetics traces were corrected for the time delay between initial mixing of reagents, and the time at which the first spectrum was acquired. The absolute rate constants were obtained according to the method described on page 16.

Final prepared sample contains: 23.4 mM hydrazone (**1a**-**1g**), 117 mM (5.0 eqv.) hydrazide residue **3** (or **5** for **Study 2**) dissolved in a total volume of 1.00 mL phosphate/D_2O buffer, pD 7.8.

Study 3: Stock solutions of aldehydes **a, d** and **g** were prepared by dissolving in d_6-DMSO. Concentrations were as follows: **g** (87 mg/mL, 536.4 mM), **a** (67.5 mg/mL, 429.5 mM), **d** (84 mg/mL, 791.6 mM). A 304.8 mg/mL, 1.82 M stock solution of Girard's Reagent T (**4**) in 100 mM phosphate/D_2O buffer, pD 7.8.

A typical ^{1}H NMR experiment was prepared by adding aldehyde stock (29.5 – 54.4 µL) and d_6-DMSO (345.6 – 370.5 µL) to a clean NMR tube, then diluting with 100 mM phosphate/D_2O, pD 7.8 (389.3 µL). The reaction was initiated by addition of the Girard's Reagent T stock solution (128.4 µL), the sample was rapidly mixed by pipetting up and down 10 times, then loaded into the NMR instrument for analysis. The kinetics traces were corrected for the time delay between initial mixing of reagents, and the time at which the first spectrum was acquired. The absolute rate constants were obtained according to the method described on page 17.

Final prepared sample contains: 25.5 mM aldehyde, 254.4 mM Girard's Reagent dissolved in a total volume of 400 µL d_6-DMSO + 517.7 µL phosphate/D_2O buffer, pD 7.8. d_6-DMSO was necessary to solubilize the aldehyde stating material.

Determination of Second Order Reversible Rate Constants:

The kinetic data for hydrazone exchange reactions (**Study 1** and **Study 2**) were analysed according to a second order reversible reaction mechanism:

$$A + B \leftrightarrow C + D \qquad (1)$$

Where *A* is the starting hydrazone (**1a**-**g**), *B* is glycol hydrazide **3** (see **Study 1**) or morpholine hydrazide **5** (see **Study 2**), *C* is product hydrazone (**2a-g**) and D is the free hydrazide (Girard's Reagent T, **4**) liberated by the exchange process.

Differential rate law:

$$\frac{\delta[A]}{\delta t} = -k_f\,[A][B] + k_r[C][D] \qquad (2)$$

Where k_f is the second order rate constant of the forward process and k_r is the second order rate constant for the reverse process. The differential rate law (2) was integrated numerically by explicit finite difference using the experimental time data, the initial values of the concentrations and trial values of k_f and k_r. The values of the two rate constants and the initial mole fraction of A (χ_A) were then optimized by least square fitting of the integrated rate law to the experimental data for [A] obtained by integration of the trimethylammonium (-NMe_3^+) signals associated with the starting hydrazone (**1a-g**) and exchange product **4** (Girard's Reagent T) in the ^{1}H NMR spectra recorded during the reaction. Each spectrum required about 2 minutes to collect, which is a much shorter time than the half-life of the reactions at the concentrations employed.

Statistical errors on the fitted values of rate constant are reported as ±1 σ confidence intervals estimated under the usual assumption of i. i. d. and normal measurement errors.

The kinetics of hydrazone exchange (**Study 3**) were analysed according to a second order irreversible reaction mechanism:

$$A + B \rightarrow C + D \qquad (3)$$

Where *A* is the starting aldehyde (**a**, **d**, **g**), *B* is Girard's Reagent T **4**, *C* is the product hydrazone (**2a-g**) and D is the water molecule liberated by the condensation reaction.

Differential rate law:

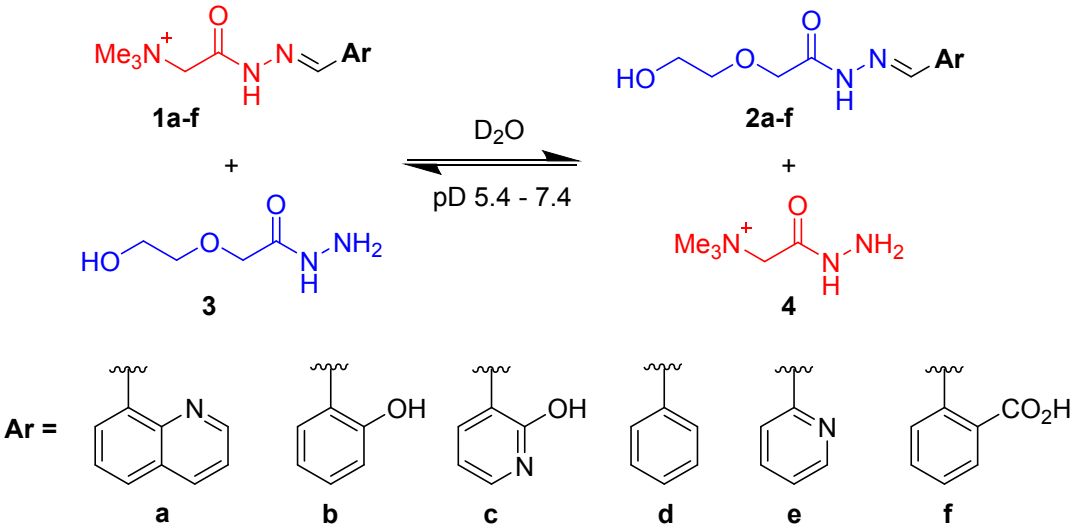
$$\frac{\delta[A]}{\delta t} = -k[A][B] \qquad (4)$$

Where *k* is the second order rate constant. The differential rate law (4) was integrated numerically by explicit finite difference using the experimental time data, the initial values of the concentrations and trial values of *k*. The values of rate constant *k* and the initial mole fraction of A (χ_A) were then optimized by least square fitting of the integrated rate law to the experimental data for [A] obtained by integration of the aldehyde (-C*H*O) signal and signals (*syn*- and *anti*-) associated with the hydrazone (-*H*C=N-N-) product in the ^{1}H NMR spectra recorded during the reaction. Each spectrum required about 2 minutes to collect, which is a much shorter time than the half-life of the reactions at the concentrations employed.

Statistical errors on the fitted values of rate constant are reported as ±1 σ confidence intervals estimated under the usual assumption of i. i. d. and normal measurement errors.

Kinetics Studies

Study 1: Hydrazones **1a-f** (23.4 mM) were exchanged with hydrazide **3** (117 mM) in buffered D_2O at pD 7.8, pD 6.8 and pD 5.8. See **S13** for kinetics traces.



Scheme S9: Hydrazones **1a-f** undergoing component exchange with hydrazide **3** to afford product hydrazones **2a-f**.

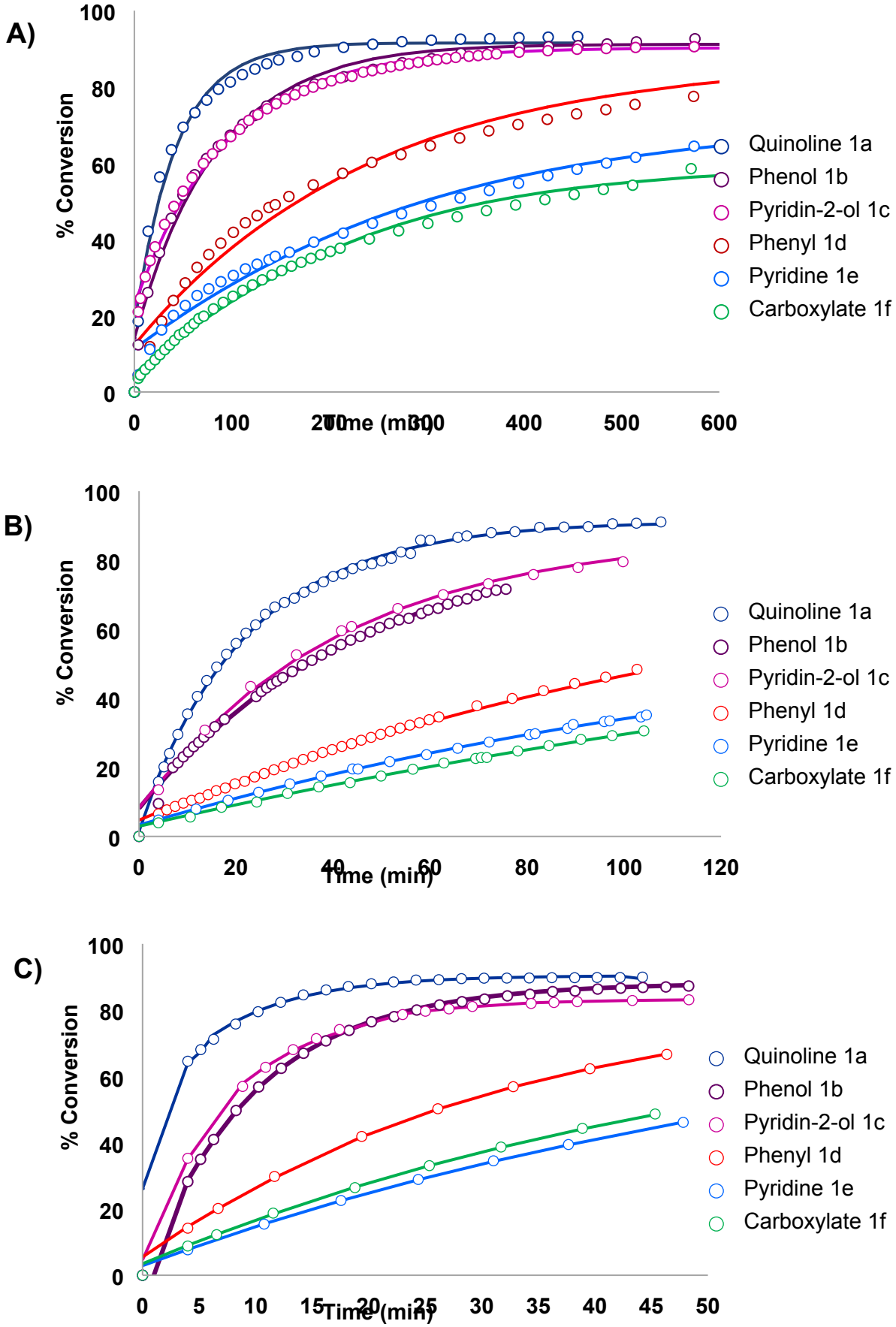


Figure S10: Kinetics traces of hydrazones **1a**-**1f** reacting with hydrazide **3** at pD 7.8 (**A**), pD 6.8 (**B**) and pD 5.4 (**C**). Experimental data and theoretical fit are shown as circles and solid lines, respectively. The fitting procedure and treatment of statistical errors is described on page 16.

Second Order Rate Constants:

		k_f (M^{-1} s^{-1})			k_r (M^{-1} s^{-1})		
	k_{rel}	**pD 7.8**	**pD 6.8**	**pD 5.8**	**pD 7.8**	**pD 6.8**	**pD 5.8**
1a	30.3	0.159 (± 2.9 %)	0.344 (± 0.6 %)	0.852 (± 0.5 %)	0.107 (± 10.6 %)	0.154 (± 4.3 %)	0.858 (± 2.2 %)
1b	26.5	0.087 (± 1.9 %)	0.156 (± 0.4 %)	0.744 (± 0.1 %)	0.055 (± 0.6 %)	0.116 (± 2.6 %)	0.368 (± 0.7 %)
1c	5.7	0.076 (± 0.9 %)	0.162 (± 0.5 %)	0.162 (± 1.6 %)	0.071 (± 3.3 %)	0.128 (± 1.0 %)	0.776 (± 1.3 %)
1d	7.4	0.030 (± 2.4 %)	0.052 (± 0.4 %)	0.207 (± 0.2 %)	0.030 (± 9.3 %)	0.043 (± 2.7 %)	0.206 (± 0.6 %)
1e	3.8	0.018 (± 2.1 %)	0.036 (± 0.3 %)	0.107 (± 0.1 %)	0.067 (± 12.3 %)	0.220 (± 5.9 %)	0.090 (± 1.4 %)
1f	4.4	0.020 (± 1.1 %)	0.028 (± 0.2 %)	0.122 (± 0.1 %)	0.121 (± 4.9 %)	0.035 (± 1.1 %)	0.157 (± 0.3 %)

Table S11: Second-order rate constants (k_f, k_r) for hydrazone exchange of **1a**-**1f** with glycol hydrazide **3** (**Study 1**). Where, k_f is the rate constant for the forward reaction and k_r is that of the reverse process. The statistical errors are reported as percentages. They correspond to 68 % (1 σ) confidence intervals (see page 16 for details).

Preliminary Kinetics Experiment: Exchange of **1g** with hydrazide **2**

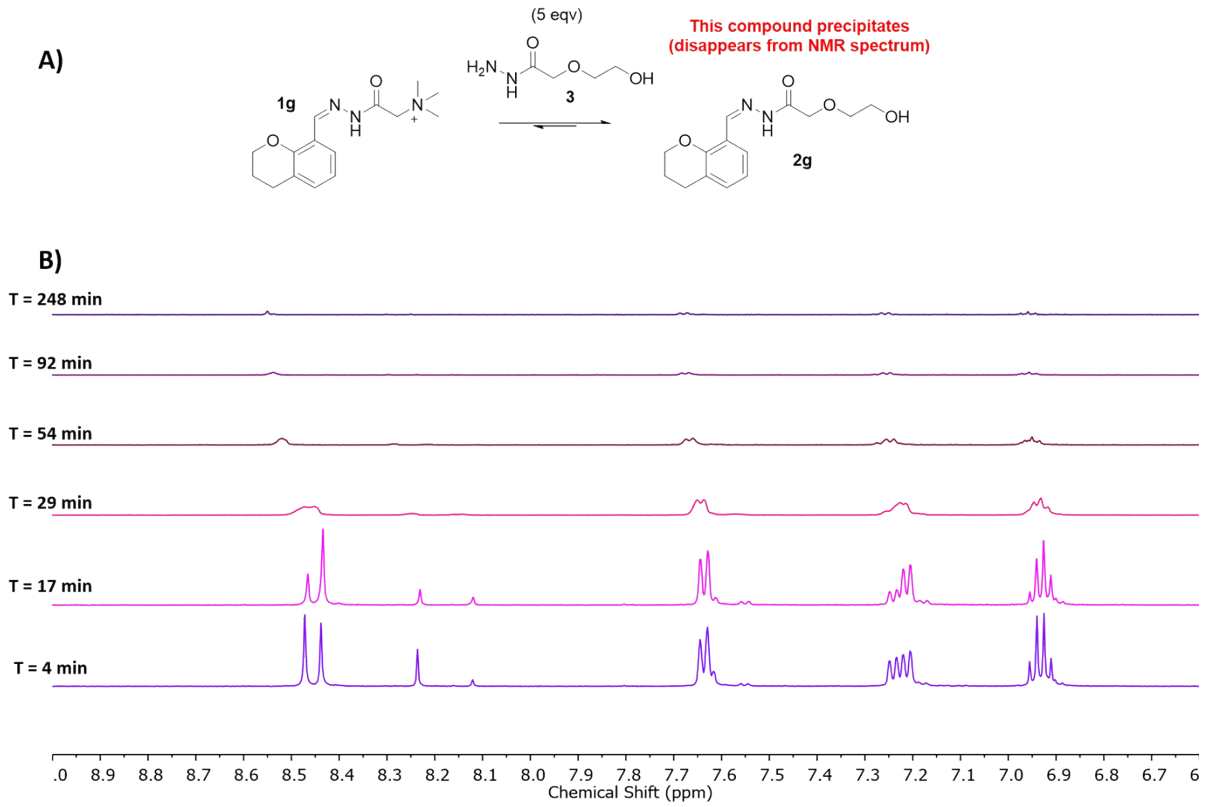
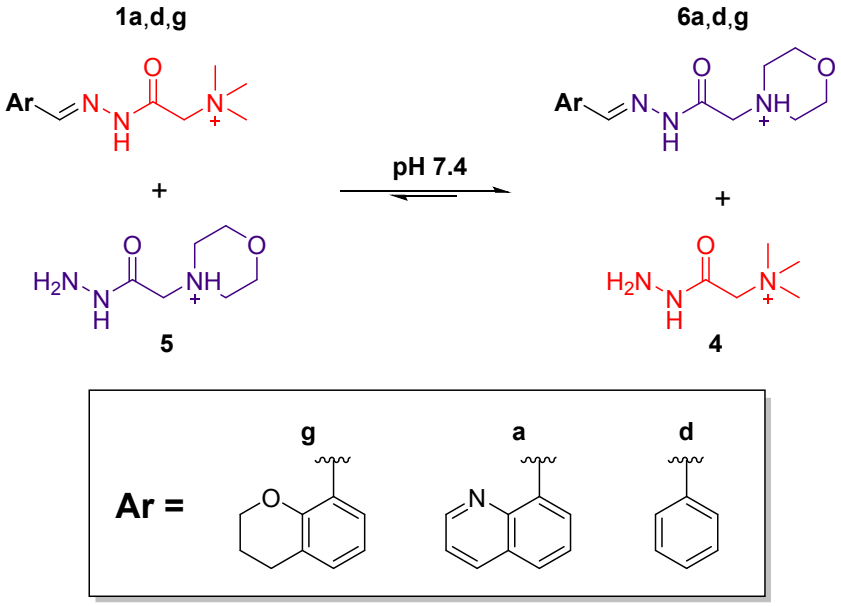


Figure S12: A preliminary experiment revealed that hydrazone exchange of **1g** with hydrazide **3** (**A**) resulted in precipitation of the product hydrazone (**2g**)**,** which led to signal broadening in the ^{1}H NMR spectra. (**B**). Convolution of the NMR spectra ultimately prevented accurate monitoring of the hydrazone exchange kinetics, thus an alternative exchange process was investigated (see **S13** and **S14**).

Study 2: Hydrazones **1a**, **1d**, and **1f** (23.4 mM) were exchanged with hydrazide **4** (117 mM) in buffered D_2O at pD 7.8. See **Fig. S16** for kinetics traces.



Scheme S13: Hydrazones **1a**,**d**,**g** undergoing component exchange with hydrazide **5** to afford product hydrazones **6a**,**d**,**g**.

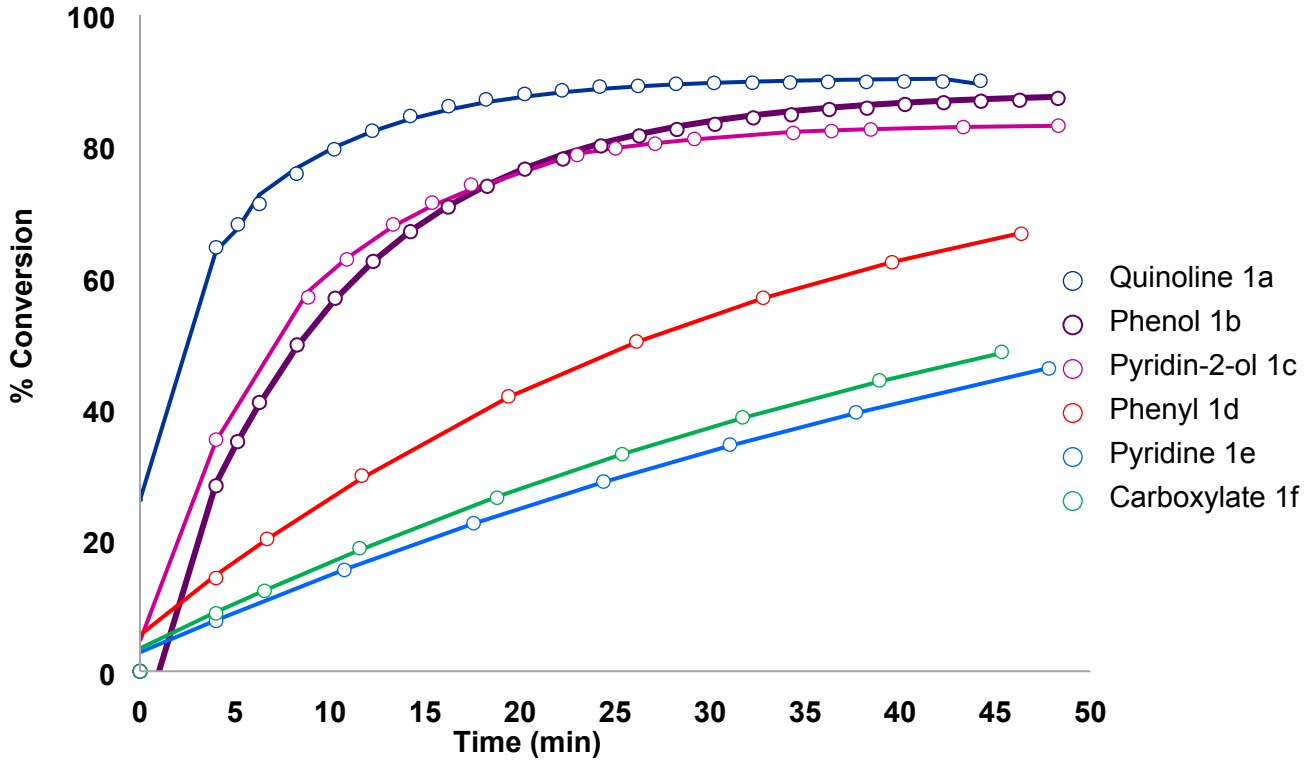


Figure S14: Kinetics traces of BenzoDHP **1g**, Quinoline **1a** and Phenyl **1d** reacting with hydrazide **5** at pD 7.8. Experimental and fitted data are shown as circles and solid lines, respectively. See page 16 for details of fitting the kinetics data.

		k_f (M^{-1} s^{-1})	k_r (M^{-1} s^{-1})
	k_{rel}	**pD 7.8**	**pD 7.8**
1a	10.3	0.078 (± 9.9 %)	0.037 (± 30.4 %)
1d	6.0	0.046 (± 9.3 %)	0.032 (± 22.2 %)
1g	1.0	0.008 (± 2.5 %)	0.021 (± 10.1 %)

Table S15: Second-order rate constants (k_f, k_r) for hydrazone exchange of **1a**,**d**,**g** with morpholine hydrazide **5** (Study 2). Where, k_f is the rate constant for the forward reaction, k_r is that of the reverse process and k_{rel} is the relative rate as deduced from k_f. The statistical errors are reported as percentages. They correspond to 68 % (1 σ) confidence intervals.

Study 3: Hydrazone formation kinetics of aldehydes **6**-**8** with Girard's Reagent T was studied by ^{1}H NMR spectroscopy. Hydrazone formation was observed to be significantly faster than hydrazone exchange under similar conditions. See page 17 for details on sample preparation.

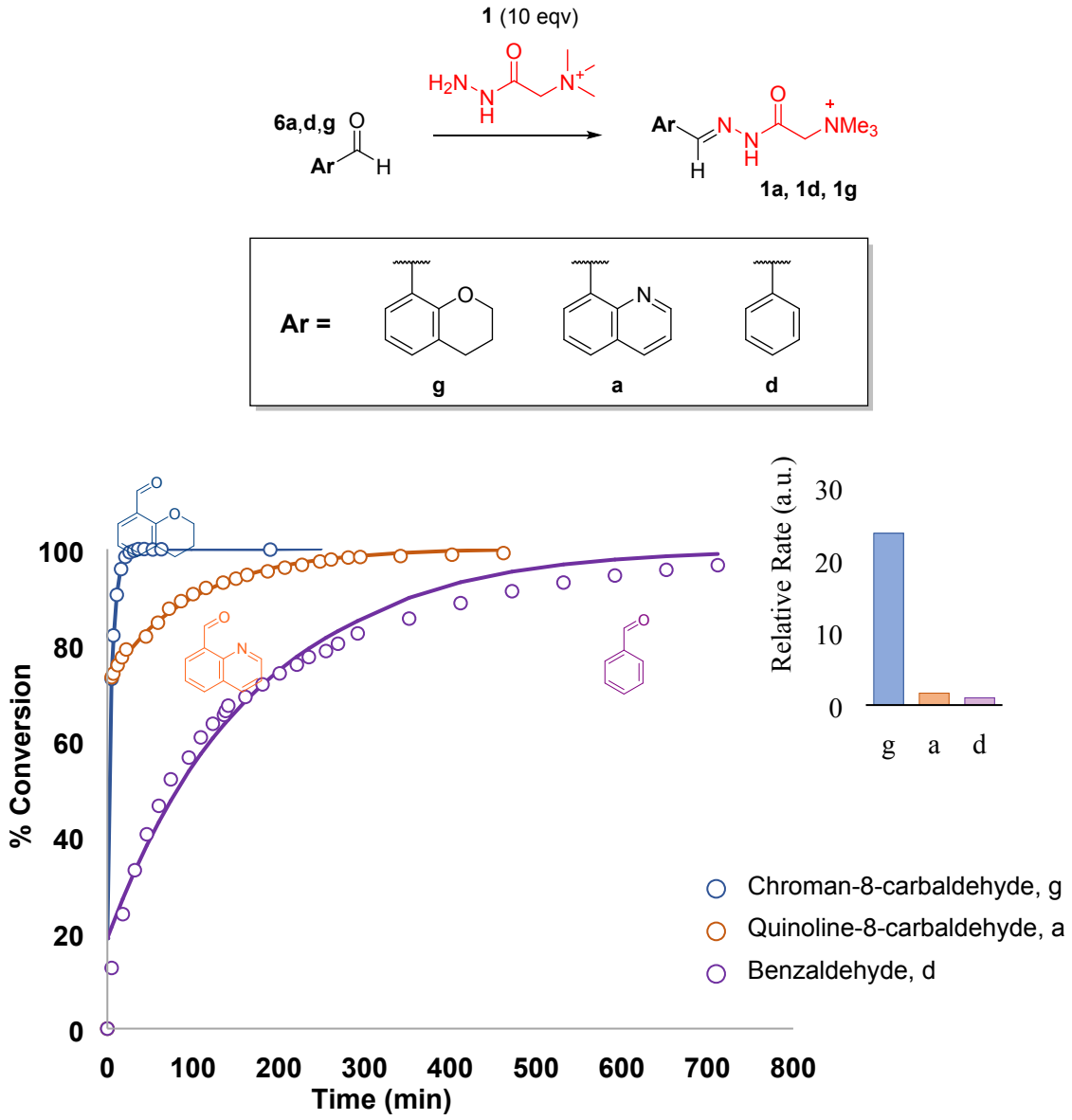


Figure S16: (**A**) Hydrazone formation of aromatic aldehydes **a**,**d**,**g** with Girard's Reagent T (**5**). 1H NMR monitored the reaction kinetics at pD 7.8. (**B**) Kinetics traces of hydrazone formation of aldehydes **a**,**d**,**g**. Inset shows the relative rates of hydrazone formation.

		k_2 (M^{-1} s^{-1})
	k_{rel}	**pD 7.8**
Chroman-8-carbaldehyde, **g**	23.6	1.266 (± 0.5 %)
Quinoline-8-carbaldehyde, **a**	1.6	0.024 (± 13.8 %)
Benzaldehyde, **d**	1.0	0.002 (± 6.9 %)

Table S17: Second-order rate constants (*k*) for hydrazone formation of **a**, **d** and **g** with Girard's reagent T (**4**) (Study 3). The statistical errors are reported as percentages. They correspond to 68 % (1 σ) confidence intervals.

Computational Studies

Hydrazone Exchange Studies: In order to gain insights to our experimental observations, computational studies were undertaken. Reaction mechanisms were studied at the M06-2X/6-31G* level of theory. To simplify the calculations, the hydrazide employed in modelling the exchange processes was $AcNHNH_2$, which was also used as the hydrazide component within the hydrazone. The process modelled is therefore a symmetrical exchange but provided the mechanistic insight required. Protonation free energies were computed using H_3O^+ as the proton source and corrected by adding the difference between the computed and experimental values of K_w. Corrections to 1 M concentrations were applied using an ideal gas approximation. Concentrations of H^+ and ^-OH that are appropriate to the pH were applied and water was assumed to be present at 55.5 M.

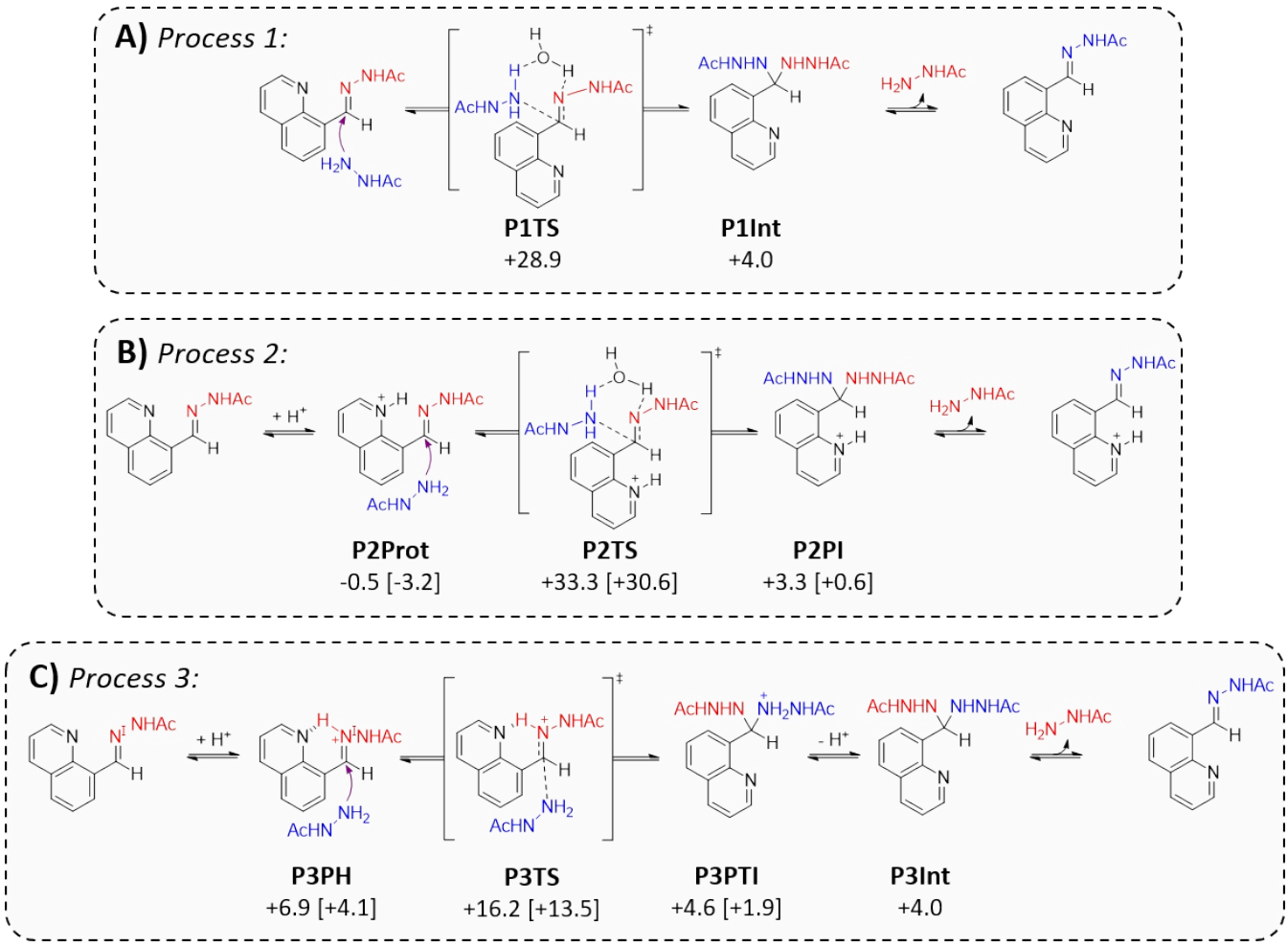


Figure S18: Three mechanisms of hydrazone exchange which were explored computationally. (**A**) Process (1): No protonation of hydrazone prior to hydrazide attack (uncatalysed reaction). (**B**) Process (2): Protonation of proximal acid/base group within aldehyde component of hydrazone. (**C**) Process (3): Protonation of hydrazone nitrogen (N^1) prior to attack. See tables **S19-21** for energetics.

Process 1:

Substrate	P1TS	P1Int
quinoline **1a**	+28.9	+4.0
phenyl **1d**	+27.1	+3.0
pyridine **1e**	+26.2	+3.7
carboxylate **1f**	+23.0	+3.0

Table S19: Free energies computed for intermediates and transition states of **1a**-**f** at pH 7.4. Values computed at pH 5.4 are in brackets (where given).

Process 2:

Substrate	P2Prot	P2TS	P2PI	ΔG†
quinoline **1a**	-0.5 [-3.2]	+33.3 [+30.6]	+3.3 [+0.6]	+33.8 [+33.8]
phenyl **1d**	0.0	+27.1	+3.0	+27.1
pyridine **1e**	+3.4 [+0.7]	+33.2 [+30.5]	+3.2 [+0.5]	+33.2 [+30.5]
carboxylate **1f**	-16.2 [-19.0]	+15.3 [+12.7]	-14.4 [-17.1]	+31.6 [+31.6]

Table S20: Free energies computed for intermediates and transition states of **1a**-**f** at pH 7.4. Values computed at pH 5.4 are in brackets (where given).

Process 3:

Substrate	P3PH	P3TS	P3PTI	ΔG†
quinoline **1a**	+6.8 [+4.1]	+16.2 [+13.5]	+4.6 [+1.9]	+16.7 [+16.7]
phenol **1b**	+11.1 [+8.3]	+19.4 [+16.7]	+23.2 [+20.4]	+19.4 [+16.7]
phenyl **1d**	+15.0 [+12.2]	+20.3 [+17.6]	+7.9 [+5.2]	+20.3 [+17.6]
pyridine **1e**	+13.4 [+10.6]	+20.2 [+17.5]	+6.7 [+3.9]	+20.2 [+17.5]
carboxylate **1f**	-4.3 [-9.8]	+10.8 [+5.3]	+4.3 [-1.1]	+27.0[a] [+24.3]

[a] *this is the free energy relative the lowest free energy state available pre-rate-limiting transition state,* **P2Prot**

Table S21: Free energies computed for intermediates and transition states of **1a**-**f** at pH 7.4. Values computed at pH 5.4 are in brackets (where given).

Hydrazone Formation versus Hydrazone Exchange: In order to gain insight to the mechanistic differences between hydrazone exchange and hydrazide, both reactions were studied in an identical way, with three possible mechanisms being considered: Process (1) hydrazide directly attacks the unprotonated aldehyde (**Fig. S23A**); process (2) protonation of acid/base groups within the aldehyde, followed by hydrazide attack; process (3) protonation of the aldehyde, followed by hydrazide attack.

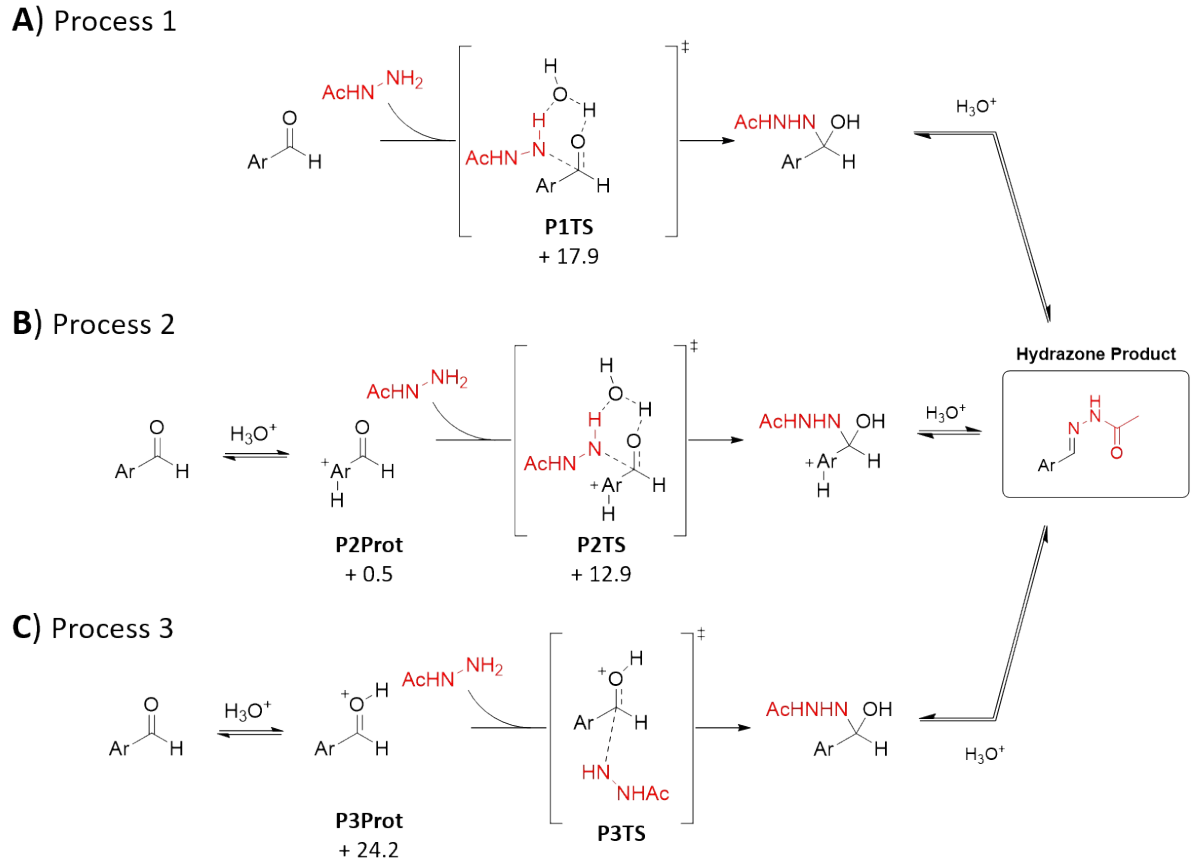


Figure S22: Three potential mechanisms of hydrazone formation were explored computationally for quinoline-8-carbaldehyde (Ar = quinoline). Free energy barriers (kcal/mol) were calculated relative to the lowest energy species. (**A**) No protonation prior to hydrazide attack on aldehyde (uncatalysed reaction). (**B**) Protonation of proximal acid/base group within the aromatic aldehyde, and subsequent hydrazide attack to form the hemiaminal intermediate. (**C**) Protonation of aldehyde oxygen prior to hydrazide attack.

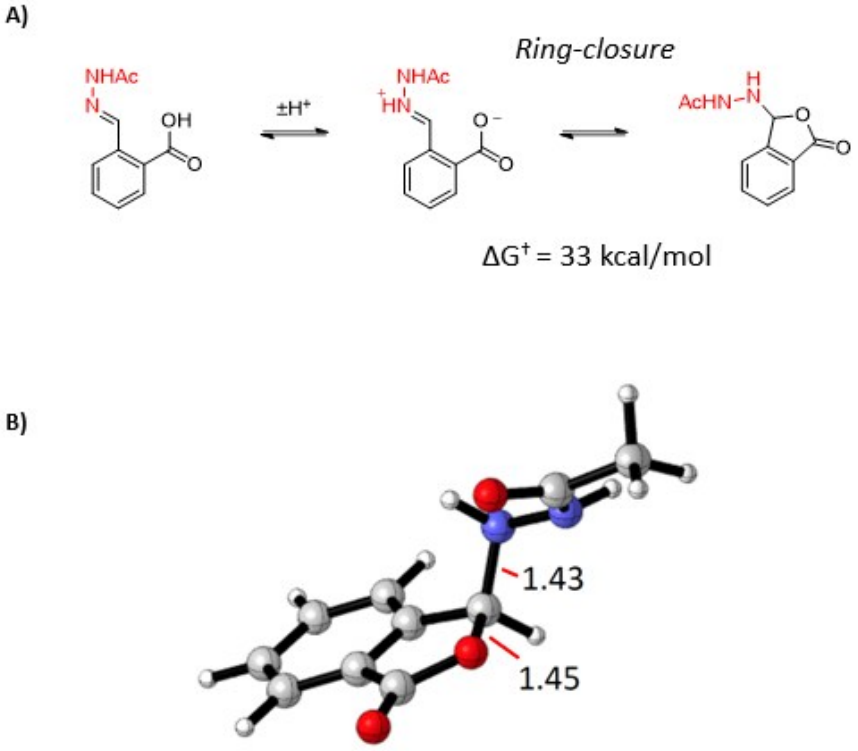


Figure S23: Computational modelling revealed that hydrazone **1f** forms a meta-stable cyclic intermediate, formed by carboxylate ring-closing upon tetrahedral (aminal) intermediate to form a 5-membered ring (**A**). Annotations indicate key bond lengths: 1.45 Å (O-C), 1.43 Å (C-N) are shown for the computed structure of the ring-closed intermediate (**B**).

Computational data

Below are geometries obtained at the M06-2X/6-31G* level in Gaussian09 with solvation incorporated using the IEFPCM model for water (geometry optimization and second derivatives were also computed with solvation included). In most cases, many conformations were considered and only the lowest energy structure has been included here for each species. Energies are in Hartrees.

Reactants

QUINOLINE
SCF energy = -703.088841077
Zero-point correction = 0.214283
Thermal correction to Energy = 0.227883
Thermal correction to Enthalpy = 0.228827
Thermal correction to Gibbs Free Energy = 0.172008
G(1M) = -702.914

Coordinates:
6 -4.15556 1.4352 0.001235
6 -4.09601 0.06806 -0.000217
6 -2.83085 -0.57378 -0.000646
6 -1.6715 0.249945 0.000396
6 -2.93969 2.16357 0.002259
1 -5.10133 1.96513 0.001614
1 -4.99851 -0.537225 -0.001039
1 -2.96909 3.25161 0.003443
6 -0.379329 -0.36608 -0.000151
6 -0.289798 -1.74416 -0.001545
1 0.693589 -2.20411 -0.002368
6 -1.44392 -2.55463 -0.002398
1 -1.33587 -3.63428 -0.003642
6 -2.69333 -1.98364 -0.002072
1 -3.58872 -2.59877 -0.002935
7 -1.74856 1.61163 0.001872
6 0.816638 0.485613 -0.000506
1 0.661402 1.56648 -0.003577
7 1.98586 -0.034851 0.001887
7 3.0374 0.818708 -0.000988
1 2.88756 1.8269 -0.006822
6 4.33581 0.374509 -0.001295
6 4.52913 -1.12072 0.00763
1 4.04216 -1.57727 -0.857223
1 4.08196 -1.55817 0.903722
1 5.59898 -1.32378 -0.012794
8 5.25193 1.18148 -0.00674

PYRIDINE

SCF energy = -549.505184199
Zero-point correction = 0.167229
Thermal correction to Energy = 0.177973
Thermal correction to Enthalpy = 0.178917
Thermal correction to Gibbs Free Energy = 0.129579
G(1M) = -549.373

Coordinates:
6 -0.001175 0.914593 2e-06
1 -0.081175 2.00576 0.000114
7 -1.02 0.14441 -8.1e-05
7 -2.23952 0.726063 -2.2e-05
1 -2.33245 1.74124 0.000173
6 -3.39838 -0.01427 -3e-06
6 -3.23226 -1.51218 -0.000234
1 -2.67249 -1.83532 0.880737
1 -2.67197 -1.83506 -0.880952
1 -4.22389 -1.96272 -0.000572
8 -4.47621 0.556314 0.000222
6 1.36451 0.363645 7e-06
6 1.60994 -1.01382 0.000157
6 3.60141 0.844373 -8.3e-05
6 2.92717 -1.44978 0.000131
1 0.777351 -1.70844 0.00027
6 3.94963 -0.503475 2e-06
1 4.37359 1.61034 -0.000237
1 3.15492 -2.51101 0.000226
1 4.9929 -0.798738 -2.8e-05
7 2.34063 1.28223 -9.5e-05

CARBOXYLIC ACID

SCF energy = -721.504519988
Zero-point correction = 0.181256
Thermal correction to Energy = 0.194798
Thermal correction to Enthalpy = 0.195742
Thermal correction to Gibbs Free Energy = 0.139045
G(1M) = -721.362

Coordinates:
6 0.407293 0.391287 0.202965
1 0.306242 1.44982 0.440838
7 1.54908 -0.159156 0.0232
7 2.6365 0.642521 0.196524
1 2.51948 1.61807 0.467132
6 3.91422 0.186843 0.024927
6 4.05831 -1.26125 -0.372687
1 3.55003 -1.45094 -1.32119
1 3.60316 -1.91279 0.377193
1 5.12066 -1.48325 -0.466602
8 4.86082 0.942605 0.194321
6 -0.83019 -0.403395 0.085347
6 -0.740462 -1.80394 0.119903
6 -3.22965 -0.609324 -0.050512
6 -1.87656 -2.59716 0.045374
1 0.240053 -2.25983 0.217354
6 -3.13311 -1.99566 -0.038671
1 -4.19593 -0.118198 -0.100766
1 -1.78505 -3.67899 0.067525
1 -4.02982 -2.60671 -0.086821
6 -2.09607 0.207977 -0.00535
6 -2.31639 1.73162 -0.09414
8 -1.36135 2.41801 -0.53352
8 -3.446 2.13655 0.25974

PHENYL

SCF energy = -533.467137249
Zero-point correction = 0.179020
Thermal correction to Energy = 0.189916
Thermal correction to Enthalpy = 0.190860
Thermal correction to Gibbs Free Energy = 0.141260
G(1M) = -533.323

Coordinates:
6 -0.023479 0.909808 -1.1e-05
1 -0.13557 1.99993 3.2e-05
7 -1.04082 0.135999 -6.5e-05
7 -2.26301 0.721474 -6.8e-05
1 -2.35342 1.7368 3.2e-05
6 -3.42162 -0.013962 -2.1e-05
6 -3.25917 -1.51279 -7.8e-05
1 -2.69973 -1.83729 0.880609
1 -2.69957 -1.83724 -0.880678
1 -4.25177 -1.96133 -0.000171
8 -4.50056 0.557213 7.1e-05
6 1.34475 0.37623 8e-06
6 1.60008 -1.00208 3e-05
6 3.72896 0.801701 2.7e-05
6 2.90791 -1.4685 4.9e-05
1 0.76458 -1.69508 3.3e-05
6 3.97615 -0.568721 4.7e-05
1 4.55546 1.50522 2.7e-05
1 3.09884 -2.53716 6.7e-05
1 4.99715 -0.937469 6.3e-05
6 2.41838 1.27201 9e-06
1 2.22354 2.34141 -4e-06

PHENOL

SCF energy = -608.671411256
Zero-point correction = 0.183918
Thermal correction to Energy = 0.195541
Thermal correction to Enthalpy = 0.196486
Thermal correction to Gibbs Free Energy = 0.145794
G(1M) = -608.523

Coordinates:
6 -0.070578 1.07555 -5e-06
1 -0.188446 2.16394 -4e-06
7 -1.09196 0.299915 -2e-05
7 -2.32549 0.861044 -3.1e-05
1 -2.42711 1.87449 1e-05
6 -3.47188 0.105688 -1.1e-05
6 -3.28424 -1.39057 -7.3e-05
1 -2.72443 -1.70887 0.883617
1 -2.72435 -1.7088 -0.88374
1 -4.26952 -1.85477 -0.000132
8 -4.55884 0.659324 -1.8e-05
6 1.29108 0.549822 1e-05
6 1.57139 -0.834903 2.4e-05
6 3.67734 1.02082 2.7e-05
6 2.89909 -1.27089 3.8e-05
6 3.93939 -0.352072 4e-05
1 4.49137 1.73725 2.8e-05
1 3.08735 -2.3396 5e-05
1 4.9645 -0.709556 5.2e-05
6 2.36154 1.45623 1.3e-05
8 0.604353 -1.77569 2.7e-05
1 -0.269419 -1.32828 2.5e-05
1 2.13931 2.52037 2e-06

BENZOFURAN

SCF energy = -684.843775903
Zero-point correction = 0.195711
Thermal correction to Energy = 0.208640
Thermal correction to Enthalpy = 0.209584
Thermal correction to Gibbs Free Energy = 0.154143
G(1M) = -684.687

Coordinates:
6 0.616325 0.54991 0.00012
1 0.51589 1.63971 0.000251
7 1.76013 -0.022252 2.3e-05
7 2.85181 0.777953 0.000105
1 2.75395 1.79248 0.000245
6 4.12657 0.267849 -1.7e-05
6 4.24305 -1.23512 -0.000263
1 3.75341 -1.65748 -0.881048
1 3.75339 -1.65778 0.880363
1 5.30135 -1.49255 -0.000296
8 5.08161 1.02779 2.9e-05
6 -0.615356 -0.242092 4.8e-05
6 -0.642727 -1.63951 -1.6e-05
6 -3.08531 -0.297104 -1.8e-05
6 -1.85002 -2.34857 -8.2e-05
1 0.301757 -2.1739 -1.1e-05
6 -3.07878 -1.69653 -8.4e-05
1 -1.82126 -3.43337 -0.000128
1 -4.00741 -2.25787 -0.000132
6 -1.86181 0.385677 4.5e-05
8 -2.06808 1.7297 9.8e-05
6 -4.09626 0.736911 7e-06
6 -3.42624 1.90889 5.5e-05
1 -5.1687 0.610487 -2.1e-05
1 -3.75088 2.93851 8.3e-05

DIHYDROBENZOPYRAN

SCF energy = -725.349234326
Zero-point correction = 0.249153
Thermal correction to Energy = 0.263568
Thermal correction to Enthalpy = 0.264512
Thermal correction to Gibbs Free Energy = 0.206526
G(1M) = -725.14

Coordinates:

6	0.91059	0.429891	-0.065375
1	0.74276	1.50723	-0.137271
7	2.09065	-0.061008	0.001569
7	3.12223	0.820369	-0.03228
1	2.94693	1.82092	-0.116577
6	4.4295	0.414118	0.033009
6	4.66074	-1.07108	0.155311
1	4.23489	-1.59695	-0.702738
1	4.17477	-1.46249	1.05222
1	5.73501	-1.24376	0.205031
8	5.32613	1.24284	-0.009094
6	-0.26852	-0.442466	-0.053286
6	-0.150838	-1.83564	-0.064505
6	-1.55208	0.135229	-0.039758
6	-1.28134	-2.64132	-0.061034
6	-2.70313	-0.666241	-0.026929
6	-2.54332	-2.0511	-0.038943
1	-1.1832	-3.72172	-0.071
1	-3.43418	-2.67455	-0.0235
1	0.843471	-2.27078	-0.081265
8	-1.60429	1.49655	-0.011929
6	-4.07758	-0.036325	0.021818
6	-3.98495	1.42072	0.468568
6	-2.86829	2.09602	-0.306645
1	-3.05027	2.02172	-1.38718
1	-2.75394	3.14785	-0.040535
1	-4.9275	1.94658	0.293556
1	-3.75876	1.48189	1.53898
1	-4.53835	-0.083902	-0.973164
1	-4.72109	-0.613518	0.693228

DIHYDROBENZOFURAN

SCF energy = -686.048925520
Zero-point correction = 0.219162
Thermal correction to Energy = 0.232825
Thermal correction to Enthalpy = 0.233769
Thermal correction to Gibbs Free Energy = 0.176627
G(1M) = -685.869

Coordinates:
6 -0.676316 0.518686 -0.000684
1 -0.561051 1.60705 -0.004647
7 -1.82946 -0.035933 0.003027
7 -2.90812 0.786328 -0.00279
1 -2.79012 1.79857 -0.012793
6 -4.19096 0.30244 0.003509
6 -4.33693 -1.19826 0.019225
1 -3.86065 -1.61999 0.907684
1 -3.85048 -1.64075 -0.85335
1 -5.39999 -1.43527 0.016419
8 -5.13307 1.07969 -0.002837
6 0.545605 -0.285828 -0.00079
6 0.543204 -1.69207 -0.037269
6 2.99061 -0.378592 0.025083
6 1.72616 -2.4172 -0.044243
1 -0.414172 -2.20299 -0.067085
6 2.96643 -1.7613 -0.008503
1 1.69132 -3.50105 -0.077568
1 3.89064 -2.3316 -0.00769
6 1.79242 0.335558 0.028456
8 1.96943 1.68193 0.074012
6 4.11899 0.620159 0.120815
6 3.37551 1.94183 -0.154099
1 4.91416 0.445978 -0.607293
1 3.66822 2.76057 0.5029
1 3.48928 2.2539 -1.19685
1 4.56665 0.607208 1.12022

CARBOXYLATE

SCF energy = -721.504519988
Zero-point correction = 0.181256
Thermal correction to Energy = 0.194798
Thermal correction to Enthalpy = 0.195742
Thermal correction to Gibbs Free Energy = 0.139045
G(1M) = -721.362

Coordinates:
6 0.407293 0.391287 0.202965
1 0.306242 1.44982 0.440838
7 1.54908 -0.159156 0.0232
7 2.6365 0.642521 0.196524
1 2.51948 1.61807 0.467132
6 3.91422 0.186843 0.024927
6 4.05831 -1.26125 -0.372687
1 3.55003 -1.45094 -1.32119
1 3.60316 -1.91279 0.377193
1 5.12066 -1.48325 -0.466602
8 4.86082 0.942605 0.194321
6 -0.83019 -0.403395 0.085347
6 -0.740462 -1.80394 0.119903
6 -3.22965 -0.609324 -0.050512
6 -1.87656 -2.59716 0.045374
1 0.240053 -2.25983 0.217354
6 -3.13311 -1.99566 -0.038671
1 -4.19593 -0.118198 -0.100766
1 -1.78505 -3.67899 0.067525
1 -4.02982 -2.60671 -0.086821
6 -2.09607 0.207977 -0.00535
6 -2.31639 1.73162 -0.09414
8 -1.36135 2.41801 -0.53352
8 -3.446 2.13655 0.25974

Addition transition states

QUINOLINE
SCF energy = -1043.87944049
Zero-point correction = 0.332513
Thermal correction to Energy = 0.353279
Thermal correction to Enthalpy = 0.354224
Thermal correction to Gibbs Free Energy = 0.282715
G(1M) = -1043.59

Coordinates:
6 0.891846 -0.039226 0.416038
1 1.46389 -0.824501 0.915382
7 1.47799 1.24894 0.610844
7 2.80189 1.14766 1.06839
7 0.988073 -0.398485 -1.10981
1 1.04019 0.587173 -1.62993
7 0.007137 -1.24383 -1.64222
1 3.00461 1.65909 1.91677
6 3.80202 0.506483 0.441835
6 5.16153 0.613306 1.09538
1 5.86799 1.0108 0.362735
1 5.49899 -0.388208 1.37365
1 5.16657 1.25141 1.98089
8 3.6436 -0.159332 -0.592018
1 -0.824538 -0.748016 -1.94621
6 -0.083061 -2.50869 -1.10938
6 -1.3587 -3.23913 -1.43355
1 -2.08138 -3.02865 -0.637456
1 -1.16184 -4.31083 -1.45174
1 -1.78673 -2.91982 -2.3856
8 0.820891 -2.96306 -0.428956
8 1.37278 2.03993 -1.74094
1 1.45392 1.85551 -0.583963
1 0.479662 2.40845 -1.8236
6 -0.543959 -0.146741 0.884809
6 -2.11732 -1.03578 2.52504
6 -2.91451 0.51555 0.855383
6 -3.14536 -0.306748 1.98866
1 -2.28822 -1.67976 3.38145
1 -4.14645 -0.354855 2.40775
1 1.9253 -0.807782 -1.22302
6 -1.61191 0.593783 0.291597
6 -0.819675 -0.954494 1.96405
1 -0.01807 -1.5426 2.40314
6 -3.94848 1.26275 0.236944
6 -3.66938 2.008 -0.877475
1 -4.43338 2.5882 -1.38194
6 -2.34777 1.99285 -1.38163
1 -2.11092 2.55646 -2.28219
7 -1.3562 1.3245 -0.832989
1 -4.95155 1.22469 0.653415

PYRIDINE
SCF energy = -890.297666291
Zero-point correction = 0.284428
Thermal correction to Energy = 0.302895
Thermal correction to Enthalpy = 0.303839
Thermal correction to Gibbs Free Energy = 0.236113
G(1M) = -890.059

Coordinates:
6 0.062209 0.379999 0.307849
1 0.406631 -0.030226 1.26347
7 0.717066 1.59962 -0.047433
7 2.00312 1.72624 0.491695
7 0.391744 -0.67641 -0.761325
1 0.206411 -0.12696 -1.70628
7 -0.237938 -1.92125 -0.649422
1 2.13515 2.52829 1.09377
6 3.0767 0.985707 0.166373
6 4.38448 1.4174 0.787379
1 5.10691 1.59334 -0.013179
1 4.76486 0.600858 1.40584
1 4.29737 2.31885 1.39632
8 3.02388 -0.006585 -0.574019
1 -1.22135 -1.8938 -0.897726
6 0.287992 -2.81493 0.246135
6 -0.551506 -4.04191 0.488378
1 -1.31828 -4.18271 -0.274792
1 -1.0346 -3.94374 1.46464
1 0.1037 -4.91355 0.518298
8 1.36814 -2.60859 0.776599
8 0.289128 1.20074 -2.45164
1 0.590801 1.60408 -1.33671
1 -0.626958 1.48766 -2.58789
6 -1.44165 0.604364 0.313502
6 -3.47966 0.358528 -0.70748
6 -3.36029 1.62792 1.31261
6 -4.12261 1.1114 0.265605
1 -4.03572 -0.065024 -1.53968
1 -3.8246 2.21945 2.09526
1 -5.19089 1.28529 0.204883
1 1.42535 -0.791734 -0.708361
7 -2.16419 0.10426 -0.690792
6 -1.99641 1.37604 1.33567
1 -1.35813 1.77099 2.11943

CARBOXYLATE

SCF energy = -1062.30449348
Zero-point correction = 0.299565
Thermal correction to Energy = 0.320110
Thermal correction to Enthalpy = 0.321054
Thermal correction to Gibbs Free Energy = 0.249793
G(1M) = -1062.05

Coordinates:
6 0.561929 -0.050273 0.44805
1 0.981203 -0.903554 0.985528
7 1.36105 1.12632 0.627539
7 2.64279 0.821239 1.11164
7 0.635414 -0.466022 -1.05598
1 0.792479 0.496111 -1.61282
7 -0.433509 -1.22433 -1.55685
1 2.90987 1.31079 1.95518
6 3.53326 -0.003972 0.538105
6 4.8692 -0.114388 1.23903
1 5.66003 0.059043 0.505732
1 4.98569 -1.13236 1.61996
1 4.98351 0.590294 2.06492
8 3.29515 -0.670514 -0.479954
1 -1.19591 -0.591239 -1.8555
6 -0.650131 -2.4412 -0.974053
6 -2.00035 -3.04227 -1.27057
1 -2.67769 -2.7667 -0.454874
1 -1.91458 -4.12881 -1.29839
1 -2.41823 -2.67433 -2.20943
8 0.194002 -2.97571 -0.267974
8 1.35325 1.875 -1.73228
1 1.42828 1.69639 -0.546658
1 0.576737 2.45632 -1.81592
6 -0.884649 0.115328 0.880409
6 -2.56463 -0.480179 2.5406
6 -3.07147 1.14313 0.839293
6 -3.4592 0.41416 1.96088
1 -2.85256 -1.06448 3.40891
1 -3.77077 1.83601 0.37784
1 -4.4554 0.540454 2.37411
1 1.53079 -0.969869 -1.13381
6 -1.79984 0.997489 0.28018
6 -1.28975 -0.620585 1.99805
1 -0.587643 -1.31683 2.45069
6 -1.50727 1.77482 -1.00076
8 -1.60379 1.11521 -2.0741
8 -1.21844 2.98224 -0.892584

PHENYL
SCF energy = -874.255679535
Zero-point correction = 0.296010
Thermal correction to Energy = 0.314803
Thermal correction to Enthalpy = 0.315747
Thermal correction to Gibbs Free Energy = 0.247103
G(1M) = -874.006

Coordinates:
6 0.284689 0.378406 0.320764
1 0.552979 -0.266753 1.16146
7 1.19212 1.45735 0.136448
7 2.43852 1.23106 0.736465
7 0.40151 -0.559074 -0.946362
1 0.523864 0.136926 -1.78045
7 -0.605056 -1.50934 -1.15968
1 2.72948 1.94303 1.3931
6 3.28832 0.230375 0.456545
6 4.6126 0.272103 1.18329
1 5.41447 0.223617 0.442853
1 4.69236 -0.612854 1.81954
1 4.74156 1.16668 1.79512
8 3.02449 -0.69929 -0.321347
1 -1.44045 -1.14462 -1.60288
6 -0.701035 -2.53587 -0.247714
6 -1.96935 -3.3414 -0.343309
1 -2.75486 -2.82405 0.21805
1 -1.80124 -4.32059 0.103465
1 -2.30201 -3.45248 -1.37746
8 0.195951 -2.7421 0.551339
8 1.1455 1.45234 -2.3341
1 1.25662 1.64971 -1.15565
1 0.524611 2.09351 -2.70854
6 -1.16204 0.798093 0.413398
6 -2.03193 0.112277 1.26256
6 -1.65385 1.84273 -0.372939
6 -3.37841 0.466958 1.33147
1 -1.65026 -0.700697 1.87741
6 -2.99773 2.19748 -0.30561
1 -0.977691 2.3777 -1.03223
6 -3.86247 1.51028 0.546137
1 -4.045 -0.070618 1.9988
1 -3.37129 3.01212 -0.918325
1 -4.91025 1.78952 0.597379
1 1.32722 -1.01633 -0.834365

Addition intermediates

QUINOLINE
SCF energy= -967.529528342
Zero-point correction = 0.312536
Thermal correction to Energy = 0.332013
Thermal correction to Enthalpy = 0.332957
Thermal correction to Gibbs Free Energy = 0.263609
G(1M) = -967.263

Coordinates:
6 -0.383984 -0.155987 -0.507082
1 -0.992262 -0.796928 -1.15655
7 -0.557307 1.20194 -1.00774
7 -1.89365 1.50316 -1.28333
7 -0.839224 -0.3221 0.898863
7 -1.41062 -1.5812 1.08795
1 -1.55606 0.380613 1.09017
1 -2.16104 1.41939 -2.25377
6 -2.77442 1.94816 -0.358494
6 -4.18043 2.16095 -0.859271
1 -4.77523 1.30676 -0.522903
1 -4.24315 2.22842 -1.94697
1 -4.58785 3.06771 -0.410042
8 -2.45178 2.14867 0.812071
1 -0.887814 -2.23494 1.65325
6 -2.69004 -1.83475 0.710641
6 -3.21286 -3.2093 1.05611
1 -2.44492 -3.86847 1.46481
1 -3.63294 -3.65927 0.15414
1 -4.01941 -3.10482 1.78638
8 -3.37066 -0.989491 0.137039
1 -0.181852 1.87123 -0.336392
6 1.05934 -0.59909 -0.614349
6 3.44823 -0.301398 -0.110476
6 2.69771 -2.27193 -1.29126
6 3.72016 -1.54129 -0.747633
1 2.89819 -3.22059 -1.77851
1 4.74711 -1.89309 -0.794025
6 1.36532 -1.79293 -1.22042
6 2.11205 0.177494 -0.03845
1 0.564856 -2.38727 -1.65376
6 2.77681 2.071 1.08414
1 2.49507 3.01182 1.55333
6 4.13827 1.68182 1.06584
6 4.4687 0.495823 0.466313
1 4.88803 2.32147 1.51763
1 5.49924 0.153261 0.422747
7 1.80085 1.3639 0.561976

PYRIDINE
SCF energy= -813.945592233
Zero-point correction= 0.265193
Thermal correction to Energy= 0.282094
Thermal correction to Enthalpy= 0.283038
Thermal correction to Gibbs Free Energy= 0.218650
G(1M)= -813.724

Coordinates:
6 -0.210432 0.35462 0.098124
1 0.104381 -0.043254 1.07311
7 0.351785 1.69295 0.013145
7 1.65053 1.77437 0.519754
7 0.277179 -0.520706 -0.987522
7 0.25992 -1.86319 -0.594491
1 1.25284 -0.277547 -1.16672
1 1.72917 2.23909 1.41374
6 2.75555 1.51048 -0.220724
6 4.07161 1.71691 0.486392
1 4.54256 0.73772 0.607509
1 3.96556 2.18363 1.46694
1 4.71946 2.32967 -0.143205
8 2.68394 1.11979 -1.38321
1 -0.630702 -2.32216 -0.734025
6 1.22587 -2.35778 0.218529
6 1.03974 -3.79208 0.65466
1 0.132479 -4.24523 0.251265
1 1.00355 -3.82334 1.74636
1 1.90644 -4.37376 0.332044
8 2.20471 -1.68724 0.53944
1 0.353838 2.02258 -0.953141
6 -1.73425 0.417345 0.066063
6 -2.42288 1.53162 0.54608
6 -3.81365 1.51725 0.525869
1 -1.86825 2.38697 0.912859
6 -3.69292 -0.673631 -0.410203
6 -4.46833 0.391842 0.037255
1 -4.37649 2.37382 0.884018
1 -4.16568 -1.5737 -0.796594
1 -5.55053 0.335051 0.000897
7 -2.35794 -0.670468 -0.40191

CARBOXYLATE

SCF energy= -985.944934950
Zero-point correction= 0.279167
Thermal correction to Energy= 0.298577
Thermal correction to Enthalpy= 0.299521
Thermal correction to Gibbs Free Energy= 0.228937
G(1M)= -985.713

Coordinates:
6 0.683301 -0.261981 -0.001845
1 1.00677 0.264181 0.899776
7 1.82372 -0.245111 -0.912807
7 2.97399 -0.792769 -0.345162
7 0.296088 -1.65903 0.30871
7 -0.85961 -1.69706 1.11498
1 1.0478 -2.07208 0.861227
1 3.06751 -1.79794 -0.230267
6 4.08003 -0.040926 -0.074753
6 3.95859 1.44191 -0.333998
1 3.12474 1.86886 0.228935
1 3.76377 1.62853 -1.39275
1 4.89283 1.91642 -0.035726
8 5.09295 -0.567409 0.365926
1 -0.95988 -0.89979 1.76386
6 -2.01583 -2.22009 0.616881
6 -1.90319 -3.08691 -0.616103
1 -1.11067 -3.82986 -0.505375
1 -1.65142 -2.46888 -1.48221
1 -2.86323 -3.57601 -0.780501
8 -3.08428 -2.01996 1.18661
1 1.61506 -0.754591 -1.76903
6 -0.499046 0.465966 -0.612412
6 -1.24063 1.41266 0.112808
6 -0.855741 0.184285 -1.93563
6 -2.28627 2.08423 -0.529579
6 -1.91874 0.836791 -2.55166
1 -0.304129 -0.562768 -2.50133
6 -2.63564 1.79966 -1.84455
1 -2.82716 2.83558 0.036947
1 -2.18001 0.597243 -3.57785
1 -3.46276 2.32183 -2.31627
6 -1.00785 1.74779 1.59524
8 -1.23284 2.92503 1.93268
8 -0.644857 0.80071 2.35154

PHENYL
SCF energy= -797.906499987
Zero-point correction= 0.277051
Thermal correction to Energy= 0.294172
Thermal correction to Enthalpy= 0.295116
Thermal correction to Gibbs Free Energy=0.230057
G(1M)= -797.673

Coordinates:
6 -0.297196 0.269397 0.129011
1 0.032167 -0.072746 1.11889
7 0.142527 1.65847 0.031511
7 1.45421 1.84981 0.473612
7 0.305043 -0.583798 -0.914325
7 0.519837 -1.87912 -0.441264
1 1.21109 -0.189015 -1.17289
1 1.53679 2.24238 1.40078
6 2.54707 1.67608 -0.305911
6 3.87009 1.92307 0.373317
1 4.34419 0.949358 0.525431
1 3.77161 2.42339 1.33815
1 4.50541 2.51661 -0.286099
8 2.4623 1.32681 -1.48215
1 -0.053725 -2.60813 -0.842656
6 1.62696 -2.17153 0.291131
6 1.80842 -3.62797 0.647142
1 0.955055 -4.24624 0.363268
1 1.96882 -3.70616 1.72446
1 2.70471 -4.0028 0.146207
8 2.42213 -1.29957 0.627118
1 0.066677 1.99739 -0.928201
6 -1.81602 0.229058 0.072362
6 -2.54037 0.862293 1.08762
6 -2.50478 -0.41878 -0.950592
6 -3.93011 0.847893 1.08047
1 -2.00265 1.3728 1.88285
6 -3.90068 -0.434582 -0.959743
1 -1.94387 -0.905493 -1.74142
6 -4.61576 0.196699 0.052938
1 -4.48039 1.3428 1.87501
1 -4.42698 -0.942188 -1.76258
1 -5.7014 0.182796 0.045814

Reactants - protonated on aromatic

QUINOLINE
SCF energy= -703.536921399
Zero-point correction= 0.228374
Thermal correction to Energy= 0.241955
Thermal correction to Enthalpy= 0.242899
Thermal correction to Gibbs Free Energy= 0.186184
G(1M)= -703.348

Coordinates:
6 2.31843 -2.63748 0.004844
6 3.17857 -1.56305 0.009867
6 2.68541 -0.237005 0.006561
6 1.28388 -0.036427 -0.001907
6 0.943443 -2.39125 -0.003816
1 2.67686 -3.65829 0.007302
1 4.253 -1.71999 0.016606
1 0.199896 -3.17905 -0.008532
6 0.733769 1.28057 -0.005103
6 1.61976 2.33997 -0.000231
1 1.22145 3.35029 -0.002557
6 3.01931 2.15425 0.007684
1 3.66895 3.02177 0.011035
6 3.54774 0.890346 0.011389
1 4.62029 0.727045 0.018115
7 0.482045 -1.14819 -0.006897
6 -0.706168 1.55848 -0.012078
1 -1.01637 2.60666 -0.011
7 -1.5381 0.589338 -0.018616
7 -2.8612 0.816585 -0.025048
1 -3.21917 1.76831 -0.007146
6 -3.71122 -0.274191 -0.012281
6 -5.17312 0.088244 0.044585
1 -5.4022 0.962204 -0.56954
1 -5.44617 0.315844 1.07968
1 -5.75807 -0.765961 -0.294155
8 -3.28493 -1.41263 -0.021204
1 -0.537215 -0.966585 -0.013347

PYRIDINE
SCF energy= -549.948571229
Zero-point correction= 0.181067
Thermal correction to Energy= 0.191890
Thermal correction to Enthalpy= 0.192834
Thermal correction to Gibbs Free Energy= 0.143472
G(1M)= -549.802

Coordinates:
6 -0.014349 1.10418 1.9e-05
1 -0.108285 2.19004 3.9e-05
7 -1.00363 0.292237 2e-05
7 -2.24372 0.771991 4.6e-05
1 -2.41919 1.77659 5.6e-05
6 -3.35257 -0.067105 4.4e-05
6 -3.07221 -1.54505 -1.9e-05
1 -2.49178 -1.82552 0.882347
1 -2.49179 -1.82544 -0.882415
1 -4.02755 -2.06755 -3.7e-05
8 -4.45837 0.432271 2.1e-05
6 1.32793 0.52691 -1e-06
6 2.49368 1.2817 -3e-06
6 2.60527 -1.47583 -3.8e-05
6 3.72418 0.633662 -2.3e-05
1 2.42439 2.36286 1e-05
6 3.78654 -0.760219 -4e-05
1 2.55176 -2.55655 -5e-05
1 4.63779 1.2175 -2.5e-05
1 4.73142 -1.28755 -5.6e-05
7 1.43481 -0.819648 -1.7e-05
1 0.557185 -1.34412 -1.5e-05

CARBOXYLIC ACID

SCF energy= -721.976329582
Zero-point correction= 0.194215
Thermal correction to Energy= 0.208022
Thermal correction to Enthalpy= 0.208966
Thermal correction to Gibbs Free Energy= 0.151850
G(1M)= -721.821

Coordinates:
6 0.440634 0.396328 0.273443
1 0.339285 1.43337 0.592269
7 1.58529 -0.125504 0.040657
7 2.66833 0.660966 0.241248
1 2.56083 1.61922 0.571643
6 3.94599 0.216048 0.004169
6 4.07819 -1.20216 -0.489337
1 3.55314 -1.32734 -1.43941
1 3.63495 -1.90054 0.22454
1 5.13803 -1.41824 -0.617292
8 4.89044 0.964022 0.197943
6 -0.775637 -0.425793 0.126413
6 -0.658971 -1.8208 0.171772
6 -3.18431 -0.69629 -0.078833
6 -1.7767 -2.639 0.077604
1 0.32816 -2.25305 0.295716
6 -3.04717 -2.07748 -0.043874
1 -4.16609 -0.248555 -0.180295
1 -1.65771 -3.71728 0.112491
1 -3.92508 -2.71152 -0.107505
6 -2.06197 0.135852 -0.005216
6 -2.25694 1.60922 -0.126983
8 -1.40142 2.40812 -0.442605
8 -3.51789 1.98448 0.135366
1 -3.56859 2.94721 -0.006076

Addition transition states - protonated on aromatic

QUINOLINE
SCF energy= -1044.31943225
Zero-point correction= 0.345286
Thermal correction to Energy= 0.365461
Thermal correction to Enthalpy= 0.366406
Thermal correction to Gibbs Free Energy= 0.296578
G(1M)= -1044.02

Coordinates:
6 0.820396 0.475027 0.157046
1 0.864997 -0.227232 0.994151
7 1.83284 1.46446 0.256332
7 2.86997 1.09171 1.11841
7 1.13724 -0.38838 -1.11786
1 1.49787 0.382196 -1.85487
7 0.144445 -1.2319 -1.63072
1 3.05434 1.74176 1.87107
6 3.67679 0.029074 0.966208
6 4.79587 -0.098959 1.97144
1 5.74401 -0.136181 1.42961
1 4.68024 -1.04439 2.50657
1 4.82535 0.721221 2.69058
8 3.52048 -0.825107 0.080045
1 -0.128376 -1.06364 -2.59113
6 -0.104304 -2.41049 -0.996952
6 -0.964164 -3.39285 -1.73933
1 -1.68006 -3.82833 -1.04078
1 -0.320482 -4.1941 -2.11356
1 -1.49155 -2.93989 -2.5798
8 0.347383 -2.60597 0.12975
8 2.26681 1.58743 -2.17054
1 2.19469 1.73076 -1.0117
1 1.76122 2.28166 -2.61837
6 -0.564732 1.07074 -0.013812
6 -3.01115 1.03476 0.336783
6 -1.98146 2.91763 -0.761219
6 -3.1111 2.29957 -0.293219
1 -4.08907 2.75978 -0.388571
1 1.99578 -0.910651 -0.838831
6 -0.717988 2.30503 -0.606378
6 -1.73556 0.423566 0.454447
6 -2.75015 -1.44653 1.53683
6 -4.1417 0.360737 0.853969
6 -4.01819 -0.869638 1.45834
1 0.170677 2.82983 -0.939112
1 -2.04575 3.88823 -1.23989
1 -5.11524 0.833269 0.764531
1 -4.87046 -1.40115 1.86036
1 -2.56792 -2.41994 1.97558
7 -1.68734 -0.811328 1.05559
1 -0.793106 -1.31194 1.09284

PYRIDINE
SCF energy= -890.732752319
Zero-point correction= 0.297880
Thermal correction to Energy= 0.316627
Thermal correction to Enthalpy= 0.317571
Thermal correction to Gibbs Free Energy= 0.249266
G(1M)= -890.48

Coordinates:
6 0.201719 0.39532 0.224122
1 0.505029 -0.087235 1.15842
7 0.969521 1.54769 -0.097046
7 2.20486 1.56942 0.557992
7 0.386359 -0.680717 -0.874014
1 0.459643 -0.091152 -1.83112
7 -0.556774 -1.71547 -0.848794
1 2.39212 2.40589 1.09427
6 3.16181 0.631494 0.435592
6 4.45876 0.915184 1.15363
1 5.2737 0.859475 0.428196
1 4.62321 0.135864 1.90158
1 4.47704 1.89111 1.64163
8 2.99809 -0.419871 -0.198055
1 -1.09769 -1.84291 -1.69608
6 -0.301177 -2.75983 0.013962
6 -1.2037 -3.95236 -0.141542
1 -2.1693 -3.68393 -0.573529
1 -1.3469 -4.41134 0.836653
1 -0.714794 -4.67806 -0.798341
8 0.598744 -2.6669 0.829405
8 0.976695 1.0937 -2.51892
1 1.04798 1.53744 -1.4201
1 0.403103 1.63095 -3.08445
6 -1.26528 0.754245 0.255449
6 -3.24809 0.879603 1.55849
6 -3.2594 1.70131 -0.682913
6 -3.93313 1.46813 0.518314
1 -3.68106 0.660763 2.52543
1 -3.77816 2.16289 -1.51573
1 -4.97307 1.73803 0.647935
1 1.35303 -1.02719 -0.700198
7 -1.95386 0.540943 1.39052
6 -1.92282 1.34782 -0.811897
1 -1.3718 1.5253 -1.72751
1 -1.47321 0.100081 2.17361

CARBOXYLIC ACID
SCF energy= -1062.76183422
Zero-point correction= 0.312487
Thermal correction to Energy= 0.333740
Thermal correction to Enthalpy= 0.334684
Thermal correction to Gibbs Free Energy= 0.261820
G(1M)= -1062.5

Coordinates:
6 -0.486333 -0.000527 -0.450497
1 -0.946013 -0.782817 -1.05732
7 -1.18319 1.24145 -0.568584
7 -2.4576 1.08193 -1.13037
7 -0.657912 -0.512595 1.01503
1 -0.695027 0.374758 1.64384
7 0.246759 -1.4821 1.46413
1 -2.64435 1.65453 -1.94252
6 -3.43395 0.298223 -0.643164
6 -4.74868 0.347797 -1.3854
1 -5.54232 0.571415 -0.668841
1 -4.94984 -0.639303 -1.80922
1 -4.76498 1.09071 -2.18469
8 -3.28239 -0.452713 0.331846
1 1.10101 -1.09671 1.85348
6 0.208303 -2.70535 0.840553
6 1.36948 -3.61093 1.15205
1 2.13983 -3.45836 0.389398
1 1.03175 -4.64601 1.10258
1 1.80283 -3.40562 2.1325
8 -0.716275 -2.9955 0.099586
8 -1.25097 1.84792 1.82338
1 -1.26941 1.73203 0.602042
1 -0.662629 2.59225 2.01673
6 0.979991 0.087216 -0.830929
6 2.68119 -0.549576 -2.45028
6 3.17935 1.12369 -0.797886
6 3.57224 0.361558 -1.89528
1 2.97609 -1.15689 -3.29968
1 3.87007 1.82907 -0.345727
1 4.56931 0.478446 -2.30625
1 -1.62833 -0.879033 1.01988
6 1.90391 0.974849 -0.255006
6 1.39699 -0.674395 -1.92358
1 0.695649 -1.37033 -2.376
6 1.61592 1.77095 0.9789
8 1.5319 0.972157 2.0618
8 1.53326 2.9716 1.04466
1 1.3252 1.52236 2.84128

Addition intermediates - protonated on aromatic

QUINOLINE
SCF energy= -967.977639934
Zero-point correction= 0.326177
Thermal correction to Energy= 0.345651
Thermal correction to Enthalpy= 0.346595
Thermal correction to Gibbs Free Energy= 0.277577
G(1M)= -967.697

Coordinates:
6 -0.443754 0.446609 -0.411479
1 -0.982653 0.317454 -1.35599
7 -0.889864 1.72055 0.132262
7 -2.27024 1.90155 0.055439
7 -0.757788 -0.707601 0.473219
7 -1.06784 -1.84804 -0.270948
1 -1.56513 -0.454895 1.05319
1 -2.57803 2.51548 -0.685751
6 -3.1473 1.40378 0.961638
6 -4.59845 1.68308 0.673381
1 -5.01985 0.770995 0.240128
1 -4.74643 2.50785 -0.025716
1 -5.11477 1.89395 1.61061
8 -2.77658 0.748238 1.93365
1 -0.432986 -2.63062 -0.193024
6 -2.30967 -1.98256 -0.819951
6 -2.57386 -3.29267 -1.51917
1 -1.69868 -3.94343 -1.55095
1 -2.90433 -3.08136 -2.53838
1 -3.38698 -3.80701 -1.00139
8 -3.13592 -1.08245 -0.742158
1 -0.58074 1.86514 1.09356
6 1.04538 0.548308 -0.724099
6 3.45195 0.26501 -0.225142
6 2.77013 1.44647 -2.21116
6 3.77482 0.976319 -1.40574
1 3.00403 1.99099 -3.11896
1 4.81914 1.13925 -1.65144
6 1.41932 1.23138 -1.86129
6 2.08734 0.050664 0.101305
1 0.639297 1.62725 -2.50601
6 2.74018 -1.12555 2.06565
1 2.38697 -1.67308 2.9309
6 4.09737 -0.920161 1.79513
6 4.44295 -0.236823 0.65271
1 4.84076 -1.30907 2.47823
1 5.48786 -0.070456 0.40814
7 1.81401 -0.653383 1.24737
1 0.796236 -0.839373 1.38879

PYRIDINE
SCF energy= -814.394547595
Zero-point correction= 0.279141
Thermal correction to Energy= 0.296013
Thermal correction to Enthalpy= 0.296957
Thermal correction to Gibbs Free Energy= 0.233725
G(1M)= -814.158

Coordinates:
6 -0.316589 0.212351 0.259327
1 0.008083 -0.165979 1.23437
7 0.065933 1.61155 0.191232
7 1.396 1.84105 0.532815
7 0.22147 -0.640082 -0.815409
7 0.648742 -1.88313 -0.348644
1 0.997466 -0.14824 -1.26829
1 1.54292 2.24361 1.44788
6 2.41098 1.71071 -0.358275
6 3.78592 1.99575 0.182157
1 4.26401 1.02902 0.364726
1 3.77112 2.56559 1.11271
1 4.36133 2.53338 -0.572515
8 2.20882 1.36179 -1.51925
1 0.16495 -2.68971 -0.718641
6 1.84827 -2.01776 0.289399
6 2.24765 -3.43549 0.617035
1 1.45191 -4.15791 0.428468
1 2.53736 -3.48028 1.66862
1 3.12097 -3.6998 0.015216
8 2.5346 -1.04536 0.571041
1 -0.114293 2.0045 -0.733213
6 -1.83919 0.180587 0.21265
6 -2.6601 0.776465 1.1571
6 -4.03866 0.694331 0.998422
1 -2.20895 1.29578 1.99419
6 -3.72836 -0.545971 -1.02148
6 -4.58215 0.026563 -0.101773
1 -4.69546 1.15081 1.7307
1 -4.05154 -1.08035 -1.90503
1 -5.65225 -0.049482 -0.245068
7 -2.40132 -0.446778 -0.828734
1 -1.72731 -0.845833 -1.49464

CARBOXYLIC ACID

SCF energy= -986.419659617
Zero-point correction= 0.292253
Thermal correction to Energy= 0.312013
Thermal correction to Enthalpy= 0.312957
Thermal correction to Gibbs Free Energy= 0.242683
G(1M)= -986.174

Coordinates:
6 -0.042632 -0.129207 0.328733
1 -0.341879 0.007915 -0.712444
7 -0.23882 1.16925 0.972352
7 -1.34502 1.84894 0.456156
7 -0.877564 -1.17083 0.958364
7 -1.22415 -2.15726 0.031554
1 -1.74004 -0.718998 1.27265
1 -1.12554 2.43344 -0.340381
6 -2.61625 1.61113 0.852866
6 -3.68301 2.33449 0.071867
1 -4.14668 1.60303 -0.59646
1 -3.28975 3.16032 -0.523609
1 -4.44298 2.70591 0.760816
8 -2.87605 0.859636 1.79256
1 -0.853601 -3.08291 0.195694
6 -2.189 -1.93528 -0.899927
6 -2.53408 -3.11723 -1.77485
1 -1.86728 -3.9683 -1.62572
1 -2.49099 -2.80215 -2.81944
1 -3.56054 -3.42472 -1.55886
8 -2.74085 -0.844657 -1.00772
1 -0.369793 1.06032 1.97825
6 1.43725 -0.477418 0.371633
6 3.74674 0.038546 -0.188067
6 3.24499 -1.91924 1.10947
6 4.17826 -1.10015 0.485414
1 4.46616 0.688322 -0.673478
1 3.56834 -2.80545 1.64692
1 5.23588 -1.33934 0.523499
6 1.88753 -1.60348 1.05444
6 2.38746 0.354229 -0.255849
1 1.1616 -2.23038 1.55992
6 1.98272 1.56918 -1.02676
8 0.89977 1.7714 -1.53542
8 2.98462 2.4557 -1.13763
1 2.65604 3.19222 -1.68447

Reactants - protonated on hydrazone

QUINOLINE
SCF energy= -703.525684514
Zero-point correction= 0.227900
Thermal correction to Energy= 0.241456
Thermal correction to Enthalpy= 0.242400
Thermal correction to Gibbs Free Energy= 0.186548
G(1M)= -703.336

Coordinates:
6 0.62866 1.58958 7.9e-05
1 0.938577 2.63197 0.000393
7 1.54052 0.678645 -0.000262
7 2.87896 0.872876 0.000134
1 3.23094 1.82339 0.004467
6 3.67278 -0.26437 -0.000102
6 5.14863 0.00966 0.001029
1 5.4263 0.59003 0.884855
1 5.42813 0.582238 -0.887352
1 5.67593 -0.942789 0.005667
8 3.14547 -1.35862 -0.002064
6 -0.783052 1.26956 -0.0001
6 -1.2758 -0.078023 5.9e-05
6 -1.67719 2.32632 -0.000296
6 -2.67614 -0.292462 0.000206
6 -3.06847 2.10415 -0.000364
1 -1.29906 3.34441 -0.000384
6 -3.55749 0.821134 -5.6e-05
1 -3.74372 2.95167 -0.000782
1 -4.62788 0.637241 3e-06
6 -0.849511 -2.34132 0.00024
6 -3.13578 -1.63227 0.000462
6 -2.22519 -2.65789 0.000429
1 -0.104823 -3.13275 0.000118
1 -2.53726 -3.69539 0.000619
1 -4.20422 -1.82762 0.00068
7 -0.388611 -1.10739 1e-06
1 1.2285 -0.32669 -0.000389

PYRIDINE

SCF energy= -549.931673027
Zero-point correction= 0.179955
Thermal correction to Energy= 0.190534
Thermal correction to Enthalpy= 0.191478
Thermal correction to Gibbs Free Energy= 0.142423
G(1M)= -549.786

Coordinates:
6 0.091007 1.12056 0.008245
1 -0.029057 2.1991 0.011179
7 -0.946466 0.365978 0.012313
7 -2.24554 0.731307 0.024162
1 -2.46752 1.72039 -0.015066
6 -3.17853 -0.30279 0.008983
6 -4.6071 0.147716 -0.031505
1 -4.83983 0.524679 -1.03184
1 -4.78685 0.947831 0.689832
1 -5.24435 -0.706622 0.19089
8 -2.78269 -1.44958 0.017106
1 -0.817529 -0.661002 0.01199
6 1.40859 0.486491 0.000877
6 2.56168 1.26308 -0.002419
6 3.78731 0.596719 -0.007075
1 2.50245 2.34608 -0.000961
6 2.56792 -1.47449 -0.005009
6 3.79146 -0.789877 -0.008292
1 4.71563 1.15688 -0.009524
1 2.54271 -2.56019 -0.005984
1 4.71998 -1.34895 -0.011751
7 1.39657 -0.855293 -0.00054

CARBOXYLIC ACID

SCF energy= -722.402725011
Zero-point correction= 0.206918
Thermal correction to Energy= 0.221016
Thermal correction to Enthalpy= 0.221960
Thermal correction to Gibbs Free Energy= 0.164024
G(1M)= -722.236

Coordinates:
6 0.240828 1.28279 -0.027506
1 0.422007 2.3546 -0.041196
7 1.28482 0.534242 -0.02695
7 2.55913 0.987456 -0.046715
1 2.71119 1.98949 -0.020009
6 3.57447 0.040278 0.002447
6 4.95678 0.623691 0.041902
1 5.13735 1.06681 1.02569
1 5.07647 1.40299 -0.714311
1 5.67462 -0.176416 -0.13084
8 3.28961 -1.13854 0.019193
1 1.18044 -0.513988 -0.016917
6 -1.16283 0.87866 -0.0095
6 -2.01516 1.99337 -0.001278
6 -1.74983 -0.418933 0.000357
6 -3.39904 1.8648 0.017059
1 -1.58111 2.98791 -0.009086
6 -3.13954 -0.525429 0.017967
6 -3.9637 0.598757 0.02678
1 -4.02178 2.75209 0.02315
1 -3.58639 -1.51117 0.025127
1 -5.04059 0.473235 0.041032
6 -0.980395 -1.69843 -0.007755
8 0.235302 -1.809 -0.014676
8 -1.75794 -2.77164 -0.006748
1 -1.18517 -3.56131 -0.011961

PHENYL
SCF energy= -533.889342364
Zero-point correction= 0.192610
Thermal correction to Energy= 0.203942
Thermal correction to Enthalpy= 0.204886
Thermal correction to Gibbs Free Energy= 0.154163
G(1M)= -533.732

Coordinates:
6 0.183028 -0.237924 -0.523806
1 0.588495 -1.22343 -0.732953
7 1.02913 0.738752 -0.609254
7 2.37354 0.499515 -0.748419
1 2.86336 1.20141 -1.29204
6 3.02677 -0.186347 0.28759
6 4.52396 -0.087798 0.215274
1 4.84012 0.852354 0.677434
1 4.87428 -0.099399 -0.818885
1 4.95704 -0.920892 0.76707
8 2.39382 -0.801962 1.11319
1 0.752386 1.70763 -0.447665
6 -1.21438 -0.090632 -0.208165
6 -2.02256 -1.22497 -0.388857
6 -1.77918 1.11455 0.248035
6 -3.38623 -1.14937 -0.141761
1 -1.57793 -2.15512 -0.729714
6 -3.13972 1.17883 0.495119
1 -1.16701 1.99166 0.434477
6 -3.94194 0.050849 0.296514
1 -4.01229 -2.02265 -0.286576
1 -3.579 2.1035 0.85207
1 -5.00716 0.109694 0.495289

PHENOL

SCF energy= -609.097565398
Zero-point correction= 0.196470
Thermal correction to Energy= 0.209010
Thermal correction to Enthalpy= 0.209954
Thermal correction to Gibbs Free Energy= 0.156448
G(1M)= -608.938

Coordinates:
6 -0.012607 1.06496 0.036674
1 -0.150448 2.14364 0.042564
7 -1.08343 0.341166 0.04915
7 -2.35953 0.810932 0.079584
1 -2.5023 1.80971 -0.017302
6 -3.36153 -0.140776 0.005009
6 -4.75368 0.410016 -0.085777
1 -5.02171 0.505467 -1.1423
1 -4.84275 1.3886 0.388541
1 -5.43668 -0.296897 0.384632
8 -3.06097 -1.3195 0.003037
1 -1.04898 -0.688632 0.044963
6 1.32941 0.551003 0.012113
6 2.38212 1.48594 -0.006354
6 1.63405 -0.827871 0.005869
6 3.69829 1.06655 -0.031322
1 2.14239 2.54503 -0.000665
6 2.96039 -1.24891 -0.020247
6 3.97877 -0.304027 -0.038291
1 4.50377 1.79107 -0.045513
1 3.1869 -2.31064 -0.025026
1 5.00913 -0.643708 -0.057827
8 0.591327 -1.68537 0.026617
1 0.887392 -2.6106 0.023524

BENZOFURAN

SCF energy= -685.272495918
Zero-point correction= 0.209459
Thermal correction to Energy= 0.222561
Thermal correction to Enthalpy= 0.223505
Thermal correction to Gibbs Free Energy= 0.168737
G(1M)= -685.101

Coordinates:

6	-0.430076	1.45856	0.042347
1	-0.700453	2.51131	0.054951
7	-1.39154	0.595622	0.040142
7	-2.72106	0.878539	0.059385
1	-3.00298	1.83366	-0.132038
6	-3.57162	-0.217231	0.013499
6	-5.02654	0.121129	-0.109364
1	-5.25524	0.329712	-1.15883
1	-5.28475	1.00037	0.483978
1	-5.61061	-0.737764	0.21805
8	-3.09534	-1.3342	0.067523
1	-1.22892	-0.423078	0.040788
6	0.95464	1.07646	0.020422
6	1.95721	2.05729	0.003781
6	1.38769	-0.255393	0.00819
6	3.30831	1.70561	-0.024037
1	1.66913	3.10379	0.011506
6	2.73141	-0.630967	-0.02052
6	3.70871	0.371403	-0.036727
1	4.0568	2.48956	-0.037111
1	4.76245	0.11392	-0.058931
8	0.586376	-1.34315	0.020654
6	2.71933	-2.07711	-0.026448
6	1.42188	-2.44084	-0.001653
1	3.57068	-2.74057	-0.046137
1	0.91818	-3.39472	0.00472

DIHYDROBENZOPYRAN

SCF energy= -725.784554268
Zero-point correction= 0.262844
Thermal correction to Energy= 0.277615
Thermal correction to Enthalpy= 0.278559
Thermal correction to Gibbs Free Energy= 0.219844
G(1M)= -725.562

Coordinates:
6 0.724367 -1.57829 0.053777
1 1.07071 -2.60857 0.086625
7 1.631 -0.656746 0.046949
7 2.97537 -0.853863 0.081411
1 3.32329 -1.80419 0.030151
6 3.7602 0.283716 0.017237
6 5.23754 0.030091 -0.045358
1 5.52054 -0.152276 -1.08647
1 5.52799 -0.836449 0.551385
1 5.75558 0.919689 0.310882
8 3.22275 1.37503 -0.003121
6 -0.691564 -1.33452 0.016355
6 -1.53537 -2.4597 0.022428
6 -1.25846 -0.038766 -0.03485
6 -2.90758 -2.30191 -0.018808
6 -2.64729 0.129531 -0.063613
6 -3.44485 -1.01341 -0.055285
1 -3.55968 -3.16722 -0.013518
1 -4.52411 -0.88387 -0.069349
1 -1.09345 -3.45073 0.060363
8 -0.391337 0.99772 -0.033613
6 -3.24329 1.51804 -0.073416
6 -2.22101 2.53702 0.425703
6 -0.90916 2.31793 -0.30067
1 -1.03411 2.41356 -1.38475
1 -0.122193 2.99392 0.032519
1 -2.56521 3.55818 0.243732
1 -2.05831 2.42331 1.50282
1 1.37957 0.341586 0.016647
1 -3.55354 1.77598 -1.09326
1 -4.14417 1.531 0.546562

DIHYDROBENZOFURAN

SCF energy= -686.482760246
Zero-point correction= 0.233282
Thermal correction to Energy= 0.246985
Thermal correction to Enthalpy= 0.247929
Thermal correction to Gibbs Free Energy= 0.191973
G(1M)= -686.288

Coordinates:
6 -0.476873 1.49474 0.025932
1 -0.767447 2.54243 0.018755
7 -1.42602 0.615557 0.033716
7 -2.7604 0.882957 0.041889
1 -3.05326 1.82882 -0.175115
6 -3.59902 -0.21877 0.027996
6 -5.05852 0.10066 -0.102224
1 -5.31885 0.128747 -1.16454
1 -5.30672 1.06436 0.345788
1 -5.62986 -0.693067 0.378209
8 -3.11653 -1.33215 0.111271
1 -1.23519 -0.398812 0.050698
6 0.912255 1.14153 0.017765
6 1.90337 2.1491 -0.006827
6 1.35068 -0.188273 0.020253
6 3.24505 1.81911 -0.028972
1 1.59253 3.18939 -0.01166
6 2.69851 -0.530832 6e-05
6 3.65053 0.471135 -0.022201
1 3.99213 2.60404 -0.050975
1 4.70743 0.222977 -0.033889
8 0.519863 -1.24613 0.044688
6 2.79092 -2.03678 0.051878
6 1.31755 -2.45723 -0.130729
1 3.18885 -2.36982 1.01461
1 3.42464 -2.44668 -0.737033
1 0.966334 -3.17596 0.607459
1 1.111 -2.82617 -1.1368

CARBOXYLATE

SCF energy= -721.984949019
Zero-point correction= 0.197089
Thermal correction to Energy= 0.209889
Thermal correction to Enthalpy= 0.210833
Thermal correction to Gibbs Free Energy= 0.156563
G(1M)= -721.825

Coordinates:
6 -0.162059 -0.459981 0.822991
1 -0.320763 -0.75691 1.86241
7 -1.05835 -1.21307 -0.0068
7 -2.3997 -1.01506 0.342462
1 -2.84156 -1.81759 0.773689
6 -3.16511 -0.151573 -0.394225
6 -4.64325 -0.194286 -0.090953
1 -5.0137 0.829928 -0.023384
1 -4.8695 -0.725086 0.835429
1 -5.15903 -0.686667 -0.919968
8 -2.67409 0.579999 -1.24053
1 -0.946585 -0.93376 -0.983379
6 1.26188 -0.61545 0.357113
6 1.76727 0.64029 0.065737
6 2.03064 -1.75606 0.174384
6 3.06123 0.82691 -0.405135
6 3.33282 -1.58314 -0.295951
6 3.84455 -0.31016 -0.579922
1 3.43714 1.82067 -0.626592
1 3.96372 -2.45308 -0.448795
1 4.86184 -0.214268 -0.944575
1 1.63584 -2.74447 0.385771
6 0.703296 1.63659 0.327573
8 -0.39313 0.971003 0.771596
8 0.726133 2.83391 0.200191

Addition transition states - protonated on hydrazone

QUINOLINE
SCF energy= -967.951891105
Zero-point correction= 0.322615
Thermal correction to Energy= 0.342690
Thermal correction to Enthalpy= 0.343634
Thermal correction to Gibbs Free Energy= 0.272421
G(1M)= -967.676

Coordinates:
6 1.18273 0.455889 -0.276951
1 1.62457 1.32455 -0.753974
7 2.01432 -0.304934 0.395643
7 3.30842 0.104915 0.617216
7 0.290566 1.79104 1.24702
7 -0.730916 2.64153 0.802804
1 0.943006 2.3255 1.82289
1 3.57842 0.189722 1.59
6 4.2523 -0.091439 -0.378198
6 5.67097 0.135661 0.075618
1 6.07151 -0.806768 0.461352
1 5.73476 0.887133 0.865149
1 6.26798 0.445333 -0.781604
8 3.92585 -0.401401 -1.50493
1 -0.446527 3.34798 0.136362
6 -2.00899 2.1623 0.824697
6 -3.03659 3.01722 0.131896
1 -2.59891 3.86158 -0.403496
1 -3.74044 3.39226 0.878933
1 -3.59045 2.38795 -0.568818
8 -2.27547 1.12077 1.41222
1 1.67168 -1.19071 0.783749
6 -0.120061 -0.003797 -0.751062
6 -0.751912 0.762922 -1.71053
6 -0.788262 -1.14323 -0.197189
6 -2.05154 0.44378 -2.16191
1 -0.241369 1.62645 -2.12822
6 -2.09752 -1.44971 -0.645678
6 -2.71332 -0.634322 -1.63179
1 -2.51957 1.06132 -2.92049
1 -3.71793 -0.884424 -1.96092
1 -0.176123 1.10455 1.84857
6 -2.74548 -2.56899 -0.070204
6 -2.09608 -3.30333 0.888449
1 -2.55838 -4.16518 1.35488
6 -0.79227 -2.91568 1.26729
1 -0.25569 -3.48263 2.02362
1 -3.74947 -2.82778 -0.394441
7 -0.157237 -1.88332 0.751812

PYRIDINE
SCF energy= -814.361273051
Zero-point correction= 0.274959
Thermal correction to Energy= 0.292709
Thermal correction to Enthalpy= 0.293653
Thermal correction to Gibbs Free Energy= 0.227499
G(1M)= -814.131

Coordinates:
6 0.962851 -0.028829 -0.236559
1 1.24149 0.533172 -1.11774
7 1.82346 -0.131171 0.726464
7 3.05784 0.466221 0.67081
7 -0.374014 1.90456 0.33202
7 -1.59856 2.05405 -0.344805
1 0.05138 2.82694 0.431389
1 3.36983 0.867599 1.5475
6 3.97157 0.009298 -0.279059
6 5.37532 0.498466 -0.04933
1 5.86628 -0.161101 0.672731
1 5.38768 1.51579 0.347377
1 5.91782 0.459236 -0.993
8 3.61338 -0.692674 -1.19889
1 -1.51661 2.20334 -1.34222
6 -2.69172 1.42643 0.172862
6 -3.91755 1.42074 -0.703499
1 -3.7021 1.69103 -1.73891
1 -4.64483 2.1277 -0.29551
1 -4.36001 0.422918 -0.669569
8 -2.66486 0.942865 1.29961
1 1.59476 -0.734839 1.5208
6 -0.252335 -0.847619 -0.183942
6 -2.28954 -1.6425 -1.12998
6 -1.56837 -2.1973 1.09315
6 -2.52122 -2.29682 0.070842
1 -2.99979 -1.70928 -1.94738
1 -1.71941 -2.70936 2.0391
1 -3.41827 -2.88569 0.225463
1 -0.639405 1.59075 1.27054
7 -0.450568 -1.49486 0.97274
6 -1.12369 -0.888192 -1.26682
1 -0.895922 -0.353338 -2.18291

CARBOXYLIC ACID

SCF energy= -986.821527902
Zero-point correction= 0.302144
Thermal correction to Energy= 0.322535
Thermal correction to Enthalpy= 0.323479
Thermal correction to Gibbs Free Energy= 0.251561
G(1M)= -986.567

Coordinates:
6 -1.13621 -0.190654 0.61469
1 -1.51052 -0.0983 1.62979
7 -1.85433 0.416428 -0.282254
7 -2.9136 1.21707 0.103126
7 0.516538 1.49839 1.12464
7 1.83204 1.02714 1.11071
1 0.357341 2.11739 1.9209
1 -2.76454 2.21246 -0.041998
6 -4.23026 0.768108 -0.056933
6 -4.41456 -0.715573 -0.234898
1 -3.98006 -1.26814 0.603311
1 -3.9289 -1.05938 -1.15282
1 -5.48297 -0.917117 -0.289284
8 -5.12731 1.57747 0.005905
1 1.97874 0.128194 1.5559
6 2.94623 1.74344 0.755284
6 2.69277 3.11273 0.171511
1 2.1449 3.748 0.873265
1 2.10226 3.03811 -0.74836
1 3.65465 3.56823 -0.0584
8 4.05539 1.25011 0.875715
1 -1.55121 0.42939 -1.25897
6 -0.146702 -1.24303 0.355018
6 0.530065 -3.45386 1.10149
6 1.64235 -2.42147 -0.769251
6 1.47439 -3.50991 0.086571
1 0.409124 -4.28113 1.79178
1 2.41001 -2.44703 -1.53347
1 2.10186 -4.38661 -0.031545
1 0.337675 2.01438 0.26418
6 0.841111 -1.28923 -0.656359
6 -0.259355 -2.3154 1.24582
6 1.12127 -0.122165 -1.54273
8 0.355323 0.803984 -1.73867
8 2.32306 -0.183179 -2.10521
1 2.42598 0.590574 -2.69076
1 -0.987186 -2.26728 2.04981

PHENYL
SCF energy= -798.320269593
Zero-point correction= 0.286939
Thermal correction to Energy= 0.304951
Thermal correction to Enthalpy= 0.305895
Thermal correction to Gibbs Free Energy= 0.238278
G(1M)= -798.079

Coordinates:
6 -0.92629 -0.093754 0.127998
1 -1.19336 0.387216 1.06174
7 -1.86131 -0.102167 -0.782376
7 -3.05869 0.535669 -0.558277
7 0.275725 1.91532 -0.286641
7 1.46126 2.02823 0.461235
1 -0.180617 2.82825 -0.309144
1 -3.31852 1.22877 -1.25033
6 -4.00299 -0.094603 0.244857
6 -5.35848 0.557919 0.213478
1 -5.95352 0.090546 -0.576908
1 -5.29377 1.6289 0.012826
1 -5.85023 0.387184 1.17073
8 -3.70969 -1.06601 0.907495
1 1.33445 2.00889 1.46464
6 2.61474 1.55831 -0.094267
6 3.79583 1.46224 0.836171
1 3.54168 1.67993 1.87517
1 4.56363 2.16331 0.499668
1 4.20529 0.451619 0.766298
8 2.66911 1.27384 -1.28517
1 -1.77304 -0.630864 -1.64734
6 0.287501 -0.888514 0.051473
6 1.04389 -1.0118 1.22429
6 0.739417 -1.47198 -1.14154
6 2.24036 -1.72017 1.20782
1 0.685729 -0.563464 2.14683
6 1.93477 -2.17328 -1.15178
1 0.18235 -1.36638 -2.06779
6 2.68581 -2.29548 0.019891
1 2.82313 -1.81756 2.11752
1 2.28951 -2.61862 -2.07473
1 3.6226 -2.84316 0.0034
1 0.593149 1.71022 -1.23913

PHENOL
SCF energy= -873.525343997
Zero-point correction= 0.291503
Thermal correction to Energy= 0.310377
Thermal correction to Enthalpy= 0.311322
Thermal correction to Gibbs Free Energy= 0.242179
G(1M)= -873.28

Coordinates:
6 0.922517 0.045785 0.3743
1 1.29261 -0.132687 1.37815
7 1.79646 -0.161623 -0.584218
7 3.03088 -0.691069 -0.291667
7 -0.20488 -1.90663 0.474432
7 -1.50862 -1.81724 0.98628
1 0.256412 -2.72283 0.878364
1 3.25198 -1.5667 -0.751053
6 4.02473 0.159214 0.172735
6 5.39379 -0.467151 0.208232
1 5.87903 -0.306004 -0.759235
1 5.34833 -1.54136 0.397934
1 5.98272 0.022961 0.982906
8 3.76865 1.2914 0.523691
1 -1.57033 -1.38416 1.90024
6 -2.52186 -1.63302 0.086249
6 -3.84665 -1.22814 0.674966
1 -3.84659 -1.23472 1.76619
1 -4.61591 -1.90934 0.305759
1 -4.08653 -0.221272 0.320647
8 -2.33497 -1.80811 -1.11193
1 1.58602 0.085152 -1.5494
6 -0.287449 0.83274 0.214821
6 -0.87835 1.38031 1.36391
6 -0.925325 0.991206 -1.02916
6 -2.0553 2.10649 1.27809
6 -2.11119 1.71694 -1.11726
6 -2.66383 2.27303 0.031035
1 -2.49955 2.53493 2.16875
1 -2.59552 1.83809 -2.08145
1 -3.58769 2.83707 -0.048755
1 -0.32625 -2.07715 -0.529473
8 -0.343681 0.396407 -2.09419
1 -0.899202 0.477281 -2.88646
1 -0.392899 1.23457 2.32503

BENZOFURAN
SCF energy= -949.702123937
Zero-point correction= 0.303656
Thermal correction to Energy= 0.323377
Thermal correction to Enthalpy = 0.324321
Thermal correction to Gibbs Free Energy= 0.252855
G(1M)= -949.446

Coordinates:
6 -1.1785 -0.208818 -0.590601
1 -1.67388 -0.727235 -1.40363
7 -1.92192 0.05049 0.46004
7 -3.20094 -0.445535 0.54696
7 -0.146851 -2.16123 -0.036443
7 1.18872 -2.27382 -0.455371
1 -0.629254 -3.03918 -0.232756
1 -3.38222 -1.05288 1.33773
6 -4.22382 0.240311 -0.095483
6 -5.60172 -0.234795 0.28212
1 -5.93316 0.316538 1.16731
1 -5.61731 -1.3017 0.513373
1 -6.28318 -0.021738 -0.540758
8 -3.98357 1.122 -0.891814
1 1.32222 -2.16206 -1.45359
6 2.15138 -1.8238 0.406797
6 3.53892 -1.7145 -0.168684
1 3.54975 -1.741 -1.25992
1 4.14253 -2.54253 0.213194
1 3.9825 -0.779775 0.180076
8 1.88049 -1.58771 1.57821
1 -1.58277 0.638936 1.2199
6 0.083043 0.460555 -0.833592
6 0.661631 0.440591 -2.10703
6 0.845621 1.03556 0.185991
6 1.92576 0.996483 -2.33675
6 2.12094 1.57384 -0.011413
6 2.66603 1.55939 -1.30138
1 2.33783 0.970933 -3.33914
1 3.65413 1.96753 -1.48745
1 -0.093343 -2.05334 0.981669
8 0.492176 1.10538 1.4883
1 0.114856 -0.015904 -2.92688
6 2.55995 1.99135 1.30057
6 1.55474 1.68114 2.14512
1 1.42177 1.80037 3.20917
1 3.49994 2.45256 1.5639

DIHYDROBENZOPYRAN

SCF energy= -990.213879702
Zero-point correction= 0.357549
Thermal correction to Energy= 0.378516
Thermal correction to Enthalpy= 0.379460
Thermal correction to Gibbs Free Energy= 0.306658
G(1M)= -989.904

Coordinates:
6 -1.31037 -0.523502 -0.434903
1 -1.82568 -1.36383 -0.88883
7 -2.07075 0.258459 0.301395
7 -3.35408 -0.12025 0.618563
7 -0.376566 -1.872 1.05983
7 0.82357 -2.47099 0.651347
1 -0.966472 -2.57305 1.51059
1 -3.51901 -0.336027 1.59519
6 -4.39182 0.273988 -0.213071
6 -5.75955 0.025309 0.368482
1 -6.05177 0.894012 0.966255
1 -5.777 -0.857827 1.01026
1 -6.47126 -0.094094 -0.44771
8 -4.17851 0.757384 -1.30445
1 0.769887 -2.95519 -0.237294
6 1.99129 -1.8654 1.02166
6 3.22564 -2.34631 0.308324
1 3.55883 -1.55606 -0.372237
1 3.05409 -3.2603 -0.262716
1 4.01197 -2.51535 1.04584
8 2.00067 -0.996383 1.88672
1 -1.70414 1.12705 0.685231
6 -0.029303 -0.118328 -0.990612
6 0.419843 -0.75939 -2.15273
6 0.812283 0.79611 -0.326734
6 1.66946 -0.46236 -2.67431
6 2.08591 1.08549 -0.831209
6 2.48317 0.45565 -2.00991
1 2.01335 -0.942995 -3.58291
1 3.46669 0.689737 -2.41059
1 -0.104531 -1.18148 1.76841
1 -0.226205 -1.48279 -2.64213
8 0.321489 1.34049 0.810051
6 2.98667 2.04464 -0.091458
6 2.16011 2.94254 0.825909
6 1.2311 2.07633 1.65405
1 1.79096 1.3446 2.24361
1 0.586717 2.66348 2.30844
1 2.80476 3.51888 1.4946
1 1.56787 3.65126 0.236664
1 3.70297 1.46897 0.509249
1 3.56708 2.6339 -0.807395

DIHYDROBENZOFURAN

SCF energy= -950.911968966
Zero-point correction = 0.327943
Thermal correction to Energy= 0.348030
Thermal correction to Enthalpy= 0.348975
Thermal correction to Gibbs Free Energy= 0.277587
G(1M)= -950.631

Coordinates:

6	-1.16538	-0.322629	-0.582395
1	-1.6584	-0.940508	-1.32547
7	-1.93872	0.121767	0.389723
7	-3.21325	-0.368068	0.546034
7	-0.230861	-2.10919	0.292134
7	1.06857	-2.39042	-0.153233
1	-0.77692	-2.97197	0.300362
1	-3.37519	-0.925268	1.3769
6	-4.25466	0.250661	-0.12614
6	-5.62111	-0.215204	0.305076
1	-6.2809	-0.212944	-0.562569
1	-6.01352	0.492053	1.04163
1	-5.60042	-1.21037	0.752709
8	-4.04764	1.07906	-0.987752
1	1.15399	-2.49605	-1.15741
6	2.10251	-1.84957	0.560424
6	3.45492	-1.92585	-0.094883
1	3.41937	-2.36009	-1.09537
1	4.11513	-2.52495	0.536611
1	3.86574	-0.914483	-0.153013
8	1.9114	-1.37186	1.67307
1	-1.59451	0.807727	1.05997
6	0.094872	0.313977	-0.912266
6	0.685344	0.121873	-2.17786
6	0.829265	1.02854	0.034277
6	1.93301	0.649931	-2.46846
6	2.09168	1.54924	-0.239222
6	2.64506	1.37095	-1.49429
1	2.36683	0.497636	-3.45004
1	3.62762	1.77271	-1.72357
1	-0.116698	-1.79436	1.26192
8	0.410737	1.25261	1.29529
1	0.144575	-0.44807	-2.92835
6	2.57819	2.24425	1.00888
6	1.54167	1.77805	2.05106
1	1.15926	2.57659	2.68476
1	3.59034	1.94521	1.28983
1	1.91868	0.95383	2.65827
1	2.56662	3.33093	0.880181

CARBOXYLATE
SCF energy= -986.370214307
Zero-point correction= 0.289713
Thermal correction to Energy= 0.309789
Thermal correction to Enthalpy= 0.310733
Thermal correction to Gibbs Free Energy= 0.238807
G(1M)= -986.128

Coordinates:
6 0.174171 -0.040832 0.274861
7 -0.498093 -0.732358 1.18689
7 -1.84189 -0.971953 1.03213
1 -2.45265 -0.152457 1.07302
6 -2.28163 -2.20019 0.602374
6 -3.77888 -2.26261 0.417586
1 -4.2226 -2.75235 1.28893
1 -3.99736 -2.8676 -0.463206
1 -4.22518 -1.27188 0.305695
8 -1.53031 -3.14057 0.430302
1 -0.098163 -0.915226 2.10303
6 1.62385 0.165067 0.502746
6 2.56312 -0.196362 -0.475325
6 2.0376 0.736352 1.7118
6 3.91173 0.044534 -0.212043
6 3.38812 0.951192 1.9607
6 4.32808 0.604402 0.991747
1 4.626 -0.230773 -0.980953
1 3.70183 1.39405 2.90023
1 5.3846 0.772648 1.17682
1 1.29959 1.03544 2.45348
6 2.17326 -0.895032 -1.79168
8 1.0225 -1.40025 -1.82557
8 3.0452 -0.905518 -2.68249
7 -0.499925 1.88796 0.411464
1 0.256574 2.57509 0.433967
1 -1.0466 1.98628 1.27441
7 -1.36995 2.21085 -0.637527
1 -0.94031 2.41933 -1.52968
6 -2.68721 1.93561 -0.496737
6 -3.54807 2.16543 -1.70569
1 -3.93776 1.20022 -2.03964
1 -3.00918 2.6404 -2.52641
1 -4.39475 2.78942 -1.41353
8 -3.12334 1.52868 0.583539
1 -0.212314 -0.088214 -0.735186

Addition intermediates - protonated on hydrazone

QUINOLINE
SCF energy= -967.973307978
Zero-point correction= 0.325063
Thermal correction to Energy= 0.344730
Thermal correction to Enthalpy= 0.345674
Thermal correction to Gibbs Free Energy= 0.275349
G(1M)= -967.695

Coordinates:
6 -0.475951 0.115083 -0.558731
1 -1.12676 -0.48614 -1.20039
7 -0.817886 1.51558 -0.606085
7 -2.11919 1.78151 -1.01749
7 -0.824277 -0.299495 0.871435
7 -0.967935 -1.67789 1.07705
1 -1.7148 0.196531 1.12364
1 -2.31905 1.80472 -2.01218
6 -3.1366 1.73878 -0.118557
6 -4.50462 2.01319 -0.681
1 -5.04761 1.06527 -0.733909
1 -4.47504 2.4674 -1.67235
1 -5.03636 2.67008 0.009257
8 -2.95571 1.46129 1.0667
1 -0.10324 -2.20117 1.16101
6 -2.13113 -2.23766 0.578644
6 -2.17928 -3.73862 0.617133
1 -1.62577 -4.14294 1.4664
1 -1.73847 -4.12792 -0.305647
1 -3.22199 -4.05096 0.666108
8 -3.01687 -1.51415 0.162631
1 -0.152652 2.08347 -1.11871
6 0.975394 -0.150171 -0.861815
6 1.31037 -0.688852 -2.08252
6 2.00988 0.220114 0.051243
6 2.6615 -0.862553 -2.46151
1 0.523261 -0.977668 -2.77342
6 3.36468 0.057134 -0.33665
6 3.66873 -0.488614 -1.6097
1 2.89029 -1.28915 -3.43181
1 4.71069 -0.607357 -1.89235
1 -0.055832 0.095713 1.46619
6 4.36482 0.456301 0.585825
6 3.9978 0.963903 1.80389
1 4.73319 1.28092 2.53388
6 2.62066 1.05384 2.11321
1 2.30345 1.42195 3.08519
1 5.41079 0.351459 0.311677
7 1.66487 0.702786 1.28165

PYRIDINE

SCF energy= -814.386831614
Zero-point correction = 0.278154
Thermal correction to Energy = 0.295273
Thermal correction to Enthalpy = 0.296217
Thermal correction to Gibbs Free Energy = 0.231505
G(1M) = -814.152

Coordinates:
6 0.155116 0.429615 -0.106954
1 -0.240652 0.036952 -1.04952
7 -0.445181 1.67235 0.248649
7 -1.68028 1.94611 -0.311556
7 -0.304719 -0.568236 0.954613
7 -0.175269 -1.92241 0.602043
1 -1.30911 -0.329032 1.16576
1 -1.71335 2.39027 -1.22322
6 -2.80093 1.40956 0.239284
6 -4.09203 1.75712 -0.448773
1 -4.48316 0.851461 -0.919821
1 -3.97943 2.53824 -1.20148
1 -4.80859 2.07964 0.308968
8 -2.7584 0.667158 1.21997
1 0.789647 -2.24276 0.622717
6 -1.09869 -2.38934 -0.319707
6 -0.804388 -3.76156 -0.855271
1 -0.383953 -4.41139 -0.085498
1 -0.080002 -3.6753 -1.67103
1 -1.72784 -4.18797 -1.24514
8 -2.05554 -1.70128 -0.62011
1 0.16195 2.48128 0.294445
6 1.67081 0.470498 -0.096501
6 2.35238 1.32436 -0.95819
6 3.74201 1.32788 -0.902653
1 1.81184 1.961 -1.65153
6 3.60859 -0.336427 0.811668
6 4.38393 0.484537 -0.000949
1 4.31455 1.97806 -1.55547
1 5.46484 0.456919 0.07229
1 0.253551 -0.412595 1.80437
1 4.06889 -1.01368 1.52471
7 2.27281 -0.345756 0.768944

CARBOXYLIC ACID

SCF energy = -986.836961269
Zero-point correction = 0.306283
Thermal correction to Energy = 0.325973
Thermal correction to Enthalpy = 0.326917
Thermal correction to Gibbs Free Energy = 0.256685
G(1M) = -986.577

Coordinates:
6 -0.669087 0.099894 0.514686
1 -0.510692 0.80951 1.32914
7 -1.92201 -0.611782 0.59098
7 -2.97405 0.255787 0.902896
7 -0.823267 0.986174 -0.731583
7 0.228597 1.90352 -0.972012
1 -1.70152 1.51883 -0.61852
1 -2.98669 0.657937 1.84012
6 -4.23799 0.02659 0.369138
6 -4.32342 -0.919935 -0.800051
1 -4.06079 -1.93297 -0.482982
1 -3.6332 -0.639372 -1.59841
1 -5.34733 -0.904184 -1.17094
8 -5.1935 0.601662 0.850455
1 0.475235 2.3929 -0.11013
6 1.36604 1.51606 -1.70766
6 1.2007 0.481395 -2.78872
1 0.244029 0.560509 -3.31172
1 1.30244 -0.525318 -2.37043
1 2.00631 0.632641 -3.50666
8 2.39921 2.0983 -1.47419
1 -1.84883 -1.37766 1.26152
6 0.503335 -0.830555 0.320784
6 1.80385 -0.533509 0.777492
6 0.277935 -2.0227 -0.370888
6 2.84183 -1.43113 0.512452
6 1.32218 -2.90717 -0.629187
1 -0.723671 -2.25882 -0.716507
6 2.60788 -2.60563 -0.19482
1 3.84052 -1.19895 0.862178
1 1.12561 -3.82501 -1.17254
1 3.42925 -3.28376 -0.398657
1 -0.958079 0.386997 -1.55891
6 2.12763 0.712856 1.54187
8 1.44404 1.71845 1.57941
8 3.27733 0.615007 2.20316
1 3.4406 1.46644 2.65025

PHENYL
SCF energy = -798.344188170
Zero-point correction = 0.290079
Thermal correction to Energy = 0.307473
Thermal correction to Enthalpy = 0.308417
Thermal correction to Gibbs Free Energy = 0.242404
G(1M) = -798.099

Coordinates:
6 -0.47414 0.484776 -0.307171
1 -0.780787 0.321664 -1.34462
7 -1.4418 1.23744 0.445135
7 -2.72603 1.28144 -0.091138
7 -0.511999 -0.913627 0.332137
7 0.183506 -1.88021 -0.407152
1 -1.53057 -1.14358 0.495462
1 -2.96509 2.05562 -0.700792
6 -3.5612 0.227116 0.045619
6 -4.94797 0.414306 -0.504941
1 -5.12404 -0.340456 -1.27432
1 -5.11147 1.40837 -0.922304
1 -5.65991 0.242085 0.305544
8 -3.20583 -0.830968 0.574467
1 -0.375189 -2.42096 -1.05702
6 1.32892 -2.38118 0.188435
6 1.95737 -3.54047 -0.52699
1 1.74346 -3.52324 -1.59682
1 1.56138 -4.468 -0.102797
1 3.03363 -3.51123 -0.35879
8 1.74316 -1.87364 1.21364
1 -1.13087 2.17185 0.686064
6 0.923833 1.02592 -0.213372
6 1.73001 1.05596 -1.35044
6 3.03507 1.53492 -1.26354
1 1.33744 0.705846 -2.30083
6 2.72846 1.94714 1.09682
6 3.53252 1.98245 -0.042316
1 3.66001 1.55798 -2.15006
1 4.5489 2.35698 0.024863
1 -0.036252 -0.868671 1.25182
1 3.11643 2.29187 2.04952
6 1.4269 1.4651 1.01563
1 0.809934 1.42911 1.91088

PHENOL

SCF energy = -873.525161676
Zero-point correction = 0.294847
Thermal correction to Energy = 0.312976
Thermal correction to Enthalpy = 0.313920
Thermal correction to Gibbs Free Energy = 0.247940
G(1M) = -873.274

Coordinates:
6 -0.520341 0.064366 -0.708261
1 -0.484017 -0.33693 -1.72808
7 -1.73538 0.764628 -0.389249
7 -2.86394 0.056249 -0.813615
7 -0.559861 -1.19731 0.172824
7 0.500579 -2.10949 -0.04051
1 -1.45532 -1.68129 -0.002852
1 -3.02644 -0.008707 -1.81837
6 -4.02721 0.097233 -0.053206
6 -3.89615 0.589841 1.3648
1 -3.62769 1.64983 1.37076
1 -3.11474 0.053368 1.90717
1 -4.85653 0.449687 1.85894
8 -5.07108 -0.276438 -0.549929
1 0.638725 -2.2908 -1.03378
6 1.71266 -1.98202 0.666582
6 1.65884 -1.39095 2.0505
1 0.813646 -1.77655 2.62845
1 1.5976 -0.298236 2.00664
1 2.58483 -1.66211 2.55597
8 2.7069 -2.43126 0.148086
1 -1.70661 1.70884 -0.775122
6 0.708976 0.853909 -0.377678
6 1.90453 0.562096 -1.05093
6 0.701956 1.817 0.635694
6 3.08137 1.22199 -0.696844
6 1.87145 2.48237 0.981998
1 -0.225036 2.0293 1.16069
6 3.05786 2.17497 0.314439
1 4.00677 0.981437 -1.21191
1 1.86083 3.22683 1.76994
1 3.97879 2.68117 0.584952
1 -0.572791 -0.911588 1.16208
8 1.85574 -0.392499 -2.01443
1 2.74216 -0.556159 -2.37403

H transfer transition states

QUINOLINE
SCF energy = -967.977639934
Zero-point correction = 0.326177
Thermal correction to Energy = 0.345651
Thermal correction to Enthalpy = 0.346595
Thermal correction to Gibbs Free Energy = 0.277577
G(1M) = -967.697

Coordinates:
6 -0.443754 0.446609 -0.411479
1 -0.982653 0.317454 -1.35599
7 -0.889864 1.72055 0.132262
7 -2.27024 1.90155 0.055439
7 -0.757788 -0.707601 0.473219
7 -1.06784 -1.84804 -0.270948
1 -1.56513 -0.454895 1.05319
1 -2.57803 2.51548 -0.685751
6 -3.1473 1.40378 0.961638
6 -4.59845 1.68308 0.673381
1 -5.01985 0.770995 0.240128
1 -4.74643 2.50785 -0.025716
1 -5.11477 1.89395 1.61061
8 -2.77658 0.748238 1.93365
1 -0.432986 -2.63062 -0.193024
6 -2.30967 -1.98256 -0.819951
6 -2.57386 -3.29267 -1.51917
1 -1.69868 -3.94343 -1.55095
1 -2.90433 -3.08136 -2.53838
1 -3.38698 -3.80701 -1.00139
8 -3.13592 -1.08245 -0.742158
1 -0.58074 1.86514 1.09356
6 1.04538 0.548308 -0.724099
6 3.45195 0.26501 -0.225142
6 2.77013 1.44647 -2.21116
6 3.77482 0.976319 -1.40574
1 3.00403 1.99099 -3.11896
1 4.81914 1.13925 -1.65144
6 1.41932 1.23138 -1.86129
6 2.08734 0.050664 0.101305
1 0.639297 1.62725 -2.50601
6 2.74018 -1.12555 2.06565
1 2.38697 -1.67308 2.9309
6 4.09737 -0.920161 1.79513
6 4.44295 -0.236823 0.65271
1 4.84076 -1.30907 2.47823
1 5.48786 -0.070456 0.40814
7 1.81401 -0.653383 1.24737
1 0.796236 -0.839373 1.38879

PYRIDINE
SCF energy = -814.394547595
Zero-point correction = 0.279141
Thermal correction to Energy = 0.296013
Thermal correction to Enthalpy = 0.296957
Thermal correction to Gibbs Free Energy = 0.233725
G(1M) = -814.158

Coordinates:
6 -0.316589 0.212351 0.259327
1 0.008083 -0.165979 1.23437
7 0.065933 1.61155 0.191232
7 1.396 1.84105 0.532815
7 0.22147 -0.640082 -0.815409
7 0.648742 -1.88313 -0.348644
1 0.997466 -0.14824 -1.26829
1 1.54292 2.24361 1.44788
6 2.41098 1.71071 -0.358275
6 3.78592 1.99575 0.182157
1 4.26401 1.02902 0.364726
1 3.77112 2.56559 1.11271
1 4.36133 2.53338 -0.572515
8 2.20882 1.36179 -1.51925
1 0.16495 -2.68971 -0.718641
6 1.84827 -2.01776 0.289399
6 2.24765 -3.43549 0.617035
1 1.45191 -4.15791 0.428468
1 2.53736 -3.48028 1.66862
1 3.12097 -3.6998 0.015216
8 2.5346 -1.04536 0.571041
1 -0.114293 2.0045 -0.733213
6 -1.83919 0.180587 0.21265
6 -2.6601 0.776465 1.1571
6 -4.03866 0.694331 0.998422
1 -2.20895 1.29578 1.99419
6 -3.72836 -0.545971 -1.02148
6 -4.58215 0.026563 -0.101773
1 -4.69546 1.15081 1.7307
1 -4.05154 -1.08035 -1.90503
1 -5.65225 -0.049482 -0.245068
7 -2.40132 -0.446778 -0.828734
1 -1.72731 -0.845833 -1.49464

Addition intermediates – deprotonated

QUINOLINE
SCF energy = -967.529528342
Zero-point correction = 0.312536
Thermal correction to Energy = 0.332013
Thermal correction to Enthalpy = 0.332957
Thermal correction to Gibbs Free Energy = 0.263609
G(1M) = -967.263

Coordinates:
6 -0.383984 -0.155987 -0.507082
1 -0.992262 -0.796928 -1.15655
7 -0.557307 1.20194 -1.00774
7 -1.89365 1.50316 -1.28333
7 -0.839224 -0.3221 0.898863
7 -1.41062 -1.5812 1.08795
1 -1.55606 0.380613 1.09017
1 -2.16104 1.41939 -2.25377
6 -2.77442 1.94816 -0.358494
6 -4.18043 2.16095 -0.859271
1 -4.77523 1.30676 -0.522903
1 -4.24315 2.22842 -1.94697
1 -4.58785 3.06771 -0.410042
8 -2.45178 2.14867 0.812071
1 -0.887814 -2.23494 1.65325
6 -2.69004 -1.83475 0.710641
6 -3.21286 -3.2093 1.05611
1 -2.44492 -3.86847 1.46481
1 -3.63294 -3.65927 0.15414
1 -4.01941 -3.10482 1.78638
8 -3.37066 -0.989491 0.137039
1 -0.181852 1.87123 -0.336392
6 1.05934 -0.59909 -0.614349
6 3.44823 -0.301398 -0.110476
6 2.69771 -2.27193 -1.29126
6 3.72016 -1.54129 -0.747633
1 2.89819 -3.22059 -1.77851
1 4.74711 -1.89309 -0.794025
6 1.36532 -1.79293 -1.22042
6 2.11205 0.177494 -0.03845
1 0.564856 -2.38727 -1.65376
6 2.77681 2.071 1.08414
1 2.49507 3.01182 1.55333
6 4.13827 1.68182 1.06584
6 4.4687 0.495823 0.466313
1 4.88803 2.32147 1.51763
1 5.49924 0.153261 0.422747
7 1.80085 1.3639 0.561976

PYRIDINE
SCF energy = -813.945592233
Zero-point correction = 0.265193
Thermal correction to Energy = 0.282094
Thermal correction to Enthalpy = 0.283038
Thermal correction to Gibbs Free Energy = 0.218650
G(1M) = -813.724

Coordinates:
6 -0.210432 0.35462 0.098124
1 0.104381 -0.043254 1.07311
7 0.351785 1.69295 0.013145
7 1.65053 1.77437 0.519754
7 0.277179 -0.520706 -0.987522
7 0.25992 -1.86319 -0.594491
1 1.25284 -0.277547 -1.16672
1 1.72917 2.23909 1.41374
6 2.75555 1.51048 -0.220724
6 4.07161 1.71691 0.486392
1 4.54256 0.73772 0.607509
1 3.96556 2.18363 1.46694
1 4.71946 2.32967 -0.143205
8 2.68394 1.11979 -1.38321
1 -0.630702 -2.32216 -0.734025
6 1.22587 -2.35778 0.218529
6 1.03974 -3.79208 0.65466
1 0.132479 -4.24523 0.251265
1 1.00355 -3.82334 1.74636
1 1.90644 -4.37376 0.332044
8 2.20471 -1.68724 0.53944
1 0.353838 2.02258 -0.953141
6 -1.73425 0.417345 0.066063
6 -2.42288 1.53162 0.54608
6 -3.81365 1.51725 0.525869
1 -1.86825 2.38697 0.912859
6 -3.69292 -0.673631 -0.410203
6 -4.46833 0.391842 0.037255
1 -4.37649 2.37382 0.884018
1 -4.16568 -1.5737 -0.796594
1 -5.55053 0.335051 0.000897
7 -2.35794 -0.670468 -0.40191

CARBOXYLIC ACID

SCF energy = -986.419659617
Zero-point correction = 0.292253
Thermal correction to Energy = 0.312013
Thermal correction to Enthalpy = 0.312957
Thermal correction to Gibbs Free Energy = 0.242683
G(1M) = -986.174

Coordinates:
6 -0.042632 -0.129207 0.328733
1 -0.341879 0.007915 -0.712444
7 -0.23882 1.16925 0.972352
7 -1.34502 1.84894 0.456156
7 -0.877564 -1.17083 0.958364
7 -1.22415 -2.15726 0.031554
1 -1.74004 -0.718998 1.27265
1 -1.12554 2.43344 -0.340381
6 -2.61625 1.61113 0.852866
6 -3.68301 2.33449 0.071867
1 -4.14668 1.60303 -0.59646
1 -3.28975 3.16032 -0.523609
1 -4.44298 2.70591 0.760816
8 -2.87605 0.859636 1.79256
1 -0.853601 -3.08291 0.195694
6 -2.189 -1.93528 -0.899927
6 -2.53408 -3.11723 -1.77485
1 -1.86728 -3.9683 -1.62572
1 -2.49099 -2.80215 -2.81944
1 -3.56054 -3.42472 -1.55886
8 -2.74085 -0.844657 -1.00772
1 -0.369793 1.06032 1.97825
6 1.43725 -0.477418 0.371633
6 3.74674 0.038546 -0.188067
6 3.24499 -1.91924 1.10947
6 4.17826 -1.10015 0.485414
1 4.46616 0.688322 -0.673478
1 3.56834 -2.80545 1.64692
1 5.23588 -1.33934 0.523499
6 1.88753 -1.60348 1.05444
6 2.38746 0.354229 -0.255849
1 1.1616 -2.23038 1.55992
6 1.98272 1.56918 -1.02676
8 0.89977 1.7714 -1.53542
8 2.98462 2.4557 -1.13763
1 2.65604 3.19222 -1.68447

PHENYL
SCF energy = -797.906499987
Zero-point correction = 0.277051
Thermal correction to Energy = 0.294172
Thermal correction to Enthalpy = 0.295116
Thermal correction to Gibbs Free Energy = 0.230057
G(1M) = -797.673

Coordinates:
6 -0.297196 0.269397 0.129011
1 0.032167 -0.072746 1.11889
7 0.142527 1.65847 0.031511
7 1.45421 1.84981 0.473612
7 0.305043 -0.583798 -0.914325
7 0.519837 -1.87912 -0.441264
1 1.21109 -0.189015 -1.17289
1 1.53679 2.24238 1.40078
6 2.54707 1.67608 -0.305911
6 3.87009 1.92307 0.373317
1 4.34419 0.949358 0.525431
1 3.77161 2.42339 1.33815
1 4.50541 2.51661 -0.286099
8 2.4623 1.32681 -1.48215
1 -0.053725 -2.60813 -0.842656
6 1.62696 -2.17153 0.291131
6 1.80842 -3.62797 0.647142
1 0.955055 -4.24624 0.363268
1 1.96882 -3.70616 1.72446
1 2.70471 -4.0028 0.146207
8 2.42213 -1.29957 0.627118
1 0.066677 1.99739 -0.928201
6 -1.81602 0.229058 0.072362
6 -2.54037 0.862293 1.08762
6 -2.50478 -0.41878 -0.950592
6 -3.93011 0.847893 1.08047
1 -2.00265 1.3728 1.88285
6 -3.90068 -0.434582 -0.959743
1 -1.94387 -0.905493 -1.74142
6 -4.61576 0.196699 0.052938
1 -4.48039 1.3428 1.87501
1 -4.42698 -0.942188 -1.76258
1 -5.7014 0.182796 0.045814

Others:

WATER

SCF energy= -76.3811217565

Zero-point correction= 0.021452

Thermal correction to Energy= 0.024287

Thermal correction to Enthalpy= 0.025231

Thermal correction to Gibbs Free Energy= 0.003789

G(1M)= -76.3743

G(55.5M)= -76.370525

Coordinates:

8 -0 -0 -0.119699

1 -0 -0.759495 0.478795

1 -0 0.759495 0.478795

HYDRONIUM

SCF energy= -76.7766326997

Zero-point correction= 0.035131

Thermal correction to Energy= 0.037995

Thermal correction to Enthalpy= 0.038939

Thermal correction to Gibbs Free Energy= 0.017025

G(1M)= -76.7566

G(pH 7)= -76.771801

Coordinates:

8 -0 -0 -0.088954

1 -0 -0.929587 0.23721

1 -0.805046 0.464793 0.23721

1 0.805046 0.464793 0.23721

Kw based correction = 19.4559942 kcal/mol

HYDROXIDE

SCF energy= -75.8262734362

Zero-point correction= 0.008337

Thermal correction to Energy= 0.010698

Thermal correction to Enthalpy= 0.011642

Thermal correction to Gibbs Free Energy = -0.007933

G(1M) = -75.8312

G(pH 7) = -75.8463994

Coordinates:

8 -0 -0 -0.108219

1 -0 -0 0.865756

References:

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