Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Feeding sequence-regulated divergent (4 + 1 + 1') annulations of α-bromo carbonyls and 1-azadienes via computational calculations-based mechanism elucidation

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Supporting Information

1. General methods

^{1}H NMR or ^{13}C NMR spectra were recorded on Agilent 600 or 150 MHz NMR spectrometer, respectively (Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard in $CDCl_3$ solution, unless otherwise noted). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, td = triple doublet, dt = double triplet, m = multiplet, and coupling constants (*J*) are reported in Hertz (Hz). ESI-HRMS was recorded on a Waters SYNAPT G2. Melting points were determined using a capillary melting point apparatus. Column chromatography was performed on silica gel (300-400 mesh) eluting with ethyl acetate (EtOAc) and petroleum ether (PE) or dichloromethane (CH_2Cl_2)/methanol (MeOH). TLC was performed on glass-backed silica plates. UV light, I_2, and solution of potassium permanganate were used to visualize products or the starting materials. All chemicals were used without purification as commercially available unless otherwise noted. Anhydrous acetonitrile (MeCN) was distilled over CaH_2 and deoxygenated with argon. Petroleum ether (60–90 °C) was redistilled. Unless otherwise noted, all reactions were carried out under ambient atmosphere.

2. General procedure for the preparation of 1-azadienes and ammonium salts

The 1-azadienes were prepared according to the reported methods,[1] and all the ^{1}H and ^{13}C NMR spectra of the obtained 1-azadienes were accordant with the literature data.

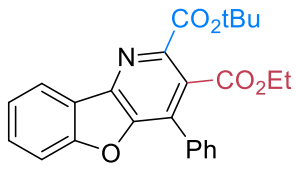
Ammonium salts can be easily prepared from amine and α-bromide. DABCO or DMAP was dissolved in a small amount of acetonitrile, and equimolar α-bromide was added and stirred for 3 hours. The white ammonium salt was filtered and washed by chilled acetonitrile. After drying, the ammonium salt was obtained in a nearly quantitative yield.

3. General procedure for (4 + 1 + 1') annulations

Procedure A: DABCO (0.2 mmol, 2.0 equiv) or DMAP (0.2 mmol, 2.0 equiv) was dissolved in MeCN (2.0 mL), and the 1st *α*-bromide **2** (0.2 mmol, 2.0 equiv) was added and stirred for 60 min at 40 ℃. Then, Cs_2CO_3 (0.4 mmol, 4.0 equiv) and 1-azadiene **1** (0.1 mmol, 1.0 equiv) were added to the solution. After 15 minutes, the 2nd *α*-bromide **2** (0.2 mmol, 2.0 equiv) was added and the reaction was continued for 20 hours. After removal of the solvent, the residue was subjected to chromatography on a silica gel (300-400 mesh) column using petroleum ether (PE):EtOAc (15: 1-5: 1) as eluent to afford the product **4**.

Procedure B: The ammonium salt was obtained by the reaction of tertiary amine and *α*-bromide in MeCN. Ammonium salt (0.105 mmol, 1.05 equiv), Cs_2CO_3 (0.4 mmol, 4.0 equiv), 1-azadiene **1** (0.1 mmol, 1.0 equiv) were added to MeCN (2.0 mL) and were stirred at 40 ℃ until **1** disappeared. This process took about 5 to 15 minutes, which could be easily judged from the

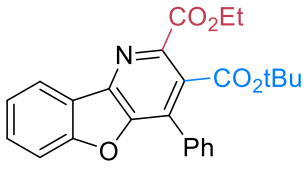
disappearance of the yellow color of the substrate. Then the 2nd α-bromide **2** (0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After removal of the solvent, the residue was subjected to chromatography on a silica gel (300-400 mesh) column using PE: EtOAc (15: 1-5: 1) as eluent to afford the product **4**.



4a

2-(*Tert*-butyl) 3-ethyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4a):

Through procedure B: Ethyl bromoacetate-DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry MeCN (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. *Tert*-Butyl bromoacetate (29.3 mg, 21.9 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4a**: 25.0 mg (0.060 mmol), as a white solid, yield 60%. M.p. = 142–144 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.7 Hz, 1H), 7.71–7.50 (m, 7H), 7.50–7.45 (m, 1H), 4.15 (q, *J* = 7.2 Hz, 2H), 1.65 (s, 9H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.81, 164.20, 158.81, 147.77, 144.58, 144.13, 131.91, 131.57, 130.30, 129.33, 129.22, 128.55, 128.40, 124.10, 122.63, 122.58, 112.40, 83.40, 61.79, 27.94, 13.53 ppm. HRMS (ESI) calcd. for $[C_{25}H_{23}NO_5+Na]^+$ 440.1468, found 440.1472.

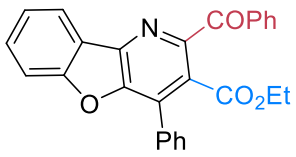


4b

3-(*Tert*-butyl) 2-ethyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4b):

Through procedure B: *Tert*-Butyl bromoacetate-DABCO salt (32.1 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Ethyl bromoacetate (25.1 mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4b**: 24.6 mg (0.059 mmol), as a white solid, yield 59%. M.p. = 139–141 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.8 Hz, 1H), 7.65–7.51 (m, 7H), 7.50–7.45 (m, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 1.49 (t, *J* = 7.1 Hz, 3H), 1.30 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.44, 165.30, 158.84,

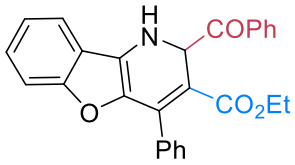
148.19, 144.13, 142.89, 132.02, 131.47, 130.29, 130.11, 129.52, 129.26, 128.47, 124.09, 122.55, 122.46, 112.45, 83.13, 62.40, 27.56, 14.28 ppm. HRMS (ESI) calcd. for $[C_{25}H_{23}NO_5+Na]^+$ 440.1468, found 440.1471.



4c

Ethyl 2-benzoyl-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4c):

Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. 2-Bromoacetophenone (30.0 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4c**: 38.0 mg (0.090 mmol), as a white solid, yield 90%. M.p. = 145–146 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.8 Hz, 1H), 8.11 (d, *J* = 7.7 Hz, 2H), 7.67–7.60 (m, 5H), 7.54 (dq, *J* = 15.6, 7.7, 7.0 Hz, 5H), 7.49–7.44 (m, 1H), 4.09 (q, *J* = 7.2 Hz, 2H), 0.96 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) 193.47, 166.81, 158.91, 151.28, 147.46, 143.83, 135.95, 133.35, 132.92, 131.69, 131.10, 130.39, 129.37, 129.24, 128.59, 128.25, 127.79, 124.17, 122.65, 122.17, 112.57, 61.91, 13.39 ppm. HRMS (ESI) calcd. for $[C_{27}H_{19}NO_4+H]^+$ 422.1387, found 422.1389.

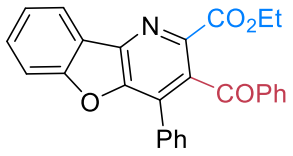


4c'

Ethyl 2-benzoyl-4-phenyl-1,2-dihydrobenzofuro[3,2-*b*]pyridine-3-carboxylate (4c'):

Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. 2-Bromoacetophenone (30.0 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 5 hours. A intermediate product was found and purified by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave intermediate product **4c'**: 9.7 mg (0.023 mmol), as a white solid, yield 23%. M.p. = 142–143 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06–8.00 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.44–7.39 (m, 3H), 7.36 (d, *J* = 8.3 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.26–7.22 (m, 1H), 7.20 (q, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 1H), 5.54 (s, 1H), 3.79 (qt, *J* = 6.9, 3.4 Hz, 2H), 0.85 (t, *J* = 7.1 Hz, 3H) ppm.^{13}C NMR (150 MHz, $CDCl_3$) 192.92, 166.30, 153.95, 144.91, 144.04,

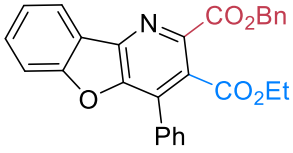
141.09, 135.40, 133.93, 128.90, 128.89, 128.37, 128.17, 126.96, 124.43, 122.78, 120.02, 117.31, 117.17, 111.99, 102.48, 60.41, 41.61, 13.54 ppm. HRMS (ESI) calcd. for $[C_{27}H_{21}NO_4+Na]^+$ 446.1363, found 446.1368.



4d

Ethyl 3-benzoyl-4-phenylbenzofuro[3,2-*b*]pyridine-2-carboxylate (4d) :

Through general procedure B: Bromoacetophenone-DMAP salt (33.6 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (260 mg, 0.8 mmol, 8.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Ethyl bromoacetate (25.1 mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4d**: 27.4 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 143–144 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.8 Hz, 1H), 7.66–7.62 (m, 3H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.54–7.50 (m, 1H), 7.46–7.42 (m, 1H), 7.41–7.37 (m, 2H), 7.33 (q, *J* = 2.9 Hz, 3H), 7.30 (t, *J* = 7.7 Hz, 2H), 4.31 (q, *J* = 7.2 Hz, 2H), 1.21 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) 194.48, 165.09, 158.84, 148.39, 144.73, 142.74, 137.60, 135.19, 133.15, 132.26, 130.68, 130.52, 129.80, 129.24, 128.98, 128.43, 128.41, 124.27, 122.57, 122.55, 112.54, 62.52, 13.79 ppm. HRMS (ESI) calcd. for $[C_{27}H_{19}NO_4+Na]^+$ 444.1206, found 444.1211.

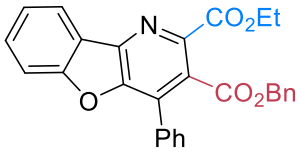


4e

2-Benzyl 3-ethyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4e):

Through general procedure B: Ethyl bromoacetate-DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Benzyl bromoacetate (34.4 mg, 23.8 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4e**: 41.9 mg (0.093 mmol), as a white solid, yield 93%. M.p. = 155–156 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.8 Hz, 1H), 7.62 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.60–7.55 (m, 3H), 7.56–7.51 (m, 4H), 7.50 (s, 1H), 7.48 (d, *J* = 7.3 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.1 Hz, 1H), 5.49 (s, 2H), 3.97 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.60, 165.02, 158.89, 148.13, 144.73, 142.31, 135.21, 132.01, 131.24, 130.51, 129.46,

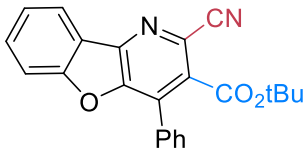
129.33, 129.27, 128.68, 128.58, 128.55, 128.44, 124.23, 122.55, 122.47, 112.48, 68.05, 61.86, 13.53 ppm. HRMS (ESI) calcd. for $[C_{28}H_{21}NO_5+Na]^+$ 474.1312, found 474.1318.



4f

3-Benzyl 2-ethyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4f) :

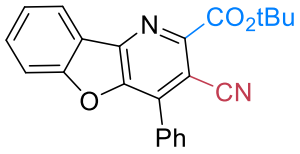
Through general procedure B: Benzyl bromoacetate-DABCO salt (35.7 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Ethyl bromoacetate (25.1 mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4f**: 33.8 mg (0.075 mmol), as a white solid, yield 75%. M.p. = 150–151 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.8 Hz, 1H), 7.62 (td, *J* = 7.7, 7.0, 1.4 Hz, 1H), 7.60–7.53 (m, 3H), 7.53–7.44 (m, 4H), 7.28 (d, *J* = 6.9 Hz, 3H), 7.09 (dd, *J* = 7.4, 2.2 Hz, 2H), 5.16 (s, 2H), 4.49 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.67, 165.11, 158.89, 148.11, 144.71, 142.49, 134.77, 132.04, 131.05, 130.52, 129.53, 129.31, 128.98, 128.68, 128.58, 128.46, 128.31, 124.22, 122.57, 122.44, 112.49, 67.93, 62.57, 14.21 ppm. HRMS (ESI) calcd. for $[C_{28}H_{21}NO_5+Na]^+$ 474.1312, found 474.1319.



4g

***Tert*-butyl 2-cyano-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4g):**

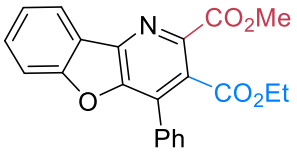
Through general procedure B: *Tert*-Butyl bromoacetate-DABCO salt (32.1 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Bromoacetonitrile (24.0 mg, 13.9 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4g**: 31.8 mg (0.086 mmol), as a white solid, yield 86%. M.p. = 143–145 ºC ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.8 Hz, 1H), 7.67 (ddd, *J* = 8.5, 7.1, 1.4 Hz, 1H), 7.63–7.58 (m, 3H), 7.57 (q, *J* = 3.2, 2.5 Hz, 3H), 7.53 (t, *J* = 7.5 Hz, 1H), 1.45 (d, *J* = 1.4 Hz, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.77, 159.05, 148.04, 146.08, 132.43, 132.36, 131.27, 130.91, 129.84, 129.27, 128.78, 127.30, 124.76, 122.35, 121.77, 116.22, 112.62, 84.85, 27.58 ppm. HRMS (ESI) calcd. for $[C_{23}H_{18}N_2O_3+Na]^+$ 393.1209, found 393.1214.



4h

***Tert*-butyl 3-cyano-4-phenylbenzofuro[3,2-*b*]pyridine-2-carboxylate (4h):**

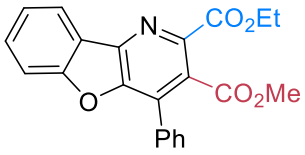
Through general procedure B: Bromoacetonitrile-DABCO salt (24.3 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. *Tert*-Butyl bromoacetate (29.3 mg, 21.9 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4h**: 11.8 mg (0.032 mmol), as a white solid, yield 32%. M.p. = 142–144 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.8 Hz, 1H), 7.82–7.77 (m, 2H), 7.69 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.63 (dd, *J* = 8.7, 6.8 Hz, 4H), 7.53 (t, *J* = 7.5 Hz, 1H), 1.75 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.95, 159.40, 149.52, 146.84, 146.61, 137.41, 131.63, 130.61, 129.98, 129.90, 128.96, 124.69, 123.01, 122.15, 115.61, 112.66, 105.48, 85.05, 28.00 ppm. HRMS (ESI) calcd. for $[C_{23}H_{18}N_2O_3+Na]^+$ 393.1209, found 393.1214.



4i

3-Ethyl 2-methyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4i):

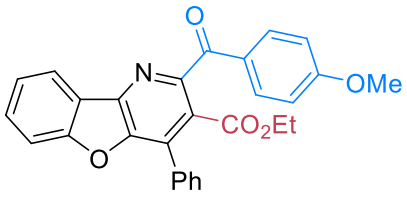
Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Methyl bromoacetate (23.0mg, 14.2 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4i**: 24.4 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 142–143 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.7 Hz, 1H), 7.63 (td, *J* = 7.5, 6.9, 1.2 Hz, 1H), 7.61–7.57 (m, 3H), 7.57–7.52 (m, 3H), 7.50 (t, *J* = 7.2 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 4.07 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.71, 165.50, 158.91, 148.28, 144.62, 141.73, 132.05, 131.09, 130.57, 129.77, 129.53, 129.33, 128.61, 124.27, 122.43, 122.40, 112.54, 62.01, 53.38, 13.70 ppm. HRMS (ESI) calcd. for $[C_{22}H_{17}NO_5+H]^+$ 376.1180, found 376.1184.



4j

2-Ethyl 3-methyl 4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4j):

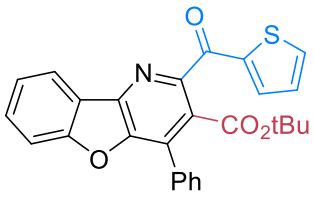
Through general procedure B: Methyl bromoacetate-DMAP salt (28.8 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. Ethyl bromoacetate (25.1mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4j**: 26.3 mg (0.070 mmol), as a white solid, yield 70%. M.p. = 141–143 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.8 Hz, 1H), 7.64–7.61 (m, 1H), 7.61–7.57 (m, 3H), 7.57–7.52 (m, 3H), 7.51–7.47 (m, 1H), 4.53 (q, *J* = 7.2 Hz, 2H), 3.73 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.33, 165.12, 158.90, 148.13, 144.74, 142.32, 132.01, 131.13, 130.54, 129.56, 129.22, 129.16, 128.68, 124.23, 122.57, 122.45, 112.50, 62.60, 52.74, 14.21 ppm. HRMS (ESI) calcd. for $[C_{22}H_{17}NO_5+Na]^+$ 398.0999, found 398.1001.



4k

Ethyl 2-(4-methoxybenzoyl)-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4k):

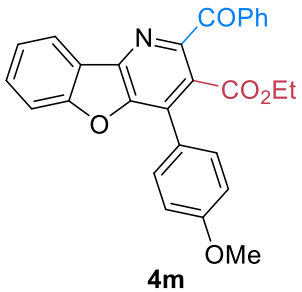
Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. 2-bromo-1-(4-methoxyphenyl)ethan-1-one (34.2mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4k**: 29.3 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 146–148 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29–8.23 (m, 1H), 8.16–8.11 (m, 2H), 7.64–7.60 (m, 4H), 7.55 (qd, *J* = 7.4, 6.2, 3.6 Hz, 3H), 7.47 (dt, *J* = 9.2, 4.0 Hz, 1H), 7.02–6.97 (m, 2H), 4.09 (qd, *J* = 7.2, 1.2 Hz, 2H), 3.91 (d, *J* = 1.3 Hz, 3H), 0.96 (td, *J* = 7.1, 1.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 192.01, 166.89, 163.86, 158.89, 151.87, 147.35, 143.70, 133.57, 132.92, 131.82, 130.31, 129.34, 129.26, 128.91, 128.59, 127.69, 124.13, 122.74, 122.13, 113.60, 112.57, 61.86, 55.53, 13.41 ppm. HRMS (ESI) calcd. for $[C_{28}H_{21}NO_5+Na]^+$ 474.1312, found 474.1321.



4l

***Tert*-butyl 4-phenyl-2-(thiophene-2-carbonyl)benzofuro[3,2-*b*]pyridine-3-carboxylate (4l):**

Through general procedure B: *Tert*-Butyl bromoacetate-DMAP salt (33.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 1-azadiene **1a** (37.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1a** disappeared. 2-bromo-1-(thiophen-2-yl)ethan-1-one (30.6mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4l**: 25.9 mg (0.057 mmol), as a white solid, yield 57%. M.p. = 142–143 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (dt, *J* = 7.8, 1.0 Hz, 1H), 8.22 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.80 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.61 (ddt, *J* = 7.2, 5.6, 2.7 Hz, 4H), 7.58–7.53 (m, 3H), 7.50 (ddd, *J* = 8.0, 6.5, 1.6 Hz, 1H), 7.22 (dd, *J* = 5.0, 3.8 Hz, 1H), 1.32 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 183.64, 165.46, 158.88, 148.51, 148.19, 143.06, 140.83, 136.75, 136.15, 132.49, 131.46, 130.28, 129.73, 129.55, 129.31, 128.51, 127.70, 124.24, 122.75, 122.05, 112.64, 83.16, 27.57 ppm. HRMS (ESI) calcd. for $[C_{25}H_{17}NO_4S+Na]^+$ 478.1084, found 478.1092.

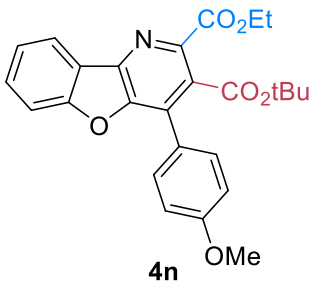


4m

Ethyl 2-benzoyl-4-(4-methoxyphenyl)benzofuro[3,2-*b*]pyridine-3-carboxylate (4m):

Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-4-methoxybenzylidene) benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1b** (40.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1b** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4m**: 26.1 mg (0.058 mmol), as a white solid, yield 58%. M.p. = 146–148 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.14–8.08 (m, 2H), 7.67–7.56 (m, 5H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.46 (ddd, *J* = 8.0, 5.7, 2.3 Hz, 1H), 7.09 (d, *J* = 1.9 Hz, 1H), 7.08 (d, *J* = 2.2 Hz, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 3H), 1.04 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ

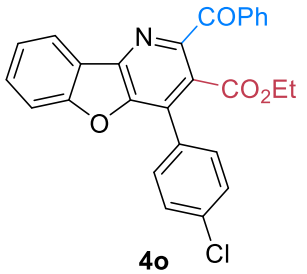
193.52, 167.08, 160.51, 158.83, 151.24, 147.64, 143.66, 136.02, 133.33, 132.71, 131.14, 130.78, 130.29, 128.25, 127.73, 124.13, 123.69, 122.76, 122.15, 114.15, 112.55, 61.95, 55.39, 13.55 ppm. HRMS (ESI) calcd. for $[C_{28}H_{21}NO_5+Na]^+$ 474.1312, found 474.1315.



4n

3-(*Tert*-butyl) 2-ethyl 4-(4-methoxyphenyl)benzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4n):

Through general procedure B: *Tert*-Butyl bromoacetate -DMAP salt (33.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-4-methoxybenzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1b** (40.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1b** disappeared. Ethyl bromoacetate (25.1 mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4n**: 28.2 mg (0.063 mmol), as a white solid, yield 63%. M.p. = 141–142 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.62–7.56 (m, 2H), 7.54 (d, *J* = 1.7 Hz, 1H), 7.53 (d, *J* = 2.3 Hz, 1H), 7.47 (ddd, *J* = 8.1, 6.7, 1.4 Hz, 1H), 7.07 (d, *J* = 1.7 Hz, 1H), 7.06 (d, *J* = 2.3 Hz, 1H), 4.54 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H), 1.36 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ165.54, 165.46, 160.40, 158.76, 148.42, 143.97, 142.83, 131.85, 130.96, 130.21, 130.20, 124.05, 123.50, 122.61, 122.45, 113.97, 112.43, 83.13, 62.39, 55.42, 27.69, 14.31 ppm. HRMS (ESI) calcd. for $[C_{26}H_{25}NO_6+H]^+$ 448.1755, found 448.1758.

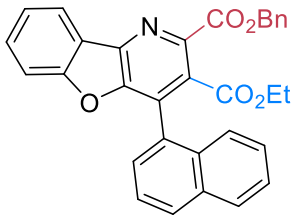


4o

Ethyl 2-benzoyl-4-(4-chlorophenyl)benzofuro[3,2-*b*]pyridine-3-carboxylate (4o):

Through general procedure B: Ethyl bromoacetate -DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-4-chlorobenzylidene) benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1c** (40.9 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1c** disappeared.

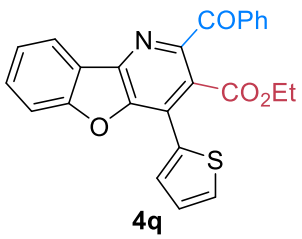
2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4o**: 29.6 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 151–152 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.7 Hz, 1H), 8.09 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.66–7.60 (m, 3H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.52 (dd, *J* = 15.1, 7.9 Hz, 4H), 7.47 (ddd, *J* = 8.0, 6.4, 1.7 Hz, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 1.01 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 193.34, 166.59, 158.92, 151.46, 147.28, 144.00, 135.88, 135.69, 133.44, 131.71, 131.09, 130.68, 130.58, 130.08, 128.95, 128.30, 127.45, 124.33, 122.58, 122.25, 112.56, 62.11, 13.47 ppm. HRMS (ESI) calcd. for $[C_{27}H_{18}ClNO_4+Na]^+$ 478.0816, found 478.0823.



4p

2-Benzyl 3-ethyl 4-(naphthalen-1-yl)benzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4p) :

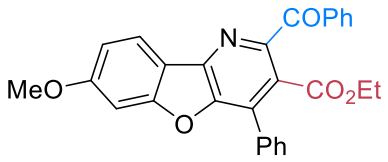
Through general procedure B: Ethyl bromoacetate-DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 4-methyl-*N*-((2*Z*,3*E*)-2-(naphthalen-1-ylmethylene)benzofuran-3(2*H*)-ylidene)benzenesulfonamide **1d** (42.5mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1d** disappeared. Benzyl bromoacetate (34.4 mg, 23.8 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4p**: 35.1 mg (0.070 mmol), as a white solid, yield 70%. M.p. = 165–166 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.8 Hz, 1H), 8.08 (s, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.92 (dd, *J* = 11.8, 7.8 Hz, 2H), 7.67 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.0 Hz, 3H), 7.54–7.47 (m, 3H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 1H), 5.51 (s, 2H), 3.94 (q, *J* = 7.2 Hz, 2H), 0.88 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.66, 165.05, 158.93, 148.34, 144.77, 142.39, 135.23, 133.42, 132.93, 132.05, 130.55, 129.46, 129.16, 128.70, 128.61, 128.58, 128.47, 128.42, 128.35, 127.86, 127.19, 126.77, 126.37, 124.28, 122.58, 122.48, 112.51, 68.08, 61.92, 13.57 ppm. HRMS (ESI) calcd. for $[C_{32}H_{23}NO_5+Na]^+$ 524.1468, found 524.1472.



4q

Ethyl 2-benzoyl-4-(thiophen-2-yl)benzofuro[3,2-*b*]pyridine-3-carboxylate (4q):

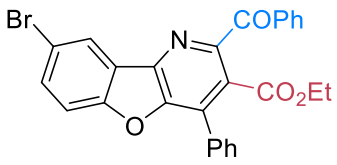
Through general procedure B: Ethyl bromoacetate-DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and 4-methyl-*N*-((2*Z*,3*Z*)-2-(thiophen-2-ylmethylene)benzofuran-3(2*H*)-ylidene)benzenesulfonamide **1e** (38.1 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1e** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4q**: 25.6 mg (0.060 mmol), as a white solid, yield 60%. M.p. = 139–141 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.8 Hz, 1H), 8.09 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.68–7.59 (m, 5H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.48–7.43 (m, 1H), 7.24 (dd, *J* = 5.2, 3.8 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.14 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 193.24, 167.02, 158.74, 150.62, 146.94, 143.72, 136.02, 133.32, 131.22, 131.17, 130.61, 130.44, 129.27, 128.21, 127.62, 127.44, 125.83, 124.32, 122.66, 122.16, 112.58, 62.24, 13.55 ppm. HRMS (ESI) calcd. for $[C_{25}H_{17}NO_4S+Na]^+$ 450.0770, found 450.0777.



4r

Ethyl 2-benzoyl-7-methoxy-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4r):

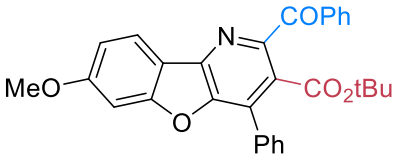
Through general procedure B: Ethyl bromoacetate-DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-benzylidene)-6-methoxybenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1f** (40.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1f** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4r**: 30.2 mg (0.067 mmol), as a white solid, yield 67%. M.p. = 145–147 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12–8.07 (m, 3H), 7.66–7.58 (m, 3H), 7.57–7.48 (m, 5H), 7.10 (d, *J* = 2.2 Hz, 1H), 7.04 (dd, *J* = 8.7, 2.2 Hz, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.91 (s, 3H), 0.94 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 193.66, 166.90, 162.41, 160.72, 151.40, 147.37, 144.25, 136.03, 133.31, 132.27, 131.89, 131.06, 129.25, 129.23, 128.56, 128.25, 126.30, 122.71, 115.53, 113.19, 96.63, 61.83, 55.87, 13.39 ppm. HRMS (ESI) calcd. for $[C_{28}H_{21}NO_5+Na]^+$ 474.1312, found 474.1310.



4s

Ethyl 2-benzoyl-8-bromo-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4s):

Through general procedure B: Ethyl bromoacetate -DABCO salt (29.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-benzylidene)-5-bromobenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1g** (45.3 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1g** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4s**: 33.4 mg (0.067 mmol), as a white solid, yield 67%. M.p. = 155–157 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (d, *J* = 2.1 Hz, 1H), 8.13–8.05 (m, 2H), 7.71 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.65 (d, *J* = 7.4 Hz, 1H), 7.61 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.58–7.49 (m, 6H), 4.10 (q, *J* = 7.1 Hz, 2H), 0.97 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 93.23, 166.59, 157.51, 151.64, 148.03, 142.44, 135.82, 133.47, 133.37, 133.16, 131.35, 131.09, 129.56, 129.21, 128.67, 128.54, 128.31, 124.92, 124.62, 117.30, 114.15, 62.03, 13.41 ppm. HRMS (ESI) calcd. for $[C_{27}H_{18}BrNO_4+Na]^+$ 522.0311, found 522.0315.

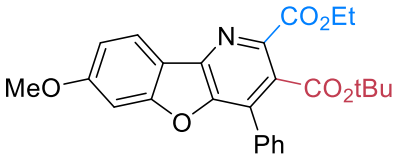


4t

***Tert*-butyl 2-benzoyl-7-methoxy-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (4t):**

Through general procedure B: *Tert*-Butyl bromoacetate-DMAP salt (33.2 mg,0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-benzylidene)-6-methoxybenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1f** (40.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1f** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4t**: 31.1 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 149–151 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.7 Hz, 1H), 8.07–8.04 (m, 2H), 7.63–7.58 (m, 3H), 7.57–7.52 (m, 3H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.08 (d, *J* = 2.1 Hz, 1H), 7.03 (dd, *J* = 8.6, 2.2 Hz, 1H), 3.90 (s, 3H), 1.18 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 193.91, 165.53, 162.29, 160.65, 151.75, 147.35, 143.97, 136.19, 133.30, 132.15, 132.12, 130.91, 129.38, 129.11, 128.48, 128.30, 127.11, 122.69, 115.58, 113.07, 96.62, 83.09, 55.85, 27.31 ppm. HRMS (ESI) calcd. for $[C_{30}H_{25}NO_5+H]^+$ 480.1806,

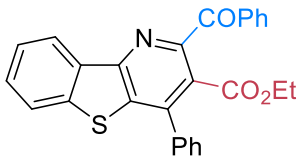
found 480.1811.



4u

3-(*Tert*-butyl) 2-ethyl 7-methoxy-4-phenylbenzofuro[3,2-*b*]pyridine-2,3-dicarboxylate (4u):

Through general procedure B: *Tert*-Butyl bromoacetate-DMAP salt (33.2 mg,0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-benzylidene)-6-methoxybenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1f** (40.5 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40 ℃ until **1f** disappeared. Ethyl bromoacetate (25.1mg, 16.6 μL, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4u**: 31.7 mg (0.071 mmol), as a white solid, yield 71%. M.p. = 149–151 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24–8.19 (m, 1H), 7.58–7.49 (m, 5H), 7.05 (d, *J* = 8.1 Hz, 2H), 4.53 (q, *J* = 7.1 Hz, 2H), 3.88 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H), 1.29 (s, 9H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ165.56, 165.45, 162.29, 160.61, 148.11, 144.45, 142.71, 131.60, 131.33, 129.50, 129.17, 128.91, 128.44, 122.99, 115.39, 112.97, 96.60, 82.97, 62.36, 55.82, 27.56, 14.29 ppm. HRMS (ESI) calcd. for $[C_{26}H_{25}NO_6+H]^+$ 448.1755, found 448.1759.



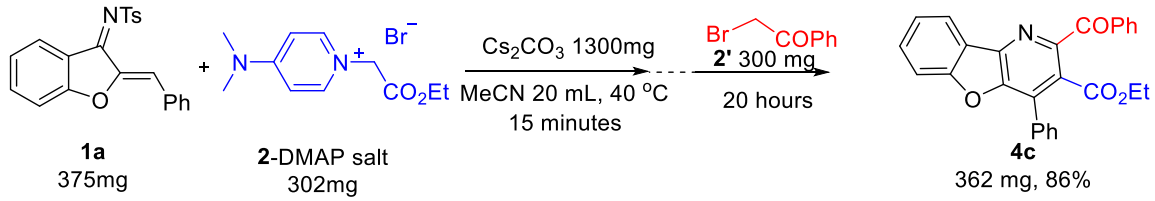
4v

Ethyl 2-benzoyl-4-phenylbenzo[4,5]thieno[3,2-*b*]pyridine-3-carboxylate (4v):

Through general procedure B: Ethyl bromoacetate-DMAP salt (30.2 mg, 0.105 mmol, 1.05 equiv), Cs_2CO_3 (130 mg, 0.4 mmol, 4.0 equiv) and *N*-((*Z*)-2-((*Z*)-benzylidene)benzo[*b*]thiophen-3(2*H*)-ylidene)-4-methylbenzenesulfonamide **1h** (39.1 mg, 0.1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (2.0 mL) and were stirred at 40, ℃ until **1h** disappeared. 2-bromo-1-phenylethan-1-one (29.9 mg, 0.15 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **4v**: 28.4 mg (0.065 mmol), as a white solid, yield 65%. M.p. = 144–145 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.9 Hz, 1H), 8.17 (d, *J* = 7.7 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.54 (dd, *J* = 14.7, 4.7 Hz, 8H), 4.07 (q, *J* = 7.1 Hz, 2H), 0.94 (t, *J* = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 193.49, 167.01, 152.35, 151.28, 144.29, 141.34, 136.38, 136.28, 136.00, 134.35, 133.30, 131.19, 129.47, 129.40, 128.85, 128.20, 128.12, 126.49, 125.43, 124.15, 122.89, 61.79, 13.43 ppm. HRMS (ESI)

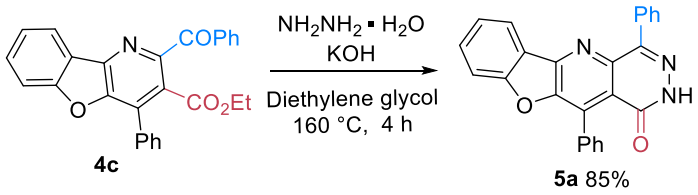
calcd. for $[C_{27}H_{19}NO_4S+H]^+$ 438.1158, found 438.1160

4. (4 + 1 + 1') annulation at a 1.0 mmol scale

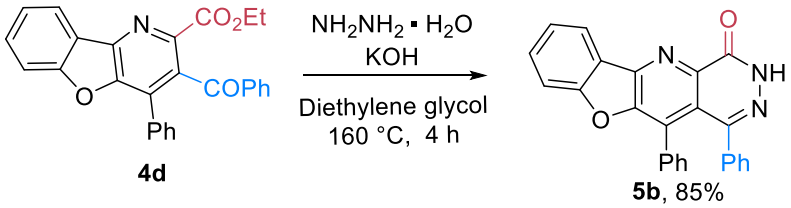


Ethyl bromoacetate-DMAP salt (302 mg, 1.05 mmol, 1.05 equiv), Cs_2CO_3 (1.3 g, 4 mmol, 4.0 equiv) and 1-azadiene **1a** (375 mg, 1 mmol, 1.0 equiv) were dissolved in dry acetonitrile (20 mL) and were stirred at 40 ℃ until 1a disappeared. 2-Bromoacetophenone (300 mg, 1.5 mmol, 1.5 equiv) was added and stirred for 20 hours. After completion, purification by flash chromatography on silica gel (PE: EtOAc: = 10: 1) gave product **4c**: 362 mg (0.86 mmol), as a white solid, yield 86%.

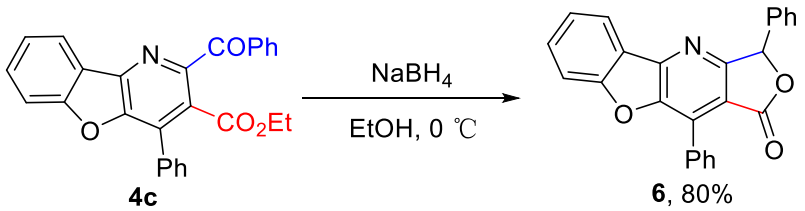
5. Transformation of products 4c and 4d



A solution of ethyl 2-benzoyl-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate **4c** (30 mg, 0.071 mmol, 1.0 equiv), KOH (16 mg, 0.28 mmol, 4.0 equiv) and 80% hydrazine hydrate (5.3 mg, 5.3 μL, 0.085 mmol, 1.2 equiv) in diethylene glycol (4.0 mL) was stirred at 160 ℃ for 4 h. After completion, H_2O (5.0 mL) was added and extracted with toluene (5.0 mL). The organic phase was washed with water (5.0 mL) three times and purified by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **5a**: 23.5 mg (0.060 mmol), as a yellow solid, yield 85%; M.p. = 163–165 ºC; ^{1}H NMR (600 MHz, Chloroform-d_1 : Toluene- d_8 : Methanol-d_4 = 4:1:1) δ 9.26 (dd, J = 7.9, 1.3 Hz, 1H), 9.06–9.02 (m, 2H), 8.61 (td, J = 7.7, 7.1, 1.3 Hz, 1H), 8.57 (dd, J = 8.2, 6.5 Hz, 2H), 8.56–8.49 (m, 7H), 8.43 (t, J = 7.5 Hz, 1H) ppm; ^{13}C NMR (150 MHz, Chloroform-d_1 : Toluene-d_8 : Methanol-d_4 = 4:1:1) δ (ppm) 157.08, 156.02, 145.39, 144.66, 144.29, 139.99, 131.23, 129.44, 128.65, 128.18, 126.68, 125.34, 125.17, 124.74, 124.05, 123.96, 120.42, 119.07, 118.40, 116.30, 108.78 ppm; HRMS (ESI) calcd. for $[C_{25}H_{15}N_3O_2$ +Na$]^+$ 412.1057, found 412.1060.

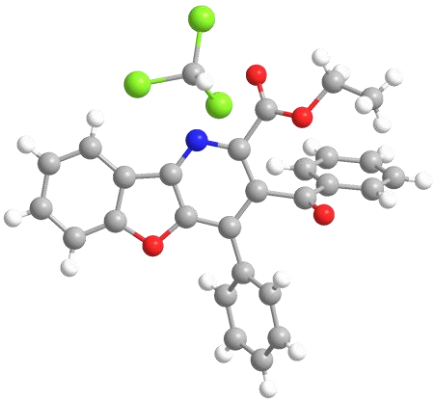


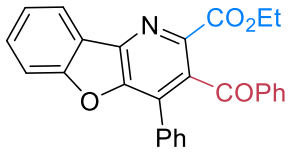
A solution of ethyl 3-benzoyl-4-phenylbenzofuro[3,2-*b*]pyridine-2-carboxylate **4d** (30 mg, 0.071 mmol, 1.0 equiv), KOH (16 mg, 0.28 mmol, 4.0 equiv) and 80% hydrazine hydrate (5.3 mg, 5.3 μL, 0.085 mmol, 1.2 equiv) in diethylene glycol (4.0 mL) was stirred at 160 ℃ for 4 h. After completion, H_2O (5.0 mL) was added and extracted with toluene (5.0 mL). The organic phase was washed with water (5.0 mL) three times and purified by flash chromatography on silica gel (PE: EtOAc = 10: 1) gave product **5b**: 23.5 mg (0.060 mmol), as a yellow solid, yield 85%; M.p. = 163–164 °C; ^{1}H NMR (600 MHz, DMF-d_7) δ 13.40 (s, 1H), 8.66 (d, *J* = 7.7 Hz, 1H), 7.99 (dt, *J* = 15.9, 8.0 Hz, 2H), 7.83 (t, *J* = 7.3 Hz, 1H), 7.56–7.52 (m, 2H), 7.40–7.35 (m, 2H), 7.32 (dd, *J* = 5.2, 1.9 Hz, 3H), 7.18 (dt, *J* = 14.7, 7.2 Hz, 3H) ppm; ^{13}C NMR (150 MHz, DMF-d_7) δ163.91, 163.13, 153.91, 151.67, 146.85, 142.22, 136.32, 135.41, 135.08, 133.81, 132.68, 132.03, 131.74, 131.67, 129.20, 127.40, 126.90, 126.80, 126.79, 117.06 ppm; HRMS (ESI) calcd. for $[C_{25}H_{15}N_3O_2$ +Na$]^+$ 412.1057, found 412.1061.



Ethyl 2-benzoyl-4-phenylbenzofuro[3,2-*b*]pyridine-3-carboxylate (**4c**, 21 mg, 0.05 mmol, 1.0 equiv) was dissolved in ethanol (1.0 mL). Sodium borohydride (37.8 mg, 0.1 mmol, 2.0 equiv) was added slowly under ice bath conditions. Monitor the reaction by TLC until the substrate disappeared. Quenched with ice water and extracted with DCM. The organic phase was concentrated, and purified by flash chromatography on silica gel (PE: EtOAc = 5: 1) gave product **6**: 15.0 mg (0.043 mmol), as a white solid, yield 80%. M.p. = 150–151 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.8 Hz, 1H), 7.93 – 7.88 (m, 2H), 7.65 (d, *J* = 7.4 Hz, 1H), 7.62 (dq, *J* = 10.9, 6.7, 6.0 Hz, 4H), 7.56 (d, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.40 (d, *J* = 7.1 Hz, 1H), 6.54 (s, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.80, 165.39, 159.60, 150.45, 147.33, 135.70, 133.40, 131.45, 130.89, 130.32, 129.12, 128.82, 128.32, 128.17, 127.06, 124.18, 122.64, 122.22, 113.06, 112.68, 81.30 ppm. HRMS (ESI) calcd. for $[C_{25}H_{15}NO_3$+Na$]^+$ 400.0944, found 400.0948.

6. Crystal data and structural refinement for product 4d

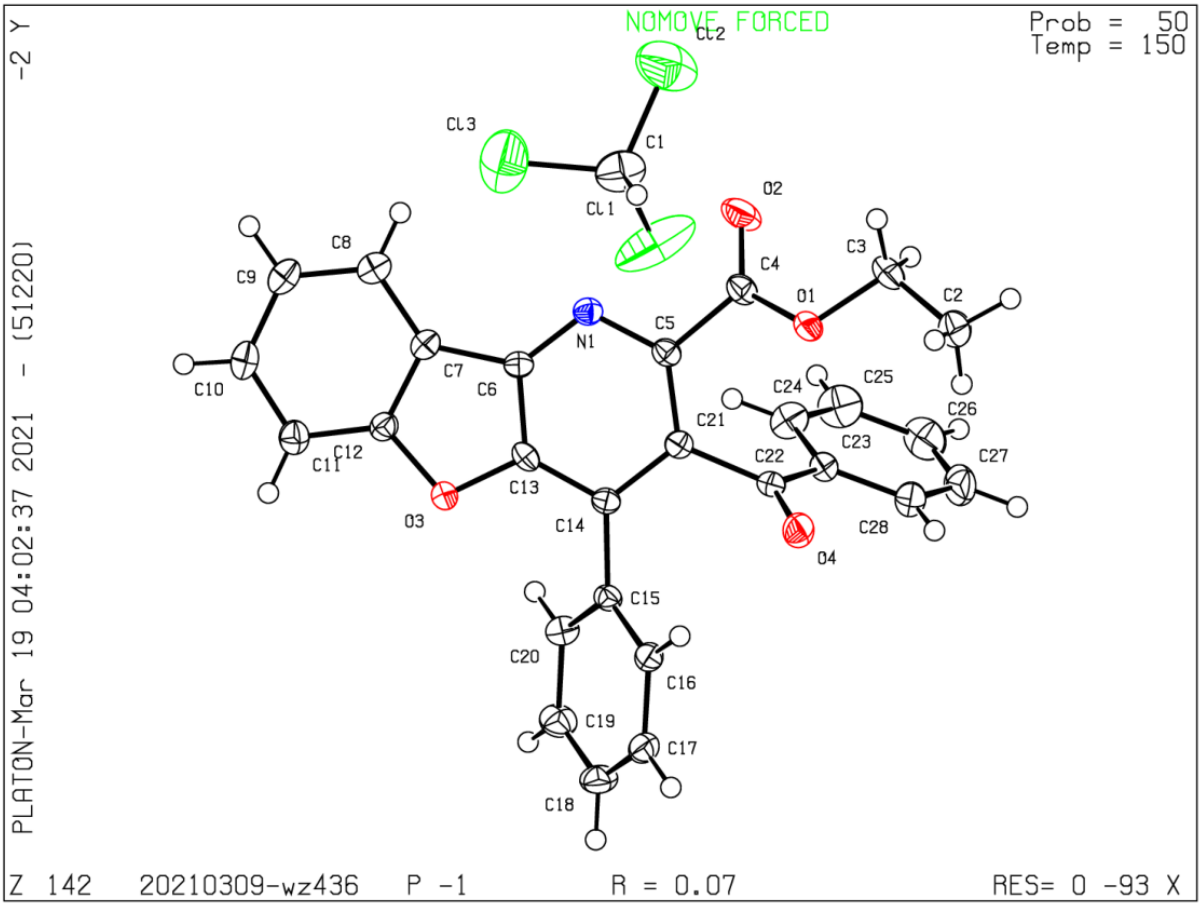




4d

Datablock: 4d

Bond precision		C-C = 0.0050 A	Wavelength = 0.71073
Cell	a = 10.4027(7)	b = 11.0987(7)	c = 12.0924(9)
	alpha = 87.255(6)	beta =73.730(6)	gamma = 70.545(6)
Temperaure: 150K			
		Calculated	Reported
Volume		1262.12(16)	1262.12(16)
Space group		P -1	P -1
Hall group		-P 1	-P 1
Moiety formula		C27 H19 N O4, C H Cl3	C H Cl3, C27 H19 N O4
Sum formula		C_{28} H_{20} Cl_3 N O_4	C_{28} H_{20} Cl_3 N O_4
Mr		540.80	540.80
Dx, g/cm^{-3}		1.423	1.423
Z		2	2
Mu (mm^{-1})		0.399	0.399
F000		556.0	556.0
F000’		557.11	
h, k, lmax		14,15,16	13,14,16
Nref		6713	5743
Tmin, Tmax		0.880,0.887	0.883,1.000
Tmin’		0.880	
Correction method= # Reported T Limits: Tmin=0.883 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness=0.856			Theta(max)= 28.999
R(reflctions)= 0.0739(4071)			wR2(reflections)= 0.2279(5743)
S= 1.034		Napr = 326	


NOMOVE FORCED
Prob = 50
Temp = 150
-2 Y
PLATON-Mar 19 04:02:37 2021 - (51220)
Cl2
Cl3
C1
Cl1
O2
C4
C3
C8
C9
O1
C2
C5
N1
C10
C7
C6
C24
C25
C26
C21
C23
C27
C22
C12
C11
C13
O3
C14
C28
O4
C15
C20
C16
C19
C17
C18
Z 142 20210309-wz436 P -1 R = 0.07 RES= 0 -93 X

7. Mechanistic study by computational calculations

In this article, all calculations were performed by Gaussian 09 software packages.[2] The conformations of intermediates were generated by SYBYL-X 2.0 GA Conf. search module and manual adjustment.[3] The recently developed M06-2X functional[4] together with the standard 6-31G(d) basis set,[5] were used for optimizing the geometry of all the minima and transition states. The optimized structures or transition structures were confirmed by normal vibrational mode analysis. The optimized structures were no imaginary frequency but transition structure had only one imaginary frequency. Transition structures were also verified by intrinsic reaction coordinate (IRC) calculations[6] or vibration direction. Considering the influence of solvation effect, SMD implicit solvent model[7] was used at M06-2X/6-311++G (2d, p) theoretical level[8] to obtain high accuracy single point energy in acetonitrile. This method has been applied successfully to investigate the mechanisms of several organic reaction, which is generally considered to be more accurate for energetic. Solution-phase single-point energies corrected by the gas-phase Gibbs free energy corrections were used to describe all the reaction energetics. All energies reported throughout the text are in kcal/mol, and the bond length unit is angstroms (Å). Structures were generated by GaussView 6[9] and CYL view.[10]

To gain more sight into the (4 + 1 + 1) annulation reaction, we carried out DFT calculations on the (4 + 1 + 1) annulation between **1a** and **2a** under the assist of DABCO and Cs_2CO_3 as a model reaction.

7.1. Formation of ylides

The core step in the formation of *N*-ylides is S_N2 nucleophilic substitution by DABCO to **2a** (Figure S1). The activation energy of **N-TS1** is 18.0 kcal/mol. Subsequently, the ammonium salt is deprotonated into *N*-ylide **N-INT2** by assistance of alkali. The relatively low energy of product (-32.2 kcal/mol) means that the formation of *N*-ylide is an irreversible process. It shows that **2a** can react with the same equivalent of DABCO, and the ammonium salt is its main form.

A similar calculation was performed by replacing DABCO with dimethyl sulfide (Figure S1). This process needs to cross the energy barrier of 25.8 kcal/mol via **S-TS1**. Then the sulfur salt is converted into sulfur ylide **S-INT2** by assistance of alkali. It should be noted that the control experiment used a pre-prepared sulfur salt **S-INT1** to participate in the reaction. In order to comprehensive comparison with *N*-ylide, the same in situ generation process was simulated in this calculation.

The relative energy of sulfur salt formation is much higher (25.8 kcal/mol vs. 18.0 kcal/mol), which means that the rate of sulfur salt formation is much lower than the rate of ammonium salt formation. This is why most of the *S*-ylide reactions using sulfur salts prepared in advance to

participate in the reaction, while *N*-ylide reaction can be processed using prepared ammonium salt as well as in situ generation one.

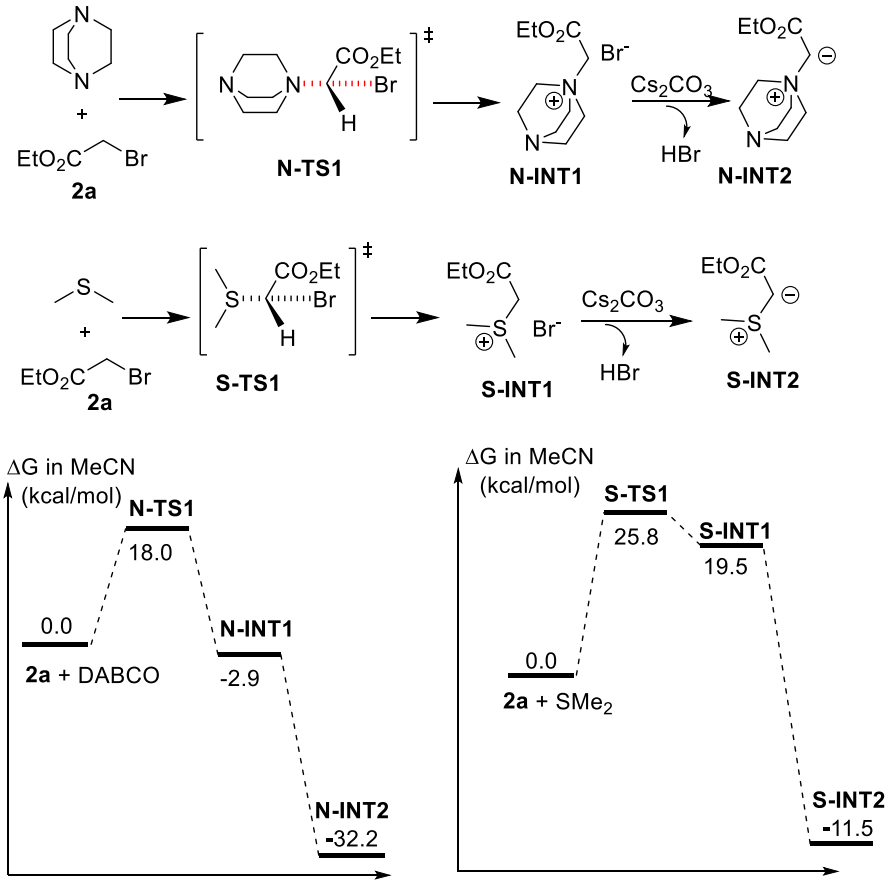


Figure S1. Gibbs free energy profile of ylides formation

7.2 [4 + 1] annulations

The cases where the newly formed ylides attack to **1a** in different orientations was examined (Figure S2). The Michael addition energy barrier for *N*-ylide (**N-TS2-SR** is 15.4 kcal/mol and **N-TS2-RR** is 15.2 kcal/mol) is significantly lower than that for *S*-ylide (**S-TS2-SR** is 23.0 kcal/mol and **S-TS2-RR** is 19.1 kcal/mol), showing better nucleophilic addition ability for *N*-ylide. However, the energy barrier of bond rotation and [4 + 1] ring-closure are completely opposite. The total energy barrier via **N-TS3-SR** and **N-TS3-RR** is 31.1 kcal/mol and 28.5 kcal/mol respectively. Such a high energy barrier obviously could not complete the [4 + 1] ring closure under normal conditions, which was also confirmed by the experimental results. For *S*-ylide, the total energy barrier via **S-TS3-SR** and **S-TS3-RR** is 19.5 kcal/mol and 15.2 kcal/mol respectively. This is also consistent with the fact that we only got the [4 + 1] product **7** in the ***trans*** configuration when reacted *S*-ylide to **1a**.

Such calculation results are also consistent with the calculation conclusions of Waser's group[11], suggesting that the nucleophilicity of *N*-ylide may not be weaker than the *S*-ylide, but in

the final elimination cyclization step, the energy barrier required for *N*-ylide to eliminate cyclization is much higher than that for *S*-ylide. The above theoretical calculations well explain why the [4 + 1] cyclization reaction occurred with *S*-ylide and **1a**, but not for *N*-ylide.

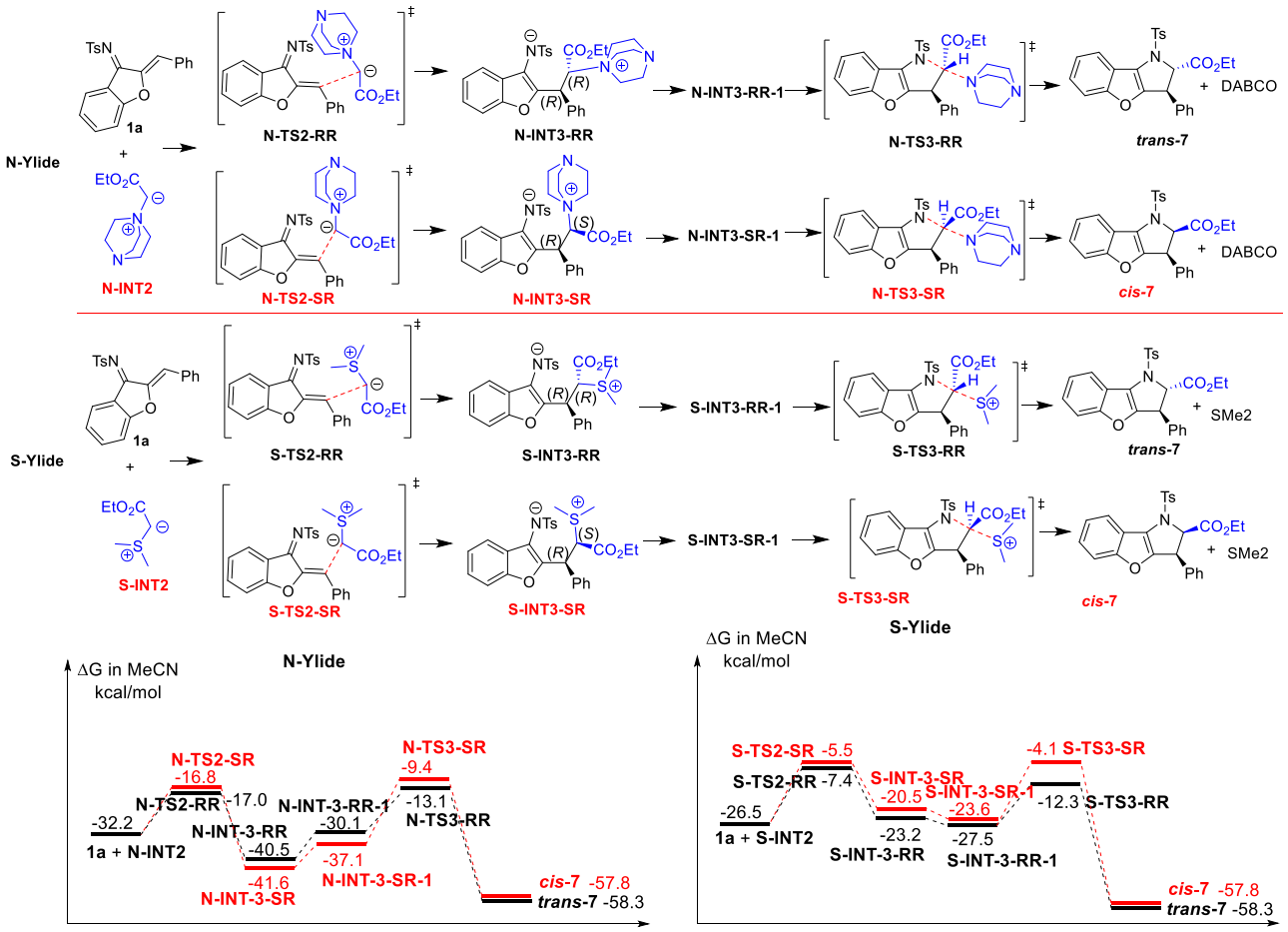


Figure S2. Gibbs free energy profile of Micheal additions and ring closures

7.3 The cyclopropane pathway

The cyclopropane pathway was also considered (Figure S3). **2a** becomes enol form **2a-1** with the assistance of carbonate anion via **2a-TS1**. Then **2a-1** is adducted to **1a** from different directions to generate **INT1-A** and **INT1-B**. We cannot rule out the possibility of generating cyclopropane intermediates, because the energy barriers of cyclopropane ring-closure is relatively low (**TS2-A**, **TS2-A-1**, **TS2-B**, **TS2-B-1**). However, we can exclude the cyclopropane ring closure process mediated by DABCO, because the energy barrier of DABCO-mediated S_N2 substitution via **TS1-A** and **TS1-B** is as high as 38.8 kcal/mol and 46.3 kcal/mol respectively.

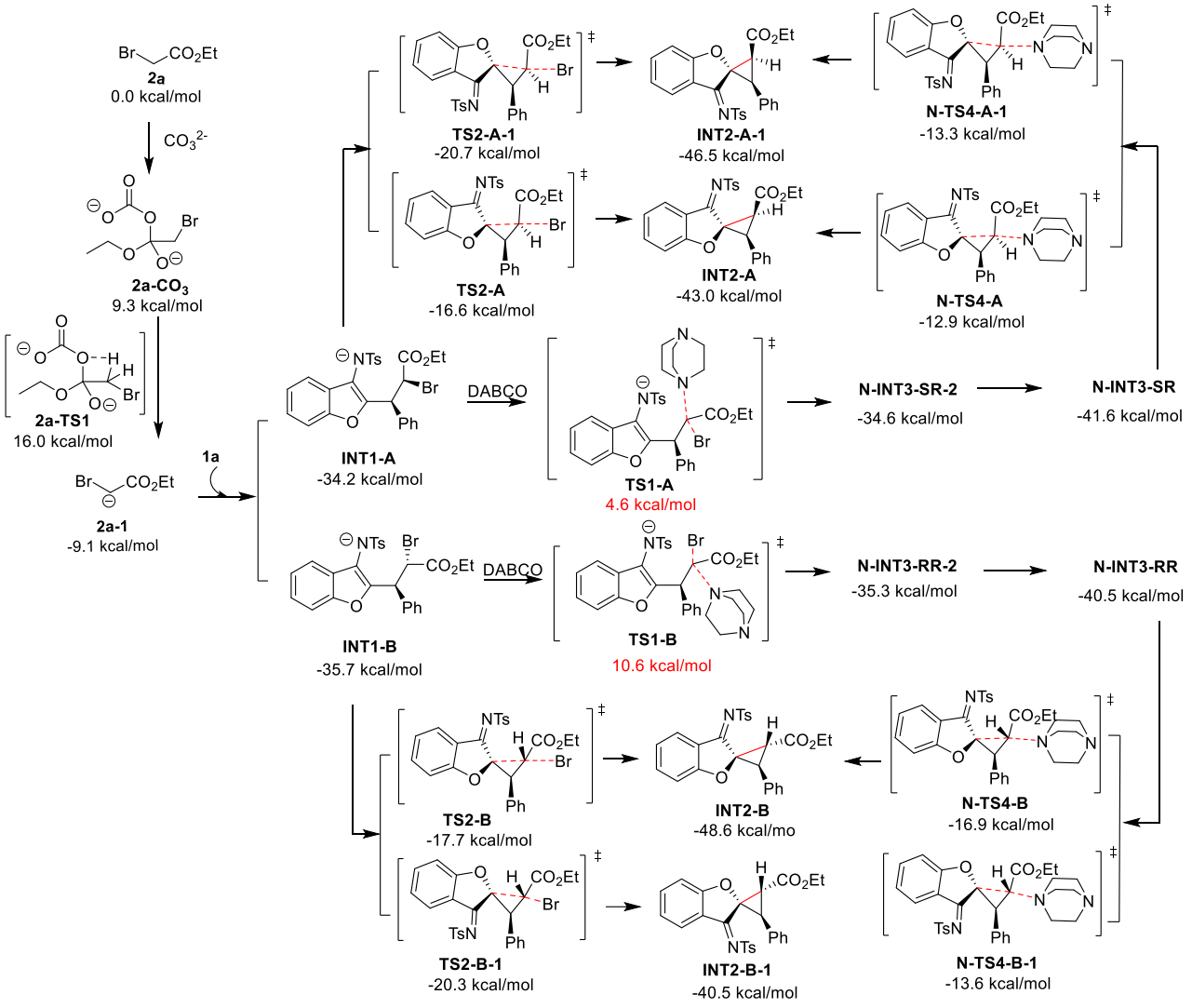


Figure S3. Gibbs free energy profile of formation of cyclopropane intermediate

Even assuming that the cyclopropane intermediate **INT2** has been formed, it is almost impossible to open the cyclopropane through the *N*-ylide. Eight configurations of the cyclopropane opening process were all calculated (Figure S4). The results show that the energy barrier of this process is 32.6 kcal/mol at least. Therefore, we can conclude that the mechanism of cyclopropane intermediate might be not reasonable.

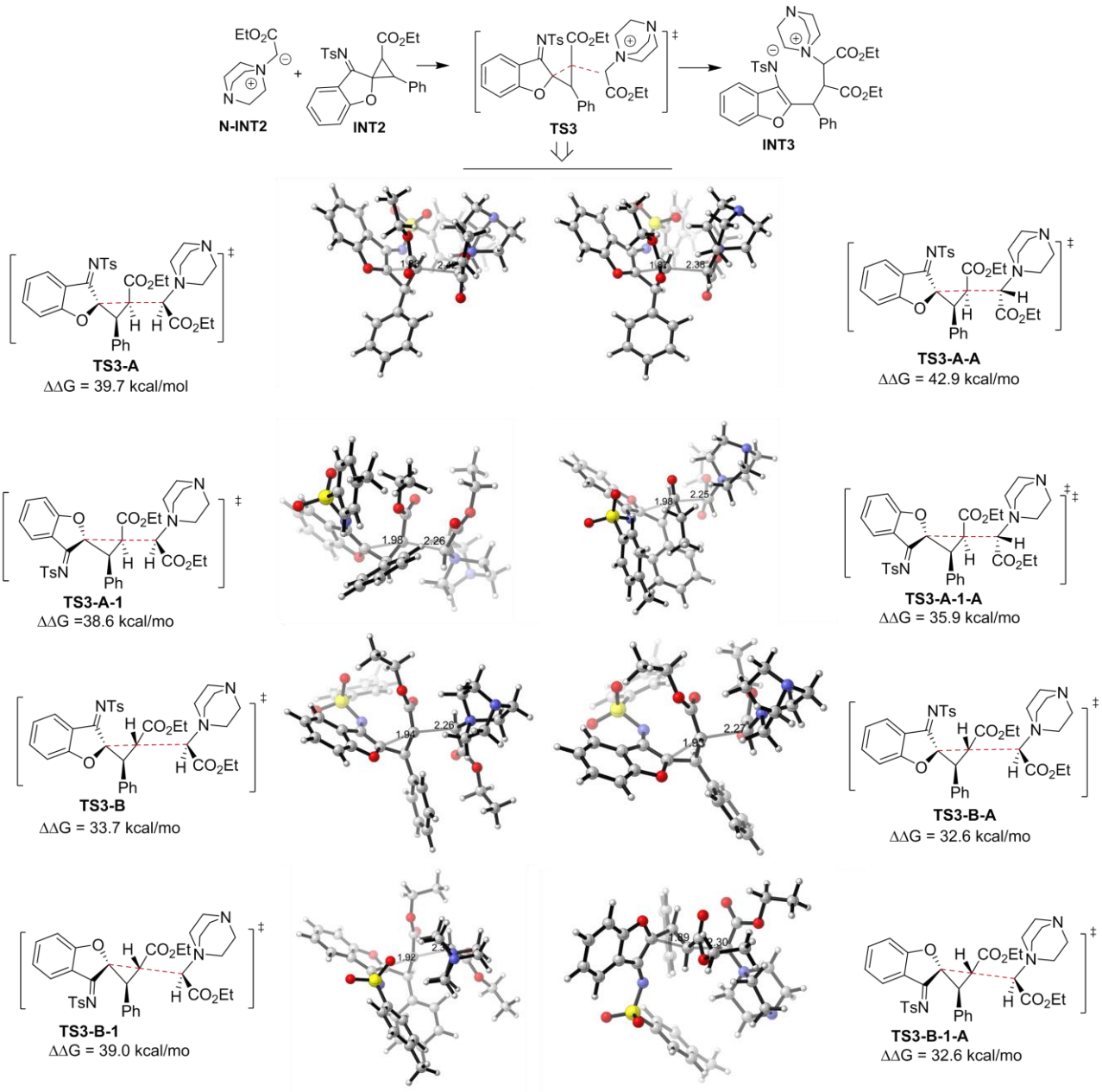


Figure S4. Gibbs free energy profile and transition structure of cyclopropane opening

7.4 Hoffman Elimination Pathway

From the above calculation, we can know that **2a** was mainly combined with DABCO and exists in the form of ammonium salt. And *N*-ylide is easy to process Michael addition to **1a**. However, the Michael addition product **N-INT3** could not perform [4 + 1] or [2 + 1] ring closure at room temperature. Therefore, it must be other transformations of **N-INT3** created the unexpected (4 + 1 + 1) reaction.

From the quaternary ammonium salt and alkaline conditions, we think of the Hoffman elimination reaction.**N-INT3-RR** can easily be combined with **-CO_3^{2-}** to form **N-INT4** (Figure S5). Then the Hoffman elimination reaction occurs through **N-TS5** with the energy barrier of 6.2 kcal/mol. Next, the negative electron on the nitrogen is transferred to the terminal double bond to

attack to the free **2a** in the system. It is worth mentioning that as electrons are transferred on the conjugated double bond, **N-INT6** will have four different configurations. Among them, the lowest energy barrier is the process through **N-TS6-B** to afford **N-INT7**. **N-INT7** and DABCO are combined into **N-INT7-A**. Due to the acidity of the α-position of the carbonyl group, DABCO can act as a base to assist the removal of H^+ via **N-TS7-A** with the energy barrier of 11.8 kcal/mol. The fallen $DABCOH^+$ stabilizes the substrate through hydrogen bonding. Subsequently, another α-hydrogen abstraction occurs through **N-TS7-B** with the energy barrier of 8.6 kcal/mol, which is actually a formal 1,6-hydrogen transfer. Afterward, the chain conjugation system **N-INT9-B** could be generated after Ts-group elimination through **N-TS8-D** with the energy barrier of 24.8 kcal/mol. Then electrocyclization reaction can easily occur through the transition state **N-TS9** to afford **N-INT10** with the energy barrier of 15.9 kcal/mol. Then, **N-INT10** is subsequently oxidized by air to obtain the final product.

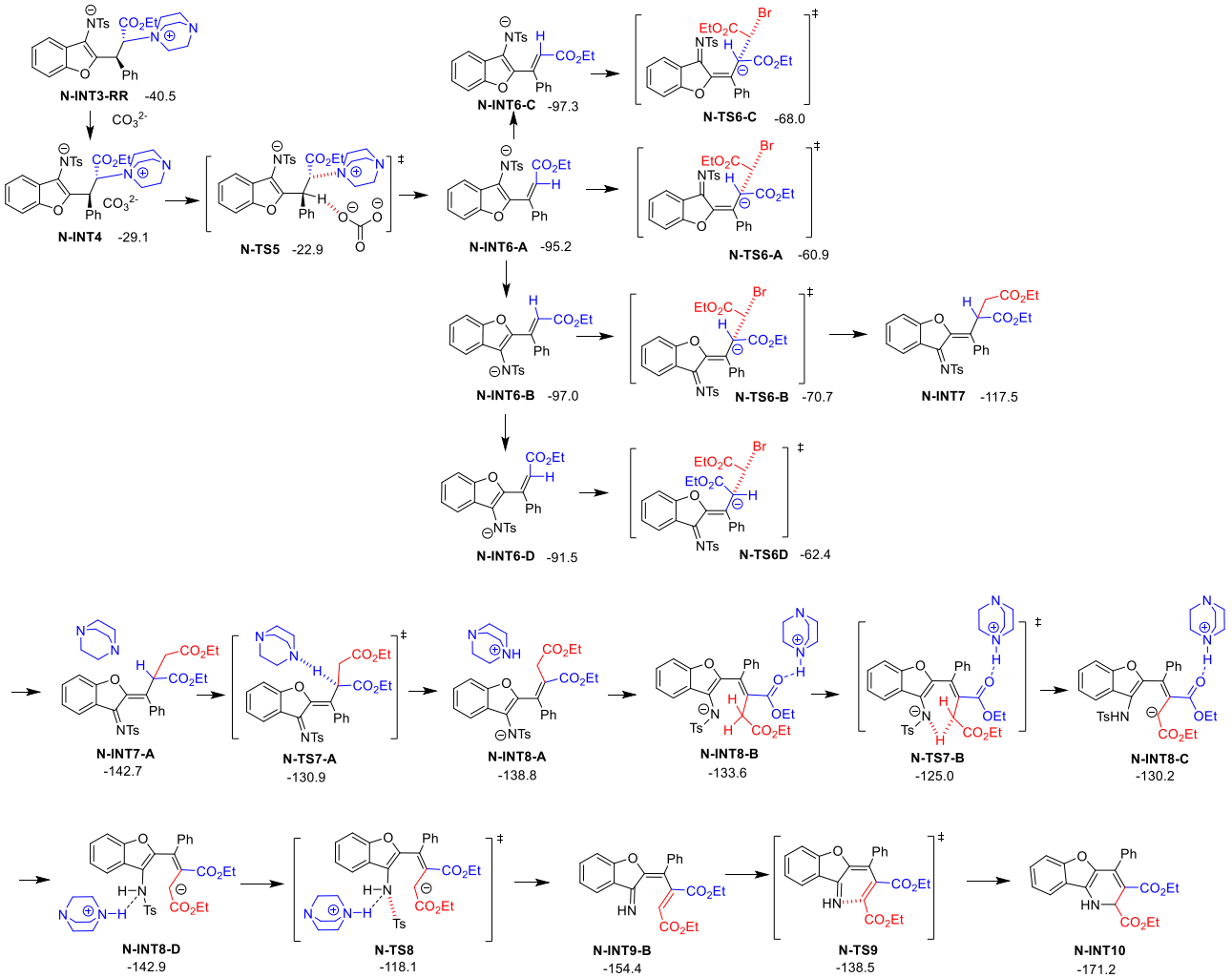
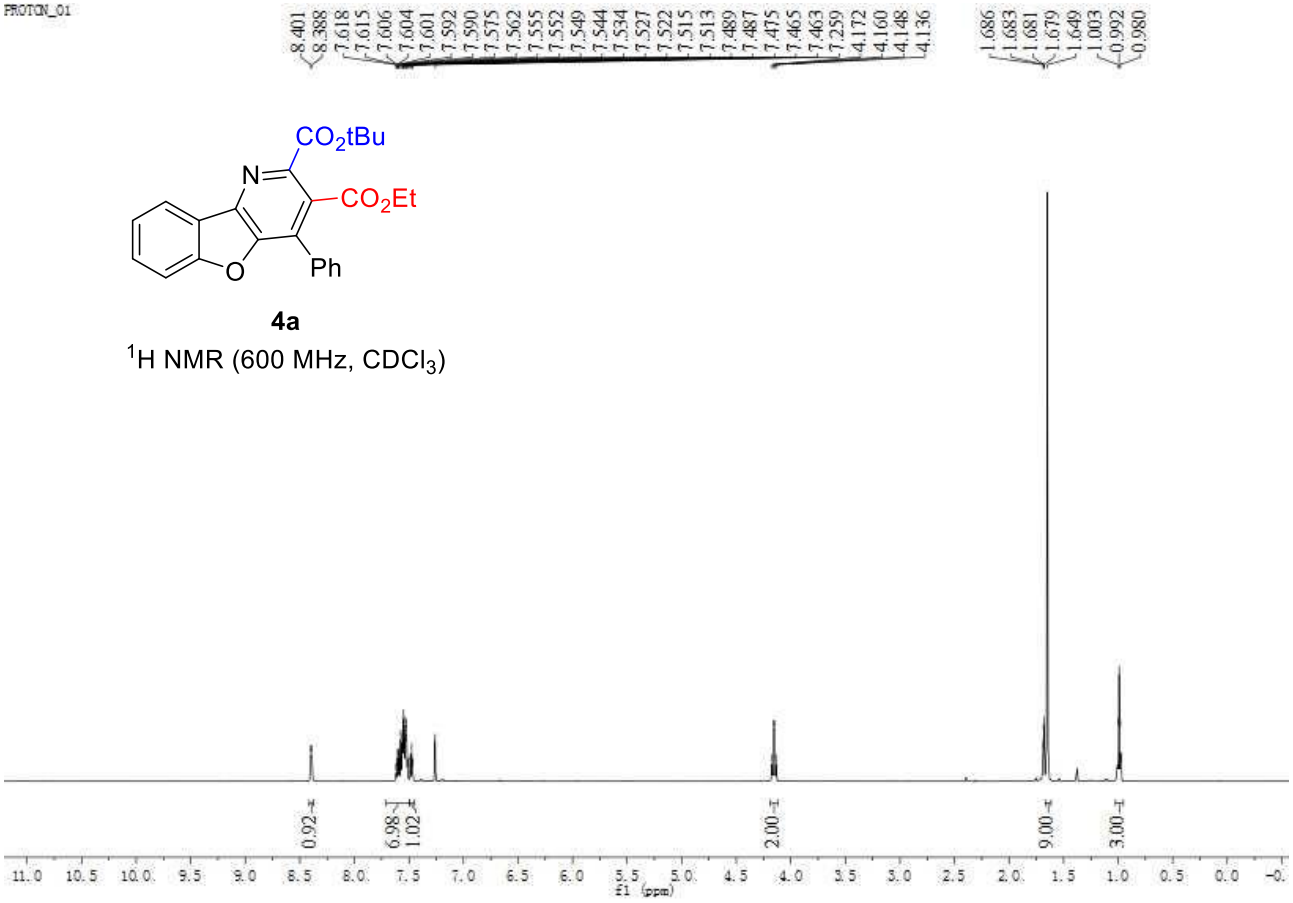


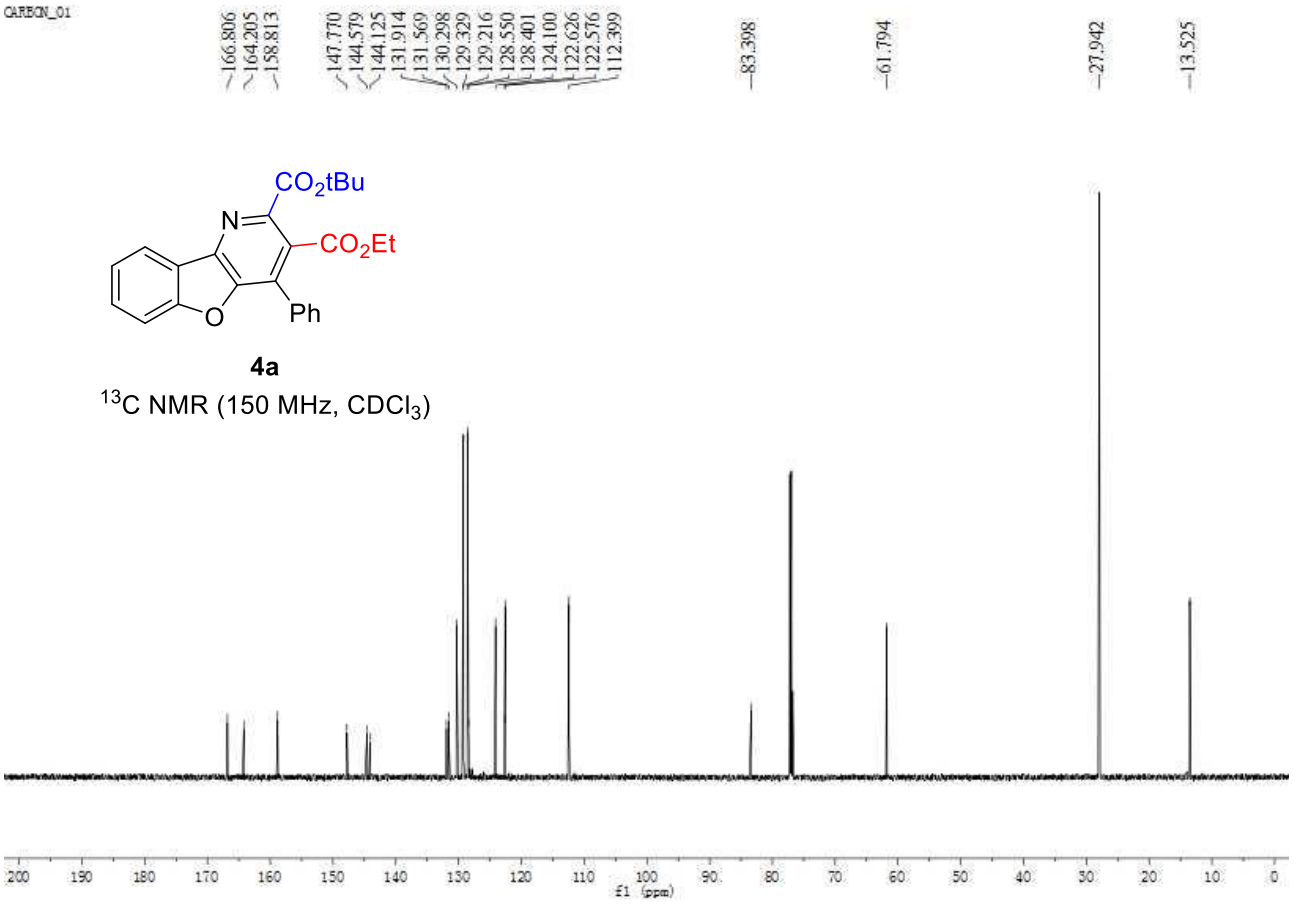
Figure S5. Gibbs free energy profile of Hoffman Elimination Pathway

8. NMR Spectra



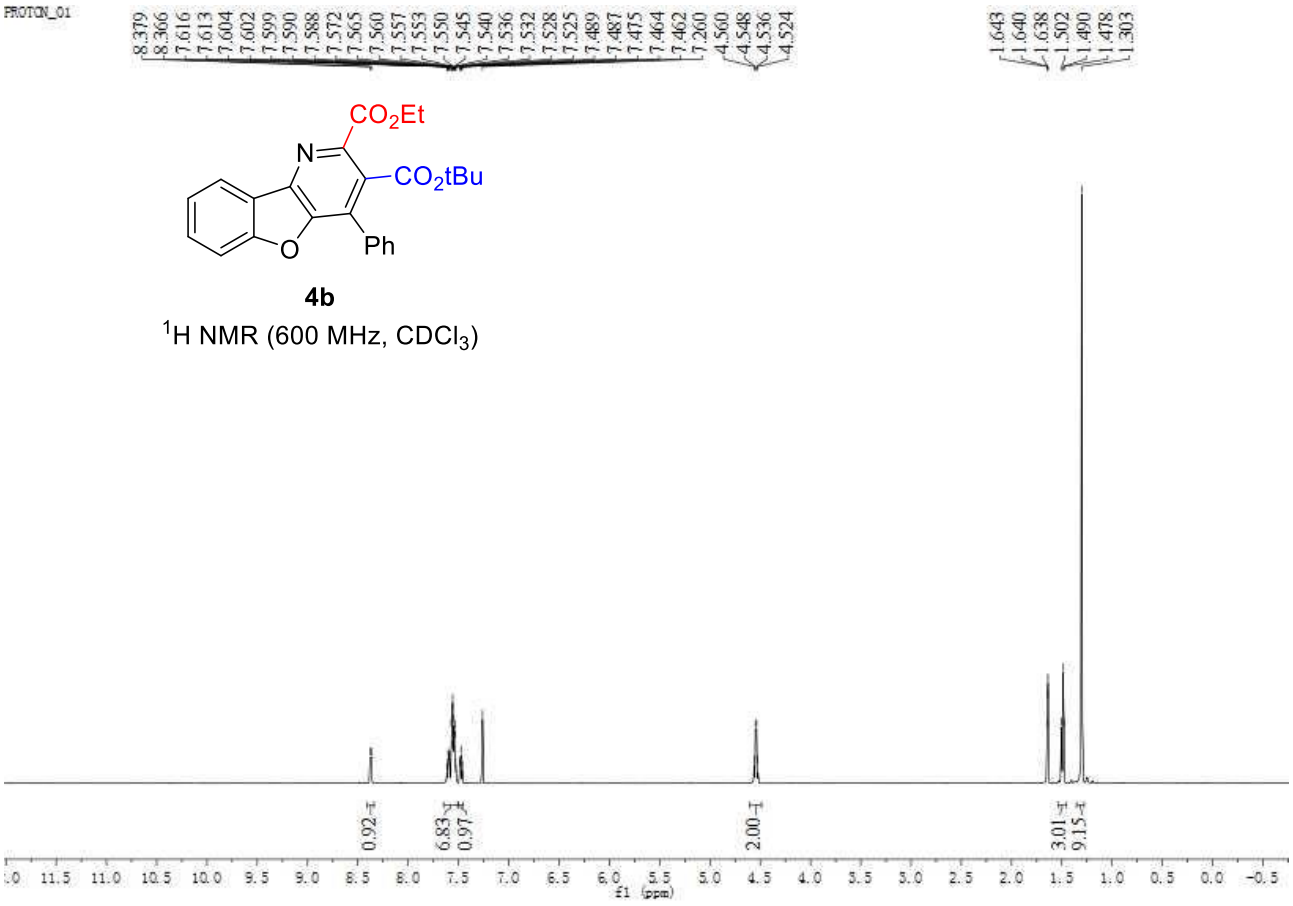
4a

^{1}H NMR (600 MHz, $CDCl_3$)



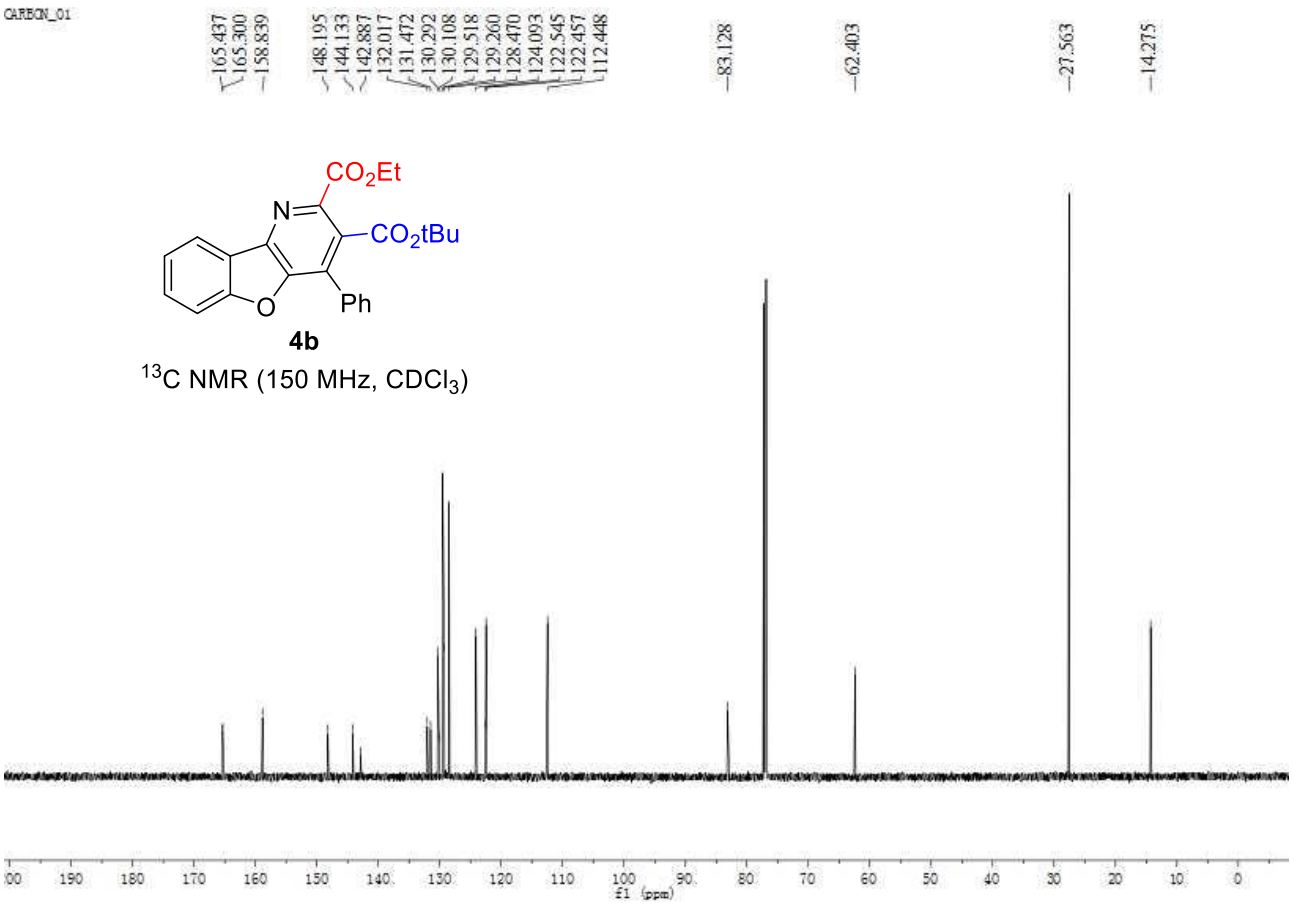
4a

^{13}C NMR (150 MHz, $CDCl_3$)



4b

^{1}H NMR (600 MHz, $CDCl_3$)

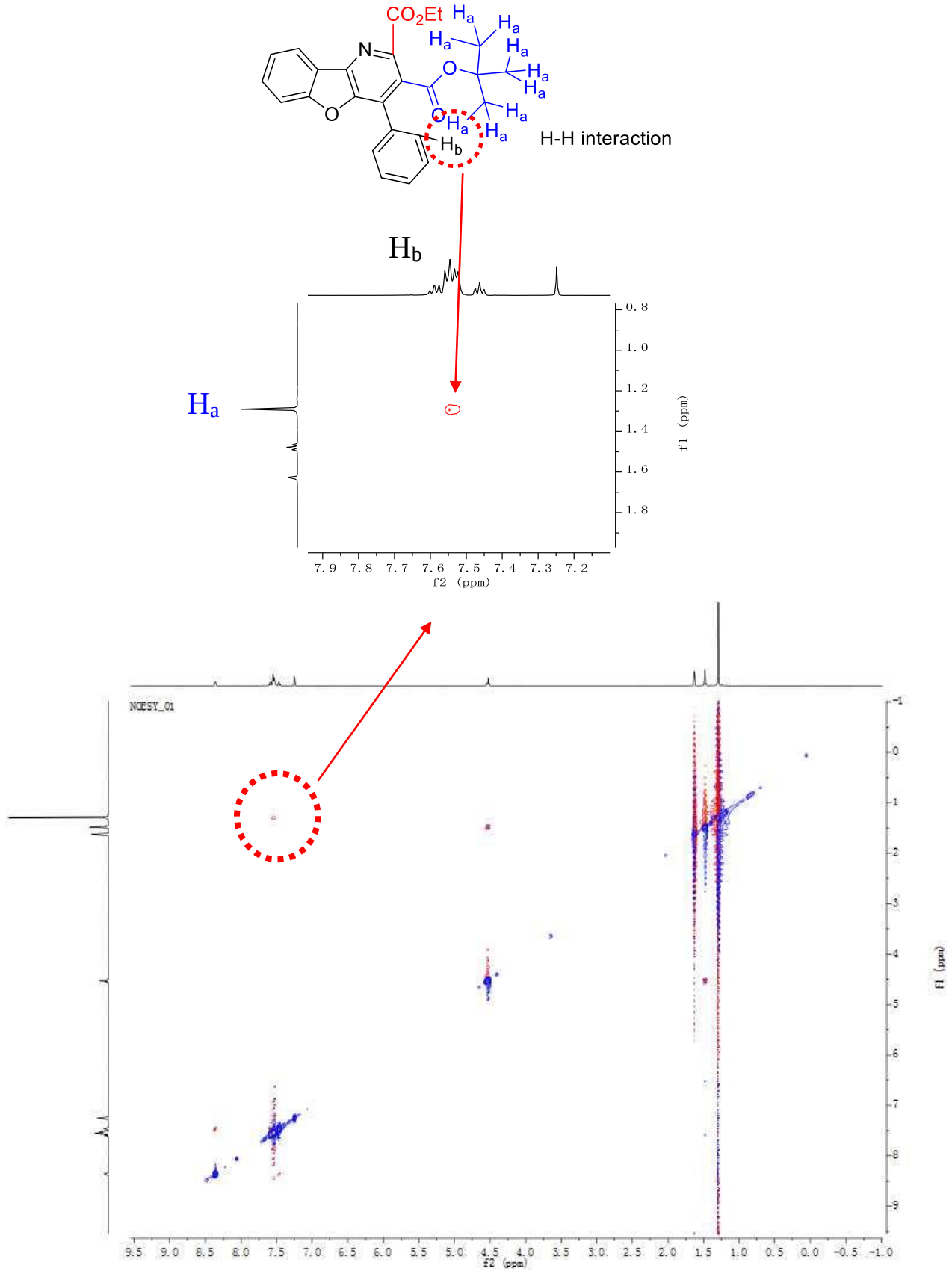


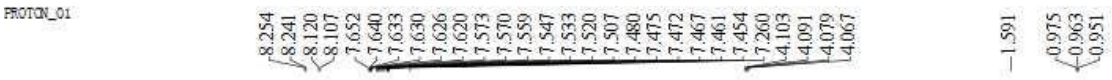
4b

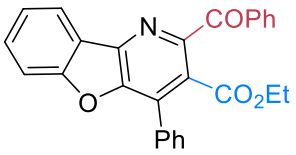
^{13}C NMR (150 MHz, $CDCl_3$)

4b

NOESY (600 MHz, $CDCl_3$)

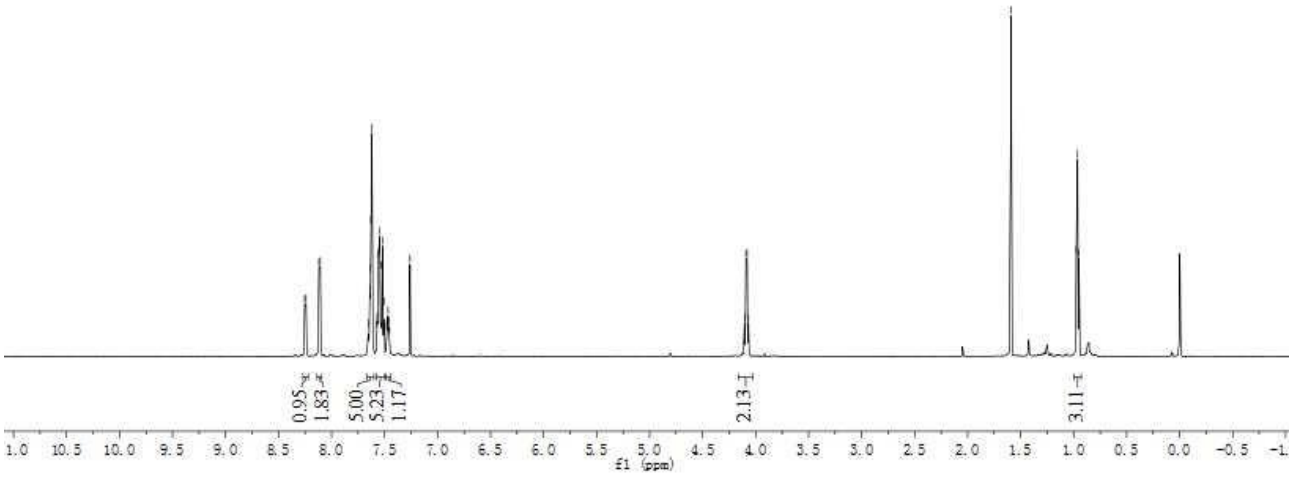


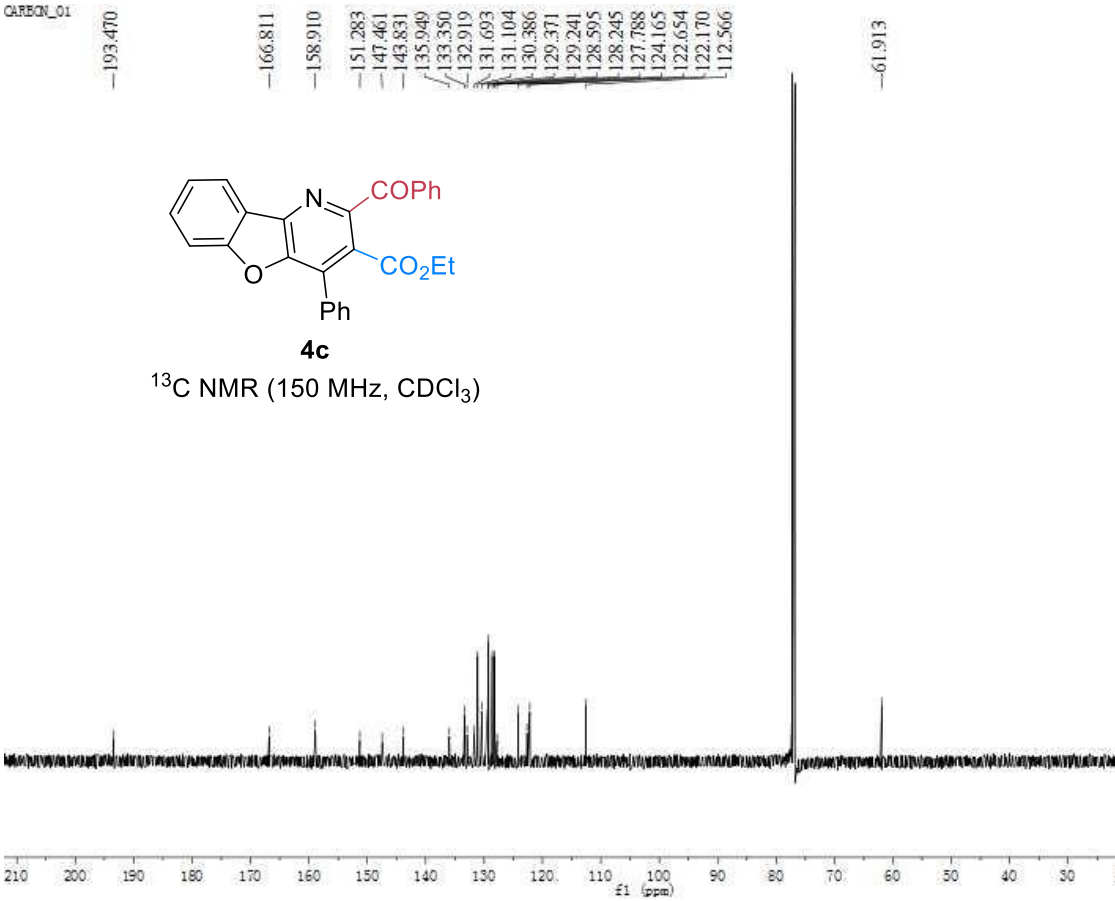




4c

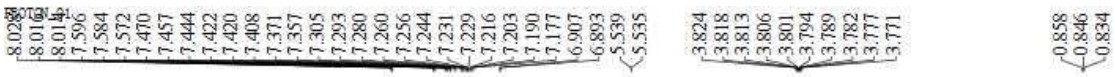
^{1}H NMR (600 MHz, $CDCl_3$)

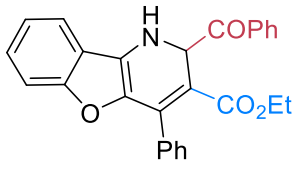




4c

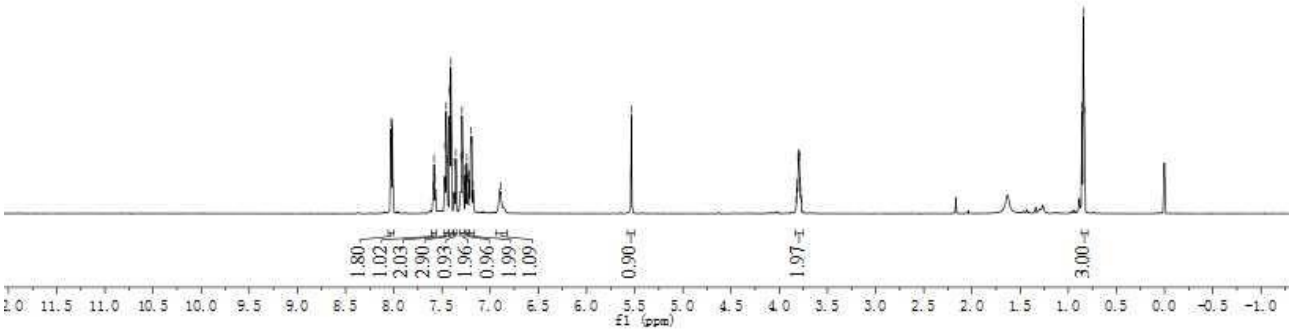
^{13}C NMR (150 MHz, $CDCl_3$)

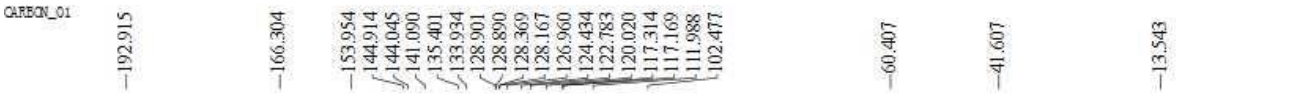


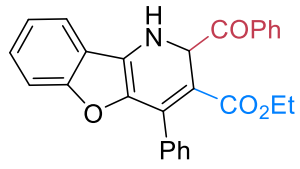


4c'

^{1}H NMR (600 MHz, $CDCl_3$)

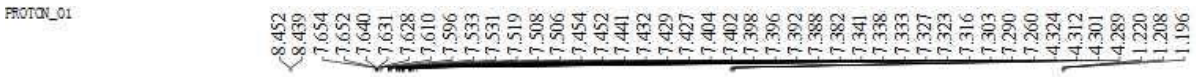


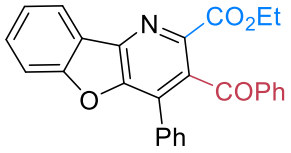




4c'

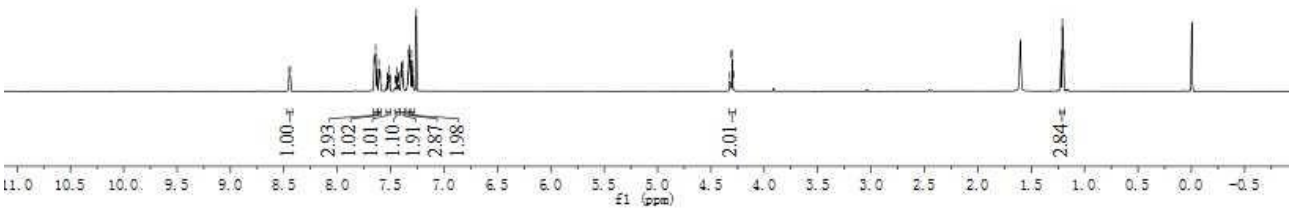
^{13}C NMR (150 MHz, $CDCl_3$)

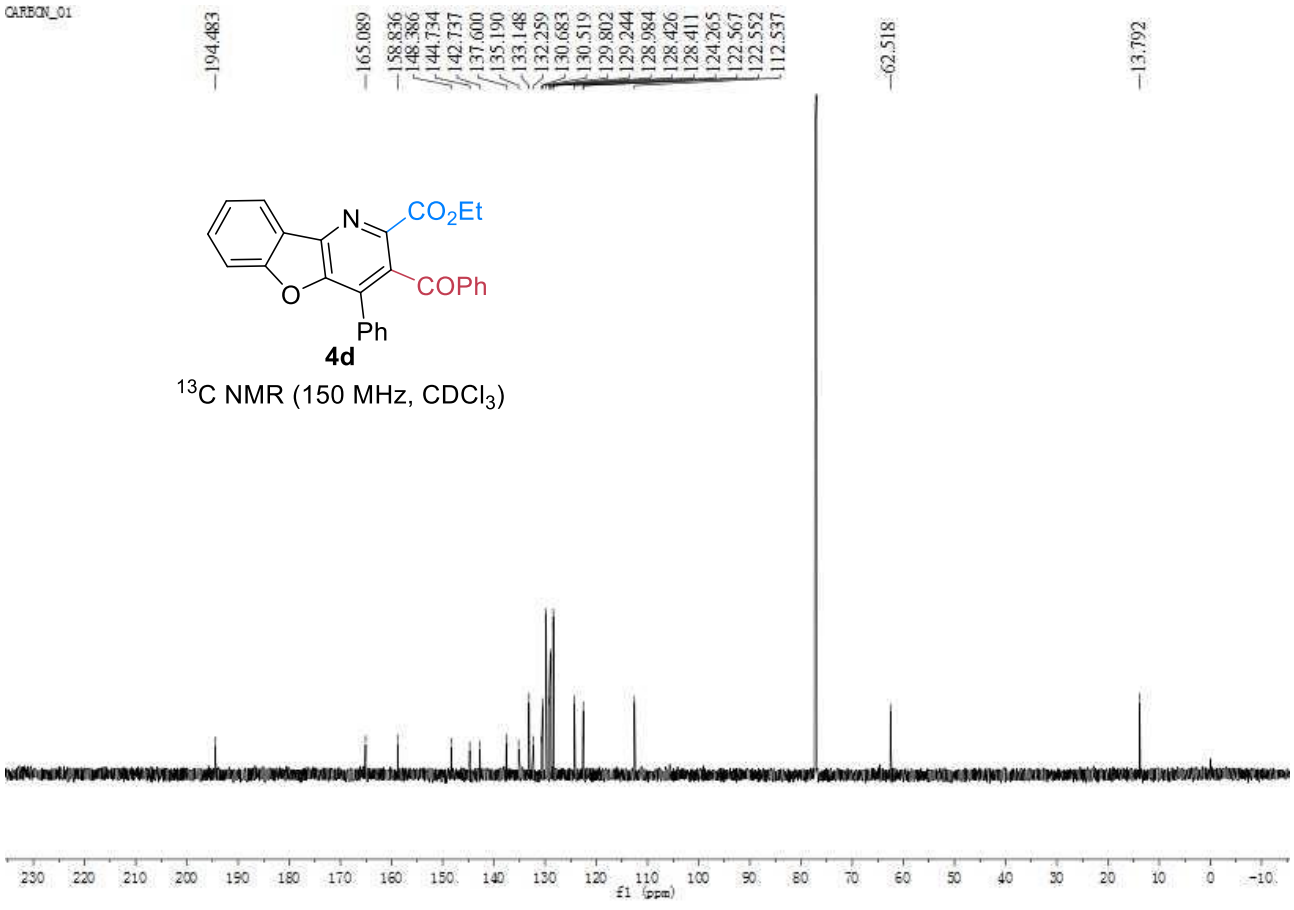




4d

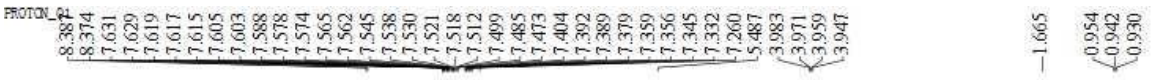
^{1}H NMR (600 MHz, $CDCl_3$)

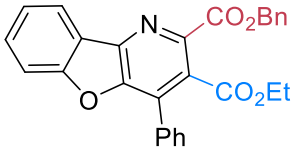




4d

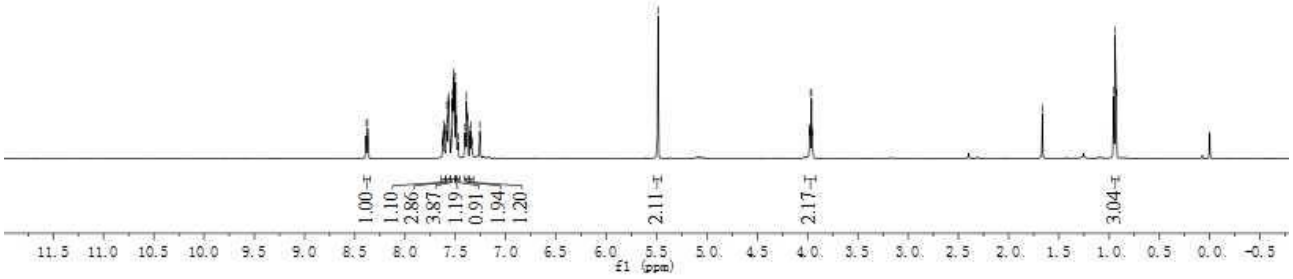
^{13}C NMR (150 MHz, $CDCl_3$)

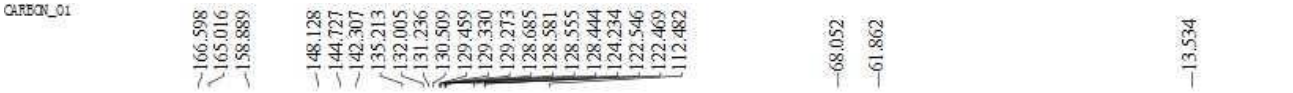


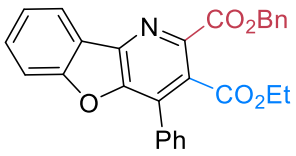


4e

^{1}H NMR (600 MHz, $CDCl_3$)

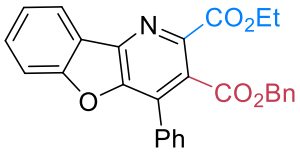






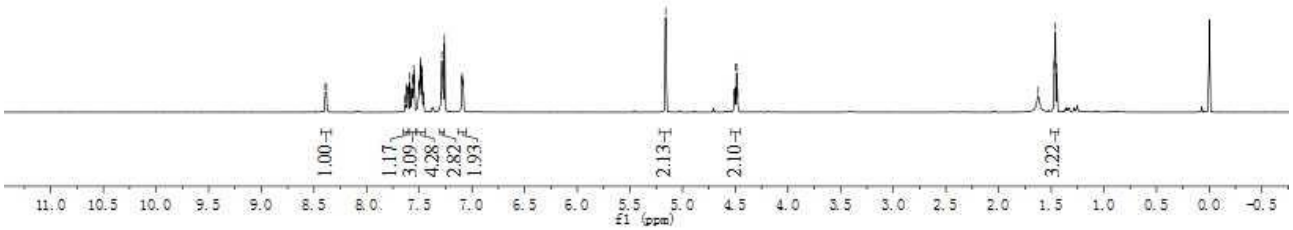
4e

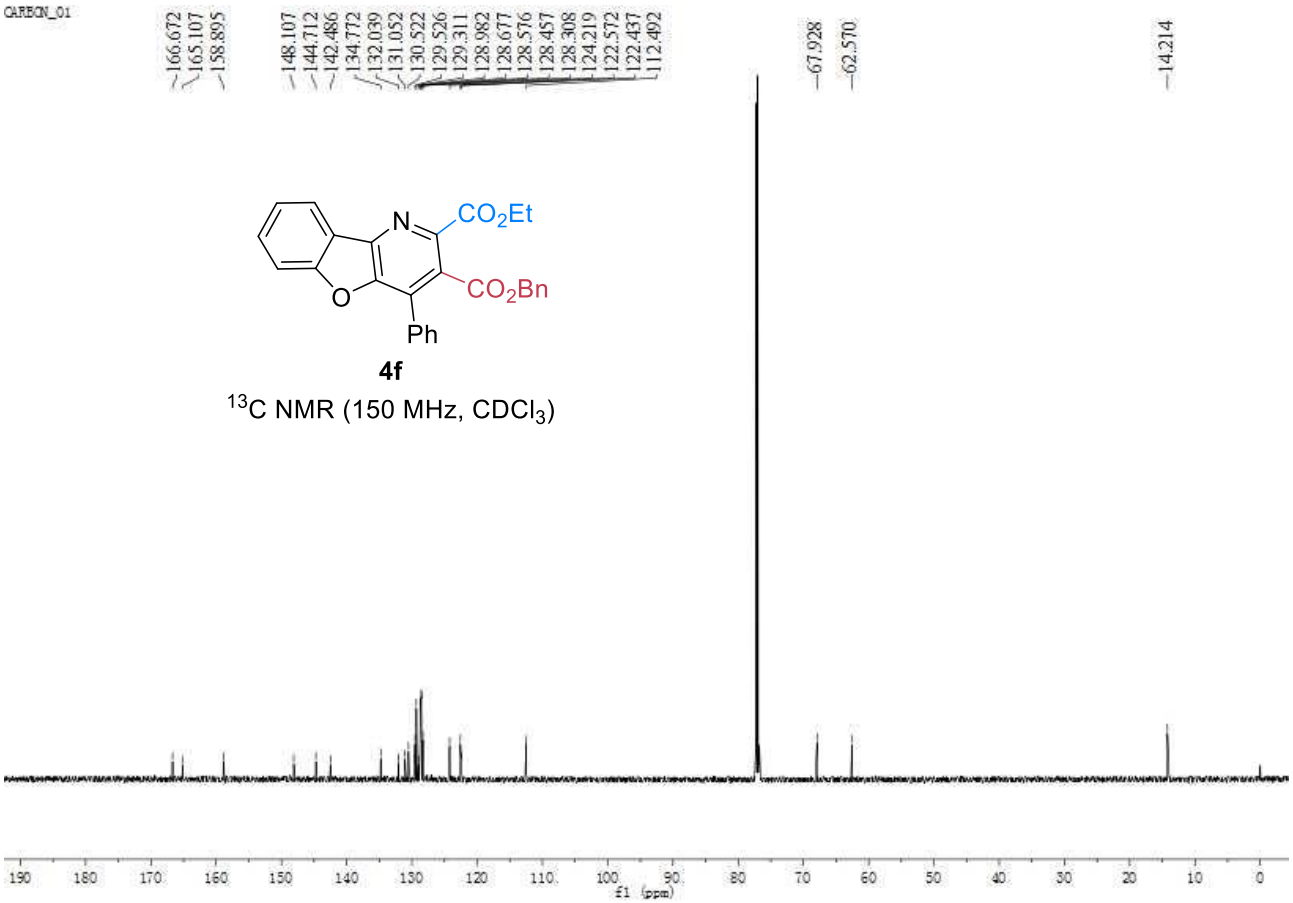
^{13}C NMR (150 MHz, $CDCl_3$)



4f

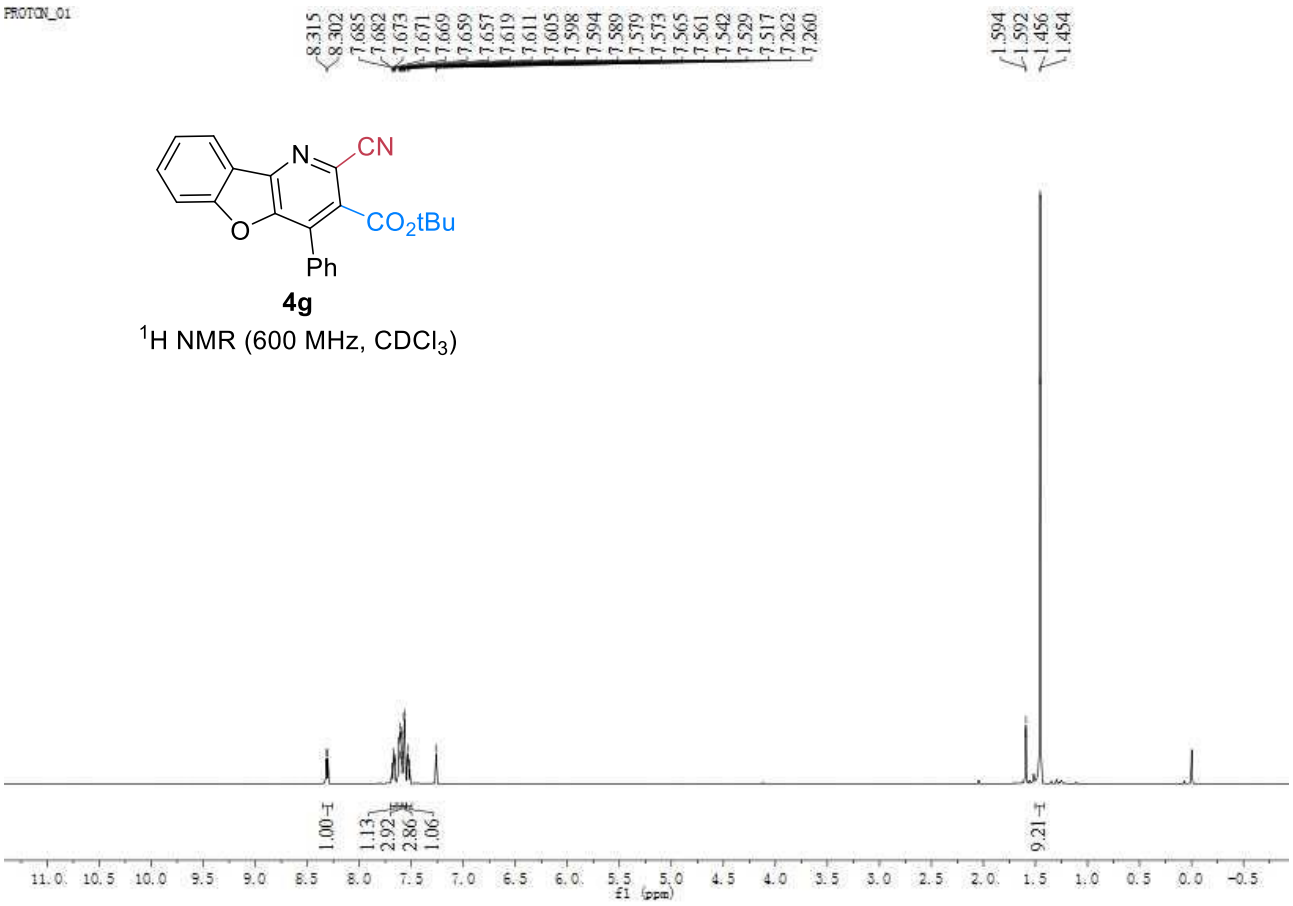
^{1}H NMR (600 MHz, $CDCl_3$)





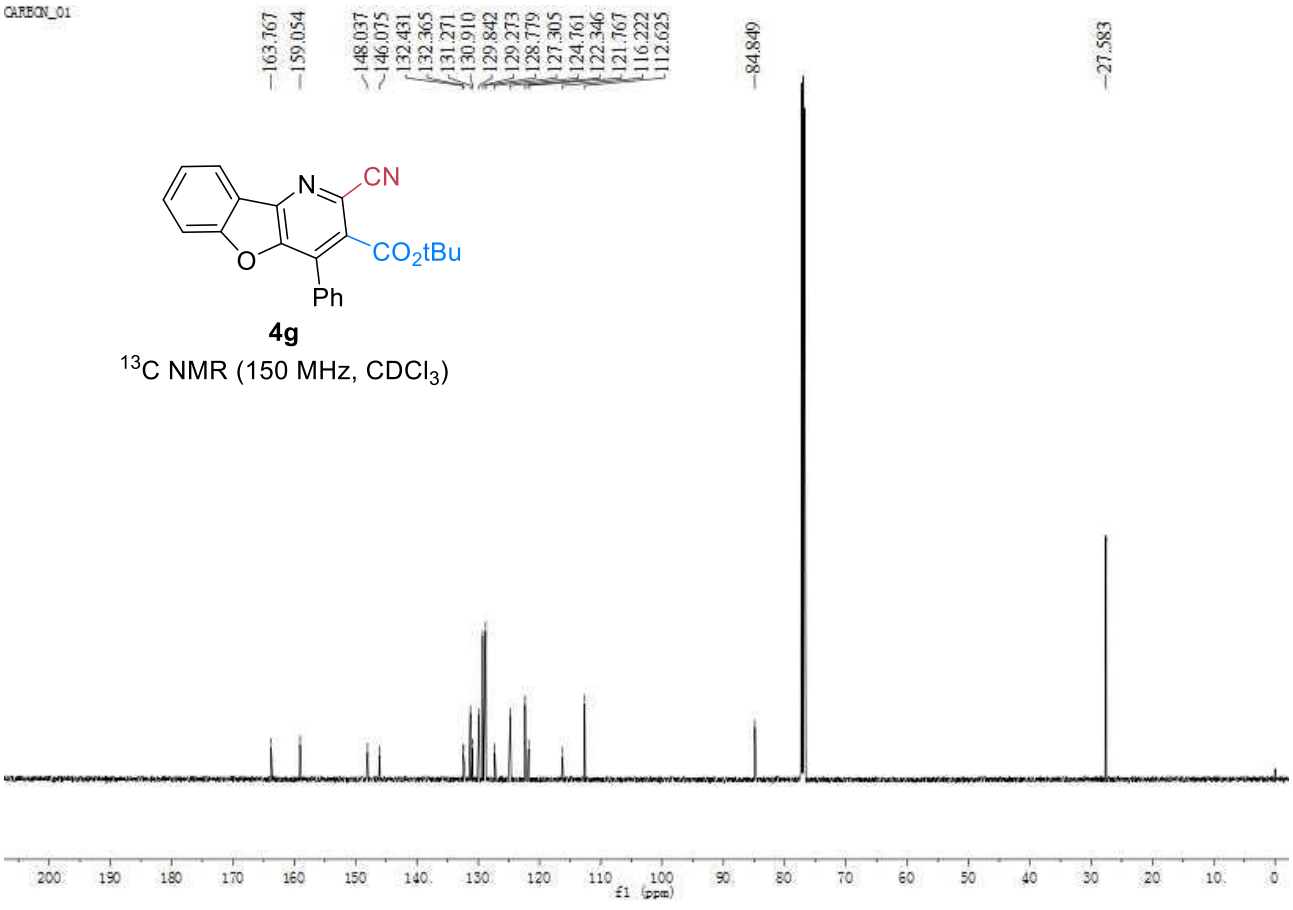
4f

^{13}C NMR (150 MHz, $CDCl_3$)



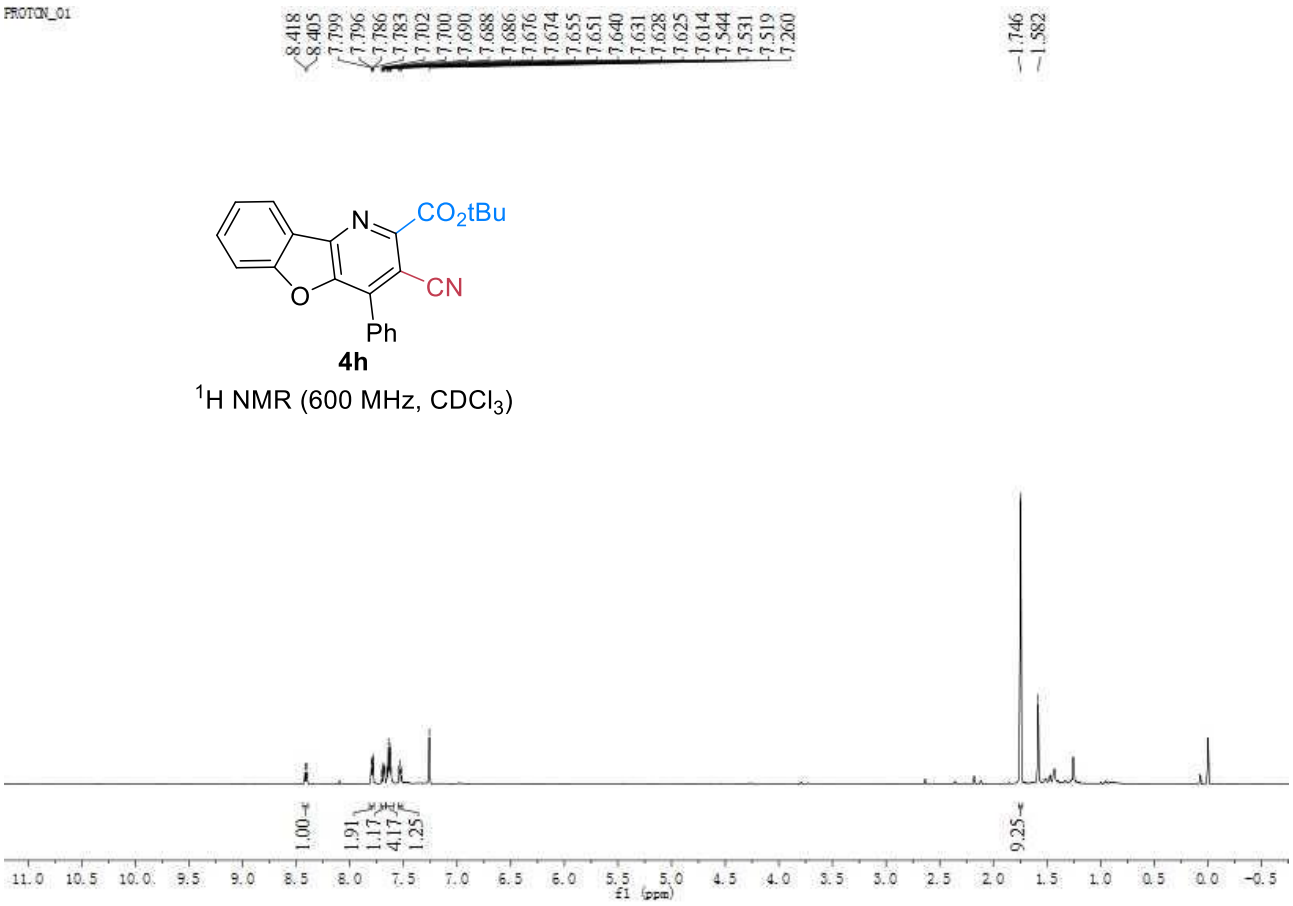
4g

^{1}H NMR (600 MHz, $CDCl_3$)



4g

^{13}C NMR (150 MHz, $CDCl_3$)


PROTON_01
8.418
8.405
7.799
7.796
7.786
7.783
7.702
7.700
7.690
7.688
7.686
7.676
7.674
7.655
7.651
7.640
7.631
7.628
7.625
7.614
7.544
7.531
7.519
7.260
1.746
1.582
CO2tBu
N
CN
O
Ph
4h
1H NMR (600 MHz, CDCl3)
1.00
1.91
1.17
4.17
1.25
9.25
f1 (ppm)
CARBON_01
162.954
159.396
149.525
146.842
146.615
137.411
131.626
130.615
129.979
129.898
128.963
124.694
123.008
122.147
115.614
112.657
105.475
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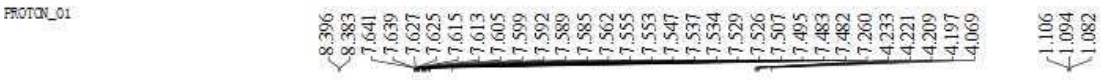
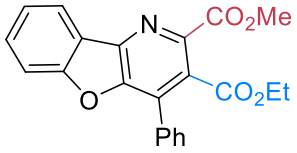
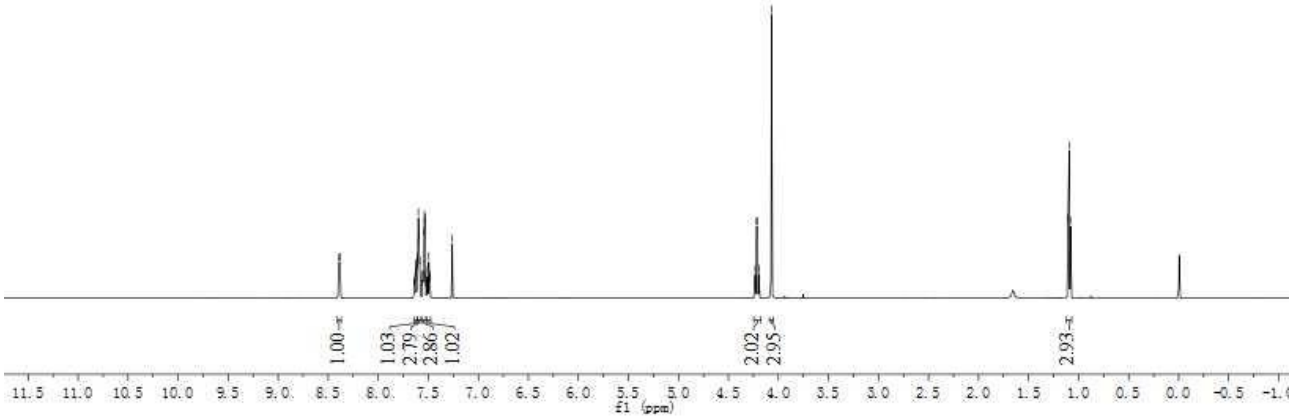
28.004
CO2tBu
N
CN
O
Ph
4h
13C NMR (150 MHz, CDCl3)
f1 (ppm)

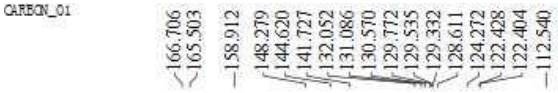


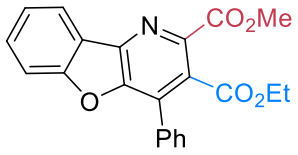


4i

^{1}H NMR (600 MHz, $CDCl_3$)

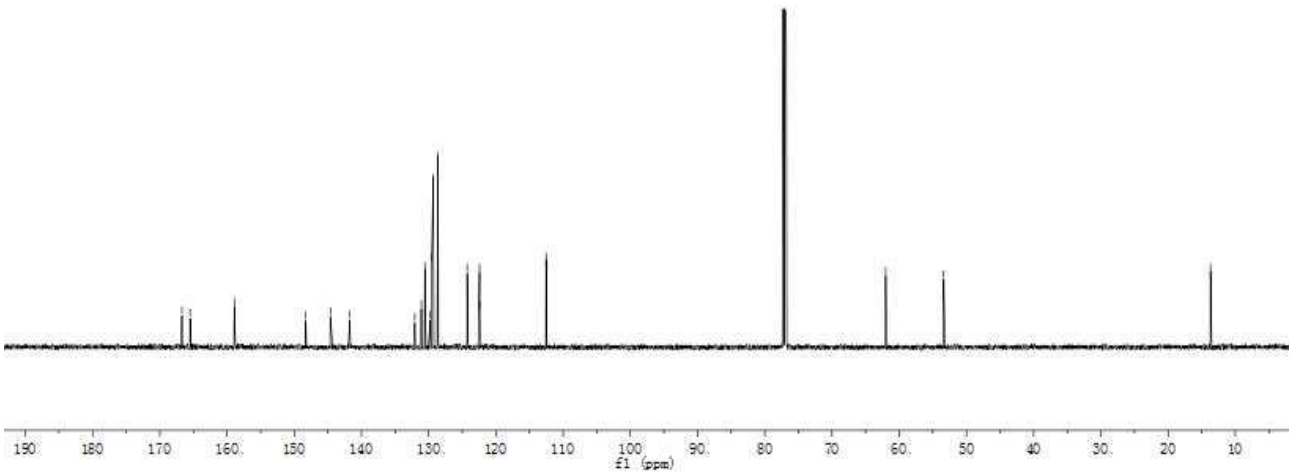


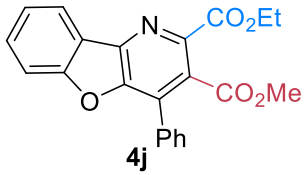




4i

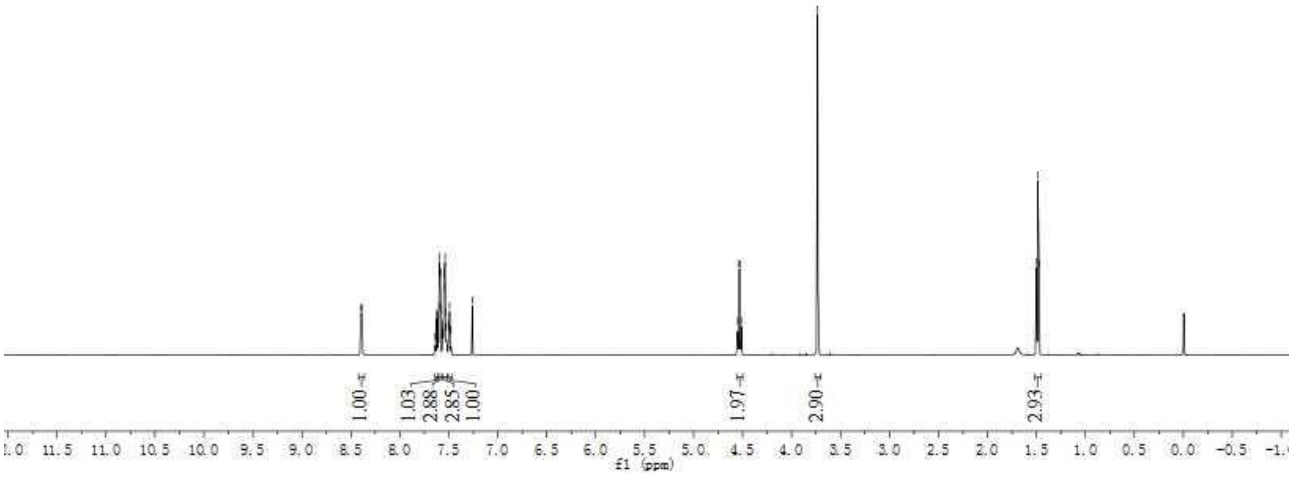
^{13}C NMR (150 MHz, $CDCl_3$)

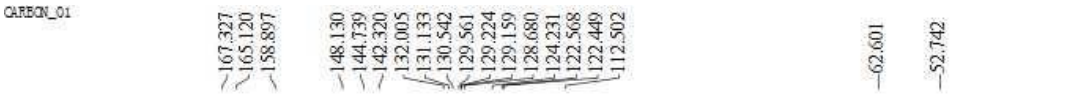


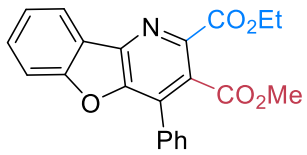


4j

^{1}H NMR (600 MHz, $CDCl_3$)

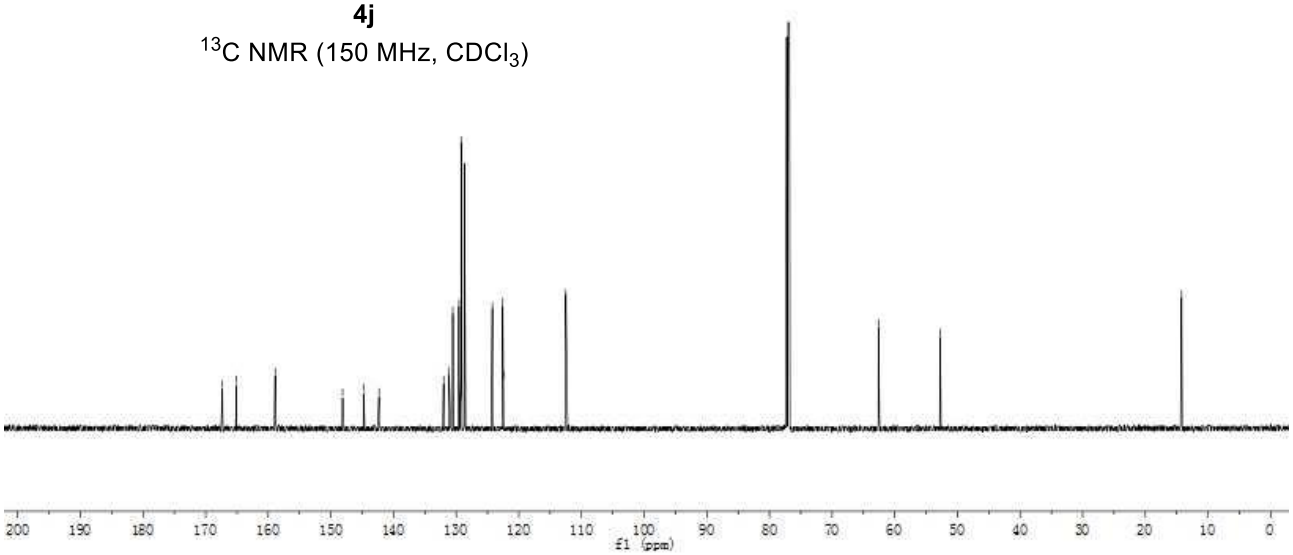


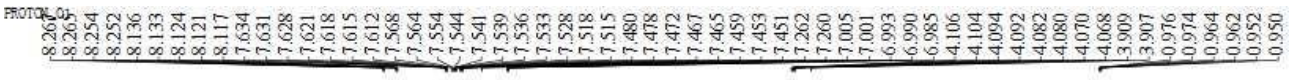


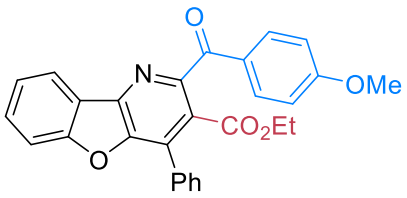


4j

^{13}C NMR (150 MHz, $CDCl_3$)

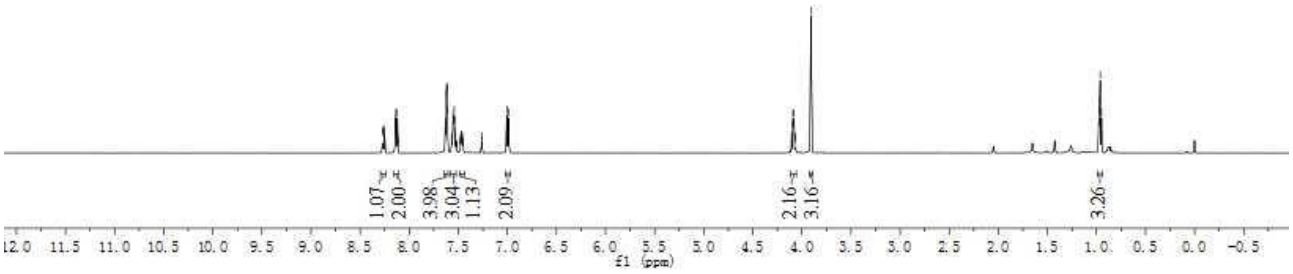


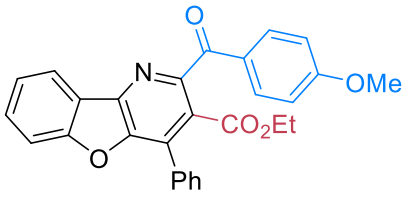




4k

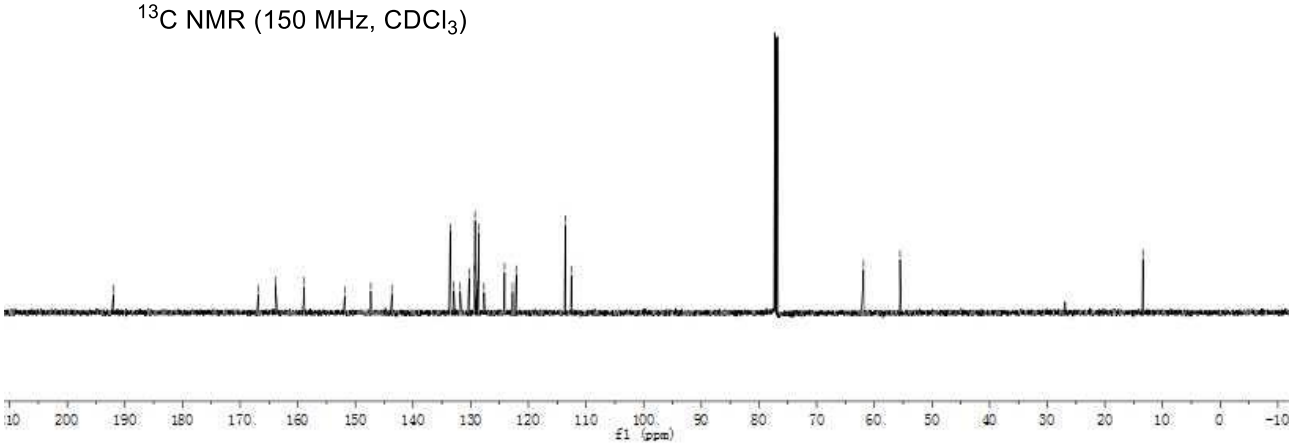
^{1}H NMR (600 MHz, $CDCl_3$)

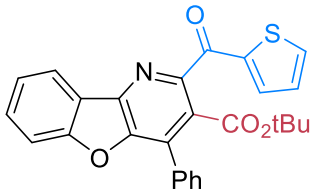




4k

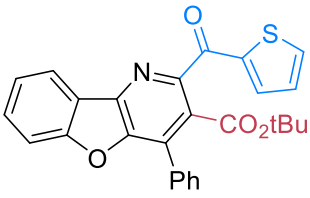
^{13}C NMR (150 MHz, $CDCl_3$)





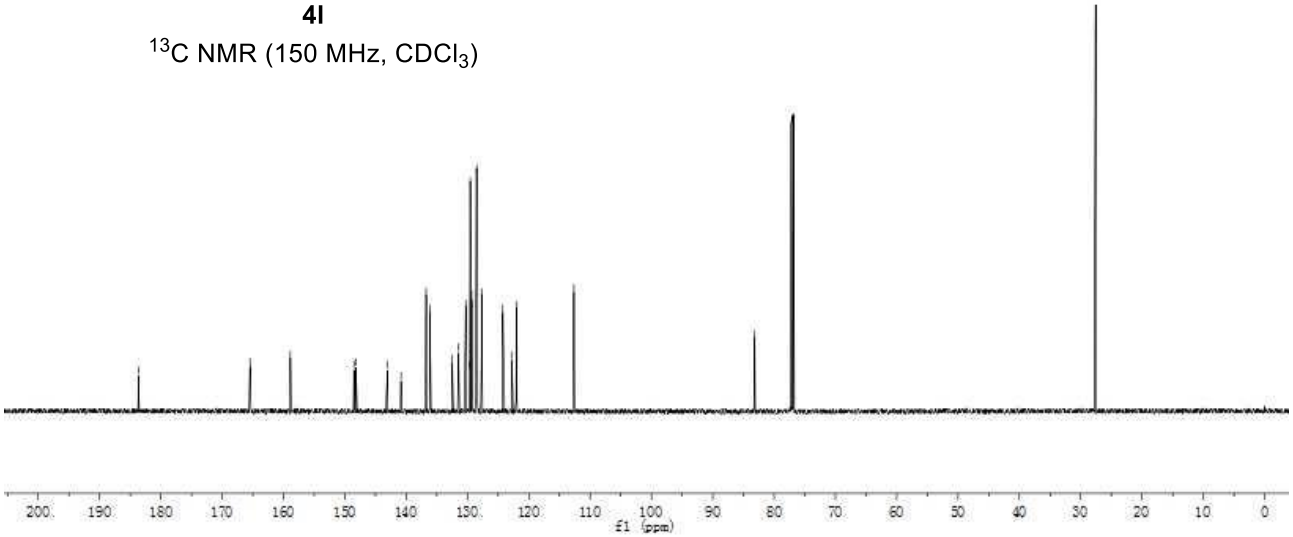
4l

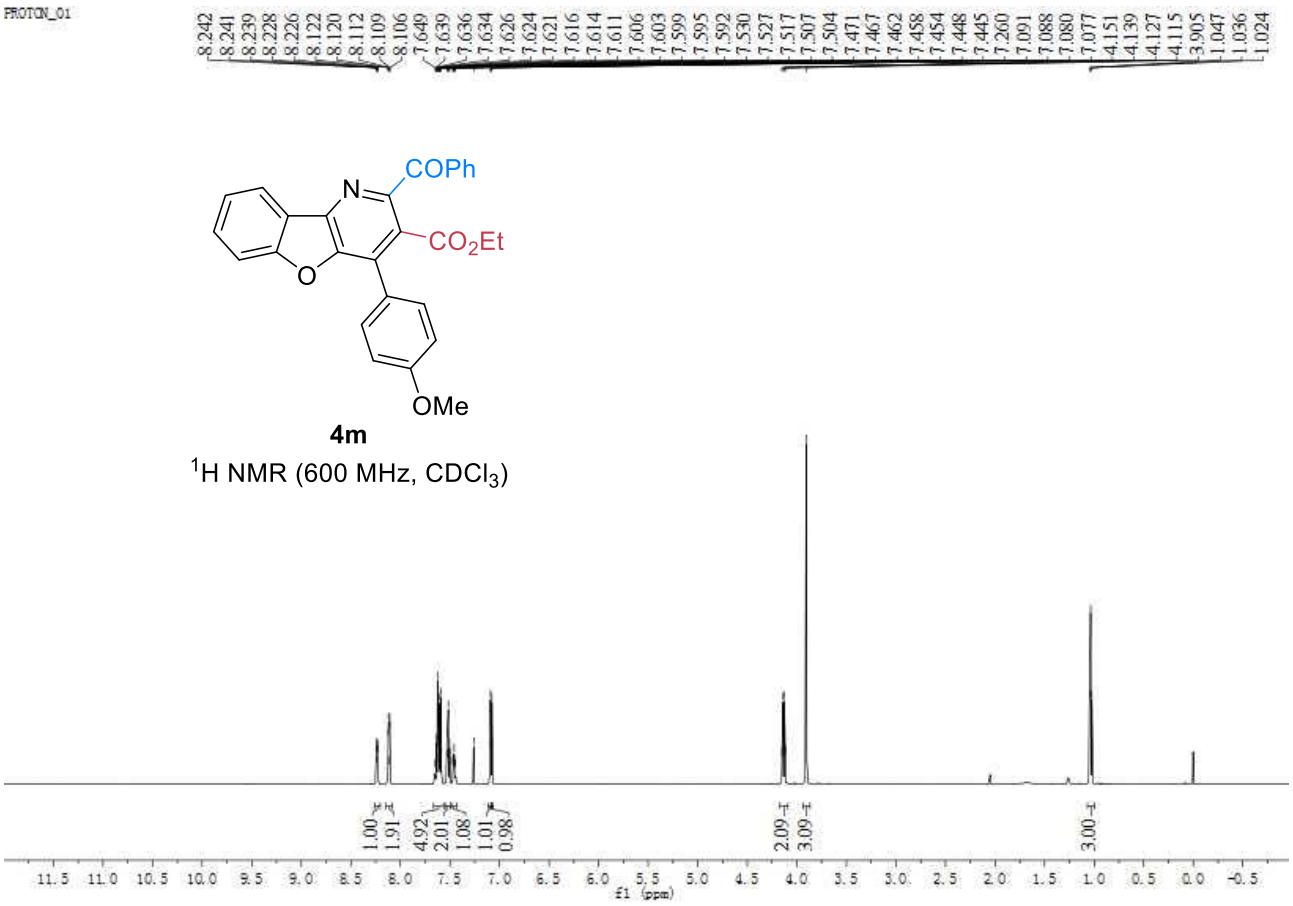
^{1}H NMR (600 MHz, $CDCl_3$)



4l

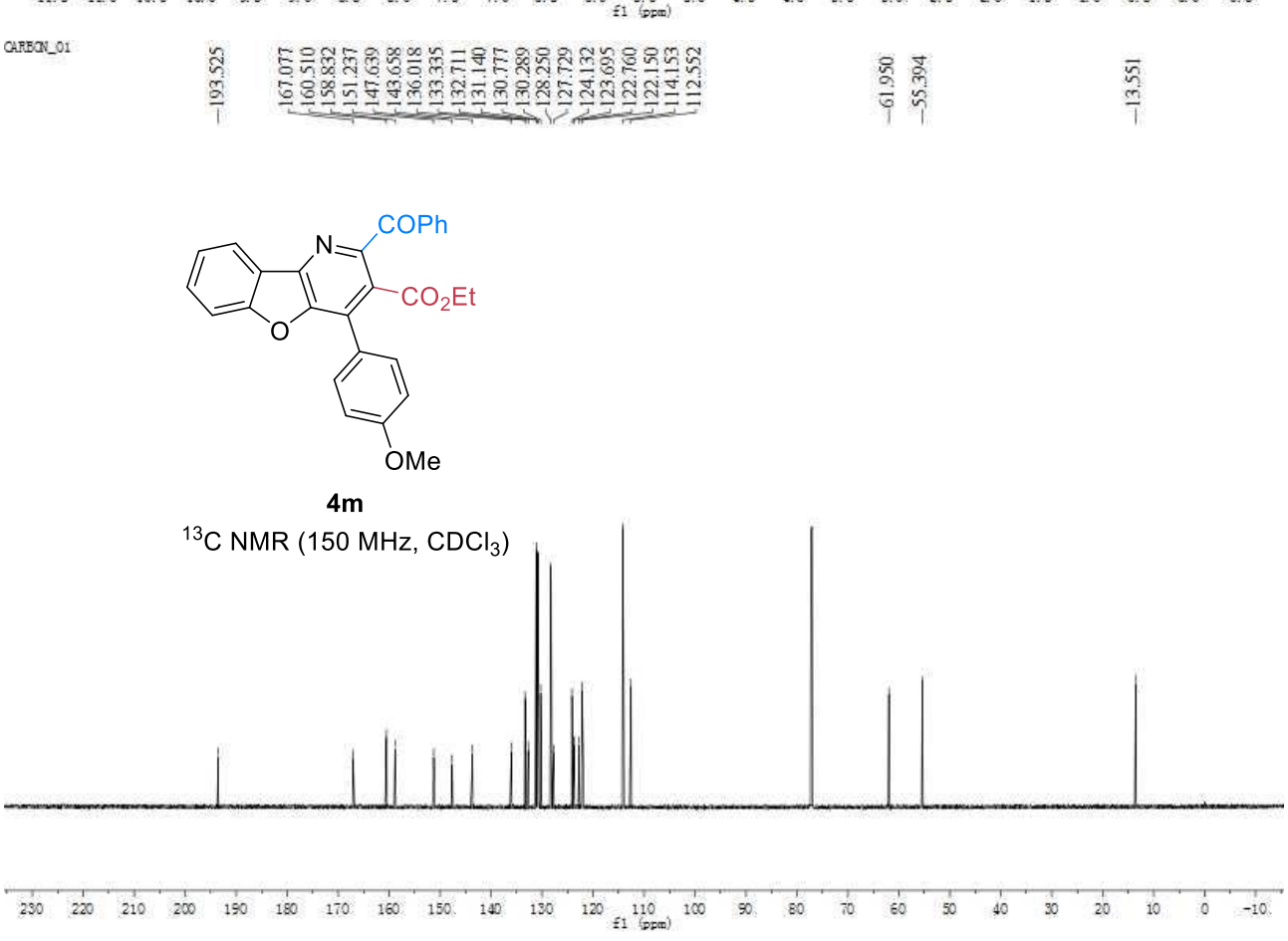
^{13}C NMR (150 MHz, $CDCl_3$)





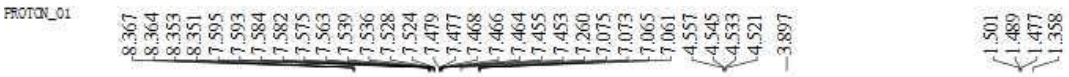
4m

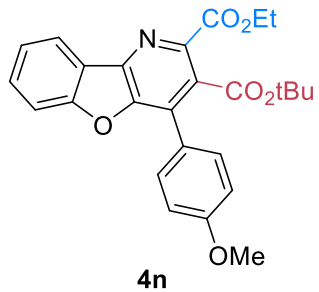
^{1}H NMR (600 MHz, $CDCl_3$)



4m

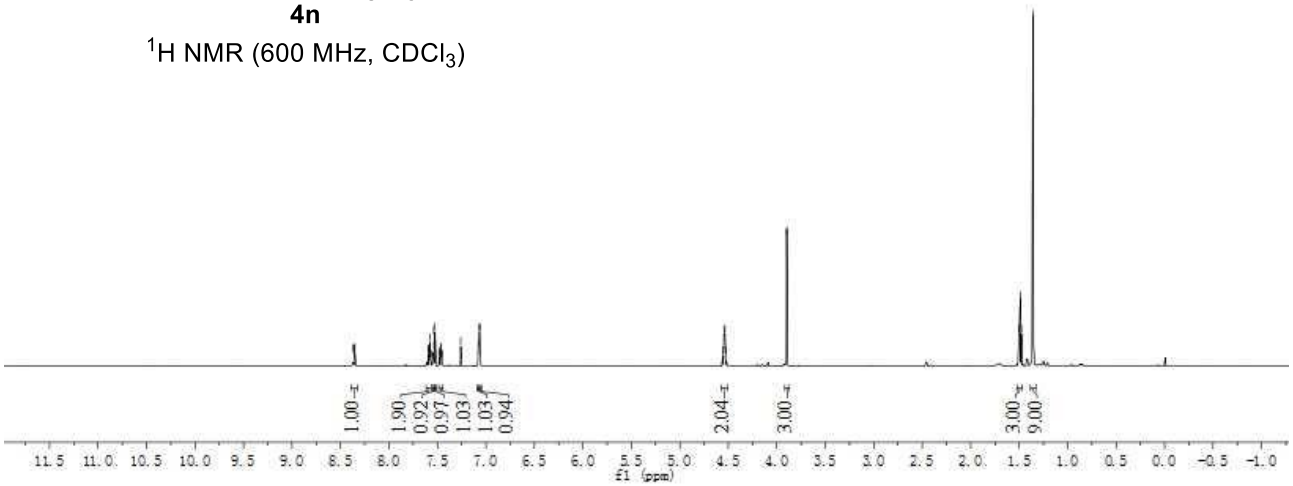
^{13}C NMR (150 MHz, $CDCl_3$)

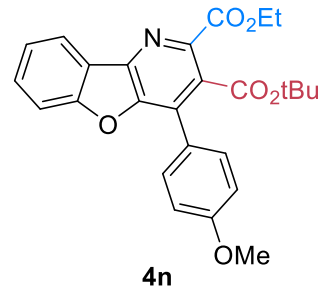




4n

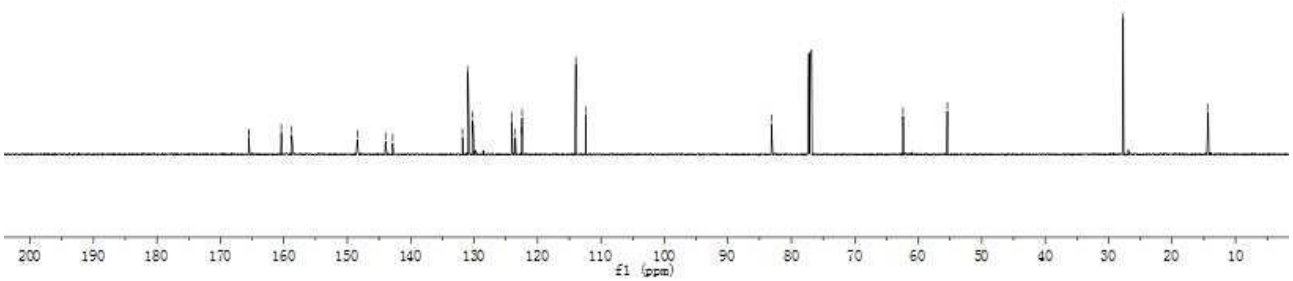
^{1}H NMR (600 MHz, $CDCl_3$)

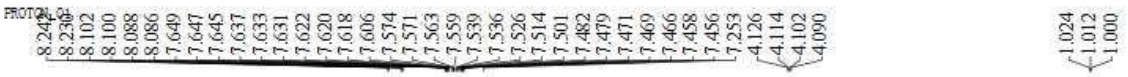


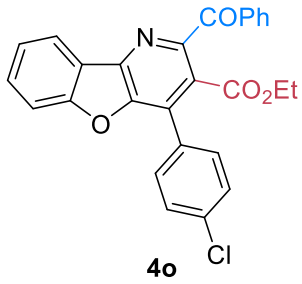


4n

^{13}C NMR (150 MHz, $CDCl_3$)

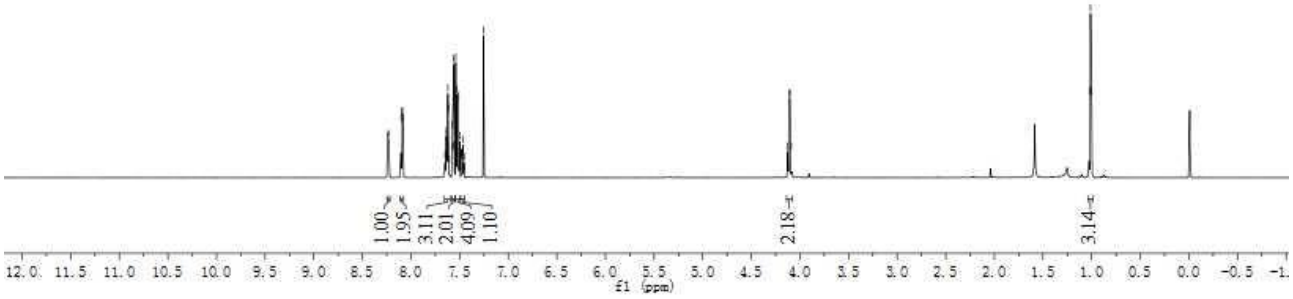


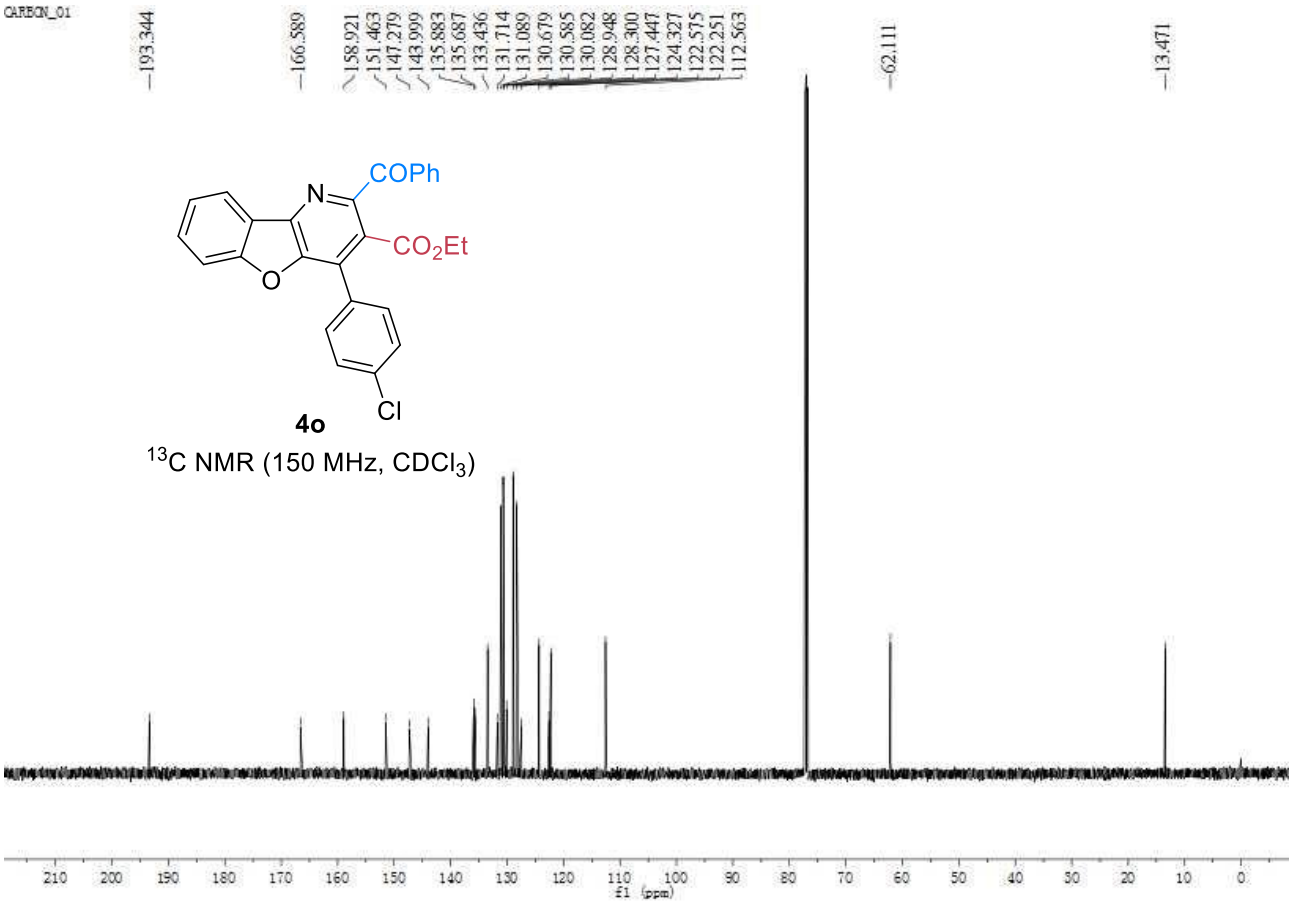




4o

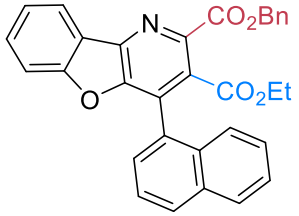
^{1}H NMR (600 MHz, $CDCl_3$)





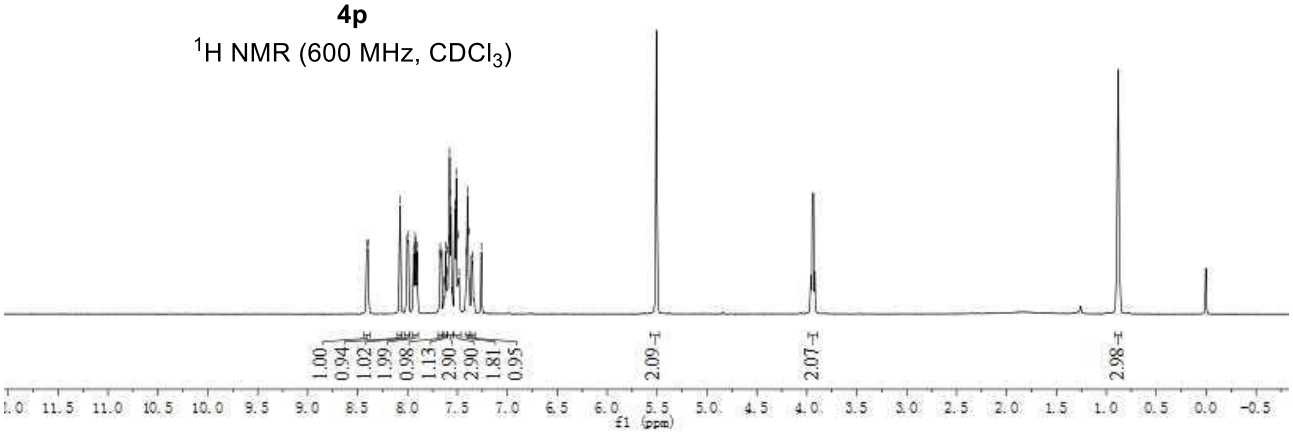
4o

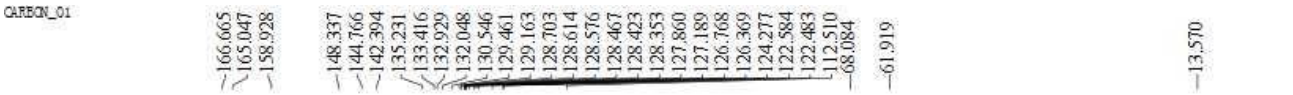
^{13}C NMR (150 MHz, $CDCl_3$)

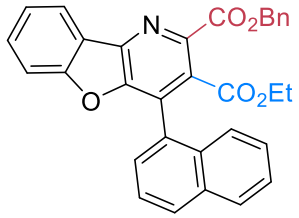


4p

^{1}H NMR (600 MHz, $CDCl_3$)

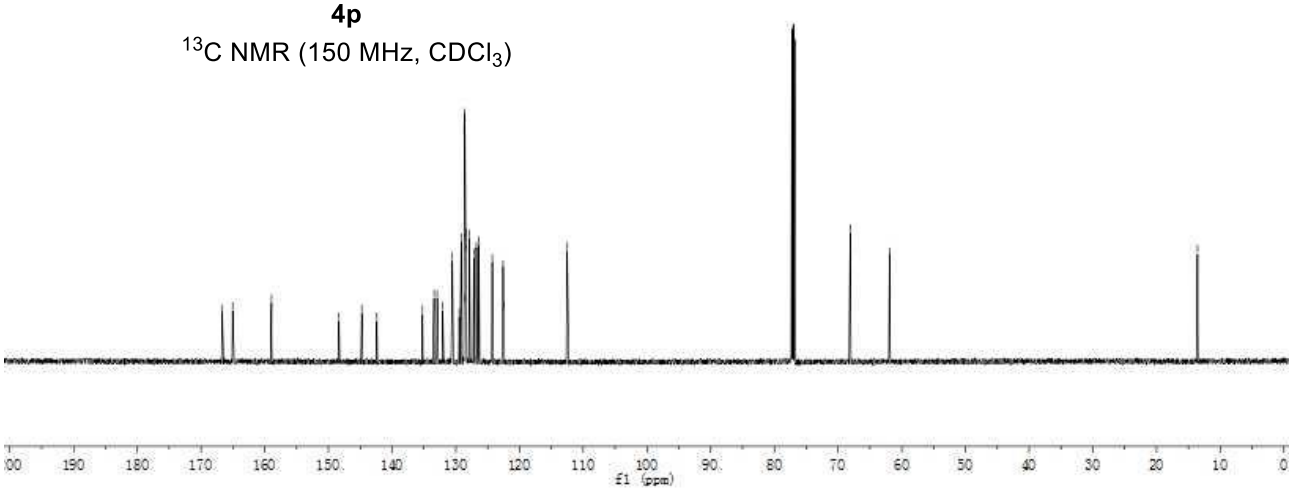


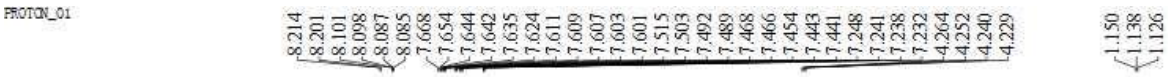


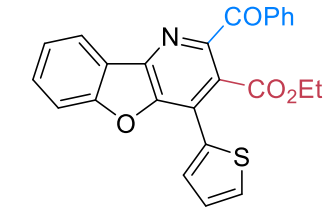


4p

^{13}C NMR (150 MHz, $CDCl_3$)

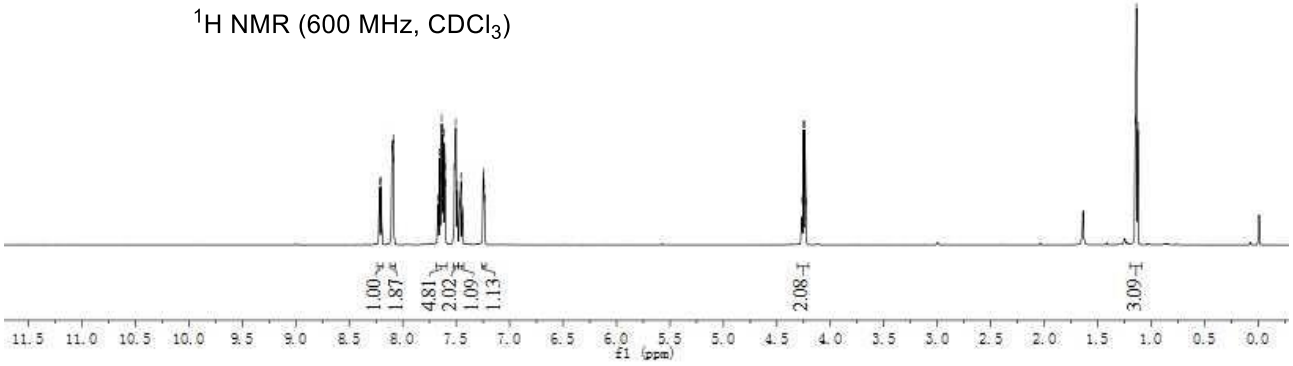


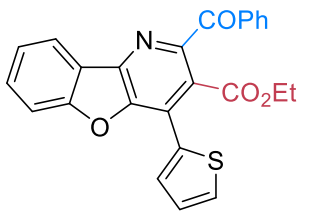




4q

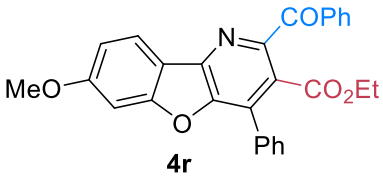
^{1}H NMR (600 MHz, $CDCl_3$)





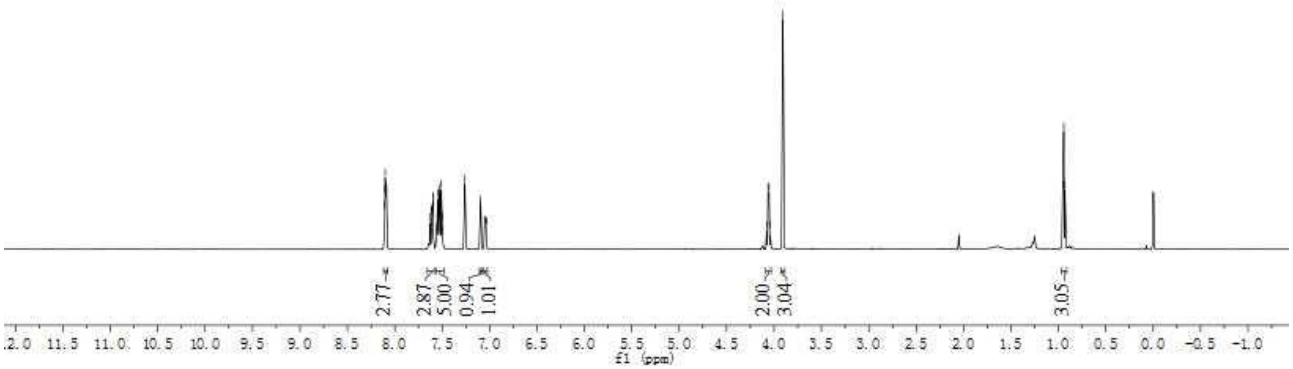
4q

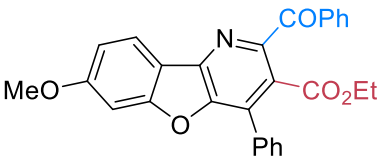
^{13}C NMR (150 MHz, $CDCl_3$)



4r

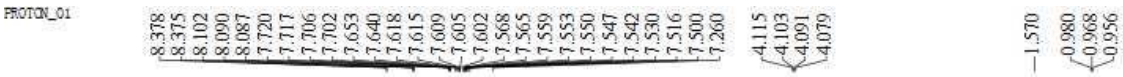
^{1}H NMR (600 MHz, $CDCl_3$)

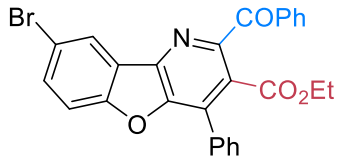




4r

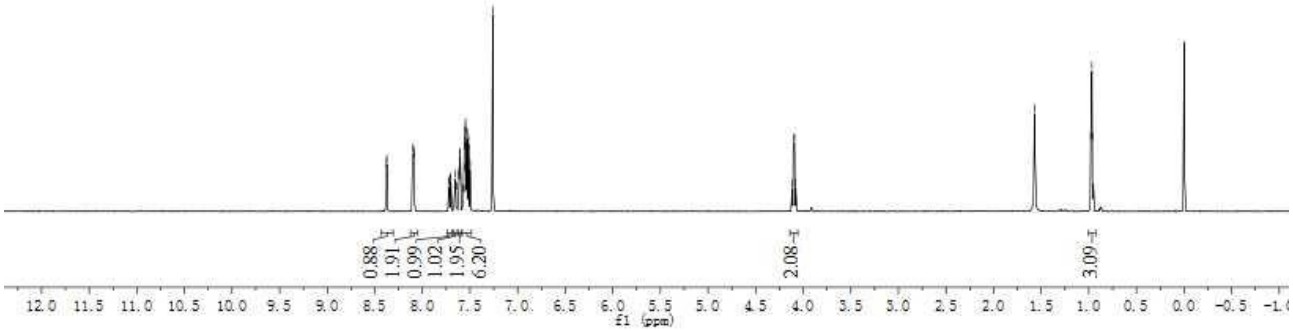
^{13}C NMR (150 MHz, $CDCl_3$)

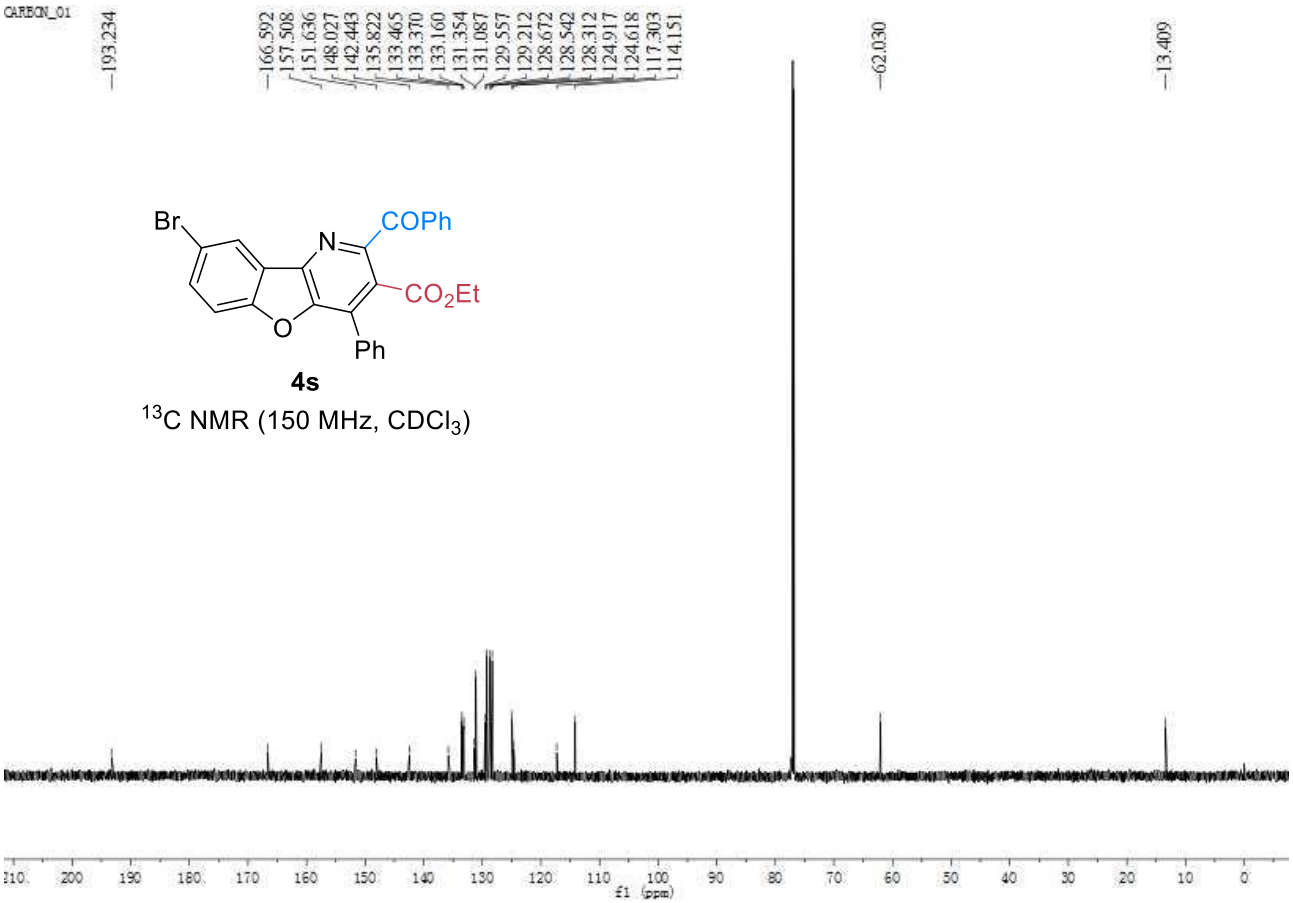




4s

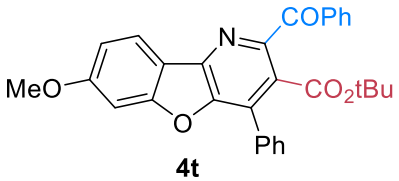
^{1}H NMR (600 MHz, $CDCl_3$)





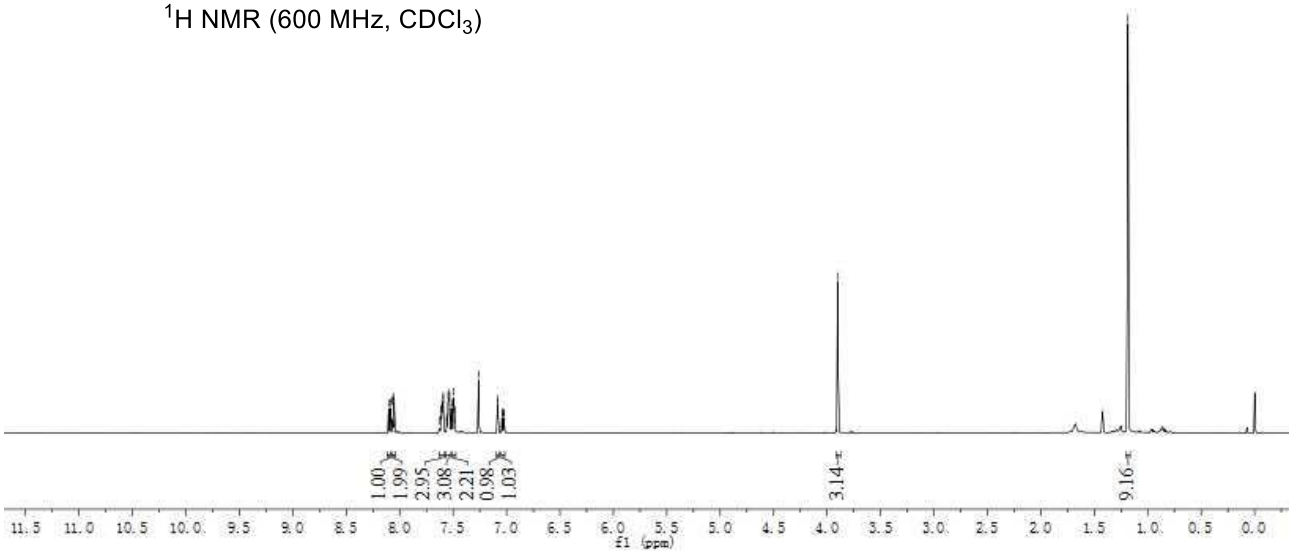
4s

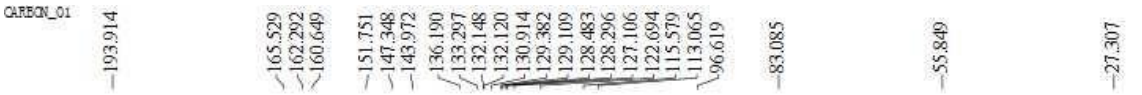
^{13}C NMR (150 MHz, $CDCl_3$)

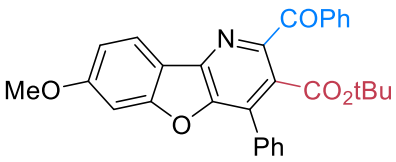


4t

^{1}H NMR (600 MHz, $CDCl_3$)

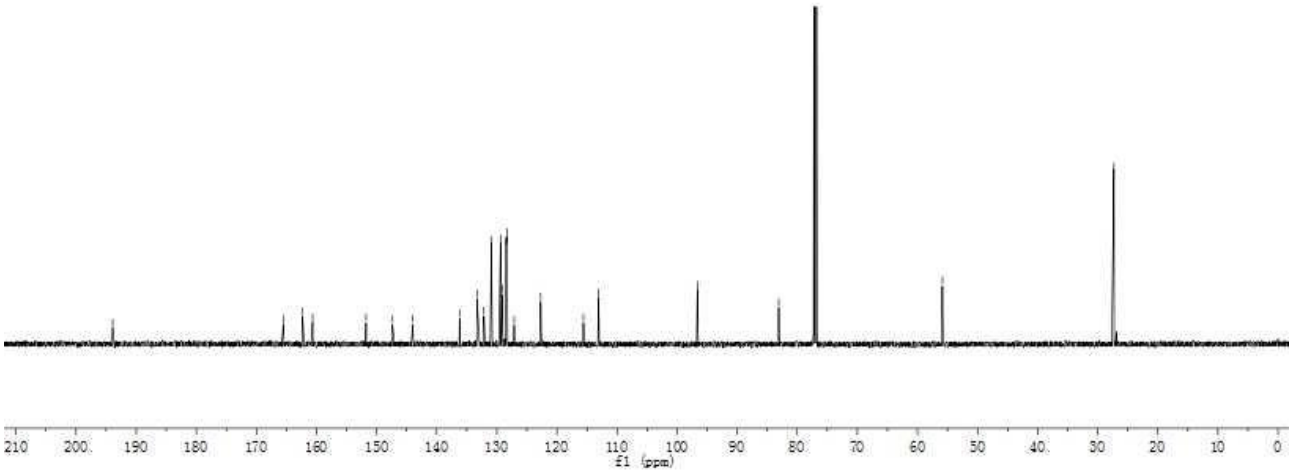


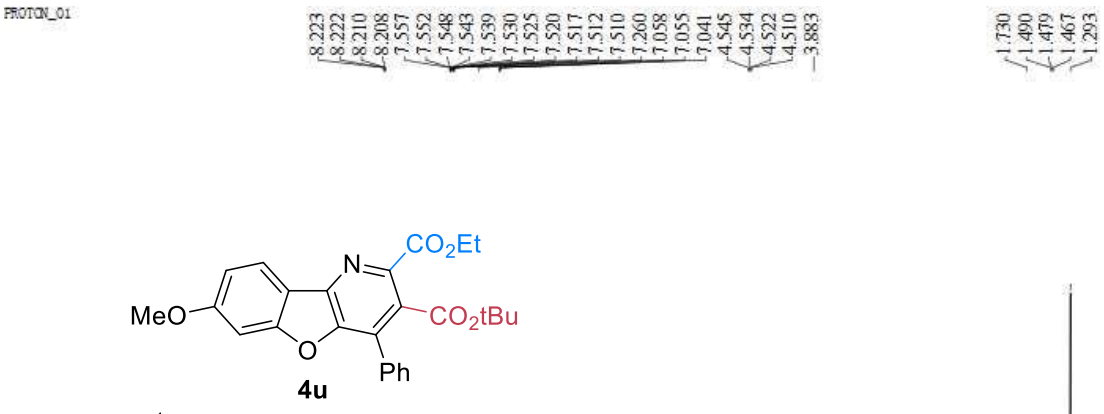




4t

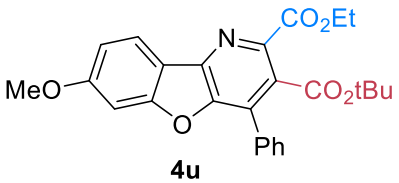
^{13}C NMR (150 MHz, $CDCl_3$)





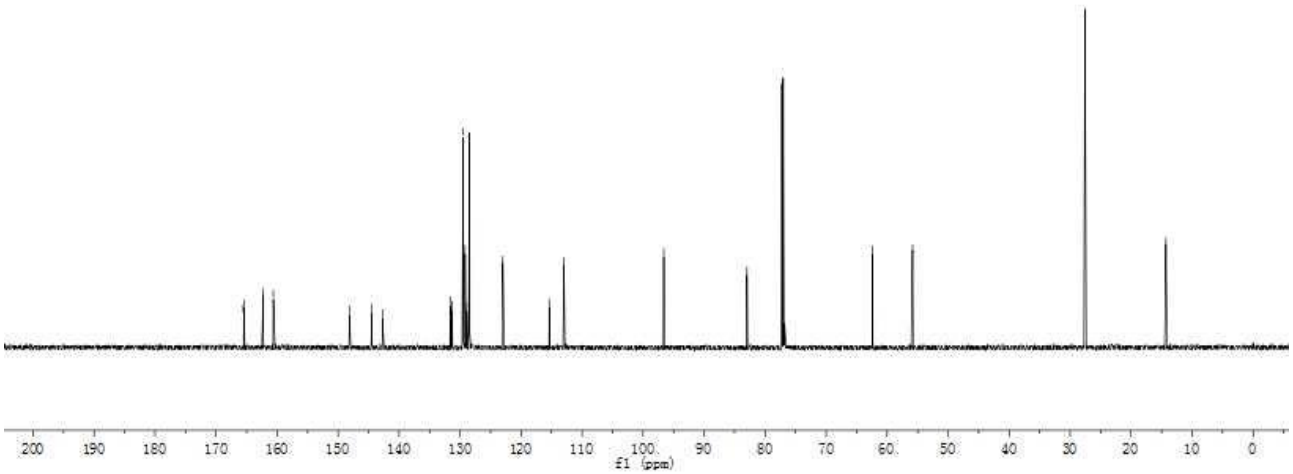
4u

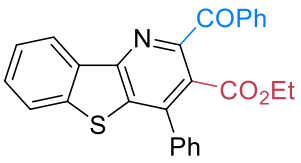
^{1}H NMR (600 MHz, $CDCl_3$)



4u

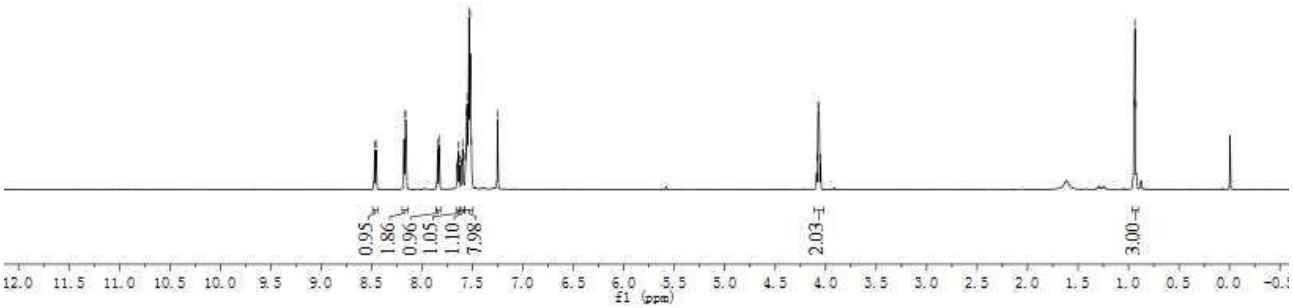
^{13}C NMR (150 MHz, $CDCl_3$)

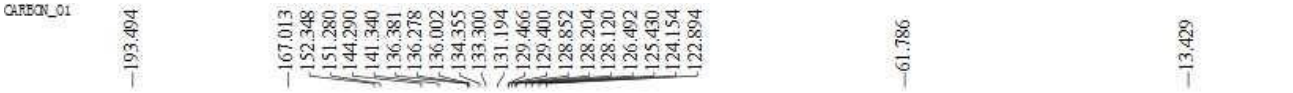


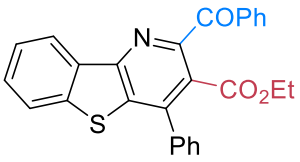


4v

^{1}H NMR (600 MHz, $CDCl_3$)

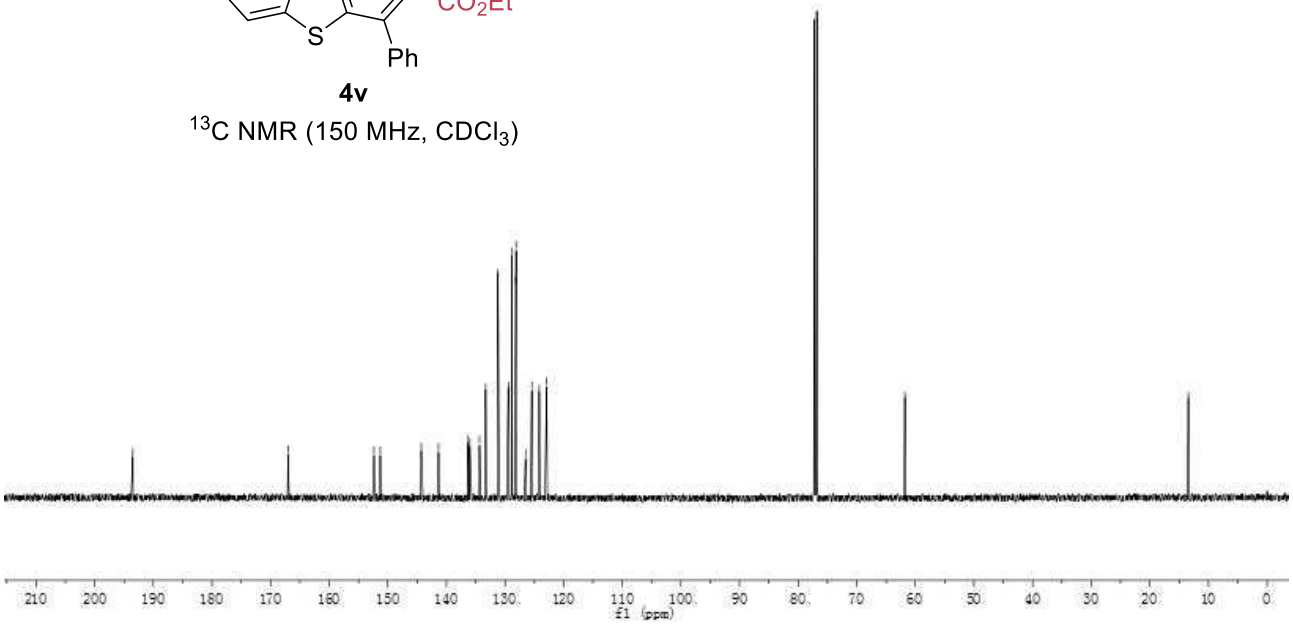


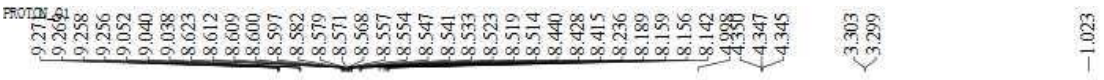


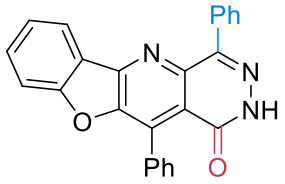


4v

^{13}C NMR (150 MHz, $CDCl_3$)

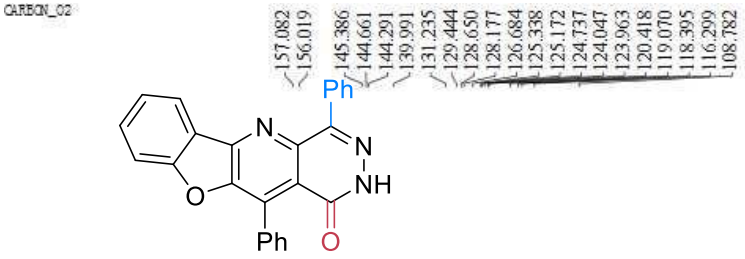






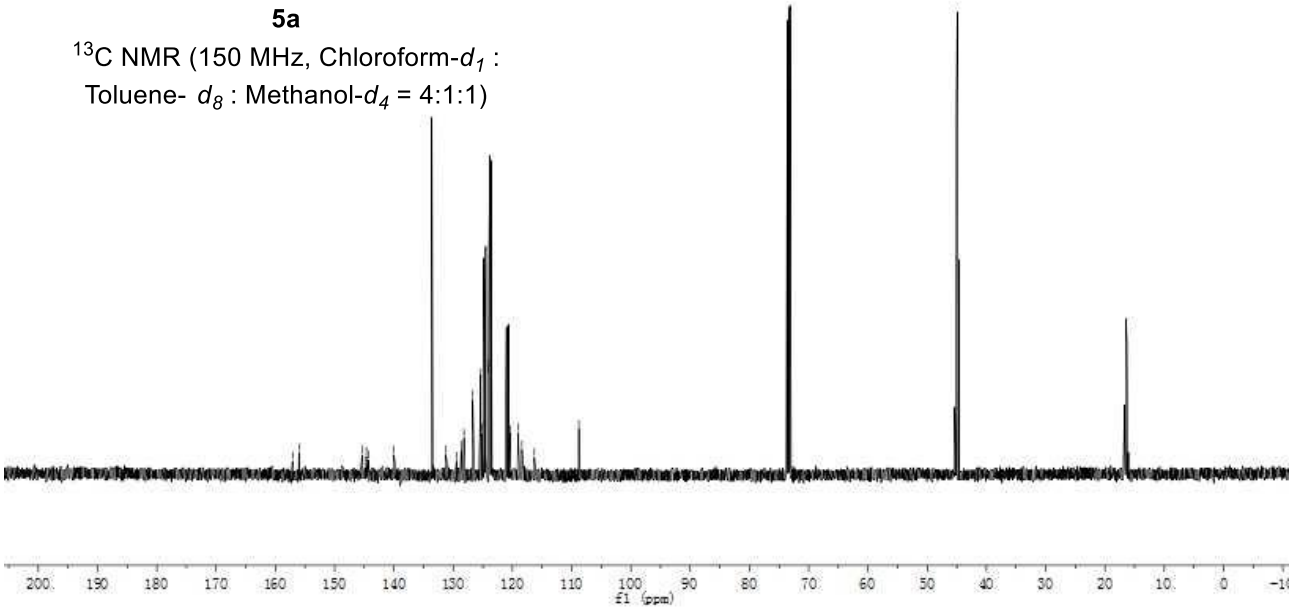
5a

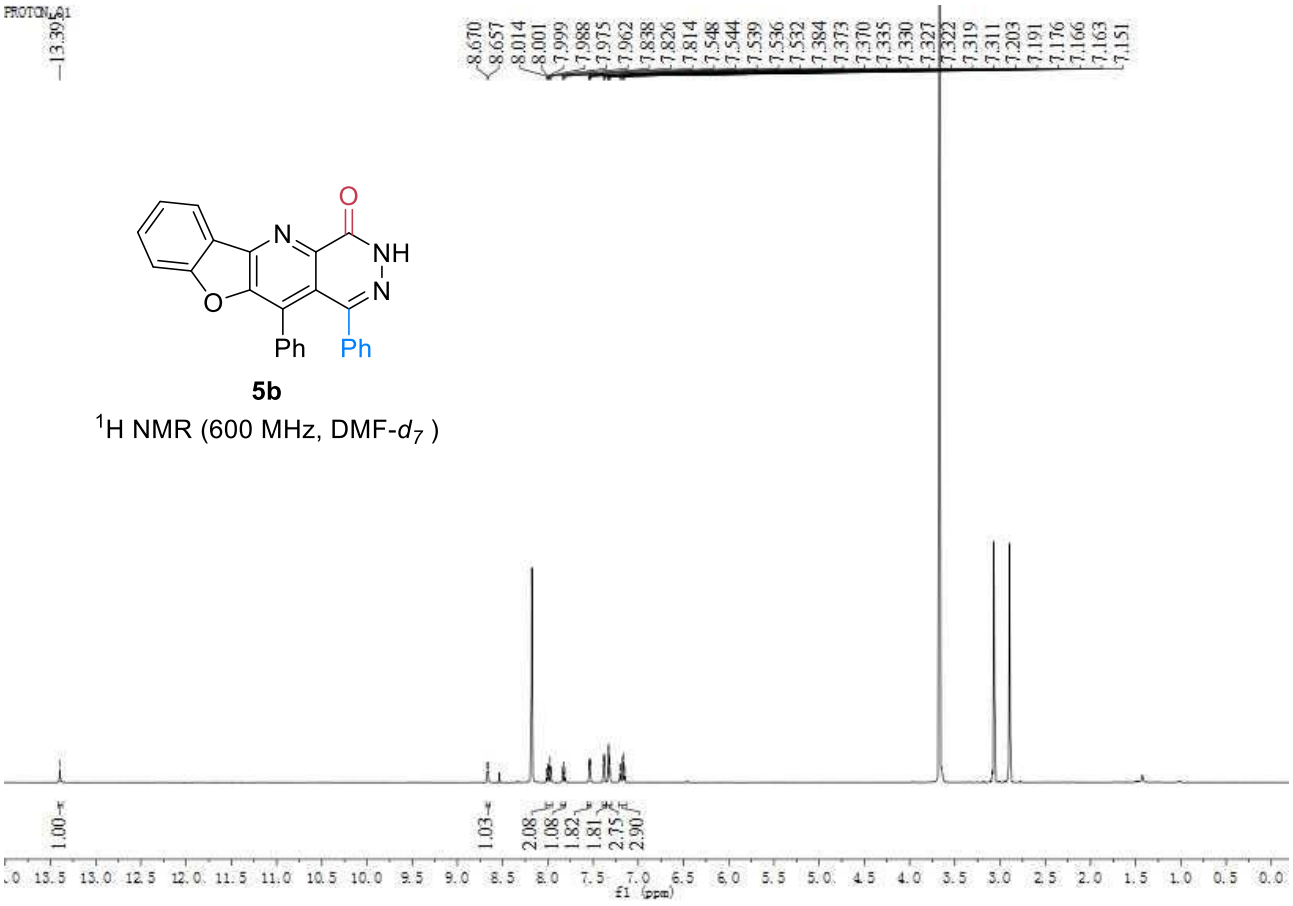
^{1}H NMR (600 MHz, Chloroform-d_1 : Toluene- d_8 : Methanol-d_4 = 4:1:1)



5a

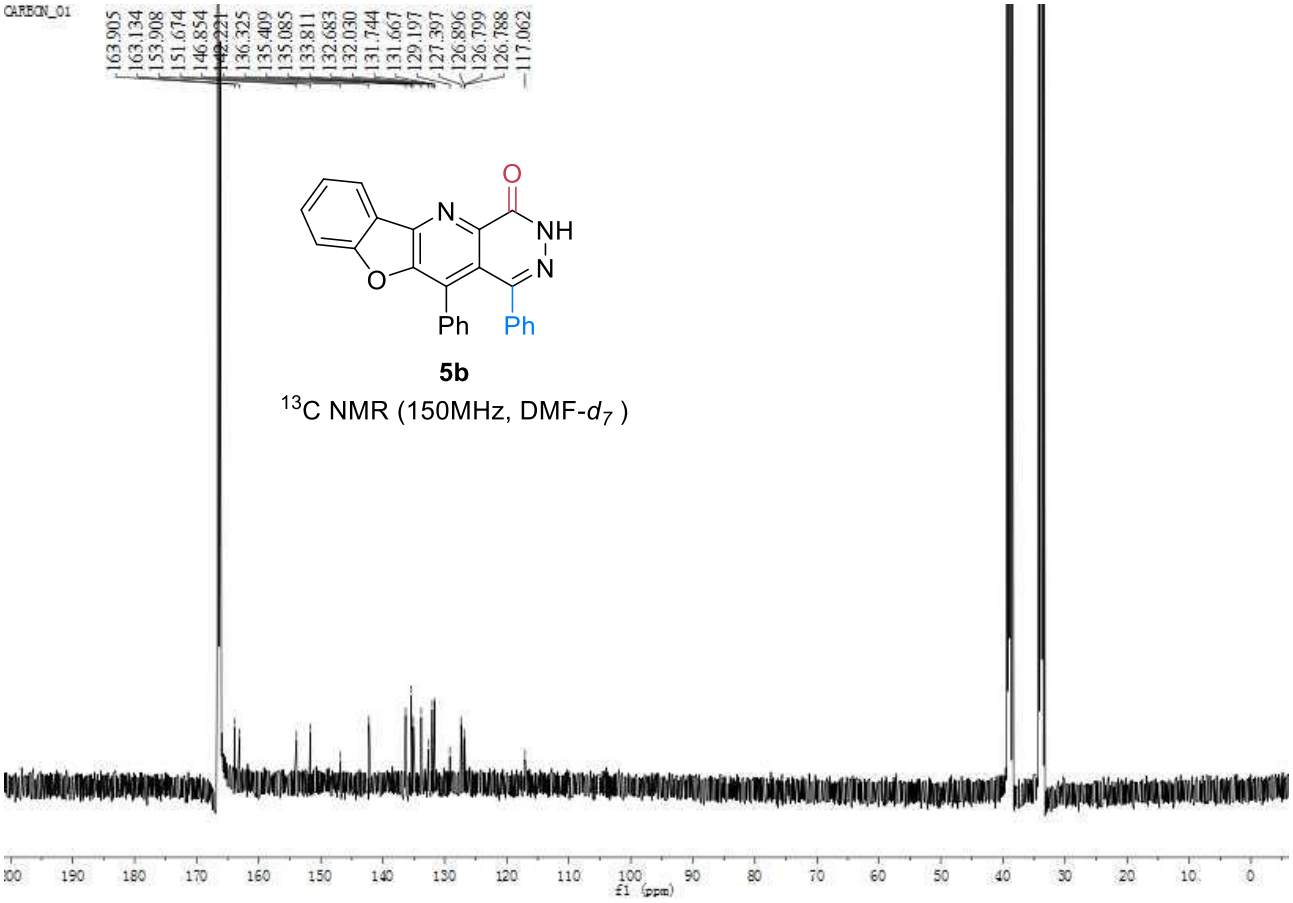
^{13}C NMR (150 MHz, Chloroform-d_1 : Toluene- d_8 : Methanol-d_4 = 4:1:1)





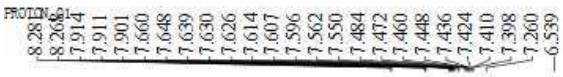
5b

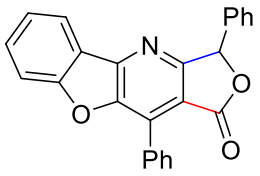
^{1}H NMR (600 MHz, DMF-d_7)



5b

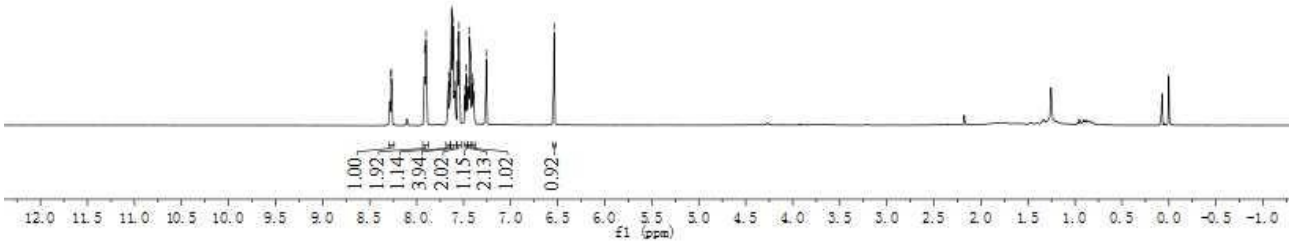
^{13}C NMR (150MHz, DMF-d_7)

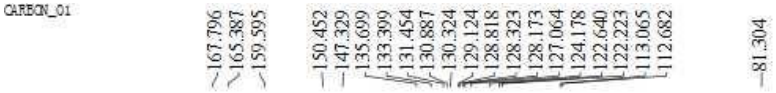


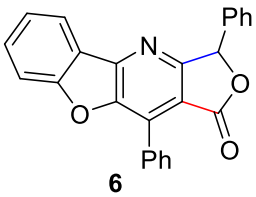


6

^{1}H NMR (600 MHz, $CDCl_3$)







6

^{13}C NMR (150 MHz, $CDCl_3$)

9. References

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10. Computational data

2a

Zero-point correction= 0.111168 (Hartree/Particle)
Thermal correction to Energy= 0.119362
Thermal correction to Enthalpy= 0.120307
Thermal correction to Gibbs Free Energy= 0.076420
E(solv) = -2881.25344310 A.U.

Br	2.26028200	-0.03387400	-0.04585100
C	0.51455300	-0.82001700	0.14556300
C	-0.59431000	0.21544400	0.07199000
O	-0.46513900	1.40805800	0.06545000
O	-1.77239100	-0.42420400	0.03223400
C	-4.14470200	-0.46904400	-0.09431100
C	-2.93037600	0.42872800	-0.00929100
H	0.38225400	-1.56057200	-0.64206500
H	0.47506200	-1.32338400	1.11214100
H	-5.05400400	0.13713000	-0.11902900
H	-4.10969600	-1.07991700	-0.99976200
H	-4.19365400	-1.13386700	0.77161800
H	-2.93706100	1.05127600	0.89022900
H	-2.84353000	1.09342300	-0.87351500

Br-

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.016176
E(solv) = -2574.36309940 A.U.

Br	0.00000000	0.00000000	0.00000000

CO_3^{2-}

Zero-point correction= 0.014441 (Hartree/Particle)
Thermal correction to Energy= 0.017608
Thermal correction to Enthalpy= 0.018553
Thermal correction to Gibbs Free Energy= -0.011113
E(solv) = -264.089319664 A.U.

C	-0.00005700	0.00004200	-0.00002600
O	-0.74186700	1.07328600	0.00000600
O	-0.55863200	-1.17908800	0.00000600
O	1.30054200	0.10577100	0.00000600

HCO_3^-

Zero-point correction= 0.027102 (Hartree/Particle)
Thermal correction to Energy= 0.030566

Thermal correction to Enthalpy= 0.031511
Thermal correction to Gibbs Free Energy= 0.001368
E(solv) = -264.575748370 A.U.

C	0.15217100	-0.07379100	0.00002000
O	1.24729600	0.49634300	-0.00001900
O	-0.17437500	-1.27996200	0.00000600
O	-0.97360700	0.81574700	0.00002900
H	-1.70754000	0.18572100	-0.00023800

N-INT1

Zero-point correction= 0.303235 (Hartree/Particle)
Thermal correction to Energy= 0.318218
Thermal correction to Enthalpy= 0.319162
Thermal correction to Gibbs Free Energy= 0.259780
E(solv) = -3226.61543723 A.U.

N	1.51496900	-0.26291700	-0.16085500
C	2.05554300	-0.66765800	1.18976300
C	3.31703600	1.39473800	-0.50586800
C	3.76821200	-0.89437300	-0.95748000
C	2.24832300	-1.03898500	-1.21713700
C	1.78689800	1.20496400	-0.36886000
C	3.51104100	-0.15517000	1.29062700
N	4.02643800	0.20669600	-0.03138600
H	1.37653100	-0.25358500	1.93728600
H	1.98801900	-1.75861500	1.22309600
H	3.63820500	2.26245900	0.07590100
H	3.59932900	1.56910600	-1.54822800
H	4.29295600	-0.70601000	-1.89776600
H	4.17775100	-1.81113700	-0.52435500
H	1.93946700	-0.61989700	-2.17850200
H	1.89602400	-2.07172700	-1.16119500
H	1.22004900	1.51772400	-1.24915100
H	1.37471500	1.71614800	0.50399900
H	3.56800800	0.72834100	1.93264200
H	4.15221000	-0.92519300	1.72781900
Br	-2.85172400	-1.36799300	-0.06292000
C	0.02487000	-0.57210000	-0.25373300
C	-0.76587400	0.45088500	0.54947700
O	-0.65821400	0.55858200	1.75287300
O	-1.33002500	1.35670000	-0.25074200
C	-3.44651100	2.25503300	-0.82317900
C	-2.46668700	2.04696900	0.30973400
H	-0.14003400	-1.56598900	0.15916600
H	-0.26836500	-0.55065400	-1.30286900
H	-4.33880600	2.77110700	-0.45727200

H	-3.00320700	2.85003700	-1.62731200
H	-3.72883000	1.26980000	-1.20471200
H	-2.89582300	1.40164600	1.08010900
H	-2.11888400	2.98166000	0.76213200

N-INT2

Zero-point correction= 0.287938 (Hartree/Particle)
Thermal correction to Energy= 0.301215
Thermal correction to Enthalpy= 0.302159
Thermal correction to Gibbs Free Energy= 0.247402
E(solv) = -651.759166809 A.U.

N	-3.26270200	0.38677500	-0.04537300
C	-3.20099000	-1.05880100	0.15502600
C	-2.59298000	0.72021400	-1.30309100
C	-2.55047200	1.04694000	1.05078900
C	-1.74495400	-1.58023600	0.05168400
C	-1.13245800	0.45628000	1.22384200
C	-1.08586500	0.37410400	-1.23449000
N	-0.80883800	-0.41467900	0.02937600
C	0.57958300	-0.89561800	0.09450700
C	1.58367500	0.06388800	0.03757700
O	1.44384000	1.30306900	0.03839600
O	2.84000000	-0.49229100	0.00035400
C	5.19669600	-0.35047300	-0.03845900
C	3.90681100	0.44564600	-0.01609600
H	-3.62123500	-1.28297800	1.14006700
H	-3.83177000	-1.54668200	-0.59376400
H	-2.73577800	1.78635100	-1.50115200
H	-3.08706600	0.16574600	-2.10733100
H	-2.50452600	2.11642600	0.82544300
H	-3.12987900	0.92679500	1.97133600
H	-1.44742300	-2.19828900	0.90186900
H	-1.55539400	-2.14147900	-0.86724500
H	-0.34215300	1.20639900	1.25956500
H	-1.04368700	-0.20414700	2.08889300
H	-0.42529900	1.24047600	-1.17592700
H	-0.75245300	-0.26678300	-2.05245400
H	0.71970100	-1.95330400	-0.05501600
H	6.06059500	0.32045400	-0.05270900
H	5.26584600	-0.98980200	0.84589700
H	5.23630200	-0.98909400	-0.92516000
H	3.82049300	1.09508400	-0.89437800
H	3.84950900	1.09226400	0.86630200

N-TS1

Zero-point correction= 0.300124 (Hartree/Particle)
Thermal correction to Energy= 0.315413
Thermal correction to Enthalpy= 0.316358
Thermal correction to Gibbs Free Energy= 0.254898
E(solv) = -3226.56945575 A.U.
Imaginary Frequency 449.05*i*

N	1.45926900	-0.29052200	-0.09683700
C	2.03814000	-0.66018200	1.21696800
C	3.20833300	1.40219400	-0.48765800
C	3.66660800	-0.86797500	-1.02933500
C	2.13019800	-1.06652500	-1.16097000
C	1.68088300	1.15574300	-0.33532100
C	3.52066400	-0.19509600	1.25020500
N	3.96056800	0.21188700	-0.08650300
H	1.41873700	-0.19945200	1.99046400
H	1.94966100	-1.74749200	1.31169700
H	3.52600200	2.24618700	0.13132100
H	3.46772300	1.63411000	-1.52526200
H	4.10964500	-0.62205900	-1.99885100
H	4.14933400	-1.77962900	-0.66396000
H	1.74788200	-0.70361600	-2.12035400
H	1.83241700	-2.11456400	-1.05313000
H	1.11143700	1.44403600	-1.22377900
H	1.26091000	1.68905600	0.52248400
H	3.64742400	0.65838500	1.92315700
H	4.17251000	-0.99826500	1.60638300
Br	-2.75107900	-1.54576900	-0.13426900
C	-0.40330000	-0.80007100	-0.12759700
C	-0.93561400	0.38937400	0.59727600
O	-0.82623100	0.56246500	1.79001500
O	-1.41778300	1.29975900	-0.25756600
C	-2.90231300	3.06682600	-0.78930000
C	-2.26129600	2.29366800	0.34142100
H	-0.21565300	-1.69917600	0.43942000
H	-0.46678300	-0.83892900	-1.20578100
H	-3.58059400	3.82491900	-0.38883900
H	-2.14434400	3.56639100	-1.39918200
H	-3.47208700	2.38617300	-1.42640300
H	-3.00557500	1.77037800	0.95014200
H	-1.66143600	2.93038300	0.99956900

S-INT1

Zero-point correction= 0.190789 (Hartree/Particle)
Thermal correction to Energy= 0.204459
Thermal correction to Enthalpy= 0.205403

Thermal correction to Gibbs Free Energy= 0.149140

E(solv) = -3359.23571858 A.U.

Br	-1.97594300	-1.30014800	-0.08719900
C	0.78359800	-0.69367400	-0.63010300
C	0.15493400	0.23243900	0.39327200
O	0.44575500	0.18992800	1.57457600
O	-0.37065700	1.30768200	-0.21624200
C	-2.44359100	2.44528900	-0.39304900
C	-1.34832100	2.02570100	0.56203900
H	0.73751500	-1.73421200	-0.31527200
H	0.38513500	-0.56041100	-1.63283500
H	-3.22295700	2.99423900	0.14303100
H	-2.05093800	3.08373000	-1.18987200
H	-2.87386800	1.53985000	-0.82925600
H	-1.73433100	1.34419900	1.32390400
H	-0.85299600	2.87207600	1.05019600
S	2.63106000	-0.30571800	-0.71834600
C	2.68954900	1.46825100	-0.35967100
H	2.10829900	1.97628700	-1.13045700
H	2.24269300	1.64242900	0.62128000
H	3.73386700	1.78166100	-0.39345400
C	3.18440400	-0.99715500	0.86033800
H	2.47223300	-0.69416400	1.63216100
H	3.19792100	-2.08243700	0.74727000
H	4.19425700	-0.63255500	1.05518600

S-INT2

Zero-point correction= 0.176994 (Hartree/Particle)

Thermal correction to Energy= 0.188633

Thermal correction to Enthalpy= 0.189577

Thermal correction to Gibbs Free Energy= 0.138964

E(solv) = -784.419307007 A.U.

C	-0.45922000	1.04440700	-0.00208500
C	0.51141900	0.00768400	0.00003000
O	0.28454400	-1.20412100	0.00242900
O	1.78258600	0.48877300	-0.00093500
C	4.13297500	0.22962800	-0.00028100
C	2.80699700	-0.50271400	0.00084300
H	-0.21947000	2.09529300	-0.00395600
H	4.96139100	-0.48433400	0.00097100
H	4.21944900	0.86276900	-0.88731900
H	4.21931500	0.86572400	0.88465000
H	2.69623400	-1.14146200	0.88342400
H	2.69639200	-1.14443100	-0.87960200
S	-2.09324200	0.64963500	-0.00139300

C	-2.40282600	-0.51236700	-1.36943900
H	-2.28148500	0.05266500	-2.29404700
H	-1.66269100	-1.31040000	-1.30107600
H	-3.42254600	-0.89538400	-1.28999300
C	-2.40326000	-0.50654700	1.37150400
H	-1.66335300	-1.30508500	1.30650200
H	-2.28181200	0.06230400	2.29376100
H	-3.42309300	-0.88960000	1.29359900

CSC

Zero-point correction= 0.077217 (Hartree/Particle)
Thermal correction to Energy= 0.082029
Thermal correction to Enthalpy= 0.082973
Thermal correction to Gibbs Free Energy= 0.050268
E(solv) = -477.988618443 A.U.

S	-0.00000100	-0.66691100	-0.00000100
C	1.37266800	0.51677300	-0.00000400
H	1.34803300	1.14633400	0.89324100
H	2.30076400	-0.05780900	0.00017500
H	1.34821800	1.14612100	-0.89338500
C	-1.37266700	0.51677800	-0.00000300
H	-2.30075200	-0.05780700	-0.00001100
H	-1.34812900	1.14618500	0.89333000
H	-1.34812200	1.14625100	-0.89328700

S-TS1

Zero-point correction= 0.189994 (Hartree/Particle)
Thermal correction to Energy= 0.203387
Thermal correction to Enthalpy= 0.204332
Thermal correction to Gibbs Free Energy= 0.148666
E(solv) = -3359.22376084 A.U.
Imaginary Frequency 333.20*i*

Br	1.96608800	-1.34046500	0.08134400
C	-0.59432300	-0.77832500	0.50901900
C	-0.15015000	0.30107800	-0.43041200
O	-0.44211400	0.32259300	-1.60793500
O	0.37779600	1.33032800	0.24217000
C	2.44902000	2.47502200	0.40800500
C	1.28985400	2.15482000	-0.51016500
H	-0.69005600	-1.76727700	0.07845800
H	-0.25046200	-0.72279000	1.53331600
H	3.18862100	3.08596800	-0.11727700
H	2.11026900	3.02026900	1.29338200
H	2.91022300	1.53373400	0.71863700
H	1.61810900	1.58523800	-1.38273700

H	0.75301000	3.04702300	-0.84928900
S	-2.63593700	-0.35929400	0.73397600
C	-2.72226000	1.42774900	0.45200600
H	-2.14862700	1.91465700	1.24179400
H	-2.28431400	1.65919700	-0.52146600
H	-3.76804900	1.73584900	0.49737400
C	-3.20774100	-0.97164600	-0.87017600
H	-2.51885500	-0.62199400	-1.64340300
H	-3.20398400	-2.06195300	-0.82054300
H	-4.22583800	-0.61848000	-1.04243300

1a

Zero-point correction= 0.342730 (Hartree/Particle)
Thermal correction to Energy= 0.365198
Thermal correction to Enthalpy= 0.366142
Thermal correction to Gibbs Free Energy= 0.287966
E(solv) = -1527.03699334 A.U.

C	1.06087200	2.25988900	0.00117800
C	2.45607300	2.16060800	0.00261800
C	3.29731000	3.26201900	0.00371200
C	2.68400000	4.51139700	0.00324500
C	1.28771200	4.64428700	0.00175700
C	0.46236000	3.52688100	0.00072300
C	0.56798100	0.87805800	0.00067800
C	1.79711500	0.04916300	0.00129000
H	4.37496400	3.14180500	0.00485200
H	3.30359800	5.40342900	0.00403200
H	0.84469800	5.63466300	0.00141800
H	-0.61504800	3.63856300	-0.00031400
O	2.90528000	0.86941800	0.00283600
C	1.84073300	-1.29154000	-0.00027000
H	0.85523200	-1.75345800	-0.00158500
N	-0.59002500	0.30916300	-0.00012400
C	2.99060800	-2.18977500	-0.00086800
C	4.32757100	-1.75389500	0.00033700
C	2.73454900	-3.57148300	-0.00301300
C	5.36516000	-2.67993300	-0.00065500
H	4.54968900	-0.69353000	0.00198200
C	3.77447100	-4.49344500	-0.00398100
H	1.70379500	-3.91756000	-0.00399400
C	5.09595300	-4.04916200	-0.00281900
H	6.39344100	-2.33019500	0.00022800
H	3.55472300	-5.55693700	-0.00568000
H	5.91269600	-4.76510300	-0.00363200
S	-1.96822400	1.26156300	-0.00261000

O	-2.04749400	1.99411000	-1.26402300
O	-2.05040000	1.99640700	1.25735000
C	-3.21910400	0.00281100	-0.00255900
C	-3.69971000	-0.47465600	-1.21591800
C	-3.68791600	-0.48671900	1.21350600
C	-4.67071900	-1.47301000	-1.20511700
H	-3.32346900	-0.06186700	-2.14715300
C	-4.65693600	-1.48317800	1.20322300
H	-3.30221600	-0.08158200	2.14422200
C	-5.16009700	-1.98969800	-0.00189700
H	-5.05699900	-1.85355100	-2.14723000
H	-5.03477700	-1.87316800	2.14549800
C	-6.22693400	-3.05423900	0.00962900
H	-7.18583300	-2.63757400	0.33737500
H	-6.37029000	-3.48505800	-0.98466900
H	-5.96784300	-3.86379300	0.69918700

cis-7

Zero-point correction= 0.447012 (Hartree/Particle)
Thermal correction to Energy= 0.475473
Thermal correction to Enthalpy= 0.476417
Thermal correction to Gibbs Free Energy= 0.385184
E(solv) = -1833.52483597 A.U.

C	0.94894600	2.28973500	0.52609200
C	0.67552300	3.13745900	-0.57039200
C	1.10275900	4.45552900	-0.63525400
C	1.81541100	4.93351200	0.45681300
C	2.08932600	4.11575600	1.56590200
C	1.66746100	2.79507500	1.61777700
C	0.35026800	1.04122200	0.12757300
C	-0.20051700	1.23106600	-1.08497500
H	0.87711800	5.07140100	-1.49840200
H	2.16370100	5.96122900	0.45354700
H	2.64250300	4.52907400	2.40298500
H	1.87279400	2.16092500	2.47294500
O	-0.05126600	2.50004400	-1.54315100
C	-1.09928200	0.12106600	-1.51596900
H	-0.92067200	-0.23517800	-2.53453500
N	0.00496600	-0.23124400	0.64278200
C	-2.58003200	0.42627300	-1.34662400
C	-3.03092300	1.38455600	-0.43798900
C	-3.51209800	-0.33384500	-2.05643400
C	-4.39517100	1.58000700	-0.24444100
H	-2.31427300	1.97383000	0.12782300
C	-4.87700800	-0.14460900	-1.85648200

H	-3.16485300	-1.09265000	-2.75330300
C	-5.32138900	0.81361100	-0.94880700
H	-4.73506300	2.33028500	0.46291900
H	-5.59155100	-0.74363000	-2.41259600
H	-6.38508000	0.96605400	-0.79406000
S	1.12912100	-1.07940600	1.56173400
O	0.50081700	-2.35952600	1.83239300
O	1.54403900	-0.16540300	2.61022000
C	2.51598900	-1.36126600	0.48924500
C	2.62141100	-2.57749100	-0.18002200
C	3.44279600	-0.33873700	0.29126300
C	3.68069600	-2.76815000	-1.06173400
H	1.89010900	-3.35845700	0.00512900
C	4.49088400	-0.54959400	-0.59454200
H	3.34658000	0.59786500	0.83311800
C	4.62549800	-1.76264300	-1.28001500
H	3.77638400	-3.71473600	-1.58622900
H	5.22121200	0.23852100	-0.75654900
C	5.78721700	-1.98462900	-2.21309800
H	6.01843100	-1.07813300	-2.77903200
H	6.68587800	-2.25951900	-1.65014900
H	5.57945400	-2.78976800	-2.92192000
C	-0.57109000	-0.97854100	-0.50521500
H	0.21377000	-1.55033200	-1.01568400
C	-1.67279800	-1.95208700	-0.13556300
O	-2.38314100	-1.55284900	0.90808600
O	-1.90980900	-2.92018100	-0.81769800
C	-3.56067100	-2.32768700	1.18345000
H	-4.14151300	-2.40954500	0.25932600
H	-3.25265700	-3.33306200	1.48507900
C	-4.31926400	-1.60105800	2.27125000
H	-5.22815500	-2.15289500	2.52590100
H	-3.70435800	-1.50422600	3.16923600
H	-4.59921500	-0.60171500	1.92758300

N-INT3-RR-1

Zero-point correction= 0.637563 (Hartree/Particle)
Thermal correction to Energy= 0.672007
Thermal correction to Enthalpy= 0.672951
Thermal correction to Gibbs Free Energy= 0.571986
E(solv) = -2178.80140443 A.U.

C	-3.47110600	0.05464400	-0.11843400
C	-3.66716100	1.43179800	-0.28609600
C	-4.90246000	2.00660400	-0.54989400
C	-5.98376700	1.13886200	-0.62413600

C	-5.82086200	-0.24454500	-0.44182800
C	-4.57493500	-0.80271300	-0.19501300
C	-2.04915900	-0.08277300	0.13900200
C	-1.54310700	1.17303100	0.12258300
H	-5.00415500	3.07818700	-0.68061800
H	-6.97297700	1.53864400	-0.82438700
H	-6.69010500	-0.89166200	-0.50222100
H	-4.44387100	-1.87232700	-0.08346000
O	-2.49599800	2.11690700	-0.13547200
C	-0.15212600	1.64326200	0.40421800
H	-0.16328300	2.17248900	1.36844400
N	-1.28110500	-1.16477400	0.59889100
C	0.24274700	2.61660600	-0.70203900
C	0.37140100	3.97704800	-0.42873600
C	0.43402400	2.17036800	-2.01219700
C	0.72106500	4.87559000	-1.43418300
H	0.19519600	4.33658700	0.58301600
C	0.78900800	3.06388400	-3.01766000
H	0.29929700	1.11611400	-2.24668800
C	0.94002800	4.41967200	-2.73030900
H	0.81827900	5.93231000	-1.20424100
H	0.93830900	2.70224600	-4.03066700
H	1.21432700	5.11651400	-3.51610000
S	-1.27105000	-2.60173800	-0.26083100
O	-2.38260400	-2.50025300	-1.20054600
O	-1.18563700	-3.72207300	0.65201400
C	0.21833300	-2.56597800	-1.24122000
C	0.23064800	-1.79890500	-2.40268500
C	1.34241000	-3.27272300	-0.82788500
C	1.40671400	-1.71479600	-3.14435500
H	-0.67586700	-1.28862100	-2.71832000
C	2.50032700	-3.19743900	-1.59472000
H	1.29188400	-3.84644000	0.09157300
C	2.55268800	-2.41418300	-2.75364200
H	1.42887000	-1.11557700	-4.05145500
H	3.38393500	-3.75306600	-1.28855100
C	3.80980500	-2.36233100	-3.58432900
H	3.87231400	-3.23402400	-4.24496800
H	3.83556200	-1.46871600	-4.21347800
H	4.70397200	-2.36646100	-2.95402300
C	0.70323600	0.36395600	0.54619400
C	-0.01711200	-0.77606200	1.41425400
O	0.70865900	-1.78953700	1.68631400
O	-0.54603100	-0.03864600	2.52371000
C	-2.69249800	-0.46625300	3.54017700

C	-1.22676900	-0.85953300	3.47051400
H	0.87993900	-0.06266000	-0.44630400
H	-3.20219500	-1.02541900	4.33146900
H	-2.79403000	0.60291100	3.75188500
H	-3.19233700	-0.67625000	2.59034200
H	-1.10132400	-1.90927600	3.18854600
H	-0.74064300	-0.71218100	4.44371800
N	2.12293100	0.59498800	1.09621500
C	2.76854300	1.85502000	0.58003600
C	4.33675300	-0.49212400	1.39749300
C	3.58856800	1.03425200	3.05580000
C	2.16102500	0.64538900	2.61244200
C	3.00159600	-0.55638100	0.63011600
C	4.27466100	1.83016800	0.94082700
N	4.55242400	0.83778900	1.97255900
H	2.60536400	1.89893600	-0.49691300
H	2.24723500	2.69604100	1.04101400
H	5.16549000	-0.73283100	0.72476800
H	4.34665300	-1.22101600	2.21327100
H	3.88211500	0.42227100	3.91306900
H	3.63800400	2.08306800	3.36568600
H	1.85797500	-0.34950200	2.93827500
H	1.39920200	1.35639900	2.93334500
H	2.42644000	-1.46224900	0.82395900
H	3.12427400	-0.41179900	-0.44876800
H	4.87728800	1.58963000	0.05990000
H	4.58367600	2.81786300	1.29460200

N-INT3-RR

Zero-point correction= 0.636697 (Hartree/Particle)
Thermal correction to Energy= 0.672127
Thermal correction to Enthalpy= 0.673072
Thermal correction to Gibbs Free Energy= 0.569611
E(solv) = -2178.81562285 A.U.

C	2.51489100	-2.01645900	-0.68239200
C	3.62003000	-1.18211400	-0.44554300
C	4.91662400	-1.65572400	-0.27815100
C	5.08748500	-3.03215600	-0.33415900
C	3.99936800	-3.89176300	-0.56497300
C	2.71372000	-3.40323500	-0.74594000
C	1.37258200	-1.11559800	-0.79240900
C	1.89685700	0.12754000	-0.61824100
H	5.74024400	-0.97190500	-0.10324900
H	6.08003600	-3.45137000	-0.19964300
H	4.17149900	-4.96263000	-0.60715200

H	1.88134500	-4.07295900	-0.93217300
O	3.25705100	0.12476700	-0.39639200
C	1.10607900	1.38175800	-0.49867300
H	0.42548600	1.36676100	-1.35895200
N	0.00926400	-1.26774200	-0.93775400
C	1.99107500	2.61198700	-0.58871900
C	2.83349200	2.94882100	0.47424500
C	2.01213400	3.39715400	-1.74119200
C	3.65933100	4.06495100	0.39528000
H	2.86288200	2.30927200	1.35434900
C	2.83821900	4.51574200	-1.82331600
H	1.38556600	3.12378900	-2.58805900
C	3.65858400	4.85613500	-0.75191400
H	4.31309900	4.31122400	1.22626000
H	2.84285400	5.11787300	-2.72669000
H	4.30264600	5.72775000	-0.81317200
S	-0.60070000	-2.73297600	-0.74344300
O	-0.19458500	-3.36507600	0.52801700
O	-0.50554900	-3.58903000	-1.93309700
C	-2.32124200	-2.28428400	-0.56186700
C	-2.90014500	-2.28940600	0.69948300
C	-3.05003900	-1.89180500	-1.68246700
C	-4.22117700	-1.86469900	0.84327700
H	-2.30487500	-2.60624900	1.54920700
C	-4.36668400	-1.47360100	-1.52560300
H	-2.58165000	-1.93350500	-2.66181500
C	-4.96816500	-1.44647800	-0.26010000
H	-4.68324100	-1.87018200	1.82785800
H	-4.94661600	-1.17506800	-2.39663700
C	-6.39040800	-0.96794200	-0.10153800
H	-7.03609100	-1.38304200	-0.88113300
H	-6.80047300	-1.25972400	0.86885800
H	-6.45685600	0.12490500	-0.17584100
N	-3.50846700	3.05181100	-0.04999100
N	-1.20475900	2.00507800	0.47293800
C	-3.29088700	1.84004500	-0.85078200
H	-4.17754000	1.20362800	-0.80164200
H	-3.15579200	2.14227700	-1.89428100
C	-2.44067400	3.99850000	-0.35310100
H	-2.59935600	4.42234900	-1.34832100
H	-2.48752600	4.81986400	0.36862200
C	-3.40986600	2.69648100	1.36466100
H	-3.77247700	3.52629600	1.97837200
H	-4.05477900	1.83171000	1.54789900
C	-1.94759200	2.36873700	1.74523100

H	-1.42223900	3.23290500	2.16350100
H	-1.87820800	1.52633400	2.42742400
C	-2.07966400	1.04336500	-0.32583400
H	-2.37233700	0.25965700	0.37163600
H	-1.46266600	0.56959000	-1.09284600
C	-1.06507500	3.29543900	-0.30822300
H	-0.71998700	3.03071900	-1.30663200
H	-0.28690600	3.89194300	0.17459600
C	0.17764800	1.44322700	0.78875000
H	0.61247600	2.18749900	1.46696900
C	0.06914500	0.16090400	1.63120000
O	1.27510100	-0.20171200	2.01863100
O	-0.96388700	-0.34941200	2.00336900
C	1.34857200	-1.46902200	2.73148300
H	0.74548300	-1.37170400	3.63946900
H	0.90456600	-2.23349300	2.08625900
C	2.80554600	-1.72864000	3.03337100
H	2.89040200	-2.65434100	3.60911200
H	3.37829100	-1.84651900	2.11016500
H	3.23803900	-0.91350900	3.62114700

N-INT3-SR-1

Zero-point correction= 0.637389 (Hartree/Particle)
Thermal correction to Energy= 0.672574
Thermal correction to Enthalpy= 0.673518
Thermal correction to Gibbs Free Energy= 0.570299
E(solv) = -2178.81092197 A.U.

C	2.96445500	-1.53391000	-0.65147700
C	3.39277700	-0.61636100	-1.61493900
C	4.54613500	-0.77198500	-2.37369200
C	5.30079500	-1.90941600	-2.12096500
C	4.90721100	-2.84090400	-1.14504000
C	3.74596300	-2.66992200	-0.40479900
C	1.73627500	-0.97376400	-0.07929400
C	1.56174900	0.21334100	-0.74456800
H	4.83361000	-0.03287400	-3.11333700
H	6.21242100	-2.07949100	-2.68562800
H	5.52411900	-3.71703400	-0.97164300
H	3.42389000	-3.40041200	0.32704700
O	2.54566900	0.44488700	-1.68404000
C	0.53842800	1.31731600	-0.70715100
H	0.06825400	1.29863900	-1.69667600
N	0.99003600	-1.40596100	1.01138800
C	1.15289600	2.71402300	-0.58035500
C	2.34527000	2.93012800	0.11534000

C	0.56137900	3.79872900	-1.23305400
C	2.89233900	4.20559800	0.20200500
H	2.84510000	2.08418600	0.57438700
C	1.10138000	5.07999600	-1.14388900
H	-0.32271800	3.64456400	-1.85072100
C	2.26724200	5.28752200	-0.41474100
H	3.82002200	4.35330200	0.74622500
H	0.62289200	5.90653200	-1.66022500
H	2.69898900	6.28102200	-0.34611300
S	0.39886300	-2.87734500	1.06208900
O	0.02769700	-3.17777400	2.44548400
O	1.15968700	-3.87772600	0.30433900
C	-1.18663100	-2.79167400	0.18781700
C	-2.37190800	-3.06636100	0.86629800
C	-1.22197400	-2.44945900	-1.16499300
C	-3.58999500	-3.00037500	0.19192300
H	-2.31382000	-3.33713900	1.91603700
C	-2.44780700	-2.37418500	-1.82743400
H	-0.29061400	-2.26788800	-1.69711600
C	-3.64824900	-2.65258900	-1.16231900
H	-4.51209100	-3.23165600	0.72139300
H	-2.47300100	-2.12533100	-2.88710700
C	-4.96792600	-2.62610800	-1.89395100
H	-4.88814000	-2.09144100	-2.84504900
H	-5.30825400	-3.64290400	-2.11737700
H	-5.75080400	-2.14809500	-1.29591700
N	-4.46365400	1.89746100	-0.44776600
N	-1.98250200	1.35812900	0.03130600
C	-4.35065400	0.93148800	0.64752500
H	-4.63122500	1.43066200	1.57942800
H	-5.05112300	0.10692900	0.48277900
C	-3.82858500	1.31073800	-1.62555400
H	-4.23591000	0.30560200	-1.77588100
H	-4.06755600	1.90951400	-2.50873800
C	-3.72827100	3.10864000	-0.07923900
H	-3.65471200	3.74622100	-0.96569800
H	-4.29446200	3.65771400	0.67753800
C	-2.32547500	2.76068300	0.47800200
H	-1.53865200	3.42376800	0.11341000
H	-2.30062200	2.74638600	1.56618500
C	-2.91971500	0.37048200	0.72097800
H	-2.56607300	0.22803800	1.73854300
H	-2.81257500	-0.56050200	0.16241900
C	-2.29539100	1.24720200	-1.44288500
H	-1.87261000	0.30270300	-1.79446300

H	-1.79854300	2.07924300	-1.94182700
C	-0.54719100	0.93068100	0.33227500
H	-0.59457200	-0.16551100	0.30978000
C	-0.19170400	1.19357800	1.80299700
O	1.10511500	1.15070900	1.98296400
O	-1.00940800	1.31853000	2.68956300
C	1.56001700	0.70667900	3.28383100
H	1.36127500	1.49889700	4.01071300
H	0.98132600	-0.18566100	3.53589300
C	3.02907400	0.38702400	3.13442600
H	3.42221600	0.01759800	4.08533900
H	3.15394700	-0.39080200	2.37632900
H	3.59951000	1.27535100	2.84721800

N-INT3-SR

Zero-point correction= 0.637223 (Hartree/Particle)
Thermal correction to Energy= 0.672875
Thermal correction to Enthalpy= 0.673820
Thermal correction to Gibbs Free Energy= 0.567924
E(solv) = -2178.81566501 A.U.

C	1.24042800	3.04743900	0.46720700
C	2.59229700	2.70663800	0.61657600
C	3.62691200	3.63118900	0.54791600
C	3.26369300	4.94974000	0.30434700
C	1.91702400	5.31754000	0.14183400
C	0.89546800	4.38152900	0.22058800
C	0.51024300	1.79781600	0.62655900
C	1.46965200	0.85659000	0.83418900
H	4.66044000	3.32865400	0.68140400
H	4.03659500	5.70917800	0.23441400
H	1.67444100	6.35741900	-0.05425600
H	-0.14497000	4.64914900	0.07092300
O	2.74378600	1.36893100	0.84327500
C	1.20771800	-0.61858500	0.89209200
H	0.36475200	-0.71940800	1.58213300
N	-0.84645400	1.47712600	0.66826400
C	2.34148800	-1.46988900	1.43169100
C	3.62222000	-1.46294400	0.87023700
C	2.11394800	-2.27440100	2.55179500
C	4.63058100	-2.26520400	1.39551900
H	3.84238200	-0.79905600	0.04120500
C	3.12003900	-3.07639400	3.08162900
H	1.13387600	-2.26021900	3.02592000
C	4.38269200	-3.07963700	2.49704000
H	5.61897100	-2.24396000	0.94673500

H	2.91789200	-3.68963600	3.95445800
H	5.17268300	-3.70205300	2.90554000
S	-1.73440500	1.82997300	-0.59153200
O	-1.52054500	0.89269200	-1.74144300
O	-1.76617600	3.24362900	-0.99058500
C	-3.34688800	1.37066300	0.04283700
C	-4.25209600	0.76376600	-0.82069800
C	-3.70180100	1.64293700	1.36241500
C	-5.52119200	0.42172600	-0.35707500
H	-3.94993300	0.56007900	-1.84394100
C	-4.96971200	1.29554500	1.81108600
H	-2.97096300	2.10009500	2.02142500
C	-5.89799200	0.68322900	0.96073600
H	-6.23141700	-0.05027000	-1.03178600
H	-5.24868900	1.50140600	2.84207800
C	-7.27427600	0.32931200	1.46409600
H	-7.84777500	1.23222000	1.69900500
H	-7.83638000	-0.23943800	0.71891000
H	-7.22077500	-0.26858200	2.37959200
N	-2.19914700	-3.92663500	-0.74620500
N	-0.36747600	-2.12112400	-0.57921000
C	-2.06501800	-3.22302600	-2.02254100
H	-1.98969100	-3.95447600	-2.83190900
H	-2.97204100	-2.63311300	-2.18438200
C	-2.54338000	-2.93894300	0.27853500
H	-3.58195200	-2.61945500	0.15028300
H	-2.45850600	-3.41904700	1.25836200
C	-0.90719400	-4.52110700	-0.40126600
H	-1.03834000	-5.20966100	0.43818600
H	-0.55991300	-5.10479600	-1.25904500
C	0.12550000	-3.43154400	-0.02524500
H	0.20714700	-3.29738800	1.05494600
H	1.11826500	-3.61297000	-0.43688900
C	-0.81305600	-2.31618000	-2.02130900
H	0.02680400	-2.76805700	-2.54617800
H	-1.01437900	-1.31311800	-2.40996400
C	-1.62385700	-1.70724000	0.17188900
H	-2.05748300	-0.90198900	-0.42196800
H	-1.34998900	-1.29425500	1.14032200
C	0.65226500	-0.99645900	-0.53082000
H	0.08384000	-0.13405000	-0.88847400
C	1.79596400	-1.22820700	-1.50852000
O	2.37407300	-0.06232000	-1.75365300
O	2.15565800	-2.28861900	-1.96966600
C	3.56977500	-0.06286400	-2.55711800

H	4.17594700	-0.93092100	-2.28163100
H	3.27248000	-0.17281800	-3.60426900
C	4.26938100	1.25056500	-2.28450600
H	5.17043200	1.32818800	-2.89885700
H	3.60972900	2.09156300	-2.51196900
H	4.54920800	1.31957300	-1.22944900

N-TS2-RR

Zero-point correction= 0.633467 (Hartree/Particle)
Thermal correction to Energy= 0.669249
Thermal correction to Enthalpy= 0.670193
Thermal correction to Gibbs Free Energy= 0.564565
E(solv) = -2178.77309220 A.U.
Imaginary Frequency 186.25*i*

C	1.93883600	2.57741700	0.34424000
C	3.20642900	1.97741900	0.34949900
C	4.38102900	2.68245300	0.11084400
C	4.25096600	4.04036700	-0.14387500
C	2.99479300	4.66834500	-0.15191100
C	1.83273100	3.95318800	0.09156500
C	0.99800600	1.49876600	0.64483600
C	1.81637800	0.34462100	0.81976700
H	5.34348300	2.18330000	0.13303200
H	5.14228400	4.62947300	-0.33818700
H	2.93365200	5.73290200	-0.35098000
H	0.86802500	4.44618700	0.08250400
O	3.15678400	0.64836900	0.60985300
C	1.35642500	-0.92674400	1.08750200
H	0.34570900	-0.92382600	1.48756700
N	-0.31680800	1.41192400	0.76540400
C	2.21186400	-2.05949200	1.48496800
C	3.46862600	-2.28248500	0.90580600
C	1.74488800	-2.95656700	2.45304500
C	4.23364400	-3.37525300	1.29725800
H	3.82164800	-1.60566400	0.13587100
C	2.51590100	-4.04512800	2.84775700
H	0.77471400	-2.78452900	2.91469300
C	3.76405800	-4.25818000	2.26852600
H	5.20441400	-3.53996500	0.83947400
H	2.14334400	-4.72469500	3.60832200
H	4.36758500	-5.10839700	2.57101400
S	-1.23515200	2.74031400	0.51375100
O	-1.07808700	3.27968800	-0.83846000
O	-1.12998500	3.67665100	1.63370400
C	-2.84938600	1.98318800	0.58334300

C	-3.67856600	2.06084000	-0.52760700
C	-3.28410400	1.38753200	1.76555700
C	-4.96354000	1.52444600	-0.45297300
H	-3.31084500	2.54711100	-1.42591000
C	-4.56352700	0.84937900	1.82051900
H	-2.62492600	1.36279000	2.62834500
C	-5.41933700	0.90707400	0.71266100
H	-5.62302300	1.58790200	-1.31517500
H	-4.91482000	0.38738400	2.74029900
C	-6.78994700	0.28370400	0.77309600
H	-7.24081300	0.41023200	1.76132300
H	-7.46076400	0.72534700	0.03171800
H	-6.73522100	-0.79277600	0.57133600
N	-3.32416600	-2.96950000	-0.98100200
N	-0.84601800	-2.24230100	-0.95359500
C	-3.20248000	-1.58945300	-0.50093600
H	-3.89732800	-0.95283600	-1.05480100
H	-3.50821400	-1.56276700	0.54980500
C	-2.54848000	-3.83635100	-0.09921200
H	-3.05480100	-3.91063100	0.86727200
H	-2.52125500	-4.83863300	-0.53831700
C	-2.76218900	-3.04722900	-2.32837800
H	-2.98736100	-4.02884000	-2.75604200
H	-3.25654300	-2.29128700	-2.94495300
C	-1.23195400	-2.81340400	-2.30112200
H	-0.65945800	-3.73891500	-2.40880300
H	-0.89519000	-2.08859600	-3.04239900
C	-1.76086300	-1.05995600	-0.67018500
H	-1.63891000	-0.37609400	-1.51025300
H	-1.37012100	-0.55241200	0.21325800
C	-1.11670400	-3.28383200	0.09573000
H	-0.98261900	-2.78459000	1.05780400
H	-0.34691500	-4.05337700	0.00036700
C	0.59464400	-1.88623000	-0.88638900
H	1.20658400	-2.77854900	-0.80685000
C	1.02981100	-0.90256100	-1.84429500
O	2.38009400	-0.83077500	-1.86041700
O	0.33087600	-0.14936300	-2.50959500
C	2.92944700	0.27962100	-2.58016600
H	2.59429800	0.23523300	-3.62078300
H	2.54489700	1.20997200	-2.14796000
C	4.43489200	0.18111100	-2.46219000
H	4.90776700	1.02679500	-2.96922000
H	4.73231200	0.19717500	-1.40995200

H	4.79857900	-0.74650800	-2.91346700

N-TS2-SR

Zero-point correction= 0.633411 (Hartree/Particle)
Thermal correction to Energy= 0.669285
Thermal correction to Enthalpy= 0.670230
Thermal correction to Gibbs Free Energy= 0.563354
E(solv) = -2178.77166417 A.U.
Imaginary Frequency 181.74*i*

C	1.47988700	2.99485600	0.22891000
C	2.81403800	2.57817200	0.35512100
C	3.89497900	3.38788400	0.02620600
C	3.59904000	4.65282900	-0.46131300
C	2.27233400	5.09472400	-0.60247700
C	1.20437400	4.28168100	-0.25860400
C	0.68024900	1.86460800	0.68546900
C	1.62879100	0.86693900	1.03951000
H	4.91280000	3.03436400	0.14725800
H	4.41267600	5.31680800	-0.73708900
H	2.08265700	6.09314600	-0.98179100
H	0.18237000	4.63147100	-0.34798900
O	2.92386200	1.31683700	0.83676500
C	1.29200200	-0.44903700	1.28984200
H	0.26422300	-0.55766000	1.62328000
N	-0.61905000	1.58420000	0.74097100
C	2.20908600	-1.52828000	1.68101700
C	3.56379300	-1.54223700	1.32004400
C	1.71154500	-2.59068100	2.44928900
C	4.38228100	-2.59950200	1.70200900
H	3.96684400	-0.71742600	0.74640200
C	2.53189800	-3.64263100	2.83636200
H	0.67043800	-2.57499400	2.76384000
C	3.87210000	-3.65345800	2.45594800
H	5.42855500	-2.59702900	1.41129000
H	2.12832900	-4.45089400	3.43841200
H	4.51625200	-4.47553800	2.75183600
S	-1.69407400	2.56966900	0.01806200
O	-1.54769300	2.52795600	-1.44334400
O	-1.77690600	3.88929200	0.64741700
C	-3.19370400	1.67523300	0.39583000
C	-4.13485700	1.51488700	-0.61448400
C	-3.42494000	1.17415000	1.67441200
C	-5.31969900	0.83540100	-0.33978900
H	-3.92508900	1.91522500	-1.60172500
C	-4.60566100	0.48570800	1.92895200
H	-2.67529700	1.31125200	2.44765500

C	-5.56710400	0.30333500	0.92781800
H	-6.06259000	0.71233900	-1.12414600
H	-4.79083900	0.08691600	2.92324100
C	-6.82585500	-0.47840700	1.20373700
H	-7.13924600	-0.37162700	2.24556200
H	-7.64702800	-0.14658000	0.56317300
H	-6.66974900	-1.54673400	1.01361900
N	-2.79611000	-3.32628900	-1.24393400
N	-0.66043900	-1.90316500	-1.01779000
C	-2.24807900	-3.03377900	-2.56829500
H	-2.15838900	-3.96805000	-3.12976900
H	-2.96028100	-2.39329500	-3.09661000
C	-3.09540600	-2.05873400	-0.57275500
H	-3.95060600	-1.58233400	-1.06036000
H	-3.38760000	-2.27445000	0.46004000
C	-1.78064000	-4.04410200	-0.47177500
H	-2.23268000	-4.41972900	0.45066100
H	-1.45642900	-4.90851600	-1.05872600
C	-0.58234600	-3.12463800	-0.13920700
H	-0.62023400	-2.74732300	0.88417100
H	0.39243300	-3.58042100	-0.31648900
C	-0.86588600	-2.34494800	-2.45248500
H	-0.02687400	-3.00167700	-2.68354700
H	-0.78749200	-1.43956200	-3.05781200
C	-1.87610100	-1.11174300	-0.60884200
H	-1.97535300	-0.30270100	-1.33961200
H	-1.64861300	-0.64733500	0.35202400
C	0.53653900	-1.04238200	-0.84581200
H	0.29226400	-0.01089600	-1.07184900
C	1.75866500	-1.57368200	-1.37945900
O	2.69241300	-0.59699400	-1.47778300
O	2.00537500	-2.74432700	-1.65903000
C	3.97373000	-1.00569800	-1.95880000
H	4.33720800	-1.84522100	-1.35763200
H	3.87269200	-1.35909800	-2.99058700
C	4.88047500	0.20413500	-1.86413400
H	5.87311100	-0.03334600	-2.25667800
H	4.46477000	1.03851300	-2.43535400
H	4.98157100	0.52873500	-0.82407900

N-TS3-RR

Zero-point correction=	0.634369 (Hartree/Particle)
Thermal correction to Energy=	0.669820
Thermal correction to Enthalpy=	0.670764
Thermal correction to Gibbs Free Energy=	0.566223

E(solv) = -2178.76856296 A.U.

Imaginary Frequency 462.32*i*

C	2.97622500	1.39125700	0.54328500
C	2.87067100	1.36167200	1.94699300
C	3.93028400	1.64202000	2.79673300
C	5.14123500	1.96354800	2.19494100
C	5.27484600	1.99928000	0.79758900
C	4.20598900	1.71518400	-0.04234400
C	1.64718100	1.03589900	0.07552500
C	0.91296300	0.84037400	1.18837300
H	3.80673100	1.60784300	3.87353400
H	5.99994800	2.19075500	2.81895600
H	6.23731500	2.25463100	0.36525100
H	4.30128200	1.73059000	-1.12249900
O	1.60289200	1.03445900	2.34864200
C	-0.52297500	0.42415900	1.16020000
H	-1.10478300	1.13355000	1.76735000
N	0.95253600	0.99149100	-1.12500300
C	-0.63521700	-0.96446800	1.77583200
C	-0.95730300	-1.08438100	3.12813300
C	-0.35931800	-2.11572800	1.03853000
C	-1.04477800	-2.33721900	3.72785400
H	-1.14638900	-0.18667200	3.71324400
C	-0.46260900	-3.37065300	1.63328000
H	-0.06440200	-2.04244300	-0.00469200
C	-0.81084600	-3.48645700	2.97686300
H	-1.30022200	-2.41510300	4.78031400
H	-0.26416200	-4.25771400	1.03849400
H	-0.89034900	-4.46567300	3.43880400
S	1.54880700	0.18480300	-2.39949400
O	2.92361900	0.60797800	-2.66352400
O	0.53834000	0.25398200	-3.44736900
C	1.64271800	-1.53355200	-1.90892100
C	2.59745900	-1.93776800	-0.97596100
C	0.71657100	-2.43728400	-2.41950900
C	2.60187500	-3.25681900	-0.54100100
H	3.32906700	-1.22542400	-0.60425600
C	0.74280200	-3.76076100	-1.98215300
H	-0.00177700	-2.09326200	-3.15774200
C	1.68005700	-4.18606600	-1.03849300
H	3.33553200	-3.57752700	0.19445500
H	0.02860100	-4.47515600	-2.38469400
C	1.72503100	-5.62077200	-0.57715000
H	2.53142900	-6.16571500	-1.07995300
H	1.91057200	-5.68336400	0.49970600

H	0.78786700	-6.14037900	-0.79606500
C	-1.02635100	0.56238100	-0.28387200
C	-1.13053900	1.91577200	-0.93549400
O	-1.58684400	2.11665900	-2.03519600
O	-0.77013800	2.87826300	-0.07849900
C	0.34728900	4.93017400	0.31135000
C	-0.50132600	4.15820300	-0.67478000
H	-1.06949500	-0.28590000	-0.95599300
H	0.58194600	5.91957400	-0.09035500
H	-0.17738600	5.05637900	1.26233400
H	1.28268100	4.39513400	0.49684400
H	0.01842000	3.98711900	-1.62115100
H	-1.45336100	4.65573200	-0.88918500
N	-3.05231900	0.38600100	-0.03091100
C	-3.50737000	-0.58748000	0.99529500
C	-5.08956900	0.02439600	-1.38611400
C	-5.20555200	1.51007800	0.46921600
C	-3.67683200	1.70163300	0.27506800
C	-3.54258000	-0.09131600	-1.35354000
C	-5.03652400	-0.82061200	0.83063200
N	-5.62379400	0.20152800	-0.03271900
H	-2.94456900	-1.51465600	0.87424500
H	-3.26333300	-0.17336700	1.97751100
H	-5.53378900	-0.87214000	-1.82879200
H	-5.40174000	0.88258600	-1.98907400
H	-5.75486300	2.29099600	-0.06478800
H	-5.48324200	1.57130900	1.52641100
H	-3.46955500	2.36532600	-0.56620000
H	-3.19009100	2.11187500	1.16594400
H	-3.05866900	0.49913400	-2.13366900
H	-3.21295700	-1.13173600	-1.45038000
H	-5.23254800	-1.79990800	0.38263000
H	-5.53358800	-0.79527700	1.80518100

N-TS3-SR

Zero-point correction= 0.634229 (Hartree/Particle)
Thermal correction to Energy= 0.669798
Thermal correction to Enthalpy= 0.670743
Thermal correction to Gibbs Free Energy= 0.564393
E(solv) = -2178.76091300 A.U.
Imaginary Frequency 473.33*i*

C	3.41716100	-0.59437500	-0.65002200
C	3.50152000	-0.01838100	-1.93378400
C	4.60701200	-0.14285100	-2.76321500
C	5.68019400	-0.86895100	-2.26515700

C	5.63321700	-1.44419800	-0.98511000
C	4.51709900	-1.31986500	-0.16981100
C	2.09312300	-0.20916600	-0.17008200
C	1.54972900	0.51083700	-1.17575200
H	4.61896900	0.31738300	-3.74495900
H	6.57000000	-0.99004100	-2.87497900
H	6.49188200	-2.00156600	-0.62430900
H	4.47746900	-1.77084300	0.81316200
O	2.36788300	0.67431000	-2.25475900
C	0.25414900	1.23085800	-1.00652500
H	-0.26953700	1.19359300	-1.96406000
N	1.34379900	-0.22972600	1.00680300
C	0.44856900	2.70463300	-0.65649800
C	1.44981200	3.10085500	0.23444200
C	-0.34145800	3.67945000	-1.26103400
C	1.63384100	4.44580900	0.52689600
H	2.06414100	2.34265800	0.71268900
C	-0.16300700	5.03094400	-0.96483800
H	-1.09599500	3.39097200	-1.99028300
C	0.82496800	5.41598700	-0.06674600
H	2.41215300	4.74139200	1.22413700
H	-0.78569200	5.77769000	-1.44803400
H	0.97458900	6.46648100	0.16275300
S	1.32990300	-1.56520100	1.93601200
O	0.70571600	-1.20051900	3.20241200
O	2.64218500	-2.21089700	1.93620600
C	0.21646300	-2.70799200	1.12154800
C	-1.01269700	-3.00962600	1.69977100
C	0.57043200	-3.23242400	-0.12159600
C	-1.89275600	-3.84994900	1.02365700
H	-1.26106500	-2.57228200	2.66084600
C	-0.33023600	-4.05398800	-0.79349500
H	1.54463700	-3.00702300	-0.54826000
C	-1.56931100	-4.37767100	-0.22994000
H	-2.85066400	-4.09894900	1.47506800
H	-0.06119000	-4.46515000	-1.76323000
C	-2.52478800	-5.30117700	-0.94287300
H	-2.32908200	-5.32475700	-2.01823600
H	-2.42835800	-6.32582000	-0.56749500
H	-3.56389500	-4.99468500	-0.78873800
N	-4.86420800	0.28563000	-1.68513800
N	-2.44742800	0.43217400	-0.80757800
C	-4.55746300	-0.86016000	-0.82489600
H	-5.16204200	-0.77310800	0.08311700
H	-4.85681200	-1.78017300	-1.33638400

C	-3.91646700	0.28241800	-2.79631900
H	-3.96462300	-0.69585500	-3.28419600
H	-4.21802100	1.03619500	-3.52958900
C	-4.66903300	1.51574400	-0.91402300
H	-4.75856300	2.36336300	-1.60098900
H	-5.47028400	1.60189200	-0.17454100
C	-3.28128200	1.50637600	-0.21146700
H	-2.74377800	2.45406900	-0.31968000
H	-3.37718600	1.28548500	0.85405900
C	-3.04513600	-0.89277900	-0.48042500
H	-2.86141200	-1.09970300	0.57316600
H	-2.50450600	-1.64292900	-1.06959100
C	-2.47762200	0.57663100	-2.28087200
H	-1.74215700	-0.11101500	-2.71168900
H	-2.18192000	1.59904900	-2.52825300
C	-0.53140300	0.35702700	-0.01816900
H	-0.57320700	-0.69944000	-0.25685300
C	-0.99757700	0.69455900	1.37570800
O	-0.61511400	1.88500200	1.80150300
O	-1.68626100	-0.06583500	2.01913800
C	-0.81156300	2.11758300	3.21100200
H	-1.88685900	2.18024300	3.40770200
H	-0.40959700	1.25455000	3.74869000
C	-0.09070900	3.40436600	3.54439500
H	-0.24636900	3.65380900	4.59743900
H	0.98153400	3.29391600	3.36574000
H	-0.46013700	4.22762400	2.92638800

S-INT3-RR-1

Zero-point correction= 0.524884 (Hartree/Particle)
Thermal correction to Energy= 0.558867
Thermal correction to Enthalpy= 0.559811
Thermal correction to Gibbs Free Energy= 0.457551
E(solv) = -2311.48719920 A.U.

C	2.85298700	-0.86882200	0.44685800
C	2.64414400	-1.42295800	1.71595400
C	3.55107100	-2.26622200	2.34458900
C	4.72308600	-2.54014900	1.65123400
C	4.96702500	-1.98513500	0.38383100
C	4.04483000	-1.15068300	-0.23209800
C	1.67427200	-0.04607400	0.18300000
C	0.89585700	-0.18906300	1.29183800
H	3.34575800	-2.67829500	3.32653400
H	5.46437100	-3.19486100	2.09942100
H	5.89672000	-2.21888400	-0.12553600

H	4.21335800	-0.73556600	-1.21871800
O	1.45770000	-1.00886400	2.24206100
C	-0.41981500	0.41300800	1.67032500
H	-0.27409700	1.08054000	2.53451400
N	1.38983600	0.86059300	-0.82930000
C	-1.43120800	-0.66509500	2.03988800
C	-2.02123500	-0.70861900	3.30033600
C	-1.80172400	-1.60608700	1.07618400
C	-2.97823300	-1.67871200	3.59571500
H	-1.72493800	0.01387500	4.05787800
C	-2.75990900	-2.56997500	1.36716700
H	-1.31226100	-1.60052900	0.10381600
C	-3.35311900	-2.60662900	2.62888100
H	-3.42765100	-1.71023200	4.58366500
H	-3.03124500	-3.30027500	0.60936400
H	-4.09783300	-3.36227500	2.85946700
S	1.36356000	0.36546500	-2.34943600
O	2.47243200	-0.53045400	-2.69482600
O	1.10728600	1.53483800	-3.18418100
C	-0.10383100	-0.67091800	-2.46927000
C	-0.01058800	-2.03380800	-2.20702200
C	-1.34253700	-0.08667200	-2.73860300
C	-1.16687500	-2.81509900	-2.20546700
H	0.96651000	-2.47206900	-2.02500000
C	-2.48825500	-0.87744700	-2.72714900
H	-1.37658200	0.97549100	-2.97395400
C	-2.41861400	-2.25030800	-2.45477300
H	-1.09352900	-3.88149500	-2.00548800
H	-3.45500500	-0.43552900	-2.96651500
C	-3.67222600	-3.08874700	-2.44744200
H	-4.17500300	-3.05558600	-3.41956600
H	-3.44800700	-4.13451800	-2.22125100
H	-4.38527900	-2.72614400	-1.69854800
C	-0.96002600	1.24051300	0.49278300
C	-0.14048600	2.40961900	-0.05297500
O	-0.51996400	3.03322000	-1.02374800
O	0.75481000	2.83765200	0.83730900
C	3.09993500	3.24592300	0.95230700
C	1.80854300	3.66128200	0.28384100
H	-1.20465600	0.59415200	-0.35505000
H	3.91970500	3.87725900	0.59760900
H	3.03024100	3.34459300	2.03939800
H	3.32275300	2.20569000	0.70073000
H	1.83649700	3.48610000	-0.79380500
H	1.55255800	4.70834300	0.47778800

S	-2.63322900	1.90774300	0.97742000
C	-2.27807000	3.61542500	1.46505600
H	-1.54719100	3.57425400	2.27531200
H	-1.86641800	4.15783300	0.61181500
H	-3.21153800	4.05509700	1.81918900
C	-3.39696700	2.14203500	-0.64351700
H	-3.57165200	1.14174900	-1.04689700
H	-4.34492900	2.66200500	-0.49553800
H	-2.70112100	2.69917500	-1.27500500

S-INT3-RR

Zero-point correction= 0.525575 (Hartree/Particle)
Thermal correction to Energy= 0.559363
Thermal correction to Enthalpy= 0.560307
Thermal correction to Gibbs Free Energy= 0.459863
E(solv) = -2311.48275905 A.U.

C	-1.41568100	2.43278800	-0.63928500
C	-2.76656600	2.10422800	-0.43955300
C	-3.77103900	3.05020600	-0.27064300
C	-3.38109300	4.38172300	-0.29546600
C	-2.03734500	4.74202700	-0.49569800
C	-1.04748000	3.78641000	-0.67329800
C	-0.72436800	1.15191600	-0.74971000
C	-1.70728600	0.21651700	-0.62677300
H	-4.80165900	2.74704000	-0.12170800
H	-4.12858800	5.15746300	-0.16027900
H	-1.76891200	5.79357000	-0.51546200
H	-0.01541100	4.07649700	-0.83377000
O	-2.95699500	0.76050300	-0.42384600
C	-1.48651600	-1.25046900	-0.54861600
H	-0.83837700	-1.49763700	-1.40312600
N	0.59559200	0.75683500	-0.84202700
C	-2.74600400	-2.08681700	-0.64414200
C	-3.75426000	-1.93721500	0.31466000
C	-2.90664900	-3.03037600	-1.65674000
C	-4.90101600	-2.71897200	0.25671600
H	-3.63987400	-1.18493300	1.09173400
C	-4.05722900	-3.81620700	-1.71539700
H	-2.13060600	-3.14780000	-2.40943900
C	-5.05449300	-3.66285800	-0.75850600
H	-5.68073000	-2.58769600	1.00056700
H	-4.17173500	-4.54670800	-2.51025600
H	-5.95137100	-4.27283300	-0.80313500
S	1.72337000	1.89294300	-0.73100200
O	1.63454700	2.67222700	0.52029800

O	1.89927600	2.68256400	-1.95604600
C	3.16203400	0.84665900	-0.57054600
C	3.68658500	0.59290800	0.69017700
C	3.71674400	0.26625000	-1.70758200
C	4.77128500	-0.27337300	0.81261300
H	3.23202900	1.06389200	1.55531000
C	4.79311900	-0.60424500	-1.57013100
H	3.30132000	0.50577700	-2.68252100
C	5.33511200	-0.88494300	-0.31037800
H	5.19127300	-0.47390600	1.79559600
H	5.23317900	-1.06274000	-2.45291500
C	6.53133200	-1.79334400	-0.17737200
H	7.46058100	-1.23890600	-0.34936900
H	6.59101400	-2.23114000	0.82295300
H	6.49790300	-2.60693400	-0.90807000
C	-0.68366400	-1.68956900	0.75373800
H	-1.38881800	-2.19937200	1.42100600
C	0.03888400	-0.64408200	1.61174300
O	-0.83226600	0.24665100	2.02946000
O	1.19582000	-0.73170500	1.96154900
C	-0.29172600	1.38163600	2.76192000
H	0.16372200	0.99625200	3.67941700
H	0.47506000	1.84333700	2.13305600
C	-1.44616900	2.31757100	3.03527800
H	-1.08460900	3.17326600	3.61185200
H	-1.86742300	2.68997700	2.09765600
H	-2.23304200	1.81866000	3.60845500
S	0.44897600	-3.01876500	0.21086100
C	1.84293900	-2.13044500	-0.53536100
H	2.54765500	-1.83659300	0.24417200
H	2.28693300	-2.79704800	-1.27474800
H	1.42503900	-1.21738700	-0.98847800
C	1.14128200	-3.70539600	1.73124200
H	1.87638400	-4.45547900	1.43337800
H	1.59662300	-2.90202400	2.30931600
H	0.32833600	-4.18838800	2.27658000

S-INT3-SR-1

Zero-point correction= 0.525360 (Hartree/Particle)
Thermal correction to Energy= 0.559175
Thermal correction to Enthalpy= 0.560119
Thermal correction to Gibbs Free Energy= 0.459198
E(solv) = -2311.48284231 A.U.

C	2.90765800	0.80626800	-0.57392700
C	2.51324900	1.83338900	-1.43455700

C	3.40595400	2.62941600	-2.14119400
C	4.75485000	2.35880700	-1.95013100
C	5.18034500	1.33471800	-1.08595200
C	4.27069000	0.54975800	-0.39188700
C	1.67707800	0.24550800	-0.02011300
C	0.67953000	0.98102800	-0.59923200
H	3.05748700	3.41695900	-2.80022300
H	5.49488400	2.94985900	-2.48102200
H	6.24374400	1.15260100	-0.96670400
H	4.58657600	-0.26245300	0.25274100
O	1.15581200	1.94467500	-1.46264800
C	-0.82276800	0.89953500	-0.58838800
H	-1.09804100	0.49500900	-1.57617100
N	1.52769100	-0.70088800	0.98582400
C	-1.51664000	2.25558000	-0.49424200
C	-1.42571800	3.08443400	0.62920400
C	-2.26604900	2.69983000	-1.58789500
C	-2.12330700	4.28821700	0.67415500
H	-0.80036600	2.78775900	1.46167000
C	-2.96262700	3.90616800	-1.54635100
H	-2.28301300	2.10463900	-2.49912800
C	-2.90553700	4.69793600	-0.40420500
H	-2.04542900	4.91670300	1.55607800
H	-3.53565100	4.22941700	-2.40989000
H	-3.44612500	5.63820000	-0.36241100
S	2.03931400	-2.18348600	0.71753700
O	2.03907000	-2.90846500	1.98693200
O	3.21184800	-2.28089100	-0.15952100
C	0.67863700	-2.88152600	-0.23651700
C	-0.37069700	-3.51214500	0.43134400
C	0.56783100	-2.57569900	-1.59312400
C	-1.53338200	-3.83623900	-0.26383400
H	-0.26392100	-3.72124400	1.49167900
C	-0.60397000	-2.89781000	-2.27686200
H	1.40014200	-2.09101700	-2.09589100
C	-1.66780400	-3.53369900	-1.62487700
H	-2.34900400	-4.33662700	0.25404000
H	-0.68851300	-2.67036000	-3.33780300
C	-2.91521100	-3.93021300	-2.37686600
H	-3.04915800	-3.33043500	-3.28276600
H	-2.86420300	-4.97931200	-2.68762300
H	-3.81018200	-3.82303200	-1.75419800
C	-1.25432400	-0.18311100	0.41207300
H	-0.76046600	-1.11365000	0.11277900
C	-0.95437300	-0.10541300	1.91781100

O	-0.18857400	0.89727300	2.27868000
O	-1.44178800	-0.92953000	2.65846700
C	0.57884700	0.68867800	3.49393100
H	-0.07809900	0.87894500	4.34793300
H	0.90116600	-0.35491800	3.49195000
C	1.75579200	1.63278700	3.42299700
H	2.36276900	1.52800100	4.32635300
H	2.36865400	1.37860100	2.55467400
H	1.42762300	2.67369000	3.34527200
S	-3.02294900	-0.71948200	0.37616800
C	-3.50570800	-0.56463800	-1.35513600
H	-2.79409800	-1.15820900	-1.93442100
H	-4.50380300	-0.99769000	-1.44538900
H	-3.50204200	0.48024400	-1.66444800
C	-3.93964900	0.64746700	1.13173600
H	-3.77298900	1.57970100	0.59073000
H	-4.99353800	0.36294700	1.12666700
H	-3.58721300	0.72067600	2.16240400

S-INT3-SR

Zero-point correction= 0.525797 (Hartree/Particle)
Thermal correction to Energy= 0.559138
Thermal correction to Enthalpy= 0.560082
Thermal correction to Gibbs Free Energy= 0.461941
E(solv) = -2311.48055671 A.U.

C	1.37219400	2.92294800	-0.09688200
C	0.39523900	3.47837600	0.74501700
C	0.63113400	4.54799300	1.59790100
C	1.91609500	5.07361200	1.59333700
C	2.91474600	4.54193400	0.76096700
C	2.66253400	3.47274000	-0.08727700
C	0.69336600	1.83982600	-0.80305300
C	-0.58581200	1.85579800	-0.31818500
H	-0.15802300	4.94298100	2.22825500
H	2.15100500	5.91119800	2.24297900
H	3.90766000	4.98047600	0.78067500
H	3.43047200	3.05845300	-0.73000500
O	-0.80147400	2.84109000	0.60876600
C	-1.67110800	0.93332300	-0.78021800
H	-1.74061200	1.08402200	-1.86768100
N	1.03224000	0.93463400	-1.80495400
C	-3.07112500	1.05227900	-0.21697300
C	-3.34120500	1.39403500	1.11139100
C	-4.14239700	0.74796800	-1.06585500
C	-4.65452300	1.41535800	1.57337500

H	-2.52153000	1.64200700	1.77357600
C	-5.45460800	0.75562800	-0.59865100
H	-3.94614700	0.52791200	-2.11486900
C	-5.71216000	1.08975400	0.72768500
H	-4.85169100	1.68885400	2.60547500
H	-6.27212100	0.52386200	-1.27480200
H	-6.73295800	1.10908300	1.09689000
S	2.44749500	0.21029700	-1.86485200
O	3.61050500	1.09366900	-1.75897900
O	2.38588600	-0.72546100	-3.00029400
C	2.52834600	-0.87205400	-0.41822900
C	2.37467800	-0.35996300	0.87247100
C	2.74835200	-2.23346500	-0.60475800
C	2.43022700	-1.22075000	1.96333000
H	2.22549500	0.70450500	1.02897100
C	2.81716200	-3.08284000	0.49821400
H	2.88331600	-2.60676800	-1.61547100
C	2.66323800	-2.59079600	1.79564200
H	2.30662200	-0.81746900	2.96616800
H	3.01467300	-4.14283200	0.34971400
C	2.78029300	-3.50062200	2.99274200
H	3.72182000	-3.32302900	3.52353900
H	1.97046100	-3.33122500	3.71157400
H	2.75972700	-4.55364800	2.69760000
C	-1.06806500	-0.49193900	-0.63649100
H	-0.02782500	-0.35066300	-1.01564900
C	-1.01168300	-1.06080900	0.76122000
O	-0.79872400	-2.38880900	0.76410200
O	-1.09290800	-0.39556800	1.75780700
C	-0.69816300	-2.99058900	2.07098700
H	0.07662100	-2.46074000	2.62879000
H	-1.65156300	-2.84862400	2.58930700
C	-0.36268000	-4.44972700	1.86224100
H	-0.23751700	-4.94527600	2.82882400
H	-1.15804200	-4.96470000	1.31455000
H	0.57097300	-4.54084700	1.29999900
S	-1.68780500	-1.57475000	-1.96760700
C	-0.25464600	-2.62534200	-2.29978600
H	0.06293200	-3.10140200	-1.37029900
H	-0.54961000	-3.35555200	-3.05612100
H	0.53249500	-1.96229000	-2.69161100
C	-2.91516200	-2.69411500	-1.25721900
H	-3.34133400	-3.26693800	-2.08282600
H	-2.45155000	-3.34087100	-0.51449500
H	-3.68635300	-2.06243300	-0.80790000

S-TS2-RR

Zero-point correction= 0.522357 (Hartree/Particle)
Thermal correction to Energy= 0.556591
Thermal correction to Enthalpy= 0.557535
Thermal correction to Gibbs Free Energy= 0.454599
E(solv) = -2311.45224602 A.U.
Imaginary Frequency 368.46*i*

C	0.99523200	2.52442900	0.50177000
C	2.36663600	2.23298500	0.48558800
C	3.35206100	3.20973600	0.38491900
C	2.91769900	4.52427400	0.29606500
C	1.55037700	4.84635400	0.31438100
C	0.58007400	3.86171600	0.41918600
C	0.32320700	1.22967700	0.63239500
C	1.37226000	0.28699100	0.68787000
H	4.40349000	2.94386300	0.38914500
H	3.65187500	5.32030400	0.21546500
H	1.24842700	5.88626000	0.24840200
H	-0.47196500	4.12030000	0.43240100
O	2.61562400	0.90523900	0.57953400
C	1.23350200	-1.10273400	0.80085000
H	0.24249900	-1.35877300	1.17262500
N	-0.94947300	0.84523600	0.71623800
C	2.32395100	-1.96354100	1.32704700
C	3.65522500	-1.81221700	0.91818400
C	2.00579600	-2.96850500	2.24505000
C	4.64250600	-2.64150200	1.43772200
H	3.90197200	-1.05107000	0.18593500
C	2.99741800	-3.79326400	2.76764900
H	0.97319000	-3.09457900	2.56175600
C	4.31972300	-3.63037300	2.36570900
H	5.67177200	-2.51535000	1.11560900
H	2.73603200	-4.56232300	3.48818700
H	5.09539000	-4.27319700	2.77038500
S	-2.14039600	1.94739000	0.59555900
O	-2.10791200	2.66772800	-0.68180700
O	-2.27757200	2.74719800	1.81435000
C	-3.52360600	0.82234200	0.51823200
C	-4.22876800	0.69563800	-0.67045400
C	-3.86232700	0.06781800	1.63942600
C	-5.28219000	-0.21509500	-0.74076400
H	-3.94262400	1.30748800	-1.52055400
C	-4.90951000	-0.83998700	1.55200700
H	-3.30341400	0.19660200	2.56172800

C	-5.63402000	-0.99412000	0.36300700
H	-5.84272300	-0.31771100	-1.66687300
H	-5.18017100	-1.43581200	2.42042200
C	-6.79362900	-1.95535600	0.29659200
H	-7.68579900	-1.51855300	0.75861600
H	-7.04552700	-2.20469600	-0.73754700
H	-6.57189800	-2.88423700	0.83032000
C	0.99596000	-1.98734600	-1.07479700
H	1.80098600	-2.71226600	-1.00874000
C	1.20408900	-0.86521800	-1.99685700
O	2.48909800	-0.49463100	-1.99516700
O	0.33405900	-0.27300600	-2.60699600
C	2.76519300	0.78752400	-2.58809500
H	2.50152900	0.75081800	-3.64916200
H	2.12689400	1.53593100	-2.10668300
C	4.23436600	1.06584600	-2.36697800
H	4.48839900	2.05558100	-2.75597700
H	4.45936700	1.04348500	-1.29739700
H	4.85322500	0.31970300	-2.87298700
S	-0.53802100	-2.82929100	-1.23051600
C	-1.83095500	-1.59098800	-0.94949400
H	-1.72396700	-0.80227800	-1.69494500
H	-2.79250000	-2.10601600	-1.01390300
H	-1.68070500	-1.15731100	0.04083000
C	-0.81229800	-3.14300100	-3.00229700
H	-1.81293500	-3.56447300	-3.11992800
H	-0.71184300	-2.19647600	-3.53515400
H	-0.06221600	-3.86416900	-3.32911300

S-TS2-SR

Zero-point correction= 0.522663 (Hartree/Particle)
Thermal correction to Energy= 0.556625
Thermal correction to Enthalpy= 0.557569
Thermal correction to Gibbs Free Energy= 0.456108
E(solv) = -2311.44746402 A.U.
Imaginary Frequency 404.09*i*

C	1.75750900	2.67796000	0.16640800
C	0.60943600	3.27487700	0.71673000
C	0.64982900	4.30014000	1.65451200
C	1.90423200	4.73752000	2.04930500
C	3.07179900	4.17444700	1.50889400
C	3.01581900	3.15544900	0.57101700
C	1.24774400	1.67900800	-0.78141000
C	-0.15364600	1.82181600	-0.71765600
H	-0.26786100	4.72586800	2.04457400

H	1.98455500	5.53374600	2.78346600
H	4.03898000	4.54838000	1.82878000
H	3.91675700	2.72836000	0.15318400
O	-0.54014400	2.76580200	0.21716200
C	-1.06633100	0.95652300	-1.33159700
H	-0.69127500	0.56782600	-2.27637500
N	1.73357900	0.72295900	-1.57832700
C	-2.52851800	1.19569300	-1.27311600
C	-3.17716000	1.42962700	-0.05425500
C	-3.28716800	1.12760600	-2.44580200
C	-4.56075200	1.55925300	-0.01110000
H	-2.58308900	1.51384900	0.85160100
C	-4.67257300	1.27019300	-2.40266100
H	-2.78537400	0.95873900	-3.39558100
C	-5.31326400	1.47260500	-1.18255500
H	-5.05558200	1.73588100	0.93949900
H	-5.24994000	1.22169800	-3.32095300
H	-6.39326400	1.57652800	-1.14528000
S	3.20045300	0.05531100	-1.47000000
O	4.17023000	0.83707200	-0.70061300
O	3.58115300	-0.43445200	-2.78896400
C	2.83242800	-1.39544300	-0.48039000
C	2.46904400	-1.22970200	0.85512400
C	2.83459500	-2.65354500	-1.06833500
C	2.10235600	-2.34212700	1.60186400
H	2.44084300	-0.23555500	1.29403100
C	2.48429500	-3.76446000	-0.30018000
H	3.11721500	-2.74500600	-2.11256000
C	2.11815700	-3.62524600	1.04107300
H	1.80053700	-2.21183900	2.63869500
H	2.50194600	-4.75561700	-0.74878400
C	1.75162300	-4.82688200	1.87621900
H	2.58690000	-5.12513400	2.51908700
H	0.90050200	-4.61082800	2.53048900
H	1.49496400	-5.68691400	1.25071800
C	-0.75311700	-0.83407900	-0.40469600
H	0.28255900	-0.84790900	-0.74993900
C	-0.90996000	-0.57767100	1.02591900
O	-2.03041600	-1.13650900	1.56813400
O	-0.17824200	0.14538900	1.66389400
C	-2.31212700	-0.75426900	2.92082100
H	-1.54413200	-1.17529600	3.57750100
H	-2.25182700	0.33492900	3.00211500
C	-3.69662700	-1.27139200	3.24770800
H	-3.96618100	-1.00837400	4.27382900

H	-4.43509800	-0.82979900	2.57152800
H	-3.74119900	-2.36015400	3.14945600
S	-1.57837400	-2.18406300	-1.16166800
C	-1.28981500	-3.65241000	-0.12977100
H	-1.65954900	-3.45319500	0.87725200
H	-1.80242900	-4.50185300	-0.58716500
H	-0.20932100	-3.81480000	-0.12372600
C	-3.36720700	-2.00169400	-0.92707700
H	-3.81378200	-2.92332900	-1.30662300
H	-3.58463000	-1.85109100	0.12895900
H	-3.70378900	-1.15099800	-1.51967500

S-TS3-RR

Zero-point correction= 0.524121 (Hartree/Particle)
Thermal correction to Energy= 0.557923
Thermal correction to Enthalpy= 0.558867
Thermal correction to Gibbs Free Energy= 0.457846
E(solv) = -2311.46334239 A.U.
Imaginary Frequency 406.22*i*

C	2.88862500	-0.35767700	0.59243500
C	2.73300100	-0.53462900	1.97845400
C	3.72297500	-1.06096000	2.79572200
C	4.91398800	-1.41882200	2.17560500
C	5.09568000	-1.25408200	0.79252700
C	4.09516200	-0.72775400	-0.01355200
C	1.62219400	0.20580100	0.15183100
C	0.86380700	0.29807400	1.26603200
H	3.56194500	-1.18267200	3.86121500
H	5.71829800	-1.83634100	2.77339800
H	6.04024400	-1.54781700	0.34530300
H	4.22006200	-0.60937500	-1.08441200
O	1.49912200	-0.12148700	2.39968300
C	-0.52476800	0.84812100	1.31209600
H	-0.52599800	1.75314300	1.93689600
N	1.11260900	0.73098300	-1.02991700
C	-1.51295100	-0.15177500	1.89344900
C	-2.16482600	0.11239000	3.09601700
C	-1.78369200	-1.33926800	1.21265400
C	-3.09022000	-0.79392300	3.60884100
H	-1.94850900	1.03302800	3.63326600
C	-2.71637500	-2.23937100	1.71762800
H	-1.24957400	-1.56675200	0.29388700
C	-3.37303900	-1.96802900	2.91652700
H	-3.59173900	-0.58059200	4.54783800
H	-2.92334700	-3.15631200	1.17280400
H	-4.09779100	-2.67227100	3.31324300

S	1.10840800	-0.19253200	-2.36350000
O	2.45716900	-0.67098900	-2.66781500
O	0.33903000	0.52860000	-3.37103600
C	0.15461100	-1.65717700	-1.96352000
C	0.72248900	-2.66438300	-1.18391000
C	-1.16390700	-1.75420800	-2.39899100
C	-0.05012700	-3.76431800	-0.82834800
H	1.76096700	-2.58694500	-0.87324000
C	-1.92349100	-2.86636200	-2.03986100
H	-1.56528800	-0.96935000	-3.03464100
C	-1.37909700	-3.88310000	-1.25146300
H	0.38563300	-4.54949600	-0.21544600
H	-2.95040800	-2.95313600	-2.38716500
C	-2.18861500	-5.10251400	-0.88839300
H	-1.94476700	-5.94178700	-1.54901700
H	-1.98181600	-5.42402200	0.13698200
H	-3.26146300	-4.91058200	-0.98002400
C	-0.90333200	1.27996200	-0.11005000
C	-0.35337700	2.52897600	-0.73607100
O	-0.70655400	2.95615300	-1.81061100
O	0.44998700	3.17426300	0.11361600
C	2.32444200	4.56945000	0.52171800
C	1.26124100	4.19938500	-0.48772400
H	-1.27740700	0.54126800	-0.81167100
H	2.98126400	5.33839100	0.10653600
H	1.87420500	4.95660500	1.43988600
H	2.92636400	3.69198600	0.77067700
H	1.68765000	3.78831100	-1.40678400
H	0.62206100	5.04795900	-0.75300300
S	-2.99500500	2.00481200	0.23770700
C	-2.86457400	3.81252200	0.21173800
H	-2.25579300	4.10708900	1.06936800
H	-2.38509100	4.13767200	-0.71343200
H	-3.86499900	4.23785000	0.30859700
C	-3.55310100	1.68281300	-1.45401000
H	-3.67512300	0.60062100	-1.54306500
H	-4.51568300	2.17044400	-1.61742400
H	-2.79297000	2.04257000	-2.15343200

S-TS3-SR

Zero-point correction= 0.523964 (Hartree/Particle)
Thermal correction to Energy= 0.557892
Thermal correction to Enthalpy= 0.558837
Thermal correction to Gibbs Free Energy= 0.457049
E(solv) = -2311.44949969 A.U.

Imaginary Frequency	405.75*i*		
C	1.41634400	2.62359000	0.00086500
C	1.01136000	3.16562800	-1.23405600
C	1.53346600	4.33386900	-1.77062900
C	2.49985200	4.98704900	-1.01788600
C	2.91811300	4.47864700	0.22230300
C	2.38986500	3.30575300	0.74492400
C	0.61839000	1.40880100	0.14498900
C	-0.13334500	1.35119600	-0.97815300
H	1.18815200	4.70813000	-2.72802600
H	2.93506300	5.90749600	-1.39456900
H	3.67204900	5.01776000	0.78738800
H	2.71153700	2.91243800	1.70186600
O	0.04975000	2.40181500	-1.83176400
C	-1.20214400	0.32848100	-1.19274200
H	-1.22022000	0.10611000	-2.26706800
N	0.34384200	0.44513000	1.10863200
C	-2.58397400	0.84782600	-0.80744000
C	-2.77389100	1.51298000	0.40835600
C	-3.65563300	0.73804200	-1.69152600
C	-4.02394800	2.01852700	0.73944900
H	-1.93594700	1.60735800	1.09416000
C	-4.91307400	1.24461700	-1.36047600
H	-3.51029700	0.28210400	-2.66902800
C	-5.09919500	1.88167500	-0.13988700
H	-4.16084400	2.52629300	1.68958700
H	-5.73480900	1.15480100	-2.06440700
H	-6.07318500	2.28333800	0.12246900
S	1.53750300	-0.16086100	2.01609400
O	0.91436500	-1.13493600	2.91119100
O	2.37811200	0.89590400	2.58176900
C	2.58179400	-1.07678300	0.88817100
C	2.36725800	-2.44035600	0.70280600
C	3.52558300	-0.38989600	0.12707600
C	3.11403100	-3.11757900	-0.25782300
H	1.62150500	-2.94842200	1.30608000
C	4.26325300	-1.08355200	-0.82562800
H	3.68483100	0.67176900	0.29604100
C	4.07040300	-2.45334600	-1.03002700
H	2.95699100	-4.18363300	-0.40430000
H	5.00601400	-0.55493400	-1.41812100
C	4.90380600	-3.20404200	-2.03736500
H	5.15768100	-2.57356700	-2.89422600
H	5.84474600	-3.54152200	-1.58846500
H	4.37954800	-4.09033400	-2.40552900

C	-0.69476500	-0.93292800	-0.47669000
H	0.34389700	-1.17958100	-0.68119900
C	-1.18843400	-1.63357300	0.77668600
O	-2.11742500	-0.99032400	1.45025600
O	-0.77467600	-2.73973000	1.04595400
C	-2.36668800	-1.48856000	2.78431300
H	-2.89277300	-2.44595300	2.70530600
H	-1.39608900	-1.64957300	3.25970200
C	-3.18898700	-0.43233600	3.48703500
H	-3.42793200	-0.76282600	4.50139300
H	-2.61986300	0.49892200	3.54974300
H	-4.12178000	-0.23919900	2.94940500
S	-1.36150100	-2.66772800	-1.73865200
C	-1.64686500	-2.08305600	-3.42425000
H	-0.70425600	-1.68698100	-3.80786000
H	-1.95198000	-2.93287200	-4.03902000
H	-2.41539300	-1.30977600	-3.45499500
C	-3.07201100	-2.89645100	-1.18373800
H	-3.59171000	-1.93567700	-1.14170300
H	-3.57445300	-3.58499700	-1.86593000
H	-3.01778300	-3.34232900	-0.18937300

trans-7

Zero-point correction= 0.447736 (Hartree/Particle)
Thermal correction to Energy= 0.476056
Thermal correction to Enthalpy= 0.477000
Thermal correction to Gibbs Free Energy= 0.387018
E(solv) = -1833.52061891 A.U.

C	-0.66358000	2.35324600	0.18535500
C	-1.46437700	2.71409500	-0.92318200
C	-1.63797600	4.02475800	-1.34013700
C	-0.98619000	5.00606500	-0.60423000
C	-0.19384900	4.67737600	0.50749400
C	-0.02229100	3.36266400	0.91657900
C	-0.76394300	0.91645400	0.20050000
C	-1.56848800	0.56303300	-0.81534600
H	-2.25863000	4.25707200	-2.19820500
H	-1.09674100	6.04648600	-0.89237400
H	0.29194300	5.47274300	1.06360400
H	0.57306800	3.10924000	1.78614100
O	-2.03290100	1.62103100	-1.52369800
C	-1.91093200	-0.89219000	-0.85103800
H	-1.73642200	-1.34110100	-1.83470600
N	-0.41317900	-0.22802900	0.95365300
C	-3.33022900	-1.19223500	-0.40828100

C	-3.80168900	-0.71606700	0.81845500
C	-4.17005300	-1.96136500	-1.21092000
C	-5.09427700	-1.01388700	1.23411100
H	-3.14966700	-0.11350000	1.44764400
C	-5.46722800	-2.25567400	-0.79733800
H	-3.80643600	-2.33416300	-2.16532700
C	-5.93057800	-1.78362300	0.42642100
H	-5.45126700	-0.64334300	2.18995600
H	-6.11279900	-2.85569300	-1.43128000
H	-6.94039800	-2.01383000	0.75166800
S	0.83079600	-0.28514800	2.05285500
O	0.66825400	-1.54211800	2.75670900
O	0.79138000	1.00337000	2.72176500
C	2.36361800	-0.36338800	1.15305200
C	3.14457100	-1.50971400	1.23418800
C	2.77403200	0.74919000	0.41745100
C	4.37272700	-1.53219900	0.57478500
H	2.79090200	-2.36010200	1.80791400
C	3.99030100	0.69858400	-0.24701200
H	2.15467200	1.64208600	0.37956700
C	4.80811900	-0.43837100	-0.17436800
H	4.99684000	-2.41919100	0.63920500
H	4.32199700	1.55859800	-0.82372600
C	6.12113100	-0.47076000	-0.91208400
H	6.72909400	0.40616800	-0.66997300
H	6.69652400	-1.36513500	-0.66236400
H	5.95674200	-0.46553700	-1.99533700
C	-0.82067000	-1.42196200	0.16086900
C	0.36390600	-2.01630900	-0.59995100
O	0.81051400	-3.11784200	-0.40660700
O	0.83251800	-1.15678000	-1.51157600
C	2.32050700	-0.51068000	-3.24510200
C	1.98655400	-1.59691100	-2.24754900
H	-1.20648100	-2.18928800	0.83199000
H	3.21420800	-0.78802400	-3.81141800
H	1.49705100	-0.36040000	-3.94816500
H	2.51249900	0.43242100	-2.72727100
H	2.79962000	-1.76935700	-1.53675700
H	1.75037700	-2.54965800	-2.73112300

2a-1

Zero-point correction=	0.096505 (Hartree/Particle)
Thermal correction to Energy=	0.104916
Thermal correction to Enthalpy=	0.105860
Thermal correction to Gibbs Free Energy=	0.061226

E(solv) = -2880.73036199 A.U.

Br	2.29348700	-0.07002700	-0.00029200
C	0.48789600	-0.69272000	0.00068700
C	-0.54187500	0.21924000	0.00042000
O	-0.56121300	1.45853600	-0.00057300
O	-1.79416900	-0.47366500	0.00162500
C	-4.14638900	-0.49998900	-0.00212200
C	-2.90607100	0.38005100	0.00154500
H	0.37117600	-1.76265500	0.00166500
H	-5.06103500	0.10410900	-0.00205100
H	-4.15174100	-1.14285800	-0.88792000
H	-4.15426000	-1.14675500	0.88083500
H	-2.89883400	1.03843800	0.88095800
H	-2.89566000	1.04222700	-0.87485100

2a-CO_3

Zero-point correction= 0.126483 (Hartree/Particle)
Thermal correction to Energy= 0.138141
Thermal correction to Enthalpy= 0.139085
Thermal correction to Gibbs Free Energy= 0.086744

E(solv) = -3145.27282467 A.U.

Br	-2.67224900	-0.04334100	-0.17913200
C	-0.83242800	-0.84354500	-0.05692800
C	0.15454200	0.16797200	0.59603100
O	-0.26963200	0.80190200	1.60722100
O	0.50832900	1.02590300	-0.59852200
C	2.77658700	1.87309100	-0.60359800
C	1.31092300	2.10280500	-0.22798300
H	-0.96643700	-1.71518300	0.57901700
H	-0.58308600	-1.12552000	-1.07034400
H	3.14130000	0.95648400	-0.12724100
H	2.87331700	1.74662500	-1.68976000
H	3.40458400	2.72746500	-0.30241200
H	0.94198100	3.01517500	-0.73685600
H	1.20590500	2.26691600	0.85368400
C	2.06958800	-1.40447500	0.01105800
O	1.38813100	-0.55688600	0.90876300
O	1.39321800	-2.09678700	-0.78211200
O	3.30943900	-1.39039800	0.17115500

2a-TS1

Zero-point correction= 0.124730 (Hartree/Particle)
Thermal correction to Energy= 0.136323
Thermal correction to Enthalpy= 0.137267
Thermal correction to Gibbs Free Energy= 0.085331

E(solv) = -3145.26084838 A.U.

Imaginary Frequency 104.86*i*

Br	-2.83888600	-0.09851000	-0.13765200
C	-0.86385200	-0.31426800	-0.25003900
C	-0.15699600	0.95073300	0.14216500
O	-0.50885100	1.73414700	0.99659500
O	0.96903000	1.08585400	-0.57799400
C	3.29927100	1.46565200	-0.76042300
C	2.10390100	1.55707200	0.16446300
H	-0.44376800	-1.04460500	0.49994700
H	-0.61982600	-0.66333200	-1.24691800
H	3.44420500	0.39336500	-0.95272800
H	3.14261600	2.04750800	-1.67960200
H	4.18910000	1.85707700	-0.24950300
H	1.90408400	2.58059600	0.51389600
H	2.22186600	0.85158000	0.99797700
C	1.86252800	-1.58698200	0.24328000
O	1.14998800	-1.12401300	1.26325600
O	1.27438400	-2.26587700	-0.67122400
O	3.12215500	-1.30606000	0.20162500

INT1-A

Zero-point correction= 0.444646 (Hartree/Particle)

Thermal correction to Energy= 0.475879

Thermal correction to Enthalpy= 0.476823

Thermal correction to Gibbs Free Energy= 0.376916

E(solv) = -4407.83508942 A.U.

C	1.76685000	5.32102500	0.13335500
C	3.10442500	4.99167900	0.41029600
C	3.50265800	3.66861300	0.56106500
C	2.51620900	2.70017900	0.42633300
C	1.17194200	3.00274000	0.15799900
C	0.79118400	4.34083400	0.00477100
O	2.70954200	1.36025500	0.53086500
C	1.46237100	0.79353300	0.34281600
C	0.48857500	1.71773200	0.10013100
C	1.22053500	-0.67679100	0.39376600
C	0.80963200	-1.18597300	-1.01625300
Br	2.28131700	-1.11566900	-2.27633400
N	-0.80302000	1.32714100	-0.18420800
C	-3.34183300	1.16377800	0.08928700
C	-4.04608400	0.98370800	1.27073100
C	-5.07721300	0.04677900	1.31999300
C	-5.41147100	-0.71297200	0.19893000
C	-4.69466200	-0.50618600	-0.98630200

C	-3.66595100	0.42563200	-1.04686700
C	-6.49688600	-1.75886600	0.26458700
S	-1.99676100	2.34883900	0.03669200
O	-2.27232800	3.22633800	-1.11715500
O	-1.98755800	3.03325600	1.34358500
C	2.26286800	-1.55627600	1.04528400
C	1.83536600	-2.58489400	1.88985500
C	2.74593100	-3.45947200	2.47616800
C	4.10656500	-3.31415100	2.22446900
C	4.54361000	-2.29322100	1.38418500
C	3.63265100	-1.42122600	0.79514100
C	0.22050400	-2.58397300	-0.96006000
O	0.61235500	-3.58206600	-1.50488800
O	-0.87075900	-2.54537000	-0.17244800
C	-2.78636800	-3.47594300	0.84430000
C	-1.57734100	-3.77697200	-0.01684600
H	1.49210100	6.36562400	0.01781000
H	3.84203600	5.78344000	0.50875600
H	4.53025800	3.39178900	0.77318000
H	-0.24230100	4.59222100	-0.21382300
H	0.28173000	-0.77842000	0.95619400
H	0.04610900	-0.49465300	-1.38490800
H	-3.76990600	1.58033300	2.13450000
H	-5.63053700	-0.09831500	2.24564600
H	-4.95239400	-1.08545100	-1.87104400
H	-3.10950700	0.59254900	-1.96420600
H	-7.17711400	-1.57278300	1.10082400
H	-7.08764000	-1.77904700	-0.65668300
H	-6.07155600	-2.76082400	0.40159900
H	0.77117800	-2.69334800	2.08953300
H	2.39158500	-4.25010900	3.13165500
H	4.82306500	-3.99222700	2.67982900
H	5.60460400	-2.17265400	1.18391100
H	3.97741500	-0.62872000	0.14189700
H	-3.39009100	-4.37885600	0.97890800
H	-2.47537200	-3.11181400	1.82725900
H	-3.39857200	-2.69900600	0.37696900
H	-1.85758800	-4.15284700	-1.00628400
H	-0.90869300	-4.51504500	0.44004500

INT1-B

Zero-point correction=	0.445316 (Hartree/Particle)
Thermal correction to Energy=	0.476129
Thermal correction to Enthalpy=	0.477073
Thermal correction to Gibbs Free Energy=	0.379892

E(solv) = -4407.84042104 A.U.

C	2.44931400	5.00883000	0.10196200
C	1.71473300	5.27359900	1.26968900
C	0.71275400	4.41191300	1.70717300
C	0.47863800	3.28435100	0.93013000
C	1.19886100	3.00127500	-0.23131000
C	2.19965600	3.87209600	-0.65764600
O	-0.43543700	2.31393700	1.16130200
C	-0.28949800	1.38110900	0.12698800
C	0.69009100	1.74282800	-0.76464500
C	-1.26194400	0.25948900	0.15999200
C	-1.51951500	-0.31598700	1.56238200
Br	0.14609500	-0.76120300	2.48906300
N	1.22485000	1.27949500	-1.94424800
C	2.21979700	-1.15067800	-1.33431300
C	1.68707000	-1.97026900	-0.35086500
C	2.54004400	-2.61813100	0.54394000
C	3.92059600	-2.46217000	0.46068700
C	4.44078900	-1.63955200	-0.54808600
C	3.60184800	-0.98224900	-1.43485600
C	4.84386000	-3.14164700	1.44107700
S	1.16214400	-0.21242300	-2.45139900
O	1.82450900	-0.27822900	-3.75625600
O	-0.15489000	-0.89064800	-2.36206500
C	-2.62212000	0.59819600	-0.44130600
C	-3.11644900	-0.18463600	-1.48719600
C	-4.37679600	0.07250500	-2.02180900
C	-5.15263200	1.11245100	-1.51850300
C	-4.65802400	1.90448900	-0.48360800
C	-3.40039100	1.64832800	0.05330700
C	-2.33685300	-1.58953300	1.43770100
O	-3.39643200	-1.79530500	1.97275700
O	-1.74106200	-2.43902700	0.59073000
C	-1.69165500	-4.20084500	-0.96538600
C	-2.51706200	-3.54282800	0.12125000
H	3.22446300	5.70511400	-0.20596600
H	1.93289600	6.16877400	1.84563900
H	0.14030800	4.60267100	2.60899300
H	2.75436500	3.64151700	-1.56186000
H	-0.83885200	-0.53201700	-0.45502400
H	-2.04355700	0.37785900	2.21737200
H	0.61242400	-2.11396500	-0.28636900
H	2.11256200	-3.24113500	1.32733300
H	5.51912200	-1.51500900	-0.62945400
H	3.99573700	-0.34147800	-2.21827600

H	4.31571500	-3.90810100	2.01555700
H	5.68573400	-3.62062600	0.92976000
H	5.26280900	-2.42169200	2.15365200
H	-2.47762600	-0.95951000	-1.90310600
H	-4.74687000	-0.53550300	-2.84278100
H	-6.13535500	1.31268800	-1.93670500
H	-5.25395900	2.72597800	-0.09526900
H	-3.00437300	2.27438600	0.84932100
H	-2.25432500	-5.01257200	-1.43561000
H	-1.41722100	-3.46274500	-1.72578400
H	-0.76740100	-4.61052500	-0.54820000
H	-2.73278600	-4.21650500	0.95719600
H	-3.46954300	-3.15663100	-0.25771200

INT2-A-1

Zero-point correction= 0.444623 (Hartree/Particle)
Thermal correction to Energy= 0.473302
Thermal correction to Enthalpy= 0.474246
Thermal correction to Gibbs Free Energy= 0.384551
E(solv) = -1833.50761404 A.U.

C	-3.07265600	-0.66171700	0.04917200
C	-3.99521300	0.32788100	0.41615900
C	-5.36811900	0.12659100	0.34873200
C	-5.79552500	-1.11459200	-0.10520400
C	-4.89038700	-2.12116800	-0.47712100
C	-3.52271200	-1.90980900	-0.40080700
C	-1.75571100	-0.08267300	0.28797600
C	-2.03093100	1.32041800	0.70199500
H	-6.05815300	0.90944100	0.64038800
H	-6.86138000	-1.31038800	-0.17245200
H	-5.26719800	-3.07662000	-0.82448500
H	-2.82007800	-2.68749800	-0.67639000
O	-3.42427300	1.48427900	0.84110400
C	-1.23203200	2.47954400	0.14306900
H	-1.87015500	3.35355700	0.01697600
N	-0.53288400	-0.46220800	0.20350200
C	-0.21386800	2.31618200	-0.94797500
C	-0.54028700	1.60478000	-2.10570800
C	1.02386200	2.95798300	-0.87556700
C	0.35378200	1.52877100	-3.16970500
H	-1.49529700	1.08888800	-2.17038300
C	1.92051500	2.88363600	-1.93892700
H	1.28738500	3.50561100	0.02301400
C	1.58832800	2.17052500	-3.08922300
H	0.08812600	0.95599100	-4.05234600

H	2.87899900	3.38998100	-1.86877100
H	2.28821000	2.11229500	-3.91740300
S	-0.14449300	-1.94349900	-0.46902900
O	-0.51694300	-1.90882100	-1.87990600
O	-0.61203600	-3.04682800	0.36263200
C	1.61608000	-1.82071800	-0.31570900
C	2.27073800	-0.80609700	-1.01116800
C	2.29491100	-2.69165400	0.52313400
C	3.64272900	-0.67551600	-0.85838000
H	1.70835300	-0.12508600	-1.64445900
C	3.67302900	-2.53768700	0.66884300
H	1.74548600	-3.45865000	1.05925600
C	4.36142100	-1.53419800	-0.01525600
H	4.16603700	0.11485300	-1.39166500
H	4.21983000	-3.20616400	1.32819500
C	5.85316900	-1.37887200	0.13091100
H	6.13657800	-0.32294800	0.17616600
H	6.21844700	-1.87244000	1.03493200
H	6.37463800	-1.82133600	-0.72488300
C	-1.10404900	2.08935900	1.59379000
C	0.03841800	1.33264000	2.23006100
O	-0.12808600	0.54553400	3.12486700
O	1.22324300	1.67864000	1.72809600
C	3.58906100	1.60701200	1.66995700
C	2.34798900	0.91264900	2.18721000
H	-1.62305700	2.73137500	2.30050700
H	4.47756900	1.02121400	1.92376800
H	3.53609300	1.70731900	0.58234500
H	3.68816100	2.60303100	2.11089900
H	2.32314600	0.86141500	3.27892100
H	2.24984500	-0.10442500	1.79193800

INT2-A

Zero-point correction= 0.444643 (Hartree/Particle)
Thermal correction to Energy= 0.473664
Thermal correction to Enthalpy= 0.474609
Thermal correction to Gibbs Free Energy= 0.382192
E(solv) = -1833.49973911 A.U.

C	-2.88728000	-4.36289000	0.28521100
C	-4.16031500	-3.80762700	0.49249800
C	-4.36741300	-2.43538900	0.50155700
C	-3.25082900	-1.63492000	0.29610000
C	-1.96854500	-2.16282500	0.09258600
C	-1.78206800	-3.55285300	0.08161000
O	-3.30231400	-0.28109900	0.27105600

C	-1.99335400	0.17008800	0.03870100
C	-1.09486700	-1.01085300	-0.11566400
C	-1.57445900	1.42711200	0.77962700
C	-1.76584700	1.44340800	-0.71222000
N	0.14802600	-0.81003600	-0.37674900
C	2.72882400	-1.26264300	-0.59165600
C	3.48488200	-1.41175000	-1.74600800
C	4.70308700	-0.74432700	-1.83538600
C	5.16072900	0.06194900	-0.79069000
C	4.36874000	0.19567300	0.35549200
C	3.15449200	-0.46742900	0.46740700
C	6.49612300	0.75403100	-0.88436900
S	1.18997100	-2.12412700	-0.43687900
O	1.16611500	-2.80512800	0.85355300
O	0.95897700	-2.89381600	-1.65438900
C	-0.24631200	1.59207700	1.44662400
C	0.78954600	2.31341800	0.85388500
C	1.98695100	2.52195100	1.53284000
C	2.16552500	1.99878400	2.81051200
C	1.14545600	1.25253600	3.39941400
C	-0.05295200	1.05318000	2.72182200
C	-2.94273000	2.15216200	-1.33860500
O	-3.89696800	1.58210100	-1.78520400
O	-2.88413600	3.49977800	-1.38408400
C	-2.00594100	5.68070800	-1.14477600
C	-1.72407900	4.20690400	-0.94104900
H	-2.76838000	-5.44064700	0.28267100
H	-5.00771900	-4.46904700	0.64654600
H	-5.34446000	-1.99116200	0.64983400
H	-0.80087600	-3.98373000	-0.07598100
H	-2.42249200	1.82264300	1.33994100
H	-0.85015600	1.42652700	-1.30420500
H	3.11603100	-2.03823200	-2.55179100
H	5.30757700	-0.84890800	-2.73256700
H	4.70849400	0.82851200	1.17208600
H	2.53702900	-0.36407300	1.35633400
H	6.74750400	0.99397900	-1.92085100
H	6.50455700	1.68098400	-0.30467100
H	7.29206800	0.11170500	-0.49132200
H	0.66155700	2.71604600	-0.14674200
H	2.78293100	3.08686300	1.05707800
H	3.09779500	2.16345200	3.34276000
H	1.28176700	0.82707700	4.38872500
H	-0.84948600	0.47429300	3.18264500
H	-1.14537300	6.27576800	-0.82821500

H	-2.20921400	5.88591400	-2.19825000
H	-2.87740200	5.98219400	-0.55904300
H	-1.52172200	3.98531200	0.11259800
H	-0.85332800	3.89329100	-1.53049000

INT2-B-1

Zero-point correction= 0.444309 (Hartree/Particle)
Thermal correction to Energy= 0.472596
Thermal correction to Enthalpy= 0.473540
Thermal correction to Gibbs Free Energy= 0.382166
E(solv) = -1833.51037382 A.U.

C	-1.54670300	2.30367400	0.01434900
C	-2.87536600	1.97562700	0.31580300
C	-3.87583200	2.93351900	0.42580200
C	-3.49983900	4.25426400	0.22136500
C	-2.17588100	4.60890700	-0.08275300
C	-1.18812700	3.64316000	-0.19263000
C	-0.82809800	1.03321400	-0.03997400
C	-1.84507900	0.01331200	0.35150600
H	-4.89334000	2.64471600	0.66087300
H	-4.25219400	5.03326500	0.29948000
H	-1.92377200	5.65242400	-0.23462900
H	-0.16729900	3.91622400	-0.42990900
O	-3.09361300	0.64755800	0.48663500
C	-1.53430800	-1.12682400	1.27745000
H	-2.40592600	-1.37460200	1.88419400
N	0.36371200	0.64241000	-0.31435100
C	-0.19877700	-1.31396100	1.92403100
C	0.30123800	-0.34926900	2.80248800
C	0.53344900	-2.48014900	1.70507400
C	1.50390700	-0.55934900	3.46942900
H	-0.25096600	0.57526300	2.95248200
C	1.73637600	-2.69496300	2.37473300
H	0.15312900	-3.22601300	1.01218200
C	2.22056300	-1.73830100	3.26354500
H	1.88575400	0.20132500	4.14272000
H	2.29317100	-3.61107300	2.20199300
H	3.15756100	-1.90366000	3.78667000
S	1.55743300	1.78331700	-0.60504600
O	1.75482000	2.55887300	0.61556500
O	1.30522100	2.49119800	-1.85642700
C	2.92971300	0.69065400	-0.84235000
C	3.21543400	-0.25422300	0.14070500
C	3.71188600	0.82370700	-1.97924900
C	4.31238300	-1.08311800	-0.03292300

H	2.57748700	-0.34170700	1.01555600
C	4.81494900	-0.01460300	-2.13129800
H	3.45090600	1.56445900	-2.72796000
C	5.12806600	-0.97341200	-1.16776500
H	4.54042200	-1.83062400	0.72339000
H	5.43851900	0.07621900	-3.01628400
C	6.31495000	-1.88674900	-1.33594500
H	7.00088100	-1.79729600	-0.48761600
H	5.99804600	-2.93337900	-1.39069800
H	6.87039900	-1.65373500	-2.24737800
C	-1.77482100	-1.39966800	-0.18049600
C	-3.06586500	-2.05189400	-0.55470500
O	-4.02326000	-2.14164200	0.17384200
O	-3.01801100	-2.51270500	-1.81083300
C	-4.30387900	-4.58244900	-1.78655100
C	-4.21407800	-3.15330800	-2.28825100
H	-0.91871300	-1.57985200	-0.82485500
H	-5.17917700	-5.07477600	-2.21967400
H	-3.41212300	-5.14498200	-2.07509200
H	-4.40143000	-4.59723400	-0.69895300
H	-5.07769800	-2.56565400	-1.96881100
H	-4.12736800	-3.11229100	-3.37509100

INT2-B

Zero-point correction= 0.444478 (Hartree/Particle)
Thermal correction to Energy= 0.473589
Thermal correction to Enthalpy= 0.474533
Thermal correction to Gibbs Free Energy= 0.380444
E(solv) = -1833.50690567 A.U.

C	-1.11809700	2.18554200	-0.61913300
C	-2.50384000	2.04352500	-0.45073500
C	-3.39893500	3.07591800	-0.70197300
C	-2.85863000	4.28282400	-1.12440500
C	-1.47567900	4.45482900	-1.29195900
C	-0.59369200	3.41462500	-1.04561700
C	-0.54422100	0.89065700	-0.26177500
C	-1.71069200	0.07584300	0.18183300
H	-4.46345700	2.92878800	-0.56332200
H	-3.52530100	5.11531600	-1.32813000
H	-1.09284900	5.41425600	-1.62156700
H	0.47240200	3.53822900	-1.18966400
O	-2.88881600	0.81525300	-0.02325500
C	-1.74722600	-1.42749600	0.11420600
H	-0.81146500	-1.84348400	-0.26238200
N	0.61922800	0.34479800	-0.20921200

C	-3.00995200	-2.12544800	-0.27485200
C	-3.60001000	-1.87386100	-1.51490400
C	-3.59448500	-3.05491000	0.58546400
C	-4.75859500	-2.54595200	-1.88987700
H	-3.15004900	-1.14191500	-2.18008700
C	-4.75262900	-3.73018700	0.20982400
H	-3.13230600	-3.25109700	1.54946500
C	-5.33659700	-3.47596000	-1.02814800
H	-5.21328800	-2.34118800	-2.85414000
H	-5.19873000	-4.45397500	0.88482100
H	-6.24144600	-3.99952200	-1.32075800
S	2.01191500	1.21614000	-0.49021600
O	2.32484300	1.94092800	0.74018300
O	1.95362500	1.96441800	-1.74362400
C	3.15544000	-0.12050700	-0.70955600
C	3.14222800	-1.21280400	0.15785200
C	4.09821300	-0.00508500	-1.72261500
C	4.10237700	-2.20078600	-0.00787800
H	2.37971200	-1.30306700	0.92717400
C	5.05491300	-1.00651200	-1.86658200
H	4.06978500	0.85088600	-2.38868000
C	5.07113700	-2.11183800	-1.01569400
H	4.09876800	-3.06256900	0.65442900
H	5.79695800	-0.92822700	-2.65621600
C	6.09599000	-3.20445200	-1.17782400
H	6.62036700	-3.39243700	-0.23588800
H	5.61966000	-4.14318700	-1.47942200
H	6.83884400	-2.94431600	-1.93552600
C	-1.62039200	-0.75548100	1.44025000
C	-0.30525200	-0.78300600	2.17399200
O	0.44361200	-1.72897400	2.20078900
O	-0.08772800	0.38125200	2.78085100
C	1.30194800	1.96813200	3.86992000
C	1.19350600	0.52862500	3.42339200
H	-2.51105600	-0.69008700	2.06095500
H	2.25611200	2.12391400	4.38026800
H	1.26504100	2.62532600	2.99856000
H	0.49144400	2.22609600	4.55681200
H	1.24774200	-0.18129800	4.25460400
H	1.97261100	0.28129600	2.69785000

N-INT3-RR-2

Zero-point correction=	0.637125 (Hartree/Particle)
Thermal correction to Energy=	0.672778
Thermal correction to Enthalpy=	0.673722

Thermal correction to Gibbs Free Energy= 0.567489

E(solv) = -2178.80526130 A.U.

C	-0.34189000	3.41226200	0.37873600
C	-1.73566900	3.47791100	0.33264900
C	-2.44501400	4.65627900	0.13535500
C	-1.68958400	5.81061200	-0.02185700
C	-0.28595100	5.77507700	0.02425200
C	0.40418400	4.58775500	0.22562700
C	-0.00732800	2.00483400	0.60809600
C	-1.21682400	1.36090200	0.68917600
H	-3.52932300	4.66182000	0.11154600
H	-2.19440700	6.75899200	-0.17950900
H	0.26974700	6.69952300	-0.09759600
H	1.48825900	4.55554100	0.26135600
O	-2.28059800	2.25073800	0.52265900
C	-1.77655500	-0.03083600	0.80975200
H	-2.76937900	0.16319400	1.22973200
N	1.22829300	1.41422400	0.76037600
C	-1.15063000	-1.06908700	1.72969000
C	0.21010400	-1.12215600	2.04043100
C	-1.99757700	-2.05938000	2.24634000
C	0.71127700	-2.17072000	2.81160600
H	0.87151500	-0.33787300	1.67527000
C	-1.49502500	-3.10455400	3.01329400
H	-3.06854100	-2.00547400	2.05826400
C	-0.13080600	-3.17018100	3.28914200
H	1.77462300	-2.19844500	3.03287200
H	-2.16982700	-3.86119000	3.40182500
H	0.26656800	-3.98597500	3.88539900
S	2.41999200	1.81767800	-0.21246500
O	3.13750200	3.05452900	0.12711000
O	2.05883800	1.68328600	-1.64602300
C	3.52636300	0.45491900	0.14709300
C	4.24175200	-0.11655000	-0.89717900
C	3.70377500	0.00357000	1.45503100
C	5.12192700	-1.16644000	-0.63536300
H	4.10492300	0.26849000	-1.90372100
C	4.58378600	-1.04202800	1.70133700
H	3.14610300	0.47375200	2.25967500
C	5.30234800	-1.64567800	0.66129500
H	5.68042100	-1.61556700	-1.45296900
H	4.72646000	-1.39573100	2.72049000
C	6.24505500	-2.78645800	0.94952000
H	5.69859400	-3.67715800	1.27885600
H	6.82344400	-3.05719800	0.06259000

H	6.94858500	-2.52358000	1.74574300
C	-2.19311700	-0.60931900	-0.60690700
C	-3.41925300	-1.52284600	-0.49491400
O	-3.52209700	-2.65770800	-0.89791300
O	-4.41012300	-0.86504100	0.10092500
C	-6.59535700	-0.69135700	1.01723000
C	-5.63416300	-1.60500200	0.29223700
H	-2.52649600	0.26978100	-1.17150300
H	-7.54119700	-1.21189000	1.18743200
H	-6.18551700	-0.38898300	1.98402900
H	-6.79357700	0.20704600	0.42804200
H	-6.00631800	-1.91458900	-0.68830900
H	-5.40193000	-2.50827800	0.86423300
N	-1.12141100	-1.24131800	-1.47847600
C	-0.63142900	-2.60827000	-1.01946200
C	1.01505400	-0.80013800	-2.68950000
C	-0.61617100	-2.18230000	-3.72251000
C	-1.64766100	-1.38115200	-2.89325500
C	0.08757600	-0.31384000	-1.55527800
C	0.61780300	-2.97328200	-1.85394100
N	0.68873900	-2.17468800	-3.07443300
H	-0.41253100	-2.54450500	0.04374300
H	-1.45484800	-3.30026800	-1.17731300
H	2.04749900	-0.74798000	-2.34468000
H	0.93170600	-0.15076700	-3.56494600
H	-0.52965100	-1.74054600	-4.71910700
H	-0.94273900	-3.22000600	-3.84176100
H	-1.77028700	-0.36016900	-3.26493200
H	-2.61611500	-1.87626900	-2.85053900
H	-0.27440800	0.70105200	-1.71923400
H	0.57119900	-0.33897300	-0.57661600
H	1.53306300	-2.79356600	-1.28145000
H	0.58097500	-4.03628800	-2.11015000

N-INT3-SR-2

Zero-point correction= 0.637410 (Hartree/Particle)
Thermal correction to Energy= 0.672741
Thermal correction to Enthalpy= 0.673685
Thermal correction to Gibbs Free Energy= 0.568907
E(solv) = -2178.80556335 A.U.

C	0.46165300	2.81081000	0.98805100
C	1.85157800	2.70579300	1.00451800
C	2.70863500	3.79920300	1.02419500
C	2.10274100	5.04963000	1.02213500
C	0.70324400	5.18593300	0.99863400

C	-0.13094700	4.07738600	0.97975400
C	-0.04797400	1.44328700	0.97851900
C	1.05684200	0.64358300	0.96334400
H	3.78651900	3.67649400	1.04338500
H	2.72451800	5.93949000	1.03445700
H	0.27153700	6.18164300	0.98767500
H	-1.21042100	4.16434100	0.92637500
O	2.23322700	1.39311500	0.99485500
C	1.08104400	-0.84952300	0.91241500
H	0.03265000	-1.07313600	1.14511100
N	-1.36430000	1.00772300	0.98952200
C	1.92049100	-1.56080300	1.97559200
C	2.93090200	-0.94537800	2.71578400
C	1.63242400	-2.90817600	2.23111200
C	3.64846900	-1.66853300	3.66918500
H	3.15347800	0.10359800	2.55940900
C	2.34682200	-3.62906600	3.18046000
H	0.81632800	-3.38611900	1.69067100
C	3.36598200	-3.00970800	3.90155600
H	4.42991100	-1.17191200	4.23644100
H	2.09894100	-4.66946300	3.36747600
H	3.92552200	-3.56675000	4.64645000
S	-2.03397800	1.22626800	-0.43167000
O	-1.42367800	0.36115700	-1.48269800
O	-2.17960700	2.63052400	-0.85398200
C	-3.67185800	0.57811100	-0.14533400
C	-4.38196800	0.08762000	-1.23670300
C	-4.24810400	0.60721300	1.12090700
C	-5.67317800	-0.39689600	-1.05162500
H	-3.91025000	0.07551600	-2.21546900
C	-5.53835200	0.11562600	1.29169800
H	-3.66590300	0.98474600	1.95490000
C	-6.26894100	-0.39047600	0.21267800
H	-6.22843200	-0.78789100	-1.90091800
H	-5.98788700	0.12225900	2.28179400
C	-7.67853400	-0.89011600	0.40423100
H	-8.39824700	-0.06873300	0.31435400
H	-7.94045400	-1.64042400	-0.34689500
H	-7.81110100	-1.33556100	1.39414200
C	1.27281100	-1.56514800	-0.48684500
C	-0.04920900	-1.92059300	-1.20410000
O	-0.19773500	-1.98373800	-2.40062300
O	-0.93314100	-2.32719300	-0.31185600
C	-3.15990300	-2.80064100	0.36338100
C	-2.24783300	-2.63749300	-0.82970900

H	1.71563100	-2.54442100	-0.26336500
H	-4.19091700	-2.93024600	0.02221800
H	-2.87402500	-3.66727700	0.96632000
H	-3.11768300	-1.90220800	0.98432300
H	-2.53986500	-1.80294800	-1.46920600
H	-2.16872400	-3.54571900	-1.43546100
N	2.26467200	-0.94006700	-1.44781100
C	3.56495800	-0.65821900	-0.72049400
C	2.90557100	1.04982500	-2.76678800
C	3.45399800	-1.10468100	-3.61531400
C	2.64380300	-1.90022700	-2.56585500
C	1.72344300	0.33379900	-2.08576600
C	4.63160600	-0.23785200	-1.76044700
N	4.00602200	0.11513300	-3.03156400
H	3.37276300	0.13276500	-0.00289000
H	3.82788900	-1.57204400	-0.18081400
H	3.28698500	1.85742800	-2.13466000
H	2.57100100	1.49273200	-3.70834700
H	2.81703800	-0.82629400	-4.45927900
H	4.26728100	-1.72687300	-4.00001100
H	1.73269900	-2.32136000	-2.97748100
H	3.23828500	-2.68599200	-2.09061900
H	0.94642800	0.01061500	-2.77868900
H	1.23747000	0.92764400	-1.31317200
H	5.18722000	0.62373500	-1.38128600
H	5.34887200	-1.04409900	-1.94180400

N-TS4-A-1

Zero-point correction= 0.633263 (Hartree/Particle)
Thermal correction to Energy= 0.669275
Thermal correction to Enthalpy= 0.670220
Thermal correction to Gibbs Free Energy= 0.562993
E(solv) = -2178.76574656 A.U.
Imaginary Frequency 474.38*i*

C	-1.36506400	2.95212200	-0.78696700
C	-0.28915100	3.64296900	-1.35504500
C	-0.28413200	5.01629700	-1.56399700
C	-1.41810600	5.70806600	-1.16203400
C	-2.50883700	5.04519000	-0.57712600
C	-2.50029600	3.67120600	-0.38509700
C	-0.95863700	1.54190600	-0.73661200
C	0.34037400	1.53791900	-1.27493500
H	0.56948800	5.50791400	-2.01685700
H	-1.46106500	6.78383000	-1.30344500
H	-3.37921300	5.61860200	-0.27592300

H	-3.35444500	3.16640400	0.05033800
O	0.73800700	2.81436200	-1.66784300
C	1.40994800	0.49933000	-1.44821300
H	2.17109100	0.97970800	-2.06880800
N	-1.54070700	0.43710900	-0.26960200
C	1.16000200	-0.88731600	-1.99715800
C	0.20831200	-1.77761400	-1.49118700
C	1.97440000	-1.30079000	-3.05737600
C	0.09400400	-3.05511100	-2.03199300
H	-0.45294500	-1.46303800	-0.69404700
C	1.86117300	-2.58035600	-3.59419900
H	2.70585100	-0.60964000	-3.47283600
C	0.91925200	-3.46460100	-3.07652800
H	-0.65695800	-3.72910700	-1.62976800
H	2.50068800	-2.87945800	-4.41913200
H	0.82130500	-4.46253700	-3.49319500
S	-3.04518700	0.45996900	0.32589500
O	-4.03395800	1.02125000	-0.60016200
O	-3.07115700	0.99160500	1.69931200
C	-3.33825500	-1.29641700	0.40600800
C	-4.49605200	-1.80164300	-0.16915300
C	-2.43359100	-2.13254300	1.05740400
C	-4.75169900	-3.16837100	-0.08987900
H	-5.17109500	-1.12344100	-0.68094900
C	-2.70122200	-3.49451200	1.12033200
H	-1.51919500	-1.72562100	1.48183300
C	-3.86385400	-4.03054700	0.55450200
H	-5.65434100	-3.57224400	-0.54146000
H	-1.99641300	-4.15679000	1.61769200
C	-4.16035500	-5.50459300	0.66349500
H	-4.79180700	-5.84470400	-0.16170700
H	-3.24070200	-6.09649000	0.65800600
H	-4.68857000	-5.72707900	1.59753900
C	1.74237200	0.76105000	-0.02065600
C	0.91151300	0.27323400	1.14228200
O	0.67840100	-0.88943000	1.38368300
O	0.57117700	1.29379600	1.91463200
C	-0.85723600	2.30814100	3.51790200
C	-0.27772500	0.99567200	3.04710100
H	2.18964900	1.73815200	0.14940000
H	-1.51352500	2.12804500	4.37332800
H	-0.07042500	3.00737300	3.81509400
H	-1.45798700	2.74445600	2.71676600
H	-1.06812400	0.32000600	2.71862400
H	0.33813200	0.50097500	3.80723000

N	5.70604900	-1.12311200	1.18563000
C	5.84406400	-0.28308400	-0.00321200
C	3.71157100	0.14146100	1.93119400
C	3.43058400	-1.64261600	0.32308700
C	4.76445000	-2.20730500	0.89232600
C	5.15998400	-0.30884800	2.27125300
C	4.49196900	0.41353400	-0.33555400
N	3.43175300	-0.16972900	0.51081500
H	6.62825200	0.45839100	0.17604500
H	6.16814100	-0.91790000	-0.83337900
H	3.56140900	1.21642200	2.08220500
H	2.96874600	-0.39492100	2.52857300
H	2.54652000	-2.04424200	0.82134200
H	3.33033700	-1.83406500	-0.74833300
H	4.59214500	-2.76258800	1.81965100
H	5.22853800	-2.89286900	0.17718800
H	5.17422500	-0.89522500	3.19443500
H	5.81809800	0.55410100	2.41410200
H	4.52368400	1.49069300	-0.13752500
H	4.20551100	0.26387100	-1.38102400

N-TS4-A

Zero-point correction= 0.633631 (Hartree/Particle)
Thermal correction to Energy= 0.669469
Thermal correction to Enthalpy= 0.670414
Thermal correction to Gibbs Free Energy= 0.563998
E(solv) = -2178.76609348 A.U.
Imaginary Frequency 449.69*i*

C	-1.90964600	2.91994500	-0.10857900
C	-3.08344300	2.20872300	0.18025700
C	-4.23249900	2.80049900	0.68714600
C	-4.18305000	4.17143300	0.89859600
C	-3.02684500	4.91355400	0.60772500
C	-1.88670400	4.30523500	0.10471700
C	-0.97613100	1.92867100	-0.64624500
C	-1.69139700	0.71663700	-0.59546700
H	-5.11729900	2.20956500	0.89593900
H	-5.05757500	4.67877500	1.29412300
H	-3.02570900	5.98423900	0.78262700
H	-0.98897600	4.87472800	-0.10079300
O	-2.97312200	0.88129000	-0.10961700
C	-1.13109100	-0.59320700	-1.03631800
H	-0.39292500	-0.35836700	-1.80930800
N	0.27581300	1.91195800	-1.10729700
C	-2.01819700	-1.71927800	-1.52207700

C	-3.32142100	-1.94770600	-1.06748900
C	-1.52717100	-2.53444300	-2.54865400
C	-4.07839700	-2.99397700	-1.58574500
H	-3.74617800	-1.29631000	-0.31716000
C	-2.27973900	-3.58706700	-3.06268000
H	-0.55205000	-2.32189800	-2.97918300
C	-3.55877100	-3.82770500	-2.57271400
H	-5.08857200	-3.15077700	-1.21868600
H	-1.87172900	-4.20269500	-3.85832100
H	-4.15432300	-4.64280300	-2.97189900
S	1.34003900	3.11140900	-0.87291900
O	1.04932200	3.92646200	0.31128900
O	1.63498000	3.79432900	-2.12909200
C	2.77767600	2.12194600	-0.46800000
C	3.31142400	2.17085600	0.81270000
C	3.34211700	1.30473200	-1.44702200
C	4.42105600	1.38114100	1.11922400
H	2.85391400	2.82232700	1.55057200
C	4.44067300	0.51709000	-1.12495400
H	2.92005100	1.30106900	-2.44809300
C	4.99876800	0.54587600	0.16137700
H	4.84597000	1.41900300	2.11926800
H	4.89235900	-0.11534400	-1.88666200
C	6.22298000	-0.27563800	0.48050800
H	6.33677100	-0.41934000	1.55854900
H	6.17968200	-1.26159200	0.00615400
H	7.12865500	0.22123800	0.11581300
C	-0.42102300	-0.55620900	0.29004800
C	-1.08256500	-0.80145200	1.60757900
O	-0.57500700	-0.50081700	2.66506100
O	-2.25130200	-1.43422200	1.50749800
C	-4.32685400	-2.17522000	2.38963200
C	-2.95474400	-1.64347900	2.74230300
H	0.36149700	0.19691500	0.32477800
H	-4.88137500	-2.40940000	3.30206800
H	-4.89204600	-1.42962000	1.82360300
H	-4.24489900	-3.08299800	1.78559300
H	-2.38181100	-2.34887600	3.35301500
H	-3.00219200	-0.69498900	3.28355500
N	2.99856500	-3.52999800	0.60641000
C	2.92559100	-2.92014200	-0.72281100
C	2.05201100	-1.37731000	1.38774000
C	0.55503200	-3.23587700	0.96435500
C	1.74388000	-4.23913400	0.87170800
C	3.14959900	-2.45487900	1.59124900

C	1.62225700	-2.08492200	-0.86333800
N	1.01874200	-1.92374800	0.47492100
H	3.80593100	-2.28104200	-0.84973800
H	2.96506900	-3.70810700	-1.48098400
H	2.45368500	-0.47683000	0.91066500
H	1.56588500	-1.08483100	2.31980200
H	0.21860900	-3.09646400	1.99721100
H	-0.30474200	-3.53924100	0.35722000
H	1.84799300	-4.80249900	1.80363300
H	1.58413100	-4.95892500	0.06281100
H	3.08828500	-2.89875900	2.58996700
H	4.14393800	-2.00958400	1.48187400
H	1.81248400	-1.08407100	-1.26842900
H	0.88579000	-2.59100700	-1.49084300

N-TS4-B-1

Zero-point correction= 0.632990 (Hartree/Particle)
Thermal correction to Energy= 0.668871
Thermal correction to Enthalpy= 0.669815
Thermal correction to Gibbs Free Energy= 0.564617
E(solv) = -2178.76784910 A.U.
Imaginary Frequency 426.25*i*

C	-3.37517500	-0.06243000	0.64963100
C	-3.66937800	-1.31166100	0.09493500
C	-4.90771600	-1.64151900	-0.44537700
C	-5.88454500	-0.65750600	-0.39469000
C	-5.63085200	0.59671900	0.18836900
C	-4.38687700	0.90700600	0.71562600
C	-1.97977100	-0.13246200	1.08962100
C	-1.57512000	-1.45271900	0.75542500
H	-5.08544800	-2.62246700	-0.87132700
H	-6.86796200	-0.86460600	-0.80550300
H	-6.42440100	1.33545500	0.22450400
H	-4.19180400	1.88030000	1.14718300
O	-2.61546600	-2.16167800	0.16719500
C	-0.23809700	-2.13522100	0.65226400
H	-0.41843400	-3.10240100	0.17531800
N	-1.15313600	0.75536400	1.64085300
C	0.71728500	-2.28984800	1.80721100
C	0.88010800	-1.31853900	2.79907900
C	1.49354200	-3.45150300	1.85754100
C	1.82637100	-1.50547200	3.80379400
H	0.27289500	-0.41824300	2.76969200
C	2.44177500	-3.63313600	2.86101100
H	1.35022300	-4.22360300	1.10450900

C	2.61371900	-2.65452300	3.83576200
H	1.94453800	-0.74568000	4.57049700
H	3.03574500	-4.54160800	2.88536300
H	3.34900900	-2.79187500	4.62260200
S	-1.28182700	2.35212200	1.38887600
O	-1.42794800	3.05376100	2.65956700
O	-2.18185600	2.69738500	0.28347300
C	0.37353100	2.70918000	0.79752900
C	0.57952300	2.93554900	-0.55932800
C	1.43420100	2.76417200	1.69843500
C	1.86580100	3.22311400	-1.01497000
H	-0.27042400	2.89954100	-1.23484000
C	2.71238300	3.04854000	1.22865400
H	1.24663300	2.60080100	2.75557800
C	2.94655600	3.28983300	-0.13083800
H	2.02962800	3.41943000	-2.07286300
H	3.54299900	3.09887800	1.92830600
C	4.32376000	3.66214500	-0.62052600
H	4.45525700	4.74981300	-0.61120900
H	5.10344500	3.23258200	0.01491900
H	4.49181400	3.32150900	-1.64679200
C	-0.06590400	-1.09555900	-0.39220700
C	-0.76700200	-1.33325700	-1.69581900
O	-0.75011000	-2.37702700	-2.30488000
O	-1.43662900	-0.24120300	-2.06153100
C	-3.30111400	0.79439800	-3.09115500
C	-2.34571100	-0.37610300	-3.16905800
H	0.09172400	-0.07127600	-0.07147900
H	-4.01328500	0.74874800	-3.91957100
H	-3.85249300	0.77052000	-2.14674700
H	-2.75924100	1.74195300	-3.14448800
H	-1.76453200	-0.38815500	-4.09748900
H	-2.85928300	-1.33703200	-3.07539400
N	4.20152500	-0.67700100	-2.10423300
C	3.81333600	-2.08769300	-2.20664700
C	1.79285900	-0.19260700	-2.41463900
C	2.67442100	-0.34922200	-0.17591600
C	4.13492400	-0.26643300	-0.69912800
C	3.24482400	0.13182600	-2.86114200
C	2.43252700	-2.33220500	-1.52339900
N	1.84113400	-1.02401500	-1.19384500
H	3.77774700	-2.35085200	-3.26859700
H	4.59164500	-2.69798500	-1.73887700
H	1.25329500	-0.76412300	-3.17717500
H	1.21831300	0.71128500	-2.18673600

H	2.24463600	0.64216700	0.00034300
H	2.60603600	-0.91921900	0.75347600
H	4.51686200	0.75654600	-0.61414700
H	4.79619400	-0.92090500	-0.12253900
H	3.47767600	1.18684400	-2.67876000
H	3.37910400	-0.06424100	-3.92938700
H	1.72826400	-2.86892000	-2.16587700
H	2.53716800	-2.88464500	-0.58482700

N-TS4-B

Zero-point correction= 0.633417 (Hartree/Particle)
Thermal correction to Energy= 0.669450
Thermal correction to Enthalpy= 0.670394
Thermal correction to Gibbs Free Energy= 0.563280
E(solv) = -2178.77177055 A.U.
Imaginary Frequency 472.73*i*

C	-1.16873500	2.90499100	0.03767200
C	0.08025400	3.53280200	0.11051500
C	0.28409400	4.87429500	-0.18560100
C	-0.83095200	5.59815800	-0.58439400
C	-2.09569100	4.99619800	-0.67531700
C	-2.28247700	3.65688700	-0.36457600
C	-0.94182400	1.50895800	0.44250000
C	0.44325200	1.44335400	0.67082200
H	1.26989200	5.31869000	-0.10530500
H	-0.72071600	6.65037600	-0.82892800
H	-2.94683900	5.59235200	-0.98720500
H	-3.26584300	3.20606300	-0.42197600
O	1.06043900	2.67960900	0.50718400
C	1.28796500	0.25731000	1.00251900
H	0.60827700	-0.54908300	1.29715300
N	-1.72314500	0.43881600	0.58795800
C	2.41122200	0.42823200	1.99582800
C	3.35624100	1.45448700	1.88524400
C	2.51578700	-0.46997600	3.05999900
C	4.38855900	1.56372400	2.81191900
H	3.27845300	2.17367700	1.07604600
C	3.54904100	-0.36091000	3.98826300
H	1.77426900	-1.25850000	3.16488500
C	4.49080400	0.65539200	3.86389600
H	5.11345900	2.36625700	2.71507500
H	3.61229700	-1.06740100	4.81014600
H	5.29562300	0.74584000	4.58667000
S	-3.27489300	0.53737500	0.12555600
O	-3.37805900	0.69759800	-1.33648800

O	-4.06526000	1.47737900	0.92918300
C	-3.83578900	-1.09974700	0.54123900
C	-4.99333200	-1.22738100	1.29624000
C	-3.15913000	-2.21788400	0.06039500
C	-5.48331600	-2.50111000	1.57374700
H	-5.48636000	-0.33304100	1.66300600
C	-3.66161600	-3.47978100	0.34921300
H	-2.24080200	-2.09400300	-0.50668200
C	-4.83065800	-3.63994000	1.10190200
H	-6.38700800	-2.61055400	2.16822200
H	-3.13842600	-4.36181500	-0.01286500
C	-5.38344300	-5.01574900	1.37435700
H	-6.01681900	-5.01996300	2.26540500
H	-5.99342700	-5.36331200	0.53279700
H	-4.58151100	-5.74504500	1.52087100
C	1.56819000	0.16500400	-0.46187500
C	0.45201900	-0.40814600	-1.29031500
O	-0.08273400	-1.46177300	-1.02549800
O	0.18379100	0.34942700	-2.34421000
C	-1.47143400	1.21684500	-3.81846300
C	-0.95914000	-0.03564400	-3.14785700
H	2.12202700	0.98799800	-0.90905600
H	-2.33705200	0.96619000	-4.43726000
H	-1.79757500	1.92646100	-3.05465700
H	-0.70468400	1.67644300	-4.44862400
H	-0.61947900	-0.79437000	-3.86224100
H	-1.71998600	-0.45834400	-2.49129300
N	4.72206200	-2.90149900	-1.55405200
C	3.76615200	-3.47318500	-0.60173700
C	2.80024900	-1.56846900	-2.37060300
C	4.27976200	-0.60341000	-0.73253800
C	5.33931500	-1.72084000	-0.95153500
C	3.99812800	-2.48240800	-2.75382400
C	2.77620700	-2.38418300	-0.09606500
N	2.93138700	-1.17888400	-0.94389500
H	3.23315900	-4.28571500	-1.10489200
H	4.32095000	-3.90788400	0.23494100
H	1.84657700	-2.09135500	-2.47702400
H	2.75906000	-0.65265400	-2.96948300
H	4.39688600	0.22031000	-1.44516300
H	4.32341500	-0.19266000	0.27773500
H	6.14440400	-1.37005800	-1.60416300
H	5.78811700	-2.01966100	0.00076000
H	4.70069800	-1.95845700	-3.40954200
H	3.64588500	-3.37131100	-3.28522500

H	1.73037300	-2.69558400	-0.15427000
H	2.99523700	-2.08209200	0.93236300

TS1-A

Zero-point correction= 0.632970 (Hartree/Particle)
Thermal correction to Energy= 0.670992
Thermal correction to Enthalpy= 0.671936
Thermal correction to Gibbs Free Energy= 0.559670
E(solv) = -4753.08990167 A.U.
Imaginary Frequency 383.86*i*

C	0.33373300	3.27084700	-0.03551600
C	1.71412700	3.06278300	-0.11396600
C	2.61780100	4.03186100	-0.53319500
C	2.08583100	5.26890900	-0.87667300
C	0.70499400	5.51191200	-0.79199900
C	-0.18120000	4.52715900	-0.37407600
C	-0.23953000	2.01673500	0.45892700
C	0.83199400	1.17521400	0.60781500
H	3.68282400	3.82430400	-0.57695700
H	2.75039200	6.06037800	-1.21213000
H	0.32327800	6.49191500	-1.06303900
H	-1.24820600	4.71493700	-0.31320900
O	2.04215600	1.80611100	0.28353200
C	0.80265200	-0.22107800	1.14352400
H	-0.23376000	-0.26898100	1.51608900
N	-1.51089300	1.67806800	0.80573200
C	1.72034400	-0.49263300	2.33688500
C	2.41186400	0.54825300	2.96370600
C	1.86023500	-1.78737900	2.85488800
C	3.24971000	0.29844600	4.04802500
H	2.29710500	1.56126100	2.59528800
C	2.70149400	-2.03507100	3.93614500
H	1.26700200	-2.59927900	2.44256500
C	3.41051800	-0.99581500	4.53227800
H	3.77881100	1.12480000	4.51466000
H	2.79011700	-3.04712600	4.32160100
H	4.06819800	-1.19111900	5.37470800
S	-2.73263500	2.35711800	0.04960600
O	-2.45324000	2.67120300	-1.36407800
O	-3.37650500	3.45785000	0.79446600
C	-3.92589800	1.01653700	0.07880000
C	-5.27871200	1.32252200	-0.01454700
C	-3.50736600	-0.30802400	0.14020800
C	-6.21257800	0.28991100	-0.06036800
H	-5.58614400	2.36381200	-0.03314800

C	-4.44747700	-1.33066300	0.10821200
H	-2.45218500	-0.52851700	0.24330800
C	-5.81215400	-1.04678000	0.00206800
H	-7.27280100	0.52472900	-0.13429900
H	-4.09833300	-2.35932500	0.18727400
C	-6.82753300	-2.16285800	-0.00709400
H	-6.95949300	-2.58611000	0.99558600
H	-7.80473800	-1.80941900	-0.34984600
H	-6.51191000	-2.98044200	-0.66341600
C	0.85462900	-1.36519800	0.12286100
C	0.00943900	-1.29994400	-1.11788900
O	-0.62875100	-0.34441400	-1.46537400
O	0.07353800	-2.45334600	-1.82239200
C	-1.29500500	-4.25258300	-2.51767600
C	-1.10606200	-2.75170100	-2.58503100
H	1.37424200	-2.28681300	0.32923200
H	-2.20187000	-4.54724100	-3.05407100
H	-0.44169100	-4.77744800	-2.95832600
H	-1.38377800	-4.53601600	-1.46540900
H	-1.95059200	-2.22214400	-2.13453700
H	-0.97594800	-2.38251100	-3.60787500
N	2.68131700	-1.00265300	-1.00849700
C	3.79013700	-0.58208800	-0.11789800
C	3.88001900	0.25291900	-2.75452600
C	4.27005900	-2.08695800	-2.55699500
C	3.07231600	-2.30813600	-1.58940000
C	2.49611600	-0.04266800	-2.12199100
C	5.12288200	-0.60599200	-0.91998300
N	4.86175500	-0.76340300	-2.35293000
H	3.56412400	0.41190100	0.25909500
H	3.81255100	-1.27123700	0.73231300
H	4.25444200	1.22844600	-2.42644800
H	3.81324100	0.27149100	-3.84746100
H	3.94381000	-2.15360200	-3.60065000
H	5.04248900	-2.84783500	-2.40162000
H	2.20948400	-2.74144800	-2.09555200
H	3.34500700	-2.96504900	-0.75575200
H	1.82117200	-0.52037700	-2.83950200
H	2.00292300	0.85440000	-1.74761400
H	5.67920800	0.32419200	-0.76523900
H	5.76587900	-1.43474000	-0.60264000
Br	-1.05342300	-2.78307500	1.01002400

TS1-B

Zero-point correction= 0.633710 (Hartree/Particle)

Thermal correction to Energy= 0.671651

Thermal correction to Enthalpy= 0.672595

Thermal correction to Gibbs Free Energy= 0.560588

E(solv) = -4753.08133386 A.U.

Imaginary Frequency 386.71*i*

C	-0.83867500	3.37330400	-0.42532300
C	0.50118500	3.72826200	-0.25376600
C	0.91995100	5.00157000	0.11348600
C	-0.07732900	5.94932600	0.30662800
C	-1.43273900	5.62293000	0.13272800
C	-1.83034700	4.34327900	-0.23200900
C	-0.84402400	1.95869500	-0.80101500
C	0.47746300	1.59796400	-0.82480800
H	1.97397600	5.22825200	0.23407700
H	0.19739400	6.96081900	0.59290500
H	-2.18596100	6.38999900	0.28724400
H	-2.87853100	4.09413600	-0.36875700
O	1.30796300	2.67272800	-0.50340700
C	1.33067200	0.40478100	-1.17028400
H	2.08540900	0.86203300	-1.81773400
N	-1.92368100	1.13584800	-1.05294400
C	0.76482700	-0.73116200	-2.00952400
C	-0.44301400	-1.38474400	-1.76821000
C	1.56385300	-1.16989400	-3.07088600
C	-0.83615500	-2.45640800	-2.56860300
H	-1.10811900	-1.02890900	-0.99093300
C	1.16932000	-2.23334900	-3.87327300
H	2.53063300	-0.69629700	-3.22817300
C	-0.03539600	-2.88442600	-3.62213400
H	-1.78293900	-2.94859000	-2.36260500
H	1.80878200	-2.55838400	-4.68913800
H	-0.34789800	-3.71883900	-4.24434300
S	-3.24329300	1.35281400	-0.20327800
O	-4.27386200	2.19245400	-0.84141600
O	-3.00119800	1.66036200	1.22712000
C	-3.89340300	-0.31956700	-0.22947500
C	-4.42001200	-0.84596500	0.94271900
C	-3.89679900	-1.07252400	-1.40410100
C	-4.94709500	-2.13734100	0.94485900
H	-4.40834400	-0.23473100	1.84017600
C	-4.42904100	-2.35555900	-1.38906500
H	-3.45510300	-0.65302900	-2.30362000
C	-4.96135500	-2.90756400	-0.21690800
H	-5.35386000	-2.55108300	1.86504500
H	-4.43005300	-2.94687900	-2.30314300

C	-5.54039600	-4.30021500	-0.22571000
H	-4.82580800	-5.02506700	-0.62962300
H	-5.81390500	-4.62134100	0.78322400
H	-6.44072700	-4.34920200	-0.84856500
C	2.21407400	-0.03182800	0.01223200
C	2.83254500	-1.39205800	0.14269700
O	2.56619400	-2.36453100	-0.51561400
O	3.69898600	-1.42199000	1.18198200
C	5.96063900	-1.80433500	1.73969800
C	4.73950300	-2.39804900	1.06921800
H	2.53927000	0.73330700	0.70395200
H	6.80945100	-2.49128700	1.66989500
H	6.20637100	-0.86834000	1.23085600
H	5.76567000	-1.59485900	2.79568200
H	4.41168800	-3.33574200	1.53274800
H	4.92269500	-2.58314400	0.00727300
N	0.80922500	-0.60631300	1.66936900
C	0.50441500	-2.05652000	1.65598200
C	-1.23134800	-0.12850400	3.00175900
C	0.72107300	-0.87499700	4.12450300
C	1.51782200	-0.27973700	2.92734700
C	-0.46624700	0.15351200	1.68151800
C	-0.53112200	-2.37355400	2.76709300
N	-0.62939100	-1.26103900	3.71499000
H	0.14949000	-2.32559100	0.65758400
H	1.44217100	-2.59227100	1.83002500
H	-2.27814600	-0.34876700	2.78338400
H	-1.21219000	0.74665600	3.65883600
H	0.64740900	-0.14497800	4.93761900
H	1.22403800	-1.76514500	4.52043000
H	1.57268900	0.81251400	2.98625500
H	2.53296700	-0.67475600	2.87741200
H	-0.24331300	1.21489300	1.57727000
H	-1.05114000	-0.13949500	0.81000600
H	-1.52645900	-2.53288800	2.33830800
H	-0.24618600	-3.28346000	3.30761900
Br	4.48875600	0.41605300	-1.09606400

TS2-A-1

Zero-point correction= 0.443183 (Hartree/Particle)
Thermal correction to Energy= 0.473994
Thermal correction to Enthalpy= 0.474938
Thermal correction to Gibbs Free Energy= 0.378744
E(solv) = -4407.81538612 A.U.
Imaginary Frequency 457.22*i*

C	2.48585400	-2.08460100	0.18809500
C	3.66502100	-1.43163600	0.56958700
C	4.90472100	-2.06073500	0.59879500
C	4.93457700	-3.39677800	0.22401700
C	3.76799600	-4.07401300	-0.16674300
C	2.53827700	-3.43203300	-0.19094400
C	1.42047200	-1.08364500	0.29599400
C	2.09306500	0.10161300	0.69344200
H	5.79429300	-1.51778400	0.89768300
H	5.88232400	-3.92763300	0.23055200
H	3.83077500	-5.11750800	-0.45809500
H	1.64107800	-3.95820300	-0.49479900
O	3.45332200	-0.13990800	0.90526600
C	1.57255300	1.44832100	1.07871000
H	2.32298800	1.97352600	1.67539700
N	0.11040100	-1.11252300	0.10460300
C	0.21320800	1.53049900	1.72980800
C	-0.07684400	0.65190700	2.77537500
C	-0.71307200	2.51534700	1.38398300
C	-1.27307400	0.75646300	3.47967300
H	0.63786100	-0.12832700	3.02678100
C	-1.91896700	2.60318000	2.07626200
H	-0.47517300	3.20486000	0.57952000
C	-2.20310400	1.73223200	3.12587300
H	-1.48420800	0.06499600	4.29091000
H	-2.63886800	3.36626800	1.79373200
H	-3.14243700	1.81367700	3.66696600
S	-0.65129400	-2.47829700	-0.31377300
O	-0.52047300	-3.52107800	0.71282900
O	-0.39182600	-2.89689000	-1.69837800
C	-2.32572100	-1.86397200	-0.26496000
C	-2.76322600	-1.13757100	0.84000500
C	-3.18249500	-2.15456100	-1.31686800
C	-4.08031800	-0.70152200	0.88312400
H	-2.06437400	-0.88714500	1.63221400
C	-4.50263900	-1.71012800	-1.25812400
H	-2.80304900	-2.70797900	-2.17017900
C	-4.96668600	-0.97895600	-0.16457800
H	-4.41882100	-0.11507000	1.73451700
H	-5.17972200	-1.92600000	-2.08135800
C	-6.37976300	-0.45419500	-0.12662600
H	-6.40650100	0.60855900	-0.39318800
H	-7.02220100	-0.98994200	-0.83100000
H	-6.81273600	-0.55138400	0.87364800
Br	1.60897800	4.16061800	-0.82158700

C	1.85579600	1.64788000	-0.35239300
C	0.99568100	1.27369100	-1.52230100
O	1.46448500	0.86570800	-2.55705900
O	-0.30550700	1.41538000	-1.28405700
C	-2.57716800	1.31523400	-1.91549600
C	-1.17033100	0.91829300	-2.30718400
H	2.88742000	1.82477600	-0.61734800
H	-3.29837800	0.91613300	-2.63539000
H	-2.81606000	0.91917600	-0.92499300
H	-2.66802200	2.40521500	-1.88649800
H	-0.86965200	1.35049700	-3.26623000
H	-1.04577900	-0.16947700	-2.36711700

TS2-A

Zero-point correction= 0.443612 (Hartree/Particle)
Thermal correction to Energy= 0.474833
Thermal correction to Enthalpy= 0.475777
Thermal correction to Gibbs Free Energy= 0.376087
E(solv) = -4407.80890505 A.U.
Imaginary Frequency 395.56*i*

C	0.23658200	2.97696400	0.05437300
C	1.62938600	2.89825600	-0.09040700
C	2.41277800	3.98141200	-0.46972000
C	1.75047600	5.18000100	-0.69956700
C	0.35766900	5.28768300	-0.55359400
C	-0.41167500	4.19562800	-0.17888300
C	-0.18809300	1.64705600	0.48566400
C	1.00595900	0.88977400	0.51257500
H	3.48695500	3.87771500	-0.57685700
H	2.32402900	6.05249700	-0.99946600
H	-0.12454700	6.24132700	-0.74367100
H	-1.48952800	4.26657100	-0.08568000
O	2.11659000	1.66391700	0.19801800
C	1.08884900	-0.54878200	0.88895100
H	0.23037800	-0.79272700	1.52333200
N	-1.33565700	1.06477800	0.80534700
C	2.37791900	-1.08651300	1.45824300
C	3.17364700	-0.27052100	2.26266100
C	2.75683400	-2.41503000	1.24621400
C	4.34007800	-0.76789400	2.84109600
H	2.88527700	0.76353800	2.42594400
C	3.92079700	-2.90766200	1.82609400
H	2.13817200	-3.04443800	0.61253400
C	4.71962400	-2.08783600	2.62266600
H	4.95224000	-0.11865900	3.46121500

H	4.20713700	-3.94110800	1.65019400
H	5.63060900	-2.47706000	3.06932400
S	-2.76783600	1.72935100	0.45407400
O	-2.77130200	2.37464600	-0.86572500
O	-3.31135100	2.52935300	1.55811200
C	-3.76191700	0.24510700	0.35232700
C	-3.22493000	-0.97767700	-0.04335300
C	-5.12012000	0.36546100	0.62584200
C	-4.06074700	-2.07946800	-0.17343700
H	-2.16265100	-1.10173900	-0.22122200
C	-5.94613600	-0.74611000	0.48662800
H	-5.51231700	1.31973700	0.96394000
C	-5.43095400	-1.97932000	0.08210100
H	-3.61982200	-3.02770400	-0.47304300
H	-7.00791900	-0.65687600	0.70542000
C	-6.32871500	-3.17927600	-0.08545400
H	-7.30024300	-3.02003900	0.39130200
H	-6.50748400	-3.38951400	-1.14607600
H	-5.87564200	-4.07482400	0.35077900
Br	-0.00233000	-3.06760700	-0.93955100
C	0.69382900	-0.68056000	-0.53362500
C	1.65697000	-0.58353100	-1.67135800
O	1.35525000	-0.29798800	-2.80264900
O	2.91499400	-0.80564000	-1.26563400
C	5.25052700	-0.79291000	-1.50925000
C	3.93500100	-0.62614400	-2.24196800
H	-0.33321100	-0.47431800	-0.78690100
H	6.09324000	-0.65923200	-2.19424600
H	5.32262600	-0.05710600	-0.70344500
H	5.30960700	-1.78782300	-1.05976800
H	3.80339800	-1.36600000	-3.03850800
H	3.83094900	0.36802300	-2.68934600

TS2-B-1

Zero-point correction= 0.443620 (Hartree/Particle)
Thermal correction to Energy= 0.474362
Thermal correction to Enthalpy= 0.475306
Thermal correction to Gibbs Free Energy= 0.378764
E(solv) = -4407.81475738 A.U.
Imaginary Frequency 339.79*i*

C	-1.05034300	2.81643700	0.21399300
C	-2.29106800	2.67232300	0.84928700
C	-3.19279600	3.72007700	0.99911800
C	-2.80959500	4.95031200	0.48324600
C	-1.57305800	5.12110700	-0.16111200

C	-0.68524200	4.06486300	-0.30572300
C	-0.42448900	1.49247000	0.26391800
C	-1.37345900	0.68364400	0.92757700
H	-4.14464300	3.56363100	1.49420100
H	-3.48294800	5.79771100	0.57828100
H	-1.30875400	6.09768500	-0.55446400
H	0.26700300	4.19865300	-0.80585800
O	-2.49743100	1.41301600	1.29662200
C	-1.24218100	-0.73112400	1.38409200
H	-2.07519300	-0.97726600	2.04900800
N	0.72981300	0.99616000	-0.16903900
C	0.10134600	-1.11297200	1.96663200
C	0.67911100	-0.25351900	2.90575400
C	0.76076100	-2.29680100	1.63678700
C	1.88153900	-0.57572500	3.52357100
H	0.18540900	0.68798700	3.13453400
C	1.96991600	-2.61701100	2.25491800
H	0.32277700	-2.96520000	0.90258300
C	2.53256000	-1.76634000	3.20189400
H	2.31800700	0.11058500	4.24339900
H	2.47392100	-3.54180100	1.98667200
H	3.47620600	-2.01968600	3.67779900
S	1.87321100	1.97411900	-0.76341900
O	2.29008300	2.98732500	0.21652700
O	1.58546700	2.48066500	-2.11355300
C	3.18430900	0.77678200	-0.92669700
C	3.38776100	-0.17527700	0.06986700
C	4.01827400	0.84560600	-2.03317700
C	4.44148700	-1.06895600	-0.05740900
H	2.70648300	-0.22466800	0.91400200
C	5.07651400	-0.05481400	-2.14214400
H	3.81825500	1.58588400	-2.80139600
C	5.29972200	-1.02177700	-1.16227800
H	4.59062200	-1.82448400	0.71135600
H	5.73049200	-0.01380700	-3.01007000
C	6.42415200	-2.01827600	-1.29470500
H	7.04649700	-2.03577100	-0.39390300
H	6.03430200	-3.03166600	-1.44103900
H	7.06683900	-1.78001700	-2.14686900
Br	-1.82501100	-3.46832800	-0.43860900
C	-1.61011900	-1.01395800	-0.01468300
C	-3.05677700	-0.92803300	-0.37117600
O	-3.96303300	-0.91575000	0.42720500
O	-3.21229300	-0.81690200	-1.70049300
C	-4.92718300	-2.45897800	-2.17102400

C	-4.55020100	-0.98743500	-2.17062700
H	-0.86185300	-0.91020700	-0.79154700
H	-5.92793800	-2.59129900	-2.59596000
H	-4.20349100	-3.03270600	-2.75504300
H	-4.91261700	-2.85045100	-1.15115300
H	-5.22862000	-0.40168500	-1.54417000
H	-4.54345000	-0.57156900	-3.18091900

TS2-B

Zero-point correction= 0.444001 (Hartree/Particle)
Thermal correction to Energy= 0.474694
Thermal correction to Enthalpy= 0.475638
Thermal correction to Gibbs Free Energy= 0.379639
E(solv) = -4407.81154498 A.U.
Imaginary Frequency 382.40*i*

C	-0.20928100	2.69786700	-0.05361800
C	-1.60119700	2.85516200	-0.05570700
C	-2.23300000	4.06702900	0.19945000
C	-1.41285200	5.15192000	0.47472300
C	-0.01496400	5.02377100	0.48808900
C	0.60033300	3.80850500	0.22283700
C	0.03270700	1.28772400	-0.38981600
C	-1.26417600	0.72574800	-0.47586000
H	-3.31475700	4.13903700	0.18522300
H	-1.86331500	6.11818400	0.68403800
H	0.59671200	5.89293100	0.70859800
H	1.68019200	3.72165400	0.22083200
O	-2.24887800	1.70522000	-0.33979800
C	-1.73515400	-0.66618200	-0.74485200
H	-0.90215800	-1.26979000	-1.11811400
N	1.12844300	0.56696000	-0.60111200
C	-2.97820700	-0.77184500	-1.59259200
C	-3.00708400	-0.06126700	-2.79606500
C	-4.06835800	-1.56656600	-1.24150300
C	-4.10384000	-0.14715000	-3.64454000
H	-2.15981900	0.56858800	-3.05737100
C	-5.16991500	-1.64634300	-2.09370300
H	-4.04683300	-2.11777400	-0.30560000
C	-5.19314400	-0.94311500	-3.29348700
H	-4.11203900	0.41277900	-4.57553600
H	-6.01625500	-2.26604100	-1.81056400
H	-6.05569100	-1.00873500	-3.95120500
S	2.57846700	1.18759600	-0.24258700
O	2.72588100	1.41807300	1.20496700
O	2.97545800	2.31102600	-1.10614700

C	3.61798800	-0.18636600	-0.69918400
C	3.29249000	-1.48372300	-0.30682200
C	4.78651500	0.08455100	-1.39701800
C	4.16523200	-2.51500000	-0.62932600
H	2.35829200	-1.67576400	0.21553800
C	5.65053900	-0.96350400	-1.70770200
H	4.99695600	1.10557100	-1.69838600
C	5.35254000	-2.27187300	-1.32968000
H	3.91715600	-3.53304900	-0.33747600
H	6.56691300	-0.76072700	-2.25715400
C	6.27531600	-3.41272500	-1.67844300
H	6.53508600	-3.99667200	-0.78934400
H	5.80225000	-4.09829100	-2.39022600
H	7.20346700	-3.04923800	-2.12833600
Br	-2.77095900	-2.71929400	1.84846500
C	-1.74132400	-0.67474600	0.73143700
C	-0.45516100	-1.02442300	1.40980400
O	0.34663000	-1.81420200	0.97384400
O	-0.27779200	-0.28241000	2.50602900
C	1.18682600	0.77156200	4.04070600
C	0.97931900	-0.45118500	3.17524300
H	-2.49302400	-0.12438500	1.27777700
H	2.12794000	0.68053700	4.59119300
H	1.24723700	1.65626100	3.40247500
H	0.36825400	0.89126600	4.75645300
H	0.93706600	-1.37948800	3.75601700
H	1.77208600	-0.53040500	2.42867900

TS3-A-1-A

Zero-point correction= 0.734501 (Hartree/Particle)
Thermal correction to Energy= 0.777172
Thermal correction to Enthalpy= 0.778116
Thermal correction to Gibbs Free Energy= 0.656586
E(solv) = -2485.21124463 A.U.
Imaginary Frequency 482.66*i*

C	1.08885200	3.38492100	-0.29003600
C	-0.00538500	3.93726100	0.38289000
C	-0.42402500	5.25235300	0.22585500
C	0.29416000	6.02762900	-0.67322600
C	1.38280100	5.49721800	-1.38325200
C	1.79149500	4.18393900	-1.20473100
C	1.17402100	1.98401200	0.15150600
C	0.08267200	1.83817000	1.04915900
H	-1.27244200	5.63546200	0.78144600
H	0.00500500	7.06200200	-0.83272900

H	1.91828900	6.12819900	-2.08462500
H	2.63835600	3.79397600	-1.75409700
O	-0.60892800	3.03712900	1.19640000
C	-0.57472900	0.70299500	1.77057900
H	-1.30773600	1.12789800	2.46025400
N	1.99956500	0.98369200	-0.15499700
C	0.23922500	-0.36386500	2.46627200
C	1.62441000	-0.26912700	2.59128900
C	-0.42452500	-1.44440800	3.05592700
C	2.34016300	-1.26939500	3.24695000
H	2.14366900	0.57793100	2.16052400
C	0.29313700	-2.44344000	3.70540700
H	-1.50990600	-1.47265100	3.03959100
C	1.68169200	-2.36692500	3.79184300
H	3.42035400	-1.18676900	3.32922100
H	-0.23570600	-3.27598700	4.16052300
H	2.24255100	-3.14659800	4.29855700
S	3.29661600	1.25007900	-1.09926900
O	4.11565400	2.36134400	-0.60518800
O	2.95903800	1.24118600	-2.52685000
C	4.20916800	-0.24709800	-0.77310700
C	4.69436600	-0.48492800	0.51155000
C	4.47666400	-1.12531400	-1.81232400
C	5.42757800	-1.63731500	0.75534500
H	4.49986600	0.23571800	1.30077400
C	5.22353200	-2.27484400	-1.55421100
H	4.10354500	-0.89636800	-2.80594000
C	5.69737500	-2.55123000	-0.27231500
H	5.80748200	-1.83398200	1.75528300
H	5.44108600	-2.96716900	-2.36375500
C	6.47813700	-3.80805800	0.01578200
H	7.37815700	-3.58924100	0.59825500
H	5.87692800	-4.51610600	0.59677900
H	6.78322300	-4.30660000	-0.90766600
C	-1.21088200	0.47617200	0.43665000
C	-0.52318800	-0.27004800	-0.65596000
O	-0.65635000	-0.01036400	-1.83493400
O	0.15977600	-1.30765300	-0.19140000
C	1.93707900	-2.85186500	-0.26572800
C	1.04564700	-1.96804800	-1.10849800
H	-1.91728300	1.22914100	0.10728000
H	2.62943400	-3.40881000	-0.90234900
H	2.51472100	-2.23431900	0.42776700
H	1.33739600	-3.55715200	0.31789800
H	0.44659500	-2.54553300	-1.82525000

H	1.60074600	-1.20554900	-1.66156200
C	-3.65279300	-0.26471800	1.49580800
O	-3.38745400	-0.14283600	2.67854900
O	-4.66080600	0.45420000	0.92105100
C	-2.86043200	-1.04146600	0.56546000
C	-5.33883500	1.36682200	1.79887900
C	-6.40036600	2.06741500	0.97839700
H	-4.60675300	2.06770600	2.20923900
H	-5.76543500	0.80632200	2.63530300
H	-6.94743900	2.77841400	1.60269200
H	-5.94721900	2.61598000	0.14828800
H	-7.11557100	1.34671800	0.57149900
H	-2.31613200	-1.85156000	1.03810900
C	-2.59664000	-2.54277600	-1.35534600
C	-4.82541100	-2.24256000	-0.40936900
C	-3.78194600	-0.43870200	-1.70810300
C	-3.37266200	-3.26487600	-2.47980600
H	-2.24034900	-3.22093400	-0.57726300
H	-1.75659900	-1.97506600	-1.75203000
C	-5.51637100	-2.57519500	-1.75329400
H	-5.42070600	-1.57619300	0.21207300
H	-4.56286600	-3.13353200	0.16699400
H	-4.57959200	0.17256600	-1.29035700
H	-2.86799500	0.14951600	-1.79198900
C	-4.17022100	-1.10363400	-3.04992000
H	-3.69140300	-4.26345100	-2.16587200
H	-2.72554500	-3.38045500	-3.35335800
H	-6.32848600	-1.87092700	-1.95618800
H	-5.94788100	-3.57949600	-1.71440500
H	-5.00104900	-0.56001100	-3.50774600
H	-3.32857600	-1.07798000	-3.74815300
N	-3.51444600	-1.53526200	-0.69112500
N	-4.56091900	-2.50198300	-2.85582800

TS3-A-1

Zero-point correction= 0.734489 (Hartree/Particle)
Thermal correction to Energy= 0.777016
Thermal correction to Enthalpy= 0.777960
Thermal correction to Gibbs Free Energy= 0.658094
E(solv) = -2485.20843784 A.U.
Imaginary Frequency 499.51*i*

C	1.09940800	3.44226200	-0.26052300
C	-0.12635700	3.93060200	0.20520100
C	-0.57019200	5.22337400	-0.03655700
C	0.27211900	6.04044900	-0.78082100

C	1.50761400	5.57736500	-1.25773500
C	1.93693500	4.28214900	-1.00386600
C	1.19563000	2.05858100	0.22393500
C	-0.04515200	1.83586000	0.88086400
H	-1.52575800	5.56697800	0.34347900
H	-0.03343600	7.06013400	-0.99560800
H	2.13905900	6.24440300	-1.83500100
H	2.89401500	3.93005000	-1.37075500
O	-0.81446700	2.99962200	0.92118600
C	-0.57274600	0.66266200	1.62351300
H	-1.29529500	1.01377400	2.37124400
N	2.13140700	1.13447400	0.18259600
C	0.42053100	-0.26529400	2.28431900
C	1.30149500	0.29685400	3.21238100
C	0.44065400	-1.64076000	2.06743000
C	2.18387500	-0.50466000	3.92686100
H	1.30291200	1.37467800	3.35867700
C	1.33589700	-2.44194300	2.77634400
H	-0.21687500	-2.09365100	1.33164300
C	2.20185000	-1.88266400	3.71063200
H	2.86523400	-0.05399400	4.64229200
H	1.35160700	-3.51179100	2.58909400
H	2.89212400	-2.51261000	4.26481100
S	3.48852600	1.33893000	-0.68934300
O	4.38137700	2.33260100	-0.08766100
O	3.21117800	1.48566700	-2.12523200
C	4.18072700	-0.28542300	-0.45751000
C	4.11852800	-0.90319700	0.78942200
C	4.79199000	-0.90743400	-1.53841800
C	4.68530200	-2.16126300	0.94587700
H	3.59508000	-0.41793000	1.60801400
C	5.35741000	-2.16881900	-1.36242000
H	4.80003000	-0.41090300	-2.50401800
C	5.31600600	-2.80895500	-0.12322100
H	4.62030700	-2.65707500	1.91182600
H	5.83165100	-2.66669700	-2.20447900
C	5.94405300	-4.16580600	0.06926300
H	5.31746300	-4.80644800	0.69669300
H	6.09982900	-4.67082700	-0.88769200
H	6.91916500	-4.07723900	0.56130500
C	-1.27739700	0.38854800	0.33912200
C	-0.72695600	-0.19190200	-0.91835800
O	-1.35211500	-0.11657800	-1.96073600
O	0.41651400	-0.81796600	-0.74196500
C	1.69916100	-2.69852600	-1.40907900

C	1.06813500	-1.40673700	-1.88215800
H	-2.06305500	1.10035300	0.13016100
H	2.27036600	-3.15585100	-2.22260200
H	2.37934400	-2.50140900	-0.57551400
H	0.92144000	-3.39208700	-1.07549200
H	0.32300000	-1.56661200	-2.66536100
H	1.80732100	-0.68028300	-2.23566800
C	-2.48339800	-2.29198800	-0.34215300
O	-1.52042200	-3.02132700	-0.18318000
O	-3.24556600	-2.34797600	-1.46921200
C	-2.83430900	-1.23017000	0.58403200
C	-2.68332400	-3.05444000	-2.58740200
C	-3.10955300	-2.32490300	-3.84380800
H	-3.04592900	-4.08721700	-2.56054800
H	-1.59741400	-3.07050800	-2.47772200
H	-2.73522600	-2.84834000	-4.72818400
H	-4.20049600	-2.27082700	-3.91622500
H	-2.69699200	-1.31251100	-3.83240200
H	-2.61673900	-1.48768400	1.61811200
C	-4.42095700	0.25903200	1.68471300
C	-4.43335000	0.19382500	-0.74298000
C	-5.28620600	-1.72048900	0.56929900
C	-5.75647000	1.02094000	1.49695400
H	-3.55683300	0.92355500	1.74063600
H	-4.42221000	-0.38386300	2.56920100
C	-5.93585800	0.53980300	-0.82691900
H	-4.04722100	-0.36083800	-1.59490200
H	-3.82573700	1.08928700	-0.61547600
H	-5.21468800	-2.27251400	-0.36682000
H	-5.00071900	-2.38045900	1.39121000
C	-6.66359300	-1.05007100	0.77702100
H	-5.57208400	2.05400900	1.18839700
H	-6.30618100	1.04924300	2.44171500
H	-6.45027900	-0.10835200	-1.54279000
H	-6.05901300	1.57185100	-1.16711900
H	-7.40888100	-1.51154000	0.12329200
H	-7.00920300	-1.16602400	1.80875700
N	-4.21200100	-0.64966900	0.50114500
N	-6.58327800	0.37825100	0.47743000

TS3-A-A

Zero-point correction= 0.734739 (Hartree/Particle)
Thermal correction to Energy= 0.777142
Thermal correction to Enthalpy= 0.778086
Thermal correction to Gibbs Free Energy= 0.658829

E(solv) = -2485.20238186 A.U.

Imaginary Frequency 484.38*i*

C	-0.87816700	-4.50650500	-2.98710900
C	-2.22514400	-4.63930100	-2.60974200
C	-2.72521700	-3.99293500	-1.48780500
C	-1.82821100	-3.20834500	-0.77340400
C	-0.47891400	-3.05313100	-1.12309400
C	0.00503200	-3.72507700	-2.25668200
O	-2.15619300	-2.52213800	0.35106300
C	-1.00462800	-1.85357500	0.73869800
C	0.09210800	-2.18163300	-0.09405700
C	-1.06488600	-0.79068700	1.79249100
C	-1.16220800	-0.00626700	0.52884400
N	1.29403900	-1.65902600	0.16403400
C	3.81889400	-1.01854700	-0.15836500
C	4.91282600	-0.62292500	-0.92794200
C	6.14640600	-0.44796000	-0.31710900
C	6.30872700	-0.66738700	1.05623800
C	5.20080200	-1.07133300	1.80184500
C	3.95472000	-1.25256700	1.20349900
C	7.66056200	-0.49583000	1.70055800
S	2.26351300	-1.15994400	-1.01746600
O	2.47631400	-2.10131000	-2.12295000
O	1.87008800	0.20470900	-1.42942600
C	-2.18436500	-0.84624600	2.80264300
C	-2.77076000	-2.06170100	3.15617600
C	-3.76023400	-2.10924200	4.13526100
C	-4.16995100	-0.94427100	4.77381300
C	-3.57178200	0.26820600	4.43831200
C	-2.58237500	0.31858700	3.46339600
C	-2.45811900	0.04878600	-0.21461700
O	-3.54717800	0.28065800	0.24612500
O	-2.24474500	-0.23546600	-1.51488500
C	-2.93674900	-0.92162500	-3.66736800
C	-3.41506900	-0.42140700	-2.32202800
H	-0.52078600	-5.03048600	-3.86761400
H	-2.88720400	-5.26112400	-3.20481200
H	-3.75741900	-4.08450300	-1.16795300
H	1.04217700	-3.61718600	-2.54712300
H	-0.08530200	-0.65550500	2.25372400
H	-0.24294300	0.18215900	-0.01228100
H	4.79008200	-0.45538200	-1.99422100
H	7.00163500	-0.13755800	-0.91228300
H	5.31145700	-1.25020600	2.86824100
H	3.09185500	-1.56940900	1.77890200

H	8.31342800	-1.34348600	1.46506900
H	8.15789900	0.40988900	1.34100700
H	7.57692500	-0.43145300	2.78836400
H	-2.45909300	-2.97577500	2.66289300
H	-4.20921500	-3.06269500	4.39731900
H	-4.94336600	-0.98168100	5.53537500
H	-3.87053400	1.18064100	4.94600500
H	-2.07539600	1.25056700	3.24133400
H	-3.79036200	-1.11843300	-4.32165300
H	-2.29072000	-0.18168300	-4.14859200
H	-2.36718300	-1.84711700	-3.54169700
H	-4.06912400	-1.14049100	-1.81892300
H	-3.95900100	0.52832600	-2.39521500
C	0.08871600	2.21252900	1.64079500
O	0.11182600	1.80878700	2.79365000
O	1.23749600	2.43168600	0.94136200
C	-1.11212200	2.34578100	0.85775100
C	2.43355000	1.90119000	1.53394400
C	3.58581900	2.26385800	0.62423900
H	2.31498900	0.81605500	1.62020100
H	2.54712400	2.31293200	2.54039900
H	4.50978400	1.81101500	0.99899900
H	3.39849000	1.88025500	-0.38227800
H	3.72018200	3.34953800	0.58092900
H	-2.01732000	2.55324600	1.41783400
C	-2.49020600	3.36738600	-0.86803400
C	-0.47097900	4.52913900	-0.19730900
C	-0.32129400	2.45355800	-1.51834400
C	-2.45467900	3.97097600	-2.29008100
H	-2.95035800	4.04087800	-0.13926500
H	-3.00766400	2.40845900	-0.81318200
C	-0.74206300	5.38688100	-1.45764100
H	0.58996500	4.36748000	-0.00976800
H	-0.93238500	4.93423900	0.70603100
H	0.63081700	2.10371000	-1.12355800
H	-0.92170500	1.58419200	-1.78888200
C	-0.17272800	3.44152400	-2.69283400
H	-3.21631800	4.75041700	-2.38411400
H	-2.66785900	3.20456200	-3.04186400
H	0.15733900	5.94507700	-1.73193200
H	-1.54096400	6.11281100	-1.27621100
H	0.83109900	3.87583700	-2.71841400
H	-0.32880800	2.91704700	-3.63968900
N	-1.07387400	3.15241600	-0.39859100
N	-1.13947600	4.53934000	-2.58126800

TS3-A

Zero-point correction= 0.734042 (Hartree/Particle)

Thermal correction to Energy= 0.777089

Thermal correction to Enthalpy= 0.778033

Thermal correction to Gibbs Free Energy= 0.656182

E(solv) = -2485.20491103 A.U.

Imaginary Frequency 497.30*i*

C	1.04691100	4.62378800	-2.74083900
C	2.43258000	4.53980900	-2.51921500
C	2.95610300	3.79006000	-1.47450400
C	2.03975700	3.12464200	-0.67026200
C	0.65140700	3.18899900	-0.86733200
C	0.14406300	3.96061000	-1.92379200
O	2.38028400	2.34483900	0.38828500
C	1.19269100	1.81312700	0.85697600
C	0.07108900	2.35312600	0.17752000
C	1.20437800	0.70484300	1.85807600
C	1.05610200	0.01127400	0.55584800
N	-1.15717800	1.96705900	0.52759300
C	-3.69175400	1.32688100	0.43795900
C	-4.94598900	1.32610600	-0.17231300
C	-6.03221900	0.79267200	0.50665200
C	-5.88991900	0.26220800	1.79488600
C	-4.62880700	0.29022900	2.39028800
C	-3.52602400	0.81855500	1.72078900
C	-7.08392000	-0.30623300	2.51749900
S	-2.32850000	1.87047000	-0.57432800
O	-2.73253400	3.13303800	-1.19796200
O	-2.03874500	0.76029400	-1.50910600
C	2.40798300	0.57939900	2.75132400
C	2.85783600	1.71428600	3.42869200
C	3.91633900	1.62222900	4.32574300
C	4.53254300	0.39297500	4.54953500
C	4.08591600	-0.73699500	3.87076000
C	3.02584400	-0.64990300	2.97175200
C	2.19737200	-0.24407800	-0.37442300
O	3.29999300	-0.63185000	-0.08718100
O	1.81257800	0.08662700	-1.61895700
C	2.25441900	0.68701400	-3.86048700
C	2.83130800	0.03256400	-2.62398100
H	0.67822700	5.22462700	-3.56562500
H	3.10990900	5.07480200	-3.17814300
H	4.02044200	3.71285000	-1.28312000
H	-0.92577800	4.02687500	-2.08660800

H	0.26107800	0.70028600	2.41124600
H	0.06831100	0.00668300	0.13031700
H	-5.05975000	1.74845000	-1.16649700
H	-7.01163900	0.79061400	0.03454900
H	-4.50548800	-0.09982400	3.39739700
H	-2.54812200	0.85863900	2.18803700
H	-7.55025300	-1.10866800	1.93680700
H	-6.80314000	-0.71128300	3.49279500
H	-7.84542700	0.46368400	2.67852500
H	2.38026000	2.67353100	3.24430100
H	4.26177200	2.51069700	4.84579900
H	5.36185500	0.31915600	5.24682900
H	4.56672400	-1.69734300	4.02956400
H	2.70382400	-1.53576200	2.43261100
H	2.99076400	0.68230700	-4.66883500
H	1.36064300	0.15484500	-4.19722700
H	1.97676100	1.72265200	-3.64168900
H	3.71640900	0.55758800	-2.25169200
H	3.10716500	-1.01546500	-2.78896800
C	1.73855100	-3.07253100	0.40861200
O	2.58369300	-3.34034100	1.24484900
O	1.94399400	-3.35727600	-0.91735700
C	0.52600300	-2.34385300	0.68324500
C	3.25382600	-3.84816800	-1.22951200
C	3.25120900	-4.22813600	-2.69567600
H	3.48076000	-4.70450400	-0.58907200
H	3.97773500	-3.05875500	-1.00411500
H	4.23603100	-4.60060800	-2.99033600
H	2.51384600	-5.01256400	-2.89027800
H	3.00797600	-3.36646700	-3.32469900
H	0.24875700	-2.39133400	1.73268400
C	-1.86684700	-1.92200700	0.52172900
C	-0.59588800	-2.01333700	-1.56060300
C	-0.99748500	-4.06217700	-0.26994000
C	-3.12831200	-2.06920600	-0.36357500
H	-1.59923300	-0.87591100	0.68311700
H	-1.96918500	-2.41394700	1.49344400
C	-1.87164300	-2.40281500	-2.34682200
H	0.32108100	-2.40555600	-1.99511100
H	-0.52293300	-0.93185900	-1.46501300
H	-0.17469500	-4.48978400	-0.84551100
H	-0.95684400	-4.45883200	0.74692700
C	-2.37991200	-4.25429600	-0.94245000
H	-3.40015600	-1.09906800	-0.78464900
H	-3.96743800	-2.43532900	0.23590100

H	-1.64242700	-3.12724300	-3.13472900
H	-2.28883900	-1.50398300	-2.80791500
H	-2.30396200	-4.97647400	-1.76071800
H	-3.10883700	-4.64072700	-0.22370900
N	-0.69067700	-2.58491800	-0.15784200
N	-2.88319500	-2.99173100	-1.46987500

TS3-B-1-A

Zero-point correction= 0.734075 (Hartree/Particle)
Thermal correction to Energy= 0.777097
Thermal correction to Enthalpy= 0.778041
Thermal correction to Gibbs Free Energy= 0.655169
E(solv) = -2485.21515005 A.U.
Imaginary Frequency 492.72*i*

C	-3.79898400	-1.15383200	-0.34325100
C	-3.60507300	-2.49815600	-0.00483500
C	-4.47747300	-3.51017700	-0.38547800
C	-5.58707600	-3.12422700	-1.12487800
C	-5.81554300	-1.77939000	-1.46353100
C	-4.93264200	-0.78249200	-1.07912900
C	-2.68295900	-0.42712100	0.25438500
C	-1.90471600	-1.43621400	0.89328200
H	-4.29043500	-4.54051200	-0.10586000
H	-6.29871100	-3.87995300	-1.44327800
H	-6.70035000	-1.51835900	-2.03415500
H	-5.11433200	0.25457700	-1.33747800
O	-2.48939300	-2.68453700	0.74562200
C	-0.64698700	-1.35985800	1.70332300
H	-0.38725500	-2.36658300	2.03767500
N	-2.30322300	0.84274700	0.24433600
C	-0.46565200	-0.34860200	2.80363100
C	-0.38080900	-0.80850800	4.11801600
C	-0.33102600	1.02162700	2.55870700
C	-0.18722200	0.08030900	5.17256000
H	-0.45326900	-1.87472500	4.31322000
C	-0.12650800	1.90894000	3.61074700
H	-0.40794400	1.39212100	1.54187500
C	-0.05926300	1.44308300	4.92245900
H	-0.12527800	-0.29613600	6.18892400
H	-0.02651100	2.97143500	3.40256900
H	0.09532400	2.13727800	5.74282700
S	-2.95614500	1.91408900	-0.78993000
O	-4.17268000	2.52552500	-0.25611200
O	-2.99756500	1.41890500	-2.16956300
C	-1.64161800	3.12315600	-0.71758600

C	-1.29347700	3.69622600	0.50445000
C	-0.97061100	3.46323900	-1.88430000
C	-0.23941000	4.60061600	0.55297200
H	-1.83658200	3.41584200	1.40332300
C	0.07132500	4.38821100	-1.82279600
H	-1.27115500	2.99946700	-2.81856000
C	0.45527500	4.96240500	-0.60887500
H	0.04277900	5.04921300	1.50285900
H	0.59437000	4.67048300	-2.73421100
C	1.57098400	5.97523400	-0.55105100
H	1.17198500	6.99472900	-0.58950900
H	2.14384700	5.88484100	0.37688100
H	2.25971600	5.86010400	-1.39316000
C	-0.12464500	-1.13768600	0.34193600
C	0.14868700	-2.32192100	-0.51113400
O	0.33677500	-3.44474200	-0.10905400
O	0.12228600	-1.98645200	-1.81816300
C	1.77535700	-3.38520600	-2.92497300
C	0.30151600	-3.07435100	-2.73750500
H	-0.28057600	-0.18306800	-0.14433800
H	1.89970200	-4.26091100	-3.56844400
H	2.29731900	-2.54296200	-3.38987300
H	2.23181800	-3.59425000	-1.95365900
H	-0.23680900	-3.94394300	-2.35543900
H	-0.16625000	-2.73552600	-3.66315300
C	2.55552700	-1.91802300	1.13647600
O	2.18473900	-2.50969800	2.13268900
O	3.37767800	-2.50840500	0.21022700
C	2.07389700	-0.60550900	0.78261900
C	3.66387800	-3.89277200	0.46084400
C	4.75085400	-4.31208900	-0.50708000
H	2.73842900	-4.46201800	0.32610700
H	3.97904600	-4.00878300	1.50051900
H	4.99792600	-5.36665700	-0.35832500
H	4.43122900	-4.17938600	-1.54497700
H	5.65766700	-3.72130800	-0.34769200
H	1.80176300	-0.03347700	1.66211800
C	2.18493800	1.63569500	-0.14680500
C	4.27800200	0.44341200	0.28485500
C	2.83026800	-0.22735400	-1.57589900
C	3.07651500	2.62075200	-0.94097400
H	2.05444200	1.92867400	0.89757300
H	1.19296500	1.51379500	-0.59289100
C	5.03431100	1.28220600	-0.77437300
H	4.68315200	-0.56156600	0.40259700

H	4.23455700	0.92777200	1.26347100
H	3.39970700	-1.15651700	-1.57346100
H	1.79227600	-0.45951900	-1.81750900
C	3.44115700	0.86319800	-2.49078200
H	3.57704300	3.32259500	-0.26645000
H	2.45639600	3.20246800	-1.62670100
H	5.71891900	0.65281400	-1.35039800
H	5.62763400	2.06167800	-0.28811100
H	4.17255100	0.41821000	-3.17125500
H	2.66504100	1.33690800	-3.09900500
N	2.83907000	0.27139300	-0.15046900
N	4.09796500	1.90758200	-1.70488100

TS3-B-1

Zero-point correction= 0.734692 (Hartree/Particle)
Thermal correction to Energy= 0.777487
Thermal correction to Enthalpy= 0.778431
Thermal correction to Gibbs Free Energy= 0.657089
E(solv) = -2485.20689340 A.U.
Imaginary Frequency 440.49*i*

C	3.43535400	-1.77467800	0.24788900
C	4.28616400	-0.86776700	0.89829000
C	5.67094600	-0.94126200	0.82752000
C	6.19745300	-1.97386100	0.06336300
C	5.36900000	-2.89749200	-0.59745000
C	3.98788000	-2.81443100	-0.51449700
C	2.08446600	-1.35768200	0.59979100
C	2.26599700	-0.19601100	1.39160000
H	6.29309200	-0.22080200	1.34585700
H	7.27537600	-2.06947000	-0.02420000
H	5.82180300	-3.69144100	-1.18197800
H	3.33896800	-3.52151400	-1.01903400
O	3.60146400	0.06819000	1.60951400
C	1.20423500	0.71189500	1.90336500
H	1.64728700	1.50750800	2.50865200
N	0.85010300	-1.79261900	0.34878200
C	0.01746500	0.05832700	2.57191700
C	0.18374800	-1.13137900	3.28460000
C	-1.24376800	0.64870100	2.53582700
C	-0.89163200	-1.72244600	3.93889200
H	1.15949600	-1.60823500	3.30352400
C	-2.32551900	0.05521600	3.18523500
H	-1.38842400	1.56965900	1.98687000
C	-2.15388400	-1.13296800	3.88964000
H	-0.74573600	-2.65307800	4.47811900

H	-3.30299200	0.52820200	3.14298100
H	-2.99453500	-1.59745100	4.39627600
S	0.41486200	-2.52242800	-1.00936900
O	1.16346700	-3.72618500	-1.38242600
O	0.26611900	-1.50868200	-2.08003700
C	-1.23699000	-3.02952000	-0.57065100
C	-1.93066200	-2.45382100	0.48949200
C	-1.85586900	-3.94602900	-1.41865500
C	-3.26588900	-2.79699300	0.68788200
H	-1.42654700	-1.76064600	1.15536600
C	-3.18908700	-4.27341100	-1.20668700
H	-1.28929000	-4.39593200	-2.22856200
C	-3.91399700	-3.70267500	-0.15443100
H	-3.80560800	-2.35216900	1.52072000
H	-3.67774700	-4.98665300	-1.86564900
C	-5.35193900	-4.08948600	0.07913600
H	-5.86317000	-3.35684900	0.70886100
H	-5.89861400	-4.17194100	-0.86470800
H	-5.41628800	-5.06133100	0.58070900
C	1.21904800	1.11515800	0.46466400
C	2.27036600	2.09981100	0.08558100
O	2.83583700	2.82462900	0.86485400
O	2.53479200	2.05270900	-1.23465100
C	2.84229500	4.38795900	-1.84051200
C	3.48957200	3.02148200	-1.69664400
H	0.81921600	0.44372600	-0.27640400
H	3.57804500	5.11921000	-2.18729500
H	2.02725500	4.35385800	-2.57103900
H	2.44570500	4.72412100	-0.87827000
H	4.32509000	3.05346900	-0.99421300
H	3.83549800	2.63145100	-2.65528000
C	-0.86604200	3.48397500	0.57431700
O	-0.19736100	4.28688600	1.19428300
O	-2.18614600	3.26195200	0.88902900
C	-0.32720000	2.64636800	-0.47490800
C	-2.66310800	3.97994400	2.03440600
C	-4.14397900	3.69060300	2.15732300
H	-2.45962700	5.04518400	1.89930200
H	-2.10622600	3.64629500	2.91671100
H	-4.55682000	4.20286100	3.03023200
H	-4.68117200	4.03503200	1.26905800
H	-4.32165100	2.61733400	2.27196800
H	0.42571200	3.18323100	-1.03979700
C	-0.37066300	1.43436600	-2.58480300
C	-1.93027500	0.74751100	-0.81687500

C	-2.26805200	2.85414500	-2.04634700
C	-1.27393500	0.76407500	-3.64817000
H	0.34785600	0.72513400	-2.17803200
H	0.16520100	2.30646800	-2.96698700
C	-2.69138900	-0.03107000	-1.92016000
H	-2.58507900	1.15495400	-0.04563000
H	-1.16226200	0.13547800	-0.34119900
H	-2.81670300	3.29970700	-1.21918300
H	-1.70357900	3.63533600	-2.56183600
C	-3.17590300	2.03542800	-3.00033500
H	-0.90741700	-0.24783200	-3.83260400
H	-1.25128300	1.32591100	-4.58708000
H	-3.73283400	-0.18480900	-1.62308800
H	-2.22853900	-1.00877400	-2.07121700
H	-4.18779500	1.95981100	-2.59146300
H	-3.24513800	2.53205800	-3.97271400
N	-1.22675300	1.93786300	-1.43967800
N	-2.66034200	0.68673900	-3.19339000

TS3-B-A

Zero-point correction= 0.733936 (Hartree/Particle)
Thermal correction to Energy= 0.776903
Thermal correction to Enthalpy= 0.777848
Thermal correction to Gibbs Free Energy= 0.654551
E(solv) = -2485.21276249 A.U.
Imaginary Frequency 525.36*i*

C	-1.80933100	3.09323800	-0.46642400
C	-0.67357400	3.87496500	-0.22249900
C	-0.51112200	5.16391500	-0.71229900
C	-1.54501400	5.66802100	-1.48990100
C	-2.69398600	4.90762100	-1.75690200
C	-2.84433200	3.62481000	-1.24943400
C	-1.58275900	1.82686900	0.24354500
C	-0.27328000	1.96022600	0.77565800
H	0.38330100	5.73475900	-0.48973000
H	-1.46204800	6.67123700	-1.89686700
H	-3.48429800	5.33422100	-2.36548200
H	-3.74358000	3.05301600	-1.44315100
O	0.24253100	3.23099000	0.54641100
C	0.53899700	0.96452200	1.53798900
H	-0.10752300	0.15639900	1.88550200
N	-2.28671200	0.71989400	0.42596900
C	1.51131600	1.43030000	2.58818700
C	1.50513500	0.81190400	3.83938700
C	2.45814000	2.42768700	2.33117400

C	2.41503900	1.19235800	4.82201400
H	0.79772800	0.01130400	4.02857100
C	3.37056000	2.80451900	3.31262500
H	2.46906200	2.92933500	1.36819200
C	3.35060300	2.18957300	4.56227700
H	2.39528400	0.70205100	5.79044600
H	4.09310800	3.58781700	3.10285200
H	4.06029200	2.48678100	5.32841800
S	-3.66266900	0.50876900	-0.41910400
O	-3.36549800	0.37440400	-1.85608800
O	-4.71677100	1.46451300	-0.06262400
C	-4.17011900	-1.08067900	0.19810300
C	-3.29825100	-2.16649800	0.13362800
C	-5.46163700	-1.21958600	0.68370500
C	-3.74177400	-3.40546000	0.57273600
H	-2.28641900	-2.02626300	-0.23542100
C	-5.88990200	-2.47364400	1.11658100
H	-6.10944800	-0.35031100	0.72430400
C	-5.04103700	-3.57802600	1.06808400
H	-3.07001600	-4.26048600	0.53569600
H	-6.89942800	-2.59248000	1.50110300
C	-5.49774600	-4.93453000	1.54130900
H	-4.88192400	-5.28725400	2.37528500
H	-6.53725200	-4.90859400	1.87731300
H	-5.41931400	-5.67743900	0.74075200
C	1.04950900	0.69058900	0.17549900
C	0.27854600	-0.17380800	-0.76295600
O	-0.22792600	-1.23068600	-0.46756700
O	0.24035300	0.36439300	-1.98849000
C	-0.99113200	0.70000500	-3.99355400
C	-0.56133100	-0.32593200	-2.97030300
H	1.68938400	1.43776400	-0.28145100
H	-1.58808600	0.21464500	-4.77022700
H	-1.61420100	1.45234800	-3.50440300
H	-0.12907600	1.18437400	-4.46144300
H	0.05338500	-1.12606000	-3.40398000
H	-1.42850500	-0.76101400	-2.47322900
C	1.99496200	-1.87537800	1.10531800
O	1.44469800	-1.83207400	2.18896100
O	1.85682900	-2.94193500	0.26496800
C	2.74858000	-0.76579300	0.55603400
C	0.79213800	-3.84957500	0.59065200
C	0.36716900	-4.51622000	-0.70072200
H	-0.02324600	-3.27785100	1.03689300
H	1.15823500	-4.57025800	1.32926200

H	-0.41943800	-5.25100300	-0.50673700
H	-0.02357900	-3.76208400	-1.39010500
H	1.20763500	-5.03366000	-1.17390700
H	3.23121500	-0.16768800	1.32419000
C	4.55585100	0.21733500	-0.72982800
C	4.65915500	-2.16850600	-0.27550800
C	3.01442300	-1.26570800	-1.87645300
C	5.40197700	0.07038500	-2.01780400
H	5.16657300	0.29937200	0.17320100
H	3.87201800	1.06736700	-0.75912400
C	5.78002400	-2.17510300	-1.34318800
H	4.04482800	-3.06821200	-0.28791300
H	5.03130500	-2.01086000	0.73891800
H	2.25037700	-2.02222100	-1.69730900
H	2.52443800	-0.32459100	-2.13498400
C	4.07377800	-1.68338200	-2.92091200
H	6.42747700	0.40103500	-1.83227700
H	4.99352600	0.68807200	-2.82268200
H	5.94869400	-3.19224900	-1.70701000
H	6.72353600	-1.81090700	-0.92582500
H	4.05470700	-2.76385000	-3.09069500
H	3.86763800	-1.19356300	-3.87662300
N	3.71218900	-1.01770800	-0.55709700
N	5.41954900	-1.31878800	-2.47231800

TS3-B

Zero-point correction= 0.734105 (Hartree/Particle)
Thermal correction to Energy= 0.776966
Thermal correction to Enthalpy= 0.777910
Thermal correction to Gibbs Free Energy= 0.656011
E(solv) = -2485.21424505 A.U.
Imaginary Frequency 497.00*i*

C	-1.94965600	2.82565300	0.35475600
C	-0.72344700	3.42476600	0.66827400
C	-0.48725200	4.78885000	0.56004200
C	-1.54123000	5.56798100	0.10213900
C	-2.78005700	4.99682300	-0.22685800
C	-3.00222500	3.63266200	-0.10094400
C	-1.77682200	1.39051000	0.62933900
C	-0.41214200	1.27698600	1.00088600
H	0.47704000	5.20823500	0.82396700
H	-1.40293700	6.64001300	-0.00120600
H	-3.58323600	5.63532500	-0.57927100
H	-3.96799500	3.20396400	-0.33828200
O	0.20019200	2.52342800	1.08977100

C	0.41625400	0.07644800	1.32754700
H	-0.22639400	-0.79084200	1.49313500
N	-2.56828000	0.33069600	0.57750300
C	1.44531800	0.26362500	2.40905600
C	1.21904900	-0.30622600	3.66396900
C	2.58714400	1.04289600	2.21983700
C	2.10921900	-0.09219500	4.71210600
H	0.33727100	-0.92261100	3.81334600
C	3.48393400	1.25389700	3.26509000
H	2.76302500	1.51638400	1.25787900
C	3.24738400	0.68815100	4.51549200
H	1.91540300	-0.53890500	5.68242900
H	4.36177700	1.87395900	3.10578700
H	3.94274600	0.85746400	5.33197300
S	-4.04393100	0.48085300	-0.09715700
O	-3.92033000	0.77148700	-1.53656300
O	-4.94383500	1.35614800	0.66221500
C	-4.64945100	-1.18007200	0.09351600
C	-3.87112800	-2.26330400	-0.31095600
C	-5.93277700	-1.35665400	0.59028800
C	-4.40247400	-3.54097600	-0.20649500
H	-2.86086500	-2.10028300	-0.67491900
C	-6.44961100	-2.64751500	0.68310500
H	-6.50410200	-0.49021400	0.90625500
C	-5.69624700	-3.75171600	0.28741100
H	-3.80266500	-4.39633600	-0.50830500
H	-7.45261300	-2.79720800	1.07403500
C	-6.24977300	-5.15035900	0.38867200
H	-5.61724600	-5.77805200	1.02488100
H	-7.25806900	-5.14917200	0.81021100
H	-6.29570300	-5.62676000	-0.59626500
C	0.76721400	0.20424700	-0.10686700
C	-0.19195600	-0.33961000	-1.11060000
O	-0.76539600	-1.39515800	-1.00734900
O	-0.31053000	0.49361400	-2.15671300
C	-1.76120000	1.44812400	-3.78224300
C	-1.31737000	0.15576600	-3.13645700
H	1.35313300	1.06051600	-0.41773800
H	-2.51763900	1.23534900	-4.54228700
H	-2.21372100	2.09119700	-3.02398400
H	-0.92288600	1.96902300	-4.25463600
H	-0.86992700	-0.54468000	-3.85216800
H	-2.15221300	-0.32707500	-2.62827800
C	2.71024700	-1.91593800	0.60396900
O	1.94178800	-2.54948000	1.29790900

O	3.98137500	-1.62566500	1.01646500
C	2.32667600	-1.33707300	-0.67270600
C	4.29011100	-2.04016100	2.35627000
C	5.67809700	-1.52862300	2.67401500
H	4.23039900	-3.13137400	2.41061900
H	3.53791800	-1.62695200	3.03197000
H	5.95400600	-1.80824200	3.69443900
H	6.42091800	-1.94882200	1.98898000
H	5.70570100	-0.43775400	2.60017900
H	1.63885400	-1.98984400	-1.20204500
C	2.75353400	-0.55707500	-2.93906800
C	4.11034100	0.34875100	-1.14202300
C	4.43007300	-1.97703600	-1.88860800
C	3.80921600	0.10141100	-3.85976200
H	1.90317100	0.09488600	-2.72862500
H	2.37248700	-1.50040500	-3.34029400
C	5.30222700	0.62826500	-2.08725500
H	4.40429700	0.17887100	-0.10757100
H	3.36389200	1.14487400	-1.17700700
H	4.97424200	-2.11172800	-0.95453100
H	3.86276300	-2.88588900	-2.09981300
C	5.33431400	-1.53589800	-3.06524000
H	3.63753100	1.17892500	-3.93531700
H	3.74172600	-0.31613800	-4.86785100
H	6.24635600	0.32976700	-1.62225900
H	5.36299200	1.69807700	-2.30531400
H	6.38403900	-1.72708800	-2.82628900
H	5.09414800	-2.09213600	-3.97605300
N	3.40070300	-0.89660800	-1.61841100
N	5.15985600	-0.11112400	-3.34185100

N-INT4

Zero-point correction= 0.652095 (Hartree/Particle)
Thermal correction to Energy= 0.690954
Thermal correction to Enthalpy= 0.691898
Thermal correction to Gibbs Free Energy= 0.582449
E(solv) = -2442.84213313 A.U.

C	3.42860600	-0.48352200	-0.78195300
C	3.55239900	0.81909300	-1.28390200
C	4.67821300	1.28375200	-1.95300100
C	5.73171300	0.38895800	-2.10153500
C	5.64363700	-0.91859000	-1.59326500
C	4.50417800	-1.36849500	-0.93698300
C	2.11881400	-0.53495300	-0.14058700
C	1.59143700	0.71875600	-0.29936900

H	4.71691000	2.30059100	-2.33018400
H	6.63344300	0.70533500	-2.62021900
H	6.48336600	-1.59611100	-1.72786700
H	4.41002000	-2.38697000	-0.57802600
O	2.45435700	1.54825900	-0.99975900
C	0.25519100	1.35110000	0.01331700
H	-0.43996700	0.99675800	-0.78893000
N	1.57304200	-1.50291600	0.68413400
C	0.36356700	2.86779000	-0.16265100
C	1.12816500	3.62596400	0.73030300
C	-0.29210900	3.49979300	-1.22230200
C	1.22950800	5.00578400	0.58623200
H	1.66132700	3.11539400	1.53261000
C	-0.19327900	4.88618400	-1.35365400
H	-0.92657200	2.91634800	-1.90125600
C	0.56242700	5.64150000	-0.46092800
H	1.83160000	5.58298500	1.28455800
H	-0.72825100	5.37334200	-2.16471100
H	0.63215300	6.72131400	-0.57547500
S	1.42214800	-3.01473000	0.23597900
O	1.35155300	-3.85259300	1.44503600
O	2.38866700	-3.44029300	-0.79836400
C	-0.19639800	-3.13010500	-0.53097600
C	-1.17118300	-3.96617200	0.00542200
C	-0.50395900	-2.27369900	-1.58706200
C	-2.46001500	-3.94137900	-0.52902700
H	-0.91248800	-4.59349000	0.85258600
C	-1.79185200	-2.24876500	-2.10789600
H	0.22616100	-1.55764900	-1.95592400
C	-2.78551600	-3.08336800	-1.58393700
H	-3.23478800	-4.57515100	-0.09755100
H	-2.05842200	-1.46837500	-2.81499000
C	-4.18359200	-2.97516500	-2.13890300
H	-4.30879800	-3.60794400	-3.02789700
H	-4.93253100	-3.28910100	-1.40167500
H	-4.35710000	-1.92916200	-2.42403900
N	-4.45568400	0.43871100	1.20146200
N	-1.89163300	0.79611300	1.32519100
C	-3.74491400	-0.71605800	0.63159900
H	-3.97587400	-1.59969300	1.23897700
H	-4.08978900	-0.84731500	-0.39707300
C	-4.08110300	1.63203500	0.43897900
H	-4.28280700	1.46776400	-0.62522700
H	-4.67723400	2.47815000	0.80157800
C	-4.04201800	0.63006000	2.57783600

H	-4.52214600	1.53942900	2.95866100
H	-4.39388400	-0.21471100	3.18118800
C	-2.50321100	0.73364300	2.70479000
H	-2.18300200	1.64238700	3.22583300
H	-2.08200900	-0.13263500	3.20159100
C	-2.21632500	-0.47701600	0.55775800
H	-1.62218000	-1.27936000	0.99958600
H	-1.91543800	-0.28889600	-0.48125700
C	-2.57237100	1.95150500	0.60764100
H	-2.14265100	2.08504400	-0.38418400
H	-2.37460900	2.83849200	1.22136300
C	-0.38834800	1.04982700	1.41735200
H	-0.33145300	1.98365400	1.99185100
C	0.29748400	0.03895300	2.35271300
O	1.53106400	0.48128800	2.61086600
O	-0.22104500	-0.88157900	2.93683800
C	2.36639800	-0.44210400	3.32840800
H	2.17162800	-0.31446400	4.40142300
H	2.09372300	-1.45293700	3.01732100
C	3.79921300	-0.11916700	2.96341500
H	4.48056300	-0.75782100	3.53505500
H	3.95503200	-0.30618200	1.89776100
H	4.03666300	0.92777300	3.17895500
C	-2.70930300	1.07512800	-2.32427500
O	-2.97471800	2.33190400	-2.31848300
O	-3.65432400	0.19239300	-2.29627700
O	-1.45902600	0.68411400	-2.25697700

N-INT6-A

Zero-point correction= 0.431294 (Hartree/Particle)
Thermal correction to Energy= 0.460245
Thermal correction to Enthalpy= 0.461189
Thermal correction to Gibbs Free Energy= 0.367366
E(solv) = -1833.05214049 A.U.

C	-0.40229700	0.63819900	1.99675300
C	0.75813000	0.19582800	2.65338600
C	0.83560100	-0.04727600	4.02091400
C	-0.31270600	0.17581600	4.76544600
C	-1.48556900	0.63979200	4.14834000
C	-1.54446700	0.87814900	2.78167800
C	-0.02735800	0.76571700	0.57748000
C	1.31290500	0.40716500	0.54356000
H	1.76368600	-0.39205900	4.46442300
H	-0.30060100	-0.00255800	5.83714900
H	-2.36690400	0.82626100	4.75532500

H	-2.44588300	1.25665100	2.31656400
O	1.78883200	0.05075500	1.80198700
C	2.23822900	0.20970700	-0.54877600
N	-0.68309400	1.15814000	-0.54957700
C	3.17514700	-0.94714400	-0.42101200
C	4.49296100	-0.85116800	-0.87809500
C	2.74543100	-2.16098000	0.12951300
C	5.35626800	-1.94087800	-0.80356200
H	4.83886300	0.09682800	-1.28000900
C	3.60498100	-3.25059800	0.20160000
H	1.72331600	-2.24094900	0.48787800
C	4.91470500	-3.14573600	-0.26479200
H	6.37818900	-1.84462800	-1.15983800
H	3.25099200	-4.18761800	0.62212100
H	5.58700700	-3.99691800	-0.20331500
S	-2.25483600	1.09942500	-0.74587700
O	-2.55883600	1.65634800	-2.06545700
O	-3.05208900	1.61541300	0.38362800
C	-2.66559400	-0.64914000	-0.84903400
C	-2.57106200	-1.29300400	-2.08109900
C	-3.00394600	-1.36346600	0.29419800
C	-2.81993400	-2.65704200	-2.16169500
H	-2.31430500	-0.70675400	-2.95802100
C	-3.24641500	-2.73251900	0.20063200
H	-3.08760300	-0.84474000	1.24459100
C	-3.15619300	-3.39696400	-1.02257200
H	-2.75444400	-3.16160600	-3.12362700
H	-3.51473100	-3.29319800	1.09339600
C	-3.39748400	-4.88286100	-1.12137800
H	-4.04615800	-5.12488700	-1.96963800
H	-2.45692600	-5.42693000	-1.26550300
H	-3.86849400	-5.26921100	-0.21302500
C	2.26351900	0.91771700	-1.70376100
H	2.84827700	0.53435200	-2.53471900
C	1.53307400	2.15658600	-2.04051700
O	1.29733700	2.95078800	-0.98702700
O	1.25753400	2.46095500	-3.18156300
C	0.31006600	3.96298200	-1.20846800
H	0.76354600	4.78197600	-1.78074800
H	-0.50422500	3.53111600	-1.79645200
C	-0.17398100	4.42004600	0.15201900
H	-0.88127400	5.24770000	0.03866900
H	-0.68300200	3.59505200	0.65760700
H	0.66342600	4.75668500	0.77115000

N-INT6-B

Zero-point correction= 0.430332 (Hartree/Particle)
Thermal correction to Energy= 0.459684
Thermal correction to Enthalpy= 0.460628
Thermal correction to Gibbs Free Energy= 0.366349
E(solv) = -1833.05405302 A.U.

C	3.29495300	0.31528000	0.03343700
C	3.83298300	-0.96489700	-0.14081300
C	5.19073800	-1.19996100	-0.33167100
C	6.02211800	-0.08775900	-0.33236300
C	5.50963200	1.20655100	-0.14123200
C	4.15121000	1.42340900	0.04532100
C	1.85594000	0.12344900	0.22174900
C	1.66578900	-1.25673300	0.11662900
H	5.56574200	-2.20863200	-0.46763700
H	7.09033400	-0.22304100	-0.47852000
H	6.19061000	2.05221900	-0.13802300
H	3.75992800	2.42303400	0.20116700
O	2.88075000	-1.91674900	-0.08646900
C	0.50144700	-2.08377300	0.17663300
N	0.87666500	1.00521400	0.50572500
C	-0.82859100	-1.40312100	0.20220300
C	-1.69814300	-1.61781300	1.27122600
C	-1.22551300	-0.55891300	-0.83668900
C	-2.95349700	-1.01511900	1.29647700
H	-1.38192200	-2.26710400	2.08356400
C	-2.47983600	0.03784700	-0.81893100
H	-0.53127300	-0.35788900	-1.64771000
C	-3.35015700	-0.19141700	0.24647800
H	-3.61869500	-1.18738700	2.13859800
H	-2.76993200	0.71038100	-1.62129300
H	-4.32345200	0.29265400	0.26614700
S	1.02441700	2.55031800	0.13903900
O	1.58054100	2.80275400	-1.20268600
O	1.59599400	3.36848100	1.22284100
C	-0.71435400	2.96206600	0.05517200
C	-1.23763800	3.47285800	-1.12261000
C	-1.53001600	2.75318300	1.16570100
C	-2.59824600	3.77620800	-1.19166000
H	-0.57467400	3.61470100	-1.97015400
C	-2.88019300	3.05785700	1.08354200
H	-1.10262900	2.32493500	2.06688500
C	-3.43494400	3.57018400	-0.09642400
H	-3.01590600	4.17330700	-2.11444300
H	-3.52603200	2.87907200	1.94104400

C	-4.91023400	3.87641100	-0.17030400
H	-5.20283100	4.61103800	0.58795400
H	-5.18350100	4.27724700	-1.15042500
H	-5.50995600	2.97563100	0.00319900
C	0.62319600	-3.44473400	0.23151600
C	-0.45026600	-4.43130900	0.14999700
O	-0.37447000	-5.57528100	0.56031200
O	-1.56343100	-3.97752000	-0.47726100
C	-3.84413500	-4.05011200	-1.04901100
C	-2.70582300	-4.81717100	-0.40560600
H	-4.77279700	-4.62745500	-1.00189700
H	-3.98658700	-3.09509100	-0.53473600
H	-3.61475800	-3.83856800	-2.09693400
H	-2.50231000	-5.76464800	-0.91700000
H	-2.91760600	-5.05343000	0.64383900
H	1.60732000	-3.88086600	0.35517500

N-INT6-C

Zero-point correction= 0.430447 (Hartree/Particle)
Thermal correction to Energy= 0.459978
Thermal correction to Enthalpy= 0.460922
Thermal correction to Gibbs Free Energy= 0.365225
E(solv) = -1833.05329120 A.U.

C	-1.45240500	2.72542300	-0.08125000
C	-2.81566300	2.39979500	-0.06824900
C	-3.82967700	3.35242300	-0.10192600
C	-3.43688100	4.68203100	-0.15371600
C	-2.07738000	5.03791100	-0.16994800
C	-1.07780800	4.07621600	-0.13376400
C	-0.74133900	1.44738300	-0.03864900
C	-1.74859700	0.47655900	-0.00269200
H	-4.87142100	3.05050000	-0.09011900
H	-4.19435600	5.46055100	-0.18305200
H	-1.80380500	6.08790000	-0.21070000
H	-0.03254100	4.36184900	-0.14089600
O	-3.01415000	1.07019900	-0.02168100
C	-1.69046600	-0.95209200	0.01195500
N	0.57126700	1.13739400	-0.03361800
C	-2.99933400	-1.66986500	0.09823200
C	-3.86901100	-1.43011400	1.16446200
C	-3.38808700	-2.56544000	-0.89957000
C	-5.09474700	-2.08437900	1.24033200
H	-3.57640400	-0.72186900	1.93374400
C	-4.61711000	-3.21131100	-0.83230100
H	-2.70952800	-2.75725700	-1.72499700

C	-5.47438800	-2.97512900	0.24008300
H	-5.75696000	-1.89246200	2.08002900
H	-4.90436000	-3.90585000	-1.61672500
H	-6.43383000	-3.48225400	0.29484600
S	1.70108200	2.26576500	-0.12924200
O	1.75923600	3.18086600	1.02523400
O	1.75852900	2.92594700	-1.44432600
C	3.13741200	1.20569500	0.00604200
C	4.18834200	1.61011400	0.81619800
C	3.21623200	0.01718700	-0.71847900
C	5.33182600	0.81673700	0.90226500
H	4.08697400	2.52908600	1.38453600
C	4.35684100	-0.76690800	-0.61774100
H	2.37338600	-0.29417500	-1.32723400
C	5.43162800	-0.37766200	0.19067600
H	6.15460000	1.12590700	1.54311500
H	4.41330400	-1.70423000	-1.16692000
C	6.66485600	-1.24160600	0.28169600
H	7.21460200	-1.24857900	-0.66636600
H	7.34446000	-0.88215900	1.05947100
H	6.40348800	-2.27972400	0.51292200
C	-0.49080800	-1.60520600	-0.07453400
H	0.40948300	-1.01386900	-0.16362000
C	-0.28611800	-3.04244400	0.02593800
O	1.04295900	-3.32007500	-0.16875400
O	-1.07745500	-3.93748500	0.25332400
C	1.39750100	-4.68744000	-0.04560500
H	1.12616400	-5.05043400	0.95220700
H	0.82987200	-5.28489100	-0.76814400
C	2.89131500	-4.78168000	-0.28881800
H	3.23362400	-5.81611500	-0.18740400
H	3.13561600	-4.42992200	-1.29519300
H	3.43170100	-4.15880300	0.42949600

N-INT6-D

Zero-point correction= 0.431362 (Hartree/Particle)
Thermal correction to Energy= 0.460238
Thermal correction to Enthalpy= 0.461182
Thermal correction to Gibbs Free Energy= 0.368927
E(solv) = -1833.04776827 A.U.

C	-1.12137800	2.52875900	-0.01679100
C	-2.46993000	2.32296100	0.30447300
C	-3.38576500	3.36216500	0.43794000
C	-2.90466000	4.64752200	0.23038900
C	-1.55812800	4.87983700	-0.10106100

C	-0.65629400	3.83291900	-0.23181600
C	-0.52120400	1.19826200	-0.06474900
C	-1.55956700	0.33140100	0.26041900
H	-4.42167000	3.15875600	0.68645600
H	-3.58465000	5.49021000	0.32280700
H	-1.22004200	5.89957900	-0.26030400
H	0.38514500	3.99972400	-0.48876400
O	-2.75038100	1.01674500	0.46450100
C	-1.55585900	-1.08635000	0.49421500
N	0.71911900	0.78721400	-0.43755800
C	-0.30464000	-1.69466100	1.03926300
C	0.07201100	-2.98800600	0.66265300
C	0.49614500	-1.00383400	1.95778500
C	1.21041100	-3.58581200	1.20106700
H	-0.52285000	-3.51383800	-0.07888300
C	1.63578700	-1.59478200	2.48740800
H	0.24845600	0.01824600	2.22442800
C	1.99379800	-2.89160200	2.11845900
H	1.49114300	-4.58833400	0.88925200
H	2.25925300	-1.02116500	3.16578300
H	2.89287700	-3.34690300	2.52444800
S	2.00162400	1.60445300	0.02157400
O	2.09960700	1.73225800	1.49100400
O	2.28461800	2.85497500	-0.71470800
C	3.28116000	0.46448900	-0.50273700
C	4.53152500	0.98811200	-0.81207900
C	3.06847500	-0.91105700	-0.51565900
C	5.57819300	0.12643300	-1.12846800
H	4.66381400	2.06553400	-0.81359700
C	4.12290400	-1.76018600	-0.83241500
H	2.07864100	-1.29676800	-0.29558000
C	5.38965000	-1.25681700	-1.14193000
H	6.55720800	0.53364500	-1.37231600
H	3.95595000	-2.83568900	-0.83733100
C	6.51601500	-2.18909300	-1.51406300
H	6.50418400	-3.09209900	-0.89562400
H	6.43593000	-2.50922900	-2.55961500
H	7.48931700	-1.70505000	-1.39076500
C	-2.64649500	-1.89792800	0.37640100
C	-3.88344900	-1.59229800	-0.34060100
O	-4.09847800	-0.71204200	-1.14335000
O	-4.83643500	-2.53241800	-0.03454300
C	-5.97251100	-2.96907000	-2.13983300
C	-6.06717900	-2.39579400	-0.73465800
H	-6.94428400	-2.91665800	-2.64157200

H	-5.24639700	-2.39777000	-2.72172300
H	-5.65529700	-4.01526300	-2.10251900
H	-6.79833200	-2.94388100	-0.13390600
H	-6.34925000	-1.34006100	-0.77050700
H	-2.60450900	-2.89427900	0.80265600

N-INT7-A

Zero-point correction= 0.733893 (Hartree/Particle)
Thermal correction to Energy= 0.778139
Thermal correction to Enthalpy= 0.779083
Thermal correction to Gibbs Free Energy= 0.651407
E(solv) = -2485.29989120 A.U.

C	0.45351200	-2.77825300	0.23082100
C	1.72887000	-2.33350500	0.59161400
C	2.79276900	-3.19807600	0.80486700
C	2.54088500	-4.55406100	0.62159300
C	1.27653100	-5.02344600	0.24246000
C	0.21988300	-4.14514300	0.04511100
C	-0.37060400	-1.57164900	0.12305700
C	0.55724100	-0.45839100	0.45292200
H	3.76720500	-2.82441000	1.09990700
H	3.34689100	-5.26485200	0.77615800
H	1.11991300	-6.08773700	0.10599200
H	-0.76025500	-4.51036200	-0.23666300
O	1.81647000	-0.97644800	0.71279000
C	0.30738200	0.85533200	0.52949800
N	-1.59254200	-1.32118600	-0.18535600
C	-1.08808500	1.36205600	0.40362100
C	-1.55429700	1.91033100	-0.79315600
C	-1.94124300	1.27008400	1.50607000
C	-2.87400400	2.34195700	-0.89173300
H	-0.88918100	1.97076900	-1.65084100
C	-3.26023500	1.69985700	1.40101800
H	-1.56482600	0.83038300	2.42714900
C	-3.73076800	2.23029800	0.20132500
H	-3.23962000	2.74852800	-1.83036900
H	-3.92712900	1.60907300	2.25329500
H	-4.76515900	2.55085700	0.11686100
S	-2.67681900	-2.54169100	-0.53502600
O	-2.79410800	-3.45764600	0.59545100
O	-2.38686100	-3.07286900	-1.86220300
C	-4.15428900	-1.56352000	-0.61088400
C	-4.95693500	-1.46968200	0.51759100
C	-4.46424900	-0.88665300	-1.78673100
C	-6.09735600	-0.67287400	0.46413700

H	-4.68944500	-2.01901000	1.41451600
C	-5.60563900	-0.09706000	-1.82053500
H	-3.81911500	-0.98732200	-2.65412400
C	-6.43449100	0.02154900	-0.69872900
H	-6.73684600	-0.59295600	1.33925200
H	-5.86212200	0.43842600	-2.73138900
C	-7.67390800	0.87705000	-0.76107400
H	-7.44785700	1.86930000	-1.16476300
H	-8.42760300	0.42478400	-1.41454400
H	-8.12035500	1.00444400	0.22806500
C	1.41347600	1.83786500	0.88067700
C	1.14060800	3.10588200	0.08539300
O	1.46899300	3.26833000	-1.06668400
O	0.40570000	3.98185500	0.77475500
C	-1.36684900	5.54913500	0.82589100
C	-0.18049300	5.05836300	0.02564300
H	-1.85577600	6.37620000	0.30382400
H	-2.08853200	4.73615400	0.95178300
H	-1.05294100	5.89755500	1.81325700
H	0.57778800	5.83236000	-0.12757800
H	-0.48070200	4.67350800	-0.95276100
H	2.37296900	1.43172400	0.53478600
C	1.42917100	2.10045200	2.40471700
C	1.68465300	0.80160700	3.12646900
O	0.82522300	0.09757800	3.60081900
O	2.98615000	0.48497100	3.11326500
C	4.74780600	-1.09123000	3.20550700
C	3.31131700	-0.82333600	3.59806800
H	2.21451900	2.82432600	2.63881000
H	0.46412000	2.49436100	2.72724000
H	4.85971400	-0.99975800	2.12049600
H	5.42271600	-0.37315200	3.67838200
H	5.04245800	-2.09960600	3.51008900
H	3.16489200	-0.84816100	4.68266200
H	2.61993900	-1.54394200	3.15131800
N	4.70026400	0.13172400	-3.55575300
C	5.07712800	1.48881800	-3.14733900
C	4.59948800	-0.42118300	-1.13997800
C	2.60980100	0.30919600	-2.23014200
C	3.23709500	0.05562900	-3.63233800
C	5.16825600	-0.81241000	-2.53653300
C	4.37673500	1.86180600	-1.80725100
N	3.65808400	0.69427900	-1.27443300
H	6.16874300	1.51950000	-3.05394900
H	4.79551300	2.17784500	-3.95112200

H	5.39652000	-0.10809900	-0.45481900
H	4.06569800	-1.25813700	-0.67679800
H	2.12636300	-0.59643300	-1.84446400
H	1.86441800	1.11090900	-2.24976900
H	2.96430500	-0.93131700	-4.02183100
H	2.90152600	0.80230400	-4.36037300
H	4.84160600	-1.81536200	-2.83335600
H	6.26397200	-0.80659800	-2.54091300
H	5.10248500	2.18722000	-1.05288500
H	3.64412200	2.66307700	-1.93672100

N-INT7

Zero-point correction= 0.545456 (Hartree/Particle)
Thermal correction to Energy= 0.582091
Thermal correction to Enthalpy= 0.583035
Thermal correction to Gibbs Free Energy= 0.471017
E(solv) = -2140.00571021 A.U.

C	1.51414100	-2.56508100	-0.57846200
C	2.76911100	-1.96427900	-0.71154700
C	3.94103900	-2.69051000	-0.85371000
C	3.81540100	-4.07618100	-0.86454300
C	2.56880200	-4.70423000	-0.73987500
C	1.40564300	-3.95965600	-0.59699800
C	0.55643100	-1.46267000	-0.46508300
C	1.39401000	-0.23575600	-0.52849700
H	4.89793600	-2.19205900	-0.95935300
H	4.70782500	-4.68426800	-0.97597100
H	2.51227200	-5.78688900	-0.75525400
H	0.44273000	-4.44595100	-0.49653100
O	2.72176900	-0.59935900	-0.68534900
C	1.03026100	1.04812000	-0.42486100
N	-0.71847100	-1.36426800	-0.34835100
C	-0.38655800	1.41983400	-0.15591800
C	-1.23229100	1.79734500	-1.20121900
C	-0.87288300	1.37131500	1.15240800
C	-2.56594600	2.09924700	-0.94056000
H	-0.84647500	1.82892300	-2.21707200
C	-2.20740500	1.67237000	1.40679600
H	-0.20419100	1.06278100	1.95282800
C	-3.05719600	2.02950200	0.36177100
H	-3.22652700	2.37290700	-1.75812700
H	-2.58944500	1.61320300	2.42150900
H	-4.10266400	2.24619800	0.56149300
S	-1.69701200	-2.71257800	-0.22805800
O	-1.32990000	-3.49859700	0.94536400

O	-1.78381800	-3.36344400	-1.53031300
C	-3.22725900	-1.88121700	0.10735800
C	-3.62612800	-1.70269800	1.42505400
C	-3.97257800	-1.38245600	-0.95649400
C	-4.80324100	-1.00428900	1.67863300
H	-3.02170500	-2.10920600	2.22957200
C	-5.14348700	-0.68852800	-0.68346000
H	-3.63348200	-1.54368900	-1.97490600
C	-5.57323700	-0.48970200	0.63382900
H	-5.12965500	-0.85795300	2.70480400
H	-5.73711400	-0.29224400	-1.50350800
C	-6.85478800	0.25445800	0.90913000
H	-6.92333900	1.16105900	0.29992600
H	-7.72480900	-0.36609000	0.66885700
H	-6.93015900	0.54189000	1.96073900
C	2.07433800	2.15165200	-0.46705700
C	1.48351500	3.30078900	-1.27274900
O	1.52139700	3.36429200	-2.47589300
O	0.83904600	4.17141200	-0.49027100
C	-1.01035500	5.60341300	-0.12439100
C	-0.01543500	5.11576200	-1.15473700
H	-1.69355400	6.32778800	-0.57606800
H	-1.59262500	4.75864400	0.25586800
H	-0.49862200	6.08328200	0.71379000
H	0.60255100	5.92211100	-1.56149800
H	-0.50697000	4.60881000	-1.98960900
H	2.95771700	1.79535300	-1.00228900
C	2.46353900	2.56642500	0.97013300
C	3.03548600	1.36341300	1.67934700
O	2.42303700	0.65754600	2.44421700
O	4.29492500	1.12386400	1.28992600
C	6.20312000	-0.26352500	1.07497600
C	4.86100300	-0.10889200	1.75579500
H	3.20228000	3.37145900	0.92972700
H	1.58114900	2.90862100	1.51247200
H	6.07908100	-0.24236800	-0.01153400
H	6.87891800	0.54782600	1.35679300
H	6.66203100	-1.21441600	1.35910300
H	4.94944500	-0.07062300	2.84563100
H	4.17491400	-0.92354300	1.50412700

N-INT8-A

Zero-point correction=	0.736428 (Hartree/Particle)
Thermal correction to Energy=	0.779848
Thermal correction to Enthalpy=	0.780792

Thermal correction to Gibbs Free Energy= 0.657671

E(solv) = -2485.29980348 A.U.

C	0.72158700	-2.92925500	-0.61839000
C	-0.67220800	-2.88784000	-0.69483900
C	-1.47995300	-4.01747500	-0.67520800
C	-0.82589500	-5.23916000	-0.57835200
C	0.57408700	-5.31583500	-0.51173200
C	1.36171400	-4.17287600	-0.53931600
C	1.17619800	-1.53398000	-0.72667500
C	-0.03024500	-0.75956000	-0.81753300
H	-2.55656200	-3.92965500	-0.77847700
H	-1.41049600	-6.15414800	-0.57048900
H	1.05029700	-6.28844700	-0.44813400
H	2.44218700	-4.24417400	-0.49953200
O	-1.14336100	-1.62120500	-0.79601200
C	-0.32184300	0.60105100	-0.91350200
N	2.36751000	-0.99009100	-0.77929500
C	0.74090200	1.61519400	-0.64920800
C	1.66264000	1.49506500	0.39698300
C	0.84952600	2.70998200	-1.51142800
C	2.66786700	2.43636700	0.57165200
H	1.61977700	0.63209900	1.05414100
C	1.85187000	3.65878600	-1.33691600
H	0.14757400	2.80254900	-2.33532500
C	2.76505200	3.52314400	-0.29626800
H	3.39916400	2.30206300	1.36424300
H	1.92356800	4.49808900	-2.02202700
H	3.55854700	4.25363100	-0.16547200
S	3.71343200	-1.81495200	-0.36429300
O	4.26578300	-2.55131100	-1.50090300
O	3.54093800	-2.54239000	0.89876300
C	4.75945400	-0.41439900	-0.02493600
C	5.03146100	0.50055000	-1.03944600
C	5.26772200	-0.24317200	1.25424700
C	5.82240000	1.60380400	-0.75601300
H	4.60344300	0.35415900	-2.02633500
C	6.06512800	0.86941200	1.52164300
H	5.03274200	-0.97490600	2.02062900
C	6.35018700	1.80407800	0.52642900
H	6.02783300	2.33237400	-1.53662600
H	6.47090000	1.01210200	2.52009700
C	7.21838600	3.00314300	0.81082500
H	7.37368700	3.13671600	1.88453400
H	8.20216600	2.89303000	0.34172800
H	6.76940500	3.91922700	0.41400300

C	-1.62266500	1.00292400	-1.31892000
C	-2.15354300	2.27200700	-0.87393200
O	-1.79560700	2.90050300	0.12200100
O	-3.20218500	2.71017500	-1.62144000
C	-4.91983500	4.24771900	-2.15661800
C	-3.83105800	3.90472300	-1.16180500
H	-5.44073100	5.15872600	-1.84945300
H	-4.49234700	4.40953000	-3.14938000
H	-5.64859200	3.43543100	-2.22497200
H	-4.23974200	3.73615600	-0.15805100
H	-3.08405300	4.69940800	-1.07775800
H	-2.16981400	0.27311600	0.54706800
C	-2.37705900	0.20762400	-2.36141900
C	-3.40761900	-0.81310500	-1.93018700
O	-3.65930600	-1.82293300	-2.53589200
O	-4.12147100	-0.45466600	-0.82124100
C	-6.16082800	-0.65644100	0.44183400
C	-5.25398800	-1.30687100	-0.58294400
H	-2.91942200	0.91001100	-3.00569000
H	-1.68422800	-0.34648800	-2.99921100
H	-5.71347600	-0.63135200	1.44099700
H	-6.40298900	0.36738100	0.14188400
H	-7.09366200	-1.22219000	0.51476900
H	-5.77789500	-1.45820700	-1.52962300
H	-4.90157700	-2.29098000	-0.25296900
N	-2.64309800	0.06651300	4.07812000
C	-3.73452800	0.82795200	3.46542700
C	-2.62932200	-1.21110500	1.95494000
C	-1.04072800	0.62852100	2.26520600
C	-1.36996600	0.72973700	3.77621200
C	-2.62710600	-1.27918500	3.50296700
C	-3.41571200	1.12649000	1.98255000
N	-2.30493000	0.20017100	1.58036800
H	-4.65481300	0.24263100	3.56693500
H	-3.87378100	1.76287600	4.01493400
H	-3.60295400	-1.43474200	1.51512900
H	-1.88278000	-1.85704000	1.48968000
H	-0.29361300	-0.13762100	2.04220600
H	-0.73736300	1.57203300	1.80362600
H	-0.57728100	0.26423800	4.36757900
H	-1.44912900	1.77509200	4.08795200
H	-1.73403900	-1.79535100	3.86638700
H	-3.50063100	-1.83187400	3.85983200
H	-4.24507100	0.94866200	1.29656300
H	-3.03633400	2.13547600	1.81477200

N-INT8-B

Zero-point correction= 0.736625 (Hartree/Particle)
Thermal correction to Energy= 0.780170
Thermal correction to Enthalpy= 0.781114
Thermal correction to Gibbs Free Energy= 0.655578
E(solv) = -2485.28945871 A.U.

C	-0.96245400	3.13399500	0.45375100
C	0.37476600	3.38628800	0.77072700
C	0.91891600	4.66041800	0.87141000
C	0.05499600	5.72421900	0.65092500
C	-1.29438100	5.50621500	0.33632300
C	-1.81730100	4.22381800	0.23651800
C	-1.11045000	1.66592000	0.46357300
C	0.18968000	1.18261100	0.70873600
H	1.96498300	4.80304000	1.12112800
H	0.43119100	6.74018800	0.72626800
H	-1.94546200	6.35755300	0.16656000
H	-2.85812500	4.07266700	-0.01971300
O	1.07718600	2.24107700	0.94986300
C	0.70973600	-0.13260800	0.93644200
N	-2.17732400	0.86691200	0.39914400
C	1.53803300	-0.31961700	2.18697100
C	2.56482700	0.52982600	2.62297700
C	1.16832400	-1.37014700	3.04610300
C	3.23519900	0.29380400	3.82403500
H	2.81681400	1.41714700	2.05839200
C	1.82849700	-1.60039700	4.24404000
H	0.32772100	-2.00071700	2.77187300
C	2.88178800	-0.77695200	4.63526100
H	4.02461300	0.97350500	4.13275300
H	1.50875200	-2.41910100	4.88133400
H	3.39865600	-0.95171300	5.57366300
S	-3.64772400	1.50452900	0.13079600
O	-3.73211800	2.20261200	-1.15703800
O	-4.16107000	2.22101300	1.30449100
C	-4.58697200	-0.00227000	-0.02249500
C	-4.47273300	-0.75801000	-1.18793800
C	-5.43004800	-0.38756500	1.00835400
C	-5.21321700	-1.92717700	-1.30212000
H	-3.80764600	-0.42029200	-1.97918300
C	-6.16769800	-1.56238000	0.87507400
H	-5.49897100	0.23550000	1.89431000
C	-6.06960600	-2.34444100	-0.27538600
H	-5.13647700	-2.52821900	-2.20571700

H	-6.83153800	-1.87480200	1.67744900
C	-6.88018600	-3.60659000	-0.42945000
H	-7.38150100	-3.87295200	0.50474900
H	-7.64966400	-3.48692200	-1.19994100
H	-6.24857300	-4.44930000	-0.72853600
C	0.35319100	-1.22954800	0.17074100
C	1.02254100	-2.52450800	0.38128400
O	2.21919300	-2.67770700	0.63107800
O	0.22344300	-3.58362100	0.20242900
C	-0.24314100	-5.90564300	0.09339900
C	0.84349600	-4.87301800	0.29988300
H	0.17855300	-6.91158500	0.16697500
H	-1.02174000	-5.79680100	0.85204500
H	-0.70275000	-5.79020300	-0.89130300
H	1.63214000	-4.94635300	-0.45639800
H	1.31705600	-4.96152300	1.28199000
H	2.83951100	-0.99874000	0.12462900
C	-0.70214200	-1.21936100	-0.90473700
C	-0.58121800	-0.21228900	-2.02942400
O	-1.52681600	0.28169000	-2.58147800
O	0.69191300	-0.01177300	-2.48419100
C	2.12700900	0.74262000	-4.24939200
C	0.74227400	0.83361300	-3.64671500
H	-0.72328500	-2.19725500	-1.39760000
H	-1.69300200	-1.02655200	-0.48064800
H	2.88971600	1.12754800	-3.56660300
H	2.37101900	-0.29422600	-4.50405400
H	2.17082200	1.33771200	-5.16553700
H	-0.01861100	0.49981700	-4.35565500
H	0.48674300	1.85521400	-3.34904700
N	5.67037400	0.09791800	-1.71824800
C	4.92688800	-0.89804800	-2.48964600
C	3.49083800	0.81578700	-0.75312600
C	4.86655000	-0.86674600	0.41945000
C	6.09503200	-0.49600200	-0.45016100
C	4.80757100	1.25062100	-1.45036600
C	3.71784300	-1.43429000	-1.67880600
N	3.64651800	-0.63297600	-0.41451000
H	4.59328300	-0.43255000	-3.42049700
H	5.60556100	-1.71472800	-2.75049500
H	2.59648900	0.89006700	-1.37736700
H	3.29485900	1.35995200	0.16884000
H	4.75965200	-0.24572600	1.31148800
H	4.83570100	-1.91424900	0.72675900
H	6.73372500	0.21880200	0.07542200

H	6.69821800	-1.38060300	-0.67259400
H	5.36415400	1.95015000	-0.82032500
H	4.59755700	1.75814800	-2.39561900
H	2.75453400	-1.29838300	-2.17964300
H	3.81940900	-2.47815500	-1.37610900

N-INT8-C

Zero-point correction= 0.735809 (Hartree/Particle)
Thermal correction to Energy= 0.779666
Thermal correction to Enthalpy= 0.780611
Thermal correction to Gibbs Free Energy= 0.655518
E(solv) = -2485.28395428 A.U.

C	-0.54020800	2.99006800	1.17446600
C	0.84071200	3.13057400	1.38335000
C	1.47657300	4.34699100	1.58633900
C	0.67519200	5.48100300	1.56119200
C	-0.70807500	5.37714700	1.35062900
C	-1.33088500	4.15122000	1.16248300
C	-0.73894900	1.56324900	1.01952800
C	0.48894100	0.97354800	1.10202800
H	2.54798500	4.39363400	1.74947300
H	1.12538000	6.45764200	1.70828300
H	-1.31096600	6.27949100	1.34003400
H	-2.40257400	4.09959100	1.01775500
O	1.46682900	1.92660900	1.33325800
C	0.89125100	-0.42155700	1.00371300
N	-1.92237800	0.81403600	0.83665000
C	1.78396000	-0.95507500	2.08018500
C	2.98016000	-0.30918600	2.43329300
C	1.44677400	-2.11680200	2.79417800
C	3.81805100	-0.82344600	3.42006200
H	3.24001300	0.62726600	1.95199700
C	2.28823500	-2.63761400	3.77073200
H	0.49506100	-2.60220200	2.59484800
C	3.48525900	-1.99884900	4.08534600
H	4.73325200	-0.29513900	3.67262500
H	1.99536500	-3.53682400	4.30513400
H	4.13909700	-2.40105400	4.85279100
S	-3.30352100	1.58783700	0.27000500
O	-3.01948800	2.30726800	-0.96789400
O	-3.89610900	2.31763800	1.38254800
C	-4.29565900	0.16712500	-0.09958500
C	-4.10393800	-0.48752700	-1.31486600
C	-5.24472500	-0.25007400	0.82519200
C	-4.88925300	-1.59980300	-1.58994200

H	-3.35873900	-0.13446900	-2.02610700
C	-6.02345100	-1.36251600	0.52164800
H	-5.36528600	0.29606200	1.75534200
C	-5.85631300	-2.04836400	-0.68347700
H	-4.75421100	-2.12489700	-2.53215000
H	-6.77373600	-1.70272800	1.23019000
C	-6.71263900	-3.24223600	-1.01986500
H	-7.31381300	-3.55576800	-0.16288000
H	-7.39584100	-3.00953100	-1.84362400
H	-6.09802100	-4.09076100	-1.33581200
C	0.33205100	-1.26733300	0.04692900
C	0.75286700	-2.71245600	0.09397900
O	1.87894400	-3.08227300	-0.18493300
O	-0.23419800	-3.55513000	0.39108300
C	-1.13547400	-5.71964900	0.75517800
C	0.11877000	-4.94857700	0.40806700
H	-0.91818100	-6.79048600	0.78969100
H	-1.51897500	-5.40922100	1.73023600
H	-1.91259900	-5.54471000	0.00712800
H	0.51807400	-5.22316200	-0.57266800
H	0.91428100	-5.09213100	1.14653300
H	2.41866900	-0.78797800	-0.40581500
C	-0.47060800	-1.06182000	-1.10364700
C	-0.61966500	0.07394600	-1.97329500
O	-1.40078200	0.12243100	-2.91494100
O	0.24651100	1.11317800	-1.73670000
C	1.05332300	3.31101100	-2.22827500
C	-0.08445400	2.33277100	-2.42756100
H	-0.94257900	-1.94620400	-1.51846500
H	-1.75487500	-0.03289700	0.27290000
H	1.23493100	3.49469000	-1.16470000
H	1.97722400	2.94538800	-2.69270500
H	0.80216800	4.26730300	-2.69585600
H	-0.24453800	2.10928500	-3.48499400
H	-1.02213700	2.71628100	-2.01444300
N	5.04313300	-0.14195100	-2.71615700
C	3.96514600	-0.88466100	-3.37546800
C	3.52011100	0.85217400	-1.03072900
C	4.39323400	-1.41925400	-0.69026500
C	5.55400400	-0.93963500	-1.59747800
C	4.50223900	1.11867700	-2.19792000
C	2.73002500	-0.98367000	-2.44834200
N	3.19503200	-0.60890600	-1.07113600
H	3.69908100	-0.37675800	-4.30622800
H	4.34568100	-1.87739000	-3.63359000

H	2.57201200	1.38973600	-1.09996400
H	3.96475800	1.04888800	-0.05300400
H	4.56829200	-1.25723700	0.37626900
H	4.11756100	-2.46394500	-0.83849800
H	6.26098600	-0.32175400	-1.03583200
H	6.10389600	-1.79724900	-1.99466200
H	5.32854000	1.75154800	-1.86348100
H	3.99879500	1.63520500	-3.02053000
H	1.93932500	-0.27437100	-2.70240100
H	2.30332500	-1.98496800	-2.37457800

N-INT8-D

Zero-point correction= 0.735041 (Hartree/Particle)
Thermal correction to Energy= 0.778614
Thermal correction to Enthalpy= 0.779558
Thermal correction to Gibbs Free Energy= 0.656279
E(solv) = -2485.30514960 A.U.

C	-0.56485000	1.57064000	-0.85919500
C	-1.36631600	2.64273900	-0.37208100
O	-1.09166300	3.51780200	0.43764900
O	-2.65279100	2.59364600	-0.91379200
C	-4.72157500	3.62616500	-1.43194100
C	-3.50210500	3.66923800	-0.53272500
H	-1.01420800	0.91866100	-1.60367400
H	-5.41455400	4.43321100	-1.17850600
H	-4.42507900	3.73363500	-2.47841500
H	-5.25531300	2.67459300	-1.32910100
H	-3.77565300	3.57429900	0.52801700
H	-2.96291100	4.61499600	-0.63342400
C	-0.08567800	-2.73502200	-1.61684200
C	0.93938000	-2.66948200	-2.57152500
C	1.17140300	-3.66360200	-3.50961500
C	0.32245400	-4.76454000	-3.47272800
C	-0.70464000	-4.86106200	-2.52000900
C	-0.91712500	-3.85988500	-1.58136700
C	0.05815700	-1.51960400	-0.86487300
C	1.10039100	-0.80648100	-1.40356600
H	1.97503600	-3.57220200	-4.23155900
H	0.46200600	-5.56681600	-4.19003400
H	-1.33603300	-5.74409700	-2.51142300
H	-1.68087200	-3.95500900	-0.81580900
O	1.64506700	-1.51265800	-2.44716600
C	1.67657600	0.47282000	-1.03690700
N	-0.72940100	-1.07674800	0.22684900
C	3.15328400	0.55371600	-1.02836600

C	3.83997800	1.71593200	-1.40525200
C	3.91043400	-0.55986900	-0.63160500
C	5.22929700	1.77429600	-1.35050000
H	3.27760100	2.57512600	-1.75948000
C	5.29788900	-0.50803700	-0.59634600
H	3.39404200	-1.46776000	-0.32627400
C	5.96689600	0.66414500	-0.94840800
H	5.73862600	2.68797500	-1.64325100
H	5.85975800	-1.38437500	-0.28283500
H	7.05166100	0.70676200	-0.91997900
S	-0.46599200	-1.79555200	1.73609200
O	-0.70045800	-3.22244300	1.57801700
O	-1.34394900	-1.01711400	2.61116600
C	1.22876500	-1.50743700	2.12509900
C	2.08797100	-2.59088000	2.26485500
C	1.66967200	-0.18913700	2.23760900
C	3.42720300	-2.33782000	2.54937800
H	1.70736500	-3.60049100	2.14992000
C	3.01171100	0.03817000	2.49838600
H	0.99680700	0.65408800	2.10519200
C	3.90291300	-1.02942000	2.66610200
H	4.11610400	-3.16996600	2.66556600
H	3.36706500	1.06373700	2.53559000
C	5.35702900	-0.75106700	2.93832400
H	5.76085200	-0.07373500	2.17871200
H	5.48533900	-0.27118000	3.91427400
H	5.94853100	-1.67017400	2.93109000
C	0.84277100	1.51753900	-0.67670600
C	1.45598900	2.70695800	0.02782100
O	1.93328200	2.67211700	1.13740600
O	1.39357300	3.81106100	-0.72139100
C	1.24314400	6.16212800	-0.93440900
C	1.66930200	5.03180800	-0.02365800
H	1.43242500	7.12673200	-0.45520000
H	1.79074900	6.12861800	-1.88018300
H	0.17401500	6.07803300	-1.14620600
H	1.09809800	5.02205700	0.90830700
H	2.73608800	5.07024800	0.22159100
H	-0.67713400	-0.03476200	0.30186900
N	-5.99354600	-0.31262300	0.71912800
C	-5.65591700	-0.37074000	-0.70438100
C	-4.13143800	-1.91680400	1.04044300
C	-3.73178400	0.48164300	1.36453900
C	-5.25031800	0.78625500	1.34486800
C	-5.61064900	-1.57470500	1.35468800

C	-4.11794800	-0.39499700	-0.89635400
N	-3.52198900	-0.68702600	0.44673800
H	-6.11981100	-1.26636400	-1.12823300
H	-6.08799000	0.49757200	-1.20915700
H	-4.02425600	-2.71288300	0.29906400
H	-3.54011900	-2.17435900	1.92155400
H	-3.35303000	0.17822400	2.34135600
H	-3.12143600	1.30353100	0.98480800
H	-5.62265000	0.93224300	2.36224800
H	-5.45638500	1.70015300	0.77949500
H	-5.76364300	-1.47305600	2.43274100
H	-6.27131700	-2.36892900	0.99690000
H	-3.77710300	-1.17628400	-1.58107700
H	-3.70633600	0.56842300	-1.21332100
H	-2.49399500	-0.85775200	0.32073700

N-INT9

Zero-point correction= 0.401417 (Hartree/Particle)
Thermal correction to Energy= 0.428013
Thermal correction to Enthalpy= 0.428957
Thermal correction to Gibbs Free Energy= 0.341030
E(solv) = -1319.84583262 A.U.

C	-0.11170800	-2.44489700	0.21649400
C	-1.29694500	-2.38914600	-0.67841900
O	-1.41193300	-1.69010700	-1.65614100
O	-2.23057300	-3.25699200	-0.26612400
C	-4.39371000	-4.22411500	-0.36975200
C	-3.45584200	-3.22193400	-1.00663800
H	0.06662500	-3.36895300	0.75773600
H	-5.35032300	-4.23185000	-0.89892500
H	-3.96636200	-5.22918600	-0.40906600
H	-4.57497200	-3.96720100	0.67686000
H	-3.85217800	-2.20202000	-0.97112000
H	-3.24577300	-3.45878300	-2.05410900
C	-2.32452200	1.92870100	0.64704700
C	-1.49697500	2.70335800	-0.15796800
C	-1.79794800	4.01369600	-0.49735000
C	-2.98469200	4.53300500	0.01433300
C	-3.83328900	3.77186100	0.82866300
C	-3.50923600	2.45745300	1.14836200
C	-1.69241500	0.60125700	0.74511800
C	-0.41003400	0.76151900	-0.00635100
H	-1.13650700	4.59319700	-1.13072600
H	-3.25802200	5.55564900	-0.22628100
H	-4.74852200	4.21245200	1.20871200

H	-4.16412300	1.85979200	1.77724000
O	-0.38073300	2.03494200	-0.56139900
C	0.63176700	-0.06220600	-0.19840500
N	-2.10404000	-0.48126300	1.28056700
C	1.80514700	0.32924800	-1.02410400
C	2.27575600	-0.57335300	-1.98162200
C	2.47239000	1.54540300	-0.84387800
C	3.38767200	-0.26040000	-2.75868500
H	1.74988400	-1.51346100	-2.12440200
C	3.58749300	1.85147900	-1.61479400
H	2.11886000	2.23795100	-0.08718800
C	4.04748800	0.95089700	-2.57524000
H	3.73739900	-0.96480700	-3.50702300
H	4.10273000	2.79552400	-1.46429300
H	4.91822900	1.19405100	-3.17642400
C	0.71201300	-1.41242400	0.41362200
C	1.86772600	-1.66593600	1.34729600
O	2.17877800	-2.75205400	1.77307900
O	2.50640300	-0.53342400	1.65944700
C	4.32959300	0.68099000	2.55386300
C	3.66947700	-0.67900500	2.48485900
H	5.23377700	0.62978100	3.16617400
H	4.60124000	1.01892100	1.55025100
H	3.65086000	1.41549200	2.99508700
H	3.35936000	-1.04460300	3.46866600
H	4.32273200	-1.43446700	2.03915800
H	-3.00738800	-0.32026000	1.73609000

N-TS5

Zero-point correction= 0.647288 (Hartree/Particle)
Thermal correction to Energy= 0.685726
Thermal correction to Enthalpy= 0.686670
Thermal correction to Gibbs Free Energy= 0.578864
E(solv) = -2442.82874889 A.U.
Imaginary Frequency 1194.99*i*

C	3.23719600	-0.77198800	-0.80658900
C	3.38454500	0.45177500	-1.47624100
C	4.47092300	0.77024800	-2.27802000
C	5.47154200	-0.19123700	-2.39278700
C	5.36431900	-1.41774400	-1.71767900
C	4.26042200	-1.72335400	-0.92824200
C	1.98308400	-0.67203500	-0.07343900
C	1.50754300	0.59383000	-0.32740400
H	4.52431000	1.73229800	-2.77770700
H	6.34245700	0.01155300	-3.01152100

H	6.16037100	-2.15146300	-1.82352200
H	4.15532000	-2.68276000	-0.43568200
O	2.35038500	1.27113900	-1.19656900
C	0.29643500	1.39696800	0.01072900
H	-0.45839100	1.11824900	-1.03878600
N	1.44777000	-1.53904200	0.87764600
C	0.63299300	2.88531700	-0.10136000
C	1.48050000	3.49519000	0.83457000
C	0.10677700	3.66277000	-1.13851400
C	1.78448000	4.85078000	0.75631900
H	1.91089000	2.88036000	1.62449500
C	0.41123600	5.02362900	-1.21066200
H	-0.58052400	3.20779100	-1.85973900
C	1.24600300	5.62373900	-0.27183700
H	2.44727400	5.30263100	1.49168700
H	-0.01754900	5.61837700	-2.01395500
H	1.47782500	6.68490300	-0.33826800
S	1.16563600	-3.06027500	0.56032700
O	0.90631200	-3.75316300	1.83450100
O	2.14930900	-3.70310400	-0.33765900
C	-0.38542700	-3.11482700	-0.34506100
C	-1.48186500	-3.79708500	0.17344300
C	-0.51306800	-2.35546900	-1.50773500
C	-2.71159800	-3.71320700	-0.48075600
H	-1.35906800	-4.35145500	1.09873500
C	-1.74562900	-2.26141200	-2.14059400
H	0.32036400	-1.76551800	-1.87731700
C	-2.85993700	-2.93928400	-1.63538000
H	-3.57966100	-4.22741300	-0.06802000
H	-1.87735100	-1.55047700	-2.94953400
C	-4.19141600	-2.75714000	-2.31969300
H	-4.29028400	-3.42278600	-3.18746700
H	-5.02400600	-2.97338000	-1.63970200
H	-4.26167200	-1.71957200	-2.66807500
N	-4.48565100	0.68958300	0.93193000
N	-1.92524100	0.93475200	1.23560400
C	-3.78715700	-0.51095100	0.44695900
H	-4.10864800	-1.36864400	1.05004200
H	-4.06479300	-0.66235600	-0.59840400
C	-3.99259700	1.83516400	0.16202400
H	-4.08048100	1.61897400	-0.90777000
H	-4.60079600	2.71464300	0.40513200
C	-4.15564500	0.90937200	2.33058800
H	-4.58906200	1.86923400	2.63633700
H	-4.61830400	0.12347800	2.93853100

C	-2.62484100	0.89491400	2.57035700
H	-2.27623600	1.76362000	3.13937900
H	-2.30160900	-0.01015400	3.07183400
C	-2.24812600	-0.34654500	0.49372700
H	-1.73955800	-1.14987000	1.03067600
H	-1.83239300	-0.24114300	-0.51276800
C	-2.51284200	2.12267600	0.49882400
H	-1.96777600	2.30787900	-0.42421600
H	-2.38017500	2.97491900	1.17609600
C	-0.40239900	1.15080800	1.37035700
H	-0.36508700	2.10040300	1.92433800
C	0.20408900	0.16833800	2.38580900
O	1.45609200	0.55547500	2.64816600
O	-0.38118400	-0.67870000	3.01848600
C	2.22846800	-0.36508500	3.43450500
H	2.07551700	-0.11891600	4.49404900
H	1.86583200	-1.37389000	3.22763800
C	3.67263200	-0.20528300	3.01035500
H	4.31416900	-0.84458000	3.62621100
H	3.77404500	-0.50597400	1.96430400
H	4.00524200	0.83254100	3.11798800
C	-2.27749400	1.17892300	-2.42296700
O	-2.43729700	2.44118100	-2.46588400
O	-3.23801300	0.34836800	-2.55464300
O	-1.05902900	0.69318900	-2.14491600

N-TS6-A

Zero-point correction= 0.543231 (Hartree/Particle)
Thermal correction to Energy= 0.581476
Thermal correction to Enthalpy= 0.582420
Thermal correction to Gibbs Free Energy= 0.467585
E(solv) = -4714.26694341 A.U.
Imaginary Frequency 533.53*i*

C	-1.32650200	3.30150000	-0.56362600
C	-0.11682100	4.00034600	-0.49985300
C	0.01517800	5.33766700	-0.85945100
C	-1.13254400	5.98039400	-1.29793300
C	-2.36111800	5.30473000	-1.37799200
C	-2.47401400	3.97068000	-1.01668100
C	-1.02404600	1.93919200	-0.10554100
C	0.39117200	1.95123200	0.16295600
H	0.97617300	5.83463400	-0.79118500
H	-1.07825300	7.02613600	-1.58684300
H	-3.23900000	5.83564400	-1.73137400
H	-3.42455700	3.45911300	-1.09650400

O	0.89851500	3.23524600	-0.05913400
C	1.23084300	1.04370200	0.79126300
N	-1.79133600	0.89607100	0.14383800
C	2.44912900	1.58297700	1.47371800
C	3.44457200	2.26513500	0.76597000
C	2.62807300	1.35139700	2.84056600
C	4.59276000	2.70505300	1.41588000
H	3.32041400	2.43218600	-0.29890400
C	3.77074600	1.80592700	3.49177800
H	1.85977100	0.82030800	3.39513600
C	4.75754000	2.48226200	2.78071400
H	5.36508800	3.21674100	0.84978400
H	3.89147200	1.62343700	4.55541500
H	5.65544500	2.82630000	3.28533500
S	-3.41472900	1.02074800	0.01716400
O	-3.85243400	1.18286400	-1.37791800
O	-3.96480500	1.97272300	0.98724400
C	-3.88489400	-0.62564100	0.50368000
C	-4.95681200	-1.21344800	-0.15703000
C	-3.23137100	-1.28176800	1.54255600
C	-5.38514400	-2.47764500	0.23842500
H	-5.42823100	-0.68571200	-0.97968800
C	-3.66454600	-2.54633200	1.91600100
H	-2.36587800	-0.82676300	2.01052600
C	-4.74602500	-3.15889500	1.27503600
H	-6.22061400	-2.94725900	-0.27484200
H	-3.13800100	-3.07716600	2.70487700
C	-5.18386900	-4.54302400	1.68250100
H	-4.42043100	-5.28483800	1.42429400
H	-5.34492700	-4.60428200	2.76356900
H	-6.11352900	-4.82917700	1.18318700
C	1.07750100	-0.36799900	0.86071100
C	0.03944100	-1.14538700	0.15138500
O	-0.54011100	-2.10487200	0.62050100
O	-0.07163600	-0.75858300	-1.12879200
C	-1.38195800	-0.50185500	-3.08595100
C	-1.08968200	-1.39651200	-1.89938600
H	-2.12260500	-0.97606100	-3.73705700
H	-1.78937900	0.45379700	-2.74595100
H	-0.47066700	-0.32341500	-3.66389700
H	-0.71877400	-2.38008400	-2.20907500
H	-1.97486700	-1.54097100	-1.27247800
H	1.42110500	-0.84420300	1.77587600
Br	4.75393200	-1.71216100	-1.58768400
C	2.76089800	-1.02088200	-0.25290900

C	2.60319600	-2.43343200	0.19461400
O	2.99140000	-2.85839000	1.25737400
O	1.86727300	-3.14473300	-0.67471400
C	0.35100000	-4.92102200	-1.08419400
C	1.50428300	-4.45025900	-0.22421100
H	2.34101400	-0.69394300	-1.19049900
H	3.45250000	-0.40872200	0.30161900
H	-0.51509800	-4.27792500	-0.90816400
H	0.61856900	-4.88343000	-2.14419800
H	0.08549700	-5.95144000	-0.82750400
H	2.38046000	-5.10277200	-0.30708600
H	1.21712200	-4.39155100	0.82862200

N-TS6-B

Zero-point correction= 0.542393 (Hartree/Particle)
Thermal correction to Energy= 0.581155
Thermal correction to Enthalpy= 0.582099
Thermal correction to Gibbs Free Energy= 0.464708
E(solv) = -4714.27967410 A.U.
Imaginary Frequency 506.13*i*

C	0.38396300	3.20708200	-0.54106300
C	-0.94768200	3.26061500	-0.96775600
C	-1.64567700	4.45398700	-1.12089200
C	-0.95477100	5.62260000	-0.83006900
C	0.38228600	5.59691200	-0.40319900
C	1.06383600	4.39733200	-0.25402200
C	0.73515600	1.78358500	-0.51127000
C	-0.46243200	1.10728600	-0.93573400
H	-2.67750700	4.45386300	-1.45428900
H	-1.46239800	6.57714100	-0.93571500
H	0.88974500	6.53041800	-0.18320600
H	2.09297000	4.38276000	0.08450100
O	-1.46785200	2.03784900	-1.20655700
C	-0.73777300	-0.23236600	-1.10361700
N	1.83949000	1.13919400	-0.21327900
C	0.35262300	-1.18875000	-0.74427400
C	1.26197500	-1.62259200	-1.70733000
C	0.49199300	-1.59892200	0.58146000
C	2.31716100	-2.45313100	-1.34622000
H	1.15155100	-1.28513600	-2.73442900
C	1.54397000	-2.43812100	0.93662700
H	-0.20392900	-1.22085700	1.32653200
C	2.46027100	-2.86332200	-0.02192300
H	3.03849500	-2.76984500	-2.09492700
H	1.65988900	-2.74523200	1.97231100

H	3.29360100	-3.49977400	0.26375100
S	3.20439400	1.90295500	0.23295500
O	3.06026700	2.62754900	1.50009100
O	3.82070600	2.62393100	-0.88664600
C	4.20267400	0.46258700	0.55802000
C	4.17866100	-0.10861900	1.82472700
C	4.96655700	-0.08389800	-0.46450800
C	4.93199500	-1.25233400	2.06317600
H	3.57712500	0.34929100	2.60354400
C	5.71485500	-1.22904500	-0.21059000
H	4.97075400	0.39491600	-1.43852500
C	5.70301900	-1.82971000	1.05029300
H	4.92083600	-1.70812700	3.05053500
H	6.31818000	-1.66523600	-1.00334100
C	6.48009300	-3.09626900	1.30797300
H	5.84243200	-3.97870800	1.17713400
H	7.32274200	-3.19363800	0.61772400
H	6.86936500	-3.12341800	2.32992700
C	-2.02866600	-0.66060000	-1.51963600
C	-2.28712300	-1.96026500	-2.15752500
O	-3.15108500	-2.15812300	-2.98811200
O	-1.52136400	-2.95788000	-1.66615100
C	-0.70477000	-5.16140800	-1.57552400
C	-1.71246000	-4.24638900	-2.24153200
H	-0.77159400	-6.17206200	-1.98930700
H	0.30783000	-4.77639800	-1.72657300
H	-0.89000500	-5.20771600	-0.49924600
H	-2.74453000	-4.57005400	-2.07158500
H	-1.56047600	-4.18449900	-3.32445400
H	-2.68325800	0.11295600	-1.90915400
Br	-4.56766500	-1.87792300	2.11839100
C	-3.14818000	-1.18753100	0.24820300
C	-2.94125300	0.14081700	0.87046300
O	-2.00576000	0.43469400	1.57838700
O	-3.89340300	1.00906400	0.49155600
C	-4.80860300	3.18213000	0.36963600
C	-3.77526500	2.31340700	1.05494500
H	-4.00462100	-1.36773600	-0.38234300
H	-2.46515800	-1.98364200	0.49848900
H	-4.64174900	3.17569700	-0.71165300
H	-5.81746900	2.80726200	0.56130900
H	-4.73850100	4.21259300	0.73072400
H	-3.94379500	2.24710600	2.13512700
H	-2.75964600	2.68664900	0.89554900

N-TS6-C

Zero-point correction= 0.542810 (Hartree/Particle)
Thermal correction to Energy= 0.581499
Thermal correction to Enthalpy= 0.582443
Thermal correction to Gibbs Free Energy= 0.466143
E(solv) = -4714.27671926 A.U.
Imaginary Frequency 528.53*i*

C	-0.70103800	3.32381800	-0.30757200
C	-2.06600100	3.22845600	-0.60596400
C	-2.93768700	4.31071300	-0.53566800
C	-2.39496800	5.52331200	-0.13760500
C	-1.03202300	5.64629700	0.17947100
C	-0.17488900	4.55897400	0.09939200
C	-0.16639900	1.96944000	-0.48372100
C	-1.30324000	1.17277800	-0.86368200
H	-3.98802600	4.18826300	-0.77425200
H	-3.03995300	6.39434600	-0.06433600
H	-0.64288000	6.60917800	0.49384500
H	0.87405000	4.66377900	0.34622800
O	-2.44258700	1.97857800	-0.93539000
C	-1.43494200	-0.17219000	-1.14320300
N	1.03231700	1.44620600	-0.34571000
C	-2.82357500	-0.63095300	-1.46890500
C	-3.75097400	-0.73925700	-0.42958100
C	-3.22226100	-0.90282900	-2.77749400
C	-5.05901600	-1.13578700	-0.69763500
H	-3.43686900	-0.50963100	0.58630000
C	-4.53222100	-1.28393100	-3.04369500
H	-2.49573000	-0.83153300	-3.58016200
C	-5.45290000	-1.40529200	-2.00450000
H	-5.76905800	-1.22948500	0.11862200
H	-4.83324400	-1.49662400	-4.06544000
H	-6.47374600	-1.71190000	-2.21444900
S	2.30465900	2.38676300	0.07800700
O	2.19896100	2.79417600	1.48333500
O	2.57028600	3.45067000	-0.89828500
C	3.60550500	1.18429900	-0.08761400
C	4.70645300	1.49773100	-0.87077600
C	3.50590000	-0.03520200	0.58031700
C	5.73422900	0.56395300	-0.99274300
H	4.73905300	2.45358800	-1.38307200
C	4.53632200	-0.95397900	0.43793600
H	2.62993100	-0.26517900	1.18231000
C	5.66034200	-0.66982600	-0.34762900
H	6.60075600	0.79497800	-1.60757800

H	4.46307000	-1.91511200	0.94118200
C	6.75752700	-1.69379900	-0.49532200
H	6.37849100	-2.60781000	-0.96526800
H	7.57760600	-1.31281100	-1.11005900
H	7.16698300	-1.97644000	0.48015200
C	-0.35895300	-1.09354000	-0.98932200
C	-0.29333100	-2.34655700	-1.75180700
O	-1.16810600	-2.91908400	-2.36705900
O	0.95783800	-2.87418800	-1.64017400
C	2.57082500	-4.56437800	-1.97578000
C	1.14582400	-4.13854200	-2.26665400
H	2.78306000	-5.53101600	-2.44202900
H	3.27563600	-3.82353800	-2.36326400
H	2.72670900	-4.65336700	-0.89744800
H	0.41639700	-4.85297900	-1.87114100
H	0.95941000	-4.04322300	-3.34194500
H	0.61489400	-0.67104400	-0.77110200
Br	-1.34075100	-3.38229800	2.89556800
C	-0.77007400	-2.10948400	0.85923100
C	-0.29825000	-0.98004600	1.70311900
O	0.83534200	-0.84613400	2.10037900
O	-1.27666500	-0.09262900	1.92712500
C	-2.11670900	1.94782600	2.77221800
C	-0.89432300	1.05791900	2.69312400
H	-1.80812100	-2.23086400	0.59701200
H	-0.04700700	-2.87772600	0.63449700
H	-2.48857800	2.17082900	1.76781500
H	-2.91704000	1.45602100	3.33265400
H	-1.86577400	2.89186100	3.26412700
H	-0.56223800	0.72234600	3.68054500
H	-0.04769800	1.55322200	2.20614400

N-TS6-D

Zero-point correction= 0.543669 (Hartree/Particle)
Thermal correction to Energy= 0.581732
Thermal correction to Enthalpy= 0.582676
Thermal correction to Gibbs Free Energy= 0.469030
E(solv) = -4714.27072305 A.U.
Imaginary Frequency 527.71*i*

C	-0.59578800	2.87268600	-0.22283800
C	0.79523600	2.93155700	-0.08175900
C	1.53266000	4.08911600	-0.31355600
C	0.82049800	5.21503700	-0.69852100
C	-0.57604000	5.18538500	-0.84507200
C	-1.29638900	4.02425800	-0.61018700

C	-0.96581300	1.49632900	0.11583300
C	0.28909400	0.85428000	0.44762600
H	2.60815200	4.09473000	-0.17815500
H	1.35626700	6.14122500	-0.88652500
H	-1.10006800	6.08621700	-1.14723600
H	-2.37196200	4.00834200	-0.73273400
O	1.32982100	1.76110100	0.30717100
C	0.55087400	-0.42520800	0.88302400
N	-2.11989400	0.87399600	0.18481900
C	-0.51125200	-1.46753300	0.75016100
C	-0.94629800	-2.18844700	1.86318500
C	-0.97810300	-1.81705700	-0.52181500
C	-1.85053900	-3.23946800	1.71301000
H	-0.57208500	-1.92070500	2.84775100
C	-1.87238900	-2.87012800	-0.67020900
H	-0.61297200	-1.26140200	-1.38191900
C	-2.31008000	-3.58422800	0.44542200
H	-2.18678200	-3.79158800	2.58631200
H	-2.22700000	-3.13761500	-1.66066300
H	-3.00929800	-4.40687600	0.32374700
S	-3.52338400	1.64289500	-0.11972800
O	-3.61817200	2.16747900	-1.48716400
O	-3.86745400	2.57555700	0.95855700
C	-4.63382900	0.25064400	-0.03902700
C	-5.81415200	0.33566700	-0.77156800
C	-4.36536600	-0.85512700	0.75955800
C	-6.74321400	-0.69471900	-0.68607600
H	-5.97962400	1.19331000	-1.41597100
C	-5.30345500	-1.88000600	0.82833100
H	-3.41844400	-0.92323500	1.28633200
C	-6.50413900	-1.81229900	0.11835600
H	-7.66375400	-0.63835800	-1.26220600
H	-5.08581300	-2.75591500	1.43530000
C	-7.52619700	-2.91586900	0.22658600
H	-7.04773000	-3.88220200	0.40981600
H	-8.21850900	-2.72905200	1.05568800
H	-8.12164200	-2.99722400	-0.68731300
C	1.81415100	-0.95657400	1.28176600
C	2.90455700	-0.19185300	1.91626100
O	2.93390700	0.97118000	2.25108600
O	3.96228100	-1.02767200	2.13534400
C	5.04615900	-0.23435300	4.16538500
C	5.13588800	-0.41178800	2.65867600
H	5.98455900	0.17111600	4.55726300
H	4.23602100	0.45523800	4.41055000

H	4.85483000	-1.19625500	4.64983100
H	5.95048100	-1.08691800	2.38618700
H	5.28613000	0.54958300	2.15995500
H	1.76062200	-1.96828200	1.67385800
Br	3.91669800	-2.89048100	-2.31099600
C	2.70601700	-1.78895200	-0.47221100
C	2.72117600	-0.49718000	-1.19738000
O	1.84813000	-0.10846600	-1.93606100
O	3.80525600	0.22008800	-0.84660200
C	4.72107500	2.35535200	-0.43890600
C	3.92581500	1.51921100	-1.42138600
H	3.54146900	-2.08485800	0.13906700
H	1.87672600	-2.45322700	-0.65865200
H	4.18894100	2.39135400	0.51764100
H	5.70842200	1.91422700	-0.27099200
H	4.85840100	3.37246400	-0.82104800
H	4.43315300	1.42104200	-2.38779800
H	2.92936600	1.93085400	-1.59597600

N-TS7-A

Zero-point correction= 0.729905 (Hartree/Particle)
Thermal correction to Energy= 0.773524
Thermal correction to Enthalpy= 0.774469
Thermal correction to Gibbs Free Energy= 0.649337
E(solv) = -2485.27893918 A.U.
Imaginary Frequency 630.23*i*

C	-0.43148900	-2.92967800	0.09205900
C	0.95538600	-2.77361500	0.15416300
C	1.83985400	-3.83209900	-0.01374600
C	1.28105700	-5.08897500	-0.21748500
C	-0.10699300	-5.27621500	-0.25132800
C	-0.97622200	-4.20488200	-0.09640200
C	-0.99462800	-1.58908700	0.29558200
C	0.16865300	-0.70828300	0.40908800
H	2.91429500	-3.68189400	0.02276600
H	1.93840900	-5.94347500	-0.34745300
H	-0.50868800	-6.27221900	-0.40199900
H	-2.04866700	-4.35179100	-0.13549700
O	1.33427600	-1.48585600	0.37105000
C	0.27125700	0.65031900	0.50153800
N	-2.19939500	-1.13139800	0.41713500
C	-0.93813200	1.47180000	0.20609100
C	-1.63020200	1.32881800	-0.99885900
C	-1.38450300	2.40948700	1.13810600
C	-2.76223100	2.08702200	-1.25857600

H	-1.28246500	0.59588600	-1.72298900
C	-2.52674800	3.16536400	0.88482600
H	-0.84105500	2.53437100	2.07193400
C	-3.21828900	3.00423400	-0.31141600
H	-3.29864400	1.95789700	-2.19367200
H	-2.87621400	3.87923100	1.62496200
H	-4.11195400	3.58927800	-0.51043600
S	-3.53863900	-2.05044100	0.12925200
O	-3.88546900	-2.82304200	1.31771900
O	-3.44495400	-2.74733000	-1.15528400
C	-4.69928100	-0.72042000	-0.06771100
C	-4.98193900	0.10403100	1.01897800
C	-5.27653600	-0.50548100	-1.31001900
C	-5.85673800	1.16472700	0.84319000
H	-4.50468900	-0.07861800	1.97684700
C	-6.15662800	0.56378800	-1.46726100
H	-5.02813000	-1.16621600	-2.13422800
C	-6.45481600	1.41023000	-0.40001900
H	-6.07660300	1.82422600	1.67933800
H	-6.61560800	0.74272300	-2.43623400
C	-7.40898000	2.56523600	-0.56467300
H	-7.64318300	2.74174900	-1.61747100
H	-8.35049200	2.37246000	-0.03903500
H	-6.98780600	3.48652300	-0.14934900
C	1.52747300	1.30619000	0.88559600
C	1.64062200	2.68964800	0.43358000
O	1.28130000	3.09834700	-0.66457700
O	2.29909200	3.50637900	1.29710300
C	3.23272600	5.58533200	1.94208300
C	2.51725300	4.84012500	0.83481600
H	3.42146800	6.61958300	1.64144100
H	2.62696500	5.59239000	2.85171300
H	4.19021900	5.10943300	2.17083000
H	3.11001000	4.81332000	-0.08682900
H	1.55357900	5.29480500	0.58692600
H	2.51195200	0.77965700	-0.24943400
C	2.09466000	1.01661400	2.28060400
C	2.41820100	-0.42347200	2.59463300
O	1.76097100	-1.14029300	3.30556900
O	3.58577500	-0.82560600	2.03506400
C	5.23626100	-2.51296000	1.65468800
C	3.96076300	-2.16160500	2.39118500
H	3.01599200	1.59162500	2.40116800
H	1.39633900	1.33563900	3.06323200
H	5.07571300	-2.56890500	0.57349800

H	6.01231000	-1.76705700	1.84924800
H	5.60277400	-3.48650900	1.99174400
H	4.10236300	-2.20713100	3.47575200
H	3.13772300	-2.83968200	2.14695700
N	4.31656200	0.19108300	-3.44034200
C	4.82138000	1.40425900	-2.79136900
C	3.98390900	-0.62750100	-1.12584600
C	2.10644800	0.36648000	-2.32355400
C	2.87470500	0.33947200	-3.67118200
C	4.53718700	-0.94350500	-2.53944800
C	3.94591400	1.76155500	-1.56384500
N	3.11132200	0.56875500	-1.24240500
H	5.86135000	1.22378100	-2.50162400
H	4.81433100	2.22435400	-3.51497300
H	4.76645200	-0.38082900	-0.40338600
H	3.37721200	-1.43056700	-0.70590700
H	1.59998200	-0.57904400	-2.10799900
H	1.38374200	1.18395200	-2.23950900
H	2.53004300	-0.49011800	-4.29481400
H	2.71565100	1.26606700	-4.23088400
H	4.03768400	-1.81816000	-2.96794000
H	5.60893400	-1.15987700	-2.49638000
H	4.52947300	2.00611200	-0.67070900
H	3.25398200	2.58249400	-1.75991900

N-TS9

Zero-point correction= 0.400941 (Hartree/Particle)
Thermal correction to Energy= 0.426483
Thermal correction to Enthalpy= 0.427427
Thermal correction to Gibbs Free Energy= 0.343257
E(solv) = -1319.82268794 A.U.
Imaginary Frequency 458.64*i*

C	-0.73489700	-1.89794300	0.59623200
C	-1.60194300	-2.19508300	-0.59436800
O	-1.39610000	-1.83711500	-1.72685700
O	-2.63265500	-2.97381500	-0.23385000
C	-4.61699700	-4.18819500	-0.69668400
C	-3.53836400	-3.30937900	-1.29186000
H	-0.82564800	-2.61780100	1.40574300
H	-5.33668300	-4.47325500	-1.46864000
H	-4.18162300	-5.09711900	-0.27404500
H	-5.14956700	-3.65856200	0.09722300
H	-3.94455500	-2.38439400	-1.71284000
H	-2.98318600	-3.81771000	-2.08590900
C	-2.15333900	2.05107300	0.66726200

C	-1.42104500	2.79359100	-0.26337300
C	-1.68042700	4.13461000	-0.51827200
C	-2.70748100	4.72086400	0.21109300
C	-3.45642900	3.99427900	1.15151200
C	-3.19543400	2.65061600	1.37679000
C	-1.65645500	0.68254500	0.55666800
C	-0.50171900	0.78795800	-0.31401900
H	-1.10088100	4.68435500	-1.25077700
H	-2.93932600	5.76833400	0.04611600
H	-4.25165700	4.48964400	1.69787000
H	-3.78494500	2.08039600	2.08907800
O	-0.45416400	2.06040400	-0.86921200
C	0.59421300	-0.03458200	-0.30563300
N	-2.10845800	-0.43091900	1.05497400
C	1.87563200	0.33838300	-0.95113900
C	2.56073900	-0.65092100	-1.66380900
C	2.43793900	1.61308000	-0.83721300
C	3.78664600	-0.37114700	-2.25684600
H	2.11291600	-1.63694400	-1.75176900
C	3.67098700	1.88646000	-1.41863900
H	1.91813600	2.38051600	-0.27466300
C	4.34775000	0.89797500	-2.13088300
H	4.30521300	-1.14409000	-2.81574500
H	4.10753600	2.87500400	-1.31334800
H	5.30786800	1.11732300	-2.58808900
C	0.47736400	-1.24699800	0.46999300
C	1.52187800	-1.63819900	1.44758700
O	1.44589800	-2.59787300	2.18558900
O	2.57763900	-0.80933700	1.43764000
C	4.82756100	-0.25397900	1.86200600
C	3.69929200	-1.19283300	2.23567000
H	5.73299900	-0.50435000	2.42152700
H	5.03778000	-0.32818300	0.79103000
H	4.55325100	0.78095300	2.08270500
H	3.42838700	-1.12052400	3.29391200
H	3.94392100	-2.23870000	2.02731100
H	-2.72849600	-0.30960400	1.85956500

N-TS8

Zero-point correction= 0.732103 (Hartree/Particle)
Thermal correction to Energy= 0.776116
Thermal correction to Enthalpy= 0.777060
Thermal correction to Gibbs Free Energy= 0.651427
E(solv) = -2485.26069613 A.U.
Imaginary Frequency 190.49*i*

C	0.28838800	2.03480700	-1.02684500
C	-0.36991200	3.20380600	-0.43624200
O	0.06093100	3.95415700	0.41045600
O	-1.63279800	3.33001400	-0.93708300
C	-3.73107600	4.42011000	-1.09017500
C	-2.37403500	4.43849000	-0.41966500
H	-0.25948800	1.52123700	-1.81109300
H	-4.34153400	5.25619600	-0.73885900
H	-3.62634900	4.49569200	-2.17575900
H	-4.26145900	3.48938400	-0.86018900
H	-2.44928100	4.34408900	0.66840400
H	-1.82880500	5.36339800	-0.63088300
C	-0.47260500	-2.52683300	-1.33435600
C	0.75503800	-2.97409500	-1.81671000
C	0.96843600	-4.25783600	-2.27913800
C	-0.12522800	-5.12697500	-2.23252800
C	-1.35993400	-4.71334700	-1.72363100
C	-1.54496100	-3.41094400	-1.25995500
C	-0.27149600	-1.14782800	-0.92524200
C	1.14035300	-0.86361100	-1.17919600
H	1.93942700	-4.56761000	-2.64869100
H	-0.00597600	-6.14679900	-2.58407400
H	-2.17939700	-5.42321700	-1.67194900
H	-2.47938500	-3.10093700	-0.80094000
O	1.70166300	-1.98984300	-1.74300500
C	1.97582000	0.21101000	-0.95023800
N	-1.21178100	-0.42860400	-0.33606100
C	3.44852100	0.08749400	-1.10378000
C	4.17072200	1.14709500	-1.66899200
C	4.15857500	-1.04299200	-0.67255000
C	5.55706400	1.08866700	-1.78587700
H	3.63836800	2.02363600	-2.02747400
C	5.54030300	-1.10345400	-0.79841600
H	3.61524300	-1.87144400	-0.23187000
C	6.24840900	-0.03669900	-1.35128600
H	6.09323100	1.92281400	-2.22892800
H	6.06963400	-1.98905100	-0.45681300
H	7.32908100	-0.08677000	-1.44467200
S	-1.33819400	-0.89979000	1.91227400
O	-2.31061000	-2.03434900	1.81701000
O	-1.59856400	0.12488500	2.96032000
C	0.28075800	-1.59160000	2.18104900
C	0.56697200	-2.88197000	1.74936900
C	1.29062500	-0.72108700	2.58663000
C	1.88886800	-3.32052100	1.77251600

H	-0.23736300	-3.52553400	1.40319700
C	2.60254500	-1.17153200	2.59787000
H	1.05273900	0.30131300	2.86229000
C	2.91703700	-2.47735100	2.20220600
H	2.12563500	-4.32718500	1.43598200
H	3.39640000	-0.48960600	2.89030400
C	4.34696100	-2.95291100	2.22856000
H	5.03309800	-2.13621400	1.98429000
H	4.61543100	-3.32754900	3.22286800
H	4.50960400	-3.76514500	1.51329400
C	1.45787800	1.51256900	-0.57212600
C	2.28219900	2.31311000	0.41582900
O	2.50325200	1.95363900	1.54485900
O	2.72936400	3.45019700	-0.11810400
C	3.59917100	5.64510000	0.06109300
C	3.32738300	4.36152500	0.81379500
H	4.04953000	6.38445800	0.72895400
H	4.28279000	5.46740300	-0.77348300
H	2.66405100	6.05115900	-0.33279000
H	2.62404500	4.51011300	1.63810100
H	4.24020200	3.91051300	1.21524900
H	-0.91808700	0.53805400	-0.19194700
N	-6.28826900	0.45274500	-0.15836900
C	-5.68785400	0.68786300	-1.47155000
C	-4.77461100	-1.50834000	0.04220200
C	-4.08597000	0.65149600	0.96916100
C	-5.53434000	1.19420000	0.85450900
C	-6.22857900	-0.97707900	0.15569200
C	-4.17556600	0.34211100	-1.45270400
N	-3.88682600	-0.32364900	-0.14974900
H	-6.21865600	0.07402900	-2.20515600
H	-5.83832800	1.73653400	-1.74473800
H	-4.63414300	-2.15320700	-0.83000400
H	-4.40736300	-2.02722100	0.92989600
H	-3.89288200	0.11688300	1.90075400
H	-3.32002400	1.42612000	0.86170500
H	-6.04970800	1.10085000	1.81393200
H	-5.54068300	2.25252000	0.57757600
H	-6.61405200	-1.11706300	1.16928100
H	-6.89001600	-1.51509000	-0.52917700
H	-3.87939900	-0.35110800	-2.24453200
H	-3.52740000	1.22291600	-1.50660200
H	-2.84055000	-0.59966500	-0.18386900

N-TS7-B

Zero-point correction= 0.732039 (Hartree/Particle)
Thermal correction to Energy= 0.775180
Thermal correction to Enthalpy= 0.776125
Thermal correction to Gibbs Free Energy= 0.653409
E(solv) = -2485.27364300 A.U.
Imaginary Frequency 1193.84*i*

C	0.57592000	3.00068800	-1.22521000
C	-0.78884600	3.14168300	-1.51241000
C	-1.42332600	4.36504100	-1.68516800
C	-0.63501400	5.49947500	-1.55109100
C	0.73456500	5.39434500	-1.26324600
C	1.35429000	4.16305300	-1.10393300
C	0.79944600	1.56059000	-1.13730800
C	-0.43190100	0.97842800	-1.32773500
H	-2.48236200	4.41516000	-1.91505300
H	-1.08439800	6.48001000	-1.67505100
H	1.32685900	6.29900000	-1.16974800
H	2.41524300	4.10648300	-0.89574200
O	-1.40718200	1.93648000	-1.58450800
C	-0.86558600	-0.39713200	-1.19219800
N	1.93289900	0.80035100	-0.90268900
C	-1.90846700	-0.91280000	-2.14303700
C	-3.09272500	-0.22012500	-2.43457700
C	-1.68708400	-2.12773900	-2.81052000
C	-4.03689300	-0.74867300	-3.31383600
H	-3.25915000	0.76121000	-2.00756600
C	-2.62876000	-2.65585700	-3.68526500
H	-0.74762500	-2.65201200	-2.65794500
C	-3.81692900	-1.97386000	-3.93420900
H	-4.94255500	-0.18713700	-3.52504900
H	-2.42412000	-3.59611900	-4.18843300
H	-4.55066500	-2.38113100	-4.62272500
S	3.26018500	1.57461900	-0.30825300
O	2.94764700	2.23388000	0.96616300
O	3.91492400	2.37338000	-1.34418500
C	4.29299200	0.16958500	0.03662300
C	4.18014800	-0.46942600	1.26683800
C	5.19680300	-0.25874100	-0.92929600
C	4.99003000	-1.57174700	1.52056100
H	3.46769400	-0.11240600	2.00637500
C	5.99853800	-1.36034600	-0.65424100
H	5.26464000	0.27516600	-1.87182800
C	5.90744600	-2.02826700	0.57067900
H	4.91094600	-2.08279300	2.47679100
H	6.71000900	-1.70817400	-1.39904300

C	6.80911800	-3.19813200	0.87228300
H	7.04034300	-3.76560500	-0.03353600
H	7.75937500	-2.85542900	1.29719300
H	6.35066300	-3.87744200	1.59604800
C	-0.28326500	-1.24054200	-0.27456200
C	-0.77537100	-2.65022700	-0.16371600
O	-1.89694900	-2.94248600	0.22008700
O	0.14934700	-3.56725900	-0.43955300
C	0.94154300	-5.79449700	-0.63912200
C	-0.24439800	-4.93746500	-0.25553500
H	0.69576400	-6.85185300	-0.50993100
H	1.21581200	-5.62439700	-1.68313000
H	1.80469100	-5.55639600	-0.01294200
H	-0.53938200	-5.07977800	0.78863800
H	-1.12076900	-5.13414800	-0.88123300
H	-2.37396200	-0.79401100	0.45602400
C	0.78416300	-0.95851600	0.70427200
C	0.66206900	-0.01619700	1.81932400
O	1.31724100	-0.06763800	2.84282500
O	-0.19664300	1.01854000	1.58083600
C	-0.72244700	2.10300500	3.70883300
C	0.01350300	2.19420000	2.38375700
H	1.29192700	-1.85739600	1.04816400
H	1.59357200	-0.16642600	-0.07763900
H	-1.79996100	1.96185500	3.55276500
H	-0.33359900	1.26807300	4.29675000
H	-0.58870100	3.02604400	4.28069400
H	1.08808800	2.32607400	2.52353300
H	-0.36090400	3.01635600	1.76581500
N	-4.94849600	0.11821200	2.72414600
C	-3.87773300	-0.57632200	3.44072500
C	-3.35272200	0.95933700	1.01496300
C	-4.37565900	-1.26456900	0.74007500
C	-5.49390600	-0.76487000	1.69241300
C	-4.40701300	1.32220900	2.09391600
C	-2.69486900	-0.89822400	2.49129400
N	-3.12895500	-0.51992300	1.10647300
H	-3.53954900	0.05794900	4.26497700
H	-4.29242500	-1.49192800	3.87154000
H	-2.37867200	1.43317900	1.15001000
H	-3.69751000	1.16159800	-0.00016400
H	-4.57153600	-1.05981300	-0.31519000
H	-4.14078600	-2.32410000	0.84675800
H	-6.25714800	-0.21071500	1.13887700
H	-5.98598500	-1.61082300	2.17968300

H	-5.23155100	1.88399500	1.64681000
H	-3.96541800	1.94758600	2.87486100
H	-1.80087000	-0.31118600	2.70788200
H	-2.43015300	-1.95627800	2.45290300

N-INT10

Zero-point correction= 0.404542 (Hartree/Particle)
Thermal correction to Energy= 0.430131
Thermal correction to Enthalpy= 0.431075
Thermal correction to Gibbs Free Energy= 0.346132
E(solv) = -1319.87764548 A.U.

C	-0.40428800	-1.74692600	0.87569000
C	-0.84021700	-2.37346700	-0.46441600
O	-0.12370200	-2.53865900	-1.41636100
O	-2.12805000	-2.75383200	-0.41599500
C	-4.09426200	-3.68037300	-1.37390200
C	-2.63034700	-3.37859300	-1.60793100
H	-0.15671600	-2.58036800	1.53889800
H	-4.52415300	-4.15653800	-2.25895800
H	-4.21792300	-4.35516400	-0.52301600
H	-4.64792700	-2.75965100	-1.17227200
H	-2.47786500	-2.69649400	-2.44907000
H	-2.04544700	-4.28251500	-1.80178900
C	-2.79018700	1.13581400	0.74915900
C	-2.31782500	2.23099800	0.00236300
C	-3.11598100	3.32053800	-0.32312600
C	-4.42609000	3.29233000	0.13447800
C	-4.92111100	2.21146400	0.88717700
C	-4.11676900	1.12780600	1.19954500
C	-1.66390500	0.24739000	0.83353200
C	-0.63581700	0.85733600	0.16721700
H	-2.72083100	4.14609500	-0.90391600
H	-5.08437000	4.12439800	-0.09352500
H	-5.95147600	2.23031400	1.22649300
H	-4.50396300	0.29648000	1.78079000
O	-1.01673600	2.07478100	-0.34796700
C	0.71009500	0.35234800	0.16003500
N	-1.46177400	-0.95099700	1.48832300
C	1.79186200	1.21111800	-0.38398800
C	2.56212000	0.74644900	-1.45397400
C	2.00783400	2.49594700	0.11519700
C	3.55327200	1.55141400	-2.00177400
H	2.36817600	-0.24779100	-1.84778800
C	3.01238100	3.29455100	-0.42423300
H	1.39432000	2.86287500	0.93281700

C	3.78636400	2.82416700	-1.48138700
H	4.14452300	1.18710700	-2.83649100
H	3.18591300	4.28770700	-0.02174800
H	4.56405900	3.45123400	-1.90663300
C	0.84280100	-0.91437500	0.64645700
C	2.10415300	-1.64150900	0.89368600
O	2.14283400	-2.83062500	1.13483600
O	3.19358900	-0.86386400	0.87217100
C	5.52293000	-0.47874400	0.91448300
C	4.44588200	-1.53428500	1.04789400
H	6.51198900	-0.93205500	1.02240800
H	5.45927400	0.00625300	-0.06325900
H	5.40305400	0.28860200	1.68346300
H	4.45621700	-2.01892100	2.02908300
H	4.53745000	-2.31889900	0.29041900
H	-2.30274500	-1.48648000	1.66927700