Supporting Information

for

Synthesis and antibacterial activity of monocyclic 3-carboxamide tetramic acids

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Experimental details, calculated energies (Spartan)

for selected compounds and NMR spectra

Synthesis of compound **5**

To a solution of glycinemethyl ester hydrochloride (4.0 g, 32.4 mmol) in THF (150 mL) were added $MgSO_4$ (7.8 g, 64.8 mmol), (*R*)-citronellal (**4**, 5.0 g, 32.4 mmol) and triethylamine (3.9 g, 38.9 mmol). The reaction was stirred at room temperature overnight. Then the reaction mixture was filtered and the solvent was evaporated to give the crude imine. The crude imine was dissolved in methanol (70 mL), and sodium borohydride (2.9 g, 77.8 mmol) was slowly added to the solution at 0 °C. The reaction was stirred at room temperature for 1 hour, and then quenched with 1 N NaOH (150 mL). The mixture was extracted with ethyl acetate (100 mL x 3 times). The organic layer was dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography to afford pure compound **5** (880 mg, 3.87 mmol, 12% yield) as an oil. ^1H NMR (400 MHz, $CDCl_3$) 5.08 (t, 1H, *J* = 7.2 Hz, C$\underline{H}$=C), 3.72 (s, 3H, OC$\underline{H}_3$), 3.40 (s, 2H, COC$\underline{H}_2$NH), 2.65-2.54 (m, 2H, NHC$\underline{H}_2$CH$_2$), 2.03-2.88 (m, 2H, CH$_2$C$\underline{H}_2$CH), 1.67 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.59 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.56-1.43 (m, 2H, CH(CH$_3$)C$\underline{H}_2$(CH$_2$)$_2$CH), 1.36-1.25 (m, 2H, NHCH$_2$C$\underline{H}_2$), 1.19-1.10 (m, 1H, C$\underline{H}$(CH$_3$)), 0.88 (d, 3H, *J* = 6.8 Hz, CH(C$\underline{H}_3$)); ^{13}C NMR (100 MHz, $CDCl_3$); 172.98 ($\underline{C}$=O), 131.12 (CH=$\underline{C}$(Me)$_2$), 124.71 ($\underline{C}$H=C(Me)$_2$), 51.66 (O$\underline{C}$H$_3$), 50.85 (CO$\underline{C}$H$_2$NH), 47.52 (NH$\underline{C}$H$_2$CH$_2$), 37.14 ($\underline{C}$H$_2$CH(Me)$\underline{C}$H$_2$), 30.41 ($\underline{C}$H(Me)), 25.65 (C($\underline{C}$H$_3$)$_2$), 25.41 (CH$\underline{C}$H$_2$), 19.47 (CH($\underline{C}$H$_3$)), 17.57 (C($\underline{C}$H$_3$)$_2$); MS (ES$^+$) 228.19 (M + H), 250.20 (M + Na).

Synthesis of compound **6**

To a mixture of compound **5** (880 mg, 3.87 mmol) and triethylamine (500 mg, 4.95 mmol) in CH_2Cl_2 (50 mL) was added ethyl malonyl chloride (640 mg, 4.26 mmol) and stirred at room temperature for 1 hour. The mixture was filtered, concentrated in vacuo, and flash column chromatography gave compound **6** (840 mg, 64% yield) as an oil. ^{1}H NMR (400 MHz, CDCl$_3$, mixture of rotamers, a; major, b; minor) 5.07 (t, 1H, J = 6.8 Hz, C$\underline{H}$), 4.24-4.16 (m, 2H, OC$\underline{H}_2$CH$_3$), 4.08 (s, 2H, NC$\underline{H}_2$CO a), 4.06 (s, 2H, NC$\underline{H}_2$CO b), 3.78 (s, 3H, OC$\underline{H}_3$ b), 3.73 (s, 3H, OC$\underline{H}_3$ a), 3.49 (s, 2H, COC$\underline{H}_2$CO a), 3.38 (s, 2H, COC$\underline{H}_2$CO b), 3.44-3.26 (m, 2H NC$\underline{H}_2$CH$_2$), 2.04-1.89 (m, 2H, CHC$\underline{H}_2$), 1.68 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.60 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.56-1.13 (m, 7H, C$\underline{H}_2$CH(CH$_3$)C$\underline{H}_2$ and OCH$_2$C$\underline{H}_3$), 0.92-0.89 (m, 3H, CH(C$\underline{H}_3$)); ^{13}C NMR (100 MHz, CDCl$_3$, mixture of rotamers, a; major, b; minor) 169.53 (ester $\underline{C}$=O b), 169.39 (ester $\underline{C}$=O a), 167.37 (ester $\underline{C}$=O b), 167.24 (ester $\underline{C}$=O a), 166.34 (amide $\underline{C}$=O b), 166.03 (amide $\underline{C}$=O a), 131.65 (CH=$\underline{C}$(Me)$_2$), 124.58 ($\underline{C}$H=C(Me)$_2$ b), 124.14 ($\underline{C}$H=C(Me)$_2$ a), 61.48 (O$\underline{C}$H$_2$CH$_3$), 52.53 (O$\underline{C}$H$_3$ b), 52.13 (O$\underline{C}$H$_3$ a), 49.85 (N$\underline{C}$H$_2$C=O), 48.01 ($\underline{C}$H$_2$), 47.39 ($\underline{C}$H$_2$), 45.88 ($\underline{C}$H$_2$), 41.49 ($\underline{C}$H$_2$), 40.82 ($\underline{C}$H$_2$), 36.89 ($\underline{C}$H$_2$), 36.76 ($\underline{C}$H$_2$), 35.40 ($\underline{C}$H$_2$), 33.95 ($\underline{C}$H$_2$), 30.34 ($\underline{C}$H(CH$_3$) b), 30.24 ($\underline{C}$H(CH$_3$) a), 25.67 (C($\underline{C}$H$_3$)$_2$), 25.31 (CH$_2$$\underline{C}H_2$CH), 19.34 (CH($\underline{C}H_3$)), 17.61 (C($\underline{C}H_3$)$_2$), 14.07 (OCH$_2$$\underline{C}H_3$); MS (ES$^+$) 342.25 (M + H), 364.19 (M + Na).

Synthesis of compound **7**

To the solution of compound **6** (830 mg, 2.53 mmol) in THF (20 ml) was added potassium *tert*-butoxide (310 mg, 2.79 mmol) and the mixture wsa heated under reflux for 3 hours. After the completion of the reaction, the mixture was cooled to room temperature and 1 N HCl (50 mL) was added. The mixture was extracted with

dichloromethane (50 mL x 3 times). The organic layer was dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography to afford pure compound **7** (405 mg, 1.31 mmol, 52% yield) as a solid (mp 91 $^{\circ}$C). ^{1}H NMR (400 MHz, $CDCl_3$) 5.06 (t, 1H, J = 6.4 Hz, C$\underline{H}$=C), 4.37 (q, 2H, J = 6.8 Hz, OC$\underline{H}_2$CH$_3$), 3.94 (s, 2H, C5), 3.52-3.33 (m, 2H, NC$\underline{H}_2$), 2.00-1.88 (m, 2H, CHC$\underline{H}_2$), 1.66 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.59 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.56-1.14 (m, 8H, C$\underline{H}_2$CH(CH$_3$)C$\underline{H}_2$ and OCH$_2$C$\underline{H}_3$), 0.93 (d, 3H, J = 6.0 Hz, CH(C$\underline{H}_3$)); ^{13}C NMR (100 MHz, $CDCl_3$); 183.42 (C4), 167.42 (C2), 165.85 (ester $\underline{C}$=O), 131.33 (CH=$\underline{C}$(Me)$_2$), 124.49 ($\underline{C}$H=C(Me)$_2$), 99.83 (C3), 61.28 (O$\underline{C}$H$_2$CH$_3$), 48.87 (C5), 39.43 (N$\underline{C}$H$_2$), 36.89 (CH(Me)$\underline{C}$H$_2$CH$_2$CH), 35.08 (NCH$_2$$\underline{C}H_2$), 29.95 ($\underline{C}$H(Me)), 25.63 (C($\underline{C}H_3$)$_2$), 25.27 (C=CH$\underline{C}H_2$), 19.29 (CH($\underline{C}H_3$)), 17.60 (C($\underline{C}H_3$)$_2$), 14.13 (OCH$_2$$\underline{C}H_3$); MS (ES$^-$); 308.21 (M − H); HRMS (M − H) calcd for $C_{17}H_{26}N_1O_4$, 308.1867; found, 308.1866.

Synthesis of 1-acetyl-5-(2-(methylthio)ethyl)pyrrolidine-2,4-dione (**8a**)

To a solution of *N*-acetyl-L-methionine (5.00 g, 26.1 mmol) in dichloromethane (150 mL) was added Meldrum's acid (1.1 equiv), DMAP (1.2 equiv) and DCC (1.2 equiv), and stirred overnight at room temperature. The mixture was filtered and the solution was washed with 5% aqueous $KHSO_4$ and saturated NaCl. The organic layer was evaporated to give a solid mass. The residue was dissolved in acetone and filtered for removing impurity and the solution was evaporated. The intermediate was obtained as a solid from precipitation in ethyl acetate and petrol solution. Then the solid was dissolved in ethyl acetate, and heated under reflux for 2 hours. After completion of the reaction, the solution was evaporated to give compound **6a** (5.0 g, 26.1 mmol, 31% yield) as a white solid (mp 95 °C). ^{1}H NMR (500 MHz, $CDCl_3$, enol: keto = 35: 65) 5.06 (s, 1H, C3 enol), 4.69 (dd, 1H, J_1 = 6.0 Hz, J_2 = 3.0 Hz, C5 enol),

4.50 (d, 1H, J = 7.0 Hz, C5 keto), 3.52 (dd, 1H, J_1 = 22.5 Hz, J_2 = 2.0 Hz, C3 keto),

3.25 (d, 1H, J = 22 Hz, C3 keto), 2.60 (s, 3H, C7 keto), 2.55-2.20 (m, 4H, C8 and

C9), 2.51 (s, 3H, C7 enol), 2.07 (s, 3H, C10 enol), 1.91 (s, 3H, C10 keto); ^{13}C NMR

(125 MHz, CDCl$_3$) 202.5 (C4 keto), 178.5 (C4 enol), 172.1 (C2 enol), 170.8 (C2

keto), 170.4 (C6 enol), 170.0 (C6 keto), 94.9 (C3 enol), 65.5 (C5 enol), 59.1 (C5

keto), 43.2 (C3 keto), 28.8 (C9 keto), 28.4 (C9 enol), 28.3 (C8 enol), 27.3 (C8 keto),

26.1 (C7 enol), 25.1 (C7 keto), 15.3 (C10 enol), 14.5 (C10 keto); MS (ES⁻) 214.04;

HRMS (M − H) calcd for $C_9H_{12}N_1O_3S_1$; 214.0543; found; 214.0547.

Synthesis of 1-(cyclohexanecarbonyl)-5-(2-(methylthio)ethyl)pyrrolidine-2,4-dione

(**8b**)

Compound **8b** was prepared by using the same method as for compound **3a**. Yield;

49%; mp 121 °C; ^{1}H NMR (400 MHz, CDCl$_3$, enol: keto form = 20: 80) 5.03 (s, 1H,

C3 enol), 4.67 (dd, 1H, J_1 = 6.0 Hz, J_2 = 2.8 Hz, C5 enol), 4.52 (d, 1H, J = 6.8 Hz, C5

keto), 3.55-3.48 (m, 2H keto and 1H enol, C3 and C10 keto, and C10 enol), 3.25 (d,

1H, J = 22 Hz, C3 keto), 2.53-2.15 (m, 4H, C6 and C7), 2.08 (s, 3H, C8 enol), 1.90

(s, 3H, C8 keto), 2.01-1.09 (m, 10H, C11-C15); ^{1}H NMR (400 MHz, MeOD, only enol

form) 4.88 (brs, 2H, C3 and OH), 4.69-4.677 (m, 1H, C5), 3.59-3.51 (m, 1H, C10),

2.38-2.08 (m, 4H, C6 and C7), 2.04 (s, 3H, C8), 1.94-1.20 (m, 10H, C11-C15); ^{13}C

NMR (100 MHz, MeOD, only enol form); 180.1 (C4), 177.9 (amide carbonyl), 173.3

(amide carbonyl), 66.3 (C5), 45.1 (C10), 31.4 (CH$_2$), 29.7 (CH$_2$), 29.5 (CH$_2$), 28.6

(CH$_2$), 27.2 (CH$_2$), 27.2 (CH$_2$), 26.8 (CH$_2$), 15.5 (C8); MS (ES⁻) 282.11 (M − H);

HRMS (M − H) calcd for $C_{14}H_{20}N_1O_3S_1$, 282.1169; found, 282.1171.

Synthesis of **9a**

To a solution of tetramic acid **8a** (3.0 g, 13.9 mmol) and DMAP (3.7 g, 30.7 mmol) in dichloromethane (100 mL) was slowly added butyl chloroformate (250 mg, 1.78 mmol) under nitrogen atmosphere at 0 °C, and the mixture stirred overnight at room temperature under nitrogen atmosphere. After completion of the reaction, the mixture was washed with 2 M HCl (50 mL x 2 times). The organic layer was dried over $MgSO_4$ and evaporated in vacuo. The residue was purified by flash column chromatography to give tetramic acid **9a** (4.11 g, 13.1 mmol, 94% yield) as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) 4.81 (t, 1H, $J = 4.0$ Hz, C5), 4.28 (t, 2H, $J = 6.8$ Hz, OC$\underline{H}_2$), 2.46 (s, 3H, COC$\underline{H}_3$), 2.44-2.26 (m, 4H, SC$\underline{H}_2$C$\underline{H}_2$), 2.02 (s, 3H, SC$\underline{H}_3$), 1.73-1.65 (m, 2H, OCH$_2$C$\underline{H}_2$), 1.44-1.34 (m, 2H, O(CH$_2$)$_2$C$\underline{H}_2$), 0.90 (t, 3H, $J = 7.6$ Hz, O(CH$_2$)$_3$C$\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$) 188.2 (C4), 169.8 (N$\underline{C}$=OMe), 166.8 (ester $\underline{C}$=O), 164.1 (C2), 98.4 (C3), 65.4 (O$\underline{C}$H$_2$), 56.9 (C5), 30.2 (OCH$_2$$\underline{C}H_2$), 28.4 (S$\underline{C}H_2$), 27.8 (SCH$_2$$\underline{C}H_2$), 25.2 (NC=O$\underline{C}H_3$), 18.8 (O(CH$_2$)$_2$$\underline{C}H_2$), 15.1 (S$\underline{C}H_3$), 13.5 (O(CH$_2$)$_3$$\underline{C}H_3$); MS (ES$^-$) 314.12 (M − H); HRMS (M − H), calcd for $C_{14}H_{20}N_1O_5S_1$, 314.1068; found, 314.1069.

Synthesis of **9b**

Tetramic acid **9b** was obtained from tetramic acid **8b** by using the same method as for tetramic acid **9a**; Yield 92%; mp 80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 4.87-4.85 (m, 1H, C5), 4.39-4.28 (m, 2H, OC$\underline{H}_2$), 2.43-2.30 (m, 3H), 2.06 (s, 3H, SC$\underline{H}_3$), 1.82-1.65 (m, 7H), 1.51-1.18 (m, 9H), 0.94 (t, 3H, $J = 8.0$ Hz, O(CH$_2$)$_3$C$\underline{H}_3$); ^{13}C NMR (100 MHz, $CDCl_3$); 188.5 (C4), 176.5 (N$\underline{C}$=OCH), 167.1 (ester $\underline{C}$=O), 163.9 (C2), 98.6 (C3), 65.6 (O$\underline{C}$H$_2$), 57.0 (C5), 44.0 (NC=O$\underline{C}$H), 30.4 (CH$_2$), 30.1 (CH$_2$), 28.6 (CH$_2$), 27.9 (CH$_2$), 27.8 (CH$_2$), 25.8 (CH$_2$), 25.2 (CH$_2$), 18.9 (CH$_2$), 15.3 (S$\underline{C}$H$_3$), 13.6

(O(CH$_2$)$_3$CH$_3$). MS (ES$^-$); 382.17 (M − H); HRMS (M − H), calcd for C$_{19}$H$_{28}$N$_1$O$_5$S$_1$, 382.1694; found, 382.1698.

Synthesis of 3-carboxamide tetramic acids **2** and **3**

General method: To a solution of 3-alkoxycarbonyl tetramic acid (1.0 equiv) in toluene was added primary amine (1.0 equiv), and the mixture was heated under reflux for 4 hours. After completion of the reaction as indicated by TLC, the solvent was evaporated, and column chromatography gave metal-chelated 3-carboxamide tetramic acid. The compound was dissolved in dichloromethane (50 mL) and washed with 1 N HCl (20 mL). The organic layer was dried with MgSO$_4$ and concentrated in vacuo to give pure 3-carboxamide tetramic acid.

Synthesis of **2a**

Yield 66%; mp 97 °C; Form AB:CD = 90:10; ^{1}H NMR (400 MHz, CDCl$_3$) 9.81 (brs, 1H, NH or OH), 9.55 (brs, 1H, NH or OH AB), 9.25 (brs, 1H, NH or OH AB), 7.51 (d, 2H, J = 8.8 Hz, C14 and C15 AB), 7.39 (d, 2H, J = 8.8 Hz, C14 and C15 CD), 6.91 (d, 2H, J = 8.8 Hz, C16 and C17), 3.98 (s, 2H, C5 AB), 3.87 (t, 4H, J = 4.8 Hz, C21 and C22), 3.77 (s, 2H, C5 CD), 3.43 (t, 2H, J = 7.2 Hz, C6), 3.13 (t, 4H, J = 4.8 Hz, C19 and C20), 1.59-1.54 (m, 2H, C7), 1.34-1.25 (m, 6H, C8-10), 0.89 (t, 3H, J = 6.8 Hz, C11); ^{13}C NMR (100 MHz, CDCl$_3$, only AB tautomer) 180.5 (C4), 168.8 (C2), 163.7 (C12), 148.2 (C18), 129.7 (C13), 121.4 (C14 and C15), 116.3 (C16 and C17), 99.6 (C3), 66.7 (C21 and C22), 49.7 (C5), 49.5 (C19 and C20), 41.4 (C6), 31.4 (CH$_2$), 28.4 (CH$_2$), 26.4 (CH$_2$), 22.5 (CH$_2$), 14.0 (C11); MS (ES$^-$) 386.22; HRMS (M − H) calcd for C$_{21}$H$_{28}$N$_3$O$_4$, 386.2085; found, 386.2092.

Synthesis of **2b**

Yield 90%; mp 67 °C; Form AB:CD = 90:10; ^{1}H NMR (500 MHz, CDCl$_3$) 11.10 (s, 1H, NH), 9.70 (s, 1H, OH AB), 9.30 (s, 1H, OH CD), 7.61 (d, 2H, J = 8.0 Hz, C14 and C15 AB), 7.51 (d, 2H, J = 7.6 Hz, C14 and C15 CD), 7.34 (dd, 2H, J_1 = 8.0 Hz, J_2 = 7.6 Hz, C16 and C17), 7.34 (dd, 1H, J_1 = 7.6 Hz, J_2 = 7.6 Hz, C18), 3.97 (s, 2H, C5 AB), 3.79 (s, 2H, C5 CD), 3.43 (t, 2H, J = 7.2 Hz, C6), 1.58-1.53 (m, 2H, C7), 1.36-1.26 (m, 6H, C8-10), 0.89 (t, 3H, J = 6.8 Hz, C11); ^{13}C NMR (125 MHz, CDCl$_3$); 188.8 (C4 CD), 180.6 (C4 AB), 175.8 (C2 CD), 168.6 (C2 AB), 165.2 (C12 CD), 164.0 (C12 AB), 136.9 (C13 AB), 136.3 (C13 CD), 129.0 (C16 and C17 CD), 128.9 (C16 and C17 AB), 124.7 (C18 CD), 124.4 (C18 AB), 120.5 (C14 and C15 CD), 120.0 (C14 and C15 AB), 99.7 (C3 AB), 87.2 (C3 CD), 55.4 (C5 CD), 49.4 (C5 AB), 42.2 (C6 CD), 41.3 (C6 AB), 31.3 (C9 AB), 31.2 (C9 CD), 28.3 (C7 AB), 27.9 (C7 CD), 26.3 (C8 AB), 26.2 (C8 CD), 22.4 (C10), 13.9 (C11); MS (ES$^-$) 301.1; HRMS (M + H), calcd for C$_{17}$H$_{23}$N$_2$O$_3$, 303.1703; found, 303.1700.

Synthesis of **2c**

Yield 88% (oil); Form AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 8.88 (brs, 1H, OH), 7.65 (brs, 1H, NH), 3.90 (s, 2H, C5 AB), 3.85-3.81 (m, 1H, C13), 3.67 (s, 2H, C5 CD), 3.38 (t, 2H, J = 7.2 Hz, C6), 1.91-1.88 (m, 2H, CH$_2$), 1.74-1.71 (m, 2H, CH$_2$), 1.60-1.52 (m, 3H, CH$_2$), 1.42-1.17 (m, 11H, CH$_2$), 0.88 (t, 3H, J = 6.4 Hz, C11); ^{13}C NMR (125 MHz, CDCl$_3$); 189.8 (C4 CD), 181.4 (C4 AB), 175.2 (C2 CD), 169.1 (C2 AB), 165.7 (C12 CD), 165.1 (C12 AB), 98.4 (C3 AB), 85.4 (C3 CD), 55.0 (C5 CD), 49.8 (C5 AB), 48.9 (C13 CD), 47.3 (C13 AB), 41.5 (C6 CD), 41.3 (C6 AB), 32.8 (CH$_2$), 32.7 (CH$_2$), 31.4 (CH$_2$), 29.6 (CH$_2$), 28.4 (CH$_2$), 28.0 (CH$_2$), 26.4 (CH$_2$), 26.3

(CH$_2$), 25.4 (CH$_2$), 25.1 (CH$_2$), 24.5 (CH$_2$), 22.5 (CH$_2$), 13.9 (C11); MS (ES$^-$) 307.2 (M − H); HRMS (M + Na), calcd for C$_{17}$H$_{28}$N$_2$Na$_1$O$_3$, 331.1992; found, 331.1993.

Synthesis of compound **2d**

Yield 41% (oil); Form AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 9.14 (brs, 1H, OH), 7.70 (brs, 1H, NH), 3.90 (s, 2H, C5 AB), 3.68 (s, 2H, C5 CD), 3.39-3.16 (m, 4H, C6 and C13), 1.56-1.51 (m, 4H, C7 and C14), 1.37-1.28 (m, 12H, C8-10 and C15-17), 0.87 (t, 6H, J = 6.8 Hz, C11 and C18); ^{13}C NMR (125 MHz, CDCl$_3$) 189.8 (C4 CD), 181.1 (C4 AB), 175.2 (C2 CD), 169.1 (C2 AB), 166.6 (C12 AB), 166.0 (C12 AB), 98.6 (C3 AB), 85.6 (C3 CD), 55.0 (C5 CD), 49.7 (C5 AB), 41.5 (CH$_2$), 41.2 (CH$_2$), 39.6 (CH$_2$), 38.4 (CH$_2$), 31.4 (CH$_2$), 31.3 (CH$_2$), 29.4 (CH$_2$), 28.4 (CH$_2$), 28.0 (CH$_2$), 26.5 (CH$_2$), 26.4 (CH$_2$), 22.5 (CH$_2$), 13.9 (C11 and C18); MS (ES$^-$) 309.2; HRMS (M − H), calcd for C$_{17}$H$_{29}$N$_2$O$_3$, 309.2184; found, 309.2178.

Synthesis of **2e**

Yield 58% (oil); Form AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 9.44 (brs, 1H, OH), 7.70 (brs, 1H, NH), 3.91 (s, 2H, C5 AB), 3.68 (s, 2H, C5 CD), 3.40-3.30 (m, 4H, C6 and C13), 1.59-1.52 (m, 4H, C7 and C14), 1.35-1.25 (m, 18H, C8-10 and C15-20), 0.89-0.85 (m, 6H, C11 and C21); ^{13}C NMR (100 MHz, CDCl$_3$, Only AB tautomer) 181.1 (C4), 169.1 (C2), 166.0 (C12), 98.6 (C3), 49.7 (C5), 41.3 (CH$_2$), 38.4 (CH$_2$), 31.8 (CH$_2$), 31.4 (CH$_2$), 29.4 (CH$_2$), 29.4 (CH$_2$), 29.2 (CH$_2$), 29.2 (CH$_2$), 28.4 (CH$_2$), 26.8 (CH$_2$), 26.4 (CH$_2$), 22.6 (CH$_2$), 22.5 (CH$_2$),14.1 (CH$_3$), 14.0 (CH$_3$); MS (ES$^-$) 351.3; HRMS (M − H) calcd for C$_{20}$H$_{35}$N$_2$O$_3$, 351.2653; found, 351.2657.

Synthesis of **2f**

Yield, 55% (oil); Form AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 7.71 (brs, 1H, NH), 3.91 (s, 2H, C5 AB), 3.69 (s, 2H, C5 CD), 3.41-3.31 (m, 4H, NC$\underline{H}_2$ and NHC$\underline{H}_2$), 1.56-1.54 (m, 4H, NCH$_2$C$\underline{H}_2$ and NHCH$_2$C$\underline{H}_2$C7), 1.30-1.25 (m, 24H, C$\underline{H}_2$), 0.90-0.86 (m, 6H, C$\underline{H}_3$); ^{13}C NMR (100 MHz, CDCl$_3$, AB tautomer only) 181.09 (C4), 169.09 (C2), 165.98 ($\underline{C}$=ONH), 98.64 (C3), 49.75 (C5), 41.28 (CH$_2$), 38.41 (CH$_2$), 31.88 (CH$_2$), 31.42 (CH$_2$), 29.58 (CH$_2$), 29.47 (CH$_2$), 29.31 (CH$_2$), 29.23 (CH$_2$), 28.40 (CH$_2$), 26.85 (CH$_2$), 26.38 (CH$_2$), 22.65 (CH$_2$), 22.49 (CH$_2$),14.08 (CH$_3$), 13.97 (CH$_3$); MS (ES$^-$) 393.3; HRMS (M − H) calcd for C$_{23}$H$_{41}$N$_2$O$_3$, 393.3123; found, 393.3120.

Synthesis of **2g**

Yield 54%; mp 84 °C; Form AB:CD = 90:10; ^{1}H NMR (400 MHz, CDCl$_3$) 9.03 (brs, 1H, OH), 8.09 (brs, 1H, NH), 7.36-7.25 (m, 5H, Ar-H), 4.55 (d, 2H, J = 6.0 Hz, NHC$\underline{H}_2$), 3.94 (s, 2H, C5 AB), 3.70 (s, 2H, C5 CD), 3.39 (t, 2H, J = 7.6 Hz, NC$\underline{H}_2$), 1.56-1.53 (m, 2H, NCH$_2$C$\underline{H}_2$), 1.37-1.26 (m, 6H, CH$_2$), 0.89 (t, 3H, J = 6.4 Hz, CH$_3$); ^{13}C NMR (100 MHz, CDCl$_3$); 189.55 (C4 CD), 180.70 (C4 AB), 175.49 (C2 CD), 168.83 (C2 AB), 166.67 ($\underline{C}$=ONH CD), 165.89 ($\underline{C}$=ONH AB), 137.52 (Ar quart-C AB), 136.67 (Ar quart-C CD), 128.80 (Ar tert-C CD), 128.67 (Ar tert-C AB), 127.85 (Ar tert-C CD), 127.53 (Ar tert-C AB), 127.47 (Ar tert-C AB), 126.87 (Ar tert-C CD), 99.17 (C3 AB), 85.95 (C3 CD), 55.22 (C5 CD), 49.57 (C5 AB), 43.21 (NHC$\underline{H}_2$ CD), 42.23 (NHC$\underline{H}_2$ AB), 41.76 (NC$\underline{H}_2$ CD), 41.25 (NC$\underline{H}_2$ AB), 31.38 (CH$_2$), 28.37 (CH$_2$), 26.35 (CH$_2$), 22.47 (CH$_2$), 13.96 (CH$_3$); MS (ES$^-$) 315.2; HRMS (M + Na) calcd for C$_{18}$H$_{24}$N$_2$Na$_1$O$_3$, 339.1679; found, 339.1674.

Synthesis of **2h**

Yield 60%; mp 96 °C; Form AB:CD = 90:10; ^{1}H NMR (400 MHz, CDCl$_3$) 9.55 (brs, 1H, NH or OH AB), 9.25 (brs, 1H, NH or OH CD), 8.27 (brs, 1H, NH or OH), 7.50 (d, 2H, J = 8.8 Hz, Ar-H AB), 7.38 (d, 2H, J = 8.8 Hz, Ar-H CD), 6.89 (d, 2H, J = 8.8 Hz, Ar-H), 5.08 (t, 1H, J = 6.8 Hz, C$\underline{H}$=C), 3.96 (s, 2H, C5 AB), 3.86 (t, 4H, J = 4.8 Hz, C$\underline{H}_2$OC$\underline{H}_2$), 3.76 (s, 2H, C5 CD), 3.54-3.39 (m, 2H, NC$\underline{H}_2$), 3.13 (t, 4H, J = 4.8 Hz, C$\underline{H}_2$NC$\underline{H}_2$), 2.07-1.91 (m, 2H, CHC$\underline{H}_2$), 1.68 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.60 (s, 3H, C(C$\underline{H}_3$)$_2$), 1.64-1.17 (m, 5H, C$\underline{H}_2$C$\underline{H}$(Me)C$\underline{H}_2$), 0.96 (d, 3H, J = 6.4 Hz, CH(C$\underline{H}_3$)); ^{13}C NMR (100 MHz, CDCl$_3$, AB tautomer only) 180.52 (C4), 168.73 (C2), 163.67 ($\underline{C}$=ONH), 148.29 (Ar quart-C), 131.44 (CH=$\underline{C}$(Me)$_2$), 129.56 (Ar quart-C), 124.39 ($\underline{C}$H=C(Me)$_2$), 121.36 (Ar tert-C), 116.17 (Ar tert-C), 99.63 (C3), 66.78 ($\underline{C}$H$_2$O$\underline{C}$H$_2$), 49.56 (C5), 49.45 ($\underline{C}$H$_2$N$\underline{C}$H$_2$), 39.43 (N$\underline{C}$H$_2$), 36.81 (NCH$_2$CH$_2$CH(Me)$\underline{C}$H$_2$), 35.23 (NCH$_2$$\underline{C}H_2$), 29.98 (CH$_2$$\underline{C}$H(Me)CH$_2$), 25.64 (C($\underline{C}H_3$)$_2$), 25.29 (CH$\underline{C}H_2$), 19.27 (CH($\underline{C}H_3$)), 17.62 (C($\underline{C}H_3$)$_2$); MS (ES$^-$) 440.29 (M − H); HRMS (M − H) calcd for C$_{25}$H$_{34}$N$_3$O$_4$, 440.2555; found, 440.2553.

Synthesis of **3a**

Yield 45% (oil); AB:CD = 85:15; ^{1}H NMR (400 MHz, CDCl$_3$) 11.85 (brs, 1H, OH), 8.60 (brs, 1H, NH CD), 8.04 (brs, 1H, NH AB), 4.73 (t, 1H, J = 4.0 Hz, C5 AB), 4.41 (brs, 1H, C5 CD), 3.63-3.43 (m, 6H, cy-Hx C$\underline{H}$, NHC$\underline{H}_2$, OC$\underline{H}_2$ and OC$\underline{H}$), 2.46-2.34 (m, 2H, SC$\underline{H}_2$), 2.28-2.21 (m, 2H, SCH$_2$C$\underline{H}_2$), 2.04 (s, 3H, SC$\underline{H}_3$), 1.93-1.65 (m, 7H, NHCH$_2$C$\underline{H}_2$ and cy-Hx CH$_2$), 1.49-1.22 (m, 5H, cy-Hx CH$_2$), 1.18 (d, 6H, J = 6.0 Hz, CH(C$\underline{H}_3$)$_2$). ^{13}C NMR (100 MHz, CDCl$_3$, AB tautomer only); 189.4 (C4), 176.0 (N$\underline{C}$=O), 167.3 (C2), 166.0 ($\underline{C}$=ONH), 95.4 (C3), 72.0 (O$\underline{C}$H), 66.6 (O$\underline{C}$H$_2$), 58.6 (C5), 44.1 (cy-Hx $\underline{C}$H), 37.7 (NH$\underline{C}$H$_2$), 30.0 (CH$_2$), 29.0 (CH$_2$), 28.5 (CH$_2$), 28.0

(CH$_2$), 27.9 (CH$_2$), 25.8 (CH$_2$), 25.7 (CH$_2$), 25.4 (CH$_2$), 21.8 (CH(C$\underline{\text{H}}_3$)$_2$), 15.2 (SC$\underline{\text{H}}_3$);

MS (ES$^-$) 425.21 (M − H); HRMS (M − H) calcd for C$_{21}$H$_{33}$N$_2$O$_5$S$_1$, 425.2116; found,

425.2118.

Synthesis of **3b**

Yield 52%; mp 97 °C; AB:CD = 85:15; ^{1}H NMR (400 MHz, CDCl$_3$) 11.96 (brs, 1H,

OH), 8.31 (d, 1H, J = 8.0 Hz, NH CD), 7.46 (d, 1H, J = 8.0 Hz, NH AB), 4.75 (t, 1H, J

= 5.2 Hz, C5 AB), 4.44 (t, 1H, J = 5.2 Hz, C5 CD), 3.88-3.80 (m, 1H, NHC$\underline{\text{H}}$), 3.49-

3.44 (m, 1H, cy-Hx C$\underline{\text{H}}$), 2.47-2.36 (m, 2H, SC$\underline{\text{H}}_2$), 2.29-2.20 (m, 2H, SCH$_2$C$\underline{\text{H}}_2$), 2.05

(s, 3H, SC$\underline{\text{H}}_3$ AB), 2.04 (s, 3H, SC$\underline{\text{H}}_3$ CD), 1.94-1.60 (m, 10H, CH$_2$), 1.50-1.23 (m,

10H, CH$_2$); ^{13}C NMR (100 MHz, CDCl$_3$); 192.0 (C4 CD), 189.6 (C4 AB), 176.0

(NC$\underline{\text{C}}$=O AB), 175.7 (NC$\underline{\text{C}}$=O CD), 173.9 (C2 CD), 167.7 (C2 AB), 165.9 (C$\underline{\text{C}}$=ONH CD),

165.4 (C$\underline{\text{C}}$=ONH AB), 95.3 (C3 AB), 86.1 (C3 CD), 62.6 (C5 CD), 58.8 (C5 AB), 49.6

(NHC$\underline{\text{H}}$ CD), 48.1 (NHC$\underline{\text{H}}$ AB), 44.4 (cy-Hx C$\underline{\text{H}}$ CD), 44.1 (cy-Hx C$\underline{\text{H}}$ AB), 32.7 (CH$_2$

AB), 32.6 (CH$_2$ AB), 32.4 (CH$_2$ CD), 30.2 (CH$_2$ CD), 30.1 (CH$_2$ AB), 29.6 (CH$_2$ CD),

28.9 (CH$_2$ CD), 28.6 (CH$_2$ AB), 28.3 (CH$_2$ CD), 28.1 (CH$_2$ CD), 28.0 (CH$_2$ AB), 27.9

(CH$_2$ AB), 25.8 (CH$_2$), 25.7 (CH$_2$), 25.4 (CH$_2$ CD), 25.3 (CH$_2$ AB), 25.2 (CH$_2$ AB),

24.9 (CH$_2$ CD), 24.5 (CH$_2$ AB), 24.2 (CH$_2$ CD), 15.2 (SC$\underline{\text{H}}_3$); MS (ES$^-$) 407.20 (M −

H); HRMS (M − H) calcd for C$_{21}$H$_{31}$N$_2$O$_4$S$_1$, 407.2010; found, 407.2012.

Synthesis of **3c**

Yield, 64%; mp 46 °C; AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 11.86 (brs, 1H,

NH or OH), 8.56 (brs, 1H, NH or OH CD), 7.59 (brs, 1H, NH or OH AB), 4.72 (dd,

1H, J_1 = 6.0 Hz, J_2 = 4.0 Hz, C5 AB), 4.44 (t, 1H, J = 4.4 Hz, C5 CD), 2.55 (s, 3H,

C=OC$\underline{\text{H}}_3$ CD), 2.53 (s, 3H, C=OC$\underline{\text{H}}_3$ AB), 2.51-2.41 (m, 2H, SC$\underline{\text{H}}_2$), 2.38-2.25 (m, 2H,

SCH$_2$CH$_2$), 2.08 (s, 3H, SCH$_3$ AB), 2.06 (s, 3H, SCH$_3$ CD),1.78 (s, 2H, CCH$_2$C), 1.52 (s, 6H, NHC(CH$_3$)$_2$ CD), 1.50 (s, 6H, NHC(CH$_3$)$_2$ AB), 1.01 (s, 9H, C(CH$_3$)$_3$); ^{13}C NMR (100 MHz, CDCl$_3$); 191.8 (C4 CD), 190.6 (C4 AB), 174.4 (NC=O CD), 169.6 (NC=O AB), 169.2 (C2 CD), 168.3 (C2 AB), 166.7 (C=ONH CD),166.3 (C=ONH AB), 94.7 (C3 AB), 86.4 (C3 CD), 62.6 (C5 CD), 59.0 (C5 AB), 57.7 (NHC(Me)$_2$ CD), 56.4 (NHC(Me)$_2$ AB), 52.4 (CCH$_2$C CD), 52.1 (CCH$_2$C AB), 31.6 (C(Me)$_3$), 31.3 (C(CH$_3$)$_3$ AB), 31.2 (C(CH$_3$)$_3$ CD), 29.3 (NHC(CH$_3$)$_2$ CD), 29.2 (NHC(CH$_3$)$_2$ AB), 28.7 (SCH$_2$ CD), 28.5 (SCH$_2$ AB), 28.4 (SCH$_2$CH$_2$ CD), 28.2 (SCH$_2$CH$_2$ AB), 25.5 (C=OCH$_3$ CD), 25.3 (C=OCH$_3$ AB), 15.3 (SCH$_3$); MS (ES$^-$) 369.19 (M-H); MS (ES$^+$) 371.21 (M + H), 393.19 (M + Na); HRMS (M + Na) calcd for C$_{18}$H$_{30}$N$_2$O$_4$S$_1$, 393.1818; found, 393.1805.

Synthesis of **3d**

Yield 58%; mp 91 °C; AB:CD = 80:20; ^{1}H NMR (400 MHz, CDCl$_3$) 11.15 (brs, 1H, OH), 7.87 (d, 1H, J = 6.4 Hz, NH AB), 7.34 (d, 1H, J = 6.4 Hz, NH CD), 4.76 (t, 1H, J = 5.2 Hz, C5 AB), 4.47-4.43 (m, 1H, C5 CD), 4.28-4.26 (m, 1H, NHCH AB), 4.09-3.98 (m, 1H, NHCH CD), 2.54 (s, 3H, C=OCH$_3$ CD), 2.52 (s, 3H, C=OCH$_3$ AB), 2.51-2.42 (m, 2H, SCH$_2$), 2.38-2.26 (m, 2H, SCH$_2$CH$_2$), 2.09 (s, 3H, SCH$_3$ AB), 2.05 (s, 3H, SCH$_3$ CD),2.00-1.17 (m, 6H, cy-Hx CH$_2$), 1.08-0.93 (m, 9H, cy-Hx CH$_3$); ^{13}C NMR (100 MHz, CDCl$_3$, diastereo mixture, tautomer AB only); 189.9 and 189.8 (C4), 169.6 and 169.5 (NC=O), 168.2 and 168.1 (C2), 165.5 and 165.4 (C=ONH AB), 95.0 (C3), 58.9 and 58.8 (C5), 47.4 and 47.3 (CH$_2$), 45.7 and 45.6 (NHCH), 41.6 and 41.5 (CH$_2$), 38.3 and 38.2 (CH$_2$), 33.8 (CH$_3$), 30.6 (C(CH$_3$)), 28.6 and 28.5 (SCH$_2$), 28.2 and 28.1 (SCH$_2$CH$_2$), 27.8 (CH$_3$), 25.4 and 25.3 (C=OCH$_3$), 22.3 and 22.2 (CH$_3$) 15.3

(S$\underline{C}$H$_3$); MS (ES$^-$) 381.19 (M − H), MS (ES$^+$), 383.20 (M + H); HRMS (M + Na) calcd for C$_{19}$H$_{30}$N$_2$O$_4$S$_1$, 405.1818; found, 405.1814.

Synthesis of **3e**

Yield 63%; mp 159 °C; AB:CD = 99:1; ^{1}H NMR (400 MHz, DMSO) 10.89 (s, 1H, NH or OH), 7.67 (d, 2H, J = 8.8 Hz, Ar-H), 7.43 (d, 2H, J = 8.8 Hz, Ar-H), 4.14 (dd, 1H, J_1 = 6.0 Hz, J_2 = 4.0 Hz, C5), 3.14 (s, 6H, N(C$\underline{H}_3$)$_2$), 2.42 (s, 3H, C=OC$\underline{H}_3$), 2.38-2.31 (m, 2H, SC$\underline{H}_2$), 2.17-2.03 (m, 2H, SCH$_2$C$\underline{H}_2$), 1.99 (s, 3H, SC$\underline{H}_3$); ^{13}C NMR (100 MHz, DMSO, tautomer AB only); 190.4 (C4), 170.5 (N$\underline{C}$=O), 168.8 (C2), 162.7 ($\underline{C}$=ONH), 138.8 (Ar quart-C), 125.3 (Ar quart-C), 120.0 (Ar tert-C), 119.5 (Ar tert-C), 92.9 (C3), 59.2 (C5), 45.4 (N($\underline{C}$H$_3$)$_2$), 29.0 (S$\underline{C}$H$_2$), 27.7 (SCH$_2$$\underline{C}H_2$), 25.3 (C=O$\underline{C}H_3$), 14.7 (S$\underline{C}H_3$); MS (ES$^-$), 376.14 (M − H); HRMS (M + Na), calcd for C$_{18}$H$_{23}$N$_3$O$_4$S$_1$, 400.1301; found, 400.1290.

Synthesis of **3f**

Yield 60%; mp 170 °C; AB:CD = 99:1; ^{1}H NMR (400 MHz, CDCl$_3$) 9.21 (s, 1H, NH or OH), 8.18 (s, 1H, NH or OH), 7.48 (d, 2H, J = 8.0 Hz, Ar-H), 6.91 (d, 2H, J = 8.0 Hz, Ar-H), 4.89 (brs, 1H, C5), 3.87 (t, 4H, J = 4.4 Hz, C$\underline{H}_2$OC$\underline{H}_2$), 3.16 (t, 4H, J = 4.4 Hz, C$\underline{H}_2$NC$\underline{H}_2$), 2.58 (s, 3H, C=OC$\underline{H}_3$), 2.55-2.45 (m, 2H, SC$\underline{H}_2$), 2.41-2.36 (m, 2H, SCH$_2$C$\underline{H}_2$), 2.10 (s, 3H, SC$\underline{H}_3$); ^{13}C NMR (100 MHz, CDCl$_3$, tautomer AB only); 187.9 (C4), 169.5 (N$\underline{C}$=O), 165.5 (C2), 163.6 ($\underline{C}$=ONH), 148.9 (Ar quart-C), 128.4 (Ar quart-C), 121.8 (Ar tert-C), 116.2 (Ar tert-C), 97.6 (C3), 66.8 ($\underline{C}$H$_2$O$\underline{C}$H$_2$), 58.3 (C5), 49.3 ($\underline{C}$H$_2$N$\underline{C}$H$_2$), 28.5 (S$\underline{C}$H$_2$), 28.2 (SCH$_2$$\underline{C}H_2$), 25.4 (C=O$\underline{C}H_3$), 15.3 (S$\underline{C}H_3$); MS (ES$^-$); 418.15 (M − H), HRMS (M − H) calcd for C$_{20}$H$_{24}$N$_3$O$_5$S$_1$, 418.1442; found, 418.1449.

10a A TAUTOMER

```
Spartan '02 Mechanics Program: (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.3
  Mechanics Wall Time: 000:00:00.3
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G(D)
Number of shells: 62
Number of basis functions: 183

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
       Step      Energy         Max Grad.      Max Dist.
          1    -552.5962400      0.023621       0.138404
          2    -552.6036072      0.009644       0.032444
          3    -552.6042932      0.002787       0.016188
          4    -552.6044155      0.001086       0.004488
          5    -552.6044243      0.000538       0.001014
          6    -552.6044231      0.000090       0.000316
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:32:01.1
  Quantum Mechanics Program Wall Time: 000:21:27.0

Spartan '02 Properties Program: (PC/x86)
Release  115B
  Orientation rotated by   179.999994991044     degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.6

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
  Searching for a Minimum

  Optimization Cycle:   6


              Coordinates (Angstroms)
   ATOM           X          Y          Z
  1  N         1.553777  -0.263542   0.000000
  2  C         1.506838   1.185329   0.000000
```

```
    3  C           0.026292    1.449356    0.000000
    4  C          -0.676986    0.276958    0.000000
    5  C           0.292687   -0.845710    0.000000
    6  O           0.069098   -2.049253    0.000000
    7  O          -0.461222    2.671232    0.000000
    8  C          -2.129675    0.272786    0.000000
    9  O          -2.729402    1.365739    0.000000
   10  C          -2.881342   -1.031236    0.000000
   11  C           2.782826   -1.022101    0.000000
   12  H           1.987925    1.624171    0.887239
   13  H           1.987925    1.624171   -0.887239
   14  H          -1.459168    2.532007    0.000000
   15  H          -2.599379   -1.629735   -0.873274
   16  H          -3.955283   -0.835946    0.000000
   17  H          -2.599379   -1.629735    0.873274
   18  H           3.387361   -0.807592    0.891511
   19  H           3.387361   -0.807592   -0.891511
   20  H           2.509748   -2.079307    0.000000
    Point Group: cs   Number of degrees of freedom:  34


   Energy is   -552.604423124


 Hessian Updated using BFGS Update
  internal optimization with constraints (0)


 34 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.052511    0.055510    0.056417    0.070952    0.127769
0.130975
     0.150573    0.159305    0.177514    0.178309    0.204058
0.212112
     0.220593    0.228453    0.233546    0.254312    0.270679
0.281991
     0.296975    0.303096    0.305099    0.306704    0.307577
0.308449
     0.310524    0.329528    0.350899    0.382164    0.443485
0.464462
     0.542845    0.714131    0.813100    0.863274


 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda = -0.00000014
 Step Taken.  Stepsize is  0.000813


                      Maximum     Tolerance    Cnvgd?
         Gradient     0.000090    0.000300     YES
         Displacement 0.000316    0.001200     YES
         Energy change 0.000001   0.000001      NO
```

```
###################################################
#  Entering anlman.exe on Sun May 06 04:19:42 2012  #
###################################################
```

 Analysis of SCF Wavefunction

 Total job wall time: 1.3e+006 s

10a B TAUTOMER

Spartan '02 Mechanics Program: (PC/x86)
Release 115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.2
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release 115B

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G(D)
Number of shells: 62
Number of basis functions: 183

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation

Optimization:
       Step   Energy   Max Grad.   Max Dist.
          1   -552.5991897   0.030375   0.107548
          2   -552.6074004   0.013960   0.038609
          3   -552.6083457   0.003796   0.016282
          4   -552.6084863   0.001023   0.004150
          5   -552.6084886   0.000204   0.000945
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:26:48.4
  Quantum Mechanics Program Wall Time: 000:14:42.8

Spartan '02 Properties Program: (PC/x86)
Release 115B
   Orientation rotated by   179.999994991044   degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.3
  Properties Program Wall Time: 000:00:00.4

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

```
   Optimization Cycle:   5

                  Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N         1.586310  -0.213839   0.000000
   2  C         1.536102   1.237007   0.000000
   3  C         0.037765   1.532582   0.000000
   4  C        -0.652557   0.270741   0.000000
   5  C         0.344093  -0.824735   0.000000
   6  O         0.160021  -2.037515   0.000000
   7  O        -0.472187   2.661860   0.000000
   8  C        -2.028307   0.199699   0.000000
   9  O        -2.747710   1.314009   0.000000
  10  C        -2.824199  -1.061635   0.000000
  11  C         2.826674  -0.955457   0.000000
  12  H         2.016125   1.674619  -0.887578
  13  H         2.016125   1.674619   0.887578
  14  H        -2.111659   2.088108   0.000000
  15  H        -3.475914  -1.081288   0.881724
  16  H        -2.162637  -1.928429   0.000000
  17  H        -3.475914  -1.081288  -0.881724
  18  H         3.426266  -0.725716  -0.890975
  19  H         3.426266  -0.725716   0.890975
  20  H         2.575339  -2.017626   0.000000
   Point Group: cs   Number of degrees of freedom:  34


   Energy is   -552.608488624

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 34 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.053121    0.056099    0.056598    0.071180    0.123833
0.132122
     0.142224    0.146835    0.168981    0.182364    0.197102
0.209779
     0.210467    0.221605    0.231890    0.250398    0.270173
0.273158
     0.276082    0.292419    0.303718    0.306650    0.307709
0.310569
     0.312854    0.321230    0.341594    0.395529    0.431717
0.512594
     0.648731    0.680669    0.821649    0.866505

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda =  -0.00000076
 Step Taken.  Stepsize is  0.001862
```

```
                        Maximum     Tolerance    Cnvgd?
        Gradient        0.000204     0.000300      YES
        Displacement    0.000945     0.001200      YES
        Energy change  -0.000002     0.000001       NO


####################################################
#  Entering anlman.exe on Sun May 06 04:38:49 2012  #
####################################################

 Analysis of SCF Wavefunction

 Total job wall time:  8.8e+005 s
```

10a C TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G(D)
Number of shells: 62
Number of basis functions: 183

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.     Max Dist.
        1    -552.5871228     0.049436      0.130259   1
        2    -552.6007876     0.010505      0.187450   1
        3    -552.6026218     0.005646      0.204341   1
        4    -552.6030211     0.003783      0.161886   1
        5    -552.6029772     0.006357      0.222468
        6    -552.6034428     0.003213      0.211975
        7    -552.6037099     0.001543      0.230797
        8    -552.6038365     0.000878      0.169330
        9    -552.6038745     0.001926      0.038243
       10    -552.6039220     0.000481      0.048647
       11    -552.6039304     0.001018      0.020277
       12    -552.6039486     0.000291      0.023252
```

```
               13       -552.6039530       0.000141         0.022391
               14       -552.6039503       0.000092         0.041845
               15       -552.6039492       0.000197         0.177355
               16       -552.6039341       0.000668         0.142921    1
               17       -552.6032730       0.002955         0.091064
               18       -552.6039558       0.000396         0.183535
               19       -552.6040081       0.000446         0.187290
               20       -552.6040519       0.000825         0.186118
               21       -552.6040740       0.001373         0.168282
               22       -552.6041266       0.001100         0.178649
               23       -552.6041548       0.000841         0.135319
               24       -552.6041878       0.000604         0.141565
               25       -552.6041838       0.000745         0.016972
               26       -552.6041962       0.000174         0.045826
               27       -552.6041956       0.000051         0.064522
    Reason for exit: Sucessful completion
    Quantum Mechanics Program CPU Time : 002:43:15.1
    Quantum Mechanics Program Wall Time: 001:37:27.3


Spartan '02 Properties Program: (PC/x86)
Release 115B
   Reason for exit: Successful completion
   Properties Program CPU Time : 000:00:00.5
   Properties Program Wall Time: 000:00:01.2


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
    Searching for a Minimum

    Optimization Cycle:  27


                    Coordinates (Angstroms)
     ATOM           X          Y          Z
   1  N         1.622430    0.015427    0.036597
   2  C         1.238259    1.416276    0.206894
   3  C        -0.318129    1.394335    0.173928
   4  C        -0.680089    0.005968   -0.013348
   5  C         0.521615   -0.740254   -0.082995
   6  O         0.583479   -2.035572   -0.246280
   7  O        -1.000475    2.402077    0.293156
   8  C        -1.931839   -0.679531   -0.128346
   9  O        -1.944897   -1.928625   -0.285233
  10  C        -3.231414    0.082256   -0.064282
  11  C         2.990364   -0.461686    0.007407
  12  H         1.634059    2.039612   -0.603918
  13  H         1.600486    1.816011    1.161582
  14  H        -0.415060   -2.304435   -0.299995
  15  H        -3.794957   -0.095132   -0.987427
  16  H        -3.836403   -0.311895    0.760409
  17  H        -3.065075    1.152163    0.073285
```

```
   18  H           3.540961   -0.005807   -0.824335
   19  H           3.504271   -0.216260    0.944595
   20  H           2.982415   -1.544929   -0.121693
   Point Group: c1    Number of degrees of freedom:  54


   Energy is   -552.604195637

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 54 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.000187    0.000846    0.002519    0.006532    0.011875
0.019201
     0.021012    0.023297    0.033718    0.035985    0.052266
0.054367
     0.055015    0.055549    0.056147    0.063491    0.066917
0.089166
     0.107864    0.128599    0.131212    0.138485    0.151339
0.163736
     0.167491    0.185045    0.198706    0.212166    0.215742
0.228407
     0.229589    0.239898    0.253628    0.263287    0.270964
0.294017
     0.303656    0.305190    0.305775    0.307706    0.307857
0.308582
     0.310140    0.312733    0.327645    0.338045    0.389876
0.410328
     0.422808    0.470423    0.546972    0.755577    0.841212
0.864885

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda = -0.00000218
 Step Taken.  Stepsize is  0.102556

                         Maximum    Tolerance   Cnvgd?
        Gradient         0.000051    0.000300     YES
        Displacement     0.064522    0.001200     NO
        Energy change    0.000001    0.000001     YES


#####################################################
#  Entering anlman.exe on Sun May 06 06:19:46 2012  #
#####################################################

 Analysis of SCF Wavefunction

 Total job wall time: 5.8e+006 s
```

10a D TAUTOMER

```
Spartan '02 Mechanics Program: (PC/x86)
Release 115B


  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.3
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release 115B

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G(D)
Number of shells: 62
Number of basis functions: 183

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
       Step      Energy        Max Grad.     Max Dist.
          1    -552.6004501     0.031675      0.103239
          2    -552.6096787     0.014116      0.164904
          3    -552.6107933     0.004552      0.171504
          4    -552.6108469     0.002244      0.175373
          5    -552.6109721     0.002005      0.066418
          6    -552.6110430     0.000578      0.022524
          7    -552.6110482     0.000450      0.012837
          8    -552.6110527     0.000170      0.005036
          9    -552.6110516     0.000048      0.006513
         10    -552.6110480     0.000033      0.003052
         11    -552.6110489     0.000023      0.000682
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 001:02:06.8
  Quantum Mechanics Program Wall Time: 000:43:51.0

Spartan '02 Properties Program: (PC/x86)
Release 115B
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.4
  Properties Program Wall Time: 000:00:00.8


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum
```

```
   Optimization Cycle:  11

                    Coordinates (Angstroms)
     ATOM              X           Y           Z
    1  N           1.652107   -0.056066    0.004685
    2  C           1.319486    1.361033    0.022632
    3  C          -0.226597    1.392437    0.018981
    4  C          -0.647364   -0.000342   -0.001899
    5  C           0.545921   -0.853051   -0.009599
    6  O           0.547159   -2.099617   -0.026313
    7  O          -0.880622    2.424147    0.032311
    8  C          -1.907677   -0.554670   -0.013741
    9  O          -2.060370   -1.869668   -0.032261
   10  C          -3.179119    0.226870   -0.007635
   11  C           3.007650   -0.561340    0.001903
   12  H           1.713012    1.887466   -0.857553
   13  H           1.708407    1.863900    0.918473
   14  H          -1.137392   -2.276755   -0.034446
   15  H          -2.972802    1.297511    0.006747
   16  H          -3.770460   -0.030844   -0.894325
   17  H          -3.775646   -0.053201    0.868767
   18  H           3.549909   -0.234202    0.898274
   19  H           3.554638   -0.212033   -0.883174
   20  H           2.959762   -1.651575   -0.011828
   Point Group: c1   Number of degrees of freedom:  54



    Energy is   -552.611048871

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 54 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.001079    0.001422    0.005573    0.006824    0.010373
0.015754
     0.021829    0.024291    0.028709    0.043085    0.051379
0.054470
     0.055225    0.055876    0.056230    0.057753    0.072077
0.084283
     0.093563    0.126088    0.131003    0.145621    0.146875
0.151080
     0.169409    0.184129    0.192062    0.197186    0.209784
0.217475
     0.221151    0.236225    0.237880    0.264926    0.273176
0.283661
     0.293566    0.303092    0.304261    0.306800    0.307835
0.309369
     0.310416    0.311685    0.312857    0.324863    0.340515
0.388067
     0.417079    0.516116    0.570588    0.696533    0.841361
```

0.849564

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda = -0.00000001
 Step Taken. Stepsize is 0.001249

	Maximum	Tolerance	Cnvgd?
Gradient	0.000023	0.000300	YES
Displacement	0.000682	0.001200	YES
Energy change	-0.000001	0.000001	YES

```
####################################################
#  Entering anlman.exe on Sun May 06 07:07:50 2012  #
####################################################
```

 Analysis of SCF Wavefunction

 Total job wall time: 2.6e+006 s

11a A TAUTOMER

Spartan '02 Mechanics Program: (PC/x86)
Release 115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.2
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release 115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 92
Number of basis functions: 200

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-607.9706244	0.025132	0.108364
2	-607.9780656	0.009302	0.029426
3	-607.9787417	0.002776	0.015587

```
          4     -607.9788546        0.000895        0.003513
          5     -607.9788625        0.000408        0.001042
          6     -607.9788641        0.000074        0.000166
   Reason for exit: Sucessful completion
   Quantum Mechanics Program CPU Time : 000:27:32.4
   Quantum Mechanics Program Wall Time: 000:27:57.5


Spartan '02 Properties Program: (PC/x86)
Release 115B
  Orientation rotated by   179.999994991044     degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.6


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                   Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N        2.003578  -0.382055   0.000000
   2  C        2.116756   1.067930   0.000000
   3  C        0.672738   1.497694   0.000000
   4  C       -0.141747   0.411441   0.000000
   5  C        0.686794  -0.804587   0.000000
   6  O        0.304214  -1.975857   0.000000
   7  O        0.311315   2.768021   0.000000
   8  C       -1.597962   0.541626   0.000000
   9  O       -2.120288   1.680399   0.000000
  10  N       -2.306452  -0.604420   0.000000
  11  C        3.137000  -1.277337   0.000000
  12  C       -3.758194  -0.620521   0.000000
  13  H        2.646269   1.444047   0.887487
  14  H        2.646269   1.444047  -0.887487
  15  H       -0.694565   2.728612   0.000000
  16  H       -1.766323  -1.467083   0.000000
  17  H        3.761936  -1.133819   0.891436
  18  H        2.745511  -2.296626   0.000000
  19  H        3.761936  -1.133819  -0.891436
  20  H       -4.156683  -0.114352  -0.885978
  21  H       -4.095419  -1.658987   0.000000
  22  H       -4.156683  -0.114352   0.885978
   Point Group: cs    Number of degrees of freedom:  38


   Energy is   -607.978864132

 Hessian Updated using BFGS Update
```

```
   internal optimization with constraints (0)

 38 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.053074    0.054479    0.056089    0.071223    0.130382
0.131687
     0.143378    0.159769    0.165635    0.175288    0.182345
0.197909
     0.205124    0.210331    0.220329    0.229939    0.250684
0.260765
     0.271643    0.293684    0.298213    0.306600    0.307186
0.307528
     0.308327    0.309303    0.322285    0.331283    0.352002
0.382227
     0.404947    0.419200    0.443702    0.485579    0.538339
0.675581
     0.800994    0.851060

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000005
 Step Taken.  Stepsize is  0.000442
```

	Maximum	Tolerance	Cnvgd?
Gradient	0.000074	0.000300	YES
Displacement	0.000166	0.001200	YES
Energy change	-0.000002	0.000001	NO

```
###################################################
#  Entering anlman.exe on Sat May 19 20:40:31 2012  #
###################################################

 Analysis of SCF Wavefunction

 Total job wall time: 1.7e+006 s
```

11a B TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
```

```
Method: RB3LYP
Basis set: LACVP*
Number of shells: 92
Number of basis functions: 200

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
       Step      Energy         Max Grad.      Max Dist.
          1    -607.9634195      0.042025       0.119293
          2    -607.9757193      0.012383       0.037746
          3    -607.9771848      0.004399       0.016434
          4    -607.9773666      0.001623       0.004735
          5    -607.9773829      0.000515       0.001581
          6    -607.9773838      0.000163       0.000470
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:33:51.9
  Quantum Mechanics Program Wall Time: 000:34:14.4

Spartan '02 Properties Program: (PC/x86)
Release  115B
   Orientation rotated by   179.999994991044    degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.4
  Properties Program Wall Time: 000:00:00.6


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                  Coordinates (Angstroms)
    ATOM          X          Y          Z
  1  N       2.030824   -0.323556   0.000000
  2  C       2.140826    1.130414   0.000000
  3  C       0.678628    1.598519   0.000000
  4  C      -0.113707    0.429295   0.000000
  5  C       0.721211   -0.761873   0.000000
  6  O       0.347949   -1.942514   0.000000
  7  O       0.281703    2.780893   0.000000
  8  C      -1.512542    0.470536   0.000000
  9  O      -2.138252    1.638821   0.000000
 10  N      -2.252125   -0.636911   0.000000
 11  C       3.169764   -1.210650   0.000000
 12  C      -3.706217   -0.658161   0.000000
 13  H       2.668912    1.506016  -0.887804
```

```
14  H           2.668912    1.506016    0.887804
15  H          -1.416053    2.342721    0.000000
16  H          -1.700091   -1.496318    0.000000
17  H           3.794592   -1.059636    0.890734
18  H           2.789939   -2.234365    0.000000
19  H           3.794592   -1.059636   -0.890734
20  H          -4.108657   -0.159942    0.888188
21  H          -4.108657   -0.159942   -0.888188
22  H          -4.031551   -1.699728    0.000000
   Point Group: cs    Number of degrees of freedom:  38
```

   Energy is   -607.977383841

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 38 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
```
     0.052727    0.054623    0.056162    0.070829    0.129217
0.131888
     0.133454    0.149834    0.160627    0.169744    0.185462
0.199528
     0.208465    0.213324    0.216744    0.225666    0.239980
0.251028
     0.270389    0.285908    0.291870    0.304578    0.305262
0.306318
     0.307035    0.308725    0.311415    0.334081    0.354335
0.374813
     0.388270    0.419292    0.422847    0.542491    0.577885
0.640683
     0.824536    0.848724
```

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda = -0.00000034
 Step Taken. Stepsize is 0.001242

                        Maximum   Tolerance   Cnvgd?
          Gradient   0.000163   0.000300   YES
          Displacement   0.000470   0.001200   YES
          Energy change -0.000001   0.000001   YES

##
Entering anlman.exe on Mon May 21 04:39:33 2012
##

 Analysis of SCF Wavefunction

 Total job wall time: 2.1e+006 s

11a C TAUTOMER

```
Spartan '02 Mechanics Program: (PC/x86)
Release  115B


  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')


Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 92
Number of basis functions: 200


SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.      Max Dist.
         1   -607.9582059     0.047656       0.118759   2
         2   -607.9719615     0.010918       0.147967   2
         3   -607.9734362     0.006198       0.168650   2
         4   -607.9739292     0.003675       0.168116   2
         5   -607.9740010     0.002312       0.202365   1
         6   -607.9743363     0.001267       0.176407   1
         7   -607.9745321     0.001624       0.162645   1
         8   -607.9746194     0.001446       0.197190
         9   -607.9747249     0.001185       0.154816
        10   -607.9747570     0.000940       0.091768
        11   -607.9747739     0.000801       0.130265
        12   -607.9748132     0.001177       0.159244   1
        13   -607.9682148     0.029147       0.124393
        14   -607.9747971     0.001768       0.168932
        15   -607.9749115     0.001096       0.167406
        16   -607.9749838     0.000839       0.186742
        17   -607.9750584     0.000548       0.198997
        18   -607.9751276     0.000746       0.207746
        19   -607.9751748     0.000681       0.213777
        20   -607.9752388     0.001056       0.170694
        21   -607.9752723     0.000729       0.072714
        22   -607.9752754     0.000541       0.023168
        23   -607.9752816     0.000150       0.014099
        24   -607.9752834     0.000084       0.004780
        25   -607.9752856     0.000021       0.001262
```

```
        26    -607.9752862      0.000009      0.000502
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 001:46:04.5
  Quantum Mechanics Program Wall Time: 001:50:46.6


Spartan '02 Properties Program: (PC/x86)
Release  115B
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.8


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:  26


                  Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N         2.114878   -0.015130    0.011005
   2  C         1.790908    1.401292   -0.173150
   3  C         0.237179    1.433426   -0.181704
   4  C        -0.172813    0.077290   -0.005631
   5  C         0.973151   -0.722530    0.099126
   6  O         0.969038   -2.024062    0.264666
   7  O        -0.440530    2.453237   -0.317784
   8  C        -1.489210   -0.524337    0.068488
   9  O        -1.604927   -1.769619    0.227210
  10  N        -2.541578    0.316046   -0.041188
  11  C         3.458644   -0.549930    0.068948
  12  C        -3.923772   -0.118046    0.008214
  13  H         2.195551    1.782528   -1.118473
  14  H         2.190252    2.010876    0.646434
  15  H        -0.030965   -2.247533    0.290921
  16  H        -2.309823    1.298638   -0.166784
  17  H         4.003540   -0.336620   -0.859118
  18  H         4.015267   -0.115975    0.908839
  19  H         3.400128   -1.631068    0.204424
  20  H        -3.932287   -1.201588    0.132731
  21  H        -4.452398    0.342979    0.851232
  22  H        -4.450235    0.140126   -0.918405
   Point Group: c1   Number of degrees of freedom:  60



   Energy is   -607.975286203


 Hessian Updated using BFGS Update
  internal optimization with constraints (0)


 60 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
```

```
    0.000499    0.000980    0.003419    0.003729    0.005615
0.008627
    0.016833    0.019778    0.025269    0.028683    0.035951
0.047308
    0.053310    0.054458    0.054710    0.055602    0.056171
0.056844
    0.066640    0.090013    0.094680    0.131464    0.132030
0.144906
    0.162508    0.172483    0.181111    0.190039    0.197230
0.205641
    0.207097    0.212823    0.225486    0.229215    0.233188
0.253423
    0.262161    0.291884    0.301455    0.303157    0.305911
0.307876
    0.308053    0.308569    0.309598    0.315204    0.319104
0.324098
    0.348642    0.363864    0.390094    0.407800    0.429305
0.440071
    0.474413    0.500497    0.543644    0.739364    0.836474
0.845653

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =   0.00000000
 Step Taken.  Stepsize is  0.001100

                          Maximum    Tolerance   Cnvgd?
        Gradient         0.000009    0.000300     YES
        Displacement     0.000502    0.001200     YES
        Energy change   -0.000001    0.000001     YES


###################################################
#  Entering anlman.exe on Sat May 19 10:27:11 2012  #
###################################################

 Analysis of SCF Wavefunction

 Total job wall time:  6.6e+006 s
```

11a D TAUTOMER

```
Spartan '02 Mechanics Program: (PC/x86)
Release  115B


  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.3
  Mechanics Wall Time: 000:00:00.4
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
```

```
    (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 92
Number of basis functions: 200

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
        Step      Energy        Max Grad.       Max Dist.
          1    -607.9639061      0.043796        0.129858   1
          2    -607.9763578      0.011497        0.046744   1
          3    -607.9778463      0.003966        0.016192
          4    -607.9780374      0.001674        0.161606   1
          5    -607.9779298      0.001686        0.143172
          6    -607.9780569      0.000427        0.013233
          7    -607.9780522      0.000155        0.008005
          8    -607.9780533      0.000090        0.004550
          9    -607.9780533      0.000061        0.008815
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:39:36.5
  Quantum Mechanics Program Wall Time: 000:40:02.9

Spartan '02 Properties Program:  (PC/x86)
Release  115B
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.6


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   9


                 Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N       2.144713   -0.077092   -0.001004
   2  C       1.845657    1.351906    0.001563
   3  C       0.300412    1.410529    0.000491
   4  C      -0.128961    0.054546   -0.002557
   5  C       1.006763   -0.840187   -0.003226
   6  O       0.952954   -2.088951   -0.005297
   7  O      -0.378147    2.443385    0.002355
   8  C      -1.441723   -0.428591   -0.002888
```

```
  9  O           -1.679273   -1.731578   -0.004226
 10  N           -2.489368    0.396512   -0.001990
 11  C            3.482979   -0.620943    0.000343
 12  C           -3.876806   -0.039821    0.002655
 13  H            2.252535    1.857005   -0.885103
 14  H            2.251017    1.853441    0.890953
 15  H           -0.770840   -2.176607   -0.005503
 16  H           -2.238087    1.384838    0.001327
 17  H            4.039900   -0.305179    0.892589
 18  H            3.400582   -1.709654   -0.001884
 19  H            4.043003   -0.301735   -0.888702
 20  H           -4.105678   -0.621855    0.901635
 21  H           -4.512789    0.846693   -0.017264
 22  H           -4.098844   -0.656660   -0.874268
    Point Group: c1   Number of degrees of freedom:  60


   Energy is   -607.978053344

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 60 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.000614    0.000910    0.004371    0.005724    0.007182
0.010917
     0.014387    0.018934    0.028600    0.031023    0.036369
0.042395
     0.051947    0.054585    0.054594    0.055619    0.056116
0.056294
     0.071804    0.091920    0.093704    0.129227    0.131554
0.137022
     0.151588    0.161480    0.165527    0.167361    0.175441
0.193342
     0.198743    0.212627    0.214247    0.216035    0.223386
0.231721
     0.240650    0.270763    0.283023    0.299460    0.304822
0.305681
     0.306159    0.306560    0.307655    0.308586    0.310129
0.310947
     0.316571    0.339660    0.351386    0.382021    0.399139
0.417850
     0.426032    0.541407    0.549274    0.655806    0.824533
0.849511

 Minimum Search - Taking Simple RFO Step
  Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000028
 Step Taken.  Stepsize is  0.017131

                         Maximum    Tolerance   Cnvgd?
```

```
        Gradient           0.000061      0.000300      YES
        Displacement       0.008815      0.001200      NO
        Energy change      0.000000      0.000001      YES



##################################################
#  Entering anlman.exe on Sat May 19 08:35:47 2012  #
##################################################

 Analysis of SCF Wavefunction

 Total job wall time:  2.4e+006 s
```

11b A TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.2
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 104
Number of basis functions: 230

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.     Max Dist.
        1    -721.3170928     0.034108      0.114632
        2    -721.3263466     0.006482      0.028010
        3    -721.3270991     0.003467      0.014555
        4    -721.3272302     0.001268      0.005208
        5    -721.3272472     0.000500      0.001160
        6    -721.3272504     0.000069      0.000258
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:36:32.4
  Quantum Mechanics Program Wall Time: 000:36:53.7

Spartan '02 Properties Program:  (PC/x86)
Release  115B
```

```
   Orientation rotated by   179.999994991044      degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.6
  Properties Program Wall Time: 000:00:00.8


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES **

  Searching for a Minimum

  Optimization Cycle:   6


                    Coordinates (Angstroms)
    ATOM          X          Y          Z
  1  N        1.747191    0.273699    0.000000
  2  C        1.554297    1.728305    0.000000
  3  C        0.059598    1.845869    0.000000
  4  C       -0.527577    0.615156    0.000000
  5  C        0.507652   -0.412708    0.000000
  6  O        0.357682   -1.630162    0.000000
  7  O       -0.550909    3.009957    0.000000
  8  C       -1.985142    0.465578    0.000000
  9  O       -2.707391    1.489019    0.000000
 10  N       -2.475754   -0.787810    0.000000
 11  C        3.052005   -0.236863    0.000000
 12  C       -3.903850   -1.059040    0.000000
 13  C        3.224162   -1.736982    0.000000
 14  O        3.986018    0.547581    0.000000
 15  H        2.008773    2.190898    0.882998
 16  H        2.008773    2.190898   -0.882998
 17  H       -1.531769    2.770403    0.000000
 18  H       -1.796034   -1.543239    0.000000
 19  H       -4.383131   -0.629826   -0.886153
 20  H       -4.052865   -2.140384    0.000000
 21  H       -4.383131   -0.629826    0.886153
 22  H        2.748117   -2.187862    0.875264
 23  H        2.748117   -2.187862   -0.875264
 24  H        4.295168   -1.944799    0.000000
   Point Group: cs    Number of degrees of freedom:  42



   Energy is   -721.327250423


 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 42 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
    0.051308    0.054479    0.055506    0.074351    0.128611
0.130299
    0.143684    0.151156    0.164729    0.166957    0.176615
0.178562
```

```
    0.198665    0.205485    0.214700    0.225257    0.232870
0.239808
    0.257597    0.267002    0.279829    0.290934    0.298472
0.305334
    0.305556    0.307019    0.307852    0.308194    0.309269
0.323222
    0.348293    0.399980    0.410308    0.419374    0.447581
0.484422
    0.543271    0.576030    0.707413    0.800702    0.807014
0.847165
```

```
 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda = -0.00000012
 Step Taken.  Stepsize is  0.000731

                        Maximum    Tolerance   Cnvgd?
          Gradient      0.000069    0.000300     YES
          Displacement   0.000258    0.001200     YES
          Energy change  -0.000003    0.000001      NO
```

```
####################################################
#  Entering anlman.exe on Tue May 22 07:08:40 2012  #
####################################################

 Analysis of SCF Wavefunction

 Total job wall time:  2.2e+006 s
```

11b B TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 104
Number of basis functions: 230

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
```

```
      performed using Pulay DIIS extrapolation


Optimization:
        Step      Energy         Max Grad.      Max Dist.
          1    -721.3112034       0.040058       0.121705
          2    -721.3243264       0.011609       0.042586
          3    -721.3258197       0.004764       0.013576
          4    -721.3260139       0.001838       0.005420
          5    -721.3260289       0.000613       0.001938
          6    -721.3260354       0.000189       0.000583
   Reason for exit: Sucessful completion
   Quantum Mechanics Program CPU Time : 000:49:57.5
   Quantum Mechanics Program Wall Time: 000:51:25.1

Spartan '02 Properties Program: (PC/x86)
Release  115B
   Orientation rotated by   179.999994991044     degrees!
   Reason for exit: Successful completion
   Properties Program CPU Time : 000:00:00.7
   Properties Program Wall Time: 000:00:00.8

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                   Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N        1.762303   0.315697   0.000000
   2  C        1.574982   1.776437   0.000000
   3  C        0.059356   1.940776   0.000000
   4  C       -0.499875   0.639054   0.000000
   5  C        0.526291  -0.373992   0.000000
   6  O        0.374300  -1.597546   0.000000
   7  O       -0.564678   3.019073   0.000000
   8  C       -1.889609   0.424753   0.000000
   9  O       -2.709602   1.460972   0.000000
  10  N       -2.423048  -0.792826   0.000000
  11  C        3.062183  -0.202027   0.000000
  12  C       -3.855111  -1.058676   0.000000
  13  C        3.230524  -1.704047   0.000000
  14  O        4.003930   0.574385   0.000000
  15  H        2.033276   2.233348  -0.883032
  16  H        2.033276   2.233348   0.883032
  17  H       -2.124795   2.286701   0.000000
  18  H       -1.737131  -1.547491   0.000000
  19  H       -4.332290  -0.632859   0.888291
  20  H       -4.332290  -0.632859  -0.888291
  21  H       -4.001018  -2.139656   0.000000
```

```
   22  H            2.753861   -2.154348    0.875092
   23  H            2.753861   -2.154348   -0.875092
   24  H            4.301305   -1.913870    0.000000
   Point Group: cs   Number of degrees of freedom:  42


   Energy is   -721.326035371

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 42 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.050683    0.054613    0.056175    0.073976    0.128445
0.129220
     0.133312    0.150024    0.152524    0.160987    0.168721
0.187011
     0.200643    0.210200    0.215474    0.218866    0.233117
0.234072
     0.239895    0.255241    0.275258    0.284364    0.292792
0.304747
     0.305418    0.306020    0.306486    0.308474    0.315141
0.319688
     0.345398    0.375466    0.418989    0.422437    0.435147
0.547133
     0.605040    0.611247    0.646931    0.807260    0.824178
0.849314

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000044
 Step Taken.  Stepsize is  0.001606

                        Maximum    Tolerance   Cnvgd?
        Gradient        0.000189    0.000300     YES
        Displacement    0.000583    0.001200     YES
        Energy change  -0.000006    0.000001     NO


###################################################
#  Entering anlman.exe on Sun May 20 01:28:33 2012  #
###################################################

 Analysis of SCF Wavefunction

 Total job wall time:  3.1e+006 s
```

11b C TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B
```

```
  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 104
Number of basis functions: 230

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
        Step       Energy        Max Grad.      Max Dist.
           1    -721.3033582      0.034912       0.089320
           2    -721.3177329      0.011315       0.040481
           3    -721.3193931      0.005967       0.019894
           4    -721.3196512      0.003336       0.010243
           5    -721.3196947      0.001995       0.002734
           6    -721.3197005      0.000395       0.001764
           7    -721.3197080      0.000145       0.000366
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:54:41.0
  Quantum Mechanics Program Wall Time: 000:58:32.3

Spartan '02 Properties Program:  (PC/x86)
Release  115B
  Orientation rotated by   89.9999974955219    degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.7
  Properties Program Wall Time: 000:00:00.9

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   7


              Coordinates (Angstroms)
     ATOM         X          Y          Z
   1  N        1.733548   0.492020   0.000000
   2  C        1.193368   1.867492   0.000000
   3  C       -0.334164   1.668451   0.000000
```

```
    4  C          -0.547945    0.249293    0.000000
    5  C           0.681193   -0.394653    0.000000
    6  O           0.841959   -1.693861    0.000000
    7  O          -1.166364    2.573064    0.000000
    8  C          -1.777650   -0.528862    0.000000
    9  O          -1.726401   -1.787376    0.000000
   10  N          -2.932189    0.160811    0.000000
   11  C           3.124658    0.278444    0.000000
   12  C          -4.231221   -0.490669    0.000000
   13  C           3.631187   -1.145493    0.000000
   14  O           3.857376    1.250053    0.000000
   15  H           1.532964    2.412464   -0.884984
   16  H           1.532964    2.412464    0.884984
   17  H          -0.127446   -2.044552    0.000000
   18  H          -2.849994    1.174505    0.000000
   19  H          -4.353030   -1.121959   -0.886479
   20  H          -4.353030   -1.121959    0.886479
   21  H          -5.005439    0.278888    0.000000
   22  H           3.277313   -1.692487   -0.878760
   23  H           4.721027   -1.103591    0.000000
   24  H           3.277313   -1.692487    0.878760
    Point Group: cs    Number of degrees of freedom:  42


   Energy is   -721.319707975

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 42 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.052092    0.054479    0.055874    0.067910    0.127877
0.129760
     0.139082    0.147305    0.153811    0.167254    0.187332
0.194827
     0.205191    0.210291    0.217587    0.227745    0.234326
0.243500
     0.254040    0.260418    0.269495    0.284631    0.294569
0.304611
     0.306911    0.307199    0.308508    0.309482    0.317204
0.338603
     0.356988    0.381378    0.401817    0.416051    0.435479
0.481009
     0.572756    0.714446    0.776144    0.797048    0.834008
0.883320

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda =  -0.00000015
 Step Taken.  Stepsize is  0.000829
```

```
                          Maximum      Tolerance      Cnvgd?
          Gradient        0.000145      0.000300       YES
          Displacement    0.000366      0.001200       YES
          Energy change  -0.000007      0.000001       NO


#####################################################
#  Entering anlman.exe on Sun May 20 00:35:24 2012  #
#####################################################

 Analysis of SCF Wavefunction

 Total job wall time:  3.5e+006 s
```

11b D TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 104
Number of basis functions: 230

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.     Max Dist.
        1    -721.3108607     0.036514      0.096415
        2    -721.3241343     0.009967      0.039701
        3    -721.3256070     0.004351      0.012127
        4    -721.3257747     0.001545      0.004641
        5    -721.3258006     0.000404      0.001221
        6    -721.3258019     0.000079      0.000449
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:46:06.3
  Quantum Mechanics Program Wall Time: 000:46:38.7

Spartan '02 Properties Program:  (PC/x86)
```

```
Release  115B
  Orientation rotated by    89.9999974955219      degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.7
  Properties Program Wall Time: 000:00:00.7


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:    6


                     Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N        1.770039   0.442377   0.000000
   2  C        1.234297   1.815727   0.000000
   3  C       -0.287608   1.621661   0.000000
   4  C       -0.505706   0.211847   0.000000
   5  C        0.735346  -0.506378   0.000000
   6  O        0.864642  -1.743743   0.000000
   7  O       -1.128713   2.525541   0.000000
   8  C       -1.745564  -0.449080   0.000000
   9  O       -1.808723  -1.770923   0.000000
  10  N       -2.887226   0.231678   0.000000
  11  C        3.157220   0.242863   0.000000
  12  C       -4.209423  -0.377768   0.000000
  13  C        3.671535  -1.178336   0.000000
  14  O        3.890084   1.217765   0.000000
  15  H        1.571020   2.367120  -0.883367
  16  H        1.571020   2.367120   0.883367
  17  H       -0.857519  -2.097097   0.000000
  18  H       -2.761888   1.245929   0.000000
  19  H       -4.354981  -1.000279  -0.888544
  20  H       -4.354981  -1.000279   0.888544
  21  H       -4.951758   0.421628   0.000000
  22  H        3.313625  -1.727468   0.875398
  23  H        3.313625  -1.727468  -0.875398
  24  H        4.761638  -1.132438   0.000000
   Point Group: cs    Number of degrees of freedom:  42



   Energy is   -721.325801946


 Hessian Updated using BFGS Update
  internal optimization with constraints (0)


 42 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
    0.050586   0.054578   0.055937   0.074504   0.128512
0.129191
```

```
     0.134980    0.151494    0.155212    0.161002    0.170955
0.189399
     0.201000    0.201719    0.215909    0.221731    0.232449
0.234931
     0.240054    0.256195    0.274285    0.285822    0.296150
0.304843
     0.305328    0.305593    0.306450    0.308358    0.320199
0.323266
     0.350664    0.384698    0.420613    0.424210    0.435568
0.542090
     0.570701    0.598031    0.635346    0.809012    0.830730
0.846248

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda = -0.00000024
 Step Taken.  Stepsize is  0.001245


                     Maximum     Tolerance    Cnvgd?
          Gradient     0.000079    0.000300     YES
          Displacement  0.000449    0.001200     YES
          Energy change  -0.000001   0.000001     NO


###################################################
#  Entering anlman.exe on Sat May 19 21:55:22 2012  #
###################################################

 Analysis of SCF Wavefunction

 Total job wall time:  2.8e+006 s
```

12a A TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.2
  Mechanics Wall Time: 000:00:00.3
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 90
Number of basis functions: 198
```

```
SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy       Max Grad.      Max Dist.
        1    -627.8197226     0.025385       0.116795
        2    -627.8272691     0.009268       0.031660
        3    -627.8279874     0.002559       0.012805
        4    -627.8280714     0.001132       0.003856
        5    -627.8280759     0.000537       0.001298
        6    -627.8280770     0.000073       0.000206
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:33:22.7
  Quantum Mechanics Program Wall Time: 000:34:01.3

Spartan '02 Properties Program:  (PC/x86)
Release  115B
  Orientation rotated by   179.999994991044     degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.4
  Properties Program Wall Time: 000:00:00.6

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                 Coordinates (Angstroms)
    ATOM          X          Y          Z
  1  N        1.938595   -0.382245    0.000000
  2  C        1.949808    1.064872    0.000000
  3  C        0.482368    1.390134    0.000000
  4  C       -0.266097    0.250265    0.000000
  5  C        0.654339   -0.920700    0.000000
  6  O        0.394071   -2.111920    0.000000
  7  O        0.062570    2.641623    0.000000
  8  C       -1.716164    0.337180    0.000000
  9  O       -2.296610    1.432331    0.000000
 10  O       -2.363307   -0.827721    0.000000
 11  C        3.135488   -1.189525    0.000000
 12  C       -3.799367   -0.752094    0.000000
 13  H        2.447014    1.486040    0.887163
 14  H        2.447014    1.486040   -0.887163
 15  H       -0.934870    2.574812    0.000000
 16  H        3.748671   -1.000490   -0.891544
 17  H        3.748671   -1.000490    0.891544
 18  H        2.818598   -2.234445    0.000000
 19  H       -4.155826   -0.228112   -0.890570
```

```
  20  H           -4.139140   -1.787442    0.000000
  21  H           -4.155826   -0.228112    0.890570
  Point Group: cs    Number of degrees of freedom:  36


  Energy is   -627.828077004

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 36 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.052994    0.056066    0.071394    0.073717    0.122326
0.130845
     0.163608    0.167895    0.174458    0.187371    0.201429
0.208767
     0.221675    0.227165    0.233493    0.257927    0.275572
0.285563
     0.288059    0.301465    0.305720    0.306454    0.307020
0.308272
     0.309420    0.333076    0.340654    0.348708    0.359480
0.400755
     0.466605    0.489248    0.522195    0.688729    0.814988
0.863556

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000009
 Step Taken.  Stepsize is  0.000574

                        Maximum    Tolerance   Cnvgd?
        Gradient        0.000073    0.000300     YES
        Displacement    0.000206    0.001200     YES
        Energy change  -0.000001    0.000001      NO


####################################################
#  Entering anlman.exe on Mon May 21 07:05:29 2012  #
####################################################

 Analysis of SCF Wavefunction

 Total job wall time: 2e+006 s
```

12a B TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
```

```
   Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 90
Number of basis functions: 198

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
       Step      Energy         Max Grad.      Max Dist.
          1    -627.8026907      0.051123       0.144796
          2    -627.8174031      0.013123       0.053666
          3    -627.8191965      0.006469       0.019339
          4    -627.8195192      0.002610       0.011144
          5    -627.8195688      0.001111       0.003774
          6    -627.8195812      0.000265       0.001072
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:33:38.9
  Quantum Mechanics Program Wall Time: 000:33:58.7

Spartan '02 Properties Program:  (PC/x86)
Release  115B
  Orientation rotated by   89.9999974955219     degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.5
** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
  Searching for a Minimum

  Optimization Cycle:   6


                  Coordinates (Angstroms)
    ATOM          X          Y          Z
  1  N         1.979021   -0.321603   0.000000
  2  C         1.954366    1.128483   0.000000
  3  C         0.464571    1.449023   0.000000
  4  C        -0.239189    0.212876   0.000000
  5  C         0.718979   -0.911521   0.000000
  6  O         0.506987   -2.115050   0.000000
  7  O        -0.029667    2.596317   0.000000
  8  C        -1.628152    0.231407   0.000000
```

```
    9  O           -2.278135    1.375120    0.000000
   10  O           -2.342008   -0.872796    0.000000
   11  C            3.200949   -1.090164    0.000000
   12  C           -3.779613   -0.759885    0.000000
   13  H            2.440449    1.560351   -0.887436
   14  H            2.440449    1.560351    0.887436
   15  H           -1.563135    2.111919    0.000000
   16  H            3.807653   -0.877817    0.890970
   17  H            2.921528   -2.145585    0.000000
   18  H            3.807653   -0.877817   -0.890970
   19  H           -4.122204   -0.232683    0.893403
   20  H           -4.122204   -0.232683   -0.893403
   21  H           -4.138299   -1.788245    0.000000
   Point Group: cs    Number of degrees of freedom:  36


   Energy is   -627.819581248

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 36 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.052836    0.056231    0.070661    0.075666    0.124875
0.131939
     0.134778    0.168481    0.169766    0.171682    0.195052
0.201156
     0.212630    0.222328    0.230973    0.246609    0.259947
0.266532
     0.285422    0.289791    0.304119    0.304401    0.306692
0.307523
     0.309628    0.311013    0.323544    0.364856    0.376448
0.392704
     0.474822    0.563732    0.591853    0.787348    0.849346
0.870485


 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000155
 Step Taken.  Stepsize is  0.002558

                        Maximum      Tolerance    Cnvgd?
         Gradient       0.000265     0.000300      YES
         Displacement    0.001072     0.001200      YES
         Energy change  -0.000012     0.000001       NO


###################################################
#  Entering anlman.exe on Sun May 20 05:00:29 2012  #
###################################################
```

Analysis of SCF Wavefunction

12a C TAUTOMER

Spartan '02 Mechanics Program: (PC/x86)
Release 115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release 115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 90
Number of basis functions: 198

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation

Optimization:
       Step   Energy   Max Grad.   Max Dist.
         1   -627.8096298   0.043585   0.125322
         2   -627.8231459   0.011491   0.046944
         3   -627.8244373   0.004708   0.015806
         4   -627.8245822   0.004207   0.007997
         5   -627.8246200   0.000566   0.001812
         6   -627.8246243   0.000207   0.000516
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:34:04.1
  Quantum Mechanics Program Wall Time: 000:34:34.8

Spartan '02 Properties Program: (PC/x86)
Release 115B
   Orientation rotated by   89.9999974955219   degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.7

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle: 6

```
                     Coordinates (Angstroms)
      ATOM             X          Y          Z
    1  N           1.972316  -0.003160   0.000000
    2  C           1.742298   1.441832   0.000000
    3  C           0.189638   1.587075   0.000000
    4  C          -0.315626   0.229497   0.000000
    5  C           0.792649  -0.638905   0.000000
    6  O           0.747034  -1.953154   0.000000
    7  O          -0.375085   2.667223   0.000000
    8  C          -1.634156  -0.342024   0.000000
    9  O          -1.822400  -1.574865   0.000000
   10  O          -2.644237   0.533476   0.000000
   11  C           3.268885  -0.659275   0.000000
   12  C          -3.965340  -0.030009   0.000000
   13  H           2.170857   1.915737  -0.890658
   14  H           2.170857   1.915737   0.890658
   15  H          -0.242358  -2.161809   0.000000
   16  H           3.394104  -1.286976  -0.889132
   17  H           4.043813   0.109484   0.000000
   18  H           3.394104  -1.286976   0.889132
   19  H          -4.640371   0.825957   0.000000
   20  H          -4.123492  -0.644433  -0.890284
   21  H          -4.123492  -0.644433   0.890284
      Point Group: cs    Number of degrees of freedom:  36


     Energy is   -627.824624343

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 36 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.052539   0.055287   0.067300   0.073355   0.122118
0.130548
     0.163856   0.169524   0.170162   0.178110   0.187015
0.208028
     0.225261   0.227551   0.234060   0.256560   0.277472
0.286270
     0.292916   0.302916   0.305224   0.305743   0.306376
0.307715
     0.315827   0.341357   0.353567   0.367206   0.386008
0.424947
     0.435969   0.498045   0.528106   0.733717   0.822942
0.855689

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda = -0.00000048
 Step Taken.  Stepsize is  0.001284
```

```
                    Maximum     Tolerance    Cnvgd?
      Gradient       0.000207    0.000300     YES
      Displacement   0.000516    0.001200     YES
      Energy change  -0.000004   0.000001     NO


##################################################
#  Entering anlman.exe on Sun May 20 04:25:26 2012  #
##################################################

 Analysis of SCF Wavefunction

 Total job wall time:  2.1e+006 s
```

12a D TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.2
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 90
Number of basis functions: 198

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.    Max Dist.
         1   -627.8047267     0.050776     0.142958
         2   -627.8199879     0.019256     0.057535
         3   -627.8219336     0.008723     0.022299
         4   -627.8222923     0.002632     0.012604
         5   -627.8223695     0.000885     0.003808
         6   -627.8223734     0.000400     0.001755
         7   -627.8223743     0.000099     0.000422
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:37:01.5
  Quantum Mechanics Program Wall Time: 000:37:43.9
```

Spartan '02 Properties Program: (PC/x86)
Release 115B
  Orientation rotated by   89.9999974955219   degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.5
  Properties Program Wall Time: 000:00:00.6

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle: 7

                  Coordinates (Angstroms)
     ATOM   X   Y   Z
   1 N   1.993750   -0.073081   0.000000
   2 C   1.817724   1.372978   0.000000
   3 C   0.279588   1.579745   0.000000
   4 C   -0.276687   0.242032   0.000000
   5 C   0.804007   -0.732927   0.000000
   6 O   0.660693   -1.979211   0.000000
   7 O   -0.255063   2.675371   0.000000
   8 C   -1.581797   -0.225156   0.000000
   9 O   -1.842019   -1.513936   0.000000
  10 O   -2.607878   0.601768   0.000000
  11 C   3.283183   -0.727548   0.000000
  12 C   -3.934256   0.038606   0.000000
  13 H   2.264195   1.839033   -0.888406
  14 H   2.264195   1.839033   0.888406
  15 H   -0.923055   -1.983950   0.000000
  16 H   3.862968   -0.452893   -0.890611
  17 H   3.862968   -0.452893   0.890611
  18 H   3.114943   -1.805930   0.000000
  19 H   -4.601312   0.899820   0.000000
  20 H   -4.093074   -0.570432   -0.893084
  21 H   -4.093074   -0.570432   0.893084
     Point Group: cs   Number of degrees of freedom: 36

   Energy is   -627.822374316

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 36 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
    0.052360   0.056146   0.071671   0.075526   0.124610
0.129119
    0.131520   0.164593   0.170317   0.172341   0.192514
0.206383

```
     0.208965    0.217502    0.227339    0.241930    0.249711
0.260839
     0.285305    0.293983    0.302504    0.304684    0.306401
0.307676
     0.309849    0.312836    0.331040    0.355012    0.374657
0.411729
     0.479748    0.564567    0.628788    0.809205    0.859283
0.871055
```

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda = -0.00000016
 Step Taken. Stepsize is 0.000886

	Maximum	Tolerance	Cnvgd?
Gradient	0.000099	0.000300	YES
Displacement	0.000422	0.001200	YES
Energy change	-0.000001	0.000001	YES


```
####################################################
#  Entering anlman.exe on Sun May 20 03:49:51 2012  #
####################################################
```

 Analysis of SCF Wavefunction

 Total job wall time: 2.3e+006 s

12b A TAUTOMER

Spartan '02 Mechanics Program: (PC/x86)
Release 115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program: (PC/x86)
Release 115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 102
Number of basis functions: 228

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation

```
Optimization:
      Step      Energy        Max Grad.     Max Dist.
         1   -741.1674797      0.033171      0.128301
         2   -741.1764991      0.009202      0.028039
         3   -741.1773037      0.002734      0.009530
         4   -741.1773840      0.001031      0.003231
         5   -741.1773947      0.000449      0.001509
         6   -741.1773927      0.000083      0.002802
         7   -741.1773938      0.000042      0.002079
         8   -741.1773947      0.000044      0.000193
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:41:30.4
  Quantum Mechanics Program Wall Time: 000:41:55.8

Spartan '02 Properties Program: (PC/x86)
Release  115B
  Orientation rotated by   179.999994991044    degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.6
  Properties Program Wall Time: 000:00:00.6

** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
  Searching for a Minimum

  Optimization Cycle:   8

                 Coordinates (Angstroms)
   ATOM          X           Y           Z
  1  N        1.647789     0.259117    -0.000015
  2  C        1.365409     1.693397     0.000044
  3  C       -0.130732     1.717536    -0.000006
  4  C       -0.650996     0.453047    -0.000080
  5  C        0.455433    -0.523824    -0.000094
  6  O        0.413269    -1.737247    -0.000182
  7  O       -0.787264     2.857476     0.000028
  8  C       -2.093978     0.259808    -0.000122
  9  O       -2.868677     1.225690    -0.000332
 10  O       -2.505018    -1.005504     0.000127
 11  C        2.983058    -0.161660     0.000056
 12  C       -3.930756    -1.208452     0.000102
 13  C        3.262413    -1.645441    -0.000019
 14  O        3.861216     0.686217     0.000188
 15  H        1.785662     2.189170     0.882623
 16  H        1.785726     2.189251    -0.882458
 17  H       -1.754409     2.601206    -0.000039
 18  H       -4.379602    -0.762892    -0.891051
 19  H       -4.063394    -2.289821     0.000295
 20  H       -4.379676    -0.762563     0.891053
 21  H        2.819318    -2.129845     0.874496
```

```
  22  H              2.819385   -2.129744   -0.874624
  23  H              4.345825   -1.774922    0.000009
  Point Group: c1    Number of degrees of freedom:  63


   Energy is   -741.177394694

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 63 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.001217    0.001855    0.004788    0.006954    0.008917
 0.013630
     0.014707    0.016688    0.017941    0.021617    0.028454
 0.037869
     0.044156    0.051300    0.054304    0.055285    0.055839
 0.064094
     0.073472    0.074551    0.076415    0.096498    0.122129
 0.128392
     0.147969    0.150825    0.166107    0.169468    0.176281
 0.182830
     0.186001    0.199181    0.211768    0.215132    0.229340
 0.241369
     0.243419    0.259385    0.273933    0.280443    0.285702
 0.296180
     0.304598    0.305229    0.305467    0.305788    0.306029
 0.306725
     0.307411    0.307420    0.311098    0.341966    0.349063
 0.363231
     0.415959    0.457555    0.490336    0.532470    0.586210
 0.675908
     0.801836    0.811903    0.856555

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda =  -0.00000003
 Step Taken.  Stepsize is  0.000598

                   Maximum    Tolerance    Cnvgd?
        Gradient    0.000044    0.000300     YES
        Displacement  0.000193  0.001200     YES
        Energy change -0.000001  0.000001    YES


#####################################################
#  Entering anlman.exe on Tue May 22 07:55:47 2012  #
#####################################################

 Analysis of SCF Wavefunction
```

```
 Total job wall time:  2.5e+006 s
```

12b B TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.1
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 102
Number of basis functions: 228

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
       Step      Energy          Max Grad.      Max Dist.
          1    -741.1503465      0.052493       0.144245
          2    -741.1662310      0.013680       0.041460
          3    -741.1680629      0.007174       0.021750
          4    -741.1683874      0.002757       0.013853
          5    -741.1684544      0.001281       0.005085
          6    -741.1684670      0.000431       0.001458
          7    -741.1684682      0.000070       0.000201
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:49:54.0
  Quantum Mechanics Program Wall Time: 000:50:40.5

Spartan '02 Properties Program:  (PC/x86)
Release  115B
   Orientation rotated by   89.9999974955219     degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.7
  Properties Program Wall Time: 000:00:00.9


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   7
```

```
                  Coordinates (Angstroms)
     ATOM           X           Y           Z
   1  N         1.669146    0.295325    0.000000
   2  C         1.363475    1.729778    0.000000
   3  C        -0.151503    1.763041    0.000000
   4  C        -0.622677    0.419039    0.000000
   5  C         0.500538   -0.520573    0.000000
   6  O         0.490801   -1.737560    0.000000
   7  O        -0.855570    2.794275    0.000000
   8  C        -1.997862    0.187354    0.000000
   9  O        -2.834740    1.195671    0.000000
  10  O        -2.498179   -1.024590    0.000000
  11  C         3.011507   -0.101908    0.000000
  12  C        -3.935417   -1.174025    0.000000
  13  C         3.323458   -1.580150    0.000000
  14  O         3.875890    0.760588    0.000000
  15  H         1.777568    2.229458   -0.882404
  16  H         1.777568    2.229458    0.882404
  17  H        -2.256891    2.051555    0.000000
  18  H        -4.364798   -0.716233   -0.893787
  19  H        -4.100763   -2.250191    0.000000
  20  H        -4.364798   -0.716233    0.893787
  21  H         2.891774   -2.074780    0.874360
  22  H         2.891774   -2.074780   -0.874360
  23  H         4.409699   -1.684520    0.000000
   Point Group: cs    Number of degrees of freedom:  40
```

   Energy is   -741.168468236

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 40 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
```
     0.050755    0.056001    0.073878    0.075686    0.125084
0.128347
     0.129873    0.152817    0.161654    0.171025    0.172149
0.194800
     0.203963    0.214973    0.232089    0.234337    0.236113
0.251072
     0.257105    0.279808    0.280415    0.287861    0.303649
0.305207
     0.305650    0.307152    0.308287    0.317231    0.320475
0.364806
     0.392777    0.414562    0.457128    0.578729    0.610294
0.615740
     0.797565    0.811343    0.856214    0.873977
```

 Minimum Search - Taking Simple RFO Step

```
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda = -0.00000008
 Step Taken.  Stepsize is  0.000557


                       Maximum      Tolerance    Cnvgd?
           Gradient     0.000070     0.000300      YES
           Displacement 0.000201     0.001200      YES
           Energy change -0.000001    0.000001      NO



#####################################################
#  Entering anlman.exe on Sun May 20 09:19:56 2012  #
#####################################################

 Analysis of SCF Wavefunction

 Total job wall time: 3e+006 s
```

12b C TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.1
  Mechanics Wall Time: 000:00:00.2
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 102
Number of basis functions: 228

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
      Step      Energy        Max Grad.     Max Dist.
         1   -741.1450738      0.036836      0.129532
         2   -741.1603094      0.013328      0.048885
         3   -741.1621251      0.003855      0.014685
         4   -741.1623188      0.002042      0.005652
         5   -741.1623338      0.001410      0.002419
         6   -741.1623422      0.000142      0.000820
  Reason for exit: Sucessful completion
```

```
   Quantum Mechanics Program CPU Time : 000:43:16.4
   Quantum Mechanics Program Wall Time: 000:43:47.5


Spartan '02 Properties Program:  (PC/x86)
Release  115B
   Orientation rotated by   89.9999974955219     degrees!
   Reason for exit: Successful completion
   Properties Program CPU Time : 000:00:00.6
   Properties Program Wall Time: 000:00:00.7


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                    Coordinates (Angstroms)
     ATOM          X          Y          Z
   1  N        1.501701   -0.226595    0.000000
   2  C        1.323387    1.236774    0.000000
   3  C       -0.211749    1.449081    0.000000
   4  C       -0.782291    0.116785    0.000000
   5  C        0.256696   -0.818463    0.000000
   6  O        0.114626   -2.114239    0.000000
   7  O       -0.728105    2.551010    0.000000
   8  C       -2.148812   -0.357836    0.000000
   9  O       -2.425643   -1.569335    0.000000
  10  O       -3.081246    0.594115    0.000000
  11  C        2.747329   -0.896885    0.000000
  12  C       -4.446843    0.140969    0.000000
  13  C        3.958331    0.017623    0.000000
  14  O        2.830154   -2.105027    0.000000
  15  H        1.766380    1.693310   -0.890110
  16  H        1.766380    1.693310    0.890110
  17  H       -0.885213   -2.255821    0.000000
  18  H       -5.047430    1.050261    0.000000
  19  H       -4.652016   -0.457834   -0.890884
  20  H       -4.652016   -0.457834    0.890884
  21  H        3.974293    0.664745    0.884181
  22  H        4.847792   -0.612862    0.000000
  23  H        3.974293    0.664745   -0.884181
   Point Group: cs   Number of degrees of freedom:  40


   Energy is   -741.162342181


 Hessian Updated using BFGS Update
  internal optimization with constraints (0)


 40 Hessian modes will be used to form the next step
```

```
   Hessian Eigenvalues:
      0.051303     0.054956     0.068885     0.073387     0.122163
0.129109
      0.152342     0.170148     0.174695     0.180318     0.197616
0.208309
      0.215447     0.225991     0.230649     0.238333     0.244256
0.253523
      0.271320     0.279828     0.289447     0.295461     0.305096
0.305767
      0.306807     0.307358     0.310350     0.324279     0.337459
0.342455
      0.415601     0.460079     0.492472     0.504449     0.560668
0.602682
      0.786431     0.815408     0.831925     0.846594

 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken    Lamda =  -0.00000038
 Step Taken.  Stepsize is  0.001470

                         Maximum     Tolerance    Cnvgd?
            Gradient      0.000142     0.000300     YES
            Displacement  0.000820     0.001200     YES
            Energy change -0.000008     0.000001     NO


####################################################
#  Entering anlman.exe on Sun May 20 08:28:19 2012  #
####################################################

 Analysis of SCF Wavefunction

 Total job wall time: 2.6e+006 s
```

12b D TAUTOMER

```
Spartan '02 Mechanics Program:  (PC/x86)
Release  115B

  Reason for exit: Successful completion
  Mechanics CPU Time : 000:00:00.3
  Mechanics Wall Time: 000:00:00.3
Spartan '02 Quantum Mechanics Program:  (PC/x86)
Release  115B
  To use a standard Psuedopotential a heavy atom must exists
  (An atom larger than 'Ar')

Job type: Geometry optimization.
Method: RB3LYP
Basis set: LACVP*
Number of shells: 102
```

```
Number of basis functions: 228

SCF model:
 A restricted hybrid HF-DFT SCF calculation will be
 performed using Pulay DIIS extrapolation


Optimization:
        Step      Energy        Max Grad.     Max Dist.
           1   -741.1491326    0.052301      0.143188
           2   -741.1652810    0.013337      0.041945
           3   -741.1671069    0.005876      0.016421
           4   -741.1673897    0.002968      0.009496
           5   -741.1674386    0.000850      0.002454
           6   -741.1674457    0.000249      0.000870
  Reason for exit: Sucessful completion
  Quantum Mechanics Program CPU Time : 000:46:03.0
  Quantum Mechanics Program Wall Time: 000:46:51.1

Spartan '02 Properties Program: (PC/x86)
Release 115B
  Orientation rotated by   89.9999974955219    degrees!
  Reason for exit: Successful completion
  Properties Program CPU Time : 000:00:00.8
  Properties Program Wall Time: 000:00:01.0


** GEOMETRY OPTIMIZATION IN DELOCALIZED INTERNAL COORDINATES
**
   Searching for a Minimum

   Optimization Cycle:   6


                 Coordinates (Angstroms)
    ATOM           X          Y          Z
  1  N        1.632642   0.472492   0.000000
  2  C        1.197822   1.878034   0.000000
  3  C       -0.341395   1.811961   0.000000
  4  C       -0.667754   0.395816   0.000000
  5  C        0.542373  -0.392665   0.000000
  6  O        0.599224  -1.639736   0.000000
  7  O       -1.066503   2.790348   0.000000
  8  C       -1.893073  -0.263313   0.000000
  9  O       -1.962561  -1.575807   0.000000
 10  O       -3.023284   0.404659   0.000000
 11  C        3.006546   0.169948   0.000000
 12  C       -4.261890  -0.336768   0.000000
 13  C        3.421830  -1.282813   0.000000
 14  O        3.803079   1.091484   0.000000
 15  H        1.572622   2.402840  -0.883821
 16  H        1.572622   2.402840   0.883821
```

```
17  H         -0.996379   -1.910883    0.000000
18  H         -4.332879   -0.960409    0.893903
19  H         -5.039495    0.425511    0.000000
20  H         -4.332879   -0.960409   -0.893903
21  H          3.028413   -1.806417    0.875796
22  H          3.028413   -1.806417   -0.875796
23  H          4.512505   -1.310296    0.000000
   Point Group: cs   Number of degrees of freedom:  40


   Energy is   -741.167445698

 Hessian Updated using BFGS Update
  internal optimization with constraints (0)

 40 Hessian modes will be used to form the next step
  Hessian Eigenvalues:
     0.050649    0.055980    0.074991    0.075656    0.125061
0.128543
     0.147487    0.151569    0.169563    0.171516    0.176625
0.195465
     0.201046    0.213746    0.227332    0.233822    0.238801
0.252288
     0.261323    0.276251    0.282997    0.298527    0.304141
0.305203
     0.305970    0.306863    0.307947    0.312678    0.321083
0.365209
     0.396169    0.407953    0.465660    0.537983    0.590756
0.601848
     0.788391    0.814588    0.858671    0.874017


 Minimum Search - Taking Simple RFO Step
 Searching for Lamda that Minimizes Along All modes
 Value Taken   Lamda =  -0.00000087
 Step Taken.  Stepsize is  0.002106


                        Maximum    Tolerance   Cnvgd?
        Gradient       0.000249    0.000300     YES
       Displacement    0.000870    0.001200     YES
       Energy change  -0.000007    0.000001      NO



####################################################
#  Entering anlman.exe on Sun May 20 07:43:28 2012  #
####################################################

 Analysis of SCF Wavefunction

 Total job wall time: 2.8e+006 s
```
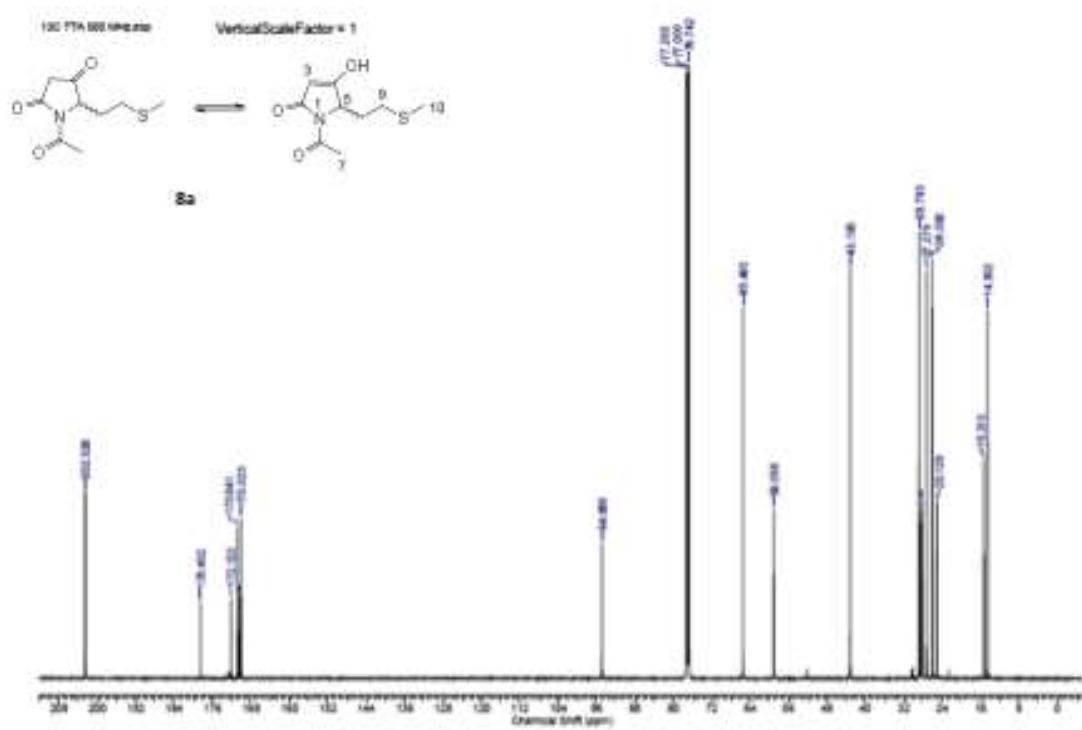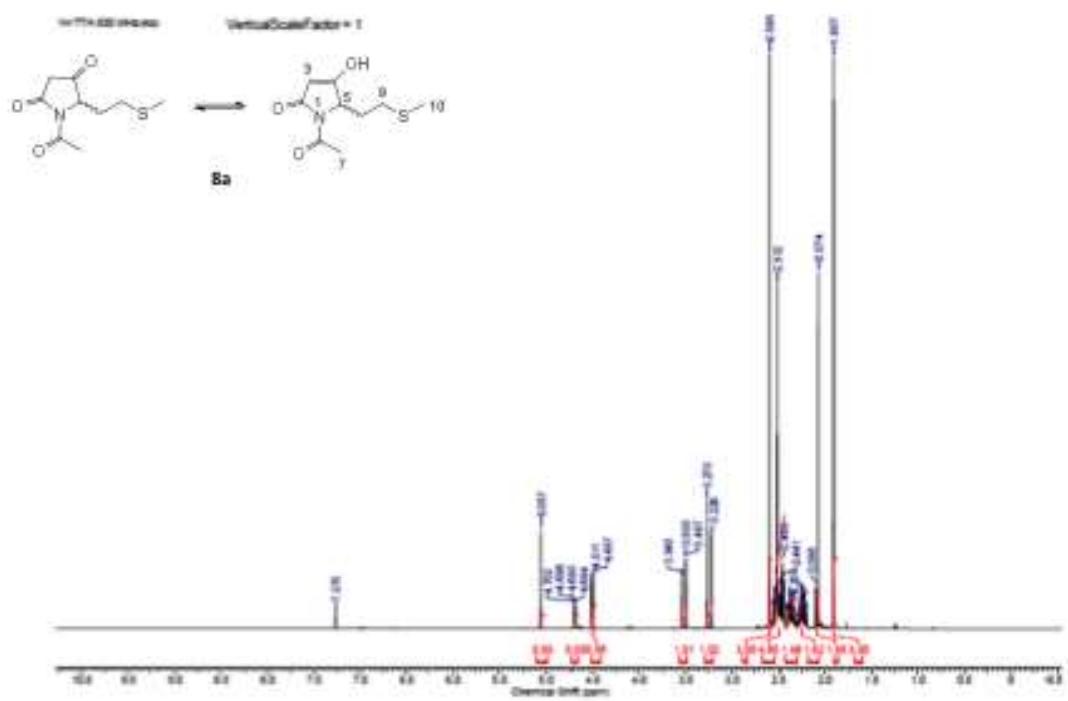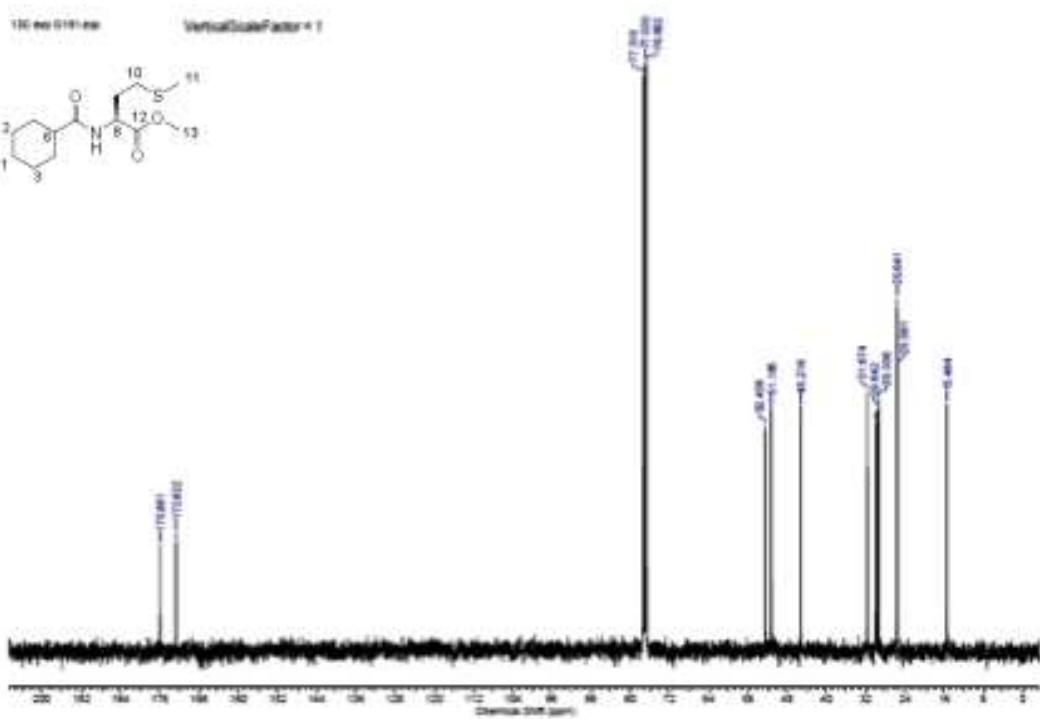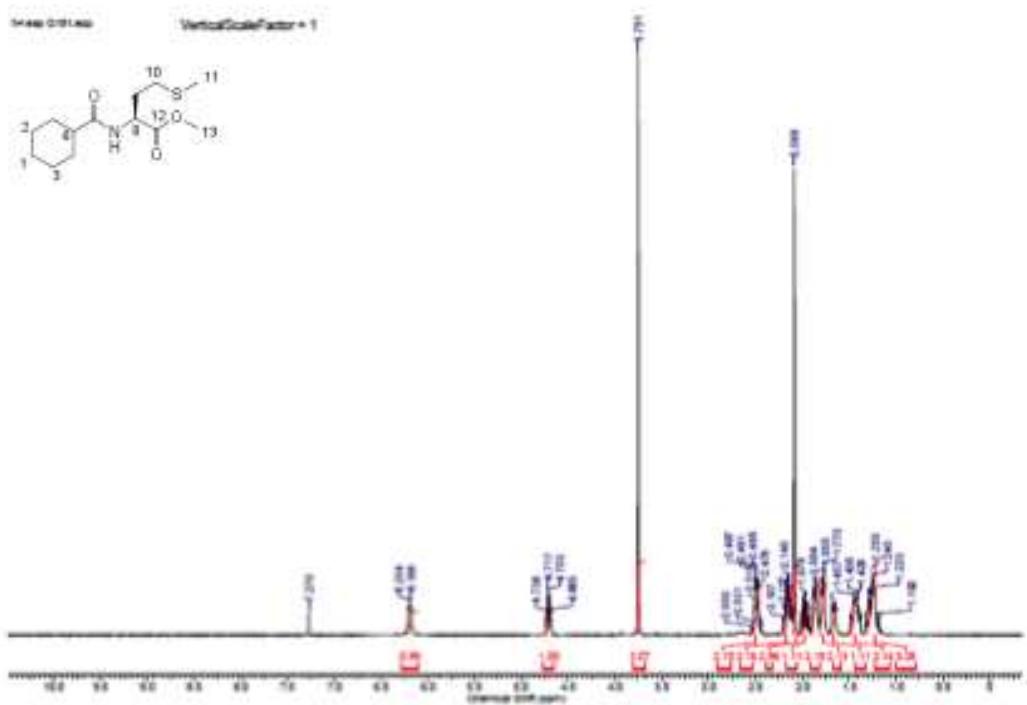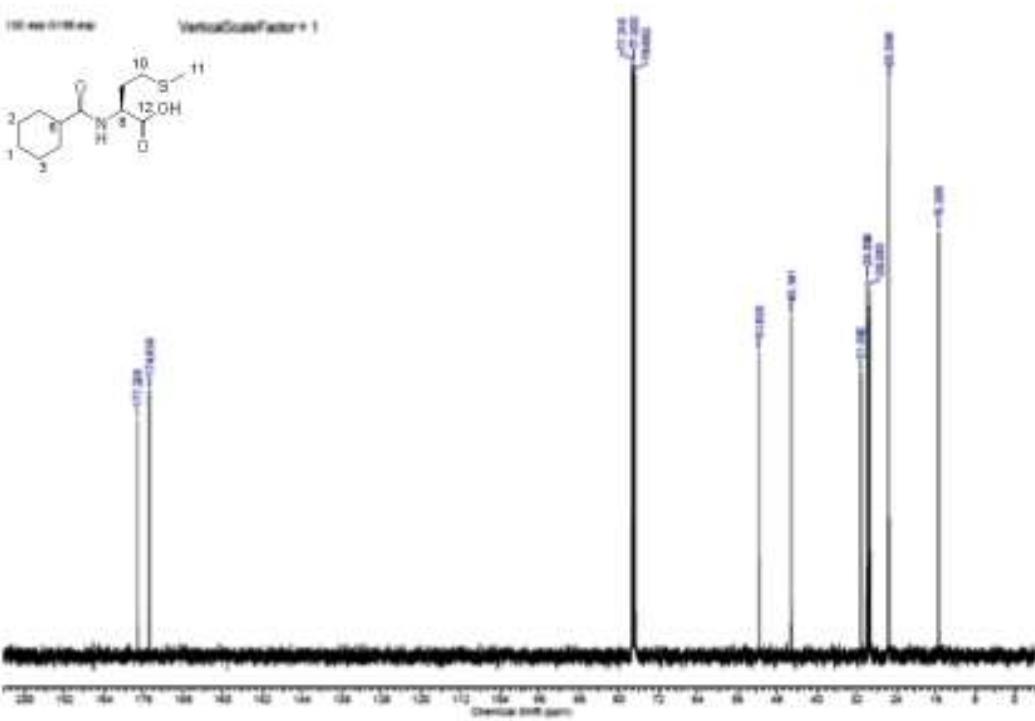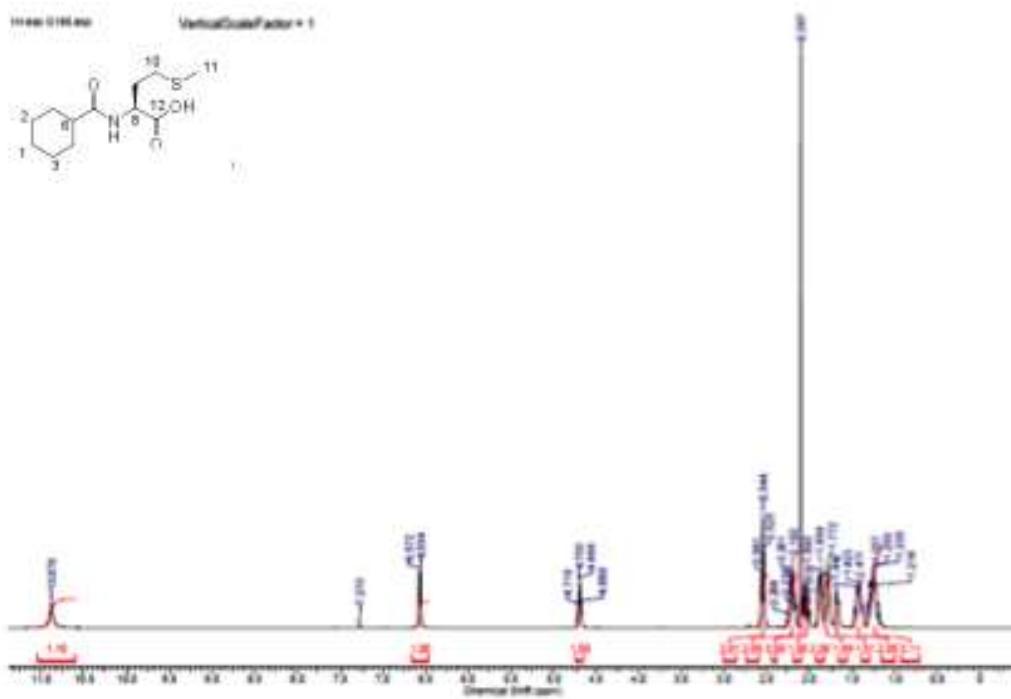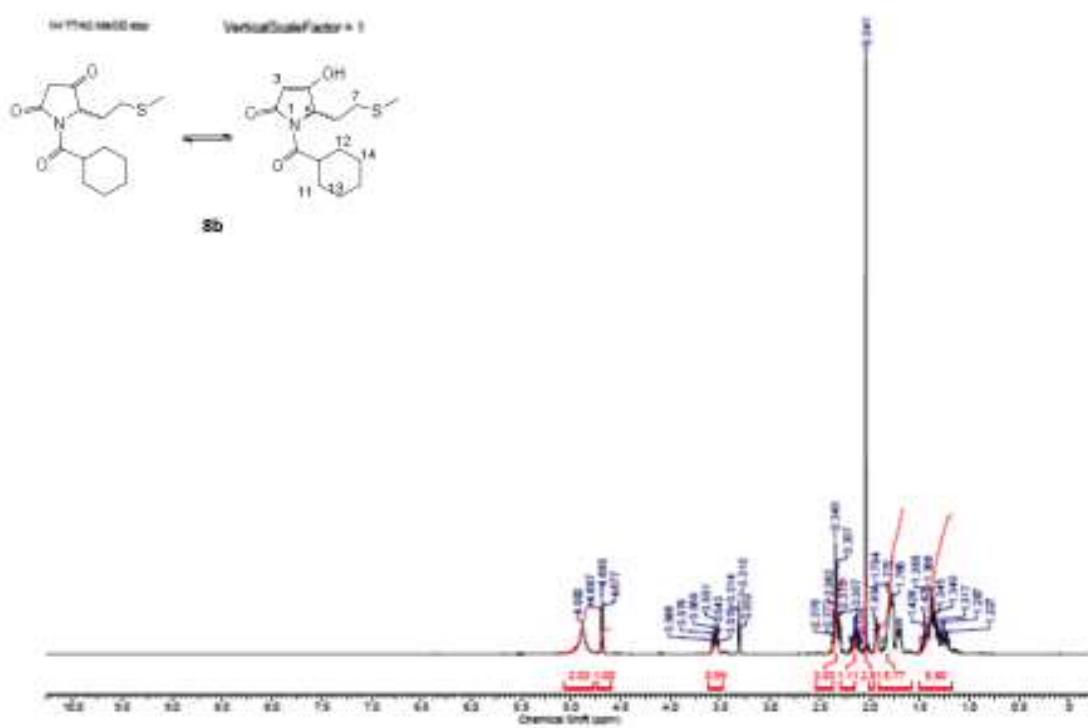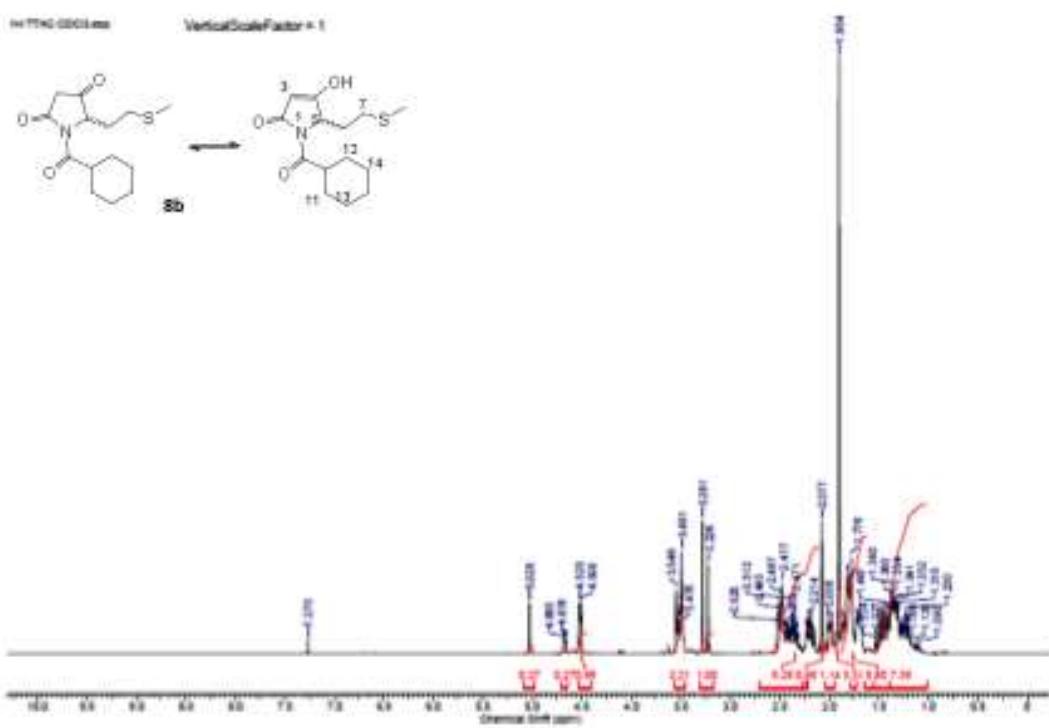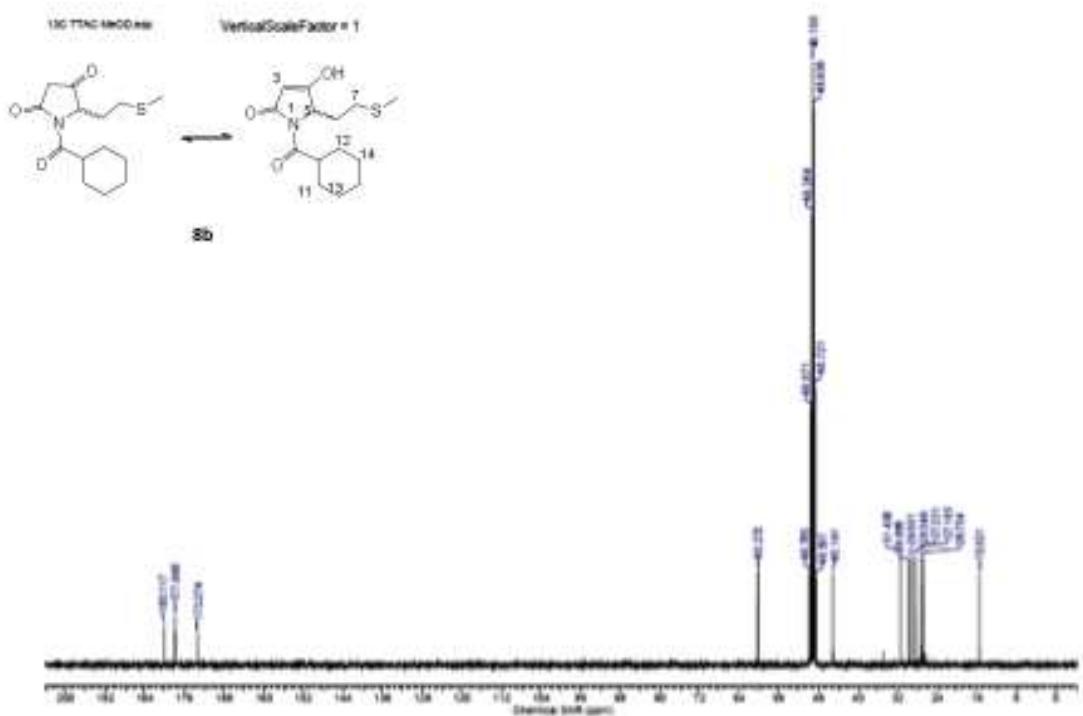
Table S1: LipE values of tetramates

|	S1	S26	S4	S2	E1	E2	P1	P9	P9B	H3	H4
2a	3.21	2.91	2.91	2.91	2.91	2.91	2.61	2.91	2.31	2.61	3.21
2b	3.63	3.63	3.63	3.33	3.33	3.03	3.03	3.03	-	3.33	2.08
2c	3.31	3.31	3.31	3.31	3.31	3.31	3.00	3.31	3.31	3.60	4.81
2d	3.5	3.5	3.5	3.5	3.5	3.5	3.20	3.80	3.20	3.80	4.72
2e	2.37	1.46	1.46	1.46	1.76	2.91	2.07	2.67	2.07	0.86	3.67
2f	0.28	0.28	0.28	0.28	0.28	0.28	0.32	0.92	0.32	0.32	0.32
2g	3.13	3.13	3.13	3.13	2.83	3.13	2.83	2.22	2.83	3.13	3.43
2h	2.55	2.55	2.55	2.55	2.55	2.55	2.93	2.25	1.04	1.04	1.95
3a	2.92	2.92	3.23	2.92	3.53	3.53	3.83	3.83	3.83	2.92	2.92
3b	3.17	2.87	3.47	3.17	3.77	3.47	4.07	4.07	4.07	2.87	3.77
3c	3.82	3.22	3.22	3.53	3.82	3.53	3.82	3.82	3.82	3.22	4.13
3d	3.62	2.71	3.02	3.02	3.62	3.32	3.62	3.62	3.92	2.71	3.92
3e	2.97	2.97	2.97	2.97	2.97	2.97	2.97	2.97	2.97	2.97	2.97
3f	3.36	3.36	3.36	3.36	3.36	3.36	3.36	3.36	3.36	3.36	3.36
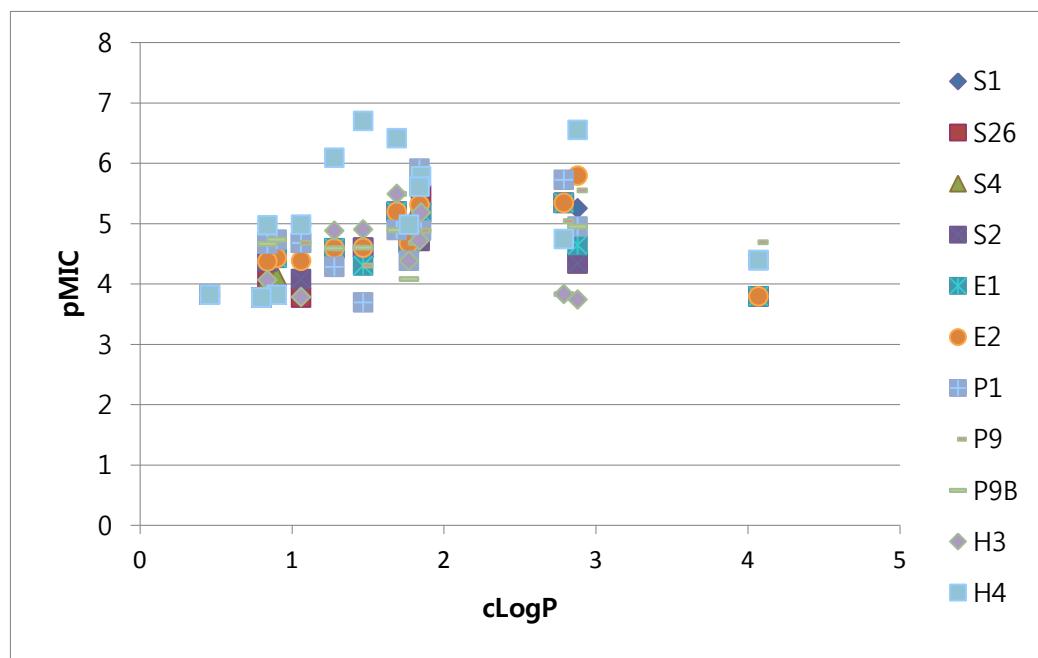
Figure S1: Plot of cLogP versus pMIC for the compounds shown in Table S1.