Chemoselective and diastereodivergent synthesis of new spirooxindolo-pyrrolizidines and pyrrolidines stemming from unsymmetrical 1,3-bis(arylidene)tetral-2-ones: A combined experimental and theoretical study.

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2.1.1. (*2R*, *3S*, *4S*, *5R*) Spiro[2,3']-oxindole-spiro[3,3'']-1''(naphtylidene)tetral-2''-one-4-naphtylpyrrolizidine (4a)

Yellow oil, (0.24 g; 39%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ:1.75-2.01 (2m, 2H, H-6_a/H-7_a); 2.08-2.13 (2m, 2H, H-6_b/H-7_b), 2.17 (d, *J*= 15 Hz, 1H, H-4''); 2.49-2.61 (m, 1H, H-8_a); 3.31-3.40 (m, 1H, H-8_b); 3.52 (d, *J* = 15 Hz, 1H, H-4''); 4.84 (d, *J* = 9 Hz, H-4) 4.95-5.04 (m, 1H, H-5); 6.22-7.97 (m, 22H, H_{arom}); 7.99 (s, 1H, $H_{ethylenic}$); 8.03 (s.l, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ: 24.3, 27.6, 34.8, 47.0, 54.2, 63.9, 65.7, 73.5, 108.4, 120.9, 125.0, 125.2, 125.4, 125.6, 125.7, 126.2, 126.4, 126.9, 127.0, 127.1, 127.3, 127.7, 127.8, 128.1, 128.9, 129.4, 129.7, 132.1, 132.2, 132.6, 132.7, 133.2, 134.0, 135.3, 135.4, 136.9, 140.5, 176.5, 200.8, **IR (ν_{max}, cm^{-1}) :** 1498; 1581; 1684; 1727; 3110 cm^{-1}; Anal. Calcd. for $C_{44}H_{39}N_2O_2$: C, 84.18; H, 6.26; N, 4.46; found: C, 84.14; H, 6.27; N, 4.43.

2.1.2. (*2R, 3S, 4S, 5R*) Spiro[2,3']-oxindole-spiro[3,3'']-1''(*p*-tolylidene)tetral-2''-one-4-(*p*-tolyl)pyrrolizidine (4b)

Yellow oil, (0.22 g; 41%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ:1.77-1.94 (2m, 2H, H-6_a/H-7_a); 2.01-2.21 (2m, 2H, H-6_b/H-7_b), 2.22 (s, 3H, CH_3); 2.26 (d, *J* = 15 Hz, 1H, H-4''); 2.27 (s, 3H, CH_3); 2.53-2.61 (m, 1H, H-8_a); 3.35-3.40 (m, 1H, H-8_b); 3.38 (d, *J* = 15 Hz, 1H, H-4''); 4.61 (d, *J*= 12 Hz, 1H, H-4); 4.85-4.94 (m, 1H, H-5); 6.30-7.42 (m, 17H, $16H_{arom}$ + $1H_{amide}$); 7.71 (S,1H, $1H_{ethylenic}$) **^{13}C NMR** ($CDCl_3$, 100 MHz) δ: 20.6; 20.8; 24.2; 27.7; 34.7; 47.4; 54.0; 63.1; 65.7; 73.8;108.7; 120.8; 125.2; 125.4, 125.6; 126.0; 126.9; 128.0; 128.2; 128.4; 128.5, 128.6; 128.7, 129.1; 129.3; 129.9; 131.9; 132.2; 132.5; 133.8; 134.7; 135.9; 136.9; 138.7; 140.8; 177.1; 201.3; **IR (ν_{max}, cm^{-1}):** 1510; 1581; 1679; 1732; 2975 cm^{-1}; Anal. Calcd. for $C_{38}H_{39}N_2O_2$: C. 82.13; H. 7.07; N. 5.04; found: C. 82.09; H. 7.05; N. 5.03.

2.1.3. (*2R, 3S, 4 S, 5R*) Spiro [2,3']-oxindole-spiro [3,3'']-1''(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (4c)

Yellow oil, (0.22 g; 40%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.75-1.95 (2m, 2H, H-6_a/H-7_a); 2.06-2.17 (2m, 2H, H-6_b/H-7_b); 2.21 (d, *J*= 15 Hz, 1H, H-4''); 2.53-2.65 (m, 1H, H-8_a); 3.35 (d, *J*= 15 Hz, 1H, H-4''); 3.28-3.48 (m, 1H, H-8_b); 4.59 (d, *J*= 9 Hz, H-4); 4.78-4.89 (m, 1H, H-5); 6.30-7.50 (m, 16H, H_{arom}); 7.66 (s, 1H, $H_{ethylenic}$); 8.00 (s.l, 1H, H_{amide}); **^{13}C NMR**

($CDCl_3$, 100 MHz) δ : 24.2; 27.6; 34.7; 47.3; 53.5; 63.0; 66.0; 73.6; 108.7; 114.6; 114.9; 115.0; 120.9; 124.8; 125.6; 125.9; 126.8; 127.1; 128.2; 129.4; 130.7; 130.9; 131.0; 131.7; 133.2; 133.3; 135.7; 140.6; 163.0; 164.0; 176.7; 200.9; **IR (ν_{max}, cm^{-1}):** 1519; 1590; 1694; 1718; 2988 cm^{-1}; Anal.Calcd. for $C_{36}H_{33}N_2O_2$: C, 76.71; H, 5.90; F, 6.74; N, 4.97; found: C, 76.65; H, 5.92; F, 6.72; N, 4.95.

2.1.4. (*2R, 3S, 4S, 5R*) Spiro [2,3']-oxindole-spiro [3,3'']-1''(*p*-cyanobenzylidene)tetral-2''-one-4-(*p*-cyanobenzyl)pyrrolizidine (4d)

Yellow powder, (0.18 g; 32%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.71-1.80 (2m, 2H, H-6_a/H-7_a); 1.82-1.94 (2m, 2H, H-6_b/H-7_b); 2.12 (d, *J*= 15 Hz, 1H, H-4''); 2.56-2.61 (m, 1H, H-8_a); 3.28 (d, *J*= 9 Hz, 1H, H-4''); 3.31-3.36 (m, 1H, H-8_b); 4.63 (d, *J*= 9 Hz, H-4); 4.85-4.89 (m, 1H, H-5); 6.24-7.65 (m, 12H, H_{arom}); 7.68 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.6; 28.1; 35.1; 47.6; 54.4; 63.6, 66.2; 73.7; 109.3; 111.0; 112.0; 118.4; 118.8; 120.4, 121.6; 125.3, 126.0, 126.2, 126.6; 127.1; 128.4; 129.1; 129.8; 130.2; 130.6; 131.4; 131.6; 132.0; 132.2; 135.0; 135.3; 140.1; 179.4, 201.0; **IR (ν_{max}, cm^{-1}):** 1478; 1596; 1688; 1714; 2225; 2923 cm^{-1}; Anal. Calcd. for $C_{38}H_{33}N_4O_2$: C, 79.00; H, 5.76; N, 9.70; found: C, 78.94; H, 5.72; N, 9.72.

2.1.5. (2R, 3S, 4S, 5R) Spiro [2,3'] *N*-methyloxindole-spiro[3,3'']-1''(naphtylidene)tetral-2''-one-4-(naphtyl)pyrrolizidine (4e)

Yellow oil, (0.33g; 52%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.81-1.93 (2m, 2H, H-6_a/H-7_a); 2.04-2.15 (2m, 2H, H-6_b/H-7_b); 2.21 (d, *J*= 15 Hz, 1H, H-4''); 2.58-2.68 (m, 1H, H-8_a); 2.78 (s, 3H, CH_3); 3.41 (d, *J*= 15 Hz, 1H, H-4''); 3.44-3.54 (m, 1H, H-8_b); 4.85 (d, *J*= 9 Hz, H-4); 5.11-5.19 (m, 1H, H-5); 6.14-7.92 (m, 22H, H_{arom}); 7.97 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 23.9; 25.3; 27.6; 35.0; 47.8; 54.5; 65.9; 73.7; 107.0; 121.0; 125.1; 125.4; 125.5; 125.6; 126.3; 126.4; 126.6; 126.9; 127.0; 127.1; 127.4; 127.7; 128.2; 128.3; 129.9 131.7; 132.1; 132.4; 132.6; 132.9; 133.0; 133.0; 134.1; 136.9; 143.2; 174.5; 201.7; **IR (ν_{max}, cm^{-1}):** 1514; 1569; 1683; 1739; 3127 cm^{-1}; Anal.Calcd. for $C_{45}H_{41}N_2O_2$: C, 84.21; H, 6.44; N, 4.36; found: C, 84.17; H, 6.39; N, 4.31.

2.1.6. (*2R, 3S, 4S, 5R*) Spiro [2,3']-*N*-methyloxindole-spiro [3,3'']-1''(*p*-tolylidene)tetral-2''-one-4-(*p*-tolyl)pyrrolizidine (4f)

Yellow oil, (0.30 g; 54%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.78-1.85 (2m, 2H, H-6_a/H-7_a); 2.04-2.18 (2m, 2H, H-6_b/H-7_b); 2.13 (d, *J*= 15 Hz, 1H, H-4''); 2.25 (s, 3H, CH_3); 2.32 (s, 3H, CH_3); 2.47-2.58 (m, 1H, H-8_a); 2.75 (s, 3H, N$\underline{CH_3}$); 3.27 (d, *J*= 15 Hz, 1H, H-4''); 3.30-3.41 (m, 1H, H-8_b); 4.57 (d, *J*= 9 Hz, 1H, H-4); 4.88-4.96 (m, 1H, H-5); 6.12-7.50 (m, 12H, H_{arom}); 7.69 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 20.5; 20.6; 23.9; 25.2; 27.5; 34.9; 47.7; 54.1; 66.0; 73.6; 106.8; 120.9; 125.3; 126.0; 126.1; 126.5; 128.0; 128.2; 128.4; 128.5; 129.0; 129.3; 129.3; 129.7; 131.8; 131.8; 132.4; 134.1; 134.6; 135.9; 136.9; 138.7; 143.1; 174.7; 201.4; **IR (ν_{max}, cm^{-1}):** 1493; 1563; 1689; 1715; 2940 cm^{-1}; Anal.Calcd. for $C_{39}H_{41}N_2O_2$: C, 82.21; H, 7.25; N, 4.92; found: C, 82.18; H, 7.26; N, 4.94.

2.1.7. (*2R, 3S, 4S, 5R*) Spiro [2,3']- *N*-methyloxindole-spiro[3,3'']-1''(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (4g)

Yellow oil, (0.32 g; 57%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.76-1.85 (2m, 2H, H-6_a/H-7_a); 2.04-2.12 (2m, 2H, H-6_b/H-7_b); 2.13 (d, *J*= 15 Hz, 1H, H-4''); 2.48-2.53 (m, 1H, H-8_a); 2.70 (s, 3H, N$\underline{CH_3}$); 3.27 (d, *J*= 15 Hz, 1H, H-4''); 3.30-3.39 (m, 1H, H-8_b); 4.59 (d, *J*= 9 Hz, H-4); 4.81-4.89 (m, 1H, H-5); 6.15-7.51 (m, 16H, H_{arom}); 7.69 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.0; 25.1; 27.5; 34.9; 47.2; 53.7; 62.8; 66.2; 73.4; 106.9; 114.5; 114.6; 114.8; 114.9; 120.9; 124.3; 125.5; 126.0; 126.3; 126.4; 128.1; 128.4; 130.8; 130.9; 131.4; 133.0; 133.5; 135.5; 143.2; 163.1; 164.0; 174.6; 201.3; **IR (ν_{max}, cm^{-1}):** 1495; 1563; 1670; 1729; 2935 cm^{-1}; Anal. Calcd. for $C_{37}H_{35}N_2O$: C, 76.93; H, 6.11; F, 6.58; N, 4.85; found: C, 76.89; H, 6.03; F, 6.54; N, 4.81.

2.1.8. (*2R, 3S, 4S, 5R*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''(*p*-cyanobenzylidene)tétral-2''-one-4-(*p*-cyanobenzyl)pyrrolizidine (4h)

Yellow powder, (0.20 g; 34%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.69-1.92 (2m, 2H, H-6_a/H-7_a); 1.95-2.08 (2m, 2H, H-6_b/H-7_b); 2.18 (d, *J*= 15 Hz, 1H, H-4''); 2.48-2.59 (m, 1H, H-8_a); 2.75 (s, 3H, N$\underline{CH_3}$); 3.24-3.37 (m, 1H, H-8_b); 3.39 (d, *J*= 9 Hz, 1H, H-4''); 4.59 (d, *J*= 9 Hz, H-4); 4.81-4.92 (m, 1H, H-5); 6.21-7.61 (m, 12H, H_{arom}); 7.69 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ: 24.3; 25.6; 28.0; 35.3; 47.5; 54.4; 62.9; 66.5; 73.8; 109.5; 111.1; 112.1; 114.3, 114.8; 118.5; 121.5; 124.7; 126.0; 126.2; 126.4; 127.1; 128.3; 129.2; 129.8; 130.1; 131.3; 131.6; 132.0; 132.2; 135.1; 135.4; 140.2; 175.6; 200.7; **IR (ν_{max}, cm^{-1}):** 1470; 1592; 1694; 1717; 2219; 2927 cm^{-1}; Anal.Calcd. for $C_{39}H_{35}N_4O_2$: C, 79.16; H, 5.96; N, 9.47; found: C, 78.91; H, 5.70; N, 9.35.

2.1.9. (*2R, 3S, 4S, 5R*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''(naphtylidene)tetral-2''-one-4-(naphtyl)pyrrolizidine (4i)

Yellow powder, (0.34g; 51%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.94-2.08 (2m, 2H, H-6_a/H-7_a); 2.10-2.19 (2m, 2H, H-6_b/H-7_b); 2.33 (d, *J*= 15 Hz, 1H, H-4''); 2.90-3.16 (m, 1H, H-8_a); 3.38 (d, *J*= 15 Hz, 1H, H-4''); 3.61-3.78 (m, 1H, H-8_b); 4.96 (d, *J*= 9 Hz, H-4); 5.30-5.40 (m, 1H, H-5); 6.40-8.11 (m, 12H, H_{arom}); 8.16 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.2; 27.8; 35.2; 48.3; 53.8; 63.5; 66.5; 73.0; 109.3; 123.1; 125.8; 126.0; 126.2; 126.4; 126.5; 126.8; 127.1; 127.3; 127.6; 127.6; 127.9; 128.1; 128.3; 130.1; 130.8; 132.3; 132.4; 132.8; 133.2; 133.4; 133.5; 133.7; 134.3; 139.9; 142.6; 147.1; 176.3; 200.1; **IR (ν_{max}, cm^{-1}):** 1523; 1588; 1682; 1728; 3125 cm^{-1}; Anal. Calcd. for $C_{44}H_{38}N_3O_4$: C, 78.55; H, 5.69; N, 6.25; found: C, 78.51; H, 5.63; N, 6.22.

2.1.10. (*2R, 3S, 4S, 5R*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''(tolylidene)tetral-2''-one-4-(tolyl)pyrrolizidine (4j)

Yellow cristal, (0.07 g; 12%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.87-2.08 (2m, 2H, H-6_a/H-7_a); 2.14-2.21 (2m, 2H, H-6_b/H-7_b); 2.27 (d, *J*= 15 Hz, 1H, H-4''); 2.32 (s, 3H, CH_3); 2.35 (s, 3H, CH_3); 2.57-2.75 (m, 1H, H-8_a); 3.23 (d, *J*= 15 Hz, 1H, H-4''); 3.33-3.38 (m, 1H, H-8_b); 4.64 (d, *J*= 9 Hz, H-4); 4.85-4.95 (m, 1H, H-5); 6.40-7.92 (m, 16H, H_{arom}); 8.05 (s, 1H, $H_{ethylenic}$); 8,17 (s.l, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 21.1; 21.4; 24.5; 27.8; 35.1; 47.9; 53.6; 63.8; 66.4; 73.2; 108.9; 123.2; 125.4; 125.7; 126.3; 126.6; 127.6; 127.9; 128.5; 129.1; 129.3; 129.6; 129.7; 130.0; 130.2; 130.6; 131.7; 131.9; 132.7; 134.0; 136.9; 139.8, 142.5; 147.0; 177.2; 200.2; **IR (ν_{max}, cm^{-1}):** 1522; 1590; 1682; 1724; 2923 cm^{-1}; Anal. Calcd. for $C_{38}H_{38}N_3O_4$: C, 75.98; H, 6.38; N, 6.99; found: C, 75.93; H, 6.32; N, 6.94.

2.1.11. (*2R, 3S, 4S, 5R*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''(*p*-fluorobenzylidene)tétral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (4k)

Yellow cristal, (0.06 g; 11%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.72-1.97 (2m, 2H, H-6_a/H-7_a); 2.00-2.16 (2m, 2H, H-6_b/H-7_b); 2.20 (d, *J*= 15 Hz, 1H, H-4''); 2.45-2.58 (m, 1H, H-8_a); 3.20 (d, *J*= 15 Hz, 1H, H-4''); 3.17-3.22 (m, 1H, H-8_b); 4.61 (d, *J*= 9 Hz, H-4); 4.68-4.79 (m, 1H, H-5); 6.41-7.93 (m, 15H, H_{arom}); 8.03 (s, 1H, $H_{ethylenic}$) 8.34 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.0; 27.7; 35.1; 48.1; 53.1; 60.3; 66.8; 72.8; 115.5; 115.8; 122.8; 126.2; 126.7; 128.3; 128.4; 130.2; 130.7; 131.3; 131.5; 131.6; 132.1; 138.7; 142.7; 161.5; 164.8; 171.0;

199.8; **IR (ν_{max}, cm^{-1}):** 1510; 1589; 1670; 1738; 2925 ; Anal. Calcd. for $C_{36}H_{32}F_2N_3O_4$: C, 71.04; H, 5.30; F, 6.24; N, 6.90; found: C, 71.00; H, 5.28; F, 6.20; N,6.85.

2.1.12. (*2R, 3S, 4R, 5S*) Spiro [2,3'] oxindole-spiro [3,3'']-1''(naphtylidene)tetral-2''-one-4-(naphtyl)pyrrolizidine (5a)

Yellow oil, (0.06 g; 11%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.79-1.89 (2m, 2H, H-6_a/H-7_a); 1.91-2.19 (2m, 2H, H-6_b/H-7_b); 2.26 (d, *J*= 15 Hz, 1H, H-4''); 2.50-2.65 (m, 1H, H-8_a); 3.34-3.45 (m, 1H, H-8_b), 3.51 (d, *J*= 15 Hz, 1H, H-4''); 4.85 (d, *J*= 9 Hz, H-4); 4.96-5.11 (m, 1H, H-5); 6.19-7.98 (m, 22H, H_{arom}); 8.01 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.3; 27.6; 34.8; 47.0; 54.2; 63.9; 65.7; 73.5; 108.4; 110.9; 111.9; 117.7; 118.0; 122.3; 125.4; 126.1; 126.4; 128.2; 128.3; 129.2; 129.9; 130.1; 130.7; 131.7; 131.9; 133.3; 133.8; 136.3; 139.2; 142.2; 142.6; 146.4; 176.2; 199.9; **IR (ν_{max}, cm^{-1}):** 1482; 1590; 1691; 1725; 2229; 2929 ; Anal.Calcd. for $C_{44}H_{39}N_2O_2$: C, 84.18; H, 6.26; N, 4.46; found: C, 84.12; H, 6.28; N, 4.44.

2.1.13. (*2R, 3S, 4R, 5S*) Spiro [2,3'] oxindole-spiro [3,3'']-1''-(tolylidene)tetral-2''-one-4-(tolyl)pyrrolizidine (5b)

Yellow oil, (0.05 g; 9%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.74-1.96 (2m, 2H, H-6_a/H-7_a); 2.06-2.18 (2m, 2H, H-6_b/H-7_b); 2.24 (s, 3H, CH_3); 2.25 (d, *J*= 15 Hz, 1H, H-4''); 2.29 (s, 3H, CH_3); 2.52-2.61 (m, 1H, H-8_a); 3.37 (d, *J*= 15 Hz, 1H, H-4''); 3.35-3.42 (m, 1H, H-8_b); 4.62 (d, *J*= 9 Hz, 1H, H-4); 4.83-4.94 (m, 1H, H-5); 6.29-7.43 (m, 16H, H_{arom}); 7.72 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 20.3; 20.6; 24.2; 27.7; 34.8; 47.6; 54.0; 63.3; 66.0; 73.9; 108.9; 121.1; 125.5; 125.6; 126.1; 126.7; 128.0; 128.1; 128.4; 128.6; 129.0; 129.3;129.9;131.9; 132.0; 132.2; 132.5; 133.6; 134.5; 135.9; 136.7; 138.6; 141.1; 177.5; 201.5; **IR (ν_{max}, cm^{-1}):** 1513; 1579; 1684; 1730; 2973 cm^{-1}; Anal. Calcd. for $C_{38}H_{39}N_2O_2$: C, 82.13; H, 7.07; N, 5.04; found: C, 82.10; H, 7.03; N, 5.06.

2.1.14. (*2R, 3S, 4R, 5S*) Spiro [2,3'] oxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (5c)

Yellow powder, (0.05g; 9%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.76-1.94 (2m, 2H, H-6_a/H-7_a); 2.09-2.18 (2m, 2H, H-6_b/H-7_b); 2.23 (d, *J*= 15 Hz, 1H, H-4''); 2.54-2.66 (m, 1H, H-8_a); 3.34 (d, *J*= 15 Hz, 1H, H-4''); 3.30-3.49 (m, 1H, H-8_b); 4.56 (d, *J*= 12 Hz, H-4); 4.78-4.89 (m, 1H, H-5); 6.29-7.55 (m, 16H, H_{arom}); 7.66 (s, 1H, $H_{ethylenic}$); 7.95 (s.l, 1H, H_{amide}); **^{13}C NMR**

($CDCl_3$, 100 MHz) δ : 24.5; 27.8; 34.7; 47.2; 53.6; 63.1; 66.3; 73.8; 108.9; 114.6; 114.7; 114.9; 120.9; 124.7; 125.4; 125.8; 126.8; 127.2; 128.1; 129.5; 130.8; 131.0; 131.7; 132.8; 133.1; 133.3; 135.7; 140.7; 163.2; 164.3; 176.8; 200.9; **IR (ν_{max}, cm^{-1}):** 1518; 1594; 1697; 1711; 2991cm^{-1}; Anal. Calcd. for $C_{36}H_{33}F_2N_2O_2$: C, 76.71 ; H, 5.90; F, 6.74; N, 4.97; found: C, 76.70; H, 5.94; F. 6.70; N, 4.93.

2.1.15. (*2R, 3S, 4R, 5S*) Spiro [2,3'] oxindole-spiro [3,3'']-1''-(*p*-cyanobenzylidene)tetral-2''-one-4-(*p*-cyanobenzyl)pyrrolizidine (5d)

Yellow powder, (0.05 g; 9%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.75-1.93 (2m, 2H, H-6_a/H-7_a); 1.84-1.98 (2m, 2H, H-6_b/H-7_b); 2.14 (d, *J*= 15 Hz, 1H, H-4''); 2.55-2.60 (m, 1H, H-8_a); 3.27 (d, *J*= 9 Hz, 1H, H-4''); 3.32-3.35 (m, 1H, H-8_b); 4.61 (d, *J*= 9 Hz, H-4); 4.83-4.87 (m, 1H, H-5); 6.22-7.69 (m, 16H, H_{arom}); 7.67 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.8; 28.0; 35.2 ; 47.8; 54.4; 62.8; 66.2; 73.8; 108.9; 111.2; 112.1; 118.2; 121.4; 125.8; 127.2; 128.6; 129.2; 129.6; 130.1; 130.4; 131.5; 131.6; 132.1; 132.2; 135.2; 135.3; 140.2; 140.8; 144.0; 179.2; 200.7; **IR (ν_{max}, cm^{-1}):** 1496; 1587; 1694; 1718; 2224; 2928 cm^{-1}; Anal. Calcd. for $C_{38}H_{33}N_4O_2$: C, 79.00; H, 5.76; N, 9.70; found: C, 78.96; H, 5.71; N, 9.74.

2.1.16. (*2R, 3S, 4R, 5S*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(naphtylidene)tetral-2''-one-4-(naphtyl)pyrrolizidine (5e)

Yellow powder, (0.07 g; 12%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.80-1.92 (2m, 2H, H-6_a/H-7_a); 2.05-2.16 (2m, 2H, H-6_b/H-7_b); 2.20 (d, *J*= 15 Hz, 1H, H-4''); 2.56-2.66 (m, 1H, H-8_a); 2.79 (s, 3H, CH_3); 3.40 (d, *J*= 15 Hz, 1H, H-4''); 3.43-3.56 (m, 1H, H-8_b); 4.86 (d, *J*= 9 Hz, H-4); 5.12-5.18 (m, 1H, H-5); 6.15-7.91 (m, 22H, H_{arom}); 7.98 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 23.8; 25.4; 27.7; 34.9; 47.8; 54.3; 65.8; 73.6; 106.9; 121.1; 125.2; 125.5; 125.6; 125.8; 126.2; 126.3; 126.5; 126.7; 126.9; 127.3; 127.4; 127.7; 128.1; 128.2; 130.0; 131.6; 132.2; 132.4; 132.6; 132.9; 133.1; 133.2; 134.1; 136.8; 143.4; 175.6; 201.8; **IR (ν_{max}, cm^{-1}):** 1521; 1579; 1680; 1742; 3134 cm^{-1}; Anal. Calcd. for $C_{45}H_{41}N_2O_2$: C, 84.21; H, 6.44; N, 4.36; found: C, 84.16; H, 6.40; N, 4.32.

2.1.17. (*2R, 3S, 4R, 5S*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(Tolylidene)tetral-2''-one-4-(*p*-tolyl)pyrrolizidine (5f)

Yellow powder, (0.07 g; 13%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.69-1.86 (2m, 2H, H-6_a/H-7_a); 2.08-2.17 (2m, 2H, H-6_b/H-7_b); 2.14 (d, *J*= 15 Hz, 1H, H-4'') ; 2.27 (s, 3H, CH_3); 2.34 (s, 3H, CH_3); 2.51-2.58 (m, 1H, H-8_a); 2.76 (s, 3H, N$\underline{CH_3}$); 3.27 (d, *J*= 15 Hz, 1H, H-4''); 3.28-3.30 (m, 1H, H-8_b); 4.61 (d, *J*= 9 Hz, 1H, H-4); 4.90-4.98 (m, 1H, H-5); 6.15-7.40 (m, 16H, H_{arom}); 7.72 (s, 1H, $H_{olefinic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ :20.8; 20.9; 24.2; 25.4; 27.6; 34.8; 47.9; 54.2; 66.1; 73.5; 107.0, 121.0; 125.4; 126.0; 126.1; 126.3; 127.9; 128.3; 128.5; 128.7; 129.1; 129.3; 129.5; 129.7; 130.9; 131.5; 132.4; 134.1; 134.5; 135.4; 136.7; 138.9; 143.2; 179.9; 201.5; **IR (ν_{max}, cm^{-1}):** 1509;1563; 1691; 1699; 2945 cm^{-1}; Anal. Calcd. for $C_{39}H_{41}N_2O_2$: C, 82.21; H, 7.25; N, 4.92; found: C, 82.18; H, 7.27; N, 4.97.

2.1.18. (*2R, 3S, 4R, 5S*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (5g)

Yellow oil, (0.06 g; 12%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.77-1.82 (2m, 2H, H-6_a/H-7_a); 2.09-2.13 (2m, 2H, H-6_b/H-7_b); 2.15 (d, *J*= 15 Hz, 1H, H-4'') ; 2.49-2.59 (m, 1H, H-8_a); 2.77 (s, 3H, N$\underline{CH_3}$); 3.30 (d, *J*= 15 Hz, 1H, H-4''); 3.29-3.39 (m, 1H, H-8_b); 4.60 (d, *J*= 9 Hz, H-4); 4.82-4.88 (m, 1H, H-5); 6.18-7.60 (m, 12H, H_{arom}); 7.70 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.2; 25.4; 27.8; 34.9; 47.2; 54.1; 63.1; 66.3; 73.2; 107.5; 114.2; 114.6; 114.8; 118.0; 120.9; 121.9; 124.5; 125.7; 126.1; 126.8; 127.9; 128.6; 129.8; 130.4;130.8; 131.5; 132.8; 133.3;133.4; 134.1; 135.4; 143.2; 160.0; 161.2; 163.3; 164.0;174.8; 200.7; **IR (ν_{max}, cm^{-1}):** 1502; 1583; 1675; 1722; 2937; Anal. Calcd. for $C_{37}H_{35}F_2N_2O$: C, 76.93; H, 6.11; F, 6.58; N, 4.85; found: C, 76.88; H, 6.10; F, 6.55; N, 4.87.

2.1.19. (*2R, 3S, 4R, 5S*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(*p*-cyanobenzylidene)tetral-2''-one-4-(*p*-cyanobenzyl)pyrrolizidine (5h)

Yellow powder, (0.05 g; 9%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.76-1. 92 (2m, 2H, H-6_a/H-7_a); 1.93-2.10 (2m, 2H, H-6_b/H-7_b); 2.18 (d, *J*= 15 Hz, 1H, H-4'') ; 2.54-2.64 (m, 1H, H-8_a); 2.76 (s, 3H, N$\underline{CH_3}$); 3.25-3.38 (m, 1H, H-8_b); 3.41 (d, *J*= 15 Hz, 1H, H-4''); 4.60 (d, *J*= 9 Hz, H-4); 4.80-4.94 (m, 1H, H-5); 6.23-7.64 (m, 12H, H_{arom}); 7.67 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.2; 25.5; 28.1; 35.4; 47.6; 54.3; 62.9; 66.5; 73.8; 109.8; 111.5; 112.3; 114.5; 114.8; 117.9; 118.6; 120.9; 124.8; 126.0; 126.3; 126.7; 127.2; 128.4; 129.3; 129.6; 129.9; 130.5; 131.2; 131.7; 132.3; 135.3; 135.6; 140.5; 175.9; 200.6; **IR (ν_{max}, cm^{-1}):** 1510; 1587; 1689; 1693; 2219; 2967cm^{-1}; Anal. Calcd. for $C_{39}H_{35}N_4O_2$: C, 79.16; H, 5.96; N, 9.47; found: C, 79.09; H, 5.90; N,9.41.

2.1.20. (*2R, 3S, 4R, 5S*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''-(naphtylidene)tetral-2''-one-4-(naphtyl)pyrrolizidine (5i)

Yellow powder, (0.07 g; 11%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.94-2.04 (2m, 2H, H-6_a/H-7_a); 2.12-2.17 (2m, 2H, H-6_b/H-7_b); 2.36 (d, *J*= 15 Hz, 1H, H-4''); 2.72-3.17 (m, 1H, H-8_a); 3.38 (d, *J*= 15 Hz, 1H, H-4''); 3.64-3.74 (m, 1H, H-8_b); 4.99 (d, *J*= 9 Hz, H-4); 5.31-5.42 (m, 1H, H-5); 6.41-8.05 (m, 12H, H_{arom}); 8.20 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.4; 27.8; 35.3; 48.2; 53.9; 63.4; 66.2; 73.2; 108.9; 123.7; 125.8; 126.1; 126.4; 126.7; 126.8; 127.0; 127.2; 127.4; 127.6; 127.8; 128.0; 128.5; 129.2; 130.3; 131.2; 132.2; 132.4; 132.6; 133.1; 133.4; 133.7; 133.9; 134.2; 139.8; 142.4; 147.0; 176.4; 200.3; **IR (ν_{max}, cm^{-1}):** 1516; 1580; 1664; 1738; 3299 ; Anal.Calcd.for $C_{44}H_{38}N_3O_4$: C, 78.55; H, 5.69; N, 6.25; found: C, 78.52; H, 5.65; N, 6.21.

2.1.21. (*2R, 3S, 4R, 5S*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''-(tolylidene)tetral-2''-one-4-(tolyl)pyrrolizidine (5j)

Yellow powder, (0.33 g; 55%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.88-2.05 (2m, 2H, H-6_a/H-7_a); 2.14-2.21 (2m, 2H, H-6_b/H-7_b); 2.28 (d, *J*= 15 Hz, 1H, H-4''); 2.31 (s, 3H, CH_3); 2.35 (s, 3H, CH_3); 2.51-2.72 (m, 1H, H-8_a); 3.24 (d, *J*= 15 Hz, 1H, H-4''); 3.30-3.46 (m, 1H, H-8_b); 4.66 (d, *J*= 9 Hz, H-4); 4.87-4.95 (m, 1H, H-5); 6.41-7.91 (m, 16H, H_{arom}); 8.07 (s, 1H, $H_{ethylenic}$); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 20.6; 20.8; 24.1; 27.3; 34.7; 47.1; 53.2; 63.5; 66.8; 72.2; 108.5; 122.7; 125.1; 125.5; 125.7; 126.2; 127.5; 128.6; 128.7; 129.2; 129.3; 129.5; 130.1; 131.2; 131.5; 132.0; 133.5; 136.3; 139.1; 142.3; 146.7; 175.9; 200.0; **IR (ν_{max}, cm^{-1}):** 1524; 1591; 1683; 1728; 2975; Anal. Calcd.for $C_{38}H_{38}N_3O_4$: C, 75.98; H, 6.38; N, 6.99; found: C, 75.96; H, 6.39; N, 6.89.

2.1.22. (*2R, 3S, 4R, 5S*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)pyrrolizidine (5k)

Yellow powder, (0.35 g; 58%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.72-1.93 (2m, 2H, H-6_a/H-7_a); 2.02-2.11 (2m, 2H, H-6_b/H-7_b); 2.21 (d, *J*= 15 Hz, 1H, H-4''); 2.42-2.50 (m, 1H, H-8_a); 3.20 (d, *J*= 15 Hz, 1H, H-4''); 3.22-3.39 (m, 1H, H-8_b); 4.60 (d, *J*= 9 Hz, H-4); 4.68-4.79 (m, 1H, H-5); 6.49-7.94 (m, 16H, H_{arom}); 8.06 (s, 1H, $H_{ethylenic}$); 8.36 (s.l, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 24.4; 27.5; 34.4; 47.9; 52.8; 61.7; 66.1; 72.6; 115.0; 115.8; 122.6; 125.1; 126.0; 127.3; 129.6; 130.4; 130.6; 131.1; 131.8; 131.9; 132.2; 132.5; 138.6; 142.1; 161.8; 164.2; 173.4; 200.1; **IR (ν_{max}, cm^{-1}):** 1505; 1579; 1677; 1733; 2938 cm^{-1};

Anal.Calcd.for $C_{36}H_{32}F_2N_3O_4$: C, 71.04; H, 5.30; F, 6.24; N, 6.90; found: C, 71.08; H, 5.25; F, 6.21; N, 6.94.

2.2.1. (*2R, 3S, 4S, 5R*) Spiro [2,3'] oxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (16a)

Yellow oil, (0.29g; 52%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.09 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$; 1.25 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$;1.88 (sept, 1H, C$\underline{H}$(CH_3)$_2$); 2.27 (d, *J*= 15 Hz, 1H, H-4''); 2.38-2.85 (s.l, 1H, NH); 2.93 (d, *J*= 15 Hz, 1H, H-4''); 4.23 (t, 1H, H-5); 4.32 (d, *J*= 9 Hz, H-4); 6.20-7.49 (m, 16H, H_{arom}); 7.59 (s, 1H, $H_{ethylenic}$); 7.81 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 19.4; 20.8; 26.9; 32.3; 35.2; 55.6; 60.2; 68.2; 72.9; 109.2; 114.7; 114.9; 115.2; 121.9; 123.1; 126.1; 126.3; 127.4; 128.7; 128.8; 129.2; 130.0; 131.0; 131.5; 131.6; 132.0; 132.1; 134.0; 135.5; 140.3; 163.1; 163.3; 163.5; 163.9; 177.9; 211.9; **IR (ν_{max}, cm^{-1}):** 1521; 1594; 1690; 1719; 2990 ; Anal.Calcd.for $C_{36}H_{35}F_2N_2O_2$: C, 76.44; H, 6.24; F, 6.72; N, 4.95; found: C, 76.39; H, 5.94; F, 6.68; N, 4.90.

2.2.2. (*2R, 3S, 4S, 5R*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene) tétral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (16b)

Yellow oil, (0.31 g; 54%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.10 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$; 1.28 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$; 1.92 (sept, 1H, C$\underline{H}$(CH_3)$_2$); 2.30 (d, *J*= 15 Hz, 1H, H-4''); 2.39-2.76 (s.l, 1H, NH); 2.75 (S, 3H, N$\underline{CH_3}$) 2.97 (d, *J*= 15 Hz, 1H, H-4''); 4.20 (t, 1H, H-5); 4.35 (d, *J*= 9 Hz, H-4); 6.18-7.51 (m, 16H, H_{arom}); 7.61 (s, 1H, $H_{ethylenic}$); 7.80 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 19.2; 20.6; 24.9; 26.7; 32.5; 35.4; 55.4; 60.4; 68.5; 72.8; 108.8; 114.5; 114.8; 115.1; 121.7; 122.8; 126.3; 126.5; 127.6; 128.9; 130.1; 129.4; 130.2; 131.3; 131.4; 131.8; 132.2; 132.0; 133.9; 135.2; 140.4; 163. 0; 163.2; 163.4; 163.6; 177.5; 210.6; **IR (ν_{max}, cm^{-1}):** 1492; 1562; 1669; 1722; 2930; Anal. Calcd. for $C_{37}H_{38}F_2N_2O_2$: C, 76.53; H, 6.60; F, 6.54; N, 4.82; found: C, 76.51; H, 6.57; F, 6.52; N, 4.80.

2.2.3. (*2R, 3S, 4S, 5R*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (16c)

Yellow oil, (0.05g; 9%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ : 1.11 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$; 1.29 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$;1.94 (sept, 1H, C$\underline{H}$(CH_3)$_2$); 2.29 (d, *J*= 15 Hz, 1H, H-4''); 2.39-2.89 (s.l, 1H, NH); 2.95 (d, *J*= 15 Hz, 1H, H-4''); 4.25 (t, 1H, H-5); 4.33 (d, *J*= 9 Hz, H-4); 6.21-7.51 (m, 16H, H_{arom}); 7.60 (s, 1H, $H_{ethylenic}$); 7.80 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100

MHz) δ: 20.1; 20.9; 27.1; 33.4; 35.7; 55.8; 60.2; 69.1; 73.4; 109.8; 115.2; 115.2; 115.5; 122.3; 123.8; 126.5; 126.8; 127.9; 128.5; 128.8; 129.7; 130.2; 131.4; 131.8; 131.9; 132.3; 132.6; 134.3; 135.7; 141.5; 163.3; 163.5; 163.7; 163.9; 177.6; 212.3; **IR (ν_{max}, cm^{-1}):** 1510; 1579; 1681; 1739; 2931; Anal. Calcd. for $C_{36}H_{34}F_2N_3O_4$: C, 70.81; H, 5.61; F, 6.22; N, 6.88; found: C, 70.78; H, 5.59; F, 6.20; N, 6.84.

2.2.4. (*2R, 3S, 4R, 5S*) Spiro [2,3'] oxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidène)tetral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (17a)

Yellow oil, (0.05g; 10%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ :1.08 (d, *J*= 3 Hz, $CH(\underline{CH_3})_2$; 1.24 (d, *J*= 3 Hz, $CH(\underline{CH_3})_2$; 1.90 (sept, 1H, $C\underline{H}(CH_3)_2$); 2.27 (d, *J*= 15 Hz, 1H, H-4''); 2.39-2.75 (s.l, 1H, NH); 2.92 (d, *J*= 15 Hz, 1H, H-4''); 4.23 (t, 1H, H-5); 4.33 (d, *J*= 9 Hz, H-4); 6.19-7.72 (m, 16H, H_{arom}); 7.57 (s, 1H, $H_{ethylenic}$); 7.75 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 20.1; 21.3; 27.0; 32.3; 35.5; 55.1; 60.0; 67.8; 72.9; 109.3; 114.7; 115.1; 115.5; 120.8; 122.6; 123.4; 125.0; 126.2; 127.3; 128.5; 128.7; 128.9; 129.1; 130.2; 131.0; 131.4; 131.5; 131.9; 132.2; 132.5; 132.7; 132.9; 133.6; 133.9; 134.3; 135.8; 140.6; 163.0; 163.2; 163.4; 163.8; 176.5; 209.7; **IR (ν_{max}, cm^{-1}):** 1517; 1596; 1692; 1723; 2987; Anal. Calcd. for $C_{36}H_{35}F_2N_2O_2$: C, 76.44; H, 6.24; F, 6.72; N, 4.95; found: C, 76.40; H, 6.22; F, 6.69; N, 4.93.

2.2.5. (*2R, 3S, 4R, 5S*) Spiro [2,3'] *N*-methyloxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (17b)

Yellow oil, (0.07 g; 12%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ : 1.08 (d, *J*= 3 Hz, $CH(\underline{CH_3})_2$; 1.26 (d, *J*= 3 Hz, $CH(\underline{CH_3})_2$; 1.91 (sept, 1H, $C\underline{H}(CH_3)_2$); 2.28 (d, *J*= 15 Hz, 1H, H-4''); 2.40-2.73 (s.l, 1H, NH); 2.76 (S, 3H, $N\underline{CH_3}$) 2.95 (d, *J*= 15 Hz, 1H, H-4''); 4.19 (t, 1H, H-5); 4.36 (d, *J*= 9 Hz, H-4); 6.19-7.53 (m, 16H, H_{arom}); 7.60 (s, 1H, $H_{ethylenic}$); 7.79 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ : 19.9; 20.8; 24.5; 26.3; 32.8; 35.6; 55.7; 60.8; 68.7; 72.6; 109.8; 114.2; 114.6; 115.2; 121.5; 122.9; 126.4; 126.3; 127.5; 128.8; 130.2; 129.2; 130.4; 131.6; 131.2; 131.5; 132.0; 132.2; 133.6; 135.0; 140.3; 163. 1; 163.3; 163.5; 163.7; 176.8; 210.2; **IR (ν_{max}, cm^{-1}): IR (ν_{max}, cm^{-1}):** 1492; 1562; 1669; 1722; 2930; Anal. Calcd. for $C_{37}H_{38}F_2N_2O_2$: C, 76.53; H, 6.60; F, 6.54; N, 4.82; found: C, 76.50; H, 6.54; F, 6.50; N, 4.77.

2.2.6. (*2R, 3S, 4R, 5S*) Spiro [2,3'] 5-nitrooxindole-spiro [3,3'']-1''-(*p*-fluorobenzylidene)tetral-2''-one-4-(*p*-fluorobenzyl)-5-isopropylpyrrole (17c)

Yellow oil, (0.29 g; 49%); **^{1}H NMR** ($CDCl_3$, 400 MHz) δ : 1.12 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$; 1.28 (d, *J*= 3 Hz, CH($\underline{CH_3}$)$_2$;1.93 (sept, 1H, C$\underline{H}$(CH_3)$_2$); 2.30 (d, *J*= 15 Hz, 1H, H-4''); 2.38-2.90 (s.l, 1H, NH); 2.94 (d, *J*= 15 Hz, 1H, H-4''); 4.26 (t, 1H, H-5); 4.32 (d, *J*= 9 Hz, H-4); 6.20-7.53 (m, 16H, H_{arom}); 7.61 (s, 1H, $H_{ethylenic}$); 7.81 (s, 1H, H_{amide}); **^{13}C NMR** ($CDCl_3$, 100 MHz) δ: 20.2; 20.9; 27.4; 33.2; 35.7; 55.7; 60.4; 69.3; 73.7; 110.5; 115.5; 115.9; 116.3; 122.7; 124.1; 126.4; 126.8; 128.0; 128.5; 128.9; 129.5; 131.2; 131.4; 131.7; 132.0; 132.4; 132.6; 135.0; 135.7; 142.2; 163.2; 163.4; 163.6; 163.8; 176.9; 211.0; **IR (ν_{max}, cm^{-1}):** 1512; 1573; 1680; 1727; 2938 ; Anal.Calcd.for $C_{36}H_{34}F_2N_3O_4$: C, 70.81; H. 5.61; F. 6.22; N. 6.88; found: C, 70.78; H, 5.59; F, 6.18; N, 6.85.

^{1}H AND ^{13}C NMR SPECTRA

Fig S1. ^{1}H NMR spectrum of **4a** in $CDCl_3$

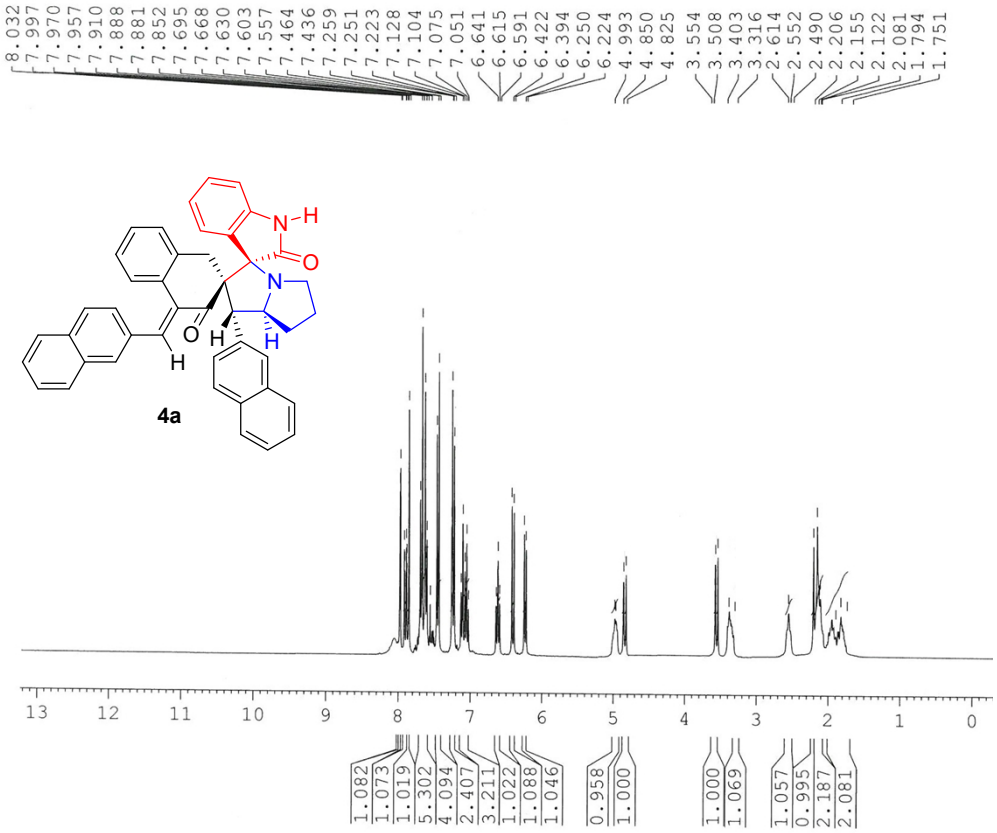

Fig S2. ^{13}C {^{1}H} NMR spectrum of **4a** in $CDCl_3$

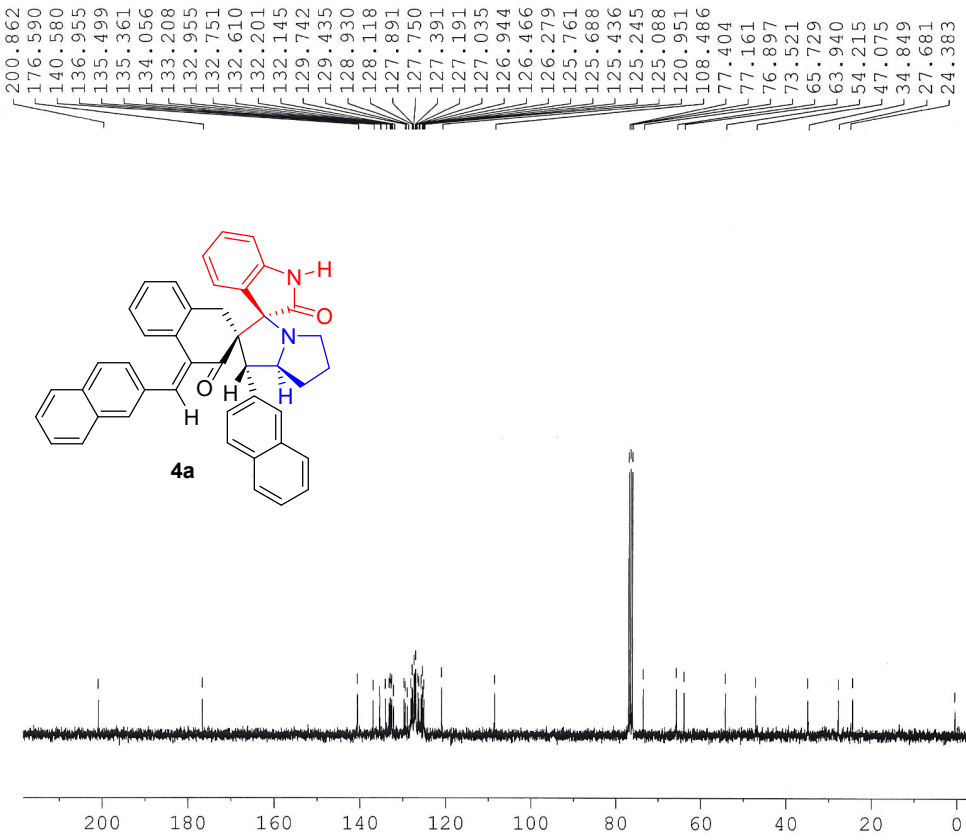

Fig S3. ^{1}H NMR Spectrum of **4b** in $CDCl_3$

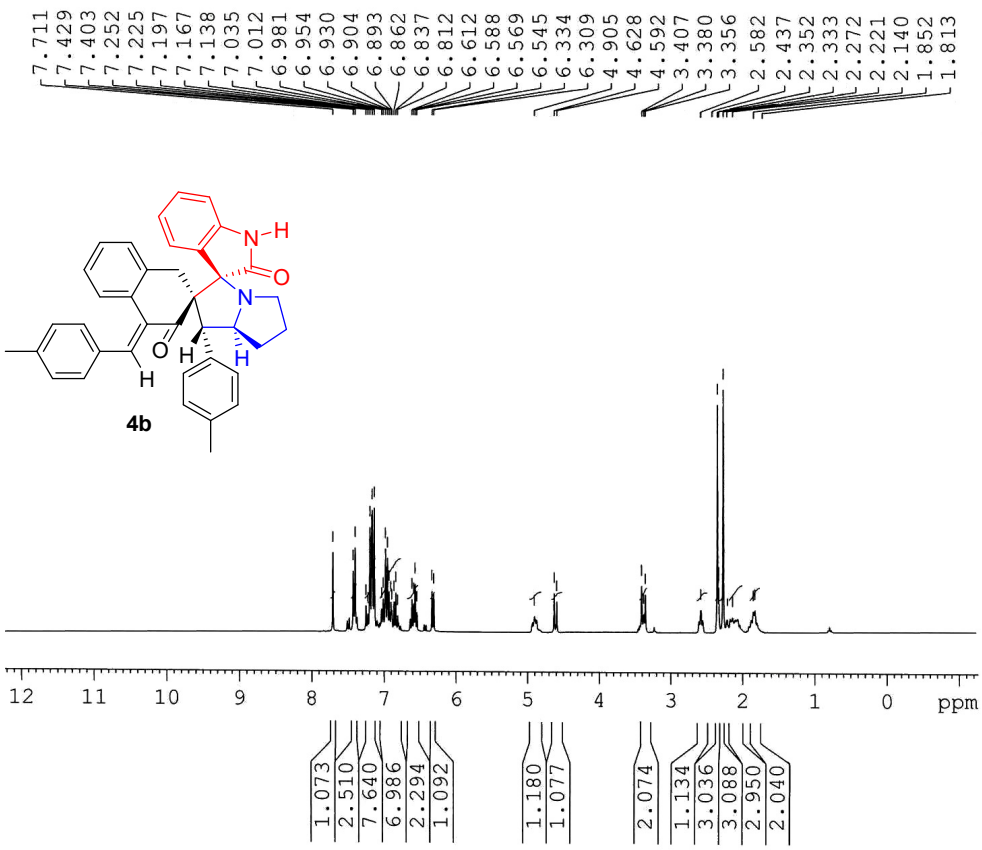

Fig S4. ^{13}C $\{^{1}H\}$ NMR spectrum of **4b** in $CDCl_3$

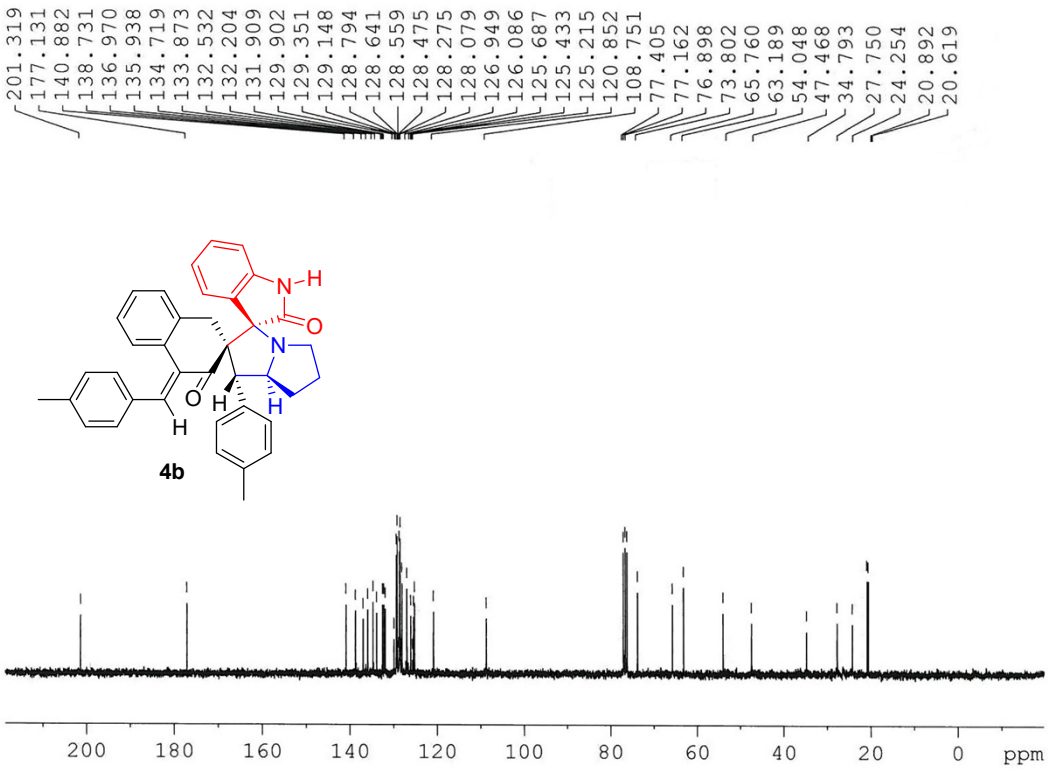

Fig S5. ^{1}H NMR Spectrum of **4c** in $CDCl_3$

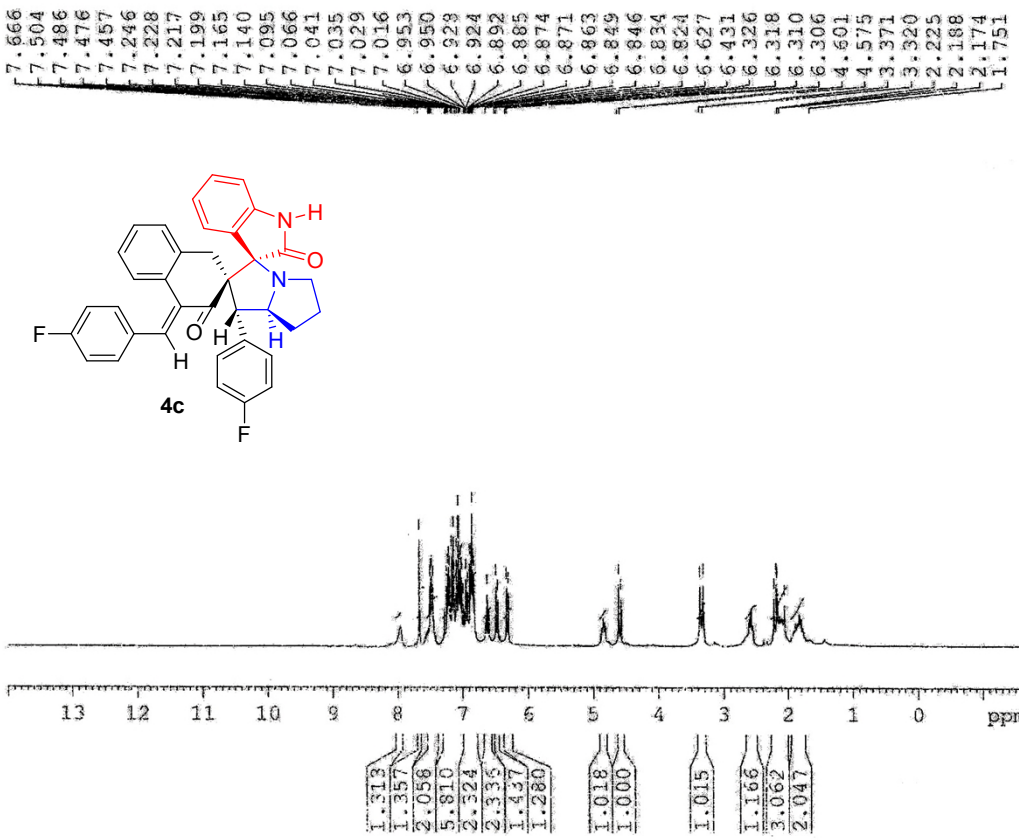

Fig S6. ^{13}C $\{^{1}H\}$ NMR Spectrum of **4c** in $CDCl_3$

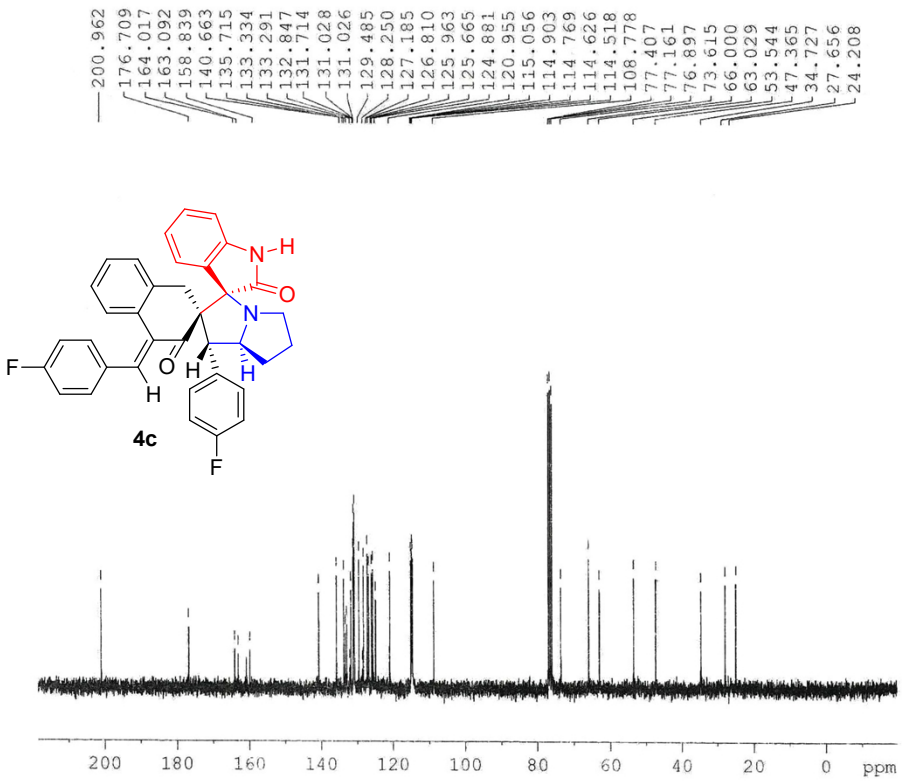

Fig S7. ^{1}H NMR Spectrum of **4d** in $CDCl_3$

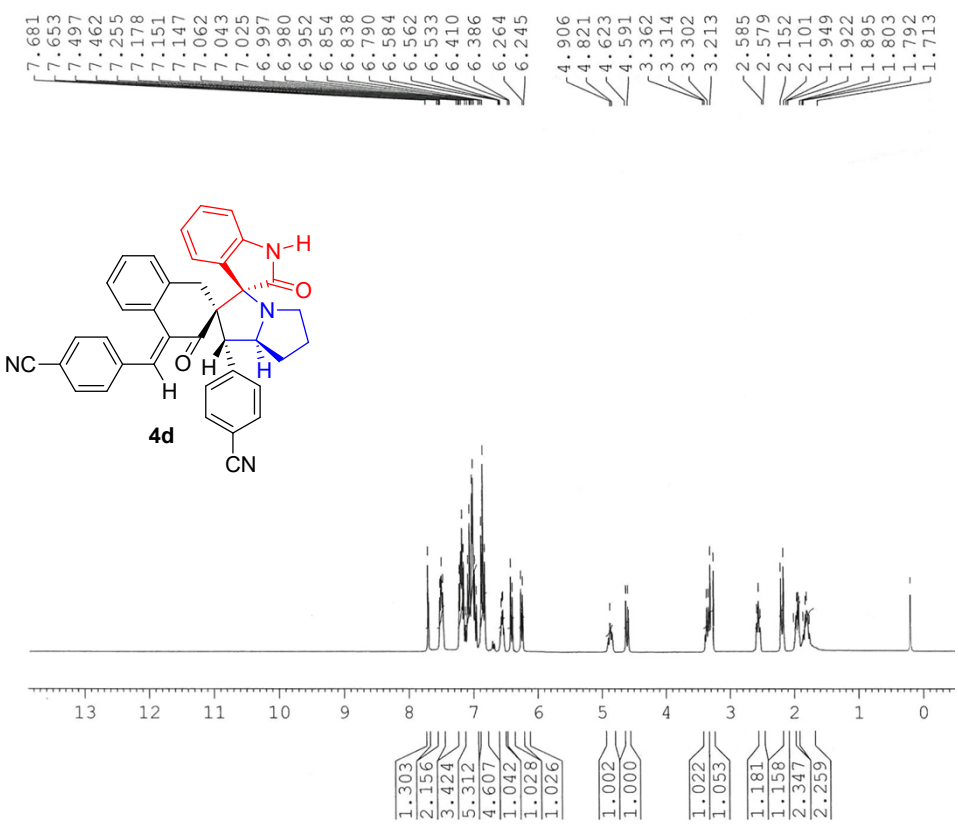

Fig S8. ^{13}C {^{1}H} NMR Spectrum of **4d** in $CDCl_3$

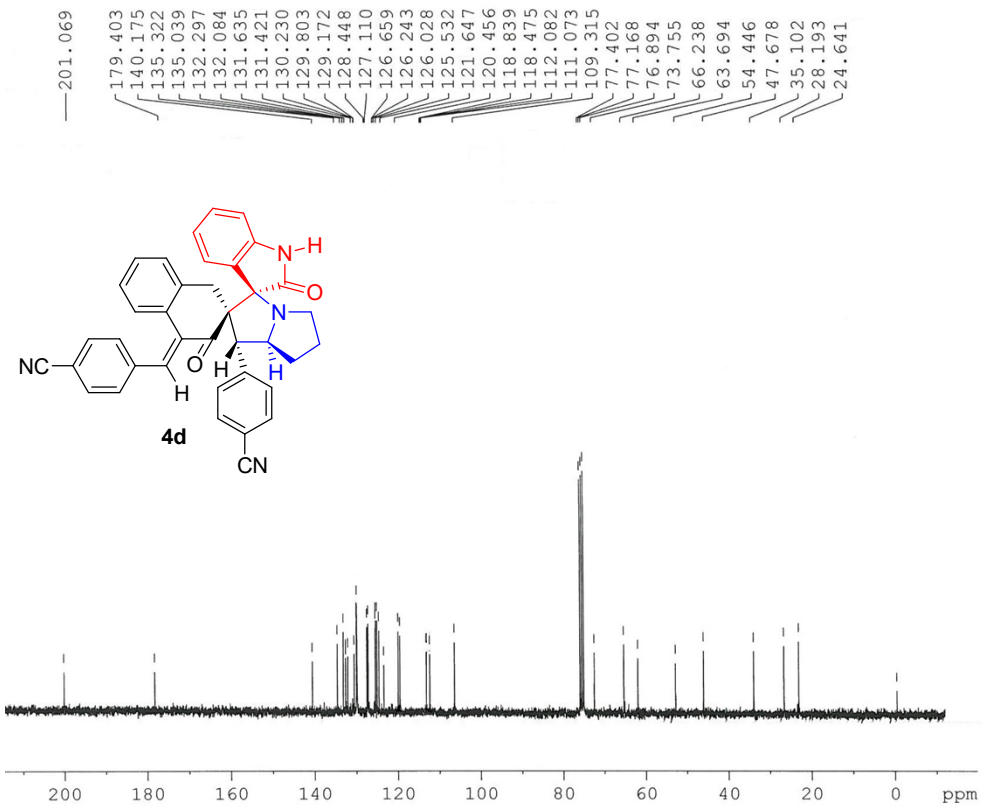

Fig S9. ^{1}H NMR Spectrum of **4e** in $CDCl_3$

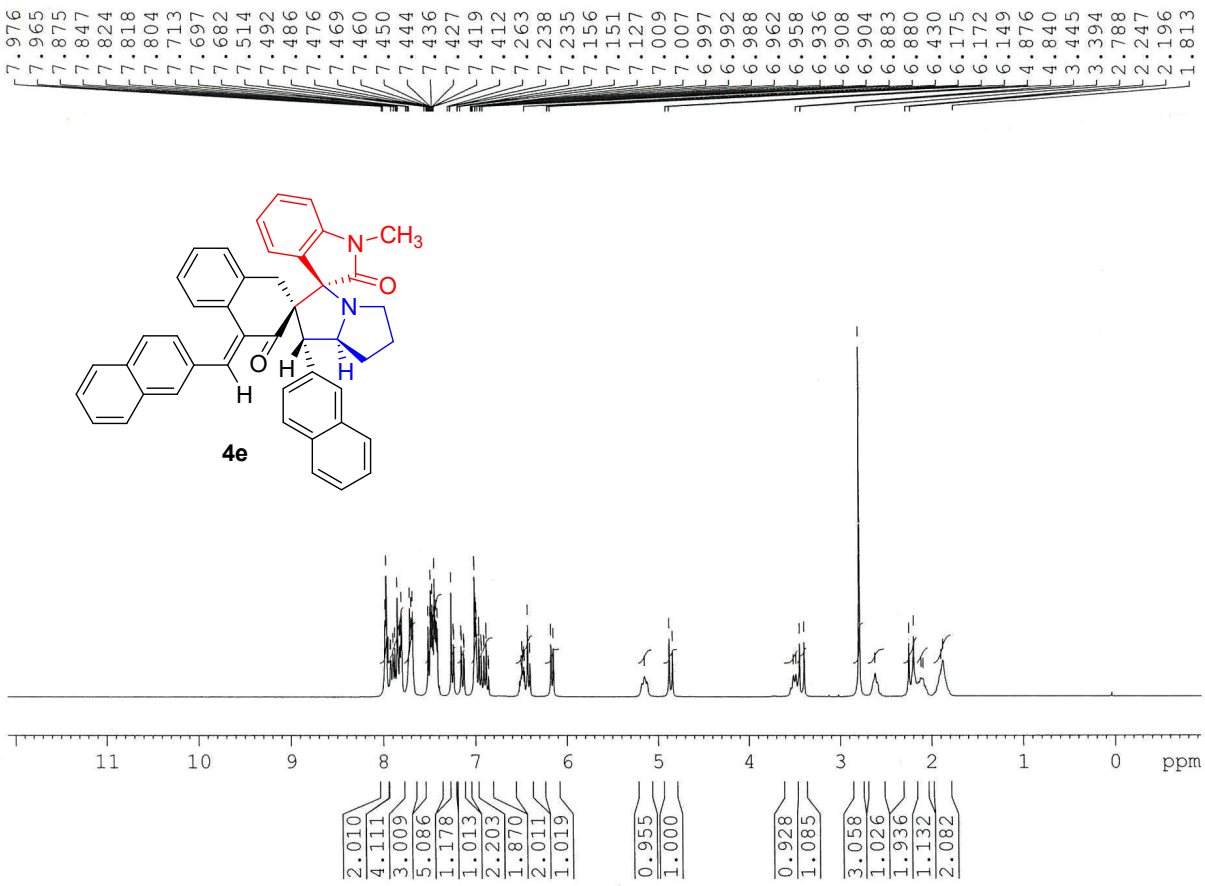

Fig S10. ^{13}C {^{1}H} NMR Spectrum of **4e** in $CDCl_3$

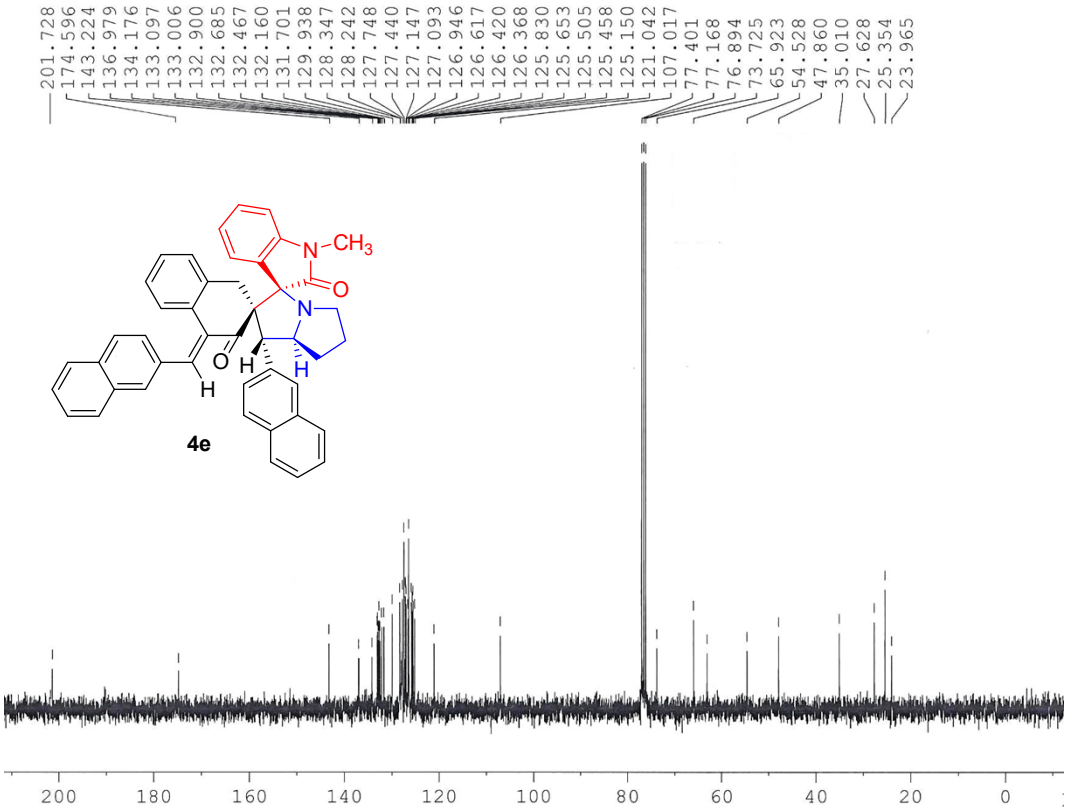

Fig S11. ^{1}H NMR Spectrum of **4f** in $CDCl_3$

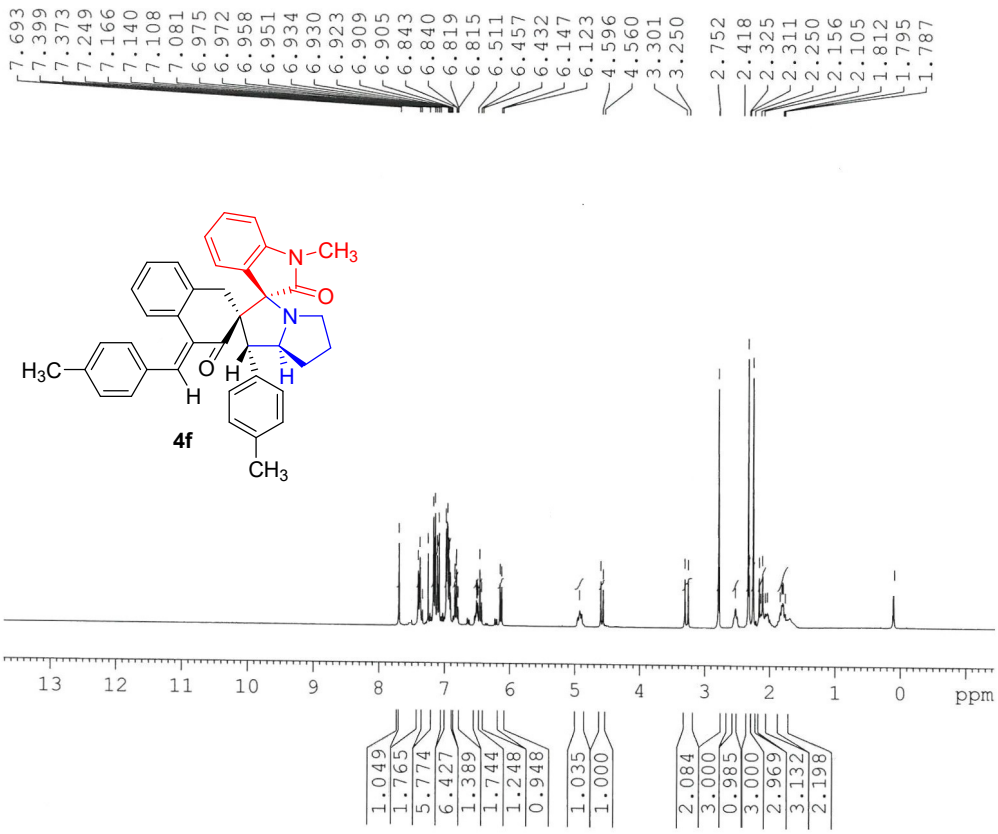

Fig S12. ^{13}C {^{1}H} NMR Spectrum of **4f** in $CDCl_3$

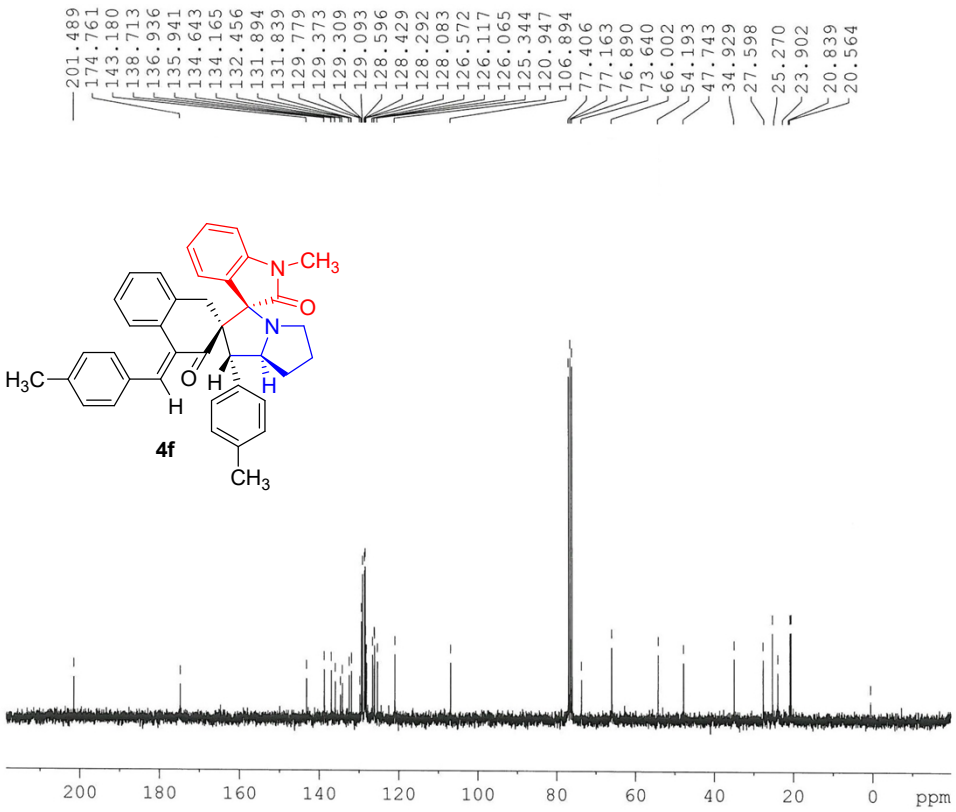

Fig S13. ^{1}H NMR Spectrum of **4g** in $CDCl_3$

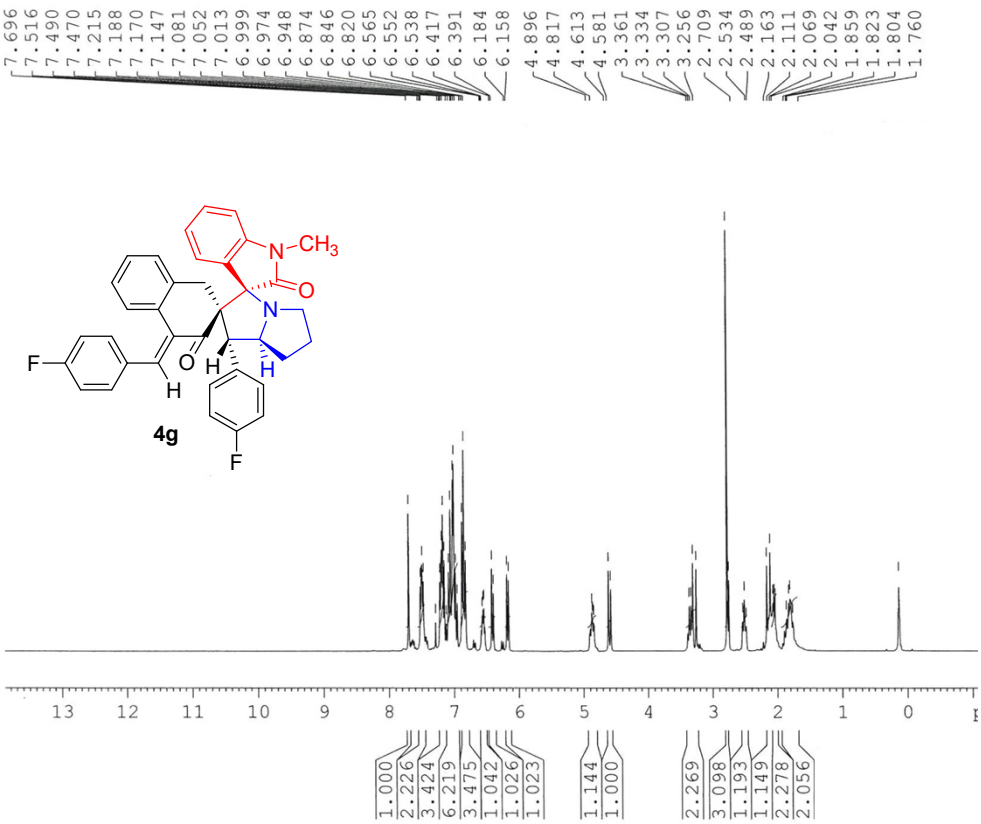

Fig S14. ^{13}C {^{1}H} NMR Spectrum of **4g** in $CDCl_3$

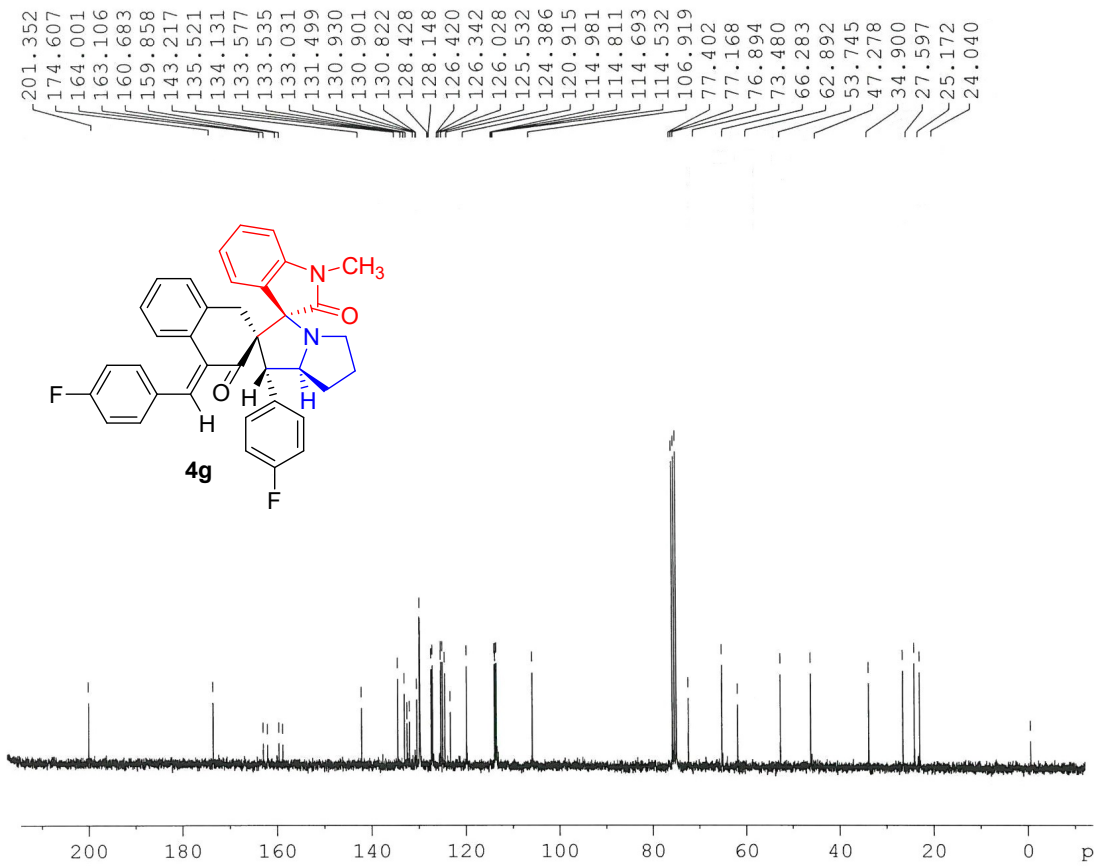

Fig S15. ^{1}H NMR Spectrum of **4h** in $CDCl_3$

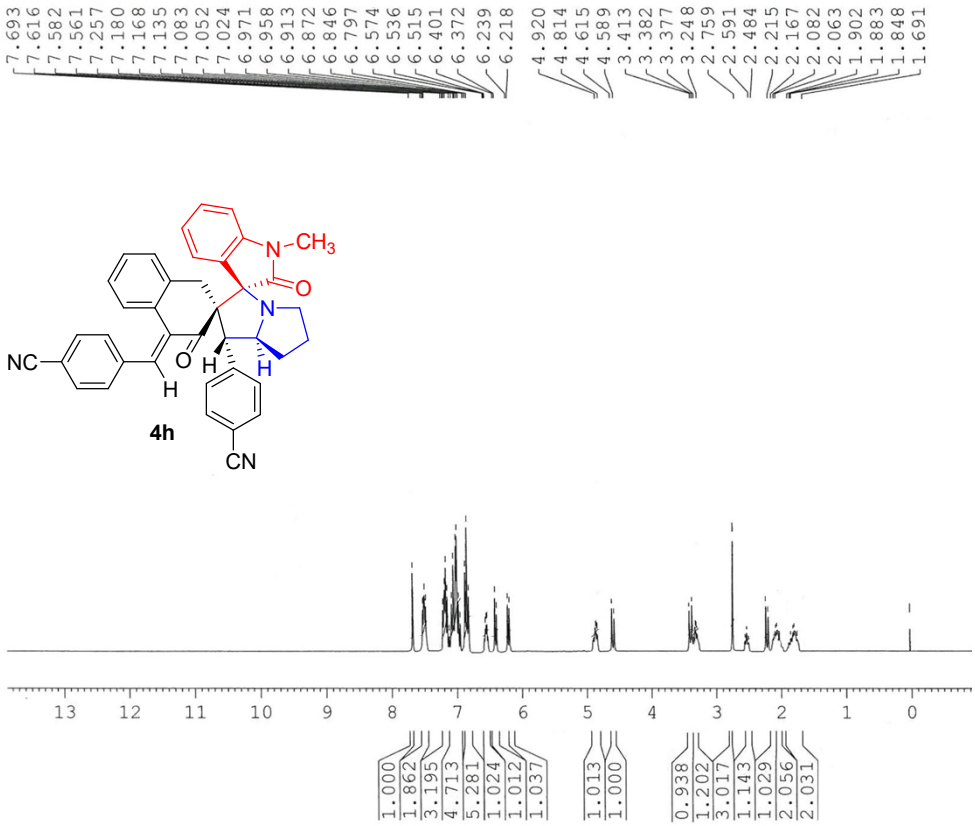

Fig S16. ^{13}C $\{^{1}H\}$ NMR Spectrum of **4h** in $CDCl_3$

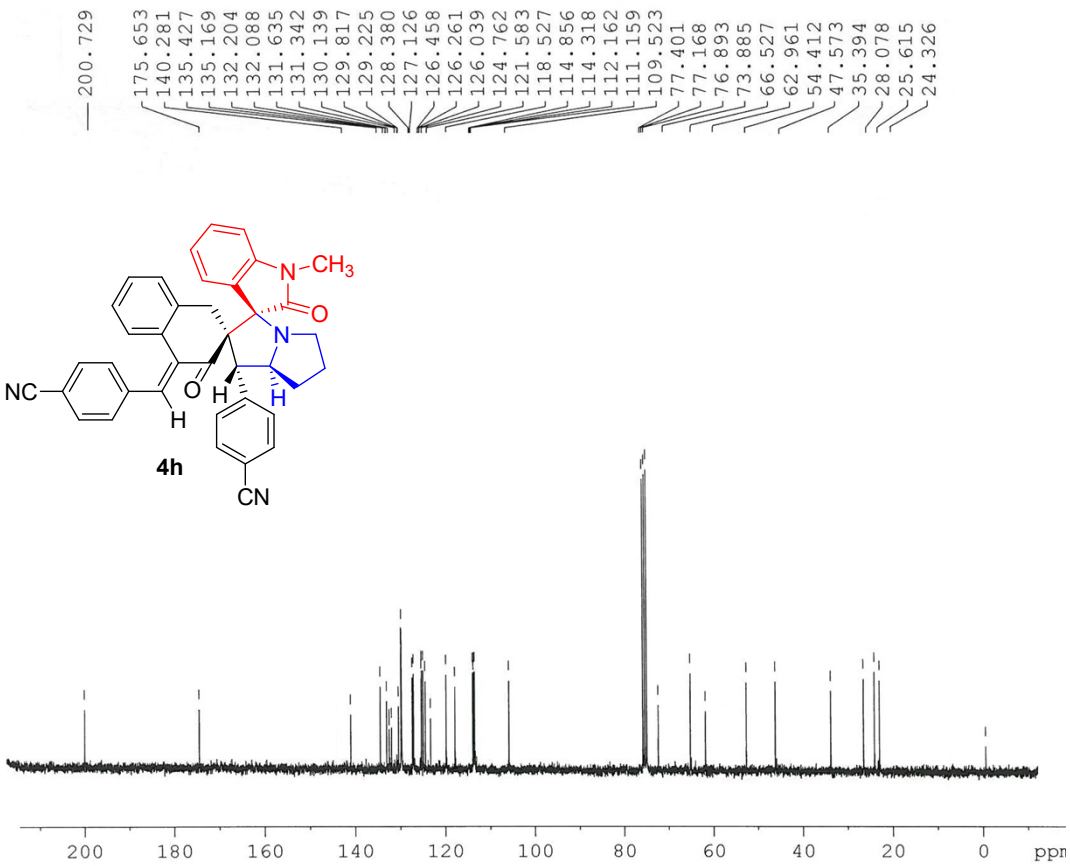

Fig S17. ^{1}H NMR Spectrum of **4i** in $CDCl_3$

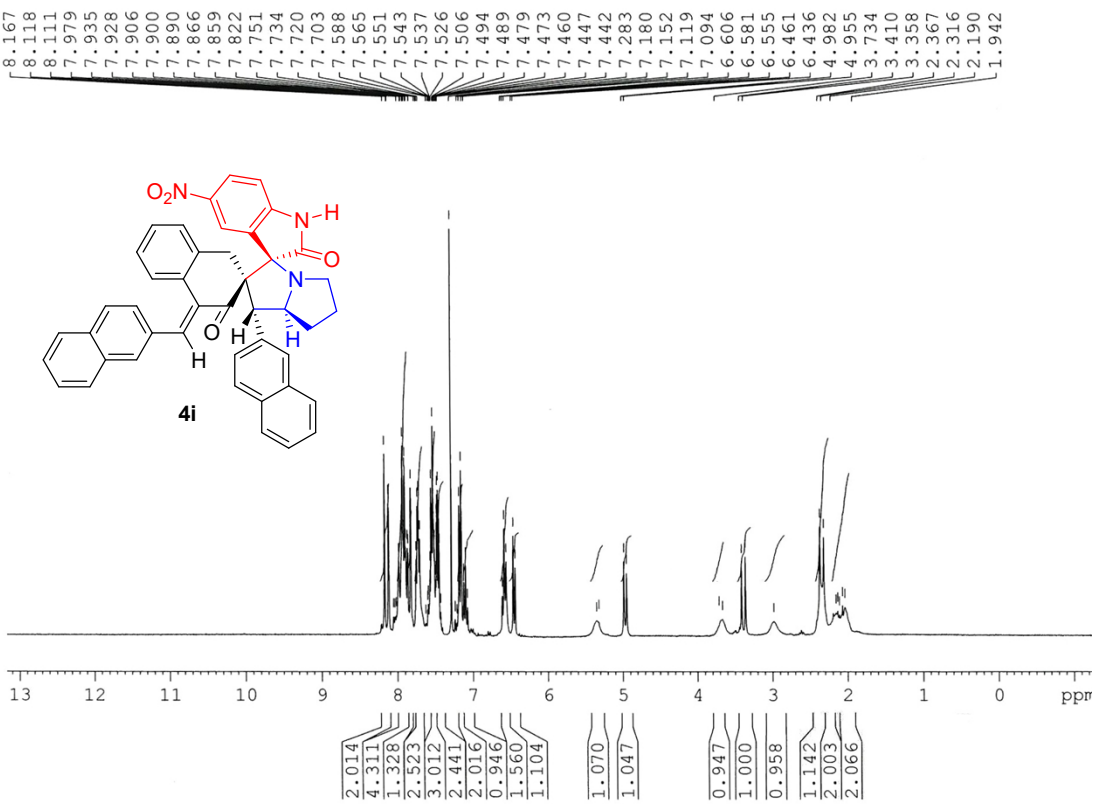

Fig S18. ^{13}C {^{1}H} NMR Spectrum of **4i** in $CDCl_3$

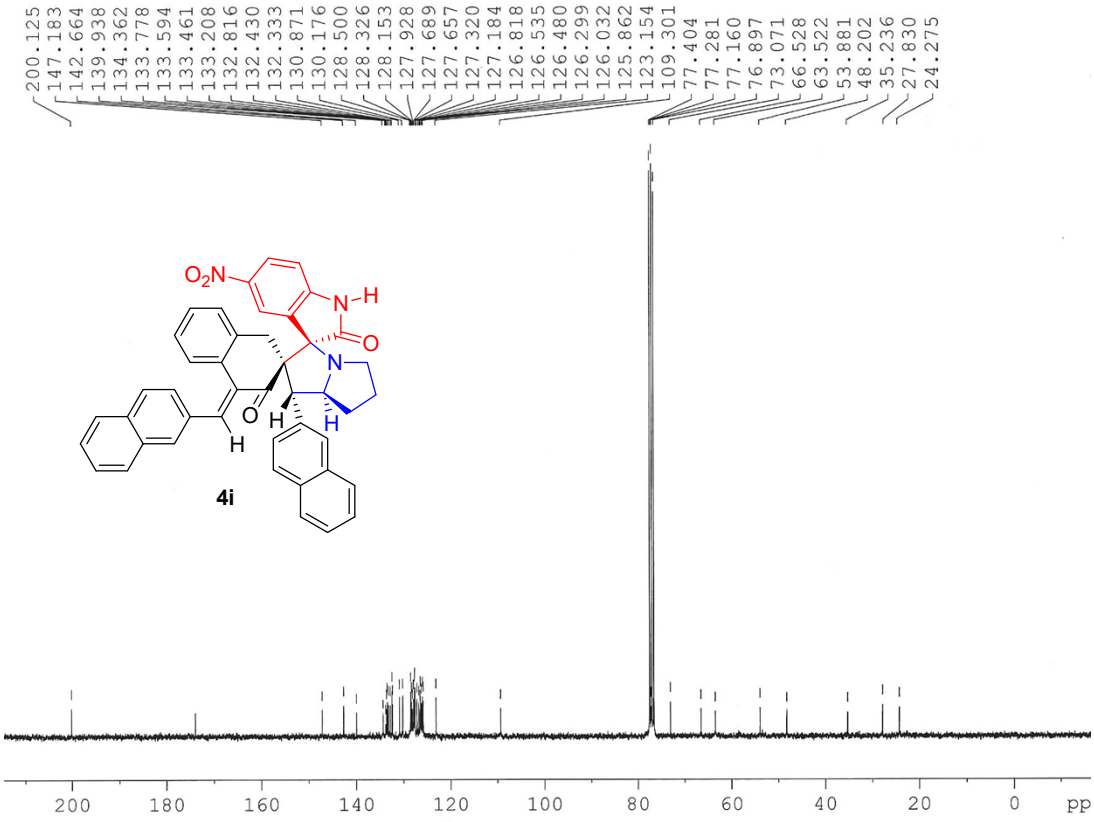

Fig S19. ^{1}H NMR Spectrum of **4j** in $CDCl_3$

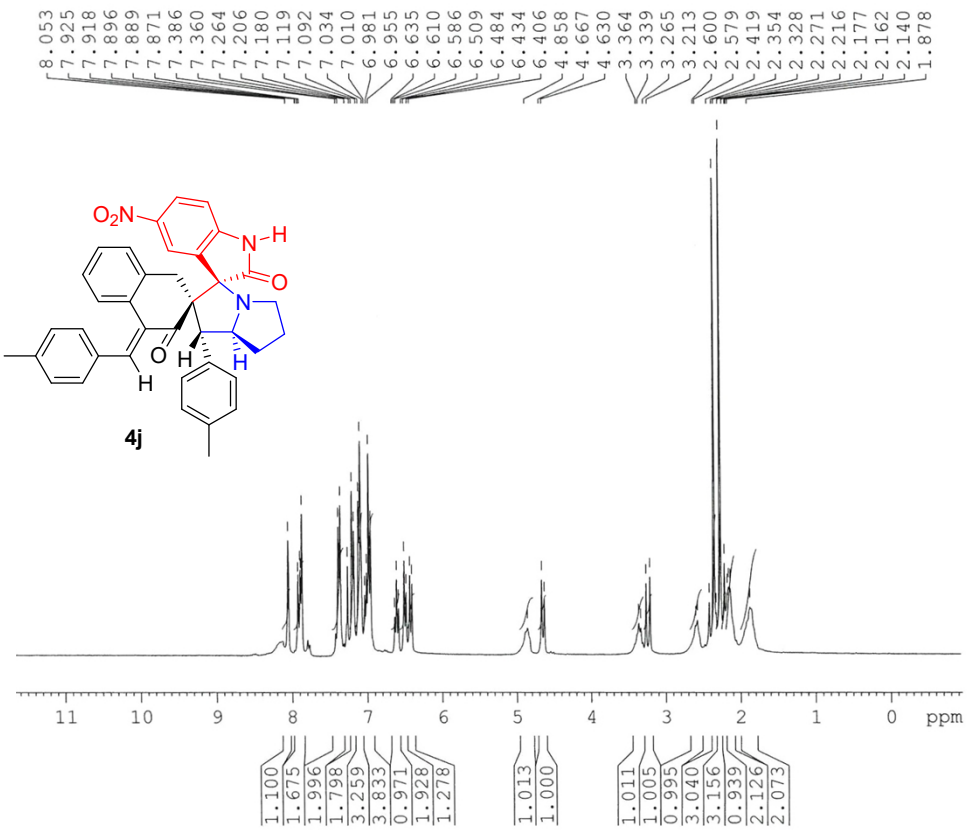

Fig S20. ^{13}C {^{1}H} NMR Spectrum of **4j** in $CDCl_3$

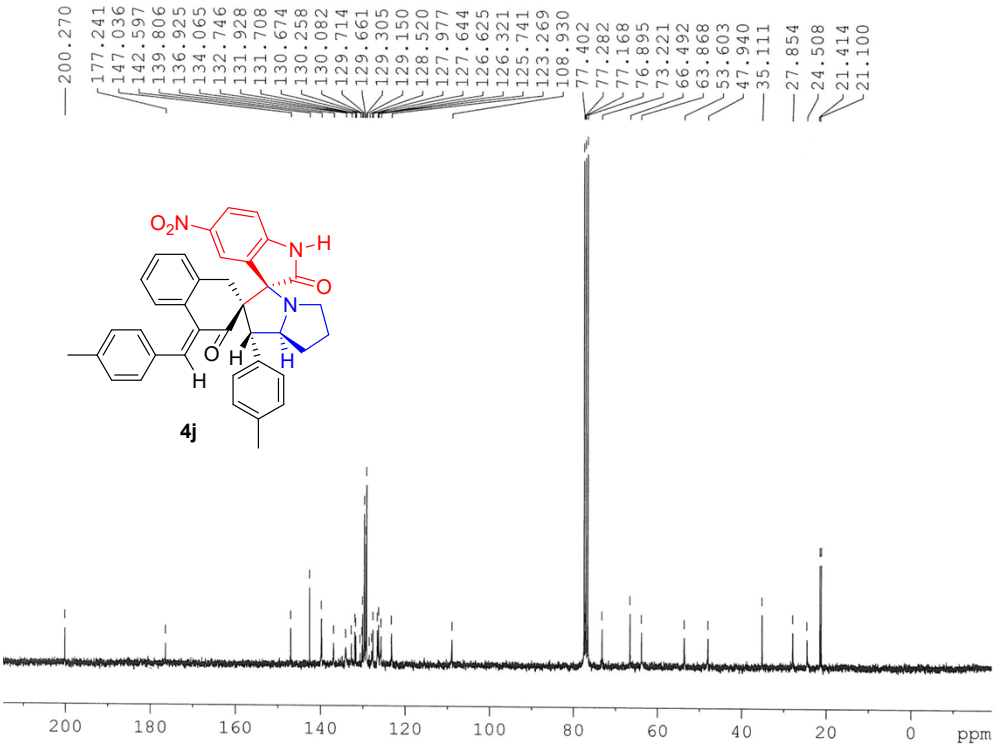

Fig S21. ^{1}H NMR Spectrum of **4k** in $CDCl_3$

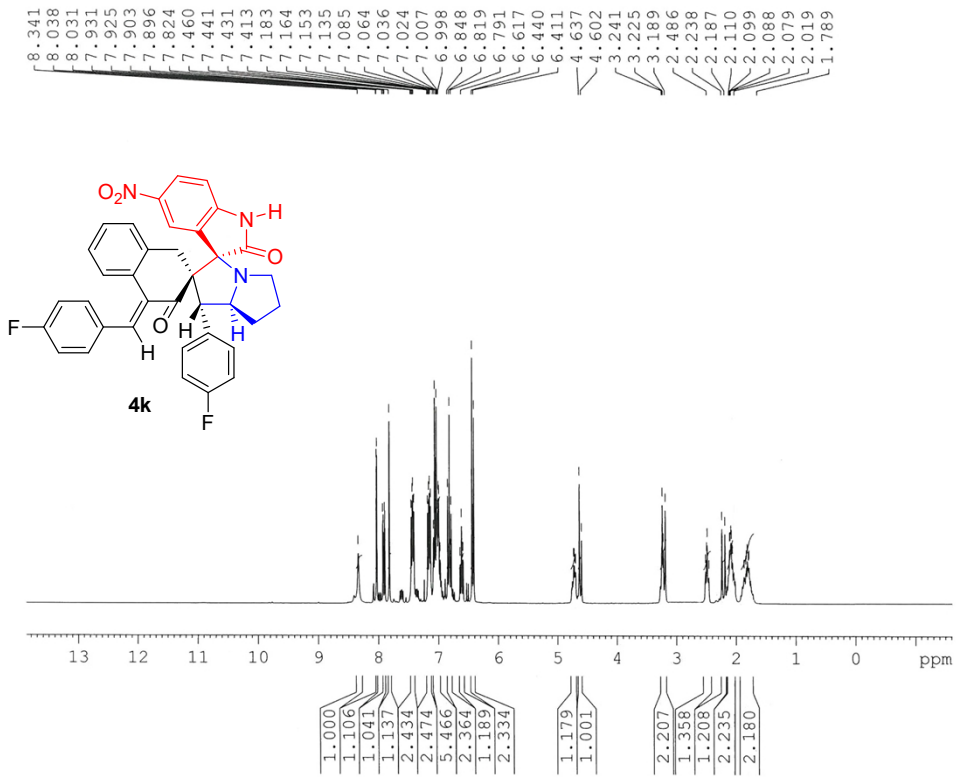

Fig S22. ^{13}C {^{1}H} NMR Spectrum of **4k** in $CDCl_3$

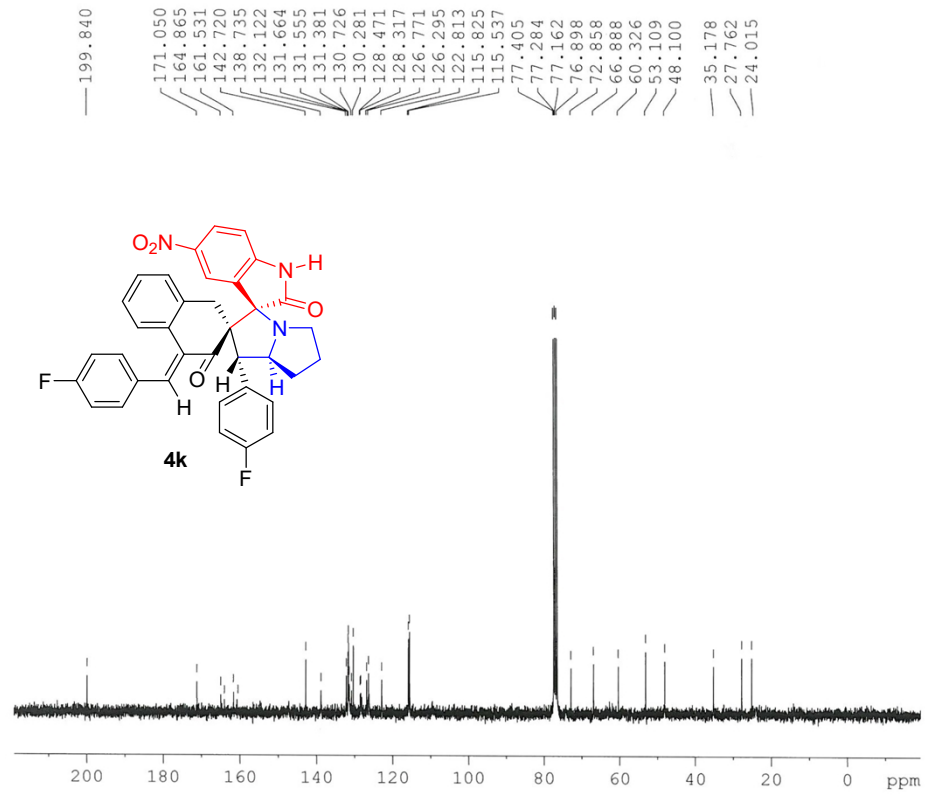

Fig S23. ^{1}H NMR Spectrum of **5a** in $CDCl_3$

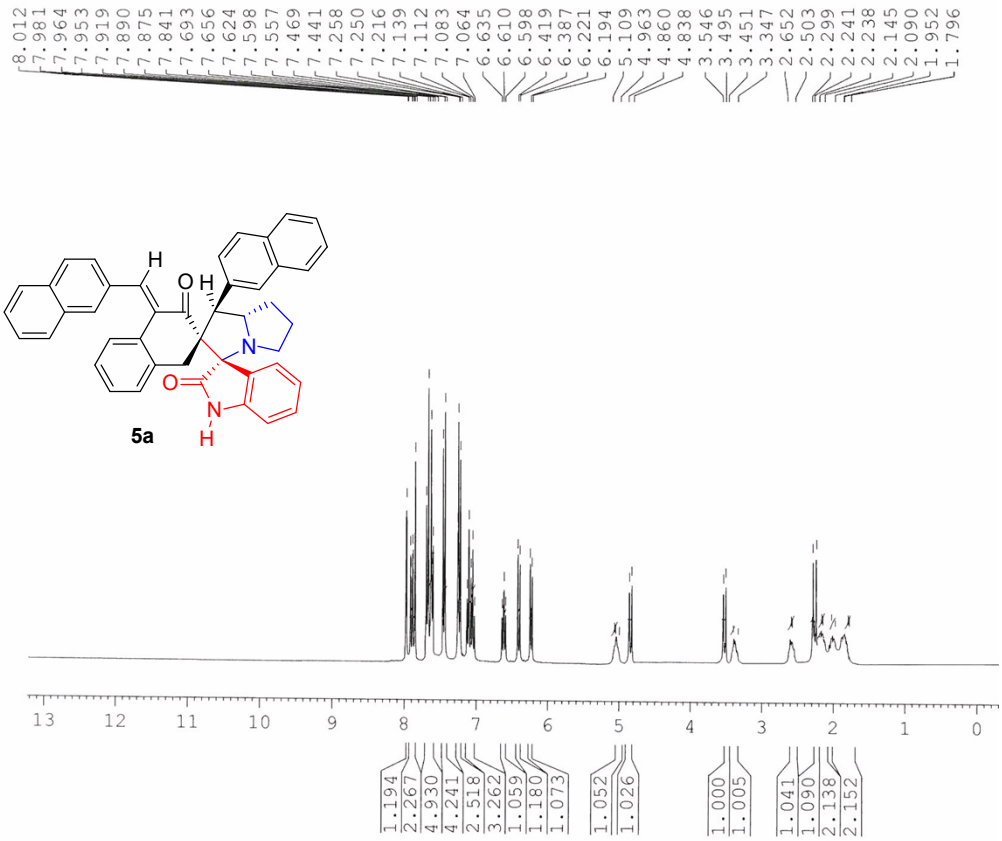

Fig S24. ^{13}C $\{^{1}H\}$ NMR Spectrum of **5a** in $CDCl_3$

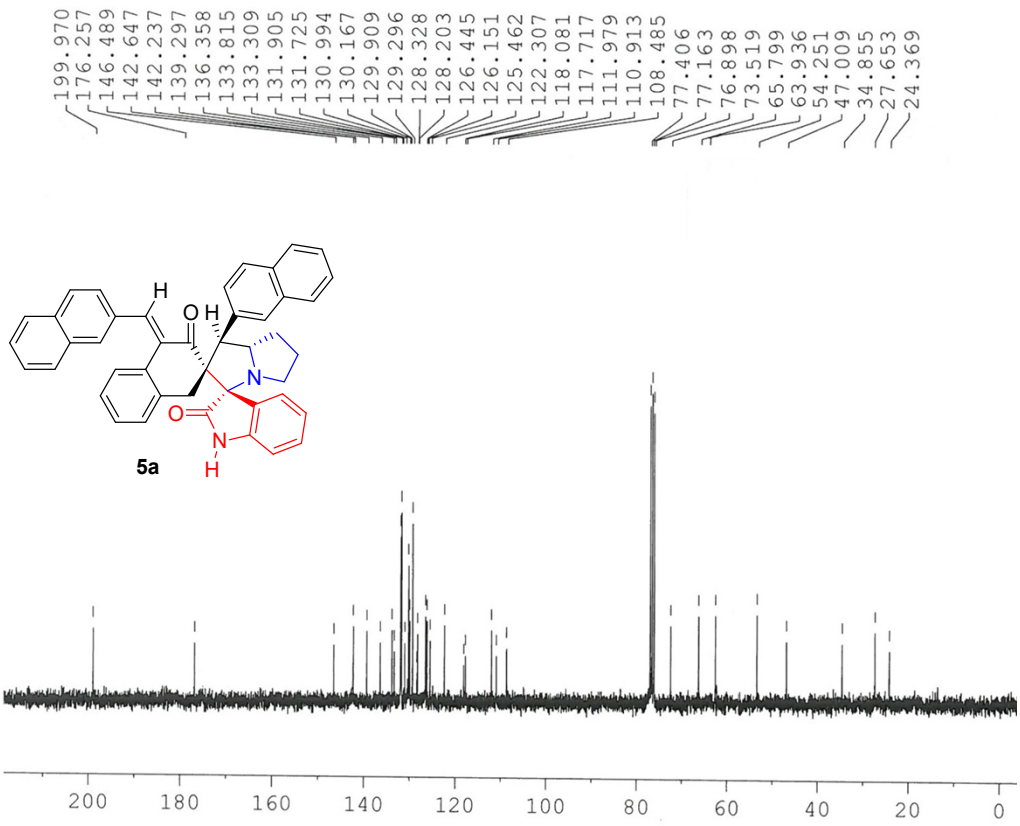

Fig S25. ^{1}H NMR Spectrum of **5b** in $CDCl_3$

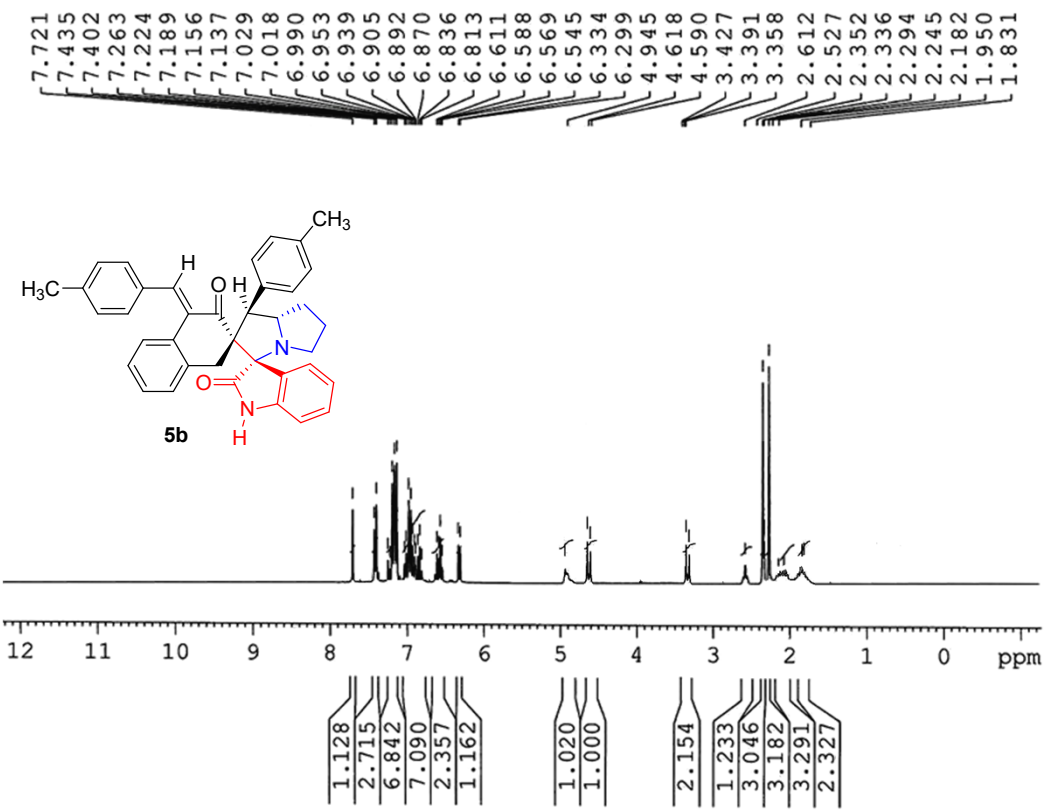

Fig S26. ^{13}C $\{^{1}H\}$ NMR Spectrum of **5b** in $CDCl_3$

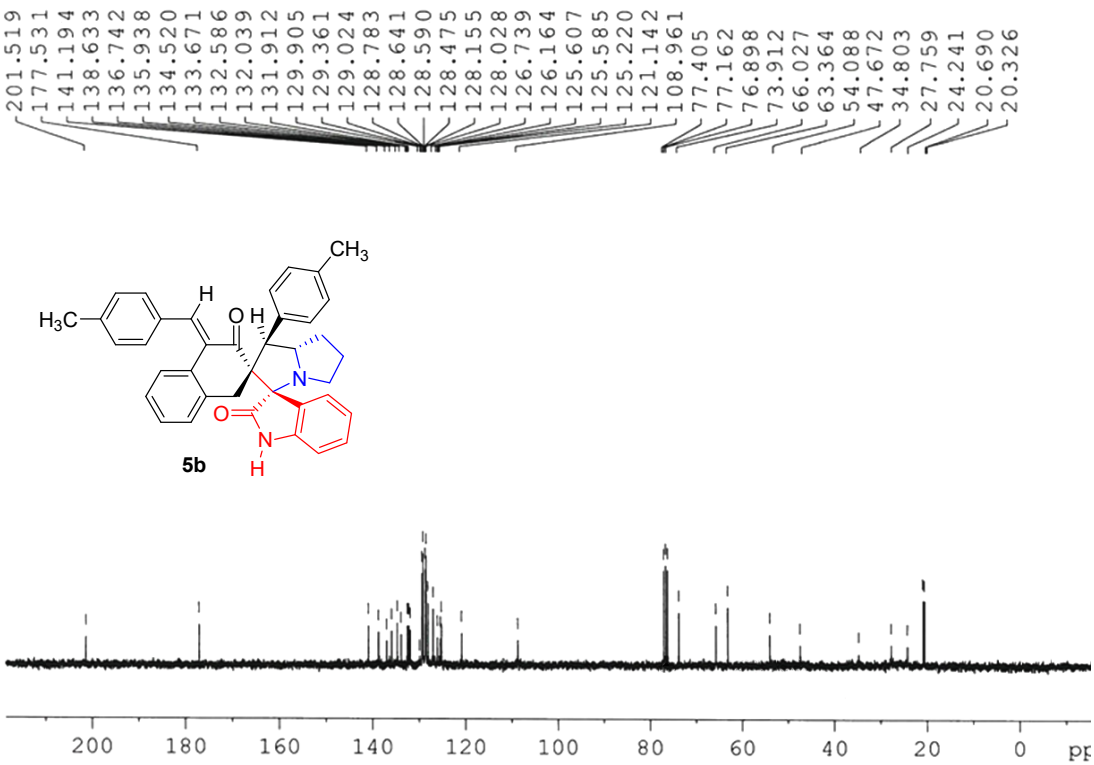

Fig S27. ^{1}H NMR Spectrum of **5f** in $CDCl_3$

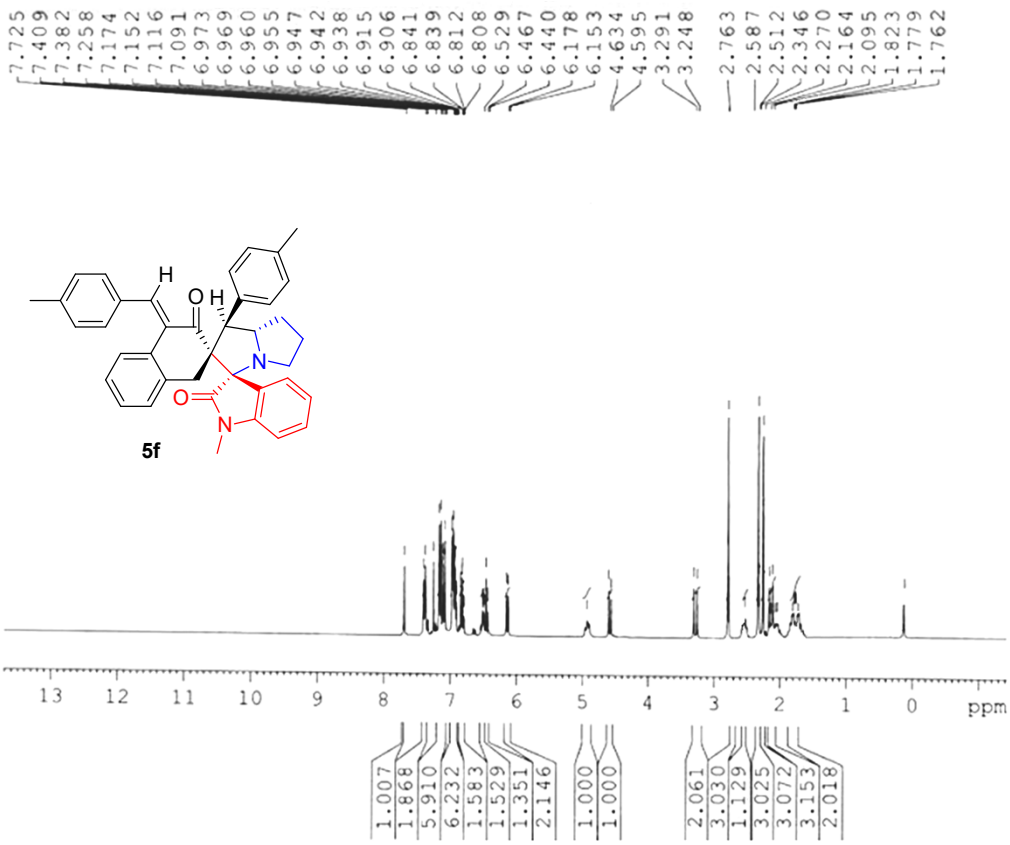

Fig S28. ^{13}C {^{1}H} NMR Spectrum of **5f** in $CDCl_3$

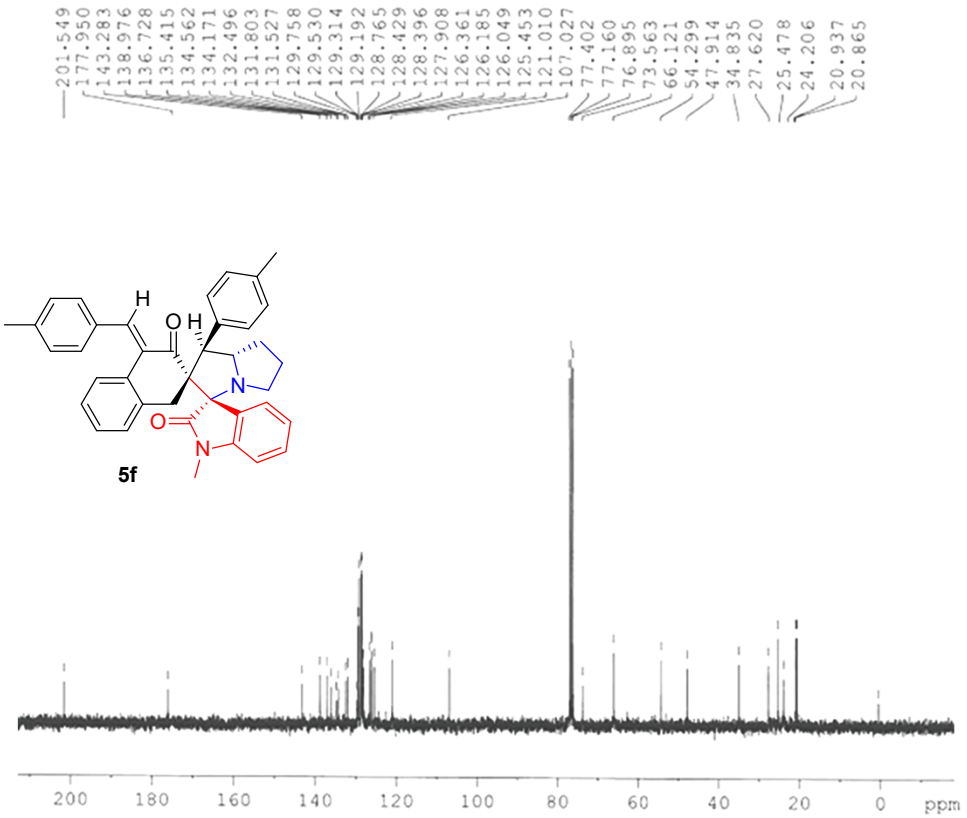

Fig S29. ^{1}H NMR Spectrum of **5g** in $CDCl_3$

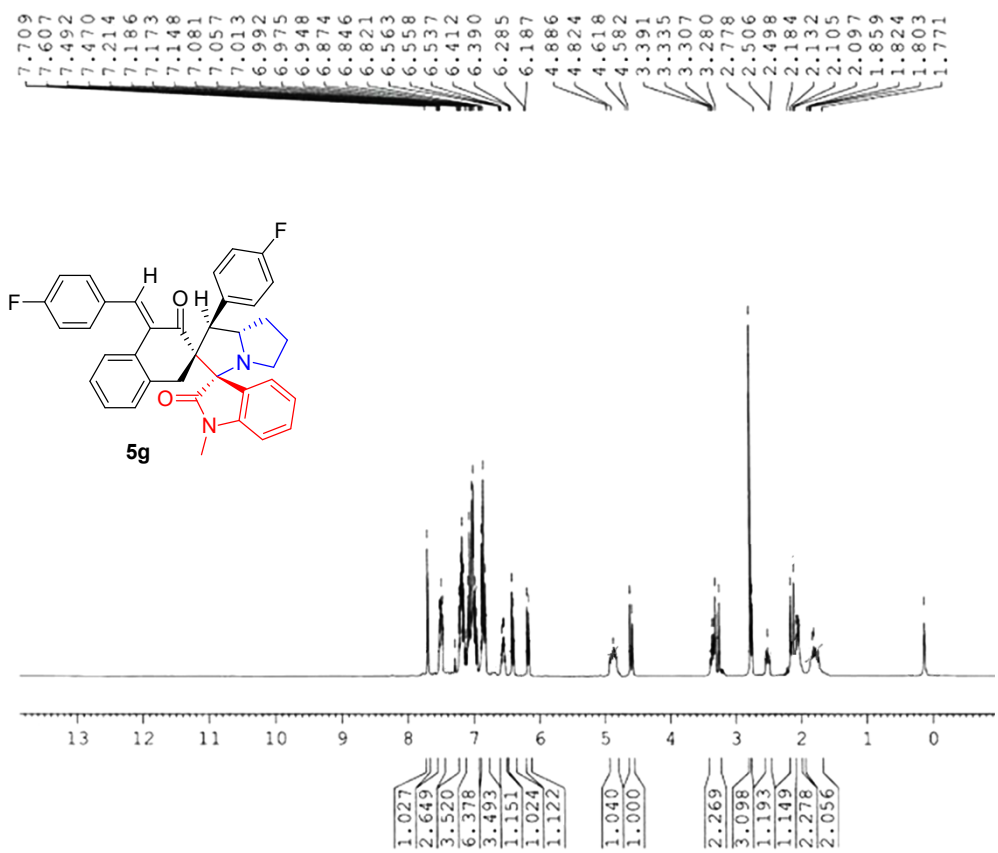

Fig S30. ^{13}C {^{1}H} NMR Spectrum of **5g** in $CDCl_3$

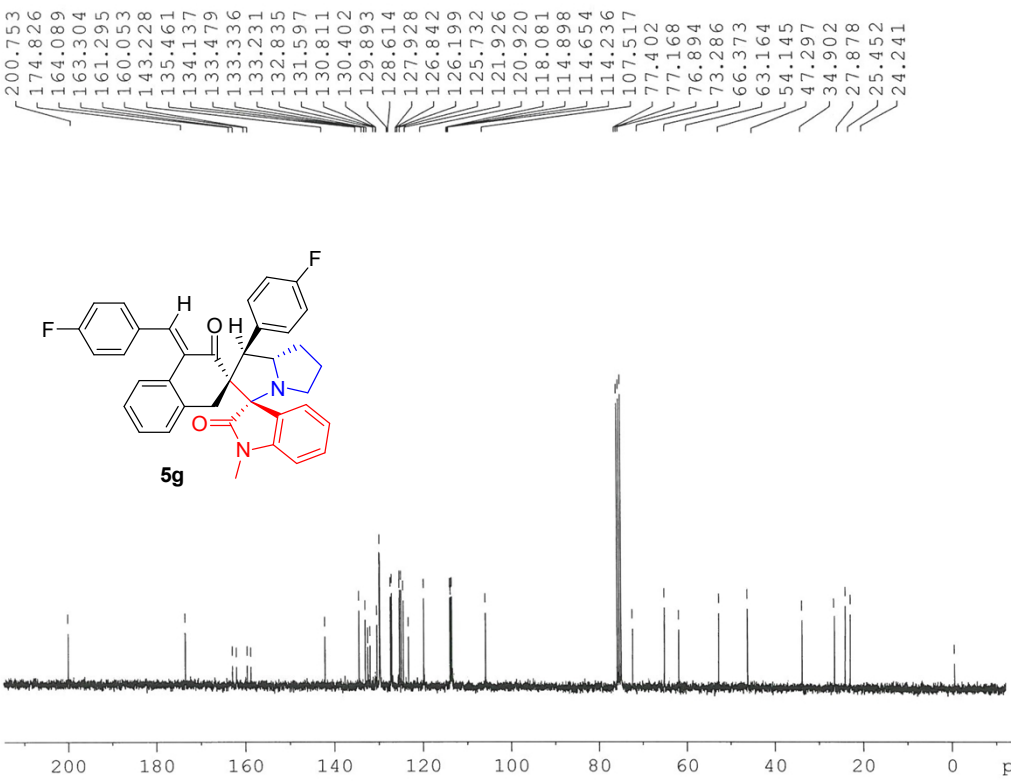

Fig S31. ^{1}H NMR Spectrum of **5h** in $CDCl_3$

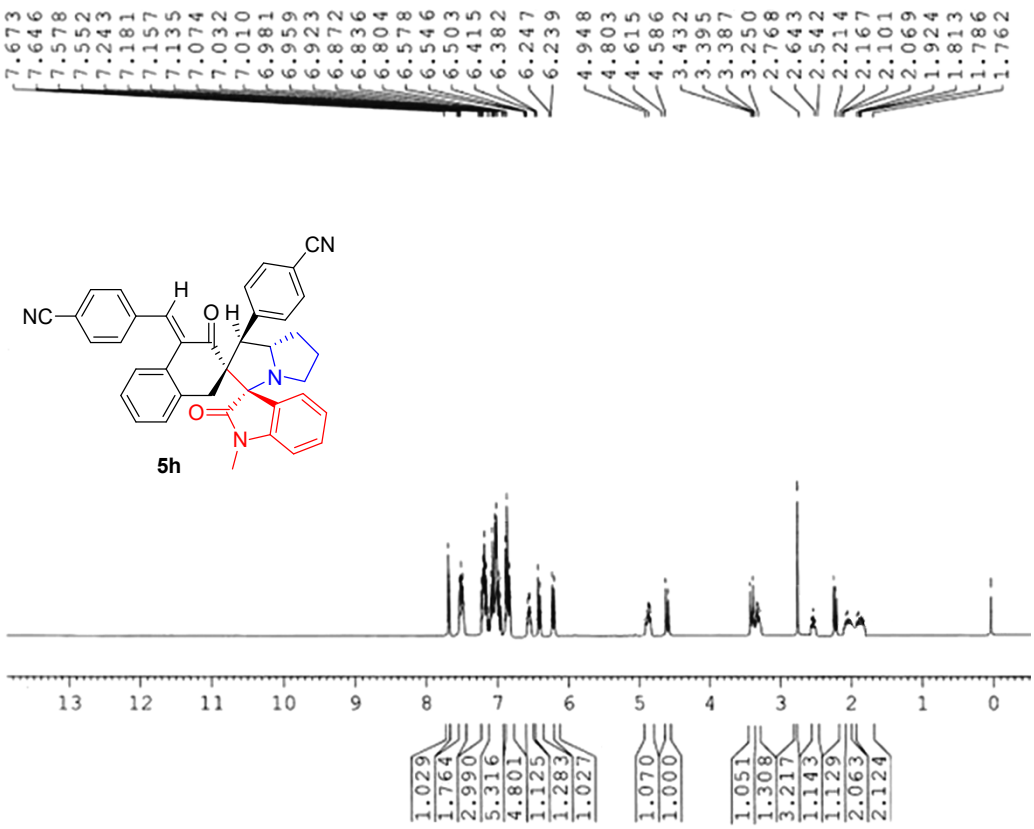

Fig S32. ^{13}C $\{^{1}H\}$ NMR Spectrum of **5h** in $CDCl_3$

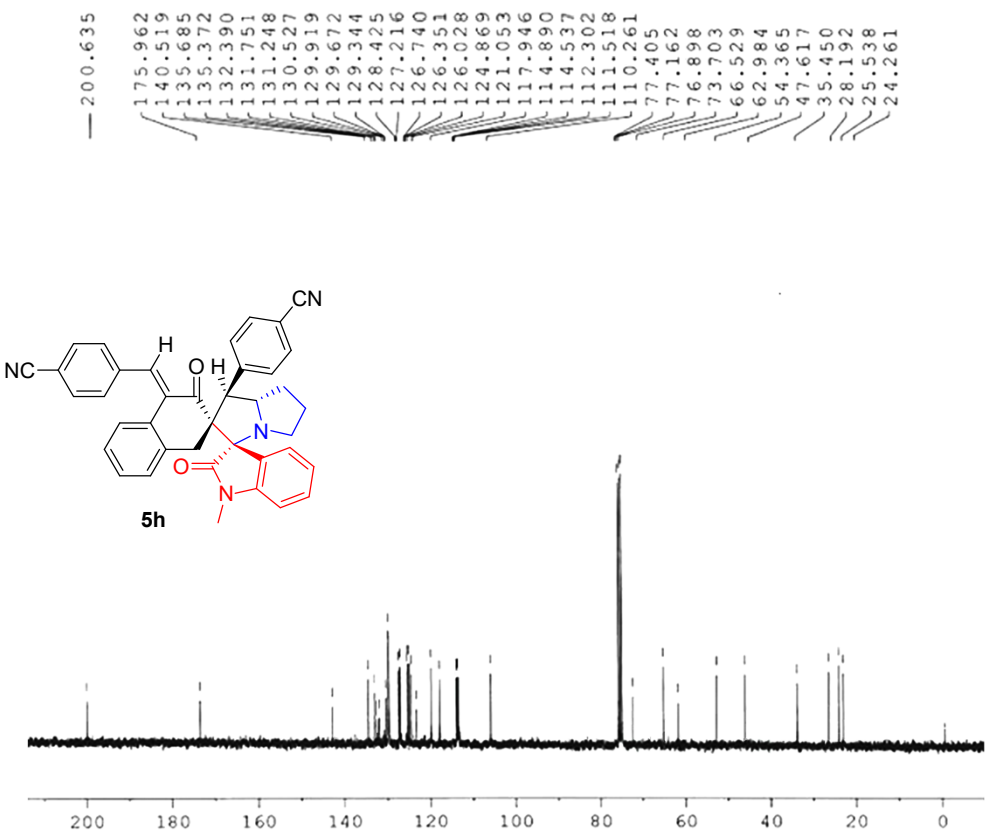

Fig S33. ^{1}H NMR Spectrum of **5j** in $CDCl_3$

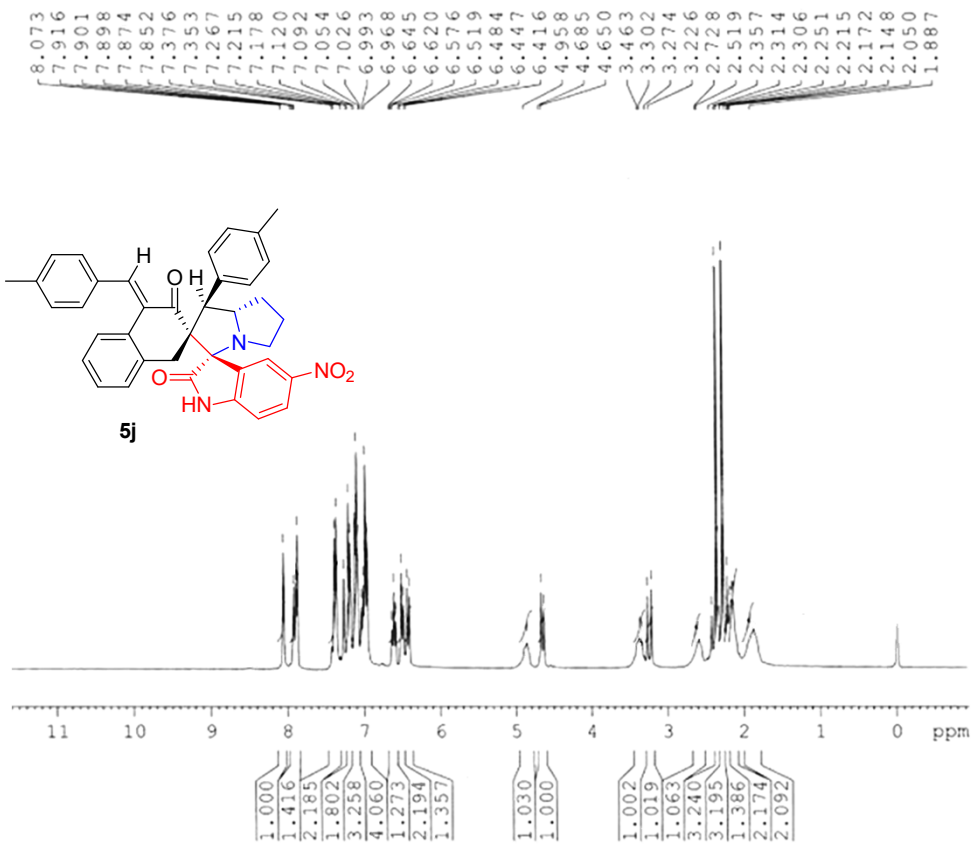

Fig S34. ^{13}C {^{1}H} NMR Spectrum of **5j** in $CDCl_3$

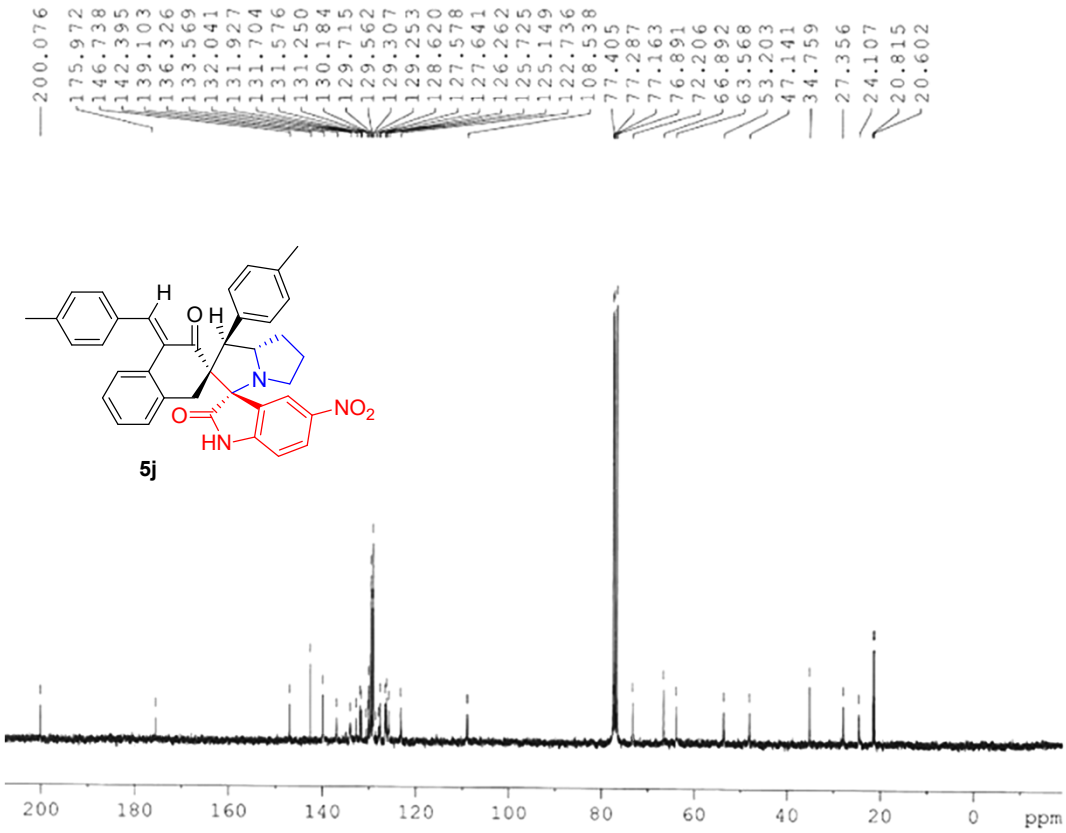

Fig S35. ^{1}H NMR Spectrum of **5k** in $CDCl_3$

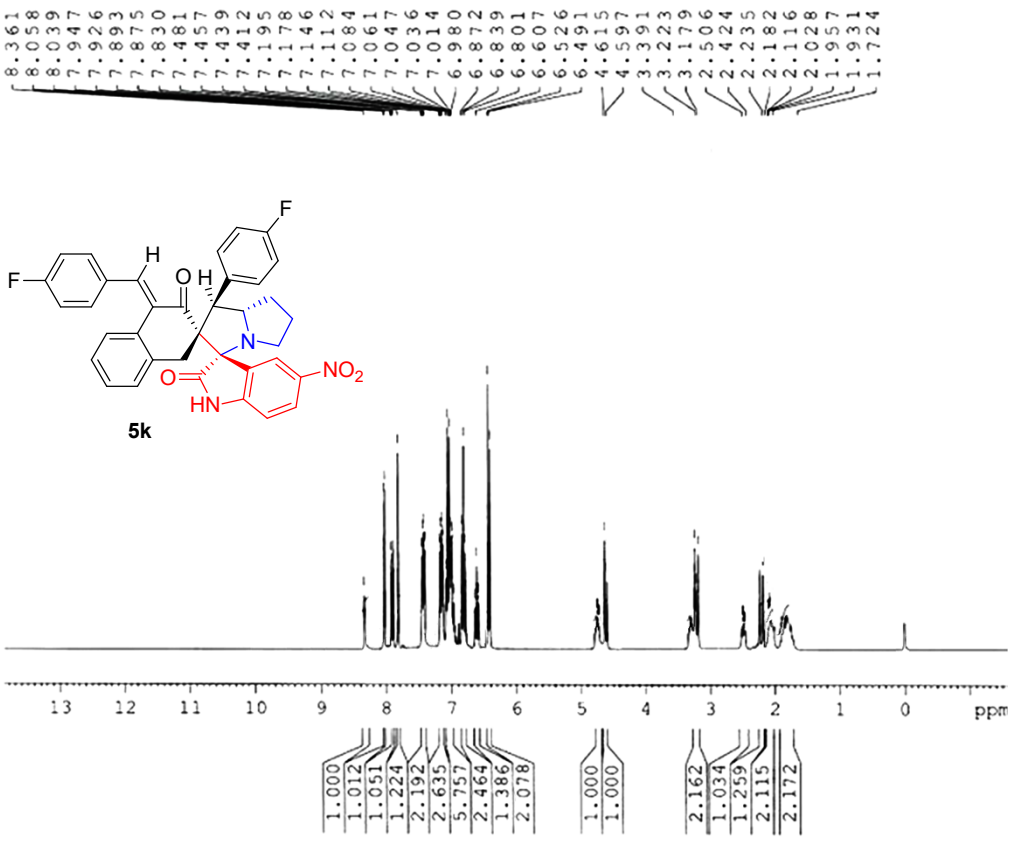

Fig S36. ^{13}C $\{^{1}H\}$ NMR Spectrum of **5k** in $CDCl_3$

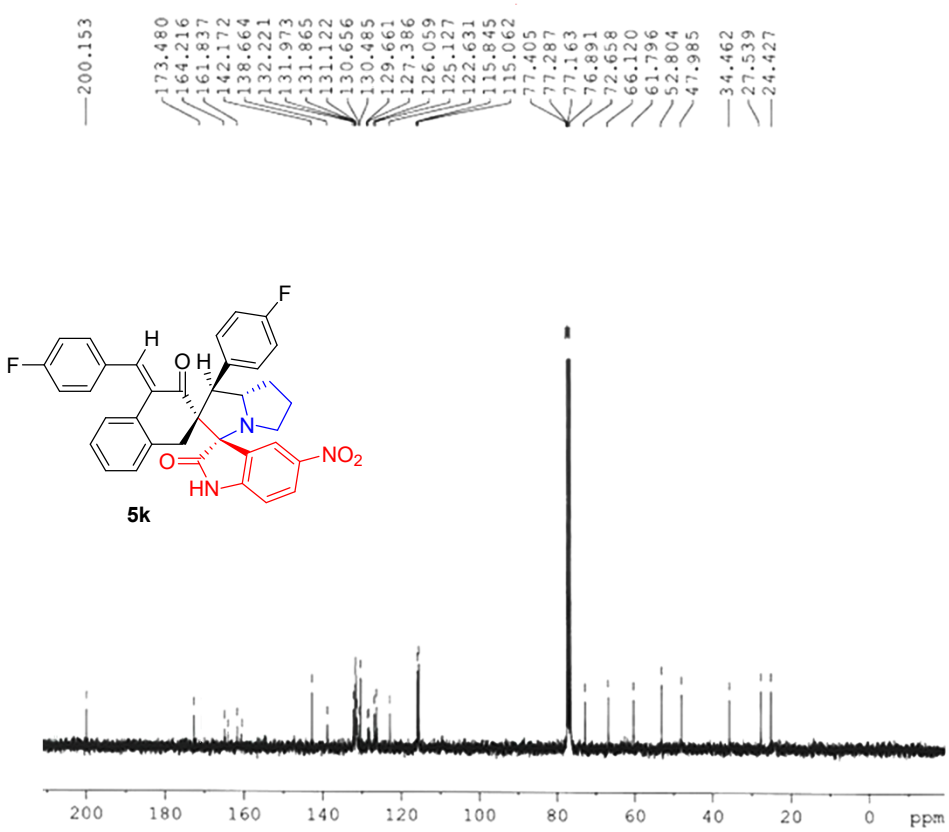

Fig S37. ^{1}H NMR Spectrum of **16a** in $CDCl_3$

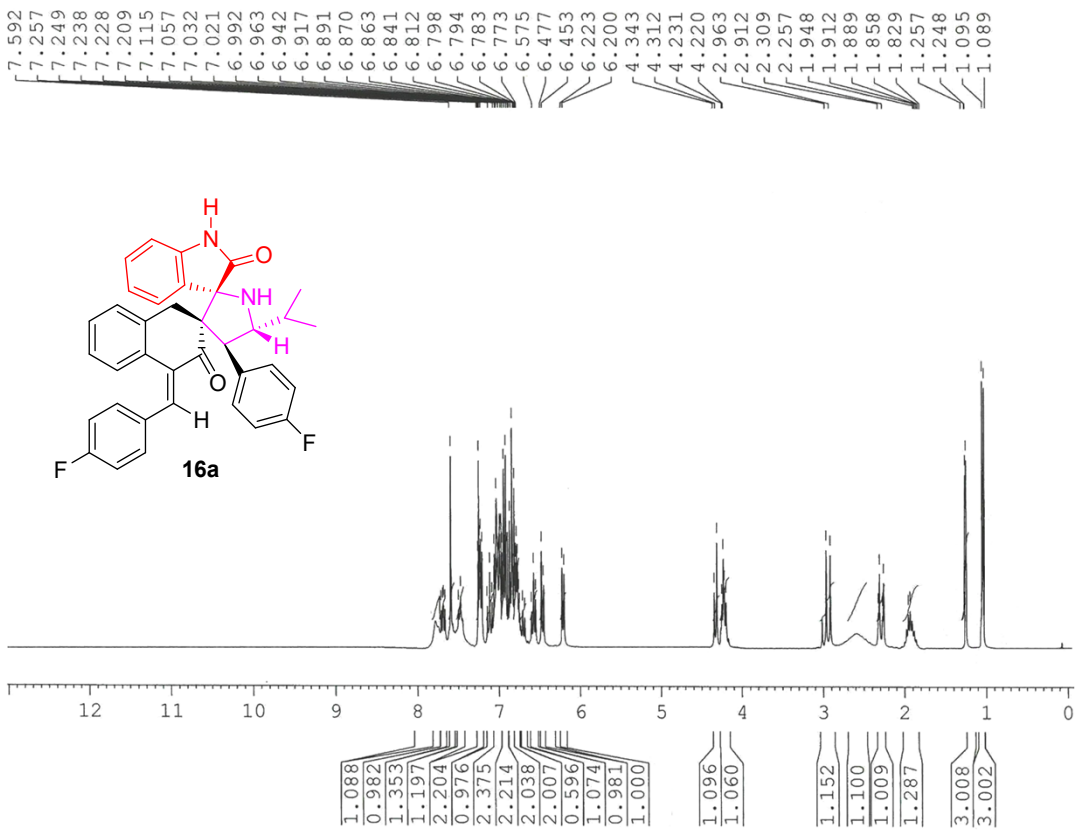

Fig S38. ^{13}C {^{1}H} NMR Spectrum of **16a** in $CDCl_3$

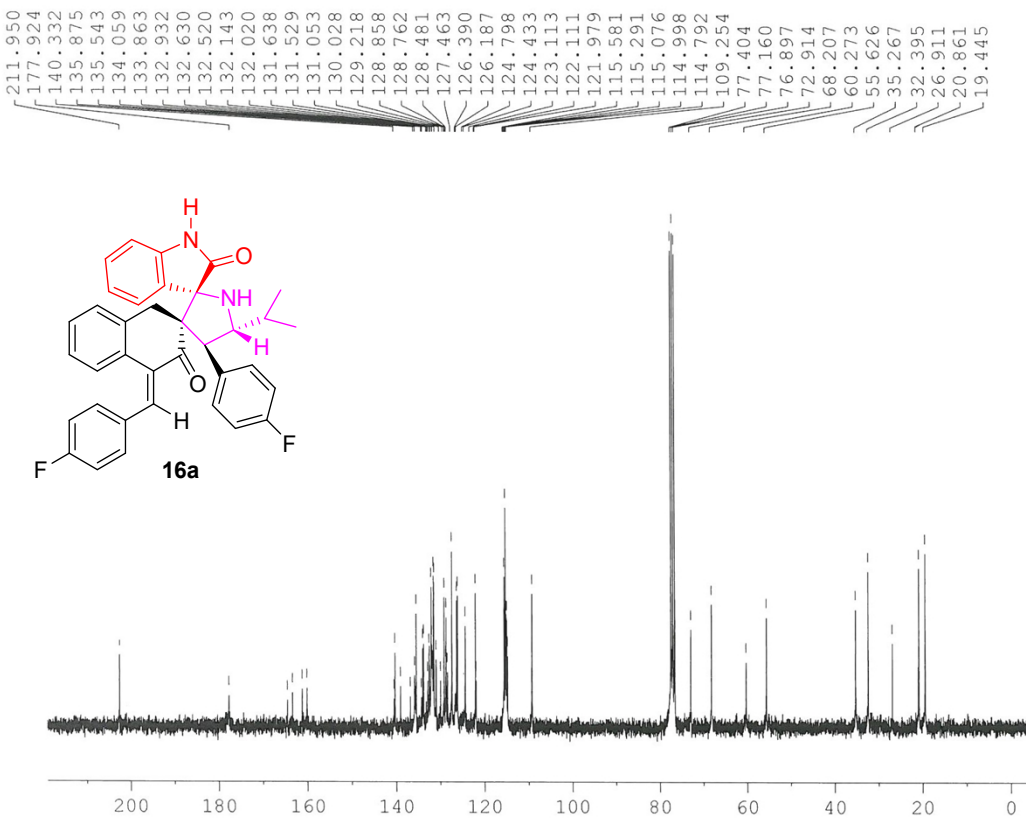

Fig S39. ^{1}H NMR Spectrum of **17a** in $CDCl_3$

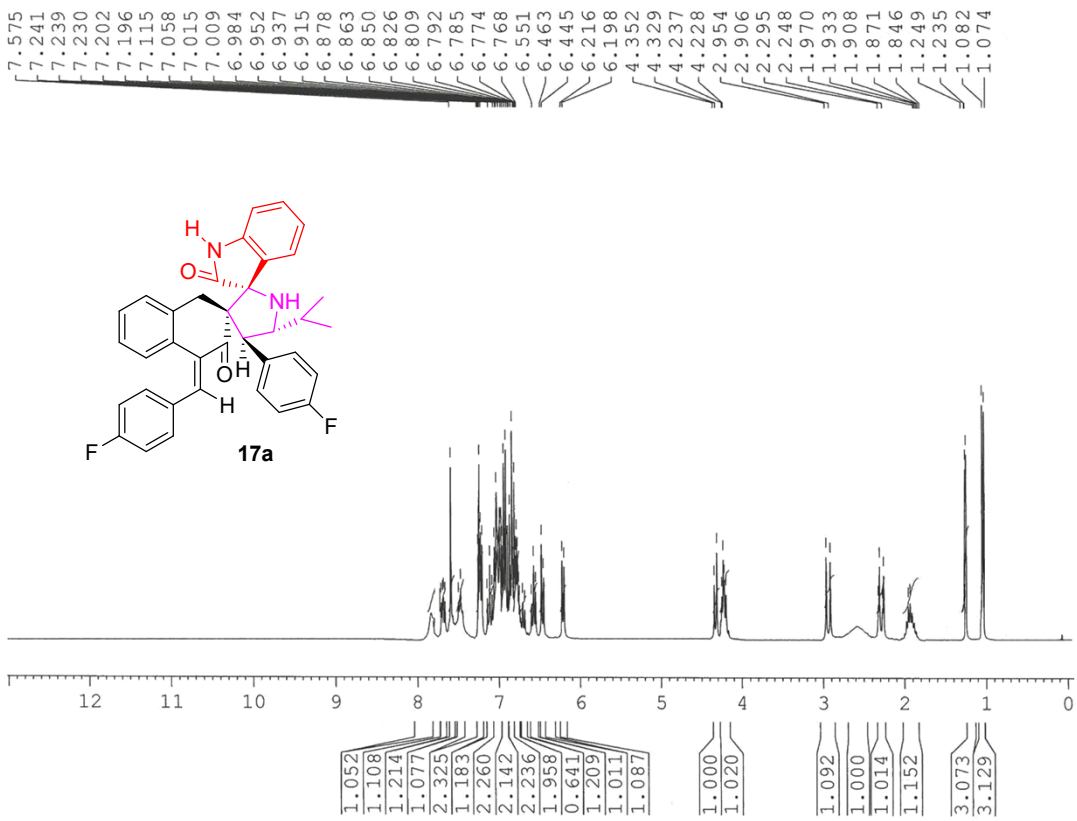

Fig S40. ^{13}C $\{^{1}H\}$ NMR Spectrum of **17a** in $CDCl_3$

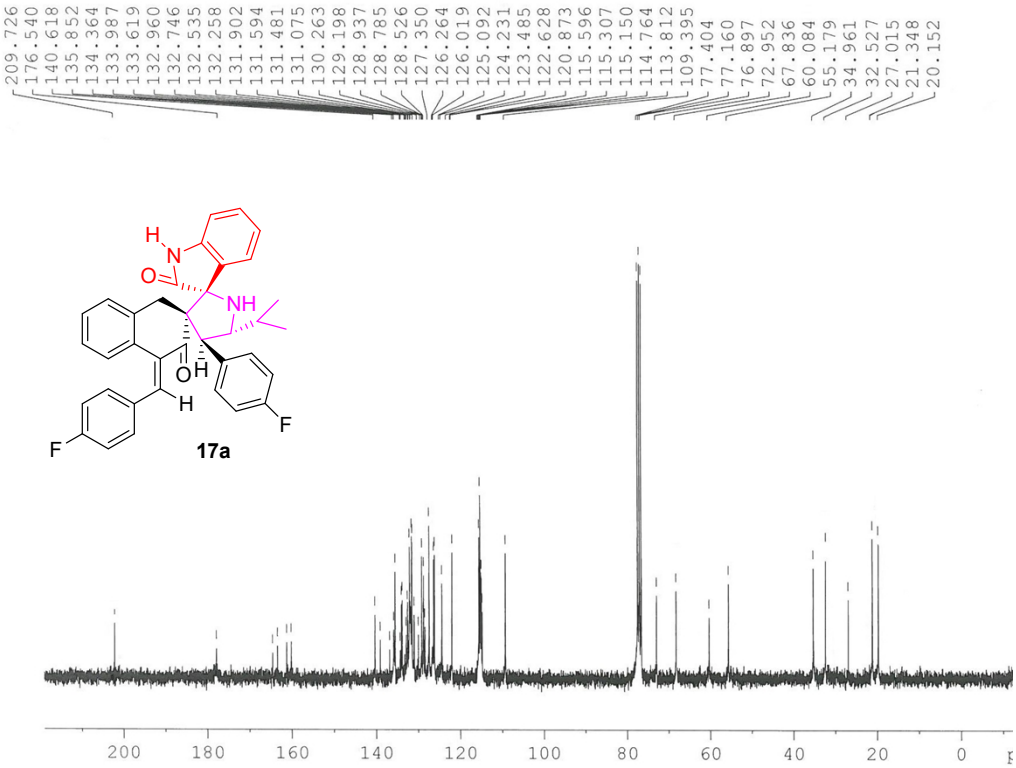

Fig S41. ^{1}H and ^{13}C chemical shifts of ~~the~~ diastereoisomer **5k**

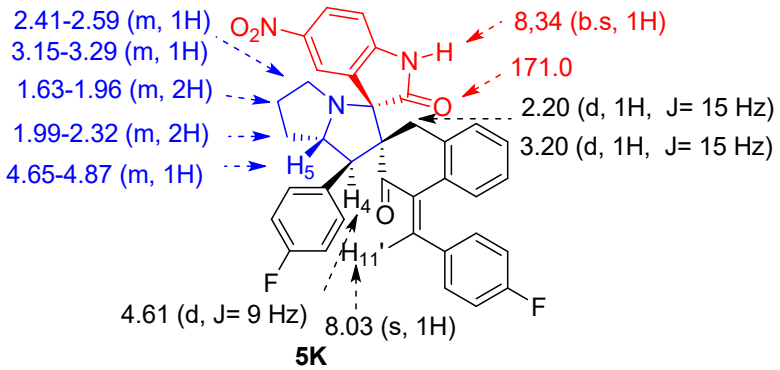

Fig S42. ^{1}H and ^{13}C chemical shifts of ~~the~~ diastereoisomer **17a**

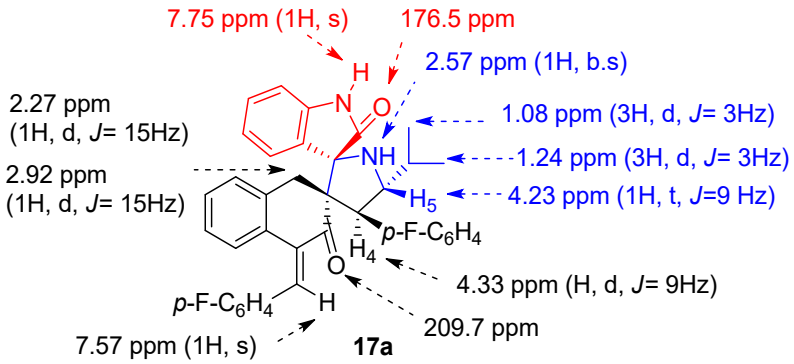

Fig S43. An alternative view of the molecular structure of **4k**.

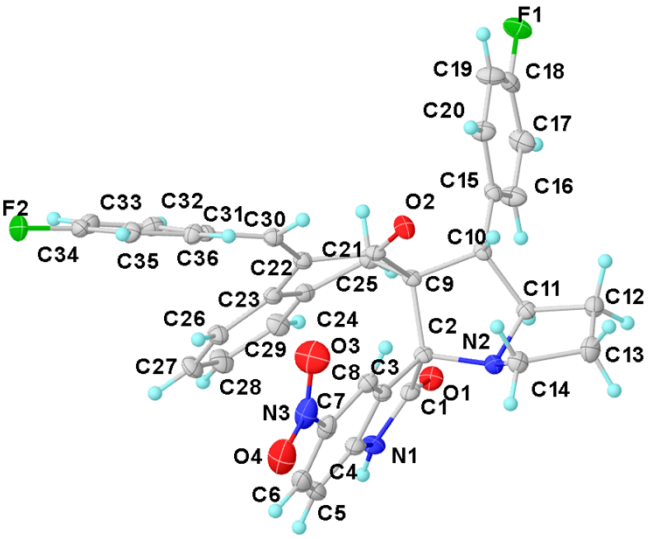

Fig S44. View of the supramolecular 2D network of **4k** resulting from intermolecular N-H….O bonding (*d*N1-H1….O3 = 1.972 Å, N1-H1-O3 = 170.6°) and weaker C17-H17….O3 contacts with the NO_2 group of a neighboured molecule

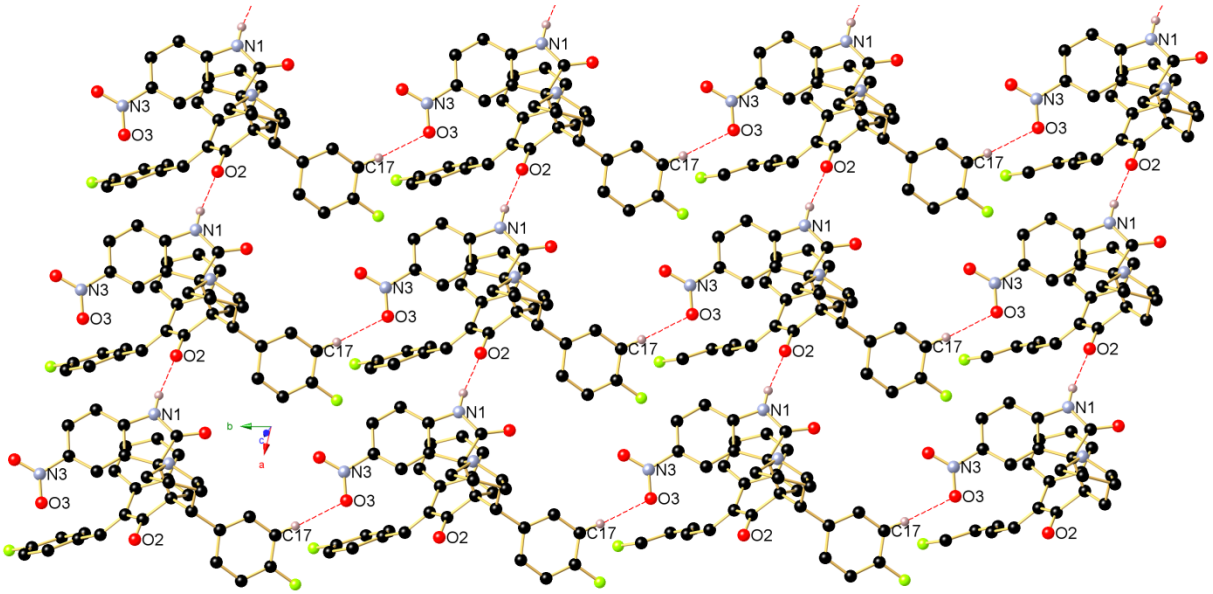

Table S2: Selected bond lengths (A) and angles (°) of **4k**

Selected bond	Lengths (A)	Selected angles	Value in (°)
N1-C1	1.371 (2)	C1-N1-C4	112.38 (2)
C1-C2	1.5645 (19)	N1-C4-C3	109.89 (13)
C2-C3	1.518 (2)	C4-C3-C2	108.5 (12)
C3-C4	1.407 (2)	C3-C2-C1	101.55 (11)
C4-N1	1.386 (2)	C2-C1-N1	107.27 (12)
N2-C2	1.4772 (19)	N2-C2-C9	107.01 (11)
C2-C9	1.6072 (19)	C2-C9-C10	102.45 (11)
C9-C10	1.5615 (19)	C9-C10-C11	105.27 (11)
C10-C11	1.545 (2)	C10-C11-N2	104.31 (11)
C11-C12	1.539 (2)	C11-N2-C2	105.83 (11)
C12-C13	1.547 (2)	C11-N2-C14	105.30 (11)
C13-C14	1.531 (2)	N2-C14-C13	102.16 (12)
C14-N2	1.4826 (18)	C14-C13-C12	104.87 (12)
N2-C11	1.4758 (19)	C13-C12-C11	104.65 (12)
C9-C21	1.5332 (19)	C12-C11-N2	105.31 (12)
C21-C22	1.506 (2)	C21-C9-C25	105.32 (11)
C22-C23	1.486 (2)	C9-C25-C24	110.05 (12
C23-C24	1.410 (2)		
C24-C25	1.509 (2)		
C25-C9	1.551 (2)		

Table S2: Hydrogen bonds occurring in **4k**.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N1	H1	O2[1]	0.88	1.97	2.8429(19)	170.6
C8	H8	O2	0.95	2.63	3.321(2)	129.8
C8	H8	O5	0.95	2.42	3.255(4)	146.6
C12	H12B	O1[2]	0.99	2.72	3.429(2)	129.0
C14	H14A	O4[3]	0.99	2.67	3.442(2)	135.4
C14	H14B	O5	0.99	2.70	3.470(4)	135.3
C17	H17	O3[4]	0.95	2.56	3.442(2)	154.4
C20	H20	O1[5]	0.95	2.60	3.443(2)	147.9
C26	H26	F2[6]	0.95	2.54	3.412(2)	153.1
C35	H35	F1[7]	0.95	2.60	3.228(2)	123.9

Table S2: Hydrogen bonds occurring in **4k**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C36	H36	F1[7]	0.95	2.70	3.289(2)	121.1
C39	H39B	O3	0.99	2.33	3.140(5)	139.0

[1]1+X,+Y,+Z; [2]1-X,1-Y,2-Z; [3]1-X,-Y,2-Z; [4]+X,1+Y,+Z; [5]-1+X,+Y,+Z; [6]1-X,-Y,1-Z; [7]+X,-1+Y,+Z

Table S3: Crystal data collection and structure refinement of **4k**.

CCDC	2097365
Compound /Formula	$C_{386}H_{31}F_2N_3O_5$
Formula weight	647.66
Temperature/K	100(2)
Wavelength/Å	0.71073
Crystal system	triclinic
Space group	P-1
a/Å	8.244(4)
b/Å	12.956(6)
c/Å	15.359(8)
α	75.195(19)°
β	80.54(2)°
γ	77.813(17)°
Volume/ Å^3	1539.6(13)
Z	2
ρ_{calc} g/cm^3	1.3794
Absorp. coefficient/mm^{-1}	0.101
F(000)	676.0
Crystal size/mm^3	0.395 x 0.207 x 0.082
2 Theta range for data collection/°	5.556 to 598.232
Index ranges	-11<=h<=11, -17<=k<=16 -21<=l<=19
Reflections collected	20681
Independent reflections	8000 [*R*(int) = 0.0364]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	8000 / 39 / 463
Goodness-of-fit on F^2	1.039
Final *R* indices [*I*>2sigma(I)]	*R*1 = 0.0470, w*R*2 = 0.1160
R indices (all data)	*R*1 = 0.06706, w*R*2 = 0.11271
Largest diff. peak and hole/e. Å^{-3}	0.45 and -0.38

DFT supplement:

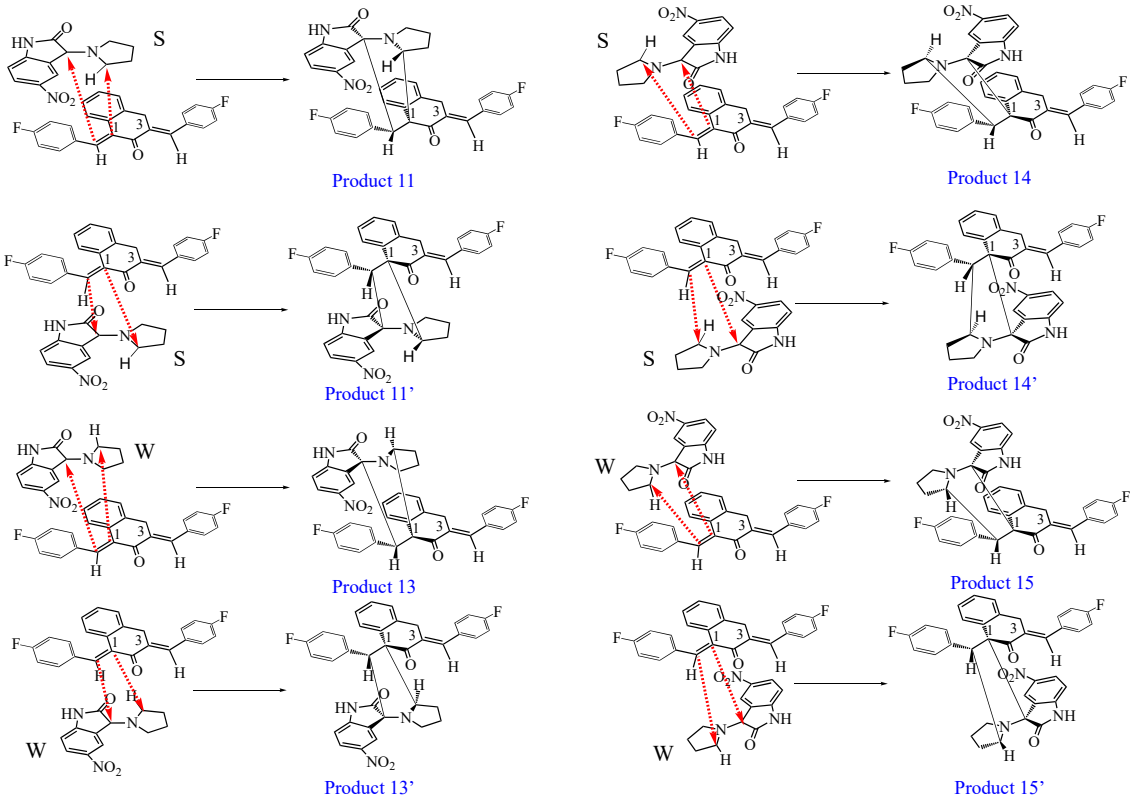

Fig 45S. The different possible approaches of the dipolarophile to the azomethine ylides on double bond at position 1.

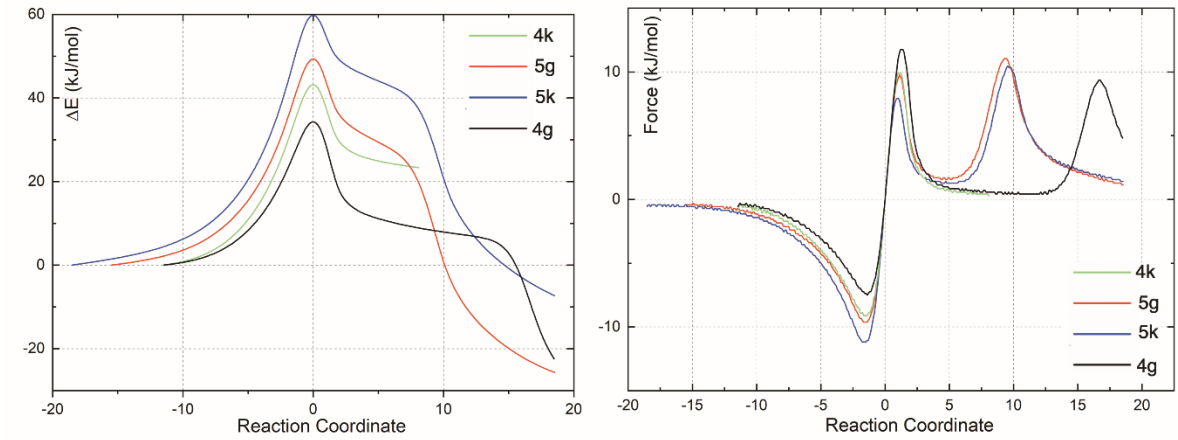

Fig 46S: The intrinsic reaction coordinate plots of the compounds ***g*** and ***k*** to lead to products **4** and **5**.

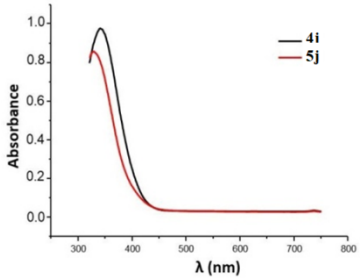

Figure 47S. Superposition of **4**j and **5**j compounds absorption spectra

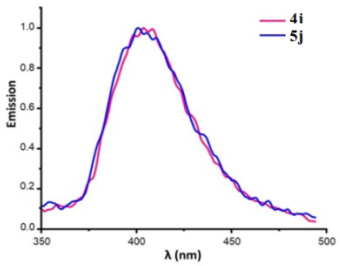

Figure 48 S. Superposition of **4j** and **5j** compounds emission spectra

Cartesian Coordinates of the optimized Structures:

Prod4a

	Atom	X	Y	Z
1	C	1.7195	-1.9411	-0.4274
2	N	2.7775	-1.9759	-1.4360
3	C	3.5270	-0.7121	-1.3371
4	C	2.4876	-2.2219	-2.8609
5	C	3.8044	-1.7942	-3.5125
6	C	4.2155	-0.5387	-2.7107
7	H	4.2544	-0.7935	-0.5305
8	C	0.6413	-2.9996	-0.6429
9	C	0.7758	-3.9931	0.3390
10	N	1.8256	-3.6646	1.1985
11	C	2.4259	-2.4753	0.8704
12	C	-0.3393	-3.1489	-1.6150
13	C	-1.1769	-4.2700	-1.5843
14	C	-1.0299	-5.2372	-0.5943
15	C	-0.0437	-5.1110	0.3863
16	O	3.3577	-1.9766	1.4670
17	H	2.2514	-3.2736	-3.0285
18	H	1.6591	-1.6110	-3.2424
19	H	4.5487	-2.5843	-3.3846
20	H	3.6949	-1.5998	-4.5816
21	H	5.2987	-0.4483	-2.6164
22	H	3.8576	0.3705	-3.2006
23	H	-0.4664	-2.4087	-2.3928
24	H	-1.6849	-6.1010	-0.5813
25	H	0.0779	-5.8629	1.1574
26	C	-0.0991	-0.6504	1.8450
27	C	1.0739	0.0543	1.2187
28	C	1.2940	-0.3834	-0.2502
29	C	-0.0244	-0.1355	-1.0221
30	C	-1.3090	-0.0970	-0.2312
31	C	-1.2931	-0.7176	1.1069
32	C	-2.3813	-1.4323	1.6274
33	C	-2.3045	-2.0180	2.8851
34	C	-2.3466	0.5168	-0.8545
35	H	-2.1472	0.7725	-1.8920
36	C	2.4677	0.3758	-0.9842
37	H	2.0395	0.7075	-1.9304
38	O	-0.0246	0.0450	-2.2280
39	H	0.8922	1.1353	1.2155
40	H	1.9735	-0.1066	1.8059
41	H	-3.2840	-1.5362	1.0388
42	H	-3.1536	-2.5675	3.2757
43	C	-1.1341	-1.9088	3.6364
44	H	-1.0736	-2.3609	4.6202
45	C	-0.0345	-1.2367	3.1096
46	H	0.8885	-1.1724	3.6762
47	C	3.0432	1.5983	-0.3002
48	C	2.7419	2.8581	-0.7751
49	C	3.9258	1.4901	0.8134
50	C	3.2744	4.0345	-0.1866
51	H	2.0783	2.9640	-1.6284

52	C	4.4599	2.6066	1.4056
53	H	4.1719	0.5087	1.2018
54	C	2.9649	5.3322	-0.6715
55	C	4.1557	3.9092	0.9315
56	H	5.1298	2.5027	2.2532
57	C	3.4989	6.4511	-0.0791
58	H	2.2961	5.4272	-1.5208
59	C	4.6910	5.0836	1.5199
60	C	4.3708	6.3260	1.0278
61	H	3.2538	7.4367	-0.4588
62	H	5.3602	4.9848	2.3686
63	H	4.7859	7.2167	1.4861
64	C	-3.6658	0.9313	-0.3778
65	C	-4.6773	1.0929	-1.3124
66	C	-3.9462	1.2593	0.9837
67	C	-5.9787	1.5132	-0.9486
68	H	-4.4736	0.8831	-2.3580
69	C	-5.1883	1.6913	1.3624
70	H	-3.1573	1.1840	1.7194
71	C	-7.0237	1.6518	-1.8998
72	C	-6.2469	1.8192	0.4221
73	H	-5.3777	1.9510	2.3987
74	C	-8.2743	2.0693	-1.5131
75	H	-6.8187	1.4207	-2.9398
76	C	-7.5458	2.2498	0.7875
77	C	-8.5380	2.3710	-0.1571
78	H	-9.0651	2.1702	-2.2477
79	H	-7.7468	2.4839	1.8277
80	H	-9.5287	2.7007	0.1348
81	H	-1.9442	-4.3831	-2.3409
82	H	2.1413	-4.2211	1.9781

Ts4a

	Atom	X	Y	Z
1	C	0.9246	-2.5212	-0.7355
2	N	1.7657	-2.0793	-1.6993
3	C	2.9312	-1.4188	-1.4440
4	C	1.4556	-2.1252	-3.1555
5	C	2.5673	-1.2843	-3.7974
6	C	3.6849	-1.2479	-2.7376
7	H	3.4268	-1.6868	-0.5233
8	C	-0.3980	-3.0977	-0.8753
9	C	-0.7428	-3.6177	0.4008
10	N	0.3194	-3.4149	1.2695
11	C	1.3728	-2.7541	0.6555
12	C	-1.3376	-3.2013	-1.9085
13	C	-2.5654	-3.8149	-1.6634
14	C	-2.8761	-4.3212	-0.4006
15	C	-1.9630	-4.2241	0.6509
16	O	2.4390	-2.4859	1.2074
17	H	1.4754	-3.1737	-3.4678
18	H	0.4747	-1.6996	-3.3339
19	H	2.8980	-1.7059	-4.7472
20	H	2.1908	-0.2780	-3.9845
21	H	4.3905	-2.0778	-2.8674
22	H	4.2680	-0.3255	-2.7568
23	H	-1.1344	-2.8102	-2.8942
24	H	-3.8367	-4.7934	-0.2303
25	H	-2.2011	-4.6085	1.6358
26	C	-0.1594	0.0028	2.1098
27	C	1.1518	0.4132	1.4866
28	C	1.1946	0.3207	-0.0147
29	C	-0.0387	0.3225	-0.7927
30	C	-1.3289	0.4915	-0.0336
31	C	-1.3536	0.0330	1.3692
32	C	-2.5271	-0.4675	1.9623
33	C	-2.5349	-0.9127	3.2759
34	C	-2.3385	1.0543	-0.7418
35	H	-2.1176	1.1617	-1.8007
36	C	2.3823	0.4559	-0.7611
37	H	2.1805	0.8081	-1.7688
38	O	-0.0303	0.2847	-2.0327
39	H	1.4003	1.4430	1.7890
40	H	1.9344	-0.2143	1.9186
41	H	-3.4351	-0.5176	1.3763
42	H	-3.4534	-1.2902	3.7112
43	C	-1.3587	-0.8828	4.0277
44	H	-1.3573	-1.2208	5.0582
45	C	-0.1818	-0.4398	3.4364
46	H	0.7446	-0.4487	4.0022
47	C	3.6675	0.9689	-0.2078
48	C	4.2417	2.0798	-0.7987
49	C	4.3498	0.3570	0.8845
50	C	5.4567	2.6400	-0.3303
51	H	3.7441	2.5557	-1.6384
52	C	5.5320	0.8700	1.3549
53	H	3.9408	-0.5409	1.3311
54	C	6.0391	3.7914	-0.9231

55	C	6.1203	2.0241	0.7758
56	H	6.0388	0.3854	2.1833
57	C	7.2191	4.3077	-0.4454
58	H	5.5341	4.2605	-1.7612
59	C	7.3381	2.5805	1.2435
60	C	7.8758	3.6964	0.6484
61	H	7.6526	5.1885	-0.9056
62	H	7.8399	2.1098	2.0826
63	H	8.8066	4.1140	1.0155
64	C	-3.6443	1.5827	-0.3365
65	C	-4.6797	1.5793	-1.2573
66	C	-3.8773	2.1906	0.9346
67	C	-5.9590	2.1055	-0.9553
68	H	-4.5139	1.1517	-2.2414
69	C	-5.0968	2.7267	1.2498
70	H	-3.0665	2.2429	1.6491
71	C	-7.0296	2.0788	-1.8877
72	C	-6.1796	2.6925	0.3299
73	H	-5.2482	3.1970	2.2161
74	C	-8.2578	2.6033	-1.5645
75	H	-6.8618	1.6344	-2.8633
76	C	-7.4566	3.2272	0.6309
77	C	-8.4742	3.1831	-0.2931
78	H	-9.0675	2.5754	-2.2851
79	H	-7.6200	3.6742	1.6062
80	H	-9.4475	3.5947	-0.0504
81	H	-3.2886	-3.8935	-2.4665
82	H	0.3102	-3.5866	2.2620

Prod5a

	Atom	X	Y	Z
1	C	2.8439	-0.8711	-0.3049
2	N	3.9847	-0.1832	0.2746
3	C	3.7541	1.2846	0.3132
4	C	5.3415	-0.4707	-0.2277
5	C	6.0487	0.8982	-0.2179
6	C	4.9075	1.8920	-0.4956
7	H	3.8414	1.6207	1.3540
8	C	2.7444	-2.3403	0.0701
9	C	2.4801	-3.0993	-1.0788
10	N	2.4617	-2.2588	-2.2017
11	C	2.8765	-0.9806	-1.8869
12	C	2.9643	-2.9875	1.2734
13	C	2.8465	-4.3805	1.3373
14	C	2.5263	-5.1122	0.1966
15	C	2.3486	-4.4794	-1.0375
16	O	3.2429	-0.1481	-2.6829
17	H	5.8482	-1.2051	0.4051
18	H	5.3167	-0.8690	-1.2490
19	H	6.4869	1.0902	0.7670
20	H	6.8536	0.9493	-0.9540
21	H	5.1457	2.9144	-0.1940
22	H	4.6559	1.8877	-1.5589
23	H	3.2388	-2.4191	2.1525
24	H	2.4318	-6.1905	0.2573
25	H	2.1389	-5.0518	-1.9338
26	C	0.3897	-1.1439	2.0234
27	C	1.3108	-0.0138	1.6435
28	C	1.6393	0.0912	0.1348
29	C	0.3630	-0.0930	-0.7167
30	C	-0.8555	-0.6997	-0.0712
31	C	-0.6653	-1.4854	1.1617
32	C	-1.4696	-2.5931	1.4761
33	C	-1.2915	-3.2882	2.6640
34	C	-2.0231	-0.4329	-0.7115
35	H	-1.8910	0.0519	-1.6754
36	C	2.3205	1.4769	-0.2056
37	H	2.3686	1.5016	-1.2933
38	O	0.3364	0.3069	-1.8652
39	H	0.8306	0.9273	1.9334
40	H	2.2383	-0.0766	2.2154
41	H	-2.2381	-2.9064	0.7810
42	H	-1.9236	-4.1390	2.8913
43	C	-0.2974	-2.8910	3.5589
44	H	-0.1622	-3.4197	4.4958
45	C	0.5426	-1.8343	3.2275
46	H	1.3408	-1.5467	3.9045
47	H	3.0079	-4.8919	2.2787
48	C	1.5927	2.7338	0.2329
49	C	0.7664	3.3762	-0.6686
50	C	1.7323	3.3007	1.5315
51	C	0.0566	4.5566	-0.3336
52	H	0.6484	2.9640	-1.6650
53	C	1.0637	4.4461	1.8887
54	H	2.3852	2.8306	2.2568

55	C	-0.7960	5.2138	-1.2600
56	C	0.2053	5.1090	0.9762
57	H	1.1913	4.8610	2.8836
58	C	-1.4683	6.3583	-0.9073
59	H	-0.9081	4.7939	-2.2541
60	C	-0.5019	6.2933	1.3090
61	C	-1.3201	6.9040	0.3901
62	H	-2.1173	6.8500	-1.6234
63	H	-0.3860	6.7101	2.3043
64	H	-1.8566	7.8082	0.6550
65	C	-3.4211	-0.6348	-0.3295
66	C	-4.3651	-0.7596	-1.3371
67	C	-3.8765	-0.6170	1.0240
68	C	-5.7431	-0.9279	-1.0608
69	H	-4.0428	-0.7379	-2.3736
70	C	-5.2053	-0.7516	1.3218
71	H	-3.1596	-0.4726	1.8208
72	C	-6.7082	-1.0864	-2.0899
73	C	-6.1791	-0.9267	0.3009
74	H	-5.5340	-0.7185	2.3554
75	C	-8.0395	-1.2398	-1.7868
76	H	-6.3764	-1.0857	-3.1230
77	C	-7.5589	-1.0841	0.5796
78	C	-8.4691	-1.2388	-0.4397
79	H	-8.7675	-1.3614	-2.5809
80	H	-7.8882	-1.0803	1.6135
81	H	-9.5226	-1.3594	-0.2138
82	H	2.4836	-2.5858	-3.1568

Ts5a

	Atom	X	Y	Z
1	C	1.0213	-2.2198	-1.4017
2	N	1.7463	-1.4678	-2.2570
3	C	2.8494	-0.7415	-1.8979
4	C	1.3273	-1.1782	-3.6675
5	C	2.2291	-0.0117	-4.0765
6	C	3.4483	-0.1302	-3.1426
7	H	3.5025	-1.1730	-1.1553
8	C	1.4653	-2.9683	-0.2406
9	C	0.3559	-3.7504	0.1841
10	N	-0.7120	-3.5122	-0.6650
11	C	-0.3816	-2.6356	-1.6929
12	C	2.6762	-3.1183	0.4460
13	C	2.7608	-4.0061	1.5217
14	C	1.6499	-4.7433	1.9283
15	C	0.4314	-4.6250	1.2547
16	O	-1.1285	-2.3168	-2.6009
17	H	1.5247	-2.0853	-4.2481
18	H	0.2675	-0.9587	-3.7006
19	H	2.5002	-0.0591	-5.1319
20	H	1.7009	0.9246	-3.8956
21	H	4.2104	-0.7996	-3.5606
22	H	3.9359	0.8243	-2.9369
23	H	3.5647	-2.5785	0.1494
24	H	1.7301	-5.4211	2.7701
25	H	-0.4318	-5.2059	1.5576
26	C	-0.3485	-0.5901	1.9179
27	C	0.9670	-0.0313	1.4305
28	C	1.0105	0.3299	-0.0284
29	C	-0.2242	0.5212	-0.7839
30	C	-1.5264	0.4181	-0.0340
31	C	-1.5412	-0.3864	1.2024
32	C	-2.7091	-1.0354	1.6465
33	C	-2.7154	-1.7918	2.8088
34	C	-2.5591	1.0899	-0.6000
35	H	-2.3332	1.4701	-1.5928
36	C	2.1820	0.7557	-0.7020
37	H	1.9239	1.3797	-1.5523
38	O	-0.2039	0.8605	-1.9745
39	H	1.2374	0.8528	2.0296
40	H	1.7358	-0.7753	1.6594
41	H	-3.6162	-0.9460	1.0639
42	H	-3.6307	-2.2751	3.1323
43	C	-1.5424	-1.9334	3.5525
44	H	-1.5378	-2.5183	4.4655
45	C	-0.3706	-1.3472	3.0936
46	H	0.5548	-1.4934	3.6415
47	H	3.7043	-4.1208	2.0424
48	C	3.4258	1.2216	-0.0241
49	C	3.9468	2.4517	-0.3857
50	C	4.1303	0.4645	0.9565
51	C	5.1256	2.9779	0.1990
52	H	3.4317	3.0491	-1.1316
53	C	5.2788	0.9401	1.5377
54	H	3.7605	-0.5091	1.2497

55	C	5.6499	4.2469	-0.1636
56	C	5.8128	2.2061	1.1864
57	H	5.7963	0.3429	2.2816
58	C	6.7965	4.7265	0.4212
59	H	5.1274	4.8348	-0.9111
60	C	6.9948	2.7290	1.7702
61	C	7.4764	3.9606	1.3973
62	H	7.1858	5.6976	0.1369
63	H	7.5137	2.1398	2.5192
64	H	8.3801	4.3517	1.8508
65	C	-3.8967	1.4310	-0.1064
66	C	-4.9311	1.5656	-1.0183
67	C	-4.1652	1.7281	1.2645
68	C	-6.2406	1.9316	-0.6228
69	H	-4.7401	1.3748	-2.0698
70	C	-5.4153	2.1057	1.6753
71	H	-3.3573	1.6707	1.9823
72	C	-7.3092	2.0428	-1.5511
73	C	-6.4953	2.2077	0.7570
74	H	-5.5944	2.3416	2.7194
75	C	-8.5676	2.4062	-1.1356
76	H	-7.1155	1.8337	-2.5981
77	C	-7.8029	2.5830	1.1525
78	C	-8.8176	2.6791	0.2292
79	H	-9.3754	2.4860	-1.8544
80	H	-7.9924	2.7944	2.1999
81	H	-9.8145	2.9661	0.5444
82	H	-1.6348	-3.9070	-0.5832

Prod4b

	Atom	X	Y	Z
1	C	1.5844	-1.3724	-0.3068
2	N	2.7427	-1.3745	-1.2001
3	C	3.3947	-0.0593	-1.0791
4	C	2.6138	-1.6832	-2.6363
5	C	3.9625	-1.1957	-3.1698
6	C	4.2201	0.1057	-2.3762
7	H	4.0296	-0.0585	-0.1941
8	C	0.6029	-2.5076	-0.5856
9	C	0.6983	-3.4555	0.4447
10	N	1.6310	-3.0281	1.3909
11	C	2.1849	-1.8122	1.0769
12	C	-0.2618	-2.7552	-1.6438
13	C	-1.0257	-3.9282	-1.6514
14	C	-0.9199	-4.8491	-0.6132
15	C	-0.0494	-4.6236	0.4552
16	O	3.0164	-1.2322	1.7438
17	H	2.4578	-2.7524	-2.7867
18	H	1.7933	-1.1378	-3.1207
19	H	4.7341	-1.9355	-2.9417
20	H	3.9498	-1.0402	-4.2508
21	H	5.2808	0.2556	-2.1690
22	H	3.8745	0.9789	-2.9354
23	H	-0.3556	-2.0514	-2.4592
24	H	-1.5169	-5.7539	-0.6305
25	H	0.0398	-5.3389	1.2646
26	C	-0.5137	-0.1226	1.7277
27	C	0.6624	0.6390	1.1786
28	C	1.0462	0.1596	-0.2427
29	C	-0.2073	0.2881	-1.1409
30	C	-1.5594	0.2675	-0.4716
31	C	-1.6266	-0.3017	0.8889
32	C	-2.7069	-1.0732	1.3399
33	C	-2.7069	-1.6065	2.6228
34	C	-2.5704	0.7925	-1.2082
35	H	-2.2895	1.0301	-2.2313
36	C	-3.9536	1.1339	-0.8735
37	C	2.2352	0.9650	-0.8981
38	C	2.6494	2.2618	-0.2337
39	H	1.8854	1.2136	-1.9008
40	O	-0.1065	0.4241	-2.3486
41	C	-4.3910	1.4916	0.4149
42	C	-5.7070	1.8648	0.6414
43	C	-6.6502	1.8899	-0.3957
44	C	-6.2152	1.5520	-1.6795
45	C	-4.8920	1.1979	-1.9170
46	C	3.4267	2.2999	0.9331
47	C	3.8028	3.5114	1.5036
48	C	3.4246	4.7336	0.9366
49	C	2.6496	4.6970	-0.2242
50	C	2.2727	3.4848	-0.7986
51	H	0.4095	1.7032	1.1092
52	H	1.5134	0.5669	1.8500
53	H	-3.5433	-1.2600	0.6783
54	H	-3.5489	-2.2014	2.9584

55	H	-3.6888	1.4953	1.2380
56	H	-6.0109	2.1499	1.6438
57	H	-6.9168	1.5796	-2.5068
58	H	-4.5745	0.9607	-2.9270
59	H	3.7315	1.3741	1.4080
60	H	4.4022	3.5070	2.4091
61	H	2.3378	5.6272	-0.6892
62	H	1.6732	3.4879	-1.7036
63	C	-1.6214	-1.3864	3.4714
64	H	-1.6217	-1.7973	4.4750
65	C	-0.5266	-0.6566	3.0173
66	H	0.3342	-0.5065	3.6605
67	C	3.8644	6.0429	1.5464
68	H	3.8360	6.0038	2.6385
69	H	4.8925	6.2875	1.2571
70	H	3.2271	6.8681	1.2210
71	C	-8.0854	2.2666	-0.1258
72	H	-8.6205	2.4890	-1.0511
73	H	-8.6173	1.4512	0.3765
74	H	-8.1514	3.1435	0.5239
75	H	-1.7030	-4.1180	-2.4756
76	H	1.8972	-3.5335	2.2219

TS4b

	Atom	X	Y	Z
1	C	-1.0511	2.1580	-0.4598
2	N	-1.9222	1.8060	-1.4346
3	C	-3.0221	1.0284	-1.2222
4	C	-1.7095	2.0932	-2.8802
5	C	-2.8036	1.2790	-3.5840
6	C	-3.8460	1.0012	-2.4840
7	H	-3.4735	1.1148	-0.2456
8	C	0.2217	2.8413	-0.5789
9	C	0.6144	3.1854	0.7422
10	N	-0.3759	2.7793	1.6241
11	C	-1.4240	2.1464	0.9717
12	C	1.0856	3.1660	-1.6322
13	C	2.2863	3.8207	-1.3609
14	C	2.6452	4.1509	-0.0533
15	C	1.8085	3.8316	1.0177
16	O	-2.4344	1.7233	1.5319
17	H	-1.8165	3.1725	-3.0258
18	H	-0.7168	1.7724	-3.1747
19	H	-3.2212	1.8132	-4.4382
20	H	-2.3757	0.3428	-3.9443
21	H	-4.6091	1.7883	-2.4448
22	H	-4.3697	0.0528	-2.6149
23	H	0.8446	2.9149	-2.6542
24	H	3.5838	4.6587	0.1366
25	H	2.0848	4.0780	2.0362
26	C	0.3624	-0.6768	1.9037
27	C	-0.9575	-1.0780	1.2930
28	C	-1.0954	-0.7719	-0.1734
29	C	0.0864	-0.5675	-1.0034
30	C	1.4288	-0.7555	-0.3461
31	C	1.5097	-0.5135	1.1090
32	C	2.6838	-0.0290	1.7139
33	C	2.7420	0.2156	3.0777
34	C	2.4244	-1.1357	-1.1829
35	H	2.1425	-1.1041	-2.2325
36	C	3.7863	-1.6217	-0.9357
37	C	-2.3160	-0.8799	-0.8693
38	C	-3.5271	-1.5670	-0.3367
39	H	-2.1542	-1.0598	-1.9285
40	O	-0.0010	-0.3447	-2.2207
41	C	4.1478	-2.4022	0.1767
42	C	5.4387	-2.8906	0.3178
43	C	6.4310	-2.6213	-0.6344
44	C	6.0706	-1.8621	-1.7502
45	C	4.7733	-1.3853	-1.9058
46	C	-4.1852	-1.2007	0.8477
47	C	-5.3144	-1.8892	1.2785
48	C	-5.8367	-2.9660	0.5540
49	C	-5.1925	-3.3206	-0.6339
50	C	-4.0659	-2.6316	-1.0735
51	H	-1.1297	-2.1544	1.4523
52	H	-1.7480	-0.5710	1.8509
53	H	3.5524	0.1657	1.0994
54	H	3.6603	0.5860	3.5198

55	H	3.4033	-2.6412	0.9254
56	H	5.6820	-3.5015	1.1819
57	H	6.8114	-1.6510	-2.5150
58	H	4.5153	-0.8137	-2.7913
59	H	-3.8291	-0.3549	1.4235
60	H	-5.8047	-1.5765	2.1953
61	H	-5.5780	-4.1440	-1.2271
62	H	-3.5863	-2.9303	-2.0001
63	C	1.6161	-0.0062	3.8737
64	H	1.6551	0.1737	4.9425
65	C	0.4360	-0.4362	3.2801
66	H	-0.4546	-0.5754	3.8849
67	C	7.8389	-3.1322	-0.4520
68	H	7.8451	-4.1682	-0.1023
69	H	8.4036	-3.0871	-1.3856
70	H	8.3814	-2.5369	0.2909
71	C	-7.0428	-3.7265	1.0491
72	H	-7.7562	-3.0639	1.5456
73	H	-7.5612	-4.2300	0.2301
74	H	-6.7529	-4.4944	1.7750
75	H	2.9508	4.0705	-2.1796
76	H	-0.3127	2.7956	2.6293

Prod5b

	Atom	X	Y	Z
1	C	2.3535	-0.5770	-0.1618
2	N	3.4063	0.1571	0.5191
3	C	3.1479	1.6202	0.4685
4	C	4.8178	-0.1209	0.1941
5	C	5.4961	1.2620	0.2333
6	C	4.3806	2.2198	-0.2201
7	H	3.1019	1.9985	1.4973
8	C	2.2301	-2.0317	0.2606
9	C	2.1177	-2.8414	-0.8787
10	N	2.2259	-2.0479	-2.0300
11	C	2.5789	-0.7496	-1.7222
12	C	2.3082	-2.6255	1.5082
13	C	2.2002	-4.0167	1.6165
14	C	2.0312	-4.7995	0.4775
15	C	1.9986	-4.2207	-0.7948
16	O	3.0288	0.0563	-2.5026
17	H	5.2570	-0.8200	0.9119
18	H	4.9226	-0.5578	-0.8061
19	H	5.8084	1.5010	1.2552
20	H	6.3834	1.3018	-0.4019
21	H	4.5636	3.2580	0.0655
22	H	4.2594	2.1685	-1.3048
23	H	2.4654	-2.0172	2.3894
24	H	1.9427	-5.8760	0.5720
25	H	1.9068	-4.8326	-1.6849
26	C	-0.3602	-0.7881	1.8817
27	C	0.5970	0.3298	1.5589
28	C	1.0908	0.3760	0.0931
29	C	-0.0755	0.1295	-0.8898
30	C	-1.3638	-0.4380	-0.3552
31	C	-1.3153	-1.1684	0.9257
32	C	-2.1520	-2.2631	1.1971
33	C	-2.1048	-2.9082	2.4247
34	C	-2.4516	-0.1882	-1.1279
35	H	-2.2091	0.2570	-2.0896
36	C	-3.8867	-0.3628	-0.8961
37	C	1.7851	1.7620	-0.2263
38	C	0.9889	3.0193	0.0671
39	H	1.9632	1.7413	-1.3009
40	O	0.0363	0.4534	-2.0571
41	C	-4.4961	-0.2845	0.3693
42	C	-5.8721	-0.3886	0.5042
43	C	-6.7040	-0.5867	-0.6069
44	C	-6.1035	-0.6473	-1.8668
45	C	-4.7265	-0.5205	-2.0109
46	C	0.2188	3.5868	-0.9591
47	C	-0.5302	4.7387	-0.7498
48	C	-0.5375	5.3837	0.4918
49	C	0.2330	4.8263	1.5133
50	C	0.9814	3.6681	1.3074
51	H	0.0885	1.2803	1.7547
52	H	1.4555	0.2952	2.2317
53	H	-2.8439	-2.6040	0.4376
54	H	-2.7599	-3.7503	2.6175

55	H	-3.8866	-0.1207	1.2483
56	H	-6.3145	-0.3086	1.4923
57	H	-6.7219	-0.7808	-2.7485
58	H	-4.2871	-0.5486	-3.0026
59	H	0.2076	3.1077	-1.9314
60	H	-1.1161	5.1469	-1.5678
61	H	0.2528	5.3038	2.4881
62	H	1.5678	3.2791	2.1314
63	C	-1.2119	-2.4727	3.4049
64	H	-1.1799	-2.9620	4.3720
65	C	-0.3395	-1.4284	3.1230
66	H	0.3812	-1.1106	3.8699
67	C	-8.1958	-0.7327	-0.4395
68	H	-8.7184	-0.6051	-1.3896
69	H	-8.4520	-1.7247	-0.0516
70	H	-8.5911	0.0022	0.2670
71	C	-1.3311	6.6500	0.7051
72	H	-1.4218	6.8893	1.7668
73	H	-0.8525	7.5038	0.2133
74	H	-2.3395	6.5623	0.2914
75	H	2.2508	-4.4862	2.5916
76	H	2.3669	-2.4125	-2.9609

TS5b

	Atom	X	Y	Z
1	C	1.1647	1.7253	1.3696
2	N	1.8910	0.9105	2.1649
3	C	2.9004	0.1015	1.7189
4	C	1.5592	0.6425	3.6022
5	C	2.3951	-0.5947	3.9376
6	C	3.5445	-0.5640	2.9126
7	H	3.5254	0.4839	0.9270
8	C	1.5774	2.4450	0.1793
9	C	0.5060	3.3183	-0.1564
10	N	-0.5088	3.1603	0.7726
11	C	-0.1726	2.2501	1.7694
12	C	2.7385	2.4999	-0.6010
13	C	2.8117	3.3867	-1.6785
14	C	1.7373	4.2164	-1.9949
15	C	0.5695	4.1927	-1.2280
16	O	-0.8712	1.9853	2.7319
17	H	1.8705	1.5261	4.1691
18	H	0.4910	0.5059	3.7156
19	H	2.7491	-0.5778	4.9692
20	H	1.7824	-1.4851	3.7953
21	H	4.3859	0.0416	3.2718
22	H	3.9391	-1.5518	2.6688
23	H	3.5991	1.8850	-0.3775
24	H	1.8070	4.8922	-2.8393
25	H	-0.2643	4.8443	-1.4614
26	C	-0.5723	0.2383	-1.8405
27	C	0.7290	-0.4235	-1.4542
28	C	0.8499	-0.8059	-0.0057
29	C	-0.3373	-0.9074	0.8391
30	C	-1.6793	-0.6989	0.1879
31	C	-1.7222	0.1176	-1.0415
32	C	-2.8658	0.8577	-1.3969
33	C	-2.8972	1.6265	-2.5502
34	C	-2.7139	-1.3022	0.8220
35	H	-2.4426	-1.7146	1.7907
36	C	-4.1080	-1.5378	0.4303
37	C	2.0319	-1.3274	0.5753
38	C	3.1786	-1.8863	-0.1980
39	H	1.7897	-1.9359	1.4416
40	O	-0.2546	-1.2576	2.0237
41	C	-4.5107	-1.8134	-0.8883
42	C	-5.8352	-2.1010	-1.1858
43	C	-6.8204	-2.1208	-0.1896
44	C	-6.4203	-1.8655	1.1244
45	C	-5.0909	-1.5951	1.4312
46	C	3.6262	-3.1772	0.1252
47	C	4.6893	-3.7695	-0.5475
48	C	5.3660	-3.0944	-1.5675
49	C	4.9309	-1.8054	-1.8872
50	C	3.8640	-1.2116	-1.2189
51	H	0.8902	-1.3172	-2.0780
52	H	1.5335	0.2642	-1.7315
53	H	-3.7347	0.8262	-0.7534
54	H	-3.7939	2.1813	-2.8039

55	H	-3.7729	-1.8192	-1.6809
56	H	-6.1113	-2.3232	-2.2121
57	H	-7.1564	-1.8906	1.9218
58	H	-4.8035	-1.4178	2.4622
59	H	3.1164	-3.7310	0.9067
60	H	4.9962	-4.7747	-0.2756
61	H	5.4337	-1.2536	-2.6754
62	H	3.5696	-0.2090	-1.5018
63	C	-1.7730	1.6884	-3.3761
64	H	-1.7890	2.2823	-4.2831
65	C	-0.6202	1.0095	-3.0067
66	H	0.2726	1.0919	-3.6184
67	C	6.5407	-3.7234	-2.2762
68	H	7.4752	-3.5326	-1.7367
69	H	6.4255	-4.8071	-2.3537
70	H	6.6588	-3.3226	-3.2855
71	C	-8.2629	-2.4018	-0.5313
72	H	-8.3494	-3.2073	-1.2656
73	H	-8.8339	-2.6887	0.3543
74	H	-8.7457	-1.5176	-0.9624
75	H	3.7174	3.4270	-2.2722
76	H	-1.4005	3.6281	0.7631

TS4c

	Atom	X	Y	Z
1	C	-1.0576	2.1383	-0.4831
2	N	-1.9179	1.7723	-1.4616
3	C	-3.0196	0.9974	-1.2514
4	C	-1.6926	2.0449	-2.9087
5	C	-2.7735	1.2147	-3.6137
6	C	-3.8278	0.9486	-2.5224
7	H	-3.4820	1.0967	-0.2812
8	C	0.2111	2.8305	-0.5971
9	C	0.5889	3.1894	0.7243
10	N	-0.4055	2.7818	1.6013
11	C	-1.4427	2.1363	0.9458
12	C	1.0809	3.1545	-1.6457
13	C	2.2732	3.8222	-1.3695
14	C	2.6176	4.1664	-0.0616
15	C	1.7746	3.8487	1.0048
16	O	-2.4551	1.7101	1.5003
17	H	-1.8067	3.1217	-3.0667
18	H	-0.6946	1.7289	-3.1895
19	H	-3.1831	1.7339	-4.4807
20	H	-2.3359	0.2756	-3.9540
21	H	-4.5948	1.7327	-2.5037
22	H	-4.3465	-0.0035	-2.6467
23	H	0.8505	2.8943	-2.6679
24	H	3.5495	4.6849	0.1321
25	H	2.0394	4.1071	2.0234
26	C	0.3701	-0.6644	1.9112
27	C	-0.9484	-1.0799	1.3066
28	C	-1.0903	-0.7898	-0.1630
29	C	0.0891	-0.5919	-0.9972
30	C	1.4335	-0.7638	-0.3388
31	C	1.5150	-0.5021	1.1128
32	C	2.6867	-0.0024	1.7099
33	C	2.7460	0.2564	3.0710
34	C	2.4287	-1.1523	-1.1712
35	H	2.1460	-1.1390	-2.2210
36	C	3.7931	-1.6289	-0.9156
37	C	-2.3105	-0.9097	-0.8562
38	C	-3.5212	-1.5859	-0.3086
39	H	-2.1514	-1.1062	-1.9128
40	O	-0.0002	-0.3871	-2.2173
41	C	4.1495	-2.3956	0.2081
42	C	5.4414	-2.8789	0.3702
43	C	6.3924	-2.5925	-0.5995
44	C	6.0826	-1.8565	-1.7320
45	C	4.7808	-1.3930	-1.8877
46	C	-4.1764	-1.1872	0.8679
47	C	-5.3041	-1.8617	1.3264
48	C	-5.7836	-2.9419	0.6017
49	C	-5.1764	-3.3603	-0.5712
50	C	-4.0526	-2.6728	-1.0204
51	H	-1.1129	-2.1558	1.4773
52	H	-1.7404	-0.5723	1.8615
53	H	3.5522	0.1944	1.0915
54	H	3.6622	0.6384	3.5074

55	H	3.4027	-2.6268	0.9562
56	H	5.7182	-3.4782	1.2288
57	H	6.8479	-1.6654	-2.4739
58	H	4.5216	-0.8288	-2.7767
59	H	-3.8178	-0.3275	1.4204
60	H	-5.8157	-1.5555	2.2306
61	H	-5.5818	-4.2048	-1.1147
62	H	-3.5681	-2.9949	-1.9358
63	C	1.6235	0.0340	3.8714
64	H	1.6637	0.2243	4.9383
65	C	0.4450	-0.4098	3.2849
66	H	-0.4430	-0.5492	3.8934
67	H	2.9421	4.0724	-2.1845
68	F	7.6522	-3.0570	-0.4405
69	F	-6.8791	-3.5989	1.0463
70	H	-0.3557	2.8163	2.6068

Prod5c

	Atom	X	Y	Z
1	C	1.1656	1.6898	1.3931
2	N	1.8906	0.8595	2.1724
3	C	2.9034	0.0626	1.7133
4	C	1.5575	0.5629	3.6044
5	C	2.3943	-0.6797	3.9163
6	C	3.5454	-0.6270	2.8941
7	H	3.5288	0.4620	0.9303
8	C	1.5793	2.4338	0.2182
9	C	0.5079	3.3132	-0.1006
10	N	-0.5086	3.1352	0.8231
11	C	-0.1737	2.2054	1.8015
12	C	2.7421	2.5063	-0.5584
13	C	2.8165	3.4155	-1.6168
14	C	1.7416	4.2504	-1.9177
15	C	0.5725	4.2098	-1.1536
16	O	-0.8733	1.9188	2.7565
17	H	1.8676	1.4358	4.1881
18	H	0.4893	0.4234	3.7139
19	H	2.7467	-0.6828	4.9484
20	H	1.7830	-1.5679	3.7556
21	H	4.3859	-0.0287	3.2672
22	H	3.9414	-1.6095	2.6317
23	H	3.6040	1.8897	-0.3443
24	H	1.8123	4.9441	-2.7473
25	H	-0.2610	4.8661	-1.3745
26	C	-0.5781	0.2676	-1.8434
27	C	0.7260	-0.3981	-1.4729
28	C	0.8499	-0.8131	-0.0336
29	C	-0.3342	-0.9323	0.8122
30	C	-1.6785	-0.7073	0.1704
31	C	-1.7250	0.1331	-1.0426
32	C	-2.8693	0.8808	-1.3798
33	C	-2.9051	1.6697	-2.5193
34	C	-2.7106	-1.3219	0.7965
35	H	-2.4365	-1.7558	1.7548
36	C	-4.1071	-1.5455	0.4039
37	C	2.0327	-1.3458	0.5345
38	C	3.1779	-1.8871	-0.2528
39	H	1.7936	-1.9717	1.3890
40	O	-0.2490	-1.3093	1.9883
41	C	-4.5070	-1.8011	-0.9197
42	C	-5.8322	-2.0762	-1.2316
43	C	-6.7724	-2.0937	-0.2106
44	C	-6.4215	-1.8648	1.1103
45	C	-5.0878	-1.6072	1.4090
46	C	3.6274	-3.1841	0.0469
47	C	4.6908	-3.7685	-0.6336
48	C	5.3251	-3.0390	-1.6263
49	C	4.9255	-1.7520	-1.9498
50	C	3.8571	-1.1849	-1.2610
51	H	0.8908	-1.2756	-2.1184
52	H	1.5261	0.3012	-1.7342
53	H	-3.7348	0.8412	-0.7323
54	H	-3.8019	2.2302	-2.7591

55	H	-3.7685	-1.7971	-1.7109
56	H	-6.1438	-2.2838	-2.2479
57	H	-7.1810	-1.9001	1.8814
58	H	-4.7971	-1.4404	2.4403
59	H	3.1223	-3.7520	0.8203
60	H	5.0286	-4.7718	-0.4054
61	H	5.4486	-1.2100	-2.7279
62	H	3.5594	-0.1767	-1.5175
63	C	-1.7844	1.7442	-3.3490
64	H	-1.8040	2.3531	-4.2459
65	C	-0.6305	1.0586	-2.9962
66	H	0.2595	1.1510	-3.6104
67	H	3.7235	3.4702	-2.2073
68	F	-8.0642	-2.3551	-0.5130
69	F	6.3618	-3.5935	-2.2927
70	H	-1.3985	3.6068	0.8245

TS5c

	Atom	X	Y	Z
1	C	1.1656	1.6898	1.3931
2	N	1.8906	0.8595	2.1724
3	C	2.9034	0.0626	1.7133
4	C	1.5575	0.5629	3.6044
5	C	2.3943	-0.6797	3.9163
6	C	3.5454	-0.6270	2.8941
7	H	3.5288	0.4620	0.9303
8	C	1.5793	2.4338	0.2182
9	C	0.5079	3.3132	-0.1006
10	N	-0.5086	3.1352	0.8231
11	C	-0.1737	2.2054	1.8015
12	C	2.7421	2.5063	-0.5584
13	C	2.8165	3.4155	-1.6168
14	C	1.7416	4.2504	-1.9177
15	C	0.5725	4.2098	-1.1536
16	O	-0.8733	1.9188	2.7565
17	H	1.8676	1.4358	4.1881
18	H	0.4893	0.4234	3.7139
19	H	2.7467	-0.6828	4.9484
20	H	1.7830	-1.5679	3.7556
21	H	4.3859	-0.0287	3.2672
22	H	3.9414	-1.6095	2.6317
23	H	3.6040	1.8897	-0.3443
24	H	1.8123	4.9441	-2.7473
25	H	-0.2610	4.8661	-1.3745
26	C	-0.5781	0.2676	-1.8434
27	C	0.7260	-0.3981	-1.4729
28	C	0.8499	-0.8131	-0.0336
29	C	-0.3342	-0.9323	0.8122
30	C	-1.6785	-0.7073	0.1704
31	C	-1.7250	0.1331	-1.0426
32	C	-2.8693	0.8808	-1.3798
33	C	-2.9051	1.6697	-2.5193
34	C	-2.7106	-1.3219	0.7965
35	H	-2.4365	-1.7558	1.7548
36	C	-4.1071	-1.5455	0.4039
37	C	2.0327	-1.3458	0.5345
38	C	3.1779	-1.8871	-0.2528
39	H	1.7936	-1.9717	1.3890
40	O	-0.2490	-1.3093	1.9883
41	C	-4.5070	-1.8011	-0.9197
42	C	-5.8322	-2.0762	-1.2316
43	C	-6.7724	-2.0937	-0.2106
44	C	-6.4215	-1.8648	1.1103
45	C	-5.0878	-1.6072	1.4090
46	C	3.6274	-3.1841	0.0469
47	C	4.6908	-3.7685	-0.6336
48	C	5.3251	-3.0390	-1.6263
49	C	4.9255	-1.7520	-1.9498
50	C	3.8571	-1.1849	-1.2610
51	H	0.8908	-1.2756	-2.1184
52	H	1.5261	0.3012	-1.7342
53	H	-3.7348	0.8412	-0.7323
54	H	-3.8019	2.2302	-2.7591

55	H	-3.7685	-1.7971	-1.7109
56	H	-6.1438	-2.2838	-2.2479
57	H	-7.1810	-1.9001	1.8814
58	H	-4.7971	-1.4404	2.4403
59	H	3.1223	-3.7520	0.8203
60	H	5.0286	-4.7718	-0.4054
61	H	5.4486	-1.2100	-2.7279
62	H	3.5594	-0.1767	-1.5175
63	C	-1.7844	1.7442	-3.3490
64	H	-1.8040	2.3531	-4.2459
65	C	-0.6305	1.0586	-2.9962
66	H	0.2595	1.1510	-3.6104
67	H	3.7235	3.4702	-2.2073
68	F	-8.0642	-2.3551	-0.5130
69	F	6.3618	-3.5935	-2.2927
70	H	-1.3985	3.6068	0.8245

Prod4d

	Atom	X	Y	Z
1	C	1.5657	-1.5632	-0.2924
2	N	2.6790	-1.6726	-1.2292
3	C	3.3972	-0.3898	-1.2292
4	C	2.4964	-2.1036	-2.6277
5	C	3.8406	-1.7055	-3.2403
6	C	4.1488	-0.3436	-2.5800
7	H	4.0865	-0.3671	-0.3858
8	C	0.5299	-2.6726	-0.4475
9	C	0.6311	-3.5447	0.6470
10	N	1.6179	-3.0869	1.5233
11	C	2.2047	-1.9237	1.0971
12	C	-0.3833	-2.9630	-1.4529
13	C	-1.1907	-4.1010	-1.3436
14	C	-1.0791	-4.9453	-0.2425
15	C	-0.1591	-4.6772	0.7732
16	O	3.0834	-1.3259	1.6839
17	H	2.3070	-3.1766	-2.6768
18	H	1.6772	-1.5786	-3.1358
19	H	4.6007	-2.4405	-2.9637
20	H	3.8010	-1.6502	-4.3300
21	H	5.2195	-0.1818	-2.4476
22	H	3.7714	0.4770	-3.1958
23	H	-0.4795	-2.3217	-2.3182
24	H	-1.7094	-5.8242	-0.1699
25	H	-0.0645	-5.3345	1.6297
26	C	-0.4504	-0.1025	1.6926
27	C	0.7492	0.5721	1.0824
28	C	1.0925	-0.0076	-0.3122
29	C	-0.1668	0.1135	-1.2002
30	C	-1.5118	0.1863	-0.5119
31	C	-1.5818	-0.2922	0.8815
32	C	-2.6878	-0.9840	1.3952
33	C	-2.6924	-1.4264	2.7119
34	C	-2.5110	0.7041	-1.2662
35	H	-2.2448	0.8697	-2.3071
36	C	-3.8753	1.1108	-0.9189
37	C	2.3004	0.7052	-1.0377
38	C	2.8172	1.9889	-0.4248
39	H	1.9292	0.9480	-2.0336
40	O	-0.0839	0.1715	-2.4138
41	C	-4.2398	1.6168	0.3420
42	C	-5.5337	2.0422	0.5921
43	C	-6.5099	1.9667	-0.4143
44	C	-6.1586	1.4810	-1.6811
45	C	-4.8556	1.0764	-1.9270
46	C	3.6168	1.9998	0.7291
47	C	4.0985	3.1908	1.2545
48	C	3.7922	4.4107	0.6340
49	C	2.9981	4.4150	-0.5198
50	C	2.5238	3.2154	-1.0353
51	H	0.5413	1.6411	0.9562
52	H	1.6045	0.5004	1.7483
53	H	-3.5388	-1.1844	0.7567
54	H	-3.5530	-1.9608	3.0975

55	H	-3.4983	1.6895	1.1260
56	H	-5.7989	2.4394	1.5640
57	H	-6.9053	1.4343	-2.4640
58	H	-4.5866	0.7181	-2.9143
59	H	3.8565	1.0672	1.2261
60	H	4.7139	3.1851	2.1458
61	H	2.7623	5.3538	-1.0056
62	H	1.9152	3.2289	-1.9331
63	C	-1.5871	-1.1931	3.5310
64	H	-1.5914	-1.5320	4.5609
65	C	-0.4686	-0.5440	3.0163
66	H	0.4045	-0.3850	3.6403
67	H	-1.9050	-4.3257	-2.1266
68	C	4.2879	5.6392	1.1734
69	N	4.6872	6.6317	1.6099
70	C	-7.8486	2.3941	-0.1522
71	N	-8.9312	2.7371	0.0605
72	H	1.9039	-3.5453	2.3752

TS4d

	Atom	X	Y	Z
1	C	-1.0510	2.2652	-0.4343
2	N	-1.8926	1.9489	-1.4448
3	C	-3.0094	1.1837	-1.2927
4	C	-1.6327	2.2809	-2.8749
5	C	-2.7048	1.4924	-3.6381
6	C	-3.7870	1.1934	-2.5830
7	H	-3.4907	1.2439	-0.3286
8	C	0.2217	2.9572	-0.4906
9	C	0.5696	3.2597	0.8526
10	N	-0.4446	2.8167	1.6900
11	C	-1.4681	2.2047	0.9863
12	C	1.1148	3.3232	-1.5054
13	C	2.3012	3.9762	-1.1746
14	C	2.6158	4.2649	0.1542
15	C	1.7490	3.9046	1.1874
16	O	-2.4940	1.7582	1.4971
17	H	-1.7340	3.3644	-2.9875
18	H	-0.6311	1.9681	-3.1464
19	H	-3.0892	2.0516	-4.4914
20	H	-2.2692	0.5636	-4.0079
21	H	-4.5470	1.9837	-2.5499
22	H	-4.3122	0.2531	-2.7593
23	H	0.9066	3.1079	-2.5427
24	H	3.5430	4.7739	0.3902
25	H	1.9907	4.1210	2.2213
26	C	0.3234	-0.6414	1.8668
27	C	-0.9865	-1.0241	1.2230
28	C	-1.1022	-0.6717	-0.2357
29	C	0.0921	-0.4466	-1.0409
30	C	1.4248	-0.6485	-0.3646
31	C	1.4823	-0.4469	1.0964
32	C	2.6464	0.0199	1.7337
33	C	2.6848	0.2134	3.1061
34	C	2.4341	-1.0035	-1.1950
35	H	2.1752	-0.9439	-2.2492
36	C	3.7909	-1.4915	-0.9281
37	C	-2.3083	-0.7546	-0.9576
38	C	-3.5323	-1.4396	-0.4600
39	H	-2.1320	-0.9084	-2.0184
40	O	0.0286	-0.1947	-2.2529
41	C	4.1129	-2.3255	0.1583
42	C	5.3973	-2.8145	0.3287
43	C	6.4087	-2.4799	-0.5860
44	C	6.1003	-1.6650	-1.6842
45	C	4.8073	-1.1944	-1.8538
46	C	-4.2034	-1.0814	0.7214
47	C	-5.3434	-1.7602	1.1283
48	C	-5.8494	-2.8190	0.3608
49	C	-5.1984	-3.1788	-0.8270
50	C	-4.0624	-2.4900	-1.2276
51	H	-1.1568	-2.1052	1.3463
52	H	-1.7849	-0.5363	1.7862
53	H	3.5218	0.2448	1.1392
54	H	3.5946	0.5709	3.5750

55	H	3.3424	-2.6018	0.8660
56	H	5.6279	-3.4627	1.1652
57	H	6.8740	-1.4146	-2.3996
58	H	4.5734	-0.5762	-2.7133
59	H	-3.8446	-0.2488	1.3137
60	H	-5.8527	-1.4704	2.0392
61	H	-5.5870	-3.9923	-1.4270
62	H	-3.5640	-2.7782	-2.1466
63	C	1.5488	-0.0434	3.8767
64	H	1.5728	0.0954	4.9519
65	C	0.3777	-0.4534	3.2520
66	H	-0.5195	-0.6188	3.8401
67	H	2.9881	4.2603	-1.9629
68	C	7.7368	-2.9759	-0.4060
69	N	8.8115	-3.3749	-0.2590
70	C	-7.0240	-3.5184	0.7801
71	N	-7.9736	-4.0832	1.1183
72	H	-0.4248	2.8248	2.6972

Prod5d

	Atom	X	Y	Z
1	C	2.4388	-0.7683	-0.1577
2	N	3.5431	-0.0914	0.4991
3	C	3.3870	1.3836	0.4192
4	C	4.9304	-0.4734	0.1712
5	C	5.7028	0.8593	0.1800
6	C	4.6538	1.8834	-0.2873
7	H	3.3722	1.7855	1.4401
8	C	2.2258	-2.2018	0.2983
9	C	2.0527	-3.0275	-0.8212
10	N	2.1962	-2.2667	-1.9921
11	C	2.6334	-0.9882	-1.7170
12	C	2.2840	-2.7718	1.5583
13	C	2.0943	-4.1510	1.6983
14	C	1.8654	-4.9467	0.5785
15	C	1.8527	-4.3949	-0.7060
16	O	3.1130	-0.2220	-2.5195
17	H	5.3239	-1.1876	0.8998
18	H	4.9961	-0.9354	-0.8209
19	H	6.0375	1.0959	1.1951
20	H	6.5861	0.8259	-0.4605
21	H	4.9109	2.9115	-0.0237
22	H	4.5231	1.8194	-1.3703
23	H	2.4897	-2.1557	2.4240
24	H	1.7151	-6.0137	0.6978
25	H	1.7161	-5.0197	-1.5811
26	C	-0.2545	-0.7746	1.8961
27	C	0.7506	0.2928	1.5461
28	C	1.2448	0.2764	0.0798
29	C	0.0604	0.0874	-0.8919
30	C	-1.2408	-0.4558	-0.3517
31	C	-1.2148	-1.1558	0.9452
32	C	-2.0887	-2.2140	1.2444
33	C	-2.0740	-2.8168	2.4936
34	C	-2.3196	-0.2052	-1.1344
35	H	-2.0726	0.2180	-2.1049
36	C	-3.7567	-0.3638	-0.8944
37	C	2.0335	1.6007	-0.2749
38	C	1.3261	2.9149	-0.0114
39	H	2.2047	1.5427	-1.3492
40	O	0.1620	0.4336	-2.0526
41	C	-4.3575	-0.1757	0.3635
42	C	-5.7303	-0.2697	0.5186
43	C	-6.5477	-0.5656	-0.5841
44	C	-5.9659	-0.7386	-1.8474
45	C	-4.5924	-0.6210	-1.9958
46	C	0.6050	3.5119	-1.0572
47	C	-0.0603	4.7173	-0.8832
48	C	-0.0146	5.3698	0.3564
49	C	0.7084	4.7934	1.4084
50	C	1.3661	3.5840	1.2206
51	H	0.2866	1.2696	1.7222
52	H	1.6078	0.2326	2.2188
53	H	-2.7810	-2.5631	0.4891
54	H	-2.7561	-3.6313	2.7084

55	H	-3.7425	0.0606	1.2215
56	H	-6.1817	-0.1116	1.4902
57	H	-6.5944	-0.9525	-2.7028
58	H	-4.1508	-0.7377	-2.9791
59	H	0.5669	3.0139	-2.0184
60	H	-0.6109	5.1621	-1.7029
61	H	0.7539	5.2975	2.3659
62	H	1.9241	3.1679	2.0498
63	C	-1.1777	-2.3740	3.4677
64	H	-1.1719	-2.8290	4.4516
65	C	-0.2677	-1.3703	3.1594
66	H	0.4564	-1.0518	3.9024
67	H	2.1301	-4.6023	2.6825
68	C	-0.6930	6.6148	0.5454
69	N	-1.2417	7.6197	0.7004
70	C	-7.9634	-0.6774	-0.4212
71	N	-9.1074	-0.7714	-0.2886
72	H	2.3056	-2.6605	-2.9156

TS5d

	Atom	X	Y	Z
1	C	1.1390	1.9518	1.2476
2	N	1.8609	1.2365	2.1348
3	C	2.9033	0.4179	1.7981
4	C	1.4998	1.1036	3.5859
5	C	2.3547	-0.0728	4.0614
6	C	3.5288	-0.1148	3.0651
7	H	3.5373	0.7347	0.9847
8	C	1.5643	2.5615	0.0015
9	C	0.4859	3.3781	-0.4365
10	N	-0.5479	3.2893	0.4817
11	C	-0.2190	2.4872	1.5676
12	C	2.7419	2.5649	-0.7563
13	C	2.8237	3.3469	-1.9109
14	C	1.7416	4.1218	-2.3259
15	C	0.5578	4.1486	-1.5846
16	O	-0.9325	2.2980	2.5357
17	H	1.7780	2.0470	4.0664
18	H	0.4326	0.9533	3.6888
19	H	2.6828	0.0558	5.0933
20	H	1.7666	-0.9884	3.9966
21	H	4.3485	0.5413	3.3827
22	H	3.9505	-1.1124	2.9301
23	H	3.6095	1.9939	-0.4560
24	H	1.8188	4.7170	-3.2282
25	H	-0.2806	4.7609	-1.8950
26	C	-0.5229	0.1319	-1.8267
27	C	0.7855	-0.4586	-1.3567
28	C	0.8883	-0.7001	0.1236
29	C	-0.3094	-0.7415	0.9567
30	C	-1.6454	-0.6113	0.2698
31	C	-1.6821	0.0777	-1.0341
32	C	-2.8323	0.7573	-1.4786
33	C	-2.8606	1.3967	-2.7081
34	C	-2.6809	-1.1585	0.9502
35	H	-2.4224	-1.4685	1.9596
36	C	-4.0660	-1.4417	0.5609
37	C	2.0663	-1.1419	0.7743
38	C	3.2332	-1.7499	0.0786
39	H	1.8206	-1.6654	1.6931
40	O	-0.2444	-0.9801	2.1689
41	C	-4.4295	-1.8859	-0.7235
42	C	-5.7424	-2.2087	-1.0239
43	C	-6.7408	-2.0925	-0.0434
44	C	-6.3921	-1.6681	1.2465
45	C	-5.0718	-1.3636	1.5409
46	C	3.7035	-2.9904	0.5443
47	C	4.7889	-3.6254	-0.0412
48	C	5.4524	-3.0242	-1.1194
49	C	5.0054	-1.7826	-1.5913
50	C	3.9159	-1.1601	-0.9983
51	H	0.9788	-1.4006	-1.8936
52	H	1.5761	0.2235	-1.6837
53	H	-3.7076	0.7864	-0.8438
54	H	-3.7612	1.9074	-3.0300

55	H	-3.6692	-1.9901	-1.4867
56	H	-6.0058	-2.5581	-2.0146
57	H	-7.1567	-1.5884	2.0093
58	H	-4.8071	-1.0487	2.5440
59	H	3.1948	-3.4695	1.3731
60	H	5.1278	-4.5849	0.3297
61	H	5.5177	-1.3111	-2.4210
62	H	3.6012	-0.1982	-1.3801
63	C	-1.7267	1.3860	-3.5232
64	H	-1.7407	1.8769	-4.4896
65	C	-0.5681	0.7710	-3.0702
66	H	0.3301	0.8011	-3.6785
67	H	3.7418	3.3506	-2.4863
68	C	-8.0974	-2.4161	-0.3549
69	N	-9.1948	-2.6755	-0.6084
70	C	6.5757	-3.6659	-1.7281
71	N	7.4847	-4.1824	-2.2199
72	H	-1.4414	3.7496	0.4151

Prod4e

	Atom	X	Y	Z
1	C	1.6850	-1.9268	-0.2951
2	N	2.7240	-2.0582	-1.3157
3	C	3.5311	-0.8267	-1.2907
4	C	2.4001	-2.3609	-2.7222
5	C	3.7235	-2.0260	-3.4131
6	C	4.2018	-0.7514	-2.6820
7	H	4.2686	-0.9026	-0.4928
8	C	0.5575	-2.9409	-0.4420
9	C	0.6609	-3.8835	0.5929
10	N	1.7369	-3.5709	1.4297
11	C	2.3794	-2.4273	1.0166
12	C	-0.4410	-3.0944	-1.3933
13	C	-1.3307	-4.1715	-1.2931
14	C	-1.2154	-5.0889	-0.2540
15	C	-0.2107	-4.9575	0.7083
16	O	3.3460	-1.9374	1.5691
17	H	2.1146	-3.4078	-2.8335
18	H	1.5935	-1.7328	-3.1223
19	H	4.4345	-2.8412	-3.2555
20	H	3.6055	-1.8808	-4.4891
21	H	5.2895	-0.7031	-2.6094
22	H	3.8739	0.1467	-3.2117
23	H	-0.5435	-2.3915	-2.2085
24	H	-1.9099	-5.9187	-0.1866
25	H	-0.1177	-5.6734	1.5156
26	C	-0.0402	-0.4464	1.9330
27	C	1.1531	0.1748	1.2585
28	C	1.3330	-0.3437	-0.1895
29	C	0.0162	-0.0744	-0.9566
30	C	-1.2546	0.0568	-0.1531
31	C	-1.2459	-0.4992	1.2132
32	C	-2.3554	-1.1420	1.7808
33	C	-2.2860	-1.6683	3.0648
34	C	-2.2741	0.6841	-0.7923
35	H	-2.0786	0.8819	-1.8432
36	C	2.5289	0.3249	-0.9738
37	H	2.1016	0.6334	-1.9282
38	O	0.0066	0.0503	-2.1695
39	H	1.0182	1.2613	1.2045
40	H	2.0531	0.0031	1.8419
41	H	-3.2694	-1.2366	1.2082
42	H	-3.1516	-2.1622	3.4916
43	C	-1.1023	-1.5706	3.7967
44	H	-1.0481	-1.9737	4.8020
45	C	0.0169	-0.9715	3.2246
46	H	0.9486	-0.9164	3.7778
47	C	2.1525	-4.3424	2.5827
48	H	1.3574	-4.3752	3.3334
49	H	2.4138	-5.3643	2.2926
50	H	3.0287	-3.8519	3.0035
51	C	3.1722	1.5485	-0.3552
52	C	2.9260	2.7979	-0.8858
53	C	4.0642	1.4491	0.7517
54	C	3.5242	3.9728	-0.3609

55	H	2.2561	2.8963	-1.7350
56	C	4.6610	2.5644	1.2833
57	H	4.2669	0.4758	1.1833
58	C	3.2721	5.2600	-0.9036
59	C	4.4145	3.8566	0.7511
60	H	5.3372	2.4674	2.1269
61	C	3.8693	6.3775	-0.3723
62	H	2.5965	5.3479	-1.7483
63	C	5.0156	5.0294	1.2758
64	C	4.7501	6.2616	0.7285
65	H	3.6676	7.3551	-0.7959
66	H	5.6915	4.9375	2.1199
67	H	5.2154	7.1511	1.1383
68	C	-3.5682	1.1759	-0.3202
69	C	-4.5849	1.3362	-1.2494
70	C	-3.8161	1.5784	1.0276
71	C	-5.8628	1.8269	-0.8904
72	H	-4.4045	1.0695	-2.2862
73	C	-5.0341	2.0790	1.4002
74	H	-3.0209	1.5046	1.7566
75	C	-6.9142	1.9647	-1.8345
76	C	-6.0994	2.2069	0.4676
77	H	-5.1984	2.3942	2.4254
78	C	-8.1412	2.4512	-1.4531
79	H	-6.7331	1.6774	-2.8650
80	C	-7.3745	2.7075	0.8278
81	C	-8.3738	2.8259	-0.1097
82	H	-8.9373	2.5507	-2.1822
83	H	-7.5515	2.9976	1.8582
84	H	-9.3461	3.2095	0.1782
85	H	-2.1125	-4.2881	-2.0341

TS4e

	Atom	X	Y	Z
1	C	1.5964	-2.1258	-0.8048
2	N	2.2677	-1.4075	-1.7351
3	C	3.1943	-0.4530	-1.4364
4	C	1.9841	-1.4740	-3.1963
5	C	2.7995	-0.3149	-3.7843
6	C	3.8617	-0.0075	-2.7117
7	H	3.7494	-0.6104	-0.5241
8	C	0.5047	-3.0589	-0.9898
9	C	0.3635	-3.7510	0.2434
10	N	1.3240	-3.3022	1.1409
11	C	2.1154	-2.3146	0.5662
12	C	-0.3840	-3.3606	-2.0273
13	C	-1.3644	-4.3341	-1.8330
14	C	-1.4778	-5.0044	-0.6154
15	C	-0.6130	-4.7146	0.4431
16	O	3.0661	-1.7750	1.1352
17	H	2.3115	-2.4550	-3.5542
18	H	0.9221	-1.3474	-3.3697
19	H	3.2350	-0.5739	-4.7500
20	H	2.1446	0.5456	-3.9253
21	H	4.7776	-0.5893	-2.8734
22	H	4.1516	1.0442	-2.6800
23	H	-0.3321	-2.8505	-2.9775
24	H	-2.2473	-5.7562	-0.4833
25	H	-0.7072	-5.2256	1.3933
26	C	-0.2369	-0.0861	2.1347
27	C	0.9515	0.6365	1.5497
28	C	1.0241	0.6396	0.0473
29	C	-0.1509	0.3323	-0.7589
30	C	-1.4523	0.1202	-0.0312
31	C	-1.3845	-0.3488	1.3662
32	C	-2.4098	-1.1286	1.9331
33	C	-2.3422	-1.5602	3.2492
34	C	-2.5615	0.4004	-0.7592
35	H	-2.3536	0.5834	-1.8103
36	C	2.1278	1.1482	-0.6668
37	H	1.8404	1.4814	-1.6599
38	O	-0.1118	0.3460	-1.9992
39	H	0.9670	1.6761	1.9127
40	H	1.8535	0.1742	1.9602
41	H	-3.2617	-1.4027	1.3255
42	H	-3.1490	-2.1544	3.6635
43	C	-1.2318	-1.2357	4.0308
44	H	-1.1744	-1.5586	5.0645
45	C	-0.1851	-0.5190	3.4640
46	H	0.6990	-0.2968	4.0535
47	C	1.5050	-3.7756	2.4970
48	H	0.6275	-3.5508	3.1091
49	H	1.6902	-4.8537	2.5082
50	H	2.3712	-3.2590	2.9073
51	C	3.2100	1.9742	-0.0622
52	C	3.4562	3.2278	-0.5923
53	C	4.0234	1.5276	1.0204
54	C	4.4589	4.0835	-0.0712

55	H	2.8550	3.5841	-1.4235
56	C	5.0075	2.3290	1.5413
57	H	3.8788	0.5305	1.4176
58	C	4.7019	5.3781	-0.6014
59	C	5.2547	3.6276	1.0253
60	H	5.6200	1.9678	2.3613
61	C	5.6831	6.1816	-0.0734
62	H	4.0963	5.7252	-1.4322
63	C	6.2609	4.4806	1.5460
64	C	6.4710	5.7288	1.0109
65	H	5.8575	7.1689	-0.4861
66	H	6.8640	4.1309	2.3776
67	H	7.2421	6.3730	1.4183
68	C	-3.9708	0.5513	-0.3843
69	C	-4.9465	0.2653	-1.3255
70	C	-4.3871	1.0762	0.8770
71	C	-6.3268	0.4257	-1.0533
72	H	-4.6501	-0.1034	-2.3027
73	C	-5.7127	1.2631	1.1632
74	H	-3.6361	1.3475	1.6072
75	C	-7.3299	0.1072	-2.0065
76	C	-6.7258	0.9346	0.2221
77	H	-6.0065	1.6773	2.1224
78	C	-8.6609	0.2802	-1.7124
79	H	-7.0271	-0.2779	-2.9748
80	C	-8.1059	1.1042	0.4930
81	C	-9.0535	0.7835	-0.4506
82	H	-9.4171	0.0319	-2.4487
83	H	-8.4052	1.4930	1.4610
84	H	-10.1069	0.9167	-0.2310
85	H	-2.0495	-4.5654	-2.6400

Prod5e

	Atom	X	Y	Z
1	C	2.3962	-0.5875	-0.1166
2	N	3.4559	0.1442	0.5574
3	C	3.1990	1.6079	0.5091
4	C	4.8627	-0.1347	0.2128
5	C	5.5433	1.2472	0.2422
6	C	4.4229	2.2063	-0.1961
7	H	3.1680	1.9868	1.5383
8	C	2.2701	-2.0412	0.2988
9	C	2.1353	-2.8396	-0.8471
10	N	2.2539	-2.0501	-2.0014
11	C	2.6005	-0.7532	-1.6754
12	C	2.3585	-2.6429	1.5403
13	C	2.2355	-4.0344	1.6411
14	C	2.0400	-4.8061	0.5000
15	C	1.9994	-4.2188	-0.7695
16	O	3.0266	0.0693	-2.4565
17	H	5.3111	-0.8344	0.9242
18	H	4.9523	-0.5719	-0.7888
19	H	5.8701	1.4860	1.2596
20	H	6.4217	1.2859	-0.4053
21	H	4.6111	3.2442	0.0874
22	H	4.2870	2.1554	-1.2790
23	H	2.5332	-2.0418	2.4232
24	H	1.9380	-5.8819	0.5885
25	H	1.8887	-4.8267	-1.6590
26	C	-0.2937	-0.8098	1.9545
27	C	0.6548	0.3137	1.6255
28	C	1.1356	0.3661	0.1549
29	C	-0.0408	0.1216	-0.8165
30	C	-1.3193	-0.4602	-0.2720
31	C	-1.2543	-1.1936	1.0051
32	C	-2.0829	-2.2937	1.2806
33	C	-2.0238	-2.9398	2.5073
34	C	-2.4163	-0.2234	-1.0367
35	H	-2.1879	0.2213	-2.0019
36	C	1.8264	1.7515	-0.1677
37	H	1.9907	1.7345	-1.2440
38	O	0.0534	0.4558	-1.9827
39	H	0.1413	1.2597	1.8291
40	H	1.5197	0.2820	2.2904
41	H	-2.7760	-2.6398	0.5244
42	H	-2.6727	-3.7856	2.7037
43	C	-1.1266	-2.5001	3.4814
44	H	-1.0850	-2.9903	4.4476
45	C	-0.2611	-1.4509	3.1947
46	H	0.4632	-1.1307	3.9369
47	C	2.3100	-2.5619	-3.3559
48	H	3.1148	-3.2962	-3.4680
49	H	1.3603	-3.0291	-3.6287
50	H	2.5007	-1.7167	-4.0151
51	H	2.2936	-4.5110	2.6124
52	C	1.0351	3.0092	0.1388
53	C	0.2965	3.5957	-0.8705
54	C	1.0279	3.6320	1.4192

55	C	-0.4654	4.7727	-0.6624
56	H	0.2914	3.1409	-1.8553
57	C	0.3052	4.7759	1.6553
58	H	1.6097	3.2067	2.2277
59	C	-1.2275	5.3726	-1.6999
60	C	-0.4646	5.3815	0.6308
61	H	0.3205	5.2340	2.6391
62	C	-1.9532	6.5155	-1.4686
63	H	-1.2272	4.9101	-2.6813
64	C	-1.2237	6.5626	0.8370
65	C	-1.9516	7.1169	-0.1875
66	H	-2.5320	6.9631	-2.2688
67	H	-1.2202	7.0222	1.8201
68	H	-2.5288	8.0192	-0.0190
69	C	-3.8458	-0.4130	-0.7884
70	C	-4.6851	-0.5771	-1.8795
71	C	-4.4337	-0.3455	0.5115
72	C	-6.0840	-0.7377	-1.7358
73	H	-4.2612	-0.5935	-2.8789
74	C	-5.7858	-0.4718	0.6802
75	H	-3.7997	-0.1700	1.3698
76	C	-6.9421	-0.9362	-2.8493
77	C	-6.6535	-0.6868	-0.4253
78	H	-6.2158	-0.4010	1.6740
79	C	-8.2973	-1.0811	-2.6748
80	H	-6.5091	-0.9731	-3.8435
81	C	-8.0543	-0.8368	-0.2796
82	C	-8.8588	-1.0312	-1.3781
83	H	-8.9427	-1.2336	-3.5323
84	H	-8.4849	-0.7953	0.7155
85	H	-9.9298	-1.1456	-1.2538

TS5e

	Atom	X	Y	Z
1	C	2.4649	-1.0289	-0.9045
2	N	2.7534	0.0827	-1.6134
3	C	3.0338	1.3009	-1.0561
4	C	2.6249	0.1735	-3.1052
5	C	2.6859	1.6776	-3.3794
6	C	3.4260	2.2556	-2.1587
7	H	3.5919	1.3022	-0.1328
8	C	2.9514	-1.4359	0.3982
9	C	2.5145	-2.7773	0.5862
10	N	1.8035	-3.1966	-0.5278
11	C	1.7769	-2.2043	-1.5073
12	C	3.7489	-0.8567	1.3908
13	C	4.0826	-1.5912	2.5328
14	C	3.6222	-2.8950	2.7011
15	C	2.8327	-3.5052	1.7215
16	O	1.2732	-2.3380	-2.6106
17	H	3.4781	-0.3661	-3.5292
18	H	1.7079	-0.3038	-3.4267
19	H	3.1895	1.8979	-4.3215
20	H	1.6700	2.0700	-3.4293
21	H	4.5135	2.2370	-2.3031
22	H	3.1495	3.2857	-1.9273
23	H	4.1390	0.1463	1.2891
24	H	3.8814	-3.4479	3.5966
25	H	2.4837	-4.5227	1.8455
26	C	-0.4312	-0.8601	1.8082
27	C	0.3435	0.4202	1.6063
28	C	0.5204	0.8474	0.1758
29	C	-0.3233	0.2918	-0.8777
30	C	-1.4297	-0.6449	-0.4661
31	C	-1.2705	-1.3758	0.8054
32	C	-1.8758	-2.6297	1.0172
33	C	-1.7224	-3.3112	2.2153
34	C	-2.4683	-0.7076	-1.3353
35	H	-2.2744	-0.1977	-2.2755
36	C	1.3015	1.9597	-0.2237
37	H	0.9444	2.3528	-1.1707
38	O	-0.2103	0.6593	-2.0548
39	H	-0.1378	1.2345	2.1708
40	H	1.3188	0.2822	2.0832
41	H	-2.4680	-3.0700	0.2263
42	H	-2.2073	-4.2711	2.3552
43	C	-0.9387	-2.7623	3.2320
44	H	-0.8151	-3.2852	4.1737
45	C	-0.2897	-1.5547	3.0139
46	H	0.3577	-1.1451	3.7827
47	C	1.1964	-4.4981	-0.7104
48	H	0.7350	-4.5023	-1.6968
49	H	1.9481	-5.2921	-0.6608
50	H	0.4304	-4.6764	0.0487
51	H	4.7072	-1.1365	3.2929
52	C	1.7644	3.0418	0.6915
53	C	1.4913	4.3536	0.3446
54	C	2.4973	2.8117	1.8920

55	C	1.8931	5.4502	1.1472
56	H	0.9356	4.5585	-0.5653
57	C	2.9088	3.8502	2.6889
58	H	2.7426	1.7993	2.1845
59	C	1.5988	6.7943	0.7960
60	C	2.6209	5.1972	2.3510
61	H	3.4663	3.6470	3.5976
62	C	2.0054	7.8346	1.5955
63	H	1.0438	6.9873	-0.1162
64	C	3.0276	6.2932	3.1539
65	C	2.7274	7.5825	2.7859
66	H	1.7731	8.8564	1.3171
67	H	3.5804	6.0970	4.0668
68	H	3.0418	8.4133	3.4074
69	C	-3.8081	-1.2927	-1.2239
70	C	-4.4313	-1.7604	-2.3694
71	C	-4.5448	-1.3139	-0.0006
72	C	-5.7400	-2.3009	-2.3473
73	H	-3.9003	-1.7236	-3.3156
74	C	-5.8197	-1.8100	0.0495
75	H	-4.0884	-0.9110	0.8942
76	C	-6.3708	-2.8068	-3.5146
77	C	-6.4558	-2.3311	-1.1097
78	H	-6.3675	-1.8030	0.9864
79	C	-7.6445	-3.3195	-3.4603
80	H	-5.8277	-2.7832	-4.4537
81	C	-7.7686	-2.8633	-1.0881
82	C	-8.3509	-3.3484	-2.2357
83	H	-8.1143	-3.7041	-4.3587
84	H	-8.3101	-2.8824	-0.1478
85	H	-9.3558	-3.7544	-2.2061

Prod4f

	Atom	X	Y	Z
1	C	1.5500	-1.3849	-0.1626
2	N	2.6846	-1.5307	-1.0745
3	C	3.4214	-0.2554	-1.0690
4	C	2.5031	-1.9400	-2.4795
5	C	3.8675	-1.5839	-3.0741
6	C	4.2253	-0.2447	-2.3898
7	H	4.0750	-0.2276	-0.1983
8	C	0.4912	-2.4674	-0.3321
9	C	0.5461	-3.3297	0.7742
10	N	1.5251	-2.9017	1.6760
11	C	2.1458	-1.7546	1.2381
12	C	-0.4087	-2.7404	-1.3526
13	C	-1.2508	-3.8551	-1.2509
14	C	-1.1858	-4.6911	-0.1413
15	C	-0.2795	-4.4392	0.8922
16	O	3.0329	-1.1760	1.8358
17	H	2.2760	-3.0051	-2.5430
18	H	1.7082	-1.3811	-2.9907
19	H	4.5957	-2.3525	-2.8026
20	H	3.8397	-1.5117	-4.1635
21	H	5.2979	-0.1485	-2.2142
22	H	3.9230	0.6034	-3.0094
23	H	-0.4715	-2.1014	-2.2224
24	H	-1.8427	-5.5511	-0.0735
25	H	-0.2254	-5.0915	1.7550
26	C	-0.4138	0.1566	1.8079
27	C	0.7950	0.7932	1.1770
28	C	1.1123	0.1802	-0.2089
29	C	-0.1519	0.3204	-1.0900
30	C	-1.4861	0.4399	-0.3948
31	C	-1.5559	-0.0154	1.0078
32	C	-2.6720	-0.6761	1.5403
33	C	-2.6753	-1.1043	2.8620
34	C	-2.4795	0.9710	-1.1505
35	H	-2.2095	1.1094	-2.1946
36	C	-3.8294	1.4274	-0.8166
37	C	2.3338	0.8531	-0.9483
38	C	2.8455	2.1678	-0.3967
39	H	1.9765	1.0451	-1.9607
40	O	-0.0725	0.3566	-2.3062
41	C	-4.2101	1.9137	0.4475
42	C	-5.4934	2.3892	0.6699
43	C	-6.4592	2.3941	-0.3464
44	C	-6.0795	1.9280	-1.6074
45	C	-4.7880	1.4701	-1.8425
46	C	3.6509	2.2454	0.7489
47	C	4.1176	3.4701	1.2144
48	C	3.8058	4.6667	0.5593
49	C	3.0029	4.5910	-0.5804
50	C	2.5353	3.3653	-1.0499
51	H	0.6094	1.8632	1.0284
52	H	1.6558	0.7173	1.8352
53	H	-3.5345	-0.8596	0.9121
54	H	-3.5454	-1.6137	3.2606

55	H	-3.4883	1.9363	1.2532
56	H	-5.7529	2.7720	1.6520
57	H	-6.7987	1.9361	-2.4199
58	H	-4.5122	1.1335	-2.8364
59	H	3.9063	1.3411	1.2898
60	H	4.7366	3.4968	2.1063
61	H	2.7408	5.5007	-1.1120
62	H	1.9163	3.3375	-1.9412
63	C	-1.5578	-0.8885	3.6695
64	H	-1.5611	-1.2147	4.7037
65	C	-0.4298	-0.2706	3.1368
66	H	0.4533	-0.1247	3.7499
67	C	1.8713	-3.5677	2.9143
68	H	1.0138	-3.5933	3.5931
69	H	2.2084	-4.5909	2.7240
70	H	2.6802	-3.0011	3.3727
71	C	4.3433	5.9876	1.0552
72	H	4.3373	6.0361	2.1473
73	H	5.3782	6.1401	0.7293
74	H	3.7535	6.8253	0.6764
75	C	-7.8601	2.8843	-0.0787
76	H	-8.4034	3.0674	-1.0079
77	H	-8.4300	2.1479	0.4985
78	H	-7.8535	3.8123	0.4994
79	H	-1.9561	-4.0648	-2.0463

TS4f

	Atom	X	Y	Z
1	C	-0.9607	2.1065	0.5073
2	N	-1.7852	2.2493	-0.5573
3	C	-3.0085	1.6556	-0.6553
4	C	-1.4066	2.9621	-1.8092
5	C	-2.5462	2.6309	-2.7819
6	C	-3.7120	2.1936	-1.8747
7	H	-3.5248	1.4924	0.2783
8	C	0.4030	2.5652	0.6689
9	C	0.7043	2.4296	2.0513
10	N	-0.4089	1.9419	2.7236
11	C	-1.4640	1.7271	1.8437
12	C	1.4057	3.0326	-0.1873
13	C	2.6560	3.3669	0.3341
14	C	2.9243	3.2324	1.6959
15	C	1.9471	2.7546	2.5728
16	O	-2.5790	1.3315	2.1886
17	H	-1.3363	4.0291	-1.5766
18	H	-0.4526	2.5935	-2.1672
19	H	-2.7985	3.4813	-3.4163
20	H	-2.2374	1.8056	-3.4243
21	H	-4.3435	3.0452	-1.5924
22	H	-4.3639	1.4504	-2.3369
23	H	1.2354	3.1345	-1.2486
24	H	3.9025	3.4957	2.0815
25	H	2.1574	2.6377	3.6287
26	C	-0.1793	-1.6338	1.7425
27	C	-1.5086	-1.4942	1.0421
28	C	-1.4801	-0.7024	-0.2359
29	C	-0.2235	-0.4430	-0.9285
30	C	1.0169	-1.0953	-0.3774
31	C	1.0327	-1.4239	1.0623
32	C	2.2309	-1.4528	1.7997
33	C	2.2382	-1.7659	3.1503
34	C	1.9908	-1.3240	-1.2920
35	H	1.7946	-0.8611	-2.2560
36	C	3.2259	-2.1147	-1.2404
37	C	-2.6456	-0.3585	-0.9498
38	C	-3.9875	-0.9571	-0.7016
39	H	-2.4348	-0.2039	-2.0043
40	O	-0.1858	0.2015	-1.9883
41	C	3.3555	-3.3122	-0.5150
42	C	4.5265	-4.0547	-0.5645
43	C	5.6242	-3.6393	-1.3301
44	C	5.4922	-2.4600	-2.0671
45	C	4.3140	-1.7214	-2.0356
46	C	-4.6612	-0.8986	0.5283
47	C	-5.9153	-1.4801	0.6830
48	C	-6.5516	-2.1410	-0.3731
49	C	-5.8895	-2.1847	-1.6026
50	C	-4.6375	-1.5995	-1.7655
51	H	-1.9264	-2.4925	0.8375
52	H	-2.2051	-1.0294	1.7455
53	H	3.1622	-1.2199	1.3015
54	H	3.1765	-1.7870	3.6935

55	H	2.5225	-3.6698	0.0770
56	H	4.5894	-4.9821	-0.0032
57	H	6.3179	-2.1203	-2.6845
58	H	4.2314	-0.8188	-2.6322
59	H	-4.2154	-0.3706	1.3627
60	H	-6.4134	-1.4111	1.6453
61	H	-6.3598	-2.6793	-2.4469
62	H	-4.1469	-1.6502	-2.7322
63	C	1.0371	-2.0434	3.8064
64	H	1.0331	-2.3009	4.8600
65	C	-0.1579	-1.9584	3.1036
66	H	-1.0994	-2.1333	3.6151
67	C	6.9034	-4.4392	-1.3487
68	H	6.7022	-5.5123	-1.4073
69	H	7.5323	-4.1660	-2.1987
70	H	7.4883	-4.2690	-0.4378
71	C	-7.8975	-2.7975	-0.1838
72	H	-8.5238	-2.2309	0.5098
73	H	-8.4350	-2.8865	-1.1305
74	H	-7.7883	-3.8073	0.2273
75	C	-0.4932	1.6765	4.1440
76	H	-1.5124	1.3554	4.3533
77	H	0.2017	0.8843	4.4350
78	H	-0.2756	2.5812	4.7196
79	H	3.4290	3.7300	-0.3331

Prod5f

	Atom	X	Y	Z
1	C	-2.1846	-0.4440	-0.7131
2	N	-3.0815	-1.3055	0.0394
3	C	-2.4350	-2.6135	0.3282
4	C	-4.4598	-1.5167	-0.4410
5	C	-4.7420	-3.0023	-0.1462
6	C	-3.3613	-3.6642	-0.2973
7	H	-2.4229	-2.7592	1.4155
8	C	-2.5004	1.0370	-0.6185
9	C	-2.4501	1.6033	-1.9014
10	N	-2.2198	0.6052	-2.8603
11	C	-2.2408	-0.6482	-2.2796
12	C	-2.8875	1.8178	0.4546
13	C	-3.1504	3.1793	0.2562
14	C	-3.0361	3.7383	-1.0126
15	C	-2.6943	2.9523	-2.1188
16	O	-2.3387	-1.6927	-2.8858
17	H	-5.1613	-0.8507	0.0701
18	H	-4.5440	-1.3294	-1.5181
19	H	-5.1092	-3.1213	0.8785
20	H	-5.4954	-3.4181	-0.8184
21	H	-3.2948	-4.6364	0.1962
22	H	-3.1181	-3.7881	-1.3552
23	H	-2.9971	1.3753	1.4361
24	H	-3.2338	4.7948	-1.1554
25	H	-2.6461	3.3823	-3.1117
26	C	0.0853	0.9203	1.4383
27	C	-0.4963	-0.4616	1.2918
28	C	-0.7572	-0.9229	-0.1626
29	C	0.4194	-0.5358	-1.0856
30	C	1.4375	0.4536	-0.5828
31	C	1.0311	1.3669	0.5021
32	C	1.5134	2.6826	0.5952
33	C	1.1351	3.5067	1.6455
34	C	2.6475	0.3753	-1.1929
35	H	2.6597	-0.2896	-2.0529
36	C	3.9454	0.9808	-0.8884
37	C	-1.0053	-2.4850	-0.2206
38	C	0.0541	-3.3783	0.3960
39	H	-1.0418	-2.7207	-1.2835
40	O	0.5453	-1.0751	-2.1691
41	C	4.3754	1.3127	0.4092
42	C	5.6474	1.8186	0.6297
43	C	6.5452	2.0289	-0.4264
44	C	6.1276	1.6836	-1.7140
45	C	4.8616	1.1545	-1.9387
46	C	1.0776	-3.8770	-0.4238
47	C	2.0756	-4.7003	0.0837
48	C	2.0927	-5.0728	1.4322
49	C	1.0721	-4.5850	2.2496
50	C	0.0725	-3.7548	1.7440
51	H	0.2101	-1.1747	1.7308
52	H	-1.4179	-0.5447	1.8703
53	H	2.1912	3.0547	-0.1624
54	H	1.5190	4.5189	1.7027

55	H	3.7135	1.1533	1.2502
56	H	5.9558	2.0509	1.6443
57	H	6.8062	1.8165	-2.5503
58	H	4.5698	0.8736	-2.9453
59	H	1.0869	-3.6054	-1.4733
60	H	2.8528	-5.0646	-0.5815
61	H	1.0532	-4.8579	3.3002
62	H	-0.7012	-3.4084	2.4190
63	C	0.2591	3.0303	2.6220
64	H	-0.0294	3.6633	3.4537
65	C	-0.2684	1.7500	2.5050
66	H	-0.9779	1.3890	3.2429
67	C	7.9127	2.6128	-0.1738
68	H	8.5756	2.4612	-1.0281
69	H	7.8513	3.6911	0.0099
70	H	8.3823	2.1619	0.7046
71	C	3.1639	-5.9896	1.9718
72	H	3.1743	-5.9909	3.0638
73	H	3.0039	-7.0216	1.6413
74	H	4.1566	-5.6893	1.6251
75	C	-2.2484	0.8075	-4.2946
76	H	-3.1990	1.2484	-4.6129
77	H	-1.4297	1.4616	-4.6058
78	H	-2.1304	-0.1683	-4.7627
79	H	-3.4443	3.7986	1.0952

TS5f

	Atom	X	Y	Z
1	C	-0.8892	-0.7109	2.1324
2	N	-1.4320	0.4542	2.5457
3	C	-2.3632	1.1638	1.8370
4	C	-0.9492	1.2164	3.7435
5	C	-1.5900	2.5954	3.5727
6	C	-2.8157	2.3349	2.6773
7	H	-3.0957	0.5984	1.2823
8	C	-1.4845	-1.7669	1.3390
9	C	-0.5700	-2.8570	1.3745
10	N	0.5304	-2.5170	2.1462
11	C	0.3845	-1.2415	2.6917
12	C	-2.6948	-1.9434	0.6602
13	C	-2.9703	-3.1623	0.0328
14	C	-2.0478	-4.2053	0.0659
15	C	-0.8335	-4.0626	0.7445
16	O	1.1790	-0.7268	3.4619
17	H	-1.3208	0.6867	4.6268
18	H	0.1332	1.2252	3.7644
19	H	-1.8550	3.0414	4.5322
20	H	-0.8831	3.2539	3.0674
21	H	-3.6939	2.0539	3.2720
22	H	-3.1011	3.1929	2.0664
23	H	-3.4421	-1.1630	0.6247
24	H	-2.2718	-5.1405	-0.4340
25	H	-0.1197	-4.8762	0.7803
26	C	0.7487	-0.8731	-1.4820
27	C	-0.4268	0.0635	-1.3372
28	C	-0.3652	0.9984	-0.1626
29	C	0.8939	1.2378	0.5363
30	C	2.1381	0.5986	-0.0244
31	C	1.9733	-0.6212	-0.8400
32	C	2.9884	-1.5932	-0.9297
33	C	2.8259	-2.7378	-1.6952
34	C	3.2901	1.2396	0.2902
35	H	3.1557	2.0248	1.0300
36	C	4.6635	1.1031	-0.2079
37	C	-1.4141	1.8810	0.1946
38	C	-2.5397	2.2633	-0.7061
39	H	-1.0215	2.7338	0.7402
40	O	0.9608	2.0267	1.4885
41	C	4.9807	0.8038	-1.5444
42	C	6.2996	0.7617	-1.9739
43	C	7.3627	1.0074	-1.0949
44	C	7.0502	1.3233	0.2297
45	C	5.7294	1.3854	0.6613
46	C	-2.7943	3.6302	-0.9007
47	C	-3.8277	4.0697	-1.7210
48	C	-4.6635	3.1633	-2.3796
49	C	-4.4249	1.8011	-2.1769
50	C	-3.3886	1.3582	-1.3602
51	H	-0.5479	0.6507	-2.2614
52	H	-1.3256	-0.5583	-1.2775
53	H	3.9123	-1.4417	-0.3882
54	H	3.6279	-3.4657	-1.7532

55	H	4.1829	0.6215	-2.2536
56	H	6.5105	0.5415	-3.0160
57	H	7.8504	1.5364	0.9315
58	H	5.5132	1.6509	1.6908
59	H	-2.1605	4.3595	-0.4071
60	H	-3.9876	5.1357	-1.8492
61	H	-5.0626	1.0703	-2.6647
62	H	-3.2518	0.2924	-1.2297
63	C	1.6289	-2.9516	-2.3818
64	H	1.4929	-3.8414	-2.9863
65	C	0.5999	-2.0290	-2.2563
66	H	-0.3495	-2.2110	-2.7496
67	C	-5.7663	3.6377	-3.2940
68	H	-6.1701	4.5988	-2.9670
69	H	-5.3985	3.7696	-4.3176
70	H	-6.5891	2.9200	-3.3332
71	C	8.7937	0.9254	-1.5664
72	H	8.9128	1.3683	-2.5589
73	H	9.4694	1.4426	-0.8818
74	H	9.1276	-0.1160	-1.6344
75	C	1.6768	-3.3596	2.4131
76	H	2.3440	-2.7975	3.0648
77	H	1.3759	-4.2839	2.9162
78	H	2.1994	-3.6059	1.4850
79	H	-3.9139	-3.2918	-0.4844

Prod4g

	Atom	X	Y	Z
1	C	1.5361	-1.3586	-0.1813
2	N	2.6504	-1.5015	-1.1163
3	C	3.3917	-0.2302	-1.1239
4	C	2.4488	-1.9222	-2.5153
5	C	3.8010	-1.5612	-3.1338
6	C	4.1549	-0.2120	-2.4689
7	H	4.0740	-0.2125	-0.2750
8	C	0.4762	-2.4426	-0.3292
9	C	0.5556	-3.3046	0.7758
10	N	1.5516	-2.8736	1.6582
11	C	2.1596	-1.7255	1.2079
12	C	-0.4424	-2.7181	-1.3321
13	C	-1.2794	-3.8348	-1.2139
14	C	-1.1903	-4.6705	-0.1056
15	C	-0.2644	-4.4163	0.9100
16	O	3.0558	-1.1416	1.7875
17	H	2.2281	-2.9892	-2.5674
18	H	1.6426	-1.3721	-3.0179
19	H	4.5401	-2.3202	-2.8649
20	H	3.7568	-1.5002	-4.2232
21	H	5.2302	-0.0928	-2.3276
22	H	3.8157	0.6247	-3.0850
23	H	-0.5225	-2.0804	-2.2017
24	H	-1.8431	-5.5323	-0.0250
25	H	-0.1914	-5.0688	1.7711
26	C	-0.4272	0.1677	1.8037
27	C	0.7801	0.8094	1.1746
28	C	1.0970	0.2058	-0.2157
29	C	-0.1683	0.3477	-1.0939
30	C	-1.5024	0.4598	-0.3957
31	C	-1.5696	-0.0036	1.0043
32	C	-2.6832	-0.6705	1.5344
33	C	-2.6841	-1.1046	2.8541
34	C	-2.4964	0.9950	-1.1465
35	H	-2.2287	1.1419	-2.1899
36	C	-3.8468	1.4470	-0.8051
37	C	2.3156	0.8854	-0.9551
38	C	2.8527	2.1771	-0.3736
39	H	1.9466	1.1105	-1.9562
40	O	-0.0919	0.3918	-2.3098
41	C	-4.2171	1.9276	0.4643
42	C	-5.4997	2.3992	0.7067
43	C	-6.4279	2.3858	-0.3263
44	C	-6.1034	1.9370	-1.5969
45	C	-4.8096	1.4863	-1.8298
46	C	3.6627	2.2058	0.7720
47	C	4.1621	3.4047	1.2724
48	C	3.8491	4.5866	0.6184
49	C	3.0554	4.6041	-0.5161
50	C	2.5652	3.3943	-1.0035
51	H	0.5937	1.8805	1.0344
52	H	1.6411	0.7292	1.8321
53	H	-3.5450	-0.8561	0.9057
54	H	-3.5518	-1.6191	3.2511

55	H	-3.4902	1.9466	1.2647
56	H	-5.7880	2.7814	1.6780
57	H	-6.8502	1.9565	-2.3806
58	H	-4.5369	1.1499	-2.8240
59	H	3.8995	1.2820	1.2868
60	H	4.7876	3.4327	2.1562
61	H	2.8360	5.5459	-1.0038
62	H	1.9476	3.3973	-1.8955
63	C	-1.5667	-0.8883	3.6615
64	H	-1.5683	-1.2188	4.6943
65	C	-0.4408	-0.2650	3.1307
66	H	0.4418	-0.1189	3.7443
67	C	1.9256	-3.5400	2.8886
68	H	1.0819	-3.5703	3.5843
69	H	2.2630	-4.5614	2.6898
70	H	2.7411	-2.9709	3.3319
71	F	4.3349	5.7543	1.1012
72	F	-7.6776	2.8359	-0.0883
73	H	-1.9990	-4.0473	-1.9956

TS4g

	Atom	X	Y	Z
1	C	-0.9564	2.0930	0.5000
2	N	-1.7790	2.2393	-0.5650
3	C	-3.0066	1.6558	-0.6633
4	C	-1.3951	2.9501	-1.8171
5	C	-2.5327	2.6205	-2.7922
6	C	-3.7033	2.1922	-1.8870
7	H	-3.5254	1.4992	0.2700
8	C	0.4078	2.5497	0.6650
9	C	0.7064	2.4099	2.0473
10	N	-0.4087	1.9214	2.7167
11	C	-1.4620	1.7106	1.8353
12	C	1.4120	3.0200	-0.1881
13	C	2.6616	3.3517	0.3365
14	C	2.9274	3.2122	1.6984
15	C	1.9483	2.7325	2.5721
16	O	-2.5784	1.3150	2.1767
17	H	-1.3233	4.0171	-1.5847
18	H	-0.4409	2.5792	-2.1718
19	H	-2.7793	3.4697	-3.4303
20	H	-2.2251	1.7915	-3.4303
21	H	-4.3323	3.0474	-1.6104
22	H	-4.3572	1.4506	-2.3493
23	H	1.2432	3.1273	-1.2491
24	H	3.9048	3.4742	2.0866
25	H	2.1566	2.6129	3.6281
26	C	-0.1691	-1.6466	1.7291
27	C	-1.5036	-1.5083	1.0381
28	C	-1.4851	-0.7156	-0.2400
29	C	-0.2345	-0.4582	-0.9431
30	C	1.0109	-1.1080	-0.3993
31	C	1.0377	-1.4339	1.0409
32	C	2.2410	-1.4593	1.7701
33	C	2.2584	-1.7731	3.1204
34	C	1.9768	-1.3389	-1.3209
35	H	1.7730	-0.8806	-2.2854
36	C	3.2128	-2.1296	-1.2741
37	C	-2.6550	-0.3702	-0.9447
38	C	-3.9970	-0.9606	-0.6779
39	H	-2.4553	-0.2198	-2.0018
40	O	-0.2045	0.1824	-2.0053
41	C	3.3392	-3.3268	-0.5474
42	C	4.5078	-4.0762	-0.5908
43	C	5.5665	-3.6252	-1.3669
44	C	5.4811	-2.4611	-2.1136
45	C	4.2986	-1.7303	-2.0724
46	C	-4.6549	-0.8813	0.5604
47	C	-5.9089	-1.4554	0.7463
48	C	-6.5129	-2.1115	-0.3152
49	C	-5.9061	-2.2011	-1.5576
50	C	-4.6543	-1.6177	-1.7300
51	H	-1.9213	-2.5072	0.8364
52	H	-2.1947	-1.0446	1.7474
53	H	3.1683	-1.2215	1.2666
54	H	3.2001	-1.7913	3.6575

55	H	2.5076	-3.6809	0.0476
56	H	4.6062	-5.0040	-0.0408
57	H	6.3231	-2.1485	-2.7186
58	H	4.2135	-0.8255	-2.6641
59	H	-4.1955	-0.3449	1.3815
60	H	-6.4226	-1.3931	1.6977
61	H	-6.4100	-2.7165	-2.3658
62	H	-4.1693	-1.6858	-2.6978
63	C	1.0625	-2.0549	3.7841
64	H	1.0665	-2.3137	4.8372
65	C	-0.1375	-1.9724	3.0896
66	H	-1.0748	-2.1504	3.6077
67	C	-0.4961	1.6561	4.1374
68	H	-1.5155	1.3349	4.3450
69	H	0.1986	0.8643	4.4296
70	H	-0.2798	2.5610	4.7129
71	H	3.4355	3.7177	-0.3278
72	F	6.7073	-4.3500	-1.4055
73	F	-7.7314	-2.6706	-0.1361

Prod5g

	Atom	X	Y	Z
1	C	-2.1690	-0.4472	-0.7091
2	N	-3.0706	-1.3084	0.0381
3	C	-2.4305	-2.6190	0.3262
4	C	-4.4484	-1.5132	-0.4473
5	C	-4.7378	-2.9976	-0.1541
6	C	-3.3596	-3.6654	-0.3024
7	H	-2.4207	-2.7663	1.4135
8	C	-2.4828	1.0339	-0.6105
9	C	-2.4287	1.6041	-1.8913
10	N	-2.1952	0.6088	-2.8531
11	C	-2.2193	-0.6459	-2.2767
12	C	-2.8740	1.8110	0.4639
13	C	-3.1365	3.1729	0.2690
14	C	-3.0183	3.7360	-0.9978
15	C	-2.6728	2.9536	-2.1054
16	O	-2.3114	-1.6893	-2.8861
17	H	-5.1484	-0.8443	0.0616
18	H	-4.5276	-1.3251	-1.5246
19	H	-5.1081	-3.1158	0.8695
20	H	-5.4911	-3.4099	-0.8284
21	H	-3.2989	-4.6384	0.1900
22	H	-3.1144	-3.7893	-1.3599
23	H	-2.9875	1.3652	1.4436
24	H	-3.2163	4.7927	-1.1379
25	H	-2.6222	3.3868	-3.0968
26	C	0.0935	0.9087	1.4455
27	C	-0.4822	-0.4758	1.2977
28	C	-0.7443	-0.9339	-0.1574
29	C	0.4362	-0.5510	-1.0765
30	C	1.4428	0.4545	-0.5801
31	C	1.0307	1.3646	0.5053
32	C	1.5017	2.6845	0.5973
33	C	1.1229	3.5035	1.6513
34	C	2.6519	0.3874	-1.1925
35	H	2.6703	-0.2802	-2.0503
36	C	3.9438	1.0079	-0.8903
37	C	-1.0000	-2.4939	-0.2209
38	C	0.0556	-3.3952	0.3905
39	H	-1.0382	-2.7254	-1.2845
40	O	0.5772	-1.1065	-2.1498
41	C	4.3689	1.3370	0.4098
42	C	5.6338	1.8594	0.6404
43	C	6.4839	2.0643	-0.4386
44	C	6.1141	1.7396	-1.7343
45	C	4.8521	1.1975	-1.9471
46	C	1.0690	-3.9006	-0.4380
47	C	2.0669	-4.7357	0.0550
48	C	2.0453	-5.0776	1.3977
49	C	1.0596	-4.6112	2.2513
50	C	0.0712	-3.7719	1.7406
51	H	0.2278	-1.1868	1.7346
52	H	-1.4027	-0.5628	1.8774
53	H	2.1700	3.0650	-0.1647
54	H	1.4976	4.5192	1.7076

55	H	3.7087	1.1673	1.2495
56	H	5.9721	2.1032	1.6398
57	H	6.8107	1.8992	-2.5477
58	H	4.5573	0.9205	-2.9532
59	H	1.0736	-3.6279	-1.4866
60	H	2.8481	-5.1261	-0.5856
61	H	1.0695	-4.9070	3.2931
62	H	-0.6995	-3.4202	2.4151
63	C	0.2577	3.0173	2.6327
64	H	-0.0304	3.6462	3.4675
65	C	-0.2603	1.7332	2.5162
66	H	-0.9628	1.3655	3.2574
67	C	-2.2221	0.8160	-4.2871
68	H	-3.1734	1.2558	-4.6050
69	H	-1.4047	1.4732	-4.5947
70	H	-2.1013	-0.1578	-4.7587
71	H	-3.4341	3.7893	1.1088
72	F	7.7106	2.5815	-0.2157
73	F	3.0074	-5.8938	1.8867

TS5g

	Atom	X	Y	Z
1	C	-0.8787	-0.6889	2.1320
2	N	-1.4211	0.4782	2.5380
3	C	-2.3593	1.1792	1.8307
4	C	-0.9348	1.2509	3.7285
5	C	-1.5803	2.6266	3.5506
6	C	-2.8098	2.3560	2.6636
7	H	-3.0923	0.6073	1.2834
8	C	-1.4749	-1.7518	1.3485
9	C	-0.5579	-2.8395	1.3885
10	N	0.5452	-2.4919	2.1534
11	C	0.3995	-1.2129	2.6895
12	C	-2.6880	-1.9359	0.6766
13	C	-2.9637	-3.1599	0.0594
14	C	-2.0383	-4.2003	0.0961
15	C	-0.8215	-4.0503	0.7685
16	O	1.1963	-0.6893	3.4509
17	H	-1.3011	0.7260	4.6167
18	H	0.1476	1.2626	3.7443
19	H	-1.8420	3.0787	4.5080
20	H	-0.8778	3.2835	3.0373
21	H	-3.6846	2.0783	3.2647
22	H	-3.1003	3.2091	2.0480
23	H	-3.4385	-1.1585	0.6413
24	H	-2.2626	-5.1398	-0.3955
25	H	-0.1064	-4.8624	0.8078
26	C	0.7552	-0.8750	-1.4849
27	C	-0.4241	0.0578	-1.3453
28	C	-0.3639	1.0038	-0.1795
29	C	0.8942	1.2527	0.5169
30	C	2.1401	0.6098	-0.0367
31	C	1.9786	-0.6164	-0.8434
32	C	2.9960	-1.5866	-0.9260
33	C	2.8376	-2.7356	-1.6858
34	C	3.2896	1.2558	0.2742
35	H	3.1535	2.0481	1.0060
36	C	4.6639	1.1155	-0.2225
37	C	-1.4141	1.8860	0.1724
38	C	-2.5431	2.2569	-0.7286
39	H	-1.0244	2.7441	0.7114
40	O	0.9603	2.0515	1.4606
41	C	4.9751	0.8140	-1.5601
42	C	6.2917	0.7620	-1.9996
43	C	7.3123	1.0110	-1.0924
44	C	7.0526	1.3291	0.2311
45	C	5.7286	1.3936	0.6521
46	C	-2.7973	3.6232	-0.9354
47	C	-3.8306	4.0621	-1.7571
48	C	-4.6331	3.1175	-2.3765
49	C	-4.4289	1.7590	-2.1943
50	C	-3.3876	1.3382	-1.3718
51	H	-0.5507	0.6348	-2.2752
52	H	-1.3188	-0.5692	-1.2765
53	H	3.9181	-1.4318	-0.3823
54	H	3.6411	-3.4620	-1.7385

55	H	4.1753	0.6316	-2.2662
56	H	6.5365	0.5406	-3.0311
57	H	7.8750	1.5305	0.9062
58	H	5.5107	1.6558	1.6814
59	H	-2.1611	4.3571	-0.4532
60	H	-4.0177	5.1161	-1.9207
61	H	-5.0796	1.0497	-2.6907
62	H	-3.2429	0.2752	-1.2317
63	C	1.6423	-2.9554	-2.3735
64	H	1.5098	-3.8482	-2.9742
65	C	0.6107	-2.0351	-2.2537
66	H	-0.3374	-2.2222	-2.7478
67	C	1.6917	-3.3329	2.4260
68	H	2.3605	-2.7656	3.0715
69	H	1.3907	-4.2522	2.9381
70	H	2.2125	-3.5881	1.4995
71	H	-3.9096	-3.2960	-0.4516
72	F	8.5952	0.9549	-1.5166
73	F	-5.6426	3.5303	-3.1745

Prod4h

	Atom	X	Y	Z
1	C	1.5417	-1.3466	-0.1759
2	N	2.6499	-1.4940	-1.1135
3	C	3.3959	-0.2275	-1.1362
4	C	2.4553	-1.9450	-2.5039
5	C	3.8059	-1.5855	-3.1260
6	C	4.1425	-0.2184	-2.4906
7	H	4.0892	-0.2073	-0.2961
8	C	0.4822	-2.4324	-0.3095
9	C	0.5638	-3.2801	0.8060
10	N	1.5612	-2.8375	1.6823
11	C	2.1678	-1.6963	1.2167
12	C	-0.4359	-2.7217	-1.3091
13	C	-1.2716	-3.8375	-1.1763
14	C	-1.1808	-4.6588	-0.0572
15	C	-0.2547	-4.3910	0.9544
16	O	3.0645	-1.1023	1.7857
17	H	2.2435	-3.0145	-2.5340
18	H	1.6461	-1.4122	-3.0200
19	H	4.5516	-2.3306	-2.8376
20	H	3.7651	-1.5487	-4.2165
21	H	5.2166	-0.0743	-2.3653
22	H	3.7777	0.5982	-3.1191
23	H	-0.5155	-2.0970	-2.1882
24	H	-1.8322	-5.5205	0.0342
25	H	-0.1799	-5.0335	1.8229
26	C	-0.4442	0.1869	1.7838
27	C	0.7683	0.8284	1.1636
28	C	1.1017	0.2190	-0.2209
29	C	-0.1541	0.3511	-1.1121
30	C	-1.4987	0.4559	-0.4263
31	C	-1.5776	0.0018	0.9746
32	C	-2.6954	-0.6627	1.4988
33	C	-2.7096	-1.0809	2.8233
34	C	-2.4892	0.9762	-1.1901
35	H	-2.2195	1.1206	-2.2334
36	C	-3.8478	1.4083	-0.8511
37	C	2.3246	0.8949	-0.9561
38	C	2.8725	2.1731	-0.3588
39	H	1.9576	1.1349	-1.9542
40	O	-0.0694	0.3925	-2.3262
41	C	-4.2042	1.9456	0.3991
42	C	-5.4920	2.3936	0.6411
43	C	-6.4701	2.3103	-0.3629
44	C	-6.1265	1.7935	-1.6195
45	C	-4.8293	1.3662	-1.8576
46	C	3.6723	2.1787	0.7950
47	C	4.1835	3.3639	1.3052
48	C	3.9078	4.5831	0.6693
49	C	3.1138	4.5926	-0.4846
50	C	2.6096	3.3987	-0.9848
51	H	0.5811	1.8990	1.0197
52	H	1.6216	0.7510	1.8313
53	H	-3.5484	-0.8611	0.8622
54	H	-3.5796	-1.5939	3.2168

55	H	-3.4609	2.0249	1.1808
56	H	-5.7510	2.8146	1.6047
57	H	-6.8744	1.7406	-2.4007
58	H	-4.5660	0.9835	-2.8373
59	H	3.8882	1.2464	1.3035
60	H	4.7987	3.3542	2.1967
61	H	2.9014	5.5308	-0.9823
62	H	2.0014	3.4160	-1.8828
63	C	-1.6021	-0.8502	3.6403
64	H	-1.6146	-1.1678	4.6769
65	C	-0.4719	-0.2296	3.1156
66	H	0.4021	-0.0721	3.7385
67	C	1.9412	-3.4924	2.9179
68	H	1.0993	-3.5208	3.6154
69	H	2.2823	-4.5138	2.7261
70	H	2.7553	-2.9167	3.3549
71	H	-1.9904	-4.0619	-1.9553
72	C	4.4342	5.8056	1.1932
73	N	4.8584	6.7931	1.6172
74	C	-7.8025	2.7614	-0.1090
75	N	-8.8802	3.1236	0.0971

TS4h

	Atom	X	Y	Z
1	C	-0.9604	2.0820	0.4961
2	N	-1.7813	2.2315	-0.5687
3	C	-3.0136	1.6606	-0.6680
4	C	-1.3917	2.9413	-1.8210
5	C	-2.5299	2.6193	-2.7976
6	C	-3.7043	2.1975	-1.8942
7	H	-3.5330	1.5013	0.2646
8	C	0.4017	2.5433	0.6662
9	C	0.6948	2.4041	2.0494
10	N	-0.4214	1.9108	2.7153
11	C	-1.4693	1.6958	1.8312
12	C	1.4065	3.0196	-0.1830
13	C	2.6524	3.3561	0.3467
14	C	2.9131	3.2163	1.7096
15	C	1.9330	2.7319	2.5794
16	O	-2.5855	1.2949	2.1652
17	H	-1.3143	4.0071	-1.5866
18	H	-0.4388	2.5650	-2.1737
19	H	-2.7708	3.4705	-3.4348
20	H	-2.2268	1.7896	-3.4371
21	H	-4.3301	3.0557	-1.6196
22	H	-4.3613	1.4597	-2.3582
23	H	1.2407	3.1292	-1.2443
24	H	3.8876	3.4831	2.1020
25	H	2.1376	2.6142	3.6362
26	C	-0.1608	-1.6498	1.7242
27	C	-1.4960	-1.5230	1.0324
28	C	-1.4833	-0.7273	-0.2447
29	C	-0.2351	-0.4680	-0.9511
30	C	1.0139	-1.1109	-0.4042
31	C	1.0448	-1.4285	1.0363
32	C	2.2492	-1.4435	1.7637
33	C	2.2697	-1.7575	3.1138
34	C	1.9801	-1.3417	-1.3255
35	H	1.7790	-0.8876	-2.2927
36	C	3.2167	-2.1279	-1.2686
37	C	-2.6525	-0.3816	-0.9491
38	C	-3.9928	-0.9677	-0.6784
39	H	-2.4557	-0.2295	-2.0063
40	O	-0.2056	0.1672	-2.0154
41	C	3.3349	-3.3300	-0.5470
42	C	4.5030	-4.0731	-0.5811
43	C	5.5994	-3.6330	-1.3400
44	C	5.4917	-2.4470	-2.0796
45	C	4.3118	-1.7196	-2.0511
46	C	-4.6452	-0.8859	0.5633
47	C	-5.8977	-1.4535	0.7501
48	C	-6.5384	-2.1191	-0.3048
49	C	-5.9060	-2.1965	-1.5531
50	C	-4.6561	-1.6208	-1.7307
51	H	-1.9012	-2.5264	0.8284
52	H	-2.1919	-1.0685	1.7424
53	H	3.1741	-1.1955	1.2607
54	H	3.2112	-1.7680	3.6511

55	H	2.4954	-3.6882	0.0341
56	H	4.5758	-5.0010	-0.0273
57	H	6.3301	-2.1101	-2.6768
58	H	4.2314	-0.8110	-2.6372
59	H	-4.1799	-0.3508	1.3818
60	H	-6.3906	-1.3791	1.7117
61	H	-6.3978	-2.7046	-2.3734
62	H	-4.1735	-1.6893	-2.6994
63	C	1.0759	-2.0497	3.7770
64	H	1.0827	-2.3093	4.8298
65	C	-0.1258	-1.9766	3.0842
66	H	-1.0606	-2.1633	3.6033
67	C	-0.5142	1.6519	4.1375
68	H	-1.5329	1.3273	4.3429
69	H	0.1832	0.8650	4.4363
70	H	-0.3043	2.5606	4.7088
71	H	3.4269	3.7276	-0.3137
72	C	6.8089	-4.3937	-1.3682
73	N	7.7879	-5.0075	-1.3890
74	C	-7.8289	-2.7041	-0.1121
75	N	-8.8719	-3.1764	0.0433

Prod5h

	Atom	X	Y	Z
1	C	-2.1431	-0.4550	-0.7044
2	N	-3.0598	-1.3031	0.0388
3	C	-2.4418	-2.6221	0.3328
4	C	-4.4383	-1.4883	-0.4541
5	C	-4.7514	-2.9672	-0.1588
6	C	-3.3829	-3.6564	-0.2983
7	H	-2.4387	-2.7672	1.4205
8	C	-2.4401	1.0294	-0.6095
9	C	-2.3750	1.5967	-1.8908
10	N	-2.1451	0.5973	-2.8504
11	C	-2.1841	-0.6553	-2.2728
12	C	-2.8309	1.8114	0.4619
13	C	-3.0803	3.1749	0.2632
14	C	-2.9506	3.7347	-1.0040
15	C	-2.6065	2.9477	-2.1086
16	O	-2.2746	-1.7005	-2.8796
17	H	-5.1303	-0.8073	0.0492
18	H	-4.5077	-1.3013	-1.5323
19	H	-5.1291	-3.0774	0.8628
20	H	-5.5068	-3.3700	-0.8363
21	H	-3.3400	-4.6289	0.1968
22	H	-3.1342	-3.7870	-1.3542
23	H	-2.9550	1.3682	1.4415
24	H	-3.1394	4.7927	-1.1470
25	H	-2.5484	3.3786	-3.1004
26	C	0.1152	0.8821	1.4511
27	C	-0.4619	-0.5029	1.3083
28	C	-0.7269	-0.9625	-0.1458
29	C	0.4610	-0.5966	-1.0606
30	C	1.4561	0.4323	-0.5795
31	C	1.0420	1.3433	0.5027
32	C	1.5097	2.6647	0.5914
33	C	1.1394	3.4802	1.6506
34	C	2.6604	0.3804	-1.2007
35	H	2.6897	-0.2921	-2.0545
36	C	3.9377	1.0360	-0.9056
37	C	-1.0076	-2.5180	-0.2097
38	C	0.0330	-3.4311	0.4066
39	H	-1.0438	-2.7503	-1.2733
40	O	0.6217	-1.1775	-2.1163
41	C	4.3801	1.3181	0.3995
42	C	5.6270	1.8769	0.6240
43	C	6.4704	2.1807	-0.4567
44	C	6.0514	1.8892	-1.7619
45	C	4.8097	1.3099	-1.9742
46	C	1.0424	-3.9517	-0.4182
47	C	2.0228	-4.7972	0.0814
48	C	2.0141	-5.1558	1.4364
49	C	1.0084	-4.6538	2.2719
50	C	0.0360	-3.8045	1.7585
51	H	0.2460	-1.2132	1.7496
52	H	-1.3830	-0.5848	1.8876
53	H	2.1664	3.0503	-0.1780
54	H	1.5103	4.4972	1.7048

55	H	3.7454	1.0830	1.2433
56	H	5.9604	2.0791	1.6343
57	H	6.7051	2.1085	-2.5969
58	H	4.4994	1.0703	-2.9851
59	H	1.0536	-3.6807	-1.4670
60	H	2.7930	-5.1889	-0.5716
61	H	0.9922	-4.9344	3.3179
62	H	-0.7334	-3.4400	2.4272
63	C	0.2871	2.9882	2.6405
64	H	0.0064	3.6143	3.4798
65	C	-0.2289	1.7031	2.5274
66	H	-0.9224	1.3325	3.2754
67	C	-2.1667	0.8030	-4.2855
68	H	-3.1147	1.2473	-4.6059
69	H	-1.3453	1.4558	-4.5911
70	H	-2.0497	-0.1717	-4.7562
71	H	-3.3781	3.7952	1.1000
72	C	3.0170	-6.0305	1.9608
73	N	3.8273	-6.7356	2.3864
74	C	7.7515	2.7714	-0.2261
75	N	8.7855	3.2523	-0.0398

TS5h

	Atom	X	Y	Z
1	C	-0.8740	-0.6639	2.1321
2	N	-1.4135	0.5053	2.5328
3	C	-2.3622	1.1974	1.8322
4	C	-0.9192	1.2887	3.7146
5	C	-1.5714	2.6607	3.5335
6	C	-2.8073	2.3805	2.6581
7	H	-3.0952	0.6198	1.2911
8	C	-1.4750	-1.7348	1.3633
9	C	-0.5600	-2.8233	1.4136
10	N	0.5477	-2.4695	2.1699
11	C	0.4082	-1.1846	2.6897
12	C	-2.6915	-1.9245	0.6987
13	C	-2.9719	-3.1549	0.0976
14	C	-2.0478	-4.1965	0.1436
15	C	-0.8283	-4.0411	0.8094
16	O	1.2092	-0.6503	3.4381
17	H	-1.2763	0.7676	4.6085
18	H	0.1632	1.3038	3.7210
19	H	-1.8276	3.1168	4.4903
20	H	-0.8759	3.3186	3.0120
21	H	-3.6770	2.1061	3.2678
22	H	-3.1045	3.2289	2.0392
23	H	-3.4414	-1.1468	0.6577
24	H	-2.2761	-5.1416	-0.3350
25	H	-0.1154	-4.8547	0.8564
26	C	0.7561	-0.8871	-1.4816
27	C	-0.4243	0.0452	-1.3473
28	C	-0.3618	1.0043	-0.1916
29	C	0.8975	1.2611	0.4988
30	C	2.1421	0.6089	-0.0496
31	C	1.9795	-0.6252	-0.8414
32	C	2.9973	-1.5957	-0.9156
33	C	2.8399	-2.7489	-1.6688
34	C	3.2929	1.2558	0.2545
35	H	3.1632	2.0544	0.9806
36	C	4.6632	1.1023	-0.2449
37	C	-1.4090	1.8915	0.1574
38	C	-2.5393	2.2538	-0.7401
39	H	-1.0177	2.7531	0.6895
40	O	0.9697	2.0706	1.4318
41	C	4.9650	0.8069	-1.5869
42	C	6.2762	0.7421	-2.0279
43	C	7.3346	0.9682	-1.1333
44	C	7.0504	1.2814	0.2033
45	C	5.7336	1.3602	0.6302
46	C	-2.8034	3.6193	-0.9470
47	C	-3.8410	4.0463	-1.7625
48	C	-4.6642	3.1058	-2.3967
49	C	-4.4236	1.7400	-2.1949
50	C	-3.3796	1.3267	-1.3791
51	H	-0.5549	0.6098	-2.2839
52	H	-1.3162	-0.5842	-1.2671
53	H	3.9175	-1.4398	-0.3690
54	H	3.6426	-3.4763	-1.7158

55	H	4.1595	0.6405	-2.2904
56	H	6.4930	0.5226	-3.0661
57	H	7.8632	1.4687	0.8942
58	H	5.5209	1.6163	1.6620
59	H	-2.1696	4.3571	-0.4681
60	H	-4.0197	5.1038	-1.9133
61	H	-5.0596	1.0089	-2.6786
62	H	-3.2260	0.2656	-1.2369
63	C	1.6455	-2.9712	-2.3575
64	H	1.5142	-3.8670	-2.9538
65	C	0.6131	-2.0509	-2.2448
66	H	-0.3334	-2.2409	-2.7405
67	C	1.6907	-3.3133	2.4519
68	H	1.3854	-4.2230	2.9776
69	H	2.2071	-3.5848	1.5277
70	H	2.3647	-2.7413	3.0877
71	H	-3.9202	-3.2963	-0.4072
72	C	8.6884	0.8919	-1.5849
73	N	9.7829	0.8273	-1.9503
74	C	-5.7403	3.5331	-3.2354
75	N	-6.6115	3.8768	-3.9120

Prod4i

	Atom	X	Y	Z
1	C	-1.3788	1.6343	0.2805
2	N	-2.3865	2.2273	-0.5976
3	C	-3.4377	1.2146	-0.8071
4	C	-2.0330	2.7930	-1.9147
5	C	-3.4107	2.9116	-2.5693
6	C	-4.1397	1.6243	-2.1223
7	H	-4.1244	1.2371	0.0383
8	C	-0.0622	2.4049	0.2903
9	C	0.0623	3.0850	1.5168
10	N	-1.0320	2.8075	2.3184
11	C	-1.9220	1.9368	1.7204
12	C	0.9229	2.5619	-0.6672
13	C	2.0168	3.3796	-0.3651
14	C	2.1411	4.0445	0.8507
15	C	1.1491	3.9011	1.8135
16	O	-2.9452	1.5413	2.2305
17	H	-1.1896	3.1750	3.2448
18	N	3.0764	3.5417	-1.3723
19	O	2.9512	2.9431	-2.4344
20	O	4.0254	4.2655	-1.0914
21	H	-1.5358	3.7571	-1.7982
22	H	-1.3860	2.1325	-2.5060
23	H	-3.9260	3.7927	-2.1785
24	H	-3.3459	3.0093	-3.6547
25	H	-5.2091	1.7874	-1.9807
26	H	-4.0300	0.8348	-2.8699
27	H	0.8849	2.0763	-1.6306
28	H	3.0104	4.6629	1.0242
29	H	1.2248	4.4114	2.7658
30	C	0.0274	-0.6534	1.9723
31	C	-1.2779	-0.8463	1.2485
32	C	-1.3716	0.0400	-0.0167
33	C	-0.1527	-0.2880	-0.9150
34	C	1.0885	-0.8269	-0.2516
35	C	1.2078	-0.6481	1.2087
36	C	2.4310	-0.3904	1.8453
37	C	2.4873	-0.2028	3.2210
38	C	1.9785	-1.4119	-1.0944
39	H	1.7352	-1.2867	-2.1463
40	C	-2.6964	-0.1551	-0.8510
41	H	-2.3612	-0.2914	-1.8794
42	O	-0.2037	-0.1251	-2.1220
43	H	-1.3676	-1.8893	0.9238
44	H	-2.1155	-0.6583	1.9147
45	H	3.3380	-0.3298	1.2573
46	H	3.4409	-0.0071	3.6983
47	C	1.3196	-0.2570	3.9824
48	H	1.3619	-0.1182	5.0570
49	C	0.0955	-0.4701	3.3543
50	H	-0.8201	-0.4869	3.9361
51	C	3.1805	-2.2055	-0.8454
52	C	4.1574	-2.2378	-1.8290
53	C	3.3640	-3.0120	0.3189
54	C	5.3440	-2.9950	-1.6840

55	H	4.0205	-1.6548	-2.7344
56	C	4.4887	-3.7756	0.4748
57	H	2.5907	-3.0341	1.0748
58	C	6.3607	-3.0049	-2.6749
59	C	5.5193	-3.7845	-0.5047
60	H	4.6036	-4.3959	1.3577
61	C	7.4971	-3.7584	-2.5063
62	H	6.2265	-2.4042	-3.5682
63	C	6.7008	-4.5525	-0.3630
64	C	7.6687	-4.5394	-1.3401
65	H	8.2683	-3.7571	-3.2681
66	H	6.8315	-5.1532	0.5310
67	H	8.5697	-5.1302	-1.2198
68	C	-3.5695	-1.3431	-0.5034
69	C	-3.5895	-2.4460	-1.3320
70	C	-4.4069	-1.3494	0.6493
71	C	-4.4063	-3.5755	-1.0660
72	H	-2.9655	-2.4593	-2.2208
73	C	-5.2106	-2.4241	0.9358
74	H	-4.4036	-0.4934	1.3139
75	C	-4.4281	-4.7124	-1.9155
76	C	-5.2389	-3.5673	0.0956
77	H	-5.8414	-2.4092	1.8189
78	C	-5.2324	-5.7890	-1.6297
79	H	-3.7963	-4.7181	-2.7978
80	C	-6.0585	-4.6941	0.3621
81	C	-6.0559	-5.7802	-0.4796
82	H	-5.2393	-6.6518	-2.2864
83	H	-6.6900	-4.6845	1.2445
84	H	-6.6864	-6.6360	-0.2658

TS4i

	Atom	X	Y	Z
1	C	1.2521	-2.2882	-0.1622
2	N	2.0545	-1.9666	-1.2052
3	C	3.1837	-1.2090	-1.0730
4	C	1.7363	-2.2616	-2.6307
5	C	2.7910	-1.4681	-3.4136
6	C	3.9148	-1.2075	-2.3928
7	H	3.7111	-1.3247	-0.1378
8	C	-0.0519	-2.9173	-0.1825
9	C	-0.3622	-3.2473	1.1692
10	N	0.6978	-2.8856	1.9676
11	C	1.7289	-2.2942	1.2335
12	C	-0.9968	-3.1943	-1.1676
13	C	-2.1936	-3.7992	-0.7857
14	C	-2.4902	-4.1255	0.5377
15	C	-1.5632	-3.8432	1.5341
16	O	2.7899	-1.9204	1.7245
17	H	0.7137	-2.9089	2.9751
18	N	-3.1867	-4.1004	-1.8270
19	O	-2.9043	-3.8193	-2.9875
20	O	-4.2426	-4.6174	-1.4794
21	H	1.8195	-3.3431	-2.7748
22	H	0.7307	-1.9303	-2.8627
23	H	3.1360	-2.0117	-4.2934
24	H	2.3549	-0.5255	-3.7461
25	H	4.6595	-2.0124	-2.3995
26	H	4.4499	-0.2730	-2.5673
27	H	-0.8532	-2.9636	-2.2098
28	H	-3.4383	-4.5915	0.7637
29	H	-1.7751	-4.0796	2.5695
30	C	0.1199	0.5701	2.3116
31	C	1.3916	0.9419	1.5901
32	C	1.4050	0.6125	0.1236
33	C	0.1533	0.4340	-0.6067
34	C	-1.1269	0.6471	0.1551
35	C	-1.0921	0.4233	1.6144
36	C	-2.2219	-0.0317	2.3192
37	C	-2.1720	-0.2635	3.6860
38	C	-2.1873	1.0173	-0.6050
39	H	-1.9958	0.9614	-1.6736
40	C	2.5694	0.6797	-0.6733
41	H	2.3211	0.8769	-1.7127
42	O	0.1426	0.2024	-1.8246
43	H	1.5882	2.0190	1.7132
44	H	2.2205	0.4373	2.0916
45	H	-3.1425	-0.2143	1.7814
46	H	-3.0588	-0.6083	4.2061
47	C	-0.9801	-0.0596	4.3839
48	H	-0.9345	-0.2290	5.4541
49	C	0.1557	0.3418	3.6910
50	H	1.0951	0.4692	4.2199
51	C	-3.5194	1.5158	-0.2518
52	C	-4.5732	1.2674	-1.1165
53	C	-3.7664	2.3251	0.8984
54	C	-5.8826	1.7423	-0.8620

55	H	-4.3993	0.6803	-2.0129
56	C	-5.0162	2.8192	1.1590
57	H	-2.9441	2.5661	1.5593
58	C	-6.9710	1.4630	-1.7299
59	C	-6.1157	2.5371	0.3036
60	H	-5.1802	3.4459	2.0297
61	C	-8.2285	1.9448	-1.4573
62	H	-6.7938	0.8581	-2.6130
63	C	-7.4232	3.0216	0.5540
64	C	-8.4572	2.7318	-0.3050
65	H	-9.0523	1.7226	-2.1262
66	H	-7.5970	3.6269	1.4378
67	H	-9.4540	3.1067	-0.1018
68	C	3.8333	1.3450	-0.2388
69	C	4.3209	2.3910	-1.0002
70	C	4.5759	0.9398	0.9083
71	C	5.5079	3.0849	-0.6548
72	H	3.7761	2.7092	-1.8840
73	C	5.7331	1.5855	1.2638
74	H	4.2338	0.0957	1.4946
75	C	6.0023	4.1706	-1.4246
76	C	6.2336	2.6763	0.5069
77	H	6.2874	1.2582	2.1375
78	C	7.1576	4.8198	-1.0628
79	H	5.4502	4.4823	-2.3052
80	C	7.4237	3.3662	0.8520
81	C	7.8759	4.4138	0.0863
82	H	7.5242	5.6487	-1.6578
83	H	7.9731	3.0529	1.7337
84	H	8.7862	4.9349	0.3604

Prod5i

	Atom	X	Y	Z
1	C	-2.2302	-0.4430	-0.6446
2	N	-3.1513	-1.2888	0.0883
3	C	-2.5285	-2.6021	0.4028
4	C	-4.5268	-1.4832	-0.4096
5	C	-4.8328	-2.9627	-0.1077
6	C	-3.4590	-3.6447	-0.2295
7	H	-2.5381	-2.7366	1.4910
8	C	-2.5324	1.0418	-0.5451
9	C	-2.4592	1.6258	-1.8222
10	N	-2.2074	0.6402	-2.7702
11	C	-2.2643	-0.6333	-2.2164
12	C	-2.9252	1.8054	0.5317
13	C	-3.1565	3.1689	0.3246
14	C	-3.0306	3.7622	-0.9288
15	C	-2.6866	2.9832	-2.0292
16	O	-2.3811	-1.6547	-2.8449
17	H	-2.2738	0.7751	-3.7690
18	N	-3.5425	4.0021	1.4693
19	O	-3.6206	3.4613	2.5687
20	O	-3.7616	5.1911	1.2672
21	H	-5.2253	-0.8047	0.0885
22	H	-4.5942	-1.3021	-1.4891
23	H	-5.2189	-3.0675	0.9112
24	H	-5.5802	-3.3738	-0.7890
25	H	-3.4149	-4.6129	0.2734
26	H	-3.1996	-3.7838	-1.2821
27	H	-3.0664	1.3801	1.5133
28	H	-3.2193	4.8218	-1.0275
29	H	-2.6179	3.4223	-3.0170
30	C	0.0107	0.9371	1.4848
31	C	-0.5530	-0.4561	1.3716
32	C	-0.8154	-0.9390	-0.0755
33	C	0.3774	-0.5844	-0.9948
34	C	1.3848	0.4215	-0.5105
35	C	0.9605	1.3635	0.5420
36	C	1.4244	2.6881	0.5938
37	C	1.0190	3.5445	1.6086
38	C	2.5997	0.3391	-1.1135
39	H	2.6223	-0.3439	-1.9587
40	C	-1.0889	-2.4953	-0.1231
41	H	-1.1097	-2.7408	-1.1842
42	O	0.5142	-1.1615	-2.0574
43	H	0.1671	-1.1528	1.8140
44	H	-1.4676	-0.5423	1.9607
45	H	2.1054	3.0436	-0.1692
46	H	1.3863	4.5641	1.6332
47	C	0.1349	3.0925	2.5889
48	H	-0.1838	3.7523	3.3874
49	C	-0.3703	1.7991	2.5153
50	H	-1.0896	1.4626	3.2543
51	C	-0.0535	-3.4000	0.5181
52	C	0.9247	-3.9638	-0.2774
53	C	-0.0500	-3.7145	1.9067
54	C	1.9227	-4.8222	0.2485

55	H	0.9382	-3.7413	-1.3390
56	C	0.8990	-4.5459	2.4492
57	H	-0.8130	-3.3015	2.5551
58	C	2.9302	-5.3991	-0.5693
59	C	1.9140	-5.1233	1.6456
60	H	0.8775	-4.7742	3.5100
61	C	3.8818	-6.2303	-0.0309
62	H	2.9359	-5.1704	-1.6298
63	C	2.9103	-5.9865	2.1708
64	C	3.8722	-6.5272	1.3527
65	H	4.6467	-6.6638	-0.6655
66	H	2.9004	-6.2132	3.2319
67	H	4.6294	-7.1851	1.7642
68	C	3.8884	0.9614	-0.8140
69	C	4.8076	1.0884	-1.8446
70	C	4.2848	1.3635	0.4980
71	C	6.0890	1.6546	-1.6447
72	H	4.5384	0.7537	-2.8417
73	C	5.5265	1.8907	0.7272
74	H	3.5993	1.2274	1.3232
75	C	7.0205	1.8138	-2.7044
76	C	6.4619	2.0701	-0.3283
77	H	5.8157	2.1752	1.7336
78	C	8.2593	2.3613	-2.4737
79	H	6.7370	1.4967	-3.7025
80	C	7.7474	2.6281	-0.1235
81	C	8.6262	2.7725	-1.1716
82	H	8.9622	2.4797	-3.2905
83	H	8.0296	2.9408	0.8764
84	H	9.6072	3.2020	-1.0026

TS5i

	Atom	X	Y	Z
1	C	-2.2528	-0.3296	1.2525
2	N	-2.2809	0.8839	1.8481
3	C	-2.3220	2.0725	1.1667
4	C	-2.0844	1.0910	3.3200
5	C	-1.8131	2.5924	3.4349
6	C	-2.4643	3.1911	2.1745
7	H	-2.9253	2.1024	0.2721
8	C	-2.8626	-0.7502	0.0069
9	C	-2.7187	-2.1699	-0.0614
10	N	-2.0727	-2.6029	1.0705
11	C	-1.7883	-1.5538	1.9544
12	C	-3.5463	-0.1098	-1.0217
13	C	-4.0383	-0.8774	-2.0808
14	C	-3.8851	-2.2605	-2.1453
15	C	-3.2185	-2.9199	-1.1174
16	O	-1.2672	-1.6990	3.0431
17	H	-1.8084	-3.5531	1.2774
18	N	-4.7281	-0.1869	-3.1760
19	O	-4.7592	1.0427	-3.1494
20	O	-5.2310	-0.8679	-4.0616
21	H	-3.0183	0.7951	3.8093
22	H	-1.2795	0.4616	3.6786
23	H	-2.2195	3.0085	4.3574
24	H	-0.7360	2.7613	3.4243
25	H	-3.5263	3.4104	2.3373
26	H	-1.9926	4.1134	1.8326
27	H	-3.7359	0.9508	-1.0421
28	H	-4.2864	-2.7962	-2.9934
29	H	-3.0912	-3.9950	-1.1436
30	C	0.3895	-0.9928	-1.6065
31	C	-0.0263	0.4540	-1.4952
32	C	-0.0605	1.0035	-0.0977
33	C	0.6887	0.3510	0.9742
34	C	1.5159	-0.8541	0.6142
35	C	1.1184	-1.6221	-0.5819
36	C	1.3755	-3.0017	-0.6932
37	C	0.9981	-3.7163	-1.8205
38	C	2.5499	-1.1021	1.4558
39	H	2.5334	-0.4873	2.3519
40	C	-0.5765	2.2827	0.2320
41	H	-0.0841	2.6669	1.1209
42	O	0.7208	0.8302	2.1149
43	H	0.6447	1.0803	-2.1048
44	H	-1.0067	0.5548	-1.9692
45	H	1.8743	-3.5129	0.1193
46	H	1.2168	-4.7765	-1.8846
47	C	0.3359	-3.0693	-2.8653
48	H	0.0442	-3.6170	-3.7543
49	C	0.0244	-1.7216	-2.7427
50	H	-0.5268	-1.2225	-3.5333
51	C	-0.8439	3.3583	-0.7711
52	C	-0.2210	4.5810	-0.5954
53	C	-1.7240	3.2109	-1.8816
54	C	-0.4120	5.6628	-1.4910

55	H	0.4504	4.7219	0.2462
56	C	-1.9416	4.2413	-2.7613
57	H	-2.2480	2.2785	-2.0453
58	C	0.2402	6.9124	-1.3192
59	C	-1.2945	5.4931	-2.6025
60	H	-2.6241	4.1017	-3.5929
61	C	0.0284	7.9420	-2.2032
62	H	0.9122	7.0411	-0.4770
63	C	-1.4933	6.5766	-3.4959
64	C	-0.8470	7.7734	-3.3020
65	H	0.5333	8.8911	-2.0625
66	H	-2.1652	6.4442	-4.3375
67	H	-1.0049	8.5950	-3.9914
68	C	3.6981	-2.0080	1.3597
69	C	4.2493	-2.5117	2.5268
70	C	4.3382	-2.3211	0.1221
71	C	5.3814	-3.3621	2.5183
72	H	3.7966	-2.2587	3.4805
73	C	5.4477	-3.1219	0.0827
74	H	3.9472	-1.8981	-0.7942
75	C	5.9313	-3.9033	3.7103
76	C	5.9987	-3.6799	1.2681
77	H	5.9288	-3.3348	-0.8665
78	C	7.0352	-4.7204	3.6678
79	H	5.4630	-3.6614	4.6586
80	C	7.1374	-4.5227	1.2589
81	C	7.6445	-5.0334	2.4307
82	H	7.4448	-5.1286	4.5849
83	H	7.6055	-4.7598	0.3090
84	H	8.5158	-5.6782	2.4108

Prod4j

	Atom	X	Y	Z
1	C	-1.3823	1.5842	0.2460
2	N	-2.4116	2.1488	-0.6268
3	C	-3.4288	1.1016	-0.8357
4	C	-2.0776	2.7207	-1.9463
5	C	-3.4601	2.8009	-2.5969
6	C	-4.1568	1.4984	-2.1407
7	H	-4.1067	1.0913	0.0167
8	C	-0.0905	2.3961	0.2545
9	C	0.0151	3.0775	1.4821
10	N	-1.0679	2.7647	2.2851
11	C	-1.9313	1.8662	1.6881
12	C	0.8872	2.5858	-0.7047
13	C	1.9554	3.4370	-0.4032
14	C	2.0616	4.1028	0.8138
15	C	1.0767	3.9265	1.7783
16	O	-2.9396	1.4378	2.2007
17	H	-1.2338	3.1235	3.2134
18	N	3.0070	3.6353	-1.4123
19	O	2.8948	3.0416	-2.4785
20	O	3.9370	4.3826	-1.1288
21	H	-1.6059	3.6980	-1.8339
22	H	-1.4145	2.0764	-2.5377
23	H	-3.9958	3.6711	-2.2093
24	H	-3.4009	2.8945	-3.6831
25	H	-5.2269	1.6412	-1.9834
26	H	-4.0434	0.7111	-2.8900
27	H	0.8624	2.1005	-1.6686
28	H	2.9115	4.7477	0.9868
29	H	1.1383	4.4369	2.7315
30	C	0.0744	-0.6616	1.9420
31	C	-1.2169	-0.8952	1.2053
32	C	-1.3255	-0.0086	-0.0581
33	C	-0.0903	-0.2990	-0.9465
34	C	1.1603	-0.8022	-0.2726
35	C	1.2612	-0.6188	1.1898
36	C	2.4690	-0.3217	1.8381
37	C	2.5057	-0.1305	3.2138
38	C	2.0691	-1.3695	-1.1065
39	H	1.8256	-1.2584	-2.1603
40	C	3.2925	-2.1290	-0.8510
41	C	-2.6387	-0.2383	-0.9016
42	C	-3.4654	-1.4669	-0.5819
43	H	-2.2934	-0.3409	-1.9310
44	O	-0.1360	-0.1360	-2.1537
45	C	3.5030	-2.9240	0.2901
46	C	4.6644	-3.6678	0.4333
47	C	5.6721	-3.6458	-0.5411
48	C	5.4582	-2.8696	-1.6833
49	C	4.2861	-2.1404	-1.8443
50	C	-4.3209	-1.5378	0.5269
51	C	-5.0763	-2.6787	0.7769
52	C	-5.0143	-3.7937	-0.0662
53	C	-4.1619	-3.7247	-1.1701
54	C	-3.4055	-2.5826	-1.4238

55	H	-1.2698	-1.9395	0.8770
56	H	-2.0679	-0.7362	1.8620
57	H	3.3798	-0.2360	1.2592
58	H	3.4477	0.0966	3.7001
59	H	2.7414	-2.9742	1.0573
60	H	4.7924	-4.2852	1.3169
61	H	6.2122	-2.8456	-2.4632
62	H	4.1356	-1.5600	-2.7484
63	H	-4.3912	-0.6985	1.2097
64	H	-5.7270	-2.7034	1.6459
65	H	-4.0891	-4.5727	-1.8440
66	H	-2.7549	-2.5568	-2.2923
67	C	1.3330	-0.2220	3.9645
68	H	1.3605	-0.0810	5.0393
69	C	0.1230	-0.4753	3.3248
70	H	-0.7977	-0.5202	3.8970
71	C	6.9466	-4.4296	-0.3535
72	H	7.4666	-4.5794	-1.3018
73	H	7.6332	-3.9042	0.3196
74	H	6.7501	-5.4108	0.0862
75	C	-5.8620	-5.0151	0.1958
76	H	-5.9363	-5.2272	1.2655
77	H	-6.8819	-4.8749	-0.1791
78	H	-5.4506	-5.8990	-0.2966

TS4j

	Atom	X	Y	Z
1	C	-0.9455	2.0876	0.4698
2	N	-1.7983	2.2526	-0.5703
3	C	-3.0219	1.6490	-0.6351
4	C	-1.4570	2.9736	-1.8285
5	C	-2.6248	2.6440	-2.7682
6	C	-3.7620	2.1991	-1.8294
7	H	-3.5155	1.4998	0.3136
8	C	0.4357	2.5060	0.5843
9	C	0.8087	2.2990	1.9449
10	N	-0.2825	1.8269	2.6358
11	C	-1.3991	1.6721	1.8095
12	C	1.3977	2.9831	-0.3027
13	C	2.6752	3.2516	0.1872
14	C	3.0343	3.0508	1.5201
15	C	2.0891	2.5639	2.4152
16	O	-2.4973	1.2960	2.2088
17	H	-0.2815	1.4970	3.5881
18	N	3.6872	3.7652	-0.7470
19	O	3.3487	3.9583	-1.9105
20	O	4.8145	3.9747	-0.3126
21	H	-1.3835	4.0399	-1.5942
22	H	-0.5130	2.6113	-2.2192
23	H	-2.8978	3.4972	-3.3896
24	H	-2.3339	1.8242	-3.4259
25	H	-4.3811	3.0486	-1.5167
26	H	-4.4298	1.4619	-2.2771
27	H	1.2077	3.1541	-1.3490
28	H	4.0436	3.2774	1.8318
29	H	2.3470	2.3928	3.4530
30	C	-0.2229	-1.5746	1.7593
31	C	-1.5424	-1.4934	1.0321
32	C	-1.5164	-0.6900	-0.2374
33	C	-0.2566	-0.4418	-0.9336
34	C	0.9832	-1.0780	-0.3652
35	C	0.9924	-1.3677	1.0842
36	C	2.1821	-1.3448	1.8354
37	C	2.1764	-1.5903	3.2004
38	C	1.9671	-1.3114	-1.2683
39	H	1.7729	-0.8703	-2.2429
40	C	3.2150	-2.0772	-1.1882
41	C	-2.6845	-0.3233	-0.9411
42	C	-4.0263	-0.9284	-0.6896
43	H	-2.4749	-0.1788	-1.9978
44	O	-0.2210	0.1923	-1.9982
45	C	3.3635	-3.2496	-0.4266
46	C	4.5507	-3.9674	-0.4462
47	C	5.6451	-3.5490	-1.2149
48	C	5.4941	-2.3943	-1.9870
49	C	4.3000	-1.6820	-1.9872
50	C	-4.7040	-0.8601	0.5370
51	C	-5.9552	-1.4473	0.6940
52	C	-6.5833	-2.1242	-0.3568
53	C	-5.9160	-2.1785	-1.5831
54	C	-4.6670	-1.5874	-1.7484

55	H	-1.9064	-2.5078	0.8033
56	H	-2.2775	-1.0708	1.7210
57	H	3.1166	-1.1232	1.3380
58	H	3.1084	-1.5717	3.7544
59	H	2.5335	-3.6088	0.1686
60	H	4.6295	-4.8770	0.1412
61	H	6.3174	-2.0533	-2.6064
62	H	4.2034	-0.7984	-2.6094
63	H	-4.2636	-0.3246	1.3697
64	H	-6.4569	-1.3711	1.6538
65	H	-6.3797	-2.6858	-2.4233
66	H	-4.1729	-1.6460	-2.7129
67	C	0.9718	-1.8530	3.8564
68	H	0.9592	-2.0562	4.9216
69	C	-0.2152	-1.8303	3.1349
70	H	-1.1600	-1.9986	3.6423
71	C	-7.9256	-2.7868	-0.1653
72	H	-8.5547	-2.2215	0.5267
73	H	-8.4627	-2.8817	-1.1116
74	H	-7.8105	-3.7946	0.2487
75	C	6.9430	-4.3179	-1.1991
76	H	7.5524	-4.0899	-2.0761
77	H	7.5366	-4.0686	-0.3123
78	H	6.7675	-5.3966	-1.1784

Prod5j

	Atom	X	Y	Z
1	C	-2.1776	-0.4492	-0.7133
2	N	-3.0745	-1.3156	0.0257
3	C	-2.4243	-2.6202	0.3220
4	C	-4.4534	-1.5300	-0.4532
5	C	-4.7303	-3.0159	-0.1550
6	C	-3.3473	-3.6743	-0.3019
7	H	-2.4136	-2.7608	1.4095
8	C	-2.4988	1.0305	-0.5979
9	C	-2.4522	1.6248	-1.8718
10	N	-2.2032	0.6499	-2.8308
11	C	-2.2328	-0.6285	-2.2857
12	C	-2.8831	1.7818	0.4905
13	C	-3.1336	3.1441	0.2972
14	C	-3.0344	3.7479	-0.9535
15	C	-2.6986	2.9811	-2.0648
16	O	-2.3482	-1.6464	-2.9200
17	H	-2.2851	0.7912	-3.8275
18	N	-3.5115	3.9641	1.4540
19	O	-3.5663	3.4145	2.5504
20	O	-3.7477	5.1520	1.2643
21	H	-5.1558	-0.8661	0.0589
22	H	-4.5400	-1.3444	-1.5306
23	H	-5.0986	-3.1327	0.8692
24	H	-5.4813	-3.4357	-0.8270
25	H	-3.2793	-4.6445	0.1946
26	H	-3.1021	-3.8031	-1.3591
27	H	-3.0037	1.3481	1.4711
28	H	-3.2370	4.8059	-1.0413
29	H	-2.6503	3.4282	-3.0503
30	C	0.0780	0.9368	1.4129
31	C	-0.4830	-0.4563	1.2851
32	C	-0.7484	-0.9250	-0.1660
33	C	0.4279	-0.5402	-1.0937
34	C	1.4462	0.4449	-0.5920
35	C	1.0274	1.3742	0.4752
36	C	1.4927	2.6972	0.5429
37	C	1.0866	3.5423	1.5666
38	C	2.6621	0.3542	-1.1901
39	H	2.6794	-0.3205	-2.0423
40	C	3.9594	0.9558	-0.8807
41	C	-0.9956	-2.4870	-0.2257
42	C	0.0653	-3.3786	0.3907
43	H	-1.0300	-2.7222	-1.2892
44	O	0.5443	-1.0805	-2.1781
45	C	4.3681	1.3331	0.4117
46	C	5.6411	1.8335	0.6372
47	C	6.5612	1.9937	-0.4087
48	C	6.1645	1.6039	-1.6903
49	C	4.8974	1.0799	-1.9191
50	C	1.0820	-3.8866	-0.4308
51	C	2.0804	-4.7091	0.0782
52	C	2.1035	-5.0702	1.4295
53	C	1.0892	-4.5716	2.2489
54	C	0.0895	-3.7430	1.7421

55	H	0.2392	-1.1571	1.7176
56	H	-1.3958	-0.5518	1.8756
57	H	2.1771	3.0594	-0.2138
58	H	1.4545	4.5614	1.6033
59	H	3.6893	1.2133	1.2457
60	H	5.9328	2.1016	1.6478
61	H	6.8604	1.6977	-2.5176
62	H	4.6217	0.7637	-2.9197
63	H	1.0873	-3.6236	-1.4826
64	H	2.8530	-5.0809	-0.5878
65	H	1.0758	-4.8347	3.3020
66	H	-0.6785	-3.3875	2.4188
67	C	0.2008	3.0799	2.5410
68	H	-0.1183	3.7310	3.3465
69	C	-0.3040	1.7876	2.4528
70	H	-1.0236	1.4428	3.1876
71	C	7.9300	2.5723	-0.1518
72	H	8.6076	2.3803	-0.9860
73	H	7.8767	3.6575	-0.0116
74	H	8.3767	2.1515	0.7530
75	C	3.1715	-5.9892	1.9713
76	H	3.2365	-5.9267	3.0596
77	H	2.9617	-7.0328	1.7127
78	H	4.1539	-5.7445	1.5590

TS5j

	Atom	X	Y	Z
1	C	-0.8371	-0.6717	2.1329
2	N	-1.4171	0.4798	2.5414
3	C	-2.3556	1.1652	1.8150
4	C	-0.9737	1.2496	3.7487
5	C	-1.6403	2.6146	3.5644
6	C	-2.8470	2.3248	2.6528
7	H	-3.0789	0.5772	1.2709
8	C	-1.3969	-1.7413	1.3313
9	C	-0.4574	-2.8170	1.3690
10	N	0.6088	-2.4443	2.1499
11	C	0.4449	-1.1648	2.6975
12	C	-2.5850	-1.9323	0.6331
13	C	-2.7954	-3.1535	-0.0131
14	C	-1.8703	-4.1945	0.0207
15	C	-0.6829	-4.0267	0.7262
16	O	1.2331	-0.6423	3.4618
17	H	1.4357	-2.9920	2.3280
18	N	-4.0380	-3.3318	-0.7719
19	O	-4.7932	-2.3658	-0.8717
20	O	-4.2570	-4.4291	-1.2714
21	H	-1.3526	0.7129	4.6248
22	H	0.1080	1.2816	3.7913
23	H	-1.9290	3.0571	4.5184
24	H	-0.9409	3.2879	3.0682
25	H	-3.7239	2.0164	3.2346
26	H	-3.1483	3.1753	2.0398
27	H	-3.3675	-1.1937	0.5742
28	H	-2.0913	-5.1133	-0.5029
29	H	0.0496	-4.8232	0.7696
30	C	0.7102	-0.8444	-1.4970
31	C	-0.4419	0.1230	-1.3726
32	C	-0.3917	1.0268	-0.1747
33	C	0.8688	1.2595	0.5285
34	C	2.1070	0.6051	-0.0234
35	C	1.9289	-0.6168	-0.8342
36	C	2.9212	-1.6132	-0.8976
37	C	2.7447	-2.7589	-1.6588
38	C	3.2665	1.2302	0.2966
39	H	3.1400	2.0212	1.0317
40	C	4.6401	1.0687	-0.1915
41	C	-1.4513	1.8913	0.2004
42	C	-2.5832	2.2628	-0.7032
43	H	-1.0596	2.7502	0.7381
44	O	0.9320	2.0466	1.4814
45	C	4.9607	0.7426	-1.5211
46	C	6.2812	0.6758	-1.9414
47	C	7.3423	0.9216	-1.0594
48	C	7.0264	1.2636	0.2578
49	C	5.7040	1.3515	0.6798
50	C	-2.8036	3.6255	-0.9540
51	C	-3.8389	4.0544	-1.7783
52	C	-4.7099	3.1415	-2.3793
53	C	-4.5050	1.7834	-2.1179
54	C	-3.4655	1.3508	-1.3006

55	H	-0.5067	0.7434	-2.2810
56	H	-1.3663	-0.4615	-1.3702
57	H	3.8386	-1.4798	-0.3402
58	H	3.5292	-3.5067	-1.6968
59	H	4.1651	0.5598	-2.2325
60	H	6.4956	0.4358	-2.9783
61	H	7.8252	1.4774	0.9608
62	H	5.4854	1.6374	1.7033
63	H	-2.1448	4.3595	-0.5016
64	H	-3.9738	5.1173	-1.9522
65	H	-5.1714	1.0458	-2.5532
66	H	-3.3653	0.2867	-1.1281
67	C	1.5581	-2.9464	-2.3705
68	H	1.4140	-3.8343	-2.9757
69	C	0.5490	-1.9983	-2.2712
70	H	-0.3919	-2.1573	-2.7884
71	C	-5.8194	3.6011	-3.2929
72	H	-6.1373	4.6185	-3.0544
73	H	-5.4931	3.5963	-4.3388
74	H	-6.6913	2.9467	-3.2215
75	C	8.7744	0.8137	-1.5216
76	H	9.4557	1.3111	-0.8282
77	H	9.0864	-0.2339	-1.5963
78	H	8.9093	1.2620	-2.5096

Prod4p

	Atom	X	Y	Z
1	C	-0.2832	-0.3357	1.1696
2	N	-1.3000	-1.3684	1.2813
3	C	-2.5036	-0.7540	1.8542
4	C	-1.6512	-2.3257	0.2081
5	C	-3.1658	-2.1574	0.0046
6	C	-3.6596	-1.6365	1.3644
7	H	-2.4421	-0.7478	2.9425
8	C	0.9382	-0.6850	0.3150
9	C	2.0552	-0.8636	1.1560
10	N	1.6915	-0.6501	2.4745
11	C	0.3626	-0.3006	2.6080
12	C	1.1089	-0.8536	-1.0484
13	C	2.3798	-1.1769	-1.5320
14	C	3.4766	-1.3572	-0.6962
15	C	3.3176	-1.1990	0.6750
16	O	-0.1752	-0.0639	3.6651
17	H	2.2955	-0.7576	3.2762
18	N	2.5637	-1.3165	-2.9848
19	O	1.6125	-1.0438	-3.7101
20	O	3.6581	-1.6906	-3.3883
21	H	-1.1014	-2.1359	-0.7105
22	H	-1.4100	-3.3422	0.5404
23	H	-3.3449	-1.4179	-0.7780
24	H	-3.6498	-3.0901	-0.2921
25	H	-4.5994	-1.0835	1.3041
26	H	-3.8093	-2.4654	2.0626
27	H	0.2986	-0.7380	-1.7501
28	H	4.4339	-1.6121	-1.1285
29	H	4.1562	-1.3304	1.3479
30	C	-0.7705	3.5868	1.0727
31	C	-0.3423	2.2384	1.5906
32	C	-1.0502	1.0574	0.8849
33	C	-1.0958	1.2911	-0.6383
34	C	-0.5809	2.5941	-1.1753
35	C	-0.8424	3.7667	-0.3183
36	C	-1.2758	4.9983	-0.8310
37	C	-1.5795	6.0496	0.0249
38	C	0.0276	2.5246	-2.3855
39	H	-0.0424	1.5513	-2.8637
40	C	0.8080	3.4936	-3.1544
41	C	-2.5387	0.7280	1.3409
42	C	-3.2262	1.6924	2.2853
43	H	-3.1296	0.7157	0.4245
44	O	-1.5277	0.4240	-1.3796
45	C	1.4039	4.6494	-2.6151
46	C	2.1750	5.4924	-3.4023
47	C	2.3530	5.1844	-4.7452
48	C	1.8015	4.0479	-5.3153
49	C	1.0449	3.2044	-4.5116
50	C	-2.9164	1.7648	3.6516
51	C	-3.5870	2.6461	4.4960
52	C	-4.5795	3.4571	3.9682
53	C	-4.9228	3.4111	2.6271
54	C	-4.2412	2.5252	1.7976

55	F	-5.2345	4.3131	4.7867
56	F	3.0960	6.0097	-5.5110
57	H	0.7378	2.1310	1.4179
58	H	-0.4923	2.1845	2.6660
59	H	-1.3822	5.1236	-1.9017
60	H	-1.9141	6.9968	-0.3827
61	H	1.2752	4.8848	-1.5679
62	H	2.6432	6.3786	-2.9924
63	H	1.9780	3.8306	-6.3611
64	H	0.6298	2.2982	-4.9382
65	H	-2.1394	1.1314	4.0614
66	H	-3.3537	2.7054	5.5521
67	H	-5.7066	4.0561	2.2500
68	H	-4.5042	2.4842	0.7460
69	C	-1.4694	5.8802	1.4057
70	H	-1.7105	6.6972	2.0760
71	C	-1.0750	4.6502	1.9228
72	H	-1.0195	4.5055	2.9960

TS4p

	Atom	X	Y	Z
1	C	-0.5458	-2.0362	0.4027
2	N	-1.3638	-2.3615	-0.6254
3	C	-2.6863	-1.9961	-0.6823
4	C	-0.9172	-3.0708	-1.8559
5	C	-2.1455	-3.0201	-2.7732
6	C	-3.3252	-2.7660	-1.8174
7	H	-3.1749	-1.9368	0.2801
8	C	0.8866	-2.1929	0.5039
9	C	1.2396	-1.8612	1.8458
10	N	0.0917	-1.5419	2.5343
11	C	-1.0457	-1.6416	1.7286
12	C	1.9071	-2.5218	-0.3861
13	C	3.2193	-2.5329	0.0845
14	C	3.5562	-2.2249	1.4016
15	C	2.5519	-1.8795	2.2994
16	O	-2.1848	-1.4311	2.1372
17	H	0.0311	-1.2751	3.5043
18	N	4.2959	-2.8630	-0.8609
19	O	3.9895	-3.0452	-2.0356
20	O	5.4390	-2.9342	-0.4262
21	H	-0.0668	-2.5593	-2.2926
22	H	-0.6382	-4.0904	-1.5720
23	H	-2.0369	-2.1902	-3.4724
24	H	-2.2583	-3.9378	-3.3509
25	H	-4.1476	-2.2198	-2.2801
26	H	-3.7364	-3.7061	-1.4318
27	H	1.7354	-2.7662	-1.4211
28	H	4.5945	-2.2518	1.6987
29	H	2.7923	-1.6246	3.3243
30	C	-0.9865	2.6195	0.9063
31	C	-1.9480	1.4601	0.7865
32	C	-1.7557	0.6331	-0.4496
33	C	-0.4627	0.5941	-1.1250
34	C	0.6534	1.4200	-0.5419
35	C	0.2606	2.6000	0.2570
36	C	1.0538	3.7615	0.2958
37	C	0.6631	4.8779	1.0196
38	C	1.9024	0.9954	-0.8593
39	H	1.9066	0.2067	-1.6063
40	C	3.2380	1.3485	-0.3717
41	C	-2.8046	-0.0807	-1.0879
42	C	-4.2456	0.2143	-0.8229
43	H	-2.5844	-0.2139	-2.1443
44	O	-0.2838	-0.1226	-2.1225
45	C	3.5041	1.8621	0.9112
46	C	4.8036	2.1063	1.3344
47	C	5.8558	1.8333	0.4701
48	C	5.6449	1.3053	-0.7935
49	C	4.3387	1.0565	-1.1987
50	C	-4.8295	0.1009	0.4485
51	C	-6.1770	0.3884	0.6479
52	C	-6.9447	0.7896	-0.4344
53	C	-6.4091	0.9052	-1.7077
54	C	-5.0617	0.6097	-1.8926

55	F	-8.2531	1.0694	-0.2446
56	F	7.1192	2.0758	0.8814
57	H	-1.8964	0.8243	1.6855
58	H	-2.9672	1.8568	0.7989
59	H	1.9798	3.7879	-0.2631
60	H	1.2924	5.7607	1.0302
61	H	2.6855	2.0624	1.5891
62	H	5.0135	2.4973	2.3224
63	H	6.4903	1.0825	-1.4320
64	H	4.1629	0.6241	-2.1775
65	H	-4.2308	-0.2309	1.2889
66	H	-6.6353	0.3001	1.6251
67	H	-7.0405	1.2200	-2.5291
68	H	-4.6317	0.7029	-2.8839
69	C	-0.5465	4.8669	1.7154
70	H	-0.8606	5.7346	2.2847
71	C	-1.3651	3.7474	1.6411
72	H	-2.3274	3.7491	2.1435

Prod5p

	Atom	X	Y	Z
1	C	-0.1431	0.6384	0.3950
2	C	-0.4540	-0.4806	1.3568
3	C	-0.7090	-1.8444	0.6708
4	C	0.2501	-2.0284	-0.5363
5	C	1.3160	-0.9869	-0.7407
6	C	0.8117	0.3943	-0.6069
7	C	1.1347	1.4146	-1.5132
8	C	0.5498	2.6696	-1.3963
9	C	2.5391	-1.4436	-1.0915
10	H	2.5879	-2.5172	-1.2537
11	C	3.8215	-0.7524	-1.2514
12	C	-2.1755	-2.1155	0.1298
13	C	-3.1406	-0.9478	0.0793
14	H	-2.0352	-2.4411	-0.9000
15	O	0.1290	-2.9658	-1.2957
16	C	4.1409	0.4707	-0.6342
17	C	5.3925	1.0500	-0.7924
18	C	6.3382	0.4044	-1.5781
19	C	6.0734	-0.8093	-2.1925
20	C	4.8207	-1.3842	-2.0131
21	C	-3.8255	-0.4564	1.1994
22	C	-4.7147	0.6112	1.1003
23	C	-4.9235	1.1930	-0.1398
24	C	-4.2758	0.7363	-1.2762
25	C	-3.3922	-0.3314	-1.1545
26	F	-5.7862	2.2284	-0.2441
27	F	7.5534	0.9704	-1.7367
28	H	0.4075	-0.5893	2.0262
29	H	-1.2955	-0.2060	1.9905
30	H	1.8356	1.2151	-2.3146
31	H	0.8062	3.4510	-2.1028
32	H	3.4072	0.9690	-0.0150
33	H	5.6472	1.9875	-0.3140
34	H	6.8403	-1.2889	-2.7876
35	H	4.6053	-2.3406	-2.4765
36	H	-3.6831	-0.9004	2.1761
37	H	-5.2460	0.9858	1.9664
38	H	-4.4662	1.2107	-2.2307
39	H	-2.8826	-0.6933	-2.0408
40	C	-0.3778	2.9175	-0.3838
41	H	-0.8403	3.8939	-0.2957
42	C	-0.7247	1.9016	0.5019
43	H	-1.4613	2.0853	1.2764
44	C	-0.4925	-3.0929	1.7156
45	N	-1.4933	-4.0826	1.3776
46	C	-2.6869	-3.3778	0.8940
47	C	-1.2307	-5.2958	0.5571
48	C	-2.2757	-5.2504	-0.5689
49	C	-3.4177	-4.4057	0.0198
50	H	-3.3249	-3.0719	1.7275
51	C	-0.6378	-2.6508	3.1818
52	C	0.6015	-2.7569	3.8342
53	N	1.5436	-3.2442	2.9415
54	C	0.9930	-3.6042	1.7212

55	C	-1.7386	-2.2606	3.9159
56	C	-1.5669	-1.9381	5.2656
57	C	-0.3318	-2.0156	5.9005
58	C	0.7782	-2.4396	5.1775
59	O	1.6057	-4.1830	0.8589
60	H	2.4909	-3.5047	3.1739
61	N	-2.7395	-1.4977	6.0360
62	O	-3.8063	-1.3903	5.4387
63	O	-2.5849	-1.2589	7.2270
64	H	-0.2165	-5.3078	0.1674
65	H	-1.3712	-6.1823	1.1865
66	H	-1.8453	-4.7588	-1.4430
67	H	-2.6042	-6.2479	-0.8679
68	H	-4.0423	-3.9263	-0.7369
69	H	-4.0700	-5.0215	0.6459
70	H	-2.7310	-2.2050	3.4999
71	H	-0.2587	-1.7539	6.9466
72	H	1.7470	-2.5283	5.6538

TS5p

	Atom	X	Y	Z
1	C	-0.5036	1.7347	-1.6864
2	C	0.6937	1.0176	-1.1027
3	C	0.7777	1.1110	0.3927
4	C	-0.4394	1.2744	1.1843
5	C	-1.7463	1.3391	0.4352
6	C	-1.6857	1.8786	-0.9396
7	C	-2.7373	2.6361	-1.4851
8	C	-2.6469	3.1774	-2.7591
9	C	-2.8336	0.9279	1.1300
10	H	-2.6346	0.7184	2.1770
11	C	-4.2127	0.6482	0.7139
12	C	1.9968	1.1634	1.1300
13	C	3.2942	1.5728	0.5022
14	H	1.8245	1.6708	2.0761
15	O	-0.4007	1.3346	2.4200
16	C	-4.5647	0.1919	-0.5696
17	C	-5.8796	-0.1237	-0.8876
18	C	-6.8589	0.0188	0.0862
19	C	-6.5565	0.4476	1.3689
20	C	-5.2335	0.7447	1.6762
21	C	3.8922	0.8969	-0.5721
22	C	5.1041	1.3200	-1.1119
23	C	5.7246	2.4335	-0.5687
24	C	5.1728	3.1289	0.4963
25	C	3.9643	2.6886	1.0264
26	F	6.9003	2.8501	-1.0859
27	F	-8.1393	-0.2827	-0.2233
28	H	0.6750	-0.0378	-1.4216
29	H	1.6002	1.4313	-1.5510
30	H	-3.6260	2.8105	-0.8927
31	H	-3.4702	3.7602	-3.1567
32	H	-3.7989	0.0782	-1.3256
33	H	-6.1551	-0.4790	-1.8730
34	H	-7.3450	0.5328	2.1062
35	H	-4.9807	1.0622	2.6815
36	H	3.4237	0.0225	-1.0067
37	H	5.5655	0.7937	-1.9379
38	H	5.6859	3.9952	0.8949
39	H	3.5237	3.2309	1.8557
40	C	-1.4906	2.9861	-3.5163
41	H	-1.4110	3.4071	-4.5122
42	C	-0.4258	2.2791	-2.9712
43	H	0.4896	2.1580	-3.5417
44	C	0.3645	-1.6849	1.3841
45	N	1.2342	-1.1721	2.2818
46	C	2.4080	-0.5333	1.9432
47	C	0.9602	-1.0987	3.7527
48	C	2.0496	-0.1582	4.2706
49	C	3.1740	-0.2785	3.2271
50	H	2.9527	-0.9569	1.1118
51	C	0.6107	-2.2319	0.0685
52	C	-0.6370	-2.7458	-0.4037
53	N	-1.5898	-2.5480	0.5661
54	C	-1.0565	-1.9473	1.7132

55	C	1.7277	-2.3722	-0.7503
56	C	1.5796	-2.9969	-1.9905
57	C	0.3596	-3.4896	-2.4469
58	C	-0.7688	-3.3630	-1.6412
59	O	-1.6976	-1.7052	2.7188
60	H	-2.5644	-2.7993	0.5072
61	N	2.7620	-3.1123	-2.8536
62	O	3.7983	-2.5652	-2.4804
63	O	2.6526	-3.7410	-3.8983
64	H	-0.0507	-0.7518	3.9270
65	H	1.0631	-2.1151	4.1471
66	H	1.6603	0.8602	4.2980
67	H	2.3755	-0.4291	5.2754
68	H	3.8075	0.6064	3.1610
69	H	3.8272	-1.1320	3.4422
70	H	2.7142	-2.0392	-0.4724
71	H	0.3098	-3.9581	-3.4192
72	H	-1.7269	-3.7452	-1.9719

Prod9

	Atom	X	Y	Z
1	C	0.0153	-3.4388	5.2768
2	C	-0.8631	-2.6238	4.3601
3	C	-0.3220	-1.1941	4.1395
4	C	1.1076	-1.3698	3.5380
5	C	1.9696	-2.4835	4.0885
6	C	1.4131	-3.3189	5.1720
7	C	2.2193	-3.9701	6.1213
8	C	1.6599	-4.7897	7.0912
9	C	3.1731	-2.6112	3.4745
10	H	3.3937	-1.8012	2.7837
11	C	4.2045	-3.6504	3.5249
12	C	-0.2872	-0.2761	5.4879
13	N	-1.0665	0.8817	5.0811
14	C	-0.9443	1.0791	3.6380
15	C	-1.1740	-0.3433	3.1035
16	C	-2.6152	-0.7778	2.9059
17	H	-0.6738	-0.4398	2.1416
18	C	-0.9882	2.1957	5.7090
19	C	-1.8279	3.0645	4.7346
20	C	-1.8659	2.2782	3.3834
21	H	0.0827	1.3616	3.3644
22	C	-0.8124	-0.8751	6.7848
23	C	0.2119	-0.8899	7.7480
24	N	1.3684	-0.3519	7.2029
25	C	1.1780	0.1086	5.9080
26	C	-2.0830	-1.2763	7.1410
27	C	-2.2892	-1.7399	8.4442
28	C	-1.2681	-1.7852	9.3894
29	C	0.0065	-1.3484	9.0454
30	O	1.9872	0.7414	5.2743
31	H	2.2214	-0.1666	7.7100
32	O	1.4745	-0.6993	2.5970
33	C	3.9224	-5.0195	3.6813
34	C	4.9338	-5.9693	3.6442
35	C	6.2440	-5.5483	3.4574
36	C	6.5666	-4.2115	3.2825
37	C	5.5406	-3.2741	3.2995
38	C	-2.9512	-1.4655	1.7324
39	C	-4.2508	-1.9002	1.4823
40	C	-5.2310	-1.6350	2.4241
41	C	-4.9484	-0.9479	3.5946
42	C	-3.6424	-0.5239	3.8265
43	F	-6.4960	-2.0525	2.1935
44	F	7.2290	-6.4700	3.4313
45	N	-3.6345	-2.1894	8.8305
46	O	-4.5124	-2.1616	7.9742
47	O	-3.8026	-2.5689	9.9836
48	H	-0.9288	-3.1034	3.3750
49	H	-1.8830	-2.5971	4.7415
50	H	3.2921	-3.8320	6.0931
51	H	2.2999	-5.2871	7.8113
52	H	-1.3990	2.1764	6.7216
53	H	0.0460	2.5695	5.7600
54	H	-2.8388	3.2050	5.1210

55	H	-1.3841	4.0549	4.6200
56	H	-2.8827	1.9594	3.1540
57	H	-1.5092	2.8809	2.5468
58	H	-2.9144	-1.2485	6.4529
59	H	-1.4888	-2.1512	10.3821
60	H	0.8090	-1.3583	9.7728
61	H	2.8993	-5.3445	3.8163
62	H	4.7229	-7.0262	3.7501
63	H	7.5983	-3.9244	3.1227
64	H	5.7753	-2.2272	3.1426
65	H	-2.1819	-1.6622	0.9930
66	H	-4.5084	-2.4311	0.5742
67	H	-5.7407	-0.7552	4.3074
68	H	-3.4143	0.0258	4.7297
69	C	0.2763	-4.9705	7.1385
70	H	-0.1662	-5.6198	7.8852
71	C	-0.5353	-4.2832	6.2446
72	H	-1.6136	-4.3825	6.3070

TS9

	Atom	X	Y	Z
1	C	-0.8285	0.8243	-1.2163
2	C	0.2434	-0.2392	-1.2305
3	C	0.1204	-1.2785	-0.1456
4	C	-1.1931	-1.5515	0.4441
5	C	-2.3669	-0.7468	-0.0494
6	C	-2.0843	0.5780	-0.6360
7	C	-3.0078	1.6368	-0.5593
8	C	-2.7274	2.8772	-1.1131
9	C	-3.5699	-1.3521	0.1040
10	H	-3.5230	-2.2607	0.6992
11	C	-4.9051	-1.0350	-0.4137
12	C	1.2668	0.3915	1.9928
13	N	2.1109	-0.6699	2.0609
14	C	1.6533	-1.9625	1.9976
15	C	1.1084	-2.2629	0.1409
16	C	2.3062	-2.5177	-0.7121
17	H	0.6351	-3.1925	0.4510
18	C	3.5901	-0.5861	2.1468
19	C	4.0559	-2.0534	2.1750
20	C	2.7741	-2.8774	2.4309
21	H	0.6518	-2.1251	2.3818
22	C	1.5415	1.7342	1.5479
23	C	0.4051	2.5245	1.9057
24	N	-0.4918	1.7305	2.5733
25	C	-0.0243	0.4096	2.7163
26	C	2.5781	2.3353	0.8388
27	C	2.4718	3.6912	0.5282
28	C	1.3678	4.4631	0.8922
29	C	0.3163	3.8744	1.5860
30	O	-0.5733	-0.4497	3.3779
31	H	-1.3821	2.0215	2.9452
32	O	-1.3461	-2.4634	1.2610
33	C	-5.1318	-0.4465	-1.6708
34	C	-6.4197	-0.2305	-2.1428
35	C	-7.4968	-0.6024	-1.3496
36	C	-7.3216	-1.2017	-0.1123
37	C	-6.0260	-1.4277	0.3389
38	C	2.5859	-3.8490	-1.0644
39	C	3.6823	-4.1879	-1.8510
40	C	4.5217	-3.1770	-2.2912
41	C	4.2920	-1.8489	-1.9653
42	C	3.1881	-1.5299	-1.1801
43	F	5.5887	-3.4918	-3.0554
44	F	-8.7505	-0.3864	-1.8043
45	N	3.5668	4.3239	-0.2170
46	O	4.5192	3.6197	-0.5432
47	O	3.4714	5.5179	-0.4766
48	H	0.2383	-0.7516	-2.2074
49	H	1.2075	0.2686	-1.1865
50	H	-3.9534	1.4779	-0.0579
51	H	-3.4592	3.6748	-1.0476
52	H	4.0070	-0.0405	1.3017
53	H	3.8399	-0.0394	3.0598
54	H	4.4963	-2.3247	1.2164

55	H	4.8103	-2.2146	2.9453
56	H	2.7708	-3.8262	1.8924
57	H	2.6514	-3.1079	3.4944
58	H	3.4653	1.8078	0.5242
59	H	1.3493	5.5095	0.6238
60	H	-0.5537	4.4560	1.8642
61	H	-4.2899	-0.1688	-2.2914
62	H	-6.6002	0.2119	-3.1146
63	H	-8.1865	-1.4918	0.4710
64	H	-5.8747	-1.9116	1.2974
65	H	1.9212	-4.6355	-0.7245
66	H	3.8879	-5.2148	-2.1264
67	H	4.9689	-1.0842	-2.3255
68	H	3.0294	-0.4911	-0.9266
69	C	-1.5034	3.0956	-1.7477
70	H	-1.2771	4.0593	-2.1893
71	C	-0.5614	2.0758	-1.7799
72	H	0.4073	2.2531	-2.2359

Prod9p

	Atom	X	Y	Z
1	C	-1.0669	1.4534	1.1156
2	C	0.2742	0.7661	1.0082
3	C	0.2655	-0.6336	0.3694
4	C	-0.8666	-1.4034	1.1089
5	C	-2.2309	-0.7527	1.1117
6	C	-2.2682	0.7221	1.2185
7	C	-3.4453	1.4264	1.5378
8	C	-3.4515	2.8063	1.6702
9	C	-3.2446	-1.6505	1.0224
10	H	-2.9163	-2.6823	1.1114
11	C	-4.6860	-1.5238	0.7695
12	C	0.0280	-0.6179	-1.2451
13	N	1.2820	-1.1730	-1.7282
14	C	1.7539	-2.1710	-0.7678
15	C	1.6370	-1.4107	0.5633
16	C	2.8366	-0.5659	0.9526
17	H	1.4674	-2.1257	1.3664
18	C	1.4701	-1.7377	-3.0613
19	C	2.8603	-2.4108	-2.9253
20	C	3.0690	-2.6525	-1.3946
21	H	1.0576	-3.0214	-0.7201
22	C	-0.3049	0.7063	-1.9120
23	C	-1.5547	0.6130	-2.5499
24	N	-2.0714	-0.6641	-2.3734
25	C	-1.1989	-1.4941	-1.6834
26	C	0.4394	1.8599	-2.0459
27	C	-0.1150	2.9256	-2.7617
28	C	-1.3678	2.8476	-3.3623
29	C	-2.1041	1.6709	-3.2671
30	O	-1.3516	-2.6816	-1.5271
31	H	-2.9031	-1.0251	-2.8181
32	O	-0.6670	-2.4641	1.6569
33	C	-5.2388	-0.5941	-0.1282
34	C	-6.6012	-0.5763	-0.4000
35	C	-7.4238	-1.4958	0.2361
36	C	-6.9201	-2.4413	1.1159
37	C	-5.5522	-2.4593	1.3619
38	C	3.3536	-0.6865	2.2484
39	C	4.4551	0.0551	2.6709
40	C	5.0484	0.9287	1.7752
41	C	4.5762	1.0757	0.4798
42	C	3.4730	0.3275	0.0778
43	F	6.1174	1.6550	2.1727
44	F	-8.7485	-1.4753	-0.0202
45	N	0.6573	4.1706	-2.8874
46	O	1.7435	4.2257	-2.3203
47	O	0.1718	5.0812	-3.5475
48	H	0.9886	1.4175	0.5068
49	H	0.6690	0.6459	2.0252
50	H	-4.3629	0.8827	1.7069
51	H	-4.3748	3.3175	1.9179
52	H	0.7047	-2.4909	-3.3044
53	H	1.4465	-0.9601	-3.8285
54	H	2.9001	-3.3387	-3.4982

55	H	3.6405	-1.7546	-3.3150
56	H	3.2533	-3.7031	-1.1659
57	H	3.9201	-2.0784	-1.0289
58	H	1.4277	1.9660	-1.6238
59	H	-1.7431	3.7038	-3.9049
60	H	-3.0694	1.5836	-3.7507
61	H	-4.5930	0.1193	-0.6237
62	H	-7.0325	0.1334	-1.0951
63	H	-7.5913	-3.1512	1.5827
64	H	-5.1438	-3.2073	2.0320
65	H	2.8883	-1.3774	2.9436
66	H	4.8541	-0.0395	3.6732
67	H	5.0682	1.7664	-0.1940
68	H	3.1049	0.4245	-0.9354
69	C	-2.2719	3.5294	1.4916
70	H	-2.2696	4.6099	1.5770
71	C	-1.0922	2.8471	1.2288
72	H	-0.1633	3.3981	1.1235

TS9p

	Atom	X	Y	Z
1	C	0.4129	0.3959	-2.3871
2	C	-0.7132	0.1299	-1.4114
3	C	-0.6669	-1.2400	-0.7809
4	C	0.5940	-1.9785	-0.7435
5	C	1.8333	-1.2444	-1.1760
6	C	1.6516	-0.2547	-2.2558
7	C	2.6397	-0.0299	-3.2305
8	C	2.4296	0.8623	-4.2714
9	C	2.9685	-1.6035	-0.5311
10	H	2.8472	-2.4615	0.1245
11	C	4.3077	-1.0047	-0.5022
12	C	-0.5162	-0.2500	2.0598
13	N	-1.6130	-1.0462	2.1337
14	C	-1.6556	-2.2788	1.5134
15	C	-1.8169	-1.9796	-0.3557
16	C	-3.2077	-1.5485	-0.6832
17	H	-1.6638	-3.0418	-0.5440
18	C	-2.8787	-0.7009	2.8263
19	C	-3.7832	-1.9257	2.6010
20	C	-2.8353	-3.0328	2.0894
21	H	-0.7006	-2.7915	1.4399
22	C	-0.4374	1.1861	2.0745
23	C	0.9537	1.5198	2.1040
24	N	1.6830	0.3608	2.1693
25	C	0.8559	-0.7799	2.1860
26	C	-1.3705	2.2160	1.9755
27	C	-0.9080	3.5313	1.9402
28	C	0.4486	3.8545	1.9853
29	C	1.3956	2.8382	2.0613
30	O	1.2544	-1.9187	2.3449
31	H	2.6885	0.2887	2.1935
32	O	0.6515	-3.1308	-0.3040
33	C	4.5582	0.3664	-0.6978
34	C	5.8416	0.8877	-0.5910
35	C	6.8916	0.0317	-0.2869
36	C	6.6904	-1.3222	-0.0692
37	C	5.3984	-1.8266	-0.1649
38	C	-4.0994	-2.4953	-1.2111
39	C	-5.4145	-2.1665	-1.5253
40	C	-5.8462	-0.8678	-1.3044
41	C	-5.0021	0.1021	-0.7848
42	C	-3.6892	-0.2452	-0.4795
43	F	-7.1197	-0.5379	-1.6057
44	F	8.1406	0.5365	-0.1881
45	N	-1.8945	4.6152	1.8427
46	O	-3.0808	4.3040	1.7777
47	O	-1.4810	5.7684	1.8290
48	H	-0.7125	0.9247	-0.6501
49	H	-1.6607	0.2489	-1.9440
50	H	3.5729	-0.5754	-3.1724
51	H	3.2045	1.0176	-5.0135
52	H	-2.6445	-0.5318	3.8809
53	H	-3.3172	0.2124	2.4266
54	H	-4.2965	-2.2135	3.5188

55	H	-4.5418	-1.6988	1.8529
56	H	-2.4806	-3.6643	2.9103
57	H	-3.3112	-3.6884	1.3591
58	H	-2.4357	2.0475	1.9376
59	H	0.7404	4.8945	1.9554
60	H	2.4529	3.0716	2.0870
61	H	3.7384	1.0326	-0.9324
62	H	6.0388	1.9425	-0.7376
63	H	7.5321	-1.9568	0.1786
64	H	5.2253	-2.8810	0.0193
65	H	-3.7526	-3.5068	-1.3917
66	H	-6.0990	-2.8959	-1.9401
67	H	-5.3724	1.1078	-0.6286
68	H	-3.0382	0.5161	-0.0703
69	C	1.2148	1.5424	-4.3703
70	H	1.0416	2.2400	-5.1818
71	C	0.2150	1.2967	-3.4375
72	H	-0.7422	1.8004	-3.5288

Prod10

	Atom	X	Y	Z
1	C	0.5890	-4.6836	-0.2556
2	N	1.0166	-6.0444	-0.3790
3	C	1.8987	-6.5121	0.7053
4	C	1.3845	-6.6460	-1.6653
5	C	2.4316	-7.7104	-1.2805
6	C	3.1012	-7.1225	-0.0254
7	H	1.3826	-7.3172	1.2425
8	C	-0.8599	-4.4234	-0.7030
9	C	-0.8943	-3.3441	-1.6000
10	N	0.4020	-2.8852	-1.8297
11	C	1.3497	-3.6824	-1.2207
12	C	-2.0283	-5.1128	-0.4366
13	C	-3.2126	-4.6510	-1.0184
14	C	-3.2517	-3.5536	-1.8737
15	C	-2.0714	-2.8856	-2.1820
16	O	2.5372	-3.6167	-1.4433
17	H	0.6598	-2.2303	-2.5547
18	N	-4.4717	-5.3530	-0.7153
19	O	-4.4335	-6.2635	0.1034
20	O	-5.4859	-4.9820	-1.2953
21	H	0.5166	-7.0864	-2.1674
22	H	1.8292	-5.9087	-2.3462
23	H	1.9348	-8.6541	-1.0364
24	H	3.1367	-7.9048	-2.0909
25	H	3.6214	-7.8732	0.5734
26	H	3.8225	-6.3545	-0.3095
27	H	-2.0391	-5.9788	0.2071
28	H	-4.1993	-3.2476	-2.2938
29	H	-2.0726	-2.0459	-2.8665
30	C	1.2586	-2.3901	2.8949
31	C	1.2300	-2.8117	1.4487
32	C	0.9115	-4.3115	1.2688
33	C	-0.3003	-4.7117	2.1568
34	C	-0.8193	-3.6963	3.1374
35	C	0.1996	-2.8016	3.7204
36	C	0.2151	-2.4546	5.0796
37	C	1.2388	-1.6691	5.5946
38	C	-2.1487	-3.7680	3.3907
39	H	-2.6425	-4.6234	2.9364
40	C	-3.0520	-2.8867	4.1318
41	C	2.0600	-5.3307	1.7105
42	C	3.4626	-4.8067	1.9834
43	H	1.7404	-5.7248	2.6753
44	O	-0.7872	-5.8214	2.0777
45	C	-2.8043	-1.5231	4.3754
46	C	-3.7309	-0.7339	5.0420
47	C	-4.9179	-1.3105	5.4758
48	C	-5.2119	-2.6449	5.2433
49	C	-4.2822	-3.4189	4.5599
50	C	4.2947	-4.1898	1.0380
51	C	5.5790	-3.7661	1.3729
52	C	6.0403	-3.9644	2.6641
53	C	5.2553	-4.5723	3.6292
54	C	3.9736	-4.9851	3.2775

55	F	7.2875	-3.5538	2.9904
56	F	-5.8147	-0.5443	6.1305
57	H	0.4499	-2.2348	0.9355
58	H	2.1758	-2.5638	0.9698
59	H	-0.5733	-2.8111	5.7312
60	H	1.2395	-1.4079	6.6468
61	H	-1.8848	-1.0720	4.0284
62	H	-3.5516	0.3183	5.2247
63	H	-6.1549	-3.0548	5.5825
64	H	-4.5078	-4.4593	4.3544
65	H	3.9408	-4.0296	0.0295
66	H	6.2219	-3.2900	0.6425
67	H	5.6429	-4.7124	4.6306
68	H	3.3544	-5.4552	4.0339
69	C	2.2708	-1.2322	4.7632
70	H	3.0735	-0.6238	5.1640
71	C	2.2815	-1.6016	3.4219
72	H	3.0980	-1.2904	2.7794

TS10

	Atom	X	Y	Z
1	C	0.9170	1.8549	0.6202
2	N	2.0229	2.1139	-0.1264
3	C	2.1647	1.6636	-1.4206
4	C	3.2384	2.7965	0.3897
5	C	4.2042	2.8021	-0.8095
6	C	3.3396	2.4012	-2.0287
7	H	1.2434	1.5776	-1.9893
8	C	-0.4654	2.1173	0.3020
9	C	-1.2062	1.9039	1.5007
10	N	-0.3301	1.5089	2.4948
11	C	0.9896	1.4746	2.0364
12	C	-1.1289	2.5742	-0.8320
13	C	-2.5044	2.7912	-0.7403
14	C	-3.2305	2.5736	0.4298
15	C	-2.5731	2.1307	1.5747
16	O	1.9539	1.1068	2.6979
17	H	-0.5777	1.2483	3.4363
18	N	-3.2189	3.2632	-1.9357
19	O	-2.5509	3.5842	-2.9121
20	O	-4.4443	3.3089	-1.8901
21	H	2.9413	3.8052	0.6899
22	H	3.6235	2.2820	1.2683
23	H	4.6654	3.7812	-0.9424
24	H	5.0023	2.0774	-0.6571
25	H	2.9675	3.2831	-2.5603
26	H	3.8872	1.7950	-2.7510
27	H	-0.6304	2.7632	-1.7698
28	H	-4.2959	2.7520	0.4272
29	H	-3.1204	1.9693	2.4953
30	C	0.5661	-2.7119	0.8727
31	C	1.5927	-1.6241	0.6522
32	C	1.3636	-0.7994	-0.5872
33	C	0.0343	-0.7288	-1.1856
34	C	-1.0880	-1.4376	-0.4809
35	C	-0.7217	-2.6234	0.3193
36	C	-1.5879	-3.7241	0.4521
37	C	-1.2184	-4.8462	1.1778
38	C	-2.3204	-0.9145	-0.7004
39	H	-2.3279	-0.1435	-1.4655
40	C	-3.6283	-1.1473	-0.0848
41	C	2.4287	-0.2113	-1.3508
42	C	3.8585	-0.5188	-1.0451
43	H	2.2138	-0.2937	-2.4161
44	O	-0.1721	-0.0558	-2.2065
45	C	-3.8135	-1.6185	1.2286
46	C	-5.0829	-1.7509	1.7743
47	C	-6.1863	-1.4108	1.0020
48	C	-6.0528	-0.9222	-0.2877
49	C	-4.7741	-0.7801	-0.8146
50	C	4.4114	-0.4187	0.2427
51	C	5.7512	-0.7136	0.4772
52	C	6.5476	-1.1106	-0.5866
53	C	6.0445	-1.2190	-1.8735
54	C	4.7028	-0.9197	-2.0912

55	F	7.8475	-1.3997	-0.3623
56	F	-7.4213	-1.5465	1.5313
57	H	1.6644	-0.9948	1.5529
58	H	2.5736	-2.1021	0.5804
59	H	-2.5543	-3.6980	-0.0340
60	H	-1.9028	-5.6827	1.2630
61	H	-2.9537	-1.8741	1.8330
62	H	-5.2305	-2.1084	2.7860
63	H	-6.9341	-0.6481	-0.8537
64	H	-4.6572	-0.3754	-1.8134
65	H	3.7983	-0.0943	1.0749
66	H	6.1806	-0.6383	1.4686
67	H	6.6945	-1.5367	-2.6792
68	H	4.2993	-1.0131	-3.0938
69	C	0.0396	-4.9016	1.7801
70	H	0.3369	-5.7741	2.3508
71	C	0.9238	-3.8442	1.6117
72	H	1.9184	-3.8992	2.0430

Prod10p

	Atom	X	Y	Z
1	C	1.3317	-2.7082	-3.6607
2	N	2.4493	-2.2428	-4.4554
3	C	2.8035	-0.8756	-4.1032
4	C	2.5811	-2.4054	-5.8954
5	C	3.7960	-1.4907	-6.2265
6	C	4.0620	-0.6442	-4.9430
7	H	2.0316	-0.1546	-4.4190
8	C	-0.0510	-2.6334	-4.3283
9	C	-0.5864	-3.9318	-4.4183
10	N	0.3060	-4.8448	-3.8742
11	C	1.4822	-4.2545	-3.4559
12	C	-0.7470	-1.5798	-4.8942
13	C	-1.9797	-1.8490	-5.4987
14	C	-2.5226	-3.1289	-5.5542
15	C	-1.8169	-4.1964	-5.0099
16	O	2.4515	-4.8504	-3.0509
17	H	0.1695	-5.8437	-3.8358
18	N	-2.7327	-0.7355	-6.0979
19	O	-2.2181	0.3761	-6.0795
20	O	-3.8313	-0.9846	-6.5820
21	H	2.7578	-3.4526	-6.1567
22	H	1.6867	-2.0680	-6.4419
23	H	4.6746	-2.0824	-6.4872
24	H	3.5674	-0.8561	-7.0847
25	H	4.9448	-1.0121	-4.4203
26	H	4.2167	0.4122	-5.1690
27	H	-0.3889	-0.5617	-4.8636
28	H	-3.4834	-3.2712	-6.0284
29	H	-2.2138	-5.2032	-5.0566
30	C	0.4154	-3.4911	-0.6995
31	C	1.6665	-2.7087	-1.0080
32	C	1.5188	-1.8530	-2.2872
33	C	0.2843	-0.9301	-2.0892
34	C	-0.8412	-1.4260	-1.2186
35	C	-0.8293	-2.8520	-0.8357
36	C	-2.0031	-3.6029	-0.6661
37	C	-1.9421	-4.9404	-0.2977
38	C	-1.7441	-0.4760	-0.8657
39	H	-1.6010	0.4724	-1.3778
40	C	-2.8429	-0.4738	0.1008
41	C	2.7794	-0.9232	-2.5631
42	C	4.0859	-1.3304	-1.9065
43	H	2.5267	0.0682	-2.1897
44	O	0.2614	0.1815	-2.5836
45	C	-2.8482	-1.2374	1.2825
46	C	-3.8905	-1.1408	2.1934
47	C	-4.9452	-0.2793	1.9192
48	C	-4.9744	0.5037	0.7755
49	C	-3.9130	0.4132	-0.1165
50	C	4.7494	-2.5363	-2.1816
51	C	5.9651	-2.8410	-1.5758
52	C	6.5225	-1.9331	-0.6881
53	C	5.9008	-0.7333	-0.3877
54	C	4.6843	-0.4439	-1.0030

55	F	7.7035	-2.2294	-0.0972
56	F	-5.9630	-0.1930	2.7996
57	H	1.8944	-2.0211	-0.1838
58	H	2.5163	-3.3806	-1.0935
59	H	-2.9653	-3.1338	-0.8273
60	H	-2.8584	-5.5052	-0.1670
61	H	-2.0208	-1.8996	1.4986
62	H	-3.8957	-1.7148	3.1116
63	H	-5.8068	1.1746	0.6046
64	H	-3.9131	1.0341	-1.0054
65	H	4.3029	-3.2488	-2.8628
66	H	6.4794	-3.7720	-1.7809
67	H	6.3638	-0.0468	0.3103
68	H	4.1941	0.4972	-0.7764
69	C	-0.7040	-5.5552	-0.1015
70	H	-0.6524	-6.5964	0.1967
71	C	0.4654	-4.8336	-0.3161
72	H	1.4303	-5.3173	-0.2134

TS10p

	Atom	X	Y	Z
1	C	-1.4454	1.6969	0.9462
2	N	-2.5443	1.7911	0.1497
3	C	-2.5200	1.4734	-1.1818
4	C	-3.9152	2.0899	0.6470
5	C	-4.8095	1.9314	-0.5948
6	C	-3.8326	1.9019	-1.7943
7	H	-1.5890	1.6583	-1.7077
8	C	-0.1463	2.3123	0.7709
9	C	0.5420	2.1562	2.0068
10	N	-0.2834	1.4913	2.8951
11	C	-1.5181	1.1827	2.3232
12	C	0.4621	3.0174	-0.2611
13	C	1.7432	3.5240	-0.0387
14	C	2.4285	3.3501	1.1627
15	C	1.8193	2.6612	2.2083
16	O	-2.4144	0.5522	2.8731
17	H	-0.0044	1.1179	3.7890
18	N	2.3980	4.2723	-1.1219
19	O	1.7445	4.5058	-2.1327
20	O	3.5605	4.6257	-0.9535
21	H	-4.1720	1.4288	1.4722
22	H	-3.9045	3.1165	1.0236
23	H	-5.3693	0.9990	-0.5420
24	H	-5.5285	2.7474	-0.6732
25	H	-4.1598	1.2283	-2.5877
26	H	-3.7142	2.8950	-2.2408
27	H	-0.0032	3.1766	-1.2212
28	H	3.4229	3.7607	1.2626
29	H	2.3290	2.5321	3.1552
30	C	0.1708	-1.6964	1.5332
31	C	-1.0954	-1.6894	0.7118
32	C	-1.0907	-0.7327	-0.4527
33	C	0.1832	-0.3039	-1.0295
34	C	1.4472	-0.8548	-0.4307
35	C	1.3961	-1.2894	0.9798
36	C	2.5215	-1.2112	1.8206
37	C	2.4512	-1.5941	3.1518
38	C	2.5060	-0.8859	-1.2776
39	H	2.3268	-0.3673	-2.2161
40	C	3.8240	-1.5200	-1.1797
41	C	-2.2372	-0.4679	-1.2599
42	C	-3.5286	-1.1971	-1.0945
43	H	-1.9594	-0.3702	-2.3078
44	O	0.2171	0.4387	-2.0191
45	C	4.0526	-2.7375	-0.5137
46	C	5.3087	-3.3289	-0.5084
47	C	6.3517	-2.6958	-1.1711
48	C	6.1690	-1.5037	-1.8543
49	C	4.9013	-0.9332	-1.8670
50	C	-4.2056	-1.3424	0.1284
51	C	-5.4070	-2.0396	0.2108
52	C	-5.9431	-2.5959	-0.9410
53	C	-5.3163	-2.4688	-2.1700
54	C	-4.1161	-1.7672	-2.2354

55	F	-7.1075	-3.2754	-0.8625
56	F	7.5756	-3.2665	-1.1603
57	H	-1.2929	-2.7034	0.3264
58	H	-1.9218	-1.4769	1.3907
59	H	3.4545	-0.8355	1.4225
60	H	3.3340	-1.5294	3.7781
61	H	3.2344	-3.2333	-0.0081
62	H	5.4889	-4.2721	-0.0078
63	H	7.0038	-1.0468	-2.3707
64	H	4.7412	-0.0089	-2.4107
65	H	-3.8090	-0.8939	1.0304
66	H	-5.9294	-2.1526	1.1527
67	H	-5.7627	-2.9150	-3.0499
68	H	-3.6160	-1.6709	-3.1930
69	C	1.2435	-2.0542	3.6818
70	H	1.1817	-2.3638	4.7191
71	C	0.1135	-2.0891	2.8747
72	H	-0.8384	-2.4014	3.2909

Prod11

	Atom	X	Y	Z
1	C	-2.0748	2.4902	-1.5909
2	C	-1.9291	1.2382	-0.7582
3	C	-1.9888	-0.0222	-1.5738
4	C	-1.3620	0.0003	-2.9238
5	C	-0.9029	1.3511	-3.5465
6	C	-1.5612	2.5686	-2.8954
7	C	-1.6556	3.7985	-3.5674
8	C	-2.2642	4.9021	-2.9816
9	C	0.7013	1.3291	-3.5052
10	H	0.9338	0.2729	-3.6390
11	C	1.3933	1.7419	-2.2231
12	C	-2.5704	-1.1847	-1.2035
13	C	-3.2319	-1.5552	0.0468
14	H	-2.5662	-1.9585	-1.9668
15	O	-1.1670	-1.0314	-3.5450
16	C	1.3223	3.0323	-1.6748
17	C	1.9604	3.3367	-0.4758
18	C	2.6738	2.3452	0.1799
19	C	2.7722	1.0600	-0.3270
20	C	2.1286	0.7711	-1.5273
21	C	-4.2464	-2.5302	-0.0055
22	C	-4.9248	-2.9366	1.1349
23	C	-4.5649	-2.3798	2.3540
24	C	-3.5474	-1.4434	2.4606
25	C	-2.8871	-1.0346	1.3079
26	F	-5.2117	-2.7735	3.4700
27	F	3.2926	2.6415	1.3449
28	H	-0.9679	1.2853	-0.2253
29	H	-2.7043	1.2271	0.0097
30	H	-1.2029	3.8977	-4.5419
31	H	-2.3132	5.8372	-3.5281
32	H	0.7777	3.8111	-2.1877
33	H	1.9099	4.3308	-0.0491
34	H	3.3402	0.3101	0.2093
35	H	2.1973	-0.2341	-1.9290
36	H	-4.5096	-2.9657	-0.9629
37	H	-5.7138	-3.6772	1.0958
38	H	-3.2779	-1.0567	3.4354
39	H	-2.0675	-0.3354	1.3998
40	C	-2.7980	4.8065	-1.6995
41	H	-3.2812	5.6595	-1.2362
42	C	-2.6950	3.6036	-1.0146
43	H	-3.0957	3.5187	-0.0094
44	C	1.1888	1.9784	-4.8835
45	N	-0.0545	2.1545	-5.6012
46	C	-1.0748	1.2495	-5.0899
47	C	-0.2087	2.2225	-7.0440
48	C	-1.7528	2.2603	-7.1962
49	C	-2.3309	1.6529	-5.8758
50	H	-0.8472	0.2048	-5.3431
51	C	2.2728	1.1081	-5.5211
52	C	3.4564	1.8569	-5.6434
53	N	3.2407	3.1431	-5.1643
54	C	1.9283	3.3512	-4.7700

55	C	2.2480	-0.2048	-5.9494
56	C	3.4177	-0.7379	-6.5038
57	C	4.5917	0.0003	-6.6187
58	C	4.6223	1.3211	-6.1805
59	O	1.4672	4.4167	-4.4441
60	H	3.9105	3.8975	-5.1943
61	N	3.4070	-2.1306	-6.9791
62	O	2.3560	-2.7537	-6.8888
63	O	4.4483	-2.5855	-7.4384
64	H	0.2777	3.1110	-7.4552
65	H	0.2090	1.3392	-7.5545
66	H	-2.0944	3.2894	-7.3191
67	H	-2.0723	1.7037	-8.0787
68	H	-2.9269	2.3913	-5.3410
69	H	-2.9647	0.7856	-6.0662
70	H	1.3702	-0.8314	-5.8654
71	H	5.4647	-0.4696	-7.0491
72	H	5.5290	1.9083	-6.2611

TS11

	Atom	X	Y	Z
1	C	2.2664	1.9131	0.8714
2	C	3.1445	0.8362	0.2802
3	C	2.4970	-0.5237	0.2646
4	C	1.0215	-0.5806	0.0014
5	C	0.2613	0.6622	0.0703
6	C	0.8656	1.8450	0.6995
7	C	0.0920	2.9006	1.2220
8	C	0.6791	3.9764	1.8826
9	C	-1.0059	0.6205	-0.6509
10	H	-1.0996	-0.3927	-1.0279
11	C	-1.3657	1.5546	-1.7742
12	C	3.1280	-1.7040	0.4370
13	C	4.5452	-1.9982	0.6646
14	H	2.4728	-2.5710	0.4169
15	O	0.4795	-1.6780	-0.2442
16	C	-1.1044	2.9328	-1.8215
17	C	-1.4472	3.6959	-2.9333
18	C	-2.0628	3.0822	-4.0123
19	C	-2.3342	1.7242	-4.0156
20	C	-1.9786	0.9741	-2.8991
21	C	4.8731	-3.1507	1.4039
22	C	6.1908	-3.5010	1.6657
23	C	7.2037	-2.6992	1.1596
24	C	6.9324	-1.5747	0.3962
25	C	5.6068	-1.2302	0.1525
26	F	8.4899	-3.0339	1.4031
27	F	-2.4005	3.8254	-5.0908
28	H	3.3873	1.1239	-0.7553
29	H	4.0941	0.8046	0.8177
30	H	-0.9842	2.8919	1.1082
31	H	0.0508	4.7739	2.2648
32	H	-0.6201	3.4259	-0.9935
33	H	-1.2404	4.7584	-2.9693
34	H	-2.7976	1.2683	-4.8818
35	H	-2.1657	-0.0936	-2.9081
36	H	4.0730	-3.7766	1.7833
37	H	6.4426	-4.3822	2.2426
38	H	7.7519	-0.9926	-0.0068
39	H	5.4018	-0.3770	-0.4791
40	C	2.0600	4.0278	2.0506
41	H	2.5247	4.8601	2.5666
42	C	2.8397	2.9917	1.5412
43	H	3.9187	3.0223	1.6599
44	C	-2.5402	0.4868	0.5378
45	N	-1.9744	0.3207	1.8343
46	C	-0.9726	-0.5014	2.0458
47	C	-2.3567	1.0750	3.0687
48	C	-1.1591	0.8408	3.9994
49	C	-0.5067	-0.4529	3.4618
50	H	-0.6930	-1.2593	1.3228
51	C	-3.3624	-0.6251	-0.0287
52	C	-4.5014	-0.0543	-0.6362
53	N	-4.4868	1.3159	-0.4180
54	C	-3.4175	1.7119	0.3666

55	C	-3.1712	-1.9943	-0.0862
56	C	-4.1432	-2.7609	-0.7365
57	C	-5.2590	-2.1990	-1.3500
58	C	-5.4474	-0.8200	-1.3058
59	O	-3.2410	2.8405	0.7818
60	H	-5.1725	1.9765	-0.7510
61	N	-3.9755	-4.2240	-0.7777
62	O	-3.0412	-4.7063	-0.1500
63	O	-4.7851	-4.8723	-1.4301
64	H	-2.5374	2.1176	2.8283
65	H	-3.2817	0.6324	3.4517
66	H	-0.4587	1.6718	3.9105
67	H	-1.4654	0.7581	5.0421
68	H	0.5840	-0.4520	3.5191
69	H	-0.8510	-1.3510	3.9909
70	H	-2.3007	-2.4864	0.3239
71	H	-5.9637	-2.8477	-1.8504
72	H	-6.3130	-0.3653	-1.7718

Prod11p

	Atom	X	Y	Z
1	C	1.5427	0.7529	-0.7936
2	C	1.7368	-0.5362	-0.0301
3	C	1.8375	-1.7403	-0.9229
4	C	0.9839	-1.7677	-2.1422
5	C	0.2242	-0.4847	-2.5894
6	C	0.7985	0.7969	-1.9835
7	C	0.5865	2.0501	-2.5815
8	C	1.1180	3.2139	-2.0387
9	C	-1.3253	-0.7622	-2.2761
10	H	-1.4173	-1.8362	-2.4359
11	C	-1.8309	-0.5120	-0.8708
12	C	2.6425	-2.8092	-0.7321
13	C	3.5639	-3.1163	0.3609
14	H	2.6177	-3.5454	-1.5314
15	O	0.8379	-2.7936	-2.7861
16	C	-1.8567	0.7522	-0.2609
17	C	-2.3085	0.9071	1.0464
18	C	-2.7369	-0.2085	1.7493
19	C	-2.7310	-1.4735	1.1851
20	C	-2.2764	-1.6121	-0.1236
21	C	4.6865	-3.9166	0.0743
22	C	5.6101	-4.2525	1.0541
23	C	5.3946	-3.8043	2.3497
24	C	4.2846	-3.0446	2.6877
25	C	3.3759	-2.7031	1.6929
26	F	6.2812	-4.1318	3.3117
27	F	-3.1747	-0.0573	3.0194
28	H	2.6296	-0.4526	0.5918
29	H	0.8902	-0.6614	0.6610
30	H	-0.0427	2.1122	-3.4560
31	H	0.9283	4.1644	-2.5244
32	H	-1.5351	1.6258	-0.8082
33	H	-2.3317	1.8801	1.5212
34	H	-3.0755	-2.3231	1.7612
35	H	-2.2647	-2.5999	-0.5714
36	H	4.8365	-4.2698	-0.9397
37	H	6.4807	-4.8574	0.8339
38	H	4.1388	-2.7412	3.7168
39	H	2.4912	-2.1456	1.9676
40	C	1.8804	3.1570	-0.8753
41	H	2.3056	4.0581	-0.4477
42	C	2.0824	1.9285	-0.2614
43	H	2.6643	1.8713	0.6530
44	C	-2.1427	-0.1478	-3.5063
45	N	-1.0882	0.2492	-4.4130
46	C	0.1307	-0.5009	-4.1427
47	C	-1.2064	0.3942	-5.8536
48	C	0.2625	0.6813	-6.2647
49	C	1.1514	0.1253	-5.1041
50	H	0.0203	-1.5584	-4.4197
51	C	-3.1809	-1.1547	-4.0038
52	C	-4.4657	-0.5987	-3.8738
53	N	-4.3623	0.6869	-3.3571
54	C	-3.0466	1.0854	-3.1802

55	C	-3.0373	-2.4304	-4.5134
56	C	-4.1943	-3.1211	-4.8928
57	C	-5.4667	-2.5744	-4.7579
58	C	-5.6154	-1.2921	-4.2371
59	O	-2.6992	2.1977	-2.8700
60	H	-5.1318	1.3262	-3.2235
61	N	-4.0608	-4.4761	-5.4514
62	O	-2.9295	-4.9278	-5.5821
63	O	-5.0876	-5.0729	-5.7541
64	H	-1.5722	-0.5245	-6.3409
65	H	-1.8855	1.2092	-6.1176
66	H	0.4984	0.2148	-7.2225
67	H	0.4190	1.7553	-6.3783
68	H	1.8635	-0.6229	-5.4551
69	H	1.7160	0.9286	-4.6327
70	H	-2.0750	-2.9128	-4.6210
71	H	-6.3225	-3.1603	-5.0621
72	H	-6.5993	-0.8533	-4.1238

TS11p

	Atom	X	Y	Z
1	C	2.6445	-1.8557	0.6760
2	C	3.5203	-0.7747	0.0890
3	C	2.8730	0.5854	0.0860
4	C	1.3963	0.6447	-0.1699
5	C	0.6360	-0.5982	-0.1062
6	C	1.2430	-1.7859	0.5111
7	C	0.4714	-2.8453	1.0292
8	C	1.0613	-3.9262	1.6789
9	C	-0.6346	-0.5509	-0.8211
10	H	-0.7298	0.4652	-1.1900
11	C	-1.0002	-1.4765	-1.9495
12	C	3.5052	1.7643	0.2637
13	C	4.9236	2.0566	0.4867
14	H	2.8503	2.6316	0.2527
15	O	0.8537	1.7440	-0.4051
16	C	-0.7387	-2.8541	-2.0086
17	C	-1.0871	-3.6090	-3.1244
18	C	-1.7087	-2.9874	-4.1954
19	C	-1.9805	-1.6295	-4.1870
20	C	-1.6193	-0.8878	-3.0667
21	C	5.2552	3.2040	1.2321
22	C	6.5743	3.5522	1.4903
23	C	7.5845	2.7535	0.9742
24	C	7.3094	1.6342	0.2046
25	C	5.9826	1.2917	-0.0354
26	F	8.8720	3.0861	1.2141
27	F	-2.0519	-3.7225	-5.2776
28	H	4.4721	-0.7471	0.6228
29	H	3.7587	-1.0549	-0.9495
30	H	-0.6052	-2.8355	0.9205
31	H	0.4345	-4.7265	2.0579
32	H	-0.2497	-3.3533	-1.1870
33	H	-0.8800	-4.6710	-3.1695
34	H	-2.4487	-1.1672	-5.0472
35	H	-1.8067	0.1799	-3.0667
36	H	4.4571	3.8276	1.6194
37	H	6.8289	4.4295	2.0719
38	H	8.1269	1.0545	-0.2060
39	H	5.7744	0.4427	-0.6717
40	C	2.4430	-3.9794	1.8400
41	H	2.9098	-4.8157	2.3476
42	C	3.2206	-2.9395	1.3349
43	H	4.3001	-2.9713	1.4483
44	C	-2.1633	-0.4255	0.3761
45	N	-1.5910	-0.2688	1.6710
46	C	-0.5878	0.5515	1.8831
47	C	-1.9670	-1.0323	2.9017
48	C	-0.7645	-0.8050	3.8279
49	C	-0.1147	0.4925	3.2964
50	H	-0.3120	1.3147	1.1644
51	C	-2.9881	0.6905	-0.1783
52	C	-4.1300	0.1243	-0.7844
53	N	-4.1145	-1.2474	-0.5763
54	C	-3.0416	-1.6492	0.2003

55	C	-2.7969	2.0601	-0.2268
56	C	-3.7719	2.8315	-0.8668
57	C	-4.8908	2.2742	-1.4789
58	C	-5.0792	0.8950	-1.4439
59	O	-2.8634	-2.7808	0.6065
60	H	-4.8022	-1.9054	-0.9104
61	N	-3.6043	4.2949	-0.8981
62	O	-2.6668	4.7725	-0.2715
63	O	-4.4170	4.9481	-1.5418
64	H	-2.8898	-0.5924	3.2928
65	H	-2.1490	-2.0730	2.6545
66	H	-1.0654	-0.7300	4.8727
67	H	-0.0647	-1.6354	3.7292
68	H	-0.4561	1.3867	3.8338
69	H	0.9764	0.4910	3.3480
70	H	-1.9244	2.5492	0.1828
71	H	-5.5978	2.9266	-1.9712
72	H	-5.9471	0.4438	-1.9090

Prod13

	Atom	X	Y	Z
1	C	-1.6622	1.1810	-0.3583
2	C	-1.3132	-0.2328	0.0374
3	C	-1.6608	-1.2215	-1.0388
4	C	-1.4518	-0.7984	-2.4559
5	C	-0.9750	0.6460	-2.7546
6	C	-1.4791	1.6268	-1.6800
7	C	-1.7685	2.9740	-1.9516
8	C	-2.2424	3.8355	-0.9672
9	C	0.6210	0.4803	-2.8670
10	H	0.7863	-0.5944	-2.9595
11	C	1.5215	0.9276	-1.7331
12	C	-2.1634	-2.4612	-0.8502
13	C	-2.4440	-3.1901	0.3863
14	H	-2.4214	-2.9899	-1.7643
15	O	-1.5731	-1.5996	-3.3688
16	C	1.5824	2.2454	-1.2550
17	C	2.4471	2.5967	-0.2221
18	C	3.2607	1.6241	0.3367
19	C	3.2372	0.3118	-0.1066
20	C	2.3650	-0.0230	-1.1385
21	C	-3.4720	-4.1521	0.3681
22	C	-3.8034	-4.8849	1.4993
23	C	-3.0770	-4.6734	2.6625
24	C	-2.0320	-3.7633	2.7189
25	C	-1.7214	-3.0256	1.5825
26	F	-3.3847	-5.3859	3.7655
27	F	4.1004	1.9645	1.3399
28	H	-0.2374	-0.2820	0.2584
29	H	-1.8298	-0.4852	0.9645
30	H	-1.5846	3.3903	-2.9297
31	H	-2.4504	4.8688	-1.2209
32	H	0.9532	3.0094	-1.6870
33	H	2.4922	3.6118	0.1524
34	H	3.8892	-0.4232	0.3486
35	H	2.3415	-1.0494	-1.4889
36	H	-4.0241	-4.3156	-0.5505
37	H	-4.6016	-5.6164	1.4912
38	H	-1.4713	-3.6507	3.6384
39	H	-0.8808	-2.3464	1.6190
40	C	-2.4437	3.3743	0.3288
41	H	-2.8213	4.0356	1.1004
42	C	-2.1476	2.0500	0.6221
43	H	-2.2911	1.6750	1.6303
44	C	0.9873	0.9986	-4.3178
45	N	-0.2192	0.8299	-5.1144
46	C	-1.3651	1.0988	-4.2369
47	C	-0.4757	-0.3927	-5.8926
48	C	-1.9789	-0.2810	-6.1809
49	C	-2.5784	0.4844	-4.9708
50	H	-1.4841	2.1737	-4.1904
51	C	2.2486	0.3691	-4.8808
52	C	3.1507	1.3831	-5.2501
53	N	2.5907	2.6211	-4.9742
54	C	1.3364	2.5207	-4.3974

55	C	2.6148	-0.9532	-5.0271
56	C	3.8741	-1.2337	-5.5687
57	C	4.7600	-0.2313	-5.9514
58	C	4.4026	1.1034	-5.7887
59	O	0.6531	3.4641	-4.0741
60	H	3.0199	3.5154	-5.1607
61	N	4.2770	-2.6389	-5.7313
62	O	3.4935	-3.5022	-5.3526
63	O	5.3717	-2.8651	-6.2329
64	H	0.1251	-0.3921	-6.8046
65	H	-0.2717	-1.3114	-5.3322
66	H	-2.1371	0.2891	-7.0995
67	H	-2.4309	-1.2651	-6.3125
68	H	-3.2459	1.2802	-5.3075
69	H	-3.1569	-0.1751	-4.3300
70	H	1.9700	-1.7741	-4.7470
71	H	5.7192	-0.5103	-6.3643
72	H	5.0855	1.8957	-6.0698

Prod13p

	Atom	X	Y	Z
1	C	-0.5505	0.8887	0.5605
2	C	-1.4922	0.0106	-0.2309
3	C	-2.0408	-1.1478	0.5526
4	C	-1.1229	-1.8135	1.5182
5	C	0.0589	-1.0400	2.1415
6	C	0.1878	0.4024	1.6482
7	C	1.0501	1.2952	2.3086
8	C	1.1785	2.6190	1.9085
9	C	1.3358	-1.9822	1.9408
10	H	0.8935	-2.9208	1.6188
11	C	2.3528	-1.6408	0.8685
12	C	-3.2838	-1.6668	0.4469
13	C	-4.3987	-1.2829	-0.4201
14	H	-3.4998	-2.4831	1.1310
15	O	-1.3001	-2.9804	1.8369
16	C	3.2960	-0.6063	0.9522
17	C	4.1944	-0.3618	-0.0831
18	C	4.1483	-1.1555	-1.2174
19	C	3.2352	-2.1891	-1.3448
20	C	2.3489	-2.4221	-0.2975
21	C	-5.7080	-1.5057	0.0471
22	C	-6.8196	-1.1700	-0.7130
23	C	-6.6207	-0.6256	-1.9739
24	C	-5.3507	-0.4206	-2.4914
25	C	-4.2466	-0.7488	-1.7128
26	F	-7.6937	-0.3026	-2.7244
27	F	5.0188	-0.9175	-2.2242
28	H	-2.3078	0.6241	-0.6184
29	H	-0.9563	-0.3736	-1.1122
30	H	1.6495	0.9474	3.1405
31	H	1.8562	3.2763	2.4415
32	H	3.3411	0.0229	1.8278
33	H	4.9214	0.4383	-0.0195
34	H	3.2285	-2.7958	-2.2417
35	H	1.6371	-3.2355	-0.3888
36	H	-5.8499	-1.9423	1.0294
37	H	-7.8274	-1.3299	-0.3510
38	H	-5.2400	-0.0216	-3.4919
39	H	-3.2594	-0.6262	-2.1362
40	C	0.4363	3.0942	0.8303
41	H	0.5204	4.1274	0.5129
42	C	-0.4202	2.2269	0.1687
43	H	-1.0088	2.5865	-0.6695
44	C	1.8427	-2.3860	3.3925
45	N	0.6980	-2.1360	4.2182
46	C	-0.1377	-1.0646	3.7322
47	C	0.0582	-2.9759	5.2181
48	C	-1.4424	-2.7659	4.9419
49	C	-1.5225	-1.3309	4.3822
50	H	0.2158	-0.0897	4.0739
51	C	2.3862	-3.8058	3.4084
52	C	3.7227	-3.7938	3.8392
53	N	4.1003	-2.4906	4.1396
54	C	3.0769	-1.5820	3.9298

55	C	1.7890	-4.9949	3.0429
56	C	2.5530	-6.1637	3.1319
57	C	3.8770	-6.1570	3.5619
58	C	4.4826	-4.9564	3.9208
59	O	3.1437	-0.4009	4.1859
60	H	4.9918	-2.2136	4.5241
61	N	1.9357	-7.4465	2.7585
62	O	0.7680	-7.4282	2.3886
63	O	2.6248	-8.4569	2.8390
64	H	0.3608	-4.0197	5.1180
65	H	0.3154	-2.6558	6.2392
66	H	-1.7748	-3.4793	4.1882
67	H	-2.0499	-2.8956	5.8402
68	H	-2.3528	-1.1981	3.6878
69	H	-1.6678	-0.6119	5.1928
70	H	0.7646	-5.0452	2.6972
71	H	4.4159	-7.0929	3.6065
72	H	5.5140	-4.9359	4.2509

Prod14

	Atom	X	Y	Z
1	C	-0.4380	-0.0130	-1.7423
2	C	-1.7381	0.1117	-0.9821
3	C	-1.6724	1.1169	0.1372
4	C	-0.3342	1.4116	0.7337
5	C	0.8404	0.4395	0.4068
6	C	0.8002	0.1198	-1.0904
7	C	1.9658	-0.0756	-1.8430
8	C	1.9154	-0.3851	-3.1975
9	C	2.1895	1.0638	0.9612
10	H	1.8697	1.5601	1.8812
11	C	2.9130	2.1205	0.1285
12	C	-2.7107	1.8280	0.6298
13	C	-4.1343	1.7918	0.3046
14	H	-2.4330	2.5671	1.3766
15	O	-0.1574	2.3746	1.4510
16	C	4.2630	1.9803	-0.2203
17	C	4.9475	2.9657	-0.9296
18	C	4.2695	4.1152	-1.2932
19	C	2.9399	4.3064	-0.9544
20	C	2.2748	3.3139	-0.2417
21	C	-4.9038	2.9308	0.6139
22	C	-6.2618	2.9916	0.3358
23	C	-6.8706	1.8851	-0.2392
24	C	-6.1624	0.7291	-0.5327
25	C	-4.7999	0.6878	-0.2619
26	F	-8.1911	1.9288	-0.5068
27	F	4.9218	5.0776	-1.9855
28	H	-2.5331	0.3921	-1.6769
29	H	-2.0136	-0.8798	-0.5974
30	H	2.9328	0.0159	-1.3749
31	H	2.8370	-0.5333	-3.7479
32	H	4.8107	1.0893	0.0584
33	H	5.9908	2.8495	-1.1956
34	H	2.4416	5.2250	-1.2389
35	H	1.2487	3.4855	0.0490
36	H	-4.4180	3.7844	1.0730
37	H	-6.8515	3.8708	0.5627
38	H	-6.6813	-0.1201	-0.9593
39	H	-4.2622	-0.2275	-0.4633
40	C	0.6861	-0.4979	-3.8390
41	H	0.6356	-0.7311	-4.8963
42	C	-0.4792	-0.3088	-3.1074
43	H	-1.4435	-0.3965	-3.5975
44	C	0.7001	-0.9243	1.3226
45	N	2.0083	-1.0684	1.8654
46	C	3.0198	-0.1461	1.4013
47	C	2.4376	-1.9493	2.9357
48	C	3.8746	-1.4494	3.2330
49	C	3.9331	-0.0282	2.6300
50	H	3.5974	-0.5656	0.5603
51	C	0.1559	-2.1743	0.6302
52	C	-1.0352	-2.5798	1.2579
53	N	-1.3483	-1.6979	2.2872
54	C	-0.3518	-0.7554	2.4892

55	C	0.6935	-2.9546	-0.3735
56	C	-0.0044	-4.1015	-0.7641
57	C	-1.2013	-4.4867	-0.1663
58	C	-1.7300	-3.7217	0.8691
59	O	-0.2930	-0.0072	3.4077
60	H	-2.0838	-1.8380	2.9649
61	N	0.5520	-4.9388	-1.8388
62	O	1.6322	-4.6111	-2.3145
63	O	-0.0964	-5.9162	-2.1947
64	H	1.7886	-1.8477	3.8157
65	H	2.4363	-3.0079	2.6415
66	H	4.0950	-1.4553	4.3017
67	H	4.6055	-2.0994	2.7440
68	H	3.5054	0.6978	3.3274
69	H	4.9516	0.2841	2.3924
70	H	1.6218	-2.7046	-0.8654
71	H	-1.6940	-5.3847	-0.5112
72	H	-2.6472	-4.0193	1.3631

Prod14p

	Atom	X	Y	Z
1	C	1.4803	-0.2872	-2.0942
2	C	2.4475	-1.1095	-1.2791
3	C	1.7452	-2.3275	-0.7347
4	C	0.3492	-2.1473	-0.1866
5	C	-0.2000	-0.6596	-0.2506
6	C	0.1699	-0.0915	-1.6198
7	C	-0.7396	0.5519	-2.4688
8	C	-0.3543	1.0436	-3.7134
9	C	0.5431	-0.0737	1.0698
10	H	1.2437	-0.8495	1.3894
11	C	1.3664	1.2048	1.0368
12	C	2.2258	-3.5861	-0.7280
13	C	3.5330	-4.0980	-1.1476
14	H	1.5217	-4.3391	-0.3819
15	O	-0.2259	-3.0501	0.3653
16	C	1.1515	2.2923	0.1827
17	C	1.9267	3.4477	0.2692
18	C	2.9306	3.5137	1.2191
19	C	3.1864	2.4575	2.0801
20	C	2.4045	1.3125	1.9767
21	C	3.6004	-5.4034	-1.6685
22	C	4.8022	-5.9582	-2.0877
23	C	5.9609	-5.2059	-1.9598
24	C	5.9490	-3.9288	-1.4201
25	C	4.7358	-3.3813	-1.0173
26	F	7.1359	-5.7389	-2.3564
27	F	3.6864	4.6300	1.3067
28	H	3.2885	-1.4048	-1.9067
29	H	2.8634	-0.5009	-0.4648
30	H	-1.7656	0.6940	-2.1677
31	H	-1.0856	1.5419	-4.3396
32	H	0.3885	2.2498	-0.5800
33	H	1.7534	4.2896	-0.3888
34	H	3.9838	2.5382	2.8083
35	H	2.6058	0.4812	2.6446
36	H	2.6888	-5.9841	-1.7541
37	H	4.8550	-6.9579	-2.5004
38	H	6.8800	-3.3865	-1.3109
39	H	4.7344	-2.4011	-0.5598
40	C	0.9569	0.8912	-4.1483
41	H	1.2669	1.2748	-5.1135
42	C	1.8609	0.2113	-3.3397
43	H	2.8767	0.0470	-3.6837
44	C	-1.7328	-0.6028	0.1473
45	N	-1.6142	-0.9165	1.5622
46	C	-0.5907	-0.0647	2.1324
47	C	-2.6725	-1.1022	2.5362
48	C	-1.8777	-1.1080	3.8798
49	C	-0.4183	-0.7024	3.5143
50	H	-0.9367	0.9745	2.2755
51	C	-2.5525	0.7051	-0.0059
52	C	-3.8456	0.3715	-0.4591
53	N	-3.8984	-0.9749	-0.7674
54	C	-2.6684	-1.6154	-0.6257

55	C	-2.3043	2.0181	0.3551
56	C	-3.3355	2.9577	0.2341
57	C	-4.6050	2.6226	-0.2220
58	C	-4.8719	1.3045	-0.5739
59	O	-2.4452	-2.7087	-1.0659
60	H	-4.6489	-1.4238	-1.2718
61	N	-3.0570	4.3577	0.5890
62	O	-1.9221	4.6376	0.9595
63	O	-3.9743	5.1648	0.4933
64	H	-3.4123	-0.2845	2.5363
65	H	-3.2014	-2.0411	2.3555
66	H	-2.3189	-0.3979	4.5817
67	H	-1.9033	-2.0910	4.3512
68	H	0.0218	-0.0245	4.2481
69	H	0.2143	-1.5891	3.4327
70	H	-1.3448	2.3663	0.7004
71	H	-5.3600	3.3924	-0.2952
72	H	-5.8532	1.0148	-0.9302

Prod15

	Atom	X	Y	Z
1	C	0.8560	-0.3767	-1.5705
2	C	1.1728	1.0377	-2.0008
3	C	0.0156	1.9833	-1.8440
4	C	-1.0570	1.6021	-0.8861
5	C	-0.7649	0.5133	0.1710
6	C	-0.0407	-0.6518	-0.5205
7	C	-0.1543	-1.9826	-0.0968
8	C	0.5433	-3.0164	-0.7117
9	C	0.0794	1.0614	1.4155
10	H	-0.3341	2.0522	1.5943
11	C	1.5781	1.2543	1.2994
12	C	-0.1794	3.1279	-2.5359
13	C	0.6570	3.7965	-3.5287
14	H	-1.1311	3.6150	-2.3408
15	O	-2.1616	2.1178	-0.9357
16	C	2.5102	0.2154	1.1511
17	C	3.8762	0.4725	1.0699
18	C	4.3195	1.7838	1.1422
19	C	3.4383	2.8415	1.2960
20	C	2.0762	2.5639	1.3747
21	C	0.0296	4.6997	-4.4093
22	C	0.7405	5.3730	-5.3924
23	C	2.1088	5.1607	-5.4829
24	C	2.7767	4.3063	-4.6181
25	C	2.0497	3.6273	-3.6478
26	F	2.8119	5.8149	-6.4293
27	F	5.6457	2.0356	1.0638
28	H	2.0354	1.3843	-1.4169
29	H	1.4959	1.0306	-3.0451
30	H	-0.7948	-2.2245	0.7345
31	H	0.4119	-4.0338	-0.3618
32	H	2.1797	-0.8104	1.0809
33	H	4.5949	-0.3292	0.9528
34	H	3.8169	3.8542	1.3567
35	H	1.3809	3.3870	1.4968
36	H	-1.0385	4.8639	-4.3212
37	H	0.2575	6.0584	-6.0774
38	H	3.8495	4.1892	-4.7068
39	H	2.5824	2.9911	-2.9560
40	C	1.3913	-2.7401	-1.7797
41	H	1.9287	-3.5376	-2.2795
42	C	1.5423	-1.4243	-2.1938
43	H	2.2144	-1.1924	-3.0137
44	C	-2.1283	0.1835	0.9293
45	N	-1.7129	-0.3427	2.2194
46	C	-0.4286	0.2192	2.6391
47	C	-2.0286	-1.6112	2.8583
48	C	-0.8550	-1.7918	3.8503
49	C	0.3087	-0.9986	3.2218
50	H	-0.5689	0.9449	3.4524
51	C	-3.2441	-0.5791	0.2108
52	C	-4.4500	0.1476	0.3425
53	N	-4.2366	1.3041	1.0552
54	C	-2.8977	1.5134	1.3398

55	C	-3.2749	-1.7684	-0.4945
56	C	-4.4896	-2.2105	-1.0308
57	C	-5.6728	-1.4936	-0.8907
58	C	-5.6577	-0.2930	-0.1947
59	O	-2.4768	2.4672	1.9490
60	H	-4.9272	2.0175	1.2334
61	N	-4.5120	-3.4824	-1.7639
62	O	-3.4655	-4.1184	-1.8415
63	O	-5.5768	-3.8409	-2.2553
64	H	-2.9918	-1.5866	3.3812
65	H	-2.0818	-2.4477	2.1473
66	H	-1.1205	-1.3585	4.8186
67	H	-0.6147	-2.8441	4.0134
68	H	1.0727	-0.7206	3.9498
69	H	0.7845	-1.5946	2.4431
70	H	-2.4020	-2.3752	-0.6639
71	H	-6.5809	-1.8831	-1.3286
72	H	-6.5633	0.2894	-0.0766

Prod15p

	Atom	X	Y	Z
1	C	-1.9558	2.2357	1.0268
2	C	-2.9620	1.1123	1.0788
3	C	-2.4908	-0.1633	0.4398
4	C	-1.0229	-0.4137	0.3271
5	C	-0.0243	0.5677	1.0069
6	C	-0.5728	1.9913	1.0306
7	C	0.2860	3.0950	1.1186
8	C	-0.1946	4.3976	1.1668
9	C	1.4181	0.3798	0.3524
10	H	1.4044	-0.6771	0.0933
11	C	1.6891	1.0810	-0.9760
12	C	-3.2936	-1.1143	-0.0914
13	C	-4.7488	-1.2156	-0.1530
14	H	-2.7623	-1.9266	-0.5800
15	O	-0.6015	-1.3927	-0.2641
16	C	2.4650	2.2350	-1.1404
17	C	2.6978	2.7914	-2.3969
18	C	2.1426	2.1872	-3.5105
19	C	1.3801	1.0361	-3.4019
20	C	1.1695	0.4894	-2.1405
21	C	-5.3013	-2.0408	-1.1532
22	C	-6.6723	-2.1959	-1.2969
23	C	-7.5102	-1.5354	-0.4094
24	C	-7.0140	-0.7382	0.6115
25	C	-5.6390	-0.5798	0.7342
26	F	-8.8439	-1.6846	-0.5336
27	F	2.3602	2.7251	-4.7330
28	H	-3.2192	0.9329	2.1328
29	H	-3.8874	1.4401	0.5985
30	H	1.3482	2.9327	1.1712
31	H	0.5014	5.2257	1.2362
32	H	2.9165	2.7209	-0.2896
33	H	3.3019	3.6824	-2.5152
34	H	0.9746	0.5735	-4.2934
35	H	0.5974	-0.4253	-2.0558
36	H	-4.6351	-2.5593	-1.8335
37	H	-7.0976	-2.8200	-2.0727
38	H	-7.7023	-0.2601	1.2972
39	H	-5.2609	0.0158	1.5523
40	C	-1.5659	4.6319	1.1235
41	H	-1.9547	5.6431	1.1525
42	C	-2.4328	3.5505	1.0564
43	H	-3.5047	3.7198	1.0421
44	C	0.2952	0.0786	2.5385
45	N	1.5857	0.6794	2.7111
46	C	2.4293	0.4475	1.5410
47	C	2.4344	0.5772	3.8899
48	C	3.7766	1.1856	3.3721
49	C	3.5751	1.4247	1.8445
50	H	2.8825	-0.5548	1.5904
51	C	-0.7288	0.4440	3.5914
52	C	-1.3457	-0.7283	4.0678
53	N	-0.7750	-1.8379	3.4586
54	C	0.3026	-1.4891	2.6492

55	C	-1.0754	1.6691	4.1257
56	C	-2.0791	1.6975	5.0999
57	C	-2.7194	0.5441	5.5458
58	C	-2.3493	-0.6953	5.0317
59	O	1.1002	-2.2651	2.1864
60	H	-0.9443	-2.7970	3.7265
61	N	-2.4665	2.9917	5.6836
62	O	-1.8437	3.9850	5.3294
63	O	-3.3903	3.0003	6.4898
64	H	2.0099	1.1326	4.7289
65	H	2.5885	-0.4652	4.2104
66	H	4.0225	2.1146	3.8884
67	H	4.5966	0.4873	3.5498
68	H	3.2882	2.4633	1.6779
69	H	4.4785	1.2184	1.2684
70	H	-0.6005	2.5876	3.8135
71	H	-3.4892	0.6322	6.2995
72	H	-2.8208	-1.6036	5.3865

Prod5k

	Atom	X	Y	Z
1	C	2.3021	3.0838	1.9686
2	N	2.9783	3.6921	0.8399
3	C	3.4583	2.6554	-0.1119
4	C	4.0307	4.7011	1.0683
5	C	5.0803	4.4052	-0.0198
6	C	4.9714	2.8832	-0.2180
7	H	3.0035	2.8494	-1.0909
8	C	1.3341	4.0058	2.6888
9	C	1.5308	3.9058	4.0776
10	N	2.5968	3.0510	4.3360
11	C	3.2524	2.6783	3.1691
12	C	0.4278	4.9168	2.1930
13	C	-0.3316	5.6556	3.1055
14	C	-0.1782	5.5195	4.4826
15	C	0.7743	4.6393	4.9868
16	O	4.3572	2.1996	3.1201
17	H	3.0402	2.9436	5.2372
18	N	-1.3261	6.6050	2.5916
19	O	-1.4634	6.6847	1.3743
20	O	-1.9672	7.2617	3.4040
21	H	3.6272	5.7147	0.9913
22	H	4.4835	4.5938	2.0613
23	H	4.8210	4.9275	-0.9460
24	H	6.0796	4.7307	0.2754
25	H	5.3859	2.5442	-1.1696
26	H	5.4831	2.3603	0.5939
27	H	0.3000	5.0785	1.1339
28	H	-0.7953	6.1161	5.1395
29	H	0.9302	4.5465	6.0547
30	C	-0.8411	2.1922	1.0697
31	C	0.4891	2.0677	0.3714
32	C	1.6888	1.7620	1.3003
33	C	1.3230	0.6632	2.3251
34	C	-0.1275	0.3166	2.5208
35	C	-1.1305	1.3294	2.1389
36	C	-2.3311	1.5007	2.8470
37	C	-3.2611	2.4518	2.4503
38	C	-0.3463	-0.9246	3.0258
39	H	0.5600	-1.4300	3.3498
40	C	-1.5617	-1.7263	3.1750
41	C	2.9608	1.3233	0.4687
42	C	2.7894	0.1689	-0.5001
43	H	3.6853	1.0039	1.2171
44	O	2.2056	0.0578	2.9042
45	C	-2.6829	-1.6173	2.3317
46	C	-3.7786	-2.4549	2.4838
47	C	-3.7618	-3.4081	3.4940
48	C	-2.6729	-3.5623	4.3379
49	C	-1.5740	-2.7307	4.1599
50	C	3.1003	-1.1274	-0.0629
51	C	2.9701	-2.2308	-0.9005
52	C	2.5292	-2.0319	-2.1992
53	C	2.2197	-0.7694	-2.6774
54	C	2.3518	0.3231	-1.8228

55	F	2.4045	-3.0963	-3.0237
56	F	-4.8310	-4.2158	3.6482
57	H	0.4238	1.2428	-0.3464
58	H	0.6946	2.9674	-0.2110
59	H	-2.5309	0.8825	3.7131
60	H	-4.1822	2.5721	3.0090
61	H	-2.6903	-0.8811	1.5395
62	H	-4.6395	-2.3851	1.8307
63	H	-2.6909	-4.3275	5.1036
64	H	-0.7073	-2.8537	4.7999
65	H	3.4460	-1.2699	0.9541
66	H	3.2113	-3.2311	-0.5632
67	H	1.8865	-0.6512	-3.7010
68	H	2.1149	1.3064	-2.2098
69	C	-3.0042	3.2549	1.3382
70	H	-3.7264	3.9967	1.0179
71	C	-1.7953	3.1279	0.6635
72	H	-1.5789	3.7819	-0.1744

TS5k

	Atom	X	Y	Z
1	C	-2.3645	0.0268	-1.0529
2	N	-2.5223	-1.2761	-1.3768
3	C	-2.5485	-2.2968	-0.4631
4	C	-2.5090	-1.7888	-2.7860
5	C	-2.3301	-3.2983	-2.6131
6	C	-2.8642	-3.5811	-1.1968
7	H	-3.0445	-2.1011	0.4753
8	C	-2.8002	0.7318	0.1357
9	C	-2.5860	2.1226	-0.1101
10	N	-2.0605	2.2722	-1.3704
11	C	-1.9295	1.0489	-2.0401
12	C	-3.3785	0.3608	1.3453
13	C	-3.7030	1.3581	2.2685
14	C	-3.4850	2.7120	2.0245
15	C	-2.9208	3.1030	0.8140
16	O	-1.5328	0.9335	-3.1834
17	H	-1.7835	3.1408	-1.7996
18	N	-4.2768	0.9502	3.5556
19	O	-4.3449	-0.2546	3.7964
20	O	-4.6507	1.8270	4.3245
21	H	-3.4770	-1.5290	-3.2269
22	H	-1.7202	-1.3055	-3.3489
23	H	-2.8595	-3.8603	-3.3832
24	H	-1.2688	-3.5402	-2.6758
25	H	-3.9480	-3.7477	-1.2029
26	H	-2.4068	-4.4498	-0.7211
27	H	-3.6094	-0.6582	1.6082
28	H	-3.7560	3.4345	2.7808
29	H	-2.7448	4.1500	0.6009
30	C	0.6261	1.0518	1.3195
31	C	0.1160	-0.3493	1.5560
32	C	-0.1016	-1.1689	0.3169
33	C	0.5502	-0.8054	-0.9394
34	C	1.4768	0.3815	-0.9276
35	C	1.2633	1.4040	0.1170
36	C	1.6072	2.7536	-0.0878
37	C	1.4037	3.7071	0.8985
38	C	2.4206	0.3686	-1.8996
39	H	2.2715	-0.4179	-2.6351
40	C	3.6203	1.1853	-2.1166
41	C	-0.7192	-2.4448	0.3180
42	C	-0.9208	-3.2723	1.5470
43	H	-0.3558	-3.0371	-0.5170
44	O	0.4244	-1.5072	-1.9508
45	C	4.4260	1.6689	-1.0707
46	C	5.5909	2.3796	-1.3288
47	C	5.9554	2.6145	-2.6476
48	C	5.2014	2.1420	-3.7102
49	C	4.0470	1.4170	-3.4358
50	C	-0.3716	-4.5648	1.5610
51	C	-0.5101	-5.4073	2.6594
52	C	-1.2229	-4.9540	3.7583
53	C	-1.7947	-3.6920	3.7846
54	C	-1.6394	-2.8598	2.6798

55	F	-1.3688	-5.7659	4.8274
56	F	7.0850	3.3116	-2.9010
57	H	0.8080	-0.8896	2.2218
58	H	-0.8133	-0.2688	2.1276
59	H	2.0367	3.0509	-1.0351
60	H	1.6856	4.7384	0.7174
61	H	4.1440	1.4733	-0.0442
62	H	6.2212	2.7448	-0.5276
63	H	5.5259	2.3333	-4.7255
64	H	3.4559	1.0285	-4.2577
65	H	0.1869	-4.9121	0.6987
66	H	-0.0785	-6.4003	2.6716
67	H	-2.3557	-3.3715	4.6535
68	H	-2.1017	-1.8824	2.7205
69	C	0.8345	3.3363	2.1184
70	H	0.6804	4.0720	2.8995
71	C	0.4377	2.0202	2.3113
72	H	-0.0434	1.7340	3.2413

Prod4k

	Atom	X	Y	Z
1	C	-0.4912	1.1416	-1.6245
2	N	-0.8248	1.7030	-2.9322
3	C	-2.2893	1.8607	-2.9832
4	C	-0.3911	1.0615	-4.1892
5	C	-1.2806	1.7732	-5.2103
6	C	-2.6418	1.8922	-4.4885
7	H	-2.5629	2.7917	-2.4879
8	C	0.9261	0.5821	-1.5555
9	C	1.7234	1.4469	-0.7818
10	N	0.9539	2.4989	-0.3139
11	C	-0.3677	2.4049	-0.7030
12	C	1.5081	-0.5308	-2.1336
13	C	2.8687	-0.7608	-1.9059
14	C	3.6533	0.0917	-1.1356
15	C	3.0779	1.2191	-0.5612
16	O	-1.2317	3.1976	-0.4048
17	H	1.2863	3.2603	0.2588
18	N	3.4926	-1.9519	-2.5026
19	O	2.7805	-2.6975	-3.1653
20	O	4.6882	-2.1320	-2.3007
21	H	0.6723	1.2336	-4.3619
22	H	-0.5802	-0.0194	-4.2071
23	H	-0.8751	2.7666	-5.4184
24	H	-1.3454	1.2280	-6.1539
25	H	-3.1739	2.8037	-4.7645
26	H	-3.2907	1.0502	-4.7418
27	H	0.9563	-1.2286	-2.7450
28	H	4.7000	-0.1396	-0.9975
29	H	3.6708	1.8969	0.0404
30	C	-1.0415	-0.1230	1.2304
31	C	-2.1379	0.3515	0.3148
32	C	-1.7433	0.2141	-1.1752
33	C	-1.3742	-1.2679	-1.4310
34	C	-0.8790	-2.0837	-0.2633
35	C	-0.4182	-1.3467	0.9312
36	C	0.6613	-1.7729	1.7190
37	C	1.0730	-1.0288	2.8178
38	C	-0.9089	-3.4268	-0.4537
39	H	-1.1575	-3.7213	-1.4702
40	C	-0.7018	-4.5480	0.4636
41	C	-2.8696	0.6510	-2.1906
42	C	-4.2584	0.8844	-1.6319
43	H	-2.9412	-0.1743	-2.8995
44	O	-1.4932	-1.7605	-2.5394
45	C	-1.0048	-4.5004	1.8366
46	C	-0.8453	-5.6174	2.6442
47	C	-0.3692	-6.7933	2.0784
48	C	-0.0714	-6.8897	0.7279
49	C	-0.2570	-5.7697	-0.0733
50	C	-4.6006	2.0473	-0.9254
51	C	-5.8905	2.2440	-0.4409
52	C	-6.8479	1.2671	-0.6678
53	C	-6.5543	0.1055	-1.3624
54	C	-5.2582	-0.0737	-1.8410

55	F	-8.1033	1.4557	-0.2001
56	F	-0.2055	-7.8763	2.8653
57	H	-3.0373	-0.2546	0.4731
58	H	-2.4133	1.3764	0.5477
59	H	1.1827	-2.6868	1.4639
60	H	1.9079	-1.3727	3.4178
61	H	-1.3844	-3.5857	2.2718
62	H	-1.0886	-5.5935	3.6991
63	H	0.2857	-7.8277	0.3219
64	H	-0.0425	-5.8344	-1.1341
65	H	-3.8508	2.8078	-0.7414
66	H	-6.1602	3.1398	0.1049
67	H	-7.3291	-0.6333	-1.5256
68	H	-5.0204	-0.9776	-2.3917
69	C	0.4196	0.1609	3.1413
70	H	0.7338	0.7390	4.0031
71	C	-0.6250	0.6137	2.3407
72	H	-1.1200	1.5517	2.5694

TS4k

	Atom	X	Y	Z
1	C	1.0124	-1.9777	0.7026
2	N	1.8404	-2.2543	-0.3332
3	C	3.0519	-1.6479	-0.5030
4	C	1.4814	-3.1306	-1.4840
5	C	2.6150	-2.8950	-2.4910
6	C	3.7690	-2.3238	-1.6454
7	H	3.5672	-1.3801	0.4072
8	C	-0.3558	-2.4048	0.9086
9	C	-0.6939	-2.0449	2.2458
10	N	0.4058	-1.4719	2.8415
11	C	1.4936	-1.3950	1.9692
12	C	-1.3321	-3.0007	0.1138
13	C	-2.5888	-3.2321	0.6713
14	C	-2.9132	-2.8833	1.9823
15	C	-1.9536	-2.2768	2.7843
16	O	2.5937	-0.9511	2.2854
17	H	0.4268	-1.0382	3.7511
18	N	-3.6172	-3.8677	-0.1659
19	O	-3.3096	-4.1830	-1.3110
20	O	-4.7252	-4.0482	0.3264
21	H	1.4400	-4.1612	-1.1188
22	H	0.5188	-2.8382	-1.8871
23	H	2.8876	-3.8109	-3.0156
24	H	2.2889	-2.1634	-3.2309
25	H	4.4131	-3.1200	-1.2535
26	H	4.4100	-1.6350	-2.1975
27	H	-1.1688	-3.2906	-0.9106
28	H	-3.9078	-3.0905	2.3500
29	H	-2.1851	-1.9901	3.8026
30	C	0.2226	1.7962	1.5480
31	C	1.5317	1.6571	0.8105
32	C	1.5056	0.7024	-0.3499
33	C	0.2421	0.3430	-0.9871
34	C	-1.0050	1.0125	-0.4748
35	C	-0.9979	1.4770	0.9284
36	C	-2.1737	1.5178	1.7002
37	C	-2.1521	1.9324	3.0236
38	C	-2.0087	1.1106	-1.3801
39	H	-1.8197	0.5611	-2.2989
40	C	-3.2749	1.8516	-1.3653
41	C	2.6699	0.2775	-1.0257
42	C	4.0027	0.9319	-0.8663
43	H	2.4497	0.0047	-2.0543
44	O	0.2051	-0.4147	-1.9674
45	C	-3.4287	3.1087	-0.7547
46	C	-4.6309	3.8001	-0.8248
47	C	-5.6951	3.2283	-1.5089
48	C	-5.5841	1.9992	-2.1397
49	C	-4.3685	1.3272	-2.0762
50	C	4.6953	1.0097	0.3524
51	C	5.9359	1.6348	0.4354
52	C	6.4902	2.1845	-0.7104
53	C	5.8466	2.1189	-1.9357
54	C	4.6091	1.4856	-2.0043

55	F	7.6945	2.7927	-0.6318
56	F	-6.8675	3.8966	-1.5720
57	H	1.8643	2.6442	0.4515
58	H	2.2883	1.3415	1.5325
59	H	-3.1100	1.2102	1.2543
60	H	-3.0736	1.9593	3.5944
61	H	-2.5930	3.5557	-0.2321
62	H	-4.7525	4.7736	-0.3663
63	H	-6.4327	1.5909	-2.6741
64	H	-4.2643	0.3713	-2.5774
65	H	4.2741	0.5613	1.2439
66	H	6.4766	1.6941	1.3718
67	H	6.3119	2.5545	-2.8112
68	H	4.0964	1.4317	-2.9586
69	C	-0.9444	2.3059	3.6169
70	H	-0.9196	2.6416	4.6477
71	C	0.2307	2.2222	2.8807
72	H	1.1786	2.4767	3.3445

Prod4l

	Atom	X	Y	Z
1	C	1.3998	-1.5372	0.2282
2	N	2.4065	-2.1025	-0.6646
3	C	3.4288	-1.0691	-0.8977
4	C	2.0556	-2.7099	-1.9637
5	C	3.4273	-2.7881	-2.6365
6	C	4.1062	-1.4611	-2.2315
7	H	4.1385	-1.0774	-0.0710
8	C	0.1092	-2.3484	0.2688
9	C	0.0332	-3.0268	1.4999
10	N	1.1339	-2.7077	2.2787
11	C	1.9786	-1.8082	1.6608
12	C	-0.8906	-2.5387	-0.6668
13	C	-1.9529	-3.3861	-0.3378
14	C	-2.0284	-4.0530	0.8808
15	C	-1.0199	-3.8768	1.8213
16	O	2.9945	-1.3665	2.1475
17	H	1.3243	-3.0681	3.2019
18	N	-3.0350	-3.5723	-1.3177
19	O	-2.9693	-2.9396	-2.3656
20	O	-3.9406	-4.3446	-1.0275
21	H	1.5989	-3.6898	-1.8186
22	H	1.3745	-2.0886	-2.5589
23	H	3.9846	-3.6370	-2.2329
24	H	3.3515	-2.9139	-3.7181
25	H	5.1867	-1.5668	-2.1257
26	H	3.9288	-0.6911	-2.9865
27	H	-0.8884	-2.0581	-1.6334
28	H	-2.8739	-4.6978	1.0751
29	H	-1.0590	-4.3872	2.7757
30	C	-0.0872	0.7081	1.9061
31	C	1.2101	0.9462	1.1803
32	C	1.3401	0.0553	-0.0788
33	C	0.1127	0.3309	-0.9796
34	C	-1.1595	0.8066	-0.3160
35	C	-1.2681	0.6394	1.1468
36	C	-2.4781	0.3405	1.7905
37	C	-2.5234	0.1744	3.1689
38	C	-2.0782	1.3338	-1.1613
39	H	-1.8329	1.2235	-2.2146
40	C	-3.3314	2.0473	-0.8996
41	C	2.6577	0.2879	-0.9150
42	C	3.5095	1.4838	-0.5459
43	H	2.3177	0.4367	-1.9400
44	O	0.1710	0.1789	-2.1860
45	C	-3.5062	2.9240	0.1858
46	C	-4.6903	3.6225	0.3519
47	C	-5.7426	3.4549	-0.5624
48	C	-5.5781	2.5941	-1.6563
49	C	-4.3805	1.9161	-1.8263
50	C	4.3392	1.4944	0.5862
51	C	5.1280	2.5967	0.8851
52	C	5.1082	3.7247	0.0521
53	C	4.2875	3.7272	-1.0829
54	C	3.5042	2.6165	-1.3705

55	H	1.2609	1.9911	0.8527
56	H	2.0527	0.7927	1.8490
57	H	-3.3830	0.2288	1.2072
58	H	-3.4662	-0.0544	3.6523
59	H	-2.7009	3.0687	0.8938
60	H	-4.8102	4.3043	1.1846
61	H	-6.3843	2.4705	-2.3684
62	H	-4.2541	1.2609	-2.6807
63	H	4.3622	0.6352	1.2460
64	H	5.7636	2.5919	1.7621
65	H	4.2720	4.5938	-1.7322
66	H	2.8774	2.6258	-2.2556
67	C	-1.3573	0.2928	3.9259
68	H	-1.3918	0.1718	5.0027
69	C	-0.1449	0.5465	3.2914
70	H	0.7698	0.6130	3.8711
71	C	5.9207	4.8616	0.3582
72	N	6.5760	5.7801	0.6068
73	C	-6.9689	4.1678	-0.3841
74	N	-7.9598	4.7435	-0.2371

TS4l

	Atom	X	Y	Z
1	C	0.9246	-2.5212	-0.7355
2	N	1.7657	-2.0793	-1.6993
3	C	2.9312	-1.4188	-1.4440
4	C	1.4556	-2.1252	-3.1555
5	C	2.5673	-1.2843	-3.7974
6	C	3.6849	-1.2479	-2.7376
7	H	3.4268	-1.6868	-0.5233
8	C	-0.3980	-3.0977	-0.8753
9	C	-0.7428	-3.6177	0.4008
10	N	0.3194	-3.4149	1.2695
11	C	1.3728	-2.7541	0.6555
12	C	-1.3376	-3.2013	-1.9085
13	C	-2.5654	-3.8149	-1.6634
14	C	-2.8761	-4.3212	-0.4006
15	C	-1.9630	-4.2241	0.6509
16	O	2.4390	-2.4859	1.2074
17	H	1.4754	-3.1737	-3.4678
18	H	0.4747	-1.6996	-3.3339
19	H	2.8980	-1.7059	-4.7472
20	H	2.1908	-0.2780	-3.9845
21	H	4.3905	-2.0778	-2.8674
22	H	4.2680	-0.3255	-2.7568
23	H	-1.1344	-2.8102	-2.8942
24	H	-3.8367	-4.7934	-0.2303
25	H	-2.2011	-4.6085	1.6358
26	C	-0.1594	0.0028	2.1098
27	C	1.1518	0.4132	1.4866
28	C	1.1946	0.3207	-0.0147
29	C	-0.0387	0.3225	-0.7927
30	C	-1.3289	0.4915	-0.0336
31	C	-1.3536	0.0330	1.3692
32	C	-2.5271	-0.4675	1.9623
33	C	-2.5349	-0.9127	3.2759
34	C	-2.3385	1.0543	-0.7418
35	H	-2.1176	1.1617	-1.8007
36	C	2.3823	0.4559	-0.7611
37	H	2.1805	0.8081	-1.7688
38	O	-0.0303	0.2847	-2.0327
39	H	1.4003	1.4430	1.7890
40	H	1.9344	-0.2143	1.9186
41	H	-3.4351	-0.5176	1.3763
42	H	-3.4534	-1.2902	3.7112
43	C	-1.3587	-0.8828	4.0277
44	H	-1.3573	-1.2208	5.0582
45	C	-0.1818	-0.4398	3.4364
46	H	0.7446	-0.4487	4.0022
47	C	3.6675	0.9689	-0.2078
48	C	4.2417	2.0798	-0.7987
49	C	4.3498	0.3570	0.8845
50	C	5.4567	2.6400	-0.3303
51	H	3.7441	2.5557	-1.6384
52	C	5.5320	0.8700	1.3549
53	H	3.9408	-0.5409	1.3311
54	C	6.0391	3.7914	-0.9231

55	C	6.1203	2.0241	0.7758
56	H	6.0388	0.3854	2.1833
57	C	7.2191	4.3077	-0.4454
58	H	5.5341	4.2605	-1.7612
59	C	7.3381	2.5805	1.2435
60	C	7.8758	3.6964	0.6484
61	H	7.6526	5.1885	-0.9056
62	H	7.8399	2.1098	2.0826
63	H	8.8066	4.1140	1.0155
64	C	-3.6443	1.5827	-0.3365
65	C	-4.6797	1.5793	-1.2573
66	C	-3.8773	2.1906	0.9346
67	C	-5.9590	2.1055	-0.9553
68	H	-4.5139	1.1517	-2.2414
69	C	-5.0968	2.7267	1.2498
70	H	-3.0665	2.2429	1.6491
71	C	-7.0296	2.0788	-1.8877
72	C	-6.1796	2.6925	0.3299
73	H	-5.2482	3.1970	2.2161
74	C	-8.2578	2.6033	-1.5645
75	H	-6.8618	1.6344	-2.8633
76	C	-7.4566	3.2272	0.6309
77	C	-8.4742	3.1831	-0.2931
78	H	-9.0675	2.5754	-2.2851
79	H	-7.6200	3.6742	1.6062
80	H	-9.4475	3.5947	-0.0504
81	H	-3.2886	-3.8935	-2.4665
82	H	0.3102	-3.5866	2.2620

Prod5l

	Atom	X	Y	Z
1	C	-2.1469	0.5098	0.6995
2	N	-3.0333	1.3879	-0.0384
3	C	-2.3720	2.6861	-0.3330
4	C	-4.4106	1.6152	0.4418
5	C	-4.6741	3.1028	0.1414
6	C	-3.2857	3.7494	0.2895
7	H	-2.3573	2.8268	-1.4206
8	C	-2.4895	-0.9646	0.5826
9	C	-2.4598	-1.5593	1.8562
10	N	-2.1943	-0.5884	2.8172
11	C	-2.1971	0.6887	2.2732
12	C	-2.8842	-1.7085	-0.5077
13	C	-3.1607	-3.0652	-0.3149
14	C	-3.0798	-3.6703	0.9363
15	C	-2.7341	-2.9097	2.0492
16	O	-2.2798	1.7112	2.9056
17	H	-2.2842	-0.7286	3.8137
18	N	-3.5473	-3.8786	-1.4752
19	O	-3.5758	-3.3287	-2.5721
20	O	-3.8137	-5.0591	-1.2850
21	H	-5.1183	0.9563	-0.0686
22	H	-4.4966	1.4322	1.5195
23	H	-5.0405	3.2218	-0.8830
24	H	-5.4213	3.5303	0.8123
25	H	-3.2097	4.7187	-0.2073
26	H	-3.0408	3.8768	1.3469
27	H	-2.9939	-1.2736	-1.4890
28	H	-3.3044	-4.7240	1.0238
29	H	-2.7004	-3.3571	3.0351
30	C	0.0789	-0.9061	-1.4209
31	C	-0.4468	0.5017	-1.2960
32	C	-0.7116	0.9733	0.1546
33	C	0.4598	0.5751	1.0811
34	C	1.4394	-0.4637	0.5984
35	C	0.9977	-1.3789	-0.4698
36	C	1.4213	-2.7163	-0.5346
37	C	1.0074	-3.5425	-1.5700
38	C	2.6496	-0.4222	1.2098
39	H	2.6944	0.2556	2.0585
40	C	3.9161	-1.0952	0.9105
41	C	-0.9466	2.5362	0.2202
42	C	0.1265	3.4182	-0.3859
43	H	-0.9828	2.7681	1.2842
44	O	0.6127	1.1416	2.1459
45	C	4.3307	-1.4289	-0.3916
46	C	5.5698	-2.0038	-0.6190
47	C	6.4325	-2.2725	0.4558
48	C	6.0412	-1.9301	1.7573
49	C	4.8074	-1.3351	1.9717
50	C	1.1385	3.9151	0.4498
51	C	2.1470	4.7323	-0.0409
52	C	2.1648	5.0844	-1.3973
53	C	1.1573	4.6049	-2.2438

54	C	0.1562	3.7841	-1.7394
55	H	0.2943	1.1836	-1.7269
56	H	-1.3543	0.6176	-1.8908
57	H	2.0758	-3.1062	0.2346
58	H	1.3413	-4.5731	-1.6052
59	H	3.6818	-1.2215	-1.2317
60	H	5.8820	-2.2459	-1.6272
61	H	6.7099	-2.1224	2.5869
62	H	4.5188	-1.0557	2.9788
63	H	1.1295	3.6495	1.5001
64	H	2.9188	5.1068	0.6202
65	H	1.1620	4.8805	-3.2912
66	H	-0.6136	3.4364	-2.4167
67	C	0.1567	-3.0456	-2.5587
68	H	-0.1674	-3.6818	-3.3739
69	C	-0.3093	-1.7387	-2.4729
70	H	-1.0042	-1.3686	-3.2189
71	C	7.7058	-2.8790	0.2227
72	N	8.7337	-3.3721	0.0349
73	C	3.1971	5.9303	-1.9123
74	N	4.0311	6.6122	-2.3295

TS5l

	Atom	X	Y	Z
1	C	0.8195	0.7074	2.1125
2	N	1.4011	-0.4305	2.5498
3	C	2.3619	-1.1183	1.8579
4	C	0.9496	-1.1798	3.7696
5	C	1.6327	-2.5408	3.6237
6	C	2.8497	-2.2575	2.7239
7	H	3.0846	-0.5338	1.3095
8	C	1.3773	1.7616	1.2894
9	C	0.4375	2.8366	1.3068
10	N	-0.6310	2.4776	2.0932
11	C	-0.4685	1.2099	2.6634
12	C	2.5630	1.9370	0.5837
13	C	2.7710	3.1426	-0.0900
14	C	1.8482	4.1855	-0.0723
15	C	0.6627	4.0336	0.6408
16	O	-1.2579	0.6956	3.4306
17	H	-1.4535	3.0334	2.2676
18	N	4.0071	3.2964	-0.8669
19	O	4.7365	2.3120	-0.9805
20	O	4.2416	4.3890	-1.3657
21	H	1.3127	-0.6185	4.6365
22	H	-0.1319	-1.2214	3.7998
23	H	1.9127	-2.9591	4.5909
24	H	0.9477	-3.2328	3.1332
25	H	3.7158	-1.9305	3.3115
26	H	3.1677	-3.1184	2.1340

27	H	3.3462	1.1984	0.5392
28	H	2.0682	5.0936	-0.6149
29	H	-0.0679	4.8322	0.6710
30	C	-0.7115	0.7994	-1.5273
31	C	0.4483	-0.1561	-1.3808
32	C	0.4016	-1.0390	-0.1669
33	C	-0.8565	-1.2665	0.5393
34	C	-2.0984	-0.6197	-0.0185
35	C	-1.9266	0.5854	-0.8535
36	C	-2.9239	1.5754	-0.9377
37	C	-2.7573	2.6993	-1.7324
38	C	-3.2543	-1.2380	0.3231
39	H	-3.1270	-2.0155	1.0722
40	C	-4.6298	-1.0755	-0.1590
41	C	1.4644	-1.8864	0.2341
42	C	2.6036	-2.2658	-0.6535
43	H	1.0795	-2.7365	0.7900
44	O	-0.9209	-2.0402	1.5022
45	C	-4.9485	-0.8113	-1.5034
46	C	-6.2659	-0.7352	-1.9240
47	C	-7.3122	-0.9173	-1.0057
48	C	-7.0112	-1.1990	0.3342
49	C	-5.6888	-1.2904	0.7410
50	C	2.8308	-3.6351	-0.8732
51	C	3.8676	-4.0798	-1.6804
52	C	4.7270	-3.1539	-2.2875
53	C	4.5246	-1.7848	-2.0692
54	C	3.4779	-1.3534	-1.2653

55	H	0.5220	-0.7887	-2.2796
56	H	1.3657	0.4397	-1.3830
57	H	-3.8355	1.4578	-0.3674
58	H	-3.5445	3.4430	-1.7866
59	H	-4.1527	-0.6791	-2.2248
60	H	-6.4966	-0.5406	-2.9641
61	H	-7.8152	-1.3526	1.0432
62	H	-5.4631	-1.5222	1.7758
63	H	2.1715	-4.3614	-0.4111
64	H	4.0191	-5.1397	-1.8433
65	H	5.1895	-1.0617	-2.5249
66	H	3.3636	-0.2879	-1.1173
67	C	-1.5759	2.8699	-2.4569
68	H	-1.4403	3.7397	-3.0895
69	C	-0.5609	1.9308	-2.3359
70	H	0.3754	2.0797	-2.8641
71	C	-8.6721	-0.8285	-1.4365
72	N	-9.7714	-0.7536	-1.7849
73	C	5.8026	-3.6044	-3.1154
74	N	6.6704	-3.9722	-3.7834