SUPPORTING INFORMATION

Synergistic effect of $GO/SrFe_{12}O_{19}$ as magnetic hybrid nanocatalyst for regioselective ring-opening of epoxides with amines under eco-friendly conditions

Mouhsine LAAYATI [1,2], Ayoub Abdelkader MEKKAOUI [1,2], Lahcen FKHAR [2], Mustapha AIT ALI [2], Hafid ANANE [3], Lahoucine BAHSIS [3,4], Larbi EL FIRDOUSSI [2], Soufiane EL HOUSSAME [1,*]

[1] Laboratoire des Sciences des Matériaux, Mathématiques et Environnement, Université Sultan Moulay Slimane, Faculté Polydisciplinaire de Khouribga, BP 145, Khouribga 25000, Morocco.

[2] Laboratoire de chimie moléculaire, Equipe de Chimie de Coordination et de Catalyse, Département de Chimie, Faculté des Sciences Semlalia, BP 2390, Marrakech 40001, Morocco.

[3] Laboratoire de Chimie Analytique et Moléculaire, LCAM, Faculté Polydisciplinaire de Safi, Université Cadi Ayyad, Safi 46030, Morocco.

[4] Laboratoire de Chimie de Coordination et d'Analytique (LCCA), Département de Chimie, Faculté des Sciences d'El Jadida, Université Chouaïb Doukkali, El Jadida, Morocco.

[*] Corresponding author:

Tel.: +212 523 490359; fax: +212 523 490354. E-mail address: hous_soufiane@hotmail.com

Contents:

A- Spectral data of β-aminoalcohol compounds

2-phenyl-2-(phenylamino)ethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.13-1.25 (m, 1 H), 3.11 (s, 1 H), 3.74 (td, 2 H, J = 10.0, 8.9, 5.1 Hz), 4.33 (dt, J= 6.9, 3.4 Hz, 1 H), 6.38 (m, 2 H), 6.55 (td, *J* = 7.3, 3.6 Hz, 1 H), 6.97 (ddd, J= 9.9, 5.9, 2.3Hz, 2 H), 7.08-7.21 (m, 5 H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 59.98, 67.16, 114.01, 117.98, 126.85, 127.65, 128.87, 129.27, 140.30, 147.4.

2-(phenylamino)-1-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.27-3.37 (m, 1 H), 3.44-3.50 (m, 1H), 4.94 (dd, J= 7.3, 4.0Hz, 1H), 5.29 (s, 1H), 6.60-670 (m, 2H), 6.70-6.94 (m, 2H), 7.13-7.32 (m, 1H), 7.26-7.54 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 51.91, 72.45, 113.70, 118.30, 126.05, 128.07, 128.72, 129.48, 142.22, 147.94.

2-((2-fluorophenyl)amino)-1-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.17(s, 1H), 2.19 (s,1H), 3.32-3.49 (m, 2H), 4.96(dd, J=8.5, 4Hz,1H), 6.62-6.85 (m, 2H), 6.94-7.08 (m ,1H), 7.28-7.49(m, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 51.46, 72.56, 112.71, 114.79, 117.41, 124.58, 125.89, 128.10, 128.68, 136.22, 141.85, 153.47.

2-((2-fluorophenyl)amino)-2-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.96 (s, 1H), 3.80-3.91 (m, 2H),4.45 (dd, J=7.2, 4.2Hz, 1H), 6.40 (td, J=8.4, 1.6Hz, 1H), 6.46-6.59 (m, 1H), 6.69-6.80 (m, 1H), 6.82 (s, 1H), 6.9 (ddd, J=11.8, 8.0, 1.5Hz, 1H), 7.10-7.34 (m, 5H). 13C NMR ($CDCl_3$, 75 MHz) δ 59.81, 67.25, 113.75, 114.57, 117.38, 124.43, 126.70, 127.75, 128.88, 135.60, 139.80, 153.51.

2-((2-chlorophenyl)amino)-1-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.92 (s, 1H), 2.07-2.20 (m, 1H), 3.31-3.53 (m, 2H), 4.97 (dd, J=8.3, 4.2, 1H), 6.60-6.79 (m, 2H), 6.99-7.22 (m,1H), 7.22-7.34 (m, 1H), 7.29-7.50 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 51.37, 72.47, 111.72, 117.86, 119.77, 125.90, 127.83, 128.12, 128.69, 129.32, 141.86, 143.78.

2-((2-chlorophenyl)amino)-2-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.29 (s, 1H), 3.84 (ddd, J=11.2, 6.8, 0.8Hz, 1H), 4.00 (dd, J=11.2, 4.3Hz, 1H), 4.58 (dd, J=6.8, 4.2Hz, 1H), 6.47 (dd, J=8.2, 1.4Hz, 1H), 6.63 (td, J=7.6, 1.4Hz, 1H), 6.91-7.05 (m, 3H), 7.22-7.41 (m,4H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 59.72, 67.32, 112.91, 117.87, 119.78, 126.67, 127.65, 127.79, 128.91, 129.12, 139.53, 143.03.

2-((2-bromophenyl)amino)-1-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.94 (m, 1H), 3.29-3.53 (m, 2H), 4.96 (dd, J=8.3, 4.2Hz, 1H), 6.6 (t, J=2.5Hz, 1H), 6.63 (d, J=1.5Hz, 1H), 6.64-6.77 (m, 1H), 7.13-7.27 (m, 1H), 7.36-7.51 (m, 5H), 7.32-7.42 (m,

1H).^{13}C NMR ($CDCl_3$, 75 MHz) δ 51.5, 72.44, 110.36, 111.80, 118.39, 125.92, 128.14, 128.52, 128.70, 132.6, 141.83, 144.76.

2-((2-bromophenyl)amino)-2-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.23-1.36 (m, 1H), 3.83 (dd, J=11.2, 6.8Hz, 1H), 3.99 (dd, J=11.2, 4.2 Hz, 1H), 4.57 (dd, J=6.8, 4.2Hz, 1H), 6.45 (dd, J= 8.2, 1.5 Hz, 1H), 6.57 (td, J= 7.6, 1.5 Hz, 1H), 7.02 (ddd, J=8.1, 7.3, 1.5Hz, 1H), 7.23-7.40 (m, 4H), 7.39 (s, 1H), 7.46 (dd, J=7.9, 1.5Hz, 1H).^{13}C NMR ($CDCl_3$, 75 MHz) δ 59.89, 67.30, 110.39, 113.04, 118.41, 126.67, 127.78, 128.36, 128.91, 132.41, 139.53, 144.03.

2-(morpholin-4-yl)-1-phenylethanol： ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.98-2.20 (m, 1H), 2.64-2.40 (m, 3H), 2.71-2.82 (m, 1H), 3.20 (s, 1H), 3.51-4.03 (m, 4H), 4.76 (dt, J= 7.3, 3.7 Hz, 1H), 5.23-5.33 (m, 1H), 7.15-7.45 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 53.46, 60.77, 66.98, 68.64, 125.84, 127.58, 128.38, 141.83

2-phenyl-2-(pyrrolidin-1-yl)ethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.67-1.89 (m, 4H), 2.69-2.83 (m, 4H), 3.36-3.43 (m, 2H), 3.77-3.90 (m, 1H), 7.23-7.42 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 23.17, 51.57, 64.64, 70.54, 126.23, 127.46, 128.63, 139.90.

1-phenyl-2-(pyrrolidin-1-yl)ethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.67-1.89 (m, 4H), 2.41-2.64 (m, 4H), 2.71 (dd, J=5.5, 3.0Hz, 2H), 4.3 (s, 1H), 4.73 (dd, J=10.4, 3.2Hz, 1H), 7.2-7.45 (m, 5H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 23.66, 53.99, 64.41, 70.97, 125.90, 127.35, 128.26, 142.82.

2-(benzylamino)-2-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.92-2.01 (m, 1H), 3.49-3.67 (m, 2H), 3.83 (s, 2H), 4.36-4.50 (m, 1H), 7.21-7-51 (m, 10H). ^{13}C ($CDCl_3$, 75 MHz) δ 51.12, 56.73, 63.96, 66.73, 127.59, 128.53, 139.79, 140.25, 142.60.

2-(benzylamino)-1-phenylethanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.17 (d, J=5.8Hz, 1H), 2.74-2.91 (m, 1H), 3.53-3.89 (m, 2H), 4.32 (s, 1H), 4.67-4.92 (m, 1H), 7.31-7.39 (m, 10H). ^{13}C ($CDCl_3$, 75 MHz) δ 53.10, 56.11, 71.48, 125.95, 126.09, 127.59, 128.43, 128.53, 128.70, 138.34, 142.60.

2-(phenylamino)-cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.94-1.26 (m, 4H), 1.58-1.67 (m, 2H), 1.97-2.04 (m, 2H), 3.0 (ddd, 1H, j= 11.1, 9.1, 4.0 Hz), 3.09 (s, 1H), 3.22 (td, 1H, J = 9.8, 4.3 Hz), 6.54-6.68 (m, 3H), 7.04-7.14 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 24.36, 24.99, 31.59, 33.4, 60.04, 74.38, 114.36, 118.2, 129.36, 147.98.

2-((2-fluorophenyl)amino)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.69-1.01 (m, 1H), 1.01-1.57 (m, 4H), 1.57-1.96 (m, 2H), 1.96-2.24 (m, 2H), 2.89-3.37 (m, 2H), 3.43 (td, J= 7.6, 1.5 Hz, 1H), 4.13 (ddd, J= 10.2, 8.4, 4.3 Hz, 1H), 6.56-6.78 (m, 1H), 6.78-

7.09 (m, 1H), 7.09-7.36 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 24.22, 24.98, 31.64, 33.17, 59.89, 74.46, 113.84, 114.84, 117.70, 124.62, 136.04, 150.43.

2-((2-chlorophenyl)amino)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.67-0.94 (m, 2H), 1.00-1.44 (m, 3H), 1.53-1.77 (m, 1H), 1.90-2.31 (m, 2H), 3.13 (ddd, J=10.8, 9.0, 4.0Hz, 1H), 3.39 (ddd, J=10.2, 8.4, 4.3Hz, 1H), 4.07(S,1H), 5.2 (S, 1H), 6.49-6.65 (m, 1H), 6.77 (dd, J=8.3, 1.5Hz,1H), 6.97-7.15 (m, 1H), 7.11-7.23 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 24.2, 24.95, 31.68, 33.16, 59.83, 74.54, 112.85, 118.04, 120.26, 127.82, 129.32, 143.81.

2-((2-bromophenyl)amino)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.43 (dd, J=7.9, 1.5Hz, 1H), 7.17 (ddd, J=8.5, 7.3, 1.5Hz, 1H), 6.84 (dd, J=8.3, 1.5Hz, 1H), 6.60 (td, J=7.6, 1.5Hz, 1H), 4.05 (s, 1H), 3.46 (td, J=9.7, 4.3Hz, 1H), 3.20 (ddd, J=10.7, 9.0, 4.0Hz, 1H), 2.05-2.30 (m, 2H), 1.69-1.81 (m,2H), 1.31-1.49 (m, 2H), 1.29-1.33 (m, 2H), 0.84-0.97 (m, 2H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 24.19, 24.99, 31.62, 33.24, 59.97, 74.38, 11.02, 113.02, 118.52, 128.52, 132.74, 144.85.

2-(morpholin-4-yl)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) *δ* 1.10-1.27 (m, 2H),1.21-1.35 (m,2H), 1.73-1.88 (m, 2H), 2.00-2.31 (m, 1H), 2.44 (ddd, J=11.4, 6.0, 3.4Hz, 2H), 2.66-2.84 m, 4H), 3.99 (td, J=9.6, 4.7Hz, 1H), 3.58-3.82 (m, 4H), 4.36 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz) *δ* 22.88, 24.00, 25.40, 33.19, 48.73, 67.37, 68.43, 70.48.

2-(pyrrolidin-1-yl)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.03-1.33 (m, 4H), 1.6-1.92 (m, 6H), 1.87-2.15 (m, 2H), 2.46 (td, J=9.7, 4.3Hz, 1H), 2.53-2.80 (m, 4H), 3.25-3.43 (m, 1H), 5.43 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 21.83, 23.48, 24.11, 25.14, 33.48, 47.67, 65.48, 70.57.

2-(benzylamino)cyclohexanol: ^{1}H NMR ($CDCl_3$, 300 MHz) *δ* 1.38-0.92 (m, 2H), 1.20-1.27 (m, 2H), 1.77-1.64 (m, 2H), 1.85-2.18 (m, 3H), 3.23 (td, J=9.6Hz, 4.5Hz, 1H), 3.33 (s, 2H), 3.67 (d, J=12.9Hz, 1H), 3.93 (d, J=12.9Hz, 1H), 4.23-4.74 (m, 1H), 7.37-7.15 (m, 5H). ^{13}C ($CDCl_3$, 75 MHz) *δ* 24.39, 24.95, 30.15, 33.59, 50.82, 63.00, 73.43, 127.09, 128.24, 128.45, 140.01

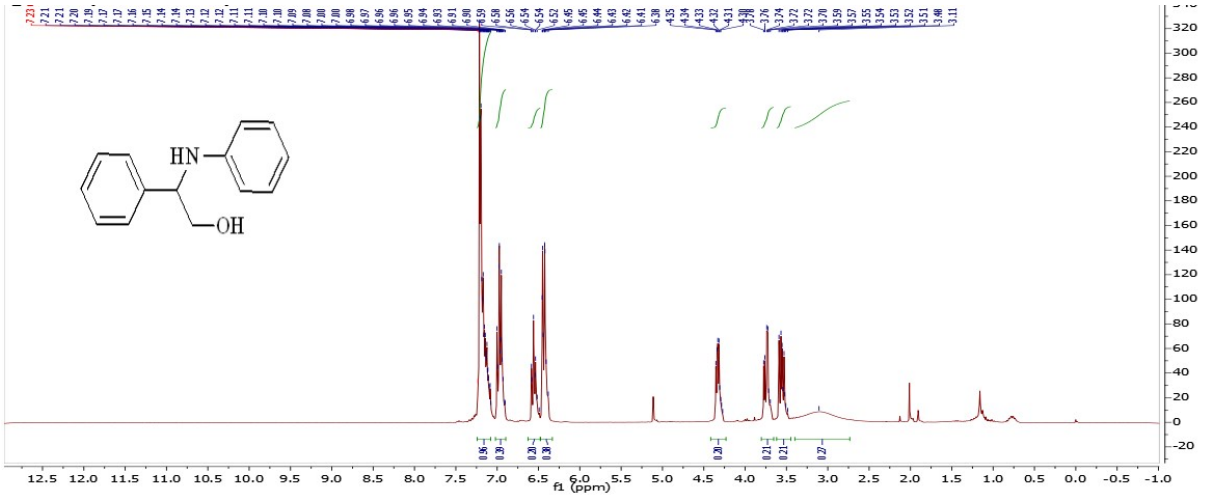

Figure S1: ^{1}H NMR spectrum of 2-phenyl-2-(phenylamino)ethanol

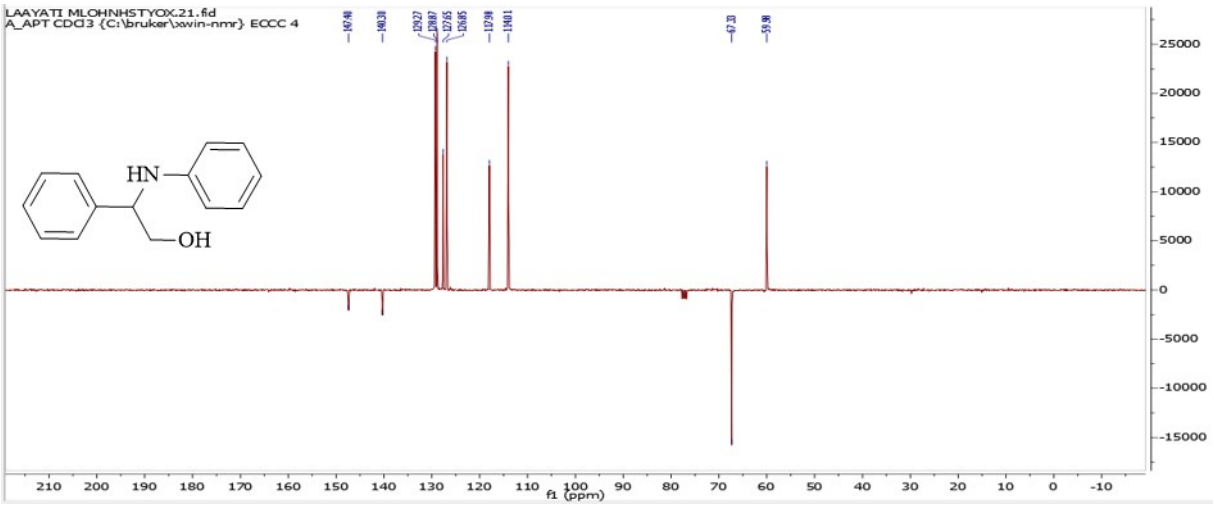

Figure S2: APT spectrum of 2-phenyl-2-(phenylamino)ethanol

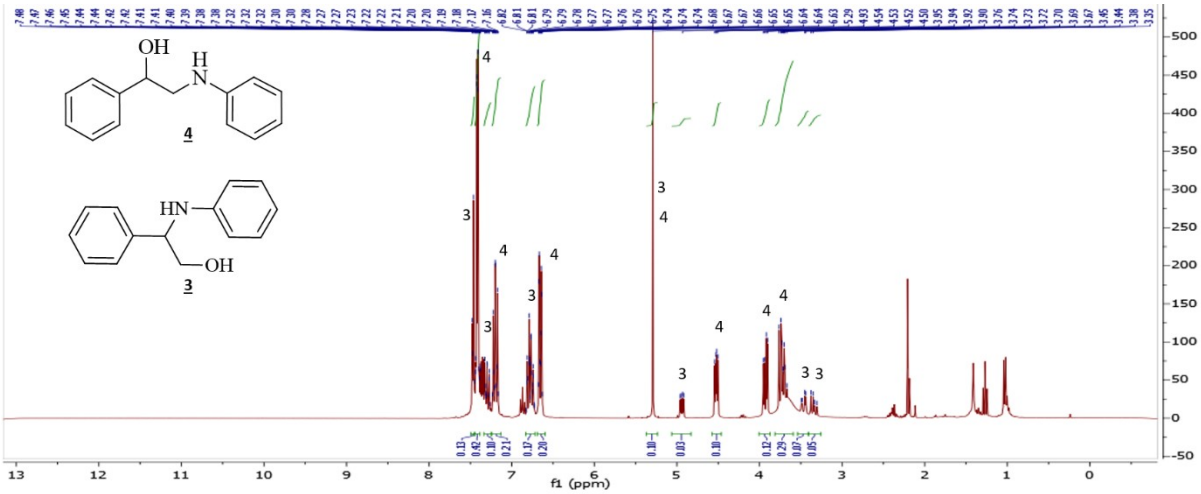

Figure S3: ^{1}H NMR spectrum of 2-phenyl-2-(phenylamino)ethanol (**3**) and 2-(phenylamino)-1-phenylethanol (**4**) mixture

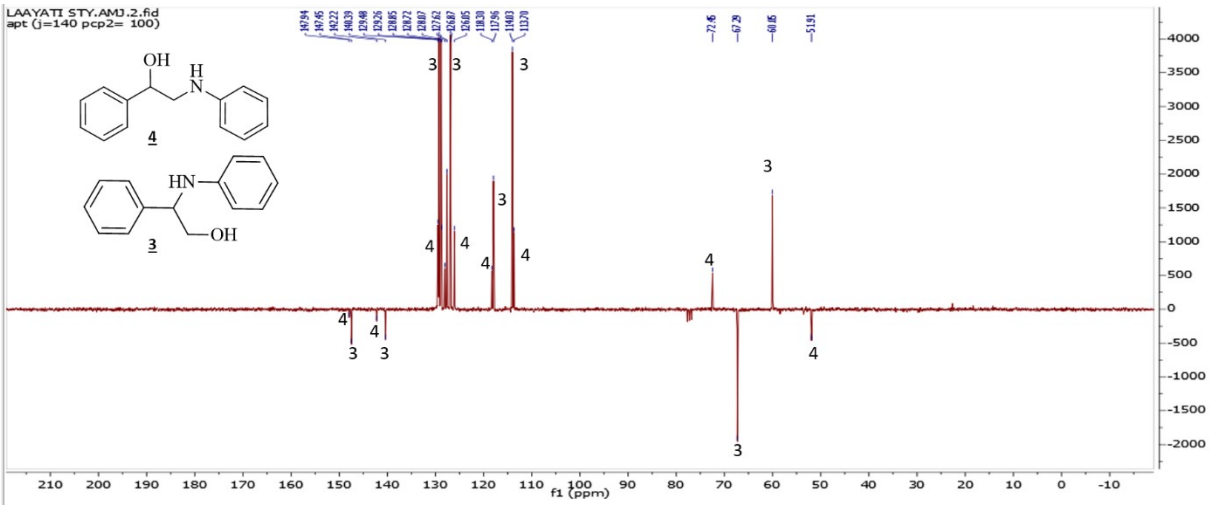

Figure S4: APT spectrum of 2-(phenylamino)-1-phenylethanol (**3**) and 2-phenyl-2-(phenylamino)ethanol (**4**) mixture

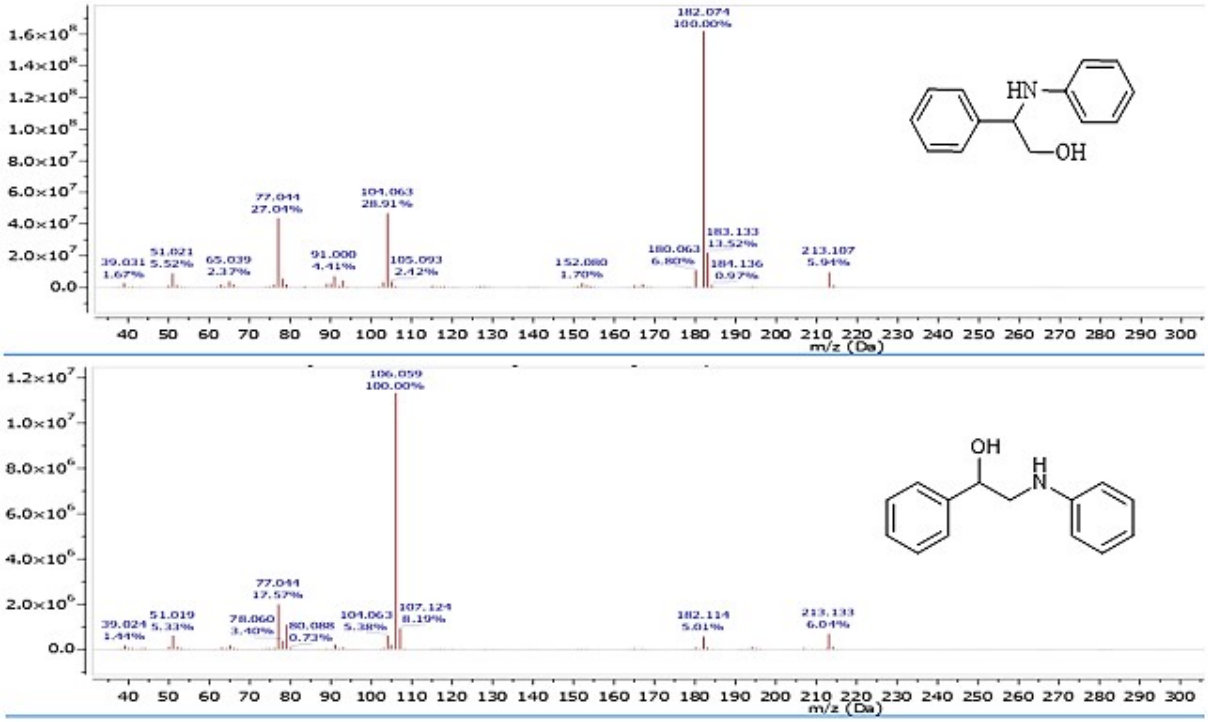

Figure S5: MS spectra of 2-phenyl-2-(phenylamino)ethanol and 1-phenyl-2-(phenylamino)ethanol

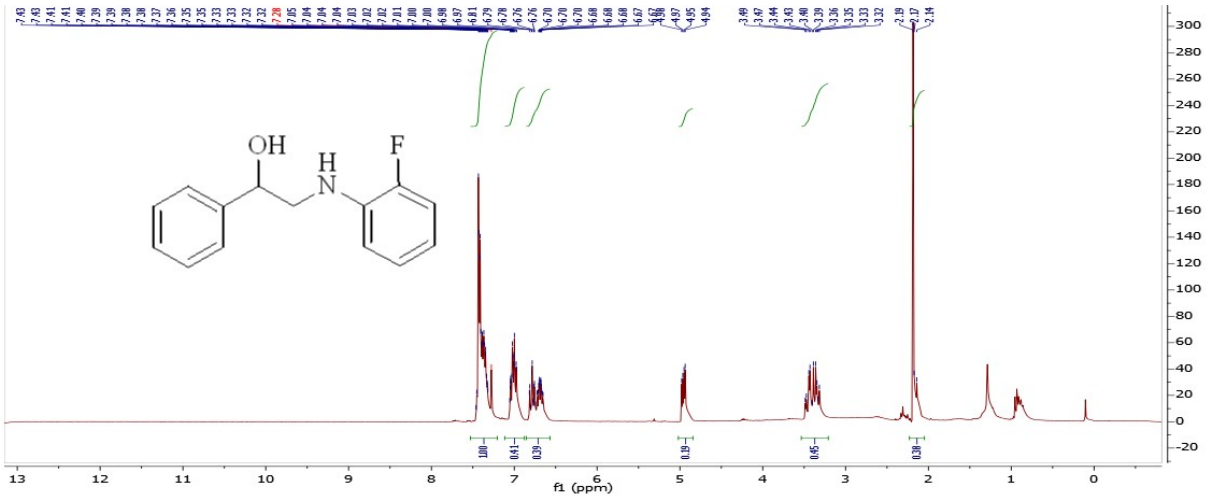

Figure S6: ^{1}H NMR spectrum of 2-((2-fluorophenyl)amino)-1-phenylethanol

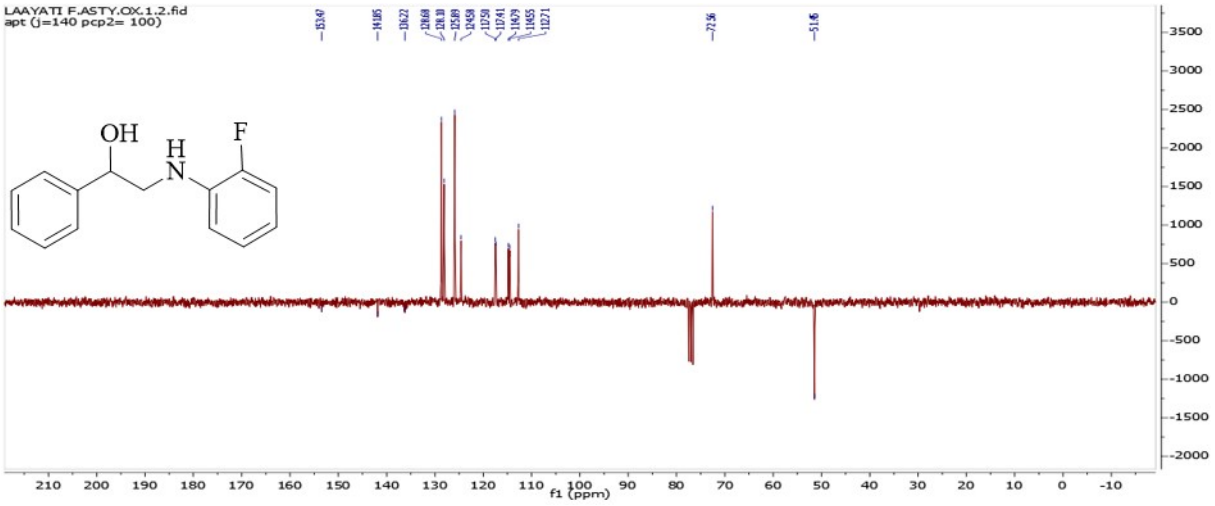

Figure S7: APT spectrum of 2-((2-fluorophenyl)amino)-1-phenylethanol

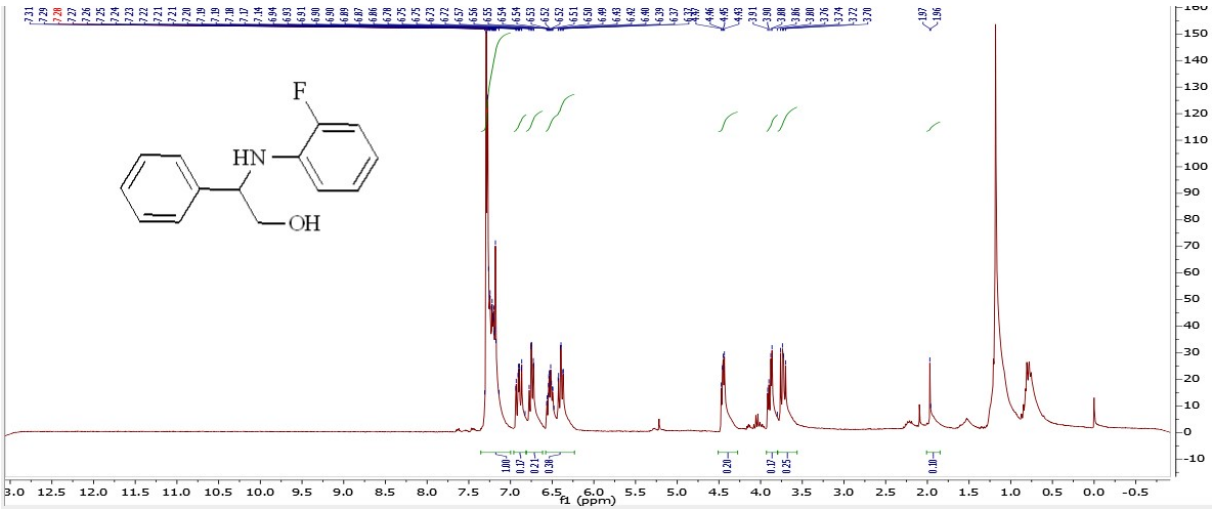

Figure S8: ^{1}H NMR spectrum of 2-((2-fluorophenyl)amino)-2-phenylethanol

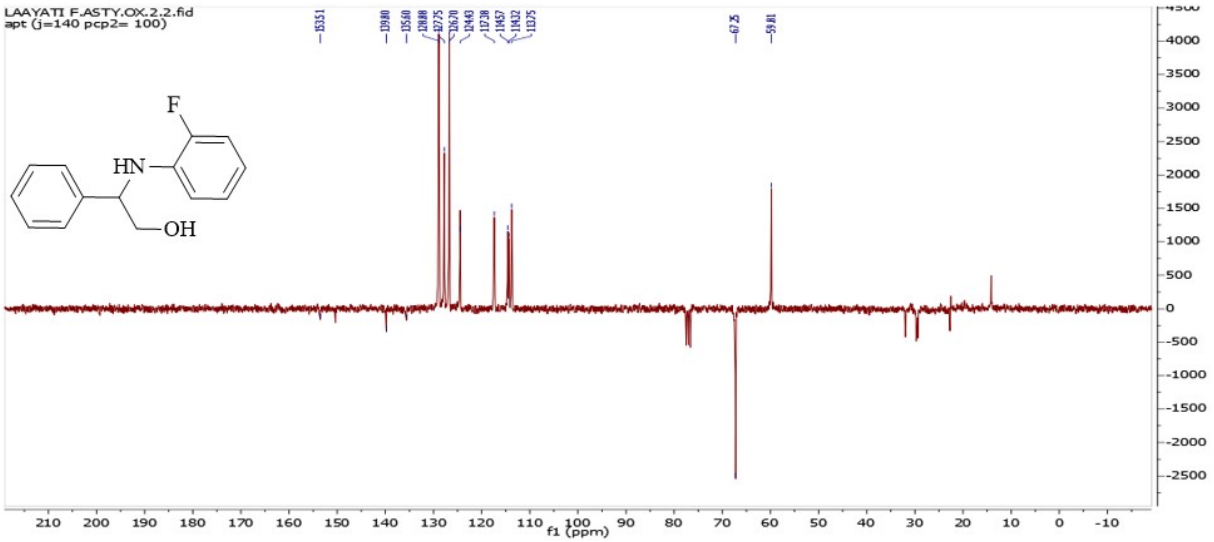

Figure S9: APT spectrum of 2-((2-fluorophenyl)amino)-2-phenylethanol

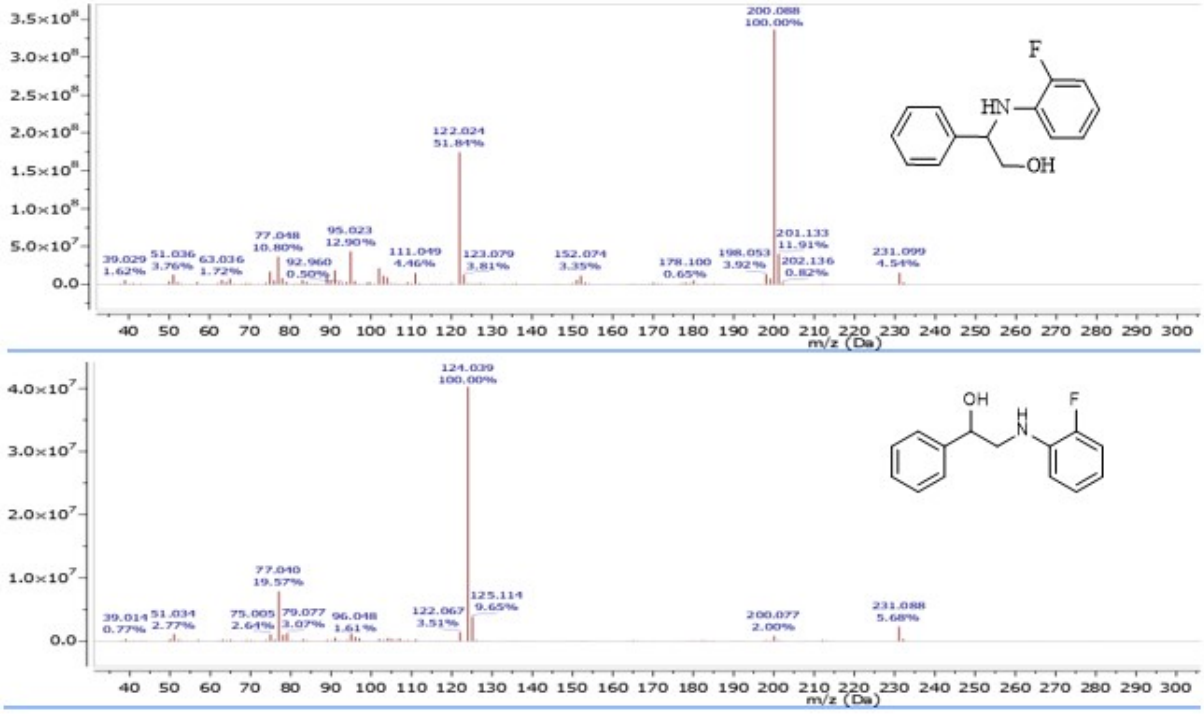

Figure S10: MS spectra of 2-((2-fluorophenyl)amino)-2-phenylethanol and 2-((2-fluorophenyl)amino)-1-phenylethanol

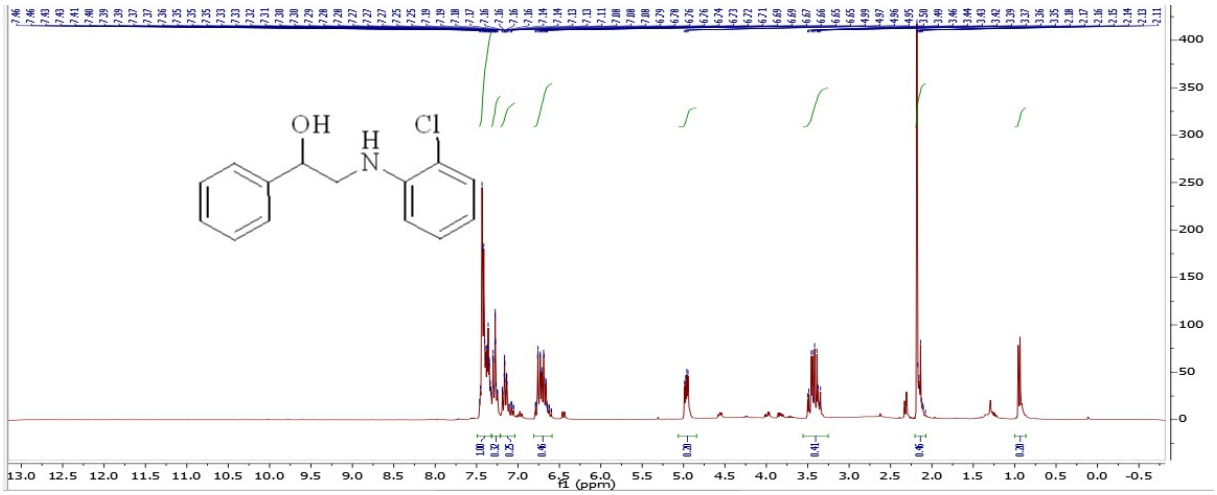

Figure S11: ^{1}H NMR spectrum of 2-((2-chlorophenyl)amino)-1-phenylethanol

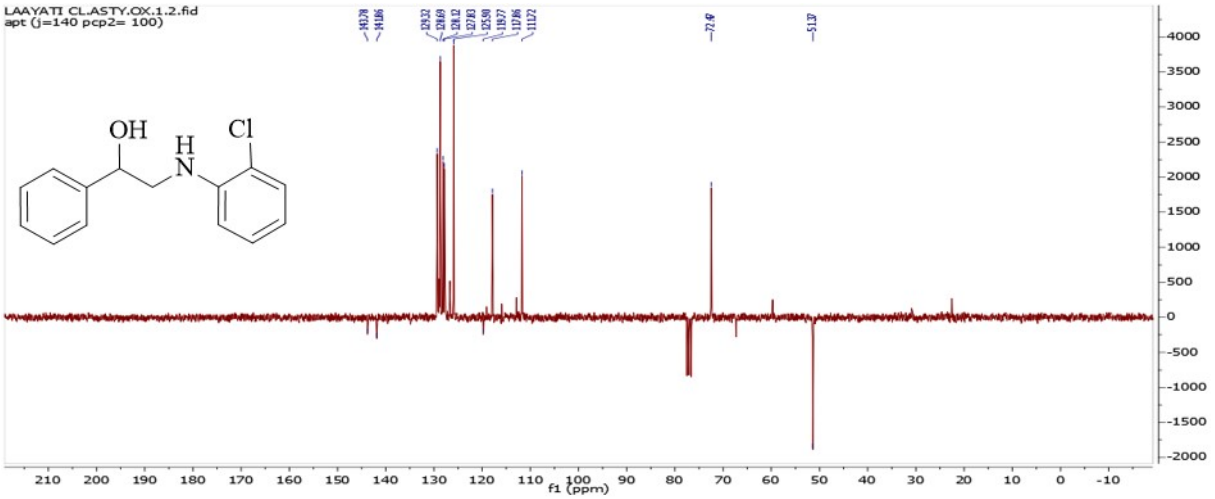

Figure S12: APT spectrum of 2-((2-chlorophenyl)amino)-1-phenylethanol

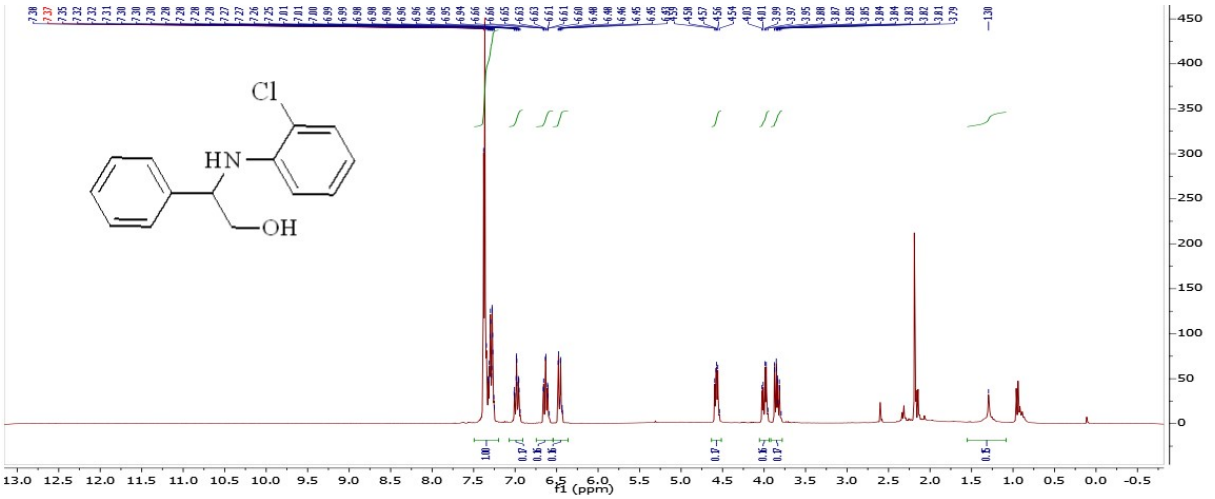

Figure S13: ^{1}H NMR spectrum of 2-((2-chlorophenyl)amino)-2-phenylethanol

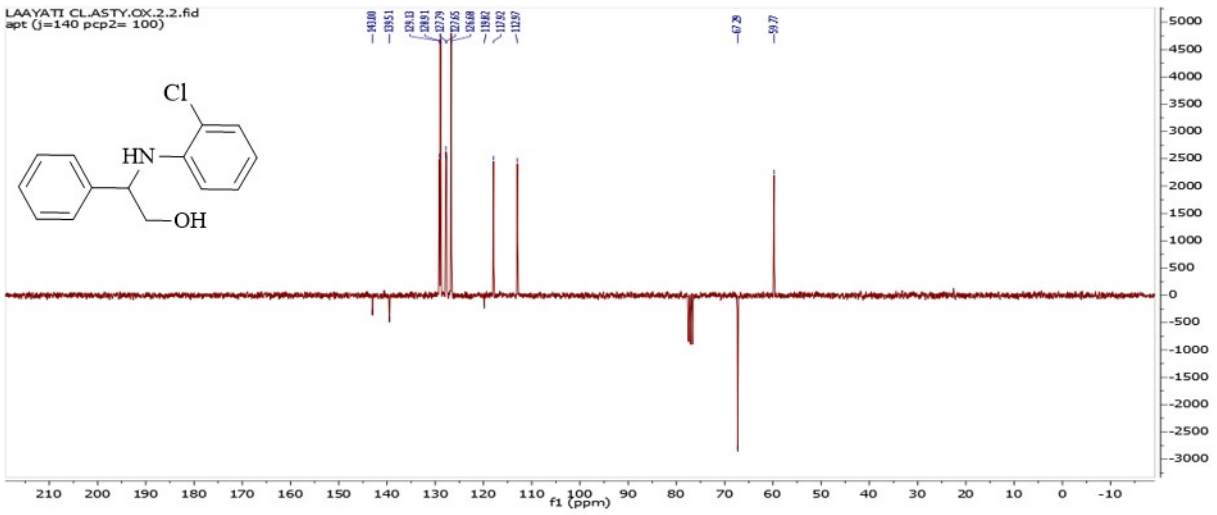

Figure S14: APT spectrum of 2-((2-chlorophenyl)amino)-2-phenylethanol

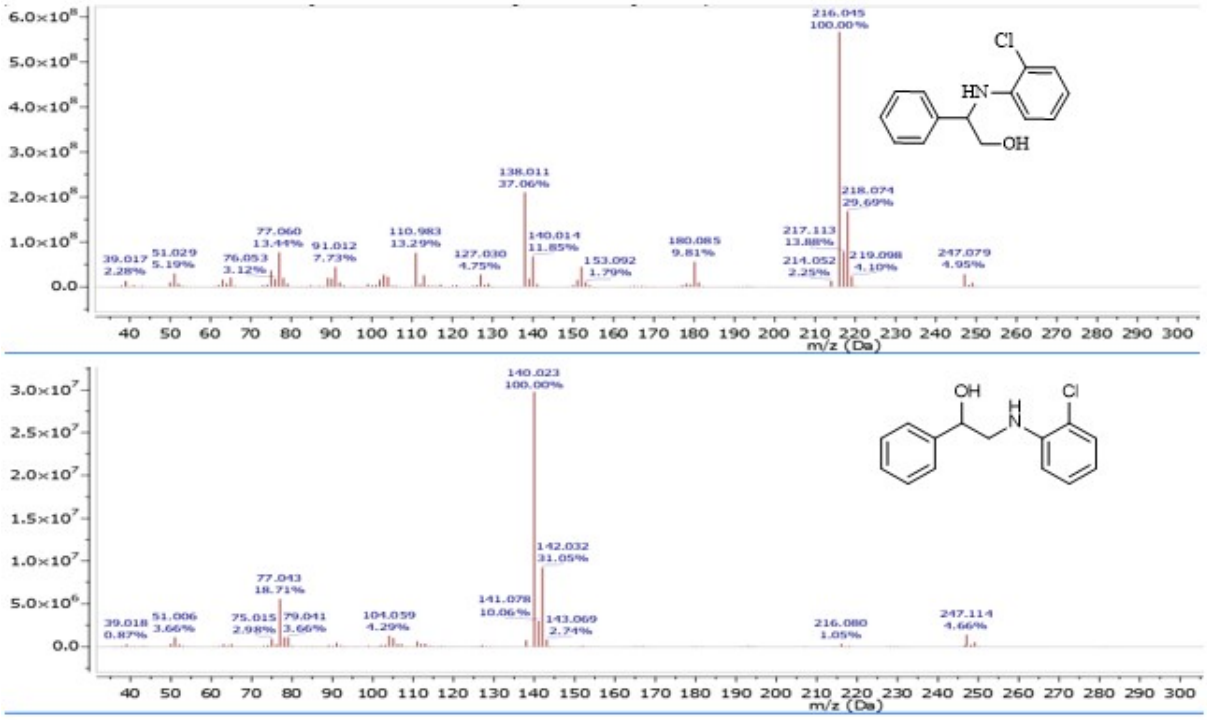

Figure S15: MS spectra of 2-((2-chlorophenyl)amino)-2-phenylethanol and 2-((2-chlorophenyl)amino)-1-phenylethanol

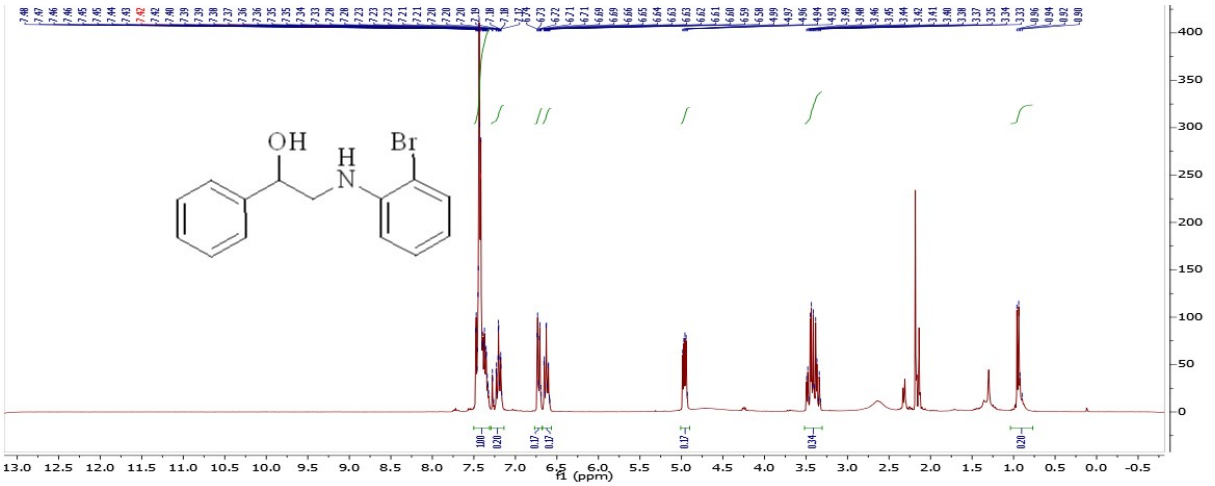

Figure S16: ^{1}H NMR spectrum of 2-((2-bromophenyl)amino)-1-phenylethanol

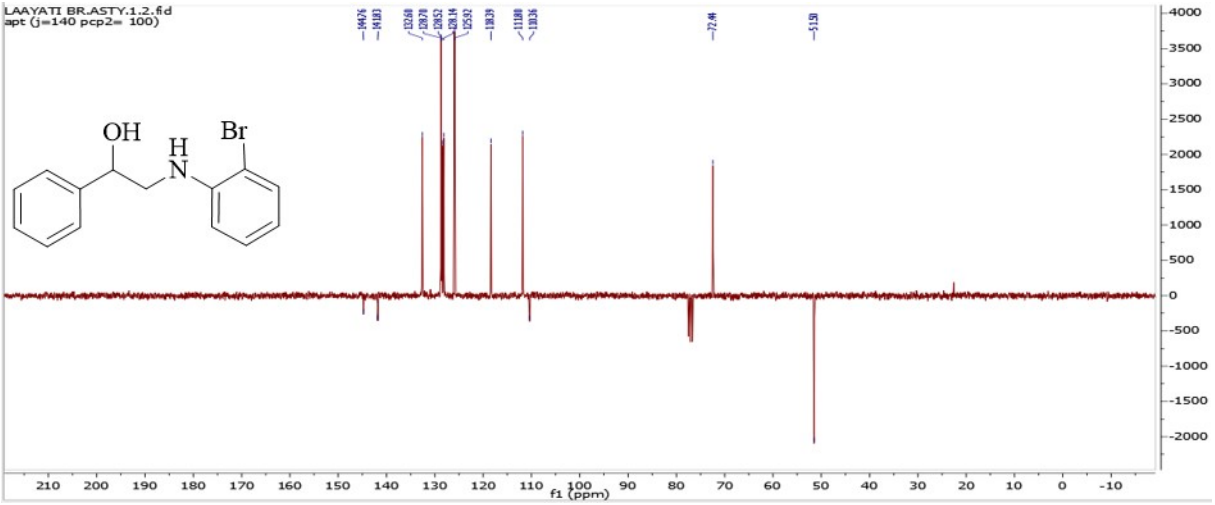

Figure 17: APT spectrum of 2-((2-bromophenyl)amino)-1-phenylethanol

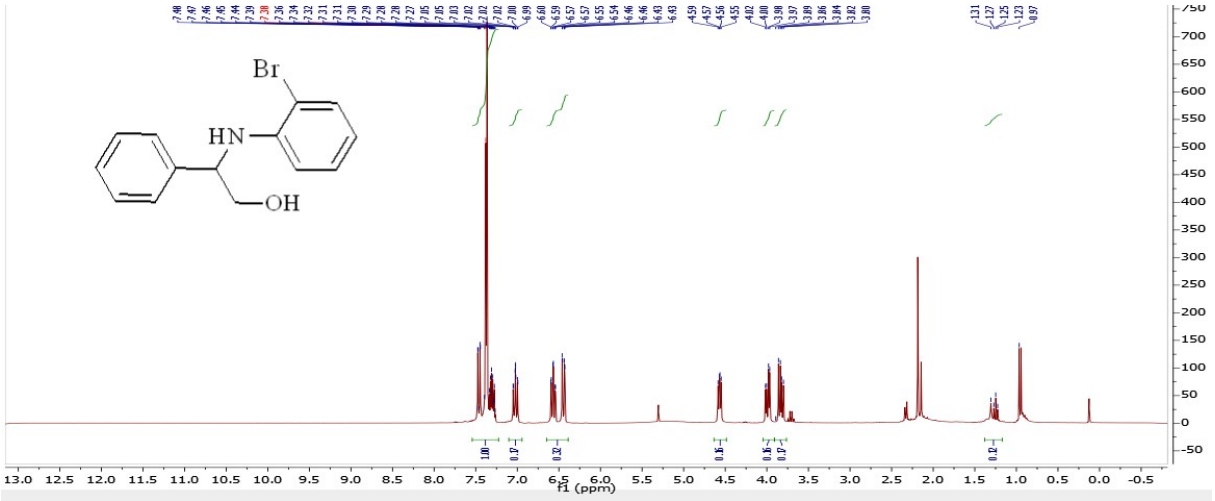

Figure S18: ^{1}H NMR spectrum of 2-((2-bromophenyl)amino)-2-phenylethanol

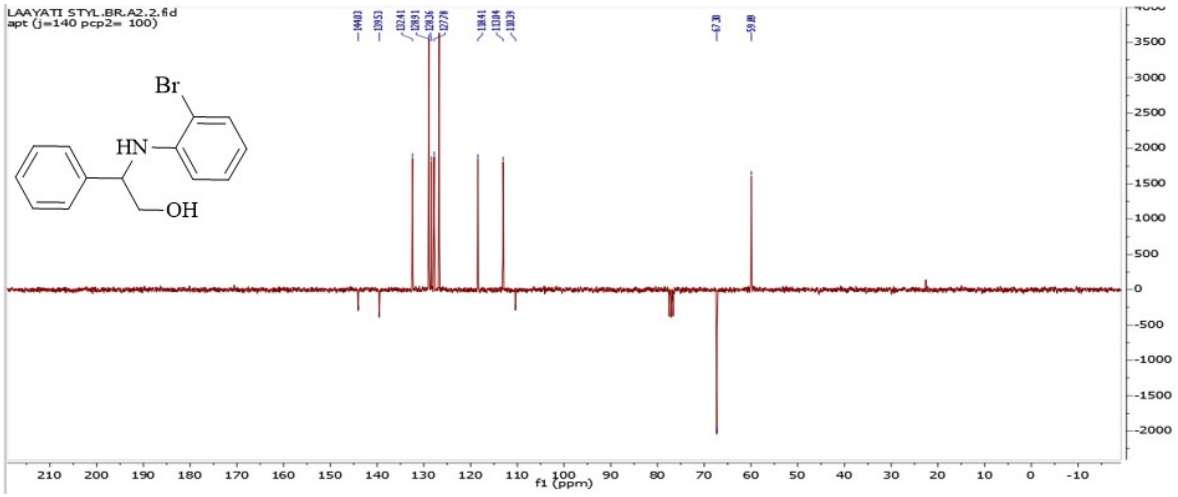

Figure S19: APT spectrum of 2-((2-bromophenyl)amino)-2-phenylethanol

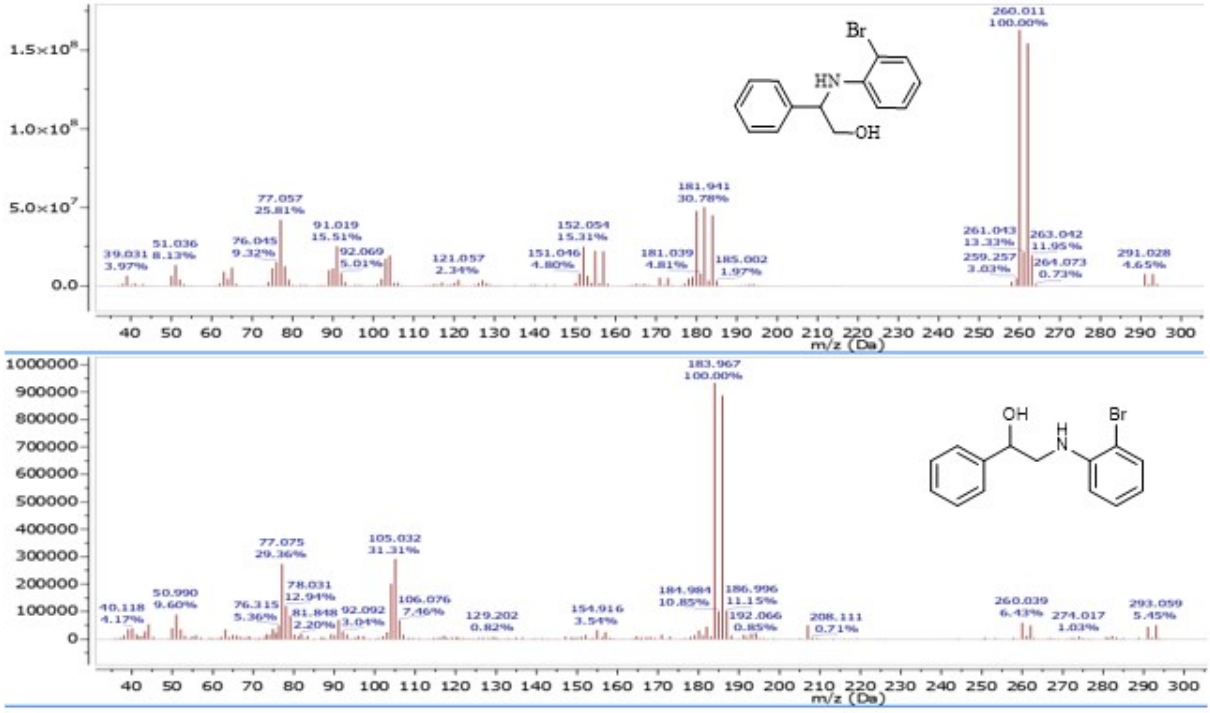

Figure S20: MS spectra of 2-((2-bromophenyl)amino)-2-phenylethanol and 2-((2-bromophenyl)amino)-1-phenylethanol

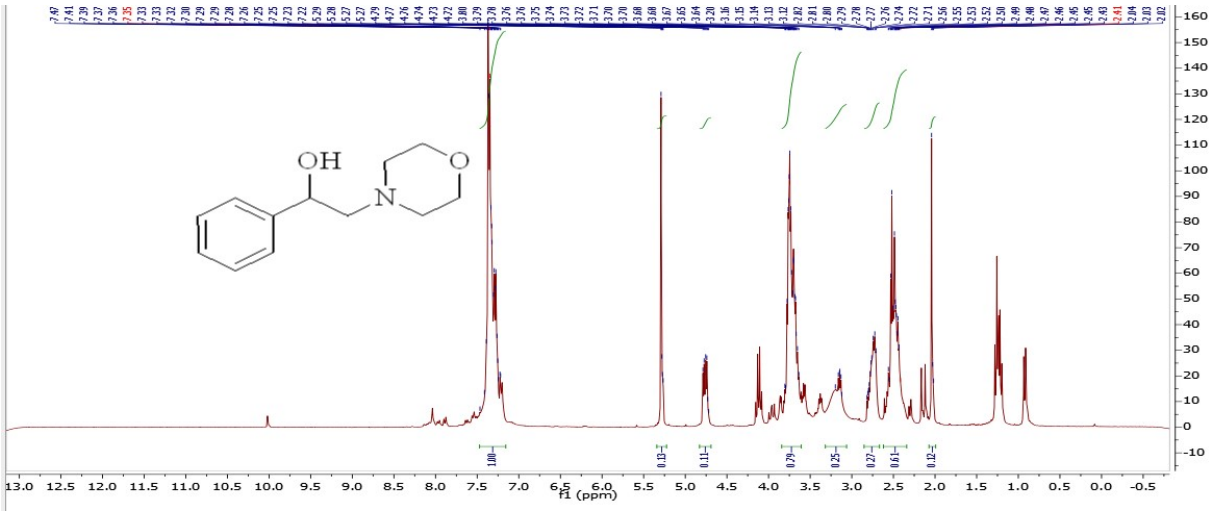

Figure S21: ^{1}H NMR spectrum of 2-(morpholin-4-yl)-1-phenylethanol

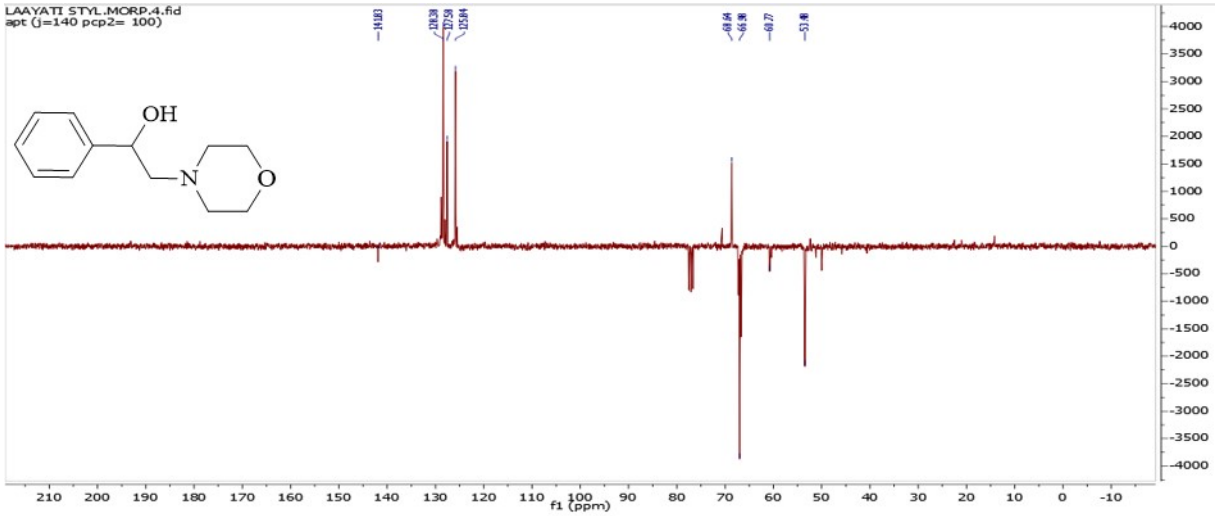

Figure S22: APT spectrum of 2-(morpholin-4-yl)-1-phenylethanol

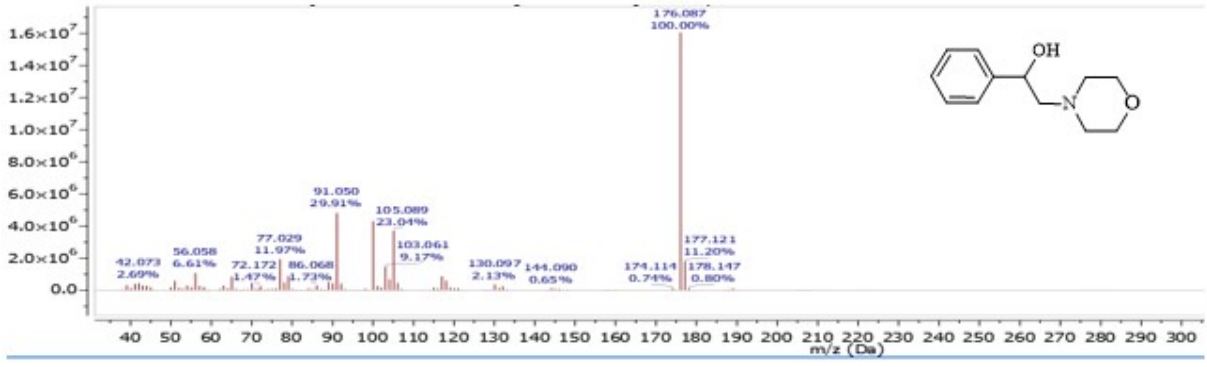

Figure S23: MS spectrum of 2-(morpholin-4-yl)-1-phenylethanol

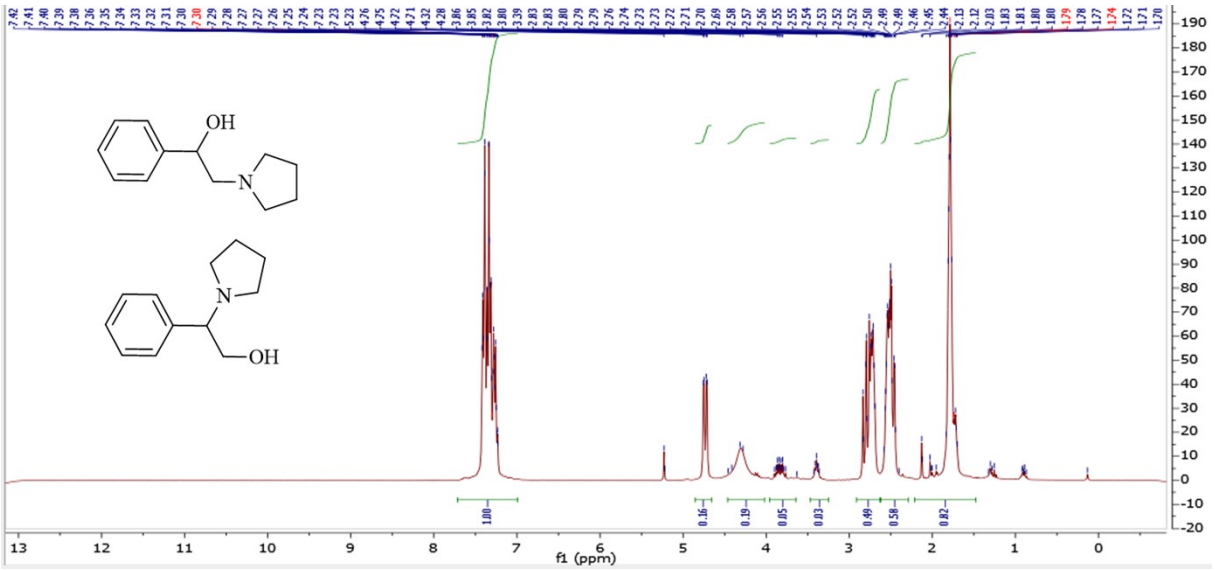

Figure S24: ^{1}H NMR spectrum of 1-phenyl-2-(pyrrolidin-1-yl)ethanol and 2-phenyl-2-(pyrrolidin-1-yl)ethanol mixture

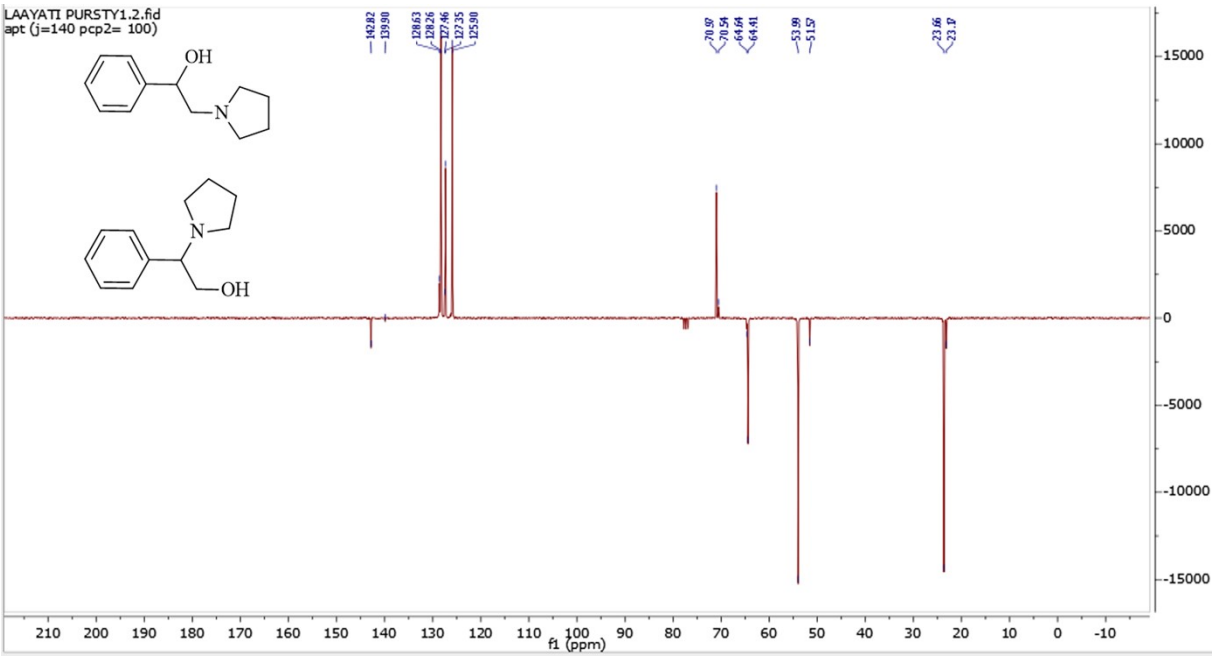

Figure S25: APT spectrum of 1-phenyl-2-(pyrrolidin-1-yl)ethanol and 2-phenyl-2-(pyrrolidin-1-yl)ethanol mixture

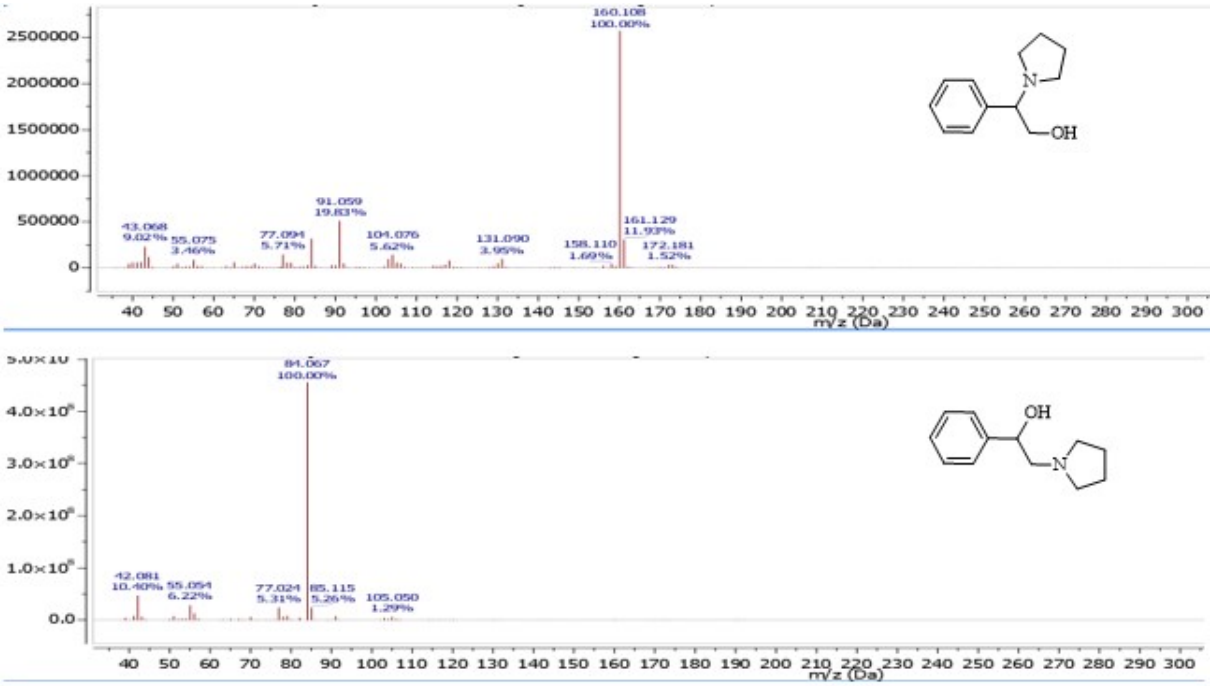

Figure S26: MS spectra of 1-phenyl-2-(pyrrolidin-1-yl)ethanol and 2-phenyl-2-(pyrrolidin-1-yl)ethanol

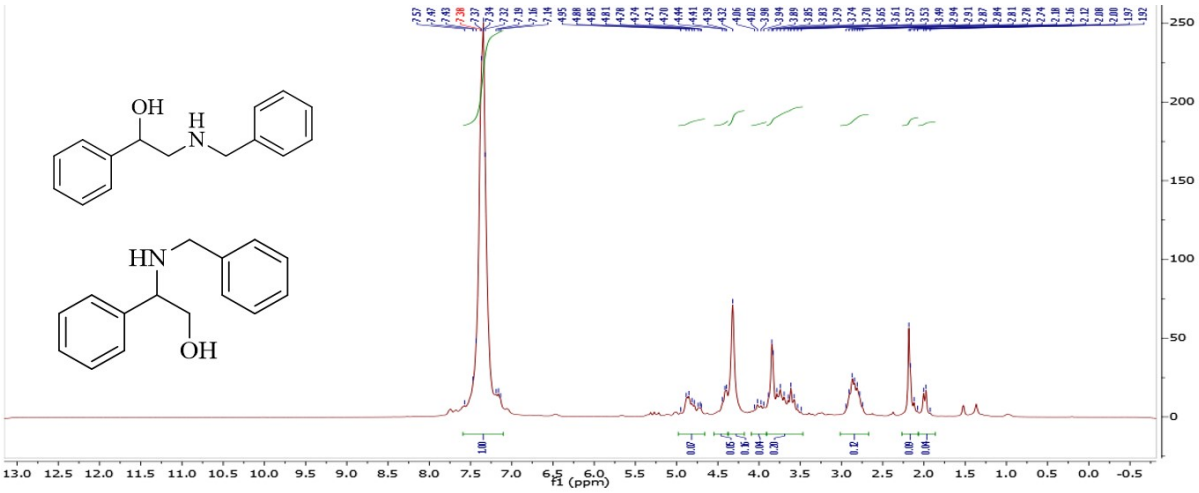

Figure S27: ^{1}H NMR spectrum of 2-(benzylamino)-1-phenylethanol and 2-(benzylamino)-2-phenylethanol mixture

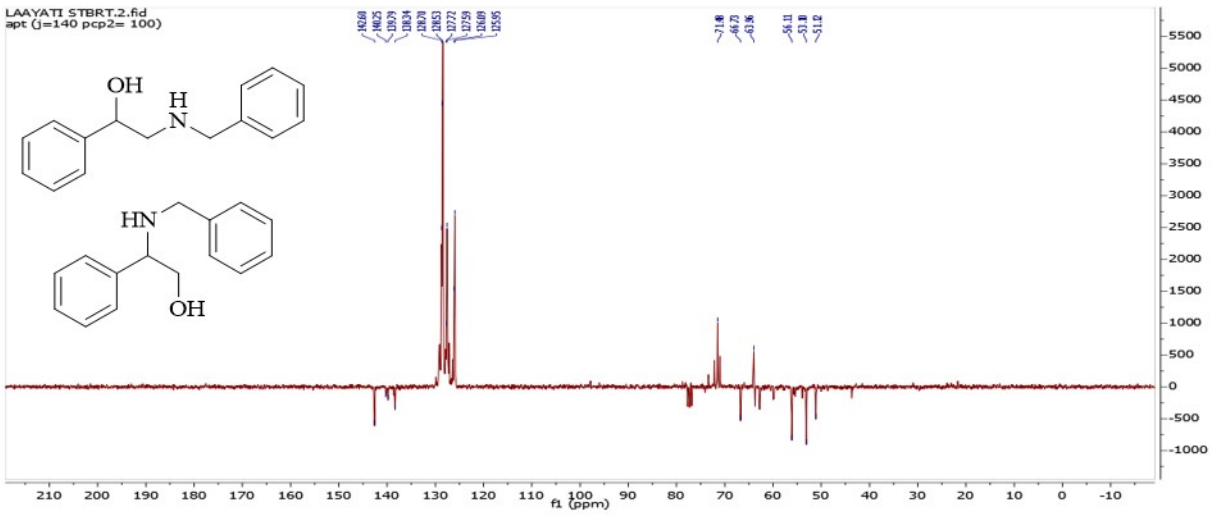

Figure S28: APT spectrum of 2-(benzylamino)-1-phenylethanol and 2-(benzylamino)-2-phenylethanol mixture

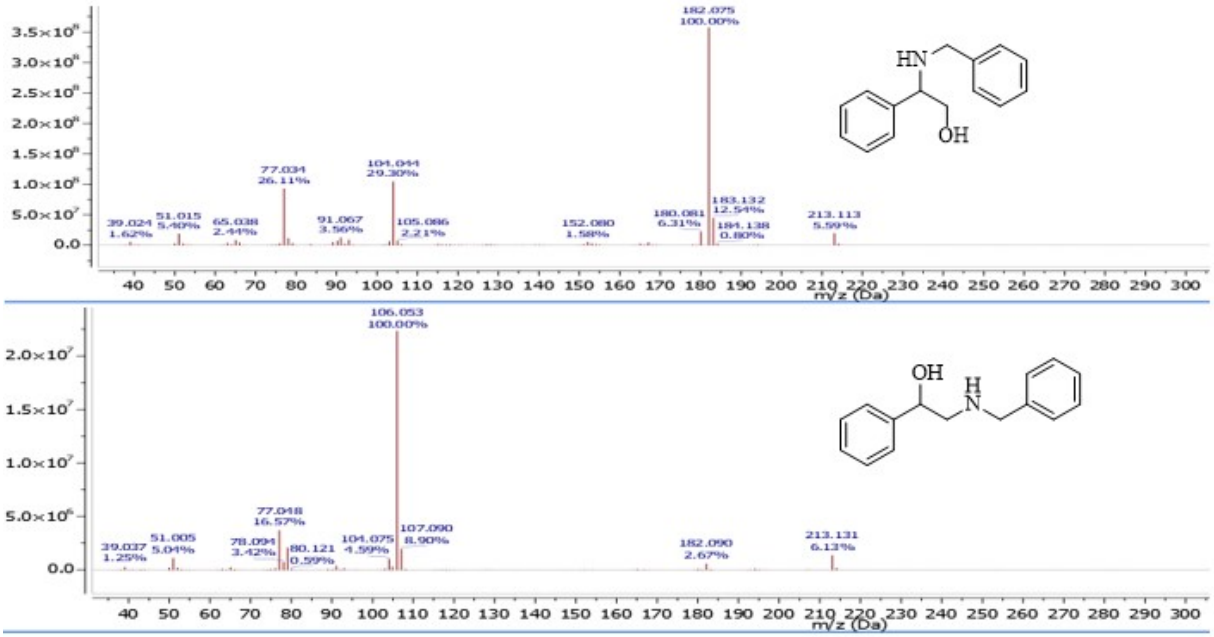

Figure S29: MS spectra of 2-(benzylamino)-2-phenylethanol and 2-(benzylamino)-1-phenylethanol

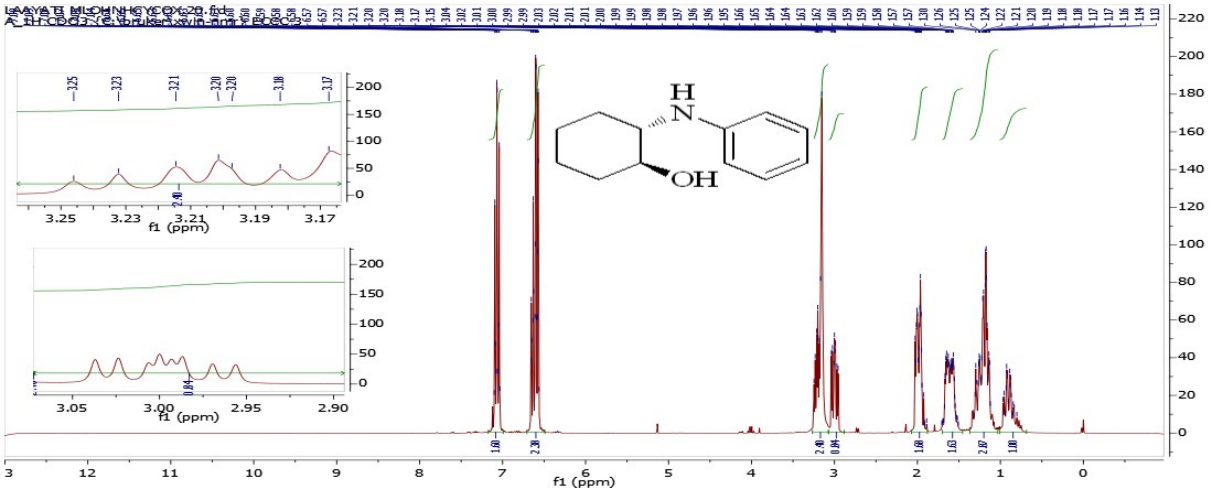

Figure S30: ^{1}H NMR spectrum of 2-(phenylamino)-cyclohexanol

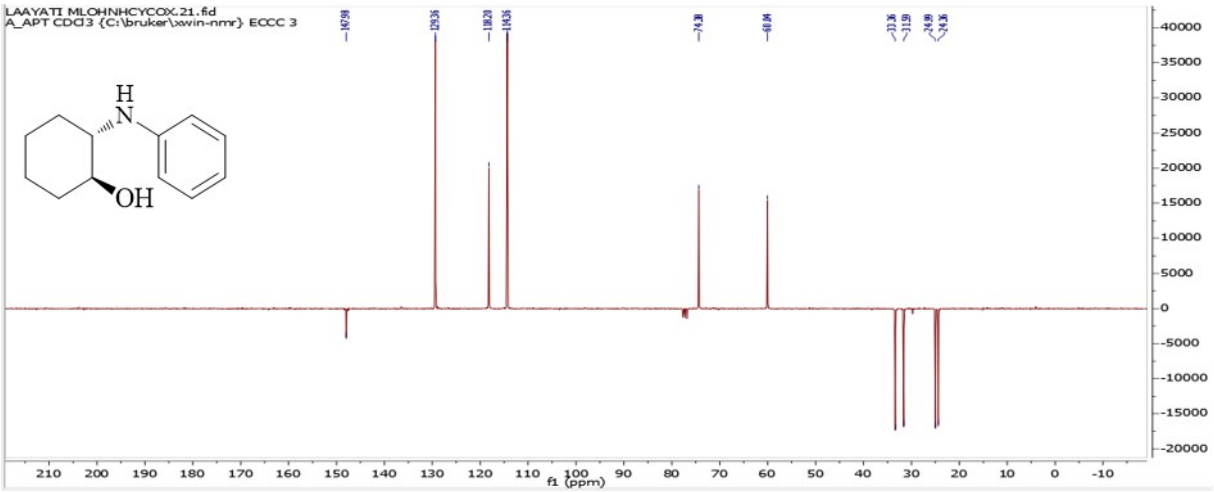

Figure S31: APT spectrum of 2-(phenylamino)-cyclohexanol

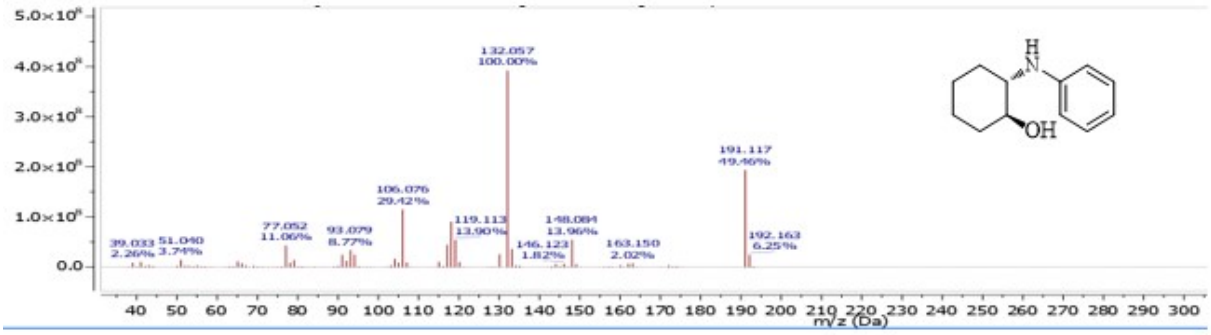

Figure S32: MS spectrum of 2-(phenylamino)-cyclohexanol

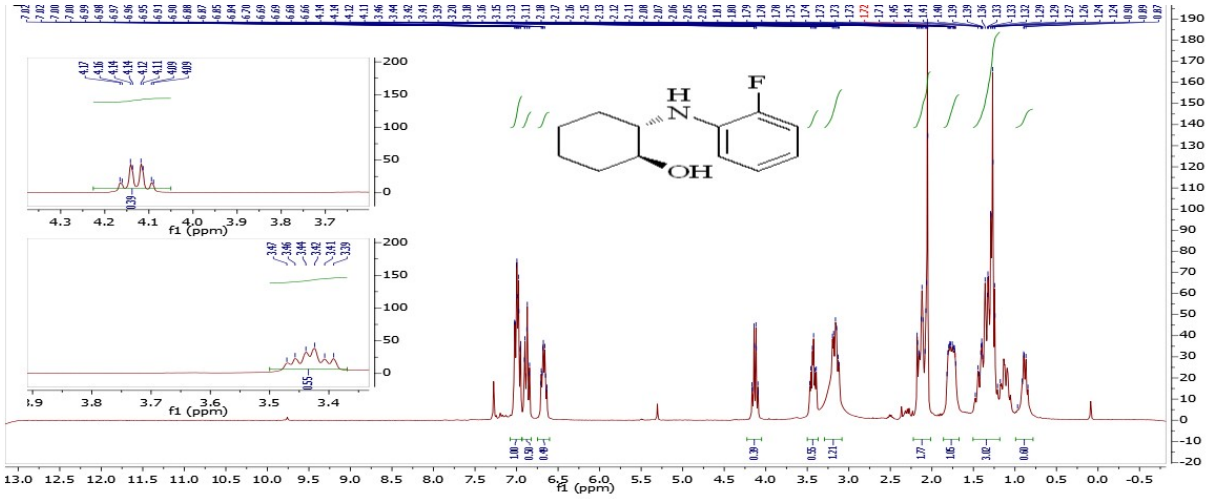

Figure S33: ^{1}H NMR spectrum of 2-(2-fluorobenzylamino)cyclohexanol

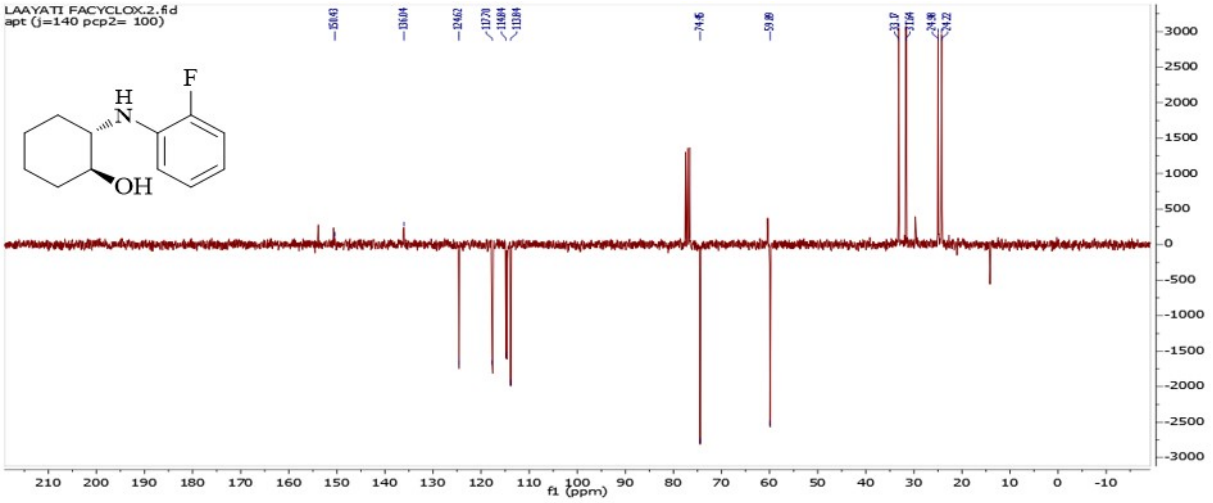

Figure S34: APT spectrum of 2-(2-fluorobenzylamino)cyclohexanol

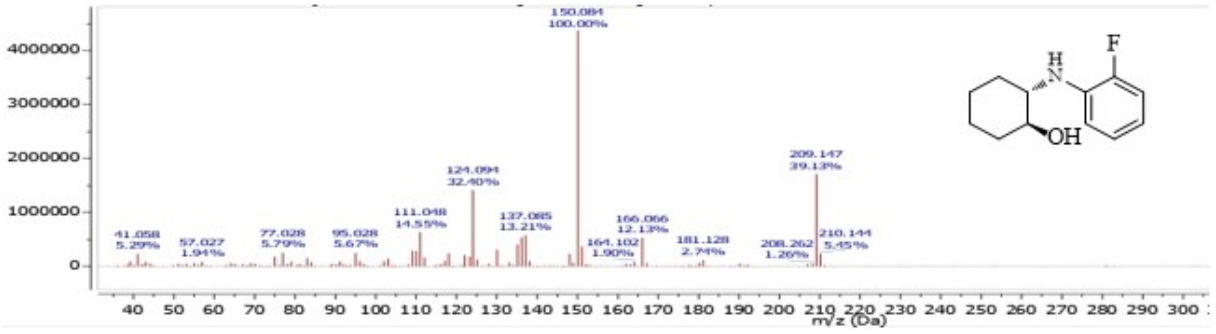

Figure S35: MS spectrum of 2-(2-fluorobenzylamino)cyclohexanol

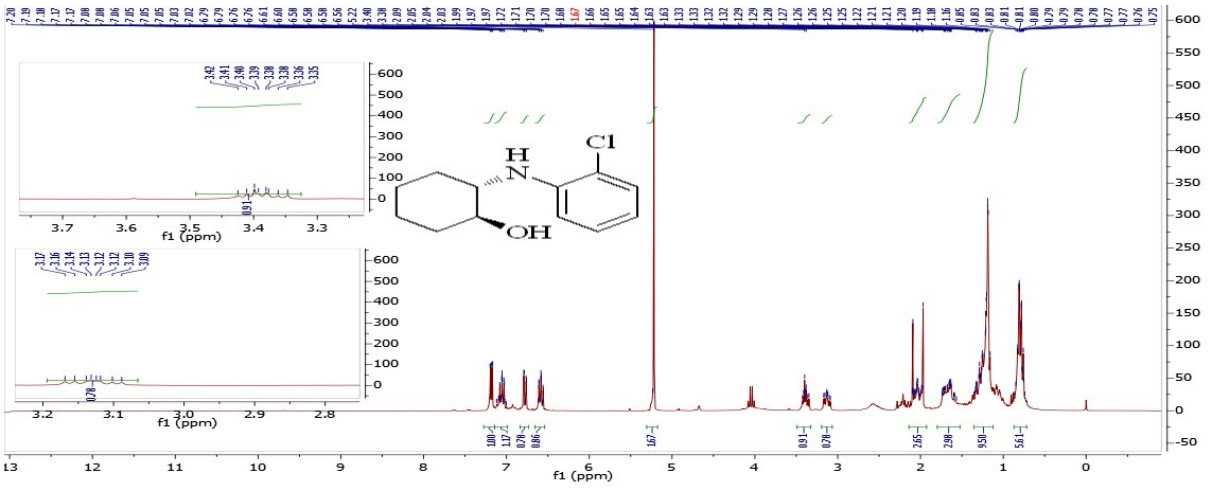

Figure S36: ^{1}H NMR spectrum of 2-((2-chlorophenyl)amino)cyclohexanol

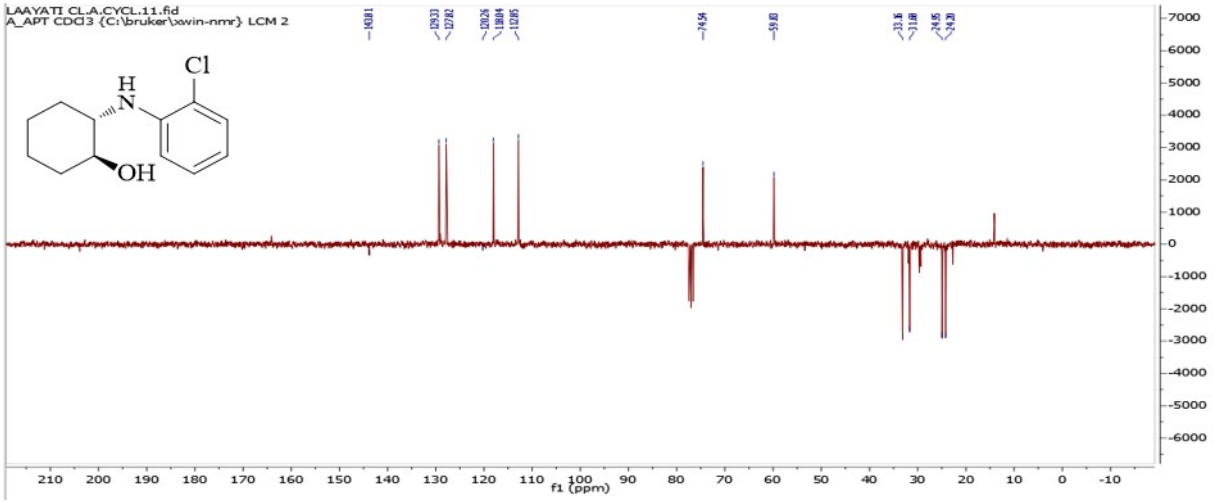

Figure S37: APT spectrum of 2-((2-chlorophenyl)amino)cyclohexanol

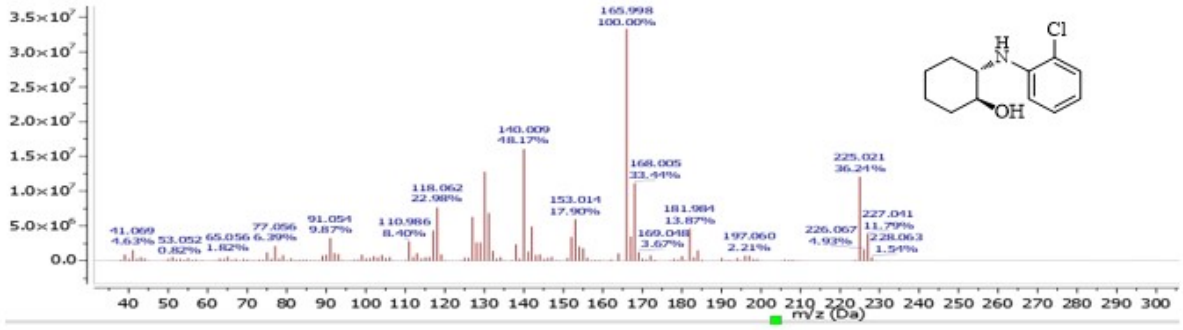

Figure S38: MS spectrum of 2-((2-chlorophenyl)amino)cyclohexanol

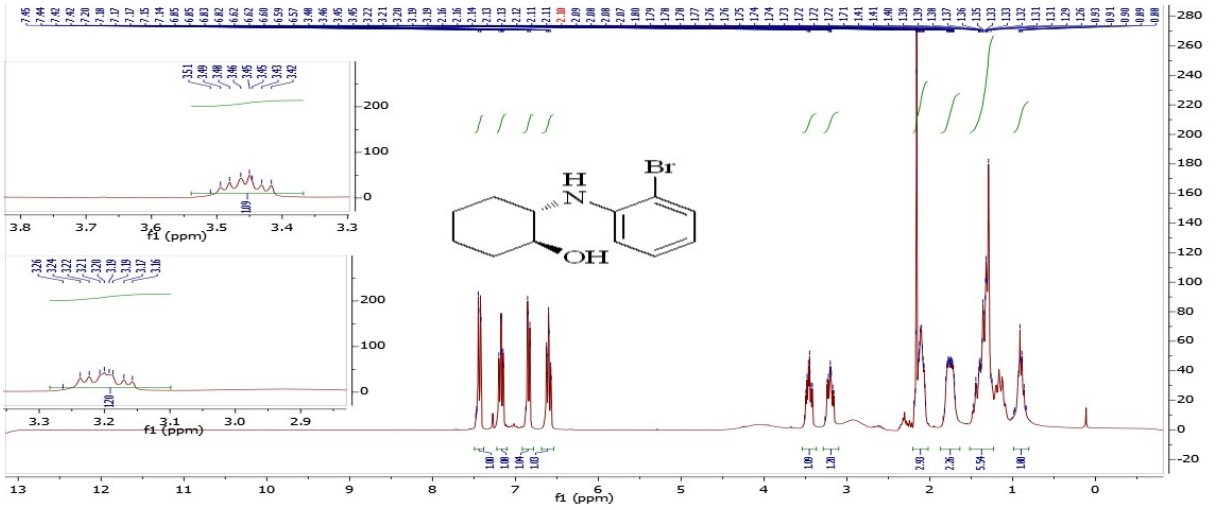

Figure S39: ^{1}H NMR spectrum of 2-((2-bromophenyl)amino)cyclohexanol

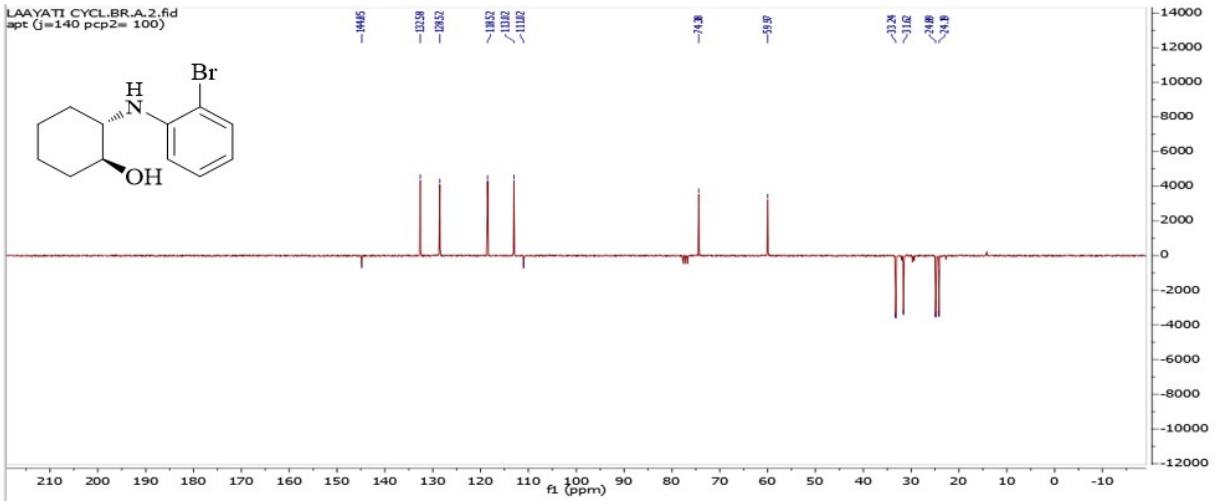

Figure S40: APT spectrum of 2-((2-bromophenyl)amino)cyclohexanol

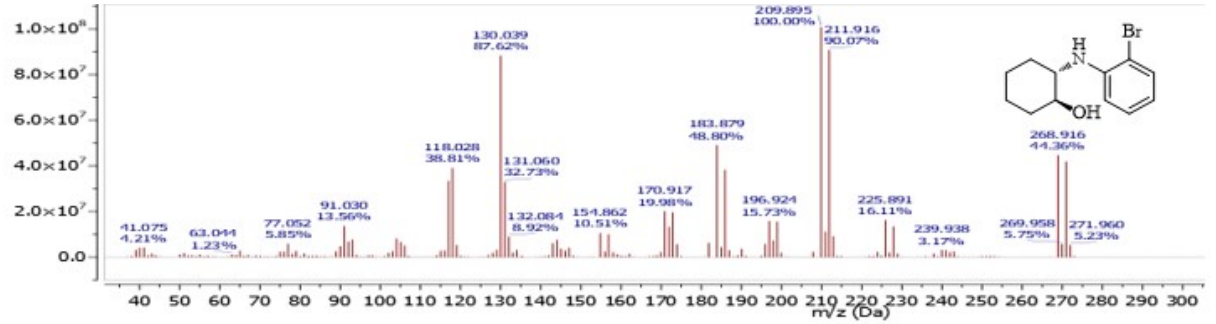

Figure S41: MS spectrum of 2-((2-bromophenyl)amino)cyclohexanol

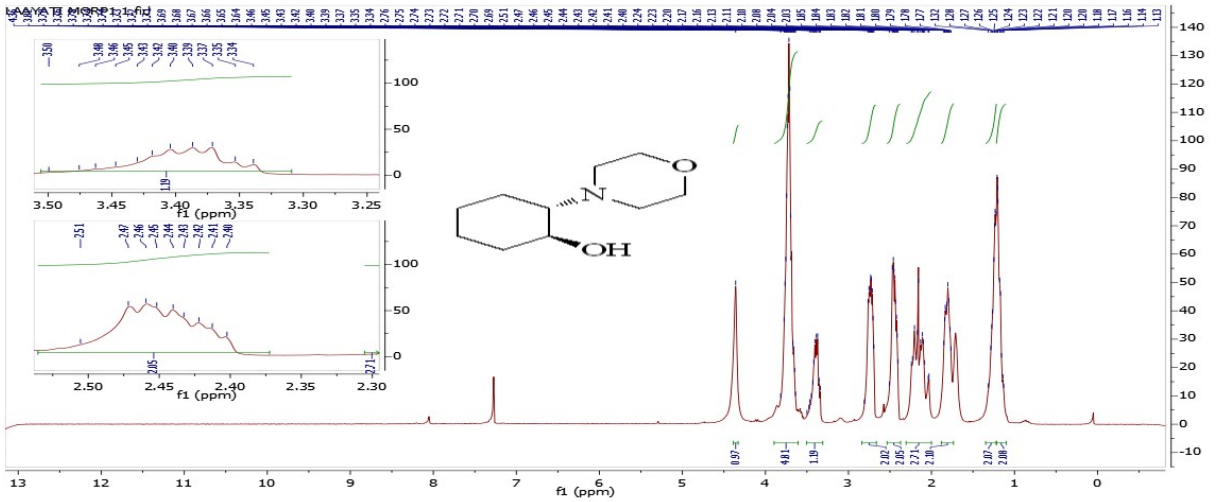

Figure S42: ^{1}H NMR spectrum of 2-(morpholin-4-yl)cyclohexanol

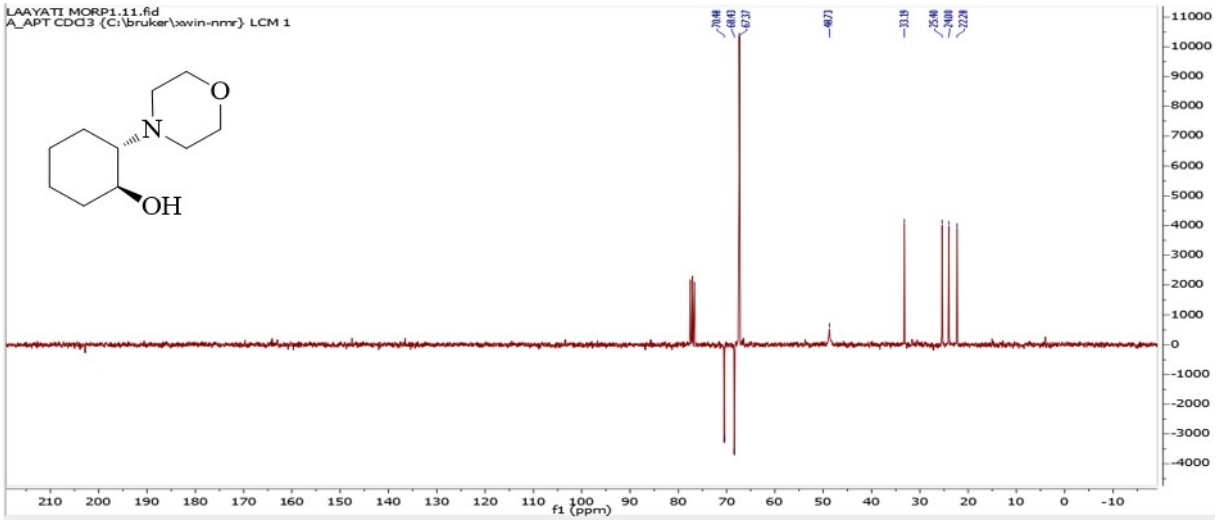

Figure S43: APT spectrum of 2-(morpholin-4-yl)cyclohexanol

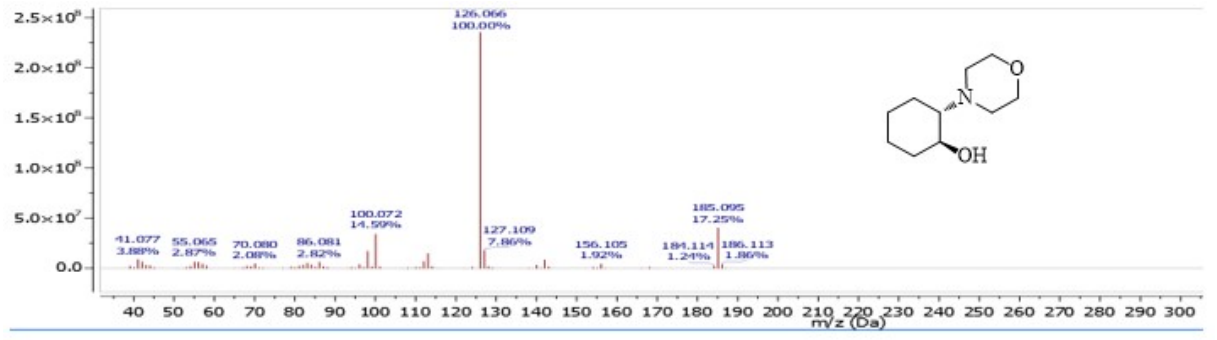

Figure S44: MS spectrum of 2-(morpholin-4-yl)cyclohexanol

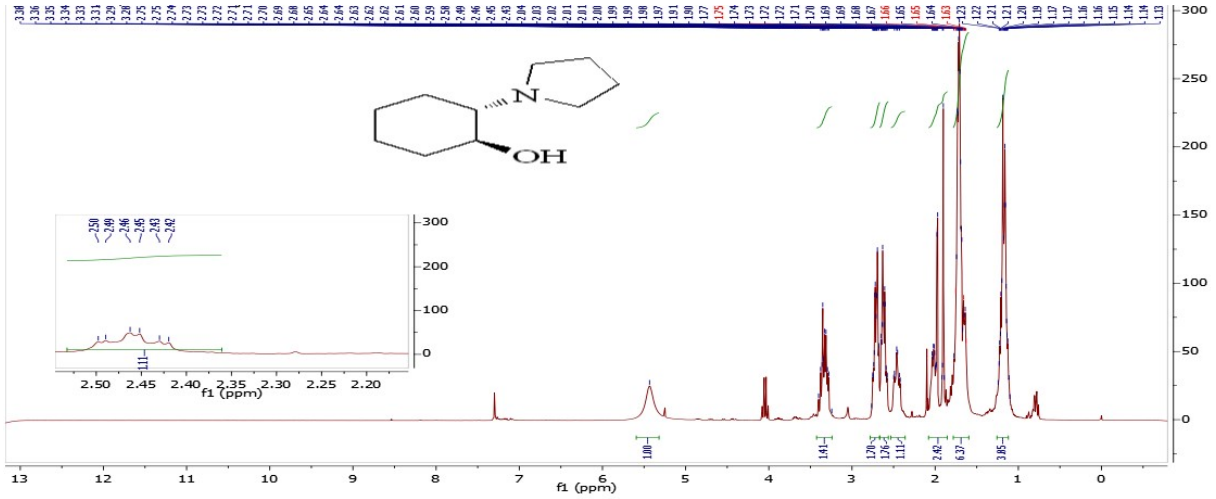

Figure S45: ^{1}H NMR spectrum of 2-(pyrrolidin-1-yl)cyclohexanol

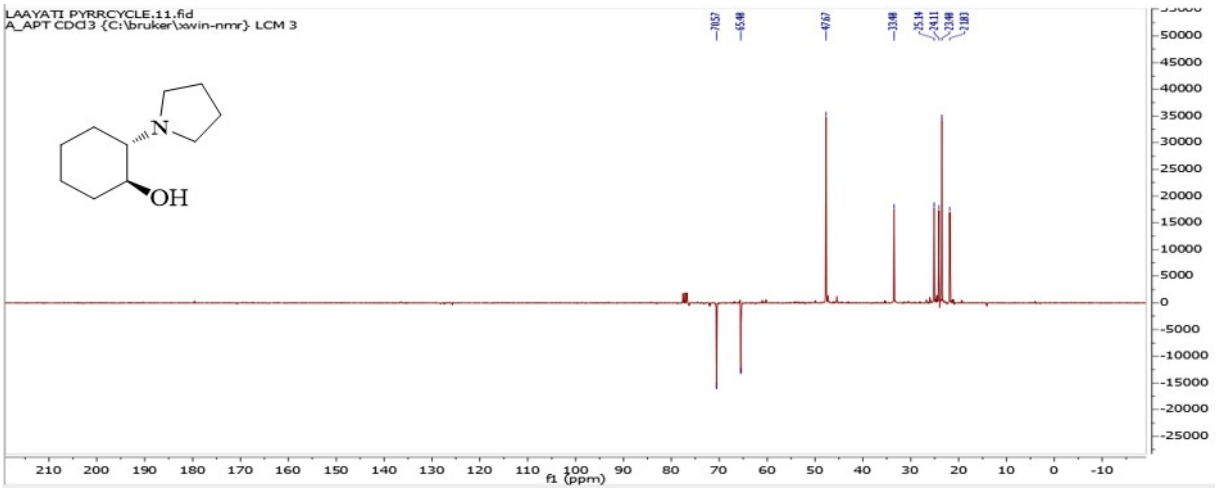

Figure S46: APT spectrum of 2-(pyrrolidin-1-yl)cyclohexanol

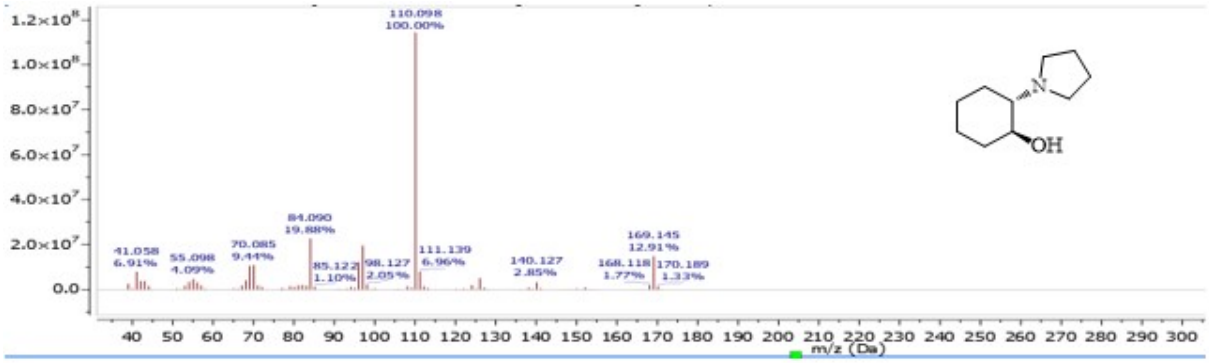

Figure S47: MS spectrum of 2-(pyrrolidin-1-yl)cyclohexanol

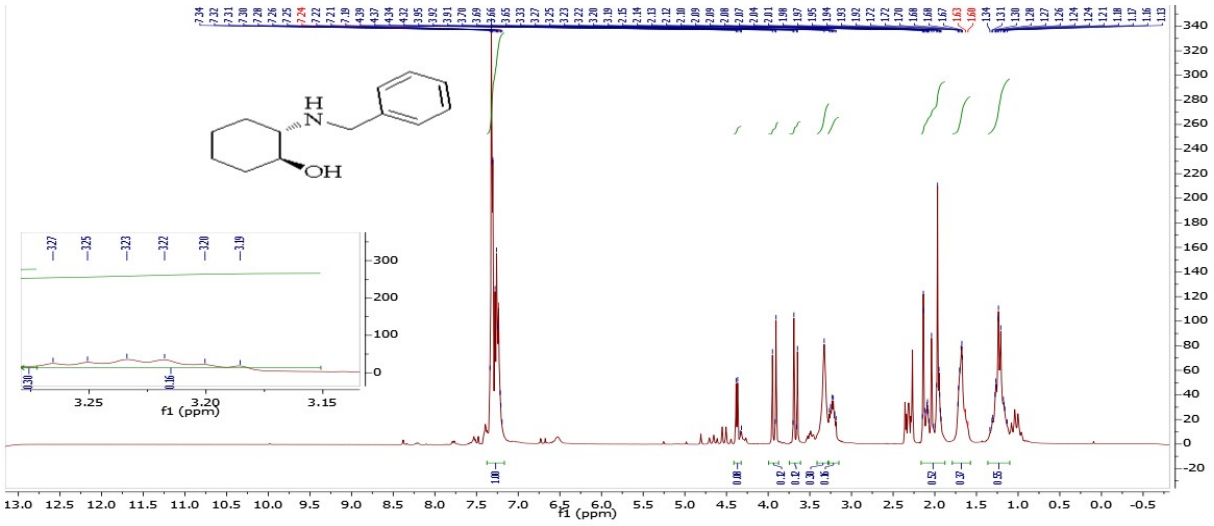

Figure S48: ^{1}H NMR spectrum of 2-(benzylamino)cyclohexanol

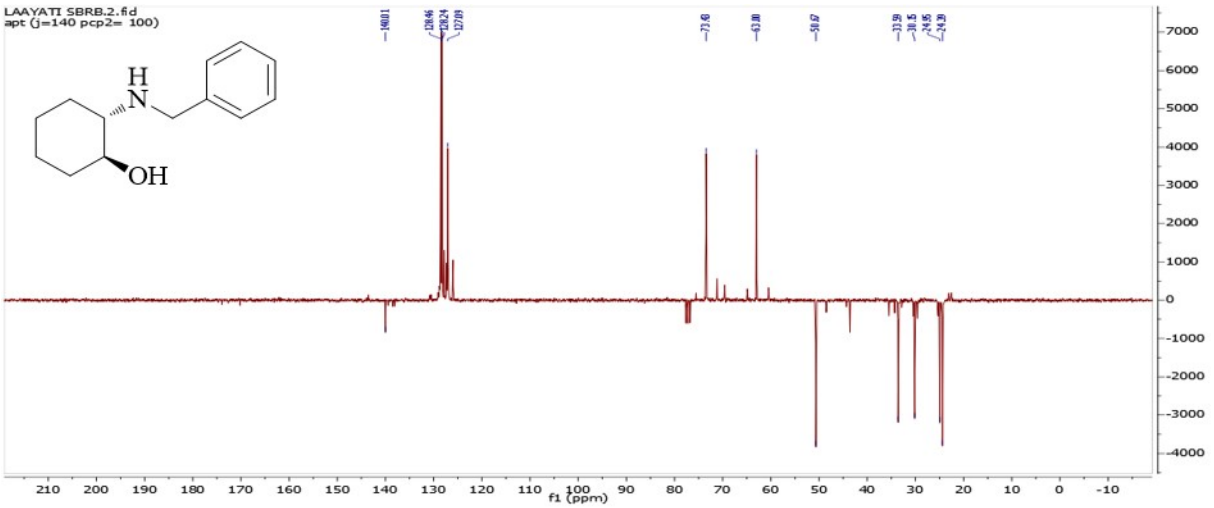

Figure S49: APT spectrum of 2-(benzylamino)cyclohexanol

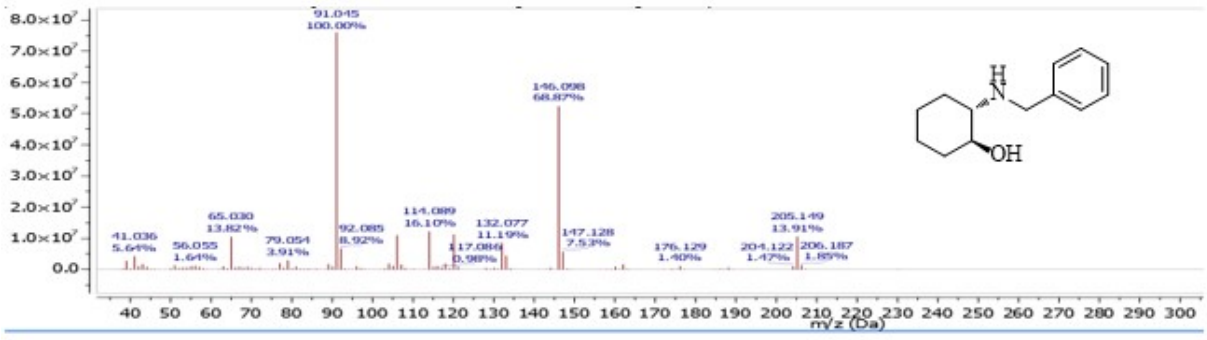

Figure S50: MS spectrum of 2-(benzylamino)cyclohexanol

B- Cartesian coordinates and energy for all optimized geometries

2-Phenyloxirane (2POX)

Energy: -384.490968 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.663876	-1.339696	0.030899
2	6	0	0.302212	-1.062140	-0.079497
3	6	0	-0.146644	0.263707	-0.118171
4	6	0	0.788040	1.304154	-0.059286
5	6	0	2.149940	1.025400	0.055298
6	6	0	2.591399	-0.297902	0.102478
7	1	0	2.002918	-2.371458	0.054507
8	1	0	-0.424922	-1.864012	-0.158607
9	1	0	0.447872	2.336109	-0.102958
10	1	0	2.865732	1.841048	0.101616
11	1	0	3.651971	-0.516015	0.186683
12	6	0	-1.602630	0.577939	-0.208060
13	6	0	-2.588668	0.023857	0.743384
14	8	0	-2.488584	-0.484026	-0.589610
15	1	0	-2.240429	-0.646962	1.528386
16	1	0	-3.499053	0.580182	0.967898
17	1	0	-1.840572	1.541393	-0.662910

Aniline

Energy: -287.3264359 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.242216	1.192298	0.000006

2	6	0	-1.152420	1.223195	0.000035
3	6	0	-1.879208	0.030692	0.000023
4	6	0	-1.203045	-1.189852	0.000003
5	6	0	0.192917	-1.218961	-0.000060
6	6	0	0.928211	-0.030163	-0.000060
7	1	0	0.808074	2.121146	0.000029
8	1	0	-1.671481	2.177634	0.000061
9	1	0	-2.965046	0.054142	0.000038
10	1	0	-1.761928	-2.121396	-0.000014
11	1	0	0.736178	-2.158400	-0.000140
12	7	0	2.369497	-0.120344	-0.000107
13	1	0	2.747868	0.364092	-0.811730
14	1	0	2.747825	0.361945	0.812818

Morpholine

Energy: -287.5372479 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.012900	-0.776102	1.177809
2	6	0	0.012900	0.754891	1.207644
3	6	0	0.012900	0.754891	-1.207644
4	6	0	0.012900	-0.776102	-1.177809
5	1	0	-0.526617	1.122240	2.088302
6	1	0	-1.025974	-1.150217	1.229193
7	1	0	0.567532	-1.195582	2.023707
8	1	0	-0.526617	1.122240	-2.088302
9	1	0	1.049213	1.108081	-1.284363
10	1	0	-1.025974	-1.150217	-1.229193
11	1	0	0.567532	-1.195582	-2.023707
12	1	0	1.049213	1.108081	1.284363
13	7	0	-0.576552	1.347881	0.000000
14	1	0	-1.579351	1.163009	0.000000

15	8	0	0.647163	-1.264087	0.000000

2POX-Fe

Energy: -508.1207002 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.553512	-1.374209	0.637547
2	6	0	1.313384	-0.740621	0.683825
3	6	0	1.110747	0.458805	-0.012542
4	6	0	2.159940	1.006879	-0.760285
5	6	0	3.402977	0.374579	-0.798370
6	6	0	3.602016	-0.816607	-0.099166
7	1	0	2.700249	-2.308020	1.172058
8	1	0	0.491670	-1.185879	1.236501
9	1	0	2.003862	1.929277	-1.314134
10	1	0	4.210679	0.807821	-1.380679
11	1	0	4.566836	-1.313745	-0.134385
12	6	0	-0.189742	1.178872	0.038895
13	6	0	-0.959353	1.372310	1.290146
14	8	0	-1.384443	0.383911	0.324723
15	1	0	-0.571789	0.951956	2.214882
16	1	0	-1.633196	2.219291	1.391410
17	1	0	-0.357096	1.902820	-0.755889
18	26	0	-3.011406	-0.570571	-0.419533

2POX-Sr

Energy: -415.2899312 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.053406	-1.418704	0.785014
2	6	0	1.890181	-0.651070	0.757230
3	6	0	1.795271	0.453262	-0.099689
4	6	0	2.874590	0.769645	-0.933425
5	6	0	4.040110	0.003353	-0.900652
6	6	0	4.132376	-1.091976	-0.040378
7	1	0	3.115833	-2.277222	1.447438
8	1	0	1.040941	-0.913172	1.380897
9	1	0	2.802614	1.617825	-1.610072
10	1	0	4.871582	0.258005	-1.551311
11	1	0	5.036760	-1.692869	-0.018375
12	6	0	0.575942	1.310554	-0.125247
13	6	0	-0.043543	1.849627	1.101422
14	8	0	-0.649767	0.744262	0.402134
15	1	0	0.392959	1.595363	2.065422
16	1	0	-0.603739	2.782860	1.063509
17	1	0	0.429198	1.881878	-1.042180
18	38	0	-3.205211	-0.435655	-0.216264

2POX-AcOOH

Energy: -805.7124119 (Hartrees)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.438595	-0.820722	-0.517560
2	6	0	4.123469	-0.959506	-0.077387
3	6	0	3.299151	0.166123	0.046288
4	6	0	3.806817	1.426994	-0.288677
5	6	0	5.125302	1.565087	-0.722503
6	6	0	5.944712	0.441311	-0.837273
7	1	0	6.068697	-1.699890	-0.616721
8	1	0	3.717884	-1.939858	0.151751
9	1	0	3.167318	2.302307	-0.207632

10	1	0	5.508979	2.548610	-0.977307
11	1	0	6.969536	0.546690	-1.180772
12	6	0	1.899011	0.053252	0.542219
13	6	0	1.540194	-0.668172	1.777034
14	8	0	1.288757	-1.264398	0.485761
15	1	0	2.321960	-1.163407	2.349148
16	1	0	0.647143	-0.359617	2.314720
17	1	0	1.215708	0.849281	0.251688
18	1	0	-0.378358	-1.274152	0.013579
19	8	0	-1.341326	-1.253907	-0.230508
20	6	0	-1.877397	-0.134755	0.266543
21	8	0	-1.236020	0.688140	0.908589
22	6	0	-3.329659	0.016514	-0.034598
23	6	0	-3.989831	1.158675	0.437155
24	6	0	-4.037509	-0.945074	-0.768424
25	6	0	-5.345837	1.338647	0.177774
26	1	0	-3.420815	1.888573	1.002652
27	6	0	-5.394922	-0.761561	-1.025846
28	1	0	-3.518969	-1.825594	-1.129751
29	6	0	-6.049571	0.378494	-0.554009
30	1	0	-5.855213	2.224844	0.544433
31	1	0	-5.942708	-1.507107	-1.594497
32	1	0	-7.107599	0.518796	-0.756427

TSA uncatalyzed

Energy: -671.763631 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.73366090087869	3.27886385805789	0.40251166462363
C	4.65760795003608	1.82094005624930	1.09490732249046
C	4.42951822784731	-0.65875852717277	0.19672048205293
C	6.28617383951788	-1.66673849704640	-1.40066494715347
C	8.36562841265877	-0.20182274448014	-2.08795839928487
C	8.58597054875289	2.27315165402055	-1.19449585715228

H	6.93094860690475	5.19069961808718	1.12363119549516
H	3.23558915814143	2.49727296835437	2.41072356663172
H	6.12044506622582	-3.59955043060218	-2.08002158546469
H	9.81467026735385	-0.98775986821086	-3.31117812944185
H	10.21132449719621	3.40982175757747	-1.72248531946796
C	2.13576851938009	-2.39390514206928	1.53918187967440
C	0.92539886451210	-1.77350794374004	-0.85755770229401
H	0.08522664823721	0.08239205904972	-1.05390021833495
H	1.23966037201086	-2.84290401078625	-2.58438938051109
H	2.99105856922136	-4.31084310783400	1.55146511082521
O	1.10624564522536	-1.53200096764258	3.59236940707651
N	-2.89997374731996	-2.82230595633957	0.57334292522032
H	-3.38034209427826	-4.64626951391762	0.24849899677501
C	-4.82239192829579	-1.05049871130996	0.12113143894291
C	-6.84307640445351	-1.58056687803231	-1.51121402373135
C	-4.65401754976709	1.34283942032524	1.26044731781182
C	-8.67459921802060	0.25284535552414	-1.97740932459671
H	-6.97611312176333	-3.42758520204967	-2.40240874333585
C	-6.49423274446119	3.15981095533602	0.77138619666348
H	-3.08119836932328	1.71776100793492	2.52580783662122
C	-8.51302718079937	2.63163271504964	-0.84603037482127
H	-10.23815810550396	-0.18330343979356	-3.23426635552311
H	-6.35344798941217	4.99983759693682	1.67070690490136
H	-9.94430581400993	4.05308449462049	-1.21736162074348
H	-1.91523738043785	-2.54527209129770	2.25727779772333

TSA_model-1

Energy: -1043.478482 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.73366090087869	3.27886385805789	0.40251166462363
C	4.65760795003608	1.82094005624930	1.09490732249046
C	4.42951822784731	-0.65875852717277	0.19672048205293
C	6.28617383951788	-1.66673849704640	-1.40066494715347
C	8.36562841265877	-0.20182274448014	-2.08795839928487

C	8.58597054875289	2.27315165402055	-1.19449585715228
H	6.93094860690475	5.19069961808718	1.12363119549516
H	3.23558915814143	2.49727296835437	2.41072356663172
H	6.12044506622582	-3.59955043060218	-2.08002158546469
H	9.81467026735385	-0.98775986821086	-3.31117812944185
H	10.21132449719621	3.40982175757747	-1.72248531946796
C	2.13576851938009	-2.39390514206928	1.53918187967440
C	0.92539886451210	-1.77350794374004	-0.85755770229401
H	0.08522664823721	0.08239205904972	-1.05390021833495
H	1.23966037201086	-2.84290401078625	-2.58438938051109
H	2.99105856922136	-4.31084310783400	1.55146511082521
O	1.10624564522536	-1.53200096764258	3.59236940707651
N	-2.89997374731996	-2.82230595633957	0.57334292522032
H	-3.38034209427826	-4.64626951391762	0.24849899677501
C	-4.82239192829579	-1.05049871130996	0.12113143894291
C	-6.84307640445351	-1.58056687803231	-1.51121402373135
C	-4.65401754976709	1.34283942032524	1.26044731781182
C	-8.67459921802060	0.25284535552414	-1.97740932459671
H	-6.97611312176333	-3.42758520204967	-2.40240874333585
C	-6.49423274446119	3.15981095533602	0.77138619666348
H	-3.08119836932328	1.71776100793492	2.52580783662122
C	-8.51302718079937	2.63163271504964	-0.84603037482127
H	-10.23815810550396	-0.18330343979356	-3.23426635552311
H	-6.35344798941217	4.99983759693682	1.67070690490136
H	-9.94430581400993	4.05308449462049	-1.21736162074348
H	-1.91523738043785	-2.54527209129770	2.25727779772333
Fe	3.56836973222128	-0.60244469242741	5.80656150962123
Fe	3.51923703438516	3.40490855657989	7.58403774783266
Fe	6.75614899514490	-3.42512860155088	6.85158000572008

TSA_model-2

Energy: -950.390074 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.73366090087869	3.27886385805789	0.40251166462363

C	4.65760795003608	1.82094005624930	1.09490732249046
C	4.42951822784731	-0.65875852717277	0.19672048205293
C	6.28617383951788	-1.66673849704640	-1.40066494715347
C	8.36562841265877	-0.20182274448014	-2.08795839928487
C	8.58597054875289	2.27315165402055	-1.19449585715228
H	6.93094860690475	5.19069961808718	1.12363119549516
H	3.23558915814143	2.49727296835437	2.41072356663172
H	6.12044506622582	-3.59955043060218	-2.08002158546469
H	9.81467026735385	-0.98775986821086	-3.31117812944185
H	10.21132449719621	3.40982175757747	-1.72248531946796
C	2.13576851938009	-2.39390514206928	1.53918187967440
C	0.92539886451210	-1.77350794374004	-0.85755770229401
H	0.08522664823721	0.08239205904972	-1.05390021833495
H	1.23966037201086	-2.84290401078625	-2.58438938051109
H	2.99105856922136	-4.31084310783400	1.55146511082521
O	1.10624564522536	-1.53200096764258	3.59236940707651
N	-2.89997374731996	-2.82230595633957	0.57334292522032
H	-3.38034209427826	-4.64626951391762	0.24849899677501
C	-4.82239192829579	-1.05049871130996	0.12113143894291
C	-6.84307640445351	-1.58056687803231	-1.51121402373135
C	-4.65401754976709	1.34283942032524	1.26044731781182
C	-8.67459921802060	0.25284535552414	-1.97740932459671
H	-6.97611312176333	-3.42758520204967	-2.40240874333585
C	-6.49423274446119	3.15981095533602	0.77138619666348
H	-3.08119836932328	1.71776100793492	2.52580783662122
C	-8.51302718079937	2.63163271504964	-0.84603037482127
H	-10.23815810550396	-0.18330343979356	-3.23426635552311
H	-6.35344798941217	4.99983759693682	1.67070690490136
H	-9.94430581400993	4.05308449462049	-1.21736162074348
H	-1.91523738043785	-2.54527209129770	2.25727779772333
Fe	3.56836973222128	-0.60244469242741	5.80656150962123
Fe	6.75614899514490	-3.42512860155088	6.85158000572008
Sr	3.51923703438516	3.40490855657989	7.58403774783266

TSA_model-3

Energy: -950.290851 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.73366090087869	3.27886385805789	0.40251166462363
C	4.65760795003608	1.82094005624930	1.09490732249046
C	4.42951822784731	-0.65875852717277	0.19672048205293
C	6.28617383951788	-1.66673849704640	-1.40066494715347
C	8.36562841265877	-0.20182274448014	-2.08795839928487
C	8.58597054875289	2.27315165402055	-1.19449585715228
H	6.93094860690475	5.19069961808718	1.12363119549516
H	3.23558915814143	2.49727296835437	2.41072356663172
H	6.12044506622582	-3.59955043060218	-2.08002158546469
H	9.81467026735385	-0.98775986821086	-3.31117812944185
H	10.21132449719621	3.40982175757747	-1.72248531946796
C	2.13576851938009	-2.39390514206928	1.53918187967440
C	0.92539886451210	-1.77350794374004	-0.85755770229401
H	0.08522664823721	0.08239205904972	-1.05390021833495
H	1.23966037201086	-2.84290401078625	-2.58438938051109
H	2.99105856922136	-4.31084310783400	1.55146511082521
O	1.10624564522536	-1.53200096764258	3.59236940707651
N	-2.89997374731996	-2.82230595633957	0.57334292522032
H	-3.38034209427826	-4.64626951391762	0.24849899677501
C	-4.82239192829579	-1.05049871130996	0.12113143894291
C	-6.84307640445351	-1.58056687803231	-1.51121402373135
C	-4.65401754976709	1.34283942032524	1.26044731781182
C	-8.67459921802060	0.25284535552414	-1.97740932459671
H	-6.97611312176333	-3.42758520204967	-2.40240874333585
C	-6.49423274446119	3.15981095533602	0.77138619666348
H	-3.08119836932328	1.71776100793492	2.52580783662122
C	-8.51302718079937	2.63163271504964	-0.84603037482127
H	-10.23815810550396	-0.18330343979356	-3.23426635552311
H	-6.35344798941217	4.99983759693682	1.67070690490136
H	-9.94430581400993	4.05308449462049	-1.21736162074348
H	-1.91523738043785	-2.54527209129770	2.25727779772333
Fe	6.75614899514490	-3.42512860155088	6.85158000572008

Sr	3.56836973222128	-0.60244469242741	5.80656150962123
Fe	3.51923703438516	3.40490855657989	7.58403774783266

IMA1_model-1

Energy: -1043.5110054 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.187531	-0.371001	-0.345840
C	0.123880	-0.780207	0.978244
C	1.264760	-0.683232	1.838593
C	2.452614	-0.116428	1.273156
C	2.500783	0.287673	-0.051516
C	1.374801	0.155784	-0.878891
H	-0.700247	-0.461795	-0.975397
H	-0.818166	-1.160618	1.375022
H	3.327569	0.011195	1.912576
H	3.418204	0.721344	-0.450070
H	1.415027	0.467298	-1.922237
C	1.248121	-1.104673	3.182175
C	0.057051	-1.648189	3.877759
O	-0.787342	-0.556161	4.336449
H	-0.549326	-2.288684	3.215636
H	0.348805	-2.246623	4.756033
H	2.152685	-0.937822	3.770634
N	0.866863	1.996159	5.064076
H	1.345258	1.598411	5.867702
C	1.628925	2.903963	4.330980
C	2.797343	3.474397	4.874533
C	1.222009	3.314051	3.045137
C	3.523542	4.428331	4.162593
H	3.132296	3.159502	5.865959
C	1.955007	4.268995	2.342404
H	0.324216	2.877188	2.604249
C	3.109200	4.837482	2.892316
H	4.424342	4.855412	4.605499

H	1.621466	4.571280	1.347606
H	3.683114	5.579150	2.337405
H	0.366079	1.272772	4.541158
Fe	-2.156482	-0.251833	5.371334
Fe	-2.873529	-0.268720	7.508355
Fe	-3.948698	-1.147901	6.005365

IMA1_model-2

Energy: -950.4204611 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.207718	-1.438824	-0.460992
C	0.292239	-1.001777	0.864958
C	1.490643	-0.467296	1.361177
C	2.597422	-0.381004	0.504945
C	2.515295	-0.821585	-0.816745
C	1.317067	-1.352728	-1.304760
H	-0.732458	-1.850815	-0.832977
H	-0.570611	-1.069802	1.529014
H	3.530711	0.045103	0.879349
H	3.384719	-0.742210	-1.470158
H	1.250569	-1.696660	-2.337951
C	1.590477	0.093534	2.774294
C	0.748268	-0.660018	3.842461
O	-0.619819	-0.370597	3.785112
H	0.918659	-1.742732	3.676943
H	1.165058	-0.425701	4.841863
H	2.646686	0.014570	3.083049
N	1.260465	1.522721	2.679322
H	-2.240034	2.108839	4.895039
C	1.490161	2.486379	3.626131
C	2.356367	2.307218	4.737592
C	0.876555	3.764168	3.459809
C	2.658688	3.395331	5.591183

H	2.844179	1.347584	4.902267
C	1.180699	4.832458	4.325087
H	0.222631	3.927613	2.601333
C	2.073909	4.659271	5.397628
H	3.380277	3.250987	6.397299
H	0.733938	5.809745	4.135422
H	2.334423	5.497919	6.045391
H	0.456632	1.697827	2.081099
Fe	-1.520875	0.704747	4.911608
Sr	-0.285911	2.918585	6.078144
Fe	-1.517045	0.393648	6.875065

IMA1_model-3

Energy: -950.36369 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.04515377554501	-0.05090706562982	-0.01028162757004
C	0.05250527126441	-0.09524689455882	2.62609416777250
C	2.34816710100094	-0.05154903016092	3.95741706040981
C	4.61779506964362	0.02842048314451	2.59168741209896
C	4.60716714787144	0.07545024461586	-0.04457659082548
C	2.31692715403685	0.03970977693509	-1.35468351691913
H	-1.74789800301808	-0.09707699037594	-1.01639566863978
H	-1.72193473642308	-0.18748479710608	3.66073003043993
H	6.41113617094563	0.05970855765356	3.60227114489338
H	6.38807793685888	0.13552320949646	-1.07105067344673
H	2.30140177457544	0.07080909048096	-3.41080039004582
C	2.43789114812727	-0.13217846228536	6.81794154465882
C	0.50361388502938	-1.89280373485048	8.07457390982567
O	-1.81352779071717	-0.48880464562893	8.05664316034072
H	0.29167540825626	-3.67034451098853	7.03406445710833
H	1.07322625277347	-2.32587550990584	10.03012754645254
H	4.33536088323175	-0.79283517210753	7.35791654389966
N	1.86233550668241	2.42898331176585	8.04885137355201

H	2.22329261538184	2.20282309821646	9.94529912965027
C	3.23632350382387	4.61177767710476	7.18119243316440
C	5.24490937696291	5.51058560815862	8.65235920888980
C	2.52895534177830	5.89185008229383	4.97127628384257
C	6.54937901192022	7.67888249733373	7.91580902485833
H	5.78678406118542	4.51483033138962	10.37368147184769
C	3.86732441464390	8.03740575405746	4.23301195569928
H	0.94239835318320	5.21511800333938	3.85872142323178
C	5.87466374128294	8.94338344775901	5.69683615332287
H	8.09856997908346	8.37001723922311	9.07696264307835
H	3.31685189607186	9.02228636940387	2.51435128506105
H	6.89561832506639	10.63115408446081	5.11900321426313
H	0.02542456047882	1.99767479858375	8.13829182758903
Sr	-4.49855057514884	-1.30090313972379	10.38307038334766
Fe	-6.72980339538084	0.21608638782296	13.41193999694440
Fe	-5.79037988118894	-5.13675115731193	10.01615263625408

IMA2_model-1

Energy: -1043.535442 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.00529123314998	0.00037794522500	0.00018897261250
C	0.00415739747499	-0.00321253441249	2.63711270349362
C	2.29091487361534	-0.00151178089999	3.98108592169933
C	4.56198770984565	-0.00510226053748	2.62142807681166
C	4.56463331508228	0.00151178089999	-0.01549575422495
C	2.28203326476281	0.00661404143748	-1.33433559229153
H	-1.78049996441759	-0.01020452107497	-1.01194832103681
H	-1.77634255371452	-0.02645616574991	3.65284054103110
H	6.34721198390654	-0.00548020576248	3.63810070938149
H	6.34683397632058	-0.00207869873749	-1.03368017336396
H	2.27523024693338	0.00604712359998	-3.38695610736985
C	2.39447192951568	-0.03477096069988	6.85176878369079
C	0.43199138272490	-1.79089349400985	8.09747615646944
O	-1.99611778897868	-0.52666665969736	8.11958624314968

H	0.20957062726179	-3.55381890530952	7.05396969260415
H	0.98738186062490	-2.23252233257359	10.04332767649865
H	4.27248183568226	-0.75343380414522	7.38278208559619
N	1.94528405606087	2.49443858325730	8.04210767989482
H	2.28033245266880	2.29148188593914	9.92748693969268
C	3.34160281265083	4.65042714949810	7.17850280864740
C	5.33866517178445	5.60436060070786	8.63245786622979
C	2.65789976078841	5.90180374033598	4.94692504433904
C	6.63048185445404	7.77546745782878	7.87637890660276
H	5.87704805030882	4.64513593902483	10.36968324222476
C	3.98203071484196	8.04550930219310	4.17856240569610
H	1.08602560025436	5.19939244896901	3.83822279861489
C	5.96681029446932	8.99660791855098	5.63667509885896
H	8.16229438238688	8.49923236905953	9.03534764993323
H	3.43533301302173	8.99604113110458	2.44341584749137
H	6.97479031914501	10.68073196397746	5.03838764894900
H	-1.56960656288338	1.28501377822372	8.25678014817489
Fe	-4.65836396520800	-1.51234782161182	10.45717743709004
Fe	-7.22593492115666	-0.08862815526220	13.71298641532505
Fe	-5.63913192423516	-5.71755528252238	9.69826364450084

IMA2_model-2

Energy: -950.400286 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.00529123314998	0.00037794522500	0.00018897261250
C	0.00415739747499	-0.00321253441249	2.63711270349362
C	2.29091487361534	-0.00151178089999	3.98108592169933
C	4.56198770984565	-0.00510226053748	2.62142807681166
C	4.56463331508228	0.00151178089999	-0.01549575422495
C	2.28203326476281	0.00661404143748	-1.33433559229153
H	-1.78049996441759	-0.01020452107497	-1.01194832103681
H	-1.77634255371452	-0.02645616574991	3.65284054103110
H	6.34721198390654	-0.00548020576248	3.63810070938149
H	6.34683397632058	-0.00207869873749	-1.03368017336396

H	2.27523024693338	0.00604712359998	-3.38695610736985
C	2.39447192951568	-0.03477096069988	6.85176878369079
C	0.43199138272490	-1.79089349400985	8.09747615646944
O	-1.99611778897868	-0.52666665969736	8.11958624314968
H	0.20957062726179	-3.55381890530952	7.05396969260415
H	0.98738186062490	-2.23252233257359	10.04332767649865
H	4.27248183568226	-0.75343380414522	7.38278208559619
N	1.94528405606087	2.49443858325730	8.04210767989482
H	2.28033245266880	2.29148188593914	9.92748693969268
C	3.34160281265083	4.65042714949810	7.17850280864740
C	5.33866517178445	5.60436060070786	8.63245786622979
C	2.65789976078841	5.90180374033598	4.94692504433904
C	6.63048185445404	7.77546745782878	7.87637890660276
H	5.87704805030882	4.64513593902483	10.36968324222476
C	3.98203071484196	8.04550930219310	4.17856240569610
H	1.08602560025436	5.19939244896901	3.83822279861489
C	5.96681029446932	8.99660791855098	5.63667509885896
H	8.16229438238688	8.49923236905953	9.03534764993323
H	3.43533301302173	8.99604113110458	2.44341584749137
H	6.97479031914501	10.68073196397746	5.03838764894900
H	-1.56960656288338	1.28501377822372	8.25678014817489
Fe	-5.63913192423516	-5.71755528252238	9.69826364450084
Sr	-7.22593492115666	-0.08862815526220	13.71298641532505
Fe	-4.65836396520800	-1.51234782161182	10.45717743709004

IMA2_model-3

Energy: -950.331519 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.00529123314998	0.00037794522500	0.00018897261250
C	0.00415739747499	-0.00321253441249	2.63711270349362
C	2.29091487361534	-0.00151178089999	3.98108592169933
C	4.56198770984565	-0.00510226053748	2.62142807681166
C	4.56463331508228	0.00151178089999	-0.01549575422495
C	2.28203326476281	0.00661404143748	-1.33433559229153

H	-1.78049996441759	-0.01020452107497	-1.01194832103681
H	-1.77634255371452	-0.02645616574991	3.65284054103110
H	6.34721198390654	-0.00548020576248	3.63810070938149
H	6.34683397632058	-0.00207869873749	-1.03368017336396
H	2.27523024693338	0.00604712359998	-3.38695610736985
C	2.39447192951568	-0.03477096069988	6.85176878369079
C	0.43199138272490	-1.79089349400985	8.09747615646944
O	-1.99611778897868	-0.52666665969736	8.11958624314968
H	0.20957062726179	-3.55381890530952	7.05396969260415
H	0.98738186062490	-2.23252233257359	10.04332767649865
H	4.27248183568226	-0.75343380414522	7.38278208559619
N	1.94528405606087	2.49443858325730	8.04210767989482
H	2.28033245266880	2.29148188593914	9.92748693969268
C	3.34160281265083	4.65042714949810	7.17850280864740
C	5.33866517178445	5.60436060070786	8.63245786622979
C	2.65789976078841	5.90180374033598	4.94692504433904
C	6.63048185445404	7.77546745782878	7.87637890660276
H	5.87704805030882	4.64513593902483	10.36968324222476
C	3.98203071484196	8.04550930219310	4.17856240569610
H	1.08602560025436	5.19939244896901	3.83822279861489
C	5.96681029446932	8.99660791855098	5.63667509885896
H	8.16229438238688	8.49923236905953	9.03534764993323
H	3.43533301302173	8.99604113110458	2.44341584749137
H	6.97479031914501	10.68073196397746	5.03838764894900
H	-1.56960656288338	1.28501377822372	8.25678014817489
Fe	-7.22593492115666	-0.08862815526220	13.71298641532505
Fe	-5.63913192423516	-5.71755528252238	9.69826364450084
Sr	-4.65836396520800	-1.51234782161182	10.45717743709004

Product 3

Energy: -671.848864 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	-5.28839867606785	-2.70174147302868	-1.78786988118726
C	-4.10127262230167	-0.38644900200982	-1.36646097421095

C	-2.58760199807153	-0.02267671349992	0.78177972436601
C	-2.30981234273515	-2.02824305751452	2.48650154455971
C	-3.49391455880133	-4.34655922639365	2.06509274907724
C	-4.98528631838051	-4.69124524891577	-0.08031336031223
H	-6.46191869795463	-2.94891766718538	-3.45404147740370
H	-4.37093645908003	1.16766179908970	-2.67282859528614
H	-1.14290633393996	-1.77426384741812	4.15777557327871
H	-3.24976197746723	-5.87685927233811	3.41095555734767
H	-5.91181937383612	-6.49158713922455	-0.41630667289499
C	-1.28274606907921	2.47402953354846	1.34132761296908
C	-2.96044488127454	4.81785673488417	0.88647052145504
O	-3.29965069047527	5.33960996681681	-1.71587130637637
H	-4.82560477073364	4.52740606568842	1.72872143646742
H	-2.08455677887631	6.44793465659954	1.85495513972727
H	-0.78725988288534	2.45173067078723	3.36427946001034
N	1.03216836600780	2.93039820565153	-0.21259418339260
H	1.78125586809567	4.59449098596745	0.39854322842279
C	3.01449100687539	1.10152133558205	-0.26399473210270
C	5.31806711733777	1.60607824686013	0.94637486985296
C	2.75748840883380	-1.15915797105600	-1.62592039762873
C	7.32136593173184	-0.10091137318493	0.80105491950259
H	5.53992128566546	3.35350803621568	2.00726699548188
C	4.74982656792823	-2.87786388740685	-1.72664273206075
H	1.00741301424162	-1.54617390035195	-2.61424705139627
C	7.04149768348263	-2.36234666097983	-0.52250924899429
H	9.09355096135973	0.33523740134578	1.74081566288039
H	4.51682319498707	-4.62113626605932	-2.78526726192873
H	8.59258455995475	-3.70102866871228	-0.62814495260951
H	-1.68469083287288	4.91990175666121	-2.48914714790662

TSB_uncatalyzed

Energy: -671.977586 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	5.54445647907708	-1.27726585386810	2.48177734641025

C	3.71576850036188	0.49945459404882	1.83265638657015
C	3.13845711059483	0.93276883608382	-0.74058367405417
C	4.41402215425865	-0.47942349523416	-2.60876683807488
C	6.21512006162908	-2.27031704593580	-1.93848104012116
C	6.78695146106243	-2.66886018932091	0.61094846376933
H	5.99874678314473	-1.58907070606601	4.45861988356056
H	2.70741069108791	1.61836147801095	3.22670732252176
H	3.98146392928529	-0.14891041864949	-4.58976701269540
H	7.18492759212374	-3.34576000036621	-3.39243632069123
H	8.19857683674839	-4.06385614329256	1.13553641717029
C	1.27764386334378	2.79566090301484	-1.49382847346154
C	0.26588446200715	4.79763668802345	0.13908384657898
O	-0.13133596379733	4.46580068220882	2.52958746461574
H	2.19208224263160	5.82602553942030	-0.48339195978090
H	-1.09547422143070	5.99137675488122	-0.94864246561390
H	1.07903357957682	3.11804806088600	-3.51980382183155
C	-4.79423506761490	1.21660571706540	-1.50554480567212
C	-2.22118412322226	-2.42432960040085	-0.37681137609564
C	-6.92868101114380	-0.70921419581283	-0.97131922635698
H	-4.64645874164315	1.53937088441224	-3.55306311312528
H	-5.21677811073265	3.02998685369691	-0.61170436744741
C	-4.33692160047947	-3.51734722133276	1.32413106743712
H	-2.38256670595082	-3.16283456815862	-2.30678872991255
H	-0.36509510057684	-2.98916875427924	0.33504845329972
H	-7.05963891066338	-2.10874545846939	-2.50880040732094
H	-8.75906935030846	0.23999522543309	-0.83790455626325
H	-3.69932785850800	-3.65529714152989	3.28698967661591
H	-4.85281683638218	-5.43031700411994	0.67689992442887
N	-2.36518126906458	0.32484392844530	-0.48773831853002
H	-2.05885651869421	1.12457599052752	1.25005378821956
O	-6.50783877823032	-1.92090659849708	1.38006700609035

TSB_Model-1

Energy: -1043.675045 (Hartrees)

Atomic	Coordinates (Angstroms)		

Type	X	Y	Z
C	5.54445647907708	-1.27726585386810	2.48177734641025
C	3.71576850036188	0.49945459404882	1.83265638657015
C	3.13845711059483	0.93276883608382	-0.74058367405417
C	4.41402215425865	-0.47942349523416	-2.60876683807488
C	6.21512006162908	-2.27031704593580	-1.93848104012116
C	6.78695146106243	-2.66886018932091	0.61094846376933
H	5.99874678314473	-1.58907070606601	4.45861988356056
H	2.70741069108791	1.61836147801095	3.22670732252176
H	3.98146392928529	-0.14891041864949	-4.58976701269540
H	7.18492759212374	-3.34576000036621	-3.39243632069123
H	8.19857683674839	-4.06385614329256	1.13553641717029
C	1.27764386334378	2.79566090301484	-1.49382847346154
C	0.26588446200715	4.79763668802345	0.13908384657898
O	-0.13133596379733	4.46580068220882	2.52958746461574
H	2.19208224263160	5.82602553942030	-0.48339195978090
H	-1.09547422143070	5.99137675488122	-0.94864246561390
H	1.07903357957682	3.11804806088600	-3.51980382183155
C	-4.79423506761490	1.21660571706540	-1.50554480567212
C	-2.22118412322226	-2.42432960040085	-0.37681137609564
C	-6.92868101114380	-0.70921419581283	-0.97131922635698
H	-4.64645874164315	1.53937088441224	-3.55306311312528
H	-5.21677811073265	3.02998685369691	-0.61170436744741
C	-4.33692160047947	-3.51734722133276	1.32413106743712
H	-2.38256670595082	-3.16283456815862	-2.30678872991255
H	-0.36509510057684	-2.98916875427924	0.33504845329972
H	-7.05963891066338	-2.10874545846939	-2.50880040732094
H	-8.75906935030846	0.23999522543309	-0.83790455626325
H	-3.69932785850800	-3.65529714152989	3.28698967661591
H	-4.85281683638218	-5.43031700411994	0.67689992442887
N	-2.36518126906458	0.32484392844530	-0.48773831853002
H	-2.05885651869421	1.12457599052752	1.25005378821956
O	-6.50783877823032	-1.92090659849708	1.38006700609035
Fe	2.88202129999964	4.23789973988048	4.17157038501855
Fe	3.20025127204514	1.87517518469826	7.85105642912920

Fe	6.40503773750190	6.30998428475786	2.58552317839157

TSB_Model-2

Energy: -950.593705 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	5.54445647907708	-1.27726585386810	2.48177734641025
C	3.71576850036188	0.49945459404882	1.83265638657015
C	3.13845711059483	0.93276883608382	-0.74058367405417
C	4.41402215425865	-0.47942349523416	-2.60876683807488
C	6.21512006162908	-2.27031704593580	-1.93848104012116
C	6.78695146106243	-2.66886018932091	0.61094846376933
H	5.99874678314473	-1.58907070606601	4.45861988356056
H	2.70741069108791	1.61836147801095	3.22670732252176
H	3.98146392928529	-0.14891041864949	-4.58976701269540
H	7.18492759212374	-3.34576000036621	-3.39243632069123
H	8.19857683674839	-4.06385614329256	1.13553641717029
C	1.27764386334378	2.79566090301484	-1.49382847346154
C	0.26588446200715	4.79763668802345	0.13908384657898
O	-0.13133596379733	4.46580068220882	2.52958746461574
H	2.19208224263160	5.82602553942030	-0.48339195978090
H	-1.09547422143070	5.99137675488122	-0.94864246561390
H	1.07903357957682	3.11804806088600	-3.51980382183155
C	-4.79423506761490	1.21660571706540	-1.50554480567212
C	-2.22118412322226	-2.42432960040085	-0.37681137609564
C	-6.92868101114380	-0.70921419581283	-0.97131922635698
H	-4.64645874164315	1.53937088441224	-3.55306311312528
H	-5.21677811073265	3.02998685369691	-0.61170436744741
C	-4.33692160047947	-3.51734722133276	1.32413106743712
H	-2.38256670595082	-3.16283456815862	-2.30678872991255
H	-0.36509510057684	-2.98916875427924	0.33504845329972
H	-7.05963891066338	-2.10874545846939	-2.50880040732094
H	-8.75906935030846	0.23999522543309	-0.83790455626325
H	-3.69932785850800	-3.65529714152989	3.28698967661591
H	-4.85281683638218	-5.43031700411994	0.67689992442887

N	-2.36518126906458	0.32484392844530	-0.48773831853002
H	-2.05885651869421	1.12457599052752	1.25005378821956
O	-6.50783877823032	-1.92090659849708	1.38006700609035
Fe	2.88202129999964	4.23789973988048	4.17157038501855
Fe	6.40503773750190	6.30998428475786	2.58552317839157
Sr	3.20025127204514	1.87517518469826	7.85105642912920

TSB_Model-3

Energy: -950.49284 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	5.54445647907708	-1.27726585386810	2.48177734641025
C	3.71576850036188	0.49945459404882	1.83265638657015
C	3.13845711059483	0.93276883608382	-0.74058367405417
C	4.41402215425865	-0.47942349523416	-2.60876683807488
C	6.21512006162908	-2.27031704593580	-1.93848104012116
C	6.78695146106243	-2.66886018932091	0.61094846376933
H	5.99874678314473	-1.58907070606601	4.45861988356056
H	2.70741069108791	1.61836147801095	3.22670732252176
H	3.98146392928529	-0.14891041864949	-4.58976701269540
H	7.18492759212374	-3.34576000036621	-3.39243632069123
H	8.19857683674839	-4.06385614329256	1.13553641717029
C	1.27764386334378	2.79566090301484	-1.49382847346154
C	0.26588446200715	4.79763668802345	0.13908384657898
O	-0.13133596379733	4.46580068220882	2.52958746461574
H	2.19208224263160	5.82602553942030	-0.48339195978090
H	-1.09547422143070	5.99137675488122	-0.94864246561390
H	1.07903357957682	3.11804806088600	-3.51980382183155
C	-4.79423506761490	1.21660571706540	-1.50554480567212
C	-2.22118412322226	-2.42432960040085	-0.37681137609564
C	-6.92868101114380	-0.70921419581283	-0.97131922635698
H	-4.64645874164315	1.53937088441224	-3.55306311312528
H	-5.21677811073265	3.02998685369691	-0.61170436744741
C	-4.33692160047947	-3.51734722133276	1.32413106743712
H	-2.38256670595082	-3.16283456815862	-2.30678872991255

H	-0.36509510057684	-2.98916875427924	0.33504845329972
H	-7.05963891066338	-2.10874545846939	-2.50880040732094
H	-8.75906935030846	0.23999522543309	-0.83790455626325
H	-3.69932785850800	-3.65529714152989	3.28698967661591
H	-4.85281683638218	-5.43031700411994	0.67689992442887
N	-2.36518126906458	0.32484392844530	-0.48773831853002
H	-2.05885651869421	1.12457599052752	1.25005378821956
O	-6.50783877823032	-1.92090659849708	1.38006700609035
Fe	6.40503773750190	6.30998428475786	2.58552317839157
Sr	2.88202129999964	4.23789973988048	4.17157038501855
Fe	3.20025127204514	1.87517518469826	7.85105642912920

IMB1_model-1

Energy: -1043.704977 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.62443507856367	-0.88628157529871	-2.72479612797415
C	4.36262163578417	0.29876568902313	-2.04808509489956
C	3.70934349200814	0.58260254354854	0.49813179143050
C	5.37740445341189	-0.31085994378199	2.35384283294612
C	7.63676152057000	-1.49004907034443	1.68072242501793
C	8.26358338899200	-1.78957069139153	-0.86719532820819
H	7.11198422417022	-1.08791530181292	-4.70957525595696
H	3.08176538164708	1.04898701733737	-3.46122227794168
H	4.92727178492472	-0.05839253726230	4.34561398160648
H	8.91270457181978	-2.16392538195071	3.14148072341743
H	10.02442998250143	-2.70363106120367	-1.39499584247780
C	1.24117206598346	1.90125356584989	1.23833756939255
C	-0.51948569097375	0.15703623909724	2.87824189688253
H	0.45410118783596	-1.25213249451596	4.02851803231886
H	-1.72947734014550	1.33679230617389	4.06064330085471
H	1.72777664332479	3.50865439045094	2.46930511052159
C	-1.23739266286635	-3.65529714152989	0.10809233434963
C	-4.93445303521752	-1.37175218279449	1.86308095828529
C	-3.01808163013206	-4.73773256639267	-1.88764741869719

H	-1.12041857793472	-4.91442176821723	1.74213846549871
H	0.65422316368579	-3.32875257106593	-0.64836505427229
C	-6.50575995855035	-2.60271983730710	-0.21826337310594
H	-4.96903467937475	-2.49613916858417	3.59671582251743
H	-5.58905420837900	0.55576842879418	2.23630196245783
H	-2.37803128577207	-6.62443507856367	-2.43226641422103
H	-3.00296379089649	-3.53038624088836	-3.58443259136661
H	-8.42704501627794	-2.92680780727226	0.46562851530869
H	-6.60232499377314	-1.32734368499756	-1.86081336063461
O	-5.50647276475648	-4.99152277364095	-0.92880037153709
N	-2.23686874801450	-1.16123667735240	1.01950724065459
H	-2.11951688226405	0.08995096543942	-0.39192918698531
O	-0.14172946504370	2.63182149302035	-0.87683289743059
Fe	-2.54300449553675	5.24266737376288	-0.67463221339463
Fe	-4.93993302366149	8.04815490742974	-3.04208108010988
Fe	-3.45857667270504	5.91635456913747	3.55967712621686

IMB1_model-2

Energy: -950.602611 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.62443507856367	-0.88628157529871	-2.72479612797415
C	4.36262163578417	0.29876568902313	-2.04808509489956
C	3.70934349200814	0.58260254354854	0.49813179143050
C	5.37740445341189	-0.31085994378199	2.35384283294612
C	7.63676152057000	-1.49004907034443	1.68072242501793
C	8.26358338899200	-1.78957069139153	-0.86719532820819
H	7.11198422417022	-1.08791530181292	-4.70957525595696
H	3.08176538164708	1.04898701733737	-3.46122227794168
H	4.92727178492472	-0.05839253726230	4.34561398160648
H	8.91270457181978	-2.16392538195071	3.14148072341743
H	10.02442998250143	-2.70363106120367	-1.39499584247780
C	1.24117206598346	1.90125356584989	1.23833756939255
C	-0.51948569097375	0.15703623909724	2.87824189688253
H	0.45410118783596	-1.25213249451596	4.02851803231886

H	-1.72947734014550	1.33679230617389	4.06064330085471
H	1.72777664332479	3.50865439045094	2.46930511052159
C	-1.23739266286635	-3.65529714152989	0.10809233434963
C	-4.93445303521752	-1.37175218279449	1.86308095828529
C	-3.01808163013206	-4.73773256639267	-1.88764741869719
H	-1.12041857793472	-4.91442176821723	1.74213846549871
H	0.65422316368579	-3.32875257106593	-0.64836505427229
C	-6.50575995855035	-2.60271983730710	-0.21826337310594
H	-4.96903467937475	-2.49613916858417	3.59671582251743
H	-5.58905420837900	0.55576842879418	2.23630196245783
H	-2.37803128577207	-6.62443507856367	-2.43226641422103
H	-3.00296379089649	-3.53038624088836	-3.58443259136661
H	-8.42704501627794	-2.92680780727226	0.46562851530869
H	-6.60232499377314	-1.32734368499756	-1.86081336063461
O	-5.50647276475648	-4.99152277364095	-0.92880037153709
N	-2.23686874801450	-1.16123667735240	1.01950724065459
H	-2.11951688226405	0.08995096543942	-0.39192918698531
O	-0.14172946504370	2.63182149302035	-0.87683289743059
Fe	-2.54300449553675	5.24266737376288	-0.67463221339463
Fe	-3.45857667270504	5.91635456913747	3.55967712621686
Sr	-4.93993302366149	8.04815490742974	-3.04208108010988

IMB1_model-3

Energy: -950.53651 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.62443507856367	-0.88628157529871	-2.72479612797415
C	4.36262163578417	0.29876568902313	-2.04808509489956
C	3.70934349200814	0.58260254354854	0.49813179143050
C	5.37740445341189	-0.31085994378199	2.35384283294612
C	7.63676152057000	-1.49004907034443	1.68072242501793
C	8.26358338899200	-1.78957069139153	-0.86719532820819
H	7.11198422417022	-1.08791530181292	-4.70957525595696
H	3.08176538164708	1.04898701733737	-3.46122227794168
H	4.92727178492472	-0.05839253726230	4.34561398160648

H	8.91270457181978	-2.16392538195071	3.14148072341743
H	10.02442998250143	-2.70363106120367	-1.39499584247780
C	1.24117206598346	1.90125356584989	1.23833756939255
C	-0.51948569097375	0.15703623909724	2.87824189688253
H	0.45410118783596	-1.25213249451596	4.02851803231886
H	-1.72947734014550	1.33679230617389	4.06064330085471
H	1.72777664332479	3.50865439045094	2.46930511052159
C	-1.23739266286635	-3.65529714152989	0.10809233434963
C	-4.93445303521752	-1.37175218279449	1.86308095828529
C	-3.01808163013206	-4.73773256639267	-1.88764741869719
H	-1.12041857793472	-4.91442176821723	1.74213846549871
H	0.65422316368579	-3.32875257106593	-0.64836505427229
C	-6.50575995855035	-2.60271983730710	-0.21826337310594
H	-4.96903467937475	-2.49613916858417	3.59671582251743
H	-5.58905420837900	0.55576842879418	2.23630196245783
H	-2.37803128577207	-6.62443507856367	-2.43226641422103
H	-3.00296379089649	-3.53038624088836	-3.58443259136661
H	-8.42704501627794	-2.92680780727226	0.46562851530869
H	-6.60232499377314	-1.32734368499756	-1.86081336063461
O	-5.50647276475648	-4.99152277364095	-0.92880037153709
N	-2.23686874801450	-1.16123667735240	1.01950724065459
H	-2.11951688226405	0.08995096543942	-0.39192918698531
O	-0.14172946504370	2.63182149302035	-0.87683289743059
Fe	-3.45857667270504	5.91635456913747	3.55967712621686
Sr	-2.54300449553675	5.24266737376288	-0.67463221339463
Fe	-4.93993302366149	8.04815490742974	-3.04208108010988

IMB2_model-1

Energy: -1043.71397 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.32472434128488	-1.50308820328360	-2.71893790517708
C	4.17421599025519	-0.14475302117451	-2.00840102012949
C	3.53038624088836	0.09788781516439	0.54443010416956
C	5.09659141013032	-1.01270422471489	2.37255107245068

C	7.24332013316549	-2.36385846644627	1.66220307686765
C	7.86088283490382	-2.62067228651714	-0.89195073666615
H	6.80131351000348	-1.67429730517035	-4.70825245333864
H	2.99805058989891	0.75211100152690	-3.42569561387469
H	4.64948235635547	-0.80540127825172	4.36829085384340
H	8.43819422278114	-3.20818808775504	3.10217443135592
H	9.53404600204299	-3.67098199308926	-1.44847506724868
C	1.21622770947943	1.57111825685597	1.40255476209559
C	-0.82467647338830	-0.00850376756247	2.80775512942781
H	0.05706973086453	-1.38498032047150	4.08691057336062
H	-1.94906345917797	1.29861981199286	3.94801585813113
H	1.81942836227671	3.11351286747438	2.63881351369790
C	-1.72267432420580	-3.76187780836310	0.19653152077879
C	-5.19202242070550	-1.20375558697434	1.72550893229055
C	-3.46235630069956	-4.74529137451661	-1.88500181346056
H	-1.79675160342336	-5.06068651171023	1.82698716851092
H	0.22695610572200	-3.69932785850800	-0.48395885872113
C	-6.81151792147433	-2.26672642078940	-0.41328311676418
H	-5.47718232918280	-2.35289803791377	3.44175824814261
H	-5.76631019576023	0.74152852577831	2.13746933147409
H	-2.98633414430476	-6.70078006692574	-2.35403183768397
H	-3.22973093534435	-3.57951916360190	-3.59652681777958
H	-8.78533707256919	-2.41015678107505	0.18103575710521
H	-6.70569326981305	-0.99324008153225	-2.05885651869421
O	-6.02690364382562	-4.74056695148974	-1.09830883140518
N	-2.51598143273633	-1.20129887309199	0.95620138523169
O	-0.06519554942255	2.71307990914714	-0.72773354396311
Fe	-1.33112308811466	6.17486919941262	-0.59469682476357
H	-1.46604950887277	1.49023807508228	-1.04558550842265
Fe	-1.79618470259339	7.28640582834411	3.62071527249525
Fe	-2.54867371359598	9.60283263392566	-3.04170307252392

IMB2_model-2

Energy: -950.605232 (Hartrees)

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	6.32472434128488	-1.50308820328360	-2.71893790517708
C	4.17421599025519	-0.14475302117451	-2.00840102012949
C	3.53038624088836	0.09788781516439	0.54443010416956
C	5.09659141013032	-1.01270422471489	2.37255107245068
C	7.24332013316549	-2.36385846644627	1.66220307686765
C	7.86088283490382	-2.62067228651714	-0.89195073666615
H	6.80131351000348	-1.67429730517035	-4.70825245333864
H	2.99805058989891	0.75211100152690	-3.42569561387469
H	4.64948235635547	-0.80540127825172	4.36829085384340
H	8.43819422278114	-3.20818808775504	3.10217443135592
H	9.53404600204299	-3.67098199308926	-1.44847506724868
C	1.21622770947943	1.57111825685597	1.40255476209559
C	-0.82467647338830	-0.00850376756247	2.80775512942781
H	0.05706973086453	-1.38498032047150	4.08691057336062
H	-1.94906345917797	1.29861981199286	3.94801585813113
H	1.81942836227671	3.11351286747438	2.63881351369790
C	-1.72267432420580	-3.76187780836310	0.19653152077879
C	-5.19202242070550	-1.20375558697434	1.72550893229055
C	-3.46235630069956	-4.74529137451661	-1.88500181346056
H	-1.79675160342336	-5.06068651171023	1.82698716851092
H	0.22695610572200	-3.69932785850800	-0.48395885872113
C	-6.81151792147433	-2.26672642078940	-0.41328311676418
H	-5.47718232918280	-2.35289803791377	3.44175824814261
H	-5.76631019576023	0.74152852577831	2.13746933147409
H	-2.98633414430476	-6.70078006692574	-2.35403183768397
H	-3.22973093534435	-3.57951916360190	-3.59652681777958
H	-8.78533707256919	-2.41015678107505	0.18103575710521
H	-6.70569326981305	-0.99324008153225	-2.05885651869421
O	-6.02690364382562	-4.74056695148974	-1.09830883140518
N	-2.51598143273633	-1.20129887309199	0.95620138523169
O	-0.06519554942255	2.71307990914714	-0.72773354396311
Fe	-1.33112308811466	6.17486919941262	-0.59469682476357
H	-1.46604950887277	1.49023807508228	-1.04558550842265
Fe	-1.79618470259339	7.28640582834411	3.62071527249525

Sr	-2.54867371359598	9.60283263392566	-3.04170307252392

IMB2_model-3

Energy: -950.560853 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	6.32472434128488	-1.50308820328360	-2.71893790517708
C	4.17421599025519	-0.14475302117451	-2.00840102012949
C	3.53038624088836	0.09788781516439	0.54443010416956
C	5.09659141013032	-1.01270422471489	2.37255107245068
C	7.24332013316549	-2.36385846644627	1.66220307686765
C	7.86088283490382	-2.62067228651714	-0.89195073666615
H	6.80131351000348	-1.67429730517035	-4.70825245333864
H	2.99805058989891	0.75211100152690	-3.42569561387469
H	4.64948235635547	-0.80540127825172	4.36829085384340
H	8.43819422278114	-3.20818808775504	3.10217443135592
H	9.53404600204299	-3.67098199308926	-1.44847506724868
C	1.21622770947943	1.57111825685597	1.40255476209559
C	-0.82467647338830	-0.00850376756247	2.80775512942781
H	0.05706973086453	-1.38498032047150	4.08691057336062
H	-1.94906345917797	1.29861981199286	3.94801585813113
H	1.81942836227671	3.11351286747438	2.63881351369790
C	-1.72267432420580	-3.76187780836310	0.19653152077879
C	-5.19202242070550	-1.20375558697434	1.72550893229055
C	-3.46235630069956	-4.74529137451661	-1.88500181346056
H	-1.79675160342336	-5.06068651171023	1.82698716851092
H	0.22695610572200	-3.69932785850800	-0.48395885872113
C	-6.81151792147433	-2.26672642078940	-0.41328311676418
H	-5.47718232918280	-2.35289803791377	3.44175824814261
H	-5.76631019576023	0.74152852577831	2.13746933147409
H	-2.98633414430476	-6.70078006692574	-2.35403183768397
H	-3.22973093534435	-3.57951916360190	-3.59652681777958
H	-8.78533707256919	-2.41015678107505	0.18103575710521
H	-6.70569326981305	-0.99324008153225	-2.05885651869421
O	-6.02690364382562	-4.74056695148974	-1.09830883140518

N	-2.51598143273633	-1.20129887309199	0.95620138523169
O	-0.06519554942255	2.71307990914714	-0.72773354396311
H	-1.46604950887277	1.49023807508228	-1.04558550842265
Fe	-1.79618470259339	7.28640582834411	3.62071527249525
Sr	-1.33112308811466	6.17486919941262	-0.59469682476357
Fe	-2.54867371359598	9.60283263392566	-3.04170307252392

Product 6

Energy: -672.058276 (Hartrees)

Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
C	5.93581859893654	-0.41328311676418	2.42017218780805
C	3.61240044919939	0.66140413240940	1.79429500103484
C	2.63711270349362	0.42518836678520	-0.66216003608748
C	4.05818692523333	-0.89780890277144	-2.46231308984404
C	6.38500647050162	-1.97230711886129	-1.83813660178126
C	7.32835795240939	-1.73817005953349	0.61170436744741
H	6.66619797301369	-0.20522425339485	4.32747275442573
H	2.56209074262727	1.73533544955901	3.18721202572240
H	3.33536658415752	-1.08640349445676	-4.37641689727883
H	7.45629223910638	-2.98671215378045	-3.26525782428876
H	9.13777022954141	-2.57097235147980	1.10662365470104
C	0.12150939172681	1.59379501759905	-1.42315270315870
C	-0.08258102788277	4.41080976346535	-0.63400311871480
O	-0.67519916902665	4.65628514741776	1.96399229556542
H	1.71983971423132	5.36153082199208	-0.98775986821086
H	-1.52009574596745	5.35038161548887	-1.81073553139488
H	0.01398397332495	1.51990674122961	-3.50865439045094
C	-4.49546957512328	1.12174138055304	-1.43014472383624
C	-1.98062194215715	-2.48007653431624	-0.18065782132884
C	-6.59778979847180	-0.82429852249412	-0.92010765403883
H	-4.32180353636650	1.39688554403636	-3.49448156923541
H	-5.01495521129498	2.94683884750541	-0.60546825044795
C	-4.04155727864160	-3.40150693428161	1.64689634627781
H	-2.20833387974764	-3.35879924668895	-2.06169112866869

H	-0.14154048865175	-3.07779697379213	0.53176892212457
H	-6.62726946177101	-2.27882064720237	-2.40883397845673
H	-8.44348543325441	0.10431288020992	-0.93239088329992
H	-3.38582230948937	-3.22765211755411	3.60125101592905
H	-4.45427346811965	-5.40764013188302	1.27348645075099
N	-2.08172239566897	0.27986844667046	-0.30122234621370
O	-6.30223669866321	-1.93564643014669	1.49288367842918
H	-1.66333698813169	3.14677193389070	2.34401620418383