Product Selectivity Control in the Brønsted Acid Mediated Reactions of 2-Alkynylanilines

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I. Computational details

Quantum chemical calculations were performed in the framework of Density Functional Theory using the wB97XD functional [1] making use of a version of Grimme's D2 dispersion model in conjunction with the 6-31G* basis set. Test calculations performed on some of the critical points (see below) using a larges basis set (6-311+G*) did not produce significant variations. All the critical points were located and characterized as true minima or first order saddle points through the calculations of the molecular vibrations in harmonic approximation. Subsequently, the effect of the solvent (either ethanol or 1,2 dichloroethane) was included in the mean field approximation, using the Polarizable Continuum Model [2] as implemented in the Gaussian16 software [3] used for all these calculations. The standard molar free energy was then calculated at 110°C, for each of the involved species, using the standard statistical mechanical relations (through the harmonic frequencies and moment of inertia from DFT calculations) and considering, as reference state, 1.0 mole/litre for all the species with the exception of the solvent, for which we utilized the experimental density in the experimental conditions.

Non-covalent Interaction Index (NCI) analysis based on promolecular density was carried using Multiwfn program. This method, which allows the visualization of the non-covalent interactions in the 3D space, is based on the determination of the strength of the non-covalent interaction through the product between electron density (ρ) and the sign of the second eigenvalue of the Hessian, sign(λ). The interactions are classified inti three types:

- $\rho \cdot \text{sign}(\lambda) < 0$ strongly attractive (pictorially represented in blue in this study)

1 D. Chai and M. Head-Gordon, "Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections," *Phys. Chem. Chem. Phys.*, **10** (2008) 6615-20.

2 J. Tomasi, B. Mennucci, and R. Cammi, "Quantum mechanical continuum solvation models," *Chem. Rev.*, **105** (2005) 2999-3093.

3 Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

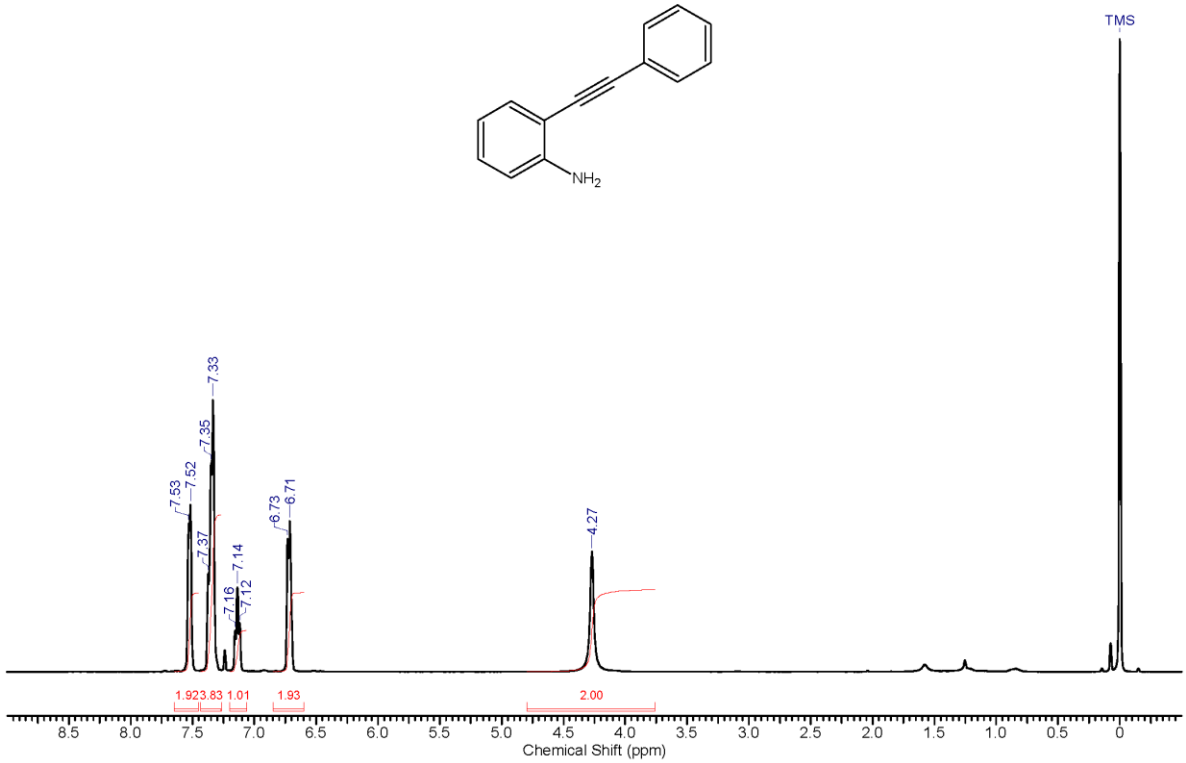
- $\rho \cdot sign(\lambda) \sim 0$ weak van der waals interactions (pictorially represented in green in this study)

- $\rho \cdot sign(\lambda) > 0$ repulsive interactions (pictorially represented in red in this study)

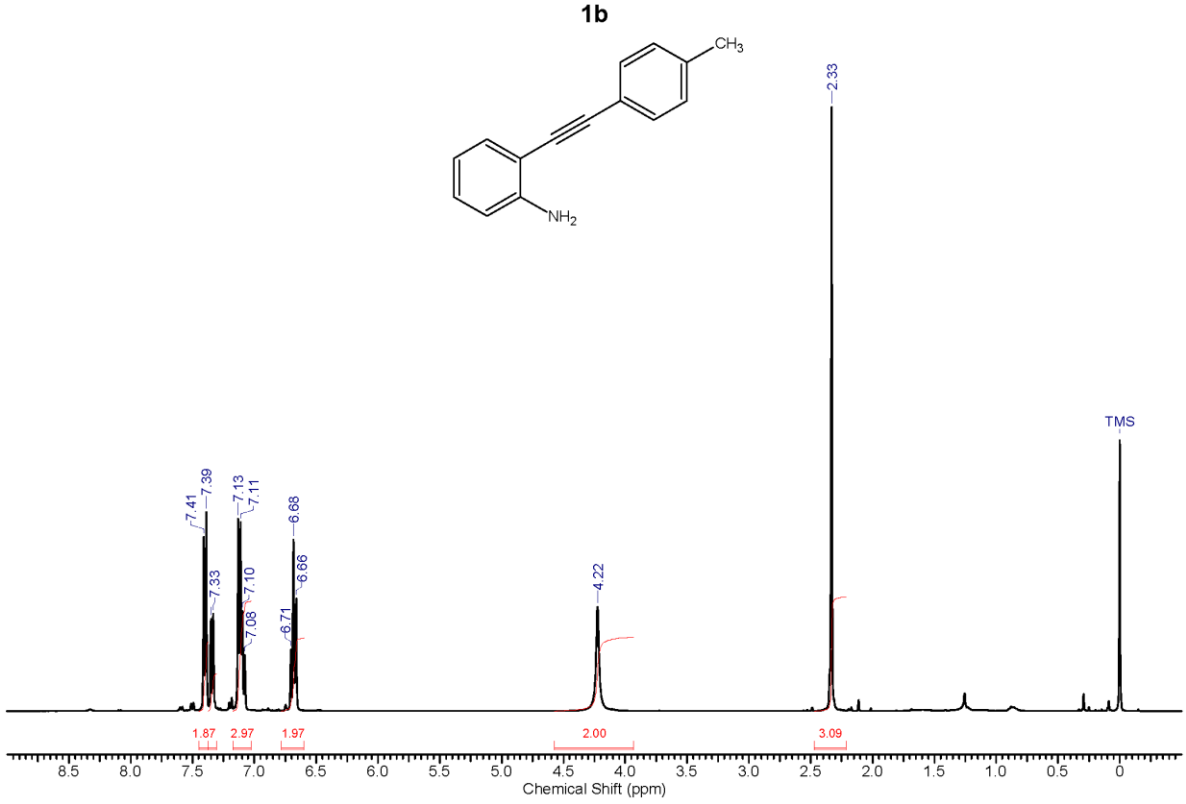
The same program was also used for performing atomic-charge calculations within the RESP scheme.

II. Copies of ^{1}H, ^{19}F and ^{13}C NMR spectra

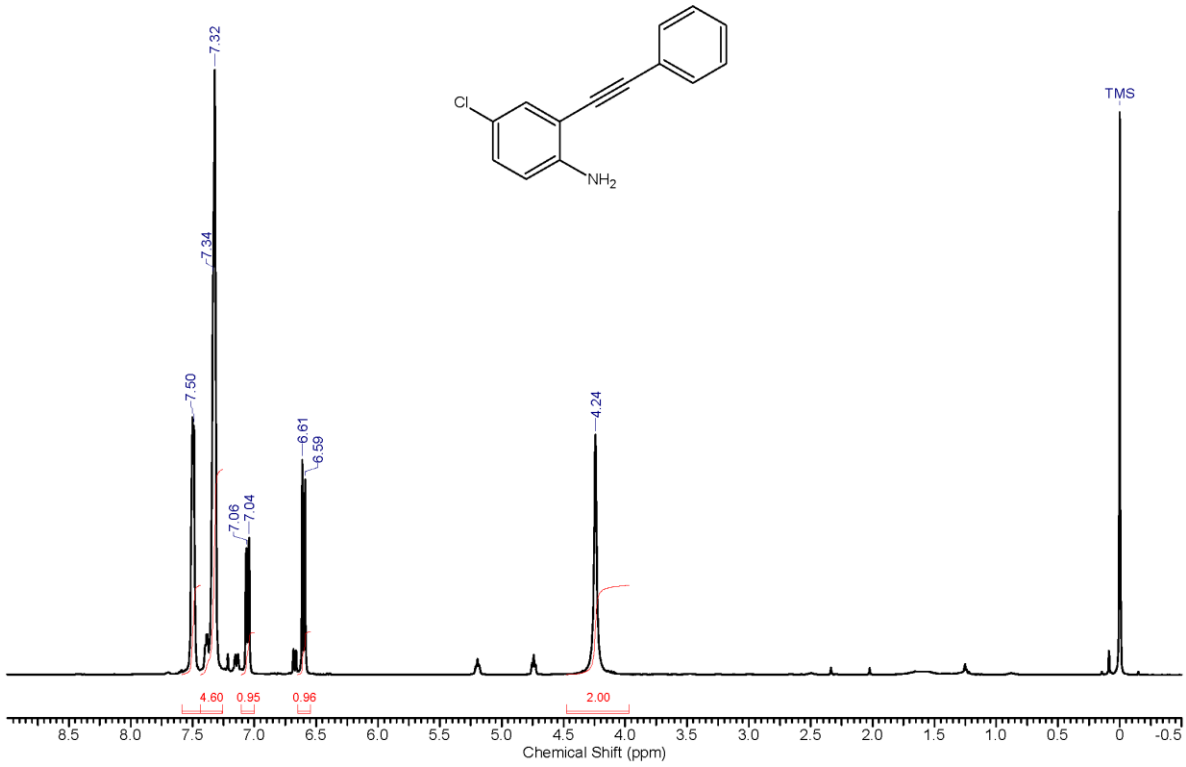
1a



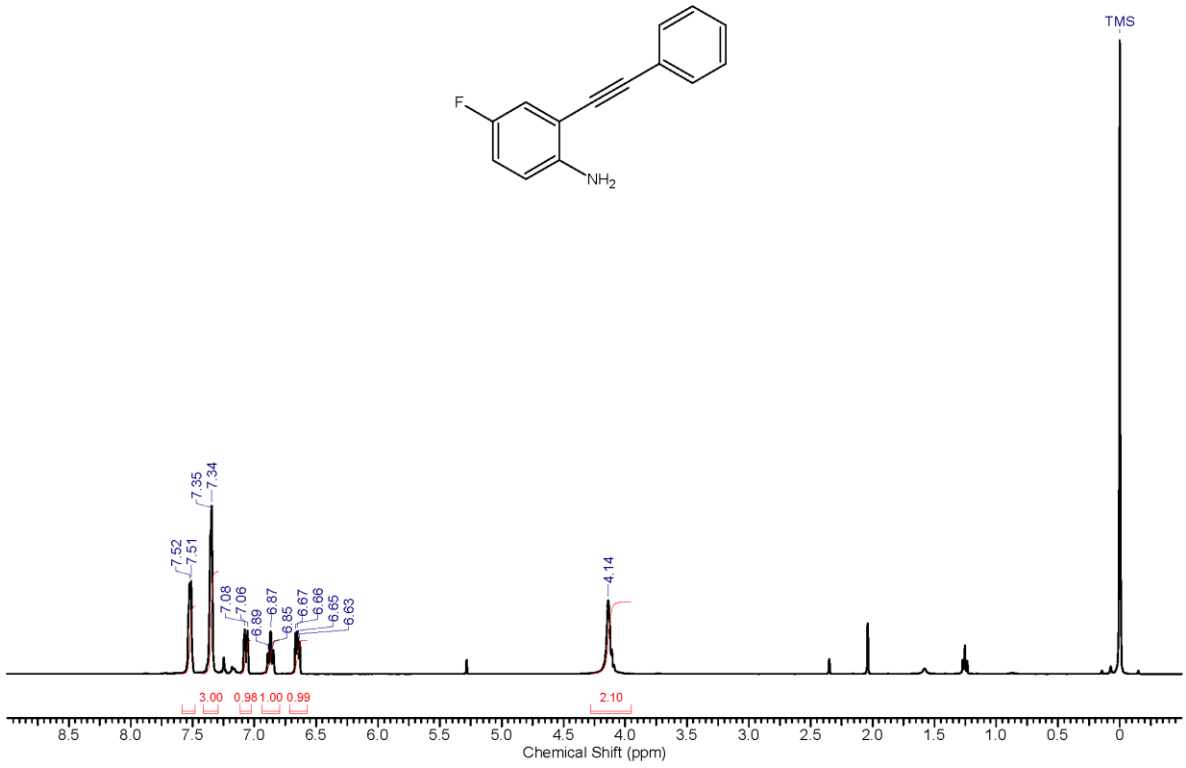
1b



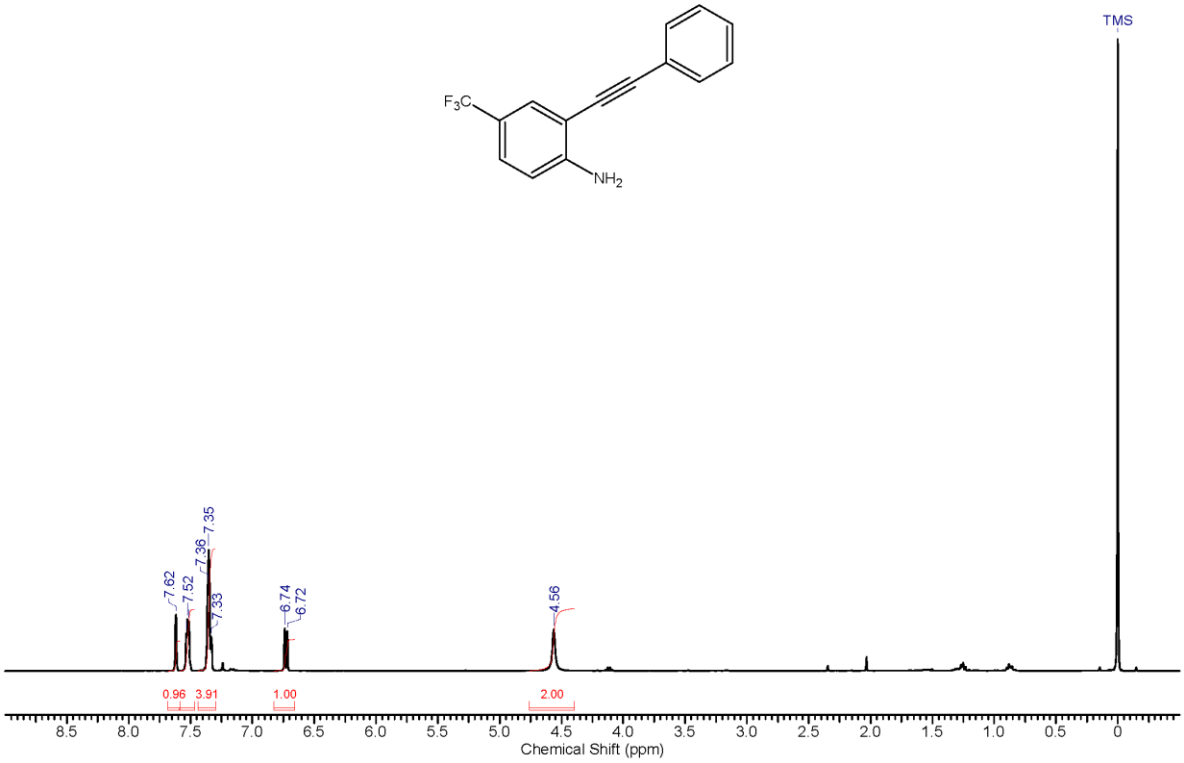
1c


Cl
NH2
7.32
7.34
7.50
7.06
7.04
6.61
6.59
4.24
TMS
4.60
0.95
0.96
2.00
Chemical Shift (ppm)

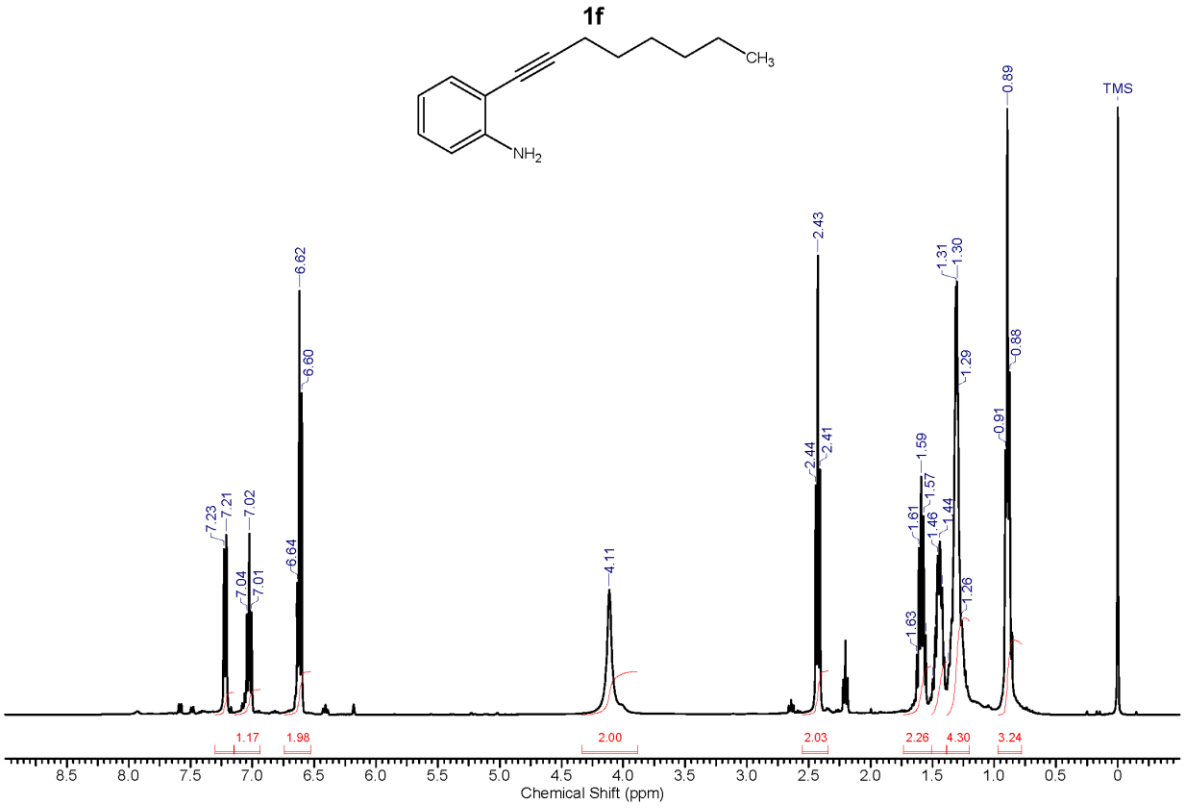
1d


F
NH2
7.35
7.34
7.52
7.51
7.08
7.06
6.89
6.87
6.85
6.67
6.66
6.65
6.63
4.14
TMS
3.00
0.98
1.00
0.99
2.10
Chemical Shift (ppm)

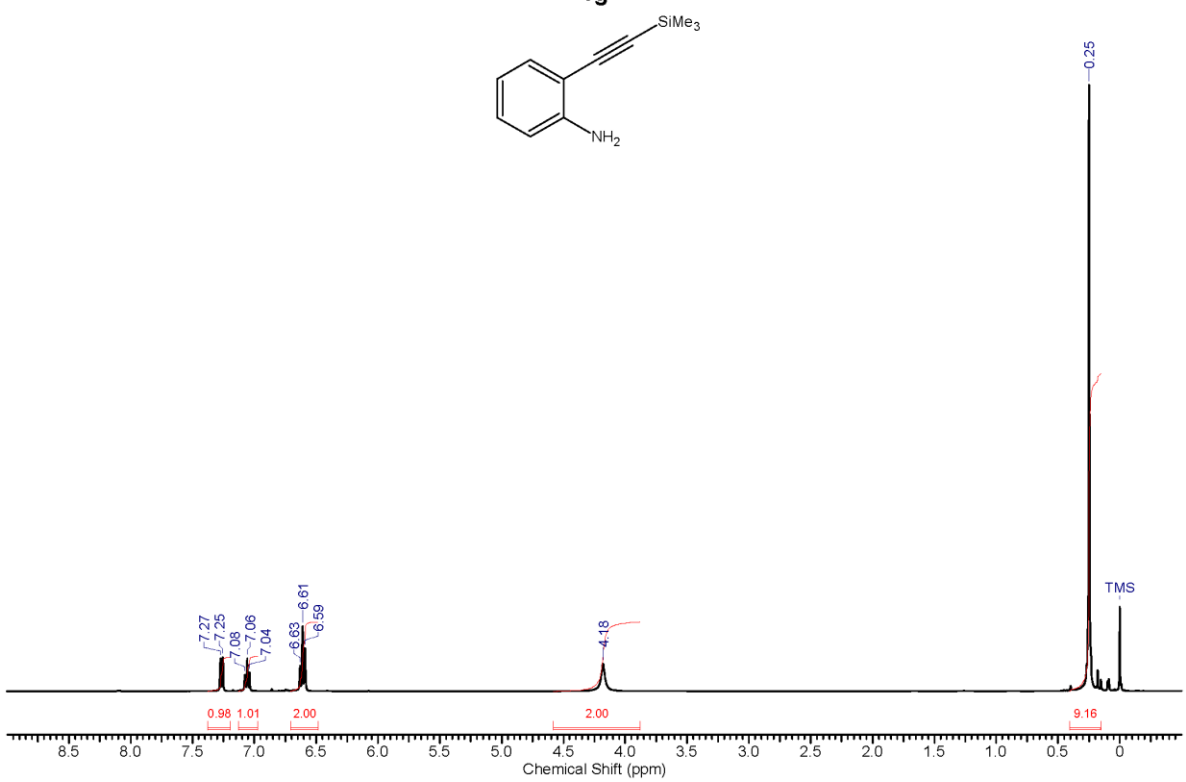
1e


F3C
NH2
TMS
7.62
7.52
7.36
7.35
7.33
6.74
6.72
4.56
0.96
3.91
1.00
2.00
Chemical Shift (ppm)

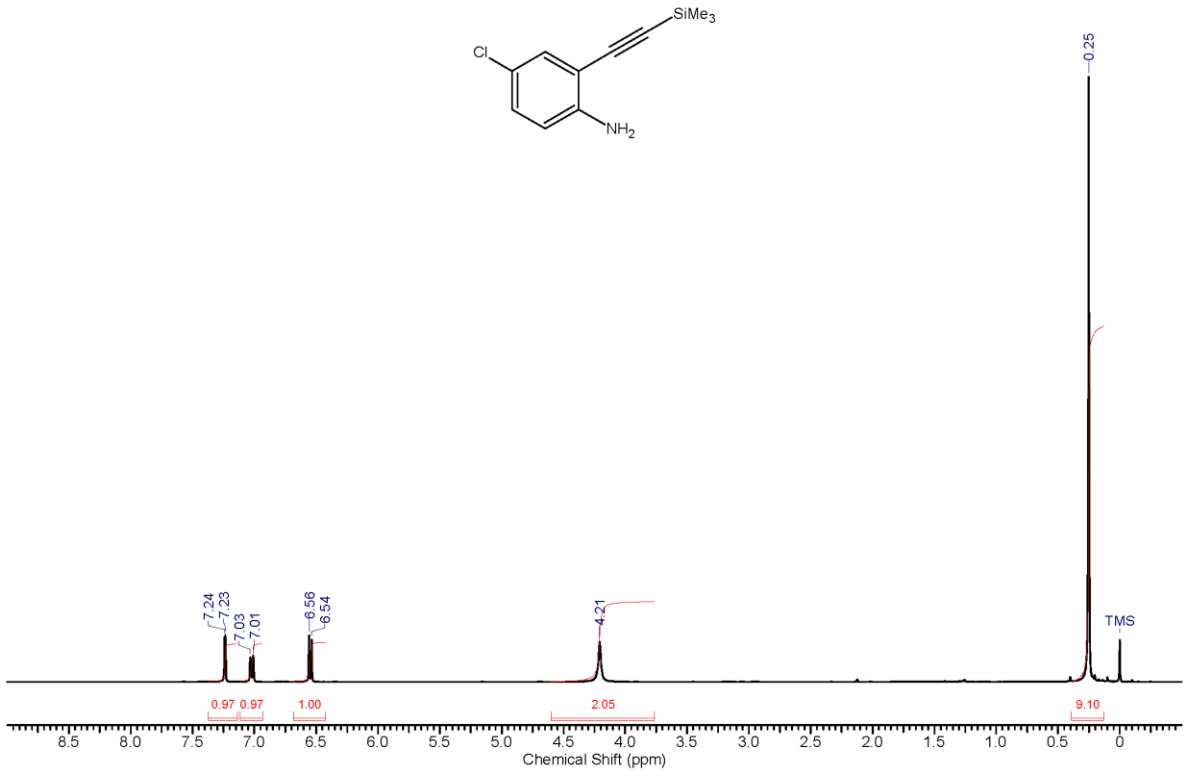
1f


CH3
NH2
TMS
0.89
6.62
6.60
2.43
1.31
1.30
0.86
1.29
0.91
2.44
2.41
1.59
1.57
1.61
1.46
1.44
7.23
7.21
7.02
6.64
4.11
7.04
7.01
1.26
1.63
1.17
1.98
2.00
2.03
2.26
4.30
3.24
Chemical Shift (ppm)

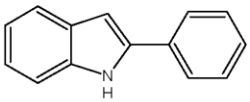
1g


SiMe3
NH2
7.27
7.25
7.08
7.06
7.04
6.63
6.61
6.59
4.18
0.25
TMS
0.98
1.01
2.00
2.00
9.16
Chemical Shift (ppm)

1h

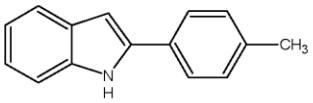

SiMe3
Cl
NH2
7.24
7.23
7.03
7.01
6.56
6.54
4.21
0.25
TMS
0.97
0.97
1.00
2.05
9.10
Chemical Shift (ppm)

5a


N
H

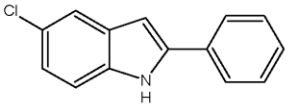
TMS
8.27
7.64
7.62
7.42
7.44
7.40
7.36
7.32
7.22
7.19
7.12
7.10
6.81
1.00
3.05
2.04
1.15
1.00
Chemical Shift (ppm)

5b


CH3
N
H

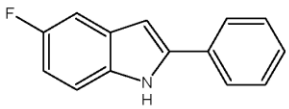
2.38
7.24
7.25
7.23
8.28
7.61
7.59
7.56
7.54
7.39
7.37
7.17
7.10
7.08
6.77
TMS
0.85
2.66
2.71
1.00
3.10
Chemical Shift (ppm)

5c


Cl
N
H

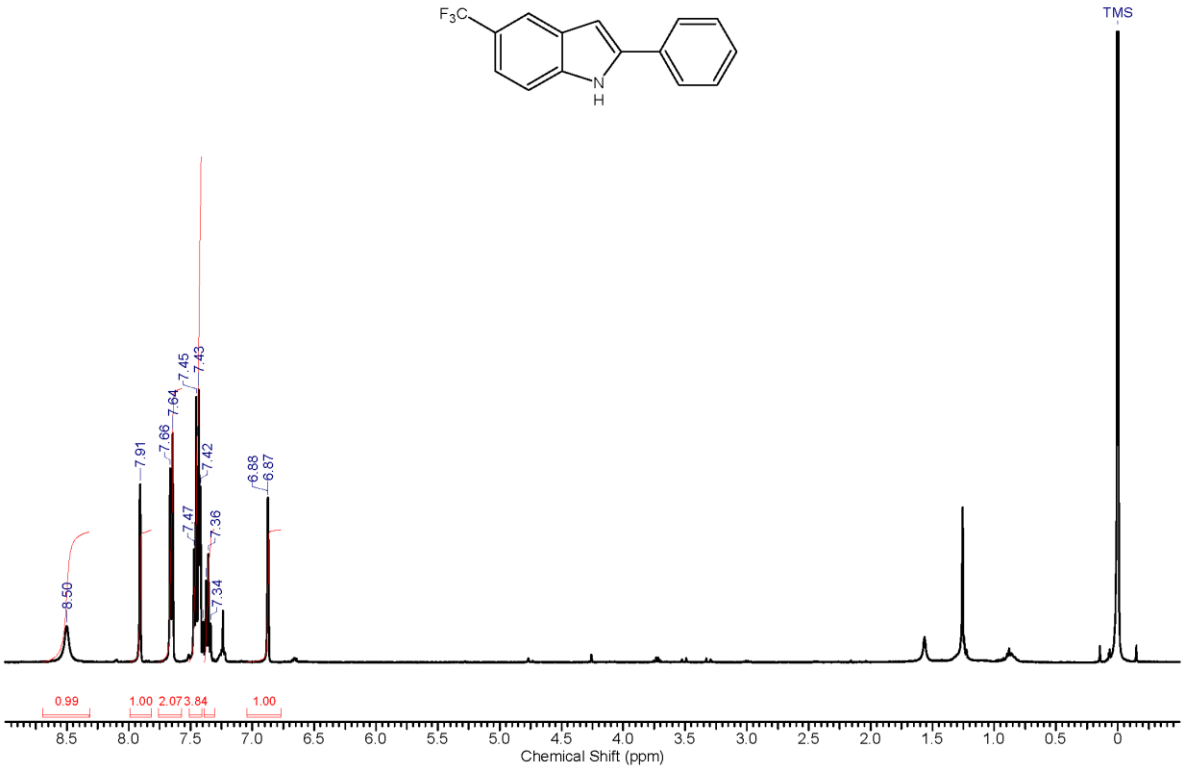
7.25
7.65
7.64
7.45
7.66
7.58
7.32
7.29
7.14
7.14
7.12
6.75
8.35
TMS
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

5d

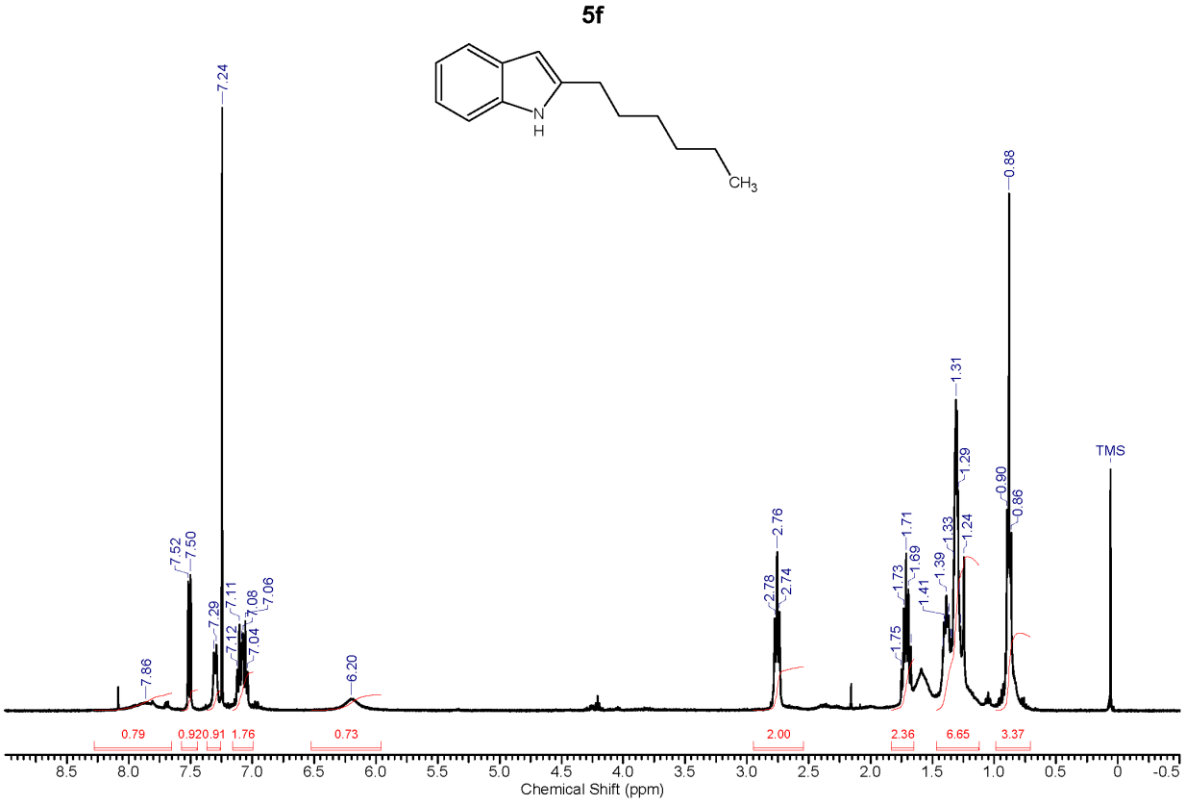

F
N
H

TMS
7.65
7.63
7.44
7.46
7.42
7.31
7.27
7.24
6.95
6.93
6.93
8.77
8.29
1.00
2.12
3.51
1.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0 -0.5
Chemical Shift (ppm)

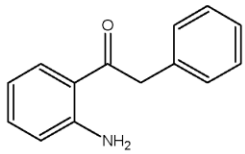
5e

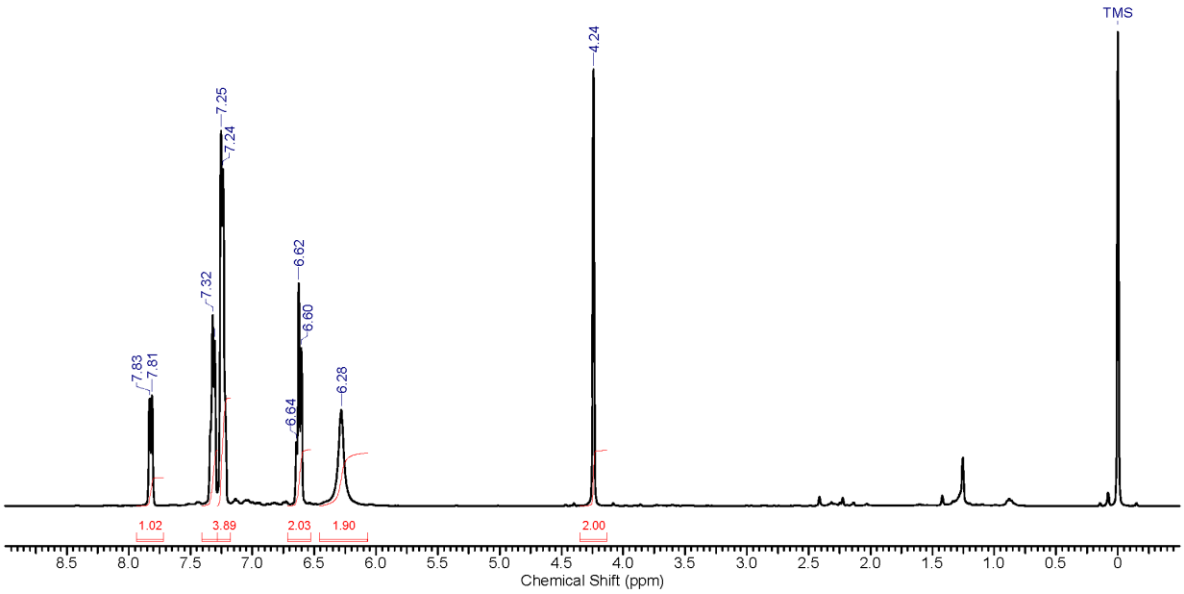

F3C
N
H
TMS
8.50
7.91
7.66
7.64
7.45
7.43
7.42
7.47
7.36
7.34
6.88
6.87
0.99
1.00
2.07
3.84
1.00
Chemical Shift (ppm)

5f

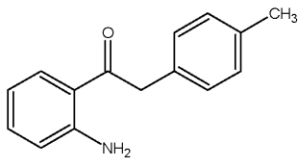

N
H
CH3
TMS
7.24
7.52
7.50
7.29
7.12
7.11
7.08
7.06
7.04
7.86
6.20
2.78
2.76
2.74
1.75
1.73
1.71
1.69
1.41
1.39
1.33
1.31
1.29
1.24
0.90
0.88
0.86
0.79
0.92
0.91
1.76
0.73
2.00
2.36
6.65
3.37
Chemical Shift (ppm)

6a


O
NH2

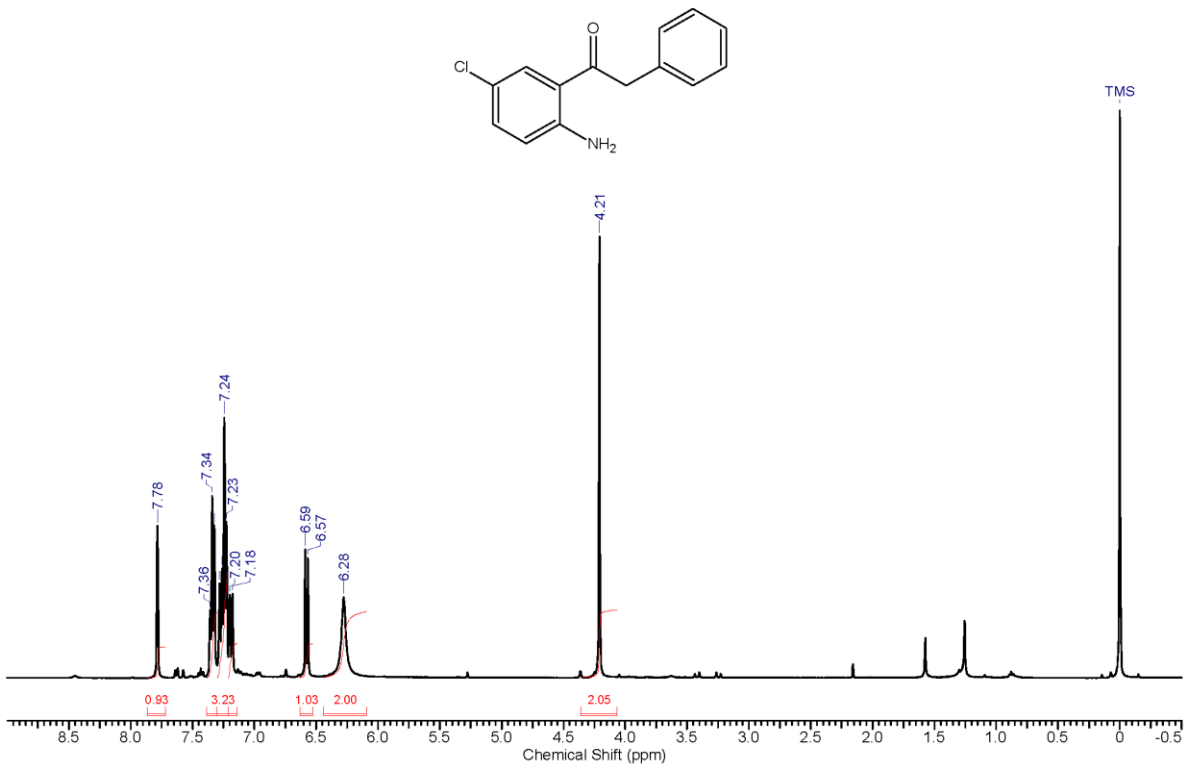

TMS
4.24
7.25
7.24
7.32
6.62
6.60
7.83
7.81
6.64
6.28
1.02
3.89
2.03
1.90
2.00
Chemical Shift (ppm)

6b

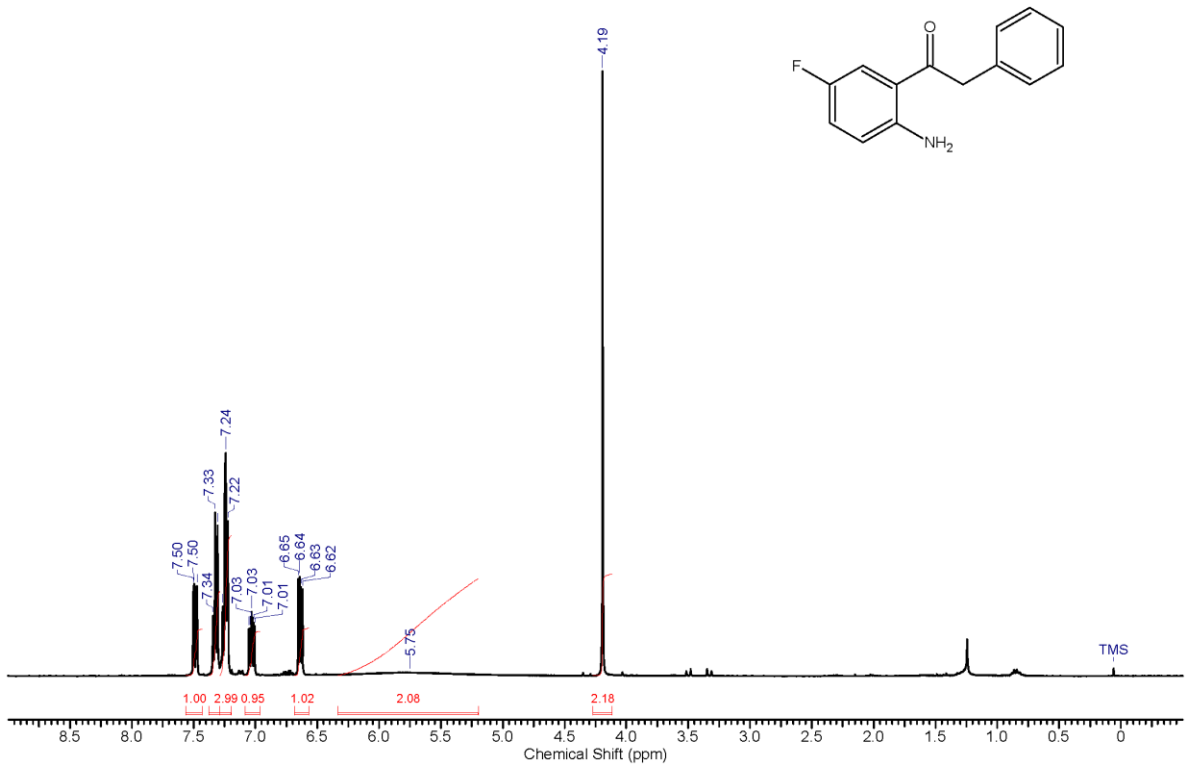

CH3
O
NH2

TMS
7.13
2.32
4.21
6.63
6.61
7.84
7.82
7.24
7.26
6.65
6.27
1.00
3.95
2.03
1.98
2.09
3.25
Chemical Shift (ppm)

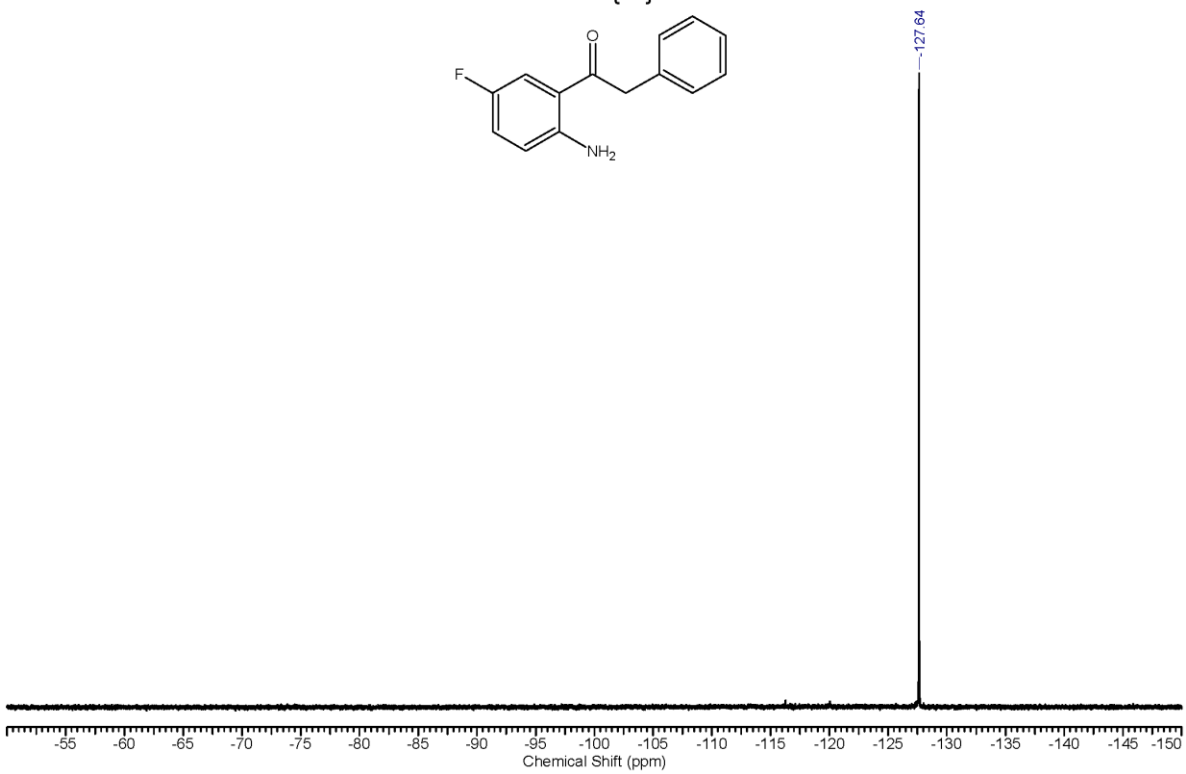
6c


Cl
O
NH2
TMS
4.21
7.24
7.34
7.23
7.78
6.59
6.57
7.36
7.20
7.18
6.28
0.93
3.23
1.03
2.00
2.05
Chemical Shift (ppm)

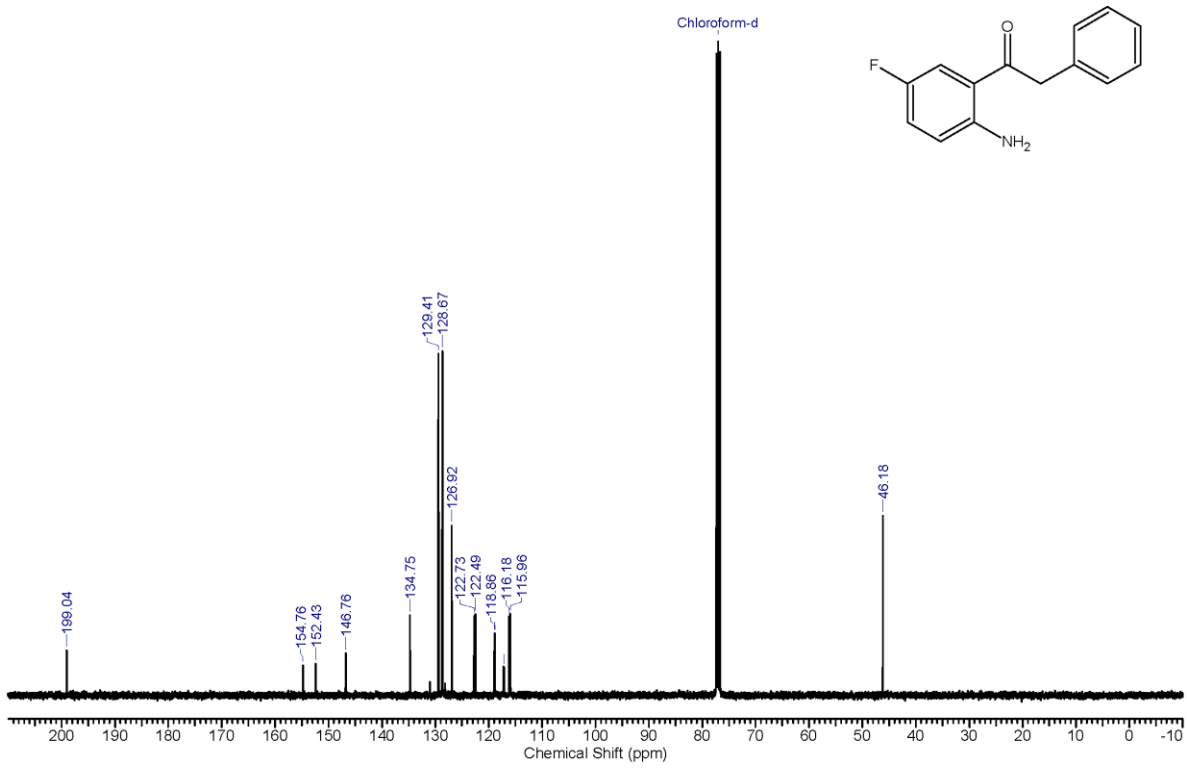
6d


F
O
NH2
4.19
7.24
7.33
7.22
7.50
7.50
7.34
7.03
7.03
7.01
7.01
6.65
6.64
6.63
6.62
5.75
TMS
1.00
2.99
0.95
1.02
2.08
2.18
Chemical Shift (ppm)

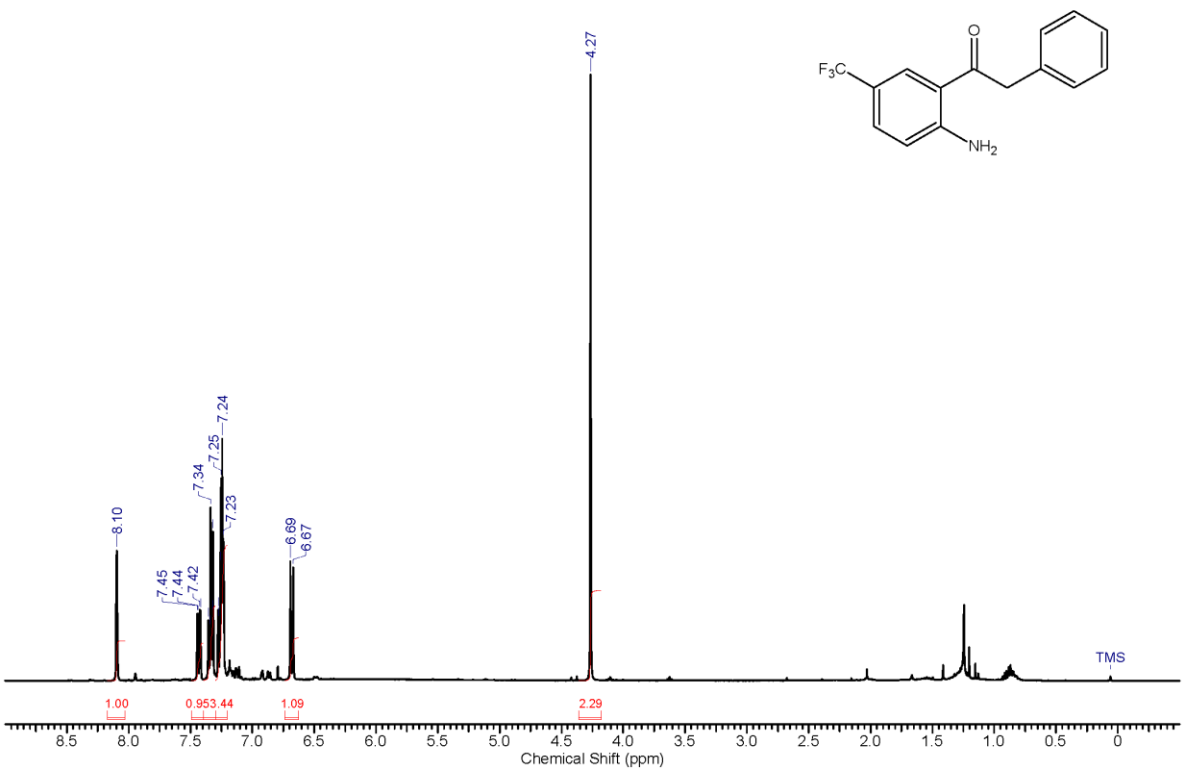
6d - $^{19}F\{^{1}H\}$


127.64
F
O
NH2
-55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
Chemical Shift (ppm)

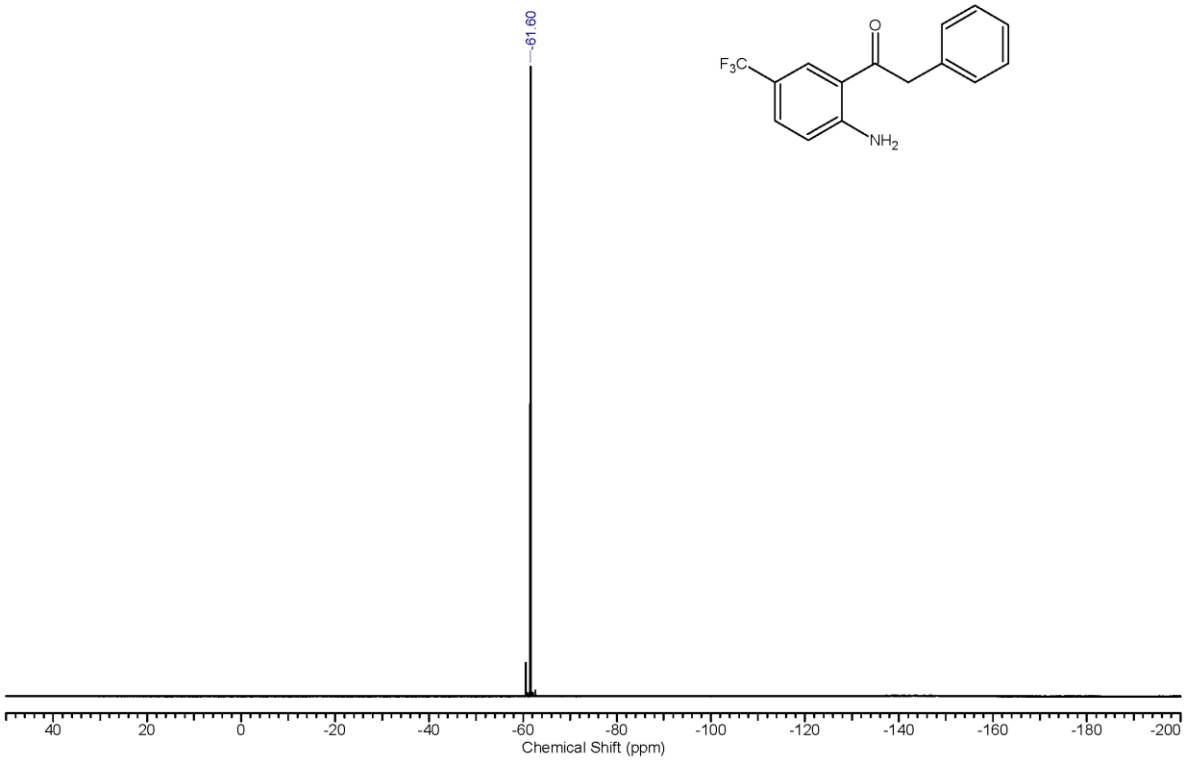
6d


Chloroform-d
F
O
NH2
199.04
154.76
152.43
146.76
134.75
129.41
128.67
126.92
122.73
122.49
118.86
116.18
115.96
46.18
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

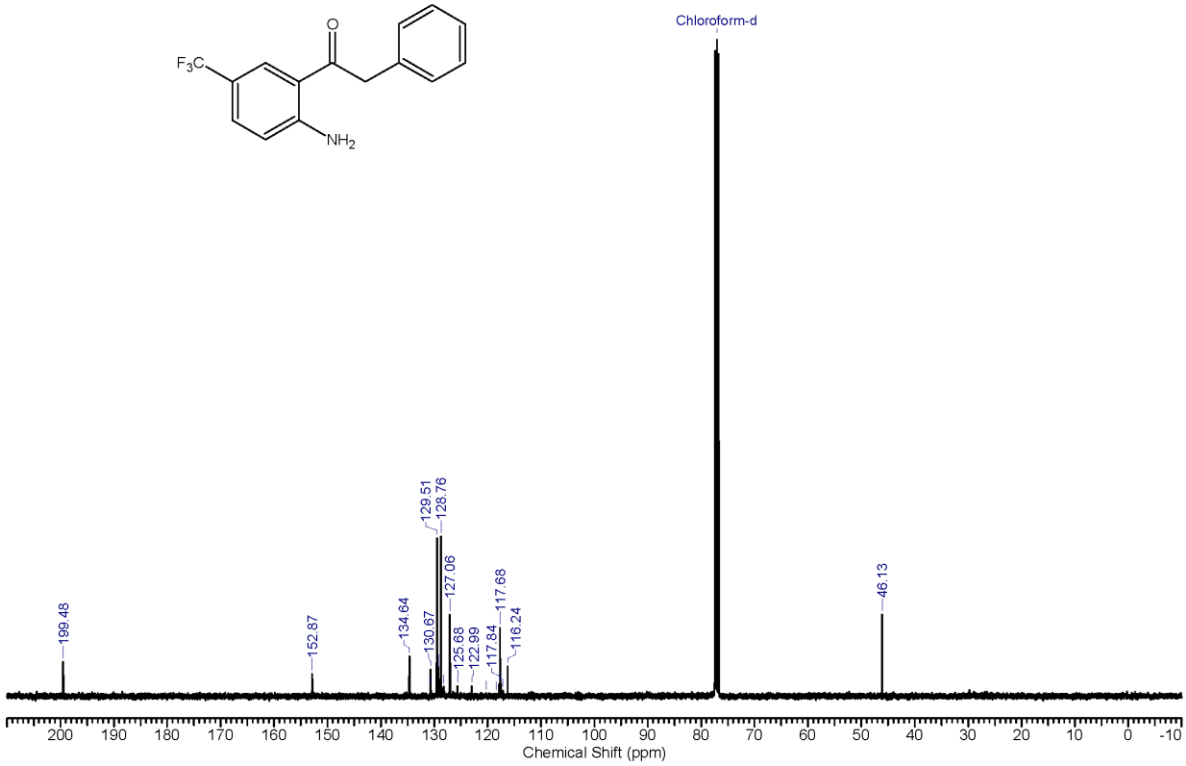
6e


4.27
8.10
7.45
7.44
7.42
7.34
7.25
7.24
7.23
6.69
6.67
TMS
1.00
0.953.44
1.09
2.29
Chemical Shift (ppm)
F3C
O
NH2

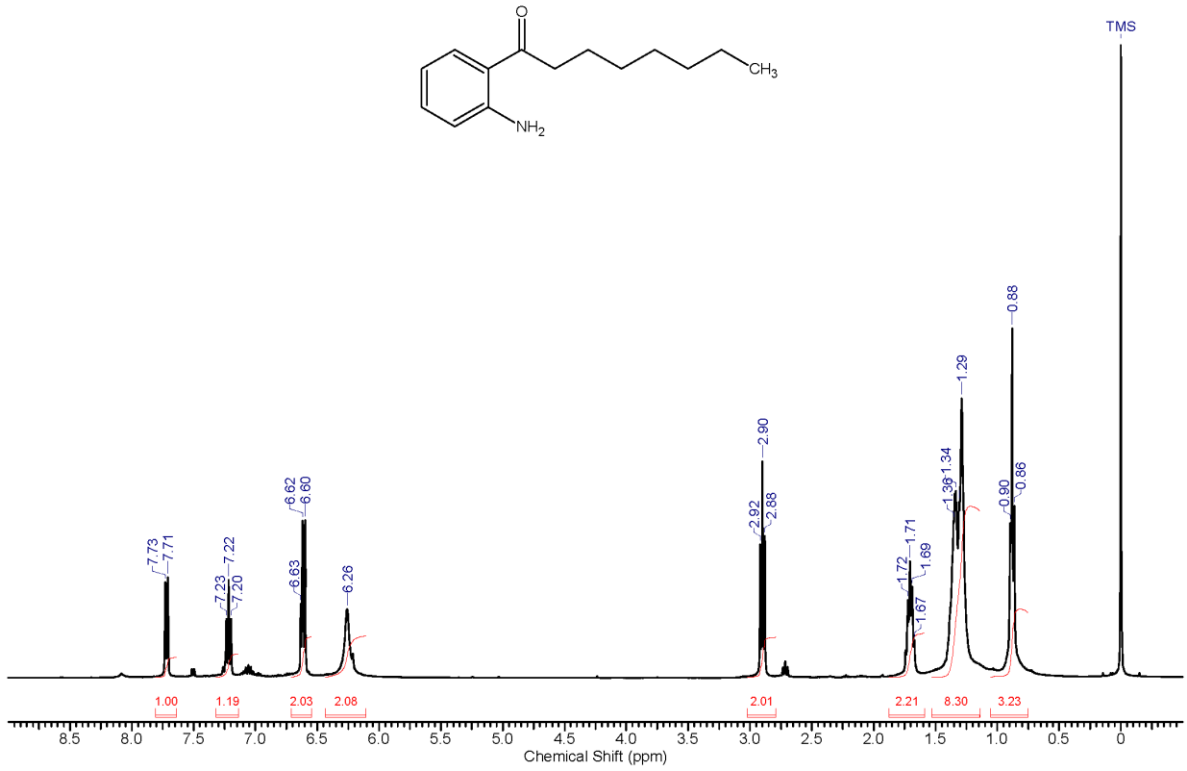
6e - $^{19}F\{^{1}H\}$


-61.60
Chemical Shift (ppm)
F3C
O
NH2

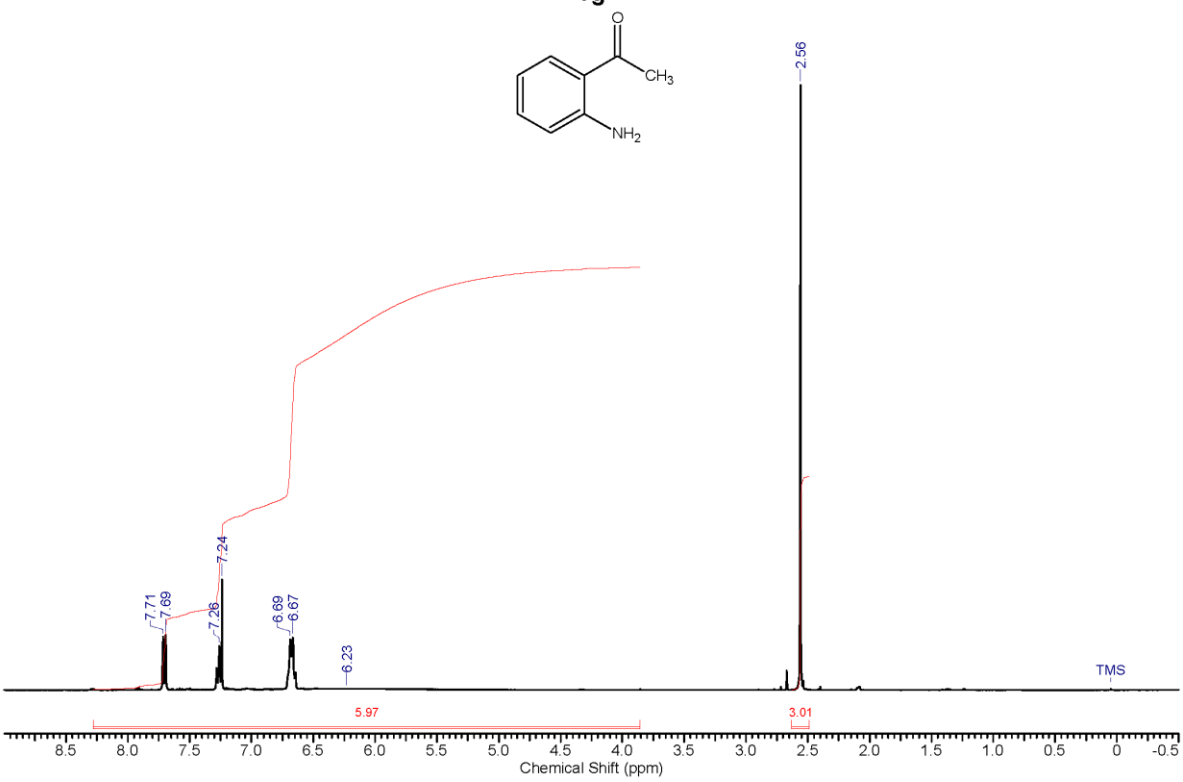
6e


O
F3C
NH2
Chloroform-d
199.48
152.87
134.64
130.67
129.51
128.76
127.06
125.68
122.99
117.84
117.68
116.24
46.13
Chemical Shift (ppm)

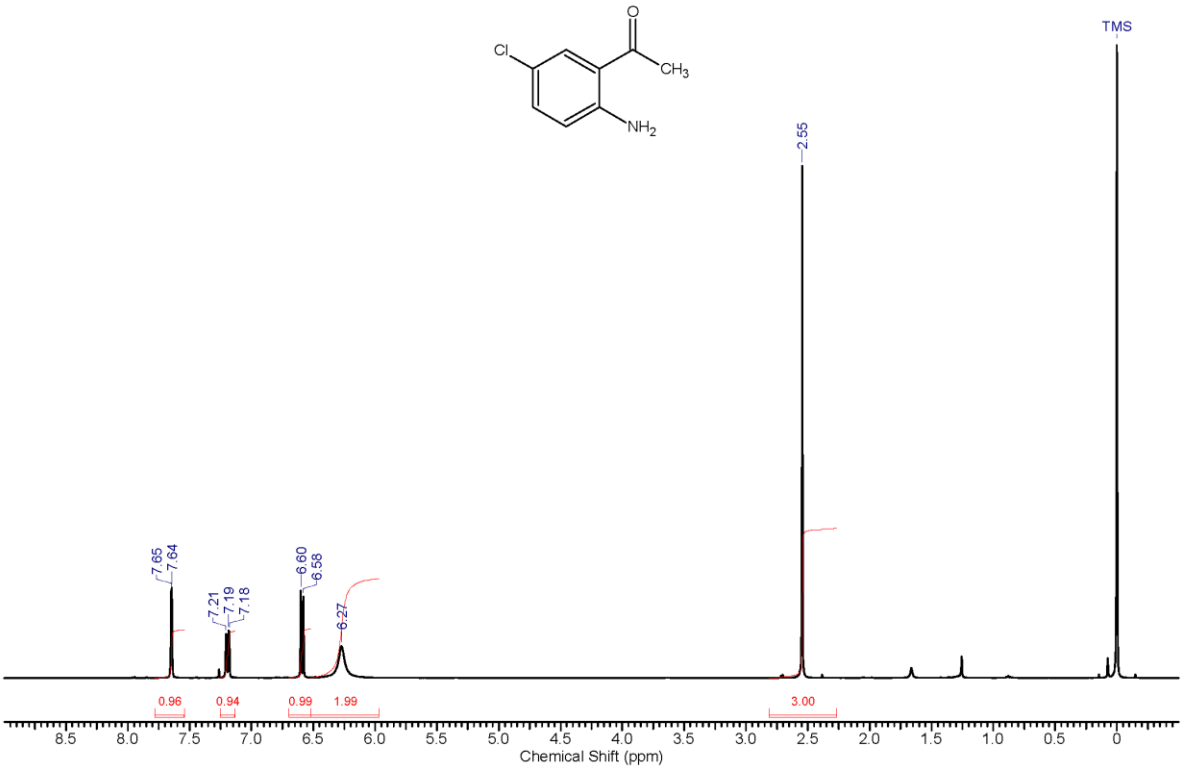
6f


O
CH3
NH2
TMS
7.73
7.71
7.23
7.22
7.20
6.63
6.62
6.60
6.26
2.92
2.90
2.88
1.72
1.71
1.69
1.67
1.38
1.34
1.29
0.90
0.88
0.86
1.00
1.19
2.03
2.08
2.01
2.21
8.30
3.23
Chemical Shift (ppm)

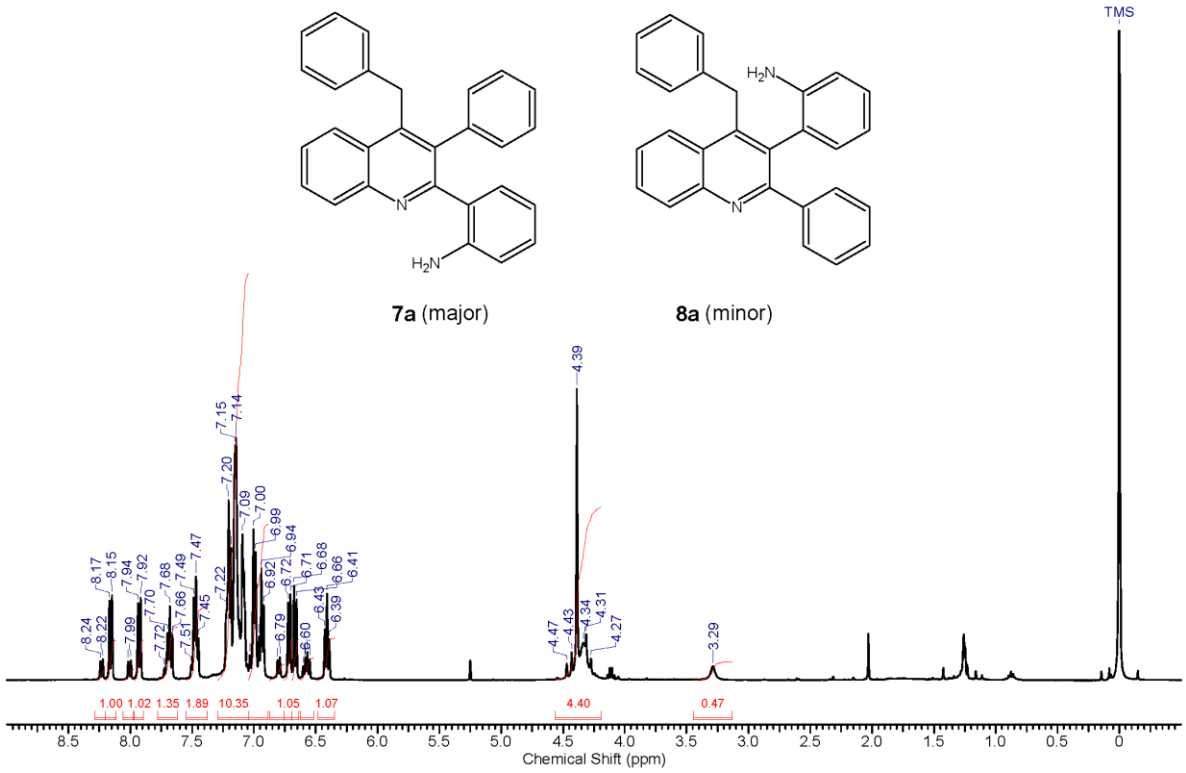
6g


O
CH3
NH2
2.56
7.71
7.69
7.24
7.26
6.69
6.67
6.23
TMS
5.97
3.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0 -0.5
Chemical Shift (ppm)

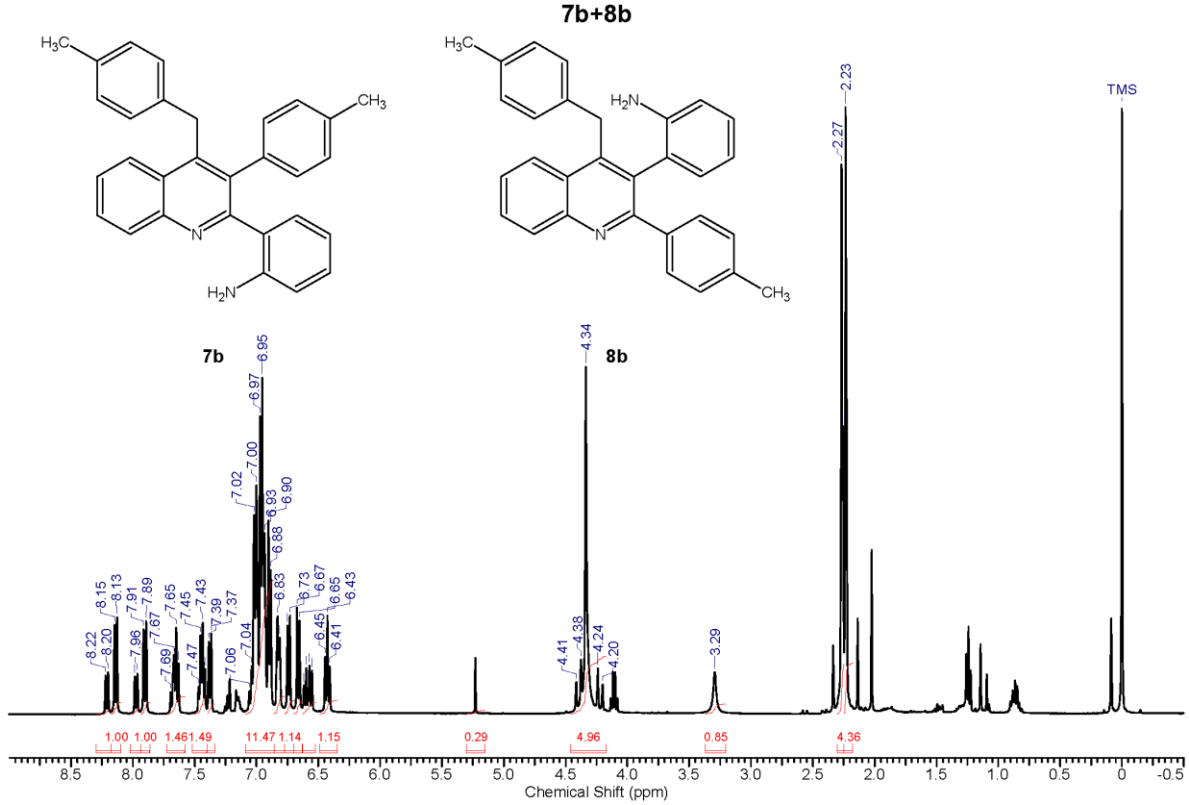
6h


O
Cl
CH3
NH2
TMS
2.55
7.65
7.64
7.21
7.19
7.18
6.60
6.58
6.27
0.96
0.94
0.99
1.99
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

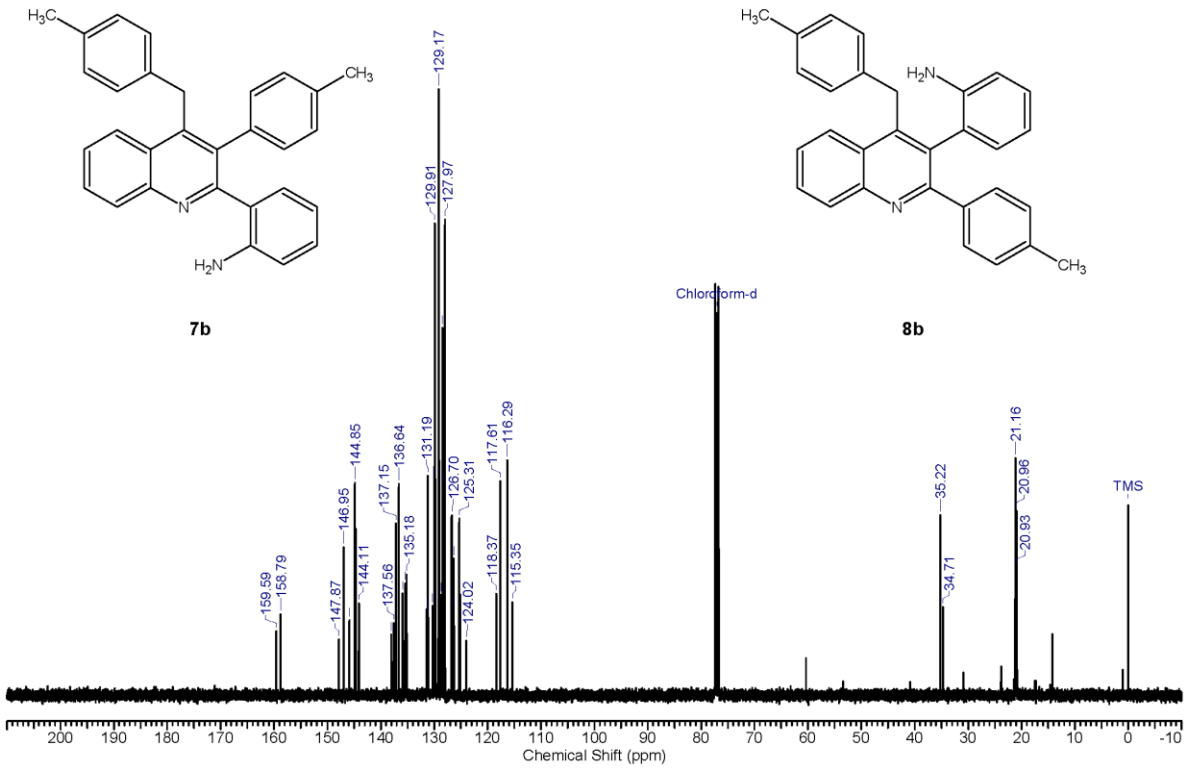
7a+8a


TMS
7a (major)
8a (minor)
Chemical Shift (ppm)

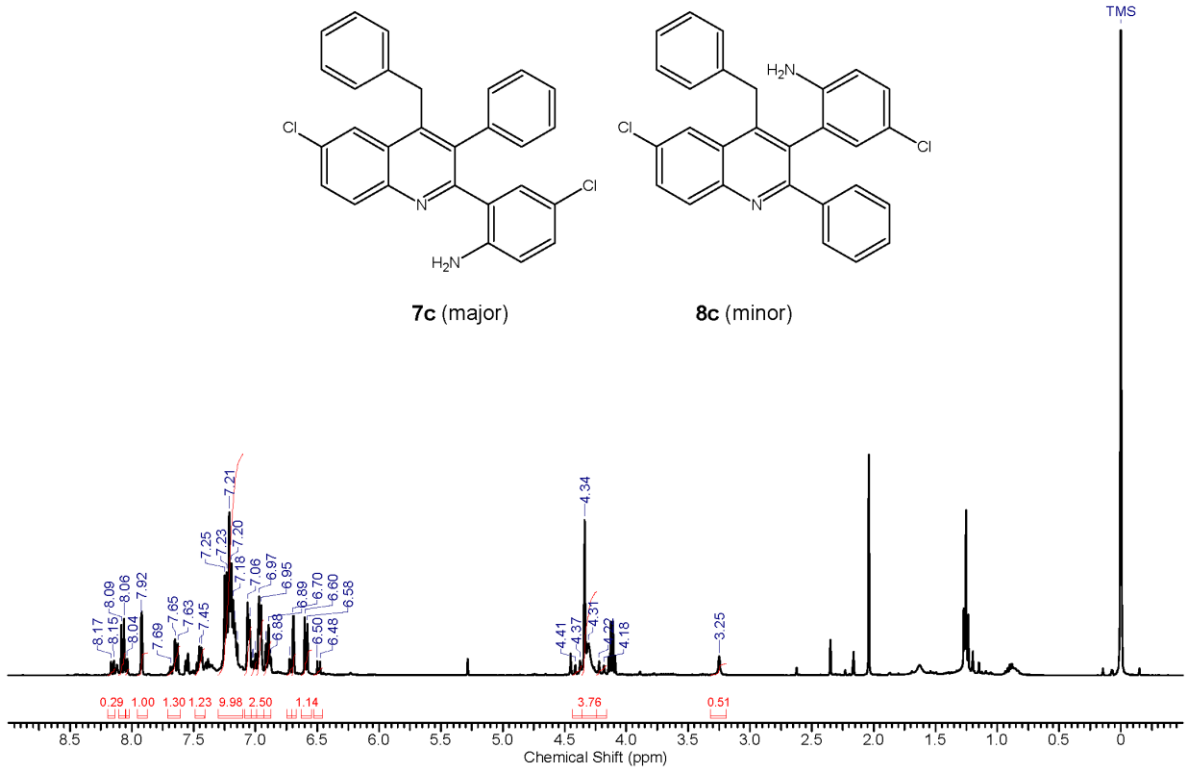
7b+8b


TMS
7b
8b
Chemical Shift (ppm)

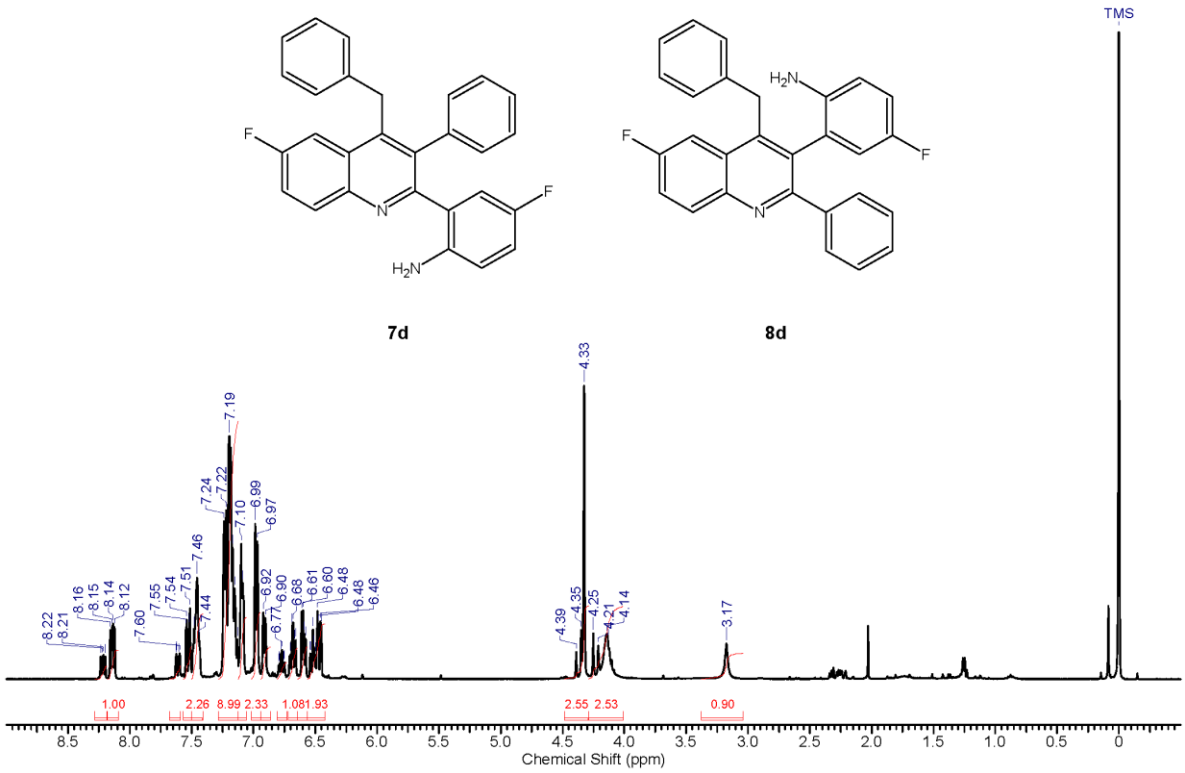
7b+8b


H3C
CH3
H2N
N
7b
H3C
H2N
CH3
N
8b
Chloroform-d
TMS
159.59
158.79
147.87
146.95
144.85
144.11
137.56
137.15
136.64
135.18
131.19
129.91
129.17
127.97
126.70
125.31
124.02
118.37
117.61
116.29
115.35
35.22
34.71
21.16
20.96
20.93
Chemical Shift (ppm)

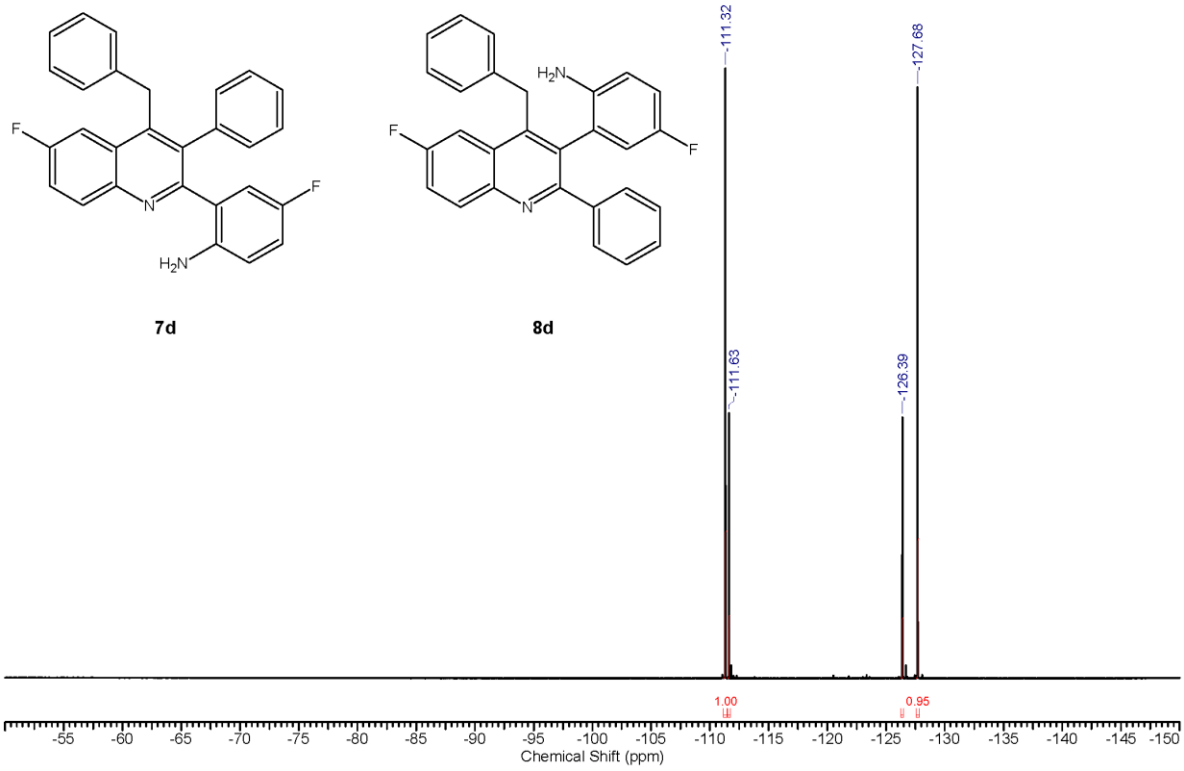
7c+8c


Cl
Cl
H2N
N
7c (major)
H2N
Cl
Cl
N
8c (minor)
TMS
8.17
8.15
8.09
8.06
8.04
7.92
7.69
7.65
7.63
7.45
7.25
7.23
7.21
7.20
7.18
7.06
6.97
6.95
6.89
6.88
6.70
6.60
6.58
6.50
6.48
4.41
4.37
4.34
4.31
4.22
4.18
3.25
0.29
1.00
1.30
1.23
9.98
2.50
1.14
3.76
0.51
Chemical Shift (ppm)

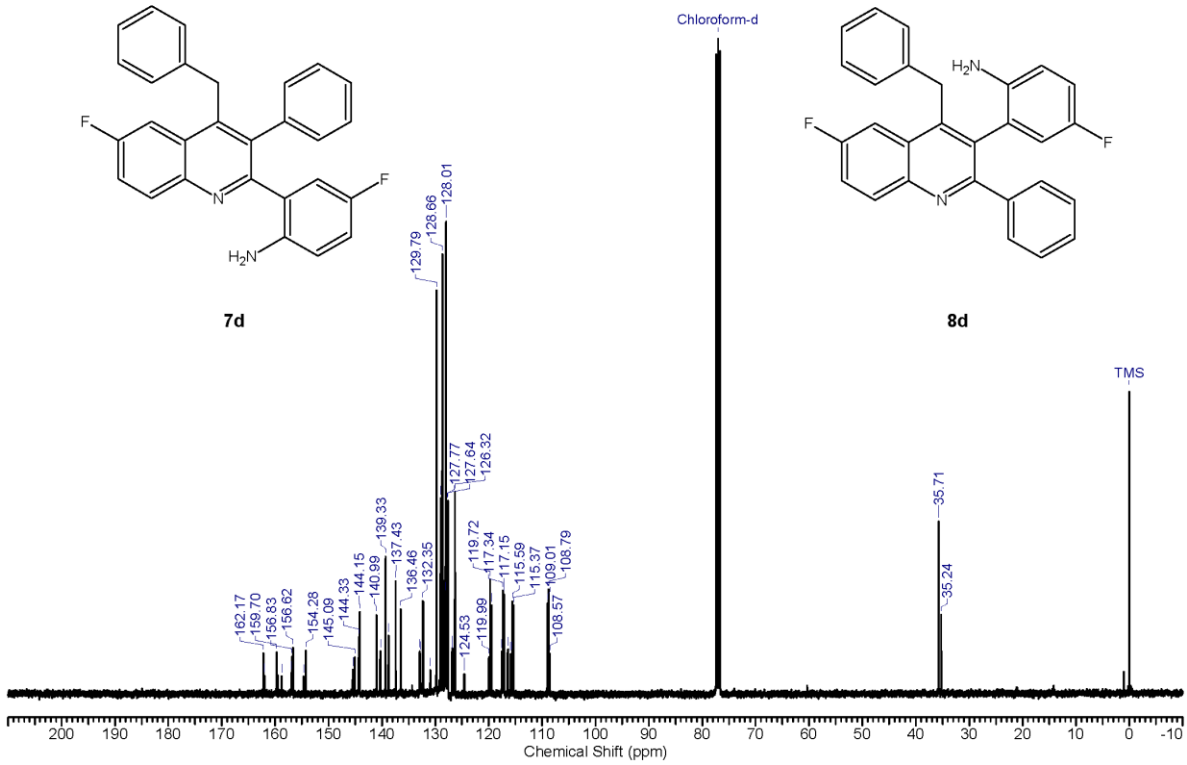
7d+8d



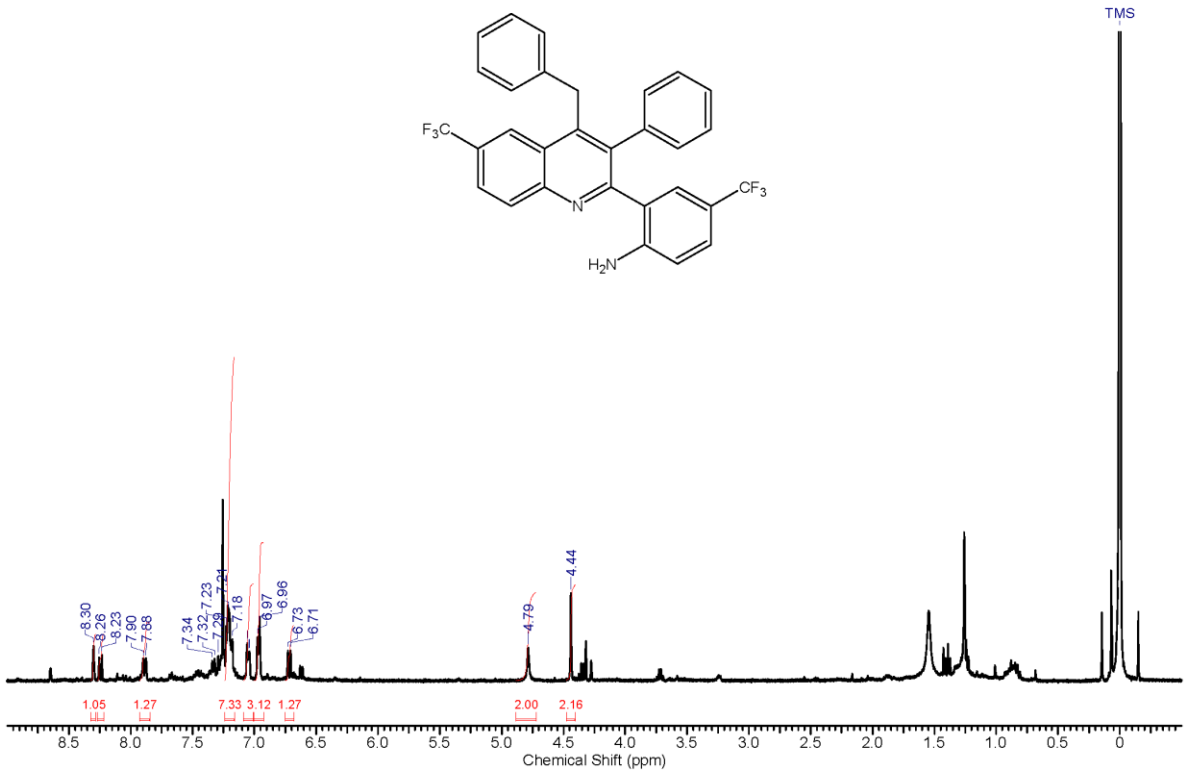
7d+8d - $^{19}F\{^{1}H\}$



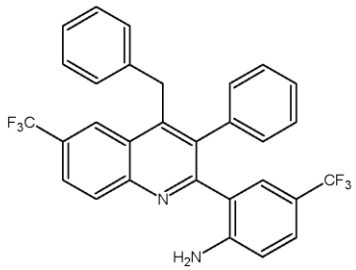
7d+8d


Chloroform-d
TMS
7d
8d
Chemical Shift (ppm)

7e

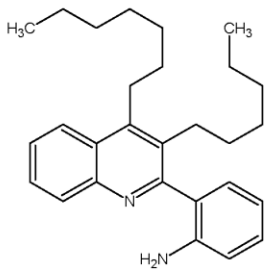

TMS
Chemical Shift (ppm)

7e - $^{19}F\{^{1}H\}$


F3C
CF3
N
H2N

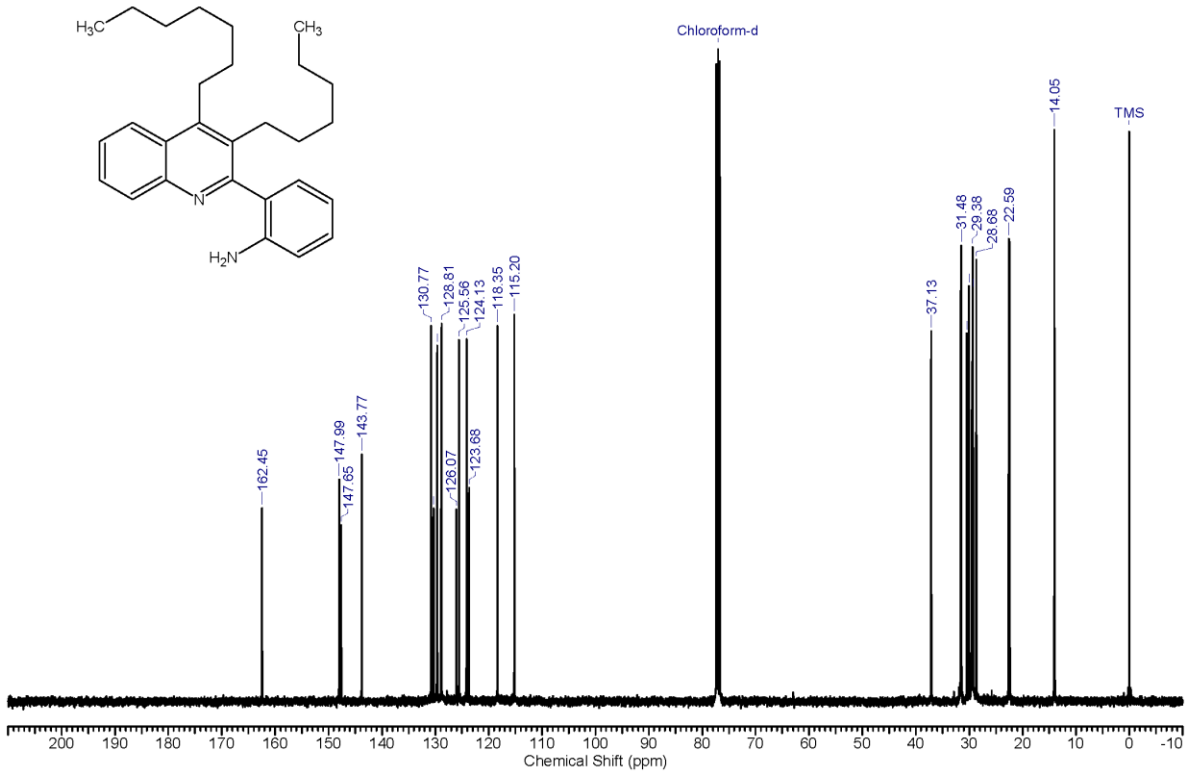
-61.58
-62.46
3.00
2.99
-51 -52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69
Chemical Shift (ppm)

7f

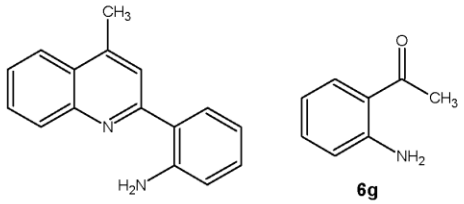

H3C
CH3
N
H2N

TMS
8.10
8.07
8.01
7.99
7.69
7.87
7.65
7.52
7.50
7.25
7.23
7.21
7.00
6.99
6.87
6.85
6.81
6.79
3.38
2.93
2.92
2.72
2.70
2.69
2.68
2.66
2.65
2.64
2.60
1.68
1.65
1.63
1.62
1.29
1.27
1.26
1.17
0.86
0.84
0.83
0.81
0.79
1.00 1.04 1.23 1.13 1.00 2.00 1.08 3.18 3.04 15.29 6.12
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

7f


H3C
CH3
N
H2N
Chloroform-d
TMS
14.05
31.48
29.38
28.68
22.59
37.13
130.77
128.81
125.56
124.13
118.35
115.20
162.45
147.99
147.65
143.77
126.07
123.68
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

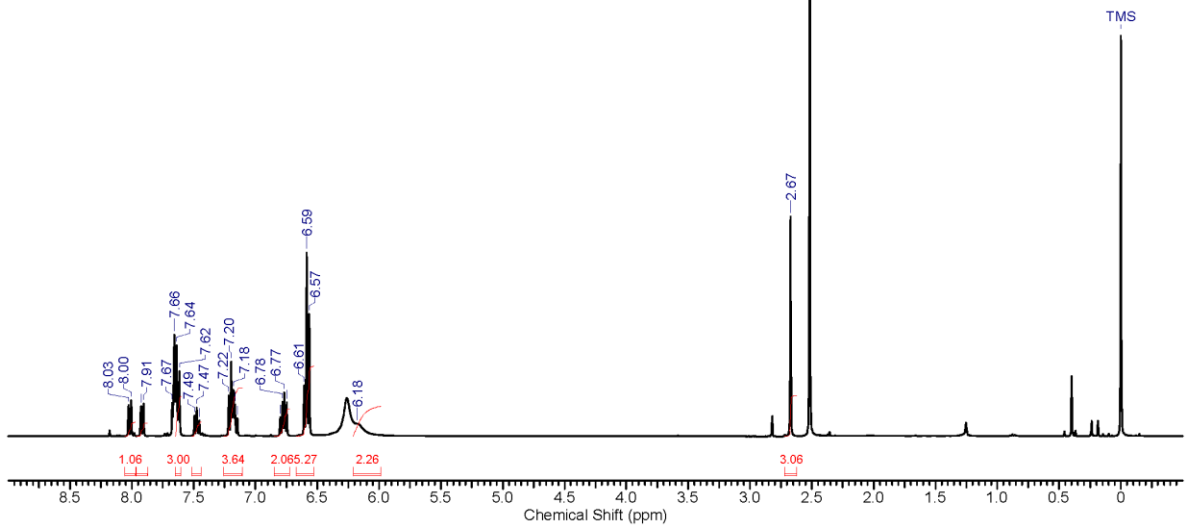
7g


CH3
N
H2N

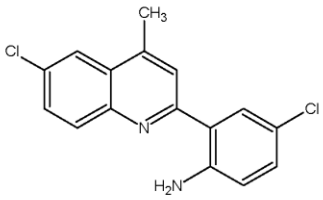
7g

O
CH3
NH2

6g

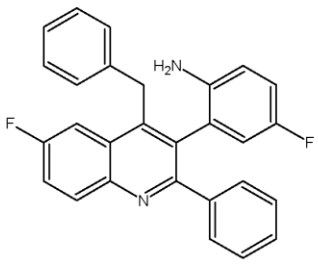

TMS
2.67
6.59
6.57
7.66
7.64
7.62
7.20
7.18
6.78
6.77
6.61
6.18
8.03
8.00
7.91
7.67
7.49
7.47
1.06
3.00
3.64
2.06
5.27
2.26
3.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)

7h


CH3
Cl
Cl
N
H2N

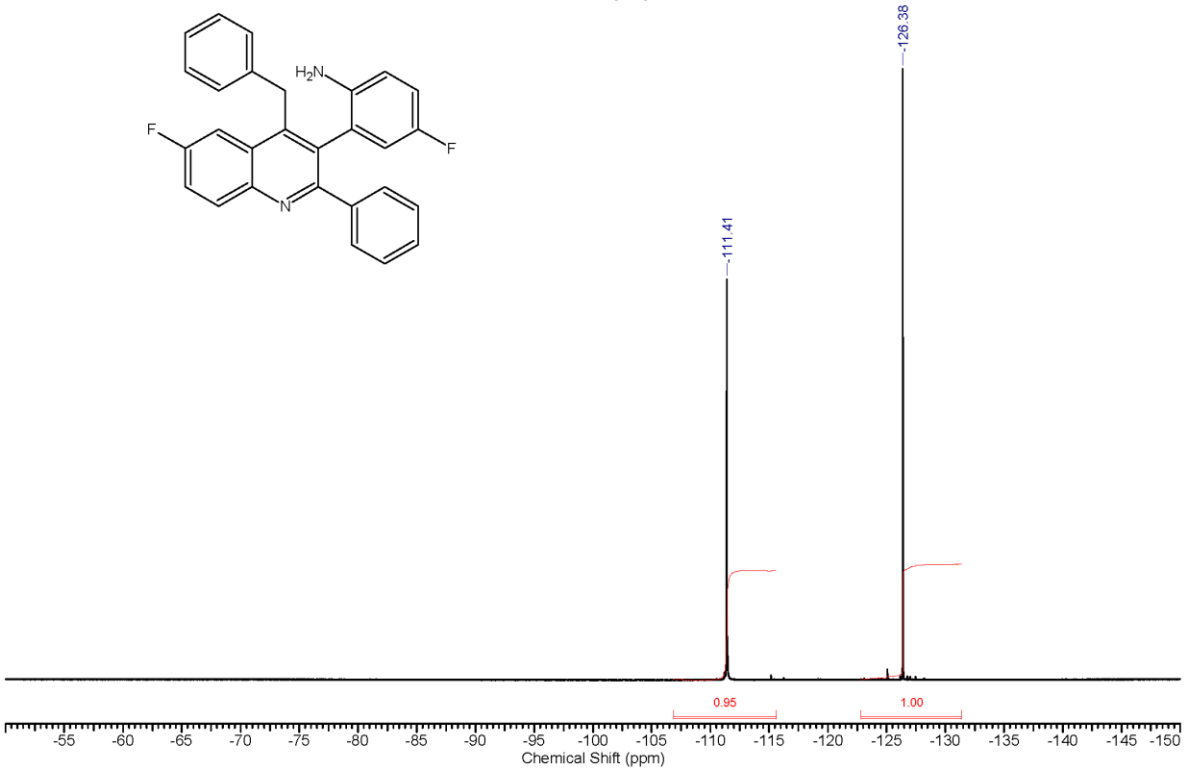
TMS
2.69
7.92
7.94
7.62
7.62
7.61
7.59
7.14
7.13
7.12
7.11
6.71
6.69
6.15
1.90
3.02
0.99
1.01
2.00
2.98
Chemical Shift (ppm)

8d

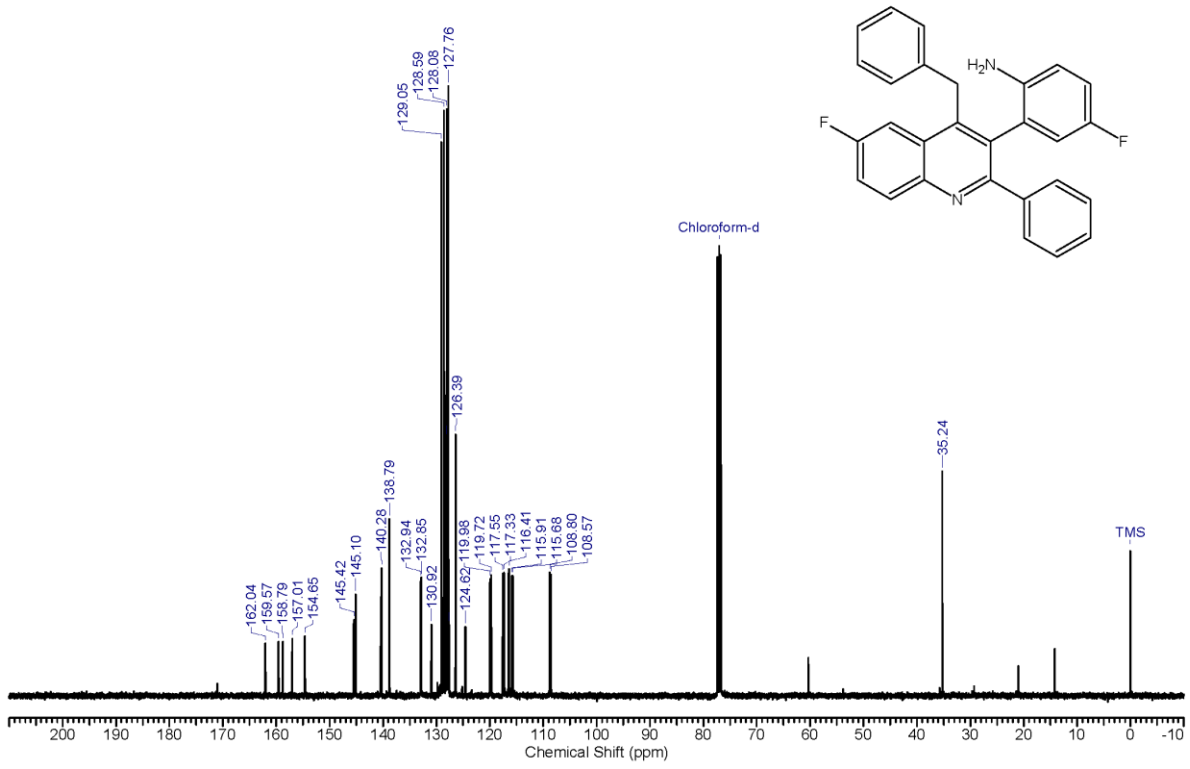

H2N
F
F
N

7.23
7.14
7.43
7.45
7.45
6.51
6.49
6.91
6.90
6.89
6.52
6.88
7.62
7.61
7.49
7.24
7.13
6.77
6.74
6.76
7.25
8.25
4.34
4.25
4.38
3.16
TMS
1.06
1.83
3.27
1.99
1.90
1.02
2.21
Chemical Shift (ppm)

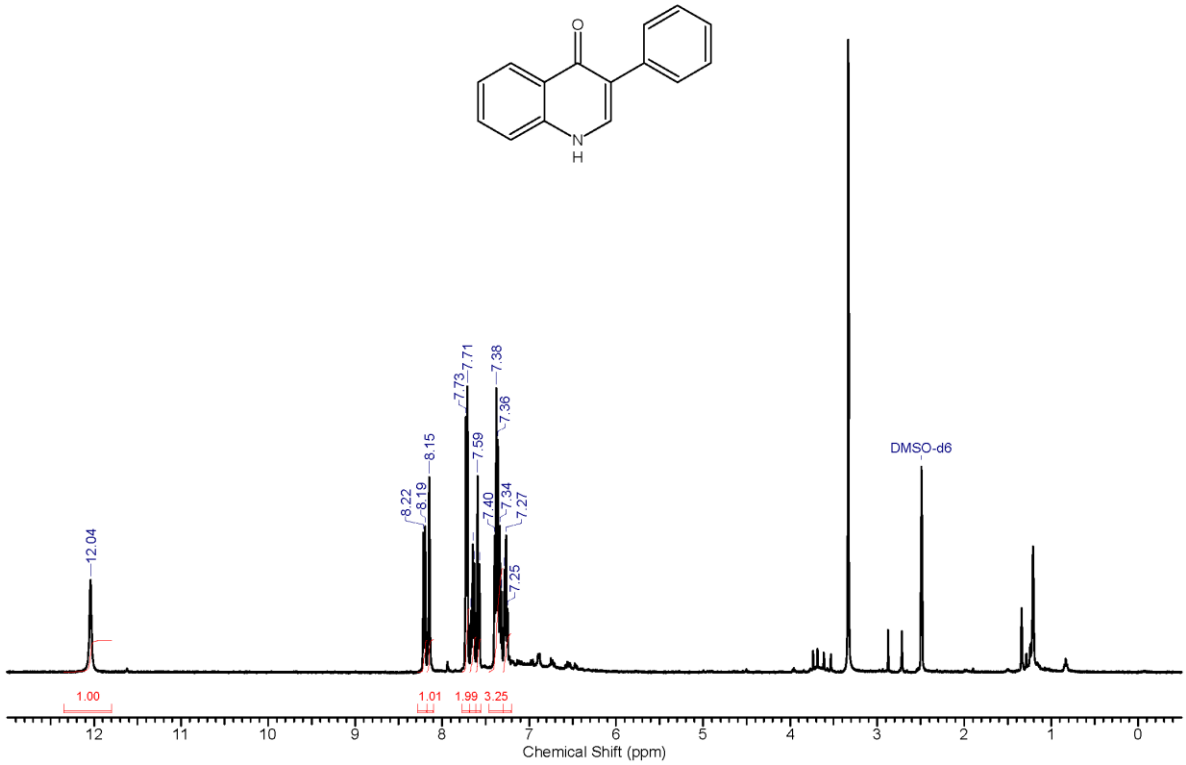
8d - $^{19}F\{^{1}H\}$


H2N
F
F
N
126.38
111.41
0.95
1.00
-55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
Chemical Shift (ppm)

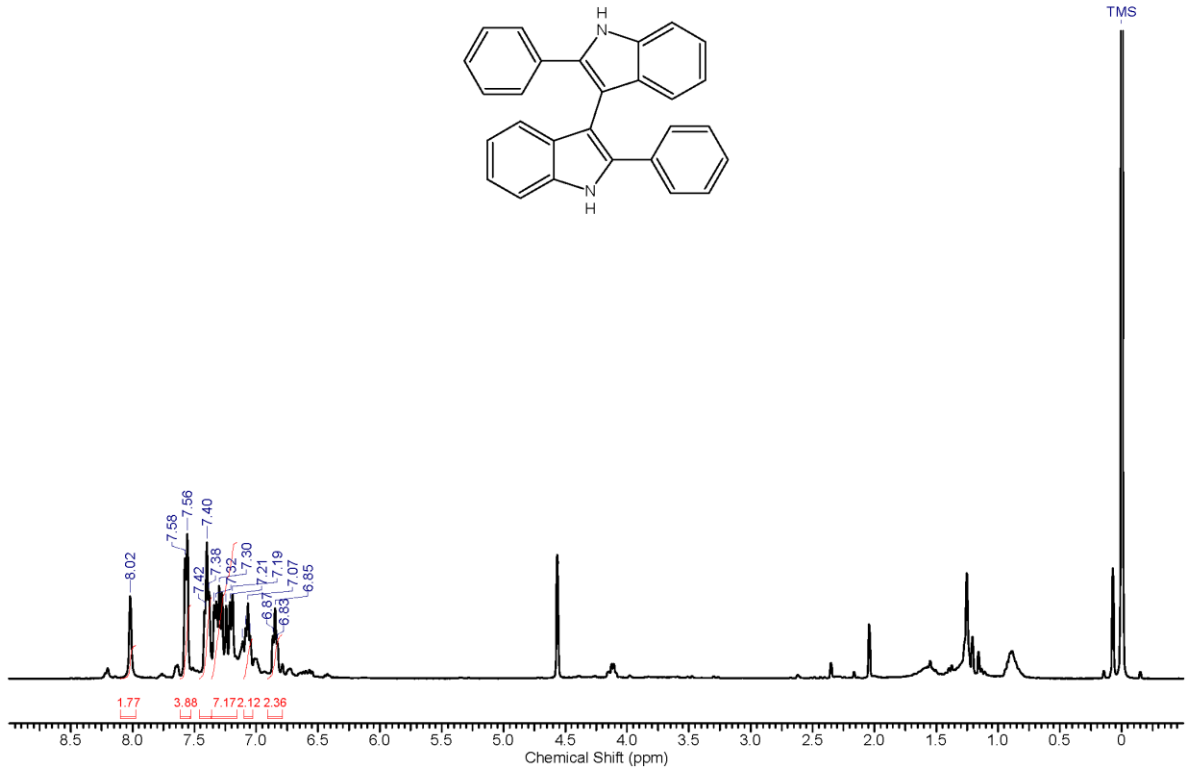
8d


H2N
F
F
N
129.05
128.59
128.08
127.76
126.39
Chloroform-d
35.24
TMS
140.28
138.79
132.94
132.85
130.92
124.62
119.98
119.72
117.55
117.33
116.41
115.91
115.68
108.80
108.57
145.42
145.10
162.04
159.57
158.79
157.01
154.65
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

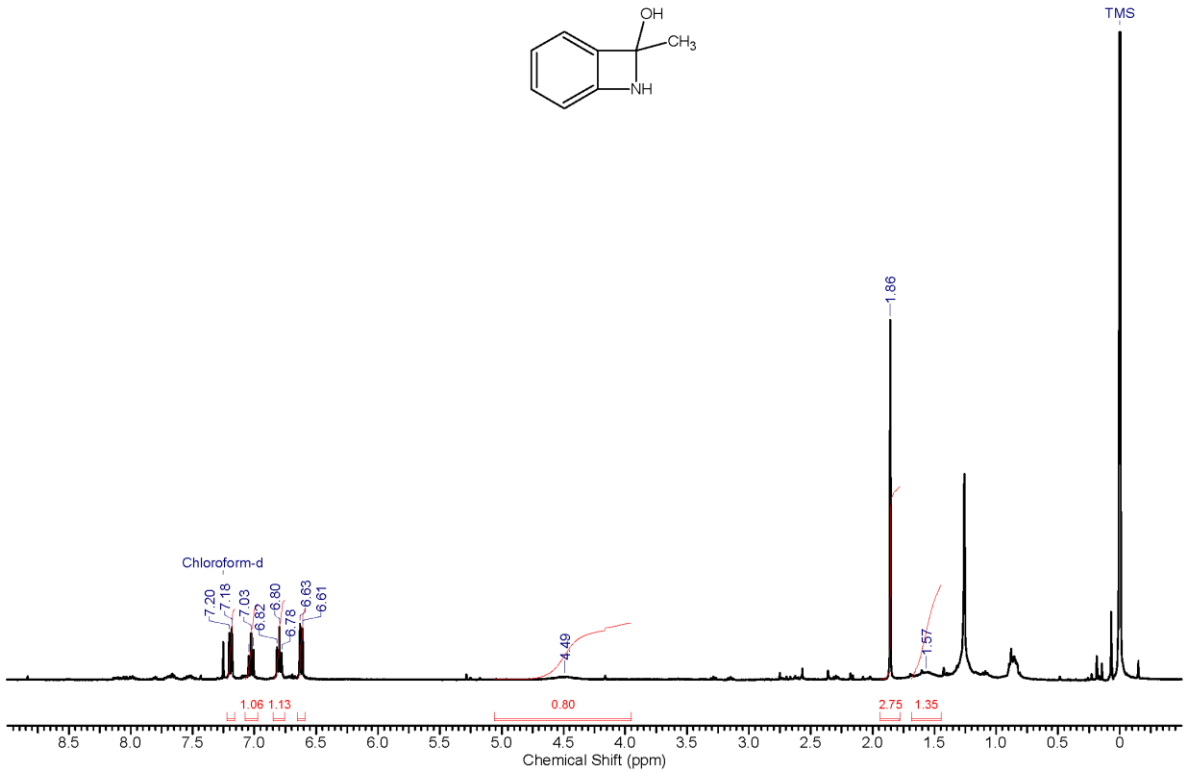
9a


12.04
8.22
8.19
8.15
7.73
7.71
7.59
7.40
7.38
7.36
7.34
7.27
7.25
DMSO-d6
1.00
1.01
1.99
3.25
Chemical Shift (ppm)

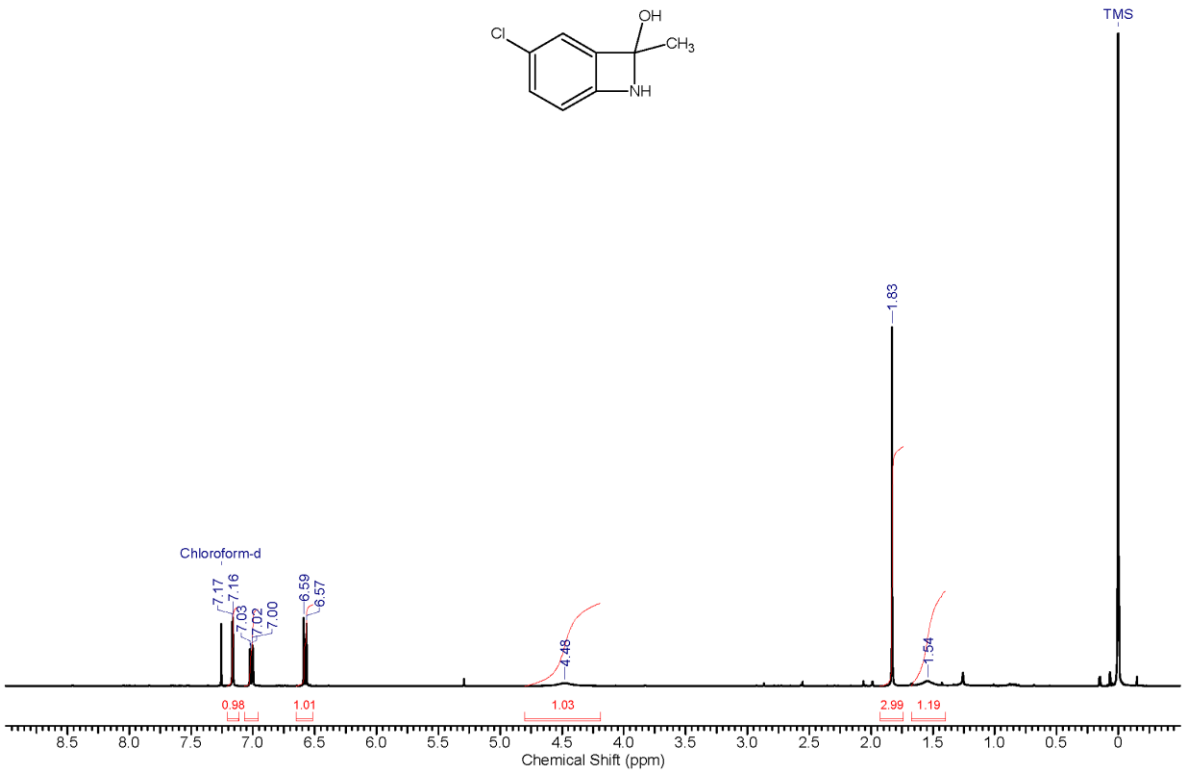
10a


TMS
8.02
7.58
7.56
7.42
7.40
7.38
7.32
7.30
7.21
7.19
7.07
6.87
6.85
6.83
1.77
3.88
7.17
2.12
2.36
Chemical Shift (ppm)

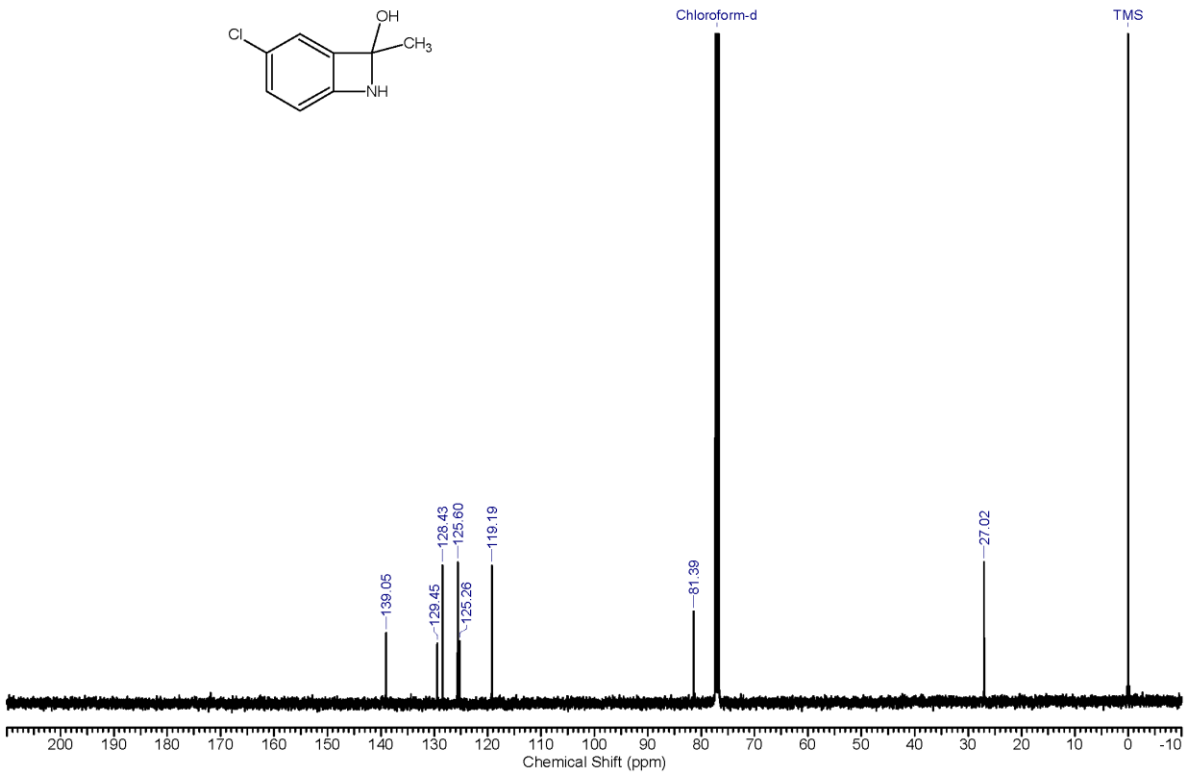
11g


OH
CH3
NH
TMS
1.86
Chloroform-d
7.20
7.18
7.03
6.82
6.80
6.78
6.63
6.61
4.49
1.57
1.06
1.13
0.80
2.75
1.35
Chemical Shift (ppm)

11h


OH
CH3
Cl
NH
TMS
1.83
Chloroform-d
7.17
7.16
7.03
7.02
7.00
6.59
6.57
4.48
1.54
0.98
1.01
1.03
2.99
1.19
Chemical Shift (ppm)

11h


OH
Cl
CH3
NH
Chloroform-d
TMS
139.05
129.45
128.43
125.60
125.26
119.19
81.39
27.02
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

III. Optimized cartesian coordinates of all the investigated species.

1a

6	1.875482	-0.288116	-0.039166
6	2.566862	-1.501520	-0.154433
6	3.952438	-1.539719	-0.146456
6	4.662949	-0.345558	-0.022110
6	3.999096	0.866660	0.091123
6	2.598992	0.921173	0.084080
1	1.990200	-2.416537	-0.247446
1	4.474604	-2.486377	-0.235992
1	5.749035	-0.358071	-0.013465
1	4.563361	1.791555	0.179447
7	1.934168	2.132936	0.150646
6	0.448380	-0.255008	-0.036587
6	-0.761646	-0.180993	-0.023466
6	-2.190715	-0.121055	-0.015709
1	0.961871	2.077376	0.421924
1	2.433599	2.884931	0.601576
6	-2.853314	1.092661	-0.249147
6	-4.241394	1.146581	-0.238526
6	-4.986543	-0.005273	0.002179
6	-4.335670	-1.214976	0.233079
6	-2.947952	-1.276477	0.226250
1	-2.269842	1.987312	-0.443240
1	-4.743721	2.091802	-0.421229
1	-6.071383	0.039498	0.008921
1	-4.912045	-2.115932	0.420706
1	-2.436653	-2.216396	0.407602

Frequencies

12.0228004
41.9788017
51.2673988
131.639893
136.701401
220.025299
248.130707
311.056305
352.641113
396.253113
411.532715
415.859802
485.420685
493.792786
529.835083

544.493225
559.784119
579.025574
584.722290
605.881470
642.820007
711.065002
713.683472
751.076904
773.516907
783.264893
832.650696
870.580505
874.019470
887.530884
945.375610
960.762695
992.004822
993.302002
1018.29968
1027.10059
1068.83826
1074.34497
1100.23987
1122.96484
1173.91846
1192.77173
1203.45459
1205.01685
1223.83264
1307.46216
1337.28979
1355.79248
1366.49524
1371.97925
1372.24609
1505.35046
1521.73816
1554.55005
1571.34631
1659.28845
1664.17065
1686.14001
1698.12500
1710.23865
2361.05151
3202.31104
3211.81177

3218.59375
3220.00122
3226.46924
3229.52515
3237.09155
3242.59448
3243.32129
3610.48096
3721.61011

Ia

6	-1.861254	-0.355846	-0.001266
6	-2.595320	-1.548276	-0.005143
6	-3.984581	-1.515647	-0.004890
6	-4.672231	-0.302912	-0.000812
6	-3.969173	0.897962	0.003090
6	-2.586979	0.840970	0.002750
1	-2.061598	-2.491715	-0.008308
1	-4.539239	-2.447660	-0.007909
1	-5.756285	-0.288242	-0.000654
1	-4.496378	1.847849	0.006279
7	-1.792758	2.089341	0.006770
6	-0.432285	-0.312467	-0.001159
6	0.778829	-0.226100	-0.000896
6	2.208548	-0.150644	-0.000555
6	2.907617	-0.108973	-1.215326
6	4.294320	-0.039836	-1.208789
6	4.986756	-0.011759	0.000068
6	4.294524	-0.054894	1.208590
6	2.907812	-0.124115	1.214507
1	2.361754	-0.140064	-2.152824
1	4.836635	-0.011927	-2.148039
1	6.070757	0.040033	0.000292
1	4.836984	-0.038684	2.148027
1	2.362100	-0.166826	2.151637
1	-0.790817	1.816468	0.006402
1	-1.966647	2.667705	-0.821788
1	-1.967470	2.662902	0.838481

Frequencies
11.1606998
46.2398987
49.9832993
131.891098
135.261993
167.709503
220.052994
248.096405
344.444611

347.502014
396.605011
411.516693
444.637512
484.670410
523.490906
544.311584
564.191406
571.291382
588.133606
641.484314
708.294006
710.660400
722.232727
785.223328
786.003906
800.126892
874.611572
876.617126
903.896973
962.878723
990.850220
1004.18140
1027.97729
1039.75415
1042.90369
1045.46741
1068.99634
1079.06738
1116.32166
1127.95886
1138.51575
1191.10693
1210.83228
1212.84082
1221.95337
1228.70093
1315.34753
1345.21399
1357.12915
1371.66394
1375.21936
1506.48376
1514.98254
1540.73145
1549.54297
1567.51355
1655.05078

1665.30725
1680.11182
1691.11243
1691.56335
1717.43835
2353.61792
3225.08325
3226.96167
3231.73291
3237.75439
3245.47168
3246.78320
3253.60913
3256.82349
3264.18481
3282.99951
3476.91284
3535.32764

IIa (first isomer)

6	3.283339	0.305059	-1.104985
6	2.064502	0.021645	-0.481439
6	2.046983	-0.423749	0.846728
6	3.238191	-0.580380	1.538612
6	4.452718	-0.295075	0.913483
6	4.474550	0.146168	-0.405956
6	0.822364	0.203880	-1.250573
6	-0.399436	0.027442	-0.835814
6	-1.656965	-0.151586	-0.416713
6	-2.397027	0.957860	0.187524
6	-3.729296	0.722876	0.610727
6	-4.287153	-0.516339	0.452309
6	-3.584479	-1.617148	-0.131009
6	-2.310371	-1.442356	-0.552641
1	1.103027	-0.653906	1.334362
1	3.300686	0.647061	-2.136044
1	3.223799	-0.928298	2.566171
1	5.382978	-0.420382	1.457824
1	5.418514	0.365365	-0.893430
1	0.922276	0.520832	-2.291831
1	-1.739570	-2.247318	-1.002242
1	-4.079372	-2.575897	-0.229636
1	-5.309259	-0.670779	0.785059
1	-4.296730	1.531876	1.059003
7	-1.831246	2.148905	0.334642
1	-2.335691	2.919706	0.749531
1	-0.879449	2.319623	0.037229

Frequencies

31.0580997
39.1110992
46.1012993
104.525902
126.455299
215.352005
265.618011
295.159790
358.987396
412.095306
414.967285
456.044495
479.773712
495.410400
517.326294
529.798218
557.180115
583.419617
602.781311
636.016479
662.899597
708.447693
741.639709
761.557190
776.523071
794.387573
843.099792
866.720703
876.788879
883.682678
888.545898
961.408630
1002.96301
1016.26593
1027.58984
1027.73303
1040.53613
1050.10889
1067.28210
1069.55786
1131.92786
1170.18188
1204.72205
1212.20020
1217.02625
1228.15503

1233.74341
1276.81702
1345.12891
1379.20569
1387.61499
1404.51648
1476.90234
1499.36047
1524.03577
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1732.29602
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3232.99438
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3245.62036
3251.87183
3253.23071
3267.25439
3610.70483
3730.33960

IIa (second isomer)

6	3.283339	0.305059	-1.104985
6	2.064502	0.021645	-0.481439
6	2.046983	-0.423749	0.846728
6	3.238191	-0.580380	1.538612
6	4.452718	-0.295075	0.913483
6	4.474550	0.146168	-0.405956
6	0.822364	0.203880	-1.250573
6	-0.399436	0.027442	-0.835814
6	-1.656965	-0.151586	-0.416713
6	-2.397027	0.957860	0.187524
6	-3.729296	0.722876	0.610727
6	-4.287153	-0.516339	0.452309
6	-3.584479	-1.617148	-0.131009
6	-2.310371	-1.442356	-0.552641
1	1.103027	-0.653906	1.334362
1	3.300686	0.647061	-2.136044
1	3.223799	-0.928298	2.566171

1	5.382978	-0.420382	1.457824
1	5.418514	0.365365	-0.893430
1	0.922276	0.520832	-2.291831
1	-1.739570	-2.247318	-1.002242
1	-4.079372	-2.575897	-0.229636
1	-5.309259	-0.670779	0.785059
1	-4.296730	1.531876	1.059003
7	-1.831246	2.148905	0.334642
1	-2.335691	2.919706	0.749531
1	-0.879449	2.319623	0.037229

Frequencies

31.0580997
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3730.33960

IIa (third isomer)

6	-2.398797	0.957702	-0.183983
6	-1.657981	-0.151369	0.419884
6	-2.309886	-1.443024	0.553894
6	-3.582128	-1.620106	0.127408
6	-4.284502	-0.520325	-0.458036
6	-3.728653	0.720505	-0.612716
6	-0.399393	0.027856	0.836531

6	0.823028	0.205294	1.249491
6	2.064910	0.023330	0.480310
6	3.284584	0.296525	1.106730
6	4.475653	0.136626	0.407595
6	4.452810	-0.295314	-0.914880
6	3.237363	-0.569706	-1.543191
6	2.046381	-0.412028	-0.851201
1	-1.739289	-2.246769	1.005784
1	1.101630	-0.632781	-1.341541
1	3.302686	0.631561	2.140030
1	3.222123	-0.909707	-2.573377
1	5.382954	-0.421484	-1.459246
1	5.420278	0.347809	0.897325
1	0.922981	0.523072	2.290618
7	-1.835885	2.150792	-0.324295
1	-4.296485	1.529087	-1.061225
1	-5.305034	-0.676544	-0.794756
1	-4.075850	-2.579679	0.224030
1	-2.339307	2.920685	-0.742153
1	-0.885834	2.323420	-0.022440

Frequencies

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3267.35986
3610.68774

3730.08032

IIIa (first isomer)

6	1.689394	0.092360	-0.086577
6	1.632916	-1.282979	0.175534
6	2.797815	-1.999219	0.383773
6	4.028018	-1.339326	0.327022
6	4.091967	0.027280	0.098606
6	2.923345	0.771083	-0.092688
1	0.673309	-1.792721	0.177906
1	2.755987	-3.066341	0.570924
1	4.946901	-1.896645	0.477486
1	5.052940	0.533276	0.087905
7	2.940785	2.152320	-0.340420
6	0.499365	0.868963	-0.452612
6	-0.747469	0.589659	-0.265217
1	0.703882	1.816732	-0.971923
6	-2.068654	0.282819	-0.117333
6	-2.732381	-0.495088	-1.115729
6	-4.064503	-0.807553	-0.957529
6	-4.746308	-0.359387	0.182172
6	-4.115613	0.403314	1.175087
6	-2.785137	0.730210	1.034813
1	-2.172967	-0.824930	-1.984909
1	-4.584782	-1.394950	-1.705468
1	-5.796331	-0.610685	0.299699
1	-4.674873	0.732446	2.043431
1	-2.265832	1.319703	1.782899
1	2.488932	2.707546	0.377419
1	3.870808	2.517515	-0.508370

Frequencies

35.4943008
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333.416992
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IIIa (the second isomer collapses into the below reported cyclized structure)

6	2.549875	-1.226103	0.211274
6	1.781635	-0.077416	-0.026197
6	2.431084	1.148156	-0.225271
6	3.818351	1.221827	-0.194026
6	4.572247	0.074667	0.032495
6	3.934405	-1.148008	0.233847
6	0.327513	-0.192508	-0.063114
6	-0.528113	-1.219523	-0.182034
6	-1.909437	-0.756688	-0.099413
6	-1.897213	0.623576	0.072321
6	-3.020162	1.412417	0.185367
6	-4.243034	0.739052	0.123903
6	-4.294183	-0.645818	-0.047221
6	-3.134300	-1.411453	-0.162294
1	-3.187623	-2.486203	-0.296737
7	-0.486573	1.060142	0.092147
1	-2.974814	2.488664	0.317008
1	-5.163724	1.304985	0.210831
1	-5.260264	-1.136891	-0.092098
1	-0.228827	-2.248659	-0.328637
1	1.875191	2.062530	-0.422909
1	4.309021	2.176115	-0.352613
1	5.655206	0.132991	0.055815
1	4.518324	-2.043060	0.419799
1	2.063202	-2.178678	0.395511
1	-0.293083	1.714556	-0.674607
1	-0.238606	1.539580	0.965789

Frequencies
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TS from Ia + 1a to Va

6	2.189060	-3.171437	-0.525289
6	2.199658	-1.931189	0.145411
6	2.353906	-1.939639	1.547537
6	2.467858	-3.140756	2.246883
6	2.467312	-4.354761	1.568087
6	2.339673	-4.358809	0.178783
6	2.002660	-0.679352	-0.546820
6	0.996073	-0.248678	-1.201504
6	-0.364369	-0.648946	-1.556184
6	-1.177945	-1.191053	-0.554736
6	-2.455113	-1.669096	-0.785534
6	-2.966232	-1.606625	-2.077306
6	-2.194998	-1.058911	-3.098894
6	-0.912473	-0.585148	-2.841922
1	2.417650	-0.990602	2.074620
7	1.184873	1.435031	-1.824222
6	1.979342	2.211578	-0.917788
6	1.394270	2.639989	0.285405
6	2.175579	3.357024	1.196507
6	3.514201	3.612213	0.922959
6	4.087609	3.145463	-0.255432
6	3.320389	2.437774	-1.177036
6	0.033623	2.301624	0.566473
6	-1.118463	1.970519	0.755820

6	-2.450451	1.489772	0.975769
6	-3.390179	1.508614	-0.062897
6	-4.653737	0.965018	0.132820
6	-4.989550	0.390578	1.356569
6	-4.061539	0.373393	2.397342
6	-2.798234	0.924869	2.214061
1	1.723612	3.704959	2.119025
1	4.112448	4.168292	1.636460
1	5.136605	3.328117	-0.461652
1	3.770000	2.064197	-2.092001
1	-3.119800	1.940128	-1.021010
1	-5.378551	0.987985	-0.674450
1	-5.978173	-0.031494	1.505616
1	-4.329755	-0.052151	3.359238
1	-2.081968	0.943969	3.031460
1	1.628458	1.372343	-2.738768
1	0.250868	1.832479	-1.937962
7	-0.647288	-1.174729	0.816175
1	-3.061026	-2.056824	0.028752
1	-3.964624	-1.977495	-2.279894
1	-2.591520	-1.009885	-4.107656
1	-0.313655	-0.189416	-3.657150
1	2.075309	-3.186523	-1.604990
1	2.344278	-5.300613	-0.361924
1	2.578171	-5.287363	2.111180
1	2.586442	-3.120186	3.326372
1	-1.391757	-1.312004	1.504996
1	0.113830	-1.864024	0.969913
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TS from Ia + 1a to IVa

6	3.766013	-1.819615	0.915678
6	3.736979	-0.918827	-0.154342
6	4.939887	-0.705778	-0.840214
6	6.134063	-1.327029	-0.521204
6	6.129917	-2.217249	0.548801
6	4.952505	-2.458063	1.258311
6	2.583357	-0.162056	-0.648166

6	1.393434	-0.148660	-0.219936
6	0.299328	-0.506763	0.637703
6	0.030479	0.253393	1.785430
6	-1.026977	-0.102494	2.612787
6	-1.815012	-1.207634	2.301874
6	-1.545511	-1.972616	1.167529
6	-0.494609	-1.623719	0.332990
7	4.791816	0.254435	-1.938738
7	0.302905	1.243558	-1.432809
6	-0.028048	2.418079	-0.719571
6	-1.315769	2.558965	-0.168438
6	-1.599684	3.693556	0.603476
6	-0.629528	4.658905	0.829407
6	0.644708	4.504095	0.284812
6	0.945106	3.387053	-0.483516
6	-2.291170	1.539716	-0.383302
6	-3.055788	0.615732	-0.554551
6	-3.936404	-0.503111	-0.682573
6	-3.713835	-1.471549	-1.670762
6	-4.535852	-2.588505	-1.750637
6	-5.585340	-2.750353	-0.848750
6	-5.814501	-1.788021	0.132441
6	-4.996731	-0.668578	0.218940
1	-2.594871	3.802507	1.020948
1	-0.865230	5.533010	1.426783
1	1.406313	5.257420	0.458044
1	1.939690	3.257380	-0.901366
1	-2.894848	-1.341637	-2.371804
1	-4.360310	-3.333370	-2.520511
1	-6.227279	-3.623128	-0.913785
1	-6.635029	-1.909914	0.832424
1	-5.166999	0.081929	0.983962
1	0.979653	1.389607	-2.173569
1	-0.522591	0.760338	-1.782469
1	0.645226	1.118614	2.010988
1	-1.240478	0.487512	3.497971
1	-2.647677	-1.475886	2.944347
1	-2.170436	-2.825518	0.924370
1	-0.282177	-2.204551	-0.559450
1	2.855229	-2.012927	1.473212
1	4.963144	-3.154227	2.090550
1	7.047415	-2.723251	0.828463
1	7.043995	-1.131545	-1.080530
1	3.709468	0.467548	-1.808735
1	5.349202	1.103264	-1.822438
1	4.979443	-0.142348	-2.861863

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3246.63501
3252.19946
3254.90381
3593.71167
3655.19507
3687.42041

Ts-to VIIa

6	-3.064358	-1.278884	-0.213060
6	-2.053570	-0.347210	0.072144
6	-2.378405	0.965587	0.404050
6	-3.723817	1.321606	0.440651
6	-4.722356	0.391148	0.153991
6	-4.401314	-0.925624	-0.176802

6	-0.729430	-0.941230	-0.031092
6	0.511672	-0.844348	0.033299
6	1.913316	-0.917068	0.040574
6	2.631104	-0.690270	-1.151327
6	4.015198	-0.747768	-1.137658
6	4.685328	-1.028267	0.054223
6	3.981660	-1.254529	1.239068
6	2.597954	-1.201655	1.239262
7	-2.535767	-2.588758	-0.530118
8	0.637585	1.867487	0.676931
1	2.090610	-0.474507	-2.067018
1	-1.585655	1.671487	0.630547
1	-3.998937	2.338960	0.698145
1	-5.764411	0.690865	0.189016
1	-5.179470	-1.649089	-0.397861
1	2.032539	-1.373017	2.149163
1	4.517525	-1.473529	2.156178
1	5.769897	-1.073088	0.059873
1	4.575660	-0.577554	-2.050409
1	1.177430	2.159621	1.422209
6	1.154906	2.481922	-0.499412
1	-1.197439	-2.128248	-0.354073
1	-2.811115	-3.316200	0.128310
1	-2.743858	-2.901548	-1.477367
6	1.176037	3.997834	-0.404733
1	2.159191	2.089486	-0.718752
1	0.490916	2.155006	-1.305756
1	1.538485	4.436287	-1.339551
1	0.172940	4.385637	-0.205148
1	1.841833	4.333382	0.398819

Frequencie

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270.181091
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364.802002

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1017.28363
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1172.40442
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1463.18018
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3232.30322
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3238.70435
3240.55103
3244.19849
3246.10522
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3254.05493
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3527.96460
3614.69116
3835.47144

VIIa

6	2.554433	-1.568966	-0.433206
6	2.036993	-0.385815	0.103795
6	2.910397	0.547453	0.675880
6	4.274357	0.290155	0.727187
6	4.780734	-0.897149	0.203044
6	3.919590	-1.824077	-0.378151
6	0.585643	-0.111984	0.077635
8	0.222848	1.215495	-0.049127
6	-0.372259	-1.043137	0.228568

6	-1.832892	-0.862354	0.113448
6	-2.559040	0.169066	0.716046
6	-3.933604	0.309575	0.592619
6	-4.639281	-0.622965	-0.156654
6	-3.957917	-1.682768	-0.750365
6	-2.581671	-1.801264	-0.609793
7	-1.825286	1.134188	1.555785
1	2.516031	1.471098	1.089838
1	-2.059784	-2.628896	-1.080108
1	-4.503284	-2.421456	-1.327795
1	-5.713775	-0.527071	-0.264402
1	-4.456535	1.128594	1.079965
1	1.891371	-2.279956	-0.917257
1	4.312986	-2.742504	-0.801356
1	5.846856	-1.095941	0.240915
1	4.943511	1.015129	1.179103
6	0.591036	1.877534	-1.285371
1	-1.009900	1.501675	0.995801
1	-2.423584	1.905370	1.859748
1	-1.438943	0.682708	2.391577
1	-0.039201	-2.063870	0.391317
6	0.114182	3.308881	-1.200541
1	1.676410	1.818268	-1.399784
1	0.115621	1.335045	-2.108860
1	0.386886	3.840414	-2.116094
1	-0.974966	3.358554	-1.098151
1	0.580309	3.826443	-0.356778

Frequencie

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145.748093
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206.128494
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270.352997
273.736511
291.222198
312.143494
357.675293
374.754700
418.807495
422.045898
446.086304
476.452911

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603.583618
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737.208191
745.814880
780.291321
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833.218323
851.441589
878.013489
894.370911
903.320679
907.173401
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3216.66968
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3237.33521
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3267.61792
3482.40918
3554.83008

TsOH

6	1.945862	-1.203577	0.019904
6	0.557067	-1.216536	-0.032629
6	-0.124999	-0.005890	-0.082537
6	0.556206	1.208472	-0.091418
6	1.943056	1.200225	-0.041568
6	2.656988	-0.001514	0.018080
16	-1.895852	-0.010507	-0.127307
8	-2.340963	-1.234999	-0.748840
8	-2.279666	-0.132953	1.449820
8	-2.364180	1.294000	-0.561814
1	0.004237	2.140173	-0.154655
1	2.483149	2.143212	-0.054937

6	4.163016	0.013824	0.068674
1	2.485573	-2.145596	0.057026
1	0.007638	-2.151691	-0.046735
1	-2.623180	0.730847	1.728234
1	4.573145	-0.997564	0.132034
1	4.578770	0.491574	-0.825179
1	4.519585	0.578745	0.936773

Frequencies

24.4405994
34.1104012
87.7325974
150.397202
171.605103
206.320694
290.361603
328.769501
354.416199
389.100311
418.624695
467.939087
480.920410
547.294678
560.688721
654.061707
672.326477
723.993225
811.954712
840.951477
848.293213
871.819397
991.791992
1001.72223
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1083.95959
1131.77686
1159.29187
1169.59033
1217.01819
1231.62854
1255.69202
1349.39331
1358.97632
1430.99316
1452.07410
1465.14160
1520.96326

1530.44751
1563.75122
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3140.25000
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3216.00610
3221.00391
3248.62695
3252.53491
3800.67139

TsO-

6	1.918578	-1.199011	0.001279
6	0.527918	-1.194121	0.002865
6	-0.170459	0.010947	0.001627
6	0.539528	1.207195	0.000925
6	1.931255	1.197502	-0.001143
6	2.642605	-0.004229	-0.000614
16	-1.982699	0.002067	-0.001658
8	-2.328503	-0.720848	-1.240450
8	-2.327059	-0.725472	1.235412
8	-2.352757	1.431108	0.005650
1	-0.022944	2.135632	0.000894
1	2.476561	2.140774	-0.002408
6	4.152632	-0.003419	-0.001357
1	2.454051	-2.147426	0.001698
1	-0.028759	-2.126454	0.004707
1	4.551194	-1.023798	-0.000488
1	4.553127	0.509404	-0.884959
1	4.554163	0.511308	0.880689

Frequencies
16.0149994
91.3380966
162.364502
212.714294
277.334991
322.752899
355.114410
393.230988
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491.482513
548.005310
568.540710
580.184204
658.800781

682.698181
728.405823
826.969604
831.430908
867.756714
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994.872620
1021.41211
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1059.50830
1079.16736
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1152.11731
1219.32690
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1282.49390
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1355.23450
1444.53625
1457.34570
1522.70178
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1564.35693
1664.50903
1698.08569
3048.44165
3110.17261
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3176.94556
3181.41553
3233.05908
3241.95068

Ethanol

6	-1.219831	-0.219927	-0.000000
1	-1.287894	-0.857199	0.886751
6	0.091696	0.545213	-0.000000
1	-1.287895	-0.857199	-0.886751
1	-2.067345	0.473236	0.000000
1	0.142084	1.196421	-0.887883
1	0.142083	1.196421	0.887883
8	1.143803	-0.398491	0.000000
1	1.977355	0.084535	-0.000000

Frequencies
252.891907
301.278412
424.402191

836.127319
929.438171
1060.68945
1160.25427
1206.27466
1309.71106
1324.50586
1433.50024
1496.64563
1520.19775
1538.76526
1570.21216
3000.15186
3030.74219
3076.64111
3158.18115
3164.75708
3858.85522

Protonated ether

6	0.027051	-0.076856	0.040253
1	0.074731	-0.130165	1.132002
1	1.049634	-0.077532	-0.344032
1	-0.501694	-0.971698	-0.303886
6	-0.700197	1.188873	-0.329358
8	-0.714631	1.306308	-1.826269
1	-1.742762	1.213081	-0.003521
1	-0.178426	2.092259	-0.014859
6	-1.442271	2.474256	-2.427244
6	-1.376080	2.353850	-3.926806
1	-2.457625	2.451222	-2.024475
1	-0.894892	3.333181	-2.040094
1	-1.866484	3.232579	-4.356231
1	-0.343011	2.335135	-4.281489
1	-1.912831	1.472960	-4.293832
1	-1.002842	0.469309	-2.237155

Frequencies
65.4321976
96.1373978
175.497299
257.637787
265.871796
380.929993
414.538788
672.644287
817.639221
827.837097
850.644714

857.299194
988.854614
1023.08960
1093.57092
1155.32983
1173.98779
1222.08215
1294.18103
1338.61084
1374.10413
1439.81274
1454.70813
1463.17639
1469.50549
1518.82422
1523.87451
1526.98645
1529.20996
1531.57104
1546.54041
3085.23120
3085.39380
3131.52686
3132.34839
3166.69727
3166.84497
3188.35498
3188.53687
3217.29370
3217.89868
3709.20239

TS-C

6	-4.776431	-2.092771	8.989843
6	-4.143011	-1.997891	7.744049
6	-2.940004	-1.287438	7.653839
6	-2.401253	-0.656788	8.769666
6	-3.050398	-0.741447	9.997965
6	-4.235150	-1.466574	10.105387
6	-4.668734	-2.655837	6.535098
6	-5.945257	-2.817727	6.166853
8	-6.174305	-3.493368	4.960608
6	-6.600669	-2.079001	3.465963
6	-6.859951	-3.117852	2.422450
6	-7.185679	-2.281167	6.784510
6	-7.256755	-0.960400	7.241503

6	-8.451743	-0.433289	7.714103
6	-9.600450	-1.220794	7.725277
6	-9.547395	-2.537629	7.281906
6	-8.347801	-3.072027	6.818718
7	-8.258492	-4.412305	6.317707
8	-6.826577	-0.468603	2.385920
6	-5.603757	0.232716	2.031031
6	-4.823019	-0.607333	1.045802
1	-6.360947	-0.347811	7.223819
1	-8.488334	0.591867	8.067263
1	-10.538540	-0.814599	8.089216
1	-10.438843	-3.158763	7.307224
1	-7.739396	-5.014567	6.954550
1	-9.174219	-4.828380	6.179460
1	-6.988320	-4.048426	5.122390
1	-5.596124	-1.768011	3.717379
1	-7.393560	-1.741250	4.120578
1	-5.973419	-3.734856	2.268319
1	-7.126082	-2.639687	1.477463
1	-7.696813	-3.754284	2.718228
1	-7.409129	0.142696	2.860826
1	-5.029557	0.432681	2.943482
1	-5.899788	1.186385	1.586067
1	-4.497814	-1.555951	1.483756
1	-3.927700	-0.059873	0.738887
1	-5.421182	-0.815078	0.154883
1	-3.929461	-3.072836	5.852910
1	-2.422795	-1.228629	6.699305
1	-1.469867	-0.106431	8.681602
1	-2.627735	-0.256467	10.872096
1	-4.733970	-1.554331	11.065445
1	-5.689263	-2.671655	9.088773

Frequencies

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3808.08960

TS-C’

6	3.160901	-0.404757	-1.396984
6	2.633267	-0.367458	-0.099925
6	3.481385	-0.052804	0.968506
6	4.831050	0.195144	0.746028
6	5.349763	0.139313	-0.544253
6	4.510158	-0.159188	-1.615138
6	1.204865	-0.638040	0.157073
8	0.735627	-0.035860	1.309781
1	3.080943	-0.014445	1.975659
6	0.378132	-1.339001	-0.644049
6	-1.086491	-1.482319	-0.508823
6	-1.876705	-1.370438	-1.663682
6	-3.262119	-1.428195	-1.607460
6	-3.896019	-1.610684	-0.380048
6	-3.136661	-1.766957	0.772744
6	-1.743804	-1.725404	0.710959
6	-0.334135	1.656596	0.797049
6	-1.078902	1.755359	2.086066
8	-1.210693	3.186400	-0.144818
6	-2.124121	2.786809	-1.199001
6	-3.318855	2.100596	-0.576239
7	-0.953602	-1.912314	1.889563
1	-3.626596	-1.956096	1.724629
1	-4.978373	-1.657804	-0.321686
1	-3.846373	-1.333814	-2.516768
1	-1.381055	-1.223523	-2.619666
1	0.814798	-1.786007	-1.531713
1	2.513940	-0.607237	-2.245238
1	4.905942	-0.191330	-2.625168

1	6.403581	0.332867	-0.716920
1	5.480017	0.428071	1.584207
1	0.631706	2.133399	0.694396
1	-0.676004	1.040169	-0.021369
1	-0.402562	1.526946	2.913414
1	-1.931942	1.074024	2.104820
1	-1.438763	2.776744	2.226219
1	0.074338	-0.678524	1.749987
1	-0.531108	3.763238	-0.523579
1	-2.423163	3.694172	-1.730998
1	-1.600212	2.123552	-1.898385
1	-4.044063	1.862239	-1.359021
1	-3.043507	1.158177	-0.093086
1	-3.800518	2.754478	0.155544
1	-1.523990	-2.054585	2.717922
1	-0.331548	-2.714273	1.793229

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Product from TS (Figure 3B)

6	2.133452	-0.468804	0.056702
6	2.699227	0.216861	-1.029488
6	4.060848	0.509281	-1.047698
6	4.873062	0.115274	0.010273
6	4.323942	-0.585700	1.083097
6	2.966670	-0.878519	1.105920
1	2.086775	0.468805	-1.892727
1	4.487846	1.028658	-1.899644
1	5.934700	0.339075	-0.006241
1	4.957813	-0.907481	1.903114
1	2.543654	-1.424879	1.944402
6	0.690314	-0.766127	0.115935
6	-0.276554	0.117665	-0.166341
6	-1.724549	-0.179660	-0.120807
6	-2.196484	-1.453474	-0.463689
6	-3.547871	-1.766412	-0.404720
6	-4.480814	-0.806547	-0.020729
6	-4.049147	0.471933	0.308667
6	-2.693609	0.757871	0.253511
1	-1.486318	-2.196995	-0.808513
1	-3.877273	-2.762579	-0.679375
1	-5.537724	-1.045248	0.013257
1	-4.764521	1.233691	0.607684
7	-2.260195	2.122365	0.640140
8	-0.014411	1.438579	-0.497480
1	-1.287622	2.260749	0.276697
1	0.941706	1.599109	-0.405696
1	-2.254043	2.248201	1.657032
1	-2.868899	2.839879	0.236790
1	0.389637	-1.748025	0.468269ù

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Product from TS-C’ (Figure 3B)

6	-2.944845	1.081749	-0.004856
6	-2.079196	-0.016868	0.078048
6	-2.609239	-1.311301	0.054164
6	-3.980155	-1.501906	-0.064689
6	-4.834997	-0.405436	-0.151238
6	-4.316149	0.886024	-0.120370
6	-0.623993	0.196325	0.206502
8	-0.242913	1.270760	0.984462
6	0.321657	-0.552364	-0.386511
6	1.781844	-0.470109	-0.198874
6	2.519943	0.715564	-0.229969
6	3.893948	0.769956	-0.045973
6	4.587241	-0.414106	0.167184
6	3.894586	-1.622936	0.174270
6	2.519134	-1.647758	-0.011581
7	1.801358	1.973466	-0.521232
1	-1.948803	-2.166850	0.156805
1	1.988110	-2.594372	0.004061
1	4.431064	-2.552771	0.329477
1	5.660969	-0.391531	0.314969
1	4.425510	1.717781	-0.075697
1	-2.550661	2.095387	-0.015535
1	-4.978480	1.742226	-0.194368

1 -5.905684 -0.557768 -0.239194
1 -4.383817 -2.508916 -0.075844
1 -0.975545 1.538414 1.558174
1 2.425347 2.782385 -0.474126
1 1.382779 1.948183 -1.457498
1 1.015707 2.091499 0.158014
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TS addition of water to Ia (Figure 3C)
6 2.114387 -0.174536 0.059613

6	2.812542	1.020364	-0.165252
6	4.199164	0.998972	-0.199601
6	4.888123	-0.198979	-0.012963
6	4.192275	-1.385030	0.210524
6	2.804794	-1.377880	0.247904
1	2.258970	1.941813	-0.308650
1	4.746694	1.919298	-0.373496
1	5.972852	-0.207422	-0.041138
1	4.731145	-2.314845	0.357198
1	2.257815	-2.298931	0.427107
6	0.673255	-0.158777	0.093504
6	-0.470185	0.354852	0.058722
6	-1.886563	0.231510	0.008664
6	-2.799001	1.275925	0.165243
6	-4.159671	1.003956	0.170710
6	-4.613910	-0.305584	0.044916
6	-3.708698	-1.352964	-0.102174
6	-2.342582	-1.106704	-0.135452
1	-2.423647	2.284953	0.272955
1	-4.867279	1.818036	0.282161
1	-5.677724	-0.516534	0.056933
1	-4.065861	-2.373108	-0.205494
7	-1.362916	-2.148271	-0.241656
8	-0.074642	2.727827	-0.070212
1	-0.235049	3.321095	-0.814864
1	0.045530	3.294366	0.702193
1	0.007689	-1.191893	0.126881
1	-1.613108	-2.963987	0.310867
1	-1.224057	-2.448318	-1.205514

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TS addition of water to Ia (Figure 3C)

6	-2.811677	-0.268993	1.223160
6	-2.110478	-0.288057	0.000031
6	-2.812147	-0.261822	-1.222695
6	-4.195978	-0.219416	-1.214984
6	-4.882502	-0.202561	0.000824
6	-4.195523	-0.226598	1.216241
6	-0.709586	-0.328021	-0.000343
8	-0.652532	2.573460	-0.001427
1	-2.258319	-0.287940	2.156149
6	0.521531	-0.522188	-0.000762
6	1.888324	-0.023201	0.000322
6	2.312761	1.302729	0.002873
6	3.681669	1.555994	0.003560
6	4.606011	0.511534	0.001736
6	4.184657	-0.818456	-0.000850
6	2.824161	-1.069593	-0.001529
1	1.575164	2.099122	0.004145
1	4.034271	2.582038	0.005542
1	5.668216	0.732062	0.002316
1	4.905177	-1.630054	-0.002281
7	2.196467	-2.373750	-0.004110
1	-2.259144	-0.275261	-2.155992
1	-4.745115	-0.201305	-2.150034
1	-5.967596	-0.171195	0.001121
1	-4.744289	-0.214022	2.151600
1	-0.925526	3.094817	-0.765308

1	-0.932451	3.093471	0.760864
1	0.892232	-1.781461	-0.003180
1	2.397646	-2.928330	-0.834983
1	2.397378	-2.931484	0.824714

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TS-D

6	3.843660	0.244127	-1.024516
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6	3.688880	-0.942440	1.072781
6	5.064139	-1.143918	1.052277
6	5.847385	-0.663722	-0.000280

6	5.218053	0.036523	-1.032637
16	1.313754	-0.024890	0.023158
8	0.888043	0.028688	1.435525
6	7.334492	-0.913395	-0.032605
8	0.779482	-1.239488	-0.688828
8	1.036584	1.206242	-0.739474
6	-1.880825	-0.569167	-0.532997
6	-2.096396	0.685842	-0.422678
6	-2.019351	2.055010	-0.186115
6	-1.179212	2.511873	0.855179
6	-1.074422	3.875537	1.080715
6	-1.801853	4.768646	0.296343
6	-2.635637	4.321117	-0.734949
6	-2.737736	2.967589	-0.989467
6	-2.744263	-1.707522	-0.251840
6	-2.322944	-3.010496	-0.519802
6	-3.205537	-4.068666	-0.347020
6	-4.503610	-3.821962	0.096805
6	-4.915064	-2.529096	0.406624
6	-4.032133	-1.461942	0.253241
7	-4.366759	-0.121354	0.543648
1	-1.307729	-3.172084	-0.868754
1	-5.916325	-2.350181	0.789635
1	-5.198654	-4.646356	0.224184
1	-2.886478	-5.082171	-0.565978
1	-0.797148	-0.797344	-0.854835
1	-3.369679	2.587564	-1.784911
1	-3.187490	5.035027	-1.337072
1	-1.714636	5.835335	0.482331
1	-0.416509	4.243843	1.860204
1	-0.591600	1.787962	1.415542
1	-5.363513	0.023070	0.661248
1	-3.886556	0.225031	1.369798
1	3.082465	-1.300203	1.898263
1	5.539273	-1.678764	1.871299
1	5.814217	0.429771	-1.852735
1	3.355467	0.801018	-1.817383
1	7.864549	-0.104083	-0.544581
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1	7.562534	-1.844345	-0.565904

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TS-A

6	1.275539	0.829954	1.581215
6	0.280859	-0.138165	1.378950
6	0.597724	-1.462532	1.724643
6	1.833137	-1.787666	2.271450
6	2.790589	-0.805942	2.482106
6	2.505823	0.509369	2.132732
6	-0.995798	0.304002	0.745688
8	-2.155046	-0.976852	0.969240
7	-0.370481	-2.540357	1.495815
7	-0.906180	-0.136017	-0.992736
6	-0.690966	-1.494135	-1.410497
6	0.630115	-1.938549	-1.603308
6	0.836294	-3.290922	-1.916724
6	-0.240002	-4.159440	-2.047238
6	-1.544022	-3.690748	-1.883821
6	-1.768991	-2.357806	-1.565605
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900.047485
902.632996
916.249878
927.989014
938.193298
957.010376
987.464600
988.231079
1011.57568

1026.99170
1029.17871
1041.87183
1043.50317
1047.95947
1049.82007
1061.51123
1070.51025
1077.03259
1078.70752
1083.43665
1088.17566
1120.19678
1131.84607
1140.39014
1157.94958
1188.95764
1198.25696
1213.64075
1224.26575
1233.34851
1239.94299
1240.18982
1240.92651
1248.79724
1255.01025
1287.63965
1312.02393
1328.34338
1338.73376
1347.64722
1355.28564
1361.03601
1372.34717
1385.28088
1398.40149
1404.86584
1409.94788
1513.92224
1518.49976
1535.32581
1536.39160
1556.94971
1557.60437
1564.30334
1575.37476
1640.82410
1646.20862

1647.15601
1656.03674
1669.17676
1679.43860
1682.71008
1691.91870
1699.69336
1707.66455
1749.98474
1937.05090
3191.76392
3192.41919
3202.30371
3206.34009
3211.28882
3213.60327
3215.73193
3220.12012
3221.96704
3223.54468
3227.26392
3230.87549
3235.06909
3235.45874
3237.10791
3240.00195
3247.96460
3249.03687
3396.62378
3581.61011
3693.99951
3750.38721

IV. Details of NCI analysis and RESP analysis

In the Figure S1 we report the comparison of the NCI 3D representations for the TSs involved in the initial 1a-Ia addition (see Figure 2A of the main text).

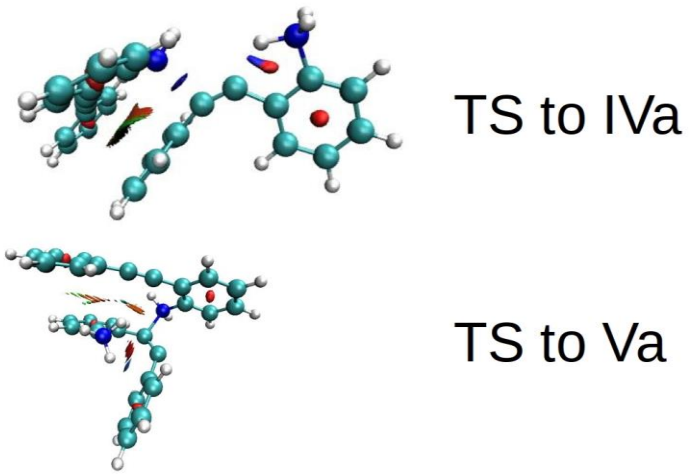


Figure S1. NCI 3D representations of the TSs involved in the 1a to Ia addition.

We observe that the two TSs are rather different. In fact, the two C-N covalent bonds, involved in the reaction, are both recognized as non-covalent strong interactions in the TS leading to Iva. On the other hand, the same C-N bonds are recognized as covalent strong, hence stronger, interactions in the TS leading to Va.

NCI analysis carried in the two high-energy TSs of the Figure 3 (i.e. TS-A and TS-B) reported in the Figure S2 shows large regions of sharp repulsive clash between the two interacting moieties. In the less stable TS-A the repulsive region appears as much larger than in TS-B. This finding could somewhat explain the difference between the two observed barriers.

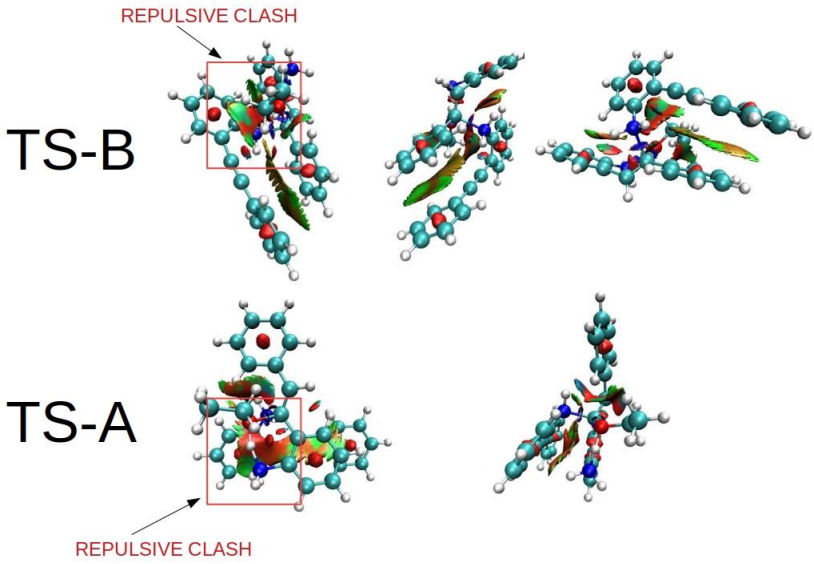


Figure S2. NCI 3D representations for TS-A (2 different views) and TS-B (three different views).

NCI analysis carried also on the two TS-D involved in the formation of 5a from 1a (see Figure 4 of the main text) produced the result reported in the Figure S3.

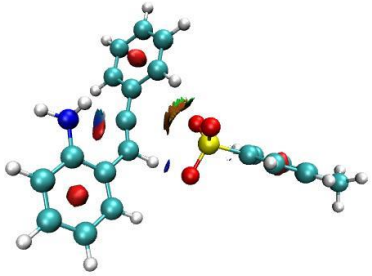


Figure S3. NCI 3D representation of TS-D (see Figure 4 of the main text).

The result nicely indicates the simultaneous presence of two strongly attractive (blue region) NCI in the regions corresponding to the proton-transfer and the ring-closure.

In the Figure S4 we report the results of the RESP analysis carried out on some of the key intermediates of the reactions reported in the Figures 2 and 3 of the main text.

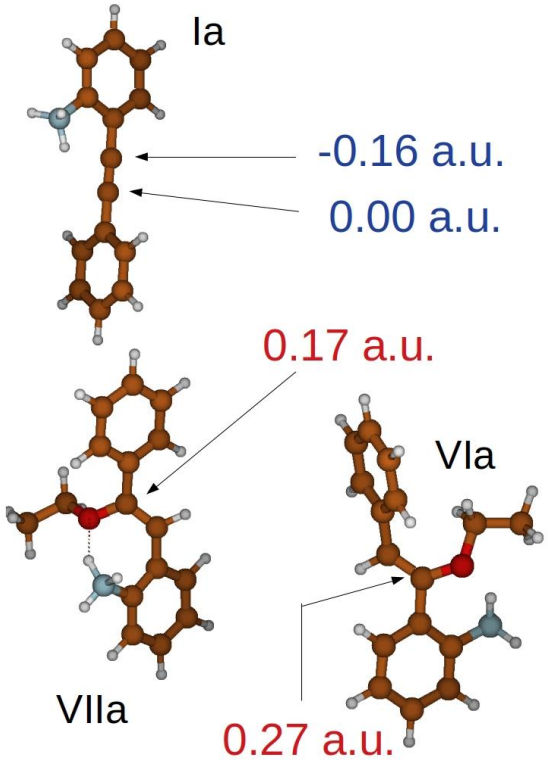


Figure S4. RESP charges for the species Ia, VIa and VIIa