Molecular Sensors for Biological Applications

Nsikak Bassey Essien

Thesis submitted in part fulfilment of the requirements for the degree of Doctor of Philosophy

University of Sussex

January 2023

Contents

S1 – Supporting information for Chapter 2 – Asymmetric salan fluorescent selective Cu^{2+} sensors

Characterisation data

Half unit.

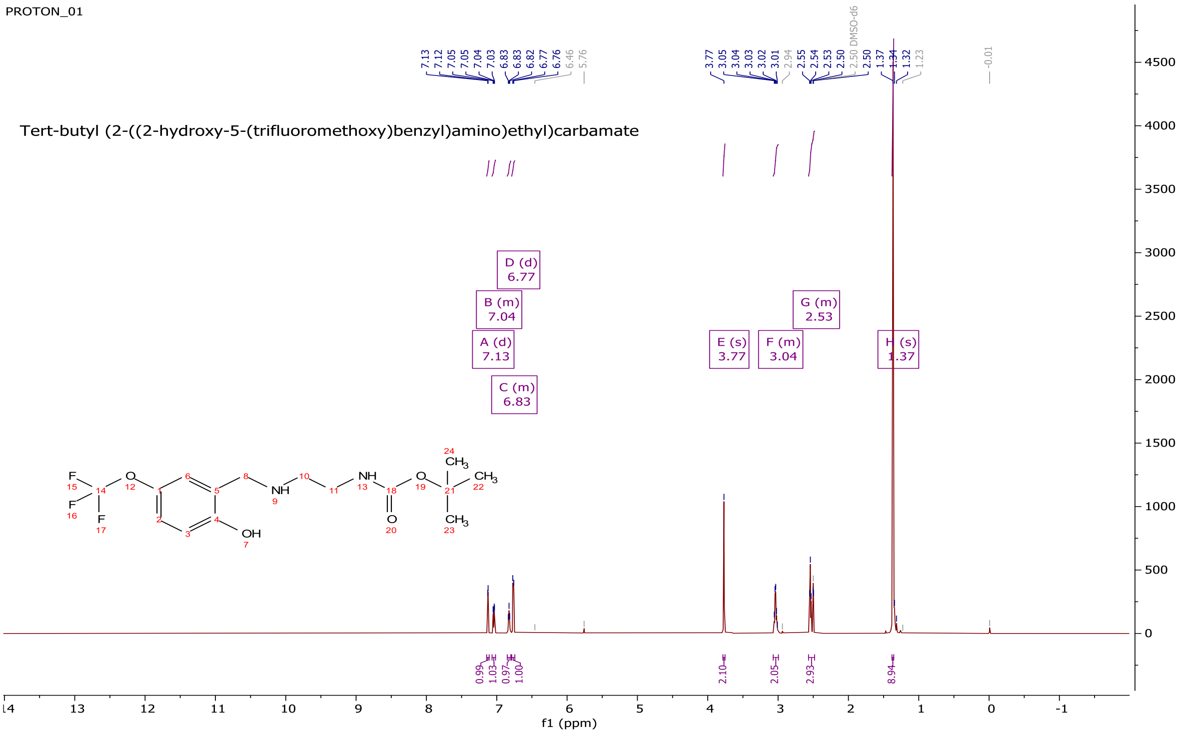


Figure S1-1. [1]H NMR of the first intermediate for **OF-nap**.

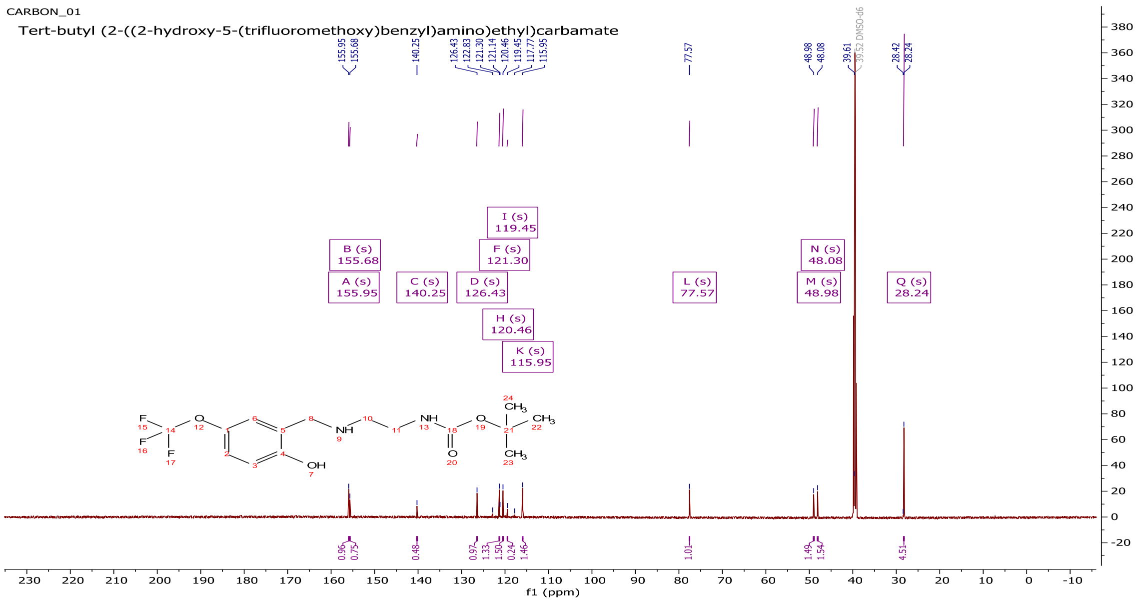


Figure S1-2. [13]C NMR of the first intermediate for **OF-nap**.

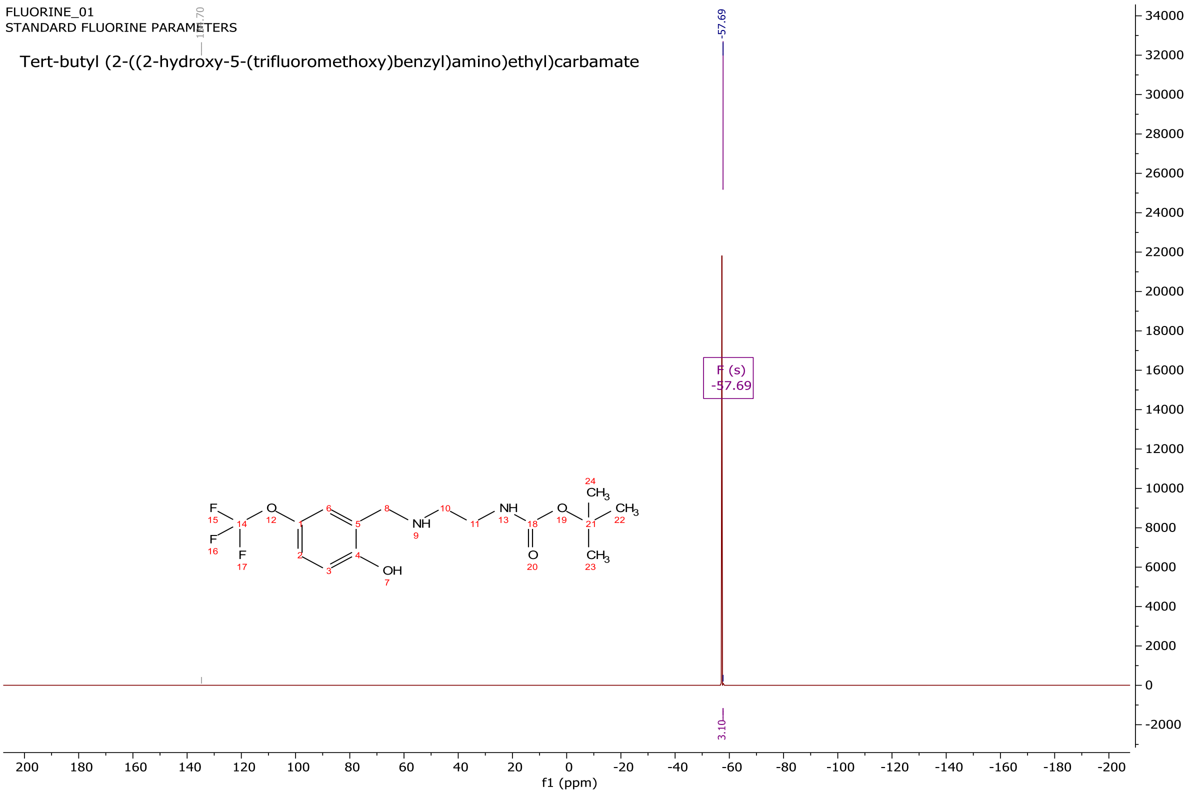


Figure S1-3. ^{19}F NMR of the first intermediate for **OF-nap**.

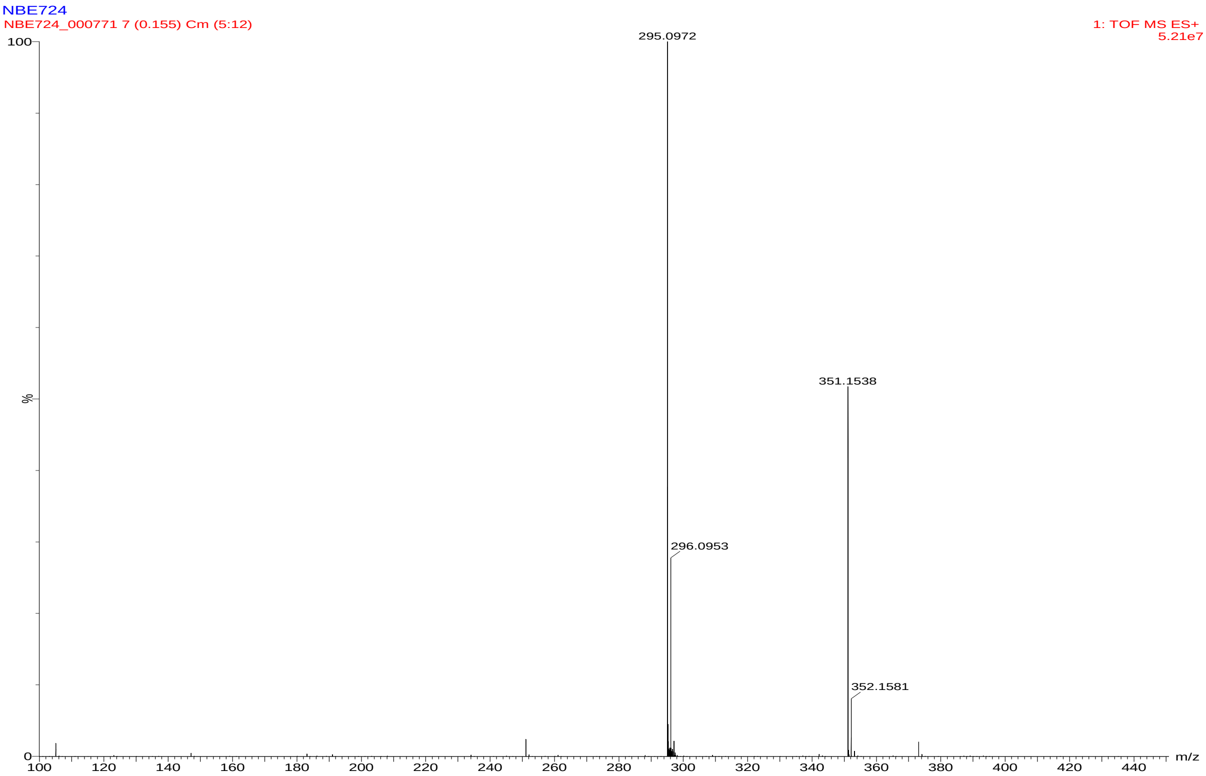


Figure S1-4. TOF MS ES+ of the first intermediate for **OF-nap**.

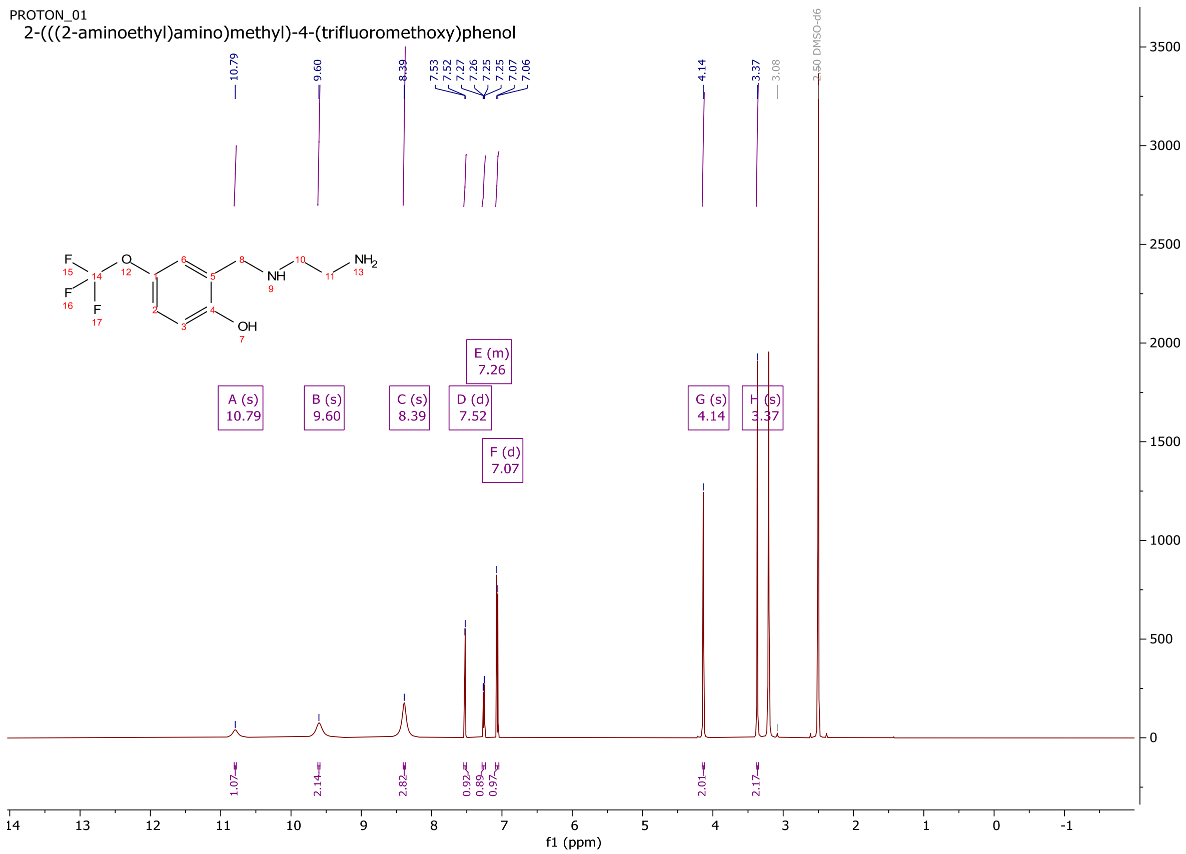


Figure S1-5. ^{1}H NMR of the second intermediate for **OF-nap**.

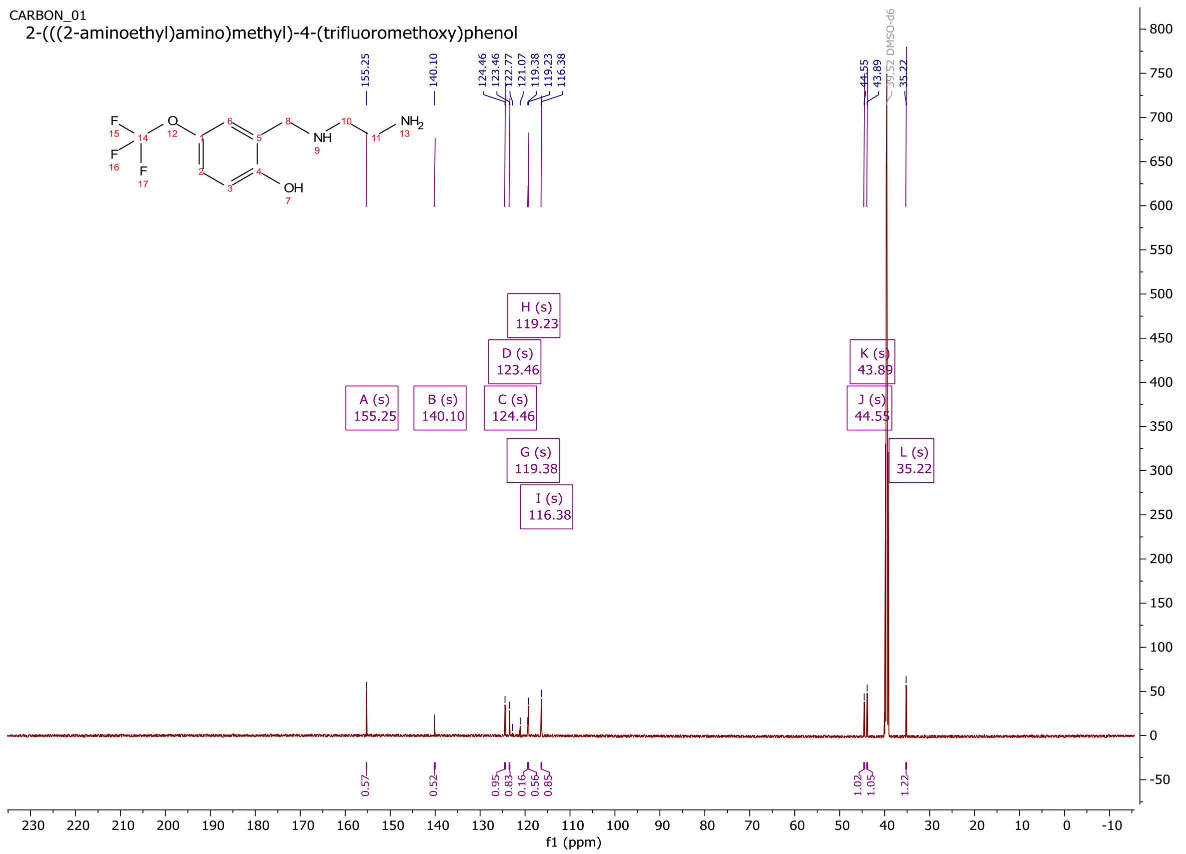


Figure S1-6. ^{13}C NMR of the second intermediate for **OF-nap**.

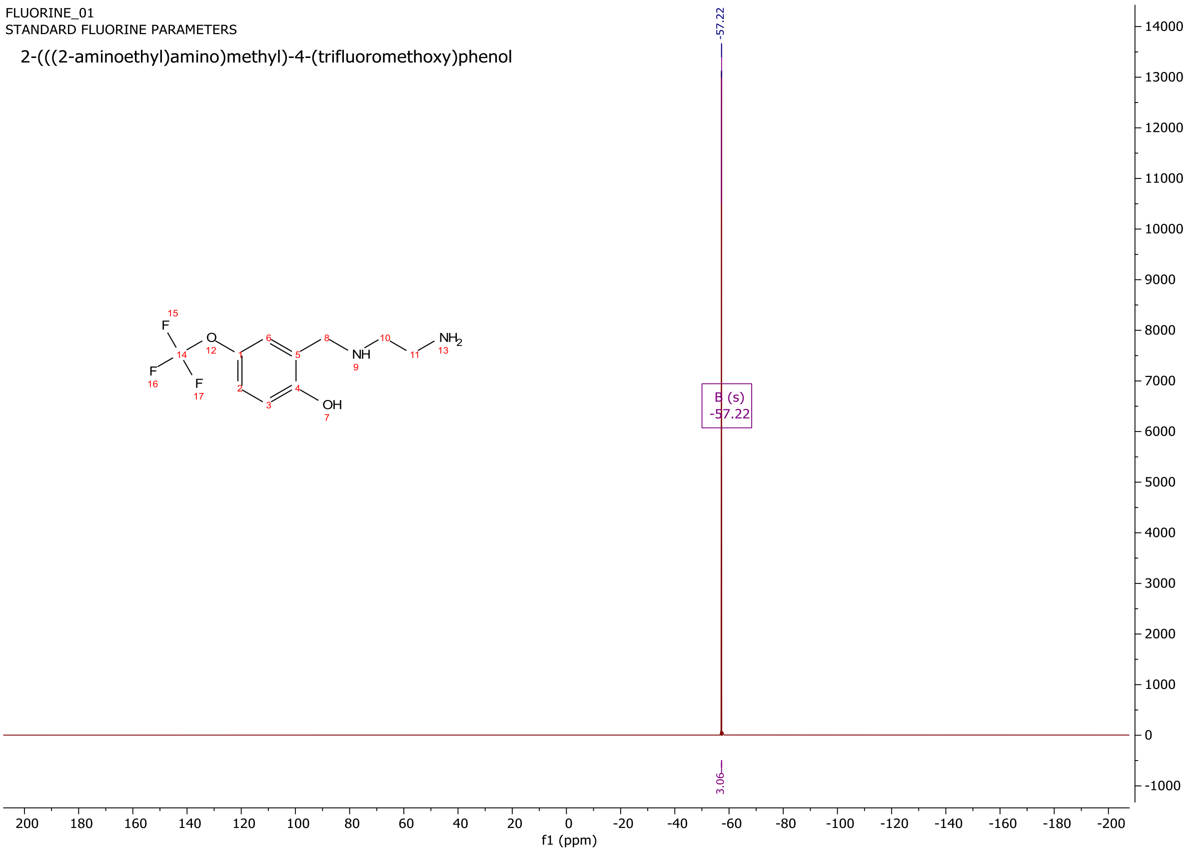


Figure S1-7. ^{19}F NMR of the second intermediate for **OF-nap**.

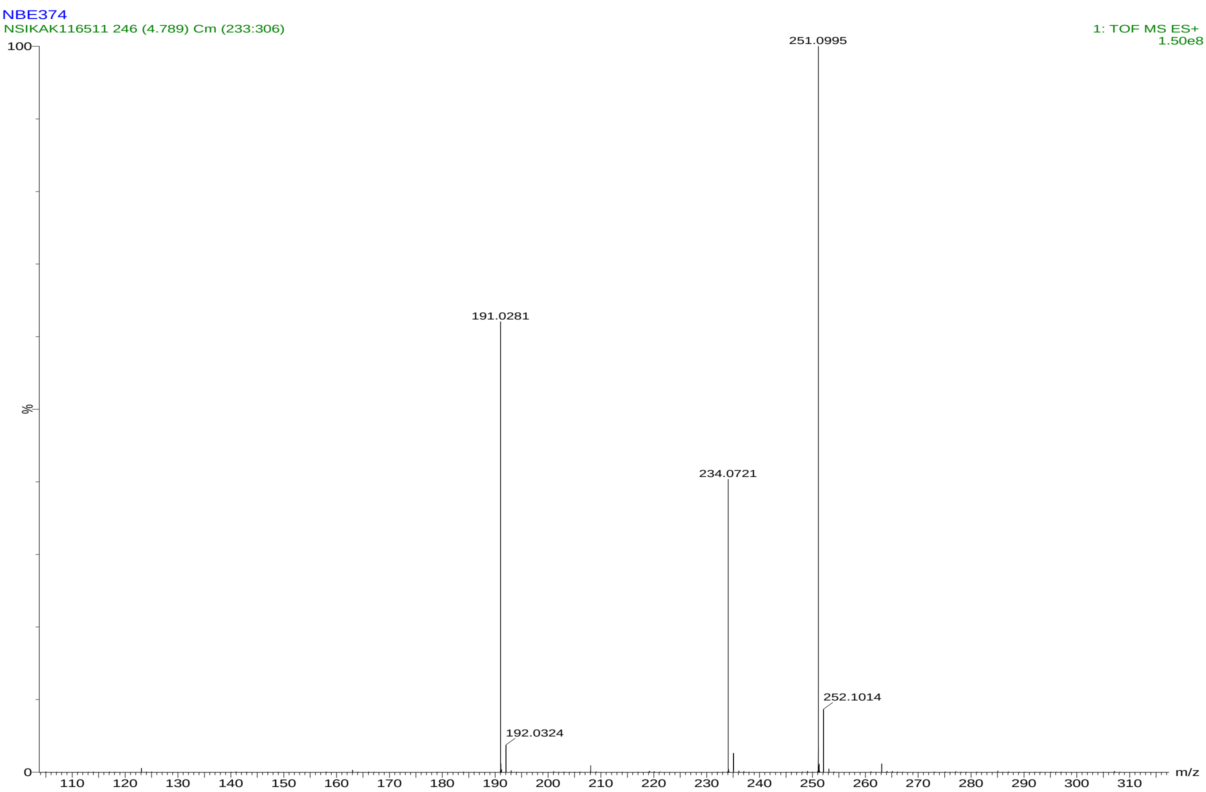


Figure S1-8. TOF MS ES+ of the second intermediate for **OF-nap**.

OF-nap.

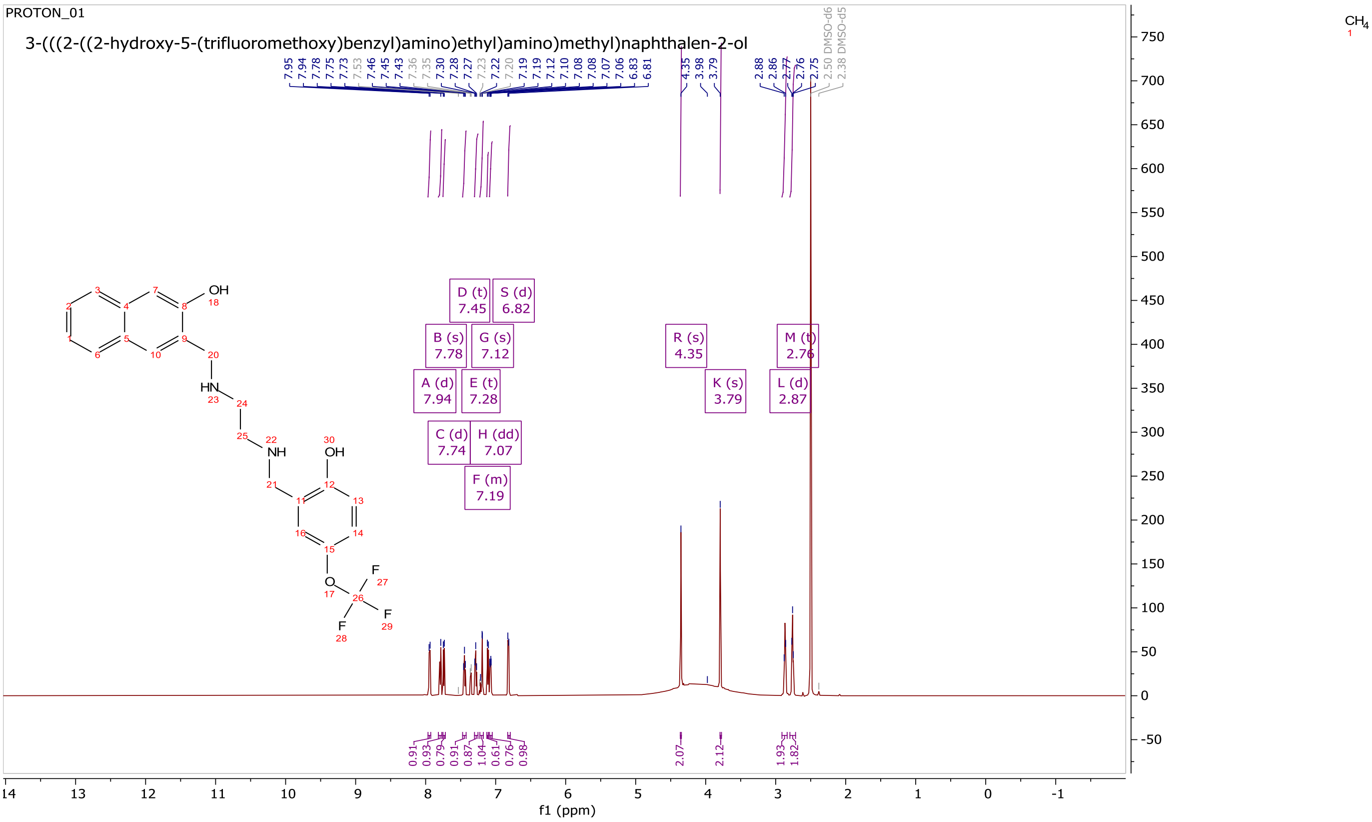


Figure S1-9. ^{1}H NMR for **OF-nap**.

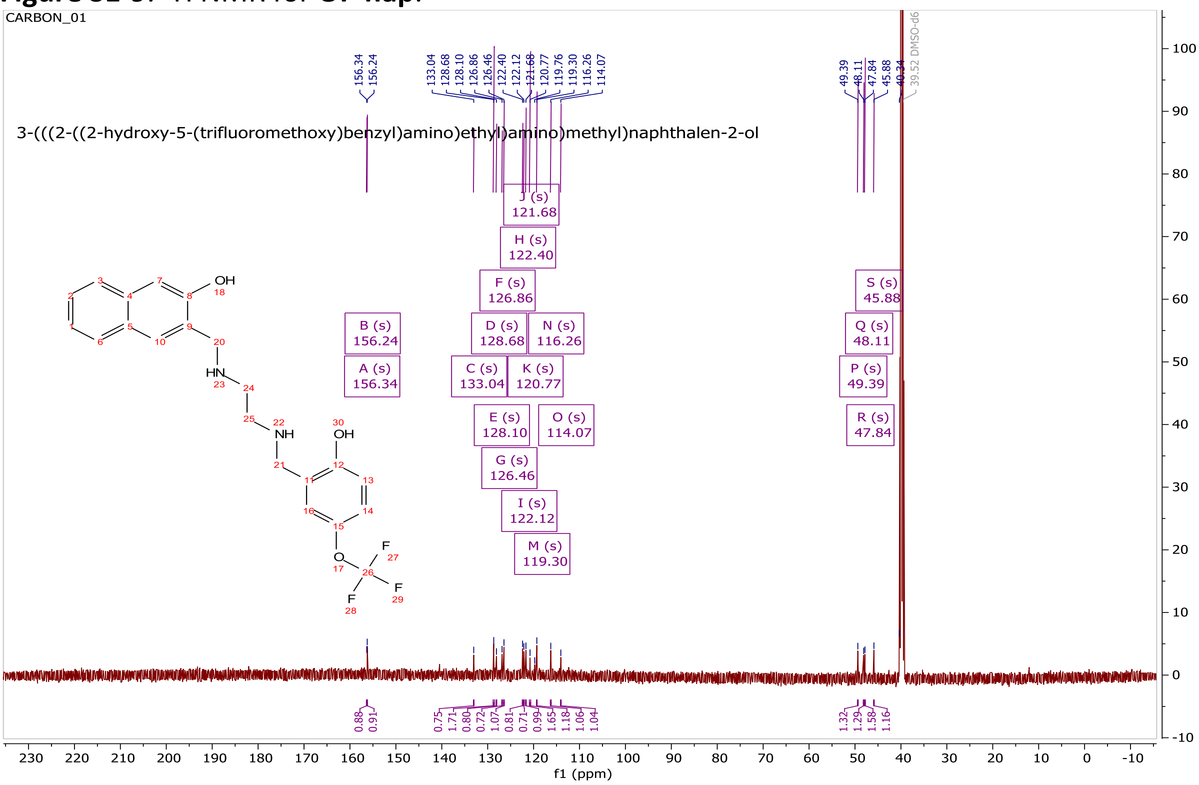


Figure S1-10. ^{13}C NMR for **OF-nap**.

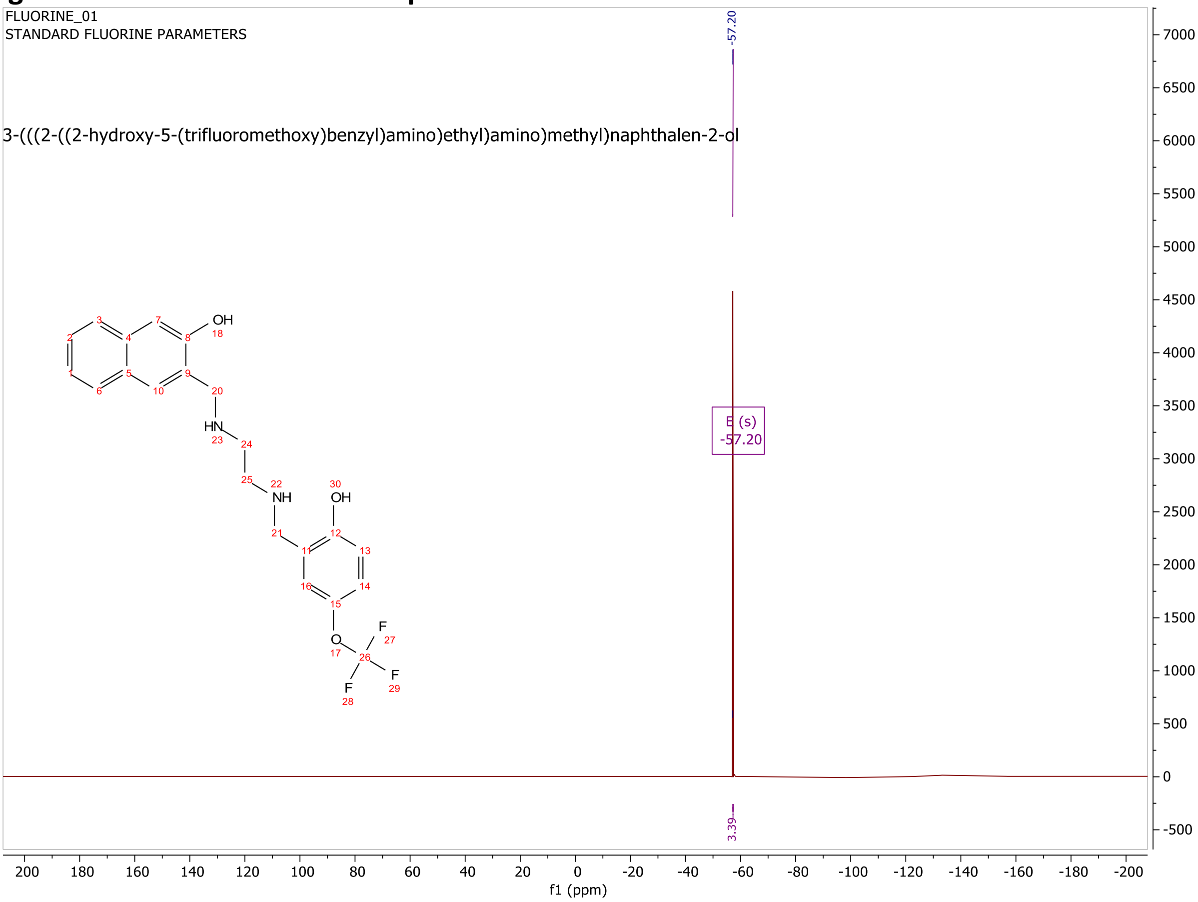


Figure S1-11. ^{19}F NMR for **OF-nap**.

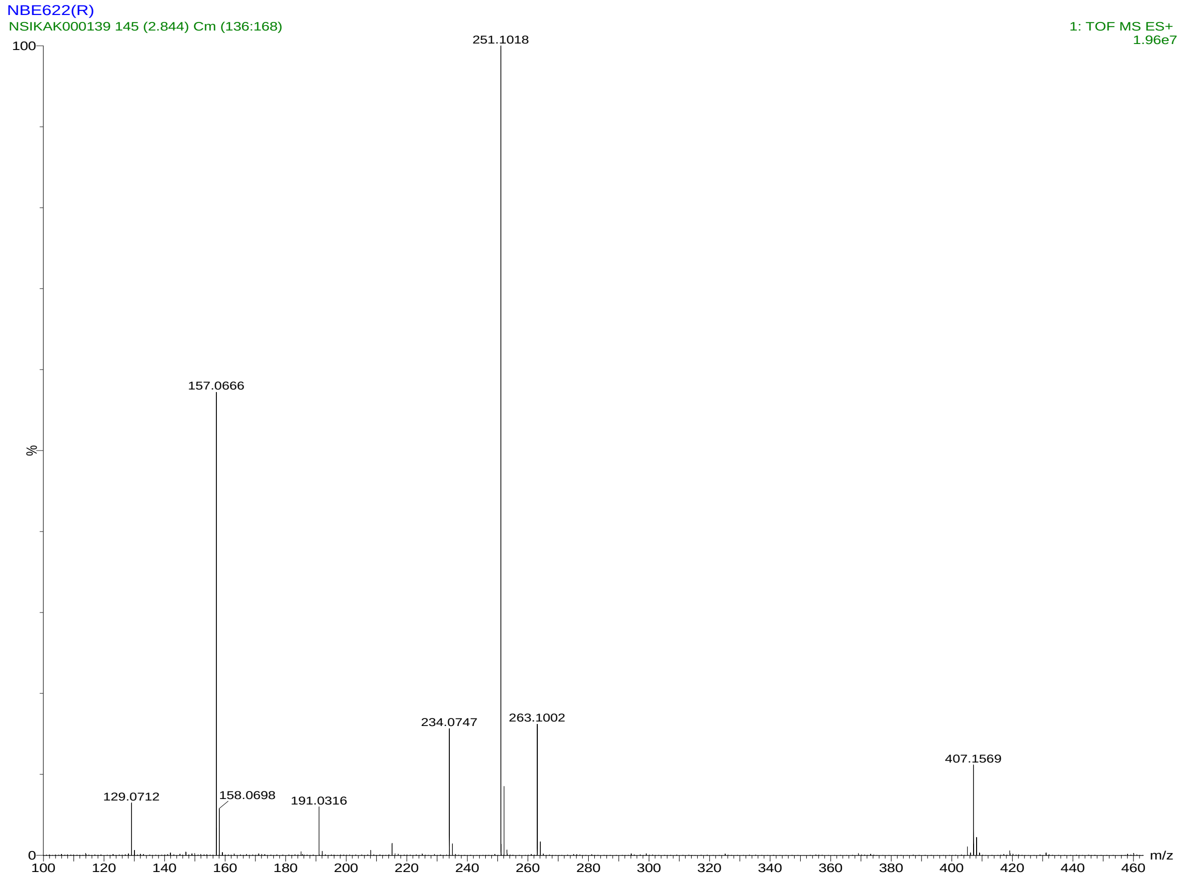


Figure S1-12. TOF MS ES+ for **OF-nap**.

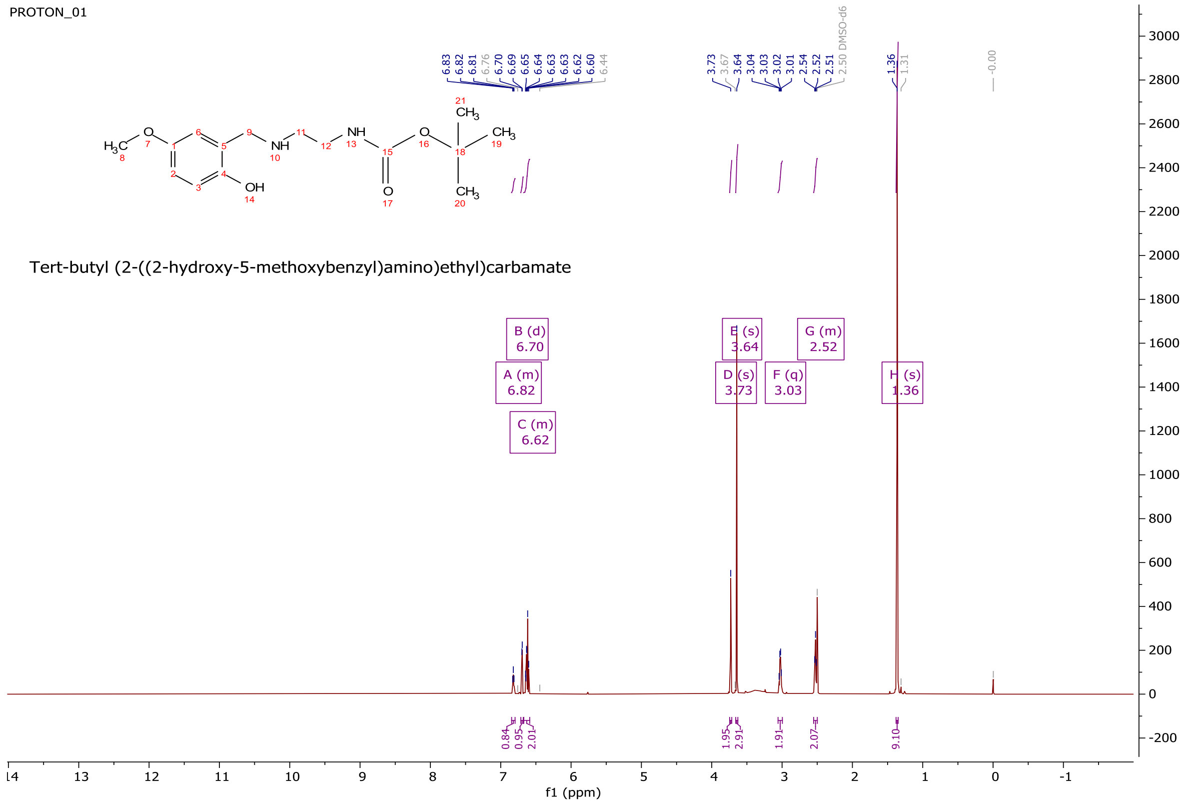


Figure S1-13 ^{1}H NMR of the first intermediate for **OH-nap**.

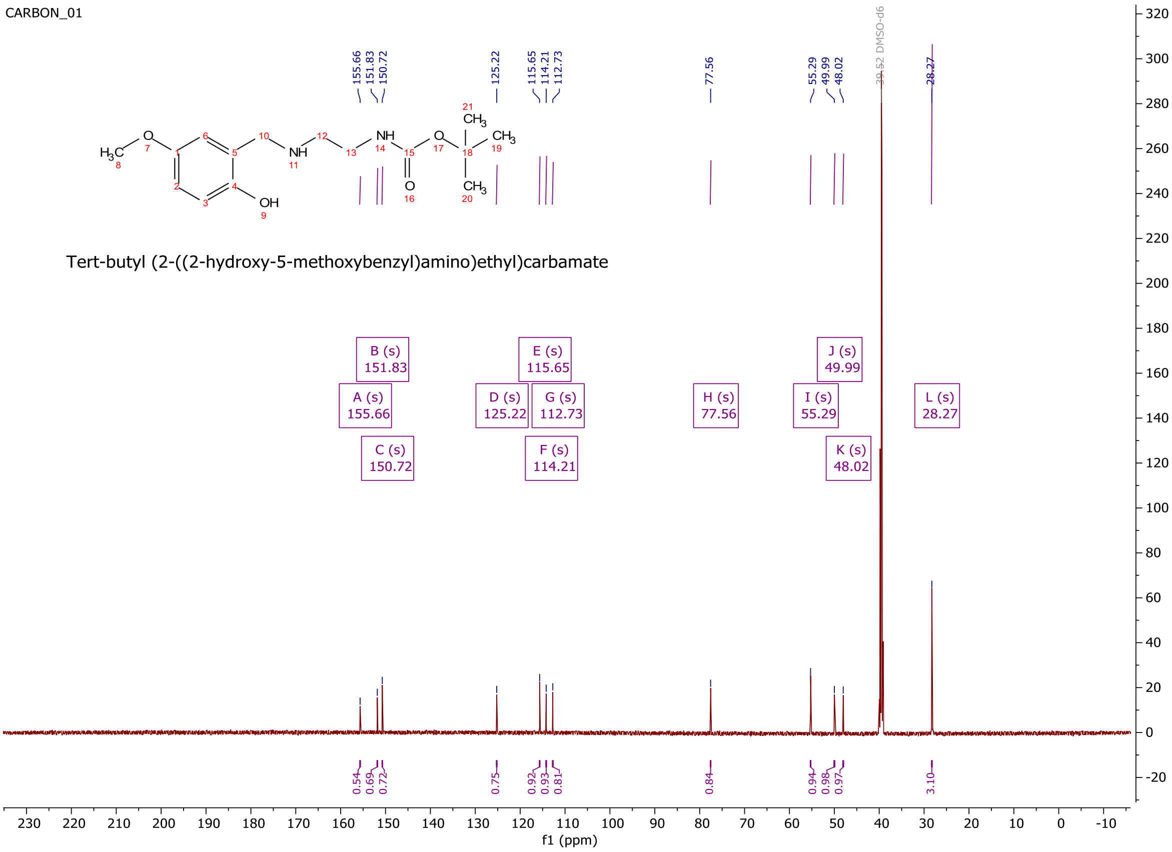


Figure S1-14. ^{13}C NMR of the first intermediate for **OH-nap**.

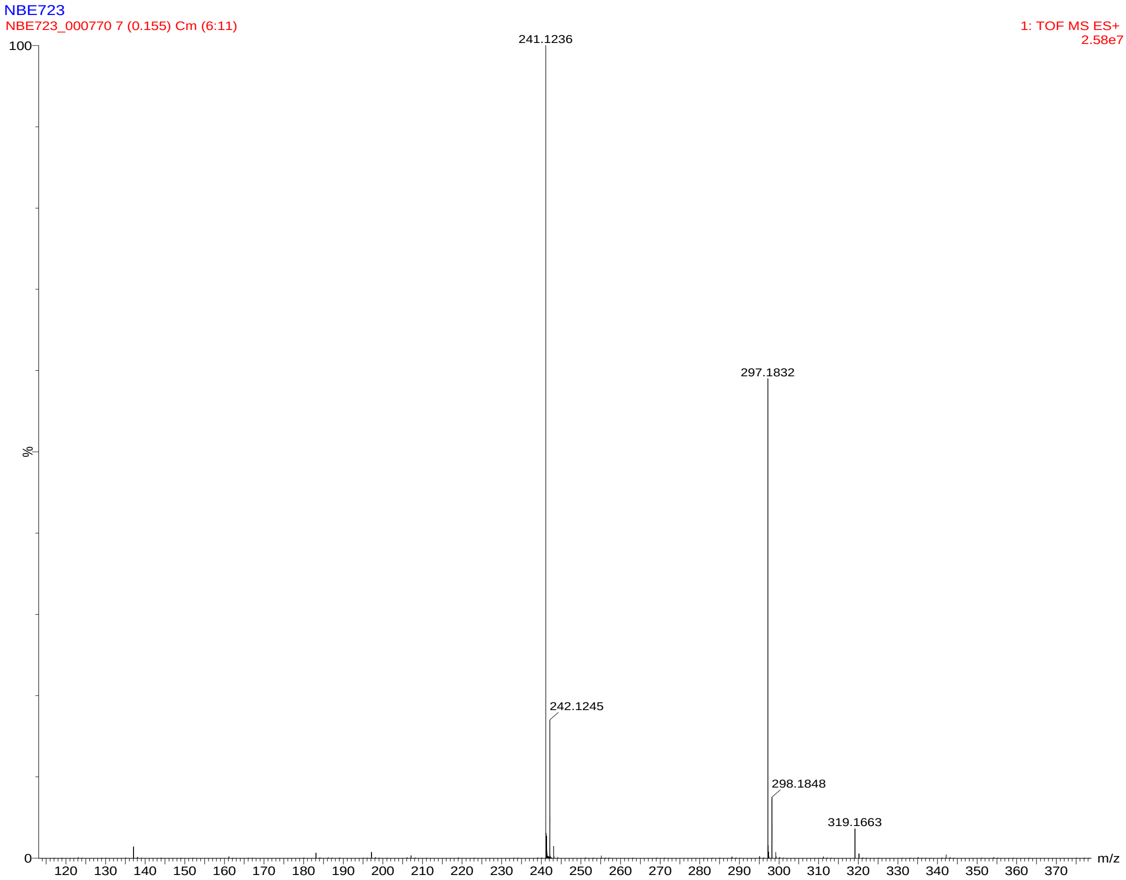


Figure S1-15. TOF MS ES+ of the first intermediate for **OH-nap**.

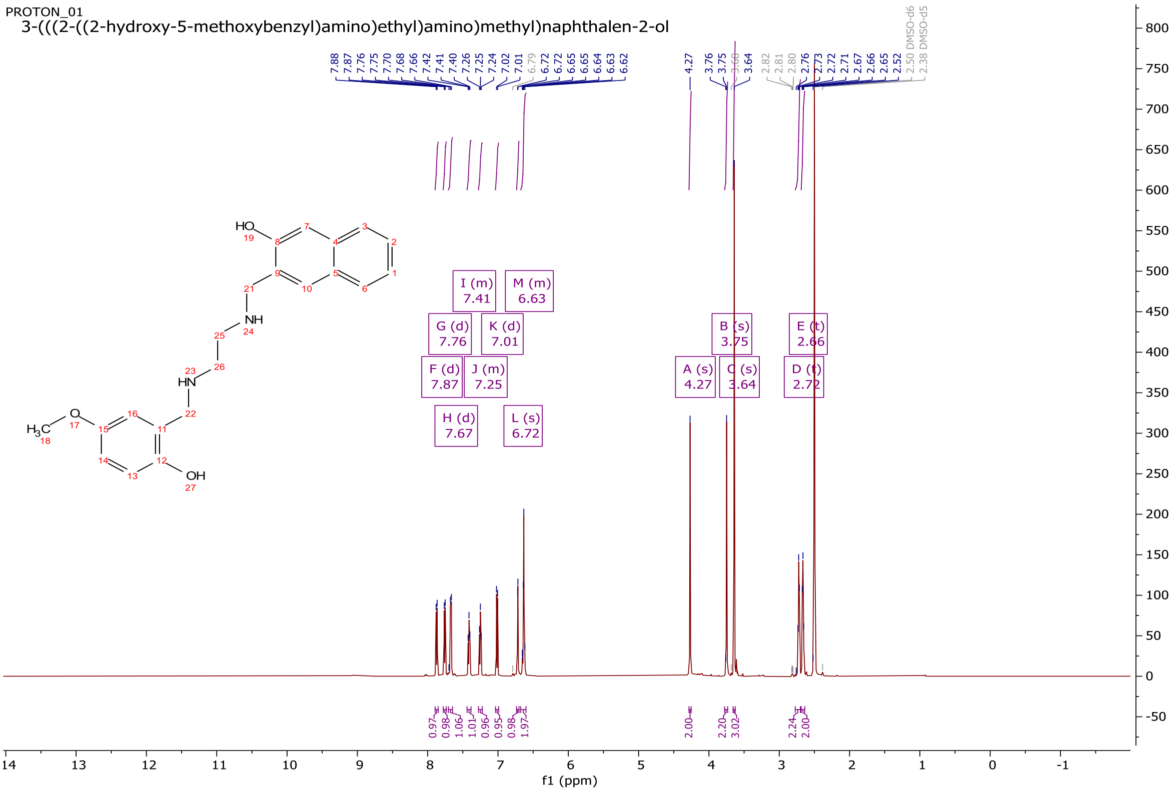


Figure S1-16. ^{1}H NMR for **OH-nap**.

OH-nap.

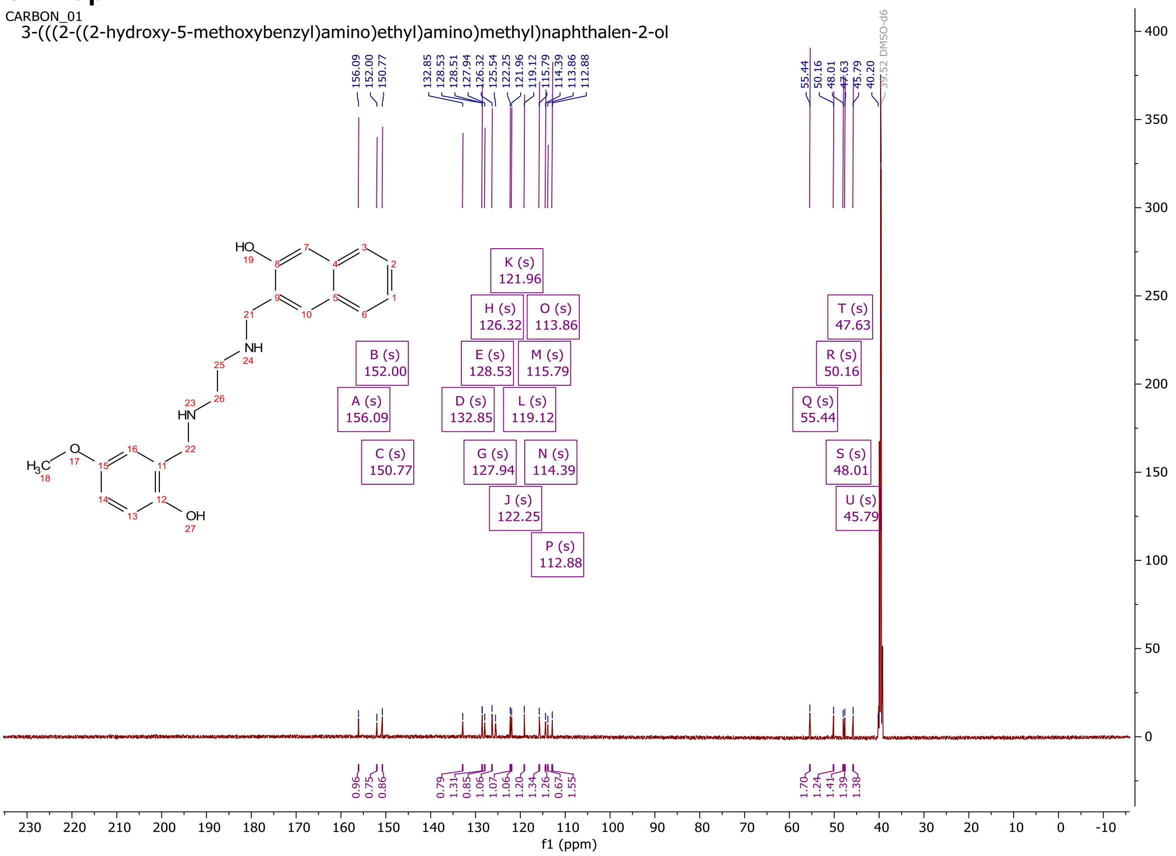


Figure S1-17. ^{13}C NMR for **OH-nap**.

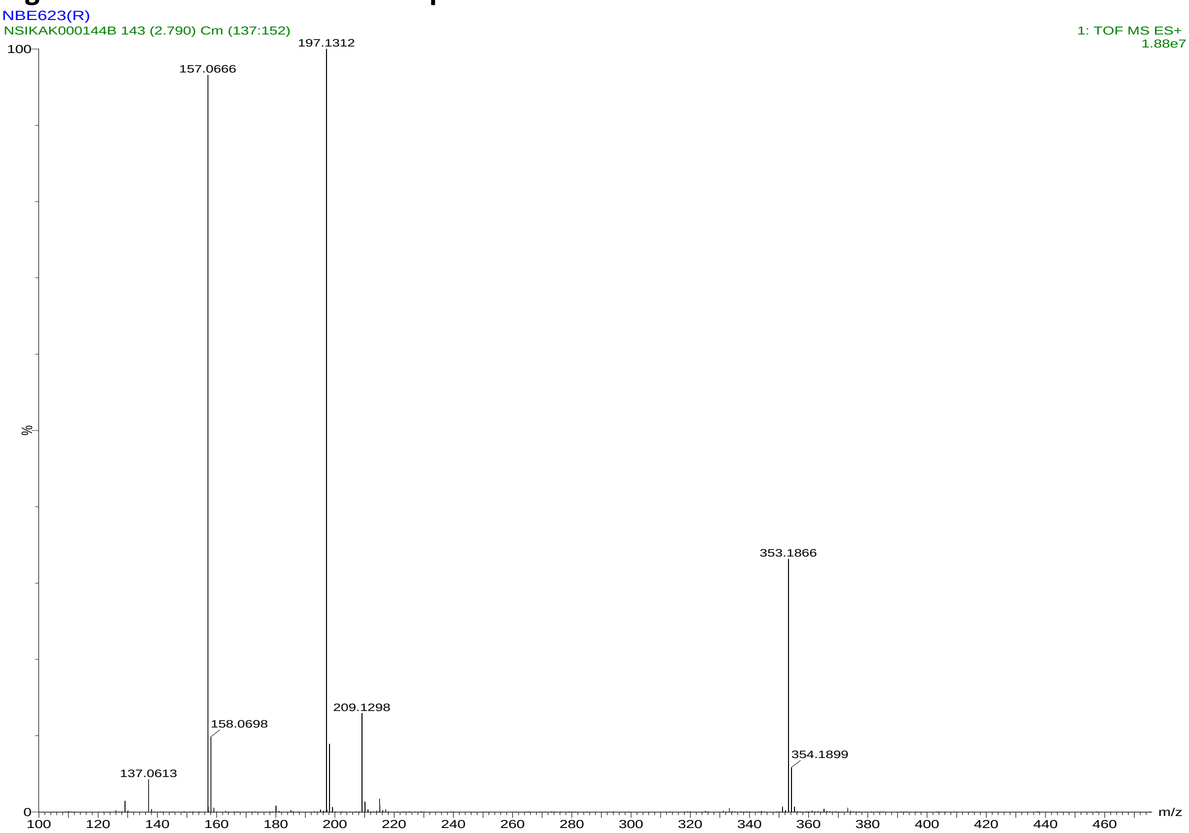


Figure S1-18. TOF MS ES+ for **OH-nap**.

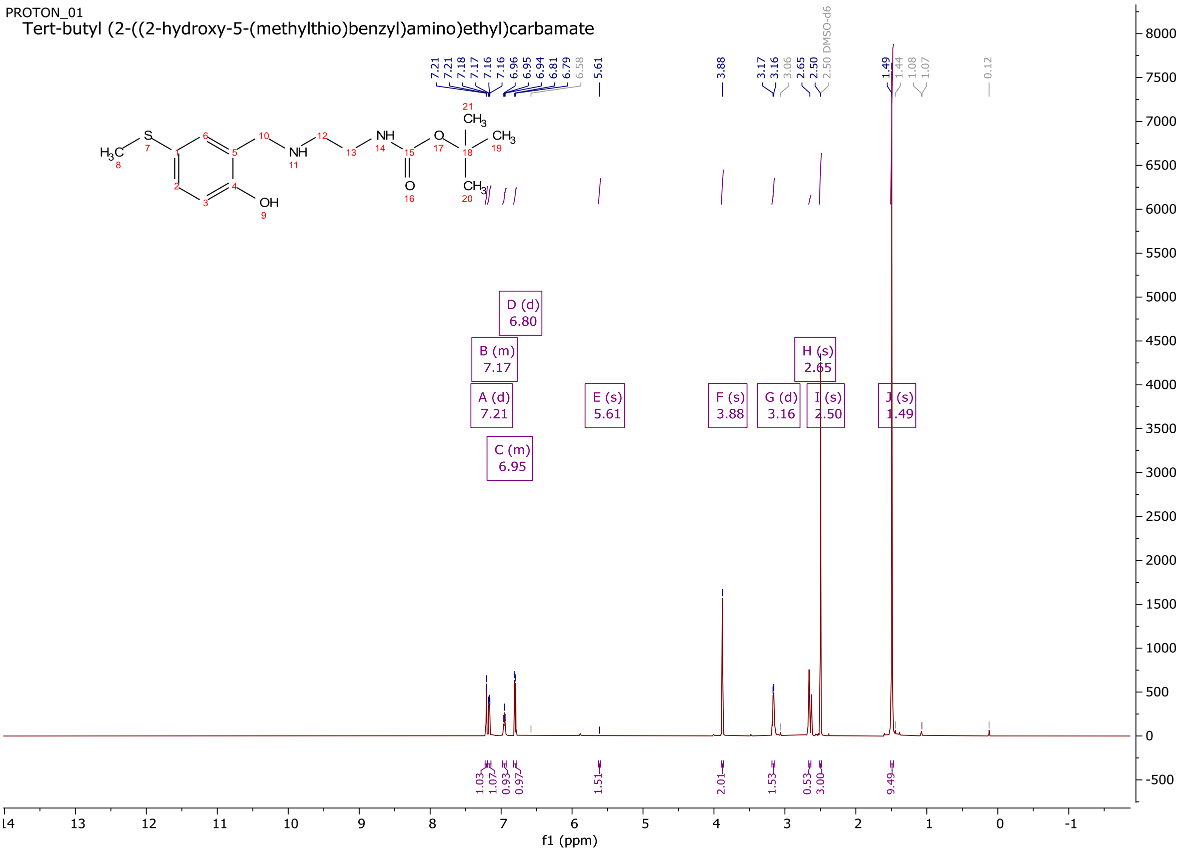


Figure S1-19. ^{1}H NMR of the first intermediate for **SH-nap**.

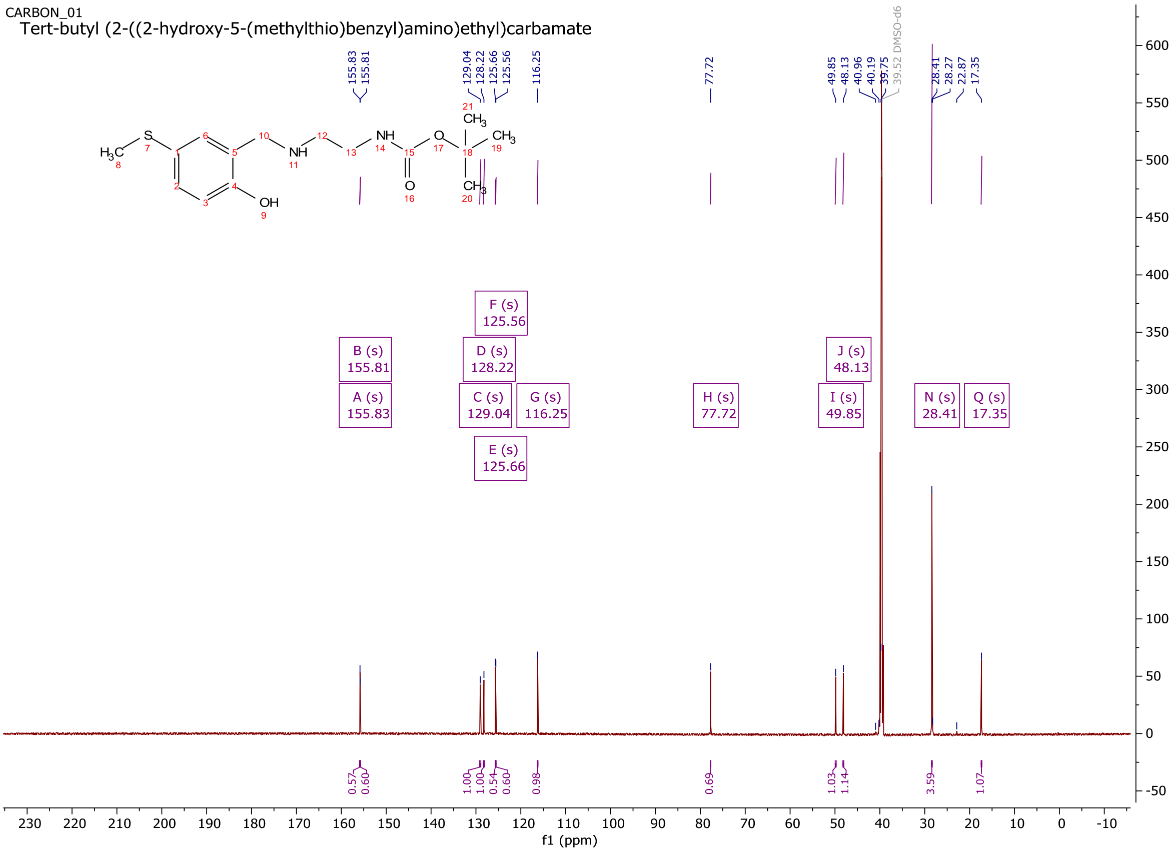


Figure S1-20. ^{13}C NMR of the first intermediate for **SH-nap**.

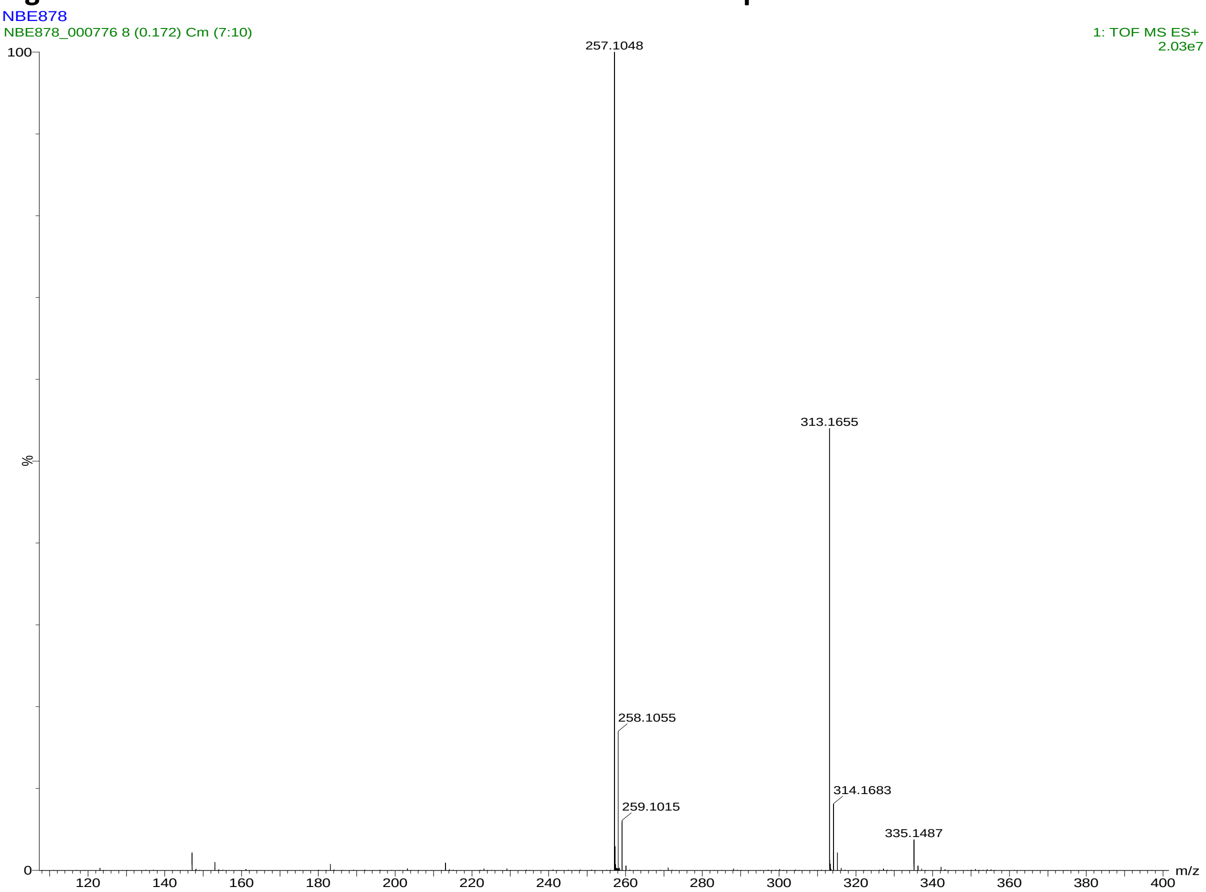


Figure S1-21. TOF MS ES+ of the first intermediate for **SH-nap**.

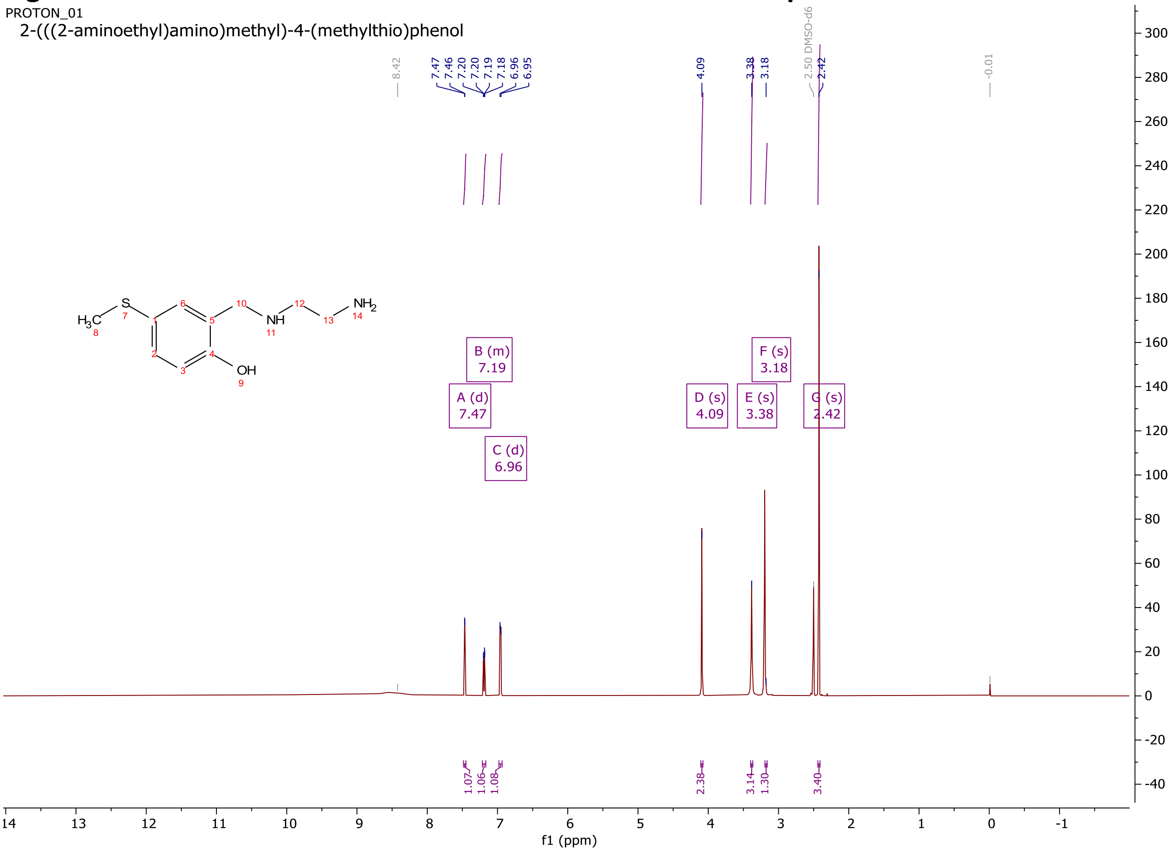


Figure S1-22. ^{1}H NMR of the second intermediate for **SH-nap**.

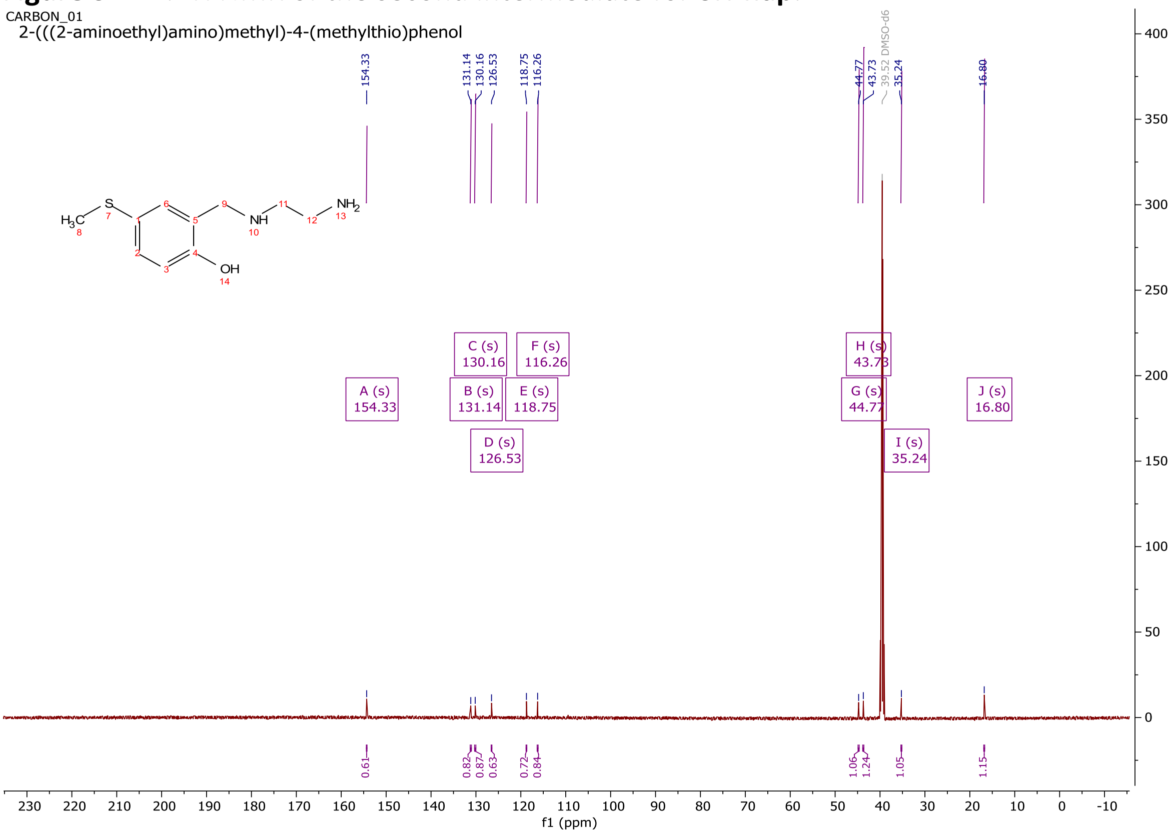


Figure S1-23. ^{13}C NMR of the second intermediate for **SH-nap**.

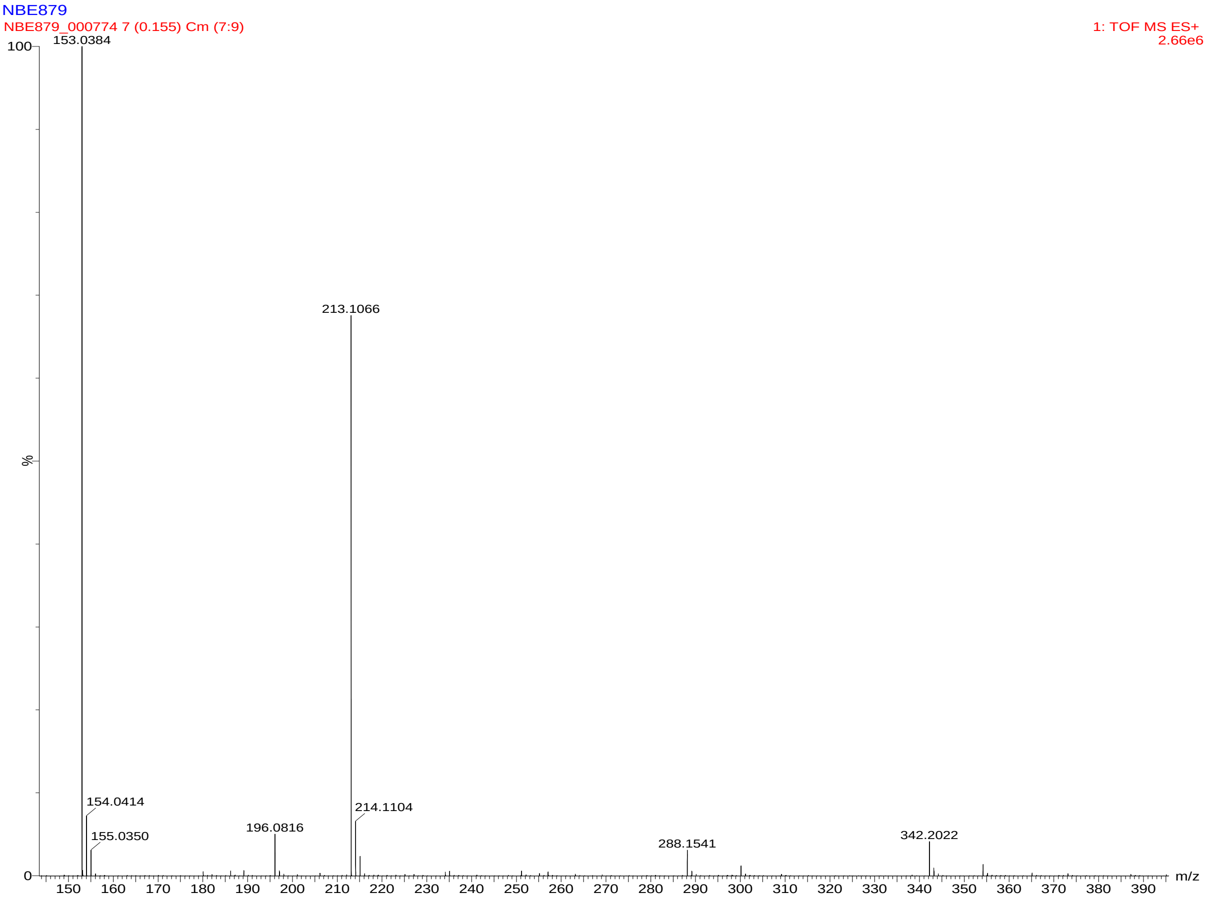


Figure S1-24. TOF MS ES+ of the second intermediate for **SH-nap**.

SH-nap.

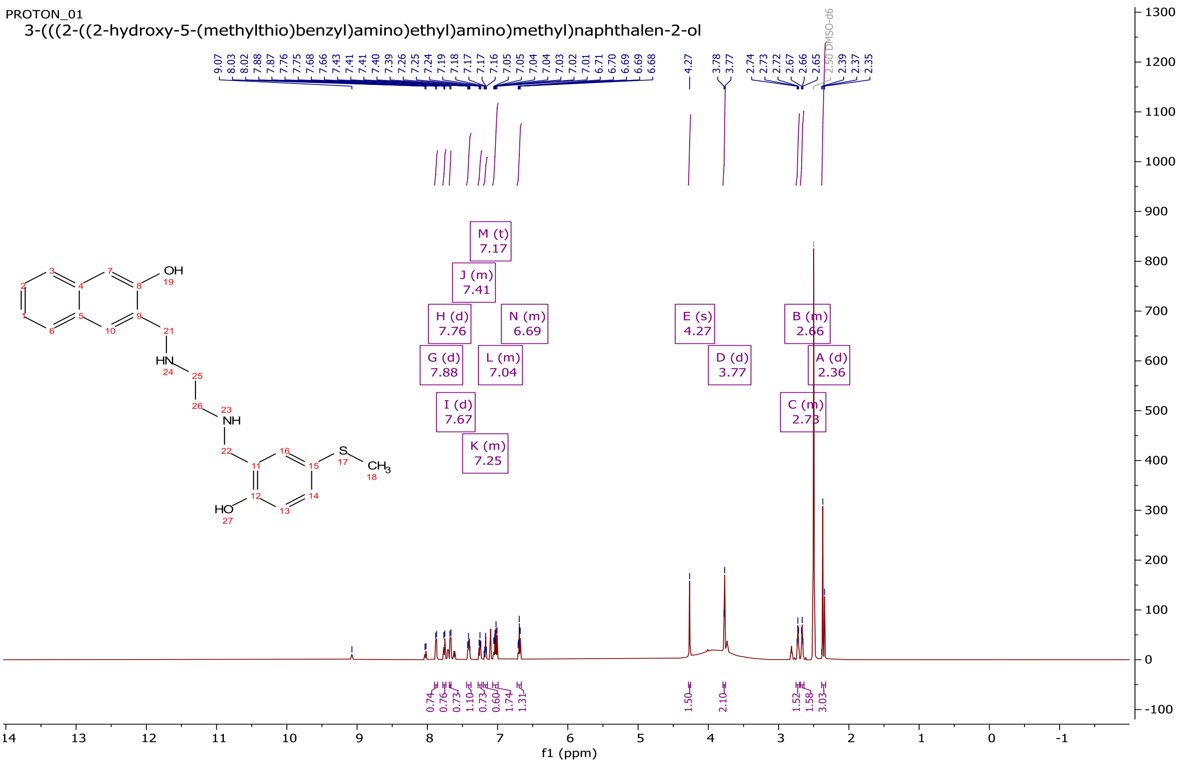


Figure S1-25. ^{1}H NMR for **SH-nap**.

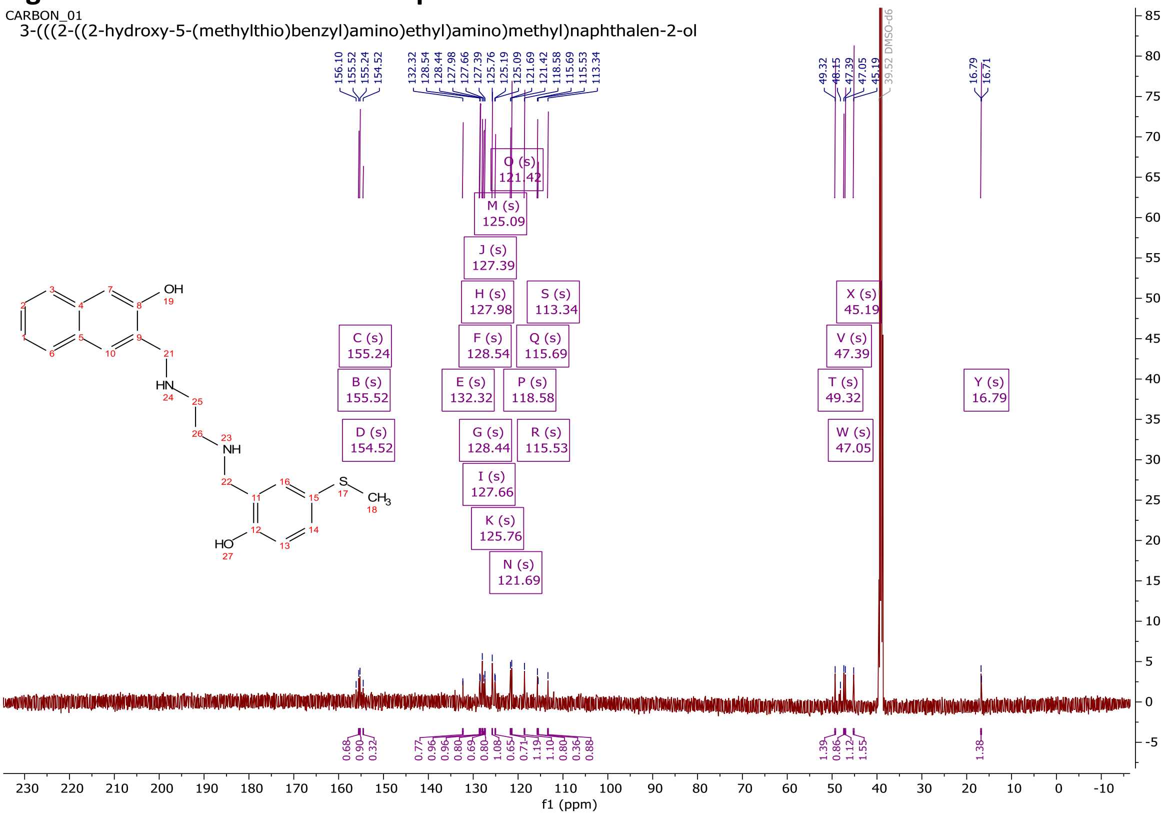


Figure S1-26. ^{13}C NMR for **SH-nap**.

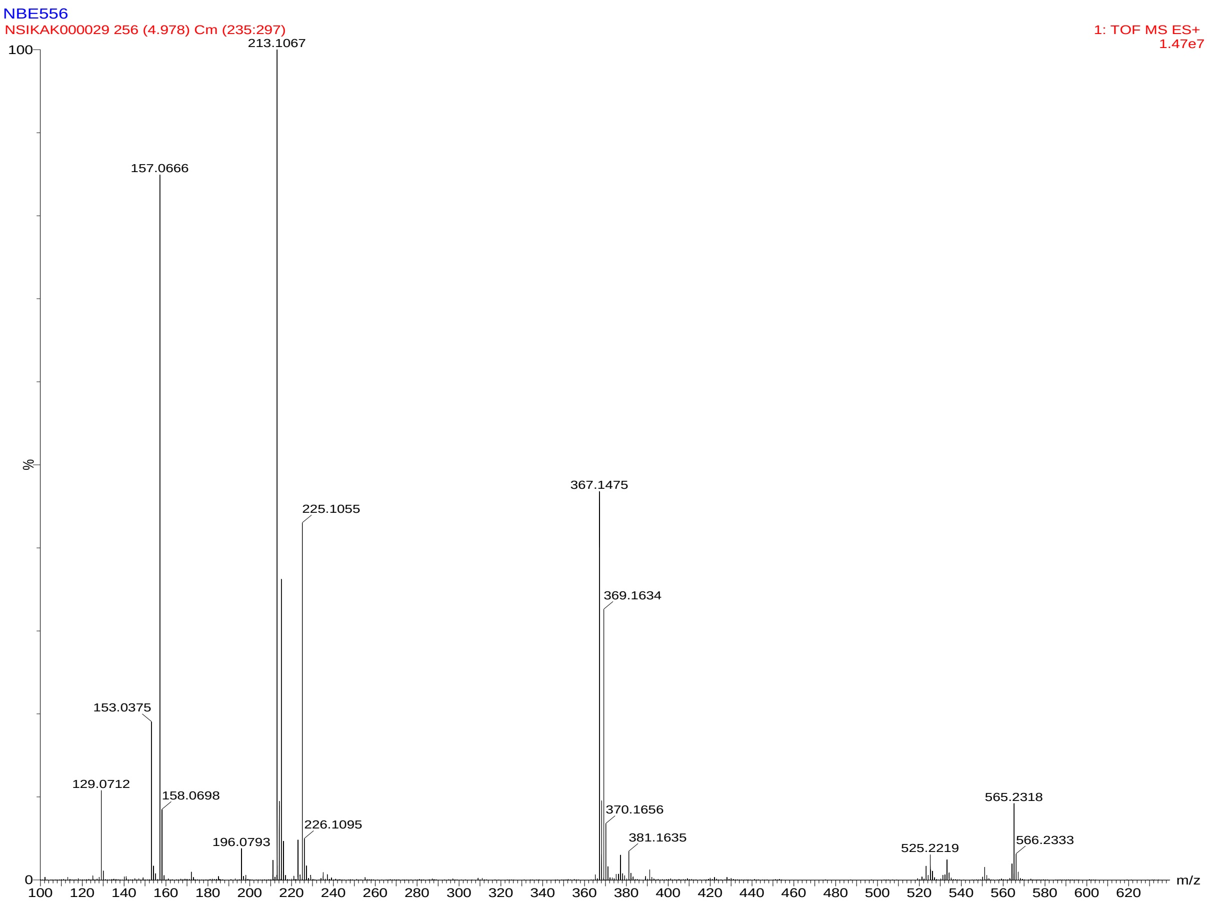


Figure S1-27. TOF MS ES+ for **SH-nap**.

Single crystal X-ray diffraction studies

Single Crystal X-Ray diffraction studies for **OH-nap** were carried out at the National Crystallography Service, University of Southampton.[1] A suitable crystal was selected and mounted on a MITIGEN holder in perfluoro ether oil on a Rigaku FRE+ equipped with VHF Varimax confocal mirror, an AFC12 goniometer, a HyPix 6000HE detector and data were collected at T = 100(2)K. The data were processed with CrysAlisPro and solved by intrinsic phasing methods with SHELXT.[2] CCDC number 2231789.

Table S1-1 Crystal data and structure refinement for **OH-nap**

Empirical formula	$C_{21}H_{24}N_2O_3$
Formula weight	352.42
Temperature/K	100.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.2168(12)
b/Å	7.3889(4)
c/Å	6.6363(4)
α/°	90
β/°	90.424(5)
γ/°	90
Volume/Å^3	893.24(9)
Z	2
ρ_{calc}g/cm^3	1.310
μ/mm^{-1}	0.708
F(000)	376.0
Crystal size/mm^3	0.15 × 0.1 × 0.03
Radiation	Cu Kα (λ = 1.54178)
2Θ range for data collection/°	4.85 to 140.08
Index ranges	$-22 \le h \le 22, -9 \le k \le 9, -8 \le l \le 8$
Reflections collected	27853
Independent reflections	1686 [R_{int} = 0.0647, R_{sigma} = 0.0145]
Data/restraints/parameters	1686/5/207
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0693, wR_2 = 0.2113
Final R indexes [all data]	R_1 = 0.0731, wR_2 = 0.2151
Largest diff. peak/hole / e Å^{-3}	0.16/-0.29

Fluorescence spectroscopy studies

Fluorescence spectra were recorded with an Edinburg F5S (slit=10, excitation at 350/405 nm) in a 1 cm quartz cell at 37°C. Typical titration experiments were performed by sequential additions of the analyte to the same 3 mL sample solution (50.0 μM) in a quartz cuvette. Kinetic studies were performed by measuring the fluorescent signal at a specific wavelength for a ten-minute period.

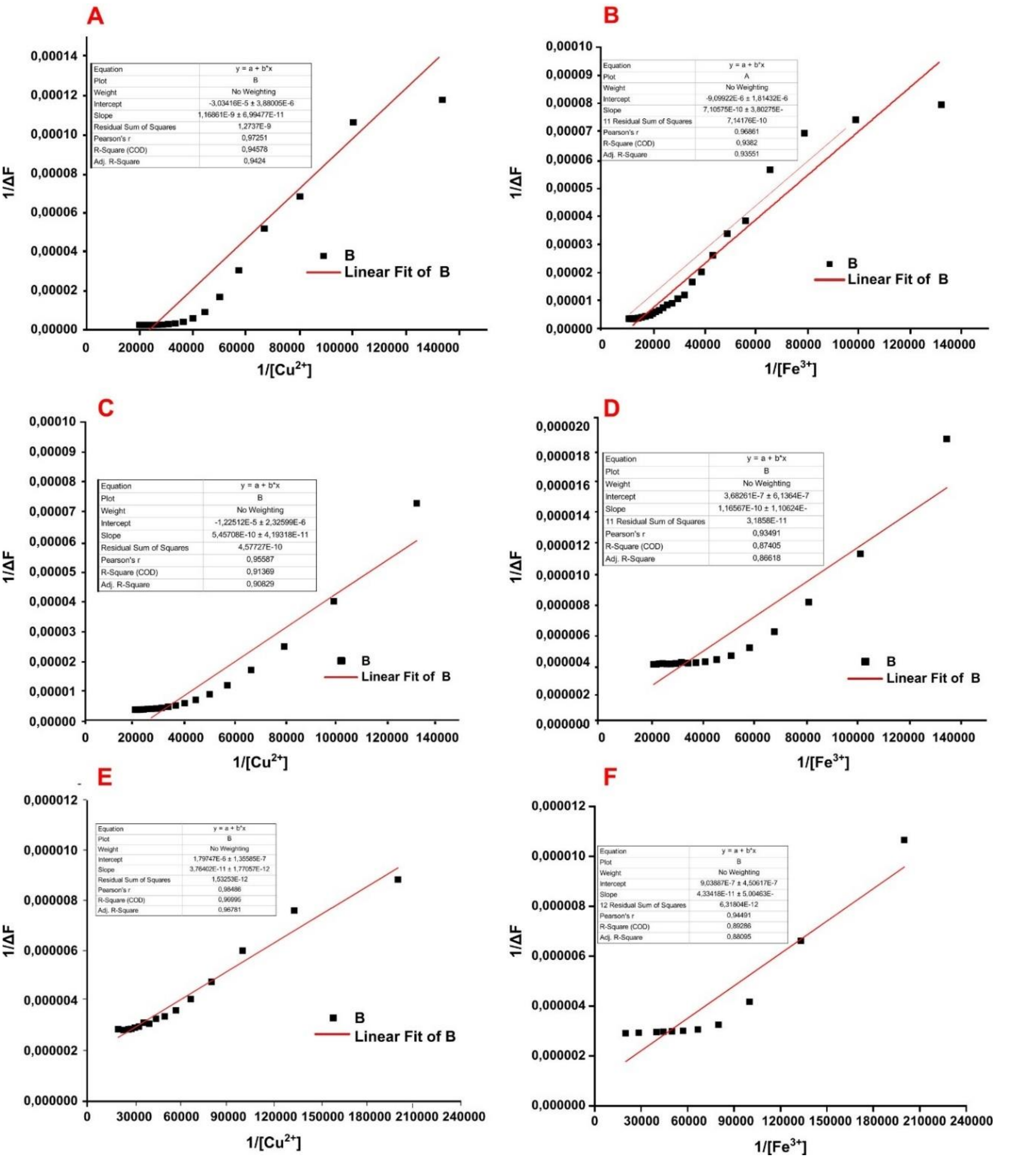


Figure S1-28. Fluorescence spectra of **SH-nap** (A/B), **OH-nap** (C/D) and **OF-nap** (E/F) upon excitation at 405 (**SH-nap**) & 350 nm (**OH-nap**/**OF-nap**), in the presence of different equivalents of Cu^{2+} and Fe^{3+}, respectively SELECTED DATA. Linear relationship between reciprocal of relative fluorescence intensity [$1/I-I_0$] and reciprocal of $1/[Cu^{2+}]$ and $1/[Fe^{3+}]$, respectively.

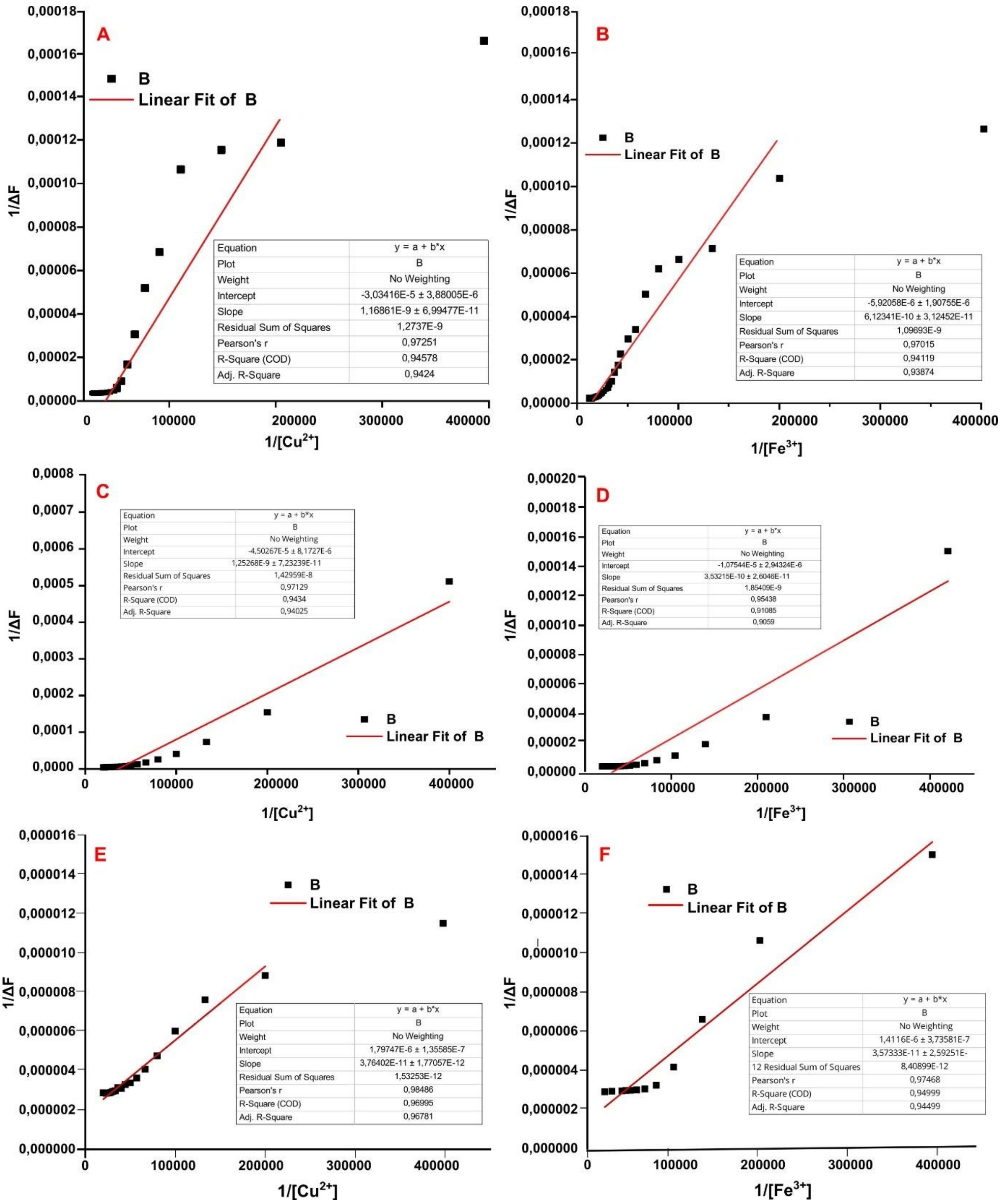


Figure S1-29. Fluorescence spectra of **SH-nap** (A/B), **OH-nap** (C/D) and **OF-nap** (E/F) upon excitation at 405 (**SH-nap**) & 350 nm (**OH-nap**/**OF-nap**), in the presence of different equivalents of Cu^{2+} and Fe^{3+}, respectively, ALL DATA. Linear relationship between reciprocal of relative fluorescence intensity [$1/I-I_0$] and reciprocal of $1/[Cu^{2+}]$ and $1/[Fe^{3+}]$, respectively.

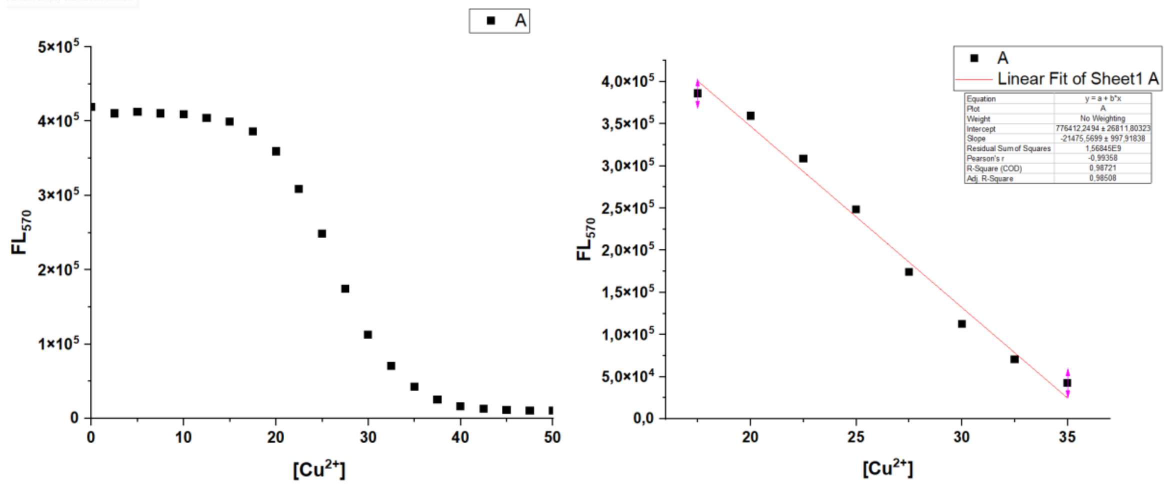


Figure S1-30. Scatter (left) and linear fit (right) of fluorescent Intensity at 570nm of **SH-nap** at 50µM in different concentrations of $CuCl_2$, T=30°C, Slit Bandwidth= 10

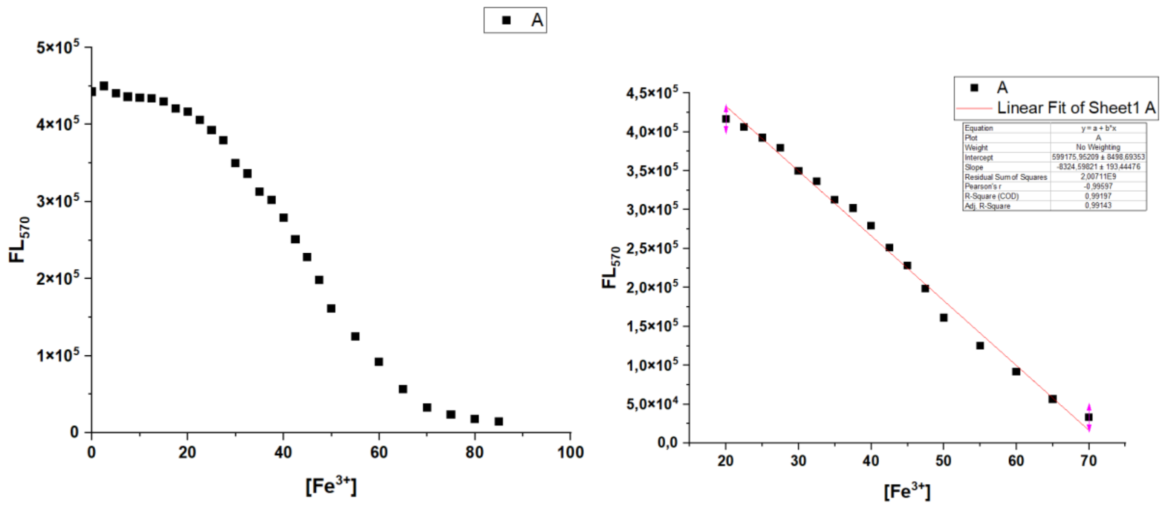


Figure S1-31. Scatter (left) and linear fit (right) of fluorescent Intensity at 570nm of **SH-nap** at 50µM in different concentrations of $FeCl_3$, T=30°C, Slit Bandwidth= 10

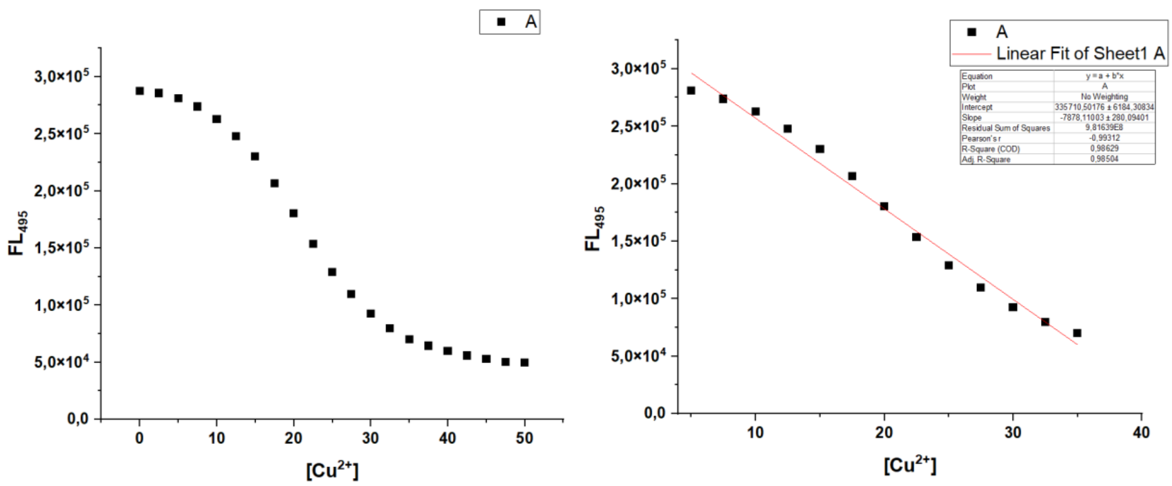


Figure S1-32. Scatter (left) and linear fit (right) of fluorescent Intensity at 495nm of **OH-nap** at 50µM in different concentrations of $CuCl_2$, T=30°C, Slit Bandwidth= 10

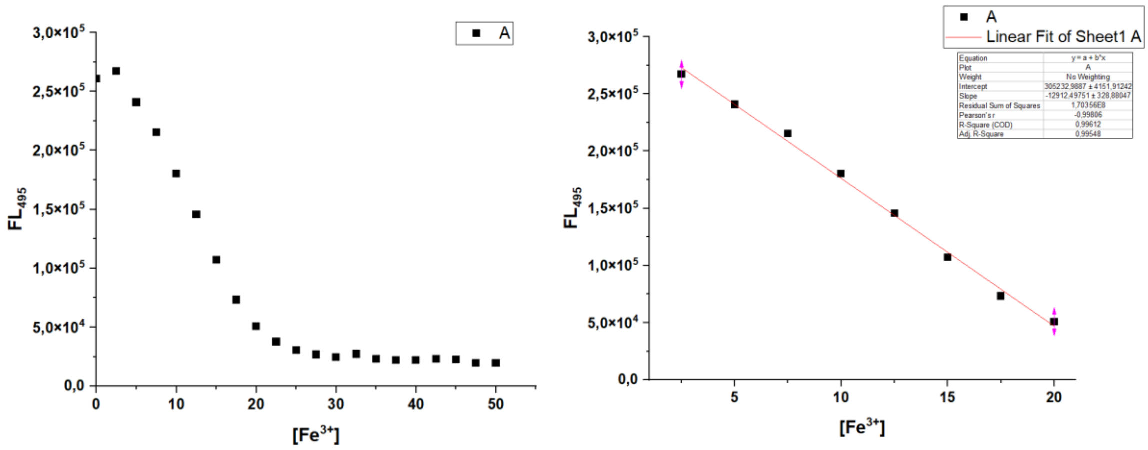


Figure S1-33. Scatter (left) and linear fit (right) of fluorescent Intensity at 495nm of **OH-nap** at 50µM in different concentrations of $FeCl_3$, T=30°C, Slit Bandwidth= 10

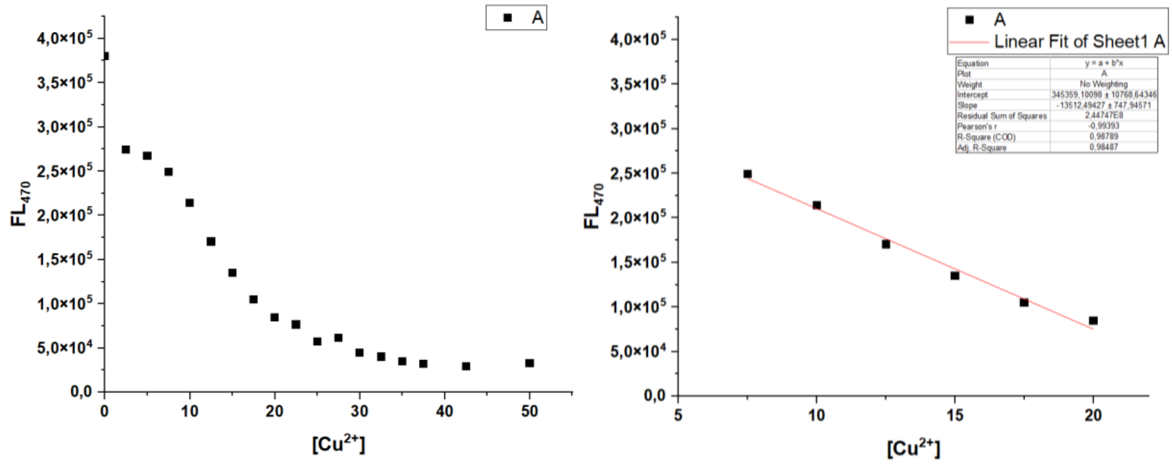


Figure S1-34. Scatter (left) and linear fit (right) of fluorescent Intensity at 470nm of **OF-nap** at 50µM in different concentrations of $CuCl_2$, T=30°C, Slit Bandwidth= 10

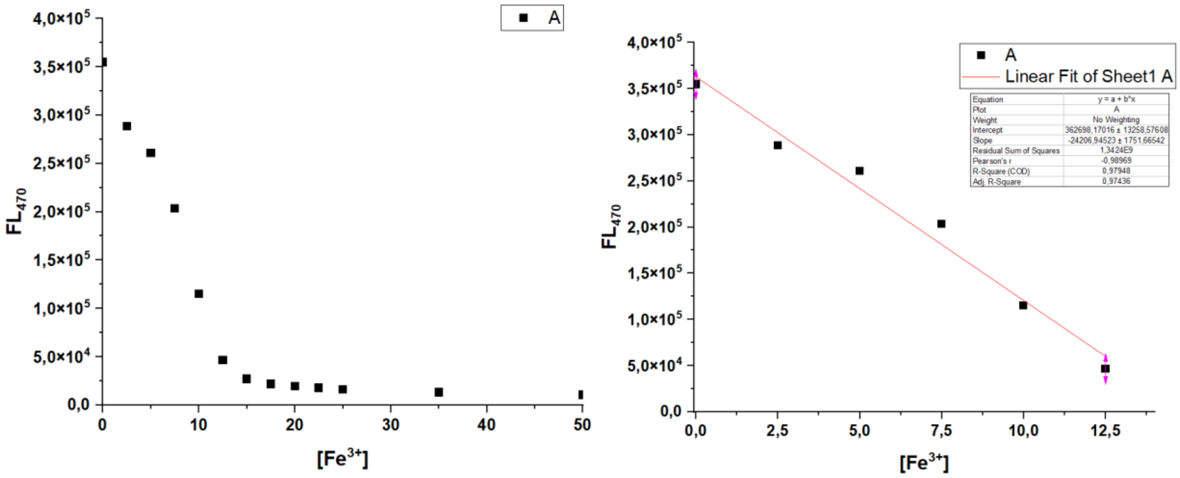
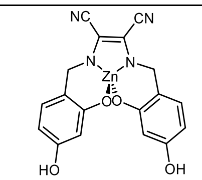
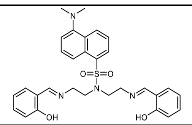
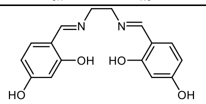
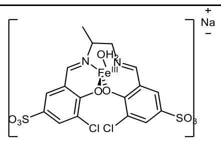
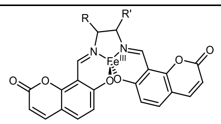
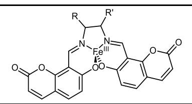
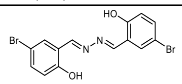
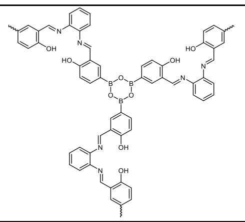
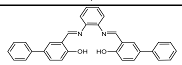
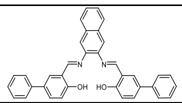
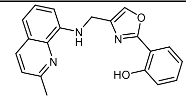
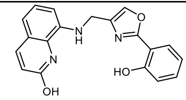
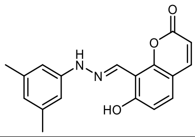
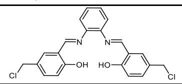
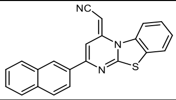
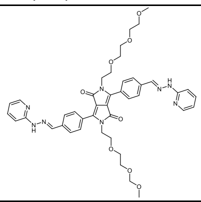
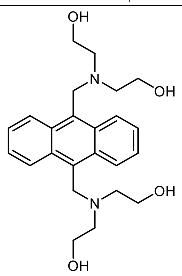
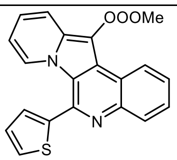
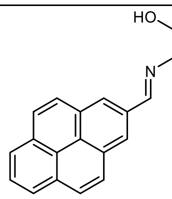


Figure S1-35. Scatter (left) and linear fit (right) of fluorescent Intensity at 470nm of **OF-nap** at 50μM in different concentrations of $FeCl_3$, T=30°C, Slit Bandwidth= 10

Chart 1 Selected Ligands used for Cu and Fe detection

Entry	Structure	Analyte	λex/λem	LOD	Ref
1		HS^- H_2S	570/630	$<10^{-5}$M	3
2		Zn^{2+}	360/523	83 nM	4
3		Al^{3+}	365/508	Not mentioned	5
4		PPi	385/500	Not mentioned	6
5		PPi	365/495	3.15×10^{-6} M	7
6		PPi	365/495	2.81×10^{-6} M	7
7		Zn^{2+}	410/513	2.18 μM	8
8		Al^{3+} Fe^{3+} Cu^{2+}	320/480	0.248/0.545/0.140 μM	9
9		Zn^{2+}	350/525	7.69nM	10

10		Zn^{2+}	350/525	5.35nM	10
11		Cu^{2+}	335/472	2.70×10^{-8} M	11
12		Cu^{2+}	335/472	2.14×10^{-8} M	11
13		Cu^{2+}	334/425	8 nM	12
14		Cu^{2+}	317/435	5.4 µg/L	13
15		Fe^{3+}	314/554	0.74 nM	14
16		Fe^{3+}	465/578	8 nM	15
17		Fe^{3+}	376/456	0.1 pM	16
18		Fe^{3+}	420/458	1 µM	17
19		Fe^{3+}	395/500	0.106 µM	18

Potentiometric studies

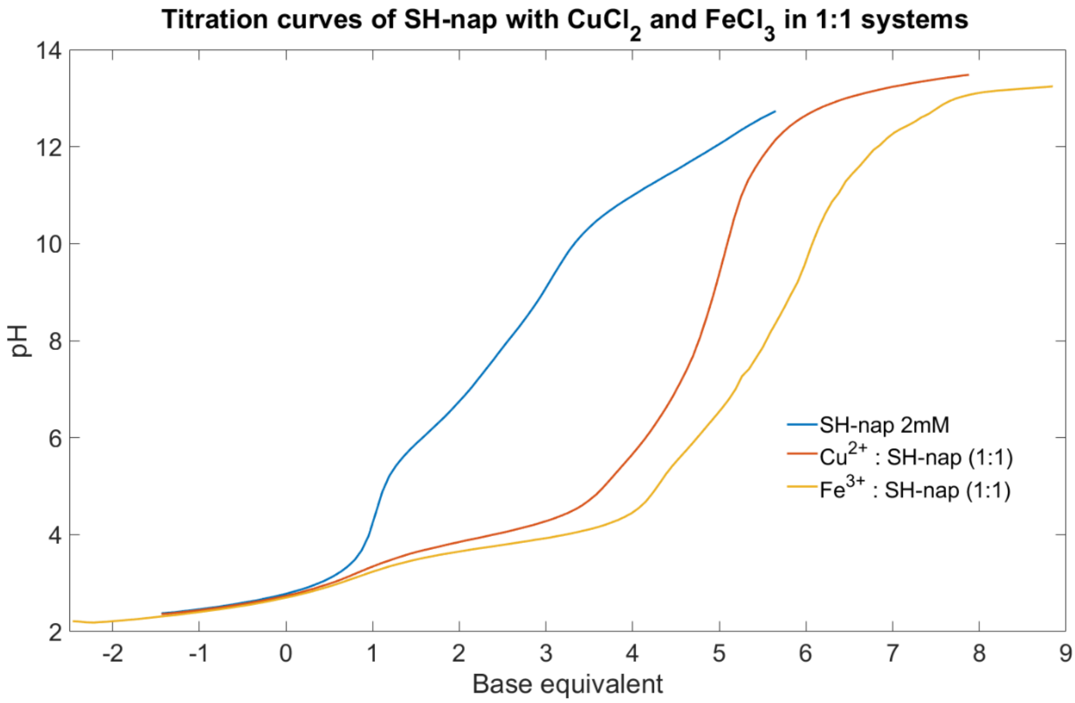


Figure S1-36. Titration curves of SH-nap and the Cu2+/Fe^{3+} containing systems

Table S1-2. Protonation constants (logβ) and pK values of SH-nap and stability constants of the formed complexes (I = 0.2 M, T = 298 K, standard deviations are in parentheses)

	logβ	pK
HL	10.99(4)	10.99(4)
H_2L	20.49(6)	9.5(6)
H_3L	27.83(8)	7.34(8)
H_4L	32.10 9)	4.27(9)
$CuLH_2$	30.84(5)	
CuLH	26.84(3)	
CuL	20.93(7)	
$CuLH_{-1}$	9.27(11)	
$FeLH_2$	30.84(11)	
FeLH	27.52(2)	
FeL	22.79(5)	
$FeLH_{-1}$	15.54(8)	

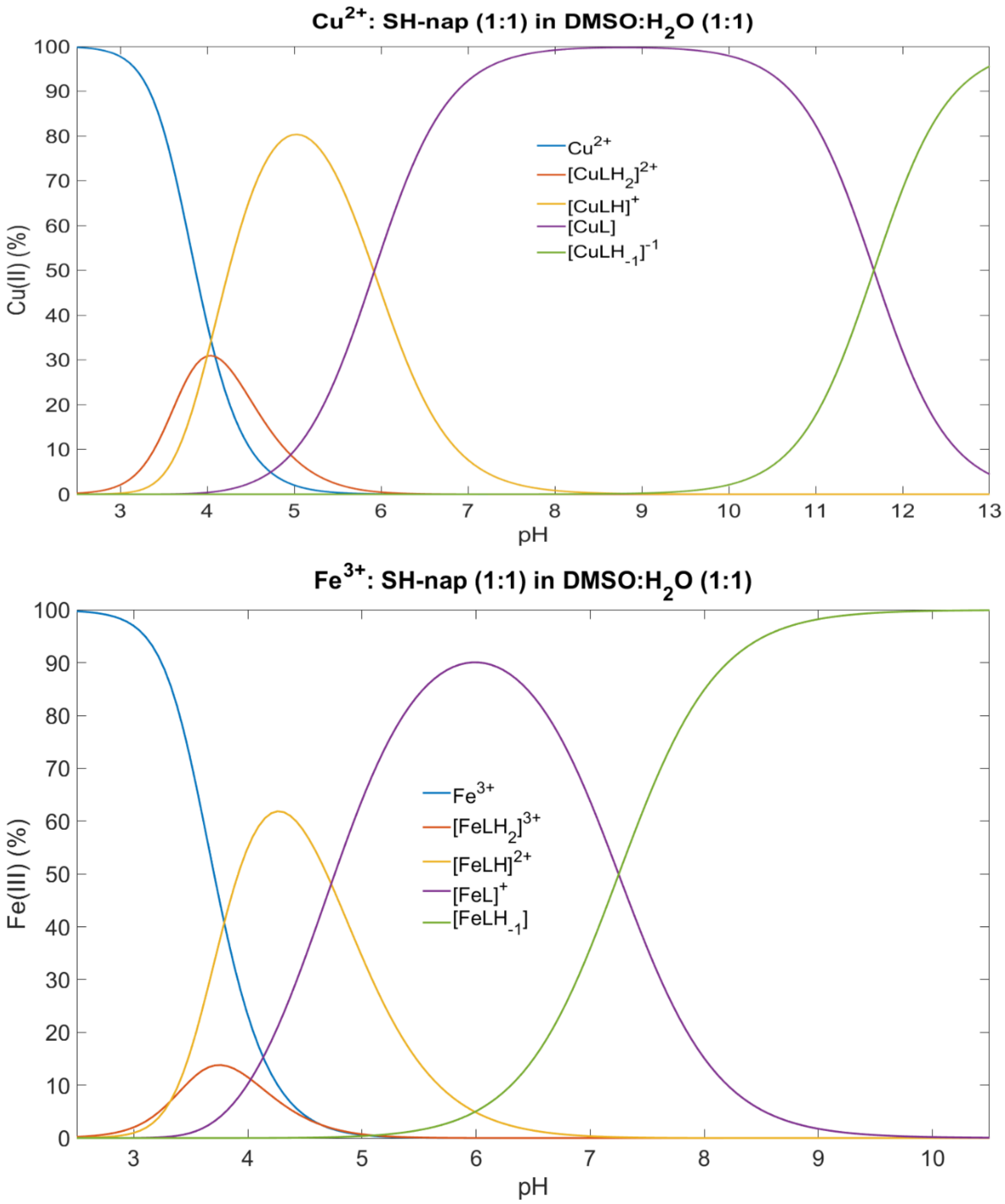
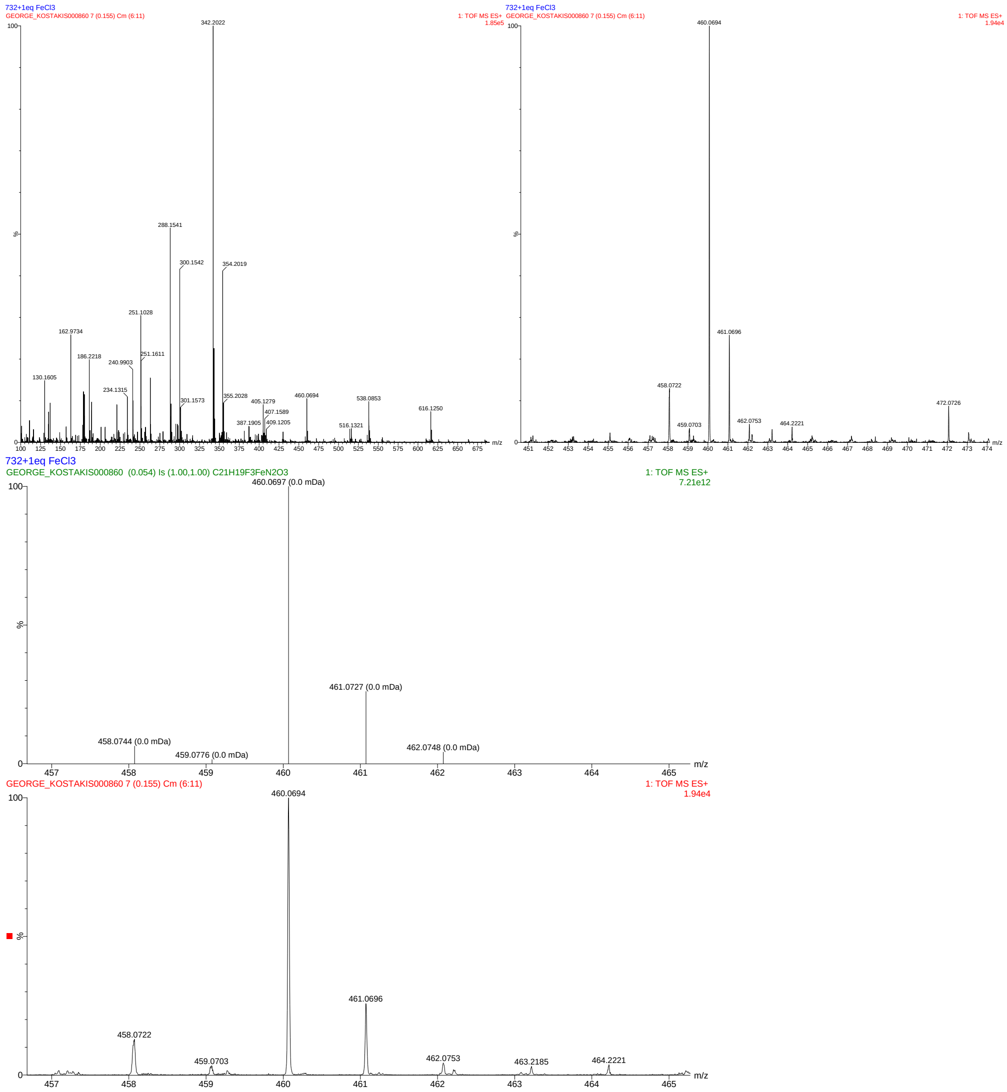


Figure S1-37. Species distribution of the Cu^{2+} and Fe^{3+} complexes

ESI-MS studies post fluorescence

OF-nap with $FeCl_3$



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

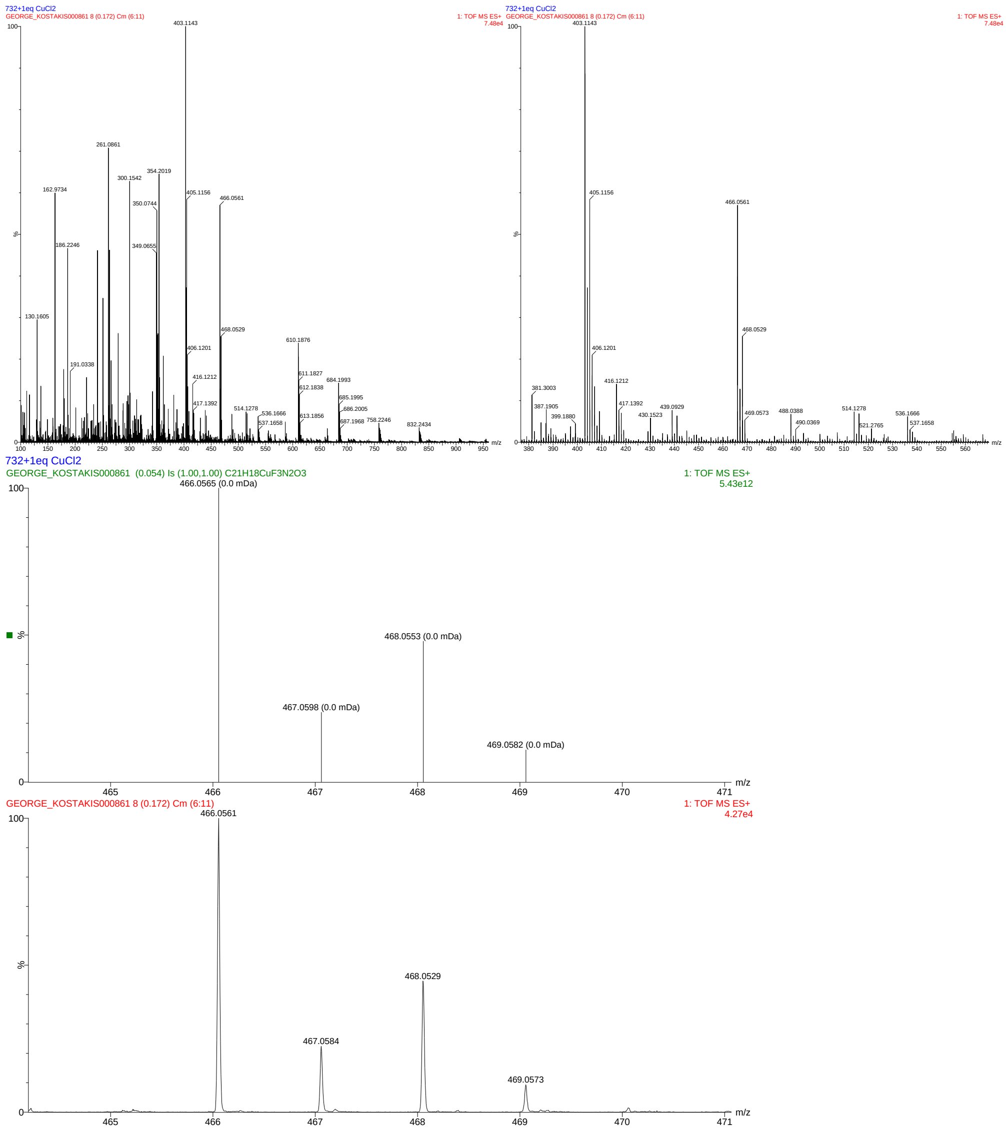
Elements Used:

C: 21-21 H: 0-100 N: 2-2 O: 3-3 F: 3-3 Fe: 0-1

Minimum:			-1.5					
Maximum:	5.0	100.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
460.0693	460.0697	-0.4	-0.9	12.0	446.1	n/a	n/a	C21 H19 N2 O3 F3 Fe

Figure S1-38. Elemental Composition Report for the sample of Fe with OF-nap, post-titration studies.

OF-nap with $CuCl_2$

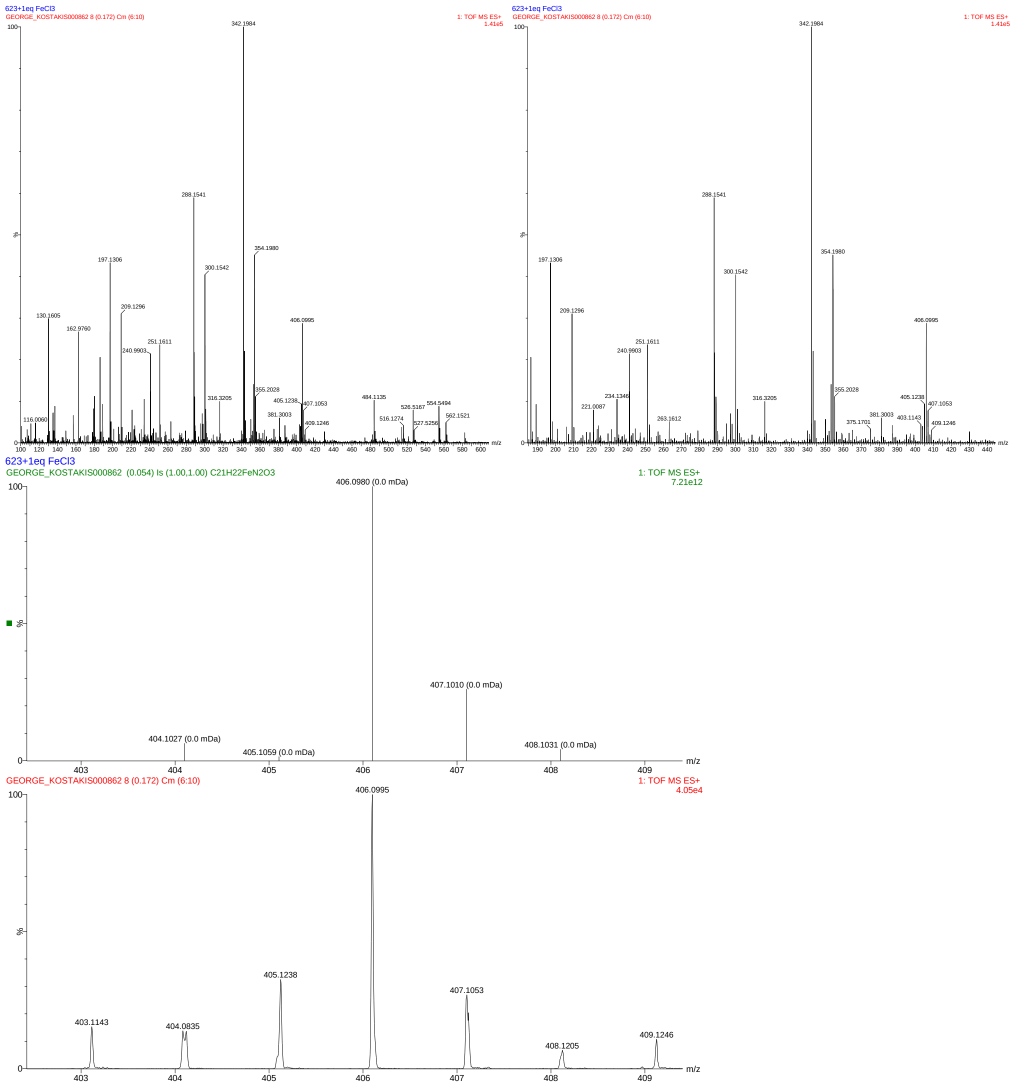


Elemental Composition Report
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 21-21 H: 0-100 N: 2-2 O: 3-3 F: 3-3 Cu: 0-1

Minimum:			-1.5					
Maximum:		5.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
466.0558	466.0566	-0.8	-1.7	12.5	353.5	n/a	n/a	C21 H18 N2 O3 F3 Cu

Figure S1-39. Elemental Composition Report for the sample of Cu with OF-nap, post-titration studies.

OH-nap with $FeCl_3$



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

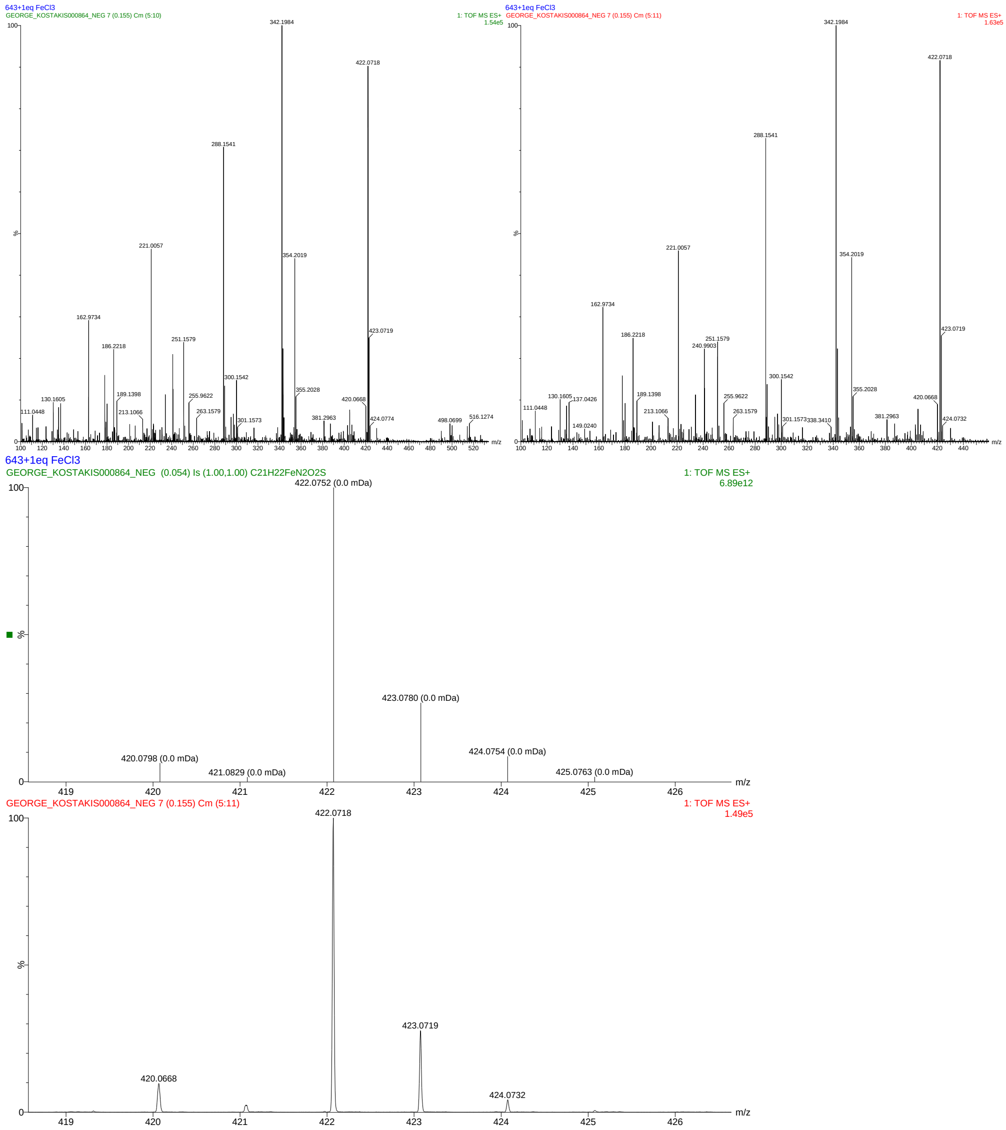
Elements Used:

C: 21-21 H: 0-100 N: 2-2 O: 3-3 Fe: 0-1

Minimum:				-1.5				
Maximum:		5.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
406.0985	406.0980	0.5	1.2	12.0	511.4	n/a	n/a	C21 H22 N2 O3 Fe

Figure S1-40. Elemental Composition Report for the sample of Fe with OH-nap, post-titration studies.

SH-nap with $FeCl_3$



Elemental Composition Report

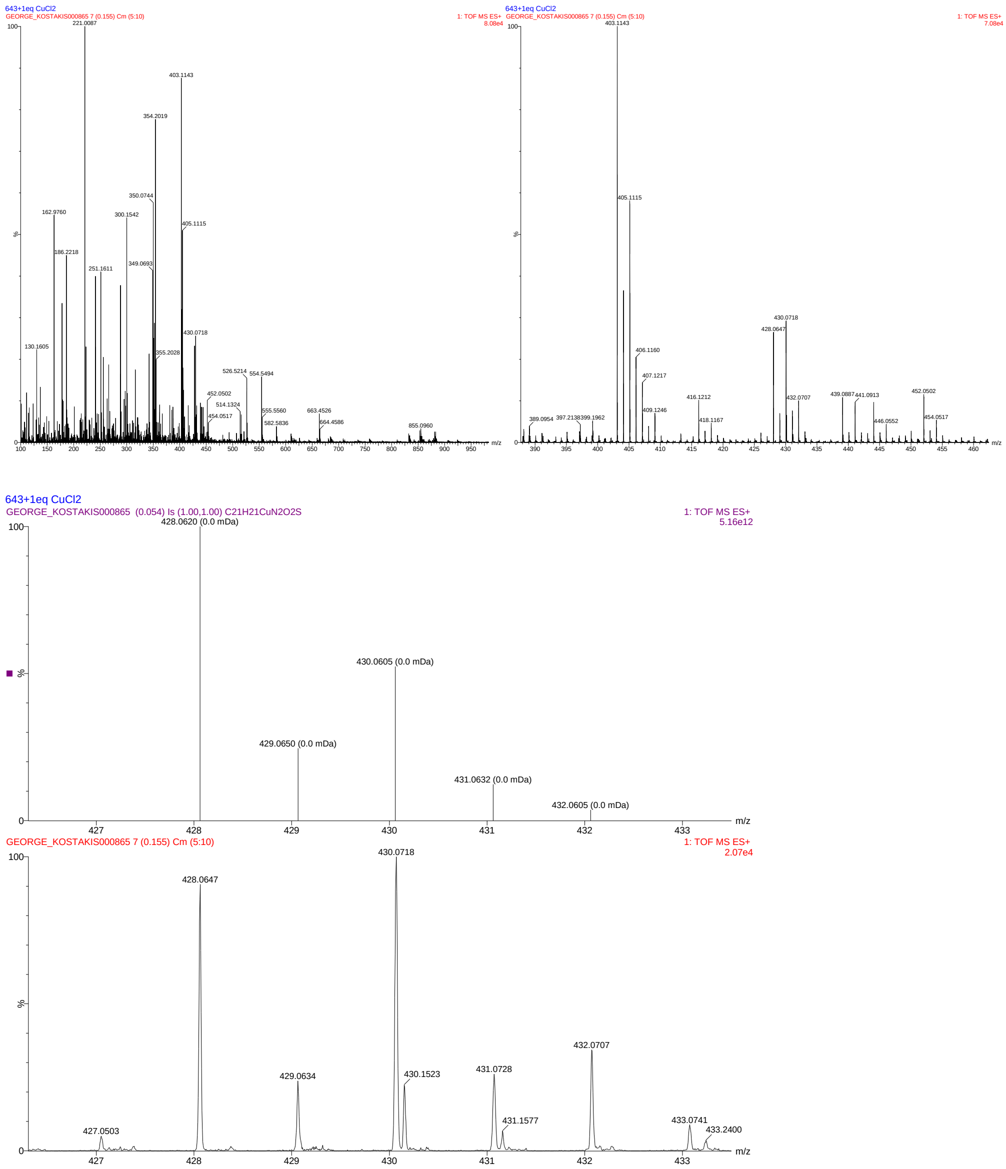
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 21-21 H: 0-100 N: 2-2 O: 2-2 S: 1-1 Fe: 0-1

Minimum:			-1.5		
Maximum:	5.0	100.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Formula
422.0760	422.0751	0.9	2.1	12.0	C21 H22 N2 O2 S Fe

Figure S1-41. Elemental Composition Report for the sample of Fe with SH-nap, post-titration studies.

SH-nap with $CuCl_2$



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 0-100 N: 2-2 O: 2-2 S: 1-1 Cu: 0-1

Minimum:			-1.5					
Maximum:	5.0	100.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
428.0619	428.0620	-0.1	-0.2	12.5	476.4	n/a	n/a	C21 H21 N2 O2 S Cu

Figure S1-42. Elemental Composition Report for the sample of Fe with SH-nap, post-titration studies.

Theoretical calculations

Geometry optimisation was carried out using the Gaussian16 [3] program at the OLYP/def2-SVP D3 with PCM implicit solvation level of theory.[4–9] To obtain the doublet state, spin-unrestricted calculations were performed, constraining the projection of the total electronic spin along a reference axis to 1/2, and for the sextet in the unrestricted formalism and set the projection to 5/2. The Jmol program was used for visualisation purposes.[10] Excitation calculations were processed using the GaussSum program.[11]

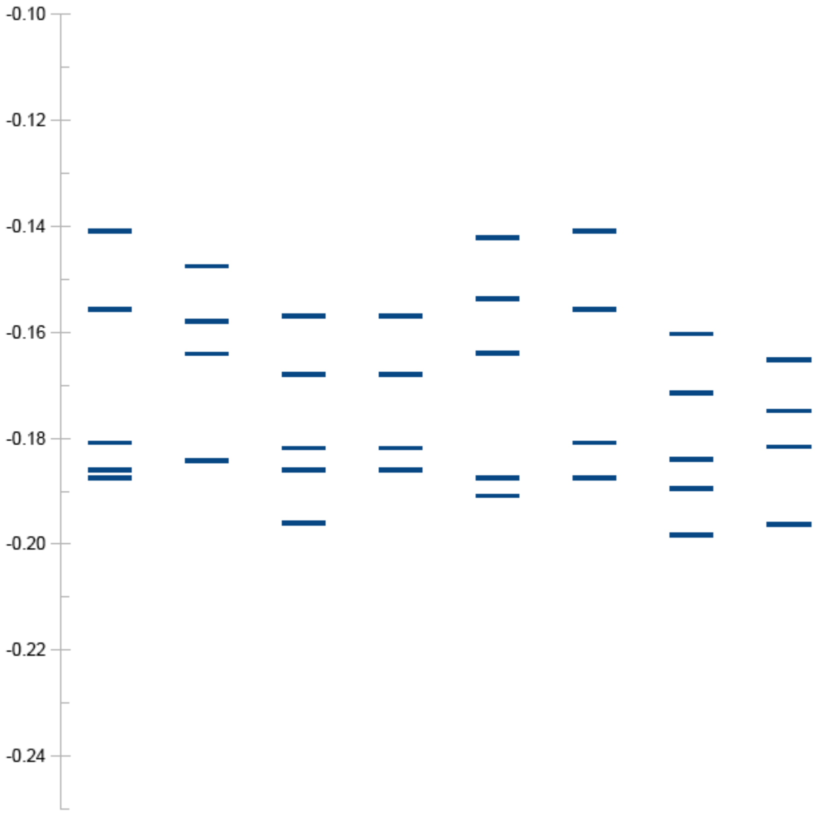


Figure S1-43: Frontier orbitals (HOMO to HOMO-5 for alpha and HOMO to HOMO-4 for beta electrons) from left to right: OH-nap Cu set 1 and 2, OF-nap Cu set 3 and 4, SH-nap set 5 and 6, and SF-nap set 7 and 8.

Table S1-3. Stabilising orbital interactions between the metal centre and the ligand from ETS-NOCV calculations. Energies are given in kcal/mol.

	Cu^{2+}	Fe^{3+}
OH-nap	-178.34	-263.81
OF-nap	-184.61	-265.02
SH-nap	-186.22	-269.43
SF-nap	-182.78	-262.51

Coordinates for the Cu^{2+} and Fe^{3+} species. No experimental evidence was recorded for Cu^{2+}- SF-nap and Fe^{3+}- SF-nap species, however, we performed theoretical studies to elucidate the impact of the secondary coordination sphere on the sensing approach.

Cu^{2+}- SH-nap

Cu	0.000000	0.000000	0.000000
O	1.317863	-1.413701	0.285056
O	-1.570850	-1.020987	0.521354
S	-7.228055	-0.694299	-1.243956
N	1.489043	1.439761	-0.272017
N	-1.288892	1.648076	-0.284992
H	-1.741647	1.787092	0.619666
C	6.469389	-1.261750	-1.864208
H	6.860206	-2.180888	-2.312933
C	7.233219	-0.107011	-1.853797
H	8.235607	-0.098970	-2.292225
C	6.703578	1.065721	-1.268955
H	7.300524	1.983669	-1.256999
C	5.437583	1.067516	-0.708524
H	5.065222	1.993033	-0.263756
C	4.620432	-0.101654	-0.698392
C	5.169373	-1.292229	-1.301672
C	4.380877	-2.478653	-1.321079
H	4.809062	-3.378320	-1.775903
C	3.110917	-2.504380	-0.800281
H	2.496587	-3.408829	-0.822533
C	2.527339	-1.336935	-0.195022
C	3.312364	-0.153961	-0.131470
C	2.665684	1.024527	0.522674
H	2.287303	0.748058	1.522746
H	3.359749	1.870281	0.641119
C	0.868381	2.713451	0.076894
H	1.510283	3.580321	-0.171544
H	0.711441	2.723682	1.168547
C	-0.469101	2.802211	-0.644001
H	-0.294866	2.758334	-1.732057
H	-0.975416	3.763447	-0.435723
C	-2.301884	1.251880	-1.269563
H	-1.746142	0.882970	-2.154850
H	-2.880248	2.133352	-1.606742
C	-2.775539	-0.894305	0.042203
C	-3.740390	-1.903427	0.350854
H	-3.388784	-2.753995	0.941142
C	-5.063698	-1.812677	-0.043794

H	-5.769161	-2.603204	0.232683
C	-5.517195	-0.710819	-0.804457
C	-4.588289	0.277540	-1.150083
H	-4.896797	1.134391	-1.751909
C	-3.242991	0.204267	-0.752845
C	-7.367520	0.789951	-2.253795
H	-8.418462	0.839022	-2.577954
H	-6.718407	0.734148	-3.143127
H	-7.128155	1.697848	-1.675996
H	1.767717	1.444252	-1.256056

Fe^{3+}- SH-nap

Fe	0.000000	0.000000	0.000000
O	0.714987	-0.966207	1.453746
O	-0.878249	-0.848590	-1.441499
S	-6.389415	-1.981565	0.356029
N	1.484797	1.545943	0.032779
N	-1.340053	1.685827	0.034892
H	-1.711558	1.780256	0.983854
C	5.714811	-2.544590	-0.463916
H	5.924415	-3.614241	-0.556273
C	6.662246	-1.608539	-0.846985
H	7.628113	-1.933099	-1.244414
C	6.377586	-0.230166	-0.725056
H	7.125001	0.507300	-1.032250
C	5.160995	0.194977	-0.219300
H	4.969748	1.267115	-0.139623
C	4.164952	-0.737809	0.187721
C	4.459360	-2.143009	0.052055
C	3.479608	-3.104508	0.439293
H	3.724246	-4.165862	0.335539
C	2.248619	-2.723988	0.918122
H	1.484798	-3.452821	1.199763
C	1.931930	-1.338997	1.047958
C	2.897414	-0.351701	0.715232
C	2.521218	1.076742	0.987670
H	2.061636	1.133933	1.986573
H	3.389266	1.750714	0.976886
C	0.804470	2.796363	0.406516
H	1.417670	3.687597	0.186226
H	0.649070	2.770065	1.497273
C	-0.536708	2.873198	-0.303566
H	-0.382909	2.862461	-1.394763
H	-1.060928	3.813064	-0.056209

C	-2.466036	1.406731	-0.889359
H	-2.058958	1.506412	-1.908128
H	-3.266051	2.155349	-0.764633
C	-2.125322	-1.078678	-1.042741
C	-2.629587	-2.400814	-0.935779
H	-1.965881	-3.228276	-1.199259
C	-3.924832	-2.631283	-0.507943
H	-4.298605	-3.656589	-0.429548
C	-4.781879	-1.551784	-0.167325
C	-4.293900	-0.233185	-0.275048
H	-4.935567	0.615624	-0.035669
C	-2.990674	0.012093	-0.706733
C	-7.181475	-0.392908	0.658127
H	-8.205892	-0.631248	0.981677
H	-7.224351	0.209564	-0.262572
H	-6.669666	0.161111	1.460428
H	1.911322	1.641662	-0.892481

Cu^{2+}- OH-nap

Cu	0.000000	0.000000	0.000000
O	-1.178259	-1.301698	-0.878090
O	1.286378	-1.205142	0.837499
O	6.641607	-0.812565	-0.438639
N	-1.450266	1.537352	-0.121026
N	1.350498	1.650057	0.116381
H	1.768799	1.742761	-0.811851
C	-6.567292	-1.275704	0.575311
H	-7.020833	-2.223843	0.882368
C	-7.313180	-0.108904	0.578069
H	-8.363179	-0.121304	0.885525
C	-6.703693	1.103322	0.180596
H	-7.286494	2.030404	0.183702
C	-5.376769	1.131294	-0.212835
H	-4.937944	2.085794	-0.512492
C	-4.576647	-0.049613	-0.231813
C	-5.206284	-1.281000	0.181918
C	-4.435253	-2.479653	0.189664
H	-4.925842	-3.408422	0.500161
C	-3.107798	-2.481411	-0.162681
H	-2.505659	-3.394038	-0.141259
C	-2.443843	-1.272090	-0.568615
C	-3.208899	-0.075018	-0.629271

C	-2.473999	1.134039	-1.109374
H	-1.922161	0.884151	-2.032048
H	-3.148649	1.976781	-1.328411
C	-0.733384	2.774302	-0.419656
H	-1.352517	3.677114	-0.255348
H	-0.471406	2.753248	-1.490940
C	0.537957	2.826776	0.413757
H	0.278720	2.786719	1.485081
H	1.083535	3.775823	0.246850
C	2.426195	1.354744	1.080296
H	1.925955	1.120548	2.036393
H	3.073514	2.239207	1.230623
C	2.546641	-1.078365	0.523027
C	3.318185	-2.195737	0.088127
H	2.806856	-3.159022	0.008644
C	4.666607	-2.075199	-0.212182
H	5.254592	-2.937993	-0.538316
C	5.318458	-0.828133	-0.112449
C	4.584980	0.296318	0.301673
H	5.063047	1.273726	0.391087
C	3.227273	0.177470	0.622332
C	7.336338	0.404341	-0.337994
H	8.377260	0.199826	-0.633731
H	7.326625	0.801986	0.696261
H	6.916486	1.177965	-1.011643
H	-1.903205	1.607925	0.792760

Fe^{3+}- OH-nap

Fe	0.000000	0.000000	0.000000
O	1.472259	-1.125201	0.114238
O	-1.558828	-1.018154	0.015228
O	-6.976859	-0.210021	0.230749
N	1.456098	1.662087	-0.065174
N	-1.337851	1.783567	-0.093908
H	-1.705193	1.938237	0.849261
C	6.991789	-0.698021	-0.440692
H	7.540698	-1.574018	-0.798325
C	7.662446	0.476796	-0.142988
H	8.747686	0.538934	-0.263754
C	6.937992	1.597771	0.320832
H	7.467071	2.525556	0.557815
C	5.565202	1.532654	0.480659
H	5.042389	2.418466	0.845724

C	4.838578	0.343005	0.182093
C	5.587850	-0.797089	-0.288978
C	4.902851	-2.010116	-0.589736
H	5.488143	-2.865489	-0.939973
C	3.541683	-2.116484	-0.448260
H	3.004411	-3.040128	-0.676122
C	2.779923	-0.996098	0.002864
C	3.423448	0.222207	0.325499
C	2.568831	1.330404	0.858867
H	2.107400	1.028610	1.817825
H	3.161234	2.233659	1.058324
C	0.774079	2.922682	0.242518
H	1.391512	3.804011	-0.007279
H	0.595853	2.950062	1.330629
C	-0.549592	2.952705	-0.496524
H	-0.373831	2.879909	-1.582867
H	-1.087296	3.901101	-0.317280
C	-2.486283	1.490461	-0.977882
H	-2.067668	1.136315	-1.938528
H	-3.051096	2.414534	-1.191277
C	-2.853339	-0.787590	0.044839
C	-3.739974	-1.791133	0.520280
H	-3.309810	-2.740921	0.847809
C	-5.102762	-1.567996	0.571266
H	-5.791260	-2.332439	0.940052
C	-5.643161	-0.331630	0.142508
C	-4.777908	0.672155	-0.340071
H	-5.176763	1.625385	-0.688615
C	-3.399070	0.454007	-0.395254
C	-7.597400	0.991675	-0.191769
H	-8.676146	0.854298	-0.030194
H	-7.408439	1.184104	-1.263725
H	-7.244699	1.854871	0.402046
H	1.849228	1.715177	-1.009048

Cu^{2+}- OF-nap

Cu	0.000000	0.000000	0.000000
O	1.089508	-1.338809	0.923058
O	-1.231635	-1.201185	-0.920082
O	-6.693036	-0.574130	-0.283825
N	1.464370	1.491899	0.266781
N	-1.291586	1.662405	-0.223045
H	-1.798097	1.753451	0.660808

C	6.583697	-1.398247	-0.042387
H	7.043481	-2.347397	-0.336191
C	7.351059	-0.250141	0.060565
H	8.424489	-0.279261	-0.149091
C	6.734691	0.964650	0.439138
H	7.335859	1.876160	0.520090
C	5.378227	1.013684	0.709843
H	4.935079	1.968764	1.000718
C	4.554945	-0.147420	0.616572
C	5.192441	-1.381697	0.224076
C	4.400661	-2.561289	0.107277
H	4.898342	-3.491482	-0.186646
C	3.046988	-2.542400	0.337018
H	2.429719	-3.438901	0.232865
C	2.377591	-1.330183	0.722619
C	3.156147	-0.151746	0.885866
C	2.401275	1.060306	1.327302
H	1.776247	0.807139	2.200977
H	3.067466	1.890730	1.608238
C	0.751057	2.742531	0.519453
H	1.403363	3.631119	0.423150
H	0.393652	2.713910	1.562453
C	-0.436773	2.831361	-0.425513
H	-0.082269	2.804681	-1.469506
H	-0.983252	3.784297	-0.291494
C	-2.275155	1.395857	-1.289694
H	-1.690979	1.154398	-2.194973
H	-2.883918	2.295680	-1.494236
C	-2.514056	-1.040913	-0.749774
C	-3.353386	-2.143003	-0.418242
H	-2.877182	-3.119594	-0.297801
C	-4.726792	-1.988683	-0.256804
H	-5.365503	-2.837331	0.000611
C	-5.305053	-0.724004	-0.412503
C	-4.521835	0.385126	-0.738917
H	-5.001964	1.359572	-0.861152
C	-3.144998	0.238788	-0.916273
C	-7.163900	-0.245221	0.939464
F	-8.493068	-0.162477	0.858013
F	-6.688264	0.946243	1.373822
F	-6.845433	-1.157181	1.881738
H	1.988717	1.561321	-0.608633

Fe^{3+}- OF-nap

Fe	0.000000	0.000000	0.000000
O	1.516968	-1.070345	0.102740
O	-1.509064	-1.079706	0.020345
O	-6.969722	-0.483896	0.285586
N	1.394475	1.711344	-0.077754
N	-1.400197	1.728821	-0.087486
H	-1.773423	1.872989	0.855309
C	7.014534	-0.461514	-0.458830
H	7.593178	-1.320664	-0.810200
C	7.645727	0.738103	-0.168875
H	8.728350	0.835071	-0.290153
C	6.885034	1.837723	0.287003
H	7.383046	2.784087	0.517312
C	5.515077	1.727870	0.447143
H	4.962862	2.598328	0.805509
C	4.828799	0.511966	0.156629
C	5.615686	-0.606221	-0.306503
C	4.972150	-1.844789	-0.598187
H	5.586436	-2.681981	-0.942500
C	3.616024	-1.996819	-0.455125
H	3.110157	-2.939718	-0.675568
C	2.817083	-0.898858	-0.012428
C	3.419418	0.345384	0.301154
C	2.529383	1.425848	0.834412
H	2.091707	1.114184	1.801323
H	3.090239	2.351499	1.021322
C	0.669045	2.947573	0.234779
H	1.252997	3.849511	-0.021022
H	0.498864	2.969625	1.324257
C	-0.659823	2.928264	-0.494678
H	-0.489971	2.863897	-1.582435
H	-1.232398	3.854512	-0.309460
C	-2.538075	1.389716	-0.969967
H	-2.108168	1.051692	-1.931251
H	-3.140138	2.289886	-1.181696
C	-2.814469	-0.900768	0.055159
C	-3.656705	-1.933994	0.536016
H	-3.193715	-2.868479	0.862040
C	-5.030159	-1.756519	0.596603
H	-5.687860	-2.544421	0.971463
C	-5.603075	-0.543925	0.173774
C	-4.791161	0.490713	-0.317678

H	-5.225663	1.427934	-0.662300
C	-3.406691	0.318771	-0.383028
C	-7.680654	0.637042	-0.056887
F	-8.953827	0.379058	0.183787
F	-7.526576	0.946074	-1.356620
F	-7.298433	1.706249	0.666144
H	1.773498	1.776887	-1.026687

Cu^{3+}- SF-nap

Cu	0.000000	0.000000	0.000000
O	1.093092	-1.286486	0.988499
O	-1.210279	-1.273155	-0.856699
S	-7.067828	-0.556937	-0.386413
N	1.446816	1.512619	0.225899
N	-1.294793	1.630905	-0.337213
H	-1.831714	1.757166	0.524292
C	6.605074	-1.325312	0.135916
H	7.080101	-2.280050	-0.111710
C	7.358963	-0.166146	0.210766
H	8.436783	-0.192190	0.024701
C	6.723500	1.055822	0.529995
H	7.314332	1.975676	0.588921
C	5.361293	1.101198	0.770513
H	4.903259	2.061814	1.016451
C	4.551366	-0.071080	0.704222
C	5.208484	-1.312979	0.372740
C	4.430887	-2.504568	0.284970
H	4.943746	-3.439910	0.037316
C	3.072685	-2.491428	0.486127
H	2.466434	-3.397656	0.404401
C	2.384465	-1.272374	0.812023
C	3.147406	-0.079837	0.944445
C	2.369905	1.140023	1.320443
H	1.733085	0.917343	2.193868
H	3.020760	1.990685	1.575137
C	0.717251	2.766317	0.407960
H	1.364288	3.655717	0.287638
H	0.335815	2.779493	1.442689
C	-0.447753	2.801011	-0.568091
H	-0.067296	2.734831	-1.601086
H	-1.008879	3.751181	-0.487932
C	-2.241132	1.302610	-1.420794
H	-1.626330	1.019905	-2.293363

H	-2.846657	2.187105	-1.690596
C	-2.495961	-1.104744	-0.753881
C	-3.349076	-2.189826	-0.397927
H	-2.876861	-3.156737	-0.204141
C	-4.724527	-2.026706	-0.294894
H	-5.363492	-2.865418	-0.005130
C	-5.315304	-0.772059	-0.538858
C	-4.501165	0.313376	-0.901489
H	-4.966344	1.284700	-1.093506
C	-3.120851	0.163788	-1.016048
C	-7.117818	0.002372	1.350550
F	-8.400175	0.226142	1.683489
F	-6.427498	1.146615	1.544053
F	-6.609262	-0.905929	2.201813
H	1.985288	1.546865	-0.643147

Fe^{3+}- SF-nap

Fe	0.000000	0.000000	0.000000
O	1.540403	-1.017688	0.207235
O	-1.483106	-1.126154	0.012781
S	-7.361572	-0.623631	0.029926
N	1.349835	1.747527	-0.101229
N	-1.441609	1.681257	-0.221606
H	-1.858467	1.858616	0.696962
C	7.037333	-0.270536	-0.170953
H	7.652897	-1.125877	-0.464082
C	7.622903	0.957741	0.092421
H	8.706289	1.081746	0.008314
C	6.814414	2.051970	0.473089
H	7.276433	3.021148	0.682670
C	5.442869	1.908378	0.585611
H	4.852955	2.775868	0.886511
C	4.802683	0.662105	0.320144
C	5.637972	-0.450196	-0.065797
C	5.041086	-1.717797	-0.329823
H	5.691343	-2.549879	-0.615487
C	3.685043	-1.903675	-0.231906
H	3.214659	-2.869256	-0.431828
C	2.839305	-0.812743	0.134290
C	3.393755	0.460028	0.417807
C	2.453121	1.535449	0.867851
H	1.984252	1.252621	1.828983
H	2.979990	2.484374	1.036238
C	0.577939	2.974072	0.124955

H	1.146176	3.880857	-0.148658
H	0.362170	3.039986	1.204536
C	-0.718609	2.881911	-0.655393
H	-0.502058	2.772190	-1.731150
H	-1.324014	3.798219	-0.537419
C	-2.531409	1.265876	-1.131996
H	-2.052138	0.889980	-2.055081
H	-3.147199	2.136556	-1.415520
C	-2.789908	-0.981691	-0.008691
C	-3.624547	-2.014022	0.486480
H	-3.150569	-2.919407	0.873640
C	-5.003244	-1.861833	0.507484
H	-5.633568	-2.652928	0.923015
C	-5.600160	-0.681891	0.013341
C	-4.782929	0.335818	-0.516117
H	-5.231878	1.233760	-0.940158
C	-3.396059	0.204261	-0.522741
C	-7.680017	1.163924	0.309479
F	-8.966631	1.279807	0.631582
F	-7.447789	1.908488	-0.789670
F	-6.923604	1.660172	1.297473
H	1.766263	1.782163	-1.035990

S2 – Supporting information for Chapter 3 – Fluorine-based Zn^{2+} complexes for amine sensing

Characterisation data

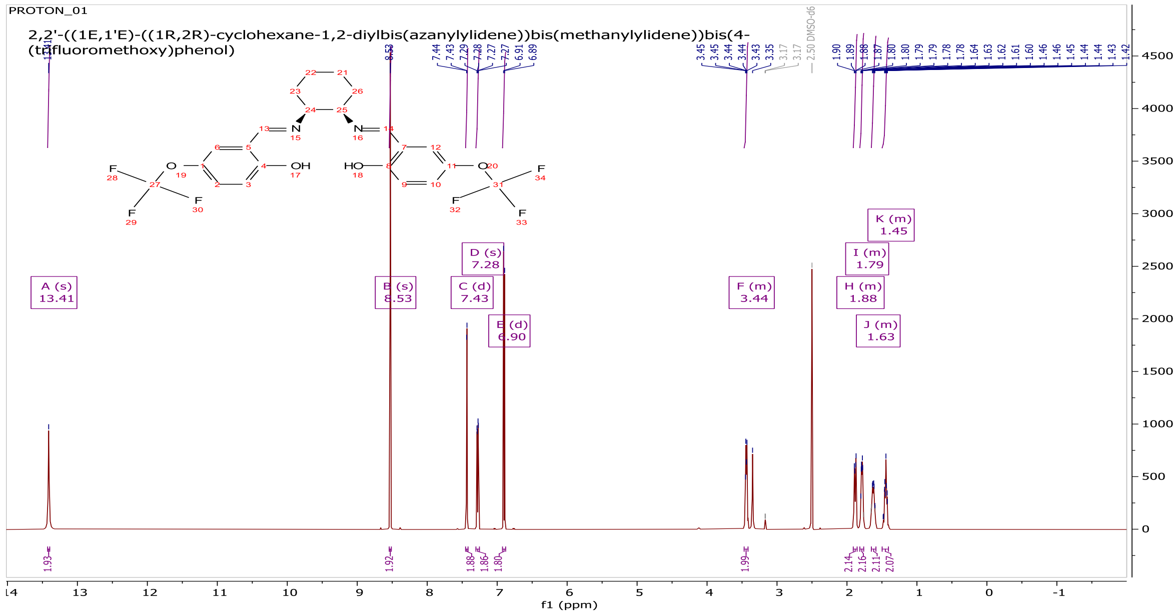


Figure S2-1. ^{1}H-NMR for 1-RR (unreduced)

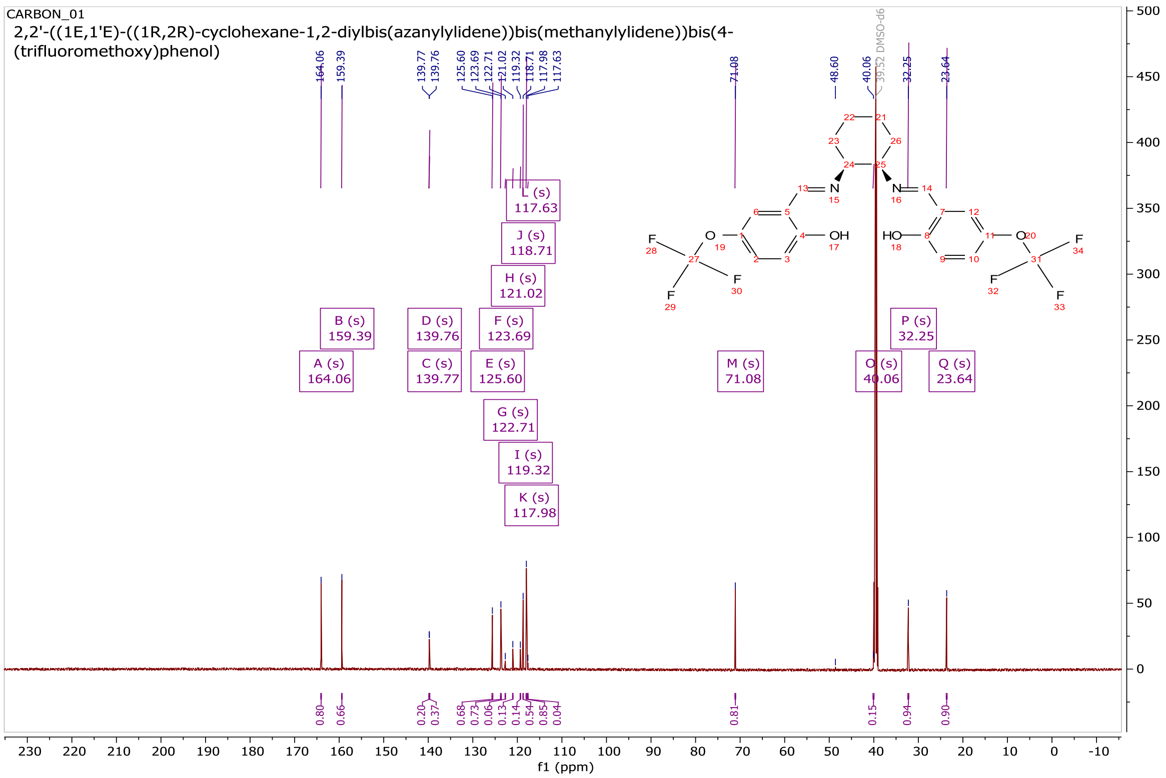


Figure S2-2. ^{13}C-NMR for 1-RR (unreduced)

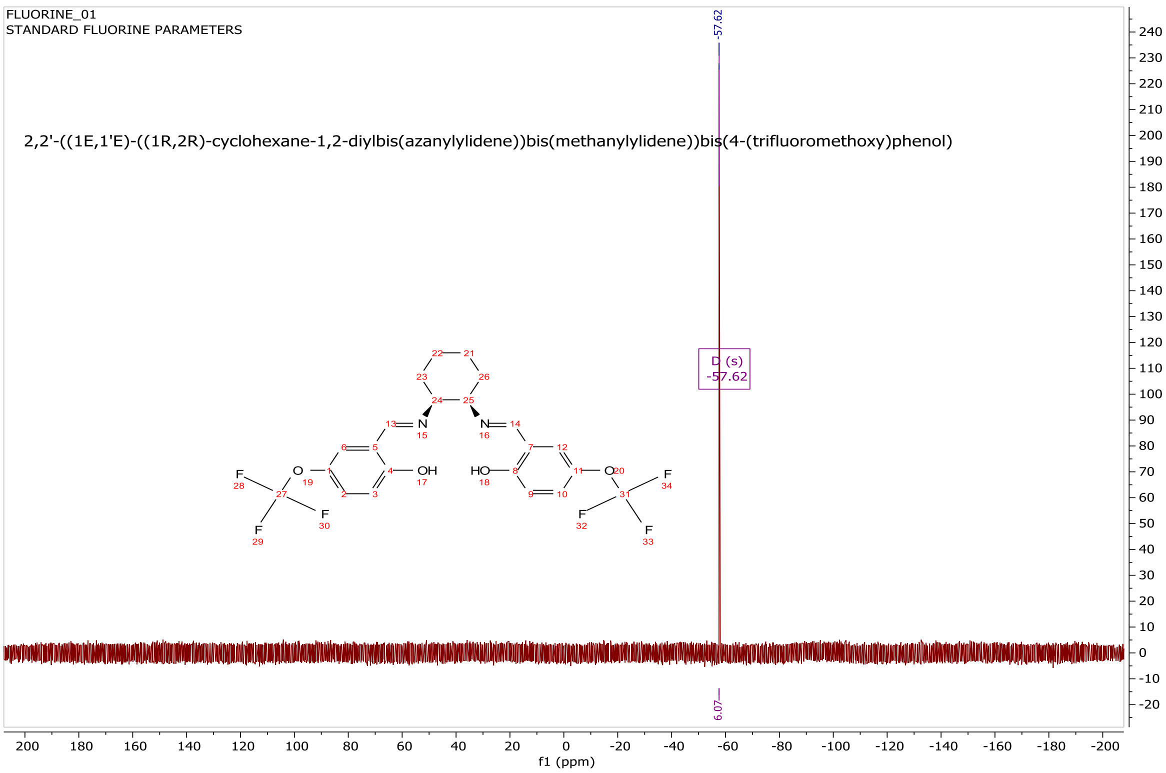


Figure S2-3. ^{19}F-NMR for 1-RR (Unreduced)

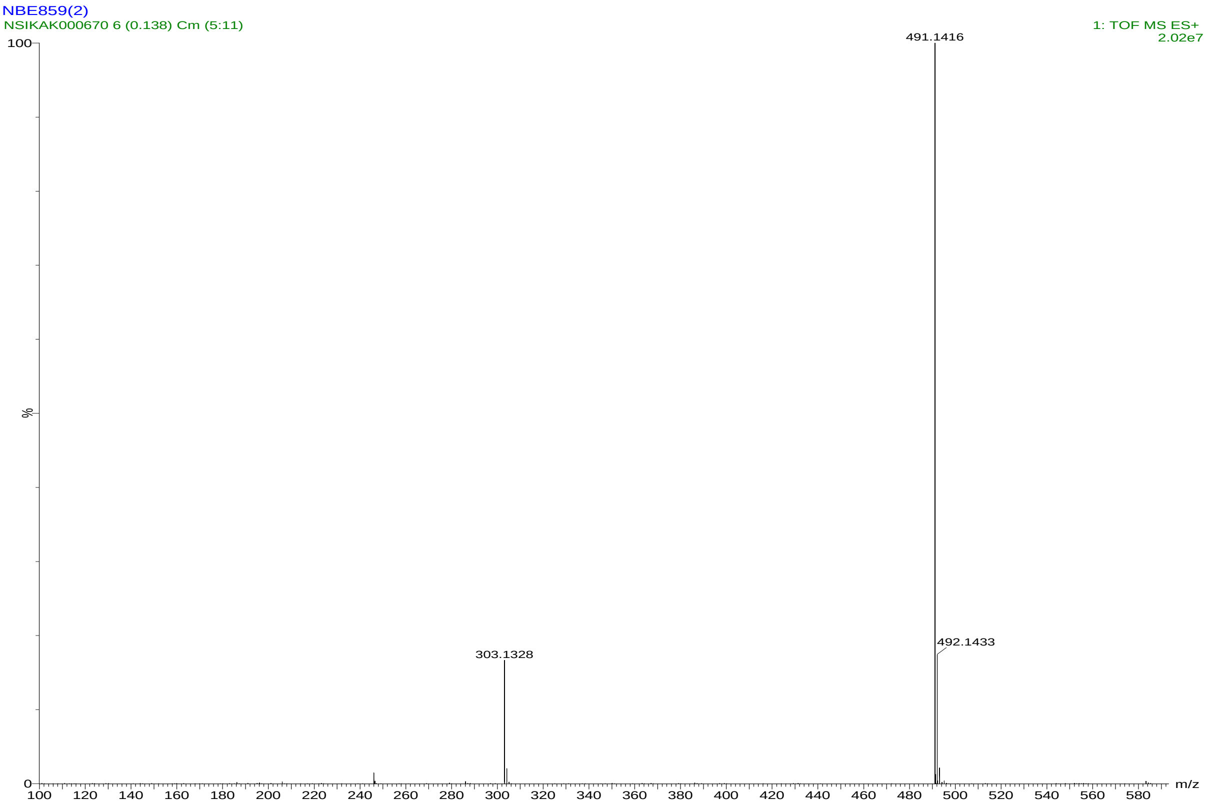


Figure S2-4. HRMS for 1-RR (Unreduced)

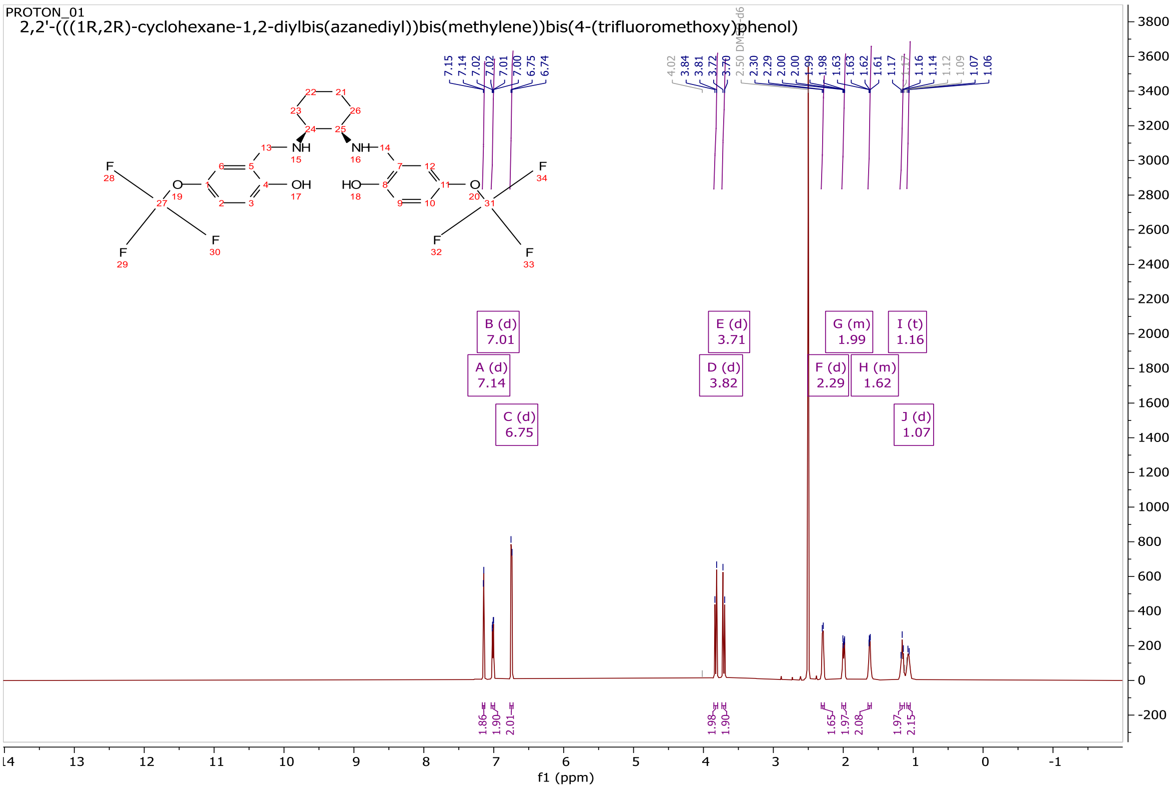


Figure S2-5. ^{1}H-NMR for **1-RR**

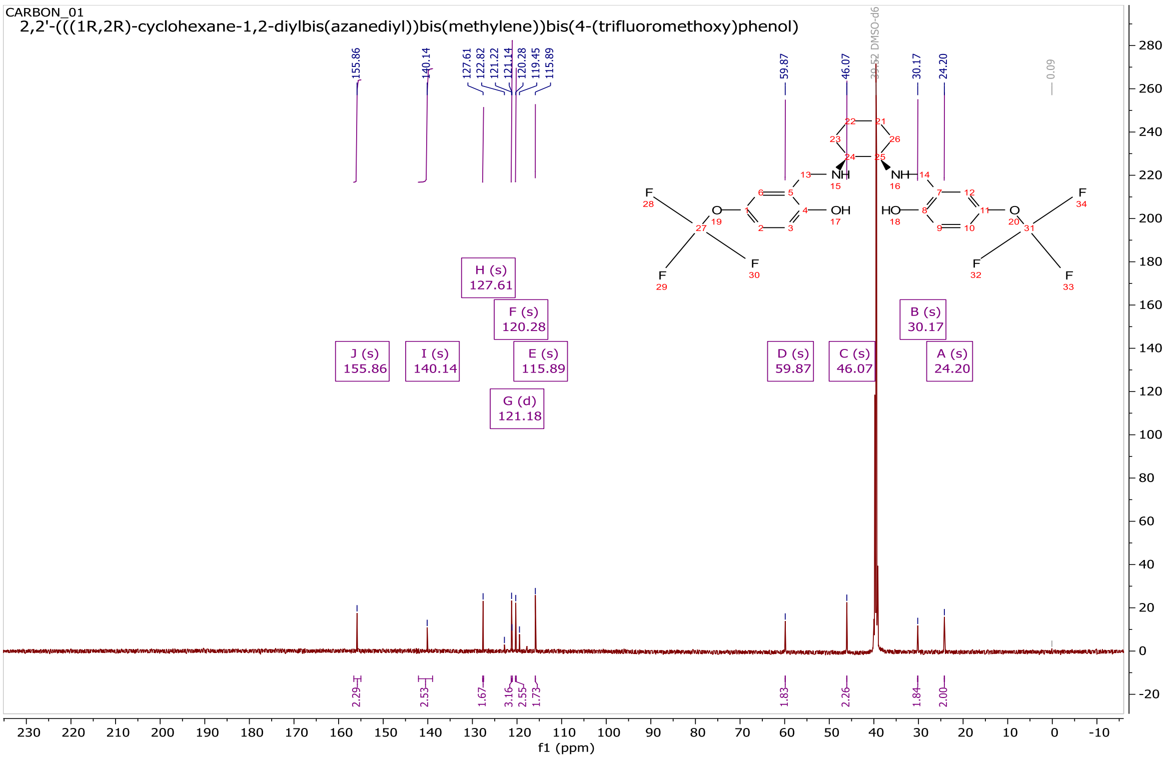


Figure S2-6. ^{13}C-NMR for **1-RR**

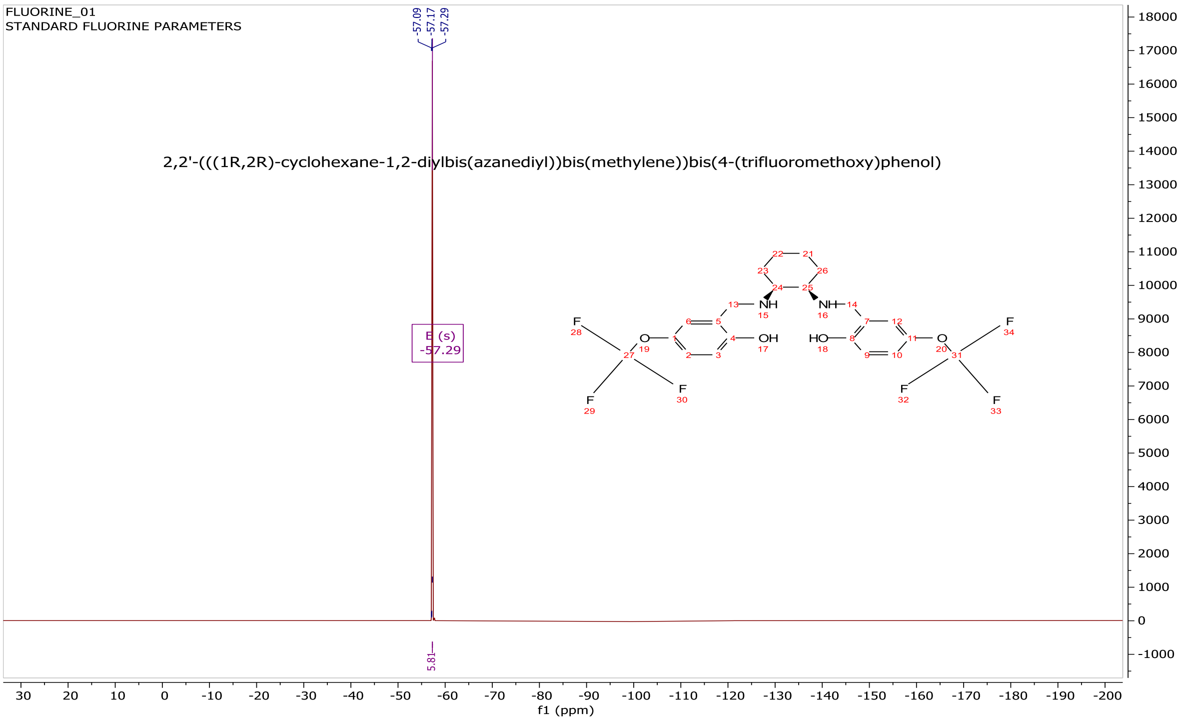


Figure S2-7. [19]F-NMR for **1-RR**

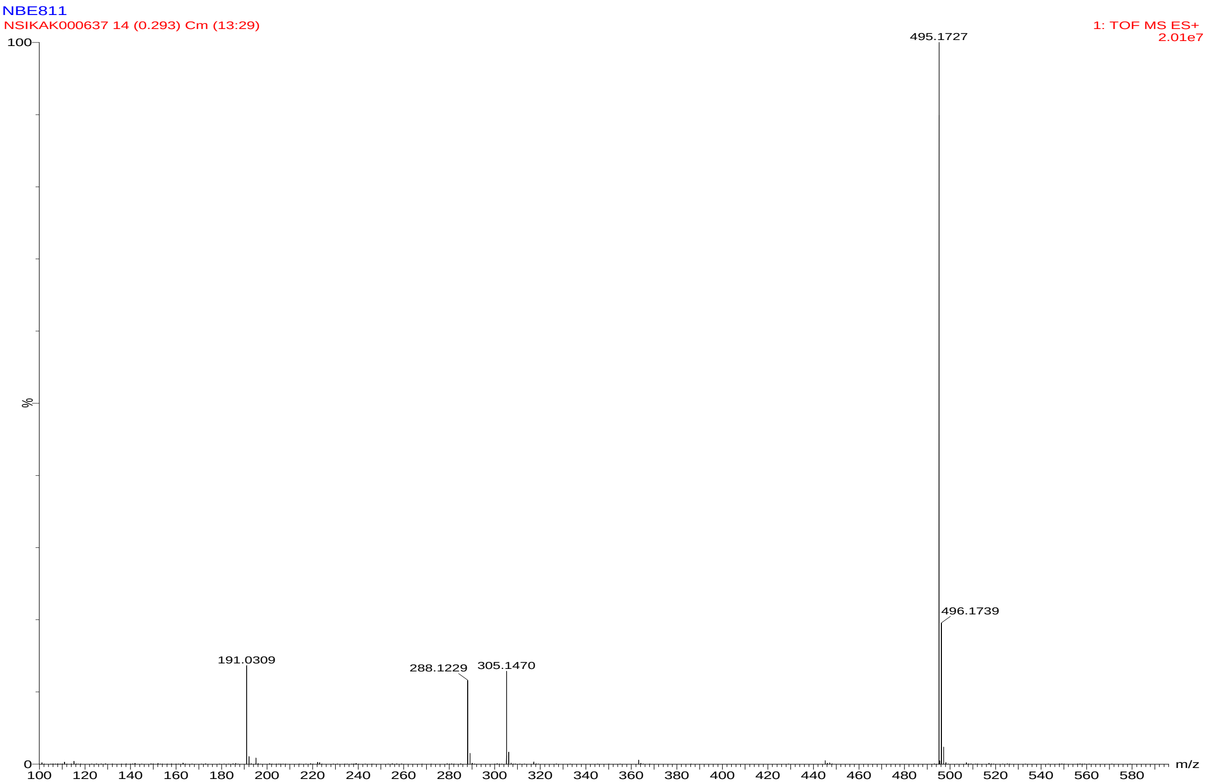


Figure S2-8. HRMS for **1-RR**

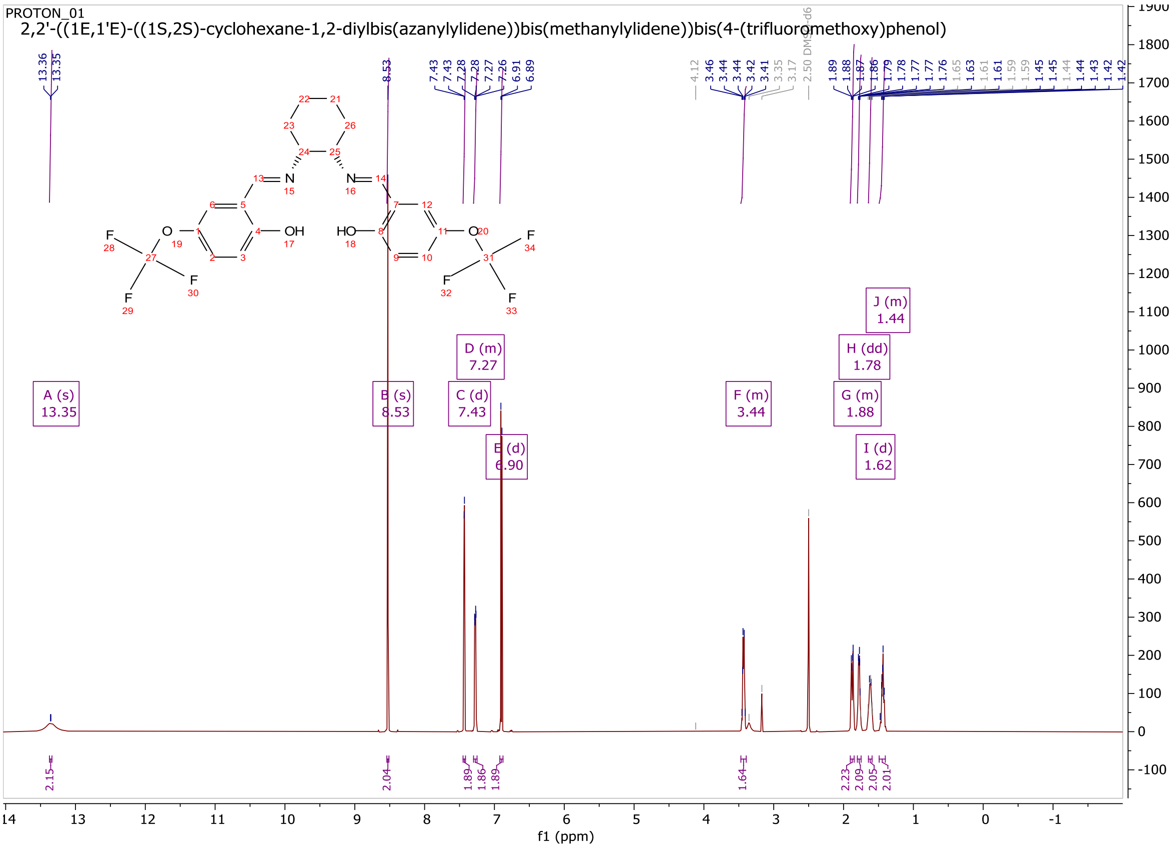


Figure S2-9. ^{1}H-NMR for 1-SS (Unreduced)

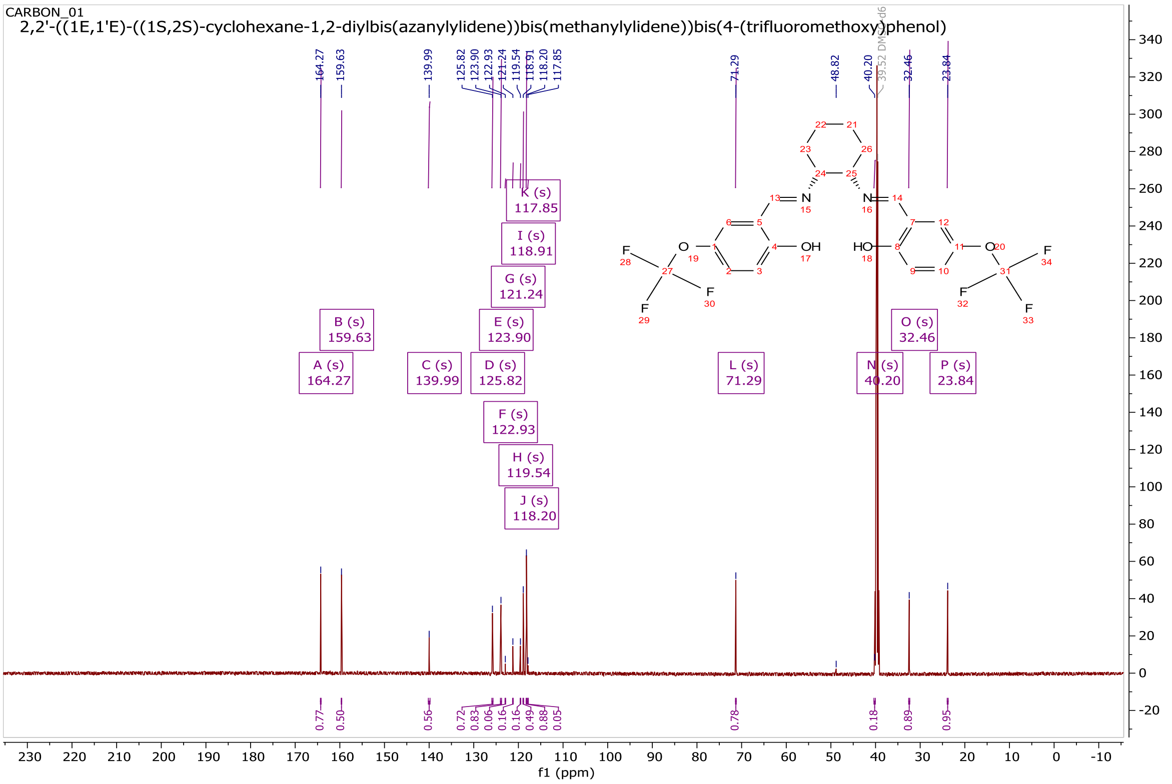


Figure S2-10. ^{13}C-NMR for 1-SS (Unreduced)

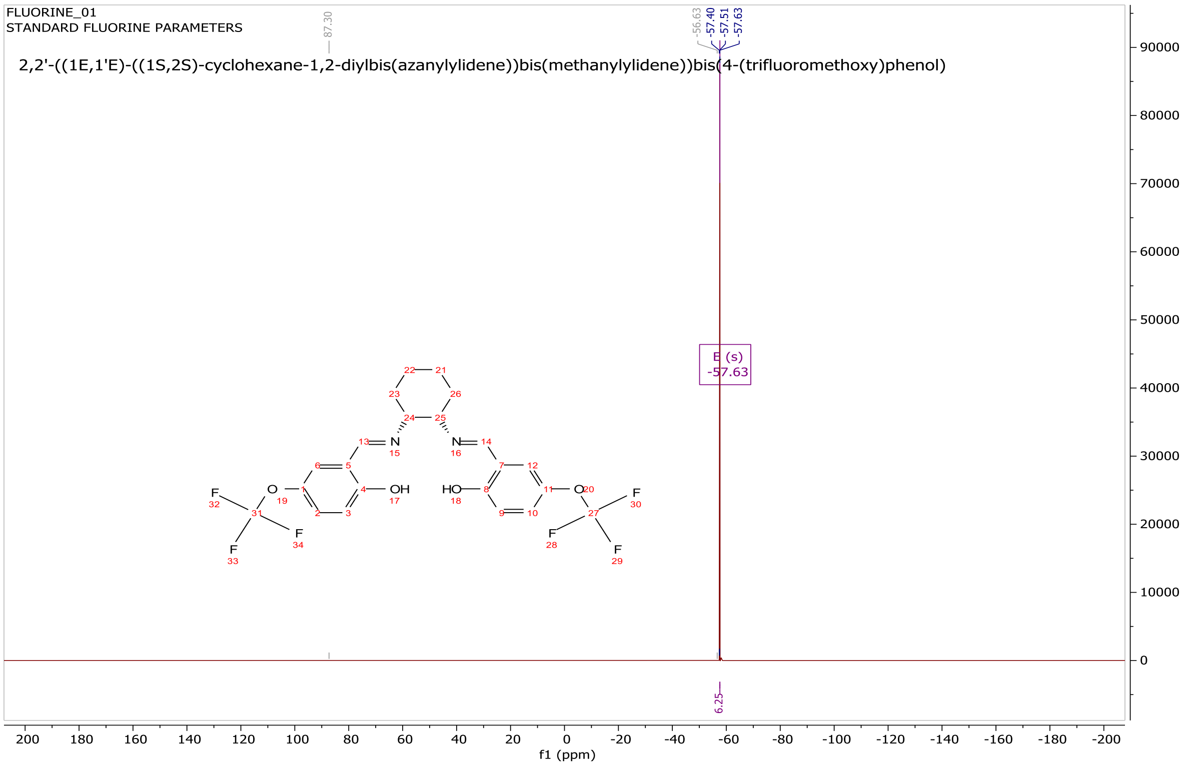


Figure S2-11. ^{19}F-NMR for 1-SS (Unreduced)

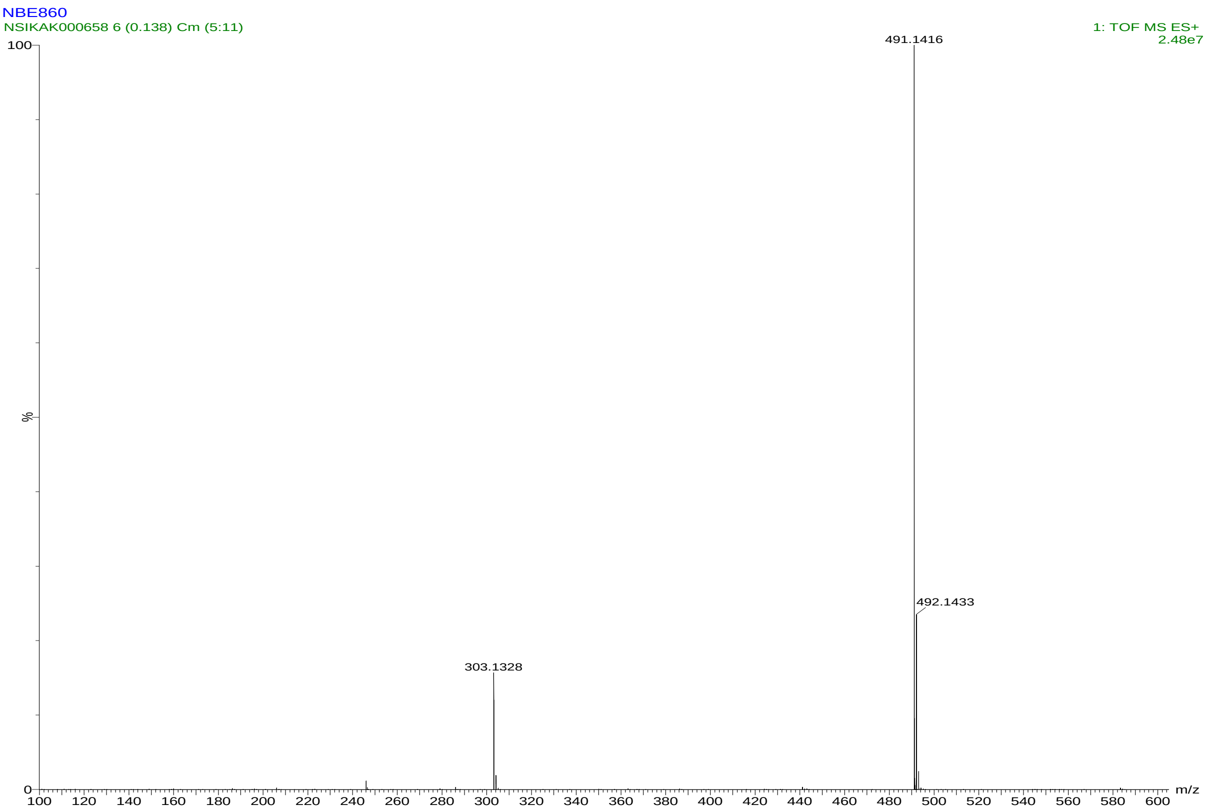


Figure S2-12. HRMS for 1-SS (Unreduced)

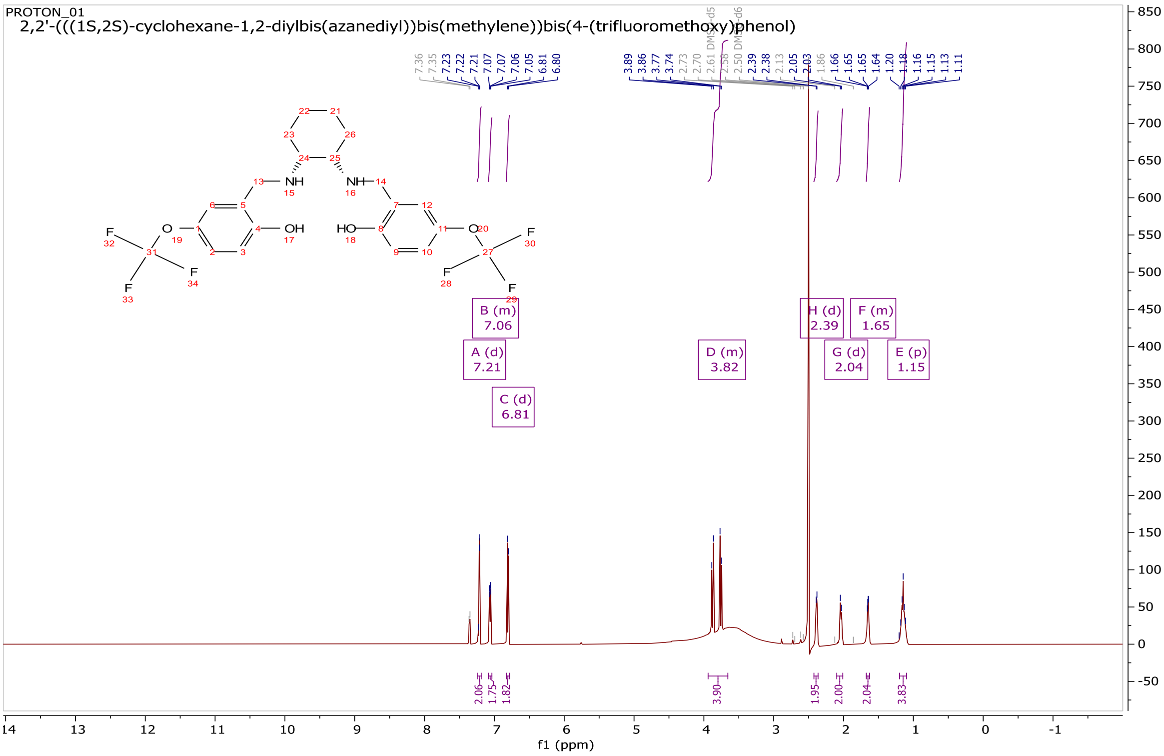


Figure S2-13. ^{1}H-NMR for **1-SS**

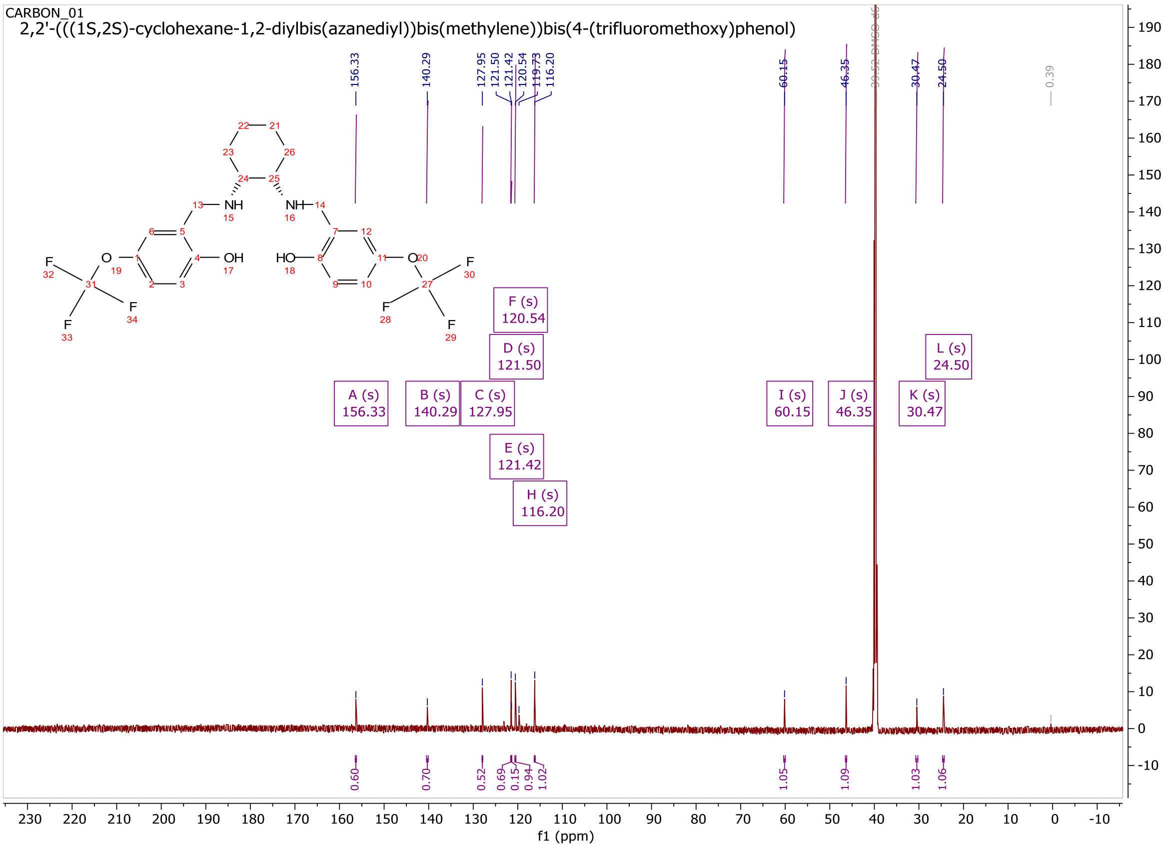


Figure S2-14. ^{13}C-NMR for **1-SS**

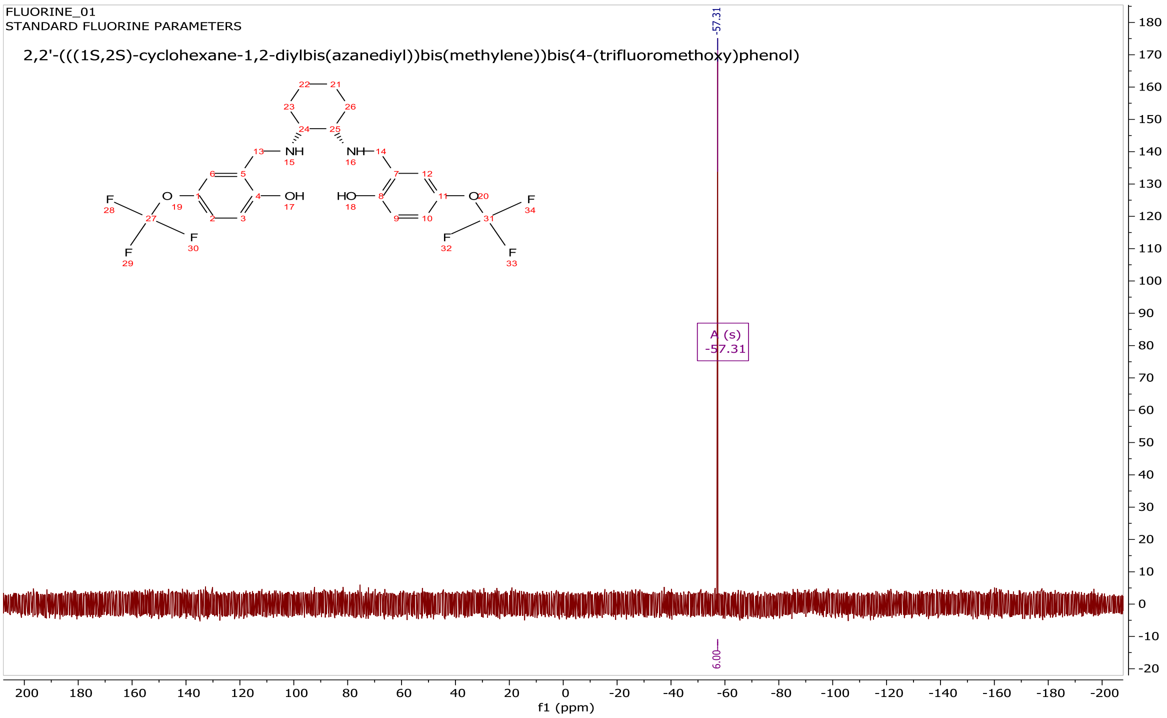


Figure S2-15. ^{19}F-NMR for **1-SS**

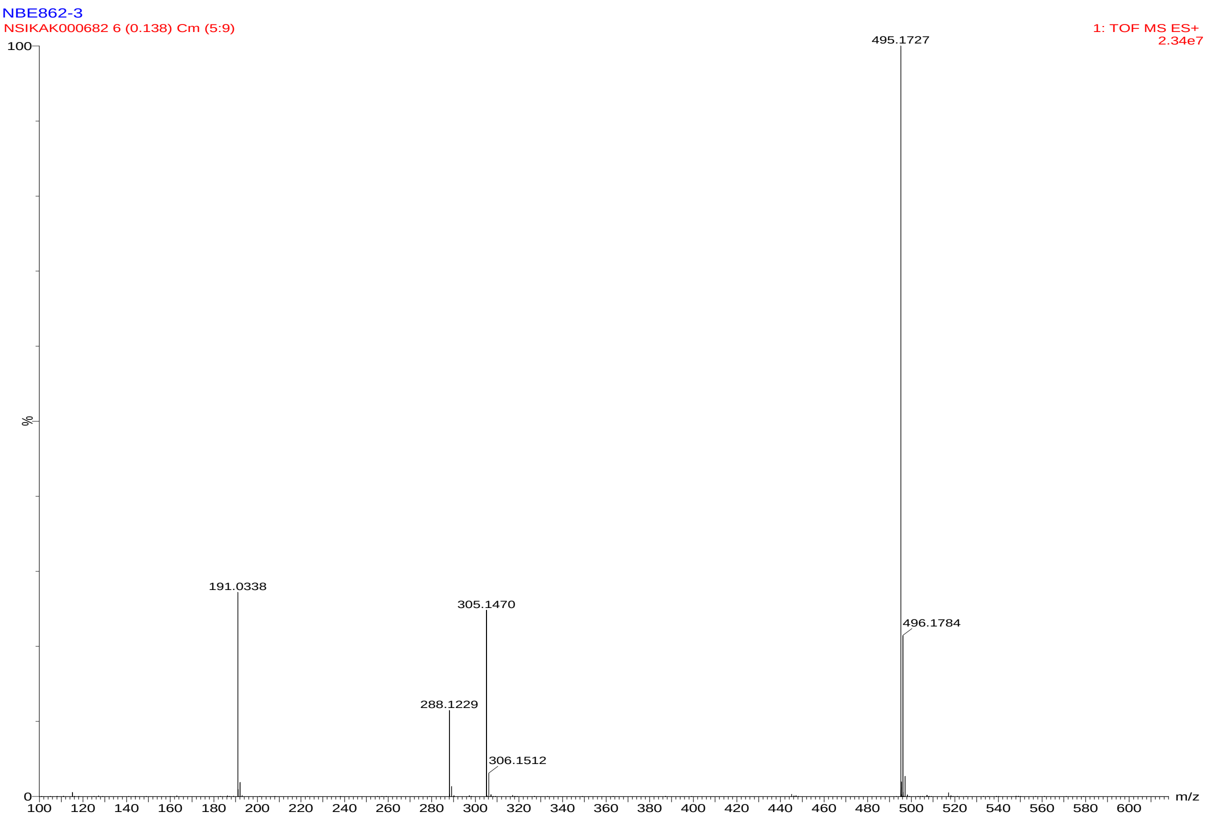


Figure S2-16. HRMS for **1-SS**

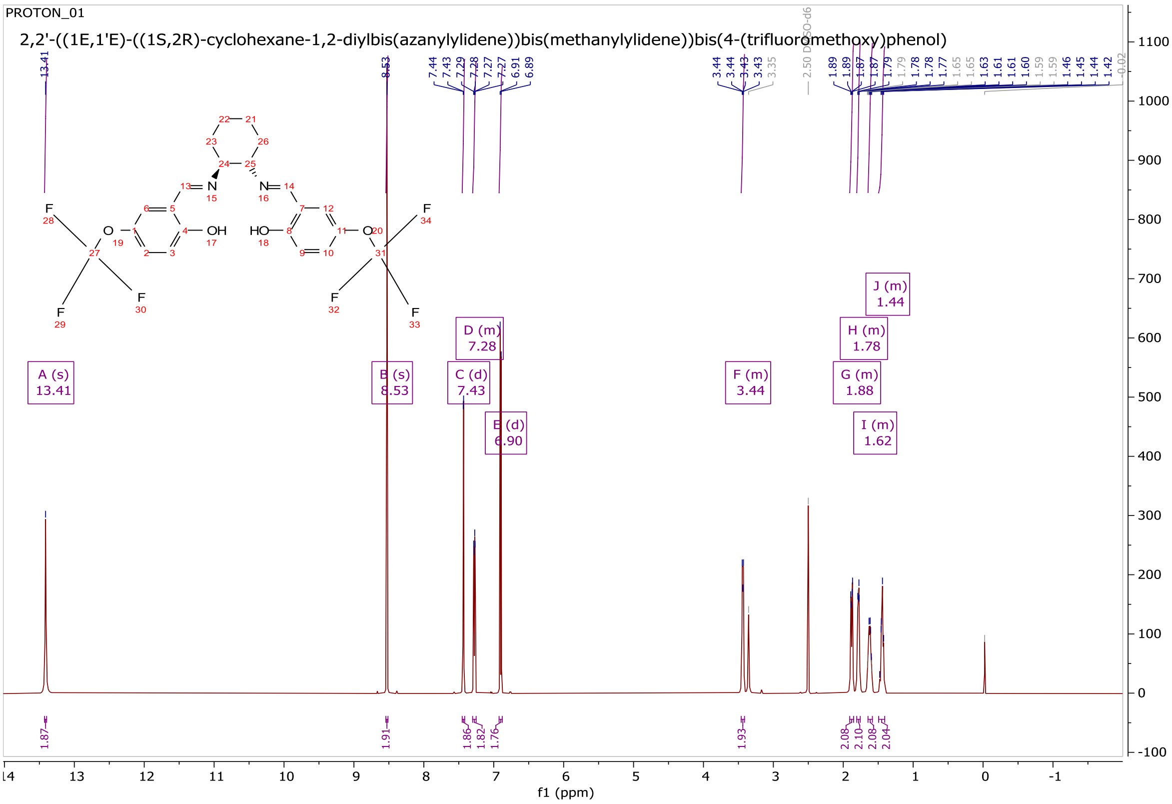


Figure S2-17. ^{1}H-NMR for 1-rac (Unreduced)

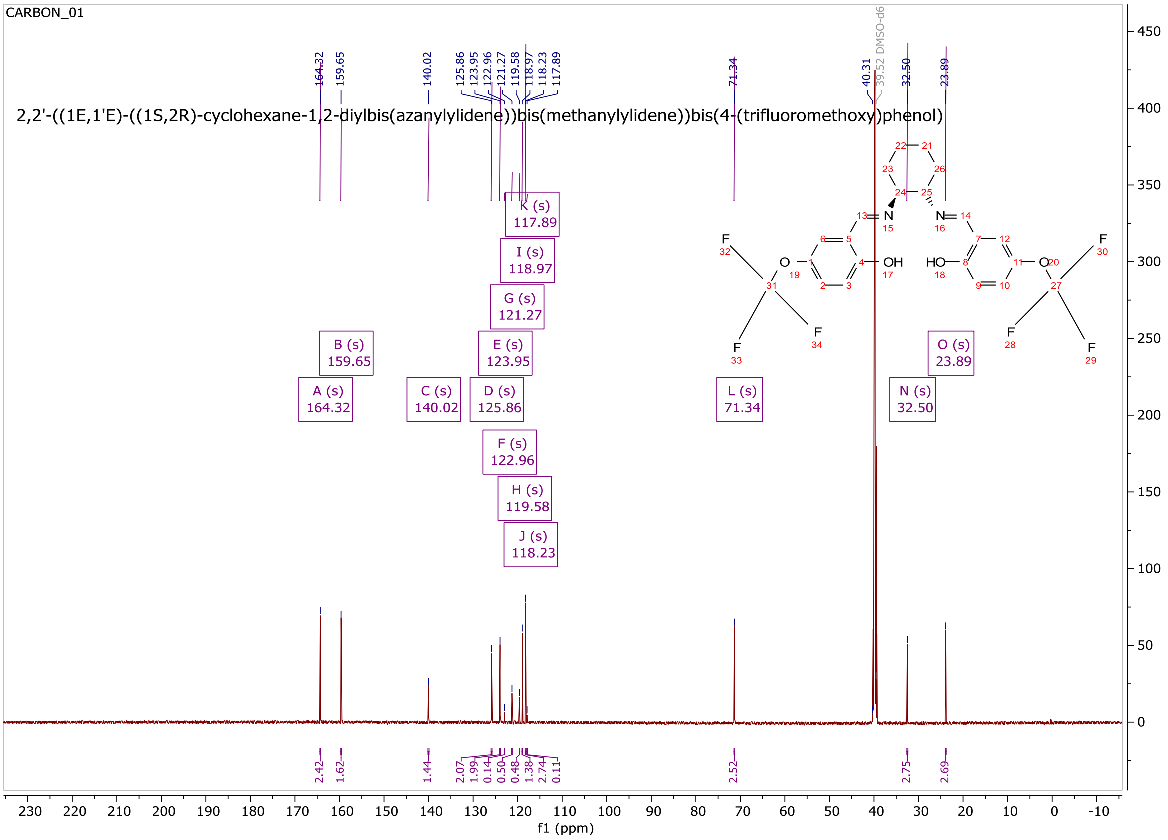


Figure S2-18. ^{13}C-NMR for 1-rac (Unreduced)

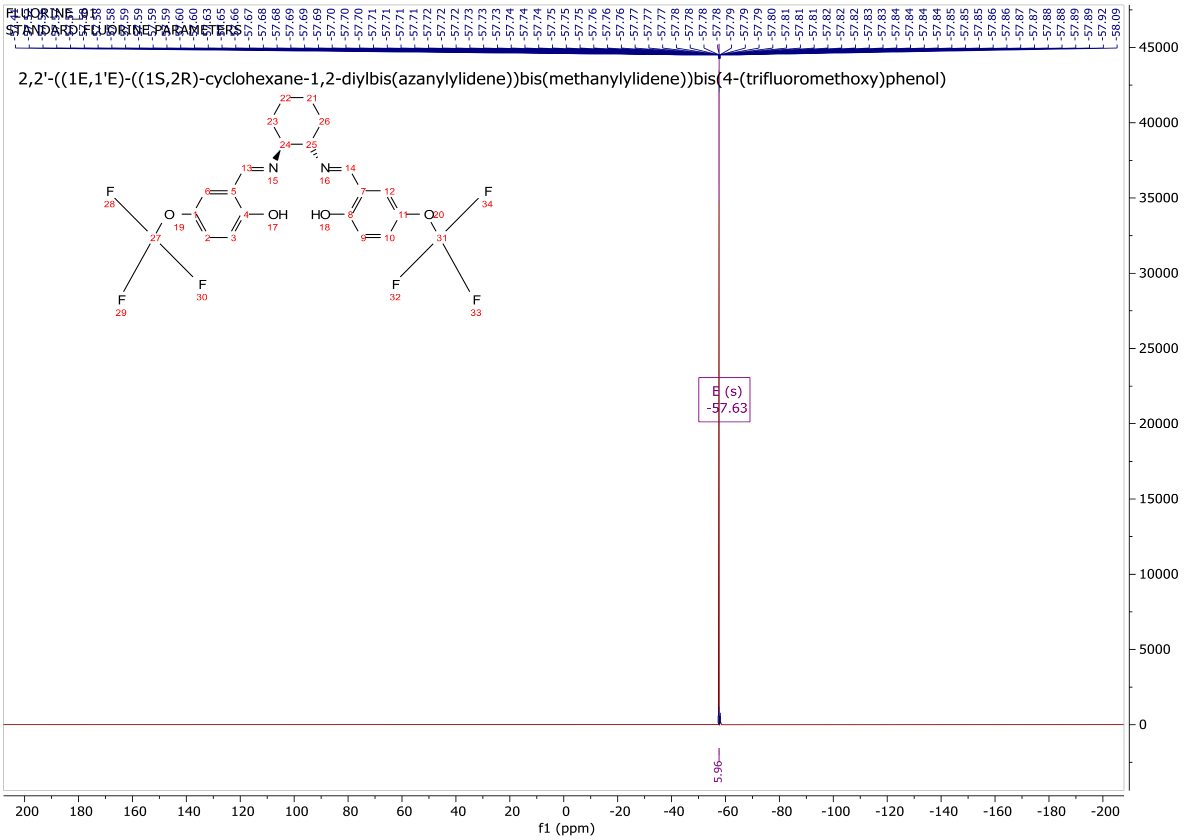


Figure S2-19. [19]F-NMR for 1-rac (Unreduced)

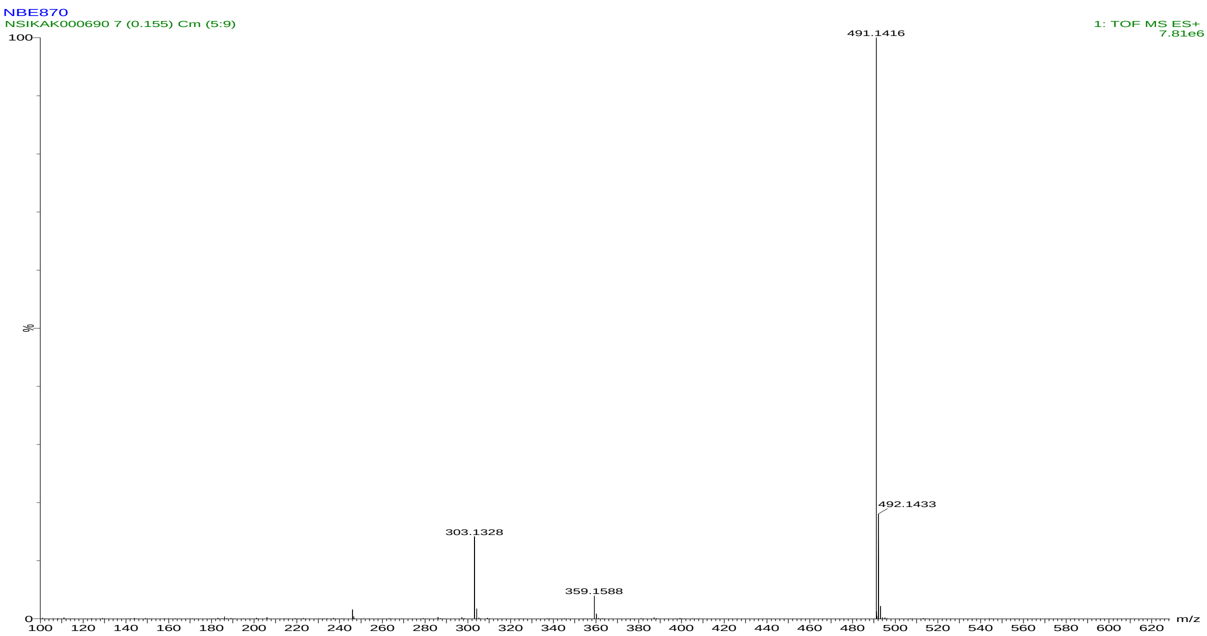


Figure S2-20. HRMS for 1-rac (Unreduced)

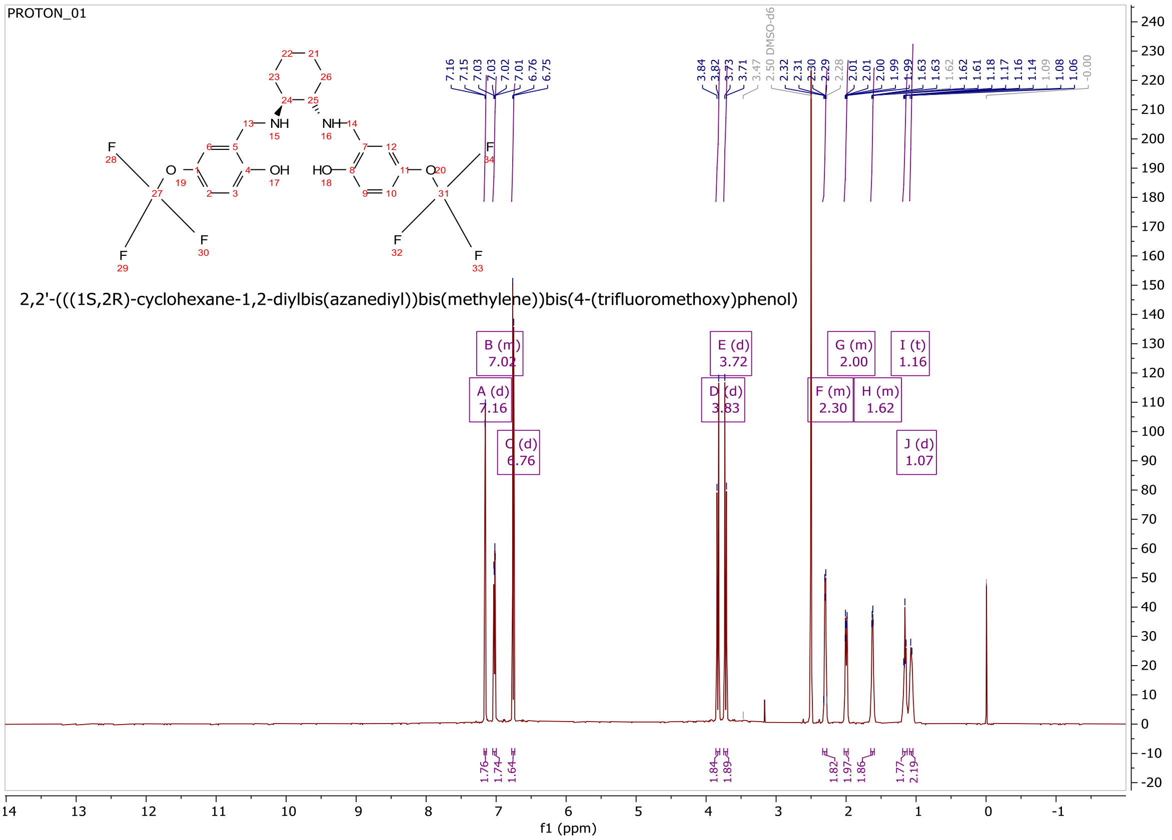


Figure S2-21. ^{1}H-NMR for 1-rac

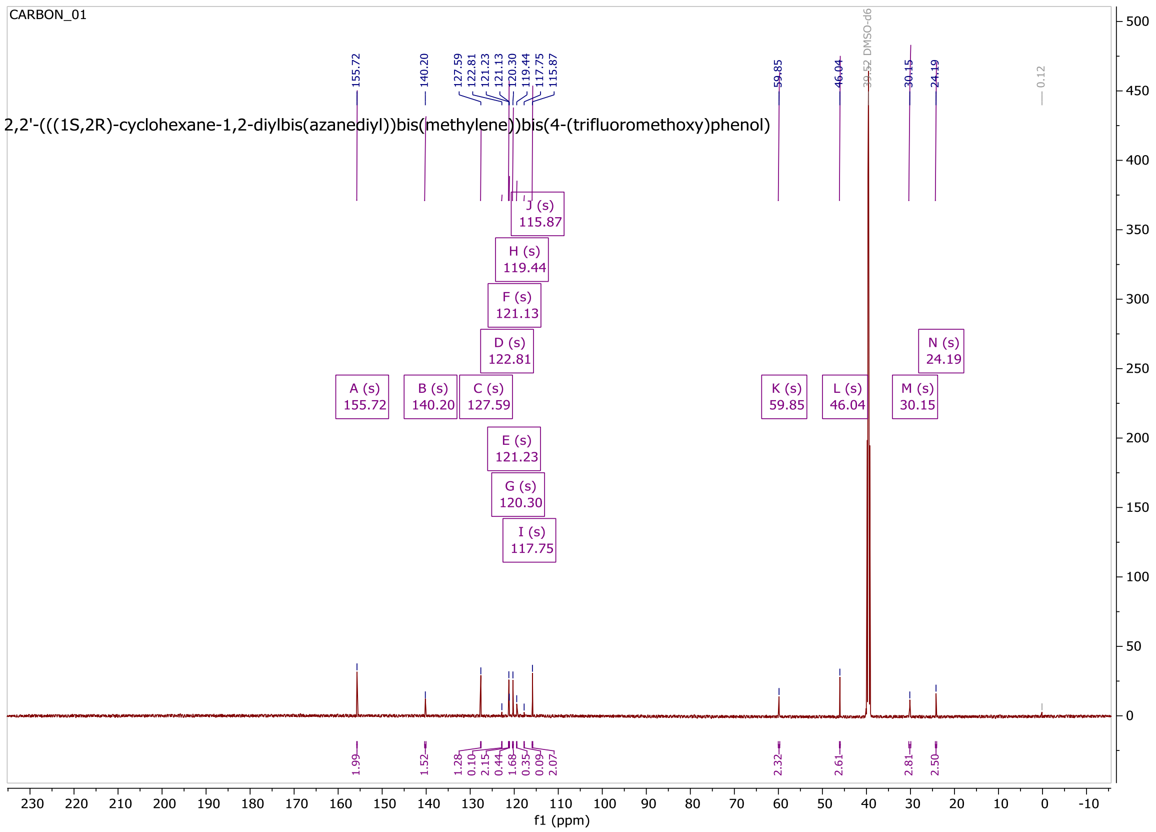


Figure S2-22. ^{13}C-NMR for **1-rac**

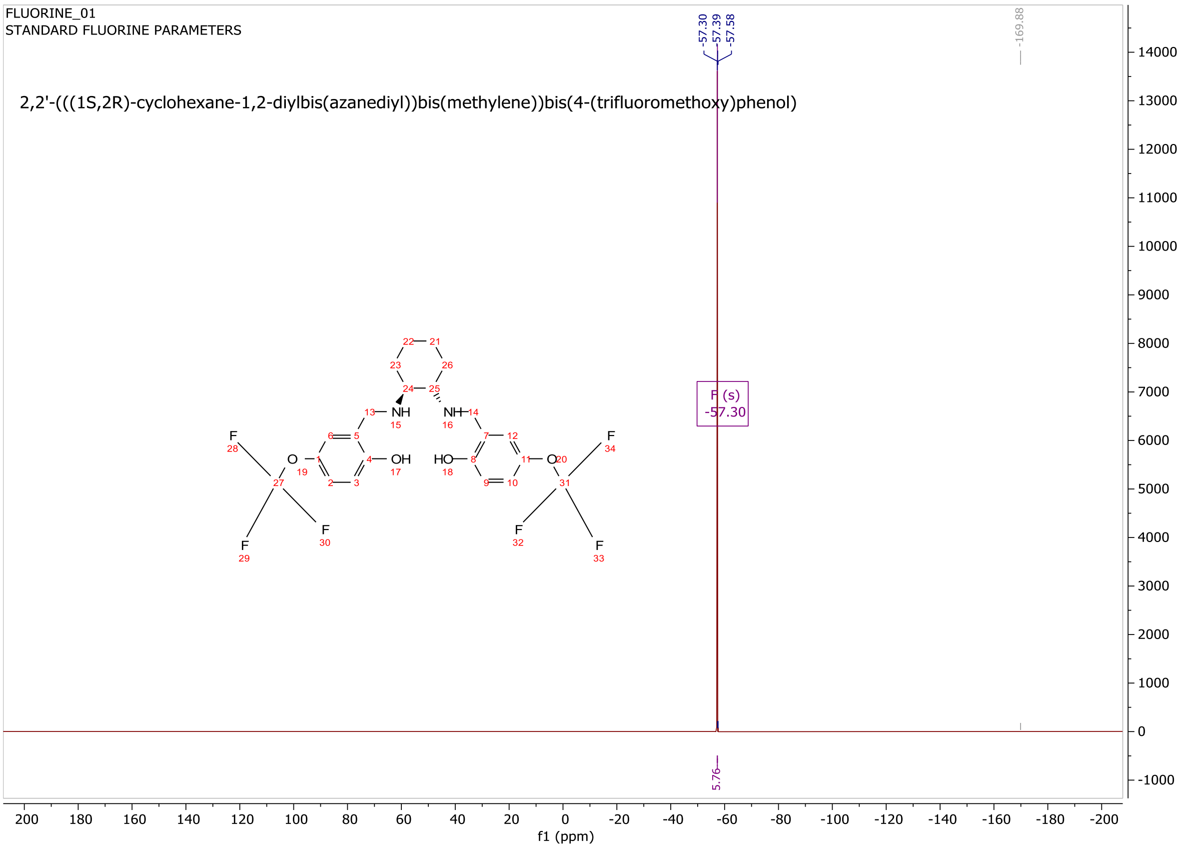


Figure S2-23. [19]F-NMR for **1-rac**

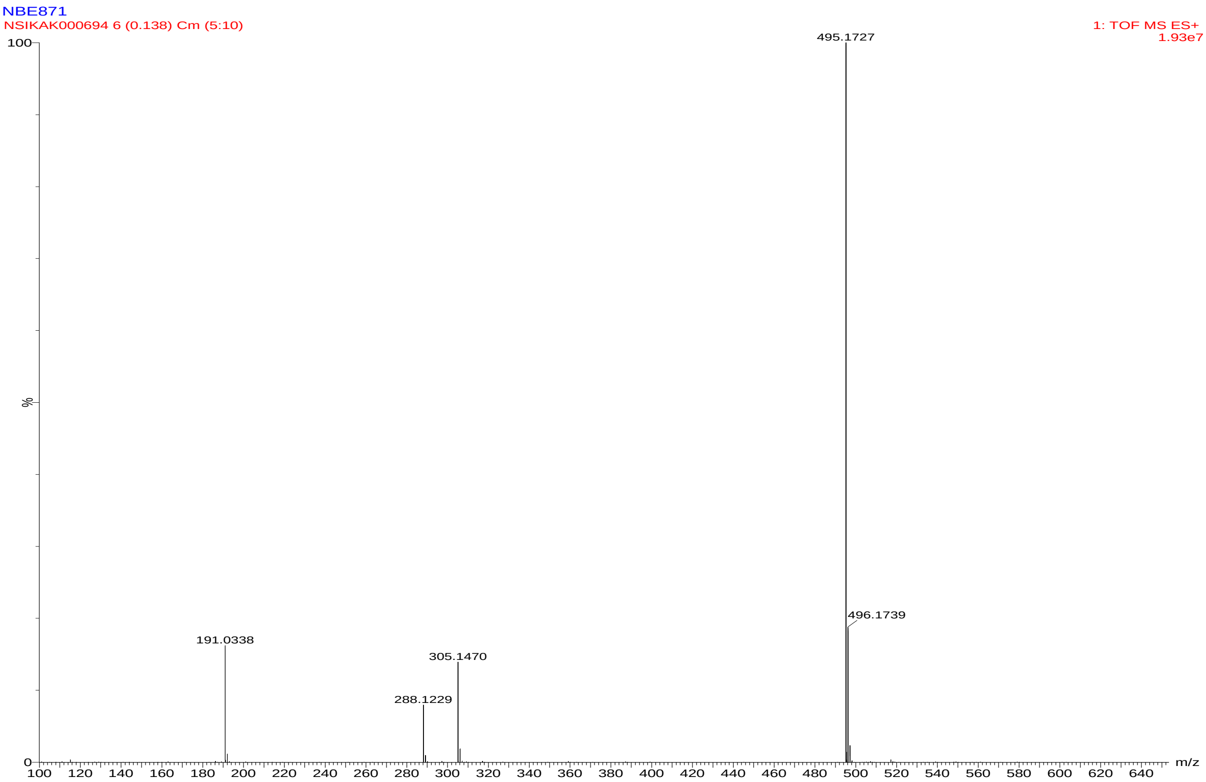


Figure S2-24. HRMS for **1-rac**

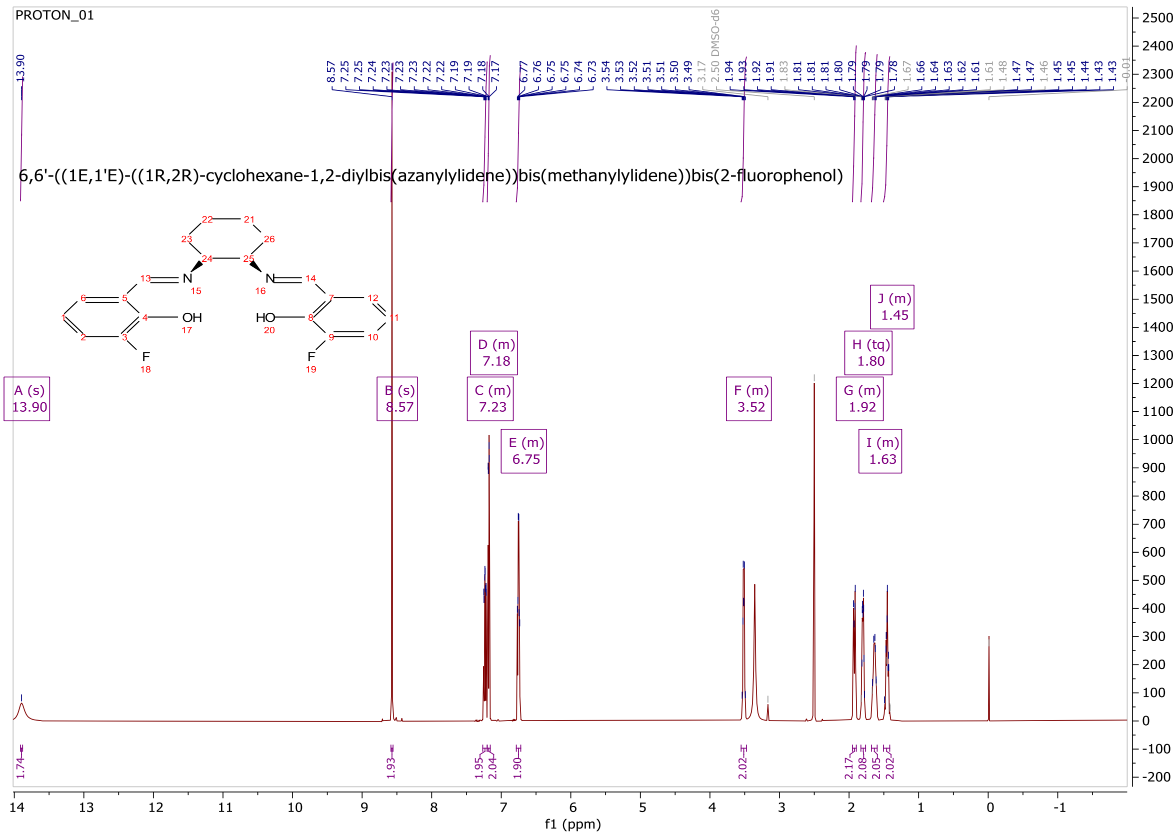


Figure S2-25. ^{1}H-NMR for 2-RR (Unreduced)

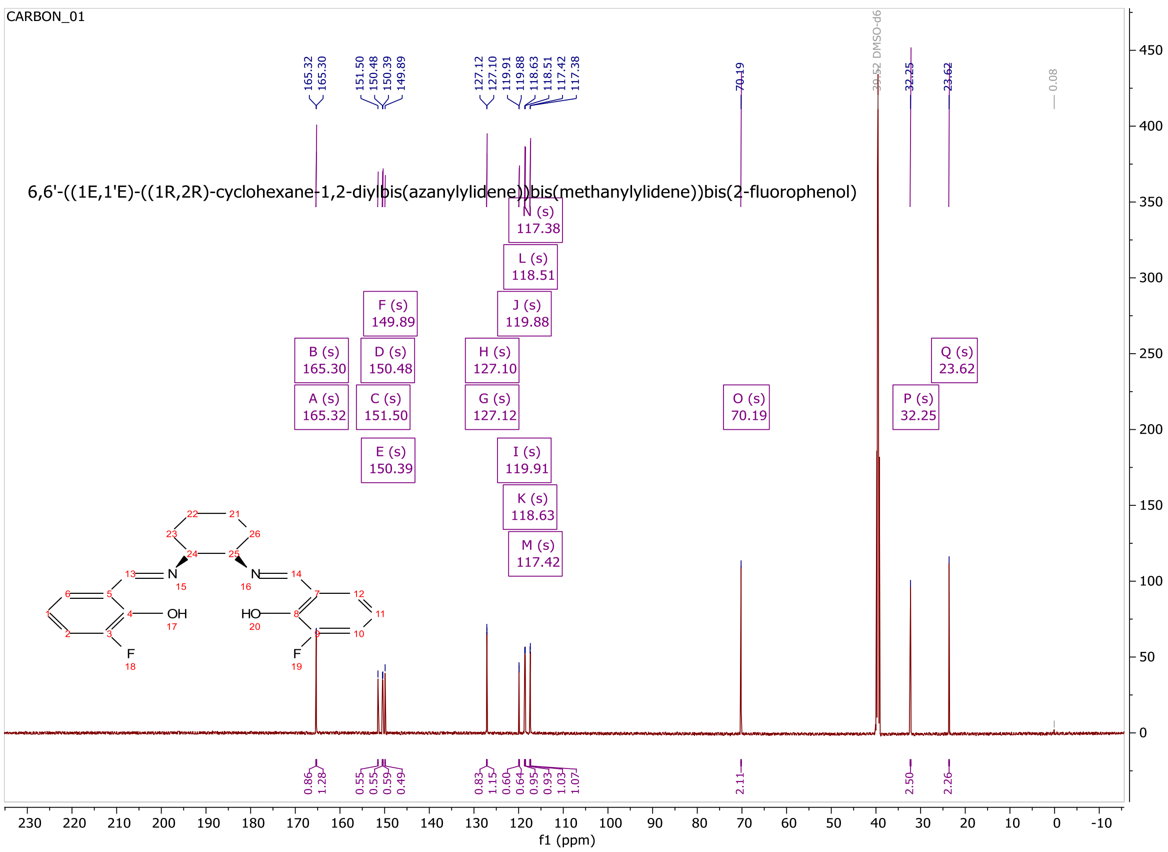


Figure S2-26. ^{13}C-NMR for 2-RR (Unreduced)

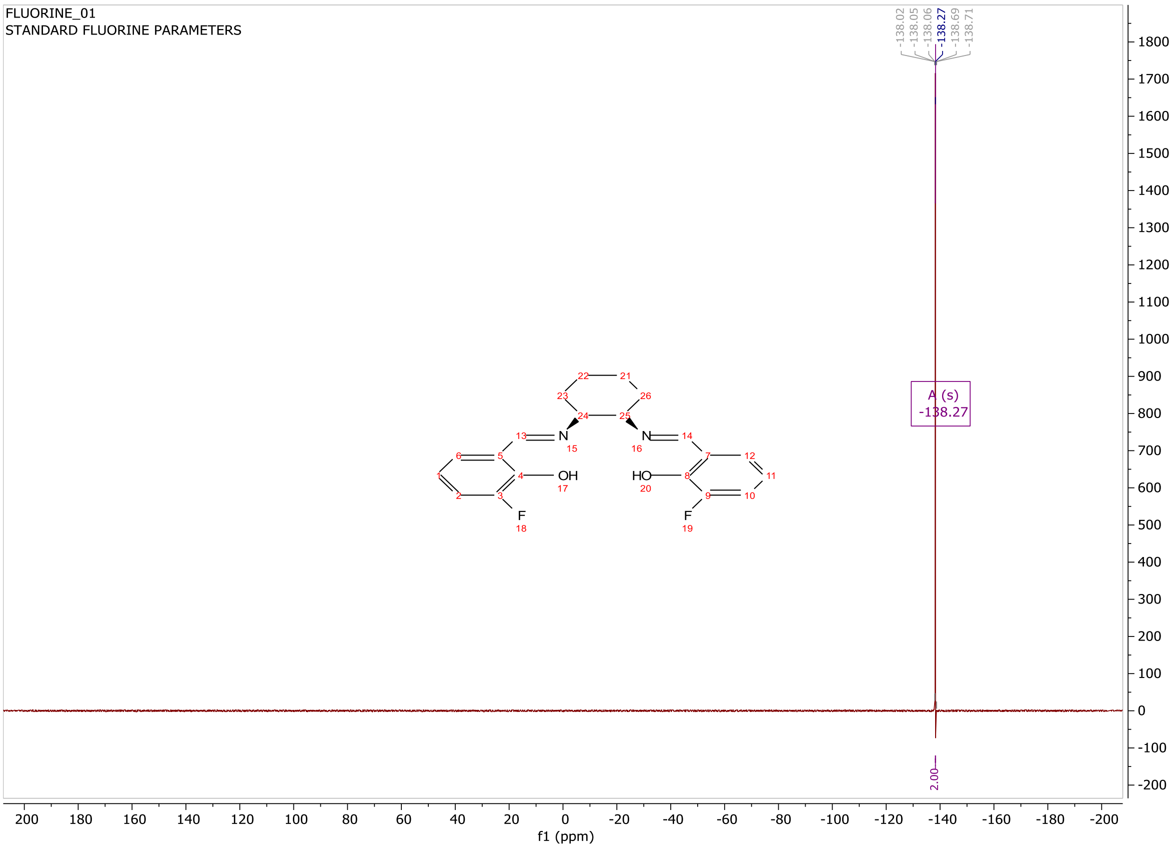


Figure S2-27. ^{19}F-NMR for 2-RR (Unreduced)

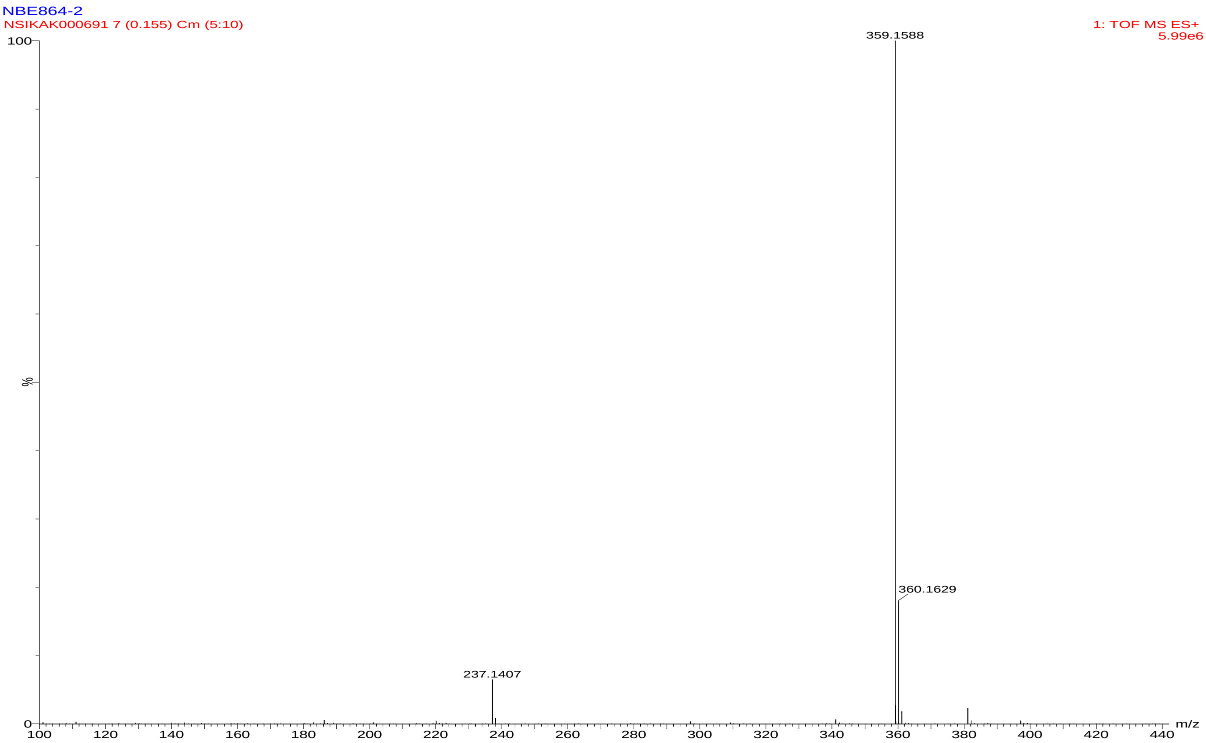


Figure S2-28. HRMS for 2-RR (Unreduced)

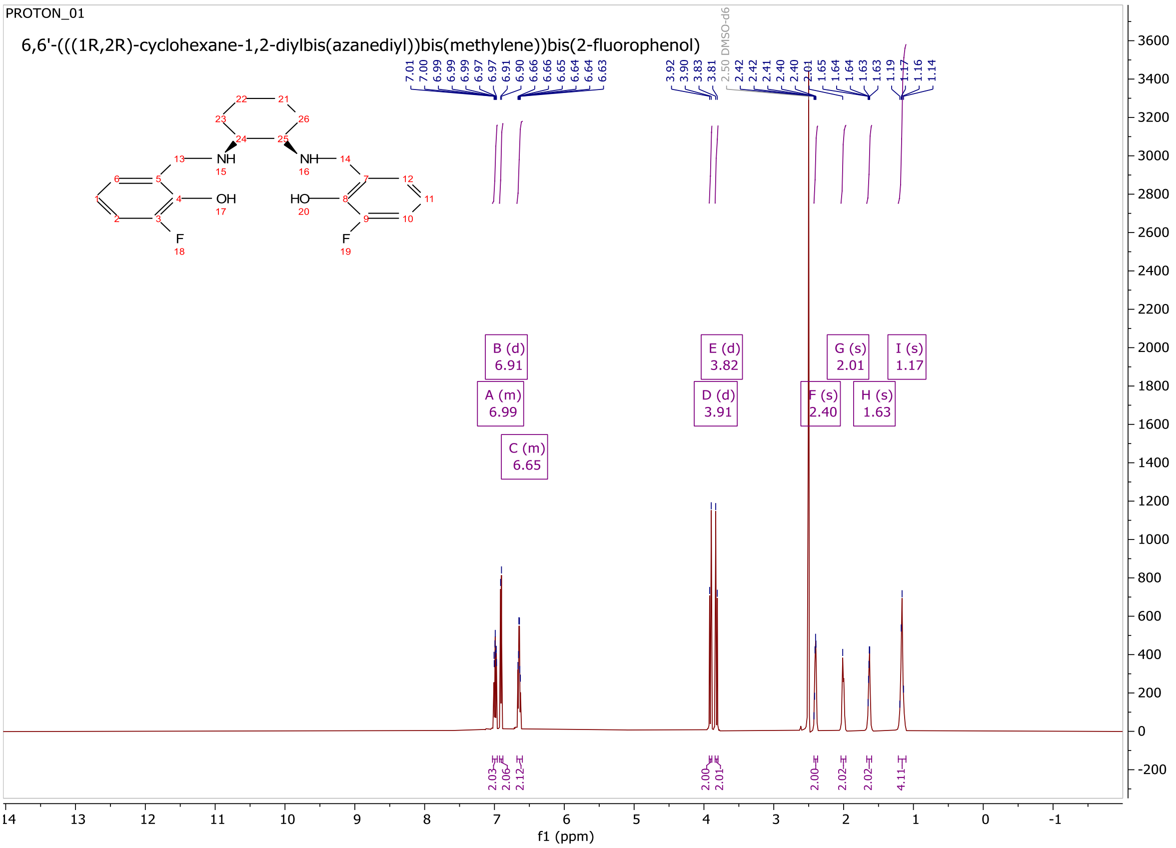


Figure S2-29. ^{1}H-NMR for 2-RR

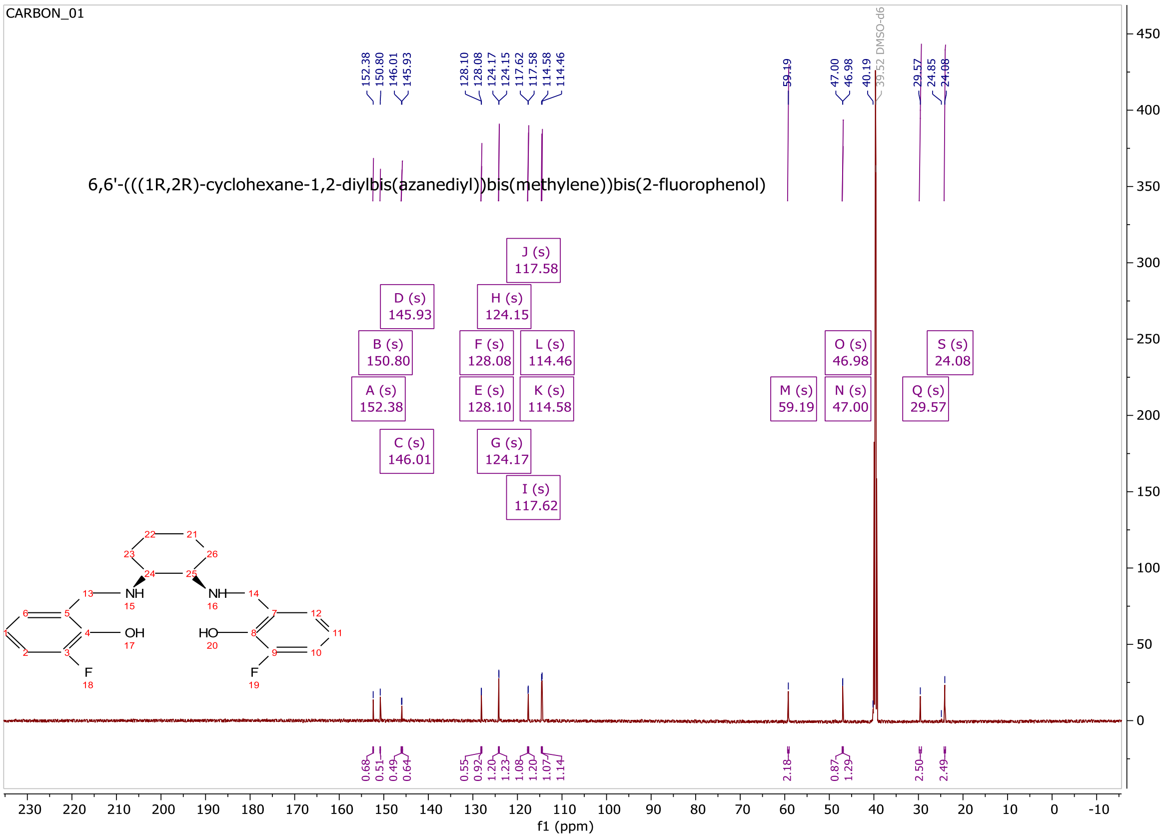


Figure S2-30. ^{13}C-NMR for **2-RR**

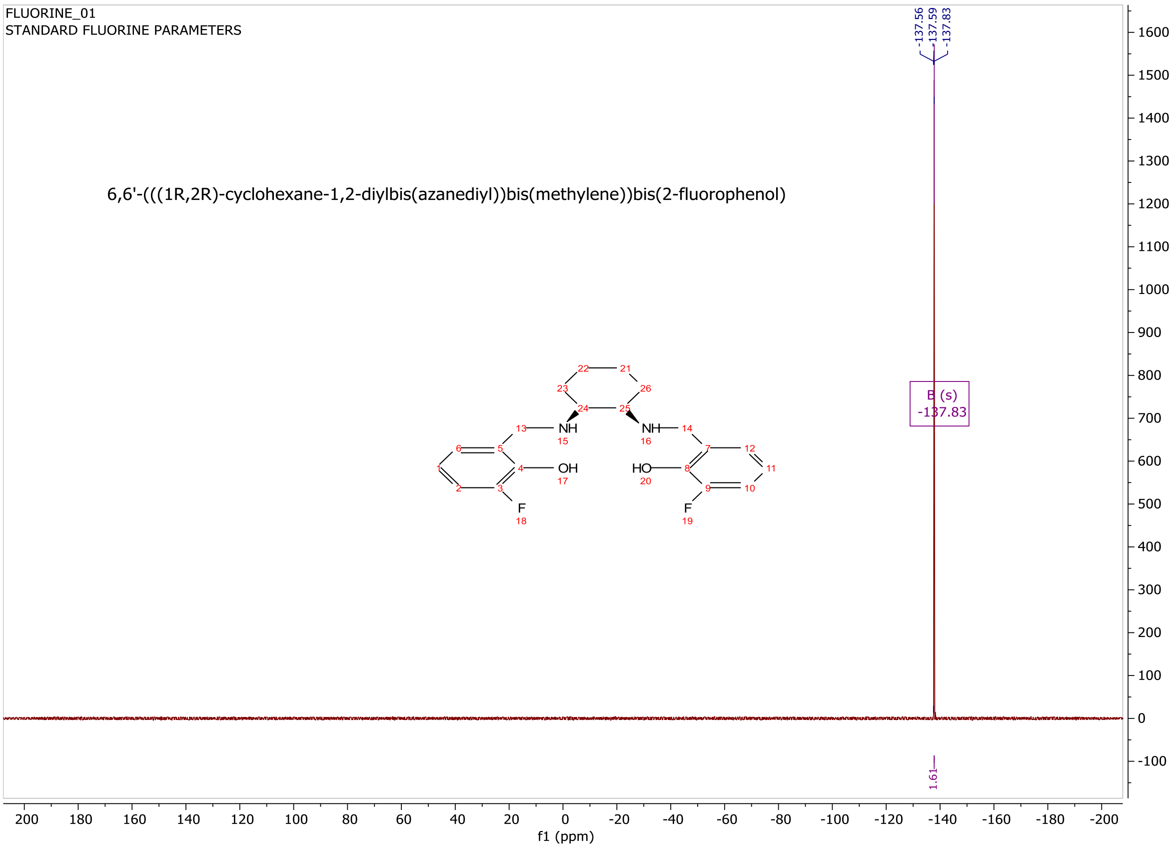


Figure S2-31. ^{19}F-NMR for **2-RR**

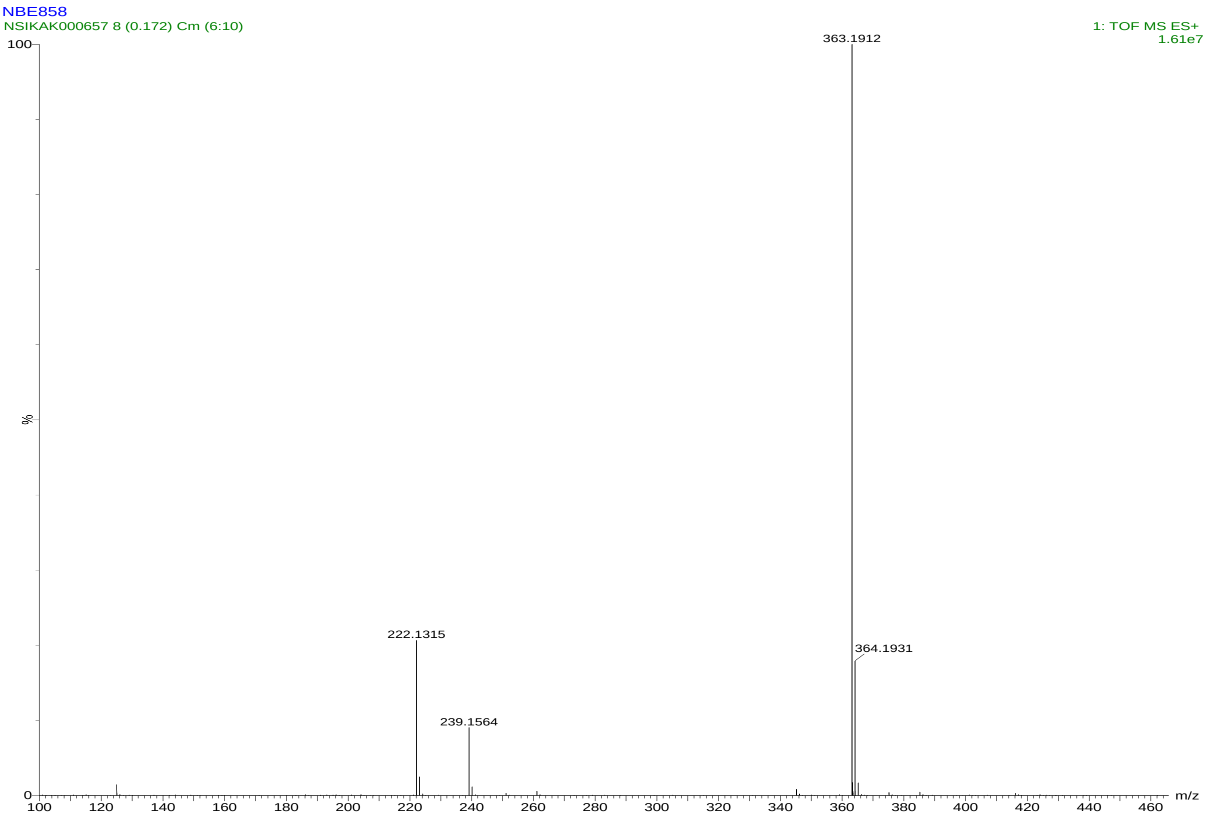


Figure S2-32. HRMS for **2-RR**

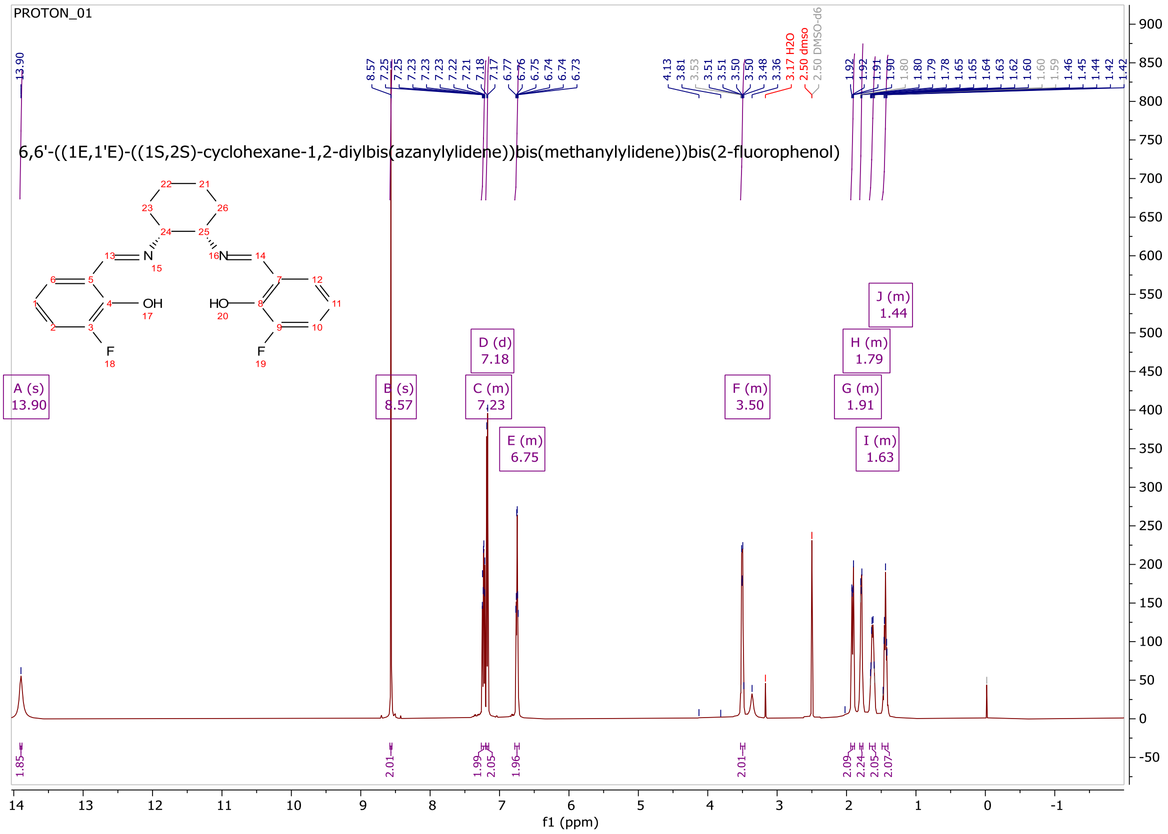


Figure S2-33. ^{1}H-NMR for 2-SS (Unreduced)

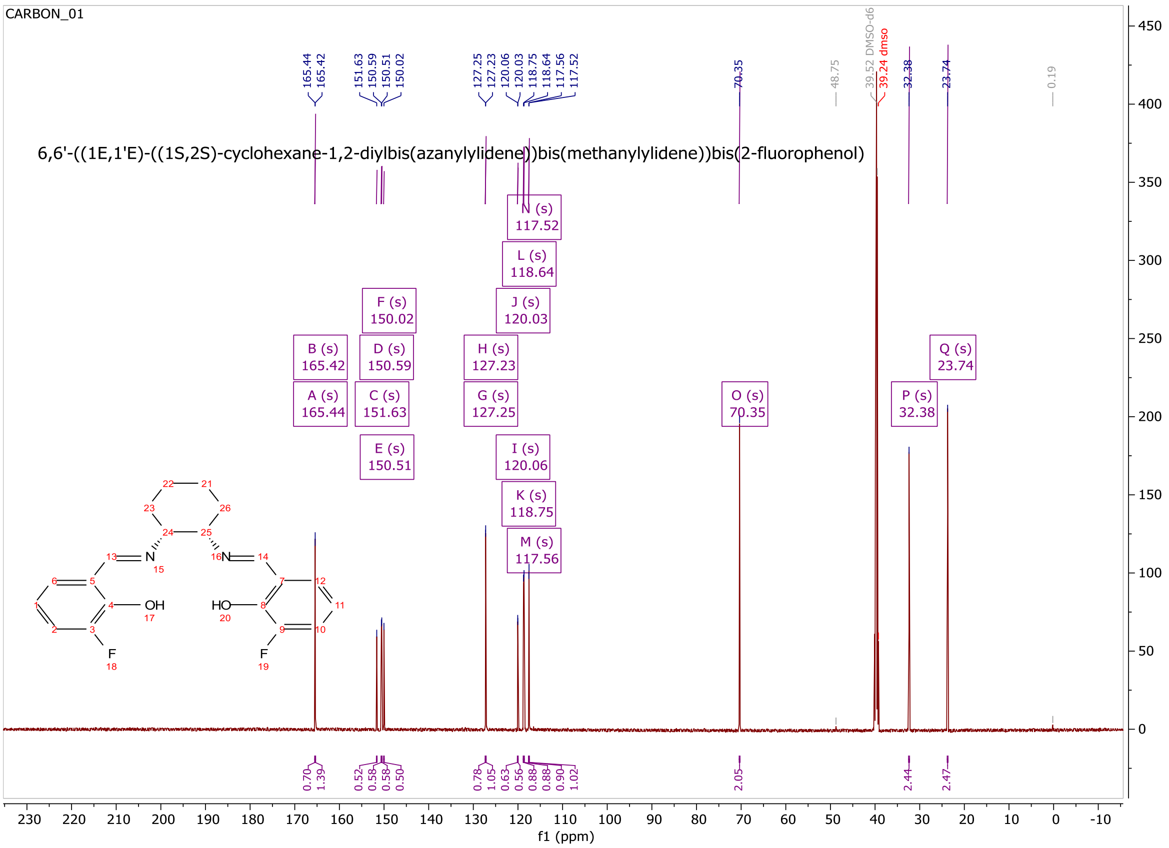


Figure S2-34. ^{13}C-NMR for 2-SS (Unreduced)

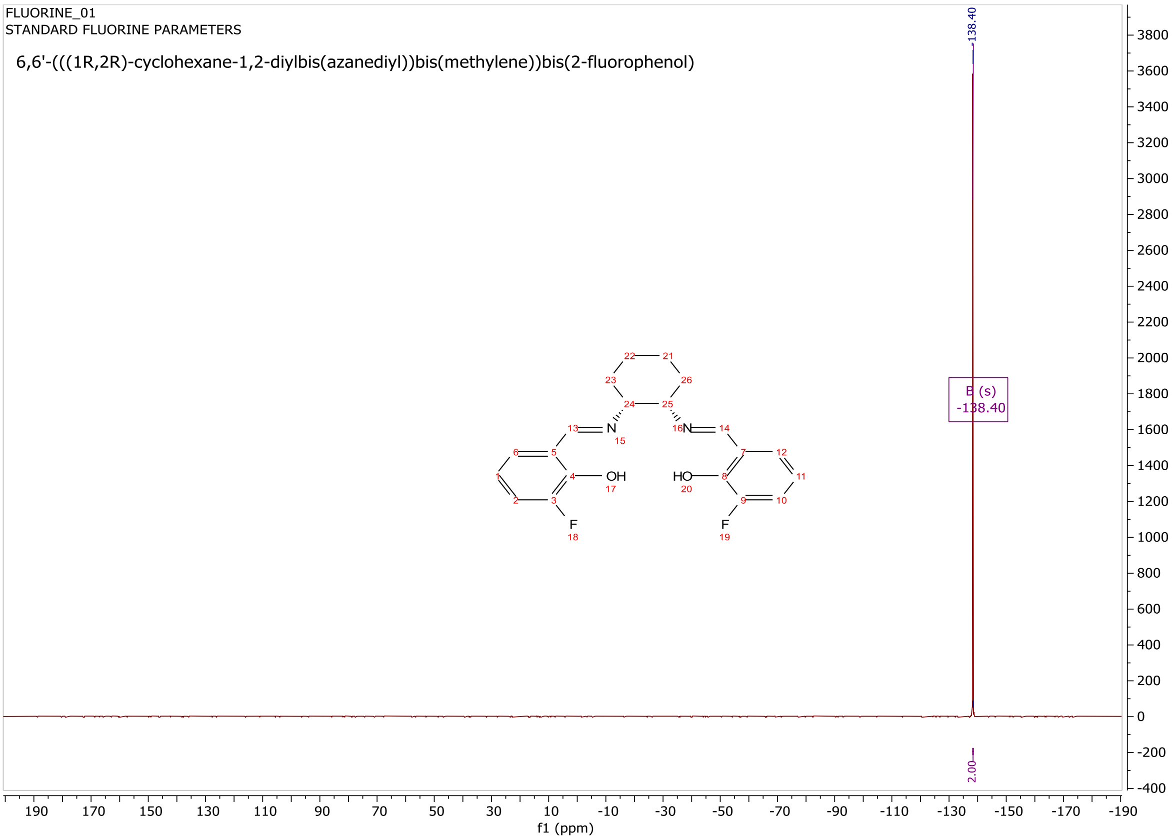


Figure S2-35. ^{19}F-NMR for 2-SS (Unreduced)

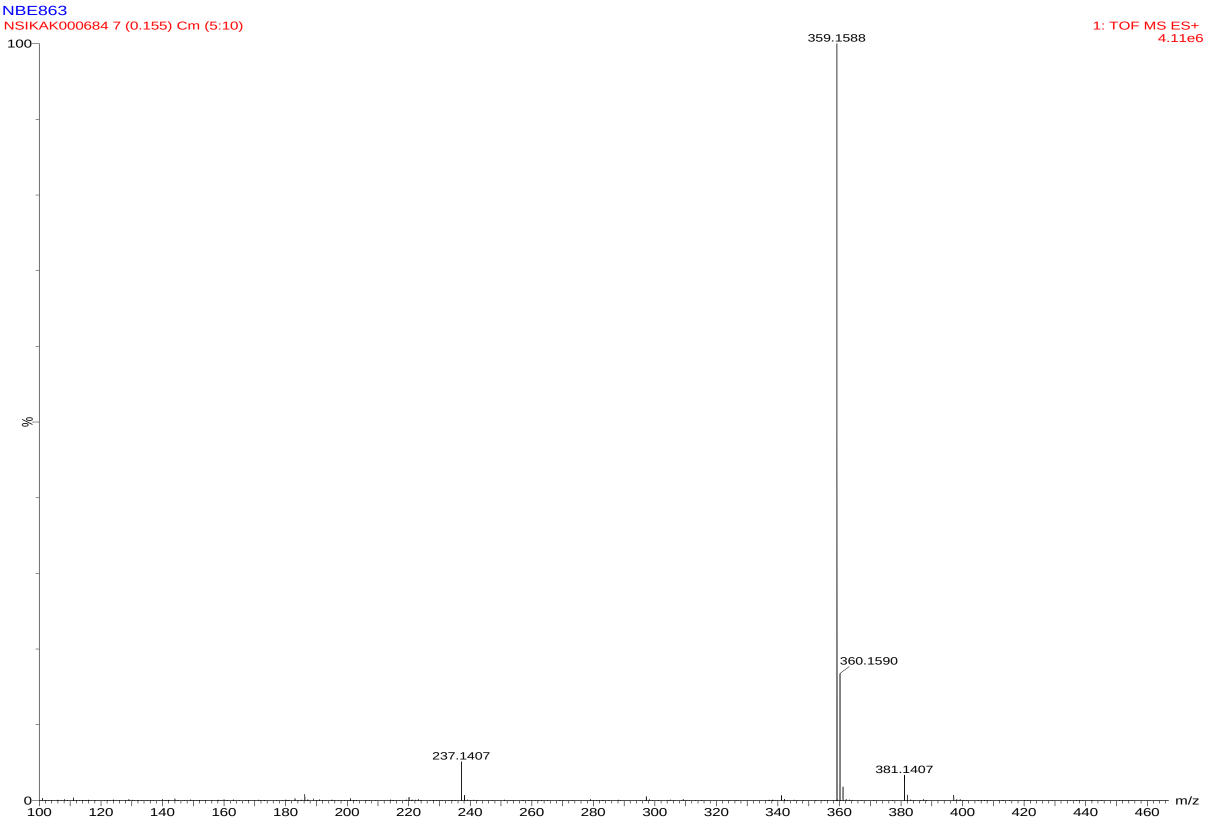


Figure S2-36. HRMS for 2-SS (Unreduced)

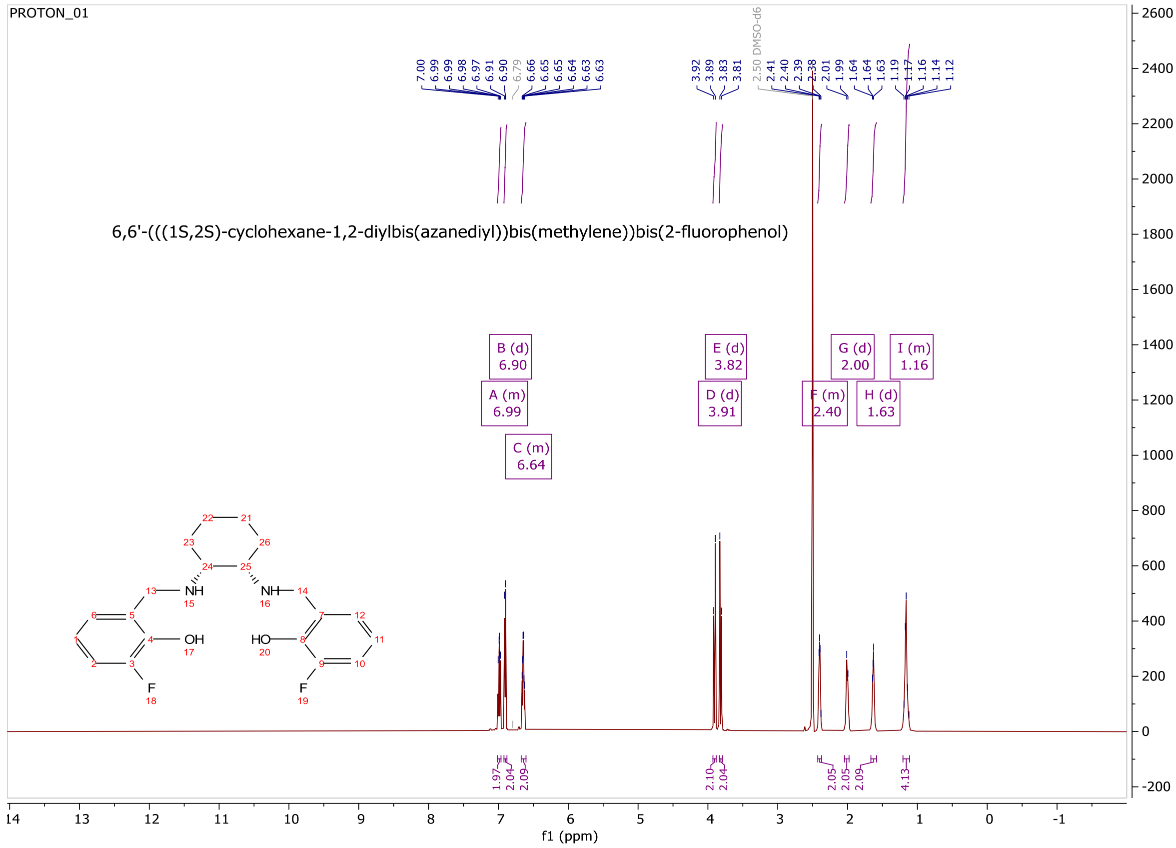


Figure S2-37. ^{1}H-NMR for **2-SS**

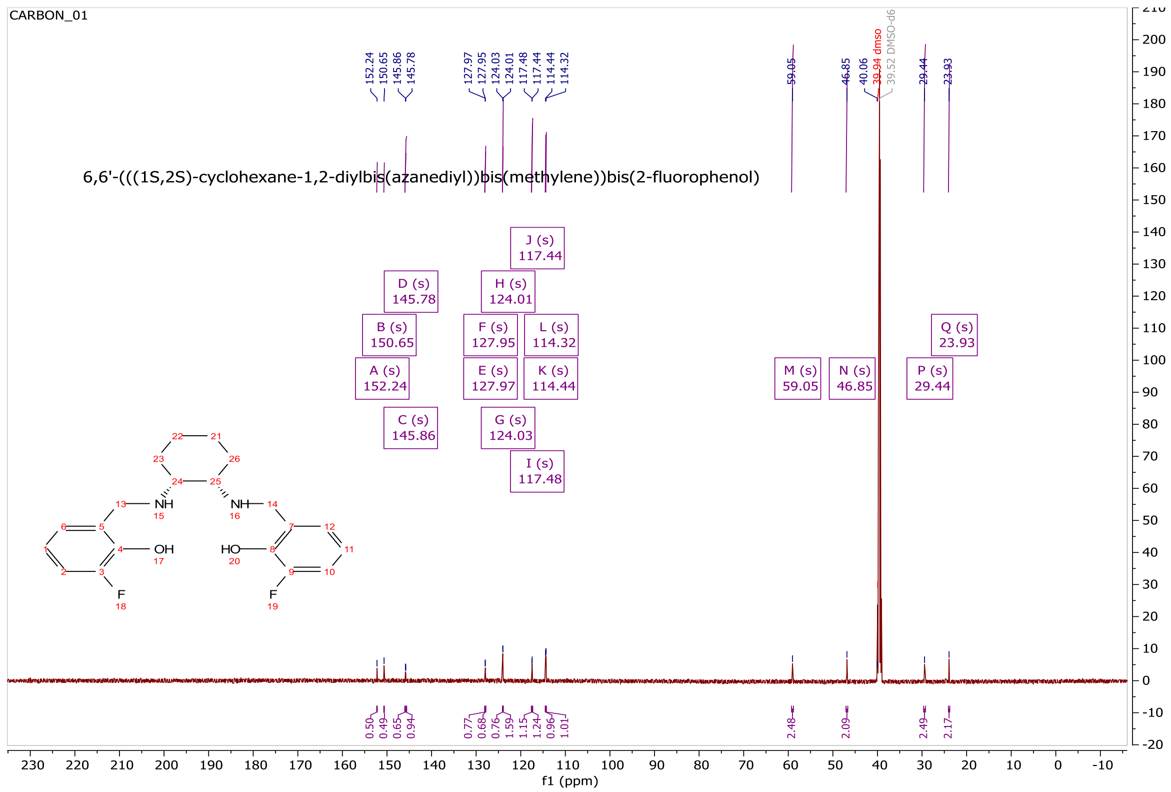


Figure S2-38. ^{13}C-NMR for **2-SS**

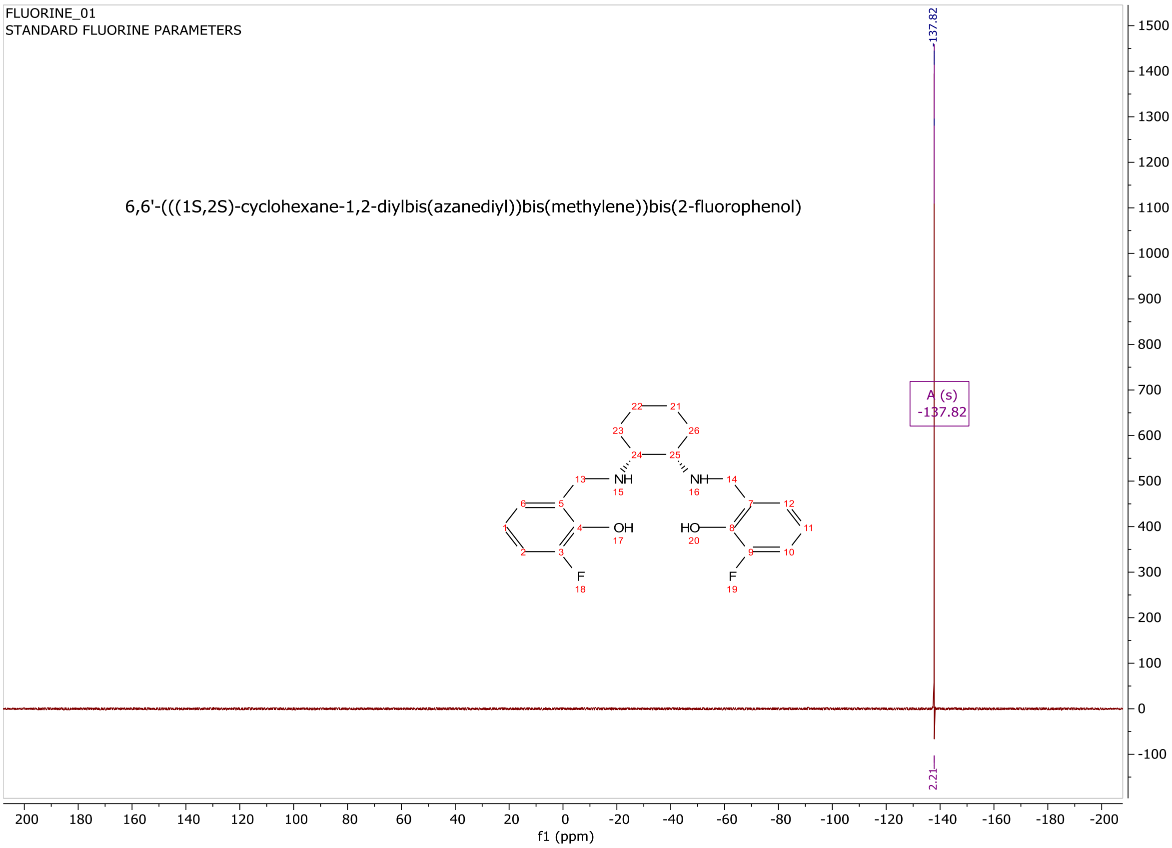


Figure S2-39. [19]F-NMR for **2-SS**

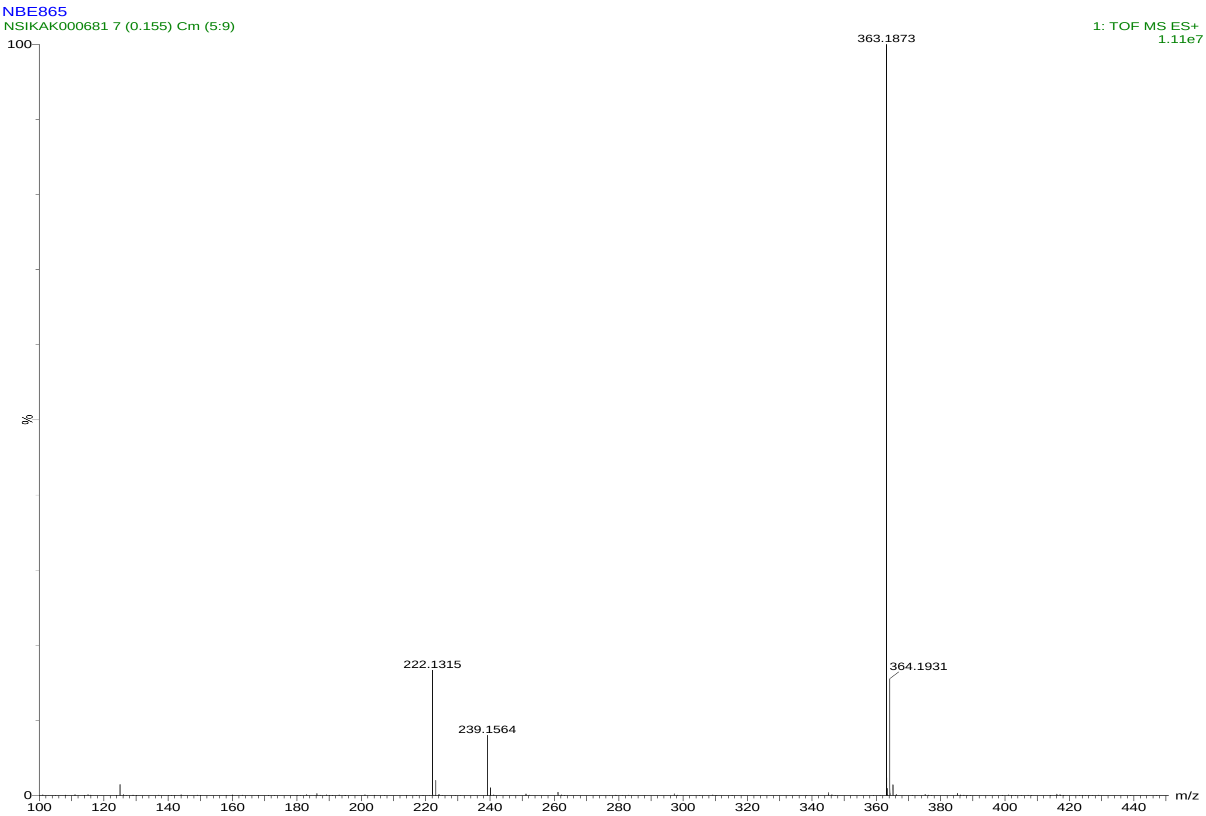


Figure S2-40. HRMS for **2-SS**

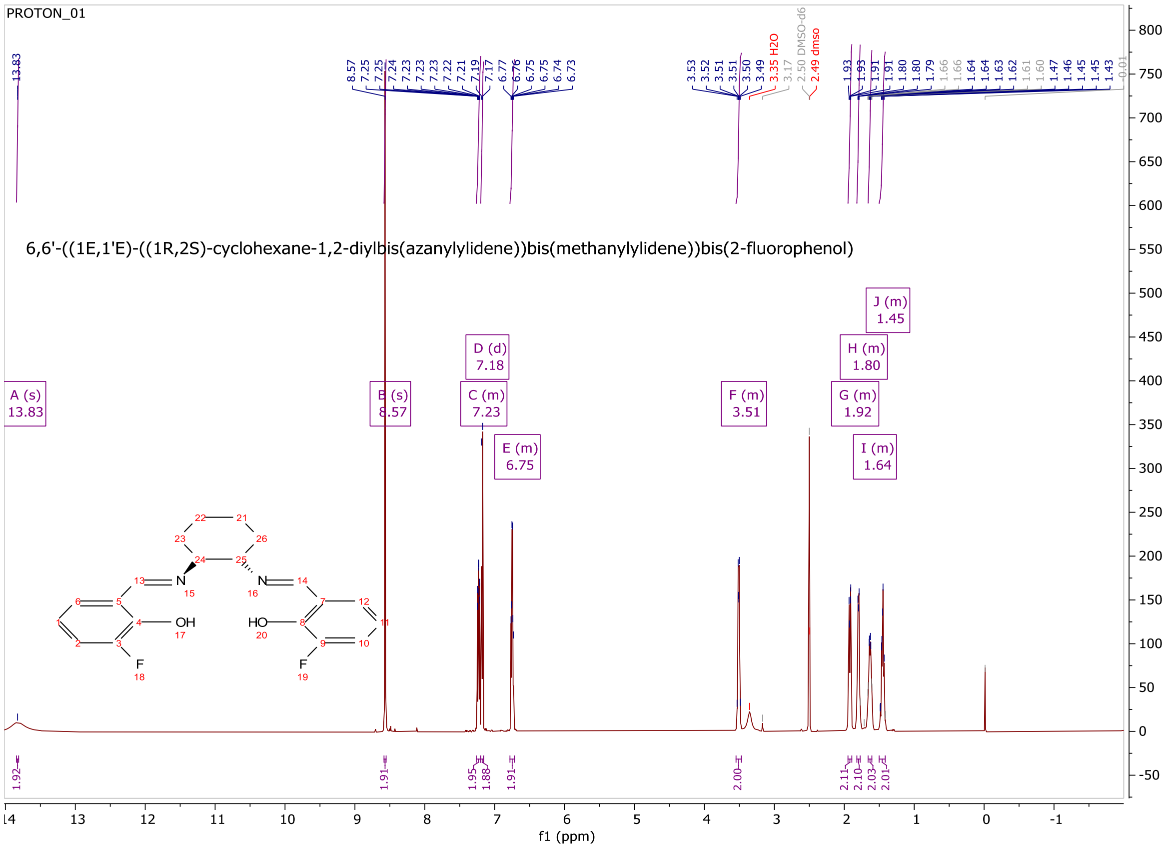


Figure S2-41. ^{1}H-NMR for 2-rac (Unreduced)

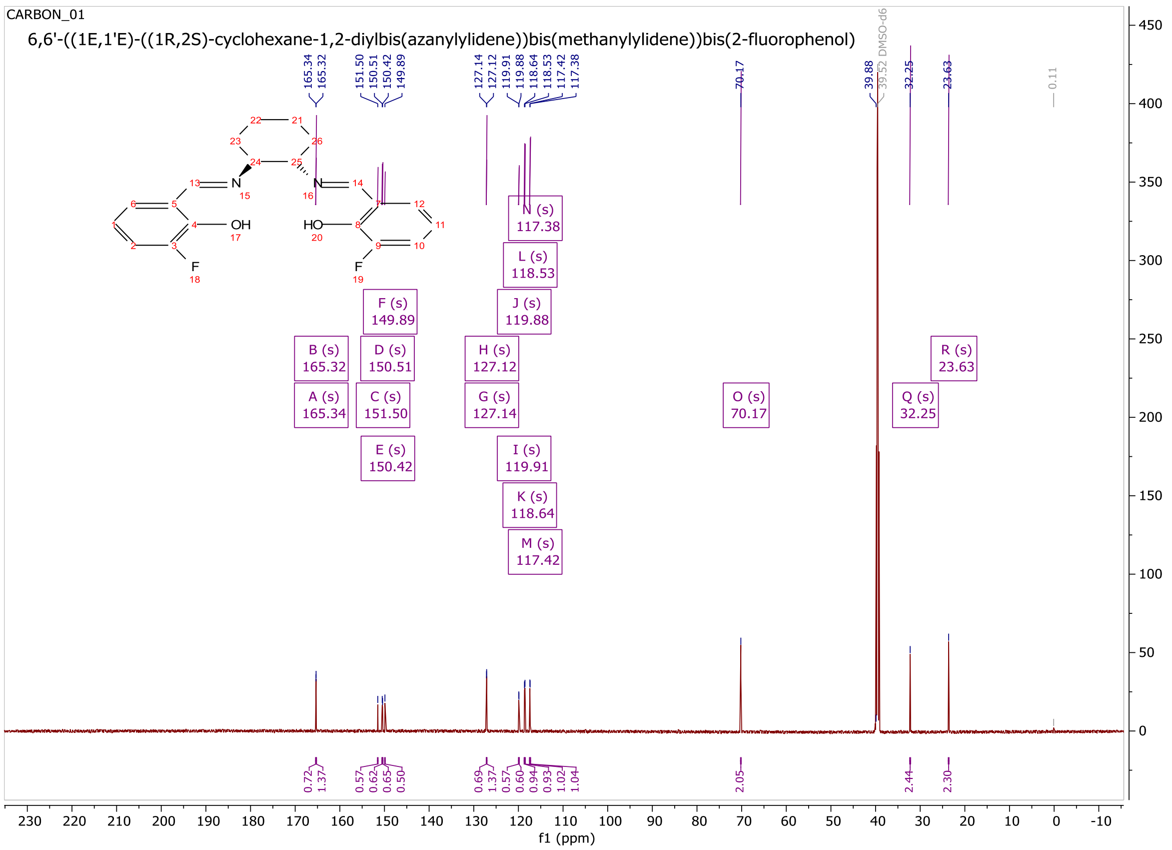


Figure S2-42. ^{13}C-NMR for 2-rac (Unreduced)

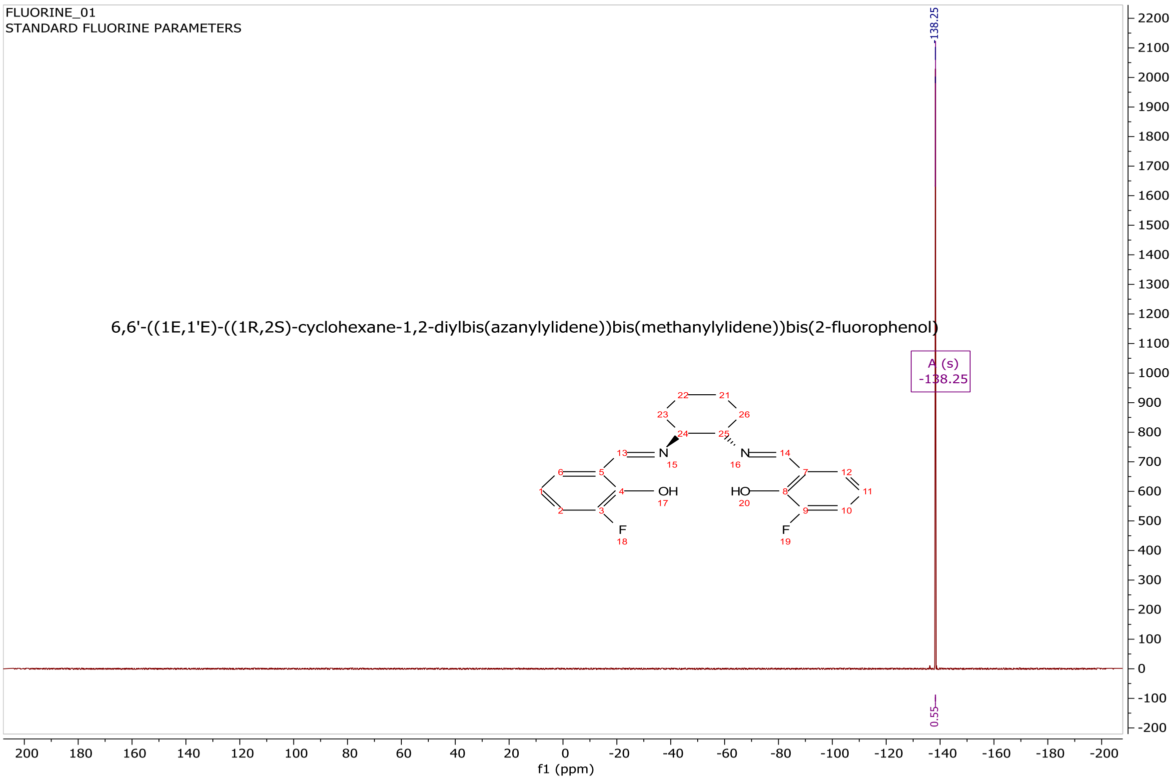


Figure S2-43. ^{19}F-NMR for 2-rac (Unreduced)

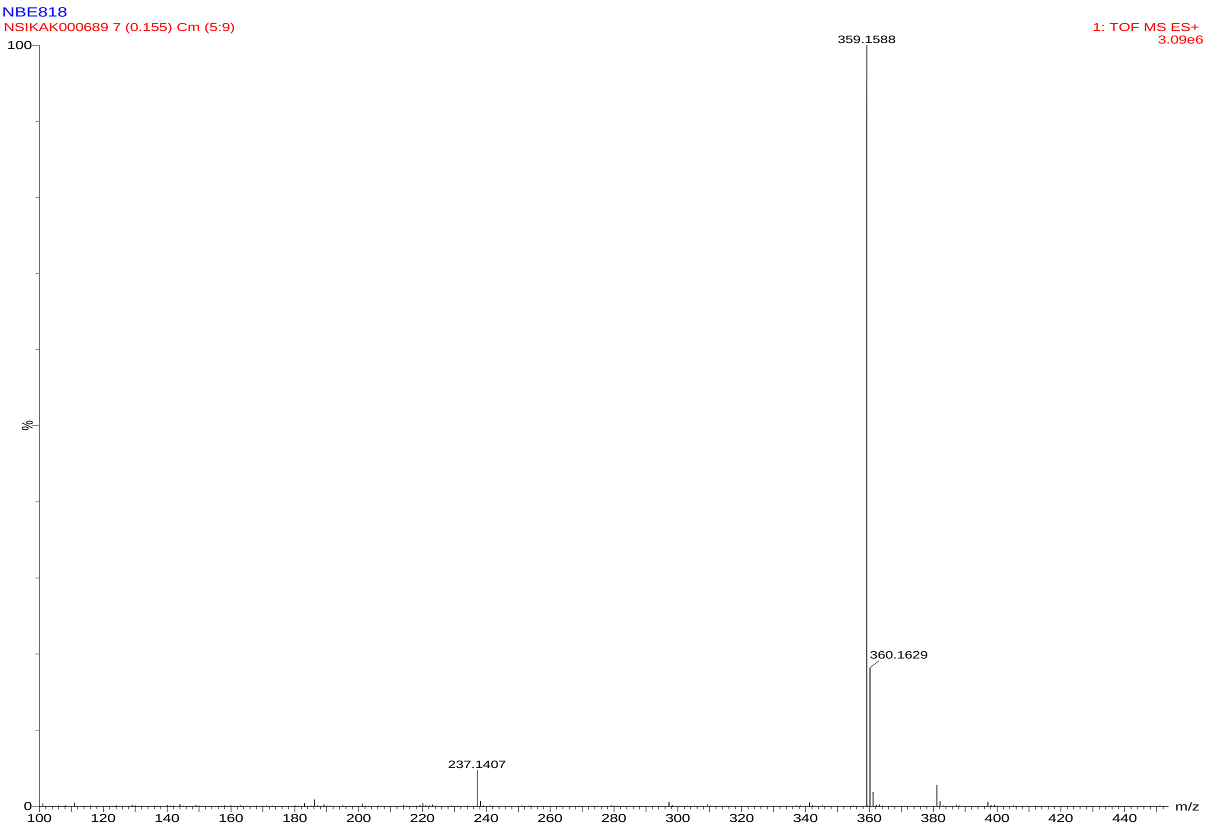


Figure S2-44. HRMS for 2-rac (Unreduced)

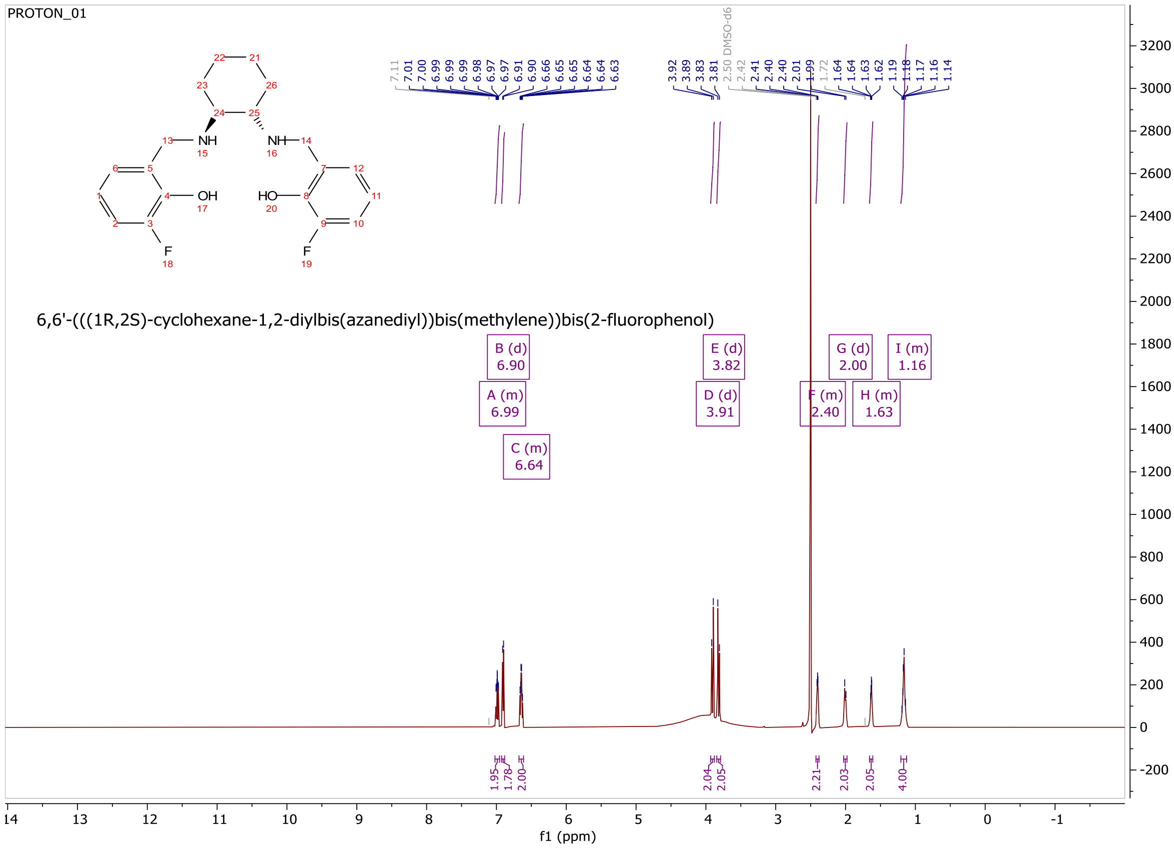


Figure S2-45. ^{1}H-NMR for **2-rac**

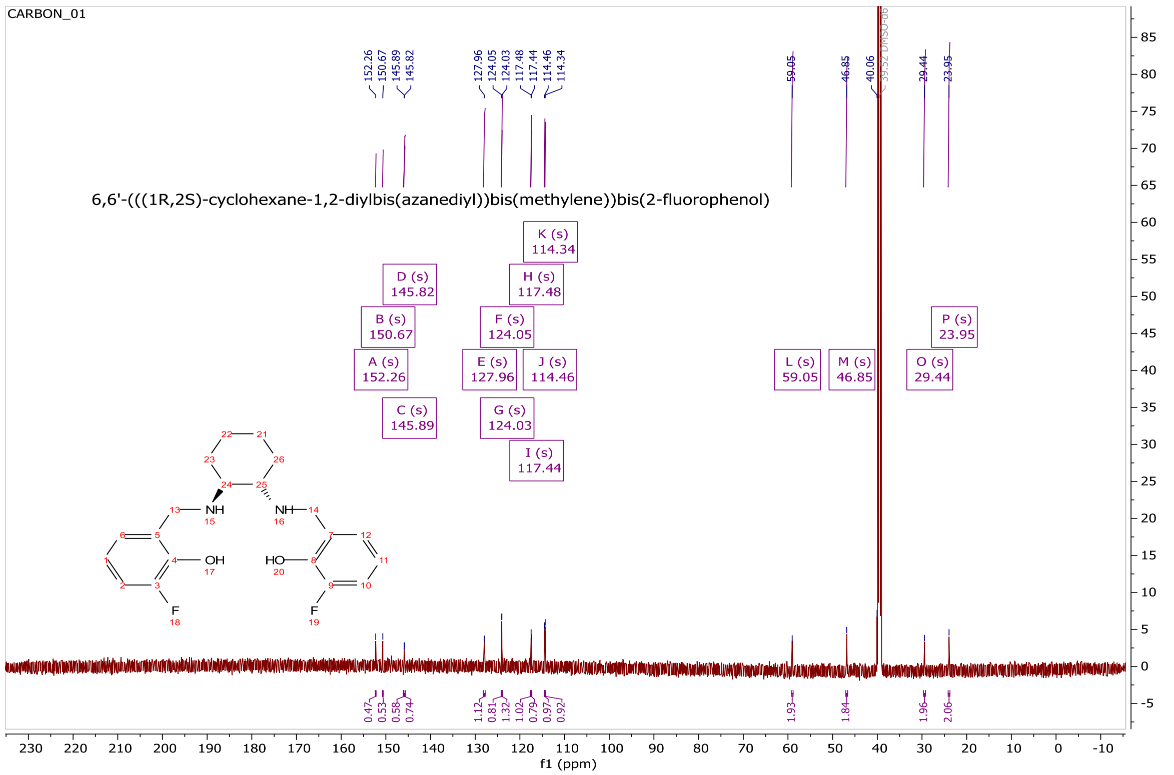


Figure S2-46. ^{13}C-NMR for **2-rac**

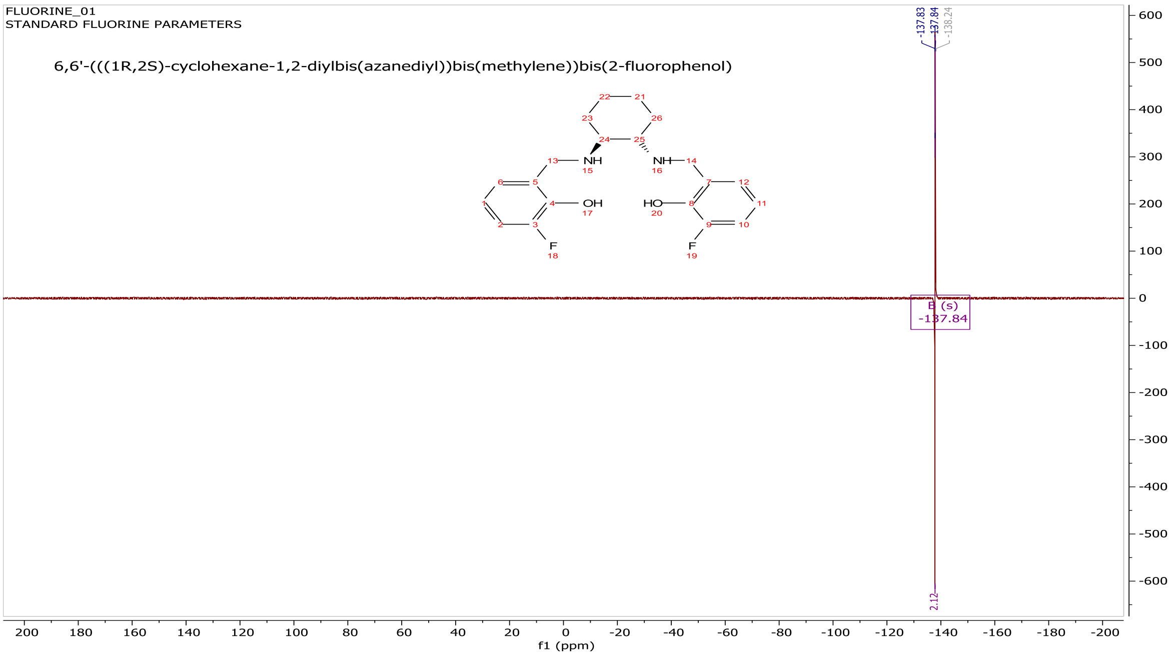


Figure S2-47. ^{19}F-NMR for **2-rac**

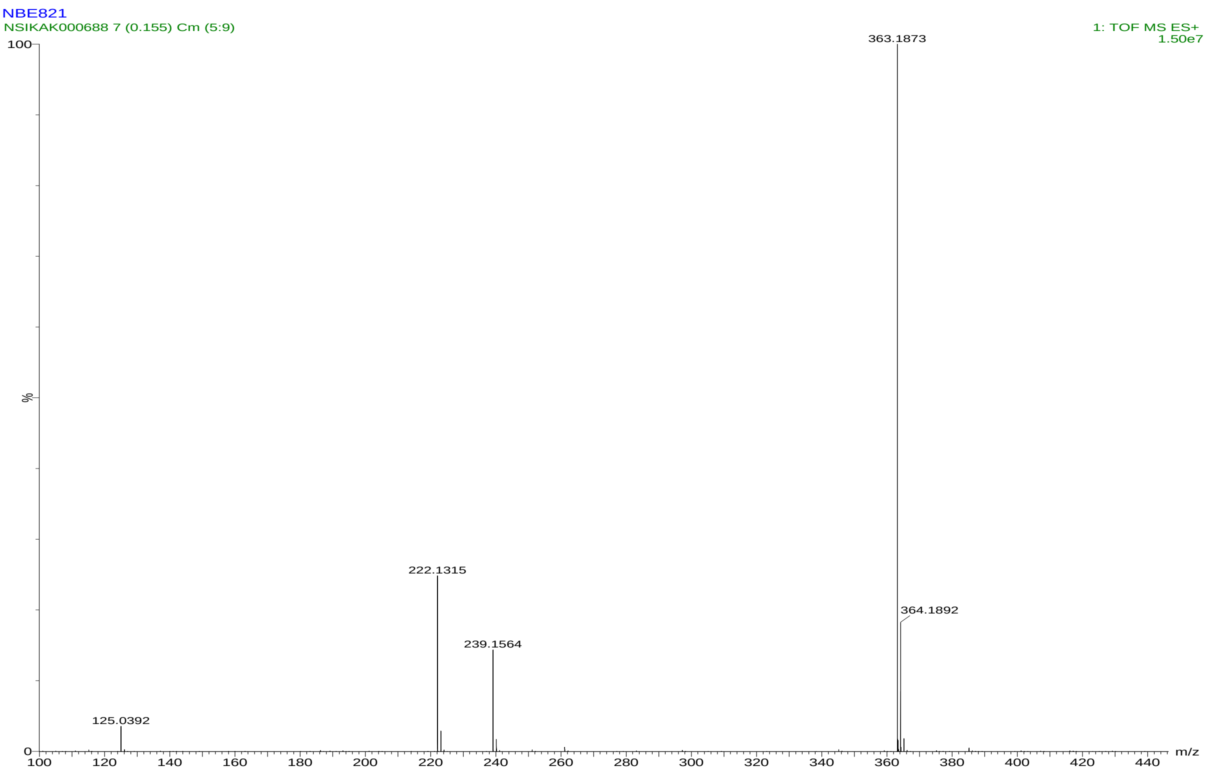


Figure S2-48. HRMS for **2-rac**

Single crystal X-ray diffraction studies

Single Crystal X-Ray diffraction studies for **Zn-1** family were carried out at the National Crystallography Service, University of Southampton[1] and for **Zn-2** family at the University of Sussex (Table S2-1). For **Zn-1**, suitable crystals were selected and mounted on a MITIGEN holder in perfluoro ether oil on a Rigaku FRE+ equipped with VHF Varimax confocal mirror, an AFC12 goniometer, a HyPix 6000HE detector and data were collected at T = 100(2)K. The data were processed with CrysAlisPro and solved by intrinsic phasing methods with SHELXT.[2] Geometric/crystallographic calculations were performed using Olex2[2]. Images and video generated using CrystalMaker®: a crystal and molecular structures program for Mac and Windows. CrystalMaker Software Ltd, Oxford, England (www.crystalmaker.com). Structures have been given CCDC deposition numbers 2231658–2231663.

Table S2-1 Crystal data and structure refinement for all compounds.

Identification code	**Zn-1-rac**	**Zn-1-RR**	**Zn-1-SS**	**Zn-2-rac**	**Zn-2-RR**	**Zn-2-SS**
Empirical formula	$C_{22}H_{22}F_6N_2O_4Zn$	$C_{46}H_{53.5}F_{12}N_4O_{10.75}Zn_2$	$C_{48}H_{60}F_{12}N_4O_{12}Zn_2$	$C_{40}H_{48}F_4N_4O_6Zn_2$	$C_{40}H_{48}F_4N_4O_6Zn_2$	$C_{40}H_{48}F_4N_4O_6Zn_2$
General forumla	[ZnL]	[ZnL 1(CH_3OH) 0.375(H2O)	[ZnL 2(CH_3OH)]	[ZnL 2(H_2O)]	[ZnL 2(H_2O)]	[ZnL 2(H_2O)]
Formula weight	557.78	1193.16	1243.74	887.56	887.56	887.56
Temperature/K	100.00(10)	100(2)	100.00(10)	100.00(10)	100.01(10)	100.00(10)
Crystal system	monoclinic	triclinic	monoclinic	triclinic	triclinic	triclinic
Space group	$P2_1/n$	P1	I2	P-1	P1	P1
a/Å	14.9548(5)	8.7181(3)	25.8902(7)	8.1340(3)	8.1202(5)	8.12372(16)
b/Å	7.7335(3)	11.4705(6)	9.1717(2)	10.6803(4)	10.6670(5)	10.6734(2)
c/Å	19.8034(6)	13.6295(4)	26.1158(6)	12.4823(5)	12.4761(8)	12.4777(3)
α/°	90	81.280(3)	90	64.938(4)	64.867(6)	64.9809(19)
β/°	102.621(3)	72.282(3)	119.476(3)	75.120(3)	75.150(6)	75.1697(17)
γ/°	90	85.815(4)	90	78.039(3)	78.068(5)	78.0265(16)
Volume/Å^3	2234.98(14)	1282.78(9)	5398.7(3)	943.32(7)	939.73(11)	941.64(4)
Z	4	1	4	1	1	1
ρ_{calc}g/cm^3	1.658	1.545	1.530	1.562	1.568	1.565
μ/mm^{-1}	2.297	2.080	2.019	2.196	2.204	2.200
F(000)	1136.0	612.0	2560.0	460.0	460.0	460.0
Crystal size/mm^3	0.05 × 0.01 × 0.01	0.09 × 0.05 × 0.005	0.15 × 0.08 × 0.01	0.04 × 0.02 × 0.02	0.04 × 0.04 × 0.02	0.04 × 0.02 × 0.02
Radiation	Cu Kα (λ = 1.54178)	Cu Kα (λ = 1.54178)	Cu Kα (λ = 1.54178)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.746 to 151.046	6.872 to 154.374	3.934 to 150.012	7.966 to 134.026	11.344 to 134.12	9.53 to 134.248
Index ranges	-18 ≤ h ≤ 18, -9 ≤ k ≤ 9, -24 ≤ l ≤ 24	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -16 ≤ l ≤ 11	-29 ≤ h ≤ 32, -11 ≤ k ≤ 10, -32 ≤ l ≤ 31	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14	-9 ≤ h ≤ 9, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected	37976	23112	38786	17027	31560	31783
Independent reflections	4532 [R_{int} = 0.0901, R_{sigma} = 0.0368]	7985 [R_{int} = 0.0651, R_{sigma} = 0.0646]	10196 [R_{int} = 0.0969, R_{sigma} = 0.0579]	3328 [R_{int} = 0.0482, R_{sigma} = 0.0305]	6398 [R_{int} = 0.0468, R_{sigma} = 0.0331]	6456 [R_{int} = 0.0420, R_{sigma} = 0.0246]

Data/restraints/parameters	4532/116/353	7985/21/703	10196/127/778	3328/0/274	6398/3/511	6456/3/511
Goodness-of-fit on F^2	1.100	1.015	1.070	1.254	1.106	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0617, wR_2 = 0.1600	R_1 = 0.0732, wR_2 = 0.1868	R_1 = 0.0823, wR_2 = 0.2211	R_1 = 0.0637, wR_2 = 0.1557	R_1 = 0.0377, wR_2 = 0.1027	R_1 = 0.0538, wR_2 = 0.1386
Final R indexes [all data]	R_1 = 0.0732, wR_2 = 0.1686	R_1 = 0.0885, wR_2 = 0.2058	R_1 = 0.0948, wR_2 = 0.2350	R_1 = 0.0658, wR_2 = 0.1566	R_1 = 0.0392, wR_2 = 0.1048	R_1 = 0.0551, wR_2 = 0.1397
Largest diff. peak/hole / e Å^{-3}	1.11/-1.06	1.03/-0.90	1.47/-0.82	0.60/-0.48	0.39/-0.33	0.53/-0.57
Flack parameter		-0.02(5)	-0.07(5)		0.00(2)	0.04(4)

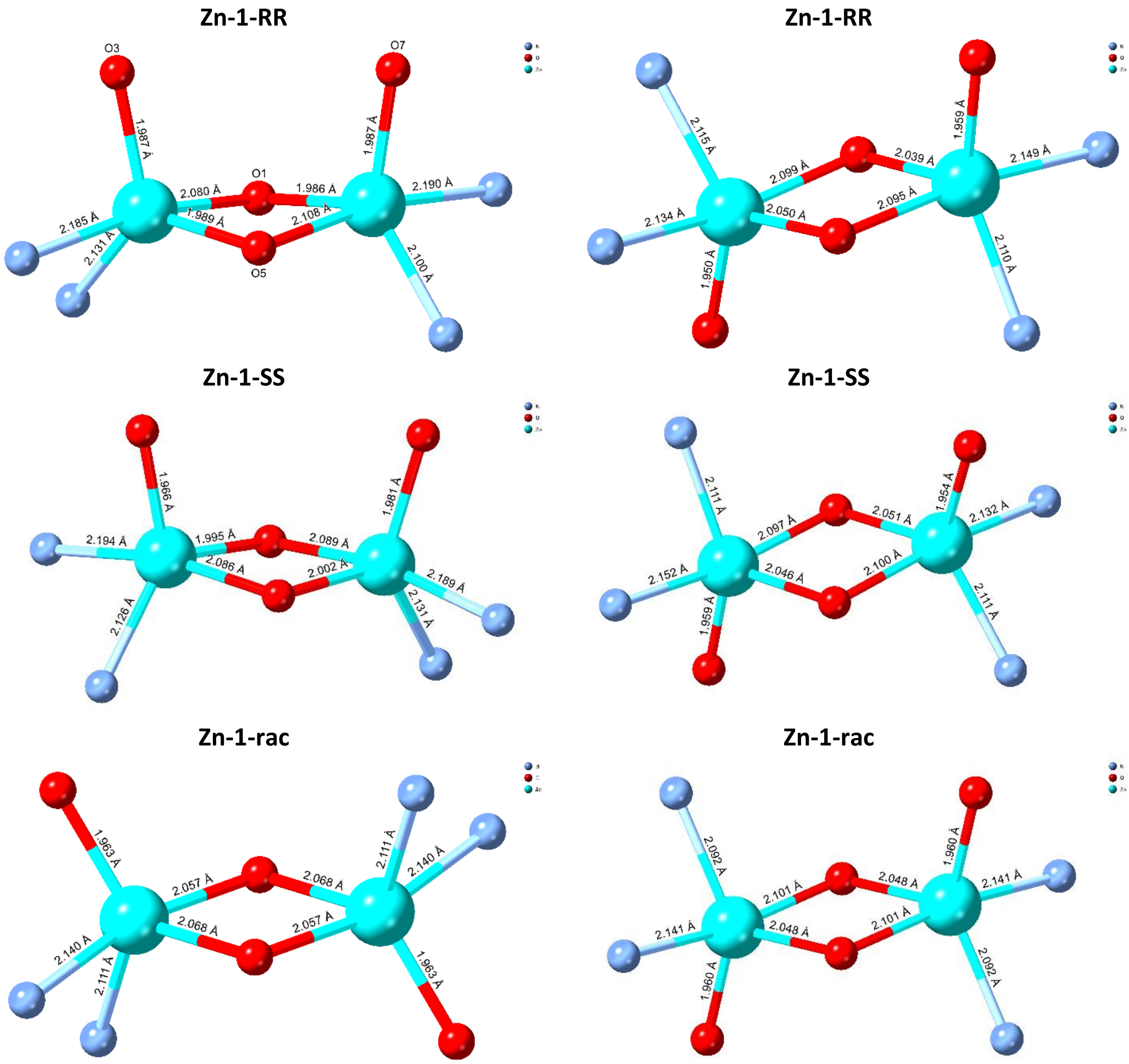


Figure S2-49. The main core defining the coordination geometry around the metal centres. Colour code; Zn (light blue), O (red), N (blue),

Thermogravimetric and elemental analyses.

Elemental analysis results for all complexes were recorded at London Metropolitan University. The samples, upon crystallisation were filtered, dried and collected. The samples were stored in Eppendorf. There is a deviation in the data; we assume this deviation is caused by losing their crystallinity and absorbing moisture from the atmosphere, therefore we provide an estimated formulae that match the experimental values. Our assumption is further supported by thermogravimetric analysis, see below. The expected lattice solvent molecule loss (up to 130^{o}C) is higher than expected, thus an estimated formula is given.

Zn-1-rac, calculated for [**ZnL**] C: 47.37; H: 3.98; N: 5.02; Found C: 44.38; H: 3.65; N: 4.58; corresponding to [**ZnL 2(H_2O)**] C: 44.50; H: 4.41; N: 4.72;

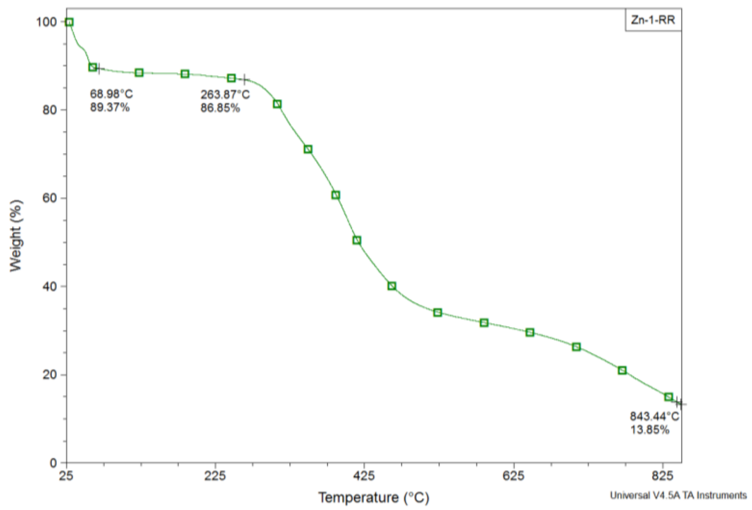
Zn-1-RR, calculated for [**ZnL 1(CH_3OH)** 0.375(H_2O)] C: 46.30; H: 4.52; N: 4.70; Found C: 43.42; H: 3.85; N: 4.63; corresponding to [**ZnL 0.5(CH_3OH) 2(H_2O)]** C: 44.31; H: 4.63; N: 4.59;

Zn-1-SS, calculated for [**ZnL 2(CH_3OH)**] C: 46.35; H: 4.86; N: 4.50; Found C: 44.89; H: 4.33; N: 4.53; corresponding to [**ZnL 2(H_2O)**] C: 44.50; H: 4.41; N: 4.72;

Zn-2-rac, calculated for [**ZnL 2(H_2O)**] C: 54.13; H: 5.45; N: 6.31; Found C: 54.43; H: 5.12; N: 6.29; corresponding to [**ZnL 1.7(H_2O)]** C: 54.46; H: 5.42; N: 6.35;

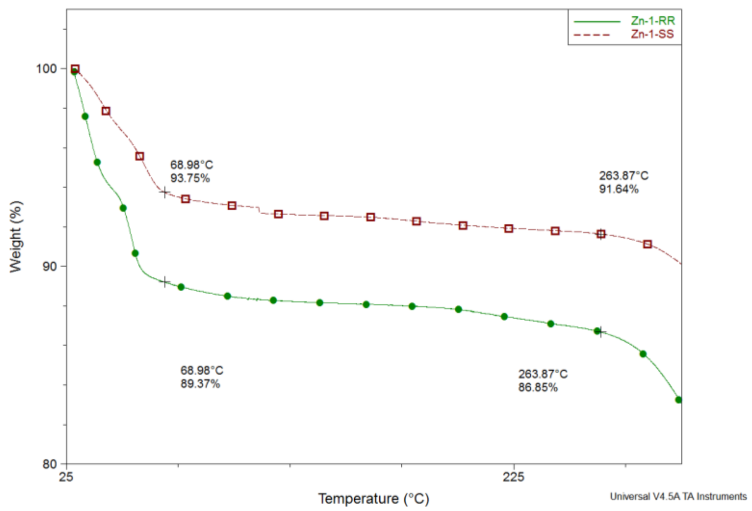
Zn-2-RR, calculated for [**ZnL 2(H_2O)**] C: 54.13; H: 5.45; N: 6.31; Found C: 54.82; H: 5.02; N: 6.34; corresponding to [**ZnL 1.4(H_2O)**] C: 54.80; H: 5.38; N: 6.39;

Zn-2-SS, calculated for [**ZnL 2(H_2O)]** C: 54.13; H: 5.45; N: 6.31; Found C: 54.60; H: 5.24; N: 6.31; corresponding to [**ZnL 1.6(H_2O)**] C: 54.57; H: 5.40; N: 6.36;



Lattice loss
10.63%
$C_{22}H_{22}F_6N_2O_4Zn$ 3.5 (H_2O)
=10.14%
$C_{22}H_{22}F_6N_2O_4Zn$ 2 (MeOH)
= 10.29%
$C_{22}H_{22}F_6N_2O_4Zn$ (MeOH)1.75(H_2O)
= 10.22%

Expected ZnO residue for [ZnL 1(CH_3OH) 0.375(H_2O)] = 13.64%



Lattice loss
6.25%

$C_{22}H_{22}F_6N_2O_4Zn$ 1.25(MeOH)
= 6.69%

Figure S2-50. Thermogravimetric analysis of **Zn-1-RR** (upper) and **Zn-1-RR** and **Zn-1-SS** (lower)

Solution studies

ESI-MS

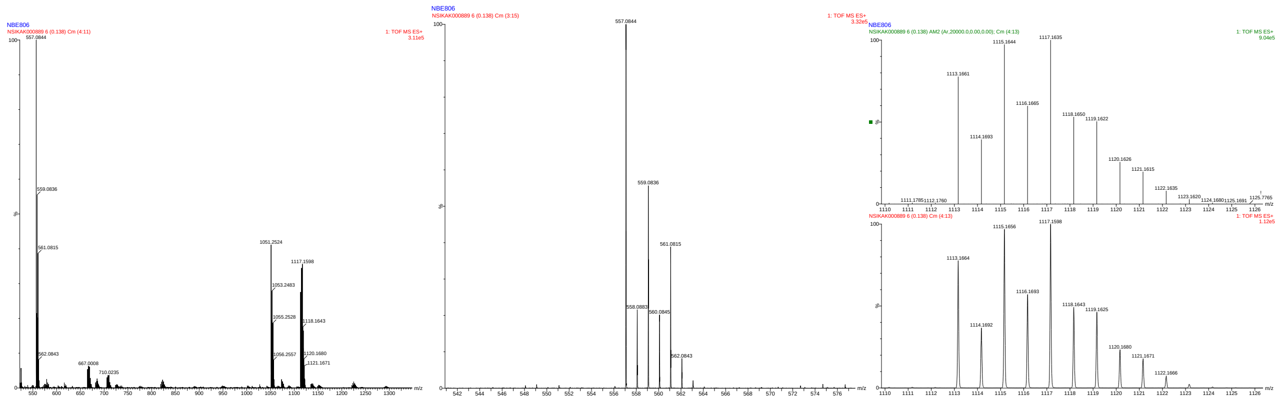


Figure S2-51. ESI-MS data for **Zn-1-RR** validating the presence of monomeric (m/z = 557) and dimeric (m/z = 1114) species.

Monomeric Elemental Composition Report

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 22-22 H: 0-100 N: 2-2 O: 4-4 F: 6-6 Zn: 0-1

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		5.0	100.0	50.0				
557.0853	557.0853	0.0	0.0	9.5	400.3	n/a	n/a	C22 H23 N2 O4 F6 Zn

Dimeric Elemental Composition Report

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 44-44 H: 0-100 N: 4-4 O: 8-8 F: 12-12 P: 0-1 Zn: 2-2

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		5.0	100.0	50.0				
1113.1661	1113.1629	3.2	2.9	18.5	184.8	n/a	n/a	C44 H45 N4 O8 F12 Zn2

NMR data.

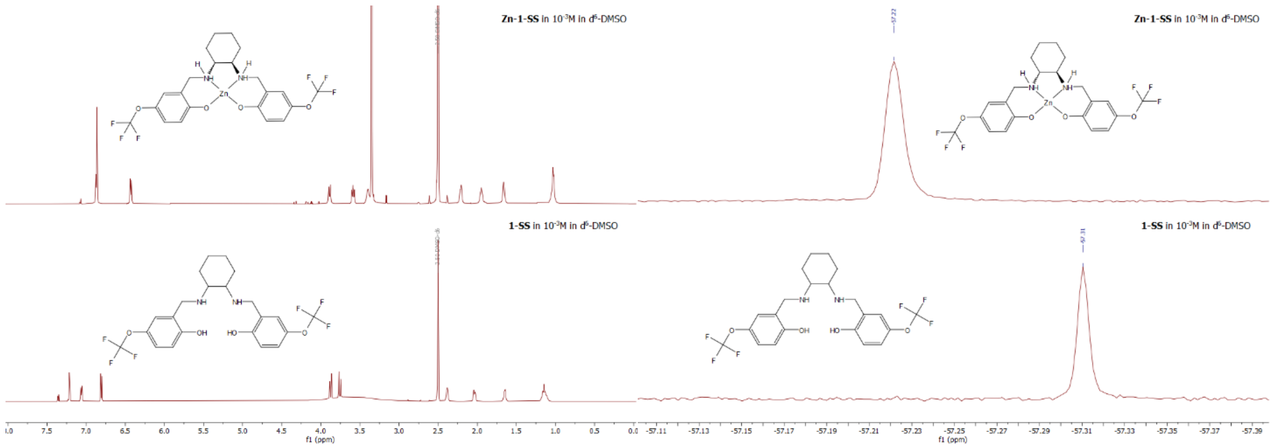


Figure S2-52. ^{1}H and ^{19}F NMR comparison of **1-SS** and **Zn-1-SS** in d^{6}-DMSO (1X 10^{-3}M).

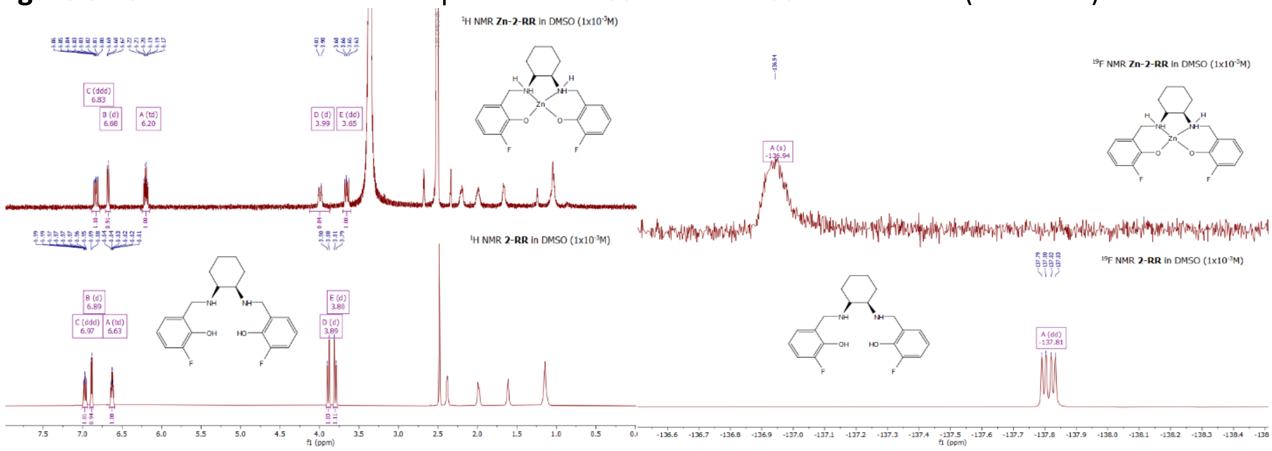
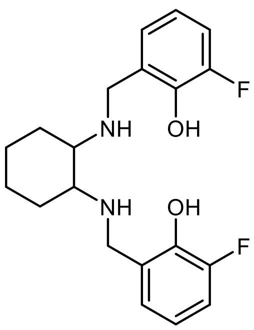


Figure S2-53. ^{1}H and ^{19}F NMR comparison of **2-RR** and **Zn-2-RR** in d^{6}-DMSO (1X 10^{-3}M).

Potentiometry



The protonation constants of **2-rac** was determined by pH-metric titration in 50%-50% DMSO-water mixture in 25, 25 and 4 ml samples at 0.2 mM, 0.4mM and 1.25 mM concentrations, respectively. The titrations were performed with carbonate free stock solution (50%-50% DMSO-water) of potassium hydroxide of known concentration. The titrations were carried out with Mettler Toledo T50 automatic titrator equipped with a 6.0234.100 combined glass electrode (Metrohm). During the measurements argon was bubbled through the samples to ensure the absence of oxygen and carbon dioxide. All pH-potentiometric measurements were carried out at a constant ionic strength of 0.2 M KCl and at a constant temperature (298 K). The samples were stirred by using a VELP Scientific magnetic stirrer.

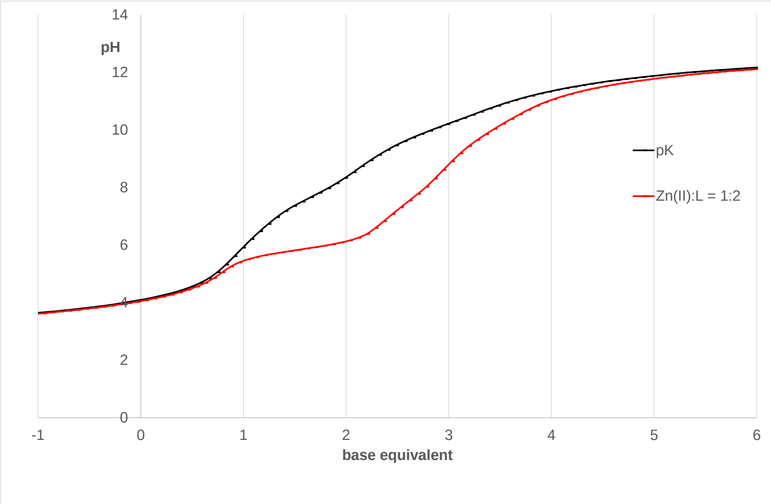


Figure S2-54. Titration curves of **2-rac** and Zn2+-ligand 1:2 system.

Sensing ^{19}F NMR studies

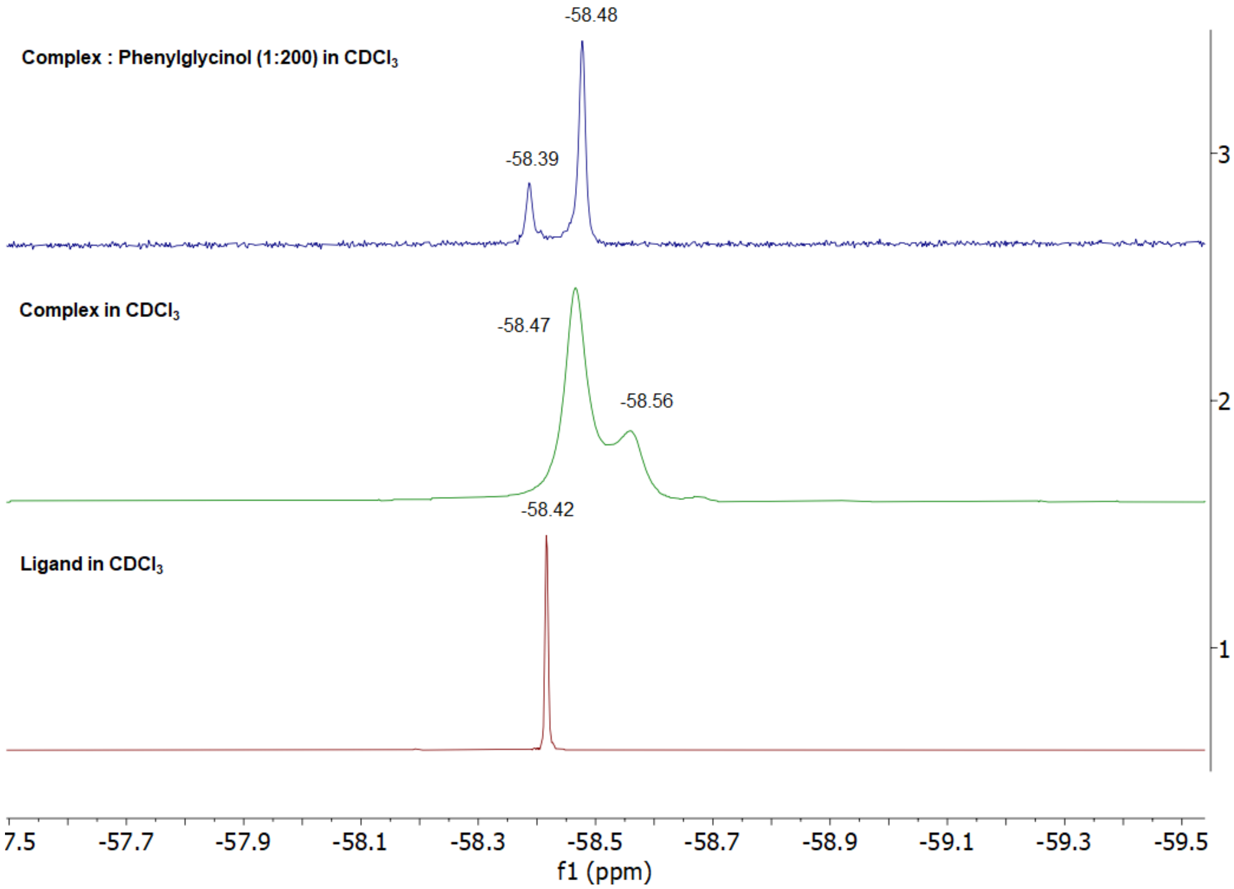


Figure S2-55. ^{19}F NMR data for ligand, complex and complex+analyte in 1:200 ratio in $CDCl_3$. Concentration 10^{-3}M, temperature 303K.

Theoretical calculations

The Conformer-Rotamer Ensemble Sampling Tool, CREST[12] (version 2.10.2), based on the semi-empirical GFNn-xTB[13] methods, was used to obtain a sample of conformers of each species with default parameters and considering solvent, chloroform or dimethyl sulfoxide (DMSO). After careful inspection of the obtained conformers, a number of structures (5 – 9)[14] were selected to be re-optimized, the selection was done considering xTB energies and structural differences to achieve a set of representative minima, and some hand constructed structures were also added. These structures were re-optimized using Gaussian[3] 16 (Rev. A.03) at DFT (Density Functional Theory) level using the B3LYP[6,15,16] functional together with the dispersion correction GD3.[17] The 6-31g(d,p)[18,19] basis sets for all atoms except for Zn for with the SDD[20] basis sets and associated Electron Core Potentials (ECPs) were used instead. Optimizations were carried under the effects of the solvent (chloroform or DMSO) as a continuum media with PCM,[21,22], some explicit solvent molecules (1 – 3) were included in some of the calculations as detailed in text. Frequency calculations have been carried for all species to ensure they correspond to minima on the Potential Energy Surface (PES) and to obtain their free energies in solution. Gaussian Gibbs Free energies are given at the 1 atm Standard State, while the reference state in solution is the 1 M State, hence all minima have been corrected from 1 atm to 1 mol.l^{-1} by adding 1.89 kcal.mol^{-1} to the Gibbs energy (298K) by using Goodvibes program.[23]

To obtain the concentration of all species in the equilibrium under the different considered conditions, systems of 9 to 19 independent non-lineal equations with the same number of unknown variables were built and solved using the equilibrium constants and mass balances together with initial concentrations as detailed in text. Equilibrium constants were obtained from the computationally obtained Standard Free Energies in solution and the isotherm equation, $K_p = \exp(-\Delta G^0/RT)$.

Systems of equations used

Zn-1-RR system in chloroform without presence of Analyte

Table S2-2: Equations and equilibrium constants,

Chemical equations	**K_{eq}**	**ΔG^0 (kcal.mol^{-1})**
Dimer ⇌ 2 * Monomer	5.08 x10^{-15}	-20.5
Dimer + H_2O ⇌ Dimer(H_2O)	5.22 x10^{+05}	8.8
Dimer(H_2O) + H_2O ⇌ Dimer(H_2O)$_2$	9.88 x10^{+05}	9.2
Dimer(H_2O)$_2$ + H_2O ⇌ Dimer(H_2O)$_3$	1.06 x10^{+06}	9.2
Monomer + H_2O ⇌ Monomer(H_2O)	1.14 x10^{+05}	7.9
Monomer(H_2O) + H_2O ⇌ Monomer(H_2O)$_2$	4.01 x10^{+05}	8.6
Monomer(H_2O)$_2$ + H_2O ⇌ Monomer(H_2O)$_3$	7.83 x10^{+04}	7.7

Mass balances,

[Dimer]$_0$ = [Dimer] + [Dimer(H_2O)] + [Dimer(H_2O)$_2$] +[Dimer(H_2O)$_3$] + 2*[Monomer] + 2*[Monomer(H_2O)]+2*[Monomer(H_2O)$_2$] + 2*[Monomer(H_2O)$_3$]

[H_2O]$_0$ = [H_2O] + [Dimer(H_2O)] + 2*[Dimer(H_2O)$_2$] + 3*[Dimer(H_2O)$_3$] + [Monomer(H_2O)] + 2*[Monomer(H_2O)$_2$] + 3*[Monomer(H_2O)$_3$]

Zn-1-RR system in chloroform in presence of Analyte

Table S2-3: Equations and equilibrium constants,

Chemical equations	**K_{eq}**	**ΔG^0 (kcal.mol^{-1})**
Dimer ⇌ 2 * Monomer	5.08 x10^{-15}	-20.5
Dimer + H_2O ⇌ Dimer(H_2O)	5.22 x10^{+05}	8.8
Dimer(H_2O) + H_2O ⇌ Dimer(H_2O)$_2$	9.88 x10^{+05}	9.2
Dimer(H_2O)$_2$ + H_2O ⇌ Dimer(H_2O)$_3$	1.06 x10^{+06}	9.2
Monomer + H_2O ⇌ Monomer(H_2O)	1.14 x10^{+05}	7.9
Monomer(H_2O) + H_2O ⇌ Monomer(H_2O)$_2$	4.01 x10^{+05}	8.6
Monomer(H_2O)$_2$ + H_2O ⇌ Monomer(H_2O)$_3$	7.83 x10^{+04}	7.7
Dimer + analyte ⇌ Dimer(analyte)	5.61 x10^{+09}	14.3
Dimer(analyte) + analyte ⇌ Dimer(analyte)$_2$	1.94 x10^{+11}	16.4
Monomer + analyte ⇌ Monomer(analyte)	9.31 x10^{+09}	14.6
Monomer(analyte) + analyte ⇌ Monomer(analyte)$_2$	2.27 x10^{+08}	12.4

Mass balances:

[Dimer]$_0$ = [Dimer] + [Dimer(H_2O)] + [Dimer(H_2O)$_2$] +[Dimer(H_2O)$_3$] + 2*[Monomer] + 2*[Monomer(H_2O)]+2*[Monomer(H_2O)$_2$] + 2*[Monomer(H_2O)$_3$] + [Dimer(analyte)] + [Dimer(analyte)$_2$] + 2*[Monomer(analyte)] + 2*[Monomer(analyte)$_2$]

[H_2O]$_0$ = [H_2O] + [Dimer(H_2O)] + 2*[Dimer(H_2O)$_2$] + 3*[Dimer(H_2O)$_3$] + [Monomer(H_2O)] + 2*[Monomer(H_2O)$_2$] + 3*[Monomer(H_2O)$_3$]

[analyte]$_0$ = [analyte] + [Dimer(analyte)] + 2*[Dimer(analyte)$_2$] + [Monomer(analyte)] + 2*[Monomer(analyte)$_2$]

Zn-1-RR system in DMSO without presence of Analyte

Table S2-4: Equations and equilibrium constants,

Chemical equations	**K_{eq}**	**ΔG^0 (kcal.mol^{-1})**
Dimer ⇌ 2 * Monomer	1.33 x10^{-12}	16.2
Dimer + H_2O ⇌ Dimer(H_2O)	5.55x10^{+1}	-2.4
Dimer(H_2O) + H_2O ⇌ Dimer(H_2O)$_2$	5.72 x10^{+4}	-6.5
Dimer(H_2O)$_2$ + H_2O ⇌ Dimer(H_2O)$_3$	6.18 x10^{+5}	-7.9
Monomer + H_2O ⇌ Monomer(H_2O)	1.06 x10^{+3}	-4.1
Monomer(H_2O) + H_2O ⇌ Monomer(H_2O)$_2$	8.63 x10^{+3}	-5.4
Monomer(H_2O)$_2$ + H_2O ⇌ Monomer(H_2O)$_3$	1.78 x10^{+4}	-5.8
Dimer + DMSO ⇌ Dimer(DMSO)	1.44 x10^{+4}	-5.7
Dimer(DMSO) + DMSO ⇌ Dimer(DMSO)$_2$	4.74 x10^{+1}	-2.3
Monomer + DMSO ⇌ Monomer(DMSO)	3.95 x10^{+5}	-7.6
Monomer(DMSO) + DMSO ⇌ Monomer(DMSO)$_2$	8.14 x10^{+3}	-5.3

Mass balances,

[Dimer]$_0$ = [Dimer] + [Dimer(H_2O)] + [Dimer(H_2O)$_2$] +[Dimer(H_2O)$_3$] + 2*[Monomer] + 2*[Monomer(H_2O)]+2*[Monomer(H_2O)$_2$] + 2*[Monomer(H_2O)$_3$] + [Dimer(DMSO)] + [Dimer(DMSO)$_2$] + 2*[Monomer(DMSO)]+2*[Monomer(DMSO)$_2$]

[H_2O]$_0$ = [H_2O] + [Dimer(H_2O)] + 2*[Dimer(H_2O)$_2$] + 3*[Dimer(H_2O)$_3$] + [Monomer(H_2O)] + 2*[Monomer(H_2O)$_2$] + 3*[Monomer(H_2O)$_3$]

[DMSO]$_0$ = [DMSO] + [Dimer(DMSO)] + 2*[Dimer(DMSO)$_2$] + [Monomer(DMSO)] + 2*[Monomer(DMSO)$_2$]

Zn-1-RR system in DMSO in presence of Analyte

Table S2-5: Equations and equilibrium constants,

Chemical equations	K_{eq}	ΔG^0 (kcal.mol^{-1})
Dimer ⇌ 2 * Monomer	1.33 x10^{-12}	16.2
Dimer + H_2O ⇌ Dimer(H_2O)	5.55x10^{+1}	-2.4
Dimer(H_2O) + H_2O ⇌ Dimer(H_2O)$_2$	5.72 x10^{+4}	-6.5
Dimer(H_2O)$_2$ + H_2O ⇌ Dimer(H_2O)$_3$	6.18 x10^{+5}	-7.9
Monomer + H_2O ⇌ Monomer(H_2O)	1.06 x10^{+3}	-4.1
Monomer(H_2O) + H_2O ⇌ Monomer(H_2O)$_2$	8.63 x10^{+3}	-5.4
Monomer(H_2O)$_2$ + H_2O ⇌ Monomer(H_2O)$_3$	1.78 x10^{+4}	-5.8
Dimer + DMSO ⇌ Dimer(DMSO)	1.44 x10^{+4}	-5.7
Dimer(DMSO) + DMSO ⇌ Dimer(DMSO)$_2$	4.74 x10^{+1}	-2.3
Monomer + DMSO ⇌ Monomer(DMSO)	3.95 x10^{+5}	-7.6
Monomer(DMSO) + DMSO ⇌ Monomer(DMSO)$_2$	8.14 x10^{+3}	-5.3
Dimer + analyte ⇌ Dimer(analyte)	1.59 x10^{+6}	-8.5
Dimer(analyte) + analyte ⇌ Dimer(analyte)$_2$	3.74 x10^{+9}	-13.1
Monomer + analyte ⇌ Monomer(analyte)	9.13 x10^{+7}	-10.9
Monomer(analyte) + analyte ⇌ Monomer(analyte)$_2$	8.25 x10^{+7}	-10.8

Mass balances,

[Dimer]$_0$ = [Dimer] + [Dimer(H_2O)] + [Dimer(H_2O)$_2$] +[Dimer(H_2O)$_3$] + 2*[Monomer] + 2*[Monomer(H_2O)]+2*[Monomer(H_2O)$_2$] + 2*[Monomer(H_2O)$_3$] + [Dimer(DMSO)] + [Dimer(DMSO)$_2$] + 2*[Monomer(DMSO)]+2*[Monomer(DMSO)$_2$] + [Dimer(analyte)] + [Dimer(analyte)$_2$] + 2*[Monomer(analyte)] + 2*[Monomer(analyte)$_2$]

[H_2O]$_0$ = [H_2O] + [Dimer(H_2O)] + 2*[Dimer(H_2O)$_2$] + 3*[Dimer(H_2O)$_3$] + [Monomer(H_2O)] + 2*[Monomer(H_2O)$_2$] + 3*[Monomer(H_2O)$_3$]

[DMSO]$_0$ = [DMSO] + [Dimer(DMSO)] + 2*[Dimer(DMSO)$_2$] + [Monomer(DMSO)] + 2*[Monomer(DMSO)$_2$]

[analyte]$_0$ = [analyte] + [Dimer(analyte)] + 2*[Dimer(analyte)$_2$] + [Monomer(analyte)] + 2*[Monomer(analyte)$_2$]

Coordinates and potential free energies

Relevant structures optimized in chloroform (coordinates/Å - potential energies/Hartree)

H_2O

ΔE -76.4231505021 h.

1	0.758319	-0.478131	-0.000000
8	-0.000000	0.119551	0.000000
1	-0.758319	-0.478279	0.000000

analyte

ΔE -441.469322871 h.

6	3.048880	-0.105837	-0.232486
6	2.362194	-1.227110	0.242882
6	0.989936	-1.156354	0.481160
6	0.276540	0.029947	0.249984
6	0.975345	1.145873	-0.223542
6	2.350921	1.080473	-0.463090
6	-1.230425	0.040877	0.475613
7	-1.885531	1.344451	0.641803
6	-1.966789	-0.666878	-0.680561
8	-3.361825	-0.690302	-0.441825
1	2.896650	-2.153794	0.432341
1	0.462137	-2.030616	0.855977

1	0.451216	2.081015	-0.396707
1	2.875688	1.959246	-0.827432
1	4.118233	-0.156348	-0.415753
1	-1.447025	-0.532672	1.385724
1	-1.614413	-1.698760	-0.778803
1	-3.537238	0.168610	-0.016990
1	-1.720163	-0.142559	-1.621819
1	-1.548511	1.818734	1.474857
1	-1.682861	1.952459	-0.149174

dimer

ΔE -4176.82437080 h.

30	-0.238183	-0.103363	1.590807
30	0.250807	-0.017412	-1.568375
9	-7.369505	-4.074817	0.896899
8	1.296618	-0.159914	0.218773
9	6.491301	-2.288653	-1.431089
9	7.195908	-4.289039	-0.935686
9	-6.565574	-2.118585	1.417394
8	-5.422317	-4.007165	1.863102
8	-1.271815	-0.019811	-0.193629
9	5.555729	-3.386966	0.185623
8	-6.371320	1.717655	-1.456809
8	5.266953	-4.113685	-1.924814
9	-5.702867	-3.230433	-0.230277
8	6.401839	1.634492	1.377964
8	0.238843	-1.803020	-2.358185
8	-0.299916	-1.915782	2.310447
9	8.152634	1.863716	2.644774
9	-7.007300	0.018512	-2.784463
7	-0.518153	1.883470	-2.348312
1	-1.000106	1.703485	-3.230471
9	-6.145914	1.790098	-3.691496
7	1.990995	0.609904	-2.747755
1	2.759476	0.742960	-2.089086
6	2.529524	0.254288	0.522961
7	0.576661	1.767789	2.375340
1	1.097487	1.574632	3.232075
7	-1.954648	0.544874	2.805515
1	-2.721778	0.720712	2.155497
9	-8.108311	1.897961	-2.750192
6	1.702554	1.889624	-3.433115
1	1.223556	1.630783	-4.387247
9	6.199826	1.804602	3.609775
6	2.360996	-0.498148	-3.677685
1	1.518749	-0.607050	-4.368724
1	3.252672	-0.238336	-4.261474
6	2.567120	-1.780161	-2.922656
6	-2.505197	0.381220	-0.514644
6	1.437842	-2.364083	-2.276634
6	-1.522027	-2.425000	2.226042
6	3.649996	-0.551182	0.246380
1	3.487024	-1.526378	-0.195020
6	-2.355077	-0.575832	3.705485
1	-1.509792	-0.739340	4.382009
1	-3.229728	-0.303461	4.309096
6	6.101090	-3.531146	-1.041948
9	7.045070	-0.008089	2.771447
6	0.372402	4.040842	-3.343468
1	-0.137164	3.809324	-4.289827
1	-0.321336	4.642031	-2.748428
6	0.683506	2.718194	-2.623035
1	1.133723	2.936353	-1.645103
6	1.639318	-3.550092	-1.534727
6	6.932212	1.322443	2.581636
6	-1.616772	1.794713	3.521046
1	-1.122294	1.494675	4.455177
6	2.903799	-4.118565	-1.413153
6	-2.619108	-1.821895	2.909036
6	1.513664	2.384299	1.392355
1	0.938579	2.502098	0.468455
1	1.831698	3.379640	1.718697
6	-3.623998	-0.425231	-0.235206
1	-3.461231	-1.391626	0.225920
6	-6.890635	1.355701	-2.651343
6	-1.492218	2.507709	-1.407771
1	-0.945732	2.665257	-0.472204
1	-1.818335	3.487575	-1.770917
6	5.098197	1.147220	1.129208
6	-3.981157	2.054300	-1.482238
1	-4.149883	3.010920	-1.967098
6	-5.069361	1.243217	-1.176713
6	-0.596053	2.620930	2.710863
1	-1.064556	2.883648	1.752777
6	2.973782	2.704471	-3.717248
1	3.470155	2.913996	-2.758512
1	3.668134	2.099389	-4.309531
6	4.935626	-0.105068	0.543628
1	5.800942	-0.718793	0.325760
6	-4.117553	-3.466088	1.989802
6	-2.857762	2.636180	3.858873
1	-3.368690	2.889486	2.918385
1	-3.556663	2.033521	4.448140
6	-3.905114	-2.347099	2.787283
1	-4.745912	-1.879472	3.289580
6	-6.239341	-3.370578	1.001694
6	-1.473631	4.745063	3.803465
1	-1.939730	5.090741	2.870447
1	-1.176853	5.641637	4.357948
6	-2.691647	1.635389	-1.148910
6	2.718262	1.522844	1.127296
6	3.986336	-3.516772	-2.049930
6	-2.491077	3.924823	4.605539
1	-3.393284	4.514333	4.800229
1	-2.062943	3.667840	5.583893
6	3.829344	-2.361256	-2.807222

1	4.694551	-1.909424	-3.281692
6	4.009470	1.958521	1.431928
1	4.178354	2.926720	1.893063
6	-4.908318	0.006356	-0.559512
1	-5.772972	-0.607971	-0.341818
6	1.647396	4.848804	-3.627228
1	1.389151	5.770284	-4.159730
1	2.101541	5.152059	-2.673805
6	-0.229788	3.909874	3.465909
1	0.291840	3.632723	4.393235
1	0.469307	4.509528	2.875579
6	-3.067732	-4.086462	1.317367
1	-3.271023	-4.950791	0.693532
6	2.659847	4.024801	-4.431786
1	3.582110	4.594231	-4.588435
1	2.247200	3.809590	-5.426762
6	-1.780126	-3.573435	1.442987
1	-0.948083	-4.026402	0.913878
1	0.782980	-3.987052	-1.031608
1	3.064563	-5.012401	-0.819130

Dimer(H_2O)
ΔE -4253.28275944 h.

6	-2.277048	1.528396	-0.943181
6	-2.373689	2.275316	0.259351
6	-3.630662	2.601704	0.777404
6	-4.781167	2.159755	0.133097
6	-4.714193	1.469019	-1.071893
6	-3.466569	1.187442	-1.618388
6	-1.133769	2.622083	1.038634
7	-0.145663	3.366888	0.207798
6	0.906356	4.047563	0.999840
6	0.430118	5.370299	1.619740
6	1.545111	6.048081	2.428422
6	2.794371	6.266924	1.565065
6	3.270217	4.947680	0.940426
6	2.155923	4.271358	0.125924
7	2.570423	2.988889	-0.487224
6	3.441907	3.136838	-1.683634
6	3.836088	1.788100	-2.214686
6	5.153596	1.340702	-2.113758
6	5.498300	0.087291	-2.606196
6	4.560422	-0.716137	-3.243653
6	3.245624	-0.273064	-3.355915
6	2.840458	0.960129	-2.799202
8	6.826110	-0.385241	-2.492559
6	7.193581	-0.788036	-1.254655
9	6.330377	-1.674548	-0.720818
8	1.556380	1.338418	-2.828399
30	0.774847	1.875488	-1.055916
8	-1.100979	1.083425	-1.405229
30	-0.622650	-0.971456	-0.894369
8	0.215092	-0.949181	-2.943200
8	-6.063979	2.408544	0.669246
6	-6.316659	1.929592	1.905051
9	-5.752712	2.688627	2.880473
8	-2.140696	-1.855781	-1.857841
6	-3.396909	-1.985682	-1.488260
6	-4.349098	-2.365937	-2.472339
6	-5.706872	-2.445738	-2.201245
6	-6.144172	-2.184402	-0.906226
6	-5.246226	-1.871601	0.104115
6	-3.876467	-1.762930	-0.159233
8	-7.534127	-2.252438	-0.627096
6	-8.181562	-1.070006	-0.621753
9	-7.971733	-0.347024	-1.746425
6	-3.021020	-1.221423	0.969896
7	-1.591630	-1.620817	0.946150
6	-1.336352	-3.082027	1.022269
6	-1.786414	-3.711933	2.349803
6	-1.454075	-5.209474	2.413567
6	0.042928	-5.453064	2.184830
6	0.495376	-4.839804	0.853197
6	0.164458	-3.342292	0.773375
7	0.570450	-2.728222	-0.511314
6	2.022384	-2.447282	-0.670762
6	2.573129	-1.591354	0.442906
6	3.630497	-2.062561	1.223919
6	4.150405	-1.284268	2.255035
6	3.620359	-0.033178	2.543321
6	2.550935	0.436600	1.783853
6	2.011547	-0.315601	0.719383
8	5.145281	-1.794570	3.117136
6	6.392510	-1.951054	2.621228
9	6.872765	-0.827242	2.056665
8	0.974619	0.153999	0.021791
9	8.396287	-1.364283	-1.346253
9	7.290481	0.243733	-0.385212
9	-7.637364	1.944501	2.097457
9	-5.861929	0.672769	2.092381
9	7.193104	-2.293064	3.637365
9	6.465190	-2.927443	1.689385
9	-9.493069	-1.313210	-0.517027
9	-7.820725	-0.279392	0.414742
1	-1.129452	-1.169214	1.735298
1	-1.902745	-3.529065	0.197535
1	-2.862100	-3.561383	2.484298
1	1.571907	-4.983498	0.709483
1	0.278049	-3.333570	-1.278218
1	-0.648326	4.063084	-0.342956
1	3.600440	6.709081	2.160016
1	4.144118	5.120630	0.304615
1	3.073501	2.428845	0.202699
1	2.500402	-0.895342	-3.837548
1	4.861563	-1.682847	-3.633840
1	5.911392	1.958794	-1.644235

1	2.853487	3.678861	-2.431565
1	4.332846	3.733170	-1.454951
1	1.864503	4.928948	-0.704961
1	3.585338	4.256486	1.735603
1	2.562862	6.982469	0.764338
1	1.185003	6.999590	2.833472
1	1.802741	5.415175	3.288507
1	-0.446616	5.192012	2.250915
1	0.107724	6.037243	0.807223
1	1.179926	3.355044	1.806439
1	-3.384910	0.608550	-2.530135
1	-5.628564	1.117174	-1.537737
1	-3.711599	3.154338	1.706612
1	-1.405341	3.200081	1.929096
1	-0.626764	1.707664	1.370960
1	2.089055	1.388433	2.023491
1	4.026639	0.545881	3.365964
1	4.052226	-3.043442	1.034737
1	2.121169	-1.924934	-1.625336
1	2.603102	-3.375869	-0.734466
1	0.723141	-2.816588	1.557959
1	-0.009942	-5.353445	0.022548
1	0.266081	-6.525488	2.198841
1	0.616066	-4.999603	3.005396
1	-1.768571	-5.619778	3.379448
1	-2.030169	-5.739231	1.642609
1	-1.281949	-3.188435	3.175459
1	-3.024779	-0.128603	0.927050
1	-3.486928	-1.494780	1.925616
1	-5.628434	-1.659230	1.097153
1	-6.426973	-2.695516	-2.973901
1	-3.975012	-2.548664	-3.475386
1	-0.658944	-0.926126	-3.360564
1	0.614145	-0.039419	-3.034293

Dimer($(H_2O)_2$)

ΔE -4329.73363033 h.

30	-0.622253	-0.986899	-0.908421
8	-2.148963	-1.791916	-1.924124
6	-3.406264	-1.937173	-1.563428
6	-4.360975	-2.243526	-2.570458
6	-5.719388	-2.331169	-2.304744
6	-6.154759	-2.154503	-0.994861
6	-5.254487	-1.916832	0.033776
6	-3.884094	-1.799899	-0.222559
6	-3.025060	-1.339267	0.939003
7	-1.598543	-1.746895	0.889426
1	-1.135122	-1.352433	1.707879
6	-1.355515	-3.212195	0.872161
1	-1.921518	-3.600507	0.017827
6	-1.816977	-3.923147	2.154177
1	-2.892305	-3.774018	2.292724
6	-1.495333	-5.424134	2.122722
6	0.001086	-5.663387	1.886280
6	0.465060	-4.969019	0.599205
1	1.541467	-5.110550	0.452650
6	0.144259	-3.467088	0.613190
7	0.558294	-2.776327	-0.628795
1	0.265274	-3.330592	-1.433112
6	2.012112	-2.496113	-0.765495
6	2.560641	-1.699555	0.392275
6	3.608806	-2.215739	1.157056
6	4.127494	-1.491315	2.227189
6	3.606224	-0.250180	2.569637
6	2.546199	0.263955	1.825840
6	2.007585	-0.433559	0.724606
8	0.979247	0.076229	0.042316
30	0.777019	1.875469	-0.901482
7	-0.127389	3.255561	0.465135
1	-0.613401	3.962127	-0.086976
6	0.930204	3.910096	1.264968
6	0.454314	5.193015	1.963889
6	1.582151	5.843407	2.776795
6	2.801135	6.128760	1.890027
1	3.618877	6.550974	2.483668
6	3.277449	4.853682	1.179784
1	4.127577	5.077831	0.527891
6	2.149728	4.200042	0.365508
7	2.570786	2.955665	-0.321890
1	3.092135	2.368827	0.331462
6	3.423918	3.174448	-1.520894
6	3.846590	1.854814	-2.104180
6	5.168883	1.421811	-2.003393
6	5.533818	0.186285	-2.526281
6	4.613298	-0.613353	-3.193042
6	3.293677	-0.183903	-3.305485
6	2.872016	1.028639	-2.721605
8	1.579918	1.388946	-2.738802
1	2.558567	-0.801446	-3.808770
1	4.930808	-1.565873	-3.604213
8	6.865911	-0.270404	-2.407494
6	7.209471	-0.733311	-1.182784
9	8.431457	-1.267092	-1.269987
9	7.246595	0.248737	-0.253967
9	6.358768	-1.674747	-0.729159
1	5.914319	2.034119	-1.507262
1	2.814887	3.733975	-2.238030
1	4.302924	3.782238	-1.278029
1	1.819976	4.887176	-0.424855
1	3.630429	4.127276	1.926165
1	2.534446	6.882651	1.137068
1	1.221221	6.765883	3.243709
1	1.874387	5.168592	3.593154
1	-0.403091	4.970578	2.607518
1	0.102452	5.895181	1.194602
1	1.237428	3.182908	2.027918

6	-1.117802	2.481724	1.256526
6	-2.358656	2.183239	0.454732
6	-3.613146	2.479919	0.996994
6	-4.769551	2.091465	0.329196
6	-4.712612	1.486205	-0.920990
6	-3.468386	1.236113	-1.489631
6	-2.273300	1.521281	-0.798516
8	-1.104368	1.104765	-1.309142
1	-3.392510	0.720370	-2.439192
1	-5.630778	1.172795	-1.406214
8	-6.048260	2.312556	0.885601
6	-6.299398	1.758633	2.090309
9	-7.619375	1.767168	2.287236
9	-5.849708	0.490637	2.197163
9	-5.729119	2.453076	3.108885
1	-3.687528	2.969594	1.961315
1	-1.392332	3.013166	2.174948
1	-0.618193	1.548257	1.544955
1	2.091781	1.207890	2.106844
1	4.011471	0.286646	3.420934
8	5.111532	-2.051723	3.070429
6	6.363706	-2.183455	2.579757
9	7.150535	-2.594258	3.580925
9	6.442522	-3.098081	1.587800
9	6.856200	-1.028207	2.094270
1	4.024113	-3.190077	0.924552
1	2.118800	-1.926650	-1.691561
1	2.588726	-3.423313	-0.872841
1	0.703740	-2.995426	1.430959
1	-0.038721	-5.424990	-0.265409
1	0.216618	-6.736097	1.832137
1	0.572877	-5.268210	2.737367
1	-1.817935	-5.893426	3.058589
1	-2.070959	-5.899103	1.316495
1	-1.313585	-3.457799	3.014690
1	-3.020933	-0.246181	0.966796
1	-3.493341	-1.670205	1.875110
1	-5.634601	-1.769034	1.039210
8	-7.545032	-2.233313	-0.720812
6	-8.184673	-1.050580	-0.624410
9	-9.497905	-1.292257	-0.541432
9	-7.821050	-0.345838	0.471382
9	-7.967426	-0.243393	-1.688896
1	-6.441264	-2.523660	-3.092011
1	-3.988019	-2.361915	-3.583533
8	0.228638	-0.872086	-2.947554
1	-0.637840	-0.815272	-3.376811
1	0.647521	0.032881	-2.989825
8	-0.002495	3.599110	-2.685086
1	-0.834405	3.103684	-2.707331
1	0.631414	2.988241	-3.110932

Dimer$(H_2O)_3$

ΔE -4406.18901906 h.

30	0.557829	-0.976740	1.041898
8	2.229867	-1.754352	1.918418
6	3.468585	-1.893111	1.456398
6	4.496147	-2.215126	2.375633
6	5.824429	-2.329124	1.988262
6	6.146918	-2.161657	0.646412
6	5.163408	-1.892684	-0.296507
6	3.826347	-1.736721	0.087396
6	2.862838	-1.257937	-0.978532
7	1.463899	-1.717063	-0.818336
1	0.915870	-1.329344	-1.586082
6	1.274310	-3.187964	-0.791527
1	1.875575	-3.554815	0.048031
6	1.720390	-3.896223	-2.080238
1	2.785471	-3.713218	-2.253534
6	1.452386	-5.407179	-2.018129
6	-0.025529	-5.698076	-1.726938
6	-0.474761	-4.998316	-0.437054
1	-1.540854	-5.173743	-0.254797
6	-0.207471	-3.487457	-0.491962
7	-0.627106	-2.777506	0.738426
1	-0.366941	-3.335373	1.551192
6	-2.083669	-2.478987	0.838224
6	-2.606262	-1.723454	-0.358807
6	-3.637045	-2.268072	-1.127922
6	-4.125816	-1.588149	-2.240634
6	-3.592777	-0.362798	-2.620133
6	-2.550469	0.179416	-1.871696
6	-2.038949	-0.473727	-0.729898
8	-1.021875	0.054246	-0.049977
30	-0.834100	1.884151	0.826474
7	0.159436	3.230978	-0.511702
1	0.581541	3.964274	0.058159
6	-0.843483	3.832780	-1.416789
6	-0.330434	5.081546	-2.151752
6	-1.404191	5.675402	-3.074267
6	-2.684400	5.994750	-2.291500
1	-3.462237	6.372796	-2.963433
6	-3.197167	4.755000	-1.545302
1	-4.093005	5.002536	-0.967127
6	-2.122842	4.162785	-0.619131
7	-2.585929	2.960749	0.114286
1	-3.087325	2.345804	-0.528212
6	-3.487293	3.253063	1.261517
6	-3.973882	1.971937	1.880006
6	-5.305828	1.577249	1.752564
6	-5.728207	0.377334	2.313887
6	-4.855573	-0.426321	3.038255
6	-3.526794	-0.035325	3.176262
6	-3.048392	1.142265	2.564825
8	-1.749931	1.465697	2.623455
1	-2.826008	-0.653985	3.725512

1	-5.217874	-1.351113	3.474942
8	-7.072937	-0.035921	2.175623
6	-7.394150	-0.557178	0.968860
9	-8.641658	-1.031420	1.041548
9	-7.354146	0.366837	-0.017619
9	-6.572065	-1.560754	0.604604
1	-6.015034	2.191936	1.208363
1	-2.896818	3.827486	1.982579
1	-4.336523	3.872666	0.951107
1	-1.850493	4.900769	0.147036
1	-3.489775	3.983366	-2.272637
1	-2.477673	6.792885	-1.565762
1	-1.017836	6.575452	-3.564114
1	-1.634423	4.955439	-3.871601
1	0.569992	4.835458	-2.723767
1	-0.036729	5.828282	-1.400374
1	-1.093305	3.060603	-2.156602
6	1.229414	2.459216	-1.194342
6	2.402366	2.201065	-0.283868
6	3.693166	2.529342	-0.710576
6	4.791059	2.166528	0.061845
6	4.630973	1.555680	1.300413
6	3.348105	1.271620	1.755405
6	2.218541	1.534240	0.954506
8	1.013578	1.096746	1.348406
1	3.194382	0.767333	2.702243
1	5.508351	1.271255	1.871051
8	6.113991	2.404224	-0.366571
6	6.451196	1.993154	-1.607205
9	7.781246	1.899623	-1.672587
9	5.910592	0.804001	-1.937831
9	6.057221	2.873925	-2.564471
1	3.841478	3.021500	-1.665187
1	1.572704	2.972790	-2.099422
1	0.772477	1.509442	-1.500943
1	-2.086122	1.110226	-2.179732
1	-3.974366	0.138966	-3.503201
8	-5.084523	-2.185201	-3.088365
6	-6.353166	-2.286754	-2.634822
9	-7.106933	-2.751073	-3.638238
9	-6.469007	-3.144995	-1.597158
9	-6.857604	-1.105238	-2.232046
1	-4.059556	-3.232439	-0.867734
1	-2.202323	-1.878523	1.742263
1	-2.666674	-3.399718	0.965165
1	-0.797200	-3.059328	-1.311801
1	0.071407	-5.420747	0.418994
1	-0.197667	-6.777079	-1.648267
1	-0.639777	-5.339774	-2.564571
1	1.759680	-5.878933	-2.957886
1	2.072049	-5.849341	-1.225925
1	1.175009	-3.458689	-2.929571
1	2.826504	-0.165195	-0.955953
1	3.260155	-1.537519	-1.963039
1	5.445897	-1.762634	-1.335401
8	7.504134	-2.321654	0.278242
6	8.132318	-1.255031	-0.258471
9	9.451799	-1.472093	-0.192119
9	7.815944	-1.070451	-1.561872
9	7.855086	-0.100172	0.381259
1	6.608136	-2.544324	2.707336
1	4.221426	-2.328128	3.419746
8	-0.401403	-0.802771	2.969294
1	0.347886	-0.690050	3.605210
1	-0.865525	0.077249	2.928744
8	-0.114063	3.632727	2.615237
1	0.706589	3.127838	2.712813
1	-0.784469	3.044399	3.016459
8	1.936807	-0.746163	4.300151
1	2.157998	-1.183075	3.424513
1	1.992473	-1.452437	4.956785

Dimer(analyte)

ΔE -4618.34128110 h.

30	0.129594	-1.135562	-0.410651
30	0.482695	1.778262	0.975772
9	7.636241	-2.897680	3.013346
8	-0.761098	0.857317	-0.365581
9	-6.003139	1.785878	1.878458
9	-7.168394	0.091636	2.599915
9	6.583173	-2.743658	1.111949
8	5.509564	-3.352713	2.996797
8	1.713006	0.300885	0.200207
9	-5.380265	-0.231773	1.393362
8	6.804875	1.320109	-1.746914
8	-5.232609	0.461065	3.527946
9	6.247610	-1.255382	2.650607
8	-5.610450	1.311858	-2.999190
8	0.222168	1.142330	2.810676
8	0.345520	-2.203702	1.337376
9	-7.501860	0.487198	-3.683241
9	7.893071	1.525294	0.209805
7	1.556583	3.294729	-0.102887
1	2.361286	3.623805	0.431697
9	7.150747	3.313467	-0.767149
7	-0.880719	3.499878	1.358810
1	-1.686805	3.372094	0.747405
6	-1.923699	1.036414	-0.982025
7	-0.263318	-1.022236	-2.641811
1	-1.000420	-1.708227	-2.809287
7	1.740422	-2.467530	-1.251855
1	2.576501	-1.889092	-1.153089
9	8.793289	2.192938	-1.658542
6	-0.168186	4.727911	0.953016
1	0.551143	4.952738	1.752954
9	-5.819186	-0.880171	-3.458606

6	-1.352953	3.467087	2.772512
1	-0.469610	3.638443	3.395962
1	-2.076729	4.266293	2.973305
6	-1.946180	2.116326	3.074872
6	2.938751	0.565928	-0.238943
6	-1.074966	0.988973	3.043564
6	1.578647	-2.486146	1.746148
6	-3.092278	1.430310	-0.298424
1	-3.038372	1.598852	0.769655
6	1.946898	-3.691188	-0.422665
1	0.987710	-4.210580	-0.358846
1	2.667045	-4.371027	-0.891808
6	-5.923090	0.517150	2.370509
9	-6.805818	-0.081169	-1.698693
6	1.378546	5.704198	-0.808070
1	2.132958	5.966568	-0.052220
1	1.919698	5.494503	-1.736119
6	0.639056	4.442697	-0.332723
1	-0.068892	4.117177	-1.107425
6	-1.635372	-0.297537	3.226237
6	-6.414542	0.228433	-2.954032
6	1.529274	-2.728134	-2.689561
1	0.772379	-3.522511	-2.760633
6	-3.007240	-0.464743	3.386732
6	2.429595	-3.291472	0.944276
6	-0.771767	0.301646	-3.095559
1	0.030058	1.019171	-2.900559
1	-0.964606	0.303234	-4.173742
6	4.027175	-0.268638	0.097099
1	3.846723	-1.097169	0.766989
6	7.637923	2.073572	-0.996347
6	2.063393	2.653818	-1.354154
1	1.212074	2.112096	-1.775407
1	2.386003	3.408940	-2.078763
6	-4.380885	1.201384	-2.308698
6	4.482886	1.956476	-1.521747
1	4.690118	2.824701	-2.140066
6	5.520180	1.086243	-1.202014
6	0.957548	-1.463590	-3.363434
1	1.693163	-0.656700	-3.234168
6	-1.105533	5.932013	0.759040
1	-1.866953	5.657348	0.014373
1	-1.635916	6.137449	1.694410
6	-4.318375	1.517787	-0.958059
1	-5.217463	1.790268	-0.420035
6	4.185137	-3.071904	2.575420
6	2.810439	-3.190484	-3.408277
1	3.576751	-2.412596	-3.277711
1	3.196253	-4.096917	-2.932380
6	3.724982	-3.588334	1.369203
1	4.392206	-4.180077	0.750844
6	6.466877	-2.572370	2.455679
6	2.009392	-2.180698	-5.573747
1	2.758788	-1.378221	-5.535864
1	1.799626	-2.366683	-6.632609
6	3.192539	1.707535	-1.050920
6	-2.017173	0.722668	-2.364848
6	-3.833812	0.655633	3.401138
6	2.576990	-3.435917	-4.903515
1	3.513493	-3.740385	-5.383006
1	1.871487	-4.268757	-5.029177
6	-3.319007	1.940458	3.262883
1	-3.994837	2.790048	3.256820
6	-3.248084	0.803072	-3.014491
1	-3.338048	0.556476	-4.068144
6	5.309664	-0.019385	-0.385074
1	6.137400	-0.664895	-0.116251
6	0.424288	6.889773	-1.005435
1	0.990200	7.771751	-1.323810
1	-0.281381	6.657231	-1.814705
6	0.731275	-1.709453	-4.866633
1	-0.053939	-2.471872	-4.977211
1	0.360136	-0.799670	-5.346998
6	3.378678	-2.266698	3.375743
1	3.781172	-1.856756	4.296262
6	-0.354885	7.182099	0.282427
1	-1.060984	8.005052	0.128098
1	0.344159	7.507346	1.064996
6	2.079531	-1.981737	2.964647
1	1.444467	-1.315950	3.538437
1	-0.970657	-1.151470	3.151532
1	-3.451052	-1.452277	3.464275
7	-2.001082	-1.735653	0.025100
1	-1.900512	-1.862129	1.032313
1	-2.598953	-0.918231	-0.073197
6	-2.719526	-2.909182	-0.530443
1	-2.878920	-2.704334	-1.596745
6	-1.786384	-4.129951	-0.439551
1	-2.344762	-5.031788	-0.710356
1	-0.993764	-3.997035	-1.195405
8	-1.233623	-4.334527	0.844129
1	-0.625874	-3.577429	1.051124
6	-4.081073	-3.072613	0.123695
6	-5.229055	-2.653558	-0.558199
6	-4.208247	-3.556435	1.435862
6	-6.483659	-2.712224	0.051975
1	-5.141664	-2.258776	-1.565984
6	-5.462107	-3.614871	2.045351
1	-3.320677	-3.890746	1.963260
6	-6.603168	-3.190505	1.356953
1	-7.357130	-2.359364	-0.487459
1	-5.548824	-3.990745	3.061161
1	-7.575689	-3.225672	1.839381

Dimer(analyte)$_2$
ΔE -5059.86139178 h.

30	-0.099506	-1.578341	0.603349
30	-0.183789	1.671538	0.150563
9	8.306357	-3.662928	-0.830173
8	-1.112802	-0.134581	-0.585477
9	-6.979640	-0.509050	0.316868
9	-6.776845	0.916592	-1.309207
9	6.658155	-2.416250	-1.514677
8	6.290007	-4.254158	-0.269359
8	1.199796	0.093237	0.601623
9	-8.647629	0.792793	-0.202530
8	6.596769	0.376733	-0.622580
8	-6.934325	1.688059	0.795285
9	7.231848	-2.394344	0.578436
8	-5.816546	-0.808959	-3.446624
8	-1.481812	1.808274	1.773007
8	1.228067	-2.863645	1.504587
9	-6.045890	-3.043068	-3.379681
9	6.669048	0.003258	-2.841743
7	1.142767	2.252870	-1.510583
1	1.847303	2.879449	-1.122487
9	8.424631	0.672383	-1.742445
7	-1.540261	2.965291	-1.020026
1	-2.085819	2.337135	-1.611425
6	-2.231944	-0.369598	-1.258079
7	-1.872797	-2.805082	0.575835
1	-1.795518	-3.259853	1.490507
7	0.330298	-2.801353	-1.167891
1	-0.148353	-2.360238	-1.952719
9	6.775102	2.045994	-2.118290
6	-0.713645	3.840052	-1.878975
1	-0.217322	4.557694	-1.210306
9	-7.323067	-1.826226	-2.116581
6	-2.488978	3.663592	-0.119541
1	-1.881304	4.220740	0.603973
1	-3.106615	4.385411	-0.667291
6	-3.372747	2.681802	0.602820
6	2.486137	0.150127	0.267211
6	-2.788523	1.831227	1.585832
6	2.395154	-3.258977	1.026771
6	-2.423745	0.185021	-2.543864
1	-1.603302	0.738542	-2.987828
6	1.774174	-2.821286	-1.473065
1	1.983208	-3.416567	-2.373189
1	2.033712	-1.786330	-1.720855
6	-7.316448	0.737470	-0.084990
9	-7.573890	-1.768279	-4.274046
6	1.286917	3.846626	-3.445039
1	1.828579	4.558068	-2.808278
1	2.041466	3.214095	-3.925061
6	0.385087	2.985181	-2.546694
1	-0.112175	2.228168	-3.166910
6	-3.658112	1.039334	2.373120
6	-6.662229	-1.844282	-3.298808

6	-0.324453	-4.097685	-0.877939
1	0.185243	-4.503929	0.002148
6	-5.022457	0.980413	2.107436
6	2.703773	-3.286680	-0.364207
6	-3.077542	-1.934303	0.566670
1	-3.986268	-2.506302	0.796154
1	-2.934725	-1.206364	1.368710
6	3.489301	-0.218837	1.187433
1	3.181666	-0.599172	2.155085
6	7.094496	0.759230	-1.808290
6	1.832562	1.030244	-1.999445
1	1.058208	0.261313	-2.096432
1	2.283838	1.195819	-2.985253
6	-4.630119	-0.744489	-2.688857
6	4.244623	0.687029	-1.343400
1	4.528247	1.052205	-2.322391
6	5.206402	0.312918	-0.408969
6	-1.798213	-3.818063	-0.500829
1	-2.274822	-3.373041	-1.383618
6	-1.516634	4.607724	-2.942758
1	-2.056498	3.877108	-3.562660
1	-2.273500	5.235330	-2.462425
6	-3.611054	0.013573	-3.250963
1	-3.752136	0.455250	-4.232119
6	4.978762	-3.938321	0.167927
6	-0.250027	-5.115499	-2.025957
1	-0.697441	-4.668032	-2.925864
1	0.796675	-5.333461	-2.262304
6	4.000472	-3.627163	-0.764488
1	4.266126	-3.619675	-1.817653
6	7.096224	-3.196597	-0.499839
6	-2.450877	-6.138757	-1.292392
1	-2.986055	-5.746070	-2.168193
1	-2.955066	-7.068105	-1.005017
6	2.888011	0.600347	-1.014615
6	-3.262046	-1.206723	-0.743540
6	-5.545327	1.744169	1.068941
6	-0.989516	-6.414730	-1.672071
1	-0.936703	-7.115953	-2.512340
1	-0.480595	-6.896835	-0.826035
6	-4.739435	2.607999	0.334283
1	-5.187742	3.223855	-0.439893
6	-4.453385	-1.367541	-1.455216
1	-5.244008	-1.969611	-1.026609
6	4.836755	-0.147384	0.852871
1	5.608023	-0.463109	1.545917
6	0.477797	4.613278	-4.498952
1	1.146010	5.239340	-5.100322
1	0.006585	3.899718	-5.188995
6	-2.536881	-5.116896	-0.150236
1	-2.088381	-5.540043	0.759733
1	-3.582358	-4.887010	0.085435
6	4.689420	-3.977115	1.528655

1	5.466215	-4.239214	2.239522
6	-0.607770	5.467603	-3.832476
1	-1.208384	5.987101	-4.586986
1	-0.131197	6.243876	-3.217746
6	3.402988	-3.659963	1.940130
1	3.143627	-3.658803	2.994777
1	-3.236878	0.470365	3.193896
1	-5.681757	0.344993	2.689435
7	-0.498349	-0.750798	2.599713
1	0.487453	-0.601953	2.808055
1	-0.890077	0.180132	2.386472
6	-1.182420	-1.319933	3.769779
1	-2.200656	-1.579735	3.454942
6	-0.513179	-2.641100	4.199645
1	0.528458	-2.427456	4.488853
1	-1.028819	-3.013329	5.092117
8	-0.571365	-3.641537	3.201884
1	0.195432	-3.474583	2.589428
6	-1.282572	-0.348913	4.943663
6	-0.416772	0.743349	5.085613
6	-2.270258	-0.546973	5.920011
6	-0.534373	1.618374	6.167712
1	0.351007	0.938202	4.345063
6	-2.388615	0.320207	7.006724
1	-2.958908	-1.383080	5.819445
6	-1.520162	1.408578	7.133598
1	0.142632	2.464970	6.235352
1	-3.164103	0.152225	7.748820
1	-1.617931	2.089608	7.974195
7	1.092194	2.683431	1.704748
1	0.488819	2.453425	2.494500
1	1.919594	2.097896	1.802732
6	1.447793	4.106935	1.828254
1	0.512472	4.667823	1.704197
6	1.996406	4.411063	3.239952
1	2.960410	3.906634	3.368105
1	2.163861	5.491818	3.349809
8	1.143115	3.896243	4.257861
1	0.314550	4.395261	4.246959
6	2.416936	4.542637	0.747460
6	2.199526	5.737360	0.048035
6	3.547844	3.772519	0.429066
6	3.085558	6.155217	-0.947698
1	1.326003	6.340934	0.281325
6	4.426357	4.179231	-0.578203
1	3.741508	2.833353	0.939555
6	4.198433	5.373008	-1.267032
1	2.898461	7.082230	-1.481594
1	5.276488	3.554279	-0.831101
1	4.879880	5.688084	-2.051431

Monomer
ΔE -2088.38421118 h.

30	-0.016163	-1.814216	-0.025890
8	-1.798759	-2.477992	0.142376
6	-2.811236	-1.615599	0.190149
6	-3.859988	-1.833183	1.112658
6	-4.944482	-0.967280	1.201882
6	-4.992220	0.144197	0.365420
6	-3.986034	0.390300	-0.560211
6	-2.898417	-0.480423	-0.669002
6	-1.839656	-0.228593	-1.713493
1	-2.120327	0.633342	-2.329420
1	-1.750326	-1.096881	-2.375532
7	-0.481124	-0.037649	-1.117724
1	0.187511	0.079944	-1.879173
6	-0.350098	1.113714	-0.185578
6	-0.243701	2.461801	-0.912908
1	-1.135413	2.619551	-1.528794
6	-0.058465	3.625208	0.071478
6	1.161540	3.392935	0.972594
6	1.047310	2.054190	1.715517
1	1.935854	1.882900	2.332157
6	0.862758	0.884374	0.739088
7	0.720143	-0.430202	1.419388
1	0.052413	-0.335905	2.184915
6	1.986866	-1.008379	1.966841
6	3.033351	-1.203026	0.898386
6	4.258249	-0.538643	1.000023
6	5.241036	-0.727860	0.037051
6	5.034531	-1.578020	-1.045310
6	3.815848	-2.237576	-1.162072
6	2.783233	-2.061677	-0.212685
8	1.633205	-2.709866	-0.377541
1	3.625306	-2.904114	-1.997323
1	5.819509	-1.708988	-1.782634
8	6.487917	-0.074877	0.182323
6	6.566602	1.164470	-0.347603
9	5.686004	2.026781	0.210024
9	6.333078	1.178400	-1.677585
9	7.800901	1.628761	-0.131172
1	4.454901	0.130142	1.832205
1	2.386799	-0.380998	2.771295
1	1.706252	-1.972709	2.404259
1	1.755020	0.802108	0.106974
1	0.184404	2.084095	2.396570
1	1.269051	4.210514	1.693186
1	2.073316	3.388494	0.359778
1	0.043958	4.565551	-0.480425
1	-0.958699	3.719571	0.693648
1	0.616356	2.422346	-1.597269
1	-1.254233	1.107255	0.435302
1	-4.058986	1.262842	-1.202129
8	-6.052584	1.071227	0.498235
6	-7.129818	0.857214	-0.288579
9	-6.830219	0.907612	-1.604916

9	-8.026834	1.813384	-0.025721
9	-7.707709	-0.341708	-0.064685
1	-5.745523	-1.138310	1.913240
1	-3.793856	-2.705180	1.755690

Monomer(H_2O)
DE -2164.83110474 h.

6	-3.931823	0.594019	-0.586057
6	-4.993816	0.231483	0.233939
6	-5.010984	-0.994956	0.890715
6	-3.935803	-1.863110	0.728307
6	-2.836031	-1.528820	-0.091307
6	-2.853296	-0.274863	-0.766731
6	-1.723751	0.102903	-1.691844
1	-1.595323	-0.669013	-2.458235
7	-0.410574	0.187317	-0.986790
1	0.311007	0.386141	-1.680150
6	-0.320097	1.197215	0.099413
6	-0.265813	2.642901	-0.415667
6	-0.110041	3.649415	0.733802
6	1.126494	3.328901	1.583814
1	1.211437	4.031700	2.419464
6	1.066346	1.890159	2.115355
1	1.966684	1.655795	2.693342
6	0.909439	0.875353	0.975113
7	0.820465	-0.527404	1.454319
1	0.199576	-0.569499	2.262344
6	2.119590	-1.164755	1.832908
6	3.095560	-1.201021	0.683029
6	4.315621	-0.528933	0.789617
6	5.235054	-0.572554	-0.250745
6	4.967441	-1.280613	-1.418565
6	3.752046	-1.945574	-1.540719
6	2.782133	-1.916872	-0.511606
8	1.632309	-2.561212	-0.680915
30	0.005662	-1.722359	-0.083918
8	-1.824987	-2.388370	-0.224050
8	-0.292075	-3.505186	1.685955
1	0.247006	-4.156419	1.216150
1	-1.132052	-3.468214	1.184740
1	3.515030	-2.502873	-2.441755
1	5.703280	-1.299104	-2.215656
8	6.481829	0.081019	-0.101797
6	6.511936	1.379177	-0.470187
9	5.659571	2.145543	0.248312
9	7.752422	1.836257	-0.272955
9	6.193249	1.560005	-1.770103
1	4.557704	0.032267	1.686892
1	1.856845	-2.178799	2.147962
1	2.570076	-0.648039	2.688150
1	1.796370	0.920874	0.331369
1	0.210176	1.787156	2.797675
1	2.031681	3.451199	0.973563
1	-0.047039	4.665792	0.330721
1	-1.006394	3.615628	1.367928
1	-1.168326	2.864112	-0.994778
1	0.587327	2.737357	-1.103081
1	-1.219478	1.064945	0.713762
1	-1.957358	1.044348	-2.202221
1	-3.922037	-2.824923	1.231801
1	-5.854048	-1.253895	1.522378
8	-6.047464	1.149969	0.449705
6	-7.070883	1.097120	-0.430988
9	-6.681258	1.363566	-1.696920
9	-7.972809	2.014815	-0.067959
9	-7.675516	-0.109117	-0.453682
1	-3.955028	1.556024	-1.088522

Monomer($(H_2O)_2$)
ΔE -2241.28493523 h.

6	-4.028422	2.275224	-0.262162
6	-2.855317	1.905280	0.435060
6	-2.916928	0.766362	1.290045
6	-4.096858	0.027851	1.384802
6	-5.220806	0.410448	0.662694
6	-5.201806	1.533989	-0.157829
8	-1.741628	2.614764	0.286631
30	-0.051698	1.682819	-0.081957
8	1.891146	4.411697	-0.977100
6	-1.692293	0.347459	2.059420
7	-0.578399	-0.038207	1.148127
6	-0.866926	-1.127680	0.186598
6	0.308772	-1.221179	-0.807144
6	0.060271	-2.309062	-1.860094
6	-0.224574	-3.669187	-1.206338
6	-1.396941	-3.572489	-0.220077
6	-1.142743	-2.489390	0.838674
7	0.565596	0.114587	-1.402554
6	1.989499	0.392778	-1.756155
6	2.896288	0.349071	-0.549725
6	2.719486	1.272978	0.518117
6	3.598955	1.206748	1.618620
6	4.621823	0.264941	1.675033
6	4.767891	-0.633627	0.622945
6	3.919935	-0.599627	-0.477585
8	1.756904	2.201628	0.501884
8	5.758965	-1.638678	0.700093
6	6.959045	-1.331700	0.158691
9	6.879330	-1.067949	-1.163396
8	-6.413229	-0.342239	0.788485
6	-6.523958	-1.402022	-0.040647
9	-7.693529	-1.999968	0.206927
8	-0.153943	2.988327	-1.919252
9	7.530314	-0.255645	0.739061
9	7.766996	-2.382684	0.329836
9	-6.493312	-1.049542	-1.343842

9	-5.537944	-2.311527	0.138125
1	0.004531	0.225531	-2.246468
1	0.230383	-0.296570	1.713797
1	3.457485	1.919886	2.424599
1	-1.940477	-0.465539	2.751775
1	-1.312548	1.187968	2.650023
1	-1.758966	-0.813772	-0.370206
1	2.346743	-0.312823	-2.515755
1	1.992940	1.393862	-2.198287
1	1.204646	-1.481954	-0.230829
1	5.298776	0.216148	2.521160
1	-0.276249	-2.767218	1.456018
1	-2.003287	-2.410919	1.510617
1	-4.148075	-0.852640	2.017660
1	0.673267	-4.007319	-0.671128
1	-0.432441	-4.417504	-1.978606
1	-1.567519	-4.538069	0.267948
1	-2.318112	-3.328419	-0.766900
1	4.064971	-1.315971	-1.280231
1	-0.801334	-2.012073	-2.475182
1	0.925059	-2.374588	-2.529866
1	-6.094104	1.810323	-0.709789
1	-3.985171	3.152974	-0.899962
1	-0.984003	3.378273	-1.597810
1	0.554826	3.655595	-1.715871
1	2.008766	3.639383	-0.365574
1	1.601686	5.135057	-0.405441

Monomer$(H_2O)_3$
ΔE -2317.73808872 h.

6	4.007612	1.998796	-0.333275
6	2.759558	1.631655	-0.878799
6	2.645571	0.380171	-1.538767
6	3.745727	-0.473835	-1.600063
6	4.951373	-0.097364	-1.020564
6	5.099129	1.135360	-0.393670
8	1.703473	2.446410	-0.772658
30	0.038279	1.759407	0.072119
8	-2.270502	4.039740	1.341556
6	1.301970	-0.046673	-2.065417
7	0.332960	-0.195138	-0.946602
6	0.742422	-1.105889	0.145506
6	-0.323590	-1.052386	1.255739
6	0.123844	-1.870756	2.473601
6	0.439383	-3.323482	2.084402
6	1.462077	-3.390552	0.940343
6	1.004721	-2.560160	-0.269125
7	-0.645689	0.357298	1.592248
6	-2.100310	0.618872	1.807745
6	-2.896768	0.407425	0.541737
6	-2.671963	1.241944	-0.589234
6	-3.410724	0.997546	-1.764849
6	-4.352006	-0.026787	-1.829753
6	-4.555019	-0.826752	-0.710241
6	-3.839438	-0.620569	0.463815
8	-1.785302	2.244902	-0.554484
8	-5.457798	-1.911507	-0.788215
6	-6.722986	-1.662420	-0.381997
9	-6.788351	-1.296560	0.916509
8	6.046992	-0.991118	-1.073637
6	6.089706	-1.908693	-0.082426
9	7.160138	-2.682619	-0.281902
8	0.213915	3.135277	1.719830
9	-7.313022	-0.681150	-1.095690
9	-7.432139	-2.784468	-0.538546
9	6.189644	-1.347998	1.141109
9	4.992572	-2.702965	-0.055828
1	-0.144643	0.635860	2.434359
1	-0.566912	-0.493761	-1.323487
1	-3.229254	1.638027	-2.622156
1	1.396544	-0.973869	-2.642804
1	0.887114	0.722693	-2.724192
1	1.672840	-0.689609	0.551999
1	-2.492941	-0.022423	2.606866
1	-2.183064	1.657225	2.140137
1	-1.238159	-1.498861	0.847631
1	-4.922369	-0.213406	-2.733369
1	0.083744	-2.983649	-0.694798
1	1.767214	-2.596716	-1.052411
1	3.668559	-1.444202	-2.079245
1	-0.488921	-3.817914	1.767271
1	0.805586	-3.872001	2.958938
1	1.626521	-4.430717	0.638959
1	2.432702	-3.006940	1.283592
1	-4.020266	-1.268482	1.315756
1	1.021054	-1.401025	2.901790
1	-0.655770	-1.836679	3.243409
1	6.051919	1.400922	0.051810
1	4.091340	2.961654	0.160971
1	0.880885	3.817881	1.448419
1	-0.661769	3.600293	1.741741
1	-2.227047	3.438991	0.551014
1	-2.347608	4.934675	0.986702
8	2.036958	4.695000	0.539253
1	1.646120	5.429319	0.048191
1	2.004113	3.914885	-0.082475

Monomer(analyte)
ΔE -2529.89387724 h.

6	0.046128	3.065984	-0.131885
6	0.416616	4.031424	-1.090995
6	1.619237	4.725471	-0.989986
6	2.467038	4.456894	0.079965
6	2.135342	3.513372	1.045937
6	0.928098	2.819166	0.956131
6	0.536524	1.813941	2.006968

7	0.414799	0.445874	1.432609
1	1.319781	0.188480	1.034834
6	0.011370	-0.594537	2.411774
6	-0.308420	-1.892525	1.645673
7	-1.321477	-1.616713	0.600602
1	-2.244168	-1.648436	1.032092
6	-1.308922	-2.568179	-0.551866
6	0.026570	-2.585411	-1.247556
6	0.796189	-3.750487	-1.256251
6	2.036049	-3.764720	-1.882237
6	2.536701	-2.629222	-2.513745
6	1.780297	-1.462461	-2.507501
6	0.518291	-1.396333	-1.867225
8	-0.166615	-0.266313	-1.867891
30	-1.035597	0.382217	-0.236871
8	-1.107429	2.407015	-0.245141
7	-3.126398	0.521878	-0.862155
1	-3.305027	-0.199328	-1.558865
1	-3.124030	1.408223	-1.367203
6	-4.207054	0.512317	0.157023
6	-5.603575	0.425871	-0.431806
6	-6.524144	-0.500816	0.073313
6	-7.824392	-0.563337	-0.431842
6	-8.220199	0.303596	-1.452599
6	-7.309971	1.233132	-1.962764
6	-6.011950	1.294819	-1.454289
1	-5.315976	2.023752	-1.861343
1	-7.610542	1.911148	-2.756183
1	-9.229738	0.254580	-1.849764
1	-8.524806	-1.290612	-0.031603
1	-6.219959	-1.178936	0.867110
6	-4.074032	1.752744	1.064146
1	-4.271680	2.652422	0.460095
8	-2.824709	1.835908	1.718392
1	-2.179217	2.220773	1.075760
1	-4.858933	1.695095	1.825575
1	-4.035171	-0.368809	0.785249
1	2.149002	-0.561533	-2.987992
1	3.509453	-2.667779	-2.993065
8	2.788403	-4.964934	-1.901950
6	3.596815	-5.164484	-0.840121
9	2.918968	-5.221196	0.330110
9	4.227453	-6.330762	-1.013396
9	4.526471	-4.194901	-0.701562
1	0.438022	-4.652292	-0.768986
1	-1.577572	-3.580885	-0.227911
1	-2.090362	-2.220627	-1.236425
1	0.604536	-2.191421	1.117333
6	-0.724022	-3.026206	2.593420
6	0.343274	-3.283159	3.664946
6	0.646227	-1.996977	4.443515
6	1.067656	-0.862693	3.498079
1	1.257597	0.049521	4.071489
1	2.011859	-1.131284	3.002374
1	1.433008	-2.171582	5.185284
1	-0.249949	-1.689750	5.000009
1	0.010652	-4.076147	4.343393
1	1.260951	-3.643864	3.180453
1	-0.913286	-3.936084	2.013550
1	-1.672183	-2.750699	3.078190
1	-0.913920	-0.228562	2.877211
1	-0.443271	2.058444	2.429068
1	1.262940	1.834938	2.827035
1	2.820463	3.331251	1.868326
8	3.667083	5.195195	0.218160
6	4.764413	4.652732	-0.351170
9	5.793026	5.479424	-0.132699
9	4.631418	4.483481	-1.683886
9	5.076515	3.443865	0.166484
1	1.907450	5.465421	-1.729135
1	-0.261948	4.217128	-1.917594

Monomer(analyte)$_2$

ΔE -2971.40910109 h.

30	0.248105	0.571031	-0.026102
9	6.257461	-2.955121	2.345984
8	-1.548053	0.034878	-1.056980
9	6.440150	-2.690213	0.201682
8	6.799735	-0.923721	1.548765
9	8.212916	-2.573513	1.463420
8	-4.831658	-4.437519	-1.106217
8	1.646704	1.129114	1.362289
9	-6.715452	-3.463646	-0.360741
6	-2.324119	-1.052211	-1.014362
7	0.371719	-1.633847	0.256559
1	1.107048	-1.787628	0.947122
7	1.844703	0.028407	-1.441684
1	1.432613	0.327553	-2.330111
9	-6.512475	-5.632432	-0.420656
6	2.871022	0.646948	1.387153
6	-3.467008	-1.095259	-1.844048
1	-3.664237	-0.231402	-2.471330
6	3.048804	0.844353	-1.136943
1	3.806930	0.746820	-1.925644
1	2.717388	1.887596	-1.124186
9	-5.423159	-4.466531	1.062782
6	-5.849337	-4.489566	-0.219526
6	2.090291	-1.428718	-1.478397
1	2.863361	-1.638905	-0.729224
6	3.647807	0.481812	0.197931
6	-0.882711	-2.212777	0.785498
1	-0.735502	-3.250857	1.109119
1	-1.123209	-1.647801	1.693961
6	-4.019078	-3.281589	-1.050027
6	0.822867	-2.185657	-1.044721
1	0.028965	-1.960674	-1.765288

6	-4.317854	-2.193530	-1.863738
1	-5.195252	-2.219298	-2.500803
6	5.478474	-0.411881	1.498080
6	2.587914	-1.920398	-2.844812
1	1.831127	-1.674008	-3.602960
1	3.500937	-1.378196	-3.115819
6	4.935519	-0.050412	0.270407
1	5.522409	-0.196909	-0.631548
6	6.914914	-2.258292	1.392906
6	1.579883	-4.193973	-2.398662
1	0.790363	-4.045358	-3.148125
1	1.774782	-5.271220	-2.356278
6	-2.045189	-2.171999	-0.184437
6	2.840101	-3.434323	-2.834865
1	3.166044	-3.769138	-3.825832
1	3.660498	-3.658087	-2.138807
6	-2.901251	-3.278204	-0.226748
1	-2.701137	-4.149952	0.388609
6	1.072594	-3.701308	-1.034686
1	1.814725	-3.931746	-0.256509
1	0.150997	-4.228839	-0.768323
6	4.757423	-0.252771	2.677745
1	5.203834	-0.545690	3.622596
6	3.471236	0.273608	2.617439
1	2.888093	0.408777	3.523829
7	-1.096377	1.131791	1.734086
1	-1.615464	0.297566	1.998813
1	-0.316923	1.212072	2.388192
6	-1.984671	2.312646	1.876091
1	-1.390182	3.186937	1.589273
6	-3.169066	2.218493	0.893847
1	-3.737586	1.298070	1.101081
1	-3.838071	3.062457	1.089651
8	-2.784478	2.283707	-0.466755
1	-2.397176	1.403874	-0.725246
6	-2.482482	2.513616	3.298699
6	-2.251694	3.721780	3.967460
6	-3.199300	1.504297	3.959137
6	-2.721407	3.919723	5.267923
1	-1.697093	4.511790	3.467084
6	-3.670532	1.698623	5.257851
1	-3.393579	0.557456	3.460918
6	-3.432232	2.908073	5.916644
1	-2.529123	4.861620	5.773589
1	-4.224055	0.907254	5.755020
1	-3.796729	3.058861	6.928494
7	0.052415	2.588306	-0.882285
1	0.648663	3.135575	-0.262406
1	-0.917049	2.806712	-0.633028
6	0.279009	3.028472	-2.284074
1	1.320250	2.800576	-2.534649
6	-0.611835	2.227815	-3.255544
1	-1.666774	2.411569	-3.005634
1	-0.440285	2.620816	-4.263397
8	-0.329603	0.839718	-3.270829
1	-0.846927	0.440653	-2.527685
6	0.043261	4.519342	-2.464606
6	1.030363	5.334033	-3.031234
6	-1.180433	5.097216	-2.088601
6	0.807442	6.700517	-3.217933
1	1.981031	4.896191	-3.326119
6	-1.403889	6.461822	-2.274686
1	-1.958993	4.479148	-1.647400
6	-0.410878	7.267806	-2.839383
1	1.585504	7.319964	-3.654888
1	-2.354594	6.896887	-1.979560
1	-0.585873	8.330322	-2.981310

Relevant structures optimized in DMSO (coordinates/Å - potential energies/Hartree)

DMSO

ΔE -553.205445321 h.

8	-0.054514	-0.270783	-0.016545
16	0.005919	0.596543	1.236067
6	1.351785	-0.057976	2.286417
1	2.291302	0.123571	1.761033
1	1.352268	0.471449	3.242527
1	1.206193	-1.131032	2.436148
6	-1.369805	0.079159	2.321883
1	-1.326832	-1.002630	2.472988
1	-1.294924	0.608311	3.275203
1	-2.299746	0.351205	1.819022

H_2O

ΔE -76.4250317442 h.

1	0.757471	-0.478651	0.000000
8	-0.000032	0.120565	0.000000
1	-0.757439	-0.478773	0.000000

analyte

ΔE -441.471698106 h.

6	3.048845	-0.104912	-0.233298
6	2.362691	-1.226888	0.242027
6	0.990058	-1.156793	0.480546
6	0.276191	0.029565	0.249566
6	0.974128	1.146422	-0.223989
6	2.350017	1.081399	-0.463617
6	-1.230843	0.039737	0.476146
7	-1.887912	1.342245	0.642197
6	-1.965607	-0.669638	-0.680085
8	-3.363633	-0.681738	-0.445517
1	2.897576	-2.153337	0.431390
1	0.463029	-2.031346	0.855639
1	0.449724	2.081245	-0.397014
1	2.874289	1.960537	-0.827702
1	4.118226	-0.154759	-0.416622
1	-1.445395	-0.533856	1.386668
1	-1.619773	-1.704410	-0.771114
1	-3.529660	0.180566	-0.022170
1	-1.714505	-0.151312	-1.622945
1	-1.553164	1.814438	1.477522
1	-1.681325	1.953291	-0.145471

Dimer

ΔE -4176.84077341 h.

30	-0.260723	-0.045546	1.580381
30	0.255523	-0.015297	-1.580276
9	-7.380210	-4.117715	0.973523
8	1.290158	-0.184556	0.231550
9	6.550513	-2.239187	-1.480668
9	7.302997	-4.244606	-1.087059
9	-6.592002	-2.136840	1.418250
8	-5.437611	-3.997229	1.943891
8	-1.292685	-0.142477	-0.228237
9	5.656512	-3.432032	0.092105
8	-6.383632	1.668845	-1.444149
8	5.359973	-4.064555	-2.047262
9	-5.714719	-3.307582	-0.180368
8	6.417680	1.514006	1.455634
8	0.284467	-1.834334	-2.334909
8	-0.321431	-1.873875	2.313155
9	8.158543	1.685145	2.745111
9	-7.020282	0.013176	-2.825854
7	-0.540537	1.867643	-2.322679
1	-1.030832	1.709496	-3.204181
9	-6.146941	1.807095	-3.674866
7	1.987030	0.629592	-2.730486
1	2.755425	0.767513	-2.072865
6	2.526398	0.216787	0.544698
7	0.583177	1.793642	2.371547
1	1.077729	1.597617	3.243012
7	-1.976680	0.613731	2.756481
1	-2.742642	0.791088	2.105737
9	-8.113475	1.895717	-2.739835
6	1.680861	1.914846	-3.403795
1	1.205816	1.658757	-4.360130
9	6.196270	1.608818	3.690173
6	2.369546	-0.460552	-3.673715
1	1.525850	-0.575452	-4.362191
1	3.252312	-0.179577	-4.260314
6	2.604464	-1.750529	-2.938591
6	-2.521047	0.287127	-0.537843
6	1.494665	-2.372911	-2.292121
6	-1.542060	-2.387074	2.249020
6	3.636414	-0.605040	0.270461
1	3.463017	-1.570264	-0.189563
6	-2.386481	-0.491331	3.670652
1	-1.548775	-0.640617	4.359767
1	-3.266174	-0.206760	4.260176
6	6.191943	-3.504924	-1.147212
9	7.035107	-0.180718	2.798173
6	0.320940	4.046152	-3.291975
1	-0.184356	3.817609	-4.241090
1	-0.381033	4.629778	-2.689394
6	0.651236	2.721304	-2.585446
1	1.096242	2.935616	-1.605330
6	1.728346	-3.582258	-1.596543
6	6.933283	1.158045	2.652285
6	-1.632621	1.869594	3.465712
1	-1.162928	1.571892	4.412630
6	3.004511	-4.132063	-1.508166
6	-2.643385	-1.758276	2.903679

6	1.553218	2.379733	1.403762
1	0.998217	2.518409	0.471143
1	1.898330	3.363487	1.735655
6	-3.646140	-0.520682	-0.285649
1	-3.491972	-1.497939	0.155551
6	-6.897597	1.346688	-2.651072
6	-1.505593	2.450030	-1.348025
1	-0.954652	2.559712	-0.409273
1	-1.831867	3.446269	-1.661321
6	5.106998	1.054945	1.183564
6	-3.990938	2.000169	-1.445115
1	-4.153129	2.975116	-1.893934
6	-5.082654	1.182066	-1.173910
6	-0.581892	2.671575	2.670329
1	-1.023080	2.934379	1.700138
6	2.941724	2.748606	-3.676651
1	3.433013	2.955315	-2.714954
1	3.644922	2.159732	-4.274876
6	4.927982	-0.187605	0.583849
1	5.783951	-0.814320	0.366674
6	-4.134672	-3.446144	2.050458
6	-2.868121	2.731325	3.767002
1	-3.353291	2.983860	2.813114
1	-3.588464	2.144741	4.346768
6	-3.926944	-2.292086	2.798800
1	-4.769658	-1.805298	3.279087
6	-6.255850	-3.400559	1.055192
6	-1.448380	4.817584	3.723480
1	-1.887919	5.161606	2.777281
1	-1.149810	5.714103	4.277185
6	-2.703354	1.565983	-1.123881
6	2.734400	1.480507	1.154782
6	4.067064	-3.487171	-2.134782
6	-2.496176	4.020700	4.510189
1	-3.393134	4.626029	4.679435
1	-2.093533	3.765098	5.499641
6	3.877911	-2.311511	-2.853755
1	4.727510	-1.829432	-3.326614
6	4.031024	1.886115	1.477098
1	4.212425	2.849069	1.944144
6	-4.928558	-0.074837	-0.597791
1	-5.796425	-0.690749	-0.397899
6	1.585420	4.874007	-3.564971
1	1.315311	5.797281	-4.088500
1	2.034149	5.172626	-2.607738
6	-0.210186	3.960628	3.421345
1	0.287351	3.684101	4.361676
1	0.509694	4.542510	2.838575
6	-3.081489	-4.095484	1.412724
1	-3.278654	-4.990700	0.831737
6	2.609333	4.072005	-4.377528
1	3.524258	4.655222	-4.527045
1	2.200061	3.861047	-5.374766
6	-1.795382	-3.572850	1.520956
1	-0.960322	-4.054587	1.021230
1	0.886514	-4.059950	-1.104315
1	3.187024	-5.045191	-0.950751

Dimer(DMSO)

ΔE -4730.07647315 h.

6	-2.272898	-2.649557	0.042614
6	-2.587530	-3.679676	0.951218
6	-3.806317	-4.350800	0.883347
6	-4.707234	-3.998086	-0.115949
6	-4.396731	-3.036306	-1.072081
6	-3.178508	-2.358961	-1.012883
6	-2.899831	-1.199483	-1.934238
7	-1.619548	-1.324415	-2.687814
1	-1.692931	-2.114472	-3.330267
6	-1.262488	-0.104907	-3.466891
6	-2.303840	0.291312	-4.524642
1	-3.271862	0.478325	-4.050461
6	-1.862700	1.535250	-5.309766
6	-0.495734	1.317135	-5.969636
1	-0.172823	2.221655	-6.496437
6	0.550795	0.920949	-4.920912
1	1.521470	0.727357	-5.390413
6	0.120049	-0.315390	-4.117374
7	1.114317	-0.682639	-3.082018
1	1.556480	0.163939	-2.725688
6	2.175523	-1.609505	-3.548605
6	3.158315	-1.898765	-2.446019
6	4.489958	-1.495320	-2.562483
6	5.390246	-1.772283	-1.538609
6	4.995475	-2.482727	-0.409828
6	3.673539	-2.899778	-0.294666
6	2.710653	-2.589466	-1.282187
8	1.441344	-2.942904	-1.116807
1	-4.754703	0.986439	3.488683
6	-4.943804	0.713354	2.447846
1	-6.013724	0.591832	2.261468
1	-4.512116	1.443594	1.763727
16	-4.101247	-0.850924	2.072050
6	-4.899919	-1.899382	3.321702
1	-4.809960	-1.433255	4.305149
1	-5.944443	-2.043400	3.038581
1	-4.380857	-2.857578	3.296062
8	-2.647147	-0.681157	2.600921
30	-1.134067	0.025448	1.170592
8	-2.593425	1.070265	0.232385
6	-2.315882	2.300379	-0.158049
6	-2.572140	2.718703	-1.487310

6	-2.258035	4.003271	-1.923410
6	-1.689466	4.901055	-1.025717
6	-1.460364	4.546671	0.300749
6	-1.778853	3.264911	0.748441
6	-1.600120	2.885723	2.195937
7	-0.575540	1.832397	2.353805
1	0.321376	2.189572	2.023688
6	-0.424918	1.288791	3.720995
1	-1.395216	0.843206	3.971743
6	-0.041986	2.313367	4.800337
1	-0.794287	3.106746	4.854186
6	0.099158	1.635620	6.173248
6	1.113373	0.483411	6.133554
6	0.759651	-0.528123	5.033205
6	0.629069	0.165447	3.672279
7	0.345812	-0.776971	2.562409
1	-0.141011	-1.595288	2.923987
6	1.563746	-1.232851	1.838808
6	2.251568	-0.093397	1.123599
6	3.538369	0.298581	1.501015
6	4.180667	1.332670	0.824624
6	3.548154	2.013189	-0.209801
6	2.252246	1.648842	-0.570175
6	1.587385	0.584277	0.068743
8	0.356040	0.228028	-0.320780
30	0.067959	-1.551586	-1.378880
8	-1.162300	-1.932231	0.205515
1	1.729893	2.181169	-1.359736
1	4.070841	2.816202	-0.718364
8	5.470142	1.799249	1.152738
6	6.368323	0.974930	1.722131
9	6.472190	-0.219585	1.105019
9	6.084454	0.713843	3.022805
9	7.560606	1.578681	1.679985
1	4.031358	-0.218138	2.315448
1	1.234660	-1.982581	1.115462
1	2.269965	-1.712290	2.529284
1	1.587074	0.645341	3.437600
1	1.520669	-1.314585	4.970037
1	-0.194359	-1.019166	5.272726
1	1.160299	-0.019294	7.105893
1	2.115443	0.888944	5.937558
1	0.391001	2.375142	6.927137
1	-0.880721	1.243320	6.479016
1	0.907884	2.790357	4.518553
1	-1.363627	3.777320	2.789531
1	-2.531929	2.463571	2.587261
1	-1.043787	5.282382	0.982616
8	-1.302720	6.189476	-1.475904
6	-2.238742	7.155287	-1.378369
9	-1.708238	8.293203	-1.841972
9	-3.349195	6.882932	-2.098784
9	-2.643429	7.365690	-0.106143
1	-2.448751	4.312356	-2.946097
1	-3.028443	2.009878	-2.169418
1	3.343562	-3.437272	0.588671
1	5.718010	-2.677644	0.375147
8	6.753305	-1.396294	-1.602857
6	7.065371	-0.148038	-1.995436
9	8.329548	0.098403	-1.629971
9	6.272214	0.802541	-1.462220
9	6.995457	0.005374	-3.343603
1	4.817815	-0.964188	-3.449389
1	1.666658	-2.533315	-3.847033
1	2.691656	-1.210210	-4.431377
1	0.038088	-1.173589	-4.798414
1	0.694066	1.755117	-4.219158
1	-0.576355	0.521752	-6.722970
1	-2.619124	1.787552	-6.060639
1	-1.800717	2.389415	-4.621512
1	-2.445719	-0.553605	-5.213638
1	-1.166372	0.701146	-2.729305
1	-3.741353	-1.075023	-2.623889
1	-2.813610	-0.293326	-1.323854
1	-5.129347	-2.794092	-1.836230
8	-5.976497	-4.625731	-0.177972
6	-6.896435	-4.149351	0.687218
9	-6.581796	-4.404911	1.980296
9	-7.061632	-2.810131	0.595310
9	-8.064207	-4.740378	0.420630
1	-4.070323	-5.116942	1.603733
1	-1.875220	-3.901311	1.739336

Dimer(DMSO)$_2$

ΔE -5283.30523054 h.

30	-0.332410	-1.084879	-0.881211
16	-0.804841	0.436996	-3.533719
6	0.083224	1.732153	-4.446575
6	3.183320	1.079592	-2.694748
6	4.503121	0.646677	-2.794983
6	5.441679	1.103572	-1.875636
6	5.090551	1.999967	-0.871623
6	3.773162	2.447528	-0.773132
6	2.778887	1.970003	-1.674867
8	1.509056	2.351785	-1.551456
1	-0.648488	2.328639	-4.997149
30	0.728160	1.764384	0.186126
16	-1.074964	5.327495	-1.065408
6	-1.700156	3.827780	-1.889715
1	-1.002438	2.999349	-1.753876
1	-2.660484	3.577787	-1.437312
1	-1.836618	4.057731	-2.949592

6	0.531415	5.398926	-1.921446
1	0.350067	5.622046	-2.976353
1	1.040242	4.436635	-1.800977
1	1.099866	6.211501	-1.464593
8	-0.777465	4.970847	0.401726
8	1.181972	-0.207894	0.421660
6	2.332153	-0.744148	0.826767
6	2.868670	-0.412687	2.089233
6	4.095055	-0.913519	2.517348
6	4.795769	-1.783516	1.690092
6	4.264054	-2.187876	0.468576
6	3.034827	-1.686464	0.030997
6	2.477540	-2.151798	-1.292624
7	1.092768	-2.687356	-1.179224
1	0.815812	-3.033419	-2.096949
6	0.889227	-3.755844	-0.174022
6	1.338978	-5.137973	-0.667902
6	1.109447	-6.220624	0.395390
6	-0.357764	-6.242712	0.844036
6	-0.804650	-4.862841	1.349150
1	-1.861016	-4.892288	1.635373
6	-0.584270	-3.772639	0.288883
7	-0.947011	-2.410248	0.741374
1	-0.373655	-2.164717	1.547782
6	-2.362042	-2.185080	1.101343
6	-3.374384	-2.391190	-0.011492
6	-4.688123	-2.645057	0.395121
6	-5.725885	-2.705581	-0.523942
6	-5.485919	-2.561337	-1.887563
6	-4.185755	-2.325332	-2.309091
6	-3.098635	-2.184954	-1.401487
8	-1.917037	-1.879890	-1.887162
1	-3.968857	-2.189865	-3.364773
1	-6.308858	-2.623220	-2.592165
8	-7.049848	-2.935953	-0.064035
6	-7.777169	-1.823230	0.167474
9	-7.920607	-1.051790	-0.933828
9	-8.997014	-2.201923	0.571317
9	-7.242478	-1.036751	1.126320
1	-4.918110	-2.766949	1.450321
1	-2.415747	-1.143202	1.435535
1	-2.656429	-2.802388	1.961155
1	-1.215944	-3.979706	-0.582175
1	-0.234215	-4.597531	2.251191
1	-0.509292	-6.993976	1.627068
1	-0.991180	-6.537812	-0.004035
1	1.407643	-7.199872	0.004739
1	1.752076	-6.016241	1.262908
1	2.396020	-5.095525	-0.953397
1	0.770914	-5.388355	-1.575681
1	1.498133	-3.481787	0.696333
1	2.413807	-1.312082	-1.987908
1	3.155992	-2.898403	-1.724741
1	4.805479	-2.875367	-0.167522
8	6.056177	-2.187029	2.178144
6	6.641575	-3.304938	1.714184
9	5.831854	-4.383922	1.763536
9	7.716854	-3.546012	2.472471
9	7.061677	-3.192946	0.430769
1	4.508858	-0.640434	3.482558
1	2.289823	0.239053	2.736214
7	-0.346242	2.565915	1.815917
1	-0.812005	3.387519	1.409338
6	0.579488	3.034756	2.873538
6	-0.093778	4.009714	3.855044
6	0.884642	4.502942	4.929334
6	2.115383	5.156721	4.288777
1	2.832147	5.466815	5.057200
6	2.790974	4.199574	3.297301
1	3.644385	4.690982	2.818933
6	1.809218	3.701053	2.224573
7	2.423977	2.770103	1.253747
1	2.943259	2.048719	1.753325
6	3.350089	3.419216	0.293162
1	2.794250	4.245704	-0.160799
1	4.226334	3.841151	0.800103
1	1.435812	4.550088	1.638189
1	3.186851	3.327575	3.838154
1	1.806496	6.067093	3.756954
1	0.379156	5.207190	5.599310
1	1.204077	3.652071	5.546928
1	-0.961029	3.533254	4.323362
1	-0.470982	4.863339	3.275243
1	0.917426	2.142725	3.420131
6	-1.341249	1.569443	2.282075
6	-2.509721	1.455810	1.338275
6	-3.811521	1.661712	1.801686
6	-4.898472	1.460749	0.959327
6	-4.717680	1.069486	-0.365645
6	-3.420233	0.903266	-0.843080
6	-2.295407	1.075569	-0.011131
8	-1.063900	0.853796	-0.479115
1	-3.248634	0.579645	-1.861318
1	-5.569306	0.865543	-1.002118
8	-6.170723	1.599409	1.558184
6	-7.135069	2.270419	0.903144
9	-6.715748	3.461341	0.426179
9	-7.640514	1.585675	-0.150303
9	-8.139595	2.484844	1.762077
1	-3.990517	1.956300	2.831485
1	-1.705814	1.817391	3.284781
1	-0.818337	0.607028	2.349749

1	5.846928	2.343643	-0.172149
8	6.790831	0.679162	-1.986123
6	7.104838	-0.455286	-1.325604
9	6.917196	-0.350717	0.007398
9	8.398462	-0.718313	-1.545733
9	6.382371	-1.518899	-1.744252
1	4.805140	-0.058626	-3.562405
1	2.424714	0.687618	-3.358669
1	0.586366	2.326893	-3.681310
1	0.808565	1.281852	-5.128021
6	-1.325512	-0.601015	-4.928643
1	-0.447319	-0.904232	-5.503506
1	-1.810602	-1.463285	-4.469537
1	-2.030271	-0.044000	-5.550929
8	0.306812	-0.393182	-2.836142

Dimer$(H_2O)_2$
ΔE -4253.29275683 h.

6	-2.277177	1.531544	-0.957294
6	-2.373573	2.272663	0.249823
6	-3.630414	2.600590	0.766565
6	-4.781535	2.165597	0.118203
6	-4.715651	1.480008	-1.089224
6	-3.467685	1.197317	-1.634983
6	-1.135289	2.613813	1.035251
7	-0.146087	3.362659	0.211447
6	0.909069	4.034979	1.008346
6	0.433624	5.351274	1.641957
6	1.551533	6.022616	2.451827
6	2.794231	6.254531	1.582459
6	3.271396	4.942631	0.943507
6	2.154544	4.268224	0.130977
7	2.571794	2.987881	-0.489006
6	3.438242	3.143920	-1.687178
6	3.843951	1.796996	-2.216687
6	5.165969	1.362884	-2.115923
6	5.523039	0.110589	-2.603491
6	4.593177	-0.708220	-3.233056
6	3.273715	-0.278486	-3.345038
6	2.856605	0.955253	-2.797216
8	6.858321	-0.345188	-2.491080
6	7.228527	-0.751347	-1.255710
9	6.379101	-1.656924	-0.731136
8	1.570044	1.320468	-2.833437
30	0.772336	1.897885	-1.066004
8	-1.102861	1.086220	-1.422821
30	-0.620991	-0.973794	-0.900680
8	0.218120	-0.947635	-2.956587
8	-6.066371	2.416661	0.652709
6	-6.321947	1.939885	1.888831
9	-5.763396	2.699883	2.864464
8	-2.152162	-1.849384	-1.866803
6	-3.405832	-1.981662	-1.491646
6	-4.361531	-2.369423	-2.470272
6	-5.718331	-2.455468	-2.193336
6	-6.150041	-2.192797	-0.896991
6	-5.248773	-1.872221	0.108667
6	-3.880987	-1.756956	-0.160582
8	-7.539292	-2.268927	-0.610345
6	-8.194287	-1.091183	-0.602684
9	-7.992208	-0.365087	-1.726528
6	-3.022316	-1.211764	0.964271
7	-1.594316	-1.613254	0.939140
6	-1.342799	-3.074675	1.028380
6	-1.792075	-3.691010	2.362689
6	-1.460748	-5.188060	2.440760
6	0.036035	-5.434263	2.213655
6	0.487187	-4.836706	0.874489
6	0.156524	-3.340222	0.778325
7	0.557607	-2.741749	-0.516165
6	2.010513	-2.469642	-0.685122
6	2.568356	-1.608038	0.420303
6	3.622565	-2.081153	1.205018
6	4.142967	-1.300117	2.233473
6	3.615834	-0.046738	2.518008
6	2.549568	0.424137	1.755148
6	2.011606	-0.327857	0.689276
8	5.137230	-1.812496	3.098244
6	6.385332	-1.960351	2.606100
9	6.863880	-0.831775	2.047997
8	0.983068	0.144723	-0.017278
9	8.441352	-1.307689	-1.348175
9	7.306138	0.273869	-0.377275
9	-7.645276	1.955227	2.075636
9	-5.870433	0.682866	2.078909
9	7.185955	-2.303964	3.622645
9	6.467039	-2.931832	1.669123
9	-9.504454	-1.343504	-0.495420
9	-7.837712	-0.299000	0.434285
1	-1.131617	-1.156441	1.725090
1	-1.911703	-3.529024	0.209066
1	-2.867538	-3.538261	2.496972
1	1.563451	-4.982079	0.731655
1	0.262549	-3.359328	-1.272045
1	-0.644609	4.065474	-0.334664
1	3.602862	6.693679	2.176391
1	4.139425	5.125158	0.302340
1	3.080437	2.429877	0.198083
1	2.534124	-0.911375	-3.821871
1	4.902589	-1.674768	-3.617146
1	5.917300	1.991616	-1.650077
1	2.843127	3.680004	-2.434045

1	4.324184	3.748211	-1.461921
1	1.857576	4.927386	-0.696064
1	3.595375	4.247316	1.730996
1	2.554457	6.976299	0.789896
1	1.190961	6.968974	2.868704
1	1.816358	5.380941	3.303111
1	-0.439852	5.165414	2.275237
1	0.107828	6.025155	0.836906
1	1.184293	3.334584	1.806947
1	-3.387654	0.622738	-2.549758
1	-5.630424	1.133020	-1.558237
1	-3.709593	3.149775	1.697875
1	-1.408864	3.185187	1.928741
1	-0.631810	1.696484	1.363676
1	2.090553	1.376590	1.995370
1	4.020325	0.534916	3.339623
1	4.038260	-3.065887	1.022021
1	2.106786	-1.954716	-1.643940
1	2.585412	-3.401801	-0.744790
1	0.717430	-2.805132	1.554462
1	-0.018829	-5.360006	0.050387
1	0.259270	-6.506494	2.239574
1	0.609375	-4.970832	3.028370
1	-1.774679	-5.588044	3.411179
1	-2.037106	-5.725704	1.675292
1	-1.286966	-3.159830	3.182428
1	-3.025367	-0.119576	0.916310
1	-3.486238	-1.479736	1.922127
1	-5.626440	-1.660767	1.103669
1	-6.440032	-2.711543	-2.962548
1	-3.992750	-2.553428	-3.475289
1	-0.650680	-0.880063	-3.379011
1	0.646038	-0.046319	-3.023156

Dimer($(H_2O)_2$)
ΔE -4329.74455275 h.

30	-0.622513	-0.971431	-0.970678
8	-2.187954	-1.690430	-1.974016
6	-3.435324	-1.848362	-1.585959
6	-4.410131	-2.143704	-2.577762
6	-5.762898	-2.242363	-2.285990
6	-6.171104	-2.087895	-0.964835
6	-5.250673	-1.861406	0.048893
6	-3.886459	-1.733576	-0.233199
6	-3.004025	-1.288836	0.916262
7	-1.585565	-1.715786	0.840502
1	-1.102515	-1.326118	1.649930
6	-1.365427	-3.184643	0.823105
1	-1.938966	-3.565694	-0.030066
6	-1.834034	-3.889524	2.105956
1	-2.907271	-3.727597	2.246224
6	-1.530955	-5.394368	2.073930
6	-0.038099	-5.652411	1.834900
6	0.431770	-4.965010	0.546250
1	1.505933	-5.119674	0.397465
6	0.129480	-3.459588	0.561763
7	0.550597	-2.772900	-0.681525
1	0.270171	-3.338220	-1.482616
6	2.007841	-2.499756	-0.805121
6	2.546081	-1.700788	0.355758
6	3.583723	-2.221611	1.132614
6	4.088981	-1.501221	2.211322
6	3.561610	-0.263060	2.555831
6	2.511984	0.254322	1.800351
6	1.992731	-0.433602	0.683765
8	0.984070	0.088367	-0.020133
30	0.820607	1.940340	-0.880075
7	-0.105377	3.307590	0.488307
1	-0.614766	4.035334	-0.013611
6	0.946036	3.946361	1.318199
6	0.458794	5.220059	2.025278
6	1.572363	5.854616	2.869942
6	2.809702	6.148460	2.011861
1	3.616329	6.559937	2.627835
6	3.297932	4.880944	1.296147
1	4.160688	5.110673	0.663323
6	2.184557	4.242099	0.450768
7	2.612646	3.002149	-0.242029
1	3.123654	2.409795	0.414274
6	3.483442	3.237305	-1.424350
6	3.917408	1.927701	-2.019981
6	5.244348	1.506806	-1.924970
6	5.624457	0.286879	-2.473180
6	4.715108	-0.509553	-3.158862
6	3.390967	-0.092267	-3.263607
6	2.953398	1.103512	-2.655364
8	1.655133	1.445188	-2.675347
1	2.667505	-0.707635	-3.786395
1	5.042710	-1.449400	-3.590601
8	6.963348	-0.155274	-2.364102
6	7.312219	-0.646343	-1.152522
9	8.541510	-1.162417	-1.253665
9	7.337177	0.309536	-0.196899
9	6.474258	-1.611059	-0.724373
1	5.980948	2.119059	-1.415819
1	2.884420	3.801870	-2.146438
1	4.356740	3.843627	-1.160398
1	1.877498	4.942815	-0.337300
1	3.633699	4.145052	2.040423
1	2.560382	6.912702	1.263418
1	1.203733	6.771942	3.340983
1	1.845706	5.167845	3.682472

1	-0.411690	4.990791	2.648262
1	0.125705	5.934949	1.259578
1	1.232436	3.205431	2.075334
6	-1.082243	2.504357	1.275090
6	-2.335347	2.226506	0.488981
6	-3.582058	2.513340	1.052827
6	-4.745733	2.140769	0.388047
6	-4.703551	1.563189	-0.875377
6	-3.465779	1.322476	-1.463159
6	-2.266674	1.594976	-0.777196
8	-1.096385	1.187883	-1.303867
1	-3.403842	0.828775	-2.425317
1	-5.627398	1.262134	-1.357681
8	-6.019973	2.352101	0.959944
6	-6.257882	1.788315	2.163364
9	-7.577544	1.794648	2.371452
9	-5.808270	0.519731	2.253955
9	-5.680381	2.474468	3.181302
1	-3.642647	2.982475	2.027979
1	-1.337694	3.012474	2.210765
1	-0.578932	1.564368	1.530659
1	2.053282	1.194881	2.083726
1	3.953162	0.270587	3.415343
8	5.069437	-2.065198	3.058857
6	6.327061	-2.170498	2.578781
9	7.111994	-2.585461	3.580452
9	6.429386	-3.068154	1.573091
9	6.807817	-1.000777	2.115176
1	3.998302	-3.197099	0.903316
1	2.129408	-1.938642	-1.734365
1	2.579393	-3.431001	-0.900114
1	0.694728	-2.995564	1.379407
1	-0.079604	-5.414981	-0.316912
1	0.163898	-6.727778	1.780852
1	0.539815	-5.263178	2.684451
1	-1.857562	-5.858876	3.010826
1	-2.113566	-5.862766	1.268715
1	-1.324086	-3.429454	2.964860
1	-2.985206	-0.196701	0.948131
1	-3.461104	-1.616276	1.858642
1	-5.609342	-1.732265	1.064726
8	-7.556144	-2.178133	-0.663237
6	-8.198665	-1.000871	-0.531280
9	-9.509824	-1.250434	-0.431249
9	-7.820604	-0.317888	0.573620
9	-8.003287	-0.169763	-1.581095
1	-6.499390	-2.425937	-3.061857
1	-4.059475	-2.243943	-3.600890
8	0.302769	-0.822771	-2.942044
1	-0.450339	-0.568837	-3.500174
1	0.833289	0.020250	-2.886371
8	-0.872230	1.609395	-3.993780
1	-1.079536	1.486416	-3.041006
1	0.092600	1.714899	-3.961201

Dimner$(H_2O)_3$

ΔE -4406.19927947 h.

30	0.546115	-0.948112	1.036435
8	2.225119	-1.688491	1.934432
6	3.463427	-1.842301	1.476727
6	4.488694	-2.150472	2.403616
6	5.817912	-2.274014	2.020329
6	6.141305	-2.131990	0.675852
6	5.159472	-1.880049	-0.273886
6	3.822569	-1.712794	0.105042
6	2.861988	-1.250298	-0.970542
7	1.462615	-1.706736	-0.807013
1	0.920662	-1.332584	-1.585814
6	1.276543	-3.178503	-0.762968
1	1.874919	-3.534556	0.083406
6	1.729265	-3.900260	-2.041781
1	2.794994	-3.718338	-2.212238
6	1.462081	-5.410624	-1.964468
6	-0.016917	-5.699130	-1.676768
6	-0.471106	-4.987580	-0.395173
1	-1.537416	-5.162205	-0.214458
6	-0.205098	-3.477347	-0.464965
7	-0.627469	-2.756174	0.759334
1	-0.372182	-3.311766	1.575377
6	-2.085350	-2.460806	0.851037
6	-2.602274	-1.713403	-0.353633
6	-3.624731	-2.267552	-1.127863
6	-4.105508	-1.595848	-2.248651
6	-3.572109	-0.372321	-2.634370
6	-2.537574	0.177982	-1.881446
6	-2.037428	-0.464209	-0.728955
8	-1.031948	0.075972	-0.038108
30	-0.877857	1.933639	0.781469
7	0.137183	3.275674	-0.532272
1	0.592636	4.020588	-0.004116
6	-0.863402	3.879312	-1.448191
6	-0.337452	5.127615	-2.173554
6	-1.399004	5.725538	-3.107450
6	-2.686274	6.048705	-2.338053
1	-3.454992	6.431509	-3.017735
6	-3.213463	4.808534	-1.602801
1	-4.113209	5.057847	-1.031680
6	-2.152120	4.208073	-0.667155
7	-2.626703	3.000112	0.051560
1	-3.125551	2.394495	-0.601505
6	-3.534098	3.287030	1.194755
6	-4.006863	2.003580	1.818862

6	-5.335959	1.596201	1.700645
6	-5.745822	0.399705	2.278942
6	-4.865194	-0.387414	3.011839
6	-3.538759	0.016216	3.139114
6	-3.072680	1.188902	2.509355
8	-1.775375	1.522827	2.559381
1	-2.832357	-0.590648	3.694104
1	-5.217152	-1.309769	3.461842
8	-7.088513	-0.026713	2.151074
6	-7.410991	-0.564396	0.952327
9	-8.652991	-1.052260	1.037939
9	-7.387752	0.348201	-0.044743
9	-6.580298	-1.563164	0.593349
1	-6.051134	2.199819	1.152044
1	-2.950969	3.866097	1.918413
1	-4.388178	3.896872	0.880200
1	-1.890438	4.941866	0.107049
1	-3.501723	4.041835	-2.336310
1	-2.484075	6.843530	-1.607468
1	-1.003049	6.625044	-3.590575
1	-1.622380	5.007239	-3.907865
1	0.568813	4.879666	-2.735087
1	-0.051859	5.872733	-1.417583
1	-1.102557	3.107236	-2.190859
6	1.186683	2.478894	-1.228378
6	2.376394	2.222184	-0.341404
6	3.661406	2.542082	-0.791097
6	4.768661	2.186689	-0.028042
6	4.626334	1.590797	1.219517
6	3.349077	1.313239	1.694112
6	2.211731	1.571874	0.905696
8	1.007012	1.146933	1.325742
1	3.207927	0.816846	2.647025
1	5.510842	1.312563	1.782056
8	6.086540	2.419712	-0.477083
6	6.416145	1.960563	-1.703390
9	7.747751	1.873037	-1.773807
9	5.883091	0.754935	-1.979596
9	6.009859	2.798354	-2.691353
1	3.797128	3.023309	-1.753054
1	1.511063	2.981369	-2.145290
1	0.715481	1.530973	-1.515194
1	-2.072919	1.106509	-2.194795
1	-3.946027	0.123000	-3.524189
8	-5.059938	-2.200811	-3.098024
6	-6.330047	-2.296509	-2.650999
9	-7.081162	-2.763887	-3.655709
9	-6.455088	-3.149067	-1.609228
9	-6.834661	-1.111776	-2.255809
1	-4.044022	-3.232661	-0.865367
1	-2.209780	-1.855449	1.750987
1	-2.665663	-3.382397	0.980686
1	-0.792788	-3.057242	-1.290025
1	0.072878	-5.400602	0.466562
1	-0.189043	-6.777379	-1.588102
1	-0.627437	-5.348480	-2.520237
1	1.773724	-5.891480	-2.898196
1	2.078076	-5.844371	-1.164652
1	1.188004	-3.471802	-2.897827
1	2.826446	-0.157689	-0.965367
1	3.260805	-1.544305	-1.949633
1	5.442286	-1.771747	-1.315086
8	7.500256	-2.297712	0.311418
6	8.126782	-1.242209	-0.247405
9	9.447254	-1.454043	-0.172403
9	7.814508	-1.086788	-1.555348
9	7.845904	-0.073059	0.365171
1	6.599688	-2.476820	2.745160
1	4.212733	-2.244520	3.449358
8	-0.409903	-0.742101	2.967479
1	0.334355	-0.619087	3.607891
1	-0.882492	0.129704	2.908765
8	0.470287	2.659052	3.642952
1	0.843950	2.046572	2.981898
1	-0.469522	2.410958	3.596716
8	1.919423	-0.682459	4.311812
1	2.143272	-1.118178	3.435743
1	1.957736	-1.394319	4.964263

Dimer(analyte)

ΔE -4618.35396652 h.

30	0.135575	-1.177178	-0.421446
30	0.416045	1.763370	0.993827
9	7.615419	-3.130841	3.092706
8	-0.740561	0.810315	-0.403039
9	-6.133920	2.118768	1.903917
9	-7.465389	0.660790	2.825602
9	6.620090	-2.865524	1.173284
8	5.498845	-3.617515	2.976882
8	1.705774	0.250432	0.414031
9	-5.831211	0.003353	1.540934
8	6.723540	1.079676	-1.797264
8	-5.439684	0.813742	3.602574
9	6.208840	-1.489843	2.795874
8	-5.703577	1.260307	-2.826160
8	0.043811	1.122215	2.821386
8	0.360611	-2.345764	1.323950
9	-7.664520	0.502610	-3.378445
9	7.904504	1.428986	0.084209
7	1.507924	3.194558	-0.159141
1	2.317439	3.546625	0.352713
9	7.125924	3.140731	-0.995372

7	-0.926530	3.505808	1.292860
1	-1.739876	3.371234	0.692547
6	-1.935829	0.962758	-0.969603
7	-0.237208	-1.011645	-2.676158
1	-0.872877	-1.779968	-2.894881
7	1.813919	-2.369836	-1.264099
1	2.630811	-1.788321	-1.069479
9	8.718576	1.938532	-1.871390
6	-0.192732	4.701430	0.824320
1	0.534309	4.952767	1.608751
9	-6.029547	-0.929451	-3.217330
6	-1.391133	3.544945	2.708271
1	-0.497065	3.687045	3.323630
1	-2.069375	4.387412	2.887043
6	-2.060771	2.238050	3.048738
6	2.914909	0.495980	-0.079625
6	-1.261892	1.056272	3.038524
6	1.579969	-2.668500	1.732657
6	-3.073419	1.353777	-0.235476
1	-2.970156	1.538235	0.825271
6	2.008049	-3.656740	-0.534315
1	1.050055	-4.182774	-0.536117
1	2.740333	-4.290596	-1.046352
6	-6.193187	0.891854	2.487176
9	-6.877497	-0.050654	-1.423160
6	1.353907	5.559834	-0.999220
1	2.119417	5.850597	-0.265532
1	1.881857	5.291212	-1.919544
6	0.601471	4.336807	-0.450407
1	-0.114424	3.976730	-1.201643
6	-1.908256	-0.189157	3.226436
6	-6.546608	0.214201	-2.707719
6	1.710594	-2.528642	-2.731530
1	1.040496	-3.380611	-2.913200
6	-3.288321	-0.268471	3.392712
6	2.461237	-3.377151	0.871380
6	-0.874178	0.251062	-3.138413
1	-0.115669	1.032918	-3.035327
1	-1.138674	0.191811	-4.199215
6	4.017857	-0.300419	0.303473
1	3.857090	-1.068073	1.048086
6	7.594028	1.883043	-1.149566
6	2.001115	2.469464	-1.368397
1	1.148695	1.894570	-1.739564
1	2.313498	3.171175	-2.148281
6	-4.447978	1.126902	-2.185391
6	4.412005	1.746590	-1.547501
1	4.595525	2.547634	-2.256999
6	5.460262	0.908269	-1.180707
6	1.061870	-1.274680	-3.346080
1	1.704716	-0.415851	-3.104612
6	-1.112949	5.907985	0.574833
1	-1.884684	5.607318	-0.148439
1	-1.631773	6.171047	1.502162
6	-4.326064	1.450308	-0.840982
1	-5.196669	1.745664	-0.270512
6	4.178709	-3.313761	2.556571
6	3.076484	-2.806373	-3.384900
1	3.746895	-1.969010	-3.142029
1	3.521868	-3.705337	-2.947815
6	3.751564	-3.698753	1.289865
1	4.439240	-4.210492	0.624541
6	6.458455	-2.787672	2.519479
6	2.321414	-1.704638	-5.520423
1	2.982808	-0.840735	-5.367834
1	2.200704	-1.822676	-6.602730
6	3.138989	1.552162	-1.008516
6	-2.090802	0.635575	-2.342476
6	-4.037582	0.905016	3.408911
6	2.967834	-2.951146	-4.907197
1	3.960276	-3.123796	-5.337496
1	2.359875	-3.834448	-5.145872
6	-3.439917	2.152054	3.248064
1	-4.057893	3.044298	3.236757
6	-3.350060	0.715063	-2.936929
1	-3.485581	0.465383	-3.984856
6	5.282166	-0.107786	-0.247959
1	6.117213	-0.732381	0.046955
6	0.414660	6.746799	-1.251021
1	0.990099	7.602115	-1.621151
1	-0.302773	6.481597	-2.039521
6	0.959008	-1.415036	-4.875814
1	0.259838	-2.233018	-5.102209
1	0.535720	-0.504637	-5.309115
6	3.338115	-2.627218	3.428296
1	3.707542	-2.330762	4.404680
6	-0.346468	7.118760	0.027099
1	-1.041405	7.943751	-0.163409
1	0.365580	7.472148	0.785291
6	2.043041	-2.317466	3.019931
1	1.374815	-1.763617	3.671535
1	-1.298690	-1.086956	3.185390
1	-3.790699	-1.226546	3.484245
7	-1.949940	-1.784531	0.068484
1	-1.810873	-1.982851	1.058956
1	-2.541319	-0.956603	0.045962
6	-2.704092	-2.911025	-0.537883
1	-2.923907	-2.619038	-1.571590
6	-1.778817	-4.138600	-0.601964
1	-2.358445	-5.010004	-0.922690
1	-1.021320	-3.946500	-1.380229
8	-1.165110	-4.460931	0.632520

1	-0.574779	-3.707710	0.895352
6	-4.022229	-3.112295	0.191457
6	-5.201946	-2.610007	-0.370144
6	-4.073333	-3.698444	1.466878
6	-6.412962	-2.688970	0.320632
1	-5.171786	-2.140744	-1.348122
6	-5.284398	-3.780312	2.156498
1	-3.161408	-4.091247	1.904025
6	-6.457414	-3.273408	1.587106
1	-7.310089	-2.272492	-0.126331
1	-5.312489	-4.238589	3.141338
1	-7.396112	-3.329247	2.130890

Dimer(analyte)$_2$
ΔE -5059.87048876 h.

30	-0.095018	-1.574760	0.598274
30	-0.179351	1.689290	0.158180
9	8.312971	-3.689436	-0.841623
8	-1.124462	-0.131370	-0.567654
9	-7.007747	-0.482696	0.310798
9	-6.783929	0.935841	-1.318133
9	6.669868	-2.434013	-1.522314
8	6.294086	-4.274913	-0.283564
8	1.198576	0.097182	0.602039
9	-8.661436	0.832370	-0.220541
8	6.595861	0.371352	-0.624964
8	-6.944974	1.715234	0.783378
9	7.242694	-2.421145	0.570626
8	-5.826008	-0.832246	-3.427881
8	-1.494249	1.801092	1.781312
8	1.240797	-2.862635	1.498884
9	-6.059533	-3.065753	-3.349053
9	6.663675	-0.014720	-2.842003
7	1.142380	2.258076	-1.506429
1	1.849463	2.886013	-1.125062
9	8.424319	0.650076	-1.748004
7	-1.539754	2.972775	-1.007559
1	-2.088624	2.348937	-1.600081
6	-2.240921	-0.372641	-1.240331
7	-1.859848	-2.816618	0.578234
1	-1.780418	-3.276382	1.489509
7	0.338798	-2.796123	-1.172088
1	-0.137573	-2.355466	-1.958655
9	6.782463	2.031230	-2.129618
6	-0.713594	3.847340	-1.869864
1	-0.214363	4.563309	-1.202441
9	-7.331166	-1.839329	-2.089274
6	-2.485845	3.673980	-0.106196
1	-1.877398	4.226301	0.619807
1	-3.098707	4.400045	-0.652846
6	-3.376184	2.692467	0.609565
6	2.484783	0.155286	0.268781
6	-2.798418	1.828932	1.586461
6	2.405155	-3.261445	1.020122
6	-2.440173	0.187561	-2.522974
1	-1.626405	0.750617	-2.966282
6	1.782532	-2.815560	-1.478099
1	1.990238	-3.404697	-2.382093
1	2.043304	-1.779770	-1.719762
6	-7.330578	0.765459	-0.095487
9	-7.586843	-1.792334	-4.246564
6	1.279028	3.846242	-3.446179
1	1.825559	4.557799	-2.813903
1	2.028592	3.210330	-3.929271
6	0.379715	2.988918	-2.541643
1	-0.120419	2.230933	-3.157834
6	-3.674714	1.030336	2.360865
6	-6.671847	-1.865024	-3.272959
6	-0.312328	-4.095839	-0.888178
1	0.200704	-4.506478	-0.011921
6	-5.038989	0.980856	2.092048
6	2.711482	-3.289220	-0.372184
6	-3.070522	-1.953485	0.577499
1	-3.973996	-2.532792	0.808353
1	-2.928498	-1.228049	1.381816
6	3.487775	-0.210005	1.190669
1	3.180233	-0.581447	2.161773
6	7.093252	0.745913	-1.813221
6	1.829762	1.034884	-1.997802
1	1.055164	0.266402	-2.094489
1	2.279336	1.200454	-2.983878
6	-4.638063	-0.761622	-2.669571
6	4.242512	0.687789	-1.344136
1	4.525179	1.052076	-2.323762
6	5.203942	0.314070	-0.408819
6	-1.785264	-3.823378	-0.504595
1	-2.265765	-3.374719	-1.383051
6	-1.520037	4.616786	-2.929480
1	-2.066573	3.888634	-3.546196
1	-2.270258	5.248693	-2.444573
6	-3.627002	0.009802	-3.228761
1	-3.772196	0.457505	-4.206578
6	4.983484	-3.954867	0.156516
6	-0.238767	-5.106615	-2.042653
1	-0.689967	-4.654846	-2.938067
1	0.807690	-5.320150	-2.284065
6	4.005305	-3.637681	-0.774717
1	4.268193	-3.631451	-1.828648
6	7.103862	-3.219377	-0.509998
6	-2.434357	-6.140517	-1.308450
1	-2.972903	-5.743037	-2.179905
1	-2.935372	-7.072938	-1.025390

6	2.886124	0.603668	-1.014166
6	-3.263426	-1.221971	-0.729030
6	-5.555047	1.760866	1.062175
6	-0.973508	-6.410102	-1.694505
1	-0.921634	-7.105454	-2.539684
1	-0.461014	-6.896680	-0.853008
6	-4.742843	2.628392	0.337859
1	-5.185170	3.255342	-0.430923
6	-4.454622	-1.390730	-1.440062
1	-5.237340	-2.005406	-1.014355
6	4.835351	-0.139850	0.855432
1	5.606776	-0.450560	1.550885
6	0.465825	4.613258	-4.496559
1	1.132925	5.236279	-5.102419
1	-0.011857	3.899657	-5.181980
6	-2.519195	-5.126262	-0.159511
1	-2.065816	-5.554694	0.745785
1	-3.564206	-4.900744	0.081837
6	4.697053	-3.993382	1.517739
1	5.473492	-4.258988	2.227809
6	-0.612341	5.472469	-3.824481
1	-1.215598	5.993300	-4.576077
1	-0.129408	6.246981	-3.212765
6	3.412576	-3.669670	1.931475
1	3.156717	-3.666642	2.987096
1	-3.258443	0.444577	3.172549
1	-5.701405	0.339457	2.663901
7	-0.492865	-0.752797	2.599720
1	0.491001	-0.591602	2.808081
1	-0.893240	0.173430	2.381510
6	-1.173329	-1.322051	3.771622
1	-2.186677	-1.599446	3.456483
6	-0.486244	-2.628918	4.215508
1	0.551477	-2.397199	4.505626
1	-0.999355	-3.000388	5.109763
8	-0.527264	-3.641083	3.227495
1	0.224626	-3.457405	2.600636
6	-1.291995	-0.343262	4.937514
6	-0.429082	0.751183	5.083776
6	-2.295092	-0.534266	5.899706
6	-0.566714	1.637039	6.154957
1	0.350956	0.938522	4.354148
6	-2.432318	0.343034	6.976615
1	-2.981082	-1.371971	5.795253
6	-1.568289	1.434883	7.106787
1	0.105839	2.486947	6.225151
1	-3.219500	0.180774	7.707551
1	-1.681485	2.124602	7.938250
7	1.086290	2.687522	1.717544
1	0.484932	2.467118	2.511344
1	1.909854	2.097105	1.820062

6	1.453521	4.110266	1.834677
1	0.523714	4.679076	1.711444
6	2.008140	4.412739	3.243592
1	2.962536	3.890886	3.374802
1	2.193631	5.490680	3.346910
8	1.143689	3.920853	4.265230
1	0.333992	4.450287	4.260241
6	2.424443	4.534988	0.751437
6	2.206601	5.722713	0.040094
6	3.556778	3.762939	0.442924
6	3.093655	6.131466	-0.958572
1	1.331400	6.326595	0.265090
6	4.436371	4.160885	-0.567122
1	3.749919	2.829295	0.963672
6	4.208085	5.347425	-1.268445
1	2.904694	7.051611	-1.503381
1	5.287268	3.534463	-0.813762
1	4.889211	5.654677	-2.056228

Monomer

ΔE -2088.39179254 h.

30	-0.018504	-1.784269	-0.084043
8	-1.800257	-2.486648	0.049957
6	-2.815418	-1.630588	0.142254
6	-3.848504	-1.878235	1.075036
6	-4.935559	-1.019889	1.205194
6	-5.000176	0.112880	0.399430
6	-4.008684	0.390607	-0.533728
6	-2.919024	-0.471141	-0.682363
6	-1.874642	-0.186237	-1.733317
1	-2.167944	0.688233	-2.324698
1	-1.788731	-1.037453	-2.417241
7	-0.510485	-0.001853	-1.151345
1	0.147230	0.119498	-1.921654
6	-0.365457	1.146335	-0.217032
6	-0.258978	2.494914	-0.943173
1	-1.156113	2.658411	-1.549347
6	-0.057552	3.654984	0.041737
6	1.170559	3.413740	0.929262
6	1.056077	2.074562	1.671402
1	1.949252	1.897903	2.279410
6	0.854947	0.907129	0.695386
7	0.703954	-0.407326	1.374333
1	0.025077	-0.312116	2.129884
6	1.958336	-0.985159	1.945512
6	3.025381	-1.192208	0.899172
6	4.255601	-0.542684	1.027410
6	5.260711	-0.751698	0.091288
6	5.071903	-1.605272	-0.991361
6	3.847377	-2.249200	-1.135243
6	2.793488	-2.055258	-0.212765

8	1.641637	-2.693695	-0.400440
1	3.670681	-2.917074	-1.972731
1	5.873351	-1.751703	-1.707800
8	6.514426	-0.117567	0.268368
6	6.635258	1.109768	-0.281152
9	5.751081	1.997708	0.225158
9	6.454855	1.101653	-1.619544
9	7.869946	1.555785	-0.025910
1	4.439033	0.128376	1.860755
1	2.346233	-0.355869	2.754016
1	1.665984	-1.945983	2.382977
1	1.740395	0.818007	0.054408
1	0.199837	2.108059	2.360030
1	1.290372	4.229117	1.650571
1	2.075407	3.405223	0.306307
1	0.044409	4.595788	-0.509685
1	-0.950460	3.752426	0.673874
1	0.593607	2.451960	-1.636101
1	-1.262756	1.143648	0.413761
1	-4.093310	1.281184	-1.148830
8	-6.064719	1.030670	0.571547
6	-7.155786	0.822814	-0.195990
9	-6.884574	0.892339	-1.517535
9	-8.052797	1.770275	0.098565
9	-7.724571	-0.382504	0.022236
1	-5.723656	-1.213655	1.925175
1	-3.769395	-2.765341	1.695892

Monomer(DMSO)
ΔE -2641.62737118 h.

6	-4.012223	0.046924	0.846532
6	-4.122086	1.226625	1.573201
6	-3.065843	1.695329	2.348933
6	-1.881747	0.966547	2.386302
6	-1.719449	-0.235929	1.652942
6	-2.831589	-0.697297	0.882836
6	-2.724897	-1.979689	0.097882
7	-1.645475	-1.919888	-0.928051
1	-1.612527	-2.820056	-1.405434
6	-1.761049	-0.834572	-1.923094
6	-2.841001	-1.092585	-2.983716
1	-3.811909	-1.221398	-2.493705
6	-2.905585	0.045413	-4.011143
6	-1.535770	0.266548	-4.665800
6	-0.455544	0.533798	-3.607690
6	-0.380214	-0.595837	-2.567483
7	0.613281	-0.341464	-1.495482
1	0.478220	0.605680	-1.140658
6	2.033162	-0.484452	-1.912993
6	2.963113	-0.081673	-0.799765
6	3.820971	1.009132	-0.945920
6	4.696073	1.349112	0.080120
6	4.735368	0.622493	1.266537
6	3.877368	-0.461874	1.424539
6	2.967511	-0.839469	0.408609
8	2.170935	-1.882774	0.577509
30	0.231915	-1.773159	0.138322
16	0.793425	-4.957372	0.983859
6	1.345993	-4.199450	2.540487
1	2.026197	-4.893723	3.039428
1	1.833511	-3.252522	2.294444
1	0.455754	-4.042672	3.151788
6	2.391751	-4.978000	0.118139
1	2.208845	-5.378871	-0.880183
1	2.755295	-3.948485	0.075585
1	3.073588	-5.633568	0.665391
8	-0.069243	-3.880248	0.261479
8	-0.573997	-0.890227	1.710540
1	3.887733	-1.044136	2.341002
1	5.428528	0.911332	2.049864
8	5.603015	2.422226	-0.108829
6	5.157479	3.642787	0.254158
9	4.830787	3.712096	1.563013
9	6.135042	4.525667	0.018471
9	4.064098	4.028171	-0.440525
1	3.820150	1.594492	-1.860490
1	2.247643	0.101636	-2.814081
1	2.175935	-1.543356	-2.158530
1	-0.069246	-1.527394	-3.060676
1	0.519344	0.668108	-4.086955
1	-0.684964	1.471381	-3.081102
1	-1.576775	1.102389	-5.372707
1	-1.261913	-0.625469	-5.245691
1	-3.663658	-0.177640	-4.769829
1	-3.222942	0.968739	-3.507204
1	-2.612143	-2.038617	-3.495028
1	-2.023033	0.071594	-1.362973
1	-2.450345	-2.812372	0.753623
1	-3.692477	-2.217272	-0.360564
1	-1.041285	1.312662	2.980678
1	-3.176452	2.620260	2.905685
8	-5.345937	1.943065	1.552811
6	-5.476901	2.851187	0.564075
9	-6.676129	3.431168	0.691893
9	-5.404696	2.298717	-0.667936
9	-4.532870	3.816422	0.611860
1	-4.855149	-0.288138	0.249604

Monomer$(DMSO)_2$
ΔE -3194.86165439 h.

6	3.544563	2.236650	-0.504577
6	4.901653	2.067261	-0.760978

6	5.484261	0.829667	-0.508754
6	4.736298	-0.224691	0.004923
6	3.376707	-0.065272	0.277003
6	2.736101	1.185823	0.005933
8	1.453740	1.396499	0.209208
30	0.014092	0.018323	-0.042121
16	-0.533704	0.669960	3.345806
6	-2.345015	0.619053	3.531230
1	-2.645454	1.384131	4.251291
1	-2.814327	0.791188	2.560432
1	-2.598425	-0.371540	3.912692
6	-0.397862	2.315377	2.584693
1	0.653625	2.459100	2.336200
1	-0.980334	2.317604	1.660283
1	-0.745022	3.059847	3.305193
8	-0.194208	-0.361577	2.245404
16	0.534211	0.591708	-3.447652
6	0.314939	2.252141	-2.740504
1	0.897170	2.315035	-1.818124
1	-0.742446	2.349970	-2.494698
1	0.623236	2.988836	-3.486310
6	2.346166	0.625854	-3.630328
1	2.649861	-0.361397	-3.982645
1	2.803903	0.849221	-2.664436
1	2.609456	1.383835	-4.372039
8	0.244649	-0.419691	-2.314834
7	-1.358963	-1.671074	-0.025298
1	-1.683036	-1.727836	0.939493
6	-2.500760	-1.364476	-0.915618
1	-2.062756	-1.070553	-1.875205
1	-3.130934	-2.246659	-1.085408
6	-3.341937	-0.246105	-0.351596
6	-4.691884	-0.464698	-0.072651
6	-5.491504	0.566627	0.409056
6	-4.971443	1.839057	0.621753
6	-3.624584	2.067954	0.357965
6	-2.764875	1.043234	-0.120799
8	-1.494715	1.310924	-0.332608
1	-3.192678	3.050430	0.523724
1	-5.615366	2.629302	0.993989
8	-6.845496	0.299992	0.738698
6	-7.740585	0.474700	-0.254383
9	-7.507748	-0.327642	-1.316863
9	-7.762689	1.742060	-0.722683
9	-8.955187	0.186114	0.228575
1	-5.134074	-1.443231	-0.235666
6	-0.597450	-2.891784	-0.357284
1	-0.409537	-2.851687	-1.437997
6	0.771512	-2.847281	0.361185
7	1.470297	-1.599355	-0.006185
1	1.799516	-1.668803	-0.968403
6	2.592343	-1.206764	0.875570
1	2.136953	-0.905112	1.824551
1	3.266329	-2.049752	1.074012
1	0.581351	-2.786743	1.440519
6	1.590942	-4.110790	0.048031
1	1.829345	-4.109288	-1.025575
1	2.544988	-4.078149	0.584335
6	0.827061	-5.394825	0.398379
1	1.431406	-6.271825	0.140951
1	0.660146	-5.432551	1.483748
6	-0.524875	-5.438562	-0.324595
1	-0.355442	-5.497173	-1.408641
1	-1.084487	-6.337618	-0.043205
6	-1.352438	-4.185689	-0.008607
1	-1.590888	-4.166614	1.064822
1	-2.306747	-4.216026	-0.544546
1	5.226368	-1.174455	0.198376
8	6.850395	0.620721	-0.829810
6	7.733884	0.869829	0.157821
9	7.691286	2.150037	0.588086
9	7.539912	0.088763	1.243724
9	8.962285	0.628450	-0.316042
1	5.505854	2.876755	-1.157651
1	3.064729	3.190824	-0.701045

Monomer(H_2O)
ΔE -2164.83988517 h.

6	-4.007339	0.569857	-0.373556
6	-4.916605	0.070520	0.550842
6	-4.766967	-1.200505	1.096978
6	-3.677339	-1.974867	0.711750
6	-2.729839	-1.503120	-0.222458
6	-2.915872	-0.203540	-0.778705
6	-1.968351	0.333831	-1.824872
1	-1.912781	-0.356185	-2.673046
7	-0.560707	0.468524	-1.326000
1	0.023430	0.755900	-2.111394
6	-0.375269	1.446233	-0.212663
6	-0.222759	2.886195	-0.718052
6	-0.002691	3.867882	0.441744
6	1.207806	3.453582	1.289038
1	1.339233	4.139869	2.132292
6	1.051818	2.017020	1.808537
1	1.936202	1.722337	2.382502
6	0.827714	1.024363	0.659721
7	0.603568	-0.372469	1.111606
1	-0.159061	-0.382928	1.789459
6	1.769587	-1.082302	1.715736
6	2.921247	-1.218522	0.750017
6	4.152811	-0.628234	1.040856

6	5.223928	-0.780080	0.167972
6	5.101773	-1.515538	-1.006143
6	3.875501	-2.101525	-1.309555
6	2.763083	-1.960844	-0.455026
8	1.596764	-2.532815	-0.785912
30	0.031054	-1.414938	-0.647931
8	-1.700877	-2.282927	-0.564145
8	-0.082060	-4.005960	1.066302
1	0.657510	-3.759127	0.483197
1	-0.846165	-3.601871	0.614424
1	3.749387	-2.676885	-2.221374
1	5.954741	-1.617504	-1.668598
8	6.476092	-0.212950	0.503766
6	6.663682	1.069309	0.122515
9	5.772219	1.915850	0.683824
9	7.890325	1.437325	0.506276
9	6.568136	1.233656	-1.214097
1	4.285914	-0.049862	1.949590
1	1.387394	-2.071536	1.986959
1	2.103075	-0.581597	2.630826
1	1.720562	1.000491	0.021890
1	0.192852	1.963374	2.492166
1	2.119636	3.521024	0.680208
1	0.131690	4.880976	0.048249
1	-0.900690	3.888968	1.073859
1	-1.108057	3.167309	-1.298211
1	0.637548	2.928817	-1.400912
1	-1.275986	1.374237	0.408708
1	-2.332733	1.296649	-2.198384
1	-3.531919	-2.967444	1.126698
1	-5.491864	-1.566303	1.816285
8	-5.982204	0.893207	0.986366
6	-7.122445	0.816677	0.266092
9	-6.949291	1.182041	-1.022712
9	-8.015045	1.643437	0.820702
9	-7.646385	-0.427574	0.251920
1	-4.157720	1.564471	-0.781482

Monomer$(H_2O)_2$
ΔE -2241.29098630 h.

6	-4.031144	2.288609	-0.281392
6	-2.868492	1.907684	0.427886
6	-2.946136	0.764000	1.275861
6	-4.133663	0.036203	1.358091
6	-5.248860	0.433875	0.629659
6	-5.212830	1.558428	-0.188851
8	-1.751000	2.615395	0.302129
30	-0.060191	1.668897	-0.062046
8	1.914547	4.397488	-0.933424
6	-1.733677	0.335145	2.059992
7	-0.605727	-0.046783	1.165697
6	-0.875306	-1.143439	0.205861
6	0.313911	-1.233564	-0.772341
6	0.090739	-2.333229	-1.818832
6	-0.189498	-3.690201	-1.156888
6	-1.377435	-3.596471	-0.189341
6	-1.148779	-2.502716	0.864081
7	0.562564	0.100120	-1.377333
6	1.980860	0.379500	-1.746531
6	2.902122	0.341498	-0.550645
6	2.730089	1.258584	0.524040
6	3.626770	1.197858	1.611303
6	4.662006	0.268422	1.648818
6	4.802315	-0.623268	0.590284
6	3.937447	-0.595651	-0.497309
8	1.758944	2.178445	0.526310
8	5.808423	-1.616601	0.648032
6	6.992830	-1.294112	0.084238
9	6.886153	-1.031060	-1.236320
8	-6.453315	-0.302274	0.750638
6	-6.580746	-1.356048	-0.083511
9	-7.761290	-1.935173	0.161081
8	-0.137364	2.989783	-1.897737
9	7.561836	-0.210066	0.653366
9	7.818738	-2.334114	0.239798
9	-6.544952	-0.997713	-1.385099
9	-5.611189	-2.282307	0.091045
1	-0.006052	0.201215	-2.217456
1	0.193158	-0.302180	1.746525
1	3.488867	1.904035	2.424139
1	-1.994879	-0.481191	2.743065
1	-1.361454	1.170015	2.663293
1	-1.761840	-0.838170	-0.364310
1	2.331836	-0.326370	-2.508239
1	1.977566	1.379477	-2.191352
1	1.205397	-1.478831	-0.182660
1	5.350981	0.224173	2.485495
1	-0.289290	-2.767656	1.496203
1	-2.019566	-2.426936	1.523102
1	-4.197382	-0.845979	1.987486
1	0.703442	-4.014071	-0.605083
1	-0.378441	-4.447259	-1.925615
1	-1.546549	-4.559392	0.304622
1	-2.291771	-3.365289	-0.753128
1	4.076587	-1.308102	-1.304362
1	-0.764739	-2.050029	-2.448505
1	0.965430	-2.396582	-2.475428
1	-6.097798	1.845631	-0.747155
1	-3.974513	3.167168	-0.917181
1	-0.967747	3.383837	-1.582426
1	0.572937	3.650369	-1.680859
1	2.010043	3.618052	-0.325774

1	1.598830	5.113094	-0.365302

Monomer($(H_2O)_3$)
ΔE -2317.74452538 h.

6	3.981769	2.085818	-0.406058
6	2.749382	1.663143	-0.947445
6	2.673777	0.377500	-1.546745
6	3.792708	-0.453666	-1.551230
6	4.981442	-0.020522	-0.975208
6	5.093379	1.245034	-0.409545
8	1.667505	2.450188	-0.892301
30	0.073551	1.697631	0.056934
8	-2.182242	4.006848	1.372687
6	1.348554	-0.100653	-2.076257
7	0.369435	-0.245091	-0.966108
6	0.758855	-1.168193	0.125415
6	-0.323492	-1.111038	1.219845
6	0.084854	-1.955222	2.433711
6	0.380959	-3.407411	2.029419
6	1.427629	-3.473988	0.907504
6	1.007792	-2.621601	-0.300281
7	-0.622629	0.299834	1.573158
6	-2.069301	0.577308	1.814744
6	-2.890361	0.393899	0.559778
6	-2.664597	1.230667	-0.569367
6	-3.430609	1.015160	-1.733281
6	-4.400648	0.017594	-1.788527
6	-4.605009	-0.783394	-0.670005
6	-3.862126	-0.607423	0.491963
8	-1.755097	2.212933	-0.542583
8	-5.543826	-1.839852	-0.735256
6	-6.798580	-1.543004	-0.332104
9	-6.850890	-1.150694	0.959223
8	6.100079	-0.888398	-0.971287
6	6.145927	-1.765962	0.055476
9	7.243896	-2.514106	-0.090615
8	0.303655	3.069342	1.713188
9	-7.359824	-0.556236	-1.062911
9	-7.544893	-2.644112	-0.467322
9	6.202232	-1.156004	1.258176
9	5.073459	-2.591188	0.088922
1	-0.105542	0.559448	2.411697
1	-0.526559	-0.539868	-1.355383
1	-3.247367	1.655605	-2.590354
1	1.472833	-1.038594	-2.629317
1	0.922024	0.640869	-2.758714
1	1.688361	-0.764110	0.546472
1	-2.458086	-0.067260	2.612536
1	-2.132072	1.612616	2.161212
1	-1.240218	-1.531643	0.789746
1	-4.991488	-0.146277	-2.683323
1	0.089005	-3.025638	-0.748408
1	1.784135	-2.661544	-1.069887
1	3.742859	-1.447980	-1.982548
1	-0.548727	-3.879372	1.683665
1	0.717915	-3.975719	2.903137
1	1.584522	-4.512074	0.594982
1	2.394851	-3.107594	1.278860
1	-4.043420	-1.257549	1.342110
1	0.982002	-1.508436	2.885504
1	-0.709107	-1.917033	3.188189
1	6.033823	1.554718	0.033918
1	4.038995	3.072951	0.041821
1	0.932849	3.767303	1.394062
1	-0.579625	3.518975	1.757590
1	-2.152217	3.410346	0.578234
1	-2.170447	4.906670	1.020164
8	1.966066	4.714112	0.405229
1	1.457250	5.416317	-0.021571
1	1.920617	3.937755	-0.220942

Monomer(analyte)
ΔE -2529.90221868 h.

6	0.129571	3.078276	-0.201979
6	0.585160	4.026400	-1.143382
6	1.781184	4.715037	-0.957831
6	2.537777	4.457779	0.180917
6	2.122327	3.531804	1.131786
6	0.920492	2.843700	0.958228
6	0.447630	1.855006	1.992761
7	0.371624	0.480700	1.425850
1	1.293768	0.241113	1.057779
6	-0.032611	-0.566794	2.398903
6	-0.329878	-1.867136	1.626679
7	-1.335367	-1.599540	0.571559
1	-2.261857	-1.637311	0.994924
6	-1.314142	-2.561041	-0.571170
6	0.017590	-2.581808	-1.276511
6	0.768919	-3.758354	-1.313351
6	1.991629	-3.788643	-1.972969
6	2.497169	-2.656883	-2.606414
6	1.760644	-1.477706	-2.569521
6	0.514097	-1.397174	-1.901061
8	-0.154413	-0.256822	-1.887356
30	-1.037393	0.401751	-0.258808
8	-1.018210	2.430888	-0.399268
7	-3.127555	0.545990	-0.864811
1	-3.323958	-0.251760	-1.467316
1	-3.151403	1.364830	-1.472703
6	-4.187741	0.647305	0.175582
6	-5.587620	0.407662	-0.358908

6	-6.444325	-0.486897	0.295196
6	-7.749187	-0.687049	-0.160297
6	-8.213518	0.007539	-1.279808
6	-7.366587	0.902612	-1.939392
6	-6.063475	1.102357	-1.480786
1	-5.416684	1.801085	-2.004705
1	-7.720406	1.446275	-2.810519
1	-9.226803	-0.148840	-1.637865
1	-8.399542	-1.387357	0.355767
1	-6.085334	-1.031440	1.165007
6	-4.098438	2.016834	0.876759
1	-4.317682	2.805527	0.138299
8	-2.863209	2.239281	1.523134
1	-2.188112	2.456343	0.834113
1	-4.888778	2.054825	1.633617
1	-3.960242	-0.114659	0.928384
1	2.133530	-0.579866	-3.053351
1	3.455582	-2.707337	-3.112780
8	2.716311	-5.005220	-2.034416
6	3.567205	-5.233324	-1.012307
9	2.943136	-5.288037	0.185717
9	4.164015	-6.411264	-1.227179
9	4.524413	-4.285924	-0.908246
1	0.406026	-4.658736	-0.827035
1	-1.575722	-3.571601	-0.236609
1	-2.100631	-2.230156	-1.257945
1	0.592111	-2.154494	1.107159
6	-0.744025	-3.005354	2.569898
6	0.312551	-3.250436	3.654817
6	0.594075	-1.961424	4.436727
6	1.015317	-0.823610	3.495491
1	1.190801	0.090871	4.069806
1	1.966538	-1.083949	3.009232
1	1.374928	-2.128071	5.186627
1	-0.311003	-1.662826	4.983077
1	-0.021614	-4.045995	4.329508
1	1.240150	-3.602400	3.182946
1	-0.915876	-3.917384	1.988458
1	-1.701116	-2.740371	3.041941
1	-0.966504	-0.214213	2.857178
1	-0.561725	2.103101	2.334517
1	1.111555	1.887228	2.863263
1	2.738204	3.356912	2.008620
8	3.729549	5.190398	0.403847
6	4.863700	4.632704	-0.069972
9	5.879138	5.453424	0.221149
9	4.836054	4.450241	-1.407900
9	5.122564	3.426917	0.482131
1	2.131699	5.441981	-1.682908
1	-0.024006	4.207015	-2.023759

Monomer(analyte)$_2$

ΔE -2971.41500169 h.

30	0.229750	0.559611	-0.001750
9	6.354106	-2.879854	2.331258
8	-1.584440	0.042929	-1.040067
9	6.496234	-2.644287	0.180612
8	6.843991	-0.850972	1.494647
9	8.287083	-2.474660	1.410382
8	-4.820042	-4.458625	-1.259943
8	1.655059	1.116411	1.373253
9	-6.737784	-3.517449	-0.560093
6	-2.353145	-1.049420	-1.039310
7	0.318813	-1.644080	0.276802
1	1.037238	-1.810330	0.982072
7	1.814035	0.005666	-1.422750
1	1.397647	0.290407	-2.313762
9	-6.507432	-5.682704	-0.645966
6	2.885717	0.651781	1.382004
6	-3.469027	-1.090700	-1.905007
1	-3.656052	-0.220098	-2.526265
6	3.020552	0.828711	-1.146741
1	3.764679	0.725885	-1.947313
1	2.686234	1.870844	-1.139616
9	-5.479452	-4.527107	0.888566
6	-5.863730	-4.535251	-0.406558
6	2.062773	-1.451640	-1.437532
1	2.824045	-1.650465	-0.673501
6	3.644756	0.484280	0.181301
6	-0.951109	-2.216211	0.781075
1	-0.812985	-3.251595	1.115156
1	-1.214154	-1.644593	1.678130
6	-4.021298	-3.294350	-1.160595
6	0.789566	-2.204487	-1.014521
1	0.006196	-1.985154	-1.748512
6	-4.307281	-2.197840	-1.967327
1	-5.164084	-2.222933	-2.631990
6	5.511806	-0.363478	1.460307
6	2.583546	-1.958852	-2.789781
1	1.839284	-1.722131	-3.563463
1	3.500489	-1.419576	-3.052260
6	4.941571	-0.027356	0.237446
1	5.513995	-0.175986	-0.673417
6	6.981423	-2.185368	1.356572
6	1.567455	-4.226810	-2.338040
1	0.791622	-4.084830	-3.103076
1	1.760529	-5.303749	-2.281248
6	-2.087579	-2.178703	-0.218180
6	2.835606	-3.472329	-2.759267
1	3.179623	-3.817191	-3.740666
1	3.642928	-3.688437	-2.045760
6	-2.929253	-3.292936	-0.302434

1	-2.737751	-4.171296	0.306089
6	1.037542	-3.720460	-0.987928
1	1.765534	-3.944618	-0.195076
1	0.111166	-4.244497	-0.731838
6	4.809556	-0.200805	2.650868
1	5.276449	-0.474142	3.591764
6	3.513855	0.303891	2.606444
1	2.944672	0.438702	3.521858
7	-1.090700	1.129043	1.758001
1	-1.617766	0.299994	2.022951
1	-0.312874	1.199368	2.414855
6	-1.966125	2.319366	1.904992
1	-1.368906	3.187323	1.605912
6	-3.166798	2.230290	0.942531
1	-3.738126	1.315136	1.164412
1	-3.825020	3.080838	1.146125
8	-2.806495	2.287461	-0.426016
1	-2.423472	1.405977	-0.687397
6	-2.444533	2.532921	3.332773
6	-2.222705	3.755735	3.978228
6	-3.137952	1.524236	4.018996
6	-2.678065	3.968707	5.281661
1	-1.687109	4.545345	3.457061
6	-3.594424	1.733733	5.321018
1	-3.324637	0.566149	3.540090
6	-3.365166	2.957448	5.956804
1	-2.493064	4.921686	5.768971
1	-4.128980	0.942521	5.838730
1	-3.718065	3.119613	6.971025
7	0.036550	2.576405	-0.867238
1	0.635625	3.125228	-0.251545
1	-0.930756	2.799190	-0.614326
6	0.260785	3.014689	-2.269929
1	1.298338	2.778505	-2.526033
6	-0.641851	2.223846	-3.237898
1	-1.693973	2.418968	-2.983454
1	-0.469825	2.615323	-4.246261
8	-0.375955	0.832256	-3.255063
1	-0.882401	0.444157	-2.497210
6	0.036402	4.507455	-2.451342
6	1.019081	5.308363	-3.045325
6	-1.172876	5.100342	-2.052773
6	0.805409	6.675911	-3.236698
1	1.958658	4.858912	-3.357372
6	-1.387212	6.466127	-2.243095
1	-1.947522	4.493279	-1.590010
6	-0.398836	7.258307	-2.835349
1	1.579838	7.284557	-3.694768
1	-2.326436	6.912863	-1.929285
1	-0.566223	8.321607	-2.980459

S3 – Supporting information for Chapter 4 – Multimodal molecular γ-aminobutyric acid (GABA) sensor

Characterisation data

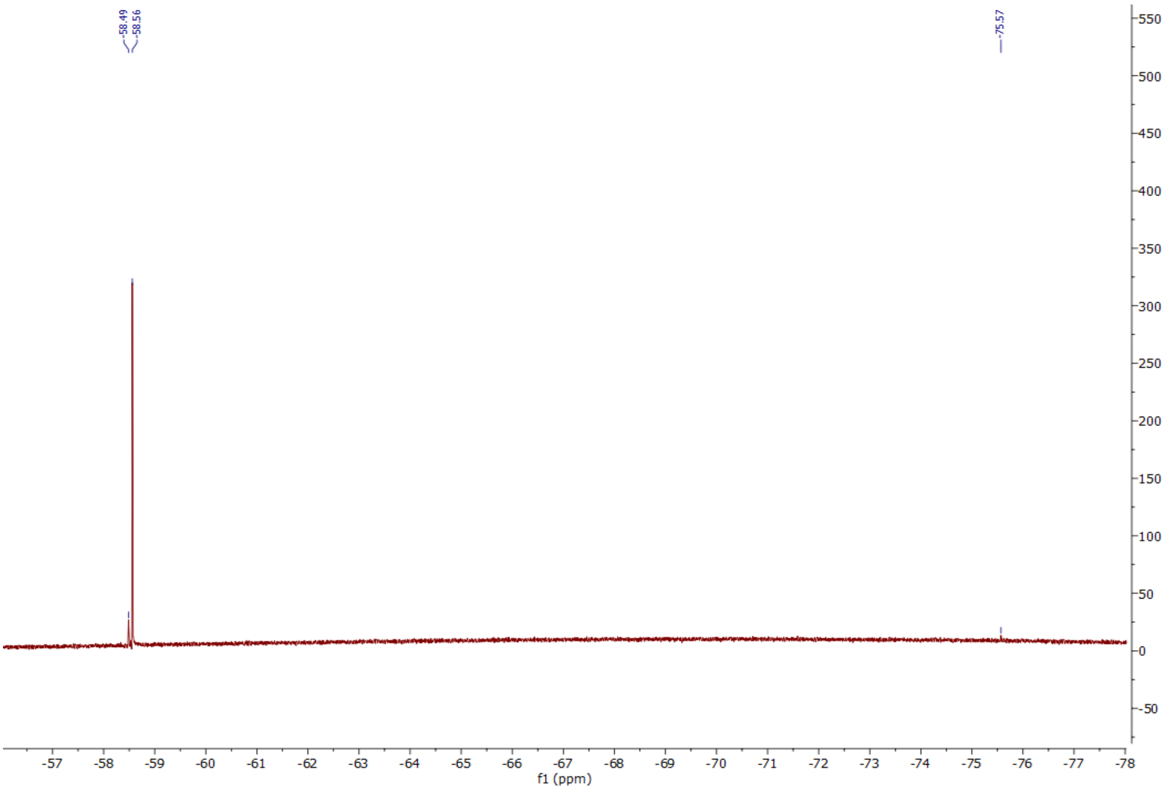


Figure S3-1: [19]F NMR spectra of [H_4oct$^{(p\text{-}OCF3)}$salox 3TFA] in D_2O.

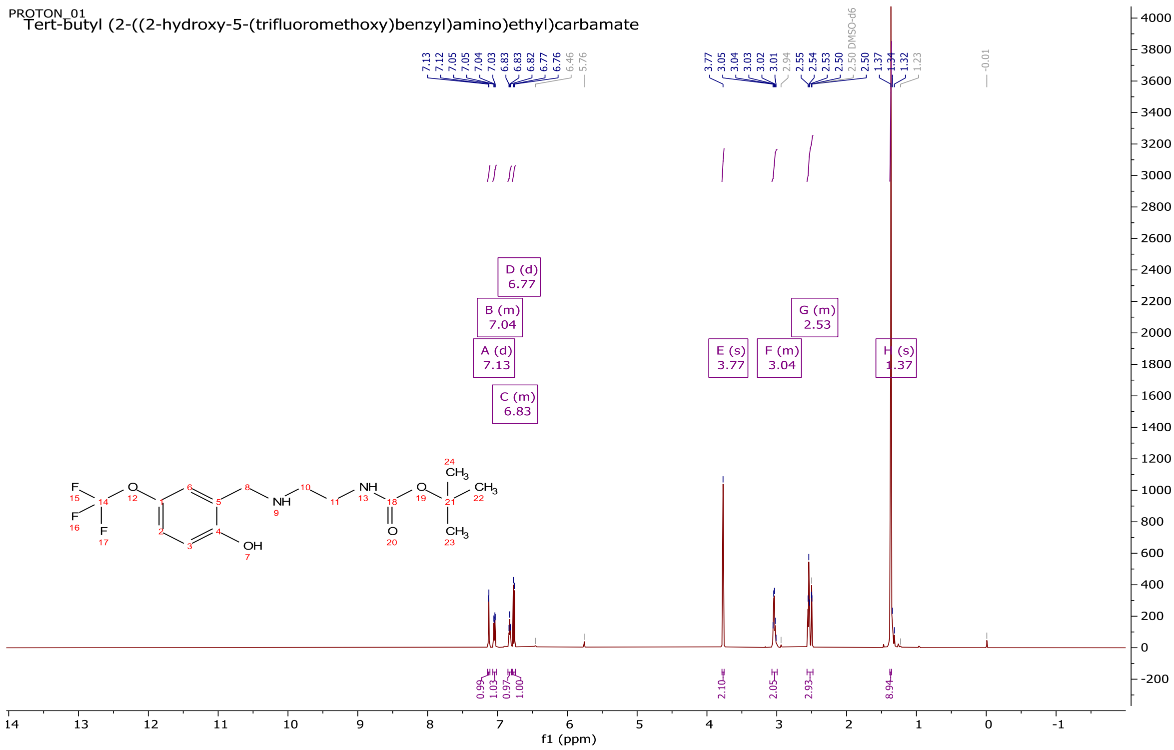


Figure S3-2. ^{1}H NMR data for compound **A.**

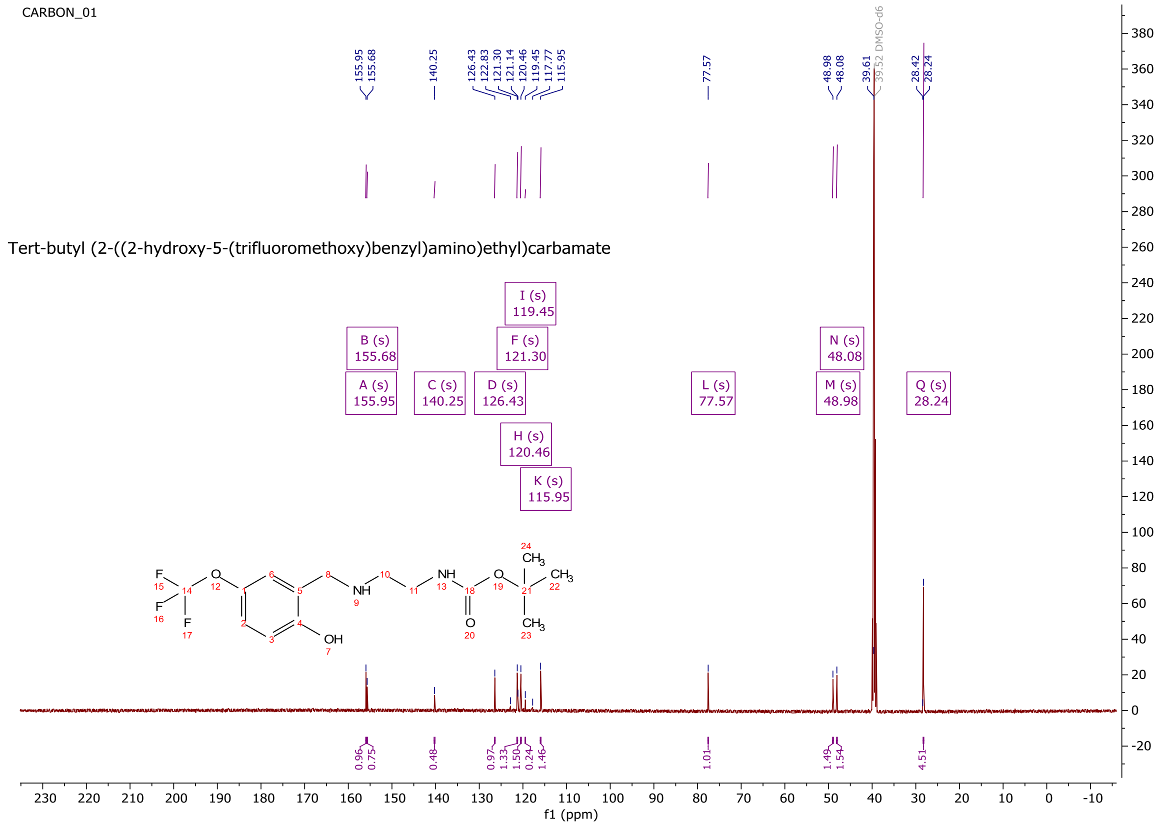


Figure S3-3. ^{13}C NMR data for compound **A.**

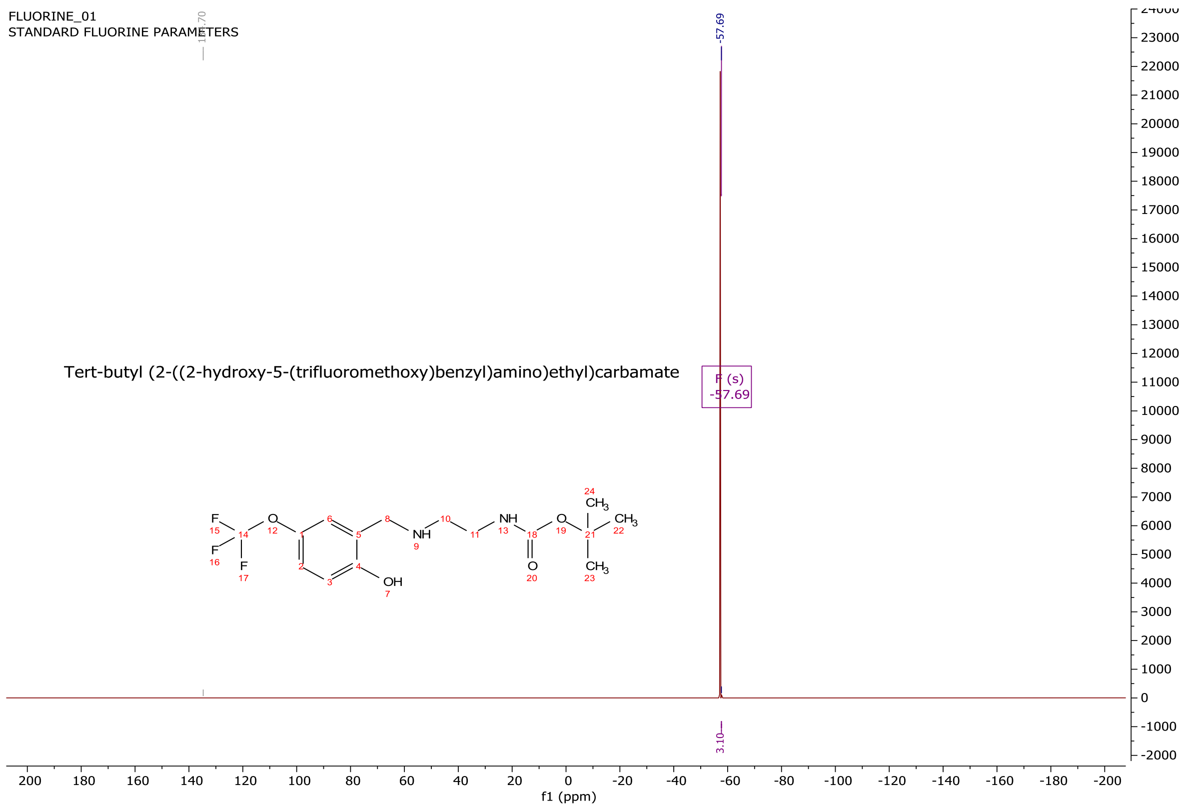


Figure S3-4. ^{19}F NMR data for compound **A.**

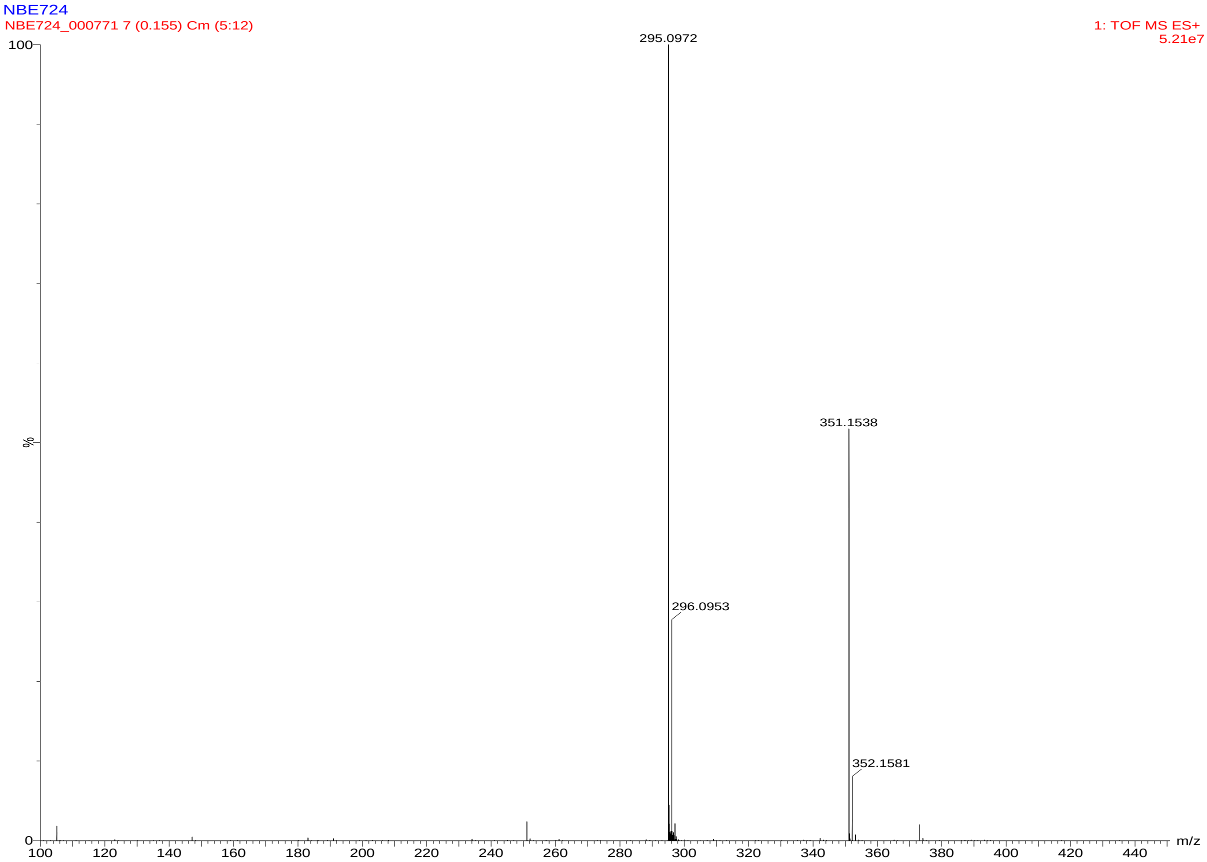


Figure S3-5. TOF MS ES+ data for compound **A.**

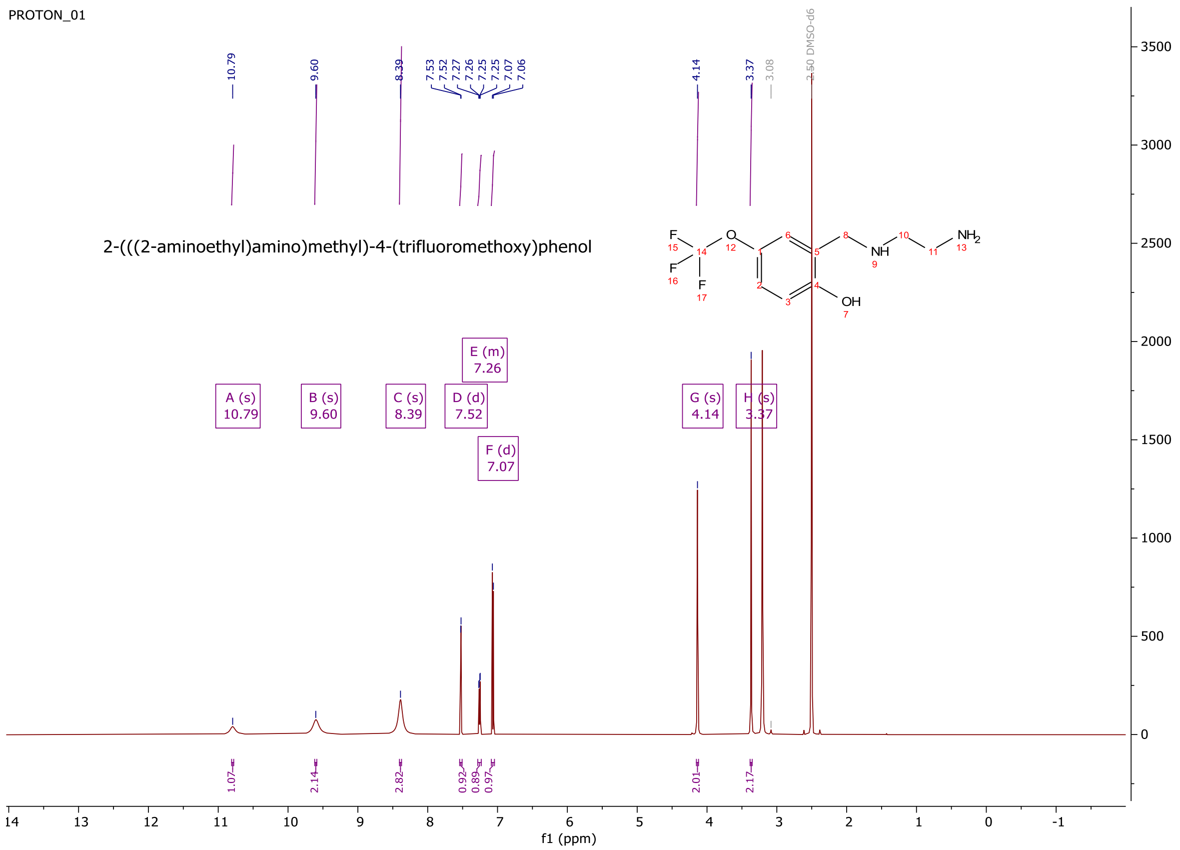


Figure S3-6. ^{1}H NMR data for precursor **B.**

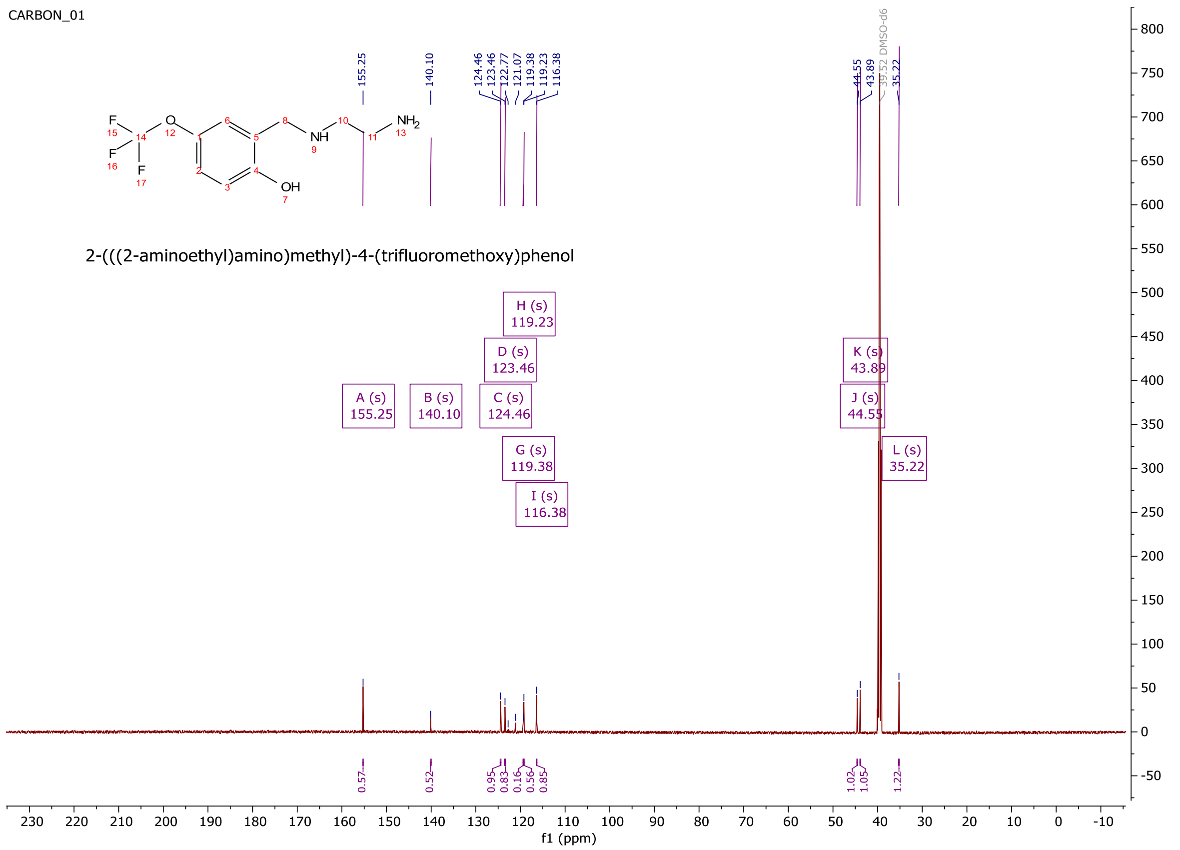


Figure S3-7. ^{13}C NMR data for precursor **B.**

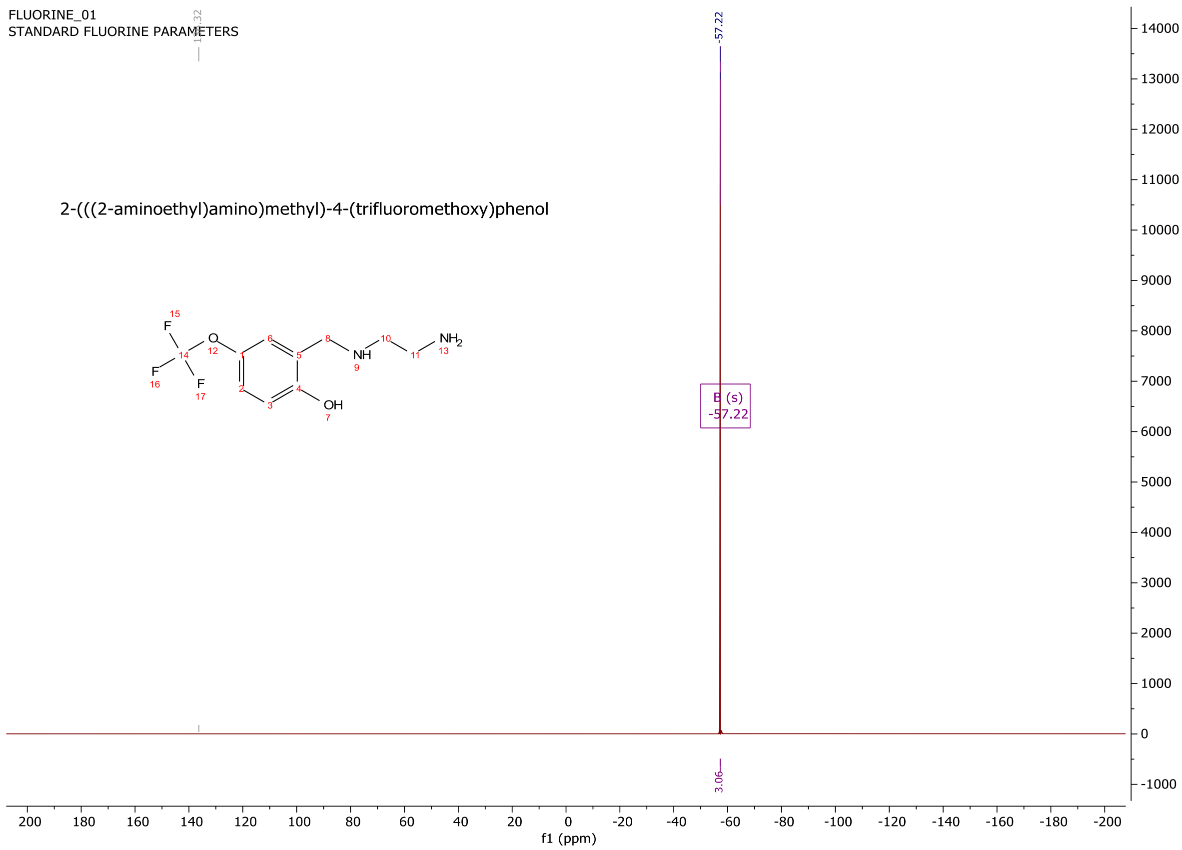


Figure S3-8. ^{19}F NMR data for precursor **B.**

Figure S3-9. TOF MS ES+ data for precursor **B.**

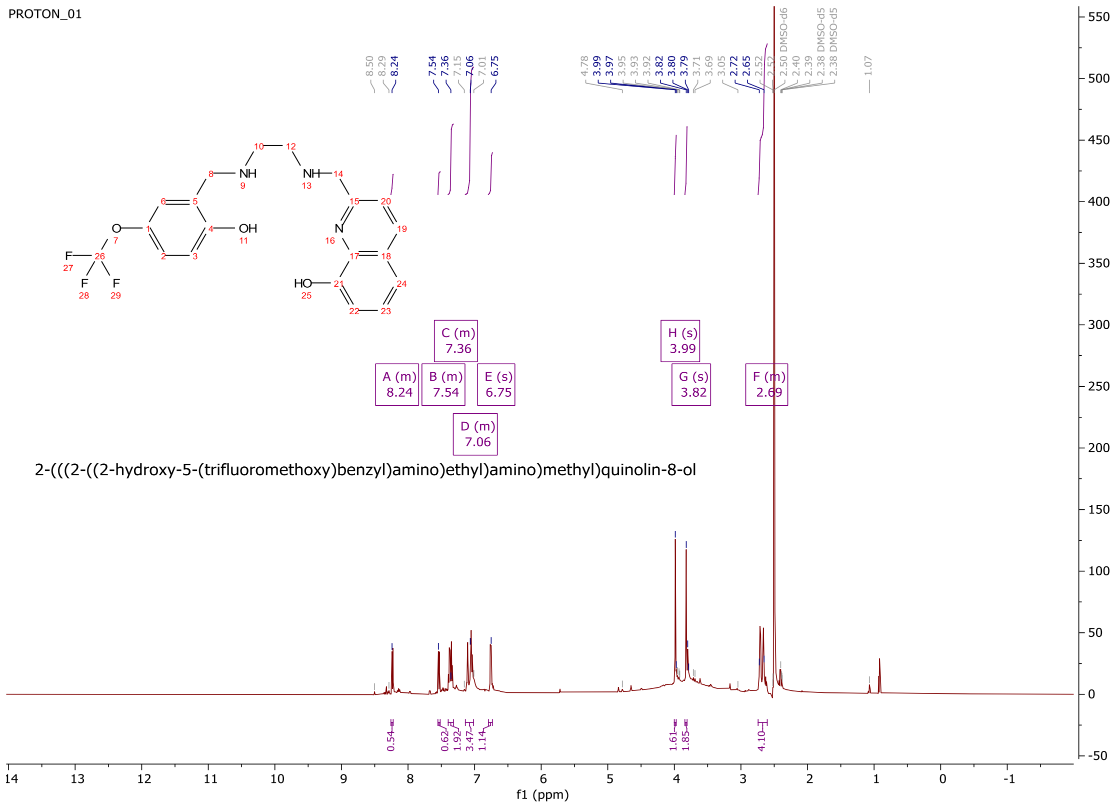


Figure S3-10. ^{1}H NMR data for precursor **C.**

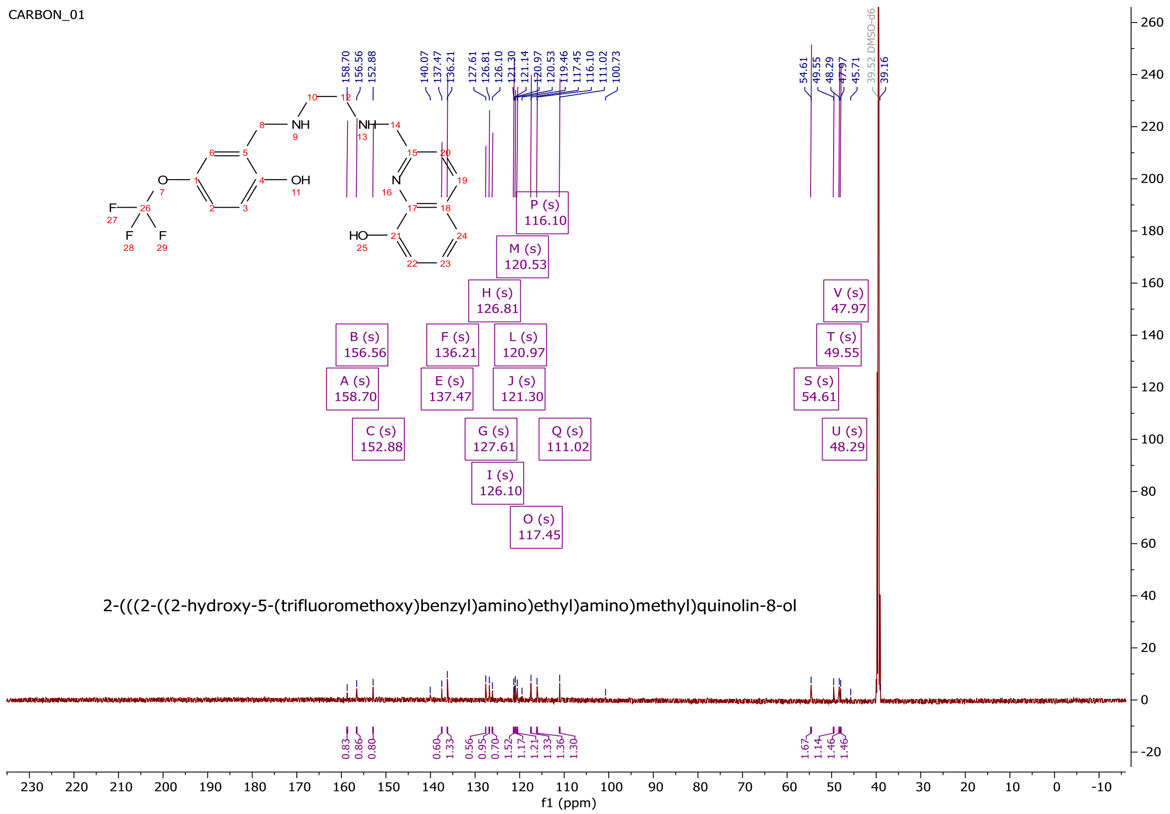


Figure S3-11. ^{13}C NMR data for precursor C.

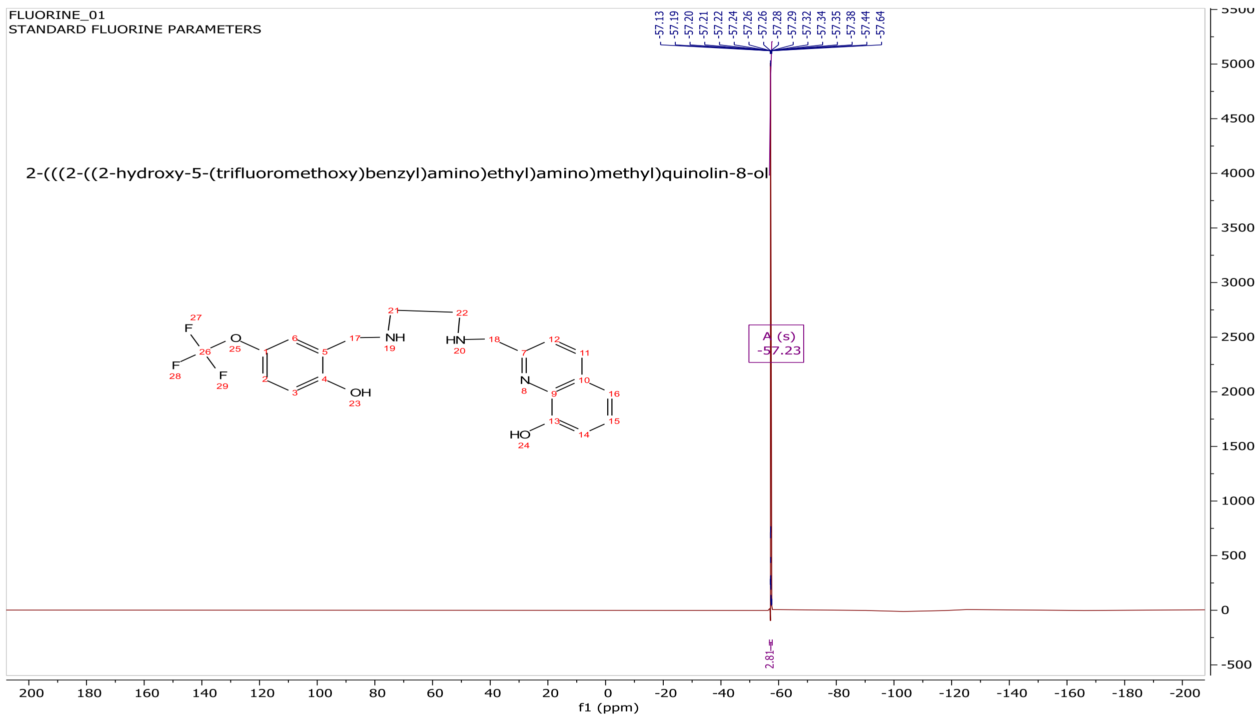


Figure S3-12. ^{19}F NMR data for precursor C.

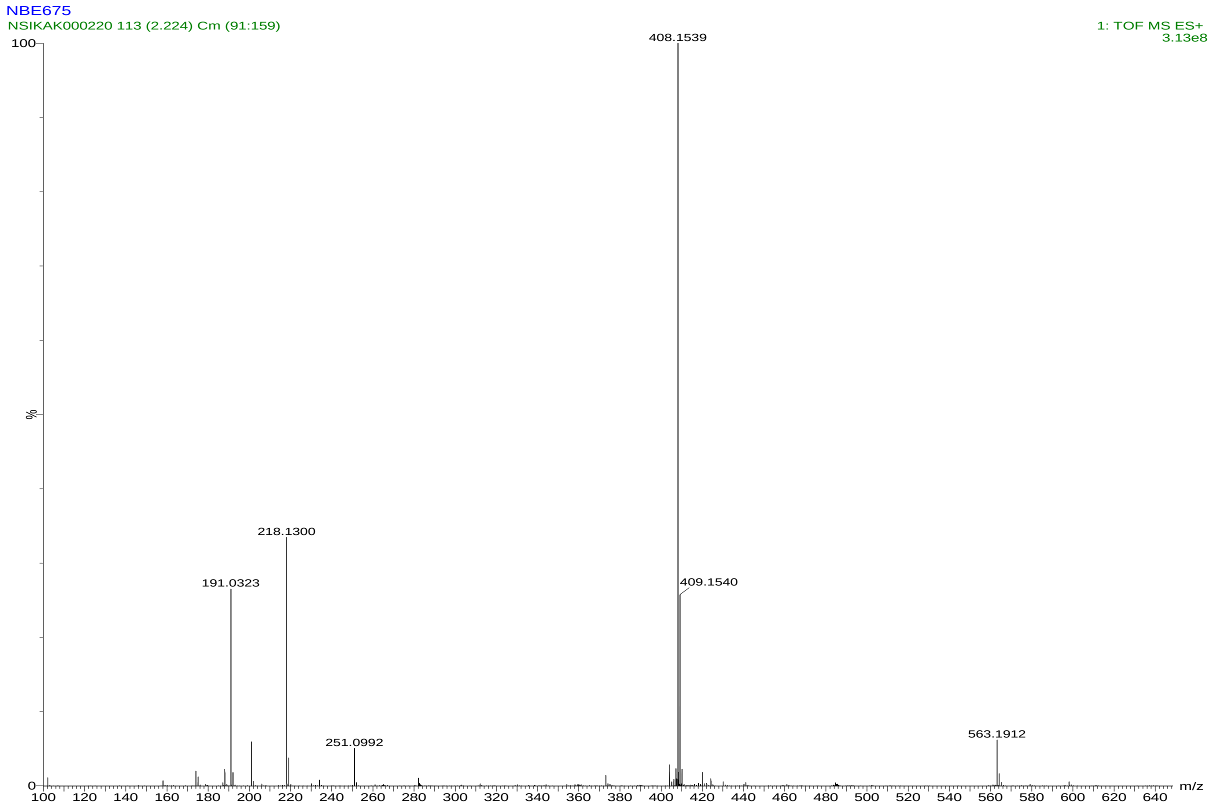


Figure S3-13. TOF MS ES+ data for precursor **C.**

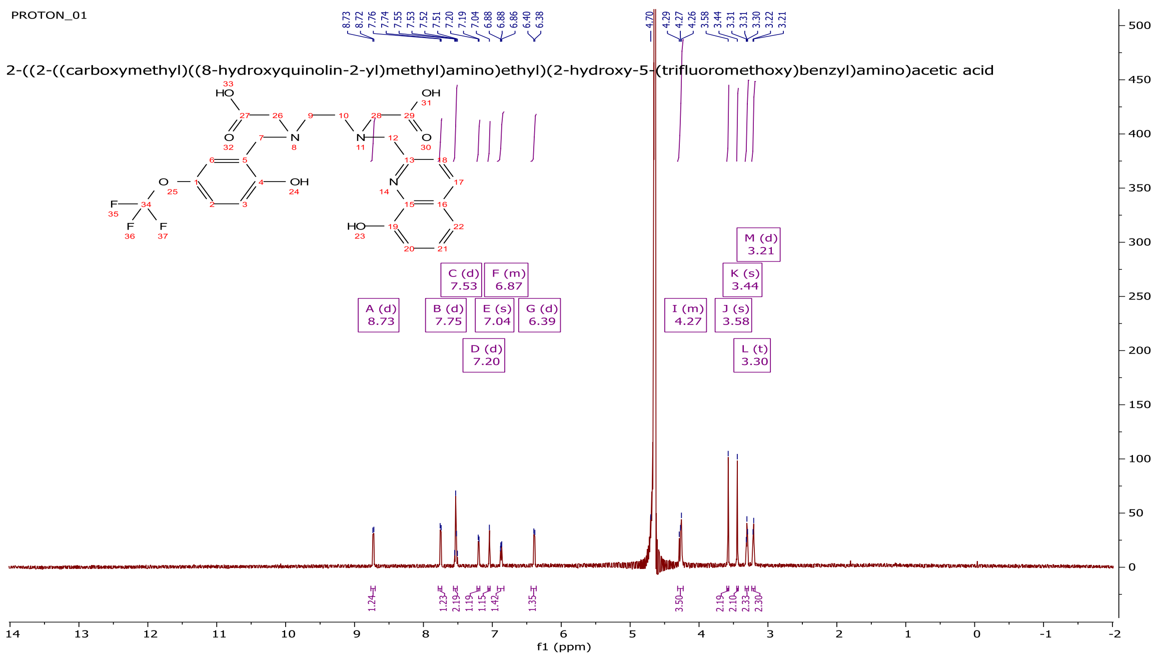


Figure S3-14. ^{1}H NMR spectra of [$H_4oct^{(p\text{-}OCF3)}$salox 3HCl] in D_2O.

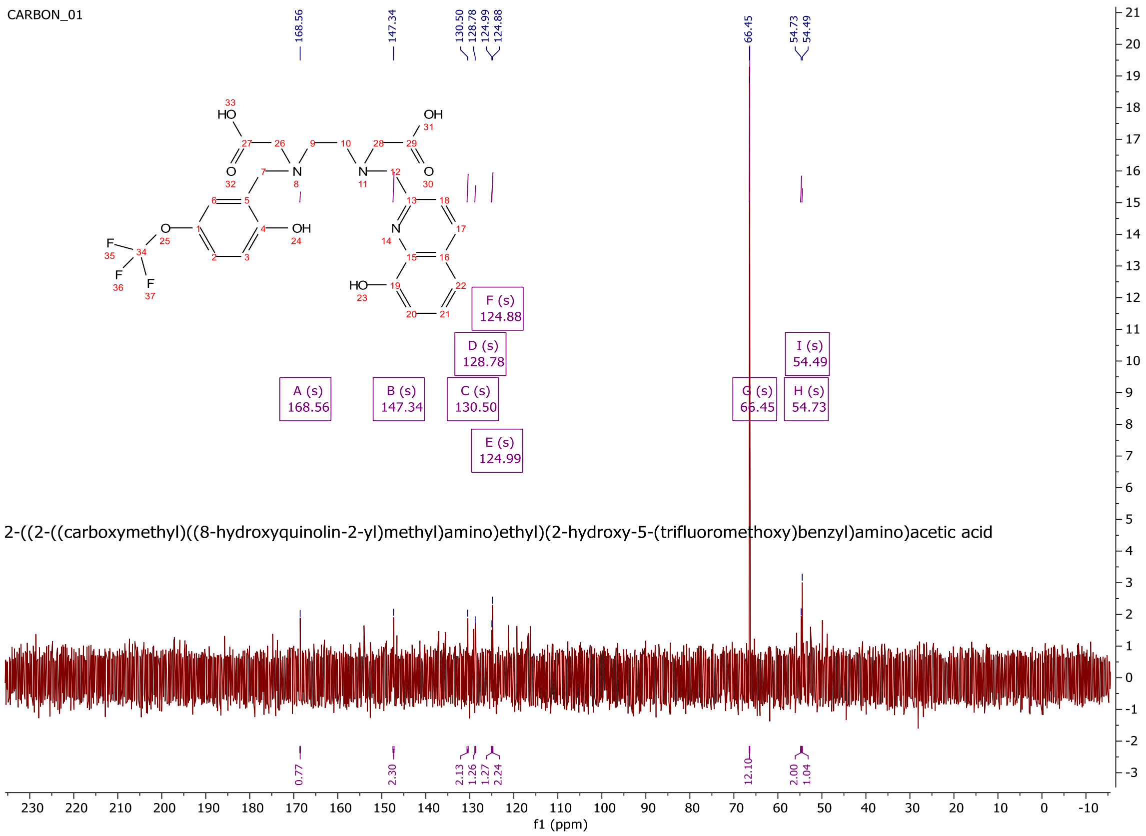


Figure S3-15. ^{13}C NMR spectra of [$H_4oct^{(p\text{-}OCF3)}$salox 3HCl] in D_2O.

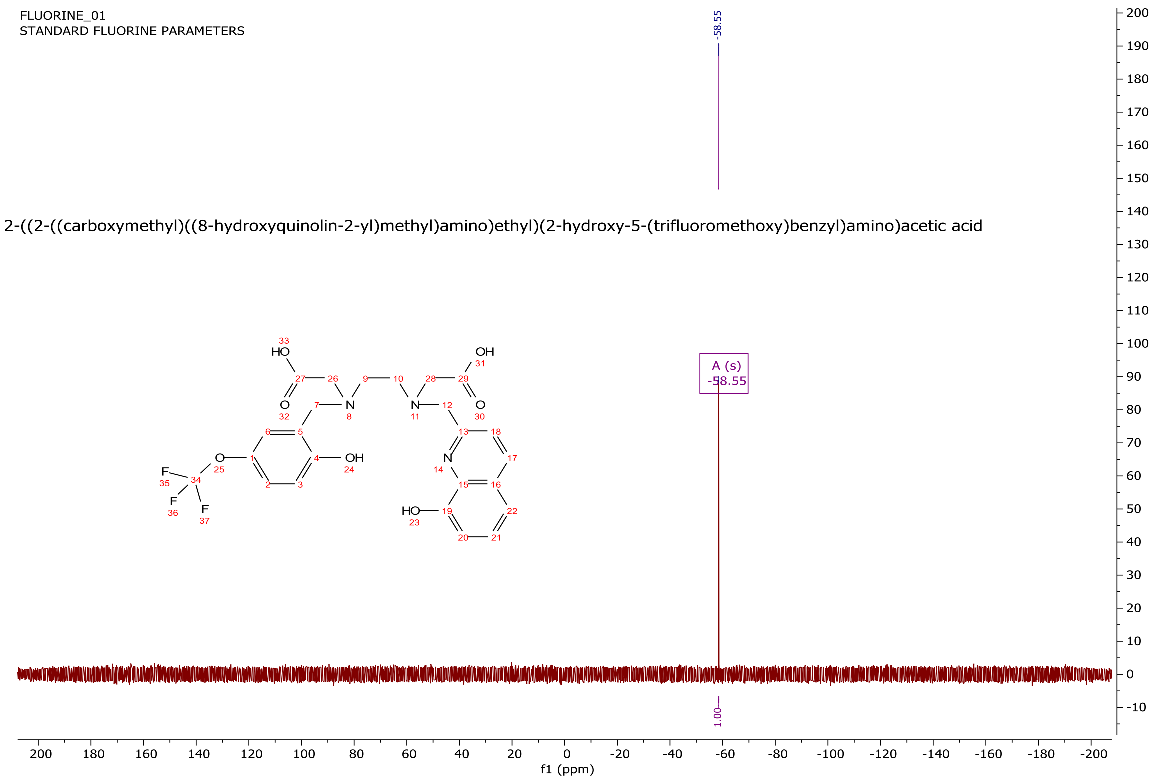


Figure S3-16. ^{19}F NMR spectra of [$H_4oct^{(p\text{-}OCF3)}$salox 3HCl] in D_2O.

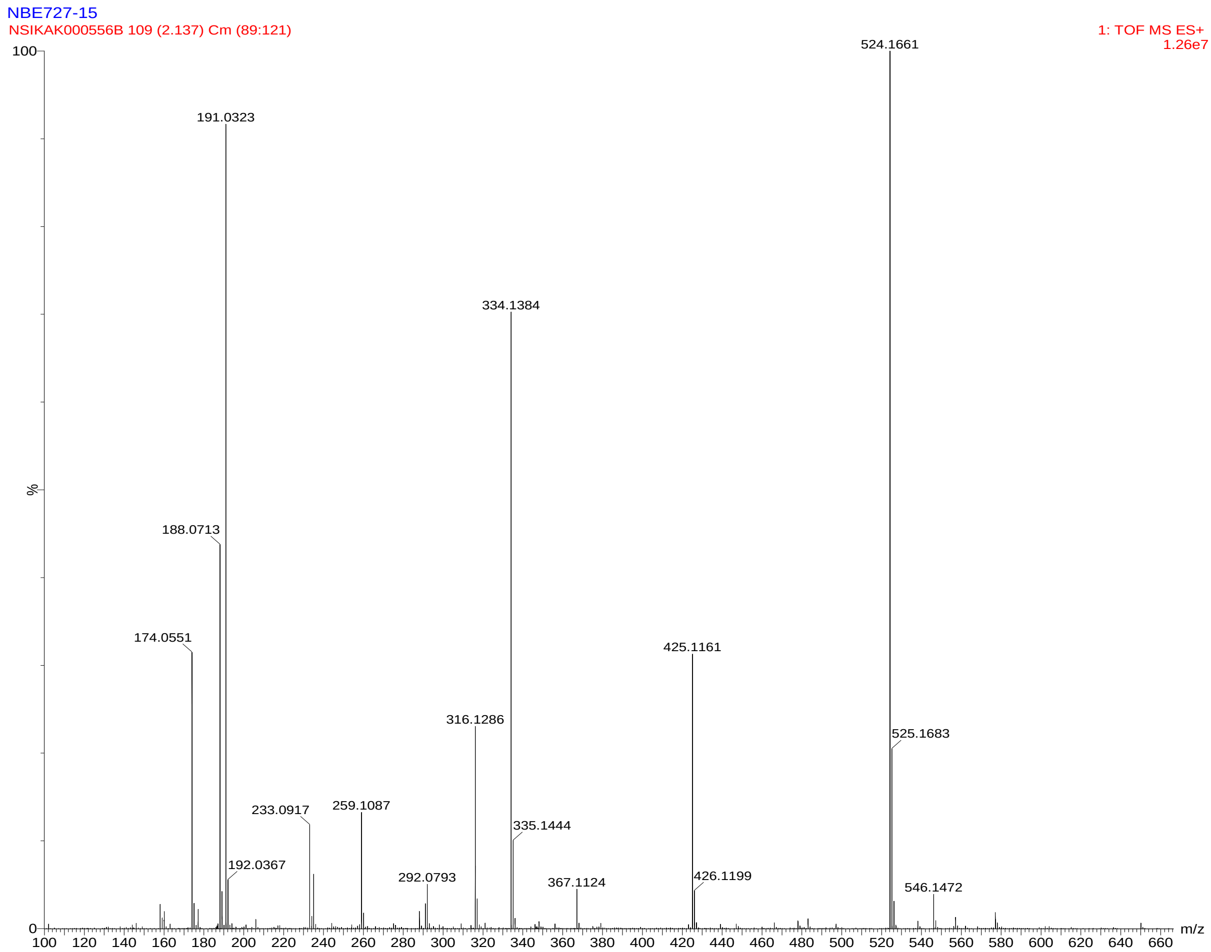


Figure S3-17. TOF MS ES+ data for [$H_4oct^{(p\text{-}OCF3)}$salox 3HCl] in D_2O.

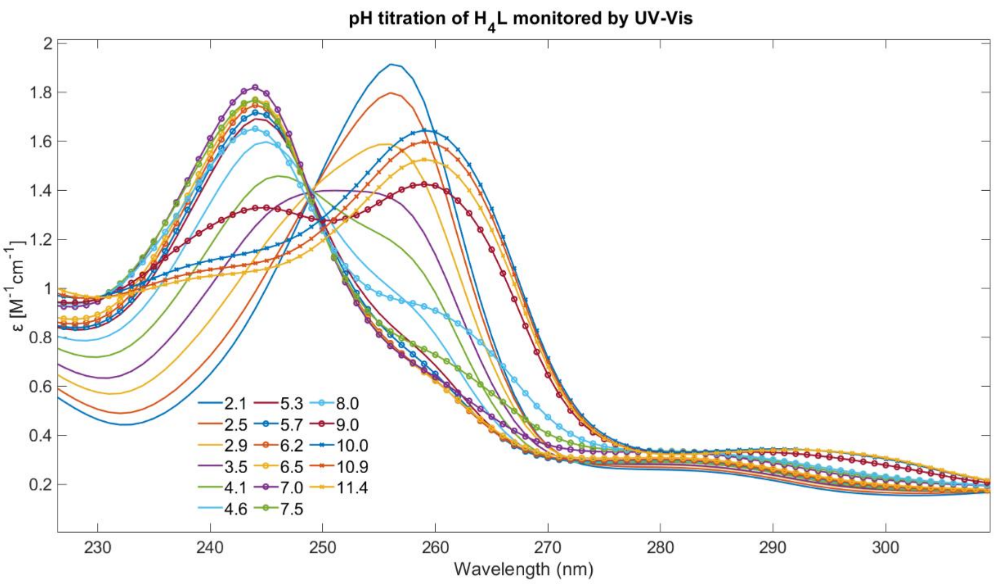


Figure S3-18. pH dependent UV-Vis studies of $H_4oct^{(p\text{-}OCF3)}$salox

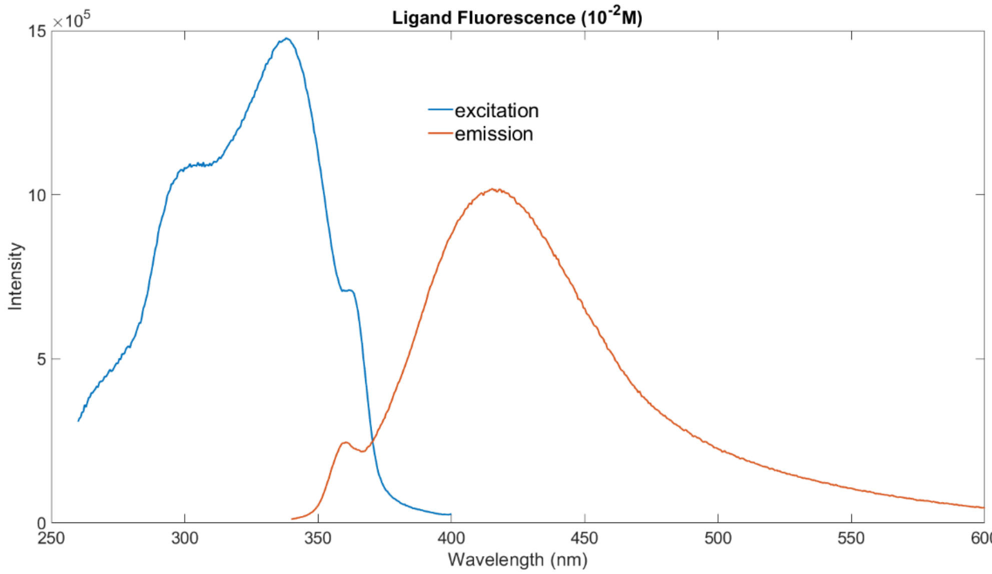
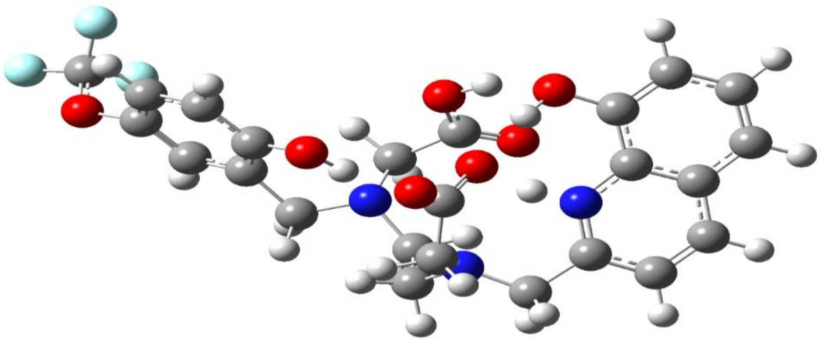


Figure S3-19. The excitation and emission spectra of $H_4oct^{(p-OCF3)}$salox (320nm excitation wavelength)

Theoretical calculations

Molecular structures, cartesian coordinates and corresponding energies for all the computed species.

$H_4oct^{(p\text{-}OCF3)}salox$, axial



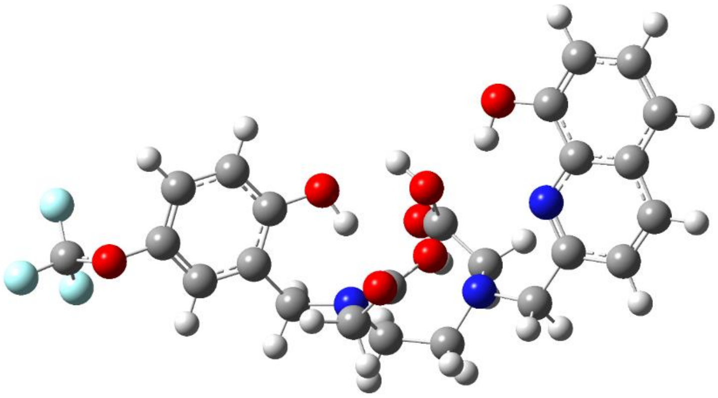
Electronic Energy (EE)	-1920.186	Hartree
EE + Zero-point Energy	-1919.718	Hartree
EE + Thermal Energy Correction	-1919.686	Hartree
EE + Thermal Enthalpy Correction	-1919.685	Hartree
EE + Thermal Free Energy Correction	-1919.786	Hartree

Tag	Symbol	X	Y	Z
1	C	4.529576	3.343543	-0.251646
2	C	3.849562	2.211710	0.145231
3	C	4.311697	0.951644	-0.315844
4	C	5.453018	0.873781	-1.155727
5	C	6.121239	2.056419	-1.534395
6	C	5.656836	3.267766	-1.086079
7	H	4.169850	4.302900	0.095944
8	C	5.859664	-0.412044	-1.587262
9	H	6.989227	1.990281	-2.176159
10	H	6.159781	4.182192	-1.370947
11	C	5.172360	-1.534710	-1.213095
12	C	4.044784	-1.408421	-0.384159
13	H	6.727298	-0.493962	-2.229651
14	H	5.476501	-2.517219	-1.544824
15	O	2.731826	2.361727	0.904674
16	N	3.666230	-0.209401	0.019913
17	C	3.259335	-2.609941	0.099721

18	H	3.903248	-3.129512	0.822820
19	H	3.164761	-3.290465	-0.750556
20	N	1.959747	-2.327799	0.668870
21	C	0.829016	-2.894612	-0.069171
22	H	1.115769	-3.855703	-0.513965
23	H	0.032720	-3.117087	0.640322
24	C	0.278828	-2.010577	-1.198402
25	H	1.104369	-1.466302	-1.654416
26	H	-0.144391	-2.652944	-1.983257
27	N	-0.742167	-1.031434	-0.763400
28	C	1.869097	-2.291365	2.121760
29	H	0.961337	-2.798190	2.452099
30	H	2.701986	-2.839304	2.577829
31	C	1.853074	-0.896992	2.794444
32	O	2.054787	0.116926	2.041887
33	O	1.653399	-0.865631	4.011923
34	C	-2.067530	-1.679550	-0.652262
35	H	-1.915884	-2.625837	-0.127677
36	H	-2.464332	-1.931798	-1.644314
37	C	-3.081978	-0.865106	0.114302
38	C	-2.734008	-0.236536	1.322961
39	C	-5.350169	-0.131499	0.443517
40	C	-3.704077	0.415975	2.082964
41	C	-5.021397	0.462968	1.650051
42	H	-3.412951	0.882878	3.014558
43	C	-0.808846	0.125439	-1.674212
44	H	-1.730785	0.671350	-1.475760
45	H	-0.804533	-0.182766	-2.725032
46	C	0.360825	1.062237	-1.438821
47	O	0.200035	1.797648	-0.334648
48	O	1.339420	1.126153	-2.147808
49	H	-5.780400	0.959965	2.238244
50	C	-4.402691	-0.792636	-0.319143
51	H	-4.696882	-1.266512	-1.246742
52	O	-1.459766	-0.261293	1.784840
53	O	-6.700178	-0.142155	0.019059
54	C	-7.131318	0.876946	-0.742356
55	F	-6.458782	0.991147	-1.905658
56	F	-7.038746	2.074140	-0.128557
57	F	-8.417564	0.659832	-1.029375
58	H	1.041042	2.250789	-0.111465
59	H	2.862969	-0.174697	0.724188
60	H	-0.875689	-0.501458	1.022845
61	H	2.521153	1.579080	1.481621

Figure S3-20(Above) and **Table S3-1**(Above) for **$H_4oct^{(p\text{-}OCF3)}salox$, axial**

$H_4oct^{(p\text{-}OCF3)}salox$, equatorial



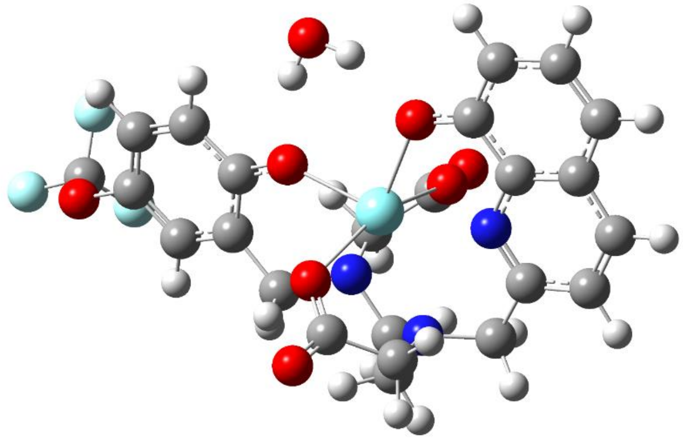
Electronic Energy (EE)	-1920.184	Hartree
EE + Zero-point Energy	-1919.716	Hartree
EE + Thermal Energy Correction	-1919.683	Hartree
EE + Thermal Enthalpy Correction	-1919.682	Hartree
EE + Thermal Free Energy Correction	-1919.785	Hartree

Tag	Symbol	X	Y	Z
1	N	-0.840426	0.368807	-0.487354
2	C	-0.454780	0.717492	0.895025
3	H	-0.622977	1.787861	1.020482
4	H	0.624523	0.557730	1.035291
5	C	-1.142547	-0.060299	2.007509
6	H	-0.685913	0.263226	2.952695
7	H	-0.915835	-1.122087	1.909100
8	N	-2.613239	0.071430	2.066221
9	C	-3.024746	1.436919	2.430406
10	H	-3.984754	1.386811	2.944996
11	H	-2.310137	1.903407	3.114464
12	C	-3.251506	2.409062	1.290786
13	O	-3.939746	1.877652	0.266210
14	O	-2.908717	3.565603	1.318322
15	C	-0.702321	-1.059000	-0.802974
16	H	-0.269348	-1.174860	-1.794608
17	H	-0.014649	-1.567178	-0.116628
18	C	-1.990886	-1.882436	-0.844853
19	O	-3.062624	-1.467257	-0.181582

20	O	-2.028430	-2.910311	-1.485463
21	C	-0.042004	1.211601	-1.412672
22	H	1.025994	0.971775	-1.335933
23	H	-0.157975	2.242331	-1.066461
24	C	-0.468335	1.135027	-2.858416
25	C	0.484704	1.046515	-3.869695
26	C	-2.199667	1.244598	-4.560398
27	C	0.094813	1.078742	-5.197430
28	H	1.534113	0.957914	-3.620572
29	C	-1.238713	1.173125	-5.558401
30	C	-3.142534	-0.906680	3.031685
31	H	-2.667476	-1.868003	2.823966
32	H	-2.849221	-0.643426	4.058414
33	C	-4.640535	-1.124375	2.996630
34	C	-5.211173	-1.993039	3.964303
35	C	-6.703496	-0.766677	2.044954
36	C	-6.555327	-2.241116	3.939206
37	H	-4.576654	-2.453942	4.710329
38	C	-7.449053	-0.100832	1.032468
39	C	-7.368840	-1.624605	2.957013
40	H	-7.007596	-2.904873	4.666100
41	C	-8.807639	-0.298173	0.940922
42	C	-8.765845	-1.809933	2.842994
43	C	-9.457666	-1.155722	1.851684
44	H	-9.369264	0.209571	0.167579
45	H	-9.275627	-2.464726	3.538197
46	H	-10.527381	-1.295056	1.760012
47	N	-5.366035	-0.535860	2.077951
48	O	-6.800806	0.718469	0.172856
49	C	-1.821791	1.226978	-3.219389
50	H	-3.250504	1.308420	-4.809528
51	H	-1.522290	1.177251	-6.601715
52	O	-2.793981	1.300511	-2.274096
53	O	1.075105	0.916793	-6.204038
54	C	1.647701	2.020798	-6.712790
55	F	2.300714	2.753040	-5.787814
56	F	0.764993	2.850816	-7.304233
57	F	2.533546	1.635820	-7.634831
58	H	-4.052773	2.559677	-0.418385
59	H	-2.399917	1.035814	-1.411609
60	H	-5.856911	0.717969	0.424475
61	H	-2.920328	-0.715452	0.467119

Figure S3-21(Above) and **Table S3-2**(Above) for **$H_4oct^{(p\text{-}OCF3)}$salox, equatorial**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, axial, H_2O



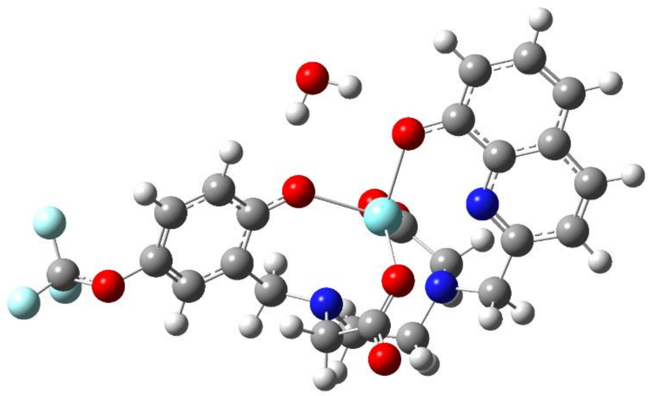
Electronic Energy (EE)	-2033.047	Hartree
EE + Zero-point Energy	-2032.602	Hartree
EE + Thermal Energy Correction	-2032.566	Hartree
EE + Thermal Enthalpy Correction	-2032.565	Hartree
EE + Thermal Free Energy Correction	-2032.671	Hartree

Tag	Symbol	X	Y	Z
1	C	4.250473	3.420853	0.338443
2	C	3.498941	2.253537	0.248757
3	C	4.189389	1.068626	-0.181392
4	C	5.568250	1.086516	-0.514037
5	C	6.285245	2.300688	-0.403393
6	C	5.621764	3.431071	0.016960
7	H	3.763496	4.333516	0.659536
8	C	6.126861	-0.141777	-0.940481
9	H	7.338449	2.327582	-0.651153
10	H	6.164694	4.364916	0.103235
11	C	5.349491	-1.269941	-1.019019
12	C	3.985880	-1.192561	-0.666050
13	H	7.177382	-0.183638	-1.202443
14	H	5.769092	-2.213544	-1.341203
15	O	2.217504	2.168292	0.522956
16	N	3.444974	-0.062552	-0.259385
17	C	3.058119	-2.379781	-0.777016
18	H	3.612241	-3.313935	-0.629284
19	H	2.664340	-2.409023	-1.795619

20	N	1.926747	-2.272675	0.164307
21	C	0.799262	-3.155538	-0.218485
22	H	1.169380	-4.127654	-0.565505
23	H	0.212775	-3.352010	0.677743
24	C	-0.086375	-2.552541	-1.295411
25	H	0.514074	-2.332345	-2.178427
26	H	-0.828210	-3.301748	-1.601432
27	N	-0.762981	-1.296736	-0.892849
28	C	2.367023	-2.588392	1.537110
29	H	2.472236	-3.667168	1.688123
30	H	3.349335	-2.142259	1.705194
31	C	1.432898	-2.003498	2.605039
32	O	0.743859	-0.984879	2.236175
33	O	1.428664	-2.508637	3.727022
34	C	-1.888855	-1.579009	0.036091
35	H	-1.451299	-1.975142	0.954789
36	H	-2.520138	-2.371848	-0.383617
37	C	-2.775826	-0.403956	0.382006
38	C	-2.259299	0.859870	0.776809
39	C	-5.022227	0.402752	0.755054
40	C	-3.179211	1.855705	1.167268
41	C	-4.546945	1.635986	1.166039
42	H	-2.791752	2.815684	1.484248
43	C	-1.190449	-0.580021	-2.105176
44	H	-1.954977	0.149811	-1.837301
45	H	-1.634592	-1.252874	-2.846044
46	C	-0.040735	0.206927	-2.748221
47	O	0.933171	0.504224	-1.966033
48	O	-0.134864	0.532047	-3.932118
49	Y	1.014269	0.216401	0.301266
50	H	-5.234219	2.410779	1.478954
51	C	-4.154684	-0.604706	0.372815
52	H	-4.557887	-1.563101	0.070463
53	O	-0.967248	1.120122	0.778786
54	O	-6.414781	0.133295	0.809209
55	C	-7.150439	0.401416	-0.278664
56	F	-6.768422	-0.299006	-1.367482
57	F	-7.122515	1.702770	-0.635377
58	F	-8.419914	0.078229	-0.009269
59	O	0.050208	3.804665	1.221807
60	H	0.945208	3.479747	1.006100
61	H	-0.478956	2.992005	1.124933

Figure S3-22 (Above) and **Table S3-3**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, axial, H_2O**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, equatorial, H_2O



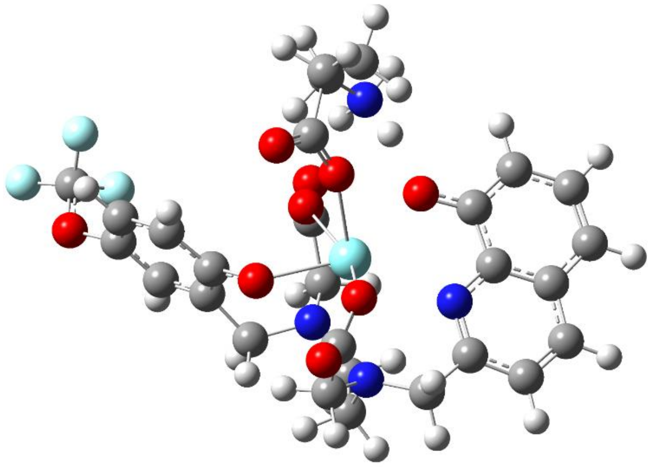
Electronic Energy (EE)	-2033.050	Hartree
EE + Zero-point Energy	-2032.605	Hartree
EE + Thermal Energy Correction	-2032.569	Hartree
EE + Thermal Enthalpy Correction	-2032.568	Hartree
EE + Thermal Free Energy Correction	-2032.675	Hartree

Tag	Symbol	X	Y	Z
1	N	-0.965104	0.300161	-0.292635
2	C	-0.431248	0.732656	1.019059
3	H	-0.662848	1.790314	1.141172
4	H	0.663806	0.649101	1.024701
5	C	-0.969591	-0.061653	2.198540
6	H	-0.419756	0.244293	3.097559
7	H	-0.763278	-1.121164	2.054932
8	N	-2.425964	0.098528	2.399658
9	C	-2.751523	1.403661	3.013111
10	H	-3.671291	1.297960	3.591790
11	H	-1.972527	1.719485	3.713307
12	C	-3.030297	2.539153	2.020730
13	O	-3.385813	2.181055	0.839653
14	O	-2.946137	3.699383	2.420076
15	C	-0.459309	-1.035521	-0.661160
16	H	-0.387965	-1.092693	-1.748286
17	H	0.547705	-1.210961	-0.269911
18	C	-1.366850	-2.205372	-0.254290
19	O	-2.598341	-1.920312	-0.019523

20	O	-0.880268	-3.335386	-0.221070
21	C	-0.601260	1.341105	-1.299948
22	H	0.481350	1.515926	-1.275147
23	H	-1.085698	2.262368	-0.967463
24	C	-1.012403	1.038501	-2.715339
25	C	-0.052053	0.998355	-3.722837
26	C	-2.713334	0.602351	-4.388755
27	C	-0.422822	0.776903	-5.037883
28	H	0.994052	1.139323	-3.480863
29	C	-1.747791	0.567839	-5.382652
30	C	-2.965201	-1.005444	3.217532
31	H	-2.502137	-1.934765	2.878768
32	H	-2.708876	-0.889732	4.277053
33	C	-4.458374	-1.148940	3.052707
34	C	-5.272986	-1.680851	4.073926
35	C	-6.284025	-0.954661	1.633128
36	C	-6.614894	-1.850255	3.843380
37	H	-4.833813	-1.946255	5.026203
38	C	-6.733404	-0.549360	0.330015
39	C	-7.177479	-1.490179	2.596586
40	H	-7.255511	-2.256520	4.617062
41	C	-8.087958	-0.707191	0.054291
42	C	-8.545671	-1.626426	2.264740
43	C	-8.970827	-1.237849	1.014851
44	H	-8.460819	-0.416583	-0.920262
45	H	-9.236523	-2.033297	2.991730
46	H	-10.017207	-1.341362	0.752893
47	N	-4.959048	-0.800765	1.883857
48	O	-5.853108	-0.063283	-0.514990
49	Y	-3.603036	0.111059	-0.027556
50	C	-2.378517	0.840024	-3.040223
51	H	-3.754229	0.441319	-4.639633
52	H	-2.018664	0.375412	-6.412404
53	O	-3.313643	0.875231	-2.111409
54	O	0.585695	0.665998	-6.030870
55	C	0.929576	1.772194	-6.704931
56	F	1.408026	2.753919	-5.911914
57	F	-0.092074	2.311864	-7.402834
58	F	1.890603	1.444066	-7.575247
59	O	-6.013422	1.628318	-2.736668
60	H	-5.044058	1.527356	-2.741140
61	H	-6.242487	1.047518	-1.985182

Figure S3-23 (Above) and **Table S3-4**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, equatorial, H_2O**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^{-}$, axial, GABA-O



Electronic Energy (EE)	-2319.796	Hartree
EE + Zero-point Energy	-2319.234	Hartree
EE + Thermal Energy Correction	-2319.193	Hartree
EE + Thermal Enthalpy Correction	-2319.192	Hartree
EE + Thermal Free Energy Correction	-2319.308	Hartree

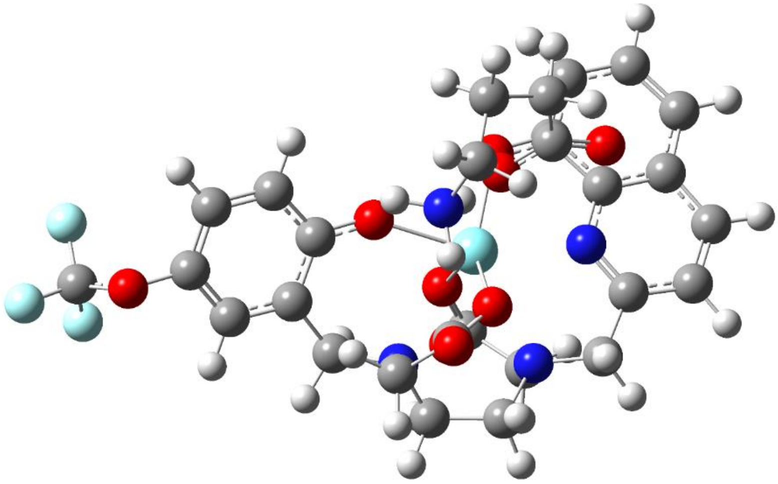
Tag	Symbol	X	Y	Z
1	C	4.024961	3.759048	-1.944185
2	C	3.392582	2.778143	-1.178881
3	C	4.171729	1.622162	-0.829441
4	C	5.519559	1.487268	-1.259673
5	C	6.107974	2.507495	-2.042504
6	C	5.358848	3.615328	-2.365327
7	H	3.473939	4.650859	-2.215988
8	C	6.194345	0.309619	-0.866036
9	H	7.134070	2.405447	-2.371473
10	H	5.802247	4.405347	-2.960211
11	C	5.550797	-0.624217	-0.098597
12	C	4.214361	-0.397276	0.294578
13	H	7.220253	0.154256	-1.178372
14	H	6.050405	-1.532325	0.211543
15	O	2.156065	2.844380	-0.764610
16	N	3.550800	0.683454	-0.066089
17	C	3.520900	-1.351357	1.226763
18	H	3.703655	-0.987573	2.240230
19	H	3.986252	-2.342054	1.165260

20	N	2.066544	-1.437284	1.022222
21	C	1.726059	-2.385837	-0.062942
22	H	2.542857	-3.097805	-0.221943
23	H	0.874602	-2.983493	0.255566
24	C	1.428977	-1.715895	-1.404186
25	H	2.320390	-1.202132	-1.762657
26	H	1.198129	-2.506501	-2.133662
27	N	0.338411	-0.721946	-1.330173
28	C	1.416691	-1.758975	2.300885
29	H	0.360628	-1.957484	2.117333
30	H	1.849525	-2.644184	2.781591
31	C	1.473003	-0.575748	3.283529
32	O	1.639503	0.581123	2.764768
33	O	1.331063	-0.814085	4.487681
34	C	-0.948421	-1.422210	-1.061082
35	H	-0.763760	-2.129041	-0.255008
36	H	-1.218707	-2.011548	-1.947542
37	C	-2.122367	-0.581137	-0.644074
38	C	-2.043290	0.151451	0.571700
39	C	-4.422062	0.073476	-0.907017
40	C	-3.211697	0.801631	1.021618
41	C	-4.392305	0.764867	0.291685
42	H	-3.169766	1.347439	1.955927
43	C	0.245771	0.072475	-2.564415
44	H	-0.333123	-0.435845	-3.344672
45	H	1.251192	0.219624	-2.965454
46	C	-0.327438	1.475279	-2.333927
47	O	-0.401796	1.868860	-1.134320
48	O	-0.621385	2.169101	-3.328122
49	Y	1.026546	1.151970	0.583654
50	H	-5.280993	1.269112	0.649039
51	C	-3.306444	-0.609063	-1.368724
52	H	-3.368528	-1.172653	-2.291911
53	O	-0.919415	0.211043	1.242430
54	O	-5.644874	-0.027025	-1.628333
55	C	-5.898863	0.896322	-2.562994
56	F	-4.983142	0.922109	-3.555552
57	F	-5.960996	2.153505	-2.073443
58	F	-7.086651	0.614988	-3.112937
59	O	0.367609	3.094848	1.568524
60	C	-0.350221	3.904690	2.247634
61	C	-0.410552	5.362343	1.752570
62	H	0.097703	5.969258	2.507240
63	H	-1.457384	5.676922	1.777156

64	C	0.213154	5.618707	0.382275
65	H	0.304164	6.693795	0.210325
66	H	1.221564	5.204137	0.381740
67	C	-0.589639	4.972716	-0.748339
68	H	-1.087091	4.071715	-0.404828
69	H	-1.334168	5.650849	-1.163090
70	N	0.296535	4.518734	-1.864047
71	H	1.084957	3.930770	-1.465608
72	H	-0.207436	3.888413	-2.515229
73	O	-0.978588	3.618188	3.276218
74	H	0.683819	5.302669	-2.384866

Figure S3-24 (Above) and **Table S3-5**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, axial, GABA-O**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, equatorial, GABA-O



Electronic Energy (EE)	-2319.797	Hartree
EE + Zero-point Energy	-2319.237	Hartree
EE + Thermal Energy Correction	-2319.196	Hartree
EE + Thermal Enthalpy Correction	-2319.195	Hartree
EE + Thermal Free Energy Correction	-2319.315	Hartree

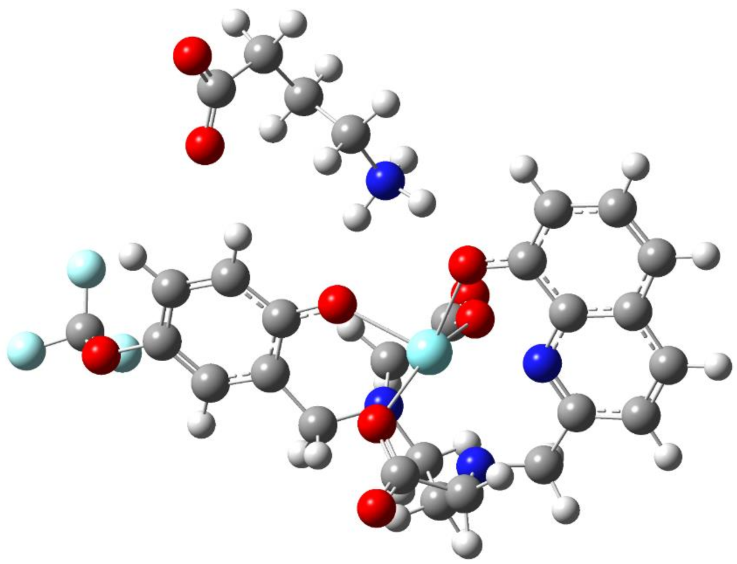
Tag	Symbol	X	Y	Z
1	N	-0.982279	-0.004388	-0.986254
2	C	-0.417718	0.291125	0.343372
3	H	-0.622439	1.336336	0.572480
4	H	0.676744	0.190409	0.324046
5	C	-0.956691	-0.592280	1.461595
6	H	-0.363602	-0.397634	2.366060
7	H	-0.824843	-1.643466	1.212095
8	N	-2.388422	-0.358994	1.722428
9	C	-2.611243	0.985749	2.294364
10	H	-3.437532	0.942935	3.004472
11	H	-1.737621	1.323416	2.859936
12	C	-2.996891	2.073390	1.280735
13	O	-3.410394	1.677059	0.140676
14	O	-2.913274	3.250701	1.649211
15	C	-0.399675	-1.224014	-1.555817
16	H	-0.305981	-1.110165	-2.635868
17	H	0.612823	-1.414778	-1.179399

18	C	-1.242736	-2.480073	-1.342927
19	O	-2.349202	-2.353338	-0.735080
20	O	-0.822605	-3.546292	-1.836624
21	C	-0.803210	1.181705	-1.864590
22	H	0.249872	1.494385	-1.868419
23	H	-1.377946	1.984698	-1.398597
24	C	-1.251237	1.010115	-3.294698
25	C	-0.366060	1.323528	-4.323115
26	C	-2.928790	0.508140	-4.977011
27	C	-0.761848	1.246163	-5.647528
28	H	0.645673	1.631506	-4.089069
29	C	-2.038117	0.831160	-5.988476
30	C	-2.960752	-1.406571	2.590502
31	H	-2.674594	-2.378163	2.179227
32	H	-2.561204	-1.359142	3.611475
33	C	-4.468814	-1.287125	2.617846
34	C	-5.249210	-1.610060	3.746045
35	C	-6.351193	-0.587876	1.451413
36	C	-6.608311	-1.412913	3.697395
37	H	-4.774243	-1.993333	4.639504
38	C	-6.829111	-0.011630	0.216228
39	C	-7.216393	-0.871114	2.540205
40	H	-7.224018	-1.651618	4.556869
41	C	-8.200236	0.252841	0.152726
42	C	-8.597356	-0.591099	2.410117
43	C	-9.054230	-0.039889	1.232259
44	H	-8.604638	0.689435	-0.752914
45	H	-9.271157	-0.804292	3.230027
46	H	-10.110543	0.181431	1.127347
47	N	-5.022370	-0.821142	1.516749
48	O	-5.979363	0.229943	-0.736048
49	Y	-3.761913	-0.467137	-0.636887
50	C	-2.572678	0.588070	-3.612141
51	H	-3.932596	0.183513	-5.221337
52	H	-2.327772	0.757653	-7.028622
53	O	-3.441025	0.272292	-2.684261
54	O	0.189336	1.502278	-6.672126
55	C	0.285636	2.752834	-7.141715
56	F	0.637686	3.653214	-6.199236
57	F	-0.860333	3.208181	-7.691464
58	F	1.227830	2.767329	-8.091745
59	O	-4.915179	-2.369445	-1.799689
60	C	-5.784997	-3.246447	-1.437345
61	O	-6.278728	-3.329659	-0.309186

62	C	-6.275037	-4.266870	-2.482913
63	H	-6.306184	-5.235597	-1.978304
64	H	-7.319123	-4.006933	-2.680678
65	C	-5.545629	-4.412469	-3.822258
66	H	-6.074855	-5.166267	-4.408971
67	H	-5.602840	-3.485685	-4.399698
68	C	-4.087960	-4.854723	-3.719182
69	H	-3.732429	-5.291504	-4.649610
70	H	-3.954483	-5.589897	-2.926528
71	N	-3.209279	-3.686446	-3.394919
72	H	-3.758226	-3.051205	-2.749403
73	H	-2.324187	-3.934183	-2.917715
74	H	-2.978666	-3.161554	-4.236088

Figure S3-25 (Above) and **Table S3-6**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, equatorial, GABA-O**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, axial, GABA-N



Electronic Energy (EE)	-2319.797	Hartree
EE + Zero-point Energy	-2319.236	Hartree
EE + Thermal Energy Correction	-2319.194	Hartree
EE + Thermal Enthalpy Correction	-2319.193	Hartree
EE + Thermal Free Energy Correction	-2319.314	Hartree

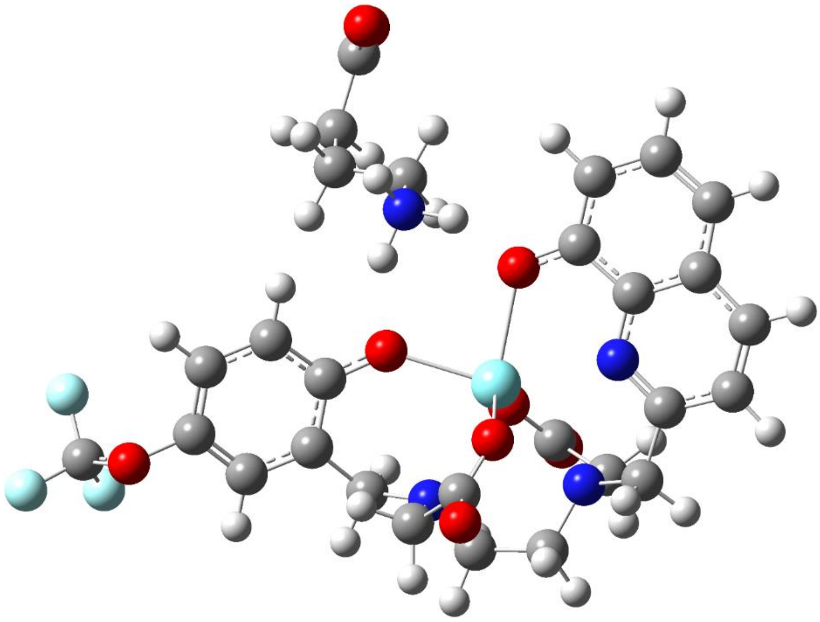
Tag	Symbol	X	Y	Z
1	C	4.431298	3.218518	-0.050723
2	C	3.649588	2.070991	-0.028344
3	C	4.317201	0.821769	-0.262295
4	C	5.711506	0.759313	-0.515277
5	C	6.461915	1.957965	-0.525598
6	C	5.817388	3.151267	-0.295671
7	H	3.960581	4.178226	0.123783
8	C	6.251696	-0.528377	-0.745732
9	H	7.526743	1.923124	-0.715777
10	H	6.385330	4.073823	-0.303480
11	C	5.443976	-1.637537	-0.723754
12	C	4.066003	-1.479741	-0.466686
13	H	7.313023	-0.630133	-0.938057
14	H	5.849898	-2.625235	-0.895882
15	O	2.346011	2.061029	0.187727
16	N	3.543164	-0.292234	-0.241100
17	C	3.104161	-2.645856	-0.483245
18	H	3.614679	-3.566927	-0.179969
19	H	2.772608	-2.796887	-1.513248

20	N	1.919671	-2.386440	0.359740
21	C	0.780975	-3.273647	0.015463
22	H	1.133714	-4.287489	-0.205611
23	H	0.147125	-3.355228	0.896932
24	C	-0.034018	-2.768384	-1.163808
25	H	0.610012	-2.677687	-2.038709
26	H	-0.795409	-3.518832	-1.412019
27	N	-0.671158	-1.445939	-0.942615
28	C	2.257919	-2.537104	1.789218
29	H	2.319607	-3.590497	2.078485
30	H	3.239742	-2.094502	1.969046
31	C	1.270430	-1.802559	2.707953
32	O	0.635304	-0.825990	2.165708
33	O	1.176720	-2.159681	3.880806
34	C	-1.847616	-1.570855	-0.048428
35	H	-1.479290	-1.932513	0.913557
36	H	-2.521109	-2.343914	-0.438618
37	C	-2.665982	-0.316861	0.192648
38	C	-2.112649	0.975213	0.399405
39	C	-4.870580	0.568626	0.646056
40	C	-2.986387	2.020678	0.763079
41	C	-4.351838	1.827663	0.892302
42	H	-2.570409	2.999848	0.968707
43	C	-1.017920	-0.861107	-2.248701
44	H	-1.744331	-0.061970	-2.098145
45	H	-1.479638	-1.595517	-2.916534
46	C	0.198332	-0.229057	-2.938840
47	O	1.173077	0.086859	-2.163234
48	O	0.155751	-0.033709	-4.153159
49	Y	1.108210	0.098432	0.121296
50	H	-5.001905	2.642495	1.182033
51	C	-4.045569	-0.488133	0.310131
52	H	-4.481493	-1.466154	0.149063
53	O	-0.819486	1.229783	0.256492
54	O	-6.256640	0.329793	0.833749
55	C	-7.073238	0.502488	-0.215092
56	F	-6.783354	-0.306824	-1.255771
57	F	-7.062105	1.762221	-0.699167
58	F	-8.320137	0.227642	0.182130
59	C	0.029536	5.000165	0.140081
60	H	-0.095447	4.750367	1.191299
61	H	0.905159	5.639505	0.032401
62	C	-1.217789	5.674517	-0.408103
63	H	-1.041093	5.966133	-1.448347

64	H	-2.045239	4.962781	-0.401102
65	C	-1.610353	6.898853	0.414444
66	H	-2.405752	7.439810	-0.106831
67	H	-0.774874	7.599854	0.490660
68	C	-2.133238	6.604244	1.842407
69	N	0.327215	3.721202	-0.574583
70	H	0.333842	3.854133	-1.584894
71	H	1.247622	3.300515	-0.294317
72	H	-0.355904	2.972355	-0.347555
73	O	-2.465533	5.421731	2.109930
74	O	-2.202262	7.593477	2.613893

Figure S3-26 (Above) and **Table S3-7**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^{-}$, axial, GABA-N**

[Y(oct$^{(p\text{-}OCF3)}$salox)]$^{-}$, equatorial, GABA-N



Electronic Energy (EE)	-2319.800	Hartree
EE + Zero-point Energy	-2319.239	Hartree
EE + Thermal Energy Correction	-2319.198	Hartree
EE + Thermal Enthalpy Correction	-2319.197	Hartree
EE + Thermal Free Energy Correction	-2319.319	Hartree

Tag	Symbol	X	Y	Z
1	N	-1.032982	0.679476	-0.284414
2	C	-1.126507	1.852330	0.615201
3	H	-1.782690	2.583359	0.145140
4	H	-0.143171	2.330857	0.711302
5	C	-1.624653	1.514694	2.011283
6	H	-1.543268	2.414064	2.634103
7	H	-0.976473	0.764765	2.462202
8	N	-3.009322	0.992827	2.030929
9	C	-3.999410	2.074235	1.836379
10	H	-4.938764	1.776225	2.306229
11	H	-3.678955	2.998773	2.325553
12	C	-4.354614	2.369450	0.373668
13	O	-4.139163	1.415027	-0.460590
14	O	-4.855303	3.457720	0.099345
15	C	0.059864	-0.221508	0.130709
16	H	0.482818	-0.693815	-0.756737

17	H	0.875350	0.324376	0.614336
18	C	-0.376432	-1.380872	1.036379
19	O	-1.627839	-1.678259	1.016572
20	O	0.484947	-1.976078	1.681805
21	C	-0.866178	1.183121	-1.680474
22	H	-0.030588	1.892004	-1.719870
23	H	-1.776285	1.742333	-1.909363
24	C	-0.645175	0.118591	-2.720333
25	C	0.509252	0.154962	-3.498894
26	C	-1.340263	-1.854856	-3.940779
27	C	0.721675	-0.787592	-4.489105
28	H	1.251755	0.924301	-3.328293
29	C	-0.189913	-1.804609	-4.712599
30	C	-3.274808	0.269773	3.290760
31	H	-2.398012	-0.338877	3.522667
32	H	-3.415754	0.957744	4.132045
33	C	-4.459229	-0.656453	3.166987
34	C	-5.252661	-1.002496	4.280472
35	C	-5.703867	-2.047811	1.787652
36	C	-6.281253	-1.895883	4.120648
37	H	-5.045559	-0.558524	5.244801
38	C	-5.881576	-2.545765	0.454476
39	C	-6.548163	-2.459160	2.851155
40	H	-6.902203	-2.171855	4.964493
41	C	-6.915077	-3.450980	0.248458
42	C	-7.587688	-3.381313	2.587985
43	C	-7.751278	-3.855758	1.307461
44	H	-7.075182	-3.849618	-0.745772
45	H	-8.237649	-3.700574	3.392210
46	H	-8.544664	-4.563091	1.097790
47	N	-4.687343	-1.166432	1.972546
48	O	-5.062360	-2.122324	-0.488592
49	Y	-3.317011	-0.641004	-0.060704
50	C	-1.605779	-0.900451	-2.939020
51	H	-2.051831	-2.653895	-4.103227
52	H	0.000052	-2.550553	-5.472828
53	O	-2.720823	-0.965415	-2.225718
54	O	1.940455	-0.768946	-5.214078
55	C	1.981712	-0.072386	-6.359322
56	F	1.734153	1.243519	-6.192117
57	F	1.100649	-0.511111	-7.282221
58	F	3.209772	-0.196051	-6.873383
59	C	-6.007010	-1.635271	-4.092204
60	H	-6.889674	-2.274392	-4.104690

61	H	-5.579730	-1.607161	-5.092110
62	C	-6.348702	-0.232374	-3.618296
63	H	-5.435758	0.364014	-3.574269
64	H	-6.758063	-0.283979	-2.605204
65	C	-7.352974	0.450771	-4.544219
66	H	-8.253609	-0.159791	-4.652983
67	H	-7.683128	1.385887	-4.081835
68	C	-6.839221	0.815379	-5.959320
69	N	-5.005117	-2.289118	-3.195278
70	H	-5.309483	-2.353268	-2.194343
71	H	-4.783541	-3.228845	-3.518428
72	H	-4.114512	-1.753902	-3.113730
73	O	-5.598960	0.791820	-6.157992
74	O	-7.723605	1.133448	-6.794101

Figure S3-27 (Above) and **Table S3-8**(Above) for **[Y(oct$^{(p\text{-}OCF3)}$salox)]$^-$, equatorial, GABA-N**

S4 - Supporting information for Chapter 5 – Molecular fluorine-based probes for heavy metals ion detection

Ligands and complex characterisation data

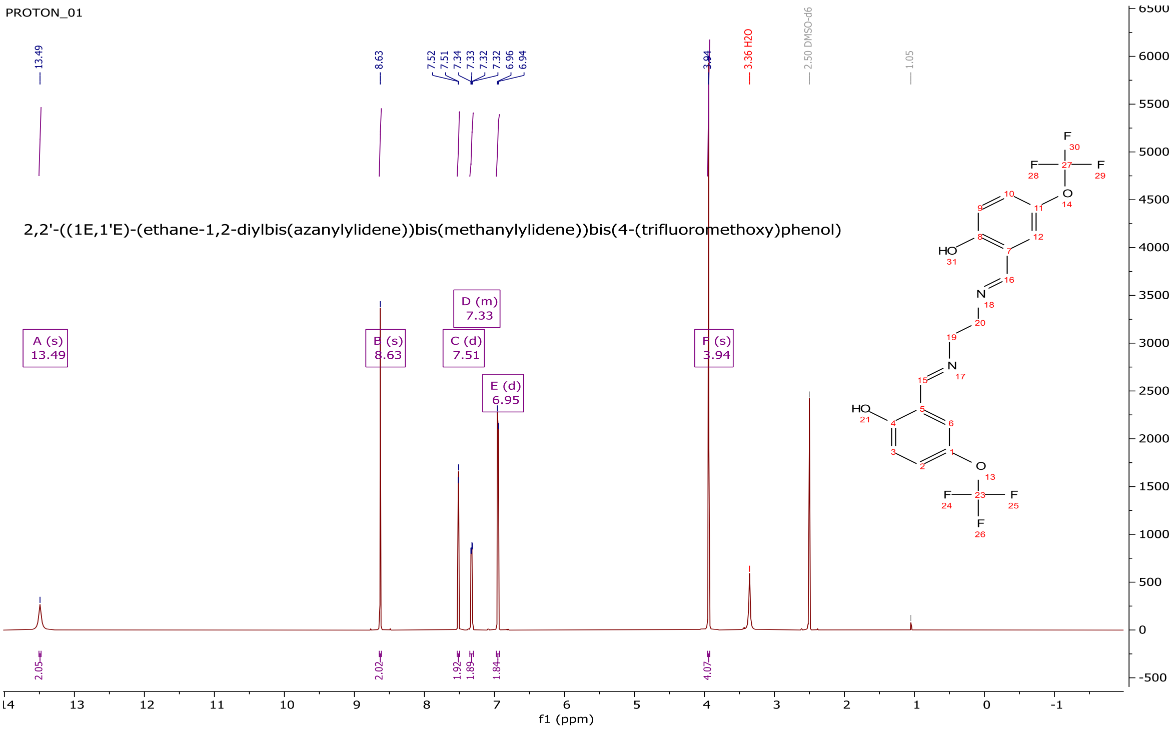


Figure S4-1. ^{1}H NMR for OCF_3/OCF_3 (Unreduced)

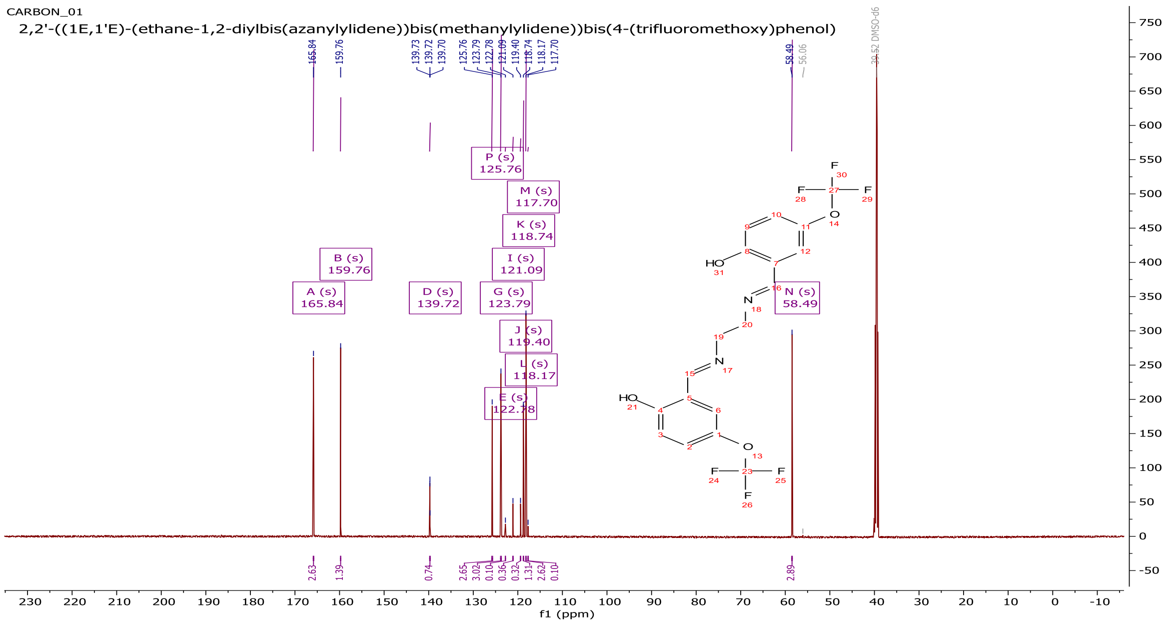


Figure S4-2. ^{13}C NMR for OCF_3/OCF_3 (Unreduced)

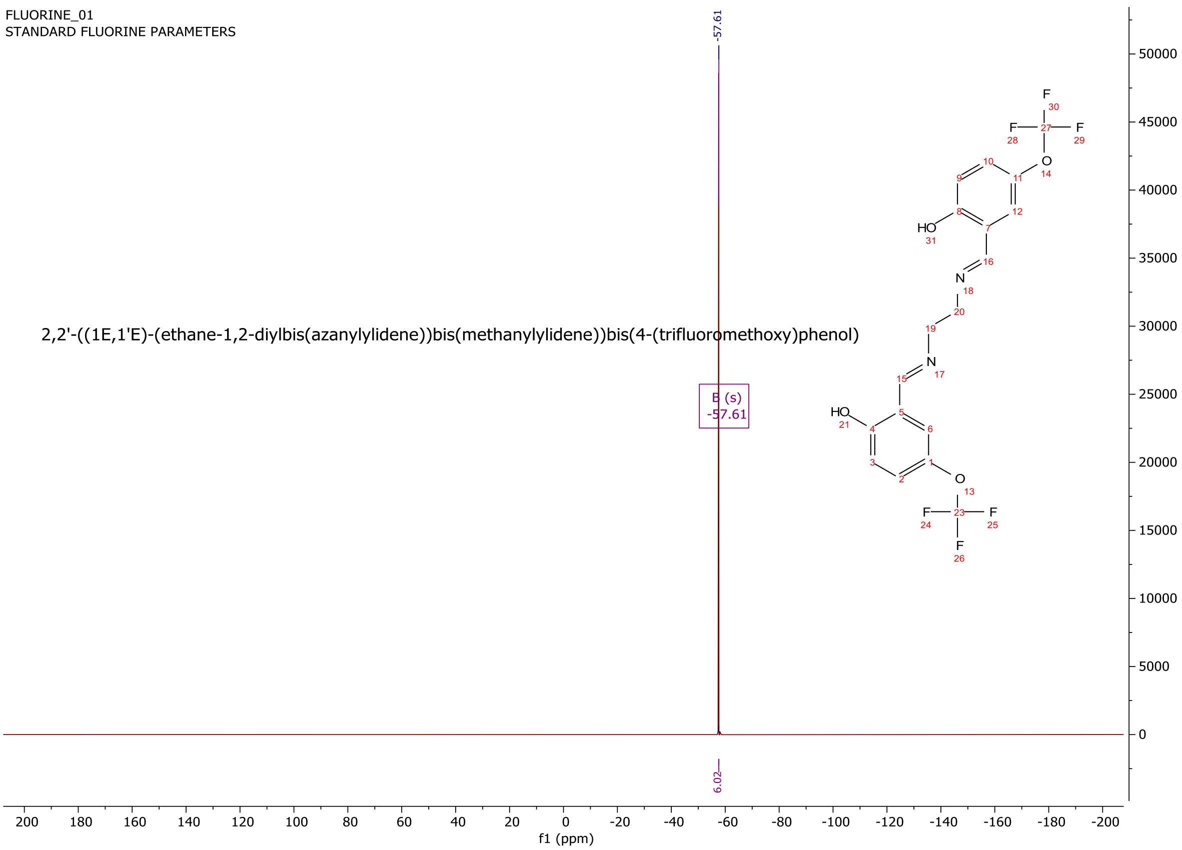


Figure S4-3. ^{19}F NMR for OCF_3/OCF_3 (Unreduced)

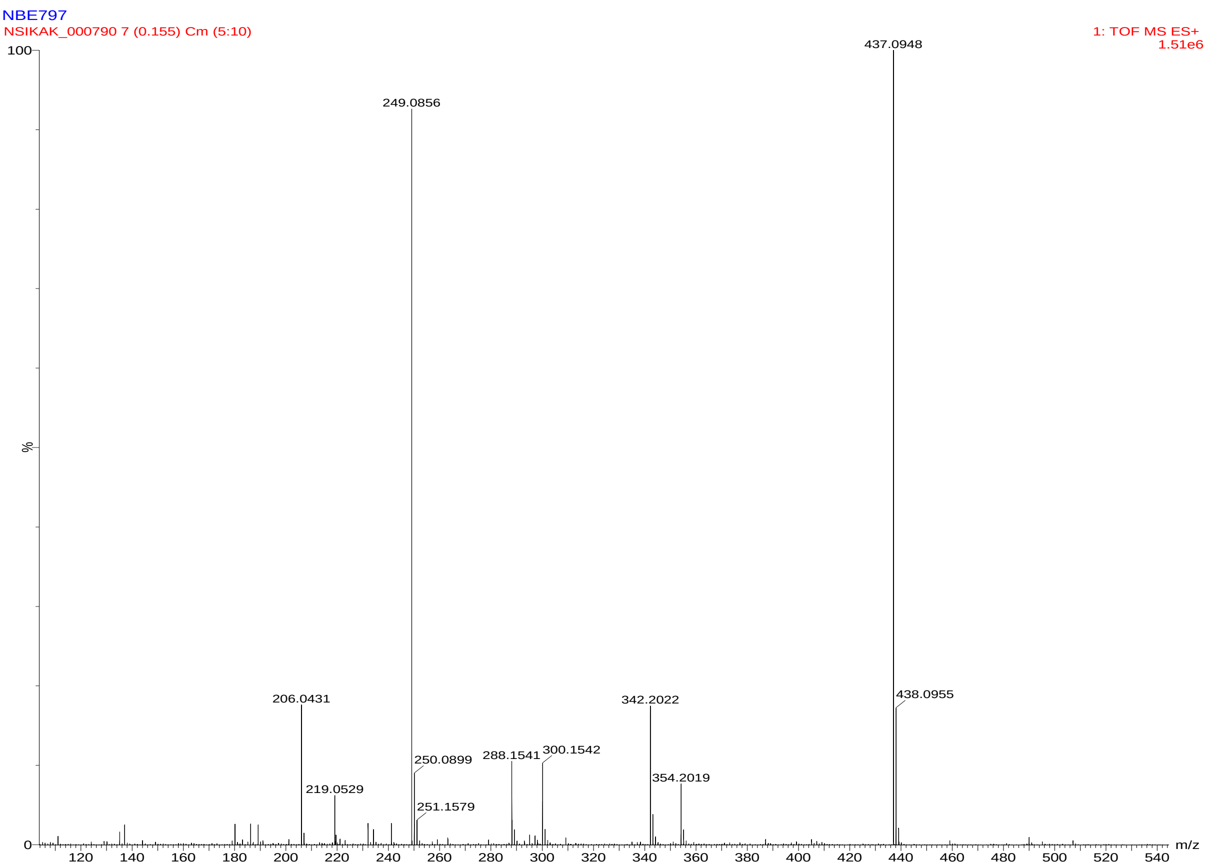


Figure S4-4. TOF MS ES+ for OCF_3/OCF_3 (Unreduced)

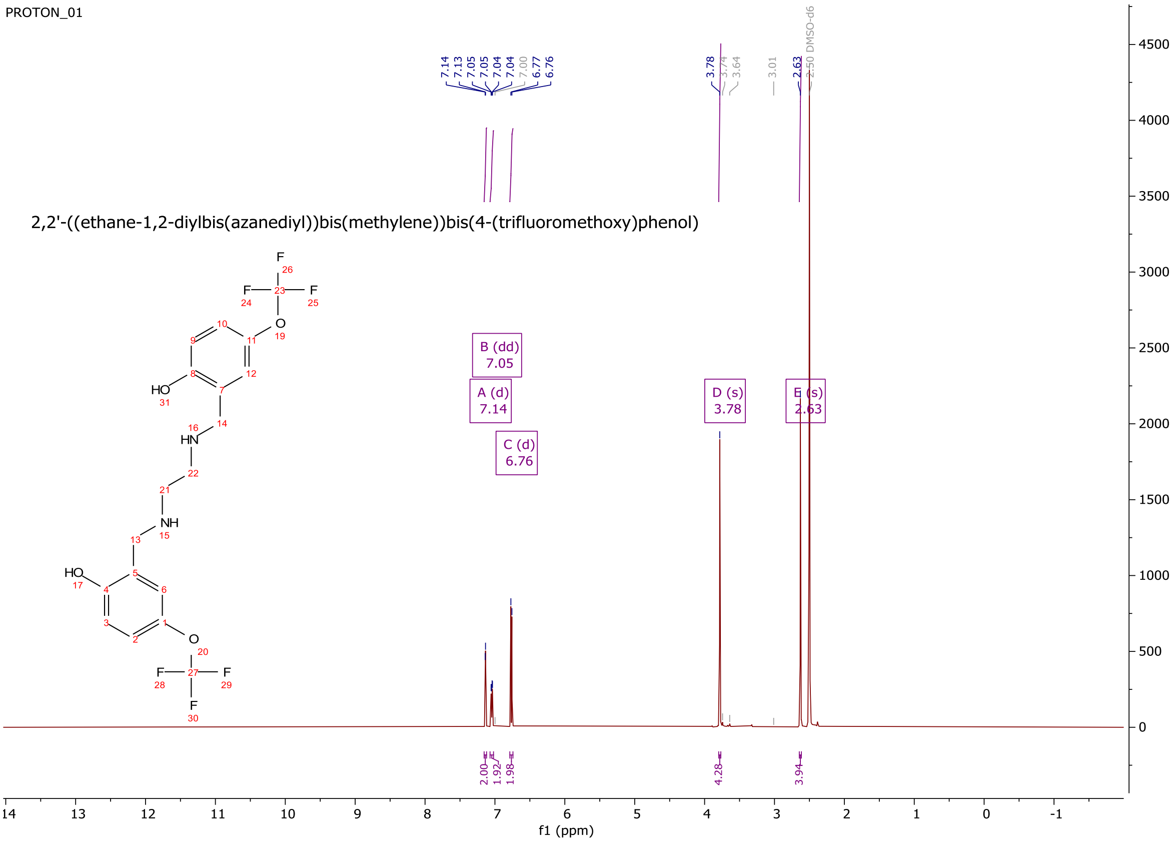


Figure S4-5. [1]H NMR for OCF_3/OCF_3

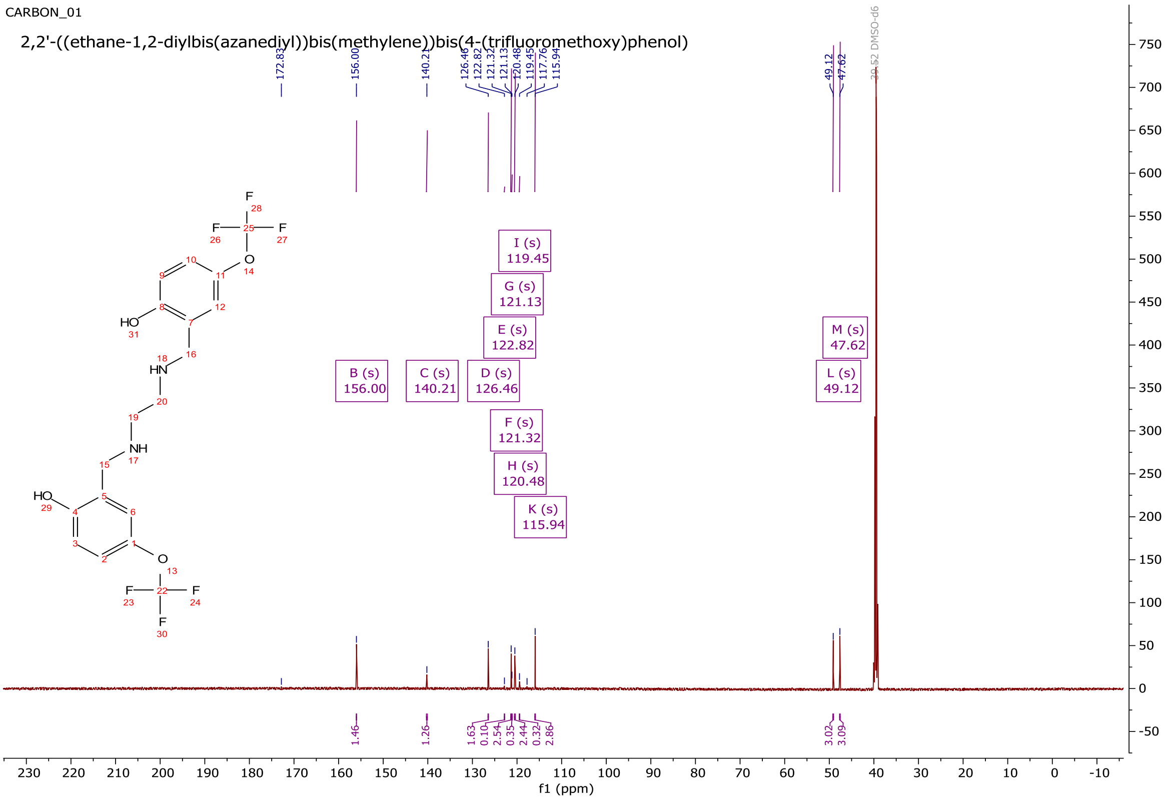


Figure S4-6. [13]C NMR for OCF_3/OCF_3

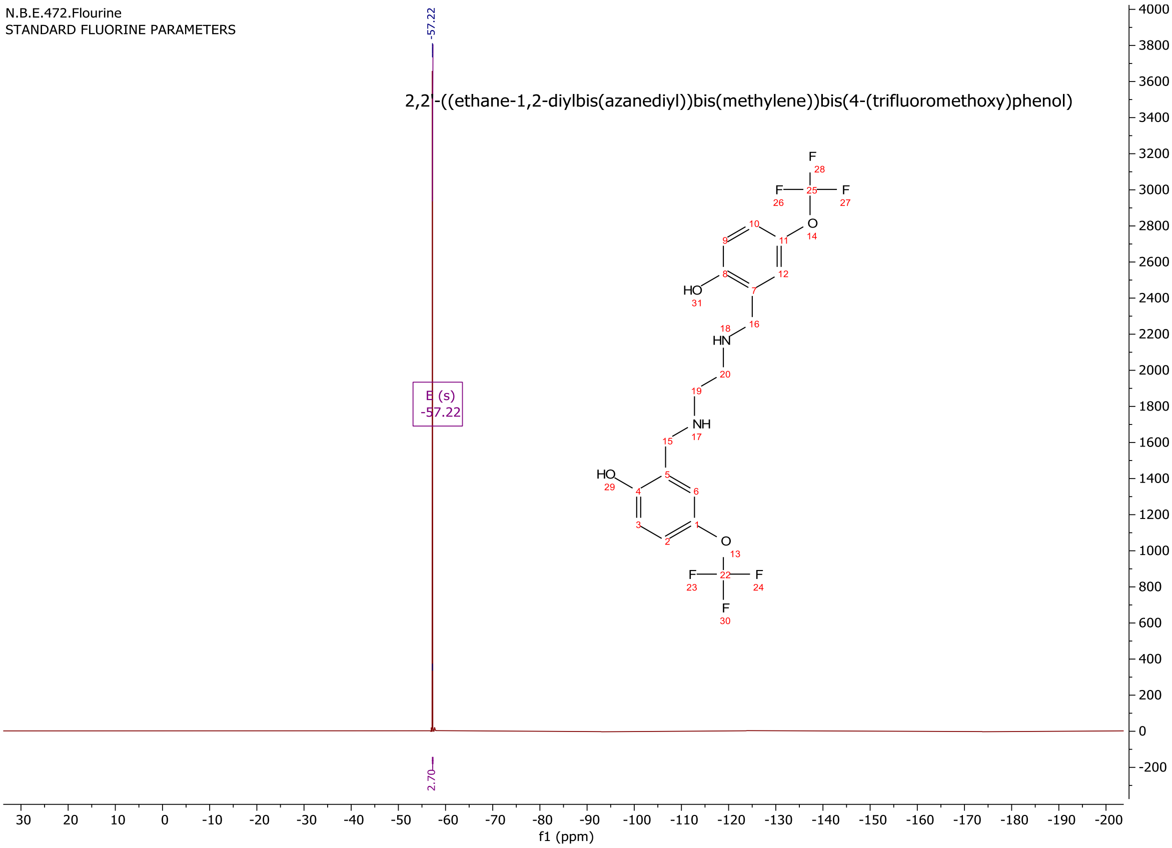


Figure S4-7. ^{19}F NMR for OCF_3/OCF_3

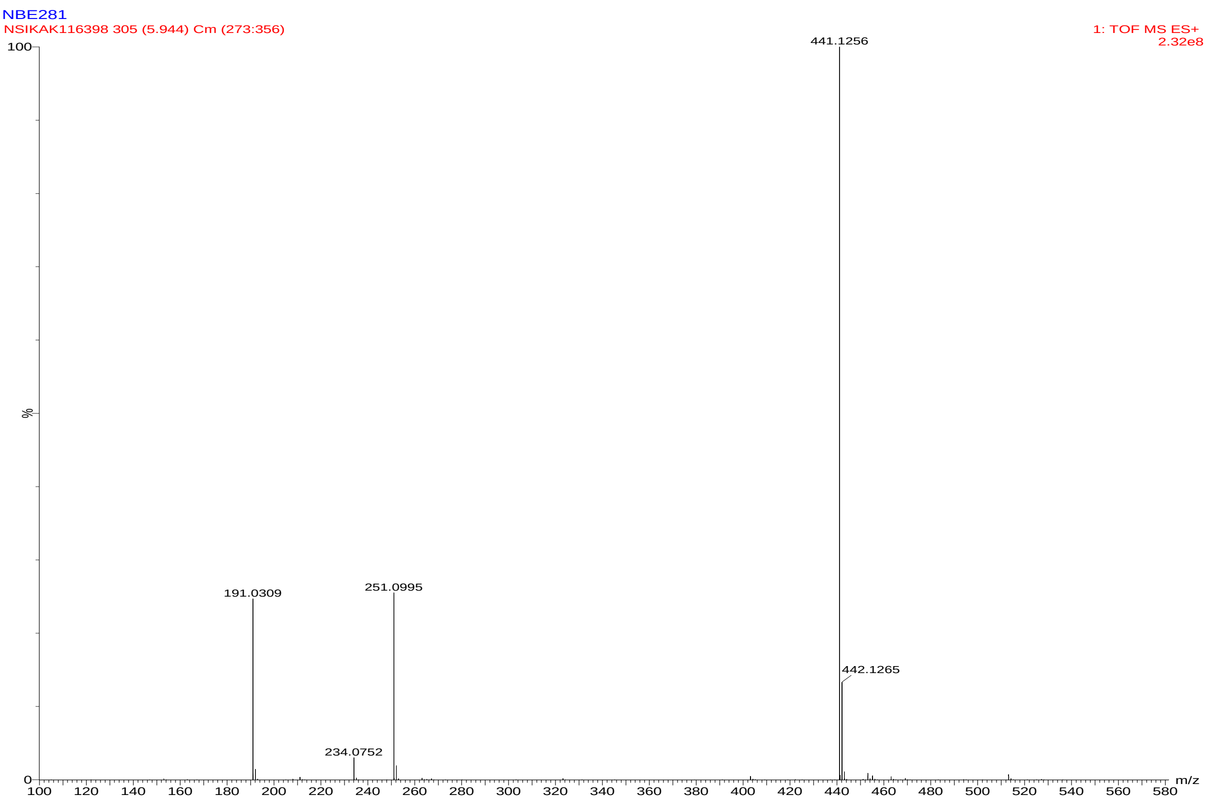


Figure S4-8. TOF MS ES+ for OCF_3/OCF_3

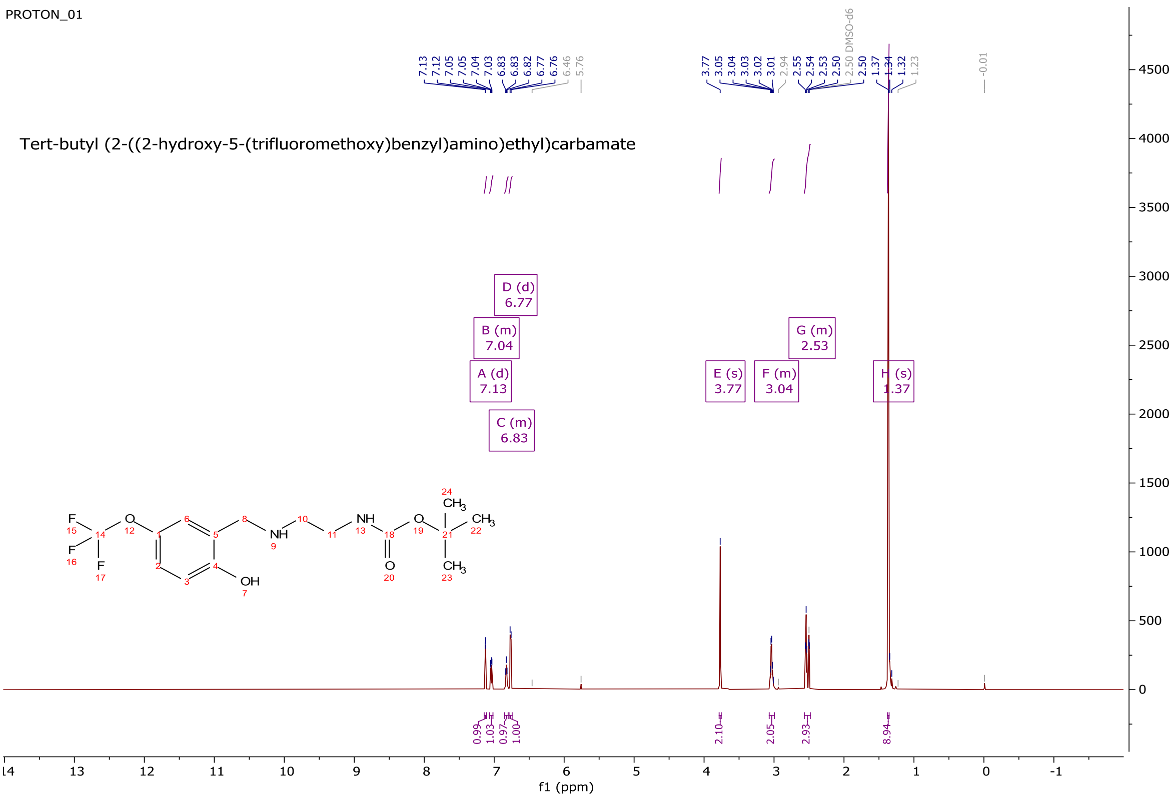


Figure S4-9. ^{1}H NMR for Half protected unit

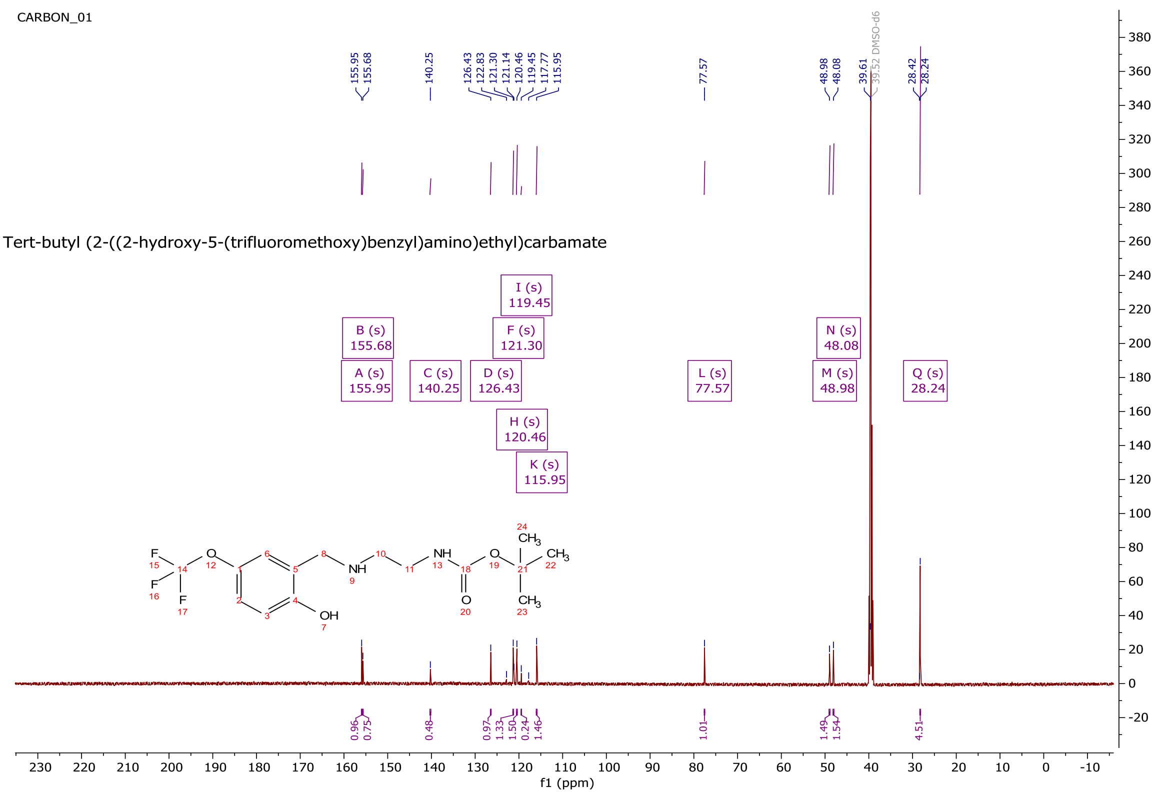


Figure S4-10. ^{13}C NMR for Half protected unit

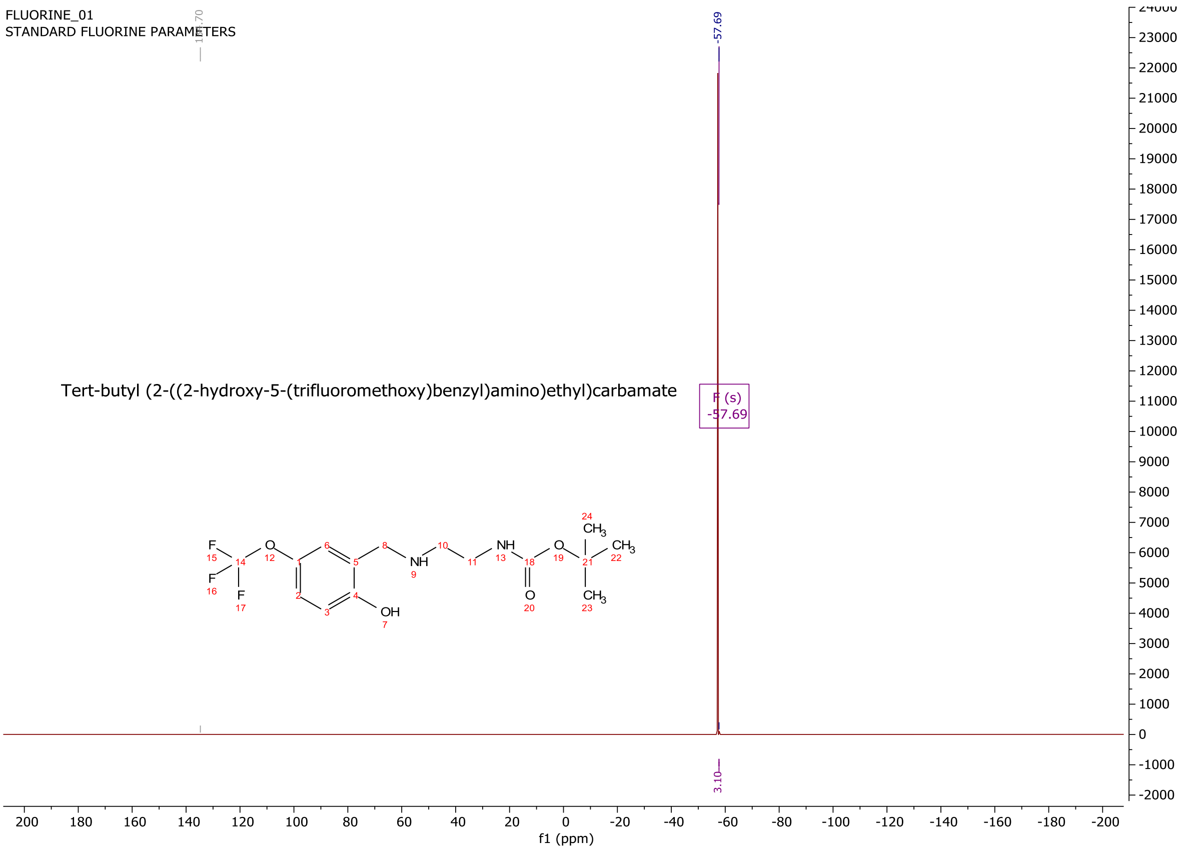


Figure S4-11. ^{19}F NMR for Half protected unit

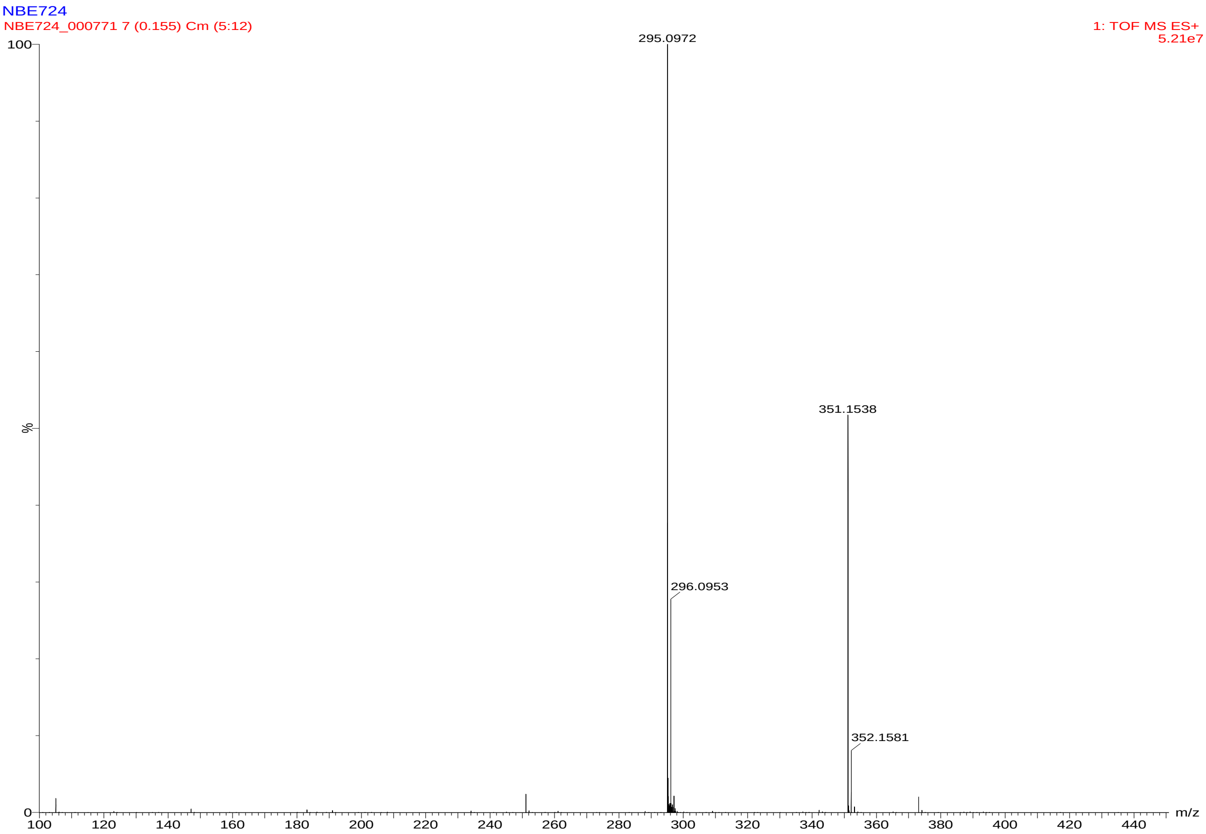


Figure S4-12. TOF MS ES+ for Half protected unit

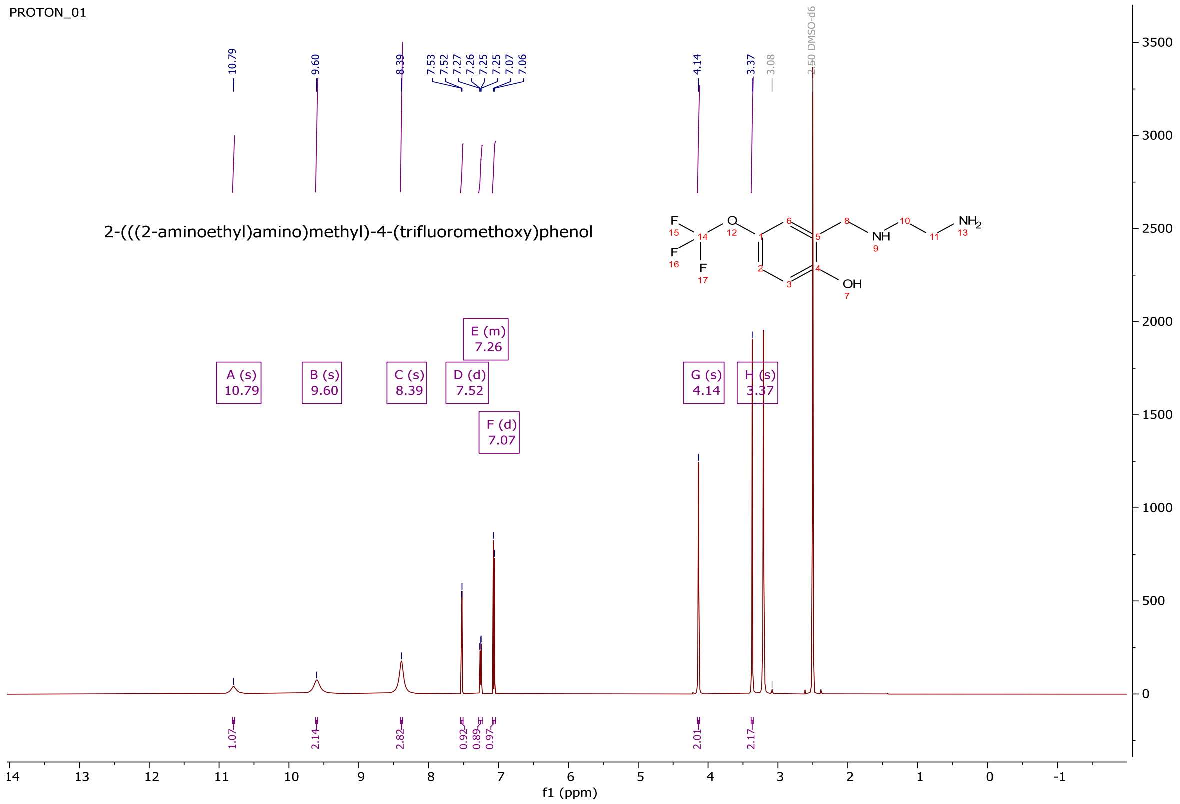


Figure S4-13. ^{1}H NMR for Half unit

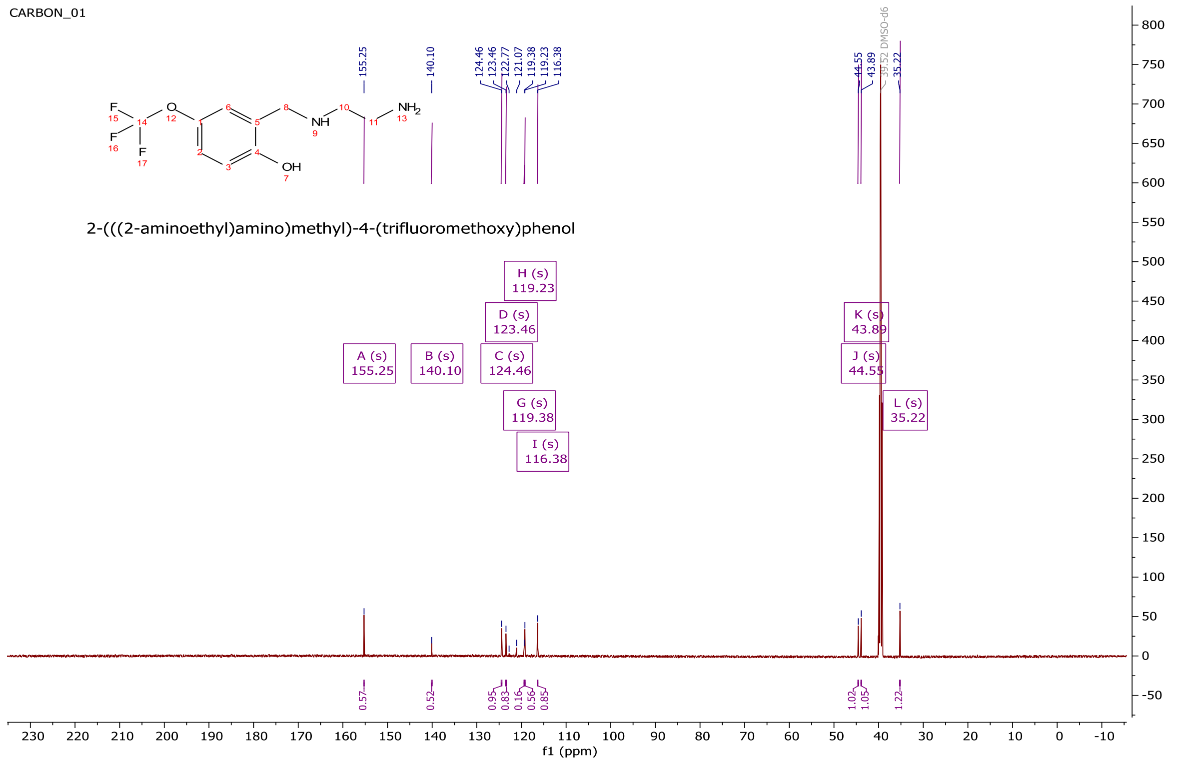


Figure S4-14. ^{13}C NMR for Half unit

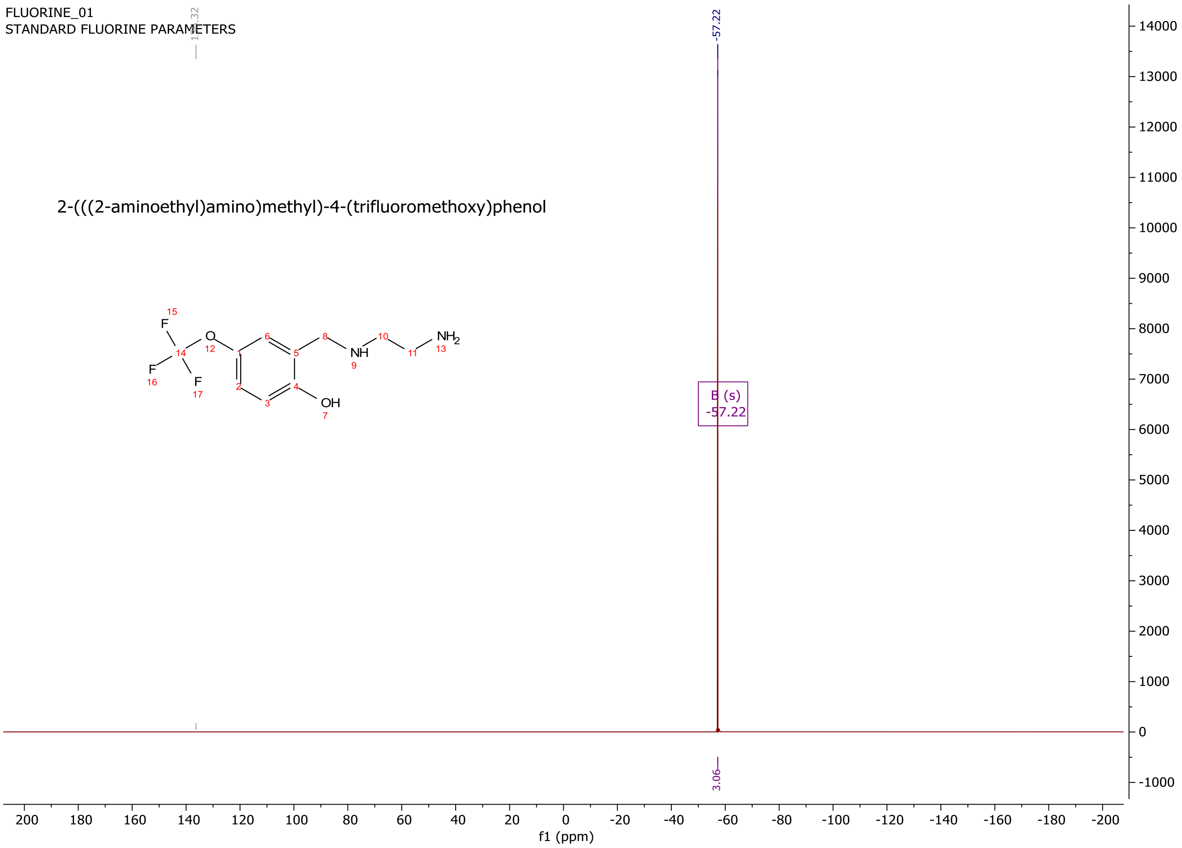


Figure S4-15. ^{19}F NMR for Half unit

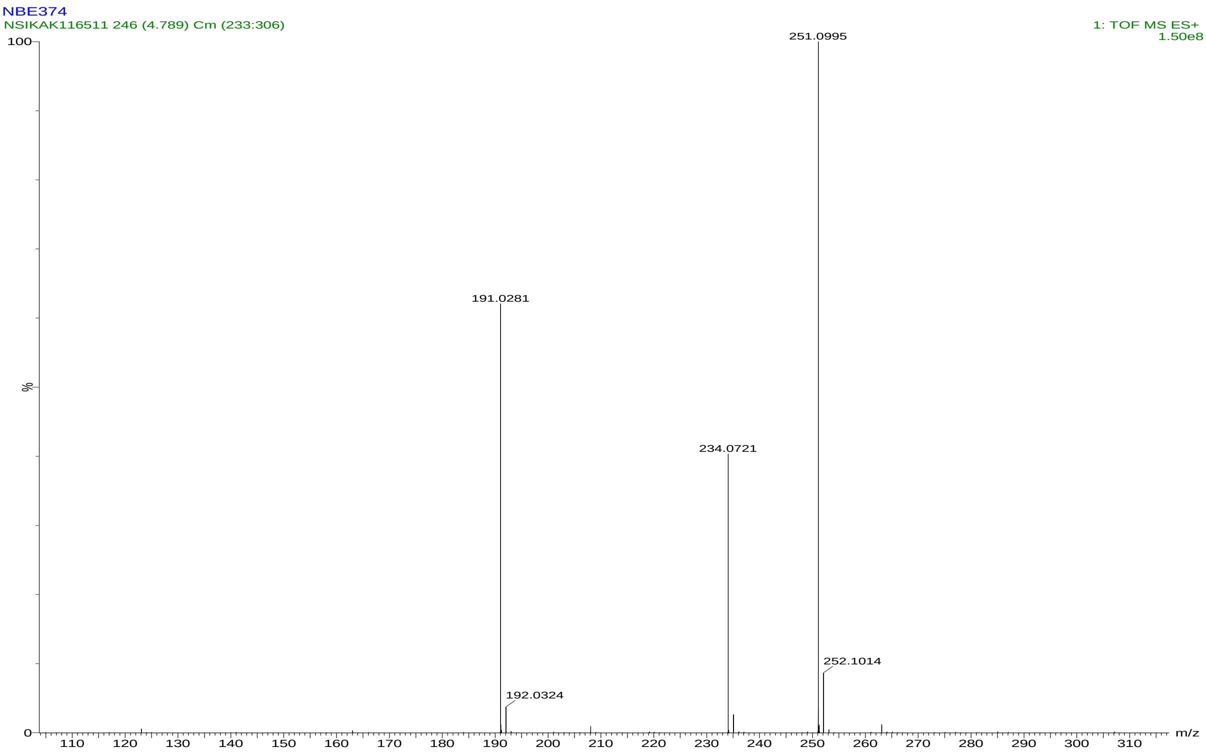


Figure S4-16. TOF MS ES+ for Half unit

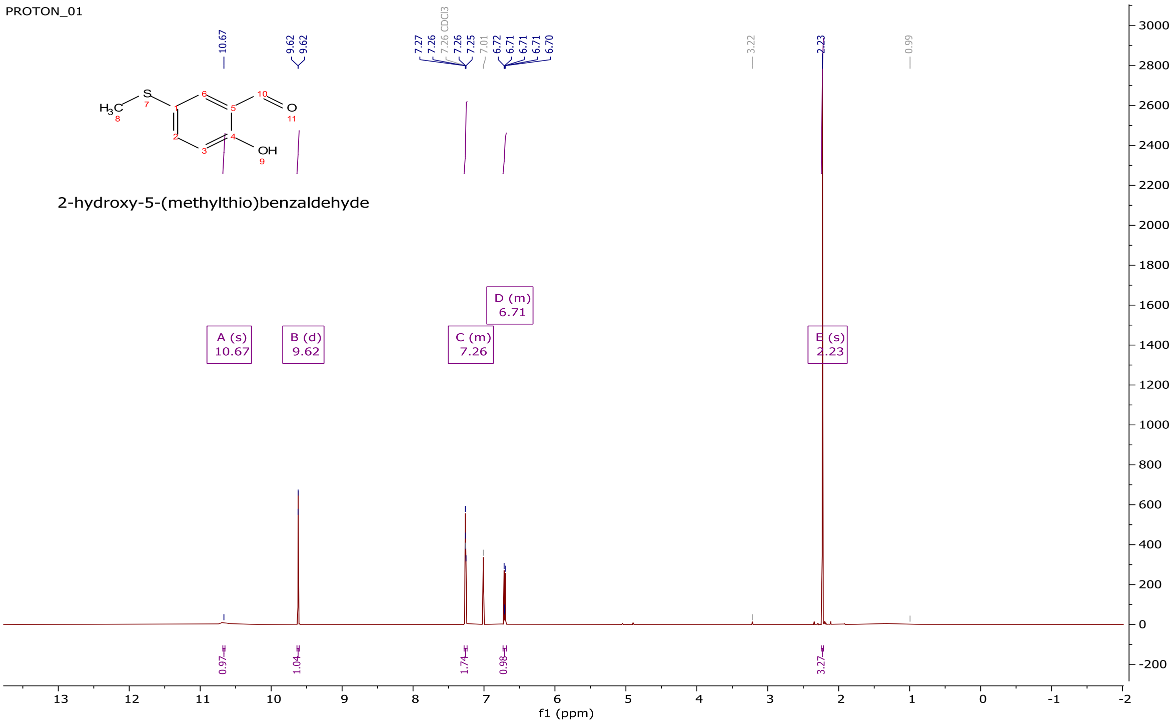


Figure S4-17. ^{1}H NMR for Half thiol Unit

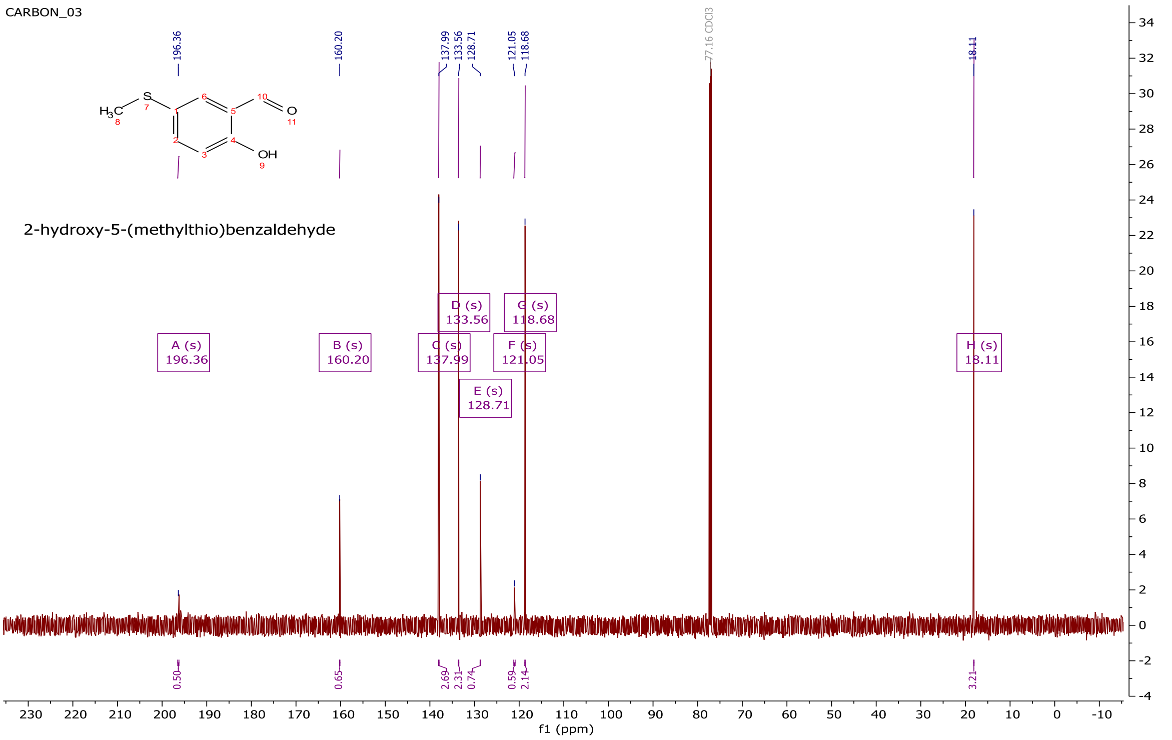


Figure S4-18. ^{13}C NMR for Half thiol unit

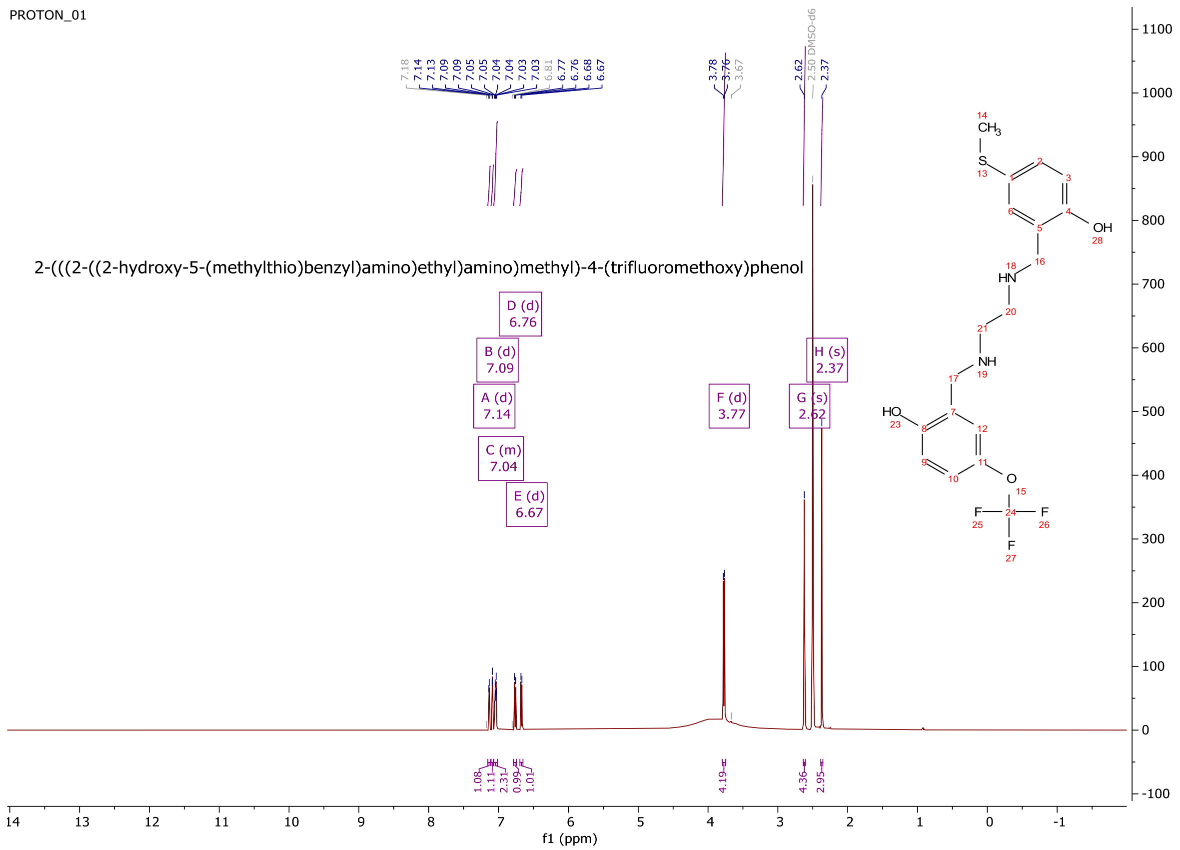


Figure S4-19. ^{1}H NMR OCF_3/SCH_3

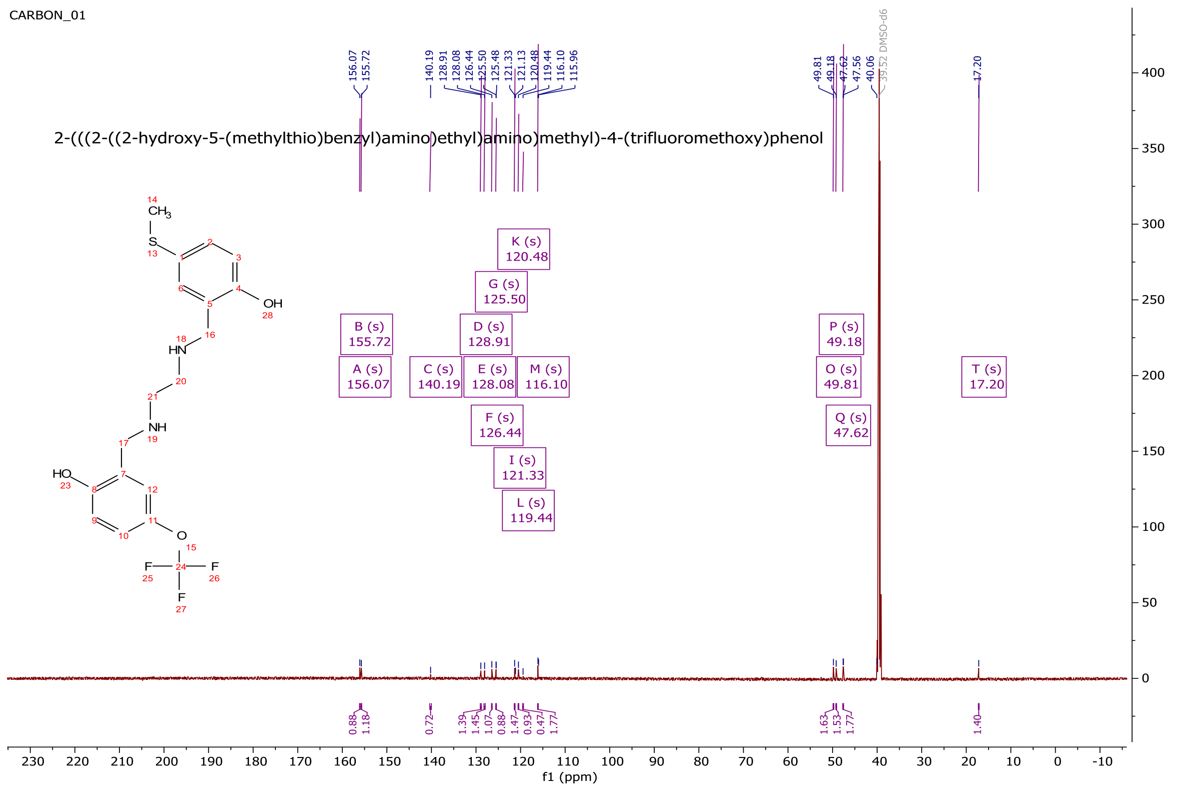


Figure S4-20. ^{13}C NMR for OCF_3/SCH_3

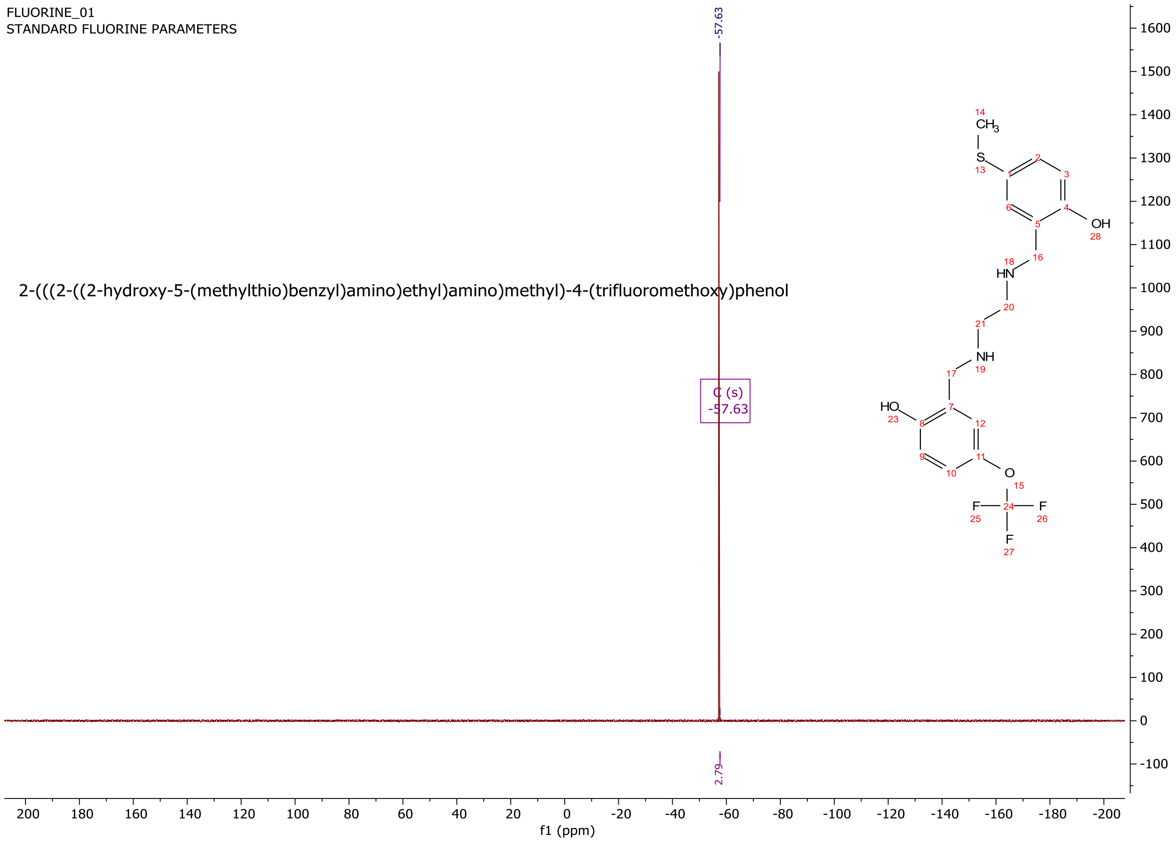


Figure S4-21. ^{19}F NMR for OCF_3/SCH_3

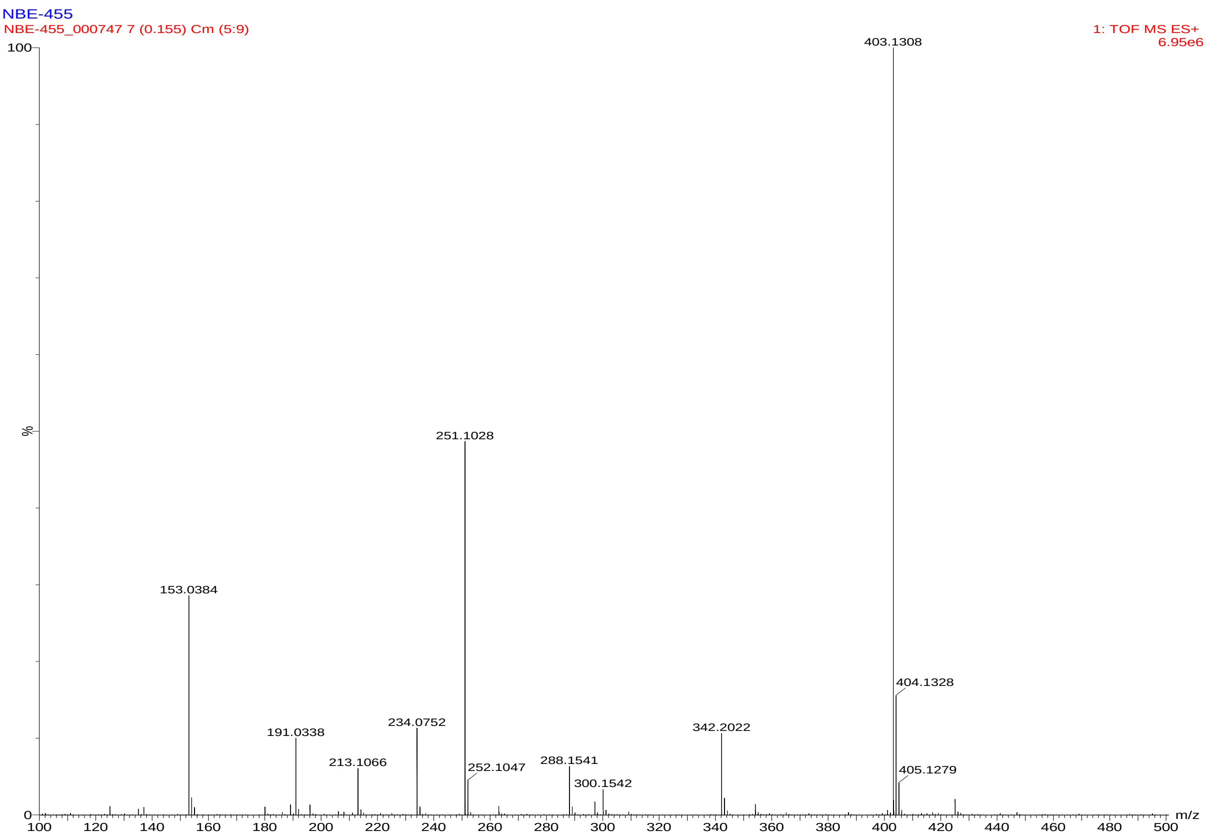


Figure S4-22. TOF MS ES+ for OCF_3/SCH_3

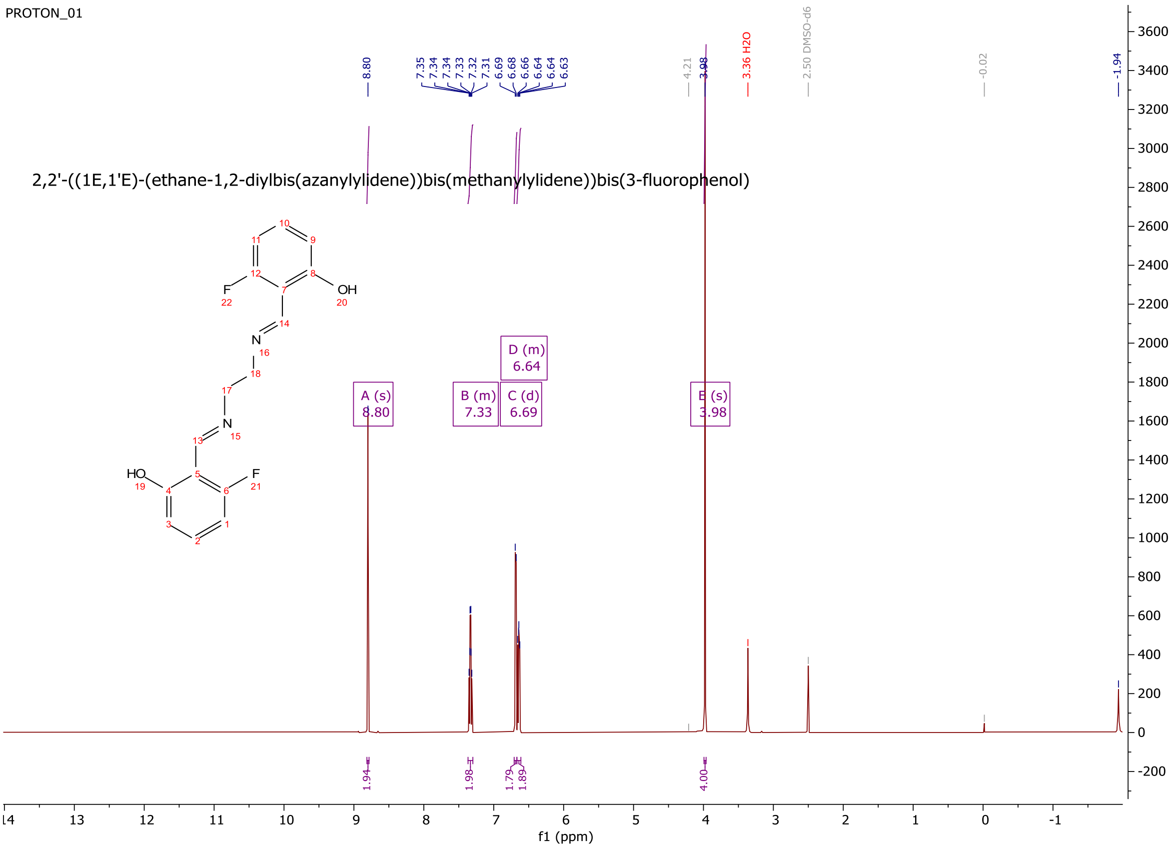


Figure S4-23. ^{1}H NMR for F/F (Unreduced)

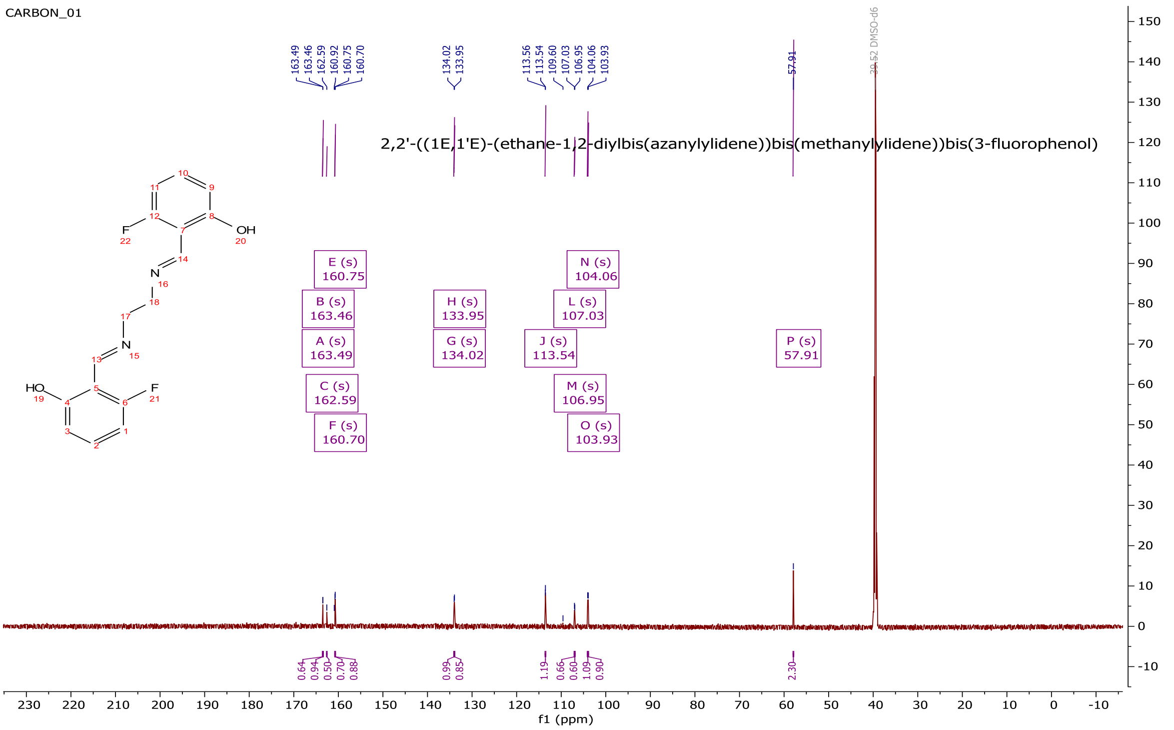


Figure S4-24. ^{13}C NMR for F/F (Unreduced)

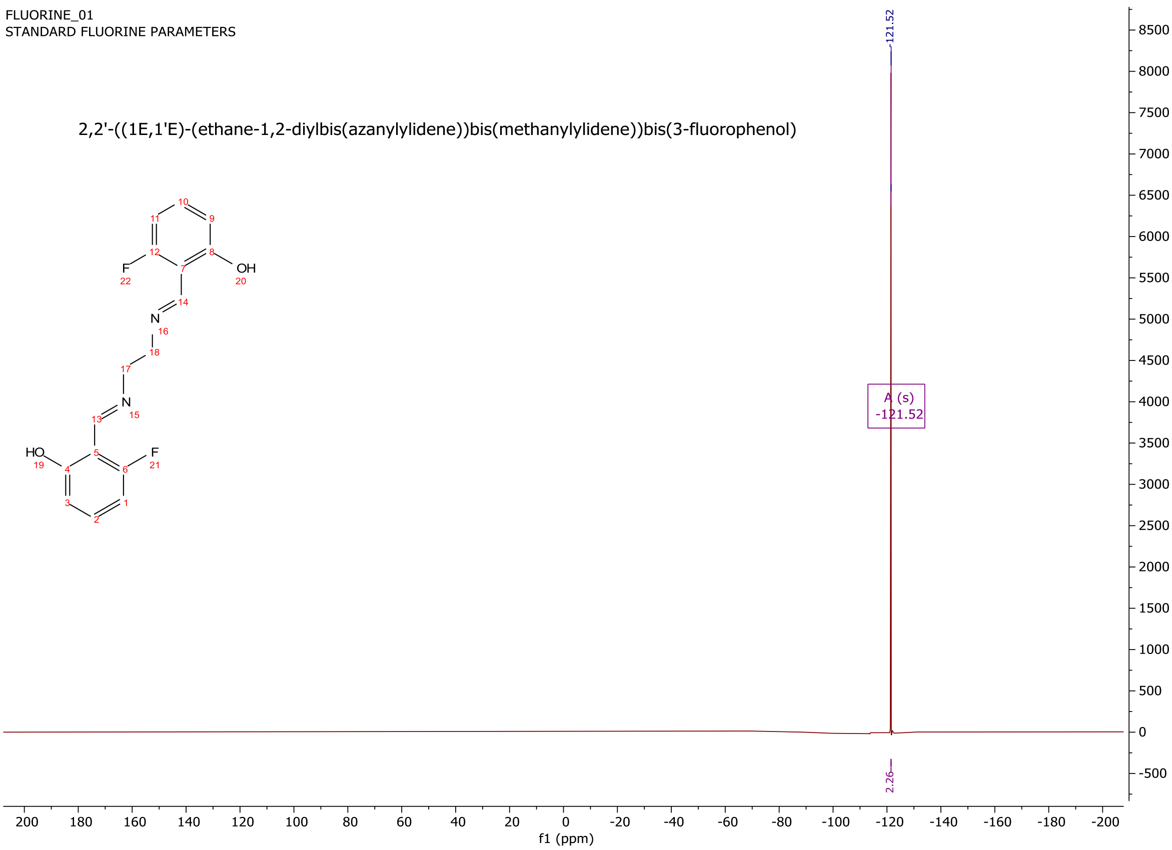


Figure S4-25. ^{19}F NMR for F/F (Unreduced)

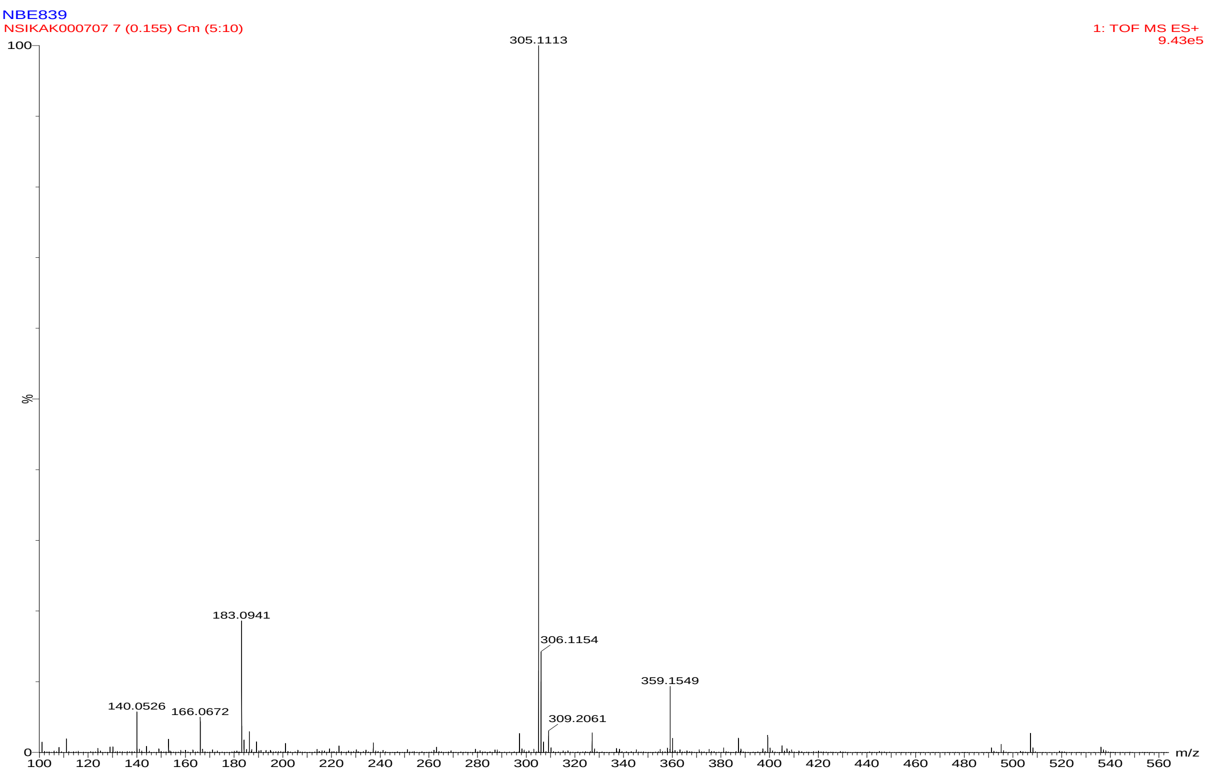


Figure S4-26. TOF MS ES+ for F/F (Unreduced)

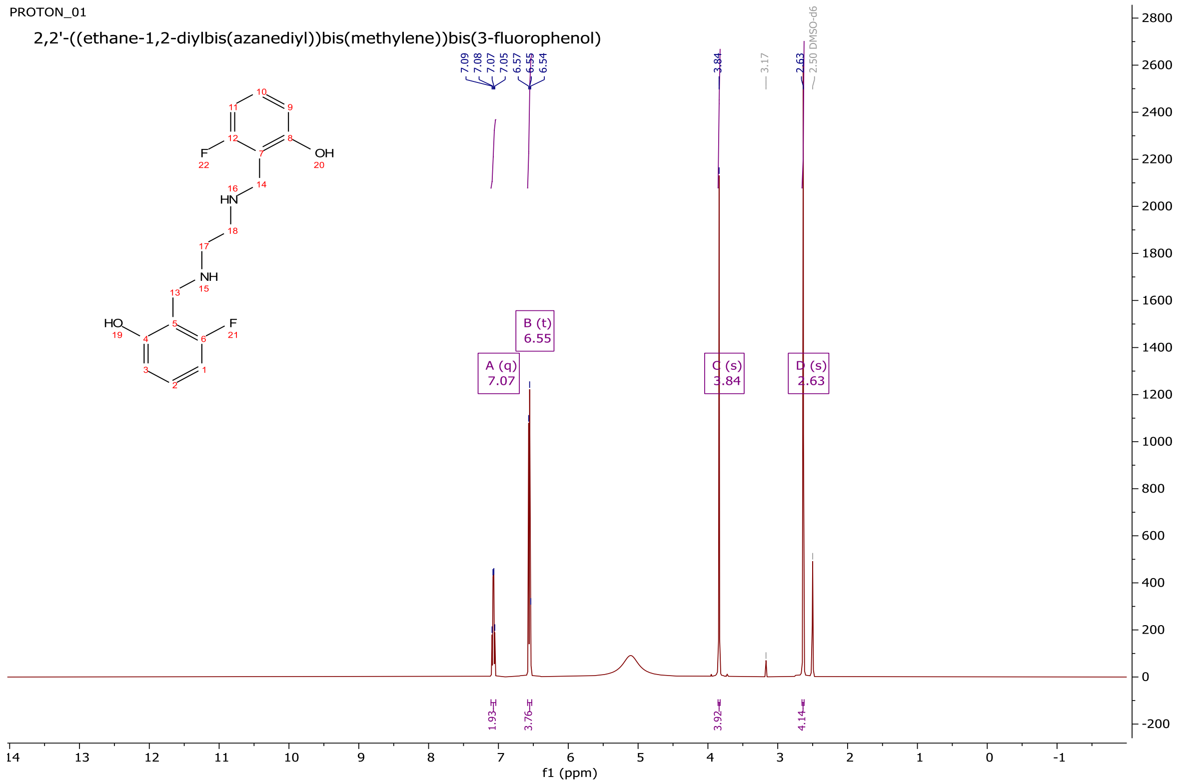


Figure S4-27. ^{1}H NMR for F/F

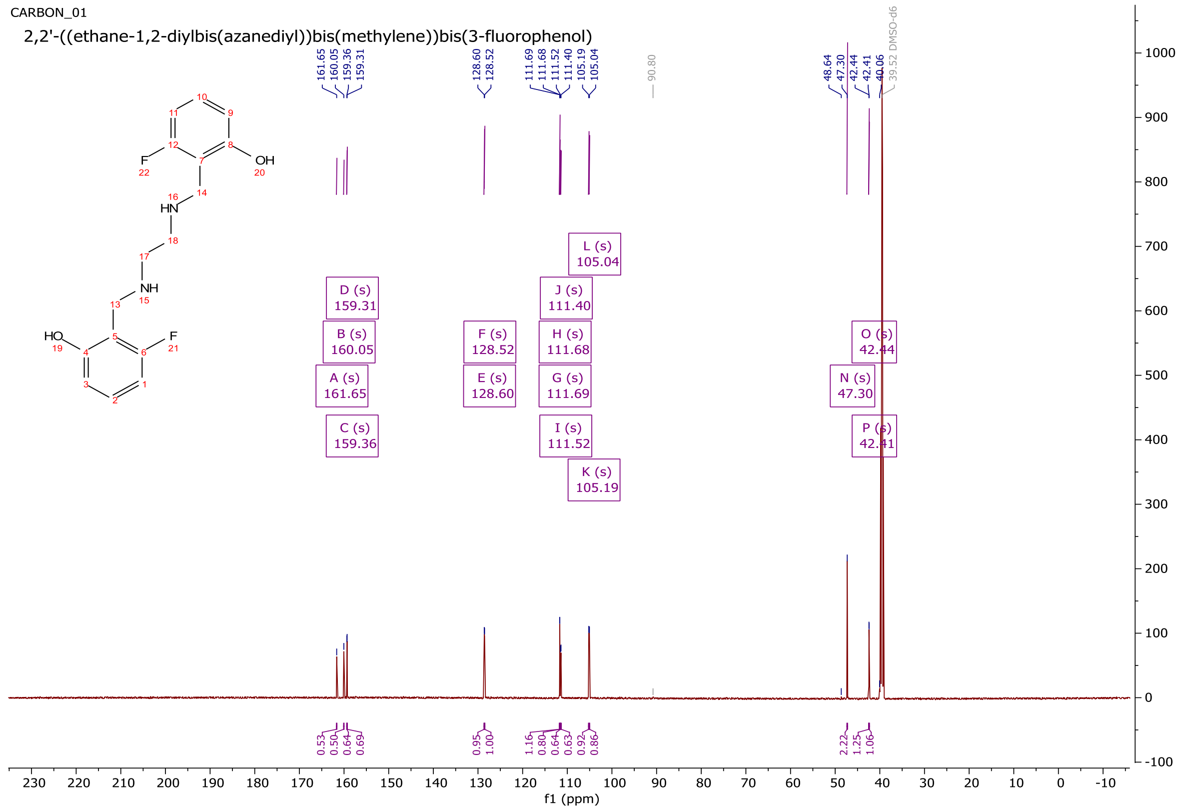


Figure S4-28. ^{13}C NMR for F/F

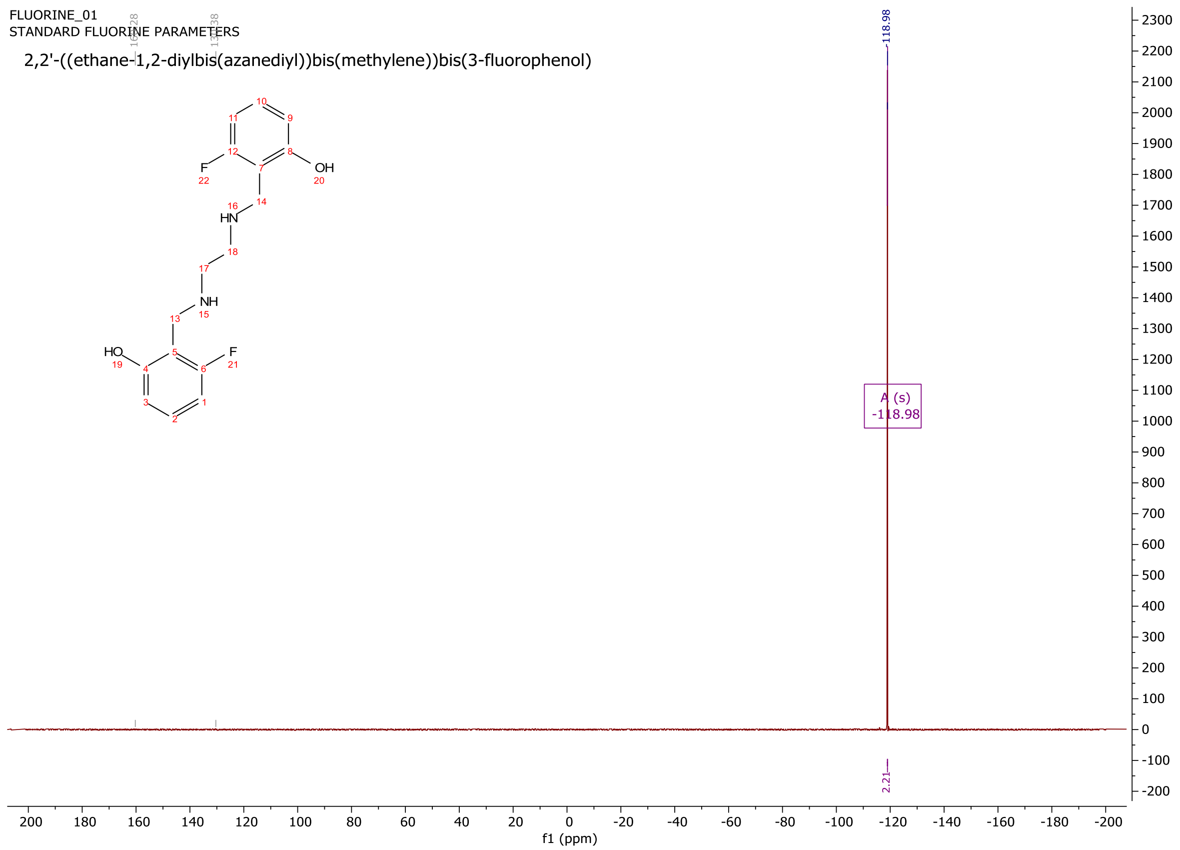


Figure S4-29. ^{19}F NMR for F/F

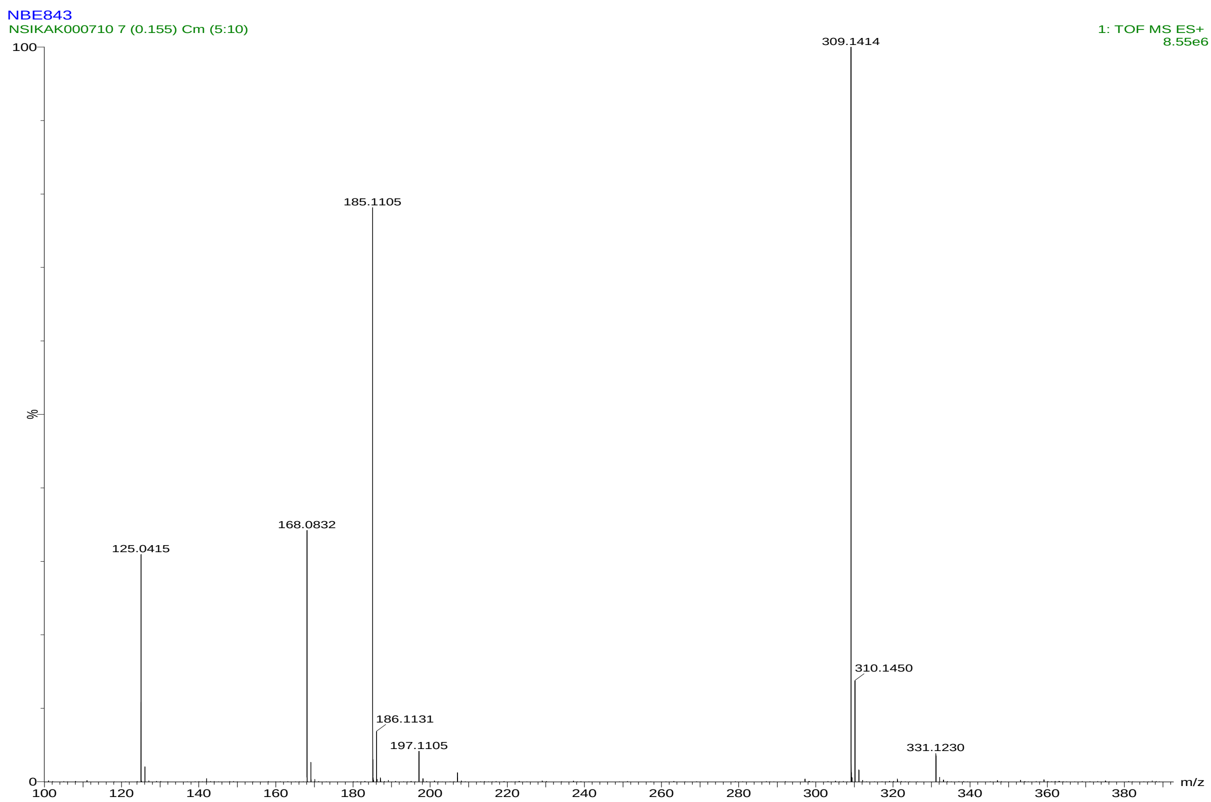


Figure S4-30. TOF MS ES+ for F/F

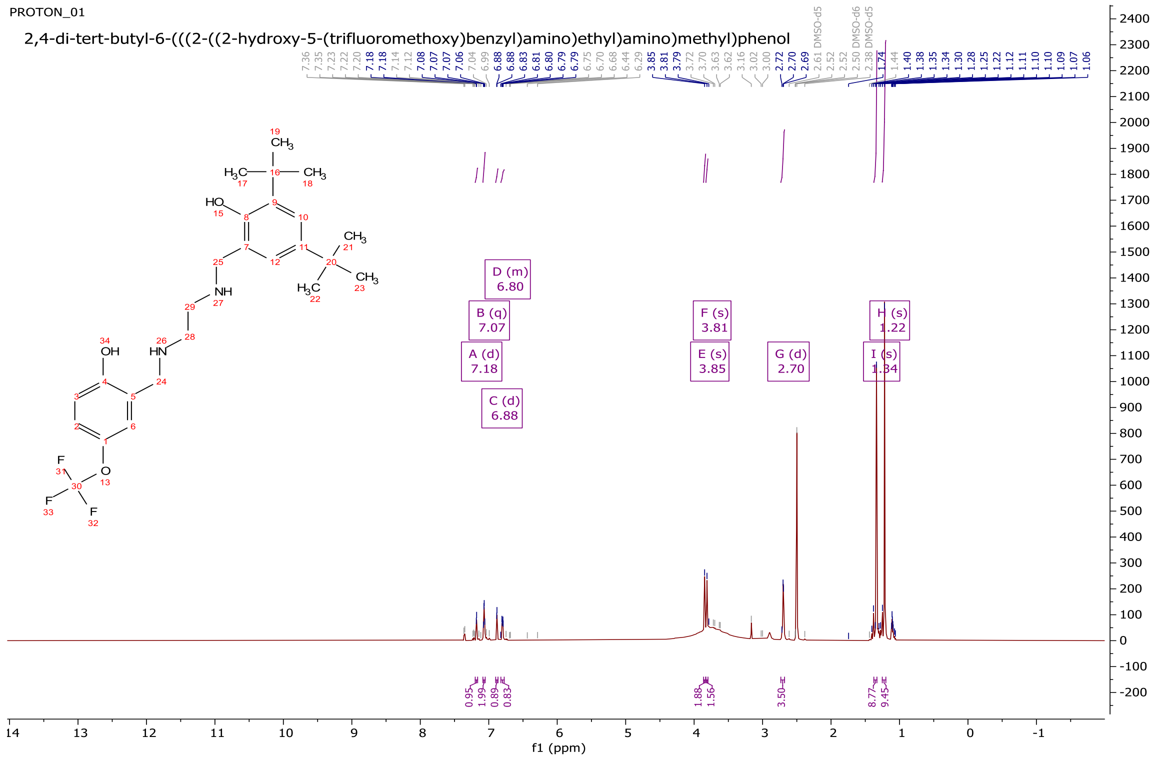


Figure S4-31. ^{1}H NMR for Bis-tert-OCF_3

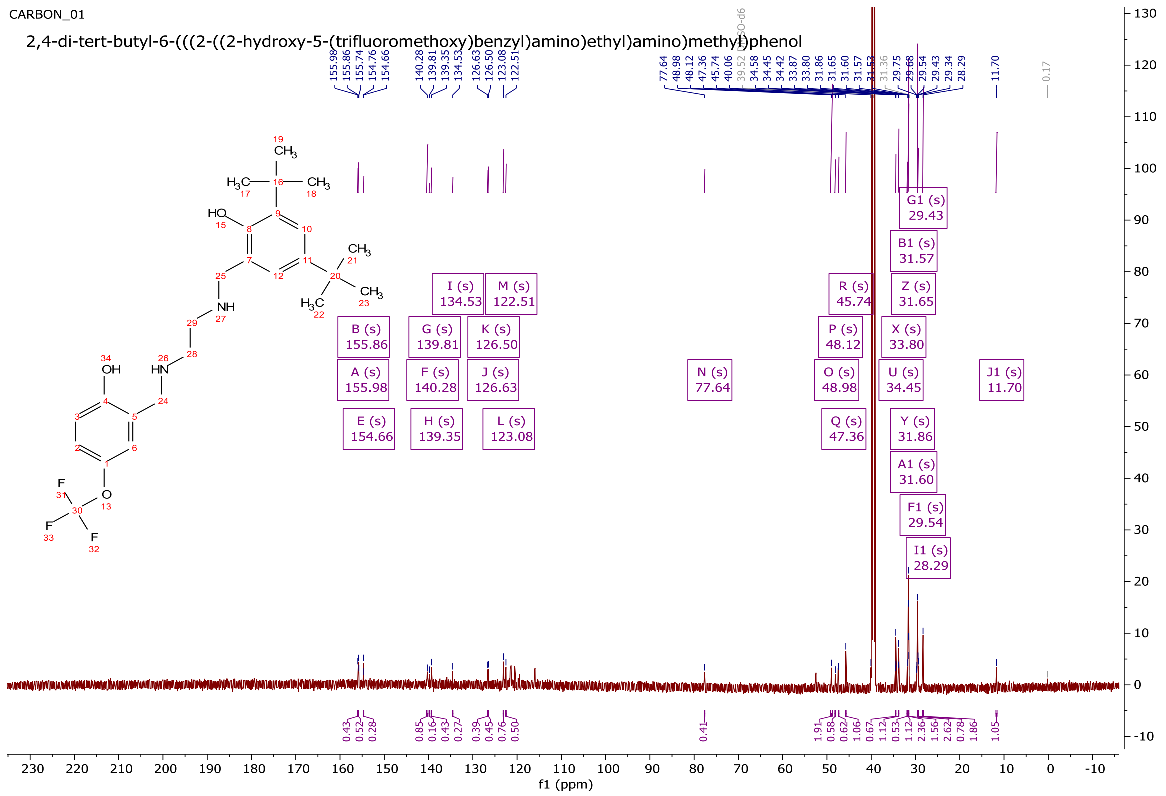


Figure S4-32. ^{13}C NMR Bis-tert-OCF_3

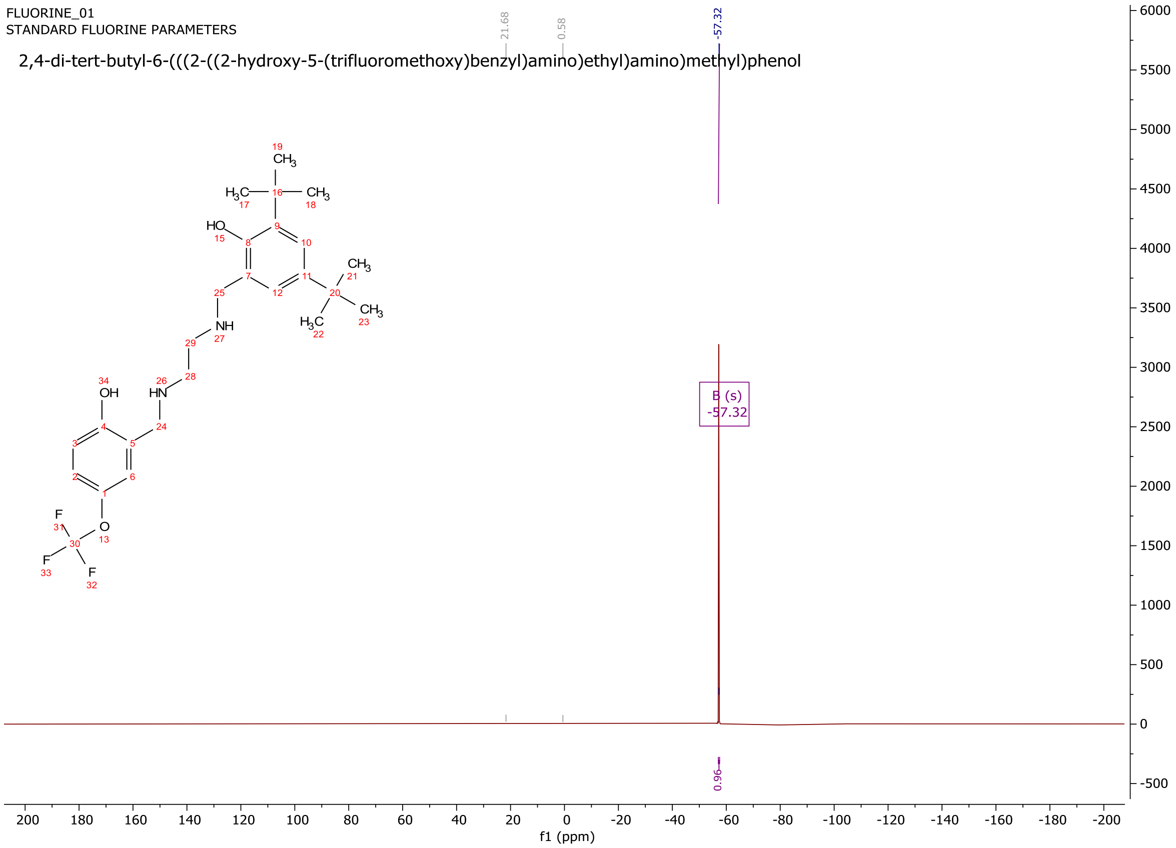


Figure S4-33. ^{19}F NMR for Bis-tert-OCF_3

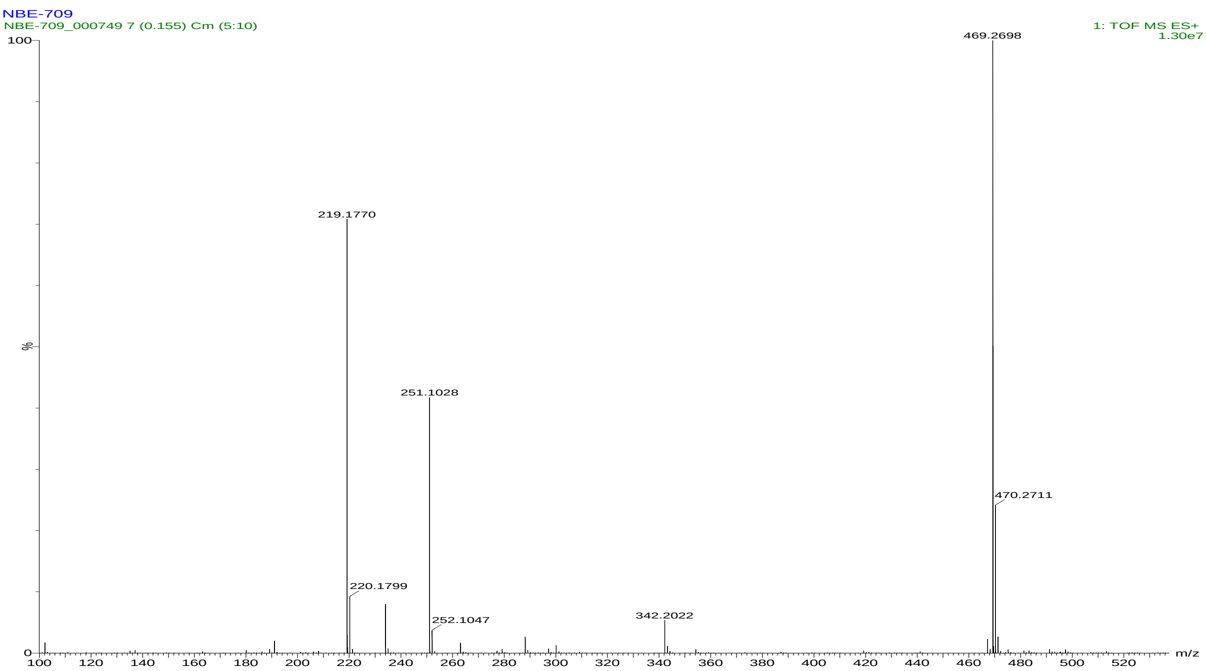


Figure S4-34. TOF MS ES+ for Bis-tert-OCF_3

Table S4-1. Selected Bond distances for all complexes and trigonality index

	Zn-O1	Zn-O2	Zn-O3	Zn-N1	Zn-N2	Trigonality index (τ)[24]
Set A	2.0207(19)	2.1131(18)	1.958(2)	2.092(2)	2.195(2)	0.17
Set B	1.986(3)	2.057(3)	2.029(2)	2.144(3)	2.118(3)	0.30
	1.981(2)	2.049(3)	2.033(2)	2.145(3)	2.109(3)	0.28
Set C	N/A	N/A	N/A	N/A	N/A	N/A
Set D	2.0026(17)	2.0918(16)	1.9701(16)	2.151(2)	2.146(2)	0.64
Set E	2.1102(19)	2.0309(19)	1.956(2)	2.080(2)	2.187(2)	0.33

Trigonality index indicates the geometry of the coordination center.[24] When τ = 0 the geometry corresponds to square pyramidal, when τ= 1 corresponds to trigonal bipyramidal.

Thermogravimetric analysis.

Thermogravimetric analysis to determine the thermal stability of the zinc complex were measure by George Kostakis in University of Sussex and results is illustrated in the figure below.

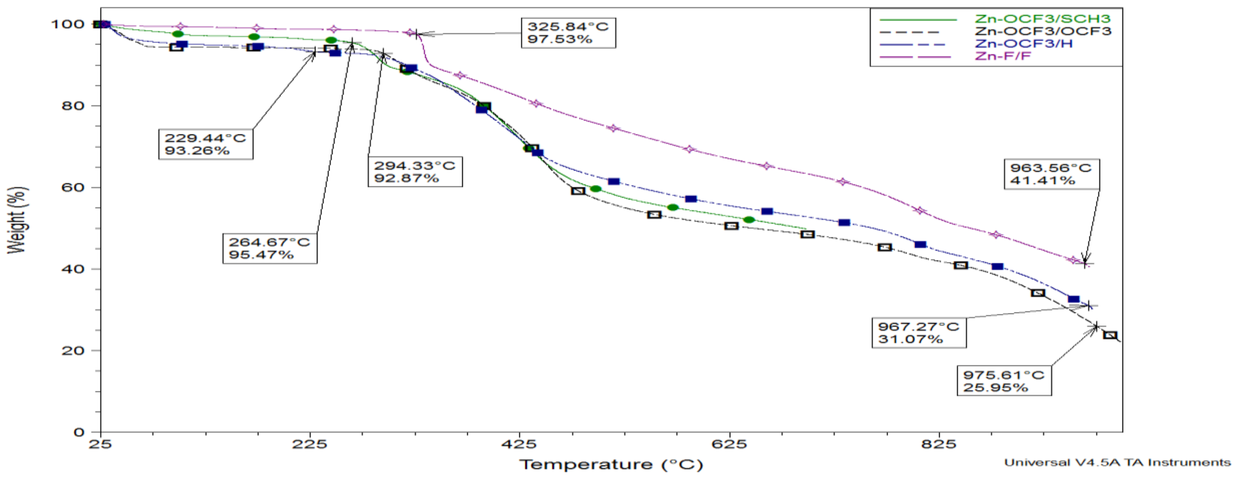


Figure S4-35: Showing Thermogravimetric analysis of the Zinc complexes

ESI-MS

Set A

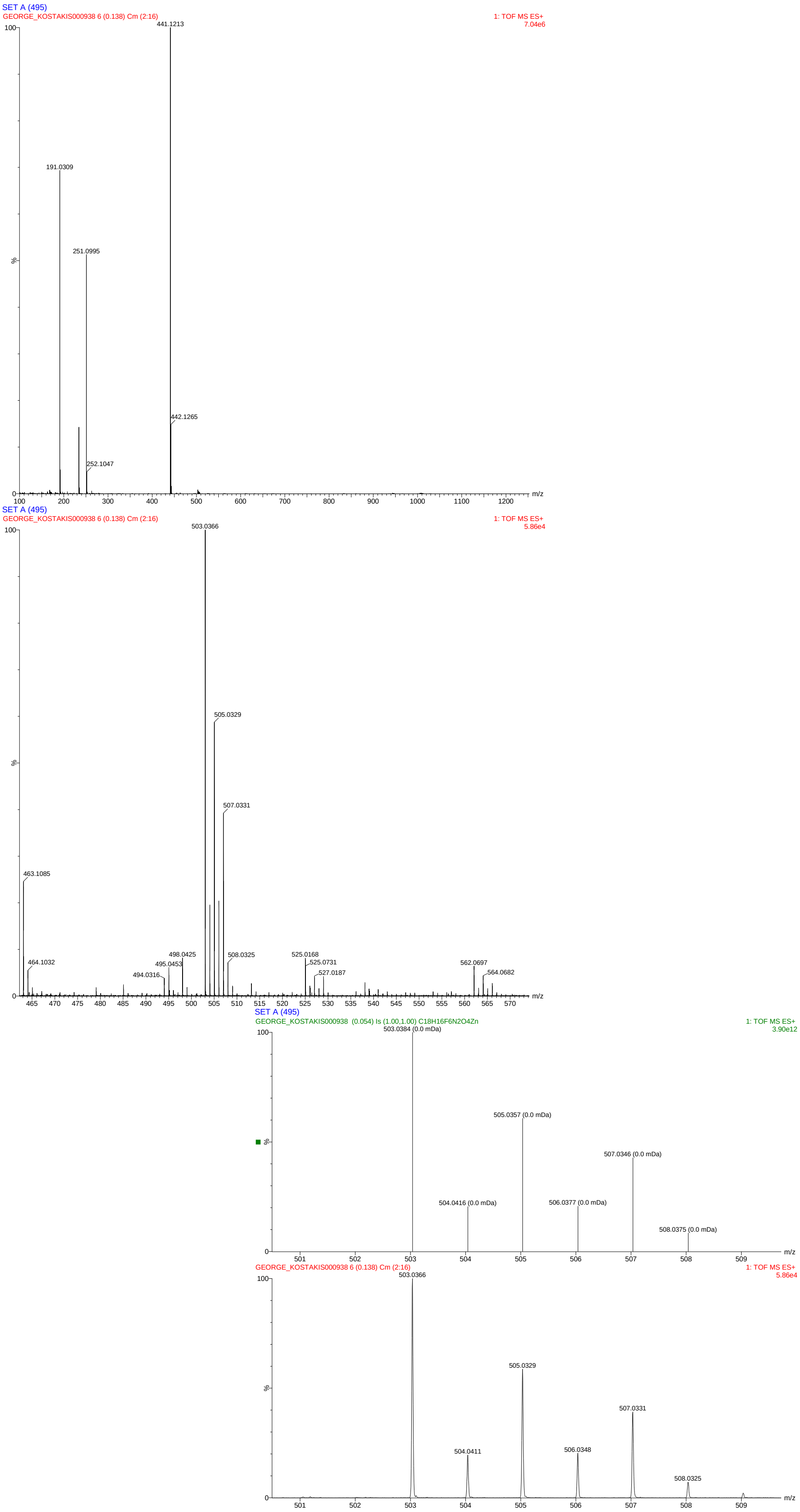
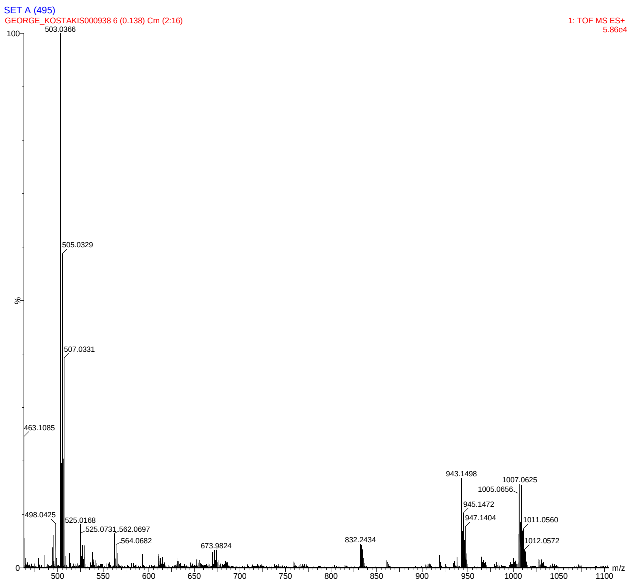


Figure S4-36. Showing ESI-MS of Zinc complexes for set A

Elemental Composition Report
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 18-18 H: 0-100 N: 2-2 O: 4-4 F: 6-6 Zn: 1-1

Minimum:			-25.0					
Maximum:	5.0	1000.0		100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
503.0360	503.0384	-2.4	-4.8	8.5	430.8	n/a	n/a	C18 H17 N2 O4 F6 Zn

Set A



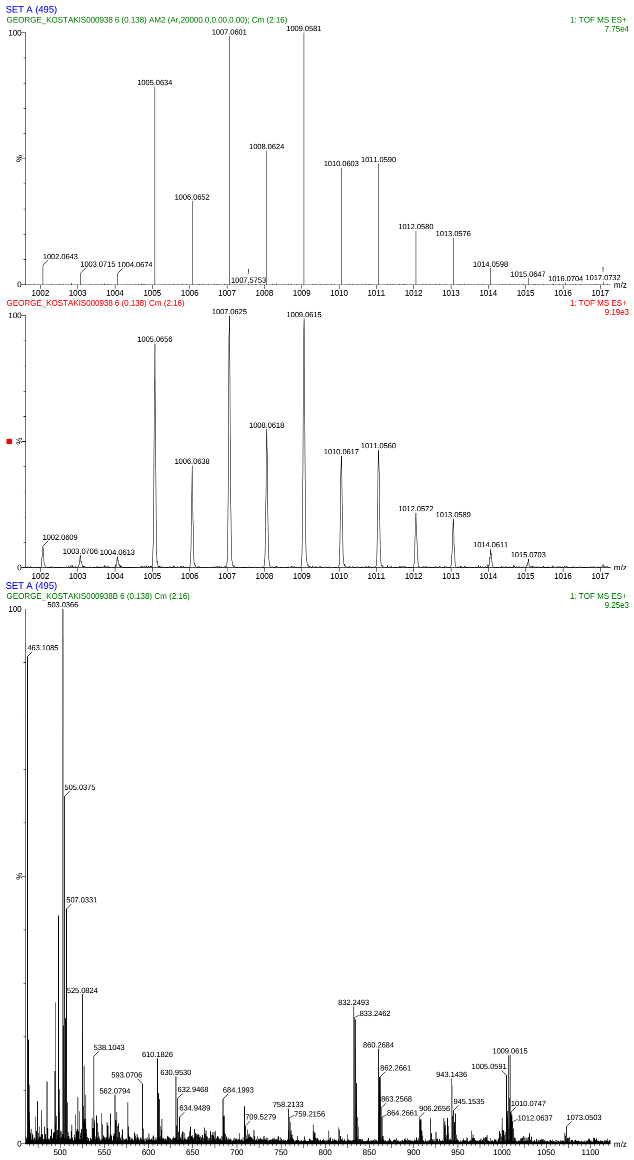


Figure S4-37. Showing ESI-MS of Zinc complexes for set A

Elemental Composition Report
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 36-36 H: 0-100 N: 4-4 O: 8-8 F: 12-12 Zn: 2-2

Minimum:				-25.0				
Maximum:		5.0	1000.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1005.0634	1005.0690	-5.6	-5.6	16.5	173.7	n/a	n/a	C36 H33 N4 O8 F12 Zn2

Set B

Same as before only very small concentrations were used to record these mass spectra, all of them (even at the lowest concentration as per the low number of counts shown) showing evidence of the dimer compounds in solution.

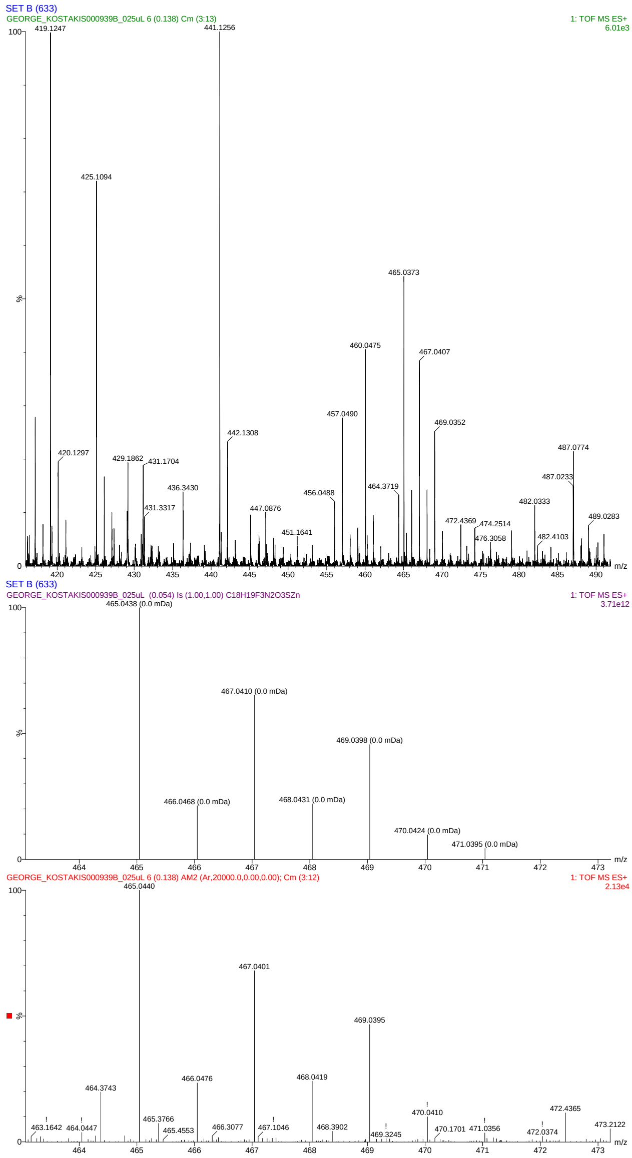


Figure S4-38. Showing ESI-MS of Zinc complexes for set B

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 18-18 H: 0-100 N: 2-2 O: 3-3 F: 3-3 S: 1-1 Zn: 1-1

Minimum:				-25.0				
Maximum:		5.0	1000.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula

465.0440 465.0438 0.2 0.4 8.5 389.2 n/a n/a C18 H20 N2 O3 F3 S Zn

Set B

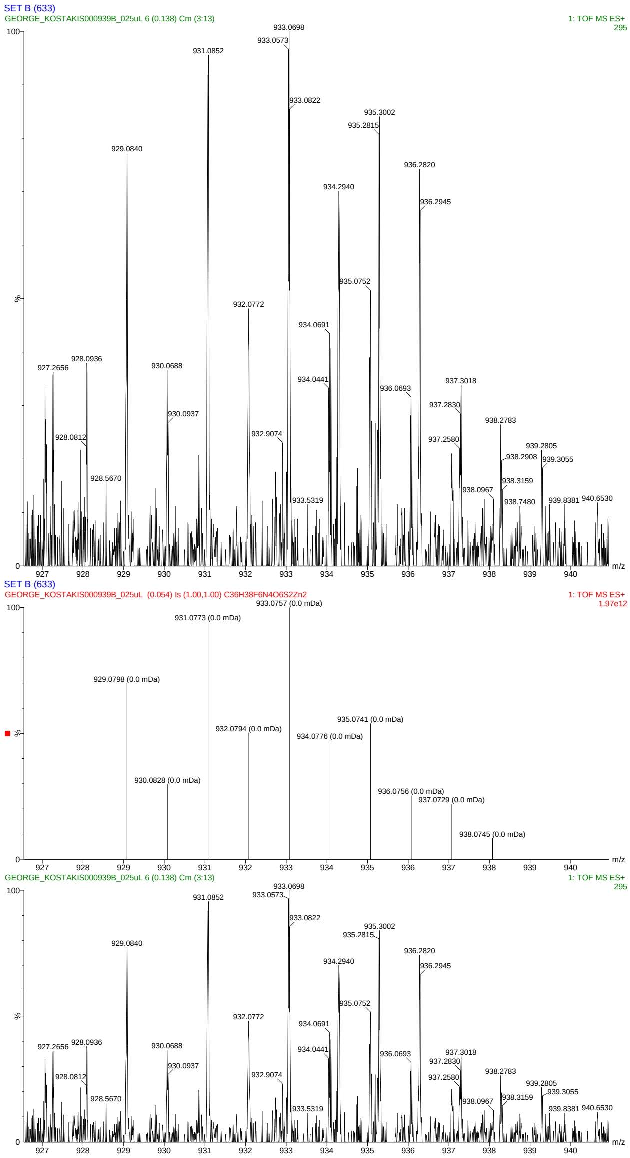


Figure S4-39. ESI-MS of Zinc complexes for set B

Elemental Composition Report

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

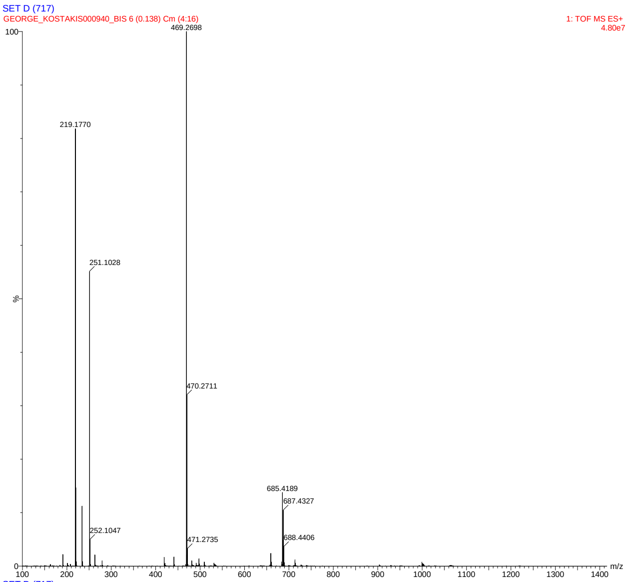
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 36-36 H: 0-100 N: 4-4 O: 6-6 F: 6-6 S: 2-2 Zn: 2-2

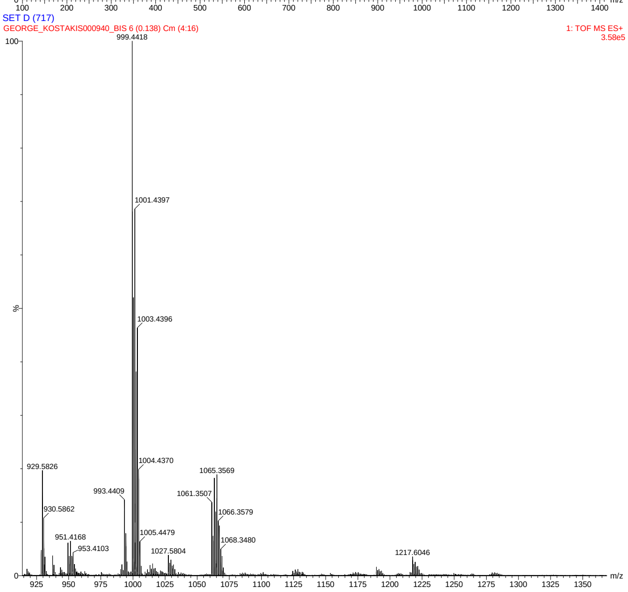
Minimum:			-25.0					
Maximum:	5.0	1000.0	100.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula

929.0776	929.0798	-2.2	-2.4	16.5	191.6	n/a	n/a	C36 H39 N4 O6 F6 S2

Set D

No traces of the monomer (mass 594.2259 u) are shown in the mass spectra.





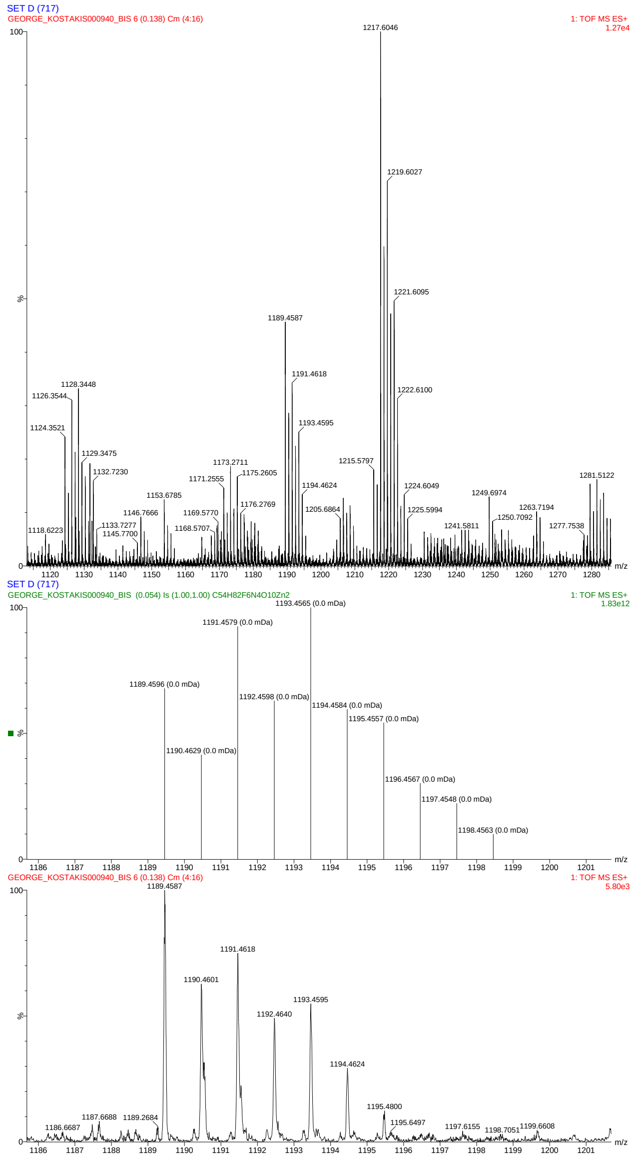


Figure S4-40. ESI-MS of Zinc complexes for set D

The isotopic pattern (as shown below) is not perfect for this compound, but accurate mass is within tolerances (+4.2 ppm)

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 54-54 H: 0-100 N: 4-4 O: 10-10 F: 6-6 Zn: 2-2

Minimum:			-25.0					
Maximum:		5.0	1000.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1189.4646	1189.4596	5.0	4.2	12.5	253.7	n/a	n/a	C54 H83 N4 O10 F6 Zn2

Set E

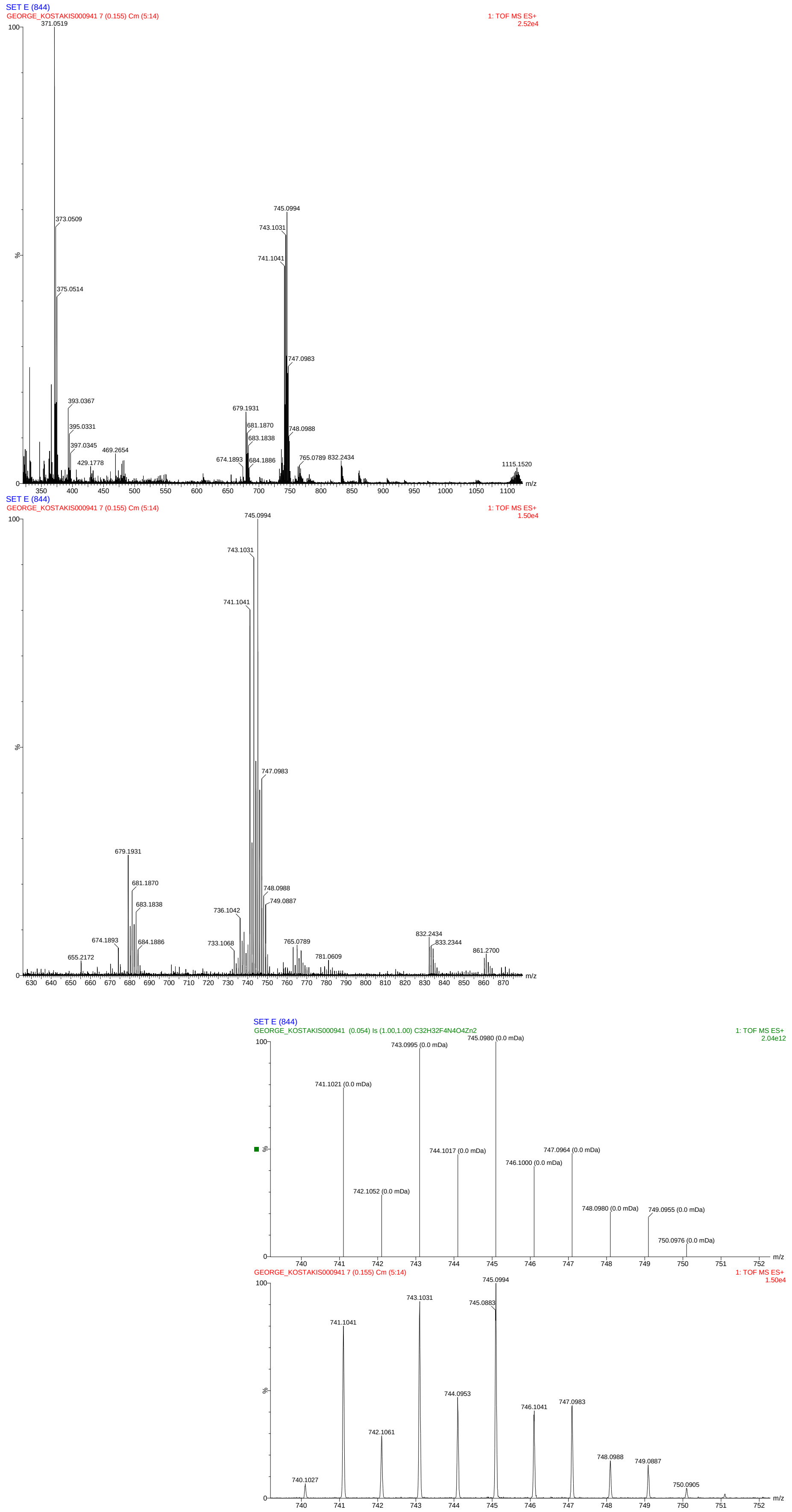


Figure S4-41. ESI-MS of Zinc complexes for set E

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 32-32 H: 0-100 N: 4-4 O: 4-4 F: 4-4 Zn: 2-2

Minimum:			-25.0					
Maximum:	5.0	1000.0	100.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
741.1023	741.1021	0.2	0.3	16.5	274.7	n/a	n/a	C32 H33 N4 O4 F4 Zn2

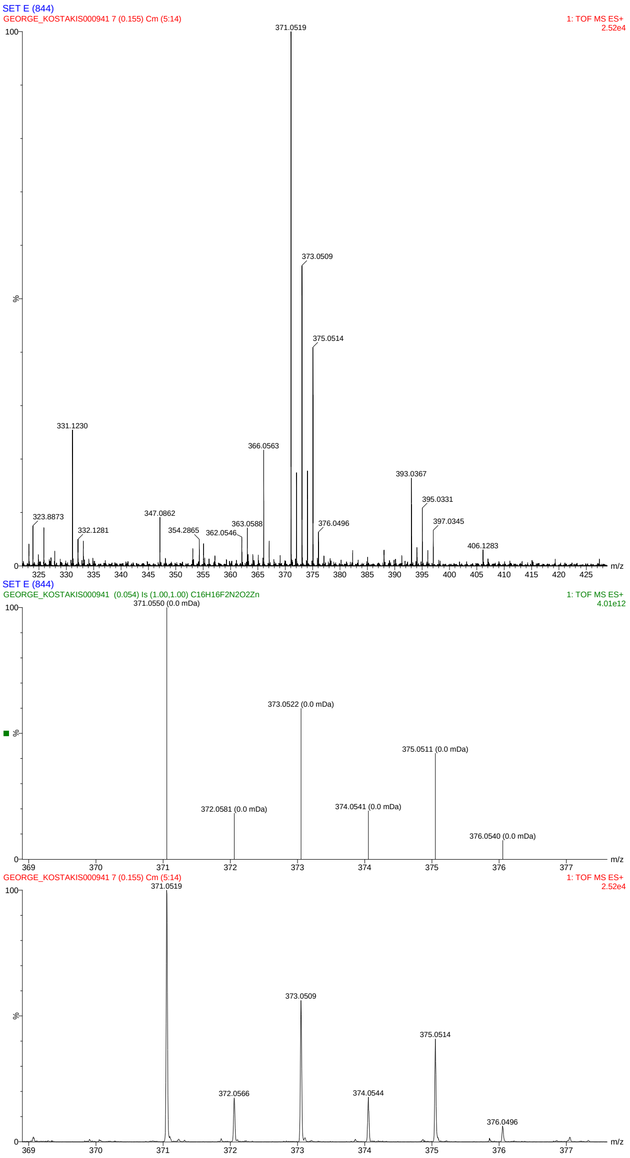


Figure S4-42. ESI-MS of Zinc complexes for set E

Elemental Composition Report

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -25.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 0-100 N: 2-2 O: 2-2 F: 2-2 Zn: 1-1

Minimum:			-25.0					
Maximum:	5.0	1000.0	100.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
371.0550	371.0550	0.0	0.0	8.5	416.6	n/a	n/a	C16 H17 N2 O2 F2 Zn
503.0375	503.0384	-0.9	-1.8	8.5	428.7	n/a	n/a	C18 H17 N2 O4 F6 Zn

S5. References

1. Coles, S. J. & Gale, P. A. Changing and challenging times for service crystallography. *Chem. Sci.* **3**, 683–689 (2012).

2. Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. OLEX2 : a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **42**, 339–341 (2009).

3. Frisch, M. J. *et al.* G16_C01. Gaussian 16, Revision C.01, Gaussian, Inc., Wallin (2016).

4. Handy, N. C. & Cohen, A. J. Left-right correlation energy. *Mol. Phys.* **99**, 403–412 (2001).

5. Hoe, W. M., Cohen, A. J. & Handy, N. C. Assessment of a new local exchange functional OPTX. *Chem. Phys. Lett.* **341**, 319–328 (2001).

6. Lee, C., Yang, W. & Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **37**, 785–789 (1988).

7. Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297–3305 (2005).

8. Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.* **8**, 1057–1065 (2006).

9. Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **132**, 154104 (2010).

10. Jmol: an open-source Java viewer for chemical structures in 3D, www.jmol.org.

11. O'Boyle, N. M., Tenderholt, A. L. & Langner, K. M. Cclib: A library for package-independent computational chemistry algorithms. *J. Comput. Chem.* **29**, 839–845 (2008).

12. Pracht, P., Bohle, F. & Grimme, S. Automated exploration of the low-energy chemical space with fast quantum chemical methods. *Phys. Chem. Chem. Phys.* **22**, 7169–7192 (2020).

13. Bannwarth, C. *et al. Extended tight-binding quantum chemistry methods*. *Wiley Interdisciplinary Reviews: Computational Molecular Science* vol. 11 (John Wiley & Sons, Ltd, 2021).

14. Besora, M., Braga, A. A. C., Ujaque, G., Maseras, F. & Lledós, A. The importance of conformational search: A test case on the catalytic cycle of the Suzuki-Miyaura cross-coupling. *Theor. Chem. Acc.* **128**, 639–646 (2011).

15. Stephens, P. J., Devlin, F. J., Chabalowski, C. F. & Frisch, M. J. Ab Initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. *J. Phys. Chem.* **98**, 11623–11627 (1994).

16. Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **98**, 5648–5652 (1993).

17. Grimme, S. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comput. Chem.* **27**, 1787–1799 (2006).

18. Ditchfield, R., Hehre, W. J. & Pople, J. A. Self-consistent molecular-orbital methods. IX. An extended gaussian-type basis for molecular-orbital studies of organic molecules. *J. Chem. Phys.* **54**, 724–728 (1971).

19. Hariharan, P. C. & Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chim. Acta* **28**, 213–222 (1973).

20. Dolg, M., Wedig, U., Stoll, H. & Preuss, H. Energy-adjusted ab initio pseudopotentials for the first row transition elements. *J. Chem. Phys.* **86**, 866–872 (1987).

21. Tomasi, J., Mennucci, B. & Cammi, R. Quantum mechanical continuum solvation models. *Chem. Rev.* **105**, 2999–3093 (2005).

22. Scalmani, G. & Frisch, M. J. Continuous surface charge polarizable continuum models of solvation. I. General formalism. *J. Chem. Phys.* **132**, 114110 (2010).

23. Luchini, G., Alegre-Requena, J. V, Funes-Ardoiz, I. & Paton, R. S. GoodVibes: automated thermochemistry for heterogeneous computational chemistry data. *F1000Research* **9**, 291 (2020).

24. Addison, A. W., Rao, T. N., Reedijk, J., Van Rijn, J. & Verschoor, G. C. Synthesis, structure, and spectroscopic properties of copper(II) compounds containing nitrogen-sulphur donor ligands; the crystal and molecular structure of aqua[1,7-bis(N-methylbenzimidazol-2';-yl)-2,6-dithiaheptane]copper(II) perchlorate. *J. Chem. Soc. Dalt. Trans.* 1349–1356 (1984) doi:10.1039/DT9840001349.