Supporting Information (82 pages)

Importance of Solvent-Bridged Structures of Fluorinated Diphenylalanines. Synthesis, Detailed NMR Analysis, and Rotational Profiles of Phe(2-F)-Phe(2-F), Phe(2-F)-Phe, and Phe-Phe(2-F)

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Synthesis of mono1 F-FF and mono2 F-FF

Synthesis of mono1 F-FF: 1.2 g (3 mMol) of Fmoc-*L*-Phe(2-F)-OH were added to the resin together with 1.7 ml (10 mMol) of *N*,*N*-diisopropylethylamine (DIPEA). The reaction was left to proceed for 1 hour and then repeated. Capping of the resin was then performed with MeOH (5 min, 15 ml) and the loading of the resin was experimentally shown to be ≈ 0.6 mMol/g by HPLC based quantitative Fmoc evaluation test. Fmoc deprotection was achieved by treatment with 20% piperidine in DMF for 20 min, repeated twice.

2.4 g (6 mMol) of the second protected amino acid, Fmoc-*L*-Phe-OH was reacted with 3.4 ml of DIPEA (20 mMol) and subsequently with 2 g (5.5 mMol) of 2-(1*H*-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) for 5 min to provide the corresponding activated ester. This activated ester was reacted in situ with the peptydil resin for 1 hour. The same coupling procedure was repeated once to afford the protected dipeptide on the resin. Capping of unreacted amino groups of the first phenylalanine residue by acylation was achieved by reaction with 5% Ac_2O and DIPEA for 5 min. Final Fmoc deprotection was performed as above to obtain the desired dipeptide on the resin.

Acid-catalyzed ester hydrolysis was used to cleave the peptide from the resin and involved treatment with 10% trifluoroacetic acid (TFA) in presence of water and triisopropylsilane (TIPS) scavangers (both 5%) in dichloromethane (DCM). After 45 min of reaction, the reaction mixture was filtered and evaporated by nitrogen to almost dryness before to be diluted with 50% water and acetonitrile and lyophilized overnight to obtain 400 mg of crude dipeptide. Crude dipeptide identity was confirmed by LC-MS analysis and its preparative purification by MS-assisted flash chromatography yielded 240 mg of 95% pure H_2N-Phe(2-F)-Phe-COOH.

As this last contained however a small amount of a quite colorful contaminant, these were furtherly purified by MS assisted preparative HPLC to yield to obtain 130 mg of final purified colorless product.

Synthesis of Mono2 F-FF: 1.2 g (3 mMol) of Fmoc-*L*-Phe-OH were added to the resin together with 1.7 ml (10 mMol) of *N*,*N*-diisopropylethylamine (DIPEA). The reaction was left to proceed for 1 hour and then repeated. Capping of the resin was then performed with MeOH (5 min, 15 ml) and the loading of the resin was experimentally shown to be ≈ 0.6 mMol/g by HPLC based quantitative Fmoc evaluation test. Fmoc deprotection was achieved by treatment with 20% piperidine in DMF for 20 min, repeated twice.

2.4 g (6 mMol) of the second protected amino acid, Fmoc-*L*-Phe(2-F)-OH was reacted with 3.4 ml of DIPEA (20 mMol) and subsequently with 2 g (5.5 mMol) of 2-(1*H*-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) for 5 min to provide the corresponding activated ester. This activated ester was reacted in situ with the peptydil resin for 1 hour. The same coupling procedure was repeated once to afford the protected dipeptide on the resin. Capping of unreacted amino groups of the first phenylalanine residue by acylation was achieved by reaction with 5% Ac_2O and DIPEA for 5 min. Final Fmoc deprotection was performed as above to obtain the desired dipeptide on the resin.

Acid-catalyzed ester hydrolysis was used to cleave the peptide from the resin and involved treatment with 10% trifluoroacetic acid (TFA) in presence of water and triisopropylsilane (TIPS) scavangers (both 5%) in dichloromethane (DCM). After 45 min of reaction, the reaction mixture was filtered and evaporated by nitrogen to almost dryness before to be diluted with 50% water and acetonitrile and lyophilized overnight to obtain 350 mg of crude dipeptide. Crude dipeptide identity was confirmed by LC-MS analysis and its preparative purification by MS-assisted flash chromatography yielded 225 mg of 95% pure H_2N-Phe(2-F)-Phe-COOH.

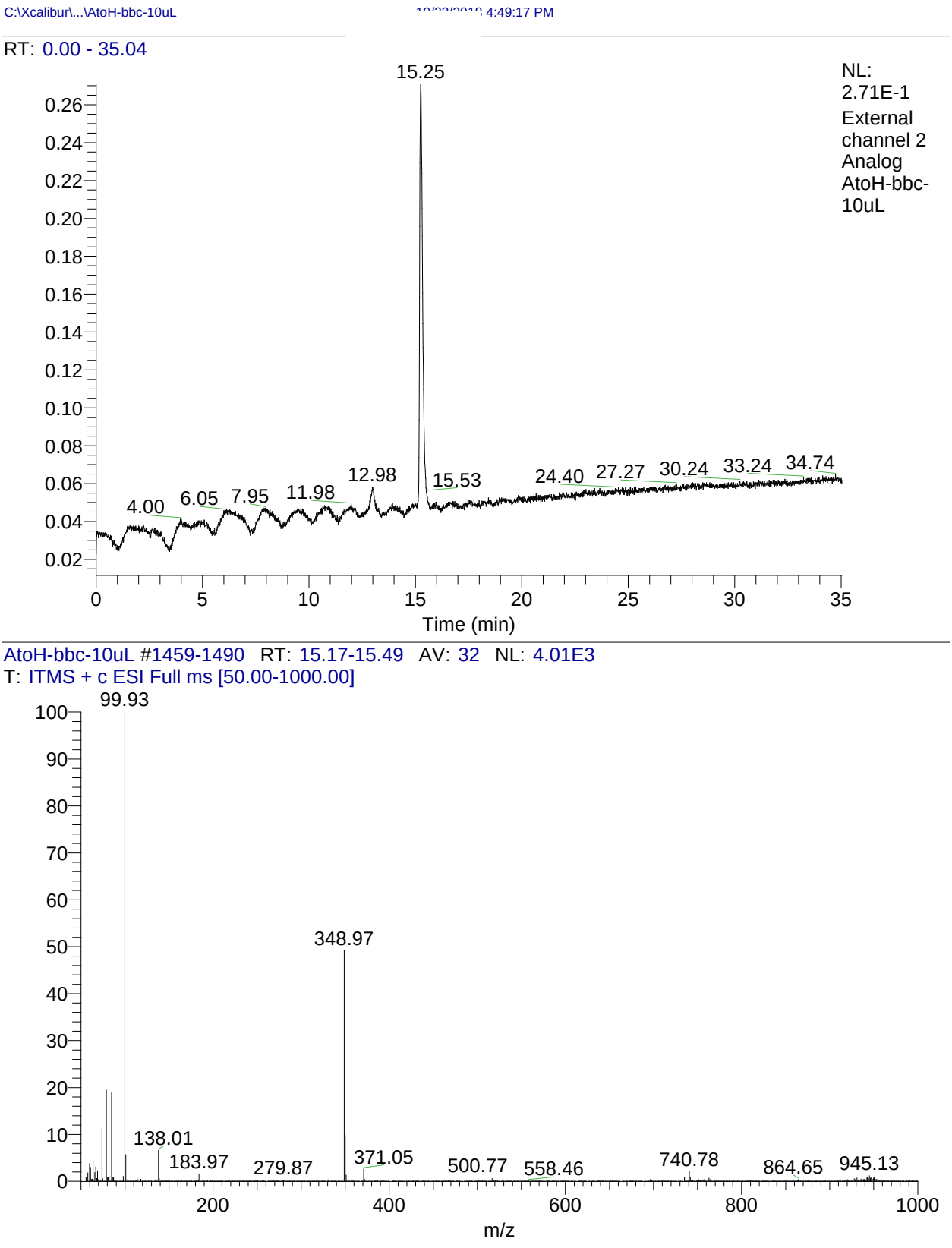


Figure S1. GC chromatogram (top) and MS spectrum of di F-FF (bottom).

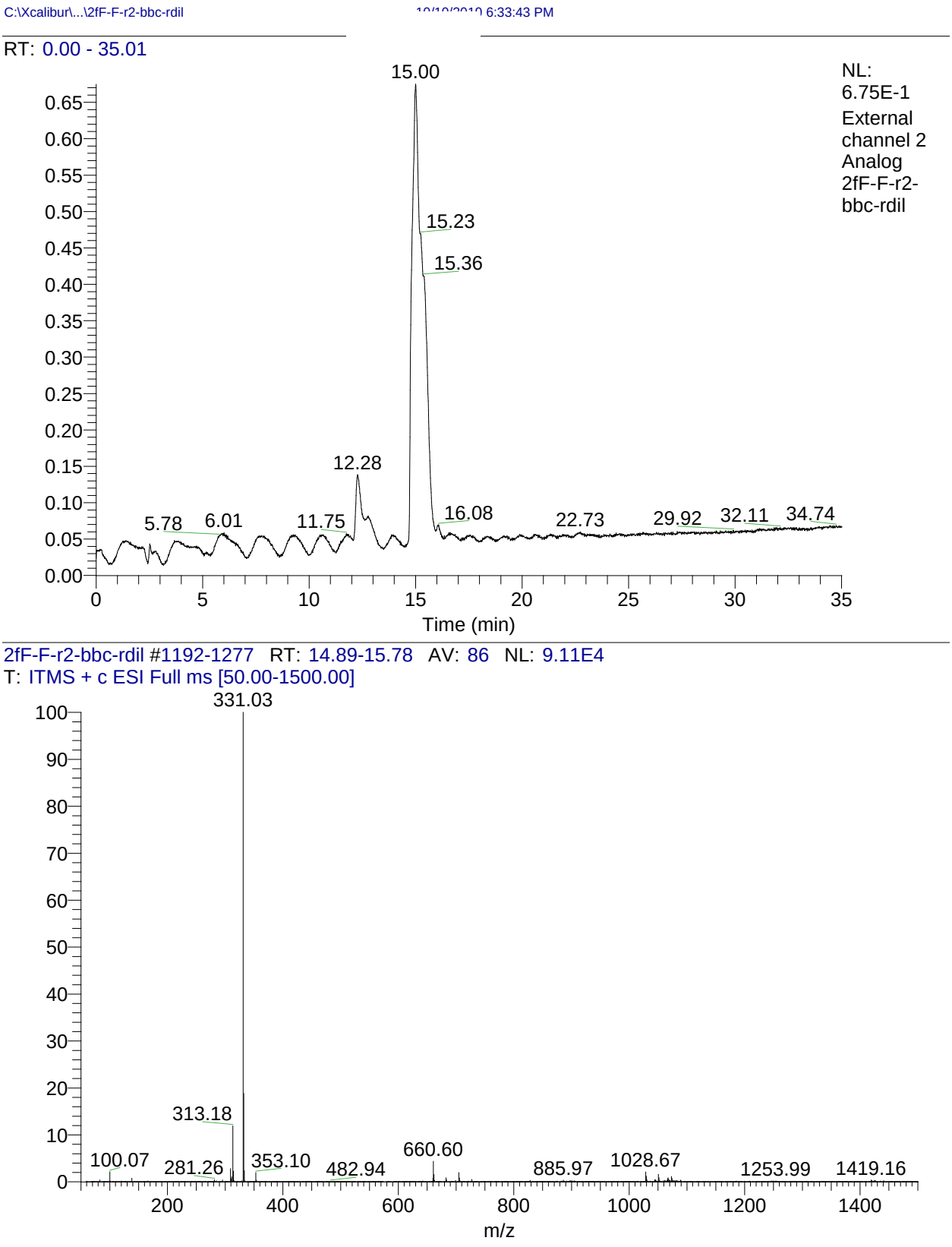


Figure S2. GC chromatogram (top) and MS spectrum of mono1 F-FF (bottom).

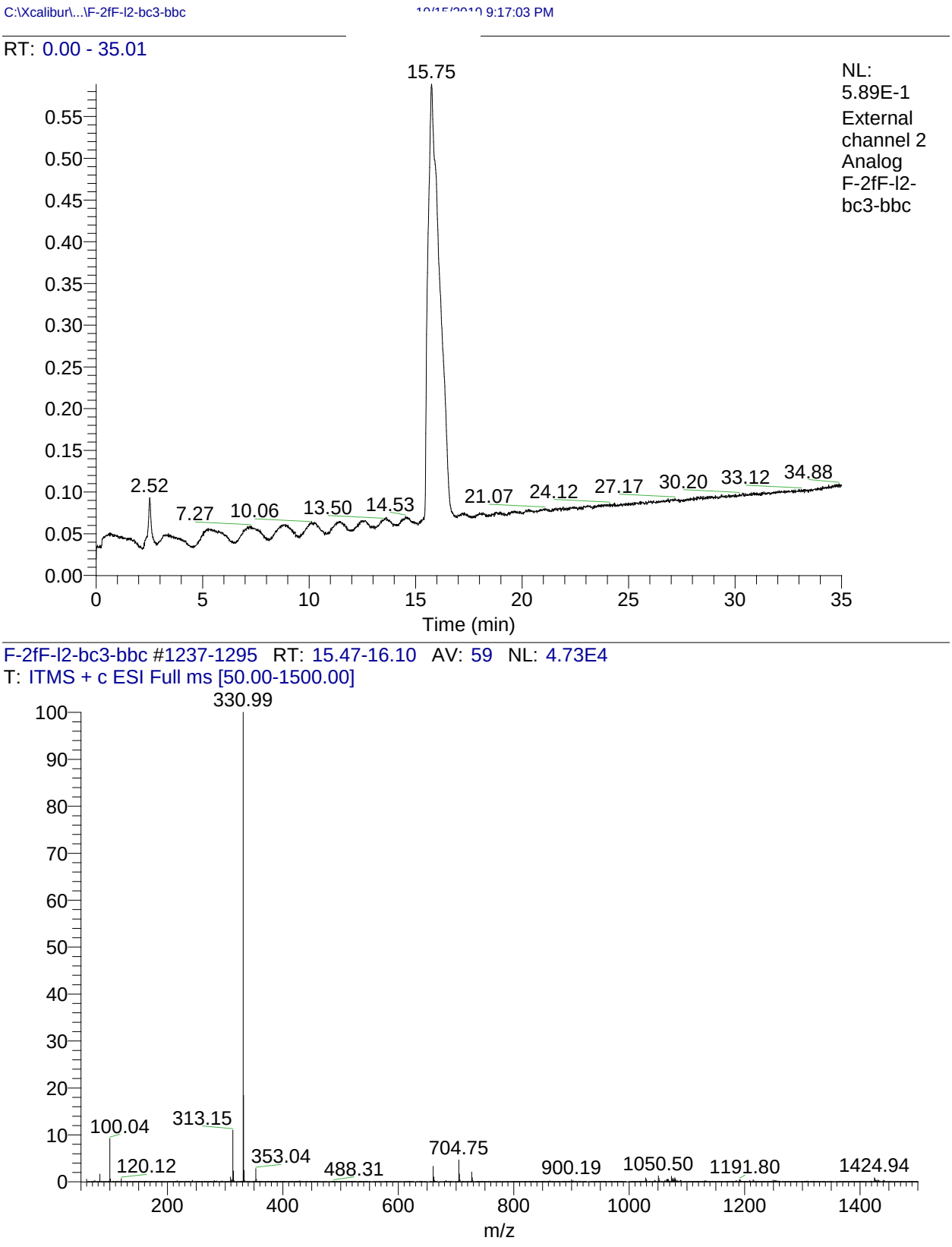


Figure S3. GC chromatogram (top) and MS spectrum of mono2 F-FF (bottom).

Experimental NMR Spectra of di F-FF

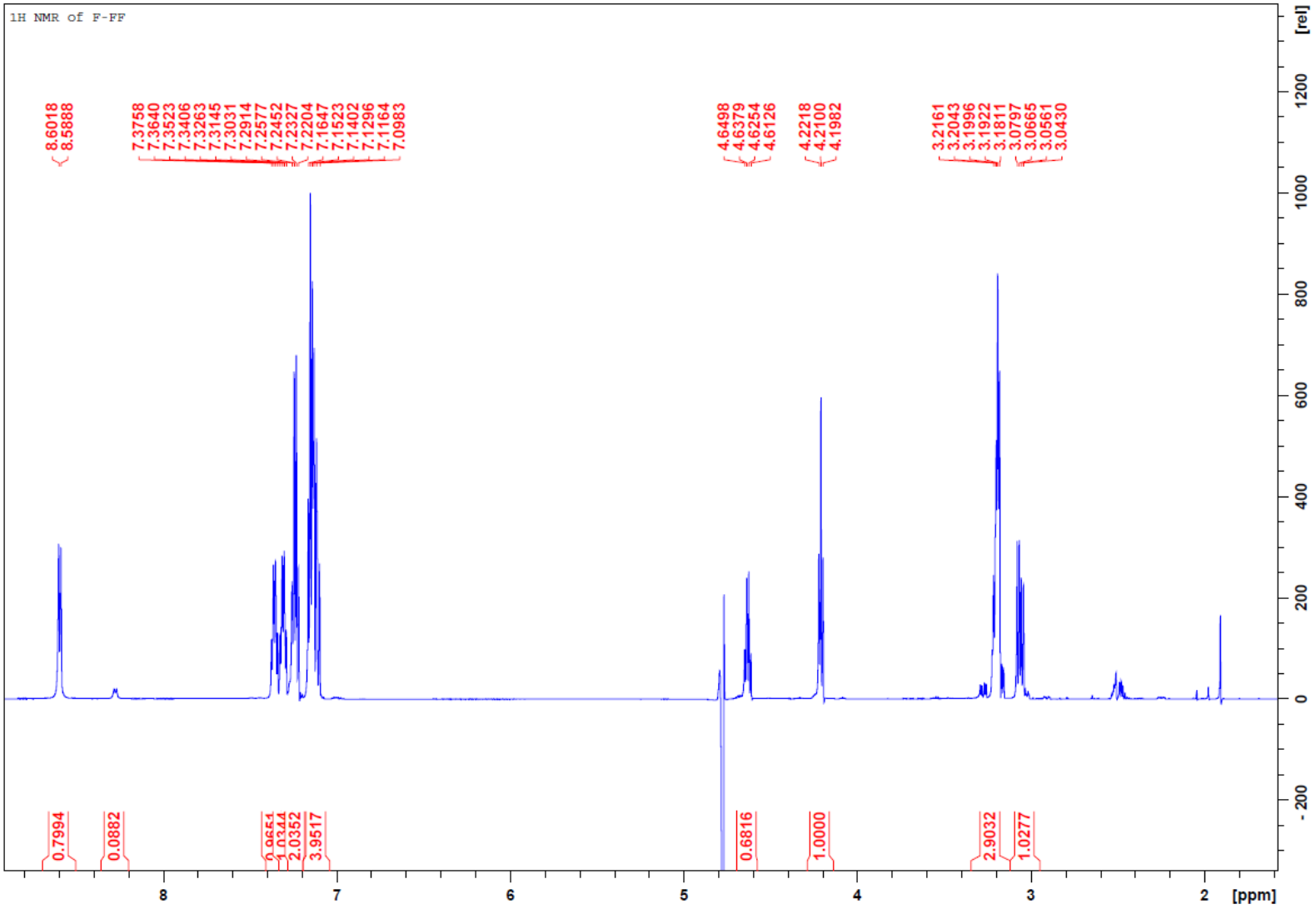


Figure S4. H-NMR spectrum of di F-FF.

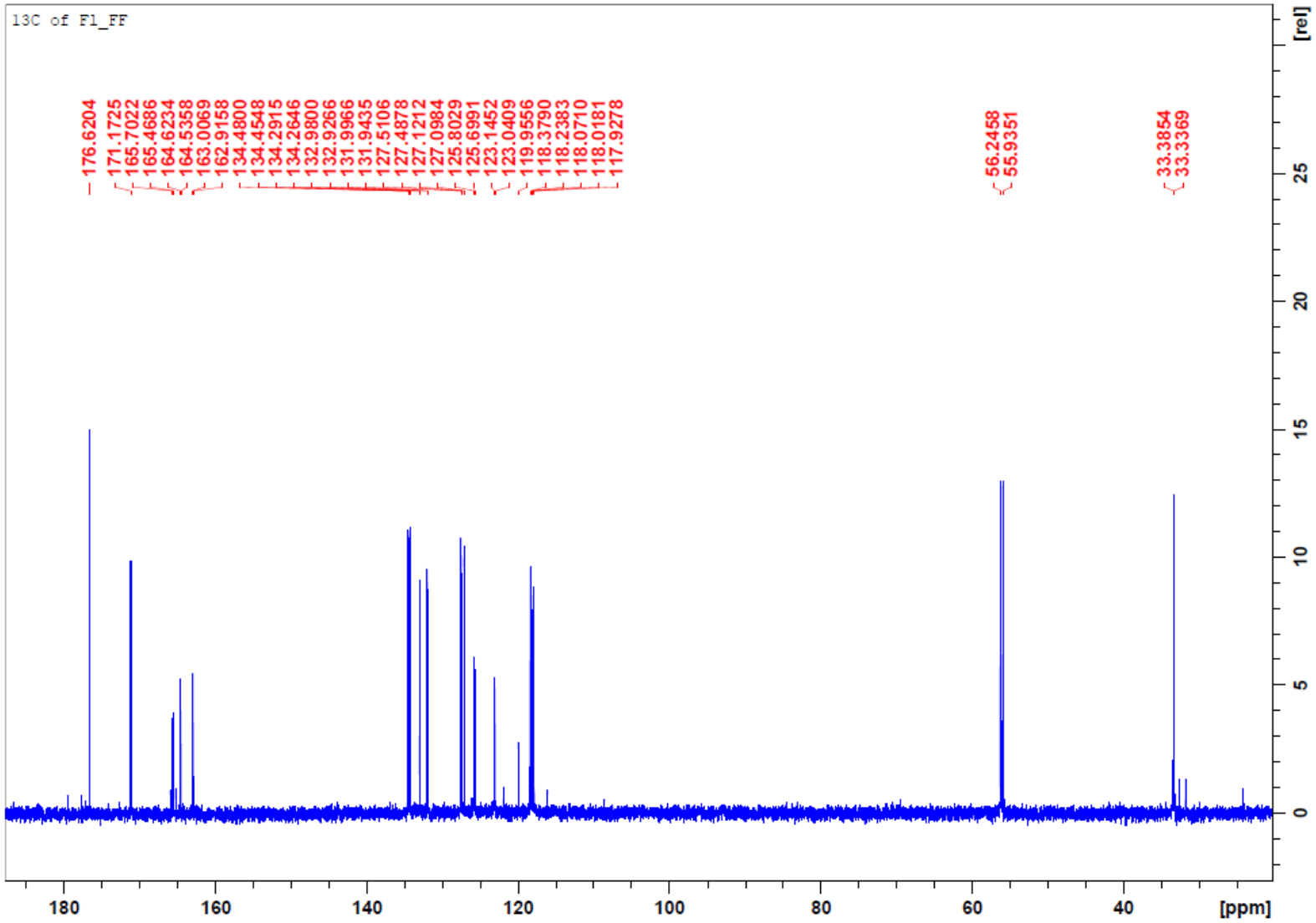


Figure S5. C-NMR spectrum of di F-FF.

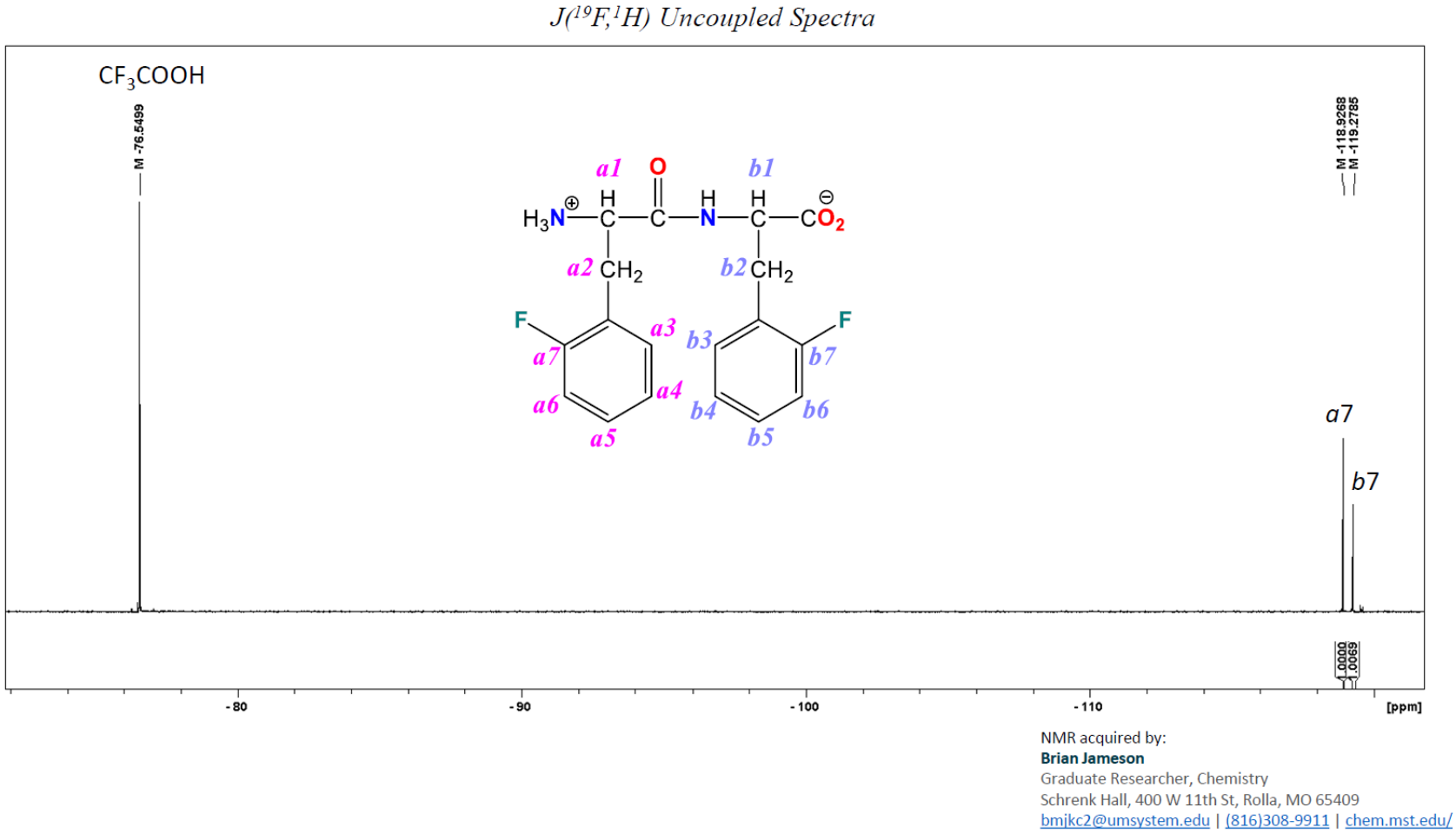


Figure S6a. F-NMR spectrum of di F-FF, decoupled.

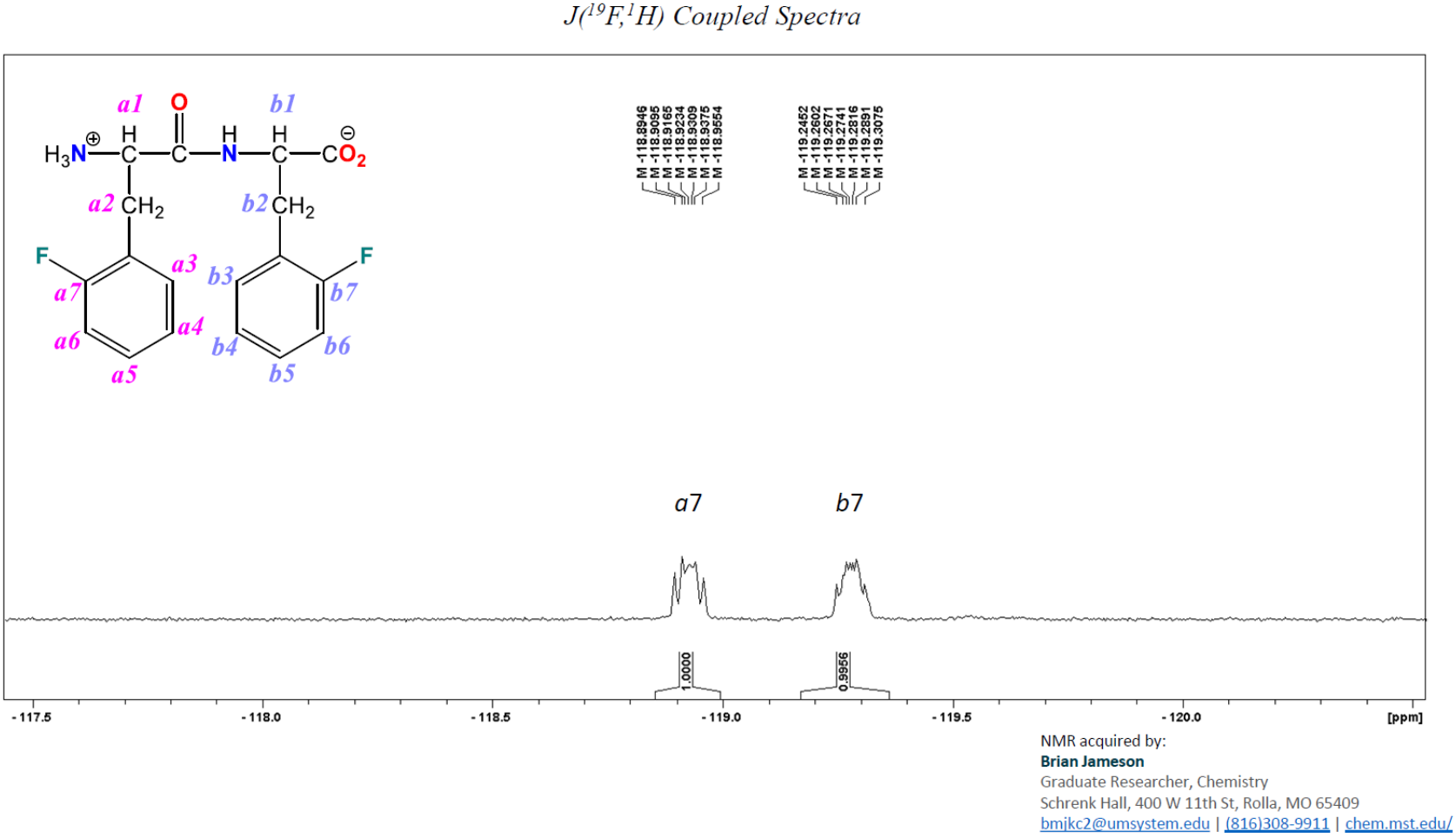


Figure S6b. F-NMR spectrum of di F-FF, coupled.

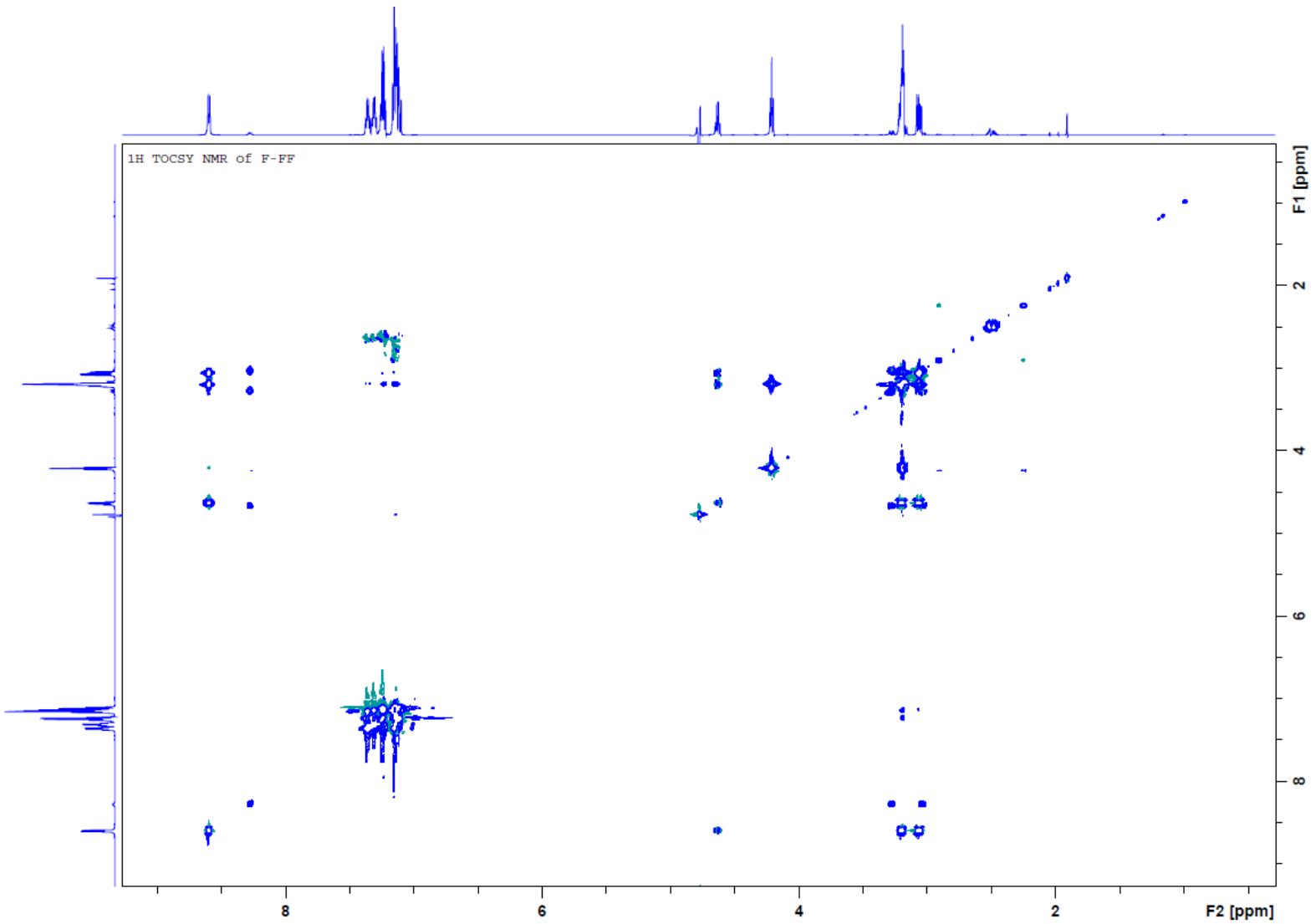


Figure S7. TOCSY spectrum of di F-FF.

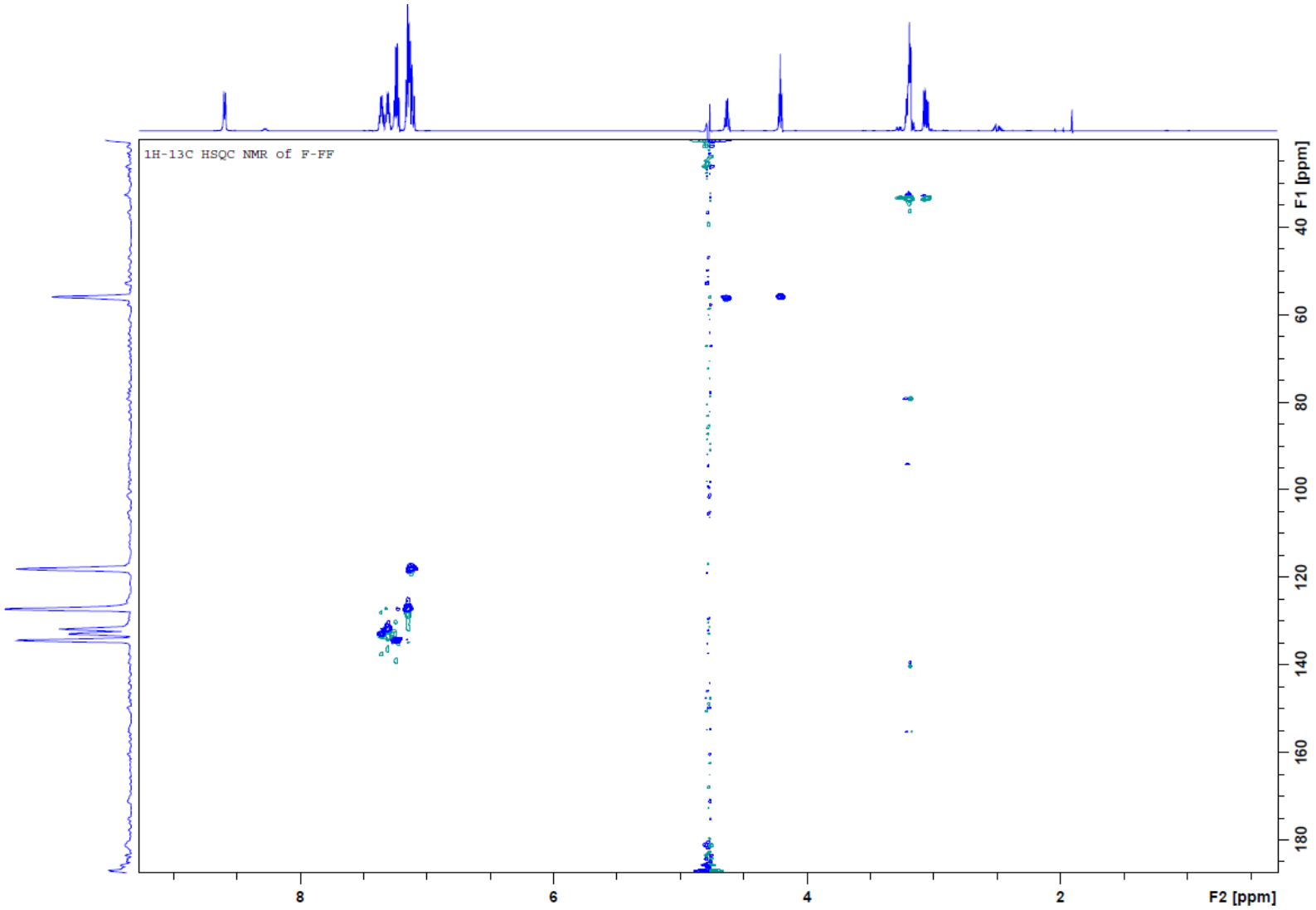


Figure S8. HSQC spectrum of di F-FF.

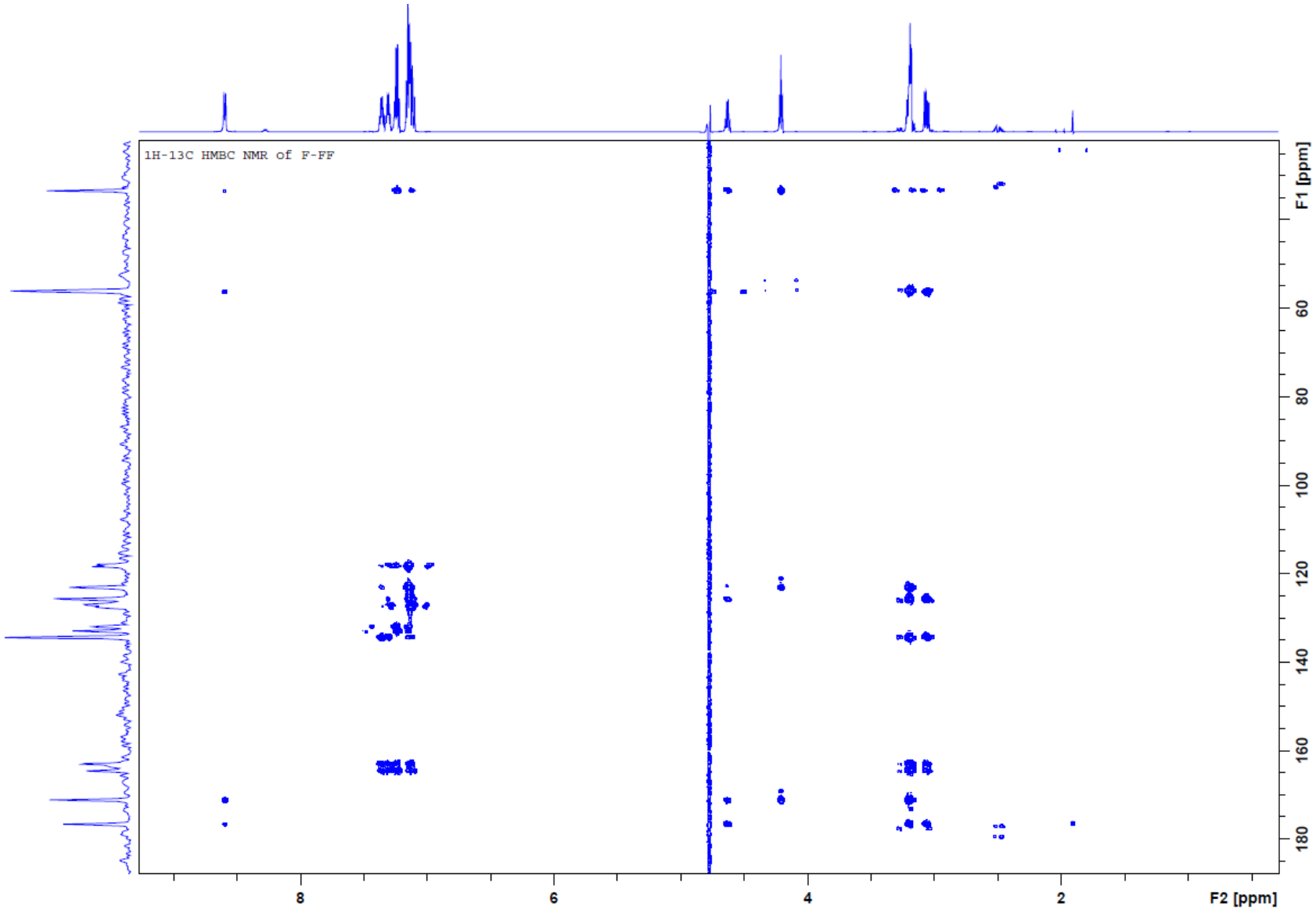


Figure S9. HMBC spectrum of di F-FF.

Experimental NMR Spectra of mono1 F-FF

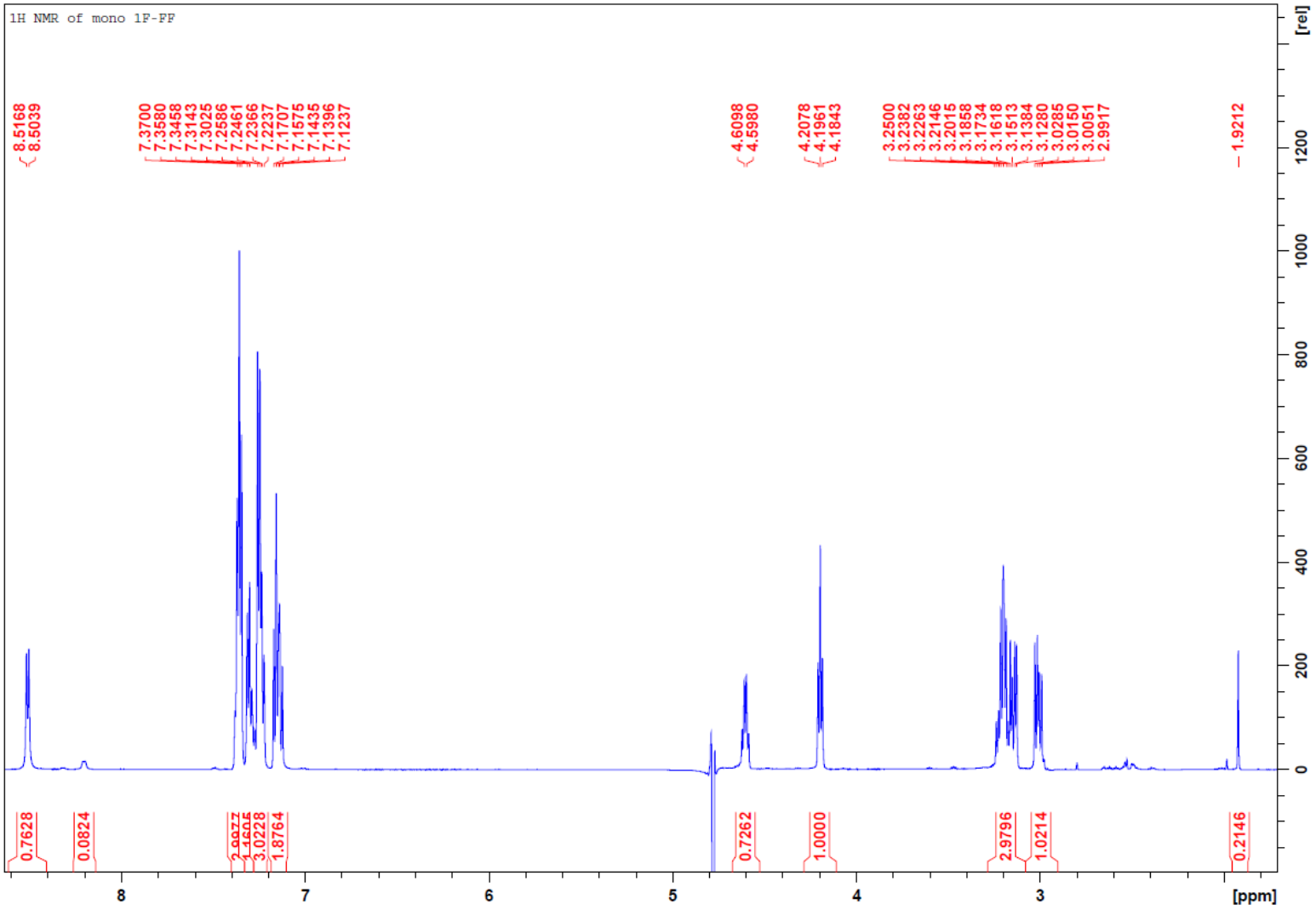


Figure S10. H-NMR spectrum of mono1 F-FF.

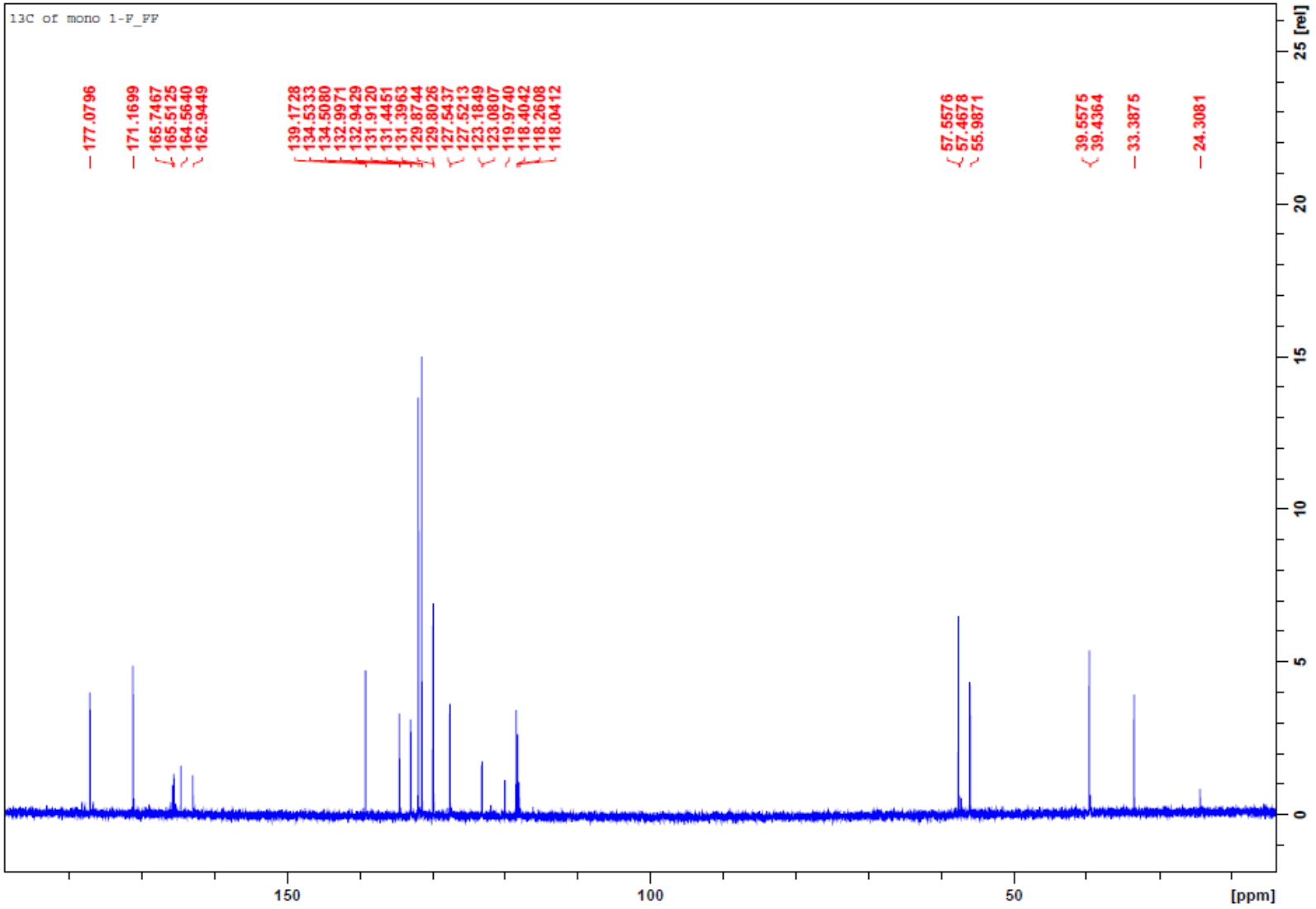


Figure S11. C-NMR spectrum of mono1 F-FF.

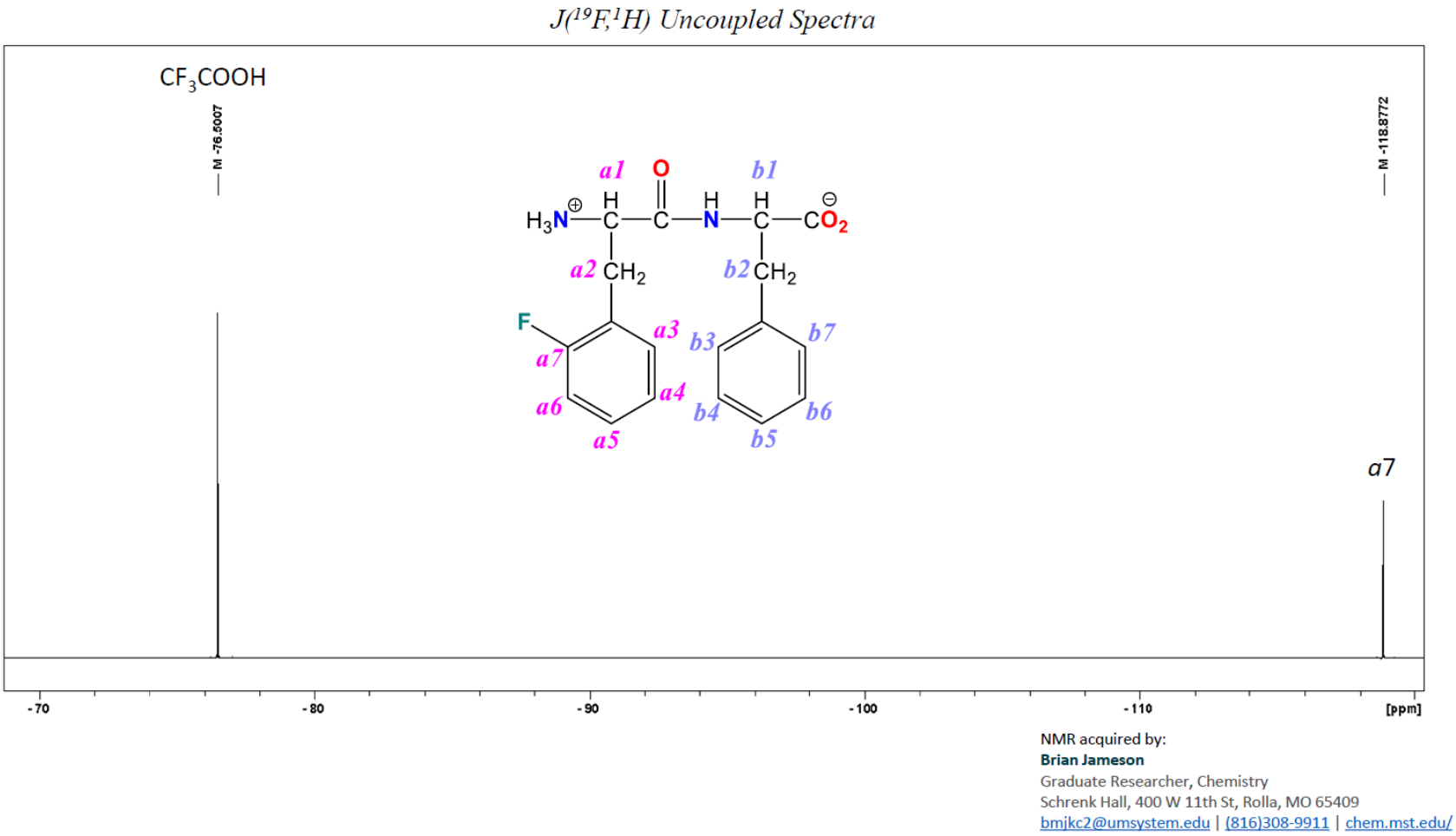


Figure S12a. F-NMR spectrum of mono1 F-FF, uncoupled.

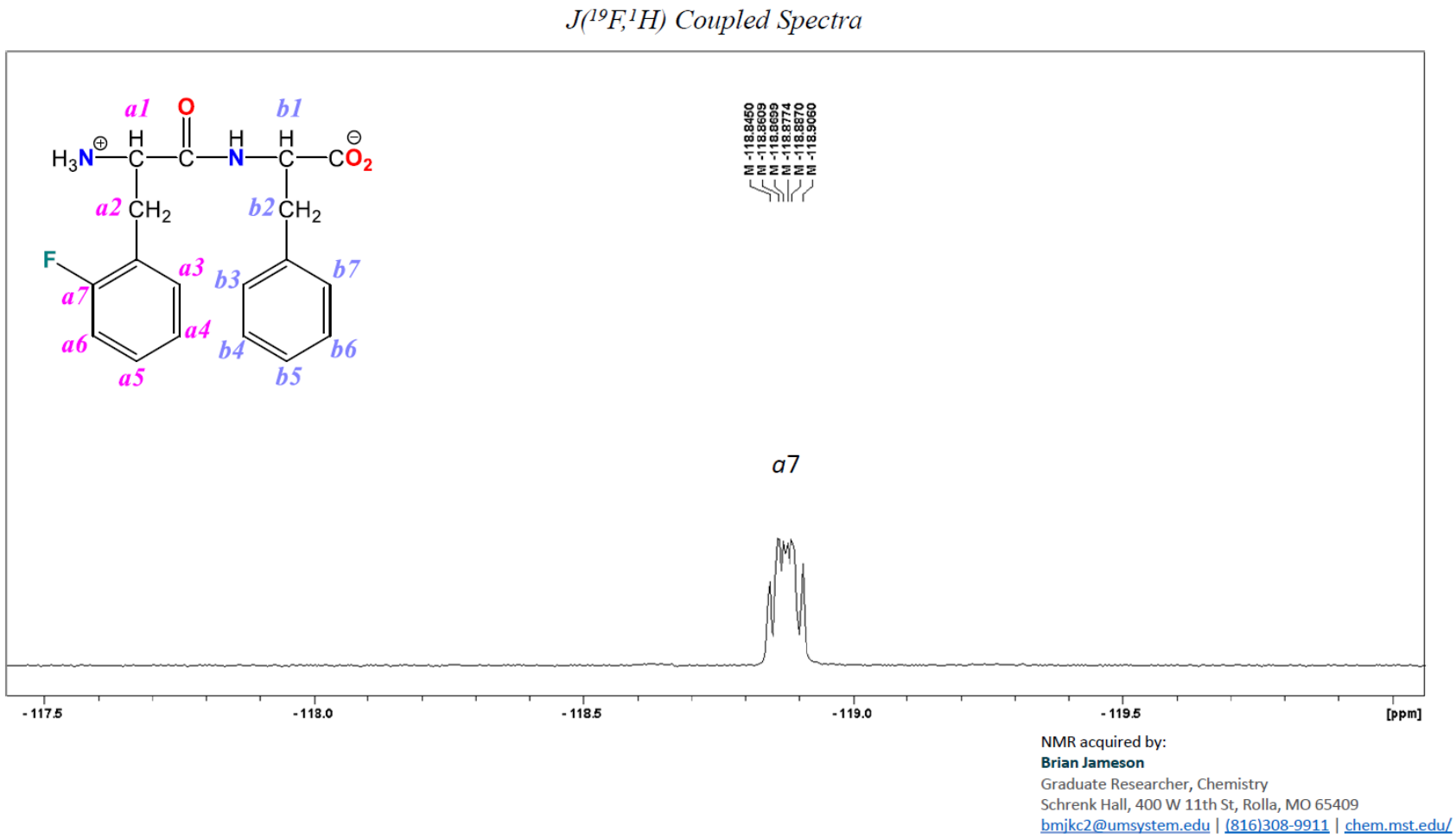


Figure S12b. F-NMR spectrum of mono1 F-FF, coupled.

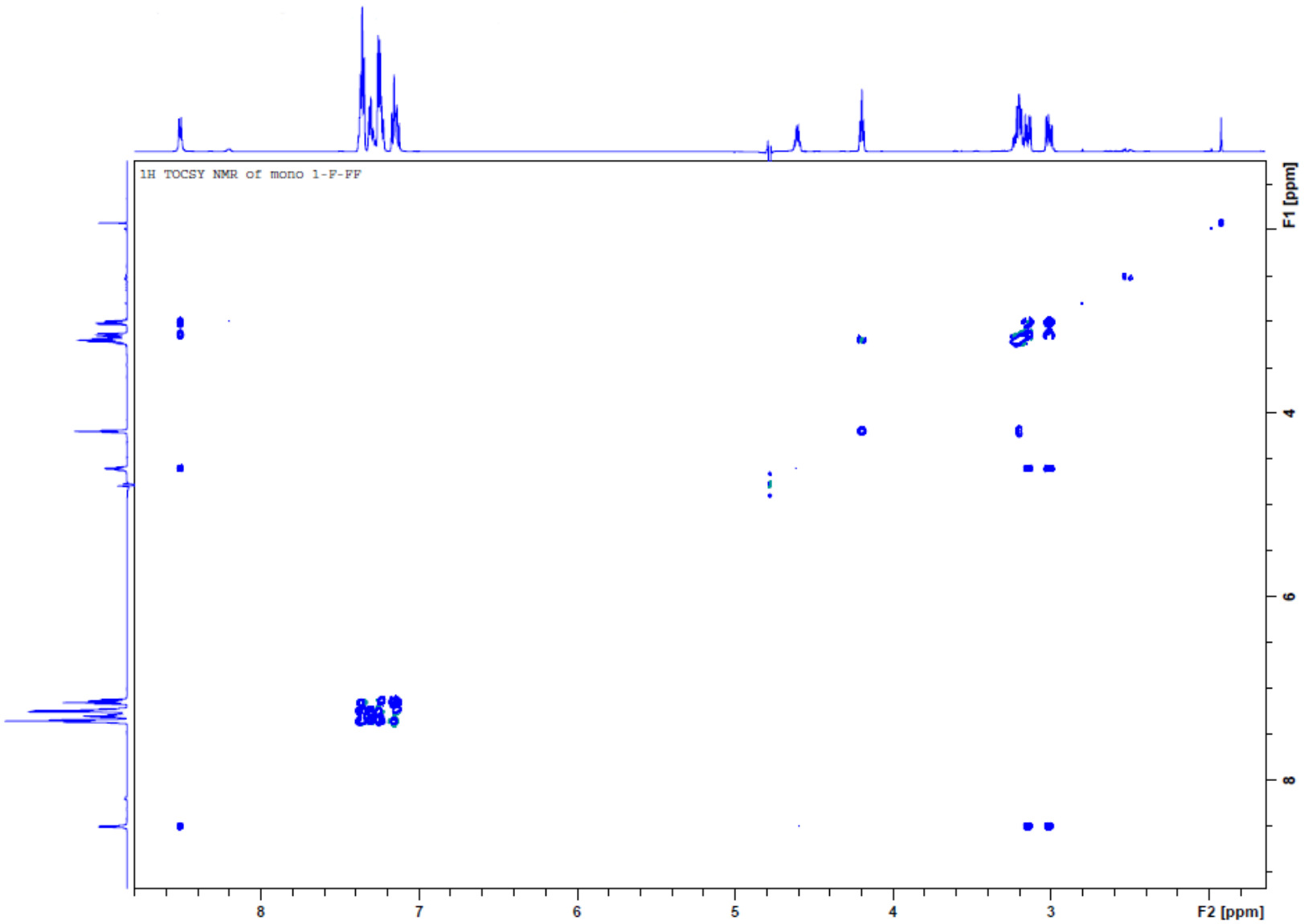


Figure S13. TOCSY spectrum of mono1 F-FF.

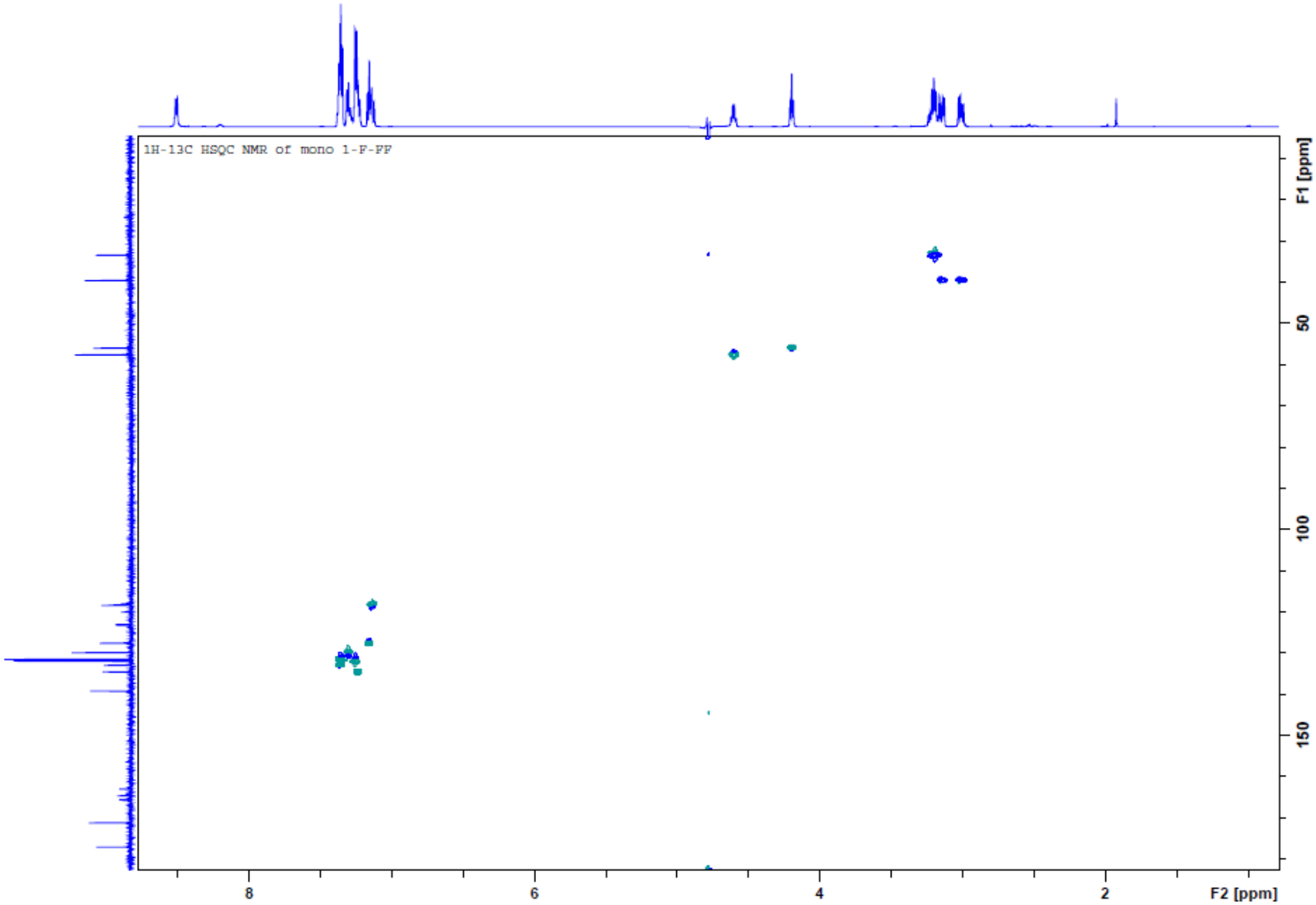


Figure S14. HSQC spectrum of mono1 F-FF.

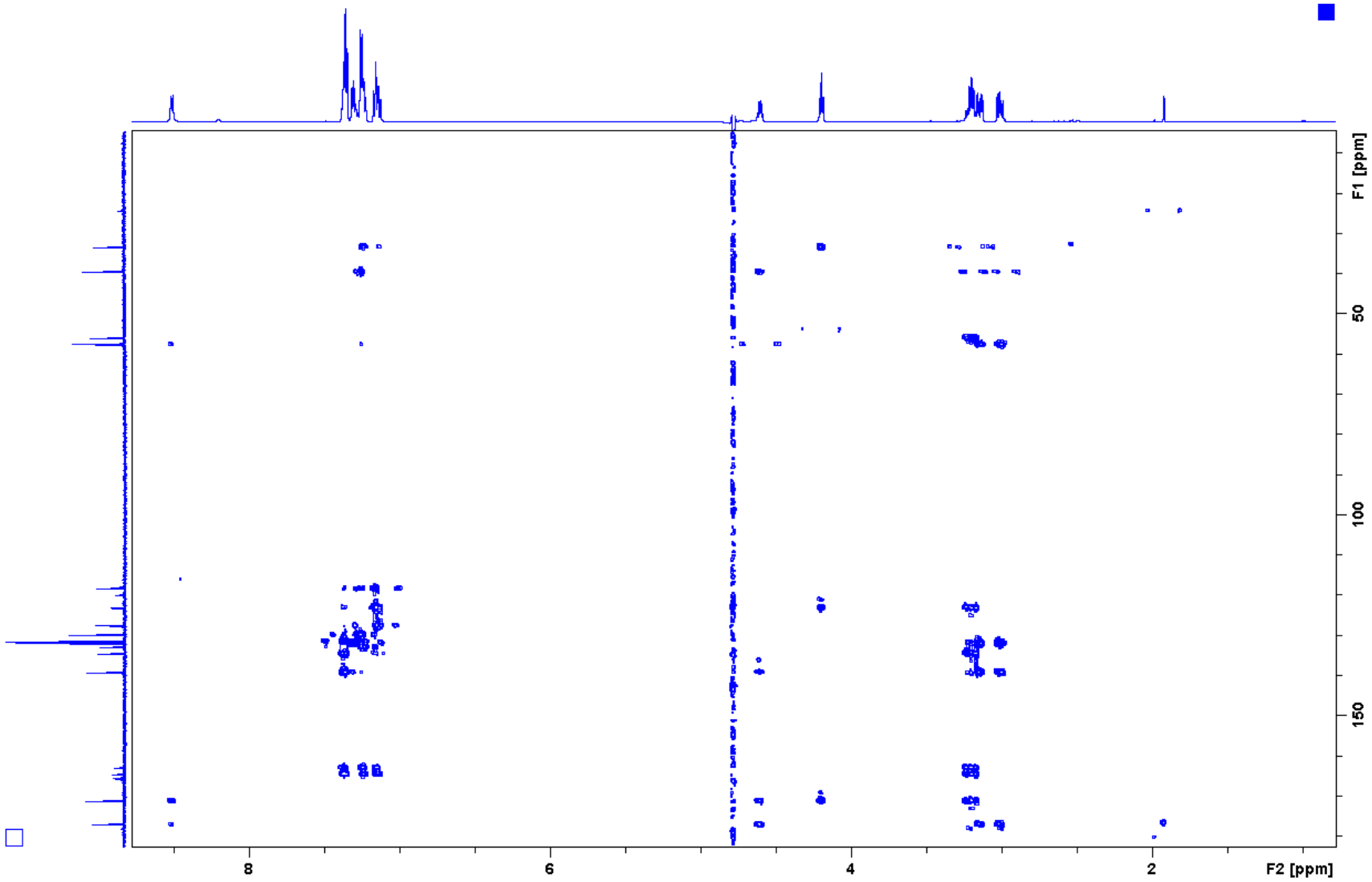


Figure S15. HMBC spectrum of mono1 F-FF.

Experimental NMR Spectra of mono2 F-FF

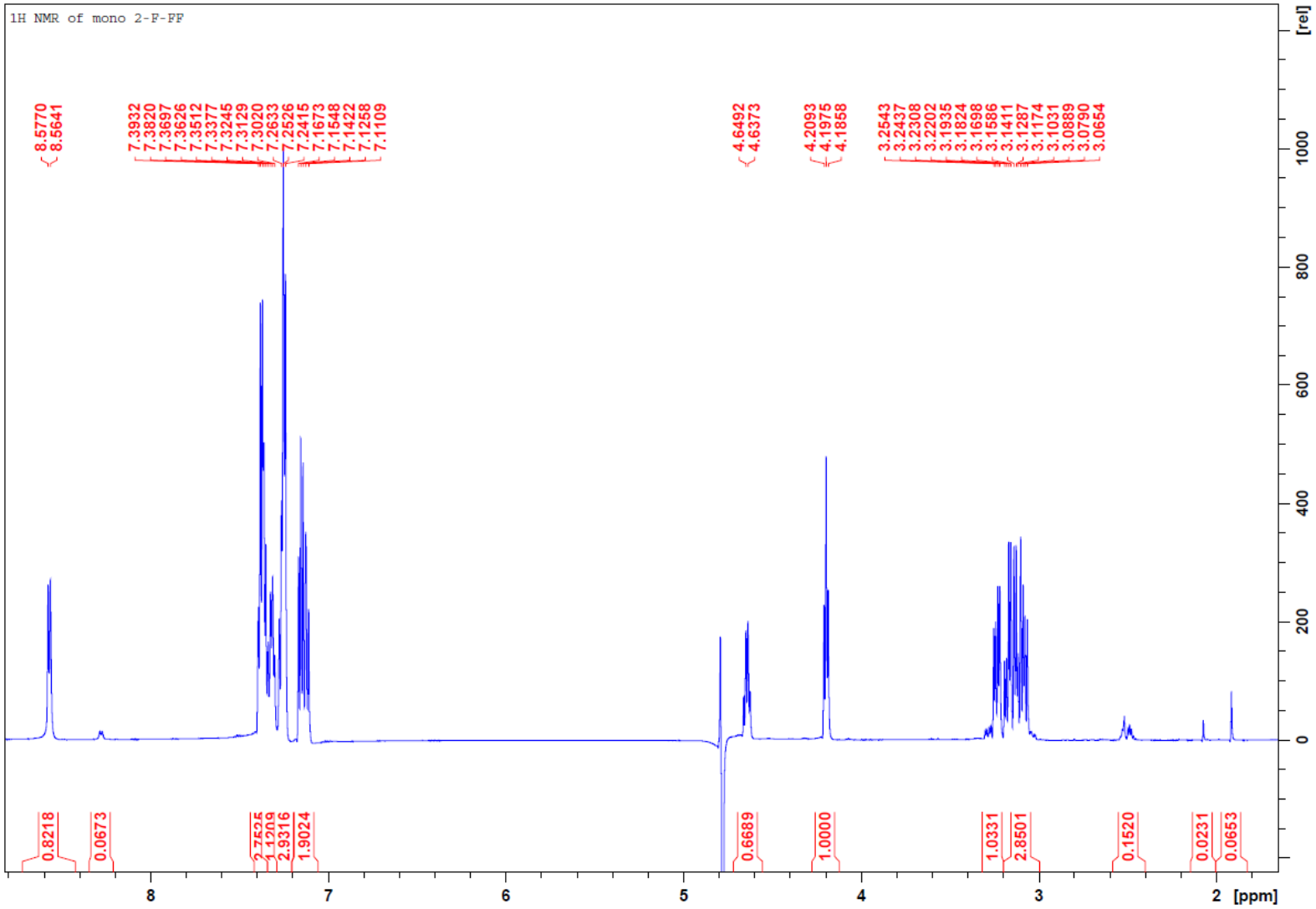


Figure S16. H-NMR spectrum of mono2 F-FF.

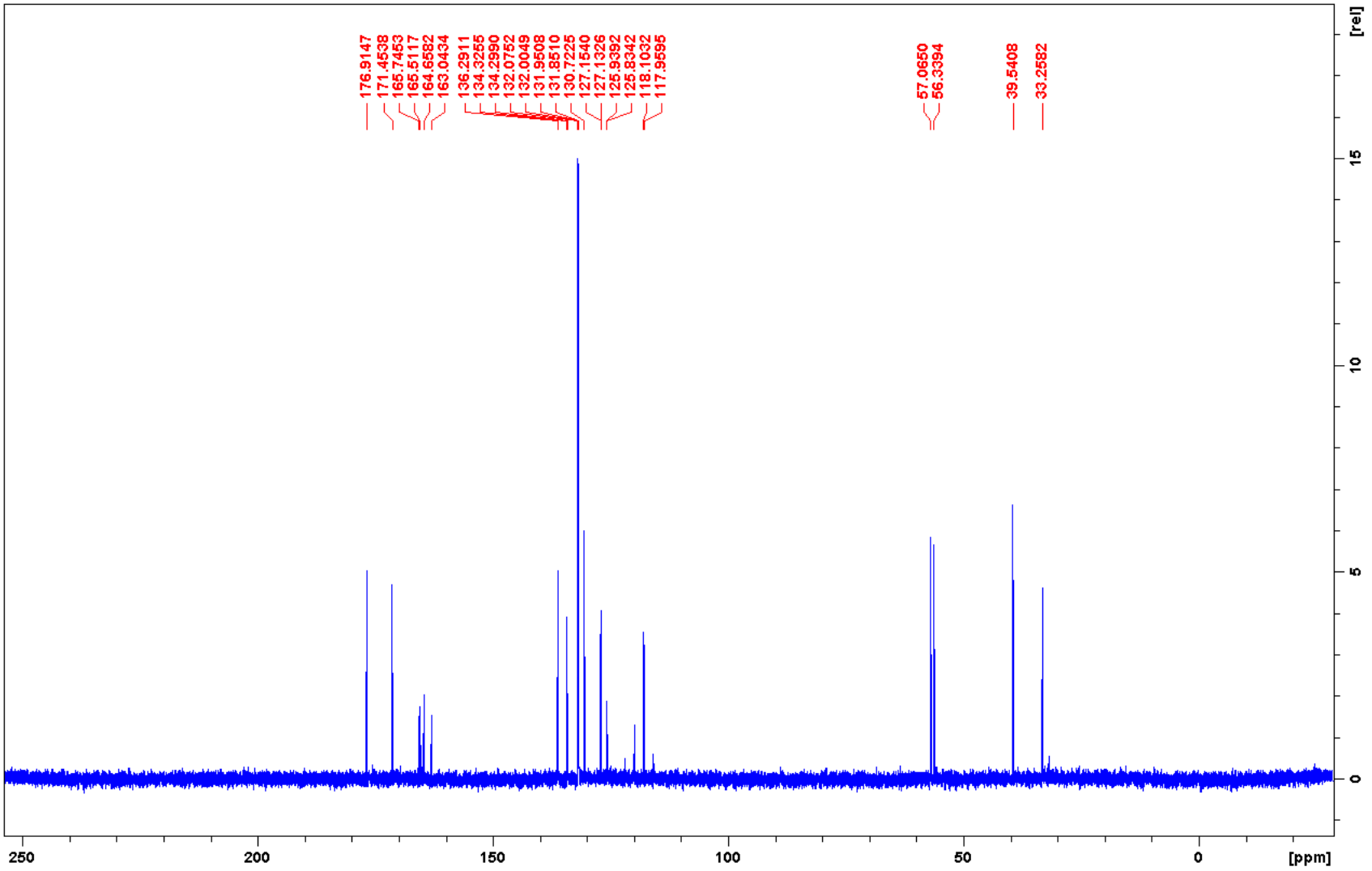


Figure S17. C-NMR spectrum of mono2 F-FF.

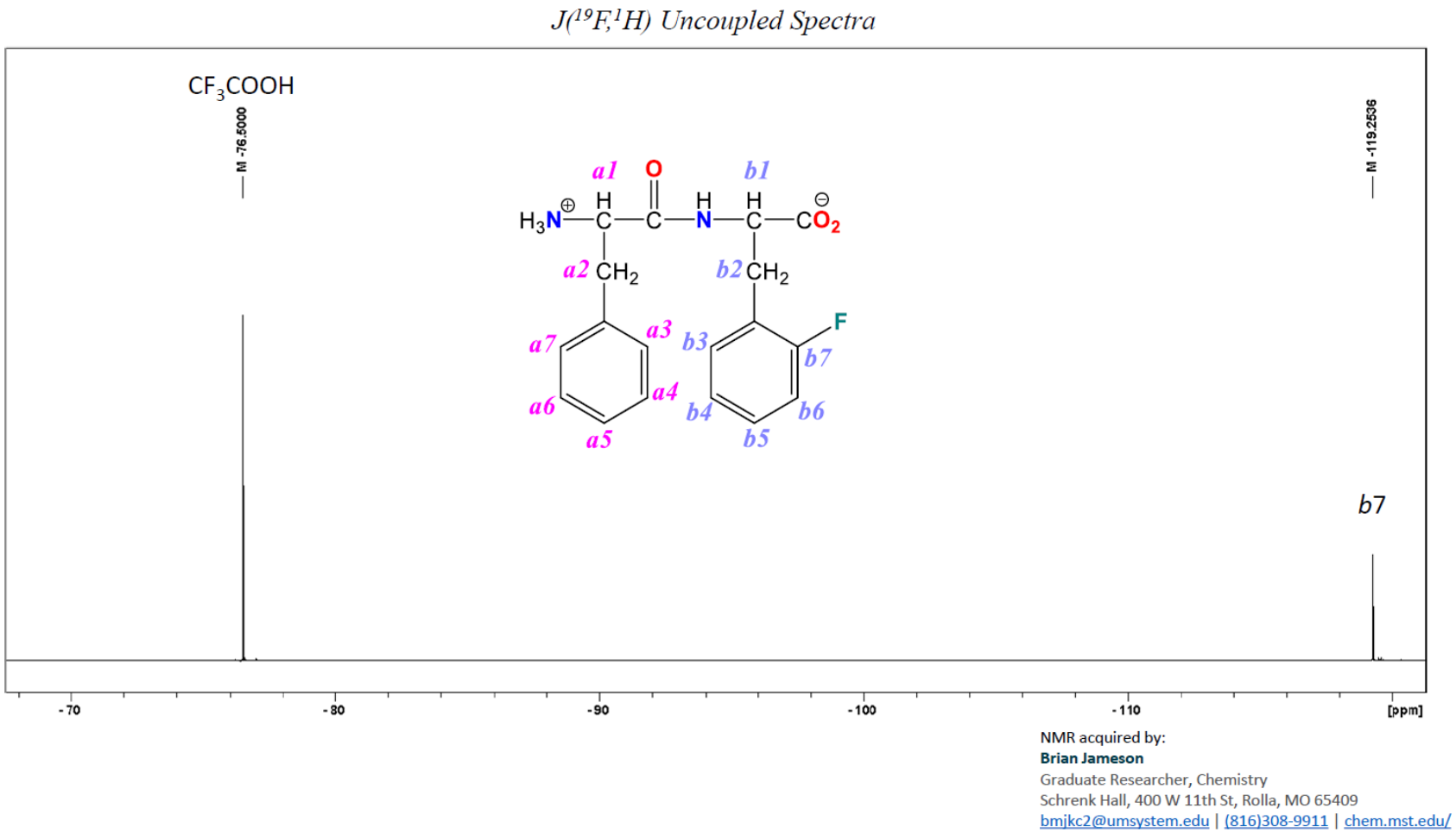


Figure S18a. F-NMR spectrum of mono2 F-FF, uncoupled.

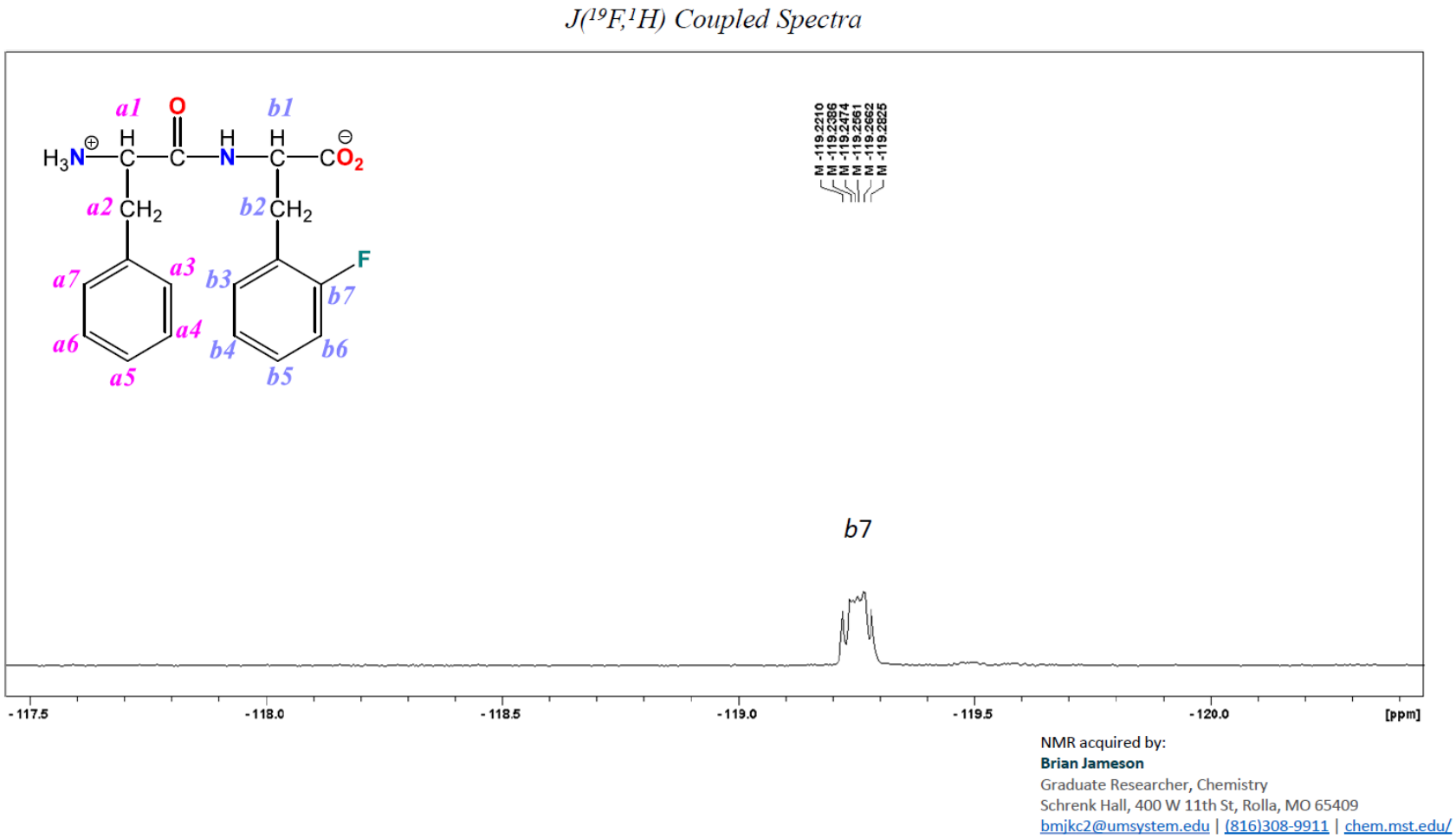


Figure S18b. F-NMR spectrum of mono2 F-FF, coupled.

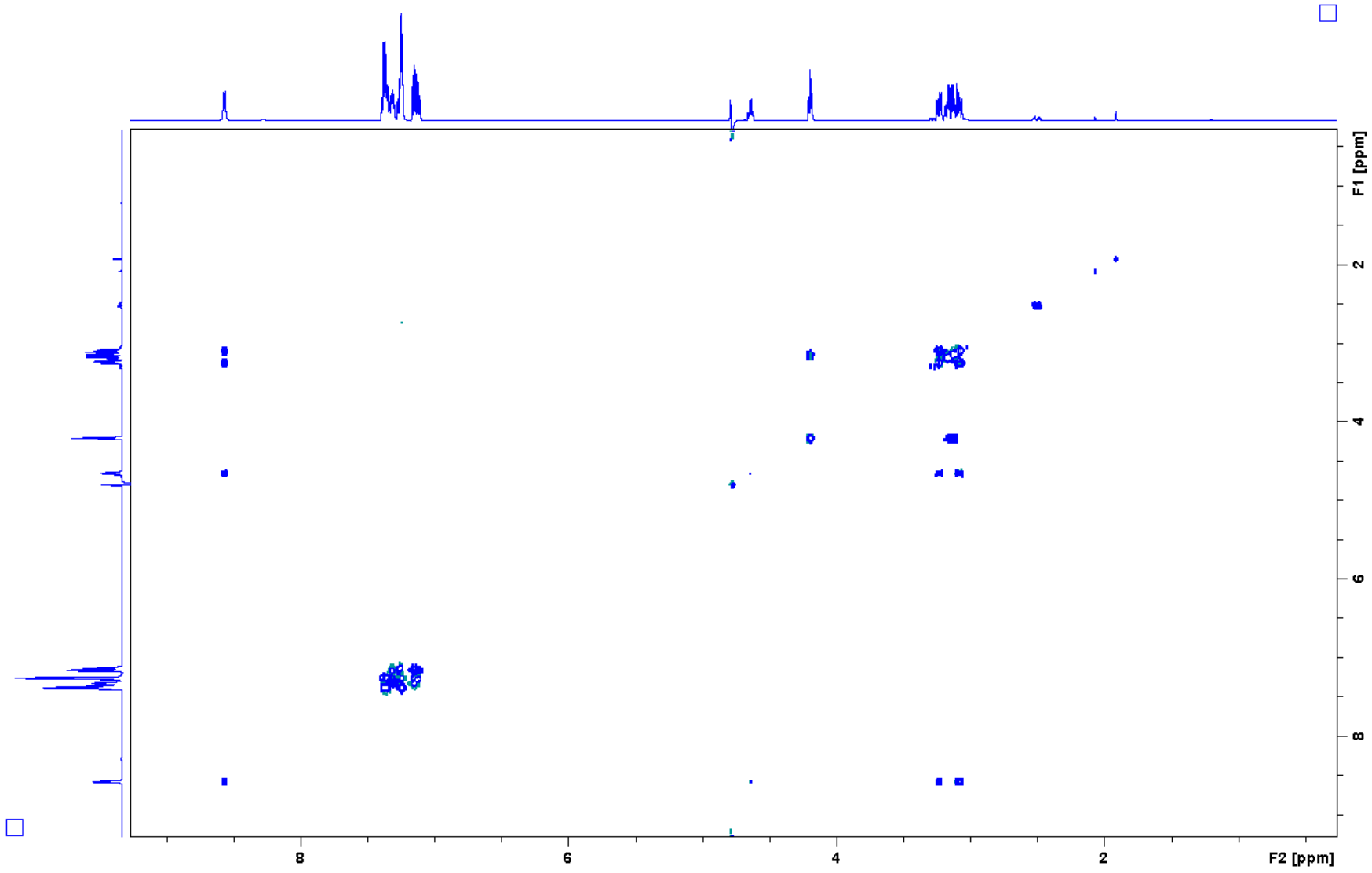


Figure S19. TOCSY spectrum of mono2 F-FF.

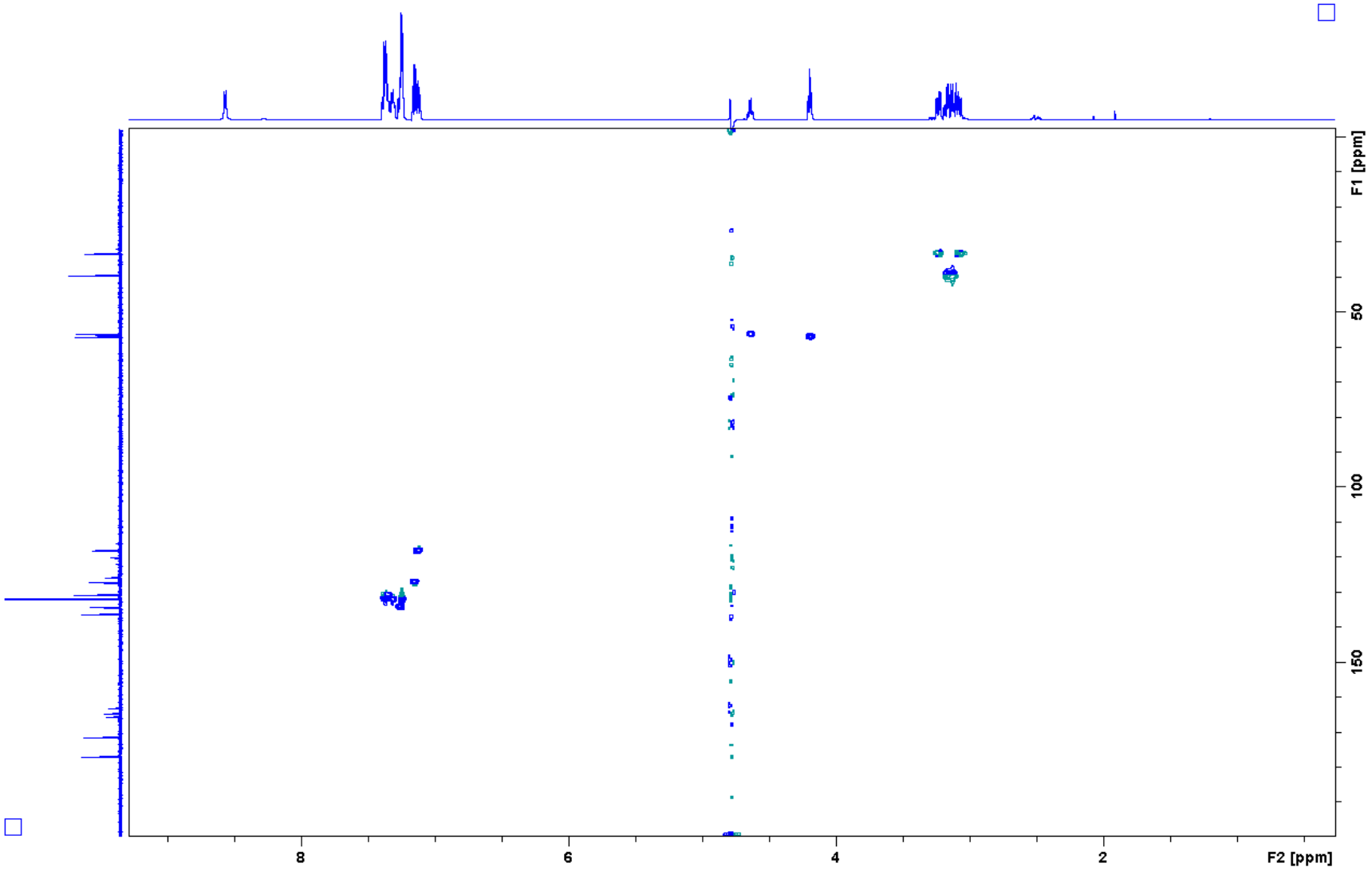


Figure S20. HSQC spectrum of mono2 F-FF.

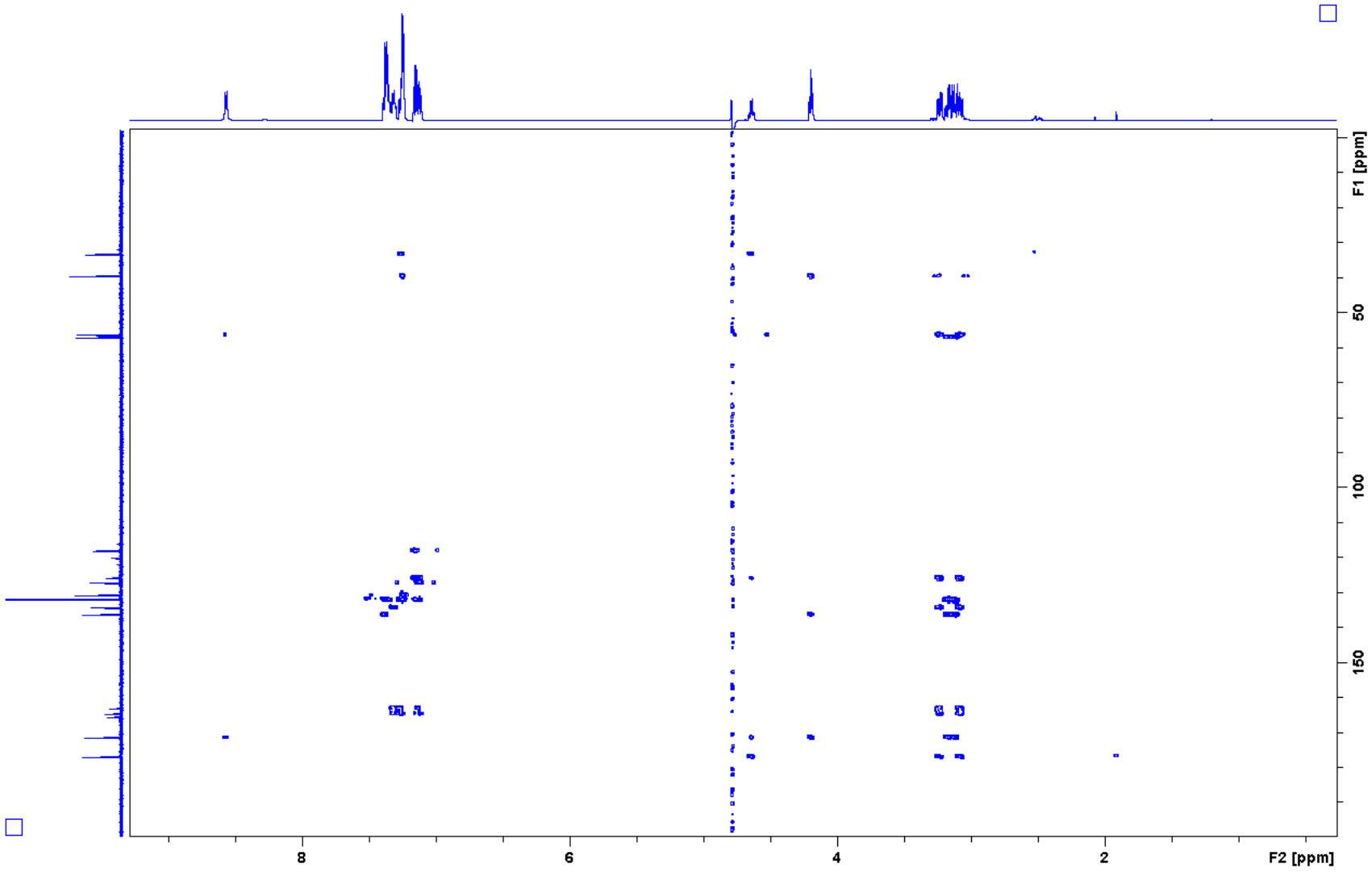


Figure S21. HMBC spectrum of mono2 F-FF.

Potential Energy Surface Analysis

Table S1. Energies and Thermochemistry of FF and Fluorinated Derivatives Computed at the SMD(B3LYP/6-31G*) Level

	Molecule	Total Energy [Hartree]	Vibrational Zero-Point Energy [kcal/mol]	Thermal Energy [kcal/mol]	Entropy S_{tot} [cal/(mol·*K*)]	Translational Entropy S_{trans} [cal/(mol·*K*)]	Lowest Vibr. Frequency [cm^{-1}]	Dipole Moment [Debye]
water		-76.422116	13.17	14.95	45.16	34.61	1677.32	2.51
FF	**M1**	-1033.189202	224.89	237.98	156.92	43.11	18.47	23.62
	M1-CIP	-1033.188540	224.49	237.58	159.31	43.11	12.65	17.41
	M1-N1	-1033.185687	223.52	236.47	156.12	43.11	14.80	10.36
	M1-N2	-1033.190247	223.21	236.51	159.00	43.11	17.19	6.27
	M1-N3	-1033.188503	223.34	236.63	159.97	43.11	16.01	5.67
	M3	-1033.196290	224.71	237.93	158.83	43.11	18.43	26.29
	M1a	-1109.633799	240.19	254.79	169.99	43.28	9.22	20.05
	M2b	-1109.630305	240.35	255.15	169.69	43.28	19.00	25.49
	M3b	-1109.631788	240.20	255.00	169.37	43.28	19.21	25.73
Mono1 F-FF	**M1**	-1132.423262	219.58	233.26	163.22	43.28	13.05	22.27
	M1-CIP	-1132.422581	219.85	233.26	159.43	43.28	14.30	17.33
	M1-N1	-1132.419385	218.53	231.96	159.10	43.28	16.19	8.81
	M1-N2	-1132.423082	218.19	231.96	161.46	43.28	18.48	5.61
	M1-N3	-1132.421443	218.31	232.08	162.32	43.28	20.46	6.12
	M3	-1132.430725	219.43	233.00	161.22	43.28	17.11	23.88
	M1a	-1208.867628	235.07	250.19	172.68	43.44	14.59	20.55
	M2b	-1208.865849	235.28	250.55	173.52	43.44	16.03	22.26
	M3b	-1208.867027	235.32	250.51	171.65	43.44	20.59	22.11
Mono2 F-FF	**M1**	-1132.424423	219.83	233.42	159.20	43.28	20.07	23.48
	M1-CIP	-1132.422366	219.86	233.32	158.91	43.28	17.64	17.29
	M1-N1	-1132.418981	218.35	231.81	158.66	43.28	18.56	10.94
	M1-N2	-1132.425944	218.19	231.95	160.14	43.28	22.47	7.86
	M1-N3	-1132.424277	218.31	232.05	160.77	43.28	21.04	7.64
	M2	-1132.428870	219.71	233.39	161.81	43.28	14.62	26.25
	M3	-1132.429441	219.49	233.29	165.31	43.28	12.40	26.18
	M1a	-1208.869801	235.14	250.19	170.27	43.44	16.17	21.13
	M2b	-1208.866864	235.59	250.71	170.53	43.44	17.73	24.43

	M3b	-1208.866727	235.16	250.45	174.31	43.44	18.13	23.75
	M3c	-1208.868508	234.85	250.22	174.62	43.44	13.03	24.65
Di F-FF	**M1**	-1231.658538	214.50	228.68	166.10	43.44	13.23	22.28
	M1-CIP	-1231.656081	214.65	228.55	162.09	43.44	14.58	16.85
	M1-N1	-1231.657278	213.09	227.35	164.39	43.44	18.85	10.36
	M1-N2	-1231.658649	212.95	227.29	166.15	43.44	13.01	7.37
	M1-N3	-1231.657088	213.21	227.48	164.66	43.44	20.24	7.92
	M2	-1308.100437	230.35	245.99	174.52	43.44	16.75	22.24
	M3	-1308.102339	229.41	245.38	179.53	43.44	10.76	22.88
	M1a	-1308.103861	230.15	245.68	172.93	43.59	22.55	19.93
	M2b	-1231.663979	214.41	228.47	164.71	43.59	15.07	23.75
	M3b	-1308.09979	230.26	245.86	173.30	43.59	14.76	23.82
	M3c	-1231.662949	214.50	228.71	167.24	43.59	9.85	23.97

Table S2. Energies and Thermochemistry of FF and Fluorinated Derivatives Computed at the SMD(MP2/6-31G*) Level

	Molecule	Total Energy [Hartree]	Vibrational Zero-Point Energy [kcal/mol]	Thermal Energy [kcal/mol]	Entropy S_{tot} [cal/(mol·*K*)]	Translational Entropy S_{trans} [cal/(mol·*K*)]	Lowest Vibr. Frequency [cm^{-1}]	Dipole Moment [Debye]
H_2O		-76.211405	13.32	15.10	45.16	34.61	1698.22	2.67
FF	**M1**	-1029.986718	226.01	239.30	156.38	43.11	20.56	25.22
	M1a	-1106.218673	241.85	256.54	164.74	43.28	23.20	21.11
Mono1 F-FF	**M1**	-1129.005608	221.26	234.93	159.83	43.28	16.47	21.61
	M1a	-1205.236987	236.64	251.91	172.24	43.44	16.45	22.21
Mono2 F-FF	**M1**	-1129.005701	221.19	234.82	157.54	43.28	20.72	24.56
	M1a	-1205.238943	236.30	251.62	170.83	43.44	17.65	22.93
Di F-FF	**M1**	-1228.025646	215.76	230.05	163.89	43.44	18.19	22.75
	M1a	-1304.258939	231.39	247.17	174.58	43.59	18.34	21.24

Table S3. Hydration Energies of FF and Fluorinated Derivatives at SMD(MP2/6-31G*).

Molecule	ΔE_{water}[a]	ΔG_{water}[a]	$\Delta^{W}A_{water}$[a]	K_{water}[b]	BR[c]
FF					
M1 + H_2O → **M1a**	-12.90	-0.37	-2.54	1.88	103.50
Mono1 F-FF					
M1 + H_2O → **M1a**	-12.53	-1.48	-3.65	474.27	26084.79
Mono2 F-FF					
M1 + H_2O → **M1a**	-13.77	-2.30	-4.47	1869.28	102810.57
Di F-FF					
M1 + H_2O → **M1a**	-13.73	-2.03	-4.20	1188.34	65358.65

a) Hydration energies in kcal/mol.

b) Equilibrium constant K_{water} computed with $\Delta^{W}A_{water} = -RT \bullet \ln(K_{water})$ at room temperature.

c) Bridging ratio BR = [bridged]/[unbridged] computed as product $K_{water} \bullet [H_2O]$.

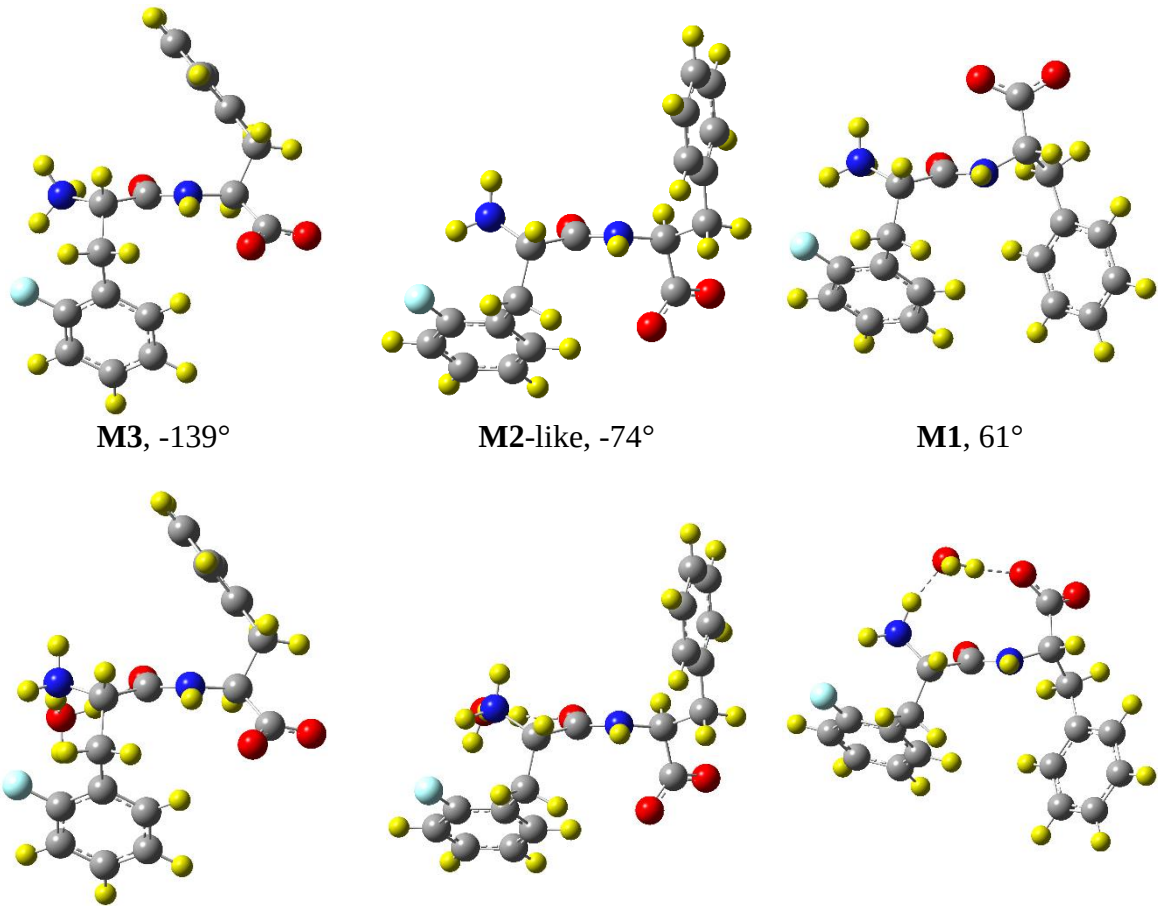


Figure S22. Minima of mono1 F-FF, unbridged structure (top) and bridged structure (bottom).

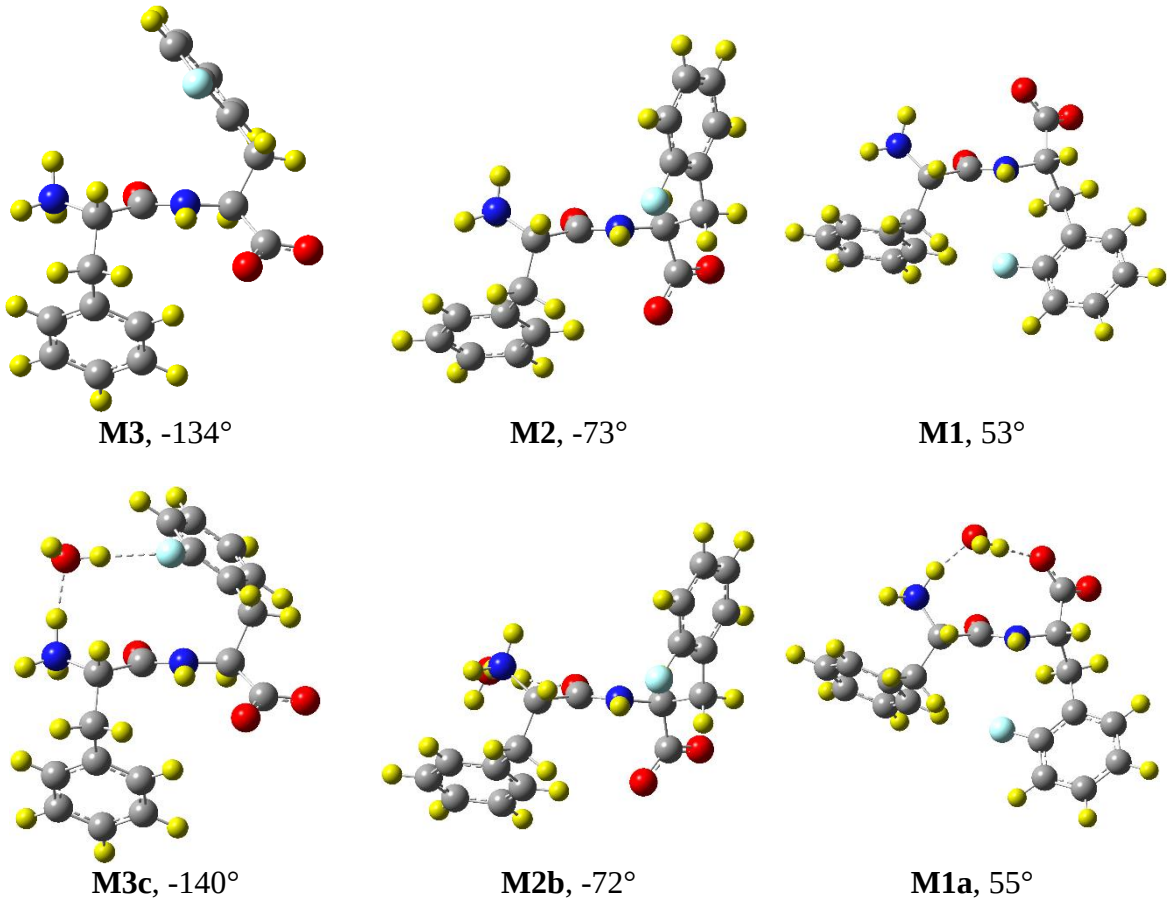
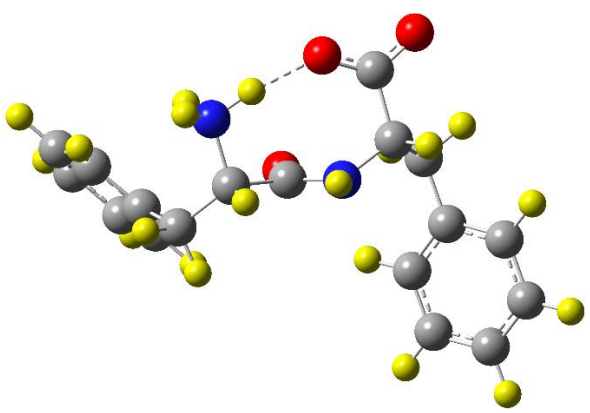
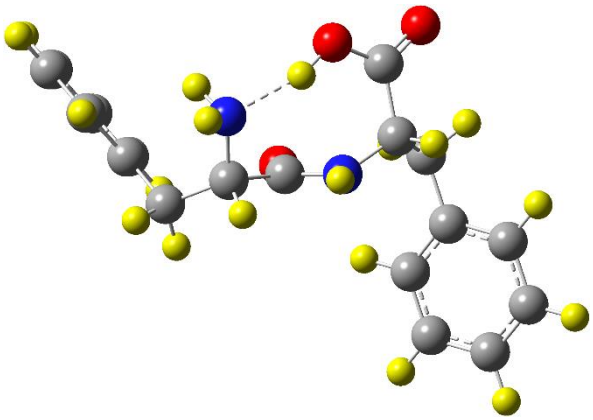


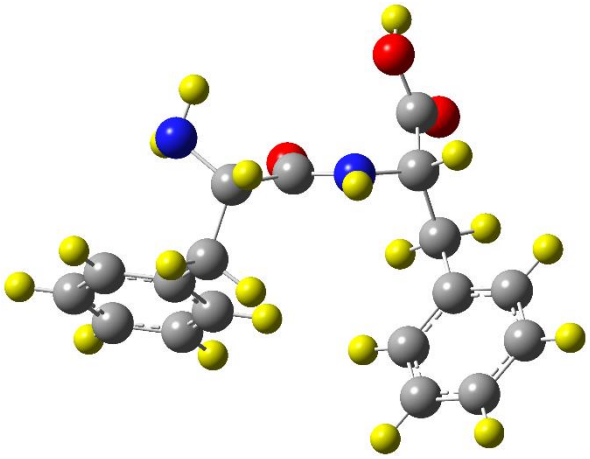
Figure S23. Minima of mono2 F-FF, unbridged structure (top) and bridged structure (bottom).



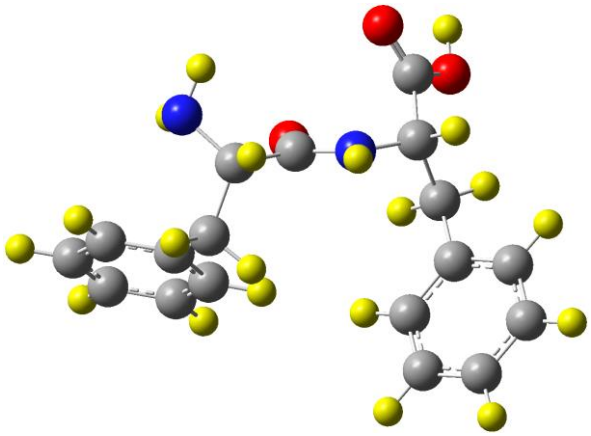
FF, **M1-CIP,**
Δ*E* = 4.86 kcal/mol
Δ*G* = 4.38 kcal/mol



FF, **M1-N1**
Δ*E* = 6.65 kcal/mol
Δ*G* = 6.00 kcal/mol

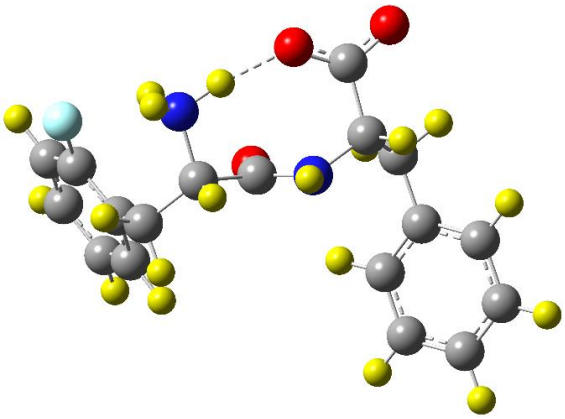


FF, **M1-N2**
Δ*E* = 3.79 kcal/mol
Δ*G* = 2.32 kcal/mol

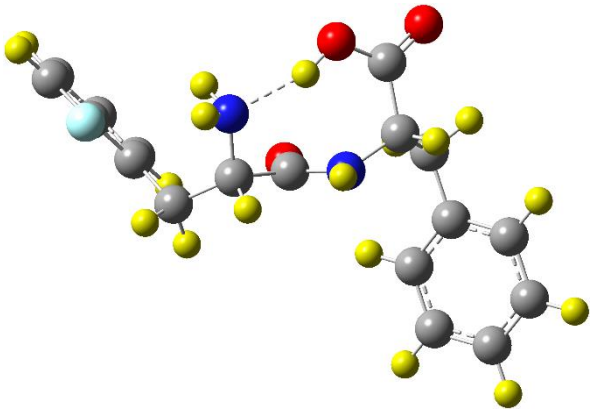


FF, **M1-N3**
Δ*E* = 4.89 kcal/mol
Δ*G* = 3.25 kcal/mol

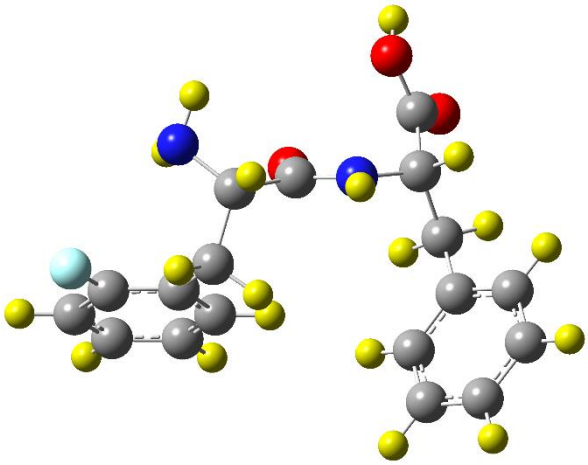
Figure S24a. Contact ion pair and neutral structures of FF, with relative energies Δ*E* and Δ*G* with respect to **M3**.



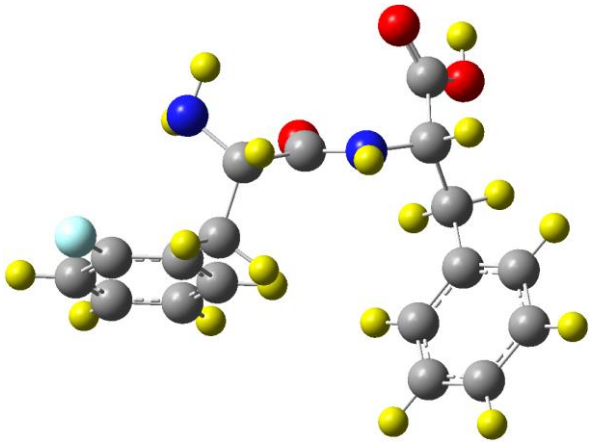
Mono1 F-FF, **M1-CIP**
Δ*E* = 5.11 kcal/mol
Δ*G* = 5.91 kcal/mol



Mono1 F-FF, **M1-N1**
Δ*E* = 7.12 kcal/mol
Δ*G* = 6.70 kcal/mol

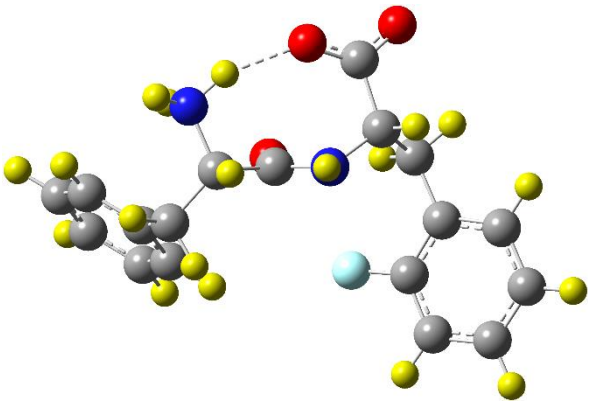


Mono1 F-FF, **M1-N2**
Δ*E* = 4.80 kcal/mol
Δ*G* = 3.68 kcal/mol

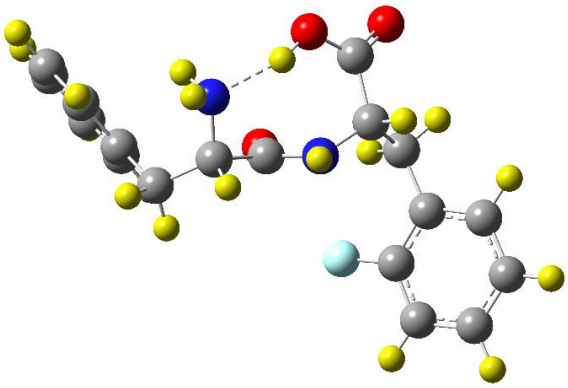


Mono1 F-FF, **M1-N3**
Δ*E* = 5.82 kcal/mol
Δ*G* = 4.57 kcal/mol

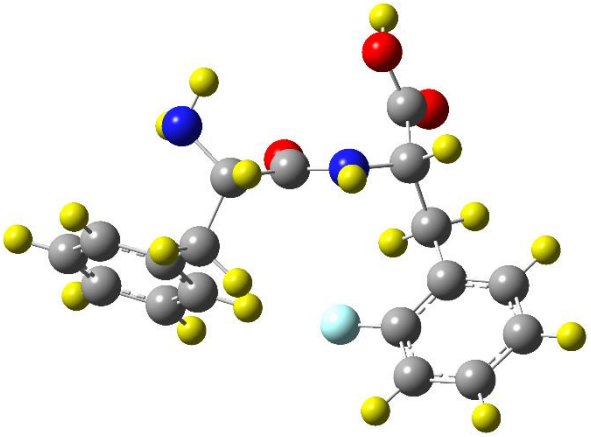
Figure S24b. Contact ion pair and neutral structures of mono1 F-FF, with relative energies Δ*E* and Δ*G* with respect to **M3**.



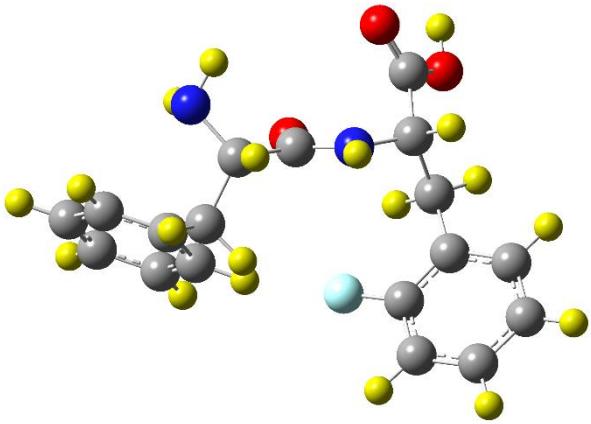
Mono2 F-FF, **M1-CIP**
Δ*E* = 4.44 kcal/mol
Δ*G* = 6.38 kcal/mol



Mono2 F-FF, **M1-N1**
Δ*E* = 6.56 kcal/mol
Δ*G* = 7.06 kcal/mol

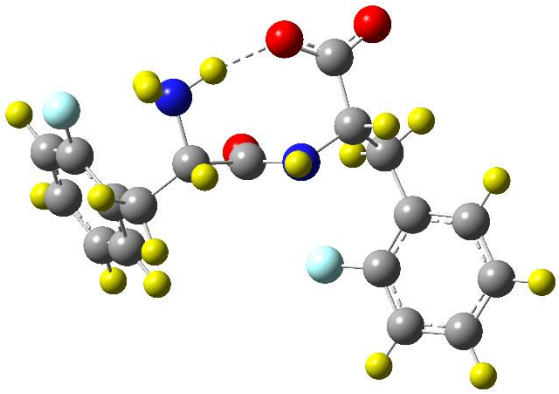


Mono2 F-FF, **M1-N2**
Δ*E* = 2.19 kcal/mol
Δ*G* = 2.39 kcal/mol

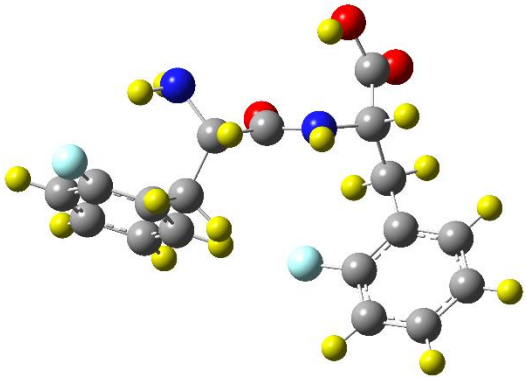


Mono2 F-FF, **M1-N3**
Δ*E* = 3.24 kcal/mol
Δ*G* = 3.35 kcal/mol

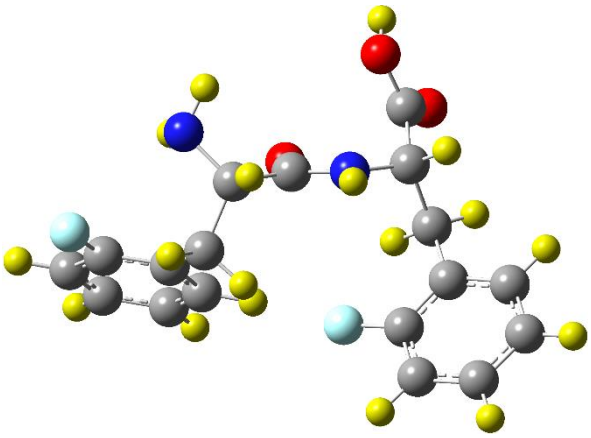
Figure S24c. Contact ion pair and neutral structures of mono2 F-FF, with relative energies Δ*E* and Δ*G* with respect to **M3**.



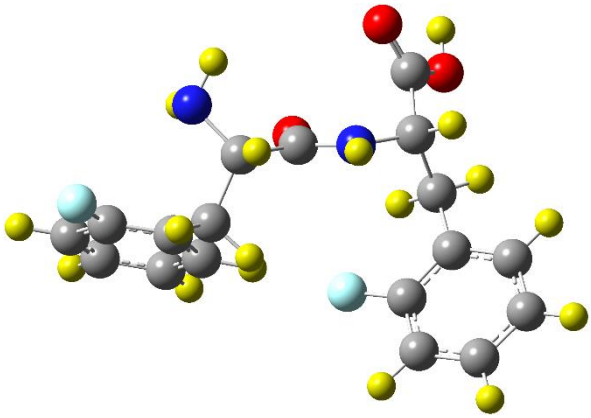
Di F-FF, **M1-CIP**
Δ*E* = 4.96 kcal/mol
Δ*G* = 5.82 kcal/mol



Di F-FF, **M1-N1**
Δ*E* = 4.20 kcal/mol
Δ*G* = 3.18 kcal/mol

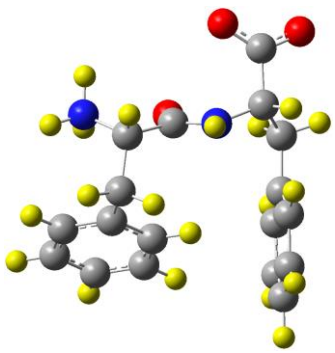


Di F-FF, **M1-N2**
Δ*E* = 3.34 kcal/mol
Δ*G* = 1.73 kcal/mol

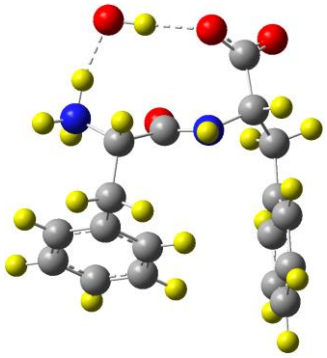


Di F-FF, **M1-N3**
Δ*E* = 4.32 kcal/mol
Δ*G* = 3.35 kcal/mol

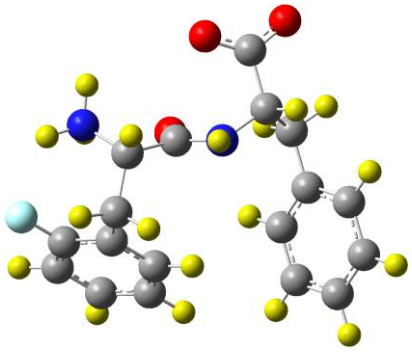
Figure S24d. Contact ion pair and neutral structures of di F-FF, with relative energies Δ*E* and Δ*G* with respect to **M3**.



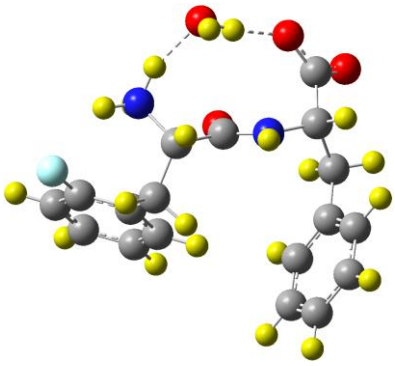
FF, **M1**



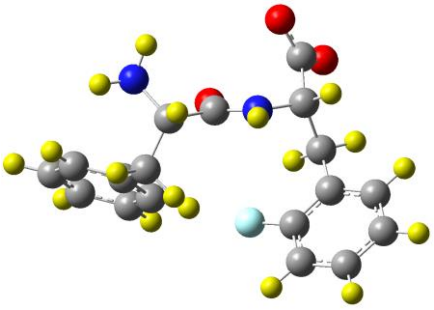
FF, **M1a**



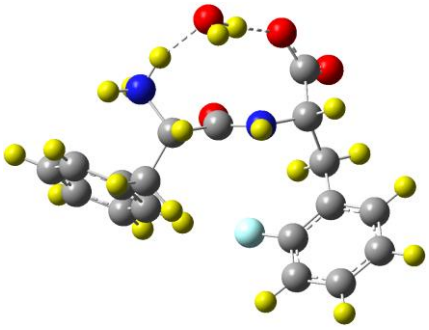
Mono1 F-FF, **M1**



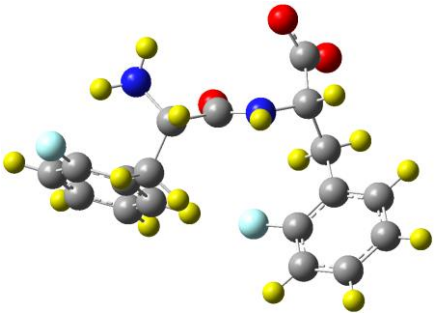
Mono1 F-FF, **M1a**



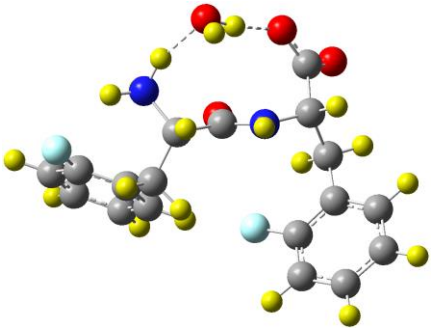
Mono2 F-FF, **M1**



Mono2 F-FF, **M1a**



Di F-FF, **M1**



Di F-FF, **M1a**

Figure S25. **M1** and **M1a** structures calculated at SMD(MP2/6-31G*) level.

Cartesian Coordinates of Stationary Structures at SMD(B3LYP/6-31G*)

Parent FF

Without water

M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.606696	1.577118	-0.914117
2	8	0	1.537035	3.740619	-0.224126
3	8	0	3.192464	2.884678	-1.491570
4	7	0	-2.512485	2.546764	0.644666
5	7	0	0.862804	1.298367	0.822866
6	6	0	-1.498352	1.662296	1.315187
7	6	0	-2.147576	0.328853	1.751410
8	6	0	-2.783361	-0.484630	0.642131
9	6	0	-2.034553	-1.428067	-0.076137
10	6	0	-2.618575	-2.169096	-1.104666
11	6	0	-3.963662	-1.977199	-1.432063
12	6	0	-4.721521	-1.045494	-0.719370
13	6	0	-4.135414	-0.307978	0.312273
14	6	0	-0.352156	1.514044	0.298910
15	6	0	2.106731	1.394249	0.047646
16	6	0	2.306561	0.233344	-0.947372
17	6	0	2.449943	-1.141610	-0.326525
18	6	0	1.612418	-2.194080	-0.722068
19	6	0	1.759106	-3.476783	-0.184351
20	6	0	2.751520	-3.729353	0.764043
21	6	0	3.597262	-2.690481	1.165172
22	6	0	3.448282	-1.412951	0.623306
23	6	0	2.274373	2.803085	-0.627612
24	1	0	-2.190569	3.521306	0.619642
25	1	0	-3.420803	2.518512	1.122357
26	1	0	-2.630513	2.237116	-0.330734
27	1	0	0.945808	1.390177	1.828358
28	1	0	-1.158521	2.195862	2.204292
29	1	0	-1.361711	-0.247867	2.249149
30	1	0	-2.896542	0.575519	2.512572
31	1	0	-0.990327	-1.587989	0.178152
32	1	0	-2.024090	-2.899504	-1.647098
33	1	0	-4.419323	-2.555051	-2.231435
34	1	0	-5.770699	-0.896555	-0.959753
35	1	0	-4.735734	0.404587	0.874116
36	1	0	2.905473	1.340415	0.794744
37	1	0	3.215749	0.475501	-1.505987
38	1	0	1.484339	0.227822	-1.668684
39	1	0	0.840657	-2.007945	-1.465287
40	1	0	1.098028	-4.276031	-0.509420
41	1	0	2.868585	-4.724543	1.184391
42	1	0	4.378284	-2.876691	1.897911
43	1	0	4.121078	-0.618784	0.938994

Rotational constants (GHZ): 0.2958733 0.2070111 0.1401292

M1-CIP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.497053	0.015780	-0.591677
2	8	0	0.077152	3.218331	-0.204803
3	8	0	1.892800	3.444616	-1.506422
4	7	0	-2.005724	1.940112	1.137949
5	7	0	0.967485	0.911871	0.929667
6	6	0	-1.355117	0.646662	1.581503
7	6	0	-2.367019	-0.497769	1.770591
8	6	0	-3.293986	-0.837517	0.618677
9	6	0	-2.996309	-1.882749	-0.268657
10	6	0	-3.868221	-2.208840	-1.307677
11	6	0	-5.056561	-1.492578	-1.480550
12	6	0	-5.370295	-0.456456	-0.599809
13	6	0	-4.498917	-0.138625	0.446034
14	6	0	-0.244155	0.450637	0.536170
15	6	0	1.881167	1.573811	-0.010875
16	6	0	2.488267	0.649037	-1.089270
17	6	0	3.232400	-0.543148	-0.528154
18	6	0	2.623403	-1.803741	-0.449179
19	6	0	3.308997	-2.900559	0.079326
20	6	0	4.619300	-2.753395	0.540437
21	6	0	5.238260	-1.502167	0.467471
22	6	0	4.549667	-0.409605	-0.063241
23	6	0	1.215021	2.847059	-0.634491
24	1	0	-1.256425	2.583913	0.768701
25	1	0	-2.522448	2.381973	1.905773
26	1	0	-2.663975	1.770399	0.367578
27	1	0	0.981818	1.328664	1.853296
28	1	0	-0.914173	0.865033	2.555209
29	1	0	-1.774271	-1.376399	2.046848
30	1	0	-2.968511	-0.234831	2.648501
31	1	0	-2.074459	-2.443457	-0.140896
32	1	0	-3.621206	-3.024510	-1.981908
33	1	0	-5.735013	-1.746825	-2.290222
34	1	0	-6.297149	0.098628	-0.716122
35	1	0	-4.766110	0.651477	1.144775
36	1	0	2.707878	1.940810	0.606665
37	1	0	3.174201	1.275308	-1.666234
38	1	0	1.700475	0.315009	-1.767989
39	1	0	1.603275	-1.924329	-0.805465
40	1	0	2.819640	-3.869957	0.128162
41	1	0	5.154965	-3.605925	0.949344
42	1	0	6.259717	-1.378362	0.818000
43	1	0	5.040827	0.559337	-0.123955

Rotational constants (GHZ): 0.3821604 0.1492470
0.1217597

M1-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.345124	-0.450792	-0.605161
2	8	0	-0.276007	3.007181	0.099048
3	8	0	1.336404	3.417212	-1.356849
4	7	0	-1.796240	1.280544	1.681835
5	7	0	0.929514	0.648959	0.950183
6	6	0	-1.256897	-0.102462	1.638730

7	6	0	-2.295232	-1.239098	1.478292
8	6	0	-3.387249	-1.045064	0.443186
9	6	0	-3.311039	-1.636025	-0.827501
10	6	0	-4.334069	-1.466531	-1.761852
11	6	0	-5.457357	-0.697606	-1.444867
12	6	0	-5.552661	-0.109691	-0.182231
13	6	0	-4.529916	-0.288927	0.753355
14	6	0	-0.183668	-0.034842	0.544653
15	6	0	1.714777	1.509517	0.068819
16	6	0	2.455421	0.785063	-1.079065
17	6	0	3.413202	-0.279719	-0.590461
18	6	0	3.046686	-1.632669	-0.580718
19	6	0	3.932911	-2.611093	-0.122835
20	6	0	5.201649	-2.249490	0.336003
21	6	0	5.578522	-0.903480	0.331669
22	6	0	4.690854	0.070717	-0.128891
23	6	0	0.897069	2.704840	-0.465720
24	1	0	-0.641345	2.366255	0.791696
25	1	0	-2.149137	1.485449	2.615713
26	1	0	-2.595546	1.347919	1.049914
27	1	0	0.901801	0.973888	1.910386
28	1	0	-0.742251	-0.270693	2.589698
29	1	0	-1.744050	-2.163395	1.271877
30	1	0	-2.766433	-1.364216	2.460007
31	1	0	-2.441996	-2.234603	-1.084433
32	1	0	-4.254598	-1.938083	-2.737881
33	1	0	-6.253723	-0.565758	-2.172306
34	1	0	-6.426750	0.479865	0.081503
35	1	0	-4.627494	0.149964	1.743621
36	1	0	2.475463	1.967623	0.711436
37	1	0	3.006281	1.556525	-1.623795
38	1	0	1.723610	0.354407	-1.764767
39	1	0	2.059713	-1.919331	-0.934747
40	1	0	3.631808	-3.655434	-0.126597
41	1	0	5.892626	-3.009548	0.690568
42	1	0	6.565695	-0.612553	0.681266
43	1	0	4.993206	1.115748	-0.136983

Rotational constants (GHZ): 0.4440538 0.1345749 0.1182037
Standard basis: 6-31G(d) (6D, 7F)

M1-N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.880014	1.678235	-0.332611
2	8	0	1.263872	3.791434	0.189655
3	8	0	1.659723	3.080697	-1.912961
4	7	0	-2.466240	1.532772	2.083440
5	7	0	0.918010	1.142044	0.940377
6	6	0	-1.315284	0.662353	1.833520
7	6	0	-1.771285	-0.793634	1.538023
8	6	0	-2.756999	-0.959548	0.398726
9	6	0	-2.320838	-1.215700	-0.910541
10	6	0	-3.233818	-1.374885	-1.954823
11	6	0	-4.606045	-1.278993	-1.708891
12	6	0	-5.055651	-1.028020	-0.410522
13	6	0	-4.138608	-0.872729	0.631837
14	6	0	-0.414362	1.195407	0.713259
15	6	0	1.907027	1.504176	-0.070116
16	6	0	2.144717	0.404652	-1.125823
17	6	0	2.712494	-0.865585	-0.527898
18	6	0	1.926266	-2.017372	-0.390808
19	6	0	2.453398	-3.184100	0.170871
20	6	0	3.779485	-3.215284	0.606186

21	6	0	4.575583	-2.073633	0.472367
22	6	0	4.045838	-0.911861	-0.090832
23	6	0	1.569411	2.846487	-0.721337
24	1	0	1.107006	4.628956	-0.291057
25	1	0	-2.959330	1.656400	1.198189
26	1	0	-2.116203	2.460965	2.324226
27	1	0	1.255256	0.692143	1.782401
28	1	0	-0.724067	0.621021	2.753574
29	1	0	-0.875938	-1.396611	1.347877
30	1	0	-2.224065	-1.166399	2.463079
31	1	0	-1.255608	-1.296361	-1.112054
32	1	0	-2.873058	-1.577716	-2.959862
33	1	0	-5.317854	-1.405703	-2.520153
34	1	0	-6.120895	-0.959448	-0.205695
35	1	0	-4.497706	-0.690481	1.641268
36	1	0	2.842975	1.680148	0.472356
37	1	0	2.839757	0.809973	-1.868345
38	1	0	1.200673	0.198706	-1.639627
39	1	0	0.895576	-2.003851	-0.736195
40	1	0	1.827221	-4.067460	0.264655
41	1	0	4.191771	-4.121206	1.042141
42	1	0	5.611059	-2.089806	0.802083
43	1	0	4.674409	-0.030304	-0.197430

Rotational constants (GHZ): 0.3205612 0.1773917
0.1391196
Standard basis: 6-31G(d) (6D, 7F)

M1-N3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.758863	1.539351	0.470682
2	8	0	-2.227109	3.057982	1.769079
3	8	0	-1.256307	3.781506	-0.127812
4	7	0	2.435279	1.740563	-1.901055
5	7	0	-0.950180	1.114080	-0.961213
6	6	0	1.341074	0.775144	-1.763507
7	6	0	1.888090	-0.664838	-1.560151
8	6	0	2.868518	-0.853146	-0.419404
9	6	0	2.439070	-1.264059	0.851858
10	6	0	3.349292	-1.448238	1.894500
11	6	0	4.712341	-1.222901	1.685140
12	6	0	5.155796	-0.817252	0.424244
13	6	0	4.241799	-0.637947	-0.616791
14	6	0	0.364554	1.167277	-0.647328
15	6	0	-2.003122	1.466579	-0.018058
16	6	0	-2.245078	0.391289	1.067642
17	6	0	-2.708363	-0.927972	0.485607
18	6	0	-1.839622	-2.022725	0.386548
19	6	0	-2.272243	-3.235518	-0.157514
20	6	0	-3.585132	-3.370628	-0.613103
21	6	0	-4.462634	-2.286320	-0.517972
22	6	0	-4.026659	-1.078004	0.027708
23	6	0	-1.754557	2.880481	0.522265
24	1	0	-2.092694	3.998600	2.003850
25	1	0	2.886613	1.829918	-0.989765
26	1	0	2.027513	2.657656	-2.087551
27	1	0	-1.221419	0.822385	-1.891174
28	1	0	0.790068	0.765115	-2.709011

29	1	0	1.031513	-1.336298	-1.430077
30	1	0	2.377072	-0.941214	-2.500627
31	1	0	1.381450	-1.446481	1.024297
32	1	0	2.993724	-1.772060	2.869246
33	1	0	5.422343	-1.368833	2.494747
34	1	0	6.214564	-0.646995	0.246901
35	1	0	-2.920852	1.563564	-0.609944
36	1	0	-3.007459	0.775125	1.751287
37	1	0	-1.324935	0.253433	1.642217
38	1	0	-1.583405	-4.073778	-0.221549
39	1	0	-3.924341	-4.313106	-1.034310
40	1	0	-5.488553	-2.383577	-0.863370
41	1	0	-4.717777	-0.241324	0.105249
42	1	0	-0.818711	-1.927327	0.747878
43	1	0	4.597274	-0.335345	-1.598112

Rotational constants (GHZ): 0.3220786 0.1747418
0.1357302
Standard basis: 6-31G(d) (6D, 7F)

M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.130917	-1.077315	0.568917
2	8	0	-0.356222	3.112499	-1.270452
3	8	0	0.910799	3.932633	0.409505
4	7	0	-1.096638	-2.684965	-1.092975
5	7	0	0.420632	0.626794	-0.934851
6	6	0	-0.973342	-1.263772	-1.561792
7	6	0	-2.367336	-0.619304	-1.737375
8	6	0	-3.162394	-0.419587	-0.462720
9	6	0	-3.038556	0.767626	0.275612
10	6	0	-3.763577	0.950351	1.454517
11	6	0	-4.624701	-0.050339	1.912783
12	6	0	-4.761076	-1.232643	1.181969
13	6	0	-4.036756	-1.413505	0.001240
14	6	0	-0.078585	-0.551225	-0.535283
15	6	0	1.052660	1.587821	-0.033775
16	6	0	2.596577	1.590145	-0.155798
17	6	0	3.248455	0.271144	0.195286
18	6	0	3.686671	-0.608156	-0.804547
19	6	0	4.269184	-1.836235	-0.477810
20	6	0	4.423711	-2.204884	0.860005
21	6	0	3.994018	-1.335629	1.867681
22	6	0	3.412709	-0.111053	1.536289
23	6	0	0.480617	3.005750	-0.325825
24	1	0	-0.200652	-3.178189	-1.178886
25	1	0	-1.803127	-3.196837	-1.633938
26	1	0	-1.354568	-2.704446	-0.097751
27	1	0	0.024164	1.064577	-1.764565
28	1	0	-0.478816	-1.301717	-2.533872
29	1	0	-2.201256	0.342968	-2.231894
30	1	0	-2.925588	-1.245390	-2.443181
31	1	0	-2.378763	1.554323	-0.082638
32	1	0	-3.660035	1.877388	2.011910
33	1	0	-5.190916	0.093999	2.828817
34	1	0	-5.435888	-2.012055	1.525306
35	1	0	-4.159068	-2.330141	-0.571742
36	1	0	0.781008	1.318921	0.991586

37	1	0	2.958543	2.378916	0.511183
38	1	0	2.864719	1.877905	-1.179443
39	1	0	3.576216	-0.325037	-1.848727
40	1	0	4.604704	-2.501540	-1.269250
41	1	0	4.878656	-3.157833	1.116669
42	1	0	4.115241	-1.610718	2.912270
43	1	0	3.083839	0.560550	2.326427

Rotational constants (GHZ): 0.3703007 0.1684556 0.1398062

With water

M1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.828896	-1.026253	-0.871847
2	8	0	-0.945201	-3.604979	-0.558527
3	8	0	-2.281650	-2.814643	-2.174049
4	7	0	2.547461	-1.826133	1.115454
5	7	0	-0.853550	-1.097751	0.674138
6	6	0	1.442119	-0.870414	1.451704
7	6	0	1.969669	0.561486	1.693284
8	6	0	2.718469	1.211208	0.547441
9	6	0	2.046325	2.014221	-0.385698
10	6	0	2.737066	2.619315	-1.436704
11	6	0	4.114981	2.429130	-1.572801
12	6	0	4.797068	1.637201	-0.646592
13	6	0	4.103688	1.037615	0.407780
14	6	0	0.431194	-0.997909	0.303388
15	6	0	-1.941668	-1.401388	-0.258921
16	6	0	-2.322187	-0.198857	-1.147703
17	6	0	-2.838219	0.998703	-0.377905
18	6	0	-2.137070	2.212021	-0.373149
19	6	0	-2.614037	3.318656	0.336219
20	6	0	-3.806625	3.228192	1.055986
21	6	0	-4.520454	2.025542	1.055137
22	6	0	-4.040892	0.925037	0.343689
23	6	0	-1.676944	-2.709073	-1.077889
24	1	0	2.142101	-2.808435	1.097533
25	1	0	3.307755	-1.770386	1.801038
26	1	0	2.928666	-1.610483	0.187007
27	1	0	-1.056071	-1.138142	1.665085
28	1	0	1.005605	-1.234359	2.383154
29	1	0	1.098513	1.165944	1.966459
30	1	0	2.615349	0.511050	2.577722
31	1	0	0.976079	2.171219	-0.279207
32	1	0	2.199976	3.241932	-2.147233
33	1	0	4.653497	2.901467	-2.389783
34	1	0	5.870163	1.492184	-0.737553
35	1	0	4.645232	0.438448	1.136666
36	1	0	-2.800706	-1.638003	0.378525
37	1	0	-3.091143	-0.555959	-1.838290
38	1	0	-1.456835	0.088932	-1.752650
39	1	0	-1.213251	2.293285	-0.940815
40	1	0	-2.052933	4.249493	0.323945
41	1	0	-4.180211	4.085955	1.608730

42	1	0	-5.454534	1.946612	1.605436
43	1	0	-4.608609	-0.003114	0.345253
44	8	0	1.135181	-4.172471	1.094670
45	1	0	0.343862	-3.880889	0.566444
46	1	0	1.597405	-4.776915	0.489819

Rotational constants (GHZ): 0.2542747 0.1805886 0.1252683

M2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.626851	-0.037772	1.275908
2	8	0	-0.158193	2.615552	-0.909254
3	8	0	1.114618	3.599927	0.676017
4	7	0	-1.432509	-2.518120	0.184391
5	7	0	0.927554	0.133655	-0.373110
6	6	0	-0.885042	-1.436046	-0.701699
7	6	0	-1.989923	-0.839785	-1.611310
8	6	0	-3.249796	-0.352953	-0.923506
9	6	0	-3.335268	0.939441	-0.382967
10	6	0	-4.504059	1.369347	0.247901
11	6	0	-5.606597	0.516209	0.347415
12	6	0	-5.535591	-0.768736	-0.194418
13	6	0	-4.366147	-1.196770	-0.826975
14	6	0	-0.184197	-0.384849	0.164907
15	6	0	1.581266	1.316810	0.179825
16	6	0	2.981482	1.491336	-0.446648
17	6	0	3.921774	0.328004	-0.215100
18	6	0	4.203454	-0.585255	-1.240533
19	6	0	5.059938	-1.668193	-1.023024
20	6	0	5.650354	-1.853390	0.228622
21	6	0	5.379446	-0.947919	1.259305
22	6	0	4.523309	0.131820	1.037659
23	6	0	0.752846	2.623242	-0.035795
24	1	0	-0.666139	-3.042869	0.621075
25	1	0	-1.984188	-3.183599	-0.369640
26	1	0	-2.043302	-2.145437	0.958975
27	1	0	1.182329	-0.151503	-1.313074
28	1	0	-0.150684	-1.920915	-1.346360
29	1	0	-1.515367	-0.023175	-2.165242
30	1	0	-2.248159	-1.617222	-2.338430
31	1	0	-2.485881	1.612209	-0.461737
32	1	0	-4.554891	2.374367	0.658291
33	1	0	-6.515906	0.853584	0.837370
34	1	0	-6.390251	-1.436872	-0.130907
35	1	0	-4.319720	-2.195293	-1.256186
36	1	0	1.685321	1.166271	1.257611
37	1	0	3.398950	2.407015	-0.016589
38	1	0	2.861693	1.663582	-1.523763
39	1	0	3.752121	-0.441871	-2.219892
40	1	0	5.267069	-2.363166	-1.832633
41	1	0	6.319138	-2.692569	0.399779
42	1	0	5.839303	-1.080713	2.235155
43	1	0	4.321414	0.834488	1.843174
44	8	0	-2.828837	-1.363701	2.339105
45	1	0	-2.148318	-0.678968	2.153140
46	1	0	-2.459242	-1.852017	3.094749

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 Rotational constants (GHZ):           0.4411152           0.1207093
0.1075689
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M3b

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 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          8           0       -0.211689   -0.984331   -0.388014
      2          8           0        0.061019    3.405326    1.010801
      3          8           0       -1.170823    3.965736   -0.797541
      4          7           0        1.136925   -2.330273    1.531171
      5          7           0       -0.550552    0.859877    0.911099
      6          6           0        0.924886   -0.861811    1.757483
      7          6           0        2.271302   -0.108036    1.869997
      8          6           0        3.096833   -0.015311    0.603006
      9          6           0        2.905901    1.045250   -0.296495
     10          6           0        3.664706    1.131499   -1.465278
     11          6           0        4.628865    0.160961   -1.750410
     12          6           0        4.833615   -0.893117   -0.857169
     13          6           0        4.074163   -0.977649    0.312026
     14          6           0       -0.000760   -0.332119    0.650872
     15          6           0       -1.231250    1.684184   -0.085055
     16          6           0       -2.773350    1.628396    0.048637
     17          6           0       -3.369458    0.257278   -0.179999
     18          6           0       -3.768572   -0.547891    0.895685
     19          6           0       -4.303392   -1.821488    0.680682
     20          6           0       -4.448323   -2.310695   -0.619028
     21          6           0       -4.056340   -1.516644   -1.701426
     22          6           0       -3.522296   -0.246433   -1.481578
     23          6           0       -0.730222    3.151415    0.055315
     24          1           0        0.251775   -2.837431    1.640747
     25          1           0        1.796266   -2.701867    2.223559
     26          1           0        1.494903   -2.552790    0.567881
     27          1           0       -0.189559    1.406700    1.690533
     28          1           0        0.413474   -0.778668    2.718770
     29          1           0        2.031644    0.897080    2.231827
     30          1           0        2.847197   -0.597179    2.663886
     31          1           0        2.170260    1.813388   -0.069855
     32          1           0        3.507905    1.961237   -2.149231
     33          1           0        5.221771    0.230275   -2.658296
     34          1           0        5.588288   -1.646646   -1.065634
     35          1           0        4.245644   -1.793934    1.010057
     36          1           0       -0.948454    1.320595   -1.077249
     37          1           0       -3.173063    2.337643   -0.683097
     38          1           0       -3.049355    1.994806    1.044628
     39          1           0       -3.666329   -0.170439    1.910453
     40          1           0       -4.609662   -2.428016    1.529139
     41          1           0       -4.866938   -3.299043   -0.788873
     42          1           0       -4.170632   -1.885916   -2.717341
     43          1           0       -3.223445    0.366822   -2.329030
     44          8           0        1.681351   -2.887062   -1.187152
     45          1           0        0.988584   -2.193338   -1.237397
     46          1           0        1.178417   -3.714599   -1.279702
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3255179           0.1610784
0.1305382
```

Mono1 F-FF

Without water

M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.201162	1.416468	1.092665
2	8	0	-1.879155	3.629357	0.270508
3	8	0	-3.880653	2.831194	0.937911
4	7	0	2.174208	2.631949	-0.128311
5	7	0	-1.092781	1.242795	-0.797836
6	6	0	1.268944	1.828128	-1.019211
7	6	0	2.006942	0.607407	-1.610955
8	6	0	2.581686	-0.376609	-0.614695
9	6	0	1.897904	-1.541780	-0.241140
10	6	0	2.451437	-2.450792	0.662424
11	6	0	3.714523	-2.213270	1.210200
12	6	0	4.424985	-1.065500	0.853126
13	6	0	3.841435	-0.184757	-0.045436
14	6	0	0.051307	1.479809	-0.137473
15	6	0	-2.423738	1.298447	-0.176852
16	6	0	-2.692087	0.194410	0.869685
17	6	0	-2.618877	-1.220448	0.338560
18	6	0	-1.588777	-2.084718	0.732569
19	6	0	-1.528887	-3.398163	0.255802
20	6	0	-2.502110	-3.867787	-0.628349
21	6	0	-3.535932	-3.015623	-1.029404
22	6	0	-3.592674	-1.706791	-0.548374
23	6	0	-2.741880	2.721763	0.401858
24	1	0	1.867982	3.610412	-0.081214
25	1	0	3.152473	2.609744	-0.436073
26	1	0	2.105355	2.243106	0.825967
27	1	0	-1.076168	1.455063	-1.789232
28	1	0	0.969309	2.481732	-1.839349
29	1	0	1.288013	0.093891	-2.255520
30	1	0	2.798590	0.993864	-2.261598
31	1	0	0.920451	-1.733930	-0.673334
32	1	0	1.899212	-3.346196	0.932028
33	1	0	4.151482	-2.917529	1.911730
34	1	0	5.409996	-0.849488	1.253632
35	1	0	-3.124816	1.147065	-1.003659
36	1	0	-3.699978	0.392324	1.246386
37	1	0	-2.003406	0.312640	1.709945
38	1	0	-0.723699	-4.053090	0.579390
39	1	0	-2.459528	-4.888501	-0.998680
40	1	0	-4.302276	-3.373493	-1.712193
41	1	0	-4.406440	-1.054713	-0.858761
42	9	0	4.541689	0.937780	-0.392198
43	1	0	-0.827793	-1.724636	1.420655

Rotational constants (GHZ): 0.2948492 0.1843368 0.1249135

M1-CIP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.400181	0.122507	-0.594821
2	8	0	0.277343	3.293892	-0.292122
3	8	0	2.089267	3.423248	-1.612115
4	7	0	-1.829919	2.128838	1.122966
5	7	0	1.101601	0.994480	0.903864
6	6	0	-1.224553	0.811892	1.571983
7	6	0	-2.264322	-0.298259	1.789253
8	6	0	-2.967999	-0.911015	0.594405
9	6	0	-2.654100	-2.200303	0.140859
10	6	0	-3.345435	-2.789038	-0.919421
11	6	0	-4.380839	-2.096744	-1.552136
12	6	0	-4.723097	-0.813467	-1.121413
13	6	0	-4.012557	-0.264960	-0.064718
14	6	0	-0.125172	0.563893	0.525217
15	6	0	2.031789	1.602555	-0.056180
16	6	0	2.610903	0.627811	-1.105923
17	6	0	3.314782	-0.571159	-0.508528
18	6	0	2.664293	-1.808135	-0.393979
19	6	0	3.313145	-2.911335	0.166624
20	6	0	4.627453	-2.794272	0.625013
21	6	0	5.287391	-1.566732	0.517110
22	6	0	4.635460	-0.467719	-0.045660
23	6	0	1.400141	2.874825	-0.717106
24	1	0	-1.066144	2.725713	0.707636
25	1	0	-2.275950	2.611520	1.910108
26	1	0	-2.546304	1.985255	0.402723
27	1	0	1.138149	1.424600	1.820838
28	1	0	-0.775609	1.026772	2.542682
29	1	0	-1.731457	-1.095251	2.317197
30	1	0	-3.006582	0.097308	2.493390
31	1	0	-1.853913	-2.744847	0.634859
32	1	0	-3.077973	-3.788906	-1.247820
33	1	0	-4.922976	-2.548987	-2.377101
34	1	0	-5.522308	-0.243688	-1.584029
35	1	0	2.869185	1.964503	0.549853
36	1	0	3.318040	1.213747	-1.699270
37	1	0	1.813979	0.299357	-1.776770
38	1	0	2.792081	-3.862288	0.242597
39	1	0	5.134530	-3.651922	1.058893
40	1	0	6.312195	-1.466652	0.865425
41	1	0	5.158308	0.482374	-0.133533
42	9	0	-4.350556	0.996580	0.350288
43	1	0	1.640837	-1.905249	-0.748007

Rotational constants (GHZ): 0.3417853 0.1461852
0.1159651
Standard basis: 6-31G(d) (6D, 7F)

M1-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.092742	-0.408839	0.733936
2	8	0	-0.010275	3.053670	0.023249
3	8	0	-1.705344	3.430853	1.391455
4	7	0	1.668402	1.313039	-1.420199
5	7	0	-1.119034	0.670811	-0.885917

6	6	0	1.107237	-0.059233	-1.459801
7	6	0	2.106878	-1.227004	-1.272856
8	6	0	3.180987	-1.056708	-0.219468
9	6	0	3.087663	-1.611946	1.065697
10	6	0	4.114281	-1.467203	2.000304
11	6	0	5.271357	-0.757998	1.667131
12	6	0	5.400795	-0.199177	0.394958
13	6	0	4.359807	-0.364535	-0.509631
14	6	0	-0.021953	-0.000840	-0.424792
15	6	0	-1.967703	1.513274	-0.047434
16	6	0	-2.750291	0.772234	1.061441
17	6	0	-3.661126	-0.310440	0.524656
18	6	0	-3.267504	-1.655764	0.531048
19	6	0	-4.110999	-2.650670	0.029960
20	6	0	-5.363126	-2.313428	-0.489088
21	6	0	-5.766535	-0.975179	-0.501642
22	6	0	-4.921637	0.015550	0.002073
23	6	0	-1.205548	2.726270	0.527200
24	1	0	0.399796	2.416917	-0.641550
25	1	0	2.187426	1.498106	-2.277521
26	1	0	2.345673	1.372627	-0.658347
27	1	0	-1.051864	0.989378	-1.846278
28	1	0	0.649214	-0.183336	-2.445435
29	1	0	1.529576	-2.132385	-1.058045
30	1	0	2.592372	-1.381869	-2.241869
31	1	0	2.191994	-2.166517	1.328254
32	1	0	4.011812	-1.910652	2.986358
33	1	0	6.073601	-0.641506	2.389823
34	1	0	6.286907	0.351428	0.095869
35	1	0	-2.703876	1.954747	-0.728926
36	1	0	-3.342925	1.531732	1.578329
37	1	0	-2.045212	0.355149	1.782596
38	1	0	-3.789659	-3.688823	0.047162
39	1	0	-6.021028	-3.086405	-0.877086
40	1	0	-6.741301	-0.703267	-0.898179
41	1	0	-5.244810	1.054333	-0.003344
42	9	0	4.505300	0.170915	-1.754341
43	1	0	-2.293443	-1.923527	0.932421

Rotational constants (GHZ): 0.4179847 0.1197109
0.1073345
Standard basis: 6-31G(d) (6D, 7F)

M1-N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.470958	1.793428	0.496333
2	8	0	-1.781366	3.738488	-0.268555
3	8	0	-2.339252	3.046149	1.803069
4	7	0	2.269193	1.803667	-1.758544
5	7	0	-1.168040	1.123332	-0.920882
6	6	0	1.159281	0.856235	-1.642176
7	6	0	1.674468	-0.584026	-1.367415
8	6	0	2.596892	-0.739927	-0.177272
9	6	0	2.118699	-0.945437	1.126453
10	6	0	2.985532	-1.099119	2.209529
11	6	0	4.367889	-1.053032	2.010808
12	6	0	4.877423	-0.859354	0.726416
13	6	0	3.985807	-0.708269	-0.328763

14	6	0	0.131735	1.289817	-0.587662
15	6	0	-2.266095	1.412172	-0.004206
16	6	0	-2.492689	0.319505	1.060799
17	6	0	-2.869007	-1.018379	0.459162
18	6	0	-1.985039	-2.104754	0.501773
19	6	0	-2.334437	-3.337430	-0.057886
20	6	0	-3.577391	-3.501110	-0.671980
21	6	0	-4.469699	-2.425562	-0.718787
22	6	0	-4.117837	-1.197726	-0.156621
23	6	0	-2.107885	2.793404	0.634446
24	1	0	-1.741520	4.596463	0.199511
25	1	0	2.678560	1.916598	-0.829906
26	1	0	1.879552	2.719310	-1.986045
27	1	0	-1.395226	0.679465	-1.801807
28	1	0	0.649322	0.819365	-2.609858
29	1	0	0.805011	-1.238259	-1.239714
30	1	0	2.196200	-0.907505	-2.272132
31	1	0	1.045156	-0.989028	1.286420
32	1	0	2.582206	-1.258286	3.205267
33	1	0	5.049669	-1.173268	2.847628
34	1	0	5.944491	-0.827568	0.530582
35	1	0	-3.165122	1.489479	-0.626082
36	1	0	-3.293233	0.669935	1.720658
37	1	0	-1.587984	0.223852	1.668692
38	1	0	-1.635170	-4.168157	-0.011122
39	1	0	-3.851467	-4.458234	-1.107339
40	1	0	-5.442367	-2.544855	-1.188831
41	1	0	-4.821461	-0.368676	-0.191441
42	9	0	4.505074	-0.543193	-1.574609
43	1	0	-1.018954	-1.987448	0.986497

Rotational constants (GHZ): 0.3034694 0.1561783 0.1254297

Standard basis: 6-31G(d) (6D, 7F)

M1-N3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.388556	1.720940	0.524588
2	8	0	-2.724595	2.981608	1.667580
3	8	0	-1.782204	3.751133	-0.225987
4	7	0	2.218939	1.844812	-1.719370
5	7	0	-1.206417	1.092111	-0.963078
6	6	0	1.140758	0.858338	-1.623300
7	6	0	1.702374	-0.563592	-1.343292
8	6	0	2.641433	-0.684877	-0.161952
9	6	0	2.185875	-0.901896	1.147917
10	6	0	3.069966	-1.024805	2.220904
11	6	0	4.447729	-0.935447	2.005677
12	6	0	4.935420	-0.728942	0.714850
13	6	0	4.026781	-0.609117	-0.329786
14	6	0	0.081883	1.254205	-0.585246
15	6	0	-2.331950	1.384323	-0.084582
16	6	0	-2.550782	0.317373	1.013264
17	6	0	-2.841676	-1.055433	0.442106
18	6	0	-1.907525	-2.094643	0.544656
19	6	0	-2.178966	-3.359250	0.013748
20	6	0	-3.392999	-3.602661	-0.631140
21	6	0	-4.334958	-2.574793	-0.737239

22	6	0	-4.060863	-1.314818	-0.203436
23	6	0	-2.215168	2.823157	0.432823
24	1	0	-2.668285	3.933035	1.890153
25	1	0	2.606950	1.970924	-0.783306
26	1	0	1.801706	2.746241	-1.954695
27	1	0	-1.403777	0.699632	-1.874513
28	1	0	0.648954	0.807322	-2.599554
29	1	0	0.854625	-1.243521	-1.203787
30	1	0	2.225942	-0.877424	-2.250350
31	1	0	1.116292	-0.976671	1.321086
32	1	0	2.683713	-1.193598	3.221827
33	1	0	5.142822	-1.031653	2.834641
34	1	0	5.998502	-0.663425	0.506079
35	1	0	-3.220473	1.400568	-0.726308
36	1	0	-3.394397	0.643358	1.629025
37	1	0	-1.667757	0.281076	1.657519
38	1	0	-1.441905	-4.152519	0.107277
39	1	0	-3.606578	-4.584775	-1.044157
40	1	0	-5.285884	-2.756272	-1.231307
41	1	0	-4.802899	-0.523284	-0.284253
42	9	0	4.525645	-0.430451	-1.581978
43	1	0	-0.964050	-1.915585	1.054281

Rotational constants (GHZ): 0.3053591 0.1551400
0.1245532
Standard basis: 6-31G(d) (6D, 7F)

M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.392551	-1.030256	0.703466
2	8	0	0.018571	3.155540	-1.348094
3	8	0	1.280729	3.973759	0.337337
4	7	0	-1.065376	-2.614910	-0.732537
5	7	0	0.580784	0.650311	-0.838574
6	6	0	-0.837752	-1.262842	-1.357637
7	6	0	-2.164123	-0.526268	-1.644173
8	6	0	-2.979131	-0.128609	-0.430630
9	6	0	-2.901434	1.155123	0.130011
10	6	0	-3.678890	1.510219	1.234123
11	6	0	-4.561227	0.586302	1.799114
12	6	0	-4.664933	-0.698512	1.261896
13	6	0	-3.874675	-1.014713	0.168078
14	6	0	0.110392	-0.516757	-0.393828
15	6	0	1.321242	1.611975	-0.024486
16	6	0	2.853277	1.525590	-0.243087
17	6	0	3.466420	0.193598	0.127214
18	6	0	3.793468	-0.749651	-0.856756
19	6	0	4.341957	-1.988161	-0.511340
20	6	0	4.573489	-2.302733	0.829124
21	6	0	4.255311	-1.369150	1.820544
22	6	0	3.707631	-0.134306	1.470797
23	6	0	0.820892	3.043389	-0.374119
24	1	0	-0.635002	-3.364645	-1.282834
25	1	0	-2.062220	-2.834598	-0.616161
26	1	0	-0.612522	-2.586390	0.202207
27	1	0	0.157126	1.079871	-1.659366
28	1	0	-0.325081	-1.430885	-2.305852
29	1	0	-1.911535	0.370967	-2.215797

30	1	0	-2.754473	-1.163577	-2.310994
31	1	0	-2.222426	1.879060	-0.312494
32	1	0	-3.599861	2.510885	1.647986
33	1	0	-5.169373	0.859323	2.656210
34	1	0	-5.339243	-1.442910	1.672163
35	1	0	1.099178	1.415572	1.028284
36	1	0	3.295479	2.324341	0.361052
37	1	0	3.065195	1.754047	-1.294460
38	1	0	4.590809	-2.703849	-1.290691
39	1	0	5.002347	-3.263776	1.100069
40	1	0	4.437836	-1.602112	2.866436
41	1	0	3.466267	0.587798	2.247829
42	9	0	-3.971063	-2.280834	-0.351456
43	1	0	3.622929	-0.508737	-1.903442

Rotational constants (GHZ): 0.3495518 0.1522307 0.1236029

With water

M1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.503776	1.028860	0.976307
2	8	0	-1.322234	3.572689	0.604009
3	8	0	-2.677172	2.726652	2.175302
4	7	0	2.267819	1.921981	-0.928914
5	7	0	-1.114123	1.078719	-0.637354
6	6	0	1.218836	0.923871	-1.318414
7	6	0	1.801515	-0.489984	-1.532022
8	6	0	2.564199	-1.095869	-0.374114
9	6	0	1.962829	-1.962890	0.549099
10	6	0	2.694772	-2.534771	1.590936
11	6	0	4.055976	-2.250627	1.729121
12	6	0	4.685605	-1.394921	0.823435
13	6	0	3.926048	-0.844055	-0.198968
14	6	0	0.155469	1.007835	-0.214734
15	6	0	-2.244380	1.343846	0.256375
16	6	0	-2.621578	0.125487	1.125178
17	6	0	-3.021077	-1.098411	0.328753
18	6	0	-2.232152	-2.256606	0.342187
19	6	0	-2.597657	-3.387335	-0.394635
20	6	0	-3.764266	-3.376487	-1.161275
21	6	0	-4.564216	-2.229519	-1.179890
22	6	0	-4.195779	-1.104580	-0.440682
23	6	0	-2.042066	2.650694	1.094137
24	1	0	1.826841	2.888146	-0.970384
25	1	0	3.086630	1.874092	-1.542882
26	1	0	2.570814	1.747859	0.037001
27	1	0	-1.277597	1.128074	-1.635056
28	1	0	0.809619	1.271203	-2.268103
29	1	0	0.955911	-1.135378	-1.788426
30	1	0	2.445781	-0.439506	-2.416028
31	1	0	0.907347	-2.193573	0.434741
32	1	0	2.204165	-3.204537	2.290752
33	1	0	4.630913	-2.693890	2.536674
34	1	0	5.741306	-1.154922	0.896496

35	1	0	-3.086396	1.559321	-0.410561
36	1	0	-3.451785	0.444528	1.761408
37	1	0	-1.784564	-0.116260	1.787177
38	1	0	-1.970742	-4.274874	-0.367148
39	1	0	-4.051410	-4.253382	-1.735261
40	1	0	-5.478771	-2.213388	-1.767152
41	1	0	-4.829157	-0.220138	-0.457939
42	8	0	0.746756	4.189780	-1.042927
43	1	0	-0.033952	3.883751	-0.506248
44	9	0	4.545140	-0.008796	-1.083158
45	1	0	0.429167	4.154812	-1.960839
46	1	0	-1.327715	-2.275586	0.945608

Rotational constants (GHZ): 0.2520610 0.1568207 0.1143770

M2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.370869	-0.030320	1.260587
2	8	0	0.084757	2.639759	-1.055654
3	8	0	1.438349	3.651256	0.442977
4	7	0	-1.378772	-2.403213	0.083688
5	7	0	1.099507	0.155065	-0.465748
6	6	0	-0.805334	-1.305303	-0.766068
7	6	0	-1.913220	-0.573752	-1.565526
8	6	0	-3.074756	-0.035799	-0.758527
9	6	0	-3.099400	1.268049	-0.241897
10	6	0	-4.191364	1.732461	0.493811
11	6	0	-5.288380	0.898756	0.727231
12	6	0	-5.295938	-0.403399	0.221218
13	6	0	-4.193533	-0.831736	-0.505275
14	6	0	-0.002146	-0.342004	0.113841
15	6	0	1.796137	1.325690	0.061403
16	6	0	3.213530	1.420185	-0.542765
17	6	0	4.112678	0.249444	-0.209158
18	6	0	4.379592	-0.750083	-1.154768
19	6	0	5.196326	-1.839122	-0.837594
20	6	0	5.761337	-1.943838	0.435045
21	6	0	5.505502	-0.951511	1.386452
22	6	0	4.689053	0.133937	1.065281
23	6	0	1.020019	2.654933	-0.207345
24	1	0	-0.631734	-3.020716	0.421184
25	1	0	-2.030156	-2.975500	-0.465378
26	1	0	-1.894341	-2.043056	0.930963
27	1	0	1.269345	-0.082802	-1.437440
28	1	0	-0.140653	-1.791715	-1.481532
29	1	0	-1.418989	0.247787	-2.091862
30	1	0	-2.277815	-1.273537	-2.323402
31	1	0	-2.248525	1.918884	-0.423115
32	1	0	-4.186567	2.746319	0.882478
33	1	0	-6.139833	1.256603	1.298328
34	1	0	-6.130954	-1.078213	0.378387
35	1	0	1.874025	1.203242	1.144430
36	1	0	3.648873	2.349950	-0.163904
37	1	0	3.123007	1.523995	-1.631601
38	1	0	5.392058	-2.602594	-1.586043
39	1	0	6.398697	-2.788165	0.683444
40	1	0	5.945815	-1.021051	2.377745

41	1	0	4.498497	0.904523	1.809126
42	8	0	-2.522091	-1.350869	2.436973
43	1	0	-3.349341	-0.928951	2.146161
44	9	0	-4.195240	-2.109602	-0.984958
45	1	0	-1.838558	-0.670655	2.249714
46	1	0	3.947384	-0.670971	-2.149860

Rotational constants (GHZ): 0.4009587 0.1127083 0.0996587

M3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.367725	-0.933251	0.429651
2	8	0	0.306661	3.422316	-1.116626
3	8	0	1.611494	3.978857	0.640853
4	7	0	-1.132627	-2.244849	-1.401336
5	7	0	0.764590	0.855346	-0.929510
6	6	0	-0.832141	-0.800485	-1.680352
7	6	0	-2.124763	0.042839	-1.777031
8	6	0	-2.888678	0.255191	-0.489133
9	6	0	-2.682815	1.381874	0.319796
10	6	0	-3.407897	1.566889	1.498938
11	6	0	-4.363253	0.625706	1.889653
12	6	0	-4.597015	-0.503199	1.100127
13	6	0	-3.855651	-0.656770	-0.063574
14	6	0	0.159563	-0.297156	-0.619335
15	6	0	1.517903	1.670396	0.021551
16	6	0	3.050265	1.512423	-0.139800
17	6	0	3.565798	0.118725	0.142531
18	6	0	3.893345	-0.758583	-0.900286
19	6	0	4.351870	-2.052111	-0.633967
20	6	0	4.491142	-2.489015	0.684833
21	6	0	4.170572	-1.622692	1.734798
22	6	0	3.712976	-0.332730	1.463815
23	6	0	1.103621	3.159315	-0.167851
24	1	0	-0.288191	-2.812696	-1.533982
25	1	0	-1.845640	-2.590891	-2.051969
26	1	0	-1.460948	-2.419337	-0.416990
27	1	0	0.410336	1.402876	-1.712007
28	1	0	-0.348882	-0.779553	-2.659371
29	1	0	-1.831584	1.015614	-2.181898
30	1	0	-2.764865	-0.428406	-2.530067
31	1	0	-1.948241	2.120488	0.009092
32	1	0	-3.230632	2.448267	2.107731
33	1	0	-4.932194	0.766928	2.803687
34	1	0	-5.337565	-1.249724	1.367847
35	1	0	1.234662	1.363430	1.032691
36	1	0	3.509670	2.227568	0.549883
37	1	0	3.325742	1.814730	-1.157201
38	1	0	4.603342	-2.715331	-1.457633
39	1	0	4.849994	-3.493131	0.894330
40	1	0	4.281284	-1.951091	2.765040
41	1	0	3.469462	0.336638	2.286144
42	8	0	-1.603316	-2.690182	1.339561
43	1	0	-2.392661	-2.186536	1.603148
44	9	0	-4.076155	-1.760561	-0.831770
45	1	0	-0.885631	-2.020927	1.357570
46	1	0	3.794634	-0.422968	-1.929983

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 Rotational constants (GHZ):           0.3085523           0.1467616
0.1195913
```

Mono2 F-FF

Without water

M1

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 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          8           0        0.891186    1.567823    0.544114
      2          8           0       -1.070445    3.884760   -0.120006
      3          8           0       -2.173429    3.263345    1.744660
      4          7           0        2.582319    1.816046   -1.593816
      5          7           0       -0.834763    1.237516   -0.920540
      6          6           0        1.444689    0.835184   -1.676054
      7          6           0        1.971400   -0.616089   -1.544054
      8          6           0        2.937507   -0.880050   -0.403232
      9          6           0        2.490077   -1.269979    0.868583
     10          6           0        3.399176   -1.512263    1.899750
     11          6           0        4.771507   -1.366764    1.679604
     12          6           0        5.229933   -0.984464    0.417528
     13          6           0        4.318864   -0.748189   -0.614575
     14          6           0        0.458590    1.248212   -0.574977
     15          6           0       -1.917176    1.626428   -0.011277
     16          6           0       -2.226029    0.536322    1.037473
     17          6           0       -2.836812   -0.714766    0.448507
     18          6           0       -2.068712   -1.805020    0.039971
     19          6           0       -2.599645   -2.961674   -0.515914
     20          6           0       -3.982725   -3.046498   -0.683199
     21          6           0       -4.795534   -1.979827   -0.290200
     22          6           0       -4.223941   -0.835493    0.268651
     23          6           0       -1.675470    3.050403    0.605128
     24          1           0        2.288796    2.750934   -1.902139
     25          1           0        3.379698    1.523952   -2.170835
     26          1           0        2.895237    1.894360   -0.616615
     27          1           0       -1.070758    0.994455   -1.874699
     28          1           0        1.000652    0.959750   -2.664342
     29          1           0        1.089958   -1.258161   -1.460139
     30          1           0        2.460442   -0.857282   -2.493961
     31          1           0        1.427521   -1.394198    1.049778
     32          1           0        3.034116   -1.818729    2.876337
     33          1           0        5.477358   -1.556902    2.483442
     34          1           0        6.295146   -0.877794    0.231243
     35          1           0       -2.799251    1.738976   -0.651459
     36          1           0       -2.932032    0.973178    1.746384
     37          1           0       -1.312502    0.300333    1.590855
     38          1           0       -1.935582   -3.770056   -0.804925
     39          1           0       -4.418551   -3.942207   -1.115829
     40          1           0       -5.872919   -2.040924   -0.413177
     41          1           0       -4.860255   -0.010791    0.580732
     42          9           0       -0.713009   -1.743860    0.194487
     43          1           0        4.684423   -0.469355   -1.600963
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3195690           0.1647050
0.1277994
```

M1-CIP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.601550	-0.170235	-0.674512
2	8	0	-0.449536	3.017829	0.153133
3	8	0	1.025636	3.347843	-1.459498
4	7	0	-1.912614	1.254691	1.795861
5	7	0	0.808795	0.643315	0.927478
6	6	0	-1.366291	-0.118512	1.647091
7	6	0	-2.397933	-1.257232	1.462711
8	6	0	-3.513727	-1.038115	0.459089
9	6	0	-3.464160	-1.598699	-0.826581
10	6	0	-4.506600	-1.407789	-1.734809
11	6	0	-5.623115	-0.647377	-1.375569
12	6	0	-5.692118	-0.090498	-0.097282
13	6	0	-4.649938	-0.291526	0.812196
14	6	0	-0.350837	0.049721	0.512809
15	6	0	1.558898	1.551659	0.065621
16	6	0	2.371373	0.864599	-1.054813
17	6	0	3.421698	-0.080697	-0.519888
18	6	0	3.188487	-1.451815	-0.402811
19	6	0	4.127855	-2.349549	0.089384
20	6	0	5.370917	-1.861473	0.494830
21	6	0	5.647915	-0.495253	0.396318
22	6	0	4.681646	0.377415	-0.107177
23	6	0	0.677079	2.689230	-0.491787
24	1	0	-0.762955	2.395200	0.881109
25	1	0	-2.239979	1.394879	2.750773
26	1	0	-2.728426	1.357695	1.190639
27	1	0	0.858609	0.863150	1.915592
28	1	0	-0.809945	-0.338585	2.562889
29	1	0	-1.841681	-2.167000	1.209147
30	1	0	-2.845105	-1.425193	2.449485
31	1	0	-2.599619	-2.189624	-1.115878
32	1	0	-4.447644	-1.855072	-2.723629
33	1	0	-6.434539	-0.498403	-2.082774
34	1	0	-6.560717	0.491767	0.198847
35	1	0	2.271623	2.060221	0.725208
36	1	0	2.860058	1.658068	-1.625166
37	1	0	1.688955	0.343604	-1.727911
38	1	0	3.878427	-3.404217	0.147937
39	1	0	6.117517	-2.548370	0.882506
40	1	0	6.615342	-0.110802	0.705693
41	1	0	4.901932	1.439059	-0.190050
42	9	0	1.983244	-1.944743	-0.795745
43	1	0	-4.727601	0.122233	1.814933

Rotational constants (GHZ): 0.4350130 0.1262131 0.1120536

M1-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.601550	-0.170235	-0.674512
2	8	0	-0.449536	3.017829	0.153133
3	8	0	1.025636	3.347843	-1.459498

4	7	0	-1.912614	1.254691	1.795861
5	7	0	0.808795	0.643315	0.927478
6	6	0	-1.366291	-0.118512	1.647091
7	6	0	-2.397933	-1.257232	1.462711
8	6	0	-3.513727	-1.038115	0.459089
9	6	0	-3.464160	-1.598699	-0.826581
10	6	0	-4.506600	-1.407789	-1.734809
11	6	0	-5.623115	-0.647377	-1.375569
12	6	0	-5.692118	-0.090498	-0.097282
13	6	0	-4.649938	-0.291526	0.812196
14	6	0	-0.350837	0.049721	0.512809
15	6	0	1.558898	1.551659	0.065621
16	6	0	2.371373	0.864599	-1.054813
17	6	0	3.421698	-0.080697	-0.519888
18	6	0	3.188487	-1.451815	-0.402811
19	6	0	4.127855	-2.349549	0.089384
20	6	0	5.370917	-1.861473	0.494830
21	6	0	5.647915	-0.495253	0.396318
22	6	0	4.681646	0.377415	-0.107177
23	6	0	0.677079	2.689230	-0.491787
24	1	0	-0.762955	2.395200	0.881109
25	1	0	-2.239979	1.394879	2.750773
26	1	0	-2.728426	1.357695	1.190639
27	1	0	0.858609	0.863150	1.915592
28	1	0	-0.809945	-0.338585	2.562889
29	1	0	-1.841681	-2.167000	1.209147
30	1	0	-2.845105	-1.425193	2.449485
31	1	0	-2.599619	-2.189624	-1.115878
32	1	0	-4.447644	-1.855072	-2.723629
33	1	0	-6.434539	-0.498403	-2.082774
34	1	0	-6.560717	0.491767	0.198847
35	1	0	2.271623	2.060221	0.725208
36	1	0	2.860058	1.658068	-1.625166
37	1	0	1.688955	0.343604	-1.727911
38	1	0	3.878427	-3.404217	0.147937
39	1	0	6.117517	-2.548370	0.882506
40	1	0	6.615342	-0.110802	0.705693
41	1	0	4.901932	1.439059	-0.190050
42	9	0	1.983244	-1.944743	-0.795745
43	1	0	-4.727601	0.122233	1.814933

Rotational constants (GHZ): 0.4350130 0.1262131
0.1120536
Standard basis: 6-31G(d) (6D, 7F)

M1-N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.971328	1.524173	-0.352061
2	8	0	0.893901	3.853529	0.241743
3	8	0	1.442380	3.225681	-1.852417
4	7	0	-2.486064	1.444581	2.149922
5	7	0	0.836301	1.184777	0.968989
6	6	0	-1.371090	0.544051	1.836474
7	6	0	-1.882525	-0.884460	1.506396
8	6	0	-2.895079	-0.994953	0.382733
9	6	0	-2.498656	-1.310419	-0.926684
10	6	0	-3.437753	-1.423991	-1.953726
11	6	0	-4.795476	-1.223006	-1.691581

12	6	0	-5.205591	-0.914558	-0.392543
13	6	0	-4.263660	-0.806085	0.633414
14	6	0	-0.490293	1.106298	0.714794
15	6	0	1.796779	1.654205	-0.023678
16	6	0	2.154525	0.601263	-1.094623
17	6	0	2.856320	-0.603391	-0.511867
18	6	0	2.165333	-1.758138	-0.145377
19	6	0	2.774886	-2.880578	0.399905
20	6	0	4.156035	-2.857603	0.598750
21	6	0	4.890887	-1.721727	0.248017
22	6	0	4.243596	-0.613994	-0.301395
23	6	0	1.336169	2.963698	-0.667891
24	1	0	0.656522	4.672974	-0.237054
25	1	0	-3.002995	1.611415	1.285627
26	1	0	-2.098590	2.352684	2.409680
27	1	0	1.200660	0.790241	1.827201
28	1	0	-0.758892	0.452052	2.739100
29	1	0	-1.012247	-1.509494	1.283322
30	1	0	-2.330531	-1.265491	2.430755
31	1	0	-1.446679	-1.476237	-1.140207
32	1	0	-3.108322	-1.673607	-2.959070
33	1	0	-5.526862	-1.313722	-2.490208
34	1	0	-6.259912	-0.765707	-0.174048
35	1	0	2.706523	1.911760	0.530921
36	1	0	2.814936	1.081741	-1.821502
37	1	0	1.243295	0.307183	-1.621373
38	1	0	2.171849	-3.745637	0.656497
39	1	0	4.652049	-3.725079	1.023942
40	1	0	5.966360	-1.700403	0.397060
41	1	0	4.818039	0.265795	-0.581040
42	9	0	0.814516	-1.798026	-0.333413
43	1	0	-4.593585	-0.580483	1.643908

Rotational constants (GHZ): 0.3224915 0.1645545
0.1313307
Standard basis: 6-31G(d) (6D, 7F)

M1-N3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.848551	1.419605	-0.450801
2	8	0	1.955278	3.240229	-1.724680
3	8	0	0.928894	3.854744	0.181879
4	7	0	-2.449840	1.605720	2.018233
5	7	0	0.880005	1.165723	0.995130
6	6	0	-1.378240	0.629540	1.787186
7	6	0	-1.957336	-0.784927	1.514010
8	6	0	-2.975384	-0.899940	0.395222
9	6	0	-2.603404	-1.326165	-0.889612
10	6	0	-3.550655	-1.449900	-1.908115
11	6	0	-4.892508	-1.147943	-1.662205
12	6	0	-5.278874	-0.728252	-0.387208
13	6	0	-4.329290	-0.610539	0.630484
14	6	0	-0.431847	1.088656	0.671916
15	6	0	1.892422	1.623566	0.053538
16	6	0	2.232347	0.586551	-1.043884
17	6	0	2.837019	-0.677159	-0.475601
18	6	0	2.062270	-1.793082	-0.159968
19	6	0	2.581893	-2.967579	0.368202

20	6	0	3.955889	-3.041564	0.602058
21	6	0	4.772770	-1.947908	0.302654
22	6	0	4.214346	-0.785271	-0.230919
23	6	0	1.508005	3.010690	-0.477303
24	1	0	1.731676	4.165293	-1.953661
25	1	0	-2.933513	1.752859	1.131411
26	1	0	-2.019359	2.504103	2.241603
27	1	0	1.174663	0.912910	1.929175
28	1	0	-0.801533	0.551813	2.714147
29	1	0	-1.117268	-1.459630	1.320311
30	1	0	-2.423640	-1.106056	2.452088
31	1	0	-1.564263	-1.568872	-1.091258
32	1	0	-3.239715	-1.786157	-2.893934
33	1	0	-5.630392	-1.246512	-2.453895
34	1	0	-6.321327	-0.500164	-0.180459
35	1	0	2.799882	1.800433	0.642689
36	1	0	2.953600	1.043044	-1.725585
37	1	0	1.329403	0.362435	-1.616053
38	1	0	1.916790	-3.797190	0.585305
39	1	0	4.382501	-3.951030	1.014613
40	1	0	5.842967	-2.001855	0.479044
41	1	0	4.852698	0.061542	-0.471028
42	9	0	0.717345	-1.736451	-0.381677
43	1	0	-4.641939	-0.298291	1.623133

Rotational constants (GHZ): 0.3222173 0.1638610
0.1293692
Standard basis: 6-31G(d) (6D, 7F)

M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.927999	0.092384	-1.533734
2	8	0	0.523477	2.490812	1.079129
3	8	0	-0.718901	3.684232	-0.381312
4	7	0	1.681617	-2.427839	-0.982420
5	7	0	-0.580975	0.104207	0.182783
6	6	0	1.138081	-1.610472	0.154059
7	6	0	2.263208	-1.251952	1.155778
8	6	0	3.519292	-0.650304	0.554481
9	6	0	3.623704	0.727140	0.306545
10	6	0	4.788786	1.263610	-0.244030
11	6	0	5.868096	0.432942	-0.557857
12	6	0	5.777018	-0.938603	-0.313069
13	6	0	4.612012	-1.473517	0.241893
14	6	0	0.475613	-0.382852	-0.479304
15	6	0	-1.220257	1.365316	-0.183128
16	6	0	-2.609905	1.477013	0.482126
17	6	0	-3.587316	0.394043	0.087348
18	6	0	-3.674299	-0.805660	0.794460
19	6	0	-4.553687	-1.829853	0.472911
20	6	0	-5.401392	-1.656289	-0.623177
21	6	0	-5.348762	-0.472699	-1.363999
22	6	0	-4.452339	0.536702	-1.006949
23	6	0	-0.376083	2.620021	0.203652
24	1	0	0.924480	-2.893800	-1.496281
25	1	0	2.337785	-3.146366	-0.655282
26	1	0	2.166708	-1.804358	-1.642752
27	1	0	-0.854048	-0.340800	1.052289

28	1	0	0.396446	-2.229139	0.661079
29	1	0	1.817916	-0.567095	1.884581
30	1	0	2.517300	-2.173919	1.689577
31	1	0	2.791793	1.381670	0.550912
32	1	0	4.854671	2.333145	-0.424819
33	1	0	6.774773	0.853094	-0.984496
34	1	0	6.613060	-1.592463	-0.546022
35	1	0	-1.341437	1.372110	-1.269829
36	1	0	-3.015126	2.450428	0.194350
37	1	0	-2.475752	1.487965	1.570072
38	1	0	-4.566332	-2.734378	1.072386
39	1	0	-6.098146	-2.444317	-0.893042
40	1	0	-6.009002	-0.332473	-2.214764
41	1	0	-4.419269	1.460461	-1.579262
42	9	0	-2.842675	-0.986740	1.864505
43	1	0	4.552514	-2.540634	0.445119

Rotational constants (GHZ): 0.4661365 0.1232890 0.1079489

M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.038382	-1.056758	0.633286
2	8	0	-0.486218	3.127443	-1.245494
3	8	0	0.719044	3.973335	0.467015
4	7	0	-1.185425	-2.672946	-1.079451
5	7	0	0.292949	0.650898	-0.858270
6	6	0	-1.064481	-1.247702	-1.535902
7	6	0	-2.459918	-0.615384	-1.744265
8	6	0	-3.286958	-0.428072	-0.488322
9	6	0	-3.200514	0.762259	0.250267
10	6	0	-3.953463	0.933049	1.413397
11	6	0	-4.805090	-0.083011	1.855289
12	6	0	-4.903849	-1.268872	1.124079
13	6	0	-4.151753	-1.437809	-0.040898
14	6	0	-0.209765	-0.531910	-0.478088
15	6	0	0.875130	1.621592	0.064881
16	6	0	2.423217	1.628417	0.027410
17	6	0	3.050818	0.317211	0.436806
18	6	0	3.476370	-0.620410	-0.505573
19	6	0	4.039288	-1.845845	-0.169294
20	6	0	4.185390	-2.166480	1.181003
21	6	0	3.772783	-1.257781	2.159799
22	6	0	3.214646	-0.034672	1.785281
23	6	0	0.316108	3.036002	-0.270238
24	1	0	-0.285574	-3.160468	-1.157891
25	1	0	-1.882205	-3.185395	-1.632280
26	1	0	-1.454705	-2.699438	-0.087254
27	1	0	-0.071402	1.082147	-1.706109
28	1	0	-0.542645	-1.272980	-2.493923
29	1	0	-2.290193	0.350485	-2.230397
30	1	0	-2.994519	-1.243800	-2.466195
31	1	0	-2.546987	1.559952	-0.095065
32	1	0	-3.878933	1.862503	1.971387
33	1	0	-5.392911	0.051896	2.759065
34	1	0	-5.570710	-2.060437	1.454935
35	1	0	0.551136	1.362496	1.077716
36	1	0	2.749628	2.417923	0.709967

37	1	0	2.750592	1.906068	-0.979545
38	1	0	4.352728	-2.523310	-0.957281
39	1	0	4.622822	-3.119689	1.463274
40	1	0	3.888413	-1.499939	3.212245
41	1	0	2.898477	0.671851	2.548998
42	9	0	3.347255	-0.322634	-1.827242
43	1	0	-4.244284	-2.357478	-0.614664

Rotational constants (GHZ): 0.3475371 0.1560377 0.1335806

With water

M1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.813620	1.011972	0.860443
2	8	0	-0.852977	3.650217	0.541898
3	8	0	-2.159611	2.899450	2.200513
4	7	0	2.480690	1.707912	-1.272817
5	7	0	-0.873332	1.130318	-0.674285
6	6	0	1.391131	0.693535	-1.454922
7	6	0	1.945885	-0.749146	-1.519516
8	6	0	2.913123	-1.160763	-0.425751
9	6	0	2.470666	-1.795514	0.745018
10	6	0	3.377900	-2.180580	1.733493
11	6	0	4.744124	-1.935946	1.570499
12	6	0	5.198069	-1.310011	0.407809
13	6	0	4.289007	-0.930913	-0.582802
14	6	0	0.404296	0.948046	-0.309009
15	6	0	-1.932818	1.483856	0.270446
16	6	0	-2.344790	0.296681	1.169718
17	6	0	-2.960558	-0.853658	0.407567
18	6	0	-2.199394	-1.909973	-0.094183
19	6	0	-2.732185	-2.978356	-0.803412
20	6	0	-4.108378	-3.003898	-1.035924
21	6	0	-4.912983	-1.967677	-0.554849
22	6	0	-4.340381	-0.912493	0.157630
23	6	0	-1.597576	2.778041	1.084191
24	1	0	2.049010	2.677205	-1.336895
25	1	0	3.212596	1.600227	-1.982960
26	1	0	2.912134	1.601265	-0.347488
27	1	0	-1.098336	1.107260	-1.660837
28	1	0	0.925649	0.925279	-2.414113
29	1	0	1.075965	-1.413127	-1.530875
30	1	0	2.440325	-0.847538	-2.492278
31	1	0	1.412102	-1.995367	0.879146
32	1	0	3.016650	-2.675315	2.631133
33	1	0	5.449081	-2.237608	2.340320
34	1	0	6.259200	-1.123783	0.265690
35	1	0	-2.794568	1.751259	-0.351512
36	1	0	-3.074095	0.680916	1.885148
37	1	0	-1.473907	-0.039320	1.739019
38	1	0	-2.075252	-3.766307	-1.157780
39	1	0	-4.545496	-3.830940	-1.587576
40	1	0	-5.984968	-1.983738	-0.728534
41	1	0	-4.970354	-0.112027	0.538153
42	8	0	1.013408	4.016880	-1.388140
43	1	0	0.294154	3.801158	-0.731953

44	9	0	-0.850963	-1.904183	0.122953
45	1	0	0.579285	3.915509	-2.251873
46	1	0	4.651648	-0.460515	-1.494531

Rotational constants (GHZ): 0.2647566 0.1590607
0.1180401
Standard basis: 6-31G(d) (6D, 7F)

M2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.825648	0.097897	1.325708
2	8	0	-0.285320	2.645811	-0.986419
3	8	0	0.969275	3.707838	0.562635
4	7	0	-1.502365	-2.494615	0.420292
5	7	0	0.773111	0.184348	-0.287586
6	6	0	-0.978466	-1.463814	-0.537798
7	6	0	-2.086395	-0.985905	-1.510707
8	6	0	-3.352165	-0.438188	-0.882680
9	6	0	-3.454101	0.909984	-0.506954
10	6	0	-4.621357	1.397417	0.083485
11	6	0	-5.706402	0.545420	0.308823
12	6	0	-5.620366	-0.796735	-0.070801
13	6	0	-4.452730	-1.281027	-0.666865
14	6	0	-0.337504	-0.323344	0.260382
15	6	0	1.415070	1.394472	0.217880
16	6	0	2.839046	1.530076	-0.365849
17	6	0	3.769718	0.387200	-0.030103
18	6	0	3.854804	-0.747803	-0.837368
19	6	0	4.690414	-1.823590	-0.573444
20	6	0	5.494746	-1.773818	0.567048
21	6	0	5.443171	-0.658766	1.407454
22	6	0	4.591037	0.405798	1.106212
23	6	0	0.608109	2.694874	-0.097171
24	1	0	-0.726854	-2.942239	0.922172
25	1	0	-2.003365	-3.230466	-0.090992
26	1	0	-2.154722	-2.089058	1.142999
27	1	0	1.097476	-0.199159	-1.168695
28	1	0	-0.212403	-1.966635	-1.129927
29	1	0	-1.618271	-0.230037	-2.149778
30	1	0	-2.331959	-1.841897	-2.148984
31	1	0	-2.615374	1.579489	-0.676275
32	1	0	-4.684242	2.444757	0.366299
33	1	0	-6.614395	0.926321	0.768106
34	1	0	-6.462079	-1.465119	0.088706
35	1	0	1.481686	1.305995	1.305818
36	1	0	3.251267	2.460139	0.033035
37	1	0	2.761561	1.647088	-1.453119
38	1	0	4.703317	-2.671957	-1.250114
39	1	0	6.156959	-2.604114	0.793719
40	1	0	6.069575	-0.615021	2.293513
41	1	0	4.559019	1.275752	1.757404
42	8	0	-3.003493	-1.244968	2.443660
43	1	0	-3.808336	-0.949832	1.982616
44	1	0	-2.346664	-0.546123	2.229184
45	1	0	-4.394842	-2.324189	-0.969731
46	9	0	3.064350	-0.808662	-1.952093

```
 Rotational constants (GHZ):           0.4085334           0.1152348
0.1034024
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M3b

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 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          8           0       -0.047152   -0.961496   -0.477333
      2          8           0        0.151942    3.413381    0.981744
      3          8           0       -1.037303    3.999069   -0.847003
      4          7           0        1.195214   -2.333416    1.492207
      5          7           0       -0.450319    0.866626    0.826745
      6          6           0        0.989024   -0.863909    1.718610
      7          6           0        2.337680   -0.122069    1.883517
      8          6           0        3.200494   -0.019884    0.642315
      9          6           0        3.025514    1.037398   -0.263483
     10          6           0        3.807045    1.122920   -1.417658
     11          6           0        4.779256    0.155253   -1.682046
     12          6           0        4.974314   -0.893435   -0.778631
     13          6           0        4.191928   -0.976447    0.376899
     14          6           0        0.112626   -0.321723    0.578166
     15          6           0       -1.085317    1.701395   -0.189647
     16          6           0       -2.631877    1.627569   -0.145638
     17          6           0       -3.190165    0.253818   -0.431053
     18          6           0       -3.538737   -0.626260    0.594696
     19          6           0       -4.038865   -1.903772    0.373063
     20          6           0       -4.198773   -2.340112   -0.942930
     21          6           0       -3.861647   -1.492696   -2.002215
     22          6           0       -3.365341   -0.214468   -1.742038
     23          6           0       -0.609802    3.171994   -0.000018
     24          1           0        0.299323   -2.830671    1.547905
     25          1           0        1.811870   -2.718228    2.215965
     26          1           0        1.604822   -2.547863    0.546892
     27          1           0       -0.132709    1.400561    1.633123
     28          1           0        0.442502   -0.779092    2.660217
     29          1           0        2.093743    0.880262    2.250466
     30          1           0        2.885899   -0.625037    2.688160
     31          1           0        2.282173    1.803275   -0.055284
     32          1           0        3.659754    1.949499   -2.107374
     33          1           0        5.388850    0.223303   -2.578747
     34          1           0        5.740220   -1.640994   -0.966246
     35          1           0       -0.745434    1.357617   -1.171197
     36          1           0       -2.999829    2.332661   -0.896254
     37          1           0       -2.973028    1.978828    0.833533
     38          1           0       -4.294354   -2.531459    1.220933
     39          1           0       -4.587950   -3.335538   -1.135983
     40          1           0       -3.988356   -1.825196   -3.028378
     41          1           0       -3.108764    0.444695   -2.567934
     42          8           0        1.952290   -2.811526   -1.188006
     43          1           0        2.787652   -2.315133   -1.256147
     44          1           0        1.266975   -2.117077   -1.290142
     45          1           0        4.354299   -1.788359    1.082046
     46          9           0       -3.393809   -0.215266    1.883900
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3102529           0.1493901
0.1252192
```

M3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.036794	-0.794472	0.653528
2	8	0	-0.668627	3.095475	-1.801820
3	8	0	0.701558	4.189288	-0.379631
4	7	0	-1.264993	-2.647490	-0.756475
5	7	0	0.088951	0.711738	-1.065111
6	6	0	-1.257859	-1.282059	-1.367264
7	6	0	-2.685114	-0.704906	-1.505460
8	6	0	-3.380117	-0.360970	-0.203444
9	6	0	-3.260089	0.924700	0.346879
10	6	0	-3.889786	1.244876	1.551087
11	6	0	-4.650687	0.284655	2.223249
12	6	0	-4.782319	-0.995917	1.681275
13	6	0	-4.153423	-1.314280	0.475289
14	6	0	-0.332387	-0.422079	-0.493388
15	6	0	0.768336	1.793924	-0.359232
16	6	0	2.311046	1.736169	-0.496787
17	6	0	2.992136	0.670921	0.333814
18	6	0	3.170837	-0.638379	-0.112010
19	6	0	3.785448	-1.636653	0.629345
20	6	0	4.264542	-1.319145	1.901820
21	6	0	4.115143	-0.020522	2.394036
22	6	0	3.489412	0.954953	1.615094
23	6	0	0.217417	3.150539	-0.899007
24	1	0	-0.319331	-3.098532	-0.892042
25	1	0	-1.988573	-3.238046	-1.178732
26	1	0	-1.440819	-2.575692	0.252700
27	1	0	-0.362592	1.027894	-1.921583
28	1	0	-0.829663	-1.395446	-2.365194
29	1	0	-2.598601	0.190585	-2.129039
30	1	0	-3.275166	-1.432294	-2.075226
31	1	0	-2.676064	1.677989	-0.177166
32	1	0	-3.790570	2.246354	1.961040
33	1	0	-5.143587	0.535031	3.158662
34	1	0	-5.379724	-1.746138	2.192281
35	1	0	0.506908	1.733180	0.702520
36	1	0	2.687659	2.711463	-0.177969
37	1	0	2.561730	1.615599	-1.556394
38	1	0	3.875354	-2.634863	0.212920
39	1	0	4.749814	-2.084443	2.500192
40	1	0	4.488746	0.235045	3.381260
41	1	0	3.380475	1.965893	1.999881
42	8	0	1.302959	-3.591251	-1.202457
43	1	0	1.751279	-2.734042	-1.325762
44	9	0	2.700086	-0.973068	-1.357000
45	1	0	1.278209	-3.970103	-2.097999
46	1	0	-4.271961	-2.308846	0.051025

Rotational constants (GHZ): 0.2822911 0.1530634 0.1269860

Di F FF

Without water

M1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.654056	1.523445	0.637119
2	8	0	-1.244795	3.880275	-0.065070
3	8	0	-2.441212	3.263888	1.743135
4	7	0	2.389311	1.817038	-1.472581
5	7	0	-1.028203	1.240610	-0.888112
6	6	0	1.272317	0.811838	-1.568612
7	6	0	1.813932	-0.626394	-1.381515
8	6	0	2.731352	-0.859557	-0.197396
9	6	0	2.277156	-1.376684	1.025114
10	6	0	3.157314	-1.619716	2.080871
11	6	0	4.520781	-1.351144	1.936806
12	6	0	5.005810	-0.836735	0.733232
13	6	0	4.101673	-0.608603	-0.293163
14	6	0	0.251670	1.226596	-0.499604
15	6	0	-2.133909	1.635714	-0.010057
16	6	0	-2.485378	0.541503	1.020566
17	6	0	-3.068480	-0.706875	0.399275
18	6	0	-2.280486	-1.795626	0.026421
19	6	0	-2.781814	-2.950000	-0.560454
20	6	0	-4.154673	-3.033612	-0.798397
21	6	0	-4.986574	-1.968322	-0.443301
22	6	0	-4.444511	-0.826147	0.148501
23	6	0	-1.896016	3.051434	0.625361
24	1	0	2.120629	2.711559	-1.899343
25	1	0	3.246728	1.482081	-1.927991
26	1	0	2.592753	1.992829	-0.477725
27	1	0	-1.235159	1.018189	-1.853906
28	1	0	0.855898	0.900946	-2.572052
29	1	0	0.941728	-1.280320	-1.304180
30	1	0	2.336644	-0.890970	-2.306042
31	1	0	1.221196	-1.598066	1.139762
32	1	0	2.777840	-2.023521	3.014610
33	1	0	5.208696	-1.540177	2.755356
34	1	0	6.057375	-0.616481	0.581689
35	1	0	-2.994548	1.761540	-0.676284
36	1	0	-3.219757	0.975454	1.701939
37	1	0	-1.595274	0.302656	1.609570
38	1	0	-2.103945	-3.757272	-0.818801
39	1	0	-4.567960	-3.927272	-1.256607
40	1	0	-6.056202	-2.028657	-0.621854
41	1	0	-5.095776	-0.002177	0.430173
42	9	0	4.582541	-0.097311	-1.469675
43	9	0	-0.934096	-1.732772	0.250028

Rotational constants (GHZ): 0.3108988 0.1439515
0.1163693

M1-CIP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.594667	0.266888	-0.630677
2	8	0	0.065452	3.329119	-0.240300
3	8	0	1.742683	3.400938	-1.731600

4	7	0	-2.003266	2.106529	1.207586
5	7	0	0.953622	1.011546	0.886276
6	6	0	-1.357230	0.790033	1.599362
7	6	0	-2.365638	-0.351435	1.800204
8	6	0	-3.078198	-0.934608	0.596445
9	6	0	-2.730073	-2.188470	0.073937
10	6	0	-3.428525	-2.751399	-0.995710
11	6	0	-4.504501	-2.068342	-1.567984
12	6	0	-4.879054	-0.818945	-1.069516
13	6	0	-4.159866	-0.294752	-0.006416
14	6	0	-0.284959	0.610041	0.513404
15	6	0	1.846945	1.662227	-0.079164
16	6	0	2.486321	0.699470	-1.102797
17	6	0	3.365726	-0.355182	-0.470928
18	6	0	2.888140	-1.628668	-0.155813
19	6	0	3.667143	-2.617296	0.432856
20	6	0	4.999295	-2.329306	0.733760
21	6	0	5.520909	-1.067183	0.437570
22	6	0	4.709515	-0.099714	-0.158039
23	6	0	1.143794	2.891808	-0.752727
24	1	0	-1.263114	2.733316	0.797494
25	1	0	-2.445073	2.552983	2.018236
26	1	0	-2.729066	1.969033	0.495711
27	1	0	1.022698	1.382166	1.826580
28	1	0	-0.888358	0.983019	2.565089
29	1	0	-1.802325	-1.153911	2.286569
30	1	0	-3.101547	-0.000014	2.533625
31	1	0	-1.895966	-2.723988	0.519428
32	1	0	-3.134626	-3.723941	-1.378992
33	1	0	-5.052523	-2.501103	-2.399506
34	1	0	-5.708626	-0.256823	-1.485751
35	1	0	2.659302	2.084703	0.522278
36	1	0	3.094390	1.317215	-1.767634
37	1	0	1.704121	0.235517	-1.706186
38	1	0	3.227653	-3.586979	0.644376
39	1	0	5.623506	-3.089880	1.193645
40	1	0	6.558191	-0.838359	0.664106
41	1	0	5.120307	0.879062	-0.394394
42	9	0	-4.524695	0.936019	0.472833
43	9	0	1.592734	-1.930883	-0.444139

Rotational constants (GHZ): 0.3409395 0.1353588 0.1098685

M1-N1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.610788	1.524170	0.555266
2	8	0	-1.228161	3.900659	-0.171637
3	8	0	-2.131806	3.278691	1.754962
4	7	0	2.250784	1.723596	-1.765195
5	7	0	-1.060022	1.228258	-0.948215
6	6	0	1.232744	0.674262	-1.626829
7	6	0	1.766916	-0.758927	-1.311421
8	6	0	2.738173	-0.869165	-0.158026
9	6	0	2.336248	-1.218602	1.140496
10	6	0	3.255549	-1.327748	2.185555
11	6	0	4.612460	-1.088669	1.953827
12	6	0	5.047416	-0.745666	0.672637

13	6	0	4.105076	-0.646059	-0.342487
14	6	0	0.243017	1.157107	-0.569573
15	6	0	-2.121228	1.620297	-0.023259
16	6	0	-2.475314	0.556900	1.037748
17	6	0	-3.059778	-0.698331	0.433050
18	6	0	-2.272654	-1.809864	0.134015
19	6	0	-2.769927	-2.978448	-0.427545
20	6	0	-4.133916	-3.050176	-0.714211
21	6	0	-4.962906	-1.960756	-0.432550
22	6	0	-4.426874	-0.804062	0.135493
23	6	0	-1.808613	2.977835	0.622233
24	1	0	-1.006188	3.507400	-1.038450
25	1	0	2.987981	1.366870	-2.372689
26	1	0	2.691762	1.846538	-0.852655
27	1	0	-1.330536	0.852210	-1.848925
28	1	0	0.703990	0.594112	-2.581277
29	1	0	0.911504	-1.417435	-1.131967
30	1	0	2.256264	-1.108511	-2.226814
31	1	0	1.284401	-1.414493	1.324647
32	1	0	2.912474	-1.602720	3.178667
33	1	0	5.333112	-1.172377	2.762026
34	1	0	6.093605	-0.560751	0.450816
35	1	0	-3.006789	1.799700	-0.644430
36	1	0	-3.209955	1.004698	1.711790
37	1	0	-1.583630	0.329487	1.626374
38	1	0	-2.096084	-3.804943	-0.628887
39	1	0	-4.543744	-3.954824	-1.153465
40	1	0	-6.025662	-2.013766	-0.649427
41	1	0	-5.074848	0.039213	0.361615
42	9	0	4.550400	-0.330234	-1.592449
43	9	0	-0.936831	-1.754335	0.408369

Rotational constants (GHZ): 0.3098457 0.1439957 0.1178938

M1-N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.643390	1.637543	0.471781
2	8	0	-1.317105	3.843540	-0.314919
3	8	0	-1.971249	3.240154	1.756135
4	7	0	2.336308	1.609687	-1.903198
5	7	0	-1.051003	1.168201	-0.956666
6	6	0	1.240918	0.661967	-1.675591
7	6	0	1.780283	-0.751387	-1.325202
8	6	0	2.731471	-0.838795	-0.149616
9	6	0	2.287364	-1.060161	1.164094
10	6	0	3.180306	-1.157581	2.232374
11	6	0	4.554687	-1.039418	2.009686
12	6	0	5.030968	-0.832579	0.714700
13	6	0	4.114399	-0.739686	-0.325823
14	6	0	0.258355	1.178341	-0.616801
15	6	0	-2.102131	1.600341	-0.042166
16	6	0	-2.464217	0.555614	1.035192
17	6	0	-3.054564	-0.704375	0.446218
18	6	0	-2.274131	-1.822790	0.154299
19	6	0	-2.780289	-2.993235	-0.395825
20	6	0	-4.145391	-3.060252	-0.678080
21	6	0	-4.967572	-1.964042	-0.403170

22	6	0	-4.423120	-0.805703	0.153305
23	6	0	-1.767867	2.953505	0.590198
24	1	0	-1.167432	4.690971	0.150579
25	1	0	2.795339	1.774510	-1.006037
26	1	0	1.927596	2.509381	-2.159757
27	1	0	-1.331061	0.752808	-1.836323
28	1	0	0.695708	0.555348	-2.618490
29	1	0	0.921424	-1.403047	-1.138890
30	1	0	2.284610	-1.120012	-2.223048
31	1	0	1.222016	-1.167372	1.342351
32	1	0	2.803205	-1.329986	3.236219
33	1	0	5.255958	-1.115067	2.835603
34	1	0	6.091403	-0.748339	0.499158
35	1	0	-2.987364	1.784123	-0.661690
36	1	0	-3.196932	1.013923	1.704800
37	1	0	-1.572919	0.331925	1.626563
38	1	0	-2.111558	-3.825113	-0.592061
39	1	0	-4.561299	-3.966395	-1.108474
40	1	0	-6.031251	-2.012754	-0.616574
41	1	0	-5.065724	0.043179	0.373810
42	9	0	4.603491	-0.564537	-1.582511
43	9	0	-0.937489	-1.775659	0.424797

Rotational constants (GHZ): 0.3076817 0.1440369 0.1183687

M1-N3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.528794	1.560556	0.541962
2	8	0	-2.406828	3.213723	1.614120
3	8	0	-1.354309	3.853333	-0.270109
4	7	0	2.308776	1.711733	-1.777258
5	7	0	-1.090278	1.142784	-0.989374
6	6	0	1.240237	0.718359	-1.626933
7	6	0	1.818118	-0.688235	-1.308714
8	6	0	2.788811	-0.772141	-0.148918
9	6	0	2.374072	-1.013057	1.170787
10	6	0	3.289121	-1.105150	2.220747
11	6	0	4.656782	-0.961811	1.973129
12	6	0	5.104465	-0.735418	0.671244
13	6	0	4.166380	-0.648431	-0.350440
14	6	0	0.201658	1.160965	-0.587995
15	6	0	-2.183389	1.569865	-0.126327
16	6	0	-2.539266	0.545657	0.977606
17	6	0	-3.038041	-0.764398	0.411580
18	6	0	-2.189629	-1.849437	0.192692
19	6	0	-2.612307	-3.064906	-0.329488
20	6	0	-3.960160	-3.215577	-0.658794
21	6	0	-4.848373	-2.155515	-0.457742
22	6	0	-4.386986	-0.949708	0.072543
23	6	0	-1.903435	2.988361	0.387716
24	1	0	-2.245030	4.153961	1.832533
25	1	0	2.723237	1.862007	-0.856162
26	1	0	1.878547	2.604425	-2.022839
27	1	0	-1.312021	0.834691	-1.927078
28	1	0	0.734248	0.629462	-2.593207
29	1	0	0.978450	-1.365155	-1.123997
30	1	0	2.320735	-1.029179	-2.218197

31	1	0	1.314503	-1.138030	1.369296
32	1	0	2.934306	-1.292933	3.229962
33	1	0	5.374911	-1.033173	2.784839
34	1	0	6.159001	-0.631652	0.436182
35	1	0	-3.058498	1.683927	-0.776479
36	1	0	-3.327004	0.980880	1.596909
37	1	0	-1.665904	0.387487	1.614177
38	1	0	-1.894068	-3.866598	-0.468024
39	1	0	-4.311225	-4.158350	-1.067749
40	1	0	-5.899028	-2.269049	-0.707926
41	1	0	-5.081351	-0.129109	0.235813
42	9	0	4.628244	-0.455826	-1.614806
43	9	0	-0.868567	-1.720025	0.508630

Rotational constants (GHZ): 0.3082778 0.1430688
0.1168757

M2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.718852	0.174322	-1.534103
2	8	0	0.253813	2.548925	1.079395
3	8	0	-1.040090	3.729960	-0.346388
4	7	0	1.605706	-2.283067	-0.926110
5	7	0	-0.793130	0.149274	0.180694
6	6	0	1.022259	-1.468504	0.193973
7	6	0	2.129651	-0.995659	1.166709
8	6	0	3.324052	-0.318016	0.527290
9	6	0	3.410554	1.073014	0.368280
10	6	0	4.540742	1.665530	-0.197830
11	6	0	5.614137	0.875880	-0.618200
12	6	0	5.556236	-0.511937	-0.478556
13	6	0	4.417216	-1.065721	0.086349
14	6	0	0.287781	-0.297748	-0.469132
15	6	0	-1.465524	1.392242	-0.188315
16	6	0	-2.866131	1.462089	0.459060
17	6	0	-3.799903	0.341028	0.065395
18	6	0	-3.856271	-0.850200	0.789940
19	6	0	-4.695184	-1.908756	0.471408
20	6	0	-5.531165	-1.781289	-0.639898
21	6	0	-5.507596	-0.608061	-1.398502
22	6	0	-4.652205	0.437201	-1.043811
23	6	0	-0.658342	2.666718	0.215322
24	1	0	0.899537	-2.901296	-1.341561
25	1	0	2.397817	-2.857831	-0.615268
26	1	0	1.926945	-1.636462	-1.663114
27	1	0	-1.033772	-0.281566	1.066898
28	1	0	0.327794	-2.113432	0.732894
29	1	0	1.652083	-0.310378	1.872808
30	1	0	2.457552	-1.871223	1.735112
31	1	0	2.577022	1.689895	0.692092
32	1	0	4.584119	2.744930	-0.307570
33	1	0	6.495487	1.334044	-1.056841
34	1	0	6.368064	-1.158272	-0.795484
35	1	0	-1.572438	1.399190	-1.276351
36	1	0	-3.300906	2.418016	0.156431
37	1	0	-2.746269	1.488743	1.548362
38	1	0	-4.686349	-2.803865	1.084952
39	1	0	-6.196330	-2.596861	-0.907675

40	1	0	-6.158798	-0.503920	-2.261340
41	1	0	-4.641980	1.352630	-1.630201
42	9	0	4.355556	-2.427953	0.207222
43	9	0	-3.035561	-0.986303	1.874515

Rotational constants (GHZ): 0.4212182 0.1137542 0.0984686

M3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.257070	-0.984082	0.792847
2	8	0	-0.137314	3.175517	-1.332447
3	8	0	1.139375	4.041566	0.317703
4	7	0	-1.147867	-2.611383	-0.650837
5	7	0	0.426923	0.687840	-0.760388
6	6	0	-0.932129	-1.262931	-1.287572
7	6	0	-2.264986	-0.555226	-1.613618
8	6	0	-3.109128	-0.146672	-0.423555
9	6	0	-3.067150	1.151530	0.106904
10	6	0	-3.870601	1.517257	1.188718
11	6	0	-4.743577	0.589312	1.761493
12	6	0	-4.811371	-0.710143	1.254669
13	6	0	-3.996065	-1.036452	0.182406
14	6	0	-0.019383	-0.486542	-0.313518
15	6	0	1.156832	1.667317	0.039527
16	6	0	2.692690	1.570562	-0.147083
17	6	0	3.298237	0.265724	0.313163
18	6	0	3.495611	-0.803876	-0.562073
19	6	0	4.037729	-2.022921	-0.174539
20	6	0	4.402338	-2.197888	1.161438
21	6	0	4.221511	-1.154705	2.073716
22	6	0	3.677631	0.058273	1.647734
23	6	0	0.668867	3.091352	-0.359429
24	1	0	-0.701188	-3.360761	-1.188507
25	1	0	-2.142947	-2.843460	-0.543624
26	1	0	-0.706179	-2.566700	0.288615
27	1	0	0.017758	1.094540	-1.599590
28	1	0	-0.393358	-1.432341	-2.221013
29	1	0	-2.016940	0.334793	-2.198601
30	1	0	-2.831745	-1.215585	-2.278453
31	1	0	-2.394781	1.878378	-0.340914
32	1	0	-3.818967	2.529109	1.579011
33	1	0	-5.372001	0.870391	2.601168
34	1	0	-5.477097	-1.458372	1.671925
35	1	0	0.916207	1.502170	1.093919
36	1	0	3.127800	2.392858	0.427852
37	1	0	2.926137	1.744623	-1.202692
38	1	0	4.166488	-2.808711	-0.912172
39	1	0	4.827377	-3.144052	1.483432
40	1	0	4.507461	-1.283637	3.113531
41	1	0	3.544202	0.870569	2.358149
42	9	0	-4.057995	-2.316787	-0.306324
43	9	0	3.143883	-0.650641	-1.867962

Rotational constants (GHZ): 0.3286054 0.1421232 0.1182828

With water

M1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.533817	1.017596	0.966793
2	8	0	-1.138182	3.646531	0.553211
3	8	0	-2.515438	2.895431	2.154203
4	7	0	2.295965	1.755611	-1.059328
5	7	0	-1.078558	1.127228	-0.647557
6	6	0	1.228883	0.733276	-1.318214
7	6	0	1.791902	-0.706444	-1.360897
8	6	0	2.723121	-1.106334	-0.236120
9	6	0	2.292499	-1.807741	0.899697
10	6	0	3.190070	-2.187406	1.899126
11	6	0	4.546628	-1.873371	1.782644
12	6	0	5.007783	-1.179179	0.662752
13	6	0	4.087358	-0.818338	-0.310561
14	6	0	0.181322	0.962449	-0.221641
15	6	0	-2.184803	1.469558	0.246247
16	6	0	-2.620759	0.280627	1.131761
17	6	0	-3.158438	-0.892250	0.344859
18	6	0	-2.340501	-1.935637	-0.090049
19	6	0	-2.797741	-3.024362	-0.820502
20	6	0	-4.153742	-3.085507	-1.146405
21	6	0	-5.013395	-2.063721	-0.734647
22	6	0	-4.516064	-0.987130	0.002065
23	6	0	-1.900780	2.772114	1.066085
24	1	0	1.865044	2.718800	-1.185577
25	1	0	3.100051	1.632651	-1.682882
26	1	0	2.624416	1.678094	-0.089133
27	1	0	-1.251050	1.126150	-1.644769
28	1	0	0.814975	0.970101	-2.299358
29	1	0	0.929878	-1.378844	-1.381685
30	1	0	2.311003	-0.816238	-2.318062
31	1	0	1.241179	-2.061200	0.991091
32	1	0	2.830029	-2.731396	2.767205
33	1	0	5.247763	-2.167216	2.558004
34	1	0	6.053890	-0.920763	0.535101
35	1	0	-3.020906	1.721534	-0.415604
36	1	0	-3.401945	0.651492	1.797811
37	1	0	-1.778376	-0.028246	1.756402
38	1	0	-2.099871	-3.800129	-1.118977
39	1	0	-4.532322	-3.928775	-1.716500
40	1	0	-6.070275	-2.107778	-0.980882
41	1	0	-5.189350	-0.198036	0.328206
42	8	0	0.794073	4.031965	-1.319125
43	1	0	0.054971	3.810516	-0.687978
44	9	0	4.541246	-0.138653	-1.405910
45	9	0	-1.010476	-1.893404	0.218699
46	1	0	0.397888	3.902109	-2.197184

Rotational constants (GHZ): 0.2584356 0.1408309 0.1082277

M2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.613937	0.311449	1.372987
2	8	0	-0.009169	2.622836	-1.106031
3	8	0	1.298887	3.762798	0.340172
4	7	0	-1.475384	-2.285296	0.580561
5	7	0	0.985049	0.195933	-0.238402
6	6	0	-0.882225	-1.325998	-0.411874
7	6	0	-1.953938	-0.784571	-1.392560
8	6	0	-3.193118	-0.177776	-0.771634
9	6	0	-3.295394	1.186710	-0.463420
10	6	0	-4.456919	1.713954	0.103927
11	6	0	-5.547878	0.882955	0.373149
12	6	0	-5.478824	-0.479556	0.072350
13	6	0	-4.308074	-0.969857	-0.489583
14	6	0	-0.157151	-0.202244	0.335237
15	6	0	1.674659	1.417474	0.166702
16	6	0	3.089647	1.466543	-0.450321
17	6	0	3.987064	0.312781	-0.065189
18	6	0	4.025175	-0.863971	-0.814281
19	6	0	4.829524	-1.951463	-0.504892
20	6	0	5.649417	-1.869912	0.622608
21	6	0	5.643921	-0.712662	1.405650
22	6	0	4.822724	0.362545	1.059601
23	6	0	0.899038	2.713573	-0.234414
24	1	0	-0.732102	-2.797695	1.069204
25	1	0	-2.062570	-2.976491	0.100480
26	1	0	-2.064214	-1.805602	1.315159
27	1	0	1.265907	-0.243827	-1.107965
28	1	0	-0.159050	-1.900076	-0.992908
29	1	0	-1.449435	-0.037416	-2.012098
30	1	0	-2.234985	-1.613724	-2.048623
31	1	0	-2.449382	1.835416	-0.671380
32	1	0	-4.511049	2.773965	0.332934
33	1	0	-6.453509	1.289494	0.813235
34	1	0	-6.306445	-1.154637	0.263719
35	1	0	1.758924	1.407637	1.256782
36	1	0	3.541992	2.403689	-0.116634
37	1	0	2.993504	1.521248	-1.540929
38	1	0	4.807188	-2.832929	-1.137562
39	1	0	6.287760	-2.708662	0.884011
40	1	0	6.282713	-0.644379	2.281238
41	1	0	4.826748	1.265189	1.665503
42	8	0	-2.812030	-0.871001	2.597500
43	1	0	-3.615772	-0.522313	2.174145
44	9	0	-4.237770	-2.303650	-0.768408
45	9	0	3.218862	-0.955535	-1.915153
46	1	0	-2.119599	-0.220481	2.345279

Rotational constants (GHZ): 0.3767310 0.1056053
0.0942457

M3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.049118	-0.012230	-0.678241
2	8	0	2.916906	-3.571117	0.496613

3	8	0	4.113349	-2.938293	-1.314369
4	7	0	-1.171710	0.251016	1.995912
5	7	0	1.293657	-1.520505	0.376497
6	6	0	-0.874546	-1.076567	1.347267
7	6	0	-2.160084	-1.787306	0.871720
8	6	0	-3.056931	-1.050078	-0.097878
9	6	0	-2.988245	-1.244798	-1.484441
10	6	0	-3.847077	-0.571729	-2.355208
11	6	0	-4.803590	0.313481	-1.851408
12	6	0	-4.903663	0.523577	-0.473869
13	6	0	-4.031762	-0.162549	0.360656
14	6	0	0.164975	-0.823113	0.244478
15	6	0	2.470206	-1.415786	-0.478211
16	6	0	3.444026	-0.299007	-0.007238
17	6	0	2.942910	1.120859	-0.149376
18	6	0	2.200820	1.760889	0.844967
19	6	0	1.728263	3.061333	0.741857
20	6	0	2.011131	3.782811	-0.419858
21	6	0	2.753618	3.187598	-1.442335
22	6	0	3.212017	1.876385	-1.300596
23	6	0	3.227331	-2.774705	-0.434650
24	1	0	-0.323384	0.615173	2.447573
25	1	0	-1.895384	0.146703	2.715094
26	1	0	-1.485659	0.982013	1.302581
27	1	0	1.388069	-2.227860	1.101899
28	1	0	-0.432067	-1.692711	2.130658
29	1	0	-1.832766	-2.728279	0.418855
30	1	0	-2.725952	-2.048306	1.772283
31	1	0	-2.248745	-1.936899	-1.877668
32	1	0	-3.771866	-0.741257	-3.425016
33	1	0	-5.475763	0.838157	-2.523693
34	1	0	-5.638593	1.197212	-0.045427
35	1	0	2.150942	-1.213484	-1.503535
36	1	0	4.351204	-0.409419	-0.608663
37	1	0	3.713393	-0.504164	1.034760
38	1	0	1.156298	3.490020	1.558449
39	1	0	1.652275	4.802843	-0.519968
40	1	0	2.980759	3.744257	-2.346789
41	1	0	3.795847	1.418749	-2.095395
42	8	0	-1.663232	2.152597	-0.006326
43	9	0	-4.123039	0.052178	1.704948
44	9	0	1.900006	1.066981	1.987002
45	1	0	-2.566298	1.995064	-0.332835
46	1	0	-1.118290	1.510747	-0.514256

Rotational constants (GHZ): 0.2799775 0.1399500 0.1158776

M3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.058029	-0.448410	0.694026
2	8	0	0.779051	3.483718	-1.821485
3	8	0	1.999473	4.218554	-0.067340
4	7	0	-1.372783	-1.993506	-1.013365
5	7	0	0.570479	1.041644	-0.929038
6	6	0	-1.166335	-0.573152	-1.439729
7	6	0	-2.494042	0.217214	-1.483657
8	6	0	-3.246332	0.305944	-0.173965

9	6	0	-3.075911	1.374824	0.717799
10	6	0	-3.790383	1.439955	1.915392
11	6	0	-4.699245	0.431082	2.244982
12	6	0	-4.893766	-0.644838	1.376677
13	6	0	-4.164105	-0.677713	0.197134
14	6	0	-0.147715	0.020785	-0.453659
15	6	0	1.466516	1.887904	-0.148059
16	6	0	2.939160	1.399845	-0.168884
17	6	0	3.200758	0.102960	0.561477
18	6	0	3.124941	-1.138699	-0.068318
19	6	0	3.352015	-2.350042	0.568220
20	6	0	3.682262	-2.333796	1.924718
21	6	0	3.775007	-1.115136	2.601651
22	6	0	3.538514	0.082012	1.923264
23	6	0	1.400658	3.331752	-0.730949
24	1	0	-0.558381	-2.584668	-1.337981
25	1	0	-2.246143	-2.382817	-1.381799
26	1	0	-1.397499	-2.025585	0.015061
27	1	0	0.332365	1.450661	-1.831733
28	1	0	-0.747656	-0.602239	-2.446778
29	1	0	-2.247668	1.224095	-1.833543
30	1	0	-3.122875	-0.243538	-2.252247
31	1	0	-2.378740	2.166669	0.457475
32	1	0	-3.641317	2.279654	2.587393
33	1	0	-5.259401	0.477837	3.174038
34	1	0	-5.592518	-1.444828	1.598251
35	1	0	1.114527	1.913488	0.887600
36	1	0	3.531580	2.190432	0.300183
37	1	0	3.260965	1.321205	-1.212874
38	1	0	3.266319	-3.275392	0.007550
39	1	0	3.865589	-3.269420	2.444563
40	1	0	4.035612	-1.095752	3.655746
41	1	0	3.617994	1.028524	2.452192
42	8	0	0.870535	-3.353948	-1.899852
43	1	0	1.525566	-2.635933	-1.818338
44	9	0	-4.351821	-1.733822	-0.648287
45	9	0	2.793510	-1.171896	-1.400084
46	1	0	0.742394	-3.442604	-2.859954

Rotational constants (GHZ): 0.2561104 0.1355261 0.1144673

Cartesian Coordinates of Stationary Structures M1 and M1a at SMD(MP2/6-31G*)

FF **M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.485657	-1.477381	-1.065512
2	8	0	-3.400895	-2.371307	-0.328264
3	8	0	-4.572865	-0.598671	-1.119945
4	7	0	0.912732	-3.343428	0.147370
5	7	0	-1.532881	-0.785942	0.859696
6	6	0	0.343835	-2.292421	1.039126
7	6	0	1.476057	-1.453299	1.646347
8	6	0	2.365914	-0.827616	0.604836
9	6	0	2.043515	0.412450	0.034085
10	6	0	2.858661	0.964082	-0.956795
11	6	0	3.996882	0.281186	-1.395568

12	6	0	4.326887	-0.952252	-0.828845
13	6	0	3.514237	-1.503257	0.165185
14	6	0	-0.616877	-1.479823	0.174641
15	6	0	-2.673939	-0.126445	0.233744
16	6	0	-2.273416	1.008154	-0.715375
17	6	0	-1.263895	1.985736	-0.165814
18	6	0	-0.418175	2.662644	-1.057720
19	6	0	0.502160	3.610184	-0.602800
20	6	0	0.600344	3.889580	0.763017
21	6	0	-0.237716	3.224242	1.661901
22	6	0	-1.169322	2.289222	1.200916
23	6	0	-3.620141	-1.134524	-0.473428
24	1	0	0.185668	-4.010136	-0.144917
25	1	0	1.663866	-3.868355	0.616007
26	1	0	1.290897	-2.910983	-0.706894
27	1	0	-1.587097	-0.956549	1.860287
28	1	0	-0.201136	-2.809707	1.832786
29	1	0	1.012143	-0.687916	2.277681
30	1	0	2.062167	-2.109184	2.301202
31	1	0	1.166719	0.955767	0.379297
32	1	0	2.601166	1.928265	-1.387497
33	1	0	4.629605	0.714368	-2.166655
34	1	0	5.216621	-1.484630	-1.157034
35	1	0	3.783758	-2.456411	0.619238
36	1	0	-3.249855	0.299112	1.063193
37	1	0	-3.196594	1.534515	-0.980266
38	1	0	-1.882906	0.580611	-1.643581
39	1	0	-0.479634	2.437803	-2.121885
40	1	0	1.142464	4.127492	-1.314378
41	1	0	1.321841	4.619068	1.123730
42	1	0	-0.174111	3.439984	2.726457
43	1	0	-1.819277	1.794290	1.918807

Rotational constants (GHZ): 0.3230049 0.2377914 0.1613625

FF **M1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.171689	-0.732782	0.894781
2	8	0	3.879529	0.617832	-0.051007
3	8	0	3.428470	2.198166	1.506129
4	7	0	1.438983	-2.936530	-0.531751
5	7	0	1.305903	0.637144	-0.932824
6	6	0	0.980155	-1.736761	-1.282996
7	6	0	-0.467170	-1.901766	-1.761802
8	6	0	-1.448848	-2.056980	-0.630763
9	6	0	-2.045585	-0.930349	-0.045523
10	6	0	-2.931270	-1.076543	1.024111
11	6	0	-3.224783	-2.347626	1.527078
12	6	0	-2.638411	-3.475196	0.947074
13	6	0	-1.755218	-3.329820	-0.126116
14	6	0	1.167445	-0.555052	-0.339589
15	6	0	1.776101	1.799119	-0.186216
16	6	0	0.734702	2.342016	0.795301
17	6	0	-0.657254	2.489069	0.230317
18	6	0	-1.758438	2.355641	1.089393
19	6	0	-3.065058	2.513243	0.619978
20	6	0	-3.293245	2.799987	-0.728464

21	6	0	-2.205082	2.940038	-1.594396
22	6	0	-0.898835	2.796798	-1.117419
23	6	0	3.137489	1.495711	0.498900
24	1	0	2.432965	-2.786261	-0.219010
25	1	0	1.374804	-3.781353	-1.113622
26	1	0	0.860789	-3.072607	0.307056
27	1	0	1.406943	0.649196	-1.944091
28	1	0	1.643007	-1.636897	-2.146998
29	1	0	-0.710056	-1.020328	-2.365460
30	1	0	-0.503969	-2.773882	-2.425882
31	1	0	-1.830539	0.061166	-0.438990
32	1	0	-3.391325	-0.195101	1.463666
33	1	0	-3.916277	-2.459024	2.358918
34	1	0	-2.870453	-4.467950	1.325769
35	1	0	-1.316874	-4.212724	-0.590400
36	1	0	1.984595	2.564407	-0.943119
37	1	0	1.099666	3.312298	1.150495
38	1	0	0.694382	1.688602	1.671440
39	1	0	-1.587750	2.116307	2.138319
40	1	0	-3.902792	2.409633	1.306557
41	1	0	-4.308484	2.913742	-1.101519
42	1	0	-2.371758	3.169939	-2.644727
43	1	0	-0.068438	2.921210	-1.809009
44	8	0	3.995052	-2.155509	0.310517
45	1	0	3.920553	-1.175132	0.203293
46	1	0	3.908736	-2.280366	1.272769

Rotational constants (GHZ): 0.2652001 0.2314249 0.1464961

Mono1 F-FF **M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.246987	-1.255560	-1.004548
2	8	0	-1.555925	-3.592544	-0.183036
3	8	0	-3.496335	-2.980601	-1.185194
4	7	0	2.122516	-2.582267	0.264396
5	7	0	-1.115769	-1.143943	0.845951
6	6	0	1.229902	-1.747191	1.121393
7	6	0	1.982811	-0.537296	1.683808
8	6	0	2.464453	0.429239	0.636970
9	6	0	1.720804	1.561032	0.276676
10	6	0	2.184004	2.447774	-0.697661
11	6	0	3.412777	2.221759	-1.324837
12	6	0	4.179462	1.105258	-0.982807
13	6	0	3.684699	0.245884	-0.012784
14	6	0	0.055283	-1.367095	0.220183
15	6	0	-2.379239	-1.332885	0.129416
16	6	0	-2.661137	-0.253357	-0.922700
17	6	0	-2.574839	1.141384	-0.365197
18	6	0	-1.547582	2.009998	-0.755622
19	6	0	-1.469827	3.305822	-0.233986
20	6	0	-2.418163	3.746613	0.692046
21	6	0	-3.447061	2.886362	1.090208
22	6	0	-3.523794	1.595718	0.563861
23	6	0	-2.469784	-2.764424	-0.471212
24	1	0	1.680871	-3.492255	0.074082
25	1	0	3.035766	-2.749135	0.704800
26	1	0	2.258389	-2.119906	-0.645867

27	1	0	-1.138300	-1.437802	1.819855
28	1	0	0.898181	-2.384407	1.944928
29	1	0	1.295267	-0.024752	2.364215
30	1	0	2.819785	-0.908486	2.286038
31	1	0	0.771492	1.745301	0.773830
32	1	0	1.591384	3.321079	-0.957359
33	1	0	3.779105	2.910872	-2.081225
34	1	0	5.140051	0.900544	-1.446748
35	1	0	-3.159226	-1.263188	0.896747
36	1	0	-3.668983	-0.444145	-1.303508
37	1	0	-1.967516	-0.365253	-1.759782
38	1	0	-0.671919	3.971597	-0.556518
39	1	0	-2.360116	4.753972	1.097735
40	1	0	-4.192949	3.224620	1.806242
41	1	0	-4.334245	0.934918	0.869611
42	9	0	4.431743	-0.855183	0.323399
43	1	0	-0.804389	1.668611	-1.474401

Rotational constants (GHZ): 0.2989012 0.1996452 0.1344930

Mono1 F-FF **M1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.245121	1.149174	0.927735
2	8	0	-1.843212	3.410735	0.593819
3	8	0	-2.940318	2.382876	2.275673
4	7	0	1.880621	1.955027	-1.119465
5	7	0	-1.414450	0.955590	-0.636543
6	6	0	0.888460	0.871985	-1.371552
7	6	0	1.557380	-0.508101	-1.427319
8	6	0	2.455368	-0.818935	-0.260531
9	6	0	2.022971	-1.564829	0.844527
10	6	0	2.883526	-1.848906	1.906190
11	6	0	4.205124	-1.393583	1.879909
12	6	0	4.668536	-0.653063	0.790343
13	6	0	3.784067	-0.393127	-0.246589
14	6	0	-0.135121	0.997778	-0.251680
15	6	0	-2.518263	1.099759	0.303895
16	6	0	-2.692789	-0.151735	1.174142
17	6	0	-2.653785	-1.415158	0.355254
18	6	0	-1.689391	-2.397691	0.615152
19	6	0	-1.612911	-3.556936	-0.163687
20	6	0	-2.506855	-3.747600	-1.219905
21	6	0	-3.484793	-2.781355	-1.479076
22	6	0	-3.555907	-1.625068	-0.699270
23	6	0	-2.398931	2.401374	1.135304
24	1	0	1.371544	2.872322	-1.206323
25	1	0	2.668240	1.913543	-1.776690
26	1	0	2.245188	1.878513	-0.160837
27	1	0	-1.621190	0.838723	-1.624192
28	1	0	0.429919	1.088641	-2.339644
29	1	0	0.756087	-1.253310	-1.485978
30	1	0	2.126394	-0.562948	-2.361768
31	1	0	0.998610	-1.926015	0.856116
32	1	0	2.525096	-2.431398	2.750833
33	1	0	4.878649	-1.612204	2.704294
34	1	0	5.690496	-0.289882	0.731893
35	1	0	-3.412688	1.221912	-0.318474

36	1	0	-3.643514	-0.057245	1.708457
37	1	0	-1.898921	-0.177070	1.927339
38	1	0	-0.856211	-4.307370	0.055363
39	1	0	-2.450497	-4.645613	-1.830576
40	1	0	-4.192024	-2.928321	-2.292514
41	1	0	-4.322790	-0.881019	-0.910360
42	8	0	0.036981	4.004070	-1.314824
43	1	0	-0.659204	3.695211	-0.676731
44	9	0	4.241554	0.329211	-1.321205
45	1	0	-0.351887	3.823629	-2.189250
46	1	0	-1.007179	-2.261001	1.452070

Rotational constants (GHZ): 0.2550707 0.1730135 0.1286466

Mono2 F-FF **M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.965551	1.473094	-0.341017
2	8	0	0.855430	3.837903	0.320806
3	8	0	1.536375	3.295661	-1.772010
4	7	0	-2.421699	1.401930	1.987778
5	7	0	0.891622	1.117655	0.948945
6	6	0	-1.280163	0.453416	1.806334
7	6	0	-1.815607	-0.949863	1.481133
8	6	0	-2.811336	-1.003267	0.347828
9	6	0	-2.401111	-1.186958	-0.981625
10	6	0	-3.340719	-1.228970	-2.013065
11	6	0	-4.702978	-1.082792	-1.734376
12	6	0	-5.122382	-0.906239	-0.414033
13	6	0	-4.182186	-0.871957	0.619141
14	6	0	-0.422104	1.053519	0.700957
15	6	0	1.833084	1.672738	-0.020185
16	6	0	2.158588	0.659431	-1.120664
17	6	0	2.824913	-0.562164	-0.553033
18	6	0	2.106520	-1.697121	-0.181888
19	6	0	2.679732	-2.829852	0.380442
20	6	0	4.058721	-2.833035	0.600145
21	6	0	4.823365	-1.716581	0.248483
22	6	0	4.207943	-0.598469	-0.317867
23	6	0	1.341624	3.051901	-0.544267
24	1	0	-2.096793	2.298627	2.376159
25	1	0	-3.134103	1.018361	2.624243
26	1	0	-2.865291	1.594705	1.078749
27	1	0	1.245881	0.727529	1.817911
28	1	0	-0.741439	0.425488	2.756272
29	1	0	-0.947337	-1.579896	1.268311
30	1	0	-2.284307	-1.332143	2.395933
31	1	0	-1.345662	-1.306100	-1.207572
32	1	0	-3.008166	-1.376873	-3.038004
33	1	0	-5.432328	-1.115491	-2.540234
34	1	0	-6.180662	-0.804001	-0.185275
35	1	0	2.750684	1.876410	0.546050
36	1	0	2.834287	1.138197	-1.833937
37	1	0	1.240586	0.397714	-1.655339
38	1	0	2.054087	-3.680746	0.635299
39	1	0	4.530610	-3.708285	1.038908
40	1	0	5.897618	-1.717866	0.414093
41	1	0	4.805443	0.267949	-0.597488

42	9	0	0.751033	-1.711039	-0.398204
43	1	0	-4.517337	-0.757002	1.649687

Rotational constants (GHZ): 0.3325756 0.1694248
0.1358847

Mono2 F-FF **M1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.885953	1.001910	0.764110
2	8	0	-0.724174	3.600217	0.550321
3	8	0	-1.584185	2.753995	2.456485
4	7	0	2.304617	1.513277	-1.600219
5	7	0	-0.942640	1.058801	-0.604495
6	6	0	1.214184	0.494903	-1.563061
7	6	0	1.788585	-0.927715	-1.512985
8	6	0	2.800834	-1.175360	-0.421549
9	6	0	2.422380	-1.713526	0.817705
10	6	0	3.374399	-1.940563	1.813053
11	6	0	4.718967	-1.630862	1.587513
12	6	0	5.108022	-1.102160	0.354712
13	6	0	4.155723	-0.883029	-0.644302
14	6	0	0.359940	0.862542	-0.357913
15	6	0	-1.865739	1.474375	0.444814
16	6	0	-2.251632	0.292970	1.341500
17	6	0	-2.892336	-0.799600	0.533519
18	6	0	-2.150094	-1.846617	-0.010290
19	6	0	-2.689225	-2.848987	-0.805255
20	6	0	-4.056034	-2.803828	-1.088770
21	6	0	-4.843000	-1.772176	-0.568123
22	6	0	-4.261810	-0.784134	0.229559
23	6	0	-1.322192	2.699036	1.224162
24	1	0	1.857303	2.460082	-1.714335
25	1	0	2.954752	1.336779	-2.377021
26	1	0	2.838544	1.495436	-0.721516
27	1	0	-1.278448	0.975560	-1.559218
28	1	0	0.649566	0.618497	-2.490866
29	1	0	0.939913	-1.611483	-1.416288
30	1	0	2.252635	-1.116240	-2.488844
31	1	0	1.379962	-1.958304	1.000579
32	1	0	3.065831	-2.362883	2.766707
33	1	0	5.458761	-1.808316	2.364401
34	1	0	6.153535	-0.870686	0.164721
35	1	0	-2.767133	1.822763	-0.075296
36	1	0	-2.956789	0.650684	2.095964
37	1	0	-1.361735	-0.072307	1.861673
38	1	0	-2.047516	-3.637757	-1.188053
39	1	0	-4.501415	-3.576693	-1.709758
40	1	0	-5.907755	-1.737276	-0.783843
41	1	0	-4.876347	0.016702	0.637978
42	8	0	0.623240	3.703265	-1.822934
43	1	0	0.078441	3.590234	-0.997545
44	9	0	-0.806241	-1.903309	0.263996
45	1	0	0.046114	3.360605	-2.528797
46	1	0	4.471600	-0.496882	-1.613184

Rotational constants (GHZ): 0.2763970 0.1634400
0.1279857

Di F-FF **M1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.662267	1.508437	0.484431
2	8	0	-1.187671	3.839693	-0.331070
3	8	0	-1.960506	3.296459	1.729103
4	7	0	2.266111	1.516355	-1.731089
5	7	0	-1.100527	1.117904	-0.924652
6	6	0	1.141069	0.533558	-1.651007
7	6	0	1.681679	-0.861781	-1.301030
8	6	0	2.629903	-0.897519	-0.129841
9	6	0	2.217898	-1.168405	1.183728
10	6	0	3.137801	-1.208594	2.232888
11	6	0	4.496298	-0.985023	1.990031
12	6	0	4.938881	-0.715424	0.693677
13	6	0	3.995462	-0.685033	-0.322727
14	6	0	0.194808	1.091422	-0.595409
15	6	0	-2.116515	1.650297	-0.019650
16	6	0	-2.473870	0.639945	1.073042
17	6	0	-3.042794	-0.619607	0.483273
18	6	0	-2.247866	-1.725819	0.190878
19	6	0	-2.724111	-2.894661	-0.387343
20	6	0	-4.081629	-2.967236	-0.706770
21	6	0	-4.920692	-1.881827	-0.436932
22	6	0	-4.401301	-0.725314	0.148351
23	6	0	-1.696660	3.048111	0.515619
24	1	0	1.964711	2.382487	-2.198857
25	1	0	3.073376	1.135640	-2.242477
26	1	0	2.567215	1.767108	-0.776927
27	1	0	-1.381714	0.748028	-1.828420
28	1	0	0.670744	0.505496	-2.636232
29	1	0	0.817973	-1.501209	-1.102148
30	1	0	2.182526	-1.252772	-2.192808
31	1	0	1.165479	-1.350991	1.377467
32	1	0	2.794381	-1.422234	3.241582
33	1	0	5.213431	-1.015858	2.806017
34	1	0	5.985959	-0.540450	0.464336
35	1	0	-3.004094	1.818217	-0.642243
36	1	0	-3.217766	1.098873	1.729258
37	1	0	-1.585303	0.427705	1.674709
38	1	0	-2.042680	-3.719229	-0.577087
39	1	0	-4.479322	-3.871695	-1.159540
40	1	0	-5.978608	-1.937524	-0.680123
41	1	0	-5.057220	0.116576	0.364566
42	9	0	4.431033	-0.414811	-1.599239
43	9	0	-0.912261	-1.668215	0.504210

Rotational constants (GHZ): 0.3192068 0.1487963
0.1230262

Di F-FF **M1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.533455	1.033955	0.928082
2	8	0	-1.115525	3.613404	0.507263

3	8	0	-2.200267	2.806399	2.313633
4	7	0	2.193678	1.622787	-1.209792
5	7	0	-1.152683	1.059832	-0.616927
6	6	0	1.112006	0.606832	-1.363356
7	6	0	1.673578	-0.821890	-1.317607
8	6	0	2.645511	-1.083837	-0.197404
9	6	0	2.269387	-1.650893	1.029208
10	6	0	3.212475	-1.892587	2.029751
11	6	0	4.558566	-1.577144	1.821754
12	6	0	4.965688	-1.015593	0.609970
13	6	0	4.000367	-0.791841	-0.360896
14	6	0	0.124855	0.910534	-0.244120
15	6	0	-2.185439	1.451058	0.335300
16	6	0	-2.593925	0.276909	1.231609
17	6	0	-3.099260	-0.878094	0.415237
18	6	0	-2.257165	-1.906161	-0.004903
19	6	0	-2.667949	-2.973821	-0.791252
20	6	0	-4.004130	-3.020019	-1.195347
21	6	0	-4.887707	-2.010266	-0.802394
22	6	0	-4.434299	-0.954410	-0.008718
23	6	0	-1.776096	2.719505	1.128864
24	1	0	1.769500	2.568829	-1.397601
25	1	0	2.978348	1.447171	-1.849050
26	1	0	2.548762	1.609667	-0.244311
27	1	0	-1.378429	1.016722	-1.606368
28	1	0	0.657207	0.783034	-2.341374
29	1	0	0.823199	-1.505029	-1.241166
30	1	0	2.163151	-1.012139	-2.278341
31	1	0	1.226009	-1.904308	1.192032
32	1	0	2.897332	-2.334903	2.971097
33	1	0	5.294022	-1.764304	2.599626
34	1	0	6.002801	-0.762948	0.409233
35	1	0	-3.052499	1.739345	-0.272431
36	1	0	-3.383743	0.621924	1.903076
37	1	0	-1.740905	-0.022533	1.846431
38	1	0	-1.954447	-3.743311	-1.072536
39	1	0	-4.350440	-3.846008	-1.811073
40	1	0	-5.928938	-2.046804	-1.112096
41	1	0	-5.124603	-0.171789	0.302324
42	8	0	0.559160	3.808164	-1.653755
43	1	0	-0.101796	3.656135	-0.927081
44	9	0	4.399831	-0.242169	-1.555281
45	9	0	-0.942647	-1.872069	0.390280
46	1	0	0.100477	3.496004	-2.454304

Rotational constants (GHZ): 0.2658006 0.1445424
0.1149406