Quaternary ammonium fluorides and difluorosilicates as nucleophilic fluorination reagents.

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SUPPORTING INFORMATION

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1. Results of preliminary computations

Preliminary computations were performed using Gaussian16[1] program suite using pure M-06L functional,[2] which enabled the use of the RI (resolution of identity) approach,[3] together with the double-ζ def2-SVP basis set,[4] which greatly accelerated the initial calculations. To better describe the anionic structures, we also used double-ζ def2-SVPD basis set with additional diffuse functions.[5] Solvent (MeCN) was simulated using the SMD variant of the IEF-PCM method.[6] The potential energy surfaces of decomposition of difluorosilicates **20**-**23** to fluorosilane-ammonium fluoride complexes **24**-**27** is show on Figure S1. Compared to higher level computations at the M06-2X/def2-TZVP level, relative transition state energies was lower for silicate **22**, but decrease analogously with increasing amount of methyl groups in the silicate.

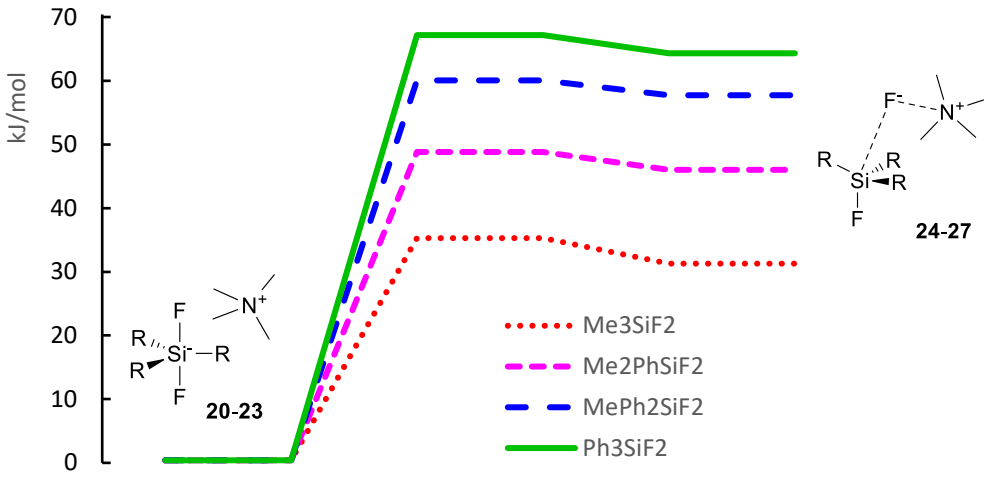

Figure S1. Preliminary calculations of potential energy surfaces of decomposition of difluorosilicates **20-23** to fluorosilane-ammonium fluoride complexes **24-27** at the SMD-M06L/def2-SVP level of theory

2. NMR spectra of the synthesized compounds

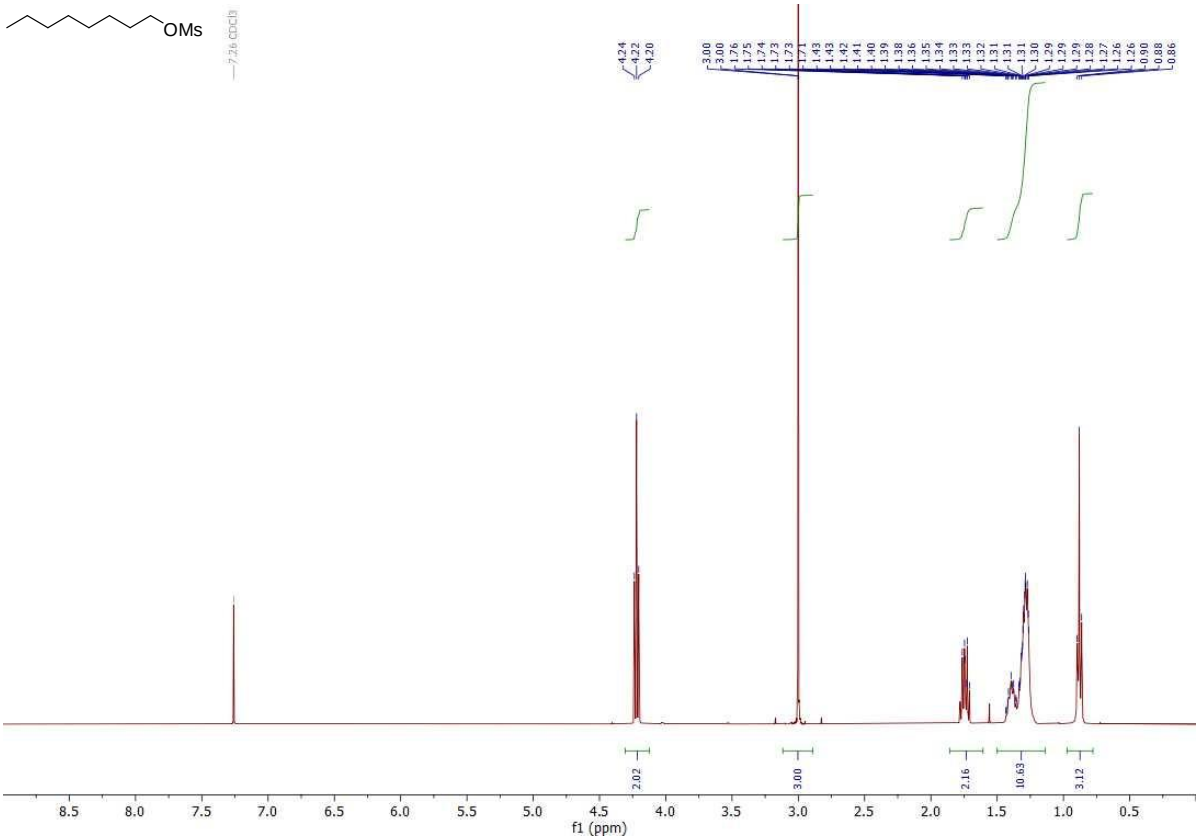

Figure S1: ^{1}H NMR spectrum of **4a** in $CDCl_3$

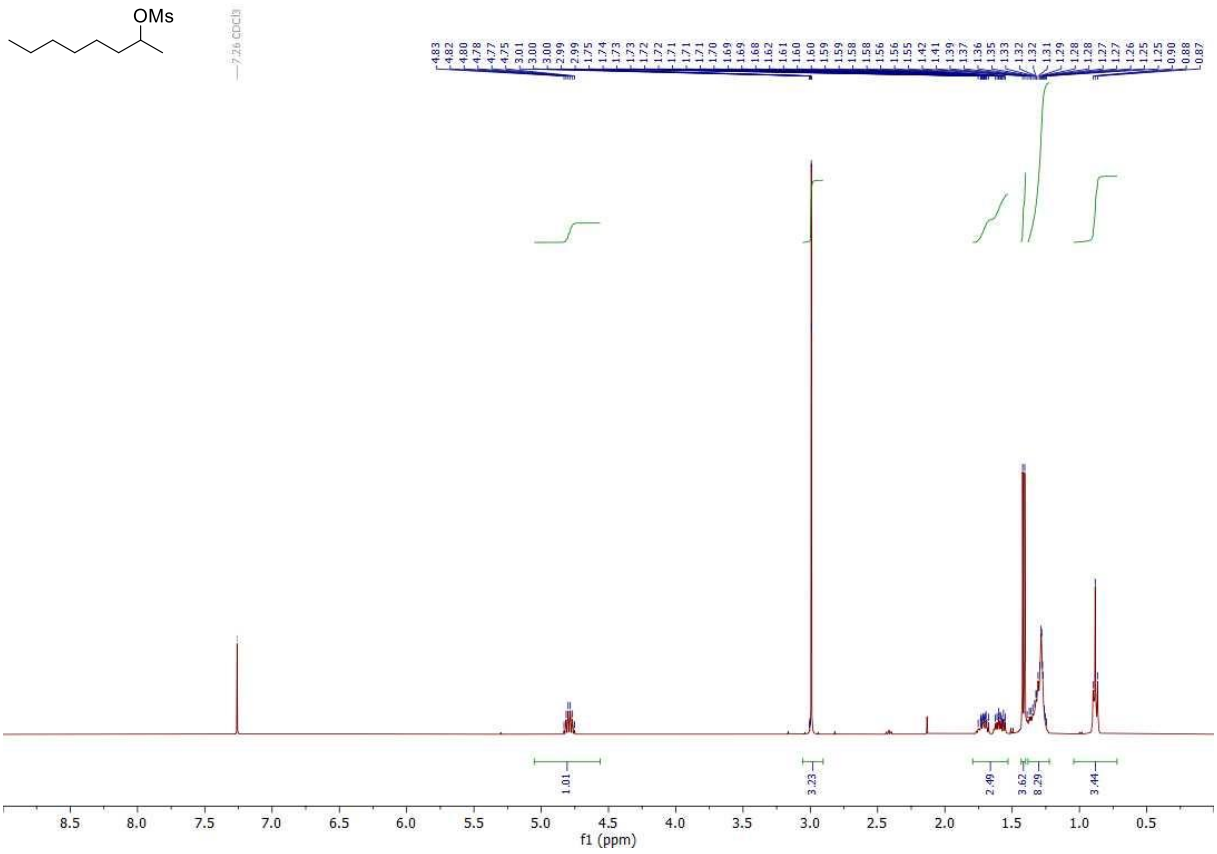

Figure S2: ^{1}H NMR spectrum of **4b** in $CDCl_3$

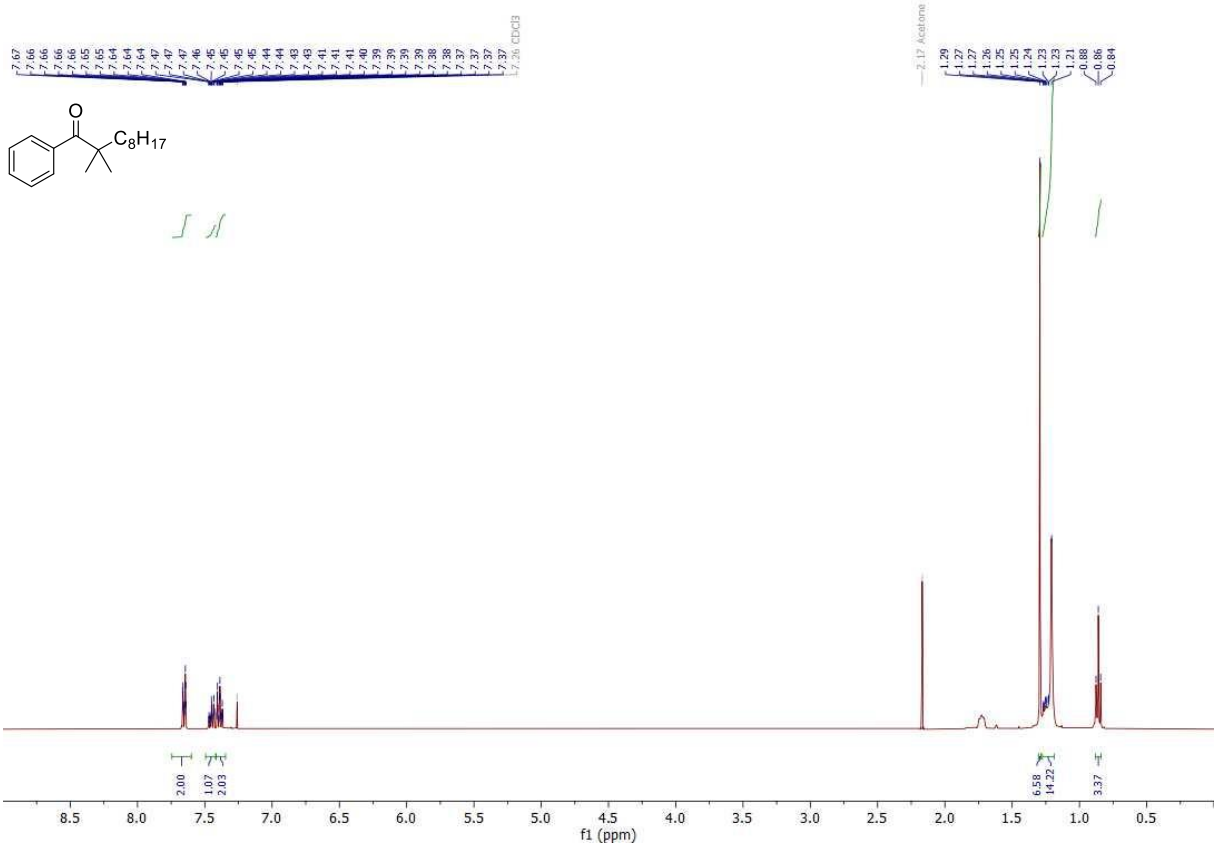

Figure S3: ^{1}H NMR spectrum of **11** in $CDCl_3$

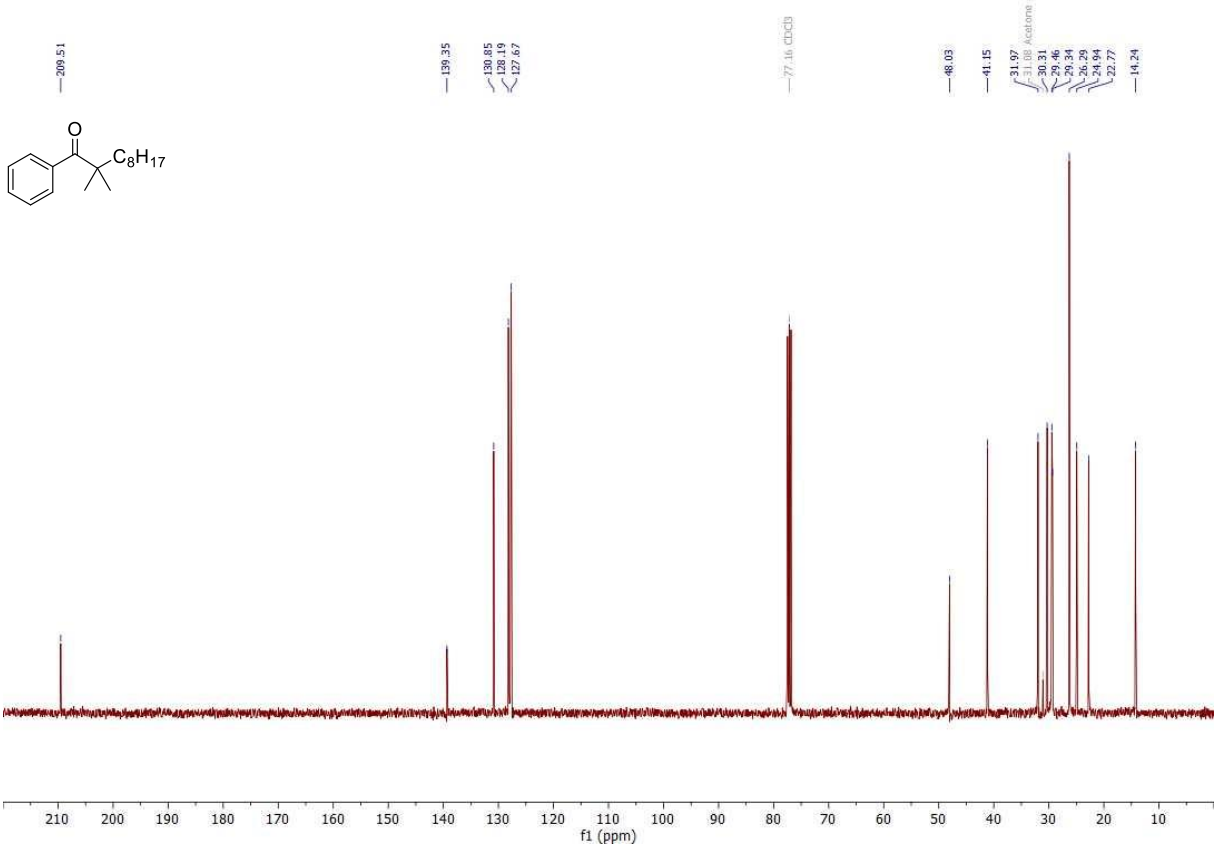

Figure S4: ^{13}C NMR spectrum of **11** in $CDCl_3$

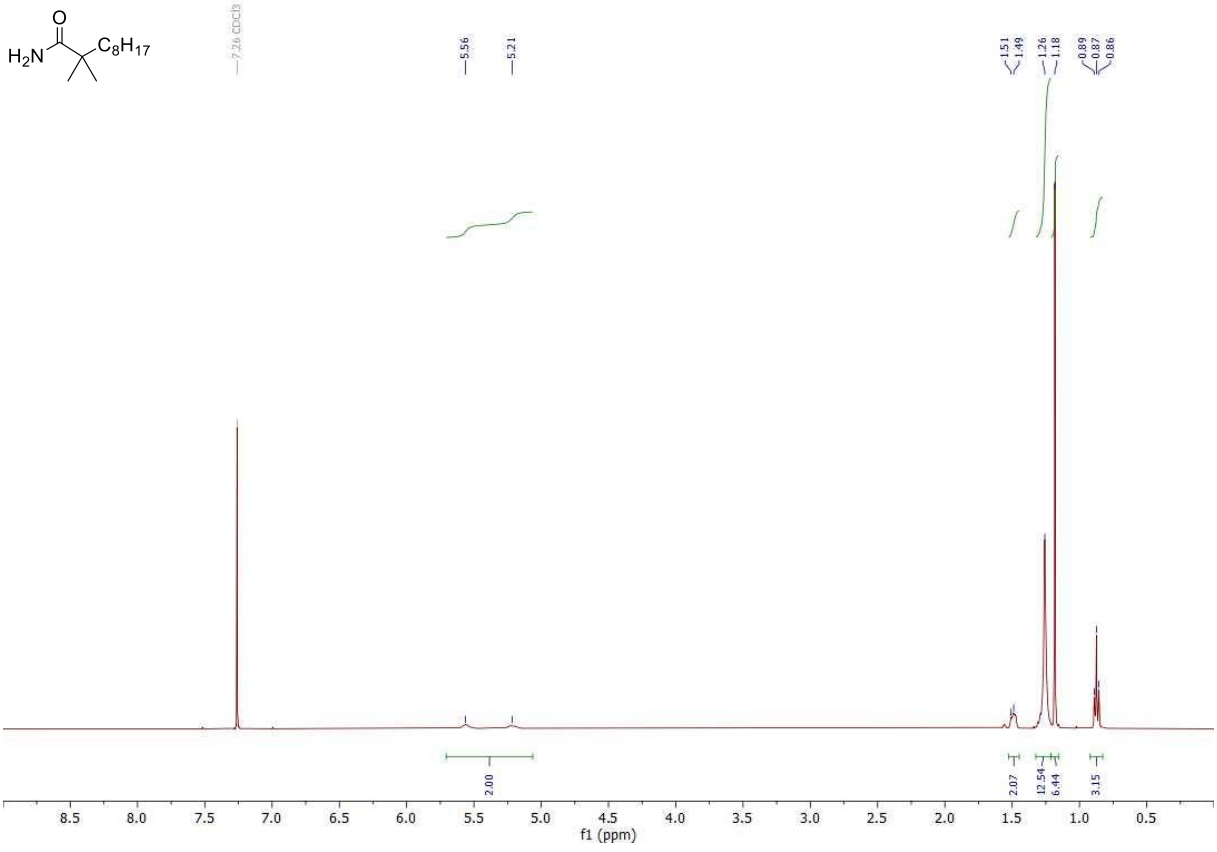

Figure S5: ^{1}H NMR spectrum of **12** in $CDCl_3$

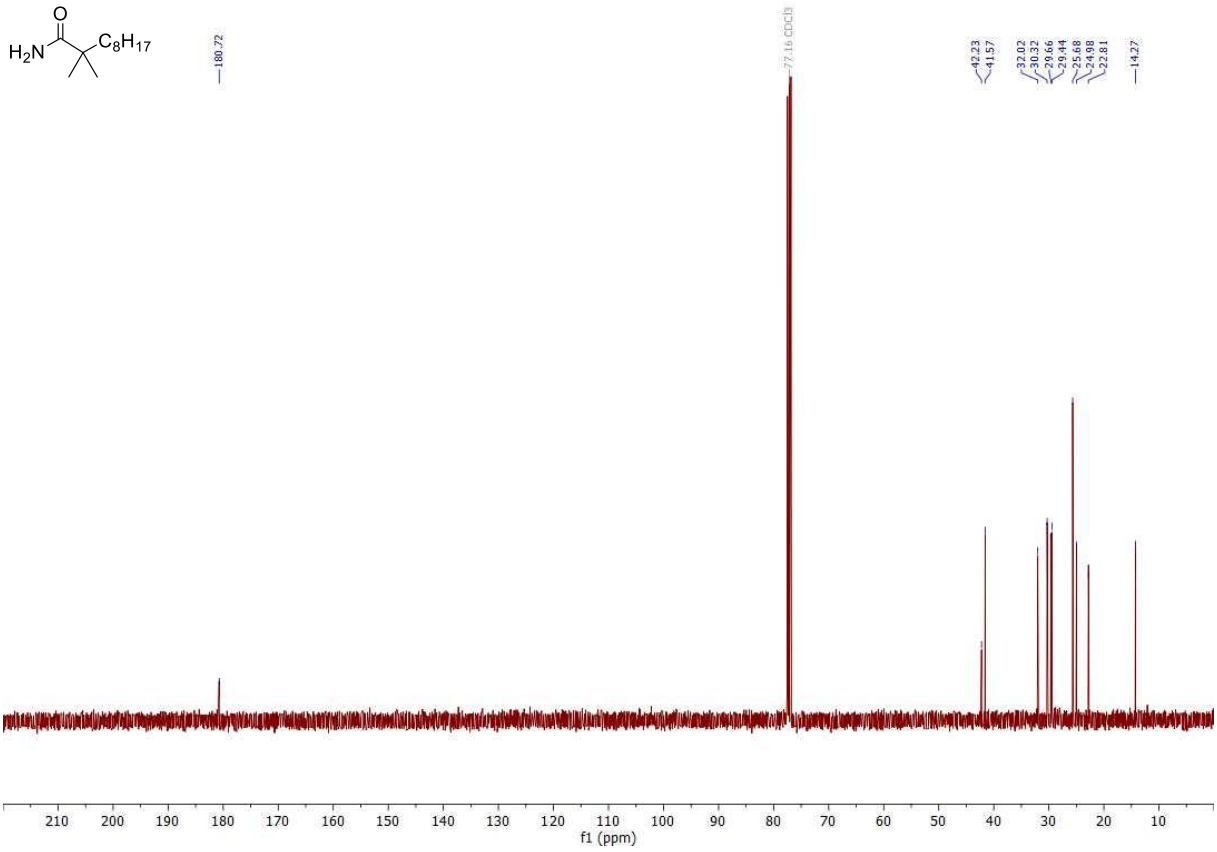

Figure S6: ^{13}C NMR spectrum of **12** in $CDCl_3$

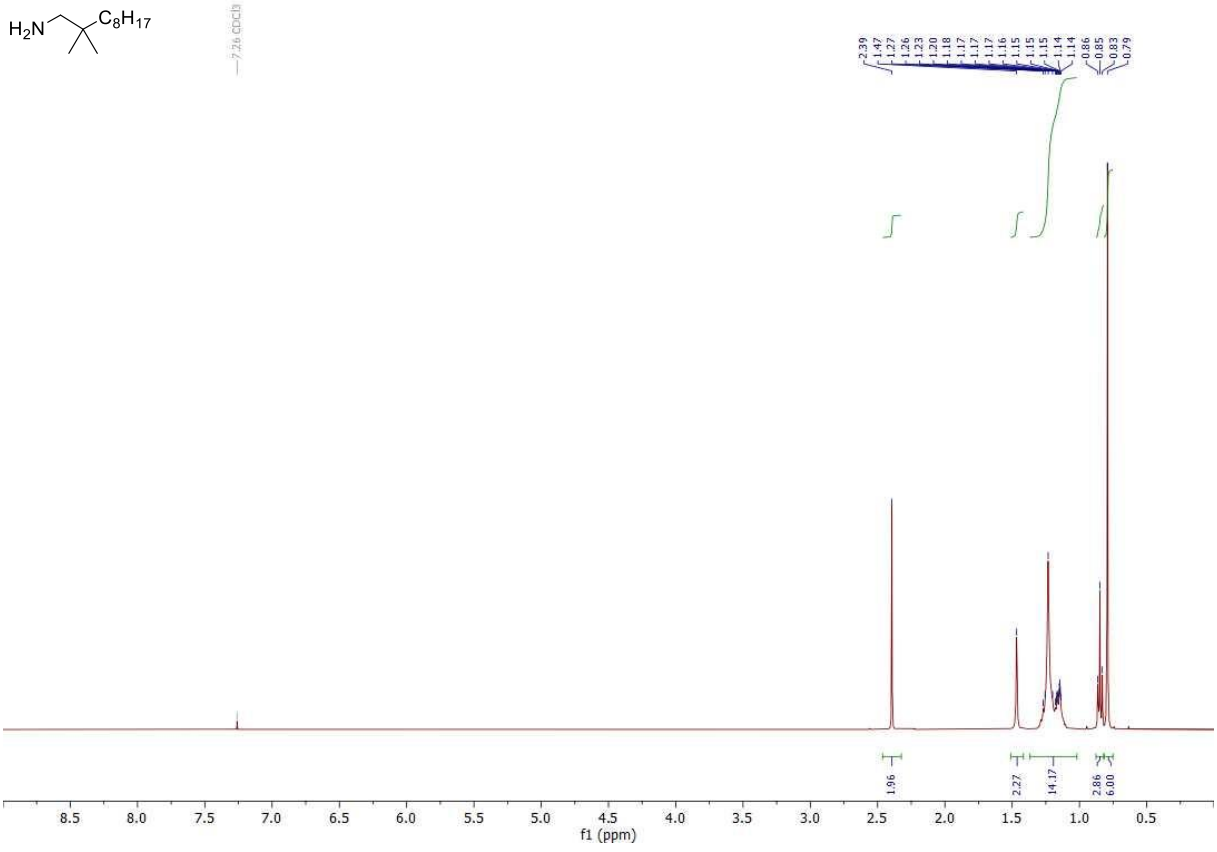

Figure S7: ^{1}H NMR spectrum of **9d** in $CDCl_3$

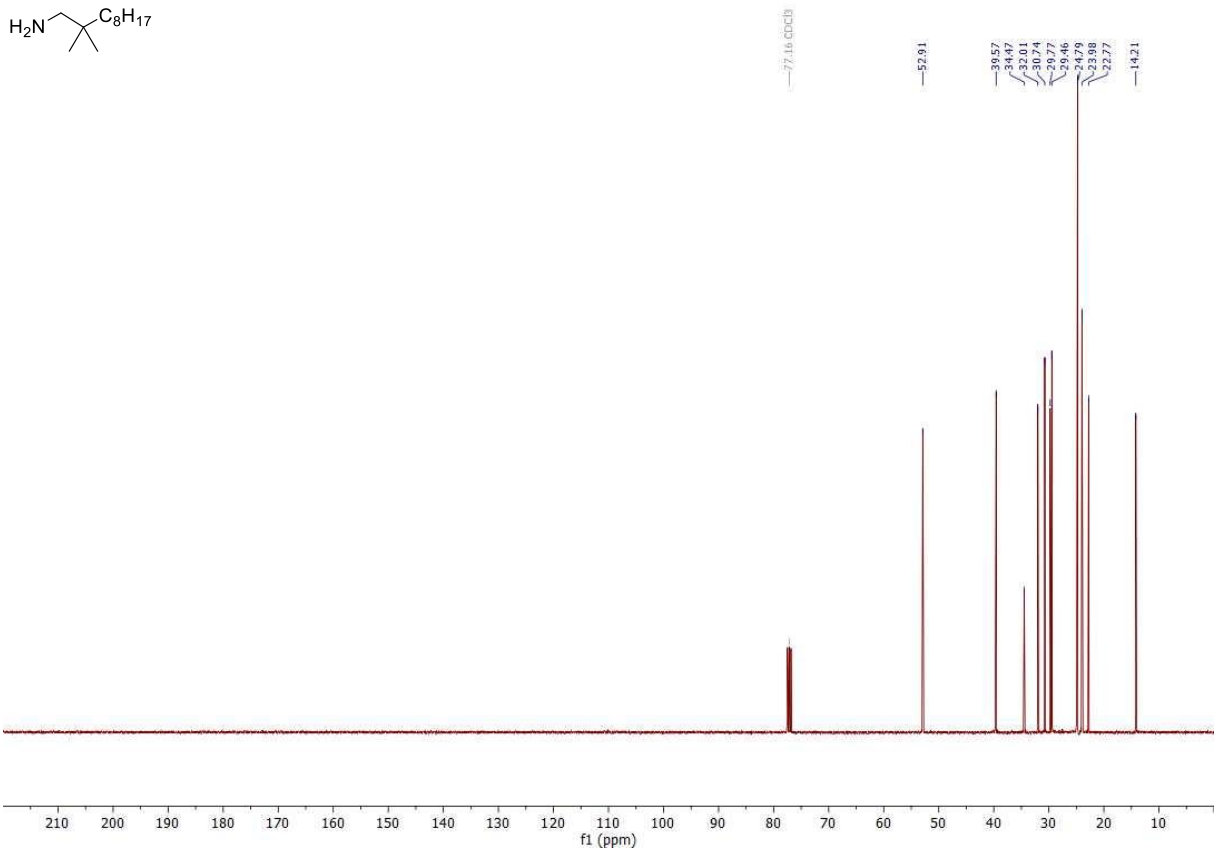

Figure S8: ^{13}C NMR spectrum of **9d** in $CDCl_3$

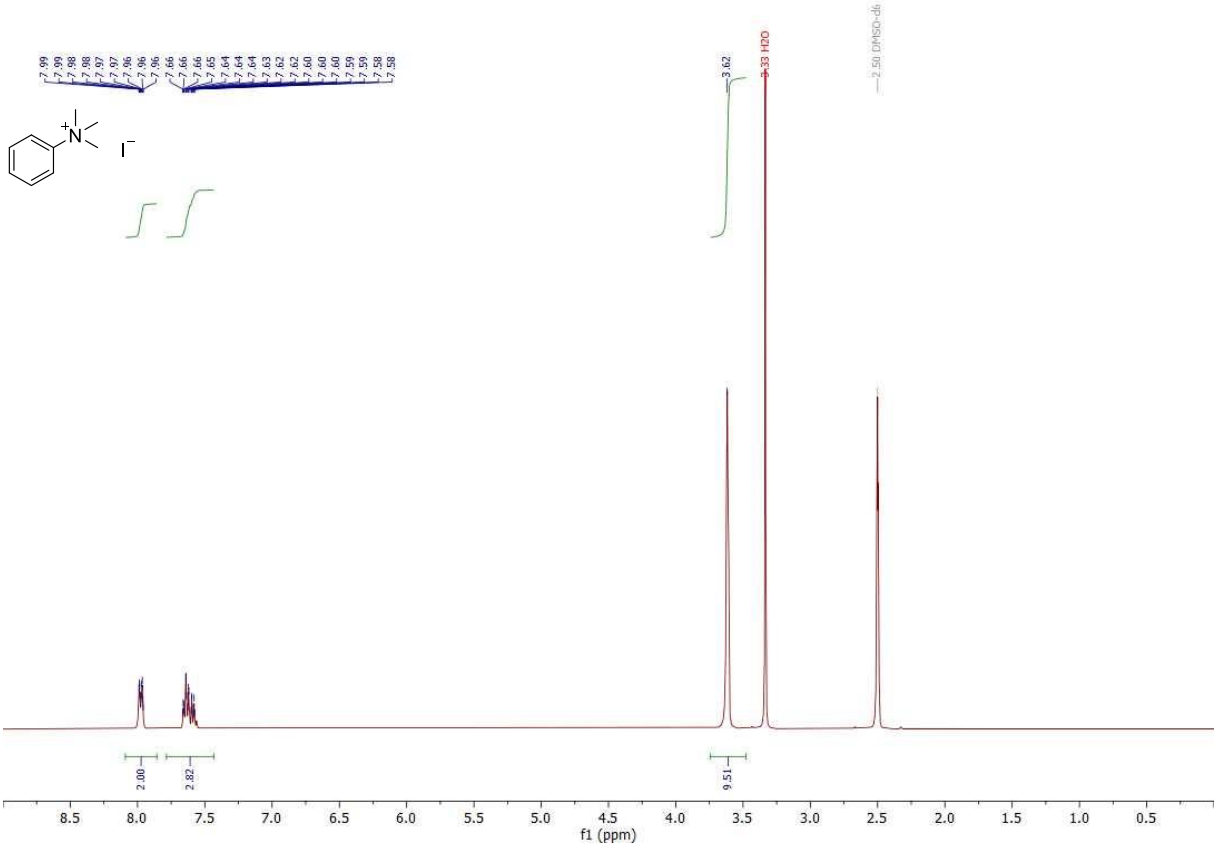

Figure S9: ^{1}H NMR spectrum of **13a** in DMSO-d_6

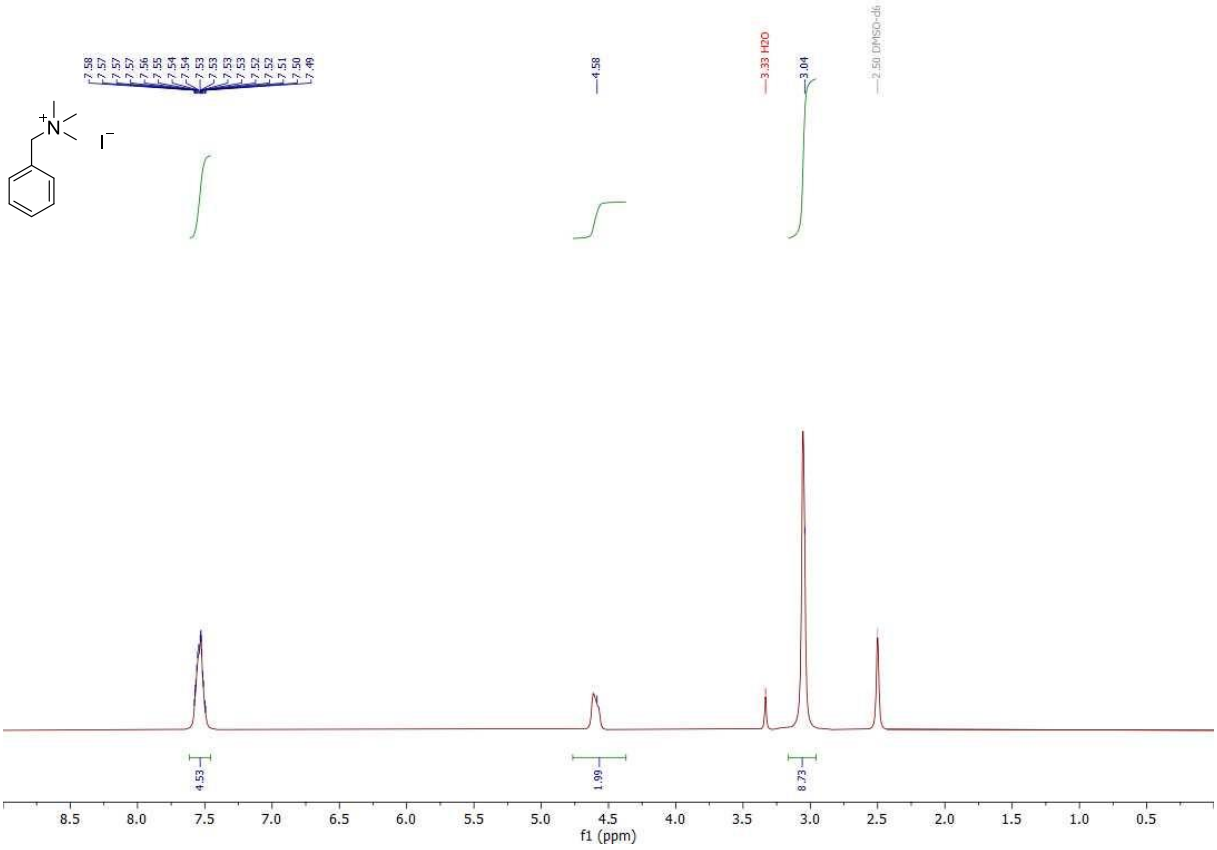

Figure S10: ^{1}H NMR spectrum of **13b** in DMSO-d_6

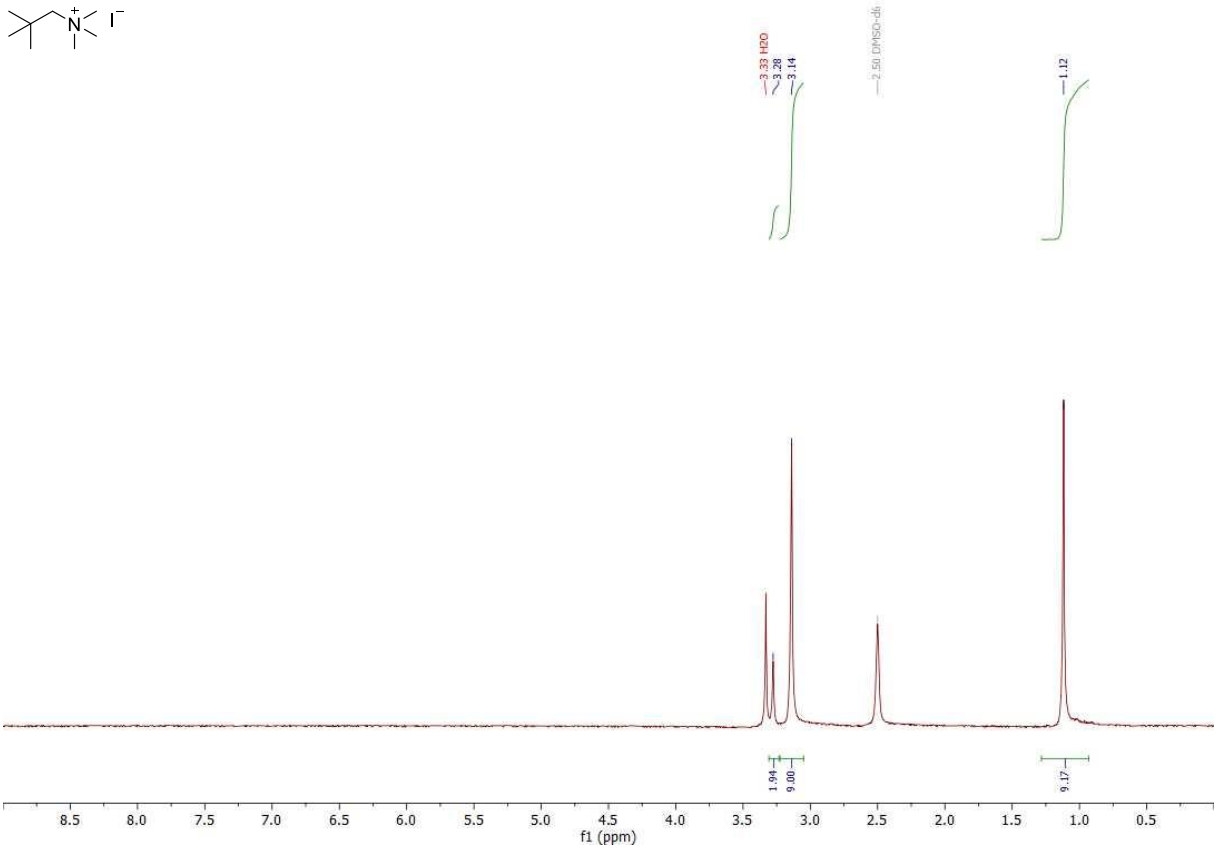

Figure S11: ^{1}H NMR spectrum of **13c** in DMSO-d_6

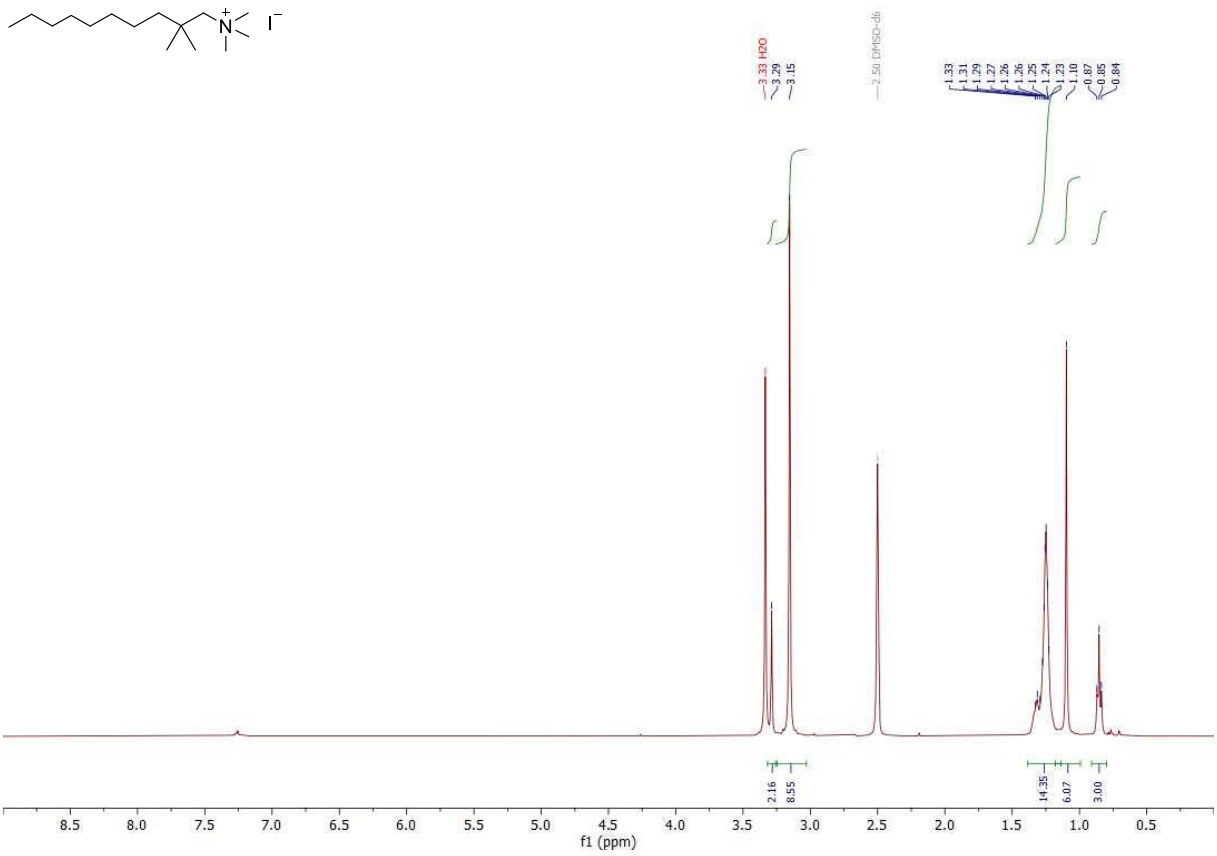

Figure S12: ^{1}H NMR spectrum of **13d** in DMSO-d_6

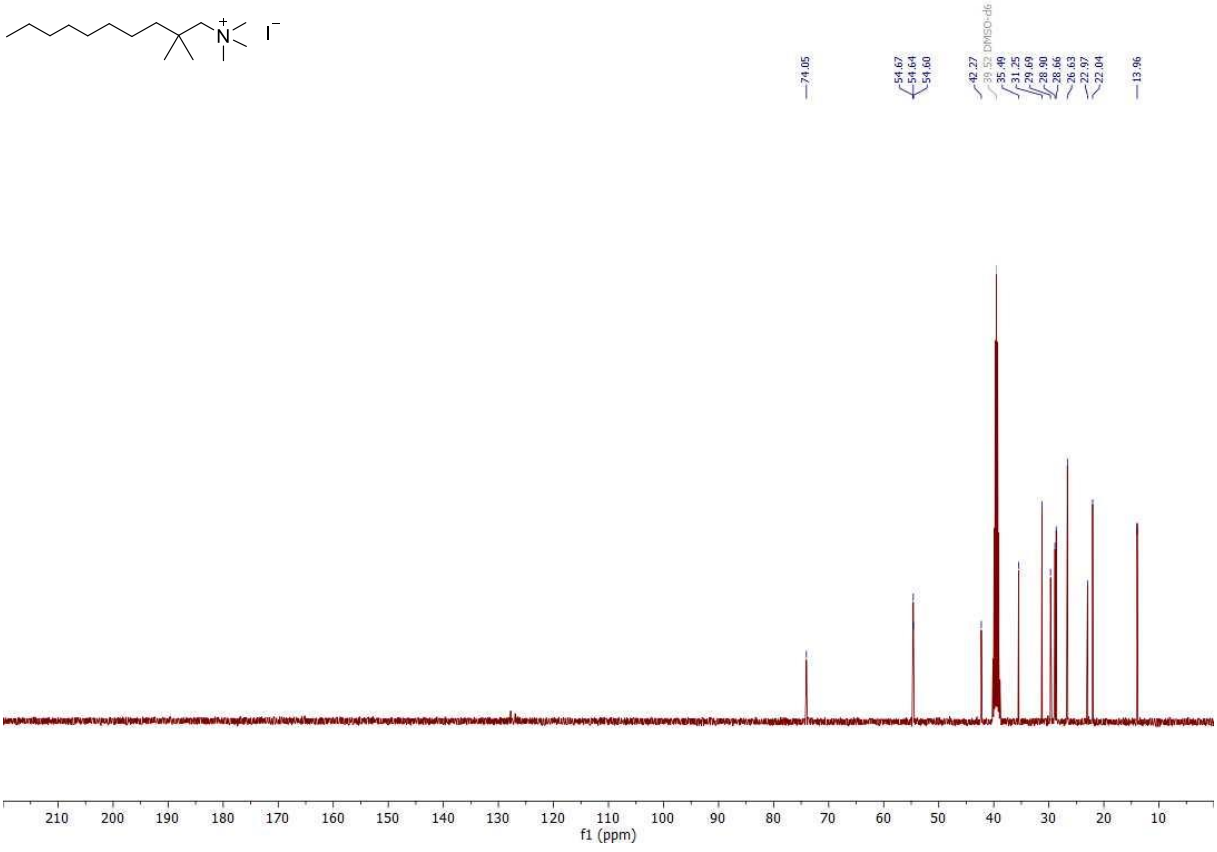

Figure S13: ^{13}C NMR spectrum of **13d** in DMSO-d_6

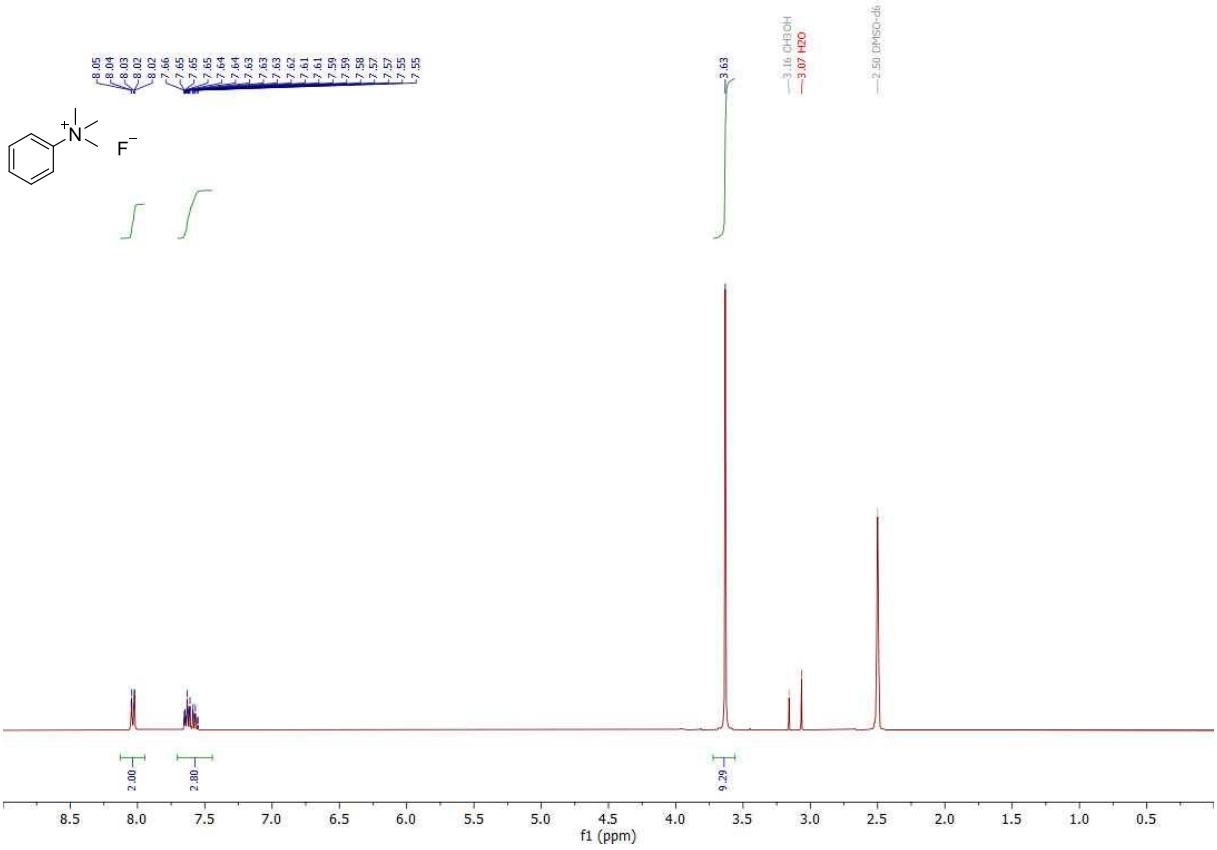

Figure S14: ^{1}H NMR spectrum of **8a** in DMSO-d_6

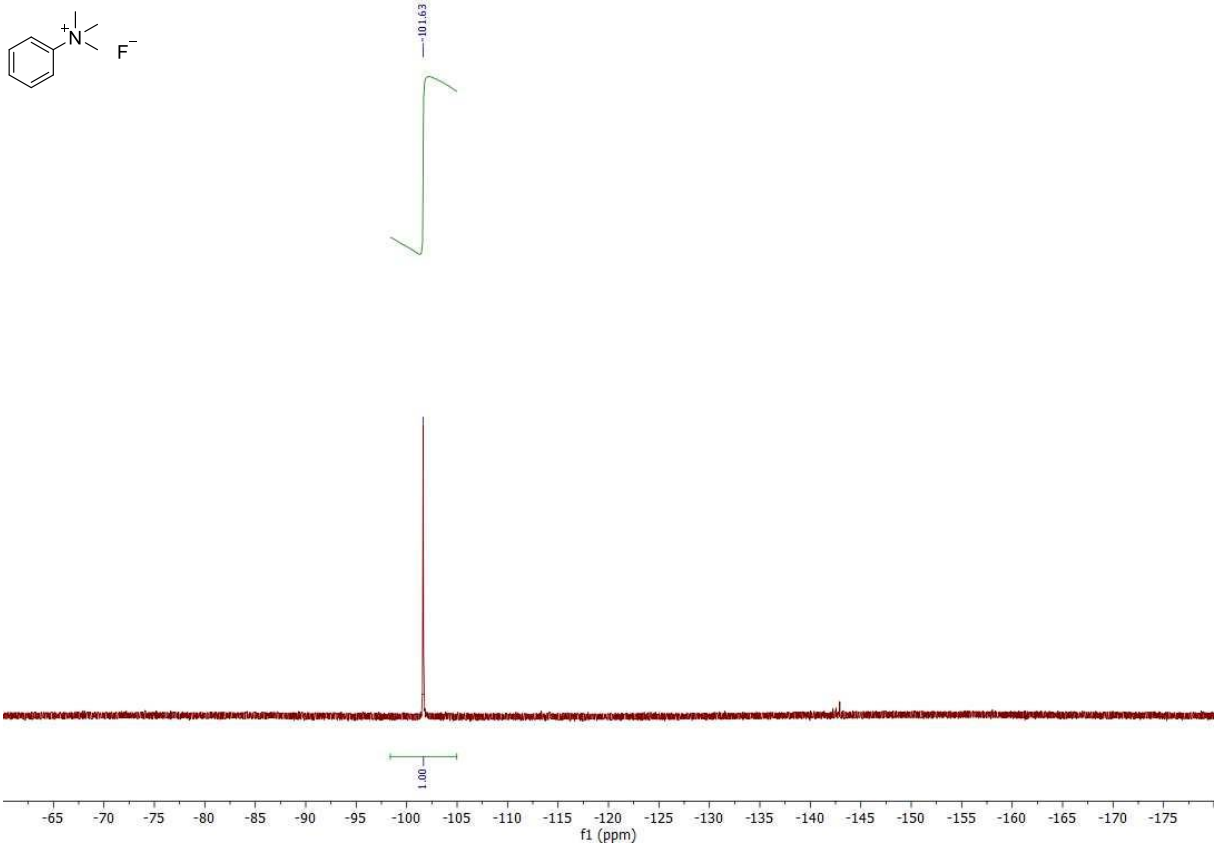

Figure S15: ^{19}F NMR spectrum of **8a** in DMSO-d_6

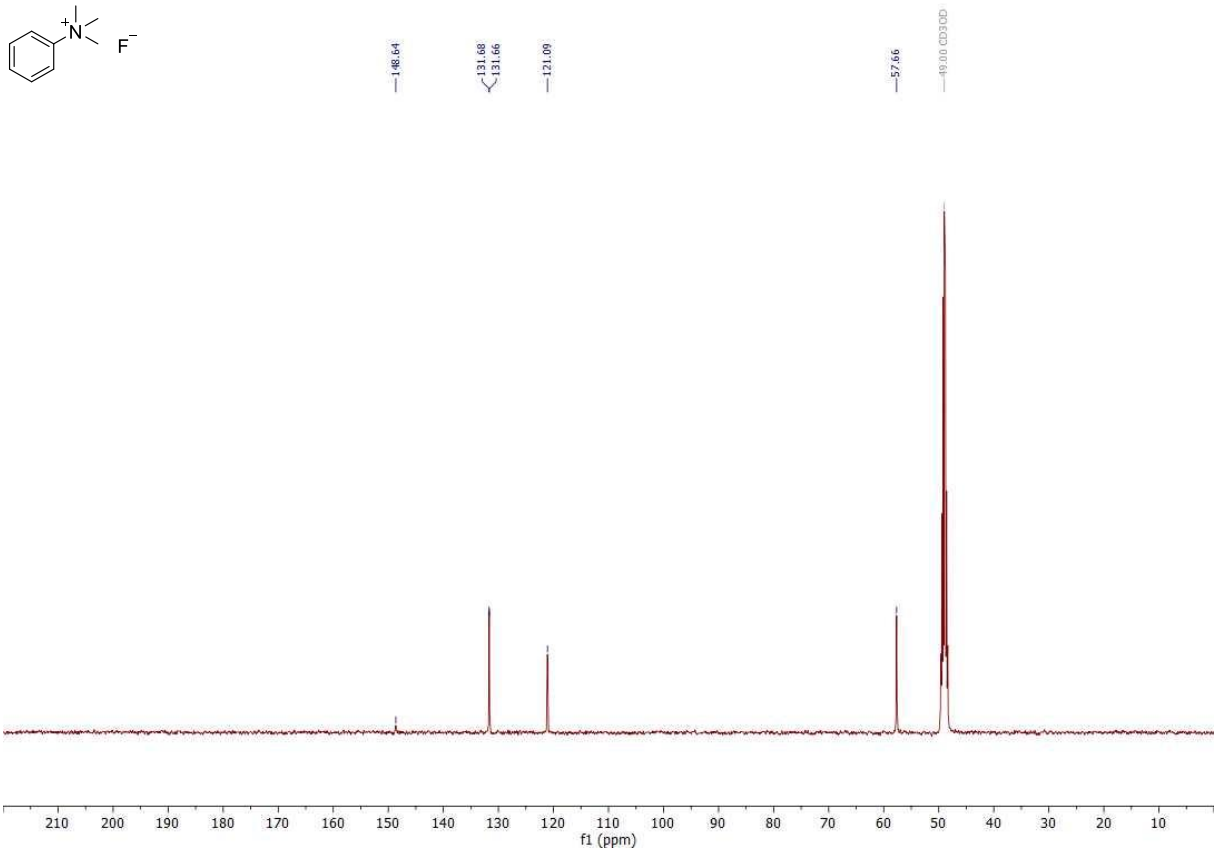

Figure S16: ^{13}C NMR spectrum of **8a** in CD_3OD

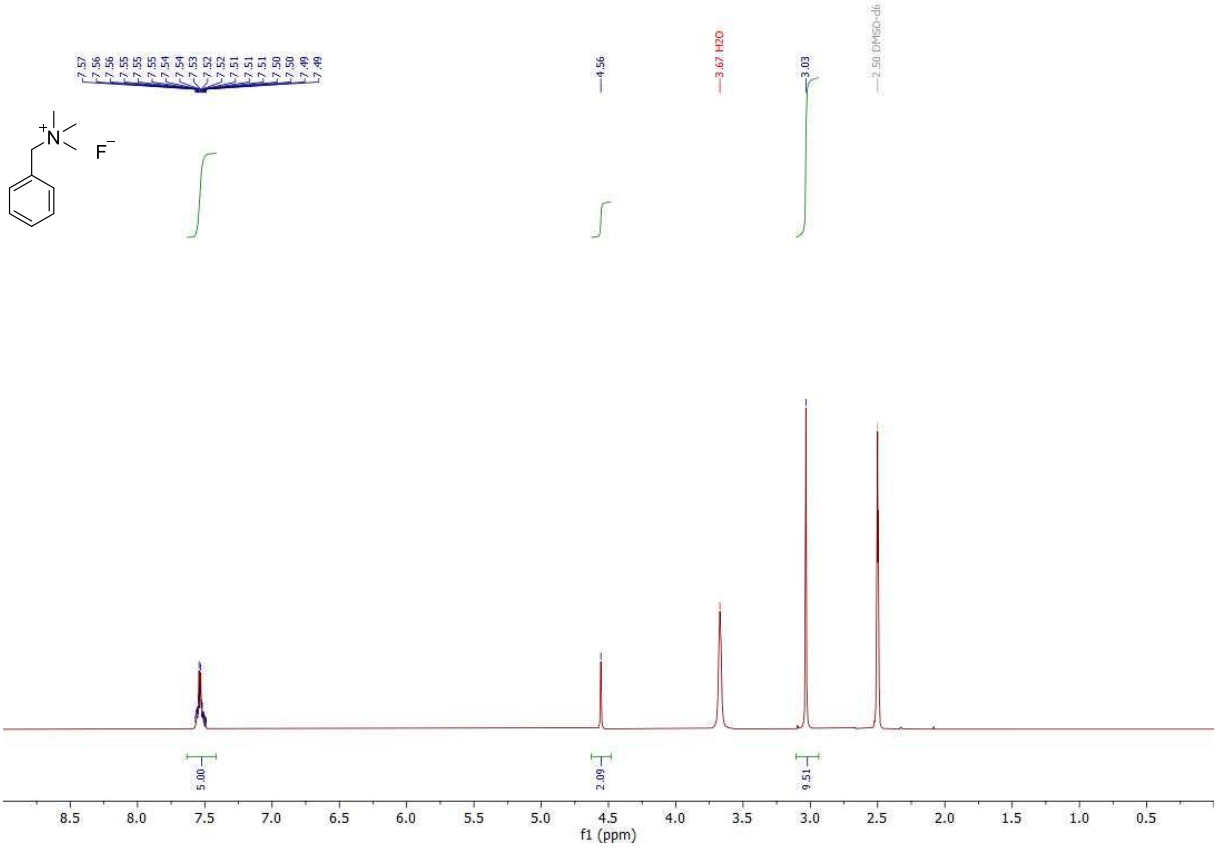

Figure S17: ^{1}H NMR spectrum of **8b** in DMSO-d_6

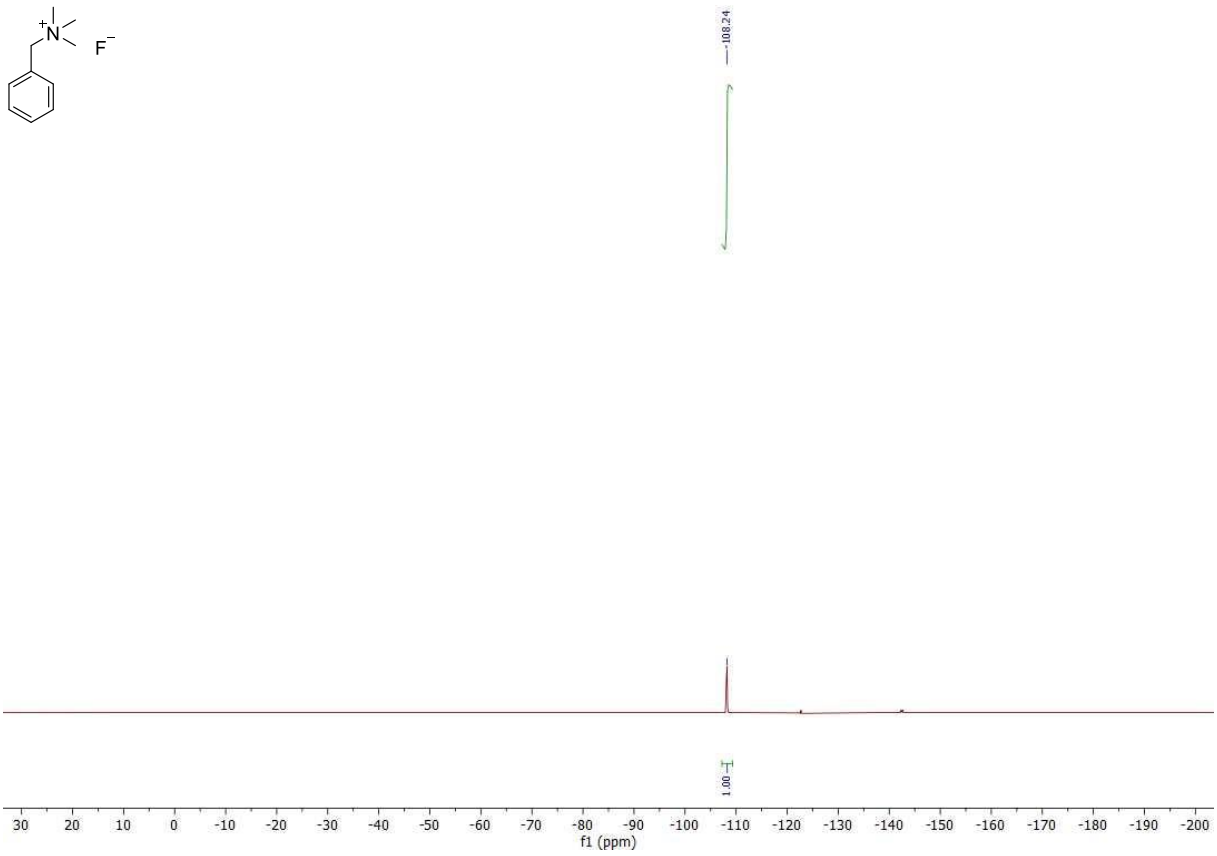

Figure S18: ^{19}F NMR spectrum of **8b** in DMSO-d_6

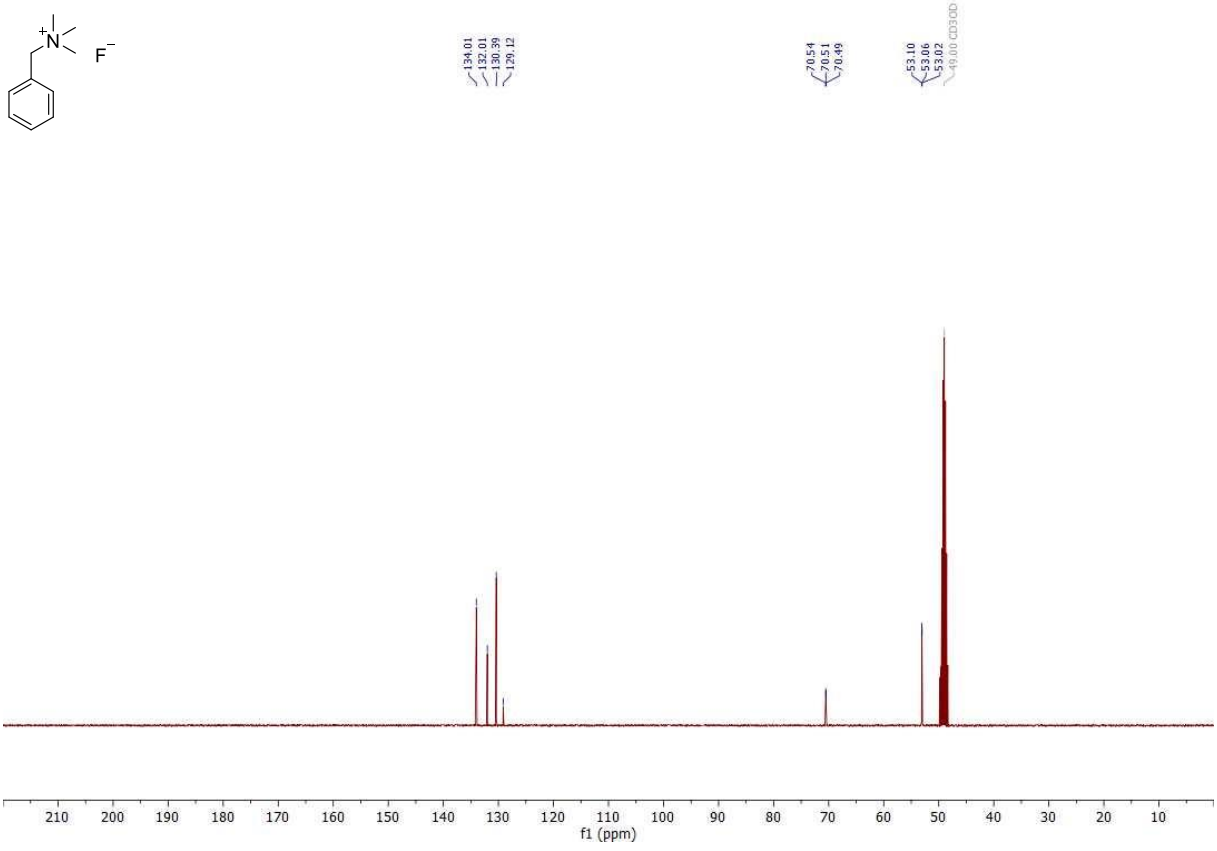

Figure S19: ^{13}C NMR spectrum of **8b** in CD_3OD

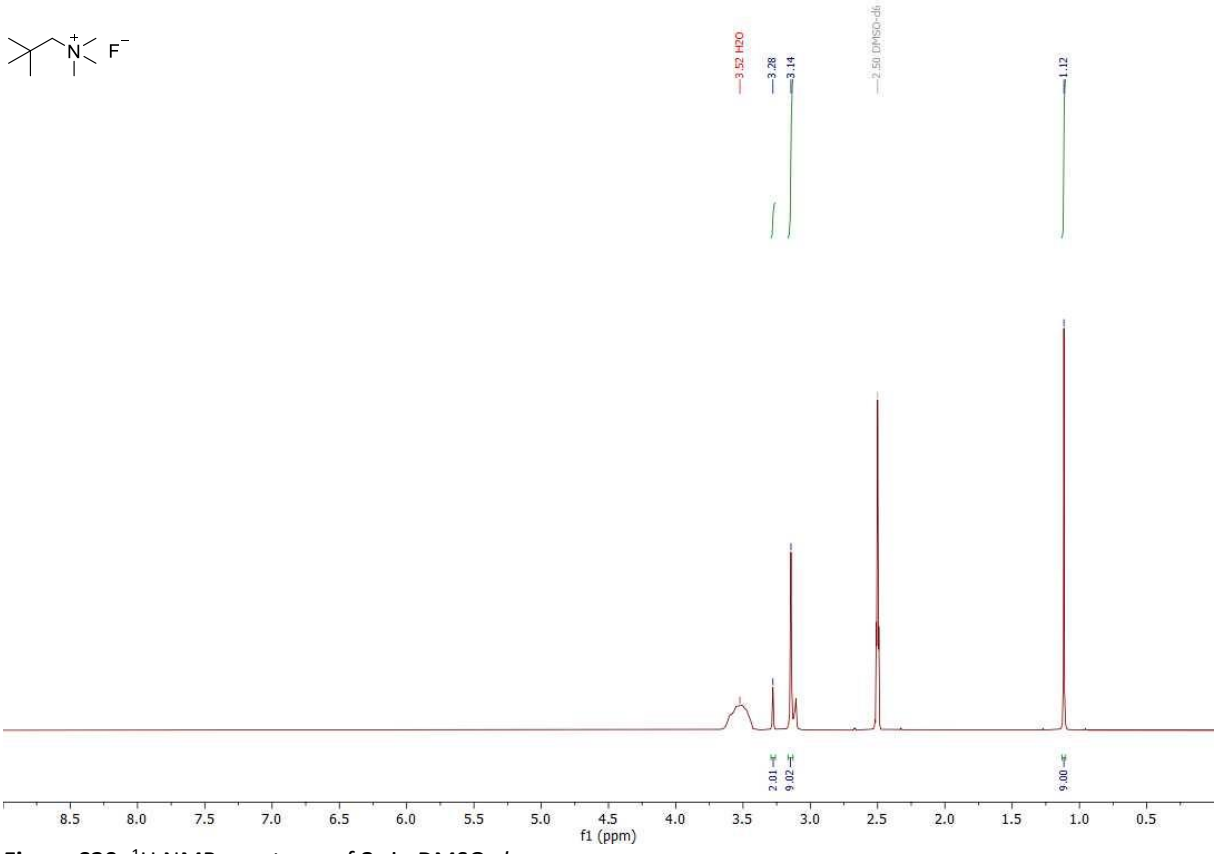

Figure S20: ^{1}H NMR spectrum of **8c** in DMSO-d_6

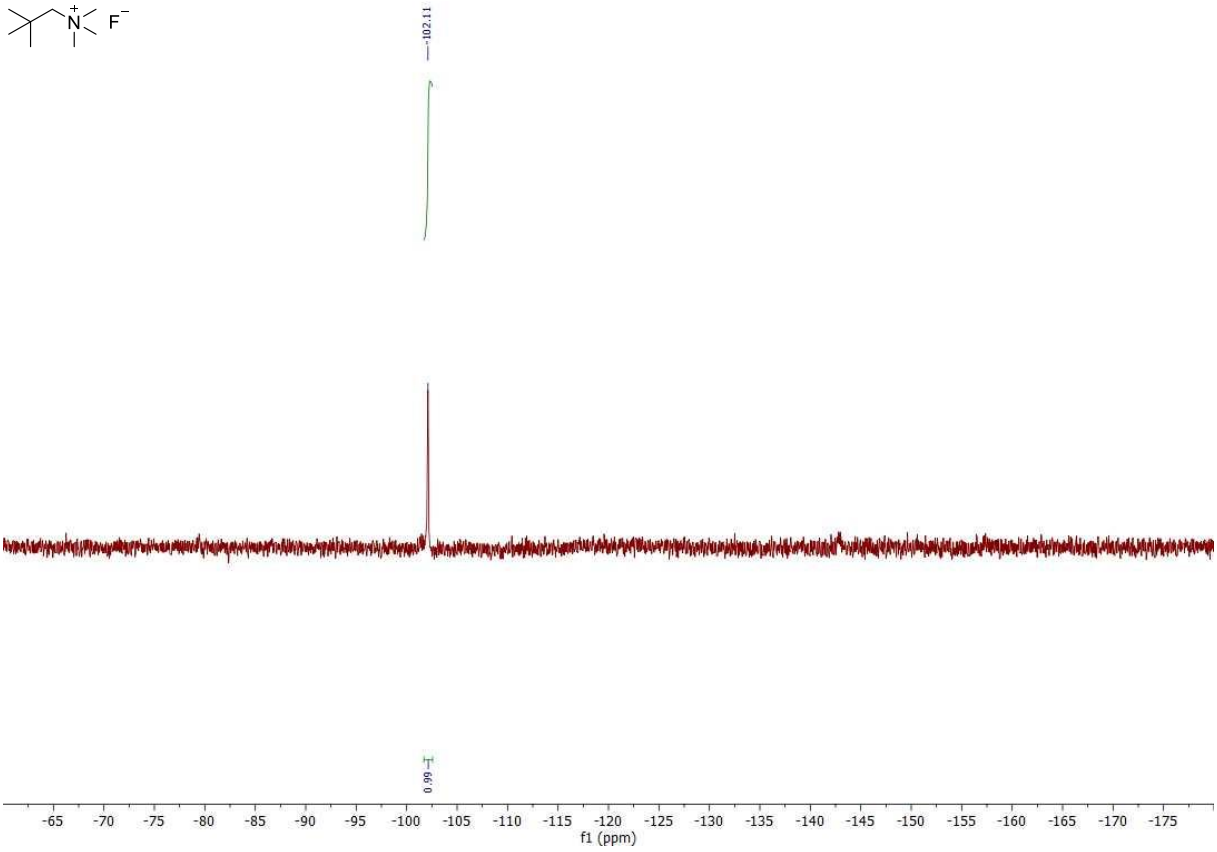

Figure S21: ^{19}F NMR spectrum of **8c** in DMSO-d_6

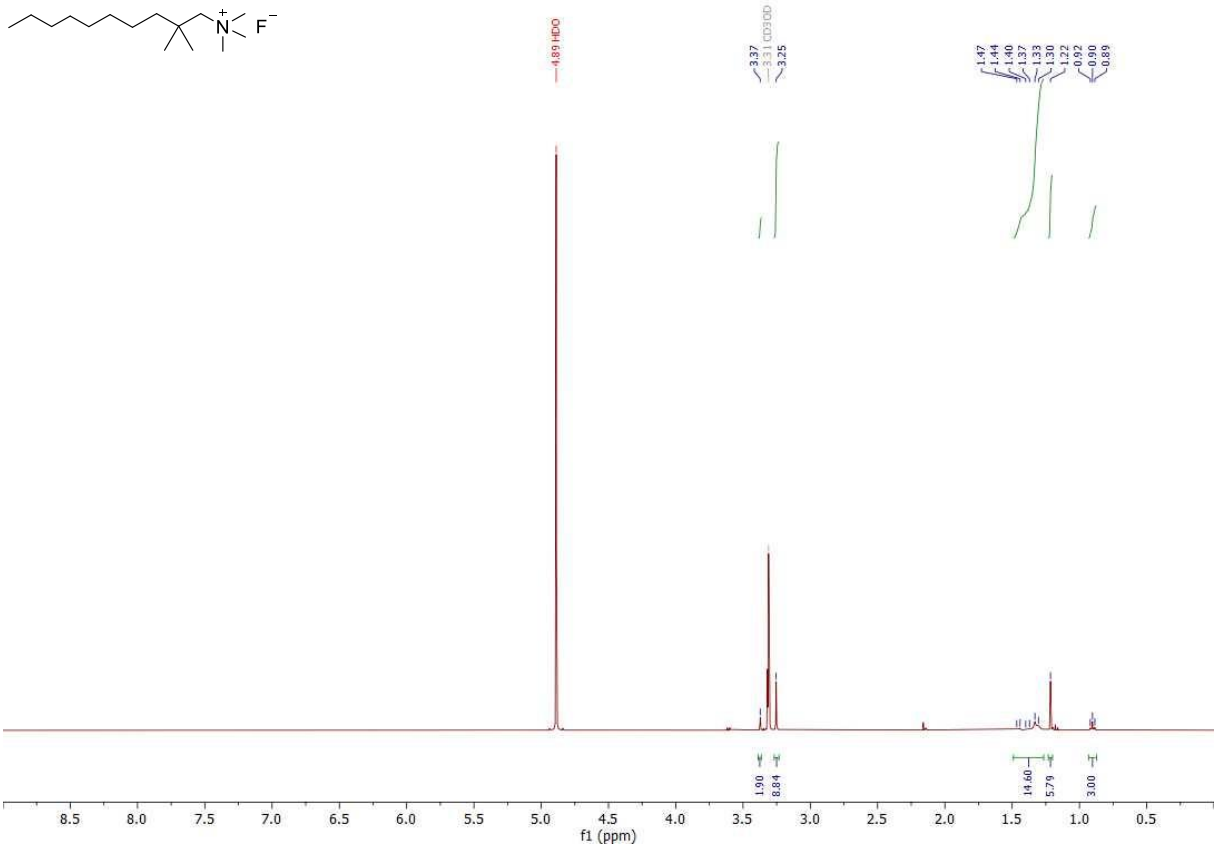

Figure S22: ^{1}H NMR spectrum of **8d** in CD_3OD

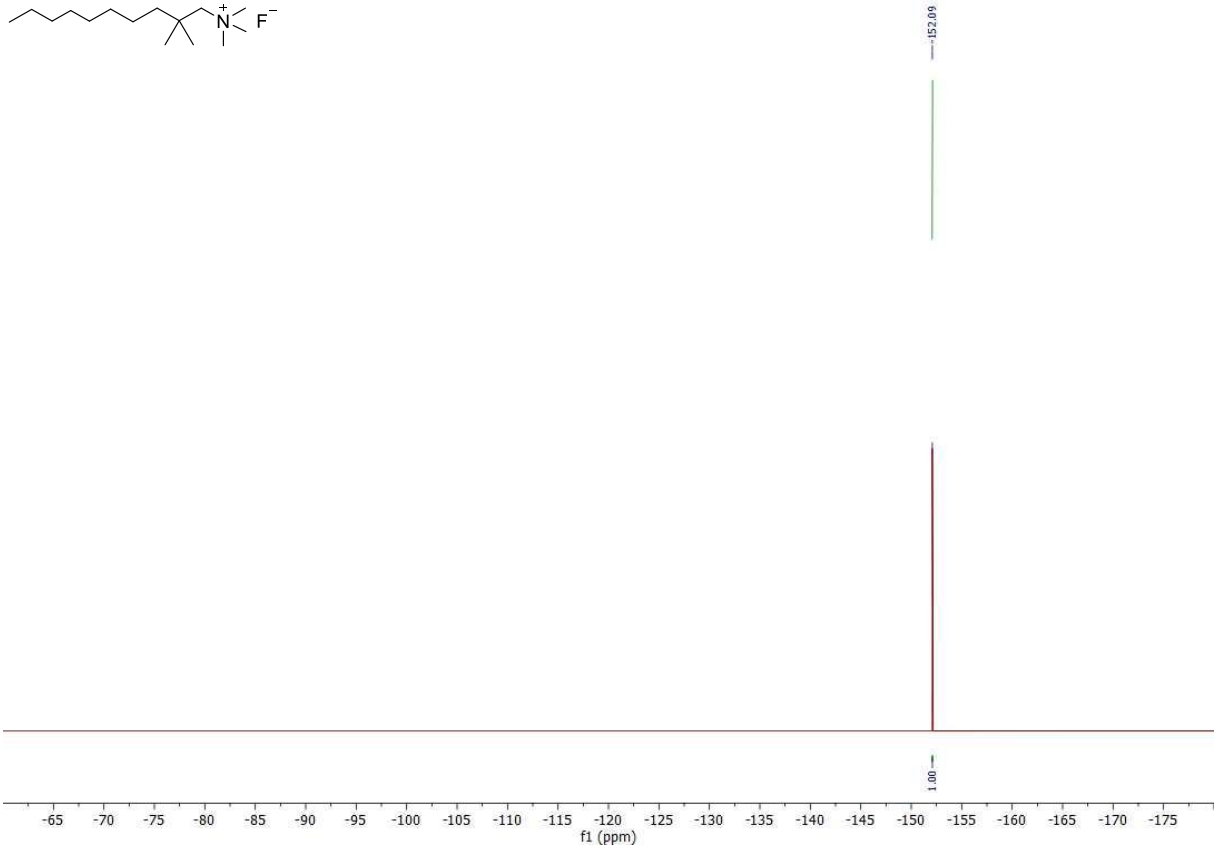

Figure S23: ^{19}F NMR spectrum of **8d** in CD_3OD

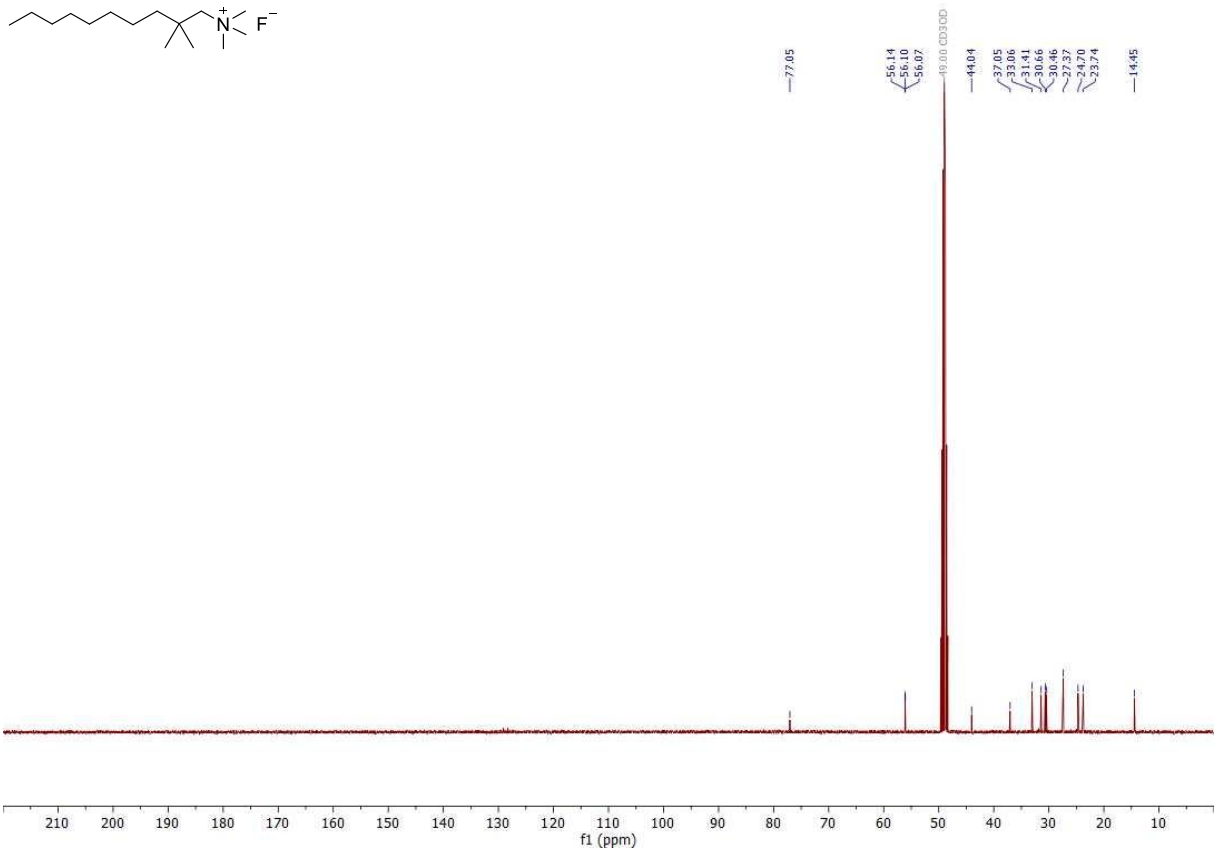

Figure S24: ^{13}C NMR spectrum of **8d** in CD_3OD

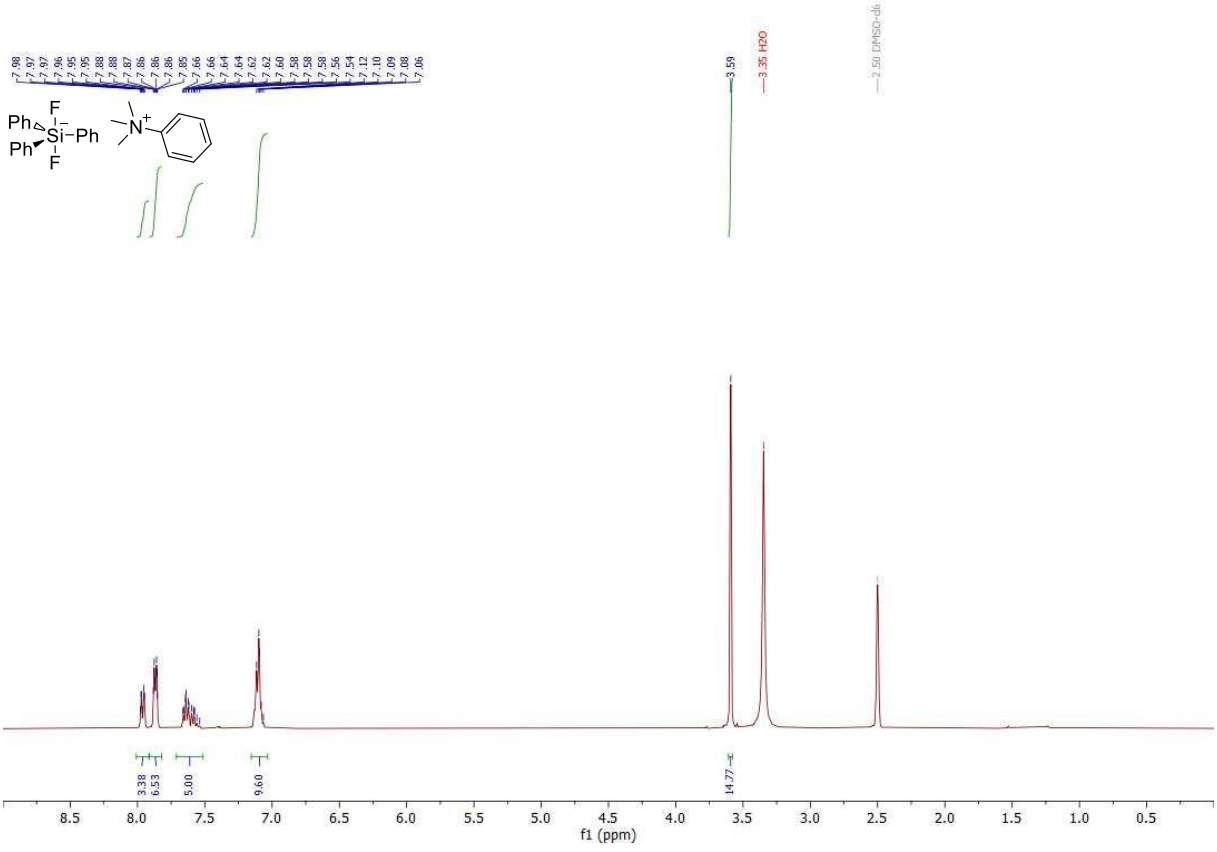

Figure S25: ^{1}H NMR spectrum of **7a** in DMSO-d_6

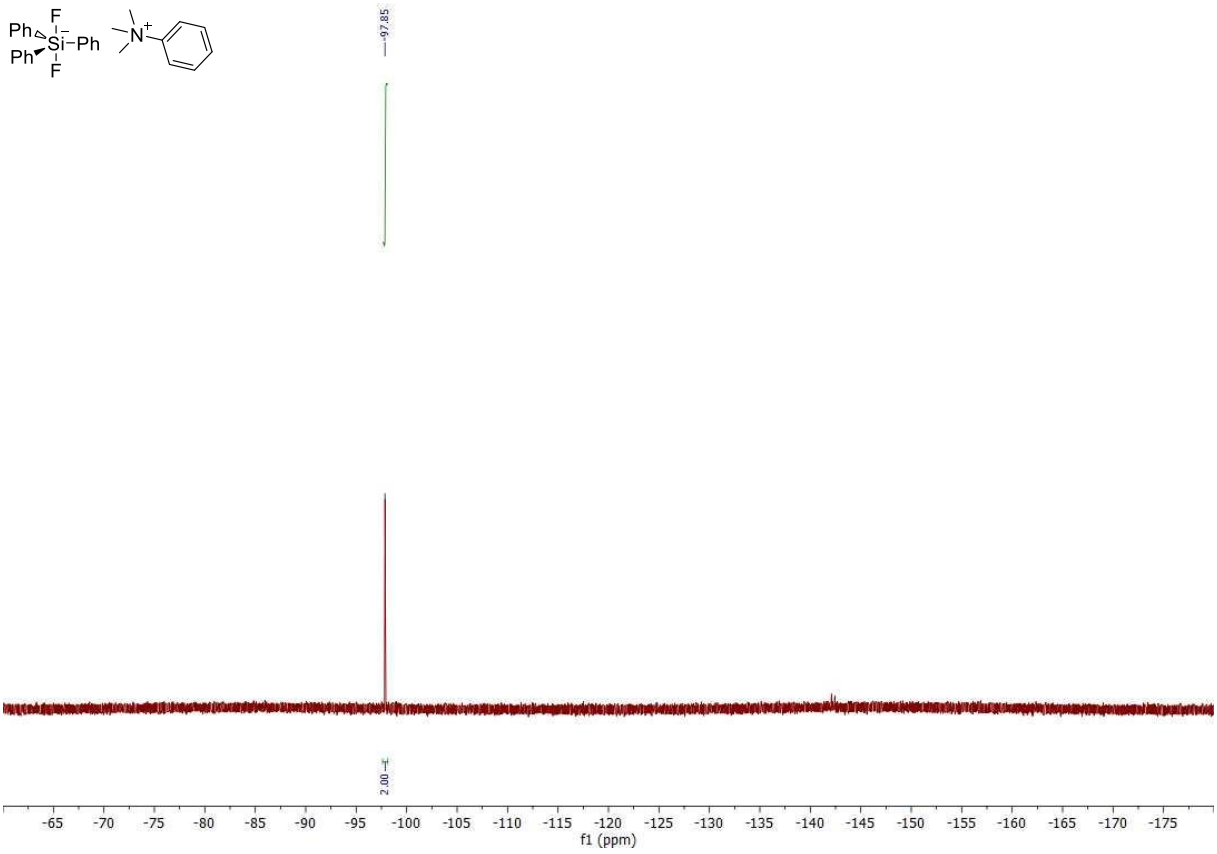

Figure S26: ^{19}F NMR spectrum of **7a** in DMSO-d_6

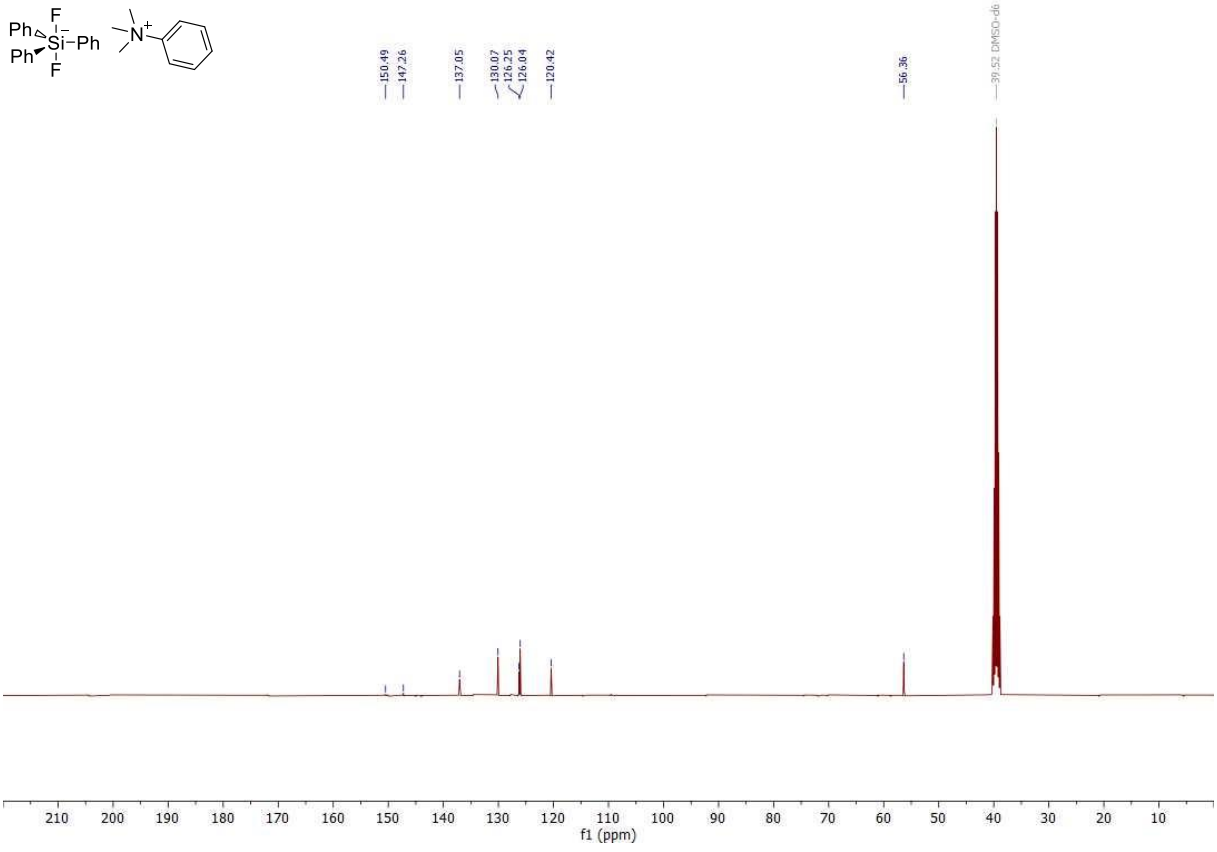

Figure S27: ^{13}C NMR spectrum of **7a** in DMSO-d_6

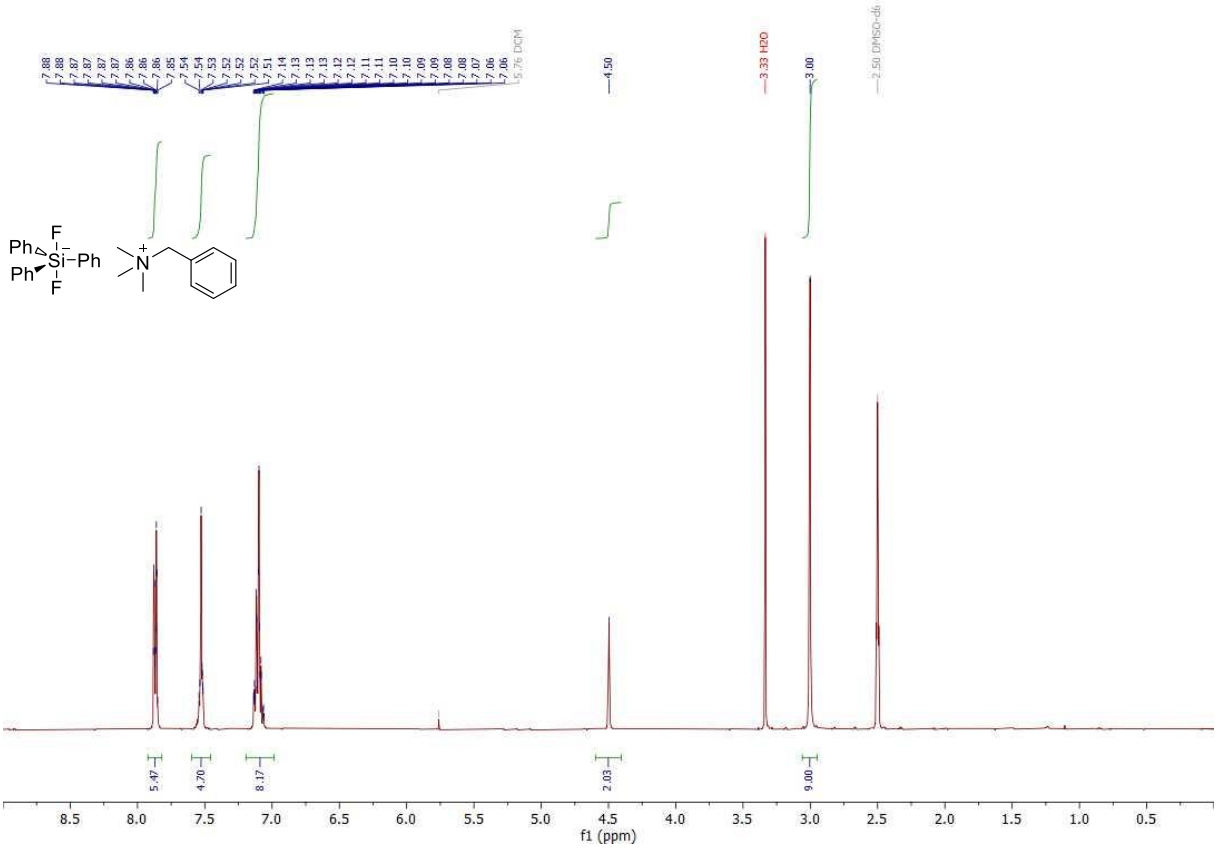

Figure S28: ^{1}H NMR spectrum of **7b** in DMSO-d_6

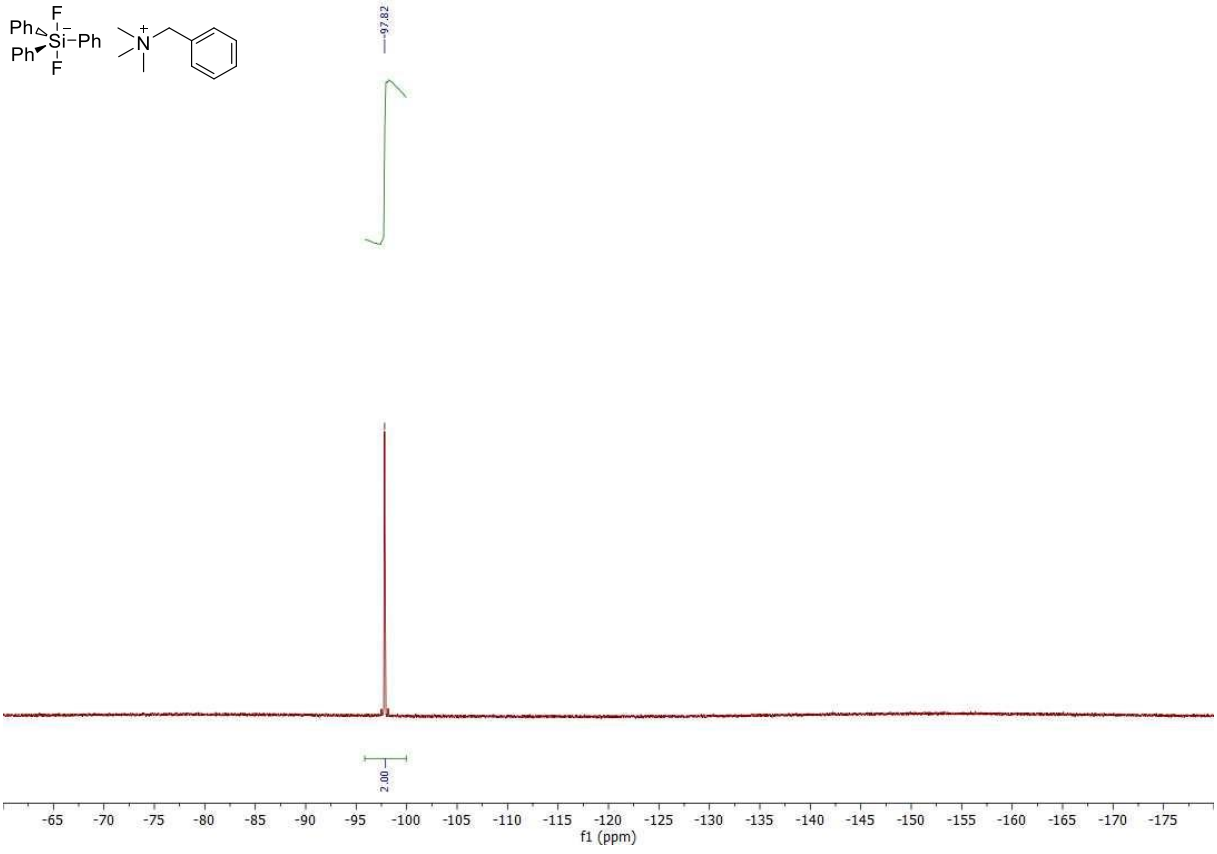

Figure S29: ^{19}F NMR spectrum of **7b** in DMSO-d_6

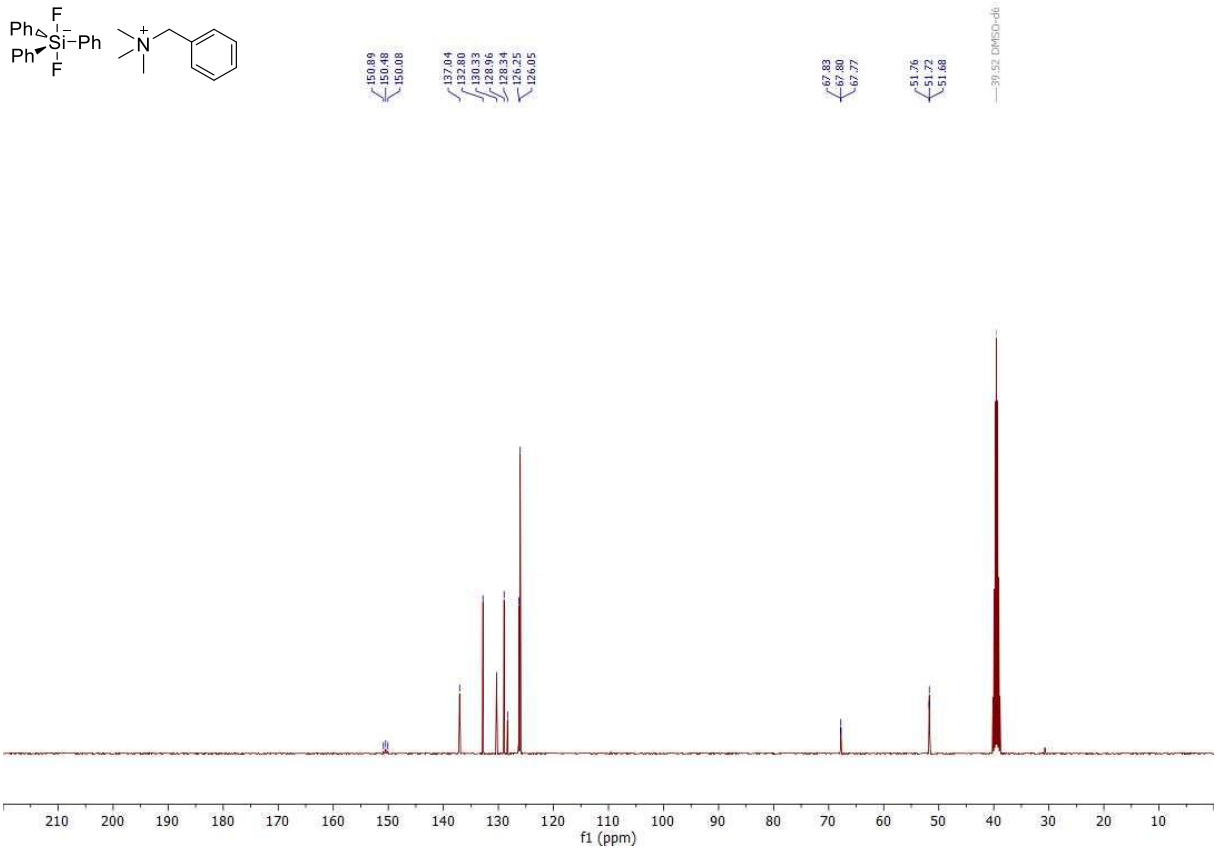

Figure S30: ^{13}C NMR spectrum of **7b** in DMSO-d_6

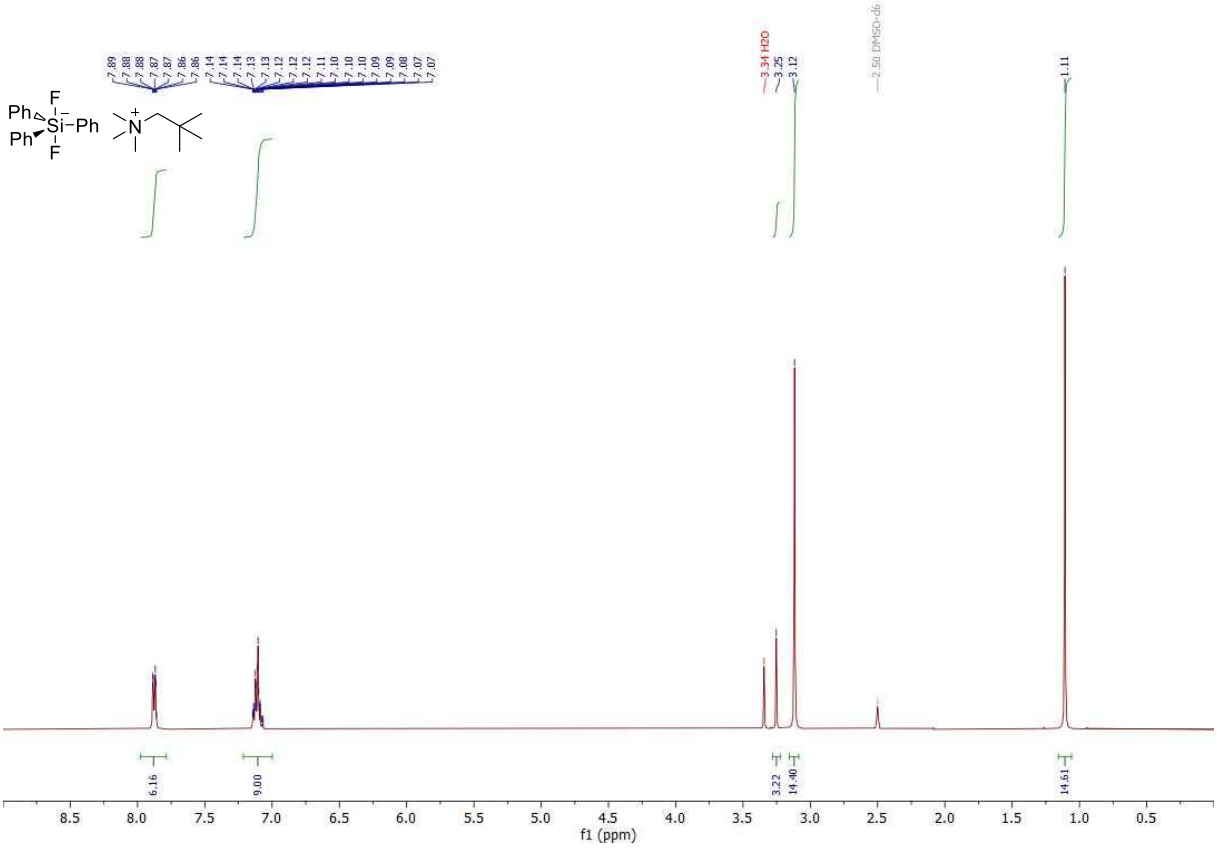

Figure S31: ^{1}H NMR spectrum of **7c** in DMSO-d_6

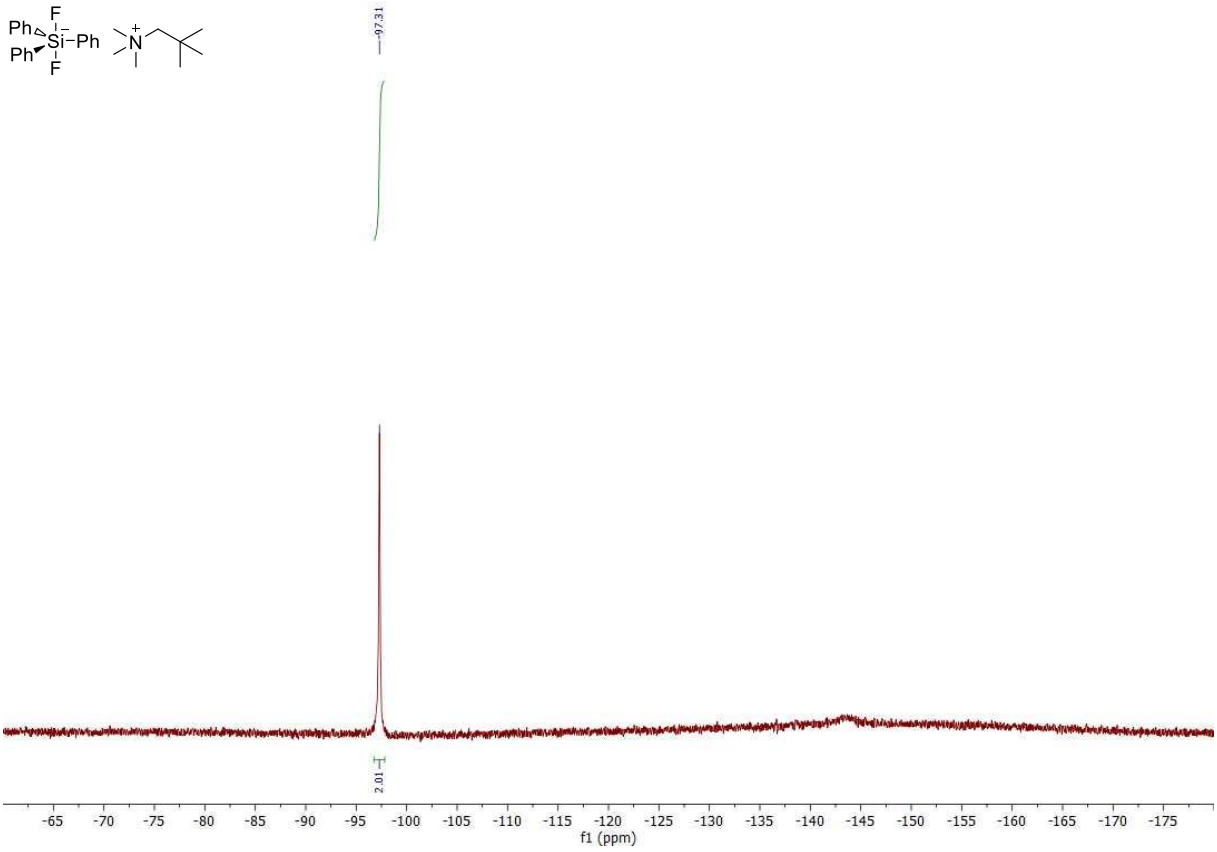

Figure S32: ^{19}F NMR spectrum of **7c** in DMSO-d_6

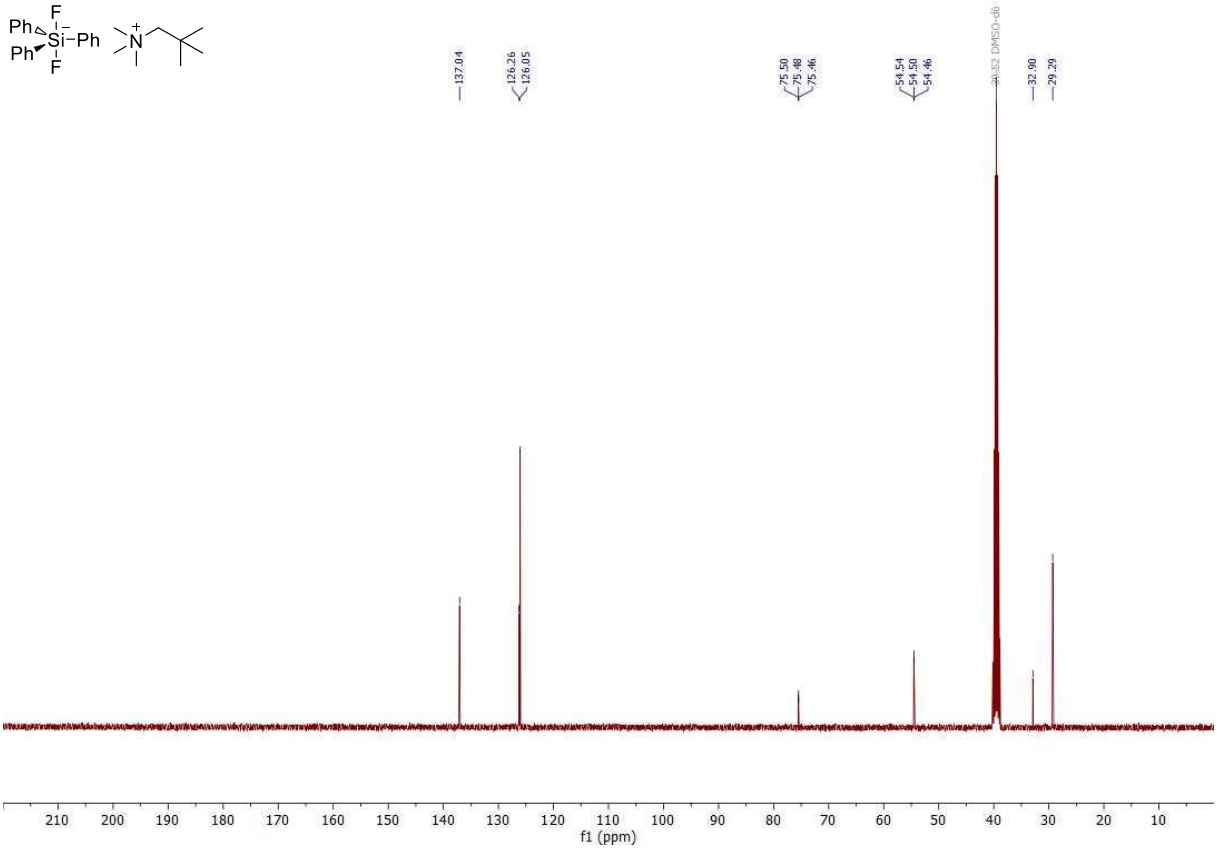

Figure S33: ^{13}C NMR spectrum of **7c** in DMSO-d_6

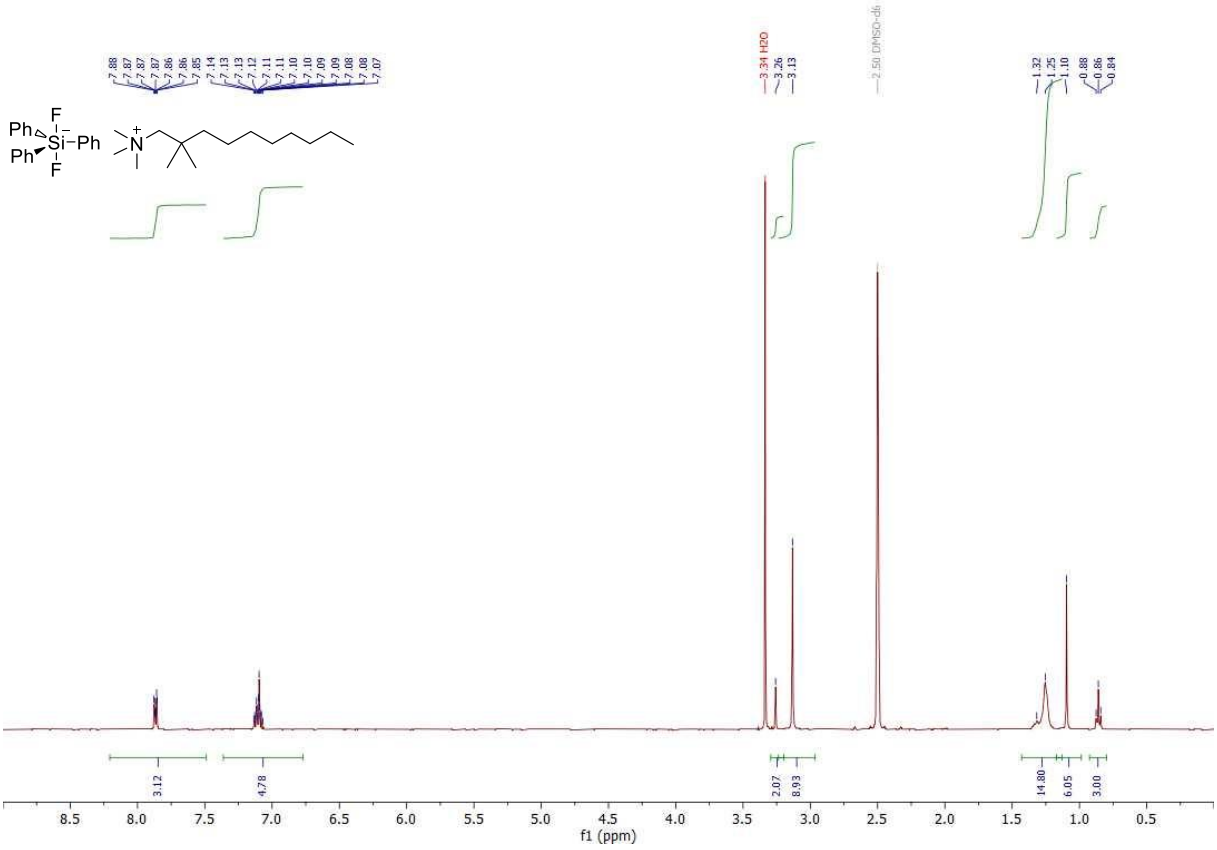

Figure S34: ^{1}H NMR spectrum of **7d** in DMSO-d_6

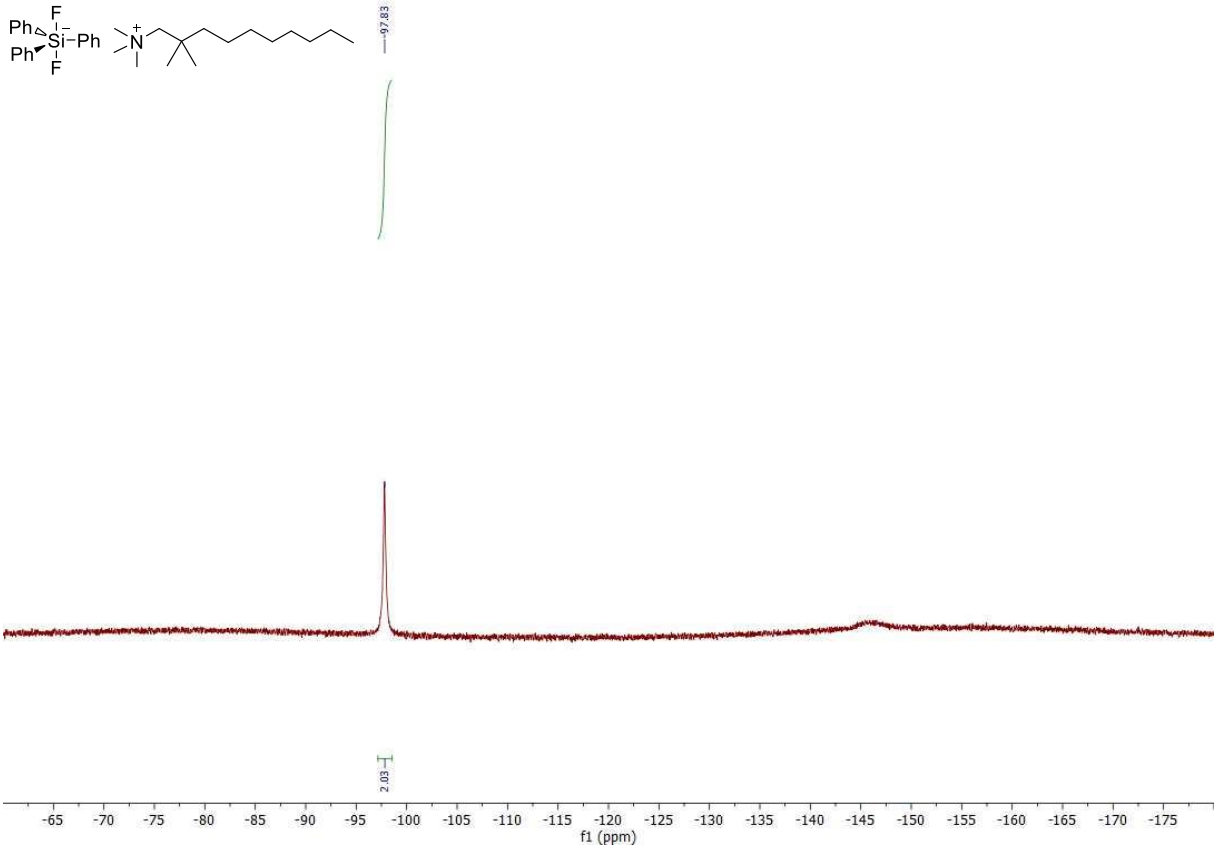

Figure S35: ^{19}F NMR spectrum of **7d** in DMSO-d_6

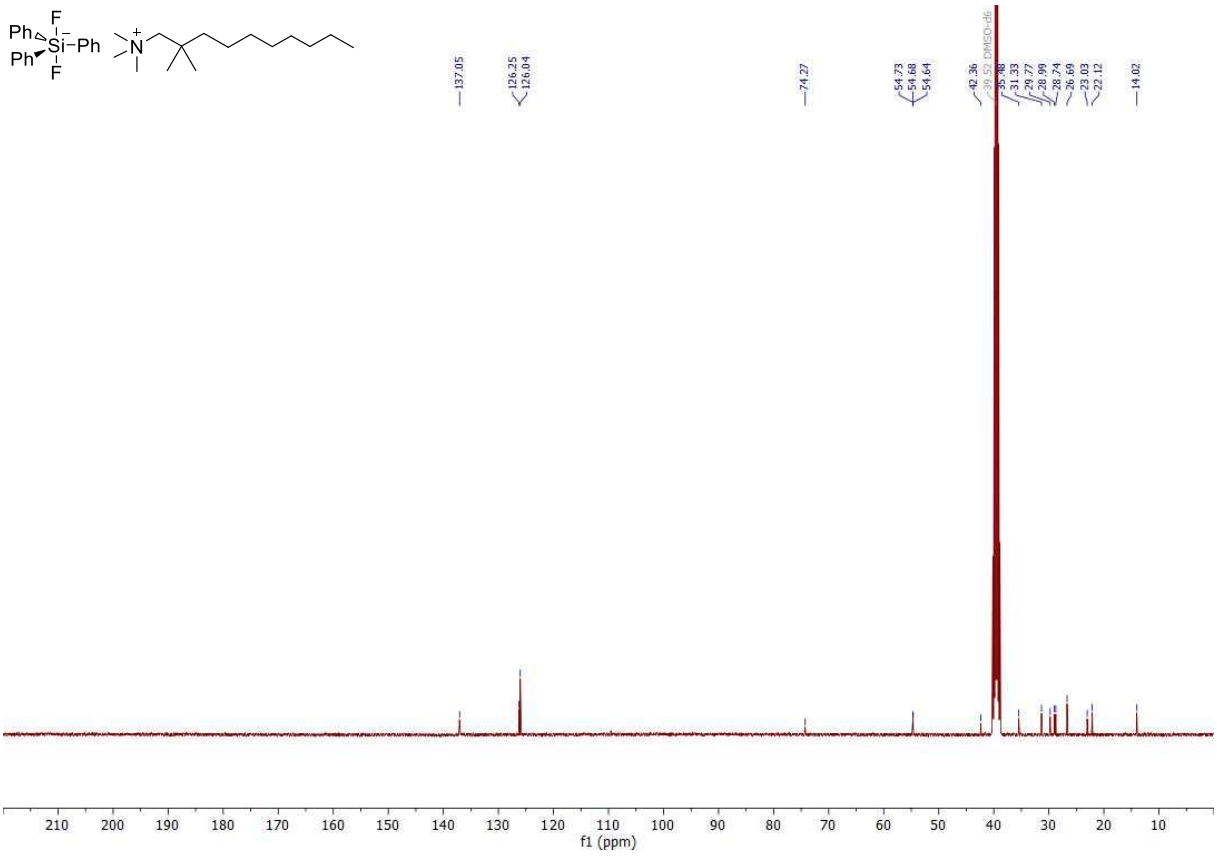

Figure S36: ^{13}C NMR spectrum of **7d** in DMSO-d_6

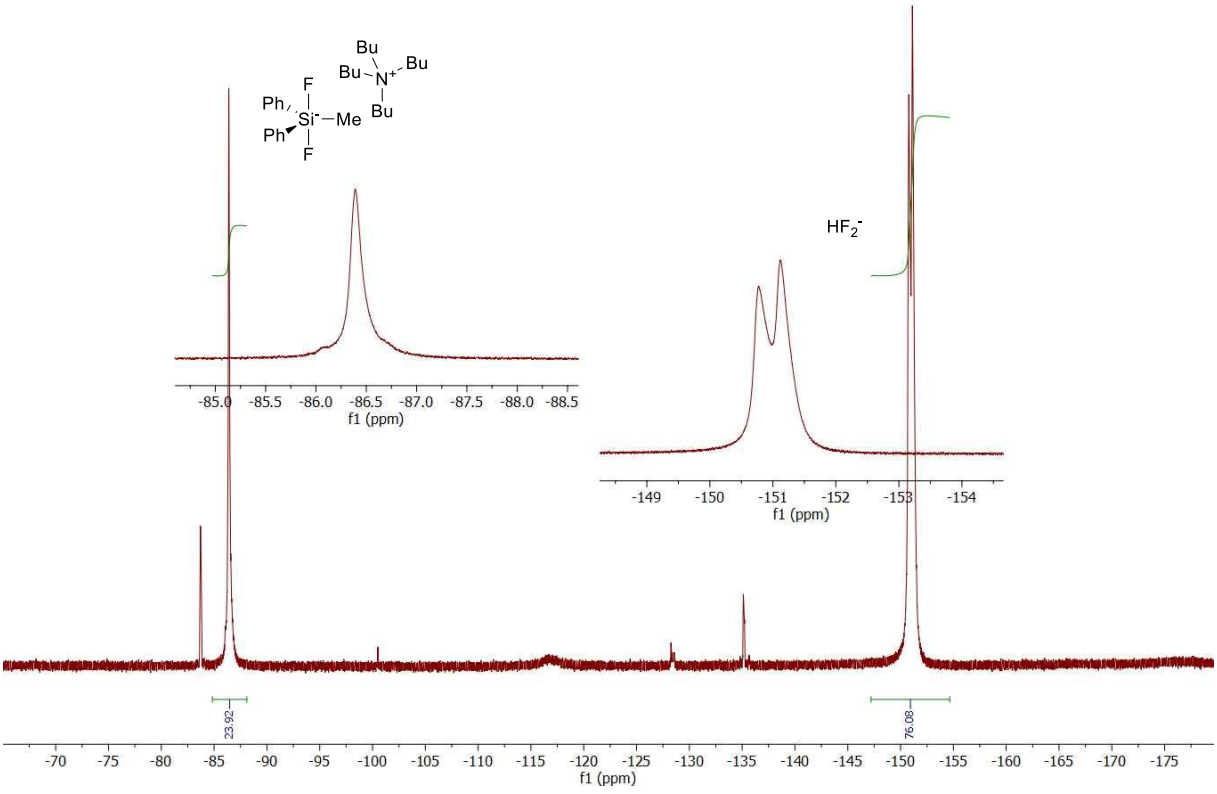

Figure S37: Low temperature (40 °C) ^{19}F NMR spectra of attempted preparation of **16** in CD_3CN

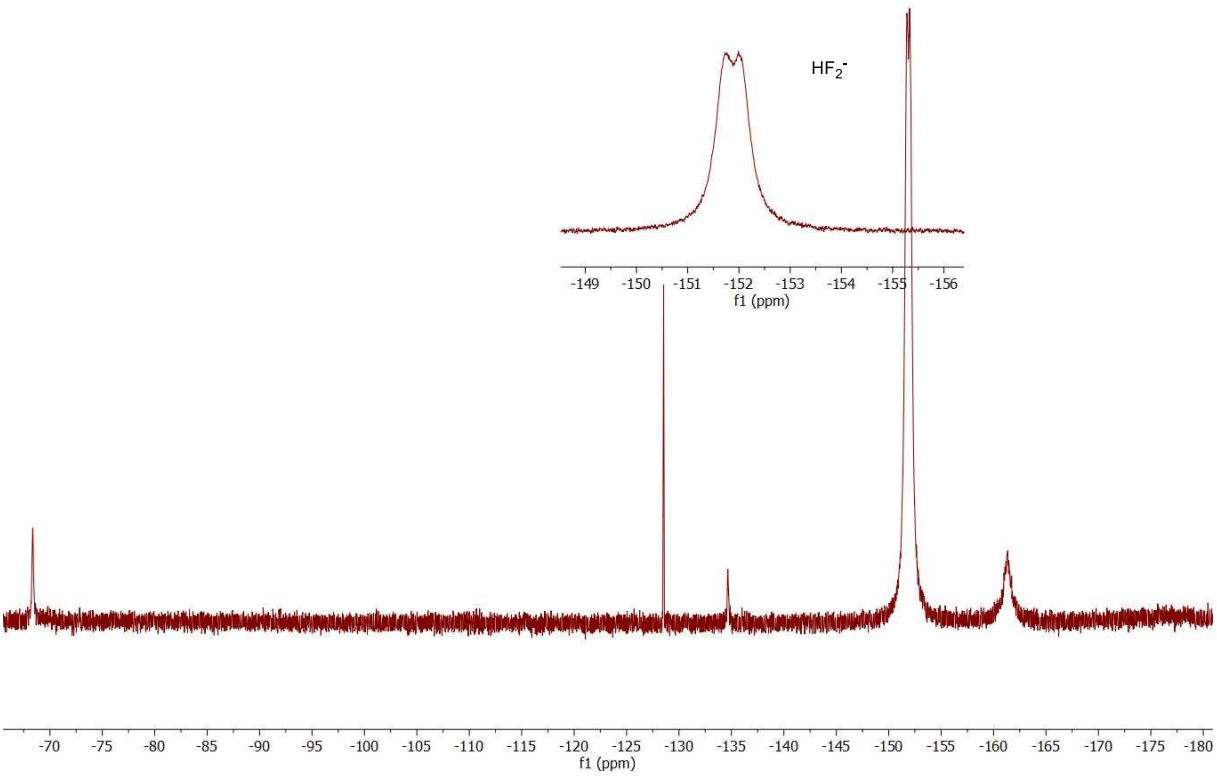

Figure S38: : Low temperature (40 °C) ^{19}F NMR spectra of attempted preparation of **16** in CD_3CN

3. Crystallographic data of 7b

A prismatic colourless single-crystal of **7b**, approximate dimensions 0.042 mm x 0.093 mm x 0.230 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were collected on a Bruker D8 VENTURE system equipped with charge-integrating pixel array detector Photon II 7, a multilayer monochromator and a CuKα Incoatec microfocus sealed tube (λ = 1.54178 Å) using combined φ and ω scans at 180 K. A total of 1343 frames were collected. The total exposure time was 3.36 hours. The frames were integrated with the Bruker SAINT software package using a wide-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 68911 reflections to a maximum ϑ angle of 70.08° (0.82 Å resolution). The final cell constants of a = 15.2943(3) Å, b = 15.8356(3) Å, c = 19.9358(4) Å, V = 4828.35(18) Å^3, are based upon the refinement of the XYZ-centroids of 9767 reflections above 20 $\sigma(I)$ with 7.129° < 2ϑ < 140.1°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.858.

The positional and anisotropical thermal parameters of all non-hydrogen atoms were refined. All hydrogen atoms were located in a difference map, but repositioned geometrically, then they were initially refined with soft restraints on the bond lengths and angles to regularise their geometry (C-H in the range of 0.93-0.98 Å) and U_{iso}(H) (in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions of the hydrogen atoms were refined with riding constraints. The refinement of 289 parameters on all 4589 reflections (3796 observed reflections, $I > 2\ \sigma(I)$) converged to the final R_1 of 0.0389 and R_{w1} of 0.0943.

Data collection: APEX4[7]; Unit Cell refinement and data reduction: SAINT[7]; program used to solve structure: SIR92[8] ; program used to refine structure: CRYSTALS[9]. CCDC 2307603 contains the

supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

4. XYZ files of computed structures (energies in kJ/mol)

Preliminary computations using Gaussian 16, method SMD-M06L/def2-SVPD

20: ΔG = -2160706.30 kJ/mol

N	-2.73352	-0.02139	0.00077
C	-4.15756	-0.42872	0.15696
H	-4.24875	-1.05283	1.04976
H	-4.77117	0.46984	0.26102
H	-4.46088	-0.99177	-0.72960
C	-2.58281	0.83470	-1.21258
H	-1.53164	1.12409	-1.29648
H	-2.89640	0.25886	-2.08737
H	-3.21582	1.71838	-1.09638
C	-1.87662	-1.23329	-0.14669
H	-0.84069	-0.90322	-0.25020
H	-1.99570	-1.85825	0.74218
H	-2.19381	-1.78007	-1.03869
C	-2.29286	0.74755	1.20225
H	-2.38702	0.10452	2.08151
H	-1.25208	1.04707	1.04923
H	-2.93486	1.62589	1.30820
F	0.55553	1.10220	-0.33988
Si	2.00420	0.00400	0.00465
C	3.14195	1.48053	-0.32538
H	2.91730	2.29966	0.37500
H	4.21281	1.25377	-0.24288
H	2.95956	1.88559	-1.33252
C	1.31731	-0.26282	1.75451
H	0.44069	-0.92971	1.73933
H	2.04548	-0.70940	2.44429
H	0.97386	0.68689	2.19028
C	1.50770	-1.12860	-1.43732
H	2.36597	-1.28013	-2.10877
H	1.23647	-2.13110	-1.06987
H	0.67066	-0.75492	-2.04231
F	3.40438	-1.10726	0.34359

20-TS: ΔG = -2160671.41 kJ/mol

N	2.79981	-0.17822	0.00283
C	3.91736	-1.15913	0.03145
H	3.60588	-2.06388	-0.49745
H	4.78856	-0.71769	-0.45989
H	4.15219	-1.39473	1.07293
C	3.20055	1.07712	0.70330

H	2.33887	1.75384	0.67434
H	3.47111	0.83054	1.73369
H	4.05958	1.50934	0.18253
C	1.59655	-0.74545	0.68323
H	0.80439	0.00982	0.59976
H	1.32195	-1.67784	0.18191
H	1.85036	-0.94304	1.72884
C	2.44137	0.15172	-1.40789
H	2.10951	-0.76327	-1.90680
H	1.63662	0.89502	-1.37091
H	3.32704	0.55269	-1.90797
F	0.20619	1.92600	0.01455
Si	-2.41441	-0.19295	-0.00579
C	-3.16391	1.48440	-0.28481
H	-3.65632	1.55889	-1.26492
H	-3.90799	1.73463	0.48484
H	-2.37088	2.24367	-0.24758
C	-1.27616	-0.71335	-1.37951
H	-0.85251	-1.71549	-1.22416
H	-1.79651	-0.71567	-2.34782
H	-0.44997	0.00686	-1.44294
C	-1.72197	-0.39040	1.71060
H	-2.51986	-0.30730	2.46230
H	-1.22517	-1.35967	1.85900
H	-0.98947	0.40025	1.92062
F	-3.70140	-1.27240	-0.07092

24: ΔG = -2160675.40 kJ/mol

N	2.84481	-0.25314	-0.00373
C	3.82642	-1.36950	-0.05898
H	3.38100	-2.20390	-0.60734
H	4.72749	-1.02159	-0.57112
H	4.06837	-1.67706	0.96192
C	3.42952	0.90500	0.73391
H	2.67113	1.69626	0.75115
H	3.68247	0.58057	1.74721
H	4.33059	1.23355	0.20846
C	1.60228	-0.69540	0.69721
H	0.91781	0.16121	0.70153
H	1.18149	-1.54435	0.15143
H	1.86459	-0.99779	1.71503
C	2.48697	0.18418	-1.38578
H	2.04601	-0.66440	-1.91640
H	1.77090	1.00859	-1.28783
H	3.39894	0.51096	-1.89275
F	0.61484	2.22194	0.11953
Si	-2.55396	-0.19786	-0.02650
C	-3.44514	1.42863	0.10205

H	-3.89754	1.73104	-0.85287
H	-4.24038	1.40798	0.86048
H	-2.73700	2.21904	0.39196
C	-1.26727	-0.18308	-1.36425
H	-0.76607	-1.15466	-1.47714
H	-1.68543	0.09812	-2.34084
H	-0.50784	0.56930	-1.09498
C	-1.87010	-0.74191	1.61651
H	-2.66336	-0.84920	2.36952
H	-1.33543	-1.70020	1.55557
H	-1.16266	0.00868	1.99883
F	-3.70144	-1.33723	-0.45494

21: ΔG = -2663704.91 kJ/mol

Si	1.77399	-1.09754	0.02053
C	2.79561	-1.86551	1.41572
H	3.30744	-1.07541	1.98749
H	2.20174	-2.45319	2.12697
H	3.58998	-2.51091	1.01364
C	1.11718	-2.13923	-1.41911
H	0.77584	-3.12312	-1.06446
H	0.23595	-1.65602	-1.86929
H	1.84929	-2.30220	-2.22027
C	1.31513	0.75831	0.05967
C	0.83061	1.38113	1.22185
C	1.39276	1.54374	-1.10284
C	0.44456	2.72282	1.22894
H	0.74413	0.80097	2.14478
C	0.98413	2.87855	-1.11564
H	1.76824	1.09666	-2.02760
C	0.51142	3.47476	0.05465
H	0.08067	3.18248	2.15128
H	1.03693	3.45860	-2.04019
H	0.19613	4.52038	0.05168
F	0.22063	-1.44057	0.93324
F	3.29283	-0.69486	-0.87356
N	-2.99514	-0.41465	-0.07399
C	-2.70061	0.01728	1.32461
H	-2.83440	1.10034	1.39189
H	-3.39608	-0.49038	1.99839
H	-1.66896	-0.26240	1.55676
C	-2.05725	0.27490	-1.00648
H	-2.27443	-0.04995	-2.02747
H	-2.20313	1.35453	-0.91437
H	-1.03739	0.00221	-0.72457
C	-4.39981	-0.06565	-0.42523
H	-4.59594	-0.39075	-1.45043
H	-5.07255	-0.57705	0.26826

H	-4.52438	1.01723	-0.34283
C	-2.80066	-1.89056	-0.18426
H	-1.76945	-2.12073	0.09748
H	-3.50293	-2.38543	0.49185
H	-2.99631	-2.19214	-1.21678

21-TS: ΔG = -2663656.50 kJ/mol

Si	2.23729	-0.86104	-0.16014
C	2.84630	-1.60236	1.42694
H	1.99780	-1.93911	2.03433
H	3.49572	-2.46739	1.23241
H	3.42834	-0.87550	2.01129
C	1.37060	-2.00256	-1.34502
H	2.02374	-2.84118	-1.62588
H	0.46028	-2.41188	-0.89146
H	1.09394	-1.47701	-2.27053
C	1.39253	0.80417	0.04422
C	0.86208	1.23572	1.27026
C	1.26177	1.65555	-1.06670
C	0.20987	2.46395	1.38048
H	0.94697	0.59645	2.15222
C	0.61387	2.88623	-0.96172
H	1.66559	1.35289	-2.03746
C	0.08213	3.29091	0.26335
H	-0.20110	2.77805	2.34225
H	0.52042	3.53048	-1.83839
H	-0.43048	4.25122	0.34792
F	-0.32834	-1.79971	1.34295
F	3.63702	-0.45092	-1.00213
N	-2.98545	-0.47505	-0.19955
C	-2.92057	-0.01073	1.21802
H	-2.86985	1.08175	1.22334
H	-3.82423	-0.34614	1.73461
H	-2.02274	-0.45624	1.66304
C	-1.73402	-0.05447	-0.89733
H	-1.78783	-0.38102	-1.94003
H	-1.65790	1.03543	-0.84582
H	-0.90275	-0.53520	-0.37068
C	-4.17163	0.11415	-0.87534
H	-4.20582	-0.24620	-1.90701
H	-5.07335	-0.19365	-0.33914
H	-4.07930	1.20358	-0.86097
C	-3.06739	-1.96542	-0.21946
H	-2.18080	-2.34445	0.30294
H	-3.98611	-2.27103	0.28902
H	-3.08573	-2.29895	-1.26076

25: ΔG = -2663659.32 kJ/mol

Si	2.49825	-0.73500	-0.21983
C	3.03170	-1.54455	1.36100
H	2.16383	-1.96198	1.89114
H	3.72322	-2.37558	1.16619
H	3.53178	-0.84191	2.04169
C	1.65200	-1.89825	-1.39603
H	2.31467	-2.72702	-1.68224
H	0.75941	-2.33921	-0.92964
H	1.33207	-1.39040	-2.31682
C	1.48755	0.81348	0.08488
C	0.84380	1.03138	1.31450
C	1.30617	1.76456	-0.93481
C	0.04036	2.15354	1.51689
H	0.96374	0.31212	2.12896
C	0.51179	2.89254	-0.73333
H	1.78845	1.62340	-1.90655
C	-0.12655	3.08650	0.49299
H	-0.45659	2.30132	2.47766
H	0.38515	3.62077	-1.53681
H	-0.75448	3.96582	0.64989
F	-0.88810	-2.16809	1.53395
F	3.87106	-0.21644	-1.01238
N	-3.03187	-0.41955	-0.32727
C	-3.09385	0.02164	1.09777
H	-2.85263	1.08738	1.14169
H	-4.10808	-0.14830	1.46944
H	-2.36277	-0.57806	1.65366
C	-1.63823	-0.22844	-0.83007
H	-1.59605	-0.56079	-1.87130
H	-1.39099	0.83464	-0.76334
H	-0.98380	-0.83258	-0.19117
C	-3.98236	0.37665	-1.14827
H	-3.92372	0.03699	-2.18585
H	-4.99415	0.22971	-0.76107
H	-3.70437	1.43231	-1.08288
C	-3.37731	-1.86905	-0.40256
H	-2.65692	-2.40755	0.22397
H	-4.39797	-2.00413	-0.03411
H	-3.30930	-2.18939	-1.44587

22: ΔG = -3166699.80 kJ/mol

Si	0.04677	-1.79876	-0.59854
C	0.10142	-3.04913	-2.01406
H	1.01160	-2.90092	-2.61478
H	0.07680	-4.09648	-1.68899
H	-0.74292	-2.88259	-2.69984
C	-1.62711	-1.14592	0.06214

C	-1.96487	-1.22504	1.42518
C	-2.55411	-0.51606	-0.78739
C	-3.14408	-0.66882	1.92415
H	-1.28436	-1.72605	2.11606
C	-3.75027	0.01646	-0.30421
H	-2.33018	-0.43090	-1.85264
C	-4.04400	-0.04628	1.05865
H	-3.36514	-0.72740	2.99245
H	-4.45286	0.49261	-0.99245
H	-4.97053	0.38521	1.44346
F	0.07227	-3.07884	0.65641
F	0.06796	-0.45835	-1.83503
C	1.65106	-1.05811	0.12536
C	1.74248	-0.69555	1.47910
C	2.77422	-0.81417	-0.68278
C	2.88816	-0.08941	1.99890
H	0.89593	-0.87996	2.14671
C	3.93598	-0.23864	-0.16636
H	2.74078	-1.06970	-1.74571
C	3.99323	0.13630	1.17732
H	2.92243	0.20149	3.05138
H	4.79783	-0.07081	-0.81666
H	4.89444	0.60188	1.58168
N	-0.05017	2.94727	-0.31686
C	-0.97323	2.68752	-1.46081
H	-0.63191	3.27109	-2.32012
H	-0.93978	1.61781	-1.68939
H	-1.98262	2.99397	-1.17352
C	-0.50982	2.17496	0.87306
H	-0.50092	1.11221	0.61605
H	0.17280	2.37131	1.70425
H	-1.52334	2.49478	1.13015
C	-0.03853	4.40196	0.00283
H	0.64293	4.57339	0.84012
H	0.30162	4.95152	-0.87870
H	-1.05186	4.71138	0.27194
C	1.32413	2.49831	-0.69073
H	1.65570	3.07639	-1.55731
H	1.99243	2.67246	0.15689
H	1.27768	1.43352	-0.93791

22-TS: ΔG = -3166640.15 kJ/mol

Si	2.31036	-0.00424	0.51127
C	2.52392	-0.03495	2.34827
H	3.08907	-0.91450	2.68335
H	3.03514	0.86363	2.71758
H	1.53160	-0.07422	2.82411
C	1.42873	1.53964	-0.07920

C	1.43923	1.90439	-1.43725
C	0.65586	2.30831	0.80759
C	0.69444	2.99033	-1.89448
H	2.03406	1.33192	-2.15417
C	-0.09241	3.39379	0.35229
H	0.62580	2.05135	1.86935
C	-0.07760	3.73447	-1.00032
H	0.71399	3.25667	-2.95306
H	-0.69093	3.97510	1.05633
H	-0.66607	4.58145	-1.35863
F	3.78698	0.01014	-0.25018
F	-1.15304	-0.15905	2.69606
C	1.42859	-1.52924	-0.12865
C	1.35634	-1.79974	-1.50681
C	0.73521	-2.37874	0.74904
C	0.61172	-2.87459	-1.98964
H	1.88536	-1.16103	-2.21946
C	-0.01903	-3.44942	0.26882
H	0.76918	-2.19625	1.82561
C	-0.08417	-3.69776	-1.10207
H	0.56844	-3.06866	-3.06308
H	-0.55847	-4.09129	0.96815
H	-0.67602	-4.53381	-1.48000
N	-3.06164	0.01716	-0.05908
C	-3.26580	1.22899	0.78873
H	-4.31103	1.25802	1.10842
H	-2.59344	1.14007	1.65057
H	-3.03217	2.11381	0.19010
C	-1.62923	-0.03815	-0.47919
H	-1.03274	-0.07547	0.43838
H	-1.47956	-0.93560	-1.08661
H	-1.40487	0.85804	-1.06506
C	-3.94148	0.07851	-1.25677
H	-3.77515	-0.81606	-1.86319
H	-4.98339	0.12212	-0.92831
H	-3.69076	0.97420	-1.83187
C	-3.δ37259	-1.20084	0.74656
H	-4.41867	-1.15148	1.06121
H	-3.21062	-2.08215	0.11956
H	-2.69806	-1.19636	1.61202

26: ΔG = -3166642.47 kJ/mol

Si	-2.38500	-0.09493	0.38444
C	-2.85928	-0.10252	2.17312
H	-3.48218	0.76400	2.43164
H	-3.41132	-1.01297	2.44140
H	-1.96058	-0.06323	2.80585
C	-1.36777	-1.59033	-0.10268

C	-1.23548	-1.96369	-1.45177
C	-0.63629	-2.30805	0.85861
C	-0.39564	-3.01095	-1.82773
H	-1.79242	-1.42841	-2.22562
C	0.21065	-3.35121	0.48475
H	-0.71657	-2.04428	1.91587
C	0.33429	-3.70300	-0.85952
H	-0.30641	-3.28647	-2.88032
H	0.77685	-3.89114	1.24618
H	0.99844	-4.51819	-1.15362
F	-3.74659	-0.16329	-0.56444
F	1.18309	0.13672	2.71817
C	-1.50531	1.47814	-0.12498
C	-1.37765	1.82927	-1.48063
C	-0.86767	2.28564	0.83143
C	-0.63182	2.94191	-1.86661
H	-1.86343	1.22496	-2.25163
C	-0.11134	3.39305	0.44786
H	-0.94959	2.04241	1.89339
C	0.00954	3.72185	-0.90235
H	-0.54489	3.19932	-2.92396
H	0.38495	4.00178	1.20625
H	0.60259	4.58746	-1.20426
N	3.06133	0.09927	-0.07996
C	3.36122	-1.10079	0.75540
H	4.41716	-1.07364	1.03784
H	2.71601	-1.05138	1.64038
H	3.15400	-1.99639	0.16307
C	1.61502	0.07692	-0.45451
H	1.04301	0.08168	0.47963
H	1.40109	0.96439	-1.05704
H	1.42243	-0.83025	-1.03476
C	3.90284	0.09039	-1.30686
H	3.66311	0.97424	-1.90442
H	4.95619	0.10814	-1.01459
H	3.68546	-0.81779	-1.87597
C	3.33156	1.33098	0.71868
H	4.38763	1.33787	1.00191
H	3.10354	2.20315	0.09953
H	2.68597	1.29240	1.60418

23: ΔG = -3669683.40 kJ/mol

Si	0.99200	-0.05400	0.40500
C	0.15100	1.63500	0.67400
C	-0.76800	1.83200	1.71700
C	0.39400	2.71600	-0.18900
C	-1.43900	3.04600	1.87700
H	-0.97500	1.01700	2.41700

C	-0.24900	3.94300	-0.01800
H	1.09500	2.59700	-1.02100
C	-1.17700	4.10900	1.01200
H	-2.16500	3.16600	2.68400
H	-0.03300	4.77200	-0.69600
H	-1.69400	5.06300	1.13900
F	1.60400	-0.01500	2.08100
F	0.36100	-0.05800	-1.28400
C	2.77200	-0.12100	-0.27200
C	3.77600	0.71900	0.23900
C	3.13400	-1.01100	-1.29700
C	5.08000	0.68200	-0.25800
H	3.53600	1.42000	1.04300
C	4.44200	-1.07600	-1.77900
H	2.37700	-1.67000	-1.73100
C	5.42000	-0.22300	-1.26500
H	5.83700	1.35700	0.14700
H	4.70000	-1.78900	-2.56500
H	6.44200	-0.26200	-1.64800
C	0.01200	-1.65600	0.77000
C	-0.28500	-2.58900	-0.23900
C	-0.50000	-1.91900	2.05400
C	-1.05700	-3.72400	0.01600
H	0.08500	-2.42000	-1.25100
C	-1.29800	-3.03500	2.31100
H	-0.27700	-1.22900	2.87000
C	-1.57800	-3.94500	1.29100
H	-1.26400	-4.43400	-0.78900
H	-1.69900	-3.19800	3.31400
H	-2.19700	-4.82200	1.49000
N	-3.40800	0.12900	-1.35200
C	-2.75100	-0.87600	-2.23900
H	-3.22300	-1.84900	-2.07500
H	-2.88500	-0.56300	-3.27800
H	-1.68700	-0.91200	-1.98700
C	-2.75500	1.45600	-1.55000
H	-2.88700	1.75900	-2.59200
H	-3.22900	2.18200	-0.88300
H	-1.69100	1.35300	-1.31600
C	-3.24800	-0.29100	0.07000
H	-3.73300	0.45000	0.71100
H	-3.71500	-1.27100	0.20200
H	-2.17900	-0.34700	0.29400
C	-4.85600	0.22600	-1.68500
H	-4.95600	0.53500	-2.72900
H	-5.31800	-0.75400	-1.53600
H	-5.31900	0.96600	-1.02700

23-TS: ΔG = -3669616.64 kJ/mol

Si	-1.32000	0.05200	1.06800
C	-0.23200	-1.46700	1.19400
C	0.48000	-1.69600	2.38500
C	-0.03900	-2.35500	0.12300
C	1.36000	-2.77100	2.49900
H	0.35400	-1.02400	3.23700
C	0.83800	-3.43300	0.23700
H	-0.55200	-2.17500	-0.82300
C	1.54100	-3.64200	1.42400
H	1.90800	-2.93100	3.43000
H	0.97700	-4.11100	-0.60800
H	2.23200	-4.48300	1.51000
F	-2.04800	0.12300	2.56500
F	0.07300	-0.21200	-2.20100
C	-2.67500	-0.08900	-0.20800
C	-3.26500	-1.33300	-0.49400
C	-3.15600	1.04200	-0.88900
C	-4.29300	-1.44300	-1.42900
H	-2.92200	-2.23400	0.02000
C	-4.18400	0.93500	-1.82400
H	-2.72600	2.02600	-0.68800
C	-4.75100	-0.30900	-2.10000
H	-4.73700	-2.41900	-1.63700
H	-4.54200	1.82600	-2.34300
H	-5.55400	-0.39500	-2.83500
C	-0.36100	1.65900	0.98300
C	0.02300	2.23100	-0.24300
C	0.03000	2.30200	2.17100
C	0.77100	3.40700	-0.27700
H	-0.22600	1.71000	-1.17200
C	0.78700	3.47300	2.13500
H	-0.25700	1.88600	3.13900
C	1.15600	4.03000	0.91100
H	1.06000	3.83800	-1.23800
H	1.08500	3.95600	3.06800
H	1.74500	4.94900	0.88300
N	3.36600	-0.08300	-1.43500
C	2.98600	1.09900	-2.26400
H	3.22900	2.00700	-1.70500
H	3.55800	1.06900	-3.19500
H	1.91000	1.02600	-2.46100
C	3.03400	-1.33100	-2.18400
H	3.60300	-1.33700	-3.11800
H	3.31500	-2.19000	-1.56900
H	1.95500	-1.31500	-2.38000
C	2.56900	-0.05800	-0.17300
H	2.83200	-0.93800	0.42200

H	2.81100	0.85600	0.37700
H	1.51500	-0.07800	-0.46900
C	4.82000	-0.04500	-1.12400
H	5.38300	-0.06400	-2.06000
H	5.03900	0.87300	-0.57200
H	5.07200	-0.91800	-0.51500

25: ΔG = -3669619.49 kJ/mol

Si	1.53600	-0.00000	1.06800
C	0.50100	1.53700	0.83300
C	-0.14000	2.16400	1.91400
C	0.24700	2.02000	-0.46300
C	-1.00900	3.23500	1.70700
H	0.03400	1.80800	2.93300
C	-0.62700	3.08500	-0.67300
H	0.72600	1.54900	-1.32600
C	-1.25600	3.69400	0.41300
H	-1.49800	3.71200	2.55900
H	-0.81900	3.43800	-1.68800
H	-1.94300	4.52700	0.25000
F	2.00000	-0.00000	2.65800
F	-1.45100	0.00000	-2.92700
C	3.03900	-0.00100	-0.04000
C	3.62500	1.20600	-0.46100
C	3.62300	-1.20800	-0.46300
C	4.75800	1.20700	-1.27200
H	3.19200	2.16100	-0.15200
C	4.75600	-1.20900	-1.27500
H	3.18800	-2.16200	-0.15700
C	5.32400	-0.00100	-1.68200
H	5.20000	2.15300	-1.59000
H	5.19500	-2.15500	-1.59500
H	6.20900	-0.00100	-2.32100
C	0.50000	-1.53700	0.83300
C	0.24400	-2.01900	-0.46300
C	-0.14000	-2.16400	1.91500
C	-0.63000	-3.08300	-0.67300
H	0.72200	-1.54700	-1.32600
C	-1.01000	-3.23500	1.70800
H	0.03500	-1.80900	2.93300
C	-1.25900	-3.69300	0.41400
H	-0.82400	-3.43500	-1.68800
H	-1.49800	-3.71100	2.56000
H	-1.94600	-4.52600	0.25100
N	-3.86200	0.00000	-0.59400
C	-3.98100	-1.21500	-1.45200
H	-3.88200	-2.10000	-0.81700
H	-4.96300	-1.20600	-1.93300

H	-3.17700	-1.16600	-2.19600
C	-3.98200	1.21500	-1.45200
H	-4.96400	1.20500	-1.93300
H	-3.88400	2.10000	-0.81800
H	-3.17800	1.16700	-2.19600
C	-2.51600	0.00100	0.05500
H	-2.43200	0.90000	0.67400
H	-2.43100	-0.89600	0.67600
H	-1.77500	0.00000	-0.75200
C	-4.92800	0.00000	0.44300
H	-5.90300	-0.00000	-0.05200
H	-4.81900	-0.89600	1.06000
H	-4.82000	0.89600	1.06000

Computations using ORCA, method CPCM-M062X/ma-def2-TZVP

20: ΔG = -2161220.33 kJ/mol

N	2.822200	-0.273030	0.006510
C	3.746330	-1.437100	-0.027180
H	3.246890	-2.258040	-0.536470
H	4.646070	-1.147020	-0.564550
H	3.987610	-1.715380	0.996040
C	3.470240	0.877310	0.701300
H	2.748760	1.693310	0.697700
H	3.716240	0.566730	1.714350
H	4.373760	1.139570	0.155480
C	1.571820	-0.633770	0.736870
H	0.941520	0.255310	0.740040
H	1.095930	-1.458600	0.210260
H	1.843250	-0.934480	1.746880
C	2.469820	0.138760	-1.383470
H	1.976540	-0.698770	-1.872120
H	1.803770	0.996750	-1.302540
H	3.389000	0.395230	-1.905520
F	0.742860	2.282670	0.121670
Si	-2.499950	-0.202630	-0.050500
C	-3.561490	1.313180	0.105040
H	-4.046500	1.549630	-0.843700
H	-4.332460	1.177090	0.865500
H	-2.946040	2.168250	0.393990
C	-1.207100	-0.012930	-1.364160
H	-0.675520	-0.952870	-1.528980
H	-1.651270	0.307860	-2.308360
H	-0.484770	0.741940	-1.035800
C	-1.784780	-0.700460	1.590590
H	-2.580050	-0.891710	2.313740
H	-1.172450	-1.600110	1.504050
H	-1.157270	0.102880	1.983720
F	-3.480940	-1.415780	-0.513550

20-TS: ΔG = -2161186.36 kJ/mol

N	0.021728	-0.027736	0.051190
C	1.506369	-0.046592	-0.026187
H	1.875477	0.951761	0.196960
H	1.880553	-0.761802	0.702850
H	1.795405	-0.342946	-1.031830
C	-0.523319	-1.384249	-0.249249
H	-1.608149	-1.311056	-0.180088
H	-0.204316	-1.663897	-1.251012
H	-0.122759	-2.081590	0.483313
C	-0.531848	0.942331	-0.938051
H	-1.615934	0.913258	-0.836002
H	-0.137564	1.929541	-0.705479
H	-0.217140	0.632033	-1.932447
C	-0.414707	0.378966	1.419347
H	-0.019465	1.372622	1.619712
H	-1.504632	0.374515	1.417985
H	-0.012356	-0.338444	2.131308
F	-3.261890	-0.007607	0.260695
Si	-4.524551	1.942405	-1.075566
C	-5.955783	1.169446	-0.173003
H	-6.441812	1.917103	0.458556
H	-6.696466	0.809314	-0.891171
H	-5.622196	0.339829	0.444461
C	-3.341182	2.945983	-0.042980
H	-2.609547	3.441124	-0.686712
H	-3.896534	3.723571	0.487333
H	-2.814177	2.325371	0.677269
C	-3.808302	0.964789	-2.492208
H	-4.599088	0.746047	-3.214068
H	-3.045429	1.555863	-3.006000
H	-3.363034	0.032605	-2.153402
F	-5.294959	3.153932	-1.909117

24: ΔG = -2161190.09 kJ/mol

N	2.822200	-0.273030	0.006510
C	3.746330	-1.437100	-0.027180
H	3.246890	-2.258040	-0.536470
H	4.646070	-1.147020	-0.564550
H	3.987610	-1.715380	0.996040
C	3.470240	0.877310	0.701300
H	2.748760	1.693310	0.697700
H	3.716240	0.566730	1.714350
H	4.373760	1.139570	0.155480
C	1.571820	-0.633770	0.736870
H	0.941520	0.255310	0.740040
H	1.095930	-1.458600	0.210260
H	1.843250	-0.934480	1.746880

C	2.469820	0.138760	-1.383470
H	1.976540	-0.698770	-1.872120
H	1.803770	0.996750	-1.302540
H	3.389000	0.395230	-1.905520
F	0.742860	2.282670	0.121670
Si	-2.499950	-0.202630	-0.050500
C	-3.561490	1.313180	0.105040
H	-4.046500	1.549630	-0.843700
H	-4.332460	1.177090	0.865500
H	-2.946040	2.168250	0.393990
C	-1.207100	-0.012930	-1.364160
H	-0.675520	-0.952870	-1.528980
H	-1.651270	0.307860	-2.308360
H	-0.484770	0.741940	-1.035800
C	-1.784780	-0.700460	1.590590
H	-2.580050	-0.891710	2.313740
H	-1.172450	-1.600110	1.504050
H	-1.157270	0.102880	1.983720
F	-3.480940	-1.415780	-0.513550

21: ΔG = -2664490.67 kJ/mol

Si	1.733520	-1.102060	-0.000680
C	2.716620	-1.831640	1.438720
H	2.499190	-1.267690	2.350090
H	2.393250	-2.859140	1.625690
H	3.793770	-1.829360	1.276530
C	1.006090	-2.180850	-1.379100
H	0.585920	-3.099150	-0.962470
H	0.177390	-1.646410	-1.855870
H	1.727630	-2.439670	-2.153580
C	1.327010	0.765500	0.009950
C	0.767800	1.388400	1.131780
C	1.500460	1.554720	-1.131620
C	0.401390	2.729950	1.121290
H	0.602560	0.806980	2.032190
C	1.111420	2.891100	-1.166390
H	1.939690	1.113540	-2.019720
C	0.562160	3.484500	-0.035970
H	-0.020050	3.185140	2.010030
H	1.239740	3.470310	-2.073230
H	0.262920	4.525370	-0.055520
F	0.237160	-1.378380	0.930760
F	3.175990	-0.798380	-0.938130
N	-2.953170	-0.417030	-0.042490
C	-2.644390	-0.061440	1.373500
H	-2.823030	1.003720	1.503390
H	-3.301880	-0.639170	2.019270
H	-1.601020	-0.306820	1.558960

C	-2.065970	0.366860	-0.948290
H	-2.303550	0.100610	-1.975860
H	-2.246430	1.425890	-0.775520
H	-1.035740	0.114840	-0.710340
C	-4.377870	-0.104530	-0.340940
H	-4.578360	-0.371660	-1.375790
H	-5.004290	-0.686160	0.331120
H	-4.535510	0.959860	-0.184410
C	-2.700780	-1.873050	-0.251460
H	-1.656780	-2.067420	-0.014930
H	-3.359950	-2.430510	0.410090
H	-2.917110	-2.110140	-1.290730

21-TS: ΔG = -2664443.35 kJ/mol

Si	0.046009	0.132198	0.048629
C	1.888088	-0.075834	0.060109
H	2.378857	0.891503	-0.013779
H	2.199341	-0.567137	0.984800
H	2.195023	-0.706991	-0.776978
C	-0.766809	0.875826	1.543344
H	-0.497602	1.926056	1.628498
H	-1.852397	0.785003	1.454108
H	-0.456847	0.345300	2.446518
C	-0.661588	0.732393	-1.575884
C	0.095042	1.432530	-2.517622
C	-2.004955	0.477833	-1.870258
C	-0.466910	1.860431	-3.714449
H	1.129826	1.666951	-2.297846
C	-2.577916	0.911351	-3.061083
H	-2.620651	-0.065019	-1.159745
C	-1.806448	1.603560	-3.986919
H	0.135977	2.403132	-4.432722
H	-3.622080	0.709426	-3.266258
H	-2.247081	1.942737	-4.916357
F	1.014499	2.827924	0.066814
F	-0.500416	-1.420514	0.098027
N	-1.067672	5.129663	-1.015844
C	0.048938	4.940973	-1.987733
H	-0.382305	4.666868	-2.948082
H	0.590347	5.881368	-2.068260
H	0.677568	4.141235	-1.595544
C	-1.779463	3.828621	-0.843816
H	-2.610034	3.984688	-0.157975
H	-2.141685	3.504002	-1.818423
H	-1.050385	3.122880	-0.448122
C	-2.006535	6.166985	-1.517044
H	-2.803922	6.292311	-0.788316
H	-1.457495	7.097317	-1.644099

H	-2.411569	5.831584	-2.469227
C	-0.500596	5.540751	0.301067
H	0.182053	4.749453	0.610158
H	0.017968	6.487860	0.169687
H	-1.322626	5.655215	1.004462

25: ΔG = -2664443.91 kJ/mol

Si	2.540890	-0.702520	-0.215420
C	2.948650	-1.551470	1.378850
H	2.039060	-1.938170	1.843880
H	3.619230	-2.393250	1.196590
H	3.429270	-0.867910	2.080890
C	1.777080	-1.839530	-1.465750
H	2.465920	-2.645700	-1.725560
H	0.867070	-2.286440	-1.059120
H	1.514320	-1.296750	-2.376050
C	1.487070	0.813320	0.060790
C	0.837790	1.041120	1.277330
C	1.290650	1.734930	-0.974410
C	0.013710	2.146580	1.454830
H	0.966760	0.344550	2.098870
C	0.477130	2.847620	-0.800330
H	1.778470	1.584990	-1.932440
C	-0.166530	3.051730	0.415820
H	-0.487070	2.301680	2.402510
H	0.339730	3.551440	-1.611670
H	-0.806530	3.914540	0.552790
F	-0.978180	-2.273460	1.509680
F	3.928600	-0.169010	-0.867770
N	-3.026350	-0.420240	-0.283080
C	-3.075360	-0.004890	1.149260
H	-2.772340	1.038520	1.210810
H	-4.097490	-0.123990	1.502700
H	-2.385350	-0.652080	1.690300
C	-1.625750	-0.275210	-0.778450
H	-1.596770	-0.596390	-1.817980
H	-1.343430	0.772510	-0.694840
H	-1.000370	-0.904150	-0.145440
C	-3.940400	0.429830	-1.090490
H	-3.882060	0.108700	-2.127930
H	-4.951910	0.307860	-0.710130
H	-3.620290	1.465140	-0.994730
C	-3.430660	-1.852060	-0.387640
H	-2.725990	-2.424730	0.214120
H	-4.446880	-1.947400	-0.011270
H	-3.386800	-2.141220	-1.435490

22: ΔG = -3167753.60 kJ/mol

Si	0.015490	-1.757120	-0.600040
C	0.102820	-2.906130	-2.094570
H	1.021650	-2.709610	-2.654450
H	0.077550	-3.962370	-1.830810
H	-0.726380	-2.690550	-2.772970
C	-1.662600	-1.200660	0.122620
C	-1.997030	-1.422650	1.463730
C	-2.595480	-0.499260	-0.652440
C	-3.180810	-0.941000	2.015260
H	-1.315250	-1.980060	2.094610
C	-3.795070	-0.038890	-0.121550
H	-2.374870	-0.301930	-1.694700
C	-4.086190	-0.247340	1.222050
H	-3.398590	-1.112050	3.062800
H	-4.499330	0.490110	-0.752720
H	-5.011750	0.123720	1.644890
F	0.088690	-3.084210	0.523550
F	-0.020930	-0.371570	-1.702720
C	1.597290	-1.014130	0.159360
C	1.624310	-0.541200	1.474700
C	2.760320	-0.848370	-0.600150
C	2.746520	0.089510	2.004170
H	0.744840	-0.651170	2.102460
C	3.895910	-0.238970	-0.077090
H	2.779900	-1.188300	-1.631150
C	3.889330	0.241080	1.228250
H	2.729430	0.461760	3.021840
H	4.783720	-0.130420	-0.688940
H	4.766500	0.728250	1.635980
N	0.035260	2.939410	-0.405100
C	-0.890370	2.756420	-1.560690
H	-0.491890	3.310010	-2.407830
H	-0.940100	1.692400	-1.781500
H	-1.867690	3.142030	-1.278200
C	-0.492980	2.184800	0.767080
H	-0.563690	1.135340	0.490590
H	0.196220	2.315580	1.598630
H	-1.476060	2.580420	1.013960
C	0.138920	4.385020	-0.065200
H	0.824650	4.491840	0.771820
H	0.516100	4.915530	-0.936220
H	-0.850860	4.746950	0.203170
C	1.382790	2.407310	-0.765550
H	1.772560	2.999560	-1.590400
H	2.029150	2.491020	0.106230
H	1.266000	1.365800	-1.053290

22-TS: ΔG = -3167691.78 kJ/mol

Si	0.005938	-0.040955	0.227381
C	1.833752	0.056840	0.000897
H	2.271326	0.785619	0.686202
H	2.292943	-0.915406	0.188047
H	2.024287	0.365217	-1.028184
C	-0.841348	-1.377945	-0.760658
C	-2.007207	-1.977746	-0.270102
C	-0.388031	-1.753696	-2.029078
C	-2.710515	-2.906055	-1.029176
H	-2.377984	-1.716397	0.715455
C	-1.081487	-2.690432	-2.786452
H	0.485766	-1.262668	-2.440075
C	-2.247759	-3.262080	-2.290684
H	-3.616127	-3.352008	-0.636968
H	-0.719170	-2.966251	-3.769493
H	-2.794593	-3.983794	-2.884972
F	-0.264360	-0.489030	1.772677
F	0.719618	0.987116	-2.754632
C	-0.877631	1.597568	0.066431
C	-2.269537	1.661853	0.189100
C	-0.183834	2.788099	-0.163060
C	-2.946975	2.871562	0.090027
H	-2.842010	0.754155	0.355630
C	-0.853457	4.001773	-0.265124
H	0.894160	2.767645	-0.276160
C	-2.237322	4.044609	-0.137128
H	-4.025812	2.898047	0.183437
H	-0.297693	4.913550	-0.446206
H	-2.761573	4.988692	-0.220185
N	-2.585218	1.248330	-4.028374
C	-1.564714	0.483615	-4.804638
H	-1.241707	1.106808	-5.636395
H	-0.726398	0.282771	-4.134925
H	-2.029134	-0.428784	-5.172674
C	-3.124198	0.384228	-2.941230
H	-2.297971	0.090605	-2.298495
H	-3.857892	0.957732	-2.378744
H	-3.583692	-0.492044	-3.393838
C	-3.697323	1.667546	-4.922650
H	-4.426265	2.216255	-4.330849
H	-3.288926	2.301669	-5.705792
H	-4.148645	0.776033	-5.352230
C	-1.932210	2.448578	-3.423386
H	-1.590856	3.087842	-4.235663
H	-2.670579	2.966784	-2.815396
H	-1.083224	2.099990	-2.830856

26: ΔG = -3167702.49 kJ/mol

Si	2.444490	0.098980	0.312620
C	2.993170	0.097560	2.076520
H	3.625030	-0.769050	2.278760
H	3.556390	1.004540	2.302550
H	2.133150	0.054810	2.748710
C	1.387590	1.572390	-0.112760
C	1.188810	1.936650	-1.449720
C	0.681470	2.265390	0.874250
C	0.306390	2.953550	-1.790060
H	1.722150	1.416720	-2.238950
C	-0.209680	3.278380	0.538890
H	0.813940	2.006280	1.919300
C	-0.400230	3.620580	-0.794420
H	0.163680	3.221910	-2.829390
H	-0.755910	3.797910	1.316470
H	-1.096340	4.407000	-1.058500
F	3.736870	0.183120	-0.656150
F	-1.508800	-0.106830	2.844710
C	1.526910	-1.456230	-0.147630
C	1.354000	-1.813780	-1.489960
C	0.886990	-2.224930	0.829170
C	0.561190	-2.897730	-1.845050
H	1.838240	-1.237480	-2.271640
C	0.083580	-3.304170	0.479070
H	1.001340	-1.974350	1.878370
C	-0.082640	-3.638870	-0.859340
H	0.437980	-3.160650	-2.888270
H	-0.413260	-3.881240	1.249230
H	-0.710350	-4.477320	-1.134780
N	-3.039270	-0.102700	-0.086900
C	-3.430280	1.100490	0.703260
H	-4.507000	1.072220	0.857260
H	-2.888510	1.046650	1.647300
H	-3.150670	1.985310	0.134480
C	-1.561370	-0.080050	-0.291290
H	-1.106840	-0.078170	0.698710
H	-1.278100	-0.969590	-0.852520
H	-1.306920	0.823450	-0.843590
C	-3.736580	-0.101090	-1.399140
H	-3.431880	-0.987230	-1.951390
H	-4.809310	-0.114350	-1.220130
H	-3.451810	0.799630	-1.938340
C	-3.398250	-1.328110	0.683760
H	-4.475860	-1.333190	0.834130
H	-3.092020	-2.196140	0.102870
H	-2.862210	-1.273260	1.630900

23: ΔG = -3671016.13 kJ/mol

Si	1.059980	-0.071880	0.227190
C	0.189280	1.626900	0.323660
C	-0.572340	1.988060	1.441870
C	0.271110	2.559100	-0.717260
C	-1.240150	3.206320	1.511340
H	-0.650700	1.295930	2.273410
C	-0.362470	3.795800	-0.645010
H	0.840390	2.310590	-1.605710
C	-1.129600	4.119090	0.467960
H	-1.839190	3.447980	2.381170
H	-0.267880	4.502410	-1.461060
H	-1.637870	5.074080	0.521840
F	1.438630	0.044880	1.913170
F	0.684090	-0.149760	-1.469520
C	2.916440	-0.198600	-0.196260
C	3.891300	0.450280	0.570210
C	3.365460	-0.942180	-1.294640
C	5.243740	0.377430	0.251440
H	3.586060	1.026560	1.435570
C	4.716770	-1.047400	-1.606490
H	2.641640	-1.450320	-1.920940
C	5.661850	-0.379070	-0.836710
H	5.972140	0.905240	0.855710
H	5.032500	-1.643220	-2.454690
H	6.714460	-0.447270	-1.083090
C	0.012010	-1.643460	0.542210
C	-0.358140	-2.507780	-0.496430
C	-0.478650	-1.950630	1.818800
C	-1.171740	-3.615500	-0.279060
H	-0.011340	-2.303880	-1.501580
C	-1.309740	-3.042690	2.045470
H	-0.213780	-1.313140	2.652640
C	-1.658810	-3.882640	0.994720
H	-1.432790	-4.265050	-1.106280
H	-1.683210	-3.239900	3.043360
H	-2.302960	-4.736280	1.166700
N	-3.548050	0.182260	-1.029810
C	-2.639400	-0.411790	-2.052700
H	-2.785250	-1.489720	-2.052340
H	-2.897150	0.009610	-3.022090
H	-1.610580	-0.170400	-1.784920
C	-3.376130	1.663970	-1.027570
H	-3.699730	2.046570	-1.993050
H	-3.982150	2.081570	-0.227100
H	-2.321780	1.879450	-0.866430
C	-3.193450	-0.355090	0.315490
H	-3.886350	0.059730	1.043950

H	-3.262120	-1.441510	0.286250
H	-2.173760	-0.053930	0.537110
C	-4.961180	-0.161530	-1.348850
H	-5.192140	0.219100	-2.340840
H	-5.064940	-1.243720	-1.321230
H	-5.603120	0.302120	-0.603450

23-TS: ΔG = -3670937.78 kJ/mol

Si	0.017033	-0.090126	-0.071379
C	1.881630	-0.057270	-0.003476
C	2.512479	1.189400	0.077813
C	2.681963	-1.199612	-0.093734
C	3.898514	1.296186	0.057267
H	1.917847	2.094215	0.151871
C	4.067460	-1.098094	-0.104817
H	2.209039	-2.166068	-0.208193
C	4.678063	0.149521	-0.035278
H	4.367951	2.270393	0.113890
H	4.673625	-1.992926	-0.179699
H	5.758232	0.227573	-0.052606
F	-0.387997	1.122564	0.940389
F	0.876065	-2.481868	-2.038044
C	-0.751345	-1.630324	0.631859
C	-0.103222	-2.341547	1.646980
C	-1.999653	-2.086459	0.197681
C	-0.677645	-3.477165	2.204980
H	0.865202	-2.010107	2.006313
C	-2.578349	-3.221904	0.751824
H	-2.526057	-1.554081	-0.587008
C	-1.915489	-3.920427	1.754269
H	-0.159244	-4.017716	2.987162
H	-3.543978	-3.563767	0.400616
H	-2.363119	-4.807982	2.184043
C	-0.725056	0.505042	-1.677852
C	-1.051616	-0.337964	-2.745384
C	-0.933009	1.881177	-1.832419
C	-1.573376	0.178871	-3.924637
H	-0.844314	-1.397996	-2.652347
C	-1.444743	2.401664	-3.015665
H	-0.694903	2.558857	-1.020402
C	-1.768260	1.549090	-4.063597
H	-1.820332	-0.487357	-4.742547
H	-1.593589	3.469550	-3.116745
H	-2.170343	1.950654	-4.985600
N	2.772460	-0.990054	-4.332018
C	1.542864	-1.553244	-4.962062
H	1.003882	-0.737608	-5.440042
H	1.845302	-2.293274	-5.699807

H	0.953913	-2.000032	-4.160939
C	3.515709	-2.088077	-3.647361
H	3.784614	-2.833381	-4.393039
H	4.409422	-1.660755	-3.196931
H	2.846634	-2.496076	-2.888916
C	2.361710	0.012705	-3.307542
H	3.257603	0.395412	-2.819635
H	1.820662	0.814317	-3.808598
H	1.725782	-0.513680	-2.600014
C	3.631607	-0.353341	-5.363200
H	3.917675	-1.110103	-6.090124
H	3.062557	0.439361	-5.843545
H	4.511984	0.055496	-4.872695

27: ΔG = -3670950.71 kJ/mol

Si	-1.535230	0.000520	1.028000
C	-0.498340	-1.523800	0.783980
C	0.159780	-2.121650	1.863560
C	-0.243030	-2.008930	-0.502600
C	1.051660	-3.168760	1.663100
H	-0.016710	-1.762500	2.871510
C	0.653870	-3.048820	-0.708830
H	-0.735860	-1.559720	-1.359530
C	1.303110	-3.628820	0.375540
H	1.554350	-3.621070	2.508760
H	0.848260	-3.405420	-1.712720
H	2.004320	-4.438700	0.216990
F	-1.984130	0.000900	2.578020
F	1.666020	-0.000210	-3.043670
C	-3.045870	0.000710	-0.051030
C	-3.646030	-1.200980	-0.442160
C	-3.646240	1.202530	-0.441400
C	-4.810370	-1.203230	-1.199130
H	-3.198730	-2.146770	-0.155620
C	-4.810550	1.205060	-1.198400
H	-3.199100	2.148220	-0.154260
C	-5.392480	0.000980	-1.577320
H	-5.262760	-2.141380	-1.494530
H	-5.263100	2.143320	-1.493230
H	-6.299280	0.001090	-2.169150
C	-0.497590	1.524270	0.783580
C	-0.242070	2.009060	-0.503080
C	0.160930	2.121910	1.863030
C	0.655430	3.048400	-0.709510
H	-0.735260	1.560040	-1.359900
C	1.053400	3.168460	1.662390
H	-0.015710	1.763000	2.871050
C	1.305070	3.628170	0.374740

H	0.849960	3.404760	-1.713460
H	1.556390	3.620610	2.507950
H	2.006760	4.437610	0.216030
N	3.843450	-0.000790	-0.562810
C	4.013390	1.215420	-1.409860
H	3.873260	2.089770	-0.777090
H	5.018630	1.204490	-1.825620
H	3.254900	1.164940	-2.190950
C	4.013270	-1.216440	-1.410720
H	5.018480	-1.205280	-1.826530
H	3.873140	-2.091210	-0.778530
H	3.254720	-1.165370	-2.191710
C	2.461710	-0.000940	0.000240
H	2.338430	-0.897780	0.605850
H	2.338650	0.895140	0.607010
H	1.778050	-0.000290	-0.847030
C	4.841970	-0.001240	0.537840
H	5.838150	-0.001210	0.101740
H	4.690270	0.891830	1.139850
H	4.690090	-0.894650	1.139290

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