

Hydroxyl radicals via Collision Induced Dissociation of Trimethylammonium Benzyl Alcohols

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Table of contents

Mass Spectra	S3 - S12
CBS-QB3 Calculations	S13 - S15
NMR Spectra	S16 - S29
Flash Laser Photolysis Spectra	S30

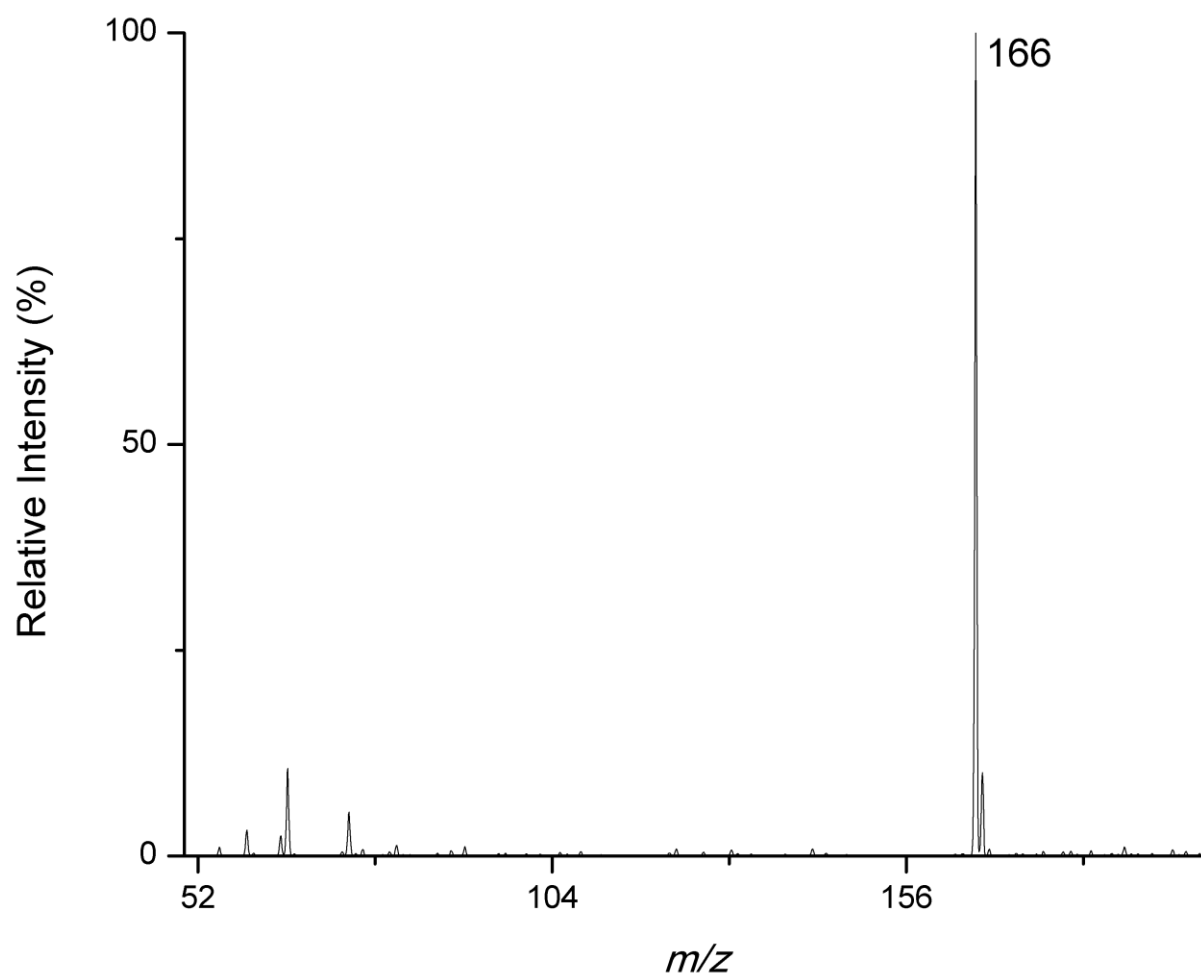


Figure S1: Electrospray ionization mass spectrometry (ESI-MS) of **9**

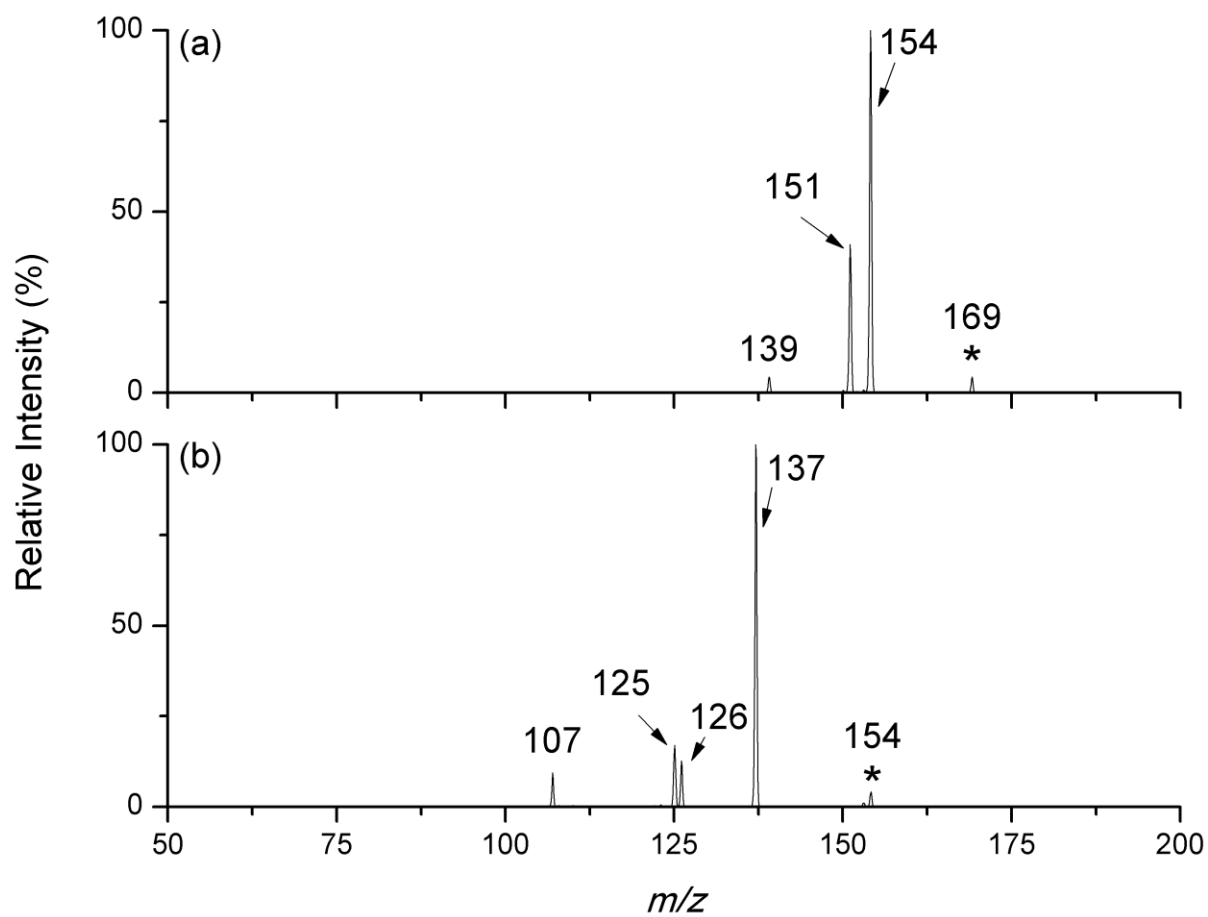


Figure S2: CID mass spectra of: (a) **17**; (b) **18**.

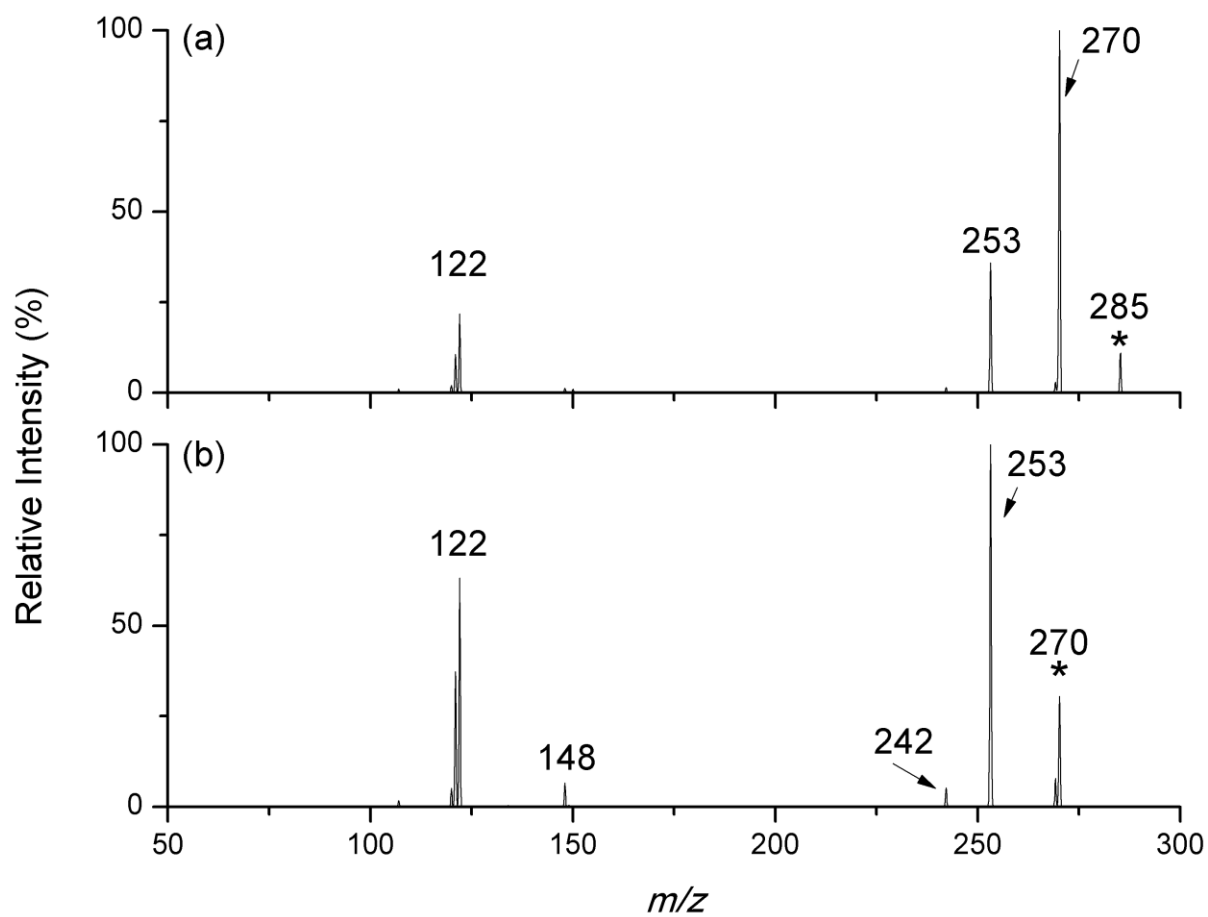


Figure S3: CID mass spectra of: (a) **24**; (b) **30**.

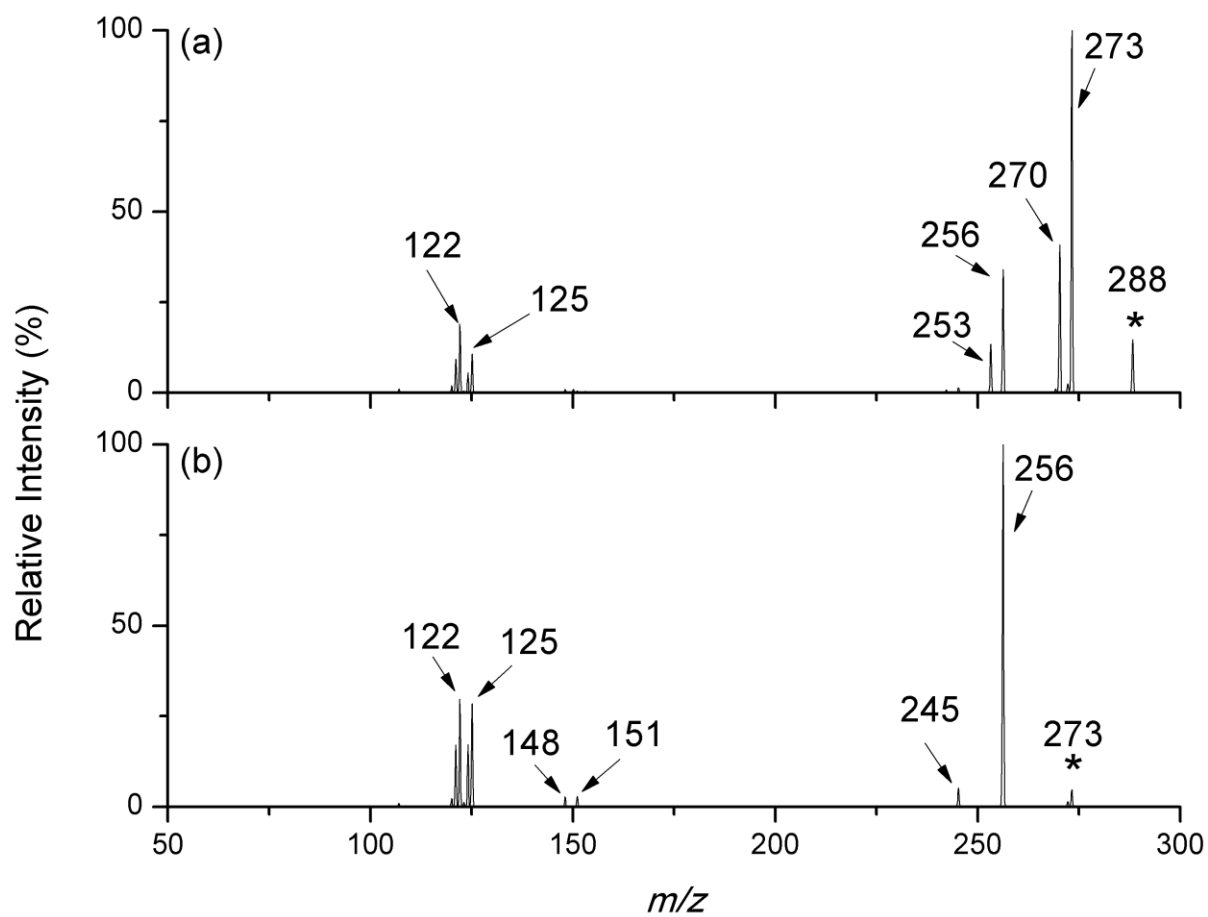


Figure S4: CID mass spectra of: (a) **25**; (b) **31**.

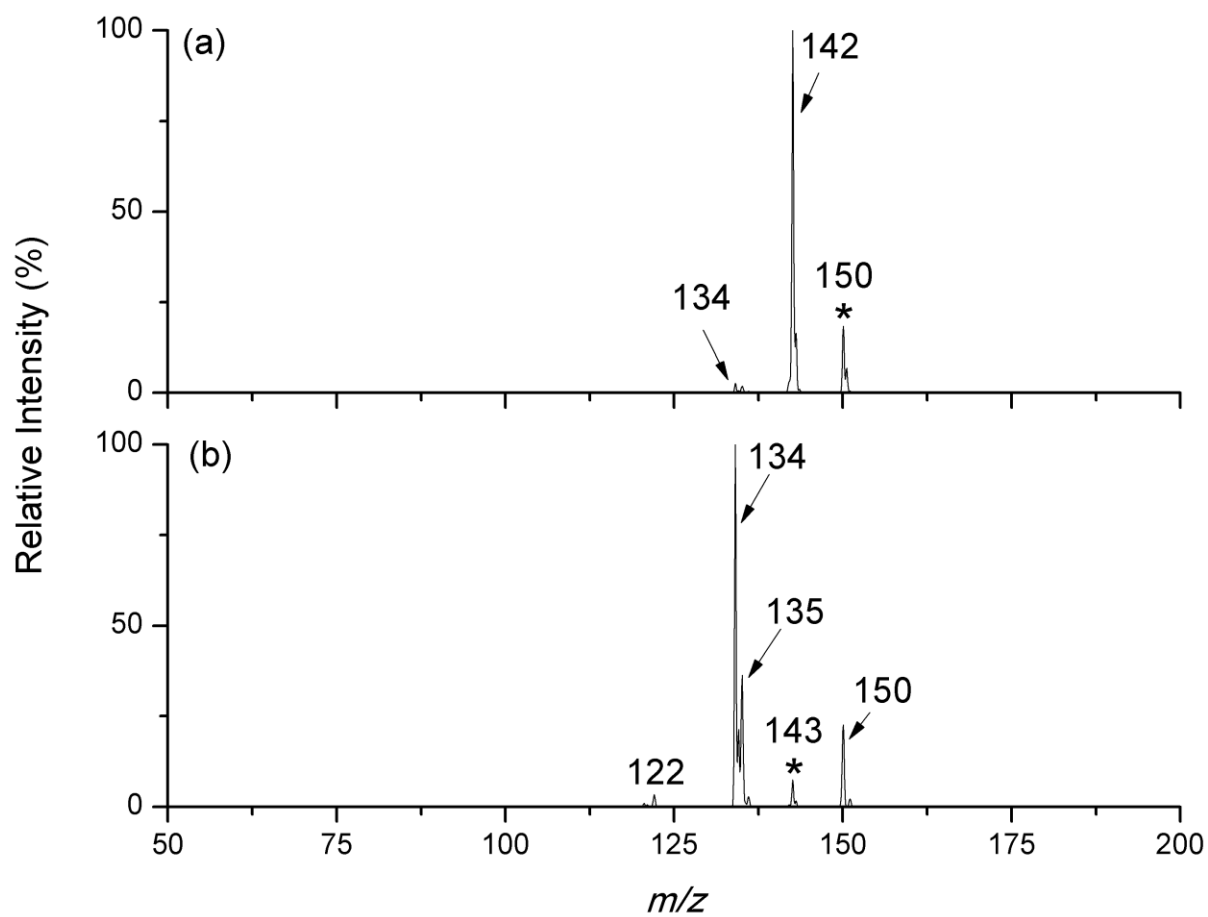


Figure S5: CID mass spectra of: (a) **34**; (b) **37**.

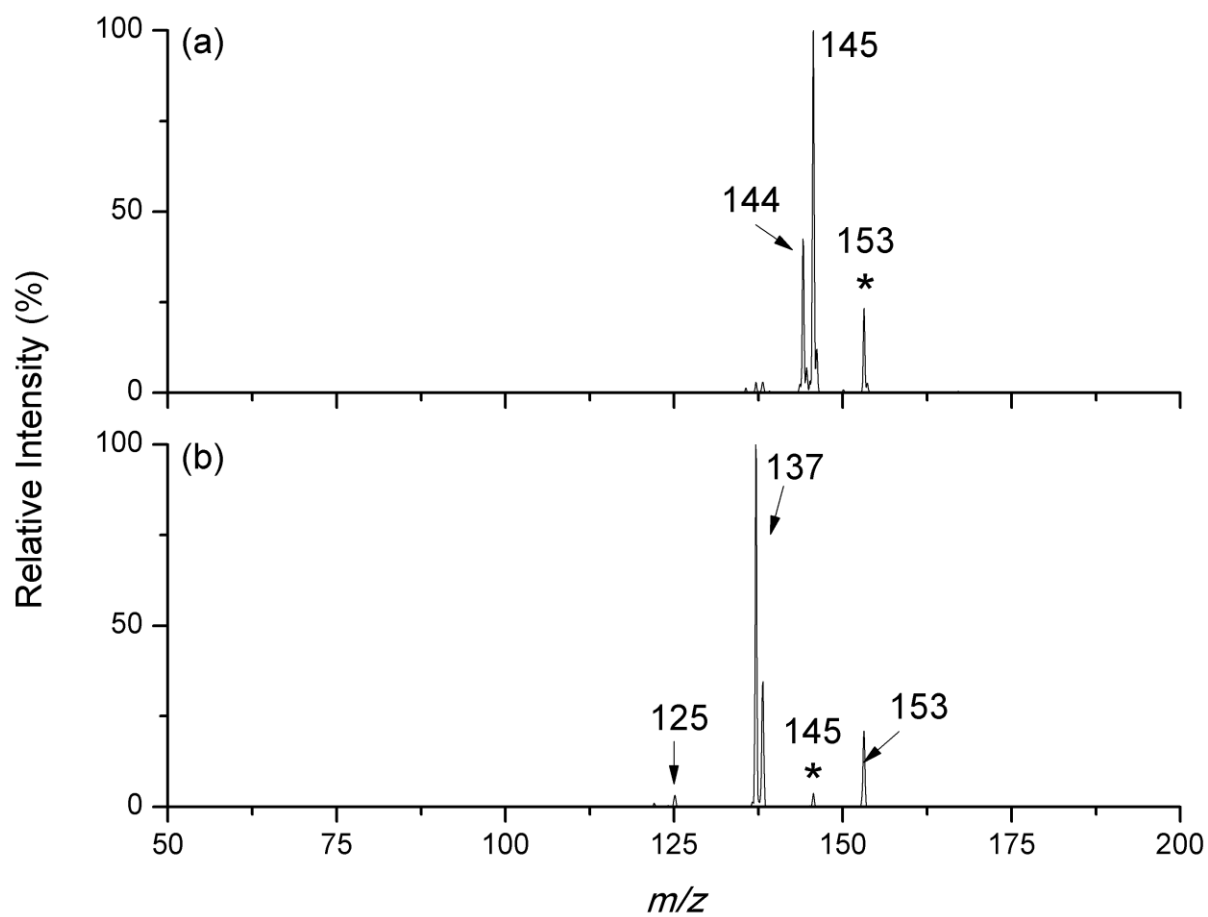


Figure S6: CID mass spectra of: (a) 35; (b) 38.

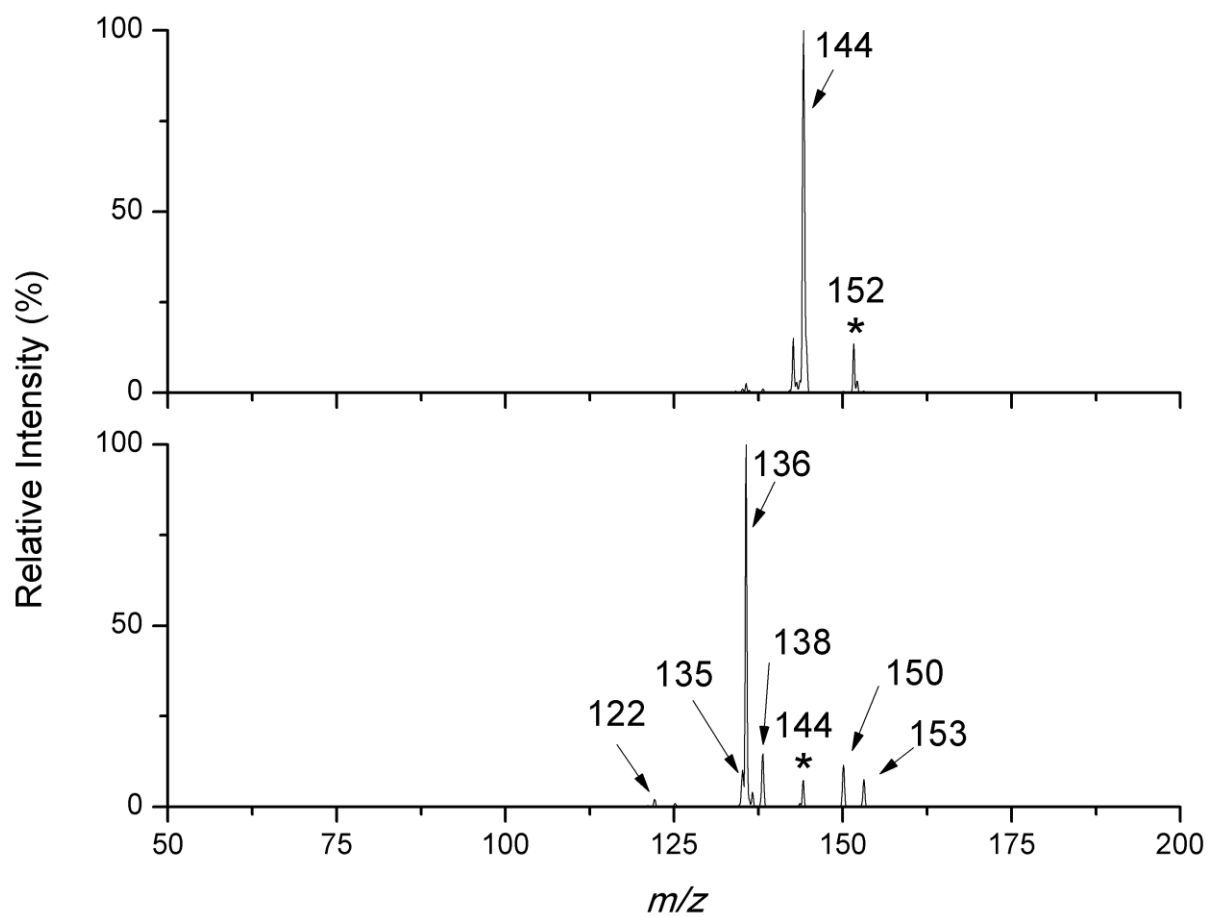


Figure S7: CID mass spectra of: (a) **36**; (b) **39**.

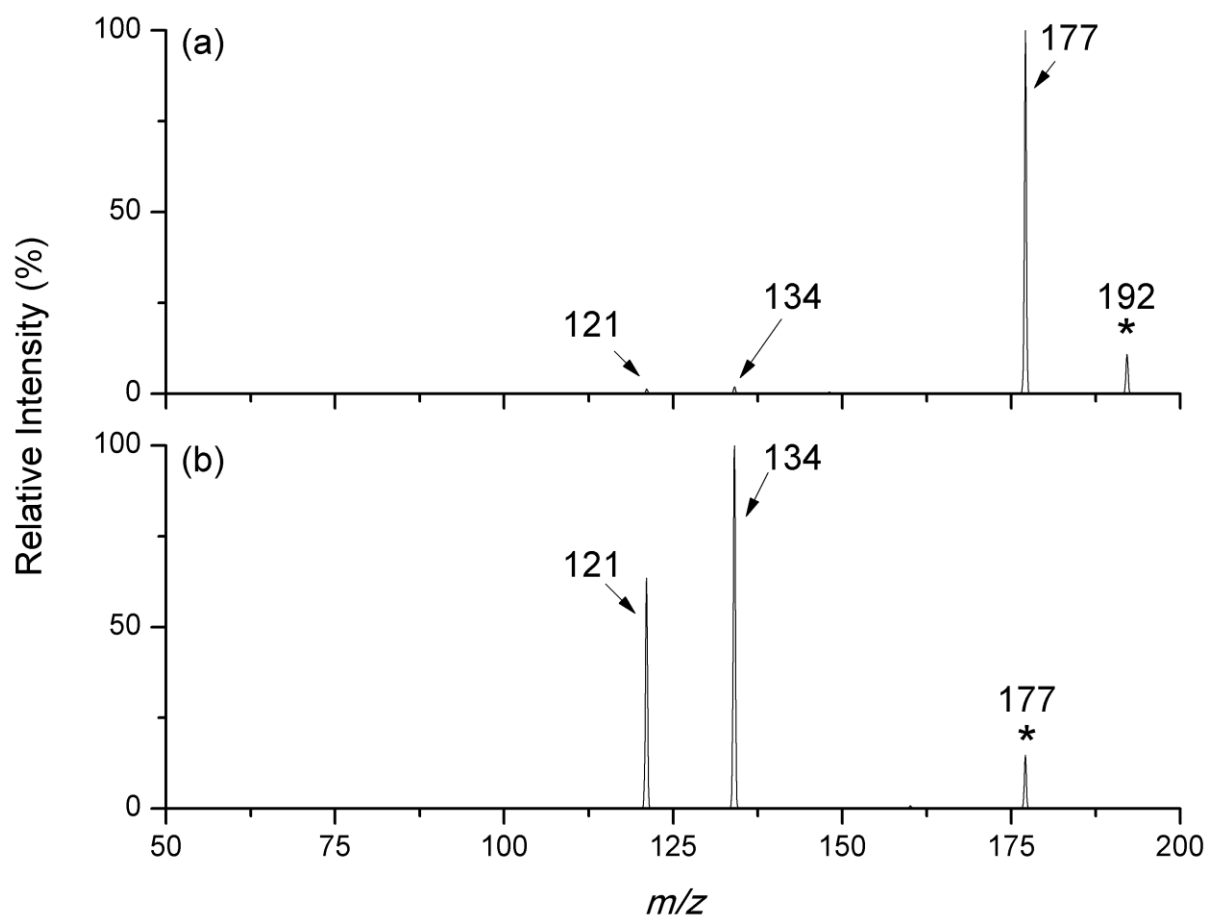


Figure S8: CID mass spectra of: (a) **43**; (b) **44**.

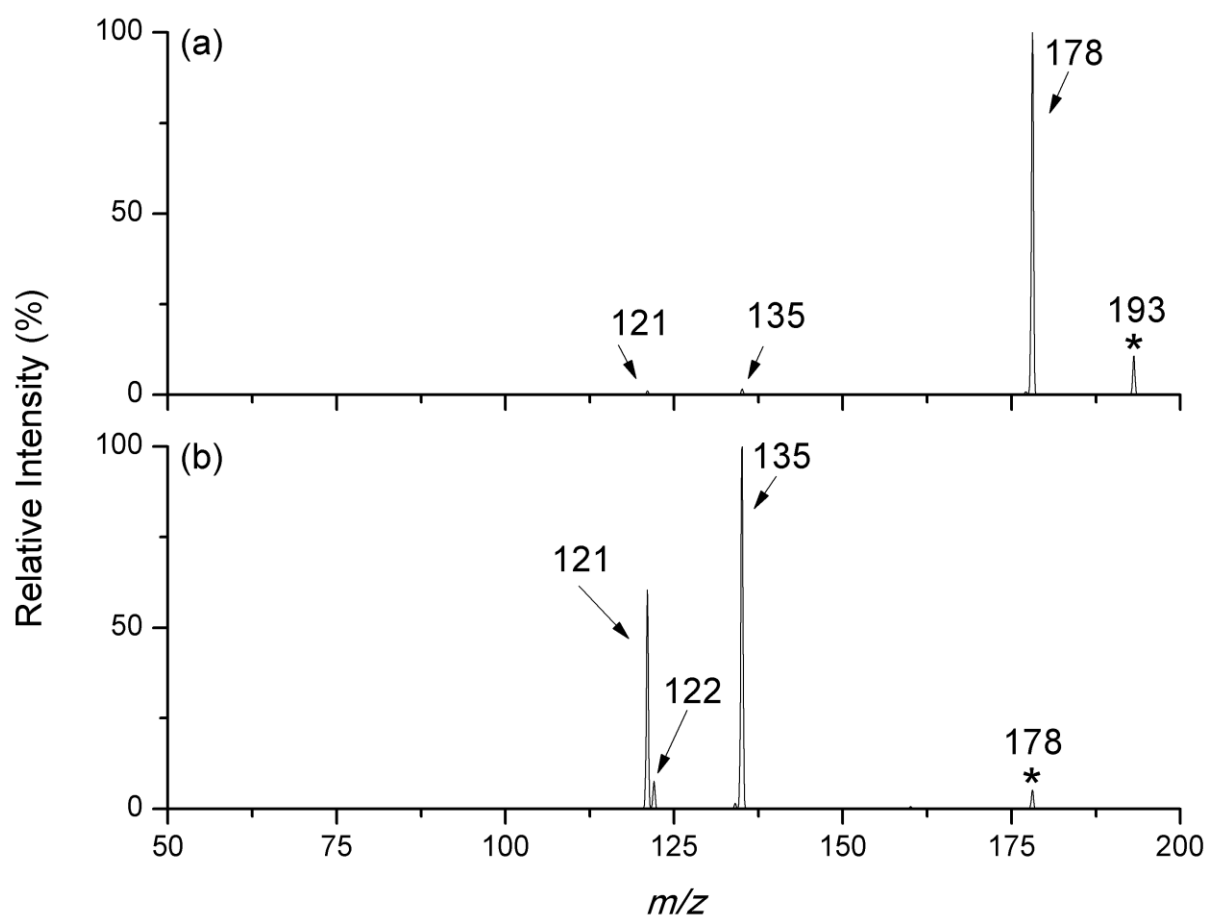


Figure S9: CID mass spectra of: (a) **46**; (b) **44(D)**.

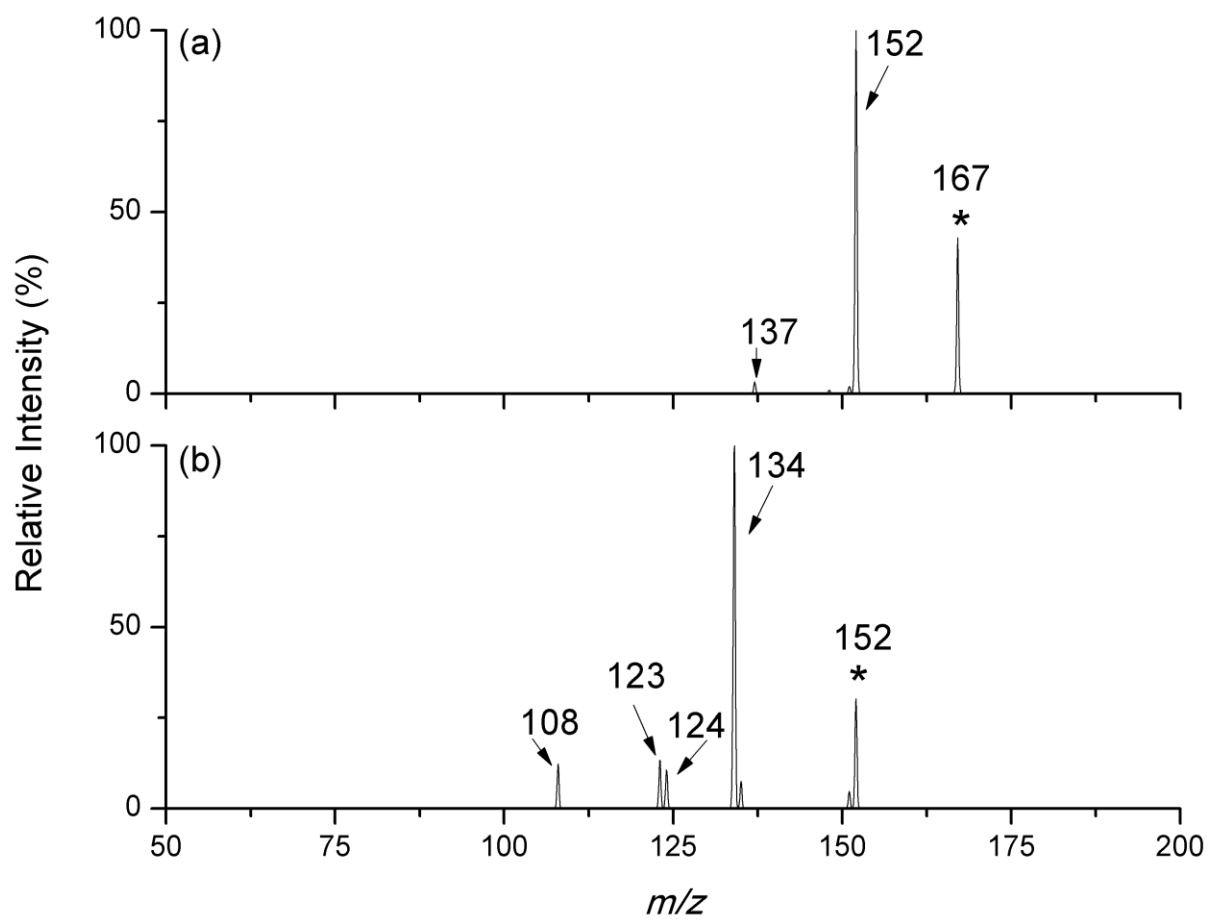


Figure S10: CID mass spectra of: (a) 47; (b) 48.

CBS-QB3 Calculations

Cartesian coordinates from CBS-QB3 calculations are listed below, together with the following energies (in Hartrees):

- CBS-QB3 total electronic energy at 0 K including zero-point energy (E)
- CBS-QB3 enthalpy at 298.15 K (H)
- CBS-QB3 Gibbs free energy at 298.15 K and 1 atm (G)

PhNMe₃⁺

N	0.491322	1.323367	0.000000
C	1.997117	1.415584	0.000000
C	-0.009125	-0.106442	-0.000000
C	-0.009125	2.039098	1.238716
C	-0.009125	2.039098	-1.238716
H	2.264572	2.470131	0.000000
H	2.389300	0.938377	0.894614
H	2.389300	0.938377	-0.894614
H	-1.094886	2.048206	1.237207
H	0.354338	1.504961	2.114056
H	0.371974	3.059207	1.227325
H	-1.094886	2.048206	-1.237207
H	0.371974	3.059207	-1.227325
H	0.354338	1.504961	-2.114056
C	-1.387775	-0.319322	-0.000000
C	-1.878751	-1.620478	-0.000000
C	-1.002284	-2.703534	-0.000000
C	0.368905	-2.478905	-0.000000
C	0.876457	-1.178709	-0.000000
H	-2.092940	0.501855	-0.000000
H	-2.949429	-1.782526	-0.000000
H	-1.388299	-3.715271	-0.000000
H	1.059914	-3.312678	-0.000000
H	1.947709	-1.044931	-0.000000

0 imaginary frequencies
E = -405.080253
H = -405.069642
G = -405.114521

Me•

C	0.000000	0.000000	0.000000
H	0.000000	0.935780	-0.540270
H	-0.000000	-0.935780	-0.540270
H	-0.000000	-0.000000	1.080540

0 imaginary frequencies
E = -39.744798
H = -39.740782
G = -39.763940

PhNMe₂⁺

N	-0.000000	-0.000000	1.526094
C	-0.000000	1.241401	2.312814
C	-0.000000	-0.000000	0.169219
C	-0.000000	-1.241401	2.312814

H	-0.460211	1.035186	3.277424
H	1.027250	1.581033	2.479439
H	-0.570908	2.018983	1.812183
H	0.570908	-2.018983	1.812183
H	0.460211	-1.035186	3.277424
H	-1.027250	-1.581033	2.479439
C	-0.206378	-1.213115	-0.561781
C	-0.210684	-1.198799	-1.937475
C	0.000000	0.000000	-2.638672
C	0.210684	1.198799	-1.937475
C	0.206378	1.213115	-0.561781
H	-0.394895	-2.140633	-0.041088
H	-0.384162	-2.118843	-2.481351
H	0.000000	0.000000	-3.721838
H	0.384162	2.118843	-2.481351
H	0.394895	2.140633	-0.041088

0 imaginary frequencies
E = -365.236186
H = -365.226273
G = -365.270285

Ph•

C	0.000000	0.000000	1.395883
C	0.000000	1.223888	0.770634
C	-0.000000	1.211888	-0.631401
C	-0.000000	0.000000	-1.321962
C	-0.000000	-1.211888	-0.631401
C	-0.000000	-1.223888	0.770634
H	0.000000	2.157687	1.321777
H	-0.000000	2.150450	-1.175978
H	-0.000000	0.000000	-2.405930
H	-0.000000	-2.150450	-1.175978
H	-0.000000	-2.157687	1.321777

0 imaginary frequencies
E = -231.108289
H = -231.102929
G = -231.135692

NMe₃⁺

C	1.242620	0.744470	0.000000
N	0.000000	-0.000000	0.000000
C	0.023420	-1.448380	0.000000
C	-1.266040	0.703910	0.000000
H	-1.315250	1.350820	0.884300
H	-1.315250	1.350820	-0.884300
H	-2.094600	-0.000180	0.000000
H	1.827470	0.463630	0.884300
H	1.827470	0.463630	-0.884300
H	1.047140	1.814070	0.000000
H	1.047460	-1.813880	0.000000
H	-0.512220	-1.814450	-0.884300
H	-0.512220	-1.814450	0.884300

0 imaginary frequencies
E = -173.817315
H = -173.809890
G = -173.847597

PhNMe₂CD₃⁺

N	-0.491323	-1.323367	0.000000
C	-1.997118	-1.415584	0.000000
C	0.009125	0.106442	-0.000000
C	0.009125	-2.039098	1.238716
C	0.009125	-2.039098	-1.238716
H(Iso=2)	-2.264572	-2.470130	0.000000
H(Iso=2)	-2.389300	-0.938376	0.894614
H(Iso=2)	-2.389300	-0.938376	-0.894614
H	1.094886	-2.048207	1.237207
H	-0.354339	-1.504961	2.114056
H	-0.371975	-3.059207	1.227325
H	1.094886	-2.048207	-1.237207
H	-0.371975	-3.059207	-1.227325
H	-0.354339	-1.504961	-2.114056
C	1.387775	0.319322	0.000000
C	1.878751	1.620477	-0.000000
C	1.002284	2.703534	-0.000000
C	-0.368904	2.478905	-0.000000
C	-0.876457	1.178709	-0.000000
H	2.092941	-0.501855	0.000000
H	2.949429	1.782525	-0.000000
H	1.388300	3.715270	-0.000000
H	-1.059914	3.312678	-0.000000
H	-1.947708	1.044932	-0.000000

0 imaginary frequencies

E = -405.090235

H = -405.079249

G = -405.124893

CD₃•

C	0.000000	0.000000	0.000000
H(Iso=2)	0.000000	0.935780	-0.540270
H(Iso=2)	-0.000000	-0.935780	-0.540270
H(Iso=2)	-0.000000	-0.000000	1.080540

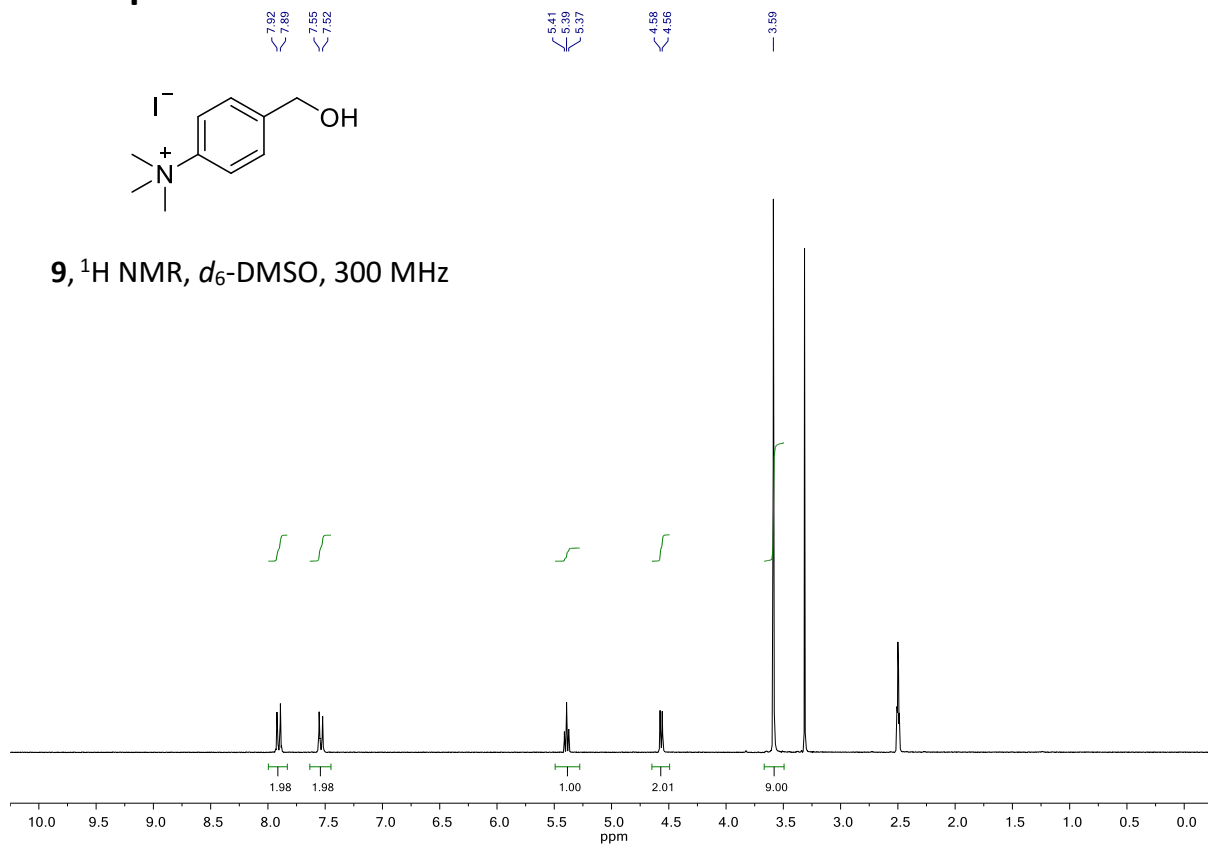
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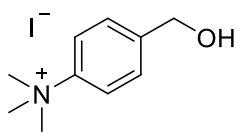
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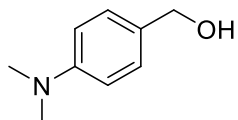
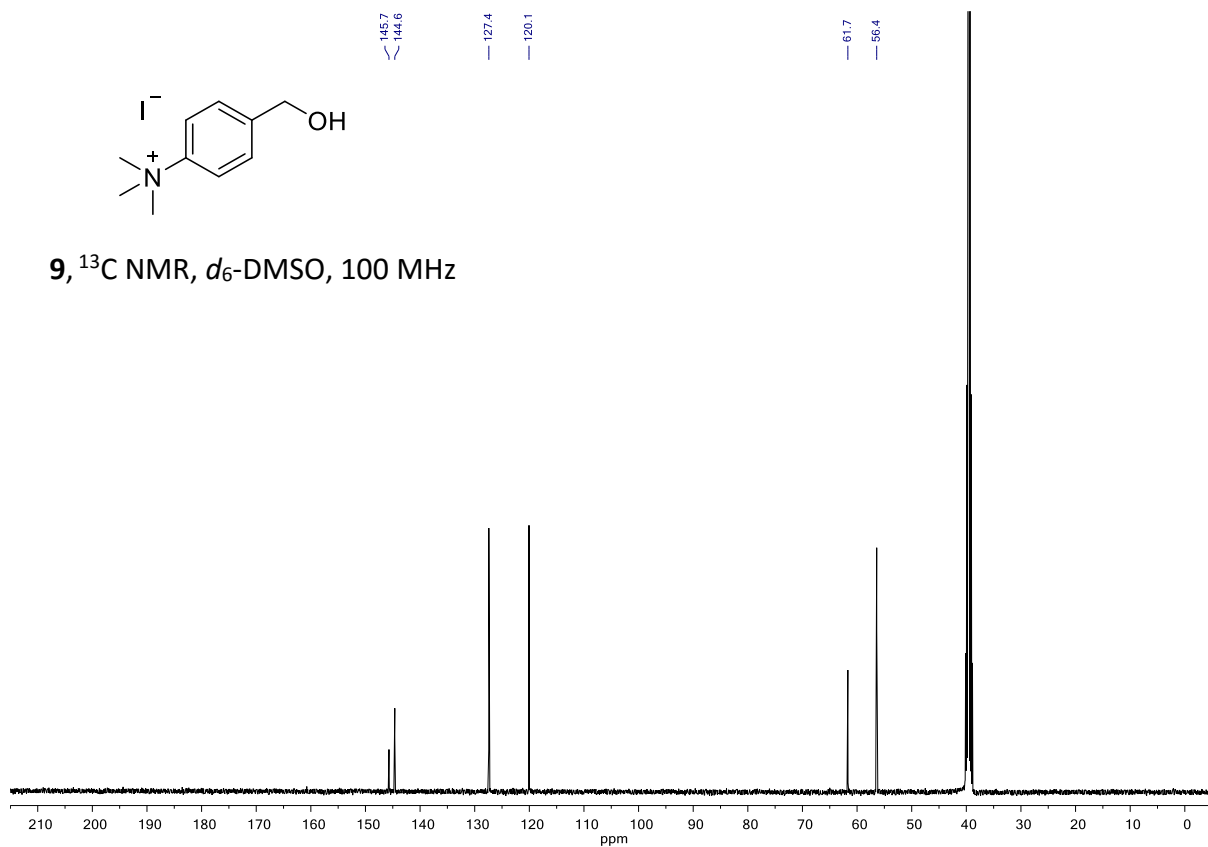
G = -39.773011

NMR Spectra

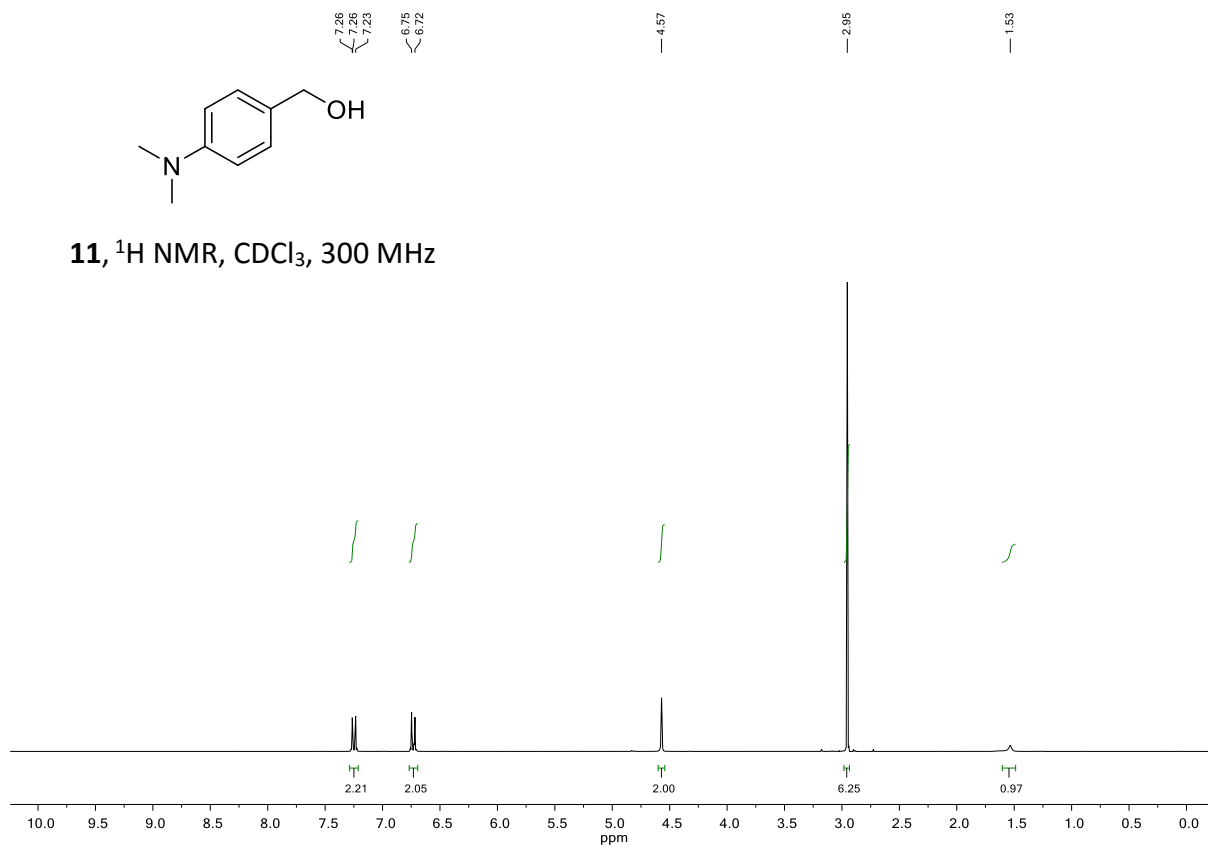


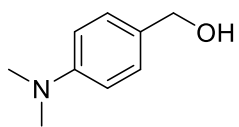


9, ^{13}C NMR, d_6 -DMSO, 100 MHz



11, ^1H NMR, CDCl_3 , 300 MHz





150.9

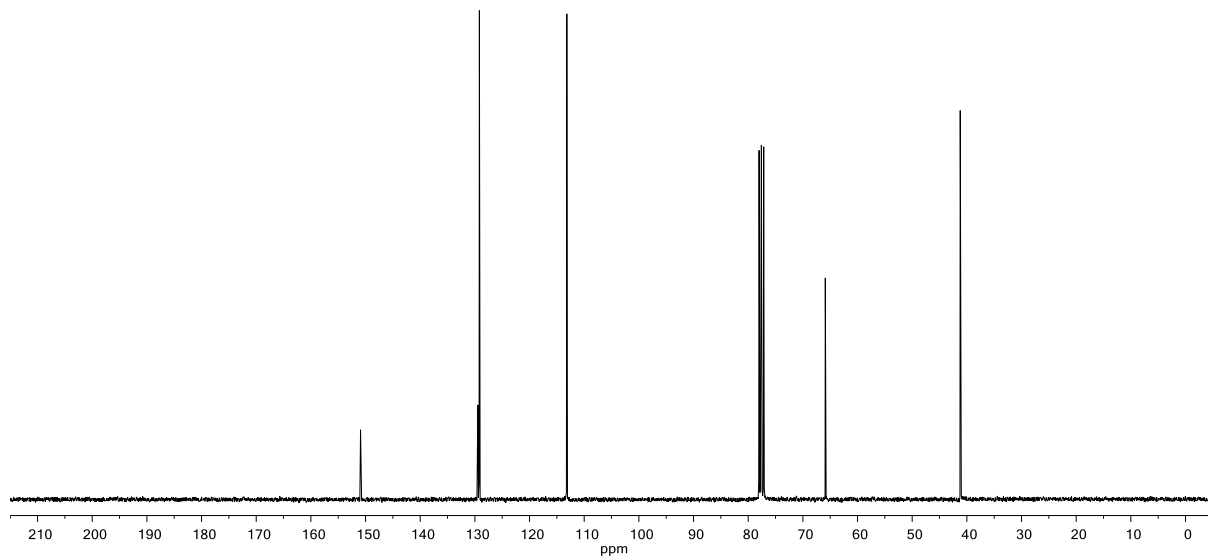
129.5
129.2

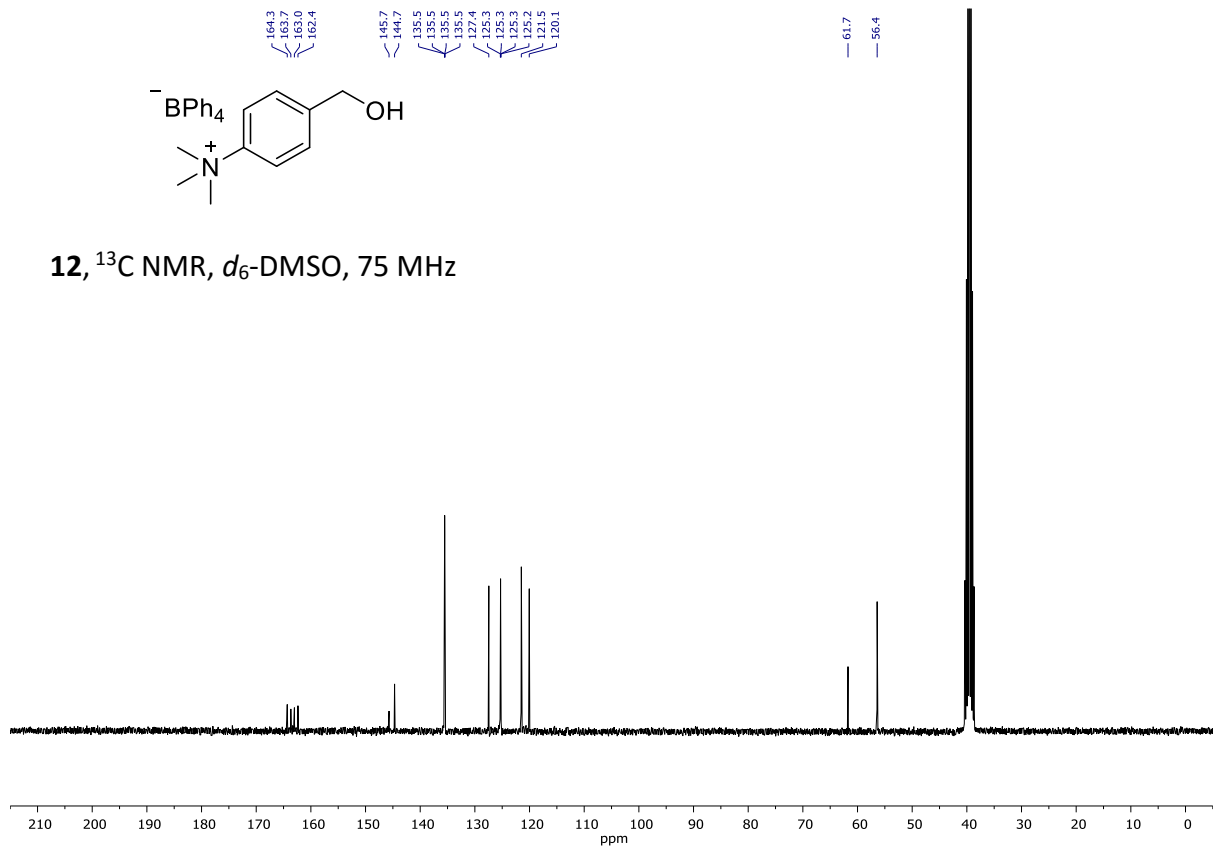
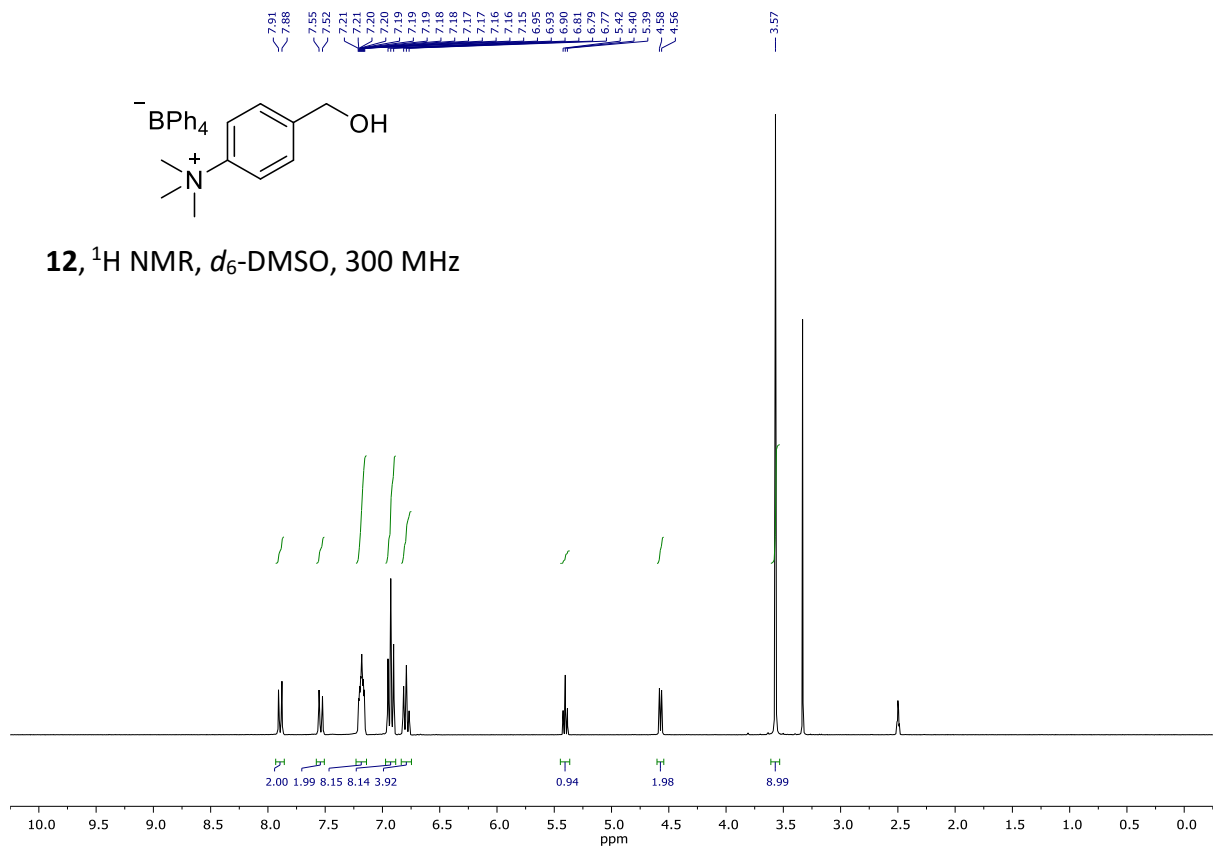
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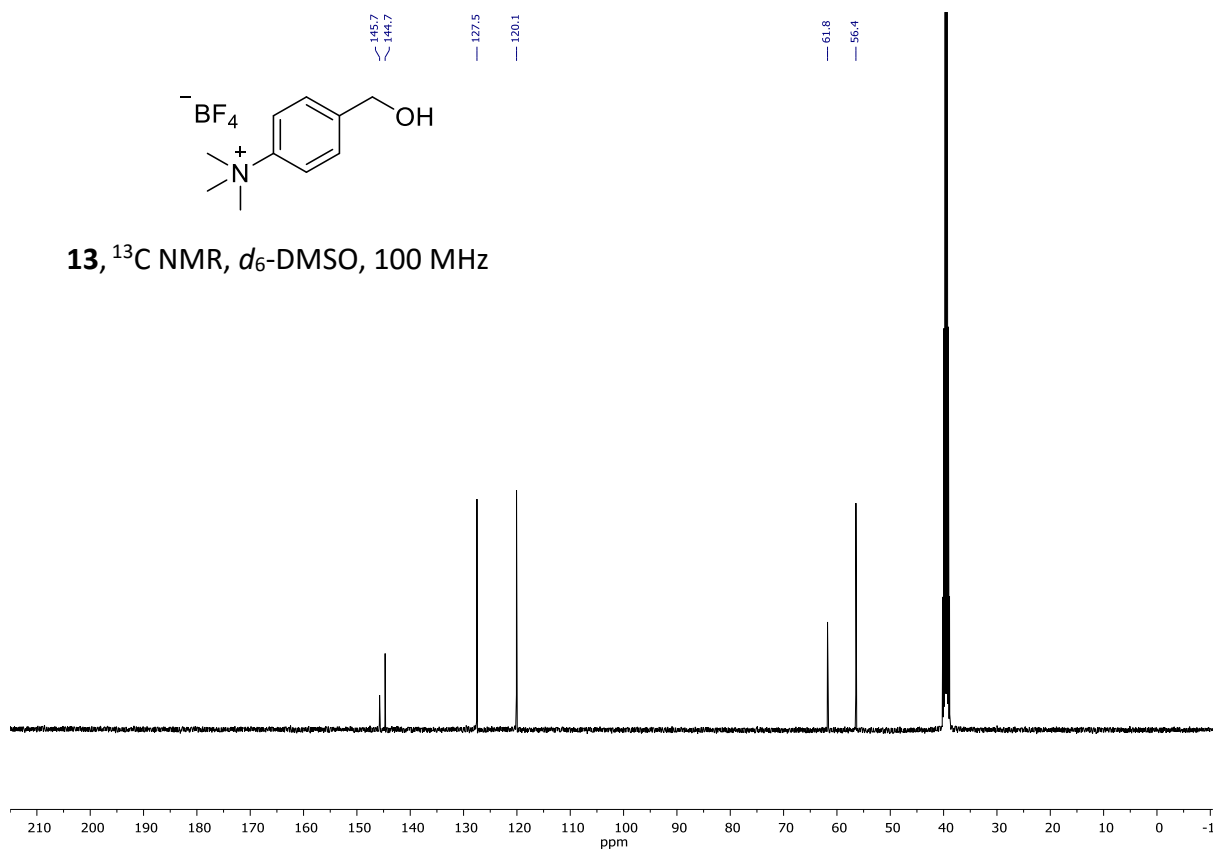
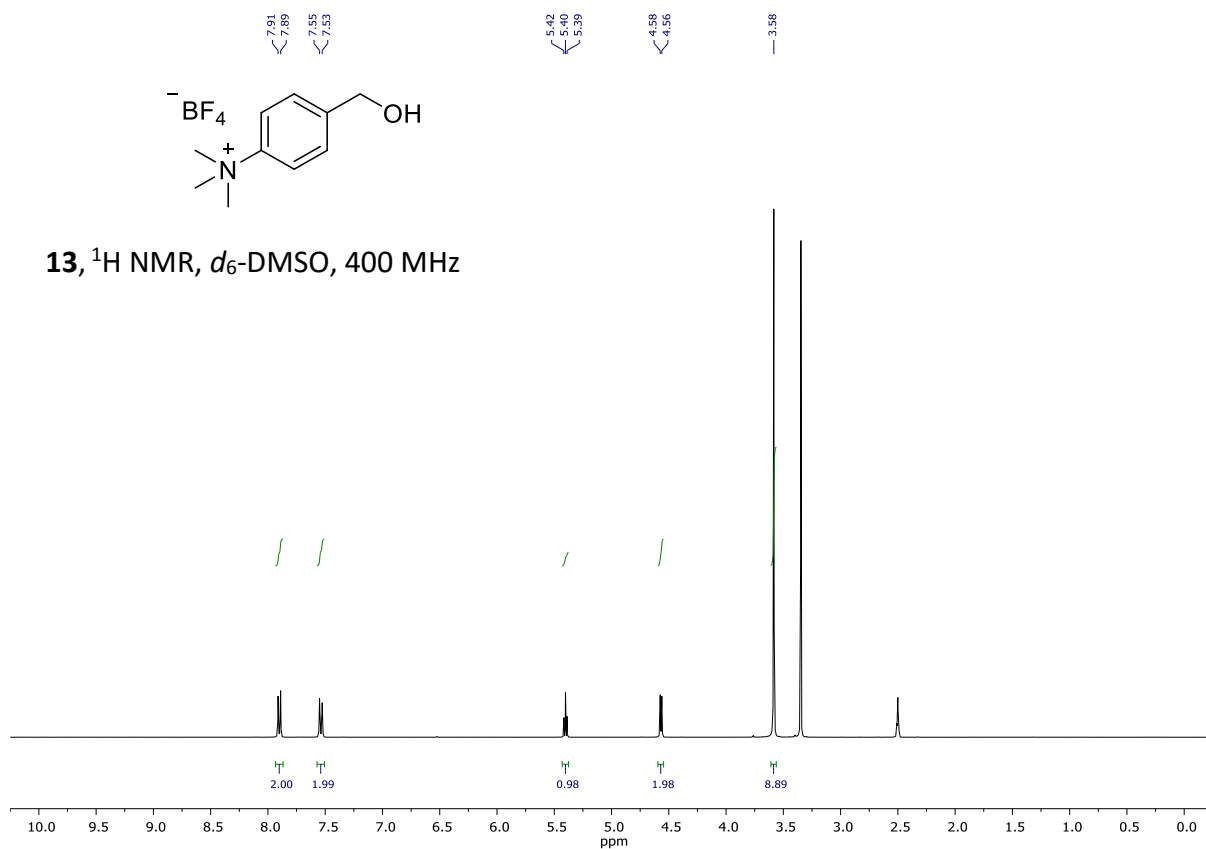
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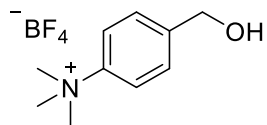
41.2

11, ^{13}C NMR, CDCl_3 , 100 MHz

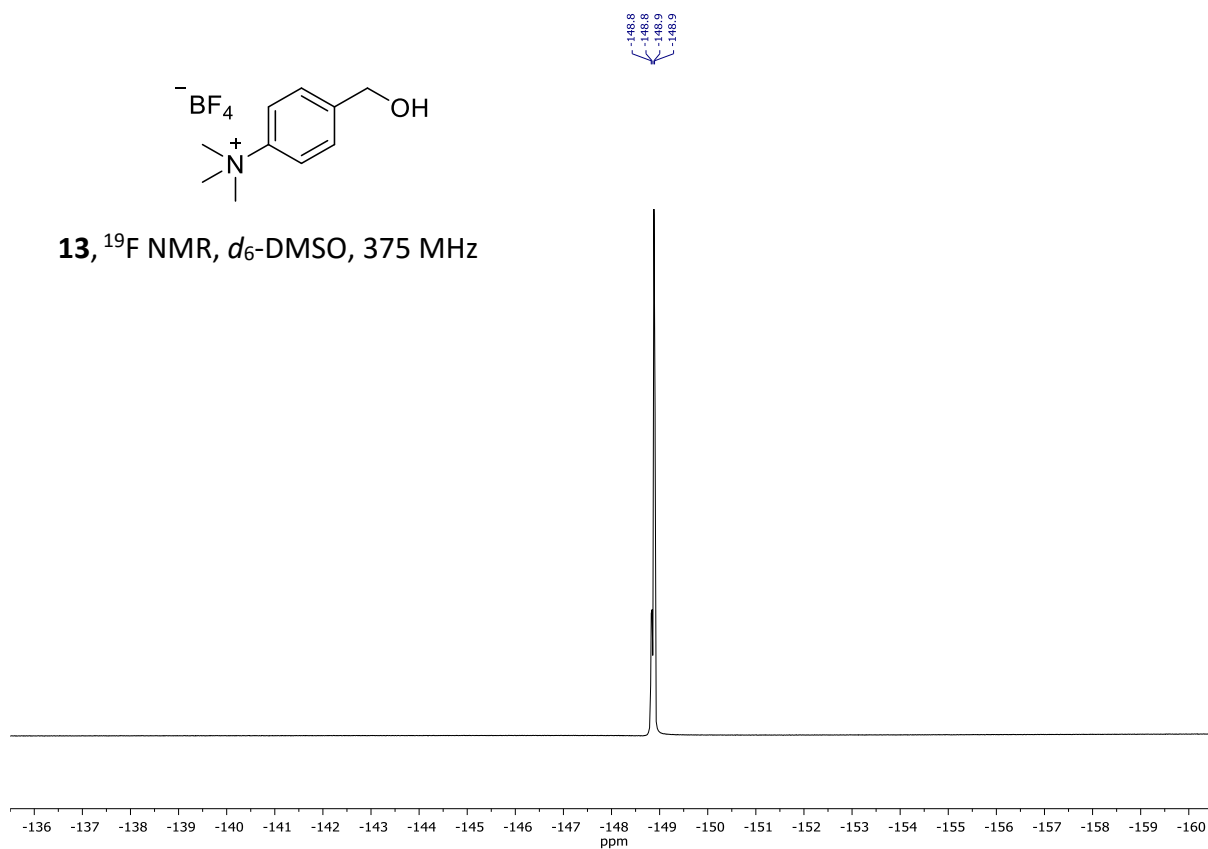


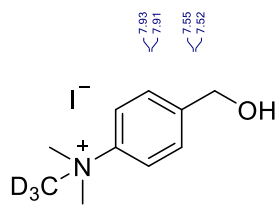




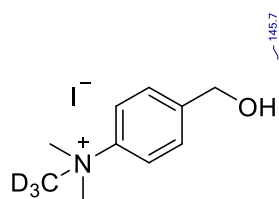
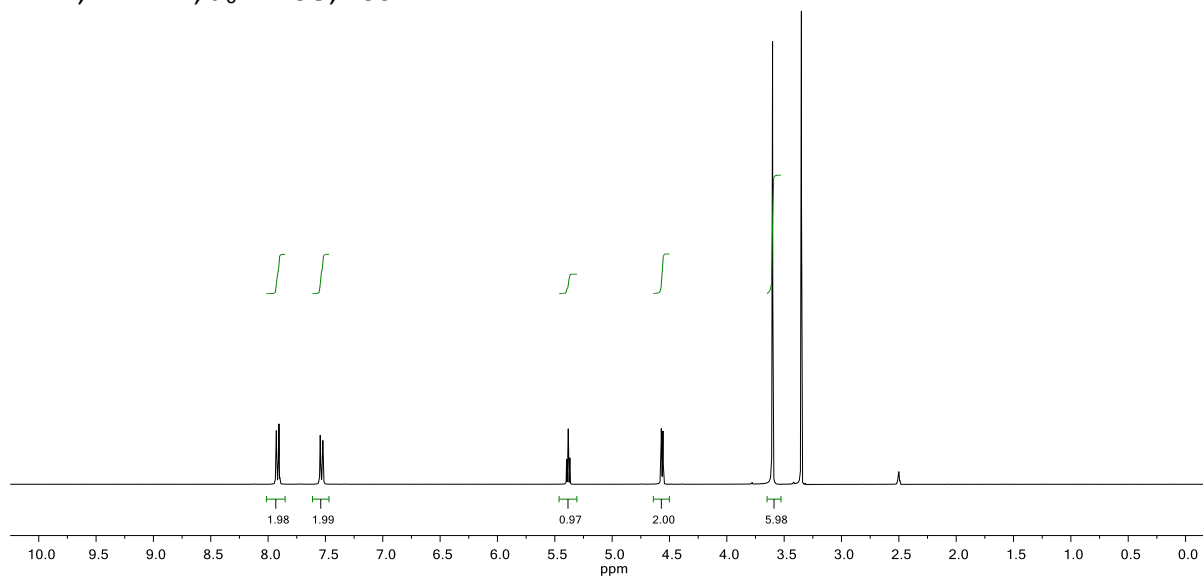


13, ¹⁹F NMR, *d*₆-DMSO, 375 MHz

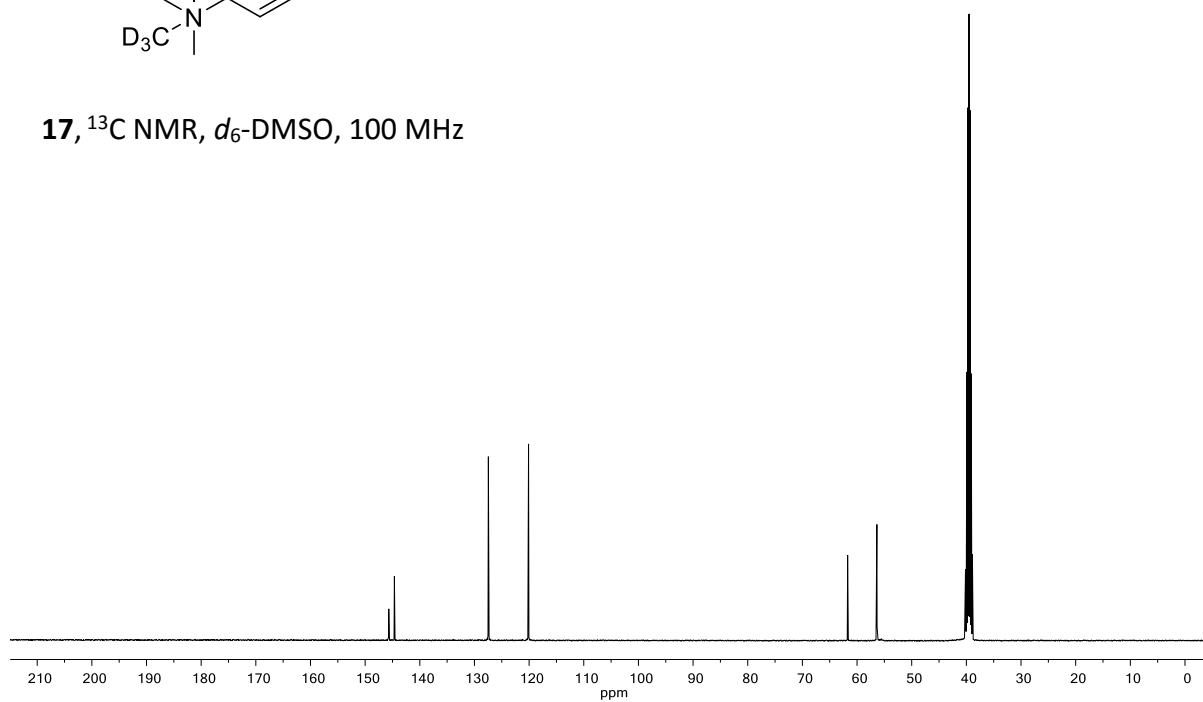


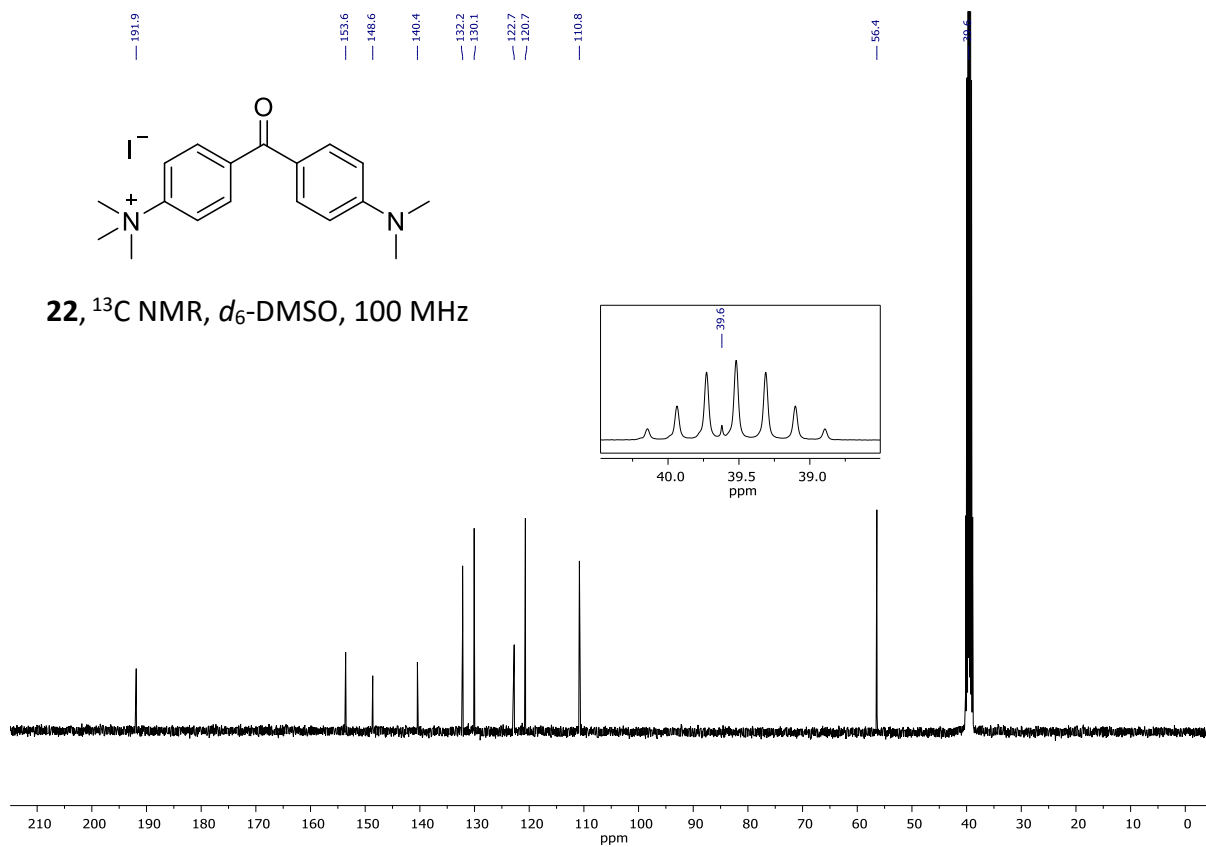
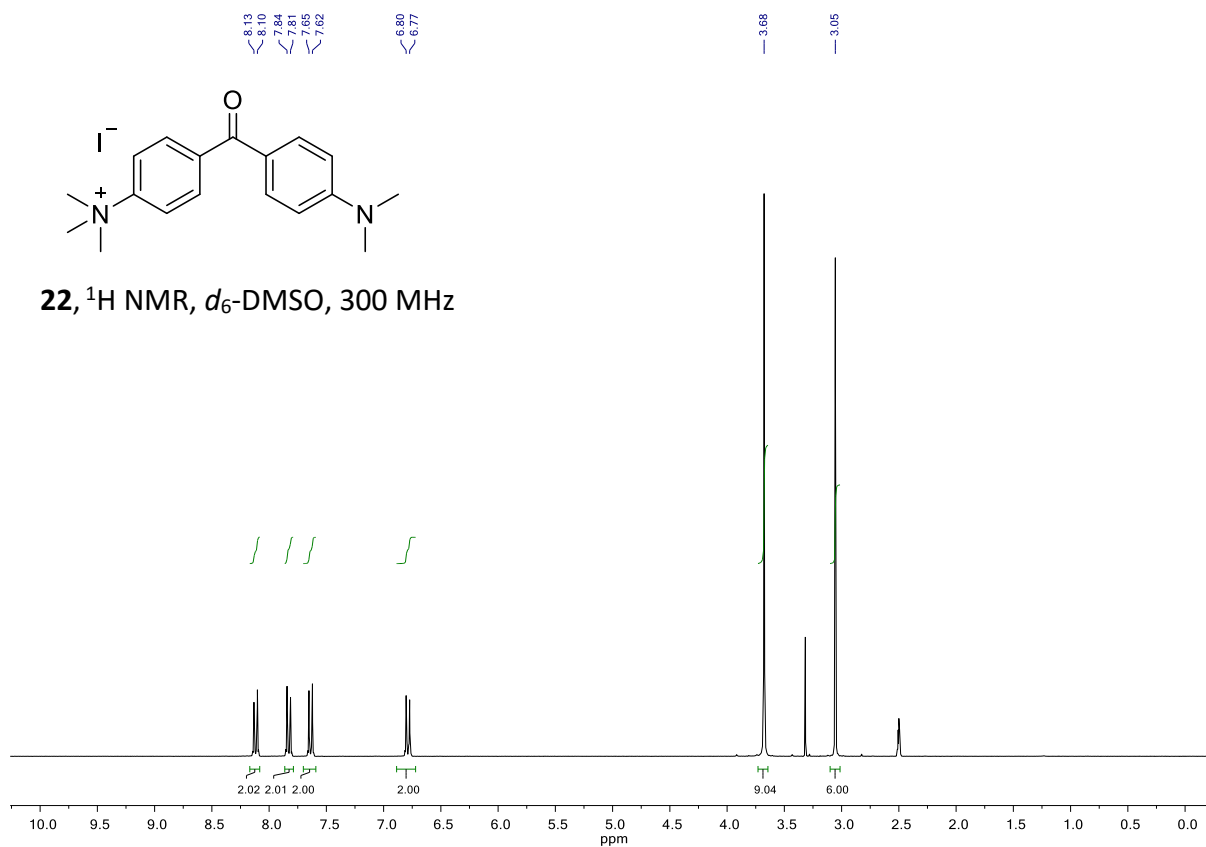


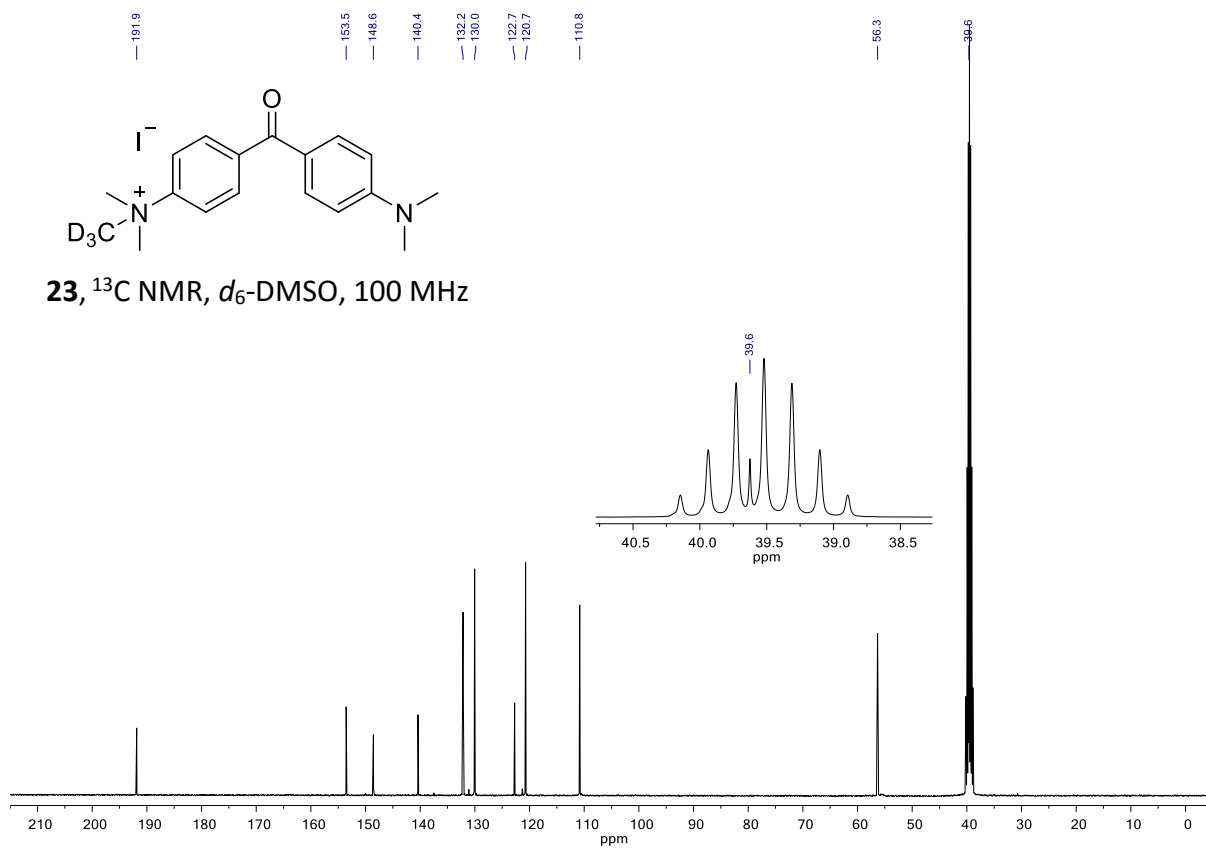
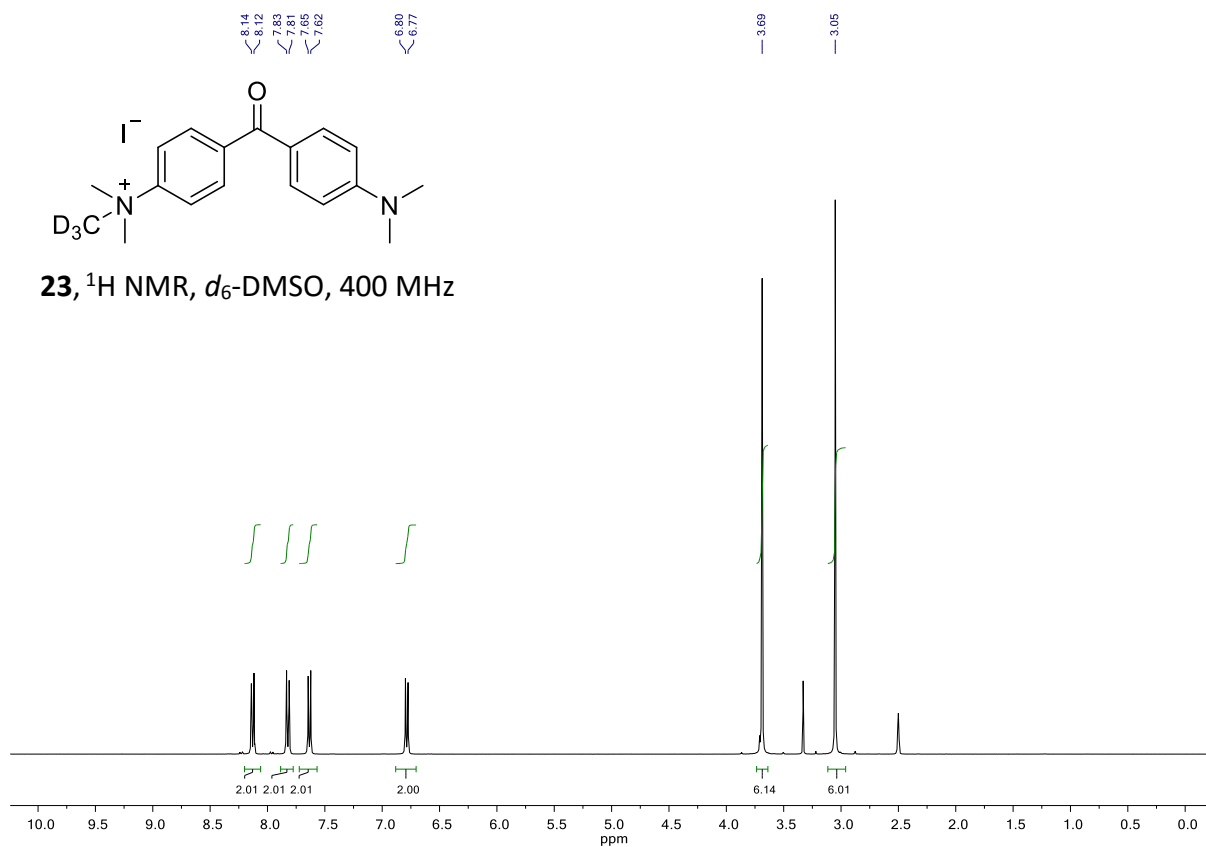
17, ^1H NMR, d_6 -DMSO, 400 MHz

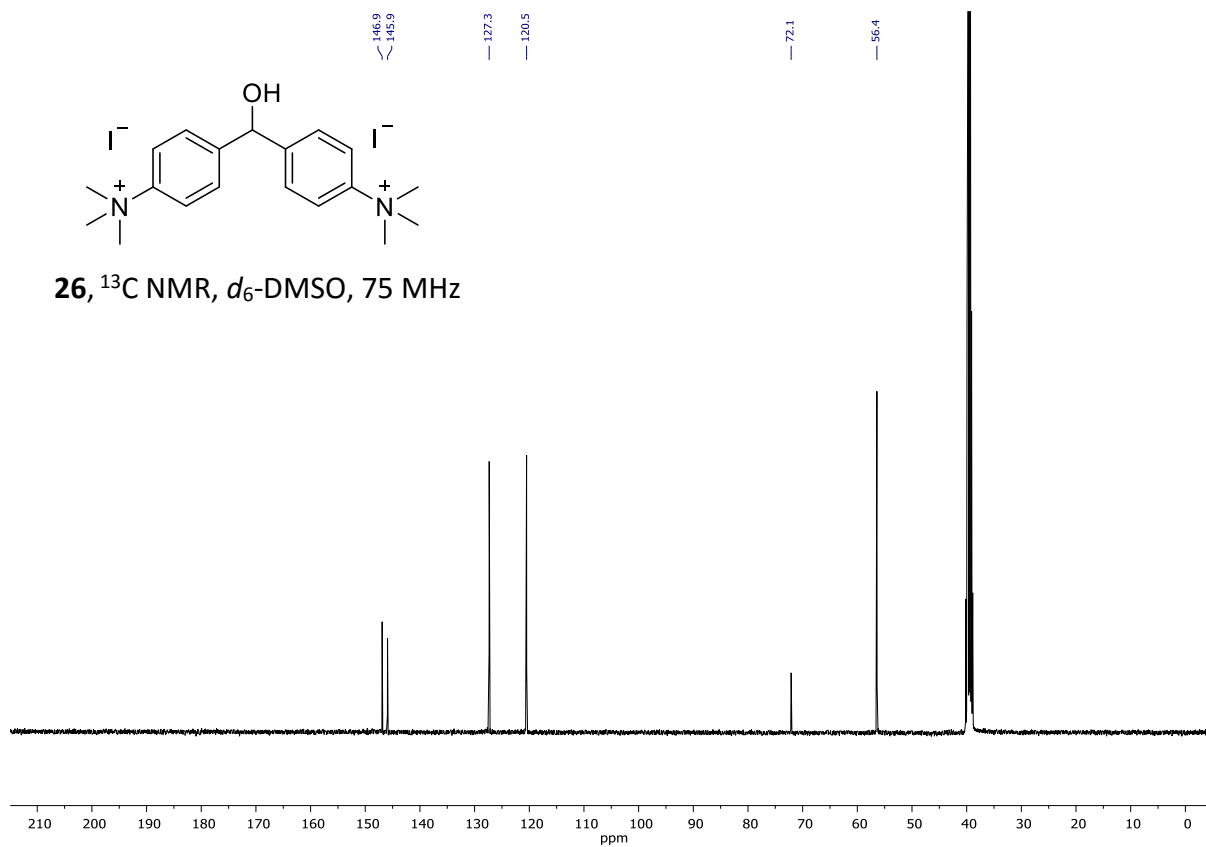
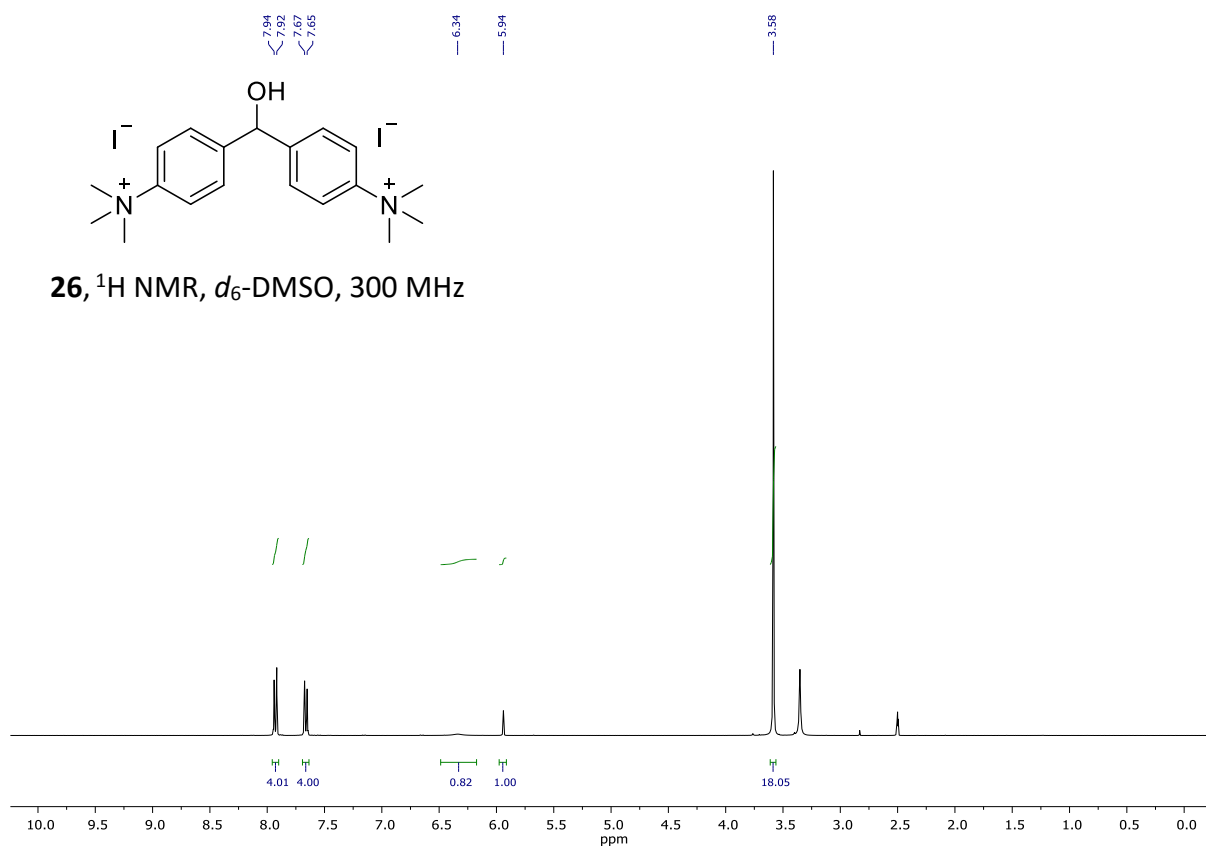


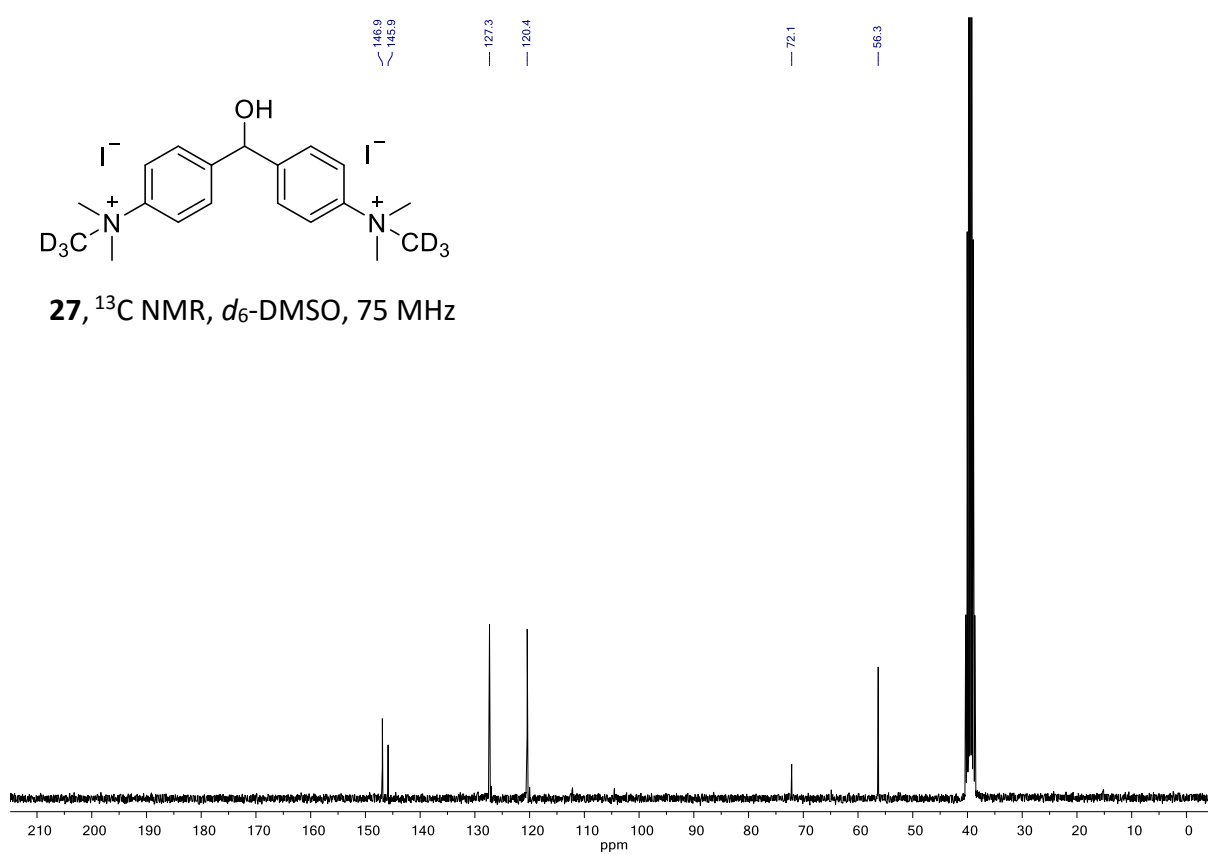
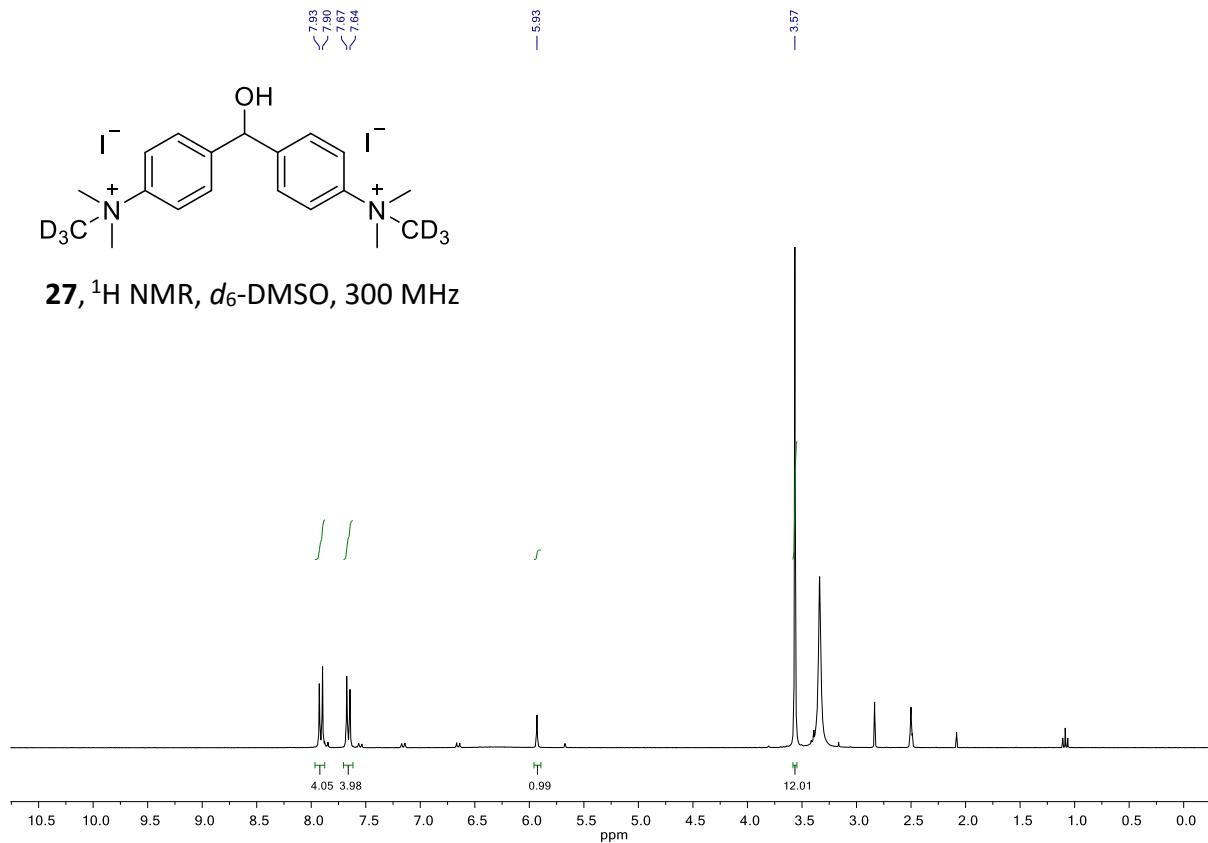
17, ^{13}C NMR, d_6 -DMSO, 100 MHz

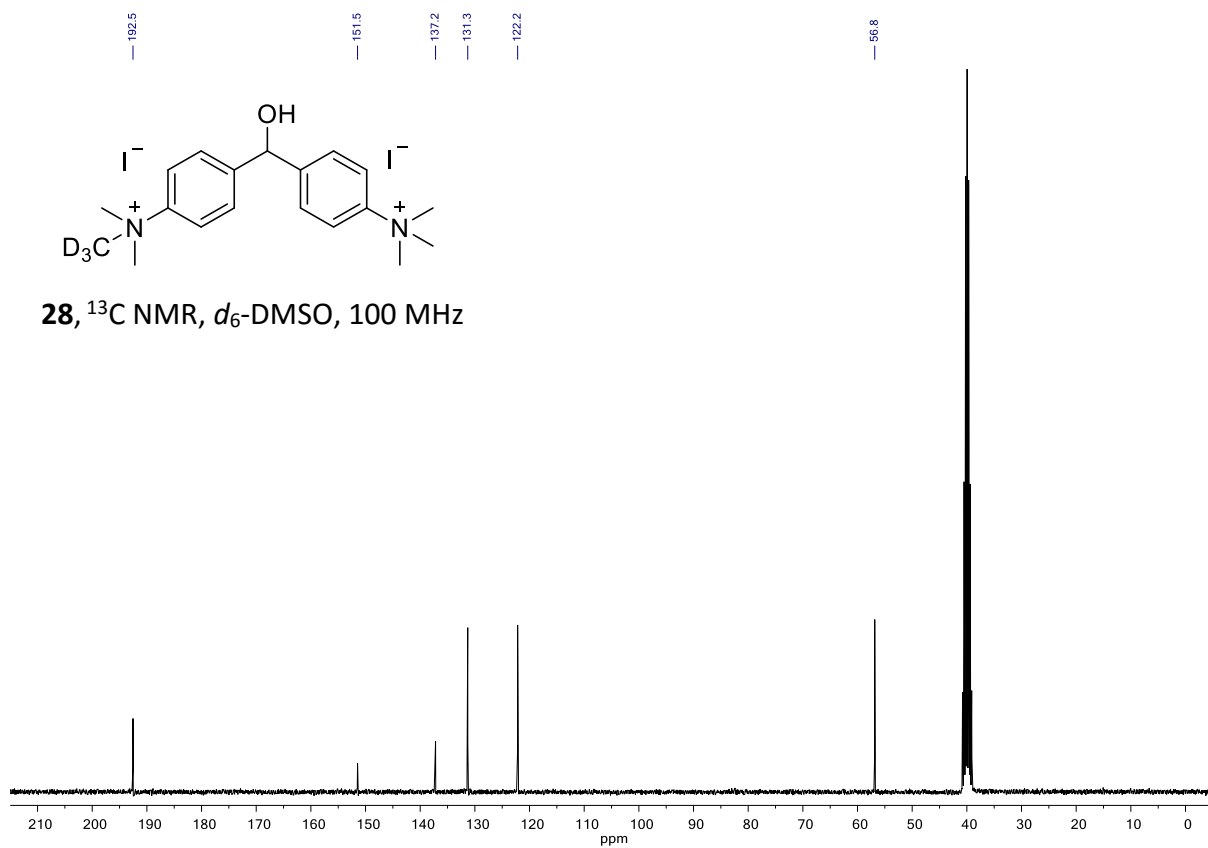
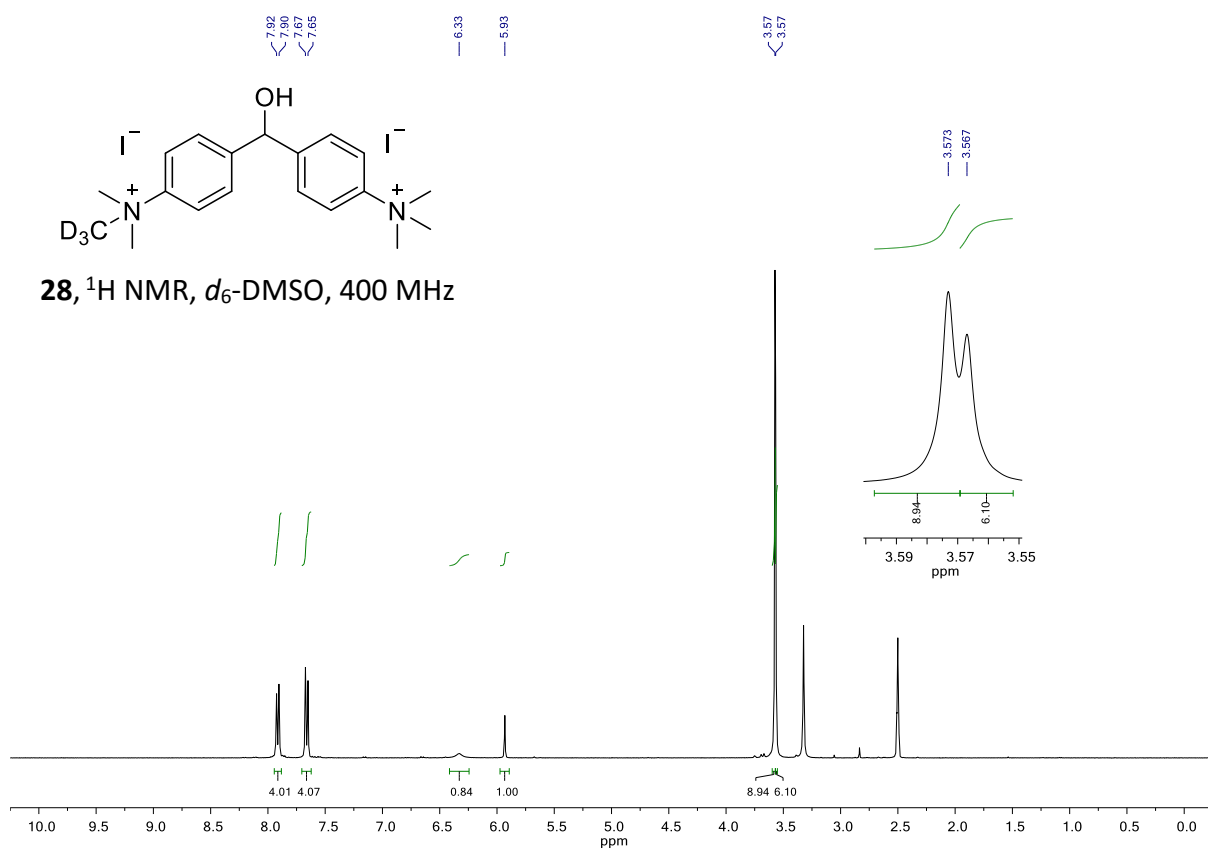


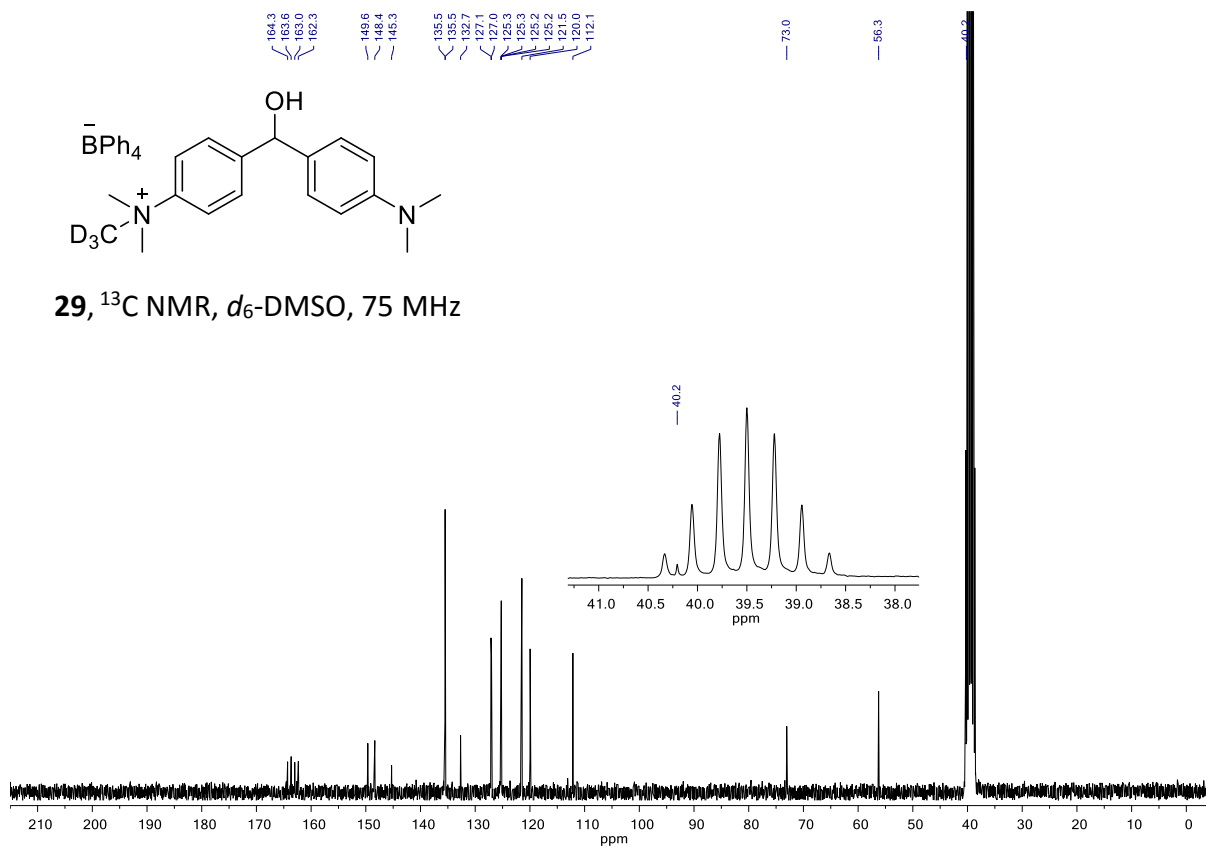
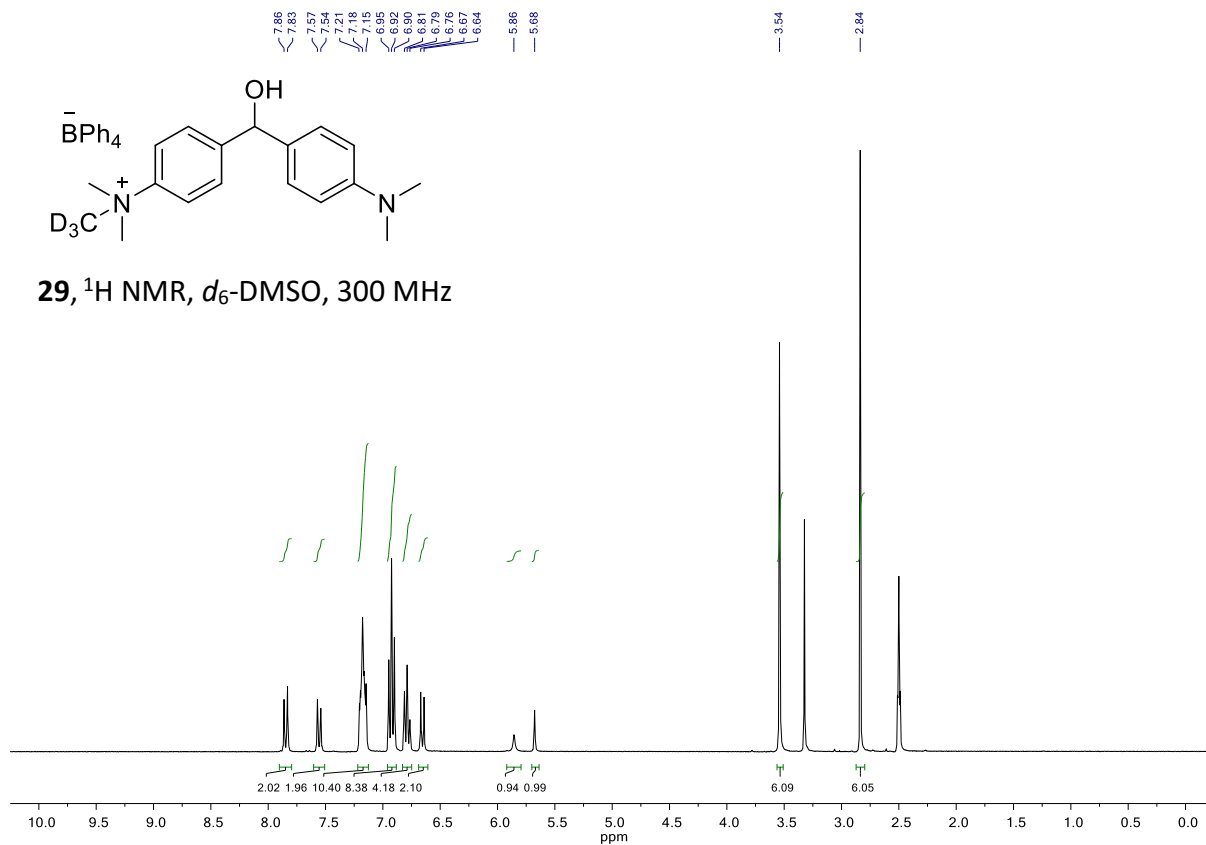


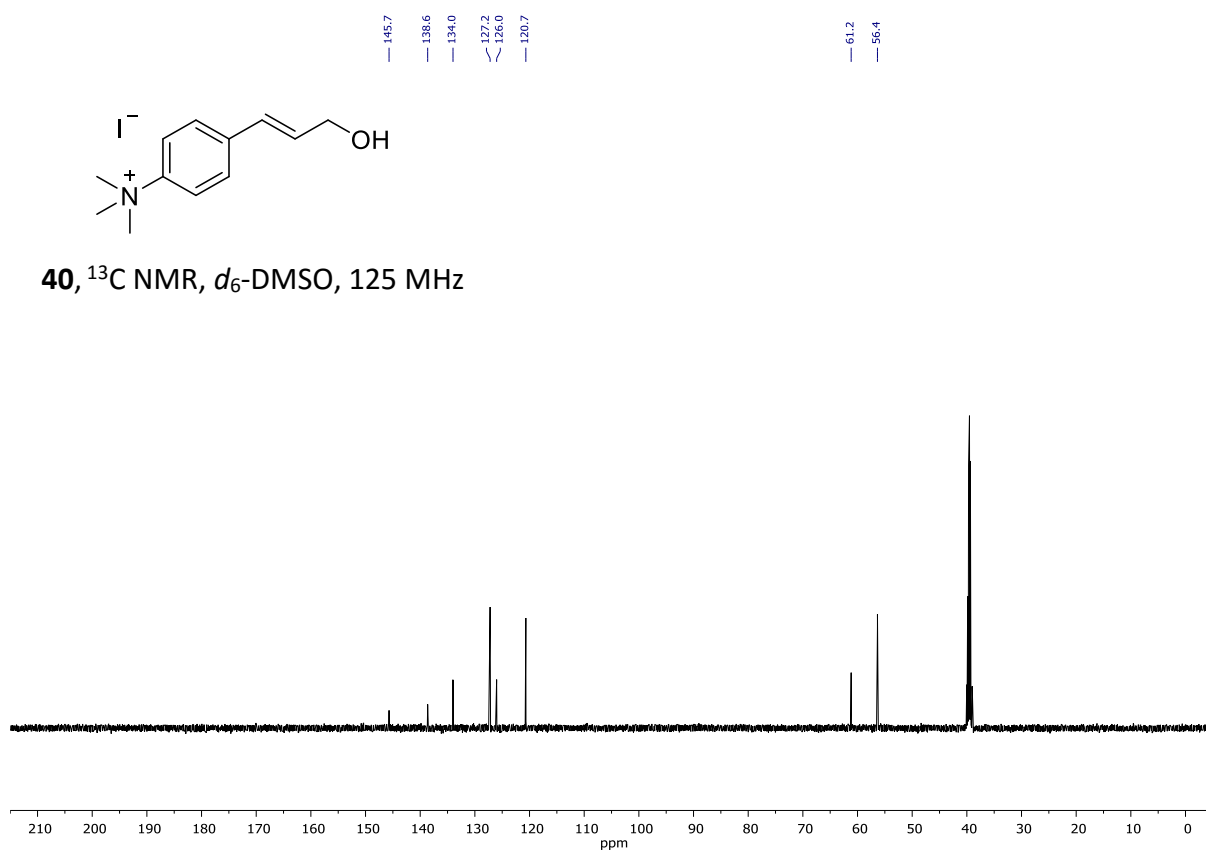
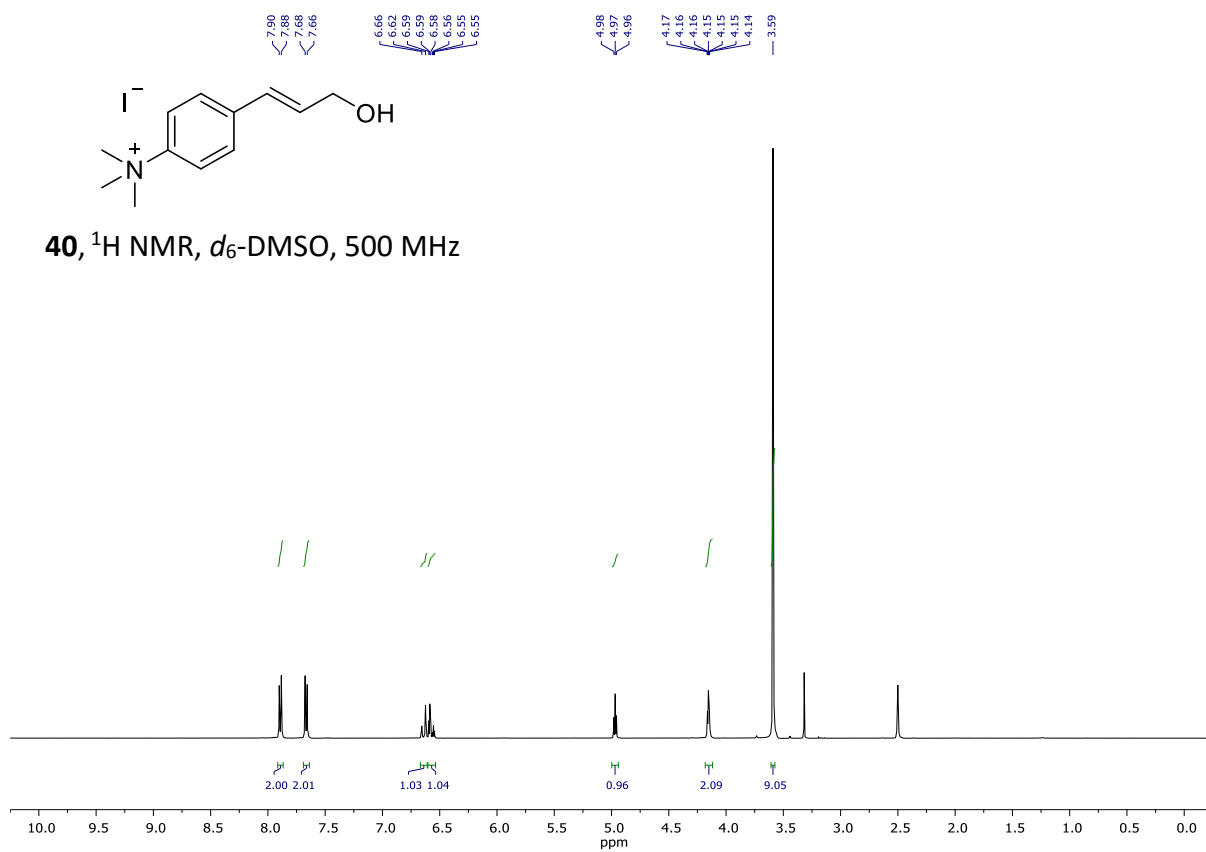












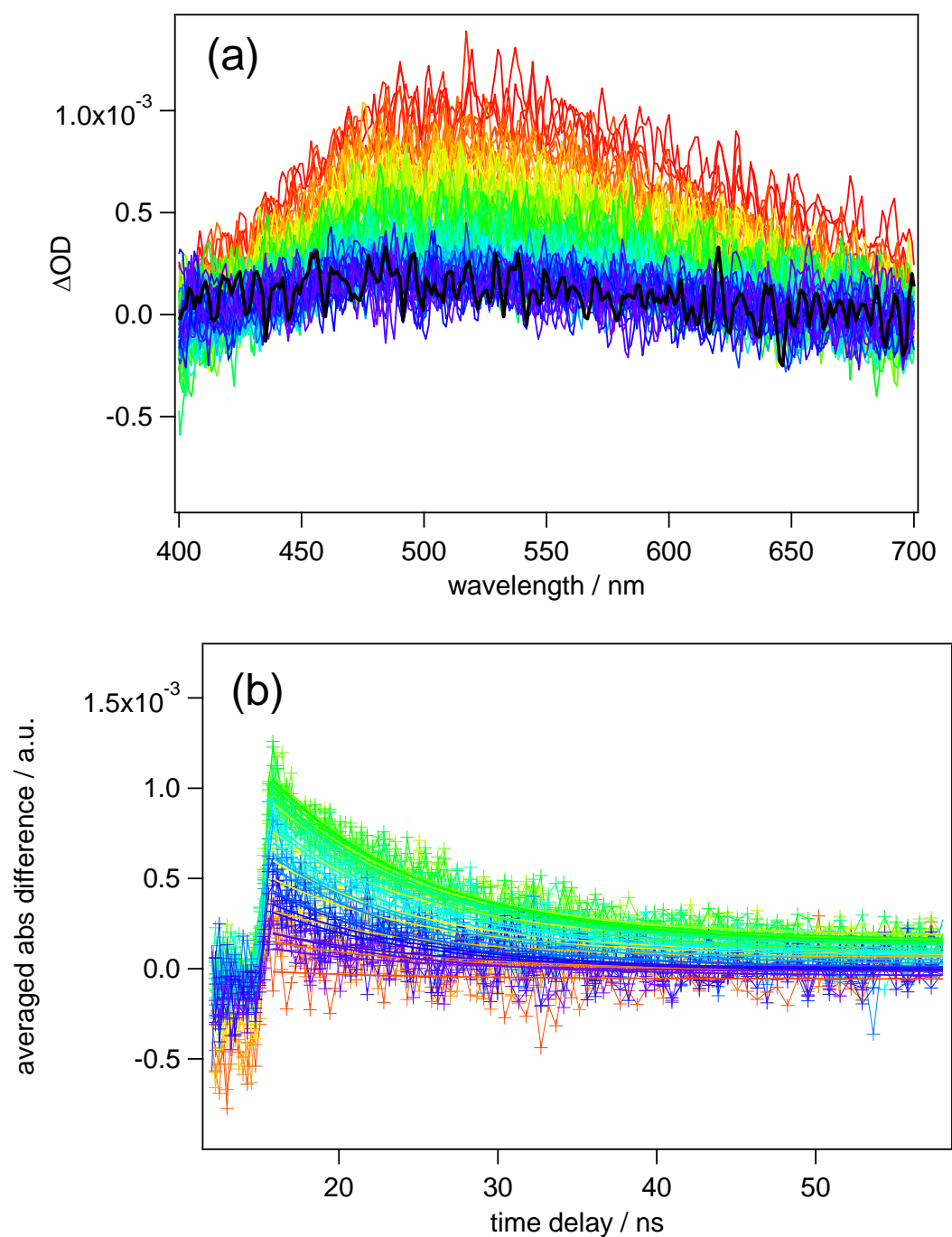


Figure S11. (a) Observed transient absorption spectra of **9** in CH_3CN ($\lambda_{\text{ex}}=250$ nm) obtained by nanosecond flash photolysis, and (b) corresponding decay kinetics integrated from 400-700 nm in 10 nm data increments, together with monoexponential fit of 9.8 ± 1 ns.