Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Macrocyclic derivatives with sucrose scaffold: insertion of a long polyhydroxylated linker between the terminal 6,6'-positions via an azide-alkyne cycloaddition, esterification, and amidation approaches

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Supplementary Information

Contents

1. Copies of the NMR spectra

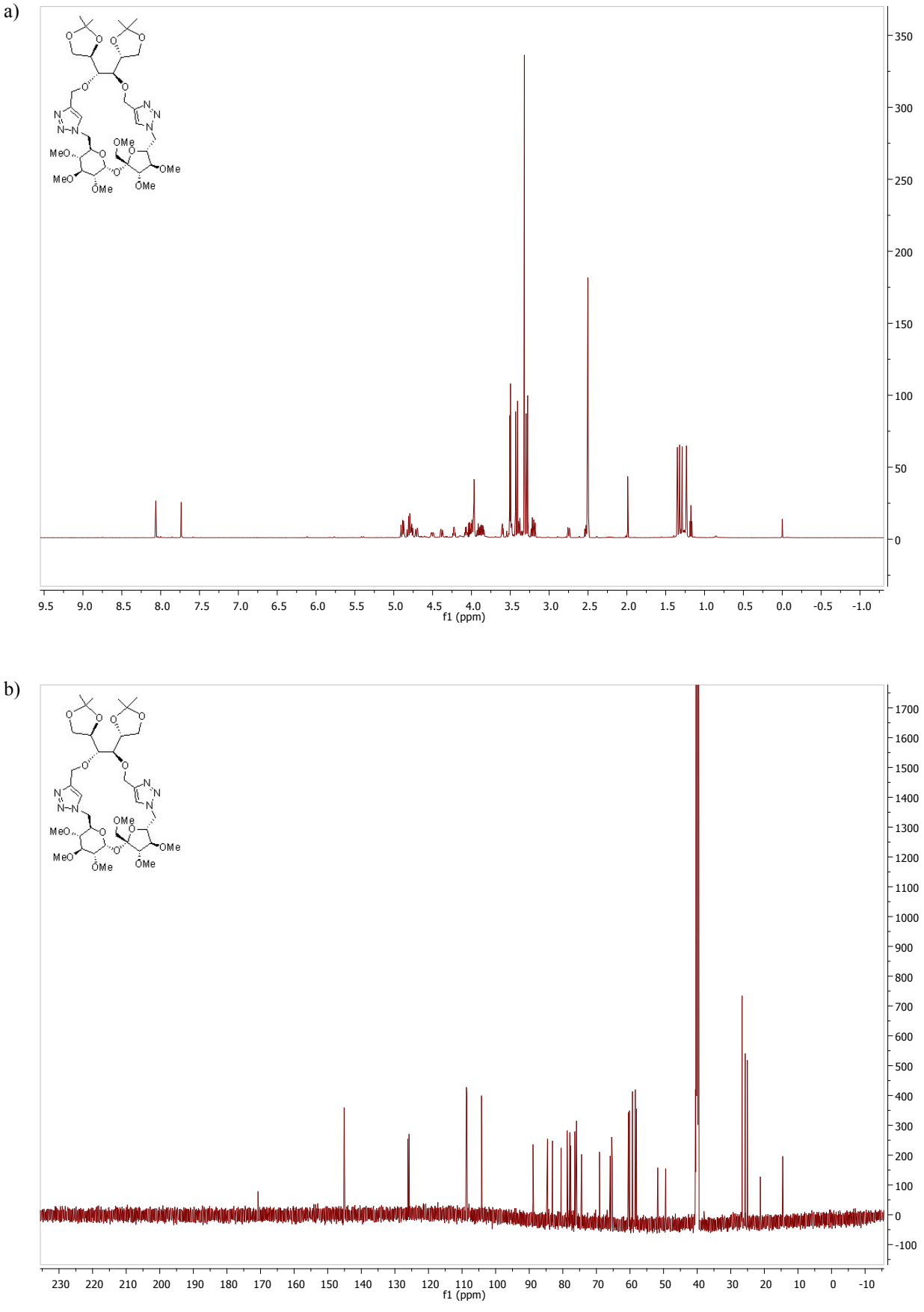
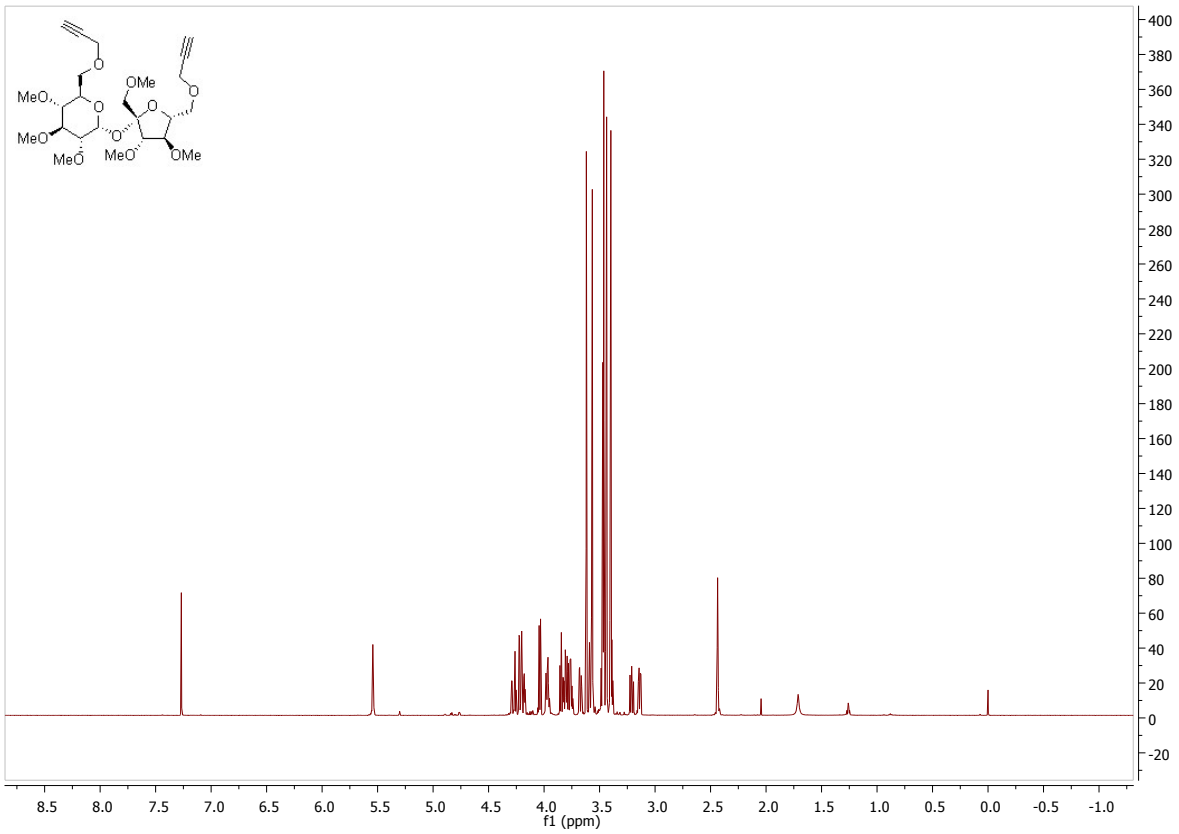


Fig. S1. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **5** in DMSO-d_6.

a)



b)

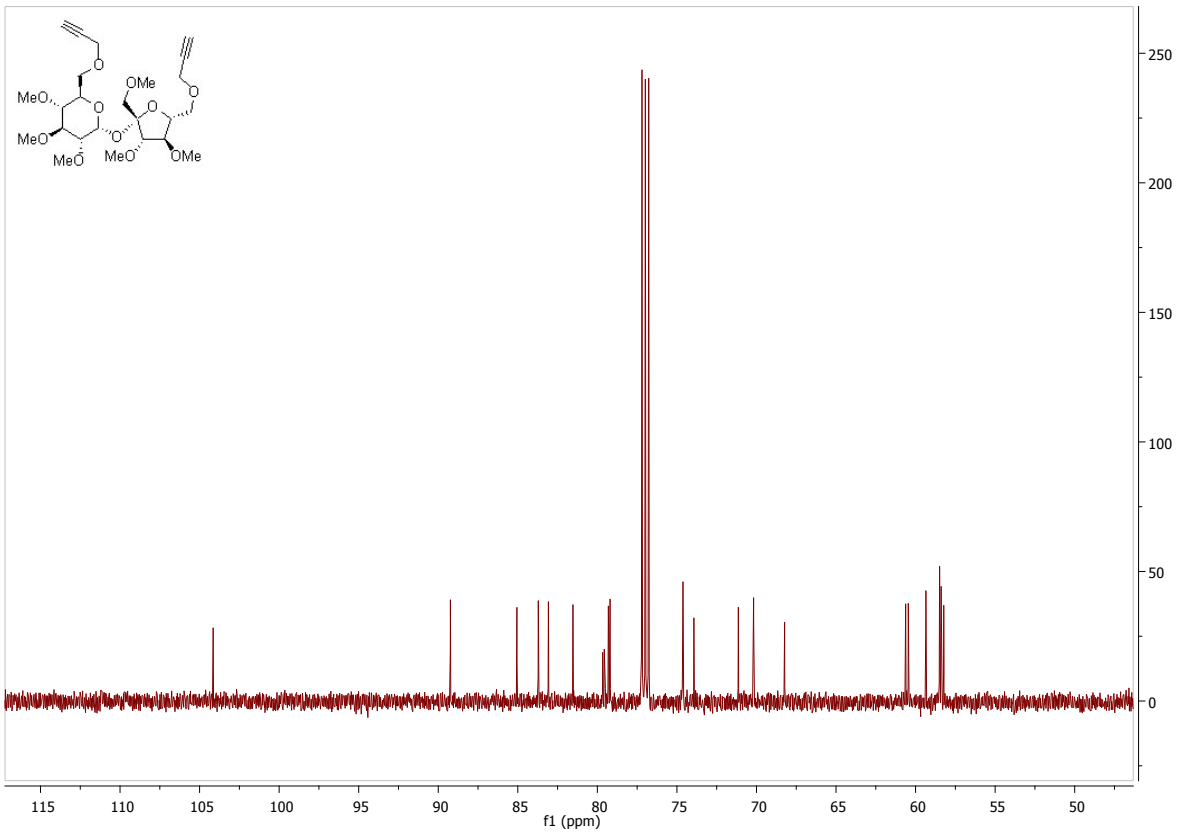


Fig. S2. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **6** in $CDCl_3$.

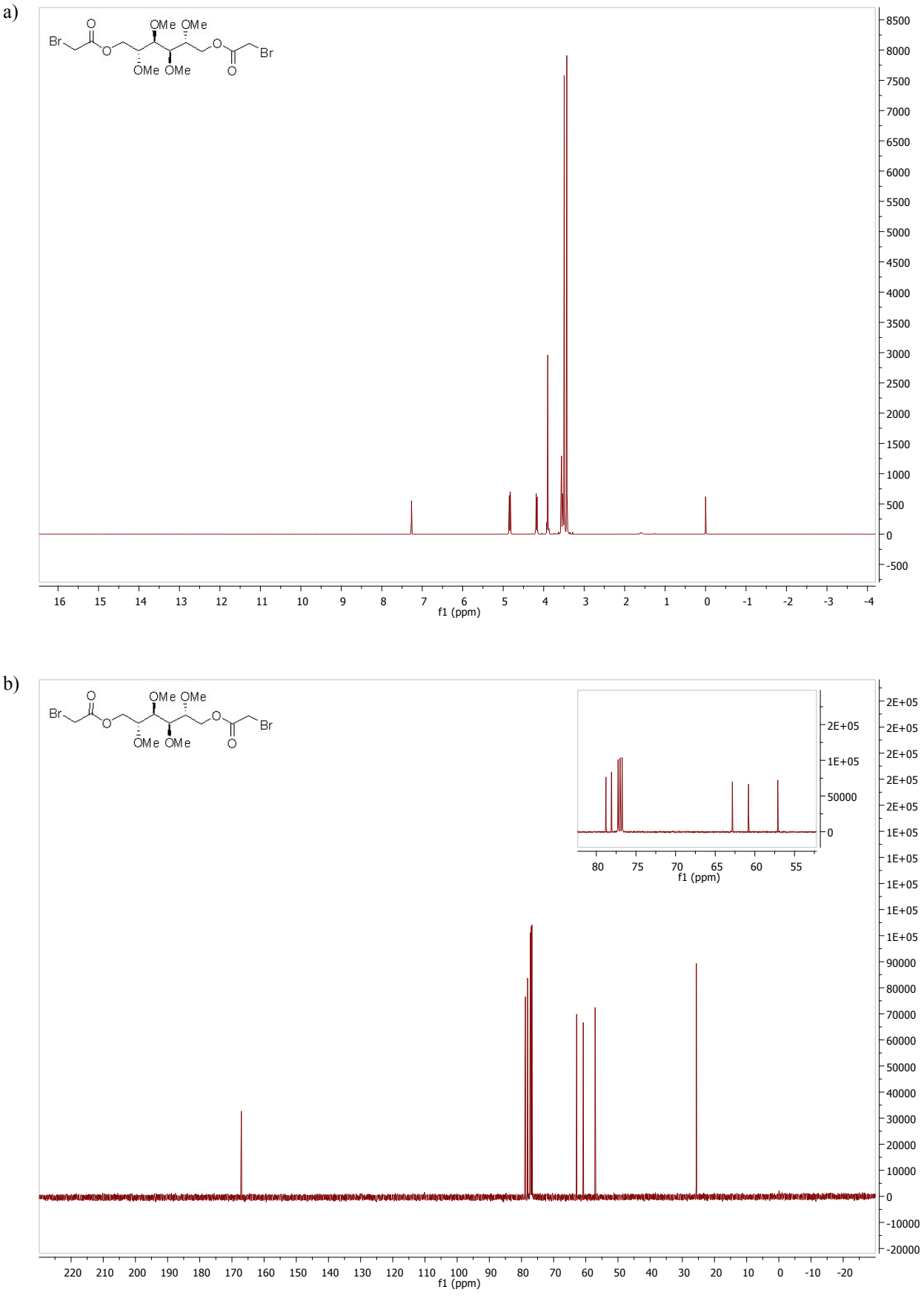


Fig. S3. ^{1}H NMR (500 MHz, a) and ^{13}C NMR (100 MHz, b) spectra of compound **8** in $CDCl_3$.

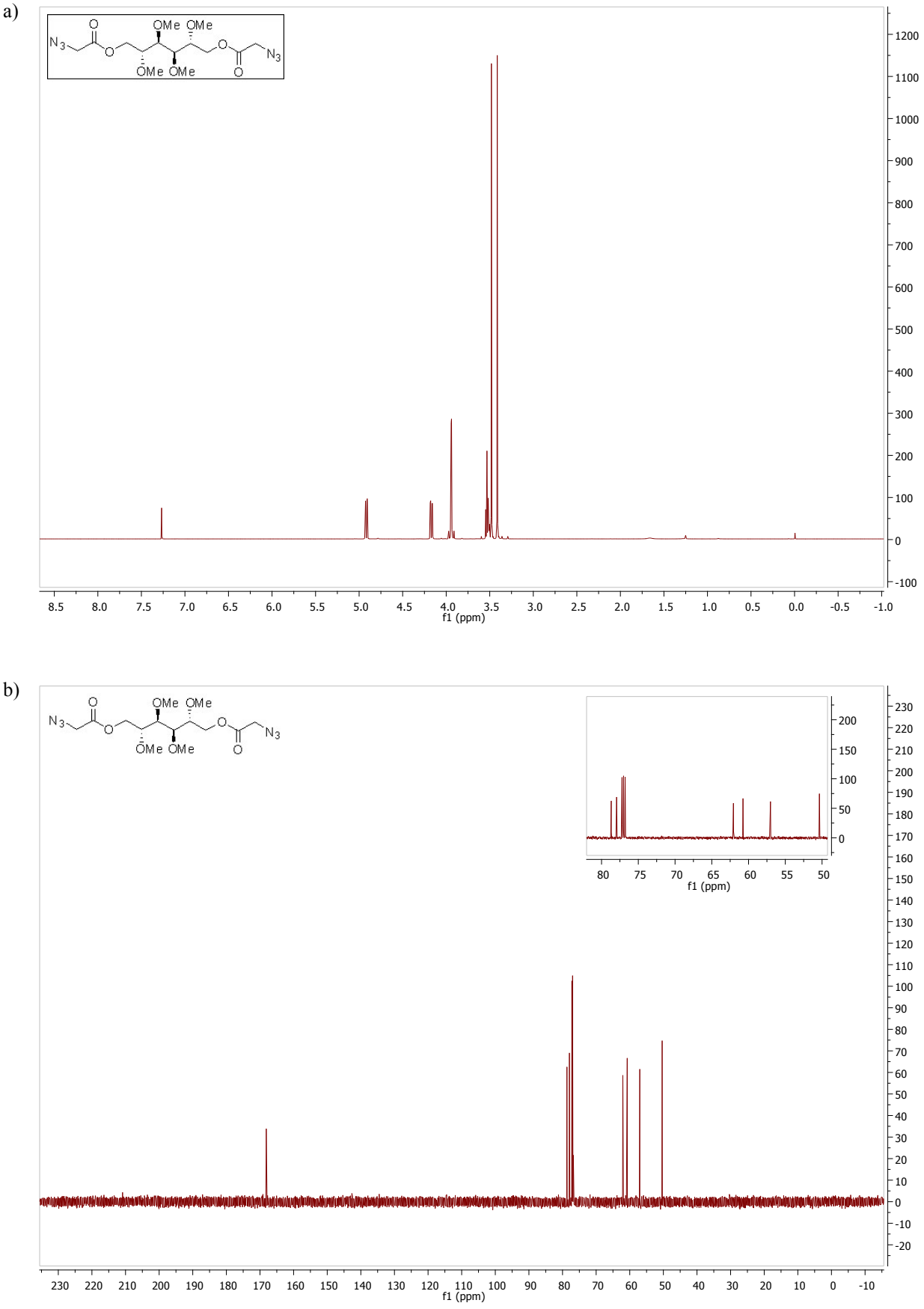


Fig. S4. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **9** in $CDCl_3$.

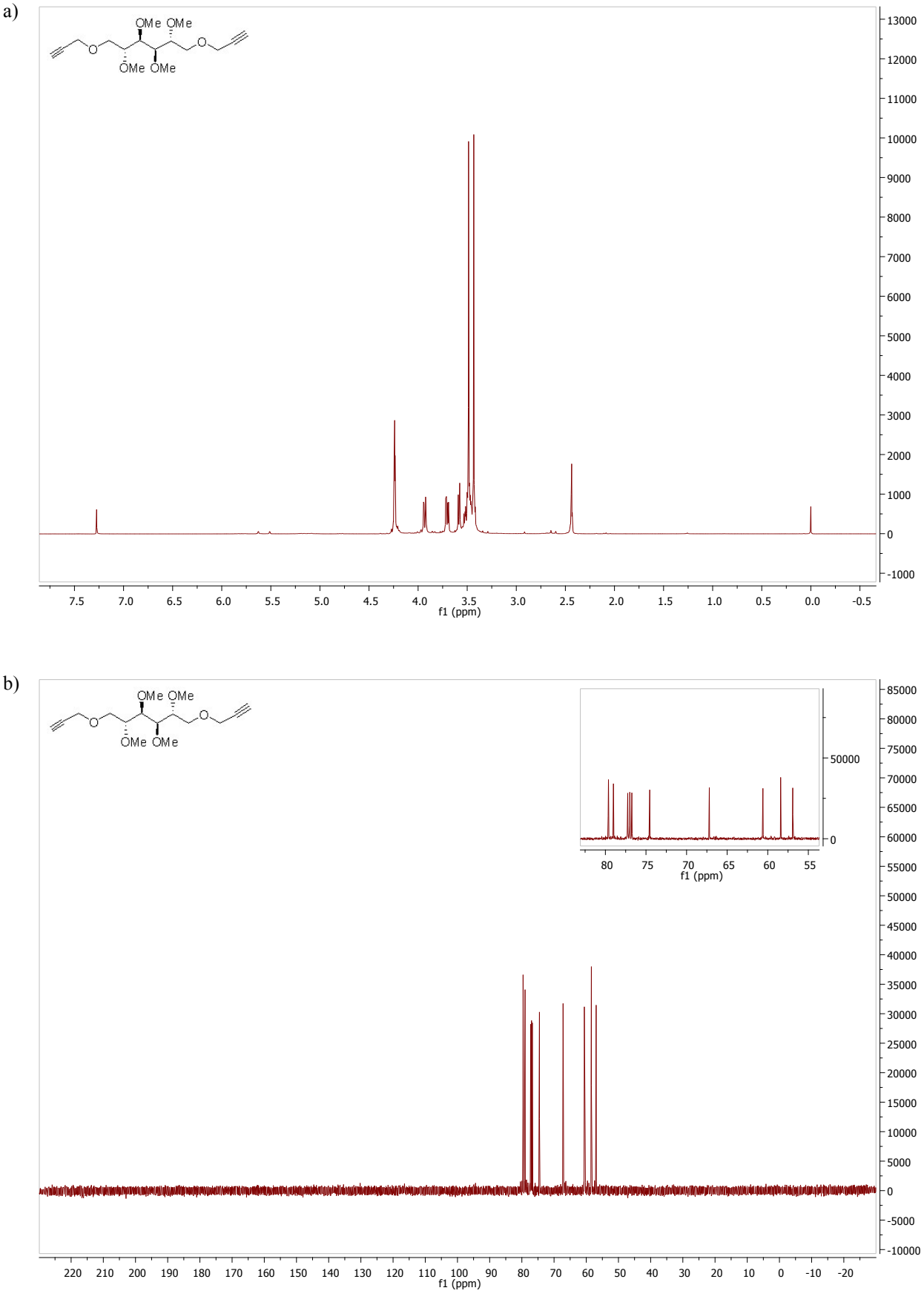


Fig. S5. ^{1}H NMR (500 MHz, a) and ^{13}C NMR (100 MHz, b) spectra of compound **10** in $CDCl_3$.

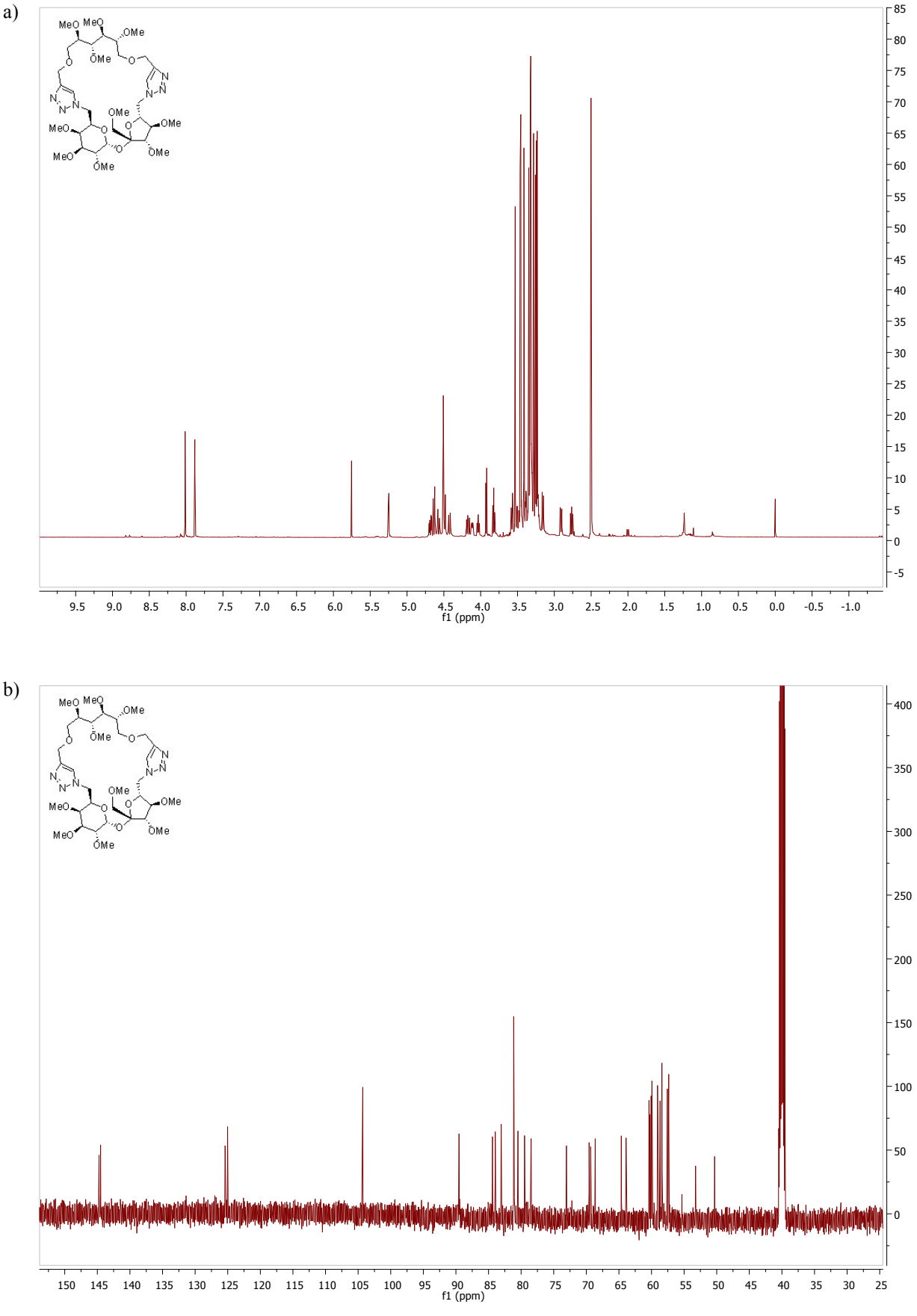
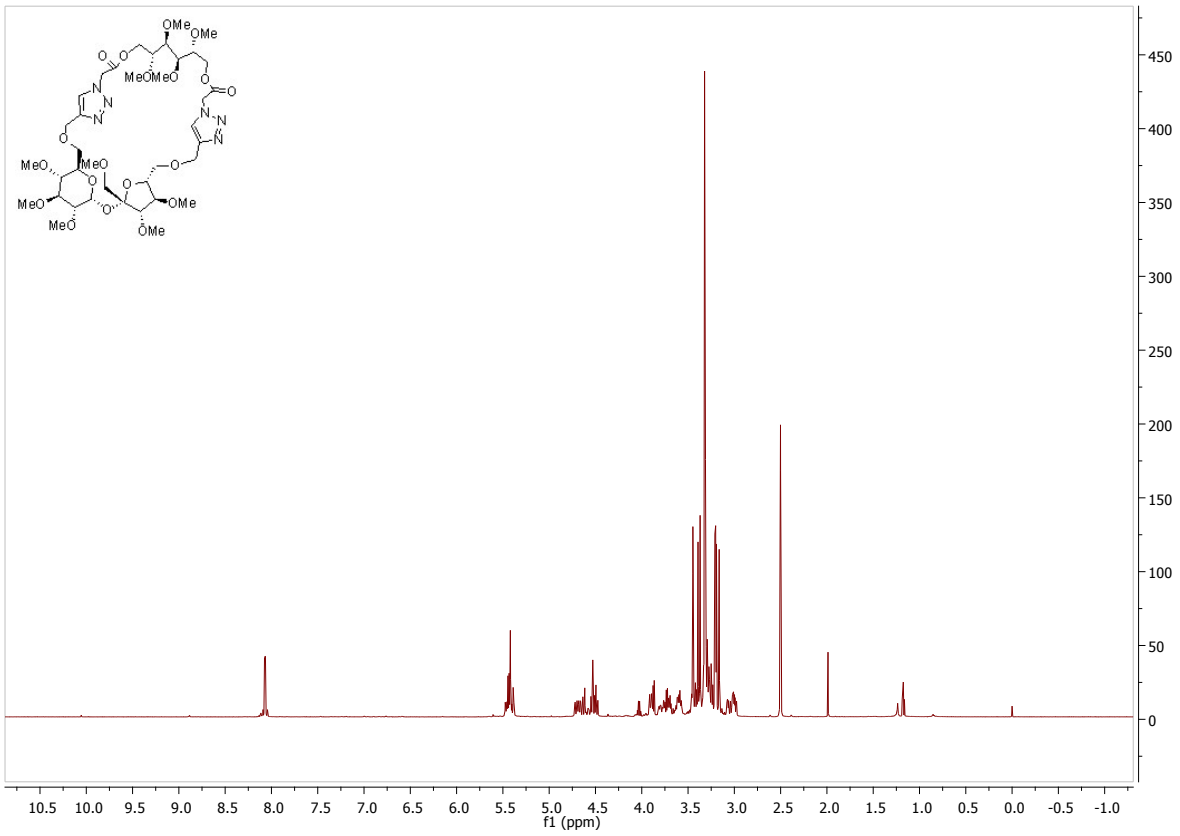


Fig. S6. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **11** in DMSO-d_6.

a)



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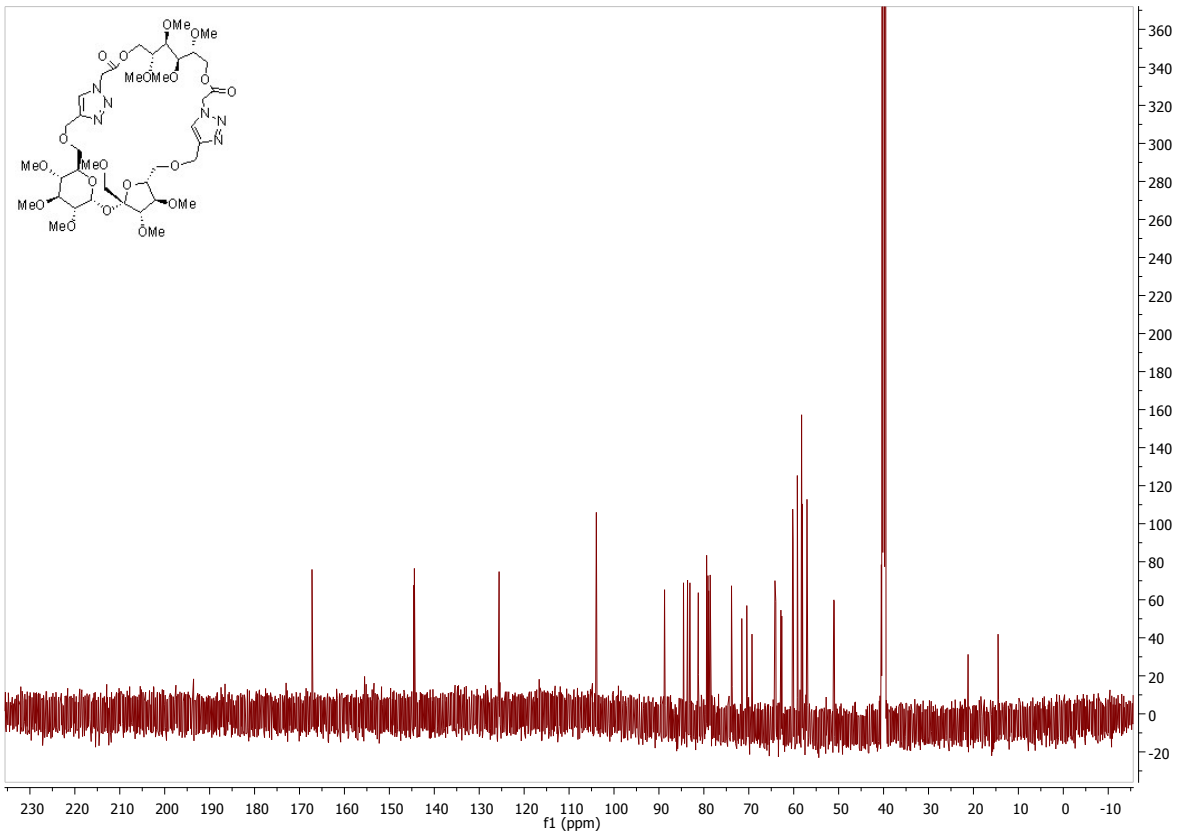
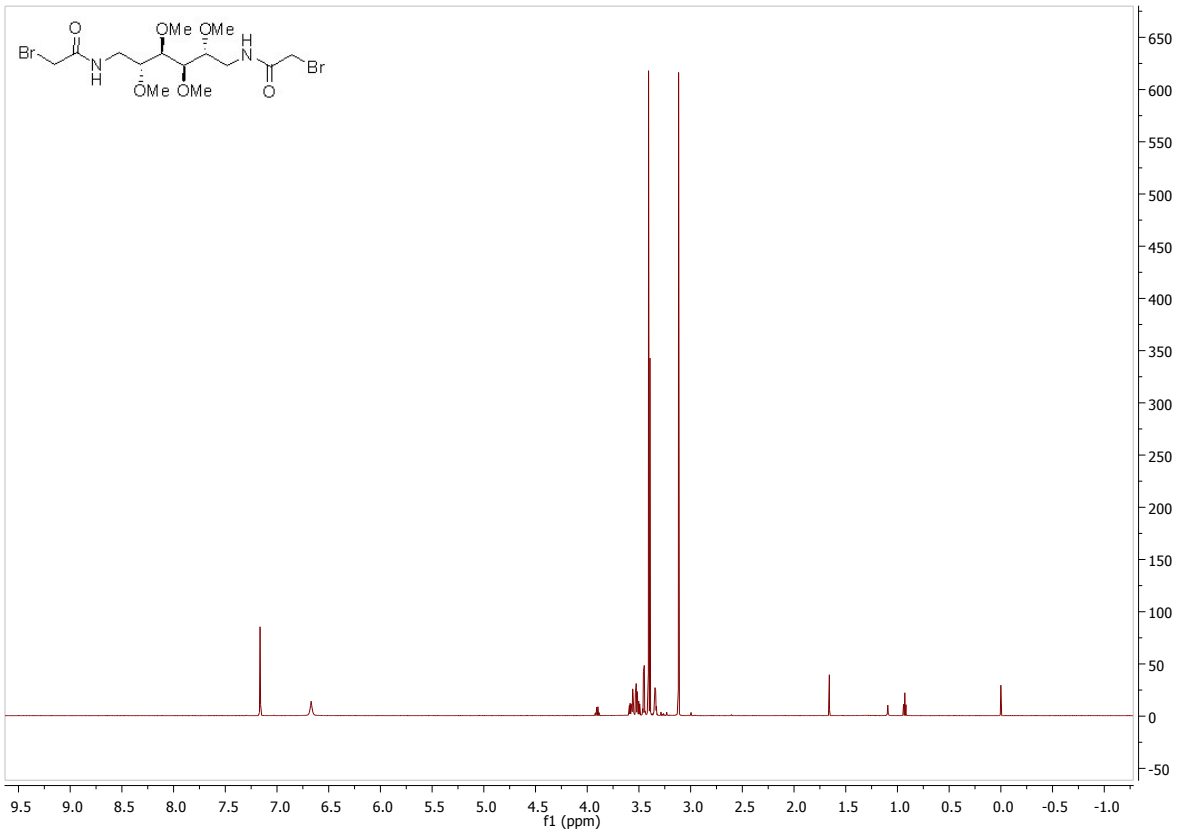


Fig. S7. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **12** in DMSO-d_6.

a)



b)

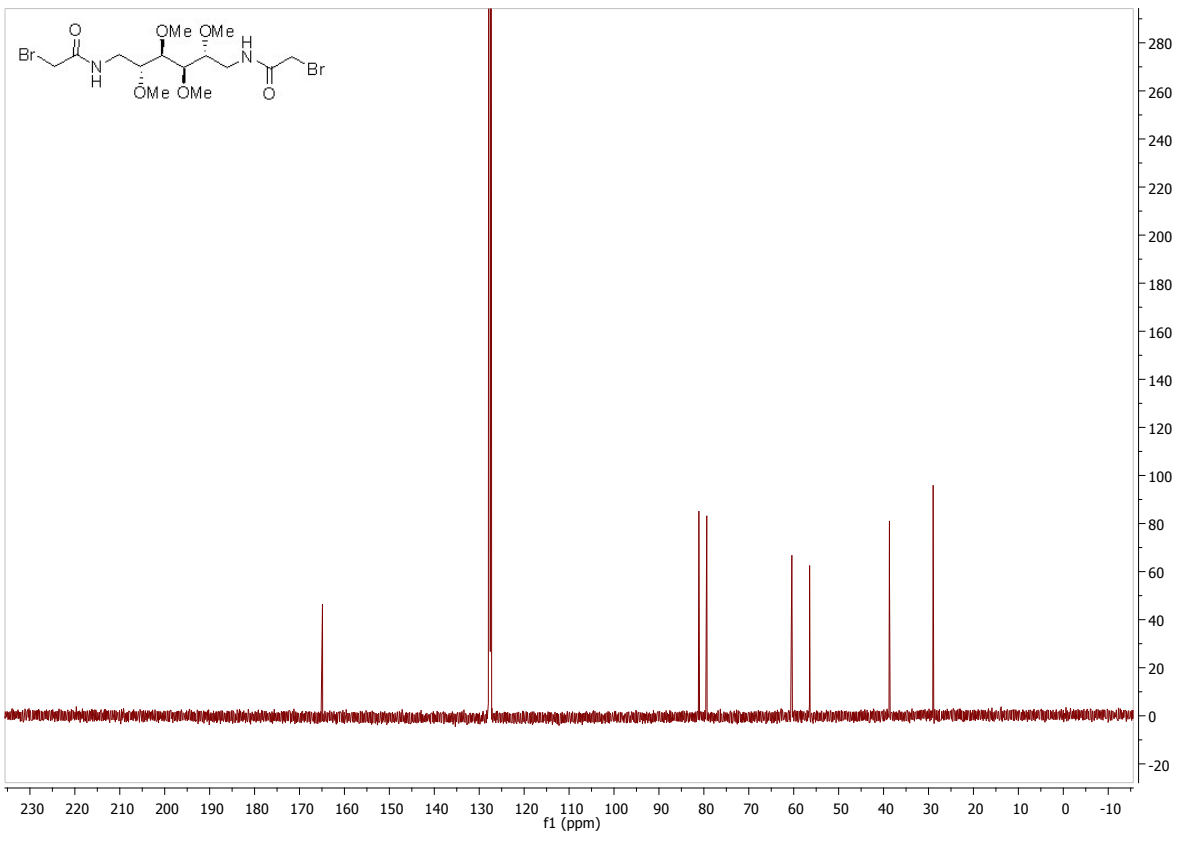


Fig. S8. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **15** in C_6D_6.

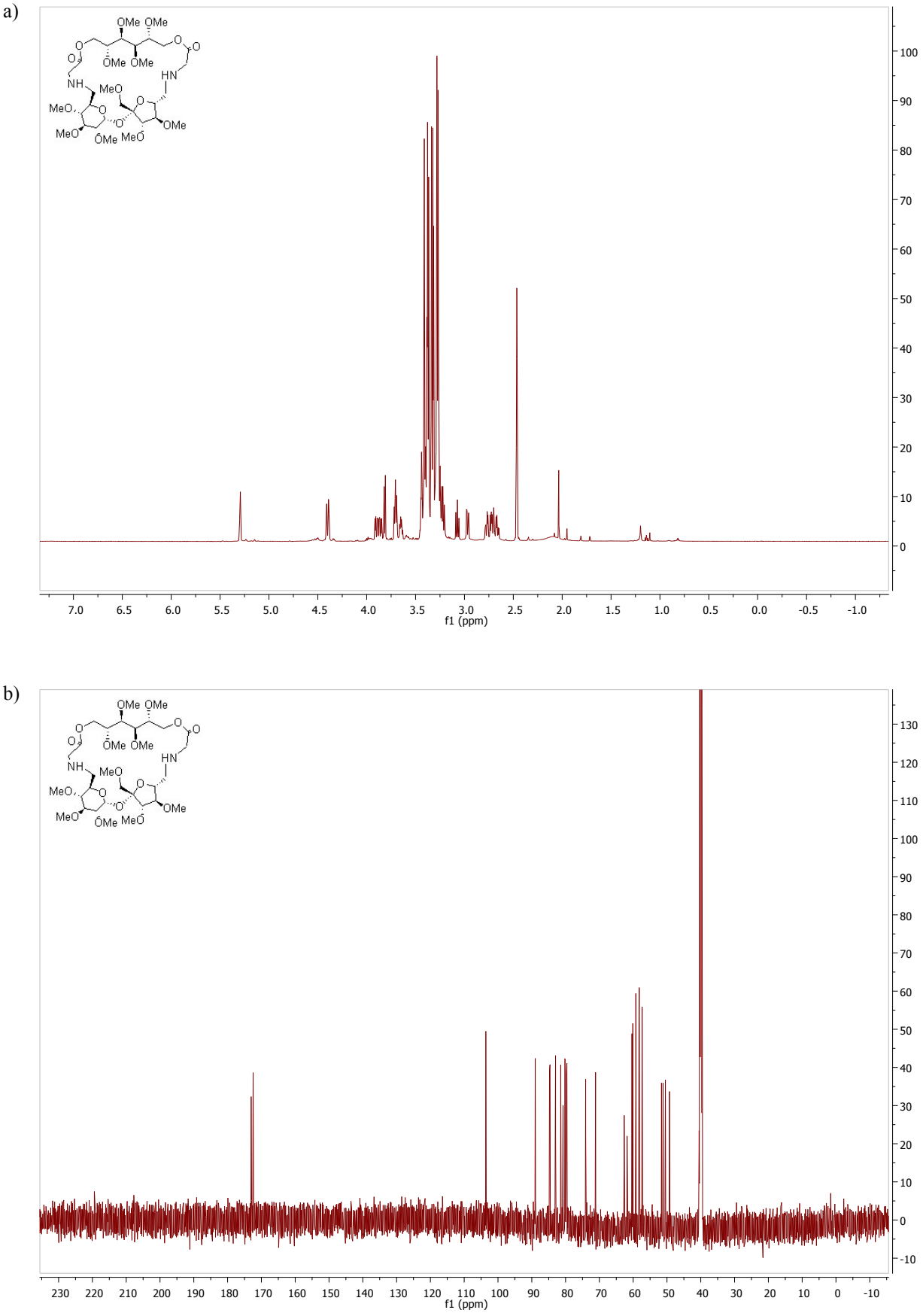
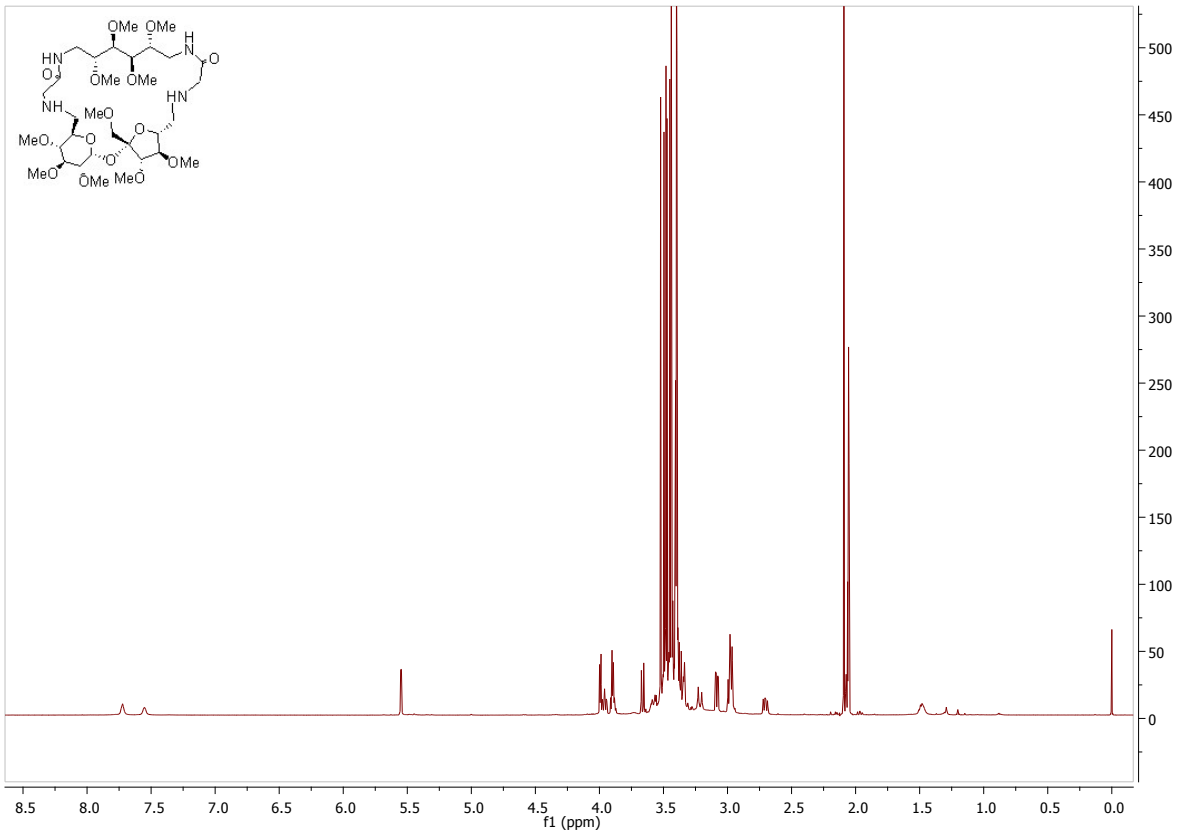


Fig. S9. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **16** in DMSO-d_6.

a)



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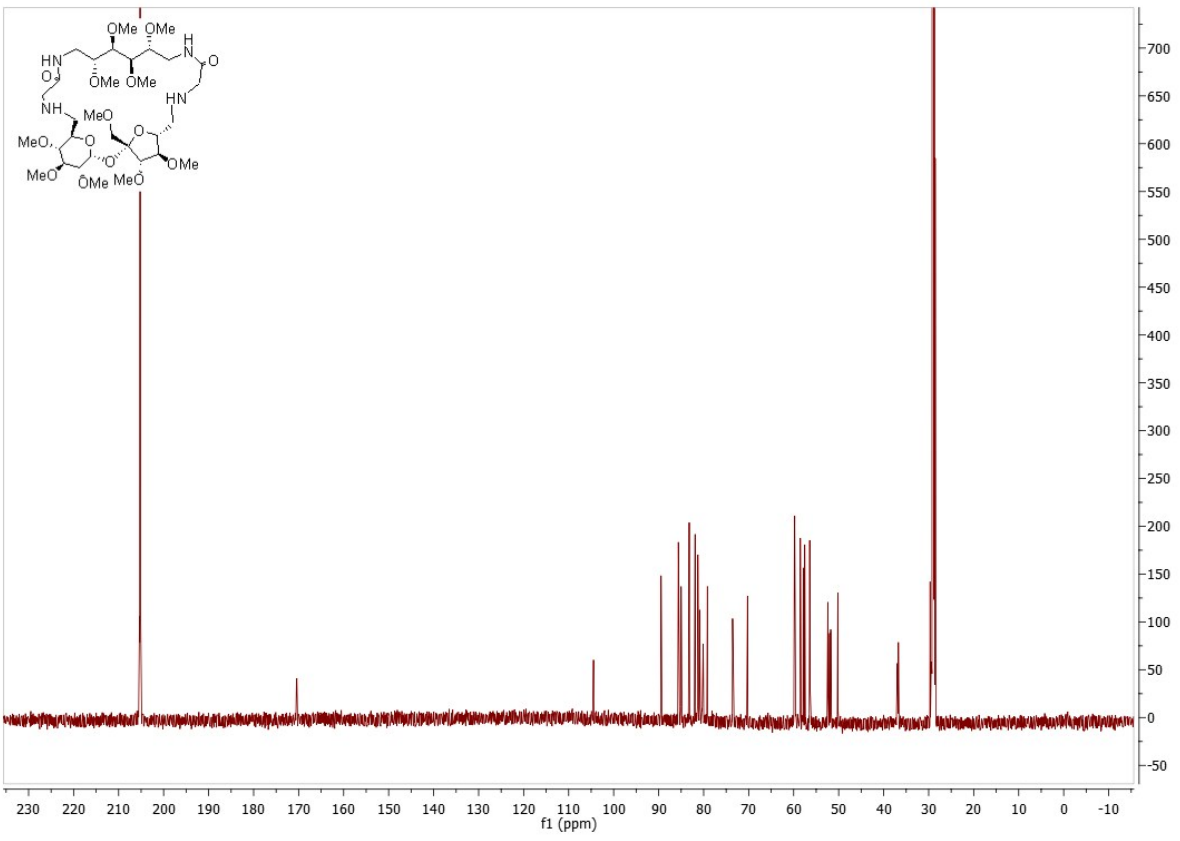

Fig. S10. ^{1}H NMR (600 MHz, a) and ^{13}C NMR (151 MHz, b) spectra of compound **17** in acetone-d_6.

2. ^{1}H NMR Titration Experiments

The (S)-α-phenylethyl ammonium and (R)- α-phenylethyl ammonium chlorides were prepared as described previously.[1] The $CDCl_3$ of 99.90% isotopic purity was used as a deuterated solvent.

A simultaneous nonlinear curve fitting for all protons belonging to host **17**, and assuming a 1:1 (host:guest) binding model was carried out with the HypNMR 2008 Software.[2-4] This procedure provides more reliable K_a's (so-called 'global association constant") than fitting of the experimental data to a single chemical signal changes.[5,6]

Table S1. Titration details, stability constants K_a (M^{-1}), and selected maximum signal shifts ($\Delta\delta_{max}$) of anomeric CH aromatic proton for host **17** with (S)-α-PEA and (R)-α-PEA cations in $CDCl_3$ at 298 K[a]

No	Guest	c_{Host} (M)	c_{Guest} (M)	K_a (M^{-1})	$\Delta\delta_{max}$ (ppm)
1	(S)-α-PEA	0.01017	0.36253	79.2±6.9	0.050
2	(R)-α-PEA	0.01017	0.33177	118.7±8.9	0.059

Job Plot experiment

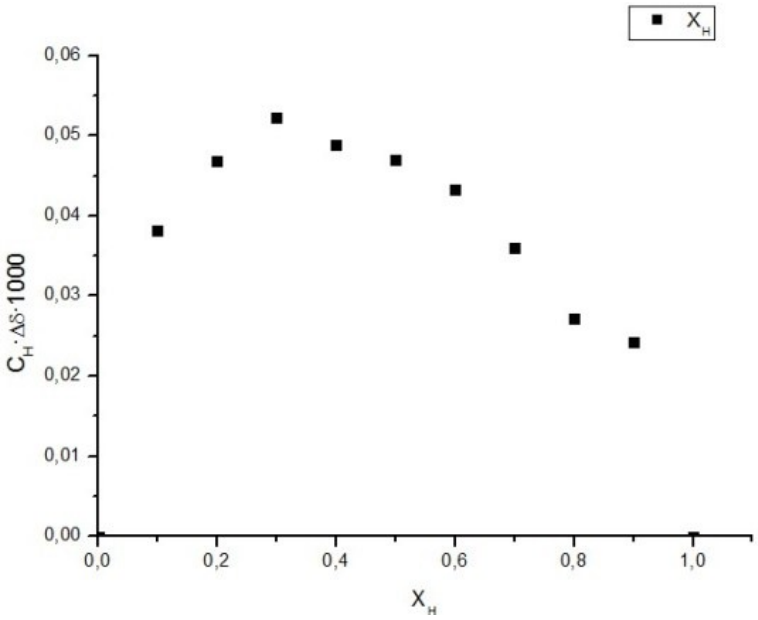

Fig. S11. Job plot for host **17** with *R*-α-phenyl-ethylamine (^{1}H NMR 400 MHz in $CDCl_3$); anomeric CH proton was tracked; amount of the host: 25.3 mg; amount of the guest: 5.2 mg.

3. Cartesian coordinates of calculated structures

Table S2. Energies, enthalpies, and Cartesian coordinates of the energy-minimized structures of two linear intermediates leading to host **17**, three lowest-energy conformation of host **17**, (S)-α-phenylethylammonium (S-α-PEA) cation, (R)-α-phenylethylammonium (R-α-PEA) cation, and complexes **17**⊃S-α-PEA and **17**⊃R-α-PEA.

Linear intermediate A E = -5177.45636 au G^0 = -5176.57064 au				Linear intermediate B E = -5177.45322 au G^0 = -5176.56646 au				Free host **17** (lowest energy) E = -2602.94013 au G^0 = -2602.06357 au			
H	-4.246110	0.893852	-0.718634	H	3.963421	-1.390313	-0.323204	H	4.049961	0.596021	-1.531839
C	-3.262884	0.480207	-0.948127	C	3.227534	-0.728893	-0.784504	C	3.261743	0.965817	-0.874643
C	-1.968466	-1.093947	-2.419127	C	2.676382	0.742844	-2.725500	C	2.580576	2.820238	0.686882
C	-1.151780	1.212073	-1.817805	C	1.013962	-0.905931	-1.746192	C	0.998835	1.745294	-1.023439
C	-1.176591	0.123625	-2.906496	C	1.457215	-0.133134	-3.008841	C	1.331678	3.006115	-0.195513
O	-2.515452	1.554590	-1.488089	O	2.128154	-1.556581	-1.105913	O	2.179207	1.295505	-1.717761
C	-3.366336	-0.655009	-1.973414	C	3.775956	-0.086360	-2.064468	C	3.727754	2.221223	-0.127236
H	-1.438002	-1.531349	-1.562513	H	2.372706	1.540898	-2.036943	H	2.371982	2.129912	1.514766
H	-0.655351	0.823471	-0.920418	H	0.552458	-0.193814	-1.051089	H	0.646466	0.942539	-0.367959
H	-1.679859	0.545951	-3.788367	H	1.717636	-0.855101	-3.796832	H	1.563875	3.814837	-0.898777
H	-3.900914	-0.263336	-2.848145	H	4.070593	-0.899236	-2.740765	H	4.038732	2.950222	-0.888825
O	-2.631679	-0.025271	0.211936	O	2.832417	0.297288	0.112335	O	2.871088	-0.031269	0.051760
C	-0.441405	2.503962	-2.248793	C	0.023235	-2.033657	-2.062679	C	-0.029444	1.990784	-2.128910
H	-0.938446	3.350475	-1.748871	H	-0.104696	-2.639649	-1.157256	H	-0.143714	1.054315	-2.686586
H	-0.561977	2.652113	-3.327583	H	0.469864	-2.689108	-2.832011	H	0.383206	2.740908	-2.829723
O	0.155126	-0.252300	-3.248045	O	0.349958	0.671984	-3.420865	O	0.219879	3.507307	0.554960
O	-2.058100	-2.047471	-3.475142	O	3.153346	1.304729	-3.948708	O	3.032439	4.071854	1.195176
O	-4.084226	-1.738529	-1.394372	O	4.897684	0.725749	-1.747563	O	4.824904	1.867946	0.699346
C	-3.274962	0.147584	1.465010	C	3.457437	0.379367	1.390402	C	3.523467	-1.300085	0.021684
C	-2.185011	-0.072304	2.555771	C	2.610971	1.390646	2.203353	C	2.551334	-2.362075	0.651693
C	-1.722492	1.351349	2.869212	C	1.521493	0.500830	2.816455	C	2.430163	-3.443012	-0.444571
C	-2.963979	2.204442	2.611467	C	2.210385	-0.861797	2.971030	C	2.790644	-2.687127	-1.722649
O	-3.734232	1.477685	1.628898	O	3.361778	-0.841635	2.098393	O	3.787245	-1.734970	-1.302492
H	-2.668401	-0.516086	3.437467	H	3.243951	1.795687	3.005096	H	3.014214	-2.777378	1.553580
C	-4.481640	-0.797878	1.581155	C	4.954265	0.722780	1.269460	C	4.857235	-1.182416	0.773907
H	-4.145390	-1.821462	1.401537	H	5.074480	1.528196	0.547214	H	4.656363	-0.668804	1.717694
H	-5.216768	-0.546145	0.807068	H	5.488349	-0.158310	0.885125	H	5.541996	-0.555064	0.188301
C	-6.133261	0.167102	3.022869	C	5.834513	0.166097	3.441776	C	6.228746	-3.018717	0.066912
O	-5.055462	-0.755759	2.878553	O	5.531478	1.176319	2.482196	O	5.440520	-2.431441	1.098657
C	-1.909709	-3.400322	-3.050282	C	3.437745	2.698966	-3.866942	C	2.473749	4.461273	2.445433
H	-2.688023	-3.685804	-2.333536	H	2.527847	3.277686	-3.652871	H	1.410839	4.710664	2.356098
C	-5.157722	-2.223779	-2.197315	C	6.011384	0.557024	-2.620781	C	5.861362	2.842378	0.770306
H	-5.908816	-1.441625	-2.376440	H	5.751726	0.820782	-3.652719	H	5.499449	3.778875	1.207122
H	-5.620734	-3.042449	-1.640097	H	6.383487	-0.477130	-2.596599	H	6.282363	3.050068	-0.224987
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H	-0.925714	1.595425	2.154059	H	0.682295	0.452803	2.107886	H	1.411181	-3.845265	-0.467320
O	-1.289275	1.595435	4.199828	O	1.058983	0.910961	4.091664	O	3.376833	-4.491957	-0.292952
O	-1.063070	-0.827535	2.152528	O	2.003650	2.429195	1.463457	O	1.251633	-1.887662	0.942806
C	-0.346785	0.654759	4.715098	C	0.286638	2.111341	4.061130	C	3.058120	-5.405163	0.746364
H	0.010906	1.067048	5.661378	H	0.887416	2.968866	3.735493	H	3.057663	-4.926277	1.735501
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H	-6.957642	-0.081540	2.337915	H	-0.065047	2.279438	5.082567	H	3.829156	-6.179640	0.732075
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C	1.944196	3.107929	-2.760269	H	6.354007	-0.682906	2.974393	H	6.977571	-2.305395	-0.309374
H	-4.796185	-2.600802	-3.162395	C	-2.707330	-4.854557	1.894842	C	-0.656005	-2.307212	-3.266496
H	-6.486637	0.074969	4.053612	C	-2.263653	-2.478293	-2.882300	C	-2.361902	2.501231	-2.624093
H	-0.812408	-0.321632	4.897399	H	6.795443	1.227438	-2.259351	H	6.643803	2.416638	1.404580
H	-0.926762	-3.565606	-2.588177	H	6.495577	0.629026	4.180139	H	6.744914	-3.869687	0.520924
H	1.401821	-0.771984	-4.765391	H	-0.574455	2.001485	3.391990	H	2.073340	-5.868432	0.582367
H	-1.766773	-2.697855	2.772331	H	3.830342	2.997940	-4.842550	H	3.028047	5.345700	2.772187
H	2.322565	4.038884	-2.315155	H	-0.015575	-0.143049	-5.311641	H	0.326265	2.008891	2.037370

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C	1.524918	2.561415	2.087257
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H	2.504358	1.088798	3.106373
C	3.173300	2.235866	-3.077784
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C	3.930058	-0.116461	-3.086538
H	3.594464	-0.969014	-3.683695
C	4.258659	-0.611880	-1.658025
H	5.131301	-1.282341	-1.714263
C	3.088997	-1.444900	-1.088951
H	2.139732	-0.918071	-1.248372
C	3.174318	-1.818863	0.406524
C	3.209229	-0.644937	1.408816
O	4.534234	0.477591	-0.796024
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C	5.814103	1.076888	-0.977251
H	5.946301	1.777321	-0.148199
H	5.866571	1.627033	-1.922990
H	6.612398	0.321428	-0.941624
C	1.832627	-3.135612	-2.281510
H	1.234887	-2.342179	-2.744830
H	1.270347	-3.556465	-1.441492
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H	4.822778	0.300008	-3.557296
H	1.536143	4.505553	2.984693
Br	2.619231	3.154661	4.817013
N	-1.999002	3.731430	0.823853
H	-2.377753	3.051711	0.163174
H	-1.020133	3.476669	0.957524
H	0.377945	3.344610	3.702602
H	3.657286	3.706135	1.591315
H	-2.411436	-3.209686	-2.083156
H	-1.985193	-3.009532	-3.806854
C	-2.720002	-3.587176	1.049522
O	-3.508959	-3.488801	0.095856
N	-1.831554	-2.655774	1.424202
H	-1.237861	-2.798520	2.256109
C	-3.516355	-1.641564	-3.132436
O	-3.599725	-0.949051	-4.155336
N	-4.422355	-1.603502	-2.122598
H	-4.211630	-2.144214	-1.282085
C	-5.318309	-0.460006	-1.954445
H	-5.181637	0.203344	-2.809712
C	-4.987461	0.277284	-0.642101
H	-5.624928	1.169272	-0.557629
C	-3.516788	0.768365	-0.655743
H	-2.899398	0.059712	-1.210903
C	-2.803631	0.984431	0.698423
C	-2.607835	-0.301453	1.527070
O	-5.235211	-0.591362	0.461180
O	-3.549813	2.006249	-1.379421
C	-1.763580	-1.345722	0.797378
O	-1.495447	1.499467	0.419585
H	-3.367937	1.707621	1.302830
O	-1.946347	-0.000621	2.764207
H	-3.588995	-0.729759	1.732228
C	-2.839143	0.259337	3.840916
H	-3.449793	-0.626035	4.069097
H	-3.506872	1.103598	3.620872
H	-2.223818	0.509690	4.708433
C	-1.339968	2.901856	0.604202
H	-0.278089	3.114977	0.459772
H	-1.622850	3.200632	1.623798
H	-1.941520	3.470498	-0.113087
C	-6.596089	-0.667124	0.867040
H	-6.621417	-1.309671	1.750676
H	-7.238769	-1.104939	0.091456
H	-6.985807	0.327063	1.128992
C	-2.653371	2.060494	-2.490379
H	-2.759704	3.058622	-2.925400
H	-2.911916	1.307150	-3.246370
H	-1.614297	1.906158	-2.181381
H	-2.079438	-1.446663	-0.237814
H	-0.723406	-1.018157	0.782340
H	-6.363030	-0.786721	-1.942280
H	-3.180710	-5.670218	1.352908
H	-0.371056	-1.292060	3.450852
H	-1.711548	-5.130786	2.241585
Br	-3.792182	-4.569995	3.533742
H	1.578862	-1.824890	3.001510
H	-1.297521	-3.104657	-3.658314
H	-2.354801	1.603776	-3.246069
H	-2.211290	3.380837	-3.272341
C	-1.513634	-1.462602	-2.321550
O	-2.397782	-0.732829	-2.796556
N	-1.233956	-1.569659	-1.008966
H	-0.491074	-2.197121	-0.724327
C	-3.691952	2.658878	-1.895782
O	-3.982856	3.721493	-1.335028
N	-4.473931	1.548624	-1.865459
H	-4.065946	0.678940	-2.203084
C	-5.648308	1.441542	-1.009006
H	-5.795866	2.401131	-0.511224
C	-5.445540	0.331697	0.036932
H	-6.364097	0.219457	0.632439
C	-4.318040	0.741277	1.012237
H	-3.560494	1.310115	0.465333
C	-3.581326	-0.376821	1.779705
C	-2.808076	-1.388680	0.905342
O	-5.144310	-0.899932	-0.611365
O	-4.962525	1.610009	1.946866
C	-1.811261	-0.690573	-0.011475
O	-2.637629	0.298380	2.622687
H	-4.314922	-0.913366	2.396278
O	-2.047328	-2.287663	1.720482
H	-3.519414	-1.952207	0.298287
C	-2.784345	-3.398276	2.206328
H	-3.231353	-3.974503	1.382148
H	-3.586042	-3.098274	2.897183
H	-2.078467	-4.034729	2.747373
C	-2.662673	-0.102964	3.983759
H	-1.904129	0.492108	4.500719
H	-2.419685	-1.166881	4.094626
H	-3.643495	0.095006	4.439857
C	-6.242589	-1.517923	-1.268709
H	-5.901605	-2.509916	-1.575670
H	-6.558694	-0.961365	-2.160957
H	-7.103732	-1.623162	-0.592515
C	-4.296147	2.852792	2.162242
H	-4.945428	3.443297	2.815613
H	-4.148763	3.390654	1.215726
H	-3.326130	2.703991	2.648304
H	-2.270724	0.133629	-0.551189
H	-1.006831	-0.277231	0.597572
H	-6.537054	1.233945	-1.614781
H	-0.409292	-1.648134	-4.115891

Table S2. Continuation

Free host **17** (#2) E = -2602.93944 au G^0 = -2602.06207 au				Free host **17** (#3) E = -2602.93711 au G^0 = -2602.05637 au				S-α-PEA cation E = -366.694622 au G^0 = -366.538053 au			
H	4.149178	0.498084	-1.301284	H	4.133413	0.028085	-1.070648	H	0.240145	-1.879542	0.574372
C	3.307973	0.841404	-0.696759	C	3.268088	0.426460	-0.536986	C	-0.425520	-1.059983	0.315025
C	2.514443	2.534272	0.966622	C	2.439649	2.108671	1.116237	C	-2.162730	1.018704	-0.364965
C	1.114415	1.769146	-1.009353	C	1.258335	1.691836	-1.106213	C	0.095548	0.167531	-0.118329
C	1.421221	2.922899	-0.030868	C	1.521758	2.691828	0.038749	C	-1.804576	-1.243551	0.412248
O	2.340912	1.309053	-1.612463	O	2.467866	1.025019	-1.529714	C	-2.675518	-0.205567	0.068272
C	3.736114	1.984898	0.233173	C	3.683781	1.492368	0.489090	C	-0.781627	1.206322	-0.452333
H	2.132647	1.747593	1.629978	H	1.886191	1.326330	1.649955	H	-2.199150	-2.197638	0.749873
H	0.655798	0.943943	-0.448465	H	0.530467	0.952982	-0.749056	H	-3.749630	-0.352867	0.137244
H	1.790826	3.779530	-0.611814	H	2.000763	3.593452	-0.370301	H	-0.384867	2.161026	-0.789038
H	4.160260	2.777030	-0.399542	H	4.226438	2.279570	-0.053028	H	-2.835390	1.827155	-0.635716
O	2.776842	-0.221075	0.079026	O	2.566603	-0.620027	0.119312	C	1.588210	0.383857	-0.225812
C	0.195550	2.161775	-2.172325	C	0.754481	2.354024	-2.406420	H	1.790046	1.388377	-0.604755
H	0.356770	1.439619	-2.991243	H	0.403663	1.555094	-3.065211	C	2.337470	-0.651923	-1.060436
H	0.481947	3.149444	-2.554070	H	1.632285	2.811755	-2.885157	H	1.928377	-0.645105	-2.074049
O	0.267179	3.298585	0.717255	O	0.271889	3.030045	0.645845	H	2.219528	-1.660193	-0.650685
O	2.904094	3.675931	1.727998	O	2.804251	3.154265	2.014040	H	3.405203	-0.414667	-1.114672
O	4.711493	1.496291	1.140379	O	4.498235	0.951784	1.517858	N	2.184884	0.393727	1.187702
C	3.376683	-1.507701	-0.026359	C	3.095109	-1.943648	0.039878	H	1.728538	1.098863	1.777168
C	2.357095	-2.560642	0.540402	C	1.957992	-2.940697	0.465930	H	3.190358	0.601114	1.172018
C	2.142338	-3.536130	-0.640270	C	1.674521	-3.759264	-0.817315	H	2.065503	-0.514093	1.651764
C	2.553672	-2.713470	-1.859766	C	2.322774	-2.934913	-1.927132				
O	3.613537	-1.865861	-1.377489	O	3.444942	-2.292652	-1.287553				
H	2.816994	-3.081749	1.387199	H	2.357115	-3.597546	1.247476				
C	4.718161	-1.514272	0.723354	C	4.358266	-2.058797	0.910601				
H	4.546218	-1.073102	1.707920	H	4.149763	-1.571347	1.864890				
H	5.435171	-0.877039	0.188493	H	5.179247	-1.519319	0.417721				
C	5.957261	-3.377595	-0.154045	C	5.386718	-4.097942	0.151863				
O	5.240517	-2.812118	0.940309	O	4.742517	-3.388243	1.208893				
C	2.359339	3.709034	3.042708	C	2.698161	2.798014	3.387348				
H	2.730531	2.869681	3.649643	H	3.330647	1.934632	3.625463				
C	5.764110	2.413110	1.423953	C	5.894069	1.093440	1.282157				
H	6.337925	2.654873	0.516670	H	6.202865	0.616592	0.341358				
H	6.425364	1.916048	2.138965	H	6.406414	0.600282	2.111987				
C	-0.264777	4.574513	0.386390	C	0.140728	4.403477	1.009436				
H	0.484035	5.363559	0.539893	H	0.989704	4.731617	1.614982				
H	-0.624720	4.604448	-0.649342	H	0.052781	5.036012	0.115565				
H	2.991835	-3.359816	-2.627065	H	2.731618	-3.585758	-2.705947				
C	1.413081	-1.880337	-2.449400	C	1.384509	-1.884445	-2.523238				
H	1.832523	-1.167088	-3.176472	H	1.971953	-1.200241	-3.154875				
H	1.091982	-3.846504	-0.682409	H	0.593471	-3.865087	-0.962501				
O	2.988504	-4.674604	-0.582520	O	2.291191	-5.039670	-0.804241				
O	1.099184	-2.030932	0.908174	O	0.756083	-2.334645	0.887943				
C	2.584524	-5.642719	0.375235	C	1.630020	-5.979526	0.032198				
H	3.265249	-6.491291	0.270381	H	2.169279	-6.924595	-0.067562				
C	1.060106	-1.451096	2.209656	C	0.774398	-1.836201	2.222116				
H	1.697263	-0.562237	2.272570	H	1.487890	-1.012032	2.335890				
H	0.019924	-1.171417	2.395274	H	-0.236343	-1.475586	2.429284				
N	0.381905	-2.754378	-3.016143	N	0.255796	-2.502854	-3.223085				
N	-1.185515	2.200713	-1.711919	N	-0.303459	3.328584	-2.196997				
H	5.289188	-3.699333	-0.956759	H	4.669086	-4.449442	-0.594708				
H	0.962187	-1.287818	-1.648241	H	0.992790	-1.282757	-1.699229				
H	0.765603	-3.274315	-3.802863	H	0.580284	-2.959676	-4.073342				
H	-1.499491	1.238862	-1.574573	H	0.049237	4.276762	-2.192274				
H	1.552877	-5.978460	0.190552	H	0.584367	-6.120845	-0.280498				
H	2.688689	4.648213	3.496163	H	3.034452	3.664022	3.964440				
H	6.692432	-2.663714	-0.554570	H	6.146608	-3.473456	-0.340134				
C	-0.805796	-2.020705	-3.450231	C	-0.774106	-1.518578	-3.557728				
C	-2.153413	2.839915	-2.593142	C	-1.567019	3.226487	-2.902355				
H	5.377208	3.339448	1.861256	H	6.183470	2.153669	1.254051				
H	6.487409	-4.248263	0.243734	H	5.878553	-4.958566	0.615401				
H	2.649532	-5.263468	1.404811	H	1.640230	-5.674181	1.088122				
H	1.264097	3.678172	3.021114	H	1.656612	2.569628	3.659329				
H	-1.110715	4.745693	1.057913	H	-0.779547	4.481558	1.593783				
H	1.379641	-2.179657	2.969852	H	1.030069	-2.634825	2.934863				
H	-1.455363	-2.701152	-4.013919	H	-1.526079	-1.995464	-4.197760				
H	-2.389104	2.268576	-3.504111	H	-1.692140	2.201470	-3.262919				
H	-1.768760	3.818681	-2.909359	H	-1.657154	3.900835	-3.766372				
C	-1.588508	-1.474591	-2.252198	C	-1.453044	-1.005915	-2.283008				
O	-2.215010	-0.408194	-2.333079	O	-1.744649	0.186603	-2.135826				
N	-1.531631	-2.225932	-1.136599	N	-1.687965	-1.947313	-1.344803				

H	-0.910311	-3.025052	-1.184241	H	-1.269235	-2.851949	-1.521287
C	-3.481167	3.065010	-1.850942	C	-2.776238	3.496856	-1.995254
O	-4.546449	3.213027	-2.454498	O	-3.867878	3.826574	-2.474269
N	-3.336609	3.125951	-0.503610	N	-2.531128	3.325198	-0.677406
H	-2.391333	2.917784	-0.191414	H	-1.574689	3.069958	-0.435042
C	-4.428045	2.991920	0.440630	C	-3.549102	3.434095	0.348330
H	-4.172674	3.526380	1.358688	H	-3.106754	3.864092	1.251723
C	-4.718521	1.518280	0.805343	C	-4.186297	2.083586	0.731705
H	-5.508183	1.514388	1.576543	H	-4.948943	2.279920	1.504150
C	-3.475788	0.839060	1.421078	C	-3.146440	1.145041	1.385801
H	-2.620561	0.979879	0.747237	H	-2.218225	1.160002	0.800132
C	-3.671050	-0.685547	1.653372	C	-3.650742	-0.317788	1.494124
C	-3.389416	-1.504878	0.370532	C	-3.459466	-1.083644	0.166347
O	-5.131774	0.750658	-0.310978	O	-4.788137	1.430905	-0.371588
O	-3.249765	1.545018	2.634235	O	-2.919511	1.733834	2.662249
C	-1.889235	-1.711396	0.180575	C	-2.025881	-1.584582	0.026617
O	-2.793787	-1.070413	2.712560	O	-2.935859	-0.943475	2.561462
H	-4.710959	-0.861475	1.968827	H	-4.722032	-0.299575	1.745846
O	-3.997818	-2.800624	0.428259	O	-4.322352	-2.225993	0.082100
H	-3.781000	-0.956536	-0.487603	H	-3.675207	-0.405152	-0.660247
C	-5.339461	-2.805231	-0.035002	C	-5.610404	-1.916817	-0.427493
H	-5.978627	-2.117549	0.537079	H	-6.136284	-1.174232	0.188884
H	-5.717288	-3.824337	0.086409	H	-6.185499	-2.847290	-0.429521
H	-5.395888	-2.521247	-1.096895	H	-5.549425	-1.525070	-1.454190
C	-3.153056	-2.274994	3.377852	C	-3.565765	-2.099319	3.099494
H	-3.074600	-3.148563	2.721429	H	-3.594721	-2.927257	2.382081
H	-4.182369	-2.220604	3.763859	H	-4.596732	-1.875683	3.413492
H	-2.461197	-2.384240	4.217749	H	-2.980731	-2.394091	3.975341
C	-6.420070	1.064541	-0.828007	C	-5.998486	2.018590	-0.834368
H	-6.690733	0.244499	-1.498962	H	-6.445175	1.298221	-1.525444
H	-6.403380	2.001297	-1.395664	H	-5.806422	2.955694	-1.366587
H	-7.166162	1.129367	-0.022015	H	-6.696689	2.194939	-0.002090
C	-1.877004	1.743784	2.965881	C	-1.586524	1.634595	3.159561
H	-1.321785	2.190981	2.130197	H	-0.857558	1.970829	2.411542
H	-1.395529	0.803091	3.253346	H	-1.346794	0.611117	3.466481
H	-1.860315	2.433444	3.815417	H	-1.534170	2.294088	4.031658
H	-1.363896	-0.764947	0.345409	H	-1.326274	-0.817696	0.369606
H	-1.511394	-2.419517	0.916364	H	-1.870388	-2.462855	0.652104
H	-5.318337	3.453764	0.008756	H	-4.320406	4.118071	-0.013833
H	-0.592379	-1.153781	-4.095538	H	-0.394500	-0.630563	-4.086897

Table S2. Continuation

R-α-PEA cation E = -366.694625 au G^0 = -366.538802 au				**17**⊃S-α-PEA E = -2969.68419 au G^0 = -2968.61751 au				**17**⊃R-α-PEA E = -2969.685736 au G^0 = -2968.62035 au			
H	-0.377124	-2.163785	-0.753496	H	4.865179	0.393512	-0.912439	H	4.865181	0.393512	-0.912440
C	-0.778217	-1.205083	-0.433688	C	4.083431	0.850278	-0.303799	C	4.083433	0.850279	-0.303799
C	-1.810086	1.254500	0.386964	C	3.395186	2.795193	1.129859	C	3.395188	2.795194	1.129860
C	0.095187	-0.154587	-0.128233	C	1.828298	1.587039	-0.527473	C	1.828298	1.587040	-0.527473
C	-2.159656	-1.026610	-0.337718	C	2.088387	2.853686	0.318368	C	2.088388	2.853688	0.318368
C	-2.676855	0.203355	0.073056	O	3.005614	1.105791	-1.184042	O	3.005615	1.105792	-1.184042
C	-0.430101	1.078861	0.283843	C	4.530967	2.185476	0.306791	C	4.530970	2.185477	0.306791
H	-2.828228	-1.847009	-0.582527	H	3.228297	2.172218	2.018590	H	3.228299	2.172219	2.018591
H	-3.751457	0.343605	0.148850	H	1.450986	0.810018	0.151767	H	1.450987	0.810018	0.151767
H	0.232341	1.906441	0.524753	H	2.159032	3.729784	-0.345372	H	2.159033	3.729785	-0.345372
H	-2.209432	2.212326	0.707509	H	4.760857	2.869088	-0.522745	H	4.760860	2.869090	-0.522746
C	1.587285	-0.375444	-0.236334	O	3.661615	-0.026562	0.721962	O	3.661616	-0.026562	0.721963
N	2.177825	-0.424135	1.179425	C	0.817936	1.794749	-1.661186	C	0.817936	1.794750	-1.661186
H	2.051150	0.468267	1.670730	H	0.781229	0.860627	-2.236000	H	0.781229	0.860628	-2.236001
H	3.184327	-0.626593	1.162602	H	1.172405	2.579301	-2.337592	H	1.172406	2.579302	-2.337593
H	1.722122	-1.149906	1.744318	O	0.938802	2.972303	1.159240	O	0.938802	2.972305	1.159240
C	2.347913	0.670868	-1.045119	O	3.716769	4.130910	1.509645	O	3.716771	4.130912	1.509646
H	2.237672	1.671276	-0.614977	O	5.664697	2.025546	1.144582	O	5.664700	2.025547	1.144583
H	1.942806	0.688017	-2.060168	C	4.318662	-1.275281	0.905770	C	4.318664	-1.275282	0.905771
H	3.413680	0.425803	-1.100525	C	3.336566	-2.222713	1.684189	C	3.336568	-2.222714	1.684190
H	1.783660	-1.372987	-0.636211	C	3.328364	-3.508979	0.830940	C	3.328366	-3.508981	0.830940
				C	3.680770	-2.994274	-0.565519	C	3.680772	-2.994275	-0.565519
				O	4.599455	-1.909870	-0.332328	O	4.599457	-1.909871	-0.332328
				H	3.725226	-2.410929	2.690156	H	3.725228	-2.410930	2.690158
				C	5.639344	-1.033629	1.652888	C	5.639347	-1.033629	1.652889
				H	5.425767	-0.362146	2.488568	H	5.425769	-0.362146	2.488569
				H	6.341001	-0.527631	0.977257	H	6.341004	-0.527632	0.977258
				C	7.062317	-2.925539	1.305960	C	7.062320	-2.925540	1.305961
				O	6.205232	-2.211495	2.193849	O	6.205235	-2.211496	2.193850
				C	4.320613	4.257538	2.794283	C	4.320615	4.257540	2.794284
				H	5.276243	3.726975	2.842672	H	5.276246	3.726977	2.842673
				C	6.909178	2.148638	0.461978	C	6.909181	2.148639	0.461978
				H	7.014166	1.402781	-0.337718	H	7.014169	1.402782	-0.337719
				H	7.692281	1.982128	1.205295	H	7.692285	1.982129	1.205295
				C	0.819187	4.179724	1.911678	C	0.819187	4.179726	1.911679
				H	1.496284	4.190563	2.770956	H	1.496285	4.190565	2.770957
				H	1.021619	5.059820	1.289022	H	1.021620	5.059823	1.289023
				H	4.232877	-3.763739	-1.114946	H	4.232878	-3.763741	-1.114946
				C	2.479769	-2.518205	-1.389392	C	2.479770	-2.518206	-1.389393
				H	2.845512	-2.149920	-2.362259	H	2.845513	-2.149921	-2.362260
				H	2.337388	-3.976502	0.869118	H	2.337389	-3.976504	0.869119
				O	4.328779	-4.443429	1.194955	O	4.328781	-4.443431	1.194955
				O	2.001809	-1.748139	1.750889	O	2.001810	-1.748139	1.750890
				C	4.070316	-5.130153	2.411107	C	4.070318	-5.130155	2.411108
				H	4.853643	-5.884815	2.515413	H	4.853645	-5.884818	2.515415
				C	1.756107	-0.861320	2.840558	C	1.756108	-0.861321	2.840559
				H	2.344719	0.057179	2.750745	H	2.344720	0.057179	2.750746
				H	0.693831	-0.613263	2.809313	H	0.693831	-0.613263	2.809314
				N	1.498536	-3.599153	-1.512476	N	1.498537	-3.599155	-1.512477
				N	-0.540695	2.117513	-1.192277	N	-0.540696	2.117514	-1.192277
				H	6.514277	-3.350610	0.461741	H	6.514280	-3.350612	0.461741
				H	2.010685	-1.669450	-0.882504	H	2.010686	-1.669451	-0.882505
				H	1.938546	-4.424727	-1.912107	H	1.938547	-4.424729	-1.912108
				H	-0.619870	1.818307	-0.222476	H	-0.619870	1.818308	-0.222476
				H	3.088050	-5.625772	2.387462	H	3.088052	-5.625775	2.387463
				H	4.482207	5.326505	2.957638	H	4.482209	5.326508	2.957639
				H	7.865126	-2.272526	0.931812	H	7.865130	-2.272527	0.931813
				C	0.311960	-3.257430	-2.282346	C	0.311960	-3.257431	-2.282347
				C	-0.970556	3.527748	-1.268045	C	-0.970556	3.527749	-1.268046
				H	7.024140	3.152260	0.029306	H	7.024143	3.152261	0.029306
				H	7.504459	-3.736946	1.890342	H	7.504463	-3.736947	1.890343
				H	4.108012	-4.461002	3.281434	H	4.108014	-4.461004	3.281435
				H	3.657356	3.873001	3.584460	H	3.657358	3.873003	3.584461
				H	-0.212844	4.215642	2.271720	H	-0.212844	4.215644	2.271721
				H	1.985351	-1.349363	3.798935	H	1.985352	-1.349363	3.798937
				H	-0.177584	-4.179342	-2.615442	H	-0.177585	-4.179344	-2.615443
				H	-0.832419	3.884483	-2.289901	H	-0.832420	3.884485	-2.289902
				H	-0.420949	4.180617	-0.578190	H	-0.420950	4.180619	-0.578191
				C	-0.726814	-2.466897	-1.483852	C	-0.726814	-2.466899	-1.483853
				O	-1.672492	-1.938422	-2.101359	O	-1.672493	-1.938422	-2.101360
				N	-0.533648	-2.428526	-0.162735	N	-0.533648	-2.428528	-0.162735

H	0.302878	-2.912018	0.151876	H	0.302878	-2.912020	0.151876
C	-2.475557	3.519920	-0.972387	C	-2.475558	3.519922	-0.972388
O	-3.319241	3.514573	-1.872779	O	-3.319243	3.514574	-1.872780
N	-2.788418	3.396808	0.341609	N	-2.788419	3.396810	0.341610
H	-2.038063	3.392189	1.020145	H	-2.038064	3.392190	1.020146
C	-4.114009	3.045297	0.833564	C	-4.114011	3.045298	0.833565
H	-4.254448	3.524751	1.803856	H	-4.254450	3.524753	1.803857
C	-4.329017	1.524724	0.996897	C	-4.329019	1.524724	0.996898
H	-5.194513	1.378979	1.659723	H	-5.194515	1.378980	1.659724
C	-3.109228	0.823536	1.619588	C	-3.109229	0.823536	1.619589
H	-2.272422	0.947410	0.918643	H	-2.272423	0.947410	0.918643
C	-3.373231	-0.707667	1.824974	C	-3.373232	-0.707668	1.824975
C	-2.751657	-1.528419	0.667968	C	-2.751659	-1.528419	0.667968
O	-4.580636	0.858070	-0.243047	O	-4.580639	0.858070	-0.243047
O	-2.827077	1.542045	2.804447	O	-2.827079	1.542046	2.804448
C	-1.236484	-1.641522	0.845163	C	-1.236484	-1.641523	0.845164
O	-2.875685	-1.090764	3.098325	O	-2.875687	-1.090764	3.098327
H	-4.459768	-0.880728	1.801084	H	-4.459771	-0.880728	1.801084
O	-3.290289	-2.843484	0.592928	O	-3.290290	-2.843486	0.592928
H	-2.978834	-0.999659	-0.257170	H	-2.978835	-0.999660	-0.257170
C	-4.472314	-2.915241	-0.196179	C	-4.472316	-2.915243	-0.196179
H	-5.274281	-2.277728	0.202647	H	-5.274284	-2.277729	0.202647
H	-4.804688	-3.956244	-0.176556	H	-4.804690	-3.956246	-0.176556
H	-4.270551	-2.614613	-1.233407	H	-4.270553	-2.614614	-1.233408
C	-3.418883	-2.304396	3.612136	C	-3.418885	-2.304397	3.612137
H	-3.083934	-3.178161	3.043652	H	-3.083935	-3.178162	3.043653
H	-4.518516	-2.278422	3.598054	H	-4.518518	-2.278423	3.598056
H	-3.074084	-2.382435	4.646703	H	-3.074086	-2.382436	4.646705
C	-5.908656	0.998608	-0.756976	C	-5.908659	0.998608	-0.756977
H	-5.997223	0.295016	-1.586221	H	-5.997226	0.295016	-1.586222
H	-6.088529	2.014490	-1.127735	H	-6.088531	2.014491	-1.127736
H	-6.646370	0.751708	0.016671	H	-6.646373	0.751708	0.016671
C	-1.472316	1.469674	3.251124	C	-1.472316	1.469675	3.251126
H	-0.770477	1.703480	2.437171	H	-0.770477	1.703481	2.437172
H	-1.240445	0.479906	3.653988	H	-1.240446	0.479907	3.653989
H	-1.366192	2.220816	4.038430	H	-1.366192	2.220818	4.038432
H	-0.803316	-0.634343	0.881015	H	-0.803316	-0.634344	0.881015
H	-1.029520	-2.111034	1.808211	H	-1.029520	-2.111035	1.808212
H	-4.853461	3.451259	0.140849	H	-4.853463	3.451260	0.140849
H	0.517308	-2.659145	-3.185432	H	0.517308	-2.659146	-3.185433
H	-3.688313	-1.753233	-3.487678	C	-3.015657	0.892127	-3.742589
C	-4.531241	-1.139616	-3.794434	H	-3.120940	1.976200	-3.817677
C	-6.710608	0.427636	-4.563860	N	-2.613199	0.630838	-2.320923
C	-4.358425	0.237844	-3.996241	H	-3.372509	0.844763	-1.651835
C	-5.786900	-1.724100	-3.964184	H	-1.776123	1.210400	-2.016197
C	-6.880570	-0.941385	-4.348386	H	-2.337559	-0.361221	-2.182959
C	-5.455114	1.014124	-4.384016	C	-1.893863	0.401941	-4.661968
H	-5.911783	-2.790204	-3.794508	C	0.137499	-0.485696	-6.326795
H	-7.858384	-1.397058	-4.478280	C	-1.015132	1.311759	-5.229032
H	-5.330239	2.084205	-4.529721	C	-1.756913	-0.951694	-4.927317
H	-7.555859	1.042133	-4.861519	C	-0.741231	-1.395514	-5.759731
C	-3.015656	0.892127	-3.742587	C	0.000549	0.867939	-6.061446
H	-3.120939	1.976199	-3.817675	H	-1.123414	2.382027	-5.019231
C	-1.894365	0.402160	-4.661554	H	-2.451691	-1.671052	-4.478962
H	-2.158598	0.597509	-5.704530	H	-0.632949	-2.465782	-5.969533
H	-1.731037	-0.673044	-4.534845	H	0.695328	1.587296	-6.509802
H	-0.957987	0.924449	-4.434314	H	0.940560	-0.836607	-6.984953
N	-2.613198	0.630838	-2.320922	C	-4.372539	0.230967	-3.998909
H	-3.372508	0.844762	-1.651834	H	-4.268552	-0.857506	-3.923882
H	-1.776122	1.210399	-2.016196	H	-4.724332	0.496043	-5.002498
H	-2.337558	-0.361221	-2.182958	H	-5.096086	0.581059	-3.253838

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