

# Electronic Supplementary Information

## Membrane-specific spin trap, 5-dodecylcarbamoyl-5-N-dodecylacetamide-1-pyrroline-N-oxide (diC<sub>12</sub>PO): Theoretical, bioorthogonal fluorescence imaging and EPR studies

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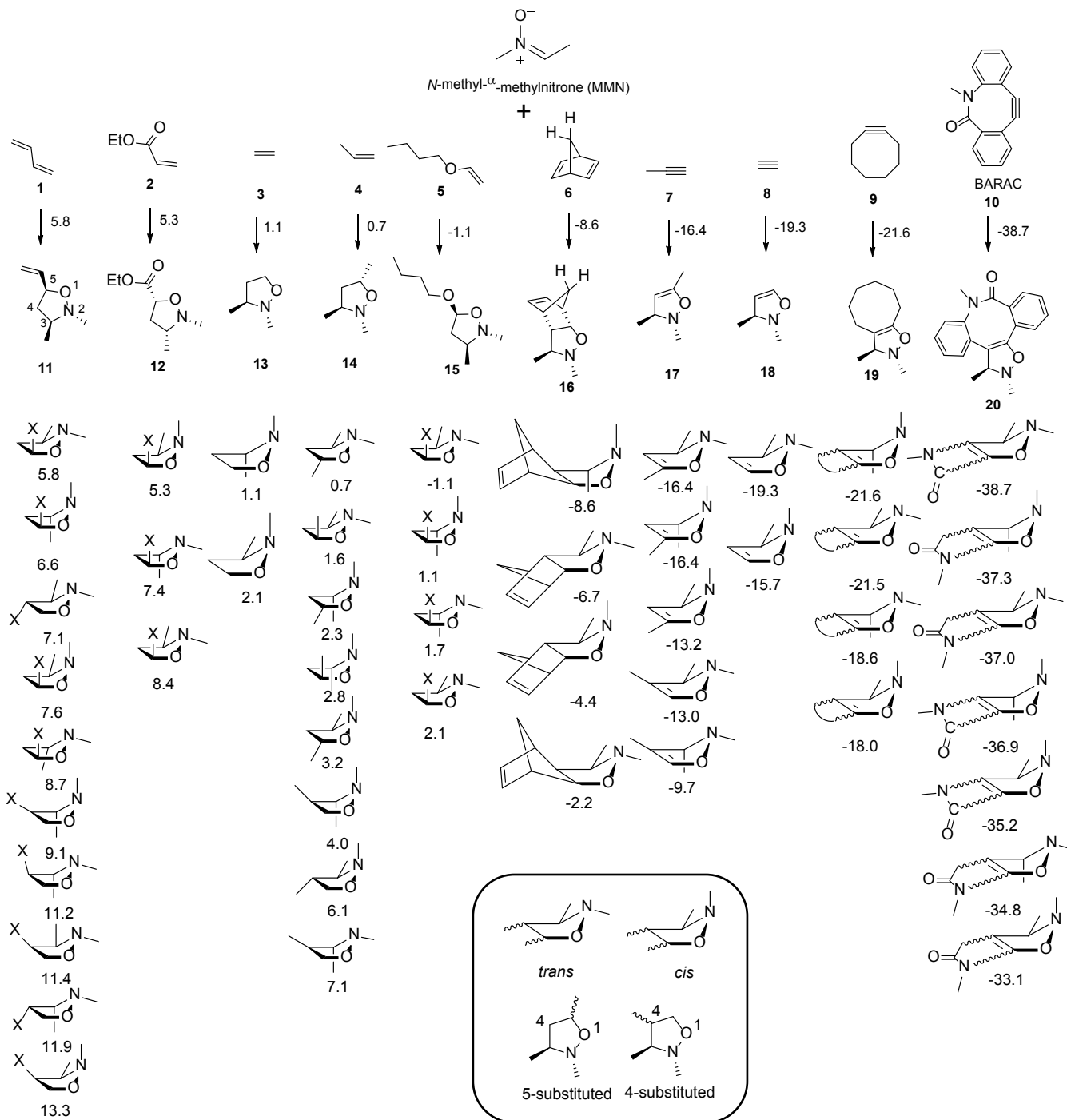
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**Scheme S1.** Gibbs free energies dipolar cycloaddition reactions (in kcal/mol) of the various alkenes and alkynes with MMN.



**Table S1.** Cartesian Coordinates**MMN**

C	-2.818857419	1.180700817	-0.122270595
N	-2.232484143	2.252167484	0.35014335
O	-1.00125131	2.305645795	0.68210498
C	-2.983621614	3.511555946	0.536034661
H	-2.487873282	4.278435696	-0.062160214
H	-4.027331085	3.400376093	0.235542864
H	-2.910992089	3.781913685	1.591175531
H	-3.870047724	1.254602307	-0.369743974
C	-2.021721246	-0.064476355	-0.292020777
H	-2.640103143	-0.87217064	-0.691517143
H	-1.172435055	0.107744906	-0.966300705
H	-1.588407941	-0.380723394	0.665958801

**1**

C	-3.804007744	0.049220754	0
H	-3.314122657	-0.922257885	0
H	-4.889730413	0.047292161	0
C	-3.09876254	1.18910166	0
H	-3.624229839	2.144810888	0
C	-1.64294774	1.254879439	0
H	-1.117480441	0.29917021	0
C	-0.937702536	2.394760344	0
H	-1.427587623	3.366238983	0
H	0.148020133	2.396688937	0

**2**

C	-3.635361638	1.424095071	0.020767445
H	-3.226348229	0.419440989	0.080519783
H	-4.715636806	1.532576321	0.008315587
C	-2.822495442	2.481083731	-0.034839773
H	-3.194821191	3.499452296	-0.095110213
C	-1.347972366	2.305510342	-0.016170146
O	-0.724968394	3.506639765	-0.081090417
O	-0.757893547	1.245700984	0.047860021
C	0.709202185	3.452211523	-0.069777808
H	1.04290782	4.488688404	-0.128489989
H	1.068929936	2.983680332	0.850455646
H	1.079111422	2.879709293	-0.924843446

**3**

C	-2.389767971	0.383301255	0
H	-1.876686249	-0.575625642	0
H	-3.476747671	0.347681358	0
C	-1.724601969	1.536012605	0
H	-2.237683692	2.494939502	0
H	-0.637622269	1.571632503	0

**4**

C	-1.248245411	0.105429962	0.173453923
H	-0.69281548	-0.819369882	0.042036995
H	-2.241300421	0.017899524	0.610437732
C	-0.741577991	1.286659526	-0.181149363
H	0.258962998	1.321978728	-0.615072021
C	-1.440090949	2.608196624	-0.034012506
H	-0.863987289	3.293037629	0.60291449
H	-1.55513455	3.106916461	-1.005933554
H	-2.435341699	2.489338178	0.407324344

**5**

C	-4.064969183	1.965876369	0.067911591
H	-3.780003293	0.908052727	0.086734694
H	-3.587623749	2.4560276	0.924999798
H	-5.150054359	2.022573524	0.216250246
C	-3.651927376	2.630332303	-1.24939282
H	-4.116907403	2.095490905	-2.089653706
H	-2.566003465	2.527248122	-1.38512953
C	-4.036727945	4.113956335	-1.3122568
H	-5.121388114	4.226941893	-1.186557092
H	-3.566520208	4.661123238	-0.484783194
C	-3.629453656	4.771822631	-2.622713862
H	-4.107843742	4.266278162	-3.475493098
H	-2.539315216	4.70963939	-2.765504464
O	-4.034320371	6.141089872	-2.581685951
C	-3.655925439	6.9026342	-3.645483316
H	-2.939822067	6.433887274	-4.322410889
C	-4.107358731	8.141933283	-3.840073898
H	-3.754050538	8.720101316	-4.685615665
H	-4.820724184	8.598804369	-3.162055414

**6**

C	-0.668009412	-1.245649236	-0.513593837
C	0.668009412	-1.245649236	-0.513593837
C	1.122814555	0	0.278464512
C	0.668009412	1.245649236	-0.513593837
C	-0.668009412	1.245649236	-0.513593837
C	-1.122814555	0	0.278464512
H	-1.338561299	-1.936984858	-1.012044722
H	1.338561299	-1.936984858	-1.012044722
H	2.160215104	0	0.61917599
H	1.338561299	1.936984858	-1.012044722
H	-1.338561299	1.936984858	-1.012044722
H	-2.160215104	0	0.61917599
C	0	0	1.361868615
H	0	0.900102598	1.985702305
H	0	-0.900102598	1.985702305

**7**

C	-1.179611617	0.959484399	0.65249246
H	-2.054512093	1.561411849	0.558875351
C	-0.188965655	0.277914836	0.758534472

C	1.009682739	-0.546697676	0.887592755
H	1.014154843	-1.093551832	1.837947792
H	1.072559606	-1.28399804	0.078470866
H	1.918186317	0.066135834	0.851415945

### 8

C	-2.073084096	2.21682845	0
H	-3.139736561	2.21682845	0
C	-0.868110924	2.21682845	0
H	0.198541541	2.21682845	0

### 9

C	-0.469885014	1.444890497	0.224052286
H	-0.123235019	2.036355818	1.081269206
H	-0.147297124	1.984825534	-0.677471645
C	0.176600385	0.031093007	0.254988419
H	0.078847848	-0.374678091	1.270200674
H	1.253095466	0.149034934	0.070796212
C	-0.401174509	-0.993712073	-0.756668607
H	0.412554122	-1.69462136	-0.982428442
H	-0.61956613	-0.483665369	-1.704689681
C	-1.636042944	-1.852865258	-0.325820467
H	-1.40938834	-2.893432109	-0.590856189
H	-1.728217719	-1.843061247	0.768708742
C	-3.0163539	-1.534321699	-0.958885143
H	-2.867643359	-1.213848159	-1.998136581
H	-3.61279607	-2.455814338	-1.001155481
C	-3.859981938	-0.453848899	-0.224995492
H	-4.727343255	-0.17370623	-0.836569466
H	-4.260051338	-0.864089228	0.71307995
C	-2.967731357	0.668921301	0.054775668
C	-1.918296837	1.253067182	0.206647393

### 10

C	0.176501031	-0.010200206	-0.401842775
C	1.570716816	0.084892981	-0.360797233
C	1.37402726	2.451147334	0.187229356
C	-0.021875932	2.338876679	0.1574467
C	-0.613640059	1.11254839	-0.143210749
H	-0.292337499	-0.96459282	-0.624279156
H	2.186226304	-0.79346149	-0.534731214
H	-0.632546432	3.210148181	0.373673532
H	-1.696667115	1.031007471	-0.168635647
H	4.904043773	6.263741149	1.457146346
C	5.378643769	5.44278047	0.92868442
C	6.758692285	5.428959401	0.731743804
C	4.590060848	4.388516943	0.449536076
C	7.366557025	4.364399464	0.063137513
H	7.362824215	6.249889188	1.107541983
C	6.594995144	3.303521624	-0.420753612
H	8.443332372	4.355795576	-0.080012497
H	7.056086658	2.466540682	-0.936176596
C	2.180195139	1.306537147	-0.088825006

C	5.217095435	3.302846675	-0.240458312
C	2.133190601	3.626727765	0.476860702
C	3.180309023	4.241497602	0.602835704
C	3.674234206	1.477725949	0.116556073
O	4.210394625	1.025746576	1.113230521
C	3.827713271	2.580266846	-2.120818889
H	4.654132662	2.68093591	-2.831286305
H	3.193717587	1.753044048	-2.446876291
H	3.237604164	3.505640025	-2.132148441
N	4.377224634	2.276194461	-0.797076766

### 11

C	-3.398262946	1.418840756	-1.084112937
H	-3.379511642	0.994480711	-2.086554958
H	-4.232260946	2.076060998	-0.853150247
C	-2.44731524	1.145298418	-0.19150414
H	-2.483870261	1.571928444	0.810495974
O	-1.177349352	-0.791309549	0.526527504
N	-0.278338525	-0.257362282	1.5539455
C	0.036722316	-1.404327552	2.390295761
H	0.491867004	-2.231195226	1.819899729
H	0.726044359	-1.079304373	3.175272411
H	-0.882941726	-1.760584376	2.861270697
C	0.847466695	0.236198894	0.739315454
H	1.392288465	-0.617380105	0.296767121
C	1.802248481	1.09945224	1.558372965
H	2.31341494	0.51641708	2.332443344
H	2.571915054	1.534077551	0.911165192
H	1.256147325	1.914577728	2.04518808
C	0.100588564	0.994557949	-0.370997707
H	0.644941089	0.973529036	-1.31955413
H	-0.044863499	2.043406986	-0.089996183
C	-1.26500487	0.255322995	-0.456764099
H	-1.389949485	-0.255037983	-1.417802279

### 12

O	-0.920555865	1.929662728	-0.504388173
C	0.482448162	1.738463554	-0.253454131
H	0.787427575	0.919673651	-0.905462726
H	1.039546937	2.648399147	-0.490741841
H	0.653015955	1.481237843	0.795428172
C	-1.509088583	2.902109476	0.223318111
O	-0.925852128	3.591755057	1.028945721
O	-3.358952871	4.327731432	-0.219723584
N	-4.747653065	4.381916898	0.258847182
C	-4.653144887	3.670836008	1.554511734
C	-5.081011676	5.79639396	0.301265673
H	-6.087229843	5.888853247	0.723107785
H	-4.378380499	6.399856632	0.893234772
H	-5.097343005	6.177856955	-0.723261456
C	-3.00365842	2.961654082	-0.073918765
H	-3.216942154	2.402639336	-0.992211202
C	-3.860429388	2.421908383	1.115243387

H -4.527860822	1.632514685	0.760867444
H -3.250548404	2.020425306	1.929058168
C -3.972018738	4.427225035	2.703362869
H -4.535138865	5.321811635	2.990144765
H -2.955549901	4.720029689	2.425162251
H -5.67792221	3.39992404	1.835649837
H -3.911947969	3.779967364	3.585927196

**13**

C -1.690047438	0.944944404	0.763795481
C -2.971033484	1.707777146	1.20736888
H -3.75388197	1.661903818	0.444384288
N -0.780558329	1.991836254	0.257109734
C -1.068255686	2.411758863	-1.115606869
H -0.435621506	3.271561301	-1.347975643
H -0.797955224	1.589073818	-1.785804787
H -2.120355786	2.684980483	-1.302184109
O -1.036144537	3.101461886	1.140534969
C -2.456882275	3.148709463	1.398731352
H -2.953091283	3.853765134	0.718129198
H -1.901589414	0.251728953	-0.058212661
C -1.021169364	0.191121485	1.914129118
H -0.102033573	-0.293792327	1.571318644
H -1.69219459	-0.575045991	2.31982075
H -0.75772661	0.88479315	2.71932613
H -3.384449043	1.287143284	2.128784492
H -2.56722568	3.522057847	2.420711854

**14**

C -1.529122317	0.849069509	0.587053811
C -2.812031549	1.481216385	1.169026296
N -0.764945356	2.040656025	0.158707021
O -0.971601407	2.952347685	1.282536006
C -2.390489171	2.945819238	1.455501398
H -2.842228649	3.608805228	0.702640834
H -3.129691789	0.958429634	2.077334614
C 0.673446314	1.8385852	0.103063516
H 0.892056588	1.138526515	-0.708856417
H 1.156481876	2.792951222	-0.122068615
H 1.082477253	1.442312876	1.047884696
H -0.984539694	0.33087968	1.396602617
C -1.764417578	-0.110544707	-0.575474844
H -0.824582217	-0.528069266	-0.954002669
H -2.392638661	-0.949221743	-0.25546567
H -2.266907963	0.406649469	-1.399843053
H -3.638816135	1.442611982	0.451675148
C -2.696291669	3.455800204	2.854539223
H -2.285211032	4.460311637	2.99936406
H -3.779435269	3.502749706	3.014020191
H -2.260786286	2.79202495	3.609434388

**15**

C -4.349337674	3.001790697	0.62740211
H -4.13945326	2.059015705	1.14525344

H -3.941951307	3.816466009	1.238387038
H -5.438305461	3.128199612	0.591943125
C -3.745225823	3.012201048	-0.780564554
H -4.145684421	2.165140988	-1.355649444
H -2.660324642	2.848998827	-0.713587387
C -4.017789391	4.318250577	-1.537271951
H -5.100003857	4.485543224	-1.621002379
H -3.612419083	5.169436055	-0.974609218
C -3.409962897	4.32911532	-2.933586696
H -3.821340801	3.504800091	-3.542502888
H -2.321265546	4.192923149	-2.88681156
O -3.716187178	5.579339678	-3.546957351
O -1.825568901	5.669621622	-4.962991216
N -1.396720639	7.071962307	-4.816755972
C -3.660098945	7.083949671	-5.396416154
H -4.318900085	7.012665937	-6.2661987
H -4.185628796	7.620208118	-4.601232606
C -3.239296418	5.704374797	-4.859483374
H -3.58051174	4.852085669	-5.46528871
C -2.321725796	7.760291355	-5.73850035
H -2.051315208	7.526583983	-6.78470679
C -2.306897997	9.270372573	-5.521062955
H -2.523658843	9.505074034	-4.473800964
H -1.33604582	9.707533065	-5.779482039
H -3.063293174	9.751641081	-6.150803664
C -0.009719115	7.072083783	-5.251169331
H 0.36571613	8.098257103	-5.192979413
H 0.575808894	6.450724605	-4.568660256
H 0.114807722	6.693925248	-6.279881521

**16**

C -0.858682783	-0.560219158	-0.419856575
C 0.336831511	-1.164165386	-0.394373884
C 1.335698401	-0.1795281	0.208918274
C 1.532118731	0.925530414	-0.869573771
C 0.135485023	1.62441119	-0.935867993
C -0.6777709	0.846055225	0.152207473
H -1.777393839	-0.935488222	-0.859996689
H 0.594513569	-2.134101165	-0.807399037
H 2.269658369	-0.598418722	0.589714772
H 1.872144455	0.5333999	-1.835732616
H -0.328498724	1.527277438	-1.921695763
H -1.587217481	1.349634656	0.491340128
C 0.417298232	0.559614618	1.211298002
H 0.881331712	1.454155139	1.635483334
H 0.061763444	-0.091109646	2.01547681
O 2.429487474	1.92686848	-0.3992351
N 1.909175903	3.171916105	-0.979491797
C 2.633294454	4.229291679	-0.293240306
H 3.697766417	4.134533434	-0.522933141
H 2.280195714	5.191920832	-0.675397633
H 2.497247945	4.19818585	0.801194763
C 0.467781543	3.10254132	-0.645939154
H 0.317330502	3.31621675	0.427413508
C -0.335443025	4.09771427	-1.480496008
H -1.406484521	3.985032628	-1.278000354

H -0.063776263 5.133880102 -1.249735784  
H -0.162155864 3.927450368 -2.548281459

17

C -3.918431389 0.715176834 -0.026659938  
H -3.896830124 1.721388669 0.417380398  
C -5.336256258 0.145206984 0.10694424  
H -5.604452866 0.026468414 1.163721449  
H -6.066930853 0.8114915 -0.365107384  
H -5.397624308 -0.834371403 -0.377390196  
C -2.84294928 -0.182714563 0.534841394  
H -2.702230525 -0.407327565 1.583347287  
C -2.160902219 -0.710933753 -0.484237527  
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H -3.470290112 2.908564618 -1.623017292  
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18

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H -3.874668159 1.206843648 1.600605216  
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19

C -0.549028747 1.22906707 0.574830475  
H -0.193579832 1.591000121 1.552849232  
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C -3.358139883 -0.683091821 0.514523463  
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O -4.26240536 1.496666331 0.148175925  
C -2.470229765 3.003760863 0.250562491  
H -1.910914851 3.527445511 -0.540241687  
C -2.380444855 3.825869938 1.543557126  
H -1.340535707 3.91052944 1.880886262  
H -2.775504684 4.835193474 1.384659474  
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20

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H -2.85559994 1.907060743 2.875589326  
H -2.39152155 -0.402387856 3.699638483  
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C 1.302191287 -0.955585289 -1.026486752  
C 2.4342789 1.130470909 -1.477335141  
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C 3.620178058 0.613522939 -0.966570683  
H 2.408603857 2.151928079 -1.847575027  
C 3.649680273 -0.688492315 -0.460269681  
H 2.508686126 -2.484238979 -0.120415729  
H 4.516355222 1.227711803 -0.951354795  
H 4.566596216 -1.098039894 -0.045958241  
N 0.196081027 -1.852722943 -1.200882746  
C -1.161714393 1.030673832 -1.321968099  
C 0.002287501 0.962311477 -1.993246297  
C 0.420838175 -3.01448766 -2.069868064  
H -0.534805298 -3.329592937 -2.4907816  
H 1.106634621 -2.725385581 -2.868725471  
H 0.842840173 -3.865056299 -1.51984264  
C -0.923639896 -1.902556092 -0.404304122  
O -1.657320906 -2.887446502 -0.40655689  
O -2.121291984 1.776070811 -1.966216581  
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C -1.257433109 3.816305511 -2.668020035

H -0.811613168	4.366803774	-3.503073473
H -2.227514638	4.261902619	-2.436324549
H -0.598880004	3.896285577	-1.78757776
C -0.192956464	1.693581018	-3.310888764
H 0.603042085	2.427034663	-3.500554388
C -0.298248154	0.746667251	-4.512425053
H 0.630467524	0.176421238	-4.629926071
H -1.123226056	0.042542372	-4.367240206
H -0.482040035	1.311949301	-5.43243021

**DMPO**

C 0.825233547	0.266373481	0.148532782
C 3.123881334	0.464804917	-0.718596641
C 1.683308103	1.011684022	-0.895107509
H 3.746200273	1.137320246	-0.108265415
H 3.64221874	0.352173091	-1.678460925
H 1.628192546	2.096829555	-0.767974425
H 1.32285513	0.778279186	-1.902532829
N 1.681162035	-0.967159097	0.439690761
C 2.896187539	-0.841676918	-0.029518363
H 3.614154124	-1.629362043	0.159219953
O 1.184903356	-1.918288982	1.111167582
C -0.52984879	-0.205776619	-0.371803821
H -1.009829761	-0.852888286	0.3663214
H -1.176019507	0.65684074	-0.567664235
H -0.417075153	-0.771164077	-1.303172345
C 0.681296885	1.021592388	1.475697083
H 0.002759247	1.872724591	1.354070134
H 0.275110017	0.35170011	2.239021646
H 1.648423726	1.399818164	1.825818707

**PBN**

C -2.485112482	2.362612253	0.909458422
C -1.422903509	2.170109451	-0.001817075
C -1.379592877	2.976831309	-1.159382553
C -2.368567756	3.933735717	-1.380747956
C -3.412278609	4.112382426	-0.471002945
C -3.466118244	3.319576668	0.67917282
H -2.533351226	1.749108272	1.806761967
H -0.57009437	2.83570949	-1.861337994
H -2.320964233	4.546982144	-2.276986286
H -4.177749987	4.861725015	-0.654235879
H -4.273290874	3.448512659	1.3954568
C -0.453076301	1.143679407	0.336207079
H -0.609130734	0.600775666	1.255763454
N 0.607919532	0.798403713	-0.363636269
O 0.946986676	1.333551533	-1.474907318
C 1.561667526	-0.307695124	0.101288049
C 1.149517222	-0.941955476	1.433580827
H 0.169222046	-1.426962501	1.377094732
H 1.882269612	-1.715534958	1.686146689
H 1.144069525	-0.217114351	2.25453517
C 2.942907343	0.353348934	0.230902303
H 3.696959387	-0.406940382	0.459683163
H 3.207689573	0.852993767	-0.702361122

H 2.945795424	1.09462047	1.038100276
C 1.5588034	-1.363806515	-1.01502719
H 1.797036774	-0.897015485	-1.972153125
H 2.302958727	-2.136403049	-0.795230068
H 0.577014949	-1.844242832	-1.094223782

**DBCO-Me**

C 1.429834154	2.311965653	-3.694631792
C 1.079886529	3.269660806	-2.739985278
C 0.397969383	2.89236723	-1.580447191
C 1.111697836	0.972045533	-3.486861233
C 0.429076036	0.589834226	-2.323696338
C 0.046931889	1.561847142	-1.355965627
C -0.799275016	1.168908164	-0.150993787
N -0.169258223	0.248394081	0.838971751
C -0.333092578	-1.590394332	-1.185689035
C 0.096071414	-0.739515161	-1.945402083
C -0.79647615	-2.028347838	0.083313558
C -0.73561823	-1.035626846	1.108273658
C 0.870684748	0.795942622	1.576659192
C -1.245182189	-1.340658422	2.373169238
C -1.758436195	-2.609202978	2.650397688
C -1.796709155	-3.58565822	1.652827007
C -1.328163845	-3.293029649	0.374463801
C 1.656773234	-0.114460605	2.508042062
O 1.166767409	1.977629632	1.446627897
H 1.959772752	2.607886016	-4.595777737
H 1.342093591	4.312588067	-2.894933657
H 0.142691422	3.636954369	-0.832097081
H 1.393278112	0.215163227	-4.212603643
H -1.085762257	2.078632138	0.383830336
H -1.710795009	0.672021721	-0.492549401
H -1.23997136	-0.574364489	3.142557643
H -2.140237763	-2.827740026	3.643636305
H -2.202171694	-4.570172739	1.867645785
H -1.368793235	-4.038453101	-0.413713652
H 1.708445511	-1.147264897	2.155245843
H 2.662303863	0.303323844	2.58893642
H 1.215665003	-0.120275137	3.510749313

**HYA-Me**

C 1.642158991	-0.555671806	2.958283749
C 1.835488349	-0.380667313	1.778176682
C 2.0531488	-0.144066175	0.349059164
H 1.645820933	-0.980367979	-0.233009115
H 3.132206744	-0.126056448	0.145997131
C 1.424940967	1.171764392	-0.162192465
H 1.663942496	1.268282795	-1.225519292
H 1.879428501	2.018417143	0.364744994
C -0.09546597	1.234511447	0.00728994
H -0.451619068	2.234877364	-0.275478567
H -0.367156785	1.088210644	1.060312898
C -0.823368409	0.223195176	-0.882344609
O -0.342658525	-0.191392494	-1.932769014
N -2.057635278	-0.152624204	-0.432062011
H 1.488451641	-0.722630627	3.999990491

C -2.914791866 -1.072722798 -1.157145711  
H -2.398163993 -1.335274974 -2.081283606  
H -3.87789516 -0.609122641 -1.402177522  
H -3.099700573 -1.986019728 -0.578666995  
H -2.370425994 0.199123028 0.461264459

**(Z)-DBCO-Me-DMPO**

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C 1.005380758 2.854626475 -1.457739004  
C 0.688242025 1.827001649 -0.55301469  
C 1.520724059 1.628194754 0.571726053  
C 1.085985039 0.722102453 1.703560856  
N 1.344164585 -0.727837936 1.555594371  
C -0.376483953 -0.407526741 -0.878706526  
C -0.450633856 0.935831911 -0.807445382  
C 0.813823519 -1.277733979 -0.815499762  
C 1.673898603 -1.334481509 0.296920667  
O -1.528531931 -1.008613607 -1.27886832  
N -2.473610876 0.069765945 -1.674273029  
C -1.858475785 1.349602468 -1.169086708  
C 2.845148897 -2.09738436 0.216412256  
C 3.153745079 -2.816617198 -0.933300698  
C 2.286056649 -2.789416686 -2.027320548  
C 1.128463077 -2.02258194 -1.965040752  
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C -2.721000838 1.842970374 0.035651342  
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H 3.887958313 4.006142666 -0.067515223  
H 3.309978529 2.257073235 1.586369485  
H 0.363790129 3.017810818 -2.319596333  
H 1.60223155 1.058016523 2.608069778  
H 0.012316694 0.881007522 1.867002372  
H 3.497436036 -2.140822296 1.08117388  
H 4.065876304 -3.405705111 -0.970396558  
H 2.514116597 -3.356403551 -2.925454237  
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H -3.377618247 2.665302814 -0.269823543  
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O 1.28161391 -2.793861135 2.55096155  
C 0.734258878 -0.940589643 3.958341439  
H 0.543906708 -1.751009705 4.662578564  
H 1.531739057 -0.304012019 4.359842482  
H -0.165223341 -0.322184254 3.867254173  
C -3.753339763 -0.131884341 -0.920227567  
C -4.834643771 0.566355425 -1.768928058  
H -4.923655164 0.074894706 -2.742340582  
H -5.803461759 0.514006073 -1.259319855  
H -4.606453902 1.622202695 -1.948552084  
C -4.104738415 -1.612737001 -0.767128855  
H -5.095825869 -1.704253586 -0.308516693  
H -4.132525235 -2.109063568 -1.742790731

H -3.381459752 -2.135928552 -0.138504317  
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**(E)-DBCO-Me-DMPO**

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C -1.285325373 1.501055341 2.646236465  
C -1.071317048 0.552179237 1.635512711  
C -2.142949532 -0.241776188 1.174402542  
C -1.941203884 -1.455959974 0.292353078  
N -1.474988368 -1.229824784 -1.091049484  
C 0.625541025 0.633631647 -0.256581466  
C 0.269847305 0.470864439 1.031316069  
C -0.293170227 0.923863682 -1.368140412  
C -1.36932882 0.067098788 -1.689698063  
C -1.163417851 -2.385055607 -1.785735271  
C 2.135499328 0.622110295 -0.326329744  
N 2.542466742 0.748221111 1.117840879  
O 1.318659616 0.405102061 1.896150859  
C -2.293615682 0.43975802 -2.672971976  
C -2.139760332 1.626996647 -3.385181424  
C -1.050641949 2.456881317 -3.111272043  
C -0.146612046 2.108705282 -2.111016935  
O -1.311451927 -3.485221637 -1.263153275  
C 2.750806941 -0.705177682 -0.879475793  
C 3.203682509 -1.450884884 0.386289823  
C 3.562435585 -0.316950235 1.375516053  
H -2.710178321 2.447382797 3.952055175  
H -4.630699755 1.109062018 3.090352846  
H -4.248448562 -0.619677024 1.365676281  
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H -1.218816242 -2.130815669 0.76563499  
H -2.880665123 -2.018262117 0.246184026  
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H 2.018582113 -1.272030262 -1.461124384  
H 3.599078751 -0.492018042 -1.539517841  
H 2.378159979 -2.043819779 0.797034679  
H 4.042006427 -2.131444741 0.204193276  
C -0.625370185 -2.250279277 -3.20361168  
H -1.430201689 -2.016467851 -3.908670917  
H 0.127368578 -1.462415079 -3.297244671  
H -0.19335398 -3.214202519 -3.477384129  
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H 5.11599339 1.175288364 1.685490808  
H 5.722522361 -0.404839141 1.137801685  
H 4.947568116 0.697829694 -0.009278445  
C 3.576042187 -0.753920024 2.841453758  
H 4.402218351 -1.455168894 3.004190319  
H 3.723300187 0.106963724 3.502294332  
H 2.643137904 -1.24639001 3.123108332  
H 2.529336364 1.488856565 -0.870025857

**(Z)-DBCO-Me-PBN**



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C -1.800812	-3.103612	-1.40887
C 0.149323	-1.55426	-2.622622
C -0.260408	-1.23491	-1.317843
C -1.235694	-2.043219	-0.689704
C -1.550151	-1.920352	0.785259
N -2.25566	-0.696689	1.230481
C -0.446226	1.017452	-0.249511
C 0.282473	-0.034359	-0.657694
C -1.907892	1.195635	-0.315648
C -2.770179	0.286563	0.329079
C -2.34998	-0.548738	2.604854
O 0.283373	2.085188	0.171454
N 1.697542	1.642844	0.187234
C -4.15314	0.410329	0.154827
C -4.685254	1.447351	-0.609794
C -3.83335	2.375355	-1.211857
C -2.453991	2.245094	-1.067601
O -1.933904	-1.425713	3.35354
H -0.080329	-2.846763	-4.327855
H -1.85342	-4.229378	-3.245113
H -2.550421	-3.724926	-0.92465
H 0.903017	-0.938177	-3.106333
H -2.146896	-2.784597	1.096934
H -0.618351	-1.973923	1.35871
H -4.8052	-0.30984	0.640365
H -5.761555	1.531997	-0.731337
H -4.24129	3.191275	-1.801716
H -1.784162	2.951495	-1.548697
C 2.504364	2.765362	-0.369415
C 2.125208	3.138833	-1.816066
H 1.073208	3.432665	-1.877803
H 2.733906	3.983972	-2.156005
H 2.295979	2.312616	-2.515387
C 3.97723	2.325627	-0.289627
H 4.234851	2.019976	0.72889
H 4.200899	1.491312	-0.961836
H 4.619965	3.165302	-0.574977
C 2.293783	3.97578	0.557712
H 2.535677	3.708215	1.591166
H 2.944583	4.801229	0.248423
H 1.258146	4.323737	0.52704
C 1.752256	0.330845	-0.525859
C 2.568723	-0.691745	0.258154
C 3.443995	-1.550237	-0.413789
C 2.41946	-0.821892	1.644504
C 4.158521	-2.527461	0.282781
H 3.568688	-1.455397	-1.490766
C 3.133397	-1.795246	2.342264
H 1.750889	-0.147459	2.170445
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H 2.208984	0.425708	-1.526904
C -2.959884	0.736156	3.146853

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H -2.767032	0.756502	4.220467

**(E)-DBCO-Me-PBN**

C -3.797700483	3.144666914	-0.030298874
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C -2.204496062	-2.500224638	2.793585766
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H 0.794834853	-1.593156221	0.752523107
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H -1.133032421	2.098636034	1.074266829
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O -2.422504463	0.752107993	2.871846685
N -4.559490795	0.259370718	2.250757023
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H -5.178387555	-1.529299128	3.188175471
H -5.712836298	-0.034079939	3.999281731
H -5.268140214	0.384133353	1.542429468

**(Z)-HYA-Me-DMPO**

C 0.187180945	2.326523449	0.018586793
O -0.465756809	0.222241239	0.52883406
N -0.958251289	0.468276139	-0.859433016
C -0.757547086	1.948086675	-1.088653822
C -3.058165221	1.554767144	-0.385798152
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H -2.124437728	3.549563535	-0.420429353
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H -2.279030001	-0.954271458	-2.696667552
H -3.866414193	-0.187778378	-2.459676301
H -2.484654766	0.773764136	-3.008108764
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H -3.899241816	-1.187185331	-0.15058276
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**(Z)-HYA-Me-PBN**

C 0.355230863	0.326278092	-1.656486512
C 0.314695628	-0.857804963	-1.041747318
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H 3.146897084	2.728105963	-0.803699509
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H 4.5908703	2.441722029	0.18727894
C 1.241192509	-0.8378776	0.149156311
C 0.517447204	-1.165292757	1.455066238
C 0.510792779	-2.479108033	1.934873536

**(E)-HYA-Me-DMPO**

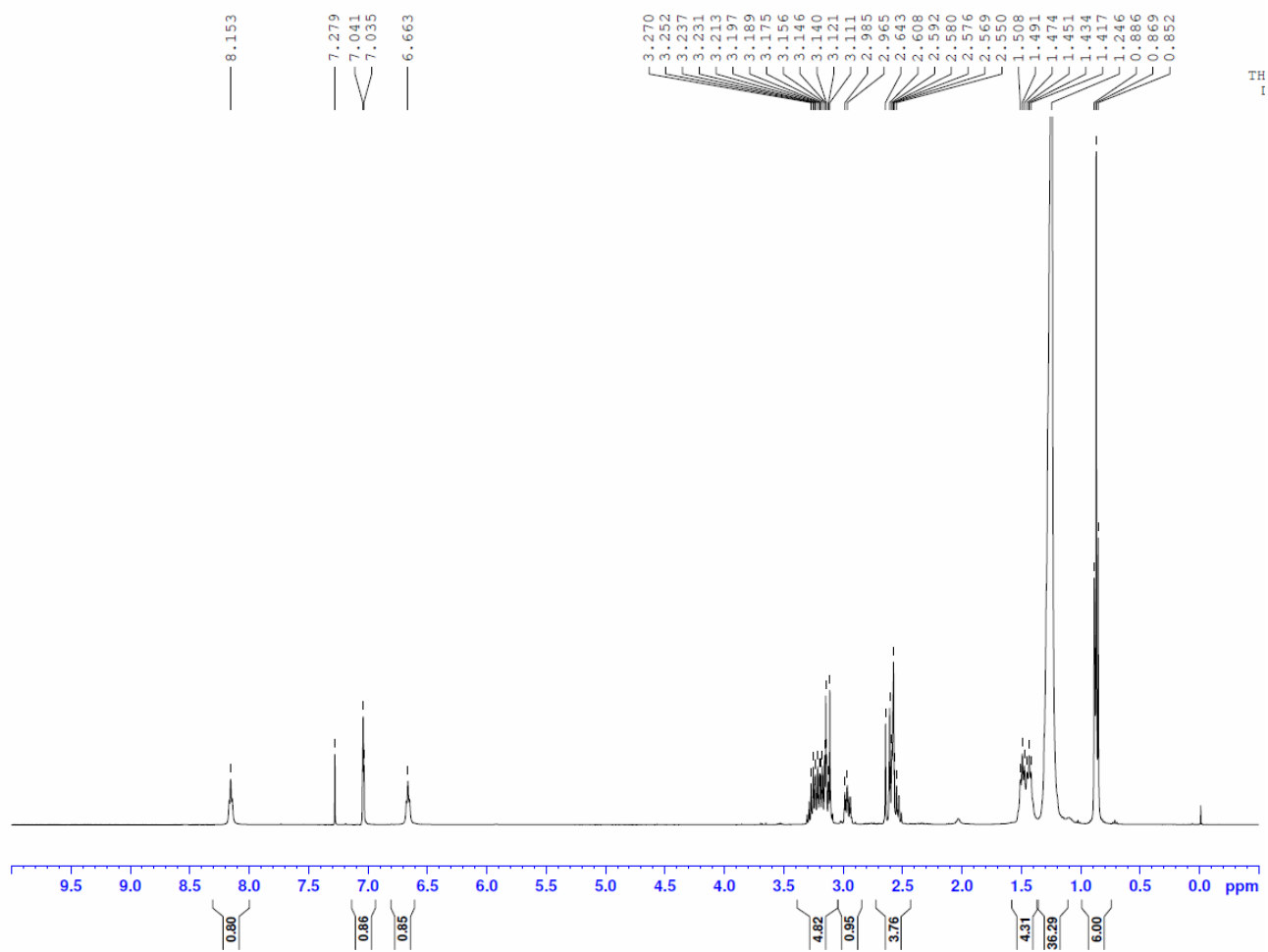
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H 0.247596631	1.166075171	-3.61433852	C -0.214426865	-1.969117348	-3.329768114
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H -1.940560887	2.329259233	-3.287788466	N 1.007835083	-2.079602069	-2.729123468
H -0.674622363	2.943554538	-2.216047277	H -3.083326965	-1.032210075	0.433663744
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H -2.814877245	2.740048496	-1.0266543	H 1.989563442	-1.882058505	-4.528490715
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C -4.202975293	-1.357482663	-0.497276351			
H -3.639780682	-2.295607668	-0.582346345			
H -4.827418869	-1.237695454	-1.38375588			
H -4.840562057	-1.411661275	0.392465626			
H -2.657725324	-0.155029552	0.332420326			

**(E)-HYA-Me-PBN**

C -2.226990201	-0.411409046	0.668918231
C -1.396046209	0.259138345	-0.130743531
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N -0.73210236	0.472370942	2.13367175
C -0.993626614	1.510961499	3.170918637
C -2.14640448	2.465664132	2.803981032
H -3.075576212	1.907968939	2.655695802
H -2.307756622	3.188821471	3.611133991
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H 1.147908998	1.601164157	3.574555238
H 0.591455272	2.872419147	2.470924798
H 0.21795823	2.982834654	4.19461677
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H -1.434102347	1.487770032	5.29857287
H -2.250588445	0.201071812	4.388980964
C -0.375753836	0.948616945	0.765481214
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C 1.850457967	1.480821481	-0.329133742
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C 2.928024556	-0.96634904	0.448905967
H 1.025727812	-1.305102501	1.418411488
C 3.700097014	-0.077347475	-0.306659146

Figure S1. 400 MHz  $^1\text{H}$ -NMR spectrum of  $\text{diC}_{12}\text{PO}$  in  $\text{CDCl}_3$ .



**Figure S2.** 100 MHz  $^{13}\text{C}$ -NMR spectrum of diC<sub>12</sub>PO in CDCl<sub>3</sub>.

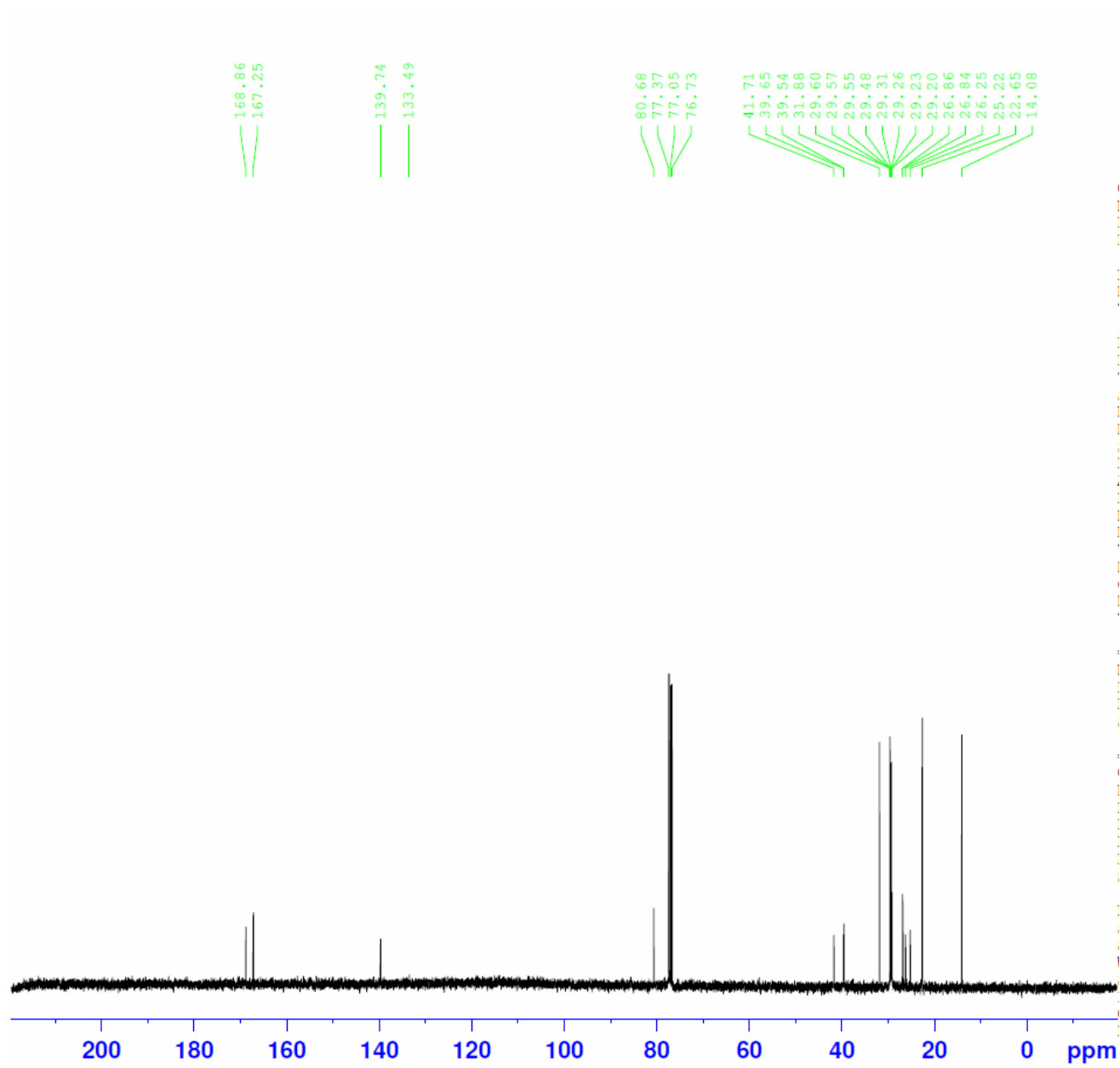


Figure S3. Neat IR spectrum of diC<sub>12</sub>PO.

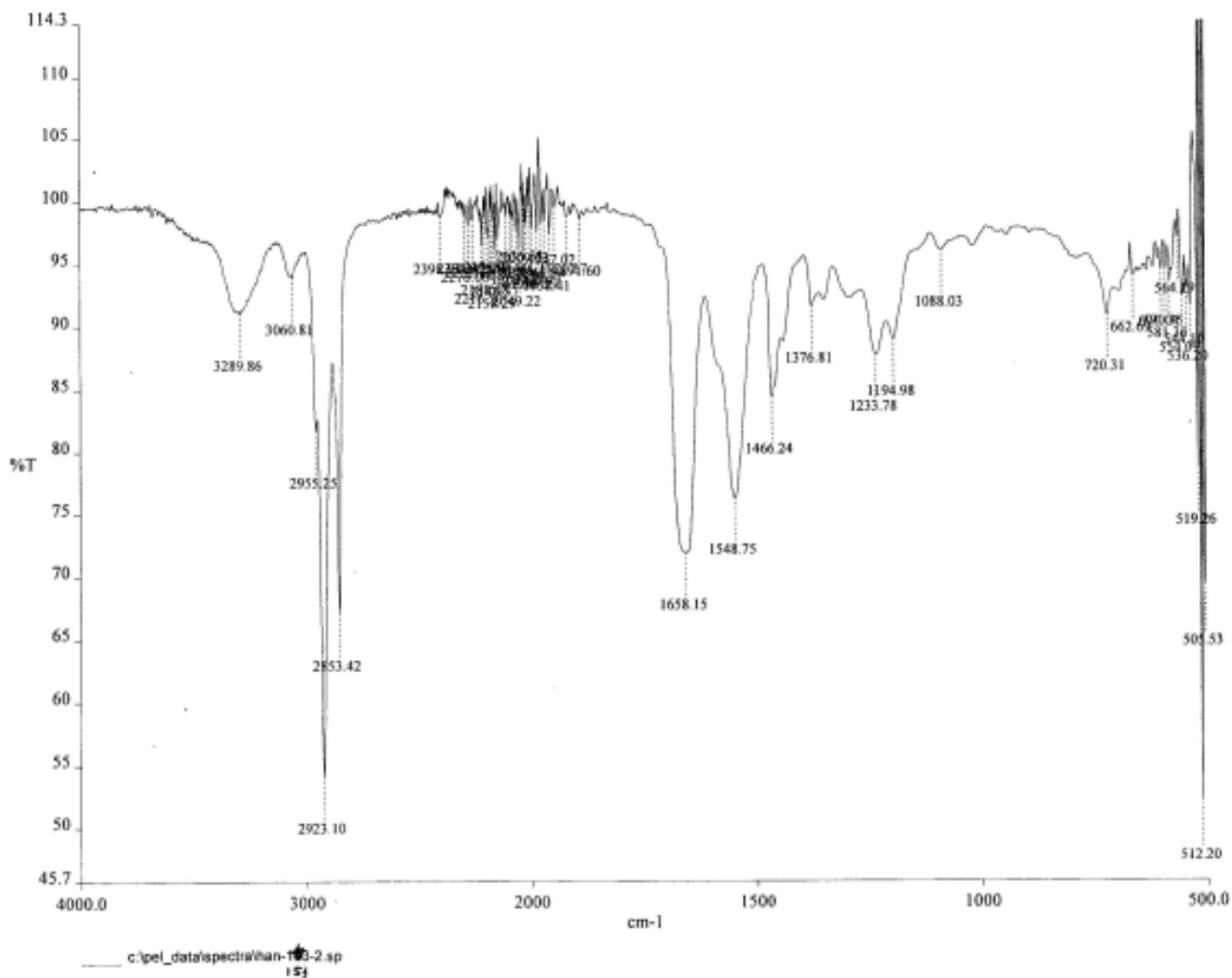
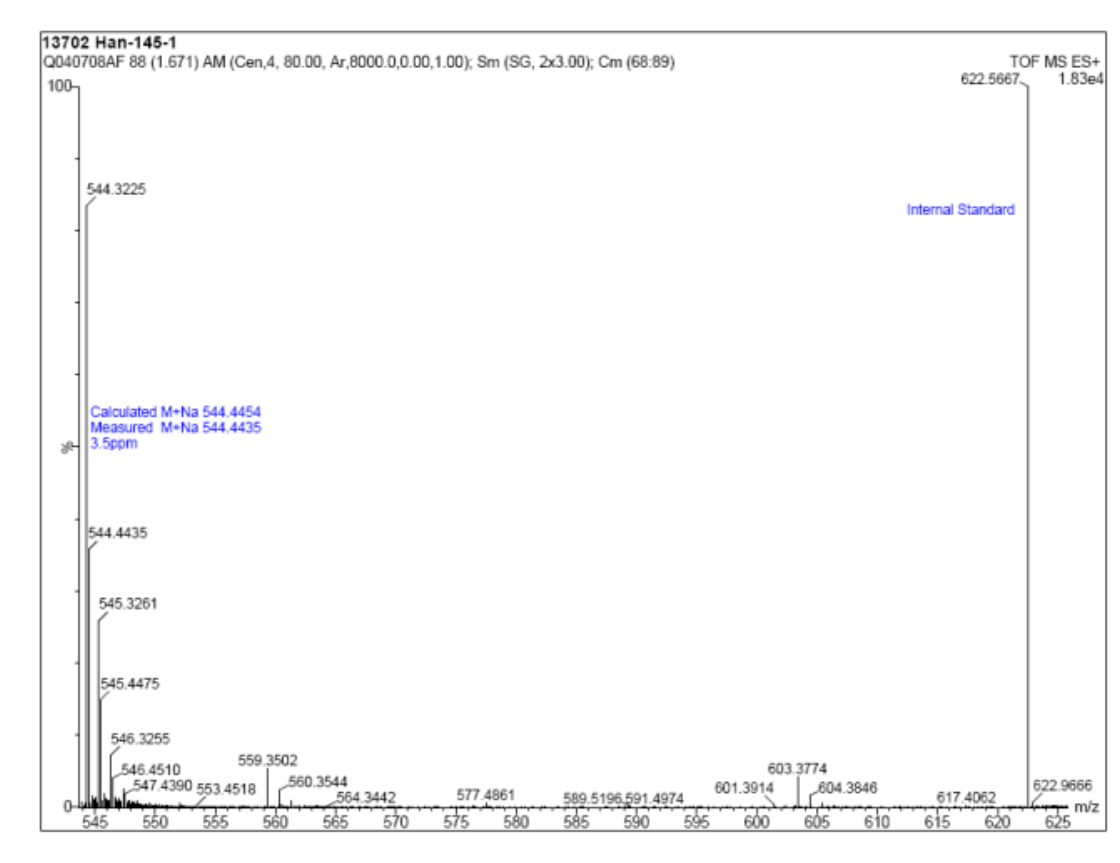
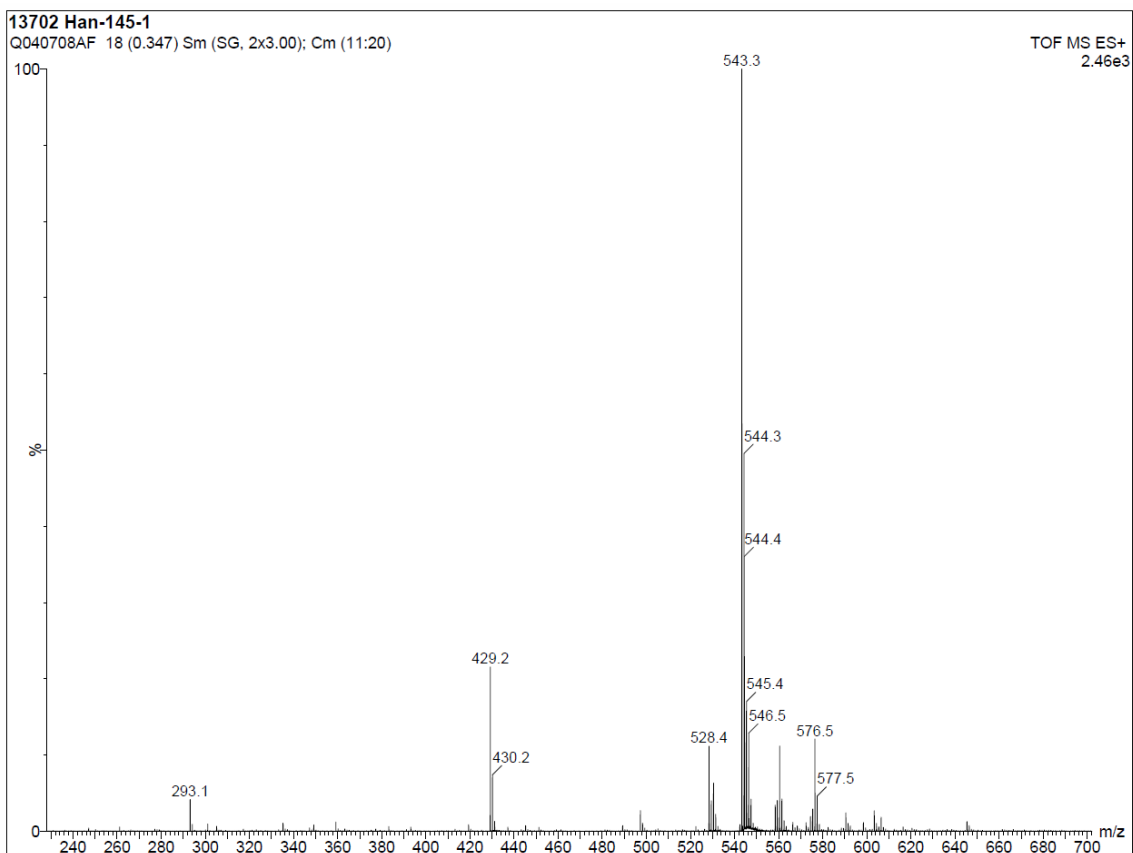


Figure S4. ESI-TOF mass spectrum of diC<sub>12</sub>PO.



**Figure S5.** Excitation and emission spectrum of HYA-FL (25  $\mu\text{M}$ ) in  $\text{H}_2\text{O}$ .

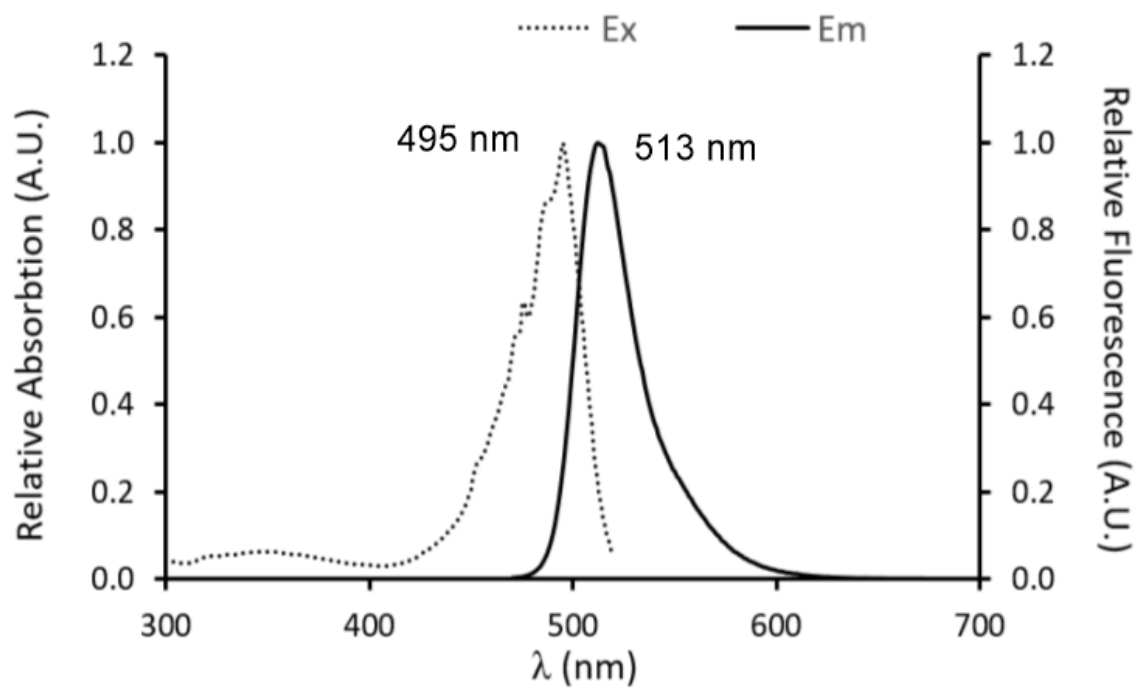
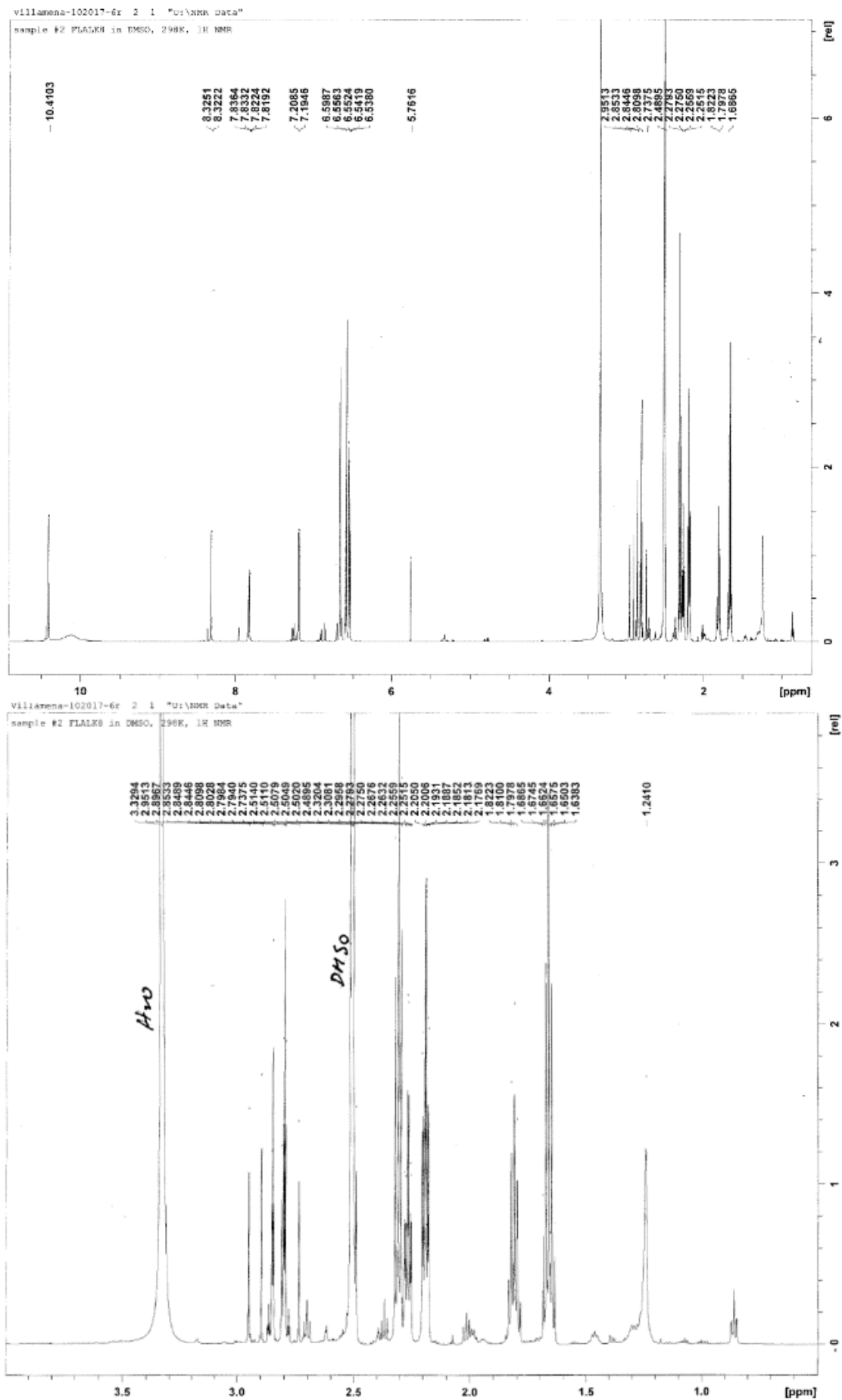


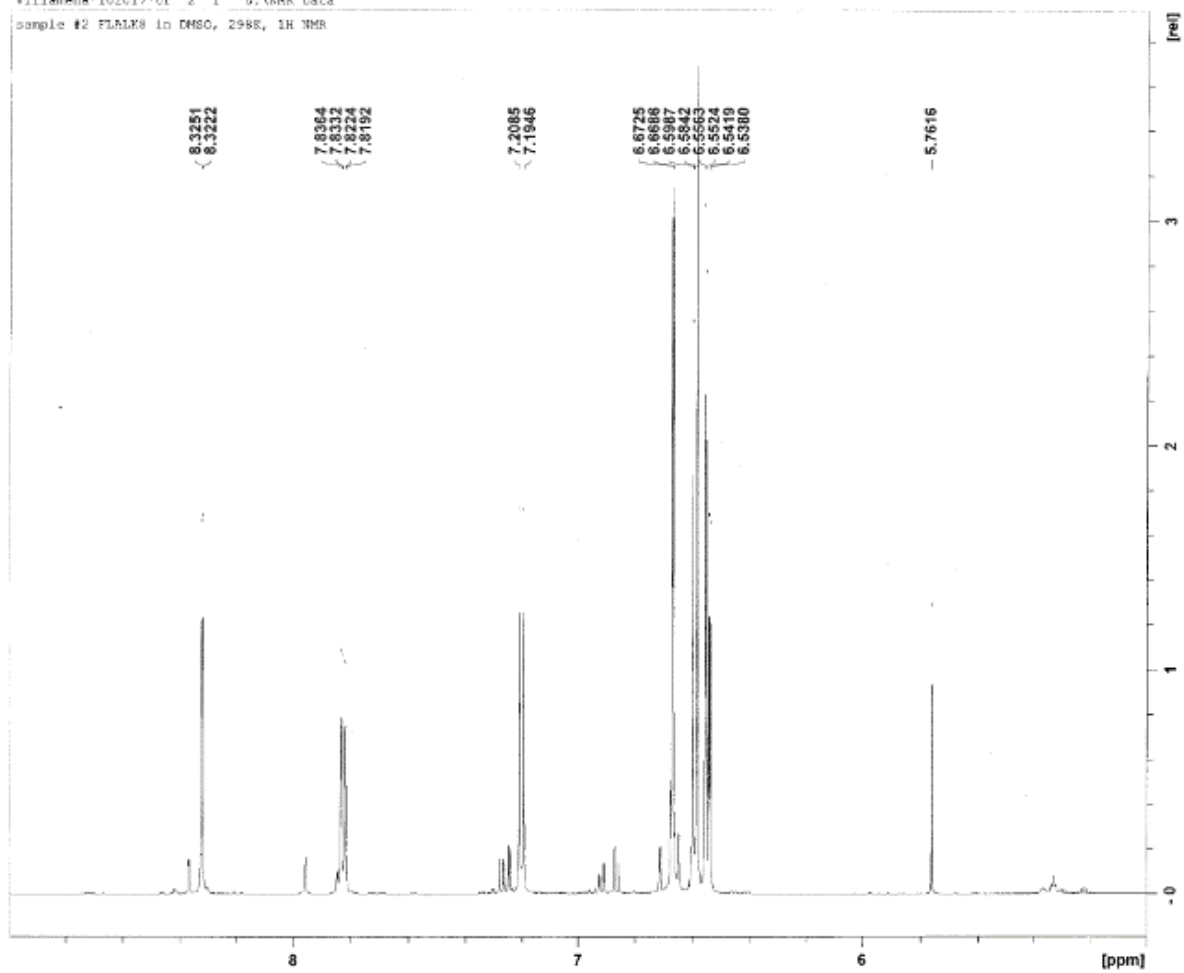


Figure S6. 400 MHz <sup>1</sup>H-NMR spectrum of HYA-FL in DMSO-d<sub>6</sub>.



Villarene-102017-0r 2 1 "D:\NMR Data"

sample #2 FLAME8 in DMSO, 298K, 1H NMR



**Figure S7.** FT-ICR ESI positive ion mode mass spectrum of HYA-FL.

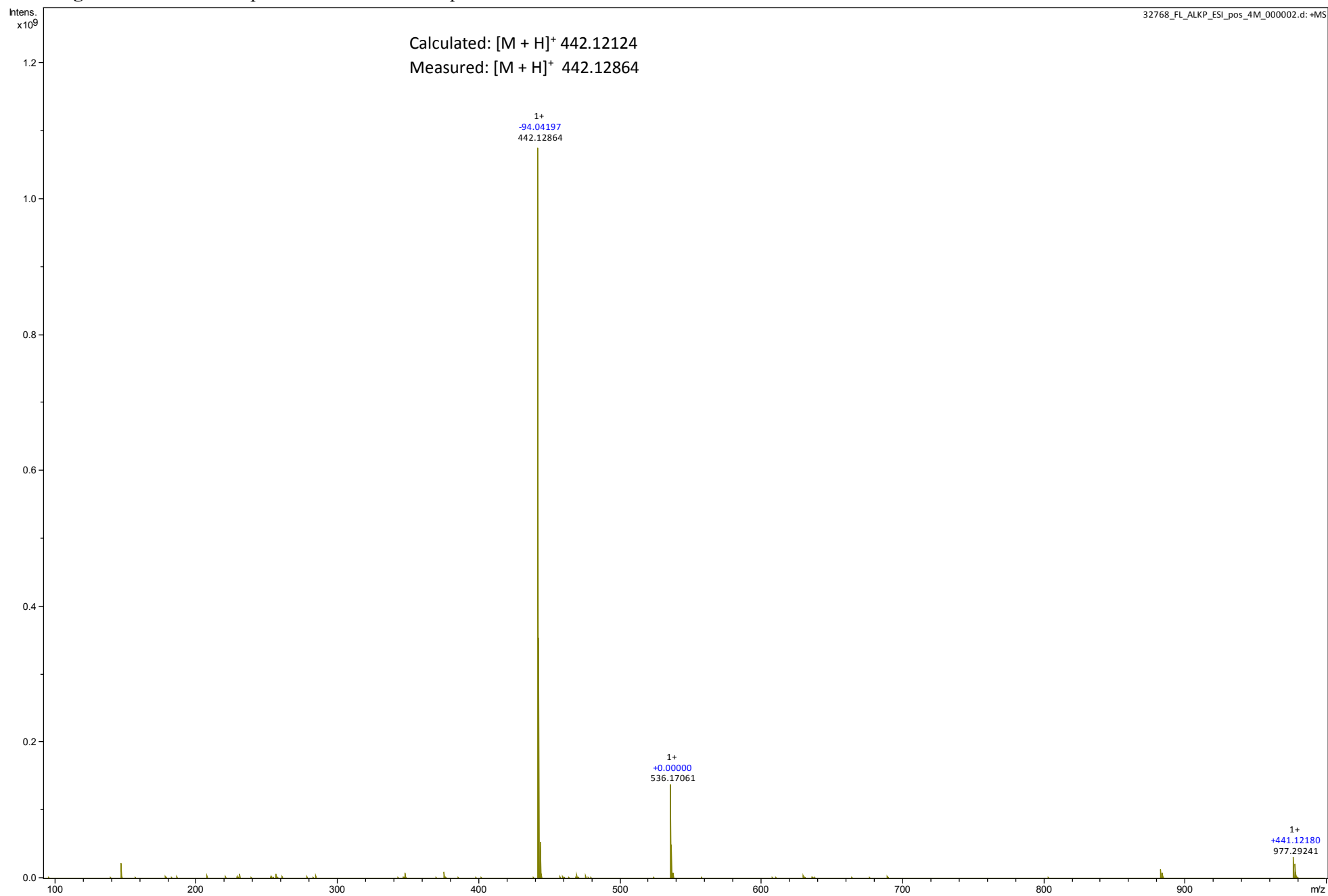
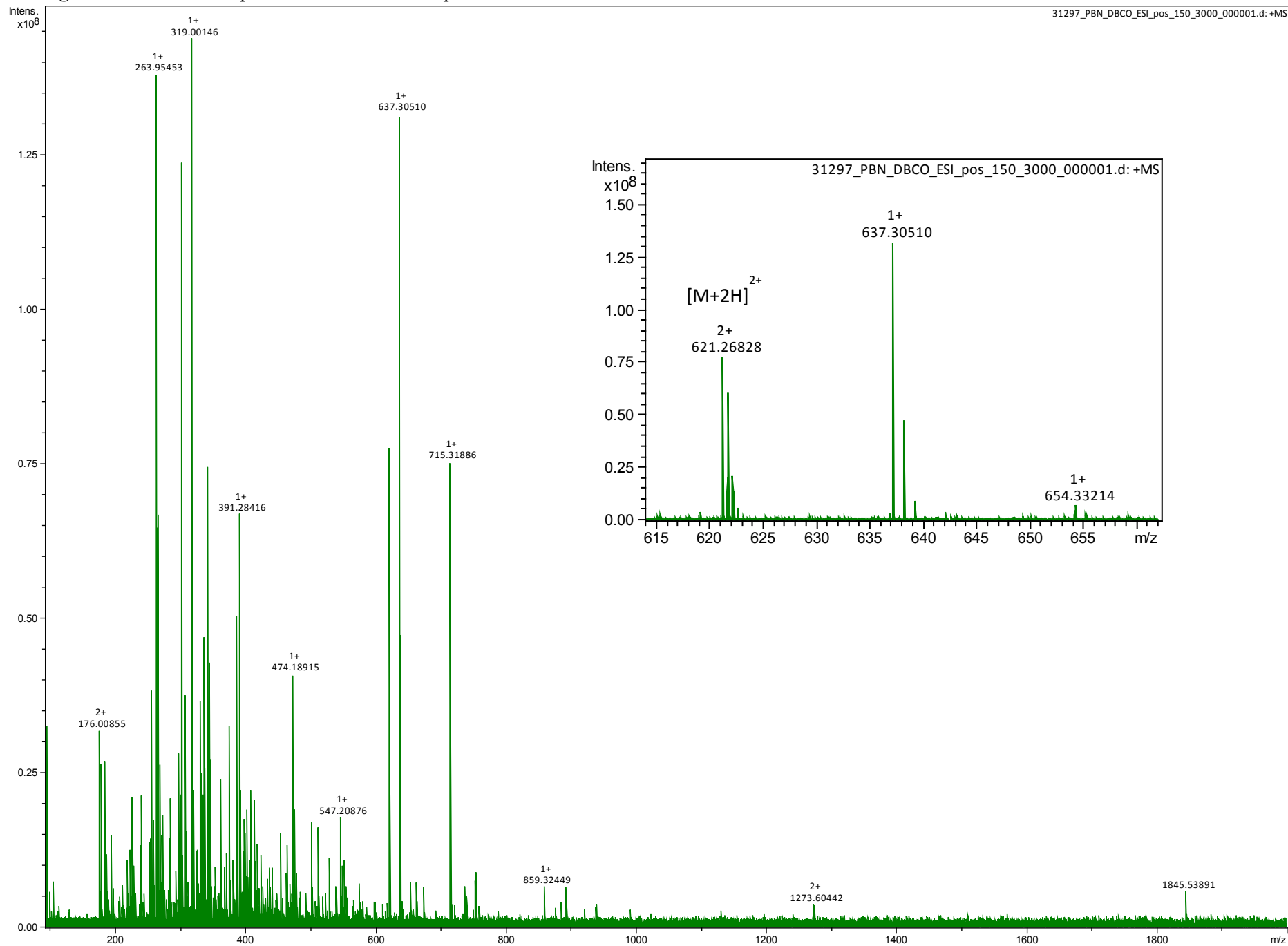
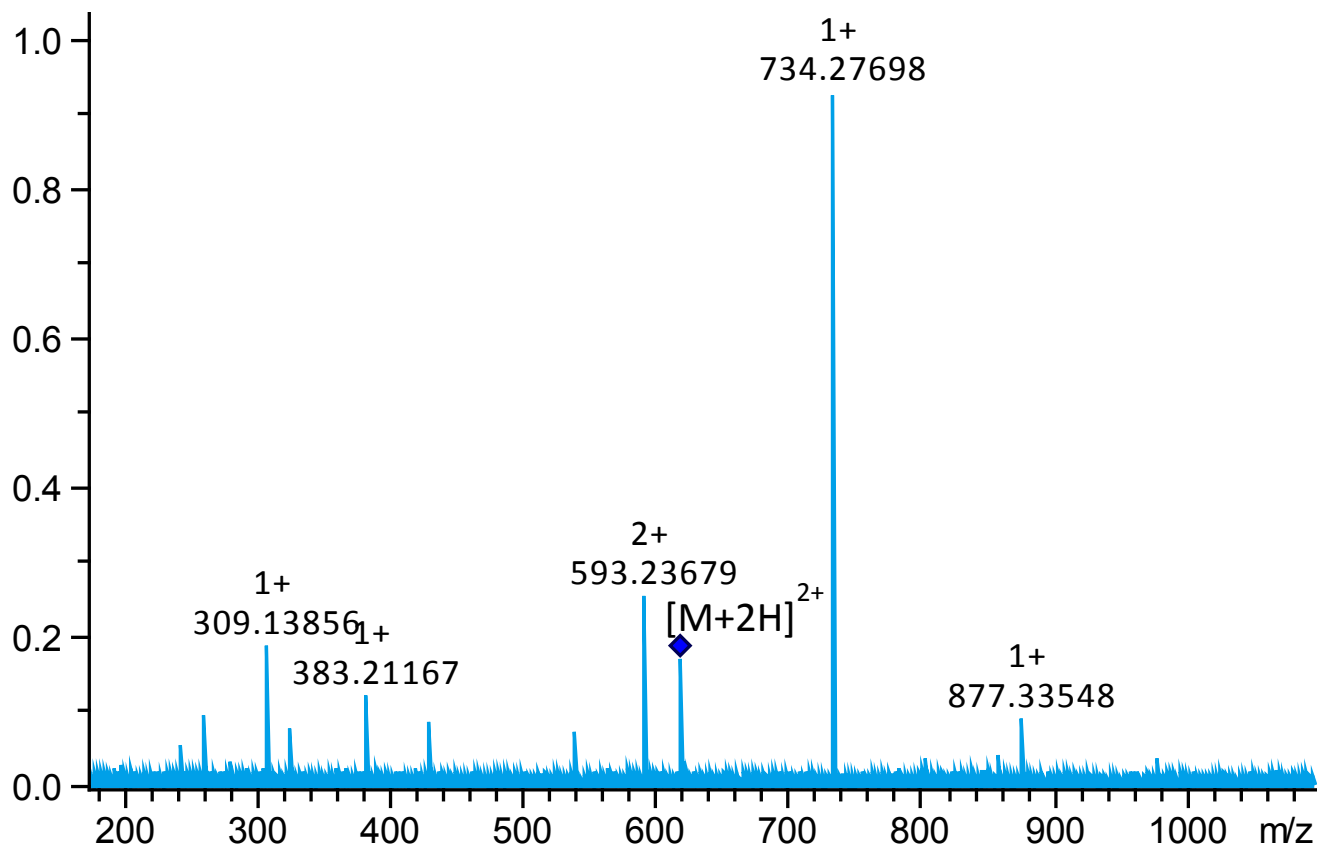


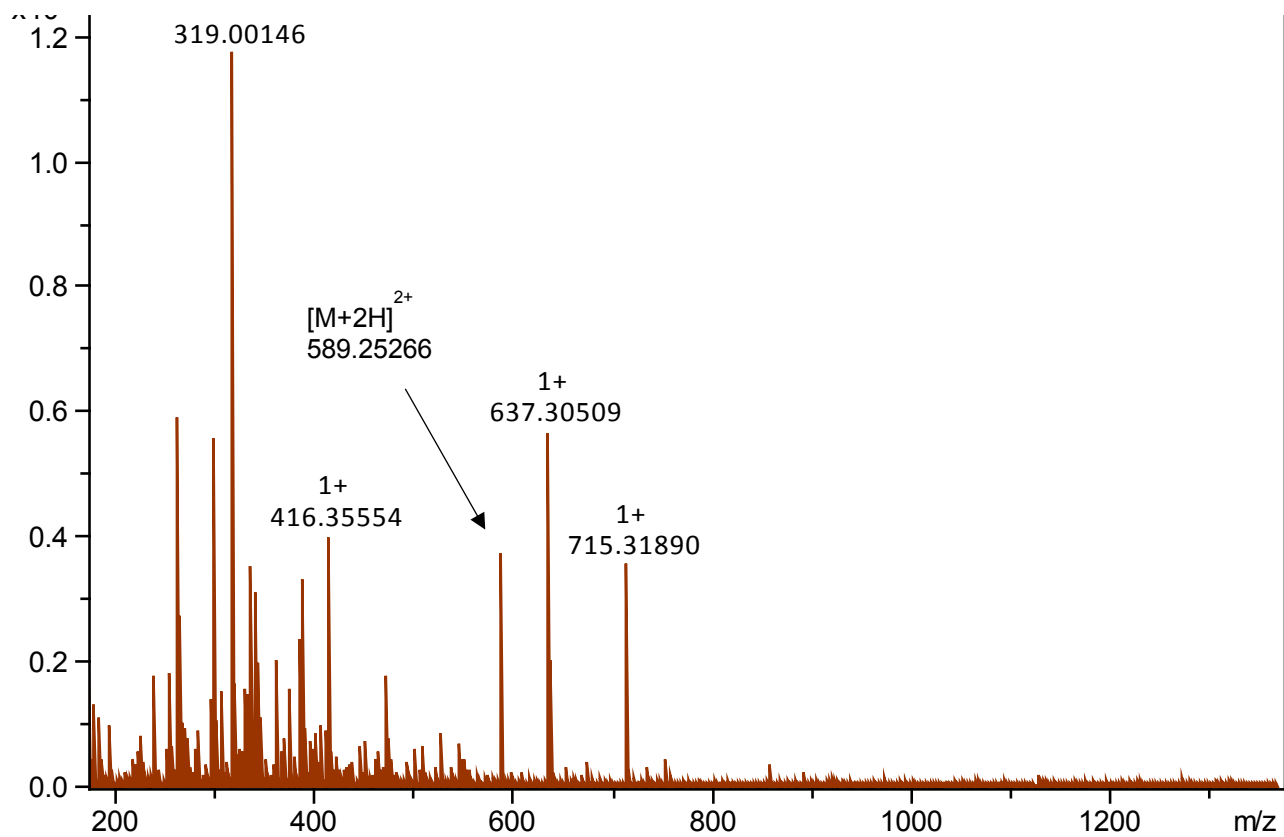
Figure S8. FT-ICR ESI positive ion mode mass spectrum of PBN-DBCO-Rhod.



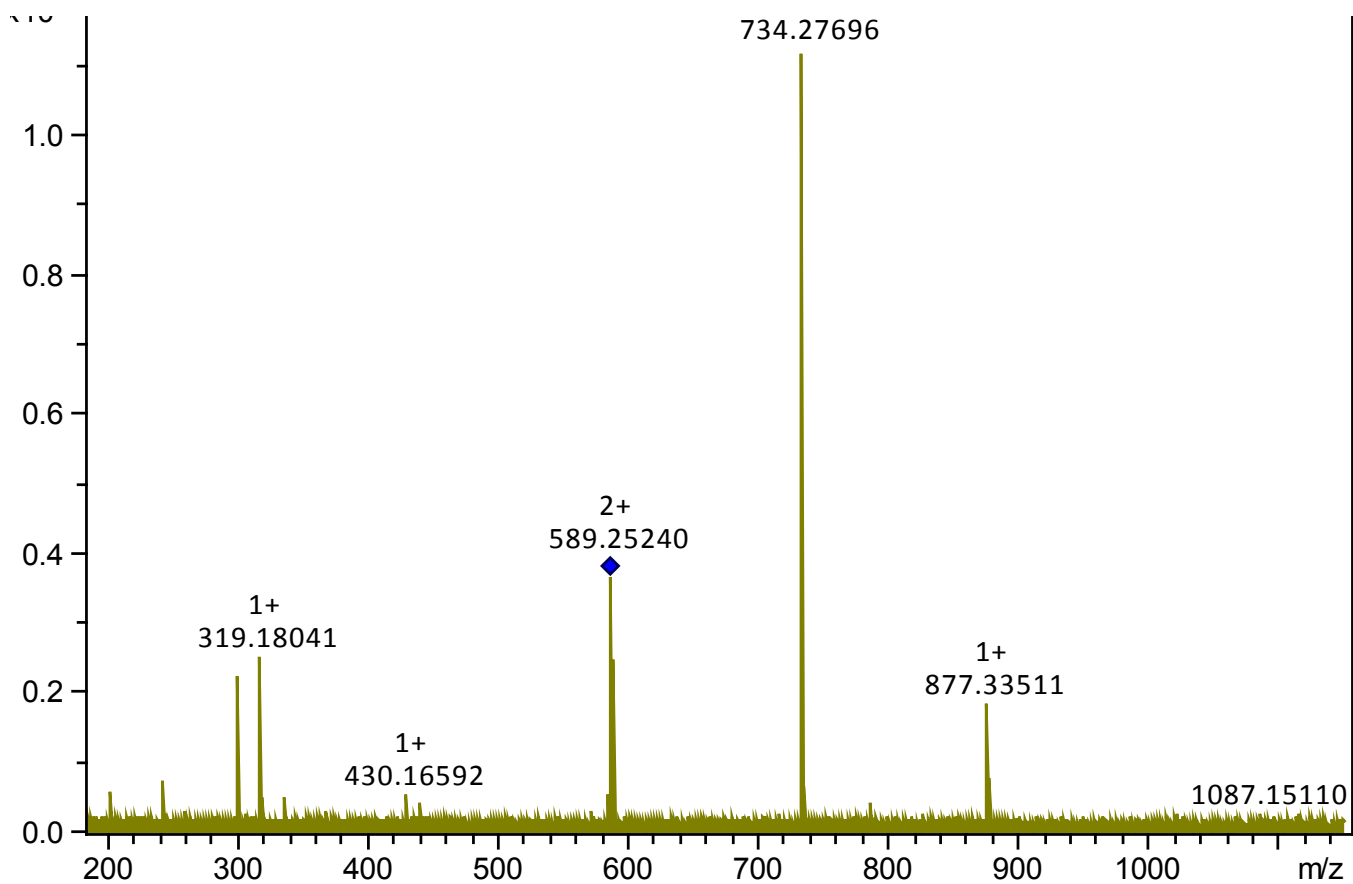
**Figure S9.** FT-ICR ESI positive ion mode ms/ms spectrum of PBN-DBCO-Rhod.



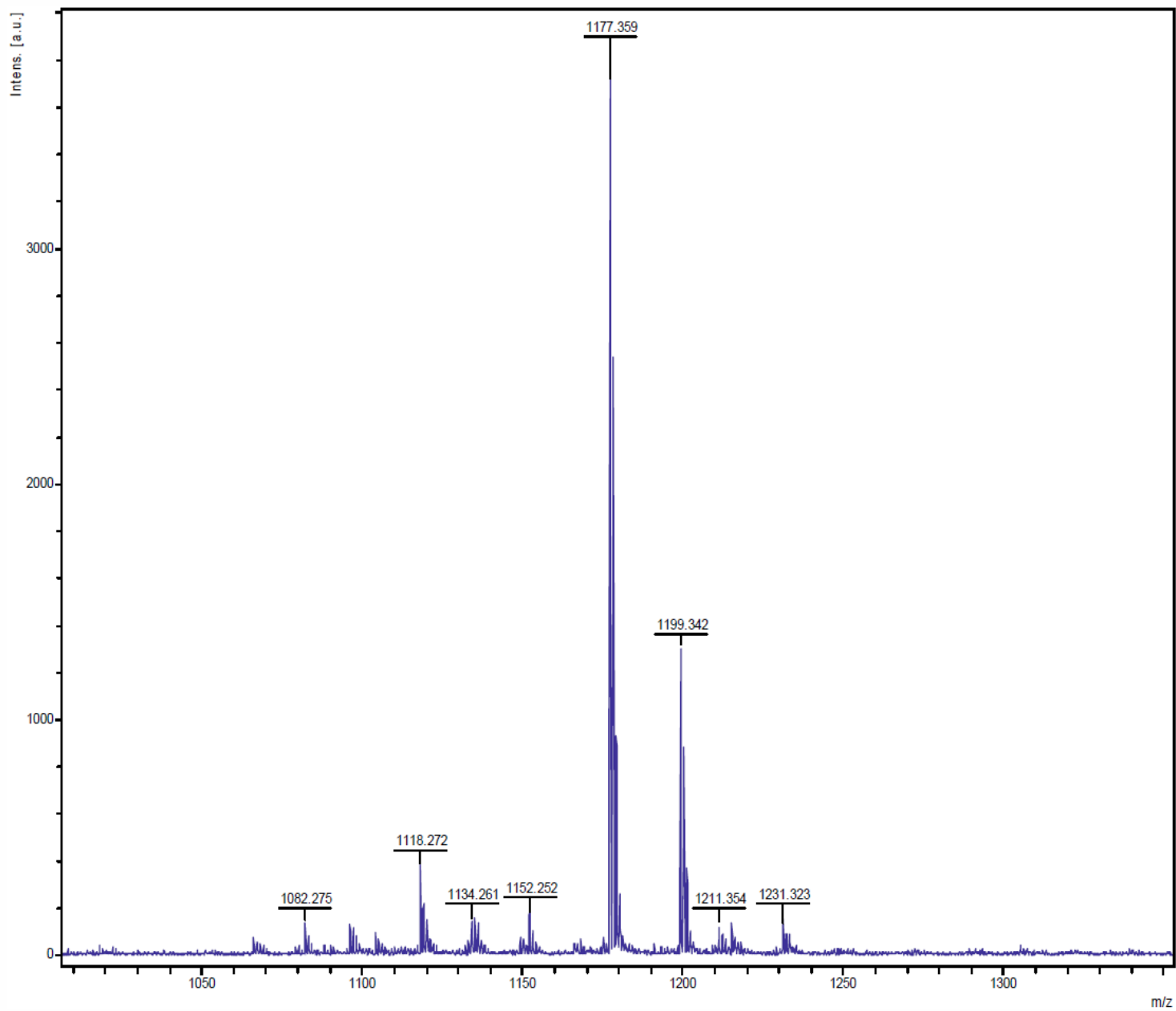
**Figure S10.** FT-ICR ESI positive ion mode mass spectrum of DMPO-DBCO-Rhod.



**Figure S11.** FT-ICR ESI positive ion mode  $m/z$  spectrum of DMPO-DBCO-Rhod.

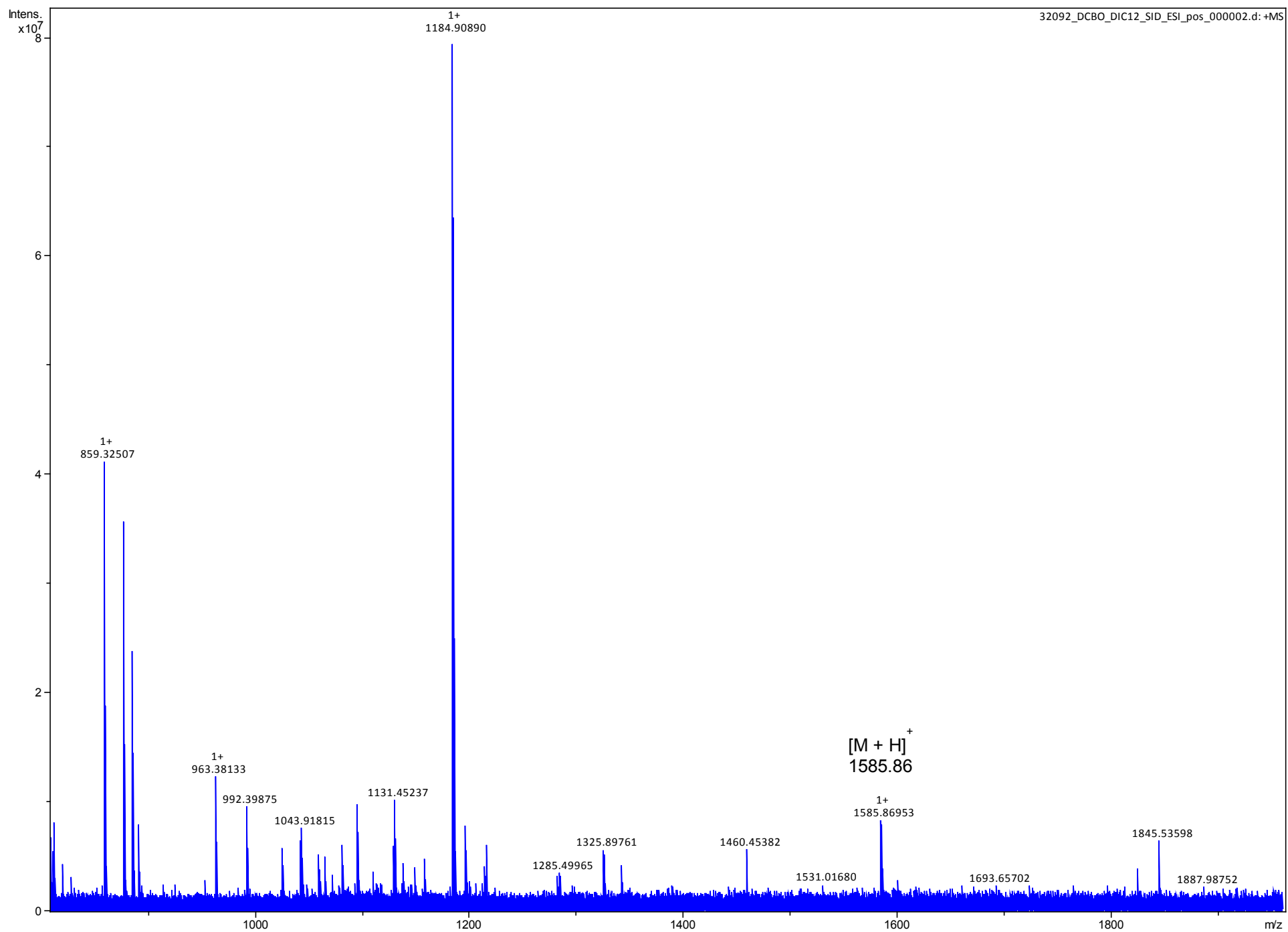


**Figure S12.** MALDI spectrum of DMPO-DBCO-Rhod.





**Figure S13.** FT-ICR ESI positive ion mode mass spectrum of diC<sub>12</sub>PO-DBCO-Rhod.



## Reference

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.