Supplementary Materials: Protonation Sites, Tandem Mass Spectrometry and Computational Calculations of *o*-Carbonyl Carbazolequinone Derivatives

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1. Optimized Geometries and Energies

DFT B3LYP/6-31G(d,p) level

1.1. Neutral Species

Table S1. Cartesian coordinates for **CQ1**.

C	−4.091623	0.700303	0.060087
C	−3.959467	−0.624404	0.152651
C	−2.927999	1.564045	−0.175800
C	−1.583404	0.914506	0.003062
C	−1.454016	−0.442176	0.025377
C	−2.660131	−1.375078	0.066322
C	−2.730824	−2.253784	−1.219336
C	−2.585069	−2.292191	1.324096
C	−0.390424	1.826709	0.146383
C	−0.071276	−1.099490	−0.019233
C	0.904159	1.155932	0.038883
C	1.074480	−0.209948	−0.030532
N	2.116335	1.776309	0.076010
C	2.490769	−0.459243	−0.047211
C	3.115075	0.818670	0.018617
C	3.288241	−1.612202	−0.107050
C	4.503921	0.968540	0.019325
C	4.666215	−1.462819	−0.103798
C	5.266221	−0.188480	−0.041793
O	−3.050775	2.716806	−0.547961
O	−0.462438	3.015301	0.398271
O	0.050939	−2.316993	−0.064045
H	−2.783011	−1.627626	−2.113145
H	−3.632004	−2.872105	−1.186756
H	−1.861784	−2.905131	−1.286370
H	−2.527352	−1.694294	2.237066
H	−1.722641	−2.952589	1.273211
H	−3.491171	−2.901650	1.377177
H	2.230811	2.777115	0.144431
H	−5.057268	1.192651	0.081090
H	−4.841116	−1.250089	0.270026
H	6.347331	−0.111392	−0.041148
H	2.825038	−2.589017	−0.155405
H	5.299770	−2.340903	−0.150684
H	4.968157	1.946614	0.068028

Table S2. Energies for **CQ1**.

Zero-point correction	0.267187 (Hartree/Particle)
Thermal correction to Energy	0.284824
Thermal correction to Enthalpy	0.285769
Thermal correction to Gibbs Free Energy	0.222144
Sum of electronic and zero-point Energies	−974.146119
Sum of electronic ad thermal Energies	−974.128481
Sum of electronic and thermal Enthalpies	−974.127537
Sum of electronic and thermal Free Energies	−974.191161

Table S3. Cartesian coordinates for **CQ2**.

C	−4.274958	0.994172	0.067551
C	−4.272262	−0.336932	0.161872
C	−3.033558	1.740238	−0.173511
C	−1.758110	0.963013	0.001975
C	−1.761533	−0.399891	0.027350
C	−3.052765	−1.210795	0.072138
C	−3.213024	−2.077493	−1.213606
C	−3.064962	−2.132137	1.329177
C	−0.480458	1.754398	0.136702
C	−0.449821	−1.189801	−0.019824
C	0.740836	0.959335	0.028716
C	0.777624	−0.417042	−0.034764
N	2.008187	1.457618	0.059464
C	2.162408	−0.804263	−0.053286
C	2.909201	0.405331	0.004168
C	2.840595	−2.031571	−0.107878
C	4.312098	0.442081	0.001386
C	4.224975	−2.008540	−0.107332
C	4.942281	−0.795446	−0.054582
O	−3.045469	2.899176	−0.546764
O	−0.434876	2.946233	0.380825
O	−0.449039	−2.413352	−0.064963
H	−3.203181	−1.449061	−2.107260
H	−4.171640	−2.602255	−1.179794
H	−2.413476	−2.812341	−1.281711
H	−2.949932	−1.543381	2.242678
H	−2.269446	−2.871620	1.276893
H	−4.025010	−2.652572	1.382450
H	2.217677	2.443029	0.122075
H	−5.188026	1.578269	0.090863
H	−5.210329	−0.873659	0.282508
C	5.067483	1.743603	0.057441
H	6.026819	−0.827243	−0.056775
H	2.286085	−2.959621	−0.149858
H	4.776727	−2.940598	−0.149704
H	4.833167	2.307517	0.967199
H	4.827831	2.385538	−0.797483
H	6.144202	1.568672	0.046728

Table S4. Energies for **CQ2**.

Zero-point correction	0.294619 (Hartree/Particle)
Thermal correction to Energy	0.314038
Thermal correction to Enthalpy	0.314982
Thermal correction to Gibbs Free Energy	0.247478
Sum of electronic and zero-point Energies	−1013.447303
Sum of electronic and thermal Energies	−1013.427885
Sum of electronic and thermal Enthalpies	−1013.426941
Sum of electronic and thermal Free Energies	−1013.494444

Table S5. Cartesian coordinates for **CQ3**.

C	−5.379772	0.746743	−0.001142
C	−4.712933	1.895332	0.129597
C	−4.673676	−0.518903	−0.234900
C	−3.184803	−0.487726	−0.020592
C	−2.506139	0.692655	0.042011
C	−3.217438	2.040752	0.092582
C	−2.808097	2.813449	1.383044
C	−2.878695	2.900268	−1.162821
C	−2.479300	−1.814698	0.108660
C	−0.975709	0.718639	0.036069
C	−1.020560	−1.738511	0.029371
C	−0.299835	−0.566326	0.004322
N	−0.173374	−2.808032	0.056440
C	1.093148	−0.927401	0.006267
C	1.130017	−2.350557	0.036292
C	2.292154	−0.205648	−0.011944
C	2.334103	−3.061595	0.041377
C	3.491864	−0.911509	−0.004375
C	3.504456	−2.326322	0.021903
O	−5.253537	−1.512930	−0.631953
O	−3.039505	−2.872464	0.326801
O	−0.358001	1.774792	0.036386
H	−3.030805	2.222943	2.275206
H	−3.382613	3.741659	1.441215
H	−1.748716	3.058869	1.370477
H	−3.156862	2.373753	−2.078829
H	−1.816926	3.136263	−1.191580
H	−3.445030	3.834785	−1.125390
H	−0.484562	−3.768005	0.095278
H	−6.462798	0.699924	−0.012756
H	−5.258883	2.828602	0.245516
H	2.352911	−4.144843	0.061864
H	4.465713	−2.824249	0.026961
H	2.282184	0.874602	−0.031871
C	4.813263	−0.219109	−0.023715
O	4.693633	1.122891	−0.054131
C	5.928274	1.881932	−0.074820
H	6.506697	1.580612	−0.951077
H	6.509301	1.624364	0.813602
C	5.561175	3.351020	−0.110723
H	6.471876	3.955735	−0.127798

H	4.979610	3.632167	0.770050
H	4.975980	3.587784	−1.002081
O	5.880855	−0.791495	−0.013683

Table S6. Energies for **CQ3**.

Zero-point correction	0.337803 (Hartree/Particle)
Thermal correction to Energy	0.361476
Thermal correction to Enthalpy	0.362420
Thermal correction to Gibbs Free Energy	0.283677
Sum of electronic and zero-point Energies	−1241.351749
Sum of electronic and thermal Energies	−1241.328076
Sum of electronic and thermal Enthalpies	−1241.327131
Sum of electronic and thermal Free Energies	−1241.405874

Table S7. Cartesian coordinates for **CQ4**.

C	−5.295181	−0.228925	0.024620
C	−4.800012	−1.462821	0.140363
C	−4.415786	0.921894	−0.214005
C	−2.945276	0.674989	−0.013259
C	−2.443401	−0.591809	0.031864
C	−3.342107	−1.823193	0.077466
C	−3.149666	−2.703134	−1.194941
C	−3.029178	−2.666189	1.350263
C	−2.056830	1.885475	0.125463
C	−0.932838	−0.838526	0.009579
C	−0.623749	1.600966	0.042351
C	−0.080372	0.335699	−0.003008
N	0.366813	2.534997	0.081038
C	1.348721	0.491171	−0.001403
C	1.592011	1.892116	0.049622
C	2.428711	−0.403739	−0.033730
C	2.886043	2.416459	0.061934
C	3.703308	0.133548	−0.018015
C	3.943210	1.520536	0.028390
O	−4.848602	1.990742	−0.604098
O	−2.458203	3.010912	0.354750
O	−0.472798	−1.972342	−0.018215
H	−3.356730	−2.125797	−2.099079
H	−3.848219	−3.543569	−1.163376
H	−2.135066	−3.093522	−1.241696
H	−3.154529	−2.065167	2.254344
H	−2.015116	−3.057477	1.317541
H	−3.727116	−3.505961	1.404693
H	0.197309	3.529088	0.133956
H	−6.360032	−0.025625	0.028768
H	−5.473868	−2.307870	0.259848
H	3.067871	3.484046	0.098620
H	4.961731	1.885525	0.038495
H	2.258015	−1.470430	−0.070089
Br	5.215121	−1.045995	−0.062003

Table S8. Energies for **CQ4**.

Zero-point correction	0.256854 (Hartree/Particle)
Thermal correction to Energy	0.276067
Thermal correction to Enthalpy	0.277011
Thermal correction to Gibbs Free Energy	0.208568
Sum of electronic and zero-point Energies	−3547.697444
Sum of electronic and thermal Energies	−3547.678231
Sum of electronic and thermal Enthalpies	−3547.677286
Sum of electronic and thermal Free Energies	−3547.745730

1.2. Protonated Species for CQ1

Table S9. Cartesian coordinates for **CQ1_O1**.

C	4.057977	0.674236	−0.000007
C	3.932355	−0.672435	0.000082
C	2.877679	1.473681	−0.000050
C	1.559621	0.857820	−0.000031
C	1.434717	−0.509823	0.000120
C	2.639516	−1.415264	0.000188
C	2.638228	−2.329162	1.280038
C	2.638120	−2.329377	−1.279518
C	0.380261	1.785872	−0.000291
C	0.036096	−1.142421	0.000167
C	−0.902213	1.158036	−0.000104
C	−1.086572	−0.224121	0.000070
N	−2.118448	1.781876	−0.000123
C	−2.495078	−0.461097	0.000006
C	−3.114421	0.829974	−0.000083
C	−3.297283	−1.617801	0.000047
C	−4.507192	0.989880	−0.000128
C	−4.671065	−1.454891	0.000005
C	−5.266898	−0.167229	−0.000081
O	3.003530	2.758192	−0.000032
O	0.545002	3.023957	−0.000398
O	−0.092665	−2.362255	0.000016
H	2.646576	−1.728376	2.192773
H	3.533413	−2.955778	1.268763
H	1.756240	−2.967133	1.269316
H	2.646450	−1.728745	−2.192354
H	1.756094	−2.967296	−1.268633
H	3.533269	−2.956044	−1.268190
H	−2.244570	2.785325	−0.000216
H	5.016734	1.180680	−0.000023
H	4.827057	−1.290376	0.000126
H	−6.349111	−0.089667	−0.000107
H	−2.838940	−2.599325	0.000128
H	−5.314379	−2.328386	0.000049
H	−4.967569	1.971995	−0.000196
H	2.057855	3.165592	0.000149

Table S10. Energies for **CQ1_O1**.

Zero-point correction	0.281366 (Hartree/Particle)
Thermal correction to Energy	0.298670
Thermal correction to Enthalpy	0.299614
Thermal correction to Gibbs Free Energy	0.237298
Sum of electronic and zero-point Energies	−974.290473
Sum of electronic and thermal Energies	−974.273169
Sum of electronic and thermal Enthalpies	−974.272225
Sum of electronic and thermal Free Energies	−974.334541

Table S11. Cartesian coordinates for **CQ1_O2**.

C	−4.058036	0.674349	−0.000194
C	−3.932514	−0.672358	−0.000298
C	−2.877667	1.473760	−0.000028
C	−1.559581	0.857801	0.000045
C	−1.434791	−0.509797	−0.000003
C	−2.639663	−1.415286	−0.000066
C	−2.638365	−2.329701	−1.279427
C	−2.638609	−2.328720	1.280156
C	−0.380223	1.785952	0.000034
C	−0.035870	−1.142710	0.000141
C	0.902214	1.157952	−0.000090
C	1.086605	−0.224150	−0.000046
N	2.118461	1.781829	−0.000267
C	2.495119	−0.461149	−0.000036
C	3.114487	0.829925	−0.000186
C	3.297362	−1.617846	0.000031
C	4.507255	0.989923	−0.000286
C	4.671162	−1.454881	−0.000056
C	5.266996	−0.167204	−0.000211
O	−3.003525	2.758269	−0.000027
O	−0.544806	3.024082	0.000045
O	0.092924	−2.362478	0.000463
H	−2.646292	−1.729350	−2.192476
H	−3.533787	−2.956023	−1.268115
H	−1.756635	−2.968046	−1.268274
H	−2.646733	−1.727622	2.192707
H	−1.756819	−2.967001	1.269578
H	−3.533995	−2.955089	1.269115
H	2.244615	2.785273	−0.000055
H	−5.016789	1.180838	−0.000291
H	−4.827315	−1.290194	−0.000510
H	6.349227	−0.089618	−0.000284
H	2.839070	−2.599416	0.000139
H	5.314476	−2.328403	−0.000016
H	4.967588	1.972078	−0.000410
H	−2.057866	3.165621	0.000039

Table S12. Energies for **CQ1_O2**.

Zero-point correction	0.281361 (Hartree/Particle)
Thermal correction to Energy	0.298664
Thermal correction to Enthalpy	0.299608
Thermal correction to Gibbs Free Energy	0.237299
Sum of electronic and zero-point Energies	−974.290478
Sum of electronic and thermal Energies	−974.273175
Sum of electronic and thermal Enthalpies	−974.272231
Sum of electronic and thermal Free Energies	−974.334540

Table S13. Cartesian coordinates for **CQ1_O3**.

C	−4.108561	0.710348	0.008778
C	−3.965030	−0.617469	0.089374
C	−2.950372	1.590246	−0.154998
C	−1.599398	0.930265	0.005332
C	−1.455406	−0.433084	0.023700
C	−2.663316	−1.376512	0.049278
C	−2.715589	−2.269797	−1.229552
C	−2.636684	−2.266624	1.331692
C	−0.412643	1.845725	0.125658
C	−0.083988	−1.012438	0.005778
C	0.897776	1.168193	0.028546
C	1.066182	−0.224313	−0.026765
N	2.087713	1.767531	0.061418
C	2.504476	−0.470947	−0.044331
C	3.109275	0.814811	0.013931
C	3.332724	−1.596902	−0.103132
C	4.489008	1.009969	0.016196
C	4.715131	−1.412905	−0.098514
C	5.285455	−0.129939	−0.038950
O	−3.042497	2.771721	−0.439050
O	−0.455057	3.041009	0.348226
O	−0.009488	−2.330200	−0.002142
H	−2.736677	−1.655460	−2.133579
H	−3.630973	−2.867353	−1.208814
H	−1.870397	−2.955904	−1.281143
H	−2.600383	−1.650711	2.234393
H	−1.794691	−2.957578	1.334876
H	−3.554850	−2.859098	1.367649
H	2.196463	2.775731	0.119531
H	−5.080955	1.191511	0.008011
H	−4.846416	−1.250166	0.167619
H	6.364919	−0.026532	−0.037762
H	2.944172	−2.610737	−0.161272
H	5.365092	−2.279969	−0.144917
H	4.923061	2.003142	0.059941
H	0.909749	−2.641588	−0.022872

Table S14. Energies for **CQ1_O3**.

Zero-point correction	0.281072 (Hartree/Particle)
Thermal correction to Energy	0.299022
Thermal correction to Enthalpy	0.299967
Thermal correction to Gibbs Free Energy	0.235403
Sum of electronic and zero-point Energies	−974.250033
Sum of electronic and thermal Energies	−974.232083
Sum of electronic and thermal Enthalpies	−974.231139
Sum of electronic and thermal Free Energies	−974.295702

Table S15. Cartesian coordinates for **CQ1_N4**.

C	−4.130669	0.685629	0.031946
C	−3.991171	−0.644907	0.089514
C	−2.972503	1.570851	−0.107969
C	−1.619711	0.902650	0.010343
C	−1.486332	−0.460150	0.016646
C	−2.688675	−1.397268	0.040911
C	−2.721145	−2.288116	−1.240126
C	−2.635434	−2.304123	1.310277
C	−0.432000	1.814150	0.102265
C	−0.116888	−1.104124	−0.021208
C	0.849486	1.132450	−0.068452
C	1.063623	−0.190563	−0.063452
N	2.139043	1.861516	−0.018301
C	2.496209	−0.465812	−0.044928
C	3.162193	0.771470	−0.012122
C	3.245240	−1.642520	−0.047928
C	4.532687	0.913844	0.007281
C	4.638675	−1.528734	−0.023602
C	5.271359	−0.280497	0.003164
O	−3.067736	2.764415	−0.339658
O	−0.432514	3.008825	0.358711
O	0.073131	−2.309504	−0.033804
H	−2.758243	−1.673663	−2.143870
H	−3.619728	−2.910960	−1.219620
H	−1.851793	−2.944426	−1.282749
H	−2.608594	−1.701260	2.222329
H	−1.769611	−2.965195	1.287376
H	−3.537148	−2.921906	1.342404
H	2.165133	2.466942	0.815423
H	−5.101743	1.169588	0.040661
H	−4.874481	−1.276530	0.158146
H	6.354453	−0.227613	0.022984
H	2.750273	−2.605767	−0.070429
H	5.244701	−2.428368	−0.026216
H	5.026329	1.879867	0.030203
H	2.234429	2.493403	−0.825882

Table S16. Energies for **CQ1_N4**.

Zero-point correction	0.281463 (Hartree/Particle)
Thermal correction to Energy	0.299421
Thermal correction to Enthalpy	0.300365
Thermal correction to Gibbs Free Energy	0.235816
Sum of electronic and zero-point Energies	−974.217276
Sum of electronic and thermal Energies	−974.199318
Sum of electronic and thermal Enthalpies	−974.198373
Sum of electronic and thermal Free Energies	−974.262923

1.3. Protonated Species for CQ2

Table S17. Cartesian coordinates for **CQ2_O1**.

C	4.238253	0.980132	−0.000136
C	4.249981	−0.372236	0.000023
C	2.982700	1.655617	−0.000206
C	1.734407	0.909301	−0.000071
C	1.748513	−0.464310	0.000034
C	3.039221	−1.242765	0.000085
C	3.130920	−2.152245	1.279639
C	3.130893	−2.152335	−1.279428
C	0.467119	1.712794	−0.000020
C	0.422160	−1.235917	0.000094
C	−0.743456	0.957881	0.000018
C	−0.787460	−0.436287	0.000058
N	−2.017304	1.453548	−0.000011
C	−2.164192	−0.815497	0.000075
C	−2.912100	0.405419	0.000024
C	−2.842522	−2.048040	0.000130
C	−4.321410	0.448620	0.000026
C	−4.224748	−2.015060	0.000124
C	−4.943361	−0.791920	0.000073
O	2.976490	2.946303	−0.000526
O	0.505888	2.961938	0.000003
O	0.418801	−2.462781	0.000140
H	3.078088	−1.554015	2.192570
H	4.085110	−2.684741	1.268292
H	2.317858	−2.875947	1.268257
H	3.078044	−1.554163	−2.192395
H	2.317824	−2.876030	−1.267973
H	4.085079	−2.684834	−1.268061
H	−2.244419	2.438722	−0.000056
H	5.140685	1.581215	−0.000234
H	5.202708	−0.896314	0.000078
C	−5.073895	1.752765	−0.000023
H	−6.028692	−0.828187	0.000072
H	−2.289628	−2.979303	0.000169
H	−4.783713	−2.944954	0.000159
H	−4.837167	2.355527	−0.885168
H	−4.837173	2.355589	0.885082
H	−6.151542	1.579680	−0.000021
H	1.992499	3.253717	−0.000754

Table S18. Energies for **CQ2_O1**.

Zero-point correction	0.308946 (Hartree/Particle)
Thermal correction to Energy	0.328025
Thermal correction to Enthalpy	0.328969
Thermal correction to Gibbs Free Energy	0.262808
Sum of electronic and zero-point Energies	−1013.585942
Sum of electronic and thermal Energies	−1013.566864
Sum of electronic and thermal Enthalpies	−1013.565919
Sum of electronic and thermal Free Energies	−1013.632081

Table S19. Cartesian coordinates for **CQ2_O2**.

C	−1.732241	0.898925	−0.000026
C	−1.758593	−0.466098	−0.000008
C	−3.057753	−1.233798	0.000047
C	−3.159034	−2.135227	−1.277265
C	−3.159095	−2.133730	1.278631
C	−0.465462	1.660813	0.000022
C	−0.436651	−1.242944	−0.000043
C	0.742144	0.952185	0.000056
C	0.788378	−0.444239	0.000026
N	2.023984	1.449863	0.000118
C	2.152941	−0.822367	−0.000043
C	2.907828	0.402293	0.000101
C	2.830770	−2.059083	−0.000266
C	4.316989	0.438276	0.000040
C	4.205903	−2.027432	−0.000319
C	4.929063	−0.801809	−0.000162
O	−2.904810	2.951583	−0.000051
O	−0.488340	2.946852	0.000032
O	−0.422360	−2.459292	0.000011
H	−3.086735	−1.537197	−2.187987
H	−4.126623	−2.640775	−1.276814
H	−2.372436	−2.886155	−1.272201
H	−3.086682	−1.534544	2.188558
H	−2.372557	−2.884722	1.274292
H	−4.126740	−2.639155	1.278696
H	2.262693	2.431909	0.000557
H	−5.138352	1.607239	−0.001216
H	−5.212901	−0.853016	−0.000579
C	5.074153	1.738056	0.000187
H	6.012625	−0.845631	−0.000208
H	2.278254	−2.988548	−0.000345
H	4.764860	−2.955353	−0.000478
H	4.840156	2.339280	0.885217
H	4.840140	2.339482	−0.884706
H	6.149414	1.560213	0.000157
H	−1.517589	3.223497	−0.000156

Table S20. Energies for **CQ2_O2**.

Zero-point correction	0.308944 (Hartree/Particle)
Thermal correction to Energy	0.328018
Thermal correction to Enthalpy	0.328963
Thermal correction to Gibbs Free Energy	0.262822
Sum of electronic and zero-point Energies	−1013.585944
Sum of electronic and thermal Energies	−1013.566870
Sum of electronic and thermal Enthalpies	−1013.565926
Sum of electronic and thermal Free Energies	−1013.632067

Table S21. Cartesian coordinates for **CQ2_O3**.

C	−4.285091	1.010815	0.010261
C	−4.274058	−0.324520	0.091467
C	−3.045377	1.772008	−0.152317
C	−1.766178	0.981622	0.004740
C	−1.758327	−0.389677	0.025424
C	−3.053826	−1.208732	0.053326
C	−3.195507	−2.094897	−1.223552
C	−3.116250	−2.094158	1.337901
C	−0.493249	1.774400	0.116733
C	−0.452118	−1.103768	0.006758
C	0.740654	0.968188	0.020162
C	0.770098	−0.434440	−0.029806
N	1.985162	1.444070	0.047016
C	2.176530	−0.823379	−0.049506
C	2.908167	0.395123	0.001216
C	2.883259	−2.028091	−0.104240
C	4.307751	0.475944	−0.000089
C	4.276536	−1.974899	−0.102917
C	4.967674	−0.754075	−0.051491
O	−3.022155	2.957673	−0.433408
O	−0.414510	2.970046	0.330215
O	−0.510301	−2.422978	0.002422
H	−3.156461	−1.483028	−2.128685
H	−4.165735	−2.598486	−1.200847
H	−2.422255	−2.861186	−1.274712
H	−3.024011	−1.481852	2.239091
H	−2.343600	−2.861785	1.345678
H	−4.086856	−2.596316	1.372420
H	2.192828	2.436438	0.100527
H	−5.204965	1.586090	0.008641
H	−5.213871	−0.866758	0.169164
C	5.034384	1.793581	0.050784
H	6.052937	−0.763876	−0.053379
H	2.397298	−2.998884	−0.156819
H	4.842867	−2.899081	−0.145837
H	4.784628	2.357390	0.957237
H	4.788268	2.422514	−0.812776
H	6.114718	1.640307	0.047517
H	0.373369	−2.824173	−0.019302

Table S22. Energies for **CQ2_O3**.

Zero-point correction	0.308505 (Hartree/Particle)
Thermal correction to Energy	0.328314
Thermal correction to Enthalpy	0.329259
Thermal correction to Gibbs Free Energy	0.260427
Sum of electronic and zero-point Energies	−1013.546671
Sum of electronic and thermal Energies	−1013.526862
Sum of electronic and thermal Enthalpies	−1013.525917
Sum of electronic and thermal Free Energies	−1013.594749

Table S23. Cartesian coordinates for **CQ2_N4**.

C	−4.319194	0.978187	0.037524
C	−4.307219	−0.359515	0.095400
C	−3.082112	1.748822	−0.105881
C	−1.799018	0.955159	0.010745
C	−1.796404	−0.414231	0.018275
C	−3.082550	−1.232588	0.043144
C	−3.202532	−2.112408	−1.240371
C	−3.114838	−2.144333	1.309694
C	−0.528645	1.748747	0.098094
C	−0.494837	−1.186779	−0.020895
C	0.680881	0.946769	−0.068826
C	0.767765	−0.391036	−0.062276
N	2.032826	1.547976	−0.022921
C	2.166626	−0.802418	−0.045390
C	2.948912	0.365461	−0.016422
C	2.796332	−2.045717	−0.047367
C	4.332518	0.402771	−0.000527
C	4.194052	−2.055837	−0.025990
C	4.936627	−0.871140	−0.003754
O	−3.064866	2.945797	−0.339283
O	−0.415046	2.939894	0.347112
O	−0.423416	−2.404880	−0.036125
H	−3.181158	−1.494482	−2.142257
H	−4.157088	−2.645531	−1.220206
H	−2.400298	−2.849023	−1.285918
H	−3.031226	−1.549477	2.223595
H	−2.314738	−2.883430	1.284185
H	−4.070596	−2.674850	1.340543
H	2.119880	2.151642	0.808076
H	−5.239617	1.552682	0.048047
H	−5.246590	−0.904060	0.165923
C	5.127953	1.682722	0.023066
H	6.020656	−0.925337	0.013551
H	2.214046	−2.958586	−0.066977
H	4.719171	−3.005084	−0.027475
H	4.901895	2.286737	0.909964
H	4.931059	2.300470	−0.861511
H	6.198277	1.472040	0.038523
H	2.187272	2.168157	−0.830693

Table S24. Cartesian coordinates for **CQ2_N4**.

Zero-point correction	0.308948 (Hartree/Particle)
Thermal correction to Energy	0.328770
Thermal correction to Enthalpy	0.329714
Thermal correction to Gibbs Free Energy	0.260831
Sum of electronic and zero-point Energies	−1013.514191
Sum of electronic and thermal Energies	−1013.494370
Sum of electronic and thermal Enthalpies	−1013.493425
Sum of electronic and thermal Free Energies	−1013.562308

1.4. Protonated Species for CQ3

Table S25. Cartesian coordinates for **CQ3_O1**.

C	5.338090	0.774345	0.000083
C	4.663849	1.947010	0.000103
C	4.597140	−0.443440	0.000030
C	3.142119	−0.431066	0.000009
C	2.460284	0.760817	0.000019
C	3.179127	2.085415	0.000056
C	2.799006	2.916132	−1.280053
C	2.798901	2.916116	1.280139
C	2.454337	−1.764911	0.000001
C	0.925138	0.755426	0.000037
C	1.026322	−1.726351	−0.000035
C	0.284447	−0.546861	−0.000014
N	0.178942	−2.800382	−0.000103
C	−1.095526	−0.917869	−0.000037
C	−1.121338	−2.349669	−0.000100
C	−2.302653	−0.197391	−0.000017
C	−2.322673	−3.073889	−0.000141
C	−3.489413	−0.916709	−0.000060
C	−3.492017	−2.339687	−0.000121
O	5.245661	−1.559375	0.000008
O	3.117224	−2.822958	−0.000072
O	0.301653	1.811044	0.000090
H	3.057264	2.373260	−2.192599
H	3.352921	3.858056	−1.268309
H	1.731658	3.130049	−1.270553
H	3.057112	2.373247	2.192700
H	1.731547	3.130004	1.270570
H	3.352790	3.858056	1.268436
H	0.481067	−3.765652	−0.000138
H	6.420648	0.712550	0.000106
H	5.220682	2.880961	0.000141
H	−2.334734	−4.158458	−0.000187
H	−4.456799	−2.834628	−0.000153
H	−2.305489	0.884687	0.000028
C	−4.829894	−0.242755	−0.000047
O	−4.728138	1.094590	0.000031
C	−5.985994	1.828513	0.000065
H	−6.557276	1.529836	0.883447
H	−6.557276	1.529919	−0.883345

C	−5.652391	3.305773	0.000135
H	−6.578085	3.888477	0.000164
H	−5.076347	3.579595	−0.888153
H	−5.076345	3.579511	0.888447
O	−5.878085	−0.855480	−0.000075
H	4.556379	−2.323061	−0.000040

Table S26. Cartesian coordinates for **CQ3_O1**.

Zero-point correction	0.352282 (Hartree/Particle)
Thermal correction to Energy	0.375646
Thermal correction to Enthalpy	0.376590
Thermal correction to Gibbs Free Energy	0.299104
Sum of electronic and zero-point Energies	−1241.421016
Sum of electronic and thermal Energies	−1241.397651
Sum of electronic and thermal Enthalpies	−1241.396707
Sum of electronic and thermal Free Energies	−1241.474193

Table S27. Cartesian coordinates for **CQ3_O2**.

C	−5.338072	0.774327	−0.000037
C	−4.663842	1.946976	−0.000151
C	−4.597158	−0.443489	0.000002
C	−3.142101	−0.431102	−0.000026
C	−2.460276	0.760788	−0.000084
C	−3.179111	2.085401	−0.000052
C	−2.799176	2.915676	1.280455
C	−2.798774	2.916491	−1.279749
C	−2.454273	−1.764893	−0.000040
C	−0.925136	0.755406	0.000076
C	−1.026280	−1.726370	−0.000079
C	−0.284411	−0.546873	−0.000083
N	−0.178883	−2.800386	−0.000066
C	1.095557	−0.917863	−0.000053
C	1.121382	−2.349663	−0.000095
C	2.302679	−0.197384	−0.000040
C	2.322729	−3.073866	−0.000123
C	3.489441	−0.916686	−0.000071
C	3.492058	−2.339665	−0.000111
O	−5.245758	−1.559327	−0.000035
O	−3.117196	−2.822930	−0.000023
O	−0.301664	1.811000	0.000441
H	−3.057615	2.372503	2.192767
H	−3.353024	3.857641	1.268939
H	−1.731810	3.129524	1.271180
H	−3.056906	2.373944	−2.192528
H	−1.731432	3.130409	−1.270083
H	−3.352665	3.858431	−1.267822
H	−0.481012	−3.765655	−0.000027
H	−6.420630	0.712531	−0.000040
H	−5.220665	2.880932	−0.000280
H	2.334799	−4.158435	−0.000142
H	4.456853	−2.834581	−0.000125
H	2.305510	0.884696	−0.000005

C	4.829895	−0.242706	−0.000060
O	4.728091	1.094592	−0.000041
C	5.985966	1.828571	−0.000039
H	6.557251	1.529861	−0.883397
H	6.557178	1.529972	0.883406
C	5.652257	3.305792	−0.000142
H	6.577914	3.888553	−0.000128
H	5.076155	3.579590	0.888113
H	5.076246	3.579486	−0.888488
O	5.878067	−0.855459	−0.000075
H	−4.556408	−2.322926	0.000004

Table S28. Energies for **CQ3_O2**.

Zero-point correction	0.352283 (Hartree/Particle)
Thermal correction to Energy	0.375649
Thermal correction to Enthalpy	0.376593
Thermal correction to Gibbs Free Energy	0.299099
Sum of electronic and zero-point Energies	−1241.421014
Sum of electronic and thermal Energies	−1241.397649
Sum of electronic and thermal Enthalpies	−1241.396704
Sum of electronic and thermal Free Energies	−1241.474198

Table S29. Cartesian coordinates for **CQ3_O3**.

C	−5.408485	0.726464	−0.039728
C	−4.737357	1.878294	0.074705
C	−4.707751	−0.547647	−0.207625
C	−3.208257	−0.500051	−0.017597
C	−2.521435	0.685404	0.037310
C	−3.238672	2.039566	0.073226
C	−2.881436	2.813951	1.381109
C	−2.891857	2.901556	−1.180582
C	−2.500190	−1.822981	0.087617
C	−1.033466	0.654617	0.049617
C	−1.025605	−1.737664	0.018073
C	−0.305245	−0.534357	0.004102
N	−0.181810	−2.770972	0.043793
C	1.108626	−0.893402	0.006303
C	1.138311	−2.315338	0.032026
C	2.317517	−0.195162	−0.012898
C	2.322429	−3.051259	0.039312
C	3.512177	−0.921954	−0.002592
C	3.509651	−2.330688	0.023789
O	−5.269251	−1.583958	−0.517077
O	−3.030503	−2.901169	0.277790
O	−0.425899	1.825186	0.081395
H	−3.122959	2.218373	2.265684
H	−3.477267	3.729716	1.421502
H	−1.830594	3.098560	1.416547
H	−3.145429	2.369636	−2.101401
H	−1.838339	3.179571	−1.205224
H	−3.480462	3.822587	−1.152806
H	−0.492443	−3.737565	0.074224

H	−6.492292	0.684722	−0.065562
H	−5.285230	2.814544	0.155289
H	2.320175	−4.135818	0.057307
H	4.468156	−2.837252	0.030096
H	2.386948	0.887901	−0.043368
C	4.850815	−0.238670	−0.022213
O	4.735203	1.097759	−0.049951
C	5.990380	1.844999	−0.072209
H	6.557505	1.528699	−0.951609
H	6.565053	1.568750	0.815763
C	5.645912	3.318772	−0.104198
H	6.568270	3.906121	−0.122018
H	5.075188	3.611269	0.781753
H	5.066663	3.570592	−0.997062
O	5.899494	−0.845821	−0.013096
H	0.541002	1.733718	0.076563

Table S30. Energies for **CQ3_O3**.

Zero-point correction	0.351992 (Hartree/Particle)
Thermal correction to Energy	0.375969
Thermal correction to Enthalpy	0.376913
Thermal correction to Gibbs Free Energy	0.297390
Sum of electronic and zero-point Energies	−1241.380729
Sum of electronic and thermal Energies	−1241.356752
Sum of electronic and thermal Enthalpies	−1241.355808
Sum of electronic and thermal Free Energies	−1241.435331

Table S31. Cartesian coordinates for **CQ3_N4**.

C	−5.380552	0.793330	0.019729
C	−4.695556	1.936410	0.122430
C	−4.696243	−0.482960	−0.184363
C	−3.194570	−0.452405	−0.002971
C	−2.501521	0.722813	0.032928
C	−3.198876	2.075662	0.075503
C	−2.772429	2.855627	1.357785
C	−2.858441	2.918349	−1.192345
C	−2.507833	−1.779768	0.112848
C	−0.988286	0.726601	0.004126
C	−1.056525	−1.710182	−0.048324
C	−0.305921	−0.603017	−0.044810
N	−0.194584	−2.915331	0.004048
C	1.109856	−0.958076	−0.024786
C	1.191351	−2.357923	0.006244
C	2.283529	−0.208942	−0.028280
C	2.371158	−3.065445	0.023877
C	3.500927	−0.899704	−0.006030
C	3.541997	−2.299342	0.019140
O	−5.262663	−1.500483	−0.526487
O	−3.025280	−2.844147	0.388368
O	−0.312949	1.733630	−0.000333
H	−2.992485	2.278521	2.258888
H	−3.340464	3.786792	1.409685

H	−1.713270	3.103970	1.337052
H	−3.141542	2.386691	−2.103480
H	−1.797724	3.160656	−1.228829
H	−3.421396	3.853660	−1.161238
H	−0.414542	−3.470740	0.842100
H	−6.463825	0.763672	0.019852
H	−5.232144	2.875841	0.223394
H	2.411460	−4.147964	0.045431
H	4.511340	−2.782256	0.036908
H	2.257597	0.871229	−0.049237
C	4.826083	−0.176677	−0.008256
O	4.671411	1.146160	−0.035129
C	5.896464	1.952012	−0.039444
H	6.482842	1.660989	−0.912391
H	6.465310	1.696902	0.856060
C	5.488159	3.407160	−0.073037
H	6.385350	4.030853	−0.076659
H	4.894464	3.672642	0.804159
H	4.912383	3.636633	−0.972060
O	5.881353	−0.760424	0.012490
H	−0.372872	−3.529808	−0.801019

Table S32. Energies for **CQ3_N4**.

Zero-point correction	0.352328 (Hartree/Particle)
Thermal correction to Energy	0.376335
Thermal correction to Enthalpy	0.377279
Thermal correction to Gibbs Free Energy	0.297641
Sum of electronic and zero-point Energies	−1241.346918
Sum of electronic and thermal Energies	−1241.322911
Sum of electronic and thermal Enthalpies	−1241.321966
Sum of electronic and thermal Free Energies	−1241.401605

Table S33. Cartesian coordinates for **CQ3_O5**.

C	−5.416776	0.718174	−0.011017
C	−4.758574	1.872553	0.120572
C	−4.699699	−0.538898	−0.238292
C	−3.206918	−0.490127	−0.017281
C	−2.538185	0.697692	0.043681
C	−3.263943	2.037001	0.088791
C	−2.866094	2.815343	1.379922
C	−2.928972	2.896191	−1.168308
C	−2.502198	−1.811524	0.116503
C	−1.016627	0.731619	0.041098
C	−1.034259	−1.730411	0.031067
C	−0.331435	−0.560017	0.008746
N	−0.175495	−2.803971	0.055994
C	1.064092	−0.913624	0.008291
C	1.110924	−2.347331	0.035517
C	2.243164	−0.189292	−0.010088
C	2.322261	−3.056591	0.036778
C	3.461924	−0.900221	−0.006266
C	3.488254	−2.327784	0.016841

O	−5.249728	−1.547573	−0.633252
O	−3.036966	−2.875497	0.345182
O	−0.378230	1.772725	0.042324
H	−3.084983	2.225658	2.273327
H	−3.451545	3.736072	1.434427
H	−1.810527	3.078146	1.371183
H	−3.197070	2.365744	−2.084801
H	−1.870916	3.150145	−1.194074
H	−3.506883	3.822885	−1.135361
H	−0.486665	−3.766755	0.092992
H	−6.499104	0.663932	−0.025935
H	−5.314046	2.800053	0.232505
H	2.343478	−4.139107	0.054624
H	4.439999	−2.841345	0.018844
H	2.219793	0.891703	−0.026768
C	4.689150	−0.174407	−0.027232
O	4.670467	1.119754	−0.050283
C	5.902476	1.939341	−0.074194
H	6.462842	1.666862	−0.973275
H	6.474331	1.702018	0.827589
C	5.478084	3.388582	−0.100023
H	6.373408	4.014334	−0.119038
H	4.900033	3.642866	0.789160
H	4.887308	3.607235	−0.990328
O	5.814426	−0.848698	−0.022703
H	6.609368	−0.295953	−0.037800

Table S34. Energies for **CQ3_O5**.

Zero-point correction	0.352173 (Hartree/Particle)
Thermal correction to Energy	0.376133
Thermal correction to Enthalpy	0.377078
Thermal correction to Gibbs Free Energy	0.298142
Sum of electronic and zero-point Energies	−1241.380763
Sum of electronic and thermal Energies	−1241.356802
Sum of electronic and thermal Enthalpies	−1241.355858
Sum of electronic and thermal Free Energies	−1241.434793

Table S35. Cartesian coordinates for **CQ3_O6**.

C	−5.321300	0.880819	−0.031144
C	−4.606354	2.003338	0.079603
C	−4.668062	−0.415235	−0.227498
C	−3.173960	−0.435478	−0.006248
C	−2.446922	0.718731	0.032908
C	−3.105203	2.092893	0.052270
C	−2.675229	2.872155	1.332737
C	−2.722168	2.912762	−1.217393
C	−2.536638	−1.787690	0.150203
C	−0.926820	0.676695	0.032038
C	−1.065806	−1.782682	0.052114
C	−0.306883	−0.649187	0.007429
N	−0.261125	−2.897374	0.088818
C	1.068686	−1.071171	0.005477

C	1.044816	−2.506013	0.053562
C	2.278172	−0.399605	−0.035063
C	2.218572	−3.275772	0.051448
C	3.454515	−1.175179	−0.029300
C	3.420043	−2.610166	0.007344
O	−5.265765	−1.405220	−0.598926
O	−3.120388	−2.818965	0.404607
O	−0.233842	1.682024	0.030113
H	−2.930541	2.310989	2.234780
H	−3.212195	3.822856	1.366607
H	−1.607464	3.080026	1.327174
H	−3.010691	2.380211	−2.126401
H	−1.653082	3.115957	−1.241606
H	−3.255022	3.866389	−1.203707
H	−0.619745	−3.843217	0.140721
H	−6.404912	0.880783	−0.049211
H	−5.115395	2.959302	0.170517
H	2.188796	−4.357891	0.083103
H	4.349105	−3.165647	0.004097
H	2.313658	0.677376	−0.090071
C	4.753011	−0.640904	−0.097007
O	4.484952	1.345908	0.201291
C	5.568612	2.172666	−0.351168
H	5.448488	2.091894	−1.430930
H	6.523880	1.726979	−0.063991
C	5.441421	3.604237	0.127785
H	6.241741	4.200550	−0.317242
H	5.548660	3.676812	1.214553
H	4.485204	4.039566	−0.167205
O	5.882408	−0.781458	−0.232400
H	4.403489	1.529089	1.149045

Table S36. Energies for **CQ3_O6**.

Zero-point correction	0.350340 (Hartree/Particle)
Thermal correction to Energy	0.375049
Thermal correction to Enthalpy	0.375993
Thermal correction to Gibbs Free Energy	0.294573
Sum of electronic and zero-point Energies	−1241.352664
Sum of electronic and thermal Energies	−1241.327955
Sum of electronic and thermal Enthalpies	−1241.327011
Sum of electronic and thermal Free Energies	−1241.408431

1.5. Protonated Species for CQ4

Table S37. Cartesian coordinates for **CQ4_O1**.

C	5.248891	−0.251905	−0.000248
C	4.753188	−1.510387	−0.000053
C	4.338026	0.844427	−0.000380
C	2.900557	0.620605	−0.000295
C	2.399354	−0.659222	−0.000097
C	3.304718	−1.864259	0.000018
C	3.048857	−2.741636	1.279821

C	3.048829	−2.741862	−1.279640
C	2.028174	1.840309	−0.000439
C	0.881665	−0.878595	0.000082
C	0.620718	1.592762	−0.000267
C	0.060943	0.316278	−0.000030
N	−0.374565	2.530093	−0.000296
C	−1.358732	0.481157	0.000027
C	−1.593884	1.892646	−0.000135
C	−2.442537	−0.412840	0.000212
C	−2.890378	2.428667	−0.000116
C	−3.715228	0.131048	0.000230
C	−3.942701	1.532890	0.000069
O	4.817969	2.042866	−0.000514
O	2.528157	2.984545	−0.000583
O	0.415129	−2.013580	0.000183
H	3.220226	−2.165921	2.192694
H	3.736418	−3.591004	1.271052
H	2.025004	−3.111318	1.266498
H	3.220147	−2.166292	−2.192614
H	2.024986	−3.111568	−1.266206
H	3.736414	−3.591209	−1.270755
H	−0.216725	3.529238	−0.000439
H	6.310788	−0.032590	−0.000299
H	5.440619	−2.352949	0.000053
H	−3.067049	3.498787	−0.000237
H	−4.963576	1.896533	0.000097
H	−2.280589	−1.482954	0.000342
Br	−5.223541	−1.015987	0.000490
H	4.026426	2.698995	−0.000522

Table S38. Energies for **CQ4_O1**.

Zero-point correction	0.271054 (Hartree/Particle)
Thermal correction to Energy	0.289893
Thermal correction to Enthalpy	0.290837
Thermal correction to Gibbs Free Energy	0.223764
Sum of electronic and zero-point Energies	−3545.399576
Sum of electronic and thermal Energies	−3545.380738
Sum of electronic and thermal Enthalpies	−3545.379794
Sum of electronic and thermal Free Energies	−3545.446867

Table S39. Cartesian coordinates for **CQ4_O2**.

C	−5.255668	−0.229803	−0.000331
C	−4.770181	−1.482842	−0.000075
C	−4.349101	0.888947	−0.000099
C	−2.893559	0.608147	−0.000028
C	−2.404623	−0.667610	−0.000091
C	−3.321967	−1.864999	0.000052
C	−3.077680	−2.738482	−1.277690
C	−3.077505	−2.737626	1.278474
C	−2.010219	1.791021	0.000054
C	−0.888878	−0.890706	−0.000185
C	−0.621635	1.586235	−0.000025

C	−0.056947	0.309524	−0.000070
N	0.378276	2.529562	−0.000142
C	1.352483	0.474384	0.000017
C	1.588300	1.890959	0.000024
C	2.438905	−0.420474	0.000020
C	2.886119	2.423884	0.000051
C	3.706055	0.121557	0.000035
C	3.932357	1.528762	0.000059
O	−4.747566	2.072723	0.000023
O	−2.516478	2.970222	0.000058
O	−0.415379	−2.012253	−0.000339
H	−3.229875	−2.155519	−2.188317
H	−3.788035	−3.567452	−1.280385
H	−2.068338	−3.143370	−1.269581
H	−3.229600	−2.153997	2.188673
H	−2.068154	−3.142482	1.270374
H	−3.787847	−3.566603	1.281754
H	0.231486	3.530038	0.000084
H	−6.316535	−0.011165	−0.000553
H	−5.462529	−2.319833	0.000069
H	3.065486	3.491868	0.000076
H	4.951606	1.893054	0.000058
H	2.273915	−1.488580	−0.000013
Br	5.221283	−1.019790	−0.000012
H	−3.586555	2.828940	0.000077

Table S40. Energies for **CQ4_O2**.

Zero-point correction	0.271053 (Hartree/Particle)
Thermal correction to Energy	0.289892
Thermal correction to Enthalpy	0.290837
Thermal correction to Gibbs Free Energy	0.223757
Sum of electronic and zero-point Energies	−3545.399578
Sum of electronic and thermal Energies	−3545.380738
Sum of electronic and thermal Enthalpies	−3545.379794
Sum of electronic and thermal Free Energies	−3545.446874

Table S41. Cartesian coordinates for **CQ4_O3**.

C	−5.309155	−0.181602	−0.020284
C	−4.818090	−1.416637	0.112050
C	−4.420932	0.956240	−0.249974
C	−2.952206	0.690851	−0.015389
C	−2.449325	−0.579097	0.036275
C	−3.363493	−1.806878	0.078415
C	−3.179675	−2.702999	−1.185397
C	−3.102926	−2.635841	1.374355
C	−2.066515	1.894956	0.137691
C	−0.974817	−0.764420	0.035215
C	−0.620864	1.603547	0.048670
C	−0.085175	0.307467	0.005022
N	0.364218	2.499373	0.090617
C	1.365806	0.457900	0.003906
C	1.601370	1.856787	0.059875

C	2.458560	−0.409003	−0.038490
C	2.879825	2.406681	0.074428
C	3.740101	0.141847	−0.019986
C	3.953933	1.529241	0.035959
O	−4.798812	2.035962	−0.652750
O	−2.447085	3.014193	0.394557
O	−0.547444	−2.010642	0.035426
H	−3.349388	−2.128384	−2.098378
H	−3.912834	−3.511573	−1.158017
H	−2.188965	−3.152017	−1.222955
H	−3.227932	−2.017398	2.265973
H	−2.110803	−3.081255	1.383999
H	−3.832441	−3.446599	1.426133
H	0.204662	3.500928	0.142248
H	−6.373362	0.022102	−0.032854
H	−5.500090	−2.254695	0.224416
H	3.040251	3.477178	0.115540
H	4.965375	1.913101	0.047590
H	2.362172	−1.487074	−0.092577
Br	5.238954	−1.019138	−0.077351
H	0.418642	−2.070435	0.019940

Table S42. Energies for **CQ4_O3**.

Zero-point correction	0.270820 (Hartree/Particle)
Thermal correction to Energy	0.290267
Thermal correction to Enthalpy	0.291211
Thermal correction to Gibbs Free Energy	0.222017
Sum of electronic and zero-point Energies	−3545.358193
Sum of electronic and thermal Energies	−3545.338746
Sum of electronic and thermal Enthalpies	−3545.337802
Sum of electronic and thermal Free Energies	−3545.406997

Table S43. Cartesian coordinates for **CQ4_N4**.

C	−5.304089	−0.270134	0.042450
C	−4.791258	−1.500962	0.135924
C	−4.443398	0.892753	−0.169998
C	−2.960797	0.643900	0.001089
C	−2.445119	−0.619746	0.025407
C	−3.331650	−1.856879	0.066155
C	−3.134071	−2.724293	−1.215654
C	−3.004903	−2.705683	1.333365
C	−2.090366	1.857484	0.123027
C	−0.948821	−0.841736	−0.016298
C	−0.663351	1.580944	−0.042368
C	−0.082672	0.376647	−0.050940
N	0.364154	2.648651	0.019159
C	1.370105	0.523706	−0.030280
C	1.652679	1.896138	0.014199
C	2.415623	−0.393933	−0.042386
C	2.927128	2.415442	0.037119
C	3.718644	0.113637	−0.014669
C	3.976345	1.489198	0.023742

O	−4.856902	1.981866	−0.510483
O	−2.447452	2.983178	0.408213
O	−0.423717	−1.934501	−0.042904
H	−3.344753	−2.144223	−2.116804
H	−3.829075	−3.566180	−1.188262
H	−2.121321	−3.120426	−1.267933
H	−3.127691	−2.114949	2.244115
H	−1.992776	−3.102945	1.293731
H	−3.699219	−3.547092	1.384426
H	0.224134	3.222060	0.862455
H	−6.371450	−0.083329	0.056140
H	−5.457663	−2.352475	0.243078
H	3.132354	3.478872	0.069110
H	4.998577	1.843413	0.045281
H	2.220604	−1.456689	−0.074299
Br	5.177420	−1.096840	−0.030366
H	0.273887	3.289556	−0.780252

Table S44. Energies for **CQ4_N4**.

Zero-point correction	0.271077 (Hartree/Particle)
Thermal correction to Energy	0.290559
Thermal correction to Enthalpy	0.291503
Thermal correction to Gibbs Free Energy	0.222218
Sum of electronic and zero-point Energies	−3545.323935
Sum of electronic and thermal Energies	−3545.304453
Sum of electronic and thermal Enthalpies	−3545.303509
Sum of electronic and thermal Free Energies	−3545.372794

1.6. Fragments for CQ1

m/*z* 292a corresponds to **CQ1_O1** and *m*/*z* 292c corresponds to **CQ1_O2**.

Table S45. Cartesian coordinates for *m*/*z* 292b.

C	−2.748930	1.492265	−0.145775
C	−1.464831	0.847832	−0.105418
C	−1.320789	−0.576581	−0.150941
C	−2.424830	−2.877511	−0.405452
C	−0.266822	1.756528	−0.033743
C	0.071001	−1.197255	−0.111259
C	1.004970	1.108022	−0.003428
C	1.193684	−0.275636	−0.039285
N	2.215338	1.734014	0.064486
C	2.595900	−0.510263	0.012317
C	3.214395	0.781543	0.076577
C	3.399013	−1.670867	0.010446
C	4.602654	0.938080	0.138336
C	4.769425	−1.510782	0.072032
C	5.361867	−0.222394	0.135005
O	−2.910115	2.811280	−0.130631
O	−0.391000	2.995123	−0.005980
O	0.223951	−2.412471	−0.128834
H	−1.777792	−3.166127	−1.237732
H	−3.428603	−3.270024	−0.577499

H	−1.986357	−3.366797	0.470565
H	2.332191	2.737762	0.100326
H	6.443239	−0.144705	0.181727
H	2.937499	−2.649622	−0.037686
H	5.413922	−2.383254	0.072683
H	5.065180	1.917917	0.186536
H	−2.010854	3.231937	−0.083669
C	−4.584353	−1.285714	1.104175
H	−4.083203	−0.945114	2.011332
H	−5.600932	−0.890653	1.083744
H	−4.626684	−2.374650	1.098027
C	−2.450552	−1.390084	−0.242698
C	−3.873308	0.693816	−0.194708
H	−4.847791	1.173733	−0.198435
C	−3.800240	−0.768171	−0.177913
H	−4.389396	−1.156917	−1.027377

Table S46. Energies for *m*/*z* 292b.

Zero-point correction	0.280268 (Hartree/Particle)
Thermal correction to Energy	0.297885
Thermal correction to Enthalpy	0.298830
Thermal correction to Gibbs Free Energy	0.235073
Sum of electronic and zero-point Energies	−974.270142
Sum of electronic and thermal Energies	−974.252525
Sum of electronic and thermal Enthalpies	−974.251581
Sum of electronic and thermal Free Energies	−974.315337

Table S47. Cartesian coordinates for *m*/*z* 292d.

C	3.448074	0.666495	1.382189
C	3.702417	−0.470553	0.720204
C	2.246723	1.449200	1.105196
C	1.590348	1.011106	−0.419233
C	1.519443	−0.414937	−0.328252
C	2.841700	−1.140722	−0.364847
C	2.830971	−2.660811	−0.072123
C	3.548231	−0.926659	−1.747434
C	0.328254	1.835900	−0.679293
C	0.197845	−1.090002	−0.004793
C	−0.904426	1.120561	−0.420938
C	−0.970357	−0.244663	−0.106851
N	−2.153903	1.638086	−0.459297
C	−2.357056	−0.566810	0.057989
C	−3.076964	0.641797	−0.168337
C	−3.055802	−1.743991	0.373033
C	−4.469035	0.709286	−0.090697
C	−4.442355	−1.678359	0.450494
C	−5.136138	−0.471935	0.222183
O	1.726041	2.331974	1.702351
O	0.410996	2.980934	−1.078941
O	0.153784	−2.281697	0.294892
H	2.433708	−2.895555	0.914037
H	3.861275	−3.022272	−0.136857

H	2.231753	−3.196343	−0.808671
H	3.681792	0.124301	−2.008530
H	2.972524	−1.419715	−2.534965
H	4.534541	−1.395062	−1.707238
H	−2.356292	2.606854	−0.673748
H	4.096783	1.047884	2.164506
H	4.591324	−1.042237	0.978716
H	−6.218674	−0.462990	0.293222
H	−2.518089	−2.667570	0.550571
H	−5.006898	−2.572454	0.692436
H	−5.008266	1.634325	−0.264437
H	2.404033	1.395129	−1.041302

Table S48. Energies for *m*/*z* 292d.

Zero-point correction	0.278804 (Hartree/Particle)
Thermal correction to Energy	0.296873
Thermal correction to Enthalpy	0.297817
Thermal correction to Gibbs Free Energy	0.232873
Sum of electronic and zero-point Energies	−974.211489
Sum of electronic and thermal Energies	−974.193420
Sum of electronic and thermal Enthalpies	−974.192476
Sum of electronic and thermal Free Energies	−974.257420

Table S49. Cartesian coordinates for *m*/*z* 292e.

C	−3.978308	0.902536	−0.293301
C	−3.950330	−0.434059	−0.193232
C	−2.756819	1.703083	−0.203538
C	−1.474546	0.908528	−0.069623
C	−1.457528	−0.447916	0.081893
C	−2.723773	−1.286669	−0.004533
C	−2.642947	−2.252071	−1.230277
C	−2.916493	−2.114741	1.301793
C	−0.217695	1.709030	−0.116720
C	−0.143821	−1.159396	0.302716
C	0.885033	1.130212	0.891639
C	1.036703	−0.285221	0.504047
N	2.201801	1.673133	0.765652
C	2.350613	−0.515406	0.145068
C	3.061160	0.746171	0.309674
C	3.038758	−1.665034	−0.352193
C	4.429895	0.858528	−0.004353
C	4.369095	−1.533459	−0.640511
C	5.051226	−0.280624	−0.467300
O	−2.735439	2.921949	−0.200289
O	0.009560	2.681237	−0.774603
O	−0.015818	−2.373896	0.294662
H	−2.502410	−1.694404	−2.160115
H	−3.582986	−2.805432	−1.306852
H	−1.830221	−2.967589	−1.109077
H	−2.985816	−1.462433	2.176792
H	−2.098471	−2.822215	1.440592
H	−3.848974	−2.681278	1.229885

H	2.419431	2.650849	0.910691
H	−4.902355	1.455714	−0.424963
H	−4.881889	−0.993439	−0.249541
H	6.106508	−0.234340	−0.718581
H	2.505740	−2.600735	−0.468311
H	4.934216	−2.382809	−1.007962
H	4.964785	1.794300	0.111201
H	0.462063	1.296603	1.891039

Table S50. Energies for *m*/*z* 292e.

Zero-point correction	0.279897 (Hartree/Particle)
Thermal correction to Energy	0.297823
Thermal correction to Enthalpy	0.298767
Thermal correction to Gibbs Free Energy	0.234465
Sum of electronic and zero-point Energies	−974.228196
Sum of electronic and thermal Energies	−974.210270
Sum of electronic and thermal Enthalpies	−974.209326
Sum of electronic and thermal Free Energies	−974.273628

Table S51. Cartesian coordinates for *m*/*z* 292f.

C	3.139187	−2.119839	−0.000207
C	4.259204	−1.379823	−0.000015
C	1.801648	−1.525958	−0.000183
C	1.723198	−0.037885	−0.000076
C	2.879962	0.679743	0.000140
C	4.259582	0.118028	0.000174
C	5.003610	0.640735	−1.268477
C	5.003594	0.640505	1.268875
C	0.470835	0.781515	−0.000156
C	−1.884540	2.516081	−0.000080
C	−0.922092	0.265183	−0.000089
C	−2.026273	1.161622	−0.000043
N	−1.390124	−0.981135	−0.000039
C	−3.237021	0.355806	0.000063
C	−2.778329	−0.989398	−0.000004
C	−4.608274	0.627139	0.000170
C	−3.656026	−2.078036	0.000013
C	−5.480606	−0.455665	0.000191
C	−5.012839	−1.787245	0.000114
O	0.813024	−2.277798	−0.000168
O	0.523058	2.014714	−0.000235
O	−1.960337	3.660836	−0.000088
H	4.514178	0.303268	−2.185142
H	6.031339	0.267304	−1.266186
H	5.037585	1.733649	−1.268131
H	4.514169	0.302894	2.185494
H	5.037576	1.733421	1.268734
H	6.031327	0.267086	1.266551
H	−0.685234	−1.762403	−0.000111
H	3.161104	−3.204516	−0.000332
H	5.231986	−1.866772	0.000006
H	−5.731248	−2.599764	0.000142

H	−4.985294	1.644309	0.000208
H	−6.550013	−0.273486	0.000265
H	−3.290131	−3.098882	−0.000033
H	2.798656	1.764764	0.000267

Table S52. Energies for *m*/*z* 292f.

Zero-point correction	0.278849 (Hartree/Particle)
Thermal correction to Energy	0.297334
Thermal correction to Enthalpy	0.298278
Thermal correction to Gibbs Free Energy	0.231759
Sum of electronic and zero-point Energies	−974.266410
Sum of electronic and thermal Energies	−974.247926
Sum of electronic and thermal Enthalpies	−974.246981
Sum of electronic and thermal Free Energies	−974.313500

Table S53. Cartesian coordinates for *m*/*z* 292g.

C	−3.231412	−1.455787	−0.721208
C	−3.113321	−0.303853	−1.374417
C	−2.448801	−1.724366	0.472652
C	−1.456218	−0.668155	0.827306
C	−1.298919	0.503587	0.153152
C	−2.240699	0.862228	−0.974024
C	−3.195689	2.002090	−0.467497
C	−1.440341	1.378556	−2.198513
C	−0.647255	−1.006433	1.919495
C	−0.226914	1.489389	0.578251
C	2.142397	1.935296	0.976230
C	1.152098	1.139614	0.426572
N	3.343996	1.414680	0.706918
C	1.836225	0.040563	−0.259004
C	3.205573	0.252855	−0.050638
C	1.448157	−1.063176	−1.029217
C	4.190142	−0.585908	−0.554552
C	2.419015	−1.903654	−1.535395
C	3.779610	−1.671925	−1.298263
O	−2.512716	−2.726478	1.162528
O	−0.036613	−1.309514	2.805945
O	−0.637009	2.525088	1.095989
H	−3.763093	1.682188	0.395390
H	−3.886479	2.231029	−1.267989
H	−2.641082	2.890566	−0.215225
H	−0.759341	0.631726	−2.583772
H	−0.880899	2.269664	−1.948483
H	−2.135681	1.637269	−2.985545
H	4.209351	1.803552	0.999185
H	−3.900249	−2.230568	−1.035101
H	−3.708312	−0.132019	−2.251431
H	4.508284	−2.343505	−1.705494
H	0.419787	−1.268403	−1.250220
H	2.128129	−2.749167	−2.126693
H	5.230224	−0.395778	−0.376422
H	2.020203	2.832385	1.542100

Table S54. Energies for *m*/*z* 292g.

Zero-point correction	0.278021 (Hartree/Particle)
Thermal correction to Energy	0.297156
Thermal correction to Enthalpy	0.298101
Thermal correction to Gibbs Free Energy	0.229406
Sum of electronic and zero-point Energies	−974.219194
Sum of electronic and thermal Energies	−974.200059
Sum of electronic and thermal Enthalpies	−974.199115
Sum of electronic and thermal Free Energies	−974.267810

Table S55. Cartesian coordinates for TS *m*/*z* 292g.

C	−4.828713	0.154314	0.100241
C	−4.115619	1.285772	−0.067979
C	−4.209707	−1.183211	0.142292
C	−2.724634	−1.054727	0.021050
C	−1.935086	0.047209	−0.138183
C	−2.609138	1.405875	−0.248067
C	−2.043952	2.383385	0.812192
C	−2.322278	1.969751	−1.668377
C	−1.536476	−1.715519	−0.107510
C	0.707650	0.153890	1.252750
C	1.305256	−0.099088	−1.144385
C	1.596291	0.063461	0.227245
N	2.457478	−0.194119	−1.803294
C	3.058966	0.054061	0.373705
C	3.558373	−0.109127	−0.935450
C	3.941677	0.165186	1.448897
C	4.921307	−0.165469	−1.218451
C	5.306251	0.108797	1.175118
C	5.788768	−0.053516	−0.135921
O	−4.794018	−2.241829	0.257834
O	−0.613964	−2.433097	−0.207031
O	0.167014	0.247589	2.262624
H	−2.188377	2.005963	1.827603
H	−2.553066	3.348455	0.733644
H	−0.976254	2.554680	0.645691
H	−2.695505	1.300982	−2.448242
H	−1.247351	2.117826	−1.809768
H	−2.815968	2.938805	−1.787490
H	2.525573	−0.324478	−2.805504
H	−5.908530	0.182091	0.209808
H	−4.651352	2.234596	−0.092335
H	6.858826	−0.092883	−0.307655
H	3.585183	0.289610	2.466087
H	6.013771	0.191620	1.993046
H	5.290429	−0.291877	−2.230679
H	0.334412	−0.144115	−1.613571

Table S56. Energies for TS *m*/*z* 292g.

Zero-point correction	0.274406 (Hartree/Particle)
Thermal correction to Energy	0.294354
Thermal correction to Enthalpy	0.295298
Thermal correction to Gibbs Free Energy	0.221997
Sum of electronic and zero-point Energies	−974.137502
Sum of electronic and thermal Energies	−974.117555
Sum of electronic and thermal Enthalpies	−974.116611
Sum of electronic and thermal Free Energies	−974.189912

Table S57. Cartesian coordinates for TS *m*/*z* 292f.

C	5.228810	0.951887	−0.222219
C	5.348728	−0.376575	−0.065849
C	3.930250	1.629462	−0.217583
C	2.744765	0.676133	−0.021061
C	2.878166	−0.671421	0.137332
C	4.205903	−1.338575	0.129841
C	4.372802	−2.087069	1.491517
C	4.199459	−2.389653	−1.027604
C	1.514970	1.341789	−0.002474
C	−1.224876	−0.512383	−0.081639
C	−2.242299	0.999020	0.258714
C	−2.543704	−0.363997	−0.025431
N	−3.454826	1.577290	0.368226
C	−3.966088	−0.621205	−0.091167
C	−4.515784	0.658288	0.172358
C	−4.799674	−1.715840	−0.324657
C	−5.890968	0.868090	0.209324
C	−6.177205	−1.506961	−0.289093
C	−6.711680	−0.235848	−0.026098
O	3.743899	2.821211	−0.351184
O	0.657677	2.085220	0.009452
O	−0.064567	−0.759749	−0.152840
H	4.376736	−1.390502	2.332967
H	5.324075	−2.625940	1.483290
H	3.569362	−2.814896	1.633925
H	4.074554	−1.911105	−2.001512
H	3.398386	−3.119605	−0.883112
H	5.153504	−2.923779	−1.023130
H	−3.601431	2.557648	0.569089
H	6.088921	1.598966	−0.360875
H	6.338653	−0.827072	−0.077731
H	−7.788916	−0.106811	−0.005309
H	−4.389513	−2.699267	−0.527298
H	−6.848632	−2.340219	−0.467184
H	−6.312865	1.847216	0.411257
H	1.995425	−1.289965	0.269353

Table S58. Energies for TS *m*/*z* 292f.

Zero-point correction	0.273587 (Hartree/Particle)
Thermal correction to Energy	0.293830
Thermal correction to Enthalpy	0.294774
Thermal correction to Gibbs Free Energy	0.219791
Sum of electronic and zero-point Energies	−974.120827
Sum of electronic and thermal Energies	−974.100585
Sum of electronic and thermal Enthalpies	−974.099640
Sum of electronic and thermal Free Energies	−974.174624

Table S59. Cartesian coordinates for product with *m*/*z* 149.

C	−4.913100	−1.132324	−0.000498
C	−5.236650	0.168157	−0.000283
C	−3.518262	−1.606363	−0.000388
C	−2.472180	−0.513865	0.000047
C	−2.823361	0.794109	0.000286
C	−4.234678	1.290754	0.000091
C	−4.441170	2.172182	1.267614
C	−4.440622	2.172526	−1.267296
C	−1.078129	−0.946273	0.000366
C	1.109355	0.061632	0.000167
C	2.141918	−0.842487	0.000191
C	2.386115	0.556216	−0.000056
N	3.276634	−1.536736	0.000205
C	3.805815	0.731035	−0.000096
C	4.343557	−0.597558	0.000054
C	4.665181	1.840776	−0.000271
C	5.713544	−0.833604	0.000012
C	6.031898	1.601324	−0.000288
C	6.541916	0.287971	−0.000153
O	−3.224256	−2.789115	−0.000671
O	−0.557504	−2.007326	0.000797
O	−0.158817	0.297175	0.000038
H	−4.302412	1.591059	2.182643
H	−5.456848	2.577845	1.268600
H	−3.741034	3.013185	1.274101
H	−4.301498	1.591635	−2.182415
H	−3.740457	3.013507	−1.273254
H	−5.456289	2.578215	−1.268585
H	3.369892	−2.544975	0.000513
H	−5.665329	−1.914485	−0.000775
H	−6.282752	0.467854	−0.000382
H	7.617246	0.142189	−0.000180
H	4.266775	2.848930	−0.000390
H	6.723200	2.436728	−0.000413
H	6.124819	−1.836993	0.000109
H	−2.054024	1.561336	0.000668

Table S60. Energies for product with *m*/*z* 149.

Zero-point correction	0.277506 (Hartree/Particle)
Thermal correction to Energy	0.296520
Thermal correction to Enthalpy	0.297464
Thermal correction to Gibbs Free Energy	0.227290
Sum of electronic and zero-point Energies	−974.149160
Sum of electronic and thermal Energies	−974.130146
Sum of electronic and thermal Enthalpies	−974.129202
Sum of electronic and thermal Free Energies	−974.199376

Table S61. Cartesian coordinates for product with *m*/*z* 144.

C	4.636945	1.585277	−0.009146
C	5.100547	0.314430	−0.005353
C	3.206580	1.981144	−0.007623
C	2.365033	0.727483	−0.001517
C	2.866590	−0.534265	0.002207
C	4.287023	−0.978558	0.001378
C	4.600083	−1.805844	1.277460
C	4.595513	−1.816388	−1.268885
C	1.483708	−0.348842	0.004125
C	−0.910125	0.290778	0.008271
C	−2.278342	−1.825129	−0.003814
C	−2.111671	−0.436517	0.002746
N	−3.595527	−2.098927	−0.008223
C	−3.438637	0.160272	0.002058
C	−4.348370	−0.919860	−0.004859
C	−3.923665	1.473399	0.006575
C	−5.731799	−0.741204	−0.007448
C	−5.301689	1.660906	0.004057
C	−6.193032	0.570750	−0.002844
O	2.774854	3.109647	−0.010764
O	0.319223	−0.833631	0.007753
O	−0.561427	1.418724	0.013101
H	4.380160	−1.242720	2.187502
H	5.662057	−2.065111	1.282604
H	4.019612	−2.732005	1.281759
H	4.371828	−1.261045	−2.182795
H	4.015480	−2.742820	−1.263155
H	5.657566	−2.075273	−1.275990
H	−3.984795	−3.031512	−0.013336
H	5.334430	2.417555	−0.013675
H	6.178907	0.164126	−0.006974
H	−7.261645	0.757443	−0.004619
H	−3.242764	2.317437	0.011910
H	−5.701197	2.669589	0.007493
H	−6.417084	−1.582500	−0.012752
H	−1.533226	−2.605592	−0.005454

Table S62. Energies for product with *m*/*z* 144.

Zero-point correction	0.277715 (Hartree/Particle)
Thermal correction to Energy	0.296995
Thermal correction to Enthalpy	0.297939
Thermal correction to Gibbs Free Energy	0.227777
Sum of electronic and zero-point Energies	−974.179513
Sum of electronic and thermal Energies	−974.160233
Sum of electronic and thermal Enthalpies	−974.159289
Sum of electronic and thermal Free Energies	−974.229451

Table S63. Cartesian coordinates for *m*/*z* 274.

C	2.722145	1.612028	0.000023
C	1.465036	1.236228	−0.000109
C	1.563602	−0.219149	−0.000090
C	2.864143	−2.419612	−0.000054
C	0.193534	2.071879	−0.000119
C	0.190662	−0.949583	−0.000116
C	−0.991594	1.259198	−0.000081
C	−1.005140	−0.135529	−0.000068
N	−2.268616	1.727917	−0.000050
C	−2.377870	−0.540713	0.000003
C	−3.145755	0.661304	0.000004
C	−3.036225	−1.783138	0.000057
C	−4.543886	0.654379	0.000060
C	−4.418028	−1.786799	0.000112
C	−5.161608	−0.583227	0.000114
O	0.247693	3.281832	−0.000069
O	0.180058	−2.161124	0.000068
H	2.359217	−2.835122	0.872892
H	3.893872	−2.764589	−0.000091
H	2.359157	−2.835100	−0.872972
H	−2.514423	2.708884	−0.000061
H	−6.243767	−0.634115	0.000158
H	−2.468663	−2.704169	0.000052
H	−4.950274	−2.730158	0.000154
H	−5.117463	1.573187	0.000061
C	5.382651	−0.835906	0.000124
H	5.508746	−1.466106	−0.884086
H	6.175780	−0.089754	0.000192
H	5.508639	−1.466148	0.884320
C	2.793895	−0.910650	−0.000024
C	3.994744	1.241019	0.000053
H	4.877856	1.864552	0.000022
C	4.021300	−0.185471	0.000065

Table S64. Energies for *m*/*z* 274.

Zero-point correction	0.250142 (Hartree/Particle)
Thermal correction to Energy	0.267113
Thermal correction to Enthalpy	0.268057
Thermal correction to Gibbs Free Energy	0.205828
Sum of electronic and zero-point Energies	−897.782219
Sum of electronic and thermal Energies	−897.765248
Sum of electronic and thermal Enthalpies	−897.764304
Sum of electronic and thermal Free Energies	−897.826532

Table S65. Cartesian coordinates for *m*/*z* 264a.

C	−3.686246	0.736895	−0.000110
C	−2.877512	1.816743	−0.000052
C	−3.102719	−0.584324	−0.000103
C	−1.719387	−0.715445	−0.000037
C	−0.840370	0.378942	0.000030
C	−1.365338	1.782878	0.000028
C	−0.862188	2.526806	1.277074
C	−0.862048	2.526848	−1.276939
C	−0.956251	−1.992561	−0.000012
C	0.452747	−1.523416	0.000023
C	0.510902	−0.120912	0.000030
N	1.687738	−2.049244	0.000066
C	1.908254	0.236215	0.000013
C	2.617647	−1.008275	0.000058
C	2.653492	1.426479	−0.000024
C	4.011586	−1.088507	0.000076
C	4.040240	1.349662	−0.000007
C	4.712292	0.109799	0.000044
O	−3.911806	−1.623931	−0.000173
O	−1.428837	−3.118130	0.000019
H	−1.226129	2.042600	2.186151
H	−1.224809	3.557920	1.263531
H	0.229152	2.544859	1.306681
H	−1.225886	2.042671	−2.186072
H	0.229297	2.544902	−1.306421
H	−1.224671	3.557961	−1.263404
H	1.910314	−3.036959	0.000088
H	−4.767546	0.819254	−0.000166
H	−3.317961	2.810541	−0.000060
H	5.796759	0.092814	0.000056
H	2.165313	2.394550	−0.000062
H	4.623126	2.264592	−0.000031
H	4.524869	−2.044397	0.000110
H	−3.391463	−2.457081	−0.000186

Table S66. Energies for *m*/*z* 264a.

Zero-point correction	0.271742 (Hartree/Particle)
Thermal correction to Energy	0.287716
Thermal correction to Enthalpy	0.288660
Thermal correction to Gibbs Free Energy	0.229445
Sum of electronic and zero-point Energies	−860.955449
Sum of electronic and thermal Energies	−860.939475
Sum of electronic and thermal Enthalpies	−860.938531
Sum of electronic and thermal Free Energies	−860.997747

Table S67. Cartesian coordinates for *m*/*z* 264b.

C	3.586233	0.247417	−0.189003
C	2.894258	1.552296	−0.239336
C	2.902267	−0.950903	−0.102008
C	1.497264	−0.855741	−0.069417
C	0.742814	0.349766	−0.133347
C	1.395156	1.554108	−0.261808
C	0.690155	2.865856	−0.429744
C	0.593099	−2.060985	0.014922
C	−0.723528	−1.476474	0.005493
C	−0.679300	−0.078085	−0.068545
N	−2.013994	−1.910964	0.077813
C	−2.022525	0.383700	−0.027400
C	−2.837777	−0.804782	0.060039
C	−2.671391	1.642715	−0.036530
C	−4.234274	−0.752094	0.121427
C	−4.048350	1.686900	0.027663
C	−4.822981	0.501121	0.102404
O	3.545537	−2.119916	−0.047789
O	1.005232	−3.219243	0.073141
H	−0.163179	2.761470	−1.104155
H	1.350228	3.633308	−0.839108
H	0.309914	3.235068	0.531871
H	−2.312204	−2.873654	0.143205
H	4.672885	0.239741	−0.203003
H	−5.904117	0.580208	0.148847
H	−2.100939	2.561777	−0.085406
H	−4.555363	2.645719	0.022418
H	−4.830597	−1.656140	0.184212
H	2.886146	−2.846662	0.009536
C	3.459339	2.475667	0.907002
H	3.197590	2.064486	1.883606
H	4.545744	2.543320	0.827671
H	3.042156	3.479248	0.817180
H	3.230787	2.039225	−1.175254

Table S68. Energies for *m*/*z* 264b.

Zero-point correction	0.270290 (Hartree/Particle)
Thermal correction to Energy	0.286517
Thermal correction to Enthalpy	0.287461
Thermal correction to Gibbs Free Energy	0.227236
Sum of electronic and zero-point Energies	−860.932227
Sum of electronic and thermal Energies	−860.916001
Sum of electronic and thermal Enthalpies	−860.915057
Sum of electronic and thermal Free Energies	−860.975281

Table S69. Cartesian coordinates for *m*/*z* 246.

C	2.855356	1.379157	−0.050717
C	1.573494	1.449210	0.186256
C	1.038985	0.071743	0.265821
C	1.344022	−2.437029	0.354945
C	0.424850	2.446246	0.040747
C	−0.742501	1.571407	0.129016
C	−0.410768	0.214533	0.190519
N	−2.071440	1.745310	0.017722
C	−1.650463	−0.509573	0.044656
C	−2.672867	0.492845	−0.022624
C	−2.049104	−1.857814	−0.008240
C	−4.029336	0.189386	−0.119889
C	−3.396695	−2.159895	−0.115175
C	−4.377462	−1.151392	−0.166824
O	0.510579	3.631633	−0.125378
H	2.099673	−3.091826	0.787732
H	1.021336	−2.888919	−0.588948
H	0.498506	−2.419926	1.039854
H	−2.540158	2.633210	−0.105183
H	−5.421626	−1.428302	−0.244910
H	−1.326607	−2.659228	0.019709
H	−3.704974	−3.197069	−0.163350
H	−4.780756	0.969008	−0.154696
C	4.202032	−2.031264	−0.308466
H	3.826903	−2.740355	−1.052423
H	5.190704	−1.702798	−0.625486
H	4.305516	−2.575088	0.635662
C	1.885914	−1.046192	0.136652
C	3.811262	0.452795	−0.159698
H	4.870734	0.608810	0.005308
C	3.255979	−0.870455	−0.176029

Table S70. Energies for *m*/*z* 246.

Zero-point correction	0.240256 (Hartree/Particle)
Thermal correction to Energy	0.255552
Thermal correction to Enthalpy	0.256496
Thermal correction to Gibbs Free Energy	0.198310
Sum of electronic and zero-point Energies	−784.447408
Sum of electronic and thermal Energies	−784.432112
Sum of electronic and thermal Enthalpies	−784.431168
Sum of electronic and thermal Free Energies	−784.489354

1.7. Fragments for CQ3

m/*z* 364 corresponds to **CQ3_O1**.

Table S71. Cartesian coordinates for *m*/*z* 346.

C	−4.529844	−0.714620	−0.000001
C	−3.229427	−0.916455	0.000151
C	−2.691511	0.441933	0.000152
C	−2.908363	2.989951	−0.000032
C	−2.439780	−2.217951	0.000283
C	−1.139599	0.509688	0.000370
C	−1.020098	−1.992269	0.000192
C	−0.407963	−0.738626	0.000216
N	−0.066861	−2.966721	0.000079
C	1.006668	−0.964440	0.000061
C	1.182519	−2.382300	−0.000010
C	2.131619	−0.122248	−0.000005
C	2.451153	−2.977682	−0.000149
C	3.387900	−0.712933	−0.000144
C	3.539147	−2.126017	−0.000216
O	−3.009883	−3.293354	0.000159
O	−0.604432	1.604644	0.000031
H	−2.270935	3.142912	0.873363
H	−3.685435	3.750783	−0.000224
H	−2.270641	3.142776	−0.873237
H	−0.270076	−3.957731	0.000058
H	4.549905	−2.518485	−0.000323
H	2.022246	0.954355	0.000054
H	2.575143	−4.055223	−0.000202
C	−5.871004	2.652539	−0.000369
H	−5.713061	3.276487	−0.885738
H	−6.910489	2.322831	−0.000458
H	−5.713251	3.276607	0.884950
C	−3.501885	1.599896	−0.000022
C	−5.517402	0.177822	−0.000167
H	−6.584770	−0.002728	−0.000273
C	−4.924533	1.475810	−0.000187
C	4.649162	0.098752	−0.000221
O	5.756963	−0.398052	−0.000384
O	4.406781	1.418701	−0.000069
C	5.580501	2.279943	−0.000058
H	6.180372	2.042819	0.883019

H	6.179948	2.043393	−0.883579
C	5.093837	3.714206	0.000514
H	4.492285	3.925455	0.889011
H	5.952945	4.391275	0.000509
H	4.491833	3.926016	−0.887543

Table S72. Energies for *m*/*z* 346.

Zero-point correction	0.321124 (Hartree/Particle)
Thermal correction to Energy	0.344111
Thermal correction to Enthalpy	0.345055
Thermal correction to Gibbs Free Energy	0.267718
Sum of electronic and zero-point Energies	−1164.912696
Sum of electronic and thermal Energies	−1164.889709
Sum of electronic and thermal Enthalpies	−1164.888765
Sum of electronic and thermal Free Energies	−1164.966102

Table S73. Cartesian coordinates for *m*/*z* 336.

C	4.192865	−2.254885	0.000053
C	2.947988	−2.774889	0.000111
C	4.360606	−0.820317	0.000060
C	3.235211	−0.005280	0.000126
C	1.922396	−0.502141	0.000193
C	1.662218	−1.978263	0.000191
C	0.851129	−2.363910	1.277237
C	0.850987	−2.363875	−1.276776
C	3.225810	1.482441	0.000151
C	1.773657	1.793288	0.000186
C	1.011761	0.614342	0.000193
N	0.976398	2.873137	0.000229
C	−0.373506	1.015798	0.000176
C	−0.353158	2.448131	0.000221
C	−1.619710	0.368430	0.000139
C	−1.513519	3.224703	0.000239
C	−2.775608	1.138410	0.000156
C	−2.725433	2.547806	0.000207
O	5.585364	−0.335166	−0.000010
O	4.204251	2.212439	0.000182
H	1.410457	−2.131401	2.186314
H	0.640277	−3.436399	1.263694
H	−0.098381	−1.825597	1.306844
H	1.410212	−2.131339	−2.185909
H	−0.098527	−1.825561	−1.306258
H	0.640137	−3.436364	−1.263241
H	1.285893	3.837157	0.000251
H	5.082763	−2.874622	−0.000003
H	2.823134	−3.854723	0.000103
H	−3.651239	3.112820	0.000219
H	−1.690380	−0.713460	0.000101
H	−1.470662	4.308838	0.000273
H	5.559847	0.646794	−0.000023
C	−4.147743	0.439234	0.000122
O	−5.205847	1.120399	0.000137

O	−4.219723	−0.988953	0.000073
C	−5.590020	−1.397840	0.000042
H	−6.076491	−1.014841	−0.872630
H	−6.075552	−1.018121	0.874669
C	−5.666765	−2.935924	−0.002803
H	−5.180380	−3.318918	0.869920
H	−6.692091	−3.241874	−0.002926
H	−5.181146	−3.315648	−0.877379

Table S74. Energies for *m*/*z* 336.

Zero-point correction	0.342709 (Hartree/Particle)
Thermal correction to Energy	0.364716
Thermal correction to Enthalpy	0.365660
Thermal correction to Gibbs Free Energy	0.291322
Sum of electronic and zero-point Energies	−1128.085892
Sum of electronic and thermal Energies	−1128.063886
Sum of electronic and thermal Enthalpies	−1128.062941
Sum of electronic and thermal Free Energies	−1128.137280

Table S75. Cartesian coordinates for *m*/z 292.

C	4.003336	−1.347698	−0.000107
C	2.988301	−2.236420	−0.000049
C	3.706399	0.065792	−0.000100
C	2.380305	0.480853	−0.000034
C	1.293500	−0.407521	0.000033
C	1.516002	−1.889790	0.000031
C	0.869554	−2.513243	1.277077
C	0.869409	−2.513256	−1.276936
C	1.898518	1.888433	−0.000009
C	0.422870	1.721591	0.000026
C	0.075215	0.361615	0.000033
N	−0.676275	2.492030	0.000069
C	−1.365816	0.301943	0.000016
C	−1.801792	1.666464	0.000061
C	−2.341626	−0.707960	−0.000021
C	−3.148813	2.033941	0.000079
C	−3.682319	−0.345315	−0.000004
C	−4.082725	1.006939	0.000047
O	4.713436	0.915074	−0.000170
O	2.594187	2.891573	0.000022
H	1.325973	−2.115009	2.186154
H	1.010529	−3.597133	1.263534
H	−0.201818	−2.304650	1.306684
H	1.325720	−2.115028	−2.186069
H	−0.201968	−2.304662	−1.306418
H	1.010385	−3.597144	−1.263401
H	−0.689245	3.504430	0.000091
H	5.044069	−1.652440	−0.000163
H	3.213149	−3.299939	−0.000057
H	−5.140109	1.248384	0.000059
H	−2.064751	−1.756207	−0.000059
H	−3.452771	3.075476	0.000113

H	4.377125	1.837999	−0.000183
C	−4.761062	−1.444366	−0.000038
O	−5.980803	−1.134846	−0.000023
H	−4.472459	−2.474710	−0.000074

Table S76. Energies for *m*/*z* 292.

Zero-point correction	0.280769 (Hartree/Particle)
Thermal correction to Energy	0.298820
Thermal correction to Enthalpy	0.299764
Thermal correction to Gibbs Free Energy	0.235606
Sum of electronic and zero-point Energies	−974.263182
Sum of electronic and thermal Energies	−974.245131
Sum of electronic and thermal Enthalpies	−974.244187
Sum of electronic and thermal Free Energies	−974.308345

1.8. Fragments for CQ4

Table S77. Cartesian coordinates for *m*/*z* 342.

C	−4.360974	−1.706516	0.000074
C	−3.238051	−2.454741	0.000094
C	−4.251554	−0.266771	0.000117
C	−2.990313	0.318940	0.000178
C	−1.797810	−0.420332	0.000202
C	−1.823917	−1.918582	0.000165
C	−1.101433	−2.452709	−1.276902
C	−1.101541	−2.452778	1.277263
C	−2.698236	1.777585	0.000271
C	−1.213381	1.805913	0.000179
C	−0.691415	0.502817	0.000133
N	−0.223496	2.713629	0.000159
C	0.744722	0.633438	0.000005
C	0.997952	2.043041	0.000053
C	1.837264	−0.245758	−0.000137
C	2.288734	2.577443	−0.000013
C	3.349961	1.685896	−0.000142
O	−5.360011	0.443686	0.000076
O	−3.519805	2.680687	0.000344
H	−1.604930	−2.116737	−2.186239
H	−1.100175	−3.545638	−1.263788
H	−0.065965	−2.107470	−1.305711
H	−1.605116	−2.116857	2.186576
H	−0.066077	−2.107545	1.306183
H	−1.100283	−3.545707	1.264090
H	−0.342814	3.719151	0.000203
H	−5.352873	−2.144834	0.000020
H	−3.322212	−3.538499	0.000055
H	4.369334	2.052892	−0.000200
H	1.708342	−1.320817	−0.000191
H	2.461934	3.648429	0.000026
H	−5.147635	1.402917	0.000063
C	3.117482	0.293823	−0.000205
Br	4.610472	−0.874112	−0.000388

Table S78. Energies for *m*/*z* 342.

Zero-point correction	0.261413 (Hartree/Particle)
Thermal correction to Energy	0.278938
Thermal correction to Enthalpy	0.279882
Thermal correction to Gibbs Free Energy	0.215928
Sum of electronic and zero-point Energies	−3432.064275
Sum of electronic and thermal Energies	−3432.046750
Sum of electronic and thermal Enthalpies	−3432.045806
Sum of electronic and thermal Free Energies	−3432.109760

Table S79. Cartesian coordinates for *m*/*z* 291.

C	4.009899	0.730976	−0.000233
C	3.909560	−0.617993	−0.000012
C	2.815050	1.508065	−0.000325
C	1.508412	0.867862	−0.000162
C	1.409530	−0.502282	0.000041
C	2.631012	−1.384848	0.000135
C	2.646871	−2.298859	1.280106
C	2.646801	−2.299249	−1.279563
C	0.312152	1.773983	−0.000259
C	0.023431	−1.161725	0.000408
C	−0.959194	1.121115	−0.000060
C	−1.115371	−0.264285	0.000182
N	−2.186195	1.721217	0.000017
C	−2.518731	−0.528965	0.000092
C	−3.165677	0.751595	0.000041
C	−3.300890	−1.708495	0.000129
C	−4.562581	0.899630	0.000014
C	−4.649142	−1.494322	0.000105
C	−5.318874	−0.266832	0.000043
O	2.917885	2.794830	−0.000603
O	0.451796	3.014474	−0.000051
O	−0.084020	−2.383486	0.000004
H	2.643051	−1.698224	2.192965
H	3.554134	−2.907870	1.269023
H	1.777602	−2.954113	1.268781
H	2.642888	−1.698890	−2.192604
H	1.777561	−2.954536	−1.267972
H	3.554087	−2.908224	−1.268368
H	−2.330857	2.722258	−0.000040
H	4.959039	1.255268	−0.000359
H	4.815809	−1.218873	0.000065
H	−5.031809	1.878186	−0.000025
H	−6.403214	−0.218379	0.000034
H	−2.840975	−2.690148	0.000208
H	1.967222	3.186252	−0.000717

Table S80. Energies for *m*/*z* 291.

Zero-point correction	0.268206 (Hartree/Particle)
Thermal correction to Energy	0.285494
Thermal correction to Enthalpy	0.286439
Thermal correction to Gibbs Free Energy	0.223525
Sum of electronic and zero-point Energies	−973.611699
Sum of electronic and thermal Energies	−973.594411
Sum of electronic and thermal Enthalpies	−973.593467
Sum of electronic and thermal Free Energies	−973.656381

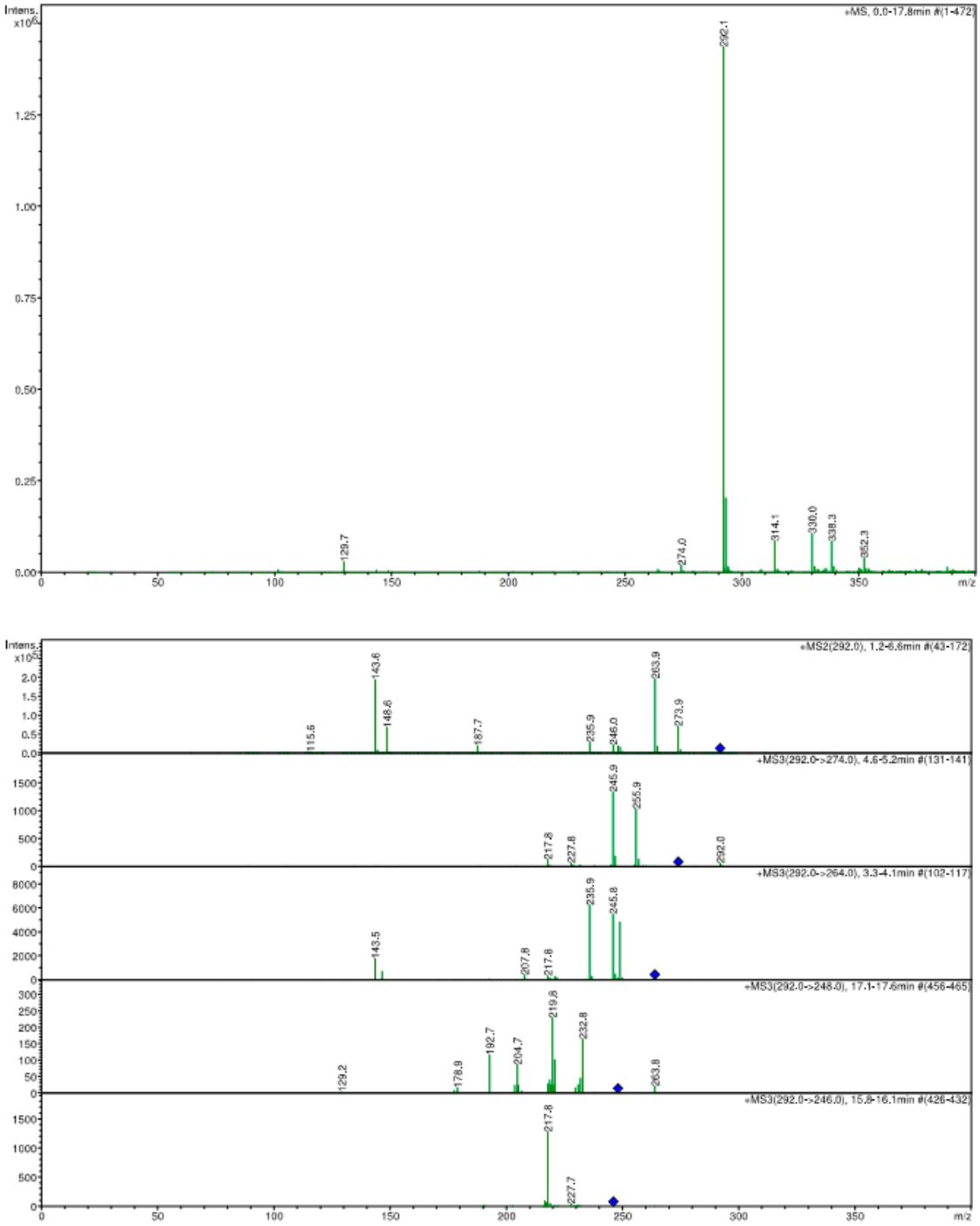
Table S81. Cartesian coordinates for *m*/*z* 263.

C	−3.666835	0.681423	−0.000110
C	−2.879464	1.776946	−0.000052
C	−3.057473	−0.628081	−0.000103
C	−1.671832	−0.732009	−0.000037
C	−0.814478	0.379430	0.000030
C	−1.366917	1.772785	0.000028
C	−0.878474	2.526451	1.277074
C	−0.878334	2.526496	−1.276939
C	−0.883762	−1.993892	−0.000012
C	0.515750	−1.497166	0.000023
C	0.546350	−0.093790	0.000030
N	1.760830	−1.998638	0.000066
C	1.936419	0.290711	0.000013
C	2.670116	−0.939607	0.000058
C	2.658138	1.495381	−0.000024
C	4.065362	−0.992448	0.000076
C	4.046127	1.445813	−0.000007
C	4.742399	0.219388	0.000044
N	−3.845987	−1.683377	−0.000173
N	−1.334152	−3.128525	0.000019
H	−1.232835	2.035191	2.186151
H	−1.261275	3.550245	1.263531
H	0.212301	2.565933	1.306681
H	−1.232594	2.035267	−2.186072
H	0.212445	2.565979	−1.306421
H	−1.261138	3.550288	−1.263404
H	2.002761	−2.981792	0.000088
H	−4.749544	0.742531	−0.000166
H	−3.339345	2.761902	−0.000060
H	5.826990	0.223704	0.000056
H	2.151041	2.453678	−0.000062
H	4.597319	−1.938074	0.000110
H	−3.309382	−2.506147	−0.000186

Table S82. Energies for *m*/*z* 263.

Zero-point correction	0.258601 (Hartree/Particle)
Thermal correction to Energy	0.274543
Thermal correction to Enthalpy	0.275487
Thermal correction to Gibbs Free Energy	0.215710
Sum of electronic and zero-point Energies	−860.276607
Sum of electronic and thermal Energies	−860.260665
Sum of electronic and thermal Enthalpies	−860.259720
Sum of electronic and thermal Free Energies	−860.319498

2. Mass Spectra



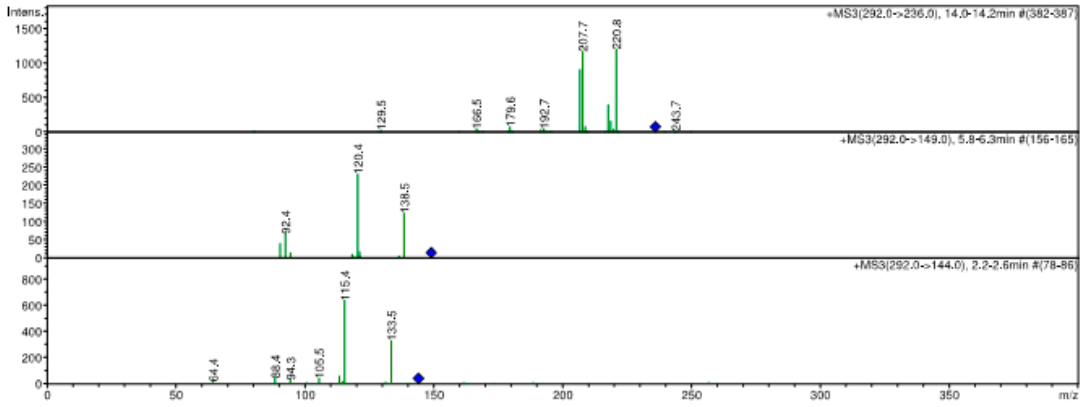
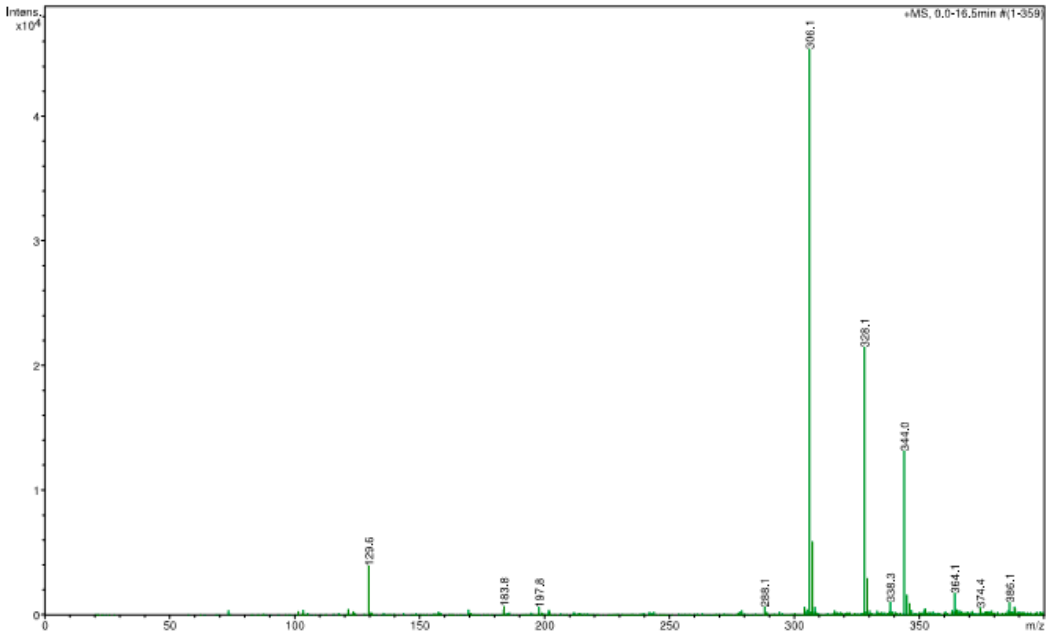
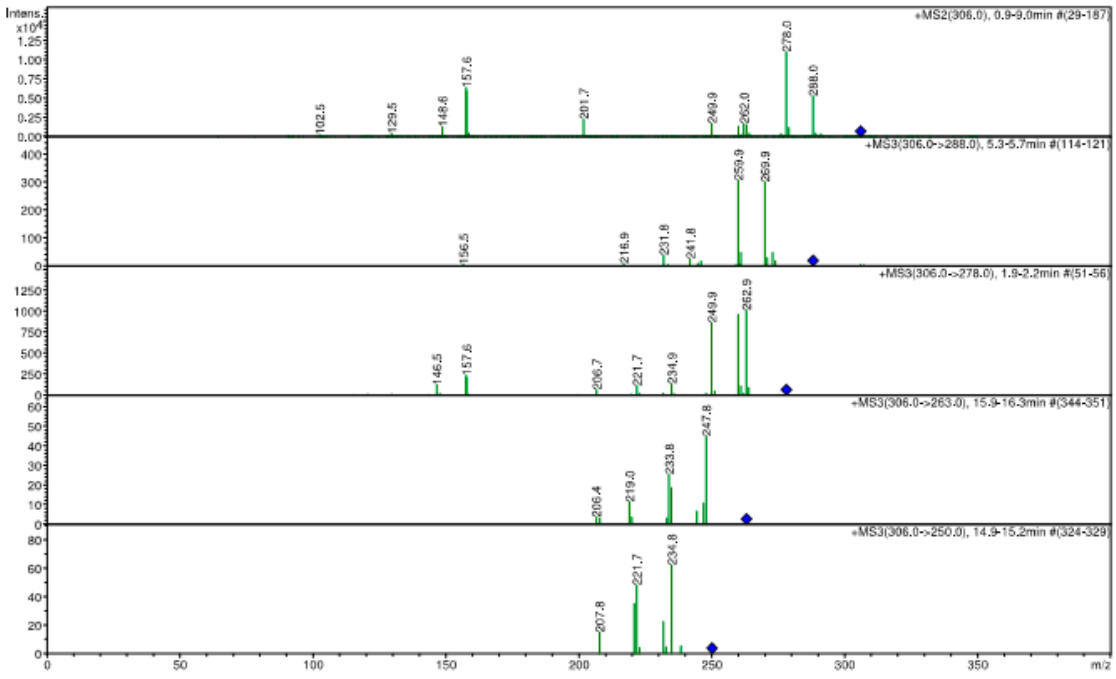


Figure S1. Mass spectrum for **CQ1**.





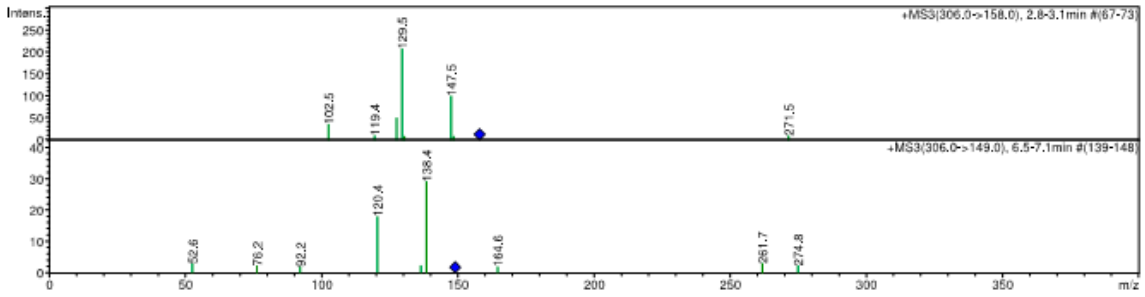
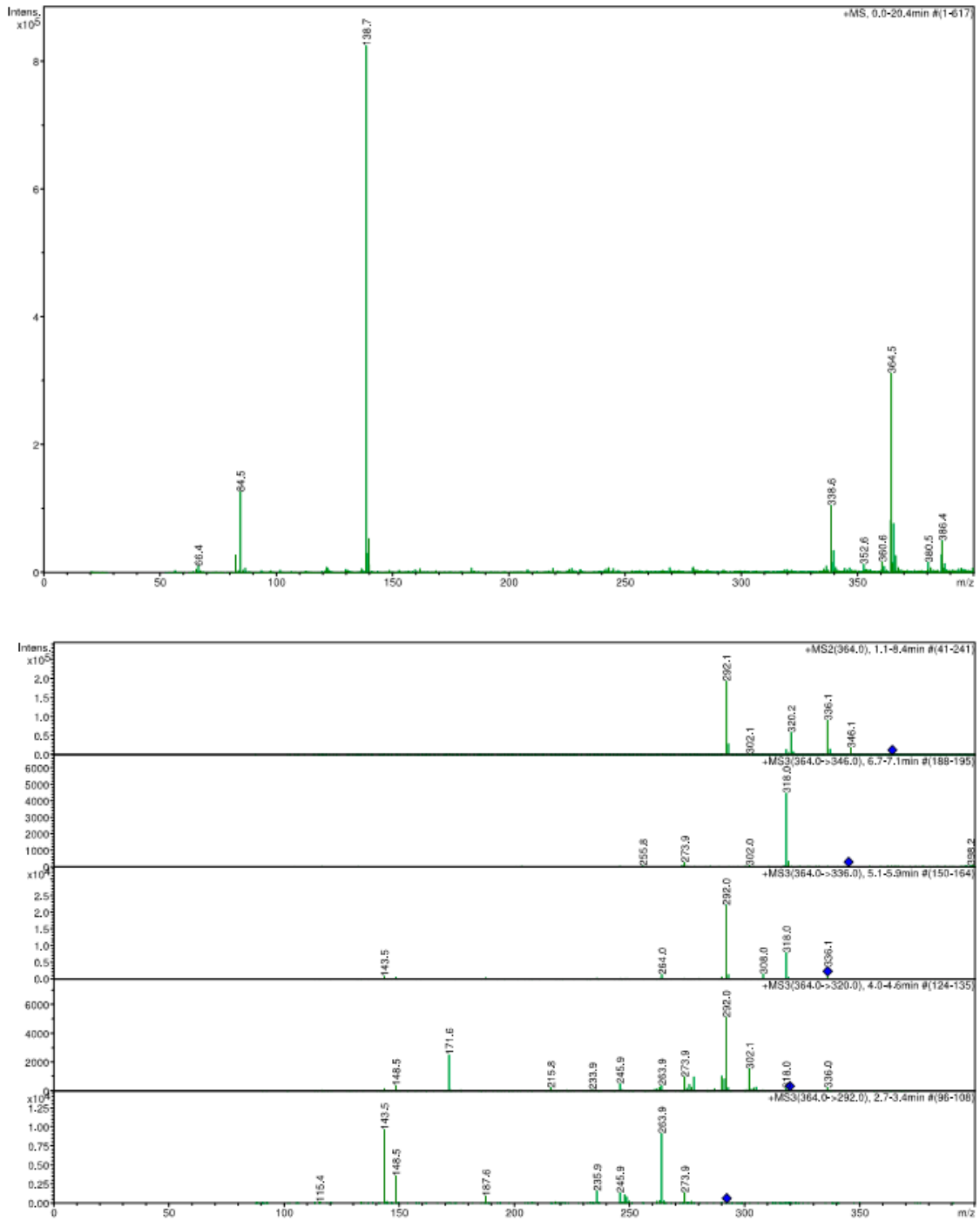


Figure S2. Mass spectrum for **CQ2**.



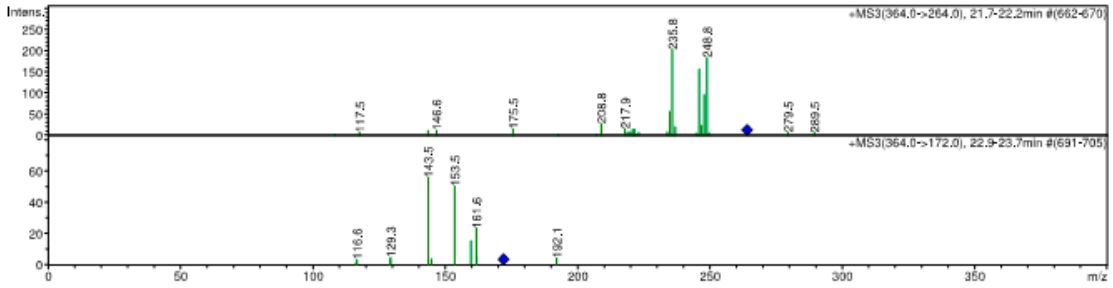
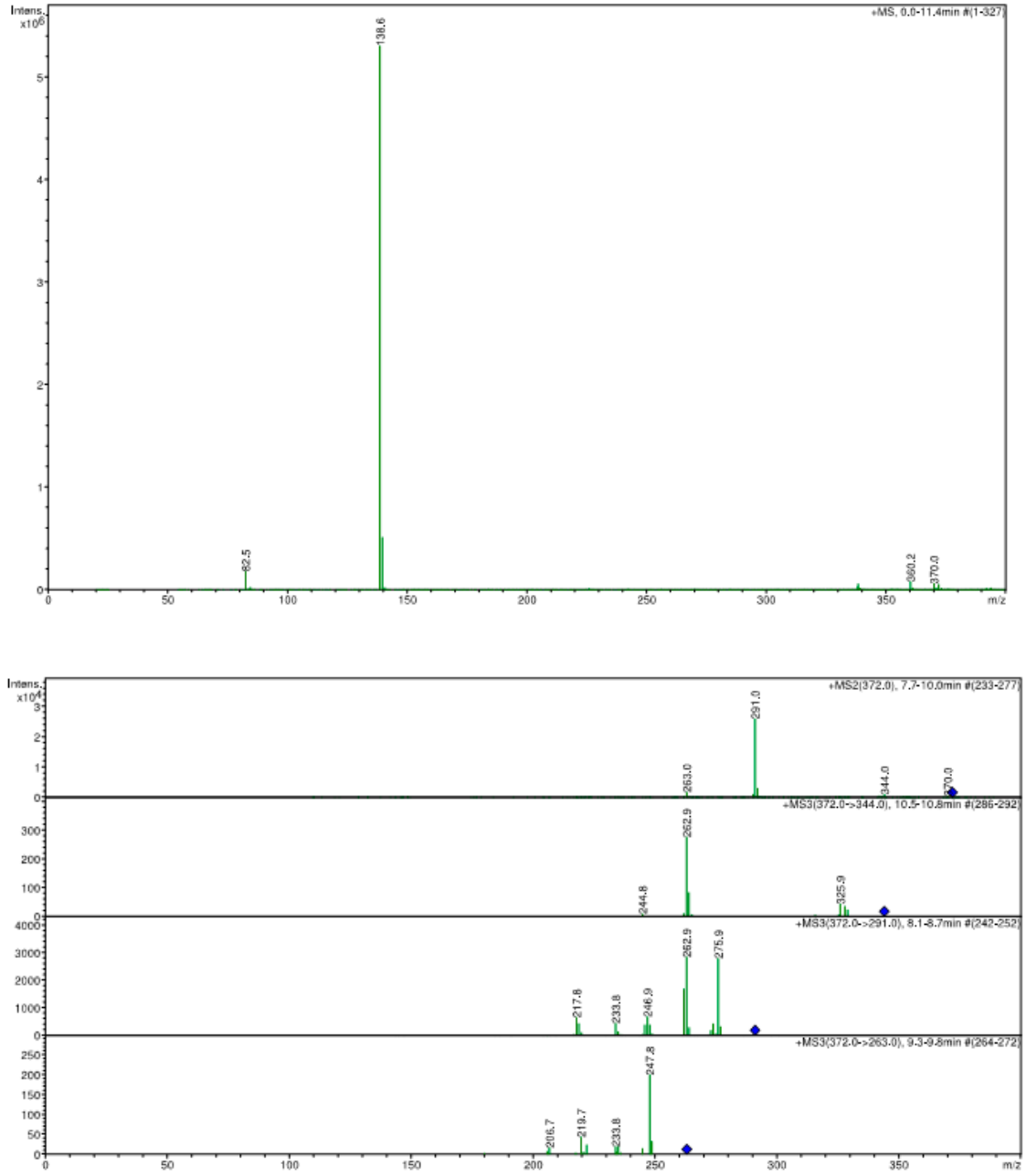


Figure S3. Mass spectrum for **CQ3**.



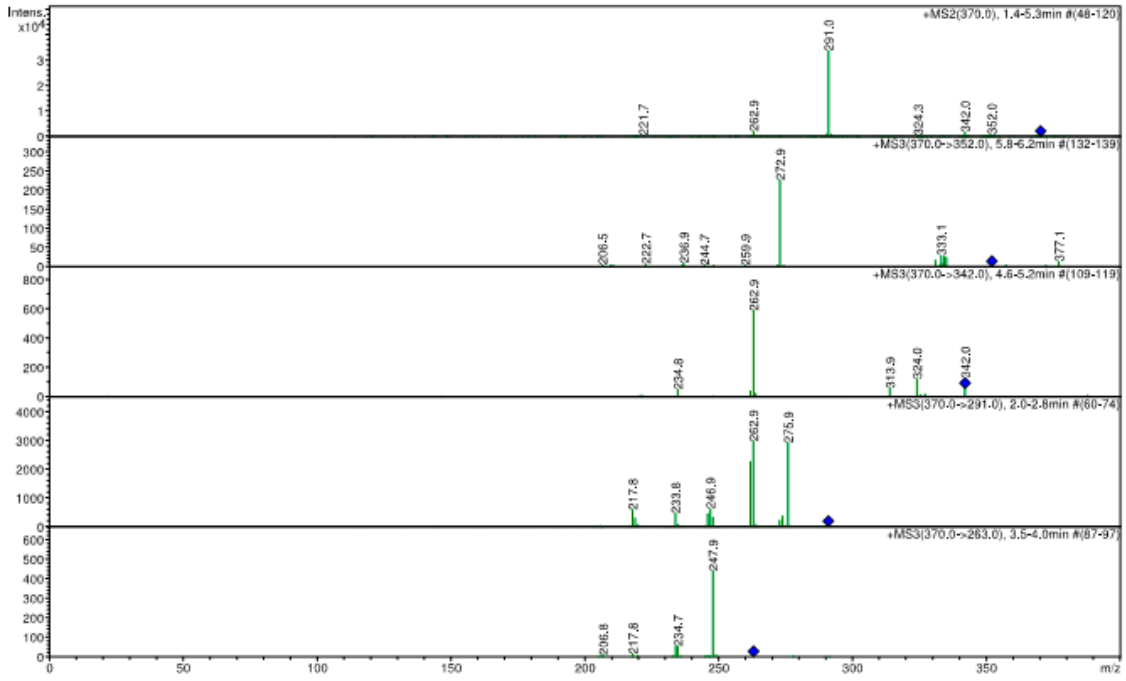


Figure S4. Mass spectra for **CQ4**.

3. Proton Affinity and Gas Phase Basicity of CQ1–CQ4 for all protonation sites studied.

Table S83. Proton Affinity (PA) and Gas Phase Basicity (GB) for O1.

Compound	PA	GB
CQ1	240.0	231.3
CQ2	241.0	232.4
CQ3	238.4	229.9
CQ4	238.1	229.5

Table S84. Proton Affinity (PA) and Gas Phase Basicity (GB) for O2.

Compound	PA	GB
CQ1	240.0	231.2
CQ2	241.0	232.4
CQ3	238.4	229.9
CQ4	238.1	229.5

Table S85. Proton Affinity (PA) and Gas Phase Basicity (GB) for O3.

Compound	PA	GB
CQ1	214.3	207.1
CQ2	215.9	209.0
CQ3	212.8	205.5
CQ4	211.8	204.5

Table S86. Proton Affinity (PA) and Gas Phase Basicity (GB) for N4.

Compound	PA	GB
CQ1	193.7	186.5
CQ2	195.5	188.6
CQ3	191.5	184.4
CQ4	190.3	183.0

Table S87. Proton Affinity (PA) and Gas Phase Basicity (GB) for O5.

Compound	PA	GB
CQ1	/	/
CQ2	/	/
CQ3	212.8	205.2
CQ4	/	/

Table S88. Proton Affinity (PA) and Gas Phase Basicity (GB) for O6.

Compound	PA	GB
CQ1	/	/
CQ2	/	/
CQ3	194.7	188.7
CQ4	/	/