

Supplementary Informations

TO

Chlorophyll and Pheophytin Protonated and Deprotonated ions: Observation and Theory

M. Diop¹, M. el-Hayek², J. Attard^{2,3}, A. Muhieddine¹, V. Veremeienko⁴, S. Soorkia¹, Ph. Carbonnière³, A. de la Lande², B. Soep¹, and N. Shafizadeh¹,

1-Institut des Sciences Moléculaires d'Orsay (ISMO) France

2- Université Paris Saclay, CNRS, Institut de Chimie Physique, UMR 8000, 91405, Orsay, France

3- Institut des sciences analytiques et de physico-chimie pour l'environnement et les matériaux (IPREM) Pau-France

4-Université Paris-Saclay, CEA, CNRS, Institute for Integrative Biology of the Cell (I2BC), 91198 Gif-sur-Yvette, France.

Corresponding author : niloufar.shafizadeh@universite-paris-saclay.fr

Figure 1: Breakdown curves of the fragmentation of deprotonated pheophytin a, in trap versus normalized fragmentation energy.

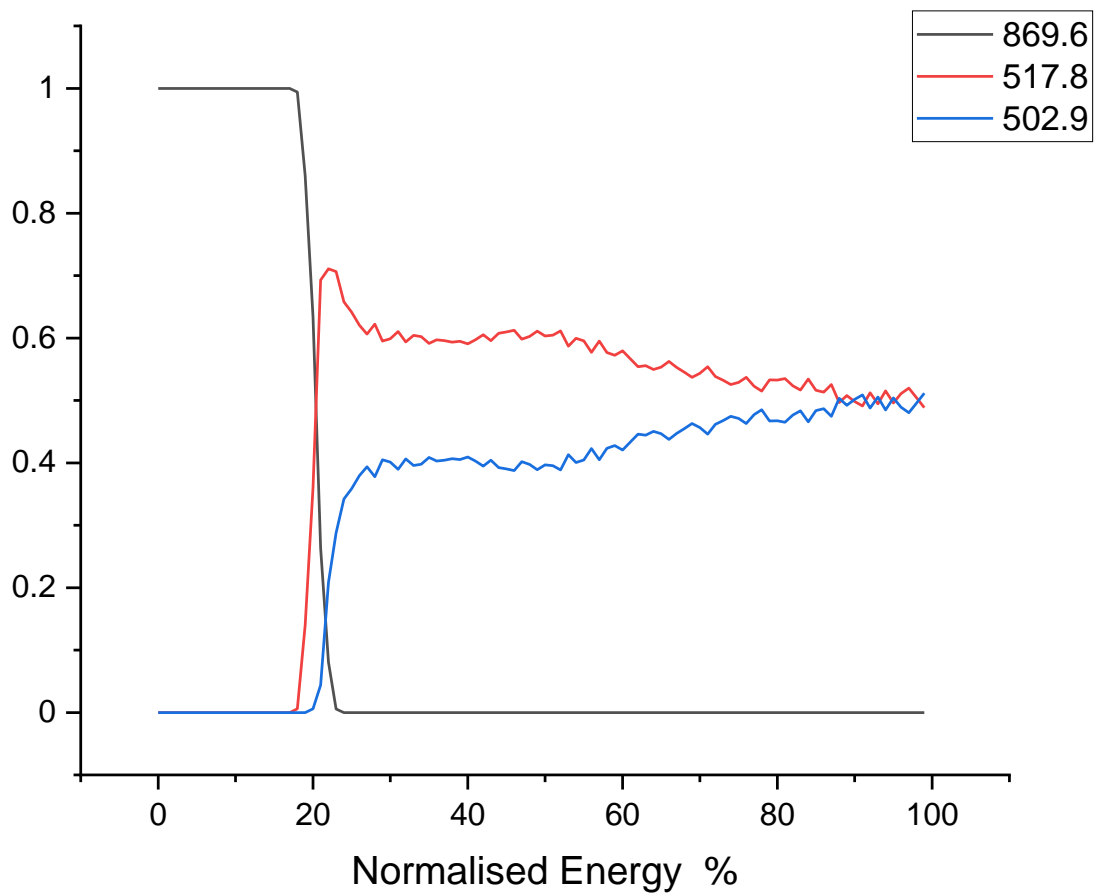
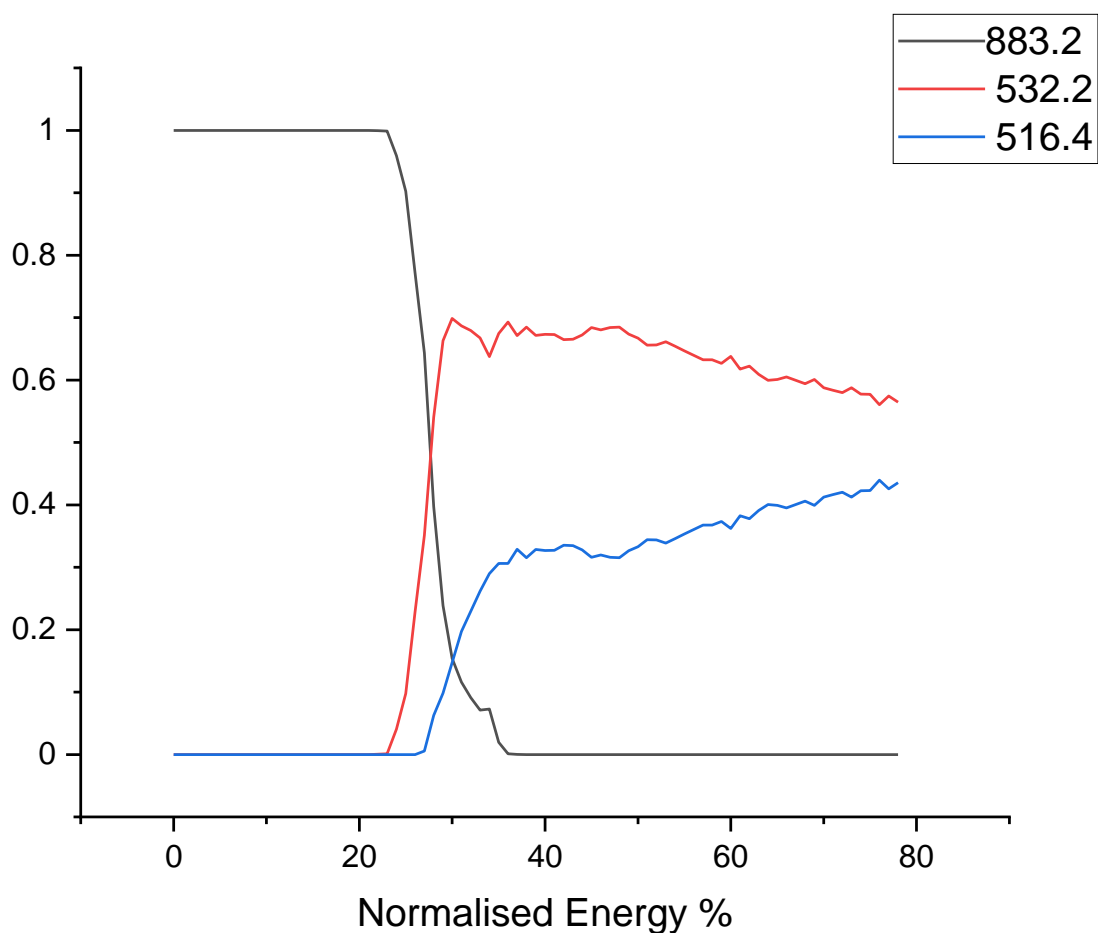


Figure 2: Breakdown curves of the fragmentation of deprotonated pheophytin b, in trap versus normalized fragmentation energy.



Cartesian Coordinates

MD simulation of Chlorophyll a

Dyn 3 Cluster 4

137

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C 5.616255378 -2.376464375 2.046828639
C 4.805626878 -2.135232238 3.300094927
N 3.492032739 -1.963748557 2.947348488
C 3.399124974 -1.970675133 1.527933109
C 4.772020632 -2.261683834 0.988639786
C 5.334279584 -2.059925883 4.571723021
C 4.609822243 -1.834479529 5.755206367
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C 1.645275501 -1.506997348 7.659545055
C 0.522584686 -1.435381747 6.748754282
C -0.746195051 -1.238593975 7.429877870
C -0.512076407 -1.183847011 8.856942188
C 1.044720398 -1.434766795 9.050295987
C -1.717705153 -1.180230014 6.433987826
C -1.018201141 -1.347969730 5.172634940
N 0.374018915 -1.518867568 5.425703274
C -1.524522443 -1.290303549 3.865797847
C -0.790071079 -1.378337242 2.706430745
N 0.623883081 -1.562902919 2.622124119
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C -0.237818065 -1.350884437 0.478046239
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Mg 1.925024126 -1.921488561 4.214693288
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C -0.222891837 -1.276353971 -0.997017717
C 2.286693373 -1.744060242 0.794392782
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C 1.164468283 -4.644837331 3.579586171
C -0.327154062 -4.623101157 3.704146516
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MD simulation of Pheophytin a

Dyn 4 Cluster 1

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C 4.588965104 -2.860759873 4.197748942
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C 5.145704335 -1.092727608 2.523753715
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H	7.134073647	2.670672907	4.615911805
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H	7.789453708	5.092407831	5.108278179
H	9.250881908	2.829913226	6.617808699
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H	7.371582967	2.974206166	8.201279861
H	10.406391793	4.993809232	7.070901691
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H	9.484234594	4.504899037	8.494767838
H	1.606246995	-3.464359873	8.437410437
H	4.256336384	-4.988190286	3.813073394
H	4.608898549	-4.832070661	6.737405343
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H	8.973510839	-0.690926336	1.817442388
H	3.636381521	0.283696418	6.011878427
H	4.395638830	0.052326045	4.187131328

Chlorophyll a

Deprotonated on site ^D1

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MG	-1.484654	1.068242	-0.901424
N	-0.153271	1.365625	0.609780
C	-0.463048	1.413127	1.953674
C	0.731924	1.630401	2.725002
C	1.792353	1.718304	1.817306
C	1.214715	1.542628	0.487713
C	-1.769251	1.269163	2.469782
C	-2.975160	1.040134	1.808326
C	-4.299141	0.969991	2.560675
C	-5.273262	0.443045	1.476341
C	-4.493221	0.642255	0.188576
N	-3.165186	0.915402	0.458460
C	-4.984993	0.546954	-1.131482
C	-4.093740	0.595247	-2.251081
C	-4.761061	0.354444	-3.472119
C	-6.206536	0.138294	-3.179386
C	-6.320176	0.286769	-1.702928
N	-2.766035	0.768981	-2.419374
C	-2.542452	0.654302	-3.792983
C	-3.808259	0.384878	-4.477955
C	-1.271326	0.776431	-4.365429
C	-0.061904	1.013371	-3.679020
C	1.247771	1.137752	-4.284509
C	2.147755	1.358236	-3.252928
C	1.380134	1.366626	-2.025258
N	0.047131	1.158829	-2.303956
C	1.550967	1.010970	-5.747249
C	1.776722	-0.448942	-6.188691
C	1.909680	1.547812	-0.729830
C	3.629802	1.549688	-3.350775
C	-4.009780	0.177452	-5.944269
O	-7.079970	-0.073652	-4.046634
C	-7.575215	0.283343	-1.007044
O	-7.816748	0.706674	0.150118
C	-5.656492	-1.041623	1.681820
C	-6.671238	-1.155499	2.843649
C	-7.010453	-2.595618	3.148301
O	-7.392205	-3.386076	2.299025
C	-4.720654	2.347122	3.103457
C	0.808096	1.705349	4.216868
C	3.205534	1.904701	2.062460
C	3.841109	2.178537	3.225679
O	-6.910279	-3.081535	4.443358
C	-6.378468	-2.262612	5.530992
C	-4.883105	-2.228179	5.500409
C	-4.082346	-1.192801	5.821566
C	-4.581013	0.141757	6.305279
C	-2.581917	-1.329022	5.701737
C	-1.806490	-1.013571	6.998185
C	-0.309548	-1.317509	6.842183
C	0.548233	-1.006487	8.087084
C	0.592516	0.501021	8.378620
C	1.967456	-1.583833	7.909231
C	2.850736	-1.517504	9.163830
C	4.185215	-2.253682	8.976324

C	5.095136	-2.267820	10.221430
C	5.595114	-0.856384	10.563060
C	6.272895	-3.241915	10.011073
C	7.108826	-3.523098	11.268263
C	8.253867	-4.510745	10.998779
C	9.149691	-4.808422	12.214881
C	8.383412	-5.519234	13.338454
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O	-8.605324	-0.251657	-1.762921
C	-9.893795	-0.202799	-1.124511
H	0.083390	-1.531638	8.954654
H	4.488093	-2.654740	11.073519
H	-6.827696	-1.256857	5.526431
H	-6.745884	-2.782583	6.437466
H	2.991614	1.705525	-0.677869
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H	-1.861720	1.367349	3.556118
H	0.890201	-1.061789	-5.955368
H	2.639193	-0.883823	-5.653835
H	1.970270	-0.504595	-7.275830
H	1.600748	1.033963	4.600285
H	-5.082911	0.018770	-6.145515
H	-0.144821	1.414852	4.692296
H	-3.995275	2.722181	3.849779
H	-6.296870	-0.605034	3.724132
H	-4.781941	3.084306	2.282790
H	-6.118561	-1.451661	0.767197
H	-5.719307	2.281459	3.580644
H	-7.605067	-0.662712	2.498955
H	-4.749310	-1.637970	1.907138
H	-3.659842	1.050001	-6.526705
H	-3.446929	-0.702788	-6.308331
H	-10.604904	-0.532775	-1.896369
H	-9.917460	-0.876519	-0.250797
H	-10.118207	0.818901	-0.777529
H	1.059235	2.729984	4.560557
H	3.840346	1.811747	1.173535
H	4.927814	2.285793	3.240935
H	3.316945	2.311022	4.171883
H	2.451008	1.607017	-5.993746
H	0.723959	1.446205	-6.342081
H	3.976000	1.498995	-4.398529
H	3.936209	2.527097	-2.932431
H	4.171679	0.771180	-2.780320
H	-4.421250	-3.162830	5.155051
H	-4.411631	0.249299	7.395148
H	-4.024436	0.962936	5.814359
H	-5.657929	0.299125	6.120337
H	-2.327901	-2.354872	5.363085
H	-2.232019	-0.638173	4.902291
H	-1.955724	0.050744	7.266991
H	-2.219211	-1.623480	7.829446
H	-0.199659	-2.399468	6.604121
H	0.097294	-0.758789	5.972336
H	1.877499	-2.644900	7.591507
H	2.471450	-1.048406	7.074393
H	3.042756	-0.458157	9.424697
H	2.305113	-1.964934	10.021303
H	3.970454	-3.304807	8.684336
H	4.741324	-1.799994	8.126914
H	5.867562	-4.206300	9.633378
H	6.931867	-2.841694	9.209692
H	7.541113	-2.579958	11.660064
H	6.438447	-3.922841	12.056167
H	7.836174	-5.468971	10.619206
H	8.888229	-4.100078	10.182860
H	9.528164	-3.837281	12.608042
H	11.038645	-5.826976	12.652739
H	10.046867	-6.621573	11.392493
H	10.948034	-5.126756	11.005213
H	9.054051	-5.737117	14.191114
H	7.542378	-4.911047	13.714658
H	7.973782	-6.480537	12.973659
H	-4.221106	0.250495	3.403507
H	-6.214720	1.024249	1.429360
H	1.075344	1.035892	7.536987
H	1.164052	0.722989	9.297576
H	-0.420047	0.922343	8.509439
H	6.205692	-0.458876	9.729030
H	6.221344	-0.852557	11.473056
H	4.758500	-0.156365	10.733511

Chlorophyll a

Deprotonated on site ^D1- Mehanol adduct at ²C Position

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MG	1.675939	0.041251	4.355431
C	0.163858	-0.212269	0.287607
C	0.009083	-0.057002	1.719070
N	1.255833	-0.079748	2.325268
C	2.188109	-0.240538	1.324067
C	1.523633	-0.323574	0.040124
C	-1.213520	0.092348	2.406779
C	-1.377949	0.233305	3.789362
C	-2.633385	0.361222	4.534415
C	-2.252784	0.470432	5.862701
C	-0.842398	0.397406	5.904660
N	-0.300299	0.250333	4.677690
C	-2.754806	0.578132	7.262963
C	-1.529477	0.566707	8.108396
C	-0.341387	0.408072	7.245034
C	1.025531	0.173193	7.504405
C	1.663454	-0.188089	8.833885
C	3.171706	0.030304	8.556831
C	3.221186	-0.037071	7.032902
N	1.969639	0.112097	6.493452
C	4.422788	-0.179079	6.338430
C	4.662164	-0.239746	4.947312
C	5.946531	-0.384173	4.313016
C	5.717262	-0.421179	2.933286
C	4.273098	-0.301458	2.749996
N	3.669072	-0.182331	3.990447
C	7.264516	-0.479109	5.014882
C	3.581557	-0.325741	1.530279
C	6.655565	-0.559939	1.840455
C	8.004241	-0.666836	1.878584
C	3.672222	1.394078	9.076451
C	1.335488	-1.672749	9.129471
C	1.886242	-2.111587	10.521328
C	2.567456	-3.445067	10.408689
O	3.932142	-3.262048	10.379022
C	4.756250	-4.423303	10.043330
C	5.707598	-4.032771	8.910966
C	7.010761	-3.327947	9.356155
C	7.887205	-3.056957	8.112212
C	9.158441	-2.241456	8.401932
C	10.192897	-2.295611	7.265544
C	11.522486	-1.589040	7.614722
C	12.560474	-1.779130	6.490667
C	13.973384	-1.296444	6.853457
C	15.013250	-1.614187	5.769926
C	16.449417	-1.163658	6.111184
C	17.454436	-1.759457	5.103601
C	18.930594	-1.574887	5.485014
C	19.882882	-2.219105	4.466488
C	21.379817	-2.030316	4.773133
C	22.236411	-2.549207	3.610121
O	-3.959337	0.673965	7.578074
C	-1.529575	0.861215	9.512109
O	-2.803295	0.909432	10.062258
C	-2.823092	1.292431	11.448119
C	-4.018723	0.339866	3.972910
C	2.208089	-0.508482	-1.279391
C	-0.953824	-0.291181	-0.708029
C	-1.476205	-1.729389	-0.901919
O	-0.540447	1.091181	10.249526
O	2.026915	-4.540324	10.303082
C	6.713977	-2.041820	10.133244
H	11.927998	-2.090161	8.525370
H	16.698968	-1.577475	7.116651
C	21.793109	-2.713987	6.083273
H	5.321324	-4.698039	10.952127
H	4.184922	-0.443445	0.624616
H	-2.121950	0.107422	1.792607
H	5.308332	-0.242617	6.979709
H	-1.827865	-2.140087	0.059242
H	-0.668233	-2.383327	-1.274840
H	-2.312557	-1.751646	-1.625079
H	7.788720	-1.419362	4.752418
H	-4.746530	0.485324	4.789172
H	7.157302	-0.440124	6.112827
H	4.733730	1.553454	8.812791
H	3.074142	2.214598	8.642186
H	0.243053	-1.824276	9.099400
H	3.568232	1.448523	10.178084
H	1.776720	-2.304218	8.332760
H	-4.163220	1.133388	3.216997

H	-4.235071	-0.625024	3.476083
H	-3.889613	1.337112	11.713797
H	-2.290239	0.553072	12.070444
H	-2.330411	2.268838	11.591709
H	7.931954	0.353180	4.711725
H	6.199715	-0.578658	0.843732
H	8.569856	-0.766156	0.949511
H	8.576278	-0.655383	2.805619
H	-0.613284	0.105531	-1.684328
H	-1.791219	0.358848	-0.387515
H	1.480222	-0.568228	-2.108323
H	2.903711	0.325907	-1.490842
H	2.807346	-1.438971	-1.288795
H	7.654408	-1.579045	10.474699
H	6.145411	-1.330182	9.504989
H	6.099773	-2.268090	11.019541
H	8.153868	-4.024981	7.638864
H	7.259876	-2.526971	7.365471
H	8.865163	-1.187576	8.575589
H	9.623015	-2.605386	9.344368
H	10.413018	-3.358539	7.019502
H	9.770981	-1.839773	6.342517
C	11.298906	-0.100373	7.919218
H	12.604647	-2.857675	6.226161
H	12.210706	-1.245305	5.579415
H	13.951932	-0.204201	7.033750
H	14.287053	-1.768632	7.807936
H	15.021198	-2.711780	5.592635
H	14.705524	-1.142609	4.811043
C	16.557501	0.368101	6.161312
H	17.247941	-2.847386	5.003612
H	17.270044	-1.310516	4.103130
H	19.173811	-0.495482	5.562552
H	19.092995	-2.016224	6.489585
H	19.667908	-3.307829	4.394268
H	19.669672	-1.789599	3.463098
H	21.575458	-0.938096	4.870457
H	23.311861	-2.382560	3.804560
H	22.077968	-3.634619	3.467420
H	21.972096	-2.040837	2.664247
H	22.876253	-2.582812	6.267244
H	21.249167	-2.305483	6.952796
H	21.586602	-3.799964	6.029679
H	3.779767	-0.779849	9.012274
H	1.263215	0.434742	9.655583
H	10.865388	0.406731	7.034426
H	12.243102	0.411510	8.176992
H	10.605094	0.045365	8.764989
H	16.320287	0.796989	5.167983
H	17.575027	0.697648	6.438544
H	15.857384	0.805812	6.894797
O	7.721849	-4.149212	10.346120
C	8.340095	-5.341886	9.848678
H	8.617817	-5.933903	10.735865
H	9.252837	-5.114767	9.265403
H	7.653604	-5.942474	9.222792
H	5.164891	-3.360573	8.213239
H	1.059970	-2.177438	11.250134
H	4.085360	-5.249247	9.755381
H	5.958197	-4.940995	8.327635
H	2.611141	-1.357148	10.876099

Pheophytin a

Deprotonated on site ^{D1}

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N	-0.122902	1.404543	0.549478
C	-0.480268	1.430967	1.884452
C	0.723388	1.630491	2.631805
C	1.789744	1.726403	1.721819
C	1.236732	1.576418	0.391861
C	-1.775319	1.278912	2.408508
C	-2.993537	1.044984	1.769708
C	-4.292168	0.949945	2.566577
C	-5.293198	0.448181	1.495265
C	-4.516979	0.652863	0.205142
N	-3.201210	0.931124	0.430987
C	-5.003940	0.565945	-1.121636
C	-4.100351	0.635192	-2.227909
C	-4.755726	0.429745	-3.452899
C	-6.204444	0.206648	-3.179751
C	-6.329289	0.317863	-1.703479
N	-2.776339	0.807075	-2.467320
C	-2.546890	0.726967	-3.838407

C	-3.816790	0.477868	-4.479903
C	-1.282600	0.868517	-4.425229
C	-0.082936	1.101197	-3.737702
C	1.223932	1.242767	-4.367807
C	2.121890	1.447711	-3.343339
C	1.345090	1.428028	-2.109510
N	0.015972	1.220196	-2.364289
C	1.511249	1.134590	-5.833951
C	1.682063	-0.323828	-6.306843
C	1.909794	1.600342	-0.830432
C	3.602436	1.647249	-3.436883
C	-4.052672	0.303725	-5.944935
O	-7.065357	0.017048	-4.063411
C	-7.587717	0.288303	-1.011768
O	-7.835374	0.668565	0.156963
C	-5.690410	-1.033986	1.692687
C	-6.673237	-1.152705	2.880552
C	-7.011988	-2.593252	3.184768
O	-7.416317	-3.377557	2.340327
C	-4.705996	2.306077	3.165503
C	0.815373	1.668377	4.124417
C	3.205724	1.884226	1.971647
C	3.827839	2.234760	3.119930
O	-6.882293	-3.087225	4.474184
C	-6.337057	-2.272111	5.558305
C	-4.841721	-2.244197	5.516478
C	-4.035372	-1.211768	5.833001
C	-4.525465	0.125342	6.318473
C	-2.536083	-1.353531	5.708452
C	-1.756844	-1.041760	7.003618
C	-0.261157	-1.350735	6.846655
C	0.601473	-1.014340	8.081697
C	0.660611	0.500266	8.330663
C	2.015082	-1.610197	7.921055
C	2.898129	-1.514268	9.174044
C	4.221752	-2.276435	9.014995
C	5.126780	-2.264164	10.263776
C	5.650579	-0.851116	10.559911
C	6.287401	-3.266048	10.092882
C	7.114059	-3.516172	11.362755
C	8.230541	-4.546995	11.138814
C	9.113354	-4.820716	12.370054
C	8.322891	-5.462224	13.518323
C	10.307593	-5.706230	11.988300
O	-8.610474	-0.223248	-1.792885
C	-9.900418	-0.214221	-1.154418
H	0.132351	-1.510336	8.964001
H	4.509524	-2.611094	11.125673
H	-6.781600	-1.264455	5.559037
H	-6.699008	-2.791319	6.467391
H	2.989718	1.766511	-0.791619
H	-1.239306	0.794961	-5.517166
H	-1.836804	1.365795	3.497128
H	0.784207	-0.915663	-6.062050
H	2.543041	-0.792159	-5.798729
H	1.848870	-0.365903	-7.398984
H	1.682596	1.072948	4.466444
H	-5.131524	0.157355	-6.121141
H	-0.093496	1.261787	4.600652
H	-3.961287	2.664829	3.901064
H	-6.271883	-0.610508	3.753905
H	-4.797203	3.066999	2.369285
H	-6.182954	-1.428658	0.787527
H	-5.688648	2.219101	3.671524
H	-7.614119	-0.652776	2.566448
H	-4.783146	-1.641510	1.883659
H	-3.710387	1.185796	-6.517449
H	-3.506825	-0.573515	-6.340995
H	-10.603617	-0.544665	-1.933043
H	-9.910263	-0.903165	-0.292706
H	-10.146785	0.796224	-0.789341
H	0.958643	2.702844	4.500369
H	3.843144	1.692768	1.099928
H	4.917011	2.301616	3.153852
H	3.288425	2.477087	4.035407
H	2.431106	1.702061	-6.073569
H	0.697215	1.611067	-6.416332
H	3.945054	1.625197	-4.486828
H	3.906590	2.614605	-2.993191
H	4.148262	0.855021	-2.888725
H	-4.386179	-3.180816	5.168267
H	-4.345982	0.233835	7.406460
H	-3.971064	0.943550	5.820003

H	-5.603446	0.286197	6.143507
H	-2.286464	-2.379049	5.366346
H	-2.185103	-0.661412	4.910365
H	-1.902258	0.023242	7.272146
H	-2.171075	-1.649548	7.835385
H	-0.153113	-2.437172	6.629237
H	0.142346	-0.809407	5.964051
H	1.915026	-2.679616	7.636210
H	2.524175	-1.105285	7.070418
H	3.105560	-0.449577	9.399075
H	2.344691	-1.923854	10.045335
H	3.991601	-3.333051	8.756519
H	4.787727	-1.859355	8.153469
H	5.865620	-4.236039	9.749143
H	6.955923	-2.907196	9.279876
H	7.572606	-2.569505	11.714241
H	6.431976	-3.862026	12.165978
H	7.785883	-5.507437	10.797319
H	8.879383	-4.189350	10.309402
H	9.519175	-3.845915	12.725022
H	10.969165	-5.876810	12.857481
H	9.958683	-6.691342	11.625117
H	10.905834	-5.240851	11.182869
H	8.984380	-5.664909	14.381816
H	7.499195	-4.814664	13.866093
H	7.885958	-6.425035	13.191058
H	-4.182122	0.205006	3.384805
H	-6.225964	1.045861	1.466586
H	1.148904	1.006810	7.474724
H	1.233817	0.742231	9.243491
H	-0.347595	0.935718	8.448369
H	6.273275	-0.493448	9.716865
H	6.271225	-0.827439	11.473439
H	4.826012	-0.130502	10.700722
H	-2.025125	0.978108	-1.795875
H	-0.765422	1.276614	-0.233970

Pheophytin a

Deprotonated on ^{D1} site and Methanol adduct at ²C position

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C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.225719
O	1.151182	0.000000	-0.760486
C	2.411066	-0.177759	-0.039907
C	-1.197473	-0.061451	-0.901138
C	2.944804	-1.588456	-0.301214
C	3.829619	-1.741702	-1.559885
O	5.004210	-0.863841	-1.466458
C	5.989049	-1.237426	-0.495311
C	3.114199	-1.232513	-2.813242
C	4.233660	-3.225520	-1.701767
C	5.137805	-3.552115	-2.902901
C	5.758040	-4.952721	-2.774321
C	6.814608	-5.289800	-3.846999
C	6.228397	-5.233103	-5.265203
C	7.442812	-6.666575	-3.553737
C	8.670159	-7.010072	-4.411024
C	9.360890	-8.301506	-3.949669
C	10.620832	-8.681436	-4.753841
C	10.266884	-9.063146	-6.198576
C	11.383056	-9.820476	-4.045774
C	12.773702	-10.122801	-4.623063
C	13.493142	-11.240904	-3.854009
C	14.881952	-11.613653	-4.403800
C	15.882655	-10.456666	-4.282497
C	15.424059	-12.861050	-3.692284
H	2.856362	-0.166386	-2.699197
H	6.703469	-0.399647	-0.453758
H	3.769551	-1.340796	-3.693099
H	-1.924474	0.725251	-0.629249
H	5.807993	-4.238064	-5.494781
H	15.555333	-9.565799	-4.846392
H	9.733952	-8.247642	-6.718351
C	-1.899165	-1.446646	-0.794306
C	-2.442870	-1.874742	-2.178071
C	-3.240452	-3.164890	-2.051190
N	-2.524670	-4.245143	-2.483137
C	-1.353492	-3.813294	-3.025546
C	-0.304901	-4.601623	-3.501048
C	-0.168817	-5.998114	-3.573416
N	-1.114357	-6.940833	-3.216725

C	-0.645923	-8.221490	-3.423551
C	-1.367208	-9.390403	-3.176169
C	-2.669920	-9.477470	-2.647035
N	-3.447937	-8.409231	-2.288385
C	-4.629433	-8.952699	-1.822274
C	-5.705820	-8.198707	-1.334416
C	-5.752814	-6.801724	-1.236743
N	-4.714348	-5.958408	-1.623899
C	-5.075267	-4.671017	-1.389061
C	-6.367607	-4.662497	-0.840416
C	-6.821021	-5.973823	-0.729302
C	-4.543750	-3.349208	-1.526303
C	0.981657	-6.716498	-4.028520
C	0.698611	-8.090299	-3.945149
C	1.542043	-9.227320	-4.241173
C	2.712985	-9.257581	-4.916627
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C	-3.363831	-10.738076	-2.411018
C	-5.590950	-2.446067	-1.017551
C	-5.555153	-1.012002	-0.968196
O	-4.648467	-0.245714	-1.369100
O	-6.696330	-0.465990	-0.398178
C	-6.697904	0.971816	-0.360980
C	-6.757059	-3.251265	-0.569444
O	-7.852274	-2.909526	-0.077048
C	-5.683963	-11.337279	-1.445916
C	-8.134113	-6.445991	-0.194500
C	2.274063	-6.091482	-4.451455
C	-2.809027	-12.101223	-2.684001
C	-1.297171	-2.293727	-3.129516
C	-5.640997	-11.626300	0.068782
C	-1.530176	-1.825017	-4.579833
H	-2.047913	-6.741495	-2.853836
H	-3.838575	-6.308558	-2.015441
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H	3.245216	-10.201719	-5.048966
H	-0.871858	-10.334653	-3.417537
H	0.550585	-4.038352	-3.885716
H	-6.596135	-8.740069	-0.996598
H	1.162425	-10.183173	-3.860128
H	-7.669424	1.242187	0.078948
H	-2.724304	-1.375479	-0.068357
H	-6.586215	1.390613	-1.374969
H	2.355445	-5.047842	-4.101491
H	-8.732273	-5.570925	0.110031
H	-5.702579	-10.686161	0.642117
H	-5.863812	1.349315	0.254514
H	-4.691812	-12.122464	0.336584
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H	-3.536942	-12.890389	-2.424056
H	6.993241	-5.455515	-6.031321
H	-2.491341	-2.218282	-4.956822
H	2.219928	-0.011552	1.033333
H	-3.065943	-1.051961	-2.578452
H	-0.721471	-2.174198	-5.247070
H	2.171129	-1.787925	-2.968893
H	-6.480213	-12.281003	0.367757
H	16.404099	-13.160212	-4.107280
H	-8.697510	-7.019432	-0.954072
H	14.727300	-13.713383	-3.798710
H	-7.999239	-7.108274	0.681197
H	15.555554	-12.663692	-2.611577
H	5.552517	-1.385031	0.510759
H	16.875459	-10.757427	-4.667345
H	-5.604890	-12.293597	-1.998096
H	6.526555	-2.159375	-0.789088
H	16.003193	-10.164447	-3.221737
H	-2.536229	-12.218095	-3.750236
H	-1.188598	-2.217556	-0.433593
H	3.124275	-6.663355	-4.036612
H	8.364585	-7.108897	-5.471199
H	-1.890026	-12.284140	-2.094176
H	9.610372	-9.955028	-6.204737
H	-1.573395	-0.719222	-4.625934
H	4.541712	-3.496150	-3.835239
H	5.413463	-5.976687	-5.370379
H	3.503060	-1.938006	0.589747
H	2.391249	-6.082904	-5.555928
H	-6.675599	-10.915205	-1.705884
H	12.689752	-10.422997	-5.687413
H	13.377219	-9.192683	-4.596354
H	2.075471	-2.270648	-0.405648

H	-0.872519	0.111518	-1.943344
H	9.396594	-6.171692	-4.365136
H	4.733370	-3.554894	-0.766141
H	-0.318412	-1.899885	-2.777857
H	3.298937	-3.822604	-1.763235
H	5.940120	-2.787248	-2.990975
H	7.736609	-6.698285	-2.482297
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H	10.761419	-10.742145	-4.075868
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H	11.496711	-9.552369	-2.972425
H	8.636930	-9.144645	-3.990887
H	6.666603	-7.452142	-3.689691
H	4.956581	-5.723018	-2.794756
H	6.244344	-5.038909	-1.776342
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