Supporting Information

Flavin Adenine Dinucleotide structural motifs: from solution to gas-phase

Juan Camilo Molano-Arevalo[1]; Diana R. Hernandez[1]; Walter G. Gonzalez[1]; Jaroslava Miksovska[1]; Mark E. Ridgeway[2], Melvin A. Park[2], and Francisco Fernandez-Lima[1,3*].

[1] *Department of Chemistry and Biochemistry, Florida International University, Miami, USA*

[2] *Bruker Daltonics Inc., Billerica, Massachusetts, USA*

[3] *Biomolecular Sciences Institute, Florida International University, Miami, FL 33199*

Abstract:

This file contains the FAD total MS spectrum (Figure S1), the open FAD conformation (Figure S2), and all the geometry files (FAD MOBCAL input files) of the FAD structures proposed.

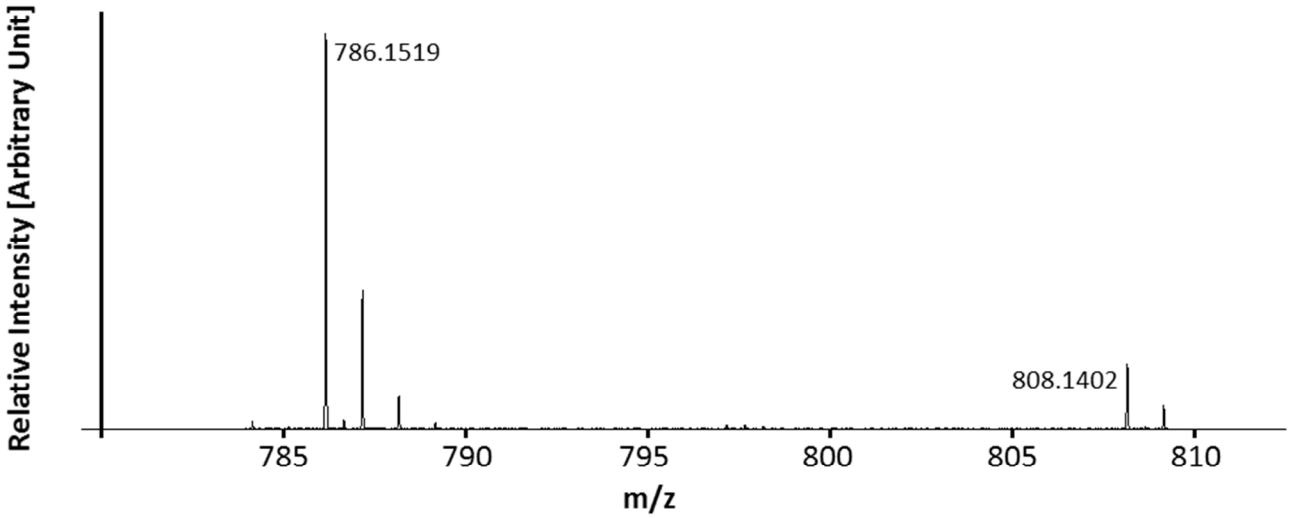


Figure S1. FAD total MS spectrum.

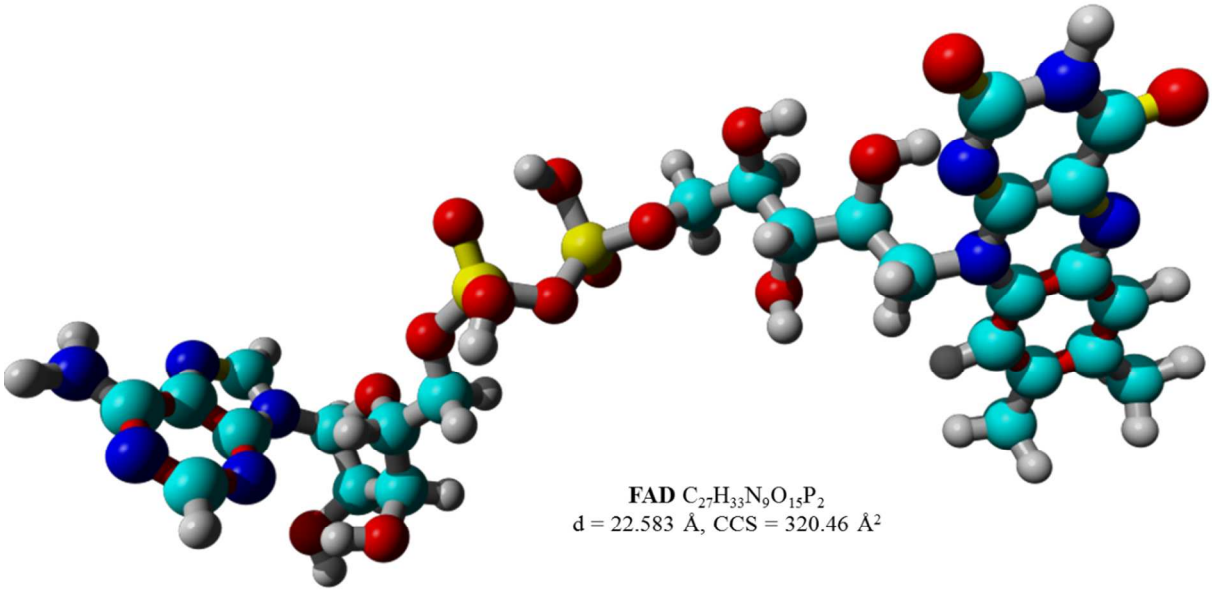
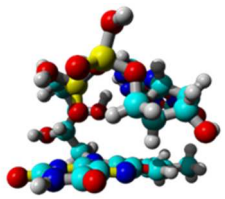


Figure S2. FAD "open" conformation theoretical structure. Optimization of the structure was done at level B3LYP/6-31G(d,P) and CCS was calculate dusing mobcal.

FAD MOBCAL INPUT FILES



$[M+H]^+$ $C_{27}H_{31}N_9O_{15}P_2$
d = 4.318 Å
CCS = 138.31 Å²
ΔE = 27.23 kcal/mol

Structure A

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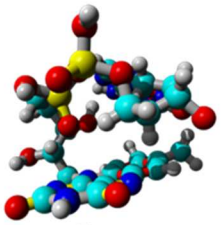
Structure B



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ang
calc
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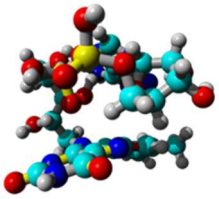
Structure C



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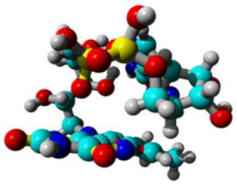
-4.703626	1.439399	-2.778669	1	0.371866

Structure D



$[M+H]^+$ $C_{27}H_{31}N_9O_{15}P_2$
d = 5.244 Å
CCS = 247.92 Å²
ΔE = 20.92 kcal/mol

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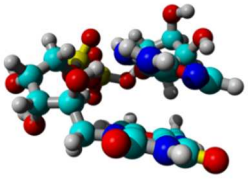
1.0000

0.892166	2.762332	-1.626065	12	0.112589
0.697704	4.245248	-1.340611	12	0.108396
-0.157580	4.296287	-0.016583	12	0.076688
0.178177	2.927119	0.652865	12	0.221920
0.299888	2.059541	-0.486444	16	-0.506330
-0.050032	4.783798	-2.386715	16	-0.622061
-1.626729	4.386353	-0.238099	16	-0.705799
2.401948	2.333832	-1.602389	12	-0.104770
3.055981	2.774062	-0.307172	16	-0.532335
3.844954	1.626847	0.537680	31	1.139617
4.705341	0.725618	-0.189362	16	-0.536625
4.593634	2.502067	1.598637	16	-0.425128
2.793226	1.033496	1.402132	16	-0.401414
-0.630465	2.425224	1.721725	14	-0.517820
-1.909959	1.889771	1.561975	12	0.666372
-2.040073	0.942364	2.570167	12	0.084452
-0.895832	0.758267	3.238398	14	-0.536735
-0.117538	1.737719	2.810983	12	0.264683
-2.975593	2.194389	0.859442	14	-0.592297
-3.272959	0.246577	2.656754	12	0.540492
-4.334793	0.579742	1.973000	14	-0.482298
-4.181687	1.555134	1.085940	12	0.196204
-3.466325	-0.757659	3.501338	14	-0.757417

2.505147	-0.393948	1.241443	31	1.129628
1.602772	-0.735563	2.567223	16	-0.579441
3.865642	-1.093416	1.586250	16	-0.641405
1.904937	-0.799535	0.008612	16	-0.550655
1.512387	-2.146615	2.978022	12	-0.081245
-0.021001	-2.525438	3.204527	12	0.068048
-0.861754	-2.482504	1.919253	12	0.114535
-0.453850	-3.530775	0.862099	12	0.066985
-1.407183	-3.494029	-0.283423	12	-0.161019
-1.028932	-2.522271	-1.299867	14	-0.526978
-0.855591	-1.181223	1.325783	16	-0.677457
-0.577586	-4.865608	1.340309	16	-0.616742
-0.700154	-1.854706	4.326124	16	-0.643692
-1.932096	-1.607948	-1.758639	12	0.405482
-1.436948	-0.410711	-2.349492	12	0.305450
-0.159416	-0.173576	-2.585161	14	-0.508159
0.654549	-1.229061	-2.518766	12	0.266876
0.197966	-2.472897	-1.897414	12	0.552486
-2.313182	0.622665	-2.677364	12	-0.192962
-3.347019	-1.726742	-1.684543	12	-0.253273
-3.707600	0.450953	-2.565158	12	0.064896
-4.229489	-0.770319	-2.140994	12	0.170387
-4.576146	1.661366	-2.969874	12	-0.508167
-5.710879	-1.106039	-2.048844	12	-0.545120
1.967440	-1.228646	-3.137620	12	0.648295
2.718430	-2.426078	-3.116412	14	-0.654340
2.312626	-3.561372	-2.550413	12	0.711592
1.060758	-3.524254	-2.006555	14	-0.545207
2.981035	-4.547955	-2.535983	16	-0.410590
2.516592	-0.297029	-3.722490	16	-0.451382
0.434742	2.533226	-2.602251	1	0.204015
1.663541	4.770616	-1.243182	1	0.189497

0.213177	5.086335	0.645860	1	0.178617
1.100093	3.026457	1.161746	1	0.188499
-0.907385	5.011306	-1.874969	1	0.432332
-2.132414	3.630037	0.147375	1	0.462241
2.496997	1.244034	-1.692916	1	0.208085
2.988308	2.849932	-2.366541	1	0.205532
0.878924	1.749707	3.176209	1	0.240724
-5.006192	1.665864	0.422051	1	0.190887
-4.419877	-1.037942	3.579689	1	0.375319
-2.704255	-1.147065	4.064878	1	0.399037
4.452830	-0.920851	0.865851	1	0.471565
2.055993	-2.220400	3.854260	1	0.214143
1.999500	-2.822664	2.227985	1	0.182719
-0.121623	-3.607287	3.435402	1	0.185420
-1.850890	-2.721245	2.209880	1	0.144864
0.558834	-3.250890	0.543248	1	0.191954
-1.568276	-4.433701	-0.737568	1	0.227204
-2.323440	-3.116721	0.129838	1	0.193354
-0.989210	-0.415809	2.046732	1	0.468242
0.123879	-5.355364	0.948144	1	0.431512
-0.386923	-0.884682	4.227600	1	0.436180
-1.958531	1.479009	-3.207075	1	0.196964
-3.790703	-2.635992	-1.238140	1	0.177404
-5.496970	1.495927	-2.423487	1	0.174476
-4.096240	2.645164	-2.702483	1	0.200789
-4.747633	1.507235	-4.038599	1	0.209053
-5.928603	-2.081539	-1.789478	1	0.202854
-6.072303	-0.520805	-1.195238	1	0.189750
-6.299830	-0.838329	-2.950836	1	0.200712
3.668372	-2.442378	-3.428952	1	0.378848

Structure E



$[M+H]^+$ $C_{27}H_{31}N_9O_{15}P_2$
d = 5.915 Å
CCS = 252.79 Å²
ΔE = 41.61 kcal/mol

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0.586021	2.823581	-1.583458	12	0.095727
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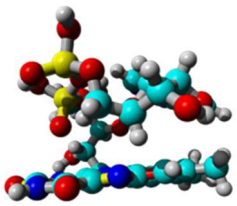
-0.703756	4.261988	-0.040943	12	0.050728
-0.253387	2.932372	0.621205	12	0.193153
-0.086233	2.066497	-0.568089	16	-0.515920
-0.768122	4.766975	-2.338181	16	-0.623881
-2.167713	4.365588	-0.165629	16	-0.650738
2.128589	2.757583	-1.498816	12	-0.109998
2.601123	3.186163	-0.210725	16	-0.472701
3.425966	2.232125	0.689214	31	1.146866
4.564678	1.523860	0.030347	16	-0.524841
3.806608	3.318116	1.681231	16	-0.426762
2.423175	1.335102	1.445874	16	-0.492534
-1.106646	2.165539	1.542490	14	-0.516529
-2.253072	1.547447	1.322339	12	0.689895
-2.503046	0.756976	2.409437	12	0.164589
-1.543821	0.776194	3.346190	14	-0.549434
-0.670477	1.691421	2.817623	12	0.229101
-3.104613	1.723149	0.351661	14	-0.540632
-3.730907	0.070563	2.431132	12	0.530055
-4.579757	0.161368	1.439809	14	-0.493804
-4.258304	1.075347	0.487991	12	0.160294
-4.078319	-0.789561	3.410804	14	-0.729389

2.506165	-0.183401	1.423730	31	1.158766
1.501215	-0.621326	2.582758	16	-0.539918
3.864428	-0.488550	2.183245	16	-0.641614
2.359959	-0.932236	0.162179	16	-0.572349
1.522999	-1.948238	3.100323	12	-0.085481
0.117644	-2.563102	3.159365	12	0.063871
-0.629878	-2.721101	1.819568	12	0.131515
0.201619	-3.627956	0.795580	12	0.097014
-0.605511	-3.877137	-0.499477	12	-0.197801
-0.491793	-2.736713	-1.480147	14	-0.552248
-0.881864	-1.369973	1.241725	16	-0.689164
0.446611	-4.927891	1.350176	16	-0.626996
-0.729577	-1.950507	4.107814	16	-0.641376
-1.473786	-1.891770	-1.857801	12	0.456611
-1.275817	-0.671862	-2.509310	12	0.352342
-0.064766	-0.353075	-2.873006	14	-0.540662
1.021005	-1.134473	-2.595058	12	0.265427
0.743275	-2.465283	-2.045867	12	0.486019
-2.255414	0.185907	-2.930675	12	-0.187643
-2.801022	-2.256626	-1.622633	12	-0.257488
-3.577754	-0.216485	-2.680013	12	0.136158
-3.805790	-1.438271	-2.013225	12	0.143375
-4.761269	0.610345	-3.137326	12	-0.558775
-5.234730	-1.916642	-1.843568	12	-0.538096
2.429164	-0.827233	-2.964334	12	0.658265
3.371749	-1.820371	-2.739046	14	-0.651905
3.119087	-3.040023	-2.174188	12	0.740240
1.787951	-3.396552	-1.924072	14	-0.539049
4.026671	-3.809316	-2.033471	16	-0.419735
2.821840	0.169106	-3.540214	16	-0.455727
0.241172	2.483484	-2.601628	1	0.196885
0.845036	4.964024	-1.350538	1	0.185058

-0.372173	5.075382	0.605130	1	0.198193
0.752120	3.093956	1.066628	1	0.215595
-1.599160	4.874157	-1.763583	1	0.421542
-2.493537	3.480463	-0.388552	1	0.432003
2.441811	1.745218	-1.638469	1	0.196780
2.676588	3.363587	-2.263098	1	0.206438
0.259294	1.999618	3.281508	1	0.242230
-5.107984	1.340308	-0.208820	1	0.180472
-4.872043	-1.303468	3.450039	1	0.369000
-3.390769	-0.794521	4.162942	1	0.383180
4.629303	-0.358631	1.590177	1	0.462299
1.937268	-1.950811	4.088778	1	0.204293
2.191296	-2.553061	2.579308	1	0.195371
0.295285	-3.644569	3.467685	1	0.183925
-1.564179	-3.221052	1.954844	1	0.151673
1.095646	-3.138214	0.581368	1	0.205357
-0.293707	-4.768757	-1.066373	1	0.222822
-1.604265	-4.150248	-0.176630	1	0.205156
-1.004493	-0.781325	2.066037	1	0.430090
1.112153	-5.418330	0.801927	1	0.429112
-0.589607	-0.994178	4.140127	1	0.430625
-2.150107	1.060585	-3.534875	1	0.203585
-3.077952	-3.250866	-1.191124	1	0.180133
-5.643002	0.692392	-2.417593	1	0.180820
-4.464191	1.667645	-3.330592	1	0.189556
-5.192572	0.203097	-4.057157	1	0.210785
-5.861008	-1.924356	-2.749937	1	0.196294
-5.183880	-2.903906	-1.413278	1	0.177079
-5.690043	-1.299870	-1.142821	1	0.206704
4.328437	-1.642848	-2.986578	1	0.381652

Structure F



$[M+Na]^+$ $C_{27}H_{31}N_9O_{15}P_2$
d = 5.204 Å
CCS = 234.28 Å²
ΔE = 16.93 kcal/mol

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-0.618793	2.955321	0.859158	12	0.115785
0.176357	4.262414	0.547258	12	0.103688
1.482275	3.775175	-0.257853	12	0.078813
0.957121	2.454762	-0.918241	12	0.217472
0.064558	1.874909	0.077865	16	-0.515635
0.635879	4.984862	1.680396	16	-0.639141
2.617417	3.516645	0.628556	16	-0.700826
-2.085846	2.936954	0.436566	12	-0.125138
-2.226138	3.325426	-0.935413	16	-0.505146
-2.974645	2.329236	-1.863823	31	1.136881
-4.361744	1.973208	-1.539595	16	-0.550121
-2.821310	3.061970	-3.230171	16	-0.587625
-1.951044	1.187548	-1.955796	16	-0.494274
1.752067	1.381974	-1.498481	14	-0.487037
3.020262	0.942473	-1.320564	12	0.589943
3.153434	-0.236985	-2.026795	12	0.324286
2.061995	-0.519521	-2.675869	14	-0.658337
1.267526	0.494602	-2.366613	12	0.312919
3.994267	1.412759	-0.484768	14	-0.529469
4.409439	-0.833820	-1.956750	12	0.575422
5.431554	-0.344498	-1.253939	14	-0.477462
5.173921	0.786749	-0.592553	12	0.198432
4.641446	-1.969210	-2.623436	14	-0.953900

4.645641	-2.927318	-2.909436	1	0.451046
-2.388355	-0.194711	-1.541237	31	1.159684
-1.195926	-1.097046	-2.138938	16	-0.568932
-3.581139	-0.476332	-2.519306	16	-0.650929
-2.777157	-0.418435	-0.131997	16	-0.532233
-1.539849	-2.489259	-2.481755	12	-0.123354
-0.257735	-3.328511	-2.546564	12	0.104267
0.418236	-3.340369	-1.160681	12	0.146231
-0.525078	-3.762319	0.000596	12	0.103598
0.096351	-3.660303	1.396275	12	-0.159468
-0.159569	-2.335422	2.027811	14	-0.601927
1.233421	-2.202081	-0.803698	16	-0.694506
-0.947496	-5.093089	-0.186743	16	-0.643294
0.648503	-2.853751	-3.529276	16	-0.660403
0.877383	-1.429053	2.392657	12	0.400963
0.561350	-0.122296	2.765622	12	0.305884
-0.620809	0.430651	2.856599	14	-0.527091
-1.625046	-0.459415	2.723473	12	0.164160
-1.427096	-1.821296	2.240222	12	0.570461
1.593344	0.815611	2.916006	12	-0.247389
2.263419	-1.784011	2.398455	12	-0.245633
2.962672	0.508532	2.858366	12	0.091953
3.301428	-0.858296	2.590230	12	0.113990
4.030536	1.504986	3.124261	12	-0.515767
4.756841	-1.369665	2.542844	12	-0.537402
-3.049651	0.080644	2.997203	12	0.616127
-4.108272	-0.807179	2.719055	14	-0.642351
-3.863635	-2.048734	2.217881	12	0.697115
-2.585995	-2.558312	2.073014	14	-0.633424
-4.771768	-2.726405	2.018544	16	-0.448279
-3.335152	1.181346	3.367585	16	-0.471928
-0.480801	2.769164	1.888050	1	0.228352

-0.543346	4.939769	0.012970	1	0.169756
1.751416	4.547839	-0.921206	1	0.174319
0.398423	2.847961	-1.774559	1	0.171184
1.589764	4.746322	1.863816	1	0.430587
3.124771	2.757683	0.207536	1	0.471218
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0.335367	0.664423	-2.796843	1	0.228809
6.004200	1.138178	0.055069	1	0.217329
5.566884	-2.360168	-2.473313	1	0.464686
3.946073	-2.260677	-3.304966	1	0.456298
-4.307266	0.081140	-2.211057	1	0.475862
-2.034443	-2.535183	-3.454560	1	0.195026
-2.274424	-2.864049	-1.806862	1	0.221097
-0.561783	-4.334326	-2.840669	1	0.188204
1.128786	-4.207979	-1.186246	1	0.100529
-1.353341	-3.116807	-0.052548	1	0.195641
-0.465978	-4.427282	1.916791	1	0.195988
1.204834	-3.779792	1.412496	1	0.170994
1.651383	-1.786902	-1.726428	1	0.413353
-1.822689	-5.251747	0.348165	1	0.421648
0.503994	-1.857009	-3.662768	1	0.414877
1.383610	1.837471	3.126569	1	0.153115
2.521186	-2.788959	2.253929	1	0.131817
3.664549	2.453383	2.978152	1	0.187700
4.251904	1.356613	4.158955	1	0.191279
4.882904	1.301869	2.454986	1	0.132939
4.706279	-2.430520	2.871762	1	0.174379
5.149302	-1.318103	1.512774	1	0.137535
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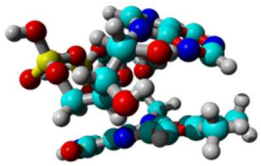
-5.012902	-0.577503	2.877613	1	0.342518

Structure G



$[M+Na]^+$ $C_{27}H_{31}N_9O_{15}P_2$
d = 5.570 Å
CCS = 241.53 Å²
ΔE = 0 kcal/mol

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87
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calc
1.0000

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-1.588591	3.986491	-0.352405	12	0.101261
-0.876624	2.893917	0.467269	12	0.186168
-0.546945	1.881853	-0.476899	16	-0.504817
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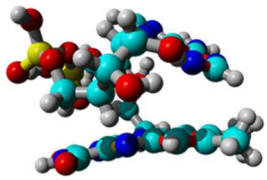
Structure H



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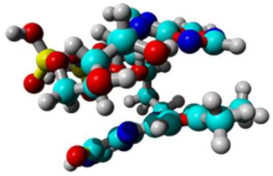
Structure I



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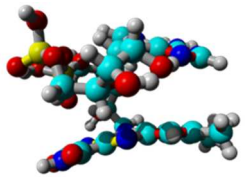
Structure J



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1.184042	2.430620	2.244036	12	0.109016
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2.108833	3.386149	0.075744	12	-0.202991
1.867527	2.377333	-0.949268	14	-0.529410
1.144707	1.063922	1.613639	16	-0.685419
0.894159	4.900515	1.618558	16	-0.626544
0.473889	1.617667	4.459144	16	-0.636925
2.680785	1.323033	-1.283507	12	0.419439
2.270210	0.243174	-2.103866	12	0.335598
1.067229	0.212731	-2.720628	14	-0.511261
0.348604	1.404094	-2.635054	12	0.218825
0.764266	2.484182	-1.813662	12	0.550852
3.086014	-0.794811	-2.357462	12	-0.220168
4.045609	1.340002	-0.959319	12	-0.247914
4.403857	-0.838367	-1.948194	12	0.116347
4.935555	0.300189	-1.296900	12	0.148733
5.285398	-2.014433	-2.345762	12	-0.534635
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-1.525184	0.718334	-4.040783	16	-0.458817
-0.867562	-1.644736	-2.829947	1	0.216283
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-2.916192	-0.357842	-1.819778	1	0.208820
-3.454840	-1.838971	-2.766335	1	0.198247
-5.720595	-2.858389	0.667622	23	0.647212
-1.244586	-1.382993	2.674116	1	0.242765
4.439226	-3.753721	0.611382	1	0.184385
4.620308	-1.224287	4.179738	1	0.362444
3.103363	-0.474486	4.500151	1	0.367946
-2.087166	2.510105	3.816303	1	0.211393
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0.521499	5.488463	0.869203	1	0.430836
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4.429323	2.163891	-0.411559	1	0.166383
5.899256	-1.722372	-3.209115	1	0.204141
5.962504	-2.234706	-1.533658	1	0.186247
4.621995	-2.975344	-2.455698	1	0.176182
7.085908	-0.119584	-1.749981	1	0.187483
6.847172	1.565754	-1.020371	1	0.184198
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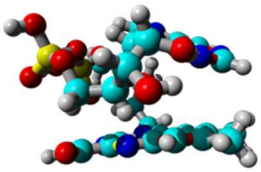
Structure K



$[M+Na]^+$ $C_{27}H_{33}N_9O_{15}P_2$
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ΔE = 0 kcal/mol

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calc
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2.689100	-0.894006	-1.492023	16	-0.486441
-0.930298	-2.066148	-1.874307	14	-0.518321
-2.220886	-1.732295	-1.682157	12	0.728966
-2.495368	-0.681184	-2.502805	12	0.147853
-1.401769	-0.327340	-3.280044	14	-0.586996
-0.456449	-1.171469	-2.852573	12	0.300159
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-4.794475	-0.712148	-1.897952	14	-0.489664
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3.855785	1.279833	-1.621815	16	-0.665368
1.891426	0.916440	0.079473	16	-0.544470
1.390304	2.474794	-2.580148	12	-0.081064
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-0.769511	3.761007	-0.512357	12	0.079945
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-1.137029	2.452540	1.652499	14	-0.580187
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-1.038542	5.087704	-0.984110	16	-0.648232
-0.684824	2.356804	-4.008162	16	-0.684588
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-2.084195	-0.930131	2.876584	12	-0.252330
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0.591407	-1.147018	-3.039766	1	0.246886
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1.984061	2.785271	-3.511464	1	0.193312
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-1.565237	-1.773993	3.251100	1	0.174497
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-5.950013	1.273087	1.578550	1	0.159696
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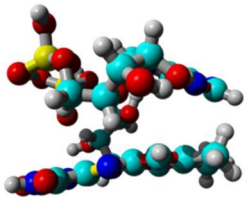
Structure L



$[M+Na]^+$ $C_{27}H_{33}N_9O_{15}P_2$
d = 5.382 Å
CCS = 248.64 Å²
ΔE = 15.07 kcal/mol

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87
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5.293148	-1.045957	0.988397	14	-0.482199
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