

Supporting Information

Sustainable Leads for Hypoxic Tumor Therapy: Allosteric Selective Inhibition of Carbonic Anhydrase IX by Abietane-Type Resin Acids

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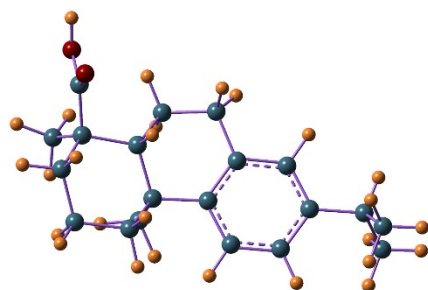
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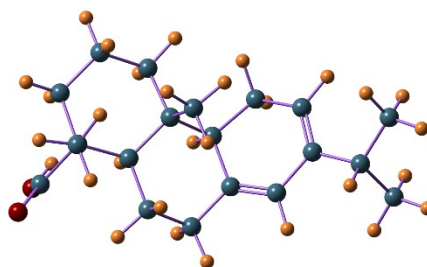
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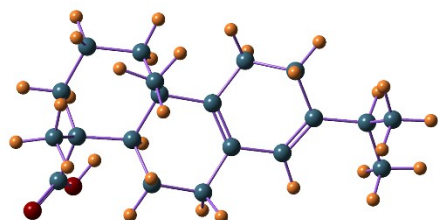
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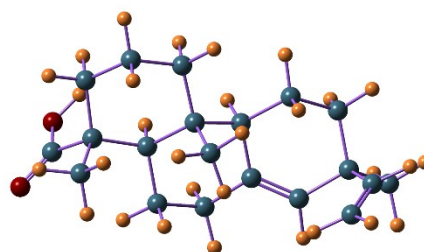
Callitrisic acid



Levopimaric acid



Palustric acid



Pimaric acid

Figure S1. Geometries of investigated compounds optimized using DFT at the B3LYP level of theory

Cartesian coordinates of DFT-calculated isolated phenolics at the B3LYP level of theory
Callitrisic acid

1	6	0	-0.972165	2.110797	-0.662536
2	6	0	-2.469883	2.482515	-0.627048
3	6	0	-3.348610	1.265769	-0.962222
4	6	0	-3.107370	0.065287	-0.007274
5	6	0	-3.786333	0.270727	1.361366
6	6	0	-3.705559	-1.157008	-0.705184
7	6	0	-1.559832	-0.239103	0.046755
8	6	0	-1.192330	-1.434655	0.950477
9	6	0	0.191316	-1.961773	0.528926
10	6	0	1.210335	-0.849275	0.293568
11	6	0	2.561496	-1.210961	0.174188
12	6	0	3.568230	-0.278067	-0.073958
13	6	0	3.192149	1.066456	-0.204071
14	6	0	1.857782	1.440537	-0.087959
15	6	0	0.839306	0.501458	0.153596
16	6	0	-0.622177	0.978105	0.345255
17	6	0	-0.701868	1.532680	1.796889
18	8	0	-3.718653	-1.366244	-1.914161
19	8	0	-4.210193	-2.088075	0.191985
20	6	0	5.026494	-0.713252	-0.195580
21	6	0	5.899935	-0.055349	0.901157
22	6	0	5.588176	-0.394985	-1.603409
23	1	0	-0.374325	3.002626	-0.444174
24	1	0	-0.710012	1.771914	-1.673387
25	1	0	-2.661963	3.274369	-1.361997
26	1	0	-2.735763	2.888407	0.355882
27	1	0	-4.411128	1.539934	-0.927271
28	1	0	-3.130433	0.925118	-1.979968
29	1	0	-3.475712	1.213895	1.811635
30	1	0	-4.873392	0.295135	1.231390

31	1	0	-3.549799	-0.545222	2.046292
32	1	0	-1.316044	-0.531911	-0.987119
33	1	0	-1.943413	-2.223965	0.857155
34	1	0	-1.174569	-1.122919	1.999347
35	1	0	0.582441	-2.658165	1.281048
36	1	0	0.078960	-2.526665	-0.408313
37	1	0	2.829027	-2.259050	0.281918
38	1	0	3.943424	1.825263	-0.394514
39	1	0	1.603723	2.488948	-0.185897
40	1	0	-1.671884	1.981155	2.018152
41	1	0	-0.502203	0.748342	2.531572
42	1	0	0.067538	2.303070	1.917583
43	1	0	-4.553213	-2.862777	-0.337025
44	1	0	5.059784	-1.801218	-0.052190
45	1	0	5.516648	-0.297722	1.897690
46	1	0	6.935588	-0.407399	0.826570
47	1	0	5.898242	1.034328	0.786912
48	1	0	4.984495	-0.877917	-2.378658
49	1	0	6.622388	-0.748384	-1.690660
50	1	0	5.577800	0.685939	-1.782186
Levopimaric acid					
1	6	0	-2.963499	0.084614	0.460001
2	6	0	-3.440396	1.462373	-0.085271
3	6	0	-2.358892	2.549864	0.043698
4	6	0	-1.072351	2.131292	-0.699528
5	6	0	-0.463809	0.810620	-0.152180
6	6	0	0.668640	0.299015	-1.137701
7	6	0	1.839764	1.298356	-1.400272
8	6	0	3.088445	1.069143	-0.569338
9	6	0	3.374732	-0.123458	-0.026500

10	6	0	2.400300	-1.224265	-0.152260
11	6	0	1.166646	-1.058102	-0.653285
12	6	0	0.111157	-2.137884	-0.624940
13	6	0	-1.067671	-1.674385	0.273309
14	6	0	-1.583484	-0.292803	-0.193554
15	6	0	-3.976580	-0.992453	0.014868
16	8	0	-4.572825	-1.743628	0.770647
17	8	0	-4.197381	-1.102412	-1.352910
18	6	0	5.446986	0.805282	1.178829
19	6	0	4.666885	-0.443782	0.721883
20	6	0	5.571958	-1.334549	-0.172290
21	6	0	0.159654	1.054635	1.241419
22	6	0	-2.973941	0.073650	2.000664
23	1	0	-4.355714	1.756109	0.442757
24	1	0	-3.699950	1.369631	-1.149151
25	1	0	-2.738106	3.487368	-0.381999
26	1	0	-2.140823	2.741276	1.099600
27	1	0	-0.333909	2.937398	-0.627251
28	1	0	-1.309663	1.996659	-1.766125
29	1	0	0.158800	0.139399	-2.099916
30	1	0	2.126541	1.210874	-2.460458
31	1	0	1.490486	2.327618	-1.267551
32	1	0	3.777560	1.903176	-0.488391
33	1	0	2.695193	-2.198241	0.231904
34	1	0	0.528328	-3.078495	-0.248259

35	1	0	-0.272660	-2.316085	-1.640410
36	1	0	-1.880357	-2.409386	0.230846
37	1	0	-0.725715	-1.616950	1.310982
38	1	0	-1.802038	-0.403207	-1.269615
39	1	0	-3.663569	-0.443790	-1.865463
40	1	0	6.320719	0.504158	1.767343
41	1	0	5.804190	1.375965	0.313850
42	1	0	4.819235	1.458287	1.794348
43	1	0	4.393567	-1.022960	1.616210
44	1	0	5.041329	-2.234127	-0.501703
45	1	0	6.470618	-1.641605	0.375383
46	1	0	5.874930	-0.769507	-1.060496
47	1	0	1.002442	1.745433	1.140053
48	1	0	-0.555781	1.490539	1.939933
49	1	0	0.545377	0.126717	1.668984
50	1	0	-4.002009	0.198767	2.352366
51	1	0	-2.614859	-0.883758	2.383711
52	1	0	-2.359793	0.874078	2.411313

Palustric acid

1	6	0	-3.130777	-0.075079	0.106480
2	6	0	-3.531865	0.986831	-0.960952
3	6	0	-2.715635	2.288391	-0.838041
4	6	0	-1.198153	2.009731	-0.925992
5	6	0	-0.713069	1.033198	0.186802
6	6	0	0.753888	0.629589	-0.044150

7	6	0	1.739895	1.696837	-0.524893
8	6	0	3.164519	1.444055	0.013337
9	6	0	3.585499	-0.006606	-0.206631
10	6	0	2.631706	-0.948645	-0.126785
11	6	0	1.216999	-0.623476	0.146820
12	6	0	0.347373	-1.788382	0.601580
13	6	0	-1.060055	-1.345848	1.050525
14	6	0	-1.576525	-0.266472	0.078333
15	6	0	-3.756183	-1.428548	-0.296550
16	8	0	-4.514446	-2.081830	0.403245
17	8	0	-3.410507	-1.918011	-1.549757
18	6	0	5.379878	-1.732122	-0.829351
19	6	0	5.066730	-0.279315	-0.417000
20	6	0	5.856667	0.083585	0.872539
21	6	0	-0.757572	1.752101	1.566321
22	6	0	-3.715927	0.275817	1.487438
23	1	0	-4.605640	1.192751	-0.874216
24	1	0	-3.364609	0.574192	-1.965290
25	1	0	-3.006813	2.970979	-1.646237
26	1	0	-2.952847	2.791022	0.105620
27	1	0	-0.973918	1.564122	-1.905522
28	1	0	-0.649239	2.955413	-0.860278
29	1	0	1.763667	1.691944	-1.626067
30	1	0	1.411355	2.692828	-0.211102
31	1	0	3.871480	2.123348	-0.477565

32	1	0	3.186822	1.663000	1.092287
33	1	0	2.876427	-2.000898	-0.233248
34	1	0	0.855817	-2.318507	1.417768
35	1	0	0.255151	-2.502526	-0.231473
36	1	0	-1.020549	-0.944071	2.067506
37	1	0	-1.737120	-2.207806	1.063759
38	1	0	-1.346902	-0.638690	-0.933702
39	1	0	-2.776638	-1.317441	-2.017909
40	1	0	6.451965	-1.840308	-1.027505
41	1	0	5.112218	-2.426827	-0.024945
42	1	0	4.828846	-2.013125	-1.733137
43	1	0	5.412538	0.388389	-1.220944
44	1	0	5.679861	1.122711	1.168916
45	1	0	6.932238	-0.050541	0.710048
46	1	0	5.539854	-0.571387	1.691496
47	1	0	-0.541786	1.053269	2.378151
48	1	0	0.012047	2.532197	1.583446
49	1	0	-1.720214	2.228678	1.759646
50	1	0	-3.362405	-0.425963	2.246738
51	1	0	-3.451182	1.288278	1.789710
52	1	0	-4.805146	0.189846	1.447178

Pimaric acid

1	6	0	-2.920376	0.093413	0.267271
2	6	0	-3.322973	1.395741	-0.482551
3	6	0	-2.298967	2.526301	-0.273054

4	6	0	-0.908150	2.088069	-0.775764
5	6	0	-0.363757	0.841755	-0.026144
6	6	0	0.909333	0.297928	-0.792684
7	6	0	2.053202	1.340099	-0.888280
8	6	0	3.368340	0.678613	-1.336215
9	6	0	3.846632	-0.353681	-0.276081
10	6	0	2.686068	-1.264270	0.082880
11	6	0	1.397375	-1.015962	-0.182701
12	6	0	0.335962	-2.090335	0.003219
13	6	0	-0.954772	-1.554432	0.661726
14	6	0	-1.437223	-0.297921	-0.094381
15	6	0	-3.800376	-1.071731	-0.235423
16	8	0	-4.457611	-1.807770	0.484285
17	8	0	-3.804687	-1.295119	-1.606772
18	6	0	4.986204	-1.219016	-0.887768
19	6	0	0.032116	1.222274	1.422261
20	6	0	-3.214916	0.230674	1.774430
21	6	0	4.415378	0.380694	0.932204
22	6	0	3.914995	0.380571	2.166019
23	1	0	-4.322178	1.702890	-0.150673
24	1	0	-3.389265	1.203234	-1.562753
25	1	0	-2.249695	2.801555	0.786049
26	1	0	-2.625909	3.416787	-0.824265
27	1	0	-0.197124	2.915248	-0.672566
28	1	0	-0.983070	1.850561	-1.848334

29	1	0	0.568638	0.073396	-1.818573
30	1	0	1.773620	2.132115	-1.591303
31	1	0	2.223736	1.796035	0.091333
32	1	0	3.217831	0.154432	-2.289465
33	1	0	4.147453	1.436681	-1.485751
34	1	0	2.960255	-2.219644	0.529436
35	1	0	0.746291	-2.926181	0.581373
36	1	0	0.067824	-2.478816	-0.992249
37	1	0	-0.764231	-1.309611	1.710667
38	1	0	-1.731470	-2.328090	0.639074
39	1	0	-1.473813	-0.577121	-1.160788
40	1	0	-3.245533	-0.634270	-2.088586
41	1	0	4.619489	-1.751552	-1.772098
42	1	0	5.828061	-0.581836	-1.184090
43	1	0	5.343945	-1.951165	-0.155423
44	1	0	0.663270	2.116127	1.414928
45	1	0	-0.839875	1.435852	2.040062
46	1	0	0.603017	0.417400	1.892271
47	1	0	-2.881008	-0.654140	2.319415
48	1	0	-2.736407	1.113606	2.197756
49	1	0	-4.295811	0.313482	1.920176
50	1	0	5.324857	0.943961	0.718616
51	1	0	4.389601	0.928278	2.974015
52	1	0	3.011323	-0.168795	2.407852

CGenFF parameters

Callitrisic acid

GROUP	!CHARGE	CH_PENALTY	Z	EL	NB	NBE	RNG1	TYP	RNG2	TYP	RNG3	TYP
TOM C1	CG311	-0.130	!	16.185	6	C	4	4	6	3	6	4
ATOM O1	OG311	-0.561	!	12.422	8	O	2	2				
ATOM C2	CG301	-0.041	!	24.633	6	C	4	4	6	3	6	4
ATOM O2	OG2D1	-0.558	!	7.574	8	O	1	2				
ATOM C3	CG301	0.117	!	22.730	6	C	4	4	6	3		
ATOM C4	CG321	-0.192	!	13.163	6	C	4	4	6	3		
ATOM C5	CG321	-0.192	!	5.682	6	C	4	4	6	4		
ATOM C6	CG321	-0.277	!	13.030	6	C	4	4	6	3		
ATOM C7	CG321	-0.184	!	7.980	6	C	4	4	6	3		
ATOM C8	CG2R61	0.090	!	24.040	6	C	3	4	6	4	6	1
ATOM C9	CG321	-0.165	!	0.256	6	C	4	4	6	4		
ATOM C10	CG331	-0.271	!	9.837	6	C	4	4				
ATOM C11	CG2R61	-0.014	!	9.957	6	C	3	4	6	4	6	1
ATOM C12	CG331	-0.284	!	9.957	6	C	4	4				
ATOM C13	CG2O2	0.840	!	21.878	6	C	3	4				
ATOM C14	CG2R61	-0.118	!	9.964	6	C	3	4	6	1		
ATOM C15	CG2R61	-0.118	!	0.496	6	C	3	4	6	1		
ATOM C16	CG2R61	0.008	!	0.000	6	C	3	4	6	1		
ATOM C17	CG2R61	-0.115	!	0.496	6	C	3	4	6	1		
ATOM C18	CG311	-0.092	!	0.000	6	C	4	4				
ATOM C19	CG331	-0.269	!	0.000	6	C	4	4				
ATOM C20	CG331	-0.269	!	0.000	6	C	4	4				
ATOM H1	HGP1	0.290	!	0.845	1	H	1	1				
ATOM H2	HGA1	0.090	!	1.082	1	H	1	1				
ATOM H3	HGA2	0.090	!	0.900	1	H	1	1				
ATOM H4	HGA2	0.090	!	0.900	1	H	1	1				
ATOM H5	HGA2	0.090	!	0.000	1	H	1	1				
ATOM H6	HGA2	0.090	!	0.000	1	H	1	1				

ATOM H7 HGA2 0.090! 0.600 1 H 1 1
 ATOM H8 HGA2 0.090! 0.600 1 H 1 1
 ATOM H9 HGA2 0.090! 0.000 1 H 1 1
 ATOM H10 HGA2 0.090! 0.000 1 H 1 1
 ATOM H11 HGA2 0.090! 0.000 1 H 1 1
 ATOM H12 HGA2 0.090! 0.000 1 H 1 1
 ATOM H13 HGA3 0.090! 0.600 1 H 1 1
 ATOM H14 HGA3 0.090! 0.600 1 H 1 1
 ATOM H15 HGA3 0.090! 0.600 1 H 1 1
 ATOM H16 HGA3 0.090! 0.600 1 H 1 1
 ATOM H17 HGA3 0.090! 0.600 1 H 1 1
 ATOM H18 HGA3 0.090! 0.600 1 H 1 1
 ATOM H19 HGR61 0.115! 0.060 1 H 1 1
 ATOM H20 HGR61 0.115! 0.000 1 H 1 1
 ATOM H21 HGR61 0.115! 0.000 1 H 1 1
 ATOM H22 HGA1 0.090! 0.000 1 H 1 1
 ATOM H23 HGA3 0.090! 0.000 1 H 1 1
 ATOM H24 HGA3 0.090! 0.000 1 H 1 1
 ATOM H25 HGA3 0.090! 0.000 1 H 1 1
 ATOM H26 HGA3 0.090! 0.000 1 H 1 1
 ATOM H27 HGA3 0.090! 0.000 1 H 1 1
 ATOM H28 HGA3 0.090! 0.000 1 H 1 1
 BOND C1 C5 !1 1
 BOND C1 C3 !1 1
 BOND C1 C2 !1 1
 BOND C1 H2 !1 0
 BOND O1 C13 !1 0
 BOND O1 H1 !1 0
 BOND C2 C10 !1 0
 BOND C2 C8 !1 1

BOND C2 C4 !1 1
BOND O2 C13 !2 0
BOND C3 C12 !1 0
BOND C3 C13 !1 0
BOND C3 C6 !1 1
BOND C4 C7 !1 1
BOND C4 H3 !1 0
BOND C4 H4 !1 0
BOND C5 C9 !1 1
BOND C5 H5 !1 0
BOND C5 H6 !1 0
BOND C6 C7 !1 1
BOND C6 H7 !1 0
BOND C6 H8 !1 0
BOND C7 H9 !1 0
BOND C7 H10 !1 0
BOND C8 C11 !2 1
BOND C8 C14 !1 1
BOND C9 C11 !1 1
BOND C9 H11 !1 0
BOND C9 H12 !1 0
BOND C10 H13 !1 0
BOND C10 H14 !1 0
BOND C10 H15 !1 0
BOND C11 C15 !1 1
BOND C12 H16 !1 0
BOND C12 H17 !1 0
BOND C12 H18 !1 0
BOND C14 C17 !2 1
BOND C14 H19 !1 0

BOND C15 C16 ! 2 1

BOND C15 H20 ! 1 0

BOND C16 C18 ! 1 0

BOND C16 C17 ! 1 1

BOND C17 H21 ! 1 0

BOND C18 C20 ! 1 0

BOND C18 C19 ! 1 0

BOND C18 H22 ! 1 0

BOND C19 H23 ! 1 0

BOND C19 H24 ! 1 0

BOND C19 H25 ! 1 0

BOND C20 H26 ! 1 0

BOND C20 H27 ! 1 0

BOND C20 H28 ! 1 0

IMPR C13 C3 O2 O1

BONDS

CG202 CG301 200.00 1.5220 ! JZ4 , from CG202 CG311, penalty= 8

ANGLES

CG301 CG202 OG2D1 70.00 125.00 20.00 2.44200 ! JZ4 , from CG311 CG202 OG2D1, penalty= 1.2

CG301 CG202 OG311 55.00 110.50 ! JZ4 , from CG311 CG202 OG311, penalty= 1.2

CG202 CG301 CG311 52.00 108.00 ! JZ4 , from CG202 CG311 CG311, penalty= 8

CG202 CG301 CG321 52.00 108.00 ! JZ4 , from CG202 CG311 CG321, penalty= 8

CG202 CG301 CG331 52.00 108.00 ! JZ4 , from CG202 CG311 CG331, penalty= 8

CG2R61 CG301 CG311 51.80 107.50 ! JZ4 , from CG2R61 CG301 CG331, penalty= 1.5

CG2R61 CG301 CG321 51.80 107.50 ! JZ4 , from CG2R61 CG301 CG331, penalty= 0.9

CG301 CG311 CG301 52.00 108.00 ! JZ4 , from CG301 CG311 CG311, penalty= 1.2

DIHEDRALS

OG2D1 CG202 CG301 CG311 0.0500 6 180.00 ! JZ4 , from OG2D1 CG202 CG311 CG311, penalty= 8

OG2D1 CG202 CG301 CG321 0.0500 6 180.00 ! JZ4 , from OG2D1 CG202 CG311 CG321, penalty= 8

OG2D1 CG202 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG2D1 CG202 CG311 CG331, penalty= 8
OG311 CG202 CG301 CG311	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG311, penalty= 8
OG311 CG202 CG301 CG321	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8
OG311 CG202 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8.9
CG301 CG202 OG311 HGP1	2.0500	2	180.00 ! JZ4 , from CG311 CG202 OG311 HGP1, penalty= 1.2
CG301 CG2R61 CG2R61 CG321	2.4000	2	180.00 ! JZ4 , from CG321 CG2R61 CG2R61 CG331, penalty= 2.7
CG2R61 CG2R61 CG301 CG311	0.2300	2	180.00 ! JZ4 , from CG2R61 CG2R61 CG301 CG331, penalty= 1.5
CG2R61 CG2R61 CG301 CG321	0.2300	2	180.00 ! JZ4 , from CG2R61 CG2R61 CG301 CG331, penalty= 0.9
CG202 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 9.8
CG202 CG301 CG311 CG321	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 8
CG202 CG301 CG311 HGA1	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 HGA1, penalty= 8
CG2R61 CG301 CG311 CG301	0.0400	3	0.00 ! JZ4 , from CG321 CG311 CG321 CG2R61, penalty= 13.8
CG2R61 CG301 CG311 CG321	0.0400	3	0.00 ! JZ4 , from CG321 CG311 CG321 CG2R61, penalty= 12
CG2R61 CG301 CG311 HGA1	0.0400	3	0.00 ! JZ4 , from CG2R61 CG301 CG331 HGA3, penalty= 11
CG321 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG321 CG301 CG311 CG311, penalty= 1.2
CG331 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG331 CG301 CG311 CG311, penalty= 1.2
CG202 CG301 CG321 CG321	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG321 CG321, penalty= 8
CG202 CG301 CG321 HGA2	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG321 HGA2, penalty= 8
CG2R61 CG301 CG321 CG321	0.0400	3	0.00 ! JZ4 , from CG2R61 CG321 CG321 CG321, penalty= 12
CG2R61 CG301 CG321 HGA2	0.0400	3	0.00 ! JZ4 , from CG2R61 CG301 CG331 HGA3, penalty= 6
CG202 CG301 CG331 HGA3	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG331 HGA3, penalty= 8
CG2R61 CG321 CG321 CG311	0.0400	3	0.00 ! JZ4 , from CG2R61 CG321 CG321 CG321, penalty= 0.6

IMPROPER

CG202 CG301 OG2D1 OG311	65.0000	0	0.00 ! JZ4 , from CG202 CG311 OG2D1 OG311, penalty= 0.8
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Levopimaric acid

GROUP	! CHARGE	CH_PENALTY	Z	EL	NB	NBE	RNG1	TYP	RNG2	TYP	RNG3	TYP
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ATOM C1 CG301 -0.041! 24.633 6 C 4 4 6 3 6 4
 ATOM O1 OG311 -0.561! 12.422 8 O 2 2
 ATOM C2 CG311 -0.130! 16.185 6 C 4 4 6 3 6 4
 ATOM O2 OG2D1 -0.558! 7.574 8 O 1 2
 ATOM C3 CG301 0.117! 22.730 6 C 4 4 6 3
 ATOM C4 CG2R61 0.090! 24.040 6 C 3 4 6 4 6 1
 ATOM C5 CG321 -0.192! 13.163 6 C 4 4 6 3
 ATOM C6 CG321 -0.192! 5.682 6 C 4 4 6 4
 ATOM C7 CG321 -0.277! 13.030 6 C 4 4 6 3
 ATOM C8 CG321 -0.184! 7.980 6 C 4 4 6 3
 ATOM C9 CG2R61 -0.014! 9.957 6 C 3 4 6 4 6 1
 ATOM C10 CG321 -0.165! 0.256 6 C 4 4 6 4
 ATOM C11 CG331 -0.271! 9.837 6 C 4 4
 ATOM C12 CG2R61 -0.118! 9.964 6 C 3 4 6 1
 ATOM C13 CG331 -0.284! 9.957 6 C 4 4
 ATOM C14 CG2O2 0.840! 21.878 6 C 3 4
 ATOM C15 CG2R61 -0.118! 0.496 6 C 3 4 6 1
 ATOM C16 CG2R61 -0.115! 0.496 6 C 3 4 6 1
 ATOM C17 CG2R61 0.008! 0.000 6 C 3 4 6 1
 ATOM C18 CG311 -0.092! 0.000 6 C 4 4
 ATOM C19 CG331 -0.269! 0.000 6 C 4 4
 ATOM C20 CG331 -0.269! 0.000 6 C 4 4
 ATOM H1 HGP1 0.290! 0.845 1 H 1 1
 ATOM H2 HGA1 0.090! 1.082 1 H 1 1
 ATOM H3 HGA2 0.090! 0.900 1 H 1 1
 ATOM H4 HGA2 0.090! 0.900 1 H 1 1
 ATOM H5 HGA2 0.090! 0.000 1 H 1 1
 ATOM H6 HGA2 0.090! 0.000 1 H 1 1
 ATOM H7 HGA2 0.090! 0.600 1 H 1 1
 ATOM H8 HGA2 0.090! 0.600 1 H 1 1

ATOM H9 HGA2 0.090! 0.000 1 H 1 1
 ATOM H10 HGA2 0.090! 0.000 1 H 1 1
 ATOM H11 HGA2 0.090! 0.000 1 H 1 1
 ATOM H12 HGA2 0.090! 0.000 1 H 1 1
 ATOM H13 HGA3 0.090! 0.600 1 H 1 1
 ATOM H14 HGA3 0.090! 0.600 1 H 1 1
 ATOM H15 HGA3 0.090! 0.600 1 H 1 1
 ATOM H16 HGR61 0.115! 0.060 1 H 1 1
 ATOM H17 HGA3 0.090! 0.600 1 H 1 1
 ATOM H18 HGA3 0.090! 0.600 1 H 1 1
 ATOM H19 HGA3 0.090! 0.600 1 H 1 1
 ATOM H20 HGR61 0.115! 0.000 1 H 1 1
 ATOM H21 HGR61 0.115! 0.000 1 H 1 1
 ATOM H22 HGA1 0.090! 0.000 1 H 1 1
 ATOM H23 HGA3 0.090! 0.000 1 H 1 1
 ATOM H24 HGA3 0.090! 0.000 1 H 1 1
 ATOM H25 HGA3 0.090! 0.000 1 H 1 1
 ATOM H26 HGA3 0.090! 0.000 1 H 1 1
 ATOM H27 HGA3 0.090! 0.000 1 H 1 1
 ATOM H28 HGA3 0.090! 0.000 1 H 1 1
 BOND C1 C2 !1 1
 BOND C1 C5 !1 1
 BOND C1 C11 !1 0
 BOND C1 C4 !1 1
 BOND O1 H1 !1 0
 BOND O1 C14 !1 0
 BOND C2 C3 !1 1
 BOND C2 C6 !1 1
 BOND C2 H2 !1 0
 BOND O2 C14 !2 0

BOND C3 C14 ! 1 0
BOND C3 C13 ! 1 0
BOND C3 C7 ! 1 1
BOND C4 C9 ! 2 1
BOND C4 C12 ! 1 1
BOND C5 C8 ! 1 1
BOND C5 H3 ! 1 0
BOND C5 H4 ! 1 0
BOND C6 C10 ! 1 1
BOND C6 H5 ! 1 0
BOND C6 H6 ! 1 0
BOND C7 C8 ! 1 1
BOND C7 H7 ! 1 0
BOND C7 H8 ! 1 0
BOND C8 H9 ! 1 0
BOND C8 H10 ! 1 0
BOND C9 C10 ! 1 1
BOND C9 C15 ! 1 1
BOND C10 H11 ! 1 0
BOND C10 H12 ! 1 0
BOND C11 H13 ! 1 0
BOND C11 H14 ! 1 0
BOND C11 H15 ! 1 0
BOND C12 C16 ! 2 1
BOND C12 H16 ! 1 0
BOND C13 H17 ! 1 0
BOND C13 H18 ! 1 0
BOND C13 H19 ! 1 0
BOND C15 C17 ! 2 1
BOND C15 H20 ! 1 0

BOND C16 C17 ! 1 1

BOND C16 H21 ! 1 0

BOND C17 C18 ! 1 0

BOND C18 C19 ! 1 0

BOND C18 C20 ! 1 0

BOND C18 H22 ! 1 0

BOND C19 H23 ! 1 0

BOND C19 H24 ! 1 0

BOND C19 H25 ! 1 0

BOND C20 H26 ! 1 0

BOND C20 H27 ! 1 0

BOND C20 H28 ! 1 0

IMPR C14 C3 O2 O1

BONDS

CG202 CG301 200.00 1.5220 ! JZ4 , from CG202 CG311, penalty= 8

ANGLES

CG301 CG202 OG2D1 70.00 125.00 20.00 2.44200 ! JZ4 , from CG311 CG202 OG2D1, penalty= 1.2

CG301 CG202 OG311 55.00 110.50 ! JZ4 , from CG311 CG202 OG311, penalty= 1.2

CG202 CG301 CG311 52.00 108.00 ! JZ4 , from CG202 CG311 CG311, penalty= 8

CG202 CG301 CG321 52.00 108.00 ! JZ4 , from CG202 CG311 CG321, penalty= 8

CG202 CG301 CG331 52.00 108.00 ! JZ4 , from CG202 CG311 CG331, penalty= 8

CG2R61 CG301 CG311 51.80 107.50 ! JZ4 , from CG2R61 CG301 CG331, penalty= 1.5

CG2R61 CG301 CG321 51.80 107.50 ! JZ4 , from CG2R61 CG301 CG331, penalty= 0.9

CG301 CG311 CG301 52.00 108.00 ! JZ4 , from CG301 CG311 CG311, penalty= 1.2

DIHEDRALS

OG2D1 CG202 CG301 CG311 0.0500 6 180.00 ! JZ4 , from OG2D1 CG202 CG311 CG311, penalty= 8

OG2D1 CG202 CG301 CG321 0.0500 6 180.00 ! JZ4 , from OG2D1 CG202 CG311 CG321, penalty= 8

OG2D1 CG202 CG301 CG331 0.0500 6 180.00 ! JZ4 , from OG2D1 CG202 CG311 CG331, penalty= 8

OG311 CG202 CG301 CG311 0.0500 6 180.00 ! JZ4 , from OG311 CG202 CG311 CG311, penalty= 8

OG311 CG202 CG301 CG321 0.0500 6 180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8

OG311 CG202 CG301 CG331 0.0500 6 180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8.9

CG301 CG202 OG311 HGP1 2.0500 2 180.00 ! JZ4 , from CG311 CG202 OG311 HGP1, penalty= 1.2

CG301 CG2R61 CG2R61 CG321 2.4000 2 180.00 ! JZ4 , from CG321 CG2R61 CG2R61 CG331, penalty= 2.7

CG2R61 CG2R61 CG301 CG311 0.2300 2 180.00 ! JZ4 , from CG2R61 CG2R61 CG301 CG331, penalty= 1.5

CG2R61 CG2R61 CG301 CG321 0.2300 2 180.00 ! JZ4 , from CG2R61 CG2R61 CG301 CG331, penalty= 0.9

CG202 CG301 CG311 CG301 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 9.8

CG202 CG301 CG311 CG321 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 8

CG202 CG301 CG311 HGA1 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG311 HGA1, penalty= 8

CG2R61 CG301 CG311 CG301 0.0400 3 0.00 ! JZ4 , from CG321 CG311 CG321 CG2R61, penalty= 13.8

CG2R61 CG301 CG311 CG321 0.0400 3 0.00 ! JZ4 , from CG321 CG311 CG321 CG2R61, penalty= 12

CG2R61 CG301 CG311 HGA1 0.0400 3 0.00 ! JZ4 , from CG2R61 CG301 CG331 HGA3, penalty= 11

CG321 CG301 CG311 CG301 0.2000 3 0.00 ! JZ4 , from CG321 CG301 CG311 CG311, penalty= 1.2

CG331 CG301 CG311 CG301 0.2000 3 0.00 ! JZ4 , from CG331 CG301 CG311 CG311, penalty= 1.2

CG202 CG301 CG321 CG321 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG321 CG321, penalty= 8

CG202 CG301 CG321 HGA2 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG321 HGA2, penalty= 8

CG2R61 CG301 CG321 CG321 0.0400 3 0.00 ! JZ4 , from CG2R61 CG321 CG321 CG321, penalty= 12

CG2R61 CG301 CG321 HGA2 0.0400 3 0.00 ! JZ4 , from CG2R61 CG301 CG331 HGA3, penalty= 6

CG202 CG301 CG331 HGA3 0.2000 3 0.00 ! JZ4 , from CG202 CG311 CG331 HGA3, penalty= 8

CG2R61 CG321 CG321 CG311 0.0400 3 0.00 ! JZ4 , from CG2R61 CG321 CG321 CG321, penalty= 0.6

IMPROPERS

CG202 CG301 OG2D1 OG311 65.0000 0 0.00 ! JZ4 , from CG202 CG311 OG2D1 OG311, penalty= 0.8

Palustric acid

GROUP	! CHARGE	CH_PENALTY	Z	EL	NB	NBE	RNG1	TYP	RNG2	TYP	RNG3	TYP
ATOM C1	CG301	0.056	!	7.383	6	C	4	4	6	3	6	4
ATOM O1	OG311	-0.561	!	12.422	8	O	2	2				
ATOM C2	CG311	-0.082	!	11.793	6	C	4	4	6	3	6	4
ATOM O2	OG2D1	-0.558	!	7.574	8	O	1	2				

ATOM C3 CG301 0.117! 21.520 6 C 4 4 6 3
 ATOM C4 CG321 -0.220! 1.776 6 C 4 4 6 3
 ATOM C5 CG321 -0.195! 10.619 6 C 4 4 6 4
 ATOM C6 CG2DC1 0.155! 2.131 6 C 3 4 6 4 6 4
 ATOM C7 CG321 -0.277! 13.030 6 C 4 4 6 3
 ATOM C8 CG321 -0.240! 4.781 6 C 4 4 6 3
 ATOM C9 CG321 -0.280! 9.732 6 C 4 4 6 4
 ATOM C10 CG2DC1 -0.024! 9.290 6 C 3 4 6 4 6 4
 ATOM C11 CG331 -0.270! 1.626 6 C 4 4
 ATOM C12 CG321 -0.185! 3.396 6 C 4 4 6 4
 ATOM C13 CG331 -0.284! 9.957 6 C 4 4
 ATOM C14 CG202 0.840! 21.878 6 C 3 4
 ATOM C15 CG321 -0.216! 6.434 6 C 4 4 6 4
 ATOM C16 CG2DC2 -0.245! 10.766 6 C 3 4 6 4
 ATOM C17 CG2DC2 -0.059! 9.538 6 C 3 4 6 4
 ATOM C18 CG311 -0.000! 8.013 6 C 4 4
 ATOM C19 CG331 -0.216! 6.515 6 C 4 4
 ATOM C20 CG331 -0.216! 6.515 6 C 4 4
 ATOM H1 HGP1 0.290! 0.845 1 H 1 1
 ATOM H2 HGA1 0.090! 0.601 1 H 1 1
 ATOM H3 HGA2 0.090! 0.000 1 H 1 1
 ATOM H4 HGA2 0.090! 0.000 1 H 1 1
 ATOM H5 HGA2 0.090! 0.000 1 H 1 1
 ATOM H6 HGA2 0.090! 0.000 1 H 1 1
 ATOM H7 HGA2 0.090! 0.600 1 H 1 1
 ATOM H8 HGA2 0.090! 0.600 1 H 1 1
 ATOM H9 HGA2 0.090! 0.000 1 H 1 1
 ATOM H10 HGA2 0.090! 0.000 1 H 1 1
 ATOM H11 HGA2 0.090! 0.450 1 H 1 1
 ATOM H12 HGA2 0.090! 0.450 1 H 1 1

ATOM H13 HGA3 0.090! 0.000 1 H 1 1
 ATOM H14 HGA3 0.090! 0.000 1 H 1 1
 ATOM H15 HGA3 0.090! 0.000 1 H 1 1
 ATOM H16 HGA2 0.090! 0.135 1 H 1 1
 ATOM H17 HGA2 0.090! 0.135 1 H 1 1
 ATOM H18 HGA3 0.090! 0.600 1 H 1 1
 ATOM H19 HGA3 0.090! 0.600 1 H 1 1
 ATOM H20 HGA3 0.090! 0.600 1 H 1 1
 ATOM H21 HGA2 0.090! 0.075 1 H 1 1
 ATOM H22 HGA2 0.090! 0.075 1 H 1 1
 ATOM H23 HGA4 0.150! 0.054 1 H 1 1
 ATOM H24 HGA1 0.090! 0.442 1 H 1 1
 ATOM H25 HGA3 0.090! 0.300 1 H 1 1
 ATOM H26 HGA3 0.090! 0.300 1 H 1 1
 ATOM H27 HGA3 0.090! 0.300 1 H 1 1
 ATOM H28 HGA3 0.090! 0.300 1 H 1 1
 ATOM H29 HGA3 0.090! 0.300 1 H 1 1
 ATOM H30 HGA3 0.090! 0.300 1 H 1 1
 BOND C1 C2 !1 1
 BOND C1 C4 !1 1
 BOND C1 C11 !1 0
 BOND C1 C6 !1 1
 BOND O1 H1 !1 0
 BOND O1 C14 !1 0
 BOND C2 C3 !1 1
 BOND C2 C5 !1 1
 BOND C2 H2 !1 0
 BOND O2 C14 !2 0
 BOND C3 C14 !1 0
 BOND C3 C13 !1 0

BOND C3 C7 !1 1
BOND C4 C8 !1 1
BOND C4 H3 !1 0
BOND C4 H4 !1 0
BOND C5 C9 !1 1
BOND C5 H5 !1 0
BOND C5 H6 !1 0
BOND C6 C10 !2 1
BOND C6 C12 !1 1
BOND C7 C8 !1 1
BOND C7 H7 !1 0
BOND C7 H8 !1 0
BOND C8 H9 !1 0
BOND C8 H10 !1 0
BOND C9 C10 !1 1
BOND C9 H11 !1 0
BOND C9 H12 !1 0
BOND C10 C16 !1 1
BOND C11 H13 !1 0
BOND C11 H14 !1 0
BOND C11 H15 !1 0
BOND C12 C15 !1 1
BOND C12 H16 !1 0
BOND C12 H17 !1 0
BOND C13 H18 !1 0
BOND C13 H19 !1 0
BOND C13 H20 !1 0
BOND C15 C17 !1 1
BOND C15 H21 !1 0
BOND C15 H22 !1 0

BOND C16 C17 ! 2 1

BOND C16 H23 ! 1 0

BOND C17 C18 ! 1 0

BOND C18 C20 ! 1 0

BOND C18 C19 ! 1 0

BOND C18 H24 ! 1 0

BOND C19 H25 ! 1 0

BOND C19 H26 ! 1 0

BOND C19 H27 ! 1 0

BOND C20 H28 ! 1 0

BOND C20 H29 ! 1 0

BOND C20 H30 ! 1 0

IMPR C14 C3 O2 O1

BONDS

CG2DC2 CG311 365.00 1.5020 ! JZ4 , from CG2DC2 CG321, penalty= 4

CG2O2 CG301 200.00 1.5220 ! JZ4 , from CG2O2 CG311, penalty= 8

ANGLES

CG2DC2 CG2DC1 CG321 48.00 113.00 ! JZ4 , from CG2DC2 CG2DC1 CG331, penalty= 0.9

CG301 CG2DC1 CG321 48.00 123.50 ! JZ4 , from CG321 CG2DC2 CG331, penalty= 2.7

CG2DC2 CG2DC2 CG311 48.00 123.50 ! JZ4 , from CG2DC1 CG2DC1 CG321, penalty= 0.6

CG311 CG2DC2 CG321 48.00 123.50 ! JZ4 , from CG321 CG2DC2 CG331, penalty= 1.5

CG301 CG2O2 OG2D1 70.00 125.00 20.00 2.44200 ! JZ4 , from CG311 CG2O2 OG2D1, penalty= 1.2

CG301 CG2O2 OG311 55.00 110.50 ! JZ4 , from CG311 CG2O2 OG311, penalty= 1.2

CG2DC1 CG301 CG311 32.00 112.20 ! JZ4 , from CG2D1 CG301 CG311, penalty= 0.5

CG2O2 CG301 CG311 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG311, penalty= 8

CG2O2 CG301 CG321 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG321, penalty= 8

CG2O2 CG301 CG331 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG331, penalty= 8

CG2DC2 CG311 CG331 32.00 112.20 ! JZ4 , from CG2D1 CG311 CG321, penalty= 1.4

CG2DC2 CG311 HGA1 45.00 111.50 ! JZ4 , from CG2D1 CG311 HGA1, penalty= 0.5

CG301 CG311 CG301 52.00 108.00 ! JZ4 , from CG301 CG311 CG311, penalty= 1.2

DIHEDRALS

CG2DC2 CG2DC1 CG2DC1 CG301 0.5600 1 180.00 ! JZ4 , from CG2DC2 CG2DC1 CG2DC1 CG321, penalty= 1.8

CG2DC2 CG2DC1 CG2DC1 CG301 7.0000 2 180.00 ! JZ4 , from CG2DC2 CG2DC1 CG2DC1 CG321, penalty= 1.8

CG321 CG2DC1 CG2DC1 CG321 10.0000 2 180.00 ! JZ4 , from CG321 CG2DC1 CG2DC1 CG331, penalty= 0.9

CG321 CG2DC1 CG2DC2 CG2DC2 1.1000 1 180.00 ! JZ4 , from CG2DC1 CG2DC1 CG2DC2 CG331, penalty= 0.9

CG321 CG2DC1 CG2DC2 CG2DC2 0.7000 2 180.00 ! JZ4 , from CG2DC1 CG2DC1 CG2DC2 CG331, penalty= 0.9

CG321 CG2DC1 CG2DC2 HGA4 1.0000 2 180.00 ! JZ4 , from CG331 CG2DC1 CG2DC2 HGA4, penalty= 0.9

CG2DC1 CG2DC1 CG301 CG311 0.5000 2 0.00 ! JZ4 , from CG2DC1 CG2DC1 CG301 CG321, penalty= 0.6

CG2DC1 CG2DC1 CG301 CG311 0.3000 3 0.00 ! JZ4 , from CG2DC1 CG2DC1 CG301 CG321, penalty= 0.6

CG321 CG2DC1 CG301 CG311 0.1900 3 0.00 ! JZ4 , from CG331 CG2DC1 CG321 CG321, penalty= 13.5

CG321 CG2DC1 CG301 CG321 0.1900 3 0.00 ! JZ4 , from CG331 CG2DC1 CG321 CG321, penalty= 12.9

CG321 CG2DC1 CG301 CG331 0.1900 3 0.00 ! JZ4 , from CG331 CG2DC1 CG321 CG321, penalty= 13.8

CG2DC2 CG2DC1 CG321 CG321 0.3000 3 0.00 ! JZ4 , from CG2DC2 CG2DC1 CG301 CG321, penalty= 12

CG2DC2 CG2DC1 CG321 HGA2 0.3000 3 180.00 ! JZ4 , from CG2DC2 CG2DC1 CG331 HGA3, penalty= 6

CG301 CG2DC1 CG321 CG321 0.1900 3 0.00 ! JZ4 , from CG331 CG2DC2 CG321 CG321, penalty= 2.7

CG301 CG2DC1 CG321 HGA2 0.1900 3 0.00 ! JZ4 , from CG331 CG2DC1 CG321 HGA2, penalty= 2.7

CG2DC1 CG2DC2 CG2DC2 CG311 0.5600 1 180.00 ! JZ4 , from CG2DC2 CG2DC1 CG2DC1 CG321, penalty= 0.6

CG2DC1 CG2DC2 CG2DC2 CG311 7.0000 2 180.00 ! JZ4 , from CG2DC2 CG2DC1 CG2DC1 CG321, penalty= 0.6

CG311 CG2DC2 CG2DC2 HGA4	5.2000	2	180.00 ! JZ4 , from CG321 CG2DC1 CG2DC1 HGA4, penalty=
	0.6		
CG2DC2 CG2DC2 CG311 CG331	0.5000	2	0.00 ! JZ4 , from CG2DC1 CG2DC1 CG321 CG331, penalty= 4
CG2DC2 CG2DC2 CG311 CG331	0.3000	3	0.00 ! JZ4 , from CG2DC1 CG2DC1 CG321 CG331, penalty= 4
CG2DC2 CG2DC2 CG311 HGA1	0.0300	3	0.00 ! JZ4 , from CG2DC1 CG2DC1 CG321 HGA2, penalty= 4
CG321 CG2DC2 CG311 CG331	0.1900	3	0.00 ! JZ4 , from CG331 CG2DC1 CG321 CG321, penalty= 5.8
CG321 CG2DC2 CG311 HGA1	0.1900	3	0.00 ! JZ4 , from CG331 CG2DC2 CG321 HGA2, penalty= 4.9
CG311 CG2DC2 CG321 CG321	0.1900	3	0.00 ! JZ4 , from CG331 CG2DC1 CG321 CG321, penalty= 1.5
CG311 CG2DC2 CG321 HGA2	0.1900	3	0.00 ! JZ4 , from CG331 CG2DC2 CG321 HGA2, penalty= 1.5
OG2D1 CG2O2 CG301 CG311	0.0500	6	180.00 ! JZ4 , from OG2D1 CG2O2 CG311 CG311, penalty= 8
OG2D1 CG2O2 CG301 CG321	0.0500	6	180.00 ! JZ4 , from OG2D1 CG2O2 CG311 CG321, penalty= 8
OG2D1 CG2O2 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG2D1 CG2O2 CG311 CG331, penalty= 8
OG311 CG2O2 CG301 CG311	0.0500	6	180.00 ! JZ4 , from OG311 CG2O2 CG311 CG311, penalty= 8
OG311 CG2O2 CG301 CG321	0.0500	6	180.00 ! JZ4 , from OG311 CG2O2 CG311 CG321, penalty= 8
OG311 CG2O2 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG311 CG2O2 CG311 CG321, penalty= 8.9
CG301 CG2O2 OG311 HGP1	2.0500	2	180.00 ! JZ4 , from CG311 CG2O2 OG311 HGP1, penalty= 1.2
CG2DC1 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG2D1 CG301 CG311 CG311, penalty= 1.7
CG2DC1 CG301 CG311 CG321	0.2000	3	0.00 ! JZ4 , from CG2D1 CG301 CG311 CG321, penalty= 0.5
CG2DC1 CG301 CG311 HGA1	0.1950	3	0.00 ! JZ4 , from CG2D1 CG301 CG311 HGA1, penalty= 0.5
CG2O2 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG311 CG321, penalty= 9.8
CG2O2 CG301 CG311 CG321	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG311 CG321, penalty= 8
CG2O2 CG301 CG311 HGA1	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG311 HGA1, penalty= 8
CG321 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG321 CG301 CG311 CG311, penalty= 1.2
CG331 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG331 CG301 CG311 CG311, penalty= 1.2
CG2O2 CG301 CG321 CG321	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG321 CG321, penalty= 8
CG2O2 CG301 CG321 HGA2	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG321 HGA2, penalty= 8
CG2O2 CG301 CG331 HGA3	0.2000	3	0.00 ! JZ4 , from CG2O2 CG311 CG331 HGA3, penalty= 8
CG2DC2 CG311 CG331 HGA3	0.1600	3	0.00 ! JZ4 , from CG2DC1 CG321 CG331 HGA3, penalty= 4
CG2DC1 CG321 CG321 CG2DC2	0.9000	1	180.00 ! JZ4 , from CG2D1 CG321 CG321 CG2D1, penalty= 1
CG2DC1 CG321 CG321 CG2DC2	0.3000	3	180.00 ! JZ4 , from CG2D1 CG321 CG321 CG2D1, penalty= 1

CG2DC1 CG321 CG321 CG311 0.1900 3 0.00 ! JZ4 , from CG2DC2 CG321 CG321 CG321, penalty= 0.6

IMPROPERS

CG2O2 CG301 OG2D1 OG311 65.0000 0 0.00 ! JZ4 , from CG2O2 CG311 OG2D1 OG311, penalty= 0.8

Pimaric acid

GROUP	! CHARGE	CH_PENALTY	Z	EL	NB	NBE	RNG1	TYP	RNG2	TYP	RNG3	TYP
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ATOM C1	CG301	0.007 !	13.530	6	C	4	4	6	3	6	4	
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ATOM O1	OG311	-0.561 !	12.422	8	O	2	2					
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ATOM C2	CG311	-0.124 !	13.071	6	C	4	4	6	3	6	4	
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ATOM O2	OG2D1	-0.558 !	7.574	8	O	1	2					
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ATOM C3	CG311	0.037 !	10.293	6	C	4	4	6	4	6	4	
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ATOM C4	CG301	0.116 !	21.513	6	C	4	4	6	3			
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ATOM C5	CG321	-0.182 !	0.902	6	C	4	4	6	3			
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ATOM C6	CG321	-0.205 !	5.622	6	C	4	4	6	4			
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ATOM C7	CG2D1	-0.021 !	9.427	6	C	3	4	6	4	6	4	
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ATOM C8	CG321	-0.277 !	13.030	6	C	4	4	6	3			
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ATOM C9	CG321	-0.188 !	4.781	6	C	4	4	6	3			
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ATOM C10	CG321	-0.186 !	3.402	6	C	4	4	6	4			
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ATOM C11	CG321	-0.161 !	4.356	6	C	4	4	6	4			
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ATOM C12	CG331	-0.269 !	5.705	6	C	4	4					
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ATOM C13	CG321	-0.173 !	5.487	6	C	4	4	6	4			
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ATOM C14	CG301	0.012 !	9.437	6	C	4	4	6	4			
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ATOM C15	CG331	-0.284 !	9.957	6	C	4	4					
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ATOM C16	CG2D1	-0.253 !	10.145	6	C	3	4	6	4			
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ATOM C17	CG2O2	0.840 !	21.878	6	C	3	4					
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ATOM C18	CG331	-0.273 !	5.772	6	C	4	4					
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ATOM C19	CG2D1	-0.168 !	10.389	6	C	3	4					
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ATOM C20	CG2D2	-0.419 !	5.994	6	C	3	4					
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ATOM H1	HGP1	0.290 !	0.845	1	H	1	1					
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ATOM H2	HGA1	0.090 !	0.600	1	H	1	1					
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ATOM H3	HGA1	0.090 !	0.345	1	H	1	1					
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ATOM H4	HGA2	0.090!	0.000	1	H	1	1
ATOM H5	HGA2	0.090!	0.000	1	H	1	1
ATOM H6	HGA2	0.090!	0.000	1	H	1	1
ATOM H7	HGA2	0.090!	0.000	1	H	1	1
ATOM H8	HGA2	0.090!	0.600	1	H	1	1
ATOM H9	HGA2	0.090!	0.600	1	H	1	1
ATOM H10	HGA2	0.090!	0.000	1	H	1	1
ATOM H11	HGA2	0.090!	0.000	1	H	1	1
ATOM H12	HGA2	0.090!	0.000	1	H	1	1
ATOM H13	HGA2	0.090!	0.000	1	H	1	1
ATOM H14	HGA2	0.090!	0.060	1	H	1	1
ATOM H15	HGA2	0.090!	0.060	1	H	1	1
ATOM H16	HGA3	0.090!	0.000	1	H	1	1
ATOM H17	HGA3	0.090!	0.000	1	H	1	1
ATOM H18	HGA3	0.090!	0.000	1	H	1	1
ATOM H19	HGA2	0.090!	0.000	1	H	1	1
ATOM H20	HGA2	0.090!	0.000	1	H	1	1
ATOM H21	HGA3	0.090!	0.600	1	H	1	1
ATOM H22	HGA3	0.090!	0.600	1	H	1	1
ATOM H23	HGA3	0.090!	0.600	1	H	1	1
ATOM H24	HGA4	0.165!	1.221	1	H	1	1
ATOM H25	HGA3	0.090!	0.000	1	H	1	1
ATOM H26	HGA3	0.090!	0.000	1	H	1	1
ATOM H27	HGA3	0.090!	0.000	1	H	1	1
ATOM H28	HGA4	0.165!	1.221	1	H	1	1
ATOM H29	HGA5	0.210!	0.090	1	H	1	1
ATOM H30	HGA5	0.210!	0.090	1	H	1	1
BOND C1	C2	!	1	1			
BOND C1	C5	!	1	1			
BOND C1	C12	!	1	0			

BOND C1 C3 !1 1
BOND O1 H1 !1 0
BOND O1 C17 !1 0
BOND C2 C4 !1 1
BOND C2 C6 !1 1
BOND C2 H2 !1 0
BOND O2 C17 !2 0
BOND C3 C7 !1 1
BOND C3 C10 !1 1
BOND C3 H3 !1 0
BOND C4 C17 !1 0
BOND C4 C15 !1 0
BOND C4 C8 !1 1
BOND C5 C9 !1 1
BOND C5 H4 !1 0
BOND C5 H5 !1 0
BOND C6 C11 !1 1
BOND C6 H6 !1 0
BOND C6 H7 !1 0
BOND C7 C11 !1 1
BOND C7 C16 !2 1
BOND C8 C9 !1 1
BOND C8 H8 !1 0
BOND C8 H9 !1 0
BOND C9 H10 !1 0
BOND C9 H11 !1 0
BOND C10 C13 !1 1
BOND C10 H12 !1 0
BOND C10 H13 !1 0
BOND C11 H14 !1 0

BOND C11 H15 ! 1 0
 BOND C12 H16 ! 1 0
 BOND C12 H17 ! 1 0
 BOND C12 H18 ! 1 0
 BOND C13 C14 ! 1 1
 BOND C13 H19 ! 1 0
 BOND C13 H20 ! 1 0
 BOND C14 C16 ! 1 1
 BOND C14 C19 ! 1 0
 BOND C14 C18 ! 1 0
 BOND C15 H21 ! 1 0
 BOND C15 H22 ! 1 0
 BOND C15 H23 ! 1 0
 BOND C16 H24 ! 1 0
 BOND C18 H25 ! 1 0
 BOND C18 H26 ! 1 0
 BOND C18 H27 ! 1 0
 BOND C19 C20 ! 2 0
 BOND C19 H28 ! 1 0
 BOND C20 H29 ! 1 0
 BOND C20 H30 ! 1 0
 IMPR C17 C4 O2 O1

BONDS

CG202 CG301 200.00 1.5220 ! JZ4 , from CG202 CG311, penalty= 8

ANGLES

CG2D2 CG2D1 CG301 48.00 126.00 ! JZ4 , from CG2D2 CG2D1 CG321, penalty= 1.8

CG301 CG2D1 HGA4 40.00 116.00 ! JZ4 , from CG311 CG2D1 HGA4, penalty= 1.2

CG311 CG2D1 CG321 50.00 113.00 ! JZ4 , from CG301 CG2D1 CG321, penalty= 1.2

CG301 CG202 OG2D1 70.00 125.00 20.00 2.44200 ! JZ4 , from CG311 CG202 OG2D1, penalty= 1.2

CG301 CG202 OG311 55.00 110.50 ! JZ4 , from CG311 CG202 OG311, penalty= 1.2

CG2D1 CG301 CG2D1 30.00 114.00 ! JZ4 , from CG2D1 CG311 CG2D1, penalty= 8
CG2O2 CG301 CG311 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG311, penalty= 8
CG2O2 CG301 CG321 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG321, penalty= 8
CG2O2 CG301 CG331 52.00 108.00 ! JZ4 , from CG2O2 CG311 CG331, penalty= 8
CG2D1 CG311 CG301 32.00 112.20 ! JZ4 , from CG2D1 CG311 CG321, penalty= 1.8
CG301 CG311 CG301 52.00 108.00 ! JZ4 , from CG301 CG311 CG311, penalty= 1.2

DIHEDRALS

CG301 CG2D1 CG2D1 CG311 0.4500 1 180.00 ! JZ4 , from CG301 CG2D1 CG2D1 CG321, penalty= 0.6
CG301 CG2D1 CG2D1 CG311 8.5000 2 180.00 ! JZ4 , from CG301 CG2D1 CG2D1 CG321, penalty= 0.6
CG301 CG2D1 CG2D2 HGA5 5.2000 2 180.00 ! JZ4 , from CG321 CG2D1 CG2D2 HGA5, penalty= 1.8
CG2D1 CG2D1 CG301 CG2D1 1.0000 1 180.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 8
CG2D1 CG2D1 CG301 CG2D1 0.1000 2 0.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 8
CG2D1 CG2D1 CG301 CG2D1 0.3000 3 180.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 8
CG2D2 CG2D1 CG301 CG2D1 1.0000 1 180.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 11.5
CG2D2 CG2D1 CG301 CG2D1 0.1000 2 0.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 11.5
CG2D2 CG2D1 CG301 CG2D1 0.3000 3 180.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG2D1, penalty= 11.5
CG2D2 CG2D1 CG301 CG321 0.5000 1 180.00 ! JZ4 , from CG2D1 CG2D1 CG301 CG321, penalty= 3.5
CG2D2 CG2D1 CG301 CG321 1.3000 3 180.00 ! JZ4 , from CG2D1 CG2D1 CG301 CG321, penalty= 3.5
CG2D2 CG2D1 CG301 CG331 0.5000 1 180.00 ! JZ4 , from CG2D1 CG2D1 CG301 CG331, penalty= 3.5
CG2D2 CG2D1 CG301 CG331 1.3000 3 180.00 ! JZ4 , from CG2D1 CG2D1 CG301 CG331, penalty= 3.5
HGA4 CG2D1 CG301 CG2D1 0.0000 3 0.00 ! JZ4 , from HGA4 CG2D1 CG311 CG2D1, penalty= 8
HGA4 CG2D1 CG301 CG321 0.1200 3 0.00 ! JZ4 , from HGA4 CG2D1 CG311 CG321, penalty= 8
HGA4 CG2D1 CG301 CG331 0.1200 3 0.00 ! JZ4 , from HGA4 CG2D1 CG311 CG321, penalty= 8.9
CG2D1 CG2D1 CG311 CG301 0.6000 1 180.00 ! JZ4 , from CG2D1 CG2D1 CG311 CG321, penalty= 1.8
CG321 CG2D1 CG311 CG301 0.1900 3 0.00 ! JZ4 , from CG331 CG2D1 CG321 CG321, penalty= 6.7
CG321 CG2D1 CG311 CG321 0.1900 3 0.00 ! JZ4 , from CG331 CG2D1 CG321 CG321, penalty= 4.9
CG321 CG2D1 CG311 HGA1 0.1900 3 0.00 ! JZ4 , from CG331 CG2D1 CG321 HGA2, penalty= 4.9
CG311 CG2D1 CG321 CG321 0.1900 3 0.00 ! JZ4 , from CG331 CG2D1 CG321 CG321, penalty= 1.5
CG311 CG2D1 CG321 HGA2 0.0300 3 0.00 ! JZ4 , from CG301 CG2D1 CG321 HGA2, penalty= 1.2
OG2D1 CG2O2 CG301 CG311 0.0500 6 180.00 ! JZ4 , from OG2D1 CG2O2 CG311 CG311, penalty= 8

OG2D1 CG202 CG301 CG321	0.0500	6	180.00 ! JZ4 , from OG2D1 CG202 CG311 CG321, penalty= 8
OG2D1 CG202 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG2D1 CG202 CG311 CG331, penalty= 8
OG311 CG202 CG301 CG311	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG311, penalty= 8
OG311 CG202 CG301 CG321	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8
OG311 CG202 CG301 CG331	0.0500	6	180.00 ! JZ4 , from OG311 CG202 CG311 CG321, penalty= 8.9
CG301 CG202 OG311 HGP1	2.0500	2	180.00 ! JZ4 , from CG311 CG202 OG311 HGP1, penalty= 1.2
CG202 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 9.8
CG202 CG301 CG311 CG321	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 CG321, penalty= 8
CG202 CG301 CG311 HGA1	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG311 HGA1, penalty= 8
CG311 CG301 CG311 CG2D1	0.2000	3	0.00 ! JZ4 , from CG311 CG311 CG321 CG2D1, penalty= 12
CG311 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG311 CG301 CG311 CG311, penalty= 1.2
CG321 CG301 CG311 CG2D1	0.1400	1	180.00 ! JZ4 , from CG2D1 CG311 CG321 CG321, penalty= 12
CG321 CG301 CG311 CG2D1	0.1700	2	0.00 ! JZ4 , from CG2D1 CG311 CG321 CG321, penalty= 12
CG321 CG301 CG311 CG2D1	0.0500	3	180.00 ! JZ4 , from CG2D1 CG311 CG321 CG321, penalty= 12
CG321 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG321 CG301 CG311 CG311, penalty= 1.2
CG331 CG301 CG311 CG2D1	0.1400	1	180.00 ! JZ4 , from CG2D1 CG311 CG321 CG331, penalty= 12
CG331 CG301 CG311 CG2D1	0.1700	2	0.00 ! JZ4 , from CG2D1 CG311 CG321 CG331, penalty= 12
CG331 CG301 CG311 CG2D1	0.0500	3	180.00 ! JZ4 , from CG2D1 CG311 CG321 CG331, penalty= 12
CG331 CG301 CG311 CG301	0.2000	3	0.00 ! JZ4 , from CG331 CG301 CG311 CG311, penalty= 1.2
CG202 CG301 CG321 CG321	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG321 CG321, penalty= 8
CG202 CG301 CG321 HGA2	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG321 HGA2, penalty= 8
CG202 CG301 CG331 HGA3	0.2000	3	0.00 ! JZ4 , from CG202 CG311 CG331 HGA3, penalty= 8
CG2D1 CG321 CG321 CG311	0.1400	1	180.00 ! JZ4 , from CG2D1 CG321 CG321 CG321, penalty= 0.6
CG2D1 CG321 CG321 CG311	0.1700	2	0.00 ! JZ4 , from CG2D1 CG321 CG321 CG321, penalty= 0.6
CG2D1 CG321 CG321 CG311	0.0500	3	180.00 ! JZ4 , from CG2D1 CG321 CG321 CG321, penalty= 0.6
IMPROPER			
CG202 CG301 OG2D1 OG311	65.0000	0	0.00 ! JZ4 , from CG202 CG311 OG2D1 OG311, penalty= 0.8