Supporting Information

Configurational and Conformational Study of (−)-Oseltamivir Using a Multi-Chiroptical Approach

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Table S1. A complete overview of the conformational search for the (−)-Oseltamivir. Conformer populations were calculated using the Gibbs free energy Δ*G* (kcal/mol) at the B3LYP/aug-cc-pVDZ level of theory using PCM model for chloroform, acetonitrile and water. Boltzmann weights are based on the Δ*G* at 298 K. The accuracy of molar fractions of particular conformers is far less than the number of decimal places given in the table. This accuracy, however, is kept to show the relative trend of the conformational composition.

B3LYP/aug-cc-pVDZ								
in $CHCl_3$ (ε = 4.71)			**in CH_3CN (ε = 35.69)**			**in H_2O (ε = 78.36)**		
	Δ*G*	*P*(%)		Δ*G*	*P*(%)		Δ*G*	*P*(%)
Conf. 1	0.00	9.98	**Conf. 5**	0.00	16.98	**Conf. 5**	0.00	16.65
Conf. 2	0.01	9.74	**Conf. 4**	0.14	13.45	**Conf. 4**	0.10	14.12
Conf. 3	0.08	8.67	**Conf. 10**	0.27	10.72	**Conf. 10**	0.24	11.01
Conf. 4	0.22	6.90	**Conf. 12**	0.30	10.21	**Conf. 12**	0.28	10.46
Conf. 5	0.24	6.66	**Conf. 9**	0.37	9.15	**Conf.9**	0.29	10.25
Conf. 6	0.28	6.22	**Conf. 1**	0.41	8.46	**Conf. 1**	0.49	7.34
Conf. 7	0.28	6.18	**Conf. 14**	0.47	7.64	**Conf. 14**	0.49	7.27
Conf. 8	0.30	6.05	**Conf. 8**	0.54	6.86	**Conf. 8**	0.61	5.94
Conf. 9	0.33	5.68	**Conf. 17**	0.83	4.17	**Conf. 17**	0.82	4.14
Conf. 10	0.48	4.42	**Conf. 13**	0.89	3.76	**Conf. 13**	0.85	3.95
Conf. 11	0.48	4.41	**Conf. 7**	1.37	1.68	**Conf. 20**	1.10	2.60
Conf. 12	0.54	4.01	**Conf. 2**	1.54	1.25	**Conf. 22**	1.59	1.13
Conf. 13	0.69	3.12	**Conf. 3**	1.56	1.21	**Conf.7**	1.65	1.02
Conf. 14	0.74	2.84	**Conf. 22**	1.57	1.20	**Conf. 2**	1.73	0.90
Conf. 15	0.75	2.83	**Conf. 6**	1.81	0.80	**Conf. 3**	1.77	0.83
Conf. 16	0.80	2.57	**Conf. 11**	1.88	0.71	**Conf. 6**	1.99	0.58
Conf. 17	0.81	2.55	**Conf. 16**	2.10	0.49	**Conf. 11**	2.03	0.54
Conf. 18	1.12	1.50	**Conf. 15**	2.23	0.39	**Conf. 16**	2.31	0.34
Conf. 19	1.12	1.51	**Conf. 19**	2.44	0.28	**Conf. 15**	2.39	0.29
Conf. 20	1.13	1.47	**Conf. 24**	2.60	0.21	**Conf. 19**	2.60	0.20
Conf. 21	1.46	0.85	**Conf. 18**	2.62	0.20	**Conf. 24**	2.71	0.17
Conf. 22	1.63	0.64	**Conf. 23**	2.99	0.11	**Conf. 18**	2.81	0.14
Conf. 23	1.65	0.61	**Conf. 21**	3.10	0.09	**Conf. 23**	3.14	0.08
Conf. 24	1.69	0.57	**Conf. 20**	14.50	0.00	**Conf. 21**	3.36	0.06

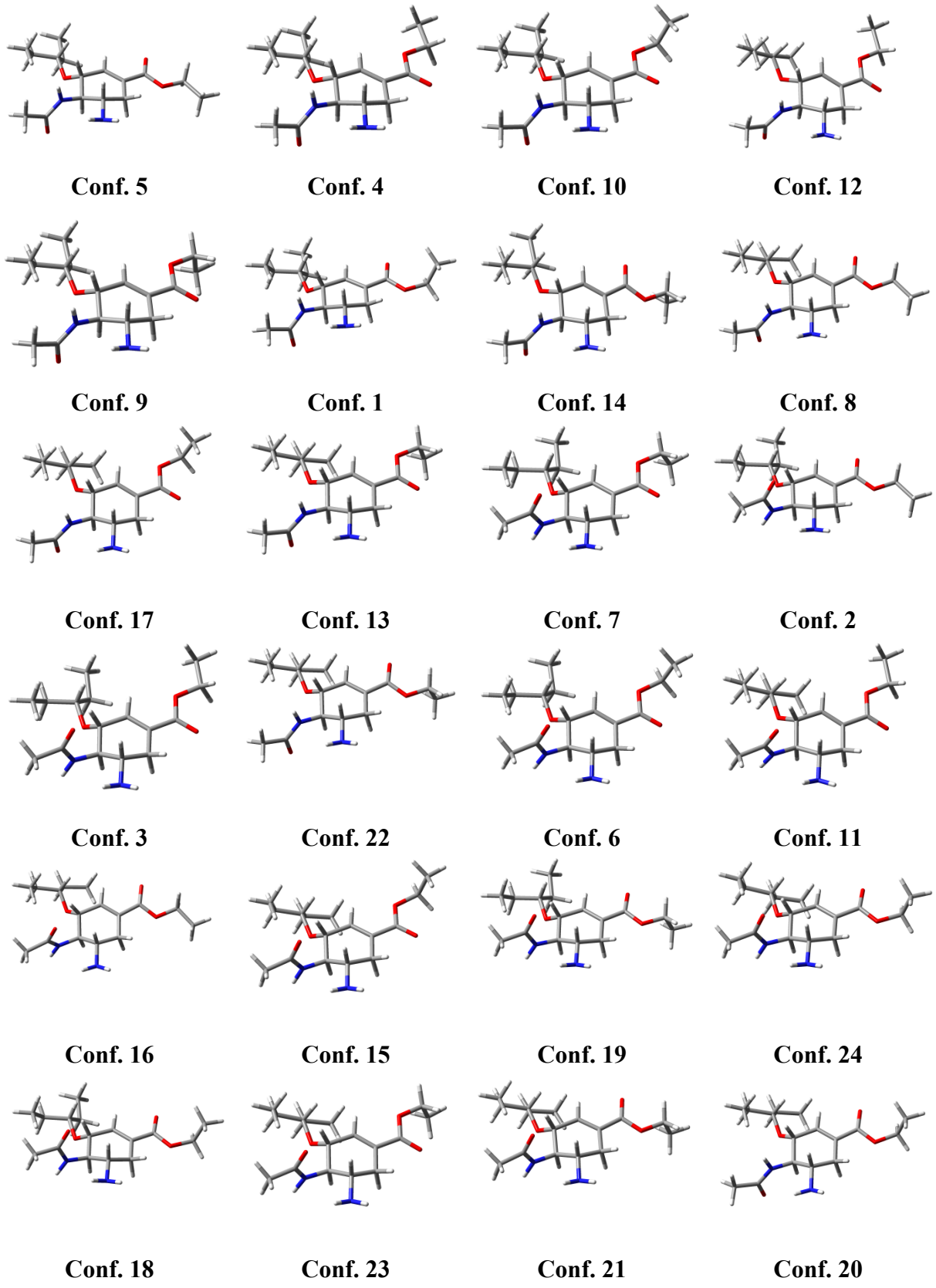


Fig. S1. Structure of conformers of (–)-Oseltamivir calculated at the B3LYP/aug-cc-pVDZ level using PCM model for acetonitrile.

Low-temperature ECD measurements

were carried out by using an Optistat Oxford optical spectroscopy cryostat attached to the sample chamber of the Jasco J-815 ECD spectrometer, in the temperature range of 298–93 K in a solution of MI_{13} (methylcyclohexane-isopentane, 1:3, by vol.). A solution with a concentration of 6.3×10^{-5} M was measured using aforementioned measurement parameters in the range 220-400 nm in a 1 cm quartz cell. Baseline correction was done by subtracting the spectrum of a reference sample of MI_{13} obtained under the same parameters and conditions. All spectra were then normalised to Δε using the volume correction for MI_{13}.

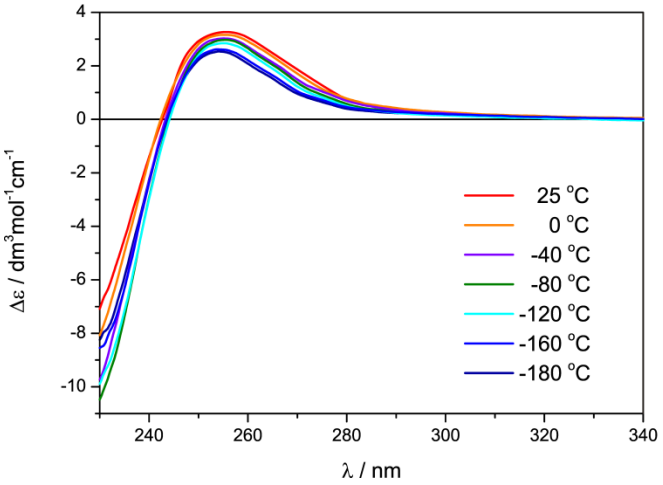


Fig. S2. Low-temperature ECD measurements of (–)-Oseltamivir recorded in MI_{13} (methylcyclohexane : isopentane = 1 : 3, *v*/*v*) as a solvent.

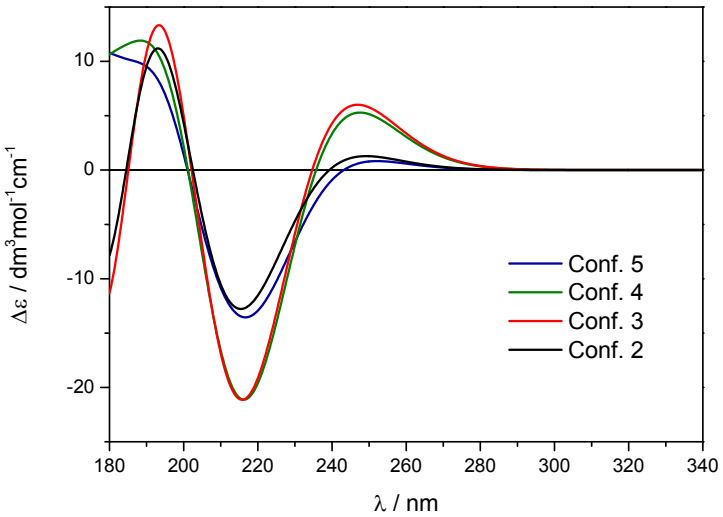


Fig. S3. Comparison of computed ECD spectra at the CAM-B3LYP/aug-cc-pVDZ/PCM(CH_3CN) level of theory for the selected representative conformers of (–)-Oseltamivir.

Table S2. Overview of calculated excited-state properties of conformer **Conf. 5** of (–)-Oseltamivir at the CAM-B3LYP/aug-cc-pVDZ/PCM(CH_3CN) level of theory.

Ex. No	λ / nm	f_{vel}	$R_{vel} \times 10^{-40}$ / cgs	θ / deg	Transition (MO→MO*)[a]	Population / %
1	240.5	0.0020	+5.5	71.3	80→86	79
2	219.5	0.4250	-31.6	98.7	84→86	76
3	212.7	0.0153	-1.3	102.2	83→86	52
4	212.0	0.0013	-0.4	91.1	81→105	10
5	203.8	0.0197	-27.0	144.9	85→86	79
6	197.8	0.0109	+30.2	54.1	85→87	35
7	190.0	0.0048	+4.2	56.3	81→86	30
8	181.5	0.0207	+19.2	49.1	84→87	17
9	180.3	0.0307	-3.3	93.6	81→87	12

[a] main molecular orbitals involved in the first nine transitions. Note: f_{vel} - oscillator strength in velocity formalism, R_{vel} – rotatory strength in velocity formalism, θ - angle between electric (μ_e) and magnetic (μ_m) transition dipole moments.

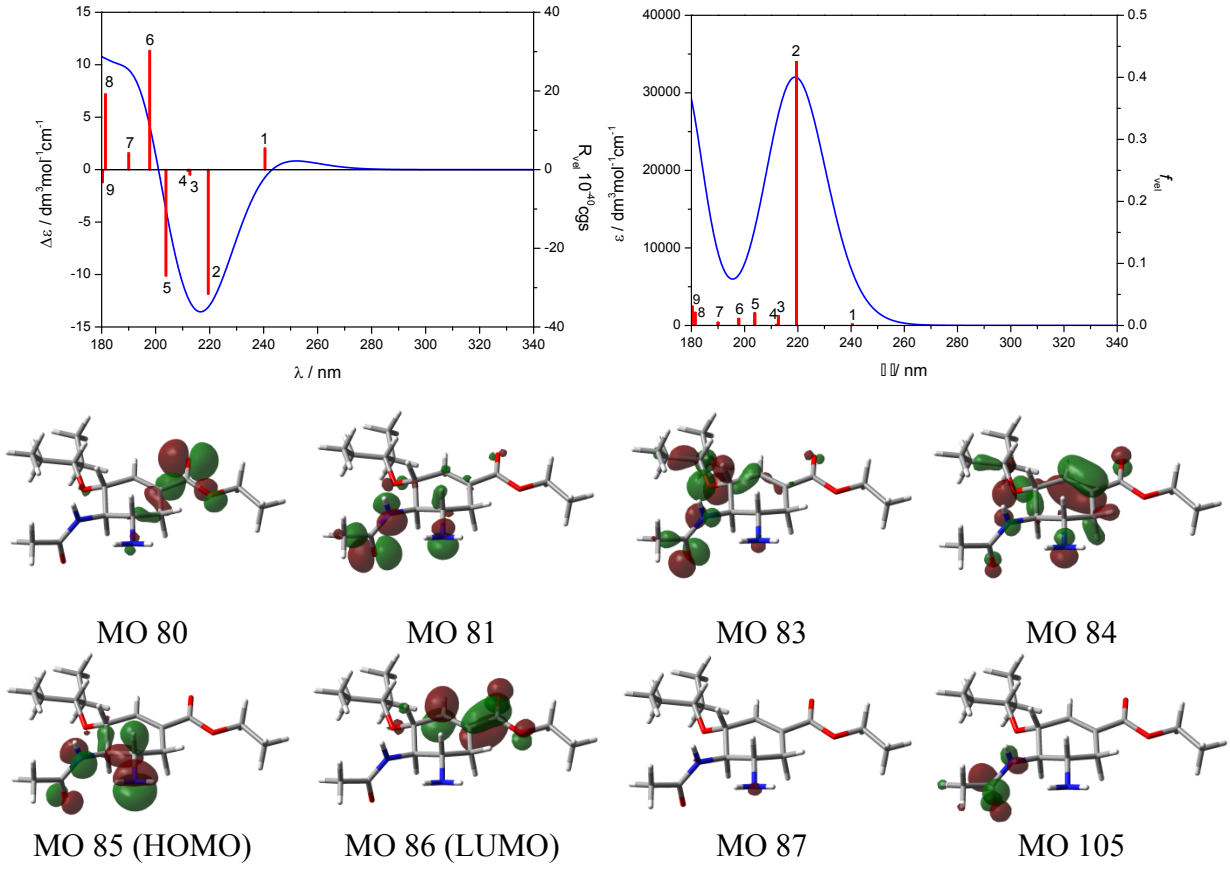


Fig. S4. Simulated ECD and UV spectra of conformer **Conf. 5** of (–)-Oseltamivir at the CAM-B3LYP/aug-cc-pVDZ/PCM(CH_3CN) level of theory with molecular orbitals involved in the key transitions.

Table S3. Comparison of the experimental and calculated[a] specific ORD values[b] of (–)-Oseltamivir using PCM solvation model for CH_3CN and CHCl3 at B3LYP/aug-cc-pVDZ and CAM-B3LYP/aug-cc-pVDZ level.

	[α] / deg cm^2 g^{-1}					
	633 nm	589 nm	574 nm	546 nm	436 nm	405 nm
exp. in CH_3CN	**-38**	**-44**	**-47**	**-54**	**-88**	**-105**
B3LYP/aug-cc-pVDZ/PCM(CH_3CN)	-29	-35	-36	-42	-75	-91
CAM-B3LYP/aug-cc-pVDZ/PCM(CH_3CN)	-24	-28	-29	-34	-61	-76
exp. in $CHCl_3$	**-57**	**-64**	**-67**	**-76**	**-157**	**-209**
B3LYP/aug-cc-pVDZ/PCM($CHCl_3$)	-51	-61	-64	-73	-129	-158
CAM-B3LYP/aug-cc-pVDZ/PCM($CHCl_3$)	-40	-47	-49	-56	-98	-119

[a] Boltzmann-weighted [b] value of specific optical rotations are given in deg cm^2 g^{-1}

Table S4. Vibrational analysis for the lowest energy conformer (**Conf. 5**) of (–)-Oseltamivir in the range of 1800-1060 cm^{-1}.

Band No.	Exp. freq.[a] / cm^{-1}	Calc. freq.[b] / cm^{-1}	Mode assignment [c]	ζ-ratio[d] / ppm
1	1068	1069	C-O stretching within 3-pentyl moiety	12
2	1115	1118	C-N stretching within amide moiety, H-C-C and C-C-C bending within 3-pentyl moiety	23
3	1157	1148	C-C stretching mods within ring	67
4	1203	1205	C-C-H bending within ring	31
5	1227	1239	C-N-H bending including NH_2 moiety, C-O stretching within ester moiety	13
6	1242	1257	C-C-H bending within 3-pentyl moiety	24
7	1271	1272	C-N-H bending and C-C stretching within amide moiety	66
8	1290	1293	C-C-H bending within 3-pentyl moiety	374
9	1323	1339	H-C-O bending and H-C-C and C-C-C bending 3-pentyl moiety	89
10	1360	1371	C=C-H bending, C-C-H bending within ester moiety	102
11	1379	1380	C-H bending mods within 3-pentyl moiety	120
12	1439	1414	H-N-C and N-C-H bending including NH_2 moiety	115
13	1487	1475	C-H bending mods within 3-pentyl moiety	41
14	1535	1550	H-N-C bending within amide moiety	0
15	1593[e]	1627	NH_2 bending	19
16	1652	1677	C=O stretching within amide moiety	36
17	1678	1691	C=C stretching, C=O stretching within ester moiety	67
18	1710	1723	C=C stretching, C=O stretching within ester moiety	24

[a] In CH_3CN

[b] B3LYP/aug-cc-pVDZ/PCM(CH_3CN)

[c] Using VEDA 4 software (M. H. Jamróz, 2004-2010, Warsaw.)

[d] Ratio between the rotational and dipole strength (*R* and *D*) of the mode, *R* and *D* values are given in the Supporting Information (Table S2)

[e] Band observed exclusively in $CDCl_3$

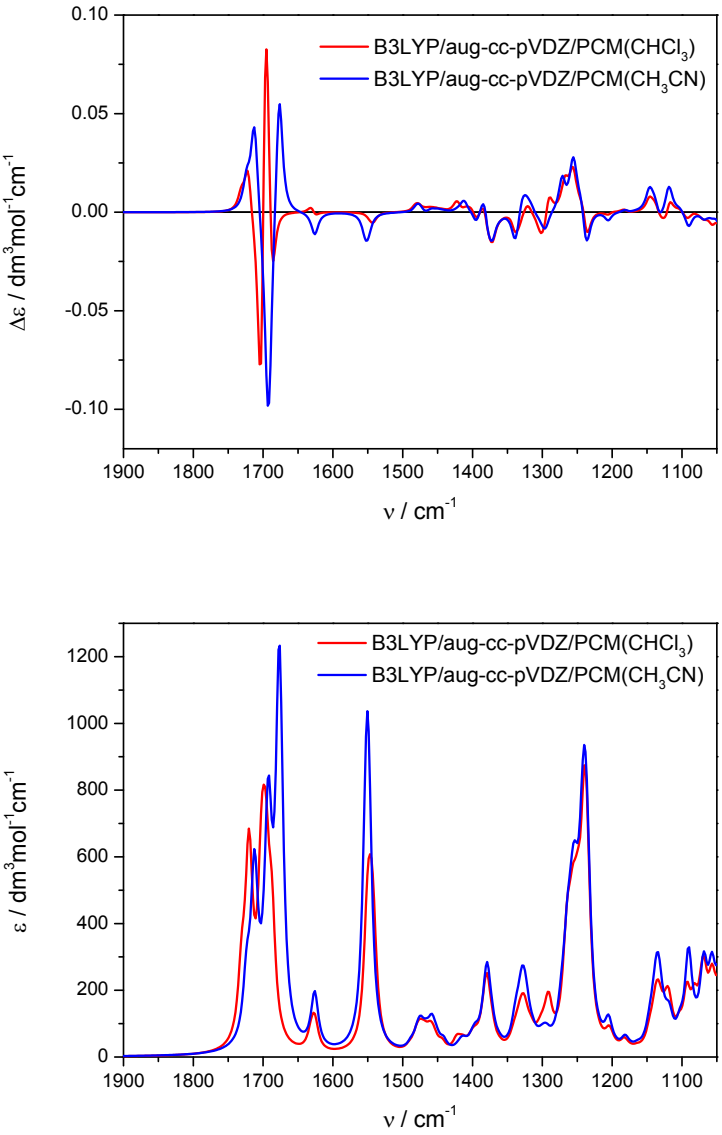


Fig. S5. Calculated VCD (top) and IR (bottom) spectra at the B3LYP/aug-cc-pVDZ level of theory using PCM model for chloroform and acetonitrile. Spectra were obtained as a population-weighted sum of the calculated spectra of individual conformers of (–)-Oseltamivir.

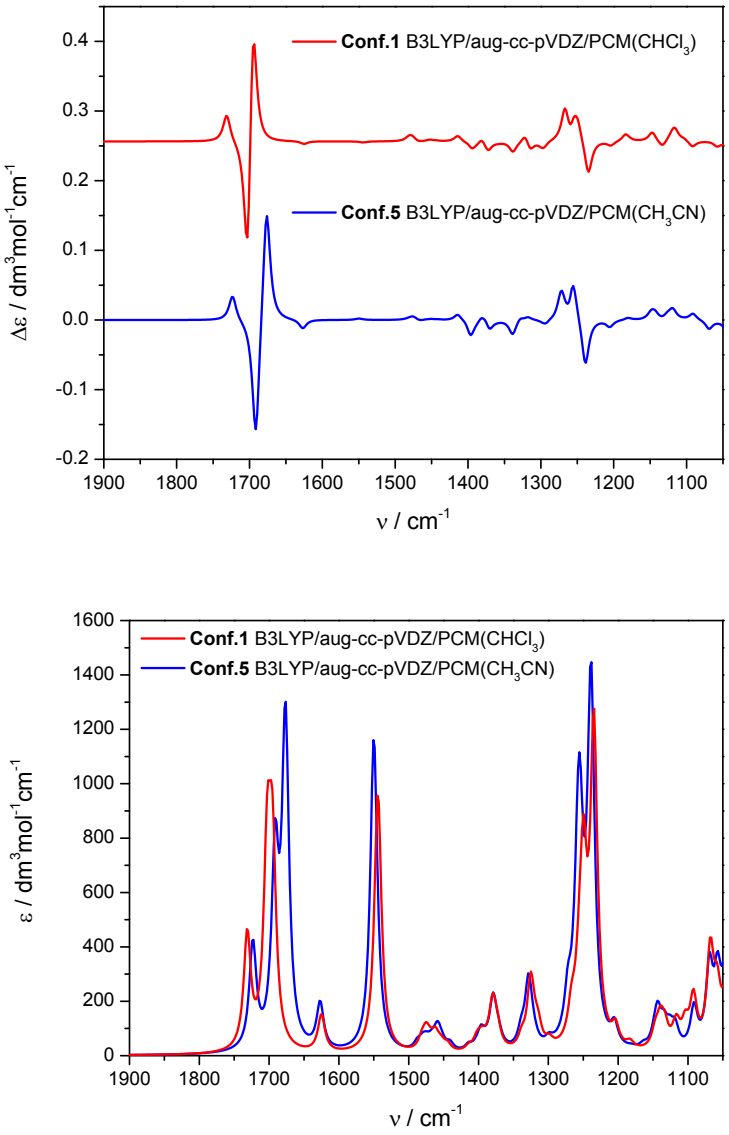
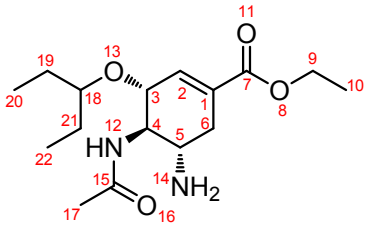


Fig. S6. Calculated VCD (top) and IR (bottom) spectra of (–)-Oseltamivir at the B3LYP/aug-cc-pVDZ level of theory using PCM model for chloroform and acetonitrile for the most abundant conformers (*i.e.* **Conf.1** in chloroform and **Conf. 5** in acetonitrile).

Table S5. Selected torsion angles (°) of (–)-Oseltamivir Phosphate determined by the X-ray diffraction data (Cambridge Crystallographic Data Centre, No CCDC 914529) compared with values calculated for the lowest energy conformer **Conf. 5** of (–)-Oseltamivir at the B3LYP/aug-cc-pVDZ(H_2O) method.



	C5-C4-N12-C15	C2-C1-C7-O11	C7-O8-C9-C10	O13-C18-C19-C20	C1-C2-C3-C4	C2-C3-C4-C5	C3-C4-C5-C6	C4-C5-C6-C7	C4-C5-C6-C1	C5-C6-C1-C2
X-Ray: Mol. A	-126.28	-6.51	-176.20	-62.78	-18.22	+47.85	-62.74	+44.06	-13.12	-0.09
X-Ray: Mol. B	-102.30	-7.61	+172.37	-176.14	-14.76	+47.81	-68.61	+50.38	-15.26	-2.69
DFT: Conf. 5	-120.82	3.36	+179.05	-172.03	-13.79	+44.01	-61.39	+46.10	-15.74	-0.84

Cartesian coordinates of all calculated conformers at the B3LYP/aug-cc-pVDZ level of theory using PCM model for acetonitrile.

Conf. 5

C	0.690663	-1.329930	0.013194
C	0.678891	0.136358	-0.453128
C	-0.707139	0.728664	-0.406797
C	-1.833994	0.011043	-0.267232
C	-1.824330	-1.494099	-0.158880
C	-0.489869	-2.103261	-0.605230
C	-3.128637	0.756187	-0.194055
O	-4.169231	-0.068095	0.025748
C	-5.484633	0.546778	0.127789
C	-6.492587	-0.562113	0.349500
O	-3.249579	1.966707	-0.309542
N	1.965357	-1.963711	-0.302703
O	1.582957	0.857699	0.388008
N	-0.442454	-3.509114	-0.179277
C	2.848850	-2.426543	0.622522
O	2.639531	-2.371708	1.840267
C	4.123657	-3.031843	0.069315
C	1.985964	2.174672	-0.066153
C	1.528384	3.200336	0.979105
C	1.710657	4.661490	0.552230
C	3.500056	2.177814	-0.292079
C	3.969116	1.267719	-1.430326
H	2.229347	-2.031405	-1.276794
H	0.392931	-3.957927	-0.548730
H	-1.231760	-4.013207	-0.579362
H	0.600904	-1.352232	1.104927
H	1.044200	0.182698	-1.495278
H	-0.785359	1.812366	-0.483418
H	-2.026342	-1.798650	0.880169

H	-2.637246	-1.918337	-0.762549
H	-0.418388	-2.002437	-1.705512
H	-5.678262	1.100720	-0.798989
H	-5.466837	1.260191	0.960997
H	-6.280734	-1.109632	1.277248
H	-6.491281	-1.270175	-0.489529
H	-7.496408	-0.124046	0.429414
H	4.980527	-2.483907	0.481075
H	4.196597	-4.071907	0.411587
H	4.175848	-3.010459	-1.025305
H	1.481614	2.387826	-1.023151
H	2.071100	3.007932	1.917369
H	0.466425	3.014438	1.190090
H	1.271368	5.335796	1.299696
H	1.211844	4.858145	-0.408380
H	2.768969	4.933602	0.445098
H	3.983883	1.885470	0.652406
H	3.814880	3.209556	-0.502086
H	3.709615	0.219434	-1.236343
H	5.059436	1.325915	-1.548865
H	3.513093	1.563562	-2.386425

Conf. 4

C	1.315151	-1.176237	0.038836
C	0.527369	0.065399	-0.412908
C	-0.964650	-0.139030	-0.302870
C	-1.550068	-1.333102	-0.108460
C	-0.757647	-2.611286	0.005380
C	0.671777	-2.458864	-0.522990
C	-3.029840	-1.458161	0.034831
O	-3.693893	-0.299513	-0.126079
C	-5.140774	-0.348031	0.019737
C	-5.670936	1.051113	-0.217858
O	-3.587621	-2.518220	0.281026
N	2.717190	-1.068461	-0.347276
O	0.965057	1.162516	0.393821
N	1.459702	-3.631191	-0.117722
C	3.757512	-1.015088	0.527900
O	3.609697	-1.070781	1.754629
C	5.133531	-0.887237	-0.094860
C	0.607258	2.491725	-0.062274
C	-0.284759	3.140681	1.004584
C	-0.917609	4.469613	0.575622
C	1.888988	3.282067	-0.336490
C	2.731931	2.734032	-1.490947
H	2.931160	-0.995596	-1.333269
H	2.385684	-3.591438	-0.538172
H	1.022988	-4.476825	-0.480112
H	1.303549	-1.220885	1.133545
H	0.770922	0.278867	-1.469777
H	-1.583821	0.751813	-0.385751
H	-0.720029	-2.938504	1.056631
H	-1.271218	-3.412897	-0.542105
H	0.620273	-2.355769	-1.624001
H	-5.374143	-0.710371	1.028705
H	-5.537623	-1.067064	-0.707532
H	-5.421269	1.401471	-1.227952
H	-5.262262	1.758559	0.515441
H	-6.764366	1.042830	-0.116572
H	5.607719	0.026671	0.284681

H	5.745889	-1.739252	0.226328
H	5.112976	-0.853224	-1.190236
H	0.036719	2.400277	-1.001244
H	0.311569	3.281491	1.919079
H	-1.080138	2.427201	1.259137
H	-1.613408	4.828209	1.346104
H	-1.486078	4.353165	-0.358969
H	-0.167183	5.255556	0.418582
H	2.481216	3.300710	0.591249
H	1.610818	4.322779	-0.553893
H	3.064977	1.708237	-1.289165
H	3.626389	3.352342	-1.645252
H	2.161120	2.731627	-2.431056

Conf. 10

C	-1.173939	-1.249686	-0.052664
C	-0.528872	0.080506	0.373296
C	0.971104	0.062209	0.200940
C	1.691713	-1.050477	-0.019332
C	1.061382	-2.417777	-0.098752
C	-0.356345	-2.441668	0.481797
C	3.169997	-0.992760	-0.217001
O	3.677437	0.253178	-0.153215
C	5.115847	0.404183	-0.322321
C	5.844176	0.266068	1.003931
O	3.850319	-1.986420	-0.427590
N	-2.562944	-1.316289	0.386637
O	-1.128311	1.117220	-0.409356
N	-1.007590	-3.703021	0.102076
C	-3.634971	-1.391044	-0.447632
O	-3.528712	-1.432487	-1.679170
C	-4.991528	-1.426283	0.227598
C	-0.931186	2.477937	0.051835
C	-0.176303	3.248548	-1.038940
C	0.281736	4.650135	-0.618896
C	-2.293465	3.088968	0.390207
C	-3.005811	2.425451	1.571683
H	-2.745791	-1.275428	1.380610
H	-1.916137	-3.776675	0.554777
H	-0.457831	-4.487841	0.447035
H	-1.197839	-1.295089	-1.147135
H	-0.754226	0.261458	1.440164
H	1.478147	1.022992	0.258921
H	1.025474	-2.755012	-1.147024
H	1.690992	-3.144656	0.431363
H	-0.278103	-2.331042	1.580706
H	5.228511	1.411134	-0.737580
H	5.462692	-0.332941	-1.053654
H	5.724909	-0.742628	1.418629
H	5.473926	0.999023	1.732585
H	6.916193	0.448586	0.845953
H	-5.585895	-0.577663	-0.133957
H	-5.509424	-2.347107	-0.068882
H	-4.933401	-1.383695	1.321271
H	-0.315723	2.454962	0.966375
H	-0.818126	3.309913	-1.931119
H	0.700413	2.652234	-1.326467
H	0.896326	5.104307	-1.407783
H	0.890608	4.609272	0.296454
H	-0.564437	5.324302	-0.431419

H	-2.923045	3.036581	-0.511219
H	-2.145983	4.155419	0.610591
H	-3.219537	1.369008	1.367010
H	-3.961310	2.925870	1.778609
H	-2.394723	2.482097	2.484338

Conf. 12

C	1.303547	-1.097262	0.050737
C	0.539993	0.146148	-0.438357
C	-0.954721	-0.040123	-0.344472
C	-1.557008	-1.226039	-0.151528
C	-0.783009	-2.513457	-0.017189
C	0.661388	-2.381398	-0.509315
C	-3.039165	-1.331084	-0.021667
O	-3.687302	-0.166147	-0.202403
C	-5.135474	-0.194485	-0.065929
C	-5.646680	1.207736	-0.326017
O	-3.612788	-2.381166	0.231354
N	2.716376	-1.012509	-0.299114
O	0.973019	1.251497	0.362110
N	1.425851	-3.555598	-0.065799
C	3.732424	-0.940896	0.602877
O	3.549250	-0.953465	1.825985
C	5.126638	-0.847620	0.015658
C	0.708386	2.585273	-0.138993
C	0.171326	3.423633	1.026370
C	-1.179455	2.967826	1.581770
C	1.979588	3.209396	-0.727344
C	2.531595	2.529491	-1.983618
H	2.960045	-0.987510	-1.280383
H	2.361210	-3.535947	-0.466293
H	0.985855	-4.402466	-0.421233
H	1.263342	-1.124807	1.145323
H	0.801012	0.334413	-1.493982
H	-1.560060	0.859193	-0.431171
H	-0.775375	-2.837971	1.035598
H	-1.292629	-3.310750	-0.574824
H	0.640552	-2.293995	-1.612750
H	-5.380269	-0.539760	0.946309
H	-5.536756	-0.918397	-0.785834
H	-5.386755	1.540906	-1.339262
H	-5.233372	1.920033	0.399923
H	-6.740721	1.214397	-0.231292
H	5.597230	0.077366	0.372333
H	5.722612	-1.690390	0.387865
H	5.137615	-0.856648	-1.080405
H	-0.059875	2.523863	-0.927080
H	0.092291	4.464996	0.681833
H	0.927680	3.413974	1.826109
H	-1.491407	3.615298	2.412459
H	-1.132246	1.938031	1.958447
H	-1.963571	3.015957	0.811898
H	2.748610	3.226950	0.059842
H	1.746810	4.258733	-0.962964
H	2.870059	1.506754	-1.776998
H	3.393945	3.087555	-2.372645
H	1.774908	2.488389	-2.780689

Conf. 9

C	1.191520	-1.238130	0.039671

C	0.553592	0.065820	-0.469973
C	-0.954880	0.002551	-0.454669
C	-1.660692	-1.129203	-0.290581
C	-1.001082	-2.473902	-0.117484
C	0.467853	-2.462736	-0.552411
C	-3.151693	-1.113943	-0.234096
O	-3.691445	0.097867	-0.467113
C	-5.140056	0.217494	-0.379232
C	-5.582570	0.509808	1.044664
O	-3.815999	-2.112564	0.002572
N	2.618741	-1.267501	-0.258134
O	1.038928	1.127962	0.356118
N	1.114765	-3.697289	-0.086891
C	3.603066	-1.285762	0.680908
O	3.373778	-1.302781	1.896246
C	5.021351	-1.290376	0.146295
C	0.851453	2.478013	-0.138344
C	-0.050792	3.230665	0.849009
C	-0.500465	4.614182	0.364857
C	2.223502	3.132520	-0.318253
C	3.092934	2.486133	-1.399913
H	2.898605	-1.236663	-1.229645
H	2.066874	-3.747586	-0.442884
H	0.627468	-4.503699	-0.473409
H	1.108328	-1.267433	1.131775
H	0.883124	0.242326	-1.510083
H	-1.481755	0.946111	-0.579977
H	-1.061861	-2.789833	0.936138
H	-1.551101	-3.231098	-0.692075
H	0.498185	-2.370645	-1.655271
H	-5.592343	-0.702448	-0.763641
H	-5.377391	1.049089	-1.050913
H	-5.108904	1.425415	1.422067
H	-5.336298	-0.322782	1.715280
H	-6.671794	0.653567	1.060195
H	5.550249	-0.416073	0.546233
H	5.533877	-2.188066	0.514473
H	5.072925	-1.271543	-0.948503
H	0.348951	2.428235	-1.118586
H	0.480239	3.318302	1.809211
H	-0.936283	2.609225	1.039284
H	-1.219149	5.051347	1.071077
H	-0.994434	4.549077	-0.615961
H	0.339503	5.315333	0.273872
H	2.741858	3.106172	0.652467
H	2.069005	4.192221	-0.564724
H	3.311410	1.437502	-1.162401
H	4.050958	3.014809	-1.494183
H	2.594862	2.519991	-2.379915

Conf. 1

C	0.802019	-1.323175	0.052210
C	0.635205	0.133360	-0.413833
C	-0.793739	0.604087	-0.297288
C	-1.843471	-0.205050	-0.078386
C	-1.694981	-1.701072	0.050793
C	-0.347031	-2.199131	-0.482188
C	-3.193062	0.424930	0.060792
O	-4.132748	-0.484360	0.385354
C	-5.501243	-0.013516	0.551763

C	-6.251039	-0.028286	-0.769655
O	-3.429056	1.614629	-0.084876
N	2.101857	-1.849932	-0.348640
O	1.514682	0.935706	0.379463
N	-0.151003	-3.592087	-0.056556
C	3.076124	-2.244807	0.515055
O	2.941759	-2.209619	1.744082
C	4.356322	-2.746670	-0.122818
C	1.774104	2.282107	-0.092108
C	1.252824	3.269735	0.960326
C	1.259187	4.734758	0.508479
C	3.273421	2.428390	-0.364425
C	3.791150	1.564569	-1.517474
H	2.305272	-1.899735	-1.338401
H	0.693528	-3.970526	-0.480018
H	-0.918836	-4.165003	-0.402056
H	0.789061	-1.345022	1.147536
H	0.941451	0.207933	-1.473259
H	-0.971271	1.674871	-0.389613
H	-1.797600	-2.002416	1.105206
H	-2.507144	-2.205377	-0.488844
H	-0.358604	-2.101846	-1.584795
H	-5.475478	0.987965	0.993084
H	-5.937604	-0.717986	1.267498
H	-6.249725	-1.034120	-1.209527
H	-5.808068	0.675965	-1.484690
H	-7.294023	0.269305	-0.594005
H	5.194581	-2.146056	0.251927
H	4.522712	-3.784853	0.191545
H	4.343293	-2.702028	-1.217910
H	1.224540	2.437285	-1.035213
H	1.851393	3.151834	1.876629
H	0.226617	2.975883	1.219471
H	0.789409	5.371863	1.269925
H	0.694810	4.861995	-0.427152
H	2.276248	5.114384	0.343509
H	3.812084	2.186036	0.564406
H	3.481584	3.485036	-0.583217
H	3.644227	0.496488	-1.313797
H	4.865384	1.730718	-1.674550
H	3.274333	1.809319	-2.456958

Conf. 14

C	0.809205	-1.325252	-0.008460
C	0.657628	0.125227	-0.497777
C	-0.787187	0.559399	-0.524556
C	-1.832239	-0.278930	-0.425538
C	-1.659409	-1.772428	-0.293985
C	-0.246185	-2.231141	-0.671254
C	-3.204656	0.315865	-0.419099
O	-4.149489	-0.620903	-0.207310
C	-5.536300	-0.179719	-0.142987
C	-5.918035	0.226731	1.270500
O	-3.455277	1.500599	-0.579967
N	2.160655	-1.816862	-0.251455
O	1.435268	0.951901	0.372566
N	-0.060657	-3.619400	-0.226393
C	3.037671	-2.179739	0.723352
O	2.756033	-2.151335	1.927318
C	4.400627	-2.637271	0.243353

C	1.703286	2.303733	-0.078820
C	1.075970	3.276741	0.928233
C	1.106564	4.745907	0.491095
C	3.215704	2.484637	-0.230960
C	3.845128	1.627901	-1.332571
H	2.485165	-1.852669	-1.208758
H	0.839800	-3.970168	-0.545684
H	-0.764050	-4.213883	-0.661049
H	0.668321	-1.346635	1.077944
H	1.064355	0.201649	-1.522719
H	-0.982005	1.626635	-0.621609
H	-1.873603	-2.087671	0.739399
H	-2.390982	-2.291300	-0.927176
H	-0.134594	-2.130524	-1.768185
H	-6.107147	-1.052489	-0.476661
H	-5.674865	0.642021	-0.852941
H	-5.340063	1.098194	1.602097
H	-5.754465	-0.600326	1.973578
H	-6.984146	0.491909	1.292206
H	5.167628	-2.007208	0.710915
H	4.564869	-3.668723	0.580092
H	4.514415	-2.593684	-0.845955
H	1.226998	2.448346	-1.062677
H	1.588835	3.156941	1.894874
H	0.033660	2.969418	1.089045
H	0.556409	5.369557	1.208569
H	0.634264	4.875656	-0.493960
H	2.129674	5.139687	0.429377
H	3.684120	2.260346	0.739540
H	3.415415	3.544839	-0.439909
H	3.708094	0.557703	-1.133454
H	4.924301	1.819235	-1.403358
H	3.400704	1.854911	-2.312620

Conf. 8

C	0.815276	-1.201044	0.040265
C	0.723583	0.245174	-0.479504
C	-0.695311	0.755616	-0.458017
C	-1.779561	-0.023486	-0.309881
C	-1.683486	-1.521555	-0.157550
C	-0.308699	-2.063607	-0.565354
C	-3.116595	0.644428	-0.267651
O	-4.107963	-0.234981	-0.032448
C	-5.458506	0.302111	0.041970
C	-6.401072	-0.858652	0.284733
O	-3.309518	1.841640	-0.418644
N	2.127861	-1.773369	-0.235512
O	1.573549	1.048424	0.346420
N	-0.184394	-3.449235	-0.091127
C	3.025467	-2.145476	0.716819
O	2.801787	-2.045898	1.929087
C	4.337378	-2.702490	0.200841
C	1.970493	2.345729	-0.163107
C	1.840039	3.354614	0.982805
C	0.412082	3.583970	1.482359
C	3.406065	2.305334	-0.701807
C	3.626765	1.420485	-1.931709
H	2.399452	-1.886781	-1.203078
H	0.682077	-3.859241	-0.432767
H	-0.936001	-4.012720	-0.484443

H	0.711449	-1.188661	1.131034
H	1.089031	0.274691	-1.520274
H	-0.835215	1.830584	-0.559022
H	-1.883826	-1.807058	0.887277
H	-2.460003	-2.011094	-0.759821
H	-0.226680	-1.995337	-1.667393
H	-5.675508	0.819049	-0.900863
H	-5.491771	1.037036	0.855839
H	-6.166048	-1.368700	1.228136
H	-6.350324	-1.586789	-0.535404
H	-7.429794	-0.479106	0.345292
H	5.156845	-2.078276	0.579148
H	4.474269	-3.713608	0.604439
H	4.392343	-2.742185	-0.893115
H	1.287667	2.631619	-0.979918
H	2.264760	4.309133	0.639615
H	2.476099	3.007493	1.811512
H	0.404815	4.314461	2.302714
H	-0.037219	2.654819	1.856006
H	-0.231135	3.977995	0.681866
H	4.069856	1.984984	0.115606
H	3.689113	3.339285	-0.950233
H	3.449856	0.361793	-1.705862
H	4.661868	1.511188	-2.287820
H	2.963406	1.713275	-2.758588

Conf. 17

C	-1.192522	-1.145067	-0.071012
C	-0.546185	0.171748	0.396216
C	0.953882	0.150548	0.231064
C	1.672258	-0.961711	0.001279
C	1.038150	-2.324837	-0.111763
C	-0.389319	-2.355083	0.443955
C	3.152286	-0.907476	-0.180653
O	3.669554	0.330400	-0.060917
C	5.111457	0.473778	-0.205422
C	5.821844	0.264064	1.121281
O	3.827021	-1.897614	-0.424088
N	-2.587940	-1.218848	0.346474
O	-1.134429	1.229414	-0.369282
N	-1.040003	-3.602221	0.018390
C	-3.649618	-1.255658	-0.503675
O	-3.528554	-1.242140	-1.734395
C	-5.014489	-1.318758	0.152650
C	-0.999437	2.579442	0.140022
C	-0.659444	3.489059	-1.045226
C	0.689641	3.203714	-1.708262
C	-2.288386	3.035496	0.836019
C	-2.656983	2.275154	2.112704
H	-2.783711	-1.235412	1.338544
H	-1.954781	-3.686699	0.456266
H	-0.497212	-4.398922	0.346752
H	-1.201418	-1.162070	-1.166541
H	-0.774278	0.322951	1.465233
H	1.462834	1.108971	0.302972
H	1.018178	-2.642589	-1.166548
H	1.655810	-3.064346	0.414982
H	-0.329714	-2.275237	1.546694
H	5.239581	1.498214	-0.570158

H	5.460007	-0.231062	-0.967170
H	5.686079	-0.761810	1.485409
H	5.450799	0.965646	1.879796
H	6.897698	0.441307	0.984904
H	-5.604612	-0.455575	-0.180330
H	-5.528411	-2.226125	-0.188891
H	-4.970069	-1.322120	1.247768
H	-0.170292	2.604966	0.866069
H	-0.678669	4.528532	-0.686770
H	-1.468839	3.396694	-1.785543
H	0.859707	3.893470	-2.546024
H	0.734855	2.179949	-2.101136
H	1.518282	3.335160	-0.996988
H	-3.112135	2.970194	0.108989
H	-2.166133	4.101914	1.078290
H	-2.888238	1.223394	1.904979
H	-3.546201	2.719840	2.579664
H	-1.841057	2.311305	2.849148

Conf. 13

C	1.216620	-1.135213	0.065283
C	0.577275	0.148400	-0.494067
C	-0.929884	0.072020	-0.495383
C	-1.628598	-1.062079	-0.317810
C	-0.962020	-2.396806	-0.100189
C	0.516200	-2.384599	-0.502434
C	-3.119878	-1.056524	-0.280800
O	-3.665396	0.139558	-0.574358
C	-5.115545	0.253039	-0.508969
C	-5.576474	0.612132	0.893709
O	-3.779917	-2.049249	-0.009298
N	2.649908	-1.163044	-0.201849
O	1.038352	1.236293	0.315071
N	1.163009	-3.597338	0.018236
C	3.614407	-1.125793	0.757129
O	3.359342	-1.080752	1.966452
C	5.043804	-1.147088	0.253381
C	0.905881	2.574824	-0.223482
C	0.364484	3.475305	0.892189
C	-1.044646	3.127248	1.376487
C	2.254300	3.089515	-0.742063
C	2.829178	2.341305	-1.948121
H	2.950660	-1.194417	-1.166994
H	2.121307	-3.654599	-0.319503
H	0.687094	-4.420460	-0.346537
H	1.111812	-1.130766	1.155923
H	0.917584	0.295532	-1.533552
H	-1.462381	1.009189	-0.640058
H	-1.042964	-2.687724	0.959249
H	-1.493145	-3.172676	-0.667842
H	0.570864	-2.328638	-1.606785
H	-5.557552	-0.687690	-0.852744
H	-5.350422	1.049008	-1.223300
H	-5.111597	1.547625	1.230940
H	-5.334005	-0.185208	1.607086
H	-6.666497	0.750413	0.889596
H	5.559064	-0.250732	0.621024
H	5.553533	-2.022240	0.675794
H	5.118617	-1.181349	-0.839638
H	0.184031	2.554247	-1.056183

H	0.378777	4.511228	0.523344
H	1.071488	3.431894	1.734835
H	-1.358586	3.816255	2.172275
H	-1.090699	2.106858	1.778227
H	-1.777513	3.207912	0.560241
H	2.972564	3.066960	0.091601
H	2.117061	4.147793	-1.010496
H	3.074881	1.301255	-1.700674
H	3.754018	2.823665	-2.292281
H	2.121921	2.338435	-2.790354

Conf. 7

C	-1.236246	-1.141888	-0.677660
C	-0.653038	0.075273	0.061734
C	0.834755	-0.050544	0.278568
C	1.542951	-1.170421	0.052197
C	0.900078	-2.445282	-0.434344
C	-0.611063	-2.462029	-0.186890
C	3.022590	-1.204927	0.240863
O	3.532587	-0.064797	0.745702
C	4.976397	0.007785	0.919472
C	5.662132	0.483993	-0.350124
O	3.704614	-2.180208	-0.039368
N	-2.703418	-1.153510	-0.642865
O	-0.964164	1.226691	-0.738314
N	-1.204407	-3.588794	-0.925383
C	-3.474435	-1.298240	0.465565
O	-2.998355	-1.459767	1.597547
C	-4.973118	-1.265181	0.237547
C	-0.787413	2.522496	-0.114176
C	0.334337	3.269016	-0.849510
C	0.791313	4.559816	-0.159444
C	-2.124706	3.266796	-0.146734
C	-3.217381	2.630951	0.715893
H	-3.179256	-0.995468	-1.518432
H	-2.190120	-3.678936	-0.688607
H	-0.766437	-4.457966	-0.624819
H	-0.977744	-1.031314	-1.738659
H	-1.146589	0.173038	1.041011
H	1.348357	0.840154	0.634857
H	1.095072	-2.577796	-1.510915
H	1.364899	-3.305570	0.065190
H	-0.784908	-2.541238	0.897578
H	5.342271	-0.975223	1.233544
H	5.107436	0.724020	1.737314
H	5.271345	1.460764	-0.663777
H	5.527249	-0.234795	-1.167827
H	6.739012	0.589248	-0.158807
H	-5.392723	-2.237271	0.527338
H	-5.412763	-0.503114	0.892645
H	-5.249887	-1.052892	-0.801374
H	-0.491442	2.370014	0.936908
H	-0.004318	3.485642	-1.874383
H	1.190192	2.586991	-0.943075
H	1.650469	4.993772	-0.688607
H	1.102181	4.364392	0.877524
H	0.000318	5.321096	-0.136487
H	-2.453900	3.325928	-1.195664
H	-1.953304	4.299321	0.188342
H	-3.442086	1.610004	0.383658

H	-4.146398	3.214088	0.659323
H	-2.912520	2.588197	1.771660

Conf. 2

C	-0.709349	-1.274785	-0.661725
C	-0.768580	0.067360	0.088784
C	0.605452	0.634702	0.339993
C	1.754955	-0.029237	0.131774
C	1.781932	-1.456574	-0.359256
C	0.439055	-2.163346	-0.146427
C	3.035696	0.699799	0.385055
O	4.109232	-0.044481	0.060584
C	5.415603	0.565751	0.258134
C	6.461616	-0.442082	-0.171835
O	3.122195	1.836745	0.825015
N	-2.008676	-1.956949	-0.665767
O	-1.555271	0.954579	-0.721300
N	0.445846	-3.435157	-0.887346
C	-2.652023	-2.456798	0.420655
O	-2.183044	-2.396105	1.565432
C	-3.988215	-3.120471	0.150029
C	-2.013252	2.177756	-0.093639
C	-1.335872	3.368100	-0.787635
C	-1.546519	4.712650	-0.081435
C	-3.540864	2.227252	-0.180073
C	-4.253431	1.148628	0.639028
H	-2.482590	-2.025800	-1.553920
H	-0.392087	-3.969735	-0.668335
H	1.228632	-4.005853	-0.572391
H	-0.502537	-1.049182	-1.715969
H	-1.274458	-0.082268	1.055056
H	0.656242	1.658943	0.707295
H	2.042132	-1.484383	-1.429688
H	2.570741	-2.015568	0.160355
H	0.295938	-2.315936	0.934588
H	5.512619	0.834183	1.317376
H	5.459909	1.485543	-0.337987
H	6.348164	-0.701611	-1.232574
H	6.395915	-1.359529	0.427626
H	7.459775	-0.007306	-0.028266
H	-3.902056	-4.188900	0.387590
H	-4.739964	-2.688421	0.821520
H	-4.323687	-3.013252	-0.887706
H	-1.715703	2.160527	0.967821
H	-1.702840	3.421975	-1.824192
H	-0.259821	3.157300	-0.849885
H	-0.967646	5.501957	-0.579843
H	-1.212912	4.665128	0.965688
H	-2.599621	5.023636	-0.086272
H	-3.821857	2.146585	-1.241564
H	-3.873716	3.218141	0.159154
H	-3.972554	0.143286	0.302243
H	-5.343340	1.242758	0.540798
H	-4.004996	1.234371	1.706845

Conf. 3

C	-1.351273	-1.106120	-0.665683
C	-0.630834	0.078628	0.002242
C	0.855799	-0.148443	0.120052
C	1.468808	-1.315258	-0.143866

C	0.707466	-2.544533	-0.573060
C	-0.776611	-2.459812	-0.204886
C	2.951165	-1.452658	-0.048292
O	3.575199	-0.345244	0.392681
C	5.025134	-0.406505	0.493565
C	5.503604	0.932458	1.016580
O	3.546363	-2.478066	-0.348658
N	-2.807882	-1.016424	-0.509621
O	-0.915036	1.235052	-0.801214
N	-1.500878	-3.552995	-0.873658
C	-3.491076	-1.099579	0.661068
O	-2.933062	-1.281802	1.751751
C	-4.998642	-0.972864	0.558069
C	-0.619458	2.526341	-0.213647
C	0.506469	3.186722	-1.021880
C	1.074652	4.460907	-0.386145
C	-1.905432	3.356706	-0.190699
C	-2.993093	2.804971	0.733846
H	-3.344399	-0.837715	-1.345221
H	-2.465631	-3.579098	-0.550442
H	-1.093052	-4.445315	-0.599581
H	-1.174663	-1.026255	-1.746149
H	-1.046166	0.229785	1.010469
H	1.450923	0.706249	0.435598
H	0.806202	-2.689112	-1.661235
H	1.153041	-3.433431	-0.107407
H	-0.865697	-2.515268	0.891271
H	5.431605	-0.628428	-0.500991
H	5.290581	-1.229653	1.168395
H	5.083243	1.141517	2.008990
H	5.225377	1.745761	0.333665
H	6.598190	0.913957	1.102947
H	-5.450649	-1.930505	0.848034
H	-5.338836	-0.213270	1.272150
H	-5.344864	-0.706860	-0.447121
H	-0.276807	2.370990	0.822775
H	0.128970	3.402763	-2.033211
H	1.313827	2.451787	-1.142228
H	1.932105	4.828457	-0.965895
H	1.422634	4.269206	0.639620
H	0.333796	5.270313	-0.345178
H	-2.281988	3.425134	-1.223059
H	-1.650665	4.379379	0.120462
H	-3.300660	1.797446	0.428380
H	-3.883257	3.448039	0.713876
H	-2.639625	2.754775	1.773983

Conf. 22

C	0.914466	-1.193118	0.019350
C	0.695088	0.230064	-0.524530
C	-0.769394	0.584063	-0.583242
C	-1.769946	-0.305384	-0.471743
C	-1.521434	-1.782873	-0.290785
C	-0.078874	-2.177750	-0.627218
C	-3.170966	0.216541	-0.498082
O	-4.068006	-0.759036	-0.253632
C	-5.475722	-0.387466	-0.213204
C	-5.886249	0.059379	1.179955
O	-3.481857	1.379043	-0.708526
N	2.293656	-1.621850	-0.180650

O	1.408292	1.126316	0.334758
N	0.169959	-3.537737	-0.128427
C	3.173006	-1.889379	0.822327
O	2.875284	-1.803247	2.019717
C	4.561122	-2.311711	0.383895
C	1.691739	2.454653	-0.169798
C	1.389329	3.453561	0.952454
C	-0.079822	3.524917	1.373706
C	3.151583	2.565427	-0.627391
C	3.537880	1.699742	-1.829831
H	2.628877	-1.709972	-1.130657
H	1.088455	-3.858166	-0.427541
H	-0.500927	-4.181178	-0.544487
H	0.754267	-1.182809	1.103195
H	1.110504	0.291891	-1.544888
H	-1.017669	1.636246	-0.711498
H	-1.739111	-2.077908	0.747787
H	-2.211893	-2.358978	-0.920782
H	0.047590	-2.110645	-1.725040
H	-5.999300	-1.301954	-0.510702
H	-5.652563	0.394660	-0.958547
H	-5.355907	0.973081	1.475353
H	-5.684204	-0.726950	1.918831
H	-6.964728	0.269654	1.186368
H	5.293074	-1.619484	0.818682
H	4.768017	-3.311837	0.785368
H	4.686276	-2.329801	-0.704918
H	1.029024	2.659121	-1.026581
H	1.721840	4.446434	0.616100
H	2.015713	3.189050	1.818180
H	-0.213637	4.260395	2.178588
H	-0.439358	2.555302	1.741451
H	-0.720100	3.832114	0.533706
H	3.798124	2.326557	0.230775
H	3.334494	3.621990	-0.874413
H	3.467630	0.629884	-1.598461
H	4.575087	1.902506	-2.129184
H	2.894581	1.909305	-2.696852

Conf. 6

C	-1.196865	-1.197538	-0.695354
C	-0.644324	0.069473	-0.018850
C	0.863032	0.073351	0.043471
C	1.638917	-0.979035	-0.268886
C	1.060762	-2.303344	-0.702049
C	-0.405590	-2.455456	-0.288209
C	3.127491	-0.888415	-0.217713
O	3.584056	0.315896	0.177596
C	5.026142	0.491520	0.272783
C	5.543290	0.072431	1.638708
O	3.860820	-1.819491	-0.518050
N	-2.643800	-1.338078	-0.493821
O	-1.134039	1.184674	-0.780249
N	-0.974332	-3.632507	-0.964800
C	-3.267646	-1.542113	0.695055
O	-2.653857	-1.647362	1.765731
C	-4.779062	-1.649591	0.640051
C	-1.025097	2.493428	-0.168109
C	-0.036971	3.337925	-0.985349
C	0.355776	4.663865	-0.322777

C	-2.422338	3.114712	-0.094380
C	-3.385044	2.387714	0.847317
H	-3.228444	-1.239378	-1.310293
H	-1.912208	-3.815819	-0.614551
H	-0.424107	-4.456477	-0.728300
H	-1.071187	-1.068192	-1.778083
H	-1.039124	0.131896	1.006753
H	1.330136	1.002432	0.363600
H	1.144502	-2.411849	-1.795728
H	1.652288	-3.121370	-0.270424
H	-0.448330	-2.547919	0.808188
H	5.173528	1.562942	0.101155
H	5.503106	-0.075926	-0.532897
H	5.392602	-1.001034	1.807560
H	5.040648	0.634253	2.436788
H	6.620501	0.282007	1.695377
H	-5.071045	-2.651234	0.981102
H	-5.209692	-0.920560	1.337432
H	-5.191040	-1.479396	-0.361081
H	-0.634609	2.371936	0.855855
H	-0.474631	3.524650	-1.978178
H	0.866652	2.736583	-1.152957
H	1.125943	5.175545	-0.915662
H	0.766392	4.495651	0.683852
H	-0.496924	5.349266	-0.228706
H	-2.835442	3.140919	-1.114565
H	-2.318324	4.159631	0.229674
H	-3.546180	1.350905	0.527680
H	-4.362443	2.888405	0.866341
H	-2.996326	2.372928	1.875936

Conf. 11

C	-1.328096	-0.995999	-0.684371
C	-0.636041	0.170811	0.043594
C	0.847979	-0.058754	0.182485
C	1.460878	-1.229230	-0.064825
C	0.706757	-2.459676	-0.503079
C	-0.792585	-2.359744	-0.205745
C	2.941686	-1.367311	0.049391
O	3.561191	-0.258366	0.493268
C	5.010042	-0.317785	0.606927
C	5.482407	1.023693	1.129226
O	3.540001	-2.394130	-0.240049
N	-2.790374	-0.891926	-0.625157
O	-0.901223	1.346529	-0.738709
N	-1.493194	-3.441365	-0.917238
C	-3.558377	-1.022721	0.486396
O	-3.084673	-1.270739	1.603722
C	-5.051615	-0.856401	0.282435
C	-0.646382	2.637808	-0.133788
C	0.057178	3.506159	-1.182841
C	1.439034	3.005520	-1.608452
C	-1.951609	3.288163	0.342285
C	-2.625213	2.611159	1.538866
H	-3.262536	-0.659716	-1.486018
H	-2.470024	-3.469559	-0.633084
H	-1.098470	-4.338373	-0.639220
H	-1.080839	-0.902419	-1.749732
H	-1.074525	0.283951	1.045901
H	1.442798	0.796783	0.494521

H	0.853381	-2.623860	-1.583019
H	1.123412	-3.344383	-0.003453
H	-0.936582	-2.421495	0.883888
H	5.425463	-0.542463	-0.383276
H	5.270830	-1.138214	1.286815
H	5.053692	1.235387	2.117429
H	5.208092	1.834102	0.441299
H	6.576281	1.007261	1.224516
H	-5.551821	-1.786106	0.582419
H	-5.410096	-0.056640	0.942607
H	-5.325756	-0.619785	-0.751839
H	0.022257	2.502656	0.731514
H	0.146727	4.522711	-0.773096
H	-0.603076	3.578098	-2.060969
H	1.873436	3.672594	-2.365373
H	1.385351	1.997441	-2.039068
H	2.131778	2.976624	-0.754683
H	-2.645227	3.328177	-0.511408
H	-1.719797	4.330569	0.607820
H	-2.945739	1.588915	1.306652
H	-3.517088	3.173955	1.846275
H	-1.945571	2.566309	2.402473

Conf. 16

C	-0.824759	-1.098201	-0.699517
C	-0.812516	0.198111	0.131387
C	0.593724	0.660839	0.415139
C	1.697074	-0.076007	0.202751
C	1.636249	-1.483275	-0.339233
C	0.238837	-2.097137	-0.203225
C	3.021436	0.553127	0.495048
O	4.044402	-0.248427	0.143794
C	5.388156	0.260129	0.374012
C	6.364909	-0.798708	-0.094921
O	3.181612	1.661050	0.985476
N	-2.167531	-1.682108	-0.795360
O	-1.529072	1.177536	-0.637842
N	0.178548	-3.324039	-1.014434
C	-2.876652	-2.234194	0.222040
O	-2.439706	-2.314568	1.378267
C	-4.249739	-2.765698	-0.139767
C	-1.958469	2.387068	0.033764
C	-1.653412	3.565916	-0.897114
C	-0.167849	3.790007	-1.186731
C	-3.452498	2.323052	0.375063
C	-3.838183	1.310697	1.456743
H	-2.617524	-1.635024	-1.697154
H	-0.695022	-3.815765	-0.838853
H	0.917622	-3.959981	-0.719470
H	-0.562230	-0.822815	-1.729322
H	-1.331002	0.022151	1.085130
H	0.711459	1.670426	0.805739
H	1.934357	-1.490999	-1.400018
H	2.362313	-2.118423	0.184691
H	0.049968	-2.297467	0.862685
H	5.495740	0.474729	1.444440
H	5.501241	1.199540	-0.181065
H	6.239829	-1.005226	-1.165951
H	6.232924	-1.733658	0.465255
H	7.389785	-0.440179	0.069540

H	-4.276023	-3.841754	0.074905
H	-4.995711	-2.279486	0.501322
H	-4.516957	-2.603780	-1.190159
H	-1.382099	2.503294	0.965762
H	-2.077789	4.472051	-0.440916
H	-2.199089	3.403655	-1.839623
H	-0.032568	4.644567	-1.863612
H	0.285031	2.909680	-1.660617
H	0.389494	4.006116	-0.263548
H	-4.006212	2.114817	-0.553193
H	-3.756609	3.328233	0.703754
H	-3.627276	0.280044	1.148679
H	-4.912434	1.375163	1.677079
H	-3.294088	1.504038	2.392875

Conf. 15

C	-1.203298	-1.053748	-0.727468
C	-0.649552	0.174869	0.016651
C	0.857126	0.149289	0.090253
C	1.612529	-0.921868	-0.208498
C	1.014646	-2.234645	-0.649889
C	-0.473284	-2.343169	-0.303725
C	3.101866	-0.864230	-0.141627
O	3.581480	0.323697	0.275404
C	5.026136	0.464283	0.388482
C	5.517910	0.013201	1.753577
O	3.817180	-1.807882	-0.446634
N	-2.663463	-1.151700	-0.623348
O	-1.108806	1.327713	-0.706085
N	-1.046412	-3.493437	-1.021292
C	-3.372237	-1.410663	0.504856
O	-2.835947	-1.615797	1.602491
C	-4.879678	-1.443341	0.345772
C	-1.033620	2.616461	-0.048829
C	-0.511884	3.626929	-1.076298
C	0.912422	3.363599	-1.569602
C	-2.405550	3.036303	0.494785
C	-2.911755	2.239451	1.700404
H	-3.189605	-0.964579	-1.463615
H	-2.000101	-3.659878	-0.707480
H	-0.524926	-4.334735	-0.780661
H	-1.006240	-0.899533	-1.796387
H	-1.054395	0.190752	1.038821
H	1.342358	1.071453	0.402191
H	1.144882	-2.358316	-1.737330
H	1.562386	-3.064353	-0.183587
H	-0.569383	-2.448464	0.787888
H	5.200237	1.534319	0.234339
H	5.498798	-0.102577	-0.420120
H	5.339298	-1.058603	1.904573
H	5.020117	0.575406	2.554407
H	6.599175	0.195579	1.824936
H	-5.245573	-2.425249	0.671522
H	-5.319978	-0.686669	1.007571
H	-5.212611	-1.259561	-0.682027
H	-0.319506	2.550651	0.787948
H	-0.561787	4.626159	-0.620046
H	-1.208884	3.635460	-1.928645
H	1.212157	4.123174	-2.304350
H	0.994842	2.379849	-2.049062

H	1.633384	3.401444	-0.739834
H	-3.130833	2.977792	-0.331034
H	-2.335356	4.097582	0.776949
H	-3.075654	1.182637	1.459838
H	-3.867820	2.647690	2.055601
H	-2.197768	2.290361	2.535600

Conf. 19

C	-0.828777	-1.260169	-0.653682
C	-0.733032	0.073664	0.108212
C	0.694768	0.455037	0.404802
C	1.754619	-0.350169	0.221309
C	1.611705	-1.762823	-0.290398
C	0.183765	-2.294342	-0.124525
C	3.110420	0.204781	0.522869
O	4.085489	-0.680236	0.236176
C	5.463467	-0.264582	0.459254
C	6.036031	0.420808	-0.769979
O	3.326267	1.320802	0.970839
N	-2.204224	-1.771447	-0.692715
O	-1.373375	1.061835	-0.714312
N	0.048842	-3.546455	-0.886700
C	-2.935469	-2.178414	0.376845
O	-2.491587	-2.176727	1.533133
C	-4.342248	-2.656543	0.073990
C	-1.706021	2.322330	-0.081922
C	-0.846140	3.430608	-0.706502
C	-0.927133	4.776847	0.022764
C	-3.207897	2.568271	-0.248505
C	-4.095346	1.568076	0.495915
H	-2.659887	-1.780904	-1.592942
H	-0.857052	-3.971119	-0.699907
H	0.742024	-4.217532	-0.559842
H	-0.571484	-1.055579	-1.701049
H	-1.281360	-0.013704	1.058686
H	0.866982	1.460294	0.787216
H	1.896667	-1.811392	-1.353761
H	2.306920	-2.425109	0.240939
H	-0.007304	-2.441886	0.949828
H	5.989842	-1.199579	0.677938
H	5.494374	0.387044	1.338337
H	5.504649	1.355866	-0.986596
H	5.977508	-0.235917	-1.647717
H	7.093053	0.659684	-0.588136
H	-4.416778	-3.717971	0.343927
H	-5.046470	-2.101235	0.705495
H	-4.626273	-2.535573	-0.977572
H	-1.474208	2.248027	0.993422
H	-1.142864	3.550594	-1.759915
H	0.197073	3.087579	-0.715182
H	-0.224322	5.495394	-0.420244
H	-0.665405	4.666488	1.085541
H	-1.930180	5.220156	-0.033192
H	-3.436376	2.551083	-1.325396
H	-3.432071	3.584512	0.104528
H	-3.925901	0.544980	0.138743
H	-5.157484	1.804296	0.346070
H	-3.896634	1.591160	1.577307

Conf. 24

C	-0.904695	-1.087300	-0.751533
C	-0.771389	0.195560	0.089364
C	0.671825	0.589865	0.270691
C	1.720250	-0.196396	-0.025775
C	1.553420	-1.595692	-0.565715
C	0.139686	-2.142593	-0.337347
C	3.090792	0.369534	0.169115
O	4.045583	-0.484136	-0.250901
C	5.433791	-0.065053	-0.113866
C	5.988872	-0.441442	1.249613
O	3.334078	1.471723	0.636747
N	-2.278507	-1.602670	-0.760643
O	-1.497797	1.216651	-0.613129
N	-0.036752	-3.356868	-1.150425
C	-2.947047	-2.122484	0.300101
O	-2.439802	-2.231721	1.424864
C	-4.366940	-2.579764	0.028817
C	-1.815261	2.436479	0.101005
C	-1.536566	3.609716	-0.845069
C	-0.070930	3.772116	-1.253456
C	-3.276662	2.434219	0.567383
C	-3.609602	1.446960	1.689455
H	-2.784195	-1.526139	-1.630355
H	-0.920982	-3.804771	-0.919740
H	0.686492	-4.032407	-0.908911
H	-0.698956	-0.812024	-1.794281
H	-1.223972	0.029753	1.077747
H	0.865407	1.589594	0.656244
H	1.778159	-1.612088	-1.644352
H	2.281641	-2.268151	-0.094112
H	0.014322	-2.344414	0.737684
H	5.493220	1.013427	-0.292389
H	5.951529	-0.598350	-0.917942
H	5.904425	-1.522290	1.422313
H	5.463618	0.091381	2.051888
H	7.052186	-0.167942	1.292705
H	-4.435228	-3.654438	0.241149
H	-5.042286	-2.059671	0.719651
H	-4.694365	-2.397080	-1.000957
H	-1.157080	2.517892	0.981105
H	-1.882382	4.529019	-0.350607
H	-2.163574	3.479721	-1.740811
H	0.047092	4.628724	-1.930965
H	0.302229	2.879069	-1.771083
H	0.568473	3.951462	-0.376717
H	-3.913916	2.241478	-0.309117
H	-3.512966	3.452864	0.910072
H	-3.464717	0.405342	1.380010
H	-4.658528	1.555842	1.997170
H	-2.982588	1.628469	2.574734

Conf. 18

C	-0.805329	-1.268155	-0.706850
C	-0.737337	0.070976	0.048371
C	0.679626	0.559219	0.210307
C	1.774326	-0.162640	-0.083073
C	1.689448	-1.582694	-0.587336
C	0.329537	-2.220763	-0.283717
C	3.107024	0.495123	0.084356
O	4.110752	-0.301047	-0.333949

C	5.469734	0.212270	-0.226831
C	6.070572	-0.103392	1.132637
O	3.281974	1.619499	0.529098
N	-2.135757	-1.880941	-0.614639
O	-1.523224	1.005083	-0.708703
N	0.216097	-3.482373	-1.033780
C	-2.721880	-2.349357	0.517241
O	-2.163687	-2.322290	1.622601
C	-4.112547	-2.930160	0.350511
C	-1.879126	2.245466	-0.049831
C	-1.174179	3.403723	-0.770420
C	-1.277090	4.752280	-0.048286
C	-3.404136	2.380404	-0.055267
C	-4.132369	1.329476	0.785831
H	-2.678401	-1.918826	-1.464538
H	-0.630997	-3.975396	-0.759537
H	0.988092	-4.096738	-0.780390
H	-0.667400	-1.046171	-1.772989
H	-1.186981	-0.053078	1.045556
H	0.811175	1.574486	0.582352
H	1.870726	-1.610726	-1.673912
H	2.482635	-2.189051	-0.131454
H	0.256514	-2.378504	0.803615
H	5.453662	1.289191	-0.423187
H	6.009334	-0.298593	-1.031114
H	6.060004	-1.184319	1.324076
H	5.525093	0.407661	1.935580
H	7.114212	0.239756	1.152264
H	-4.080948	-3.995354	0.613949
H	-4.789591	-2.431839	1.055069
H	-4.507739	-2.825960	-0.666252
H	-1.528749	2.201765	0.994659
H	-1.588469	3.484790	-1.787240
H	-0.115373	3.136615	-0.887550
H	-0.679744	5.512418	-0.569710
H	-0.897666	4.678837	0.981614
H	-2.310425	5.120860	-0.001429
H	-3.744422	2.333217	-1.101284
H	-3.661983	3.382543	0.314591
H	-3.934887	0.316514	0.414356
H	-5.218236	1.491863	0.755610
H	-3.815976	1.376609	1.837989

Conf. 23

C	1.216620	-1.135213	0.065283
C	0.577275	0.148400	-0.494067
C	-0.929884	0.072020	-0.495383
C	-1.628598	-1.062079	-0.317810
C	-0.962020	-2.396806	-0.100189
C	0.516200	-2.384599	-0.502434
C	-3.119878	-1.056524	-0.280800
O	-3.665396	0.139558	-0.574358
C	-5.115545	0.253039	-0.508969
C	-5.576474	0.612132	0.893709
O	-3.779917	-2.049249	-0.009298
N	2.649908	-1.163044	-0.201849
O	1.038352	1.236293	0.315071
N	1.163009	-3.597338	0.018236
C	3.614407	-1.125793	0.757129
O	3.359342	-1.080752	1.966452

C	5.043804	-1.147088	0.253381
C	0.905881	2.574824	-0.223482
C	0.364484	3.475305	0.892189
C	-1.044646	3.127248	1.376487
C	2.254300	3.089515	-0.742063
C	2.829178	2.341305	-1.948121
H	2.950660	-1.194417	-1.166994
H	2.121307	-3.654599	-0.319503
H	0.687094	-4.420460	-0.346537
H	1.111812	-1.130766	1.155923
H	0.917584	0.295532	-1.533552
H	-1.462381	1.009189	-0.640058
H	-1.042964	-2.687724	0.959249
H	-1.493145	-3.172676	-0.667842
H	0.570864	-2.328638	-1.606785
H	-5.557552	-0.687690	-0.852744
H	-5.350422	1.049008	-1.223300
H	-5.111597	1.547625	1.230940
H	-5.334005	-0.185208	1.607086
H	-6.666497	0.750413	0.889596
H	5.559064	-0.250732	0.621024
H	5.553533	-2.022240	0.675794
H	5.118617	-1.181349	-0.839638
H	0.184031	2.554247	-1.056183
H	0.378777	4.511228	0.523344
H	1.071488	3.431894	1.734835
H	-1.358586	3.816255	2.172275
H	-1.090699	2.106858	1.778227
H	-1.777513	3.207912	0.560241
H	2.972564	3.066960	0.091601
H	2.117061	4.147793	-1.010496
H	3.074881	1.301255	-1.700674
H	3.754018	2.823665	-2.292281
H	2.121921	2.338435	-2.790354

Conf. 21

C	-0.914446	-1.083891	-0.692893
C	-0.769851	0.198652	0.146356
C	0.674318	0.488708	0.465269
C	1.683185	-0.381616	0.291645
C	1.465262	-1.775847	-0.243549
C	-0.003177	-2.208297	-0.162733
C	3.065965	0.083735	0.619608
O	3.989302	-0.851679	0.320613
C	5.387235	-0.523198	0.563139
C	6.008675	0.157696	-0.644777
O	3.343708	1.173696	1.096731
N	-2.315216	-1.494443	-0.840241
O	-1.347425	1.259224	-0.631112
N	-0.187023	-3.418277	-0.980725
C	-3.125214	-1.953048	0.147681
O	-2.744601	-2.090530	1.318471
C	-4.541316	-2.302082	-0.266844
C	-1.642861	2.508333	0.041054
C	-1.176334	3.647259	-0.872644
C	0.333800	3.702203	-1.113125
C	-3.141406	2.623466	0.348130
C	-3.669757	1.667693	1.421107
H	-2.723202	-1.388837	-1.757011
H	-1.120761	-3.797028	-0.837842

H	0.456315	-4.141228	-0.662799
H	-0.581909	-0.842099	-1.710808
H	-1.327305	0.081294	1.087149
H	0.905312	1.480263	0.851043
H	1.802696	-1.832639	-1.291039
H	2.083444	-2.492132	0.313198
H	-0.256359	-2.382925	0.894250
H	5.856599	-1.492425	0.761568
H	5.449137	0.103551	1.458536
H	5.532506	1.125993	-0.842721
H	5.921192	-0.473697	-1.538529
H	7.075762	0.332215	-0.449158
H	-4.722830	-3.359952	-0.038189
H	-5.240709	-1.706083	0.332932
H	-4.738771	-2.126380	-1.330358
H	-1.078105	2.547834	0.986261
H	-1.509299	4.594763	-0.424598
H	-1.706694	3.550267	-1.832638
H	0.587395	4.538858	-1.778274
H	0.699964	2.778614	-1.579473
H	0.881210	3.849518	-0.170636
H	-3.694316	2.481318	-0.592967
H	-3.330691	3.658386	0.670521
H	-3.573796	0.617677	1.121418
H	-4.734012	1.858887	1.614891
H	-3.129427	1.800763	2.369867

Conf. 20

C	-0.891205	-1.222472	-0.073705
C	-0.661493	0.209634	0.443736
C	0.783240	0.625203	0.320758
C	1.798631	-0.227246	0.107476
C	1.588969	-1.714412	-0.036804
C	0.207833	-2.162963	0.457774
C	3.171368	0.354519	-0.018860
O	4.087607	-0.597775	-0.318501
C	5.461934	-0.157188	-0.473171
C	6.189163	-0.133952	0.861991
O	3.449512	1.530771	0.117805
N	-2.221955	-1.698381	0.285561
O	-1.525927	1.068370	-0.299300
N	-0.038563	-3.528768	-0.009502
C	-3.218172	-1.939643	-0.631720
O	-3.036761	-1.903746	-1.840516
C	-4.576065	-2.279794	-0.038365
C	-1.763924	2.396916	0.211090
C	-1.668362	3.370476	-0.968811
C	-0.287954	3.450911	-1.623388
C	-3.140109	2.481651	0.885204
C	-3.308509	1.639546	2.152817
H	-2.487332	-1.662828	1.259911
H	-0.965844	-3.843067	0.263645
H	0.634370	-4.175552	0.394352
H	-0.865144	-1.214339	-1.169744
H	-0.938487	0.248447	1.514557
H	1.010596	1.686980	0.403977
H	1.697313	-2.013293	-1.090802
H	2.371315	-2.258243	0.510150
H	0.201049	-2.086683	1.565904

H	5.461897	0.831630	-0.944805
H	5.901735	-0.892102	-1.156890
H	6.157980	-1.120686	1.342914
H	5.744749	0.608796	1.535485
H	7.242122	0.136245	0.698963
H	-5.297889	-1.520676	-0.365600
H	-4.904645	-3.244647	-0.443455
H	-4.579471	-2.328869	1.058373
H	-0.984305	2.645712	0.951621
H	-1.966884	4.367184	-0.610628
H	-2.416982	3.064189	-1.714845
H	-0.299906	4.162875	-2.459659
H	0.021454	2.475028	-2.017590
H	0.477551	3.791216	-0.910649
H	-3.899000	2.194476	0.142393
H	-3.323009	3.538695	1.131867
H	-3.226858	0.567218	1.934564
H	-4.297028	1.808060	2.601191
H	-2.553221	1.896205	2.910368