Electronic supplementary materials *Mendeleev Commun.*, 2021, **31**, 300–301

Structure revision of *ent*-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data

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Supporting Information

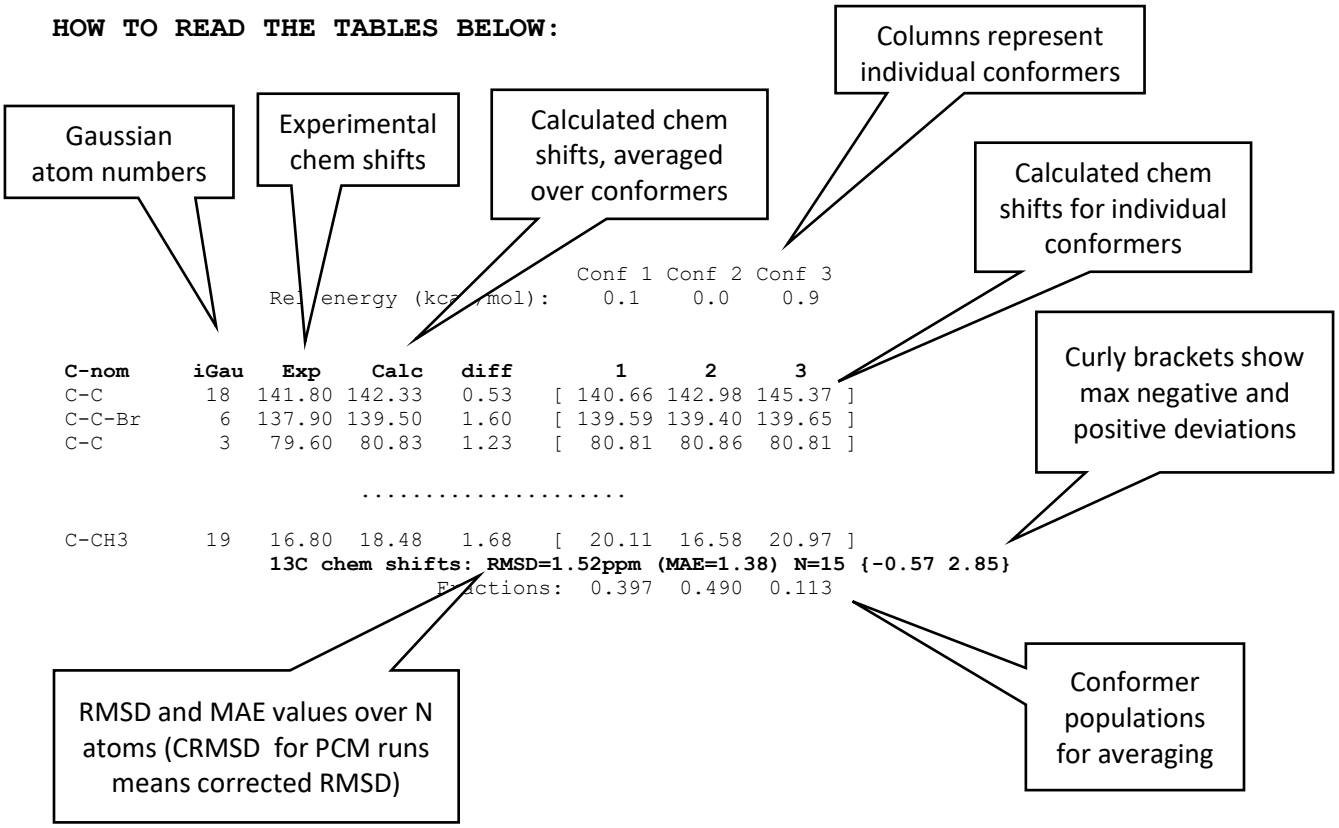
Contents

COMPUTATIONAL DETAILS

The structures of the oxetane-containing organic molecules and natural products were pre-optimized with the force field MMFF94 as implemented in OpenBabel. (O'Boyle, N. M.; Banck, M.; James, C. A.; Morley, C.; Vandermeersch, T.; Hutchison, G. R. *J. Cheminform,* **2011**, *3*, 8). For structures with freely rotatable groups, conformers were generated using OpenBabel's confab, whereas the conformers resulting from conformational changes in cyclic cores were generated manually, using Chem3D. As the empirical corrections for *DU8+* were developed on a training set of ^{1}H and ^{13}C NMR spectra recorded in $CDCl_3$, we used the Gaussian's default PCM model to account for chloroform solvent effects. For details on DU8+ method see: Kutateladze, A. G.; Reddy, D. S. *J. Org. Chem.* **2017**, *82*, 3368

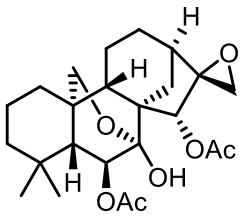
All DFT calculations were performed with Gaussian 2009, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

HOW TO READ THE TABLES BELOW:



DU8+ COMPUTATIONS

isoserrin A



Isoserrin A - original, misassigned

	Conf1
Rel energy (kcal/mol):	0.00

C-nom	iGau	Exp	Calc	diff	1
C1-CH2	8	30.90	31.90	1.00	[31.90]
C2-CH2	3	18.50	18.80	0.30	[18.80]
C3-CH2	4	41.10	39.50	-1.60	[39.50]
C4-C	5	33.50	33.03	-0.47	[33.03]
C5-CH	6	54.50	53.95	-0.55	[53.95]
C6-CH	9	75.10	78.93	3.83	[78.93]
C7-C	10	95.30	98.18	2.88	[98.18]
C8-C	11	52.70	50.95	-1.75	[50.95]
C9-CH	12	44.30	53.02	8.72	[53.02]
C10-C	7	35.80	35.19	-0.61	[35.19]
C11-CH2	16	15.60	16.71	1.11	[16.71]
C12-CH2	15	22.20	27.26	5.06	[27.26]
C13-CH	14	41.00	36.60	-4.40	[36.60]
C14-CH2	13	24.80	27.72	2.92	[27.72]
C15-CH	18	80.80	81.83	1.03	[81.83]
C16-C	17	84.20	70.27	-13.93	[70.27]
C17-CH2	19	48.60	51.84	3.24	[51.84]
C18-CH3	21	33.00	32.26	-0.74	[32.26]
C19-CH3	22	22.30	21.86	-0.44	[21.86]
C20-CH2	2	66.20	66.34	0.14	[66.34]
C-OAc-6-C	29	173.60	173.07	-0.53	[173.07]
C-OAc-6-CH3	30	21.20	20.74	-0.46	[20.74]
C-OAc-15-C	33	170.40	171.95	1.55	[171.95]
C-OAc-15-CH3	34	21.60	20.62	-0.98	[20.62]

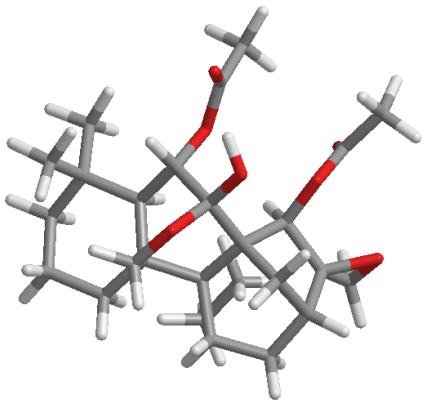
13C chem shifts: RMSD=3.93ppm (MAE=2.43) N=24 {-13.93 8.7}

Conformer 1

Energy: -1461.55861 Hartree (Rel: 0.0 kcal/mol)

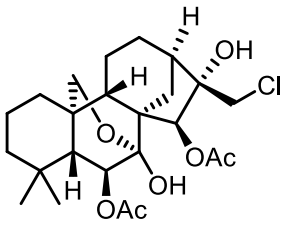
XYZ coordinates for conf 1:

O	-1.13413	-0.56259	2.25062
C	-2.07624	-1.38252	1.54445
C	-4.22530	-1.59298	-0.93143
C	-4.15030	-0.19765	-1.55528
C	-3.34980	0.81125	-0.69680
C	-1.92242	0.20323	-0.42738
C	-1.83828	-1.29621	0.03030
C	-2.82218	-2.18579	-0.76075
C	-1.04733	1.04769	0.52632
C	-0.17866	0.13748	1.42415
C	0.65062	-0.89783	0.63184
C	-0.36520	-1.77256	-0.22440
C	1.52465	-1.80475	1.53605
C	2.27674	-2.63571	0.47648
C	1.32699	-3.70849	-0.11101
C	-0.15258	-3.28696	-0.00382



C	2.64921	-1.56886	-0.56320
C	1.72140	-0.34632	-0.35136
C	3.32271	-1.84595	-1.84073
O	4.03952	-1.26616	-0.73709
C	-3.19029	2.11265	-1.51414
C	-4.16882	1.16595	0.56587
H	-1.42082	0.23328	-1.40382
O	0.62635	0.85010	2.29910
H	-0.16767	-1.57952	-1.28852
H	3.19298	-3.09877	0.85445
O	-0.26716	1.97162	-0.28478
O	-0.05614	3.42528	1.44013
C	0.09099	3.15132	0.25926
C	0.65626	4.08621	-0.77769
O	2.51258	0.69060	0.26212
O	3.05424	1.53603	-1.77362
C	3.19843	1.50574	-0.56506
C	4.14503	2.38242	0.21811
H	-3.08398	-1.05987	1.82282
H	-1.96505	-2.41686	1.89326
H	-4.81783	-2.25729	-1.57279
H	-4.74950	-1.55603	0.03175
H	-3.67487	-0.27945	-2.54435
H	-5.15814	0.20216	-1.72790
H	-2.39963	-2.35325	-1.76225
H	-2.88898	-3.17230	-0.28692
H	-1.65108	1.64642	1.21015
H	2.21036	-1.18252	2.11764
H	0.94292	-2.40859	2.23610
H	1.46456	-4.65526	0.42442
H	1.59173	-3.90458	-1.15713
H	-0.74353	-3.85330	-0.72984
H	-0.52896	-3.57520	0.98334
H	1.30421	0.04636	-1.27758
H	3.61119	-2.86653	-2.09360
H	3.16396	-1.17661	-2.68520
H	-2.70762	2.90612	-0.93357
H	-4.17533	2.48506	-1.82082
H	-2.59540	1.94819	-2.42018
H	-4.41920	0.30009	1.18309
H	-3.65726	1.89271	1.20541
H	-5.11550	1.62630	0.25848
H	0.27977	1.76122	2.36817
H	1.15384	4.92333	-0.28663
H	-0.16185	4.46930	-1.39876
H	1.35031	3.55696	-1.43577
H	4.50707	3.19418	-0.41428
H	4.99637	1.77651	0.54812
H	3.65695	2.78059	1.11210

isoserrin A – revised



Isoserrin A - revised, 16,17-chlorohydrin, epi-15,16

	Conf1	Conf2	Conf3
Rel energy (kcal/mol):	0.00	0.46	3.24

C-nom	**iGau**	**Exp**	**Calc**	**diff**		**1**	**2**	**3**	
C1-CH2	8	30.90	31.38	0.48	[	31.40	31.32	31.66	]
C2-CH2	3	18.50	18.68	0.18	[	18.69	18.67	18.76	]
C3-CH2	4	41.10	39.92	-1.18	[	39.88	40.00	40.10	]
C4-C	5	33.50	32.98	-0.52	[	33.00	32.95	32.95	]
C5-CH	6	54.50	53.69	-0.81	[	53.58	53.93	52.50	]
C6-CH	9	75.10	78.18	3.08	[	78.03	78.51	78.36	]
C7-C	10	95.30	98.10	2.80	[	98.01	98.30	98.19	]
C8-C	11	52.70	52.98	0.28	[	52.61	53.79	51.88	]
C9-CH	12	44.30	45.36	1.06	[	45.47	45.12	45.11	]
C10-C	7	35.80	35.33	-0.47	[	35.29	35.43	35.51	]
C11-CH2	16	15.60	16.55	0.95	[	16.62	16.39	16.47	]
C12-CH2	15	22.20	22.50	0.30	[	23.30	20.77	22.39	]
C13-CH	14	41.00	41.39	0.39	[	40.23	43.90	43.08	]
C14-CH2	13	24.80	26.99	2.19	[	26.66	27.69	27.91	]
C15-CH	18	80.80	84.20	3.40	[	85.79	80.72	87.35	]
C16-C	17	84.20	83.80	-0.40	[	84.42	82.46	84.07	]
C17-CH2	19	48.60	46.79	-1.81	[	45.59	49.44	41.54	]
C18-CH3	21	33.00	32.48	-0.52	[	32.43	32.58	32.77	]
C19-CH3	22	22.30	22.06	-0.24	[	22.03	22.13	22.47	]
C20-CH2	2	66.20	66.57	0.37	[	66.65	66.40	67.08	]
C-OAc-6-C	29	173.60	173.37	-0.23	[	173.07	174.04	172.90	]
C-OAc-6-CH3	30	21.20	20.65	-0.55	[	20.54	20.89	20.89	]
C-OAc-15-C	33	170.40	169.92	-0.48	[	170.57	168.50	172.12	]
C-OAc-15-CH3	34	21.60	21.04	-0.56	[	20.81	21.54	21.02	]

13C chem shifts: RMSD=1.35ppm (MAE=0.97) N=24 {-1.81 3.40}

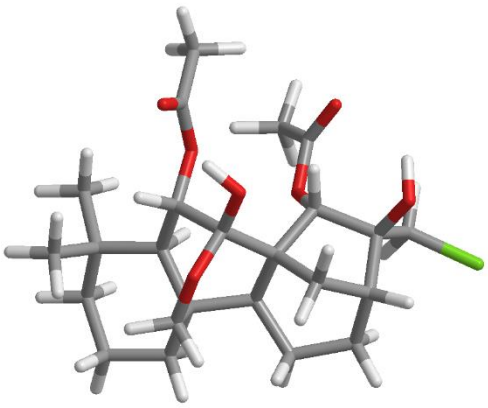
Fractions: 0.683 0.314 0.003

Conformer 1

Energy: -1922.39451 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	-1.31352	-1.05859	2.27280
C	-1.74001	-2.11513	1.39450
C	-3.38887	-2.88711	-1.34225
C	-3.82611	-1.52027	-1.87357
C	-3.59252	-0.36906	-0.86534
C	-2.07643	-0.38006	-0.44157
C	-1.42901	-1.76961	-0.07132
C	-1.88804	-2.88593	-1.03331
C	-1.73013	0.61710	0.68661
C	-0.64120	0.02947	1.60979
C	0.60348	-0.53171	0.88746
C	0.12401	-1.58461	-0.17941
C	1.59050	-1.16857	1.90038
C	2.80590	-1.43575	1.00011
C	2.46926	-2.60300	0.02790
C	0.95379	-2.88241	-0.08612
C	2.99725	-0.03810	0.34392
C	1.53138	0.54664	0.26816
C	3.70250	0.00227	-1.01568
O	3.74549	0.72541	1.29121
C	-3.89894	0.96288	-1.58557



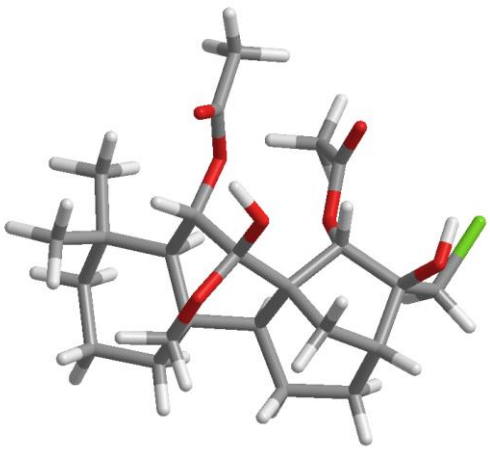
C	-4.60274	-0.50055	0.29799
H	-1.53066	-0.03951	-1.33037
O	-0.23586	0.92674	2.58993
H	0.30252	-1.16755	-1.17541
H	3.71173	-1.66703	1.56569
O	-1.35728	1.90351	0.11022
O	-2.02925	2.98587	1.98678
C	-1.60882	3.01166	0.84134
C	-1.30034	4.26837	0.07081
O	1.12294	0.90971	-1.06967
O	2.01227	2.97370	-0.80824
C	1.37277	2.17596	-1.46985
C	0.75819	2.45074	-2.81772
H	-2.80788	-2.28084	1.56451
H	-1.22153	-3.03796	1.68548
H	-3.60081	-3.66310	-2.08837
H	-3.96912	-3.15727	-0.45101
H	-3.26396	-1.30604	-2.79516
H	-4.88725	-1.53669	-2.15481
H	-1.34687	-2.75959	-1.98238
H	-1.58309	-3.86129	-0.63489
H	-2.58660	0.79988	1.33596
H	1.83616	-0.44831	2.68396
H	1.18979	-2.06205	2.38256
H	2.96187	-3.51138	0.39260
H	2.88991	-2.42528	-0.96653
H	0.77039	-3.50796	-0.96566
H	0.63738	-3.47672	0.77814
H	1.50092	1.44494	0.88348
H	3.86609	1.03521	-1.32601
H	3.15069	-0.51726	-1.79707
H	-3.82362	1.82200	-0.91081
H	-4.92014	0.94792	-1.98570
H	-3.21249	1.13135	-2.42416
H	-4.50580	-1.43331	0.85879
H	-4.52566	0.32573	1.01228
H	-5.62095	-0.47289	-0.10833
H	-0.97898	1.53190	2.78108
H	-1.57747	5.13787	0.66735
H	-1.84291	4.27678	-0.87962
H	-0.22928	4.30443	-0.15548
H	1.08568	3.42510	-3.18156
H	1.03698	1.66984	-3.53164
H	-0.33299	2.43872	-2.72436
Cl	5.35618	-0.75928	-0.95928
H	3.69927	1.65800	1.01747

Conformer 2

Energy: -1922.39378 Hartree (Rel: 0.5 kcal/mol)

XYZ coordinates for conf 2:

O	-1.45893	-1.11932	2.18156
C	-2.06162	-2.00186	1.21966
C	-3.80346	-2.22309	-1.55642
C	-3.97566	-0.76017	-1.96969
C	-3.54039	0.24061	-0.87179
C	-2.05602	-0.08740	-0.45976
C	-1.67947	-1.59720	-0.21445
C	-2.33034	-2.52471	-1.26286
C	-1.54115	0.72617	0.74767
C	-0.58134	-0.12604	1.60866
C	0.54285	-0.86047	0.84343
C	-0.11730	-1.69441	-0.31826
C	1.34164	-1.78370	1.79985
C	2.50131	-2.21485	0.89173
C	1.96888	-3.19522	-0.19218
C	0.43514	-3.13565	-0.35924
C	3.00275	-0.82825	0.38203
C	1.69751	0.05613	0.33476
C	3.78256	-0.94011	-0.93497
O	3.86260	-0.36144	1.41955
C	-3.59134	1.65996	-1.48001



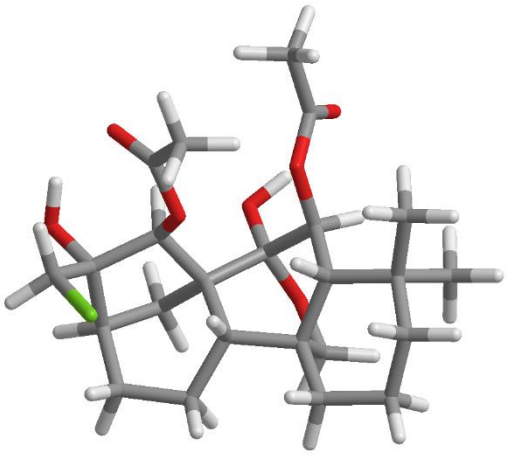
C	-4.56680	0.20427	0.28413
H	-1.44812	0.22157	-1.31962
O	-0.02818	0.59317	2.65866
H	0.14830	-1.22275	-1.26941
H	3.32669	-2.67639	1.44126
O	-0.96170	1.97695	0.27540
O	-1.40425	2.97664	2.26078
C	-1.03753	3.04716	1.09790
C	-0.62521	4.31881	0.40825
O	1.43324	0.58576	-0.97998
O	2.12605	2.66008	-0.37075
C	1.66853	1.90275	-1.20196
C	1.25756	2.29026	-2.59959
H	-3.14361	-1.98418	1.38074
H	-1.72415	-3.02570	1.42788
H	-4.15120	-2.88247	-2.36147
H	-4.42887	-2.45307	-0.68463
H	-3.37653	-0.57864	-2.87490
H	-5.01920	-0.55594	-2.24293
H	-1.76950	-2.42078	-2.20310
H	-2.21397	-3.56968	-0.95085
H	-2.35415	0.99389	1.42320
H	1.70845	-1.20977	2.65379
H	0.74945	-2.61561	2.18560
H	2.24466	-4.21534	0.09833
H	2.45401	-3.02814	-1.15926
H	0.15911	-3.61439	-1.30408
H	-0.02524	-3.74027	0.42971
H	1.82652	0.89324	1.01913
H	3.13774	-1.10073	-1.79595
H	4.52048	-1.73960	-0.86179
H	-3.37082	2.43417	-0.73806
H	-4.59353	1.86210	-1.87753
H	-2.87575	1.76865	-2.30398
H	-4.64544	-0.77152	0.76936
H	-4.34546	0.94390	1.06057
H	-5.55980	0.44917	-0.11161
H	-0.63116	1.33119	2.87968
H	-0.76353	5.16074	1.08716
H	-1.21776	4.46714	-0.50015
H	0.42618	4.24320	0.11340
H	1.70085	3.25262	-2.85889
H	1.55753	1.52749	-3.32264
H	0.16551	2.37754	-2.63513
Cl	4.74639	0.56509	-1.32480
H	4.14642	0.53903	1.18452

Conformer 3

Energy: -1922.38934 Hartree (Rel: 3.2 kcal/mol)

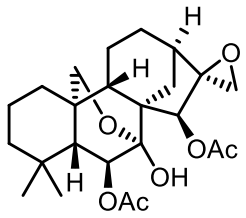
XYZ coordinates for conf 3:

O	1.30741	-0.85361	-2.39756
C	1.75640	-1.93543	-1.56079
C	3.20387	-2.88281	1.23748
C	3.53003	-1.55678	1.92671
C	3.34655	-0.32682	1.00472
C	1.88127	-0.34629	0.42617
C	1.31509	-1.72294	-0.10235
C	1.73677	-2.90383	0.79811
C	1.62245	0.70861	-0.67192
C	0.59109	0.17928	-1.69339
C	-0.68168	-0.44915	-1.08667
C	-0.24924	-1.59776	-0.10418
C	-1.62335	-0.97331	-2.20387
C	-2.85263	-1.38657	-1.38198
C	-2.52267	-2.71756	-0.66191
C	-1.00633	-2.91341	-0.40267
C	-3.07427	-0.12828	-0.48940
C	-1.65646	0.54369	-0.41606
C	-3.87434	-0.31672	0.82091
O	-3.94061	0.73080	-1.24956
C	3.52723	0.94050	1.87011



C	4.47080	-0.31743	-0.05692
H	1.23591	-0.07699	1.27081
O	0.22552	1.14258	-2.62557
H	-0.52448	-1.29625	0.91073
H	-3.75357	-1.51137	-1.99070
O	1.22546	1.97185	-0.06464
O	2.01957	3.13369	-1.84389
C	1.51774	3.10711	-0.73124
C	1.13533	4.33012	0.06192
O	-1.24507	0.93515	0.90620
O	-2.61089	2.72898	0.77265
C	-1.76541	2.08392	1.37396
C	-1.19164	2.44143	2.71941
H	2.84437	-2.01094	-1.65565
H	1.33447	-2.86763	-1.95643
H	3.38419	-3.71714	1.92685
H	3.87032	-3.04684	0.38117
H	2.87302	-1.44700	2.80269
H	4.55893	-1.56210	2.30987
H	1.11267	-2.88020	1.70305
H	1.50630	-3.84924	0.29216
H	2.52184	0.90843	-1.25524
H	-1.85911	-0.16420	-2.89994
H	-1.18563	-1.79134	-2.77952
H	-2.86342	-3.53529	-1.30834
H	-3.08684	-2.81579	0.26744
H	-0.87267	-3.61139	0.42967
H	-0.56677	-3.40214	-1.27914
H	-1.69663	1.44560	-1.02850
H	-4.77214	-0.89227	0.59389
H	-4.16942	0.65959	1.20200
H	3.47804	1.85674	1.27322
H	4.50598	0.92108	2.36522
H	2.75852	1.00445	2.64972
H	4.45181	-1.18405	-0.72260
H	4.44498	0.58185	-0.68122
H	5.44293	-0.32131	0.45060
H	0.98592	1.74096	-2.76219
H	1.47754	5.22421	-0.45989
H	1.56752	4.29096	1.06617
H	0.04548	4.36862	0.16933
H	-1.56294	3.41757	3.03302
H	-1.48776	1.68324	3.45251
H	-0.09890	2.44569	2.67186
Cl	-3.10181	-1.15654	2.25800
H	-3.84041	1.62284	-0.86646

isoserrin B



Isoserrin B - original (misassigned)

	Conf1
Rel energy (kcal/mol):	0.00

C-nom	iGau	Exp	Calc	diff		1	
C1-CH2	8	30.80	30.99	0.19	[	30.99	]
C2-CH2	3	18.50	18.71	0.21	[	18.71	]
C3-CH2	4	41.00	39.77	-1.23	[	39.77	]
C4-C	5	33.50	33.08	-0.42	[	33.08	]
C5-CH	6	54.40	54.30	-0.10	[	54.30	]
C6-CH	9	75.20	77.92	2.72	[	77.92	]
C7-C	10	95.40	98.33	2.93	[	98.33	]
C8-C	11	51.70	51.17	-0.53	[	51.17	]
C9-CH	12	44.40	45.17	0.77	[	45.17	]
C10-C	7	35.90	35.33	-0.57	[	35.33	]
C11-CH2	16	15.60	16.20	0.60	[	16.20	]
C12-CH2	15	25.60	23.41	-2.19	[	23.41	]
C13-CH	14	36.40	35.45	-0.95	[	35.45	]
C14-CH2	13	26.40	26.13	-0.27	[	26.13	]
C15-CH	18	75.70	74.41	-1.29	[	74.41	]
C16-C	17	74.00	65.87	-8.13	[	65.87	]
C17-CH2	19	48.60	55.31	6.71	[	55.31	]
C18-CH3	21	32.90	32.08	-0.82	[	32.08	]
C19-CH3	22	22.30	21.81	-0.49	[	21.81	]
C20-CH2	2	66.30	66.52	0.22	[	66.52	]
C-OAc-6-C	29	173.60	173.48	-0.12	[	173.48	]
C-OAc-6-CH3	30	21.10	20.55	-0.55	[	20.55	]
C-OAc-15-C	33	169.90	171.62	1.72	[	171.62	]
C-OAc-15-CH3	34	21.60	20.71	-0.89	[	20.71	]

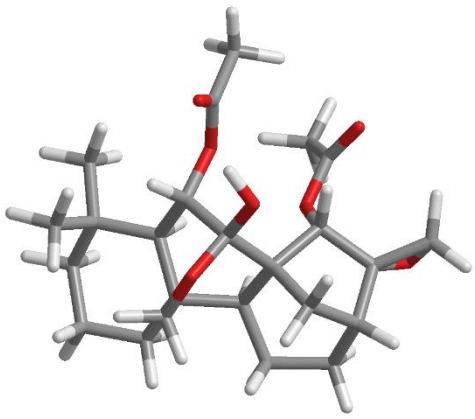
13C chem shifts: RMSD=2.44ppm (MAE=1.44) N=24 {-8.13 6.71}

Conformer 1

Energy: -1461.56520 Hartree (Rel: 0.0 kcal/mol)

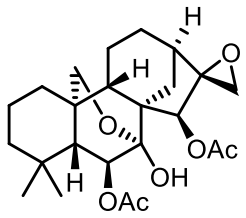
XYZ coordinates for conf 1:

O	-1.04945	-1.03619	2.21808
C	-1.67569	-1.95878	1.30957
C	-3.62061	-2.20999	-1.32279
C	-3.85000	-0.74697	-1.71081
C	-3.33453	0.25469	-0.64899
C	-1.81634	-0.05492	-0.37682
C	-1.40626	-1.55822	-0.15054
C	-2.12449	-2.49298	-1.14651
C	-1.19544	0.79059	0.75837
C	-0.20397	-0.05878	1.58025
C	0.86779	-0.79439	0.74875
C	0.14403	-1.63667	-0.36747
C	1.73761	-1.71256	1.65298
C	2.84701	-2.13506	0.67674
C	2.26821	-3.07757	-0.41819
C	0.72577	-3.06469	-0.46120
C	3.23337	-0.77115	0.10295



C	1.97323	0.12711	0.16094
C	4.58942	-0.20759	0.17102
O	4.04273	-0.70153	-1.07054
C	-3.45192	1.67856	-1.23638
C	-4.25338	0.19650	0.59320
H	-1.29791	0.24502	-1.29626
O	0.41600	0.67203	2.58763
H	0.33756	-1.15679	-1.33097
H	3.70022	-2.60590	1.17442
O	-0.59175	1.98967	0.19078
O	-0.86798	3.11101	2.14184
C	-0.54272	3.09404	0.96466
C	-0.03189	4.28579	0.19944
O	1.64026	0.60965	-1.15224
O	2.88451	2.47952	-0.84813
C	2.17550	1.78114	-1.54871
C	1.75103	2.11254	-2.95810
H	-2.74308	-1.98131	1.54636
H	-1.28252	-2.96568	1.50457
H	-4.02067	-2.86967	-2.10293
H	-4.17246	-2.45546	-0.40671
H	-3.33475	-0.55161	-2.66341
H	-4.91661	-0.55863	-1.89094
H	-1.63951	-2.38002	-2.12695
H	-1.97037	-3.53695	-0.84734
H	-1.95076	1.12356	1.47111
H	2.14391	-1.13369	2.48878
H	1.17663	-2.54786	2.07596
H	2.60516	-4.10389	-0.23253
H	2.68108	-2.79074	-1.39240
H	0.38895	-3.54147	-1.38745
H	0.34451	-3.68887	0.35534
H	2.13573	0.98341	0.81517
H	5.40021	-0.80571	0.58740
H	4.72065	0.87213	0.21349
H	-3.16636	2.44701	-0.50986
H	-4.48825	1.87858	-1.53494
H	-2.81746	1.79991	-2.12254
H	-4.29732	-0.79104	1.05824
H	-3.95699	0.91376	1.36552
H	-5.27557	0.45782	0.29402
H	-0.15435	1.43285	2.81490
H	-0.09178	5.17544	0.82700
H	-0.61381	4.42955	-0.71607
H	1.00913	4.10885	-0.09190
H	2.22669	3.04050	-3.27712
H	2.02911	1.29885	-3.63503
H	0.66209	2.22110	-3.00041

isoserrin B – revised



Isoserrin B - revised, epi-16

	Conf1
Rel energy (kcal/mol):	0.00

C-nom	iGau	Exp	Calc	diff	1
C1-CH2	8	30.80	31.04	0.24	[31.04]
C2-CH2	3	18.50	18.71	0.21	[18.71]
C3-CH2	4	41.00	39.90	-1.10	[39.90]
C4-C	5	33.50	33.05	-0.45	[33.05]
C5-CH	6	54.40	54.51	0.11	[54.51]
C6-CH	9	75.20	78.19	2.99	[78.19]
C7-C	10	95.40	98.36	2.96	[98.36]
C8-C	11	51.70	52.58	0.88	[52.58]
C9-CH	12	44.40	45.22	0.82	[45.22]
C10-C	7	35.90	35.37	-0.53	[35.37]
C11-CH2	16	15.60	16.89	1.29	[16.89]
C12-CH2	15	25.60	25.66	0.06	[25.66]
C13-CH	14	36.40	37.79	1.39	[37.79]
C14-CH2	13	26.40	28.73	2.33	[28.73]
C15-CH	18	75.70	78.40	2.70	[78.40]
C16-C	17	74.00	72.37	-1.63	[72.37]
C17-CH2	19	48.60	48.37	-0.23	[48.37]
C18-CH3	21	32.90	32.27	-0.63	[32.27]
C19-CH3	22	22.30	21.86	-0.44	[21.86]
C20-CH2	2	66.30	66.46	0.16	[66.46]
C-OAc-6-C	29	173.60	173.81	0.21	[173.81]
C-OAc-6-CH3	30	21.10	20.63	-0.47	[20.63]
C-OAc-15-C	33	169.90	171.47	1.57	[171.47]
C-OAc-15-CH3	34	21.60	21.11	-0.49	[21.11]

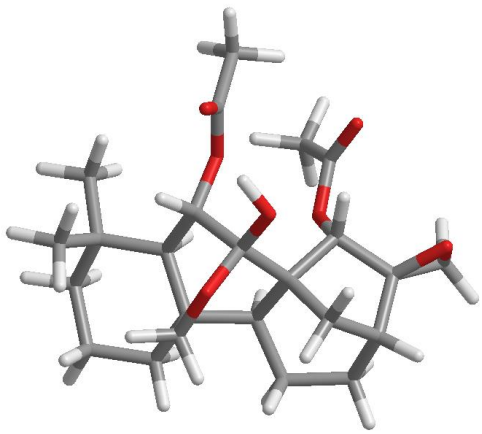
13C chem shifts: RMSD=1.35ppm (MAE=1.00) N=24 {-1.63 2.99}

Conformer 1

Energy: -1461.56237 Hartree (Rel: 0.0 kcal/mol)

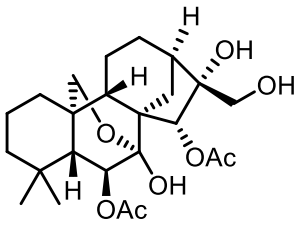
XYZ coordinates for conf 1:

O	-0.88944	-1.08336	2.21768
C	-1.52458	-2.02552	1.33637
C	-3.56566	-2.35147	-1.21326
C	-3.85876	-0.89950	-1.59872
C	-3.33699	0.12564	-0.56258
C	-1.79972	-0.13125	-0.34507
C	-1.32978	-1.61923	-0.13418
C	-2.05491	-2.58200	-1.09788
C	-1.16780	0.73237	0.76958
C	-0.10555	-0.07645	1.54426
C	0.95551	-0.78352	0.67412
C	0.21172	-1.64385	-0.41523
C	1.87198	-1.68520	1.54873
C	2.96499	-2.06377	0.53614
C	2.37847	-3.00360	-0.55939
C	0.83693	-3.05053	-0.54074
C	3.30604	-0.68258	-0.01544
C	2.02337	0.16642	0.04677
C	4.43769	-0.39314	-0.90087
O	4.50085	-0.05703	0.49469



C	-3.52660	1.53992	-1.15447
C	-4.20576	0.04540	0.71395
H	-1.32519	0.18589	-1.28245
O	0.52961	0.67762	2.52212
H	0.34780	-1.15397	-1.38358
H	3.85306	-2.50556	0.99680
O	-0.65384	1.96825	0.19150
O	-0.90665	3.04271	2.17148
C	-0.64961	3.06769	0.97796
C	-0.29355	4.30874	0.20542
O	1.62988	0.63289	-1.26322
O	2.48606	2.69922	-0.88734
C	1.88341	1.91742	-1.59624
C	1.29974	2.24387	-2.94893
H	-2.58010	-2.08100	1.61718
H	-1.09284	-3.01980	1.51424
H	-3.97488	-3.02906	-1.97303
H	-4.07076	-2.60944	-0.27395
H	-3.38732	-0.69305	-2.57155
H	-4.93710	-0.74746	-1.73848
H	-1.61510	-2.45583	-2.09787
H	-1.85228	-3.61883	-0.80289
H	-1.90582	1.01996	1.51883
H	2.29134	-1.10072	2.37368
H	1.34370	-2.53580	1.98296
H	2.76368	-4.01959	-0.41605
H	2.72867	-2.68060	-1.54826
H	0.48133	-3.53538	-1.45571
H	0.51287	-3.69211	0.28669
H	2.19484	1.03223	0.68601
H	5.09044	-1.20832	-1.21617
H	4.39989	0.45680	-1.58116
H	-3.24129	2.32412	-0.44521
H	-4.57989	1.70061	-1.41505
H	-2.93120	1.67590	-2.06539
H	-4.18991	-0.93651	1.19273
H	-3.91180	0.78546	1.46541
H	-5.24862	0.25914	0.45052
H	-0.06119	1.41311	2.77979
H	-0.37377	5.17835	0.85825
H	-0.95768	4.42277	-0.65716
H	0.73074	4.21836	-0.17076
H	1.73342	3.17231	-3.32283
H	1.47359	1.43008	-3.65790
H	0.21606	2.37045	-2.84462

isoserrin D



Isoserrin D - original (misassigned)

	Conf1	Conf2
Rel energy (kcal/mol):	0.00	3.42

C-nom	iGau	Exp	Calc	diff	1	2
C1-CH2	8	30.90	31.74	0.84	[31.74	31.48]
C2-CH2	3	18.50	18.74	0.24	[18.74	18.71]
C3-CH2	4	41.10	39.42	-1.68	[39.42	39.27]
C4-C	5	33.50	33.03	-0.47	[33.03	33.07]
C5-CH	6	54.40	54.31	-0.09	[54.31	54.56]
C6-CH	9	75.20	79.54	4.34	[79.54	79.91]
C7-C	10	95.30	98.29	2.99	[98.29	98.03]
C8-C	11	52.40	51.81	-0.59	[51.81	51.86]
C9-CH	12	44.30	53.07	8.77	[53.07	51.77]
C10-C	7	35.90	35.18	-0.72	[35.18	35.41]
C11-CH2	16	15.60	16.30	0.70	[16.30	16.35]
C12-CH2	15	21.50	20.57	-0.93	[20.56	22.93]
C13-CH	14	40.10	42.00	1.90	[42.01	40.18]
C14-CH2	13	25.30	28.88	3.58	[28.88	28.64]
C15-CH	18	81.10	87.80	6.70	[87.80	87.65]
C16-C	17	84.70	81.59	-3.11	[81.58	85.46]
C17-CH2	19	63.80	67.52	3.72	[67.52	68.36]
C18-CH3	21	32.90	32.11	-0.79	[32.11	31.97]
C19-CH3	22	22.30	21.71	-0.59	[21.71	21.60]
C20-CH2	2	66.30	65.90	-0.40	[65.90	65.50]
C-OAc-6-C	29	173.40	172.92	-0.48	[172.92	172.87]
C-OAc-6-CH3	30	21.10	20.91	-0.19	[20.91	20.97]
C-OAc-15-C	33	171.30	168.56	-2.74	[168.55	172.68]
C-OAc-15-CH3	34	21.50	21.04	-0.46	[21.04	20.63]

13C chem shifts: RMSD=2.92ppm (MAE=1.96) N=24 {-3.11 8.77}

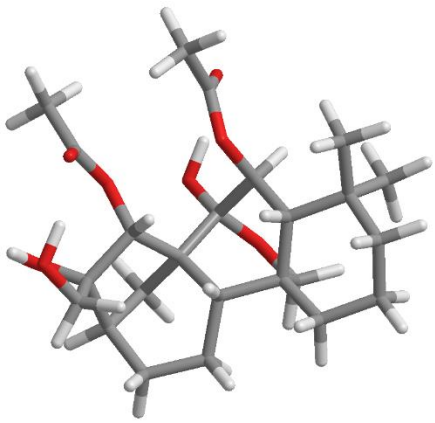
Fractions: 0.997 0.003

Conformer 1

Energy: -1538.00565 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	1.37184	-0.49370	-2.27482
C	2.22790	-1.39348	-1.55846
C	4.23978	-1.79202	1.00316
C	4.20999	-0.41133	1.66283
C	3.49956	0.66034	0.80104
C	2.05695	0.13281	0.45539
C	1.91956	-1.34340	-0.05667
C	2.81720	-2.30518	0.75226
C	1.25994	1.05303	-0.49682
C	0.40181	0.21859	-1.47616
C	-0.51948	-0.80744	-0.76845
C	0.41297	-1.75114	0.10941
C	-1.37457	-1.63950	-1.75314
C	-2.22612	-2.46782	-0.77412
C	-1.35482	-3.60381	-0.18481
C	0.14599	-3.24689	-0.16728
C	-2.72218	-1.40068	0.25218
C	-1.63236	-0.23546	0.15912
C	-2.90537	-1.88730	1.70698



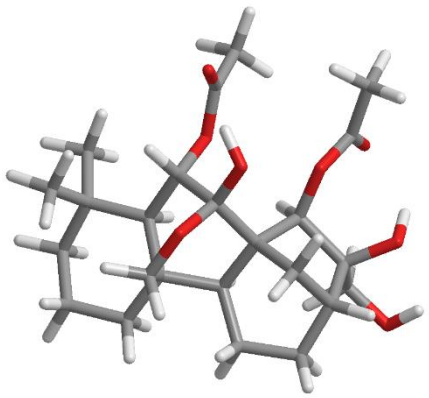
O	-3.99506	-0.94661	-0.19362
C	3.36885	1.94591	1.64794
C	4.38985	1.00668	-0.41481
H	1.51992	0.15411	1.41312
O	-0.31012	0.99779	-2.37534
H	0.17670	-1.57660	1.16817
H	-3.11833	-2.89286	-1.24143
O	0.48420	1.96984	0.32992
O	0.36818	3.50476	-1.33236
C	0.18486	3.18400	-0.16834
C	-0.36792	4.09554	0.89669
O	-2.22841	0.92616	-0.44306
O	-3.13571	1.56916	1.52971
C	-2.99720	1.70478	0.31878
C	-3.66511	2.78376	-0.49433
H	3.26466	-1.12167	-1.77748
H	2.07478	-2.40667	-1.95081
H	4.76674	-2.50354	1.65103
H	4.80910	-1.75795	0.06586
H	3.68932	-0.49372	2.62886
H	5.22886	-0.06993	1.88813
H	2.34004	-2.47664	1.72831
H	2.85531	-3.28085	0.25372
H	1.91631	1.65957	-1.12304
H	-1.99548	-0.96660	-2.35120
H	-0.78050	-2.24724	-2.44032
H	-1.49118	-4.50166	-0.79889
H	-1.69233	-3.88155	0.81889
H	0.65641	-3.85844	0.58280
H	0.58215	-3.52655	-1.13182
H	-1.25101	0.05837	1.13898
O	-3.75033	-0.99600	2.42952
H	-3.42290	-2.85158	1.71386
H	2.95361	2.77839	1.06965
H	4.35644	2.25904	2.00787
H	2.72623	1.78841	2.52206
H	4.63607	0.14326	-1.03692
H	3.93740	1.76448	-1.06291
H	5.33787	1.42366	-0.05435
H	0.04754	1.90688	-2.35162
H	-0.82931	4.96817	0.43299
H	0.45164	4.42591	1.54538
H	-1.09012	3.56678	1.52444
H	-4.04802	3.56440	0.16420
H	-4.50072	2.33685	-1.04505
H	-2.97291	3.20187	-1.22991
H	-3.37054	-0.09339	2.36677
H	-1.93764	-2.01468	2.21056
H	-4.48337	-0.72893	0.62605

Conformer 2

Energy: -1538.01110 Hartree (Rel: 3.4 kcal/mol)

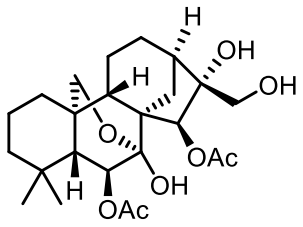
XYZ coordinates for conf 2:

O	-1.31336	-0.39752	2.29002
C	-2.07993	-1.42310	1.64576
C	-4.08867	-2.14652	-0.84038
C	-4.20846	-0.80285	-1.56395
C	-3.58122	0.37173	-0.77480
C	-2.08754	-0.00218	-0.44874
C	-1.80120	-1.42782	0.13815
C	-2.61807	-2.50928	-0.60216
C	-1.35235	1.04398	0.42014
C	-0.41914	0.34903	1.43850
C	0.58430	-0.62795	0.77192
C	-0.26457	-1.70188	-0.03687
C	1.53565	-1.31633	1.77717
C	2.43297	-2.12798	0.82253
C	1.66551	-3.39236	0.38406
C	0.13862	-3.15594	0.31062
C	2.74717	-1.11695	-0.32934
C	1.62922	-0.00634	-0.20203



C	2.80142	-1.68713	-1.75757
O	4.06337	-0.61342	-0.05442
C	-3.59037	1.62118	-1.68359
C	-4.46942	0.69397	0.44934
H	-1.58266	0.01098	-1.42378
O	0.22152	1.23997	2.28682
H	-0.06525	-1.55814	-1.10719
H	3.38396	-2.41431	1.27926
O	-0.65661	1.94939	-0.48949
O	-0.60104	3.60911	1.05140
C	-0.42284	3.21251	-0.09010
C	0.05874	4.06949	-1.23239
O	2.16228	1.19729	0.39767
O	3.25460	1.76884	-1.49714
C	2.92955	2.00549	-0.34169
C	3.35805	3.22104	0.44277
H	-3.13550	-1.24765	1.87175
H	-1.81548	-2.38977	2.09238
H	-4.55805	-2.93587	-1.44058
H	-4.63849	-2.12180	0.10880
H	-3.70781	-0.88291	-2.54063
H	-5.26102	-0.57090	-1.77323
H	-2.14626	-2.68144	-1.58067
H	-2.55214	-3.45872	-0.05823
H	-2.04420	1.64800	1.00964
H	2.10233	-0.55399	2.31855
H	1.01712	-1.93617	2.51348
H	1.85549	-4.18154	1.12155
H	2.06304	-3.76672	-0.56217
H	-0.30140	-3.83928	-0.42191
H	-0.29955	-3.42992	1.27575
H	1.21087	0.26821	-1.17244
O	3.82670	-2.66036	-1.88081
H	1.86374	-2.16654	-2.05063
H	-3.23745	2.51467	-1.15671
H	-4.61135	1.82719	-2.02714
H	-2.95928	1.47968	-2.56882
H	-4.63519	-0.16260	1.10650
H	-4.06294	1.50653	1.06042
H	-5.45428	1.02374	0.09747
H	-0.18414	2.12227	2.17830
H	0.41329	5.02780	-0.85178
H	-0.76868	4.24005	-1.93030
H	0.85313	3.56200	-1.78744
H	3.76574	3.97223	-0.23484
H	4.13444	2.92529	1.15773
H	2.52299	3.63015	1.01736
H	4.57432	-2.30129	-1.36966
H	2.97024	-0.84447	-2.44773
H	4.24605	0.07600	-0.71960

isoserrin D - revised



Isoserrin D - revised, epi-15

	Conf1	Conf2
Rel energy (kcal/mol):	0.00	0.92

C-nom	**iGau**	**Exp**	**Calc**	**diff**		**1**	**2**	
C1-CH2	8	30.90	31.60	0.70	[	31.71	31.08	]
C2-CH2	3	18.50	18.74	0.24	[	18.75	18.67	]
C3-CH2	4	41.10	40.08	-1.02	[	40.11	39.91	]
C4-C	5	33.50	32.96	-0.54	[	32.95	32.98	]
C5-CH	6	54.40	53.14	-1.26	[	52.96	54.01	]
C6-CH	9	75.20	78.20	3.00	[	78.18	78.31	]
C7-C	10	95.30	98.09	2.79	[	98.07	98.20	]
C8-C	11	52.40	52.44	0.04	[	52.47	52.32	]
C9-CH	12	44.30	45.62	1.32	[	45.77	44.91	]
C10-C	7	35.90	35.40	-0.50	[	35.41	35.37	]
C11-CH2	16	15.60	16.57	0.97	[	16.58	16.53	]
C12-CH2	15	21.50	23.13	1.63	[	23.59	20.95	]
C13-CH	14	40.10	40.39	0.29	[	39.97	42.36	]
C14-CH2	13	25.30	26.88	1.58	[	26.77	27.40	]
C15-CH	18	81.10	84.18	3.08	[	84.76	81.45	]
C16-C	17	84.70	85.87	1.17	[	85.86	85.94	]
C17-CH2	19	63.80	64.29	0.49	[	64.49	63.36	]
C18-CH3	21	32.90	32.62	-0.28	[	32.68	32.36	]
C19-CH3	22	22.30	22.28	-0.02	[	22.33	22.05	]
C20-CH2	2	66.30	66.83	0.53	[	66.91	66.43	]
C-OAc-6-C	29	173.40	173.21	-0.19	[	172.98	174.33	]
C-OAc-6-CH3	30	21.10	20.74	-0.36	[	20.68	21.02	]
C-OAc-15-C	33	171.30	170.49	-0.81	[	170.88	168.65	]
C-OAc-15-CH3	34	21.50	20.97	-0.53	[	20.85	21.56	]

13C chem shifts: RMSD=1.31ppm (MAE=0.97) N=24 {-1.26 3.08}

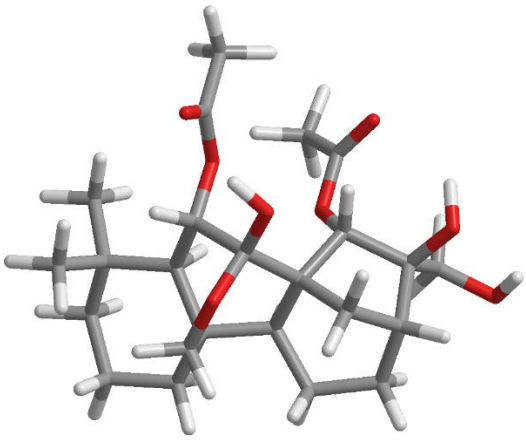
Fractions: 0.826 0.174

Conformer 1

Energy: -1538.01297 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	-1.08501	-1.07428	2.28296
C	-1.61935	-2.07707	1.40040
C	-3.36245	-2.72785	-1.31000
C	-3.72484	-1.33576	-1.83068
C	-3.41328	-0.20490	-0.82048
C	-1.89610	-0.30487	-0.40939
C	-1.31865	-1.73400	-0.06855
C	-1.85917	-2.81518	-1.02842
C	-1.48946	0.64663	0.73801
C	-0.39424	-0.00215	1.61236
C	0.79842	-0.60140	0.83753
C	0.24081	-1.63692	-0.20856
C	1.81495	-1.26226	1.80559
C	2.95947	-1.60401	0.84034
C	2.52807	-2.81203	-0.03373
C	0.99251	-2.98323	-0.11813
C	3.14415	-0.25132	0.08878
C	1.74041	0.43369	0.17619
C	3.73821	-0.34588	-1.32350



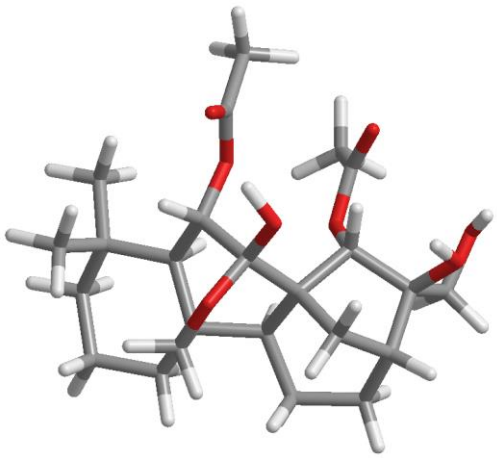
O	4.09612	0.49707	0.87688
C	-3.65061	1.14432	-1.53505
C	-4.41775	-0.28177	0.35268
H	-1.33828	0.02468	-1.29439
O	0.08349	0.86078	2.59106
H	0.42255	-1.23830	-1.21220
H	3.89561	-1.83613	1.35454
O	-1.09000	1.93726	0.19179
O	-1.66918	2.98556	2.11824
C	-1.27310	3.02913	0.96454
C	-0.91983	4.29462	0.22773
O	1.25362	0.87722	-1.11142
O	2.36925	2.82995	-0.86982
C	1.60463	2.12011	-1.50015
C	0.93099	2.49777	-2.79422
H	-2.69335	-2.16068	1.59354
H	-1.16953	-3.04202	1.66624
H	-3.63315	-3.48769	-2.05374
H	-3.94201	-2.96502	-0.40890
H	-3.16117	-1.15090	-2.75771
H	-4.78813	-1.28791	-2.10003
H	-1.32898	-2.71419	-1.98661
H	-1.60382	-3.80891	-0.64087
H	-2.32185	0.83514	1.41663
H	2.13515	-0.53497	2.55625
H	1.40358	-2.12525	2.33320
H	2.94805	-3.72243	0.40999
H	2.96581	-2.74643	-1.03318
H	0.74684	-3.60589	-0.98439
H	0.65387	-3.54300	0.76072
H	1.81892	1.30664	0.82431
O	5.00776	-0.97952	-1.27345
H	3.82919	0.66885	-1.74049
H	-3.51501	1.99671	-0.86150
H	-4.67625	1.18965	-1.92146
H	-2.96712	1.27265	-2.38316
H	-4.35546	-1.21230	0.92229
H	-4.29758	0.54770	1.05734
H	-5.43774	-0.21363	-0.04426
H	-0.63416	1.47786	2.83393
H	-1.14307	5.15683	0.85656
H	-1.47859	4.35966	-0.71100
H	0.14742	4.28714	-0.01914
H	1.30860	3.46039	-3.14030
H	1.11100	1.73034	-3.55335
H	-0.15082	2.55830	-2.63590
H	5.45932	-0.56378	-0.51663
H	3.10957	-0.92484	-2.00365
H	4.02941	1.42535	0.58765

Conformer 2

Energy: -1538.01149 Hartree (Rel: 0.9 kcal/mol)

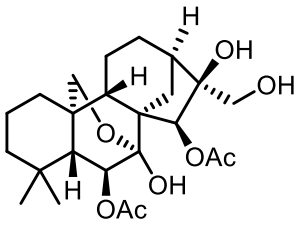
XYZ coordinates for conf 2:

O	-1.21516	-1.06845	2.21144
C	-1.83858	-1.98321	1.29314
C	-3.71483	-2.26481	-1.38760
C	-3.93148	-0.80854	-1.80472
C	-3.45249	0.20945	-0.74138
C	-1.94335	-0.09296	-0.41003
C	-1.53416	-1.59373	-0.16368
C	-2.22407	-2.54235	-1.16703
C	-1.37121	0.75173	0.75030
C	-0.37184	-0.08085	1.58293
C	0.72168	-0.81606	0.77680
C	0.02195	-1.67124	-0.34358
C	1.57183	-1.72137	1.70786
C	2.70387	-2.13844	0.75758
C	2.13790	-3.13764	-0.29389
C	0.59688	-3.10373	-0.39675
C	3.15182	-0.75754	0.19784
C	1.83874	0.10728	0.20847



C	3.89179	-0.79854	-1.14661
O	4.13579	-0.17546	1.07986
C	-3.55603	1.62268	-1.35685
C	-4.41337	0.16860	0.46938
H	-1.38971	0.20945	-1.30805
O	0.22490	0.65883	2.59657
H	0.23607	-1.20410	-1.30976
H	3.55776	-2.58609	1.27435
O	-0.81187	1.98535	0.21429
O	-1.13477	3.04447	2.19166
C	-0.83280	3.07721	1.00783
C	-0.44093	4.32271	0.26090
O	1.52302	0.61412	-1.10016
O	2.32812	2.67152	-0.57476
C	1.87911	1.88935	-1.38828
C	1.65127	2.18939	-2.84718
H	-2.91150	-1.98869	1.50604
H	-1.46593	-2.99493	1.50161
H	-4.09323	-2.93717	-2.16771
H	-4.29118	-2.49555	-0.48284
H	-3.38502	-0.62720	-2.74261
H	-4.99139	-0.62293	-2.02289
H	-1.71350	-2.44090	-2.13570
H	-2.07626	-3.58203	-0.85054
H	-2.15050	1.04082	1.45630
H	1.94739	-1.13910	2.55605
H	1.00780	-2.55715	2.12592
H	2.44139	-4.15205	-0.01059
H	2.58020	-2.96408	-1.27992
H	0.28880	-3.59412	-1.32571
H	0.17884	-3.70939	0.41501
H	1.97667	0.96421	0.86886
O	4.44835	0.46497	-1.47334
H	3.21691	-1.06762	-1.96015
H	-3.30385	2.40548	-0.63398
H	-4.58157	1.80919	-1.69852
H	-2.88888	1.73377	-2.21993
H	-4.45733	-0.80638	0.96042
H	-4.15599	0.91221	1.23072
H	-5.42856	0.40424	0.12805
H	-0.35855	1.41431	2.81300
H	-0.57217	5.19090	0.90745
H	-1.04555	4.43030	-0.64490
H	0.60701	4.23936	-0.04507
H	1.64234	3.26871	-3.00631
H	2.47868	1.75299	-3.41804
H	0.71942	1.74275	-3.20343
H	4.77226	0.82124	-0.62568
H	4.67663	-1.56937	-1.07950
H	3.69504	0.17181	1.87079

isoserrin E



Isoserrin E - original, correct

	Conf1	Conf2	Conf3
Rel energy (kcal/mol):	0.00	0.23	0.29

C-nom	**iGau**	**Exp**	**Calc**	**diff**		**1**	**2**	**3**	
C1-CH2	8	31.00	31.24	0.24	[	31.55	30.71	31.33	]
C2-CH2	3	18.50	18.74	0.24	[	18.74	18.68	18.81	]
C3-CH2	4	41.10	39.90	-1.20	[	40.04	39.64	39.95	]
C4-C	5	33.50	33.00	-0.50	[	32.94	33.12	32.98	]
C5-CH	6	54.10	54.15	0.05	[	53.86	54.88	53.82	]
C6-CH	9	75.50	78.18	2.68	[	78.47	77.79	78.13	]
C7-C	10	95.30	98.25	2.95	[	98.12	98.29	98.43	]
C8-C	11	51.60	51.24	-0.36	[	51.26	51.77	50.63	]
C9-CH	12	44.40	45.62	1.22	[	45.98	45.27	45.41	]
C10-C	7	35.90	35.36	-0.54	[	35.42	35.36	35.27	]
C11-CH2	16	14.80	16.26	1.46	[	16.09	16.49	16.30	]
C12-CH2	15	19.00	20.22	1.22	[	20.56	19.57	20.40	]
C13-CH	14	37.00	36.20	-0.80	[	36.17	35.50	37.02	]
C14-CH2	13	24.20	25.58	1.38	[	25.44	26.06	25.27	]
C15-CH	18	75.00	77.34	2.34	[	75.80	80.43	76.40	]
C16-C	17	79.40	79.35	-0.05	[	78.73	81.66	77.79	]
C17-CH2	19	70.30	68.36	-1.94	[	68.76	67.77	68.37	]
C18-CH3	21	33.00	32.29	-0.71	[	32.57	31.86	32.32	]
C19-CH3	22	22.40	21.94	-0.46	[	22.15	21.58	22.01	]
C20-CH2	2	66.50	66.54	0.04	[	66.62	66.29	66.70	]
C-OAc-6-C	29	173.50	173.30	-0.20	[	173.65	172.68	173.41	]
C-OAc-6-CH3	30	21.00	20.65	-0.35	[	20.65	20.64	20.65	]
C-OAc-15-C	33	172.20	170.18	-2.02	[	168.13	171.65	171.90	]
C-OAc-15-CH3	34	21.70	20.99	-0.71	[	21.13	20.69	21.09	]

13C chem shifts: RMSD=1.30ppm (MAE=0.99) N=24 {-2.02 2.95}

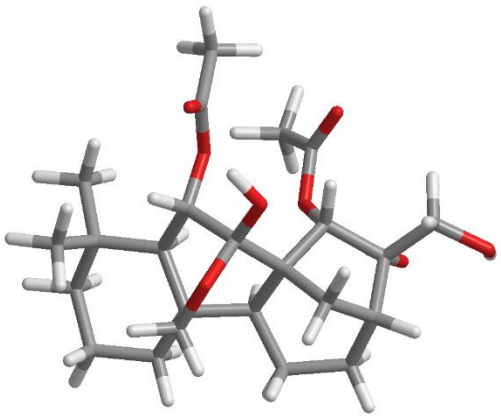
Fractions: 0.436 0.297 0.267

Conformer 1

Energy: -1538.01442 Hartree (Rel: 0.0 kcal/mol)

XYZ coordinates for conf 1:

O	-0.96722	-1.09641	2.26155
C	-1.58823	-2.07123	1.40526
C	-3.59988	-2.57782	-1.14054
C	-3.95954	-1.15808	-1.58314
C	-3.50505	-0.07105	-0.57906
C	-1.95983	-0.23986	-0.32743
C	-1.41093	-1.69612	-0.07600
C	-2.08070	-2.72692	-1.00939
C	-1.39933	0.67161	0.78656
C	-0.27129	-0.04805	1.55802
C	0.82518	-0.69193	0.68237
C	0.13123	-1.65038	-0.35714
C	1.84671	-1.46910	1.55460
C	2.91955	-1.82726	0.51628
C	2.36775	-2.90900	-0.44864
C	0.82923	-3.02737	-0.40471
C	3.16139	-0.44469	-0.16617



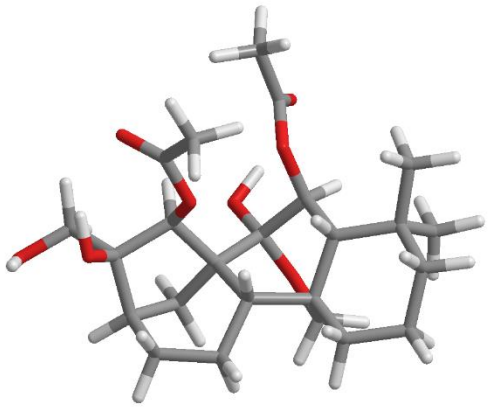
C	1.79255	0.31398	0.00422
C	4.29552	0.33514	0.52260
O	3.57220	-0.54855	-1.53082
C	-3.75872	1.30811	-1.22761
C	-4.38901	-0.14836	0.68729
H	-1.48296	0.08632	-1.26035
O	0.32421	0.76793	2.51176
H	0.23708	-1.20883	-1.35331
H	3.85510	-2.17164	0.96666
O	-0.98868	1.94788	0.21311
O	-1.32910	2.99105	2.19707
C	-1.07214	3.04081	1.00455
C	-0.81121	4.31001	0.23899
O	1.31265	0.76729	-1.28326
O	2.06897	2.87654	-0.91632
C	1.48354	2.07672	-1.61467
C	0.82765	2.38253	-2.93659
H	-2.64191	-2.14501	1.69066
H	-1.13230	-3.04943	1.60600
H	-3.96961	-3.30352	-1.87569
H	-4.09814	-2.82386	-0.19437
H	-3.48552	-0.96399	-2.55724
H	-5.04196	-1.06494	-1.74154
H	-1.64150	-2.61374	-2.01124
H	-1.82734	-3.74092	-0.67709
H	-2.15704	0.89488	1.53797
H	2.23803	-0.81316	2.33854
H	1.40719	-2.33506	2.05332
H	2.79917	-3.88252	-0.18794
H	2.70581	-2.68520	-1.46547
H	0.48541	-3.58676	-1.28092
H	0.54392	-3.62758	0.46679
H	1.92084	1.19063	0.63928
O	5.55643	-0.26442	0.27040
H	4.26981	1.37552	0.16378
H	-3.52715	2.13250	-0.54529
H	-4.81436	1.40205	-1.51053
H	-3.15565	1.44103	-2.13407
H	-4.31371	-1.10161	1.21604
H	-4.16023	0.64753	1.40366
H	-5.43929	-0.02111	0.39871
H	-0.32731	1.44066	2.79303
H	-0.96250	5.16714	0.89566
H	-1.47789	4.37686	-0.62650
H	0.21852	4.30437	-0.13291
H	1.16409	3.35539	-3.29675
H	1.04983	1.60816	-3.67603
H	-0.25867	2.40483	-2.79412
H	5.59396	-0.37752	-0.69537
H	4.15968	0.34578	1.60887
H	2.82419	-0.27769	-2.08810

Conformer 2

Energy: -1538.01478 Hartree (Rel: 0.2 kcal/mol)

XYZ coordinates for conf 2:

O	1.12457	-1.06620	-2.19996
C	1.73614	-2.01591	-1.30958
C	3.84563	-2.29739	1.18208
C	4.18141	-0.83705	1.49852
C	3.63266	0.15867	0.44754
C	2.08490	-0.08058	0.30932
C	1.58764	-1.56526	0.15288
C	2.32755	-2.50546	1.12688
C	1.41105	0.77748	-0.78585
C	0.34854	-0.05063	-1.53630
C	-0.70227	-0.73141	-0.63222
C	0.05445	-1.55658	0.47537
C	-1.62305	-1.66733	-1.45781
C	-2.72470	-1.97857	-0.43412
C	-2.13873	-2.85374	0.71366
C	-0.59791	-2.94153	0.67718



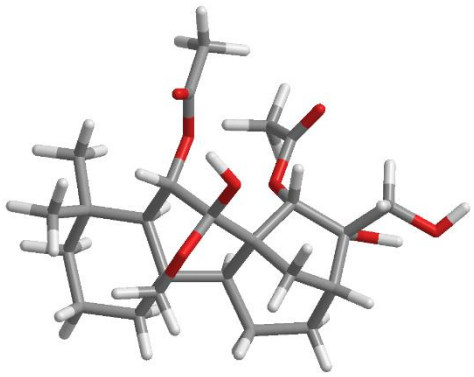
C	-3.11476	-0.54768	0.01494
C	-1.75504	0.24852	-0.02795
C	-4.13918	0.08385	-0.95262
O	-3.73171	-0.57193	1.30314
C	3.86383	1.59227	0.97413
C	4.44395	0.01662	-0.86094
H	1.66184	0.25991	1.26285
O	-0.30136	0.68519	-2.52255
H	-0.04809	-1.02636	1.42488
H	-3.59547	-2.46734	-0.87964
O	0.86683	1.98836	-0.18191
O	1.04998	3.11053	-2.14404
C	0.78244	3.09131	-0.95295
C	0.30447	4.28247	-0.16342
O	-1.32071	0.70224	1.27373
O	-2.93341	2.28024	1.37143
C	-1.93633	1.75002	1.83727
C	-1.24601	2.17162	3.11004
H	2.78103	-2.12111	-1.61306
H	1.25977	-2.99544	-1.45296
H	4.26950	-2.95206	1.95383
H	4.31273	-2.60255	0.23723
H	3.75696	-0.58472	2.48204
H	5.26759	-0.70218	1.58587
H	1.92330	-2.33459	2.13518
H	2.09787	-3.54874	0.87779
H	2.12611	1.09605	-1.54514
H	-2.01152	-1.14062	-2.33366
H	-1.10579	-2.55427	-1.82729
H	-2.54888	-3.86772	0.64211
H	-2.46771	-2.45540	1.67808
H	-0.24157	-3.38471	1.61313
H	-0.29565	-3.63365	-0.11755
H	-1.85733	1.12851	-0.66651
O	-5.37191	-0.61846	-0.91597
H	-4.27230	1.13981	-0.66806
H	3.55600	2.35096	0.24594
H	4.92910	1.75100	1.18155
H	3.31001	1.77209	1.90334
H	4.41818	-0.99045	-1.28309
H	4.10815	0.71042	-1.63854
H	5.49504	0.25365	-0.65677
H	0.27790	1.42426	-2.79257
H	0.36227	5.17830	-0.78227
H	0.90365	4.40887	0.74303
H	-0.73518	4.12200	0.14427
H	-1.77667	3.01349	3.55555
H	-1.21943	1.33434	3.81500
H	-0.21047	2.45292	2.89386
H	-5.53512	-0.79206	0.02850
H	-3.78766	0.06048	-1.98790
H	-3.92639	0.35500	1.53360

Conformer 3

Energy: -1538.01432 Hartree (Rel: 0.3 kcal/mol)

XYZ coordinates for conf 3:

O	-1.08067	-1.07321	2.24568
C	-1.71249	-2.02385	1.37040
C	-3.72817	-2.41433	-1.19393
C	-4.04050	-0.97290	-1.60268
C	-3.54962	0.07389	-0.57327
C	-2.01098	-0.15254	-0.33215
C	-1.51426	-1.63024	-0.10301
C	-2.21515	-2.61783	-1.05970
C	-1.41220	0.73017	0.78582
C	-0.33009	-0.04858	1.56390
C	0.74899	-0.72257	0.69000
C	0.02975	-1.63273	-0.37470
C	1.72667	-1.55538	1.55835
C	2.80203	-1.92581	0.52744
C	2.22550	-2.95205	-0.48396



C	0.68417	-3.02938	-0.44996
C	3.10610	-0.53195	-0.11856
C	1.75585	0.25979	0.03391
C	4.23075	0.19514	0.63645
O	3.48840	-0.58511	-1.48507
C	-3.75635	1.47720	-1.18549
C	-4.43392	-0.00570	0.69269
H	-1.52762	0.16789	-1.26346
O	0.28526	0.72951	2.53856
H	0.16269	-1.17188	-1.35775
H	3.71157	-2.32478	0.98760
O	-0.92150	1.97491	0.20816
O	-1.20207	3.06275	2.17790
C	-0.91886	3.07393	0.98972
C	-0.51693	4.30200	0.21630
O	1.28673	0.73583	-1.23637
O	2.45587	2.66616	-1.02829
C	1.72698	1.93100	-1.66920
C	1.17295	2.23954	-3.03858
H	-2.76932	-2.07970	1.64762
H	-1.27811	-3.01446	1.55941
H	-4.11817	-3.10904	-1.94841
H	-4.23912	-2.66736	-0.25634
H	-3.55966	-0.77133	-2.57186
H	-5.11935	-0.84066	-1.75843
H	-1.76704	-2.49906	-2.05685
H	-1.99847	-3.64682	-0.74774
H	-2.16245	1.00104	1.52953
H	2.12904	-0.93308	2.36404
H	1.25005	-2.41748	2.02939
H	2.62985	-3.94753	-0.26529
H	2.56868	-2.68628	-1.48850
H	0.33096	-3.55638	-1.34253
H	0.37601	-3.64326	0.40460
H	1.89953	1.12149	0.68808
O	5.44775	-0.48495	0.30591
H	4.26211	1.23789	0.30026
H	-3.49229	2.27510	-0.48326
H	-4.80908	1.61660	-1.46056
H	-3.15221	1.61158	-2.09081
H	-4.40249	-0.97932	1.18753
H	-4.16673	0.75283	1.43575
H	-5.47770	0.18030	0.41219
H	-0.33337	1.43811	2.80451
H	-0.59407	5.17968	0.85863
H	-1.15453	4.42292	-0.66498
H	0.51499	4.18808	-0.13296
H	1.55748	3.19966	-3.38452
H	1.45560	1.44959	-3.74153
H	0.07907	2.27106	-2.99791
H	6.18633	0.12579	0.44827
H	4.05565	0.17856	1.72079
H	4.45263	-0.73775	-1.45516