BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Two new aromatic polyketides from a sponge-derived *Fusarium*

Mada Triandala Sibero, Tao Zhou, Keisuke Fukaya, Daisuke Urabe, Ocky K. Karna Radjasa, Agus Sabdono, Agus Trianto and Yasuhiro Igarashi

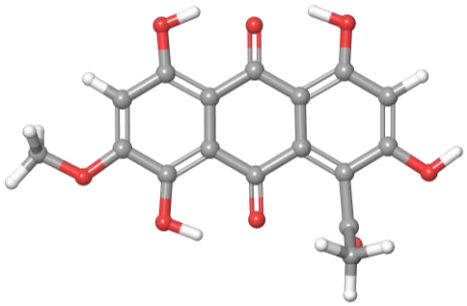
Beilstein J. Org. Chem. **2019,** *15,* 2941–2947. doi:10.3762/bjoc.15.289

NMR chemical shift calculation for compound 1

Table of contents

Cartesian coordinates of the optimized structures of a and b

Structure, energy and Cartesian coordinate of **a-conformer 1**:

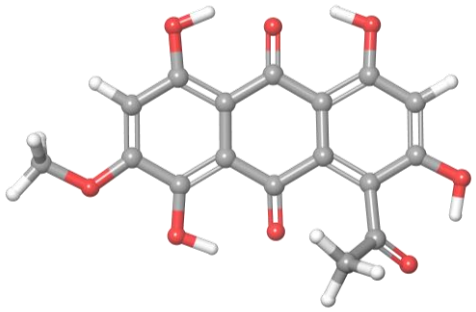


a-conformer 1 (ΔG = 0.0 kcal/mol, Boltzmann pop. (298 K) = 69%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5372187
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7588507
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.270808
	Thermal correction to Energy (a.u.)	=	0.291983
	Thermal correction to Enthalpy (a.u.)	=	0.292927
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.221632

C	2.26967	−1.23710	0.01793	O	−3.15413	−2.64916	1.19964
C	1.16475	−0.39446	0.01155	C	−3.02948	−2.84604	−1.18566
C	1.32851	1.02632	−0.00668	O	2.21109	−2.57071	0.03157
C	2.62161	1.55869	−0.01594	O	2.88072	2.86996	−0.03450
C	3.74509	0.70255	−0.00540	O	4.57948	−1.55955	0.02182
C	3.58578	−0.66363	0.01131	C	5.91238	−1.06205	0.01738
C	−0.17526	−0.98307	0.02482	H	4.72478	1.16366	−0.01178
C	−1.35663	−0.07778	0.03095	H	−4.44837	2.25736	−0.00561
C	−1.16860	1.32330	−0.00115	H	−1.27403	3.73267	−0.04828
C	0.17300	1.90527	−0.01759	H	−5.65613	0.28343	0.03290
C	−2.62284	−0.64088	0.06044	H	−2.17281	−2.61841	−1.82399
C	−3.74052	0.22032	0.04692	H	−3.11031	−3.92166	−1.02191
C	−3.58783	1.59600	0.00791	H	−3.93299	−2.48470	−1.69103
C	−2.30812	2.15901	−0.01033	H	1.25645	−2.81778	0.03247
O	0.31846	3.15309	−0.04043	H	2.01300	3.34022	−0.04179
O	−0.34834	−2.20715	0.02782	H	6.55649	−1.93902	0.02830
O	−2.23175	3.49162	−0.03950	H	6.10138	−0.47229	−0.88485
O	−4.94790	−0.37979	0.06057	H	6.09947	−0.45136	0.90597
C	−2.91452	−2.12956	0.13250				

Structure, energy and Cartesian coordinate of **a-conformer 2**:

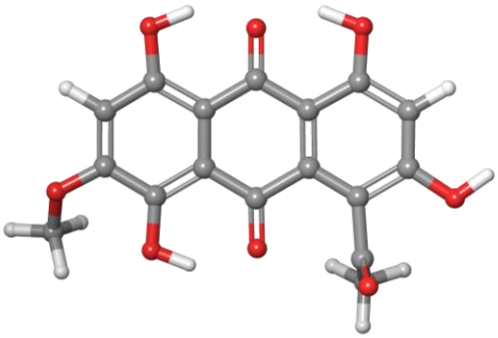


a-conformer 2 (ΔG = 0.5 kcal/mol, Boltzmann pop. (298 K) = 31%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5364662
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7598442
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.271800
	Thermal correction to Energy (a.u.)	=	0.292435
	Thermal correction to Enthalpy (a.u.)	=	0.293379
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.223378

C	−2.26776	−1.21192	−0.18932	O	3.85990	−2.66259	−0.32205
C	−1.15757	−0.37982	−0.12579	C	2.20543	−2.84128	1.35735
C	−1.30945	1.03267	0.02696	O	−2.22046	−2.53458	−0.36363
C	−2.59636	1.56872	0.13521	O	−2.84354	2.87552	0.26484
C	−3.72518	0.71997	0.10710	O	−4.57701	−1.52609	−0.09939
C	−3.57740	−0.63884	−0.05018	C	−5.90423	−1.02801	0.02404
C	0.17786	−0.96535	−0.24599	H	−4.69998	1.18177	0.20128
C	1.36890	−0.08828	−0.04666	H	4.48265	2.20658	−0.19412
C	1.19178	1.30549	−0.03743	H	1.31624	3.71318	0.05771
C	−0.14697	1.89921	0.03603	H	4.96312	−1.25195	−0.42939
C	2.63904	−0.67255	−0.02986	H	1.38484	−2.27421	1.79283
C	3.76519	0.18561	−0.15795	H	1.84104	−3.80479	0.99653
C	3.60963	1.56725	−0.13308	H	2.95765	−3.02997	2.13018
C	2.34478	2.13729	−0.04039	H	−1.27414	−2.77684	−0.49142
O	−0.27676	3.14473	0.12321	H	−1.97495	3.34277	0.25334
O	0.34200	−2.15381	−0.53852	H	−6.55459	−1.89815	−0.03805
O	2.27114	3.46806	0.00012	H	−6.04087	−0.52864	0.98813
O	5.01208	−0.28400	−0.27506	H	−6.13244	−0.33339	−0.79011
C	2.91444	−2.11754	0.23779				

Structure, energy and Cartesian coordinate of **a-conformer 3**:

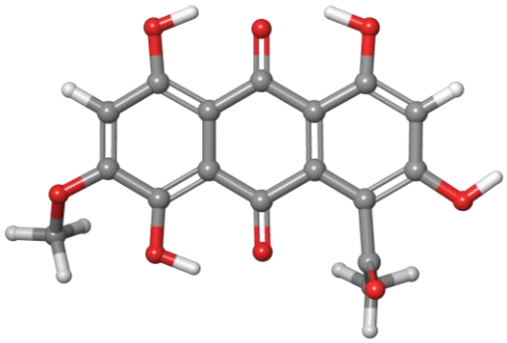


a-conformer 3 (Δ*G* = 3.3 kcal/mol, Boltzmann pop. (298 K) = 0.3%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5319414
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7519884
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.269972
	Thermal correction to Energy (a.u.)	=	0.291470
	Thermal correction to Enthalpy (a.u.)	=	0.292414
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.220047

C	−2.40509	−0.99559	0.15732	O	2.96097	−2.74633	1.23515
C	−1.24150	−0.22816	0.09695	C	2.71922	−3.00709	−1.13500
C	−1.30558	1.19619	0.05067	O	−2.42165	−2.32980	0.25260
C	−2.55726	1.82331	0.06810	O	−2.72631	3.15014	0.03199
C	−3.72799	1.04043	0.10805	O	−4.83218	−1.01587	0.22553
C	−3.67133	−0.33274	0.14036	C	−5.03130	−2.13868	−0.64462
C	0.05684	−0.90735	0.11032	H	−4.69392	1.53283	0.10361
C	1.29904	−0.09006	0.04806	H	4.54439	2.01722	−0.16179
C	1.20973	1.31932	−0.02016	H	1.48561	3.71569	−0.13686
C	−0.08659	1.99274	−0.01178	H	5.61109	−0.04309	−0.11424
C	2.52188	−0.74120	0.05293	H	2.73306	−4.08009	−0.93817
C	3.69710	0.03731	−0.02642	H	1.85338	−2.74010	−1.74513
C	3.64105	1.41874	−0.10014	H	3.62261	−2.72591	−1.68914
C	2.40413	2.07113	−0.09124	H	−1.48377	−2.63643	0.24229
O	−0.14795	3.24458	−0.05797	H	−1.83130	3.56066	−0.00978
O	0.14526	−2.13896	0.16345	H	−6.10442	−2.17869	−0.83211
O	2.42184	3.40415	−0.15590	H	−4.49983	−1.99442	−1.58885
O	4.85676	−0.64933	−0.03880	H	−4.69577	−3.06033	−0.17038
C	2.71180	−2.24429	0.16195				

Structure, energy and Cartesian coordinate of **a-conformer 4**:

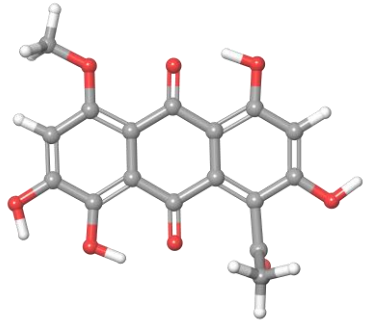


a-conformer 4 (Δ*G* = 3.4 kcal/mol, Boltzmann pop. (298 K) = 0.2%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5318302
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7520482
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.270120
	Thermal correction to Energy (a.u.)	=	0.291571
	Thermal correction to Enthalpy (a.u.)	=	0.292515
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.220218

C	2.40496	−1.00108	−0.12361	O	−2.86031	−2.81836	1.15719
C	1.24222	−0.23174	−0.07265	C	−2.82829	−2.92822	−1.23725
C	1.30720	1.19327	−0.06289	O	2.42016	−2.33700	−0.19112
C	2.55907	1.81897	−0.10375	O	2.72880	3.14620	−0.10505
C	3.72925	1.03462	−0.12737	O	4.83169	−1.02487	−0.19738
C	3.67167	−0.33890	−0.12545	C	5.03142	−2.12722	0.69846
C	−0.05642	−0.91029	−0.05738	H	4.69545	1.52637	−0.13918
C	−1.29686	−0.09135	0.01726	H	−4.54150	2.02306	0.15397
C	−1.20750	1.31963	0.02330	H	−1.48278	3.71874	0.05051
C	0.08879	1.99195	−0.01843	H	−5.60959	−0.03785	0.15991
C	−2.51880	−0.74214	0.06749	H	−2.83489	−4.01156	−1.10852
C	−3.69374	0.03900	0.11677	H	−3.77156	−2.60872	−1.69587
C	−3.63821	1.42243	0.11794	H	−2.01304	−2.62543	−1.89831
C	−2.40140	2.07379	0.07634	H	1.48187	−2.64228	−0.17646
O	0.15059	3.24463	−0.01641	H	1.83401	3.55815	−0.07366
O	−0.14668	−2.14199	−0.10398	H	6.10462	−2.16280	0.88645
O	−2.41891	3.40838	0.08614	H	4.50025	−1.96138	1.63928
O	−4.85366	−0.64667	0.14871	H	4.69581	−3.05956	0.24568
C	−2.70540	−2.24929	0.09979				

Structure, energy and Cartesian coordinate of **b-conformer 1**:

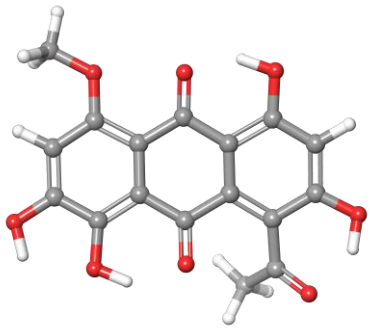


b-conformer 1 (Δ*G* = 0.0 kcal/mol, Boltzmann pop. (298 K) = 73%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5263727
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7470117
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.270485
	Thermal correction to Energy (a.u.)	=	0.291933
	Thermal correction to Enthalpy (a.u.)	=	0.292878
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.220639

C	1.95909	−1.90465	0.01726	O	−3.61776	−2.10702	1.20148
C	1.08681	−0.82104	0.01005	C	−3.54564	−2.31784	−1.18447
C	1.58085	0.51734	−0.00385	O	1.61006	−3.20355	0.02732
C	2.97419	0.72039	−0.00402	O	3.44499	1.97797	−0.01259
C	3.84747	−0.38530	0.00635	O	4.19601	−2.71783	0.02432
C	3.35466	−1.67077	0.01589	C	4.85110	2.18198	−0.00784
C	−0.35607	−1.10582	0.02188	H	4.92208	−0.25898	0.00638
C	−1.31405	0.02456	0.03188	H	−3.81873	2.96911	−0.00572
C	−0.81972	1.34369	−0.00261	H	−0.39601	3.69885	−0.05896
C	0.62751	1.63918	−0.02268	H	−5.43524	1.30376	0.03380
C	−2.67352	−0.25463	0.06368	H	−3.85936	−3.35019	−1.02289
C	−3.57665	0.82623	0.04969	H	−4.34772	−1.76684	−1.68970
C	−3.12467	2.13451	0.00843	H	−2.65953	−2.28154	−1.82234
C	−1.75238	2.40587	−0.01292	H	0.62509	−3.24746	0.02545
O	1.00316	2.81912	−0.05538	H	3.66630	−3.53551	0.03130
O	−0.78078	−2.26546	0.02110	H	5.31607	1.74882	−0.89886
O	−1.38823	3.68986	−0.04595	H	4.98743	3.26206	−0.01410
O	−4.88754	0.50309	0.06392	H	5.30838	1.76007	0.89250
C	−3.27698	−1.64565	0.13486				

Structure, energy and Cartesian coordinate of **b-conformer 2**:

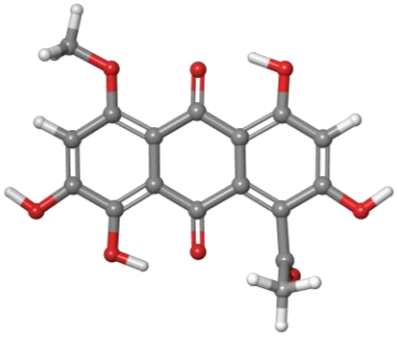


b-conformer 2 (ΔG = 0.6 kcal/mol, Boltzmann pop. (298 K) = 25%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5260183
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7485673
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.271350
	Thermal correction to Energy (a.u.)	=	0.292228
	Thermal correction to Enthalpy (a.u.)	=	0.293172
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.222549

C	1.97033	−1.86739	−0.23145	O	−4.32845	−1.98041	−0.16559
C	1.08653	−0.79573	−0.18291	C	−2.62632	−2.51863	1.38120
C	1.55951	0.53947	−0.03332	O	1.64051	−3.16091	−0.40052
C	2.94393	0.75312	0.10590	O	3.39102	2.00981	0.25519
C	3.82865	−0.34326	0.09146	O	4.20987	−2.66257	−0.10345
C	3.35634	−1.62616	−0.07737	C	4.78730	2.22432	0.41112
C	−0.35030	−1.08476	−0.29771	H	4.89713	−0.21103	0.19959
C	−1.32710	0.01048	−0.06061	H	−3.88763	2.89978	−0.18082
C	−0.85479	1.32765	−0.09026	H	−0.46385	3.69077	−0.08578
C	0.59199	1.64595	−0.06677	H	−5.09889	−0.38228	−0.28990
C	−2.69222	−0.29901	0.00424	H	−2.45945	−3.52173	0.98429
C	−3.61558	0.77370	−0.10795	H	−1.69575	−2.12104	1.78228
C	−3.16833	2.09067	−0.12754	H	−3.36058	−2.59148	2.18957
C	−1.80928	2.38337	−0.09001	H	0.67029	−3.20499	−0.56118
O	0.94786	2.83127	−0.05967	H	3.69616	−3.47905	−0.24018
O	−0.75490	−2.20635	−0.61157	H	4.90504	3.30108	0.51973
O	−1.45563	3.66840	−0.09566	H	5.16596	1.72164	1.30639
O	−4.93804	0.57901	−0.16964	H	5.33933	1.88217	−0.46964
C	−3.24825	−1.64876	0.31415				

Structure, energy and Cartesian coordinate of **b-conformer 3**:

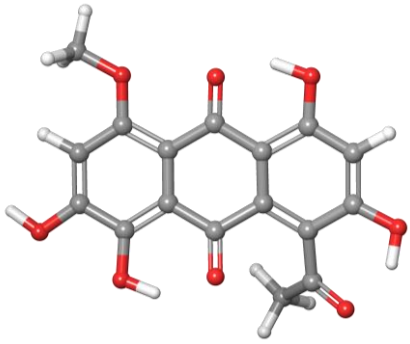


b-conformer 3 (Δ*G* = 2.5 kcal/mol, Boltzmann pop. (298 K) = 1.1%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5230671
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7430241
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.270121
	Thermal correction to Energy (a.u.)	=	0.291688
	Thermal correction to Enthalpy (a.u.)	=	0.292633
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.219957

C	1.95682	−1.92304	0.01673	O	−3.62395	−2.10780	1.20168
C	1.08582	−0.83198	0.00866	C	−3.54961	−2.31969	−1.18388
C	1.57479	0.51056	−0.00519	O	1.58605	−3.20873	0.02623
C	2.96415	0.71830	−0.00400	O	3.43636	1.97550	−0.01208
C	3.83743	−0.38880	0.00742	O	4.13844	−2.77204	0.02692
C	3.35520	−1.67878	0.01687	C	4.84191	2.18201	−0.00454
C	−0.35789	−1.10995	0.02015	H	4.91086	−0.24170	0.00808
C	−1.31554	0.02208	0.03110	H	−3.82208	2.96655	−0.00383
C	−0.82323	1.34109	−0.00380	H	−0.39759	3.69464	−0.06143
C	0.62296	1.63404	−0.02508	H	−5.43693	1.30129	0.03773
C	−2.67524	−0.25716	0.06427	H	−2.66607	−2.27865	−1.82487
C	−3.57839	0.82359	0.05148	H	−3.85812	−3.35365	−1.02234
C	−3.12743	2.13243	0.00962	H	−4.35639	−1.77208	−1.68534
C	−1.75553	2.40376	−0.01336	H	0.60079	−3.22510	0.02308
O	1.00054	2.81364	−0.05941	H	5.07296	−2.51060	0.02790
O	−0.79417	−2.26614	0.01870	H	5.30984	1.75122	−0.89524
O	−1.38994	3.68742	−0.04702	H	4.97606	3.26239	−0.01000
O	−4.88943	0.50048	0.06722	H	5.29870	1.76153	0.89681
C	−3.28006	−1.64752	0.13547				

Structure, energy and Cartesian coordinate of **b-conformer 4**:

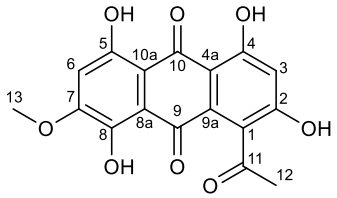


b-conformer 4 (ΔG = 3.0 kcal/mol, Boltzmann pop. (298 K) = 0.5%)

M06-2X/6-311+G(d,p)-PCM(DMSO)//M06-2X/6-31G(d)-PCM(DMSO):			
	Gibbs Free Energy (a.u.)	=	−1256.5222624
M06-2X/6-311+G(d,p)-PCM(DMSO):	*Electronic energy* (a.u.)	=	−1256.7447054
M06-2X/6-31G(d)-PCM(DMSO):	*Zero-point correction* (a.u.)	=	0.271356
	Thermal correction to Energy (a.u.)	=	0.292266
	Thermal correction to Enthalpy (a.u.)	=	0.293210
	Thermal correction to Gibbs Free Energy (a.u.)	=	0.222443

C	1.96751	−1.88359	−0.24247	O	−4.32992	−1.98510	−0.14824
C	1.08514	−0.80447	−0.19636	C	−2.60988	−2.52683	1.37713
C	1.55223	0.53450	−0.04297	O	1.61669	−3.16327	−0.42124
C	2.93167	0.75242	0.10543	O	3.37931	2.00880	0.25711
C	3.81587	−0.34592	0.09906	O	4.14938	−2.71710	−0.09989
C	3.35457	−1.63313	−0.07262	C	4.77339	2.22493	0.42810
C	−0.35227	−1.08641	−0.31471	H	4.88203	−0.19335	0.21775
C	−1.32842	0.00825	−0.06628	H	−3.89455	2.89470	−0.16470
C	−0.85957	1.32574	−0.09690	H	−0.46887	3.68754	−0.09663
C	0.58603	1.64246	−0.08085	H	−5.10072	−0.38950	−0.26673
C	−2.69283	−0.30299	0.00811	H	−2.44230	−3.52713	0.97351
C	−3.61827	0.76880	−0.09538	H	−1.67726	−2.12763	1.77192
C	−3.17348	2.08682	−0.11726	H	−3.33664	−2.60691	2.19154
C	−1.81476	2.38088	−0.08978	H	0.64604	−3.17888	−0.58125
O	0.94360	2.82755	−0.08102	H	5.07544	−2.45373	0.02177
O	−0.76808	−2.20162	−0.63929	H	5.14325	1.72382	1.32802
O	−1.46079	3.66589	−0.09780	H	5.33580	1.88426	−0.44673
O	−4.94090	0.57220	−0.14712	H	4.88851	3.30188	0.53769
C	−3.24442	−1.65376	0.32004				

• Calculated NMR chemical shifts for each conformer of **a** and **b**

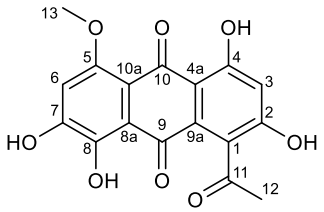


a

	a*		**a-conformer 1** (69%)**		**a-conformer 2** (31%)**		**a-conformer 3** (0.3%)**		**a-conformer 4** (0.2%)**	
position	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$
1	122.8		124.9		118.0		125.0		125.1	
2	156.7		155.5		159.4		156.0		156.0	
3	107.5	6.89	107.1	6.85	108.3	7.00	107.1	6.87	107.0	6.87
4	162.3		161.9		163.2		162.0		162.0	
4a	110.2		109.6		111.5		109.4		109.5	
5	157.1		157.0		157.5		155.8		155.8	
6	106.6	6.93	106.4	6.90	106.7	6.99	117.5	7.19	117.5	7.19
7	155.4		155.3		155.7		156.1		156.2	
8	148.3		148.3		148.4		150.6		150.5	
8a	111.9		111.8		112.2		113.4		113.4	
9	183.4		183.0		184.3		183.5		183.5	
9a	133.8		132.3		137.0		132.1		132.2	
10	182.8		182.8		182.8		183.3		183.2	
10a	104.3		104.4		104.2		107.8		107.8	
11	204.8		204.0		206.4		203.9		204.0	
12	33.7	2.58	33.5	2.66	34.3	2.39	33.4	2.66	33.7	2.68
13	56.6	4.08	56.6	4.07	56.7	4.10	62.9	4.27	62.8	4.26
4-OH		12.53		12.49		12.61		12.37		12.36

* The Boltzmann weighted chemical shifts

** Boltzmann population



b

	b*		**b-conformer 1** (73%)**		**b-conformer 2** (25%)**		**b-conformer 3** (1.1%)**		**b-conformer 4** (0.5%)**	
position	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$	$\delta_{C(calc)}$	$\delta_{H(calc)}$
1	121.7		123.6		116.0		123.5		116.0	
2	155.6		154.4		159.1		154.4		159.2	
3	108.1	6.90	107.8	6.86	109.0	7.01	107.5	6.85	108.7	6.99
4	162.4		162.0		163.5		161.9		163.5	
4a	110.9		110.5		112.0		110.5		111.9	
5	155.2		155.2		155.3		154.4		154.5	
6	104.1	7.27	104.0	7.27	104.4	7.28	104.5	7.00	104.6	7.00
7	151.3		151.2		151.7		151.0		151.5	
8	142.0		142.2		141.5		145.3		144.5	
8a	114.7		114.5		115.0		115.0		115.5	
9	185.7		185.3		186.9		185.1		186.7	
9a	132.1		130.9		135.8		131.3		136.3	
10	181.1		181.1		181.1		181.0		181.0	
10a	109.2		109.3		108.8		109.7		109.2	
11	204.7		204.2		205.9		204.2		205.9	
12	33.8	2.58	33.7	2.65	34.0	2.36	33.8	2.65	34.0	2.36
13	55.9	4.05	55.9	4.05	56.0	4.08	55.7	4.01	55.8	4.04
4-OH		13.51		13.49		13.57		13.49		13.56

* The Boltzmann weighted chemical shifts

** Boltzmann population