Supporting Information

NMR fingerprints as a predictive model to monitor punaglandins in the soft coral *Carijoa (Telesto) riisei* (Duchassaing & Michelotti, 1860).

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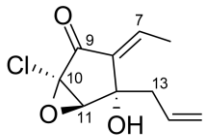
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Position	7*E*-punaglandin 3 epoxide (2)	7*Z*-punaglandin 4 (3)	punaglandin 6 (4)	punaglandin 8 (5)		carijenone (6)	
	δ^H	δ^H	δ^H	δ^C, type	δ^H	δ^C, type	δ^H
1	-	-	-	174.0	-	173.4	
2	2.30, m	2.32, m	2.34, m	33.3	2.33, t	33.5	2.29, m
3	1.6, m	1.62, m	1.6, m	24.4	1.72, m	20.5	1.58, m
4	1.6, m	1.6, m	1.6, m	27.0	2.21, m	29.8	1.58, m
5	5.20, m	5.20, m	5.11, d	133.5	5.59, dt	72.5	4.97, ddd
6	5.98, dd	6.31	5.28, m	126.3	5.83, dd	88.0	4.33, dd
7	6.54, d	6.07, d	2.13, ddd	67.9	5.96, dd	77.5	5.08
	-	-	-	-	-	-	-
8	-	-	2.66, dd	56.9	2.68, d	58.0	2.94, s
9	-	-	-	196.3	-	196.1	-
10	-	-	-	136.6	-	135.8	-
11	3.96, s	7.21, s	7.29, s	157.9	7.33, s	156.0	7.34, s
12	3.67, s	2.79, s	2.54, s	76.9	3.19, s	89.6	-
13	2.8, m	2.43, dd	2.1, m	39.3	2.39, dd	35.7	2.71, dd
13b	2.8, m	2.55, dd	2.77, ddd	-	2.55, dd	-	2.61, dd
14	5.20, m	5.20, m	5.28, m	121.1	5.34, ddd	121.7	5.32, m
15	5.58, m	5.57, dt	5.65, dt	136.1	5.66, dt	134.8	5.61, ddd
16	2.7, m	1.95, m	2.03, m	27.6	2.00, m	27.3	2.06, m
17	5.2, m	1.3, m	1.3, m	29.1	1.29, m	29.0	1.36, m
18	5.4, m	1.29, m	1.3, m	31.5	1.29, m	31.4	1.29, m
19	2.0, m	1.3, m	1.3, m	22.6	1.29, m	22.4	1.29, m
20	0.94, t	0.86, t	0.90, t	14.0	0.88, t	13.9	0.88, t
OMe	3.65, s	3.64, s	3.65, s	51.6	3.66, s	51.4	3.65, s
5-O**CO**CH_3	-	-	-	170.3	-	170.1	-
5-OCO**CH_3**	2.0, s	2.1, s	2.1, s	21.1	1.99, s	20.7	1.97, s
6-O**CO**CH_3	-	-	-	-	-	-	-
6-OCO**CH_3**	2.08, s	2.02, s	2.1, s	-	-	-	-
7-O**CO**CH_3						169.8	-
7-OCO**CH_3**						20.7	2.09, s

Table S2. GIAO DFT NMR chemical shifts for 10-chloro-10, 11-epoxy-cyclopentanone (**46**) calculated at the mPW1PW91/6-311+G(d,p) level of theory.



10-chloro-10,11-epoxy-cyclopentanone

Atom Number	Shielding tensor	Scaled chemical shift (ppm)
7	26.6	152.1
8	42.1	136.9
9	-8.7	186.7
10	100.5	79.6
11	116.2	64.2
12	108.9	71.4
13	144.3	36.6

Table S3. DFT Geometry Optimized Energies for 10-chloro-10, 11-epoxy-cyclopentanone (**46**) conformers calculated at the B3LYP-6-31G* level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
1	-673508.3701	0.00	1.00	0.52
2	-673508.0865	0.28	0.62	0.32
6	-673507.1026	1.27	0.12	0.06
3	-673506.9482	1.42	0.09	0.05
7	-673506.5121	1.86	0.04	0.02
10	-673506.0835	2.29	0.02	0.01

Table S4. DFT Geometry Optimized Coordinates for 10-chloro-10, 11-epoxy-cyclopentanone (**46**) conformers calculated at the B3LYP-6-31G* level of theory.

	Conformer 1			**Conformer 2**			**Conformer 6**			**Conformer 3**		
Gibbs free energy (hartrees)	-1073.304049			-1073.303597			-1073.302029			-1073.301783		
ΔG (kJ/mol)				1.187			5.304			5.949		
Population Proportion	51.57%			31.95%			6.07%			4.68%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-6.534863	-1.419967	-1.042942	-6.463790	-1.381222	-0.991303	-6.504992	-1.348661	-0.992822	-6.495347	-1.464275	-1.059192
C	-6.730097	-0.309505	-0.010495	-6.574755	-0.276816	0.065641	-6.708552	-0.207032	0.011389	-6.597879	-0.389554	0.021656
C	-8.260589	-0.261097	0.159222	-8.094121	-0.101229	0.224208	-8.239324	-0.144658	0.152572	-8.117611	-0.216732	0.195596
C	-8.919836	-1.245550	-0.703510	-8.828972	-1.036812	-0.638666	-8.894125	-1.159330	-0.684298	-8.856417	-1.118120	-0.693053
C	-7.841894	-2.002200	-1.476169	-7.814309	-1.876493	-1.409617	-7.810342	-1.948943	-1.414501	-7.845917	-1.932755	-1.496967
C	-5.390344	-1.977003	-1.470996	-5.362864	-2.006938	-1.443392	-5.355853	-1.917763	-1.397258	-5.397986	-2.082943	-1.524479
O	-8.027918	-2.913347	-2.252291	-8.066973	-2.784678	-2.170224	-7.988127	-2.896596	-2.147680	-8.106601	-2.802116	-2.298859

O	-8.936980	0.130698	-1.058228	-8.726084	0.330290	-1.001337	-8.895177	0.199464	-1.089636	-8.758089	0.265488	-1.006435
C	-6.184887	1.066689	-0.491050	-5.916331	1.058709	-0.344338	-6.140743	1.145913	-0.474919	-5.941333	0.957585	-0.388027
Cl	-10.458215	-2.028189	-0.378885	-10.427706	-1.692441	-0.319982	-10.440580	-1.924105	-0.351311	-10.453815	-1.780451	-0.387762
O	-6.119600	-0.704533	1.213212	-5.989651	-0.661126	1.314297	-6.111471	-0.482903	1.279492	-6.033593	-0.919605	1.223314
C	-3.990889	-1.647856	-1.059962	-3.938370	-1.763644	-1.056122	-3.959815	-1.560944	-0.994736	-3.974314	-1.874650	-1.117533
C	-6.385030	2.143238	0.542316	-6.053484	2.131921	0.703994	-6.421997	2.298125	0.452529	-5.922004	1.969198	0.730456
C	-5.426407	2.600940	1.354180	-6.704443	3.281795	0.522219	-5.487791	2.999583	1.093363	-6.755412	3.006931	0.834402
H	-8.709376	0.081336	1.088140	-8.508810	0.301269	1.143579	-8.694171	0.243918	1.059555	-8.536064	0.142555	1.132058
H	-5.509351	-2.790758	-2.187805	-5.543303	-2.806369	-2.163700	-5.467172	-2.757487	-2.084960	-5.582066	-2.855214	-2.272722
H	-5.119431	0.953094	-0.714424	-4.854961	0.862896	-0.539770	-5.061002	1.036330	-0.615256	-4.917380	0.754564	-0.720371
H	-6.697167	1.327434	-1.423022	-6.369397	1.383780	-1.285944	-6.582046	1.342244	-1.459707	-6.493587	1.350162	-1.247506
H	-6.038112	0.100977	1.757165	-6.265996	-1.571793	1.507027	-6.311338	-1.405629	1.507349	-6.100759	-0.227103	1.902829
H	-3.440007	-1.196851	-1.897448	-3.388681	-1.305511	-1.890411	-3.424990	-1.102633	-1.838577	-3.395531	-1.446902	-1.948303
H	-3.955230	-0.977228	-0.200646	-3.845655	-1.124227	-0.176819	-3.930906	-0.878966	-0.143460	-3.877140	-1.232566	-0.241224
H	-3.454399	-2.569332	-0.800633	-3.438508	-2.718398	-0.849301	-3.400692	-2.469093	-0.736350	-3.510840	-2.842483	-0.887420
H	-7.396472	2.538576	0.642911	-5.581528	1.923573	1.662685	-7.470116	2.573322	0.575786	-5.161210	1.827266	1.500430
H	-5.623990	3.365362	2.100865	-6.771008	4.030174	1.307578	-5.742388	3.836504	1.737911	-6.700130	3.704185	1.666242
H	-4.398750	2.249845	1.278829	-7.192792	3.521467	-0.420250	-4.429849	2.764288	0.997290	-7.517719	3.203599	0.083341

	Conformer 7			**Conformer 10**		
Gibbs free energy (hartrees)	-1073.301088			-1073.300405		
ΔG (kJ/mol)	7.774			9.567		
Population Proportion	2.24%			1.09%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-6.489253	-1.096796	-0.775627	-6.416331	-1.216254	-0.852544
C	-6.807743	-0.374856	0.538372	-6.636174	-0.405377	0.430634
C	-8.343507	-0.374962	0.568298	-8.164721	-0.274101	0.497631
C	-8.898493	-1.118223	-0.570655	-8.811273	-1.032932	-0.583347
C	-7.734928	-1.607733	-1.431083	-7.720520	-1.654417	-1.449642
C	-5.292229	-1.417841	-1.296010	-5.269047	-1.690593	-1.369502
O	-7.822666	-2.301466	-2.420161	-7.890067	-2.383425	-2.401853
O	-8.952891	0.299230	-0.556254	-8.741777	0.380648	-0.651433
C	-6.220524	1.047421	0.708501	-5.925785	0.963400	0.509649
Cl	-10.415157	-2.003765	-0.580475	-10.395476	-1.788448	-0.507261
O	-6.333504	-1.102689	1.680455	-6.179715	-1.117134	1.589950
C	-3.938347	-1.096751	-0.749298	-3.875813	-1.508778	-0.854973
C	-6.317434	1.954774	-0.489735	-6.222424	1.939108	-0.596588
C	-5.278434	2.610222	-1.008981	-6.585154	3.206534	-0.401021
H	-8.863915	-0.284184	1.518443	-8.651986	-0.087666	1.451246
H	-5.324643	-1.988358	-2.225277	-5.382398	-2.305786	-2.263499
H	-6.739670	1.498966	1.566987	-6.177896	1.404681	1.481564
H	-5.173883	0.938152	1.009857	-4.848398	0.755278	0.538116

H	-6.545090	-2.041103	1.545968	-6.459784	-2.043006	1.501963
H	-3.498088	-0.259158	-1.308622	-3.320812	-0.803381	-1.489574
H	-3.968970	-0.829802	0.308647	-3.852924	-1.148198	0.174731
H	-3.262516	-1.950266	-0.878428	-3.331518	-2.459711	-0.904740
H	-7.304986	2.082118	-0.927006	-6.092985	1.571099	-1.613784
H	-5.392532	3.277576	-1.858842	-6.755742	3.885186	-1.231964
H	-4.274624	2.514537	-0.598399	-6.729801	3.614837	0.597324

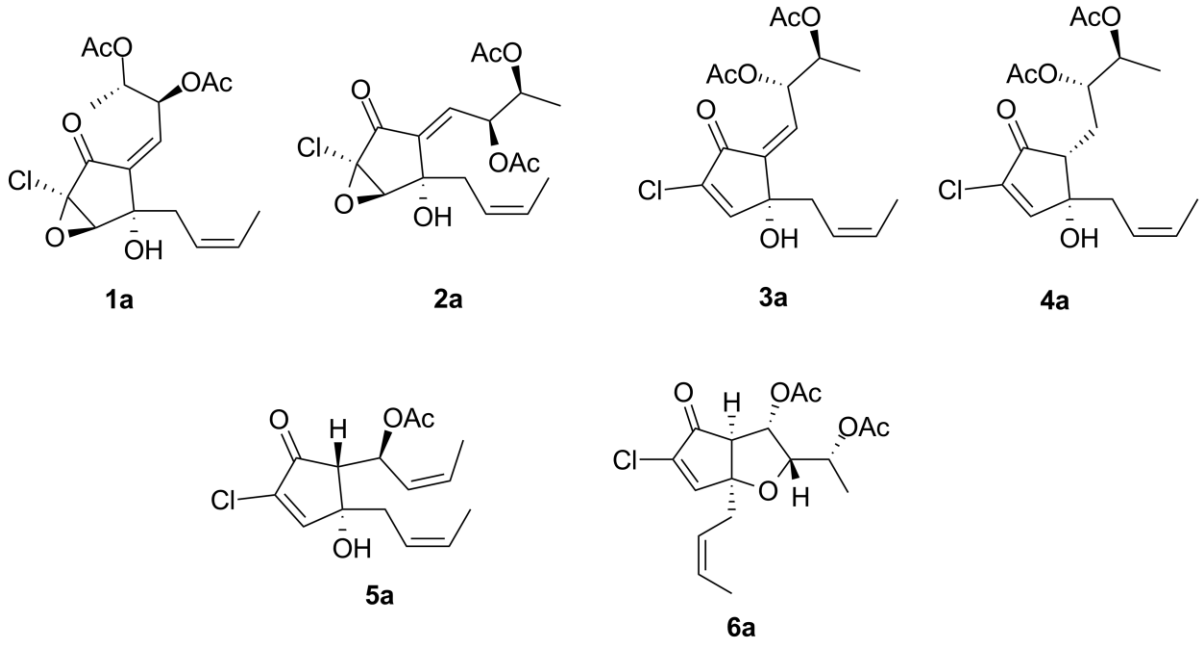


Figure S1. Truncated punaglandin input structures **1a**-**6a** for TDDFT-ECD calculations.

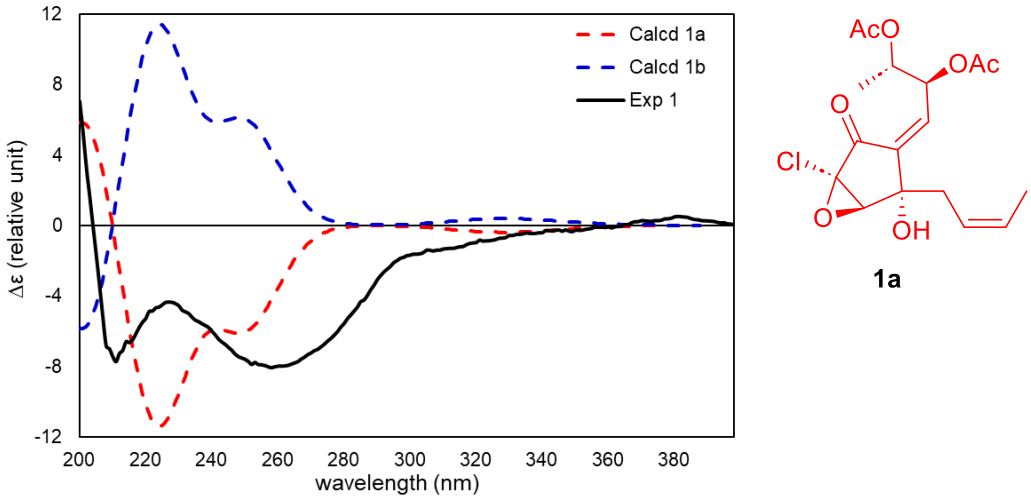


Figure S2. Comparative ECD spectra for truncated 7*Z*-punaglandin 4 epoxide (**1a**, calculated red line =5*S*,6*S*,10*S*,11*R*,12*S*, calculated blue line = 5*R*,6*R*,10*R*,11*S*,12*R*). Experimental and calculated ECD spectra matched with UV shift +6 nm and sigma/gamma value = 0.26 eV.

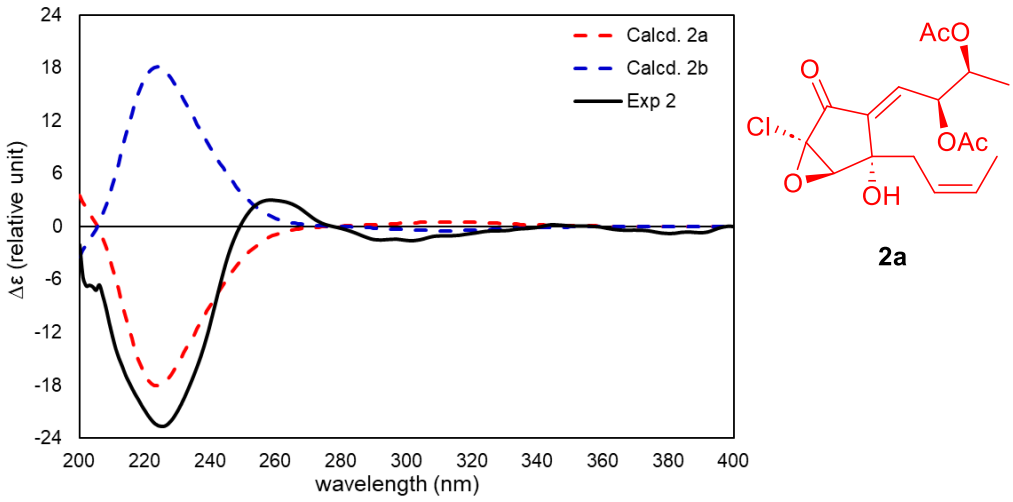


Figure S3. Comparative ECD spectra for truncated 7*E*-punaglandin 3 epoxide (**2a**, calculated red line = 5*S*,6*S*,10*S*,11*R*,12*S*, calculated blue line = 5*R*,6*R*,10*R*,11*S*,12*R*). Experimental and calculated ECD spectra matched with UV shift +18 nm and sigma/gamma value = 0.28 eV.

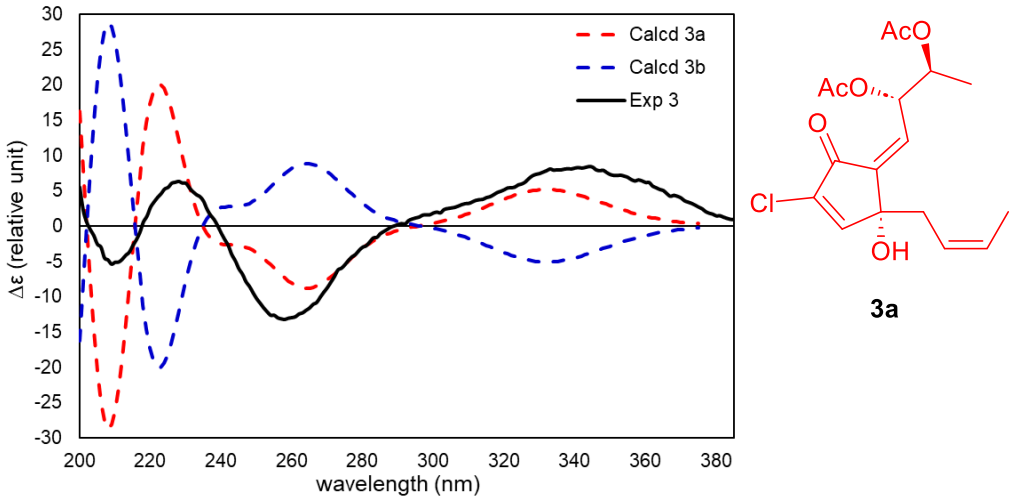


Figure S4. Comparative ECD spectra for truncated 7*Z*-punaglandin 4 (**3a**, calculated red line = 5*S*,6*S*,12*R* and calculated blue line = 5*R*,6*R*,12*S*). Experimental and calculated ECD spectra matched with UV shift +12 nm and sigma/gamma value = 0.26 eV.

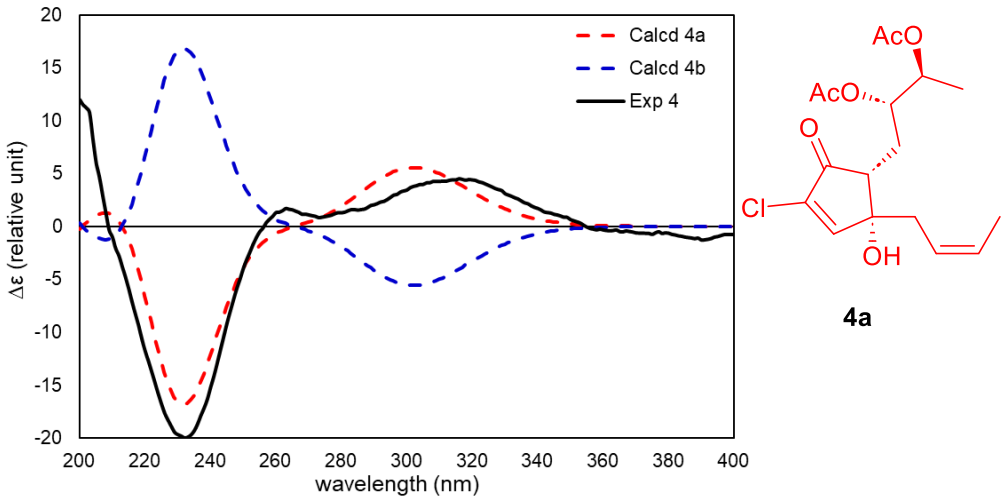


Figure S5. Comparative ECD spectra for truncated punaglandin 6 (**4a**, calculated red line = 5*S*,6*S*,8*R*,12*S* and calculated blue line = 5*R*,6*R*,8*S*,12*R*). Experimental and calculated ECD spectra matched with UV shift +8 nm and sigma/gamma value = 0.26 eV.

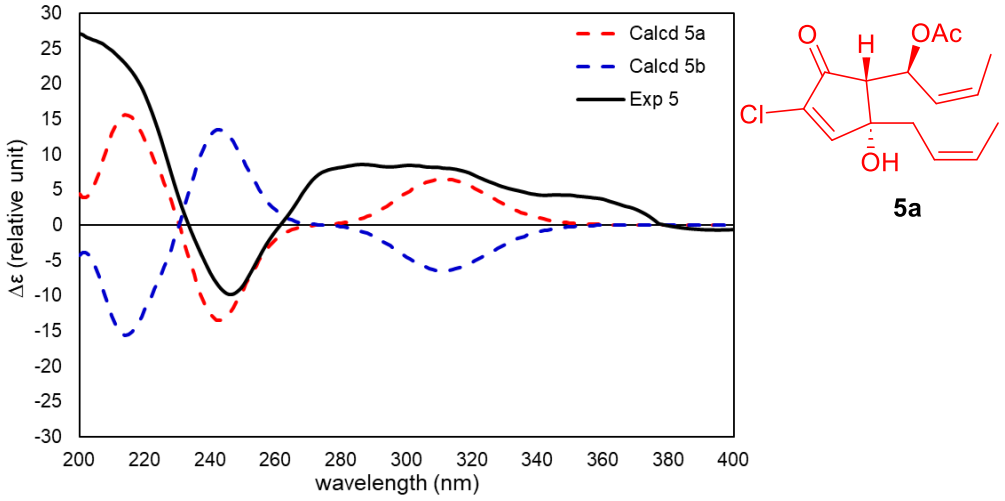


Figure S6. Comparative ECD spectra for truncated punaglandin 8 (**5a**, calculated red line = 7*S*,8*R*,12*S*, calculated blue line = 7*R*,8*S*,12*R*). Experimental and calculated ECD spectra matched with UV shift +18 nm and sigma/gamma value = 0.26 eV.

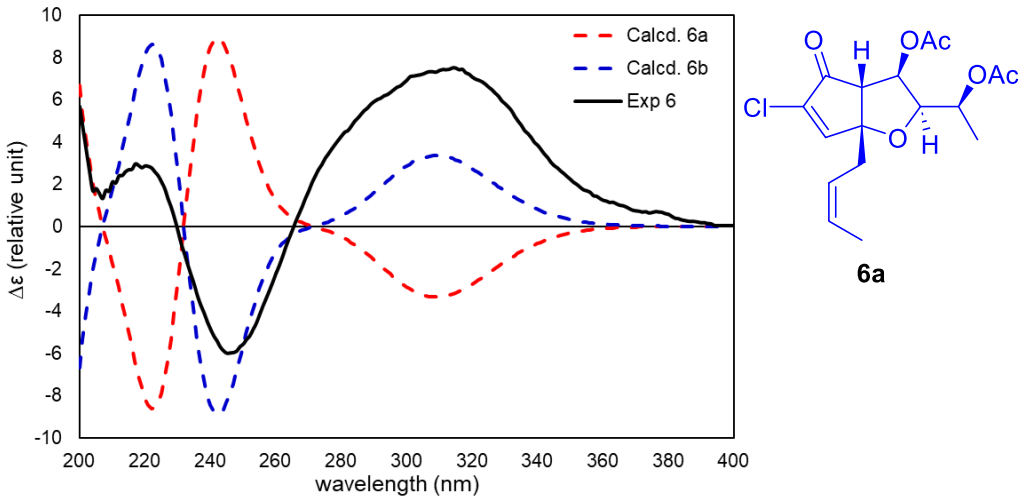


Figure S7. Comparative ECD spectra for truncated carijenone (**6a**, calculated red line = 5*R*,6*S*,7*S*,8*S*,12*R*, blue line = 5*S*,6*R*,7*R*,8*R*,12*S*). Experimental and calculated ECD spectra matched with UV shift +13 nm and sigma/gamma value = 0.30 eV.

Table S5. DFT Geometry Optimized Energies for truncated 7*Z*-punaglandin 4 epoxide (**1a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory**.**

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
43	-1033640	0	1	0.45
3	-1033640	0.35	0.55	0.25
33	-1033640	0.73	0.29	0.13
11	-1033639	1.08	0.16	0.07
25	-1033639	1.7	0.06	0.03
37	-1033638	1.9	0.04	0.02
36	-1033638	2.17	0.03	0.01
5	-1033638	2.23	0.02	0.01
19	-1033638	2.44	0.02	0.01
27	-1033638	2.5	0.01	0.01
40	-1033638	2.62	0.01	0.01
23	-1033637	2.81	0.01	0

Table S6. DFT Geometry Optimized Energies for truncated 7*E*-punaglandin 3 epoxide (**2a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
14	-1033653.004	0.00	1.00	0.47
2	-1033652.585	0.42	0.49	0.23
5	-1033652.372	0.63	0.34	0.16
20	-1033652.014	0.99	0.19	0.09
13	-1033651.291	1.71	0.06	0.03
7	-1033650.527	2.48	0.02	0.01

12	-1033650.366	2.64	0.01	0.01
1	-1033650.112	2.89	0.01	0.00

Table S7. DFT Geometry Optimized Energies for truncated 7*Z* punaglandin 4 (**3a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
12	-1572.025698	0.00	1.00	0.29
13	-1572.025422	0.17	0.75	0.22
65	-1572.024963	0.46	0.46	0.13
4	-1572.024446	0.79	0.27	0.08
69	-1572.024331	0.86	0.23	0.07
63	-1572.024108	1.00	0.19	0.05
10	-1572.02337	1.46	0.08	0.02
61	-1572.023163	1.59	0.07	0.02
27	-1572.023145	1.60	0.07	0.02
56	-1572.023041	1.67	0.06	0.02
20	-1572.022975	1.71	0.06	0.02
45	-1572.022804	1.82	0.05	0.01
30	-1572.022683	1.89	0.04	0.01
8	-1572.022668	1.90	0.04	0.01
46	-1572.022633	1.92	0.04	0.01
62	-1572.02216	2.22	0.02	0.01
18	-1572.021616	2.56	0.01	0.00
16	-1572.021424	2.68	0.01	0.00

Table S8. DFT Geometry Optimized Energies for truncated punaglandin 6 (**4a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
19	-1573.231808	0.00	1.00	0.51
24	-1573.23119	0.39	0.52	0.26
4	-1573.230321	0.93	0.21	0.10
27	-1573.230158	1.04	0.17	0.09
15	-1573.228944	1.80	0.05	0.02
11	-1573.227984	2.40	0.02	0.01
10	-1573.227743	2.55	0.01	0.01

Table S9. DFT Geometry Optimized Energies for truncated punaglandin 8 (**5a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
14	-843439.0063	0.00	1.00	0.18
2	-843438.7949	0.21	0.70	0.13
7	-843438.7353	0.27	0.63	0.12
9	-843438.7259	0.28	0.62	0.11
6	-843438.6367	0.37	0.54	0.10
5	-843438.52	0.49	0.44	0.08
19	-843438.4278	0.58	0.38	0.07
10	-843438.3374	0.67	0.32	0.06
25	-843438.0657	0.94	0.20	0.04
26	-843438.0136	0.99	0.19	0.03
13	-843437.9528	1.05	0.17	0.03
4	-843437.5625	1.44	0.09	0.02
8	-843437.2123	1.79	0.05	0.01
15	-843437.1157	1.89	0.04	0.01
11	-843437.0799	1.93	0.04	0.01
17	-843436.9506	2.06	0.03	0.01
16	-843436.8565	2.15	0.03	0.00
1	-843436.6645	2.34	0.02	0.00
12	-843436.5158	2.49	0.01	0.00

Table S10. DFT Geometry Optimized Energies for truncated carijenone (**6a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

Conformer	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction
4	-986464.7062	0.00	1.00	0.20
17	-986464.5261	0.18	0.74	0.14
26	-986464.4733	0.23	0.67	0.13
15	-986464.4169	0.29	0.61	0.12
7	-986464.3748	0.33	0.57	0.11
49	-986464.2462	0.46	0.46	0.09
28	-986464.1125	0.59	0.37	0.07
33	-986463.4781	1.23	0.13	0.02
19	-986463.4003	1.31	0.11	0.02
18	-986463.3112	1.39	0.09	0.02
46	-986463.1242	1.58	0.07	0.01
53	-986463.0577	1.65	0.06	0.01
22	-986462.9334	1.77	0.05	0.01
57	-986462.5381	2.17	0.03	0.01
51	-986462.5287	2.18	0.03	0.00
40	-986462.5105	2.20	0.02	0.00
24	-986462.24	2.47	0.02	0.00
1	-986462.1553	2.55	0.01	0.00

3	-986462.0976	2.61	0.01	0.00
11	-986462.0436	2.66	0.01	0.00
34	-986462.0116	2.69	0.01	0.00
44	-986461.91	2.80	0.01	0.00

Table S11. DFT Geometry Optimized Coordinates for truncated 7*Z*-punaglandin 4 epoxide (**1a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 43			**Conformer 3**			**Conformer 33**			**Conformer 11**		
Gibbs free energy (hartrees)	-1647.210768			-1647.210204			-1647.209612			-1647.209049		
ΔG (kcal/mol)				0.354			0.725			1.079		
Population Proportion	45.37%			24.97%			13.34%			7.35%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-5.758809	0.896398	-0.169366	-5.713176	0.845626	0.122679	-5.522476	0.632887	-0.521424	-5.474388	0.556423	-0.216219
C	-5.259206	0.224424	1.114273	-4.836700	0.182911	1.189222	-5.160276	0.062072	0.853449	-4.716538	0.018319	1.000291
C	-5.003067	1.231125	2.185530	-4.482824	1.140605	2.271051	-5.295221	1.098463	1.918680	-4.581738	1.057552	2.055993
C	-5.422975	2.574282	1.604706	-5.215789	2.433663	1.941853	-5.859324	2.332926	1.228681	-5.356772	2.267625	1.552578
C	-5.878803	2.373509	0.230614	-5.950459	2.252172	0.691107	-6.008155	2.050941	-0.197525	-5.896536	1.963002	0.228733
Cl	-4.717945	4.046515	2.256617	-4.596572	3.955741	2.566986	-5.594153	3.913854	1.948002	-4.947717	3.864513	2.161843
O	-4.546392	1.057647	3.291355	-3.763139	0.960050	3.227133	-5.016245	1.016601	3.091906	-3.987592	0.986732	3.107791
C	-4.942593	-1.074972	1.182900	-4.328174	-1.050057	1.070002	-4.640639	-1.160448	1.022488	-4.121759	-1.181033	1.032040
C	-4.319389	-1.804337	2.338599	-3.362932	-1.718860	2.011277	-4.127788	-1.768301	2.297035	-3.257205	-1.726348	2.136804
C	-7.103884	0.321301	-0.678669	-7.039418	0.090139	-0.139095	-6.601798	-0.192266	-1.259940	-6.688742	-0.314218	-0.613410
C	-7.519081	0.932997	-1.991011	-7.830593	0.707815	-1.262160	-6.875452	0.299170	-2.658375	-7.363916	0.143688	-1.880891
C	-7.398700	0.383690	-3.205680	-7.909223	0.267556	-2.523801	-7.947679	0.976254	-3.081470	-8.530399	0.787917	-1.987949
C	-6.864009	-0.973113	-3.561480	-7.271017	-0.952750	-3.121465	-9.138089	1.417571	-2.282178	-9.454524	1.217618	-0.886938
C	-5.324598	-2.687538	3.108143	-4.081856	-2.435236	3.167642	-5.097990	-2.804214	2.904233	-4.081939	-2.427124	3.230129
C	-6.475078	-1.908997	3.726701	-3.139299	-3.242463	4.047500	-6.452128	-2.226404	3.284950	-3.219557	-3.122564	4.272873
O	-4.731181	0.758187	-1.145970	-4.930986	0.949495	-1.063762	-4.301836	0.714958	-1.258169	-4.517552	0.670482	-1.270568
O	-6.811085	2.574357	1.322143	-6.616461	2.224293	1.978559	-7.144833	2.052313	0.700774	-6.729655	1.942228	1.414474
H	-5.832917	3.162973	-0.509400	-6.196369	3.085897	0.045144	-5.991023	2.836245	-0.943073	-6.120039	2.738329	-0.493850
O	-4.588918	-3.295764	4.194123	-5.069972	-3.313902	2.571842	-4.480391	-3.281296	4.121262	-4.928402	-3.399009	2.565063
O	-3.506282	-4.943752	5.152779	-7.041486	-4.277760	2.524455	-3.337593	-4.730168	5.305465	-6.810959	-4.503654	2.332042
C	-4.166756	-4.589653	4.207046	-6.316563	-3.491793	3.083265	-3.867531	-4.489847	4.248389	-6.214617	-3.642528	2.930585
C	-4.554218	-5.504692	3.071928	-6.731691	-2.692995	4.295503	-3.897642	-5.458275	3.092029	-6.828801	-2.820417	4.038163
O	-3.339825	-2.732140	1.806995	-2.611195	-2.714458	1.283929	-2.928969	-2.520634	1.982000	-2.349910	-2.703069	1.581482
O	-1.322485	-3.255874	1.120022	-0.938998	-3.315713	-0.006566	-0.761770	-2.701684	1.687539	-0.467932	-3.253557	0.592547
C	-2.041395	-2.391681	1.552033	-1.493491	-2.410211	0.562320	-1.678679	-1.970059	1.959991	-1.152321	-2.360954	1.023616
C	-1.598133	-0.977600	1.824338	-1.022726	-0.977627	0.527604	-1.529302	-0.504465	2.276509	-0.760640	-0.904872	0.987537

H	-5.102680	-1.694484	0.303704	-4.600680	-1.649280	0.206228	-4.525099	-1.799256	0.150350	-4.234703	-1.846312	0.181249
H	-3.857989	-1.121331	3.048604	-2.694481	-0.989001	2.467549	-3.922628	-1.013389	3.052895	-2.706842	-0.926589	2.631324
H	-7.864318	0.512300	0.083232	-7.624466	0.102191	0.784389	-7.505498	-0.191688	-0.648661	-7.382374	-0.331514	0.228604
H	-6.995717	-0.761268	-0.762941	-6.795211	-0.951693	-0.353183	-6.247642	-1.226853	-1.307853	-6.326829	-1.337925	-0.751240
H	-7.942591	1.932863	-1.931943	-8.375014	1.615369	-1.012104	-6.116600	0.052722	-3.398056	-6.841636	-0.099919	-2.803595
H	-7.743124	0.975486	-4.051340	-8.522720	0.846172	-3.211463	-7.980685	1.240673	-4.136569	-8.870749	1.030734	-2.992689
H	-6.030719	-0.881396	-4.266076	-6.650692	-1.505555	-2.416065	-9.066114	1.163702	-1.224504	-9.075555	0.987760	0.108986
H	-6.513418	-1.539867	-2.698976	-8.038980	-1.631380	-3.507916	-9.265570	2.502717	-2.359622	-9.629999	2.297589	-0.938945
H	-7.634853	-1.562899	-4.069051	-6.644786	-0.675277	-3.975939	-10.054259	0.969438	-2.682131	-10.433564	0.739546	-1.001408
H	-5.704750	-3.453689	2.432917	-4.575261	-1.654333	3.745570	-5.221202	-3.623421	2.196289	-4.693257	-1.650954	3.689878
H	-7.103007	-2.591778	4.300777	-3.689309	-3.695429	4.874291	-7.055063	-3.004676	3.754880	-3.846832	-3.562289	5.050317
H	-7.090369	-1.446177	2.953850	-2.365615	-2.594950	4.466971	-6.983795	-1.868166	2.402287	-2.544369	-2.405058	4.745292
H	-6.102710	-1.129947	4.394039	-2.663062	-4.032516	3.467026	-6.337978	-1.399231	3.987549	-2.628510	-3.912216	3.809172
H	-5.119893	0.986828	-2.003695	-5.537777	1.167827	-1.787075	-4.504684	1.039145	-2.145401	-4.975537	0.975382	-2.064693
H	-4.151280	-5.135379	2.128050	-6.778436	-1.627170	4.058273	-3.397215	-5.031160	2.222032	-6.918290	-1.773458	3.737584
H	-4.145387	-6.489937	3.283526	-7.720500	-3.030725	4.596116	-3.382018	-6.364117	3.402085	-7.821903	-3.215697	4.237361
H	-5.639781	-5.581281	2.975381	-6.037791	-2.821268	5.128193	-4.922889	-5.709113	2.809846	-6.235134	-2.857212	4.953242
H	-2.198471	-0.261365	1.260024	-1.806837	-0.305072	0.173728	-2.127250	0.108080	1.598935	-1.518093	-0.297253	0.488255
H	-1.691618	-0.734430	2.885056	-0.719484	-0.644440	1.523240	-1.850817	-0.289974	3.298323	-0.628940	-0.512712	1.999094
H	-0.555718	-0.887073	1.529094	-0.166992	-0.919292	-0.140450	-0.479853	-0.240752	2.171057	0.181419	-0.822011	0.451216

	Conformer 25			**Conformer 37**			**Conformer 36**			**Conformer 5**		
Gibbs free energy (hartrees)	-1647.208057			-1647.207744			-1647.207305			-1647.207221		
ΔG (kcal/mol)	1.701			1.898			2.173			2.226		
Population Proportion	2.57%			1.84%			1.16%			1.06%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-5.809116	0.602072	0.082402	-5.505363	1.404800	-0.376049	-5.813375	1.122472	-0.260882	-5.824637	0.948740	0.239777
C	-5.076157	-0.195988	1.166103	-5.138208	0.573219	0.867243	-5.341019	0.379389	1.007659	-4.958230	0.214949	1.284031
C	-4.973412	0.585502	2.432673	-5.050878	1.451038	2.077310	-5.161946	1.331729	2.146287	-4.582903	1.123930	2.403326
C	-5.751513	1.872069	2.192874	-5.558442	2.816078	1.640995	-5.580871	2.697764	1.622807	-5.239243	2.463071	2.098596
C	-6.250522	1.873796	0.819301	-5.837979	2.775752	0.208272	-5.965427	2.564096	0.218951	-5.967196	2.348754	0.835513
Cl	-5.371582	3.294035	3.154946	-5.109288	4.239211	2.565268	-4.943713	4.144700	2.387972	-4.546717	3.933775	2.765850
O	-4.382038	0.306320	3.449631	-4.660171	1.172671	3.186348	-4.754044	1.107420	3.261896	-3.890224	0.883186	3.365974
C	-4.464914	-1.362802	0.925739	-4.815042	-0.727655	0.844441	-4.948683	-0.902134	1.029343	-4.436767	-1.008287	1.118028
C	-3.643843	-2.166785	1.891654	-4.316546	-1.567147	1.988123	-4.329154	-1.654313	2.173205	-3.473572	-1.713278	2.035332
C	-7.008468	-0.160143	-0.533114	-6.699924	0.877848	-1.207194	-7.157276	0.622651	-0.858114	-7.229135	0.330772	0.000551
C	-7.653671	0.610723	-1.654888	-6.420171	-0.355454	-2.022142	-7.058348	-0.715160	-1.542830	-7.196633	-0.975151	-0.749235
C	-7.487306	0.406778	-2.967302	-7.093007	-1.510369	-2.005220	-6.890589	-0.927814	-2.854312	-7.382805	-1.142051	-2.064791
C	-6.660314	-0.647466	-3.644268	-8.266212	-1.887696	-1.149658	-6.785620	0.089597	-3.953458	-7.687853	-0.097411	-3.099290

C	-4.432912	-3.321447	2.564925	-5.390438	-2.526707	2.541768	-5.315763	-2.615067	2.870793	-4.198515	-2.503234	3.139124
C	-5.066338	-4.305681	1.594981	-6.607361	-1.817264	3.115177	-6.519740	-1.919680	3.486646	-3.264065	-3.376241	3.962502
O	-4.848762	0.949275	-0.911561	-4.353222	1.650489	-1.186397	-4.789240	1.154151	-1.247883	-5.122713	1.122139	-0.985648
O	-7.116461	1.587024	1.945367	-6.899033	2.714149	1.185856	-6.952522	2.682624	1.269615	-6.648706	2.327717	2.111971
H	-6.451905	2.793707	0.284511	-5.804514	3.659727	-0.416501	-5.906564	3.384630	-0.485267	-6.166834	3.198794	0.194971
O	-5.499002	-2.738840	3.344109	-4.771426	-3.255384	3.626521	-4.585531	-3.239343	3.951587	-5.192265	-3.328736	2.478171
O	-6.385425	-2.018219	5.217839	-3.784964	-5.006405	4.503445	-3.459338	-4.881507	4.869441	-7.195855	-4.207300	2.307525
C	-5.428470	-2.523597	4.686687	-4.347117	-4.545512	3.540320	-4.109977	-4.513936	3.921948	-6.447659	-3.520238	2.959623
C	-4.186403	-2.944578	5.433160	-4.614202	-5.327593	2.278161	-4.430243	-5.394550	2.739588	-6.843944	-2.860756	4.258481
O	-2.575920	-2.832652	1.178752	-3.269079	-2.430473	1.476250	-3.294113	-2.516291	1.634594	-2.700694	-2.658218	1.262169
O	-0.564921	-2.884961	0.298945	-1.173372	-2.876052	1.000383	-1.238752	-2.921964	0.981302	-1.000131	-3.171541	-0.029006
C	-1.381336	-2.231671	0.895841	-1.951231	-2.072762	1.447830	-2.009077	-2.106278	1.419342	-1.574607	-2.303922	0.578108
C	-1.162705	-0.810414	1.347451	-1.559082	-0.716800	1.975721	-1.642989	-0.679527	1.736821	-1.120313	-0.866400	0.626418
H	-4.533833	-1.786823	-0.072493	-4.887629	-1.267510	-0.095678	-5.030918	-1.490972	0.119771	-4.692479	-1.577449	0.230044
H	-3.242821	-1.531760	2.678694	-3.946856	-0.959661	2.810139	-3.919469	-0.985422	2.926921	-2.819232	-1.003194	2.539971
H	-7.734411	-0.347972	0.262446	-6.965604	1.689827	-1.896004	-7.493693	1.388311	-1.561579	-7.811983	1.074547	-0.548292
H	-6.647308	-1.130936	-0.876754	-7.548293	0.737653	-0.536383	-7.892866	0.578706	-0.052002	-7.710945	0.194096	0.971136
H	-8.305872	1.426767	-1.352554	-5.606180	-0.262823	-2.737875	-7.138272	-1.587893	-0.900969	-7.009469	-1.864370	-0.153868
H	-8.025678	1.069071	-3.642255	-6.765777	-2.281836	-2.699480	-6.844449	-1.963656	-3.184128	-7.331111	-2.160334	-2.444662
H	-6.124625	-1.290764	-2.946273	-8.555727	-1.106308	-0.446523	-6.811013	1.118138	-3.593802	-7.709781	0.915456	-2.697264
H	-7.294441	-1.279264	-4.275443	-9.135620	-2.119608	-1.774700	-5.855149	-0.048510	-4.514075	-6.943057	-0.125469	-3.901594
H	-5.923860	-0.185125	-4.309997	-8.046101	-2.795383	-0.577537	-7.601768	-0.044987	-4.671514	-8.655801	-0.302572	-3.569273
H	-3.725596	-3.842635	3.209481	-5.690161	-3.211100	1.748512	-5.639276	-3.365595	2.149888	-4.688947	-1.760761	3.768206
H	-5.522333	-5.124992	2.153040	-7.292601	-2.557718	3.530201	-7.132677	-2.657344	4.006512	-3.816293	-3.875553	4.760555
H	-4.307655	-4.716992	0.928177	-7.134478	-1.260643	2.338997	-7.131578	-1.448017	2.716443	-2.482309	-2.765180	4.420012
H	-5.841581	-3.822015	0.997603	-6.316440	-1.126729	3.908643	-6.204748	-1.157995	4.201558	-2.797333	-4.131783	3.330795
H	-5.340194	1.264515	-1.684970	-3.978313	0.806457	-1.461831	-4.850982	0.335780	-1.759813	-5.245079	0.317800	-1.508747
H	-3.288822	-2.475230	5.026326	-4.119310	-4.860287	1.425802	-4.016455	-4.970564	1.823767	-6.887329	-1.775051	4.140097
H	-4.305107	-2.647172	6.472240	-4.225186	-6.333085	2.420150	-3.988644	-6.371392	2.922131	-7.832506	-3.222884	4.530198
H	-4.051347	-4.027959	5.386476	-5.684307	-5.384808	2.065344	-5.508915	-5.508424	2.608716	-6.141890	-3.083242	5.063655
H	-1.931239	-0.144087	0.950663	-2.103178	0.081387	1.467380	-2.262108	0.019695	1.171207	-1.904724	-0.186803	0.286812
H	-1.186247	-0.739184	2.437376	-1.770303	-0.640188	3.044805	-1.777971	-0.466049	2.799404	-0.844539	-0.578271	1.643844
H	-0.186640	-0.489273	0.992217	-0.491697	-0.587162	1.814758	-0.598529	-0.531412	1.473843	-0.250300	-0.765591	-0.017708

	Conformer 19			**Conformer 27**			**Conformer 40**			**Conformer 23**		
Gibbs free energy (hartrees)	-1647.206887			-1647.206786			-1647.206591			-1647.206288		
ΔG (kcal/mol)	2.435			2.499			2.621			2.811		
Population Proportion	0.74%			0.67%			0.54%			0.39%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**

C	-5.490788	1.146813	-0.051319	-5.516031	0.480074	-0.195804	-5.386602	1.051759	-0.007426	-5.379462	1.123286	-0.164918
C	-4.757305	0.353297	1.036267	-4.919808	-0.313001	0.971290	-4.870535	0.052194	1.031293	-4.703427	0.342393	0.965736
C	-4.523094	1.186952	2.245905	-5.084214	0.421233	2.259483	-4.883534	0.640068	2.400429	-4.539359	1.200360	2.171637
C	-5.173967	2.533761	1.964885	-5.900490	1.663681	1.929060	-5.367335	2.076482	2.236584	-5.328843	2.471265	1.890141
C	-5.751622	2.499978	0.623935	-6.163728	1.688019	0.491844	-5.666653	2.311166	0.826473	-5.872644	2.393939	0.535793
Cl	-4.592854	3.962580	2.807967	-5.789742	3.066682	2.982240	-4.855718	3.287818	3.405193	-4.939241	3.943683	2.764965
O	-3.932242	0.887715	3.259182	-4.652542	0.139586	3.353087	-4.553831	0.132561	3.448104	-3.924581	0.960709	3.185880
C	-4.213558	-0.857792	0.848295	-4.198266	-1.428254	0.801905	-4.279659	-1.106898	0.706226	-4.188504	-0.885779	0.832585
C	-3.314125	-1.595151	1.805081	-3.499487	-2.219484	1.869346	-3.651364	-2.086791	1.653821	-3.356604	-1.625118	1.848382
C	-6.821610	0.540051	-0.551204	-6.542571	-0.332892	-1.018644	-6.680234	0.608822	-0.736359	-6.461535	0.376212	-0.970233
C	-6.679784	-0.749062	-1.313658	-7.061316	0.405340	-2.225850	-6.535066	-0.607876	-1.605868	-7.612597	-0.193396	-0.184055
C	-7.443763	-1.839158	-1.198224	-8.272508	0.949272	-2.381720	-7.259828	-1.729301	-1.540964	-8.106568	-1.431230	-0.280602
C	-8.610217	-2.062939	-0.280993	-9.411748	0.966495	-1.405605	-8.360772	-2.067032	-0.577805	-7.638796	-2.559652	-1.152806
C	-4.083392	-2.449414	2.825855	-4.312873	-3.447324	2.359801	-4.562368	-3.302368	1.976712	-4.204724	-2.376717	2.888195
C	-3.164917	-3.285632	3.705211	-4.697345	-4.429853	1.265514	-4.915872	-4.163375	0.774774	-3.367681	-3.234389	3.826113
O	-4.552499	1.331862	-1.113983	-4.414965	0.927747	-0.987813	-4.315569	1.304735	-0.914648	-4.312571	1.516967	-1.041078
O	-6.574146	2.379144	1.811279	-7.181562	1.298364	1.446188	-6.714864	2.101010	1.807505	-6.697262	2.151367	1.702764
H	-5.898322	3.396741	0.033177	-6.343411	2.611824	-0.044017	-5.625646	3.297231	0.378857	-6.112875	3.282552	-0.036033
O	-4.968478	-3.316131	2.071340	-5.537051	-2.964764	2.952939	-5.800615	-2.798439	2.522712	-5.136251	-3.213055	2.155459
O	-6.847150	-4.418258	1.804790	-6.780127	-2.358664	4.656865	-7.140071	-2.257943	4.173708	-7.085453	-4.193718	1.910990
C	-6.214492	-3.651965	2.491267	-5.712144	-2.781265	4.290758	-6.070498	-2.713732	3.854024	-6.412835	-3.431379	2.562732
C	-6.750397	-3.040186	3.763102	-4.587617	-3.134005	5.233144	-5.044747	-3.209272	4.843076	-6.932078	-2.699669	3.776867
O	-2.464545	-2.487078	1.049525	-2.283307	-2.788078	1.331950	-2.476137	-2.671529	1.045174	-2.543312	-2.602096	1.163329
O	-0.669112	-2.903035	-0.144315	-0.154125	-2.678745	0.807245	-0.341281	-2.663348	0.534713	-0.745123	-3.180366	0.043041
C	-1.305384	-2.076438	0.458451	-1.102786	-2.101781	1.272849	-1.247317	-2.075047	1.066879	-1.348559	-2.288270	0.582418
C	-0.892219	-0.632281	0.597855	-1.062527	-0.687469	1.792191	-1.103416	-0.737463	1.746293	-0.859774	-0.862986	0.655219
H	-4.379671	-1.365697	-0.095330	-4.069934	-1.814196	-0.205893	-4.206451	-1.370473	-0.343742	-4.336160	-1.422135	-0.099767
H	-2.714010	-0.895466	2.386690	-3.282533	-1.594665	2.733189	-3.392716	-1.603199	2.593400	-2.730538	-0.931569	2.409732
H	-7.274730	1.297008	-1.208739	-7.351305	-0.630709	-0.349716	-6.989833	1.458861	-1.361474	-5.951333	-0.396963	-1.548056
H	-7.492364	0.436021	0.302471	-6.044415	-1.250593	-1.347112	-7.461237	0.477462	0.012175	-6.848440	1.098627	-1.703136
H	-5.888664	-0.759733	-2.058743	-6.369300	0.480238	-3.062107	-5.778374	-0.537321	-2.382984	-8.099159	0.492003	0.502536
H	-7.210942	-2.675850	-1.854038	-8.476872	1.436670	-3.333027	-7.043643	-2.500191	-2.278217	-8.963147	-1.668468	0.347315
H	-8.806003	-1.216585	0.378730	-9.169584	0.498588	-0.451343	-8.492475	-1.319976	0.205284	-7.366898	-3.421405	-0.535155
H	-9.519859	-2.251269	-0.862425	-9.723878	1.997145	-1.205226	-9.314230	-2.176006	-1.106875	-8.446481	-2.887464	-1.816785
H	-8.442647	-2.949401	0.338430	-10.284271	0.455801	-1.827655	-8.162796	-3.028567	-0.093459	-6.781767	-2.299079	-1.775086
H	-4.666119	-1.751565	3.426603	-3.695891	-3.948964	3.104951	-4.033724	-3.903717	2.716143	-4.747371	-1.613434	3.444988
H	-3.745608	-3.842475	4.442533	-5.188176	-5.296935	1.710371	-5.517285	-5.012871	1.102695	-4.004416	-3.714926	4.570911
H	-2.465315	-2.639894	4.241204	-3.806766	-4.767230	0.734062	-4.007765	-4.538955	0.302971	-2.636609	-2.616078	4.352353
H	-2.599525	-3.991743	3.097184	-5.385732	-3.972161	0.552441	-5.488408	-3.595036	0.039534	-2.840263	-4.005222	3.264434
H	-5.001734	1.768237	-1.849520	-4.764374	1.404836	-1.751693	-4.648623	1.845651	-1.642250	-4.697811	1.940716	-1.819312
H	-6.893262	-1.963618	3.639393	-3.670249	-2.593815	4.992125	-4.086963	-2.701014	4.719618	-7.933479	-3.067386	3.986778
H	-7.711728	-3.500480	3.977882	-4.902107	-2.871760	6.240399	-5.424883	-3.016329	5.843368	-6.983155	-1.625614	3.580731

H	-6.079169	-3.194107	4.609458	-4.368932	-4.204031	5.196274	-4.877348	-4.282809	4.727023	-6.300067	-2.852555	4.653142
H	-1.670134	0.044417	0.238475	-1.798453	-0.057821	1.288328	-1.771748	0.003467	1.303054	-1.592744	-0.163733	0.247716
H	-0.688045	-0.384355	1.642394	-1.273077	-0.658900	2.863879	-1.339171	-0.809353	2.810471	-0.659649	-0.573031	1.689716
H	0.014032	-0.483253	0.016043	-0.065668	-0.290860	1.616098	-0.073279	-0.409203	1.632101	0.063003	-0.793606	0.084571

Table S12. DFT Geometry Optimized Coordinates for truncated 7*E*-punaglandin 3 epoxide (**2a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 14			**Conformer 2**			**Conformer 5**			**Conformer 20**		
Gibbs free energy (hartrees)	-1647.231132			-1647.230463			-1647.230124			-1647.229554		
ΔG (kJ/mol)				1.756			2.647			4.143		
Population Proportion	47.3%			23.29%			16.26%			8.89%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
Cl	-4.707912	0.777603	-3.082055	-5.031985	1.269787	-2.990367	-6.120168	0.649216	-2.548106	-4.876191	1.039845	-2.991928
C	-3.725595	-0.163611	-1.964321	-4.186556	0.191354	-1.883500	-4.855466	-0.179482	-1.646027	-3.966132	0.005642	-1.895013
C	-2.613837	-1.042569	-2.327632	-3.300414	-0.908496	-2.265039	-3.787904	-0.998331	-2.218623	-2.977259	-0.999606	-2.284320
C	-1.585301	-1.139788	-1.189134	-2.241704	-1.167346	-1.175583	-2.533892	-0.983608	-1.323313	-1.922058	-1.202408	-1.183464
C	-1.400543	-2.613038	-0.760842	-2.377908	-2.605481	-0.602186	-2.181981	-2.420015	-0.848023	-1.904765	-2.675251	-0.708950
C	-0.835350	-3.475386	-1.858306	-1.968067	-3.644317	-1.612337	-1.773304	-3.295875	-2.004028	-1.627878	-3.662212	-1.812758
C	-1.408883	-4.542257	-2.422132	-0.866437	-4.404099	-1.584743	-0.537648	-3.713996	-2.304286	-0.508689	-4.362725	-2.011362
C	-2.750992	-5.144498	-2.121327	0.203836	-4.450862	-0.533249	0.737918	-3.463754	-1.553289	0.759440	-4.327699	-1.209944
O	-0.327699	-0.650178	-1.642500	-0.939213	-0.934333	-1.704300	-1.449377	-0.391253	-2.031130	-0.633251	-0.886291	-1.694675
C	-2.201007	-0.256783	-0.095371	-2.542293	-0.081807	-0.143421	-2.939954	-0.046514	-0.184305	-2.379554	-0.225475	-0.090783
C	-1.703313	0.129642	1.085138	-1.789451	0.314826	0.888052	-2.189380	0.490073	0.783585	-1.778376	0.137187	1.048050
C	-0.380129	-0.203595	1.717517	-0.437058	-0.209848	1.274716	-0.722211	0.295788	1.028570	-0.464430	-0.319706	1.618755
C	0.778687	0.654074	1.178328	0.687480	0.726105	0.816308	0.067523	1.607369	0.916706	0.743270	0.417786	1.011687
C	2.054391	0.534226	1.994148	2.068686	0.279158	1.271417	-0.066771	2.310223	-0.425446	2.034329	0.211511	1.784817
O	0.392657	2.061237	1.173149	0.394308	2.047320	1.348443	1.453160	1.222921	1.122053	0.482127	1.852700	0.971114
C	0.107559	2.664637	0.005042	0.759801	3.116965	0.604572	2.232362	2.022587	1.887016	0.202298	2.438109	-0.207895
C	-0.188050	4.123896	0.204372	0.369261	4.401357	1.284347	3.624839	1.462139	1.996070	0.061239	3.925771	-0.055214
O	0.076896	2.097350	-1.069263	1.319501	3.028242	-0.462819	1.844781	3.045374	2.400117	0.071063	1.837183	-1.255859
O	-0.482889	0.028857	3.141450	-0.380948	-0.314563	2.720944	-0.581678	-0.139989	2.410465	-0.477942	-0.066068	3.042991
C	-0.995991	-0.980107	3.893440	-0.655022	-1.519596	3.277251	-0.139477	-1.395552	2.657493	-1.007112	-1.033901	3.836955
C	-1.010025	-0.608741	5.349469	-0.552719	-1.451364	4.775435	-0.051242	-1.643693	4.138012	-0.936129	-0.635363	5.284161
O	-1.373249	-2.024977	3.421947	-0.936499	-2.503709	2.634613	0.136043	-2.195348	1.794454	-1.461078	-2.065192	3.404839
C	-3.481844	0.369111	-0.560452	-3.741434	0.725161	-0.527041	-4.350995	0.431710	-0.346699	-3.605657	0.527468	-0.512228
O	-4.175138	1.161227	0.029042	-4.242010	1.644350	0.072984	-4.964573	1.182745	0.370353	-4.183294	1.398457	0.090535
O	-3.911206	-1.565274	-1.944076	-4.649384	-1.139909	-1.782466	-4.932064	-1.587716	-1.548696	-4.311334	-1.364151	-1.844783
H	-2.316198	-1.209016	-3.354746	-3.114479	-1.164689	-3.300701	-3.713191	-1.181324	-3.283335	-2.740745	-1.207990	-3.319925

H	-0.716429	-2.628081	0.092599	-1.789660	-2.675276	0.312186	-1.395801	-2.355740	-0.096479	-1.171666	-2.764572	0.092457
H	-2.360920	-2.986111	-0.405838	-3.424537	-2.748903	-0.320280	-3.067147	-2.835671	-0.359129	-2.883887	-2.887812	-0.270950
H	0.149412	-3.180909	-2.209488	-2.639808	-3.769782	-2.458951	-2.577617	-3.600049	-2.670400	-2.448591	-3.821667	-2.508746
H	-0.842446	-5.055154	-3.197419	-0.723775	-5.095230	-2.413241	-0.430968	-4.330506	-3.194901	-0.496563	-5.047515	-2.857384
H	-3.310368	-4.593866	-1.364666	0.000874	-3.805252	0.321244	1.447887	-2.911830	-2.179350	0.711201	-3.645284	-0.361527
H	-3.363055	-5.184825	-3.028903	0.321020	-5.475101	-0.163465	0.594364	-2.909952	-0.626045	1.006979	-5.326148	-0.833225
H	-2.639923	-6.178566	-1.776462	1.171864	-4.164202	-0.958619	1.220502	-4.416349	-1.309139	1.599063	-4.016822	-1.841465
H	-0.306158	0.322093	-1.587057	-0.652015	-1.756270	-2.130582	-1.060362	-1.083954	-2.586321	-0.500347	0.078505	-1.684540
H	-2.307682	0.832588	1.654244	-2.146877	1.156843	1.474167	-2.687950	1.179565	1.462252	-2.269995	0.917272	1.625085
H	-0.114596	-1.248710	1.558391	-0.245264	-1.187134	0.840466	-0.287480	-0.450625	0.370451	-0.308790	-1.386831	1.462022
H	0.948474	0.341686	0.151060	0.638620	0.775959	-0.271307	-0.223103	2.271121	1.731741	0.845815	0.061721	-0.010161
H	2.851019	1.104552	1.513789	2.824561	0.955882	0.870644	0.576050	3.191919	-0.438296	2.858487	0.692247	1.255326
H	2.365446	-0.511497	2.050098	2.280426	-0.727064	0.901705	-1.095872	2.638306	-0.585030	2.254526	-0.855175	1.868531
H	1.906677	0.910367	3.006199	2.134141	0.275813	2.360113	0.212268	1.646559	-1.244850	1.959778	0.633060	2.786955
H	-0.229503	4.624447	-0.760296	-0.719411	4.461901	1.353835	3.589857	0.466190	2.442516	-0.807766	4.142048	0.570981
H	-1.154234	4.224056	0.706037	0.766151	4.423522	2.300855	4.061697	1.360954	1.000394	0.939173	4.337167	0.445232
H	0.566746	4.582720	0.843719	0.747969	5.247035	0.714617	4.238292	2.121607	2.605868	-0.068731	4.384406	-1.032601
H	-1.501540	-1.392434	5.921375	-0.800000	-2.420224	5.203089	-1.045182	-1.556608	4.582588	-1.399232	-1.404542	5.897902
H	0.015661	-0.481232	5.703493	0.461239	-1.165148	5.063035	0.348920	-2.638733	4.318536	0.107250	-0.502898	5.578742
H	-1.527704	0.341900	5.488967	-1.231983	-0.687354	5.158705	0.585970	-0.890690	4.605349	-1.444102	0.319588	5.432133

	Conformer 13			**Conformer 7**			**Conformer 12**			**Conformer 1**		
Gibbs free energy (hartrees)	-1647.228401			-1647.227184			-1647.226928			-1647.226522		
ΔG (kJ/mol)	7.17			10.365			11.038			12.104		
Population Proportion	2.62%			0.72%			0.55%			0.36%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
Cl	-4.841380	0.830019	-3.037054	-4.940513	1.184214	-3.094033	-4.951694	1.537999	-2.886747	-5.364074	1.071390	-2.792861
C	-3.752841	-0.112093	-2.023946	-3.931305	0.108361	-2.135038	-4.013370	0.299559	-2.057369	-4.325308	0.099601	-1.755101
C	-2.617401	-0.909291	-2.489411	-2.867057	-0.755693	-2.644424	-2.987558	-0.549845	-2.656781	-3.202619	-0.726531	-2.195993
C	-1.504581	-0.961250	-1.434332	-1.756204	-0.947958	-1.601034	-1.928809	-0.980226	-1.624610	-2.139146	-0.855231	-1.089081
C	-0.998656	-2.402117	-1.197088	-1.383140	-2.436226	-1.411644	-1.919585	-2.527481	-1.577852	-1.930265	-2.344393	-0.697261
C	-1.954233	-3.355553	-0.534173	-2.379207	-3.286387	-0.663077	-0.819515	-3.157269	-0.771946	-1.304332	-3.125502	-1.823360
C	-2.329568	-4.558148	-0.976525	-2.089138	-4.315049	0.138233	-0.949148	-4.092604	0.173492	-0.035678	-3.546046	-1.902947
C	-1.946324	-5.239720	-2.258425	-0.736087	-4.866234	0.484868	-2.210080	-4.702647	0.712067	1.058303	-3.397130	-0.885290
O	-0.382689	-0.241742	-1.953445	-0.579378	-0.319262	-2.114486	-0.646760	-0.551946	-2.058930	-0.922922	-0.261670	-1.532875
C	-2.138308	-0.244285	-0.234021	-2.313652	-0.219474	-0.370242	-2.404540	-0.273695	-0.340252	-2.717171	-0.003017	0.042681
C	-1.634052	0.051553	0.969389	-1.766650	0.002892	0.830412	-1.812072	-0.062031	0.843148	-2.155303	0.391563	1.191000
C	-0.277668	-0.265050	1.533776	-0.424997	-0.425393	1.349128	-0.466497	-0.479860	1.366147	-0.774663	0.097853	1.697288
C	0.813714	0.697117	1.031695	0.721725	0.474549	0.846731	0.695276	0.357009	0.799481	0.124187	1.351547	1.831610

C	2.145575	0.526603	1.742205	2.047179	0.210499	1.539564	2.020779	0.104539	1.497157	-0.425142	2.456044	2.718080
O	0.382392	2.075538	1.237102	0.381967	1.873942	1.083145	0.392132	1.777848	0.951087	0.323370	1.923971	0.517428
C	-0.002148	2.817143	0.182142	0.036280	2.661435	0.048965	0.085273	2.515607	-0.128475	1.309408	1.412120	-0.256699
C	-0.300903	4.230509	0.594420	-0.152707	4.084403	0.492008	-0.071638	3.965669	0.231664	1.375974	2.126449	-1.577214
O	-0.100464	2.394747	-0.952584	-0.104568	2.270730	-1.092874	-0.048336	2.067801	-1.250942	2.025127	0.502005	0.091578
O	-0.331801	-0.153316	2.974212	-0.502295	-0.351885	2.793317	-0.525224	-0.295301	2.804831	-0.903867	-0.424730	3.048629
C	-0.833830	-1.215856	3.654715	-0.249417	-1.476835	3.513265	-0.303924	-1.366092	3.609440	-0.659001	-1.741504	3.263452
C	-0.791660	-0.972282	5.136919	-0.456215	-1.222649	4.979966	-0.474812	-0.983891	5.053810	-0.841764	-2.083981	4.715682
O	-1.244977	-2.211214	3.109237	0.089322	-2.523942	3.018398	-0.013507	-2.463905	3.200993	-0.340116	-2.515593	2.392999
C	-3.466684	0.348688	-0.603973	-3.600418	0.480360	-0.697030	-3.680254	0.484208	-0.585436	-4.050735	0.568488	-0.333489
O	-4.167932	1.065678	0.066590	-4.243580	1.214808	0.011477	-4.309601	1.147819	0.201435	-4.759945	1.288329	0.325331
O	-3.860253	-1.520844	-2.065999	-4.159315	-1.282923	-2.246133	-4.312461	-1.052119	-2.339779	-4.474366	-1.305481	-1.805754
H	-2.370413	-1.006832	-3.539470	-2.630303	-0.826357	-3.698922	-2.731703	-0.508509	-3.708516	-2.935789	-0.822901	-3.241161
H	-0.662717	-2.773965	-2.167539	-1.221884	-2.837164	-2.421017	-2.904219	-2.862213	-1.253893	-1.321865	-2.386561	0.205127
H	-0.093508	-2.313897	-0.586804	-0.404405	-2.459574	-0.929939	-1.803835	-2.849709	-2.621554	-2.909264	-2.762585	-0.448619
H	-2.332230	-3.031919	0.432137	-3.424562	-3.044113	-0.818846	0.184117	-2.839903	-1.040314	-1.956705	-3.344906	-2.665815
H	-3.001245	-5.130427	-0.339379	-2.927868	-4.835412	0.596824	-0.033582	-4.468406	0.625101	0.249358	-4.079606	-2.807726
H	-1.297922	-4.633295	-2.891914	0.077600	-4.364808	-0.040904	-3.114832	-4.287810	0.266529	0.717962	-2.967989	0.056643
H	-1.428777	-6.183668	-2.053785	-0.546196	-4.778118	1.559296	-2.216372	-5.785233	0.543035	1.505729	-4.373792	-0.672666
H	-2.840186	-5.496154	-2.837604	-0.686023	-5.932403	0.238199	-2.267692	-4.557424	1.796106	1.864729	-2.767302	-1.277180
H	-0.443660	0.701650	-1.720821	-0.562487	0.623578	-1.870974	-0.534724	0.401232	-1.886382	-0.457096	-0.930398	-2.058322
H	-2.262679	0.658984	1.616933	-2.337502	0.626647	1.513918	-2.370906	0.564582	1.534608	-2.761219	1.034584	1.824797
H	0.031441	-1.278957	1.277459	-0.186707	-1.451772	1.069222	-0.259785	-1.528653	1.154291	-0.259645	-0.631182	1.080230
H	0.921170	0.525780	-0.037169	0.807357	0.316369	-0.226096	0.770044	0.129361	-0.260595	1.086910	0.998844	2.204492
H	2.887757	1.189201	1.294139	2.827856	0.822402	1.085211	2.811798	0.667740	0.999576	0.322580	3.243872	2.823612
H	2.495472	-0.503058	1.638047	2.324954	-0.840224	1.432921	2.272362	-0.957261	1.453336	-0.655487	2.062222	3.708783
H	2.053226	0.760216	2.802716	1.985476	0.453095	2.601205	1.975353	0.413566	2.542142	-1.329164	2.897369	2.294039
H	-0.565016	4.820039	-0.280286	-0.462668	4.694468	-0.353033	-0.341017	4.537277	-0.653242	0.477274	1.880309	-2.146410
H	-1.128655	4.233239	1.307264	-0.905635	4.126777	1.281654	-0.843749	4.072557	0.996376	1.395959	3.206843	-1.426082
H	0.566636	4.663601	1.095466	0.782001	4.466630	0.907628	0.862731	4.343055	0.652273	2.259006	1.804447	-2.125173
H	0.247193	-0.883742	5.463219	-0.148881	-2.096915	5.549218	0.152993	-0.123284	5.291473	-0.615526	-3.135916	4.873688
H	-1.293785	-0.033202	5.376236	0.113409	-0.346640	5.294615	-1.512798	-0.694474	5.233481	-0.186756	-1.462566	5.329397
H	-1.271565	-1.798498	5.656366	-1.512448	-1.013863	5.165766	-0.212490	-1.827313	5.688436	-1.870956	-1.874596	5.015086

Table S13. DFT Geometry Optimized Coordinates for truncated 7*Z* punaglandin 4 (**3a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 12	**Conformer 13**	**Conformer 65**	**Conformer 4**
Gibbs free energy (hartrees)	-1572.025698	-1572.025422	-1572.024963	-1572.024446
ΔG (kJ/mol)		0.725	1.93	3.287

Population Proportion	29.05%			21.69%			13.34%			7.71%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.146885	-0.696355	-1.268565	0.197319	-0.656254	-1.288276	0.139515	-0.533393	-0.445931	0.288281	-0.789700	-1.116037
C	0.483283	-1.561766	-2.452035	0.553513	-1.647326	-2.362752	-0.039081	-1.616860	-1.471293	0.493141	-1.569348	-2.386210
C	0.165539	-3.039653	-2.210241	0.175034	-3.083697	-1.988696	-0.876782	-2.800151	-0.965429	0.213088	-3.064461	-2.213913
C	0.411217	-3.924028	-3.423191	0.444459	-4.094595	-3.092128	-0.265857	-3.519434	0.226767	0.323590	-3.858851	-3.506406
O	-1.233136	-3.119555	-1.815349	-1.245182	-3.103772	-1.668476	-0.943190	-3.738364	-2.072399	-1.131014	-3.189681	-1.669097
C	-1.577452	-4.065593	-0.912622	-1.632986	-3.671121	-0.503850	-2.153510	-4.060689	-2.584430	-1.368855	-4.210425	-0.815011
C	-3.052566	-4.013537	-0.618447	-3.127665	-3.597390	-0.345538	-2.000346	-5.012298	-3.740881	-2.801233	-4.199737	-0.352708
O	-0.789943	-4.839070	-0.419967	-0.868333	-4.155137	0.298524	-3.203398	-3.639164	-2.160747	-0.529334	-5.013474	-0.481098
O	-0.294358	-1.119126	-3.592942	-0.158015	-1.302316	-3.577577	-0.793683	-1.047190	-2.577301	-0.412733	-1.056310	-3.395669
C	0.229520	-0.124482	-4.351525	0.417051	-0.382478	-4.391232	-0.094293	-0.530630	-3.617752	0.039557	-0.049796	-4.184815
C	-0.678832	0.203229	-5.504582	-0.421395	-0.155734	-5.619035	-1.027041	0.009055	-4.667850	-1.010527	0.359115	-5.181000
O	1.287914	0.405133	-4.112718	1.465680	0.161060	-4.140609	1.111590	-0.514373	-3.670021	1.141778	0.431702	-4.082721
C	0.963018	-0.412096	-0.249719	0.968294	-0.314921	-0.251948	1.266882	-0.229439	0.204783	1.211864	-0.568841	-0.176884
C	0.620157	0.510141	0.919929	0.619297	0.742991	0.795579	1.440335	0.959581	1.150504	1.000177	0.262219	1.082383
C	-0.400804	-0.134540	1.890285	-0.514773	0.325756	1.764268	0.823827	0.743776	2.557436	0.095804	-0.468420	2.120071
C	-0.691171	0.708219	3.102459	-0.293135	-0.973651	2.487884	-0.678807	0.688661	2.570551	-0.147008	0.361371	3.352554
C	-0.554395	0.355974	4.383974	-0.170330	-1.151394	3.806196	-1.446837	-0.231537	3.161087	-1.249606	1.063861	3.640515
C	-0.074313	-0.951731	4.944196	-0.199713	-0.115245	4.892050	-1.018373	-1.443906	3.936144	-2.516194	1.171958	2.841683
O	0.044030	1.749741	0.508896	0.165405	1.969758	0.220531	0.874788	2.170298	0.652191	0.424389	1.516895	0.727246
C	1.973860	0.712271	1.583725	1.940595	0.930403	1.522218	2.953263	1.060444	1.271105	2.423612	0.436515	1.599422
C	2.922187	-0.037773	1.015601	2.874725	0.080578	1.086972	3.570789	0.042680	0.666286	3.301742	-0.264633	0.878245
Cl	4.590202	-0.149367	1.477371	4.506433	-0.069516	1.654049	5.275677	-0.266288	0.603045	5.014401	-0.382899	1.131214
C	2.383545	-0.836940	-0.120130	2.353926	-0.796597	0.001942	2.597846	-0.879097	0.016195	2.637507	-0.990078	-0.238268
O	2.991531	-1.651809	-0.787130	2.950148	-1.702176	-0.548503	2.860688	-1.924951	-0.542923	3.164715	-1.752356	-1.025896
H	-0.853265	-0.271734	-1.273949	-0.777243	-0.187099	-1.394672	-0.742671	0.075731	-0.267890	-0.706379	-0.374168	-0.983349
H	1.542957	-1.483823	-2.691142	1.624922	-1.626012	-2.558502	0.919018	-1.974631	-1.840192	1.517640	-1.460910	-2.738987
H	0.775541	-3.370450	-1.369744	0.730638	-3.341297	-1.088184	-1.890371	-2.463837	-0.747222	0.916659	-3.444468	-1.473299
H	0.213310	-4.965895	-3.167017	0.196588	-5.098710	-2.743167	-0.880470	-4.383326	0.485494	0.161486	-4.918615	-3.304301
H	1.453242	-3.842449	-3.741900	1.502372	-4.078718	-3.365189	-0.224475	-2.858026	1.093496	1.322138	-3.741289	-3.934444
H	-0.234311	-3.631058	-4.251824	-0.151039	-3.869945	-3.977603	0.746011	-3.860138	-0.000138	-0.413681	-3.517076	-4.233694
H	-3.315061	-3.033310	-0.214752	-3.623789	-3.953060	-1.249682	-1.444701	-4.524696	-4.545087	-3.467914	-4.283172	-1.213593
H	-3.619325	-4.151898	-1.541478	-3.434878	-4.189370	0.513782	-1.428432	-5.888777	-3.430516	-2.971941	-5.028426	0.330842
H	-3.311313	-4.790726	0.097180	-3.422198	-2.555783	-0.194339	-2.981757	-5.313389	-4.100581	-3.023683	-3.253664	0.145205
H	-0.763261	-0.664537	-6.162844	-0.467621	-1.076237	-6.205635	-1.712403	-0.774189	-4.997372	-1.248275	-0.484492	-5.832821
H	-1.679976	0.436930	-5.137734	-1.442197	0.104231	-5.333158	-1.629047	0.816044	-4.244246	-1.927581	0.641946	-4.660561
H	-0.275691	1.047731	-6.058941	0.015264	0.640187	-6.218083	-0.450873	0.381663	-5.511808	-0.645282	1.193621	-5.775278
H	-1.322159	-0.272327	1.312067	-0.659860	1.157634	2.455809	1.266977	-0.151241	2.995684	-0.840886	-0.710205	1.614721
H	-0.041923	-1.128149	2.161466	-1.422151	0.260096	1.153095	1.155120	1.594814	3.165987	0.572168	-1.414833	2.392132
H	-1.059255	1.706653	2.884681	-0.252388	-1.858627	1.857204	-1.169644	1.515237	2.065535	0.672467	0.399762	4.066197

H	-0.828947	1.098104	5.131459	-0.034612	-2.173314	4.155332	-2.524076	-0.091638	3.092527	-1.251155	1.618826	4.576518
H	0.789162	-0.793840	5.599496	-1.012521	-0.321191	5.597217	-1.356801	-1.372390	4.975994	-3.365344	0.801096	3.425797
H	-0.852204	-1.412250	5.563335	0.728519	-0.144328	5.473129	-1.479554	-2.347513	3.523475	-2.733448	2.220325	2.611466
H	0.213141	-1.671026	4.176621	-0.329385	0.900005	4.515830	0.062312	-1.590414	3.946669	-2.482258	0.621786	1.901434
H	0.636398	2.164027	-0.130664	0.810916	2.251612	-0.439683	1.187767	2.304208	-0.250984	0.097912	1.921041	1.544430
H	2.099245	1.381603	2.423605	2.058399	1.673728	2.299490	3.422453	1.870839	1.813191	2.653867	1.057227	2.454854

	Conformer 69			**Conformer 63**			**Conformer 10**			**Conformer 61**		
Gibbs free energy (hartrees)	-1572.024331			-1572.024108			-1572.02337			-1572.023163		
ΔG (kJ/mol)	3.589			4.175			6.112			6.656		
Population Proportion	6.83%			5.39%			2.47%			1.98%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.234517	-0.790939	-1.073459	0.028928	-0.427135	-0.613147	0.168542	-0.741072	-1.315078	0.283452	-0.680448	-0.932220
C	0.456333	-1.561978	-2.345932	-0.082512	-1.594016	-1.552921	0.509476	-1.629111	-2.480795	0.429496	-1.461347	-2.210327
C	0.146460	-3.053425	-2.196577	-0.978013	-2.720136	-1.014523	0.197786	-3.103413	-2.210700	0.147909	-2.956311	-2.045032
C	0.282241	-3.837524	-3.493066	-0.454603	-3.358725	0.262193	0.447209	-4.009394	-3.406827	0.246368	-3.737164	-3.347514
O	-1.214762	-3.160550	-1.692869	-1.001241	-3.739191	-2.048943	-1.200736	-3.181595	-1.814361	-1.190604	-3.083962	-1.487382
C	-1.493967	-4.182778	-0.852966	-2.184305	-4.063648	-2.620175	-1.542397	-4.116392	-0.899255	-1.441271	-4.161183	-0.709695
C	-2.938869	-4.151342	-0.432697	-1.985931	-5.106443	-3.687674	-3.017785	-4.064938	-0.606091	-2.882235	-4.191290	-0.275986
O	-0.677534	-5.001370	-0.500182	-3.245256	-3.579427	-2.304995	-0.752806	-4.880966	-0.396034	-0.608500	-4.991035	-0.428094
O	-0.413859	-1.027639	-3.375431	-0.734201	-1.114849	-2.761722	-0.270390	-1.207806	-3.628210	-0.506469	-0.938186	-3.186834
C	0.044319	0.034462	-4.083192	0.056028	-0.709421	-3.786572	0.277812	-0.273433	-4.444919	-0.100855	0.124855	-3.924450
C	-0.957059	0.455882	-5.123253	-0.779919	-0.250480	-4.950380	-0.645964	0.042110	-5.589128	-1.168244	0.536978	-4.900665
O	1.118297	0.549716	-3.885943	1.262315	-0.720957	-3.745495	1.364278	0.218270	-4.257971	0.979718	0.648167	-3.796019
C	1.139519	-0.591006	-0.111292	1.097255	-0.081201	0.110042	0.979796	-0.442474	-0.296802	1.249704	-0.469137	-0.032507
C	0.915300	0.250937	1.145595	1.198694	1.189759	0.957374	0.632245	0.491476	0.855175	1.133476	0.413428	1.211504
C	-0.026275	-0.459584	2.153545	0.339584	1.159881	2.244684	-0.417172	-0.135965	1.816563	0.382394	-0.250696	2.398337
C	-0.132915	0.220511	3.493116	0.600556	0.000164	3.164500	-0.803094	0.762390	2.962193	-1.065568	-0.565537	2.135482
C	-1.136088	0.986463	3.929301	-0.303299	-0.838129	3.680151	-0.492160	0.609704	4.253305	-2.128753	0.106155	2.585467
C	-2.381976	1.382068	3.192620	-1.788535	-0.850701	3.462786	0.316054	-0.483185	4.888448	-2.148890	1.350390	3.424093
O	0.319337	1.517109	0.873605	0.759328	2.360062	0.265681	0.157237	1.724129	0.308398	0.479377	1.655113	0.968207
C	2.328139	0.400929	1.690607	2.684244	1.261048	1.264300	1.978282	0.679252	1.542029	2.591062	0.615991	1.598307
C	3.209969	-0.319250	0.991444	3.339096	0.187555	0.813502	2.927281	-0.078970	0.988120	3.413379	-0.130516	0.856228
Cl	4.912349	-0.469731	1.286084	5.030506	-0.155001	0.973397	4.590306	-0.199358	1.468139	5.138094	-0.251506	0.993050
C	2.558754	-1.037389	-0.138987	2.424760	-0.763073	0.119409	2.395902	-0.875269	-0.151659	2.665759	-0.909733	-0.168525
O	3.091386	-1.811895	-0.910528	2.724848	-1.849702	-0.332522	3.005001	-1.694533	-0.812574	3.132163	-1.716936	-0.949520
H	-0.756047	-0.359054	-0.959888	-0.853884	0.207361	-0.570026	-0.829950	-0.314164	-1.335396	-0.694698	-0.240091	-0.764475
H	1.491751	-1.468690	-2.670766	0.896909	-1.990670	-1.808824	1.568499	-1.551169	-2.721926	1.441746	-1.359847	-2.599667
H	0.821677	-3.452083	-1.439534	-1.994706	-2.348892	-0.884699	0.809104	-3.415684	-1.364115	0.859462	-3.343515	-1.315743

H	0.094046	-4.895829	-3.306540	-1.115889	-4.174198	0.560021	0.253733	-5.047136	-3.131329	0.082293	-4.798417	-3.156651
H	1.295776	-3.735082	-3.888579	-0.422213	-2.629408	1.073196	1.488842	-3.929331	-3.727221	1.242707	-3.618168	-3.780162
H	-0.425156	-3.474864	-4.239553	0.551176	-3.755728	0.112790	-0.199718	-3.734772	-4.240713	-0.494009	-3.383816	-4.066064
H	-3.144172	-4.983582	0.236868	-1.356543	-4.701212	-4.483180	-3.284022	-3.079443	-0.218029	-3.496654	-4.525132	-1.116757
H	-3.158836	-3.206515	0.068733	-1.471229	-5.974338	-3.271113	-3.583754	-4.219964	-1.526979	-3.000980	-4.889423	0.550118
H	-3.581396	-4.213848	-1.313461	-2.950170	-5.402631	-4.094758	-3.273949	-4.831778	0.121535	-3.224125	-3.196506	0.010299
H	-0.598024	1.344431	-5.637617	-0.132171	0.028196	-5.778521	-0.214694	0.831984	-6.199956	-0.844887	1.422248	-5.443565
H	-1.103164	-0.353905	-5.841708	-1.461836	-1.045595	-5.257718	-0.798729	-0.853440	-6.195694	-1.359737	-0.278245	-5.602063
H	-1.921562	0.657205	-4.653345	-1.387449	0.606197	-4.650123	-1.620727	0.351754	-5.207534	-2.100395	0.740863	-4.370347
H	-1.000751	-0.534575	1.666426	0.542665	2.103015	2.766649	-1.304830	-0.347172	1.211056	0.913693	-1.173248	2.650793
H	0.342630	-1.480307	2.291181	-0.703107	1.197687	1.925195	-0.033992	-1.095002	2.169958	0.488549	0.422341	3.252065
H	0.698588	0.046970	4.172528	1.637517	-0.139889	3.461129	-1.422118	1.617574	2.698110	-1.246607	-1.448661	1.529121
H	-1.054735	1.382957	4.939796	0.065808	-1.606394	4.356748	-0.871598	1.359012	4.945271	-3.109806	-0.282482	2.318001
H	-2.428403	0.973871	2.183245	-2.313665	-0.655239	4.404545	-0.274270	-0.999492	5.653192	-2.684536	1.175854	4.363818
H	-3.274782	1.058904	3.739305	-2.123774	-0.112160	2.733903	0.672424	-1.226976	4.175223	-1.152213	1.723207	3.659804
H	-2.443906	2.473037	3.113562	-2.119519	-1.838039	3.124007	1.187837	-0.063356	5.402043	-2.688452	2.148734	2.902846
H	0.846887	1.962202	0.198726	1.225976	2.407546	-0.578074	-0.087428	2.304521	1.039741	0.894595	2.071891	0.202788
H	2.545043	1.023348	2.547785	3.111826	2.100667	1.796511	2.102311	1.347621	2.383528	2.872494	1.280391	2.404682

	Conformer 27			**Conformer 56**			**Conformer 20**			**Conformer 45**		
Gibbs free energy (hartrees)	-1572.023145			-1572.023041			-1572.022975			-1572.022804		
ΔG (kJ/mol)	6.703			6.976			7.149			7.598		
Population Proportion	1.94%			1.74%			1.62%			1.36%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.234159	-0.594453	-0.969238	0.281909	-0.821354	-0.904486	0.350128	-0.645670	-0.873570	0.220882	-0.664730	-1.271200
C	0.418056	-1.578765	-2.090950	0.427444	-1.644937	-2.153620	0.431423	-1.545649	-2.075778	0.530872	-1.547510	-2.450601
C	-0.239090	-2.932962	-1.817778	-0.026816	-3.095970	-1.966736	-0.186818	-2.924939	-1.838480	0.220769	-3.022273	-2.182221
C	-0.074481	-3.925919	-2.959210	0.101129	-3.937502	-3.227212	-0.112248	-3.838409	-3.053386	0.441640	-3.921689	-3.388897
O	-1.653667	-2.683913	-1.582142	-1.424032	-3.086783	-1.558864	-1.579292	-2.717999	-1.470602	-1.169205	-3.098979	-1.756709
C	-2.301501	-3.496952	-0.719821	-1.775229	-3.738202	-0.427192	-2.129642	-3.563255	-0.572061	-1.493642	-4.036379	-0.837840
C	-3.750687	-3.109443	-0.600048	-3.258756	-3.638851	-0.194876	-3.579498	-3.231301	-0.342913	-2.963289	-3.985980	-0.516954
O	-1.765646	-4.403232	-0.123969	-0.990516	-4.305646	0.297240	-1.520201	-4.458732	-0.033360	-0.694800	-4.802508	-0.351996
O	-0.192230	-1.029737	-3.289771	-0.396281	-1.059567	-3.196403	-0.295741	-0.921892	-3.168137	-0.276592	-1.115940	-3.575168
C	0.577419	-0.229314	-4.067998	0.155825	-0.068393	-3.938576	0.388613	-0.054608	-3.954100	0.257330	-0.184502	-4.404957
C	-0.190299	0.238838	-5.274045	-0.810688	0.417297	-4.984018	-0.495930	0.490836	-5.041862	-0.693519	0.139296	-5.524414
O	1.722995	0.049371	-3.808178	1.276793	0.345749	-3.766133	1.551700	0.221613	-3.784939	1.352108	0.298420	-4.246244
C	1.154142	-0.268179	-0.057046	1.264781	-0.514194	-0.051961	1.351937	-0.377831	-0.029559	1.061022	-0.359836	-0.278408
C	0.990003	0.824572	1.001513	1.126474	0.407500	1.160387	1.294522	0.626441	1.122138	0.757579	0.577376	0.894997
C	0.083383	0.417125	2.190326	0.531657	-0.281853	2.420641	0.589876	0.094051	2.397452	-0.294225	-0.031240	1.861646

C	0.528081	-0.805377	2.944015	-0.858768	-0.836781	2.257514	-0.887931	-0.133152	2.242678	-0.532193	0.800923	3.092243
C	-0.201096	-1.885643	3.237380	-2.000572	-0.265606	2.650833	-1.570747	-1.230976	2.580887	-0.451495	0.403176	4.365034
C	-1.630982	-2.168522	2.881216	-2.183491	1.074059	3.301352	-1.046583	-2.512231	3.162853	-0.102732	-0.957489	4.894938
O	0.394134	2.016667	0.490321	0.321125	1.554659	0.912838	0.634603	1.843872	0.783569	0.372679	1.889951	0.478560
C	2.423179	1.065016	1.444797	2.573335	0.782793	1.444452	2.767943	0.852218	1.427419	2.113316	0.717944	1.560683
C	3.265839	0.180221	0.904857	3.426233	0.071145	0.702750	3.551993	0.015332	0.743606	3.035455	-0.055668	0.984123
Cl	4.973606	0.054768	1.174431	5.159132	0.122039	0.750724	5.278396	-0.119853	0.833023	4.694231	-0.234291	1.453643
C	2.559695	-0.763592	-0.007199	2.708881	-0.844454	-0.227123	2.756632	-0.864197	-0.157829	2.474702	-0.814258	-0.167234
O	3.049990	-1.716036	-0.580615	3.214376	-1.664619	-0.967994	3.186629	-1.768759	-0.846055	3.061145	-1.630535	-0.851428
H	-0.731187	-0.096069	-0.942030	-0.715300	-0.436004	-0.712247	-0.609184	-0.160906	-0.720318	-0.787100	-0.257690	-1.265754
H	1.476610	-1.750170	-2.275830	1.464780	-1.657384	-2.482635	1.468011	-1.689125	-2.373714	1.583379	-1.470548	-2.717622
H	0.193623	-3.334079	-0.900536	0.561471	-3.524138	-1.155475	0.326621	-3.378888	-0.990344	0.849052	-3.341846	-1.350941
H	-0.529768	-4.879737	-2.689171	-0.203297	-4.965104	-3.020499	-0.535605	-4.814252	-2.810379	0.250632	-4.960534	-3.115808
H	0.986500	-4.096967	-3.156483	1.139658	-3.949218	-3.566497	0.929183	-3.982246	-3.350964	1.476479	-3.842980	-3.730842
H	-0.545918	-3.549511	-3.867802	-0.525580	-3.536854	-4.024874	-0.662903	-3.410095	-3.891779	-0.222010	-3.639834	-4.207100
H	-4.196799	-3.000138	-1.589649	-3.542810	-4.276534	0.639334	-4.116949	-3.236023	-1.293124	-3.222998	-3.001322	-0.122431
H	-4.285069	-3.862776	-0.025386	-3.518900	-2.602103	0.032531	-4.018918	-3.956068	0.338782	-3.546204	-4.140024	-1.427387
H	-3.826737	-2.143675	-0.094347	-3.803469	-3.926019	-1.095517	-3.664157	-2.227448	0.078656	-3.205447	-4.754150	0.214051
H	-0.463512	-0.620134	-5.891213	-1.037235	-0.394177	-5.679395	-0.830291	-0.324512	-5.687322	-0.277412	0.934496	-6.138841
H	-1.115134	0.727662	-4.962175	-1.748513	0.720169	-4.514670	-1.384524	0.950487	-4.605056	-0.858329	-0.751634	-6.134734
H	0.421554	0.927698	-5.852096	-0.374270	1.254163	-5.524615	0.054823	1.223000	-5.628085	-1.659880	0.443820	-5.118339
H	0.063845	1.282683	2.863705	1.209038	-1.092546	2.703756	1.105561	-0.808979	2.726023	-1.229378	-0.118205	1.291331
H	-0.926101	0.305571	1.791299	0.567680	0.458422	3.223490	0.754670	0.854858	3.171083	0.007628	-1.049577	2.111627
H	1.550775	-0.780596	3.312828	-0.915017	-1.819795	1.798250	-1.441689	0.711384	1.843346	-0.804115	1.835207	2.899828
H	0.286921	-2.665947	3.818292	-2.918674	-0.827024	2.486619	-2.648580	-1.205578	2.431042	-0.670780	1.147103	5.128662
H	-1.708984	-3.105549	2.320734	-1.247767	1.619808	3.419149	-1.507412	-2.706263	4.137817	0.138252	-1.677448	4.112162
H	-2.231254	-2.295742	3.789102	-2.857634	1.696022	2.702361	-1.305874	-3.359264	2.519376	0.754805	-0.895607	5.573572
H	-2.089364	-1.378214	2.285525	-2.652520	0.966684	4.285842	0.035552	-2.512085	3.298708	-0.933416	-1.364142	5.482410
H	0.886539	2.289635	-0.293913	0.637735	1.978566	0.105306	1.007890	2.172043	-0.043771	-0.546292	1.862454	0.186786
H	2.676761	1.859235	2.134791	2.828090	1.520993	2.193544	3.086966	1.596704	2.144867	2.260373	1.372457	2.408295

	Conformer 30			**Conformer 8**			**Conformer 46**			**Conformer 62**		
Gibbs free energy (hartrees)	-1572.022683			-1572.022668			-1572.022633			-1572.02216		
ΔG (kJ/mol)	7.916			7.955			8.047			9.289		
Population Proportion	1.19%			1.17%			1.13%			0.69%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.309780	-0.698960	-1.006559	0.320593	-0.699439	-1.020623	-0.157693	-0.495146	-1.262325	-0.103442	-0.384627	-1.285724
C	0.449775	-1.533261	-2.251511	0.486016	-1.521471	-2.270611	-0.132727	-1.497539	-2.378549	-0.147695	-1.479146	-2.310939
C	0.131284	-3.013318	-2.026839	0.197933	-3.008975	-2.055515	-1.200325	-2.609020	-2.254918	-1.301940	-2.487542	-2.107324

C	0.187935	-3.843952	-3.300416	0.293209	-3.835709	-3.329215	-2.620882	-2.123535	-2.027377	-2.682839	-1.874675	-1.955905
O	-1.201545	-3.084781	-1.443416	-1.142369	-3.112984	-1.496101	-0.844076	-3.449926	-1.130904	-1.028061	-3.245144	-0.903381
C	-1.464287	-4.123813	-0.619987	-1.390781	-4.146318	-0.660543	-0.013436	-4.494773	-1.365903	-0.281247	-4.370552	-1.024000
C	-2.868128	-4.053490	-0.080182	-2.832868	-4.158704	-0.229376	0.305462	-5.231457	-0.095038	-0.041342	-5.008204	0.315797
O	-0.656812	-4.981287	-0.346809	-0.555805	-4.956100	-0.330974	0.417082	-4.772183	-2.460376	0.139044	-4.781837	-2.079410
O	-0.468090	-1.023853	-3.252241	-0.437482	-1.026965	-3.273760	-0.450362	-0.819969	-3.623162	-0.398463	-0.890762	-3.614767
C	-0.005395	-0.063801	-4.091598	0.007020	-0.049861	-4.103072	0.578761	-0.260239	-4.309321	0.678756	-0.473247	-4.328068
C	-1.070758	0.345506	-5.071342	-1.061743	0.340476	-5.086916	0.085196	0.386793	-5.574145	0.251495	0.095853	-5.653055
O	1.115554	0.381236	-4.040060	1.116511	0.421820	-4.041306	1.723806	-0.292045	-3.930390	1.813480	-0.558477	-3.926987
C	1.264047	-0.485157	-0.096067	1.272070	-0.454415	-0.115069	0.659644	-0.451983	-0.206173	0.714850	-0.308300	-0.232440
C	1.156150	0.424684	1.133648	1.139167	0.446602	1.118635	0.611636	0.629361	0.874737	0.745722	0.863392	0.751439
C	0.365474	-0.231351	2.312262	0.399864	-0.249572	2.307869	-0.614818	0.464045	1.806544	-0.483785	0.919316	1.692131
C	-1.118932	-0.252133	2.067172	-1.085486	-0.343401	2.087063	-0.646126	1.453740	2.939383	-0.756867	-0.346279	2.456195
C	-2.027830	0.580271	2.591045	-2.024693	0.447172	2.622118	-0.698265	1.184525	4.247019	-0.766272	-0.504629	3.782436
C	-1.807932	1.703325	3.562588	-1.843155	1.584778	3.584758	-0.730541	-0.156829	4.920894	-0.491472	0.521472	4.842980
O	0.626619	1.711688	0.841023	0.543880	1.706981	0.838202	0.526784	1.951304	0.342951	0.762572	2.137543	0.106471
C	2.606170	0.590848	1.538339	2.585562	0.679551	1.502854	1.916725	0.407501	1.621620	2.031158	0.614623	1.519895
C	3.416838	-0.204597	0.835793	3.421326	-0.081952	0.792131	2.565719	-0.670562	1.173816	2.605446	-0.538553	1.167761
Cl	5.129642	-0.387614	1.025491	5.142653	-0.190226	0.961281	4.066024	-1.311855	1.761472	4.060838	-1.226642	1.811751
C	2.666382	-0.977444	-0.191035	2.692494	-0.889645	-0.223373	1.834581	-1.331243	0.056488	1.826771	-1.241565	0.109849
O	3.122689	-1.817280	-0.943204	3.175083	-1.713282	-0.976978	2.158150	-2.359737	-0.504358	2.075606	-2.335720	-0.356907
H	-0.661617	-0.230256	-0.880783	-0.667222	-0.268843	-0.886288	-0.918352	0.277051	-1.351507	-0.810403	0.426730	-1.443832
H	1.466174	-1.470745	-2.637728	1.502849	-1.434067	-2.650391	0.847224	-1.960951	-2.463729	0.792743	-2.023976	-2.339416
H	0.843915	-3.392232	-1.294340	0.906318	-3.373861	-1.311916	-1.132864	-3.204639	-3.165499	-1.270204	-3.169621	-2.957102
H	0.005022	-4.893336	-3.066779	0.130004	-4.889649	-3.100149	-3.306831	-2.972273	-2.035931	-3.432712	-2.665315	-1.896718
H	1.177800	-3.762087	-3.755935	1.287930	-3.731847	-3.769334	-2.911088	-1.436277	-2.823984	-2.908106	-1.248767	-2.821103
H	-0.558617	-3.501006	-4.017666	-0.449830	-3.508765	-4.057523	-2.717058	-1.611122	-1.067992	-2.752351	-1.264636	-1.053007
H	-2.869228	-3.430371	0.818653	-3.444621	-4.535078	-1.053914	1.149645	-4.726944	0.382523	0.798102	-4.493058	0.790162
H	-3.548287	-3.606876	-0.804370	-2.951861	-4.815308	0.630065	-0.537868	-5.217330	0.594470	-0.912820	-4.909101	0.962405
H	-3.200913	-5.053198	0.193955	-3.178172	-3.152005	0.006793	0.595093	-6.254462	-0.329209	0.219357	-6.056151	0.179351
H	-0.695928	1.144890	-5.706536	-1.319242	-0.518603	-5.710462	-0.439499	-0.348042	-6.187854	1.128992	0.392237	-6.223220
H	-1.356383	-0.512265	-5.684303	-1.965489	0.643809	-4.554873	-0.625360	1.179258	-5.329155	-0.324080	-0.646730	-6.209073
H	-1.961719	0.678459	-4.535442	-0.703852	1.155842	-5.711478	0.926619	0.801165	-6.124804	-0.395654	0.960614	-5.490710
H	0.737196	-1.249866	2.452728	0.823509	-1.248690	2.440079	-1.497930	0.606250	1.172528	-0.338916	1.774133	2.355019
H	0.602956	0.329492	3.218606	0.624100	0.320969	3.211575	-0.641208	-0.565779	2.164643	-1.340212	1.156685	1.050572
H	-1.472752	-1.015724	1.380219	-1.413112	-1.128169	1.411008	-0.632267	2.495933	2.633760	-0.987852	-1.215317	1.844450
H	-3.064551	0.424445	2.299574	-3.057442	0.239846	2.349212	-0.729389	2.035539	4.925002	-1.005951	-1.497150	4.159145
H	-2.358237	1.513903	4.490552	-2.285349	2.500948	3.179615	-1.647067	-0.267488	5.511033	0.336635	0.197363	5.482652
H	-0.758705	1.859195	3.813254	-2.370220	1.375006	4.521780	-0.678435	-0.992483	4.222210	-0.240660	1.502486	4.438341
H	-2.200876	2.640982	3.155892	-0.798737	1.790736	3.818852	0.103597	-0.252219	5.624486	-1.361433	0.638343	5.498593
H	-0.333503	1.659951	0.952848	-0.410773	1.608726	0.964529	1.258039	2.079255	-0.273993	1.486582	2.144861	-0.532183
H	2.893409	1.265850	2.333433	2.852767	1.368513	2.292945	2.230420	1.061999	2.423103	2.390946	1.313303	2.263575

	Conformer 18			Conformer 16		
Gibbs free energy (hartrees)	-1572.021616			-1572.021424		
ΔG (kJ/mol)	10.717			11.221		
Population Proportion	0.39%			0.31%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-0.064097	-0.260350	-1.072137	0.008406	-0.334700	-0.907711
C	-0.186250	-1.342623	-2.105380	-0.208534	-1.312815	-2.025419
C	-1.387393	-2.292976	-1.904808	-1.366575	-2.307571	-1.787031
C	-2.737897	-1.614651	-1.760375	-2.698529	-1.679695	-1.417886
O	-1.149314	-3.061087	-0.699877	-0.980348	-3.186503	-0.701795
C	-0.456749	-4.220388	-0.819407	-0.294818	-4.312053	-1.018704
C	-0.234852	-4.858154	0.523506	0.091138	-5.078385	0.215583
O	-0.065560	-4.658447	-1.875362	-0.024463	-4.632296	-2.152026
O	-0.418662	-0.722370	-3.399105	-0.593373	-0.577029	-3.218101
C	0.671100	-0.373459	-4.129733	0.403465	-0.126944	-4.022050
C	0.258730	0.240181	-5.439618	-0.159667	0.603187	-5.210405
O	1.804983	-0.543460	-3.753915	1.574483	-0.300805	-3.788691
C	0.818923	-0.210652	-0.070762	0.980462	-0.374241	0.009207
C	0.983674	0.978880	0.878792	1.218535	0.697861	1.073143
C	-0.116424	1.065681	1.967819	0.273746	0.585028	2.299277
C	-0.218507	-0.133881	2.867939	-1.167213	0.891657	2.000561
C	-1.284915	-0.915179	3.060114	-2.226459	0.123351	2.272127
C	-2.638969	-0.814955	2.421548	-2.251410	-1.235249	2.910709
O	0.928560	2.240437	0.213659	1.077215	2.029322	0.584113
C	2.353783	0.726212	1.482992	2.645511	0.408846	1.512375
C	2.844462	-0.461871	1.119773	3.111796	-0.719665	0.972157
Cl	4.345222	-1.174437	1.614528	4.657538	-1.456369	1.244762
C	1.921017	-1.179198	0.195516	2.112057	-1.344701	0.061048
O	2.069999	-2.304587	-0.237833	2.230294	-2.410864	-0.510088
H	-0.746075	0.577804	-1.194804	-0.689091	0.497587	-0.877730
H	0.723726	-1.935526	-2.153531	0.698555	-1.875423	-2.231808
H	-1.386671	-2.976913	-2.753746	-1.455955	-2.903098	-2.695806
H	-3.524047	-2.368613	-1.692625	-3.461872	-2.455473	-1.336225

H	-2.932740	-0.989783	-2.633614	-3.003289	-0.975942	-2.194462
H	-2.779221	-0.990862	-0.865659	-2.638318	-1.148365	-0.466081
H	0.025990	-5.906469	0.391373	1.016964	-4.646174	0.604625
H	-1.116039	-4.758082	1.157017	-0.674222	-4.999835	0.986997
H	0.596048	-4.342377	1.011846	0.271463	-6.120231	-0.043399
H	-0.373330	-0.456308	-5.994046	-0.857489	-0.041038	-5.748583
H	-0.328140	1.142642	-5.255256	-0.714908	1.481009	-4.872292
H	1.143547	0.486352	-6.022231	0.650574	0.909721	-5.868075
H	0.118727	1.956226	2.562757	0.394525	-0.406565	2.736749
H	-1.055018	1.269429	1.450131	0.646791	1.307292	3.036298
H	0.677737	-0.365793	3.438476	-1.342884	1.859220	1.539907
H	-1.176186	-1.730665	3.772559	-3.204901	0.522771	2.011494
H	-3.414368	-0.694619	3.186016	-1.258053	-1.624931	3.135164
H	-2.724401	0.017159	1.722074	-2.822484	-1.209388	3.845468
H	-2.874573	-1.737547	1.880960	-2.756293	-1.955999	2.258761
H	1.559836	2.226057	-0.516679	1.610602	2.117352	-0.215476
H	2.824245	1.444673	2.141465	3.165215	1.057699	2.204913

Table S14. DFT Geometry Optimized Coordinates for truncated punaglandin 6 (**4a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 19			**Conformer 24**			**Conformer 4**			**Conformer 27**		
Gibbs free energy (hartrees)	-1573.231808			-1573.23119			-1573.230321			-1573.230158		
ΔG (kJ/mol)				1.623			3.904			4.332		
Population Proportion	50.51%			26.25%			10.46%			8.8%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-1.358681	0.221553	-1.575352	-0.688866	0.736769	-1.484632	-0.547268	0.737203	-1.566035	-1.256761	0.319025	-1.377437
C	-0.889177	-1.131996	-1.048030	-0.284006	-0.661275	-1.034856	-0.147681	-0.678402	-1.166011	-0.745469	-1.039267	-0.900588
C	-0.958876	-2.236138	-2.102517	0.081852	-1.627428	-2.174205	0.169842	-1.610639	-2.351595	-0.842320	-2.117789	-1.980725
C	-0.426194	-3.582400	-1.633458	1.178339	-1.152797	-3.116221	1.265320	-1.129669	-3.286632	-0.247750	-3.461782	-1.586196
O	-0.194915	-1.789450	-3.259517	-1.156112	-1.827107	-2.911964	-1.038314	-1.748319	-3.151591	-0.157753	-1.613825	-3.162900
C	-0.627188	-2.162500	-4.483535	-1.389631	-3.049234	-3.440963	-1.967093	-2.648213	-2.757667	-0.646367	-1.964814	-4.372579
C	0.266563	-1.608023	-5.560751	-2.705889	-3.073824	-4.170735	-3.165801	-2.617066	-3.666664	0.169371	-1.351956	-5.479438
O	-1.607101	-2.846340	-4.669608	-0.627783	-3.981654	-3.336134	-1.839711	-3.363896	-1.791300	-1.613909	-2.673915	-4.524862
O	0.489169	-0.984846	-0.596451	0.894031	-0.533411	-0.189355	1.058949	-0.598912	-0.355012	0.646288	-0.860356	-0.507927
C	0.806028	-1.325988	0.671541	0.968386	-1.284662	0.934380	1.090127	-1.232365	0.840508	1.059818	-1.316176	0.695876

C	2.265437	-1.080713	0.944412	2.265230	-1.040789	1.656658	2.437590	-1.075921	1.491514	2.514849	-1.000612	0.915036
O	0.009447	-1.751276	1.477720	0.096296	-2.040557	1.295877	0.152877	-1.835026	1.310581	0.341195	-1.881307	1.488027
C	-1.470966	1.320616	-0.506777	-1.152835	1.649726	-0.338851	-1.127709	1.566385	-0.409978	-1.474210	1.355017	-0.256586
C	-2.673929	1.216937	0.482567	-2.538583	1.333370	0.305246	-2.555061	1.171375	0.083869	-2.866666	1.271066	0.468750
C	-2.206688	1.066243	1.956341	-2.408904	0.890557	1.788283	-2.545314	0.648673	1.547028	-2.752155	1.402892	2.019834
C	-3.355807	0.924645	2.919100	-3.735166	0.542249	2.410371	-3.902779	0.186330	2.006250	-2.278234	0.129791	2.665867
C	-3.769398	-0.201108	3.513931	-4.206267	-0.685331	2.661624	-4.317920	-1.080989	2.126726	-3.015985	-0.724513	3.386960
C	-3.178472	-1.577573	3.409609	-3.529954	-2.006108	2.432641	-3.537149	-2.341220	1.886964	-4.463817	-0.617011	3.768260
O	-3.504496	0.111568	0.116249	-3.199623	0.316701	-0.453450	-3.108698	0.179091	-0.786752	-3.620969	0.110209	0.131995
C	-3.439697	2.513199	0.263684	-3.311206	2.637112	0.167282	-3.358013	2.455945	-0.056311	-3.616673	2.471126	-0.064634
C	-2.851089	3.305898	-0.632674	-2.599372	3.587368	-0.439585	-2.626330	3.462385	-0.536128	-2.829582	3.297859	-0.755320
Cl	-3.394374	4.867321	-1.172011	-3.110821	5.207662	-0.809648	-3.158345	5.085830	-0.861371	-3.268381	4.826077	-1.454047
C	-1.620182	2.690229	-1.178715	-1.252333	3.101444	-0.817777	-1.231944	3.042409	-0.806344	-1.455560	2.757547	-0.876786
O	-0.874770	3.166655	-2.003931	-0.392364	3.724904	-1.396970	-0.342018	3.727114	-1.256832	-0.504971	3.301693	-1.390518
H	-0.653807	0.564624	-2.335267	0.158991	1.227949	-1.968339	0.327409	1.268505	-1.949083	-0.525283	0.717953	-2.082800
H	-2.327525	0.081606	-2.058901	-1.483480	0.633771	-2.224406	-1.277701	0.670144	-2.372893	-2.193272	0.169681	-1.917581
H	-1.496134	-1.446570	-0.201191	-1.081150	-1.118919	-0.453832	-0.927773	-1.147631	-0.573417	-1.297330	-1.397595	-0.032379
H	-2.001844	-2.335025	-2.408785	0.361272	-2.583000	-1.728687	0.415274	-2.591719	-1.941872	-1.898211	-2.237256	-2.230577
H	-0.574988	-4.333239	-2.410631	1.423410	-1.942737	-3.827943	1.459552	-1.884338	-4.050893	-0.425287	-4.192113	-2.376793
H	-0.957007	-3.906847	-0.735553	2.078256	-0.912177	-2.546815	2.184677	-0.962822	-2.723125	-0.712514	-3.826956	-0.667923
H	0.639744	-3.518545	-1.407749	0.868934	-0.266761	-3.673608	0.986658	-0.198827	-3.784289	0.828431	-3.376219	-1.425271
H	-0.045823	-1.991265	-6.529678	-2.662844	-2.392534	-5.023758	-3.779260	-3.499060	-3.494478	1.221610	-1.616361	-5.359059
H	0.207352	-0.517055	-5.559997	-2.913661	-4.083533	-4.517896	-3.752185	-1.721880	-3.442344	-0.197152	-1.701972	-6.441920
H	1.304811	-1.881506	-5.364313	-3.505925	-2.728347	-3.513566	-2.858773	-2.561681	-4.711394	0.095668	-0.263096	-5.430125
H	2.878472	-1.466224	0.129037	2.360785	0.019099	1.901050	3.200908	-1.552488	0.872300	2.878187	-1.536820	1.789025
H	2.439896	-0.003456	1.009764	2.295543	-1.637041	2.565793	2.693066	-0.017705	1.572424	3.100663	-1.264987	0.033884
H	2.545402	-1.547647	1.886235	3.103685	-1.306066	1.009167	2.423386	-1.534713	2.477545	2.627245	0.074588	1.077178
H	-0.530940	1.358523	0.052954	-0.380685	1.643523	0.437768	-0.426597	1.530948	0.430889	-0.640303	1.302248	0.448331
H	-1.546480	0.198571	2.002002	-1.728057	0.037777	1.818272	-1.816175	-0.161589	1.601408	-2.061161	2.221898	2.241677
H	-1.608858	1.946349	2.215925	-1.936158	1.704294	2.348353	-2.185163	1.455196	2.194293	-3.730188	1.694640	2.407447
H	-3.911227	1.834893	3.133020	-4.375757	1.383932	2.663168	-4.618782	0.970580	2.240992	-1.236468	-0.131277	2.502547
H	-4.631994	-0.122110	4.172950	-5.198374	-0.750936	3.104259	-5.344664	-1.233849	2.453846	-2.508543	-1.608231	3.768971
H	-2.901236	-1.942972	4.404521	-2.523698	-1.917118	2.023335	-3.576317	-2.980058	2.775769	-4.958095	0.261025	3.352253
H	-3.921344	-2.282310	3.019952	-3.467735	-2.563385	3.373721	-3.984870	-2.920236	1.071653	-5.012460	-1.504256	3.435270
H	-2.296700	-1.625211	2.770956	-4.122163	-2.623824	1.748599	-2.490545	-2.164852	1.639624	-4.565481	-0.581698	4.858373
H	-4.092840	-0.063063	0.864875	-3.932961	-0.010932	0.086880	-3.859072	-0.219175	-0.322001	-3.472769	-0.545206	0.829455
H	-4.363242	2.727234	0.785554	-4.331257	2.737924	0.514023	-4.409510	2.504324	0.195020	-4.666434	2.615623	0.155161

	Conformer 15	**Conformer 11**	**Conformer 10**
Gibbs free energy (hartrees)	-1573.228944	-1573.227984	-1573.227743

ΔG (kJ/mol)	7.519			10.04			10.673		
Population Proportion	2.43%			0.88%			0.68%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-1.058682	-0.077786	-1.261929	-0.598919	0.564440	-1.356225	-0.627637	0.772928	-1.474864
C	0.438796	-0.246011	-0.980292	-0.272914	-0.910594	-1.152068	-0.137633	-0.615616	-1.076928
C	0.793319	-0.901327	0.353235	0.322245	-1.603433	-2.394083	0.225636	-1.525774	-2.269425
C	2.287957	-1.097793	0.558049	1.584576	-0.971865	-2.954459	1.337693	-1.006603	-3.164050
O	0.162411	-2.215704	0.423875	-0.676826	-1.564292	-3.451406	-0.950625	-1.672351	-3.114950
C	-0.760937	-2.449466	1.376894	-1.620637	-2.532368	-3.474486	-1.917289	-2.534600	-2.731510
C	-1.273282	-3.862701	1.302927	-2.596025	-2.304370	-4.597570	-3.071873	-2.516650	-3.695711
O	-1.143881	-1.615898	2.169194	-1.666304	-3.443826	-2.681702	-1.856291	-3.206108	-1.727006
O	0.992753	-1.084373	-2.033812	0.723611	-1.015786	-0.095943	1.060388	-0.432553	-0.271527
C	1.479244	-0.472131	-3.136309	0.506598	-1.876752	0.925201	1.273989	-1.261317	0.778625
C	2.028846	-1.479401	-4.110581	1.666976	-1.869855	1.883218	2.565571	-0.921347	1.471607
O	1.469477	0.726041	-3.297361	-0.496190	-2.542227	1.045331	0.516284	-2.145935	1.100547
C	-1.819704	0.837428	-0.278366	-1.434988	1.191069	-0.225419	-1.353007	1.524843	-0.342407
C	-3.333152	1.030299	-0.668231	-2.938213	0.775325	-0.159563	-2.857827	1.121896	-0.126343
C	-4.285921	0.830864	0.550290	-3.337417	0.124495	1.190452	-3.210721	0.882460	1.374116
C	-4.407501	-0.617830	0.942803	-3.166865	1.004591	2.399570	-2.690063	-0.436347	1.877433
C	-5.440573	-1.430815	0.686908	-2.507019	0.720080	3.526206	-3.408349	-1.536345	2.137643
C	-6.729553	-1.106047	-0.011157	-1.759568	-0.532657	3.878614	-4.893955	-1.725817	2.038677
O	-3.765288	0.219309	-1.754025	-3.220712	-0.141375	-1.225620	-3.274129	0.001523	-0.906121
C	-3.404323	2.466985	-1.130089	-3.689604	2.072515	-0.404404	-3.624601	2.325105	-0.627211
C	-2.277609	3.136592	-0.880407	-2.871880	3.119490	-0.519460	-2.829804	3.363908	-0.890175
Cl	-1.972948	4.821727	-1.167329	-3.317451	4.776607	-0.794581	-3.312992	4.950287	-1.405632
C	-1.249261	2.257922	-0.274772	-1.451618	2.714486	-0.391573	-1.403497	3.017147	-0.688743
O	-0.164587	2.600849	0.143352	-0.485034	3.440714	-0.428735	-0.454378	3.759199	-0.798985
H	-1.165264	0.315945	-2.274397	0.331644	1.132829	-1.429171	0.233827	1.370445	-1.783198
H	-1.528062	-1.063470	-1.260383	-1.127218	0.666811	-2.304820	-1.293300	0.676424	-2.332718
H	0.940580	0.720000	-1.017703	-1.155632	-1.465662	-0.847073	-0.869054	-1.144356	-0.470471
H	0.382567	-0.286944	1.153236	0.496589	-2.648713	-2.134937	0.476299	-2.509862	-1.869905
H	2.478286	-1.525965	1.543736	1.963643	-1.572094	-3.783581	1.554440	-1.736413	-3.946066
H	2.802643	-0.135881	0.496942	2.351519	-0.928686	-2.179466	2.243608	-0.848057	-2.577546
H	2.698723	-1.764057	-0.201474	1.398656	0.040237	-3.318919	1.060285	-0.063707	-3.639508

H	-2.065185	-3.908039	0.549791	-3.245096	-1.464757	-4.334634	-3.671364	-3.415542	-3.565587
H	-0.484274	-4.552226	1.005067	-2.071719	-2.044236	-5.517684	-3.689521	-1.641956	-3.473187
H	-1.692580	-4.149229	2.265653	-3.202912	-3.195657	-4.742663	-2.723568	-2.431325	-4.724806
H	2.333245	-0.975852	-5.025447	1.743501	-0.887306	2.354806	2.694505	-1.563292	2.340131
H	2.888375	-1.986958	-3.666392	1.518172	-2.631278	2.645512	3.400503	-1.060393	0.781227
H	1.275836	-2.238204	-4.330707	2.599458	-2.051020	1.345981	2.561513	0.126904	1.776360
H	-1.725700	0.436605	0.733223	-0.945962	0.986661	0.731516	-0.770360	1.427778	0.577924
H	-3.897897	1.415085	1.390106	-4.397050	-0.155983	1.105416	-2.788757	1.704626	1.960003
H	-5.259119	1.250087	0.287105	-2.771280	-0.804334	1.281630	-4.296043	0.937377	1.478481
H	-3.555272	-1.035577	1.472611	-3.667791	1.968532	2.347803	-1.614780	-0.501492	2.020526
H	-5.359338	-2.456842	1.040662	-2.517289	1.479620	4.305819	-2.859038	-2.409913	2.482777
H	-6.775640	-0.080625	-0.377953	-0.736297	-0.292570	4.186875	-5.307092	-1.985920	3.019202
H	-6.881494	-1.776536	-0.863571	-2.231020	-1.026873	4.735860	-5.420398	-0.845069	1.670541
H	-7.577149	-1.267050	0.663834	-1.706347	-1.252007	3.061640	-5.127149	-2.563307	1.372850
H	-4.049126	-0.629316	-1.384155	-4.109030	-0.494969	-1.095353	-3.205957	-0.786350	-0.346691
H	-4.305971	2.869081	-1.573488	-4.770427	2.099448	-0.470166	-4.703281	2.303706	-0.712079

Table S15. DFT Geometry Optimized Coordinates for truncated punaglandin 8 (**5a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 14			**Conformer 2**			**Conformer 7**			**Conformer 9**		
Gibbs free energy (hartrees)	-1344.105791			-1344.105454			-1344.105359			-1344.105344		
ΔG (kJ/mol)				0.885			1.134			1.174		
Population Proportion	18.18%			12.73%			11.51%			11.33%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.473874	4.847958	-1.663231	0.107491	5.835641	-1.443642	0.649640	5.748375	-1.218757	0.790724	5.729158	-1.005446
C	1.210580	6.144025	-1.862902	1.334424	5.132730	-1.956501	-0.195865	5.765820	-2.460578	0.349373	5.605905	-2.437369
C	0.963998	7.084167	-2.779646	1.476804	4.505913	-3.128307	0.005974	5.073854	-3.586555	0.858887	4.803426	-3.376811
C	-0.104535	7.098565	-3.834735	0.464432	4.336400	-4.224557	1.106120	4.100702	-3.896127	1.985524	3.819711	-3.248991
C	-0.063661	4.651413	-0.221141	-0.373544	5.299372	-0.067614	-0.043876	5.217233	0.068653	-0.295106	5.394314	0.040962
O	1.075995	4.656041	0.616927	0.713631	5.480622	0.819090	0.963426	5.301814	1.060201	0.332020	5.664123	1.299108
C	-0.939962	3.347790	-0.149728	-0.908773	3.827348	-0.192476	-0.648618	3.784104	-0.152619	-0.846357	3.933673	-0.087792
C	-0.695729	2.426888	1.073689	-0.463951	2.836925	0.914133	-0.379448	2.750670	0.971094	-0.383872	2.954438	1.001284
C	-1.116053	1.012801	0.803985	-0.529923	1.412124	0.450831	-0.478964	1.340357	0.470761	-0.684992	1.520808	0.667091
C	-0.336123	-0.067331	0.887317	0.486424	0.547140	0.424720	0.475138	0.410233	0.551770	0.208087	0.536636	0.539278
C	1.111712	-0.149885	1.269425	1.909123	0.760854	0.848320	1.844119	0.523137	1.153682	1.696338	0.596627	0.710804

O	-1.519885	2.865617	2.219182	-1.381124	2.912317	2.070692	-1.406826	2.862070	2.028236	-1.110454	3.344429	2.220788
C	-0.999449	3.634305	3.183763	-1.066497	3.644685	3.145960	-1.164448	3.553707	3.148352	-0.592444	2.948853	3.411558
C	-1.954566	3.798437	4.331191	-2.040366	3.422760	4.267577	-2.262950	3.371086	4.156261	-1.520952	3.298310	4.543445
O	0.108950	4.135286	3.132720	-0.108924	4.394447	3.203111	-0.175300	4.241357	3.324326	0.469973	2.387546	3.521301
C	-2.387944	3.857271	-0.156102	-2.436901	3.973476	-0.198781	-2.156997	4.025232	-0.307834	-2.372388	4.085663	-0.185339
O	-3.386486	3.205825	-0.356730	-3.245458	3.131691	-0.513989	-2.979106	3.246165	-0.730797	-3.194991	3.203815	-0.266602
C	-2.314154	5.310263	0.132332	-2.722560	5.356242	0.257084	-2.403326	5.408099	0.171377	-2.648104	5.544926	-0.203025
Cl	-3.755388	6.249752	0.377989	-4.351800	5.889520	0.540928	-4.017739	6.031009	0.324090	-4.270717	6.145315	-0.347056
C	-1.053397	5.751249	0.129030	-1.604862	6.079846	0.361292	-1.260385	6.057352	0.409235	-1.529028	6.263768	-0.100570
H	-0.778707	2.732018	-1.036502	-0.590468	3.390130	-1.140173	-0.270435	3.346455	-1.077191	-0.523498	3.518798	-1.047490
H	-0.353768	4.742576	-2.366450	0.331617	6.899499	-1.301928	1.547783	5.141259	-1.347100	1.649411	5.090441	-0.788782
H	1.158519	4.009123	-1.840259	-0.718985	5.775125	-2.153392	0.985993	6.764879	-0.986168	1.105411	6.759526	-0.803025
H	2.037249	6.305206	-1.177039	2.187110	5.158321	-1.284832	-1.052361	6.435304	-2.435544	-0.466732	6.262187	-2.731903
H	1.616656	7.955366	-2.781121	2.449533	4.063327	-3.335463	-0.704513	5.230071	-4.396040	0.418287	4.864775	-4.370064
H	-0.727130	7.994656	-3.738047	0.820574	4.801840	-5.150355	0.689357	3.123187	-4.162076	1.651444	2.815998	-3.533113
H	0.343307	7.139598	-4.833958	0.316480	3.274585	-4.449519	1.680683	4.438590	-4.765612	2.799356	4.080501	-3.934512
H	-0.760061	6.227828	-3.797006	-0.507969	4.768373	-3.985399	1.801946	3.957810	-3.068811	2.399349	3.765529	-2.241631
H	0.799636	4.557283	1.548135	0.465290	5.173823	1.712091	0.603411	5.008584	1.919080	-0.306312	5.477214	1.998669
H	0.348925	2.492256	1.365960	0.531357	3.107209	1.256773	0.588761	2.954356	1.420543	0.675333	3.110523	1.192391
H	-2.153374	0.896612	0.504428	-1.506785	1.094409	0.098741	-1.423041	1.092038	-0.004827	-1.735442	1.308281	0.498643
H	-0.797791	-1.021862	0.643293	0.269798	-0.448165	0.042257	0.244590	-0.563386	0.124271	-0.181284	-0.444463	0.273849
H	1.543973	0.809616	1.554324	2.093504	1.745595	1.278369	2.037442	1.489041	1.620936	2.054846	1.572741	1.035257
H	1.240881	-0.843289	2.106871	2.199097	0.007019	1.587487	1.987538	-0.255127	1.910341	2.019119	-0.145649	1.448232
H	1.701106	-0.553397	0.439087	2.582861	0.633415	-0.005796	2.610520	0.357188	0.388983	2.199046	0.341124	-0.228426
H	-1.536019	4.486076	5.062228	-1.812261	4.095556	5.090864	-2.092056	4.024329	5.008675	-2.383241	2.626786	4.515546
H	-2.911907	4.173692	3.964916	-3.059002	3.590354	3.913348	-3.228747	3.590939	3.698148	-1.001566	3.178381	5.491883
H	-2.136953	2.826244	4.794442	-1.974866	2.385798	4.604689	-2.283012	2.329303	4.484558	-1.893714	4.318050	4.439500
H	-0.733792	6.771390	0.294699	-1.539622	7.119222	0.657219	-1.164885	7.080565	0.750301	-1.462487	7.344266	-0.086340

	Conformer 6			**Conformer 5**			**Conformer 19**			**Conformer 10**		
Gibbs free energy (hartrees)	-1344.105202			-1344.105016			-1344.104869			-1344.104725		
ΔG (kJ/mol)	1.546			2.035			2.421			2.799		
Population Proportion	9.74%			8.0%			6.85%			5.88%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.080379	5.569091	-1.543494	0.306487	5.813917	-1.357537	-0.113766	5.501535	-1.764417	0.041612	5.688490	-1.456901
C	1.312401	4.785143	-1.909369	1.596164	5.042904	-1.439493	0.902506	4.624088	-2.445108	1.463997	5.201645	-1.377745
C	2.580865	5.210608	-1.856275	2.036332	4.308347	-2.465602	2.172281	4.928678	-2.724556	2.530231	5.904432	-0.979756
C	3.092534	6.566149	-1.464143	1.369101	4.057843	-3.787273	2.911933	6.194664	-2.404652	2.580501	7.334789	-0.527417
C	-0.531536	5.096054	-0.189980	-0.560785	5.426843	-0.140243	-0.451014	5.070092	-0.308946	-0.833664	5.209204	-0.257689

O	0.463329	5.137156	0.826797	0.220357	5.747394	1.013644	0.769986	5.104349	0.401135	-0.259686	5.656610	0.964984
C	-1.252837	3.704636	-0.322049	-1.047863	3.936430	-0.186832	-1.214876	3.694223	-0.279409	-1.129097	3.670375	-0.323114
C	-0.799418	2.649897	0.705061	-0.446651	3.011452	0.884117	-0.747339	2.674412	0.791462	-0.827010	2.822738	0.930004
C	-1.300765	1.268268	0.393452	-0.737632	1.558409	0.637498	-1.080432	1.263832	0.406542	-1.590771	3.193161	2.170646
C	-0.546606	0.180566	0.214916	0.167153	0.593456	0.455905	-0.207904	0.267327	0.241159	-2.421930	2.391056	2.842351
C	0.946650	0.056795	0.287255	1.662617	0.698326	0.470991	1.283127	0.291906	0.400642	-2.793037	0.967522	2.549947
O	-1.337815	3.079064	1.996529	-1.054006	3.433978	2.157423	-1.457189	2.905504	2.066392	0.609994	2.968317	1.177884
C	-0.573440	2.886248	3.092039	-0.406082	3.095991	3.302769	-0.887614	3.613772	3.049361	1.299532	1.866507	1.561792
C	-1.246065	3.444714	4.318012	-1.221987	3.470917	4.510521	-1.700387	3.555197	4.311055	2.739088	2.205625	1.839858
O	0.509876	2.349994	3.073503	0.676724	2.564701	3.321393	0.158528	4.224886	2.931248	0.803559	0.770738	1.669803
C	-2.748473	4.029445	-0.189623	-2.582658	4.014479	-0.143470	-2.685677	4.074347	-0.056004	-2.623722	3.568711	-0.654426
O	-3.676158	3.274764	-0.371598	-3.364107	3.092224	-0.163030	-3.649009	3.357838	-0.199519	-3.234005	2.554751	-0.902239
C	-2.838959	5.459794	0.187688	-2.931878	5.456381	-0.113104	-2.686688	5.495750	0.365547	-3.162343	4.948013	-0.607656
Cl	-4.372130	6.208630	0.508157	-4.589426	5.973459	-0.084746	-4.151891	6.281326	0.870911	-4.848858	5.266014	-0.867370
C	-1.637938	6.038647	0.221060	-1.845946	6.230762	-0.122512	-1.471435	6.040091	0.261309	-2.203525	5.841565	-0.356365
H	-1.095930	3.270104	-1.312090	-0.782810	3.499357	-1.153582	-1.134698	3.186058	-1.240902	-0.581433	3.210305	-1.149605
H	0.304547	6.633984	-1.457266	0.527726	6.883179	-1.256013	0.229109	6.537208	-1.723263	0.002534	6.779462	-1.472845
H	-0.680372	5.460793	-2.322479	-0.293005	5.695301	-2.261831	-1.044733	5.496552	-2.341133	-0.419425	5.335388	-2.384887
H	1.142319	3.760519	-2.231701	2.228680	5.118172	-0.559728	0.545986	3.643433	-2.752559	1.626569	4.167325	-1.669966
H	3.350708	4.500361	-2.151229	3.007887	3.831625	-2.349033	2.759771	4.174477	-3.245208	3.491032	5.393153	-0.989740
H	3.813182	6.478956	-0.644331	1.997295	4.422497	-4.607544	3.781909	5.975813	-1.775635	3.011336	7.400438	0.477373
H	3.630376	7.023406	-2.301683	1.236993	2.983220	-3.953235	3.298436	6.659862	-3.318198	3.233212	7.921239	-1.183392
H	2.305786	7.252039	-1.149975	0.392502	4.535040	-3.876121	2.299048	6.927543	-1.879809	1.600770	7.811483	-0.502066
H	1.307068	4.895698	0.417578	-0.299080	5.525718	1.796313	0.611234	4.874987	1.336716	0.615529	5.249988	1.034486
H	0.283356	2.672020	0.780837	0.621107	3.202283	0.954639	0.316441	2.807372	0.969720	-1.008195	1.784138	0.664609
H	-2.378618	1.182644	0.300549	-1.792406	1.310850	0.585790	-2.137460	1.076936	0.242173	-1.435310	4.207532	2.518709
H	-1.070481	-0.744988	-0.016575	-0.217938	-0.407408	0.269687	-0.618355	-0.695748	-0.055240	-2.907274	2.817231	3.718449
H	1.357032	-0.208283	-0.693464	2.023234	1.695116	0.721545	1.670688	1.253034	0.739233	-2.191392	0.517252	1.761215
H	1.437425	0.966554	0.630860	2.080460	-0.007003	1.196853	1.598201	-0.474049	1.116774	-2.681034	0.358939	3.452872
H	1.222625	-0.754419	0.968783	2.073897	0.420410	-0.505591	1.770231	0.047358	-0.549399	-3.846667	0.900549	2.257240
H	-2.289174	3.128538	4.360474	-2.098467	2.820243	4.566354	-1.270335	4.219770	5.056642	2.797164	2.789493	2.762234
H	-0.713821	3.118591	5.209116	-0.620995	3.348985	5.409078	-2.733264	3.838603	4.101754	3.314019	1.289398	1.956230
H	-1.231776	4.536473	4.265765	-1.579683	4.498575	4.430419	-1.709638	2.529941	4.688161	3.151865	2.815541	1.035310
H	-1.429095	7.070243	0.472799	-1.830608	7.313061	-0.106139	-1.206459	7.064044	0.492435	-2.335270	6.911443	-0.259864

	Conformer 25	**Conformer 26**	**Conformer 13**	**Conformer 4**
Gibbs free energy (hartrees)	-1344.104292	-1344.104209	-1344.104112	-1344.10349
ΔG (kJ/mol)	3.936	4.154	4.408	6.041
Population Proportion	3.72%	3.4%	3.07%	1.59%

Element	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
C	0.281844	6.289617	-0.212982	0.057154	5.444430	-1.764033	0.930863	5.136527	-1.401352	0.165045	5.711312	-1.217500
C	0.442614	6.270824	-1.707997	1.197839	4.487379	-1.996300	0.109799	5.092304	-2.659751	1.575088	5.253572	-0.954369
C	1.497711	5.839263	-2.406041	2.503259	4.748193	-1.887249	-0.246391	6.125457	-3.428991	2.559081	5.969985	-0.398720
C	2.781621	5.258738	-1.888143	3.156698	6.037047	-1.483044	0.056802	7.581044	-3.226128	2.509546	7.389013	0.087608
C	-0.879683	5.419653	0.351005	-0.683698	5.232593	-0.425019	0.187128	4.803335	-0.074409	-0.849578	5.208593	-0.144722
O	-0.963180	5.640453	1.760266	0.266184	5.529547	0.599810	1.207975	4.838247	0.905853	-0.452961	5.664635	1.143819
C	-0.750260	3.916108	-0.066386	-1.335509	3.811018	-0.293710	-0.603126	3.448215	-0.166991	-1.100465	3.664590	-0.249892
C	-0.628229	2.867752	1.056660	-0.668506	2.869475	0.721816	-0.482062	2.507500	1.060288	-0.959696	2.822795	1.040348
C	-1.829274	2.719522	1.947988	-1.139116	1.447528	0.603342	-0.786401	1.082882	0.703322	-1.882842	3.188891	2.166434
C	-2.519369	1.591978	2.142069	-0.378768	0.386809	0.321815	0.013868	0.034591	0.909998	-2.837612	2.404809	2.674994
C	-2.280142	0.233453	1.553694	1.099477	0.334591	0.076926	1.373201	0.004368	1.542642	-3.226228	1.012287	2.275739
O	0.531763	3.291456	1.855226	-1.021337	3.402473	2.047627	-1.478211	2.874068	2.088550	0.411415	2.961996	1.537236
C	1.352108	2.326572	2.345812	-0.232536	3.045554	3.094008	-1.132073	3.629296	3.138400	1.318374	2.028001	1.158855
C	2.441637	2.927582	3.191246	-0.798987	3.556600	4.391421	-2.244177	3.715411	4.144127	2.648943	2.277835	1.814582
O	1.202238	1.150814	2.120849	0.780424	2.401611	2.973223	-0.050400	4.174963	3.258020	1.068448	1.125216	0.395610
C	-1.981724	3.630489	-0.933525	-2.824690	4.074905	-0.016160	-2.064977	3.874216	-0.367090	-2.531276	3.532811	-0.784955
O	-2.230860	2.597034	-1.509003	-3.690607	3.253899	0.177307	-2.981007	3.178406	-0.739397	-3.079053	2.507468	-1.118007
C	-2.794616	4.871026	-0.932648	-3.008915	5.545886	-0.074033	-2.125477	5.311333	-0.004152	-3.102890	4.899563	-0.806506
Cl	-4.303286	4.958554	-1.786449	-4.577117	6.258590	0.146144	-3.643445	6.152072	0.082679	-4.745048	5.181886	-1.292331
C	-2.215559	5.839799	-0.221314	-1.860092	6.182101	-0.308019	-0.906276	5.820756	0.190194	-2.207511	5.811938	-0.423848
H	0.123407	3.791395	-0.711519	-1.295817	3.303007	-1.261580	-0.280065	2.864522	-1.029745	-0.435910	3.211144	-0.989777
H	1.194233	5.960540	0.290234	0.401989	6.480389	-1.781520	1.743809	4.404518	-1.466379	0.105687	6.801357	-1.236441
H	0.084733	7.313264	0.124742	-0.675893	5.337030	-2.570502	1.397975	6.112517	-1.259531	-0.162656	5.352497	-2.198196
H	-0.397697	6.670193	-2.271356	0.912175	3.482885	-2.300264	-0.204080	4.103482	-2.986068	1.805104	4.233474	-1.252090
H	1.438926	5.919404	-3.489818	3.191484	3.936083	-2.114627	-0.828162	5.900604	-4.320831	3.526214	5.482408	-0.291774
H	2.951765	4.264390	-2.314897	3.782013	5.882062	-0.597003	0.599192	7.983799	-4.088529	2.802858	7.439575	1.141553
H	3.631935	5.877102	-2.196273	3.822894	6.398521	-2.274214	-0.872193	8.156637	-3.148853	3.226693	8.007075	-0.463649
H	2.808320	5.168596	-0.801720	2.439988	6.824170	-1.249489	0.649333	7.777626	-2.332164	1.522091	7.840354	-0.006255
H	-0.186397	5.228675	2.163477	-0.171335	5.419861	1.453167	0.820266	4.684176	1.788468	0.420709	5.291114	1.325287
H	-0.374907	1.918046	0.593274	0.410729	2.948457	0.617976	0.507476	2.614794	1.496392	-1.092695	1.784637	0.745640
H	-2.144632	3.625773	2.451912	-2.206257	1.312079	0.743504	-1.749621	0.928858	0.226135	-1.743661	4.183968	2.571334
H	-3.377805	1.655804	2.808125	-0.885991	-0.573988	0.256856	-0.354844	-0.933375	0.576910	-3.428325	2.823791	3.487458
H	-1.328588	0.152062	1.029653	1.590823	1.300436	0.188059	1.701448	0.973365	1.919362	-2.591976	0.587298	1.498005
H	-2.298756	-0.524074	2.343459	1.570542	-0.368911	0.771399	1.383530	-0.705147	2.376455	-3.194925	0.348494	3.146008
H	-3.082076	-0.025588	0.853544	1.304958	-0.039607	-0.931938	2.119524	-0.350872	0.823965	-4.258949	0.997846	1.911030
H	2.001934	3.368305	4.089353	-0.077788	3.400553	5.190764	-1.963559	4.395117	4.945200	3.358331	1.513265	1.505850
H	3.151432	2.153564	3.474541	-1.052133	4.614967	4.311410	-3.157509	4.062191	3.657338	3.019274	3.265593	1.532378
H	2.949675	3.724724	2.646079	-1.719909	3.013741	4.619045	-2.444141	2.721545	4.550718	2.534043	2.265902	2.900360
H	-2.610272	6.834523	-0.058398	-1.726904	7.253190	-0.390762	-0.675084	6.846683	0.447172	-2.374297	6.878068	-0.341670
	Conformer 8			**Conformer 15**			**Conformer 11**			**Conformer 17**		

Gibbs free energy (hartrees)	-1344.102932			-1344.102778			-1344.102721			-1344.102515		
ΔG (kJ/mol)	7.506			7.911			8.06			8.601		
Population Proportion	0.88%			0.75%			0.7%			0.57%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-0.003410	6.219143	-0.707349	-0.444356	4.183185	-2.061340	-0.595188	4.696402	-2.199359	0.732568	5.674088	-0.740056
C	1.428786	6.028180	-0.289442	0.324604	5.174491	-2.895534	0.423524	3.673112	-2.623957	0.480378	5.583900	-2.220261
C	2.418117	5.479934	-1.002283	1.640387	5.167777	-3.140910	1.637395	3.913623	-3.133245	1.077427	4.773540	-3.099714
C	2.360786	4.907415	-2.388588	2.663529	4.168580	-2.684841	2.274707	5.240257	-3.427938	2.143318	3.748084	-2.844310
C	-1.015132	5.405836	0.153692	-0.797729	4.730126	-0.656045	-0.665848	4.867496	-0.651666	-0.488312	5.342545	0.153643
O	-0.898358	5.775656	1.528017	0.385455	5.151690	0.032042	0.615296	5.211336	-0.138143	-0.167479	5.631863	1.517212
C	-0.911405	3.870377	-0.129342	-1.546398	3.688969	0.231120	-1.343949	3.634711	0.056106	-1.040266	3.894401	-0.064460
C	-0.786825	2.924499	1.089165	-0.663698	2.933879	1.244231	-0.529444	3.089209	1.257673	-0.539621	2.798295	0.887892
C	-1.942191	2.935317	2.047398	0.362380	2.046182	0.598857	0.705500	2.343832	0.834453	-0.811952	1.409238	0.380446
C	-2.730649	1.893106	2.324961	1.675282	2.037204	0.838942	1.945720	2.528670	1.294147	0.098116	0.448309	0.202647
C	-2.674308	0.497154	1.780246	2.457280	2.925662	1.758628	2.426057	3.532486	2.298713	1.575698	0.494611	0.458737
O	0.410223	3.310728	1.846398	-1.554121	2.043218	1.989827	-1.361822	2.108919	1.950841	-1.225922	2.931185	2.177864
C	1.581406	2.691863	1.539915	-1.689785	2.235309	3.318515	-1.877193	2.440972	3.155317	-0.499534	3.239115	3.267115
C	2.689519	3.165369	2.438742	-2.711107	1.287729	3.887709	-2.725541	1.321729	3.694621	-1.360316	3.286391	4.498594
O	1.686551	1.872527	0.659873	-1.079491	3.065014	3.952580	-1.682046	3.500221	3.704969	0.691172	3.474829	3.243476
C	-2.186009	3.524416	-0.907947	-2.721170	4.472877	0.848064	-2.723814	4.161513	0.483269	-2.562818	4.056064	-0.139946
O	-2.440001	2.463490	-1.429335	-3.480031	4.116115	1.718490	-3.662692	3.509307	0.877631	-3.402192	3.186815	-0.134355
C	-3.037176	4.737407	-0.884143	-2.776227	5.769107	0.128085	-2.700999	5.629950	0.282533	-2.810060	5.515916	-0.273695
Cl	-4.620515	4.741476	-1.596312	-4.046899	6.912517	0.442145	-4.042316	6.624179	0.755327	-4.409770	6.130994	-0.547943
C	-2.423633	5.754932	-0.277278	-1.751028	5.914489	-0.709431	-1.576778	6.024197	-0.315100	-1.688234	6.222606	-0.141684
H	-0.056244	3.657168	-0.774790	-2.013650	2.944234	-0.424218	-1.512229	2.805650	-0.635969	-0.742320	3.586612	-1.074125
H	-0.271301	7.275429	-0.590797	-1.377792	3.917800	-2.568656	-0.369367	5.674200	-2.629015	1.554502	5.020343	-0.435761
H	-0.153089	5.964530	-1.758515	0.123153	3.261972	-1.921865	-1.587492	4.406517	-2.558630	1.032070	6.695398	-0.478232
H	1.673431	6.403248	0.701204	-0.258948	5.983225	-3.328877	0.134761	2.634012	-2.487583	-0.268133	6.273200	-2.605334
H	3.400071	5.441277	-0.534542	2.030914	5.971480	-3.762046	2.247076	3.047924	-3.384639	0.769781	4.861603	-4.139897
H	1.373428	4.979577	-2.846029	3.138733	3.691825	-3.549101	3.229865	5.329167	-2.899612	1.812366	2.760165	-3.182267
H	3.075090	5.418460	-3.043032	3.463749	4.669122	-2.129414	2.503020	5.323392	-4.496122	3.046082	3.985055	-3.417967
H	2.651503	3.851289	-2.376688	2.249098	3.387552	-2.047505	1.653994	6.090014	-3.143854	2.424097	3.668615	-1.793651
H	-0.136304	5.309987	1.898150	0.937693	5.619654	-0.610334	1.255570	4.586667	-0.507899	0.578047	5.084789	1.803420
H	-0.611219	1.927245	0.694109	-0.217603	3.631129	1.945143	-0.308213	3.894623	1.951119	0.523826	2.938953	1.067536
H	-2.136771	3.885750	2.530684	-0.045317	1.318589	-0.099327	0.531151	1.553775	0.108389	-1.851219	1.205685	0.146825
H	-3.534360	2.068784	3.037372	2.267821	1.300675	0.299530	2.718431	1.875093	0.894302	-0.266134	-0.502741	-0.180932
H	-1.829462	0.320145	1.114840	1.829946	3.590170	2.351475	1.626769	4.144610	2.715155	1.910418	1.424000	0.920094
H	-2.621538	-0.224864	2.601631	3.061712	2.321129	2.442879	2.933387	3.022242	3.124156	1.868417	-0.332189	1.114046

H	-3.591540	0.270857	1.226019	3.157601	3.542901	1.185542	3.166074	4.200930	1.845620	2.130153	0.360142	-0.476351
H	2.403570	3.036773	3.484235	-2.657201	1.295450	4.974448	-2.183437	0.376075	3.647550	-0.731081	3.298316	5.386032
H	3.596657	2.604600	2.224990	-3.703360	1.618244	3.570141	-3.016858	1.541337	4.719521	-1.958356	4.201396	4.469955
H	2.866910	4.229894	2.271547	-2.556827	0.278294	3.504661	-3.618023	1.225261	3.071669	-2.046539	2.439681	4.524021
H	-2.829041	6.746271	-0.121528	-1.552636	6.782783	-1.323474	-1.309430	7.038174	-0.581711	-1.604102	7.300952	-0.181417

	Conformer 16			**Conformer 1**			**Conformer 12**		
Gibbs free energy (hartrees)	-1344.102365			-1344.102059			-1344.101822		
ΔG (kJ/mol)	8.995			9.798			10.421		
Population Proportion	0.48%			0.35%			0.27%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	0.237346	6.263069	0.039354	0.302788	5.817207	-1.135869	-0.128924	5.366818	-1.937971
C	0.587639	6.259553	-1.423039	1.607994	5.069078	-1.105553	1.105854	4.578326	-2.278275
C	1.719232	5.824572	-1.986210	2.110753	4.270725	-2.052767	1.202186	3.544190	-3.119926
C	2.922875	5.226982	-1.317034	1.511923	3.910258	-3.381112	0.116229	2.897996	-3.929805
C	-0.988372	5.389558	0.439509	-0.683221	5.397851	-0.015552	-0.527163	5.303458	-0.434905
O	-1.245454	5.585167	1.831792	-0.144137	5.703639	1.272329	0.508030	5.839775	0.388145
C	-0.818116	3.893663	0.011248	-1.185656	3.919569	-0.168793	-1.026662	3.873511	-0.014469
C	-0.856337	2.822757	1.124760	-0.576727	2.866562	0.772096	-0.344855	3.312475	1.258775
C	-2.159689	2.678916	1.855218	-0.844057	1.453804	0.331996	1.112033	2.997129	1.051366
C	-2.922036	1.581923	1.871873	0.079635	0.509071	0.137545	2.121606	3.346851	1.855792
C	-2.689378	0.262138	1.198992	1.567680	0.600637	0.304841	2.066562	4.146204	3.123103
O	0.166744	3.174124	2.119872	-1.164642	3.028662	2.106895	-0.993512	2.042668	1.569295
C	1.406555	2.638596	1.972541	-0.356538	3.360672	3.130437	-1.721877	1.953438	2.705390
C	2.318875	3.084392	3.081838	-1.117814	3.426350	4.424766	-2.350166	0.591872	2.824004
O	1.711049	1.912114	1.057596	0.826942	3.600809	3.007689	-1.849261	2.856148	3.499340
C	-1.927302	3.638426	-1.014012	-2.718092	4.009394	-0.117469	-2.542420	4.043282	0.181947
O	-2.104120	2.621070	-1.642781	-3.508378	3.095269	-0.097175	-3.360747	3.167254	0.339024
C	-2.729805	4.883698	-1.085794	-3.049497	5.455574	-0.144508	-2.820745	5.498199	0.115036
Cl	-4.118350	5.000709	-2.120666	-4.698117	5.995042	-0.217723	-4.417676	6.121241	0.386823
C	-2.240677	5.831941	-0.285055	-1.956469	6.215914	-0.098878	-1.728339	6.192173	-0.201321
H	0.130466	3.765354	-0.516627	-0.947896	3.586920	-1.184751	-0.871719	3.147505	-0.816476
H	1.079074	5.928671	0.650841	0.498120	6.886399	-0.993186	0.046287	6.423920	-2.168958
H	-0.000452	7.283245	0.360986	-0.197129	5.707799	-2.100733	-0.983704	5.045683	-2.536406
H	-0.171276	6.672052	-2.083992	2.212974	5.225037	-0.214886	2.021814	4.915256	-1.798325

H	1.798529	5.915448	-3.067835	3.083735	3.824762	-1.855977	2.190423	3.108414	-3.253904
H	3.127466	4.228197	-1.717526	2.185486	4.201716	-4.194327	0.352933	2.953156	-4.997996
H	3.813021	5.831547	-1.522798	1.381628	2.825608	-3.460948	0.038648	1.833133	-3.684932
H	2.818514	5.139916	-0.235125	0.544437	4.379970	-3.561549	-0.864383	3.350468	-3.778887
H	-0.532012	5.156547	2.324035	0.594173	5.115304	1.482357	1.269368	5.245269	0.354360
H	-0.554831	1.882491	0.670871	0.492220	3.042336	0.857994	-0.502795	3.985347	2.096584
H	-2.491880	3.559732	2.391790	-1.889265	1.215689	0.169321	1.328610	2.397405	0.171600
H	-3.847714	1.642725	2.440961	-0.281297	-0.465292	-0.186103	3.116089	3.013629	1.566327
H	-3.477068	0.069990	0.462528	1.904569	1.558618	0.701153	1.053270	4.404820	3.428999
H	-1.729755	0.194733	0.686690	1.917170	-0.186824	0.980598	2.535170	3.582906	3.936514
H	-2.744876	-0.549001	1.932294	2.070902	0.432653	-0.653417	2.640941	5.072662	3.016898
H	3.260965	2.544435	3.018146	-0.420636	3.478043	5.258299	-1.605229	-0.187738	2.658169
H	2.506229	4.157091	2.988416	-1.739926	4.325479	4.419076	-2.804345	0.480291	3.806224
H	1.847778	2.913743	4.051026	-1.777958	2.564792	4.528027	-3.116356	0.490149	2.051591
H	-2.647874	6.825687	-0.149424	-1.929929	7.297852	-0.093300	-1.658927	7.265614	-0.318961

Table S16. DFT Geometry Optimized Coordinates for truncated carijenone (**6a**) conformers calculated at the B3LYP/6-311G(d,p) level of theory.

	Conformer 4			**Conformer 17**			**Conformer 26**			**Conformer 15**		
Gibbs free energy (hartrees)	-1572.031782			-1572.031495			-1572.031411			-1572.031321		
ΔG (kJ/mol)				0.754			0.974			1.21		
Population Proportion	19.91%			14.69%			13.44%			12.22%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-2.831411	-2.017785	1.659262	-2.408603	-1.972138	1.402410	-2.179379	-3.073219	1.302055	-2.141506	-3.083822	1.386705
C	-1.405172	-2.340659	1.308243	-2.410013	-2.556682	2.788792	-1.757335	-1.733865	1.844008	-1.663246	-1.742910	1.875353
C	-0.531965	-3.034769	2.043435	-1.493035	-3.368147	3.323675	-1.614993	-1.385727	3.125882	-1.469776	-1.362193	3.141179
C	-0.744970	-3.678556	3.383330	-0.242161	-3.903586	2.689496	-1.842165	-2.225928	4.349322	-1.682088	-2.159141	4.395846
C	-3.851693	-2.444569	0.590676	-3.612116	-2.389702	0.541897	-3.450957	-3.009853	0.440994	-3.434482	-3.005504	0.559231
C	-3.901336	-3.954692	0.223570	-3.732062	-3.902921	0.212256	-3.852105	-4.344026	-0.246090	-3.894921	-4.345606	-0.078227
C	-3.599055	-4.006964	-1.284905	-3.515646	-3.992114	-1.304097	-3.669165	-4.080825	-1.748277	-3.752041	-4.130843	-1.590378
O	-2.191055	-4.267668	-1.473047	-2.104702	-4.192722	-1.552035	-2.323965	-4.404900	-2.163100	-2.424568	-4.546483	-1.986445
C	-1.825226	-5.406575	-2.119726	-1.719680	-5.306582	-2.231453	-2.068419	-5.703327	-2.472566	-2.306185	-5.546926	-2.900683
C	-0.327919	-5.524359	-2.173381	-0.221742	-5.372851	-2.332293	-0.641672	-5.880425	-2.909833	-0.859628	-5.880002	-3.134895
O	-2.613375	-6.192852	-2.585813	-2.494947	-6.112697	-2.684866	-2.901967	-6.572306	-2.392852	-3.249242	-6.073109	-3.439220
C	-3.930006	-2.574932	-1.736922	-3.930896	-2.588581	-1.768803	-3.836847	-2.559160	-1.827035	-3.873704	-2.604836	-1.707862

C	-3.224563	-2.087638	-2.998238	-3.358219	-2.117143	-3.100511	-3.203575	-1.860543	-3.025609	-3.254166	-1.966200	-2.946353
C	-3.638517	-2.852447	-4.246825	-3.824249	-2.951682	-4.284502	-3.767445	-2.320687	-4.360872	-3.918104	-2.404025	-4.243252
O	-3.613785	-0.699582	-3.186440	-3.840438	-0.759760	-3.299805	-3.507204	-0.444440	-2.885416	-3.451755	-0.530830	-2.821444
C	-2.686547	0.266310	-2.996337	-2.945962	0.254532	-3.299536	-2.503681	0.410324	-2.583996	-2.383588	0.254098	-2.553786
C	-3.306168	1.629492	-3.152756	-3.649838	1.578038	-3.439553	-3.036614	1.807439	-2.407151	-2.812277	1.688136	-2.389424
O	-1.525928	0.054270	-2.734970	-1.751027	0.107644	-3.197553	-1.344843	0.087101	-2.470337	-1.248398	-0.149061	-2.459165
O	-3.551183	-1.746953	-0.631499	-3.476781	-1.715704	-0.727468	-3.228643	-2.065350	-0.627691	-3.213230	-2.099585	-0.541973
H	-5.015865	-2.509463	-1.892532	-5.028271	-2.561157	-1.825972	-4.913011	-2.335656	-1.819795	-4.941285	-2.344907	-1.673907
C	-5.326679	-4.412034	0.552603	-5.147782	-4.306591	0.639634	-5.314590	-4.585275	0.148211	-5.348750	-4.536277	0.369962
O	-5.768965	-5.528611	0.426026	-5.650251	-5.397843	0.517919	-6.017292	-5.494569	-0.222753	-6.085006	-5.438284	0.049460
C	-6.053398	-3.209296	1.032582	-5.775760	-3.088137	1.211628	-5.689313	-3.475136	1.059870	-5.665171	-3.390116	1.258636
Cl	-7.727245	-3.295625	1.483346	-7.402411	-3.119158	1.814684	-7.278644	-3.386084	1.752701	-7.228064	-3.237900	1.998971
C	-5.270248	-2.127917	1.034662	-4.954911	-2.036051	1.155181	-4.688544	-2.605553	1.220971	-4.637215	-2.543506	1.361947
H	-3.188860	-4.566944	0.776091	-3.015191	-4.526180	0.747185	-3.262871	-5.201717	0.078954	-3.312715	-5.208652	0.246859
H	-3.127038	-2.467204	2.609396	-2.427618	-0.877190	1.462090	-1.387801	-3.470513	0.656232	-1.381731	-3.525135	0.731360
H	-2.940269	-0.932357	1.777493	-1.510680	-2.243972	0.845790	-2.341110	-3.801322	2.099886	-2.302383	-3.782490	2.210591
H	-1.068396	-1.940216	0.357079	-3.249776	-2.268332	3.417097	-1.540926	-0.987150	1.085232	-1.448919	-1.025693	1.088104
H	0.470928	-3.151472	1.636759	-1.652978	-3.682692	4.353184	-1.285616	-0.367941	3.326851	-1.104338	-0.349449	3.301150
H	-1.764528	-3.573835	3.756174	-0.118825	-3.594536	1.651099	-2.183153	-3.236517	4.121826	-2.055900	-3.166556	4.209490
H	-0.510378	-4.747486	3.336872	0.640830	-3.573116	3.247591	-0.920551	-2.304893	4.936533	-0.745592	-2.245429	4.957926
H	-0.068547	-3.245660	4.128763	-0.235843	-4.998442	2.720608	-2.586148	-1.757864	5.003069	-2.393570	-1.651902	5.056553
H	-4.169731	-4.771549	-1.806940	-4.077426	-4.796643	-1.772759	-4.378703	-4.636788	-2.358137	-4.487284	-4.679404	-2.174396
H	-0.051802	-6.463009	-2.648279	0.066965	-6.250796	-2.905593	-0.464393	-6.923529	-3.161560	-0.326641	-4.992068	-3.481066
H	0.085317	-4.686813	-2.739920	0.158595	-4.469441	-2.813182	-0.436315	-5.246736	-3.774998	-0.397261	-6.197298	-2.197928
H	0.085792	-5.475286	-1.164520	0.212817	-5.421582	-1.331599	0.031769	-5.570952	-2.107730	-0.782786	-6.672737	-3.875470
H	-2.147777	-2.118863	-2.848115	-2.272738	-2.082762	-3.035813	-2.123636	-1.981050	-2.984096	-2.183721	-2.160766	-2.954842
H	-3.121838	-2.444521	-5.117033	-3.404107	-2.548094	-5.207195	-3.323992	-1.734708	-5.167530	-3.454120	-1.888970	-5.085893
H	-3.380549	-3.910001	-4.163640	-3.497561	-3.988733	-4.187440	-3.532248	-3.371823	-4.537593	-3.806609	-3.478791	-4.398436
H	-4.715362	-2.771058	-4.413319	-4.913908	-2.937552	-4.364999	-4.852073	-2.192639	-4.395893	-4.984077	-2.163730	-4.234908
H	-3.987968	1.810051	-2.317783	-4.228675	1.774113	-2.533505	-3.680616	2.078440	-3.245062	-3.449066	1.992725	-3.221334
H	-2.527380	2.389028	-3.156633	-2.917980	2.370040	-3.582784	-3.642172	1.847053	-1.498137	-3.398469	1.783954	-1.471981
H	-3.890402	1.679229	-4.072798	-4.347934	1.550299	-4.277636	-2.208983	2.508443	-2.323083	-1.935352	2.329070	-2.329152
H	-5.567017	-1.125028	1.313225	-5.188543	-1.029112	1.476167	-4.718192	-1.700097	1.811871	-4.624904	-1.620642	1.925983

	Conformer 7			**Conformer 49**			**Conformer 28**			**Conformer 33**		
Gibbs free energy (hartrees)	-1572.031254			-1572.031049			-1572.030836			-1572.029825		
ΔG (kJ/mol)	1.386			1.924			2.484			5.138		
Population Proportion	11.38%			9.16%			7.31%			2.51%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**

C	-2.783435	-2.081932	1.621300	-2.125045	-2.550710	1.224303	-2.479586	-2.007087	1.326698	-2.444708	-3.018257	1.634484
C	-1.370625	-2.412465	1.225946	-2.075578	-3.333643	2.509149	-2.487171	-2.632890	2.694916	-2.047276	-1.690582	2.223535
C	-0.485347	-3.131232	1.922268	-2.016532	-2.847713	3.752130	-1.552030	-3.426419	3.225210	-0.974827	-0.960336	1.906531
C	-0.668821	-3.799988	3.254171	-1.992956	-1.412156	4.189527	-0.269046	-3.895836	2.603088	0.081133	-1.263608	0.884063
C	-3.832633	-2.467623	0.565427	-3.396942	-2.782379	0.393725	-3.654971	-2.433856	0.432342	-3.644067	-2.949805	0.672669
C	-3.903789	-3.965504	0.155422	-3.613452	-4.208931	-0.184722	-3.721813	-3.938337	0.053143	-4.057067	-4.314755	0.052036
C	-3.608352	-3.975689	-1.356775	-3.485533	-4.037019	-1.706187	-3.464151	-3.971164	-1.461143	-3.779702	-4.158653	-1.451643
O	-2.206494	-4.198600	-1.614648	-2.112527	-4.203233	-2.123279	-2.051049	-4.093071	-1.735792	-2.433179	-4.576074	-1.766192
C	-1.770275	-5.484257	-1.595106	-1.684137	-5.473498	-2.347109	-1.527178	-5.347013	-1.737617	-2.234985	-5.899857	-2.002562
C	-0.299469	-5.557010	-1.894421	-0.249855	-5.485621	-2.795196	-0.059304	-5.315189	-2.058029	-0.794374	-6.177213	-2.328124
O	-2.495610	-6.419592	-1.358590	-2.390326	-6.439969	-2.193466	-2.183593	-6.332367	-1.504185	-3.121556	-6.716446	-1.944574
C	-3.945541	-2.534785	-1.765192	-3.864888	-2.564023	-1.894133	-3.913280	-2.570074	-1.892356	-3.862378	-2.638775	-1.634544
C	-3.259007	-2.006194	-3.020386	-3.345256	-1.881041	-3.154250	-3.322213	-2.032195	-3.190609	-3.132754	-2.054568	-2.838923
C	-3.643501	-2.766316	-4.280363	-3.861019	-2.509939	-4.439581	-3.668691	-2.875292	-4.408317	-3.659883	-2.566352	-4.170615
O	-3.698135	-0.629009	-3.182413	-3.828859	-0.509890	-3.103014	-3.900633	-0.711002	-3.382648	-3.358594	-0.617508	-2.793155
C	-2.798107	0.364043	-3.002371	-2.928493	0.493523	-2.997293	-3.083477	0.366163	-3.363361	-2.304061	0.201545	-2.586793
C	-3.464409	1.708510	-3.125962	-3.629545	1.820925	-2.881250	-3.881392	1.635640	-3.500191	-2.758410	1.632417	-2.474917
O	-1.625307	0.186626	-2.770953	-1.730617	0.335286	-2.994398	-1.882118	0.306722	-3.248486	-1.158082	-0.173821	-2.497216
O	-3.553014	-1.736056	-0.642826	-3.318595	-1.901328	-0.747256	-3.519783	-1.714462	-0.812196	-3.291907	-2.099124	-0.436608
H	-5.033369	-2.468230	-1.904871	-4.961521	-2.491767	-1.880985	-5.008470	-2.578685	-1.982109	-4.924614	-2.363657	-1.700326
C	-5.335208	-4.412173	0.475764	-5.025432	-4.619228	0.252420	-5.136637	-4.394523	0.428989	-5.546587	-4.480768	0.373242
O	-5.799421	-5.513835	0.305150	-5.595121	-5.644796	-0.033727	-5.608361	-5.491884	0.252640	-6.254503	-5.400703	0.040264
C	-6.036796	-3.218859	1.013557	-5.549258	-3.501943	1.077278	-5.810104	-3.215680	1.031696	-5.940917	-3.283196	1.156312
Cl	-7.705704	-3.298262	1.483610	-7.136097	-3.575077	1.776359	-7.447886	-3.313915	1.596220	-7.570919	-3.079116	1.716926
C	-5.238154	-2.149598	1.046623	-4.675312	-2.495647	1.160605	-5.018476	-2.140140	1.031260	-4.920637	-2.436144	1.315915
H	-3.205437	-4.605232	0.693705	-2.909920	-4.954731	0.184310	-3.007498	-4.559663	0.592922	-3.518303	-5.168097	0.464094
H	-3.061816	-2.553596	2.565940	-2.052572	-1.476587	1.405977	-2.532826	-0.915485	1.417965	-1.620521	-3.469877	1.079077
H	-2.875227	-0.998788	1.771009	-1.278736	-2.823534	0.584290	-1.564234	-2.235149	0.778896	-2.709923	-3.711478	2.440890
H	-1.055540	-1.994811	0.274807	-2.074626	-4.415968	2.397707	-3.349576	-2.394437	3.313436	-2.709015	-1.302234	2.994489
H	0.504947	-3.249133	1.486056	-1.973121	-3.572071	4.563204	-1.721587	-3.778108	4.241049	-0.839285	-0.022166	2.441625
H	-1.676009	-3.690037	3.657752	-2.831898	-1.204028	4.862457	-0.131263	-3.542886	1.580616	-0.023890	-2.254718	0.442009
H	-0.449486	-4.870530	3.179580	-1.080623	-1.200193	4.757756	0.588482	-3.557738	3.195234	0.041602	-0.534541	0.067610
H	0.033888	-3.390645	3.988484	-2.044012	-0.707276	3.359223	-0.226030	-4.990257	2.593182	1.079357	-1.188988	1.328151
H	-4.191117	-4.727412	-1.886274	-4.116499	-4.730861	-2.258273	-3.998398	-4.778809	-1.957977	-4.482625	-4.717766	-2.066150
H	-0.087523	-5.078627	-2.852512	0.381025	-5.034244	-2.026449	0.102675	-4.824097	-3.019516	-0.167510	-5.911531	-1.473926
H	0.256432	-5.016446	-1.125120	0.065600	-6.509973	-2.979724	0.470306	-4.735930	-1.298446	-0.670319	-7.231956	-2.562701
H	0.016974	-6.597344	-1.917308	-0.138730	-4.890398	-3.703783	0.329589	-6.330489	-2.086688	-0.476390	-5.564083	-3.173442
H	-2.182075	-2.002120	-2.871827	-2.258453	-1.857293	-3.130142	-2.246658	-1.917613	-3.078757	-2.064879	-2.232745	-2.738346
H	-3.169102	-2.304196	-5.147622	-3.499075	-1.941340	-5.297788	-3.266582	-2.404962	-5.307197	-3.140012	-2.065219	-4.988767
H	-3.306620	-3.802999	-4.222601	-3.502815	-3.536311	-4.538639	-3.232536	-3.872380	-4.324373	-3.486735	-3.639762	-4.267402
H	-4.725713	-2.756540	-4.431154	-4.953444	-2.515751	-4.463884	-4.750786	-2.973951	-4.523702	-4.730657	-2.372899	-4.270574
H	-4.122740	1.860927	-2.266846	-4.373074	1.927922	-3.672635	-3.208215	2.481371	-3.622467	-3.479054	1.869669	-3.258323

H	-2.709977	2.491968	-3.148373	-4.156156	1.866823	-1.924732	-4.561778	1.566482	-4.350413	-3.256789	1.770824	-1.511738
H	-4.080523	1.747862	-4.025407	-2.901081	2.627022	-2.935438	-4.488038	1.777208	-2.602253	-1.898795	2.296715	-2.533879
H	-5.516743	-1.154343	1.367828	-4.830653	-1.558999	1.679544	-5.286759	-1.152350	1.383207	-4.967182	-1.477374	1.814058

	Conformer 19			**Conformer 18**			**Conformer 46**			**Conformer 53**		
Gibbs free energy (hartrees)	-1572.029701			-1572.029559			-1572.029155			-1572.028957		
ΔG (kJ/mol)	5.464			5.836			6.897			7.417		
Population Proportion	2.2%			1.89%			1.23%			1.0%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-2.813013	-2.371910	1.890102	-2.504774	-3.119927	1.722981	-2.355719	-2.446515	2.029204	-2.796607	-2.401068	1.812049
C	-1.419018	-2.841755	1.572629	-2.036036	-1.821934	2.325438	-2.502273	-3.455501	3.135791	-1.398845	-2.842776	1.470754
C	-0.372929	-2.079574	1.244418	-0.916564	-1.156906	2.028117	-1.689244	-4.480847	3.406079	-0.368800	-2.058796	1.142469
C	-0.329462	-0.588188	1.081162	0.133556	-1.518715	1.018843	-0.437955	-4.890603	2.685057	-0.351357	-0.564439	1.003704
C	-3.851067	-2.643108	0.784853	-3.691696	-2.974332	0.754505	-3.521275	-2.438626	1.026880	-3.841022	-2.666171	0.711234
C	-4.066895	-4.122979	0.351739	-4.175113	-4.306906	0.114219	-3.725222	-3.736760	0.197837	-4.029424	-4.138957	0.244477
C	-3.734423	-4.149262	-1.150145	-3.878539	-4.151040	-1.383205	-3.409578	-3.338535	-1.253897	-3.696523	-4.122511	-1.259574
O	-2.360064	-4.559746	-1.319408	-2.553420	-4.670496	-1.640632	-2.021407	-3.617294	-1.530424	-2.314956	-4.468883	-1.490104
C	-2.108104	-5.705022	-2.008264	-2.420248	-5.688553	-2.532999	-1.736935	-4.604011	-2.422365	-2.008577	-5.791027	-1.543866
C	-0.633753	-5.995874	-2.026502	-0.988035	-6.136173	-2.614181	-0.251345	-4.737618	-2.612444	-0.545768	-5.991782	-1.823903
O	-2.966908	-6.374037	-2.529356	-3.341206	-6.147584	-3.163534	-2.578587	-5.261364	-2.983402	-2.828734	-6.662039	-1.384057
C	-3.896691	-2.672759	-1.547138	-3.879565	-2.624647	-1.549230	-3.680838	-1.827441	-1.221805	-3.891158	-2.643398	-1.623441
C	-3.112672	-2.214453	-2.771579	-3.115936	-2.069613	-2.746176	-3.062015	-0.917489	-2.291651	-3.111901	-2.135005	-2.831757
C	-3.553847	-2.897874	-4.057635	-3.702668	-2.495056	-4.084116	-1.575684	-0.619082	-2.163743	-3.492461	-2.827192	-4.131597
O	-3.372754	-0.790644	-2.918950	-3.216446	-0.620677	-2.661212	-3.348232	-1.593921	-3.547154	-3.442455	-0.724002	-2.966131
C	-2.350252	0.078094	-2.760651	-2.095017	0.098762	-2.437384	-3.630666	-0.833292	-4.630292	-2.465770	0.192783	-2.790157
C	-2.841079	1.497480	-2.864967	-2.424587	1.559096	-2.279979	-3.918211	-1.696904	-5.828778	-3.026107	1.587121	-2.882817
O	-1.204100	-0.249454	-2.557535	-0.985120	-0.375817	-2.365476	-3.649087	0.374569	-4.612547	-1.306129	-0.079182	-2.581307
O	-3.456423	-1.934690	-0.401765	-3.284448	-2.132829	-0.342840	-3.248297	-1.391653	0.069032	-3.473349	-1.919334	-0.460612
H	-4.965594	-2.485194	-1.721255	-4.925232	-2.291215	-1.612905	-4.772199	-1.721108	-1.303122	-4.962790	-2.476626	-1.800003
C	-5.544327	-4.422719	0.630094	-5.673240	-4.395905	0.424764	-5.191504	-4.130517	0.406941	-5.501159	-4.472500	0.518354
O	-6.109900	-5.472756	0.439713	-6.427144	-5.271970	0.074541	-5.761066	-5.071225	-0.091881	-6.050231	-5.525973	0.301642
C	-6.136691	-3.167483	1.154830	-6.006424	-3.189462	1.222375	-5.770737	-3.118063	1.327475	-6.113192	-3.242822	1.080351
Cl	-7.819579	-3.077231	1.569783	-7.625381	-2.905290	1.780158	-7.434204	-3.199682	1.814168	-7.795430	-3.194797	1.505285
C	-5.233730	-2.186142	1.220622	-4.942924	-2.400217	1.396863	-4.874889	-2.186969	1.665082	-5.228100	-2.247414	1.169246
H	-3.453599	-4.844243	0.891111	-3.680717	-5.192221	0.515377	-3.094056	-4.564142	0.522563	-3.408406	-4.861516	0.772156
H	-3.170730	-2.866554	2.800013	-1.704518	-3.613787	1.168717	-2.297206	-1.437194	2.453987	-3.137035	-2.919693	2.715231
H	-2.829594	-1.298082	2.089586	-2.814589	-3.803428	2.521774	-1.441760	-2.603269	1.454606	-2.828127	-1.331826	2.033388
H	-1.261771	-3.915832	1.628540	-2.683797	-1.397822	3.089372	-3.362387	-3.314422	3.786464	-1.223084	-3.914894	1.509063
H	0.570393	-2.588847	1.055486	-0.732011	-0.231431	2.570615	-1.947231	-5.102827	4.261043	0.580135	-2.549946	0.934670

H	0.491075	-0.159223	1.665822	-0.023661	-2.500543	0.571643	-0.515309	-5.928520	2.343875	-1.278777	-0.094097	1.332210
H	-0.144268	-0.327355	0.033473	0.148573	-0.786268	0.204638	-0.214780	-4.266337	1.819330	0.474473	-0.132787	1.578727
H	-1.255769	-0.097710	1.382194	1.128205	-1.504974	1.476763	0.423084	-4.850540	3.361344	-0.193152	-0.282634	-0.042925
H	-4.373158	-4.824077	-1.715167	-4.593095	-4.666532	-2.020474	-4.023286	-3.863840	-1.980679	-4.331293	-4.798251	-1.829926
H	-0.265752	-6.103116	-1.004085	-0.351680	-5.294833	-2.895855	0.111586	-3.891995	-3.202914	0.051593	-5.482015	-1.065488
H	-0.448370	-6.909120	-2.587238	-0.655703	-6.487377	-1.635037	0.263683	-4.717708	-1.651555	-0.317704	-7.055220	-1.827309
H	-0.097769	-5.161391	-2.483316	-0.896062	-6.934789	-3.346663	-0.034041	-5.662371	-3.142686	-0.291789	-5.554162	-2.791799
H	-2.048256	-2.346155	-2.591130	-2.065404	-2.340502	-2.664731	-3.613092	0.023589	-2.289270	-2.045821	-2.215199	-2.634900
H	-2.973979	-2.512029	-4.897637	-3.131891	-2.042445	-4.896601	-1.281127	0.084000	-2.944965	-2.944251	-2.377902	-4.961330
H	-3.397643	-3.976908	-4.004546	-3.662539	-3.579394	-4.203546	-1.381073	-0.158070	-1.194376	-3.237615	-3.887779	-4.092981
H	-4.612624	-2.710931	-4.252658	-4.743623	-2.174602	-4.171748	-0.975457	-1.522872	-2.245654	-4.562485	-2.729803	-4.330619
H	-3.487949	1.615548	-3.735293	-3.139506	1.877463	-3.039334	-3.094760	-2.393733	-5.995025	-3.670116	1.683081	-3.757984
H	-3.433093	1.735167	-1.977305	-2.887894	1.711891	-1.301528	-4.817870	-2.288911	-5.645135	-3.637371	1.784486	-1.998323
H	-1.993137	2.176222	-2.926761	-1.513392	2.150413	-2.341780	-4.063282	-1.070159	-6.705836	-2.212694	2.308043	-2.928822
H	-5.420314	-1.168573	1.538580	-4.941165	-1.447213	1.908113	-5.056872	-1.327525	2.297418	-5.430840	-1.242637	1.516577

	Conformer 22			**Conformer 57**			**Conformer 51**			**Conformer 40**		
Gibbs free energy (hartrees)	-1572.028327			-1572.028312			-1572.028283			-1572.027852		
ΔG (kJ/mol)	9.071			9.11			9.187			10.318		
Population Proportion	0.51%			0.5%			0.49%			0.31%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-2.332508	-2.456058	1.964980	-2.155820	-3.475586	1.771283	-2.746401	-2.602504	2.282674	-2.057784	-3.010988	1.854827
C	-2.467854	-3.478811	3.060420	-1.685248	-2.375108	2.684154	-1.339405	-2.959044	1.889216	-2.270666	-4.128504	2.841018
C	-1.648276	-4.502846	3.315518	-1.640308	-2.393327	4.019235	-0.590943	-3.948332	2.385496	-2.342628	-4.031572	4.171462
C	-0.398030	-4.898572	2.584989	-2.047187	-3.499356	4.949508	-0.955609	-4.956563	3.436800	-2.241371	-2.798593	5.021320
C	-3.503714	-2.442796	0.969734	-3.323079	-3.059461	0.862668	-3.733604	-2.542184	1.105121	-3.233516	-2.789516	0.889695
C	-3.703167	-3.730425	0.122723	-3.787962	-4.137945	-0.156920	-3.874236	-3.823184	0.233821	-3.554675	-3.938197	-0.107979
C	-3.383817	-3.305635	-1.322150	-3.454837	-3.545468	-1.538417	-3.494126	-3.383756	-1.195435	-3.246420	-3.363402	-1.500704
O	-1.987236	-3.528817	-1.604163	-2.135277	-3.959528	-1.946390	-2.118394	-3.723976	-1.454118	-1.899394	-3.723057	-1.870835
C	-1.650716	-4.727013	-2.148334	-2.043132	-5.109633	-2.663240	-1.862780	-4.675906	-2.390367	-1.727423	-4.488412	-2.982203
C	-0.176261	-4.793521	-2.434432	-0.617137	-5.391748	-3.046530	-0.381460	-4.883668	-2.544270	-0.266510	-4.733464	-3.238735
O	-2.453981	-5.599919	-2.371118	-2.999642	-5.789689	-2.945186	-2.721267	-5.254335	-3.010246	-2.636573	-4.893250	-3.664529
C	-3.684296	-1.802924	-1.267704	-3.471696	-2.043417	-1.231634	-3.695995	-1.861888	-1.118541	-3.386012	-1.854403	-1.250285
C	-3.108895	-0.854378	-2.326947	-2.782135	-1.045282	-2.169352	-2.981658	-0.945008	-2.120043	-2.691659	-0.864628	-2.202507
C	-1.614057	-0.577348	-2.275583	-1.261642	-1.062086	-2.212191	-1.490169	-0.728948	-1.912732	-1.192961	-0.692768	-2.023743
O	-3.476287	-1.465680	-3.594622	-3.336754	-1.342422	-3.480714	-3.242151	-1.556227	-3.414183	-2.926349	-1.321877	-3.563870
C	-3.812315	-0.648237	-4.619413	-3.560232	-0.307931	-4.324033	-3.431186	-0.740595	-4.477122	-4.053877	-0.914035	-4.192612
C	-4.159477	-1.445653	-5.847640	-4.134708	-0.794695	-5.627087	-3.716462	-1.539945	-5.719962	-4.095531	-1.436839	-5.602837
O	-3.822748	0.557148	-4.537618	-3.322329	0.843793	-4.047154	-3.381918	0.464841	-4.411965	-4.895921	-0.220339	-3.672636

O	-3.244984	-1.379119	0.024738	-2.904711	-1.922119	0.074443	-3.315674	-1.493866	0.209137	-2.900584	-1.642340	0.078467
H	-4.778837	-1.719200	-1.334914	-4.534345	-1.761102	-1.203615	-4.775284	-1.700488	-1.251784	-4.463208	-1.642034	-1.288902
C	-5.168376	-4.131571	0.325790	-5.292351	-4.306888	0.082364	-5.344268	-4.238345	0.349514	-5.043523	-4.247886	0.089489
O	-5.736777	-5.064304	-0.188861	-6.039685	-5.032568	-0.528530	-5.861021	-5.202375	-0.162526	-5.692977	-5.062724	-0.521059
C	-5.748817	-3.137619	1.265804	-5.643002	-3.395503	1.201171	-6.006351	-3.212012	1.195203	-5.523198	-3.338178	1.159986
Cl	-7.410602	-3.234933	1.755015	-7.272096	-3.290364	1.791062	-7.704256	-3.299288	1.543928	-7.177683	-3.366965	1.683360
C	-4.855756	-2.209197	1.617803	-4.583717	-2.703940	1.629001	-5.146655	-2.271386	1.593309	-4.550355	-2.536812	1.601160
H	-3.072903	-4.561801	0.438399	-3.305581	-5.106123	-0.020404	-3.239865	-4.647178	0.559669	-2.981386	-4.849359	0.062994
H	-2.277254	-1.451463	2.401356	-1.337517	-3.776666	1.106962	-3.145801	-3.297721	3.023812	-1.874041	-2.060748	2.359947
H	-1.420855	-2.600812	1.383743	-2.458478	-4.362522	2.331898	-2.755916	-1.608495	2.747228	-1.177624	-3.219388	1.236673
H	-3.325449	-3.349886	3.716910	-1.341788	-1.478215	2.176178	-0.899080	-2.318821	1.131133	-2.361787	-5.122767	2.408873
H	-1.899469	-5.135617	4.164563	-1.255435	-1.502395	4.512055	0.419921	-4.045424	1.993577	-2.488118	-4.956614	4.726049
H	-0.180304	-4.263119	1.726050	-2.441504	-4.375314	4.433259	-1.980929	-4.856809	3.794802	-3.144428	-2.679440	5.629813
H	0.465253	-4.863020	3.258660	-1.194748	-3.821469	5.557773	-0.829505	-5.974344	3.052076	-1.404634	-2.884945	5.723150
H	-0.472329	-5.932674	2.231776	-2.812048	-3.148054	5.650606	-0.287847	-4.867665	4.300957	-2.102915	-1.885052	4.442274
H	-3.984378	-3.834795	-2.057799	-4.171981	-3.833550	-2.303136	-4.113156	-3.849451	-1.957658	-3.925457	-3.731378	-2.265574
H	0.062423	-4.117660	-3.259645	0.029655	-5.334057	-2.169666	-0.198225	-5.783918	-3.126931	0.258465	-4.957388	-2.309978
H	0.396728	-4.469343	-1.564631	-0.550327	-6.377754	-3.500920	0.048993	-4.024278	-3.065368	-0.153502	-5.549572	-3.949311
H	0.095621	-5.810099	-2.709944	-0.276007	-4.637380	-3.759842	0.098976	-4.955282	-1.567955	0.175298	-3.827728	-3.663370
H	-3.647621	0.090569	-2.245560	-3.118452	-0.047570	-1.884037	-3.484714	0.022585	-2.103669	-3.187902	0.099697	-2.088266
H	-1.363880	0.184689	-3.016032	-0.910128	-0.232638	-2.828612	-1.124164	-0.012442	-2.650313	-0.829629	0.049565	-2.737365
H	-1.348674	-0.197502	-1.287738	-0.866881	-0.932588	-1.203261	-1.319430	-0.315625	-0.917609	-0.986863	-0.333660	-1.015143
H	-1.034671	-1.476973	-2.471444	-0.885183	-1.998977	-2.616870	-0.932905	-1.658896	-2.003756	-0.656674	-1.627573	-2.174925
H	-3.299212	-2.045214	-6.153069	-3.445749	-1.501665	-6.094033	-2.955207	-2.309610	-5.857043	-3.281311	-0.992862	-6.180509
H	-4.977796	-2.133624	-5.625751	-5.073401	-1.321938	-5.444433	-4.679674	-2.044843	-5.613227	-3.948352	-2.518274	-5.603886
H	-4.446088	-0.772432	-6.652421	-4.305780	0.050244	-6.290312	-3.744560	-0.878281	-6.582873	-5.049875	-1.185002	-6.059847
H	-5.039237	-1.361948	2.265932	-4.581353	-1.960622	2.414625	-5.382909	-1.403189	2.194845	-4.651039	-1.769812	2.357722

	Conformer 24			**Conformer 1**			**Conformer 3**			**Conformer 11**		
Gibbs free energy (hartrees)	-1572.027717			-1572.027625			-1572.027539			-1572.027488		
ΔG (kJ/mol)	10.673			10.914			11.14			11.274		
Population Proportion	0.27%			0.24%			0.22%			0.21%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-2.785318	-2.661110	2.304030	-2.202348	-3.509821	1.847382	-2.504992	-2.526119	1.782594	-1.989156	-3.429957	1.209005
C	-1.369816	-3.042757	1.969055	-1.750363	-2.448802	2.814696	-1.244171	-2.817425	1.016253	-1.308544	-2.358833	2.018234
C	-0.681979	-4.083926	2.446584	-1.774227	-2.505627	4.149255	-0.331799	-3.754054	1.290502	-0.896525	-2.438502	3.286568
C	-1.137180	-5.137311	3.415021	-2.257442	-3.625431	5.024948	-0.330626	-4.753906	2.410894	-1.008195	-3.600896	4.230360
C	-3.706191	-2.522912	1.079705	-3.308177	-3.036015	0.890692	-3.766485	-2.486707	0.904235	-3.377685	-3.017842	0.693886
C	-3.841560	-3.765892	0.155132	-3.752937	-4.078459	-0.172962	-4.095310	-3.771087	0.090450	-4.071128	-4.055581	-0.232804

C	-3.383422	-3.289343	-1.238135	-3.373422	-3.461441	-1.529535	-4.088785	-3.324524	-1.386381	-4.158739	-3.368265	-1.605745
O	-2.016649	-3.690103	-1.456944	-2.082882	-3.965120	-1.931648	-2.831289	-3.630674	-2.017702	-3.025846	-3.720105	-2.424973
C	-1.756915	-4.525819	-2.496851	-2.008551	-4.671007	-3.091827	-2.730075	-4.838399	-2.631498	-3.172728	-4.795619	-3.243613
C	-0.282933	-4.803528	-2.600859	-0.590585	-5.083213	-3.374228	-1.396867	-4.987869	-3.308532	-1.952032	-4.994618	-4.096785
O	-2.605453	-4.963452	-3.235383	-2.960884	-4.910390	-3.793262	-3.616147	-5.658263	-2.625938	-4.171210	-5.473347	-3.268395
C	-3.522358	-1.762455	-1.113018	-3.319661	-1.964747	-1.185465	-4.274769	-1.804477	-1.268024	-4.099262	-1.884140	-1.223078
C	-2.696105	-0.854112	-2.040351	-2.502137	-1.016955	-2.081179	-3.821012	-0.907806	-2.420053	-3.668310	-0.863654	-2.277628
C	-1.230273	-0.677908	-1.683454	-0.994899	-1.042314	-1.893772	-4.350533	0.515497	-2.286777	-3.979069	0.568953	-1.860284
O	-2.761239	-1.413773	-3.382211	-2.780792	-1.365969	-3.466235	-2.372188	-0.831453	-2.442008	-2.235334	-0.956602	-2.483443
C	-3.799115	-1.060080	-4.176077	-3.853146	-0.799836	-4.068002	-1.717605	-1.199380	-3.561429	-1.769156	-1.213737	-3.721527
C	-3.670702	-1.695831	-5.533686	-3.947648	-1.235148	-5.505143	-0.231384	-1.031628	-3.388667	-0.264078	-1.254216	-3.722405
O	-4.694020	-0.329447	-3.820973	-4.614413	-0.046938	-3.507342	-2.257921	-1.615830	-4.560991	-2.470928	-1.393758	-4.690865
O	-3.205766	-1.458718	0.248486	-2.814450	-1.898958	0.151146	-3.617278	-1.425811	-0.056144	-3.232934	-1.814555	-0.087607
H	-4.581370	-1.540924	-1.301898	-4.360561	-1.613971	-1.204750	-5.358097	-1.644320	-1.165662	-5.122749	-1.609712	-0.927797
C	-5.326944	-4.140471	0.186290	-5.266970	-4.231033	0.010191	-5.482715	-4.214572	0.568750	-5.443560	-4.316583	0.399319
O	-5.845032	-5.070342	-0.384224	-5.999972	-4.938581	-0.638337	-6.096521	-5.185318	0.195784	-6.308008	-5.039782	-0.034405
C	-5.999633	-3.123586	1.034626	-5.647245	-3.328169	1.125704	-5.927056	-3.205531	1.564068	-5.498006	-3.495725	1.635040
Cl	-7.714468	-3.170649	1.298772	-7.297144	-3.201118	1.650055	-7.479518	-3.328382	2.330871	-6.901480	-3.511318	2.657018
C	-5.133640	-2.223107	1.505436	-4.594173	-2.661237	1.604922	-5.011838	-2.250040	1.741052	-4.384750	-2.777767	1.803631
H	-3.246432	-4.620099	0.477235	-3.283778	-5.055287	-0.051561	-3.387090	-4.583546	0.250465	-3.537022	-5.003496	-0.303592
H	-3.242514	-3.374261	2.992778	-1.358553	-3.816987	1.218504	-2.668927	-3.247758	2.585509	-1.385664	-3.655970	0.322219
H	-2.791818	-1.687342	2.809582	-2.559073	-4.402431	2.365517	-2.424929	-1.540009	2.257329	-2.094354	-4.358984	1.773310
H	-0.867300	-2.375897	1.275275	-1.357643	-1.547917	2.351312	-1.076367	-2.172657	0.159426	-1.137844	-1.428063	1.484516
H	0.345969	-4.193392	2.105700	-1.391635	-1.639953	4.686828	0.533314	-3.806859	0.631972	-0.409119	-1.558893	3.703106
H	-2.176424	-5.020340	3.724275	-2.649239	-4.474561	4.463911	-1.222224	-4.701805	3.036820	-1.513195	-4.463857	3.794995
H	-1.025262	-6.134984	2.976894	-1.445759	-3.989232	5.664651	-0.253128	-5.772761	2.016316	-0.014644	-3.922813	4.561529
H	-0.514544	-5.123825	4.316505	-3.046601	-3.272259	5.697587	0.541946	-4.605153	3.056778	-1.555771	-3.309809	5.133351
H	-3.990926	-3.699803	-2.040805	-4.092872	-3.690779	-2.311407	-4.885898	-3.794195	-1.960212	-5.071034	-3.627106	-2.140079
H	0.206950	-3.941390	-3.062096	-0.581959	-5.859802	-4.136183	-0.590050	-4.784608	-2.602298	-2.040934	-5.927718	-4.648551
H	0.155538	-4.949415	-1.613708	-0.036796	-4.215583	-3.743604	-1.301690	-5.994857	-3.708414	-1.867289	-4.158695	-4.795268
H	-0.120386	-5.678673	-3.226652	-0.099014	-5.431192	-2.465602	-1.323322	-4.258471	-4.118472	-1.052826	-5.004758	-3.478671
H	-3.187260	0.119348	-2.065123	-2.876087	-0.006262	-1.913995	-4.153803	-1.354622	-3.357455	-4.166154	-1.105327	-3.217289
H	-0.765833	0.001591	-2.401097	-0.537796	-0.317739	-2.570835	-4.005103	1.123856	-3.124458	-3.651833	1.264148	-2.635405
H	-1.150016	-0.238383	-0.688824	-0.751115	-0.760179	-0.869246	-5.443028	0.515291	-2.290127	-5.054559	0.696500	-1.716831
H	-0.695010	-1.625427	-1.688672	-0.578407	-2.028392	-2.090157	-4.002669	0.967108	-1.355971	-3.469050	0.816112	-0.927404
H	-4.550915	-1.468255	-6.130741	-3.085794	-0.855159	-6.058825	-0.004698	-0.069105	-2.928761	0.139526	-0.371928	-3.223370
H	-2.776538	-1.315235	-6.032824	-3.923963	-2.324640	-5.566122	0.141339	-1.813598	-2.722000	0.072119	-2.131629	-3.164439
H	-3.554025	-2.775959	-5.427612	-4.865280	-0.851772	-5.945612	0.262386	-1.117500	-4.354389	0.102374	-1.310882	-4.745150
H	-5.373977	-1.368493	2.124490	-4.610728	-1.927428	2.399277	-5.103284	-1.389936	2.391682	-4.187699	-2.084560	2.610152

Conformer 34	**Conformer 44**

Gibbs free energy (hartrees)	-1572.027326			-1572.027115		
ΔG (kJ/mol)	11.699			12.253		
Population Proportion	0.18%			0.14%		
Element	**X**	**Y**	**Z**	**X**	**Y**	**Z**
C	-2.714720	-2.623607	2.206450	-2.198170	-2.278682	1.457361
C	-1.305522	-2.950891	1.795947	-1.988783	-3.255872	2.581767
C	-0.543503	-3.947256	2.256367	-1.081661	-4.235262	2.640934
C	-0.892369	-4.994110	3.274762	-0.051817	-4.610912	1.615271
C	-3.712301	-2.553459	1.038590	-3.585886	-2.360920	0.799676
C	-3.844300	-3.819346	0.143624	-3.934824	-3.703299	0.099866
C	-3.456517	-3.347833	-1.274835	-4.022346	-3.362405	-1.397225
O	-2.066048	-3.614178	-1.537707	-2.762612	-3.613840	-2.052302
C	-1.756021	-4.834714	-2.043362	-2.600512	-4.841034	-2.614795
C	-0.278752	-4.951527	-2.296827	-1.285982	-4.934511	-3.336570
O	-2.580515	-5.691476	-2.252771	-3.429133	-5.715453	-2.539108
C	-3.701741	-1.836304	-1.172091	-4.321281	-1.857682	-1.366116
C	-3.039440	-0.868088	-2.159624	-4.002888	-1.010603	-2.598667
C	-1.539408	-0.653853	-2.026542	-4.635553	0.374282	-2.527240
O	-3.369163	-1.407051	-3.469835	-2.567566	-0.826472	-2.705867
C	-3.620512	-0.531469	-4.470361	-1.940277	-1.229592	-3.828446
C	-3.940055	-1.257873	-5.749112	-0.467271	-0.927893	-3.749719
O	-3.585092	0.668545	-4.333807	-2.491528	-1.766262	-4.762616
O	-3.316789	-1.482039	0.158112	-3.624304	-1.347662	-0.225968
H	-4.787421	-1.707491	-1.289622	-5.406368	-1.772377	-1.206806
C	-5.313898	-4.241566	0.245482	-5.277811	-4.140001	0.696465
O	-5.829000	-5.190480	-0.295277	-5.914521	-5.120069	0.393037
C	-5.978987	-3.243115	1.121890	-5.643768	-3.110873	1.703283
Cl	-7.675061	-3.351016	1.474132	-7.117535	-3.232673	2.611277
C	-5.124290	-2.307599	1.541851	-4.735611	-2.133753	1.763921
H	-3.214083	-4.649358	0.461465	-3.205380	-4.491974	0.284218
H	-3.098349	-3.340107	2.935632	-2.085280	-1.253703	1.830747
H	-2.734542	-1.639892	2.692066	-1.463534	-2.408634	0.661354
H	-0.875564	-2.280821	1.058049	-2.648259	-3.132401	3.437928

H	0.467062	-4.018878	1.858232	-1.067380	-4.841143	3.544843
H	-1.917358	-4.918009	3.639324	-0.101459	-4.002299	0.711868
H	-0.756365	-5.996947	2.855747	0.956434	-4.513991	2.032856
H	-0.222168	-4.926446	4.138928	-0.166466	-5.660549	1.324059
H	-4.057541	-3.820432	-2.048234	-4.798723	-3.931618	-1.905054
H	0.021824	-4.229546	-3.059651	-1.307960	-4.266663	-4.201083
H	0.275749	-4.719974	-1.385597	-0.470683	-4.612147	-2.686972
H	-0.044878	-5.959277	-2.632664	-1.123188	-5.958081	-3.666463
H	-3.544824	0.093453	-2.059936	-4.347143	-1.545254	-3.484658
H	-1.224853	0.127625	-2.720752	-4.385600	0.947248	-3.421877
H	-1.308459	-0.325487	-1.011883	-5.723067	0.291420	-2.465106
H	-0.986271	-1.567353	-2.233324	-4.274290	0.914417	-1.650269
H	-4.157164	-0.537761	-6.534841	-0.002251	-1.109144	-4.716379
H	-3.092272	-1.881740	-6.040383	-0.307313	0.105780	-3.439643
H	-4.797267	-1.917175	-5.598357	-0.007553	-1.573136	-2.997038
H	-5.364091	-1.457047	2.166700	-4.787115	-1.254808	2.393499

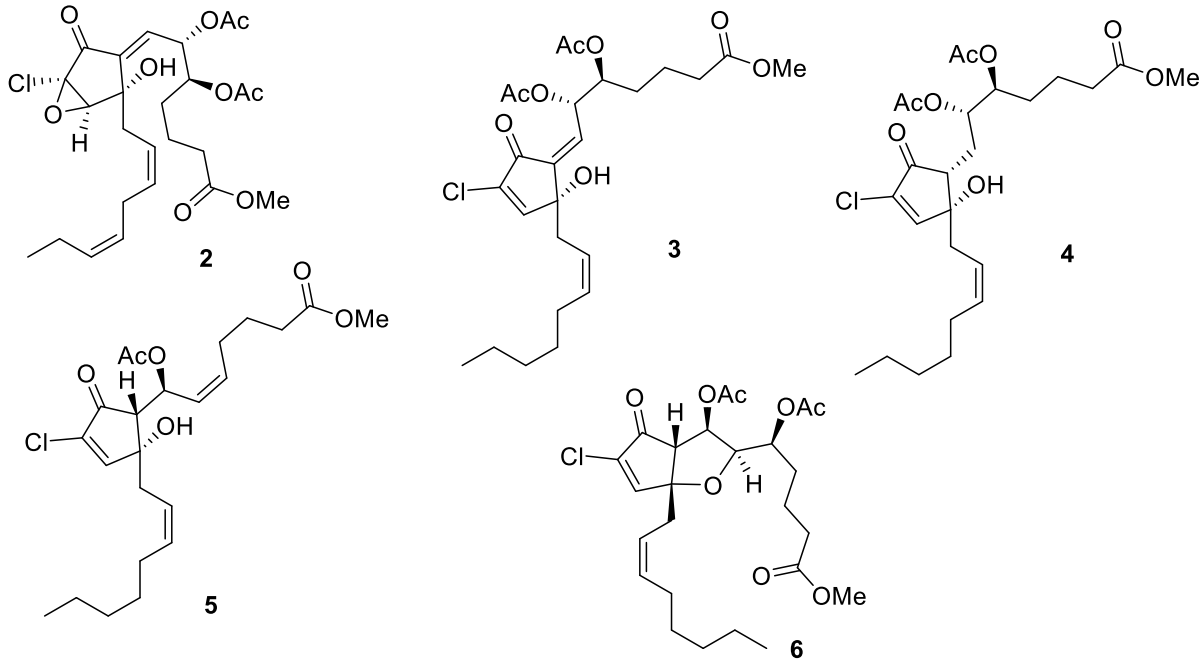


Figure S08. Structures of known punaglandins **2**-**6**.

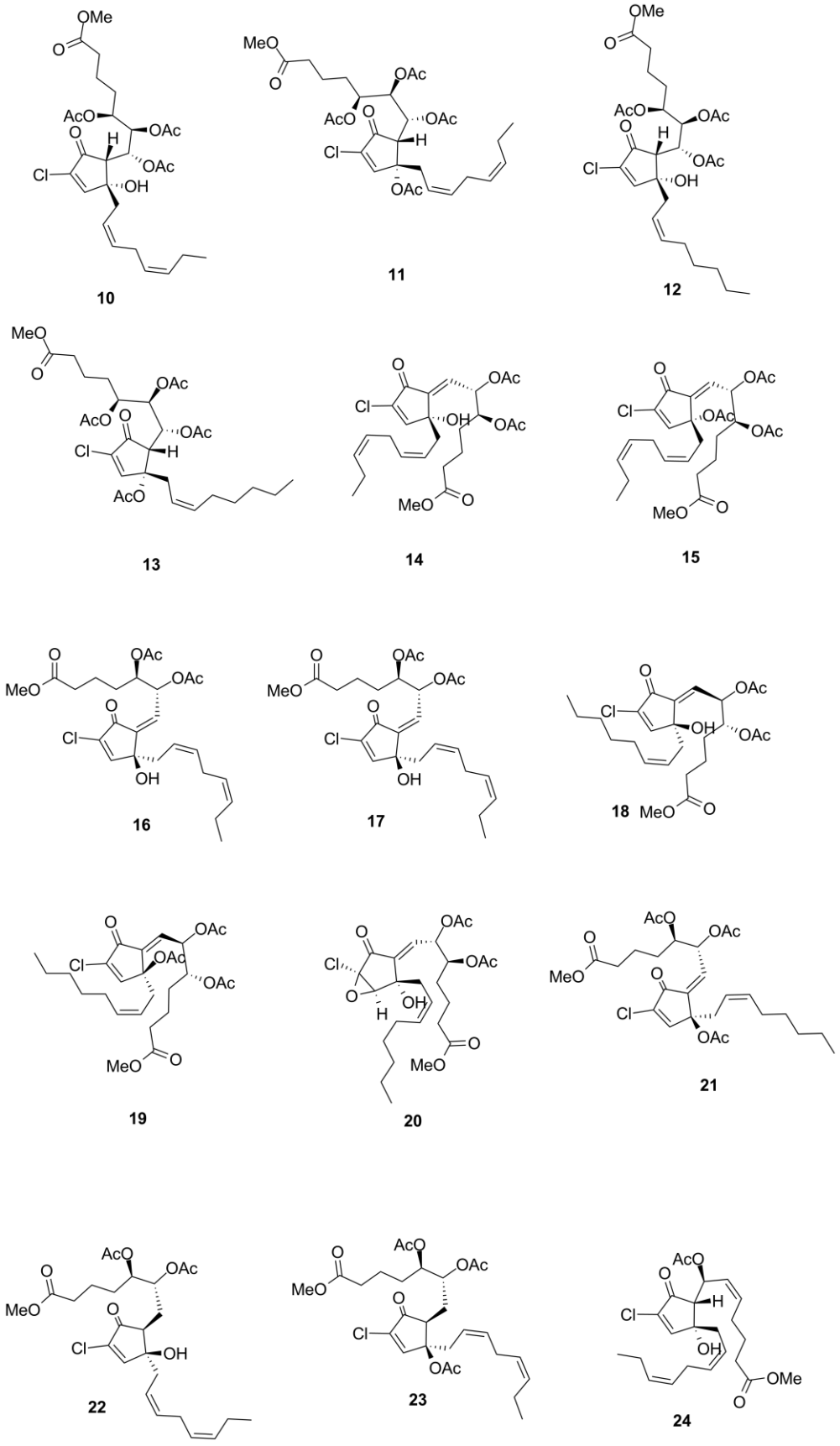


Figure S09. Structures of known punaglandins **10**-**24**.

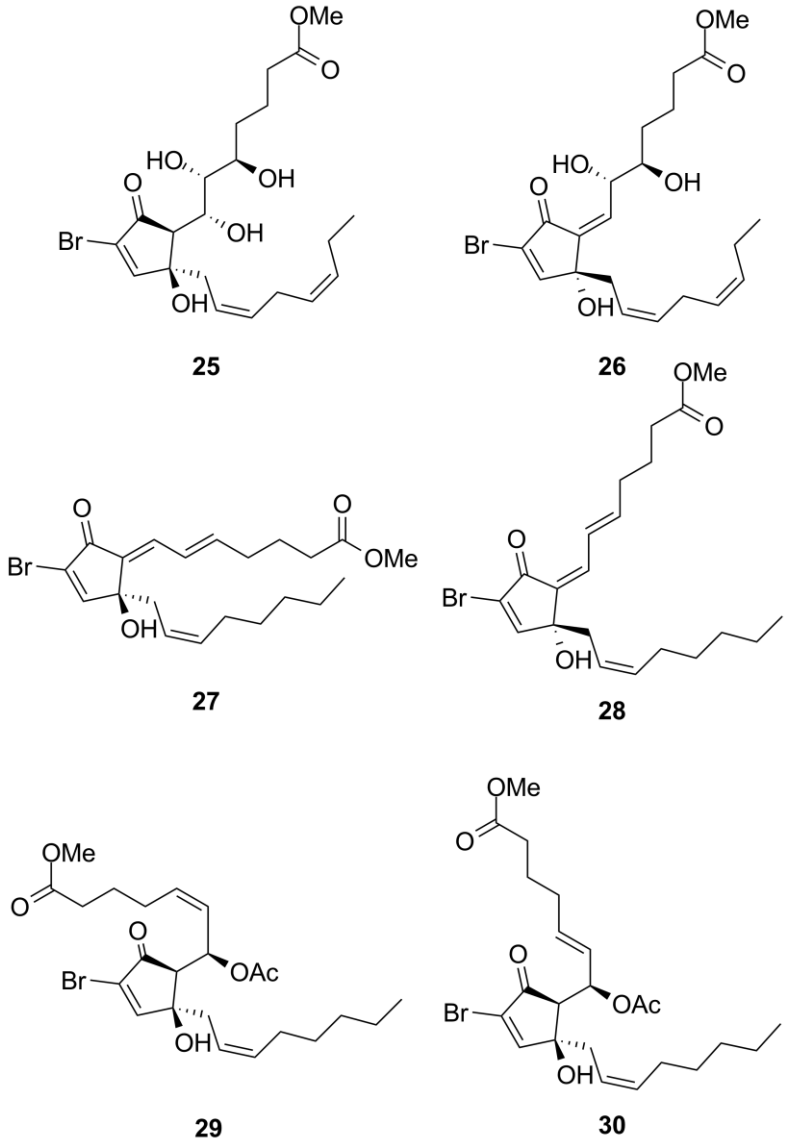


Figure S10. Structures of known brominated prostanoids **25**-**30**.

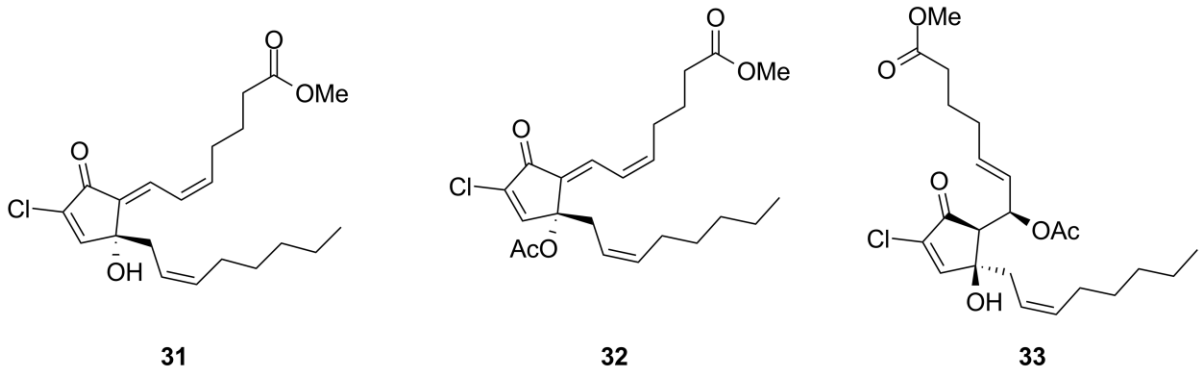


Figure S11. Structures of known chlorinated prostanoids **31**-**33**.

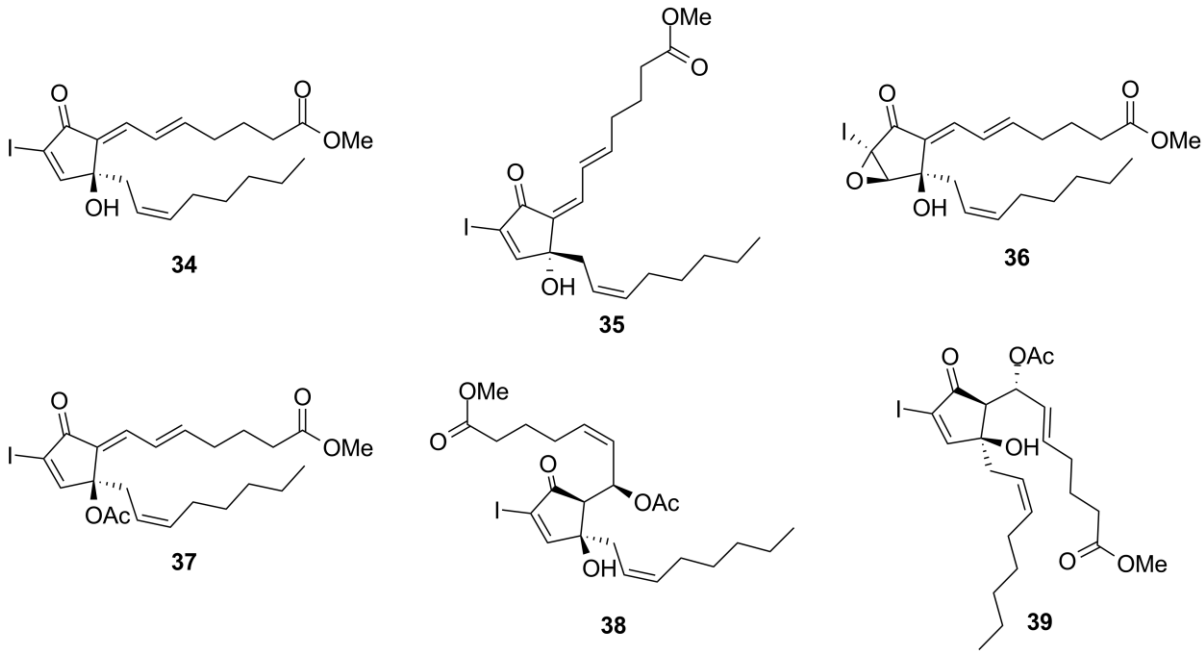


Figure S12. Structures of known iodinated prostanoids **34**-**39**.

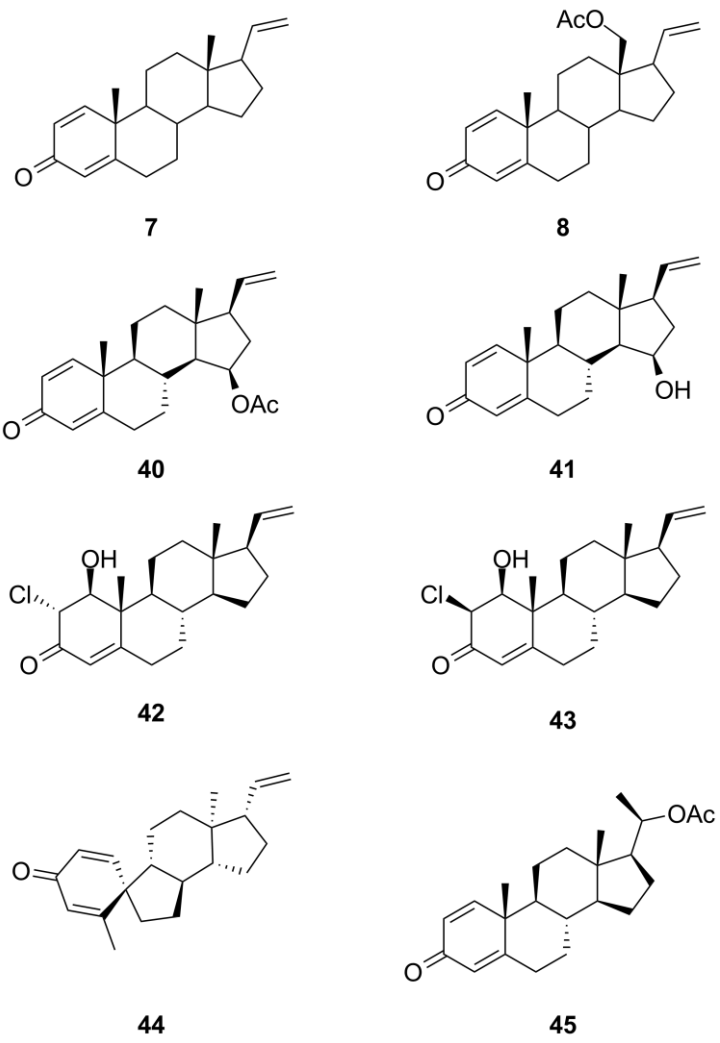


Figure S13. Structures of known pregnane steroids **7**-**8**, and **40**-**44**.

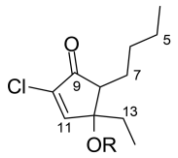


Table S17. Published proton and carbon chemical shifts of the halogenated prostanoids used to generate the PCA plots.

Name	*Structure Class*	*^{1}H-5*	*^{1}H-6*	*^{1}H-7*	*^{1}H-8*	*^{1}H-11*	*^{1}H-13*	*^{13}C-5*	*^{13}C-6*	*^{13}C -7*	*^{13}C -8*	*^{13}C -9*	*^{13}C -10*	*^{13}C -11*	*^{13}C - 12*	*^{13}C - 13*
*(**2**) 7E-Punaglandin 3 epoxide*[1]	*10,11-epoxy-7E-enone*	5.2	5.98	6.54	0	3.96	2.8	69.5	73.6	132.8	139.9	187.3	79.6	66.7	71.4	34.2
*(**3**) 7Z-Punaglandin 4*[1-3]	*7Z,10-dienone*	5.2	6.32	6.07	0	7.2	2.44	73.9	70.5	135.5	140.4	186.7	138.5	153.6	76.5	37.3
*(**4**) Punaglandin 6*[4]	*10-enone*	5.11	5.28	2.12	2.66	7.29	2.1	72.1	72.2	25.5	55.1	196.7	134.4	157.6	78.9	35.8
*(**5**) Punaglandin 8*[1]	*7-OAc,10-enone*	5.59	5.83	5.96	2.68	7.33	2.39	133.5	126.3	67.9	56.9	196.3	136.6	157.9	76.9	39.3
*(**6**) Carijenone*[5]	*Bicyclic*	4.97	4.33	5.08	2.94	7.34	2.61	72.5	88	77.5	58	196.1	135.8	156	89.6	35.7
*(**10**) Punaglandin 1*[1]	*7-OAc,10-enone*	5.18	5.61	5.34	2.75	7.26	2.53	71.6	72.9	70	53.4	196	134.6	158.1	77.2	39.4
*(**11**) Punaglandin 1 acetate*[1]	*12-acetoxy-7-OAc,10-enone*	5.3	5.3	5.3	3.1	7.8	2.9	71.1	72.7	69.5	52.9	195	137.7	155.1	83.8	33.4
*(**12**) Punaglandin 2*[1]	*7-OAc,10-enone*	5.18	5.61	5.31	2.74	7.26	2.4	71.7	72.9	70	53.5	196	136	158.2	77.2	39.5
*(**13**) Punaglandin 2 acetate*[1]	*12-acetoxy-7-OAc,10-enone*	5.27	5.33	5.5	3.01	7.82	2.77	71.1	72.7	69.5	52.9	195	137.7	155.1	83.8	33.4
*(**14**) 7E-Punaglandin 3*[1]	*7E,10-dienone*	5.25	6.02	6.35	0	7.27	2.68	69.8	73.7	130.5	140.5	186.6	137.2	155.7	77.2	35.6
*(**15**) 7E-Punaglandin 3 acetate*[1]	*12-acetoxy-7E,10-dienone*	5.2	5.86	6.47	0	7.59	2.8.0	69.9	73.3	130.4	140.9	185.4	135.4	151.5	83.3	33.9
*(**16**) 7Z-Punaglandin 3*[1]	*7Z,10-dienone*	5.1	6.32	6.08	0	7.2	2.47	73.9	70.5	135.5	140.4	186.7	138.5	153.6	76.5	37.3
*(**17**) 7Z-Punaglandin 3 acetate*[1]	*12-acetoxy-7Z,10-dienone*	5.18	6.46	6.1	0	7.53	2.63	74	69.9	136	139.6	193.8	136.5	150.1	82.1	35.3
*(**18**) 7E-Punaglandin 4*[1-4]	*7E,10-dienone*	5.25	6.01	6.33	0	7.25	2.62	69.8	73.7	130.6	140.4	186.8	137.2	155.7	77.3	35.7
*(**19**) 7E-Punaglandin 4 acetate*[1]	*12-acetoxy-7E,10-dienone*	5.07	5.86	6.47	0	7.6	2.77	70	73.7	130.8	139	185.6	137.6	152.1	83.3	34.4
*(**20**) 7E-Punaglandin 4 epoxide*[1]	*10,11-epoxy-7E-enone*	5.2	5.97	6.55	0	3.95	2.76	69.5	73.6	132.8	139.9	187.3	79.6	66.7	71.4	34.2

(21) *7Z-Punaglandin 4 acetate*[1]	*12-acetoxy-7Z,10-dienone*	5.2	6.46	6.09	0	7.53	2.58	74	69.8	135.7	142.5	190.8	136.5	149	82.3	35.4
(22) *Punaglandin 5*[1]	*10-enone*	5.11	5.1	2.16	2.67	7.3	2.65	73.7	72.2	25.7	55.1	196.6	134.6	157.5	77	35.9
(23) *Punaglandin 5 acetate*[1]	*12-acetoxy-10-enone*	5	5.3	1.9	3.2	7.5	2.3	72.8	72.3	26.4	52.2	197	138	155.6	85.5	36
(24) *Punaglandin 7*[1]	*7-OAc,10-enone*	5.3	5.8	5.9	2.6	7.3	2.4	133.5	126.3	67.9	56.9	196.3	136.6	157.9	76.9	39.3
(25) *bromopunaglandin I*[6]	*10-enone*	3.49	3.72	3.87	2.63	7.35	2.41	70.9	80.1	67.4	64.1	198.7	120.6	154.1	70.8	36.3
(26) *5-epi-bromo-Z-punagladin-3*[6]	*7Z,10-dienone*	3.35	3.98	6.47	0	7.32	2.4	76.9	74.2	147.2	142.9	196.1	122.6	158.4	76.3	37.9
(27) *Bromovulone II*[7]	*7E,10-dienone*	6.28	6.77	7.04	0	7.42	2.69	148	126.1	134.3	133.9	193.2	126.8 s	158.3	79.6	36.8
(28) *Bromovulone III*[7]	*7Z,10-dienone*	6.21	7.56	6.72	0	7.37	2.57	147.5	126	133.9	134.3	188.2	126.5	158.4	79.2	36.2
(29) *7-acetoxy-7,8-dihydrobromovulone I*[8]	*7-OAc,10-enone*	5.6	5.84	5.94	2.68	7.53	2.54	133.6	126.6	68	56.7	196.9	126.6	162.7	78.6	39.3
(30) *7-acetoxy-7,8-dihydrobromovulone II*[8]	*7-OAc,10-enone*	5.73	5.82	5.63	2.73	7.52	2.53	133.6	126.6	68	56.7	196.9	126.6	162.7	78.6	39.3
(31) *chlorovulone I*[9]	*7E,10-dienone*	6.11	6.77	7.33	0	7.21	2.67	127.9	123.8	143.6	137.9	187.7	136.4	154	77.7	33.6
(32) *12-O-acetyl-chlorovulone I*[10]	*12-acetoxy-7E,10-dienone*	6.09	6.53	7.32	0	7.39	2.71	127.3	123	144.5	133.4	186.5	138.7	150.3	83.3	35.5
(33) *7-acetoxy-7,8-dihydrochlorovulone II*[8]	*7-OAc,10-enone*	5.74	5.82	5.64	2.73	7.32	2.54	133.7	126.5	68	57	196.5	136.4	158.1	77	39.4
(34) *iodovulone II*[10]	*7E,10-dienone*	6.28	6.76	7.03	0	7.67	2.64	147.5	125.9	133.8	132.8	189.8	106.2	165.1	81.5	36.5
(35) *Iodovulone III*[10]	*7Z,10-dienone*	6.2	7.58	6.62	0	7.64	2.53	147.5	125.9	135.1	136.3	189.8	106.2	159	79.5	36.4
(36) *10,11-Epoxyiodovulone II*[10]	*10,11-epoxy-7E-enone*	6.23	6.82	7.2	0	3.88	2.69	149	125.8	141.9	130.4	188.6	29.7	67	77	35.4
(37) *12-O-acetyliodovulone II*[10]	*12-acetoxy-7E,10-dienone*	6.28	6.52	7.02	0	7.85	2.66	148.2	125.5	133.3	130.3	189.1	106.6	162.9	87.1	35.7
(38) *7-acetoxy-7,8-dihydroiodovulone I*[8]	*7-OAc,10-enone*	5.59	5.84	5.92	2.67	7.77	2.51	133.5	126.6	68	55.7	198.9	103.4	170.7	81	39.2
(39) *7-acetoxy-7,8-dihydroiodovulone II*[8]	*7-OAc,10-enone*	5.73	5.82	5.6	2.72	7.77	2.51	134.8	126.8	73.1	55.6	198.8	103.4	170.8	81	39.1

*^{13}C highlighted in green are corrected shifts based on TDDFT calculations.

Table S18. Published proton and carbon chemical shifts of pregnane steroids used to generate the PCA plots.

Name	***^{1}H-5***	***^{1}H-6***	***^{1}H-7***	***^{1}H-8***	***^{1}H-11***	***^{1}H-13***	***^{13}C-5***	***^{13}C-6***	***^{13}C -7***	***^{13}C -8***	***^{13}C -11***	***^{13}C -12***	***^{13}C -13***
*(**7**) pregna-1,4,20-trien-3-one*[11]	0	2.47	1.97	1.00	1.7	0	170	33.1	33.8	54.8	22.7	37.2	43.8
*(**8**) 18-acetyl-18-hydroxymethyl-1,4,20-pregnatrien-3-one*[12]	0	2.48	1.98	1.72	1.77	0	168.9	32.9	33.9	35.8	22.7	32.7	46.5
*(**40**) 15B-acetoxypregna-1,4,20-trien-3-one*[13]	0	2.46	1.98	1.73	1.78	0	168.5	32.7	33.7	35.6	22.5	32.5	46.3
*(**41**) 15B-hydroxypregna-1,4,20-trien-3-one*[13]	0	2.48	2.27	1.94	1.68	0	170.1	32.4	32.7	31.7	22.3	38.3	43.3
*(**42**) 4,20-pregnadien-1B-hydroxy-2a-chloro-3-one*[14]	0	2.35	1.88	1.62	1.58	0	170.7	33.8	32.7	36.3	24.0	37.8	43.5
*(**43**) 4,20-pregnadien-1B-hydroxy-2b-chloro-3-one*[14]	0	2.26	2.02	1.07	1.59	0	170.5	33.4	35.4	36.3	22.9	37.5	44.0
*(**44**) carijodienone*[15]	0	1.57	1.54	1.31	0.96	0	160.6	35.0	30.2	42.3	21.7	37.3	44.8
*(**45**) Pregna-1,4-dien-3-one, 20β-hydroxy-, acetate*[15]	0	2.45	1.96	1.65	1.74	0	169.3	32.9	33.7	35.4	22.8	38.9	42.5

Table S19 Chemical shift bins and bit string numbers used for HMBC fingerprinting matrix in **Figure 7A**

Carbon bin Number	^{13}C Bin range	
C1	33.4	36.7
C2	36.7001	37.3
C3	39.3	39.6
C4	52.2	53.2
C5	53.20001	57
C6	57.001	58
C7	66.4	71
C8	71.001	76.8
C9	76.8001	78.9
C10	82	85.5
C11	85.5001	90
C12	90.001	93.2
C13	138.5	143
C14	149	155.7
C15	155.7001	157
C16	157.001	159
C17	185	189
C18	190	198
C19	133	138

Proton Bin Number	^{1}H Bin range	
H1	1.7	2.37
H2	2.37001	2.5
H3	2.5001	2.7
H4	2.7001	2.8
H5	2.8001	2.9
H6	2.9001	3.97
H7	3.92	3.98
H8	5.05	5.65
H9	6.05	6.25
H10	6.25001	6.6
H11	7.15	7.39
H12	7.5	7.61
H13	7.75	7.85

Bitstring number	H/C coordinates
1	H1/C10
2	H1/C14
3	H1/C18
4	H1/C4
5	H1/C9
6	H10/C10
7	H10/C17
8	H10/C8
9	H10/C9
10	H11/C1
11	H11/C13
12	H11/C3
13	H11/C5
14	H11/C6
15	H12/C1
16	H12/C13
17	H12/C4
18	H13/C1
19	H13/C4
20	H2/C13
21	H2/C14
22	H2/C16
23	H2/C5
24	H3/C13
25	H3/C14
26	H3/C15

Bitstring number	H/C coordinates
27	H3/C6
28	H4/C13
29	H4/C14
30	H4/C15
31	H4/C16
32	H4/C5
33	H4/C6
34	H4/C7
35	H5/C13
36	H5/C14
37	H5/C4
38	H5/C7
39	H6/C1
40	H6/C13
41	H6/C14
42	H6/C4
43	H8/C10
44	H8/C11
45	H8/C18
46	H8/C9
47	H9/C10
48	H9/C17
49	H9/C18
50	H9/C8
51	H11/C2

Table S20 Chemical shift bins and bit string numbers used for HMBC fingerprinting in **Figure 15A**

Carbon bin Number	^{13}C Bin range (ppm)	
C1	33.4	36.7
C2	36.7001	37.3
C3	39.3	39.6
C4	52.2	53.2
C5	53.2001	57
C6	57.001	58
C7	66.4	71
C8	71.001	76.8
C9	76.8001	78.9
C10	82	85.5
C11	85.5001	90
C12	90.001	93.2
C13	138.5	143
C14	149	155.7
C15	155.7001	157
C16	157.001	159
C17	185	189
C18	190	198
C19	133	138

Proton Bin Number	^{1}H Bin range (ppm)	
H1	1.7	2.37
H2	2.37001	2.5
H3	2.5001	2.7
H4	2.7001	2.8
H5	2.8001	2.9
H6	2.9001	3.97
H7	3.92	3.98
H8	5.05	5.65
H9	6.05	6.25
H10	6.25001	6.6
H11	7.15	7.39
H12	7.5	7.61
H13	7.75	7.85

Bitstring numbers	H/C bin coordinates
1	H1/C10
2	H1/C14
3	H1/C18
4	H1/C4
5	H1/C9
6	H10/C10
7	H10/C17
8	H10/C8
9	H10/C9
10	H11/C1
11	H11/C13
12	H11/C3
13	H11/C5
14	H11/C6
15	H12/C1
16	H12/C13
17	H12/C4
18	H13/C1
19	H13/C4
20	H2/C13
21	H2/C14
22	H2/C16
23	H2/C5
24	H2/C7
25	H3/C13
26	H3/C14
27	H3/C15

Bitstring numbers	H/C coordinates
28	H3/C6
29	H3/C7
30	H4/C13
31	H4/C14
32	H4/C15
33	H4/C16
34	H4/C5
35	H4/C6
36	H4/C7
37	H5/C13
38	H5/C14
39	H5/C4
40	H5/C7
41	H6/C1
42	H6/C13
43	H6/C14
44	H6/C4
45	H8/C10
46	H8/C11
47	H8/C18
48	H8/C9
49	H9/C10
50	H9/C17
51	H9/C18
52	H9/C8
53	H11/C2

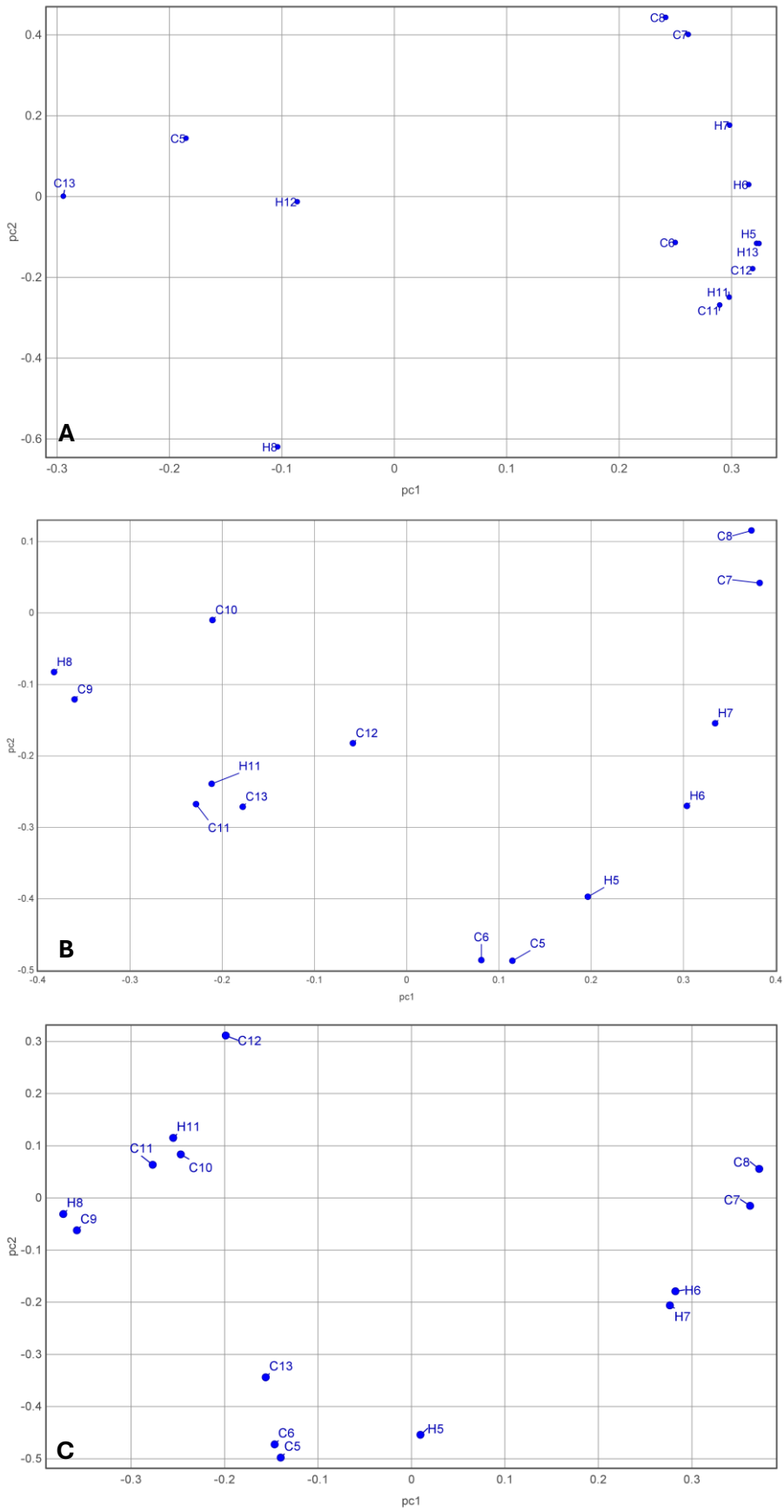


Figure S14. Loading plots of PCA's performed on the ^{1}H and ^{13}C resonances taken from the literature data. (A) pregnane steroids and halogenated prostanoids, (B) halogenated prostanoids, and (C) punaglandins.

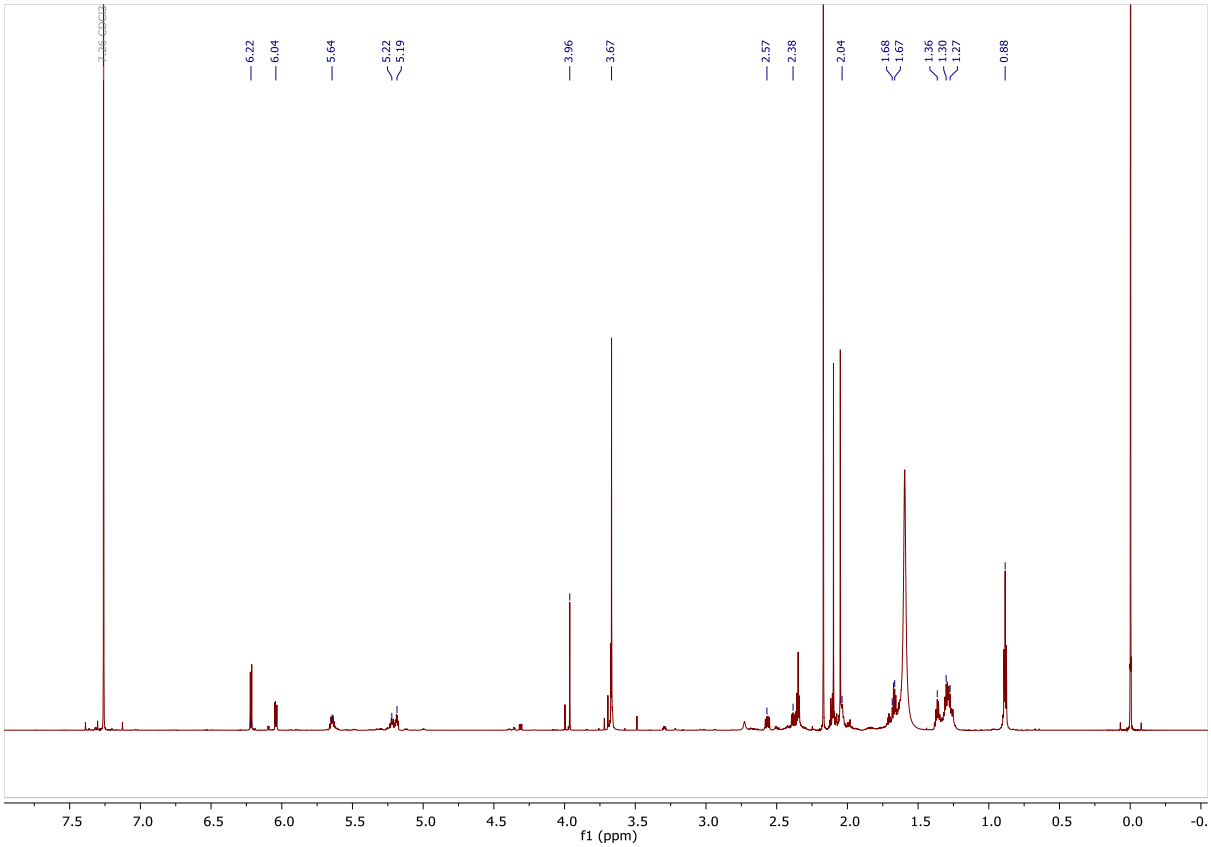


Figure S15. ^{1}H NMR spectrum (800 MHz) of **I** in $CDCl_3$.

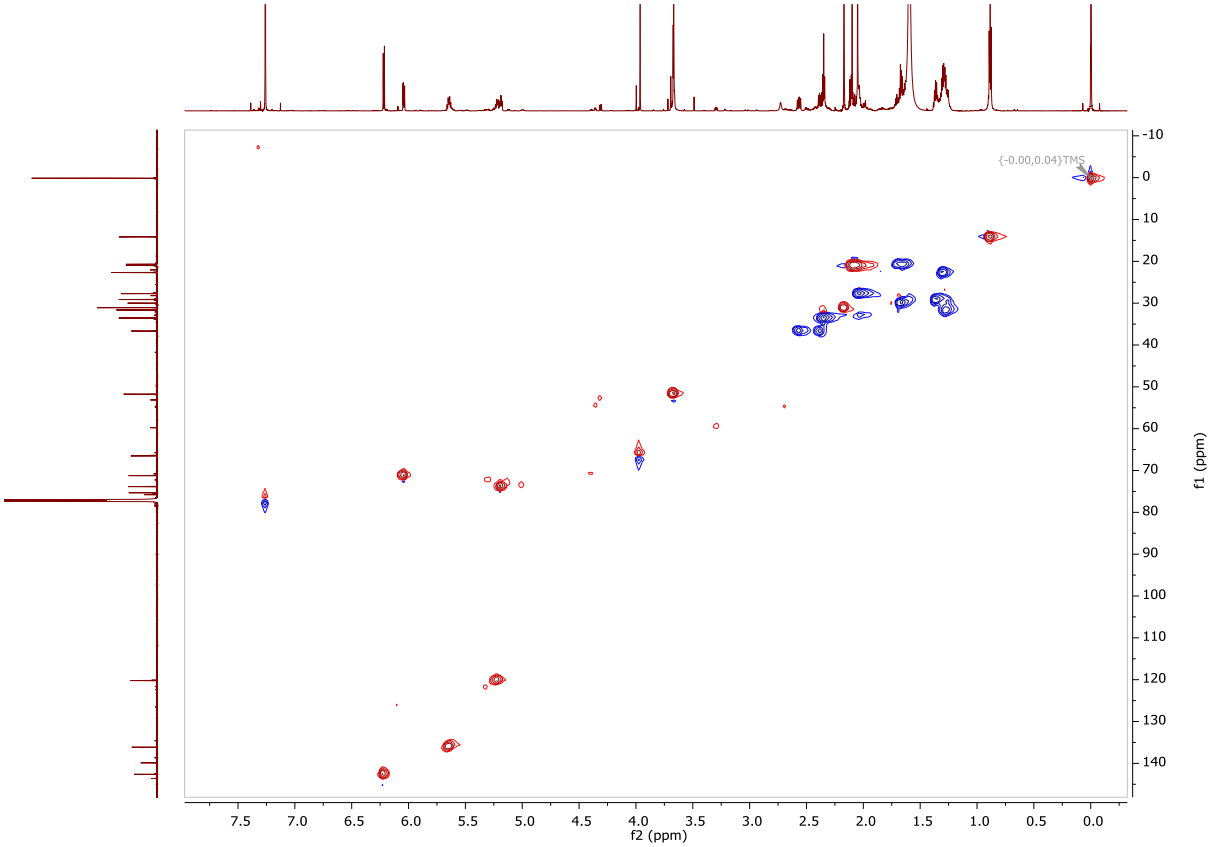


Figure S16. HSQC spectrum (800 MHz) of **I** in $CDCl_3$.

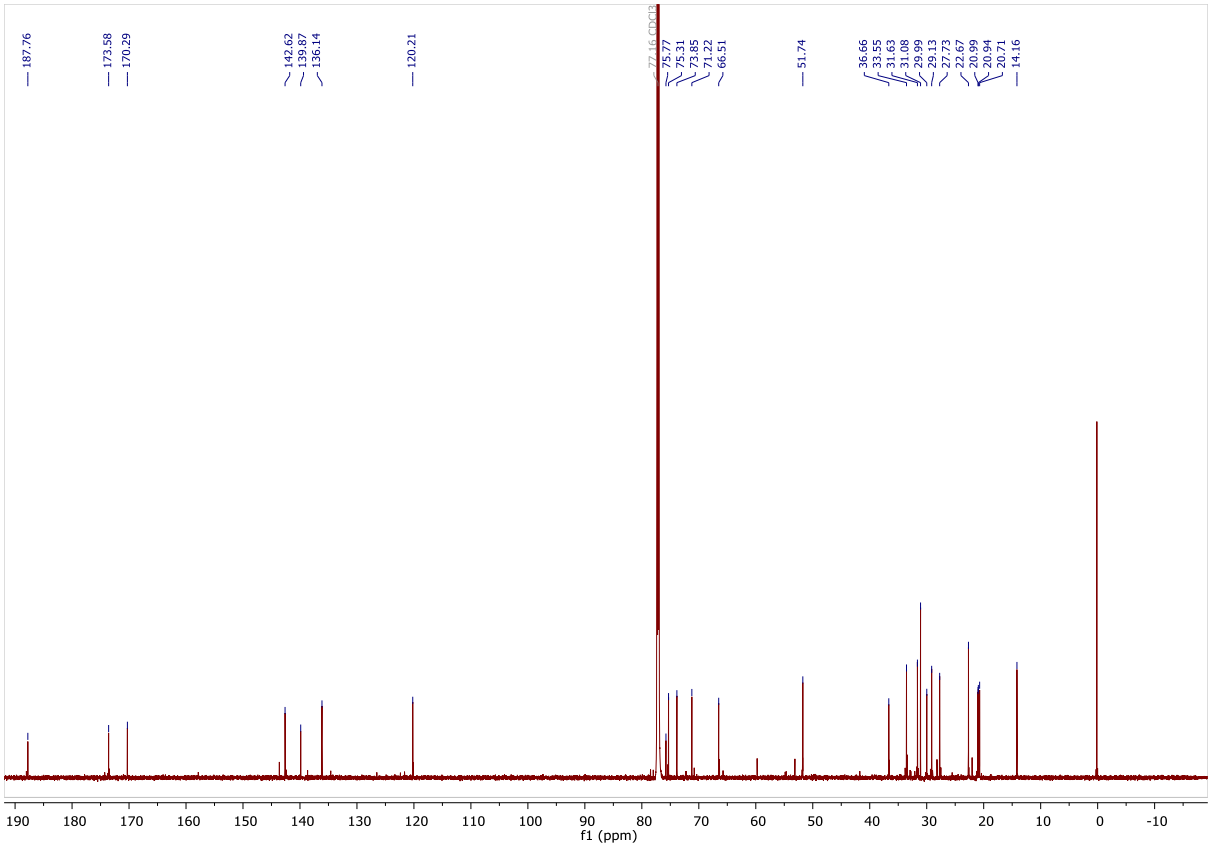


Figure S17. ^{13}C NMR spectrum (200 MHz) of **I** in $CDCl_3$.

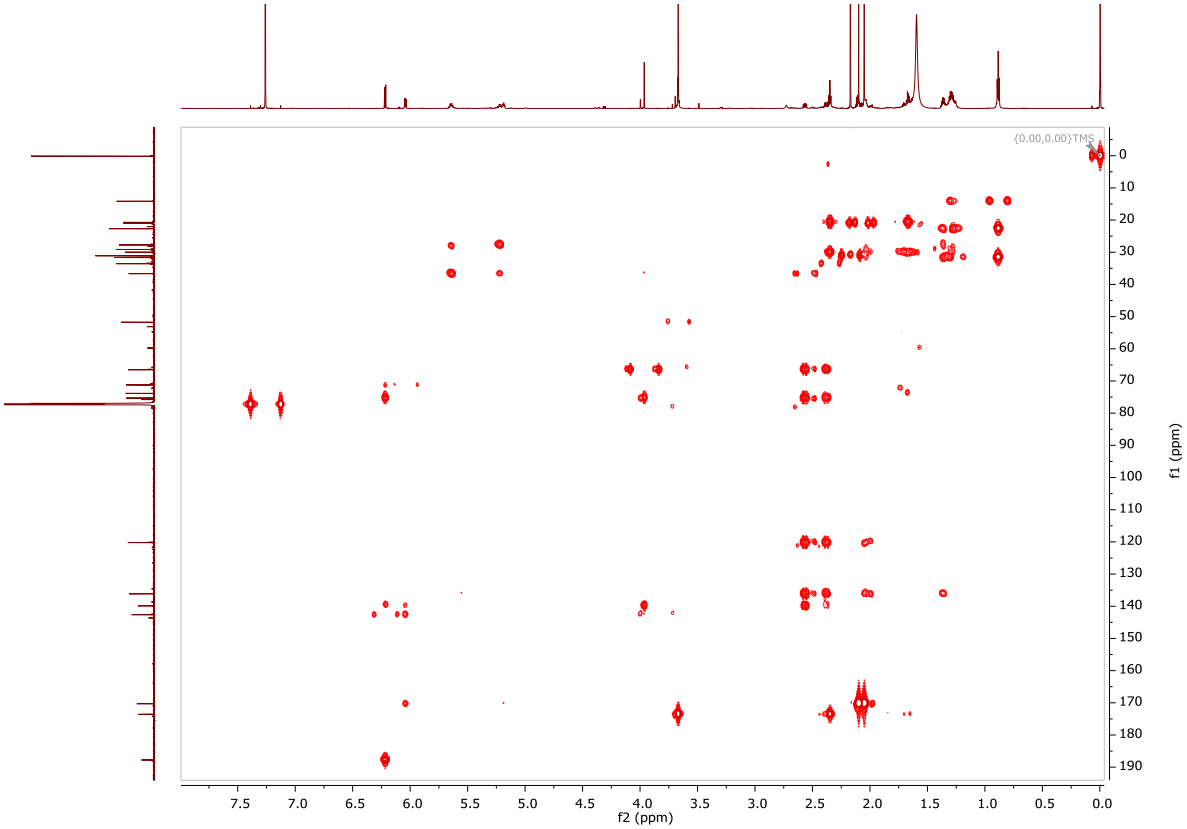


Figure S18. HMBC spectrum (800 MHz) of **I** in $CDCl_3$.

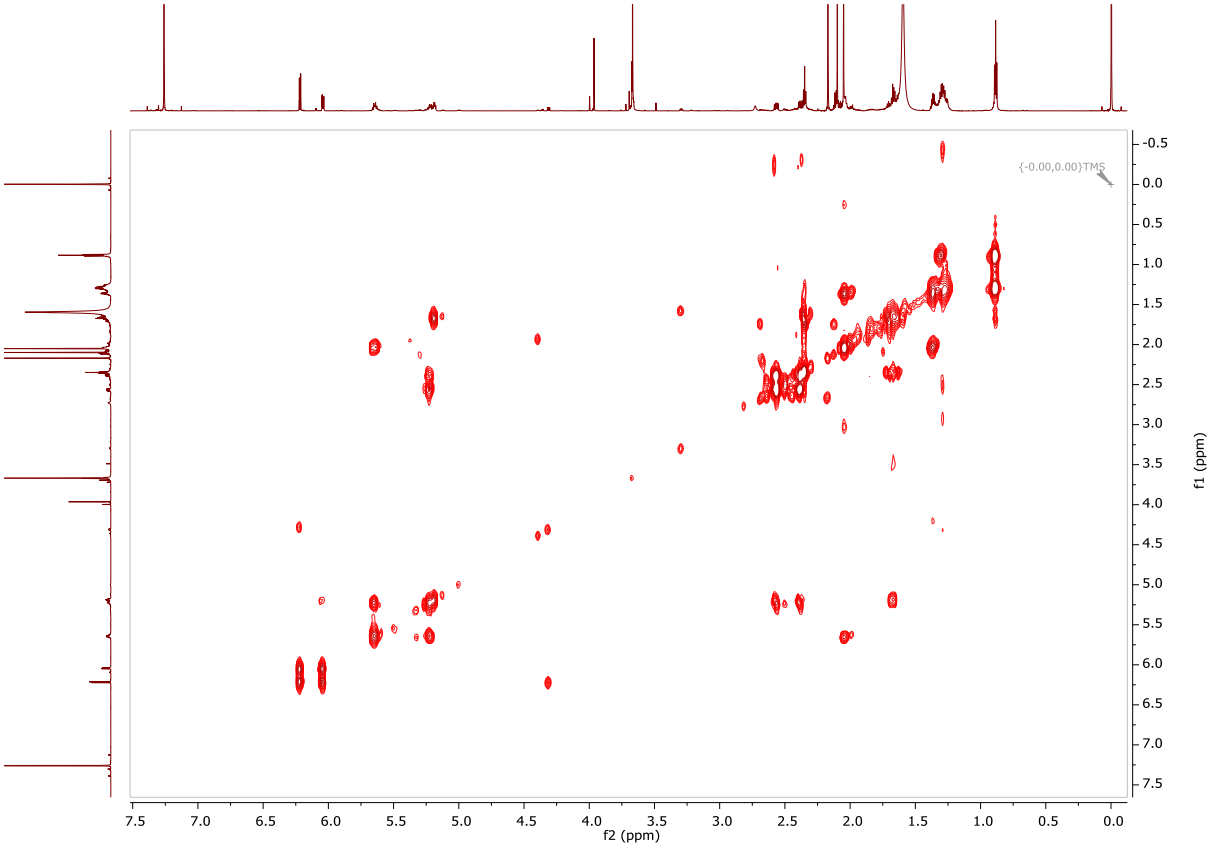


Figure S19. COSY spectrum (800 MHz) of **I** in $CDCl_3$.

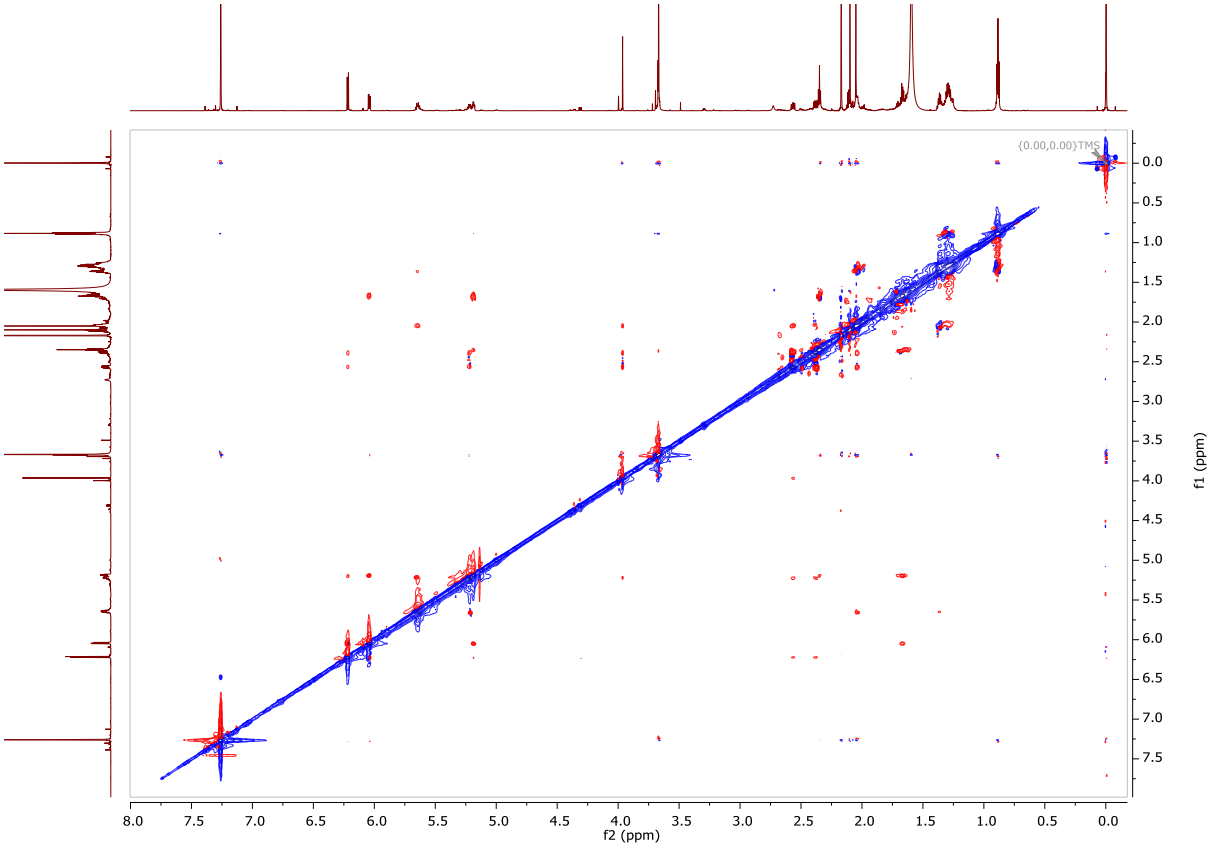


Figure S20. ROESY spectrum (800 MHz) of **I** in $CDCl_3$.

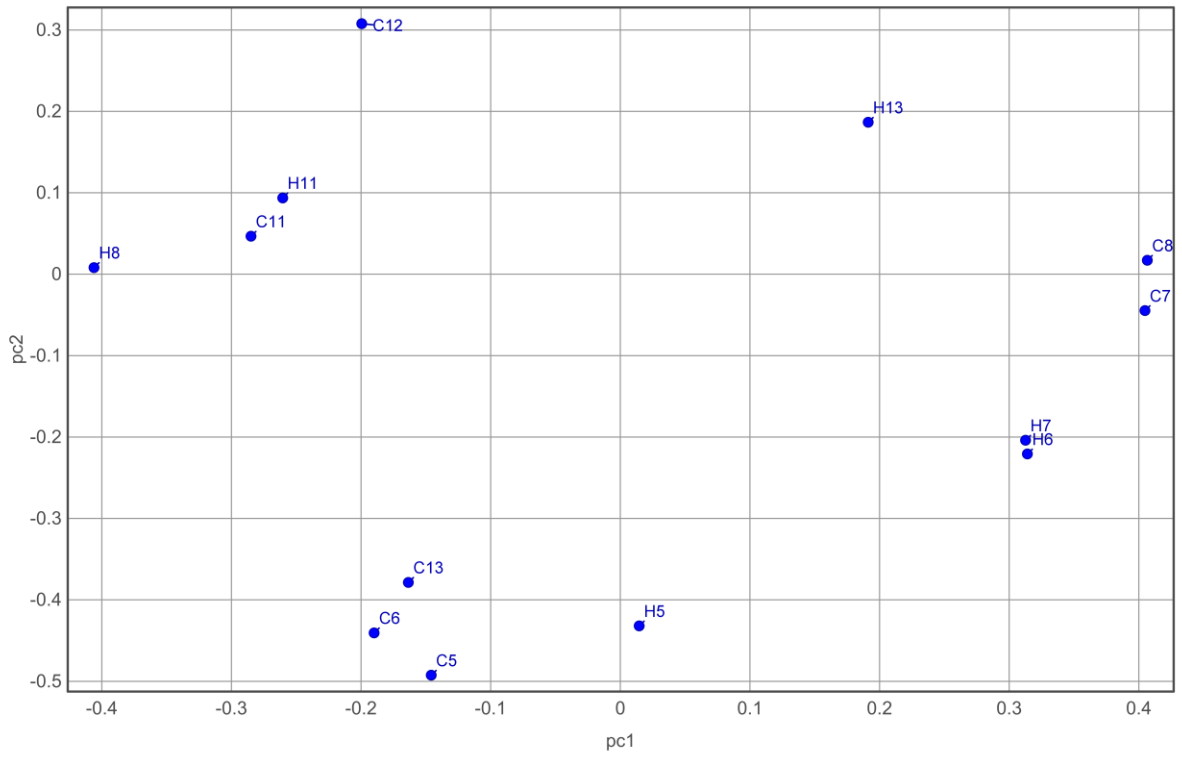


Figure S21. Loading plots of PCA's performed on the ^{1}H and ^{13}C resonances of punaglandins taken from the literature data and experimental data for the new compound 7Z-punaglandin 4 epoxide (**I**).

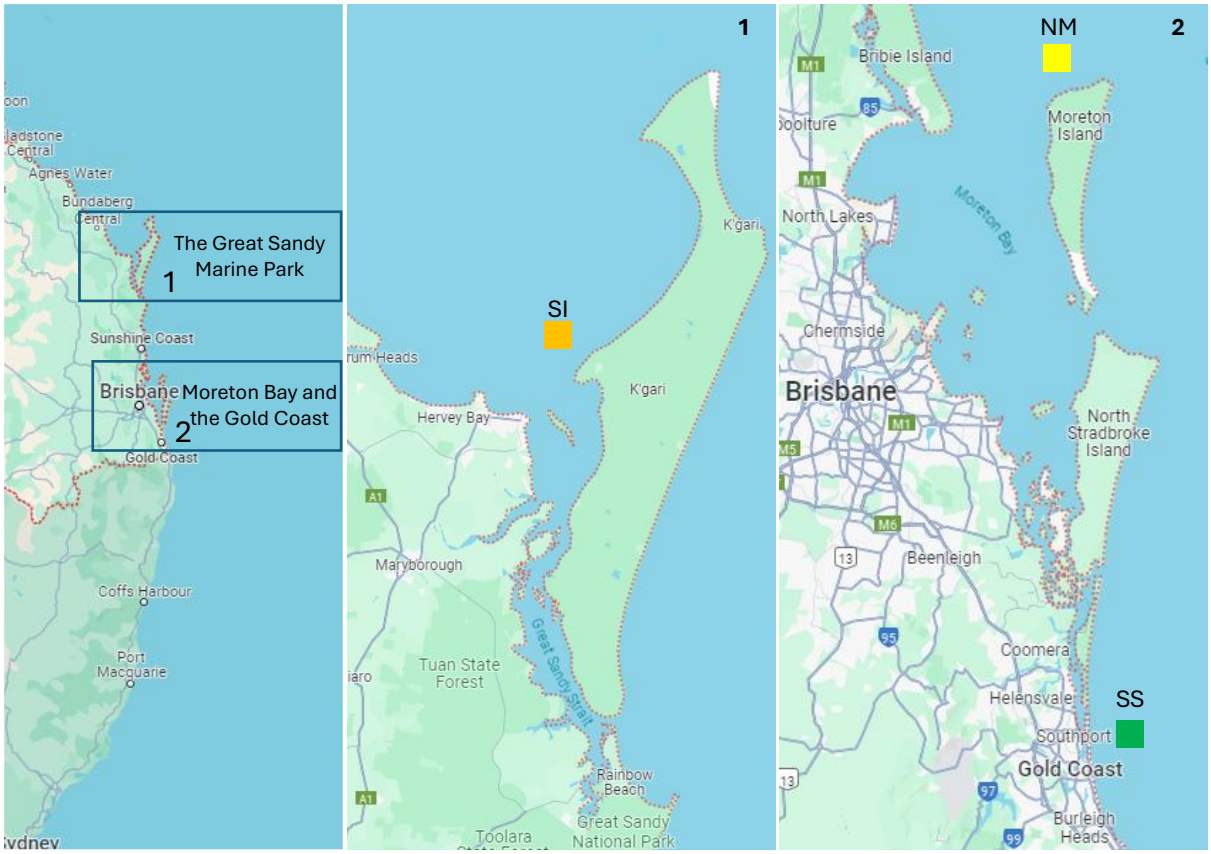


Figure S22. Map of artificial reef locations used for the collection of *C.riisei* extract in 1) the Great Sandy Marine Park (*SI:* Simpson AR), Moreton Bay (*NM:* North Moreton AR), and the Gold Coast (*SS:* South Stradbroke AR).

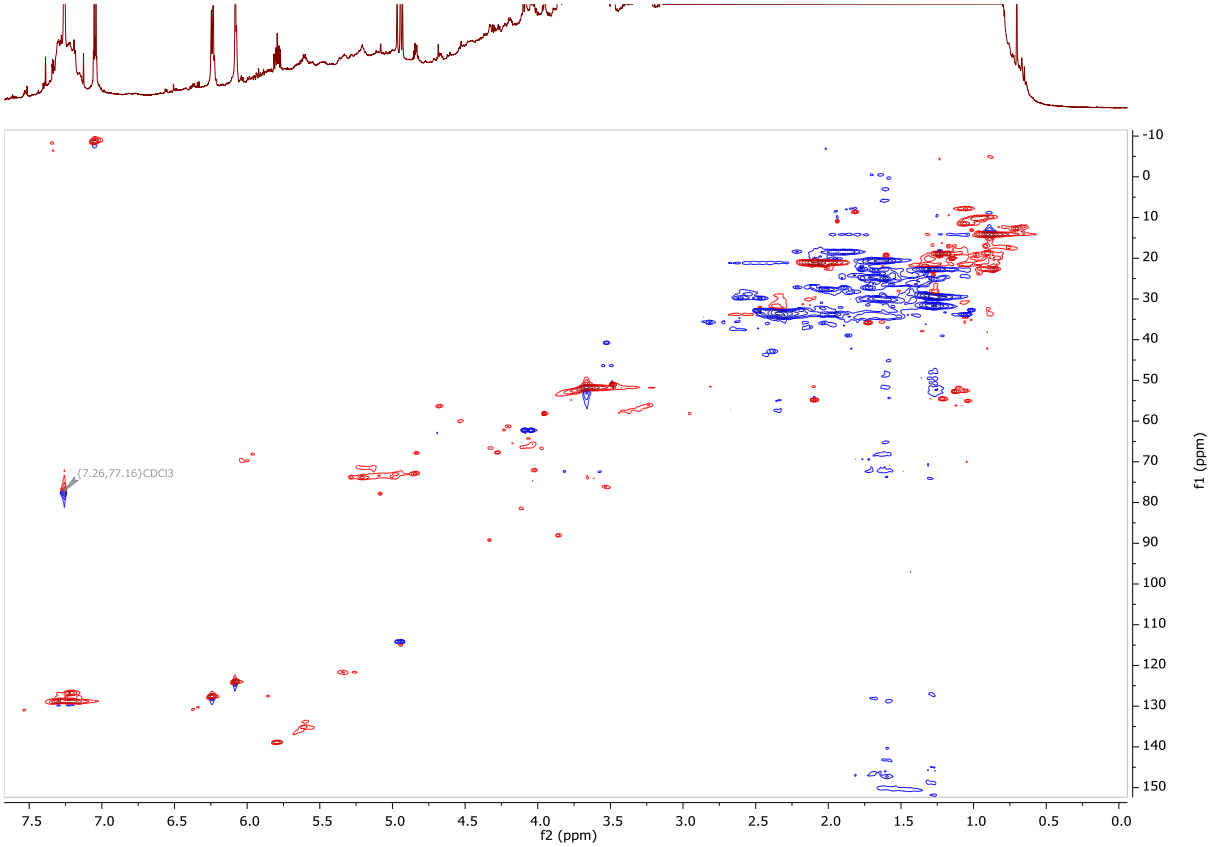


Figure S23. HSQC spectrum (800 MHz) of the SS extract (CH_2Cl_2) containing punaglandins in $CDCl_3$.

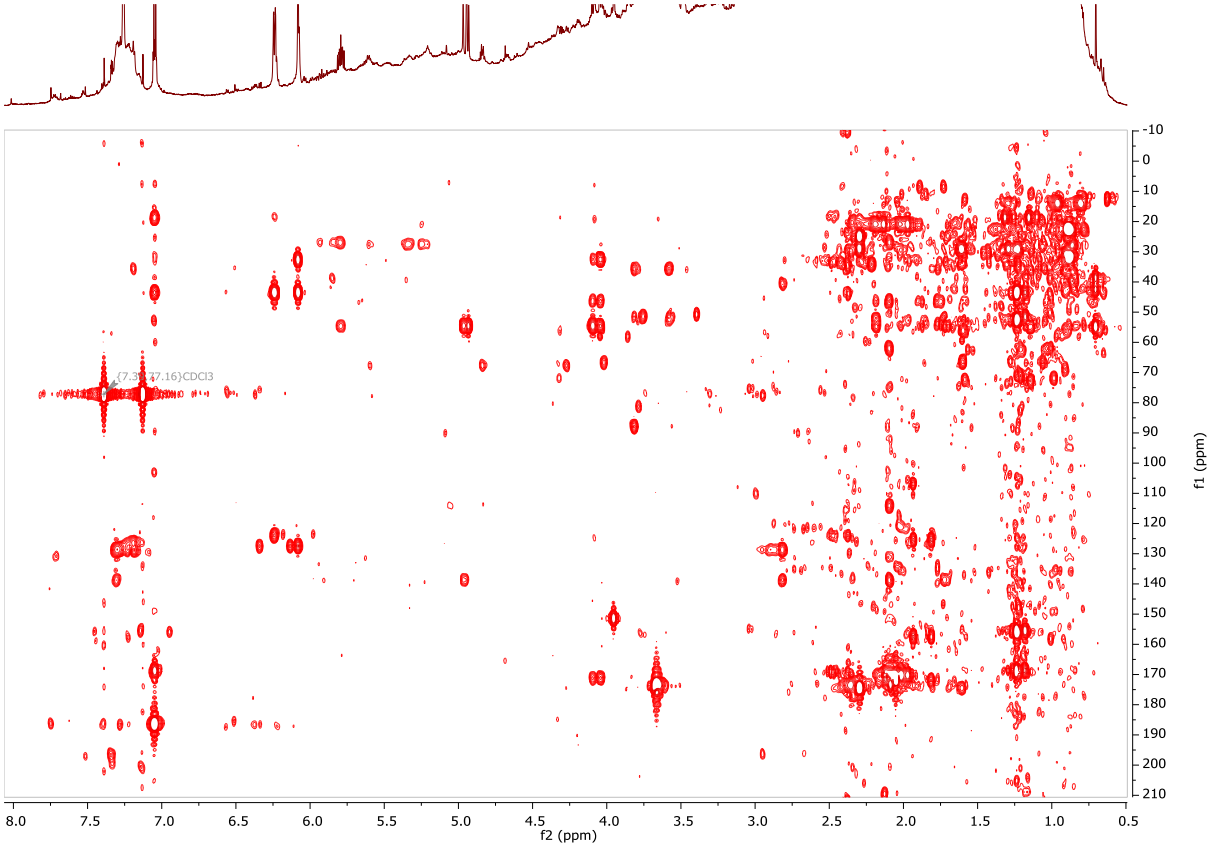


Figure S24. HMBC spectrum (800 MHz) of the SS extract (CH_2Cl_2) containing punaglandins in $CDCl_3$.

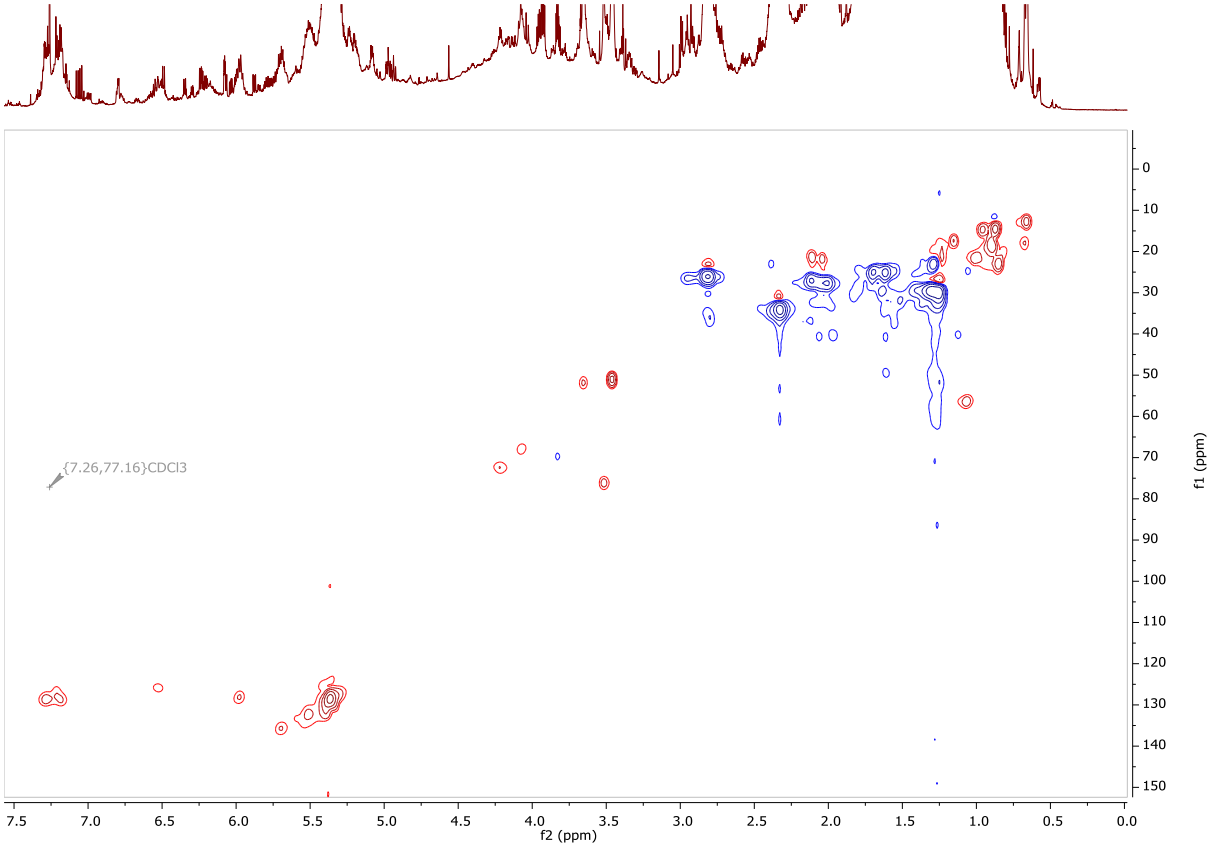


Figure S25. HSQC spectrum (800 MHz) of the SI extract (CH_2Cl_2) containing punaglandins in $CDCl_3$.

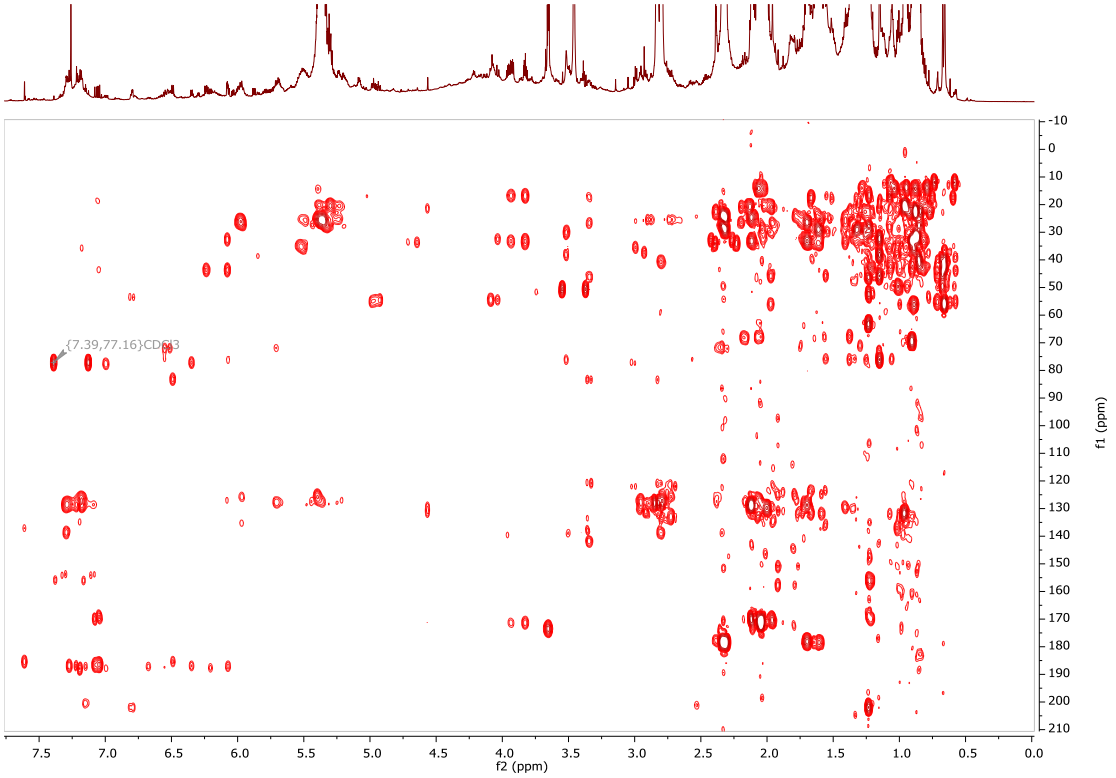


Figure S26. HMBC spectrum (800 MHz) of the SI extract (CH_2Cl_2) containing punaglandins in $CDCl_3$.

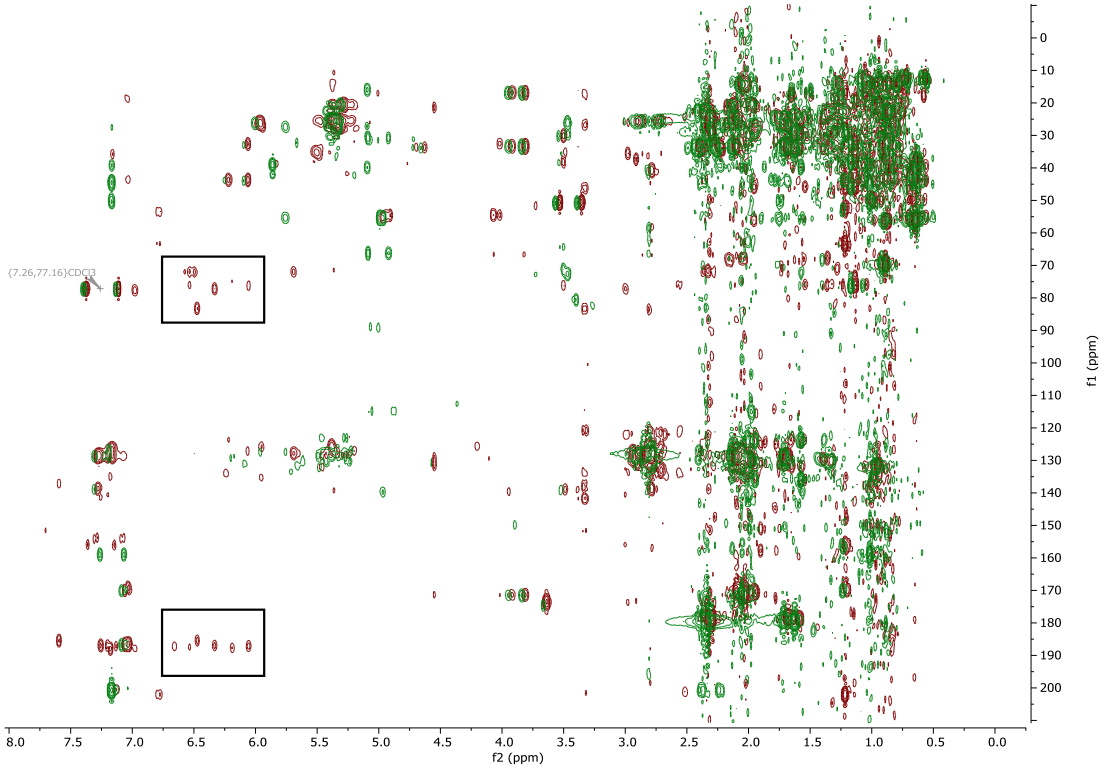


Figure S27. Overlay of HMBC spectra of DCM extracts from Simpson and North Moreton AR containing a mixture of punaglandins and pregnane steroids or only pregnane steroids. The Simpson extract (red) contains punaglandins and pregnane steroids, whereas the North Moreton extract (green) only contains pregnane steroids (green). Boxes highlight punaglandin chemical shifts.

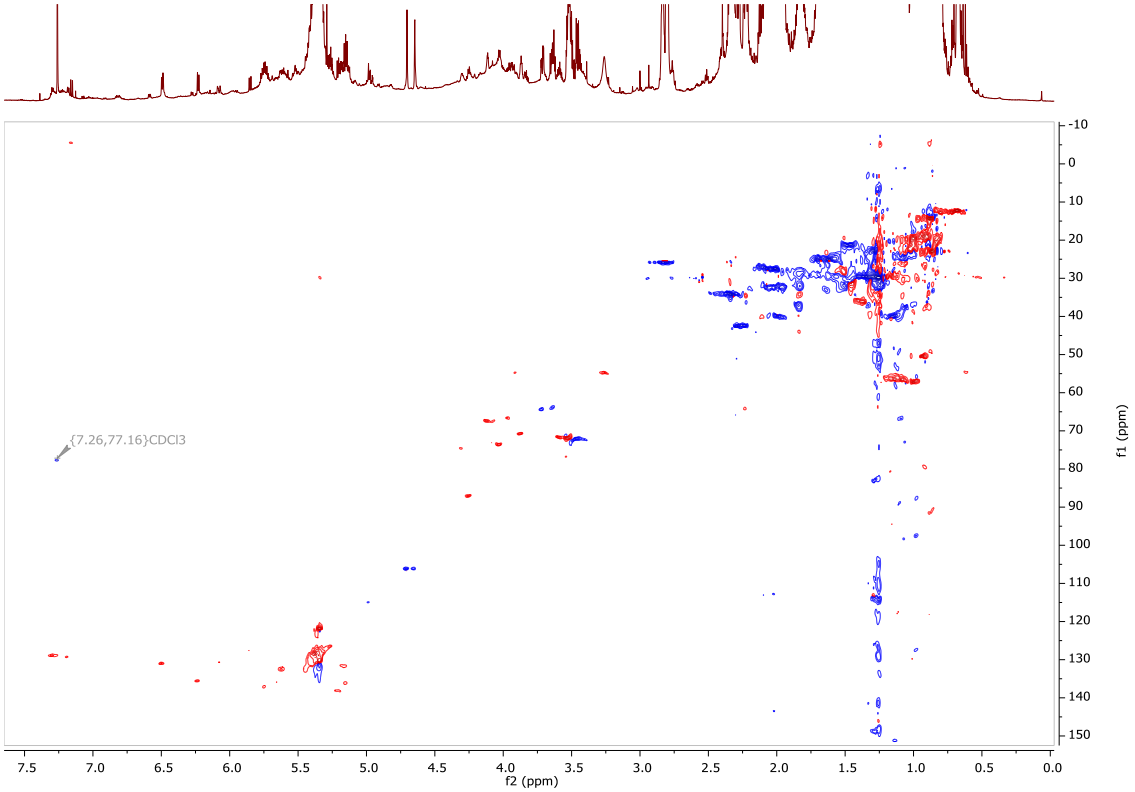


Figure S28. HSQC spectrum (800MHz) of SS_2 in $CDCl_3$.

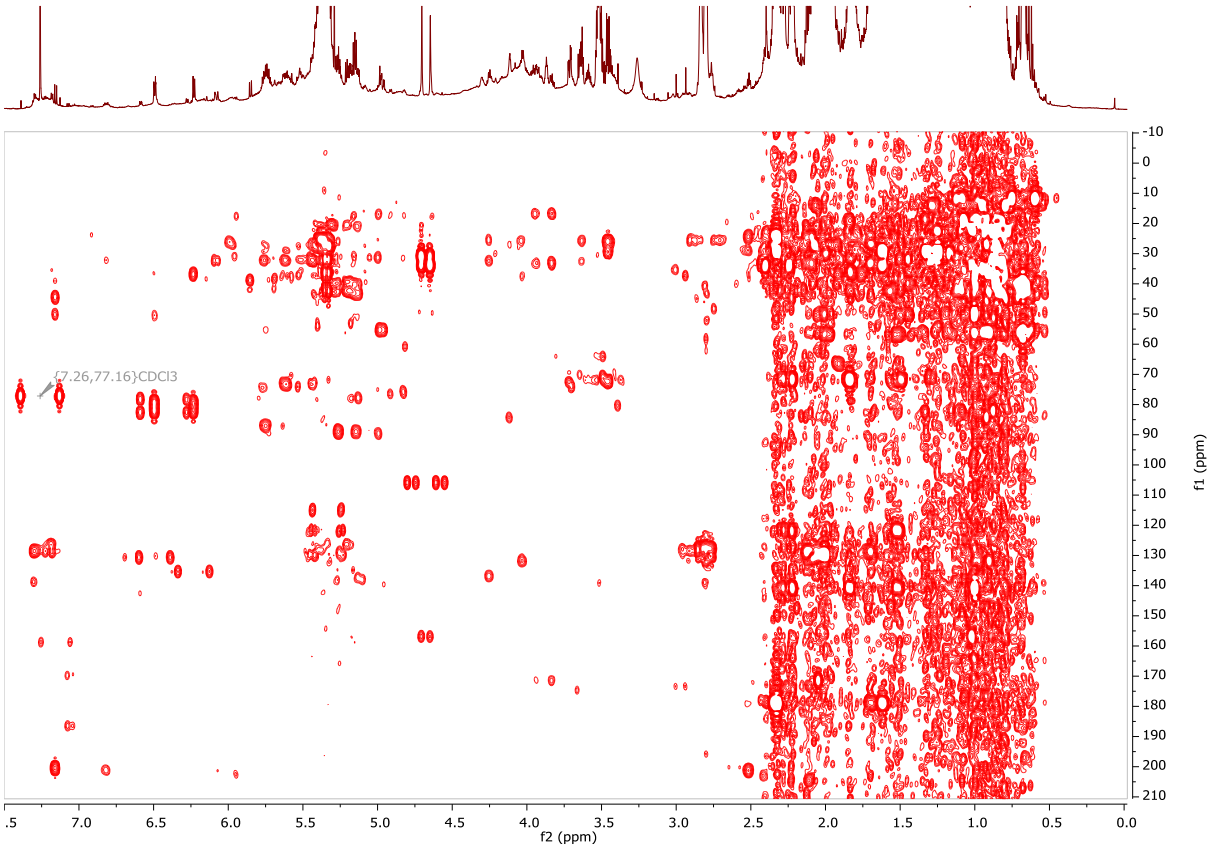


Figure S29. HMBC spectrum (800MHz) of SS_2 in $CDCl_3$.

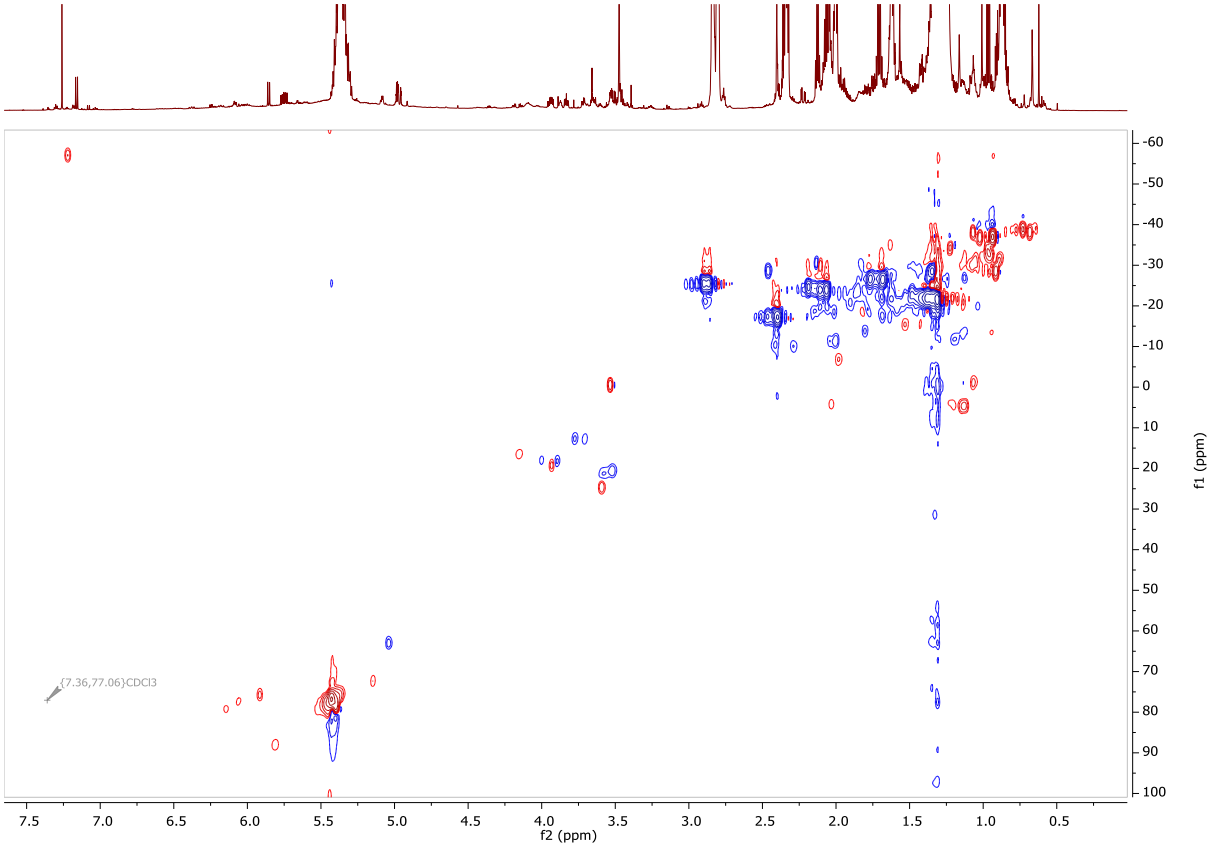


Figure S30. HSQC spectrum (800MHz) of SI_2 in $CDCl_3$

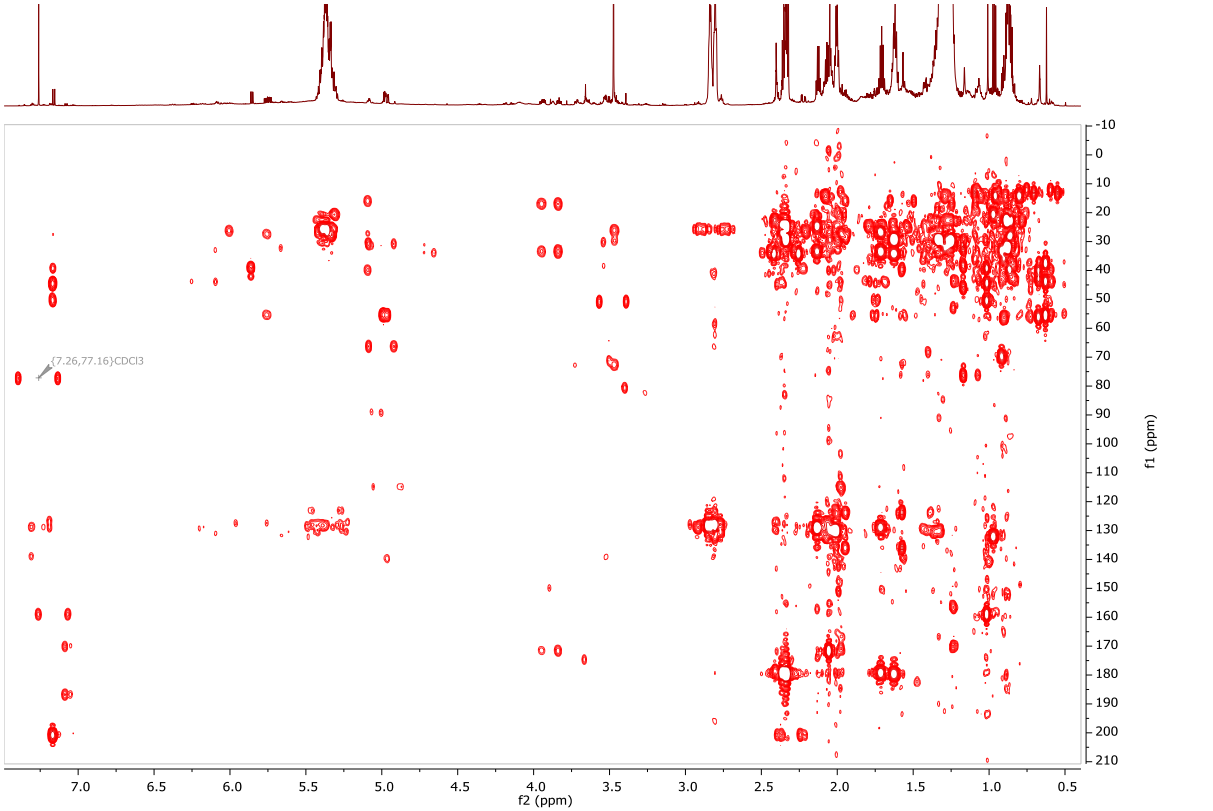


Figure S31. HMBC spectrum (800MHz) of SI_2 in $CDCl_3$

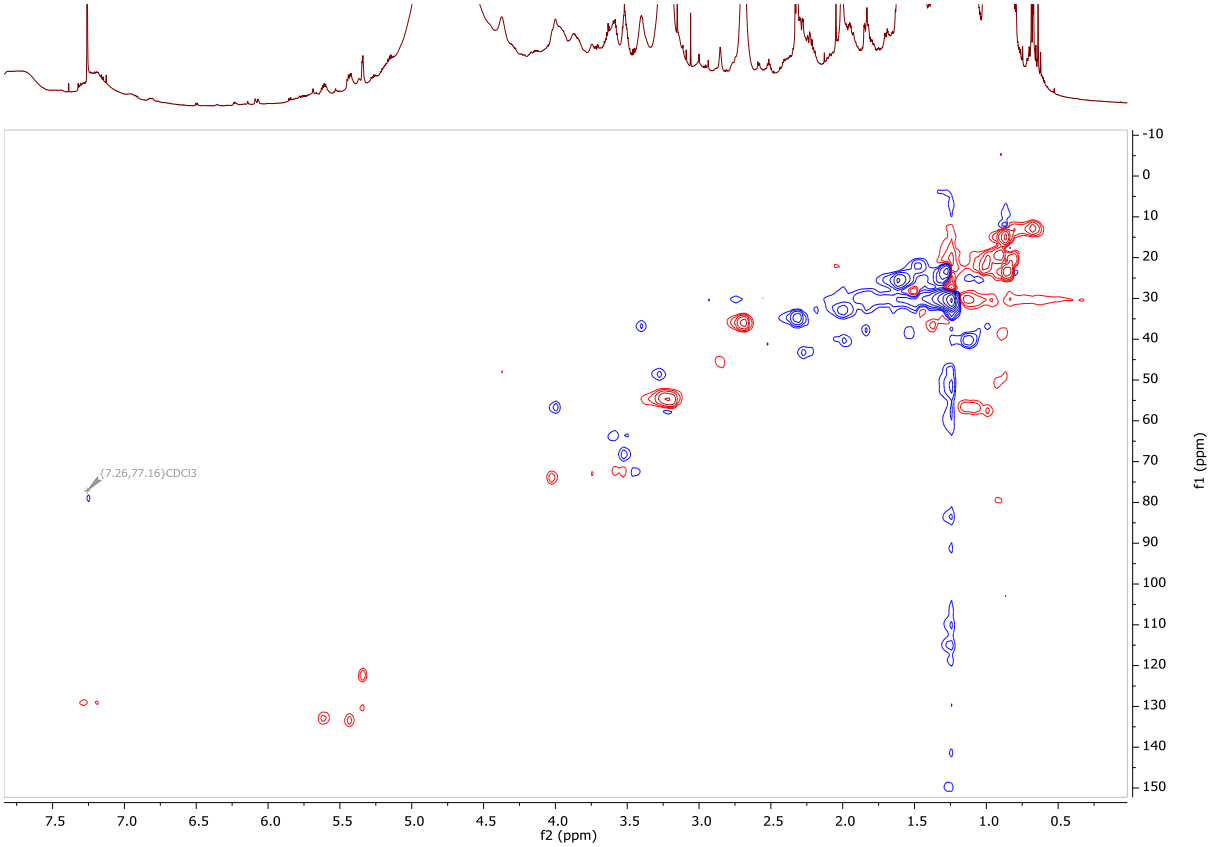


Figure S32. HSQC spectrum (800MHz) of NM in $CDCl_3$.

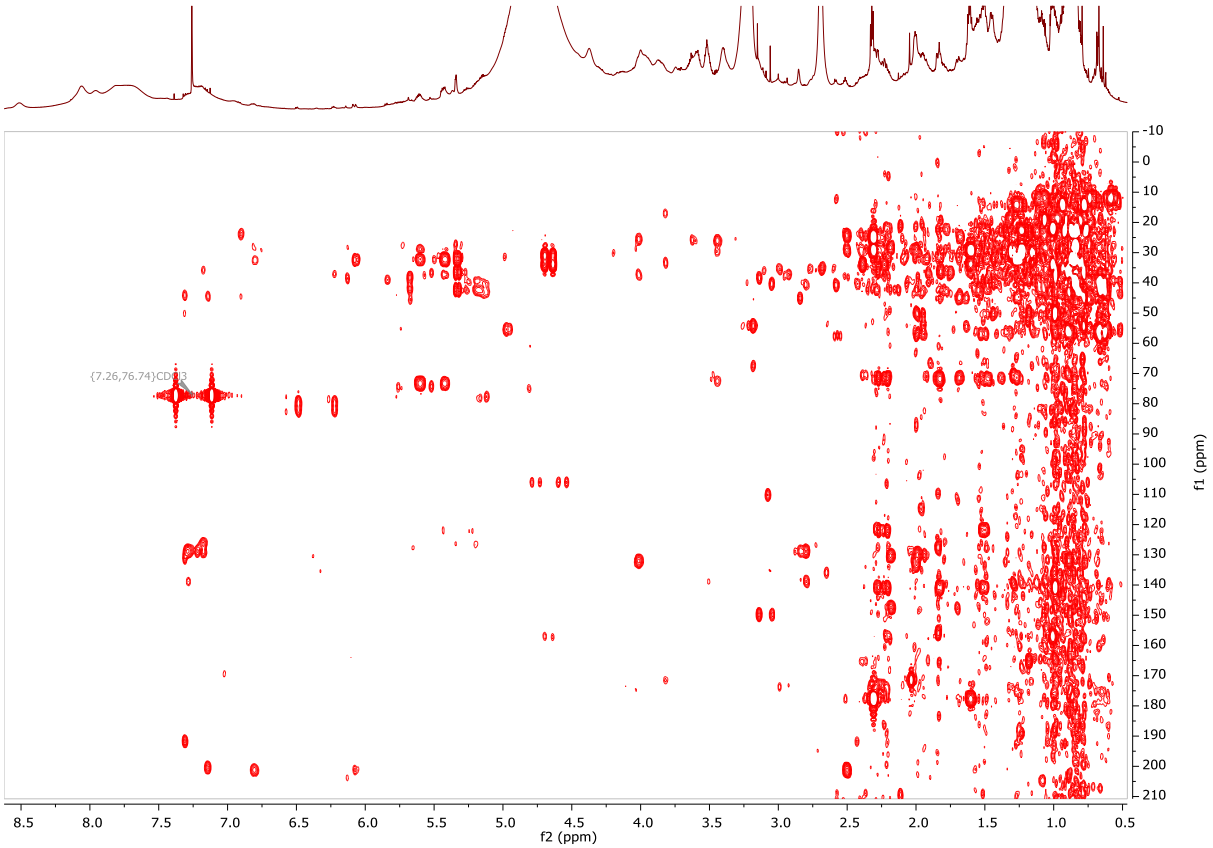


Figure S33. HMBC spectrum (800MHz) of NM in $CDCl_3$.

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