Supporting Information

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Nocardiopyrone C, a New Antimicrobial Pyran-2-one Derivative from a Marine-derived Actinomycete Strain *Nocardiopsis aegyptia* ZSN1

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S1:Experimental Section

General experimental procedures

Optical rotation and UV spectrum were measured on an AUTOPOL I digital polarimeter (Rudolph Research Analytical) and a Shimadzu UV-1800 (SHIMADZU, Japan), respectively. IR and electronic circular dichroism (ECD) spectra were acquired on a Thermo Scientific Nicolet iS10 FT-IR spectrometer and a JASCO J-1500-150ST spectrophotometer, respectively. HRESIMS data were obtained from a 6230 Time of Flight Liquid Chromatography/Mass Spectrometry (TOF LC/MS) spectrometer. 1D and 2D NMR data were recorded on a JEOL 600 NMR spectrometer (JEOL, Tokyo, Japan). Silica gel (100–200 mesh or 300-400 mesh, Qingdao Ocean Chemical Company, Qingdao, China) and Sephadex LH-20 (Amersham Pharmacia Biotech) were used for column chromatography, and further purified by preparative HPLC (SHIMAZU LC-20AP) equipped with an Agilent Pursuit C-18 column (10 μm, 21.2×250 mm). All solvents used in this study were purchased from the Shanghai Sinopharm Chemical Reagent Co., Ltd. *Escherichia coli* (ATCC 25922), *Staphylococcus aureus* (ATCC 43300), and *Candida albicans* (ATCC 10231) were gifts from Dr. Zhongjun Ma. Ampicillin (99.6%) and amphotericin B (99.0%) were ordered from Sigma-Aldrich. Components were detected by TLC under UV light (254 or 365 nm), and spots were visualized by heating silica-gel plates sprayed with 8-10% H_2SO_4 in ethyl alcohol.

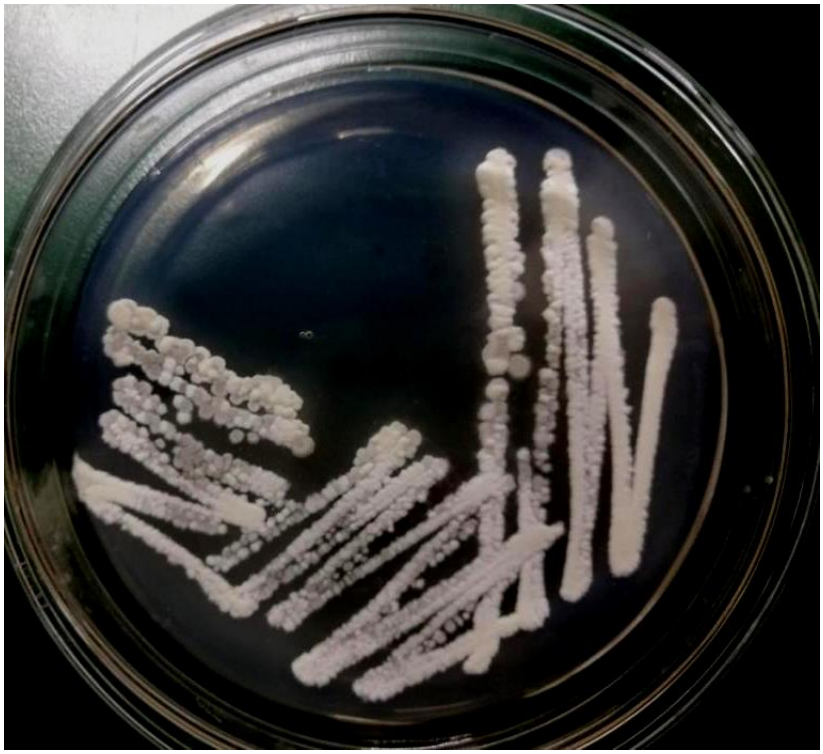

Figure S1: Colonies of *Nocardiopsis aegyptia* ZSN1

CAGGCTCAGGACGAACGCTGGCGGCGTGCTTAACACATGCAAGTCGAGCGGTAAGGCCCTTCGGGGTACAC
GAGCGGCGAACGGGTGAGTAACACGTGAGCAACCTGCCCCTGACTCCGGGATAAGCGGTGGAAACGCCGT
CTAATACCGGATACGACCTGTCACCTCATGGTGGCGGGTGGAAAGTTTTTCGGTCGGGGATGGGCTCGCGGC
CTATCAGCTAGTTGGTGGGGTAAAGGCCTACCAAGGCGATTACGGGTAGCCGGCCTGAGAGGGCGACCGGC
CACACTGGGACTGAGACACGGCCCAGACTCCTGCGGGAGGCAGCAGTGGGGAATATTGCGCAATGGGCGAA
AGCCTGACGCAGCGACGCCGCGTGGGGGATGACGGCCTTCGGGTTGTAAACCTCTTTTACCACCAACGCAG
GCTCCCAGTTCTCTGGGGGTTGACGGTAGGTGGGGAATAAGGACCGGCTAACTACGTGCCAGCAGCCGCGG
TAATACGTAGGGTCCGAGCGTTGTCCGGAATTATTGGGCGTAAAGAGCTCGTAGGCGGCGTGTCGCGTCTGC
TGTGAAAGACCGGGGCTTAACTCCGGTTCTGCAGTGGATACGGGCATGCTAGAGGTAGGTAGGGGAGACTG
GAATTCCTGGTGTAGCGGTGAAATGCGCAGATATCAGGAGGAACACCGGTGGCGAAGGCGGGTCTCTGGGC
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CGTTGGGCGCTAGGTGTGGGGACTTTCCACGGTTTCCGCGCCGTAGCTAACGCATTAAGCGCCCCGCCTGGG
GAGTACGGCCGCAAGGCTAAAACTCAAAGGAATTGACGGGGGCCCGCACAAGCGGCGGAGCATGTTGCTTA
ATTCGACGCAACGCGAAGAACCTTACCAAGGTTTGACATCACCCGTGGACCTGCAGAGATGTGGGGTCATTT
AGTTGGTGGGTGACAGGTGGTGCATGGCTGTCGTCAGCTCGTGTCGTGAGATGTTGGGTTAAGTCCCGCAAC
GAGCGCAACCCTTATTCCATGTTGCCAGCACGTAGTGGTGGGGACTCATGGGAGACTGCCGGGGTCAACTCG
GAGGAAGGTGGGGACGACGTCAAGTCATCATGCCCCTTATGTCTTGGGCTGCAAACATGCTACAATGGCCGG
TACAATGGGCGTGCGATACCGTAAGGTGGAGCGAATCCCTAAAAGCCGGTCTCAGTTCGGATTGGGGTCTGC
AACTCGACCCCATGAAGGTGGAGTCGCTAGTAATCGCGGATCAGCAACGCCGCGGTGAATACGTTCCCGGGC
CTTGTACACACCGCCCGTCACGTCATGAAAGTCGGCAACACCCGAAACTTGTGGCCTAACCCTTCGGGG

Figure S2: 16S rDNA sequence of *Nocardiopsis aegyptia* ZSN1

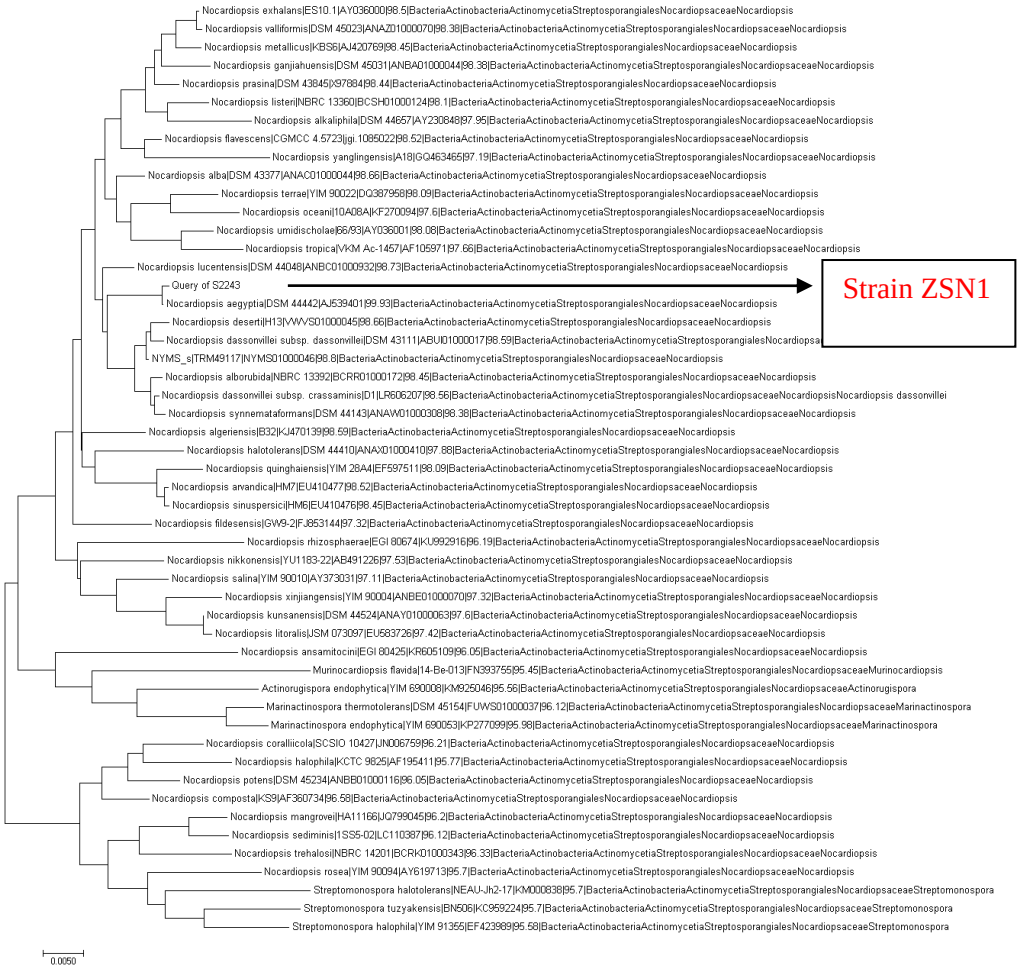

Figure S3: Evolutionary relationships of *Nocardiopsis aegyptia* ZSN1 (The evolutionary history was inferred using the Neighbor-Joining method)

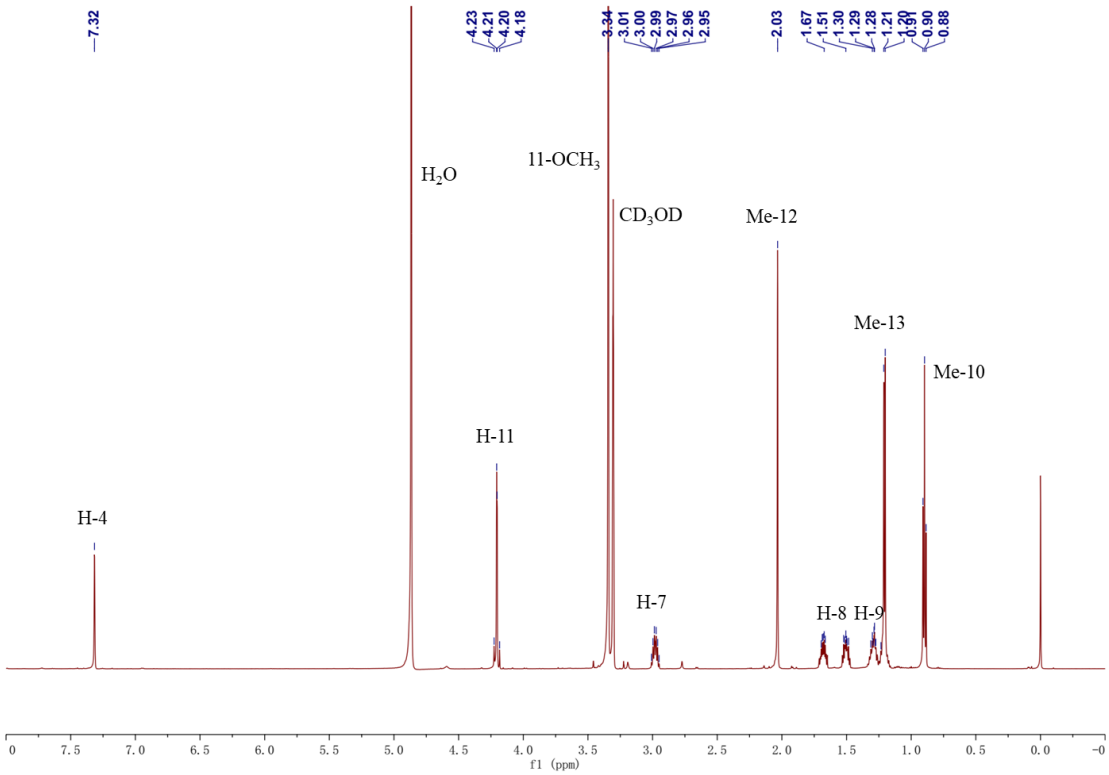

Figure S4: [1]H NMR spectrum of compound **1** in Methanol-*d*$_4$

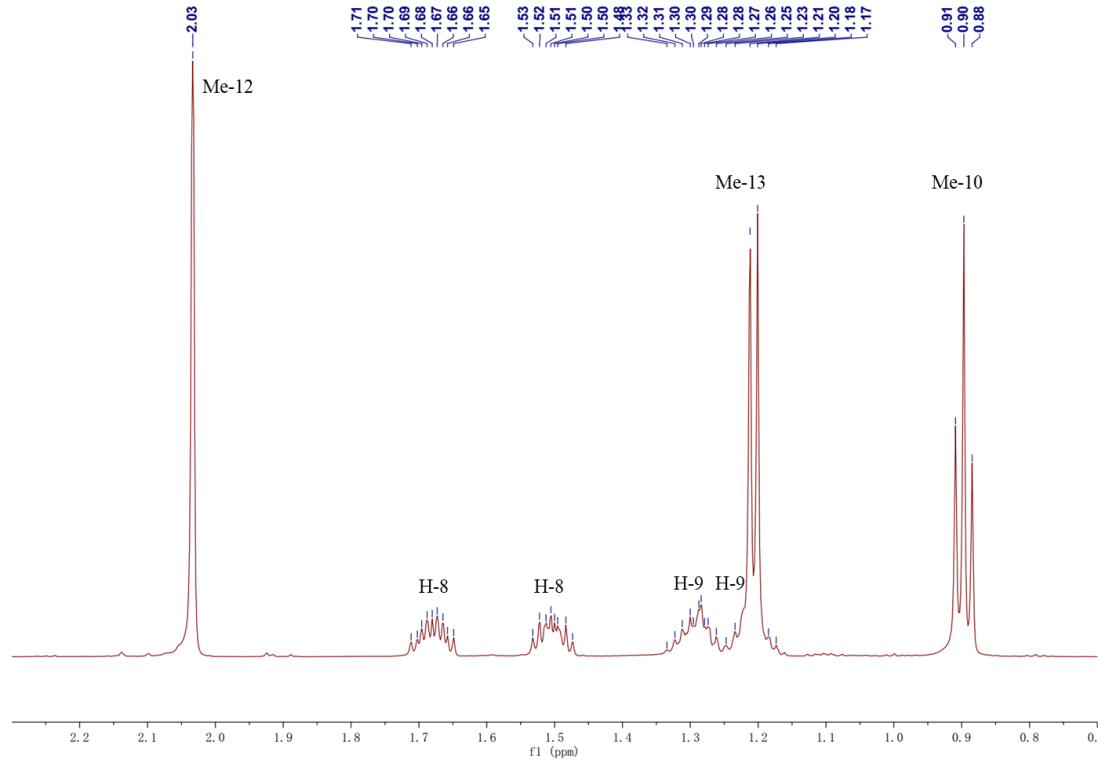

Figure S5: Enlarge [1]H NMR spectrum of compound **1** in Methanol-*d*$_4$

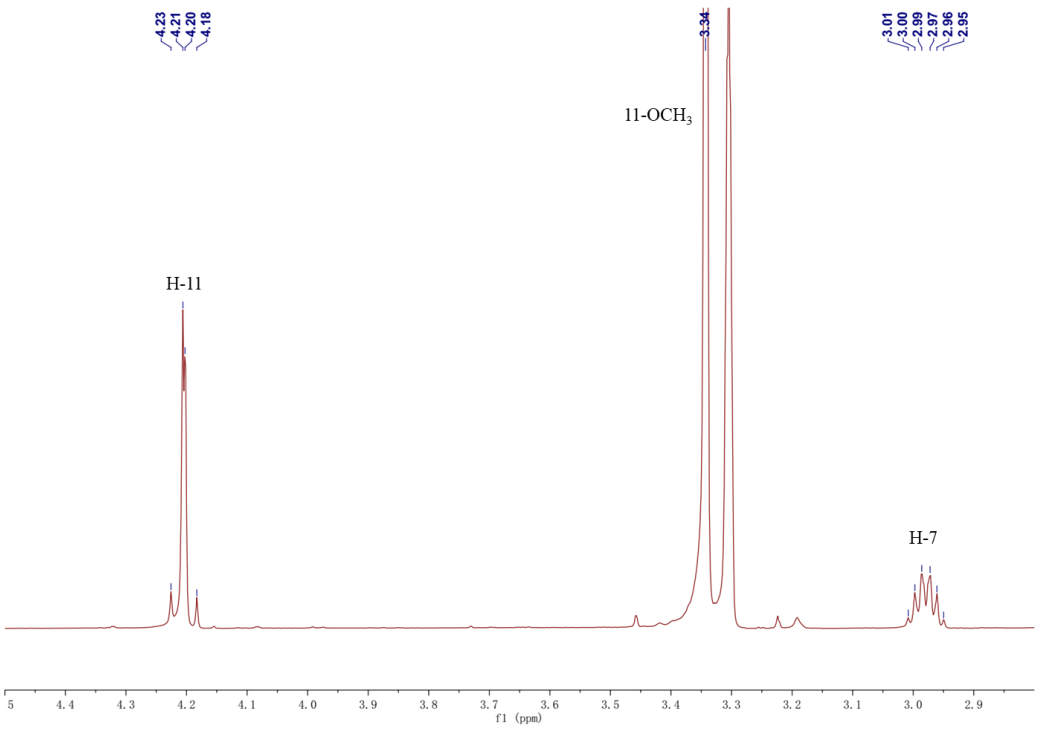

Figure S6: Enlarge ^{1}H NMR spectrum of compound **1** in Methanol-d_4

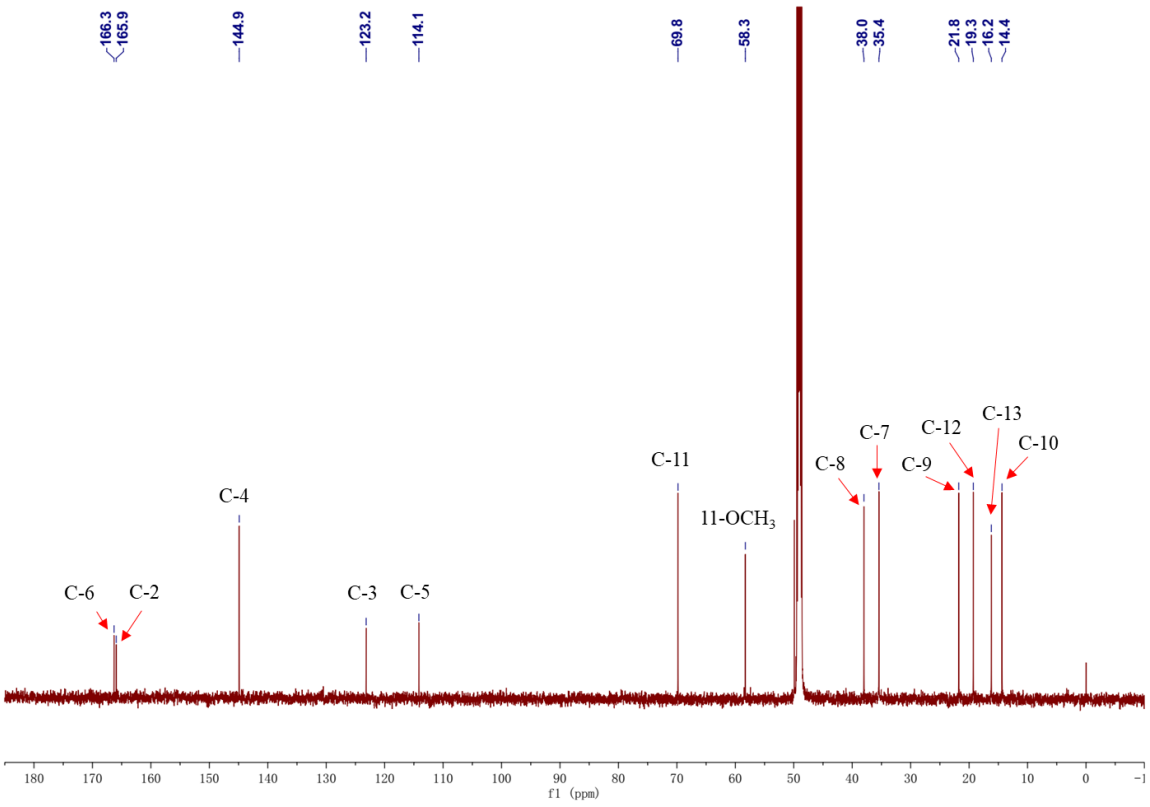

Figure S7: ^{13}C NMR spectrum of compound **1** in Methanol-d_4

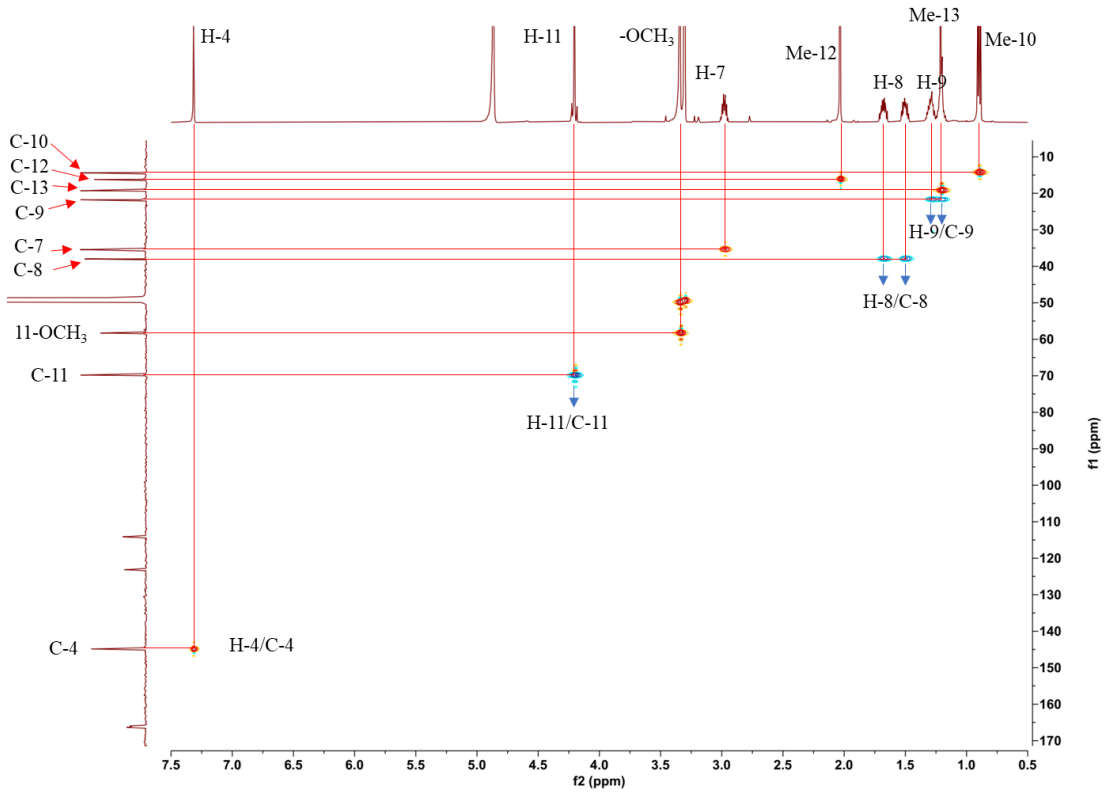

Figure S8: HSQC spectrum of compound **1** in Methanol-d_4

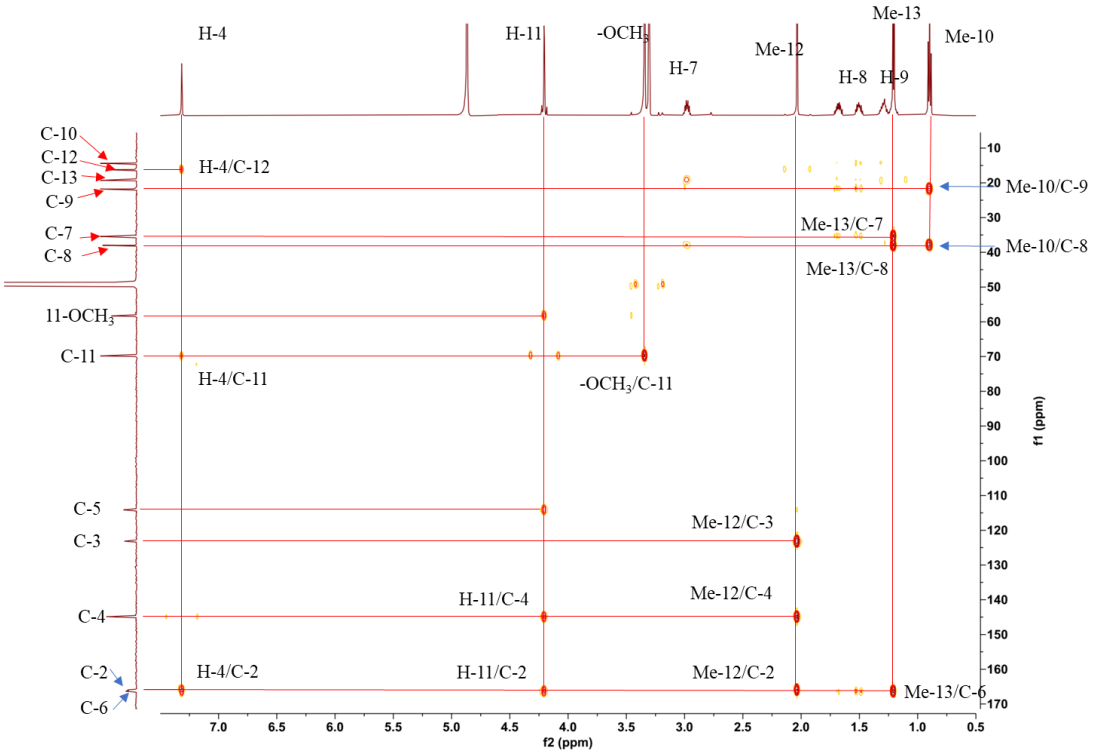

Figure S9: HMBC spectrum of compound **1** in Methanol-d_4

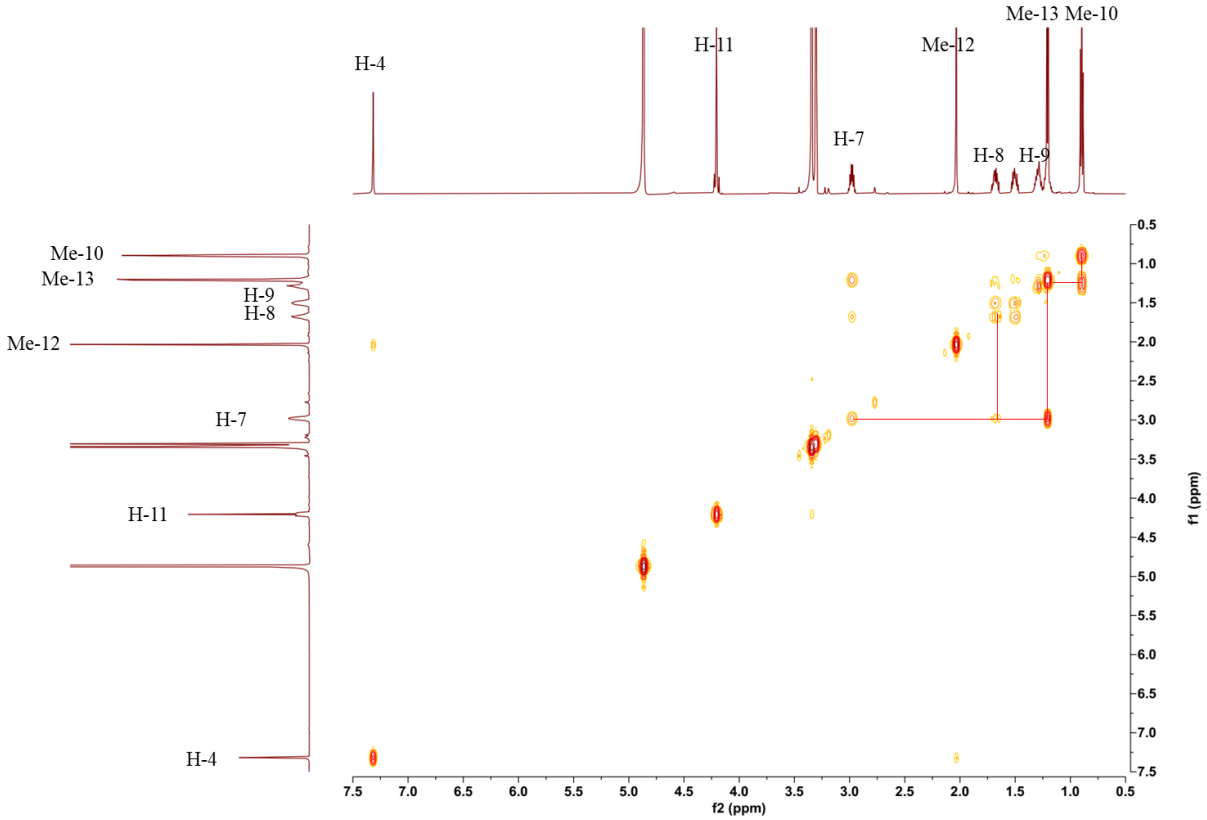

Figure S10: ^{1}H-^{1}H COSY spectrum of compound **1** in Methanol-d_4

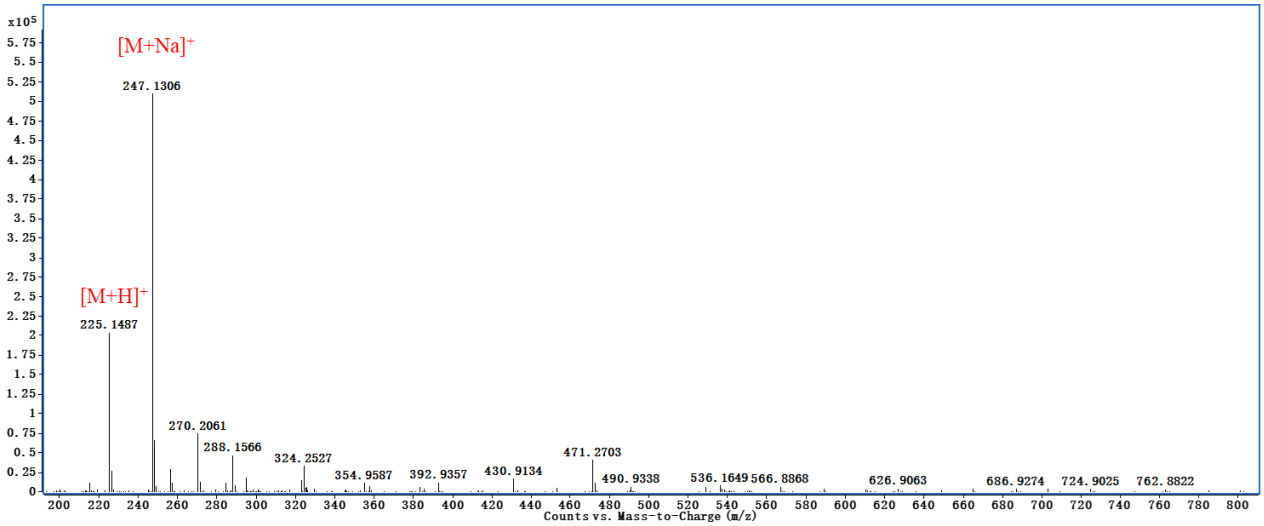

Figure S11: HR-ESI-MS spectrum of compound **1**

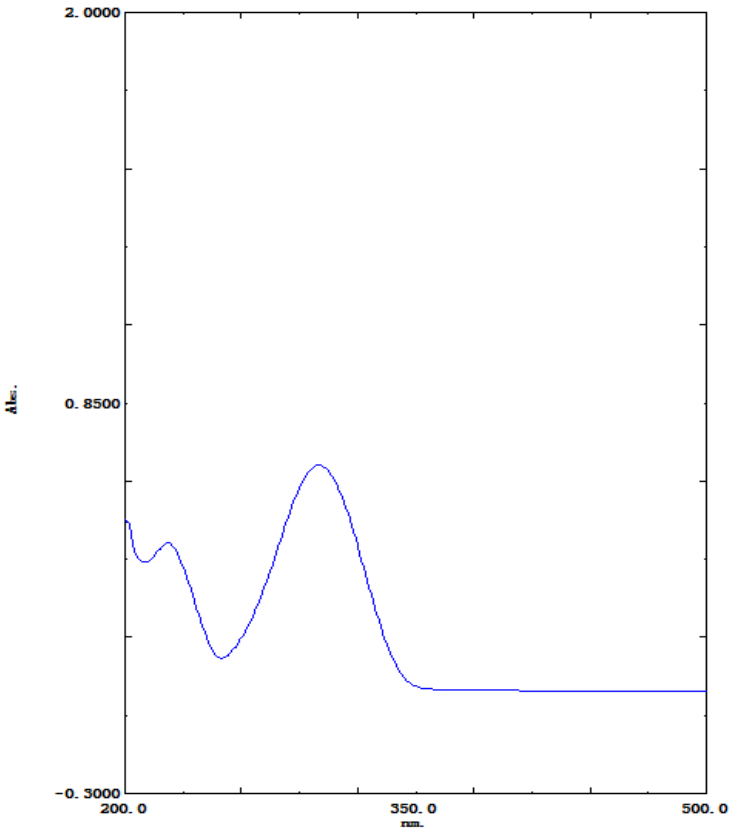

Figure S12: UV spectrum of compound **1**

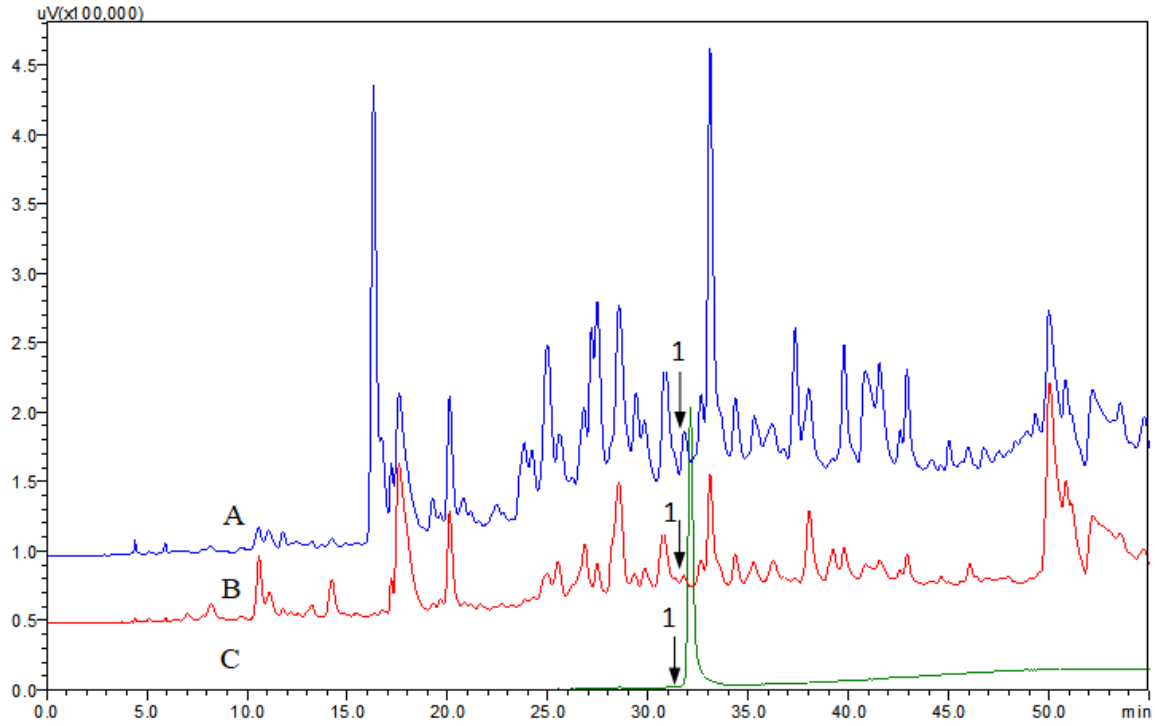

Figure S13: HPLC profile of compound **1** and ethanol crude extract (A: compound **1** + crude extract; B: crude extract; C: compound **1**).

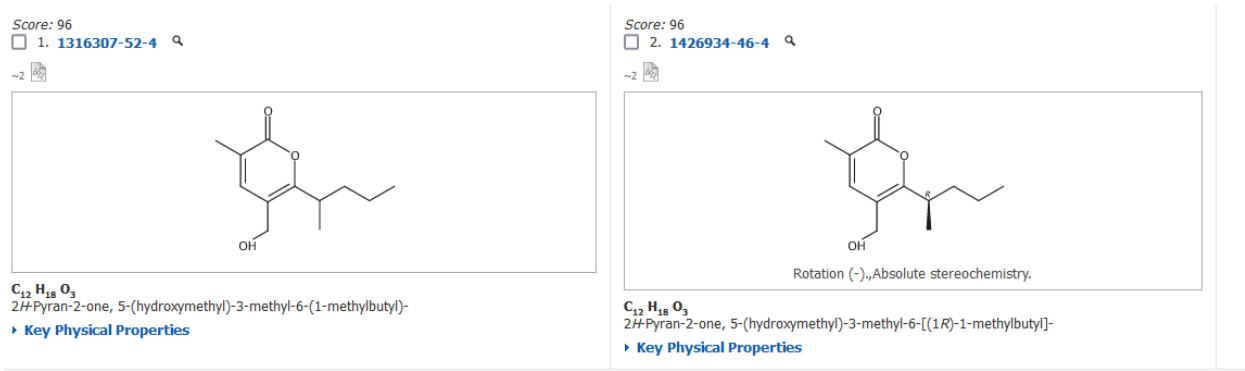

Figure S14: The Scifinder similarity report for new compound **1**

Table S1: Equilibrium populations of low-energy conformers of **1**.

Conformers	In MeOH
	P (%)
1-1	17.5
1-2	15.3
1-3	12.7
1-4	10.8
1-5	6.6
1-6	6.0

Table S2: Cartesian coordinates for the low-energy reoptimized MMFF conformers of **1** at B3LYP/6-311+G(d,p) level of theory in CH_3OH.

1-1		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	2.04826	0.676678	0.047948
2	6	0	0.726349	0.914607	0.556149
3	6	0	-0.10978	-0.15817	0.672073
4	8	0	0.333991	-1.40029	0.313858
5	6	0	1.595484	-1.68111	-0.18694
6	6	0	2.499072	-0.55752	-0.32207
7	6	0	3.878002	-0.82738	-0.85471
8	8	0	1.830924	-2.85182	-0.46578
9	6	0	0.372797	2.333543	0.956389
10	8	0	0.580584	3.27375	-0.09967
11	6	0	-0.39288	3.197451	-1.13938
12	6	0	-1.51712	-0.21778	1.215707
13	6	0	-1.51844	-0.85902	2.621806
14	6	0	-2.49047	-0.95687	0.268261
15	6	0	-2.64769	-0.32008	-1.11855
16	6	0	-3.66691	-1.05824	-1.99456
17	1	0	2.713548	1.531519	-0.04672
18	1	0	4.414258	-1.53894	-0.21682
19	1	0	4.458202	0.096854	-0.90886

20	1	0	3.832961	-1.27008	-1.85609
21	1	0	1.040398	2.661518	1.759586
22	1	0	-0.65573	2.405584	1.326624
23	1	0	-1.40173	3.386901	-0.7474
24	1	0	-0.38099	2.218443	-1.63441
25	1	0	-0.13765	3.970567	-1.8666
26	1	0	-1.86965	0.812687	1.316805
27	1	0	-2.53329	-0.85295	3.0319
28	1	0	-1.17423	-1.89729	2.577485
29	1	0	-0.86821	-0.31002	3.310039
30	1	0	-3.46891	-0.98084	0.765071
31	1	0	-2.16963	-2.00065	0.162836
32	1	0	-1.67718	-0.30115	-1.6313
33	1	0	-2.95556	0.727796	-1.003
34	1	0	-3.76421	-0.58377	-2.97702
35	1	0	-4.65866	-1.06516	-1.52691
36	1	0	-3.36775	-2.10081	-2.15526

1-2		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	1.868208	-0.16289	-0.84215
2	6	0	0.728564	0.645665	-0.50979
3	6	0	-0.21045	0.104584	0.320014

4	8	0	-0.03819	-1.16533	0.795835
5	6	0	1.044718	-1.98207	0.510926
6	6	0	2.053266	-1.43005	-0.36983
7	6	0	3.236613	-2.29221	-0.70813
8	8	0	1.048307	-3.09465	1.026392
9	6	0	0.657181	2.035242	-1.1101
10	8	0	1.773774	2.851173	-0.74458
11	6	0	1.746645	3.29374	0.610868
12	6	0	-1.49345	0.706043	0.839095
13	6	0	-1.45279	0.839949	2.376716
14	6	0	-2.73669	-0.0981	0.385192
15	6	0	-2.93937	-0.17213	-1.13354
16	6	0	-4.21733	-0.92551	-1.52137
17	1	0	2.616878	0.267708	-1.50296
18	1	0	3.784698	-2.58027	0.195963
19	1	0	3.920776	-1.7629	-1.37557
20	1	0	2.920668	-3.22058	-1.19711
21	1	0	-0.27801	2.542698	-0.85019
22	1	0	0.707732	1.963656	-2.201
23	1	0	1.799179	2.452509	1.313668
24	1	0	0.837014	3.875016	0.816373
25	1	0	2.621326	3.931723	0.750885
26	1	0	-1.57634	1.711089	0.416919

27	1	0	-2.36098	1.340337	2.726868
28	1	0	-1.39767	-0.1421	2.856246
29	1	0	-0.59139	1.431	2.703267
30	1	0	-3.61451	0.376157	0.842721
31	1	0	-2.67823	-1.11212	0.801119
32	1	0	-2.07481	-0.66163	-1.60047
33	1	0	-2.97599	0.845867	-1.54485
34	1	0	-4.34041	-0.96526	-2.60905
35	1	0	-5.10601	-0.43917	-1.10186
36	1	0	-4.19577	-1.9568	-1.14958

1-3		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	1.804457	1.182183	-0.08964
2	6	0	0.471002	1.042078	0.420149
3	6	0	0.006214	-0.2228	0.642116
4	8	0	0.8198	-1.2907	0.404528
5	6	0	2.117832	-1.20995	-0.08251
6	6	0	2.623972	0.120045	-0.34672
7	6	0	4.023626	0.243938	-0.87956
8	8	0	2.713087	-2.26984	-0.24087
9	6	0	-0.347	2.282562	0.662108
10	8	0	-0.93734	2.703441	-0.57135

11	6	0	-1.67057	3.917645	-0.43355
12	6	0	-1.33912	-0.65718	1.167695
13	6	0	-1.20418	-1.22153	2.599311
14	6	0	-2.03503	-1.67407	0.231794
15	6	0	-2.32047	-1.15686	-1.18398
16	6	0	-3.07683	-2.17733	-2.04278
17	1	0	2.17358	2.188407	-0.27519
18	1	0	4.749502	-0.19517	-0.18599
19	1	0	4.284595	1.293013	-1.03813
20	1	0	4.130629	-0.2895	-1.83073
21	1	0	0.307771	3.080278	1.044029
22	1	0	-1.12981	2.116416	1.412654
23	1	0	-1.02006	4.738829	-0.10101
24	1	0	-2.49473	3.803941	0.284727
25	1	0	-2.08	4.157415	-1.41671
26	1	0	-1.96932	0.235628	1.212942
27	1	0	-2.19367	-1.47752	2.990861
28	1	0	-0.589	-2.12692	2.608169
29	1	0	-0.74894	-0.48947	3.273835
30	1	0	-2.98212	-1.95629	0.70941
31	1	0	-1.42913	-2.58718	0.177669
32	1	0	-1.37754	-0.89414	-1.68087
33	1	0	-2.90343	-0.2282	-1.12007

34	1	0	-3.26586	-1.78739	-3.04877
35	1	0	-4.04513	-2.4306	-1.59495
36	1	0	-2.5051	-3.10715	-2.14691

1-4		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	1.98652	-0.0408	-0.71532
2	6	0	0.776607	0.651453	-0.37833
3	6	0	-0.16175	-0.02771	0.345705
4	8	0	0.068034	-1.32362	0.699733
5	6	0	1.215968	-2.042	0.39044
6	6	0	2.231908	-1.33744	-0.36164
7	6	0	3.490029	-2.08257	-0.70827
8	8	0	1.26053	-3.20274	0.782084
9	6	0	0.614212	2.088072	-0.79881
10	8	0	1.158118	2.937932	0.216214
11	6	0	1.105113	4.31518	-0.1461
12	6	0	-1.48496	0.465338	0.874041
13	6	0	-1.45971	0.524259	2.417625
14	6	0	-2.67333	-0.38789	0.369626
15	6	0	-2.86285	-0.39154	-1.15279
16	6	0	-4.08188	-1.21086	-1.59285
17	1	0	2.739128	0.499983	-1.28491

18	1	0	4.00729	-2.423	0.195806
19	1	0	4.170578	-1.44629	-1.27908
20	1	0	3.267723	-2.97618	-1.30223
21	1	0	-0.4379	2.346358	-0.97354
22	1	0	1.153297	2.254253	-1.74312
23	1	0	0.068951	4.642716	-0.31092
24	1	0	1.688232	4.508299	-1.05755
25	1	0	1.534232	4.880824	0.683139
26	1	0	-1.61843	1.485656	0.502996
27	1	0	-2.3995	0.947691	2.785366
28	1	0	-1.34438	-0.476	2.846446
29	1	0	-0.63827	1.150869	2.778572
30	1	0	-3.58117	0.006069	0.844406
31	1	0	-2.55474	-1.41733	0.730937
32	1	0	-1.9632	-0.79159	-1.6386
33	1	0	-2.97032	0.6427	-1.50699
34	1	0	-4.19817	-1.19664	-2.6819
35	1	0	-5.00455	-0.81425	-1.1527
36	1	0	-3.98753	-2.25762	-1.28033

1-5		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	1.469319	1.477069	0.131659

2	6	0	0.215757	0.901986	0.527774
3	6	0	0.108137	-0.45935	0.51257
4	8	0	1.186041	-1.21406	0.151651
5	6	0	2.419579	-0.70891	-0.23533
6	6	0	2.550636	0.732589	-0.24381
7	6	0	3.872562	1.314247	-0.65869
8	8	0	3.28231	-1.52817	-0.53078
9	6	0	-0.90513	1.827911	0.918055
10	8	0	-1.48824	2.378	-0.26672
11	6	0	-2.49499	3.343402	0.023794
12	6	0	-1.06984	-1.32531	0.88606
13	6	0	-0.79021	-2.07254	2.209321
14	6	0	-1.44208	-2.32237	-0.23942
15	6	0	-1.87519	-1.69601	-1.57559
16	6	0	-3.21314	-0.9462	-1.52063
17	1	0	1.553413	2.561476	0.137263
18	1	0	4.679269	0.964301	-0.00488
19	1	0	3.842426	2.405786	-0.62077
20	1	0	4.134519	1.008105	-1.67773
21	1	0	-0.50314	2.643985	1.537762
22	1	0	-1.67335	1.317063	1.510735
23	1	0	-2.08191	4.188336	0.592646
24	1	0	-3.31886	2.897068	0.598323

25	1	0	-2.87726	3.704901	-0.93272
26	1	0	-1.92031	-0.65997	1.05269
27	1	0	-1.67246	-2.65073	2.501267
28	1	0	0.050521	-2.76484	2.098954
29	1	0	-0.55652	-1.37381	3.018788
30	1	0	-2.25741	-2.95113	0.141376
31	1	0	-0.58896	-2.98955	-0.40864
32	1	0	-1.95057	-2.50164	-2.31672
33	1	0	-1.09003	-1.02137	-1.94246
34	1	0	-3.49355	-0.57574	-2.51273
35	1	0	-3.17235	-0.08197	-0.84972
36	1	0	-4.0169	-1.60565	-1.17125
2	6	0	0.776607	0.651453	-0.37833
3	6	0	-0.16175	-0.02771	0.345705
4	8	0	0.068034	-1.32362	0.699733
5	6	0	1.215968	-2.042	0.39044
6	6	0	2.231908	-1.33744	-0.36164
7	6	0	3.490029	-2.08257	-0.70827
8	8	0	1.26053	-3.20274	0.782084
9	6	0	0.614212	2.088072	-0.79881
10	8	0	1.158118	2.937932	0.216214
11	6	0	1.105113	4.31518	-0.1461
12	6	0	-1.48496	0.465338	0.874041

13	6	0	-1.45971	0.524259	2.417625
14	6	0	-2.67333	-0.38789	0.369626
15	6	0	-2.86285	-0.39154	-1.15279
16	6	0	-4.08188	-1.21086	-1.59285
17	1	0	2.739128	0.499983	-1.28491
18	1	0	4.00729	-2.423	0.195806
19	1	0	4.170578	-1.44629	-1.27908
20	1	0	3.267723	-2.97618	-1.30223
21	1	0	-0.4379	2.346358	-0.97354
22	1	0	1.153297	2.254253	-1.74312
23	1	0	0.068951	4.642716	-0.31092
24	1	0	1.688232	4.508299	-1.05755
25	1	0	1.534232	4.880824	0.683139
26	1	0	-1.61843	1.485656	0.502996
27	1	0	-2.3995	0.947691	2.785366
28	1	0	-1.34438	-0.476	2.846446
29	1	0	-0.63827	1.150869	2.778572
30	1	0	-3.58117	0.006069	0.844406
31	1	0	-2.55474	-1.41733	0.730937
32	1	0	-1.9632	-0.79159	-1.6386
33	1	0	-2.97032	0.6427	-1.50699
34	1	0	-4.19817	-1.19664	-2.6819
35	1	0	-5.00455	-0.81425	-1.1527

36	1	0	-3.98753	-2.25762	-1.28033

1-6		Standard Orientation (Ångstroms)			
No.	Atom	Type	X	Y	Z
1	6	0	1.469319	1.477069	0.131659
1	6	0	1.745199	0.605953	-0.79678
2	6	0	0.375582	0.803219	-0.41104
3	6	0	-0.22743	-0.18554	0.311472
4	8	0	0.481919	-1.30753	0.639156
5	6	0	1.804914	-1.54132	0.299756
6	6	0	2.463425	-0.5084	-0.47302
7	6	0	3.895031	-0.73441	-0.86957
8	8	0	2.294579	-2.5988	0.680894
9	6	0	-0.29025	2.096182	-0.83755
10	8	0	0.389899	3.25385	-0.34534
11	6	0	0.212835	3.477797	1.052043
12	6	0	-1.63354	-0.25814	0.855941
13	6	0	-1.6199	-0.26107	2.400633
14	6	0	-2.40084	-1.4921	0.315544
15	6	0	-2.60437	-1.54629	-1.20763
16	6	0	-3.54889	-0.47157	-1.76257
17	1	0	2.225045	1.393085	-1.37348
18	1	0	4.531282	-0.86597	0.012837

19	1	0	4.27297	0.112045	-1.44783
20	1	0	3.99763	-1.64322	-1.47309
21	1	0	-1.34384	2.127658	-0.53998
22	1	0	-0.24636	2.187487	-1.92722
23	1	0	0.627393	2.656687	1.650637
24	1	0	-0.85114	3.598624	1.298632
25	1	0	0.745546	4.399781	1.29254
26	1	0	-2.1567	0.643991	0.531116
27	1	0	-2.64716	-0.24858	2.778037
28	1	0	-1.12512	-1.15738	2.787178
29	1	0	-1.10075	0.616927	2.797372
30	1	0	-3.3815	-1.50665	0.808735
31	1	0	-1.87443	-2.39571	0.644688
32	1	0	-3.00978	-2.53475	-1.45769
33	1	0	-1.63284	-1.4822	-1.71574
34	1	0	-3.69217	-0.59698	-2.84124
35	1	0	-3.1654	0.541675	-1.60115
36	1	0	-4.53444	-0.53247	-1.28543