Supporting Information

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A Neoprzewaquinone Analogue from *Salvia miltiorrhiza* Bunge

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Table of Contents **Page**

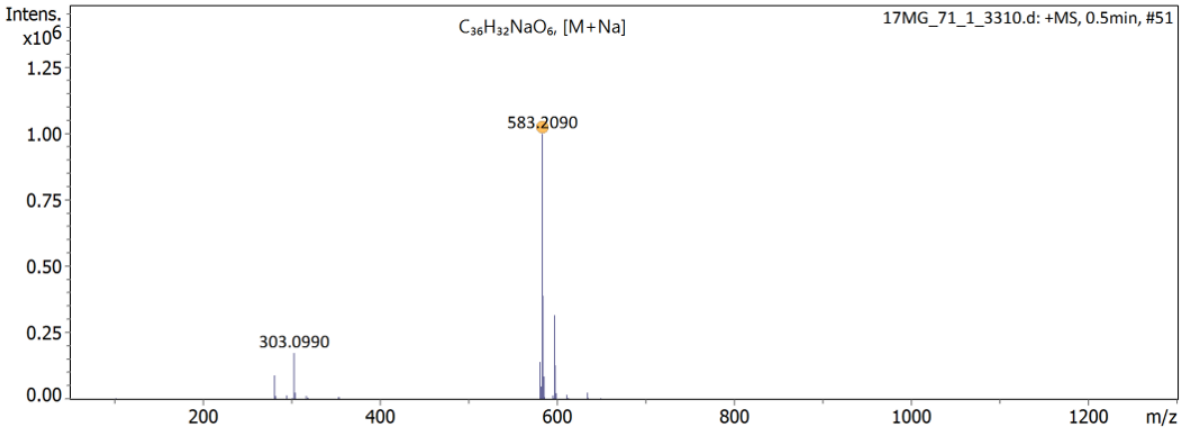

Figure S1: HR-ESI-MS spectrum of compound **1**

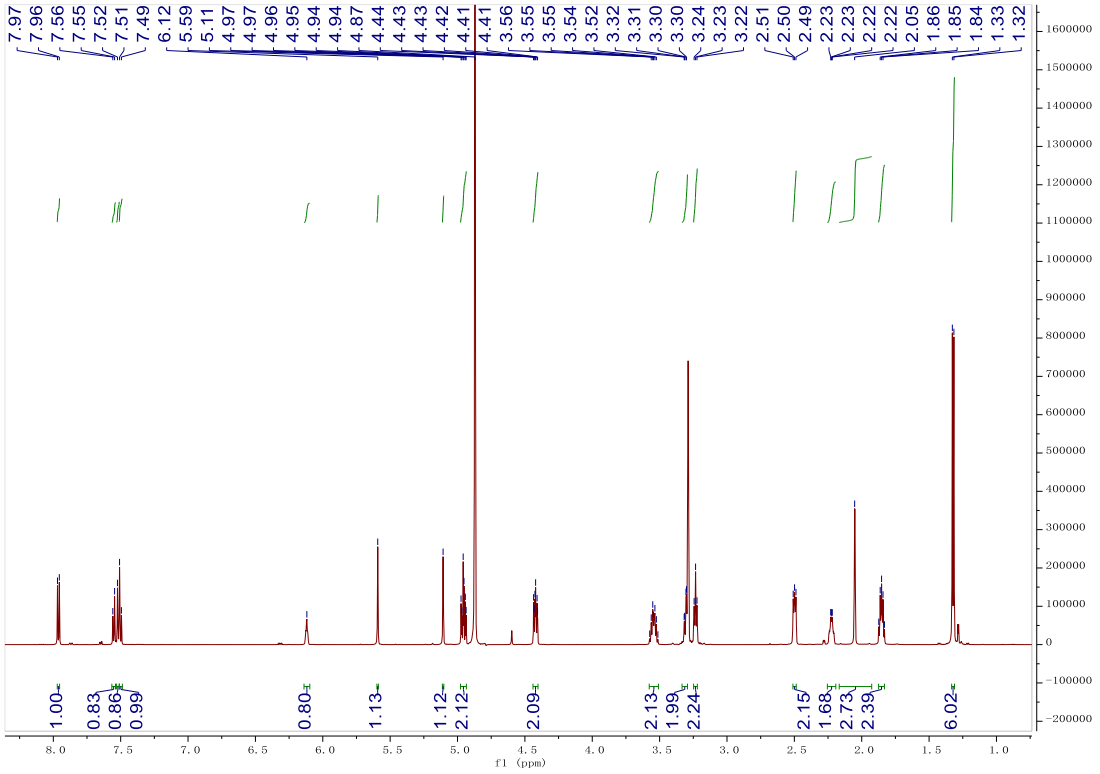

Figure S2: ^{1}H-NMR (600 MHz, CD_3OD) spectrum of compound **1**

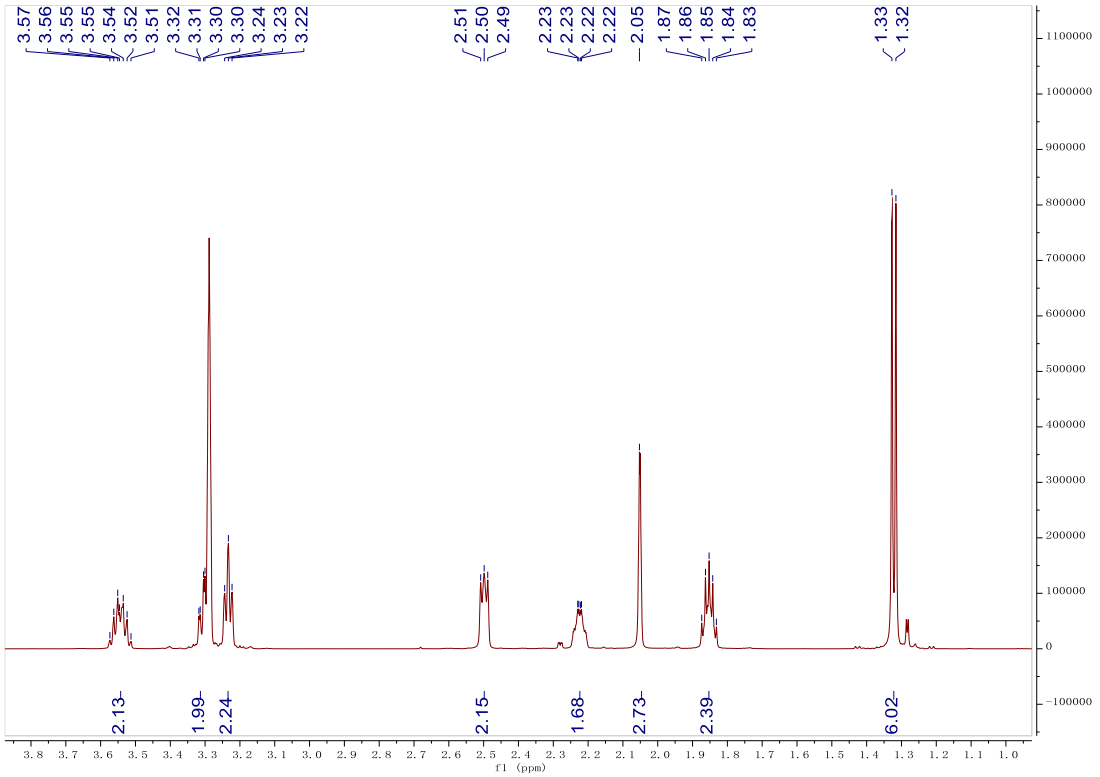

Figure S2a : ^{1}H-NMR (600 MHz, CD_3OD) spectrum of compound **1** (From δ_H1.0 ppm to δ_H 3.8 ppm)

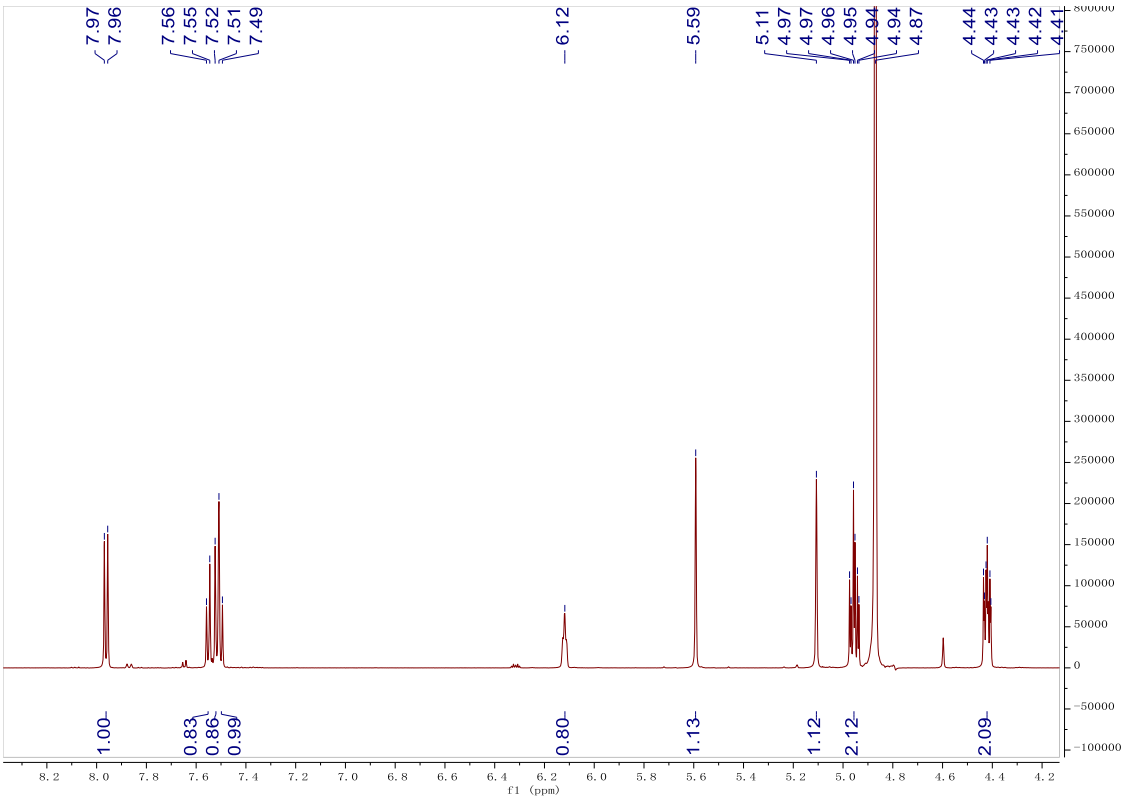

Figure S2b : ^{1}H-NMR (600 MHz, CD_3OD) spectrum of compound **1** (From δ_H4.2 ppm to δ_H 8.2 ppm)

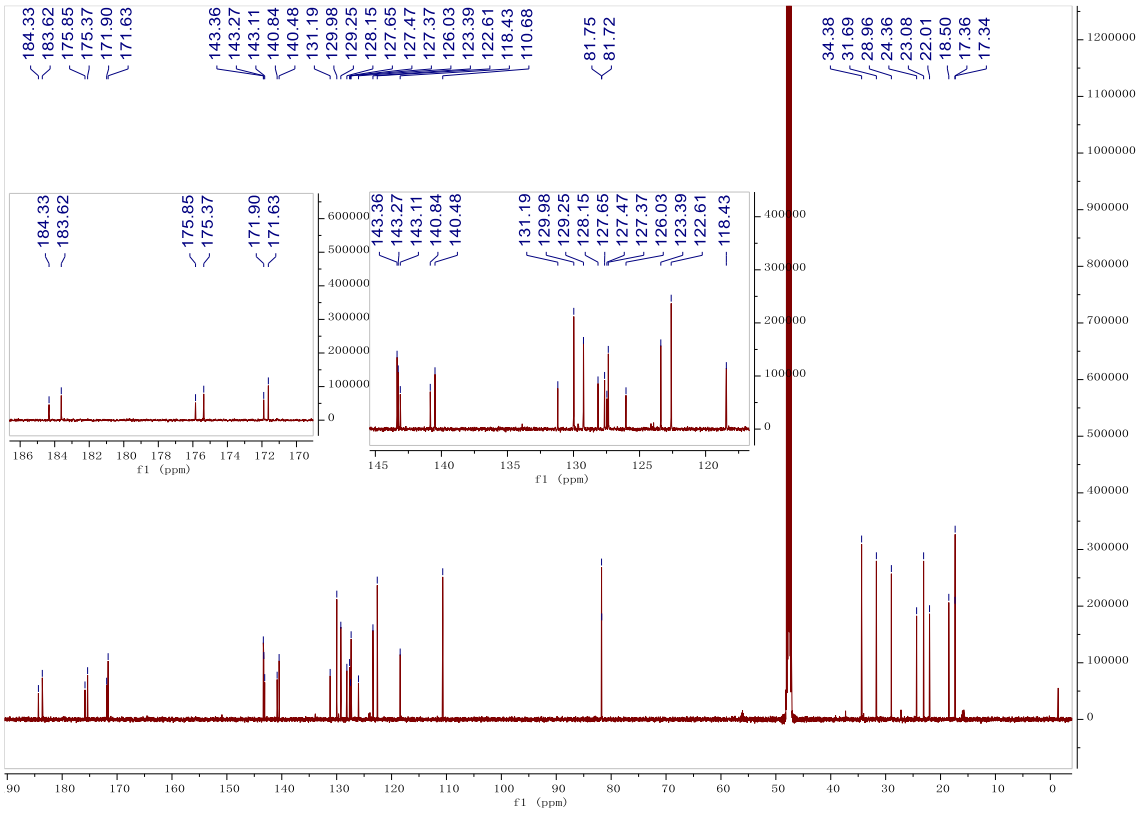

Figure S3: ^{13}C-NMR (150 MHz, CD_3OD) spectrum of compound **1**

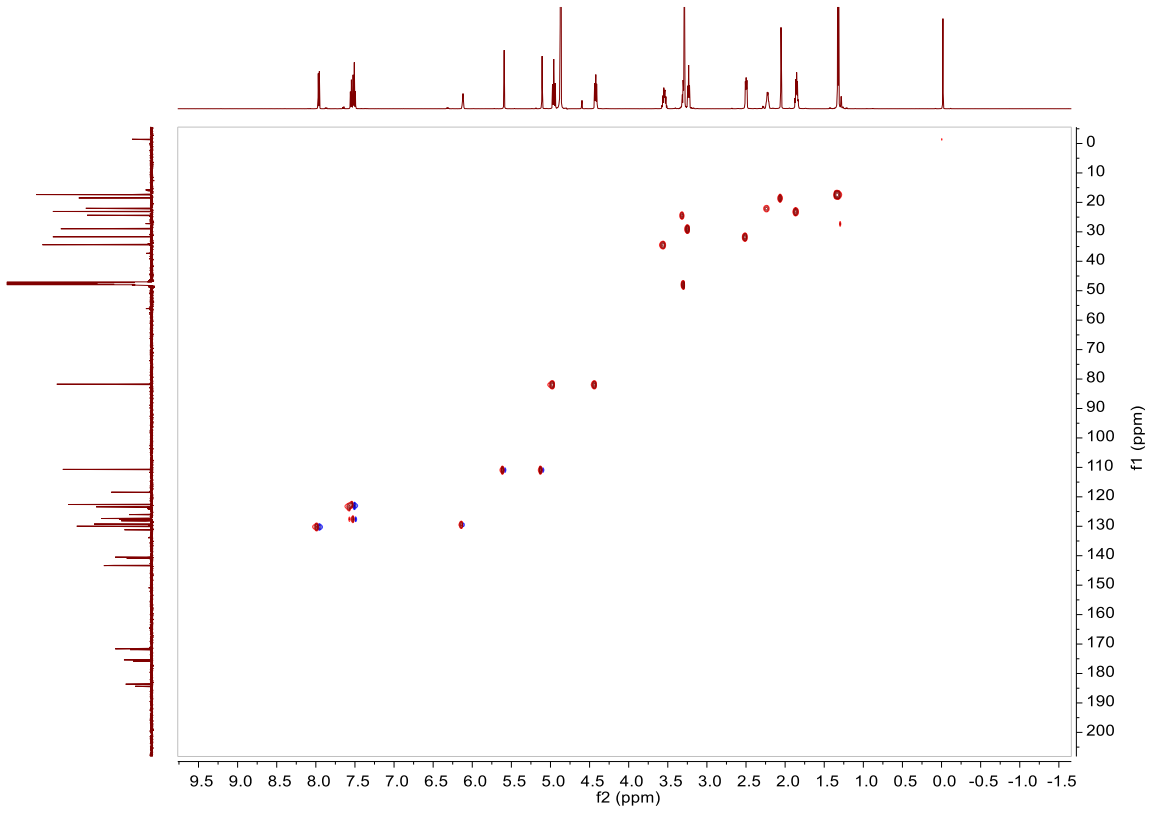

Figure S4: HSQC spectrum of compound **1**

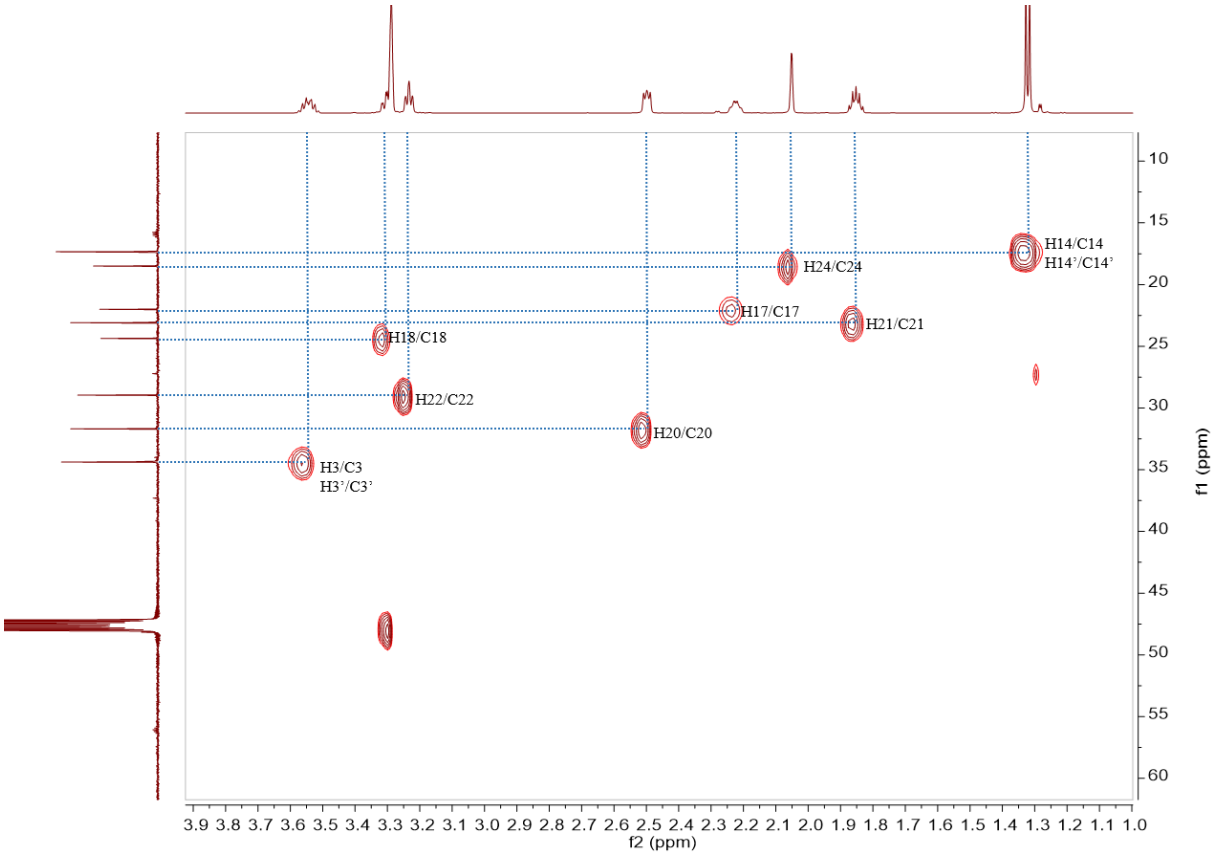

Figure S5: HSQC spectrum of compound **1** (From δ_C10 ppm to δ_C60 ppm)

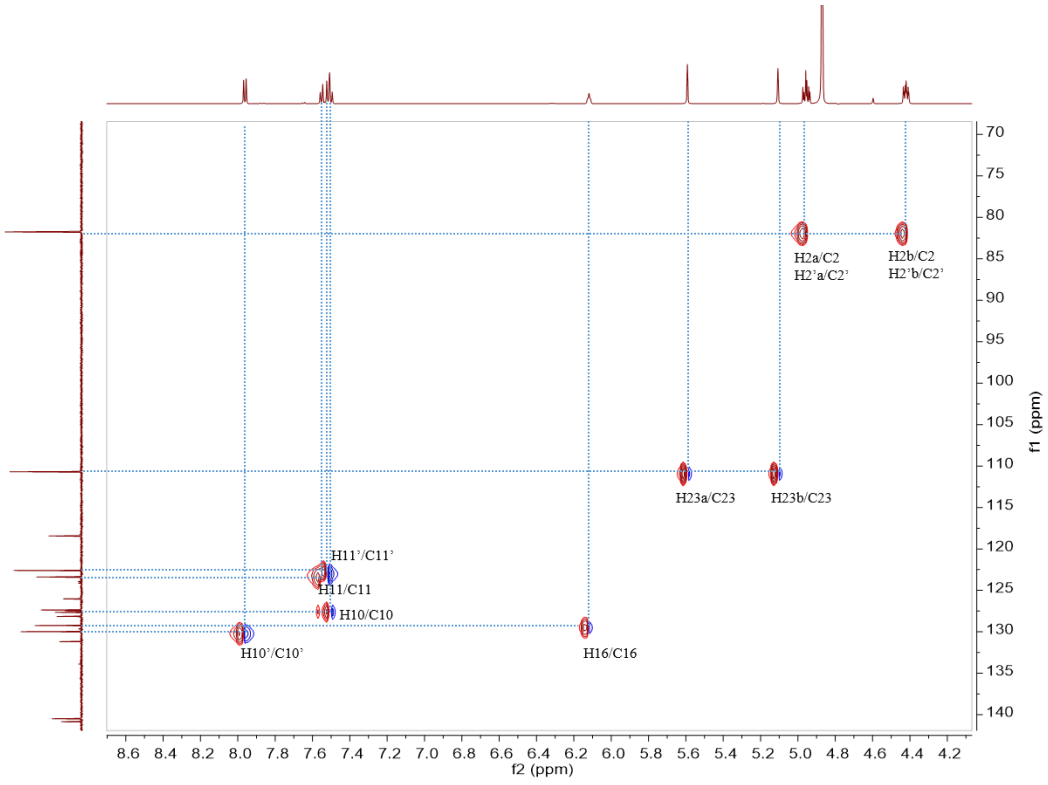

Figure S6: HSQC spectrum of compound **1** (From δ_C70 ppm to δ_C140 ppm)

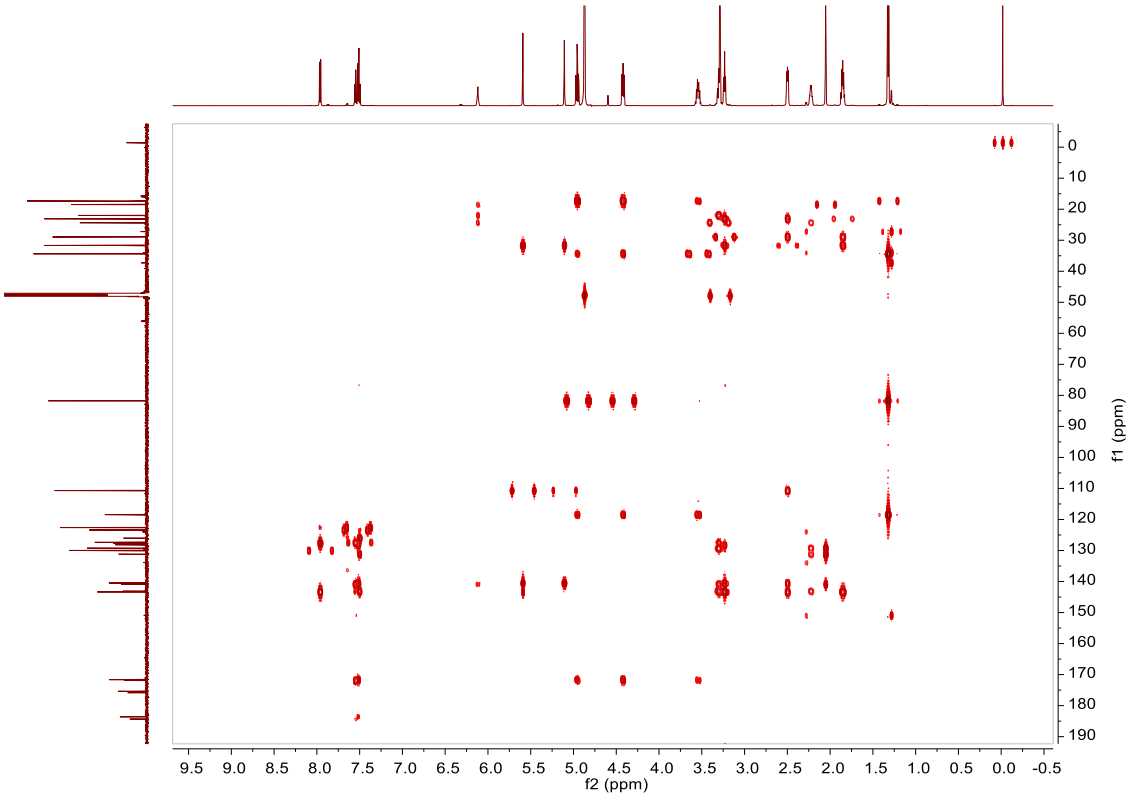

Figure S7: HMBC spectrum of compound **1**

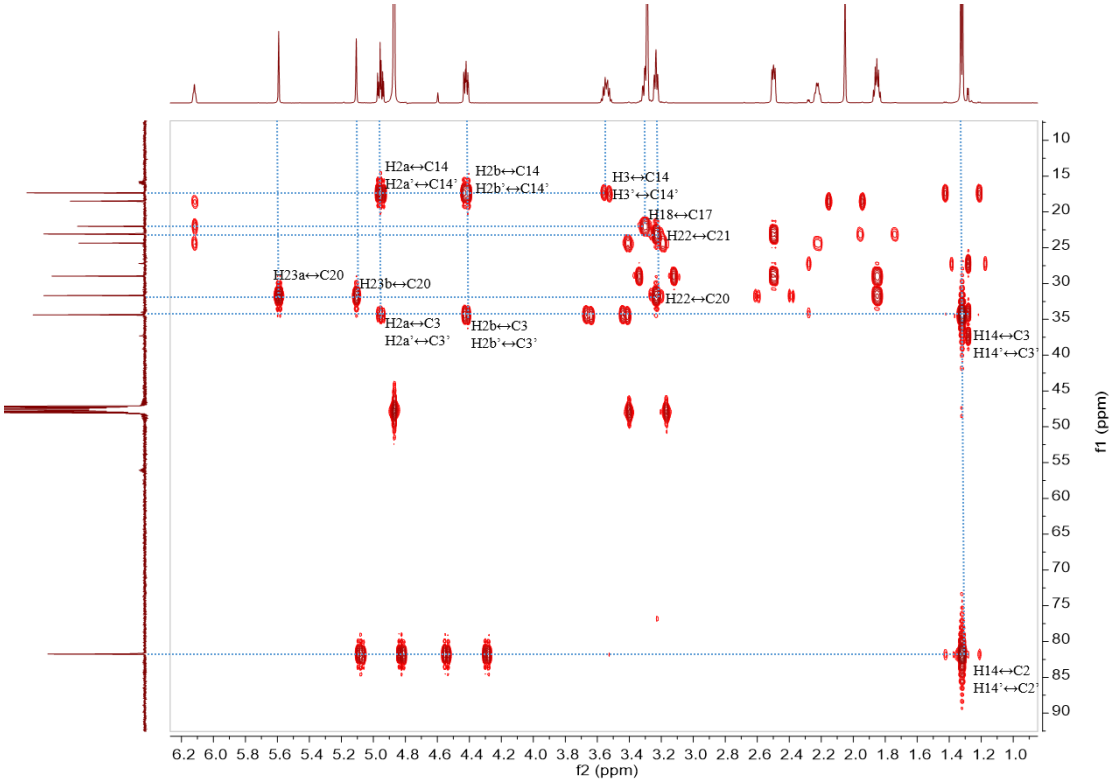

Figure S8: HMBC spectrum of compound **1** (From δ_C10 ppm to δ_C90 ppm)

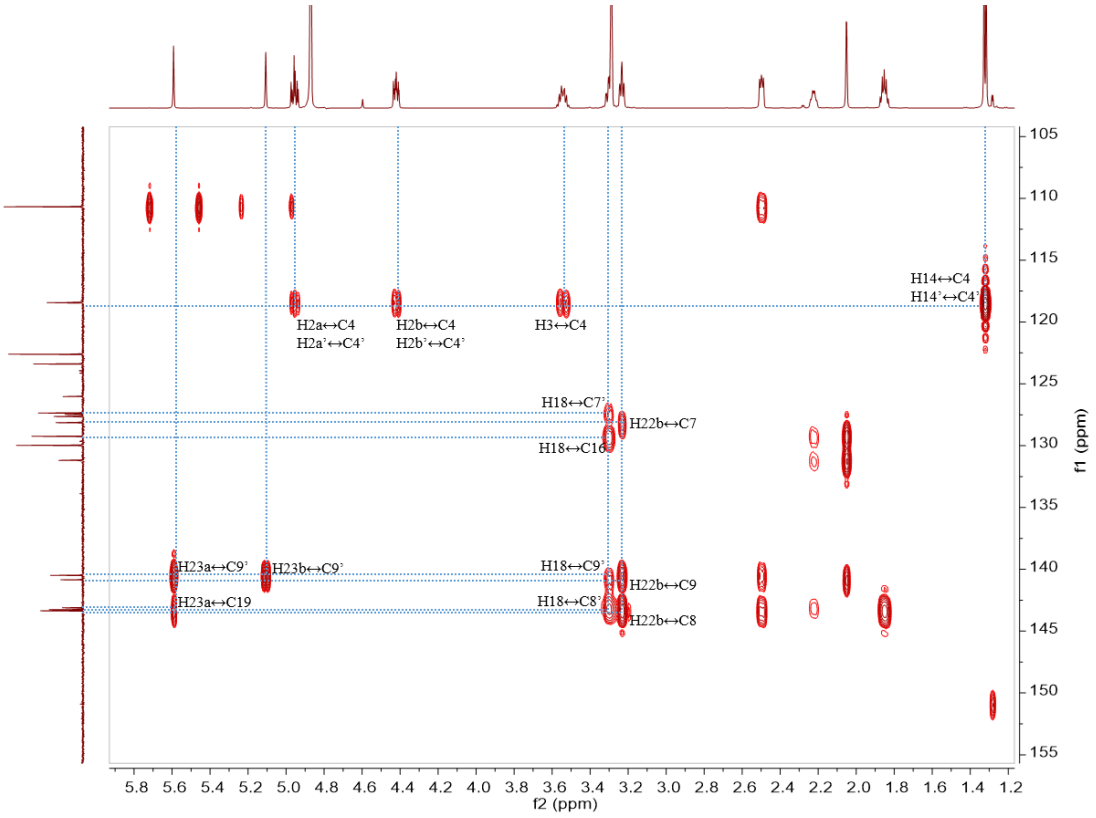

Figure S9: HMBC spectrum of compound **1** (From δ_C105 ppm to δ_C155 ppm)

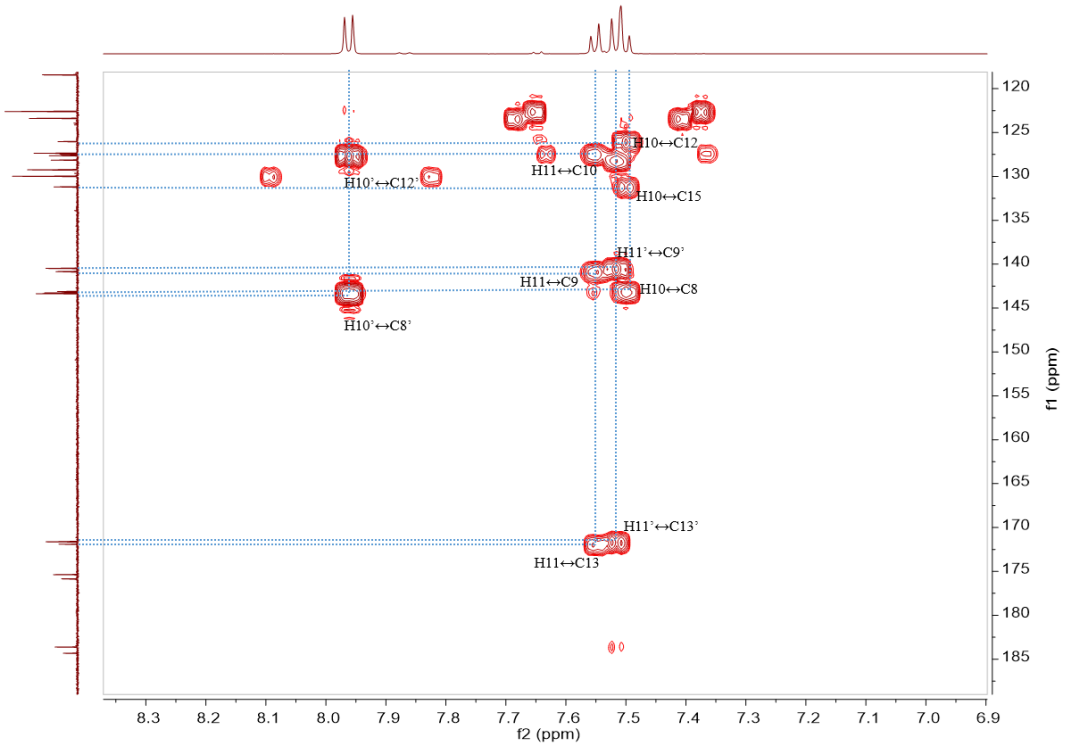

Figure S10: HMBC spectrum of compound **1** (From δ_C120 ppm to δ_C185 ppm)

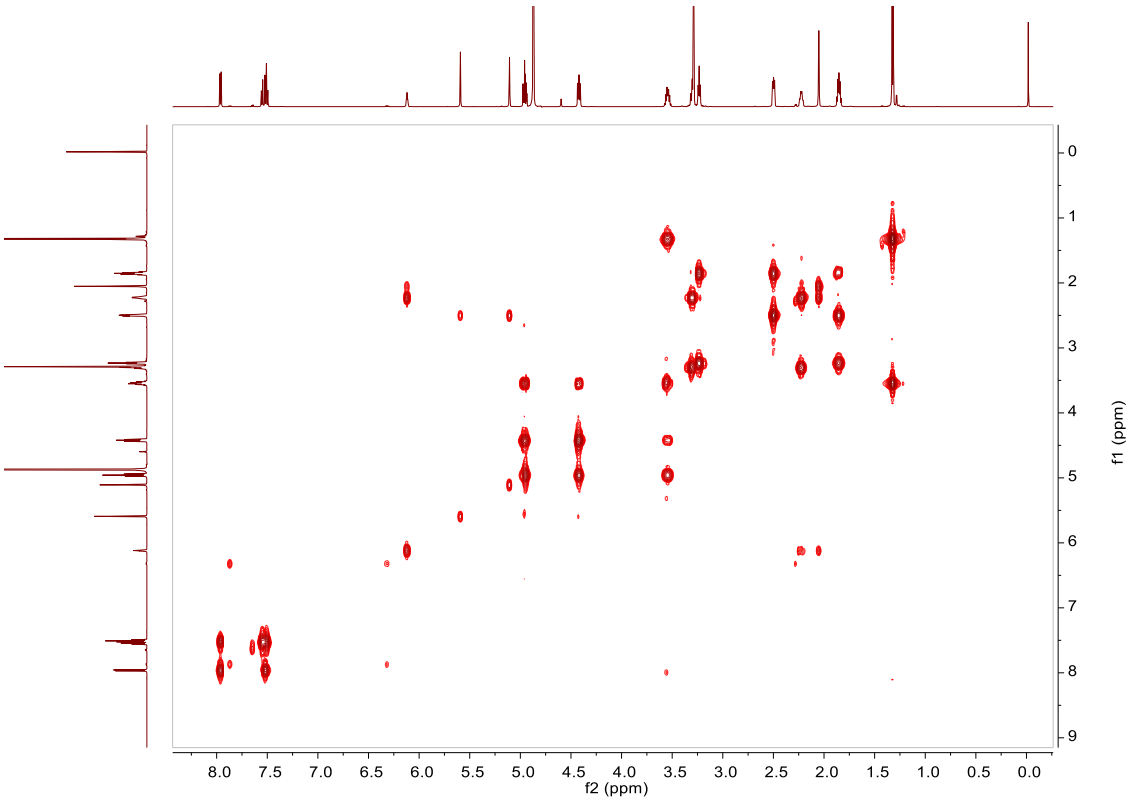

Figure S11: $^{1}H-^{1}H$ COSY spectrum of compound **1**

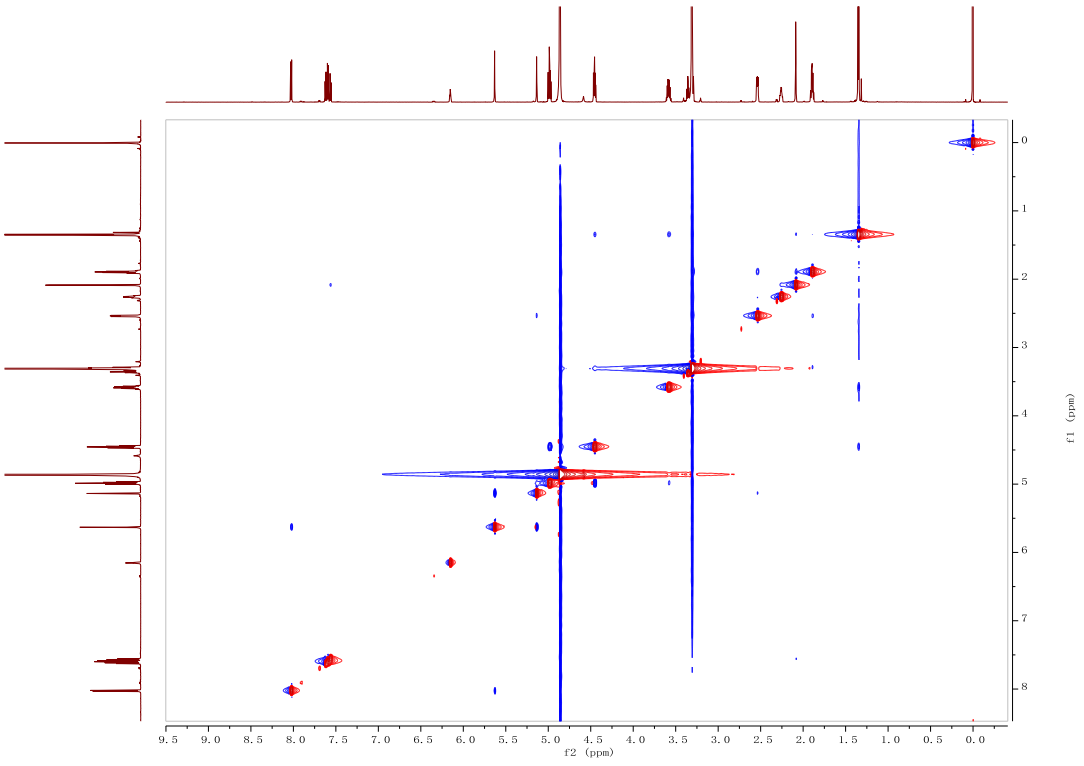

Figure S12: NOESY spectrum of compound **1**

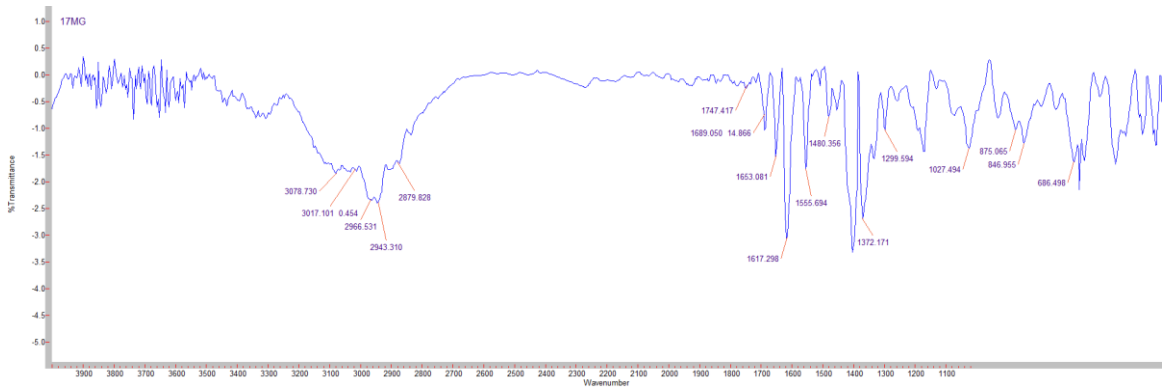

Figure S13: The IR spectrum of compound **1**

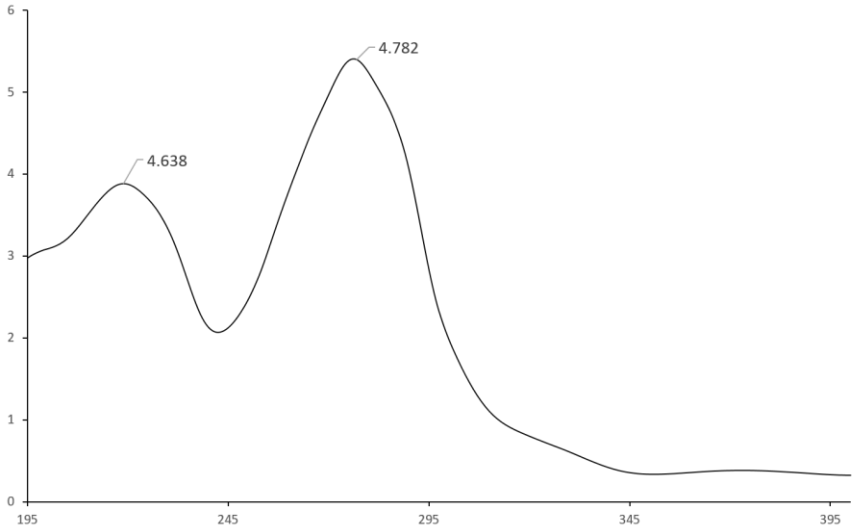

Figure S14: The UV spectrum of compound **1**

2. Computational Details

The theoretical calculations of compound **1** were performed using Gaussian 16 [1]. Conformational analysis was initially carried out using Conflex 8 to generate conformations by Boltzman Jump, then minimize them by Smart Minimizer using the MMFF molecular mechanics force field. All geometries with relative energy from 0-5.0 kcal/mol were used in optimizations at the B3LYP/6-31G (d, p) in the gas and further at WB97XD/DGDZVP in the methanol. Room-temperature equilibrium populations were calculated according to the Boltzmann distribution law. The theoretical calculation of ECD was performed using TD-DFT at the CAM-B3LYP/DGDZVP level in the methanol. The ECD spectra were obtained by weighing the Boltzmann distribution rate of each geometric conformation. SpecDis 1.71[2] was used to sum up single CD spectra after a Boltzmann statistical weighting, and for the Gauss curve generation (σ = 0.2-0.3 eV) and for the comparison with experimental data. The shielding tensors calculations for ωB97XD/DGDZVP-optimized conformers (Boltzmann distribution≥ 1%) were carried out at PCM/mPW1PW91/6-311+G (d, p) level in methanol with GIAO method. The isotropic values of TMS was calculated in the same level and used as references. The DP4+ parameters were calculated using the excel file provided by Ariel M. Sarotii[3].

References

1. Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Petersson, G.A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A.V.; Bloino, J.; Janesko, B.G.; Gomperts, R.; Mennucci, B.; Hratchian, H.P.; Ortiz, J.V.; Izmaylov, A.F.; Sonnenberg, J.L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V.G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J.A.Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.J.; Heyd, J.J.; Brothers, E.N.; Kudin, K.N.; Staroverov, V.N.; Keith, T.A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.P.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Millam, J.M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT, 2016.
2. Bruhn T., Schaumlöffel A., Hemberger Y., Pescitelli G., SpecDis version 1.71, Berlin, Germany, 2017

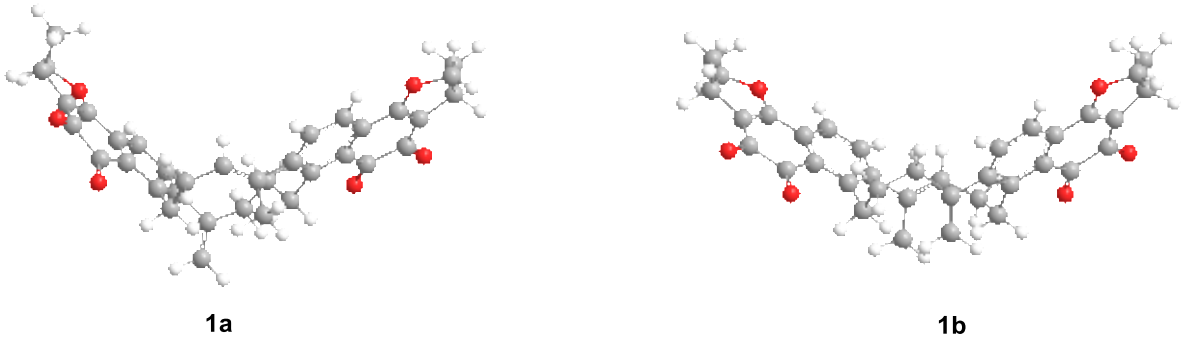

Figure S15: Most stable conformers of 3R, 3R'-**1** calculated with DFT at the CAM-B3LYP/DGDZVP level.

Table S1 : Optimized Z-Matrixes of 3R, 3R'-**1** with simplified structures in the methanol at WB97XD/DGDZVP level.

	1a			**1b**		
C	-1.09725	-2.70693	-1.59555	0.779806	-1.63649	1.823466
C	-2.17266	-1.68755	-1.35899	2.065147	-0.93642	1.491666
C	-2.85199	-1.51015	-0.1265	2.861522	-1.23271	0.355976
C	-2.40303	-2.23389	1.127971	2.417451	-2.30224	-0.61955
C	-1.87039	-1.29455	2.234732	1.759075	-1.73346	-1.89469
C	-0.53028	-0.71053	1.881	0.433298	-1.08052	-1.61548
C	0.178446	-2.2261	-2.25598	-0.44076	-0.73497	1.850268
C	0.990733	-1.23208	-1.41618	-1.79878	-1.40921	2.040448
C	1.821292	-1.93052	-0.33095	-2.31546	-2.14511	0.788286
C	2.540015	-0.93059	0.544584	-2.81769	-1.186	-0.27114
C	1.922538	-0.55419	1.76014	-2.00775	-0.93624	-1.40555
C	0.66168	-1.21837	2.21541	-0.7515	-1.70217	-1.66155
C	2.503603	0.404165	2.584452	-2.38386	0.024702	-2.34238
C	3.705732	1.011421	2.238233	-3.56131	0.748395	-2.19878
C	4.332315	0.644947	1.056335	-4.3827	0.492314	-1.11149
C	3.759479	-0.31701	0.191203	-4.02861	-0.47246	-0.13929
C	5.614059	1.244585	0.696485	-5.63494	1.22686	-0.9598
C	6.356485	0.956863	-0.3994	-6.53172	1.090131	0.046147
C	5.901802	-0.0121	-1.34165	-6.30153	0.144143	1.087677
C	4.497794	-0.64915	-1.0696	-4.99529	-0.71438	0.981338
C	-2.53479	-0.90862	-2.46384	2.460526	0.066482	2.378473
C	-3.54552	0.036218	-2.39838	3.627765	0.789842	2.18649
C	-4.24437	0.191737	-1.2098	4.418205	0.512879	1.081405
C	-3.92909	-0.59387	-0.08222	4.0513	-0.4918	0.157787
C	-5.30793	1.187555	-1.1098	5.655595	1.259782	0.875471
C	-6.03777	1.477698	-0.00531	6.536552	1.094002	-0.13895
C	-5.82686	0.742096	1.198262	6.297851	0.103852	-1.13611
C	-4.8481	-0.47164	1.098425	4.985324	-0.74168	-0.99123

O	-5.59087	1.947171	-2.16828	5.993815	2.212674	1.745114
C	-6.74661	2.772392	-1.81462	7.327425	2.689126	1.376099
C	-6.90699	2.678916	-0.28282	7.632458	2.123769	-0.02773
O	6.15558	2.159514	1.501093	-5.96793	2.143324	-1.8696
C	7.486258	2.473237	0.979254	-7.31279	2.617496	-1.54188
C	7.581619	1.835498	-0.42409	-7.6324	2.107631	-0.12041
O	-6.36948	0.961896	2.277177	7.030049	-0.13008	-2.09282
O	-4.92664	-1.30286	1.98262	4.796808	-1.57672	-1.85478
C	-1.30136	-4.00159	-1.32819	0.774674	-2.92843	2.163429
O	6.51274	-0.36569	-2.34599	-7.04081	-0.04685	2.048853
O	4.06645	-1.38877	-1.93379	-4.84083	-1.56274	1.839123
C	-6.43154	3.933269	0.457135	7.565134	3.177672	-1.13737
C	7.551837	2.859156	-1.56323	-7.58482	3.206292	0.946078
C	0.887368	-2.45331	3.052906	-0.91003	-3.15651	-2.05763
H	-1.60402	-2.92988	0.880791	1.694867	-2.95426	-0.13367
H	-3.23126	-2.8192	1.526893	3.269063	-2.91584	-0.90772
H	-2.57416	-0.48277	2.427056	2.428732	-1.01141	-2.36703
H	-1.81298	-1.8693	3.161312	1.637166	-2.55681	-2.60335
H	-0.54433	0.182166	1.256773	0.455534	-0.0305	-1.32712
H	-0.06772	-1.75014	-3.21	-0.44888	-0.13573	0.932757
H	0.800591	-3.09118	-2.50322	-0.29916	-0.01008	2.660364
H	0.319875	-0.50001	-0.95324	-2.52028	-0.64365	2.3341
H	1.662044	-0.67433	-2.07313	-1.75845	-2.11087	2.87832
H	2.528237	-2.60877	-0.80773	-3.1099	-2.83058	1.078828
H	1.15094	-2.53336	0.284921	-1.50111	-2.74463	0.380616
H	2.00936	0.674564	3.512392	-1.74482	0.199839	-3.20155
H	4.157004	1.754902	2.884869	-3.84588	1.493212	-2.93278
H	-2.02267	-1.05079	-3.40879	1.851874	0.275998	3.252047
H	-3.80069	0.633669	-3.26572	3.925769	1.556071	2.892393
H	-7.59947	2.357209	-2.35271	8.010939	2.315355	2.138984

H	-6.53765	3.778834	-2.17413	7.29501	3.777164	1.411924
H	-7.95082	2.481425	-0.02918	8.618522	1.653938	-0.03424
H	8.201822	2.051212	1.685193	-7.97967	2.202741	-2.29836
H	7.574232	3.558896	0.971565	-7.29338	3.703376	-1.62355
H	8.492662	1.237541	-0.50052	-8.61588	1.63253	-0.10706
H	-0.53924	-4.74451	-1.54594	-0.13532	-3.45162	2.438668
H	-2.23195	-4.36037	-0.89776	1.691815	-3.51034	2.17401
H	-6.49225	3.787281	1.537515	7.713361	2.714414	-2.11506
H	-7.05167	4.793481	0.191442	8.340507	3.935126	-0.99562
H	-5.39375	4.163439	0.199157	6.591534	3.676344	-1.13706
H	7.549525	2.354031	-2.53143	-7.74054	2.782109	1.940183
H	8.428917	3.510111	-1.51848	-8.3638	3.951639	0.765136
H	6.65554	3.482908	-1.49856	-6.61474	3.711714	0.935814
H	1.551619	-3.14937	2.530374	-1.89507	-3.53852	-1.78256
H	1.386242	-2.18736	3.990716	-0.81236	-3.26634	-3.14275
H	-0.03545	-2.98256	3.290348	-0.15743	-3.79484	-1.58875

Table S2 : Energy analysis for 3R, 3R'of **1**

Conf.	Steric Energy (kJ/mol)	Relative Energy (kJ/mol)	Distribution (%)
1a	-1841.6683299	0	90.87
1b	-1841.6661619	0.002168	9.13