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Supporting Information

Cytosporins A-D, novel benzophenone derivatives from the endophytic fungus *Cytospora rhizophorae* A761

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General Experimental Procedures

Optical rotation was measured on an Anton Paar MCP-500 spectropolarimeter (Anton Paar, Graz, Austria). UV spectra were measured on a SHIMADZU UV-2600 UV-visible spectrophotometer (Shimadzu, Kyoto, Japan). 1D and 2D NMR spectra were recorded on a Bruker Avance-500 spectrometer (Bruker, Fällanden, Switzerland) with TMS as internal standard, δ in ppm, J in Hz. HREIMS was measured on Thermo MAT95XP or Bruker maXis Q-TOF high resolution mass spectrometer and EIMS on a Thermo DSQ EI mass spectrometer (Thermo Scientific, Massachusetts, USA). A Shimadzu LC-20AT (Shimadzu Corporation, Kyoto, Japan) equipped with an SPD-M20A PDA detector (Shimadzu Corporation, Kyoto, Japan) was used for HPLC separation. A YMC-pack ODS-A column (250 × 10 mm, 5 μm) was used for semipreparative HPLC separation, and a CHIRALPAK IC column (250 × 10 mm, 5 μm) for chiral semipreparative HPLC separation. All solvents were analytical grade (Guangzhou Chemical Plant, Guangzhou, China). Silica gel (200-300 mesh) was used for column chromatography, and precoated silica gel GF_{254} plates (Qingdao Marine Chemical Inc., Qingdao, China) were used for TLC spotting. C_{18} reversed-phase silica gel (40-63 μm, Merck, German), and Sephadex LH-20 gel (Pharmacia Fine Chemical Co. Ltd., Sweden) were also used for column chromatography. TLC spots were visualized under UV light and by dipping into 10% H_2SO_4 in alcohol followed by heating.

Fungal Material and Identification

The strain A761 was isolated from the plant *Morinda officinalis*, which was collected from Gaoyao city of Guangdong province in January 2015. The strain was identified by sequence analysis of rDNA ITS (internal transcribed spacer) region. The sequence of ITS region of the fungus A761 has been submitted to GenBank (Accession No. KU529867). By using BLAST (nucleotide sequence comparison program) to search the GenBank database, A761 has 99.5% similarity to *Cytospora rhizophorae* M225 (Accession No. KR056292). The strain is preserved at the Guangdong Provincial Key Laboratory of Microbial Culture Collection and Application,

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Fermentation, Extraction and Isolation

Cytospora rhizophorae A761 was cultured in potato dextrose broth (potato 20%, glucose 2%, K_2HPO_4 0.3%, $MgSO_4$•$7H_2O$ 0.15%, vitamin B 10 mg/L). The fungus *C. rhizophorae* A761 was maintained on potato dextrose agar (PDA) medium at 28 °C for 5 days, and then three pieces (0.5 × 0.5 cm^2) of mycelial agar plugs were inoculated into 20 × 500 mL Erlenmeyer flasks, each containing 250 mL potato dextrose broth. After 4 days of incubation at 28 °C on a rotary shaker at 120 r/m, 25 mL seed cultures were aseptically transferred into each of a total of 100 flasks (1000 mL) containing 500 mL of potato dextrose broth. The liquid cultivation that followed was kept for 7 days at 28 °C and 120 r/m on a rotary shaker.

The culture (50 L) was centrifuged to give the broth and mycelia. The broth was exhaustively extracted with EtOAc for four times, and then the EtOAc layers were combined and evaporated under reduced pressure at a temperature not exceeding 40 °C to yield a dark brown gum (26 g). The crude EtOAc extract was subjected to reversed-phase silica gel C_{18} (MeOH/H_2O, 30%→100%) column chromatography to afford 6 fractions (Fr.1–Fr.6).

Fr. 2 was subjected to CC on Sephadex LH-20 (CH_2Cl_2/MeOH, 1:1, v/v) to yield three sub-fractions Fr.2-1 to Fr. 2-3. Fr. 2-2 was further purified by silica gel flash column chromatography (*n*-hexane/EtOAc, 2:1→1:5, v/v) to yield compound **1** (10.0 mg).

Fr. 3 was further purified by CC over reversed-phase silica gel C18 (MeOH/H_2O, 20%→100%) and silica gel flash column chromatography (*n*-hexane/EtOAc, 5:1→1:2, v/v) to yield three sub-fractions Fr.3-1 to Fr. 3-3. Fr. 3-1 was further purified by repeated silica gel and semiprep-HPLC (ACN/H_2O, 40:60, v/v, 3 mL/min) to obtain compound **2** (6.0 mg, t_R = 9.6 min). Fr. 3-3 was further purified by repeated silica gel and semiprep-HPLC (ACN/H_2O, 50:50, v/v, 3 mL/min) to obtain mixture of **3** and **4** (4.8 mg, t_R = 5.1 min). **3** (1.5 mg, t_R = 10.0 min) and **4** (1.5 mg, t_R = 13.0 min) were then successively separated from each other by chiral semi-preparative HPLC with *n*-hexane/2-propanol (2:1, v/v, 3.0 mL/min).

Cytosporin A (**1**): white powder; $[\alpha]^{20}_D$ = –54.6 (*c* 0.5, MeOH); CD (MeOH, 0.5 mg/mL): 270 (–6.88), 286 (0), 294 (+0.74); UV (MeOH) λ_{max} (log ε) 266 (5.10) , 385 (4.38) nm; IR ν_{max} 3179, 2980, 2943, 2837, 1624, 1586, 1454, 1418, 1362, 1223, 1153, 1084, 1022, 912, 858, 802, 762, 712 cm^{-1}. ^1H and ^{13}C NMR, see Table 1; HRESIMS: *m*/*z* 373.1279 $[M - H]^-$ (calcd for $C_{20}H_{21}O_8$, 373.1293).

Cytosporin B (**2**): brown solid; $[\alpha]^{20}_D$ = +22.7 (*c* 0.2, MeOH); CD (MeOH, 0.36 mg/mL): 288 (–2.68), 310 (0), 326 (+0.87); UV (MeOH) λ_{max} (log ε) 280 (5.09), 332 (4.80) nm; ^1H and ^{13}C NMR, see Table 1; HRESIMS: *m*/*z* 387.1068 $[M - H]^-$ (calcd for $C_{20}H_{19}O_8$, 387.1085).

Cytosporin C (**3**): white powder; $[\alpha]^{20}_D$ = + 12.6 (*c* 0.05, MeOH); CD (MeOH) 238 (Δε –1.39) 278 (Δε –0.72) nm; UV (MeOH) λ_{max} (log ε) 204 (5.11), 283 (3.82) nm; IR ν_{max} 3267, 2943, 2918, 2833, 1647, 1614, 1470, 1225, 1136, 1094, 1017, 930, 860, 818, 785, 721, 662, 602, 556 cm^{-1}. ^1H and ^{13}C NMR, see Table 2; HRESIMS: *m*/*z* 377.1589 $[M + H]^+$ (calcd for $C_{20}H_{25}O_7$, 377.1595).

Cytosporin D (**4**): white powder; $[\alpha]^{20}_D$ = –11.2 (*c* 0.06, MeOH); CD (MeOH) 238 (Δε +0.83) 278 (Δε +0.42) nm; UV (MeOH) λ_{max} (log ε) 204 (3.77), 283 (5.06) nm; IR ν_{max} 3256, 2943, 2918, 2835, 1645, 1470, 1225, 1018, 856, 785, 654, 631, 598, 556 cm^{-1}. ^1H and ^{13}C NMR, see Table 2; HRESIMS: *m*/*z* 377.1600 $[M + H]^+$ (calcd for $C_{20}H_{25}O_7$, 377.1595).

X-ray crytallographic data of compound 1

The single-crystal X-ray diffraction data was collected at 100K for **1** on Agilent Xcalibur Nova single-crystal diffractometer using CuKα radiation. The crystal structure was refined by full-matrix least-squares calculation. Hydrogen atoms bonded to carbons were located by the geometrically ideal positions by the "ride on" method. Hydrogen atoms bonded to oxygen were placed on the difference Fourier method and were included in the calculation of structure factors with isotropic temperature factors. Crystallographic data for **1** reported in this paper have been deposited in the Cambridge Crystallographic Data Centre. (Deposition number: CCDC 1879706). Copies of these data can be obtained free of charge via www.ccdc.cam.au.ck/conts/retrieving.html.)

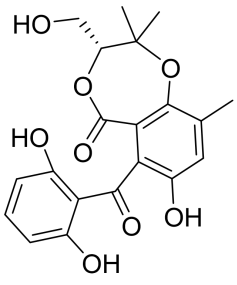
Table 1 Crystal data and structure refinement for 1

Identification code	liuhongxin_M20_collect
Empirical formula	$C_{20}H_{24}O_8$
Formula weight	392.39
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.50260(10)
b/Å	13.1145(2)
c/Å	21.4093(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1825.75(5)
Z	4
ρ_{calc}g/cm^3	1.428
μ/mm^{-1}	0.930
F(000)	832.0
Crystal size/mm^3	0.5 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.26 to 147.496
Index ranges	-3 ≤ h ≤ 7, -14 ≤ k ≤ 16, -25 ≤ l ≤ 26
Reflections collected	8427
Independent reflections	3563 [R_{int} = 0.0266, R_{sigma} = 0.0298]
Data/restraints/parameters	3563/0/263
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0275, wR_2 = 0.0724
Final R indexes [all data]	R_1 = 0.0283, wR_2 = 0.0729
Largest diff. peak/hole / e Å^{-3}	0.17/-0.19
Flack parameter	-0.08(7)

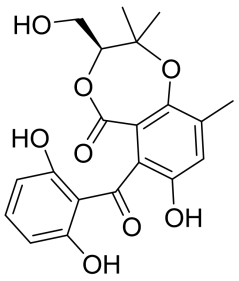
Computational methods

1. Computational Details

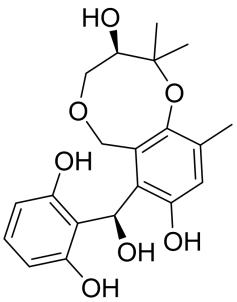
1.1. Computational method: The ECD spectra of configurations **2*S***, **3(7*R*,2'*R*)** and **3(7*S*,2'*R*)** were generated by TDDFT calculations as following, while the ECD spectra of other configurations were given by mirror inversion from their corresponding enantionmers. Conformational search was carried out to access all the possible stable conformations. The initial conformers were optimized at B3LYP/6-31G(d) theoretical level[1] with the D3BJ version of Grimme's dispersion[2] in methanol using SMD solvent model[3] by using Gaussian09 software.[4] The optimized conformers within 5.0 kcal/mol from the lowest conformer of each configuration were then used for TDDFT calculation at the CAM-B3LYP[5]/6-31G(d) level in methanol using SMD solvent model. The number of excitation states was chosen to be 40. Single point calculations were performed at B3LYP/def2-TZVP[6] theoretical level with the D3BJ version of Grimme's dispersion. Then Gibbs free energy was given by adding the thermal corrections at the B3LYP-D3BJ/6-31G(d) level to the electronic energies with solvation effect at B3LYP-D3BJ/def2TZVP level. The overall ECD curves of each configuration were weighted by Boltzmann distribution based on Gibbs free energies. The ECD spectra were generated with the help of SpecDis 1.7 software,[7] with a half-bandwidth of 0.3 eV. The most stable conformation of each configuration was illustrated using CYLview software.[8] A UV shift was made for the calculated ECD spectra to improve the superposition between experimental and calculated results.



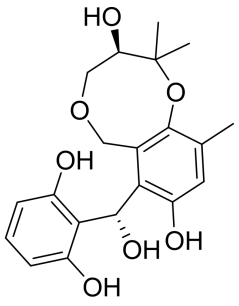
2R



2S

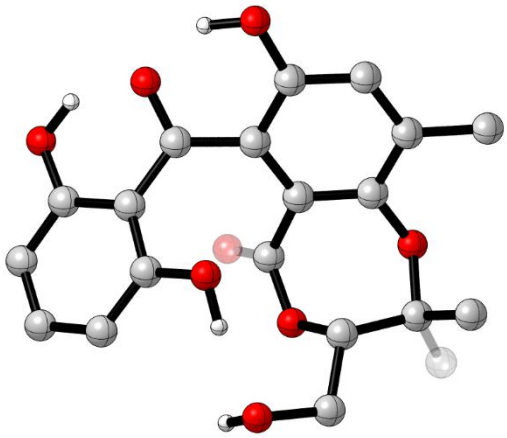


3 (7R,2'R)

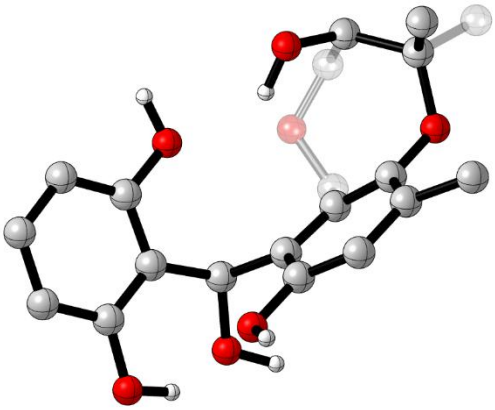


4 (7S, 2'R)

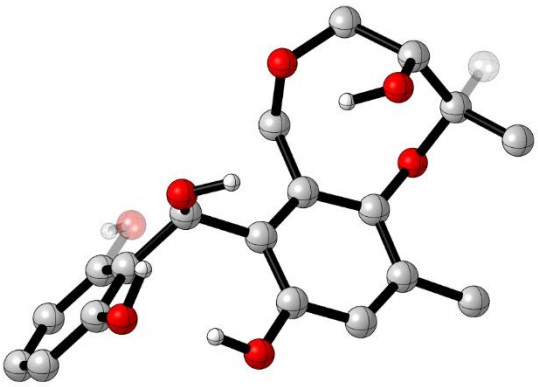
1.2. The most stable conformation of configurations **2S**, **3(7R,2'R)** and **4(7S,2'R)**. (Nonpolar hydrogen atoms omitted for clarity)



2S



3(7R,2'R)



4(7S,2'R)

1.3. Tables of energies and other thermodynamic parameters.

Conformers	E_{ele}	E_{ele}(SP)	E_0	E	H	G
2S_36	-1376.11169	-1376.66575	-1375.73360	-1375.70899	-1375.70805	-1375.78584
2S_103	-1376.10600	-1376.66358	-1375.72828	-1375.70327	-1375.70232	-1375.78084
2S_93	-1376.10600	-1376.66358	-1375.72828	-1375.70327	-1375.70232	-1375.78084
2S_5	-1376.10774	-1376.66323	-1375.73005	-1375.70522	-1375.70427	-1375.78223

Conformers	E_{ele}	E_{ele}(SP)	E_0	E	H	G
3(7R,2'R)_71	-1303.25300	-1303.78314	-1302.83414	-1302.80887	-1302.80793	-1302.88674
3(7R,2'R)_63	-1303.25345	-1303.78274	-1302.83361	-1302.80871	-1302.80776	-1302.88621
3(7R,2'R)_78	-1303.25255	-1303.78156	-1302.83186	-1302.80703	-1302.80609	-1302.88541
3(7R,2'R)_66	-1303.25307	-1303.78141	-1302.83338	-1302.80845	-1302.80751	-1302.88582
3(7R,2'R)_92	-1303.24814	-1303.77985	-1302.82896	-1302.80360	-1302.80266	-1302.88231
3(7R,2'R)_99	-1303.24738	-1303.77967	-1302.82852	-1302.80301	-1302.80207	-1302.88156
3(7R,2'R)_208	-1303.25027	-1303.78132	-1302.83077	-1302.80574	-1302.80480	-1302.88275
3(7R,2'R)_96	-1303.25007	-1303.78092	-1302.83061	-1302.80557	-1302.80463	-1302.88272
3(7R,2'R)_5	-1303.24975	-1303.78017	-1302.82972	-1302.80474	-1302.80379	-1302.88286
3(7R,2'R)_84	-1303.25469	-1303.78267	-1302.83392	-1302.80942	-1302.80847	-1302.88523

3(7R,2'R)_94	-1303.24826	-1303.77991	-1302.82851	-1302.80334	-1302.80239	-1302.88128
3(7R,2'R)_67	-1303.25214	-1303.78126	-1302.83144	-1302.80673	-1302.80579	-1302.88373
3(7R,2'R)_73	-1303.24768	-1303.77943	-1302.82839	-1302.80310	-1302.80216	-1302.88107
3(7R,2'R)_80	-1303.25188	-1303.78133	-1302.83167	-1302.80706	-1302.80611	-1302.88328
3(7R,2'R)_9	-1303.25190	-1303.78056	-1302.83150	-1302.80687	-1302.80592	-1302.88348
3(7R,2'R)_209	-1303.25190	-1303.78056	-1302.83148	-1302.80686	-1302.80592	-1302.88342
3(7R,2'R)_288	-1303.25144	-1303.78033	-1302.83111	-1302.80664	-1302.80570	-1302.88306
3(7R,2'R)_292	-1303.25162	-1303.78022	-1302.83123	-1302.80668	-1302.80573	-1302.88331
3(7R,2'R)_89	-1303.25162	-1303.78022	-1302.83123	-1302.80667	-1302.80573	-1302.88330
3(7R,2'R)_61	-1303.25205	-1303.78125	-1302.83148	-1302.80702	-1302.80607	-1302.88268
3(7R,2'R)_204	-1303.24962	-1303.77988	-1302.82935	-1302.80449	-1302.80355	-1302.88150
3(7R,2'R)_31	-1303.24879	-1303.77899	-1302.82903	-1302.80400	-1302.80305	-1302.88129
3(7R,2'R)_33	-1303.24979	-1303.77995	-1302.82942	-1302.80472	-1302.80378	-1302.88116
3(7R,2'R)_77	-1303.24979	-1303.77995	-1302.82942	-1302.80472	-1302.80378	-1302.88116
3(7R,2'R)_68	-1303.25165	-1303.78011	-1302.83116	-1302.80661	-1302.80566	-1302.88251
3(7R,2'R)_38	-1303.24984	-1303.77938	-1302.82919	-1302.80447	-1302.80353	-1302.88123
3(7R,2'R)_64	-1303.24754	-1303.77911	-1302.82711	-1302.80243	-1302.80148	-1302.87886
3(7R,2'R)_210	-1303.24723	-1303.77700	-1302.82812	-1302.80298	-1302.80204	-1302.88047
3(7R,2'R)_69	-1303.24731	-1303.77721	-1302.82772	-1302.80268	-1302.80174	-1302.88034
3(7R,2'R)_211	-1303.24783	-1303.77759	-1302.82755	-1302.80271	-1302.80176	-1302.87990

Conformers	**E_{ele}**	**E_{ele}(SP)**	**E_0**	**E**	**H**	**G**
4(7S,2'R)_160	-1303.24975	-1303.77995	-1302.83048	-1302.80528	-1302.80434	-1302.88413
4(7S,2'R)_42	-1303.24543	-1303.77808	-1302.82733	-1302.80154	-1302.80060	-1302.88137
4(7S,2'R)_43	-1303.25140	-1303.78136	-1302.83100	-1302.80620	-1302.80526	-1302.88382
4(7S,2'R)_152	-1303.25239	-1303.78126	-1302.83254	-1302.80762	-1302.80668	-1302.88473
4(7S,2'R)_6	-1303.24687	-1303.77931	-1302.82857	-1302.80359	-1302.80265	-1302.88084
4(7S,2'R)_133	-1303.24599	-1303.77899	-1302.82668	-1302.80134	-1302.80039	-1302.88014
4(7S,2'R)_33	-1303.24583	-1303.77838	-1302.82711	-1302.80157	-1302.80063	-1302.88048
4(7S,2'R)_59	-1303.24560	-1303.77826	-1302.82626	-1302.80101	-1302.80007	-1302.88016
4(7S,2'R)_148	-1303.24593	-1303.77852	-1302.82617	-1302.80106	-1302.80012	-1302.88013
4(7S,2'R)_61	-1303.24579	-1303.77705	-1302.82709	-1302.80147	-1302.80052	-1302.88046
4(7S,2'R)_5	-1303.24731	-1303.77796	-1302.82790	-1302.80272	-1302.80178	-1302.88081
4(7S,2'R)_159	-1303.24684	-1303.77901	-1302.82622	-1302.80127	-1302.80032	-1302.87920
4(7S,2'R)_179	-1303.24509	-1303.77664	-1302.82565	-1302.80034	-1302.79940	-1302.87964
4(7S,2'R)_63	-1303.24517	-1303.77698	-1302.82556	-1302.80028	-1302.79934	-1302.87930
4(7S,2'R)_14	-1303.24668	-1303.77817	-1302.82659	-1302.80168	-1302.80073	-1302.87942
4(7S,2'R)_186	-1303.24686	-1303.77776	-1302.82661	-1302.80173	-1302.80079	-1302.87934
4(7S,2'R)_158	-1303.24694	-1303.77714	-1302.82714	-1302.80212	-1302.80117	-1302.87970
4(7S,2'R)_32	-1303.24693	-1303.77618	-1302.82773	-1302.80242	-1302.80147	-1302.88058
4(7S,2'R)_16	-1303.24344	-1303.77663	-1302.82348	-1302.79828	-1302.79734	-1302.87638
4(7S,2'R)_58	-1303.24642	-1303.77648	-1302.82648	-1302.80167	-1302.80073	-1302.87894
4(7S,2'R)_46	-1303.24594	-1303.77566	-1302.82625	-1302.80119	-1302.80024	-1302.87925

4(7S,2'R)_139	-1303.24666	-1303.77706	-1302.82633	-1302.80146	-1302.80051	-1302.87854
4(7S,2'R)_162	-1303.24465	-1303.77507	-1302.82541	-1302.80016	-1302.79921	-1302.87852
4(7S,2'R)_40	-1303.24561	-1303.77553	-1302.82606	-1302.80104	-1302.80009	-1302.87870

1.4. Coordinates for the stable conformations of each configuration.

2S_103

C	-1.646204	-1.693759	-0.089603
C	-3.009783	-1.092124	0.294760
C	-1.861061	1.074008	0.350793
C	-0.499283	0.799294	0.453309
O	-2.780115	0.218088	0.914534
C	-3.879131	-0.905952	-0.946292
C	-3.720604	-1.883066	1.384447
C	-0.095998	-0.396139	1.252917
O	-0.716993	-1.564841	1.019789
C	-2.317088	2.297321	-0.188429
C	0.465221	1.733970	0.001868
C	0.005300	2.980794	-0.471989
C	-1.369635	3.228785	-0.588688
C	-3.787294	2.596107	-0.268472
O	0.838716	3.978030	-0.856352
C	1.920948	1.476308	0.023280
C	2.504703	0.153284	-0.224115
C	3.706252	-0.196297	0.457147
C	1.936106	-0.810746	-1.095133
C	4.224270	-1.490092	0.375329
C	2.478921	-2.089235	-1.202050
C	3.603058	-2.423009	-0.447279
O	2.682058	2.444093	0.280057
O	0.880053	-0.429014	-1.864557
O	4.373014	0.689407	1.231946
O	0.735680	-0.343579	2.142394
C	-1.677957	-3.180385	-0.426347
O	-0.423285	-3.634168	-0.923890
H	-1.232873	-1.147055	-0.940044
H	-3.375950	-0.272039	-1.684143
H	-4.825234	-0.435467	-0.664120
H	-4.103638	-1.867769	-1.416860
H	-4.600577	-1.326526	1.721773
H	-3.059483	-2.044196	2.241197
H	-4.055140	-2.853347	1.006424
H	-1.681615	4.194710	-0.974008
H	-4.282178	2.401297	0.688814
H	-3.954938	3.640687	-0.544061
H	-4.276706	1.961878	-1.016100
H	1.737162	3.758773	-0.520948
H	5.120943	-1.731255	0.936150
H	2.029687	-2.806908	-1.880810
H	4.016064	-3.424421	-0.526891
H	0.614128	-1.174035	-2.431790
H	3.993748	1.583326	1.057913
H	-2.481974	-3.378776	-1.144123
H	-1.874327	-3.759954	0.479050
H	-0.304571	-3.257440	-1.811519

2S_36

C	-1.745094	-1.622105	-0.219630
C	-3.078238	-1.096932	0.323268
C	-1.895873	1.051540	0.419207
C	-0.531901	0.762690	0.438864
O	-2.790205	0.177864	1.003172
C	-4.063556	-0.851543	-0.815180
C	-3.670096	-1.972556	1.417717
C	-0.131015	-0.478398	1.169070
O	-0.764073	-1.624173	0.851152
C	-2.376071	2.279738	-0.083033
C	0.424281	1.680010	-0.072077
C	-0.068093	2.931261	-0.527044
C	-1.445079	3.194859	-0.547287
C	-3.844425	2.595843	-0.070513
O	0.728506	3.927489	-0.974311
C	1.888109	1.450095	-0.115371
C	2.558766	0.143973	-0.202819
C	3.830742	0.001481	0.434127
C	2.031287	-0.995693	-0.865975
C	4.456702	-1.244269	0.519991
C	2.689985	-2.224566	-0.816436
C	3.880688	-2.344177	-0.101732
O	2.621120	2.475464	-0.038094

O	0.893159	-0.850768	-1.591157
O	4.471287	1.039795	1.016188
O	0.700744	-0.494951	2.056962
C	-1.736505	-3.026842	-0.798323
O	-0.445057	-3.325275	-1.349772
H	-1.398117	-0.944154	-0.999706
H	-3.626787	-0.202773	-1.581534
H	-4.966917	-0.376465	-0.422440
H	-4.353295	-1.795625	-1.287153
H	-4.529287	-1.465409	1.867937
H	-2.932069	-2.171384	2.200264
H	-4.012979	-2.925688	1.004026
H	-1.765893	4.165548	-0.912826
H	-4.375906	2.021000	-0.837460
H	-4.294322	2.337190	0.893177
H	-4.012349	3.658132	-0.267087
H	1.652082	3.696066	-0.709963
H	5.402682	-1.315578	1.045928
H	2.280329	-3.070590	-1.358487
H	4.380823	-3.307487	-0.058878
H	0.498467	-1.742112	-1.756114
H	4.004293	1.864572	0.738343
H	-2.450376	-3.086008	-1.622058
H	-2.002727	-3.772330	-0.042743
H	0.130814	-3.576929	-0.607277

2S_5

C	-1.790121	-1.603625	-0.127207
C	-3.148865	-1.074161	0.337987
C	-1.960051	1.070568	0.400088
C	-0.600140	0.772005	0.549786
O	-2.903495	0.237681	0.968746
C	-4.088283	-0.889104	-0.849954
C	-3.775875	-1.910426	1.443255
C	-0.216074	-0.455330	1.297689
O	-0.862939	-1.595817	0.991881
C	-2.364486	2.248512	-0.247340
C	0.396912	1.606977	0.019549
C	-0.012312	2.763282	-0.662976
C	-1.371938	3.073743	-0.774384
C	-3.819449	2.611350	-0.366260
O	0.947226	3.555439	-1.221552
C	1.865671	1.387084	0.254457
C	2.603733	0.179586	-0.124759
C	3.935280	0.013647	0.381285
C	2.071079	-0.893639	-0.898010
C	4.647247	-1.172053	0.177970
C	2.791893	-2.070206	-1.095403
C	4.067636	-2.203387	-0.547438
O	2.448150	2.331842	0.831571
O	0.849156	-0.752278	-1.466332
O	4.553322	0.978529	1.087294
O	0.646931	-0.480419	2.157264
C	-1.726245	-3.006244	-0.705931
O	-0.413694	-3.255944	-1.235388
H	-1.409171	-0.927439	-0.891874
H	-3.621925	-0.277199	-1.629089
H	-5.005661	-0.395970	-0.516285
H	-4.359686	-1.855773	-1.286016
H	-4.668354	-1.404525	1.824992
H	-3.073885	-2.054765	2.269451
H	-4.075353	-2.890137	1.058043
H	-1.657083	3.987371	-1.290659
H	-4.346732	2.451326	0.579657
H	-3.932105	3.659763	-0.656351
H	-4.320847	1.996804	-1.122571
H	0.521393	4.293378	-1.691762
H	5.646122	-1.254461	0.592822
H	2.354067	-2.863652	-1.693189
H	4.621454	-3.124310	-0.707114
H	0.483361	-1.647664	-1.668728
H	3.918480	1.748697	1.129850
H	-2.418778	-3.089200	-1.545314
H	-1.982334	-3.761703	0.043710
H	0.176094	-3.434269	-0.481857

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C	-1.646188	-1.693858	-0.089565
C	-3.009709	-1.092131	0.294847
C	-1.861009	1.073995	0.350847
C	-0.499204	0.799294	0.453086
O	-2.779961	0.218049	0.914698
C	-3.879036	-0.905815	-0.946190
C	-3.720571	-1.883106	1.384475
C	-0.095775	-0.396133	1.252653
O	-0.716844	-1.564839	1.019711
C	-2.317132	2.297354	-0.188223
C	0.465211	1.734037	0.001571

C	0.005205	2.980855	-0.472226
C	-1.369758	3.228835	-0.588643
C	-3.787359	2.596122	-0.268038
O	0.838556	3.978071	-0.856737
C	1.920921	1.476412	0.022958
C	2.504633	0.153311	-0.224152
C	1.936069	-0.810809	-1.095126
C	3.706137	-0.196209	0.457229
C	2.478869	-2.089319	-1.201836
C	4.224081	-1.490060	0.375657
C	3.602924	-2.423044	-0.446894
O	2.682044	2.444192	0.279844
O	4.372817	0.689576	1.231974
O	0.880149	-0.429162	-1.864784
O	0.736186	-0.343540	2.141864
C	-1.678009	-3.180526	-0.426117
O	-0.423392	-3.634391	-0.923700
H	-1.232937	-1.147291	-0.940135
H	-4.103614	-1.867586	-1.416818
H	-3.375784	-0.271923	-1.684006
H	-4.825101	-0.435262	-0.664019
H	-4.055069	-2.853380	1.006398
H	-4.600560	-1.326589	1.721795
H	-3.059479	-2.044271	2.241239
H	-1.681821	4.194768	-0.973880
H	-4.276795	1.962141	-1.015862
H	-4.282143	2.400919	0.689217
H	-3.955077	3.640792	-0.543235
H	1.737029	3.758927	-0.521347
H	2.029802	-2.807026	-1.880675
H	5.120685	-1.731210	0.936598
H	4.015911	-3.424476	-0.526351
H	3.993558	1.583455	1.057675
H	0.614176	-1.174370	-2.431750
H	-2.482073	-3.379026	-1.143814
H	-1.874343	-3.759968	0.479373
H	-0.304618	-3.257507	-1.811248

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C	3.354288	-1.578332	0.280878
C	3.703162	-0.167457	-0.271582
C	1.703044	1.202591	0.260956
C	0.673215	0.497795	0.896411
C	1.876963	-2.015670	0.180800
O	3.020814	0.861931	0.522153
C	5.178604	0.128578	-0.011326
C	3.378205	-0.050148	-1.758910
O	4.168478	-2.492734	-0.467748
C	1.072926	-0.550246	1.909923
O	1.146271	-1.886311	1.398294
C	1.422227	2.323794	-0.538593
C	-0.681689	0.794133	0.625744
C	-0.963010	1.922623	-0.171641
C	0.085183	2.664818	-0.724977
C	2.508795	3.164458	-1.155003
O	-2.212165	2.379033	-0.490024
C	-1.745228	-0.134470	1.192258
C	-2.814853	-0.551134	0.198593
C	-2.561786	-1.623396	-0.674516
C	-4.057934	0.090306	0.095760
C	-3.513349	-2.037551	-1.610160
C	-5.022209	-0.310514	-0.829335
C	-4.738797	-1.375879	-1.680321
O	-2.392453	0.412793	2.378952
O	-4.333289	1.193072	0.881056
O	-1.338181	-2.226519	-0.571713
H	3.644628	-1.607523	1.340164
H	1.857718	-3.086779	-0.039535
H	1.354547	-1.503526	-0.634994
H	5.394002	0.075648	1.061824
H	5.816315	-0.591137	-0.529196
H	5.426412	1.134262	-0.365339
H	3.839495	-0.882508	-2.296922
H	2.302114	-0.078660	-1.950228
H	3.776306	0.882352	-2.165496
H	4.111929	-3.356776	-0.026511
H	2.040690	-0.261908	2.332517
H	0.356742	-0.596488	2.732751
H	-0.172391	3.537554	-1.318720
H	3.451305	3.058555	-0.612755
H	2.691733	2.879113	-2.198004
H	2.220510	4.220877	-1.154344
H	-2.913576	2.068893	0.120316
H	-3.286601	-2.868333	-2.272909
H	-5.968021	0.219829	-0.870330
H	-5.479305	-1.697600	-2.406984
H	-3.768048	1.098676	1.695973
H	-1.282141	-2.962529	-1.205648

H	-1.793764	1.073116	2.768352
H	-1.242924	-1.051014	1.498524

3(7R,2'R)_33

C	2.984328	-1.881956	0.047434
C	3.516480	-0.522575	0.588996
C	1.499164	0.920481	0.540853
C	0.318341	0.271867	0.144934
C	1.894757	-1.815656	-1.043460
O	2.441965	0.211569	1.270939
C	4.511782	-0.787129	1.716691
C	4.162692	0.307307	-0.519015
O	4.134508	-2.554706	-0.482504
C	0.157506	-1.176164	0.516822
O	0.565095	-2.053870	-0.556702
C	1.688670	2.287821	0.289095
C	-0.632305	0.934554	-0.651083
C	-0.394598	2.279721	-0.977609
C	0.724525	2.945489	-0.477611
C	2.873022	3.054218	0.817301
O	-1.302758	2.923638	-1.776151
C	-1.852821	0.220591	-1.222742
C	-2.883394	-0.231641	-0.177978
C	-3.437468	0.731008	0.688391
C	-3.379179	-1.547989	-0.068784
C	-4.377604	0.399233	1.666809
C	-4.321431	-1.892748	0.910359
C	-4.808816	-0.921728	1.776123
O	-1.427926	-0.860171	-2.094868
O	-2.969449	-2.556674	-0.893519
O	-3.020160	2.024634	0.524308
H	2.584164	-2.451807	0.896175
H	2.072473	-2.626448	-1.753795
H	1.926966	-0.873023	-1.599902
H	4.039807	-1.371421	2.514509
H	5.377871	-1.339902	1.346076
H	4.856273	0.162154	2.138930
H	3.431992	0.672815	-1.245383
H	4.687469	1.166555	-0.095452
H	4.890645	-0.308032	-1.054032
H	3.883714	-3.481061	-0.635753
H	0.736654	-1.398813	1.414661
H	-0.882089	-1.436500	0.709206
H	0.853114	4.002156	-0.703209
H	3.623438	3.224326	0.036267
H	2.555229	4.038627	1.178271
H	3.360051	2.524632	1.638830
H	-1.005053	3.836544	-1.932457
H	-4.765860	1.175381	2.321083
H	-4.659470	-2.923124	0.960513
H	-5.539094	-1.189205	2.534764
H	-2.402961	-2.135982	-1.587739
H	-3.461834	2.588542	1.182221
H	-0.640009	-1.302655	-1.698542
H	-2.355603	0.922659	-1.890406

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C	3.336792	-1.584825	0.279728
C	3.691184	-0.173699	-0.282241
C	1.712432	1.209619	0.280144
C	0.682023	0.499305	0.907526
C	1.861960	-2.013466	0.162819
O	3.031352	0.861413	0.526758
C	5.173883	0.113689	-0.049017
C	3.346224	-0.055653	-1.764424
O	4.081742	-2.590545	-0.422435
C	1.074463	-0.562991	1.908396
O	1.131755	-1.894850	1.381315
C	1.432224	2.337929	-0.509903
C	-0.672707	0.795039	0.636731
C	-0.952955	1.929111	-0.149922
C	0.095591	2.680245	-0.692682
C	2.520429	3.178479	-1.123564
O	-2.202628	2.386702	-0.469008
C	-1.728232	-0.157756	1.175100
C	-2.806274	-0.545361	0.176196
C	-4.046168	0.104694	0.110322
C	-2.572523	-1.598403	-0.724073
C	-5.027833	-0.266737	-0.808273
C	-3.541573	-1.985631	-1.653551
C	-4.763686	-1.314375	-1.687942
O	-2.292478	0.400888	2.397499
O	-1.350776	-2.210192	-0.651336
O	-4.296342	1.188487	0.930476
H	3.611397	-1.602457	1.342855
H	1.845224	-3.080271	-0.072987
H	1.343252	-1.483056	-0.642530
H	5.429454	-0.001423	1.010453

H	5.805887	-0.557941	-0.638179
H	5.404724	1.139458	-0.351996
H	3.760759	-0.916941	-2.295533
H	2.267255	-0.037386	-1.938847
H	3.779782	0.851577	-2.192061
H	5.018770	-2.491863	-0.187983
H	2.046151	-0.290773	2.332839
H	0.357820	-0.608198	2.730738
H	-0.162746	3.558586	-1.277722
H	2.732958	2.867309	-2.153494
H	2.216941	4.229891	-1.158204
H	3.452327	3.101580	-0.557941
H	-2.900374	2.079021	0.146450
H	-5.971231	0.269226	-0.822926
H	-3.331279	-2.802888	-2.338237
H	-5.517782	-1.614594	-2.409797
H	-1.310161	-2.936645	-1.297143
H	-3.708961	1.079741	1.726624
H	-2.664476	-0.341620	2.907898
H	-1.218220	-1.080841	1.443344

3(7R,2'R)_5

C	-2.456898	-2.067733	-0.107376
C	-3.267107	-0.769230	0.191900
C	-1.751188	1.055810	-0.523645
C	-0.509625	0.614507	-1.011437
C	-0.934784	-1.994446	0.120489
O	-2.879909	0.286827	-0.755377
C	-4.739746	-0.996911	-0.145545
C	-3.111124	-0.330080	1.645814
O	-2.918860	-3.134539	0.732968
C	-0.491763	-0.657452	-1.825533
O	-0.186175	-1.843110	-1.081290
C	-1.891837	2.306071	0.101487
C	0.656159	1.356643	-0.737244
C	0.513491	2.581485	-0.067819
C	-0.736369	3.058313	0.312807
C	-3.231504	2.845728	0.528422
O	1.617578	3.342809	0.277097
C	2.024702	0.805698	-1.111205
C	2.579361	-0.181913	-0.098211
C	2.716386	0.071165	1.285047
C	2.948281	-1.465939	-0.559692
C	3.166863	-0.930128	2.157170
C	3.395810	-2.464778	0.305349
C	3.495262	-2.187222	1.667111
O	2.935377	1.912819	-1.377968
O	2.840964	-1.705170	-1.903180
O	2.416599	1.253694	1.893119
H	-2.625350	-2.332192	-1.159825
H	-0.613536	-2.953467	0.533911
H	-0.662718	-1.212445	0.838698
H	-5.294983	-0.061234	-0.029726
H	-4.853424	-1.343221	-1.179026
H	-5.188959	-1.736243	0.524500
H	-3.292768	-1.190350	2.295929
H	-2.109233	0.050937	1.860381
H	-3.837169	0.447208	1.895478
H	-3.830134	-3.349227	0.475054
H	-1.466943	-0.768704	-2.309938
H	0.263751	-0.616660	-2.611224
H	-0.795437	4.029309	0.796622
H	-3.408048	2.678983	1.597785
H	-3.278369	3.926419	0.357212
H	-4.046939	2.369209	-0.020426
H	2.332466	3.099478	-0.371798
H	3.250952	-0.693077	3.212871
H	3.659589	-3.441124	-0.091745
H	3.841270	-2.958768	2.349164
H	3.061622	-2.636102	-2.078811
H	2.280658	2.004794	1.276733
H	3.835948	1.615719	-1.161527
H	1.926934	0.266600	-2.050564

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C	3.214627	-1.651177	0.233036
C	3.681829	-0.234870	-0.230271
C	1.721784	1.206685	0.286538
C	0.652842	0.548550	0.910649
C	1.722155	-1.987748	0.036803
O	3.019821	0.808051	0.566335
C	5.152848	-0.051701	0.135067
C	3.466861	-0.019435	-1.727249
O	4.017173	-2.654675	-0.402934
C	1.002258	-0.570023	1.856180
O	0.930376	-1.866139	1.230375
C	1.497712	2.337633	-0.515953
C	-0.687461	0.900017	0.629027

C	-0.910476	2.004922	-0.221182
C	0.177023	2.709608	-0.747988
C	2.621563	3.152927	-1.098689
O	-2.126374	2.481517	-0.614264
C	-1.810059	0.077016	1.248589
C	-2.786733	-0.519448	0.247156
C	-4.002817	0.108655	-0.081103
C	-2.493055	-1.739303	-0.398310
C	-4.887372	-0.419313	-1.017797
C	-3.375486	-2.276295	-1.344991
C	-4.559488	-1.615767	-1.652898
O	-2.552924	0.821886	2.253101
O	-1.371538	-2.480767	-0.169438
O	-4.339491	1.319993	0.499324
H	3.448528	-1.748148	1.297455
H	1.648266	-3.044289	-0.228494
H	1.269266	-1.402103	-0.770342
H	5.293218	-0.160993	1.216279
H	5.771641	-0.795474	-0.371692
H	5.491772	0.946455	-0.159673
H	3.951119	-0.822085	-2.292281
H	2.408587	-0.001280	-2.001620
H	3.922710	0.921200	-2.043067
H	3.743016	-2.721431	-1.333323
H	2.009186	-0.411042	2.246543
H	0.325479	-0.625399	2.708936
H	-0.038720	3.577058	-1.365730
H	2.372902	4.219003	-1.065664
H	3.554411	2.995280	-0.552829
H	2.800828	2.895762	-2.149360
H	-2.891443	2.116208	-0.118962
H	-5.809636	0.110866	-1.231248
H	-3.109880	-3.214386	-1.822011
H	-5.237161	-2.040953	-2.387769
H	-0.732038	-2.095584	0.470780
H	-3.871887	1.348657	1.377668
H	-1.966421	1.508373	2.615722
H	-1.361423	-0.760209	1.781025

3(7R,2'R)_63

C	-1.969604	-2.040539	0.625716
C	-3.168288	-1.114755	0.279902
C	-1.866265	0.807633	-0.560954
C	-0.579556	0.492180	-1.030477
C	-1.219897	-2.695379	-0.547097
O	-2.877406	-0.115229	-0.758947
C	-4.293131	-1.934563	-0.350096
C	-3.657815	-0.442514	1.562592
O	-1.018309	-1.420282	1.492435
C	-0.404835	-0.794980	-1.802902
O	-0.096001	-1.929231	-0.973454
C	-2.156904	2.069346	-0.016213
C	0.494995	1.368049	-0.778571
C	0.214279	2.582768	-0.132965
C	-1.088401	2.942598	0.193388
C	-3.561246	2.516200	0.298824
O	1.225584	3.451490	0.239021
C	1.920530	0.955161	-1.126515
C	2.512567	-0.004996	-0.111000
C	2.562211	0.238329	1.279996
C	2.989720	-1.253284	-0.568516
C	3.034129	-0.742973	2.162880
C	3.460973	-2.231668	0.307123
C	3.471118	-1.968057	1.675121
O	2.746113	2.139052	-1.334243
O	2.960112	-1.481161	-1.918065
O	2.154716	1.391101	1.883733
H	-2.426993	-2.856256	1.199427
H	-1.885769	-2.905040	-1.391190
H	-0.792581	-3.640368	-0.200686
H	-3.976721	-2.393722	-1.291474
H	-4.621577	-2.726437	0.330048
H	-5.148465	-1.284444	-0.560010
H	-3.870160	-1.207694	2.317409
H	-2.904874	0.231681	1.975560
H	-4.578358	0.115629	1.376673
H	-0.248504	-1.197624	0.936047
H	-1.314624	-1.003600	-2.372384
H	0.422059	-0.718553	-2.508238
H	-1.259091	3.921516	0.632746
H	-4.299915	1.895900	-0.212898
H	-3.772076	2.472234	1.373389
H	-3.702235	3.555947	-0.016269
H	1.984604	3.270420	-0.378636
H	3.048682	-0.517160	3.224229
H	3.809468	-3.182659	-0.086115
H	3.832730	-2.724886	2.365463
H	3.249313	-2.393635	-2.090909

H	1.982355	2.136013	1.270805
H	3.642220	1.936537	-1.014670
H	1.904558	0.438937	-2.083586

3(7R,2'R)_64

C	3.200755	-1.665855	0.211854
C	3.670896	-0.255210	-0.247256
C	1.741505	1.210106	0.301896
C	0.660684	0.557812	0.914110
C	1.705023	-1.991883	0.024658
O	3.033902	0.782673	0.571249
C	5.151649	-0.086496	0.087447
C	3.424507	-0.040230	-1.739303
O	3.975055	-2.594258	-0.559229
C	0.999583	-0.571237	1.851309
O	0.919566	-1.866250	1.221809
C	1.539622	2.357215	-0.480694
C	-0.675577	0.931031	0.640957
C	-0.872232	2.060610	-0.181172
C	0.224785	2.757608	-0.698297
C	2.678407	3.155450	-1.058167
O	-2.081475	2.572626	-0.556942
C	-1.811501	0.099962	1.253147
C	-2.775843	-0.499579	0.230278
C	-2.497774	-1.743787	-0.376854
C	-3.983898	0.118941	-0.132133
C	-3.389905	-2.311406	-1.298180
C	-4.883654	-0.433118	-1.037650
C	-4.572218	-1.659665	-1.622938
O	-2.454403	0.760625	2.352488
O	-4.247779	1.342844	0.463552
O	-1.388297	-2.492351	-0.122976
H	3.447020	-1.775666	1.276304
H	1.616669	-3.046986	-0.244872
H	1.254163	-1.404193	-0.781901
H	5.316954	-0.221250	1.162265
H	5.485521	0.917846	-0.191518
H	5.756896	-0.819048	-0.450952
H	2.360280	0.031777	-1.979616
H	3.918951	0.872175	-2.079899
H	3.840474	-0.882879	-2.297634
H	3.841290	-3.474897	-0.170690
H	0.320526	-0.624537	2.702488
H	2.007276	-0.423938	2.244002
H	0.021231	3.641317	-1.297166
H	2.443577	4.224881	-1.033734
H	3.604664	2.989202	-0.503237
H	2.865094	2.889362	-2.105387
H	-2.841038	2.203463	-0.059036
H	-3.132364	-3.269149	-1.738958
H	-5.802102	0.095413	-1.276860
H	-5.259067	-2.106822	-2.335509
H	-5.073492	1.726735	0.116431
H	-0.729245	-2.085425	0.484652
H	-3.179973	1.308718	2.007168
H	-1.344745	-0.754985	1.735977

3(7R,2'R)_66

C	-1.716382	-2.231003	0.594788
C	-2.957923	-1.466933	0.060978
C	-1.861530	0.649023	-0.594499
C	-0.465575	0.568140	-0.753026
C	-0.703463	-2.711038	-0.460661
O	-2.630280	-0.449728	-0.945742
C	-3.860831	-2.427925	-0.711493
C	-3.718582	-0.857440	1.237670
O	-1.018146	-1.525001	1.622128
C	0.062898	-0.649744	-1.484024
O	0.359331	-1.783980	-0.654027
C	-2.488012	1.851829	-0.236331
C	0.362909	1.643440	-0.363012
C	-0.273907	2.845357	0.023124
C	-1.665726	2.935247	0.062789
C	-3.985383	2.020706	-0.223228
O	0.401322	3.996257	0.329928
C	1.902502	1.563737	-0.405956
C	2.502337	0.223175	-0.038220
C	3.287143	-0.514453	-0.933851
C	2.331361	-0.290939	1.255130
C	3.857423	-1.736719	-0.563108
C	2.892572	-1.504986	1.649079
C	3.653913	-2.221570	0.726249
O	2.509029	2.559556	0.466870
O	1.569829	0.471854	2.107344
O	3.438880	-0.007323	-2.196841
H	-2.133704	-3.126176	1.071131
H	-1.191078	-2.947148	-1.412924
H	-0.214754	-3.616398	-0.090438

H	-4.736375	-1.888367	-1.086124
H	-3.341526	-2.868813	-1.568157
H	-4.207453	-3.237306	-0.061528
H	-3.923191	-1.634552	1.982359
H	-3.137021	-0.073107	1.726262
H	-4.673715	-0.443982	0.906014
H	-0.247110	-1.111514	1.193299
H	0.986337	-0.407980	-2.008130
H	-0.673304	-0.948917	-2.235933
H	-2.103202	3.892599	0.333641
H	-4.475722	1.273988	-0.851952
H	-4.397245	1.926402	0.788153
H	-4.254645	3.016770	-0.590965
H	1.360647	3.756693	0.378235
H	4.451049	-2.292013	-1.284341
H	2.731747	-1.874090	2.657944
H	4.095094	-3.170438	1.017435
H	1.551897	0.063012	2.990339
H	3.984385	-0.616755	-2.723856
H	2.326867	2.263220	1.381032
H	2.247839	1.844347	-1.403154

3(7R,2'R)_67

C	-3.177620	-1.617559	0.587750
C	-3.667920	-0.610756	-0.486860
C	-1.631110	0.806110	-0.558540
C	-0.436930	0.174770	-0.169154
C	-2.117996	-2.648408	0.160656
O	-2.582347	0.051732	-1.222274
C	-4.420014	-1.351094	-1.591379
C	-4.586059	0.414514	0.179758
O	-2.732830	-0.974512	1.783033
C	-0.252842	-1.273977	-0.548109
O	-0.788767	-2.197976	0.417737
C	-1.800068	2.194767	-0.424035
C	0.555809	0.899571	0.524666
C	0.356194	2.281674	0.705859
C	-0.788514	2.907971	0.218622
C	-2.976517	2.932148	-1.008896
O	1.268005	3.081273	1.359363
C	1.778520	0.247113	1.170265
C	2.880264	-0.213099	0.218960
C	3.232399	-1.556309	-0.028842
C	3.644892	0.775699	-0.424814
C	4.277807	-1.877576	-0.905827
C	4.686533	0.471133	-1.298967
C	4.993564	-0.868415	-1.537145
O	1.400557	-0.861787	2.013763
O	3.312326	2.082114	-0.151690
O	2.579854	-2.613193	0.540547
H	-4.079341	-2.182967	0.853975
H	-2.230162	-2.941058	-0.888561
H	-2.232525	-3.540937	0.781734
H	-3.776807	-2.073623	-2.102613
H	-5.282112	-1.883412	-1.177992
H	-4.782964	-0.632923	-2.333498
H	-5.388563	-0.106735	0.713299
H	-4.047063	1.025672	0.906487
H	-5.042757	1.065496	-0.569233
H	-1.758772	-1.014557	1.755107
H	-0.721276	-1.456571	-1.519102
H	0.802082	-1.514373	-0.637174
H	-0.871623	3.985156	0.332824
H	-3.439282	2.362187	-1.817770
H	-3.749022	3.131970	-0.257751
H	-2.650811	3.899785	-1.405051
H	2.162147	2.839400	1.037276
H	4.507378	-2.925633	-1.070412
H	5.241292	1.273996	-1.776514
H	5.802590	-1.122056	-2.216127
H	3.905899	2.691739	-0.623431
H	1.952743	-2.247120	1.209695
H	0.502407	-0.706414	2.348885
H	2.219803	1.002114	1.828320

3(7R,2'R)_68

C	3.131069	-1.775918	0.013473
C	3.591691	-0.394362	0.562498
C	1.496110	0.942965	0.539902
C	0.347055	0.237991	0.148356
C	2.035241	-1.757054	-1.072267
O	2.480361	0.275203	1.251644
C	4.601820	-0.612367	1.686851
C	4.187216	0.476809	-0.541572
O	4.311758	-2.384807	-0.525345
C	0.271248	-1.221617	0.501194
O	0.721764	-2.066270	-0.581404
C	1.609291	2.325959	0.320427

C	-0.657521	0.868848	-0.611656
C	-0.521945	2.245510	-0.862478
C	0.580098	2.952211	-0.382705
C	2.765615	3.138006	0.842029
O	-1.453580	2.958139	-1.585232
C	-1.830124	0.096004	-1.215398
C	-2.900931	-0.326704	-0.201084
C	-3.250675	-1.660332	0.091623
C	-3.638979	0.677717	0.449741
C	-4.236314	-1.963422	1.040222
C	-4.624376	0.394027	1.394702
C	-4.910496	-0.938192	1.691706
O	-1.370890	-1.011601	-2.027671
O	-3.344026	1.977674	0.111175
O	-2.647100	-2.721713	-0.521296
H	2.762917	-2.371320	0.859099
H	2.250294	-2.553061	-1.788857
H	2.016575	-0.810781	-1.623008
H	4.905529	0.351420	2.107274
H	4.159087	-1.216511	2.486557
H	5.489854	-1.127317	1.313652
H	4.942013	-0.095944	-1.086963
H	3.432760	0.810144	-1.259039
H	4.670467	1.358110	-0.114237
H	4.111096	-3.323913	-0.675503
H	0.866720	-1.418972	1.394320
H	-0.749707	-1.543120	0.696921
H	0.619593	4.022731	-0.563872
H	3.505935	3.334568	0.057554
H	2.412350	4.110109	1.202684
H	3.276951	2.628744	1.662046
H	-2.339085	2.708861	-1.246318
H	-4.460101	-3.007387	1.236322
H	-5.156497	1.208307	1.878716
H	-5.675243	-1.173402	2.426365
H	-3.935139	2.592826	0.578716
H	-2.135044	-2.346044	-1.278523
H	-0.511901	-1.351246	-1.681527
H	-2.316268	0.763730	-1.930745

3(7R,2'R)_69

C	-3.115530	-1.827727	-0.038468
C	-3.611856	-0.414392	-0.450767
C	-1.548027	0.966440	-0.537340
C	-0.373929	0.278848	-0.185195
C	-1.917836	-1.887038	0.933726
O	-2.556361	0.281738	-1.197035
C	-4.725869	-0.551293	-1.486668
C	-4.089737	0.389359	0.756894
O	-4.248322	-2.470043	0.563944
C	-0.259220	-1.155942	-0.646808
O	-0.671334	-2.150531	0.299448
C	-1.674606	2.352894	-0.346956
C	0.651852	0.950518	0.512180
C	0.522442	2.338729	0.699228
C	-0.612585	3.019225	0.261858
C	-2.881528	3.125822	-0.810300
O	1.493294	3.091750	1.324264
C	1.833337	0.239371	1.162861
C	2.899405	-0.306345	0.217331
C	3.127021	-1.675268	-0.025881
C	3.750969	0.611525	-0.419736
C	4.152289	-2.093731	-0.884802
C	4.772917	0.211523	-1.278965
C	4.963432	-1.151834	-1.506568
O	1.299773	-0.784379	2.039718
O	3.524081	1.942629	-0.152611
O	2.360540	-2.655716	0.536779
H	-2.829220	-2.363668	-0.954078
H	-2.073848	-2.737469	1.603618
H	-1.849335	-0.986806	1.556276
H	-5.055677	0.439184	-1.815796
H	-4.365133	-1.104733	-2.360852
H	-5.582531	-1.084308	-1.067808
H	-4.809829	-0.206671	1.323630
H	-3.269803	0.656366	1.429346
H	-4.586416	1.307105	0.434660
H	-4.020981	-3.407790	0.678839
H	-0.848623	-1.260354	-1.563408
H	0.772448	-1.402902	-0.887778
H	-0.653319	4.095563	0.403795
H	-3.586195	3.298901	0.012072
H	-2.580835	4.108629	-1.188732
H	-3.418338	2.597321	-1.601419
H	2.365901	2.795740	0.988738
H	4.290119	-3.157989	-1.047939
H	5.403470	0.958246	-1.753524
H	5.756054	-1.478005	-2.173915

H	4.163048	2.501363	-0.628236
H	1.735341	-2.218269	1.164426
H	1.931040	-0.892189	2.772990
H	2.321643	0.975032	1.805320

3(7R,2'R)_71

C	2.867845	-1.719622	-0.343569
C	3.670483	-0.386206	-0.357664
C	1.807469	1.107489	0.256875
C	0.760934	0.461626	0.934983
C	2.493449	-2.310648	1.027509
O	3.101836	0.674906	0.484096
C	5.051353	-0.602528	0.260256
C	3.810075	0.091699	-1.803569
O	1.716339	-1.694391	-1.186559
C	1.125130	-0.565595	1.984815
O	1.208281	-1.908455	1.490527
C	1.568509	2.247730	-0.525946
C	-0.576623	0.820397	0.678883
C	-0.816263	1.943361	-0.133741
C	0.242511	2.650516	-0.700136
C	2.681491	3.065264	-1.127425
O	-2.110637	2.341377	-0.319006
C	-1.726359	0.016648	1.263140
C	-2.737976	-0.451196	0.223014
C	-4.034180	0.079155	0.068322
C	-2.357457	-1.490722	-0.643836
C	-4.901857	-0.412268	-0.916750
C	-3.209431	-1.982951	-1.634043
C	-4.484593	-1.433513	-1.762555
O	-2.406542	0.741934	2.322058
O	-1.097296	-2.007543	-0.470039
O	-4.510516	1.085693	0.854697
H	3.558650	-2.435348	-0.805837
H	3.258894	-2.090762	1.780721
H	2.418314	-3.396622	0.923514
H	4.981798	-0.906979	1.308955
H	5.603784	-1.371209	-0.288913
H	5.623006	0.329938	0.215330
H	4.243479	-0.708109	-2.414011
H	2.841900	0.353128	-2.235379
H	4.473368	0.958521	-1.856901
H	0.937313	-1.507329	-0.629650
H	2.079402	-0.285151	2.440880
H	0.372253	-0.582120	2.775104
H	0.025932	3.538769	-1.289992
H	2.855302	2.803705	-2.177464
H	2.426647	4.129859	-1.095626
H	3.620306	2.915418	-0.589247
H	-2.129565	3.098376	-0.929824
H	-5.892074	0.025021	-0.999174
H	-2.869049	-2.784441	-2.284314
H	-5.157414	-1.810470	-2.527877
H	-0.947607	-2.729764	-1.105048
H	-3.821657	1.256489	1.542996
H	-1.812032	1.445928	2.631772
H	-1.309729	-0.886818	1.712403

3(7R,2'R)_73

C	3.378592	-1.578786	0.310356
C	3.726066	-0.168516	-0.242949
C	1.707800	1.190312	0.258448
C	0.672144	0.481340	0.888163
C	1.905594	-2.023536	0.184032
O	3.024247	0.856435	0.537969
C	5.195670	0.139148	0.036398
C	3.421912	-0.058665	-1.735350
O	4.212020	-2.491651	-0.418613
C	1.063298	-0.567326	1.903038
O	1.149991	-1.901423	1.387192
C	1.434765	2.308308	-0.545408
C	-0.673535	0.785059	0.610377
C	-0.942837	1.903502	-0.195881
C	0.097339	2.650279	-0.749871
C	2.526044	3.147158	-1.156258
O	-2.246688	2.261326	-0.396716
C	-1.785535	-0.070239	1.193455
C	-2.849323	-0.507237	0.191940
C	-4.146792	0.034521	0.127435
C	-2.526176	-1.530401	-0.715792
C	-5.080478	-0.436135	-0.805137
C	-3.444921	-2.004078	-1.655144
C	-4.723480	-1.447865	-1.690106
O	-2.347751	0.644006	2.326771
O	-1.255943	-2.040367	-0.634199
O	-4.559638	1.036100	0.957442
H	3.650175	-1.600458	1.374720
H	1.895936	-3.094073	-0.040064

H	1.396444	-1.510861	-0.639473
H	5.440615	1.145843	-0.316777
H	5.397207	0.090369	1.112426
H	5.845422	-0.577093	-0.471317
H	3.892988	-0.891936	-2.263559
H	2.348785	-0.090574	-1.942129
H	3.823127	0.873320	-2.140168
H	4.152963	-3.353826	0.025853
H	2.023497	-0.276198	2.341026
H	0.335167	-0.618388	2.714574
H	-0.146385	3.523511	-1.351567
H	2.708558	2.867306	-2.200899
H	2.243381	4.205214	-1.149643
H	3.467302	3.033545	-0.613681
H	-2.280663	3.026282	-0.996664
H	-6.070775	0.008439	-0.818673
H	-3.154644	-2.795008	-2.341638
H	-5.446748	-1.810412	-2.415402
H	-1.151234	-2.758099	-1.282281
H	-3.821301	1.209297	1.589371
H	-2.768362	-0.018244	2.904334
H	-1.328234	-0.984421	1.572384

3(7R,2'R)_77

C	2.984283	-1.882048	0.047569
C	3.516546	-0.522570	0.588840
C	1.499423	0.920548	0.540941
C	0.318570	0.271942	0.145158
C	1.894656	-1.816022	-1.043240
O	2.442356	0.211719	1.270946
C	4.512194	-0.787080	1.716289
C	4.162575	0.307220	-0.519412
O	4.134397	-2.554917	-0.482370
C	0.157867	-1.176103	0.517207
O	0.564989	-2.053838	-0.556361
C	1.688907	2.287910	0.289187
C	-0.632246	0.934657	-0.650729
C	-0.394488	2.279780	-0.977323
C	0.724697	2.945563	-0.477398
C	2.873284	3.054328	0.817238
O	-1.302682	2.923765	-1.775784
C	-1.852681	0.220669	-1.222538
C	-2.883452	-0.231643	-0.177906
C	-3.379101	-1.548072	-0.068811
C	-3.438003	0.730978	0.688146
C	-4.321683	-1.892872	0.910002
C	-4.378492	0.399142	1.666250
C	-4.809570	-0.921855	1.775516
O	-1.427779	-0.859898	-2.094830
O	-3.020814	2.024664	0.524250
O	-2.968894	-2.556780	-0.893299
H	2.584208	-2.451747	0.896464
H	2.072163	-2.627144	-1.753230
H	1.927053	-0.873602	-1.600029
H	5.378181	-1.339866	1.345468
H	4.856765	0.162250	2.138352
H	4.040465	-1.371306	2.514296
H	3.431652	0.672760	-1.245538
H	4.687446	1.166466	-0.095959
H	4.890362	-0.308125	-1.054594
H	3.883328	-3.481072	-0.636355
H	0.737378	-1.398642	1.414835
H	-0.881661	-1.436315	0.710066
H	0.853195	4.002240	-0.702991
H	3.623749	3.224207	0.036202
H	2.555553	4.038812	1.178033
H	3.360298	2.524921	1.638905
H	-1.004027	3.836099	-1.933557
H	-4.659593	-2.923291	0.960071
H	-4.767024	1.175310	2.320330
H	-5.540160	-1.189365	2.533835
H	-3.463497	2.588659	1.181386
H	-2.402674	-2.135993	-1.587743
H	-0.640045	-1.302632	-1.698437
H	-2.355423	0.922826	-1.890133

3(7R,2'R)_78

C	-2.843741	-1.686903	0.632260
C	-3.473992	-0.869240	-0.539602
C	-1.648380	0.768624	-0.648947
C	-0.410639	0.226854	-0.265376
C	-1.702495	-2.673448	0.334854
O	-2.534701	-0.051965	-1.321913
C	-4.055183	-1.815722	-1.588441
C	-4.577036	0.021591	0.036074
O	-2.534644	-0.902684	1.785779
C	-0.089337	-1.184681	-0.686906
O	-0.381390	-2.129579	0.361256

C	-1.947600	2.121097	-0.424484
C	0.469091	0.969555	0.545651
C	0.120205	2.294912	0.854687
C	-1.040096	2.865764	0.331320
C	-3.177575	2.783828	-0.987914
O	0.966077	3.018371	1.652770
C	1.703891	0.346234	1.185052
C	2.804050	-0.082527	0.206631
C	3.365700	-1.375170	0.154239
C	3.349360	0.887047	-0.656927
C	4.376486	-1.691495	-0.764282
C	4.355873	0.583142	-1.576226
C	4.860042	-0.715580	-1.627052
O	1.290975	-0.726025	2.075580
O	2.848896	2.157375	-0.551611
O	2.956361	-2.386298	0.975415
H	-3.676593	-2.323278	0.952140
H	-1.866682	-3.186470	-0.619627
H	-1.697634	-3.422958	1.130143
H	-3.275586	-2.416277	-2.065707
H	-4.789293	-2.490186	-1.137007
H	-4.557246	-1.233008	-2.367386
H	-5.312915	-0.594353	0.564551
H	-4.177162	0.746948	0.747019
H	-5.090595	0.552916	-0.769389
H	-1.716207	-0.409453	1.608410
H	-0.647872	-1.450152	-1.586576
H	0.973736	-1.293793	-0.896298
H	-1.248361	3.914619	0.532530
H	-3.576165	2.222647	-1.835818
H	-3.974264	2.868634	-0.240238
H	-2.936357	3.798250	-1.322991
H	0.593950	3.906294	1.793613
H	4.767116	-2.704284	-0.773084
H	4.735692	1.362421	-2.231853
H	5.643414	-0.961676	-2.338500
H	3.298510	2.731810	-1.194768
H	2.332384	-1.981883	1.627563
H	0.536004	-1.208183	1.666766
H	2.137793	1.094552	1.850649

3(7R,2'R)_80

C	3.220094	-1.642242	0.230542
C	3.676353	-0.229108	-0.235387
C	1.719554	1.208225	0.290244
C	0.651462	0.548431	0.913212
C	1.729459	-1.987956	0.036161
O	3.017787	0.808265	0.567646
C	5.150868	-0.037638	0.113570
C	3.441664	-0.027992	-1.731058
O	4.011189	-2.565769	-0.528923
C	1.002767	-0.571614	1.856387
O	0.935381	-1.867034	1.228691
C	1.495831	2.339614	-0.511379
C	-0.688870	0.900479	0.632656
C	-0.912054	2.007241	-0.215224
C	0.175245	2.712733	-0.741689
C	2.620916	3.150802	-1.097085
O	-2.127932	2.485098	-0.606567
C	-1.810917	0.075142	1.249860
C	-2.785100	-0.521454	0.246110
C	-2.488915	-1.740263	-0.400290
C	-4.001054	0.105968	-0.083934
C	-3.368717	-2.276461	-1.349886
C	-4.882925	-0.421216	-1.023576
C	-4.552430	-1.616348	-1.659808
O	-2.556352	0.817445	2.254554
O	-4.340508	1.315814	0.498112
O	-1.368000	-2.482022	-0.169189
H	3.460993	-1.742195	1.297164
H	1.655737	-3.045196	-0.228957
H	1.275698	-1.409721	-0.775565
H	5.306533	-0.162076	1.191052
H	5.771167	-0.766075	-0.413074
H	5.474586	0.968831	-0.169602
H	3.874906	-0.867990	-2.280133
H	2.378867	0.027109	-1.982075
H	3.926070	0.889452	-2.072604
H	3.885604	-3.445541	-0.135644
H	2.008654	-0.410335	2.248173
H	0.324850	-0.630060	2.708114
H	-0.040810	3.580614	-1.358689
H	3.551903	2.998593	-0.546436
H	2.804708	2.883089	-2.144320
H	2.371407	4.216911	-1.075161
H	-2.893338	2.115906	-0.114697
H	-3.101143	-3.213488	-1.827886
H	-5.805104	0.108545	-1.238435

H	-5.227812	-2.040826	-2.397195
H	-3.875022	1.343265	1.377633
H	-0.726697	-2.095061	0.468244
H	-1.972130	1.505881	2.617170
H	-1.361532	-0.762073	1.781757

3(7R,2'R)_84

C	2.828505	-1.696559	-0.404997
C	3.651927	-0.375165	-0.376537
C	1.809466	1.119002	0.292869
C	0.769052	0.463624	0.962143
C	2.453100	-2.336753	0.942876
O	3.104142	0.674354	0.493666
C	5.028566	-0.633564	0.235239
C	3.801572	0.143038	-1.807749
O	1.672742	-1.624921	-1.239883
C	1.135674	-0.597051	1.976107
O	1.181755	-1.925784	1.436290
C	1.561521	2.274946	-0.466692
C	-0.578082	0.814202	0.721777
C	-0.830291	1.954798	-0.065790
C	0.235055	2.673822	-0.615751
C	2.667492	3.104873	-1.064464
O	-2.068546	2.453108	-0.371966
C	-1.667292	-0.105779	1.248879
C	-2.696233	-0.488802	0.196877
C	-3.942039	0.142755	0.080015
C	-2.391144	-1.507067	-0.721281
C	-4.862828	-0.221953	-0.903103
C	-3.296082	-1.884022	-1.715733
C	-4.528849	-1.236031	-1.797639
O	-2.274735	0.482782	2.433661
O	-1.162033	-2.099821	-0.594998
O	-4.261685	1.199591	0.908790
H	3.509002	-2.403337	-0.895989
H	3.229960	-2.167824	1.697330
H	2.351669	-3.415144	0.792598
H	4.952885	-0.962885	1.275991
H	5.567026	-1.398364	-0.332913
H	5.618057	0.288565	0.214548
H	4.226955	-0.642920	-2.441457
H	2.838315	0.430288	-2.233992
H	4.475571	1.002965	-1.833186
H	0.893324	-1.497249	-0.667086
H	2.103548	-0.350254	2.422082
H	0.396658	-0.622523	2.779530
H	0.001021	3.570522	-1.182992
H	2.406454	4.167502	-1.022077
H	3.609465	2.955941	-0.531143
H	2.839706	2.854024	-2.117369
H	-2.778439	2.136257	0.220994
H	-5.814443	0.296973	-0.955386
H	-3.030306	-2.674276	-2.412480
H	-5.235057	-1.527300	-2.569811
H	-1.049434	-2.780184	-1.281883
H	-3.706573	1.097762	1.727524
H	-2.641702	-0.248677	2.962775
H	-1.191330	-1.034212	1.557623

3(7R,2'R)_89

C	-3.064762	-1.513722	0.667590
C	-3.593445	-0.646895	-0.516476
C	-1.603950	0.787744	-0.660103
C	-0.431794	0.140193	-0.244528
C	-2.018849	-2.601225	0.391765
O	-2.562881	0.035107	-1.311030
C	-4.289379	-1.534061	-1.547517
C	-4.578353	0.382543	0.042948
O	-2.582913	-0.744946	1.772603
C	-0.243834	-1.306224	-0.620482
O	-0.652240	-2.195368	0.433191
C	-1.766545	2.173231	-0.506076
C	0.512072	0.826796	0.539192
C	0.298775	2.193573	0.767755
C	-0.789969	2.861973	0.217635
C	-2.919056	2.926549	-1.117774
O	1.241643	2.860485	1.525693
C	1.706442	0.140475	1.196777
C	2.849627	-0.197036	0.229725
C	3.574682	0.855785	-0.370934
C	3.257777	-1.514241	-0.078984
C	4.610480	0.605648	-1.278269
C	4.293633	-1.767331	-0.985256
C	4.958280	-0.705087	-1.588213
O	1.285927	-1.003899	1.980754
O	2.658097	-2.612634	0.472736
O	3.324807	2.181467	-0.140015
H	-3.957864	-2.073217	0.979328

H	-2.225273	-3.100234	-0.562244
H	-2.098028	-3.344547	1.189252
H	-4.704917	-0.910453	-2.345571
H	-3.593341	-2.245970	-2.000469
H	-5.109150	-2.092715	-1.085485
H	-5.370905	-0.125065	0.604316
H	-4.083245	1.086538	0.715880
H	-5.044222	0.943553	-0.770682
H	-3.349788	-0.400210	2.257077
H	-0.800579	-1.535606	-1.531430
H	0.807755	-1.524105	-0.799765
H	-0.884311	3.935489	0.365146
H	-3.700375	3.145900	-0.381112
H	-2.570871	3.885258	-1.516929
H	-3.377073	2.356781	-1.929208
H	1.072385	3.819066	1.497436
H	5.128209	1.452188	-1.718307
H	4.558927	-2.799627	-1.191538
H	5.762384	-0.898776	-2.292876
H	2.070240	-2.276979	1.193543
H	2.695881	2.356630	0.591675
H	0.396083	-1.303285	1.689647
H	2.107578	0.835566	1.938185

3(7R,2'R)_92

C	-2.320471	-2.136186	-0.124161
C	-3.192466	-0.872673	0.112996
C	-1.738503	1.020163	-0.546575
C	-0.443925	0.653989	-0.951943
C	-0.805837	-1.994723	0.141740
O	-2.801464	0.176162	-0.836132
C	-4.638425	-1.169730	-0.279555
C	-3.113107	-0.400017	1.563323
O	-2.863429	-3.144795	0.740012
C	-0.317087	-0.610210	-1.771757
O	-0.027323	-1.804363	-1.032901
C	-1.990936	2.265310	0.049026
C	0.661332	1.468042	-0.629055
C	0.411904	2.690756	0.026328
C	-0.895642	3.083097	0.319491
C	-3.383807	2.734021	0.382306
O	1.400307	3.558666	0.399272
C	2.074941	0.990544	-0.971637
C	2.558504	-0.139530	-0.086239
C	2.575349	-0.046476	1.316068
C	2.981270	-1.350611	-0.660719
C	2.957520	-1.127298	2.117546
C	3.365789	-2.441137	0.125679
C	3.344188	-2.320633	1.512679
O	3.060110	2.059560	-0.925749
O	2.989421	-1.429695	-2.027116
O	2.208397	1.147229	1.867204
H	-2.447480	-2.438738	-1.173097
H	-0.447335	-2.940278	0.559514
H	-0.588174	-1.210977	0.877649
H	-5.246756	-0.266637	-0.168241
H	-4.691733	-1.498655	-1.323425
H	-5.058982	-1.954602	0.353424
H	-3.322602	-1.242342	2.227875
H	-2.125776	-0.005571	1.817217
H	-3.854753	0.378381	1.756387
H	-2.452204	-3.989402	0.492067
H	-1.250142	-0.747375	-2.327810
H	0.492184	-0.534062	-2.498721
H	-1.042573	4.052787	0.788088
H	-3.601944	2.620782	1.451202
H	-3.496171	3.797144	0.142546
H	-4.137953	2.171323	-0.172434
H	2.251044	3.168654	0.082472
H	2.952228	-1.020799	3.198968
H	3.673952	-3.366615	-0.352986
H	3.638943	-3.164545	2.130074
H	3.235052	-2.332119	-2.293592
H	2.197148	1.066281	2.836474
H	2.981084	2.558187	-1.758592
H	2.071260	0.616882	-1.995017

3(7R,2'R)_94

C	-1.972407	-2.041948	0.658747
C	-3.176251	-1.130960	0.292893
C	-1.880107	0.787485	-0.562580
C	-0.587708	0.472438	-1.020293
C	-1.212752	-2.711552	-0.499309
O	-2.885871	-0.141114	-0.756023
C	-4.290188	-1.967089	-0.334653
C	-3.679620	-0.445988	1.563403
O	-1.029495	-1.398372	1.517535
C	-0.410581	-0.822559	-1.779366

O	-0.093661	-1.943340	-0.934797
C	-2.181128	2.052656	-0.035032
C	0.485233	1.351768	-0.771404
C	0.186939	2.557852	-0.123602
C	-1.114954	2.927094	0.186822
C	-3.589411	2.499757	0.259715
O	1.255134	3.377342	0.213021
C	1.916439	0.961822	-1.146359
C	2.539270	0.012571	-0.120894
C	2.629508	0.262328	1.264677
C	3.014226	-1.236771	-0.575685
C	3.129323	-0.706405	2.146367
C	3.514654	-2.206695	0.294488
C	3.560594	-1.933942	1.659772
O	2.764292	2.060445	-1.513050
O	2.952327	-1.481825	-1.923619
O	2.230390	1.422157	1.865597
H	-2.426415	-2.851156	1.244354
H	-1.873341	-2.941951	-1.342050
H	-0.778831	-3.646541	-0.134523
H	-3.963407	-2.436672	-1.267273
H	-4.617974	-2.752083	0.353708
H	-5.148740	-1.326363	-0.559719
H	-3.894289	-1.203364	2.325386
H	-2.933199	0.236574	1.974588
H	-4.601279	0.105374	1.363260
H	-0.254794	-1.189707	0.962222
H	-1.322278	-1.041961	-2.341262
H	0.411808	-0.753166	-2.490221
H	-1.297707	3.905203	0.626573
H	-3.728633	3.536448	-0.065964
H	-4.319795	1.873254	-0.256261
H	-3.813209	2.463585	1.331915
H	0.949907	4.153234	0.717000
H	3.171130	-0.468552	3.204573
H	3.857877	-3.158828	-0.101107
H	3.944904	-2.682990	2.346463
H	3.234644	-2.397410	-2.090319
H	2.067624	2.155011	1.236980
H	2.648439	2.775977	-0.864957
H	1.856157	0.392570	-2.068950

3(7R,2'R)_96

C	3.261212	-1.631019	0.286488
C	3.702842	-0.219580	-0.214688
C	1.717433	1.204251	0.257920
C	0.656479	0.538531	0.894959
C	1.776321	-1.999606	0.091055
O	3.019836	0.831537	0.551889
C	5.169419	0.000815	0.147040
C	3.485641	-0.048747	-1.716984
O	4.084332	-2.635632	-0.321422
C	1.012827	-0.552966	1.868480
O	0.969781	-1.862802	1.272485
C	1.480234	2.317958	-0.562227
C	-0.679780	0.876572	0.609591
C	-0.911460	1.974164	-0.239364
C	0.152836	2.683059	-0.794574
C	2.595262	3.131209	-1.164349
O	-2.203617	2.340878	-0.478886
C	-1.835101	0.111086	1.241744
C	-2.818919	-0.497301	0.246713
C	-2.457498	-1.673005	-0.446346
C	-4.097370	0.044740	-0.024495
C	-3.311442	-2.256863	-1.389691
C	-4.953950	-0.543046	-0.962584
C	-4.552957	-1.685597	-1.646263
O	-2.556205	0.940210	2.185446
O	-4.576828	1.156718	0.604137
O	-1.269928	-2.330164	-0.277974
H	3.493257	-1.695282	1.353873
H	1.723771	-3.063514	-0.148896
H	1.320428	-1.442663	-0.734282
H	5.308971	-0.071486	1.231449
H	5.801707	-0.748044	-0.334923
H	5.492429	0.994830	-0.178146
H	3.986881	-0.855534	-2.260874
H	2.427377	-0.059062	-1.992154
H	3.921615	0.892710	-2.057513
H	3.811708	-2.733335	-1.249663
H	2.010863	-0.366608	2.270534
H	0.321309	-0.599691	2.709983
H	-0.062740	3.546550	-1.420434
H	3.532814	2.984930	-0.623576
H	2.767844	2.860688	-2.212897
H	2.342048	4.196583	-1.143684
H	-2.217135	3.093448	-1.095234
H	-2.981090	-3.157224	-1.897852

H	-5.923380	-0.085506	-1.134209
H	-5.216407	-2.140352	-2.376894
H	-3.903240	1.423181	1.273810
H	-0.704371	-2.010819	0.457435
H	-1.926745	1.578364	2.562594
H	-1.419072	-0.716061	1.821603

3(7R,2'R)_99

C	3.378697	-1.572968	0.334179
C	3.722874	-0.167572	-0.245066
C	1.698897	1.187729	0.245012
C	0.665537	0.479511	0.880354
C	1.913175	-2.021546	0.188332
O	3.017574	0.865348	0.525976
C	5.191718	0.155509	0.026465
C	3.418762	-0.082349	-1.738261
O	4.155247	-2.580267	-0.329911
C	1.059059	-0.566226	1.898665
O	1.151171	-1.901212	1.386875
C	1.422222	2.298048	-0.568779
C	-0.680958	0.783176	0.601687
C	-0.953602	1.899116	-0.208996
C	0.084613	2.639580	-0.773659
C	2.512984	3.128640	-1.191391
O	-2.258586	2.254011	-0.403832
C	-1.800325	-0.049398	1.204228
C	-2.857693	-0.510997	0.209147
C	-2.510610	-1.537708	-0.686627
C	-4.165344	0.006163	0.128943
C	-3.412532	-2.037481	-1.628266
C	-5.081569	-0.491444	-0.807844
C	-4.700301	-1.504751	-1.680134
O	-2.439581	0.646976	2.309158
O	-4.606060	1.008430	0.942115
O	-1.232473	-2.023609	-0.593986
H	3.627287	-1.565996	1.403898
H	1.914589	-3.090558	-0.038254
H	1.407701	-1.504455	-0.633713
H	5.411722	1.178301	-0.294418
H	5.415895	0.070997	1.095843
H	5.854938	-0.516735	-0.526556
H	3.864594	-0.943990	-2.242945
H	2.345017	-0.088291	-1.943533
H	3.846411	0.826354	-2.168735
H	5.086372	-2.454155	-0.085255
H	2.018425	-0.269918	2.335498
H	0.332571	-0.619384	2.711403
H	-0.159960	3.507175	-1.382993
H	3.450755	3.033889	-0.639138
H	2.705641	2.822810	-2.226891
H	2.223834	4.184594	-1.213767
H	-2.297462	3.015681	-1.007848
H	-3.101003	-2.830228	-2.303307
H	-6.079817	-0.065497	-0.832464
H	-5.411220	-1.887559	-2.407246
H	-3.887991	1.173228	1.601780
H	-1.109616	-2.738294	-1.242151
H	-1.838309	1.350420	2.606614
H	-1.352335	-0.956015	1.615065

3(7R,2'R)_9

C	3.131768	-1.766199	0.019657
C	3.577253	-0.370638	0.560479
C	1.468237	0.934173	0.542692
C	0.342384	0.207568	0.125145
C	2.053557	-1.760542	-1.078850
O	2.459070	0.284234	1.258950
C	4.598773	-0.563148	1.680040
C	4.152074	0.504531	-0.550007
O	4.255204	-2.441086	-0.561654
C	0.274253	-1.251984	0.479402
O	0.742446	-2.091865	-0.598129
C	1.554772	2.320922	0.334971
C	-0.652171	0.821060	-0.657126
C	-0.526110	2.193205	-0.909050
C	0.535909	2.932773	-0.397397
C	2.686512	3.148666	0.883582
O	-1.526022	2.794584	-1.645903
C	-1.834876	0.056027	-1.248487
C	-2.903705	-0.315436	-0.207147
C	-3.597090	0.711233	0.472037
C	-3.271255	-1.644962	0.100643
C	-4.550083	0.424268	1.455548
C	-4.225758	-1.935204	1.081631
C	-4.852744	-0.898196	1.763023
O	-1.390961	-1.074063	-2.036676
O	-2.705890	-2.722285	-0.524435
O	-3.385734	2.047329	0.254637

H	2.752864	-2.352622	0.866276
H	2.295135	-2.552009	-1.790520
H	2.020503	-0.812171	-1.623907
H	5.525176	-1.003813	1.299186
H	4.847769	0.405115	2.124536
H	4.196541	-1.213458	2.464944
H	3.385808	0.839869	-1.253715
H	4.645482	1.384884	-0.131501
H	4.894500	-0.071895	-1.108660
H	4.868094	-2.681796	0.152053
H	0.861431	-1.442618	1.379573
H	-0.746428	-1.580782	0.665000
H	0.570103	4.004799	-0.577355
H	3.444146	3.350618	0.117143
H	2.313513	4.117428	1.232742
H	3.181907	2.645158	1.716744
H	-1.396394	3.759741	-1.647485
H	-5.043810	1.252407	1.954008
H	-4.460350	-2.976191	1.281396
H	-5.593677	-1.120461	2.525993
H	-2.188111	-2.362145	-1.285379
H	-2.888559	2.249394	-0.565047
H	-0.531237	-1.413182	-1.691770
H	-2.309485	0.710259	-1.983300

3(7R,2'R)_208

C	3.271782	-1.609967	0.302490
C	3.688474	-0.206517	-0.236612
C	1.708332	1.209806	0.260953
C	0.653093	0.535602	0.898685
C	1.798495	-1.997900	0.089200
O	3.015198	0.843141	0.541444
C	5.163732	0.042504	0.072976
C	3.423333	-0.074479	-1.734214
O	4.031616	-2.632011	-0.356364
C	1.015119	-0.560148	1.866034
O	0.984436	-1.868963	1.266083
C	1.463530	2.323775	-0.556366
C	-0.685483	0.872321	0.621225
C	-0.924514	1.976812	-0.216609
C	0.134642	2.690116	-0.776207
C	2.576289	3.129201	-1.172693
O	-2.218911	2.344530	-0.442367
C	-1.836727	0.094570	1.246063
C	-2.815925	-0.507219	0.242329
C	-4.098670	0.027623	-0.022120
C	-2.442803	-1.668628	-0.468110
C	-4.949837	-0.555028	-0.968212
C	-3.291013	-2.247002	-1.419880
C	-4.538046	-1.683993	-1.667939
O	-2.563276	0.908316	2.198220
O	-1.248073	-2.315271	-0.309301
O	-4.587513	1.127360	0.620722
H	3.485815	-1.636537	1.378444
H	1.761157	-3.060705	-0.156941
H	1.341908	-1.443194	-0.735831
H	5.361258	-0.080477	1.143932
H	5.805832	-0.645999	-0.484587
H	5.436691	1.062246	-0.214860
H	3.832379	-0.949427	-2.247229
H	2.356284	-0.015529	-1.964917
H	3.911800	0.817079	-2.134476
H	4.951706	-2.564864	-0.052907
H	2.009970	-0.366662	2.272804
H	0.321975	-0.616343	2.705563
H	-0.086533	3.555399	-1.397578
H	2.758624	2.829044	-2.211562
H	2.316155	4.192881	-1.183520
H	3.511465	3.003289	-0.622454
H	-2.238681	3.096926	-1.058894
H	-5.923358	-0.104060	-1.134048
H	-2.952169	-3.136509	-1.941409
H	-5.197214	-2.134532	-2.405051
H	-0.687961	-2.002048	0.432552
H	-3.914637	1.392942	1.291316
H	-1.936269	1.538936	2.591801
H	-1.416844	-0.737365	1.816389

3(7R,2'R)_210

C	2.939812	-1.738023	-0.266399
C	3.636888	-0.374065	-0.495418
C	1.744864	1.065332	0.185322
C	0.707954	0.380440	0.850892
C	2.789930	-2.134819	1.205710
O	3.070570	0.696379	0.328837
C	5.085197	-0.440497	-0.011276
C	3.582558	-0.003434	-1.977484
O	1.724073	-1.895783	-1.011255

C	0.951735	-0.754554	1.851887
O	2.297226	-1.129594	2.084109
C	1.479968	2.235506	-0.555008
C	-0.630476	0.797350	0.656662
C	-0.883749	1.941644	-0.115829
C	0.161791	2.660802	-0.688935
C	2.586540	3.053431	-1.169743
O	-2.180815	2.349209	-0.258241
C	-1.801164	0.047024	1.278779
C	-2.785343	-0.487269	0.242299
C	-4.087857	0.006330	0.031904
C	-2.361430	-1.558203	-0.564457
C	-4.921396	-0.555421	-0.945906
C	-3.178855	-2.121123	-1.545377
C	-4.463316	-1.609156	-1.728110
O	-2.502166	0.863568	2.252400
O	-1.091180	-2.024596	-0.340023
O	-4.604970	1.042147	0.752173
H	3.604982	-2.489688	-0.705778
H	3.769374	-2.407973	1.606802
H	2.142714	-3.023837	1.249864
H	5.578790	0.518848	-0.196489
H	5.635700	-1.221396	-0.545027
H	5.136172	-0.645654	1.061924
H	3.968730	-0.832107	-2.580847
H	2.559830	0.198754	-2.304160
H	4.198956	0.877888	-2.171136
H	1.059631	-1.251758	-0.713291
H	0.571842	-0.419054	2.823911
H	0.378759	-1.642923	1.563158
H	-0.060892	3.567058	-1.247941
H	2.314152	4.113826	-1.174128
H	3.524346	2.934373	-0.622680
H	2.773474	2.760838	-2.209455
H	-2.210069	3.119655	-0.851546
H	-5.918475	-0.145267	-1.073429
H	-2.805355	-2.945501	-2.146549
H	-5.110497	-2.039931	-2.487093
H	-0.889762	-2.749338	-0.957203
H	-3.922572	1.286739	1.423788
H	-1.903486	1.575352	2.534179
H	-1.420162	-0.817311	1.822055

3(7R,2'R)_211

C	-2.114014	-2.274501	-0.090274
C	-3.100114	-1.073352	-0.035884
C	-1.720594	0.926423	-0.559167
C	-0.345996	0.681681	-0.739069
C	-0.661883	-1.989440	0.344789
O	-2.636742	-0.034033	-0.963504
C	-4.443819	-1.494526	-0.625116
C	-3.277874	-0.541002	1.384820
O	-2.645462	-3.378003	0.657921
C	0.009647	-0.577872	-1.504486
O	0.232061	-1.767359	-0.735223
C	-2.192579	2.170268	-0.114707
C	0.610161	1.644635	-0.344615
C	0.127254	2.894608	0.104425
C	-1.244007	3.135856	0.207187
C	-3.660791	2.496988	-0.022559
O	0.934193	3.953595	0.422681
C	2.124090	1.379694	-0.473434
C	2.567804	-0.003544	-0.050693
C	2.383260	-0.422230	1.275096
C	3.211593	-0.883035	-0.930413
C	2.779651	-1.686111	1.710975
C	3.619731	-2.155079	-0.514585
C	3.394342	-2.547128	0.802117
O	2.913590	2.342654	0.281315
O	3.392209	-0.457723	-2.219904
O	1.799117	0.491616	2.118590
H	-2.080120	-2.629449	-1.125472
H	-0.284229	-2.891100	0.834582
H	-0.601395	-1.165528	1.066643
H	-4.873838	-2.319254	-0.051534
H	-5.144713	-0.653752	-0.609415
H	-4.318362	-1.823182	-1.662962
H	-3.582049	-1.357815	2.047046
H	-2.360947	-0.101560	1.786178
H	-4.065817	0.213940	1.415901
H	-2.557147	-3.173558	1.604168
H	-0.802503	-0.765092	-2.215522
H	0.923380	-0.438508	-2.081910
H	-1.560438	4.121523	0.538720
H	-4.259930	1.824808	-0.641036
H	-4.028248	2.419532	1.007890
H	-3.841933	3.526239	-0.350978
H	1.866903	3.631806	0.348038

H	2.616261	-1.979253	2.744253
H	4.102543	-2.822851	-1.222797
H	3.707622	-3.534944	1.127824
H	3.801901	-1.169611	-2.741705
H	1.795644	0.144730	3.027965
H	2.815037	2.095060	1.221989
H	2.425468	1.547847	-1.509321

3(7R,2'R)_204

C	-2.441342	-2.082261	-0.113242
C	-3.257448	-0.787550	0.189836
C	-1.757360	1.052139	-0.523954
C	-0.513632	0.619242	-1.013858
C	-0.911584	-2.009114	0.090030
O	-2.879787	0.274308	-0.755939
C	-4.727265	-1.031622	-0.142897
C	-3.100746	-0.333336	1.640117
O	-2.979568	-3.177437	0.640833
C	-0.491939	-0.643367	-1.842171
O	-0.173963	-1.836154	-1.115834
C	-1.904397	2.301423	0.101850
C	0.648899	1.364249	-0.734833
C	0.500609	2.586022	-0.061000
C	-0.751910	3.057472	0.317209
C	-3.246831	2.839559	0.522801
O	1.601550	3.349317	0.289791
C	2.019572	0.817790	-1.106762
C	2.572145	-0.172527	-0.095145
C	2.947869	-1.453296	-0.560028
C	2.699176	0.074560	1.290107
C	3.391192	-2.455234	0.303684
C	3.145319	-0.929769	2.160964
C	3.479984	-2.183924	1.667449
O	2.929150	1.927479	-1.365773
O	2.392339	1.253763	1.901191
O	2.850718	-1.686344	-1.905239
H	-2.624899	-2.349861	-1.158714
H	-0.583088	-2.976658	0.478551
H	-0.630874	-1.240702	0.820895
H	-5.136045	-1.830193	0.480429
H	-5.307214	-0.119582	0.030014
H	-4.838786	-1.320152	-1.194162
H	-3.347670	-1.159010	2.314905
H	-2.084173	-0.002180	1.867918
H	-3.789079	0.485468	1.859959
H	-2.691070	-3.082556	1.564065
H	-1.468979	-0.755514	-2.322561
H	0.259210	-0.587182	-2.631338
H	-0.815926	4.027356	0.802696
H	-4.061140	2.335069	-0.001809
H	-3.411386	2.709999	1.599269
H	-3.308419	3.913093	0.314286
H	2.319176	3.110017	-0.357539
H	3.660426	-3.428991	-0.096090
H	3.221644	-0.697235	3.218268
H	3.822809	-2.957886	2.348387
H	2.263237	2.007920	1.287003
H	3.072129	-2.616660	-2.083171
H	3.829294	1.631492	-1.146084
H	1.925444	0.281730	-2.048343

3(7R,2'R)_288

C	-2.663849	-1.944131	-0.093067
C	-3.292626	-0.601474	0.392572
C	-1.750055	1.152361	-0.421747
C	-0.596304	0.620930	-1.020791
C	-1.127350	-2.037845	-0.056114
O	-2.950010	0.475478	-0.550969
C	-4.813989	-0.679623	0.272405
C	-2.882597	-0.268974	1.824761
O	-3.125585	-3.023469	0.729404
C	-0.780336	-0.562074	-1.937783
O	-0.530078	-1.848620	-1.342947
C	-1.737014	2.402403	0.217831
C	0.650255	1.248728	-0.824039
C	0.652271	2.503338	-0.196400
C	-0.517381	3.075874	0.292878
C	-2.988499	3.024808	0.776938
O	1.828502	3.217166	-0.028964
C	1.947778	0.557129	-1.217521
C	2.545797	-0.332610	-0.128152
C	3.101982	0.127433	1.091796
C	2.620150	-1.725934	-0.380282
C	3.727772	-0.766157	1.973990
C	3.243541	-2.608061	0.501324
C	3.806130	-2.119640	1.677953
O	2.884734	1.565645	-1.683562
O	2.104094	-2.266309	-1.539989

O	3.104748	1.416488	1.530655
H	-2.985080	-2.107430	-1.130172
H	-0.858706	-3.056163	0.230187
H	-0.679687	-1.348356	0.665999
H	-5.109312	-0.953194	-0.746899
H	-5.252683	0.293553	0.511898
H	-5.230482	-1.413006	0.969298
H	-3.045830	-1.149536	2.452145
H	-1.829448	0.012877	1.904397
H	-3.489716	0.549029	2.220656
H	-4.070340	-3.156975	0.549921
H	-1.803106	-0.546490	-2.321951
H	-0.101726	-0.508974	-2.790631
H	-0.461071	4.059670	0.749766
H	-3.149225	2.733883	1.822028
H	-2.917458	4.116847	0.750156
H	-3.873292	2.717639	0.213093
H	2.447061	2.901056	-0.741544
H	4.143709	-0.362953	2.892194
H	3.269953	-3.663306	0.250024
H	4.293094	-2.798102	2.372893
H	1.114666	-2.176623	-1.510636
H	2.645126	2.056278	0.943251
H	3.785103	1.211663	-1.581269
H	1.753162	-0.101318	-2.063135

3(7R,2'R)_292

C	-3.064784	-1.513864	0.667376
C	-3.593231	-0.647199	-0.516901
C	-1.603833	0.787794	-0.659933
C	-0.431707	0.140324	-0.244267
C	-2.018689	-2.601247	0.391860
O	-2.562611	0.035156	-1.311094
C	-4.288522	-1.534550	-1.548218
C	-4.578676	0.381975	0.042031
O	-2.583431	-0.744913	1.772533
C	-0.243665	-1.306123	-0.620119
O	-0.652160	-2.195228	0.433510
C	-1.766519	2.173299	-0.505908
C	0.512114	0.826962	0.539482
C	0.298758	2.193692	0.767993
C	-0.790020	2.862050	0.217853
C	-2.919035	2.926467	-1.117762
O	1.241661	2.860636	1.525874
C	1.706571	0.140734	1.197003
C	2.849513	-0.196993	0.229728
C	3.258093	-1.514206	-0.078335
C	3.574073	0.855784	-0.371611
C	4.293976	-1.767341	-0.984540
C	4.609808	0.605610	-1.278951
C	4.958104	-0.705174	-1.588160
O	1.286184	-1.003310	1.981506
O	3.323571	2.181474	-0.141346
O	2.658536	-2.612576	0.473624
H	-3.957901	-2.073437	0.978893
H	-2.224945	-3.100299	-0.562159
H	-2.097927	-3.344541	1.189356
H	-4.704221	-0.911008	-2.346248
H	-3.592066	-2.246016	-2.001224
H	-5.108112	-2.093681	-1.086448
H	-5.371412	-0.125797	0.602990
H	-4.084114	1.086103	0.715220
H	-5.044239	0.942831	-0.771881
H	-3.350618	-0.400862	2.257002
H	-0.800227	-1.535576	-1.531178
H	0.807963	-1.523955	-0.799273
H	-0.884311	3.935585	0.365251
H	-3.376394	2.356891	-1.929705
H	-3.700813	3.145063	-0.381365
H	-2.571068	3.885519	-1.516260
H	1.072651	3.819237	1.497080
H	4.559682	-2.799623	-1.190376
H	5.127129	1.452087	-1.719582
H	5.762213	-0.898956	-2.292789
H	2.695837	2.356588	0.591358
H	2.070407	-2.276818	1.194232
H	0.396517	-1.303195	1.690414
H	2.107990	0.835991	1.938116

3(7R,2'R)_209

C	3.131766	-1.766046	0.019467
C	3.577359	-0.370495	0.560270
C	1.468309	0.934152	0.542669
C	0.342396	0.207538	0.125071
C	2.053458	-1.760508	-1.078908
O	2.459085	0.284116	1.258863
C	4.598933	-0.563021	1.679751
C	4.152168	0.504719	-0.550103

O	4.254922	-2.441059	-0.561976
C	0.274181	-1.251986	0.479287
O	0.742428	-2.091976	-0.598162
C	1.554577	2.320949	0.335267
C	-0.652170	0.821037	-0.657144
C	-0.526273	2.193233	-0.908924
C	0.535594	2.932786	-0.396949
C	2.686011	3.148920	0.884153
O	-1.526224	2.794594	-1.645681
C	-1.834808	0.055960	-1.248556
C	-2.903662	-0.315546	-0.207239
C	-3.270853	-1.645118	0.100840
C	-3.597274	0.711083	0.471754
C	-4.225220	-1.935344	1.082023
C	-4.550233	0.424129	1.455297
C	-4.852491	-0.898343	1.763180
O	-1.390895	-1.074129	-2.036794
O	-3.386119	2.047182	0.254094
O	-2.705202	-2.722424	-0.523887
H	2.752760	-2.352320	0.866193
H	2.295124	-2.551935	-1.790634
H	2.020282	-0.812160	-1.624048
H	4.847844	0.405228	2.124343
H	4.196826	-1.213473	2.464610
H	5.525388	-1.003562	1.298871
H	4.645133	1.385260	-0.131511
H	4.895007	-0.071562	-1.108340
H	3.386093	0.839775	-1.254172
H	4.869387	-2.679149	0.151306
H	0.861214	-1.442629	1.379559
H	-0.746548	-1.580770	0.664706
H	0.569665	4.004859	-0.576695
H	3.181071	2.645651	1.717687
H	3.444005	3.350771	0.118053
H	2.312764	4.117720	1.232946
H	-1.396598	3.759786	-1.647424
H	-4.459422	-2.976356	1.282102
H	-5.044185	1.252271	1.953544
H	-5.593386	-1.120596	2.526197
H	-2.889006	2.249188	-0.565630
H	-2.187603	-2.362301	-1.284980
H	-0.530947	-1.412958	-1.692243
H	-2.309419	0.710239	-1.983333

4(7S,2'R)_14

C	-3.695018	-1.459864	0.232487
C	-3.900285	0.007688	-0.256667
C	-1.590734	0.824613	-0.637374
C	-0.591476	-0.115423	-0.345699
C	-2.471338	-1.717781	1.132820
O	-2.803184	0.394999	-1.155581
C	-5.120847	0.072025	-1.174089
C	-4.057138	0.973478	0.915641
O	-4.829871	-1.876658	1.004976
C	-0.897752	-1.558374	-0.671414
O	-1.367657	-2.313953	0.453549
C	-1.348147	2.202028	-0.510570
C	0.636147	0.289905	0.226605
C	0.847085	1.671496	0.424330
C	-0.123203	2.593432	0.021380
C	-2.357709	3.239247	-0.925915
O	1.971036	2.241120	0.955193
C	1.653421	-0.763829	0.642796
C	3.041777	-0.564040	0.061090
C	3.288015	-0.987418	-1.256382
C	4.101916	0.036259	0.757131
C	4.538243	-0.819985	-1.855506
C	5.359511	0.209903	0.176814
C	5.567571	-0.219818	-1.131001
O	1.762139	-0.861312	2.089378
O	3.912140	0.530571	2.033643
O	2.236757	-1.555675	-1.923185
H	-3.604403	-2.100503	-0.654404
H	-2.766760	-2.449035	1.889011
H	-2.148880	-0.808371	1.652933
H	-5.027568	-0.648751	-1.994264
H	-6.041908	-0.140105	-0.622846
H	-5.211318	1.075409	-1.601141
H	-4.788693	0.563700	1.617566
H	-3.119609	1.127140	1.456233
H	-4.419851	1.945101	0.571677
H	-5.592927	-1.940776	0.407816
H	-1.644088	-1.579044	-1.470492
H	-0.018885	-2.089842	-1.033656
H	0.098667	3.649151	0.151704
H	-3.046152	2.848910	-1.679242
H	-2.958390	3.577324	-0.073140
H	-1.851918	4.120097	-1.335059

H	2.556904	1.618133	1.429925
H	4.693142	-1.156687	-2.876905
H	6.147344	0.679838	0.756349
H	6.541559	-0.088732	-1.593605
H	3.153727	0.020482	2.424963
H	2.520763	-1.814695	-2.816860
H	0.898948	-0.629851	2.473070
H	1.299189	-1.732863	0.297719

4(7S,2'R)_16

C	-3.260162	-1.799441	0.032043
C	-3.694743	-0.387415	-0.467848
C	-1.559856	0.879748	-0.542011
C	-0.437028	0.138442	-0.140200
C	-2.135779	-1.833717	1.084932
O	-2.589952	0.238233	-1.209944
C	-4.774503	-0.533484	-1.538953
C	-4.191047	0.489911	0.678402
O	-4.375682	-2.464560	0.641115
C	-0.391318	-1.329930	-0.489354
O	-0.860867	-2.193365	0.554970
C	-1.610273	2.273810	-0.376984
C	0.616919	0.758714	0.554024
C	0.539887	2.143359	0.736372
C	-0.535927	2.888816	0.268170
C	-2.756893	3.105179	-0.887822
O	1.613479	2.760301	1.360456
C	1.761960	-0.085608	1.117534
C	2.908379	-0.359015	0.145978
C	3.329726	-1.699753	-0.001869
C	3.589771	0.610285	-0.620317
C	4.344661	-2.072260	-0.884519
C	4.607743	0.243891	-1.512600
C	4.975953	-1.088868	-1.643275
O	2.213041	0.367460	2.405333
O	3.313355	1.947397	-0.594203
O	2.682286	-2.646711	0.751093
H	-2.924328	-2.375590	-0.839878
H	-2.376875	-2.623390	1.800251
H	-2.062439	-0.890589	1.637864
H	-4.433286	-1.190089	-2.347218
H	-5.697021	-0.944175	-1.117384
H	-5.009468	0.446824	-1.964371
H	-4.916222	-0.075969	1.269773
H	-3.381715	0.800962	1.344132
H	-4.686335	1.385044	0.294579
H	-5.015371	-2.683135	-0.055908
H	-0.978922	-1.490830	-1.398756
H	0.627991	-1.658131	-0.692764
H	-0.531667	3.967676	0.405079
H	-3.285718	2.598799	-1.698704
H	-3.485577	3.315124	-0.095643
H	-2.393225	4.070054	-1.256833
H	1.495046	3.727310	1.367637
H	4.629599	-3.117725	-0.967609
H	5.097624	1.026086	-2.083759
H	5.766982	-1.366557	-2.334284
H	2.818873	2.229156	0.205095
H	3.023934	-3.526074	0.514698
H	2.461567	1.304521	2.328852
H	1.326448	-1.055350	1.344372

4(7S,2'R)_133

C	3.702359	-1.467121	-0.203733
C	3.906916	0.008553	0.259728
C	1.592626	0.829916	0.608583
C	0.592523	-0.122129	0.345517
C	2.481510	-1.739896	-1.103262
O	2.803311	0.414126	1.142198
C	5.119582	0.087545	1.186569
C	4.075767	0.951950	-0.929175
O	4.839136	-1.898959	-0.965034
C	0.896882	-1.559330	0.693205
O	1.377493	-2.328366	-0.418538
C	1.352100	2.201543	0.436895
C	-0.629713	0.271867	-0.231304
C	-0.835740	1.642187	-0.473949
C	0.125421	2.583412	-0.108673
C	2.361582	3.250777	0.821483
O	-2.005331	2.023413	-1.069531
C	-1.671553	-0.754319	-0.654502
C	-3.054153	-0.540443	-0.054315
C	-3.231329	-0.858375	1.304210
C	-4.175131	-0.057697	-0.758752
C	-4.458788	-0.703007	1.950278
C	-5.414944	0.095673	-0.121869
C	-5.548374	-0.222806	1.224361
O	-1.785087	-0.799479	-2.098631

O	-4.126350	0.283946	-2.078432
O	-2.129625	-1.329686	1.971155
H	3.607825	-2.091742	0.694117
H	2.780244	-2.481772	-1.847770
H	2.158973	-0.839099	-1.638138
H	6.044759	-0.142774	0.649641
H	5.013968	-0.613378	2.022271
H	5.211803	1.100050	1.591190
H	4.438384	1.928848	-0.600532
H	4.811246	0.527278	-1.617971
H	3.142741	1.098171	-1.479572
H	5.601646	-1.947959	-0.365824
H	1.634857	-1.571954	1.500621
H	0.011831	-2.084301	1.048408
H	-0.084205	3.639163	-0.268599
H	2.946080	3.581510	-0.045350
H	1.856695	4.134050	1.226947
H	3.063525	2.874939	1.569489
H	-2.022649	2.992666	-1.154138
H	-4.549671	-0.956108	3.003087
H	-6.252251	0.468678	-0.703459
H	-6.509133	-0.099403	1.716581
H	-3.215276	0.077628	-2.396505
H	-2.373025	-1.535232	2.890326
H	-0.903846	-0.629643	-2.472274
H	-1.328162	-1.739371	-0.335812

4(7S,2'R)_139

C	3.513904	-1.912825	0.076911
C	3.653277	-0.376537	0.016826
C	1.516948	0.829396	-0.356982
C	0.358246	0.208721	0.141451
C	2.182636	-2.404256	0.633957
O	2.579403	0.108262	-0.869223
C	3.602583	0.241541	1.411624
C	4.958386	-0.002400	-0.684488
O	3.696982	-2.494463	-1.216804
C	0.110561	-1.295599	0.104118
O	1.155610	-2.145471	-0.326687
C	1.616859	2.233115	-0.444103
C	-0.700651	1.018407	0.630151
C	-0.578299	2.411007	0.535076
C	0.555036	3.012191	-0.001046
C	2.837417	2.889858	-1.031034
O	-1.651383	3.176905	0.949740
C	-1.995318	0.480628	1.247580
C	-2.922154	-0.215848	0.253477
C	-3.219190	-1.597787	0.267286
C	-3.538086	0.566740	-0.748572
C	-4.046566	-2.172927	-0.704707
C	-4.363080	-0.007185	-1.720761
C	-4.605686	-1.377033	-1.698103
O	-1.748235	-0.381120	2.379552
O	-3.368563	1.920560	-0.861847
O	-2.721684	-2.456978	1.208336
H	4.322602	-2.300780	0.705361
H	1.946437	-1.949450	1.600755
H	2.238932	-3.490525	0.773611
H	2.646142	0.082045	1.914878
H	3.788058	1.318259	1.368235
H	4.387976	-0.210870	2.026364
H	5.096612	1.081808	-0.687569
H	5.810207	-0.456905	-0.166497
H	4.955201	-0.360630	-1.716825
H	2.907332	-2.232371	-1.724537
H	-0.237676	-1.626334	1.085363
H	-0.702811	-1.475198	-0.606087
H	0.602782	4.095701	-0.075914
H	3.166429	2.378025	-1.940171
H	2.629001	3.936401	-1.272544
H	3.679115	2.872167	-0.328621
H	-1.497425	4.110823	0.720320
H	-4.236737	-3.240446	-0.654094
H	-4.803681	0.638022	-2.474174
H	-5.246187	-1.824716	-2.453000
H	-2.906048	2.333669	-0.103490
H	-2.249745	-1.916741	1.883604
H	-0.919020	-0.101555	2.802124
H	-2.535489	1.342796	1.646407

4(7S,2'R)_32

C	-1.418864	-1.996823	0.636845
C	-2.788383	-1.535037	0.060586
C	-1.877555	0.645327	-0.588263
C	-0.499864	0.573697	-0.881172
C	-0.384536	-2.430399	-0.422374
O	-2.694215	-0.424591	-0.903142
C	-3.422562	-2.660047	-0.755893

C	-3.706649	-1.127698	1.212770
O	-0.879860	-1.115453	1.632085
C	0.035182	-0.506995	-1.806643
O	-0.512120	-1.811895	-1.695633
C	-2.444740	1.806570	-0.040323
C	0.359205	1.597506	-0.434655
C	-0.212260	2.735695	0.162777
C	-1.590457	2.851771	0.314323
C	-3.932584	1.965122	0.138976
O	0.628941	3.731272	0.589764
C	1.879419	1.525222	-0.502277
C	2.467116	0.259699	0.125754
C	2.193565	0.006410	1.482659
C	3.286163	-0.667875	-0.548046
C	2.672239	-1.128911	2.138434
C	3.780839	-1.806864	0.101059
C	3.466987	-2.033811	1.436089
O	2.310381	1.719062	-1.878387
O	3.610987	-0.530542	-1.868596
O	1.419258	0.929620	2.137117
H	-1.654285	-2.897801	1.212815
H	-0.518012	-3.497271	-0.621881
H	0.624685	-2.288173	-0.012075
H	-2.801123	-2.926568	-1.614086
H	-3.570701	-3.549223	-0.134930
H	-4.400190	-2.336061	-1.128353
H	-3.290766	-0.289509	1.774776
H	-4.692820	-0.849484	0.831152
H	-3.829332	-1.967814	1.905361
H	-0.576325	-0.296981	1.205052
H	-0.197967	-0.198928	-2.833042
H	1.119869	-0.572379	-1.735256
H	-2.003248	3.762719	0.742436
H	-4.486043	1.279592	-0.505958
H	-4.238992	1.769317	1.173066
H	-4.232765	2.990984	-0.100328
H	0.103604	4.428969	1.017862
H	2.418891	-1.290971	3.182729
H	4.398878	-2.497210	-0.464364
H	3.844734	-2.920271	1.937758
H	3.215084	0.324898	-2.171367
H	1.270356	0.633534	3.052088
H	3.002537	2.402012	-1.877075
H	2.253396	2.371483	0.074197

4(7S,2'R)_33

C	-3.181898	-1.820051	0.102652
C	-3.640033	-0.444207	-0.472276
C	-1.535961	0.871795	-0.557404
C	-0.399713	0.182932	-0.107137
C	-2.077753	-1.776017	1.175960
O	-2.536946	0.174116	-1.220230
C	-4.694209	-0.670388	-1.555523
C	-4.184107	0.470008	0.622481
O	-4.292223	-2.485778	0.721140
C	-0.322504	-1.297440	-0.392962
O	-0.784549	-2.124318	0.685772
C	-1.627940	2.268642	-0.443459
C	0.625637	0.857833	0.584519
C	0.500038	2.250269	0.756606
C	-0.598166	2.929874	0.221562
C	-2.781927	3.048660	-1.017356
O	1.418040	3.015880	1.418314
C	1.795109	0.045175	1.140929
C	2.844448	-0.380080	0.130376
C	3.526605	0.536096	-0.692023
C	3.212093	-1.736367	0.032966
C	4.506591	0.116078	-1.596963
C	4.189528	-2.170501	-0.867877
C	4.828613	-1.236281	-1.678272
O	2.401891	0.782804	2.236897
O	2.560620	-2.624321	0.845842
O	3.199390	1.853718	-0.568392
H	-2.814081	-2.427860	-0.734404
H	-2.311551	-2.537943	1.923425
H	-2.040267	-0.806855	1.685442
H	-4.951622	0.282924	-2.027114
H	-4.317012	-1.349909	-2.328319
H	-5.611967	-1.092934	-1.134532
H	-4.902154	-0.090098	1.228022
H	-3.396867	0.838100	1.285150
H	-4.700005	1.330140	0.188731
H	-4.921030	-2.734190	0.024120
H	-0.901474	-1.510235	-1.296873
H	0.700259	-1.620224	-0.575980
H	-0.633930	4.009461	0.343041
H	-3.272820	2.498957	-1.824259
H	-3.540365	3.267127	-0.255910

H	-2.433734	4.009616	-1.411043
H	2.071834	2.389343	1.813188
H	5.008678	0.850955	-2.220422
H	4.439279	-3.226765	-0.920025
H	5.589583	-1.565411	-2.380117
H	2.881122	-3.523292	0.658316
H	3.723448	2.375503	-1.200629
H	3.324215	0.485832	2.314649
H	1.373968	-0.865240	1.570012

4(7S,2'R)_40

C	-1.763128	-2.092718	0.620453
C	-2.977025	-1.139850	0.529829
C	-1.819955	0.778052	-0.492341
C	-0.523871	0.456440	-0.931134
C	-1.343302	-2.711798	-0.711939
O	-2.847353	-0.147166	-0.540471
C	-4.221343	-1.923258	0.112974
C	-3.203624	-0.454569	1.878649
O	-0.678159	-1.411275	1.263549
C	-0.178559	-0.847089	-1.639837
O	-1.210720	-1.806216	-1.797605
C	-2.142295	2.075916	-0.053002
C	0.512592	1.404313	-0.762722
C	0.189202	2.664290	-0.238944
C	-1.120140	3.014982	0.063657
C	-3.556406	2.470019	0.288720
O	1.229646	3.545471	-0.007111
C	1.991811	1.114923	-1.027133
C	2.559814	0.089397	-0.045616
C	2.626329	0.439806	1.321174
C	2.994707	-1.207339	-0.400086
C	3.039907	-0.476750	2.292709
C	3.410548	-2.126377	0.570867
C	3.420073	-1.760244	1.912416
O	2.258796	0.702358	-2.382219
O	3.015209	-1.659322	-1.691699
O	2.279056	1.673220	1.803125
H	-2.084159	-2.930876	1.258206
H	-2.091711	-3.443131	-1.028402
H	-0.394279	-3.251911	-0.555987
H	-5.083118	-1.249374	0.077251
H	-4.097510	-2.367496	-0.878873
H	-4.435994	-2.720517	0.831089
H	-2.386255	0.225785	2.126844
H	-4.141782	0.106073	1.865675
H	-3.265221	-1.208779	2.670672
H	0.083726	-2.014561	1.275968
H	0.131293	-0.594145	-2.657781
H	0.674526	-1.321280	-1.150283
H	-1.339141	4.018250	0.421609
H	-4.284339	1.854443	-0.244626
H	-3.755935	2.361561	1.361196
H	-3.728173	3.520517	0.031561
H	0.891640	4.329183	0.461541
H	3.060354	-0.159339	3.330309
H	3.721646	-3.114410	0.246293
H	3.740188	-2.474621	2.665809
H	2.731750	-0.915894	-2.273093
H	2.132693	2.348860	1.109973
H	1.640938	1.163500	-2.973574
H	2.535056	2.052730	-0.884073

4(7S,2'R)_42

C	-3.194398	-1.815360	0.108186
C	-3.640774	-0.450204	-0.490128
C	-1.536880	0.869620	-0.558426
C	-0.399286	0.181698	-0.110731
C	-2.072958	-1.779326	1.169214
O	-2.531938	0.167786	-1.226199
C	-4.677171	-0.696974	-1.584988
C	-4.201178	0.476877	0.586337
O	-4.377982	-2.378722	0.692262
C	-0.321473	-1.296344	-0.405342
O	-0.782726	-2.127480	0.670187
C	-1.630766	2.265955	-0.440485
C	0.623520	0.854017	0.586471
C	0.494367	2.245304	0.765915
C	-0.603510	2.925246	0.230894
C	-2.779474	3.050670	-1.019011
O	1.408999	3.009354	1.434104
C	1.792888	0.039977	1.141153
C	2.844864	-0.379211	0.130872
C	3.212944	-1.734728	0.025571
C	3.529421	0.542476	-0.683352
C	4.193627	-2.162645	-0.874685
C	4.512817	0.128771	-1.587469
C	4.835499	-1.222940	-1.676511

O	2.396595	0.772790	2.242069
O	3.201005	1.859059	-0.552328
O	2.558879	-2.628483	0.830063
H	-2.853471	-2.451533	-0.720014
H	-2.294861	-2.544681	1.918271
H	-2.035188	-0.814243	1.688093
H	-4.976436	0.253730	-2.037539
H	-5.564810	-1.185203	-1.176367
H	-4.258500	-1.337931	-2.369060
H	-4.672842	1.351030	0.131704
H	-4.959695	-0.057605	1.164301
H	-3.428649	0.821212	1.278773
H	-4.179196	-3.304448	0.910886
H	-0.901586	-1.504860	-1.309339
H	0.701521	-1.617538	-0.590511
H	-0.640875	4.004318	0.356627
H	-3.285252	2.492970	-1.810854
H	-3.526855	3.296157	-0.254973
H	-2.420726	3.998345	-1.435122
H	2.063854	2.382235	1.826249
H	4.443821	-3.218496	-0.933118
H	5.016857	0.867930	-2.204256
H	5.599149	-1.547253	-2.377678
H	3.726302	2.385276	-1.179838
H	2.880932	-3.525853	0.637622
H	3.319594	0.477743	2.319107
H	1.371786	-0.872996	1.564870

4(7S,2'R)_43

C	-3.317049	-1.534829	0.671193
C	-3.742451	-0.577570	-0.476468
C	-1.638812	0.723974	-0.576784
C	-0.497508	0.035041	-0.134241
C	-2.316099	-2.655513	0.337435
O	-2.621502	0.001631	-1.229059
C	-4.502859	-1.354765	-1.549381
C	-4.627409	0.523512	0.108267
O	-2.860626	-0.840192	1.832908
C	-0.380193	-1.437123	-0.449679
O	-0.959999	-2.274563	0.566241
C	-1.724714	2.123807	-0.487125
C	0.517168	0.718471	0.559811
C	0.380982	2.104810	0.724795
C	-0.699987	2.792843	0.185004
C	-2.841477	2.910605	-1.122535
O	1.366420	2.850039	1.352226
C	1.715319	-0.041819	1.117631
C	2.859026	-0.265890	0.143014
C	3.468032	0.741130	-0.639303
C	3.355848	-1.582103	0.000702
C	4.492931	0.427143	-1.542814
C	4.377529	-1.897640	-0.895364
C	4.936813	-0.882705	-1.668933
O	2.150752	0.627095	2.338707
O	2.778333	-2.556832	0.771869
O	3.115666	2.057191	-0.618533
H	-4.253423	-2.030056	0.956529
H	-2.442933	-3.024172	-0.686337
H	-2.488148	-3.486862	1.026602
H	-4.836596	-0.668410	-2.334084
H	-3.872501	-2.119693	-2.012445
H	-5.384144	-1.842050	-1.120949
H	-5.466228	0.070996	0.648706
H	-4.074634	1.147249	0.813416
H	-5.033996	1.151764	-0.687673
H	-1.887916	-0.907307	1.821372
H	-0.856716	-1.645969	-1.411411
H	0.663514	-1.739993	-0.523458
H	-0.729005	3.873946	0.288974
H	-3.315810	2.343610	-1.926905
H	-3.619593	3.174695	-0.397648
H	-2.451917	3.846107	-1.537885
H	1.806536	2.229731	1.994861
H	4.927946	1.231805	-2.126707
H	4.723849	-2.924104	-0.977284
H	5.732879	-1.117894	-2.369774
H	3.170689	-3.417481	0.543941
H	2.594252	2.322846	0.170079
H	3.089322	0.412549	2.476938
H	1.361690	-1.024534	1.424919

4(7S,2'R)_46

C	-1.885935	-1.920320	0.950799
C	-3.159140	-1.191255	0.445538
C	-1.900463	0.682095	-0.535912
C	-0.563441	0.364185	-0.852824
C	-1.116827	-2.674794	-0.141989
O	-2.898413	-0.265352	-0.666714

C	-4.133281	-2.195865	-0.167389
C	-3.812940	-0.446852	1.609109
O	-1.039986	-1.103596	1.773529
C	-0.168432	-0.956954	-1.509109
O	-1.072978	-2.042752	-1.414196
C	-2.272605	1.988898	-0.165303
C	0.445330	1.337874	-0.645494
C	0.072841	2.598083	-0.142221
C	-1.266184	2.928240	0.038624
C	-3.715016	2.391588	0.005810
O	0.999347	3.575005	0.152799
C	1.915147	1.124038	-1.007728
C	2.657330	0.122740	-0.126577
C	2.845257	0.463106	1.225336
C	3.211605	-1.098894	-0.562025
C	3.505922	-0.370898	2.124654
C	3.879168	-1.947365	0.332503
C	4.017762	-1.584399	1.665932
O	2.075488	0.750814	-2.390406
O	3.119109	-1.542761	-1.851144
O	2.338908	1.675609	1.631225
H	-2.247851	-2.685265	1.646221
H	-1.605006	-3.636691	-0.320636
H	-0.097900	-2.870882	0.224468
H	-3.700180	-2.680303	-1.046529
H	-4.404599	-2.964446	0.562943
H	-5.046392	-1.677667	-0.478284
H	-3.160247	0.336292	2.000130
H	-4.758651	-0.000220	1.291401
H	-4.019546	-1.148062	2.425201
H	-0.661400	-0.391995	1.229739
H	-0.050596	-0.780298	-2.582501
H	0.798986	-1.282714	-1.122277
H	-1.512599	3.933565	0.368416
H	-4.382057	1.733383	-0.554905
H	-4.023714	2.358840	1.056727
H	-3.860136	3.419051	-0.344299
H	1.718577	3.148878	0.664457
H	3.615583	-0.065920	3.161577
H	4.279360	-2.882346	-0.046742
H	4.533568	-2.245547	2.356330
H	2.704535	-0.826917	-2.386079
H	2.532046	1.821443	2.573623
H	1.427092	1.241693	-2.922502
H	2.412747	2.090888	-0.887621

4(7S,2'R)_58

C	-3.208437	-1.612454	0.736031
C	-3.740470	-0.574935	-0.282706
C	-1.636186	0.706886	-0.511989
C	-0.506141	0.041910	0.007742
C	-2.301879	-2.689878	0.134252
O	-2.673889	0.008973	-1.103497
C	-4.626908	-1.263003	-1.319716
C	-4.518427	0.518478	0.448900
O	-2.642328	-1.019587	1.914946
C	-0.268540	-1.463077	-0.120515
O	-1.279560	-2.231904	-0.742718
C	-1.699172	2.115122	-0.548157
C	0.531404	0.801468	0.601556
C	0.427028	2.198892	0.601430
C	-0.656649	2.842946	0.017249
C	-2.843635	2.843158	-1.205304
O	1.442940	2.995214	1.101059
C	1.750492	0.104724	1.198079
C	2.836608	-0.255365	0.199188
C	3.412978	0.640206	-0.730846
C	3.306507	-1.589537	0.188470
C	4.376779	0.197805	-1.647921
C	4.266079	-2.031478	-0.722848
C	4.791179	-1.127685	-1.643837
O	2.257806	0.909738	2.305040
O	2.771008	-2.449713	1.110239
O	3.086904	1.958040	-0.850064
H	-4.089572	-2.145219	1.110881
H	-2.904766	-3.378519	-0.463380
H	-1.857513	-3.256908	0.965909
H	-5.465389	-1.771643	-0.834100
H	-4.061051	-1.995679	-1.902054
H	-5.030338	-0.516961	-2.011942
H	-5.001801	1.184434	-0.269812
H	-5.294683	0.063016	1.073164
H	-3.869472	1.108643	1.100505
H	-1.967313	-0.371256	1.652111
H	0.623276	-1.601375	-0.741588
H	-0.044541	-1.894134	0.864720
H	-0.671856	3.928961	0.005578
H	-2.486958	3.775039	-1.655972

H	-3.311747	2.234355	-1.981786
H	-3.621850	3.108254	-0.480331
H	1.907310	2.443506	1.789106
H	4.787294	0.917867	-2.348456
H	4.591405	-3.067933	-0.700497
H	5.538087	-1.461727	-2.358454
H	3.131642	-3.341141	0.962049
H	2.611679	2.333953	-0.077132
H	3.213006	0.741187	2.379515
H	1.416452	-0.827899	1.647572

4(7S,2'R)_59

C	3.677114	-1.477343	0.095386
C	3.939290	0.054842	0.009642
C	1.717157	1.051762	0.457734
C	0.700014	0.123854	0.721432
C	2.309956	-1.982390	-0.412711
O	3.008356	0.779997	0.883943
C	5.298845	0.365890	0.632136
C	3.875711	0.553182	-1.432799
O	4.712708	-2.080211	-0.692922
C	1.088126	-1.112605	1.488463
O	1.352917	-2.240619	0.625107
C	1.425137	2.284816	-0.144181
C	-0.616466	0.318205	0.244205
C	-0.880714	1.520460	-0.437909
C	0.117766	2.489534	-0.578619
C	2.457277	3.368277	-0.315826
O	-2.125855	1.764294	-0.949973
C	-1.627489	-0.809255	0.477494
C	-3.083429	-0.521052	0.186009
C	-3.681245	-0.792700	-1.057351
C	-3.874469	0.071019	1.180637
C	-5.033444	-0.512215	-1.282958
C	-5.225174	0.361237	0.968962
C	-5.793887	0.064738	-0.269203
O	-1.265846	-1.990447	-0.282642
O	-3.248191	0.370403	2.365225
O	-2.966132	-1.311340	-2.100204
H	3.787982	-1.782584	1.144366
H	2.463301	-2.955834	-0.885243
H	1.879375	-1.312159	-1.164753
H	5.477408	1.445689	0.620074
H	5.329553	0.020441	1.671568
H	6.100223	-0.127952	0.078126
H	2.865075	0.500804	-1.846814
H	4.221823	1.587194	-1.495993
H	4.527560	-0.064195	-2.056385
H	4.707183	-3.032335	-0.498903
H	1.968930	-0.905052	2.098462
H	0.293985	-1.453503	2.153742
H	-0.138620	3.428941	-1.064387
H	3.322932	3.198173	0.327734
H	2.813596	3.423696	-1.351256
H	2.026267	4.345024	-0.070104
H	-2.115515	2.631013	-1.392643
H	-5.461551	-0.742727	-2.253589
H	-5.809662	0.818420	1.762892
H	-6.843159	0.286953	-0.443317
H	-3.897191	0.744970	2.985712
H	-2.108125	-1.633451	-1.729153
H	-0.323108	-2.208854	-0.100305
H	-1.572355	-1.070828	1.538623

4(7S,2'R)_5

C	2.350024	-2.145394	-0.000449
C	3.231473	-0.877616	-0.159854
C	1.728522	0.984847	0.505737
C	0.432448	0.607477	0.900578
C	0.848615	-1.982775	-0.318234
O	2.789304	0.144941	0.798157
C	4.654993	-1.182871	0.300583
C	3.223946	-0.366410	-1.598942
O	2.922135	-3.124871	-0.878479
C	0.295753	-0.696851	1.652235
O	0.024342	-1.840546	0.832351
C	1.987947	2.241308	-0.066808
C	-0.661253	1.449161	0.614700
C	-0.397747	2.665900	-0.034136
C	0.897844	3.066375	-0.341661
C	3.383170	2.718591	-0.371891
O	-1.480079	3.457636	-0.364596
C	-2.120070	1.119718	0.934838
C	-2.668531	-0.018335	0.079780
C	-2.989603	-1.302111	0.572111
C	-2.849748	0.209417	-1.301772
C	-3.429891	-2.318062	-0.283988
C	-3.286658	-0.805211	-2.159254

C	-3.566663	-2.067434	-1.644844
O	-2.338766	0.839282	2.332621
O	-2.599266	1.411465	-1.909490
O	-2.887585	-1.638898	1.893025
H	2.434836	-2.486518	1.040686
H	0.502242	-2.906459	-0.791065
H	0.662301	-1.165953	-1.026474
H	5.269982	-0.279389	0.240001
H	4.653740	-1.534037	1.338438
H	5.106321	-1.955436	-0.326315
H	2.252251	0.042401	-1.888492
H	3.980653	0.408547	-1.737899
H	3.456793	-1.193717	-2.274291
H	2.507867	-3.978049	-0.667279
H	1.216860	-0.862941	2.220182
H	-0.531817	-0.654692	2.354884
H	1.056364	4.038144	-0.803800
H	4.130468	2.142321	0.177283
H	3.611064	2.632576	-1.440877
H	3.489397	3.775389	-0.103949
H	-1.183135	4.212828	-0.903018
H	-3.657610	-3.289671	0.143132
H	-3.401342	-0.580066	-3.214769
H	-3.905065	-2.858050	-2.308953
H	-2.401115	2.142586	-1.289058
H	-2.664261	-0.819117	2.391426
H	-1.708607	1.363311	2.855018
H	-2.706285	2.015569	0.714118

4(7S,2'R)_61

C	-1.697622	-2.232548	0.512217
C	-2.954561	-1.450025	0.047392
C	-1.847821	0.676578	-0.552670
C	-0.468893	0.584918	-0.813250
C	-0.724137	-2.690652	-0.588989
O	-2.660307	-0.384121	-0.919526
C	-3.877651	-2.376837	-0.741920
C	-3.680846	-0.900727	1.274883
O	-0.955990	-1.546428	1.522408
C	0.034242	-0.612503	-1.587769
O	0.340081	-1.764036	-0.781049
C	-2.415152	1.861608	-0.059234
C	0.396027	1.619901	-0.416765
C	-0.168512	2.771275	0.155780
C	-1.548618	2.897831	0.295870
C	-3.904144	2.068327	0.049646
O	0.673511	3.779257	0.556543
C	1.913566	1.548118	-0.586378
C	2.509613	0.292012	0.053563
C	3.230361	-0.714813	-0.607823
C	2.331798	0.129096	1.441849
C	3.713725	-1.843362	0.061150
C	2.790645	-0.999397	2.124933
C	3.481612	-1.985049	1.424785
O	2.219839	1.746716	-1.975813
O	1.677820	1.134864	2.100294
O	3.435229	-0.580652	-1.963306
H	-2.102601	-3.138286	0.980525
H	-1.239696	-2.891181	-1.534134
H	-0.232886	-3.610924	-0.261015
H	-4.773957	-1.828807	-1.049489
H	-3.388555	-2.759113	-1.643232
H	-4.187630	-3.227642	-0.127281
H	-3.081979	-0.147382	1.790192
H	-4.641803	-0.465168	0.991986
H	-3.872281	-1.716274	1.980938
H	-0.152479	-1.212157	1.079802
H	-0.709827	-0.895369	-2.338742
H	0.956453	-0.358491	-2.105941
H	-1.957113	3.826142	0.690391
H	-4.450499	1.350040	-0.565055
H	-4.256712	1.962690	1.082031
H	-4.167351	3.079518	-0.279855
H	0.142667	4.502358	0.932400
H	4.256036	-2.600685	-0.498348
H	2.610748	-1.087368	3.193052
H	3.845848	-2.865134	1.946544
H	1.610464	0.907301	3.043635
H	4.010964	-1.294680	-2.287522
H	2.928201	1.127482	-2.227240
H	2.330713	2.395834	-0.033665

4(7S,2'R)_63

C	-3.464218	-1.157330	1.002444
C	-3.970742	-0.174768	-0.094263
C	-1.767052	0.702237	-0.750768
C	-0.708026	-0.172527	-0.463846
C	-2.799584	-2.469947	0.551847

O	-2.983566	0.160916	-1.129858
C	-5.093980	-0.828162	-0.898058
C	-4.478401	1.096385	0.588414
O	-2.630643	-0.529144	1.978410
C	-0.941944	-1.640017	-0.738209
O	-1.382848	-2.365126	0.423823
C	-1.577563	2.091737	-0.753878
C	0.517841	0.316083	0.044166
C	0.666222	1.716349	0.142028
C	-0.347527	2.567273	-0.304230
C	-2.630468	3.055952	-1.235151
O	1.785889	2.362915	0.599153
C	1.556022	-0.684061	0.556972
C	2.983790	-0.455033	0.076756
C	3.376502	-0.993934	-1.161232
C	3.961340	0.232609	0.804904
C	4.685277	-0.866089	-1.635570
C	5.275626	0.369805	0.360095
C	5.628850	-0.188728	-0.866553
O	1.438221	-0.870385	1.978735
O	3.544186	0.807541	1.992302
O	2.412931	-1.647438	-1.880298
H	-4.384004	-1.445052	1.526432
H	-3.242033	-2.851064	-0.375480
H	-2.949947	-3.216755	1.336331
H	-5.919631	-1.121121	-0.242069
H	-5.478384	-0.117627	-1.636829
H	-4.741979	-1.715800	-1.431814
H	-5.227077	0.834312	1.343964
H	-3.669390	1.630490	1.090443
H	-4.947539	1.760019	-0.142123
H	-1.713839	-0.779418	1.759386
H	-1.683295	-1.745501	-1.533963
H	-0.027919	-2.127676	-1.076236
H	-0.162637	3.637554	-0.265327
H	-3.351809	2.562567	-1.890828
H	-3.187814	3.498451	-0.401628
H	-2.163296	3.878710	-1.787055
H	2.312323	1.827024	1.227063
H	4.951408	-1.298208	-2.596503
H	5.995268	0.914111	0.964963
H	6.647571	-0.089459	-1.229469
H	4.268525	1.312088	2.403756
H	2.808556	-2.022047	-2.686320
H	1.880553	-0.128406	2.425207
H	1.281239	-1.658428	0.164754

4(7S,2'R)_6

C	-2.104713	-2.262282	-0.178360
C	-3.114969	-1.087424	-0.111496
C	-1.719264	0.929468	-0.510841
C	-0.347916	0.689874	-0.714415
C	-0.684306	-1.974043	0.350816
O	-2.643020	0.004017	-0.971913
C	-4.426111	-1.504993	-0.773668
C	-3.352536	-0.633760	1.327673
O	-2.698119	-3.324277	0.581429
C	0.034162	-0.559316	-1.475795
O	0.269576	-1.724851	-0.672710
C	-2.176012	2.141002	0.032082
C	0.603709	1.621070	-0.260903
C	0.142448	2.806011	0.337240
C	-1.221130	3.065265	0.457484
C	-3.640568	2.475918	0.144493
O	1.072816	3.711203	0.784214
C	2.109921	1.437574	-0.422626
C	2.636332	0.095128	0.060791
C	3.283156	-0.868382	-0.735184
C	2.454353	-0.211141	1.422075
C	3.694558	-2.094183	-0.194665
C	2.848633	-1.432367	1.969448
C	3.467298	-2.373611	1.146945
O	2.495668	1.639946	-1.798880
O	1.857376	0.755008	2.191448
O	3.520181	-0.697313	-2.072465
H	-2.011048	-2.565653	-1.230390
H	-0.319839	-2.875315	0.852701
H	-0.677008	-1.164100	1.090708
H	-4.248595	-1.809271	-1.811327
H	-4.879932	-2.343039	-0.239265
H	-5.130608	-0.667154	-0.773365
H	-3.590724	-1.505477	1.942868
H	-4.193796	0.060523	1.380259
H	-2.474288	-0.146331	1.759215
H	-2.162628	-4.120725	0.430471
H	-0.761563	-0.772936	-2.197689
H	0.956855	-0.409757	-2.033508
H	-1.544564	4.009910	0.889979

H	-3.809521	3.528299	-0.108457
H	-4.244216	1.856421	-0.522305
H	-4.009808	2.327002	1.166194
H	0.611264	4.470156	1.180660
H	4.180504	-2.810353	-0.849934
H	2.674836	-1.630113	3.023866
H	3.779837	-3.328085	1.561270
H	1.795548	0.438618	3.109181
H	3.259650	0.221306	-2.308921
H	2.287991	2.555953	-2.046335
H	2.593544	2.211433	0.178558

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C	3.670868	-1.482581	0.098770
C	3.935258	0.052706	-0.001331
C	1.717044	1.049899	0.463405
C	0.699957	0.120109	0.722051
C	2.310510	-1.974408	-0.426959
O	3.010422	0.777960	0.882752
C	5.299794	0.377048	0.605623
C	3.860292	0.541680	-1.445607
O	4.646887	-2.196663	-0.671241
C	1.086596	-1.123440	1.479034
O	1.353780	-2.244679	0.607030
C	1.424954	2.285988	-0.132299
C	-0.617310	0.319069	0.248125
C	-0.882830	1.527212	-0.422944
C	0.116613	2.495790	-0.560912
C	2.460840	3.365334	-0.306294
O	-2.129949	1.777117	-0.927455
C	-1.627727	-0.811106	0.471583
C	-3.083933	-0.522452	0.182147
C	-3.877313	0.056634	1.182500
C	-3.680080	-0.782164	-1.064553
C	-5.228754	0.345049	0.973115
C	-5.032963	-0.503133	-1.288043
C	-5.795843	0.060356	-0.268595
O	-1.265023	-1.984877	-0.299480
O	-2.962812	-1.287132	-2.112645
O	-3.252689	0.345809	2.370527
H	3.757988	-1.772704	1.153847
H	2.469539	-2.938290	-0.914275
H	1.879947	-1.288888	-1.163848
H	5.370591	-0.006447	1.629764
H	5.445093	1.461295	0.630851
H	6.111638	-0.053567	0.011537
H	2.842707	0.511258	-1.844066
H	4.232138	1.565715	-1.526830
H	4.486835	-0.101254	-2.069928
H	5.512695	-2.073440	-0.249348
H	1.965576	-0.920764	2.093419
H	0.291449	-1.470485	2.139677
H	-0.139812	3.438381	-1.040414
H	2.825898	3.408490	-1.339278
H	2.030715	4.345806	-0.074640
H	3.321264	3.199393	0.345465
H	-2.121270	2.648522	-1.360799
H	-5.815111	0.791860	1.771541
H	-5.459672	-0.724217	-2.261477
H	-6.845664	0.281245	-0.441024
H	-2.104707	-1.612007	-1.744439
H	-3.903610	0.711028	2.994518
H	-0.322254	-2.204429	-0.119310
H	-1.572746	-1.082299	1.530269

4(7S,2'R)_152

C	-1.917542	-2.085842	0.759119
C	-3.130150	-1.257056	0.256746
C	-1.872509	0.710389	-0.550266
C	-0.526790	0.476987	-0.882909
C	-1.016121	-2.726881	-0.309913
O	-2.791763	-0.292522	-0.800437
C	-4.140183	-2.172887	-0.432349
C	-3.778645	-0.560092	1.452833
O	-1.095406	-1.365369	1.678850
C	-0.188423	-0.827571	-1.566945
O	0.093220	-1.898345	-0.648849
C	-2.305528	1.968321	-0.099020
C	0.448063	1.454750	-0.596294
C	0.026580	2.649919	0.017287
C	-1.326870	2.915503	0.204127
C	-3.762448	2.325048	0.045213
O	0.918282	3.623649	0.417811
C	1.931470	1.291025	-0.919655
C	2.601301	0.186969	-0.111908
C	2.724267	0.387829	1.274502
C	3.097186	-1.022653	-0.634111
C	3.263740	-0.575325	2.124940

C	3.644711	-1.999706	0.208439
C	3.716280	-1.776509	1.577703
O	2.171268	1.082761	-2.329688
O	3.068034	-1.320417	-1.967602
O	2.277666	1.594561	1.760734
H	-2.374261	-2.907083	1.325163
H	-1.577419	-3.005340	-1.208082
H	-0.566897	-3.631344	0.109358
H	-3.706766	-2.670037	-1.305426
H	-4.998973	-1.583732	-0.769529
H	-4.501112	-2.939433	0.260304
H	-4.711720	-0.075213	1.157218
H	-4.008418	-1.302634	2.224765
H	-3.109931	0.181700	1.893294
H	-0.290009	-1.121951	1.183997
H	-1.012987	-1.122819	-2.221917
H	0.703337	-0.721638	-2.175952
H	-1.612392	3.881876	0.610760
H	-4.097316	2.269307	1.086967
H	-3.929183	3.352854	-0.294903
H	-4.394553	1.657500	-0.544887
H	1.638973	3.173148	0.904891
H	3.327220	-0.378871	3.191435
H	4.006498	-2.921288	-0.236526
H	4.136910	-2.537721	2.228544
H	2.759322	-0.512669	-2.441686
H	2.397655	1.631926	2.725247
H	1.440139	1.481658	-2.830718
H	2.421147	2.233963	-0.664116

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C	-1.946270	-2.067021	0.744211
C	-3.147155	-1.173631	0.336543
C	-1.859877	0.754931	-0.525928
C	-0.546263	0.473810	-0.942965
C	-1.145529	-2.719824	-0.395995
O	-2.830790	-0.209689	-0.727348
C	-4.240633	-2.029857	-0.299947
C	-3.685654	-0.468747	1.581215
O	-1.035491	-1.404271	1.622389
C	-0.298706	-0.831923	-1.661337
O	-0.020167	-1.935481	-0.781532
C	-2.220106	2.025190	-0.047402
C	0.480570	1.412051	-0.724674
C	0.124604	2.635932	-0.137325
C	-1.196918	2.952645	0.155860
C	-3.650803	2.428060	0.199784
O	1.144168	3.530646	0.136034
C	1.963682	1.175319	-1.048378
C	2.579634	0.137393	-0.105016
C	2.968834	-1.161309	-0.484401
C	2.769525	0.482126	1.251600
C	3.491567	-2.081654	0.424252
C	3.285645	-0.435940	2.174531
C	3.640177	-1.713204	1.758706
O	2.174777	0.951896	-2.446692
O	2.470288	1.709286	1.773316
O	2.815711	-1.517305	-1.805293
H	-2.402050	-2.881226	1.321351
H	-1.775124	-2.943682	-1.263690
H	-0.716786	-3.656596	-0.029221
H	-3.886547	-2.525590	-1.208867
H	-5.093559	-1.398417	-0.568517
H	-4.587369	-2.795389	0.400972
H	-4.612605	0.062059	1.352902
H	-3.901495	-1.213769	2.354988
H	-2.958505	0.234636	1.991811
H	-0.252496	-1.188094	1.080972
H	-1.165470	-1.078603	-2.281330
H	0.569222	-0.742814	-2.306959
H	-1.433433	3.939914	0.546720
H	-3.811205	3.458608	-0.135024
H	-3.909977	2.388130	1.263732
H	-4.343665	1.776858	-0.337664
H	0.790658	4.287880	0.635452
H	3.773105	-3.071884	0.075988
H	3.403420	-0.119714	3.206084
H	4.041646	-2.425128	2.474072
H	2.165568	2.369088	1.115532
H	3.182470	-2.404680	-1.959683
H	2.503172	0.042517	-2.572112
H	2.475128	2.119155	-0.844503

4(7S,2'R)_159

C	-3.280762	-1.571460	0.663719
C	-3.745027	-0.603090	-0.459178
C	-1.663025	0.731785	-0.581465
C	-0.503720	0.053356	-0.168236

C	-2.272071	-2.672753	0.290301
O	-2.648350	0.005805	-1.224850
C	-4.515091	-1.375478	-1.528773
C	-4.635658	0.474861	0.159597
O	-2.808086	-0.887509	1.825000
C	-0.369555	-1.412048	-0.509682
O	-0.916912	-2.277917	0.500218
C	-1.766569	2.127911	-0.471441
C	0.514584	0.734942	0.522965
C	0.365445	2.117281	0.685974
C	-0.730530	2.803554	0.178007
C	-2.905849	2.908889	-1.072567
O	1.397291	2.793318	1.320029
C	1.700184	-0.036724	1.108188
C	2.871753	-0.255554	0.152281
C	3.502621	0.741736	-0.621457
C	3.374674	-1.570467	0.028139
C	4.549169	0.425065	-1.499349
C	4.418550	-1.893248	-0.840193
C	4.997584	-0.884865	-1.607738
O	2.109679	0.454574	2.395793
O	2.778316	-2.544532	0.788966
O	3.147146	2.060345	-0.615893
H	-4.203382	-2.084780	0.961738
H	-2.413633	-3.024288	-0.737438
H	-2.420281	-3.518472	0.967225
H	-4.878270	-0.682296	-2.294151
H	-5.378024	-1.885037	-1.089073
H	-3.882383	-2.121922	-2.018065
H	-4.080710	1.096315	0.865197
H	-5.065914	1.109511	-0.618715
H	-5.457844	0.000840	0.707037
H	-1.835307	-0.948248	1.795416
H	-0.858929	-1.612182	-1.466850
H	0.678494	-1.693355	-0.607689
H	-0.771436	3.885784	0.278924
H	-2.537059	3.855127	-1.482458
H	-3.389255	2.346769	-1.874953
H	-3.672435	3.152418	-0.328395
H	1.232721	3.753359	1.315992
H	4.997783	1.227876	-2.075810
H	4.766403	-2.920635	-0.905904
H	5.810740	-1.124544	-2.287222
H	3.171366	-3.405838	0.565508
H	2.642922	2.323969	0.183459
H	2.308833	1.402593	2.311550
H	1.322671	-1.027802	1.346010

4(7S,2'R)_160

C	-3.569309	-1.102546	0.952127
C	-3.968531	-0.130015	-0.194956
C	-1.695506	0.687761	-0.700400
C	-0.665258	-0.200262	-0.355016
C	-2.887936	-2.429325	0.573905
O	-2.893024	0.161228	-1.152244
C	-5.039588	-0.771523	-1.075385
C	-4.499590	1.163286	0.425642
O	-2.797639	-0.469576	1.974988
C	-0.918914	-1.669865	-0.599199
O	-1.463972	-2.336056	0.554996
C	-1.481434	2.075062	-0.708920
C	0.551972	0.281234	0.180785
C	0.721162	1.680491	0.276720
C	-0.267581	2.539551	-0.208036
C	-2.486484	3.050752	-1.263902
O	1.825989	2.319256	0.768354
C	1.604484	-0.699514	0.677020
C	2.988613	-0.499143	0.083871
C	3.253573	-1.012624	-1.197351
C	4.029493	0.177320	0.737990
C	4.502750	-0.858041	-1.802158
C	5.285255	0.341238	0.150909
C	5.511964	-0.178893	-1.120548
O	1.702627	-0.685551	2.130720
O	3.819248	0.753674	1.975783
O	2.222512	-1.657181	-1.825481
H	-4.529914	-1.368391	1.410345
H	-3.259692	-2.823083	-0.378266
H	-3.105769	-3.160634	1.357122
H	-4.670670	-1.678688	-1.563262
H	-5.342649	-0.066609	-1.856167
H	-5.922698	-1.029471	-0.482867
H	-4.889677	1.826931	-0.349740
H	-5.315449	0.929963	1.118516
H	-3.722251	1.684631	0.987445
H	-1.875935	-0.751350	1.826239
H	-1.605733	-1.781957	-1.441446
H	0.000116	-2.194870	-0.853780

H	-0.068447	3.607329	-0.176362
H	-3.181312	2.559037	-1.948479
H	-3.077786	3.522078	-0.470751
H	-1.971547	3.851540	-1.805364
H	2.424965	1.750217	1.291339
H	4.671925	-1.266220	-2.794897
H	6.057776	0.872245	0.697397
H	6.484986	-0.057328	-1.587801
H	3.074852	0.245377	2.397344
H	2.526099	-1.988395	-2.688387
H	0.869197	-0.332972	2.487480
H	1.288891	-1.705409	0.408829

4(7S,2'R)_162

C	-2.101942	-2.040009	0.826153
C	-3.245413	-1.051005	0.489807
C	-1.847610	0.752811	-0.470591
C	-0.529390	0.372363	-0.782726
C	-1.511189	-2.760484	-0.381144
O	-2.903651	-0.134809	-0.596432
C	-4.445836	-1.813444	-0.069496
C	-3.645043	-0.276248	1.747219
O	-1.019816	-1.434315	1.543532
C	-0.157286	-1.012878	-1.299512
O	-1.205377	-1.945841	-1.503975
C	-2.164387	2.084851	-0.139216
C	0.513637	1.322390	-0.650803
C	0.197262	2.614271	-0.189792
C	-1.123505	2.996158	0.016442
C	-3.588022	2.542540	0.052428
O	1.164609	3.573643	0.036414
C	1.970829	1.052830	-1.033079
C	2.697748	0.056470	-0.137549
C	2.970016	0.452883	1.183703
C	3.147687	-1.220616	-0.530352
C	3.613869	-0.377662	2.098458
C	3.796576	-2.067081	0.379874
C	4.019854	-1.646510	1.684780
O	2.111540	0.643421	-2.411755
O	2.974398	-1.713070	-1.792682
O	2.564020	1.717017	1.543518
H	-2.552040	-2.820299	1.457580
H	-2.226758	-3.500942	-0.746273
H	-0.609499	-3.294465	-0.045609
H	-4.192055	-2.319652	-1.005429
H	-5.263801	-1.114470	-0.271142
H	-4.800645	-2.559204	0.648765
H	-4.558479	0.296530	1.570245
H	-3.836448	-0.973324	2.571374
H	-2.859030	0.416727	2.060339
H	-1.359182	-1.140361	2.404129
H	0.307083	-0.888198	-2.279571
H	0.593942	-1.451570	-0.633724
H	-1.328974	4.019885	0.316406
H	-3.884704	2.512184	1.107271
H	-3.699693	3.578041	-0.286034
H	-4.288437	1.915566	-0.503957
H	1.882847	3.149181	0.550492
H	3.792420	-0.027720	3.111515
H	4.117542	-3.045146	0.035405
H	4.521104	-2.305905	2.387548
H	2.603963	-0.986069	-2.345366
H	2.822430	1.900850	2.463201
H	1.428357	1.093235	-2.936781
H	2.497143	2.006981	-0.946966

4(7S,2'R)_179

C	3.657208	-1.564670	0.185746
C	3.905229	-0.027510	0.274689
C	1.611990	0.920214	0.346586
C	0.586461	-0.039631	0.298677
C	2.443646	-2.008016	-0.653158
O	2.796528	0.611809	0.997608
C	5.100323	0.246266	1.186820
C	4.130044	0.588090	-1.104384
O	4.790737	-2.209571	-0.411932
C	0.816291	-1.359500	0.992084
O	1.311603	-2.389721	0.125088
C	1.418849	2.218019	-0.152443
C	-0.613130	0.247958	-0.366234
C	-0.776526	1.524697	-0.921588
C	0.208399	2.498902	-0.792499
C	2.460857	3.295987	-0.008476
O	-1.949722	1.758290	-1.605998
C	-1.706886	-0.787832	-0.583393
C	-3.048537	-0.468659	0.092575
C	-3.088973	-0.017095	1.427088
C	-4.292724	-0.675676	-0.544488

C	-4.289624	0.299239	2.068924
C	-5.501470	-0.360194	0.091315
C	-5.494045	0.133249	1.389331
O	-1.849050	-0.972412	-2.018464
O	-4.402993	-1.203756	-1.799180
O	-1.900001	0.087106	2.100470
H	3.519972	-1.943261	1.207087
H	2.730441	-2.910451	-1.198299
H	2.157095	-1.248381	-1.388827
H	4.959455	-0.228278	2.164642
H	5.212199	1.324301	1.337843
H	6.029956	-0.126534	0.745864
H	4.521267	1.604567	-1.015496
H	4.864366	-0.014180	-1.646339
H	3.214251	0.622331	-1.700422
H	5.538725	-2.138447	0.203056
H	1.513356	-1.202795	1.821744
H	-0.108537	-1.755168	1.410590
H	0.033558	3.490074	-1.205217
H	3.071282	3.389986	-0.914482
H	1.983913	4.266824	0.163065
H	3.135260	3.086273	0.825062
H	-1.912478	2.626965	-2.043123
H	-4.266608	0.658043	3.094601
H	-6.427129	-0.522055	-0.452171
H	-6.430258	0.377600	1.883590
H	-3.482693	-1.349799	-2.131750
H	-2.074212	0.393323	3.007263
H	-1.967368	-0.076754	-2.395537
H	-1.356909	-1.761195	-0.236517

4(7S,2'R)_186

C	-1.927048	-2.072902	0.732698
C	-3.138481	-1.230326	0.246272
C	-1.857995	0.730349	-0.542038
C	-0.527505	0.473107	-0.914119
C	-1.027158	-2.708139	-0.336148
O	-2.805981	-0.245655	-0.790646
C	-4.156191	-2.128507	-0.455444
C	-3.784424	-0.551531	1.455717
O	-1.061679	-1.368297	1.626163
C	-0.233871	-0.827784	-1.630063
O	0.072245	-1.915135	-0.755078
C	-2.256250	1.987907	-0.059418
C	0.469983	1.433050	-0.653699
C	0.078320	2.635834	-0.043180
C	-1.257269	2.925397	0.208204
C	-3.701789	2.368087	0.129723
O	1.075130	3.528270	0.300442
C	1.956962	1.246006	-0.951525
C	2.603044	0.166933	-0.087215
C	2.721086	0.405363	1.299064
C	3.084397	-1.067008	-0.575012
C	3.247225	-0.558931	2.164067
C	3.617943	-2.031201	0.287455
C	3.685819	-1.776637	1.652646
O	2.222844	0.997466	-2.349737
O	3.051356	-1.402986	-1.900791
O	2.319845	1.568245	1.903734
H	-2.391086	-2.914970	1.265830
H	-1.622399	-3.029965	-1.200185
H	-0.565464	-3.597279	0.103058
H	-3.728515	-2.609149	-1.340359
H	-5.013790	-1.528626	-0.776547
H	-4.517525	-2.907560	0.222838
H	-4.721449	-0.067777	1.171492
H	-4.009666	-1.302628	2.221627
H	-3.122244	0.196173	1.898336
H	-1.522950	-1.275601	2.474751
H	0.635316	-0.713370	-2.271938
H	-1.087719	-1.092463	-2.262599
H	-1.523874	3.898026	0.615532
H	-4.010637	2.302057	1.178877
H	-3.859318	3.403750	-0.190181
H	-4.360084	1.720817	-0.453992
H	0.692732	4.266299	0.807691
H	3.305956	-0.330752	3.223554
H	3.968230	-2.966720	-0.137347
H	4.094553	-2.527572	2.323219
H	2.752655	-0.606477	-2.398773
H	2.075583	2.283089	1.281348
H	1.509668	1.397519	-2.875010
H	2.451157	2.193510	-0.721826

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Antibacterial assay

Compounds **1-3** were dissolved in DMSO at a final concentration of 10 mg/mL. The antibacterial activity evaluation was carried out in triplicate according to the standard microdilution method and expressed as minimum inhibitory concentration (MIC), with vancomycin as the positive control. The compound was tested at concentrations ranging from 1.83 to 500 μg/mL. Test strains were *S. aureus* (CMCC 26003) and *E. coli* (ATCC 8739).

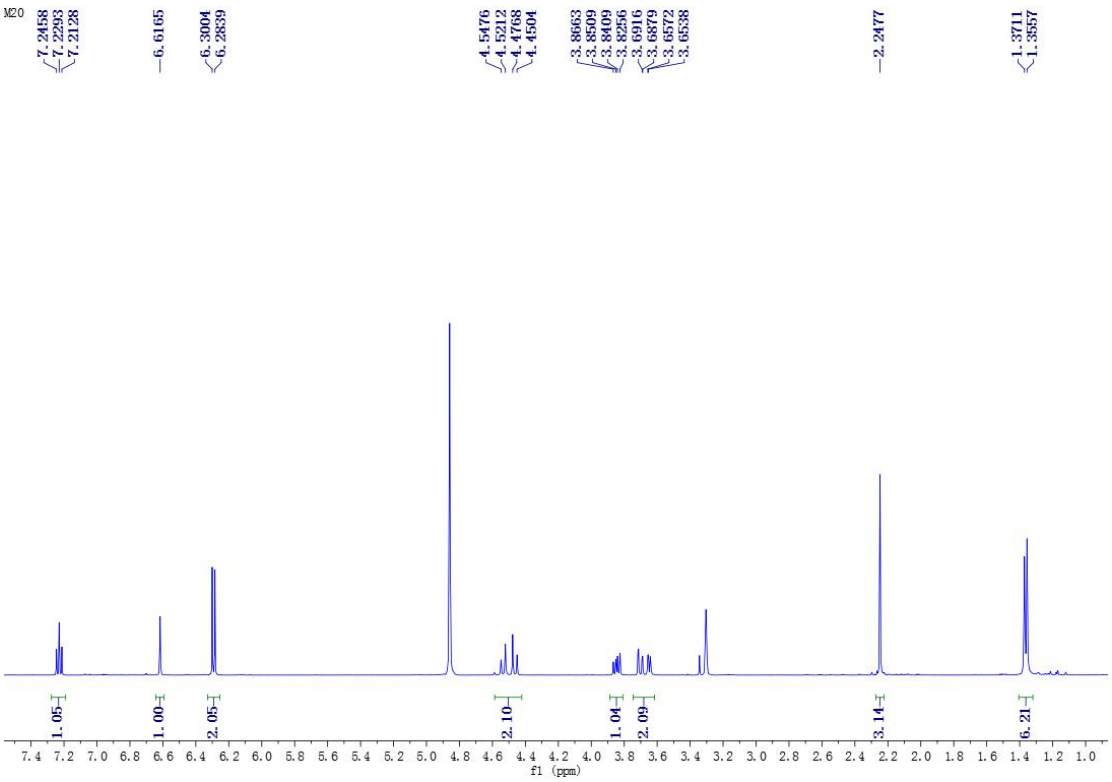


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **1**.

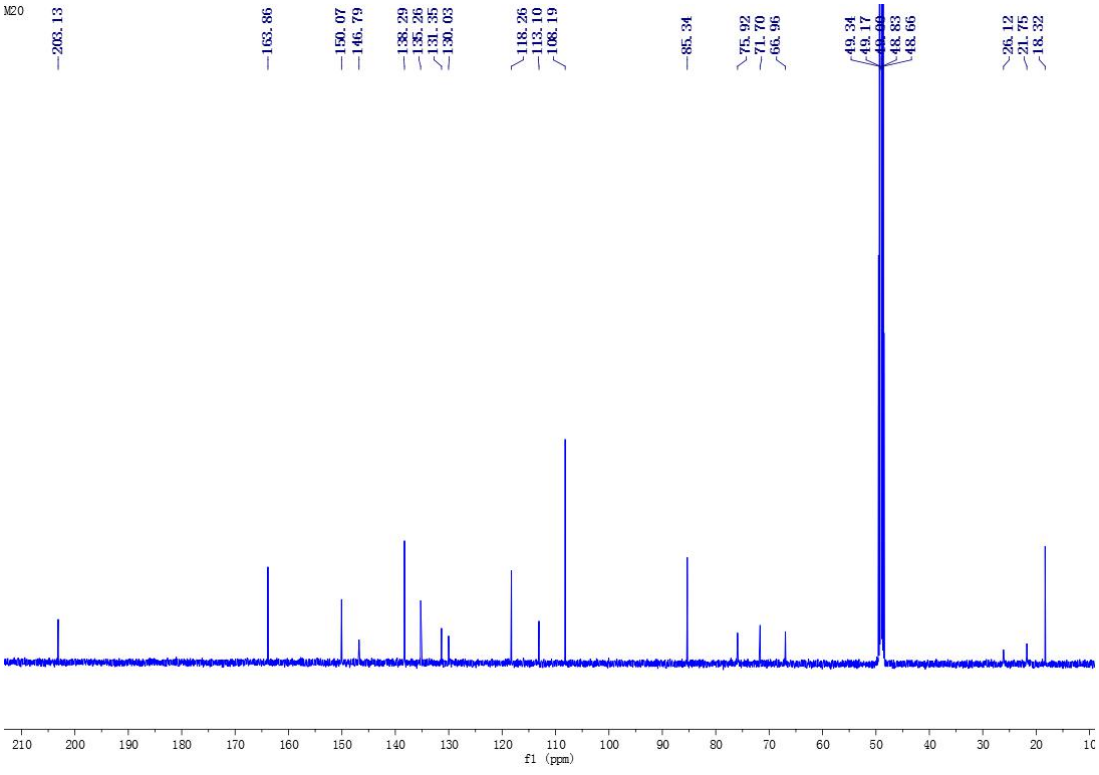


Figure S3. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **1**.

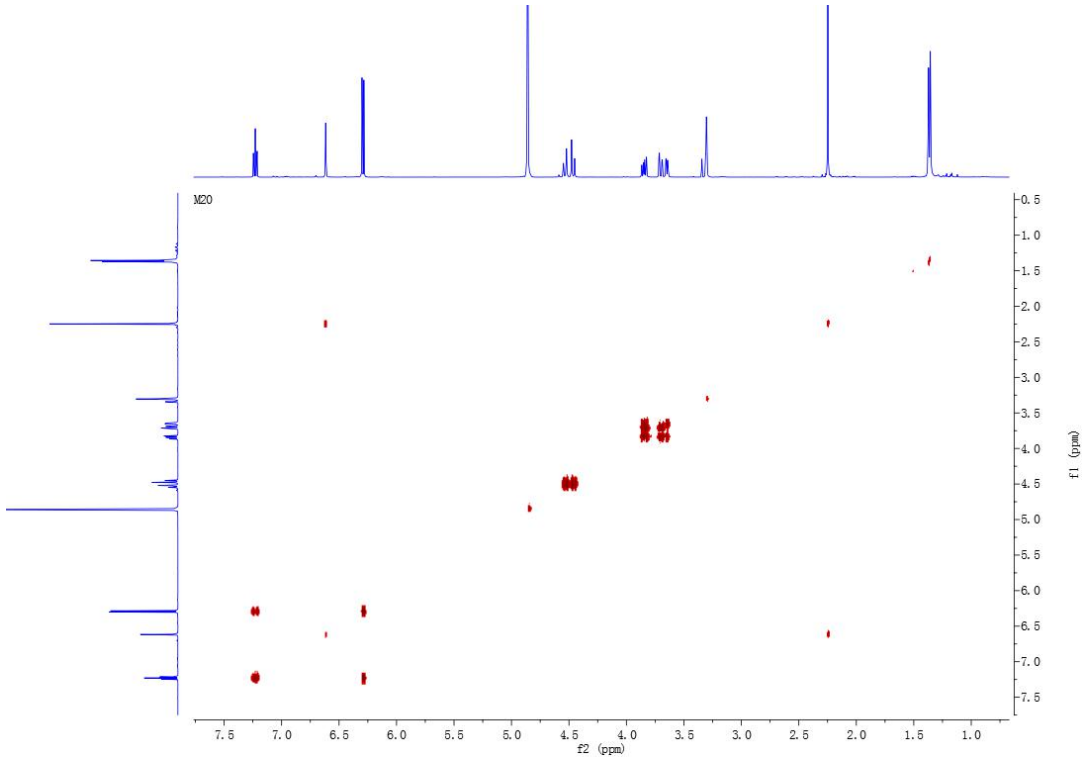


Figure S4. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **1**.

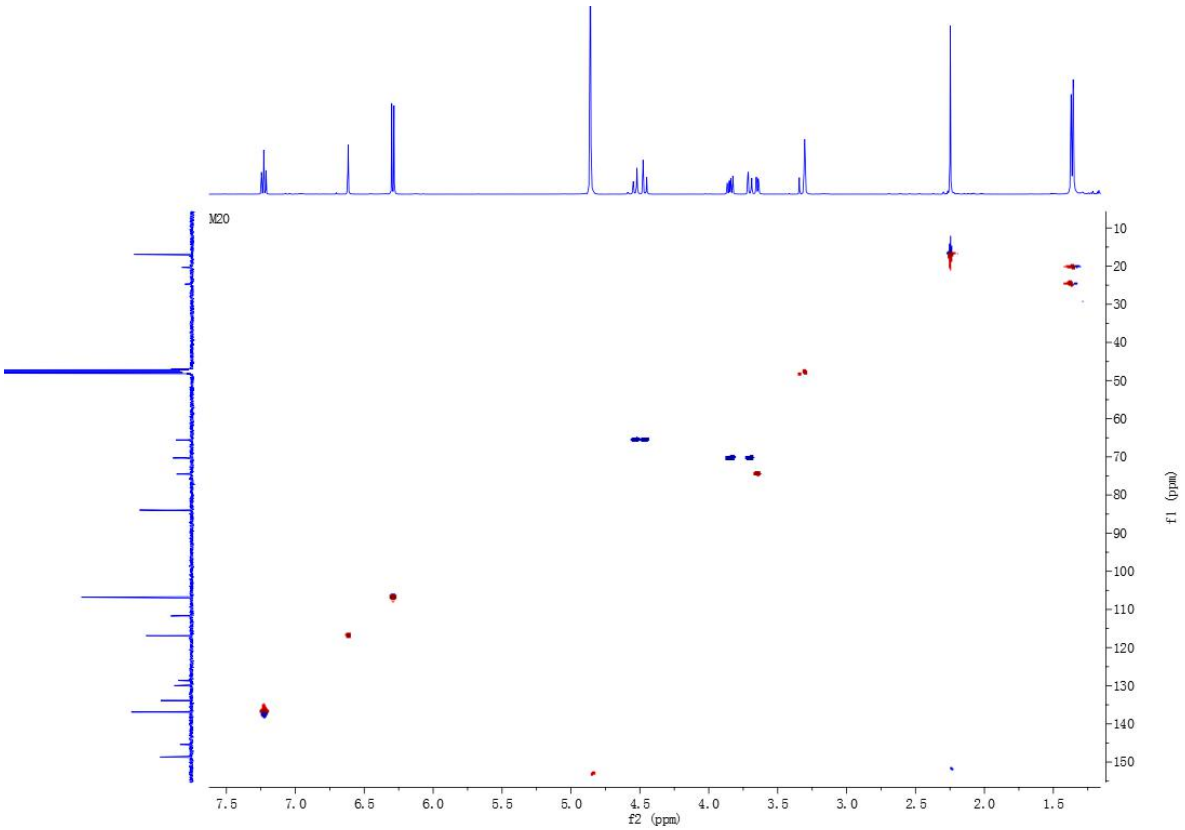


Figure S5. HSQC spectrum of **1**.

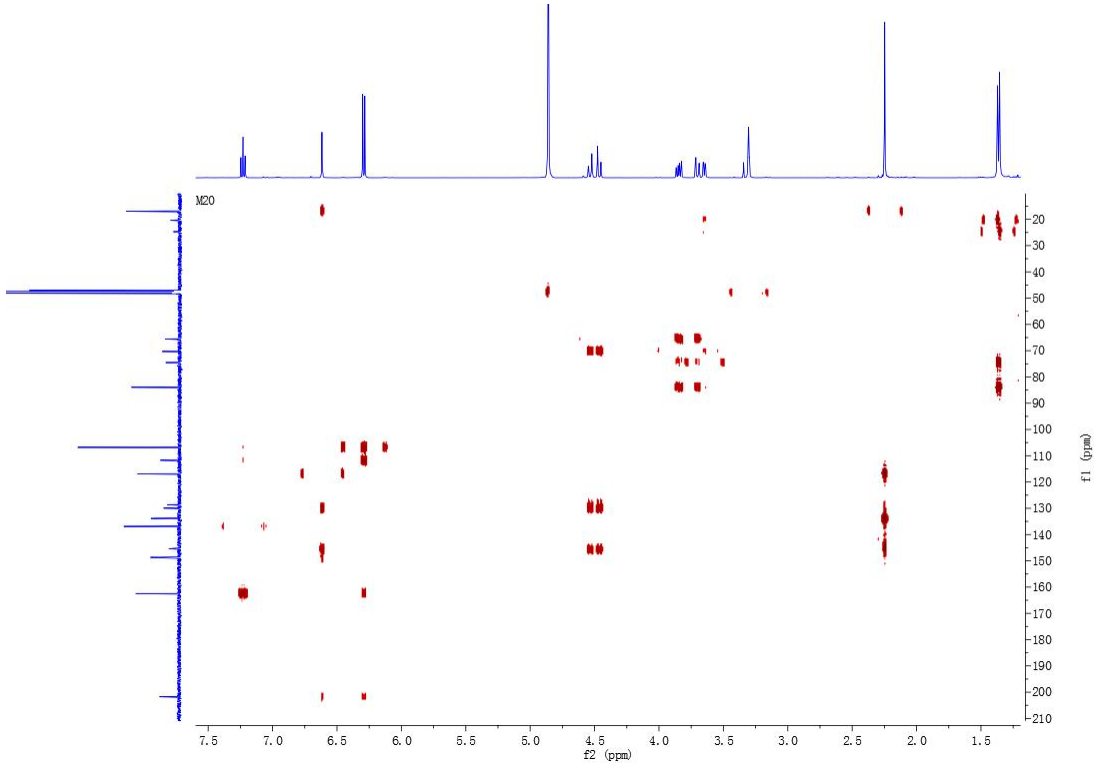


Figure S6. HMBC spectrum of **1**.

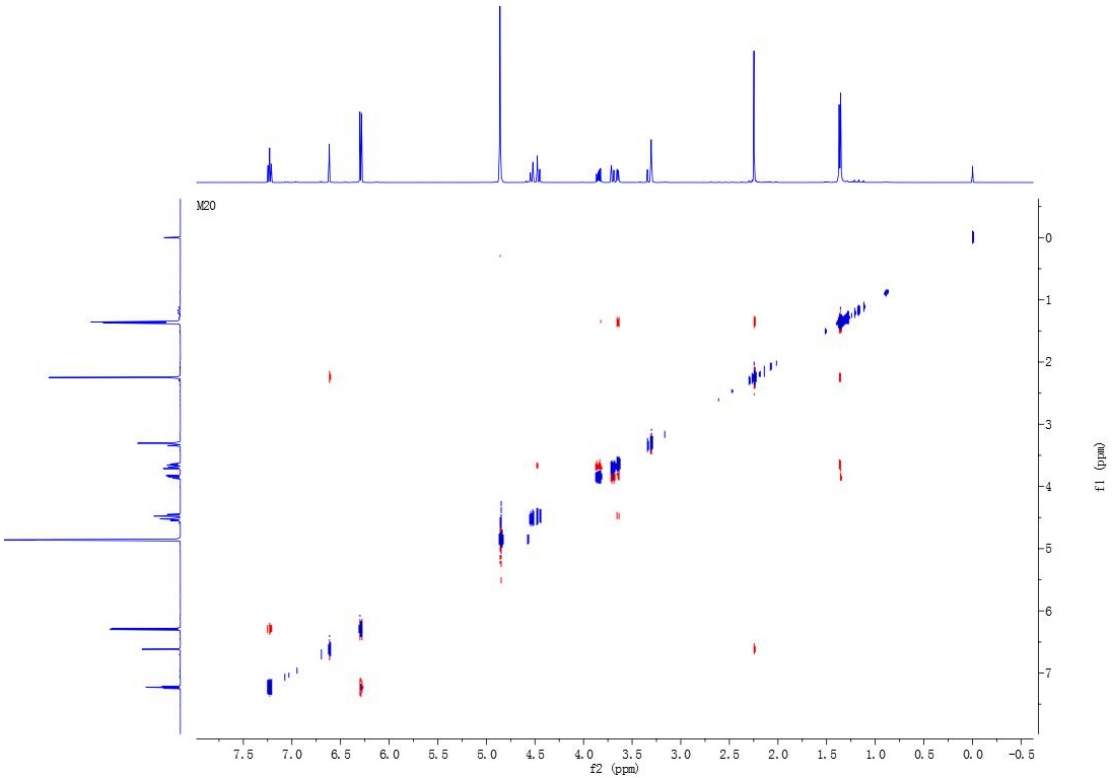


Figure S7. NOESY spectrum of **1**.

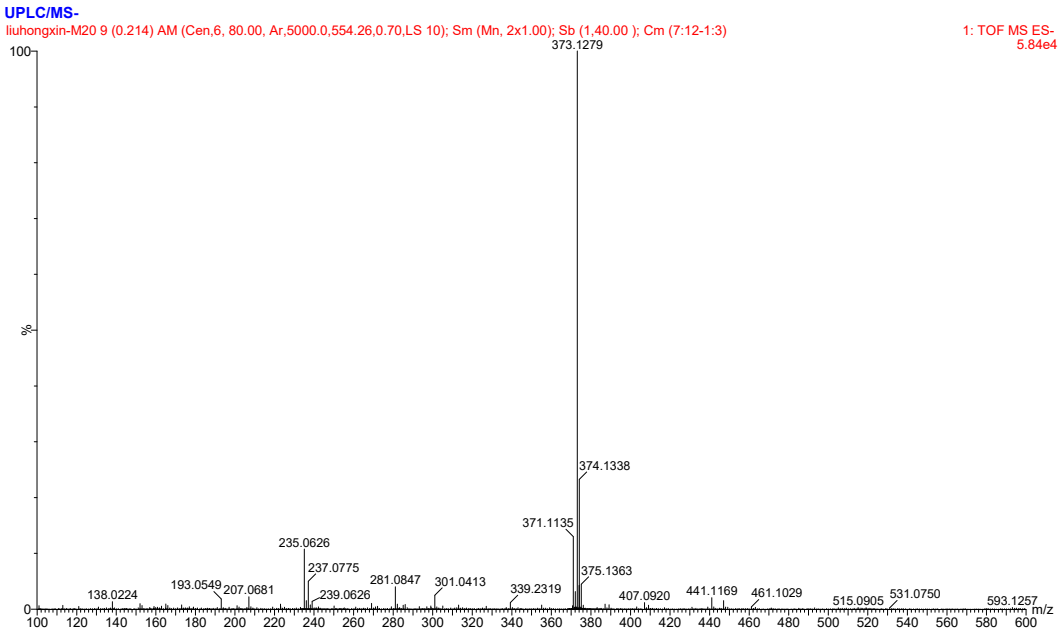


Figure S8. HRESIMS spectrum of **1**.

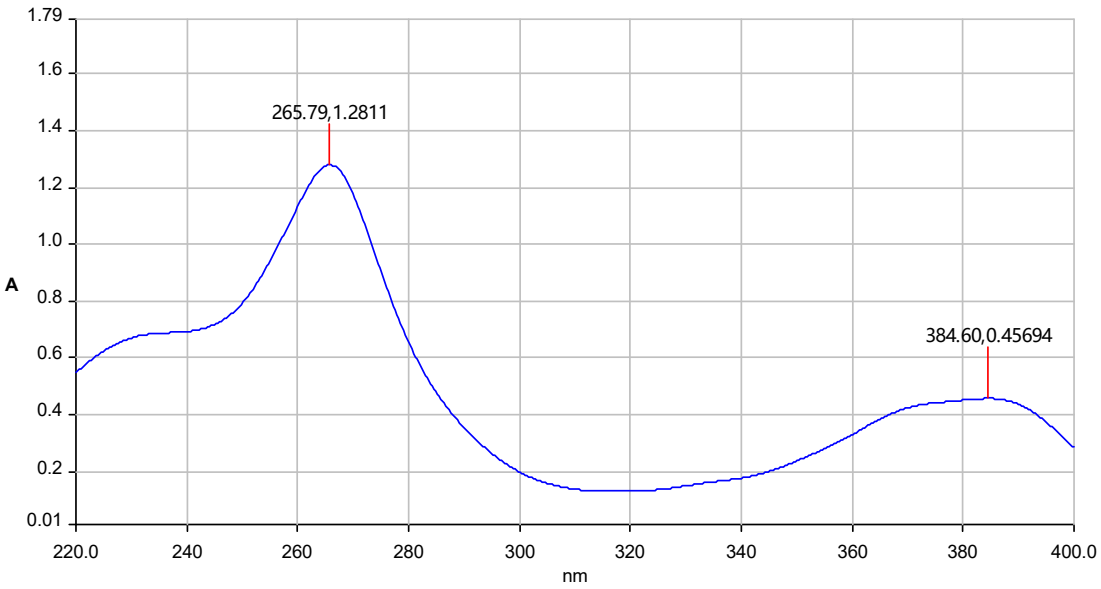


Figure S9. UV spectrum of **1**.

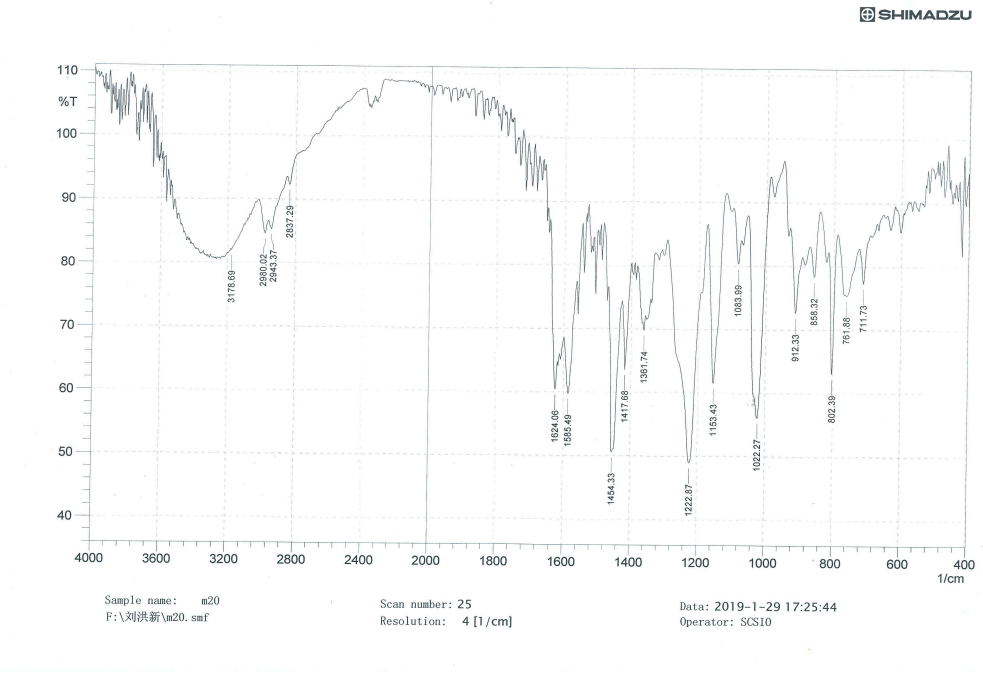


Figure S10. IR spectrum of **1**.

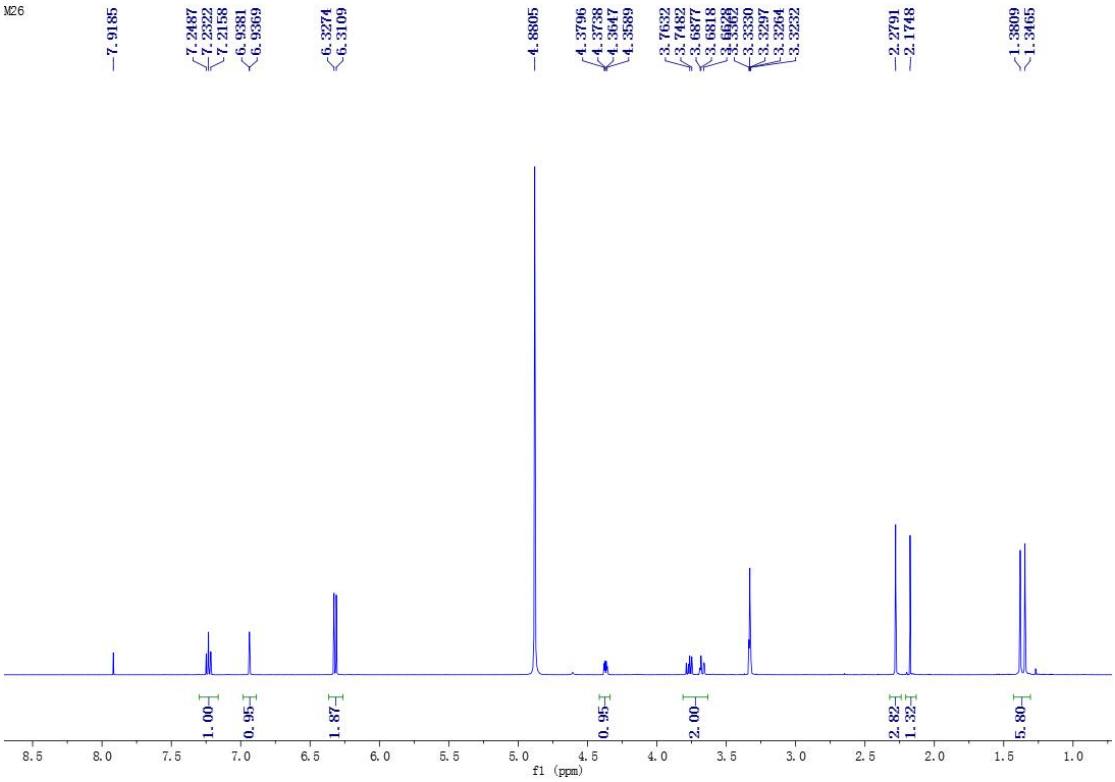


Figure S11. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2**.

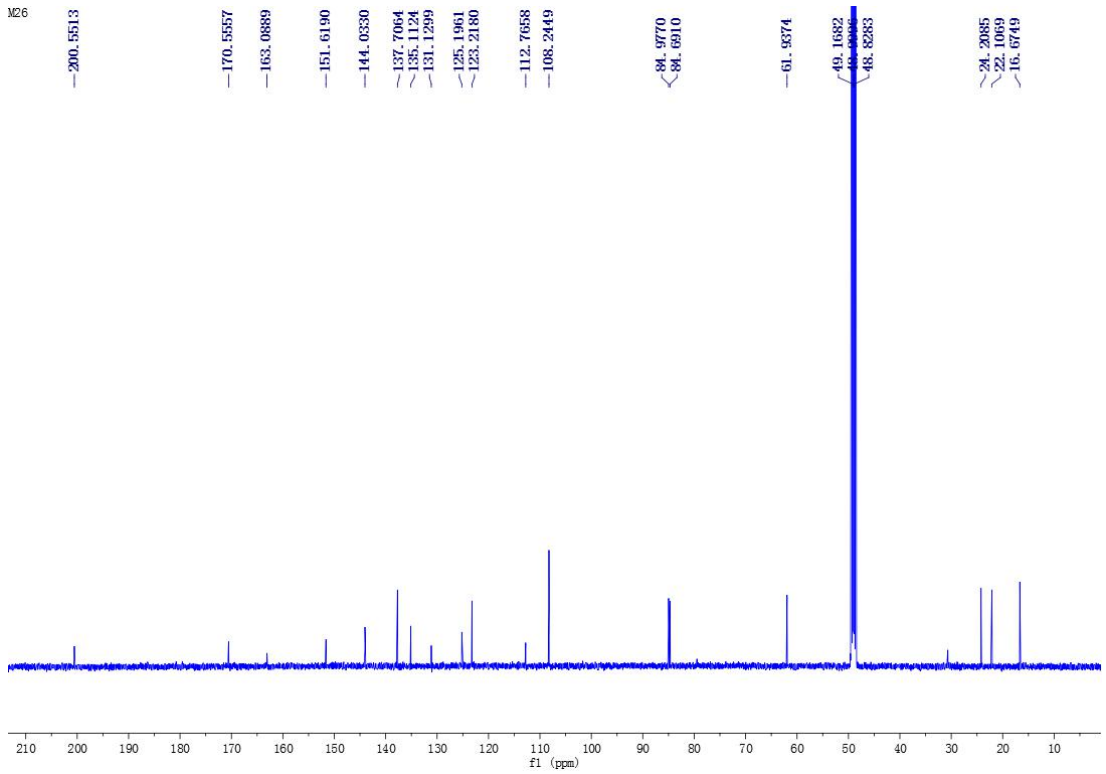


Figure S12. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2**.

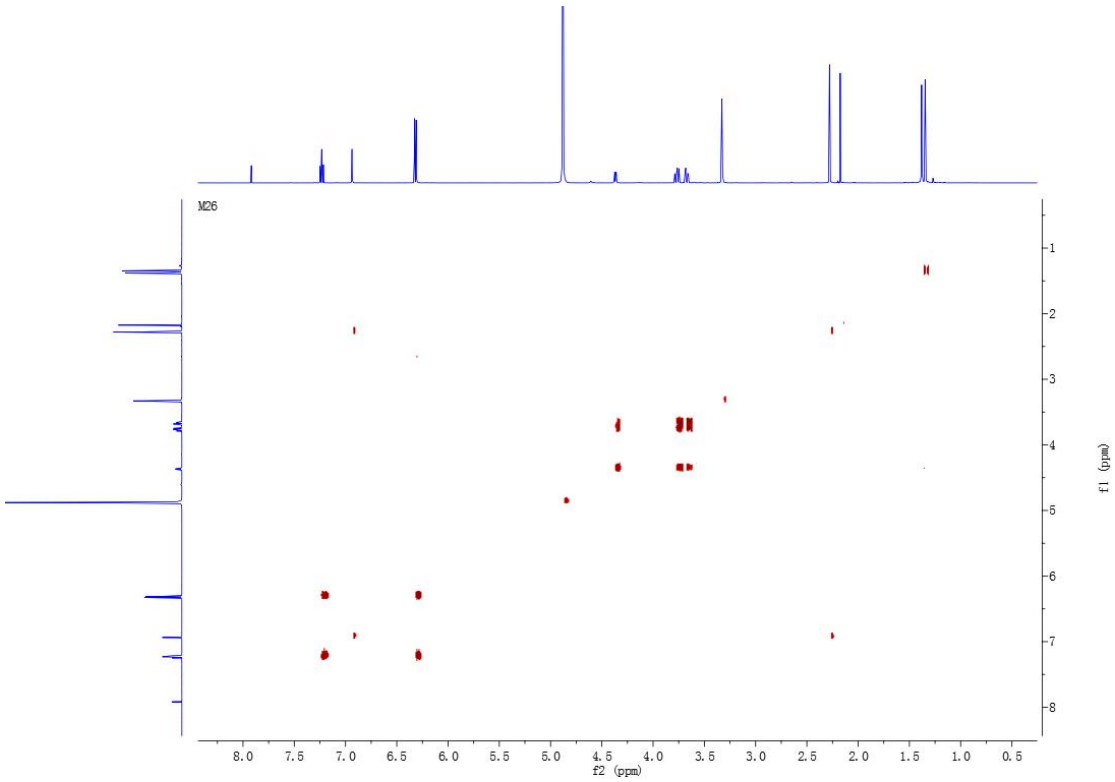


Figure S13. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **2**.

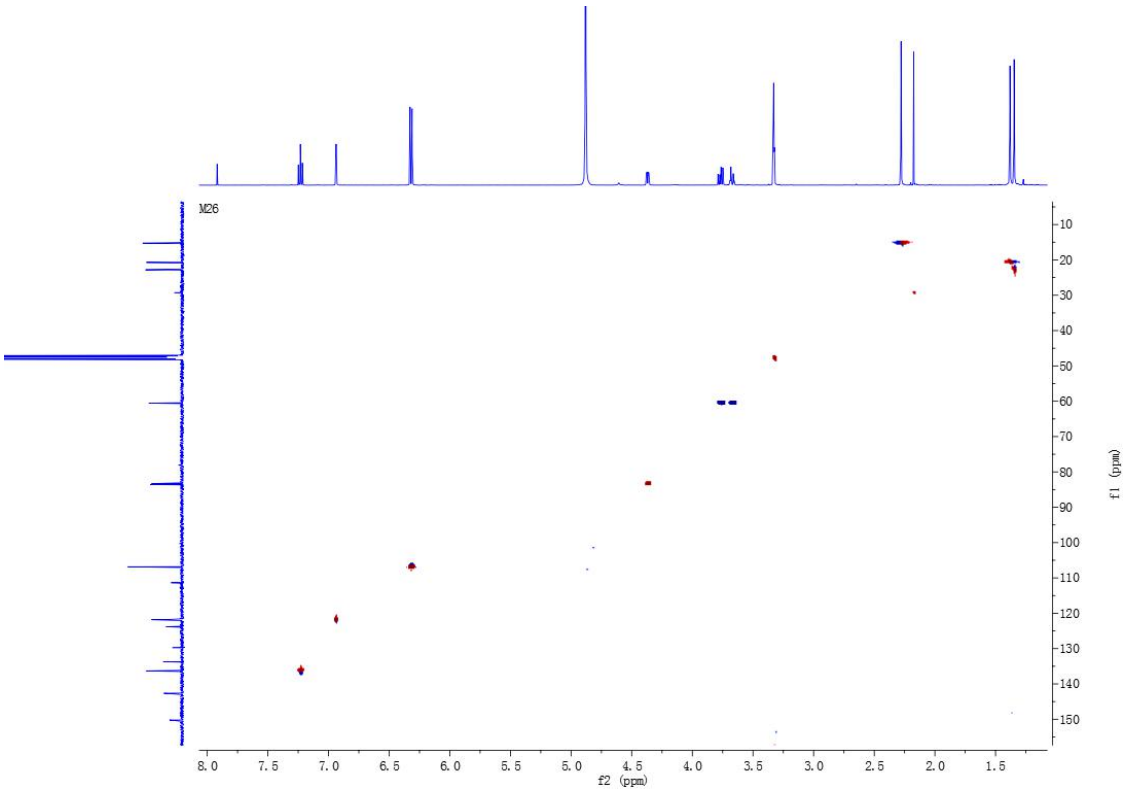


Figure S14. HSQC spectrum of **2**.

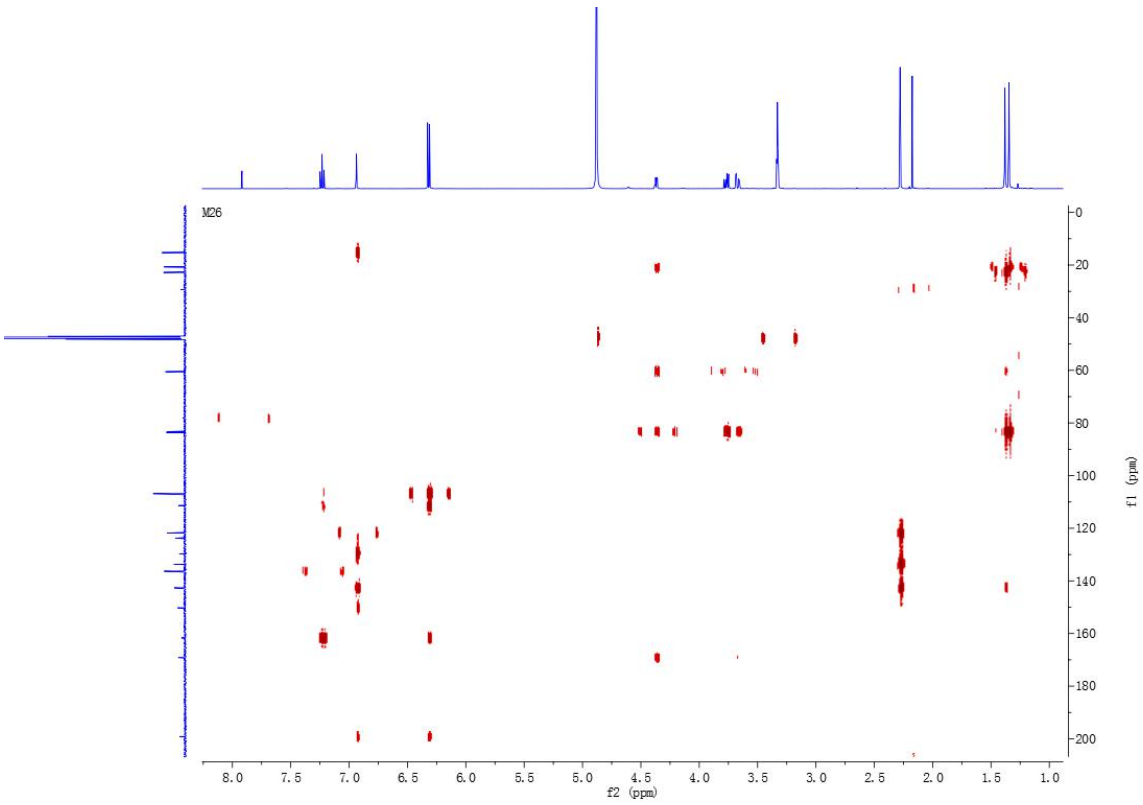


Figure S15. HSQC spectrum of **2**.

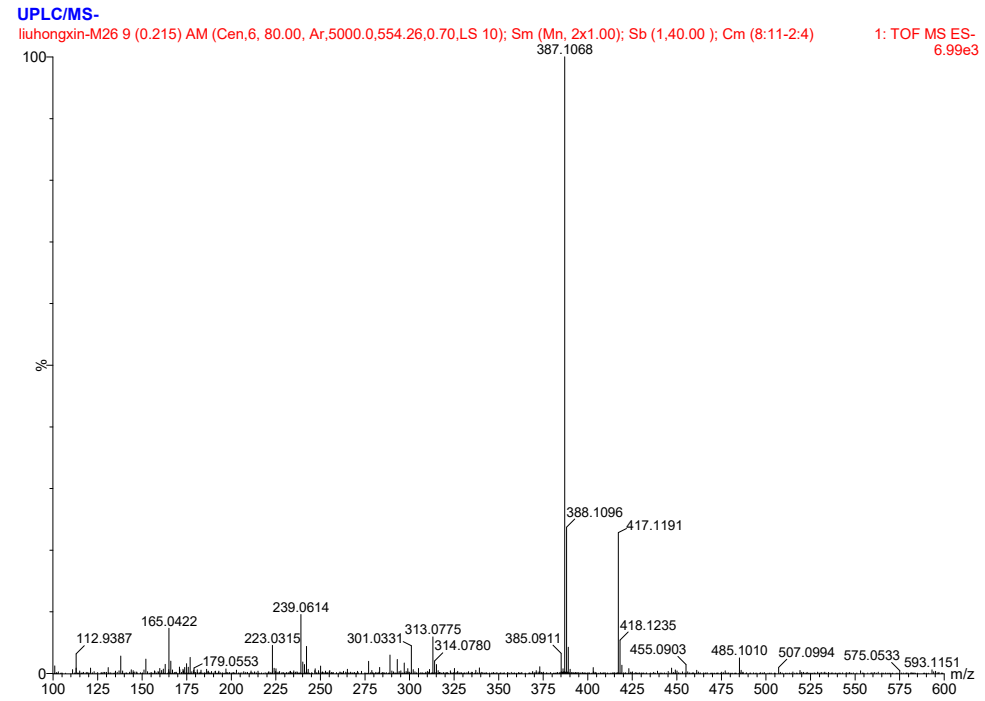


Figure S16. HRESIMS spectrum of **2**.

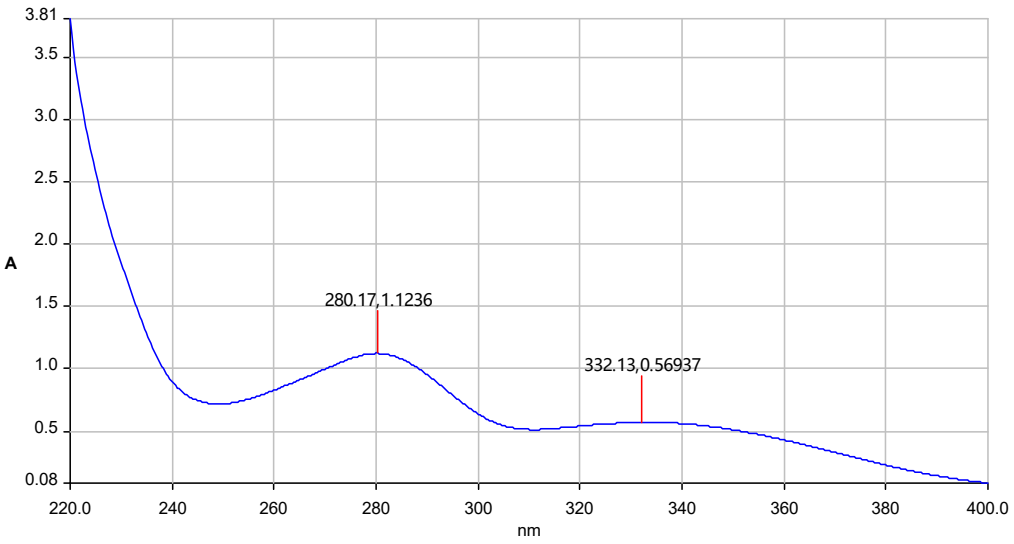


Figure S17. UV spectrum of **2**.

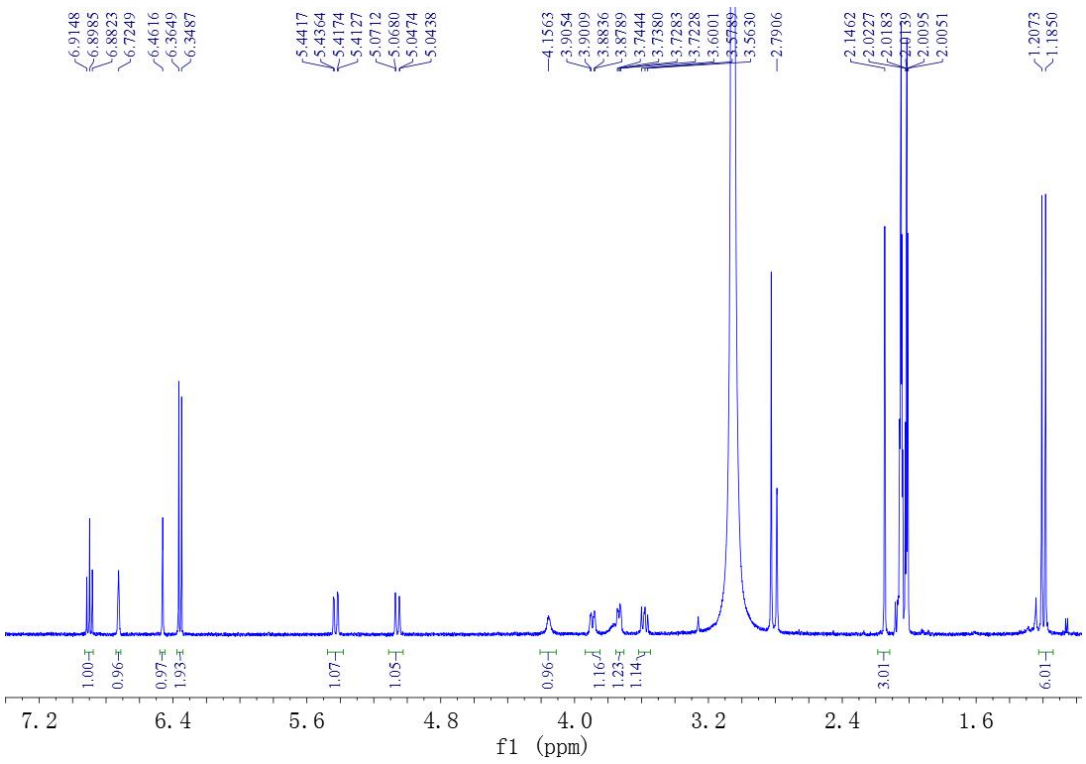


Figure S18. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **3**.

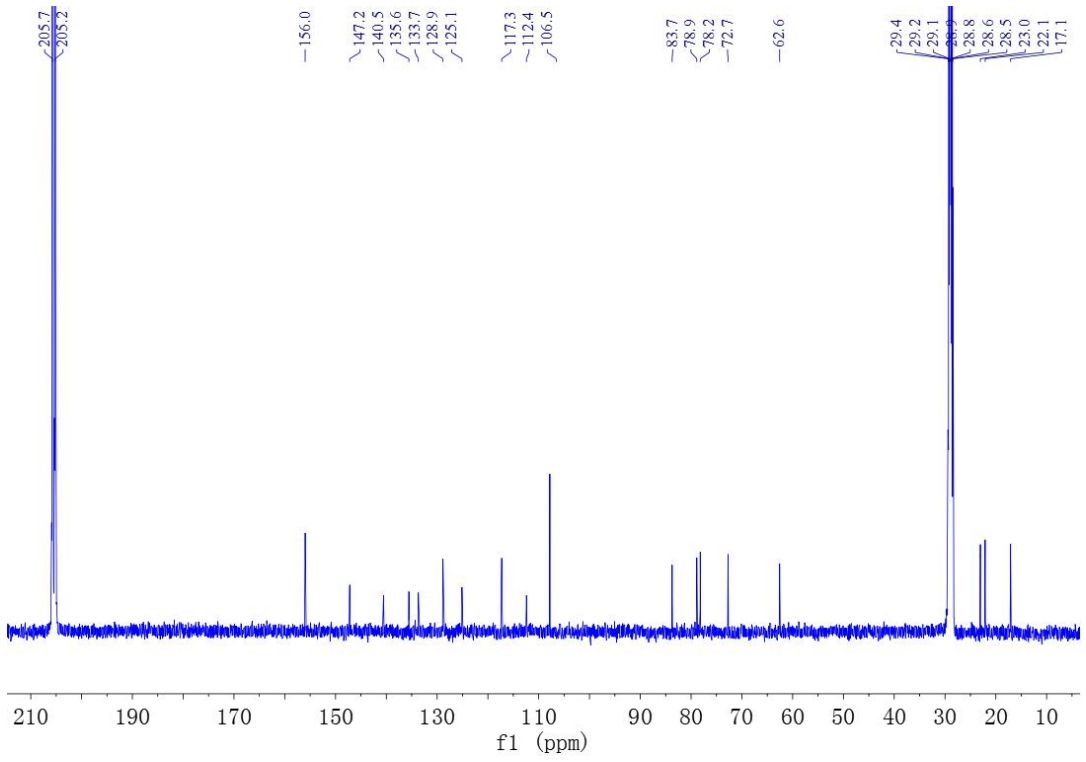


Figure S19. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **3**.

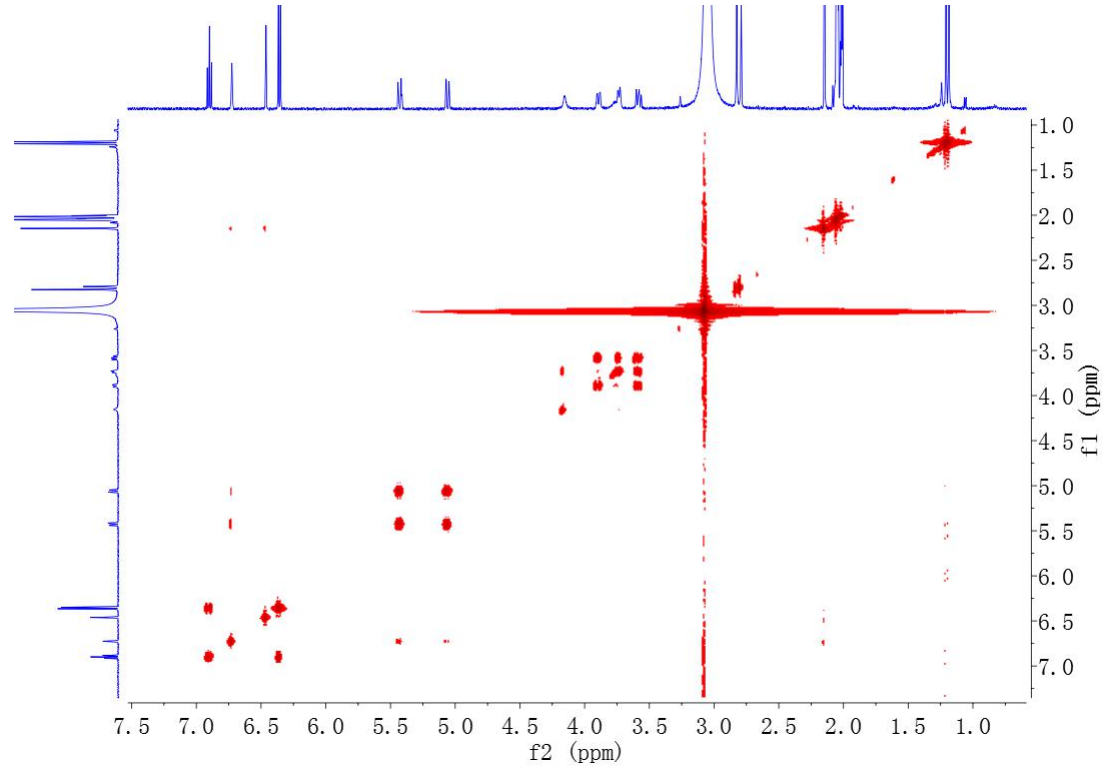


Figure S20. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **3**.

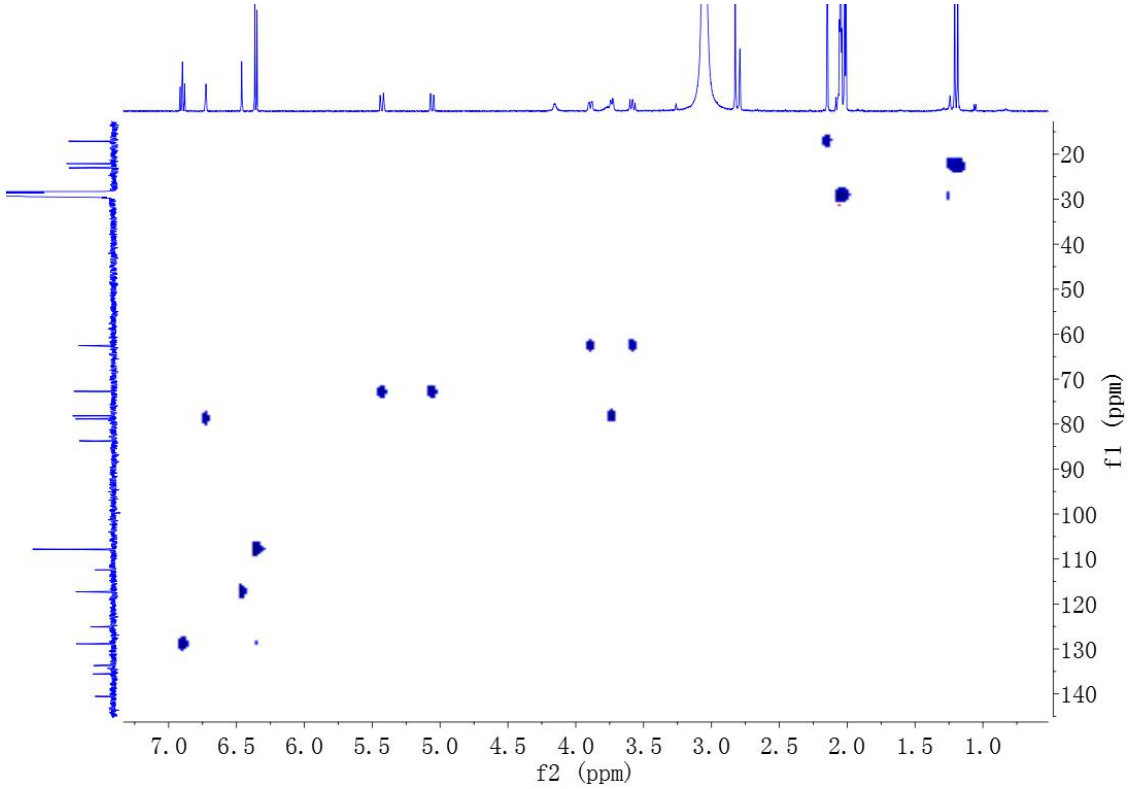


Figure S21. HSQC spectrum of **3**.

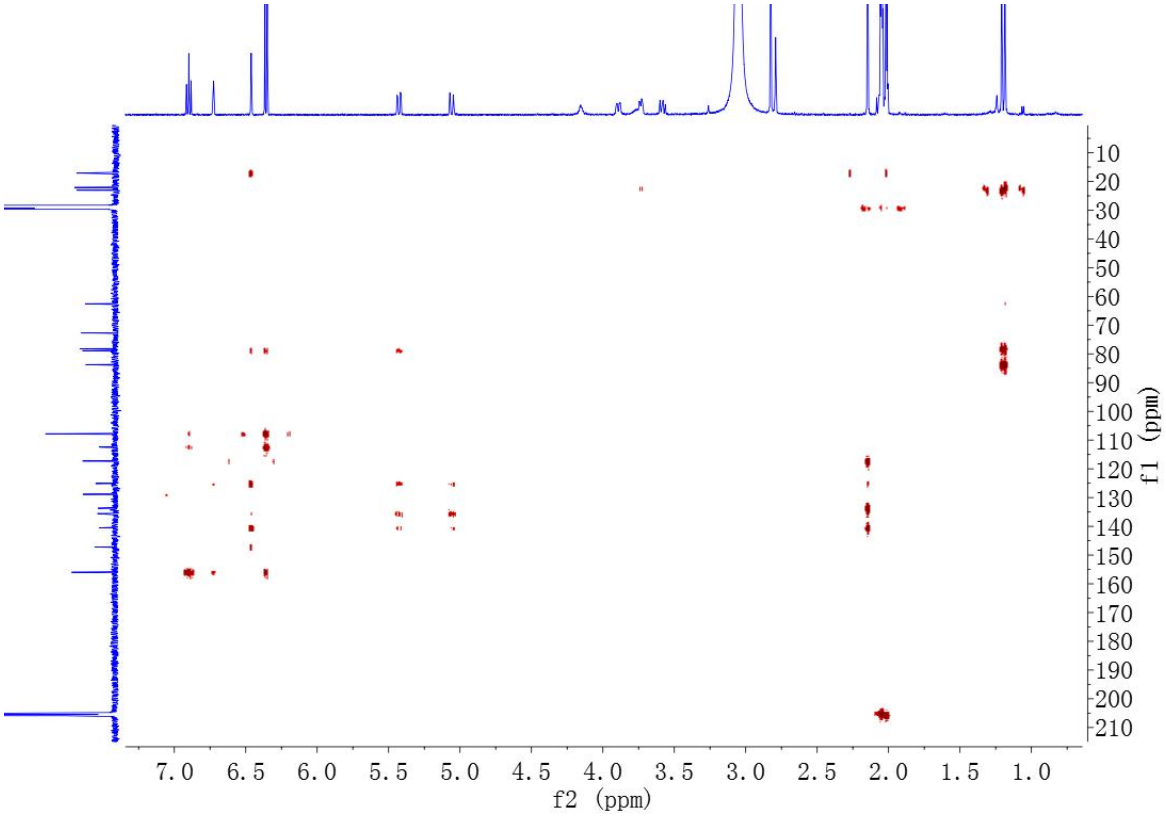


Figure S22. HMBC spectrum of **3**.

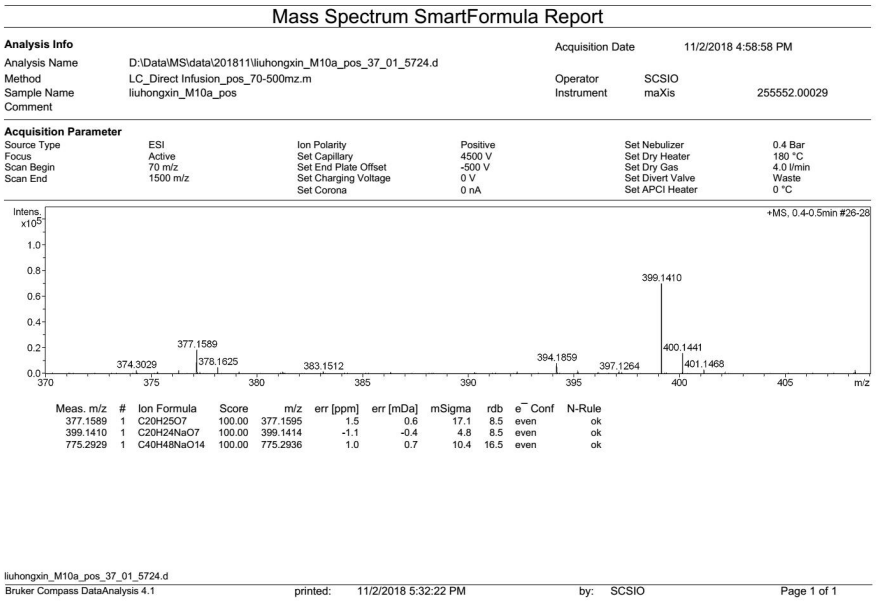
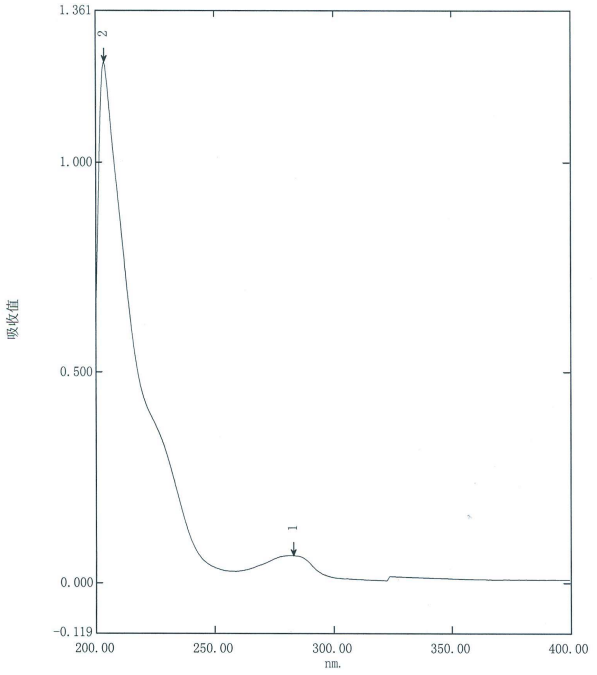


Figure S23. HRESIMS spectrum of **3**.

光谱峰值检测报告

2017-09-20 10:55:11

数据集: M10a - RawData



[测定属性]
波长范围 (nm.): 200.00 到 400.00
扫描速度: 中速
采样间隔: 0.2
自动采样间隔: 启用
扫描模式: 单个

[仪器属性]
仪器类型: UV-2600 系列
测定方式: 吸收值
狭缝宽: 2.0
积分时间: 0.1 秒.
光源转换波长: 323.0 nm
检测器单元: 直接
S/R 转换: 标准
阶梯校正: OFF

[附件属性]
附件: 无

[数据处理参数]
阈值: 0.0100000
点: 4
内插: 停用
平均: 停用

[样品准备属性]
重量:
体积:
稀释:
光程长:
附加信息:

No.	P/V	波长(nm)	吸收值	描述
1	↑	282.80	0.064	
2	↑	203.60	1.238	

Figure S24. UV spectrum of **3**.

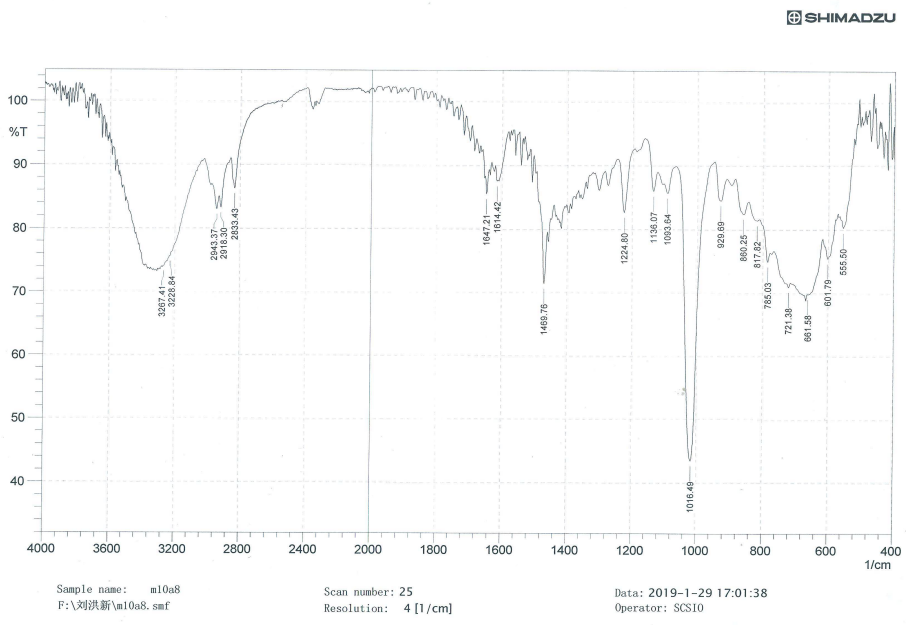


Figure S25. IR spectrum of **3**.

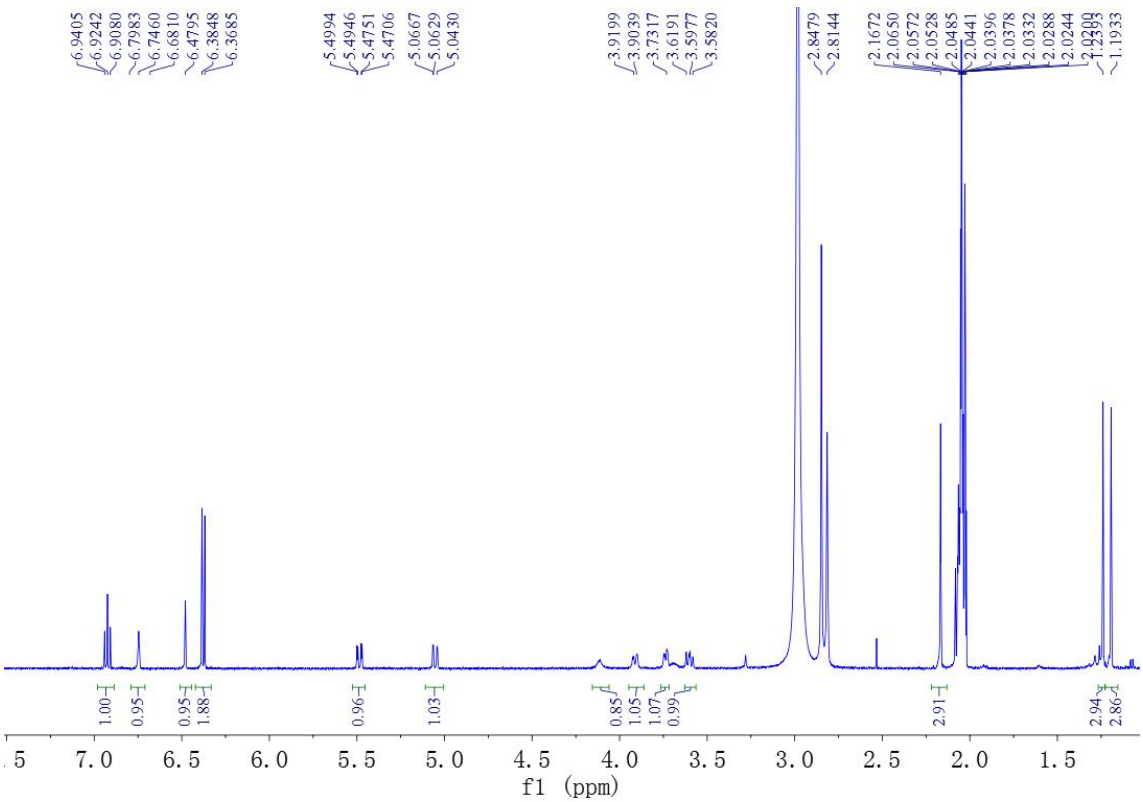


Figure S26. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **4**.

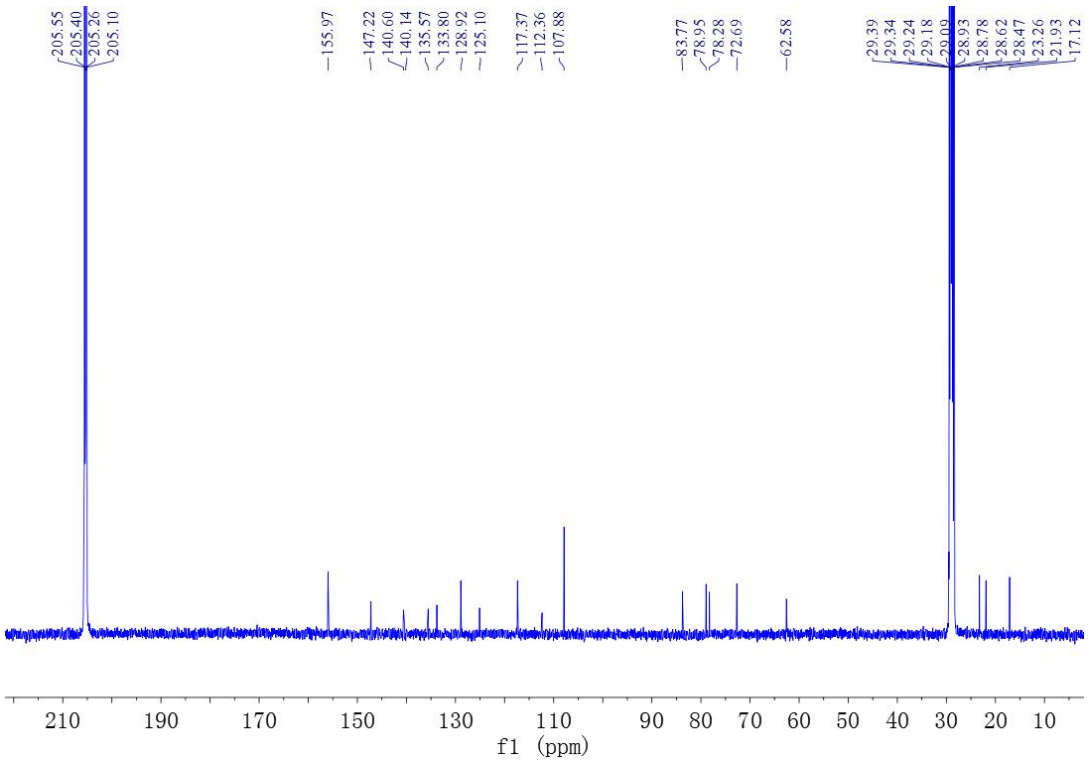


Figure S27. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **4**.

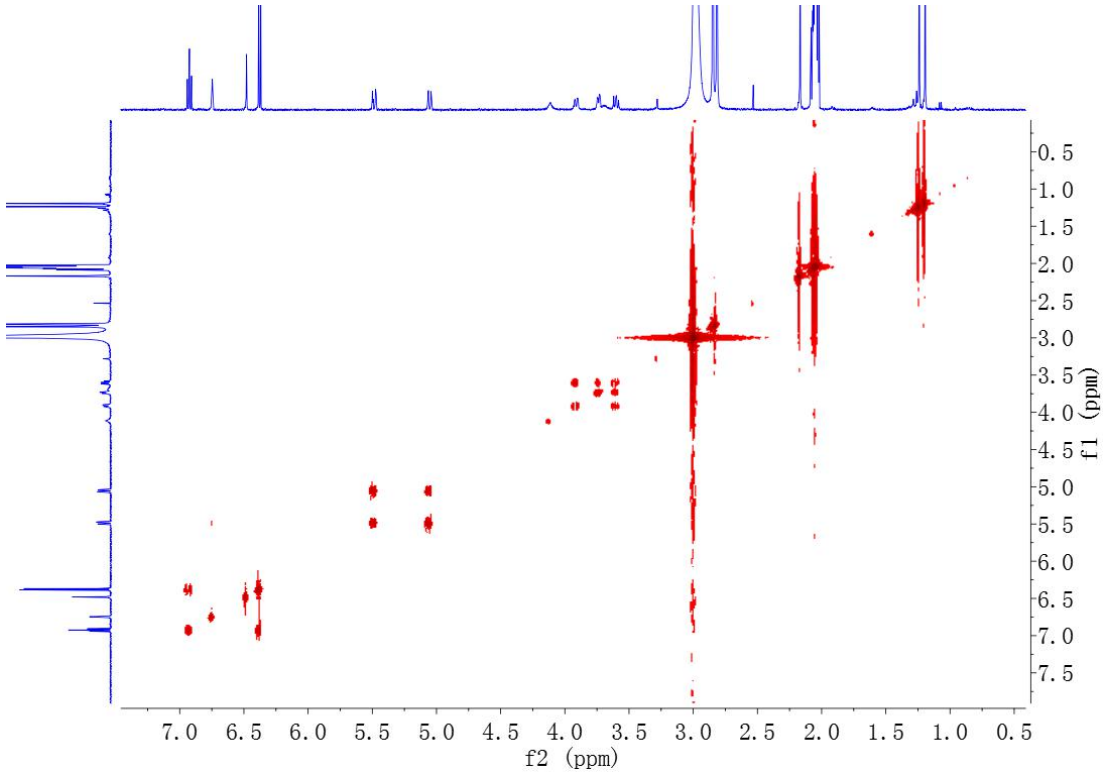


Figure S28. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **4**.

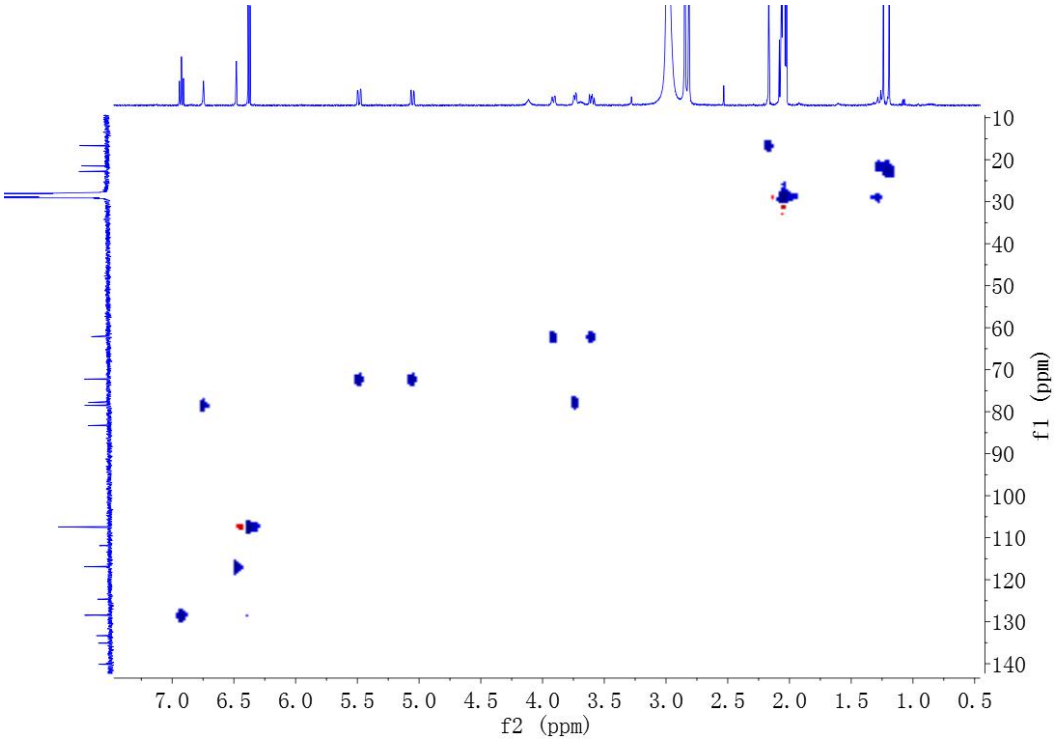


Figure S29. HSQC spectrum of **4**.

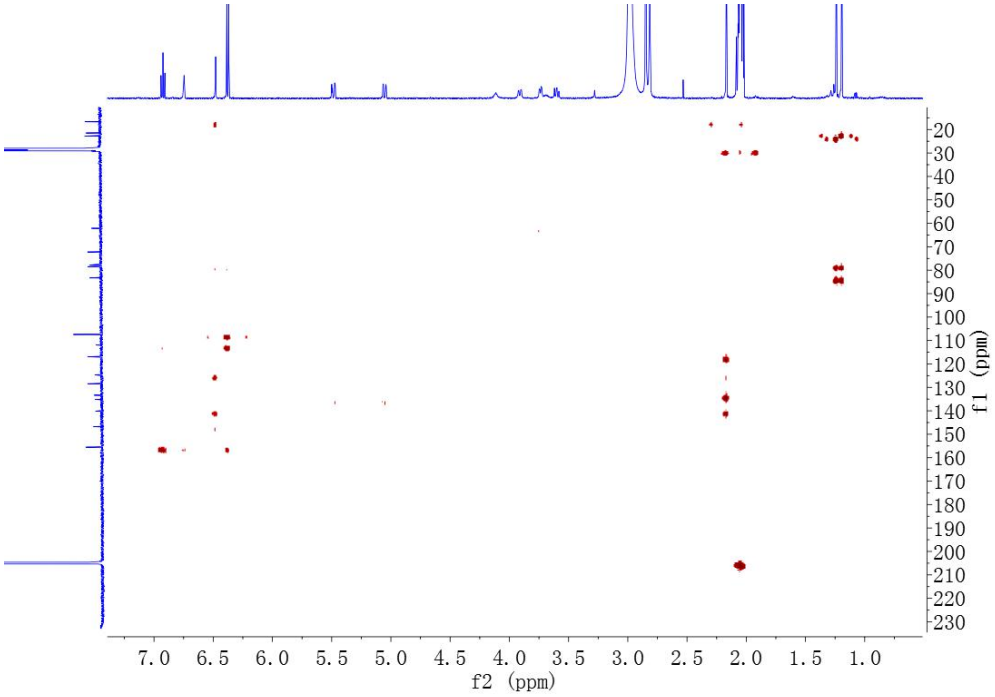
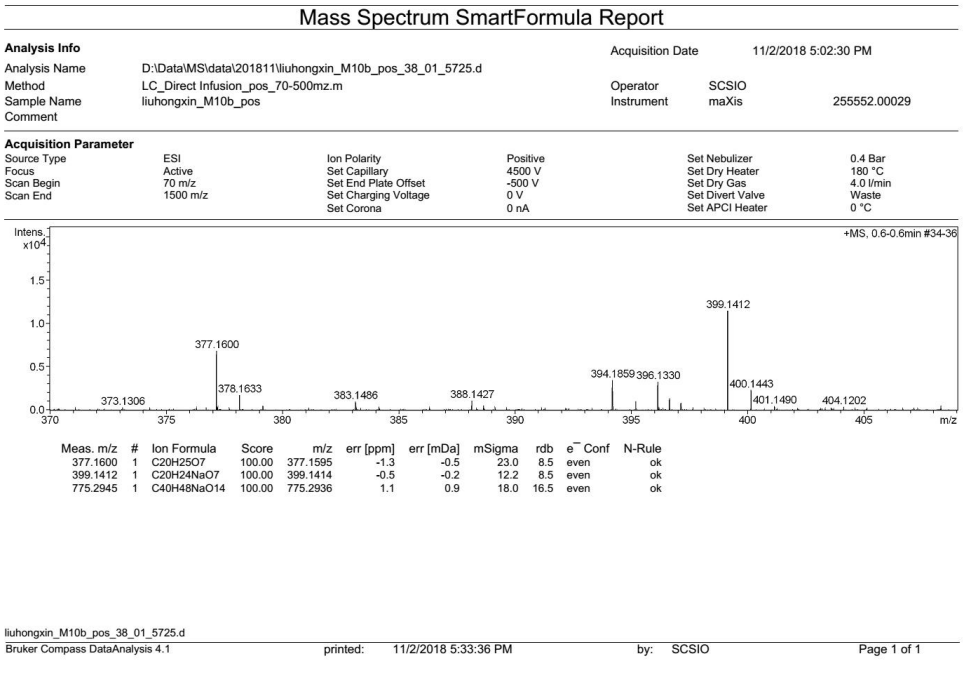


Figure S30. HMBC spectrum of **4**.



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MS\data\201811\liuhongxin_M10b_pos_38_01_5725.d			Acquisition Date	11/2/2018 5:02:30 PM
Method	LC_Direct Infusion_pos_70-500mz.m			Operator	SCSIO
Sample Name	liuhongxin_M10b_pos			Instrument	maXis 255552.00029
Comment					

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
377.1600	1	C20H25O7	100.00	377.1595	-1.3	-0.5	23.0	8.5	even	ok
399.1412	1	C20H24NaO7	100.00	399.1414	-0.5	-0.2	12.2	8.5	even	ok
775.2945	1	C40H48NaO14	100.00	775.2936	1.1	0.9	18.0	16.5	even	ok

Figure S31. HRESIMS spectrum of **4**.

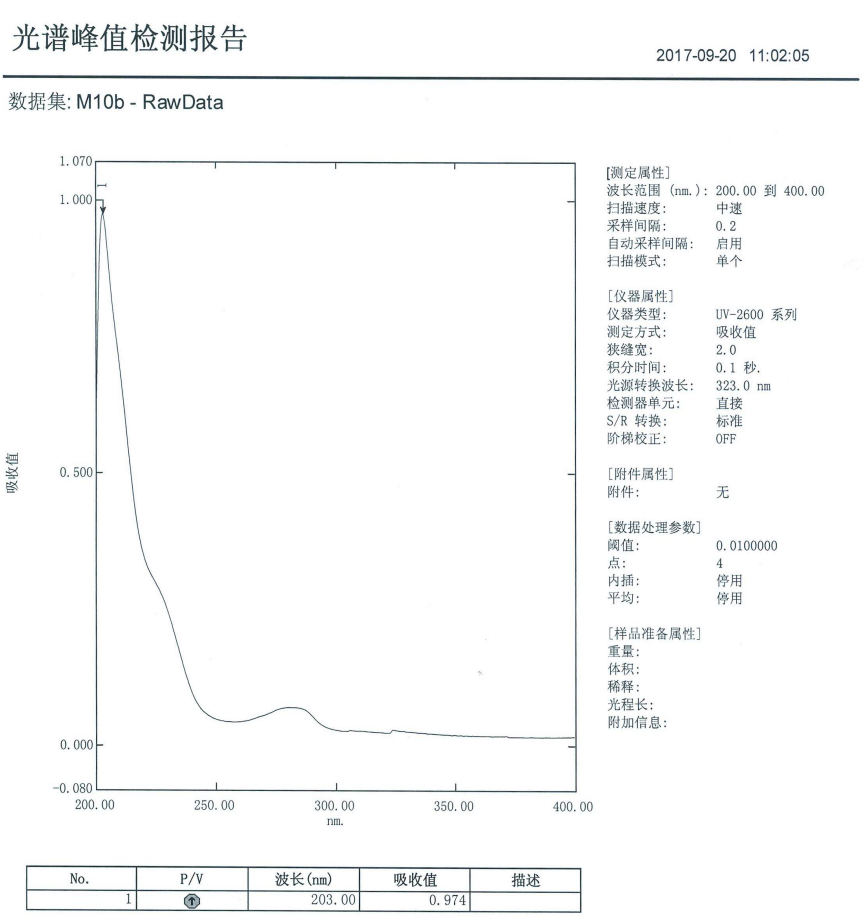


Figure S32. UV spectrum of **4**.

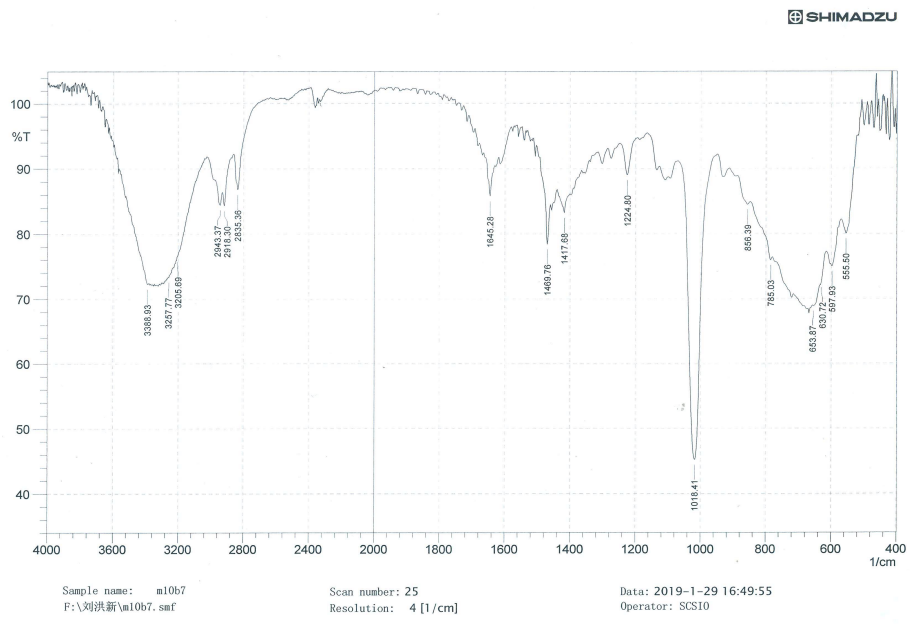


Figure S33. IR spectrum of **4**.

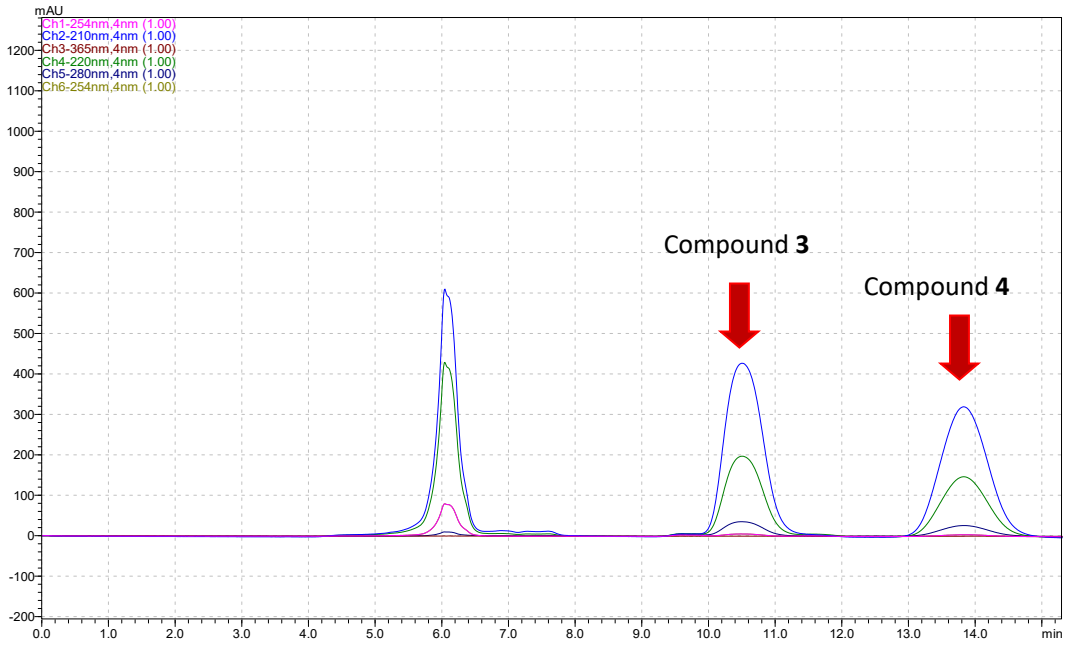


Figure S34. HPLC analysis of the mixture of compounds **3** and **4**. [CHIRALPAK IC column (250 × 10 mm, 5 μm); *n*-hexane/2-propanol (2:1, v/v, 3.0 mL/min)]