Supporting Information

Solitumergosterol A, a unique 6/6/6/6/5 steroid from the deep-sea-derived *Penicillium solitum* MCCC 3A00215

Zhi-Hui He [a], Chun-Lan Xie [a], You-Jia Hao [a], Lin Xu [a], Man-Yi Hu [a], Shu-Jing Li [a], Chao-Feng Wang [a], Tian-Hua Zhong [a] and Xian-Wen Yang [a,*]

[a] *Key Laboratory of Marine Biogenetic Resources, Third Institute of Oceanography, Ministry of Natural Resources, 184 Daxue Road, Xiamen 361005, China*

∗ Corresponding author.
E-mail address: yangxianwen@tio.org.cn (X.-W.Y.);

Content

1. General Experimental Procedures

NMR spectra were recorded on Bruker 400 MHz spectrometer using TMS as an internal standard. Chemical shifts were recorded in δ values using solvent signals ($CDCl_3$: δ_H 7.26/δ_C 77.1) as references. The HRESIMS spectra were measured on a Waters Xevo G2 Q-TOF mass spectrometer. Optical rotations were measured with an Anton Paar MCP100 polarimeter. ECD spectra were measured on a JASCO J-810 CD spectrometer. Column chromatography (CC) was performed on silica gel (Qingdao Marine Chemistry Co., Ltd., Qingdao, China), Sephadex LH-20 (Amersham Pharmacia Biotech AB, Uppsala, Sweden), and ODS (50 μm, Daiso, Japan), respectively. Preparative HPLC separations were performed on an Agilent technologies 1260 infinity instrument equipped with DAD detector using semi-preparative chromatographic column (COSMOSIL 5 C_{18}-MS-II, 10 mm i.d.×150 mm, Nacalai Tesque, Japan).

2. Fungal Material

The fungus was isolated from a sediment sample at a depth of 3034 m from the Northwest Atlantic Ocean (W 44.9801°, N 14.7532°). It was identified to be *Penicillium solitum* (GenBank accession number FJ798652) as the 16S rRNA gene sequence alignment demonstrated that it was similar to *P. solitum* ATCC 9923 (GenBank accession number IF00776501). The strain was perseved at the Marine Culture Collection of China (Xiamen, China) and numbered MCCC 3A00215.

3. Fermentation, Extraction, and Isolation

Large-scale fermentation was carried out in 48 Erlenmeyer flasks (1 L) each containing oats (80 g) and tape water (120 mL, 3% marine salt). After incubation for 30 days, the fermented broth was extracted with EtOAc for three times. The filtrate was concentrated under reduced pressure to give a crude extract (200 g), which subjected to column chromatography (CC) on silica gel using petroleum ether (PE), CH_2Cl_2, EtOAc to provide a EtOAc- soluable extract (114.5 g). The EtOAc part was subjected to medium pressure liquid chromatography (MPLC, 460 mm × 46 mm) by silica gel with gradient elution consisting CH_2Cl_2/MeOH (100%→70%, 6h; 70%→50%, 1h, 30 mL/min) to obtain five fractions (Fr.1-Fr.5). Fr.2 (4 g) was subjected to ODS chromatography (310 mm × 5 mm) eluted by gradient MeOH/H_2O (10%→40%, 4h; 40%→60%, 6h; 60%→100%, 5h) and obtain 13 subfractions. Fr.2.11 was purified by Sephadex LH-20 (1.5 m × 2 cm, MeOH) and followed by semi-preparative HPLC eluted with MeOH/H_2O (40%→100%) to lead to the isolation of compound **1** (3.0 mg).

4. Biological Assay

4.1 Cytotoxic experiment

The *in vitro* cytotoxic activities of **1** were conducted on 17 human tumor cell lines A431, A549, MB231, MCF-7, PANC1, HepG2, HCT116, H460, H1299, QGY-7701, BGC823, SKGT4, A375, U2OS, HL-60, K562, and KYSE450 by MTT method. Paclitaxel was used as a positive control, and DMSO was used as a negative control. Different cancer cells were incubated to 96-well cell plates and cultured for 24 h. Thereafter, the cells were treated with different concentrations of **1**. After 48h, 20 μL of MTT solution was added and the

incubation continued for another 4 h. The supernatant was discarded softly, and the deposited formazan formed in the cells was dissolved with 100 μL of DMSO. The absorbencies were measured at 490 nm. The percentage of cell growth rate was calculated as follows：

$$\text{Growth Rate (\%)} = (\text{OD}_{\text{sample}} - \text{OD}_{\text{blank}}) / (\text{OD}_{\text{control}} - \text{OD}_{\text{blank}}) \times 100\%$$

4.2 RXR*α* transcriptional activity

The human renal epithelial cells were seeded to 96-well plates in DMEM containing 10% FBS at 37 °C. After 24 h, two target plasmids (30 ng pBind RXRα LBD and 60 ng PG5 LUC) were transfected by Liposome 2000 into the cell. After the cells adhere to the wall, they were exposed to compound **1** for 16 h. Then the cells were rinsed with PBS and lysed by buffered solution on the oscillating platform for 15 min. According to the introduction of the Dual-Luciferase Reporter Assay System kit, the activities of firefly luciferase (FL) and rellina luciferase (RL) were checked. The activity fold was calculated as the relative luciferase activities ratio between sample and blank control. 9-*cis*-retinoic acid (9-*cis*) was used as agonist. Uvi30003 was used as antagonist.

$$\text{Relative luciferase activity (\%)} = \frac{\text{FL}}{\text{RL}} \times 100\%$$

5. ECD Calculation

Conformational analysis was firstly performed *via* random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 7.0 kcal/mol and RMSD threshold of 0.2 Å. All conformers were consecutively optimized at PM6 and HF/6-31G(d) levels. Dominative conformers were re-optimized at B3LYP/6-31G(d) level in gas phase. The theoretical ECD spectra were calculated with the time-dependent density functional theory (TD-DFT) at BP86/6-311G(d,p) level in Acetonitrile using Gaussian 09 [1]. The ECD spectrum was simulated in SpecDis [2] by overlapping Gaussian functions for each transition.

References:

[1] G.W.T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox., Gaussian 09 Revision D.01, Wallingford, CT, 2009.
[2] T. Bruhn, A. Schaumloffel, Y. Hemberger, G. Bringmann, Chirality 25 (2013) 243-249.

Table S1. Energies analysis for **1a** at MMFF94 force field.

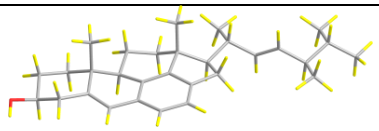
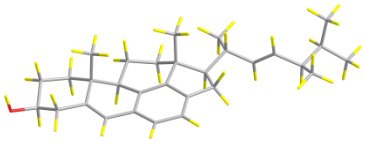
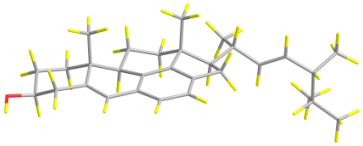
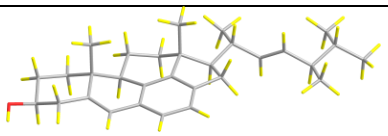
Configuration	Conformer	Structure	E (kcal/mol)	Population (%)
1a	1		112.03	80.7
1a	2		113.02	15.2
1a	3		114.05	2.7

Table S2. Standard orientations at BP86/6-311G(d,p) level in Acetonitrile.

Conformer 1a-1



SCF Energy (BP86): −1243.99364465 Hartree: −780617.79136232 kcal/mol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	6.928829	-0.046482	-0.795576
3	6	0	6.172618	1.065389	-0.054808
4	6	0	4.669834	0.891417	-0.074418
5	6	0	4.110811	-0.507260	0.249294
6	6	0	4.994273	-1.606590	-0.407333
7	6	0	3.855043	1.953521	-0.239896
8	6	0	2.404022	1.876983	-0.094100
9	6	0	1.822558	0.594211	-0.009946
10	6	0	2.671203	-0.614314	-0.346949
11	6	0	0.189949	2.892567	0.093578
12	6	0	-0.328658	-0.795067	0.328273
13	6	0	0.424963	-1.882153	-0.471530
14	6	0	1.923626	-1.940983	-0.086652
15	6	0	-0.373462	1.622557	0.194688
16	6	0	-1.816229	1.172097	0.209404
17	6	0	-1.728144	-0.325626	-0.229986
18	6	0	-2.995369	-1.136955	0.137119
19	6	0	-4.226617	-0.472092	-0.438323
20	6	0	-2.937766	-2.600296	-0.346916
21	6	0	-5.268830	-0.017868	0.263381
22	6	0	-6.498652	0.651551	-0.305044
23	6	0	-7.793068	-0.128611	0.070004
24	6	0	-9.070328	0.570262	-0.423756
25	6	0	-7.751557	-1.570741	-0.459097
26	6	0	4.110734	-0.667328	1.790894
27	6	0	-6.535998	2.121808	0.162667
28	6	0	-0.437271	-1.187864	1.822806
29	8	0	8.339546	0.069918	-0.619286
30	6	0	1.580582	3.011713	-0.024298
31	6	0	0.456670	0.496447	0.193436
32	1	0	6.808279	-1.462095	0.805404

33	1	0	7.050675	-2.196147	-0.776059
34	1	0	6.676074	-0.000547	-1.869398
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36	1	0	6.540427	1.050182	0.983472
37	1	0	4.763698	-1.639545	-1.482097
38	1	0	4.712684	-2.585478	-0.001497
39	1	0	4.290038	2.936772	-0.419263
40	1	0	2.821201	-0.548339	-1.439858
41	1	0	-0.433957	3.783473	0.084323
42	1	0	-0.017151	-2.872813	-0.316164
43	1	0	0.335464	-1.661423	-1.544896
44	1	0	2.401774	-2.746049	-0.656516
45	1	0	2.008159	-2.225471	0.967841
46	1	0	-2.456239	1.759496	-0.457278
47	1	0	-2.263211	1.253274	1.211868
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51	1	0	-3.877052	-3.115042	-0.116673
52	1	0	-2.125047	-3.157949	0.128001
53	1	0	-2.788202	-2.650948	-1.432914
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56	1	0	-7.837982	-0.172432	1.170235
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58	1	0	-9.222011	1.547789	0.044249
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60	1	0	-8.644579	-2.126258	-0.149362
61	1	0	-6.871383	-2.111232	-0.098063
62	1	0	-7.719426	-1.580928	-1.556916
63	1	0	3.814204	-1.679174	2.089271
64	1	0	3.419259	0.044538	2.254123
65	1	0	5.105829	-0.484358	2.208675
66	1	0	-6.679520	2.186078	1.249346
67	1	0	-5.592000	2.622808	-0.076804
68	1	0	-7.344003	2.683762	-0.316185
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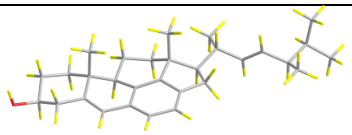
Conformer 1a-2



SCF Energy (BP86): −1243.99291910 Hartree: −780617.336104201 kcal/mol

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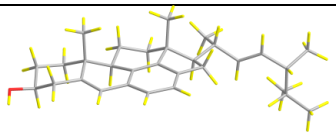
Conformer 1a-3



SCF Energy (BP86): −1243.99047270 Hartree: −780615.800965036 kcal/mol

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49	1	0	3.049298	-1.398493	-1.422055
50	1	0	4.369628	-0.332055	1.144767
51	1	0	2.121496	-3.247658	-0.022312
52	1	0	3.886160	-3.210496	0.104944
53	1	0	2.889962	-2.568039	1.420105
54	1	0	5.161662	-0.482701	-1.807619
55	1	0	6.531065	1.458486	-0.920425
56	1	0	5.938279	1.122679	1.484170
57	1	0	6.516373	-1.347321	1.695113
58	1	0	8.228132	-0.920522	1.553172
59	1	0	7.285279	-0.327660	2.923594
60	1	0	7.666117	2.743499	0.751540
61	1	0	8.063254	2.041583	2.328422
62	1	0	8.919413	1.497863	0.883086
63	1	0	-3.478313	-0.167100	-2.231221
64	1	0	-5.169031	-0.651428	-2.047382
65	1	0	-3.893018	-1.855625	-1.867798
66	1	0	7.850259	-1.304641	-0.798666
67	1	0	7.560229	-0.324539	-2.239605
68	1	0	8.709193	0.231679	-1.018036
69	1	0	-0.639905	-1.569594	-2.256665
70	1	0	0.880957	-0.736359	-2.548045
71	1	0	0.890493	-2.394274	-1.921168
72	1	0	-8.473321	1.167237	1.147415
73	1	0	-1.910600	3.978801	-0.385488

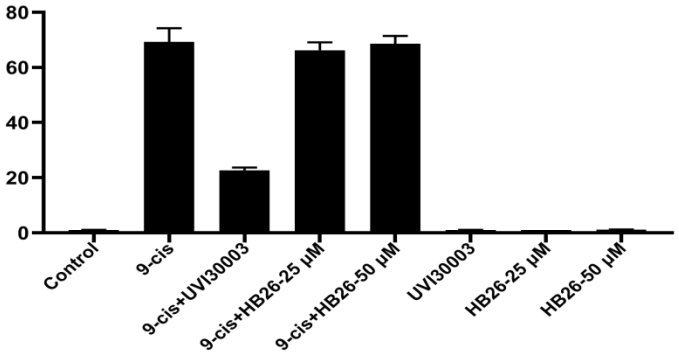
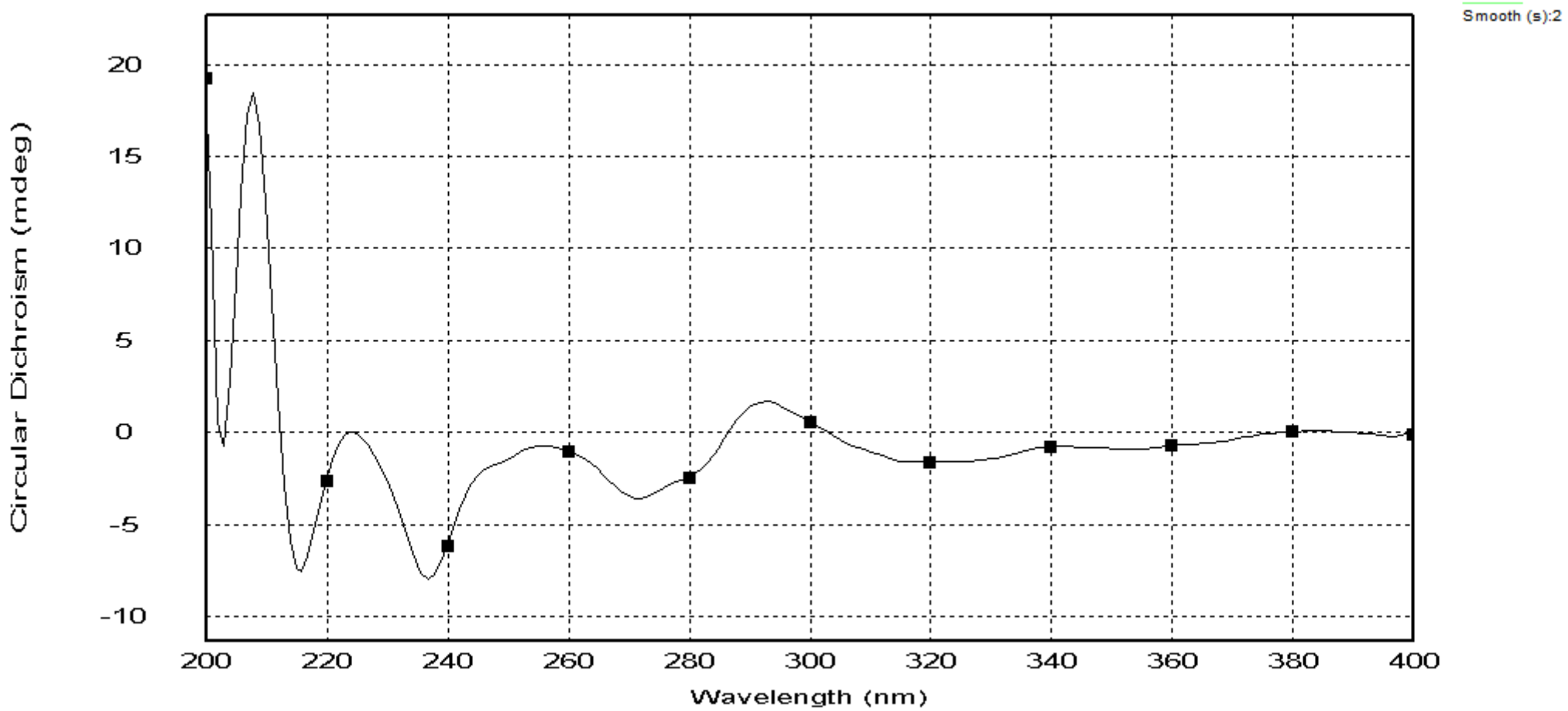


Figure S1. Effects of **1** on the transcriptional activities of RXR*α*.

Remarks :
#User: CD
#Date: 2020/07/07
#Instrument: 0536
#DetectorType: PMT
#DichOS Calibration Correction Curve: 0536/1
#HV (CDDC channel): 0 v
#Time per point: 0.25 s
#Description: Sample 1
#Concentration: 0 M
#Pathlength: 10 mm
#Temperature: ---- C

Figure S2. The CD spectrum of **1** in ACN.



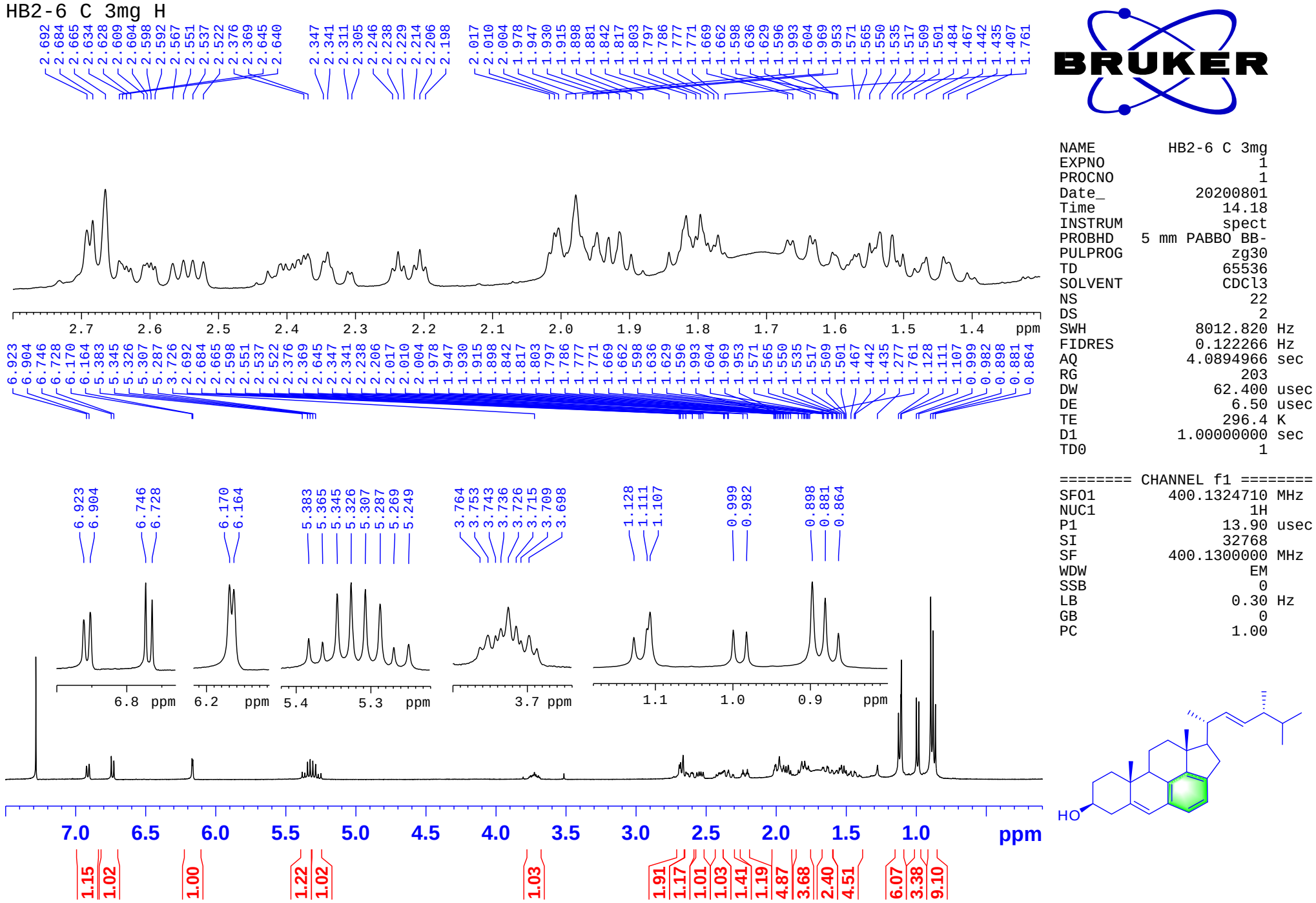
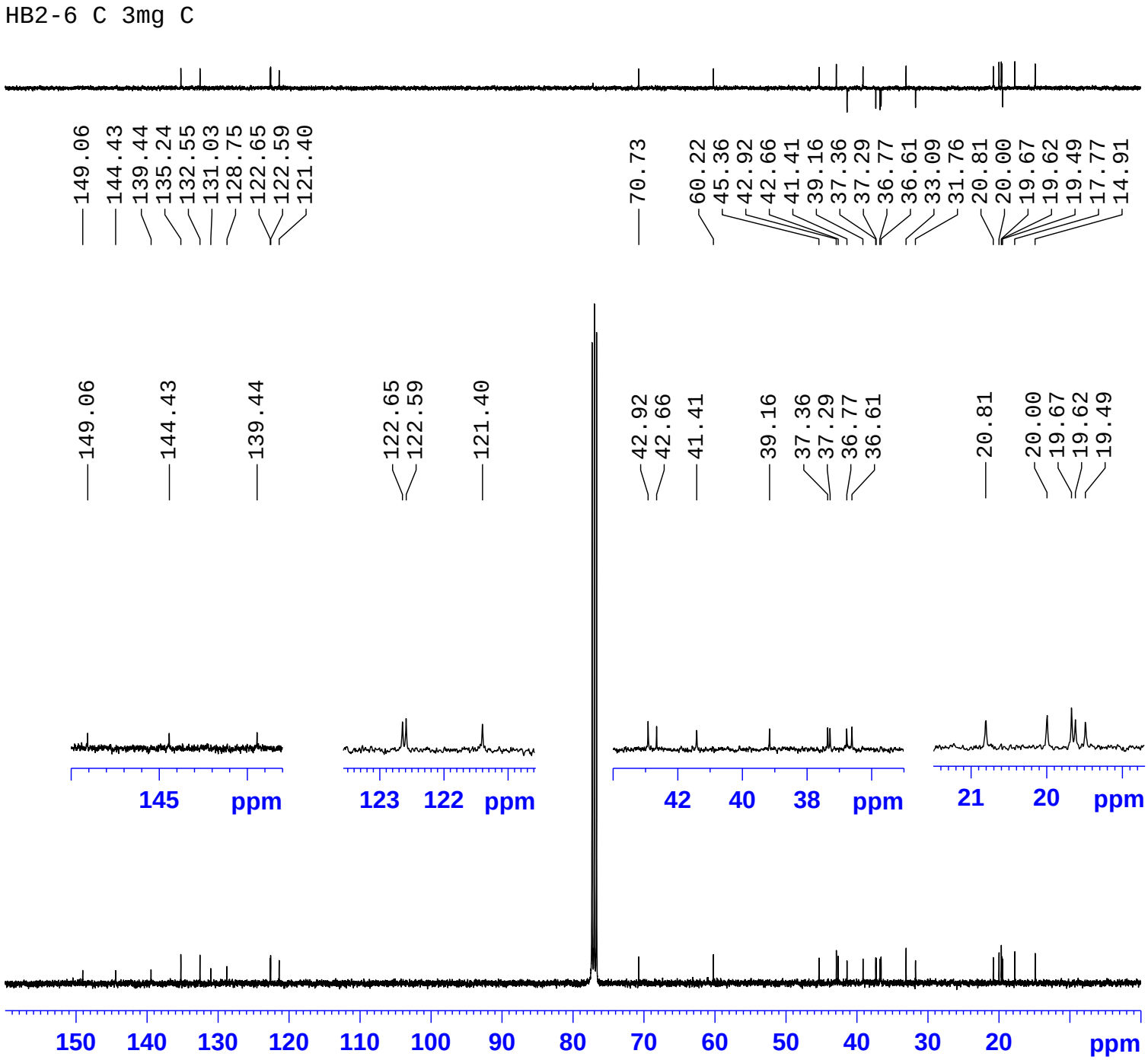


Figure S3. ^{1}H NMR spectrum of **1** in $CDCl_3$.



BRUKER

```
NAME          HB2-6 C 3mg
EXPNO                   2
PROCNO                  1
Date_            20200801
Time                14.21
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1124
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                    203
DW                20.800 usec
DE                 6.50 usec
TE                 296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                   13C
P1                 12.37 usec
SI                 32768
SF           100.6127713 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

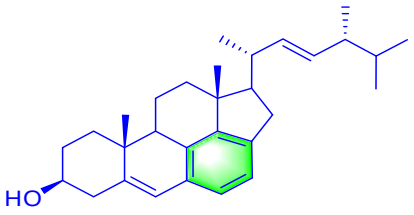


Figure S4. ^{13}C NMR spectrum of **1** in $CDCl_3$.

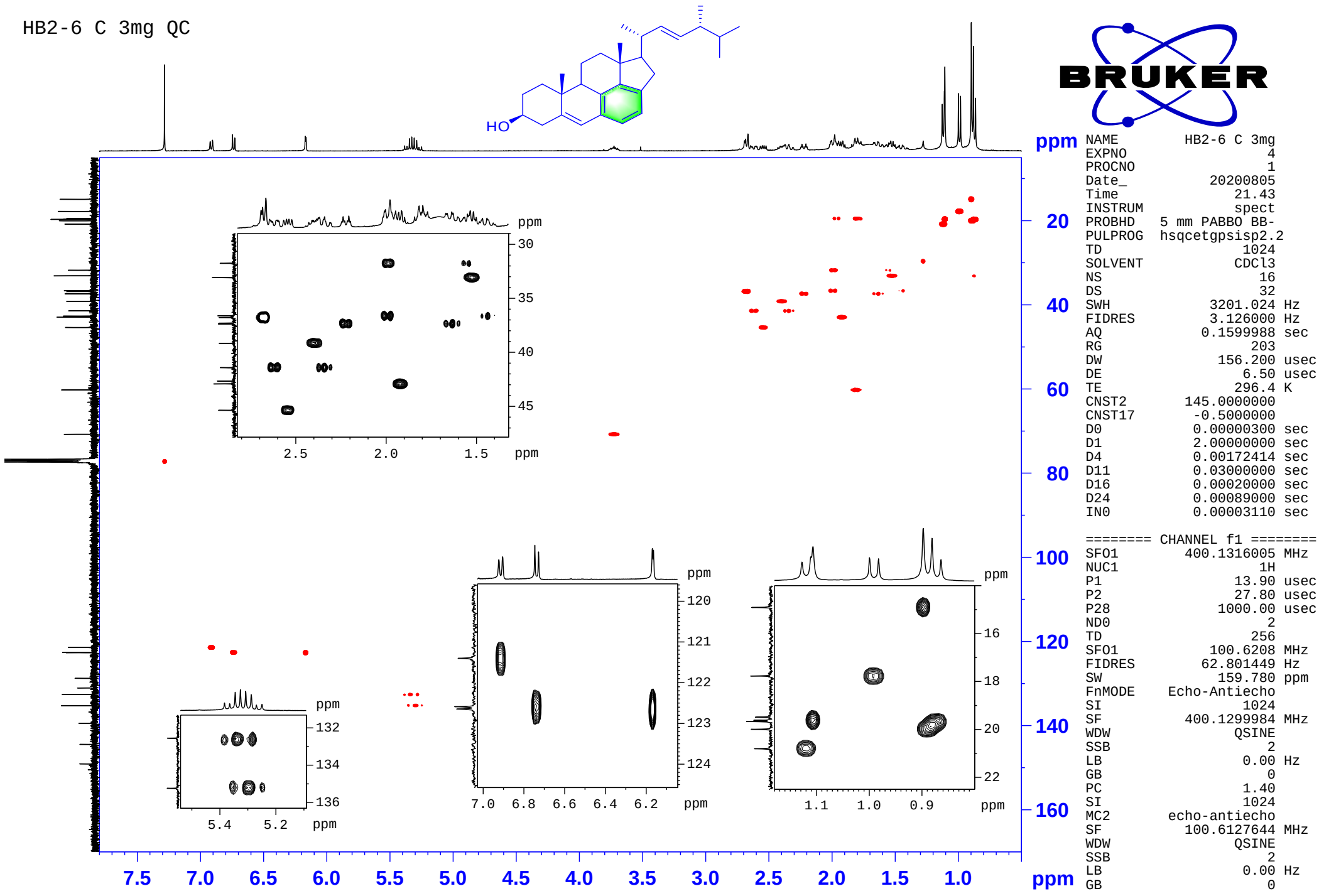


Figure S5. HSQC NMR spectrum of **1** in $CDCl_3$.

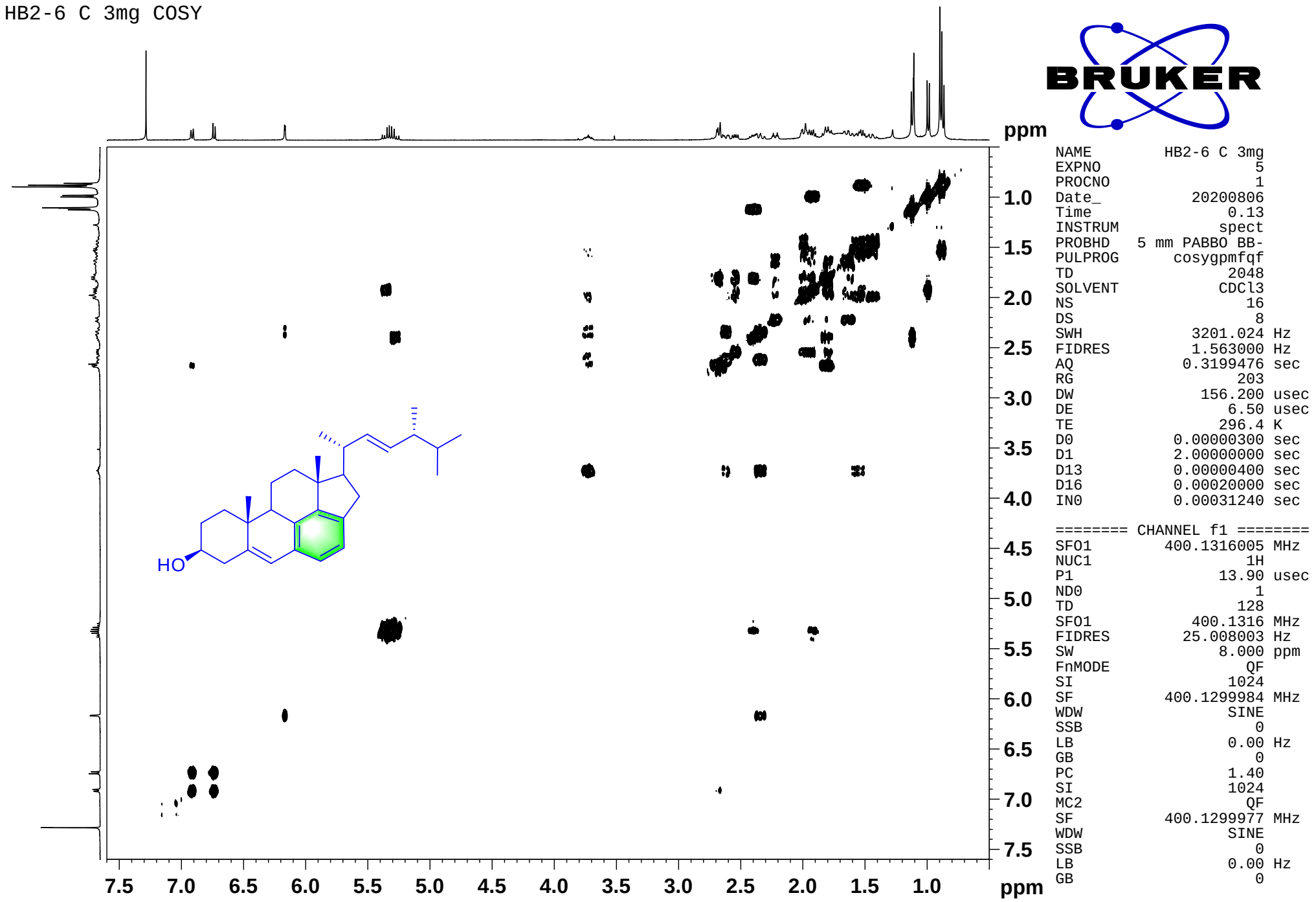


Figure S6. COSY NMR spectrum of **1** in $CDCl_3$.

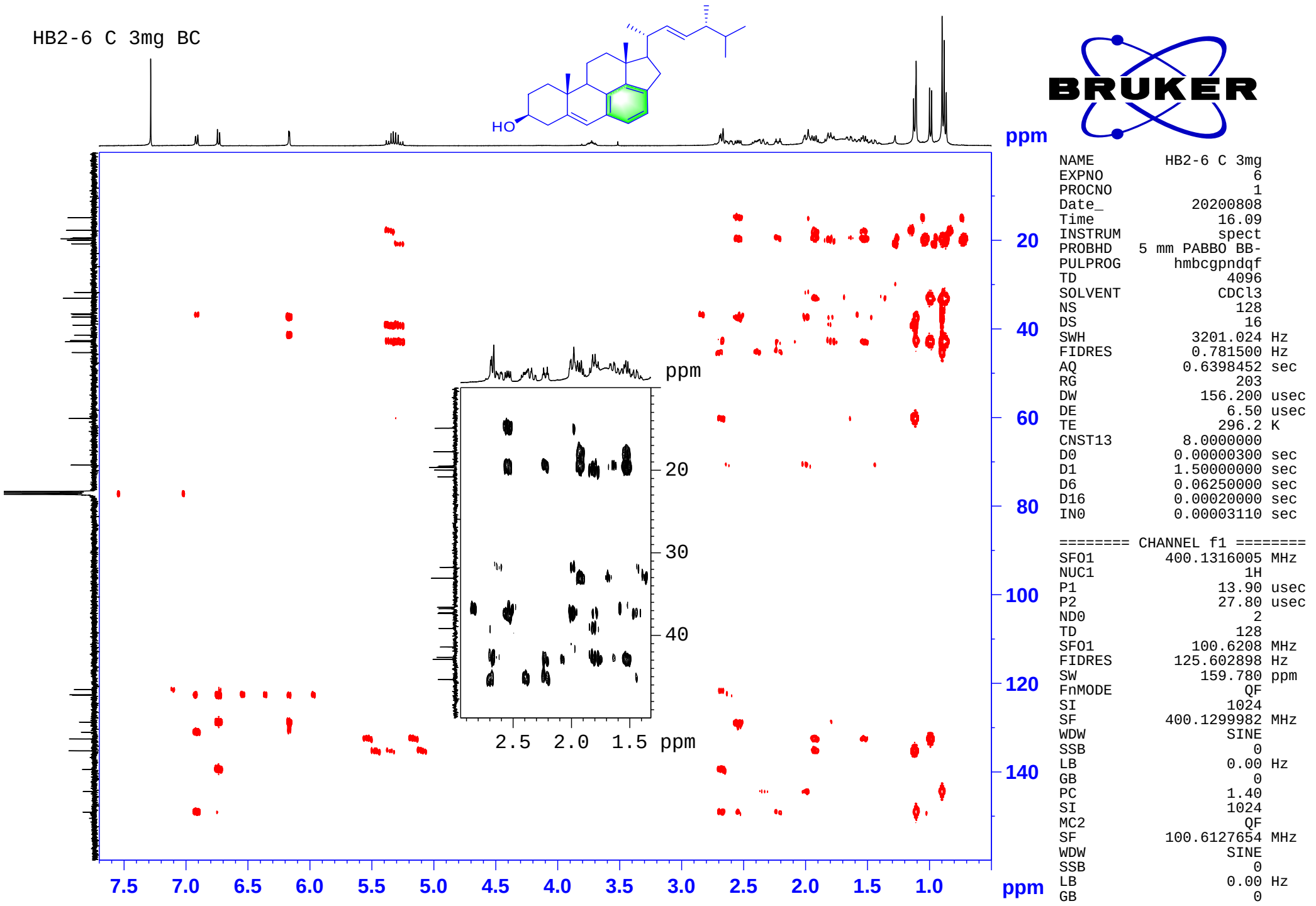
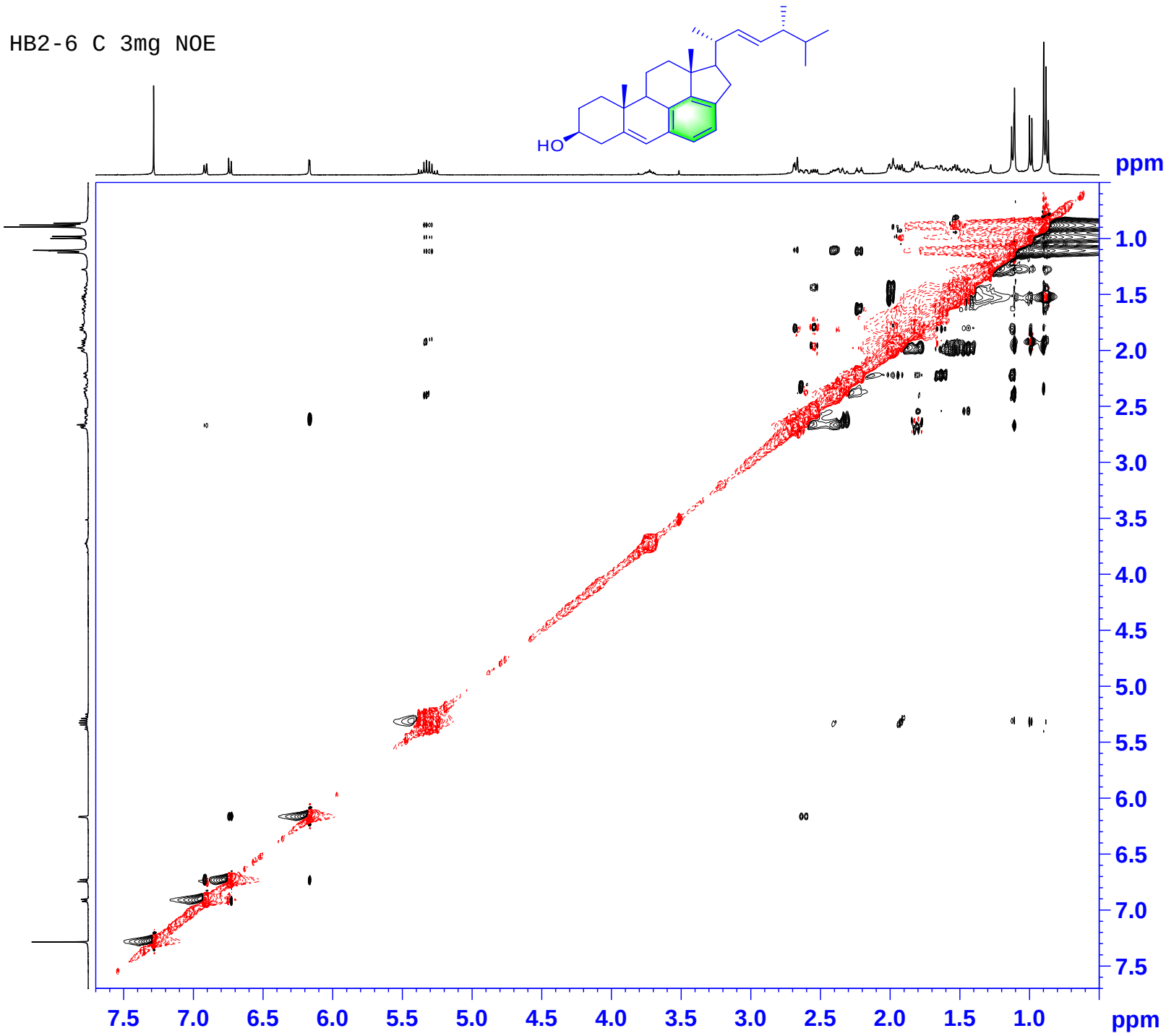


Figure S7. HMBC NMR spectrum of **1** in $CDCl_3$.



BRUKER

NAME	HB2-6 C 3mg
EXPNO	7
PROCNO	1
Date_	20200809
Time	2.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	noesygpphpp
TD	2048
SOLVENT	CDCl3
NS	32
DS	32
SWH	3201.024 Hz
FIDRES	1.563000 Hz
AQ	0.3199476 sec
RG	203
DW	156.200 usec
DE	6.50 usec
TE	296.8 K
D0	0.00013850 sec
D1	2.00000000 sec
D8	0.30000001 sec
D11	0.03000000 sec
D12	0.00002000 sec
D16	0.00020000 sec
IN0	0.00031240 sec
======== CHANNEL f1 ========	
SFO1	400.1316005 MHz
NUC1	1H
P1	13.90 usec
P2	27.80 usec
P17	2500.00 usec
ND0	1
TD	256
SFO1	400.1316 MHz
FIDRES	12.504002 Hz
SW	8.000 ppm
FnMODE	States-TPPI
SI	1024
SF	400.1299989 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	400.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

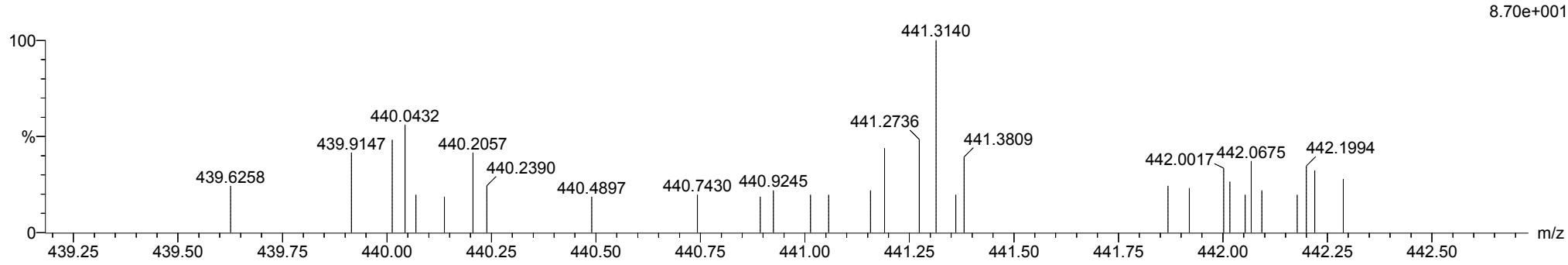
Figure S8. NOESY NMR spectrum of **1** in $CDCl_3$.

Single Mass Analysis

Tolerance = 20.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

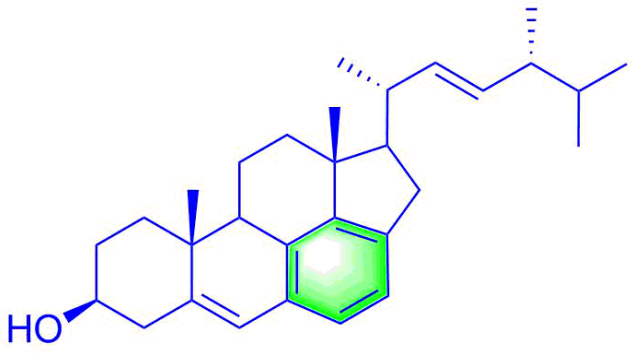
Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-30 H: 0-60 O: 0-2 23Na: 0-1

HB 2-6-re-Oct 168 (0.651)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		20.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
441.3140	441.3133	0.7	1.6	9.5	93.1	n/a	n/a	C30 H42 O 23Na

Figure S9. The HR-ESI-MS spectrum of **1**.



Chemical Formula: $C_{30}H_{42}O$

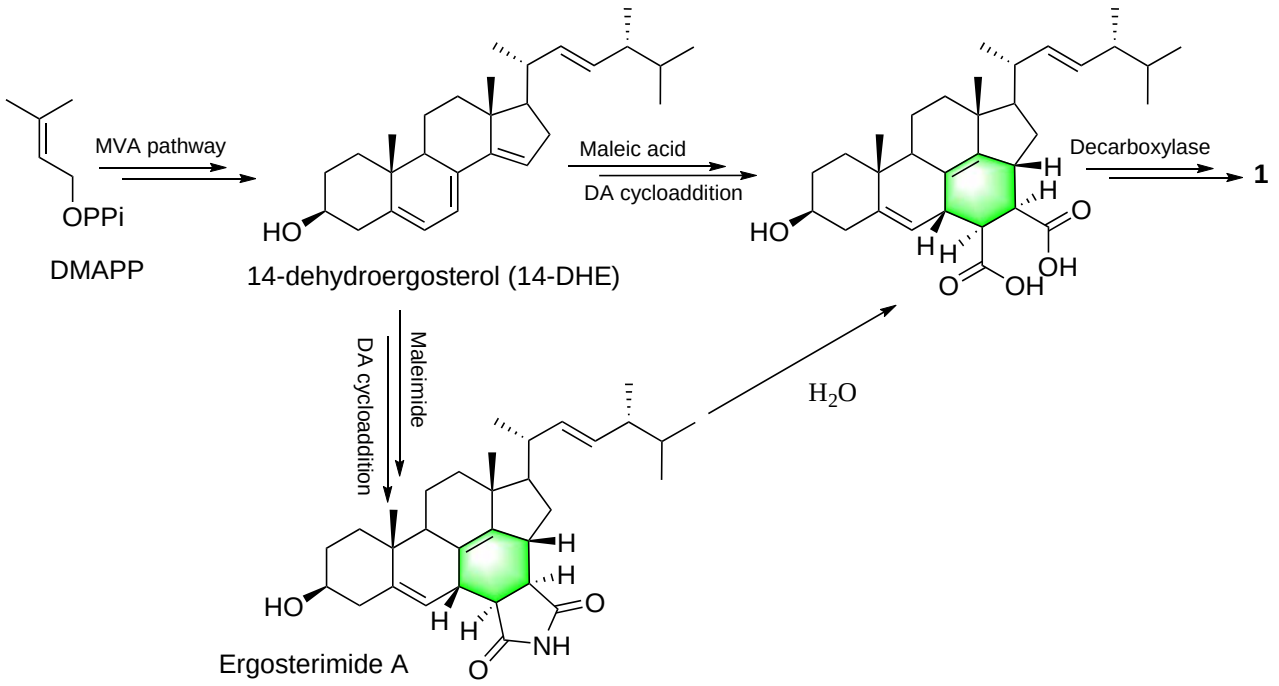


Figure S10. A biosynthetic proposal for **1**.