SUPPLEMENTARY MATERIAL

Antimicrobial Lavandulylated Flavonoids from a Sponge-Derived *Streptomyces* sp. G248 in East Vietnam Sea

Duc Danh Cao[1,2], Thi Thanh Van Trinh[1], Huong Doan Thi Mai[1,2], Van Nam Vu[1], Thi Hong Minh Le[1], Quyen Vu Thi[1], Mai Anh Nguyen[1], Thu Trang Duong[1], Dang Thach Tran[3], Van Minh Chau[1], Rui Ma[4], Gauri Shetye[4], Sanghyun Cho[4], Brian T. Murphy[5] and Van Cuong Pham[1,*]

[1] Advanced Center for Bioorganic Chemistry, Institute of Marine Biochemistry, Vietnam Academy of Science and Technology (VAST), Hanoi, Vietnam.
[2] Faculty of Chemistry, Graduate University of Science and Technology, VAST, Hanoi, Vietnam.
[3] Institute of Applied Science and Technology, University Industry Vinh, Vinh, Vietnam.
[4] Institute for Tuberculosis Research, College of Pharmacy, University of Illinois at Chicago, Chicago, USA.
[5] Department of Pharmaceutical Sciences, College of Pharmacy, University of Illinois at Chicago, Chicago, USA.
* Correspondence: phamvc@imbc.vast.vn; Tel.: +84-2437-9170-49 (V.C.P.).

Content

TD-DFT electronic CD (ECD) calculation of compounds 1 - 3: A conformational search was carried out with Spartan'14 software (Wavefunction Inc., Irvine, CA) for the proposed absolute configuration as shown at the molecular mechanics level (MMFF) [1]. All MMFF minima were re-optimized using DFT calculations at the B3LYP/6-31G(d) level with the Gaussian 09 program [2]. The geometry was optimized starting from various initial conformations with vibrational frequency calculations confirming the presence of minima. The DFT calculations (B3LYP/LanL2DZ) were performed on the lowest-energy conformations using 30 excited states and a polarizable continuum model (PCM) in methanol. The ECD spectra of the conformers were combined using Boltzmann weighting with program SpecDis 1.71 (applying a sigma value of 0.25 eV) [3]. After applying a UV-shift correction, the computed CD spectra were compared with the CD curves experimentally obtained.

[1] Spartan'14. Wavefunction: Irvine, CA, USA, **2013**.

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

[3] Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. SpecDis: Quantifying the comparison of calculated and experimental electronic circular dichroism spectra. *Chirality* **2013**, *25*, 243–249

***Streptomyces* sp. G248 isolation and characterization**

***Bacteria isolation*:** The sponge *Halichondria panicea* (Pallas, 1766) sample (0.5 g) was crushed by glass chopsticks in a falcon tube, to which sterile sea water (4.5 mL) was added. The mixture was homogenized by vortexing for 1 min, and the suspension was treated using a wet-heat technique (60 ºC for 6 min). An amount (0.5 mL) of this suspension was diluted by sterile distilled water (4.5 mL) and vortexed for 1 min, of which an aliquot of 50 µL was spread on A1 medium (soluble starch: 10 g/L, yeast extract: 4 g/L, peptone: 2 g/L, instant ocean: 30 g/L, agar: 15 g/L) supplemented with 50 µg/mL of polymycin B and cycloheximide to inhibit Gram (-) bacterial and fungal contaminations. After 21 days of aerobic incubation at 30 ºC, a colony of the actinomycete strain was transferred onto a petri dish of medium A1 for purification.

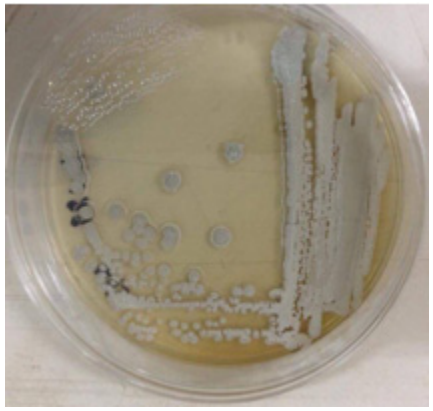

Figure 1S. Morphological appearance of strain G248

Bacteria identification: Genomic DNA was extracted with the Gen Elute Bacterial Genomic DNA kit (Sigma). The sequence of 16S rRNA was used for identification. The gene amplification was performed in a 25.0 µL mixture containing sdH_2O (16.3 µL), 10X PCR buffer (2.5 µL), 25 mM $MgCl_2$ (1.5 µL), 10 mM dNTP's (0.5 µL), Taq polymerase (0.2 µL), 0.05 mM (1.0 µL) for both primers of 9F (5'-GAGTTTGATCCTGGCTCAG3') and 1541R (5'-AAGGAGGTGATCCAACC3') and genomic DNA (2.0 µL). The reaction tube was then put into MJ Thermalcycler, which had been programmed to preheat at 94 ºC for 3 min, followed by 30 cycles of denaturation at 94 ºC for 1 min, annealing at 60 ºC for 30s and elongation at 72 ºC for 45s before a final extension of 72 ºC for 10 min. The estimated PCR

product size was about 1500 bp (Figure 2S). PCR products were purified by DNA purification kit (Invitrogen) then sequenced by DNA Analyzer (ABI PRISM 3100, Applied Bioscience). Gene sequences were handled by BioEdit v.2.7.5. and compared with bacterial 16S rRNA sequences in GeneBank database by NBCI Blast program. The results showed that the strain G248 belonged to the genus *Streptomyces*. The sequence of 16S rRNA gene of the strain G248 was registered on GenBank database with the accession number MG917690 (Figure 3S).

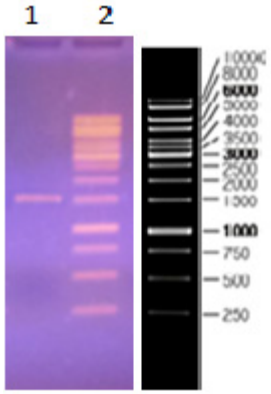

Figure 2S. Gel electrophoresis of PCR product

Lane 1: PCR product; Lane 2: One Kb DNA ladder of Fisher Scientific

Streptomyces sp. strain G248 16S ribosomal RNA gene, partial sequence

GenBank: MG917690.1

FASTA Graphics PopSet

Go to:

```
LOCUS       MG917690               1368 bp    DNA     linear   BCT 30-JUL-2018
DEFINITION  Streptomyces sp. strain G248 16S ribosomal RNA gene, partial
            sequence.
ACCESSION   MG917690
VERSION     MG917690.1
KEYWORDS    .
SOURCE      Streptomyces sp.
  ORGANISM  Streptomyces sp.
            Bacteria; Actinobacteria; Streptomycetales; Streptomycetaceae;
            Streptomyces.
REFERENCE   1  (bases 1 to 1368)
  AUTHORS   Le,T.H.M., Vu,T.Q., Nguyen,M.A., Pham,V.C., Doan,T.M.H., Tran,V.H.
            and Cao,D.T.
  TITLE     Partial 16S nRNA of strains isolated from the coastal in Viet Nam
  JOURNAL   Unpublished
REFERENCE   2  (bases 1 to 1368)
  AUTHORS   Le,T.H.M., Vu,T.Q., Nguyen,M.A., Pham,V.C., Doan,T.M.H., Tran,V.H.
            and Cao,D.T.
  TITLE     Direct Submission
  JOURNAL   Submitted (05-FEB-2018) Biotechnology, Institute of Marine
            Biochemistry, VAST, 18 Hoang Quoc Viet, Cau Giay, Ha Noi, Ha Noi
            10000, Viet Nam
COMMENT     ##Assembly-Data-START##
            Sequencing Technology :: Sanger dideoxy sequencing
            ##Assembly-Data-END##
FEATURES             Location/Qualifiers
     source          1..1368
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Figure 3S. 16S rRNA gene sequence of *Streptomyces* sp. G248 on GenBank

Table 1S. Conformational population (%) for the most stable conformers of (2*S*,2″*R*)-**1**

Conformer	Population (%)
C-1	21.41
C-2	15.78
C-3	19.94
C-4	4.38
C-5	16.57
C-6	6.18
C-7	15.74

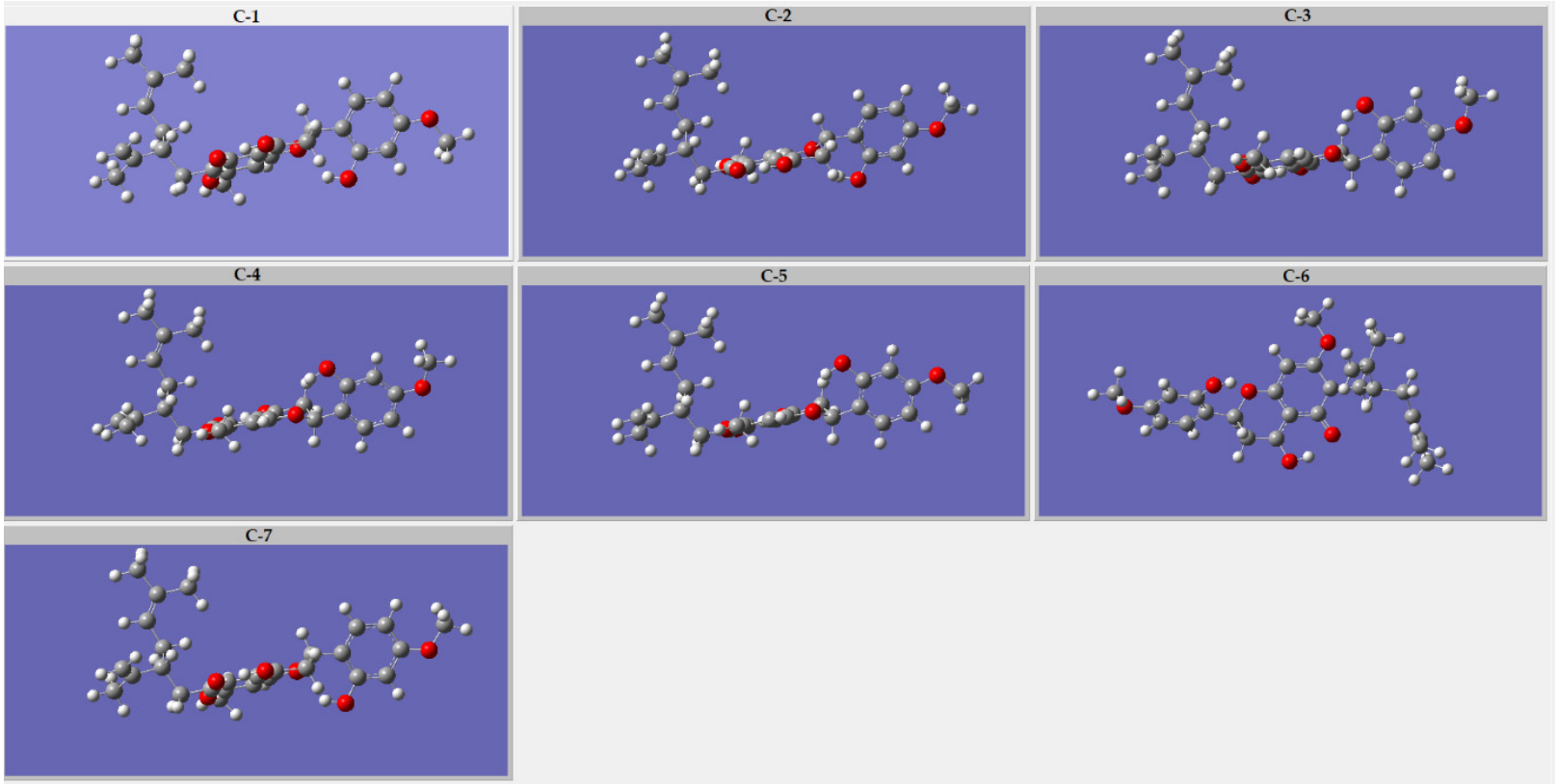


Figure 4S. Optimized conformers of (2*S*,2″*R*)-**1**

Table 2S. Conformational population (%) for the most stable conformers of (2*S*,2″*S*)-**1**

Conformer	Population (%)
C-1	13.76
C-2	8.83
C-3	19.86
C-4	12.64
C-5	3.05
C-6	10.71
C-7	6.92
C-8	15.22
C-9	9.02

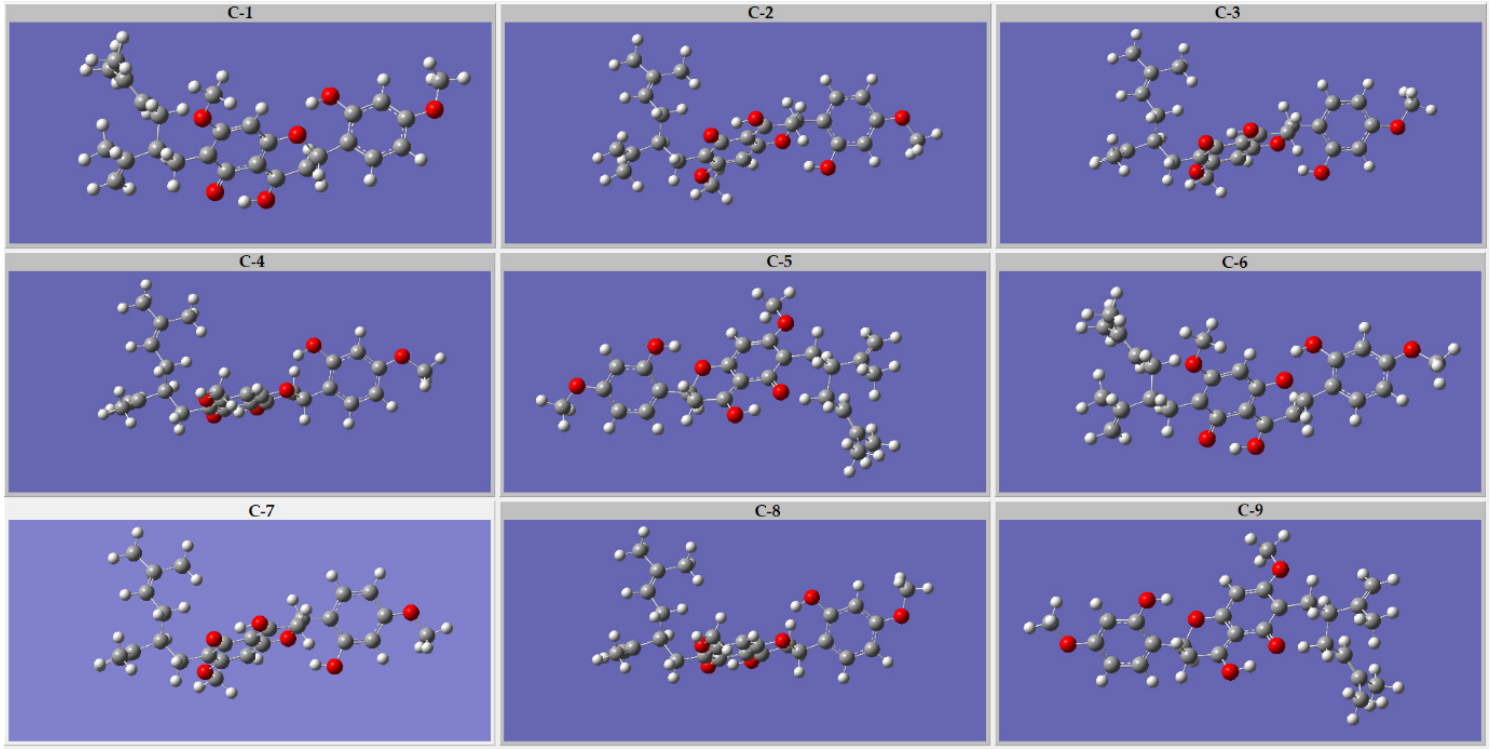


Figure 5S. Optimized conformers of (2*S*,2″*S*)-**1**

Table 3S. Conformational population (%) for the most stable conformers of (2*S*,2″*R*)-**2**

Conformer	Population (%)
C-1	8.54
C-2	36.15
C-3	8.85
C-4	8.72
C-5	37.73

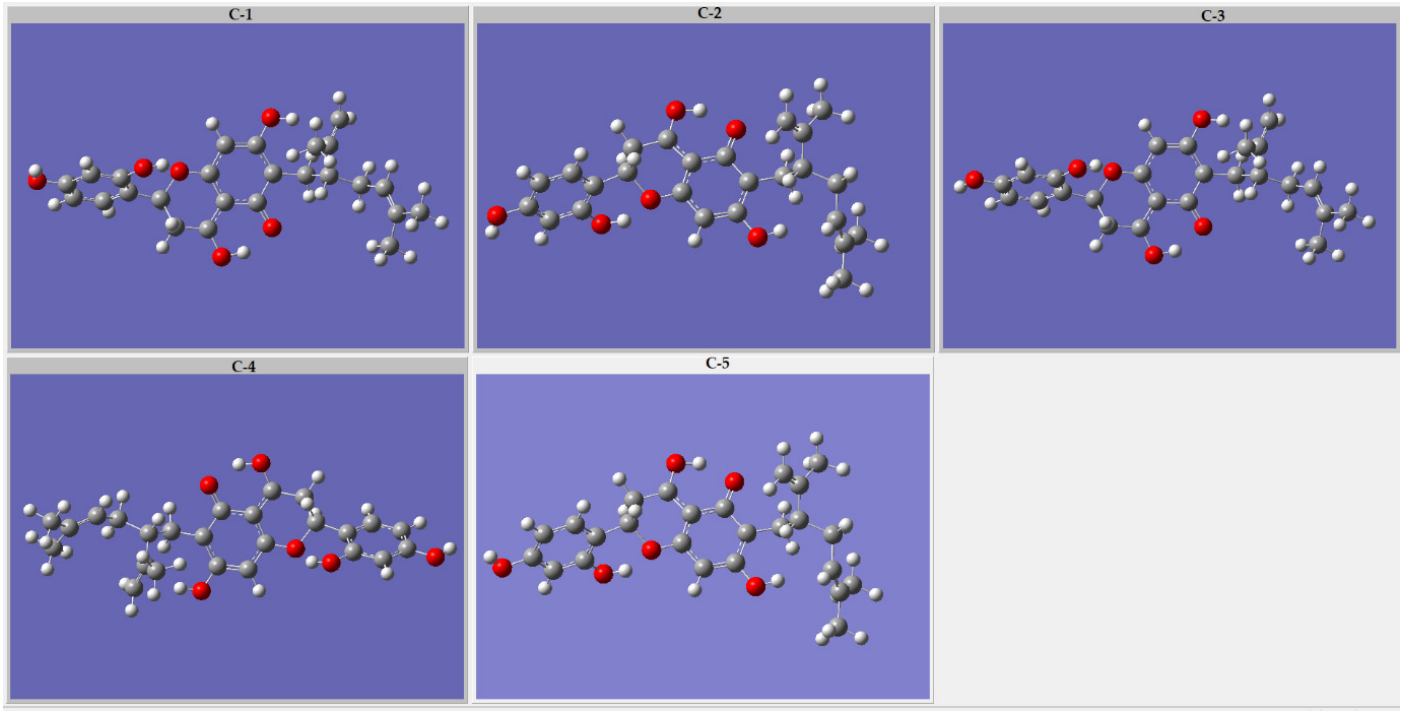


Figure 6S. Optimized conformers of (2*S*,2″*R*)-**2**

Table 4S. Conformational population (%) for the most stable conformers of (2*S*,2″*S*)-**2**

Conformer	Population (%)
C-1	30.59
C-2	2.06
C-3	1.42
C-4	31.24
C-5	31.05
C-6	2.14
C-7	1.50

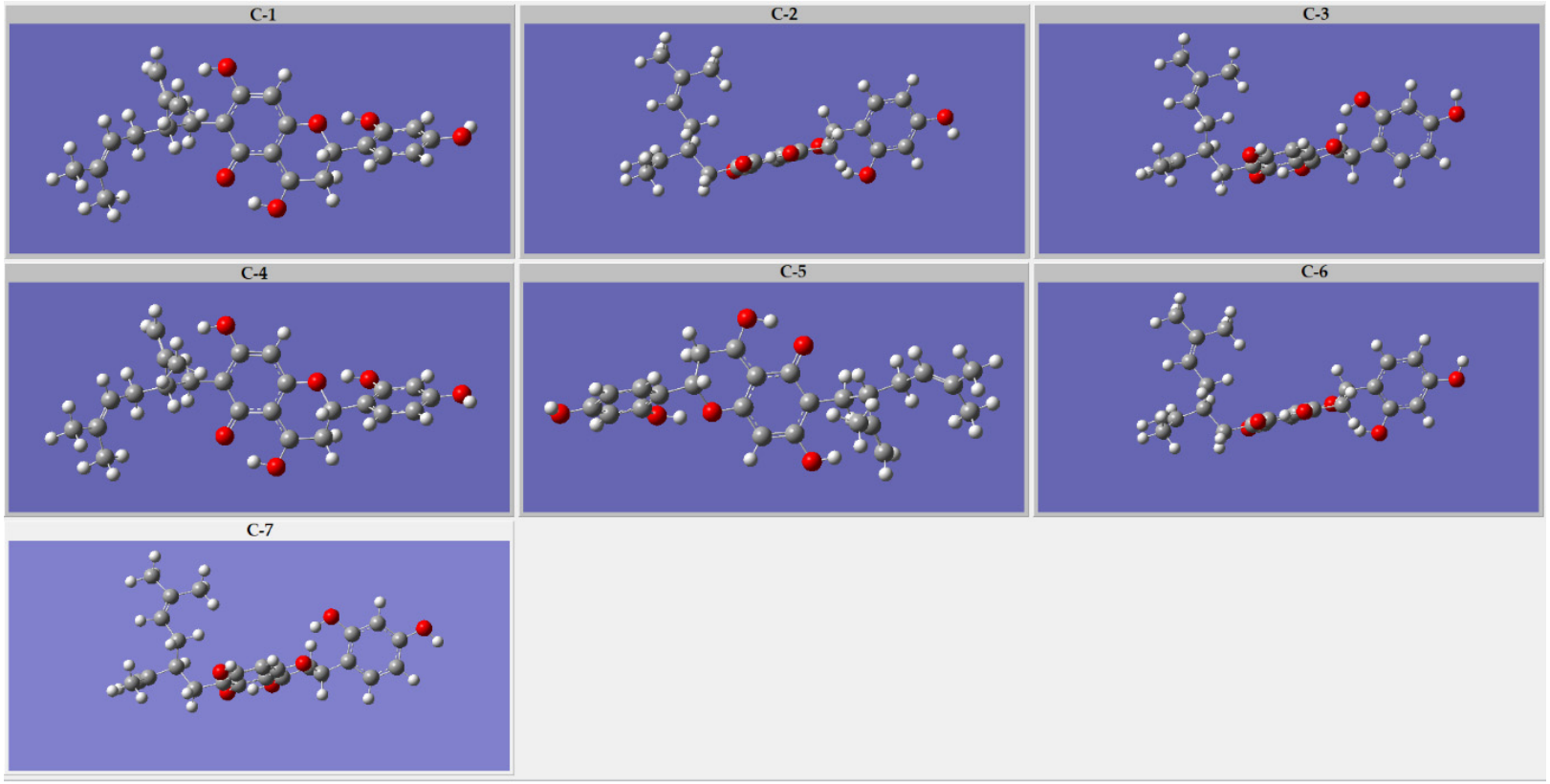


Figure 7S. Optimized conformers of (2*S*,2″*S*)-**2**

Table 5S. Conformational population (%) for the most stable conformers of (2″*S*)-**3**

Conformer	Population (%)
C-1	53.55
C-2	39.06
C-3	1.36
C-4	1.71
C-5	3.06
C-6	1.26

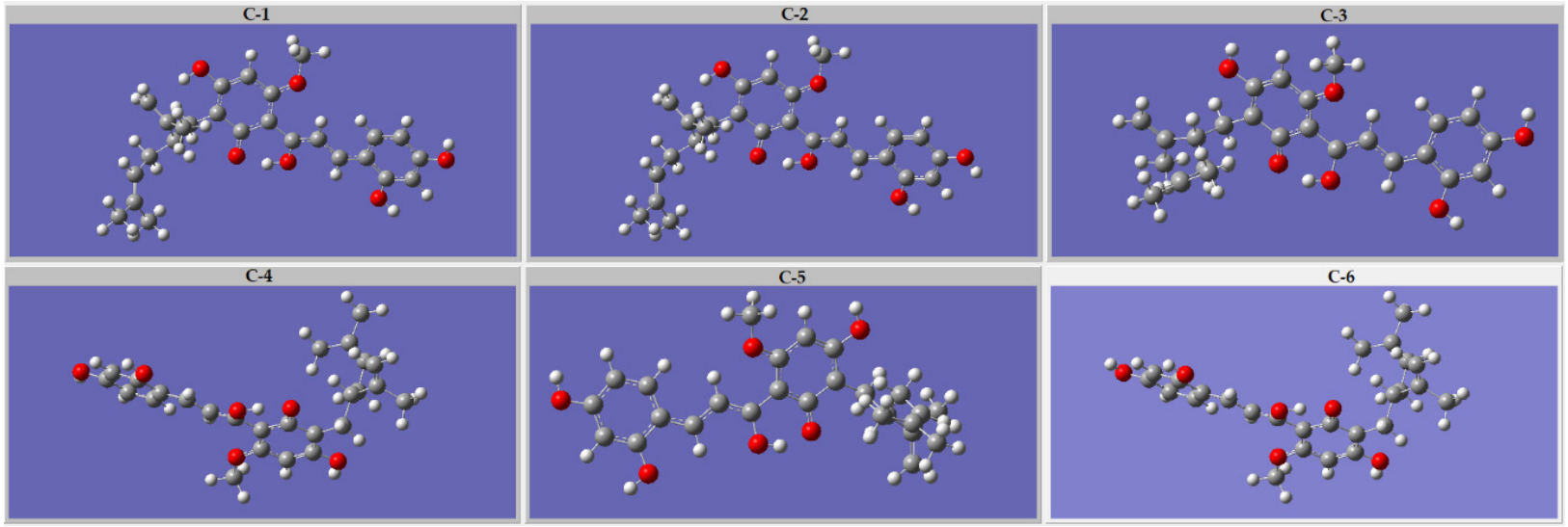


Figure 8S. Optimized conformers of (2″*S*)-**3**

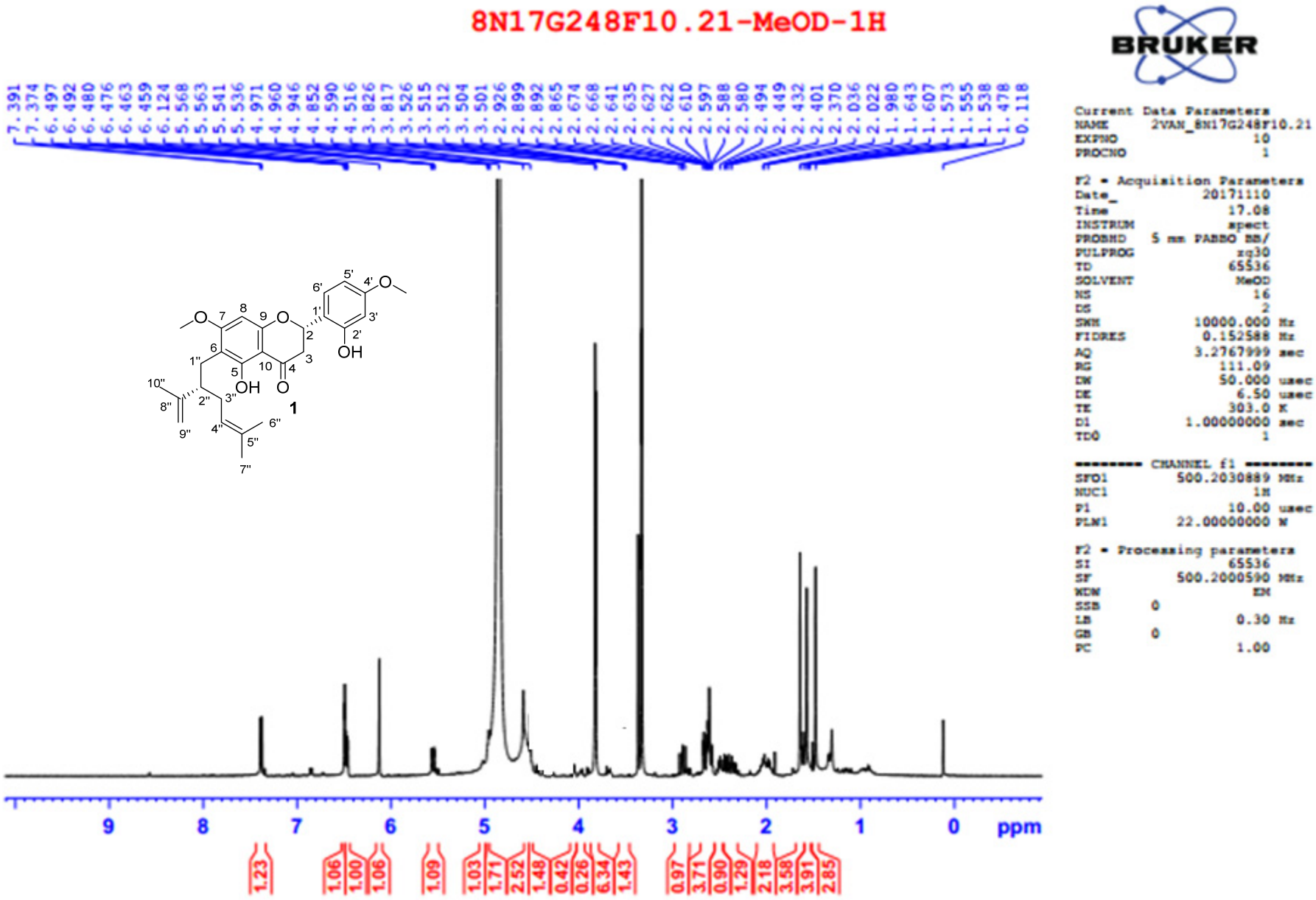
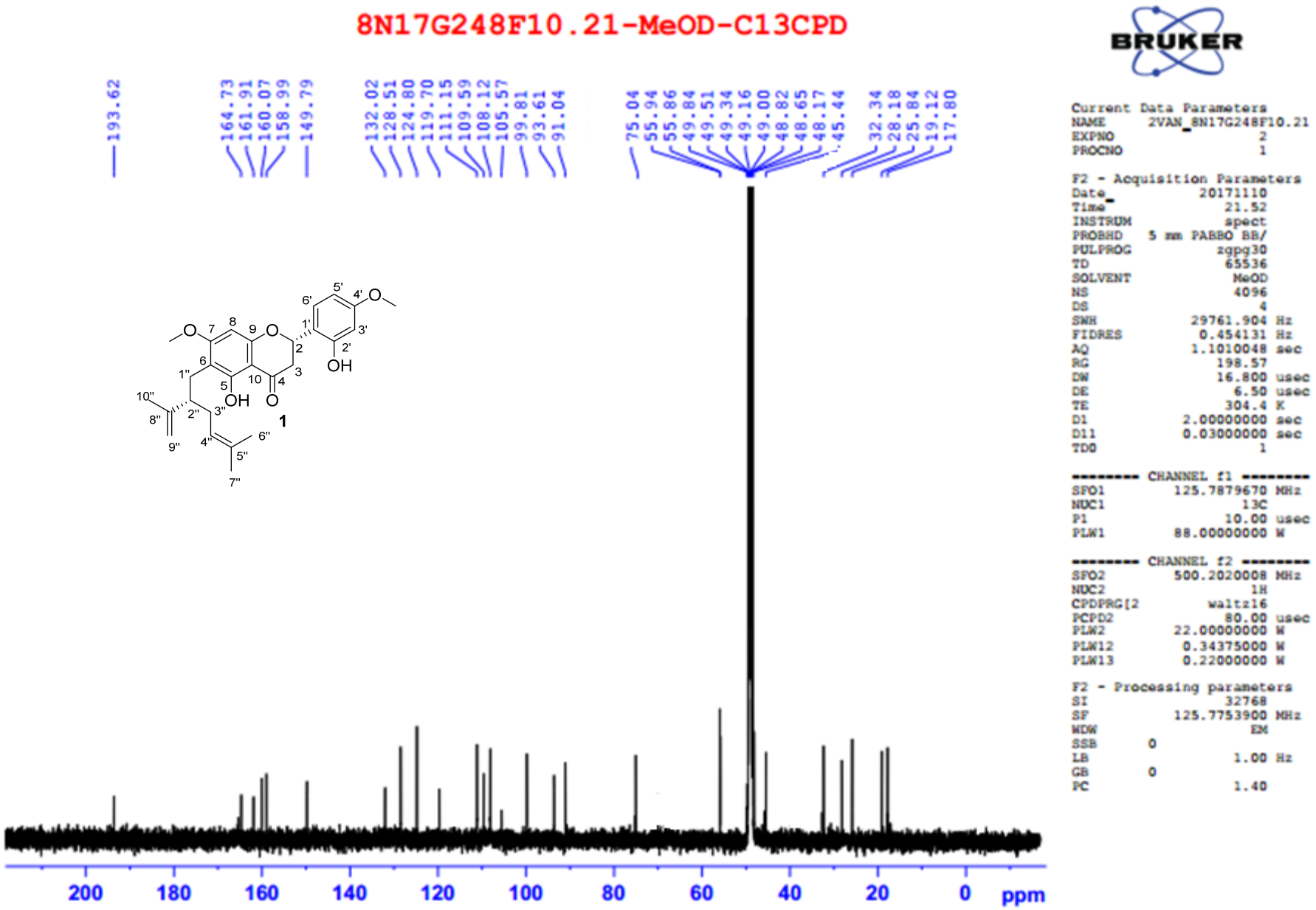


Figure 9S. ^{1}H NMR spectrum of **1** (500 MHz, CD_3OD)



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SOLVENT                MeOD
NS                     4096
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FIDRES           0.454131 Hz
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RG                   198.57
DW                 16.800 usec
DE                  6.50 usec
TE                  304.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

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NUC1                    13C
P1                   10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2          500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
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SF            125.7753900 MHz
WDW                       EM
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GB           0
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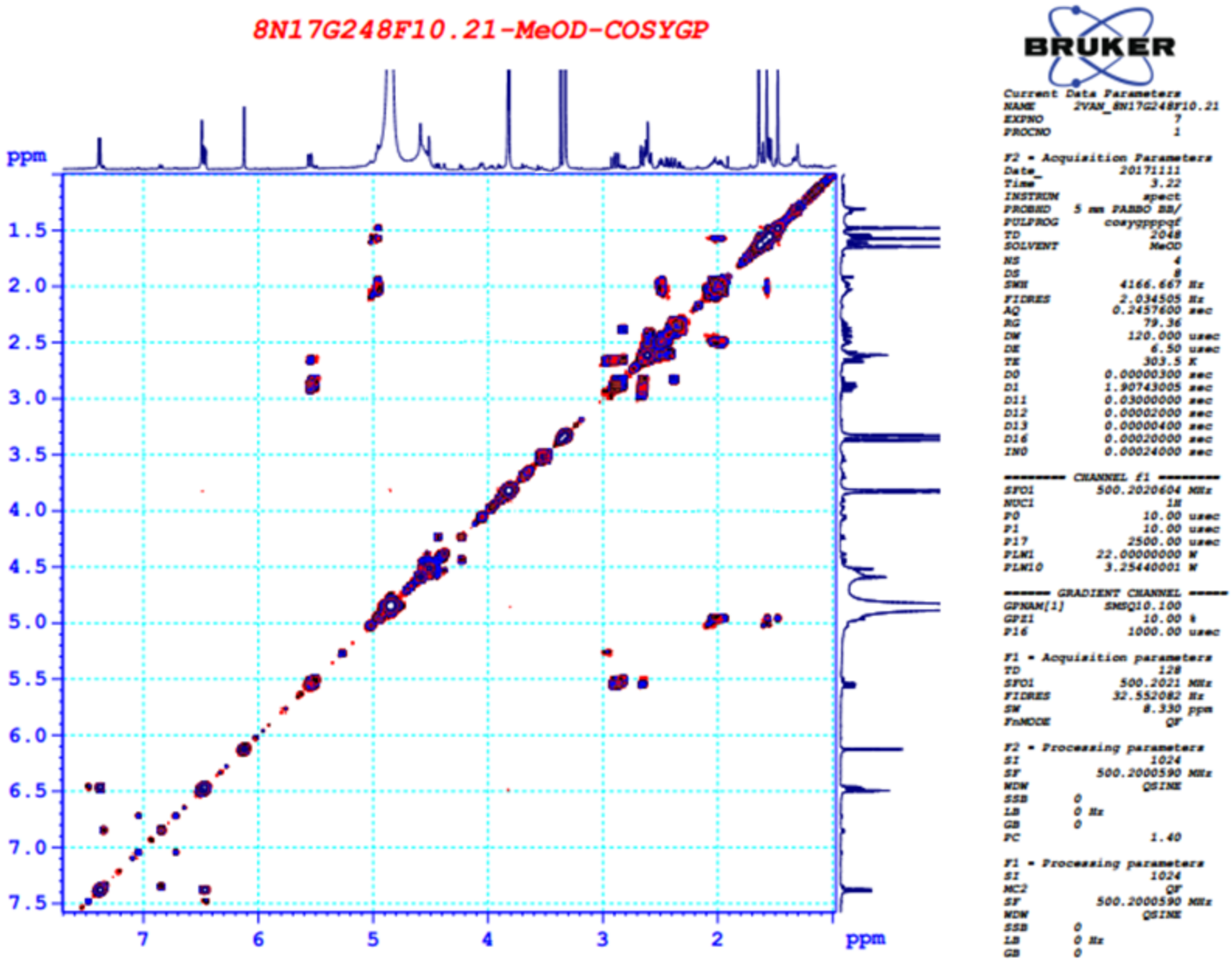
Figure 10S. ^{13}C NMR spectrum of **1** (125 MHz, CD_3OD)



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PULPROG        coxyqpppqf
TD                     2048
SOLVENT                MeOD
NS                        4
DS                        8
SWH               4166.667 Hz
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DW                  120.000 usec
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D12               0.00002000 sec
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D16               0.00020000 sec
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SFO1           500.2020604 MHz
NUC1                     1H
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P1                    10.00 usec
P17                 2500.00 usec
PLW1          22.00000000 W
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GPZ1                  10.00 %
P16                 1000.00 usec

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FnMODE                   QF

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SF             500.2000590 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
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MC2                      QF
SF             500.2000590 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
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Figure 11S. ^{1}H-^{1}H COSY spectrum of **1** (500 MHz, CD_3OD)

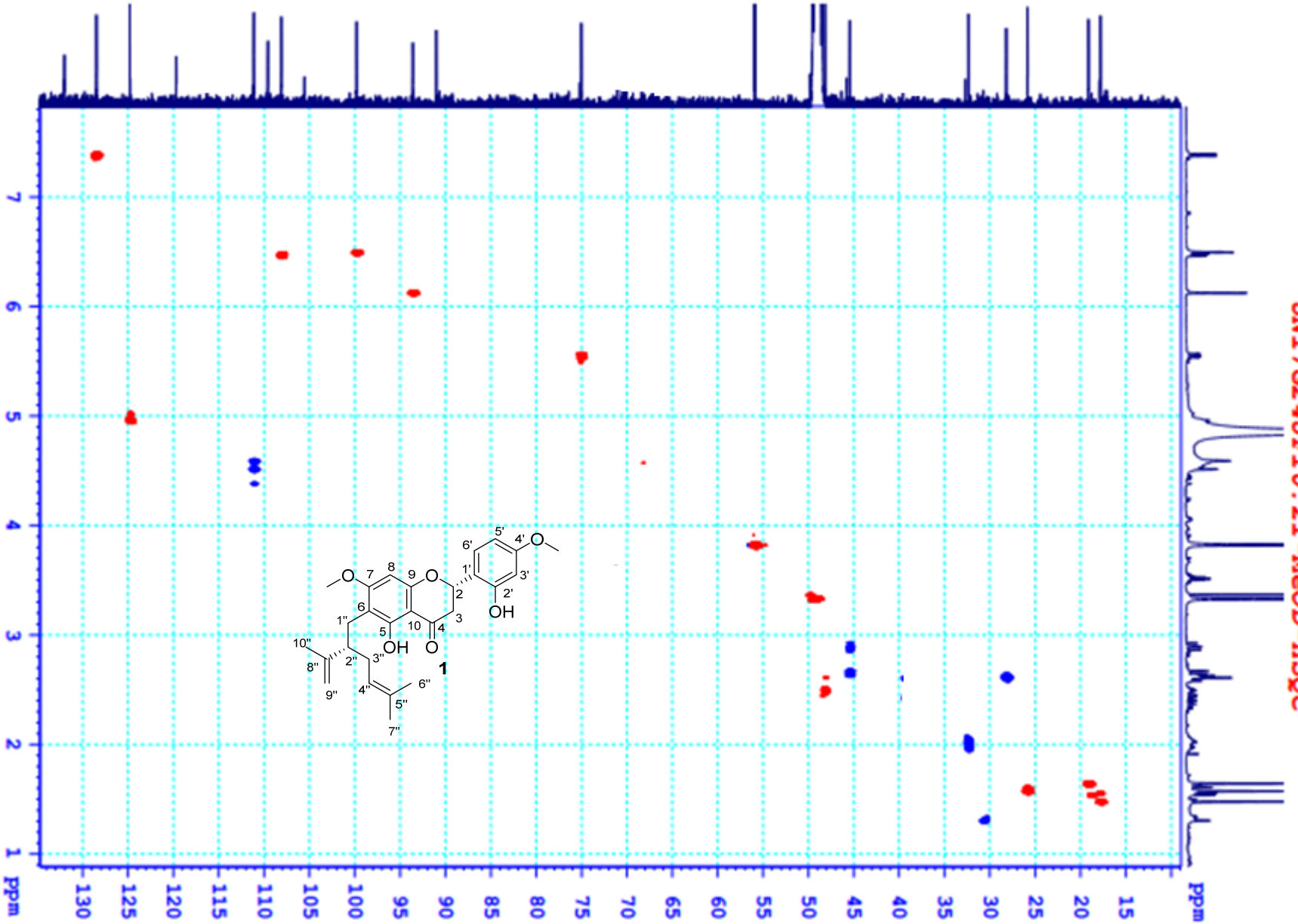


Figure 12S. HSQC spectrum of **1** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)

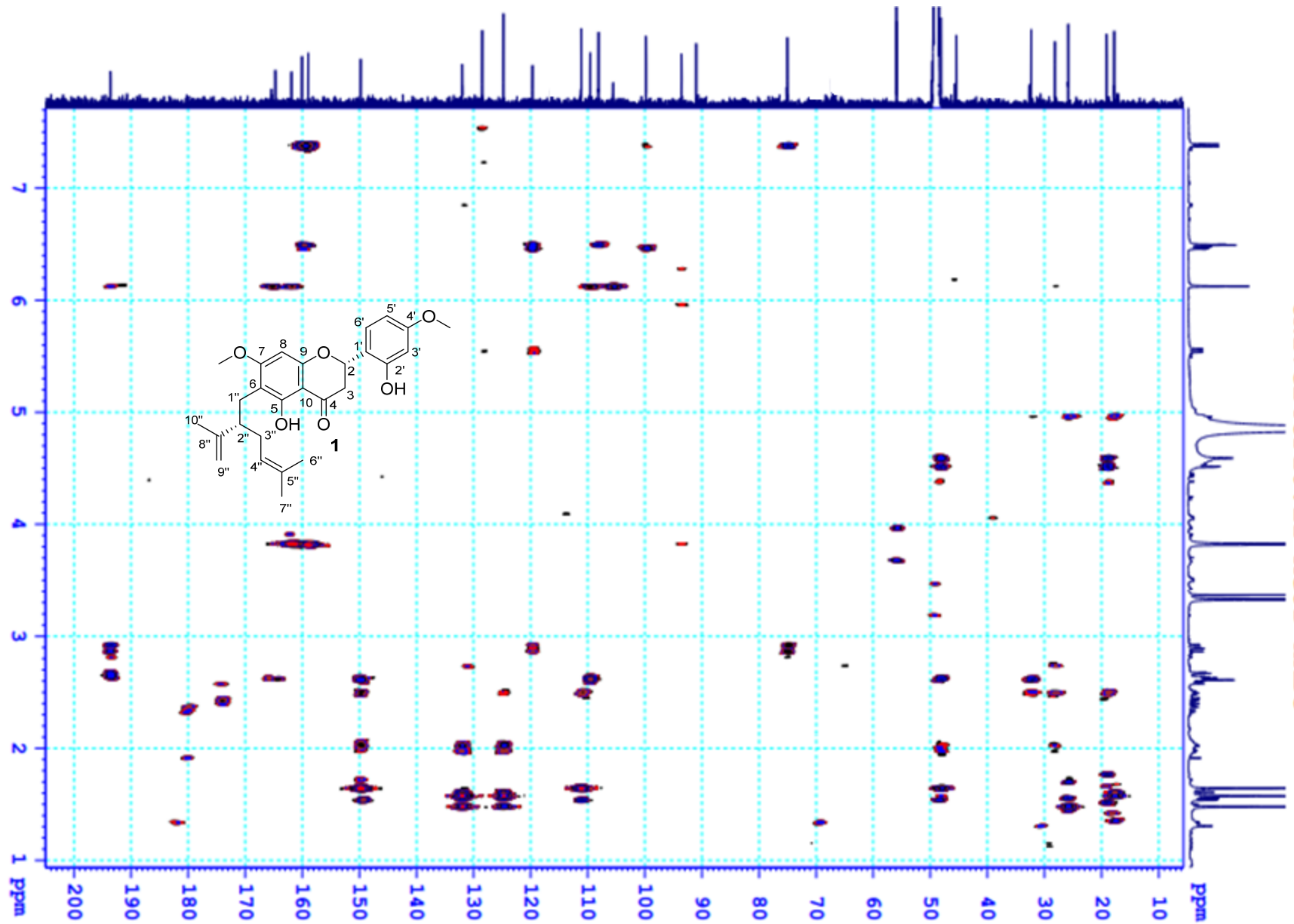
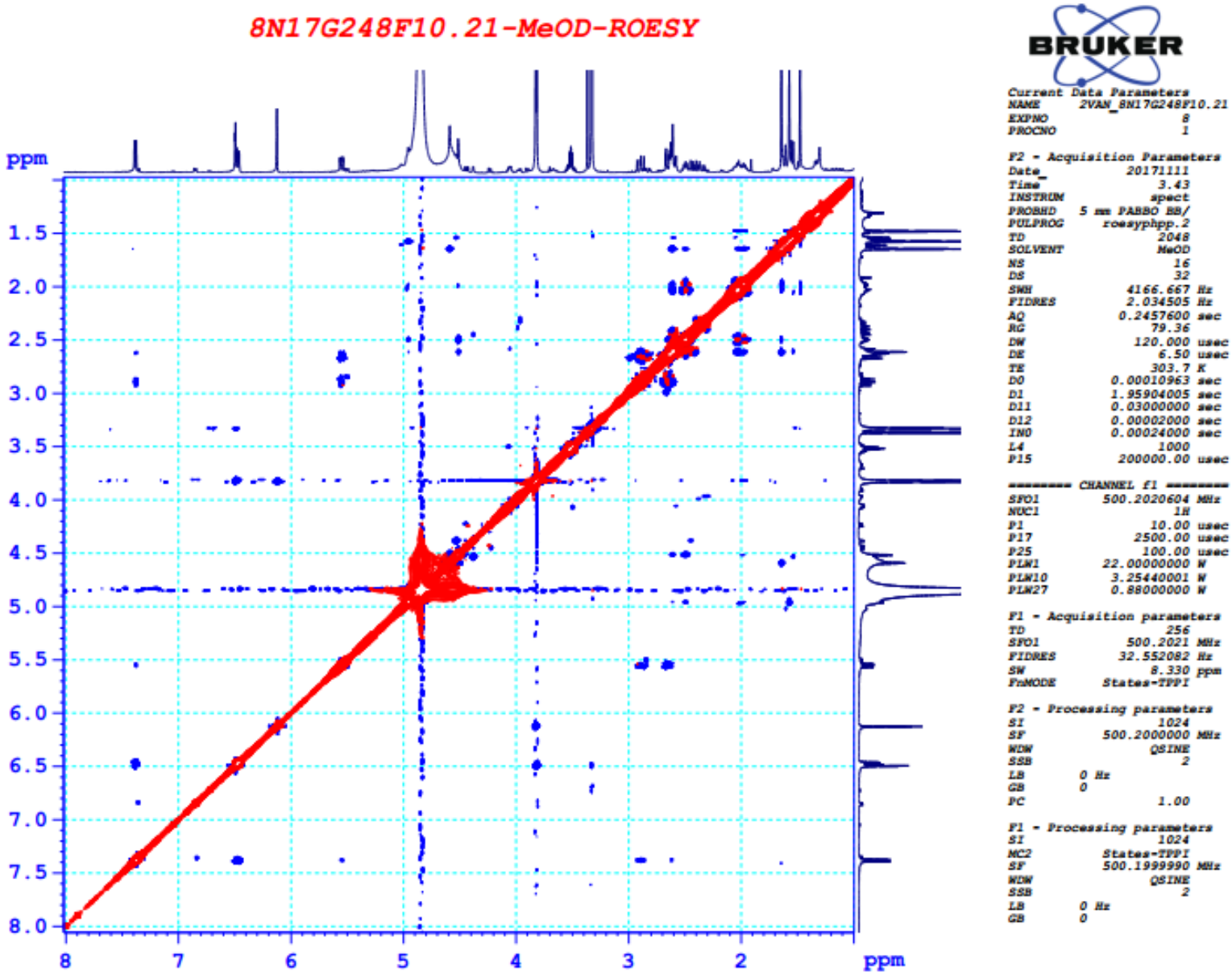


Figure 13S. HMBC spectrum of **1** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)



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SOLVENT                   MeOD
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NUC1                        1H
P1                       10.00 usec
P17                    2500.00 usec
P25                     100.00 usec
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PLW10                3.25440001 W
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FIDRES              32.552082 Hz
SW                      8.330 ppm
FnMODE              States-TPPI

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WDW                       QSINE
SSB                           2
LB          0 Hz
GB          0
PC                         1.00

F1 - Processing parameters
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SSB                           2
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GB          0
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Figure 14S. ROESY spectrum of **1** (500 MHz, CD_3OD)

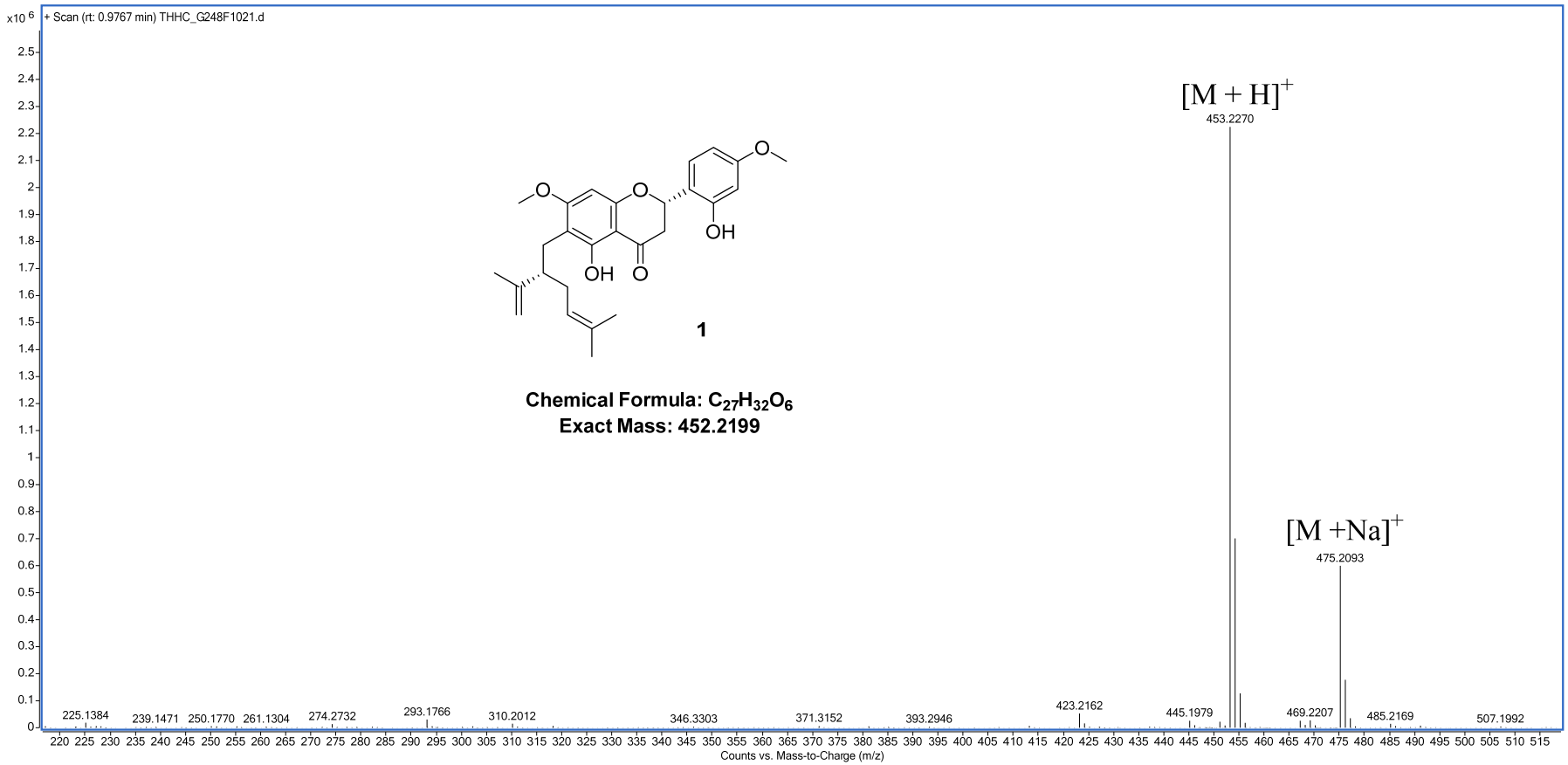


Figure 15S. HR-ESI-MS of **1**

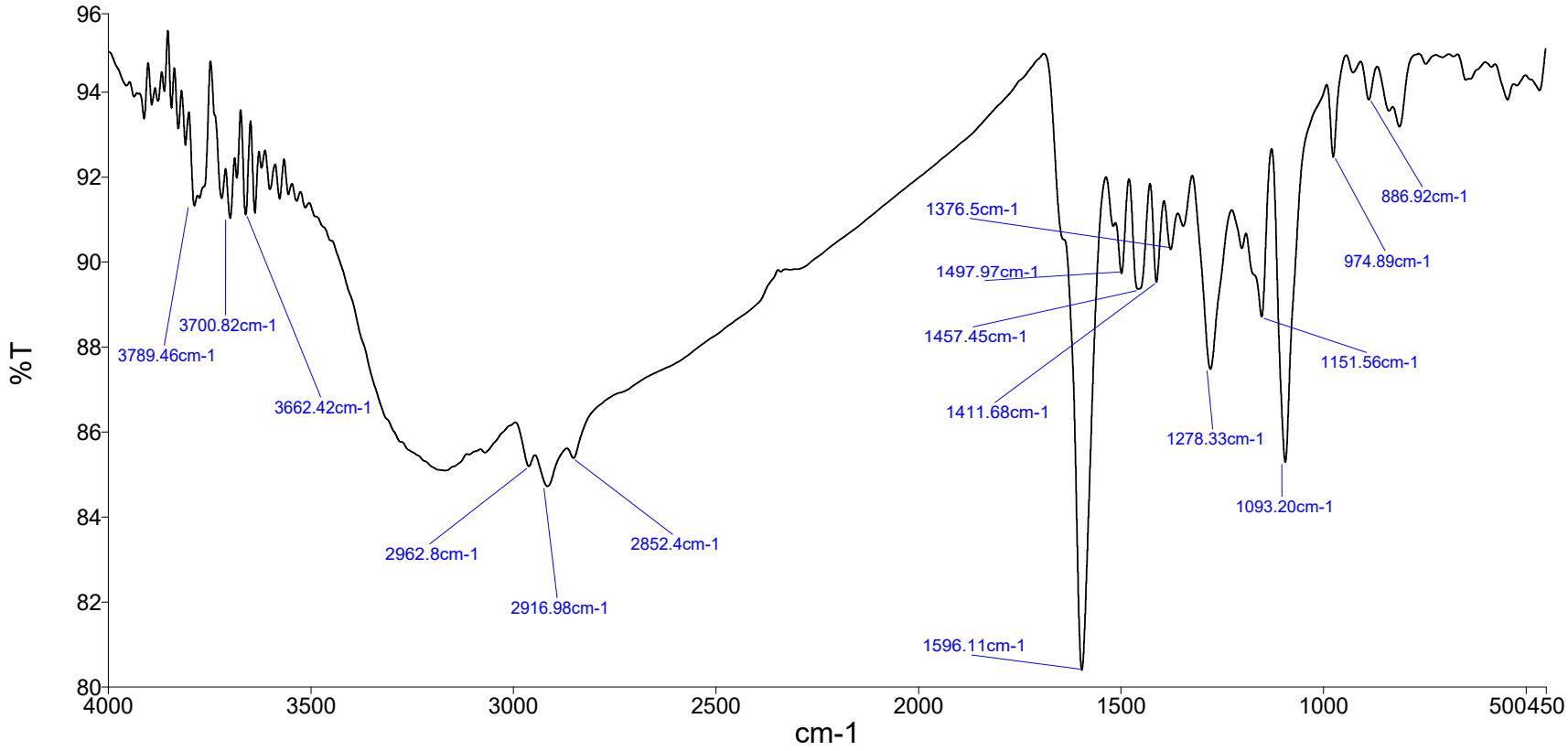


Figure 16S. IR spectrum of **1**

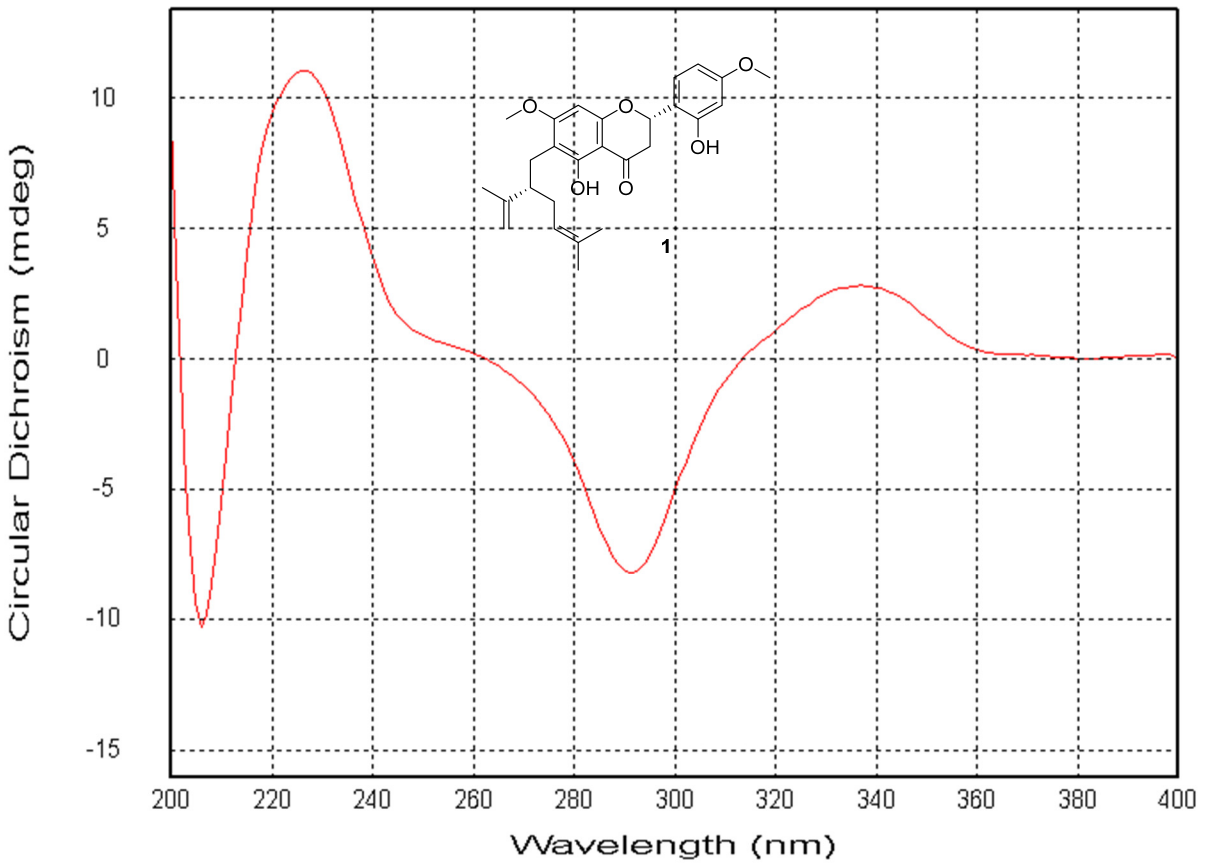


Figure 17S. CD spectrum of **1**

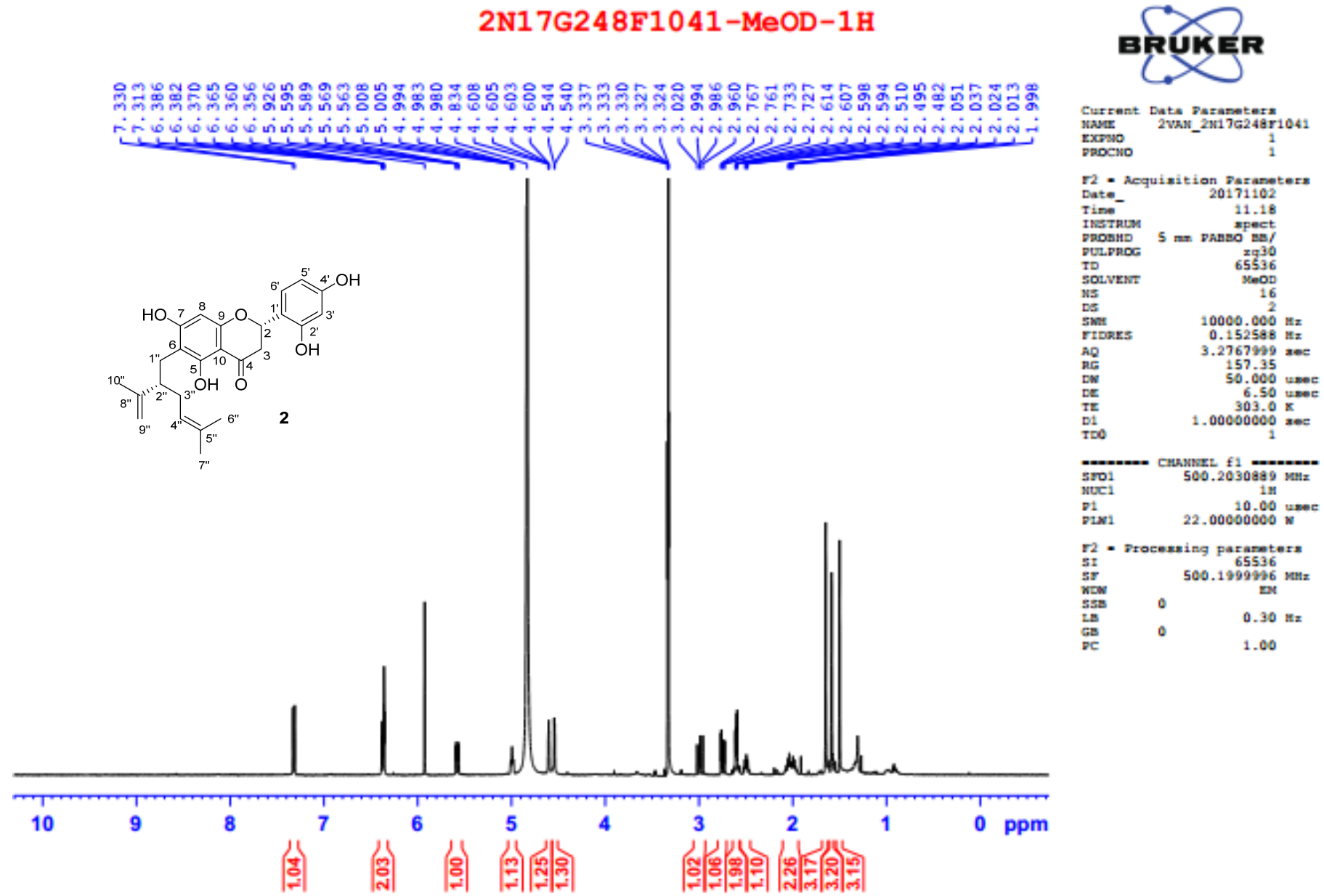
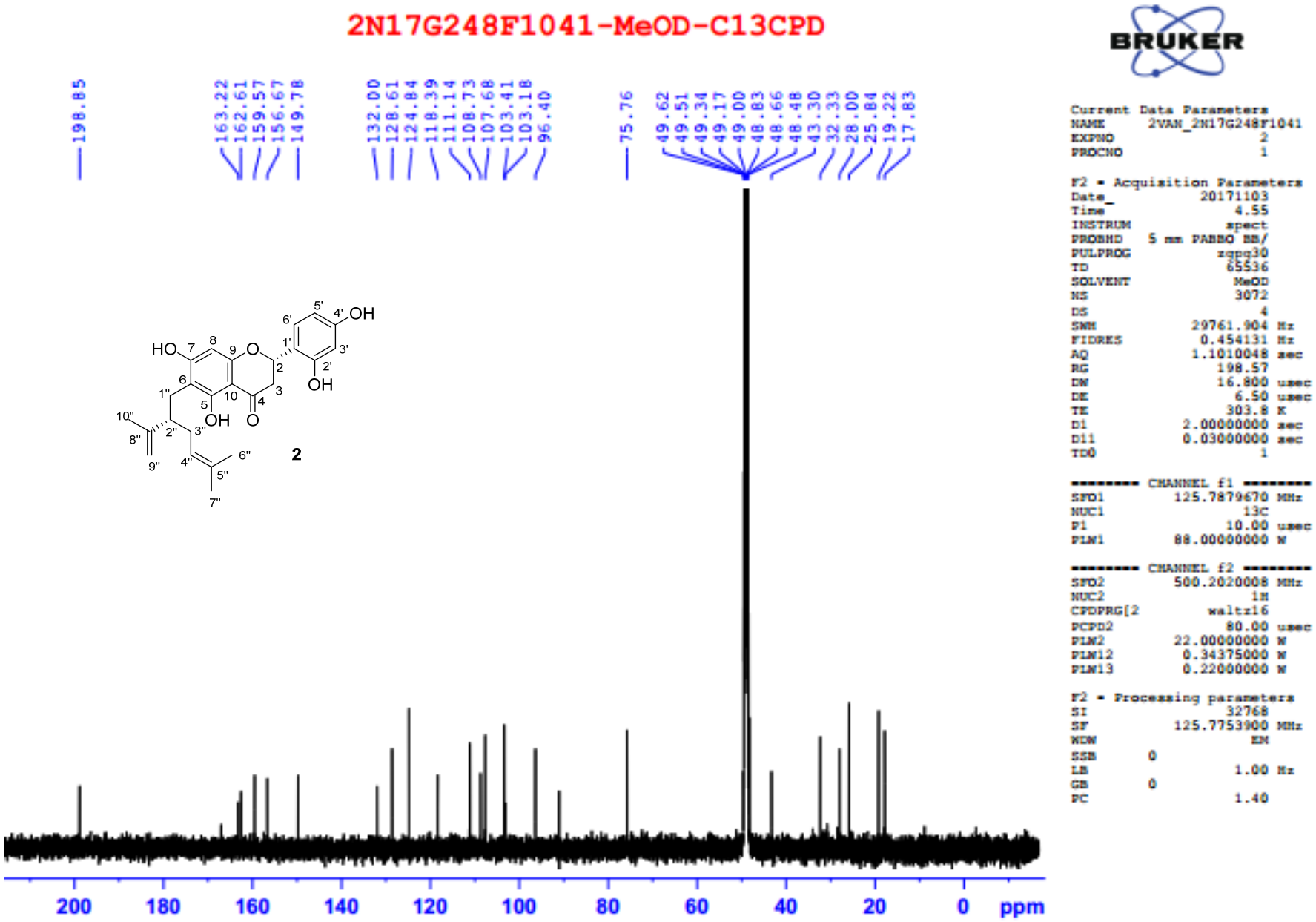


Figure 18S. ^{1}H NMR spectrum of **2** (500 MHz, CD_3OD)



BRUKER

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NS                    3072
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FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  198.57
DW                  16.800 usec
DE                   6.50 usec
TE                  303.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

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SFO1         125.7879670 MHz
NUC1                   13C
P1                   10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2         500.2020008 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

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PC                    1.40
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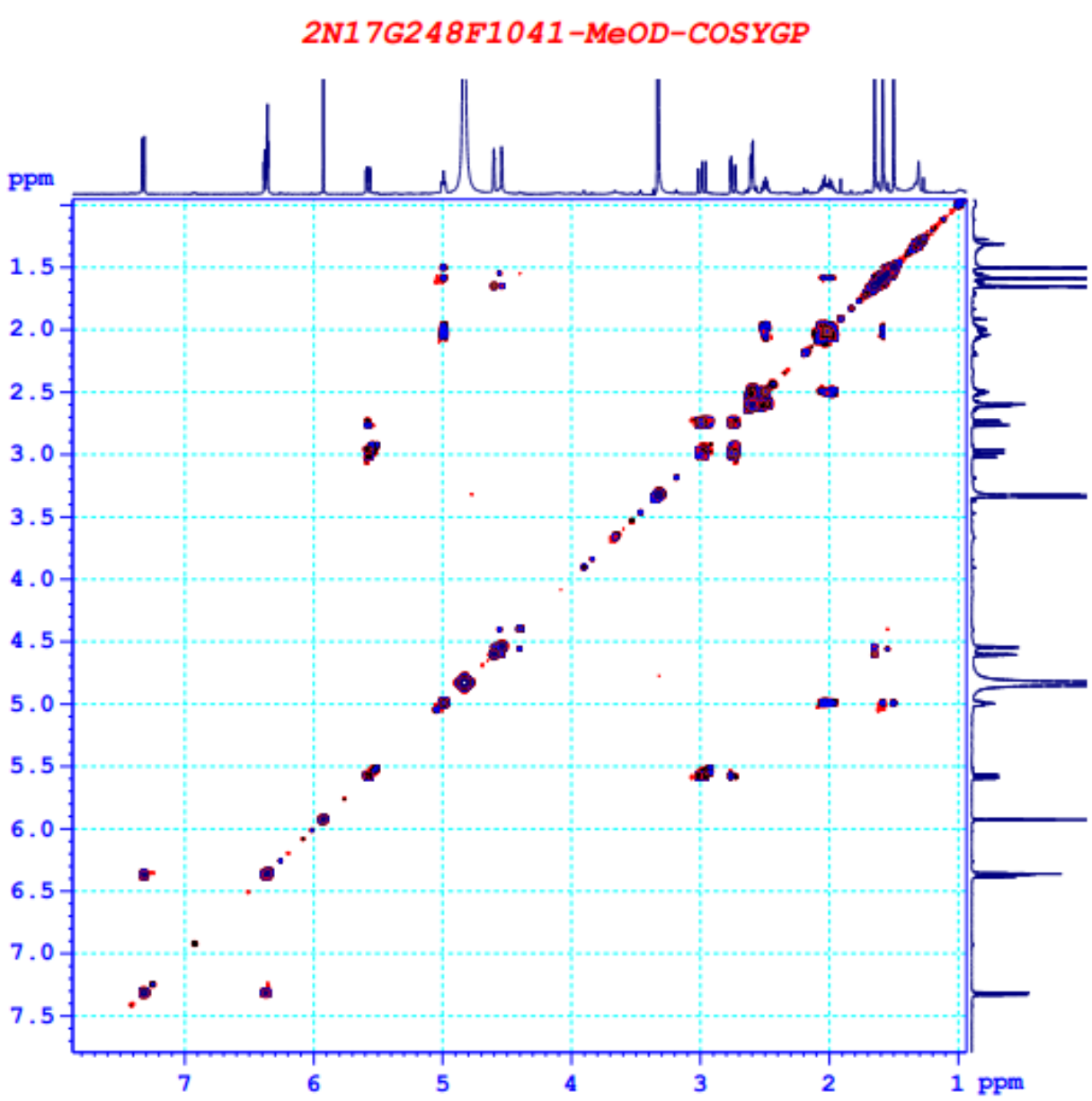
Figure 19S. ^{13}C NMR spectrum of **2** (125 MHz, CD_3OD)



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PROCNO                     1

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PULPROG       cosygpppqf
TD                    2048
SOLVENT               MeOD
NS                       4
DS                       8
SWH               3875.969 Hz
FIDRES            1.892563 Hz
AQ                0.2641920 sec
RG                   64.21
DW                 129.000 usec
DE                   6.50 usec
TE                  303.0 K
D0                0.00000300 sec
D1                1.88899803 sec
D11               0.03000000 sec
D12               0.00002000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00025800 sec

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NUC1                     1H
P0                   10.00 usec
P1                   10.00 usec
P17                2500.00 usec
PLW1          22.00000000 W
PLW10          3.25440001 W

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GPZ1                 10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
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SFO1               500.202 MHz
FIDRES           60.562016 Hz
SW                 7.749 ppm
FnMODE                  QF

F2 - Processing parameters
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WDW                 QSINE
SSB          0
LB           0 Hz
GB           0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF             500.2000027 MHz
WDW                 QSINE
SSB          0
LB           0 Hz
GB           0
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Figure 20S. ^{1}H-^{1}H COSY spectrum of **2** (500 MHz, CD_3OD)

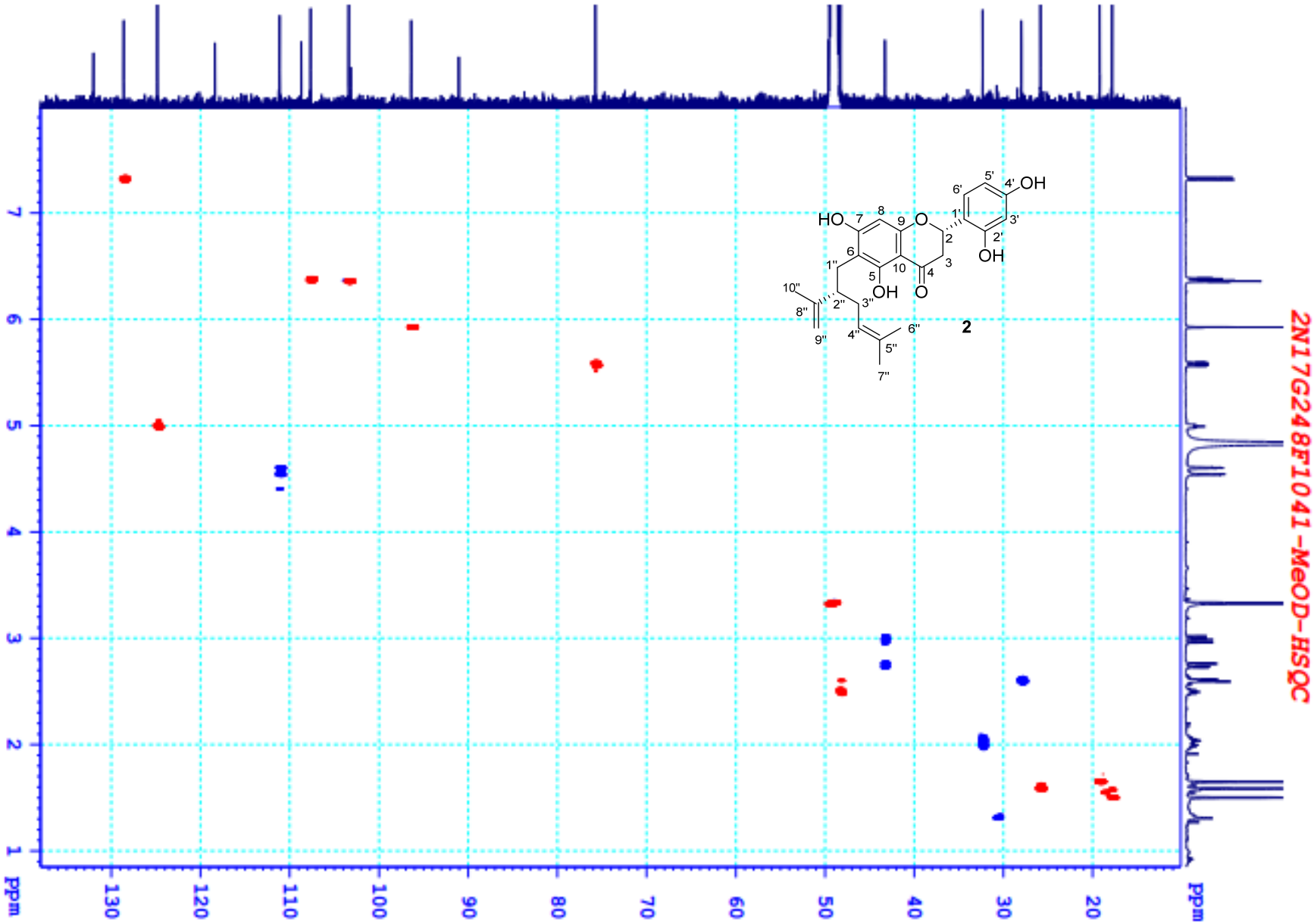


Figure 21S. HSQC spectrum of **2** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)

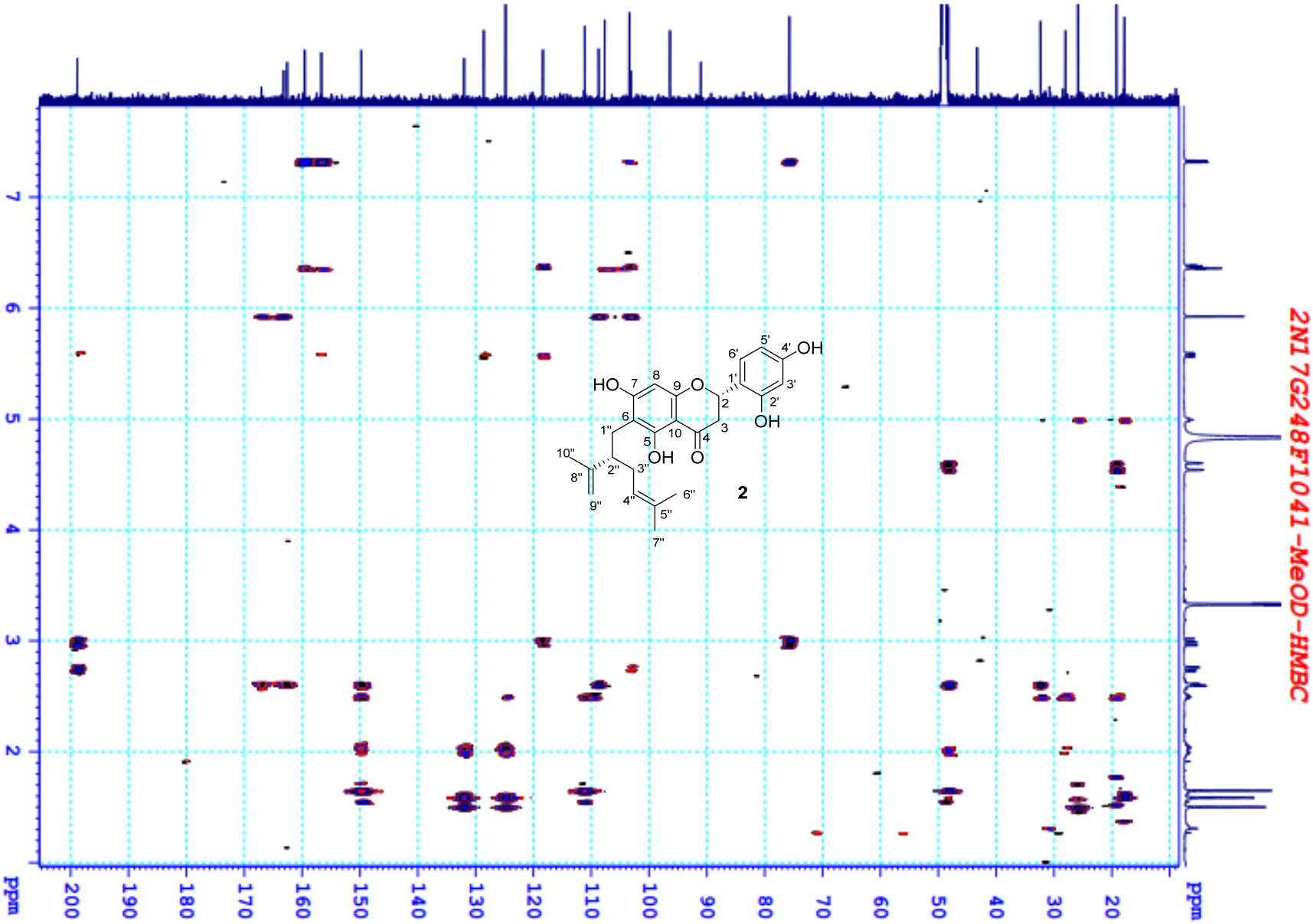


Figure 22S. HMBC spectrum of **2** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)

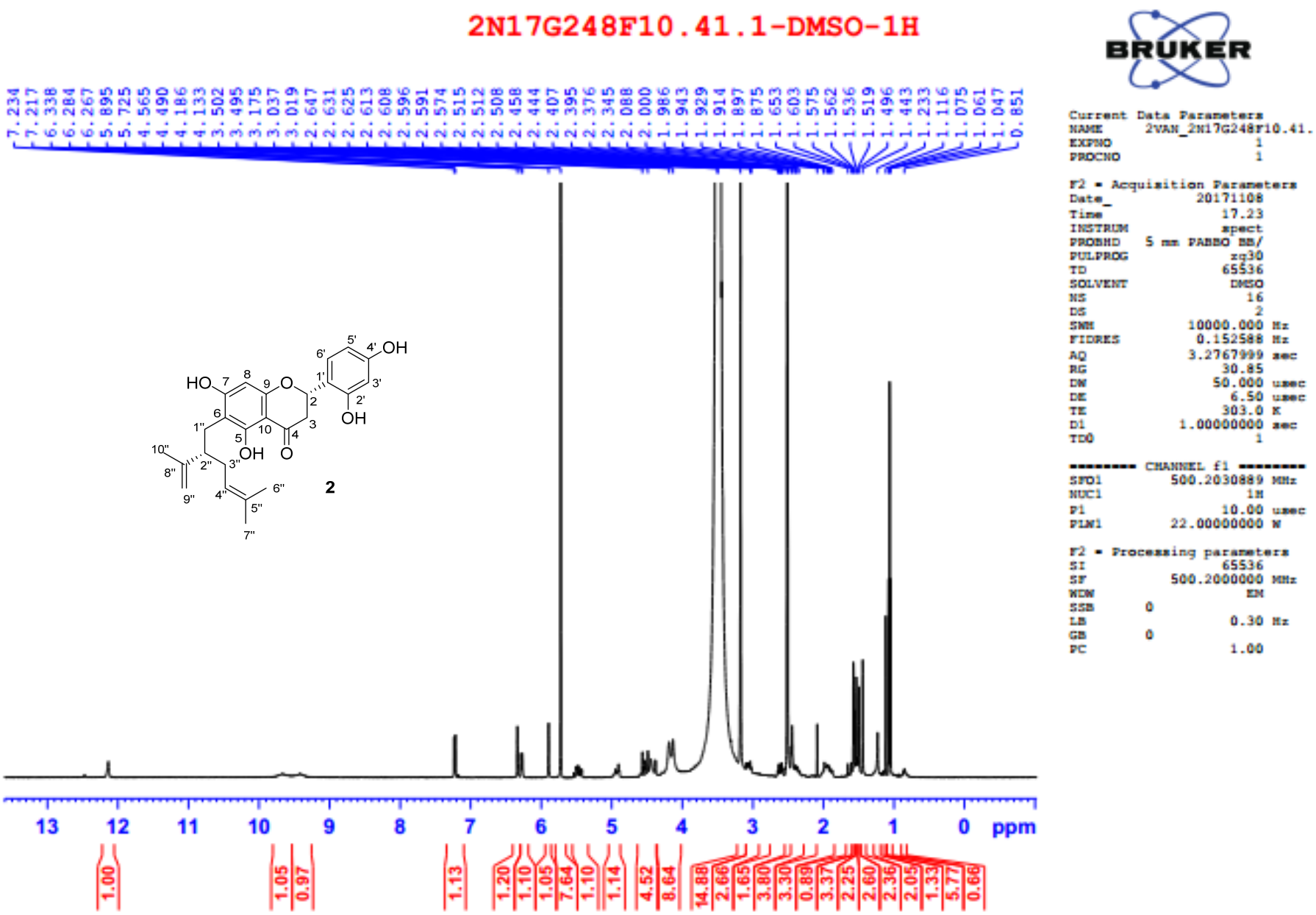


Figure 23S. ^{1}H NMR spectrum of **2** (500 MHz, DMSO-d_6)

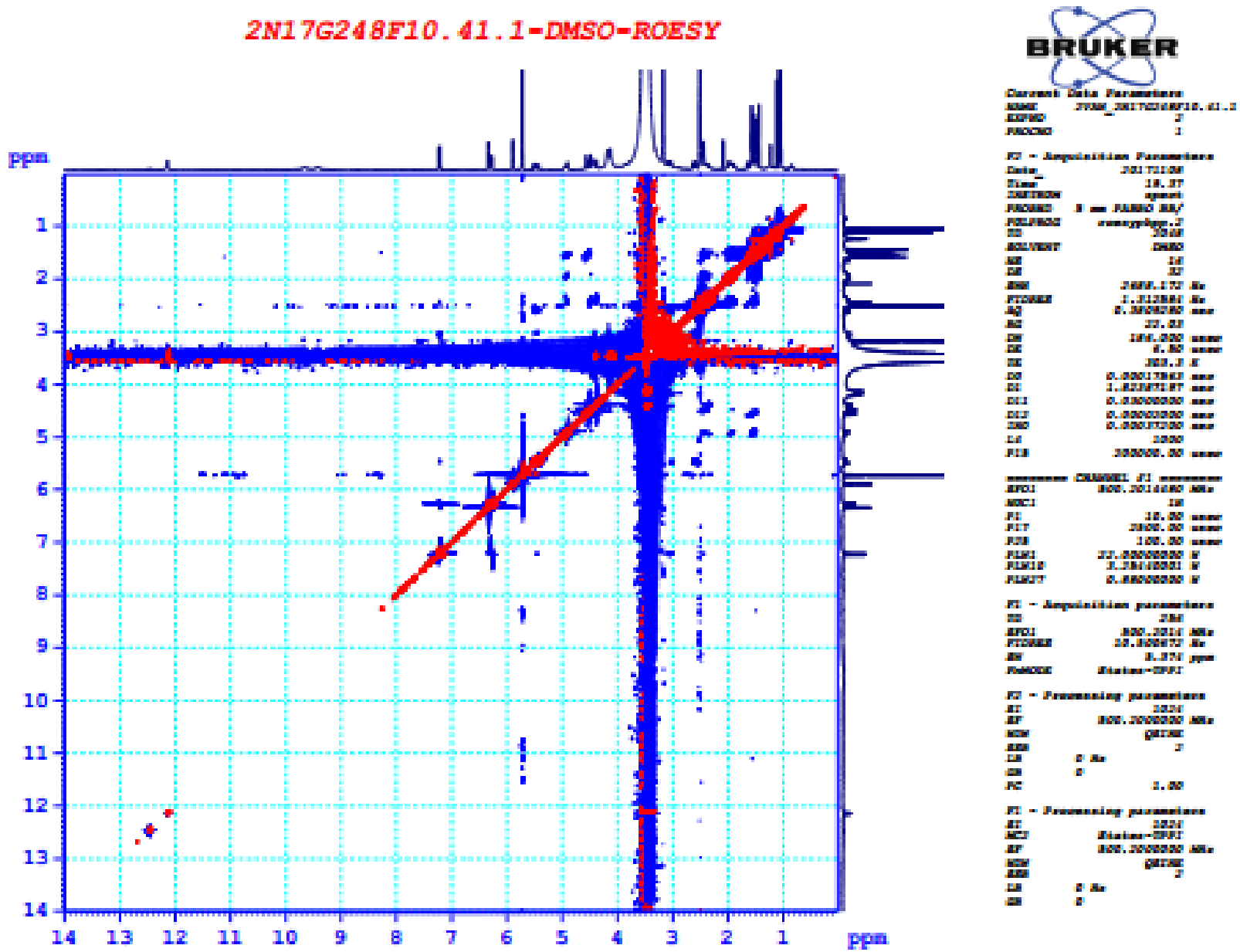


Figure 24S. ROESY spectrum of **2** (500 MHz, DMSO-d_6)

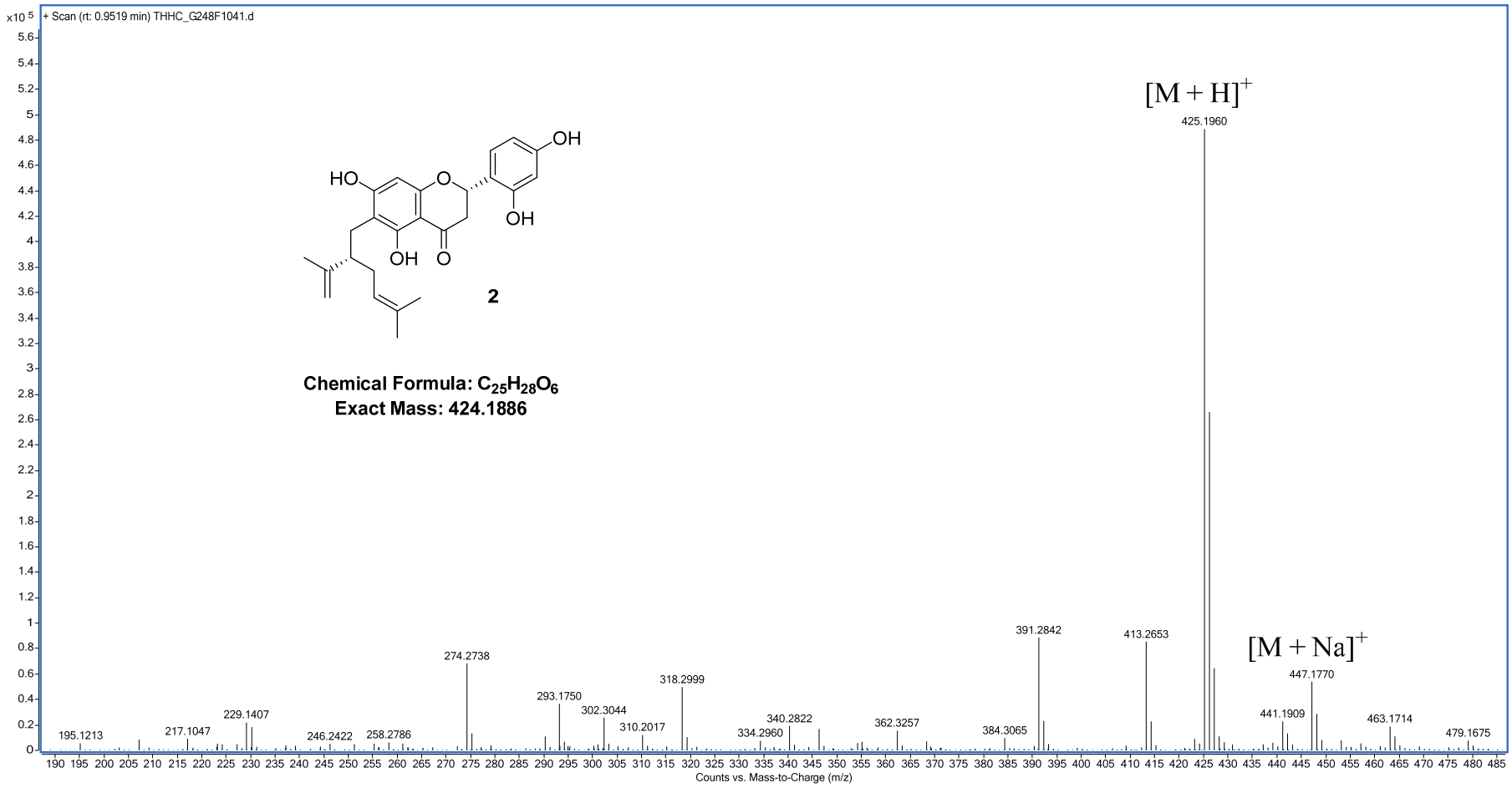


Figure 25S. HR-ESI-MS of **2**

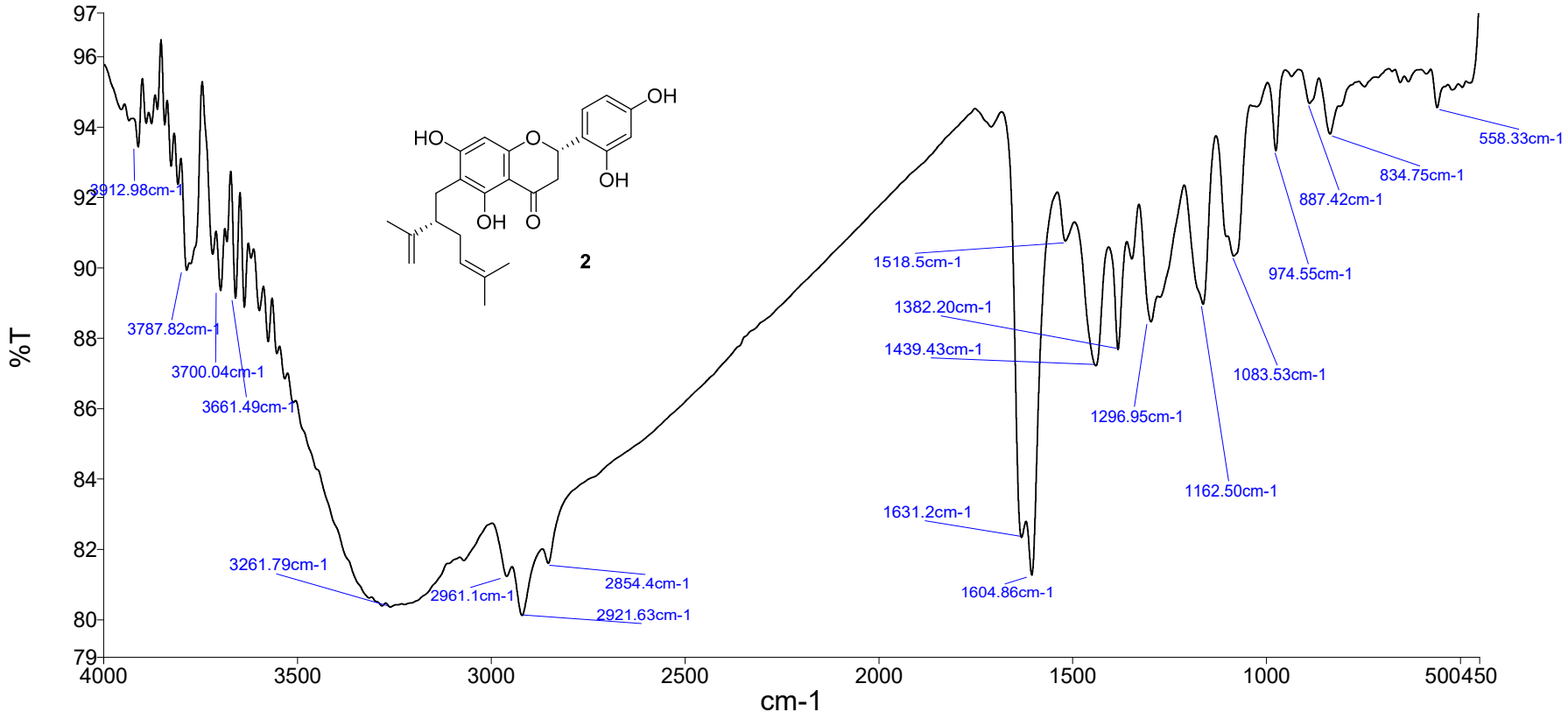


Figure 26S. IR spectrum of **2**

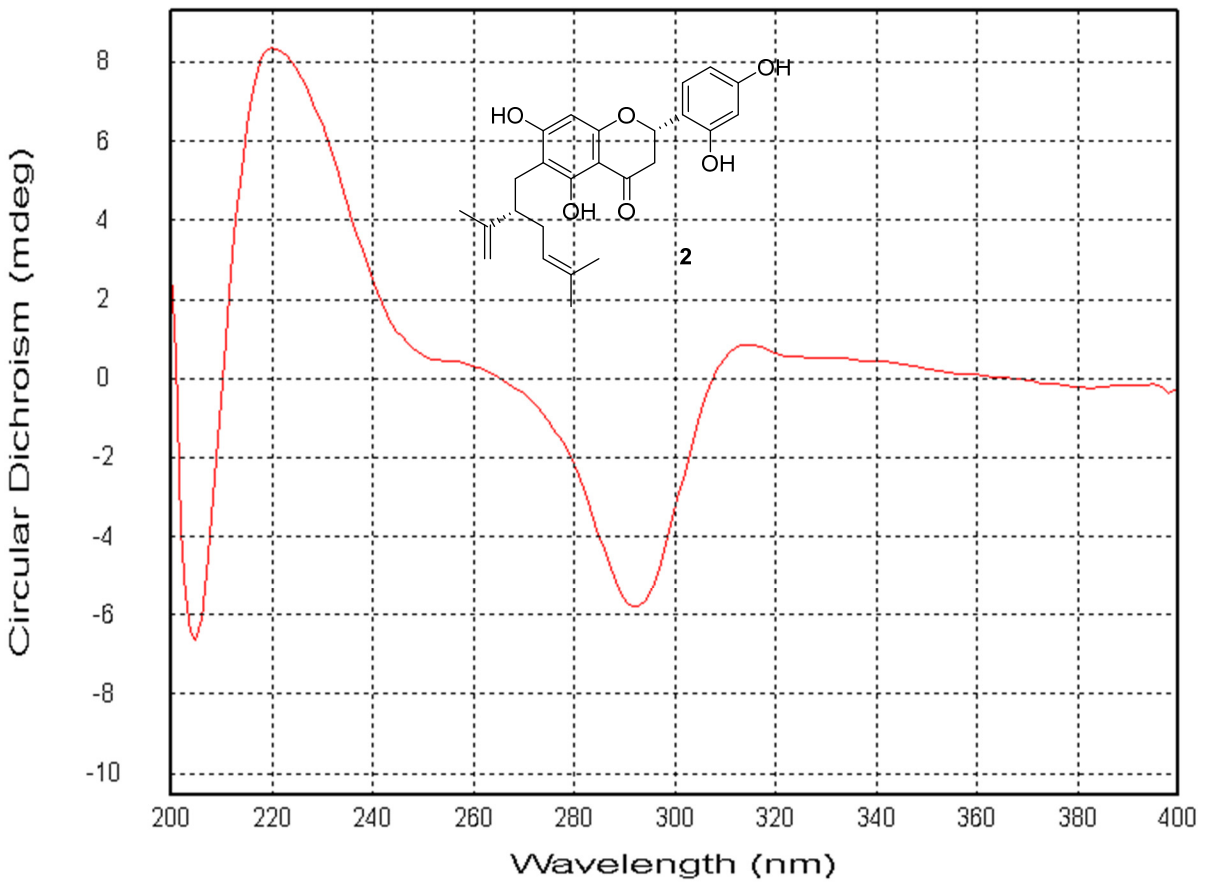
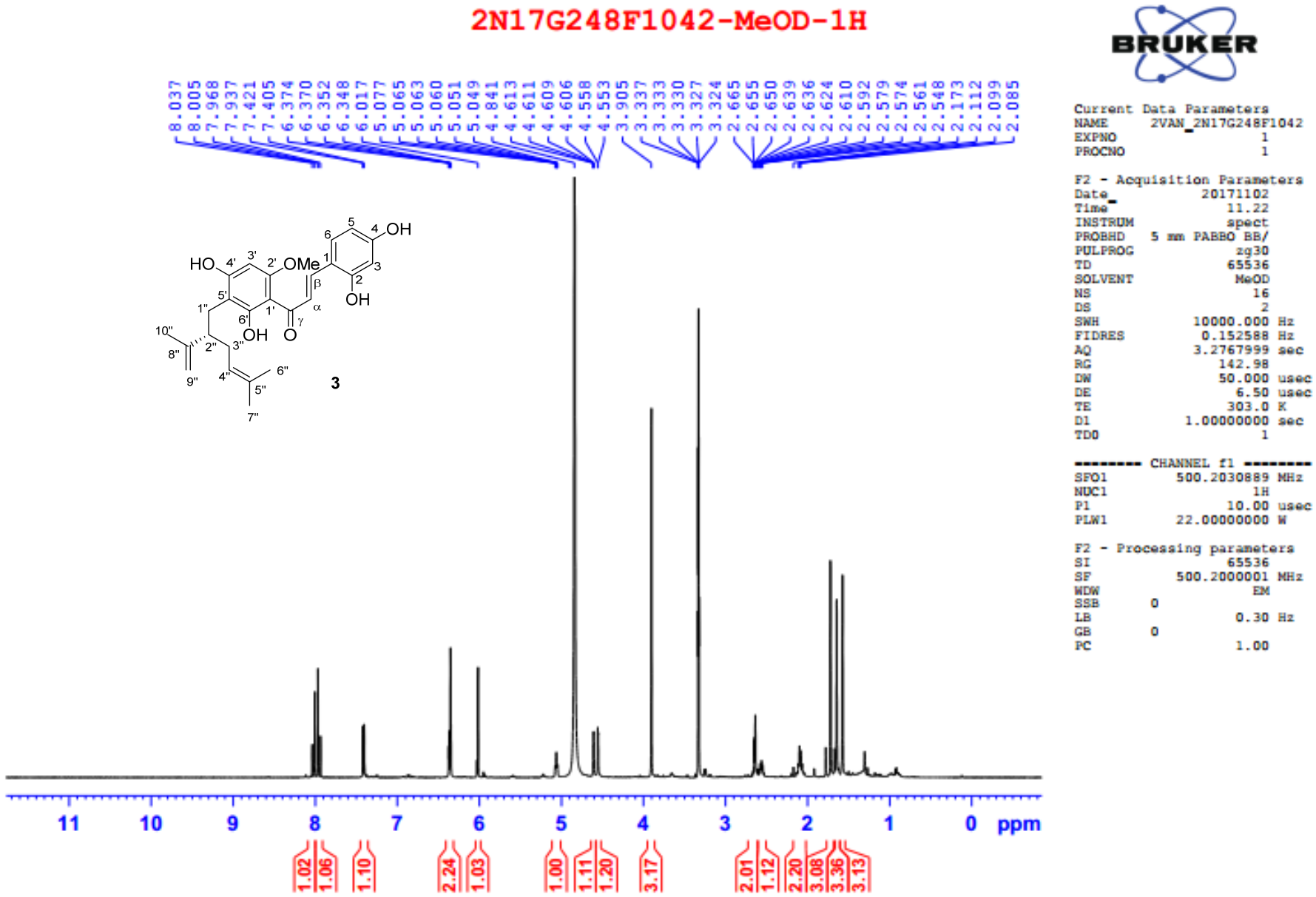


Figure 27S. CD spectrum of **2**



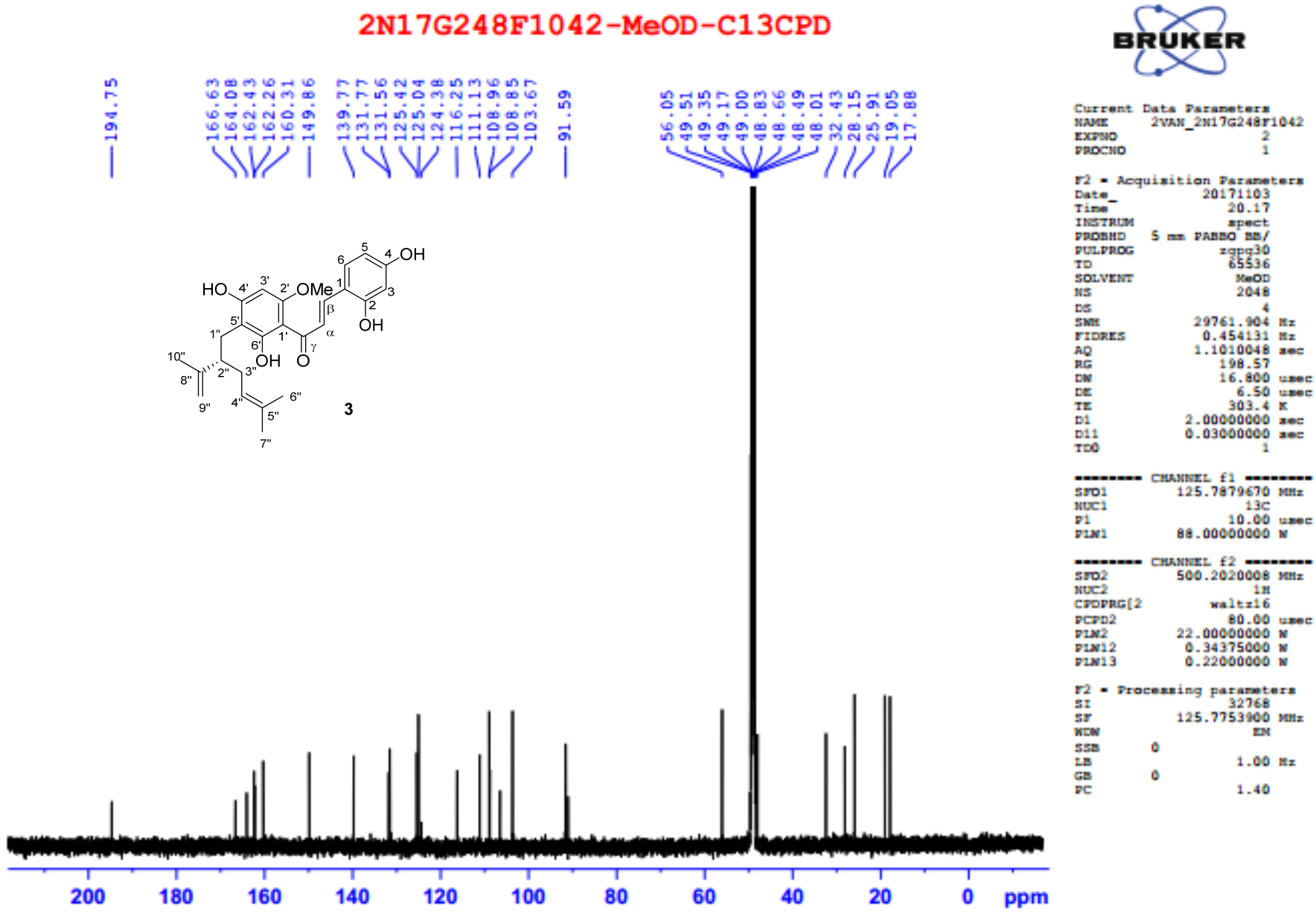

```
Current Data Parameters
NAME      2VAN_2N17G248F1042
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171102
Time                  11.22
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                MeOD
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES            0.152588 Hz
AQ                3.2767999 sec
RG                   142.98
DW                   50.000 usec
DE                    6.50 usec
TE                   303.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           500.2030889 MHz
NUC1                     1H
P1                    10.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
SI                    65536
SF               500.2000001 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

Figure 28S. ^{1}H NMR spectrum of **3** (500 MHz, CD_3OD)




```
Current Data Parameters
NAME      2VAN_2N17G248F1042
EXPNO                      2
PROCNO                     1

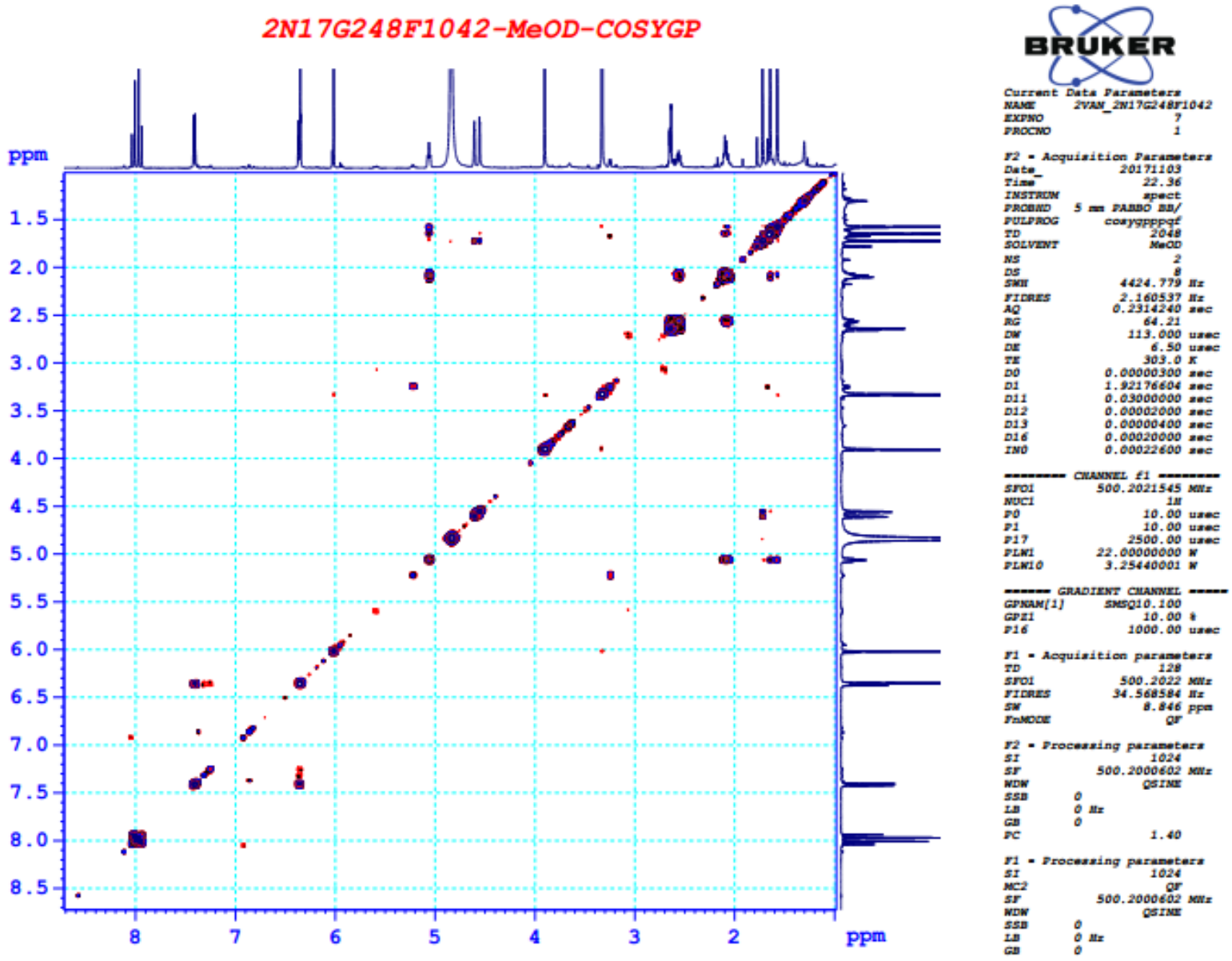
F2 - Acquisition Parameters
Date_               20171103
Time                   20.17
INSTRUM                apect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                MeOD
NS                     2048
DS                        4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                   198.57
DW                  16.800 usec
DE                   6.50 usec
TE                  303.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           125.7879670 MHz
NUC1                    13C
P1                   10.00 usec
PLW1          88.00000000 W

======== CHANNEL f2 ========
SFO2           500.2020008 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2          22.00000000 W
PLW12          0.34375000 W
PLW13          0.22000000 W

F2 - Processing parameters
SI                     32768
SF           125.7753900 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

Figure 29S. ^{13}C NMR spectrum of **3** (125 MHz, CD_3OD)



BRUKER

```
Current Data Parameters
NAME      2VAN_2N17G248F1042
EXPNO                      7
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171103
Time                  22.36
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG        cosygpppqf
TD                     2048
SOLVENT                MeOD
NS                        2
DS                        8
SWH               4424.779 Hz
FIDRES            2.160537 Hz
AQ                0.2314240 sec
RG                   64.21
DW                 113.000 usec
DE                    6.50 usec
TE                   303.0 K
D0                0.00000300 sec
D1                1.92176604 sec
D11               0.03000000 sec
D12               0.00002000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00022600 sec

======== CHANNEL f1 ========
SFO1           500.2021545 MHz
NUC1                     1H
P0                    10.00 usec
P1                    10.00 usec
P17                 2500.00 usec
PLW1          22.00000000 W
PLW10          3.25440001 W

====== GRADIENT CHANNEL =====
GPNAM[1]        SMSQ10.100
GPZ1                 10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                      128
SFO1             500.2022 MHz
FIDRES           34.568584 Hz
SW                8.846 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF            500.2000602 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                     QF
SF            500.2000602 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
```

Figure 30S. ^{1}H-^{1}H COSY spectrum of **3** (500 MHz, CD_3OD)

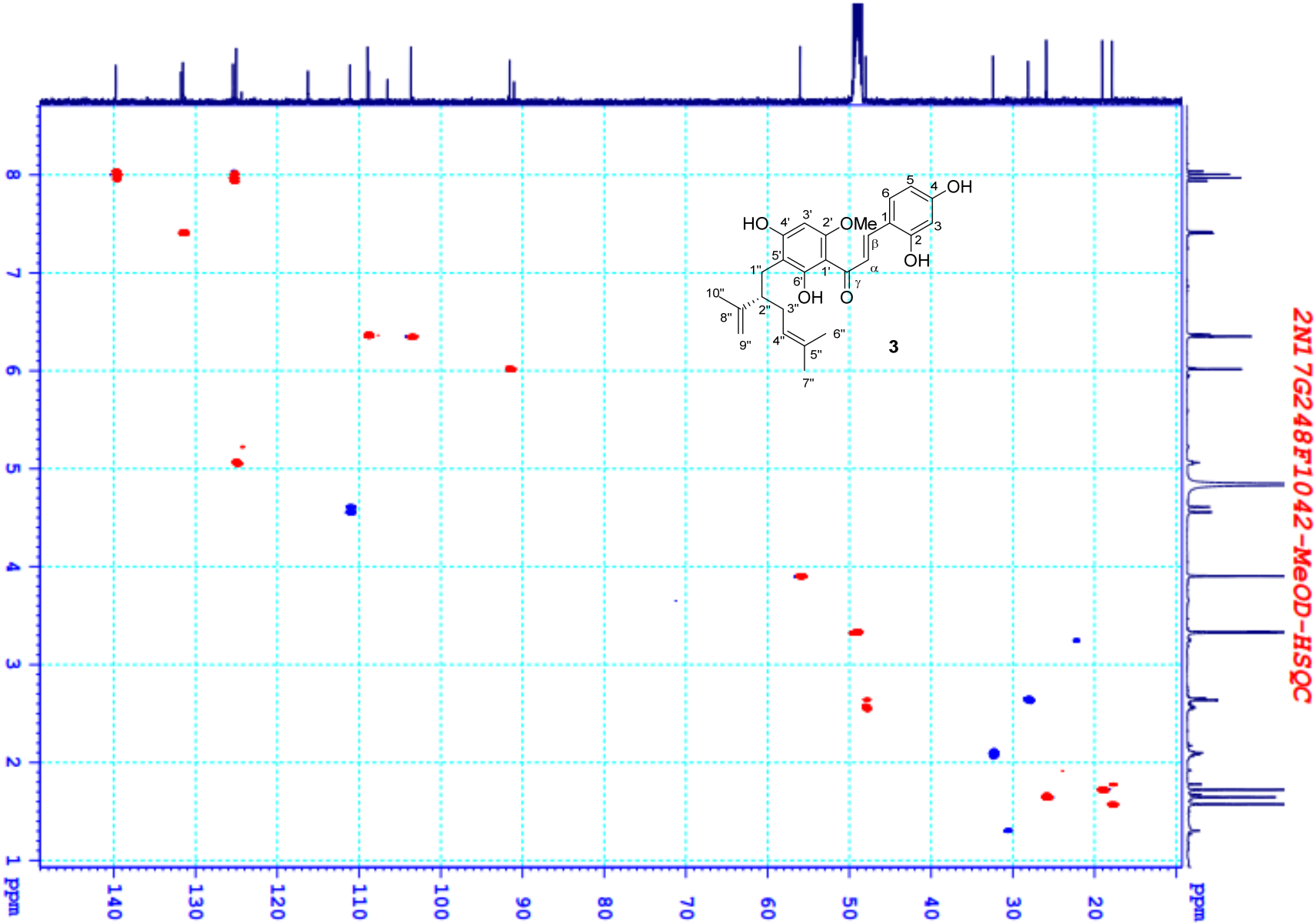


Figure 31S. HSQC spectrum of **3** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)

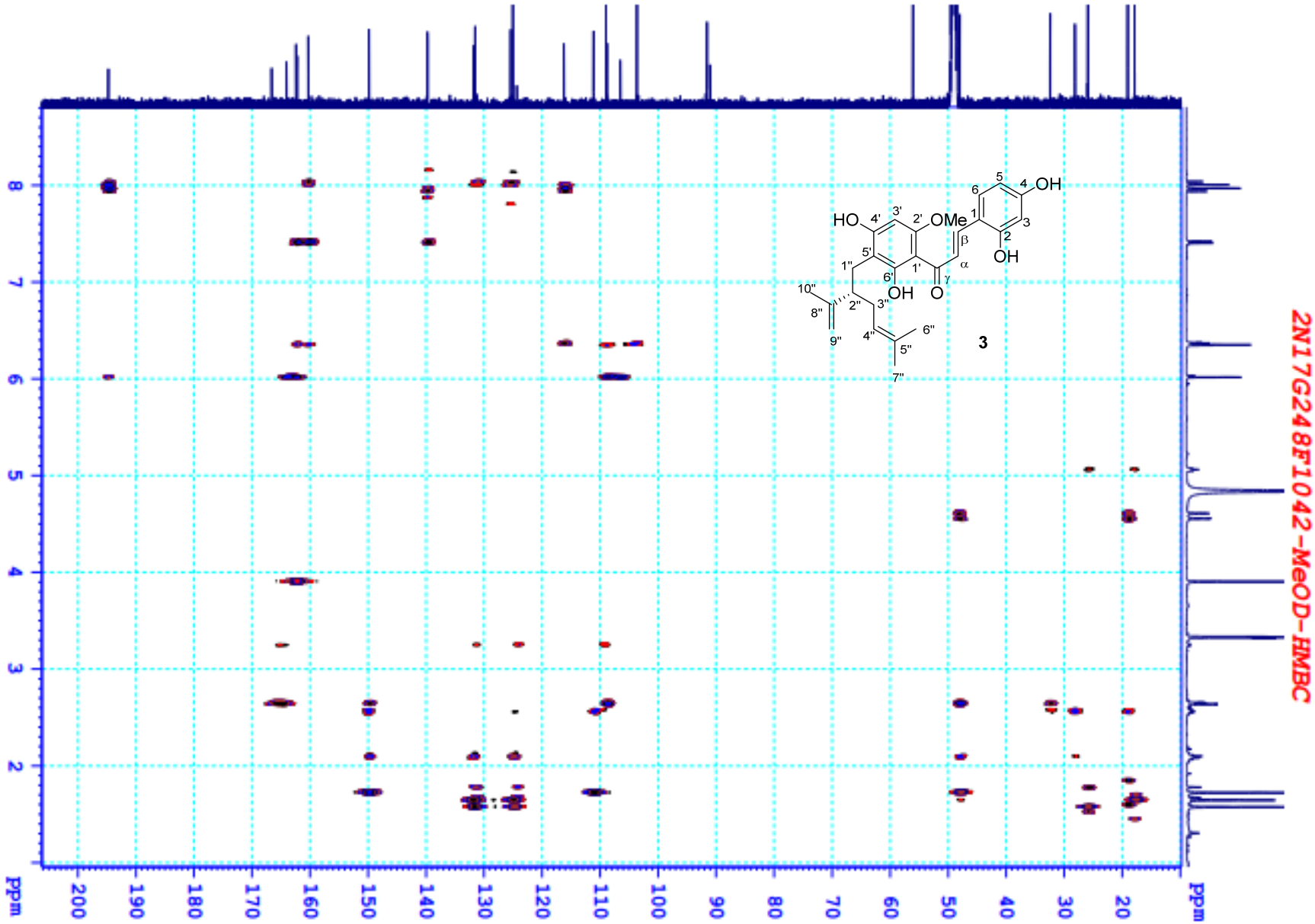


Figure 32S. HMBC spectrum of **3** (^{1}H: 500 MHz, ^{13}C: 125 MHz, CD_3OD)

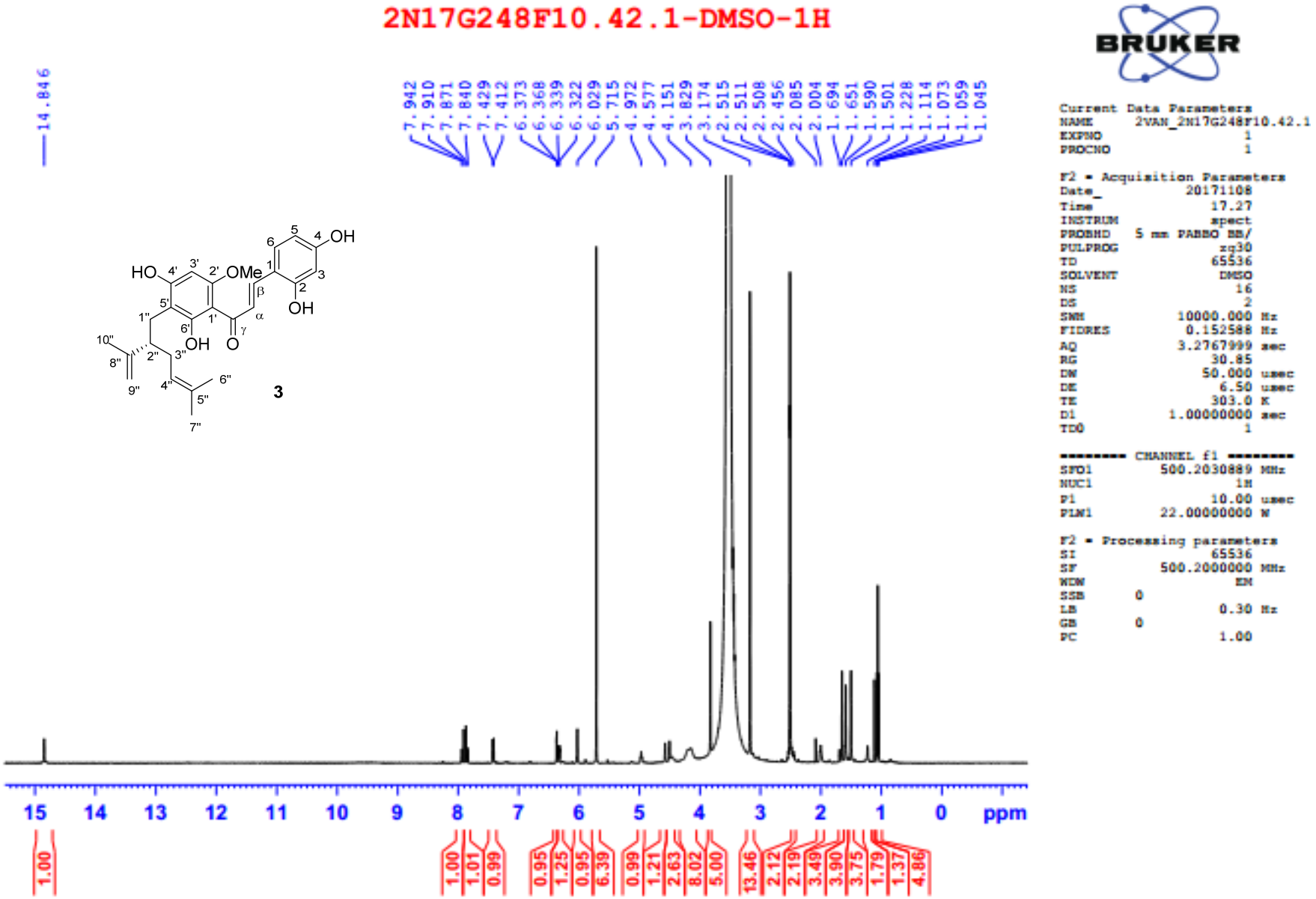
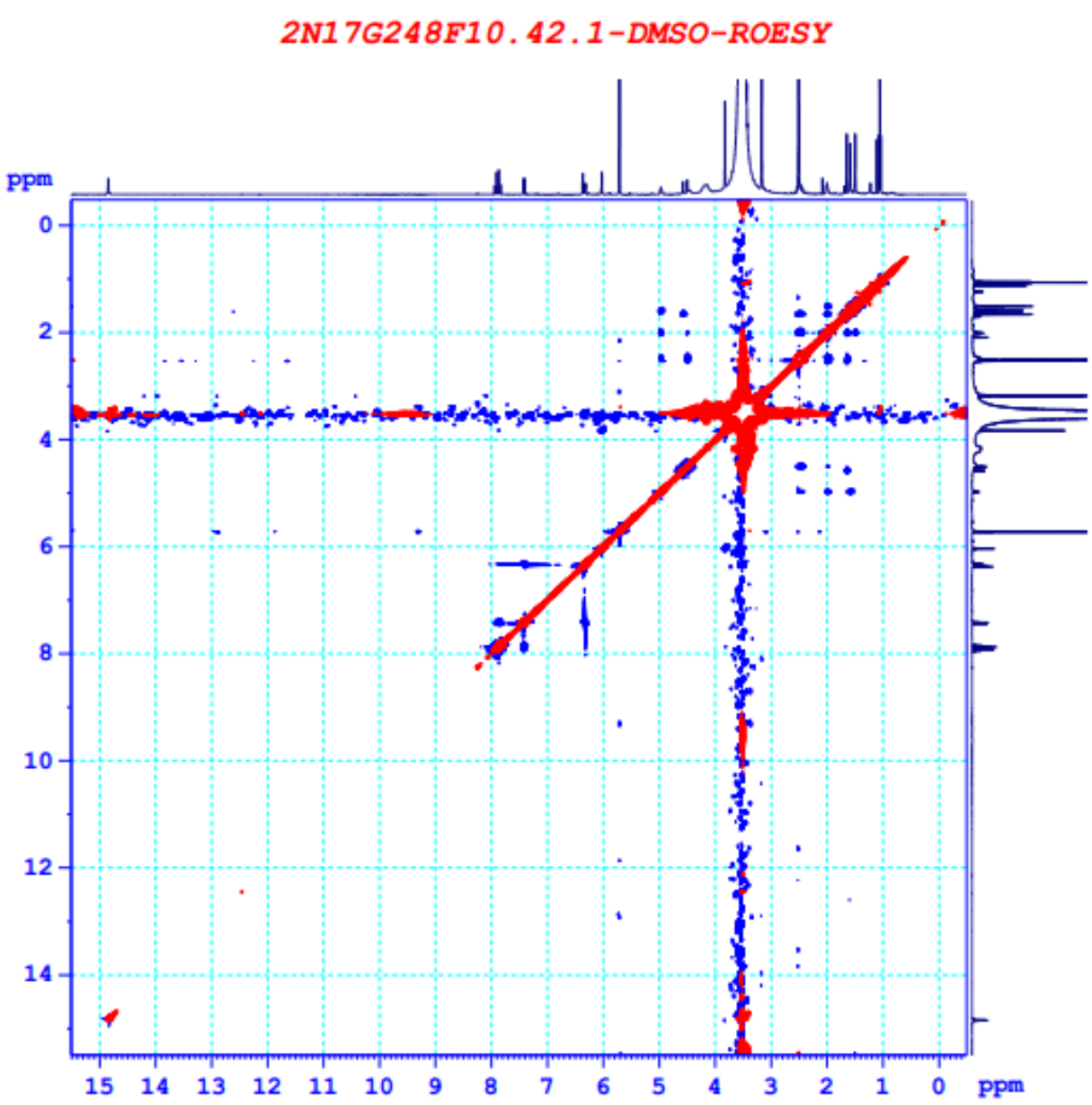


Figure 33S. ^{1}H-NMR spectrum of **3** (500 MHz, DMSO-d_6)



BRUKER

```
Current Data Parameters
NAME        2VAN_2N17G248F10.42.1
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20171109
Time                       16.17
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG          roesyphpp.2
TD                         2048
SOLVENT                    DMSO
NS                           16
DS                           32
SWH                    8012.820 Hz
FIDRES                 3.912510 Hz
AQ                     0.1277952 sec
RG                         17.93
DW                        62.400 usec
DE                         6.50 usec
TE                        303.9 K
D0                     0.00005213 sec
D1                     1.85663998 sec
D11                    0.03000000 sec
D12                    0.00002000 sec
IN0                    0.00012500 sec
L4                           1000
P15                    200000.00 usec

======== CHANNEL f1 ========
SFO1                 500.2037515 MHz
NUC1                         1H
P1                        10.00 usec
P17                     2500.00 usec
P25                      100.00 usec
PLW1                22.00000000 W
PLW10                3.25440001 W
PLW27                0.88000000 W

F1 - Acquisition parameters
TD                           256
SFO1                 500.2038 MHz
FIDRES                62.500000 Hz
SW                       15.993 ppm
FnMODE               States-TPPI

F2 - Processing parameters
SI                          1024
SF                   500.2000000 MHz
WDW                        QSINE
SSB                            2
LB          0 Hz
GB          0
PC                          1.00

F1 - Processing parameters
SI                          1024
MC2                  States-TPPI
SF                   500.2000000 MHz
WDW                        QSINE
SSB                            2
LB          0 Hz
GB          0
```

Figure 34S. ROESY spectrum of **3** (500 MHz, DMSO-d_6)

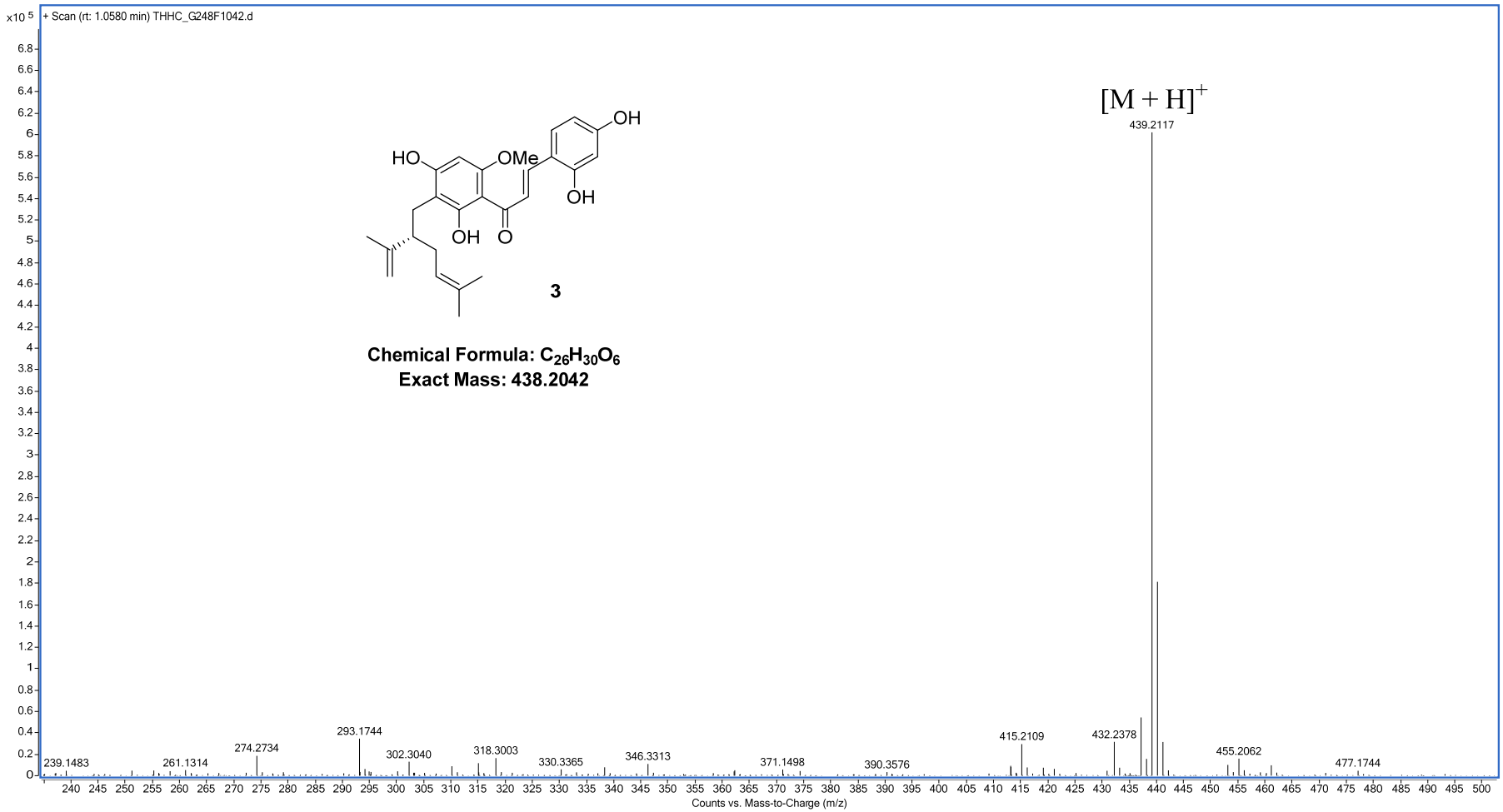


Figure 35S. HR-ESI-MS of **3**

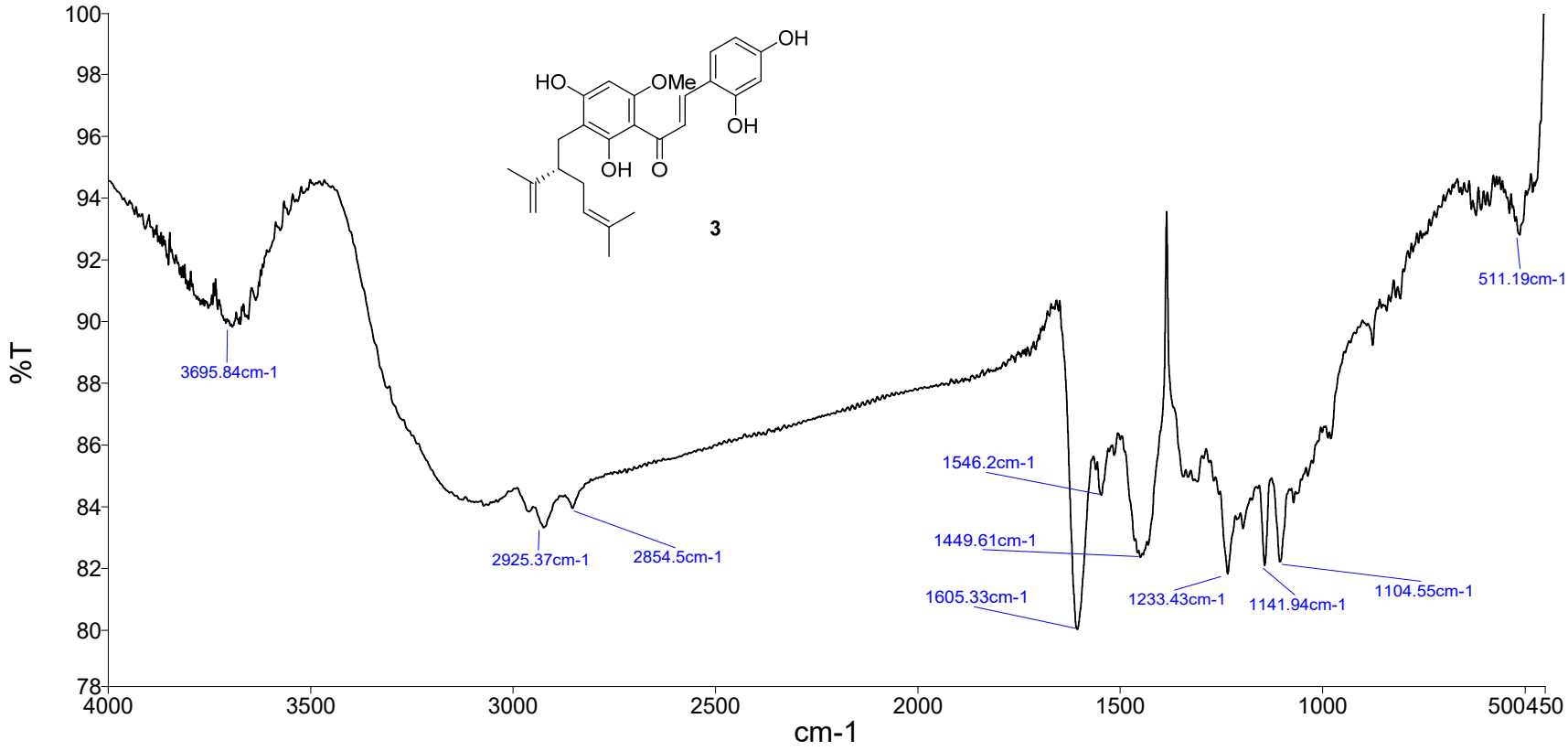


Figure 36S. IR spectrum of **3**

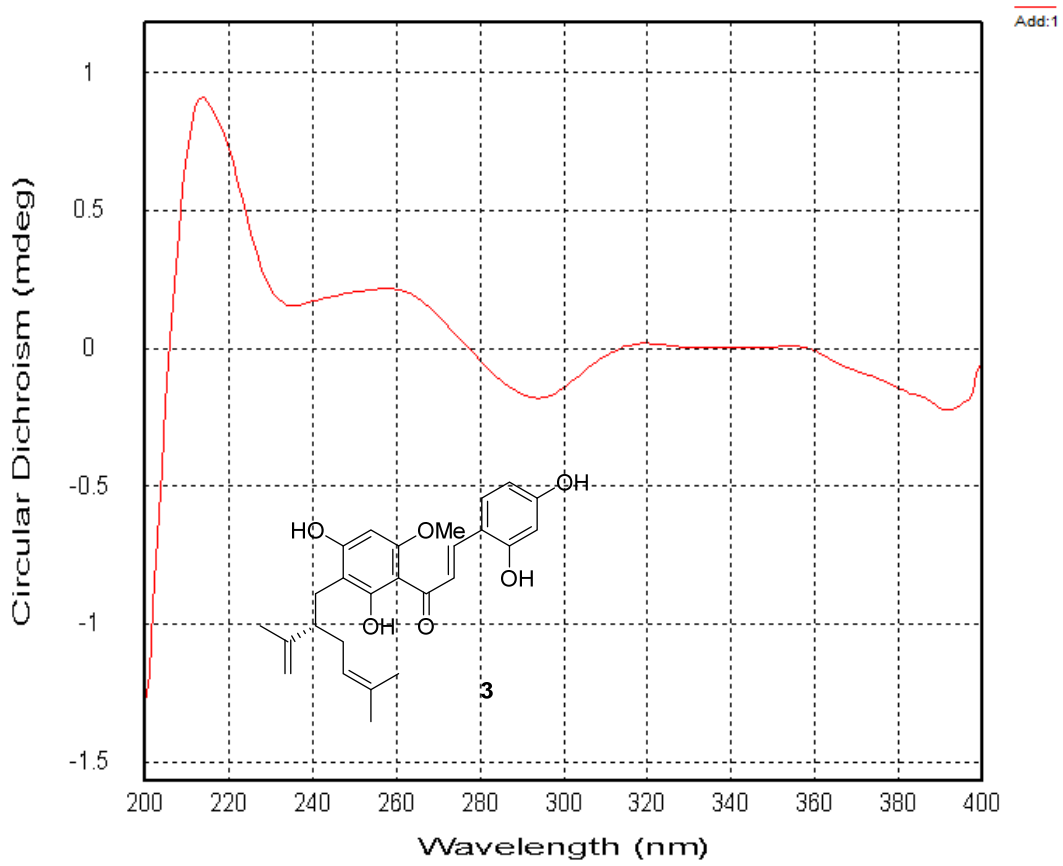


Figure 37S. CD spectrum of **3**