Supporting Information

Chemical Constituents of the Deep-Sea-Derived *Penicillium citrinum* W17 and Their Anti-Inflammatory and Anti-osteoporotic Bioactivities

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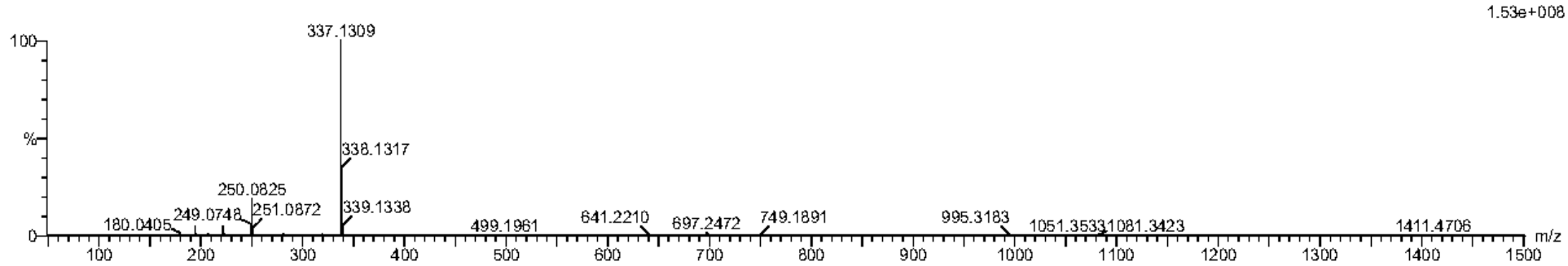
[†] These authors contributed equally to this work.

Content

Elemental Composition Report **Page 1**

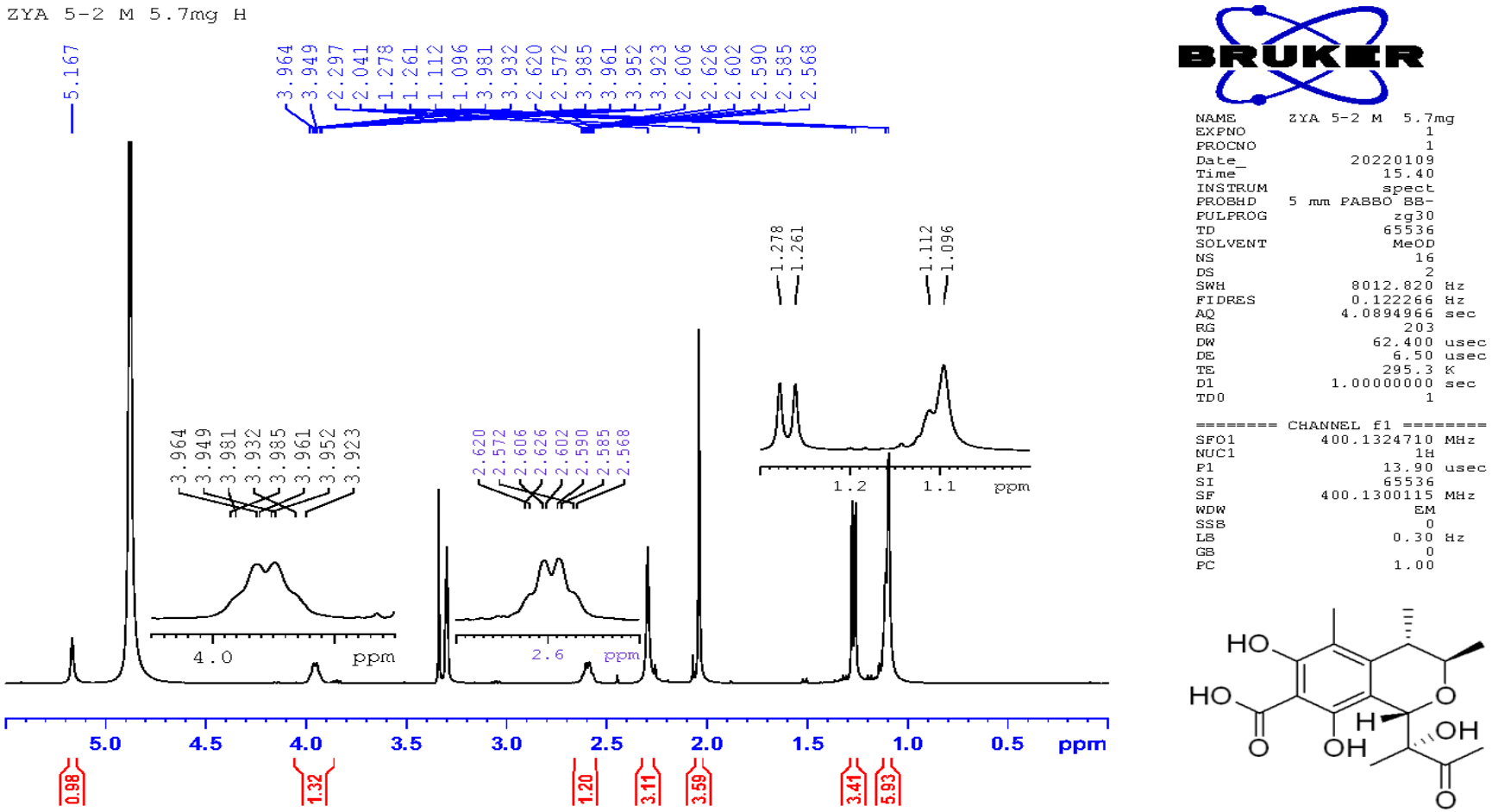
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
105 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-50 O: 0-15 23Na: 0-1
ZYA 5-2-N 86 (0.347) Cm (75:109)
1: TOF MS ES-



Minimum:	80.00				-1.5				
Maximum:	100.00		5.0	10.0	50.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1309	100.00	337.1287	2.2	6.5	7.5	2059.9	0.584	55.77	C17 H21 O7
		337.1263	4.6	13.6	4.5	2060.5	1.170	31.05	C15 H22 O7 23Na
		337.1346	-3.7	-11.0	-1.5	2061.3	2.026	13.18	C10 H25 O12

Figure S1. The HR-ESI-MS of compound **1**.

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PROCNO                     1
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Time                   15.40
INSTRUM                spect
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PULPROG                zg30
TD                    65536
SOLVENT                MeOD
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894966 sec
RG                       203
DW                  62.400 usec
DE                   6.50 usec
TE                  295.3 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                      1H
P1                   13.90 usec
SI                    65536
SF              400.1300115 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```


Figure S2. The ^{1}H NMR spectrum of compound **1** in CD_3OD.

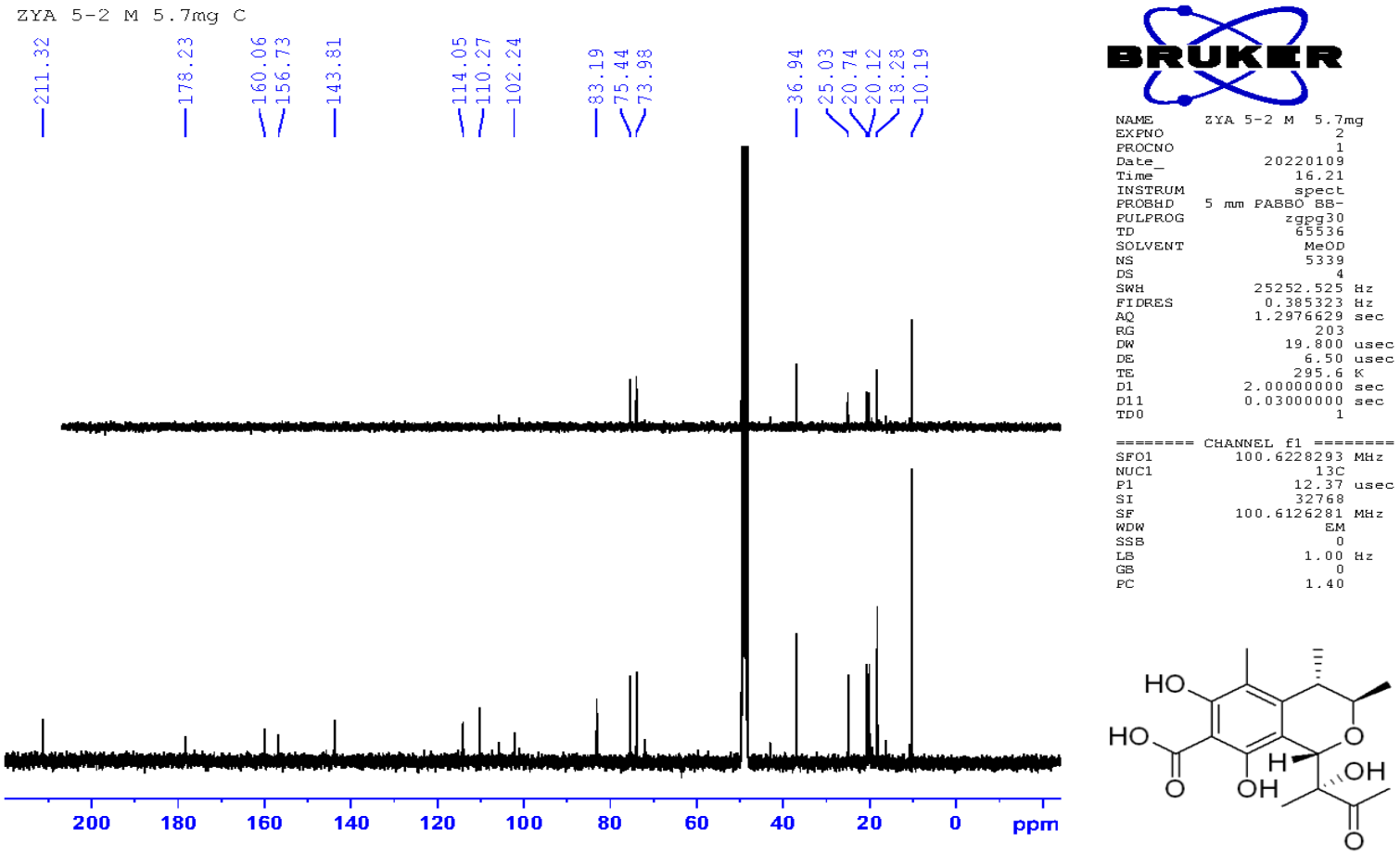


Figure S3. The ^{13}C NMR spectrum of compound **1** in CD_3OD.

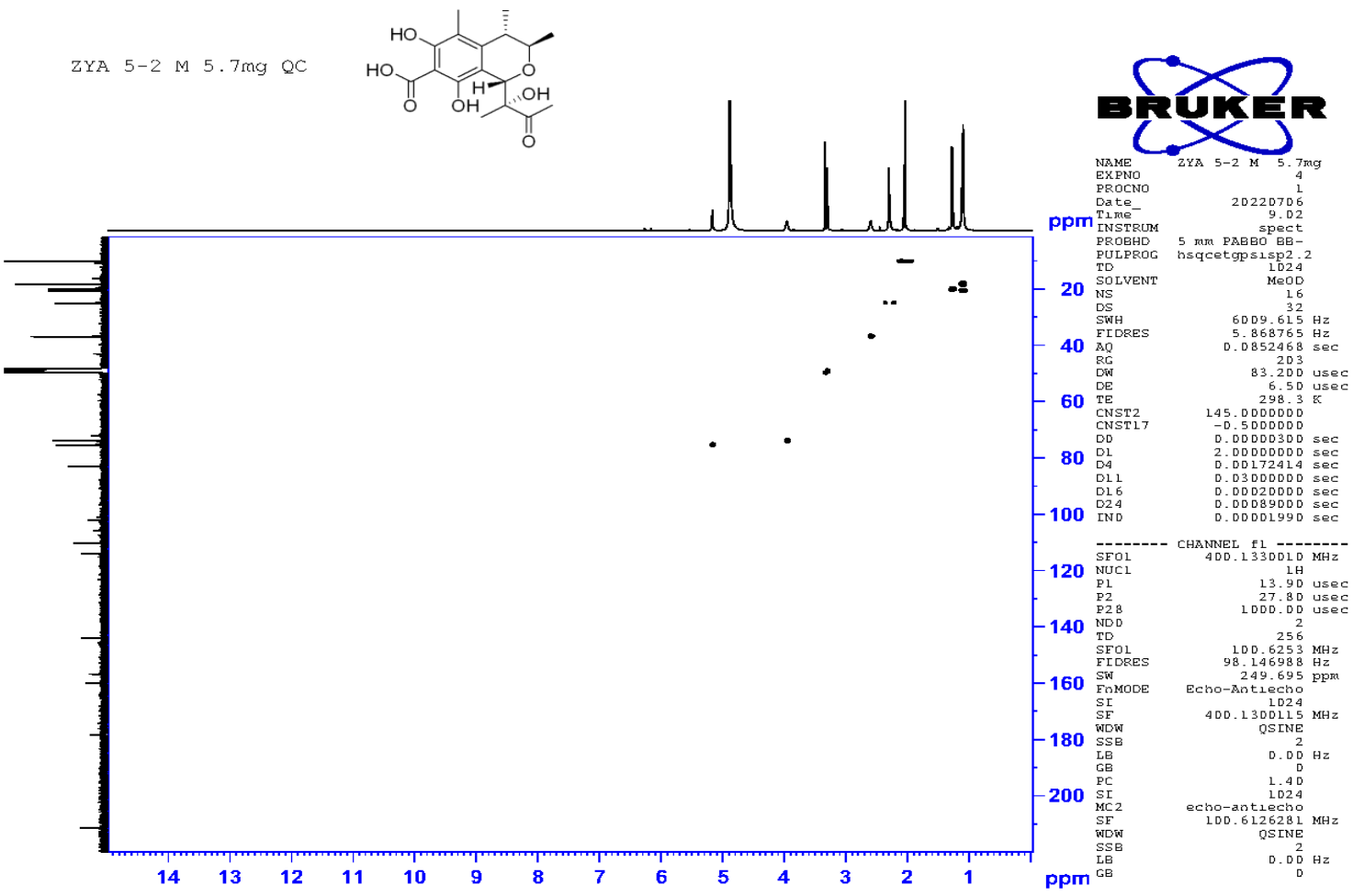


Figure S4. The HSQC spectrum of compound **1** in CD_3OD.

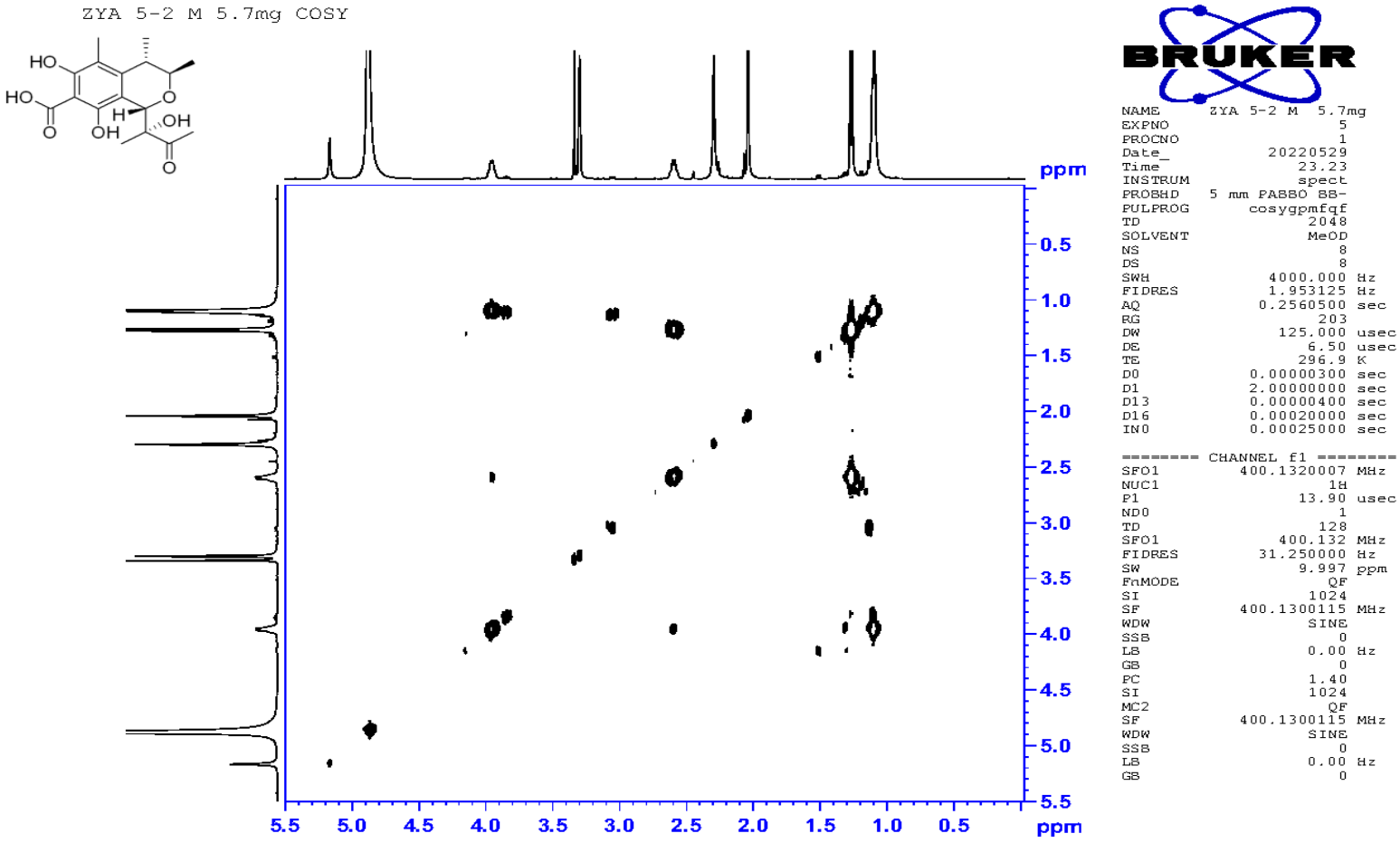


Figure S5. The ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD.

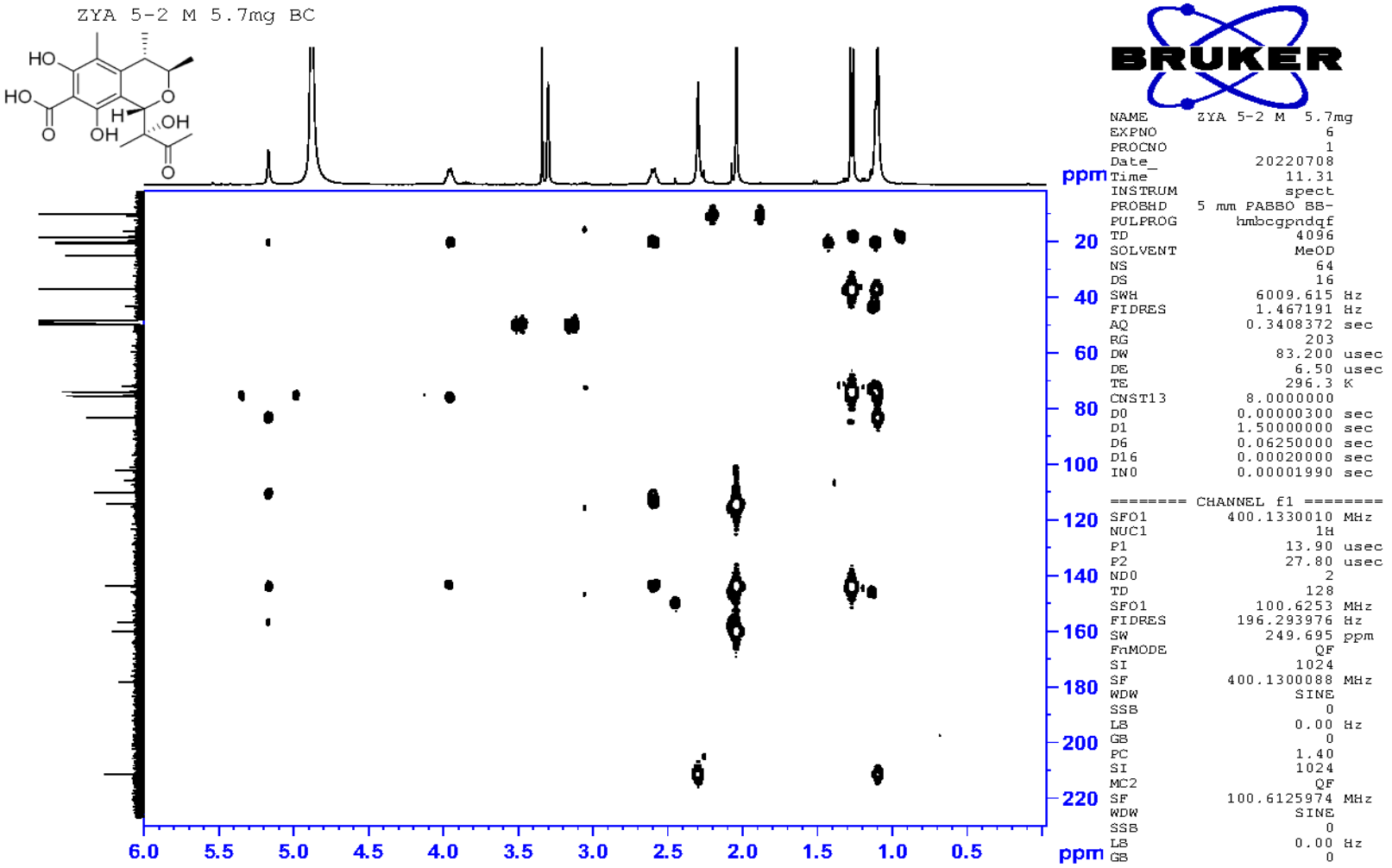


Figure S6. The HMBC spectrum of compound **1** in CD_3OD.

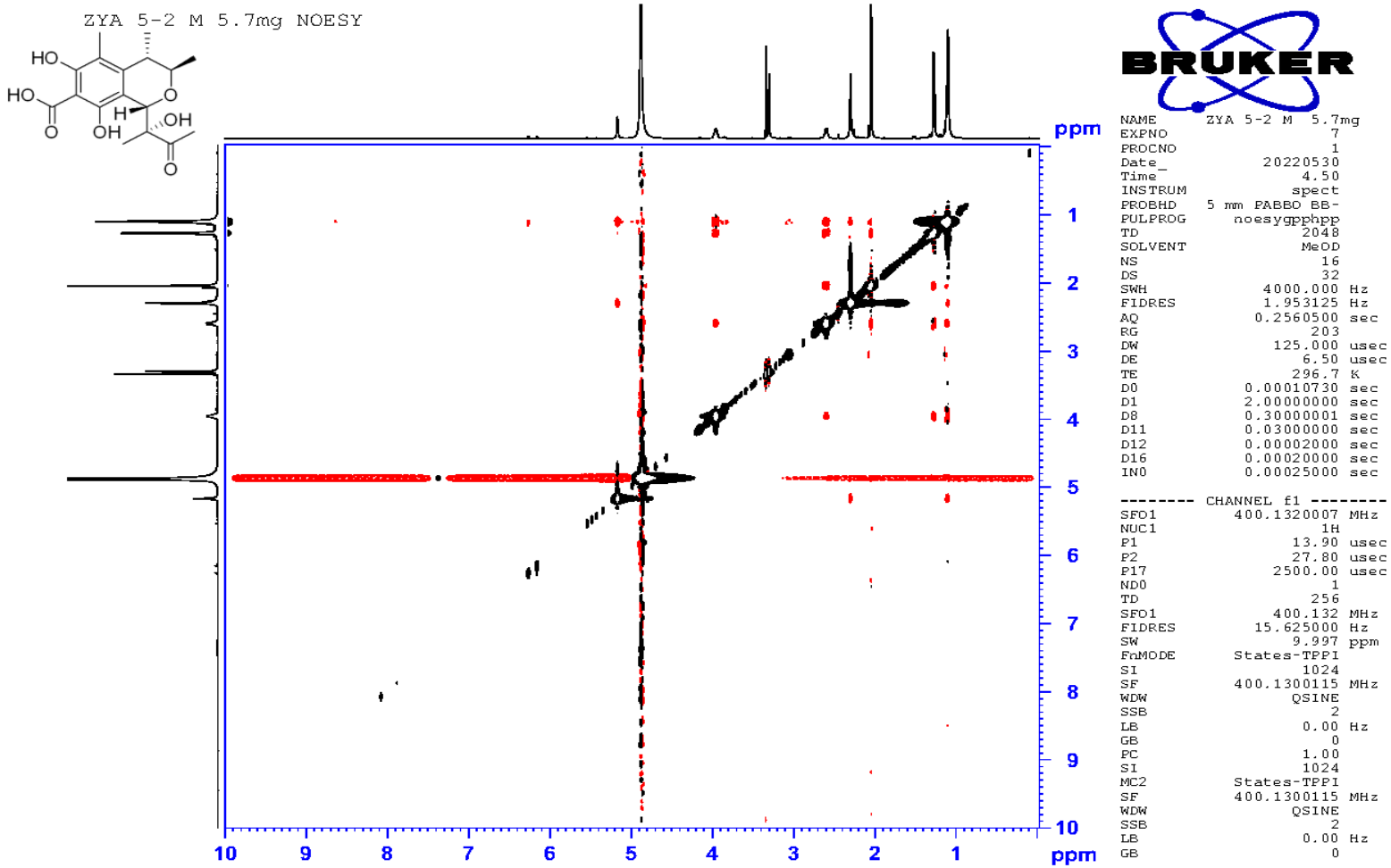
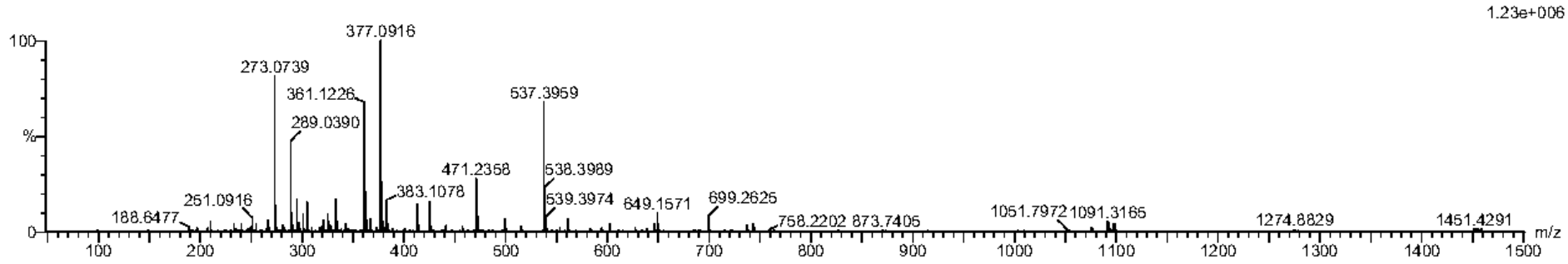


Figure S7. The NOESY spectrum of compound **1** in CD_3OD.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 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
93 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-50 O: 0-15 Na: 0-2
ZYA 8-3 70 (0.290) Cm (69:76)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
361.1226	361.1263	-3.7	-10.2	6.5	1484.8	0.581	55.91	C17 H22 O7 Na
	361.1239	-1.3	-3.6	3.5	1485.0	0.819	44.09	C15 H23 O7 Na2

Figure S8. The HR-ESI-MS of compound **2**.

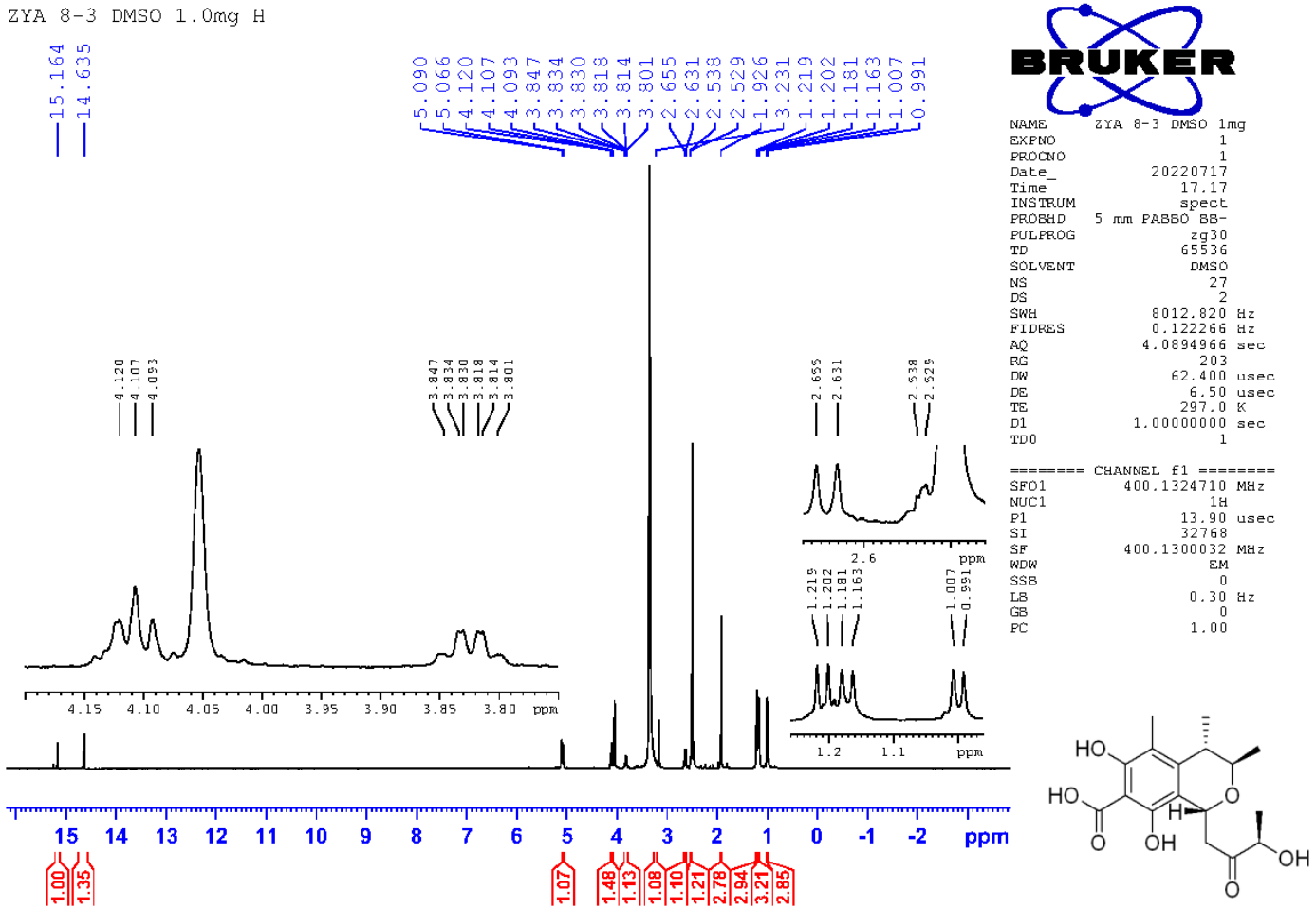


Figure S9. The ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

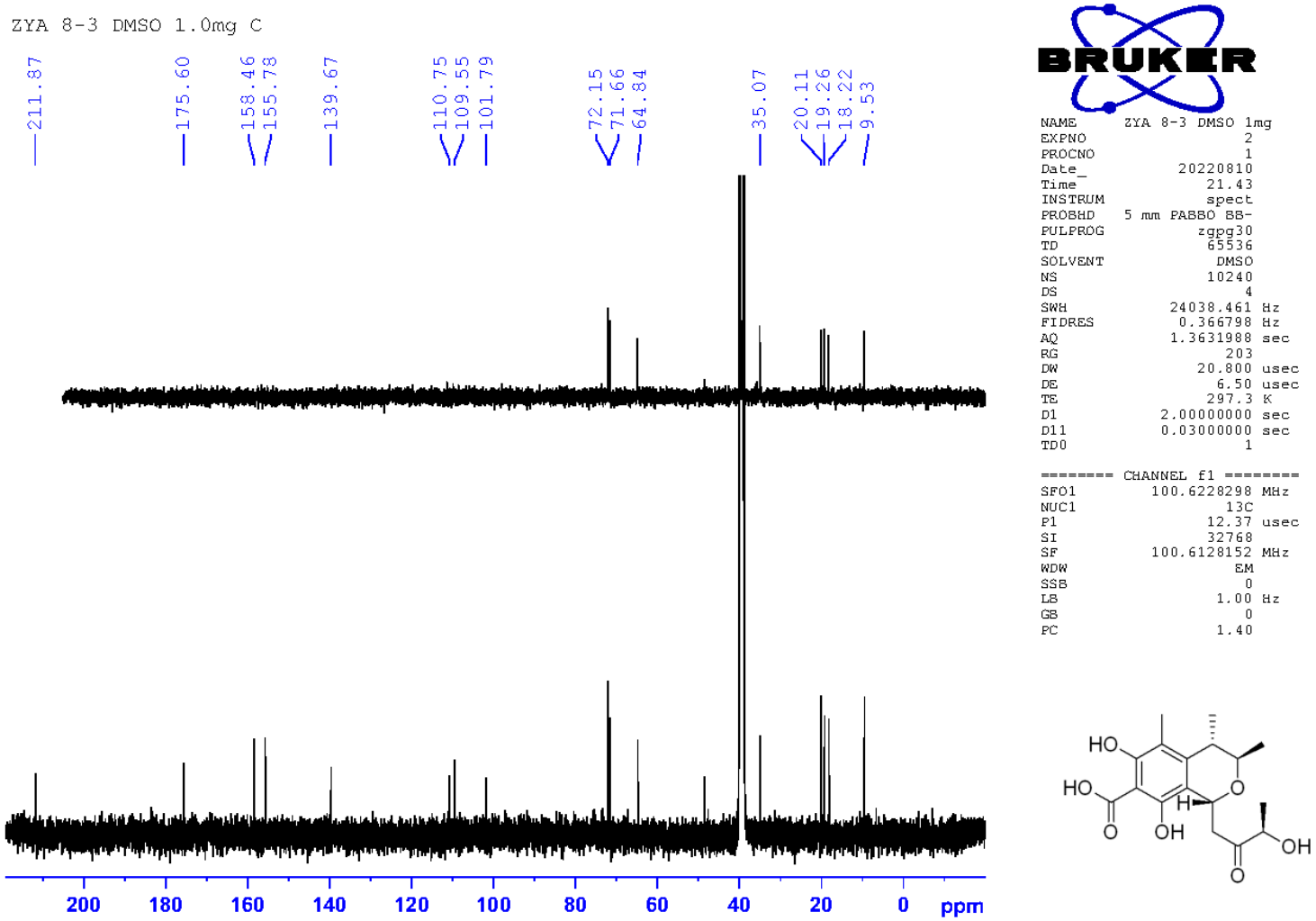


Figure S10. The ^{13}C NMR spectrum of compound **2** in DMSO-d_6.

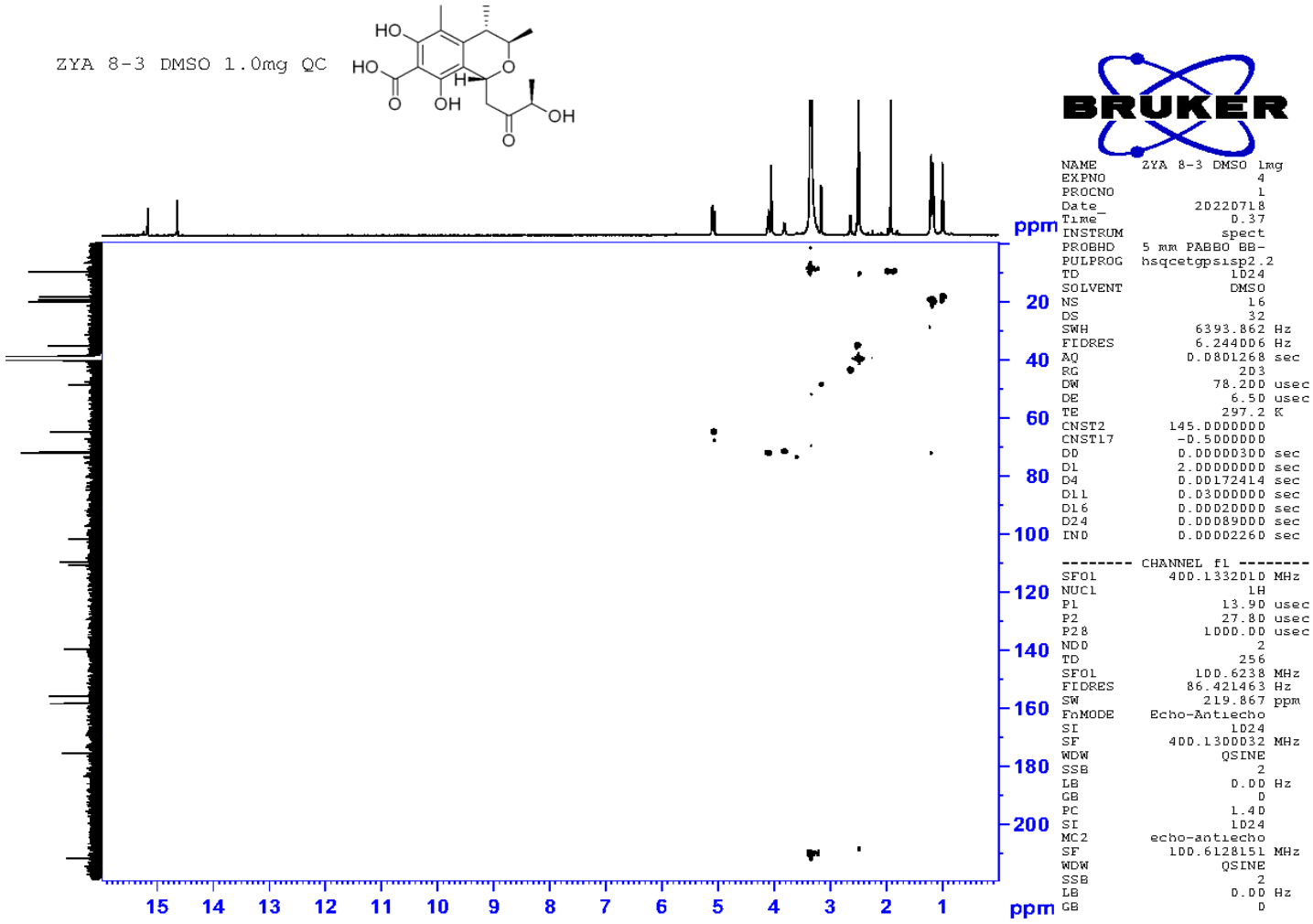


Figure S11. The HSQC spectrum of compound **2** in DMSO-d_6.

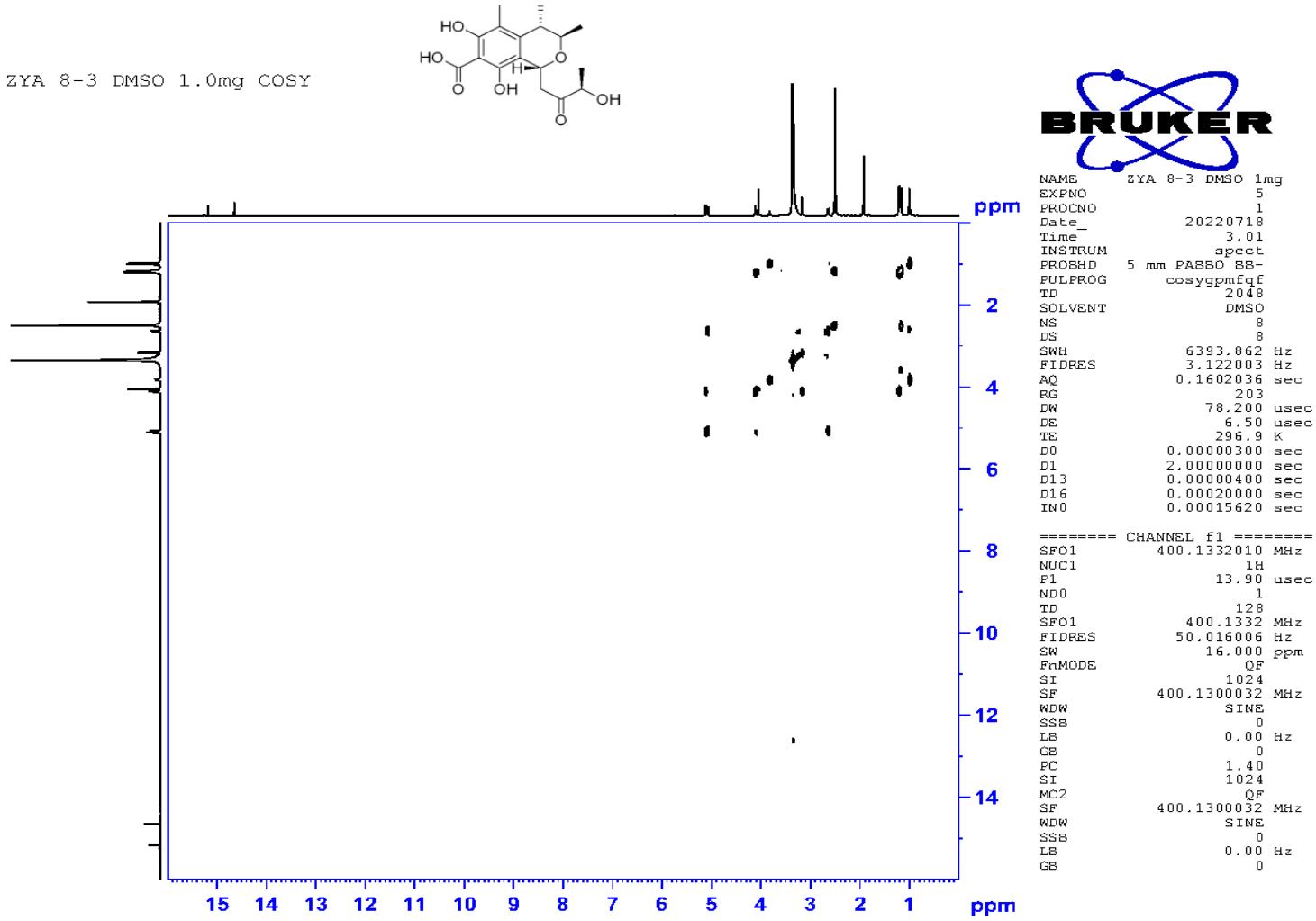


Figure S12. The ^{1}H-^{1}H COSY spectrum of compound **2** in DMSO-d_6.

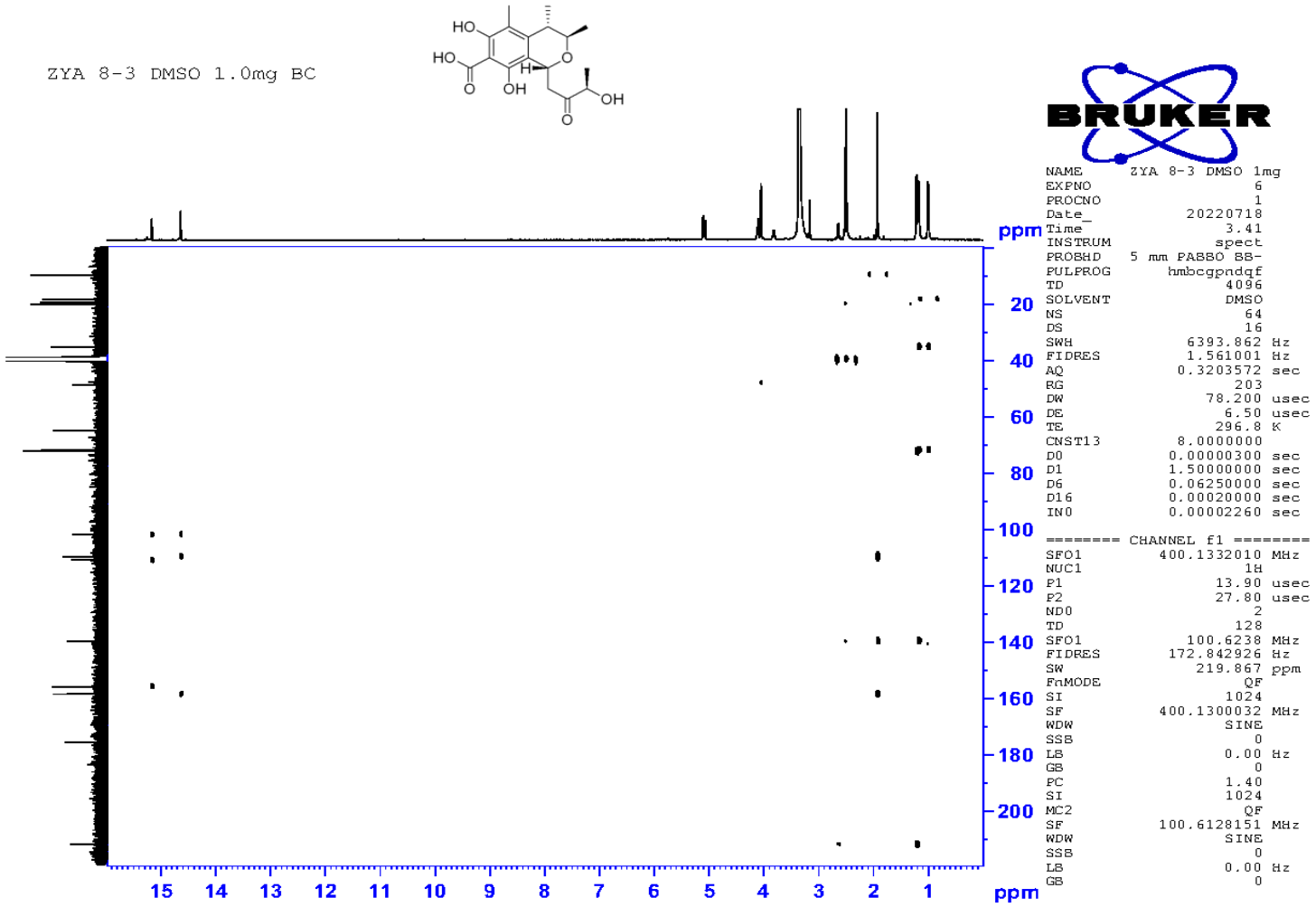


Figure S13. The HMBC spectrum of compound **2** in DMSO-d_6.

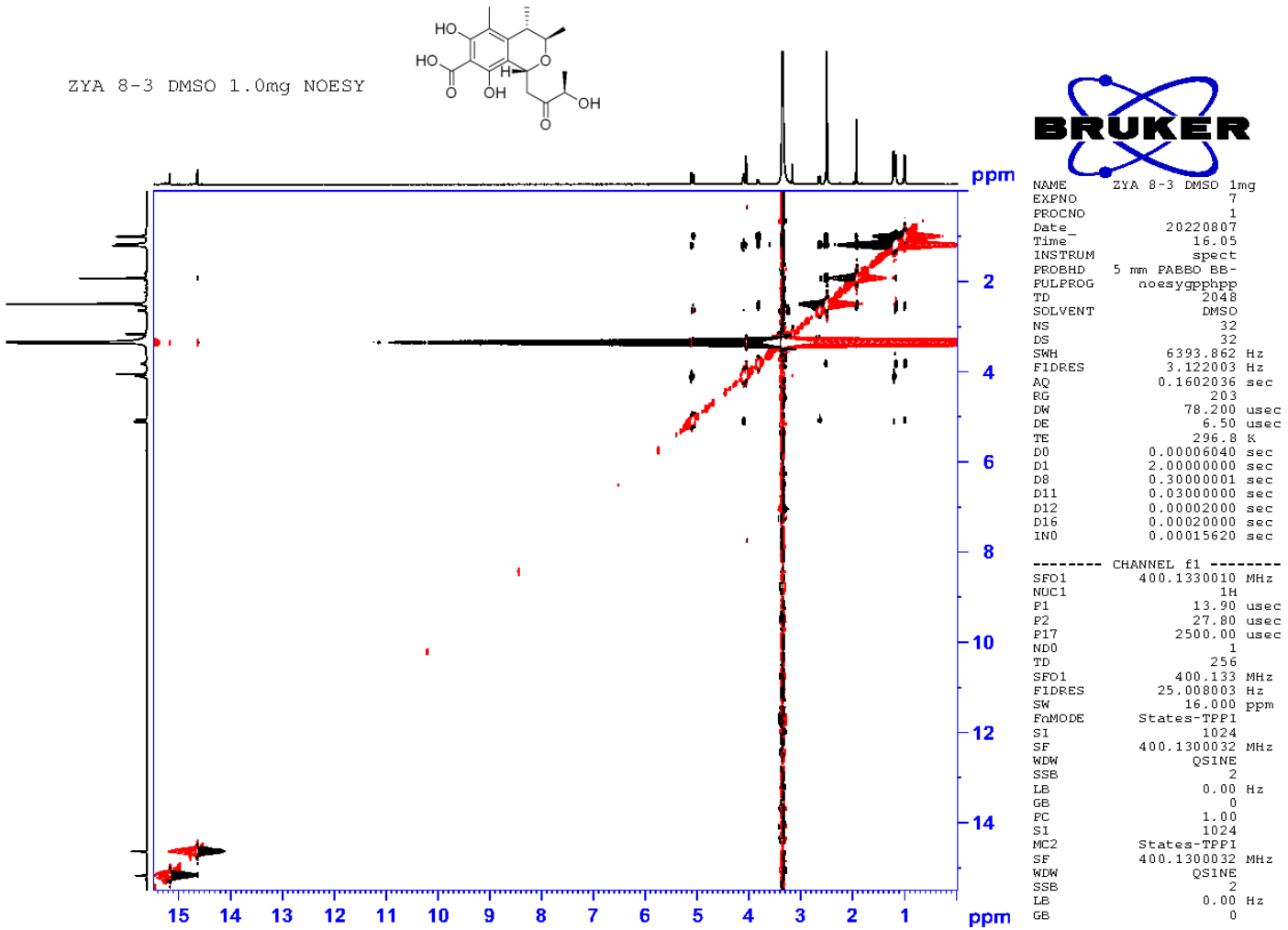
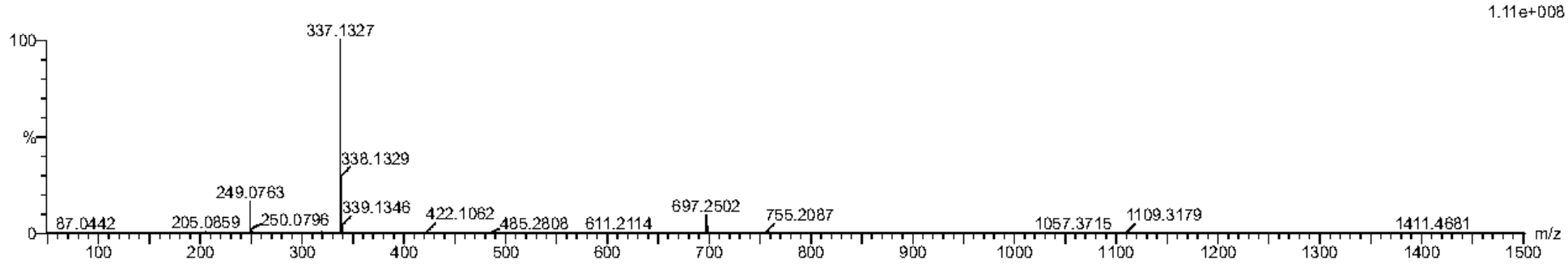


Figure S14. The NOESY spectrum of compound **2** in DMSO-d_6.

Elemental Composition Report **Page 1**

Tolerance = 5.0 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
105 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-50 O: 0-15 23Na: 0-1
ZYA 8-4-N 70 (0.290) Cm (63:89)
1: TOF MS ES-



Minimum:	80.00				-1.5				
Maximum:	100.00		5.0	10.0	50.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1327	100.00	337.1287	4.0	11.9	7.5	2032.0	0.148	86.21	C17 H21 O7
		337.1346	-1.9	-5.6	-1.5	2033.8	1.981	13.79	C10 H25 O12

Figure S15. The HR-ESI-MS of compound **3**.

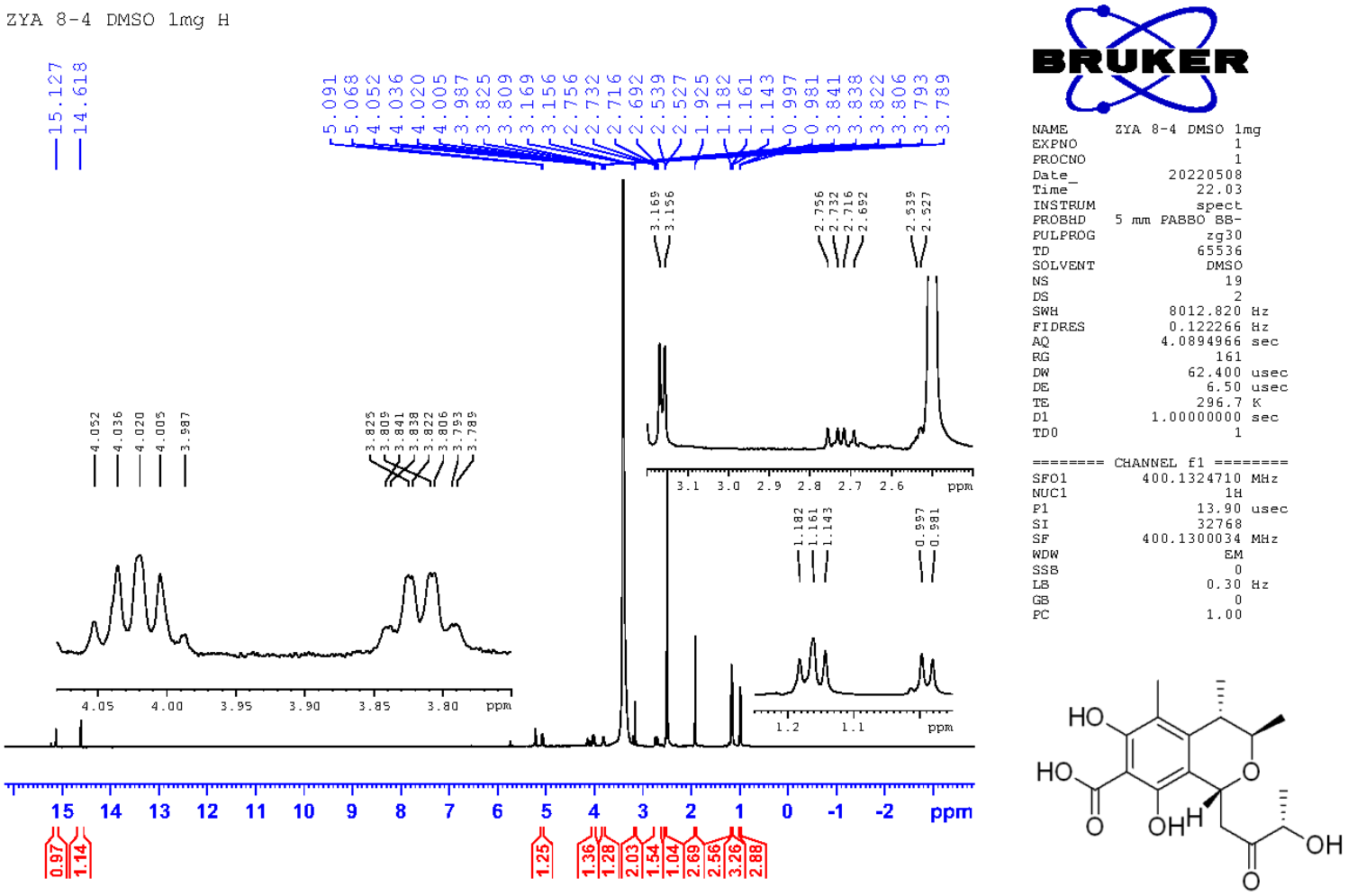


Figure S16. The ^{1}H NMR spectrum of compound **3** in DMSO-d_6.

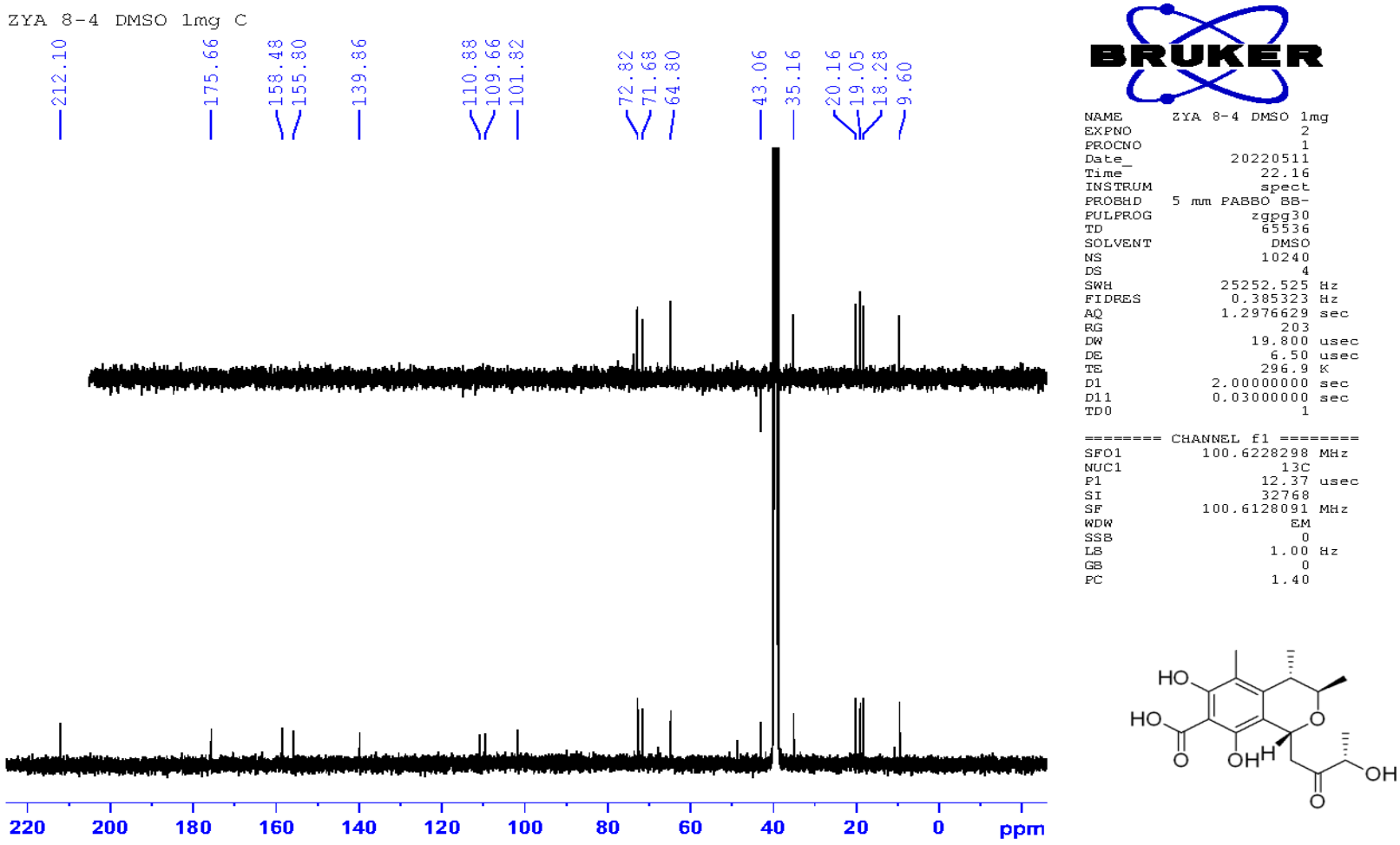
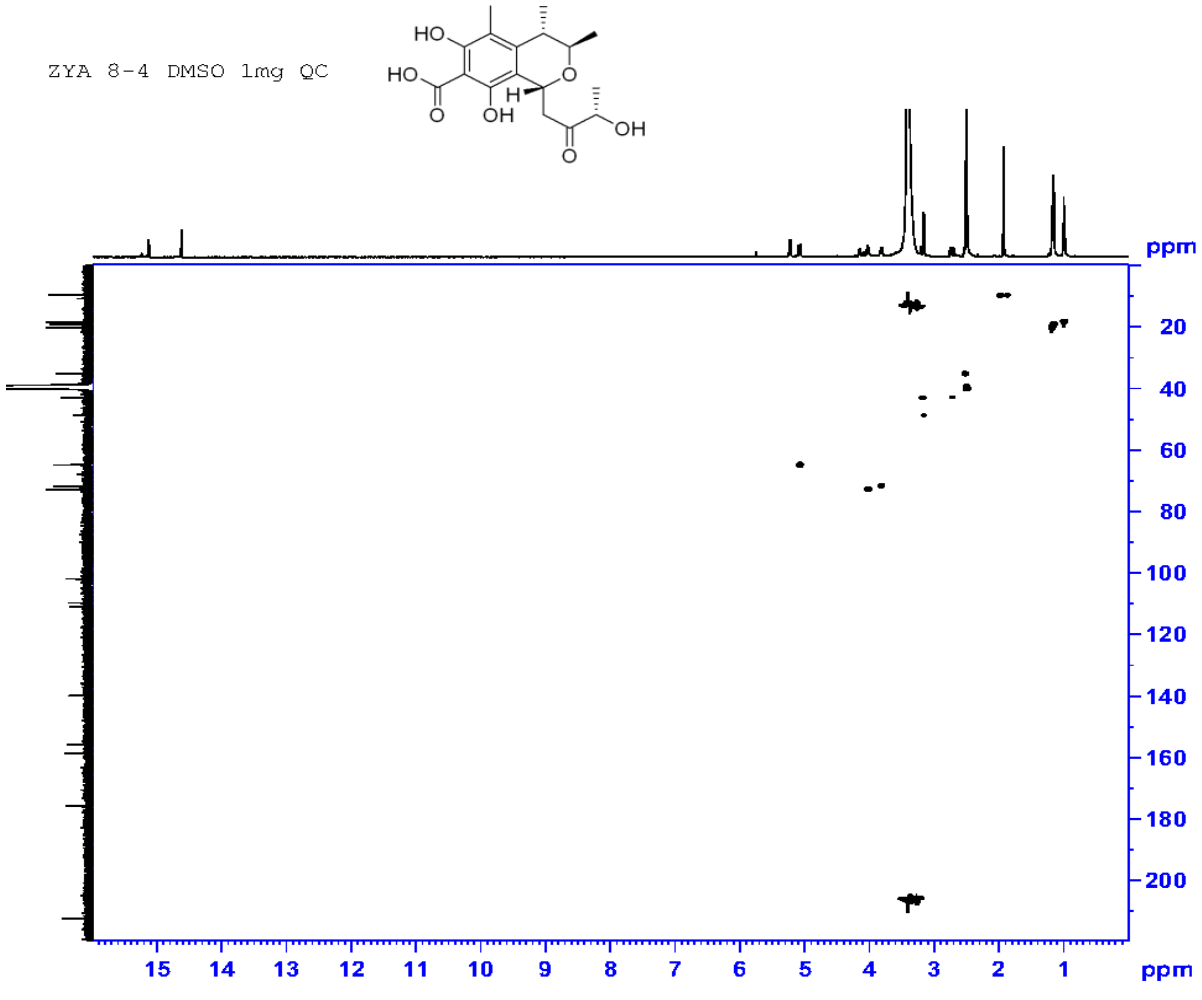


Figure S17. The ^{13}C NMR spectrum of compound **3** in DMSO-d_6.

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EXPNO                      4
PROCNO                     1
Date_            20220703
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INSTRUM              spect
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PULPROG   hsqcetgpsisp2.2
TD                    1024
SOLVENT               DMSO
NS                      16
DS                      32
SWH              8012.820 Hz
FIDRES           7.825020 Hz
AQ               0.0639476 sec
RG                     203
DW                 62.400 usec
DE                  6.50 usec
TE                 296.7 K
CNST2          145.0000000
CNST17          -0.5000000
D0              0.0000300 sec
D1              2.0000000 sec
D4              0.0017414 sec
D11             0.0300000 sec
D16             0.0002000 sec
D24             0.0008900 sec
IN0             0.0002260 sec

-------- CHANNEL f1 --------
SFO1          400.1340013 MHz
NUC1                    1H
P1                  13.90 usec
P2                  27.80 usec
P28               1000.00 usec
NDO                     2
TD                    256
SFO1            100.6238 MHz
FIDRES          86.421463 Hz
SW                219.867 ppm
FnMODE     Echo-Antiecho
SI                    1024
SF            400.1300035 MHz
WDW                 QSINE
SSB                     2
LB                  0.00 Hz
GB                      0
PC                  1.40
SI                    1024
MC2        echo-antiecho
SF              100.6128090 MHz
WDW                 QSINE
SSB                     2
LB                  0.00 Hz
GB                      0
```

Figure S18. The HSQC spectrum of compound **3** in DMSO-d_6.

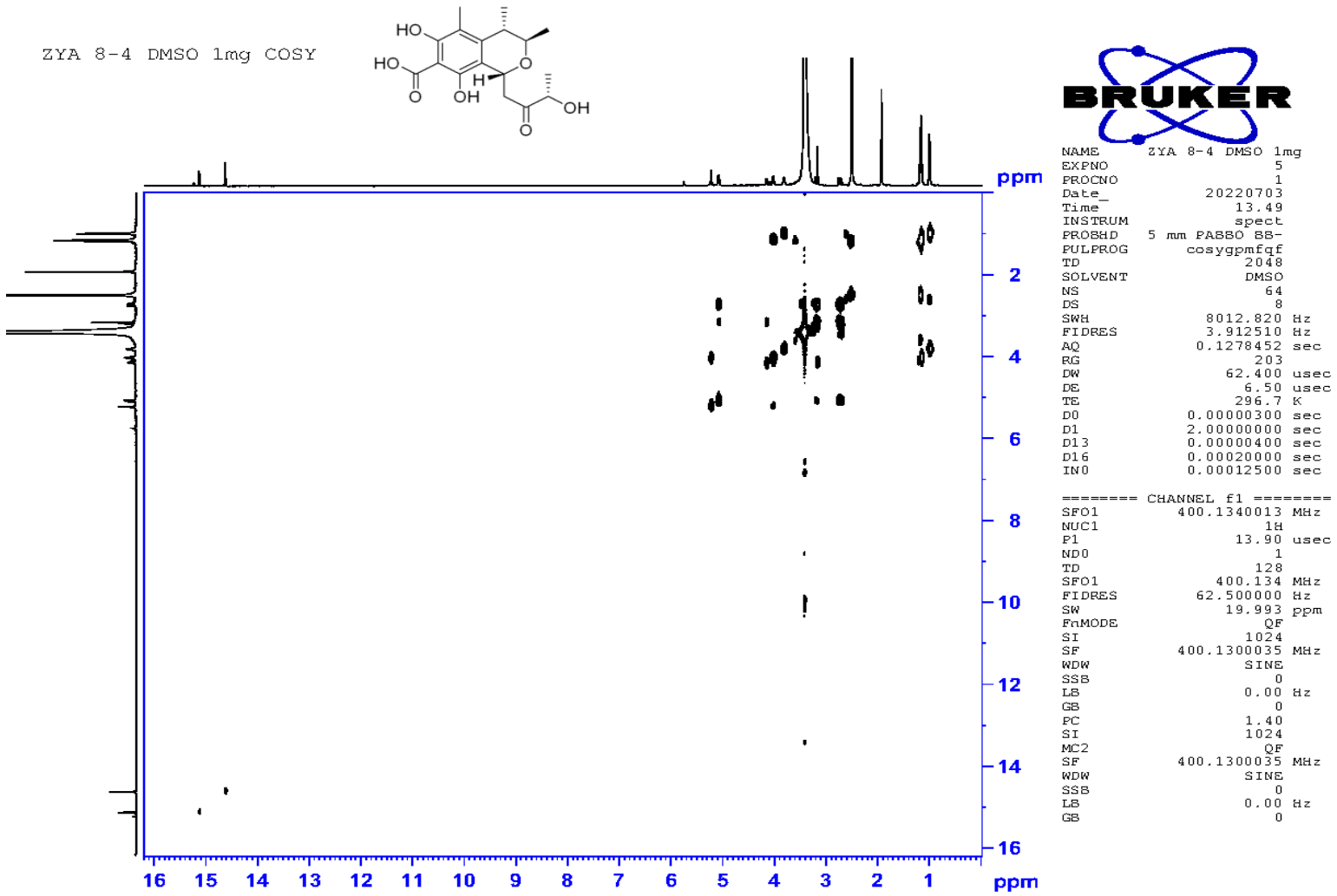
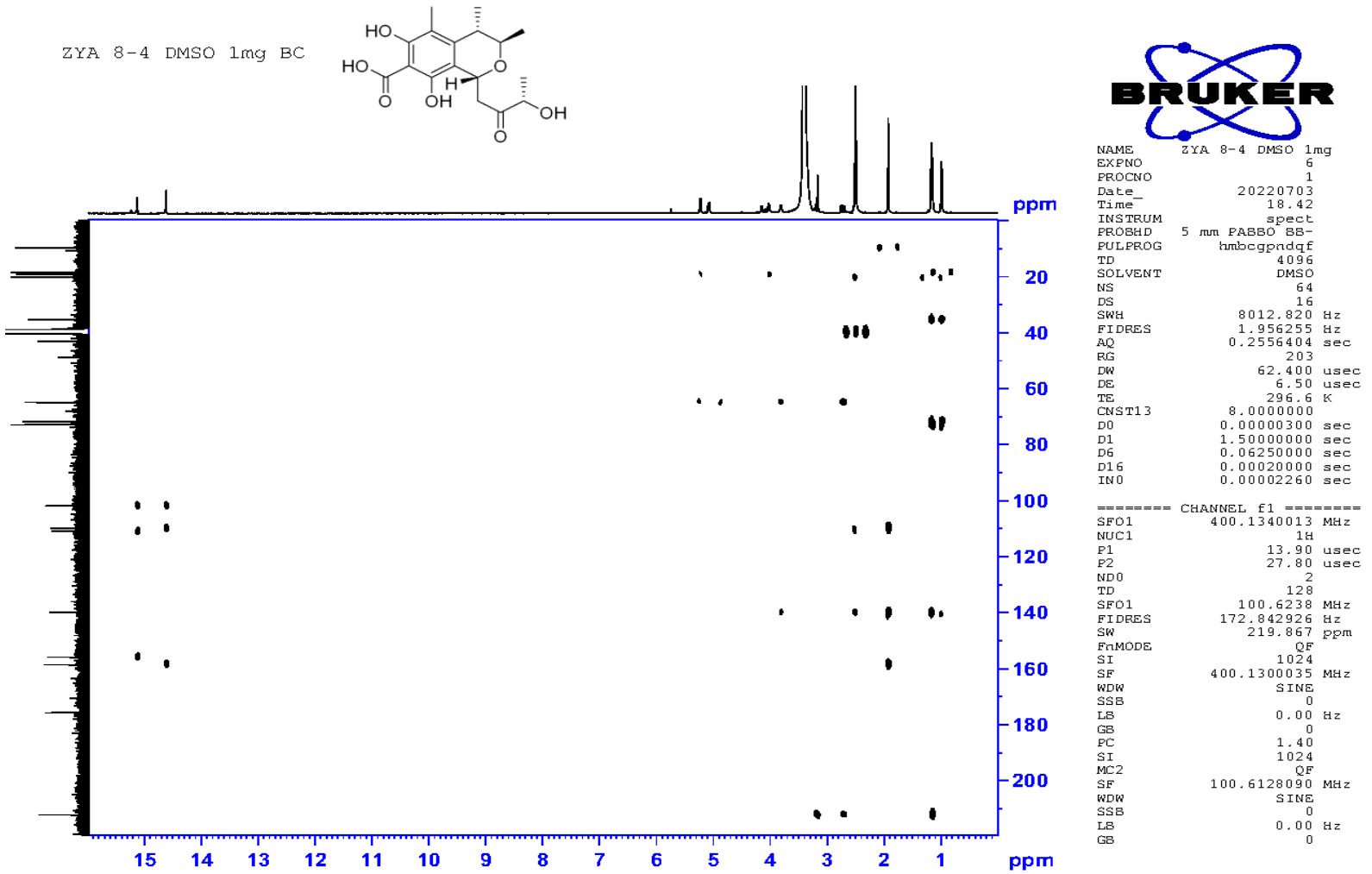


Figure S19. The ^{1}H-^{1}H COSY spectrum of compound **3** in DMSO-d_6.



BRUKER

```
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EXPNO                        6
PROCNO                       1
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INSTRUM                  spect
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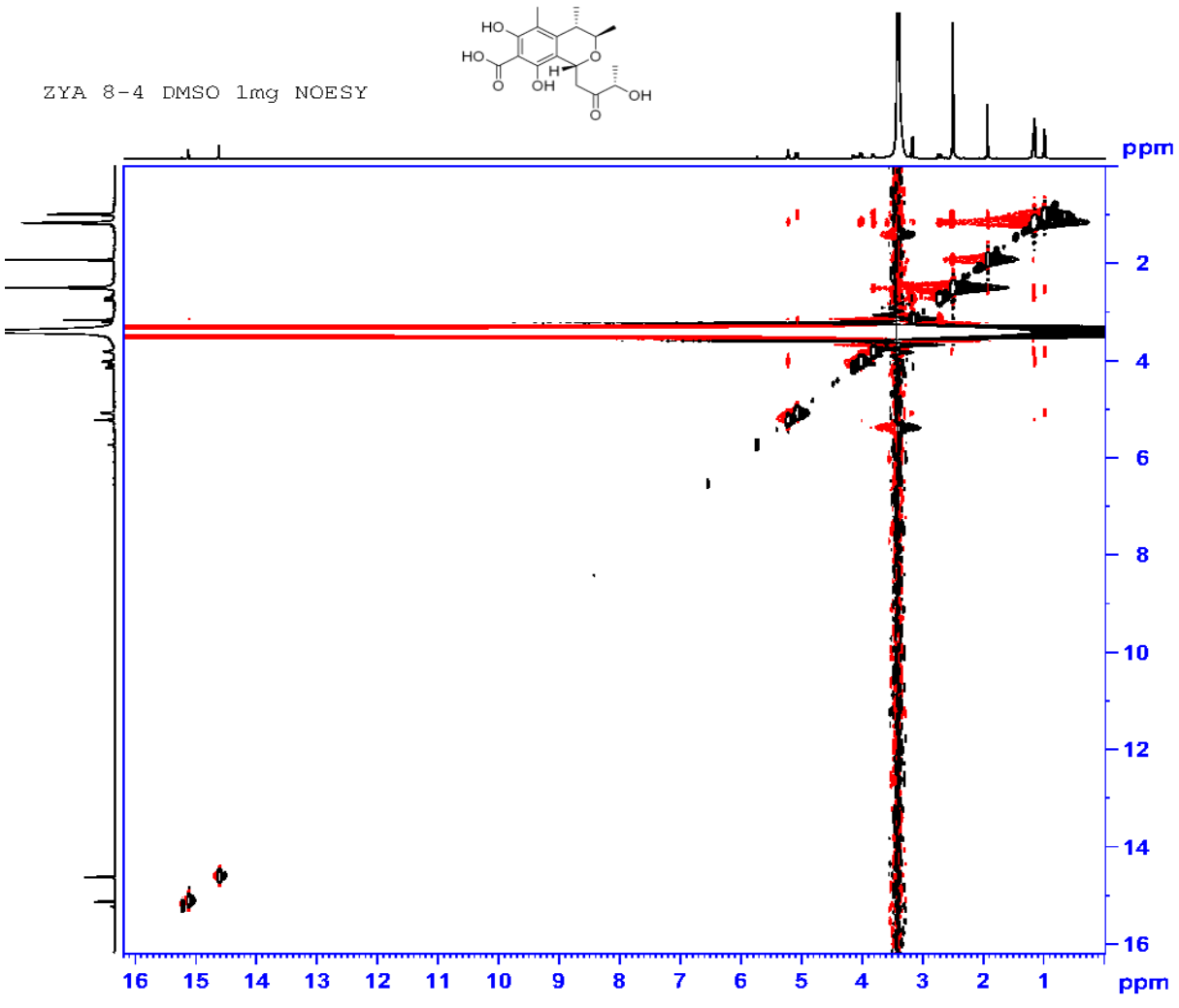
PULPROG           hmbcgpndqf
TD                        4096
SOLVENT                 DMSO
NS                          64
DS                          16
SWH                   8012.820 Hz
FIDRES                1.956255 Hz
AQ                    0.2556404 sec
RG                          203
DW                       62.400 usec
DE                        6.50 usec
TE                       296.6 K
CNST13                8.0000000
D0                    0.00000300 sec
D1                    1.50000000 sec
D6                    0.06250000 sec
D16                   0.00020000 sec
IN0                   0.00002260 sec

======== CHANNEL f1 ========
SFO1                400.1340013 MHz
NUC1                        1H
P1                       13.90 usec
P2                       27.80 usec
ND0                         2
TD                        128
SFO1                 100.6238 MHz
FIDRES               172.842926 Hz
SW                   219.867 ppm
FnMODE                     QF
SI                        1024
SF                  400.1300035 MHz
WDW                      SINE
SSB                         0
LB                    0.00 Hz
GB                          0
PC                       1.40
SI                        1024
MC2                        QF
SF                  100.6128090 MHz
WDW                      SINE
SSB                         0
LB                    0.00 Hz
GB                          0
```

Figure S20. The HMBC spectrum of compound **3** in DMSO-d_6.



BRUKER

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PROCNO                       1
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INSTRUM                  spect
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PULPROG       noesygpphpp
TD                        2048
SOLVENT                   DMSO
NS                          16
DS                          32
SWH                 8012.820 Hz
FIDRES              3.912510 Hz
AQ                  0.1278452 sec
RG                        203
DW                     62.400 usec
DE                      6.50 usec
TE                     296.7 K
D0                  0.00004480 sec
D1                  2.00000000 sec
D8                  0.30000001 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D16                 0.00020000 sec
IN0                 0.00012500 sec

-------- CHANNEL f1 --------
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NUC1                       1H
P1                      13.90 usec
P2                      27.80 usec
P17                   2500.00 usec
ND0                        1
TD                       256
SFO1                 400.134 MHz
FIDRES              31.250000 Hz
SW                     19.993 ppm
FnMODE           States-TPPI
SI                       1024
SF                400.1300035 MHz
WDW                     QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.00
SI                       1024
MC2              States-TPPI
SF                400.1300035 MHz
WDW                     QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```

Figure S21. The NOESY spectrum of compound **3** in DMSO-d_6.