Supporting Information

Penidihydrocitrinins A–C: New Polyketides from the Deep-Sea-Derived *Penicillium citrinum* W17 and Their Anti-Inflammatory and Anti-osteoporotic Bioactivities

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[2] School of Medicine, Xiamen University, South Xiangan Road, Xiamen 361005, China

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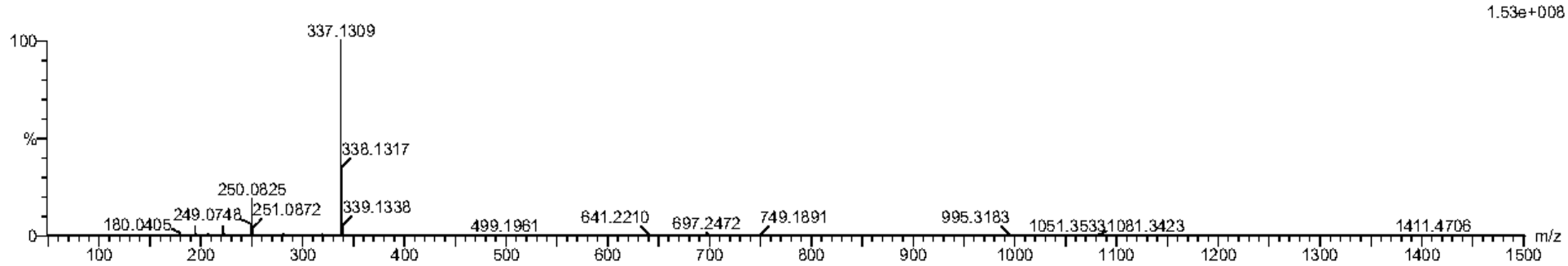
[†] These authors contributed equally to this work.

Content

Elemental Composition Report **Page 1**

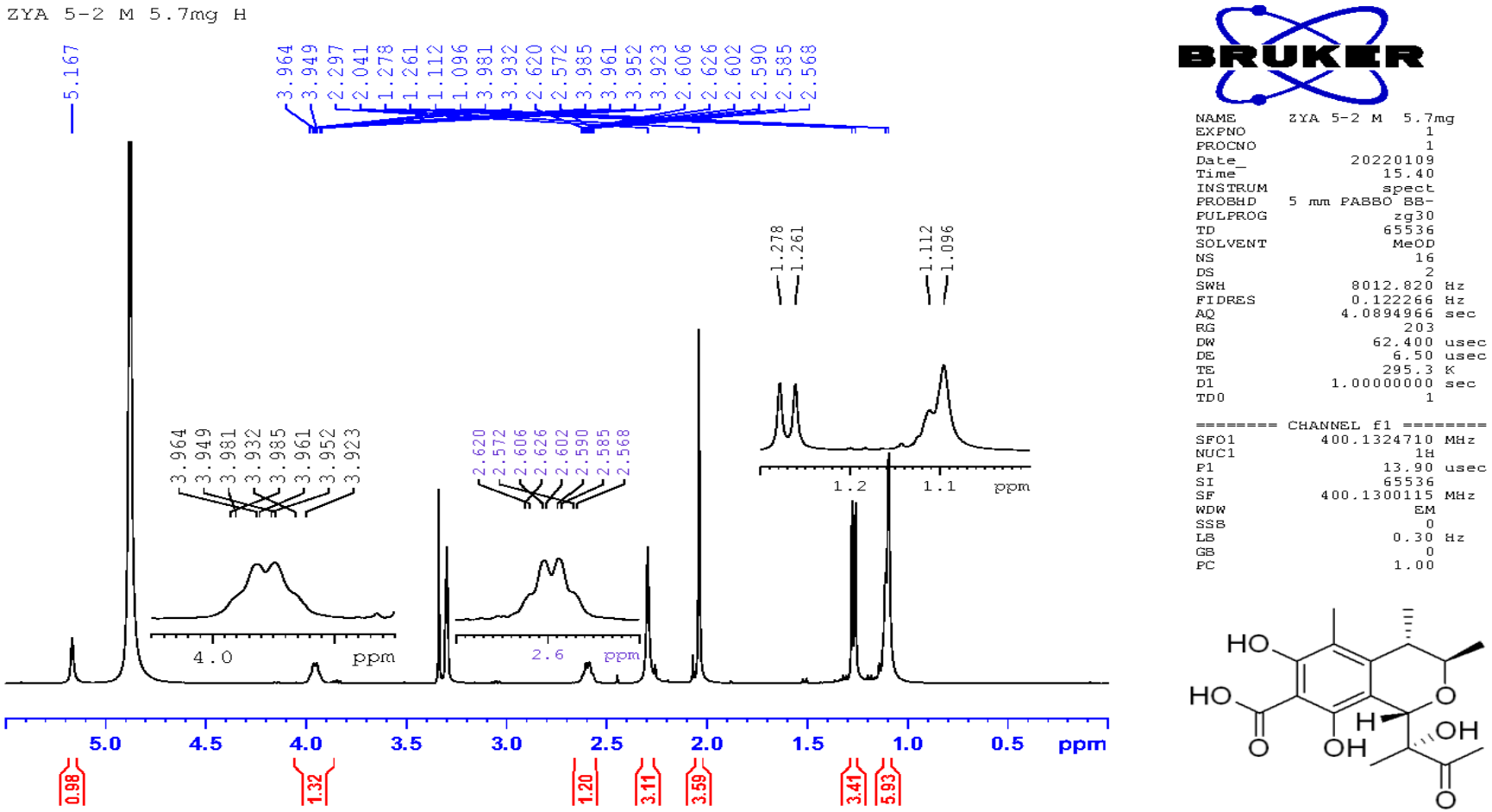
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

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**.



BRUKER

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PROCNO	1
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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.

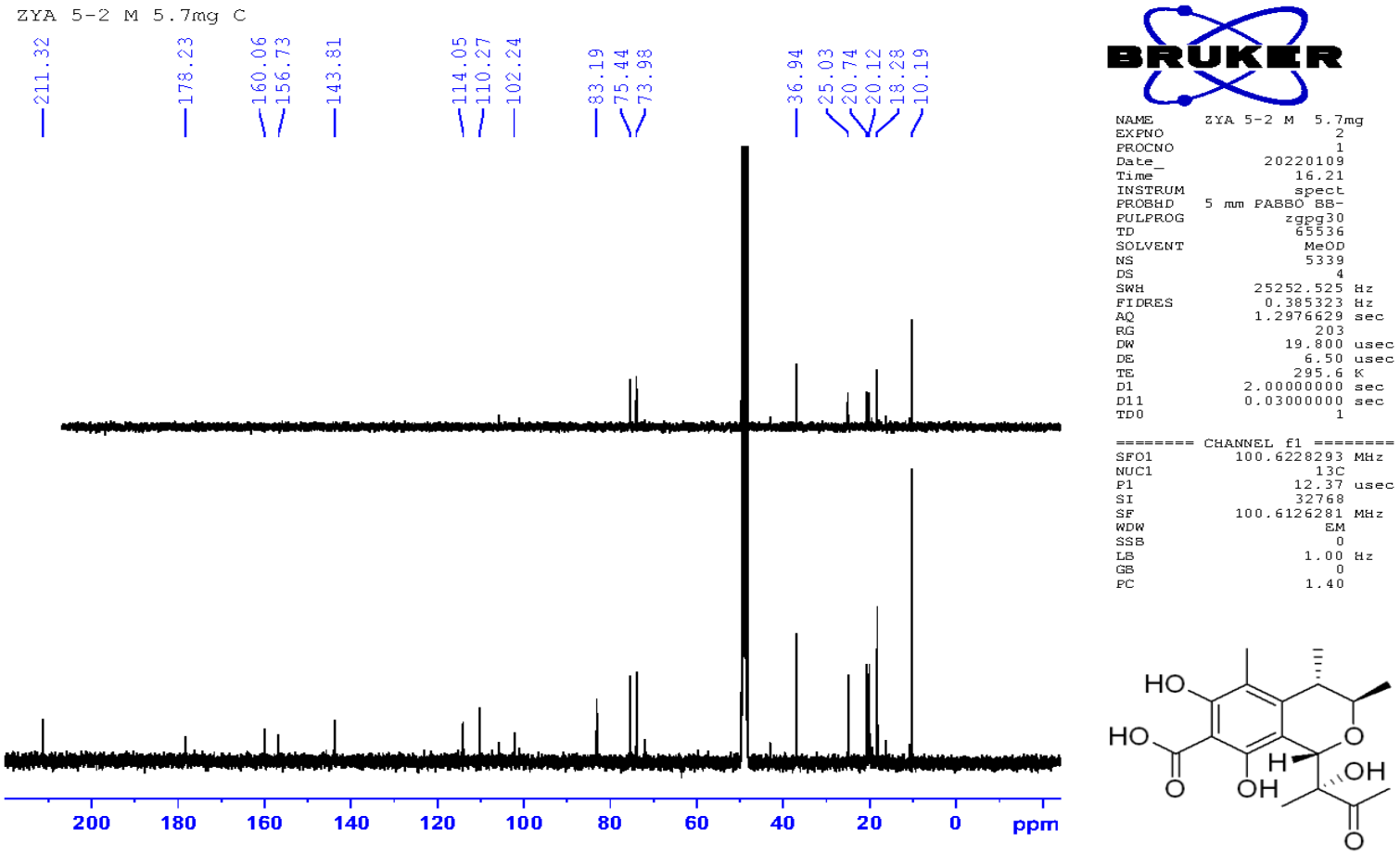


Figure S3. The ^{13}C NMR spectrum of compound **1** in CD_3OD.

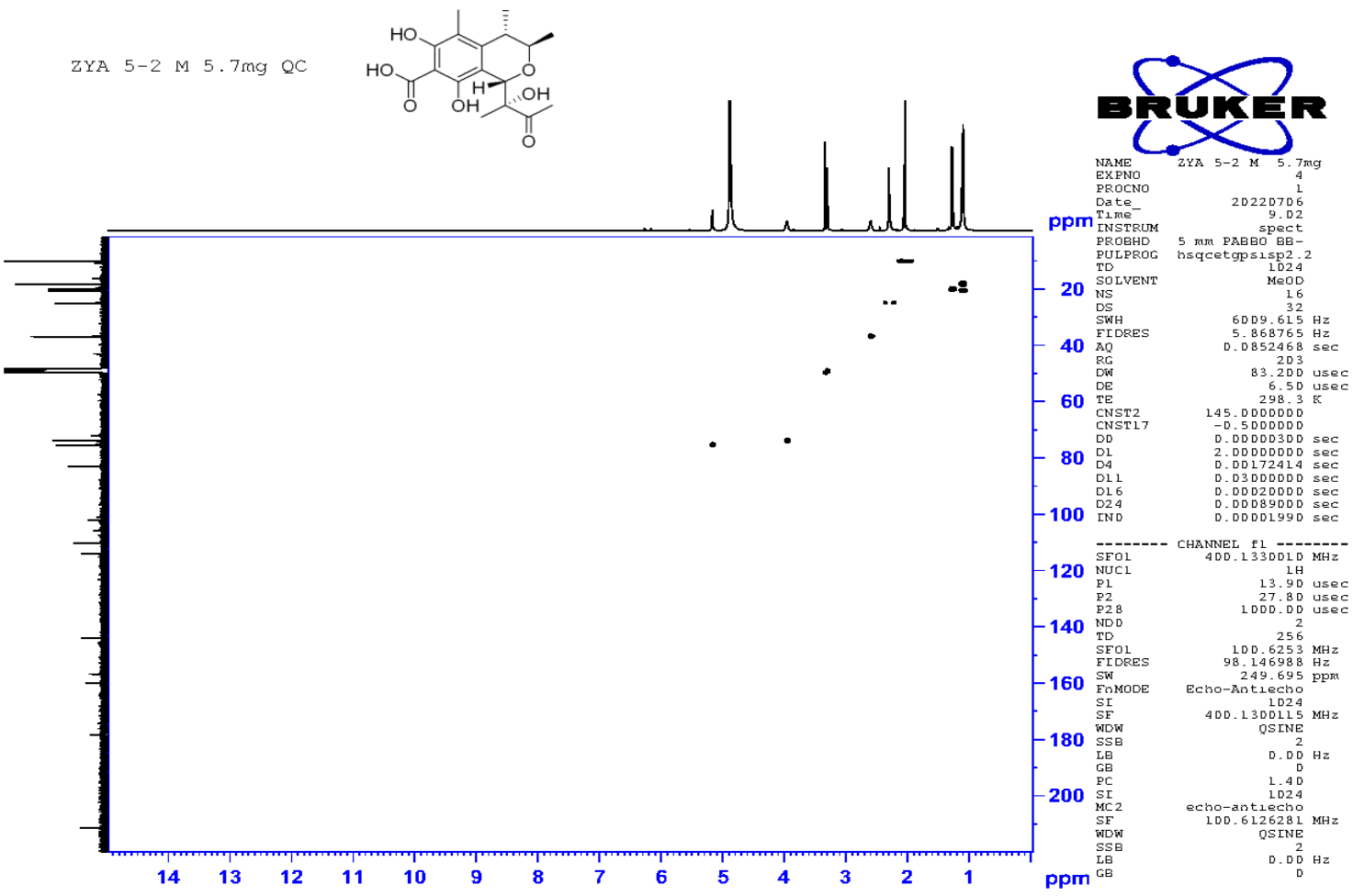


Figure S4. The HSQC spectrum of compound **1** in CD_3OD.

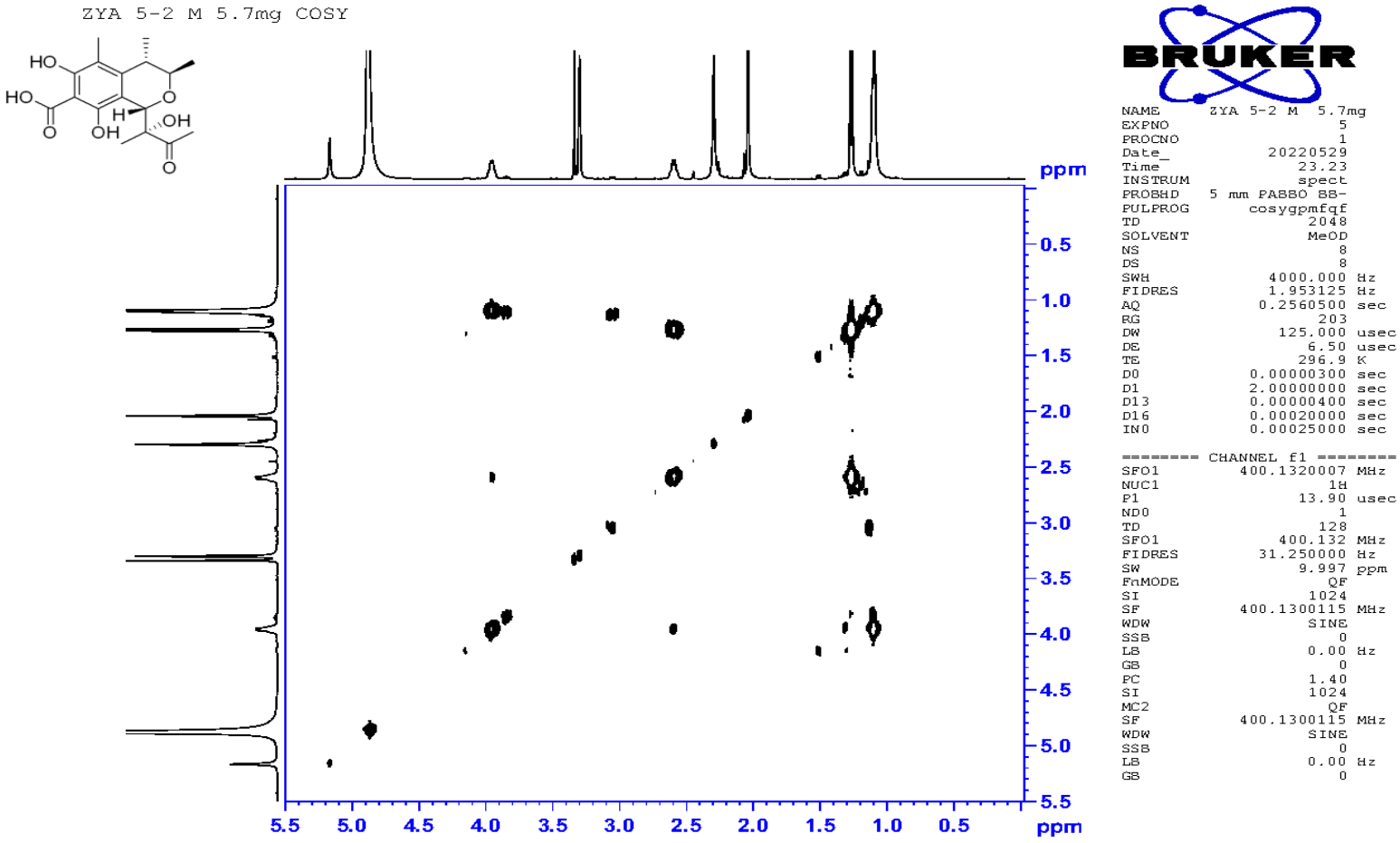


Figure S5. The ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD.

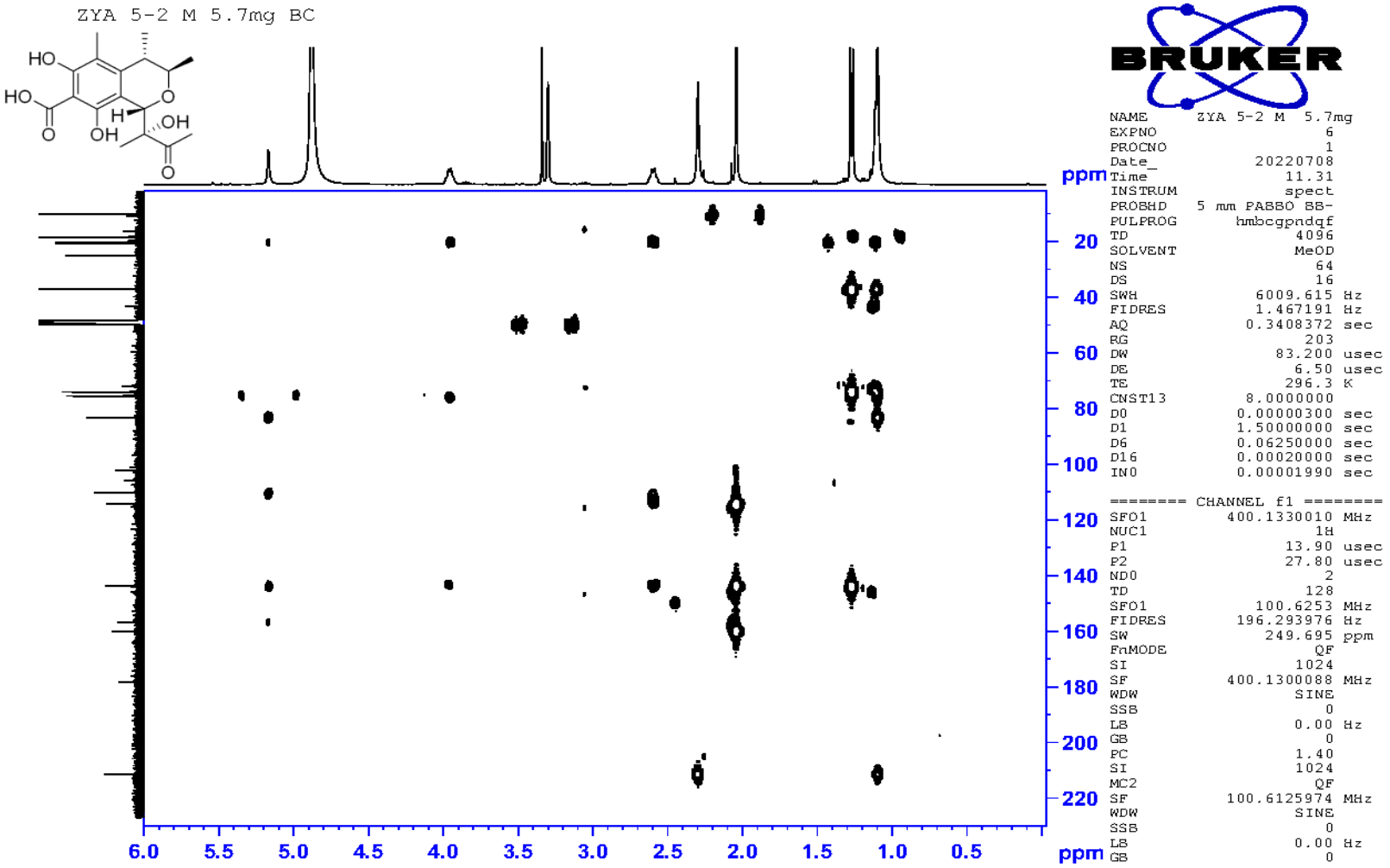


Figure S6. The HMBC spectrum of compound **1** in CD_3OD.

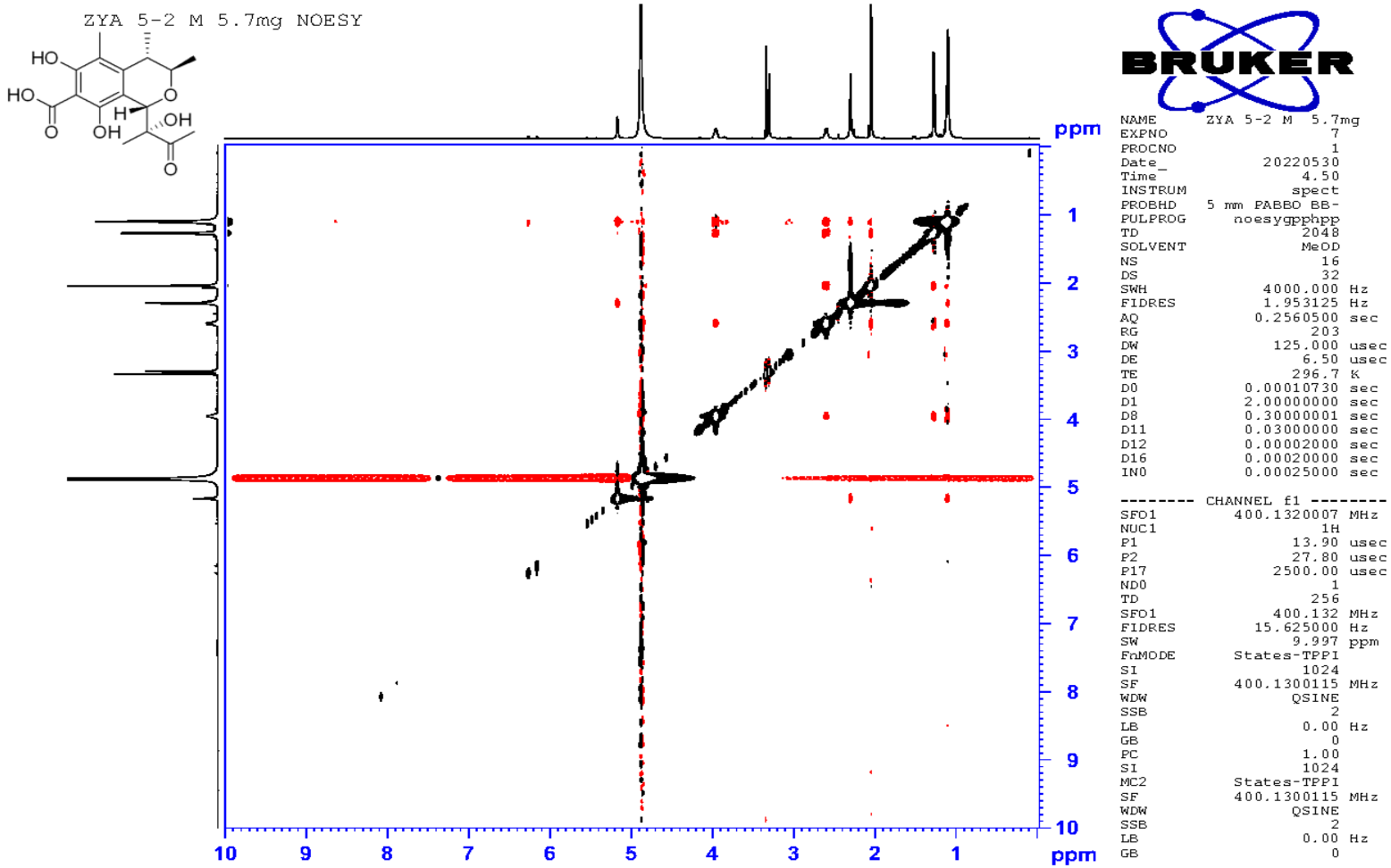
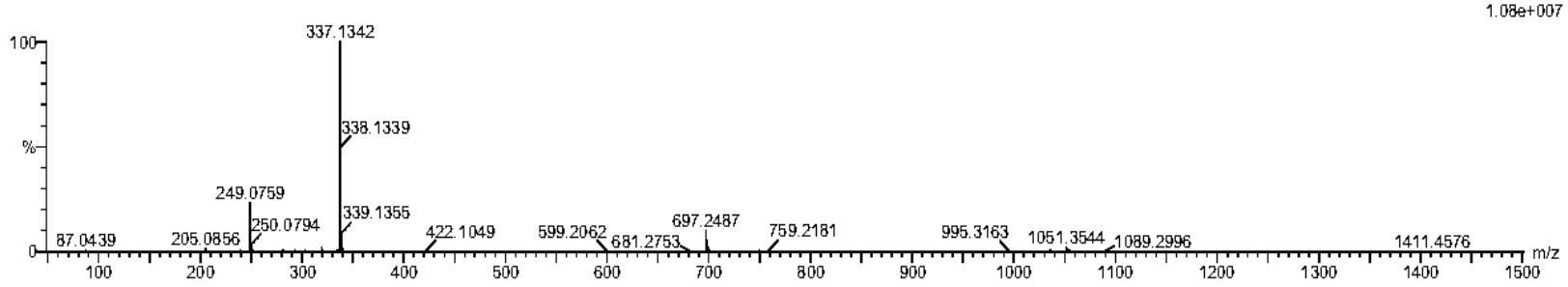


Figure S7. The NOESY spectrum of compound **1** in CD_3OD.

Elemental Composition Report **Page 1**

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

Monoisotopic Mass, Even Electron Ions
83 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-35 H: 0-60 O: 0-10 23Na: 0-1
ZYA 8-3-N 70 (0.290) Cm (70:71)
1: TOF MS ES-



Minimum:	80.00				-1.5				
Maximum:	100.00		50.0	50.0	50.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1342	100.00	337.1229	11.3	33.5	16.5	1296.8	1.570	20.81	C24 H17 O2
		337.1440	-9.8	-29.1	11.5	1297.1	1.848	15.75	C21 H21 O4
		337.1204	13.8	40.9	13.5	1297.3	1.998	13.56	C22 H18 O2 23Na
		337.1287	5.5	16.3	7.5	1297.4	2.139	11.78	C17 H21 O7
		337.1416	-7.4	-21.9	8.5	1297.4	2.151	11.64	C19 H22 O4 23Na
		337.1499	-15.7	-46.6	2.5	1297.7	2.380	9.26	C14 H25 O9
		337.1263	7.9	23.4	4.5	1297.7	2.381	9.25	C15 H22 O7 23Na
		337.1475	-13.3	-39.5	-0.5	1297.8	2.531	7.96	C12 H26 O9 23Na

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

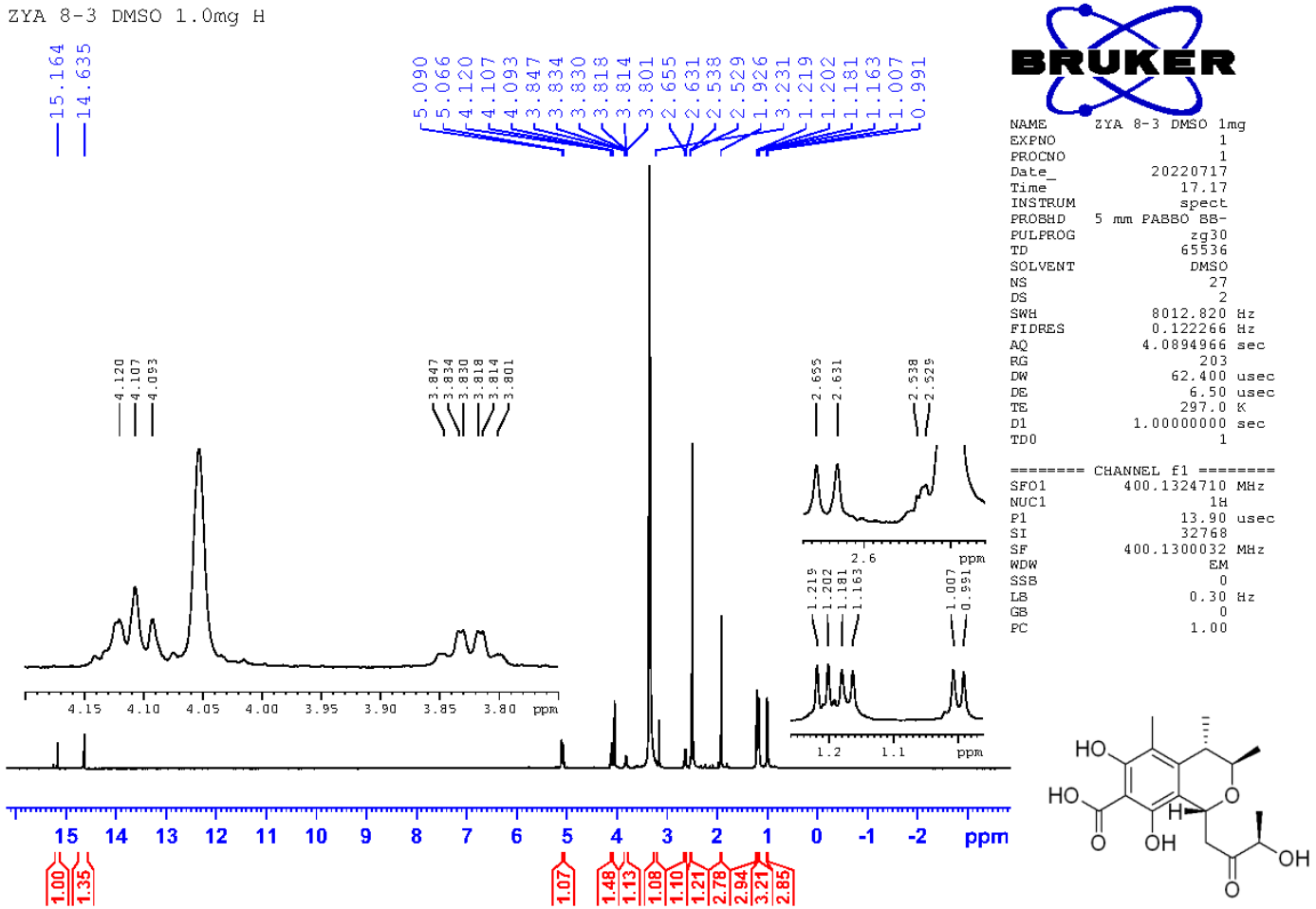


Figure S9. The ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

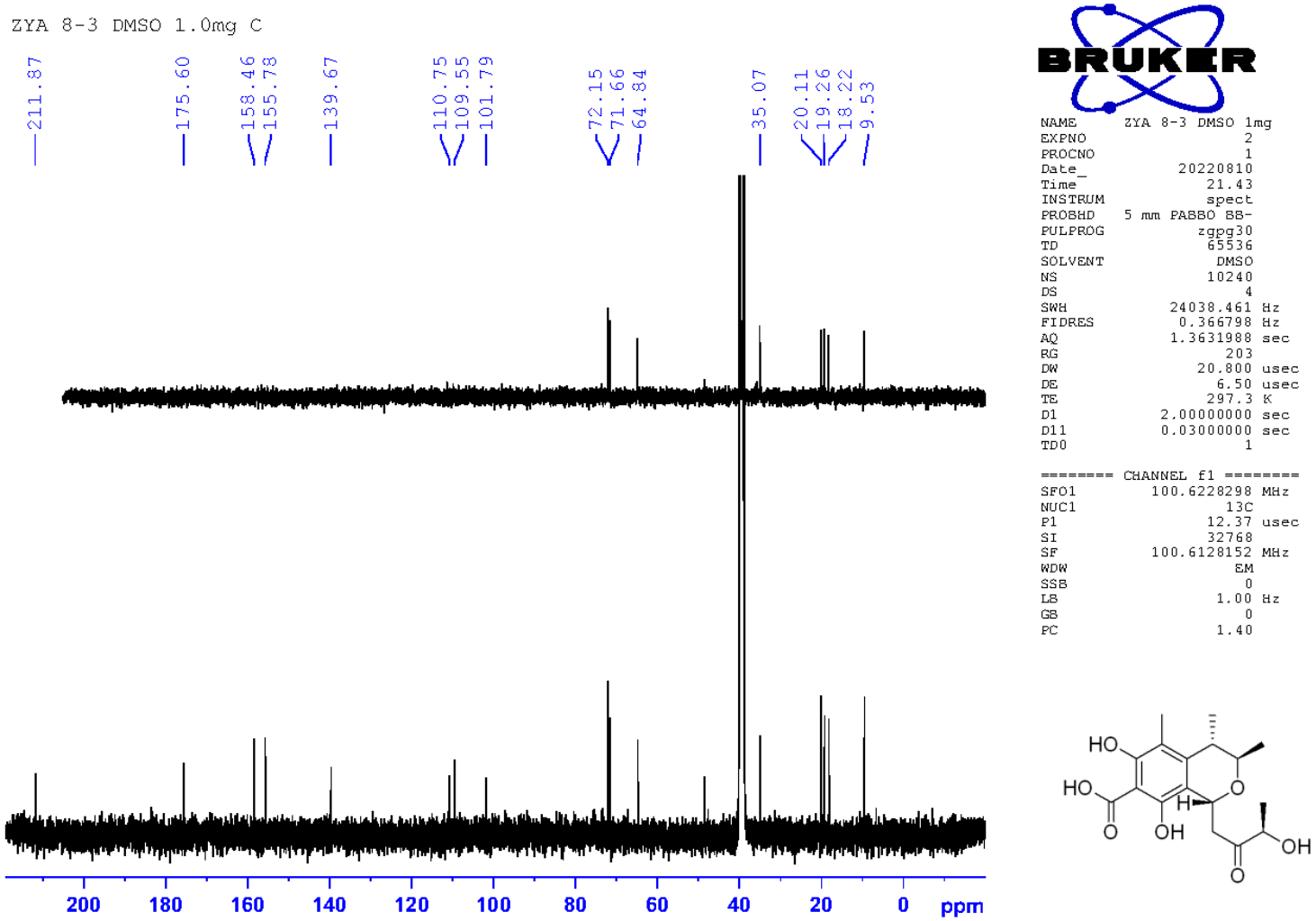


Figure S10. The ^{13}C NMR spectrum of compound **2** in DMSO-d_6.

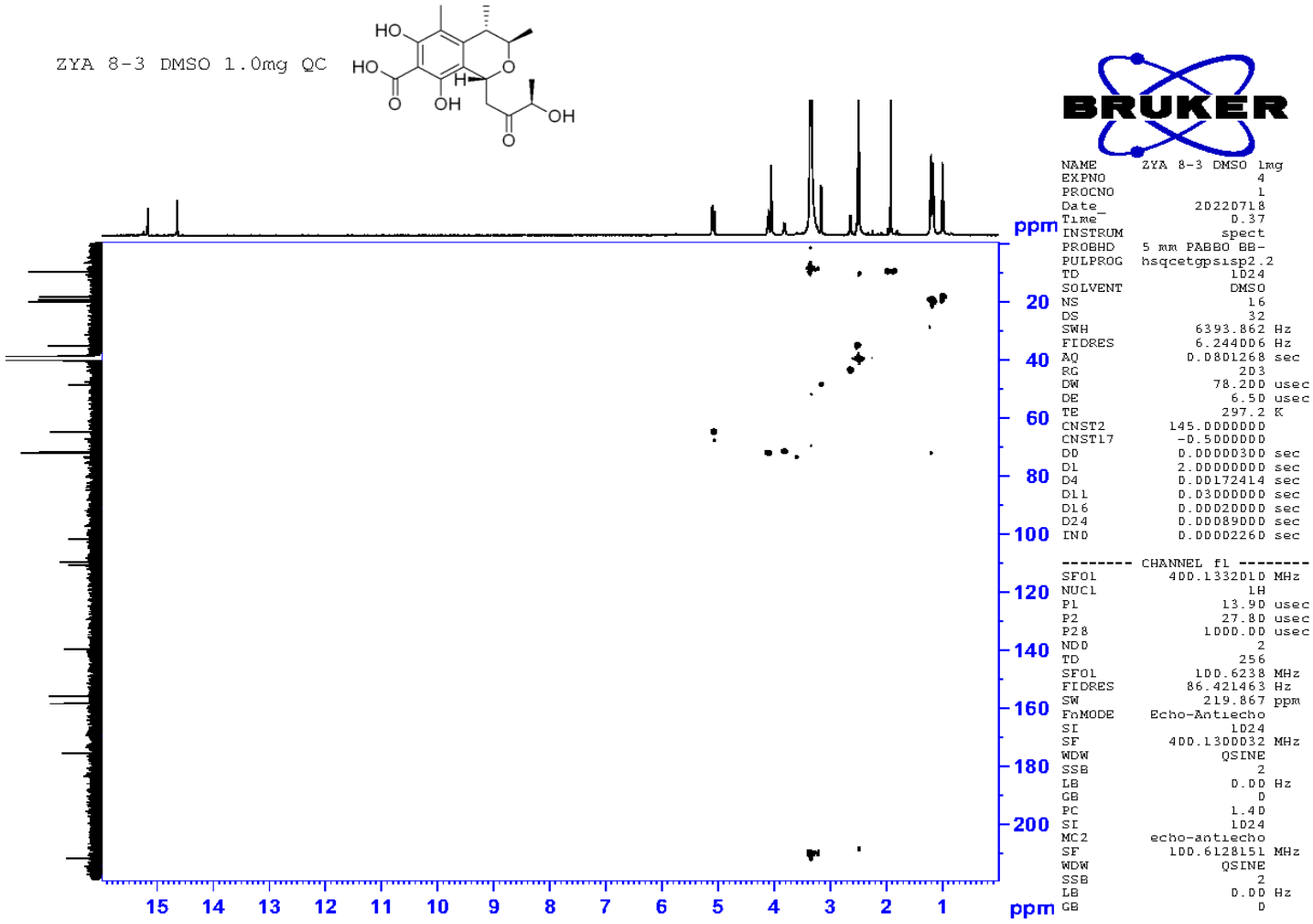


Figure S11. The HSQC spectrum of compound **2** in DMSO-d_6.

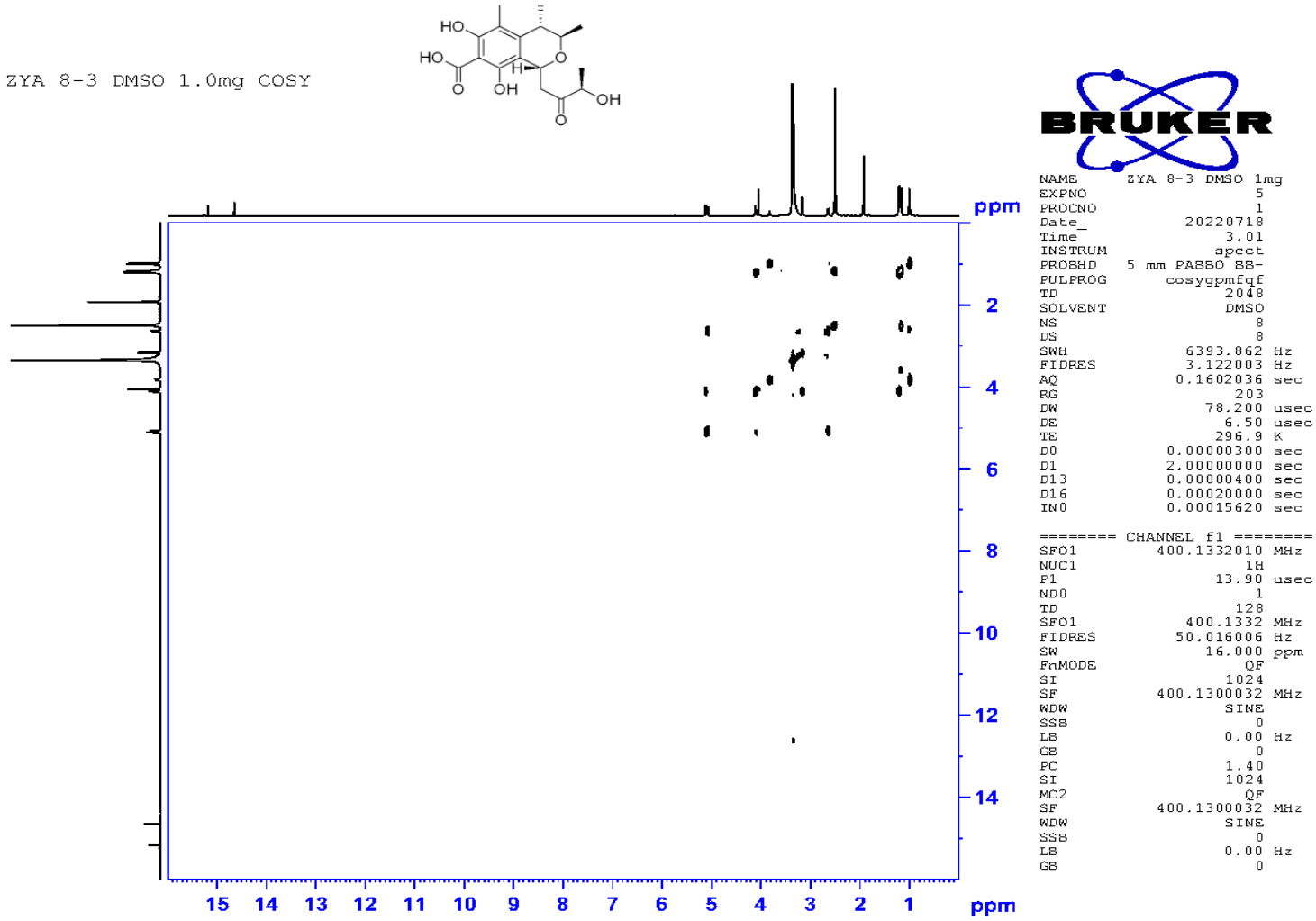


Figure S12. The ^{1}H-^{1}H COSY spectrum of compound **2** in DMSO-d_6.

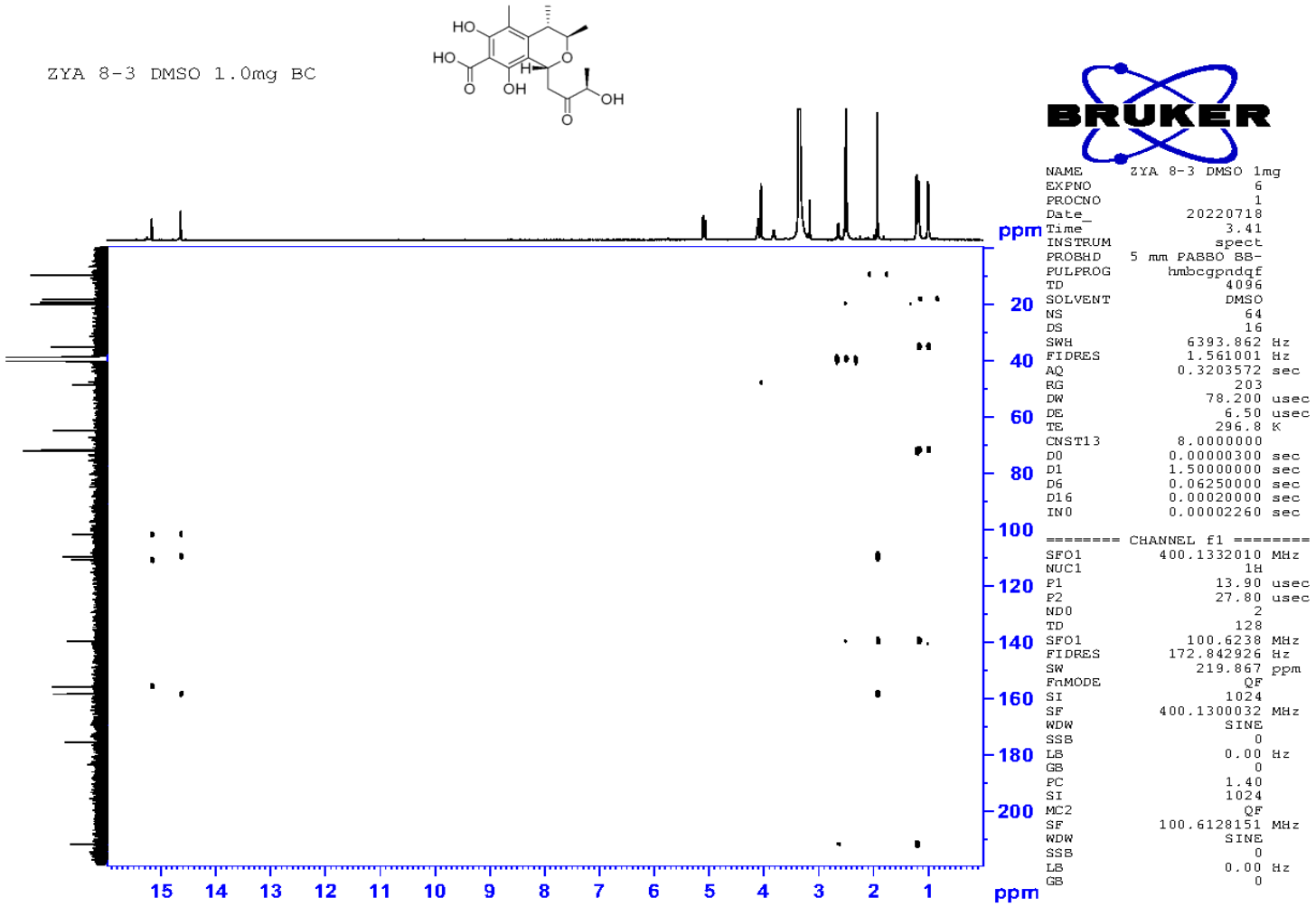


Figure S13. The HMBC spectrum of compound **2** in DMSO-d_6.

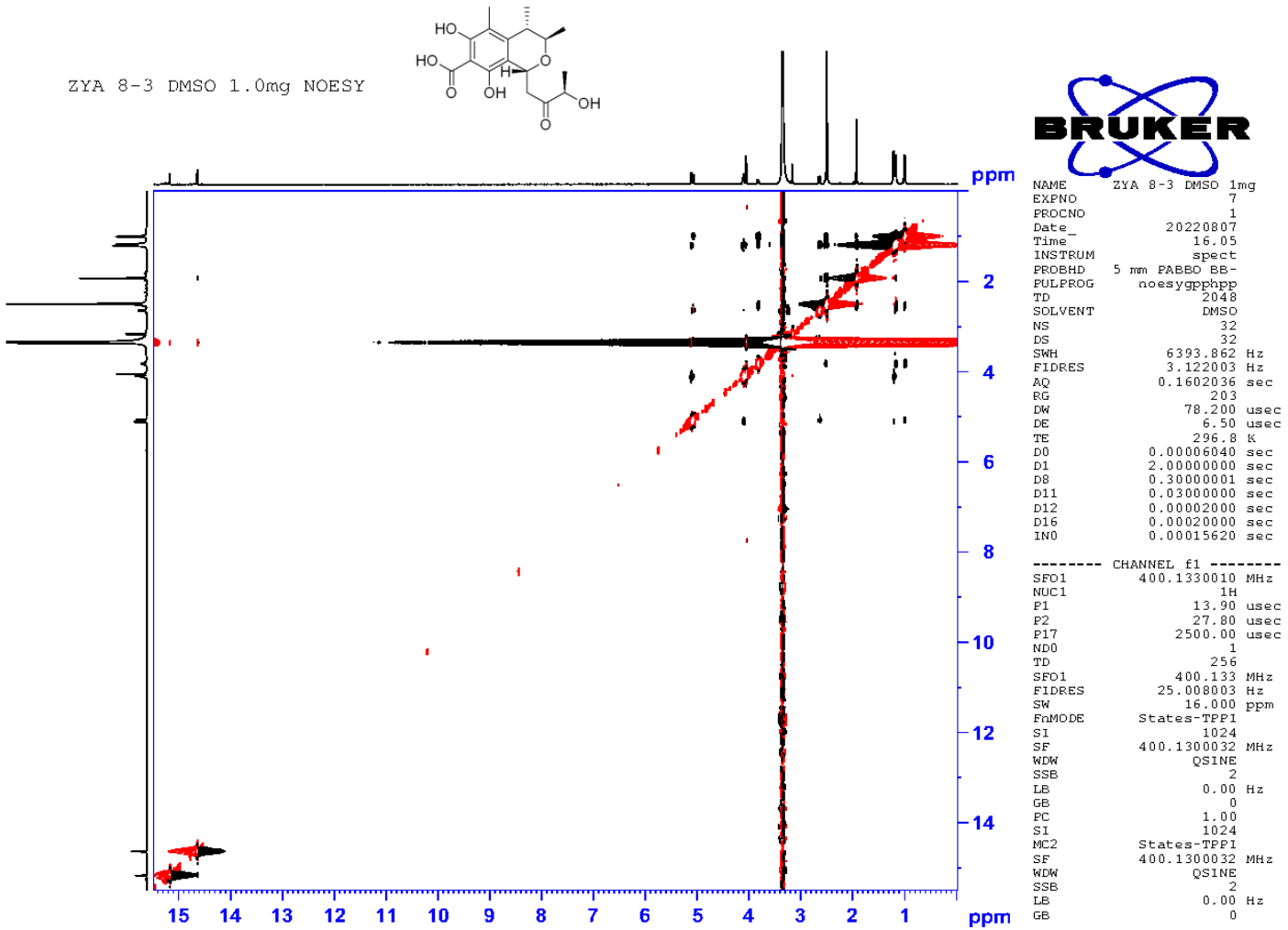
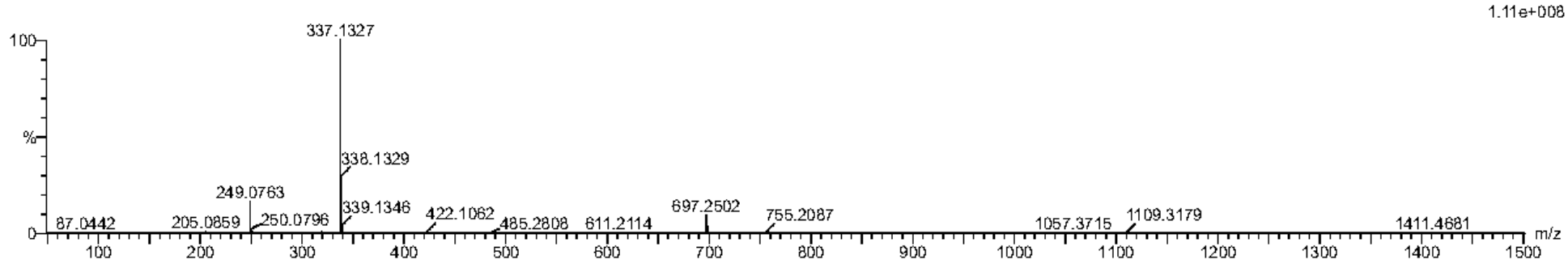


Figure S14. The NOESY spectrum of compound **2** in DMSO-d_6.

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**.

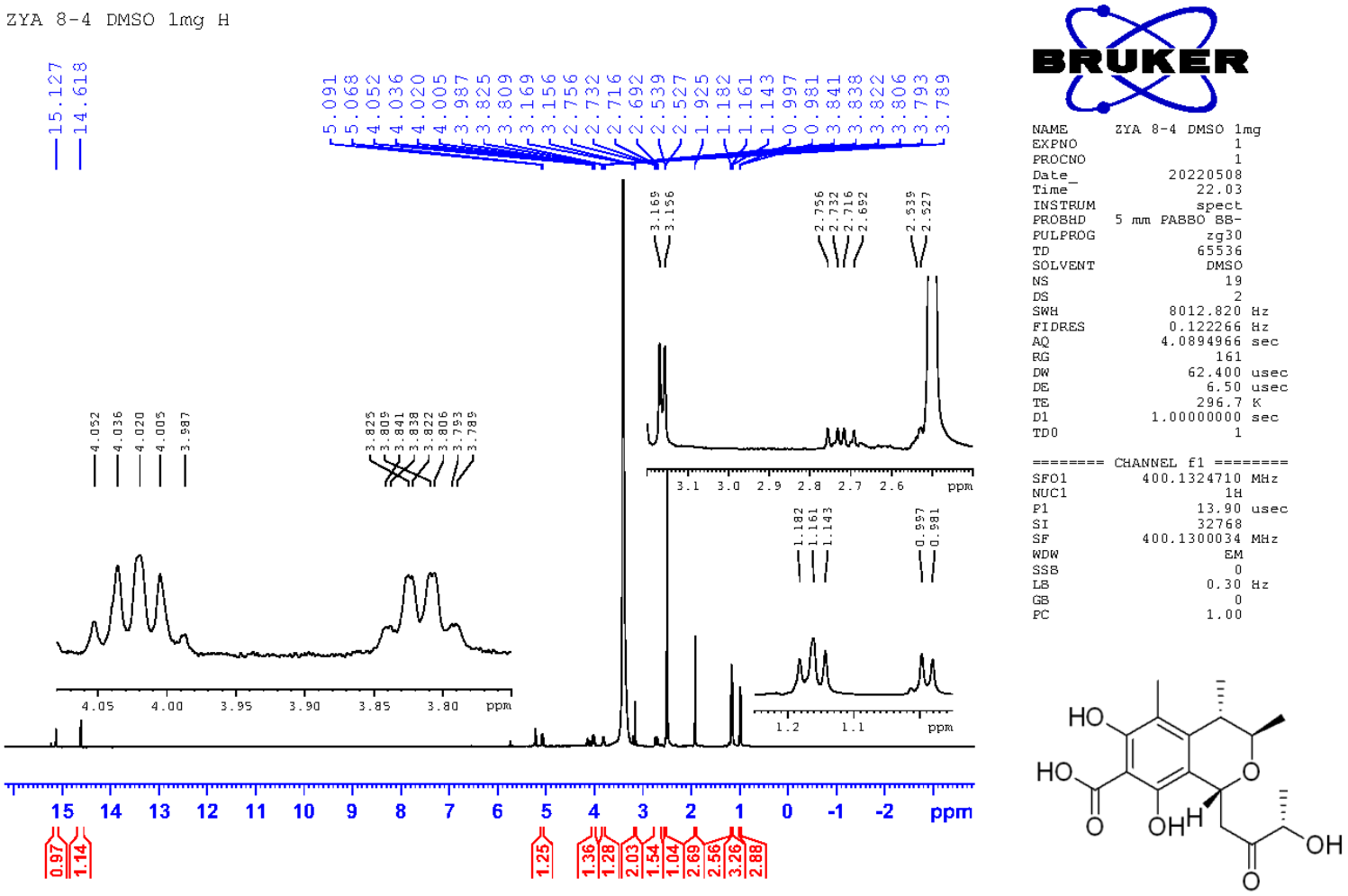


Figure S16. The ^{1}H NMR spectrum of compound **3** in DMSO-d_6.

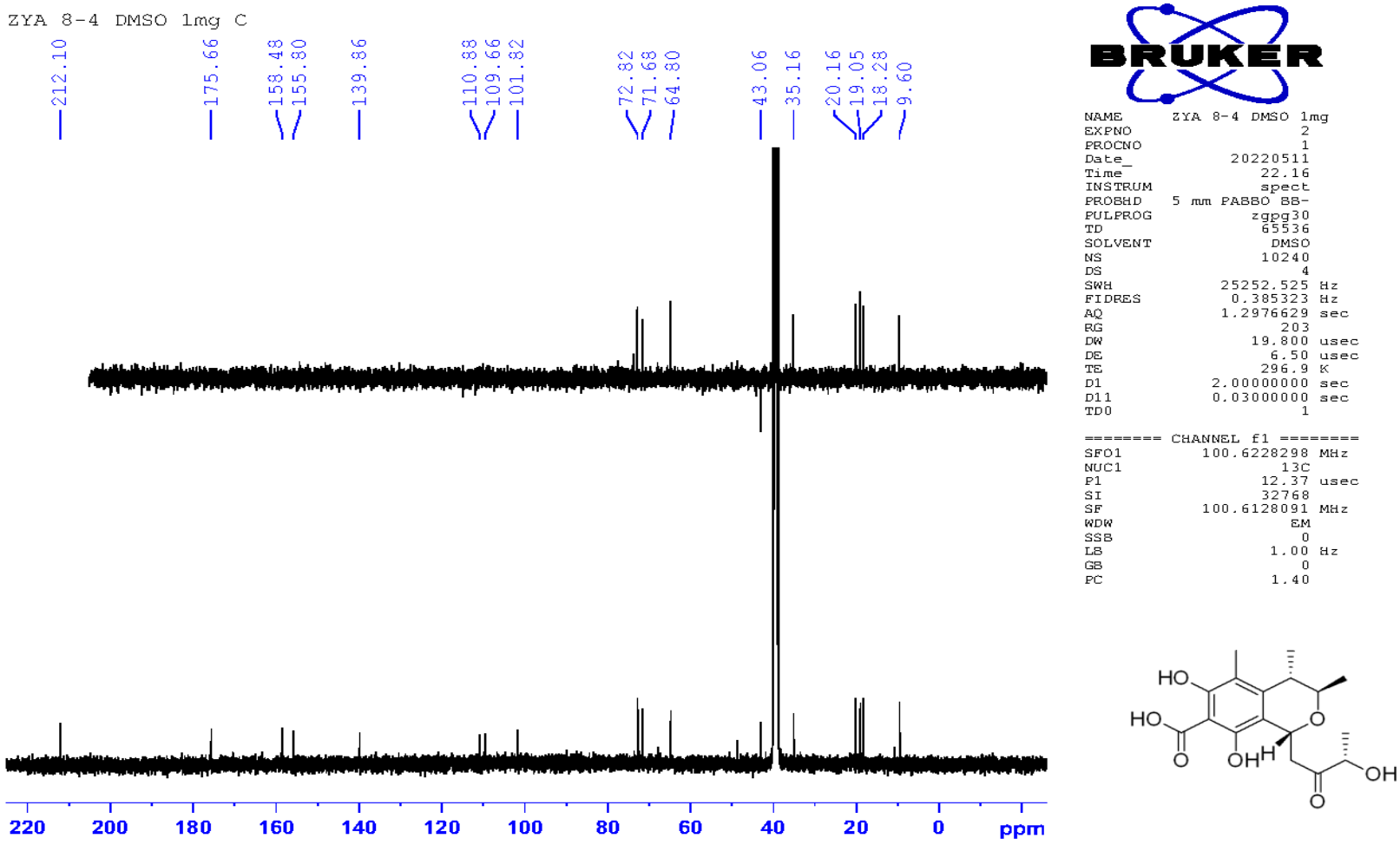
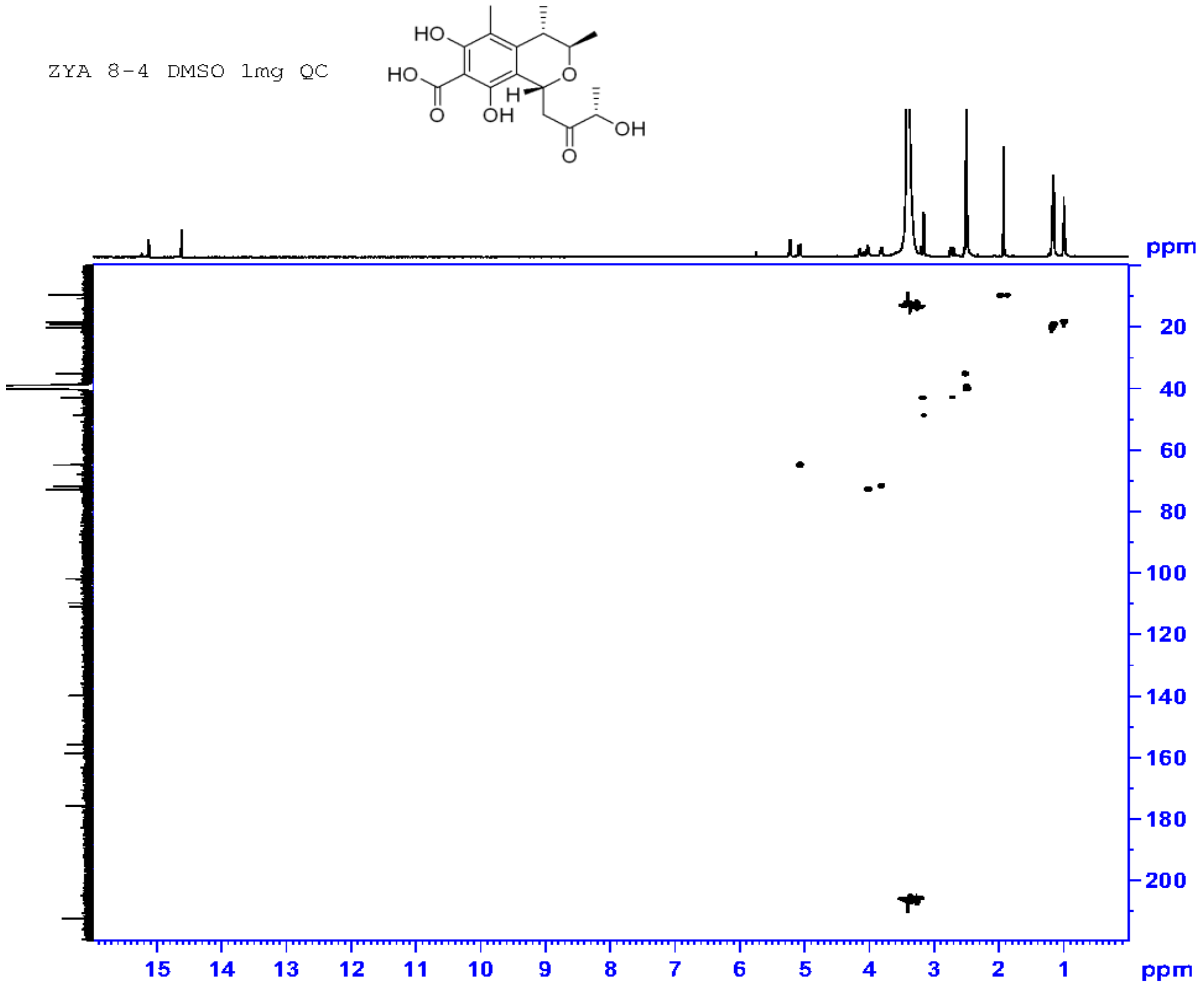


Figure S17. The ^{13}C NMR spectrum of compound **3** in DMSO-d_6.

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EXPNO                      4
PROCNO                     1
Date_            20220703
Time                 11.24
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.

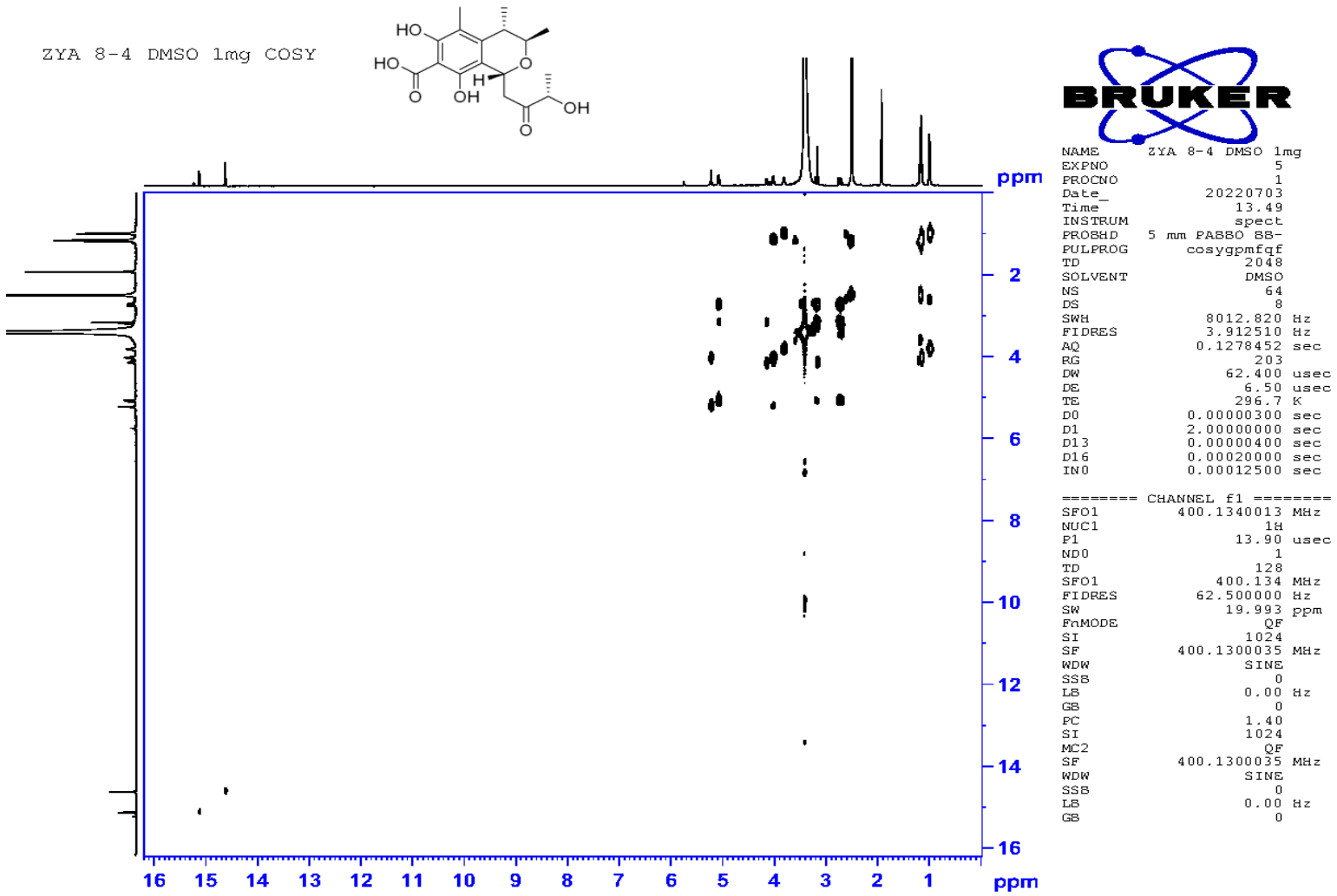
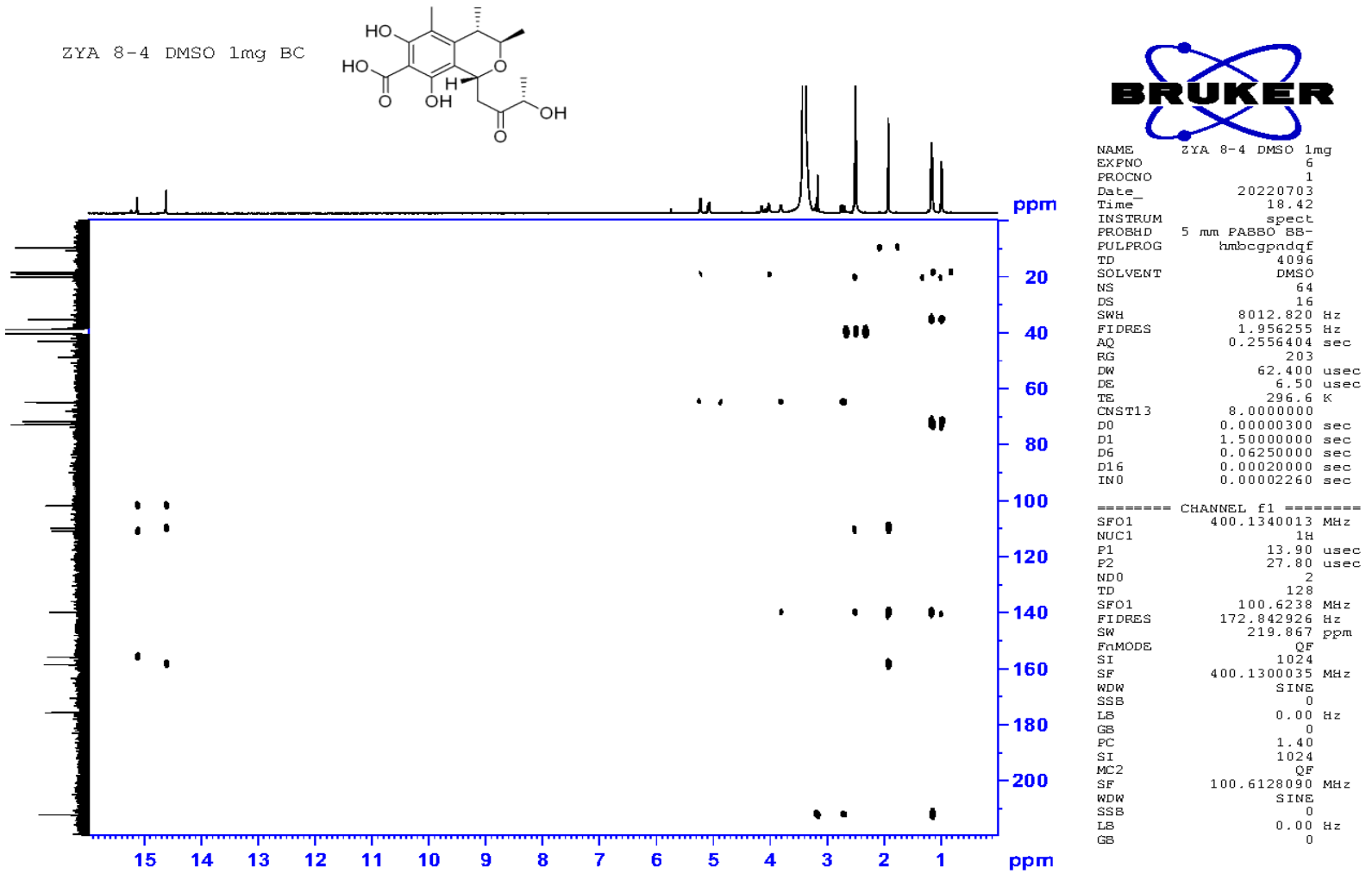


Figure S19. The ^{1}H-^{1}H COSY spectrum of compound **3** in DMSO-d_6.



BRUKER

NAME	ZYA 8-4 DMSO 1mg
EXPNO	6
PROCNO	1
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INSTRUM	spect
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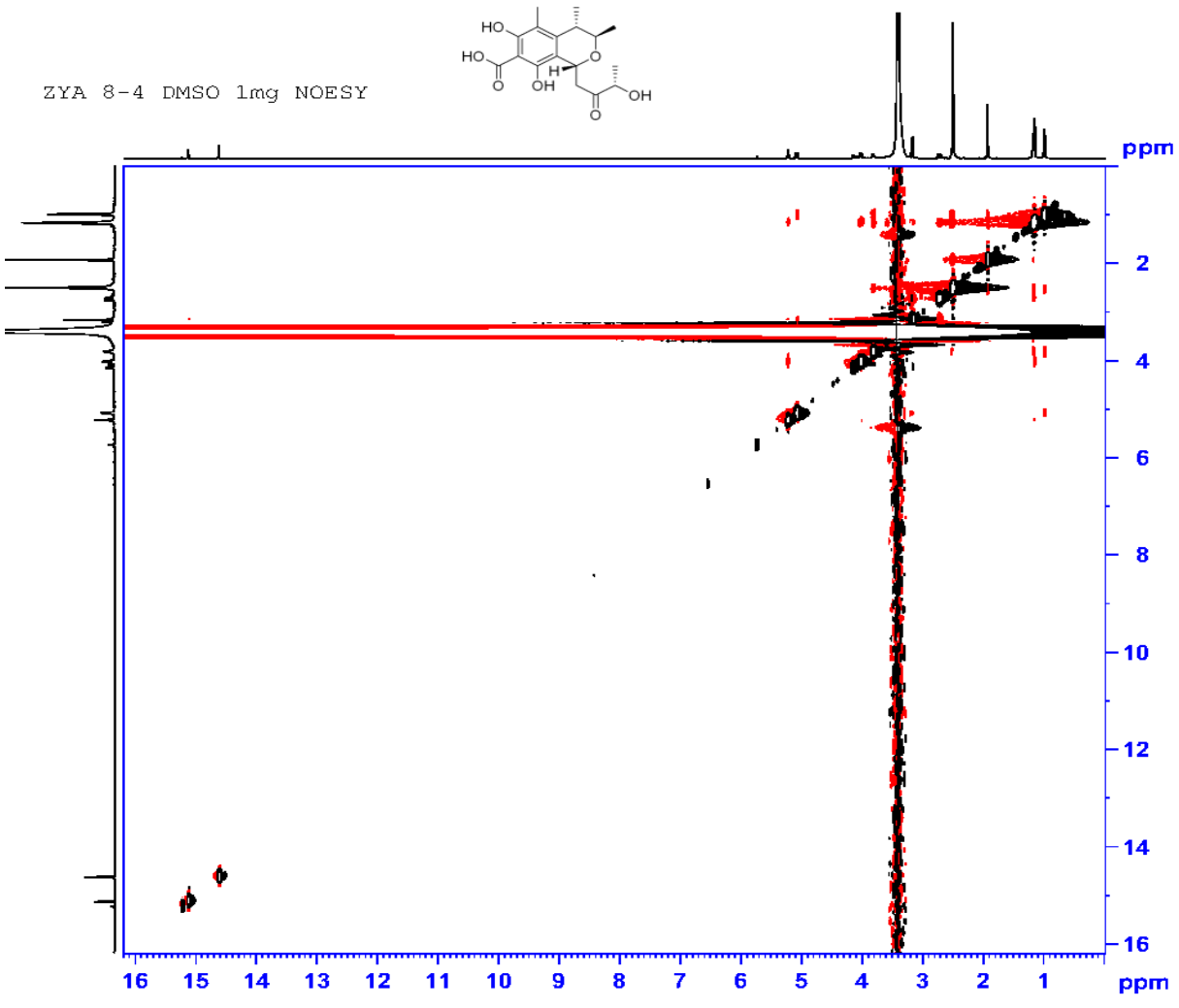
PULPROG	hmbcgpndqf
TD	4096
SOLVENT	DMSO
NS	64
DS	16
SWH	8012.820 Hz
FIDRES	1.956255 Hz
AQ	0.2556404 sec
RG	203
DW	62.400 usec
DE	6.50 usec
TE	296.6 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00002260 sec
======== CHANNEL f1 ========	
SFO1	400.1340013 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 --------
SFO1             400.1340013 MHz
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.