

Current Data Parameters  
 NAME YJA-40 C 8mg  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210912  
 Time\_ 17.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 18  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P1 13.90 usec  
 PLW1 12.14299965 W

F2 - Processing parameters  
 SI 32768  
 SF 400.1300056 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

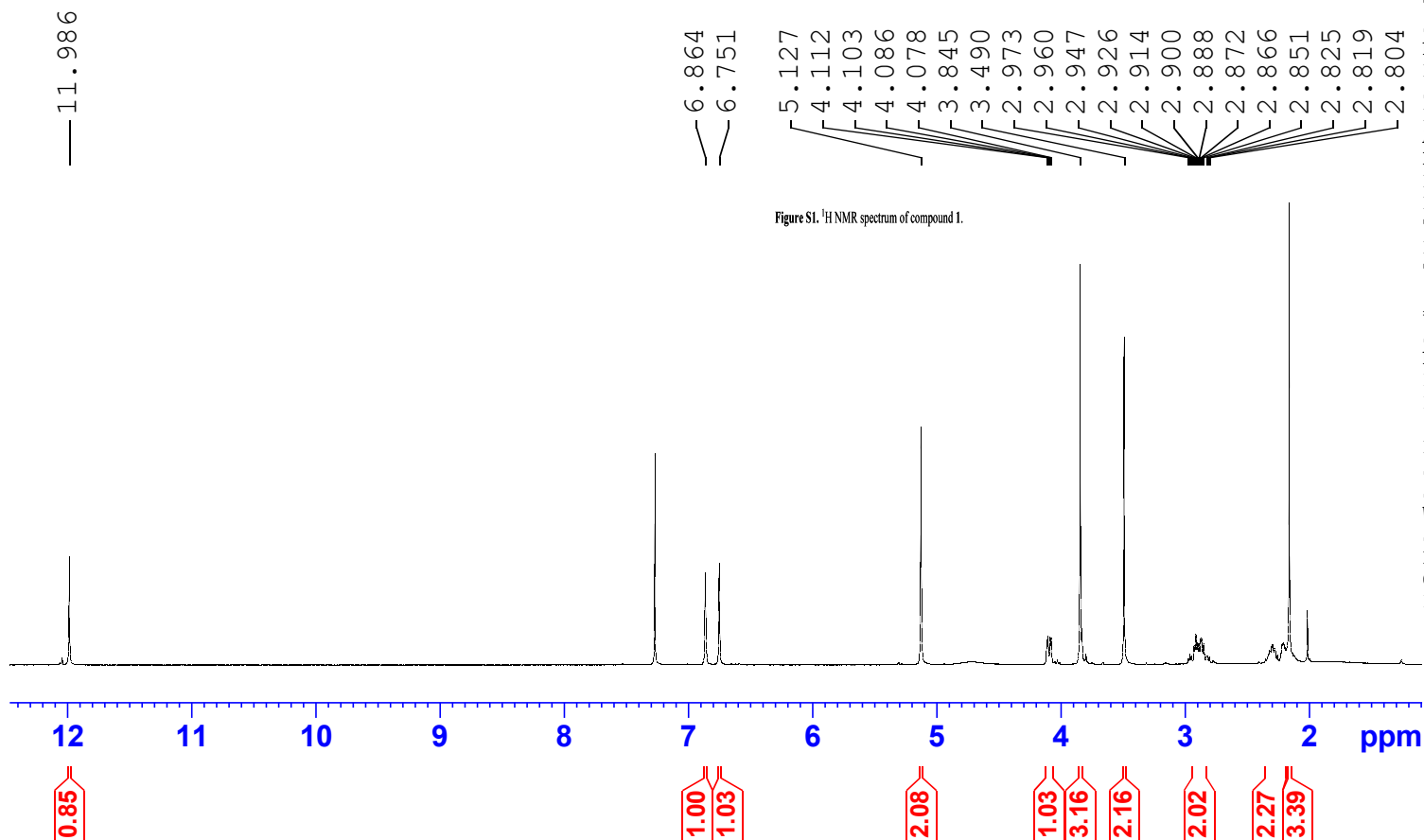
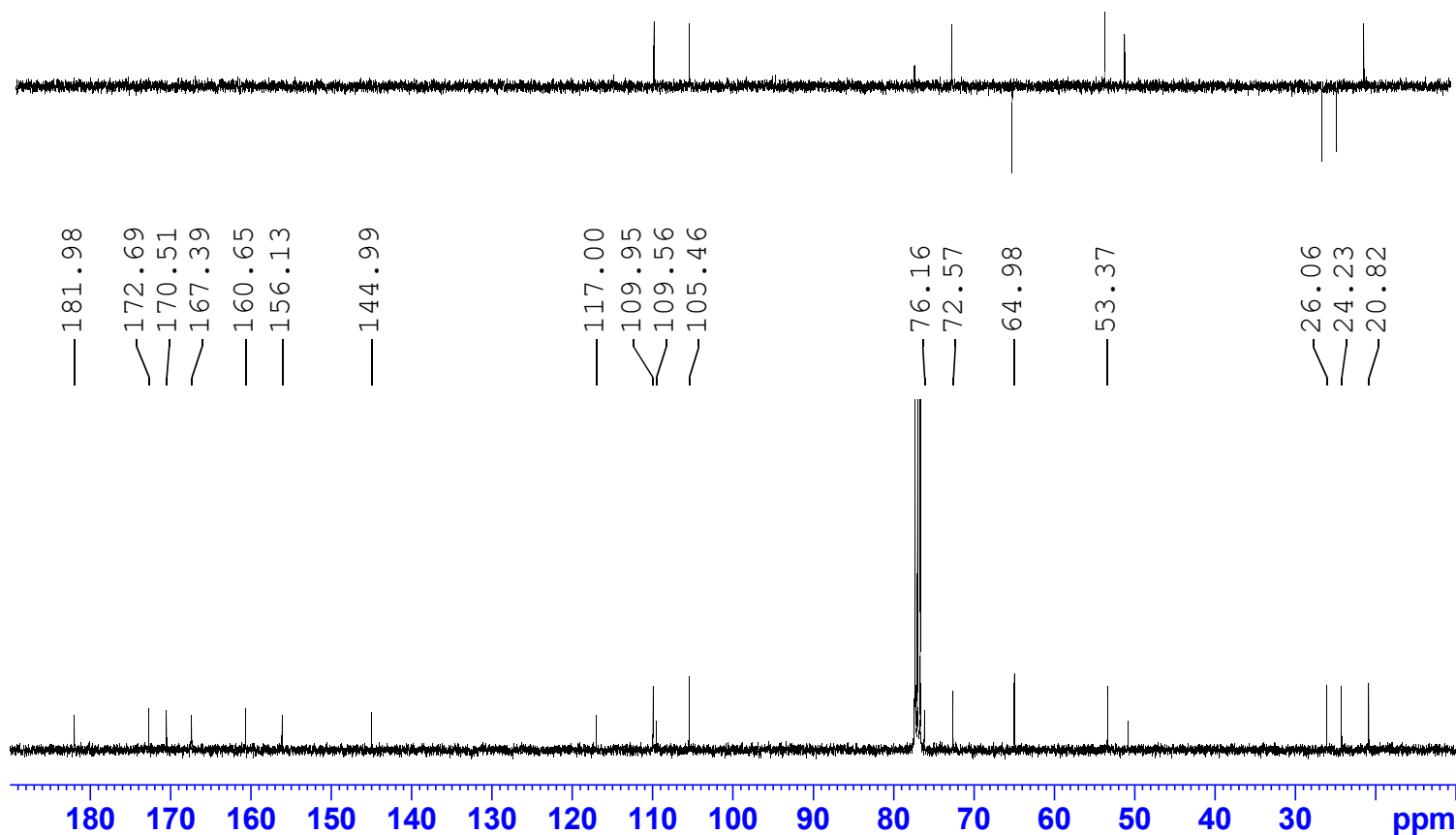
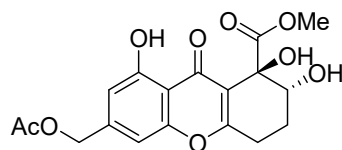
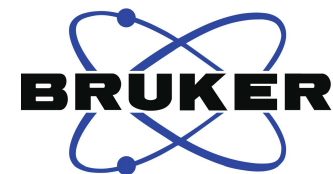


Figure S1. <sup>1</sup>H NMR spectrum of compound 1.

YJA-40 C 8mg C



Current Data Parameters  
NAME YJA-40 C 8mg  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210912  
Time\_ 17.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 484  
DS 4  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976128 sec  
RG 203  
DW 19.800 usec  
DE 6.50 usec  
TE 296.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

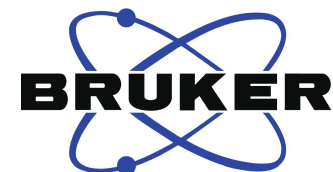
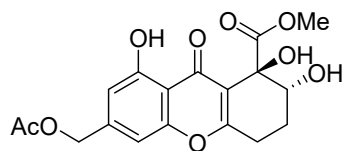
===== CHANNEL f1 =====  
SFO1 100.6228293 MHz  
NUC1 13C  
P1 12.37 usec  
PLW1 28.13500023 W

===== CHANNEL f2 =====  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.14299965 W  
PLW12 0.28964999 W  
PLW13 0.23461001 W

F2 - Processing parameters  
SI 32768  
SF 100.6127721 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure S2. <sup>13</sup>C NMR of compound 1.

YJA-40 C 8mg HSQC



Current Data Parameters  
NAME YJA-40 C 8mg  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211003  
Time 17.34  
INSTRUM spect  
PROBHD 5 mm PARBO BB-  
PULPROG hsqcetgpsisp2.2  
TD 1024  
SOLVENT CDCl3  
NS 8  
DS 32  
SWH 5597.015 Hz  
FIDRES 5.465835 Hz  
AQ 0.0914773 sec  
RG 203  
DW 89.333 usec  
DE 6.50 usec  
TE 296.3 K  
CNST2 145.000000  
CNST17 -0.500000  
D0 0.00000300 sec  
D1 2.00000000 sec  
D4 0.00172414 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.0002480 sec

===== CHANNEL f1 =====  
SFO1 400.1328009 MHz  
NUC1 1H  
P1 13.90 usec  
P2 27.80 usec  
P28 1000.00 usec  
PLW1 12.14299965 W

===== CHANNEL f2 =====  
SFO2 100.6228298 MHz  
NUC2 13C  
CPDPRG[2] garp  
P3 12.37 usec  
P14 500.00 usec  
P24 2000.00 usec  
PCPD2 70.00 usec  
PLW0 0 W  
PLW2 28.13500023 W  
PLW12 0.87860000 W  
SPNAM[3] Crp60,0.5,20.1  
SFOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 6.57779980 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPNAM[4] SMSQ10.100  
GPZ1 80.00 %  
GPZ2 20.10 %  
GPZ3 11.00 %  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 100.6228 MHz  
FIDRES 157.510086 Hz  
SW 200.365 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 400.1300096 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MZ2 echo-antiecho  
SF 100.6127726 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

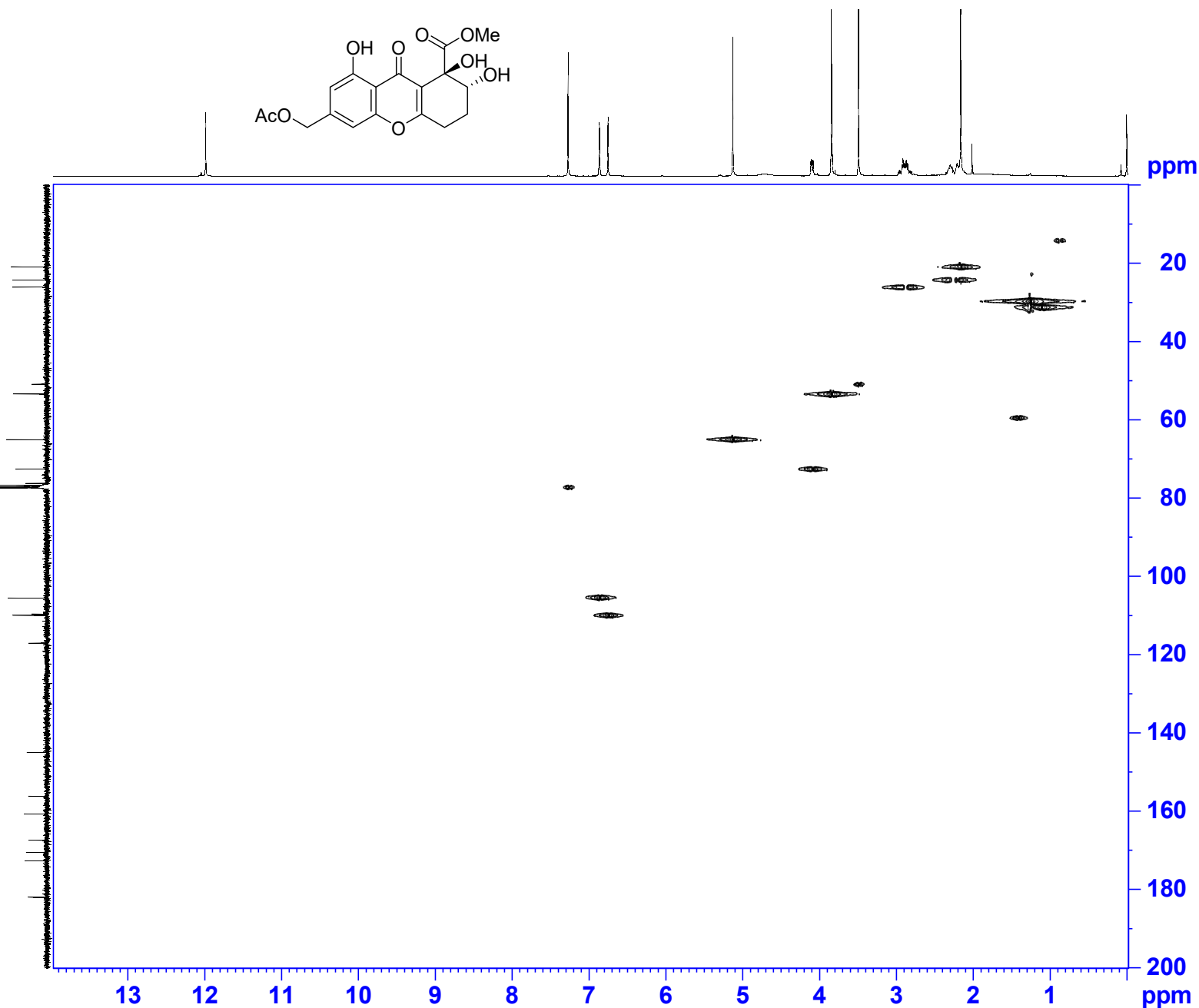
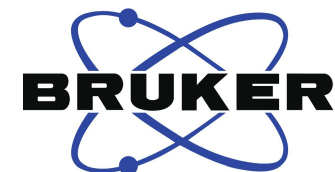


Figure S3. HSQC spectrum of compound 1.

YJA-40 C 8mg COSY



Current Data Parameters  
NAME YJA-40 C 8mg  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211003  
Time\_ 18.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpmfzf  
TD 2048  
SOLVENT CDCl3  
NS 4  
DS 8  
SWH 5597.015 Hz  
FIDRES 2.732918 Hz  
AQ 0.1829547 sec  
RG 203  
DW 89.333 usec  
DE 6.50 usec  
TE 296.3 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00017860 sec

===== CHANNEL f1 =====  
SFO1 400.1328009 MHz  
NUC1 1H  
P1 13.90 usec  
PLW1 12.14299965 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 128  
SFO1 400.1328 MHz  
FIDRES 87.486000 Hz  
SW 13.993 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 400.1300096 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 400.1300096 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

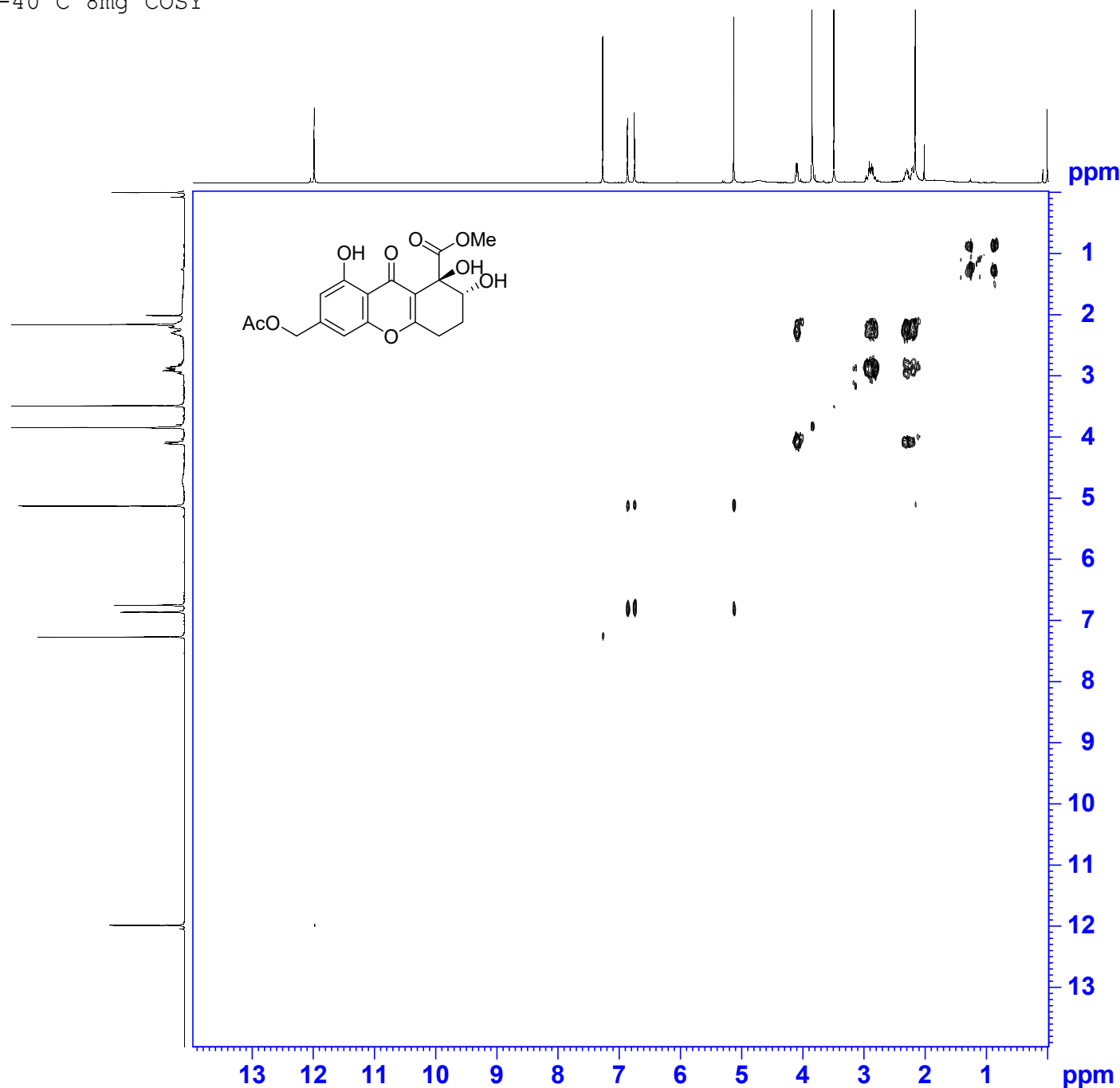
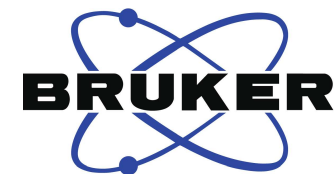


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 1.

YJA-40 C 8mg BC



Current Data Parameters  
NAME YJA-40 C 8mg  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211003  
Time 19.07

INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcgpndqf  
TD 4096  
SOLVENT CDCl3  
NS 32  
DS 16  
SWH 5597.015 Hz  
FIDRES 1.366459 Hz  
AQ 0.3659093 sec  
RG 203  
DW 89.333 usec  
DE 6.50 usec  
TE 296.1 K  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00002480 sec

===== CHANNEL f1 =====  
SFO1 400.1328009 MHz  
NUC1 1H  
P1 13.90 usec  
P2 27.80 usec  
PLW1 12.14299965 W

===== CHANNEL f2 =====  
SFO2 100.6228298 MHz  
NUC2 13C  
P3 12.37 usec  
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPZ1 50.00 %  
GPZ2 30.00 %  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 128  
SFO1 100.6228 MHz  
FIDRES 315.020172 Hz  
SW 200.365 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 400.1300096 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 100.6127726 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

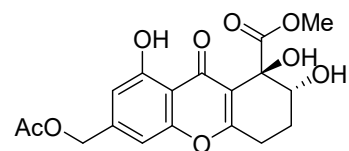


Figure S5. HMBC spectrum of compound 1.

YJA-40 C 8mg NOESY



Current Data Parameters  
 NAME HYJ1-MD-1-YJA-40 C 8mg  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220102  
 Time\_ 18.46  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG noesygpph  
 TD 2048  
 SOLVENT CDCl3  
 NS 32  
 DS 32  
 SWH 5597.015 Hz  
 FIDRES 2.732918 Hz  
 AQ 0.1829547 sec  
 RG 203  
 DW 89.333 usec  
 DE 6.50 usec  
 TE 295.3 K  
 D0 0.00007160 sec  
 D1 2.00000000 sec  
 D8 0.30000001 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec  
 D16 0.00020000 sec  
 INO 0.00017860 sec

===== CHANNEL f1 =====  
 SFO1 400.1328009 MHz  
 NUC1 1H  
 P1 13.90 usec  
 P2 27.80 usec  
 P17 2500.00 usec  
 PLW1 12.14299965 W  
 PLW10 3.47059989 W

===== GRADIENT CHANNEL =====  
 GPNAM[1] SMSQ10.100  
 GPZ1 40.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 256  
 SFO1 400.1328 MHz  
 FIDRES 21.871500 Hz  
 SW 13.993 ppm  
 FMODE States-TPPI

F2 - Processing parameters  
 SI 1024  
 SF 400.1300059 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TPPI  
 SF 400.1300098 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

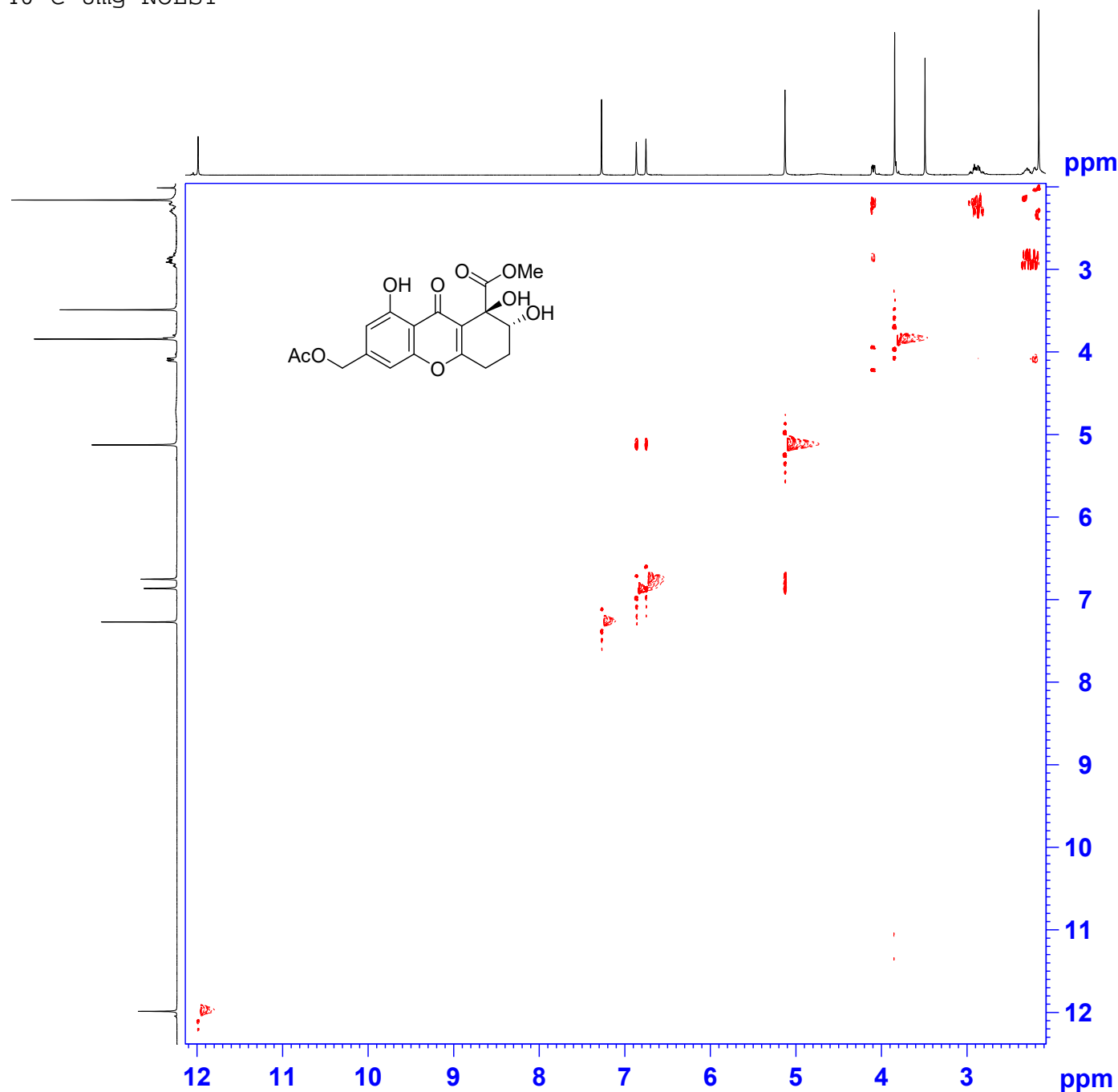


Figure S6. NOESY spectrum of compound 1.

Elemental Composition Report

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  
99 formula(e) evaluated with 9 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  
YJA-40 71 (0.293) Cm (65:85)  
1: TOF MS ES+

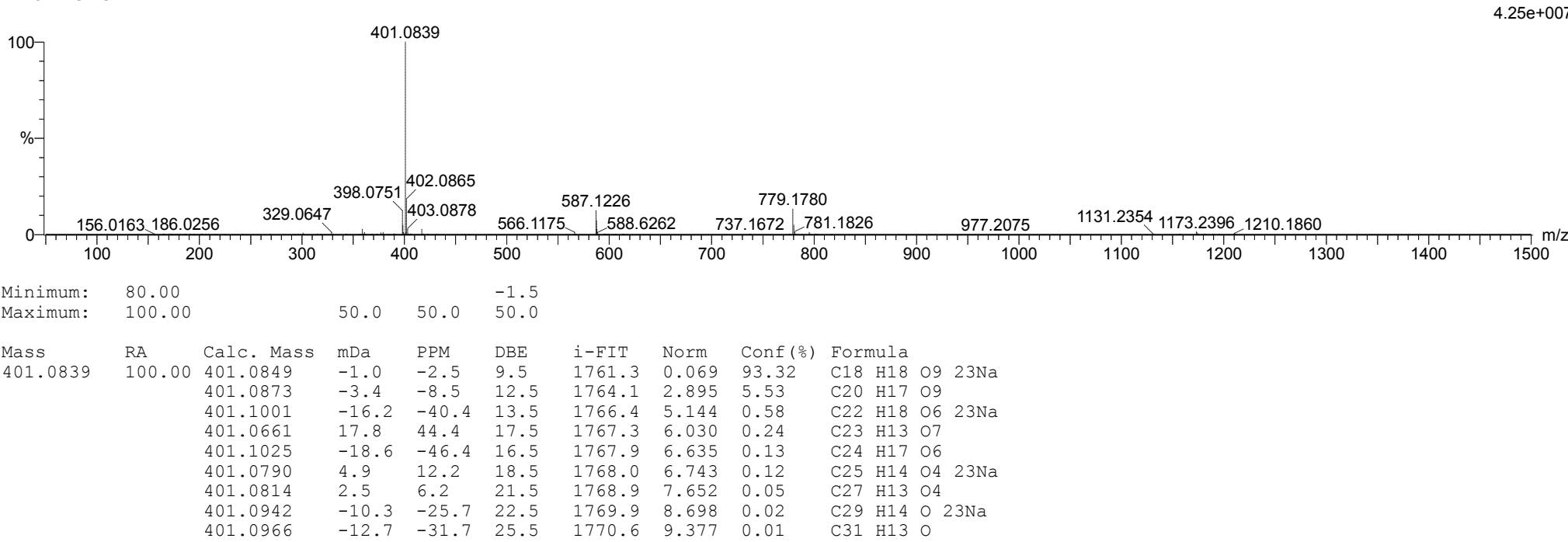
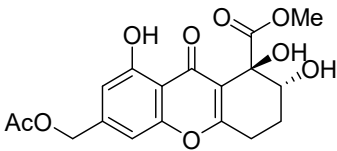
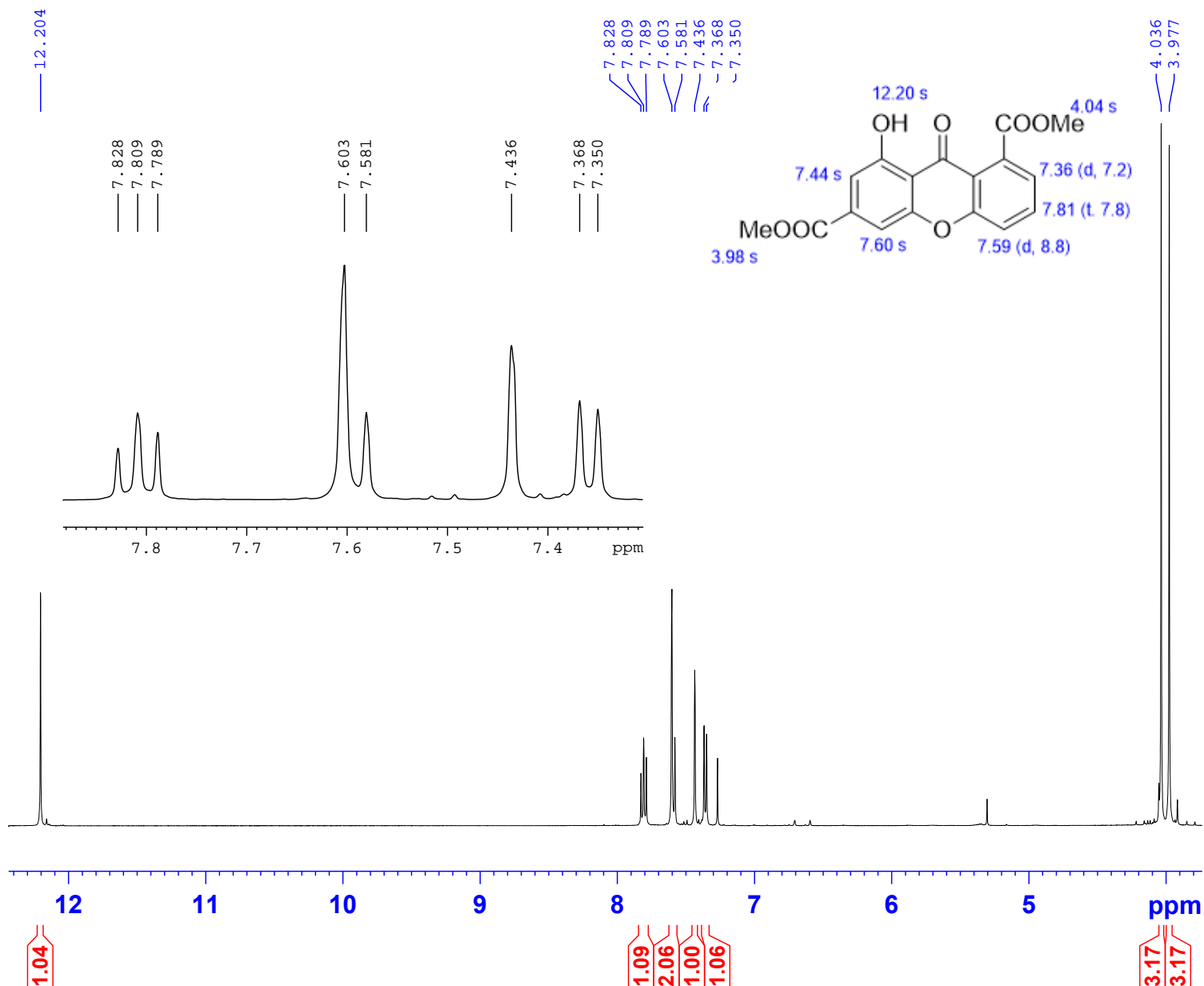


Figure S7. HR-ESI-MS spectrum of compound 1.

YJA-3 C 15 mg H



Current Data Parameters  
NAME YJA-3 C 15 mg  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210406  
Time 12.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 61  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1

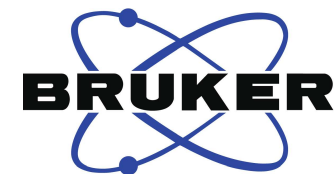
===== CHANNEL f1 =====  
SFO1 400.1324710 MHz  
NUC1 1H  
P1 13.90 usec  
PLW1 12.14299965 W

F2 - Processing parameters  
SI 32768  
SF 400.1300055 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S8. <sup>1</sup>H NMR spectrum of compound 2.



YJA-3 C 15 mg C



Current Data Parameters  
 NAME YJA-3 C 15 mg  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210406  
 Time\_ 15.14  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 342  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 100.6228293 MHz  
 NUC1 13C  
 P1 12.37 usec  
 PLW1 28.13500023 W

===== CHANNEL f2 =====  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.14299965 W  
 PLW12 0.28964999 W  
 PLW13 0.23461001 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127724 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

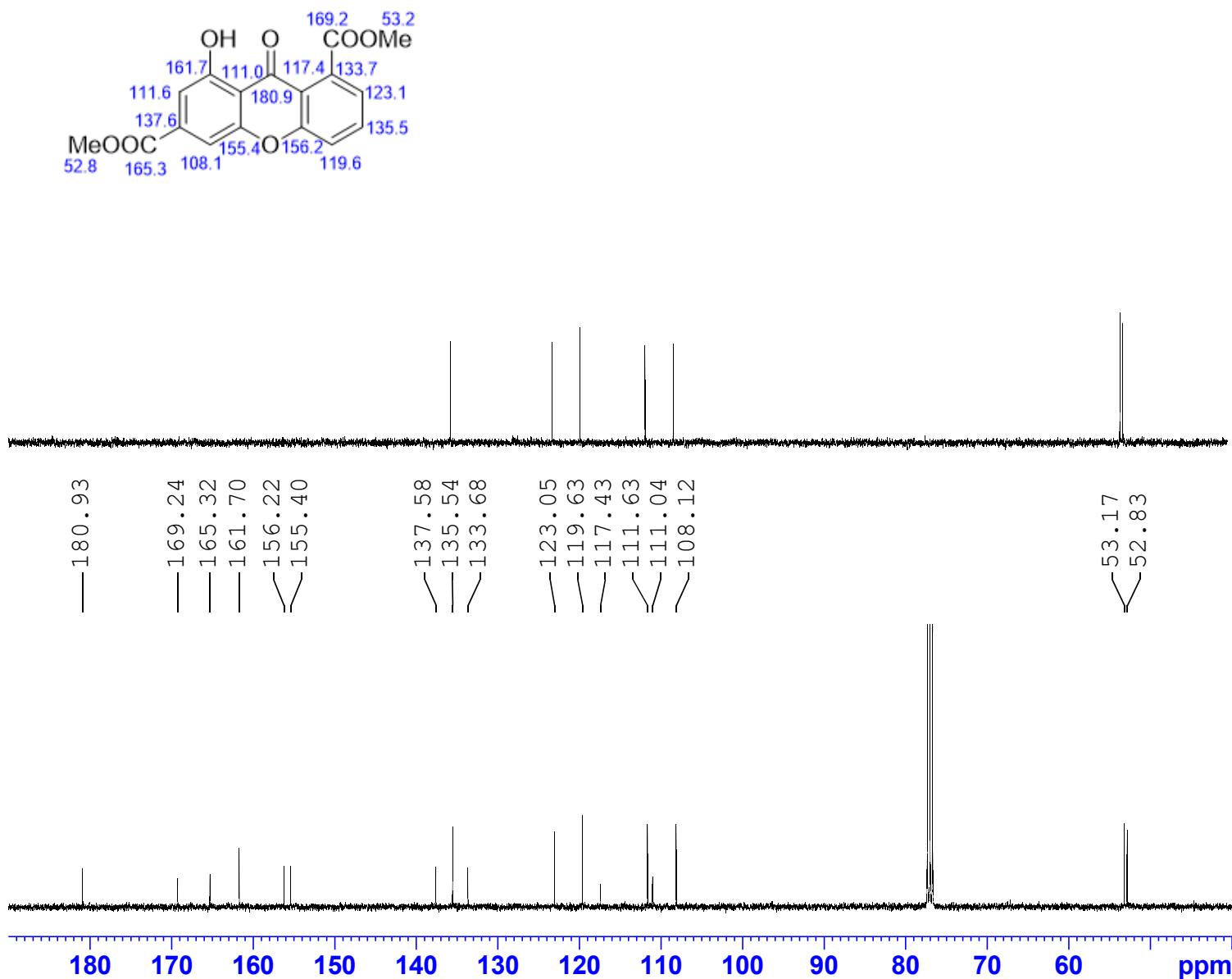
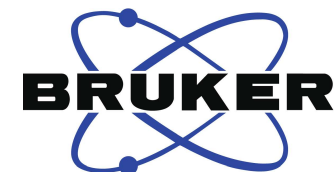


Figure S9. 13C NMR and DEPT of compound 2.

YJA-3 C 15 mg HSQC



Current Data Parameters  
NAME YJA-3 C 15 mg  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210530  
Time 20.23  
INSTRUM spect  
PROBHD 5 mm PARBO BB-  
PULPROG hsqcetgpsisp2.2  
TD 1024  
SOLVENT CDC13  
NS 8  
DS 32  
SWH 5197.505 Hz  
FIDRES 5.075689 Hz  
AQ 0.0985088 sec  
RG 203  
DW 96.200 usec  
DE 6.50 usec  
TE 296.2 K  
CNST2 145.000000  
CNST17 -0.500000  
D0 0.00000300 sec  
D1 2.00000000 sec  
D4 0.00172414 sec  
D11 0.03000000 sec  
D16 0.00020000 sec  
D24 0.00089000 sec  
IN0 0.0002620 sec

===== CHANNEL f1 =====  
SFO1 400.1326008 MHz  
NUC1 1H  
P1 13.90 usec  
P2 27.80 usec  
P28 1000.00 usec  
PLW1 12.14299965 W

===== CHANNEL f2 =====  
SFO2 100.6223267 MHz  
NUC2 13C  
CPDPRG[2] garp  
P3 12.37 usec  
P14 500.00 usec  
P24 2000.00 usec  
PCPD2 70.00 usec  
PLW0 0 W  
PLW2 28.13500023 W  
PLW12 0.87860000 W  
SPNAM[3] Crp60,0.5,20.1  
SFOAL3 0.500  
SPOFFS3 0 Hz  
SPW3 6.57779980 W  
SPNAM[7] Crp60comp.4  
SFOAL7 0.500  
SPOFFS7 0 Hz  
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPNAM[4] SMSQ10.100  
GPZ1 80.00 %  
GPZ2 20.10 %  
GPZ3 11.00 %  
GPZ4 -5.00 %  
P16 1000.00 usec  
P19 600.00 usec

F1 - Acquisition parameters  
TD 256  
SFO1 100.6223 MHz  
FIDRES 149.093506 Hz  
SW 189.659 ppm  
FMODE Echo-Antiecho

F2 - Processing parameters  
SI 1024  
SF 400.1300051 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MZ2 echo-antiecho  
SF 100.6127975 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

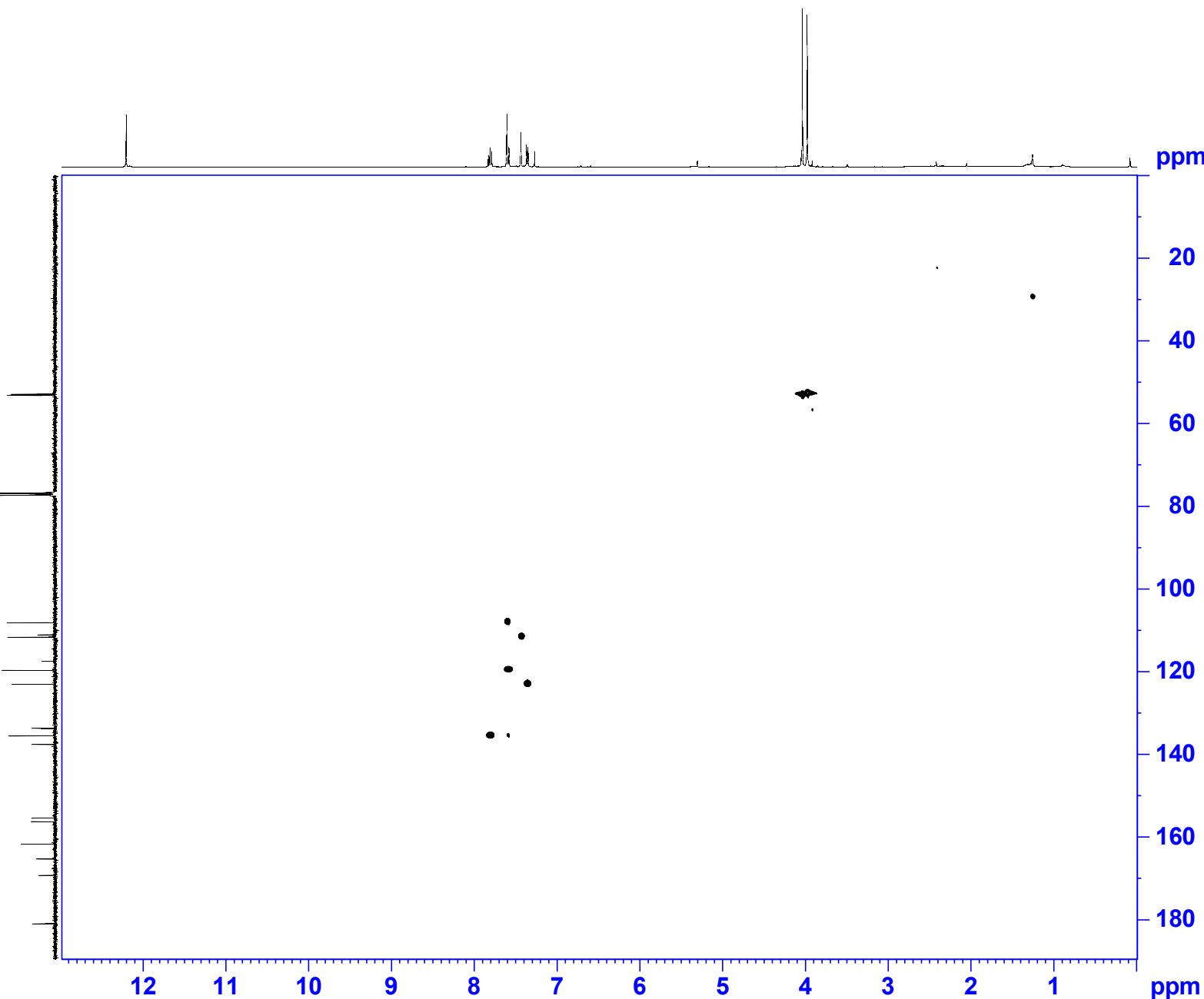
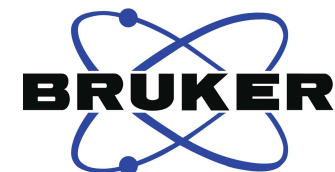


Figure S10. HMQC spectrum of compound 2.

YJA-3 C 15 mg COSY



Current Data Parameters

NAME YJA-3 C 15 mg  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20210530  
Time\_ 21.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosygpmfzf  
TD 2048  
SOLVENT CDCl3  
NS 4  
DS 8  
SWH 5197.505 Hz  
FIDRES 2.537844 Hz  
AQ 0.1970176 sec  
RG 203  
DW 96.200 usec  
DE 6.50 usec  
TE 296.3 K  
D0 0.00000300 sec  
D1 2.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00019220 sec

===== CHANNEL f1 =====

SFO1 400.1326008 MHz  
NUC1 1H  
P1 13.90 usec  
PLW1 12.14299965 W

===== GRADIENT CHANNEL =====

GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters

TD 128  
SFO1 400.1326 MHz  
FIDRES 81.295525 Hz  
SW 13.003 ppm  
FnMODE QF

F2 - Processing parameters

SI 1024  
SF 400.1300099 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters

SI 1024  
MC2 QF  
SF 400.1300099 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

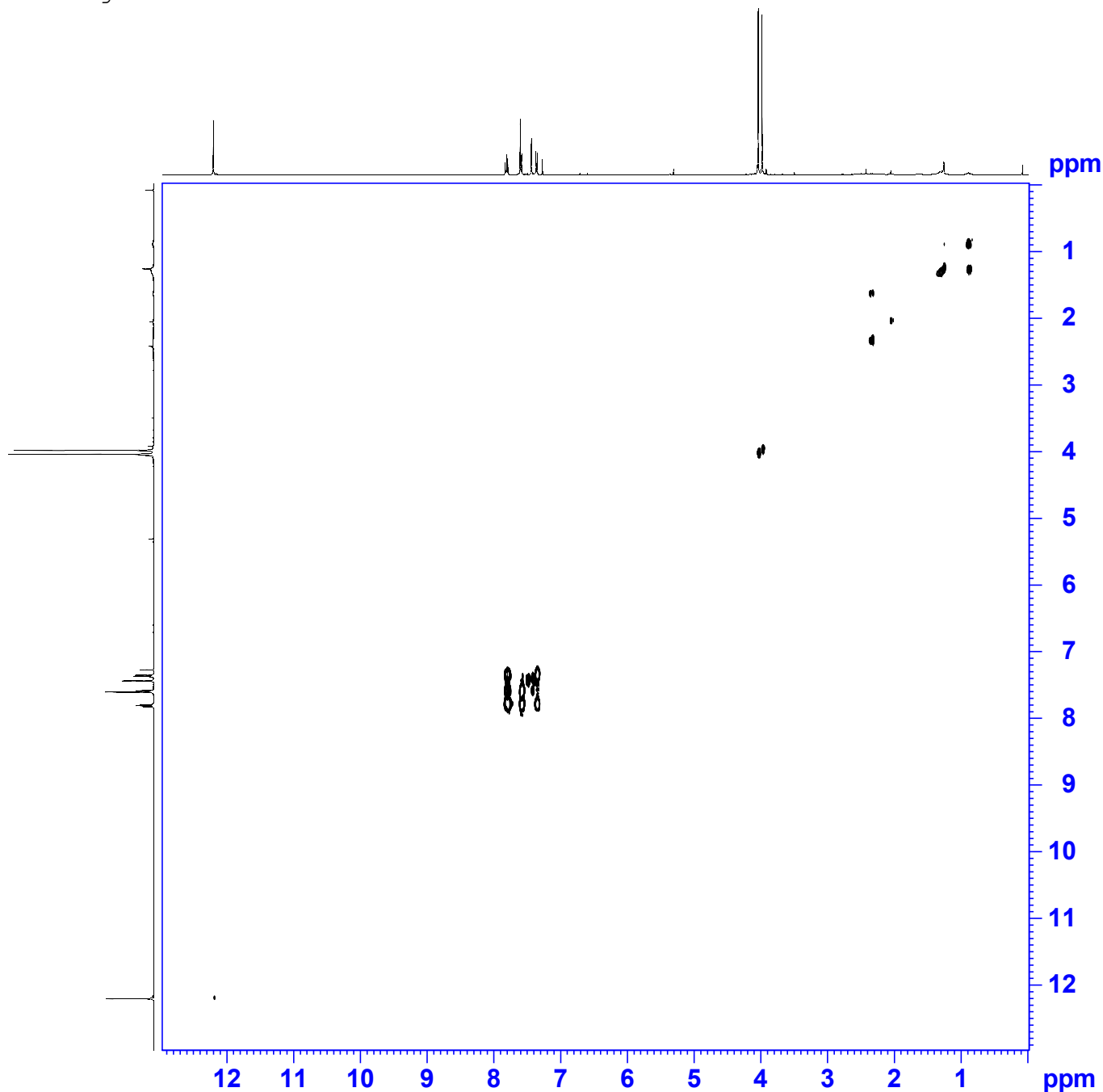
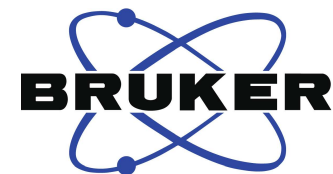


Figure S11. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 2.



Current Data Parameters  
NAME YJA-3 C 15 mg  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210530  
Time 21.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcgpndqf  
TD 4096  
SOLVENT CDCl3  
NS 32  
DS 16  
SWH 5197.505 Hz  
FIDRES 1.268922 Hz  
AQ 0.3940352 sec  
RG 203  
DW 96.200 usec  
DE 6.50 usec  
TE 295.9 K  
CNST13 8.0000000  
D0 0.00000300 sec  
D1 1.50000000 sec  
D6 0.06250000 sec  
D16 0.00020000 sec  
IN0 0.00002620 sec

===== CHANNEL f1 =====  
SFO1 400.1326008 MHz  
NUC1 1H  
P1 13.90 usec  
P2 27.80 usec  
PLW1 12.14299965 W

===== CHANNEL f2 =====  
SFO2 100.6223267 MHz  
NUC2 13C  
P3 12.37 usec  
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====  
GPNAM[1] SMSQ10.100  
GPNAM[2] SMSQ10.100  
GPNAM[3] SMSQ10.100  
GPZ1 50.00 %  
GPZ2 30.00 %  
GPZ3 40.10 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 128  
SFO1 100.6223 MHz  
FIDRES 298.187012 Hz  
SW 189.659 ppm  
FnMODE QF

F2 - Processing parameters  
SI 1024  
SF 400.1300033 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 100.6127437 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

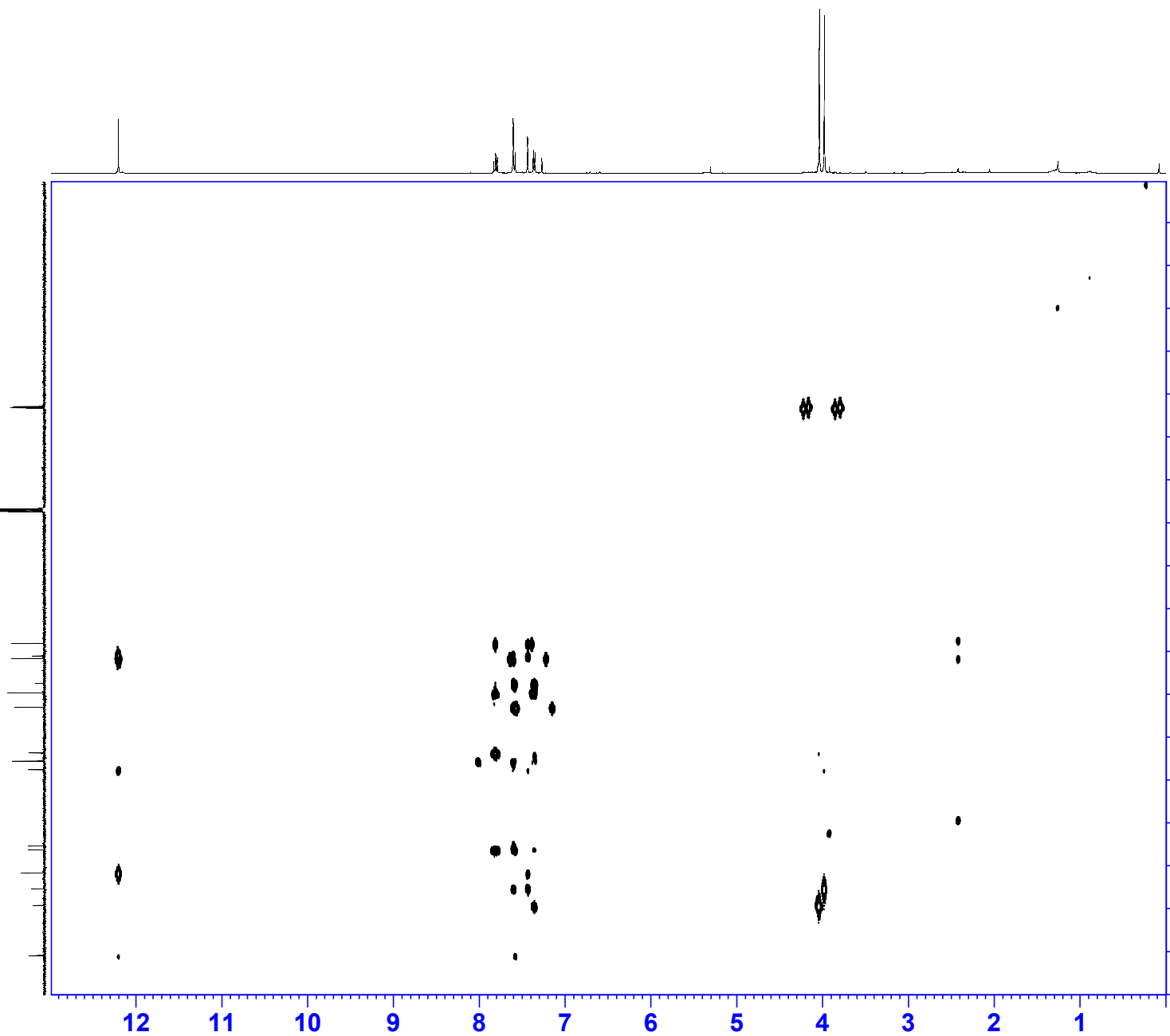


Figure S12. HMBC spectrum of compound 2.

Elemental Composition Report

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  
91 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  
YJA-3 95 (0.379) Cm (79:114)  
1: TOF MS ES+

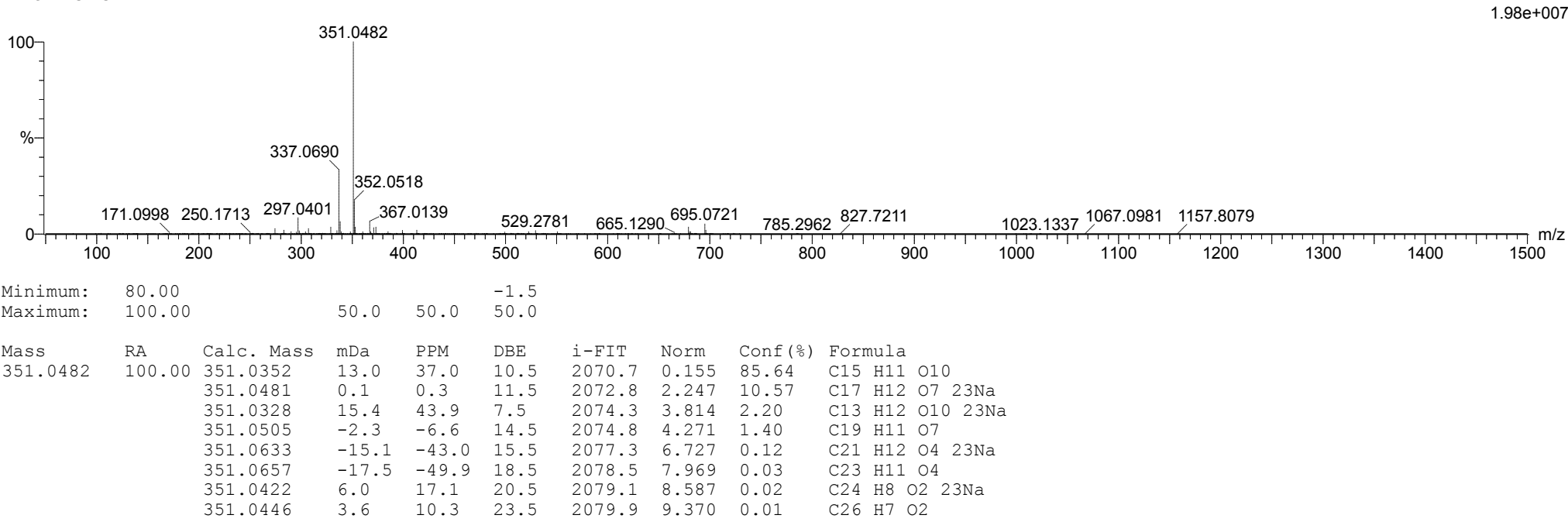


Figure S13. HR-ESI-MS spectrum of compound 2.