

## Supporting Information

# Biotransformation of Ursonic Acid by *Aspergillus ochraceus* and *Aspergillus oryzae* to Discover Anti-Neuroinflammatory Derivatives

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**Table S1.** Crystal data and structure refinement for compound **10**

Identification code	cu_20221190_0m_sq_sq
Empirical formula	C <sub>31</sub> H <sub>48</sub> O <sub>3</sub>
Formula weight	468.69
Temperature/K	173.0
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	14.3799(8)
b/Å	7.9576(4)
c/Å	24.7623(15)
$\alpha$ /°	90
$\beta$ /°	101.068(4)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2780.8(3)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.119
$\mu/\text{mm}^{-1}$	0.537
F(000)	1032.0
Crystal size/mm <sup>3</sup>	0.07 × 0.03 × 0.01
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54178)
2 $\Theta$ range for data collection/°	6.262 to 124.748
Index ranges	-16 ≤ h ≤ 16, -5 ≤ k ≤ 9, -28 ≤ l ≤ 26
Reflections collected	12677
Independent reflections	6322 [ $R_{\text{int}}$ = 0.0856, $R_{\text{sigma}}$ = 0.1046]
Data/restraints/parameters	6322/1/631
Goodness-of-fit on F <sup>2</sup>	1.142
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.1085, $wR_2$ = 0.2960
Final R indexes [all data]	$R_1$ = 0.1502, $wR_2$ = 0.3421
Largest diff. peak/hole / e Å <sup>-3</sup>	0.51/-0.39
Flack parameter	-0.4(5)

**Table S2.** Crystal data and structure refinement for compound **13**

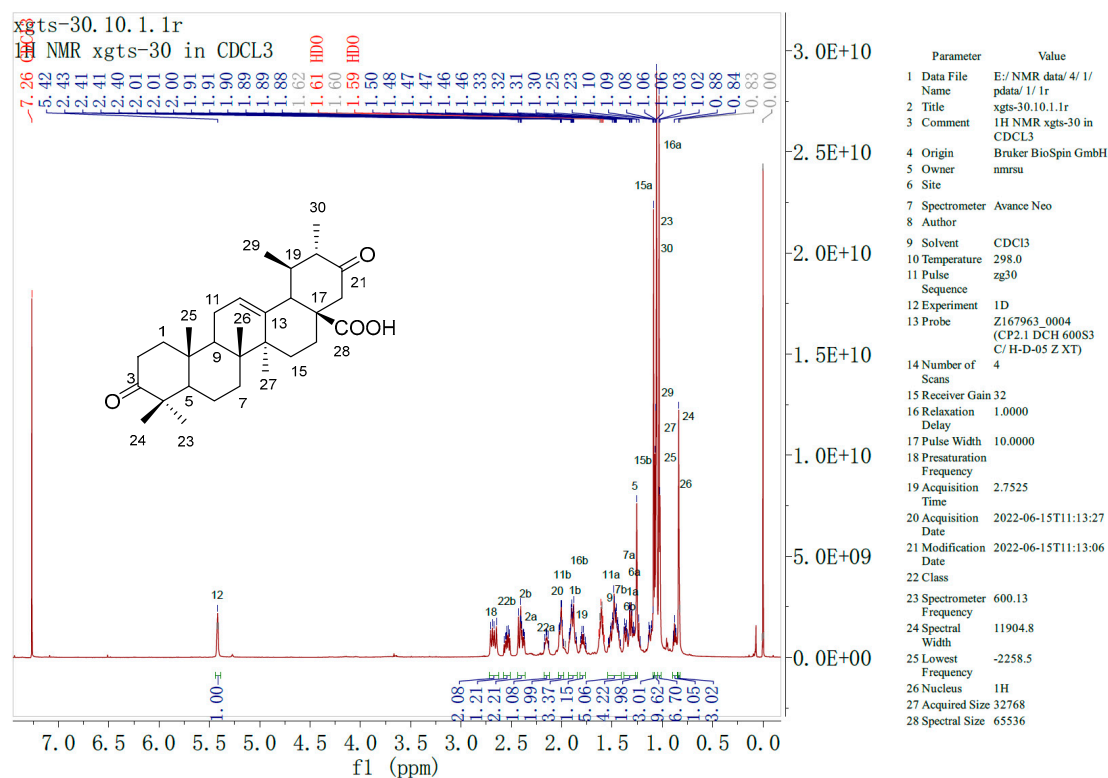
Identification code	XJTS13_0m
Empirical formula	C <sub>30</sub> H <sub>44</sub> O <sub>5</sub>
Formula weight	484.65
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	6.70930(10)
b/Å	14.3484(2)
c/Å	26.2474(4)
$\alpha$ /°	90
$\beta$ /°	90
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2526.78(6)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.274
$\mu/\text{mm}^{-1}$	0.672
F(000)	1056.0
Crystal size/mm <sup>3</sup>	0.12 × 0.08 × 0.05
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54178)
2 $\Theta$ range for data collection/°	6.736 to 149.31
Index ranges	-8 ≤ h ≤ 7, -17 ≤ k ≤ 17, -32 ≤ l ≤ 32
Reflections collected	33867
Independent reflections	5138 [R <sub>int</sub> = 0.0539, R <sub>sigma</sub> = 0.0344]
Data/restraints/parameters	5138/0/324
Goodness-of-fit on F <sup>2</sup>	1.058
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0367, wR <sub>2</sub> = 0.0887
Final R indexes [all data]	R <sub>1</sub> = 0.0406, wR <sub>2</sub> = 0.0919
Largest diff. peak/hole / e Å <sup>-3</sup>	0.28/-0.19
Flack parameter	0.08(8)

**Table S3.** Crystal data and structure refinement for compound **15**

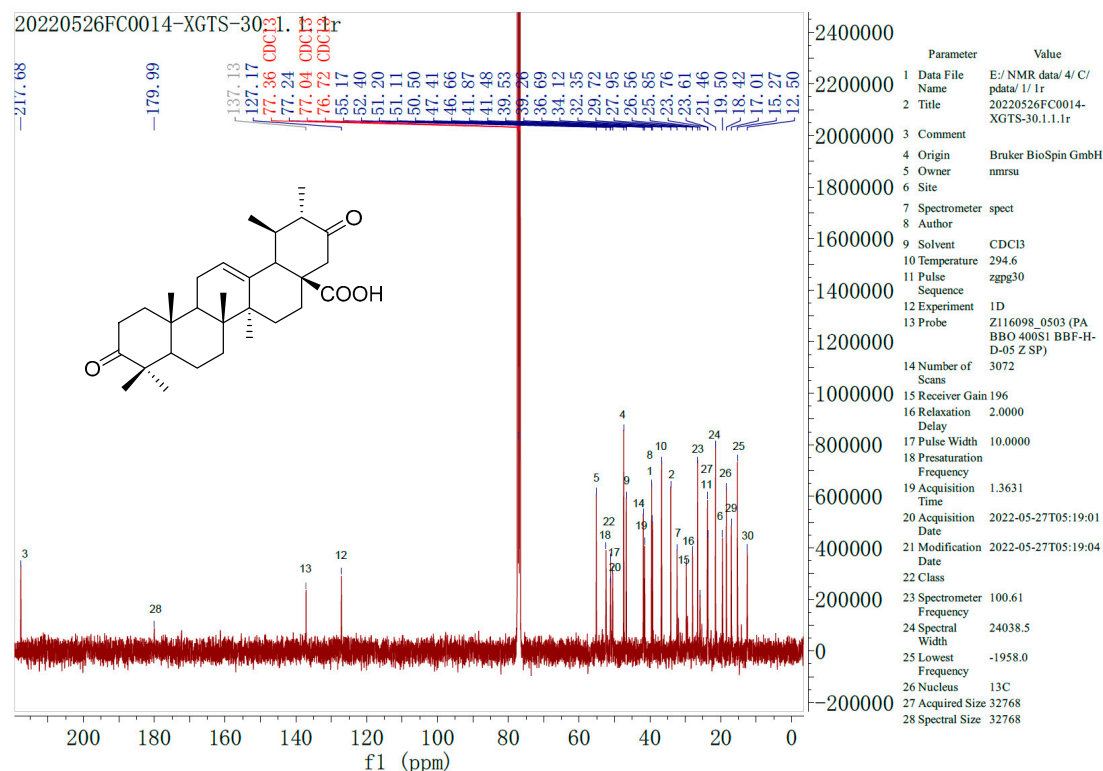
Identification code	x45_0m
Empirical formula	C <sub>30</sub> H <sub>46</sub> O <sub>7</sub>
Formula weight	518.67
Temperature/K	170.0
Crystal system	monoclinic
Space group	P2 <sub>1</sub>
a/Å	12.3958(7)
b/Å	7.8656(5)
c/Å	28.4418(17)
$\alpha$ /°	90
$\beta$ /°	96.882(3)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2753.1(3)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.251
$\mu/\text{mm}^{-1}$	0.705
F(000)	1128.0
Crystal size/mm <sup>3</sup>	0.08 × 0.05 × 0.04
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54178)
2 $\Theta$ range for data collection/°	6.26 to 150.308
Index ranges	-14 ≤ h ≤ 15, -9 ≤ k ≤ 9, -35 ≤ l ≤ 35
Reflections collected	35468
Independent reflections	10864 [R <sub>int</sub> = 0.0527, R <sub>sigma</sub> = 0.0523]
Data/restraints/parameters	10864/10/698
Goodness-of-fit on F <sup>2</sup>	1.090
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0854, wR <sub>2</sub> = 0.2337
Final R indexes [all data]	R <sub>1</sub> = 0.0877, wR <sub>2</sub> = 0.2352
Largest diff. peak/hole / e Å <sup>-3</sup>	0.49/-0.37
Flack parameter	0.04(6)

**Table S4.** Crystal data and structure refinement for compound **19**

Identification code	12_0m
Empirical formula	C <sub>30</sub> H <sub>44</sub> O <sub>6</sub>
Formula weight	500.65
Temperature/K	170.0
Crystal system	orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a/Å	6.4846(2)
b/Å	14.6936(6)
c/Å	28.2892(12)
$\alpha$ /°	90
$\beta$ /°	90
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2695.46(18)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.234
$\mu/\text{mm}^{-1}$	0.675
F(000)	1088.0
Crystal size/mm <sup>3</sup>	0.09 × 0.06 × 0.05
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54178)
2 $\Theta$ range for data collection/°	6.248 to 149.172
Index ranges	-7 ≤ h ≤ 8, -18 ≤ k ≤ 18, -33 ≤ l ≤ 34
Reflections collected	43437
Independent reflections	5462 [ $R_{\text{int}}$ = 0.0744, $R_{\text{sigma}}$ = 0.0361]
Data/restraints/parameters	5462/0/336
Goodness-of-fit on F <sup>2</sup>	1.030
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1$ = 0.0465, $wR_2$ = 0.1185
Final R indexes [all data]	$R_1$ = 0.0534, $wR_2$ = 0.1239
Largest diff. peak/hole / e Å <sup>-3</sup>	0.38/-0.17
Flack parameter	-0.09(10)



**Figure S1** <sup>1</sup>H NMR spectrum (400 MHz) of compound **4** in CDCl<sub>3</sub>



**Figure S2** <sup>13</sup>C NMR spectrum (100 MHz) of compound **4** in CDCl<sub>3</sub>

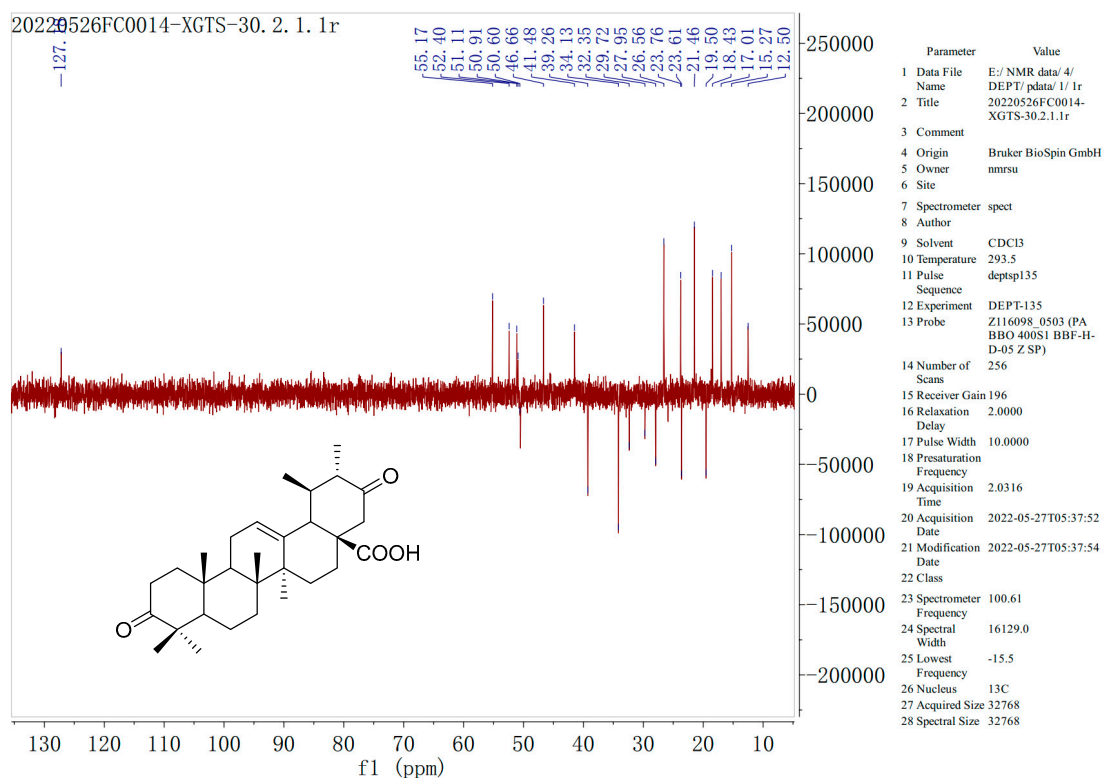


Figure S3 DEPT-135 spectrum (100 MHz) of compound **4** in CDCl<sub>3</sub>

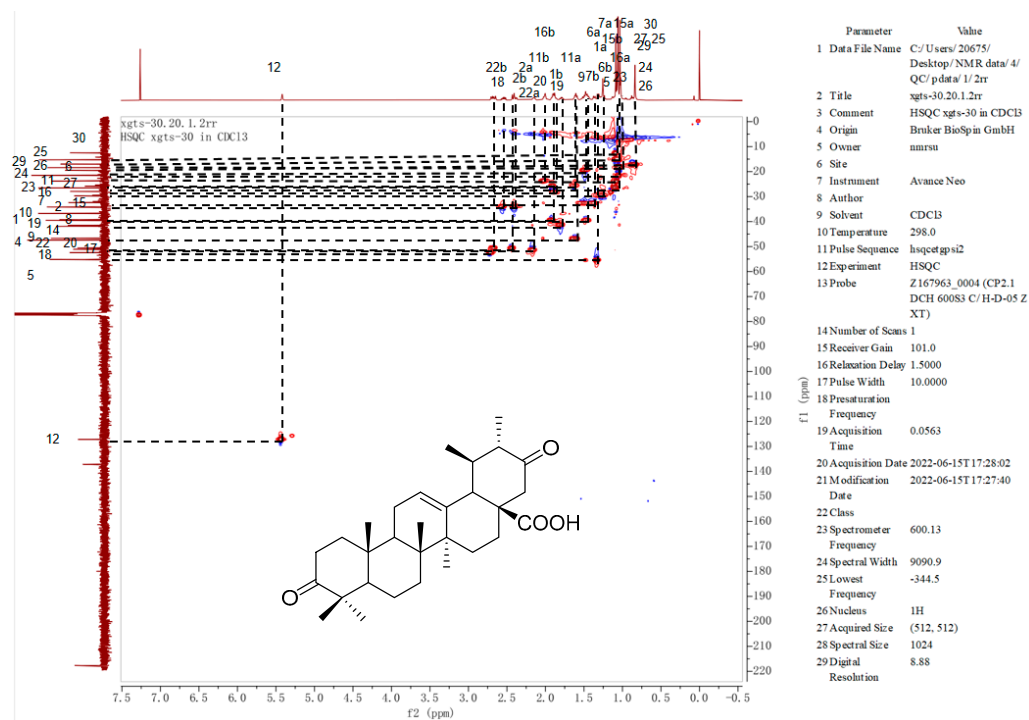
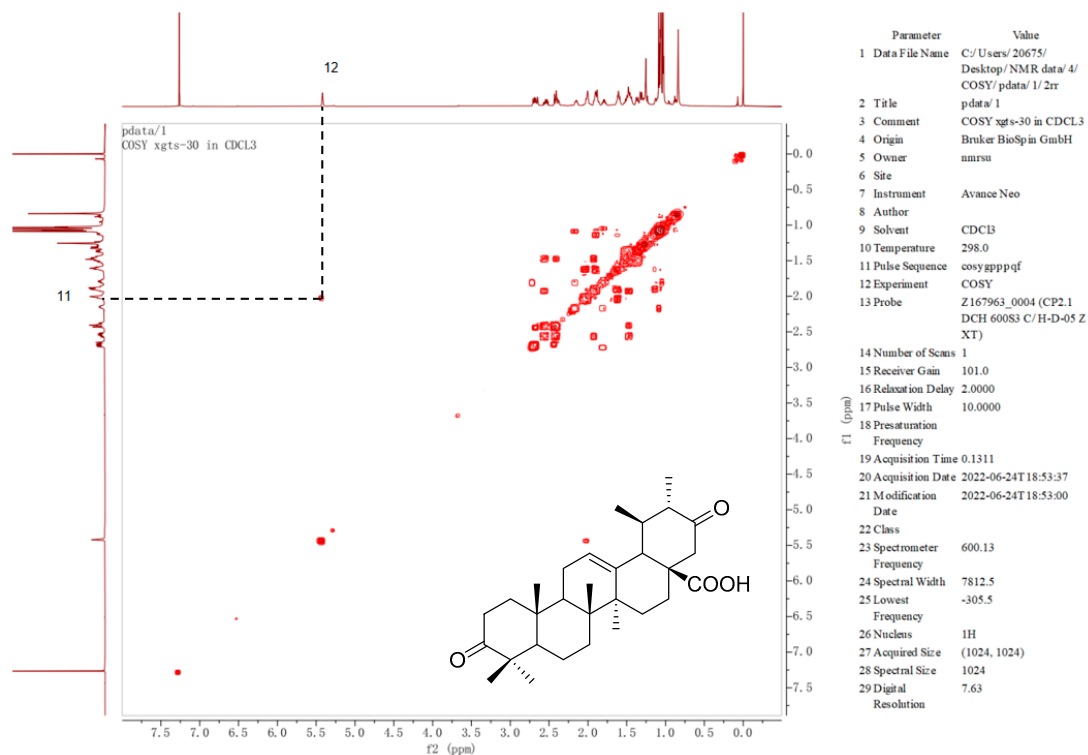
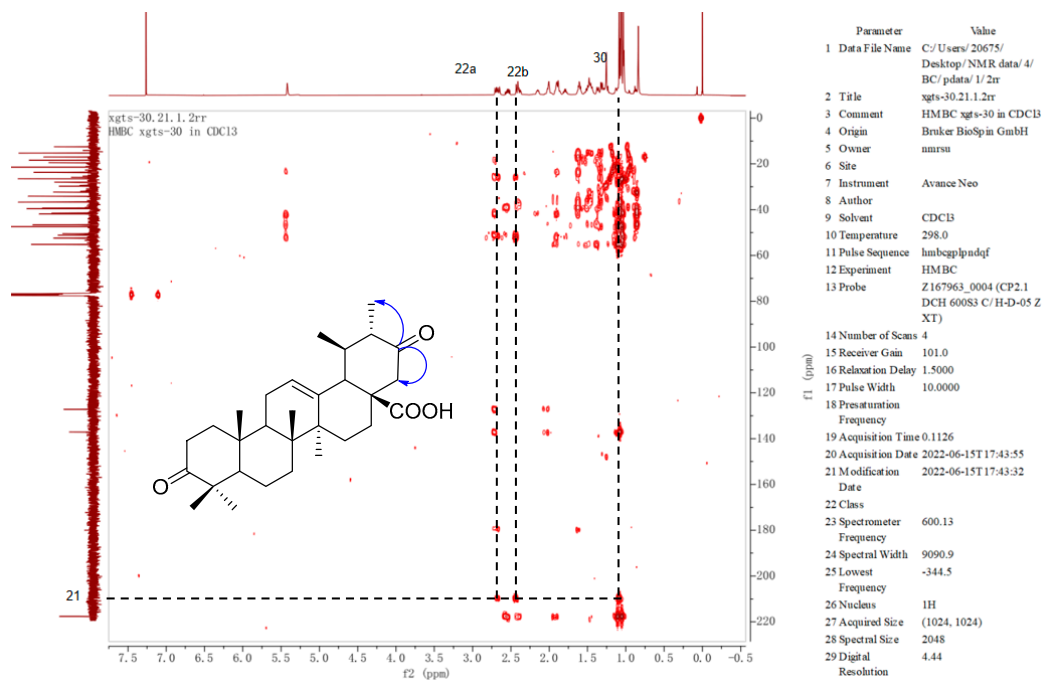


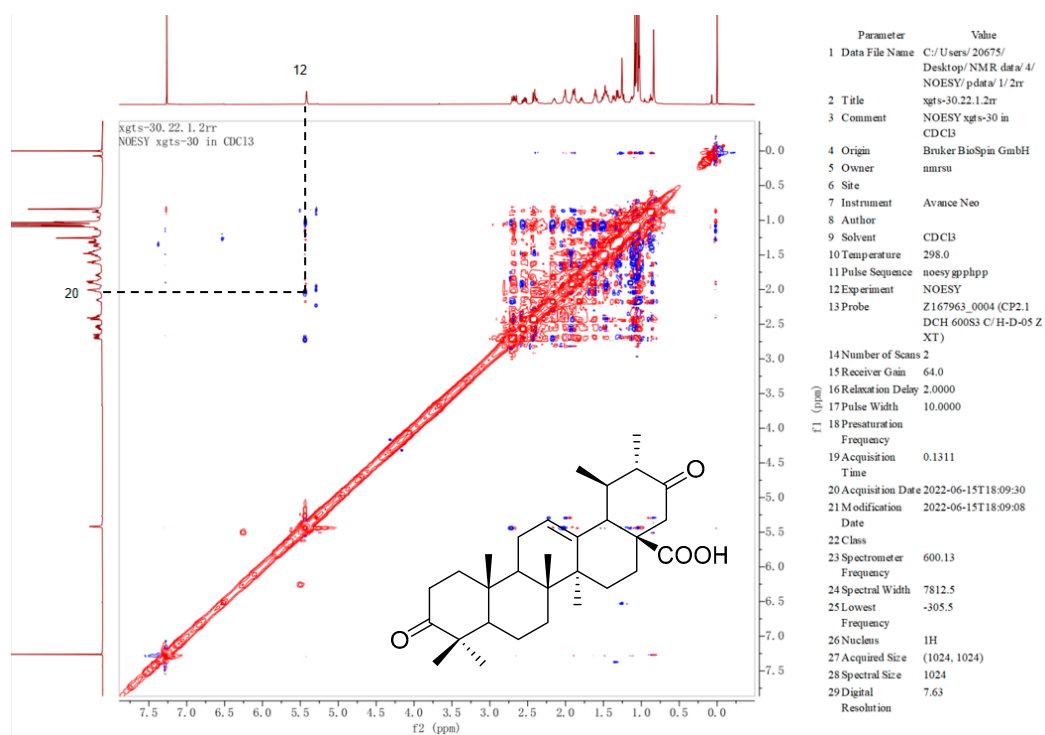
Figure S4 HSQC spectrum (100 MHz) of compound **4** in CDCl<sub>3</sub>



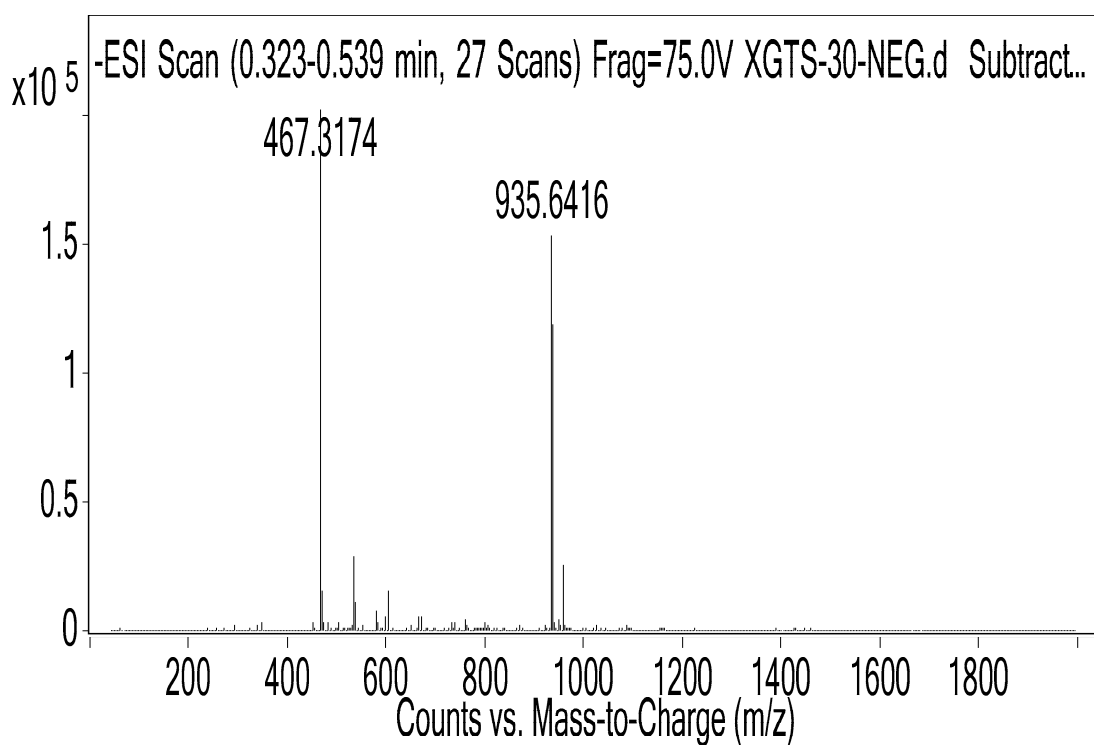
**Figure S5**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **4** in  $\text{CDCl}_3$



**Figure S6** HMBC spectrum (100 MHz) of compound **4** in  $\text{CDCl}_3$



**Figure S7** NOESY spectrum (400 MHz) of compound **4** in CDCl<sub>3</sub>



**Figure S8** HR-ESI-MS spectrum of compound **4**



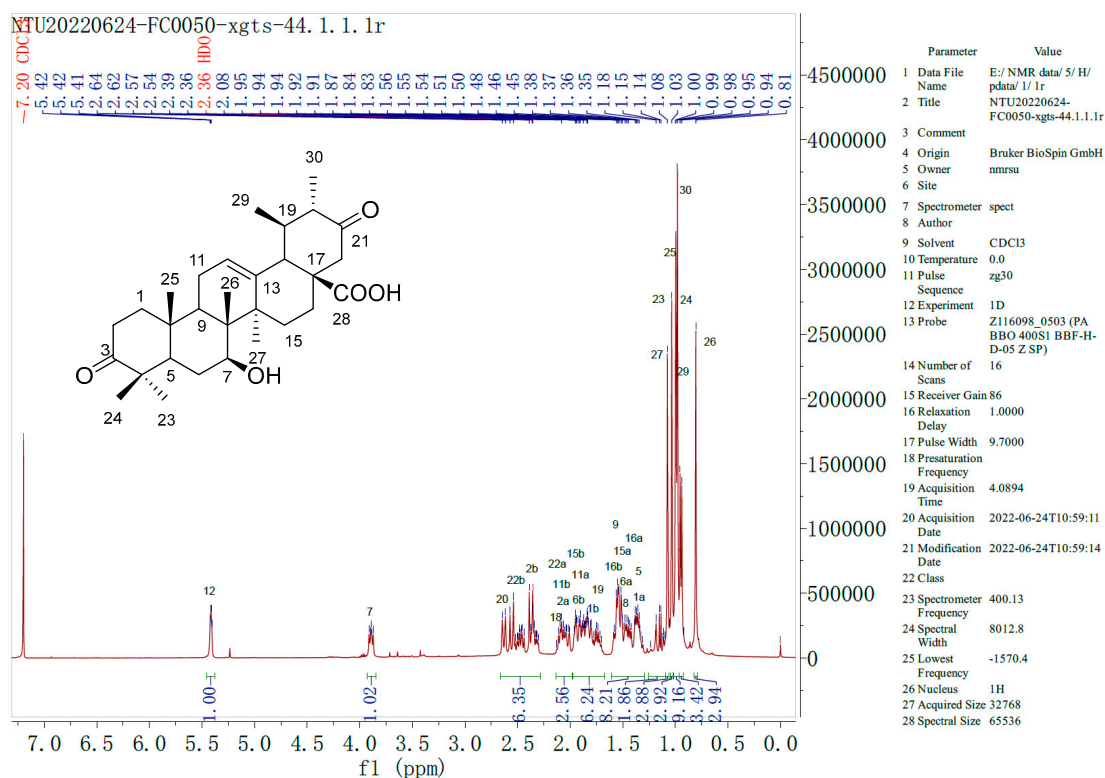


Figure S9  $^1\text{H}$  NMR spectrum (400 MHz) of compound **5** in  $\text{CDCl}_3$

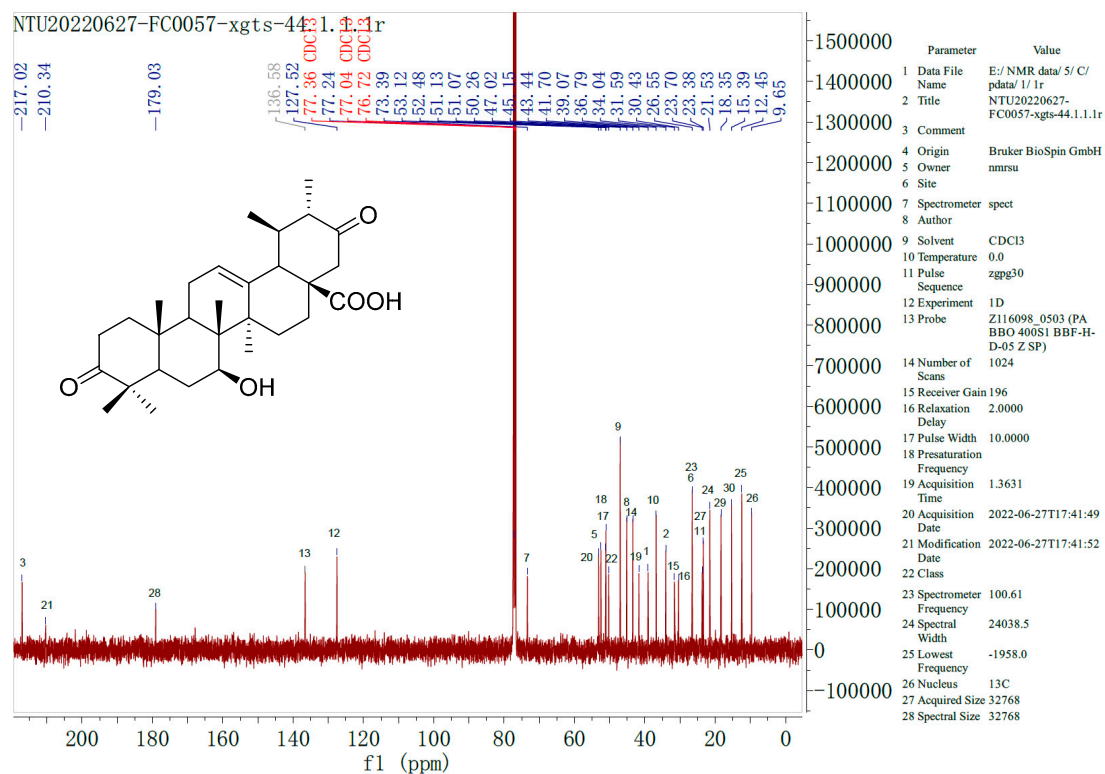


Figure S10  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **5** in  $\text{CDCl}_3$

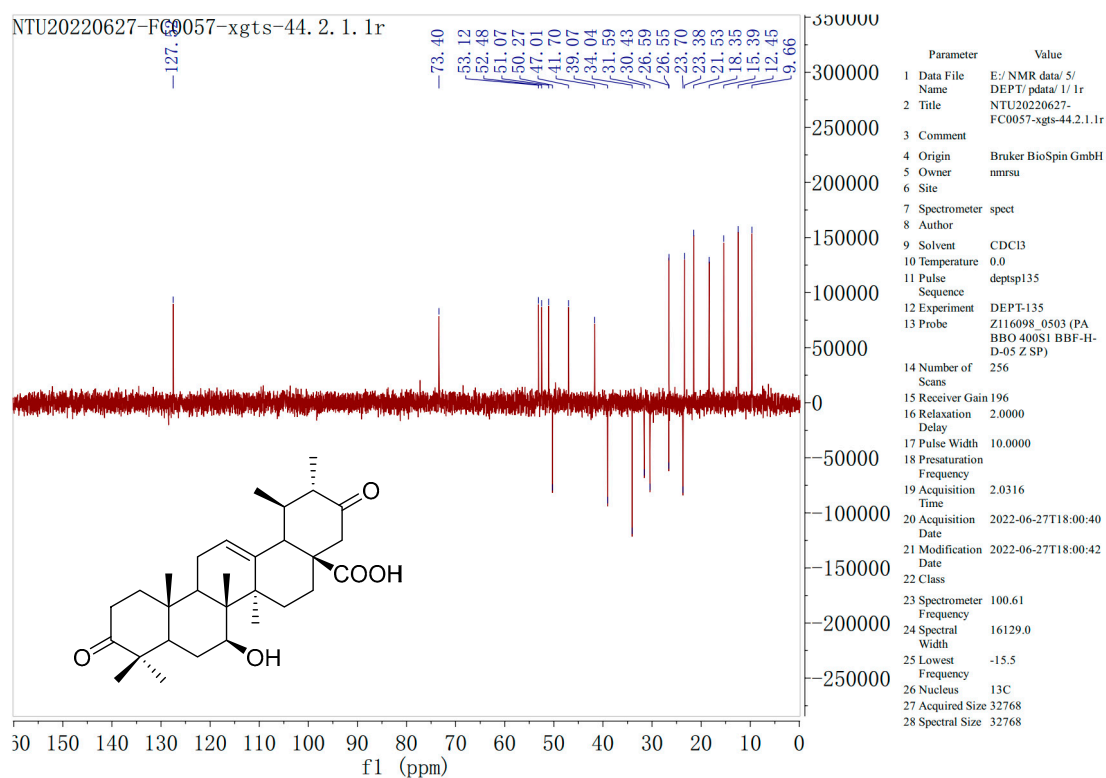


Figure S11 DEPT-135 spectrum (100 MHz) of compound **5** in CDCl<sub>3</sub>

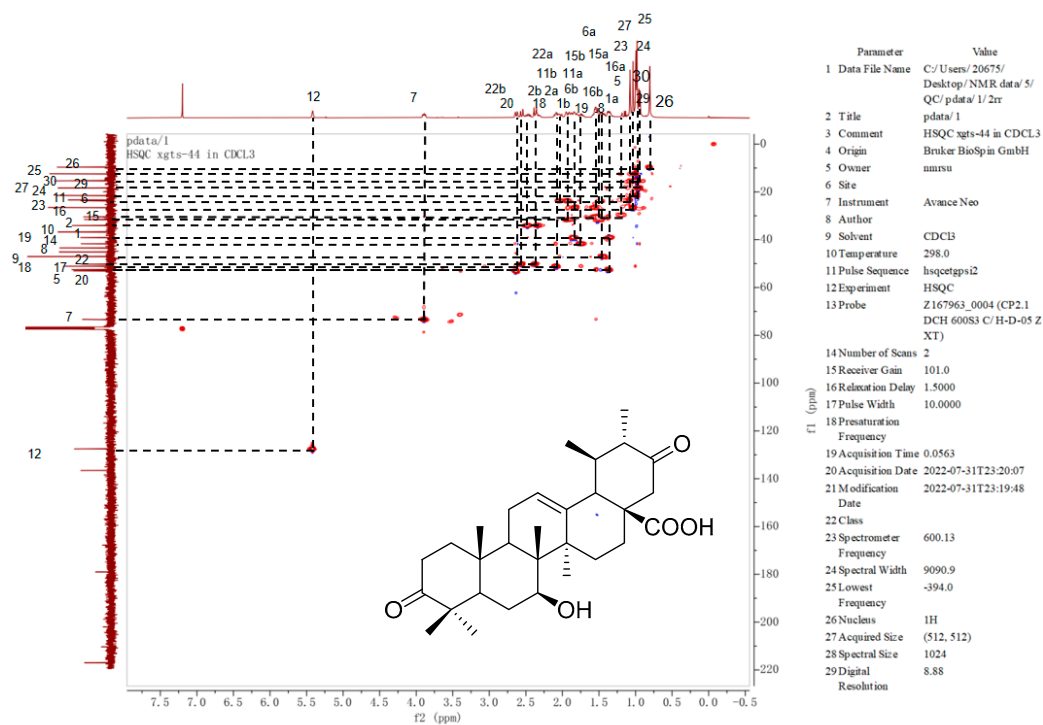
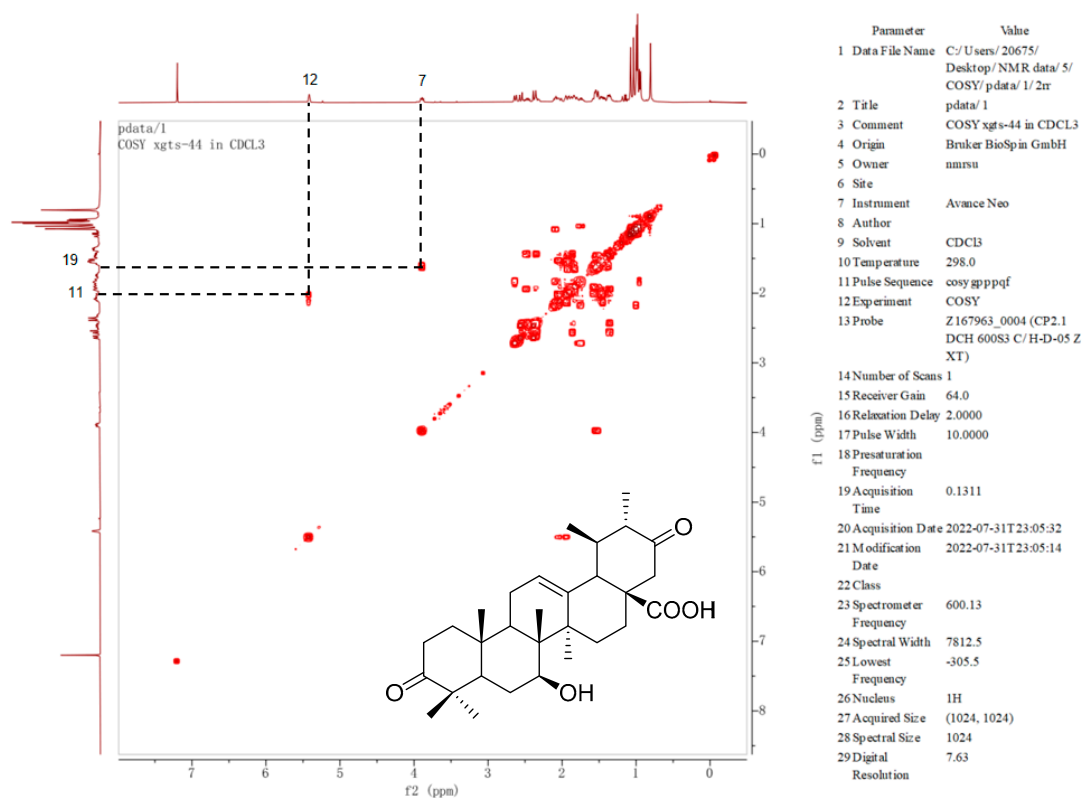
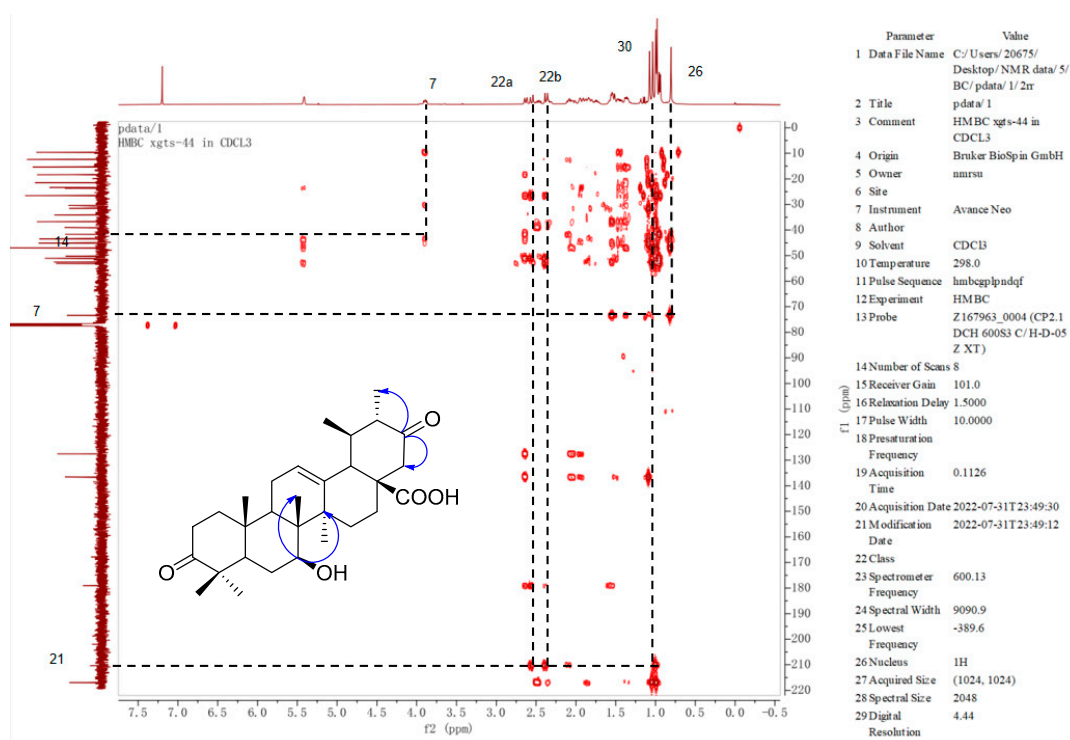


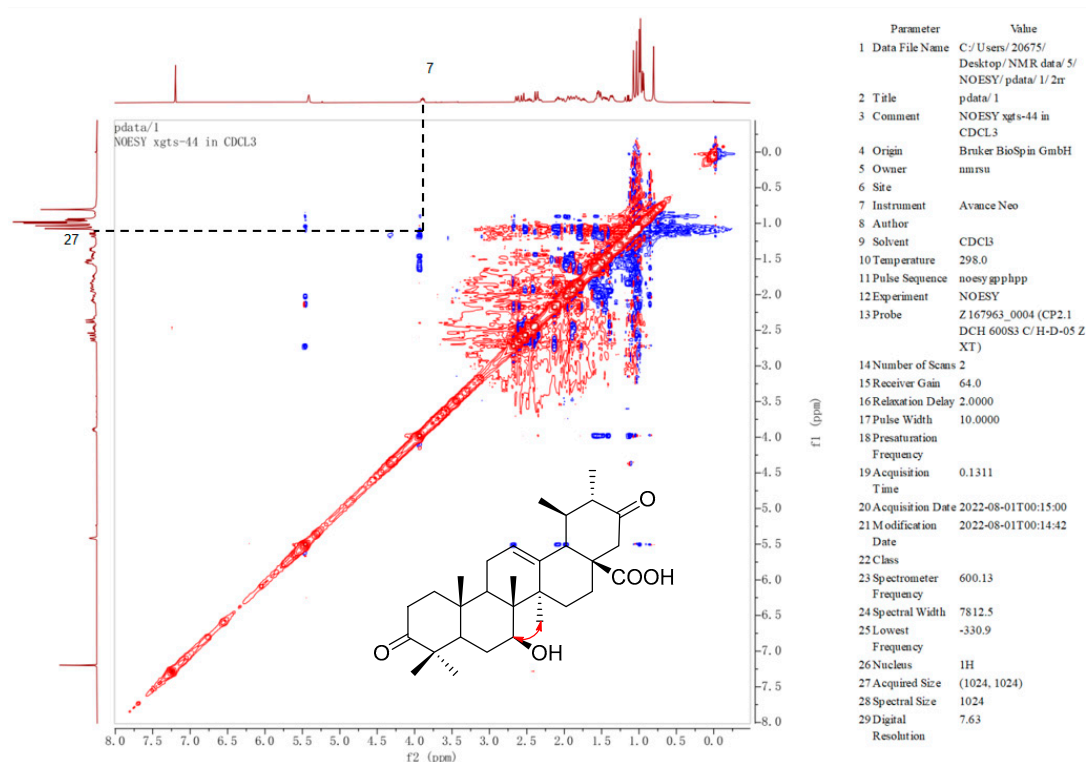
Figure S12 HSQC spectrum (100 MHz) of compound **5** in CDCl<sub>3</sub>



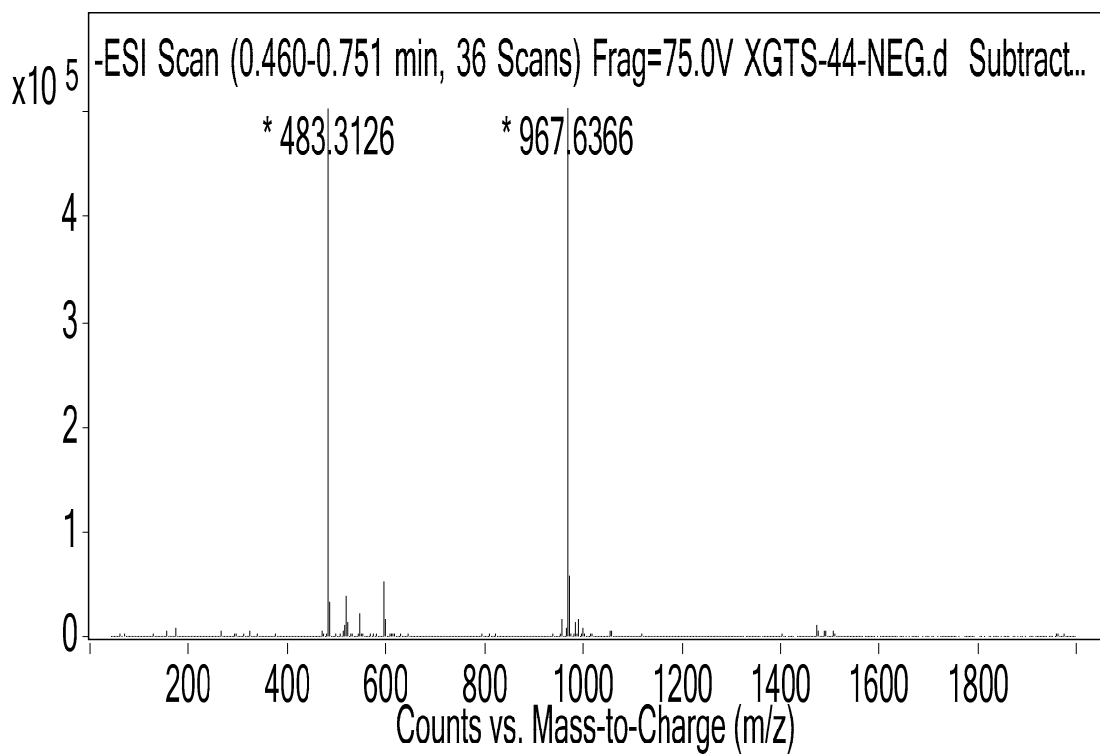
**Figure S13**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **5** in  $\text{CDCl}_3$



**Figure S14** HMBC spectrum (100 MHz) of compound **5** in  $\text{CDCl}_3$



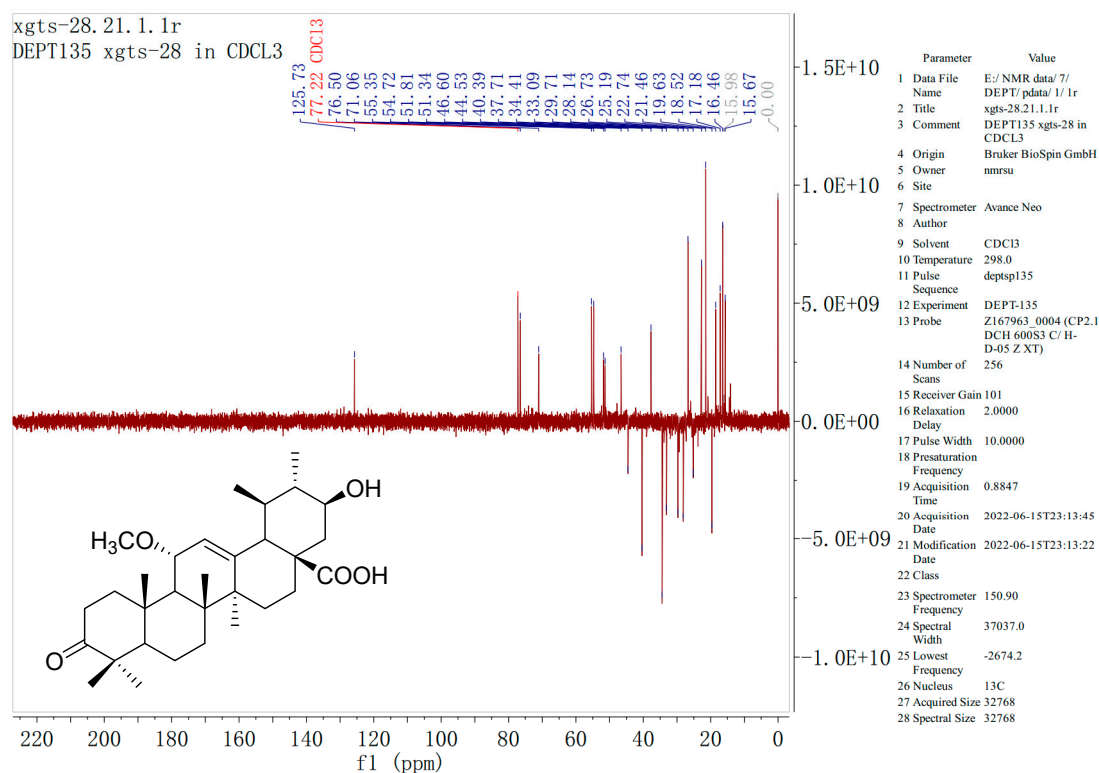
**Figure S15** NOESY spectrum (400 MHz) of compound **5** in CDCl<sub>3</sub>



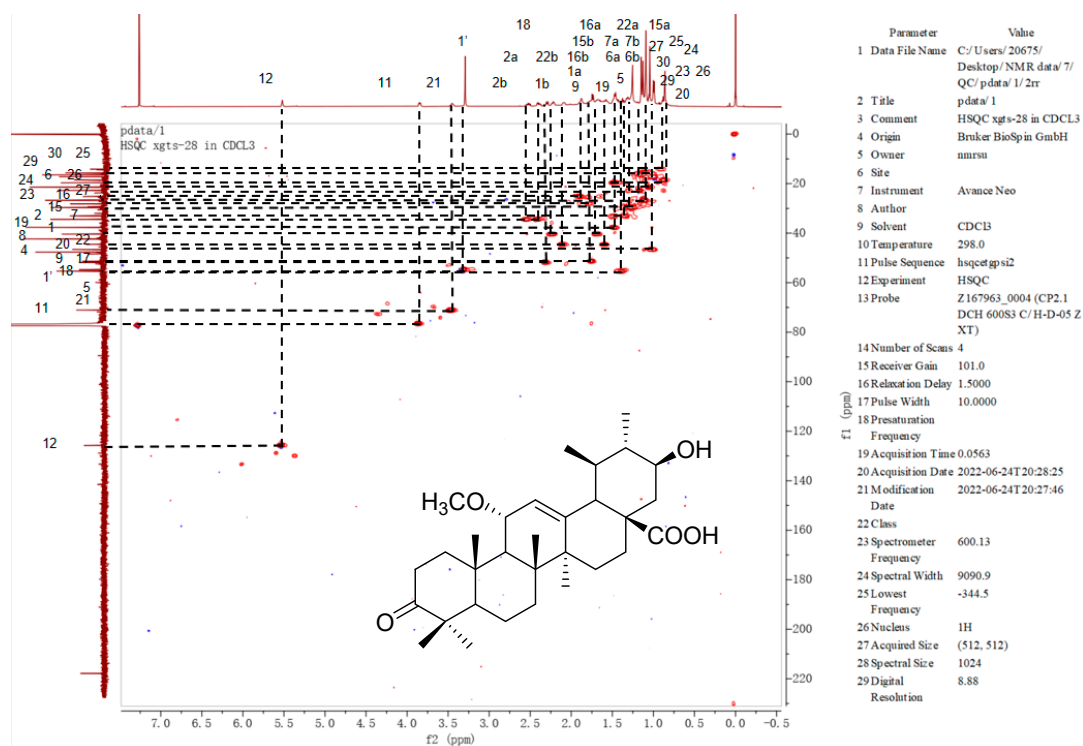
**Figure S16** HR-ESI-MS spectrum of compound **5**



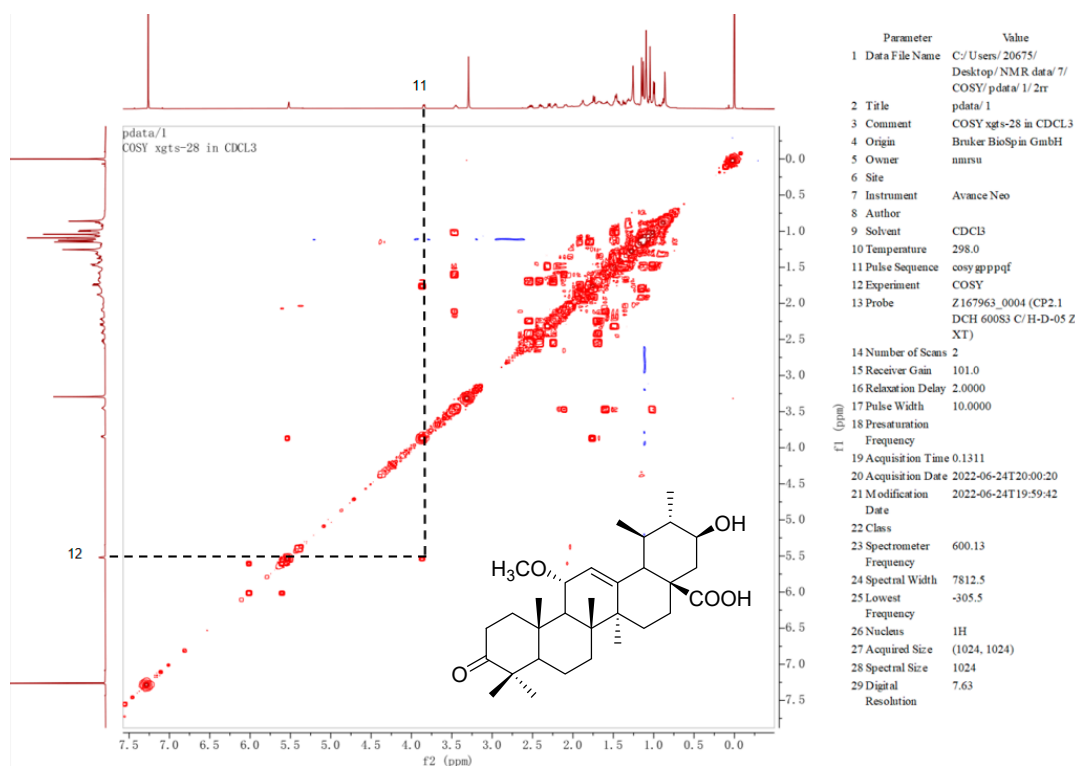




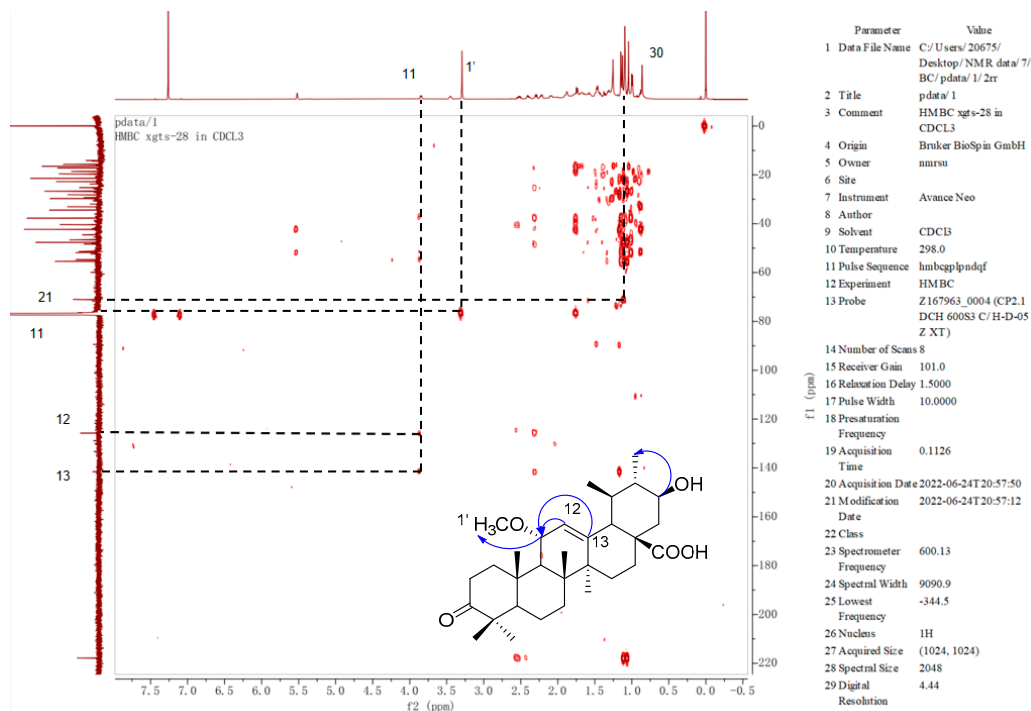
**Figure S19** DEPT-135 spectrum (150 MHz) of compound **7** in CDCl<sub>3</sub>



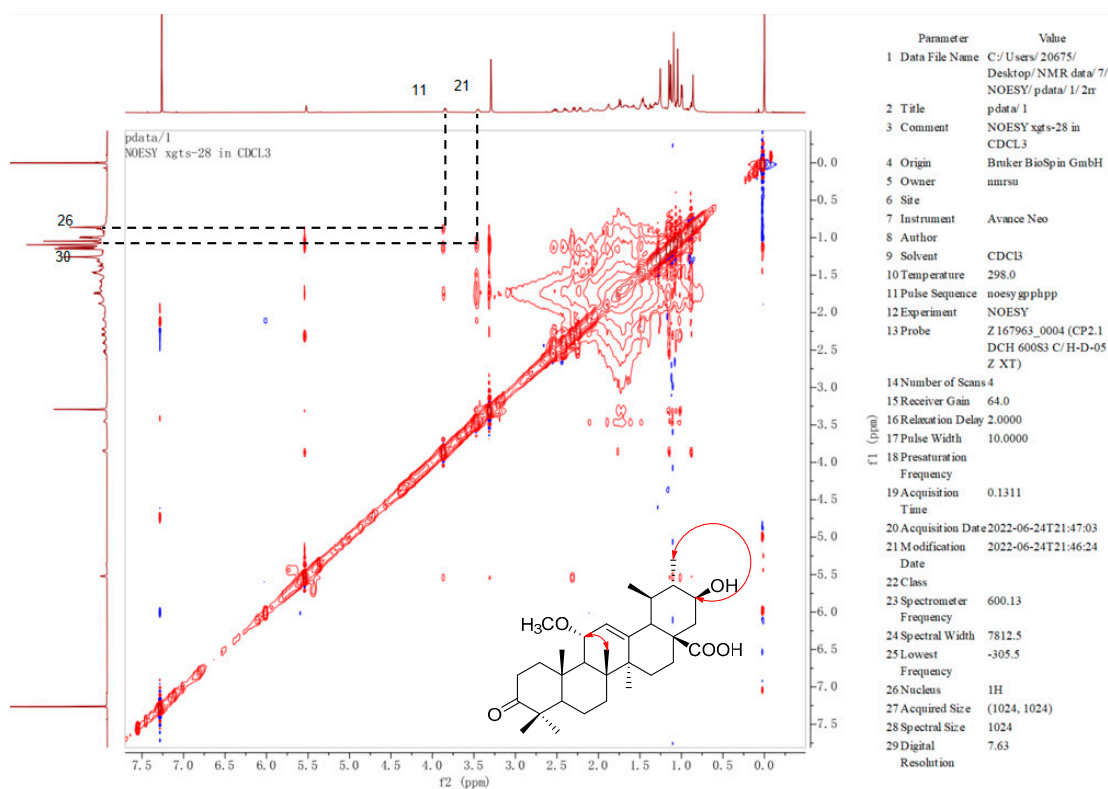
**Figure S20** HSQC spectrum (150 MHz) of compound **7** in CDCl<sub>3</sub>



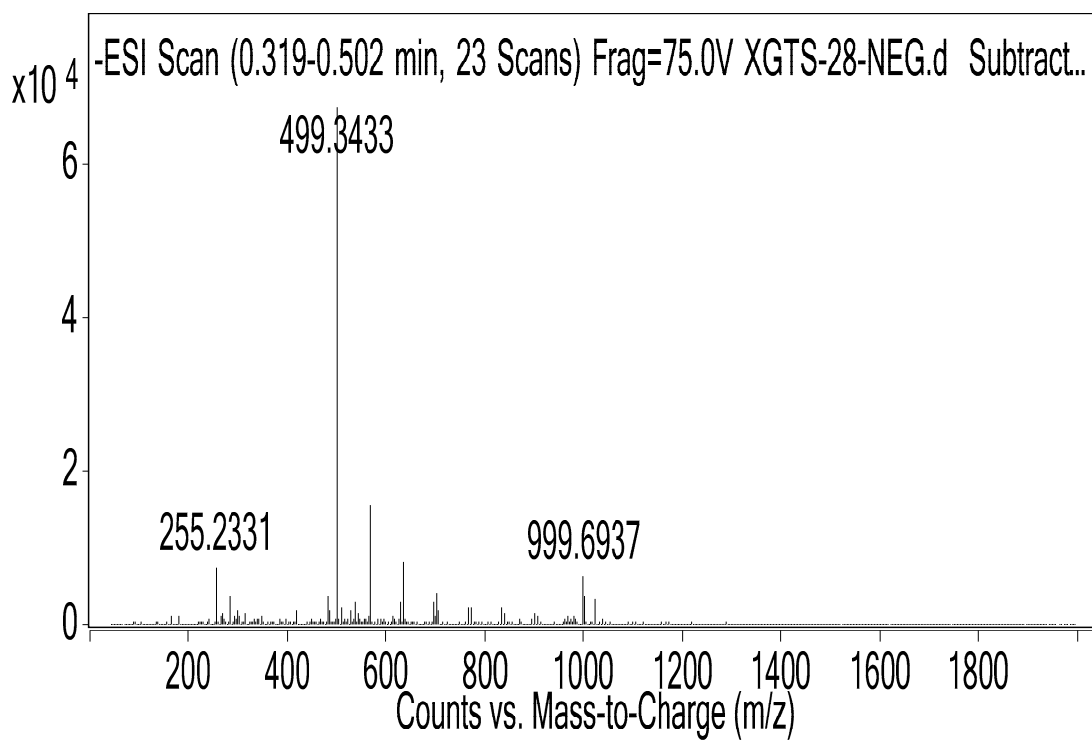
**Figure S21**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz) of compound **7** in  $\text{CDCl}_3$



**Figure S22** HMBC spectrum (150 MHz) of compound **7** in  $\text{CDCl}_3$



**Figure S23** NOESY spectrum (600 MHz) of compound 7 in CDCl<sub>3</sub>



**Figure S24** HR-ESI-MS spectrum of compound 7



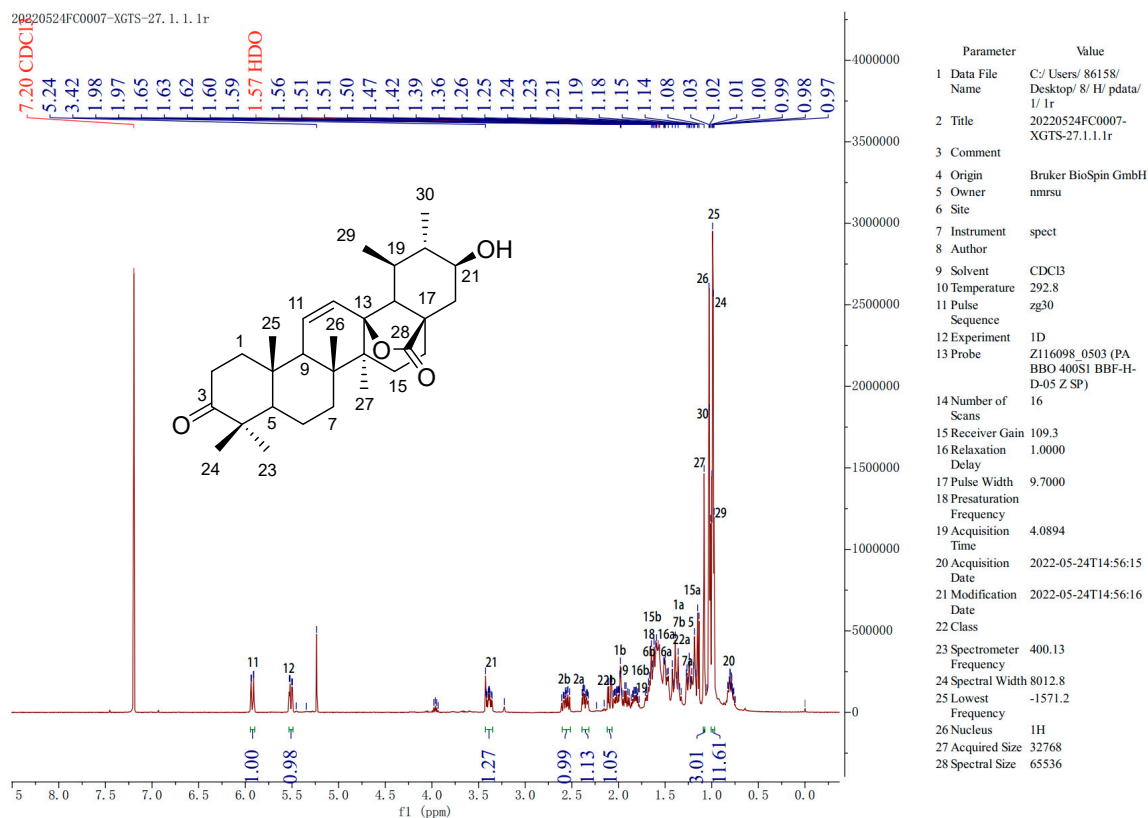


Figure S25  $^1\text{H}$  NMR spectrum (400 MHz) of compound **8** in  $\text{CDCl}_3$

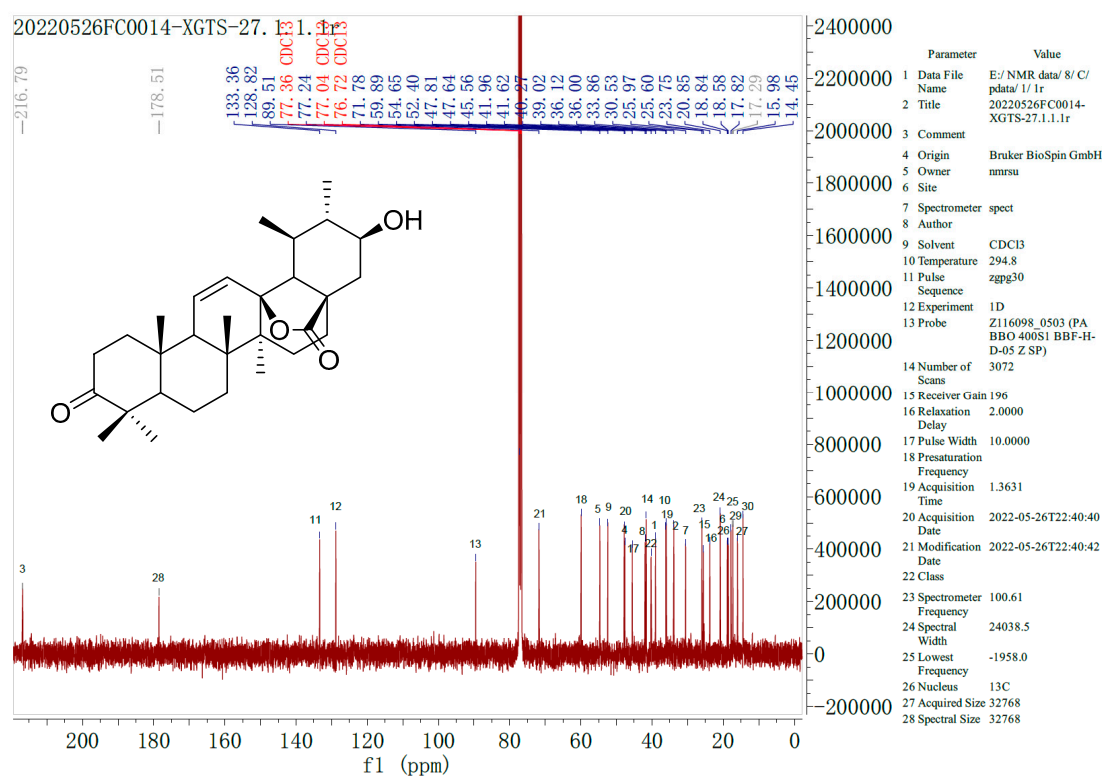


Figure S26  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **8** in  $\text{CDCl}_3$

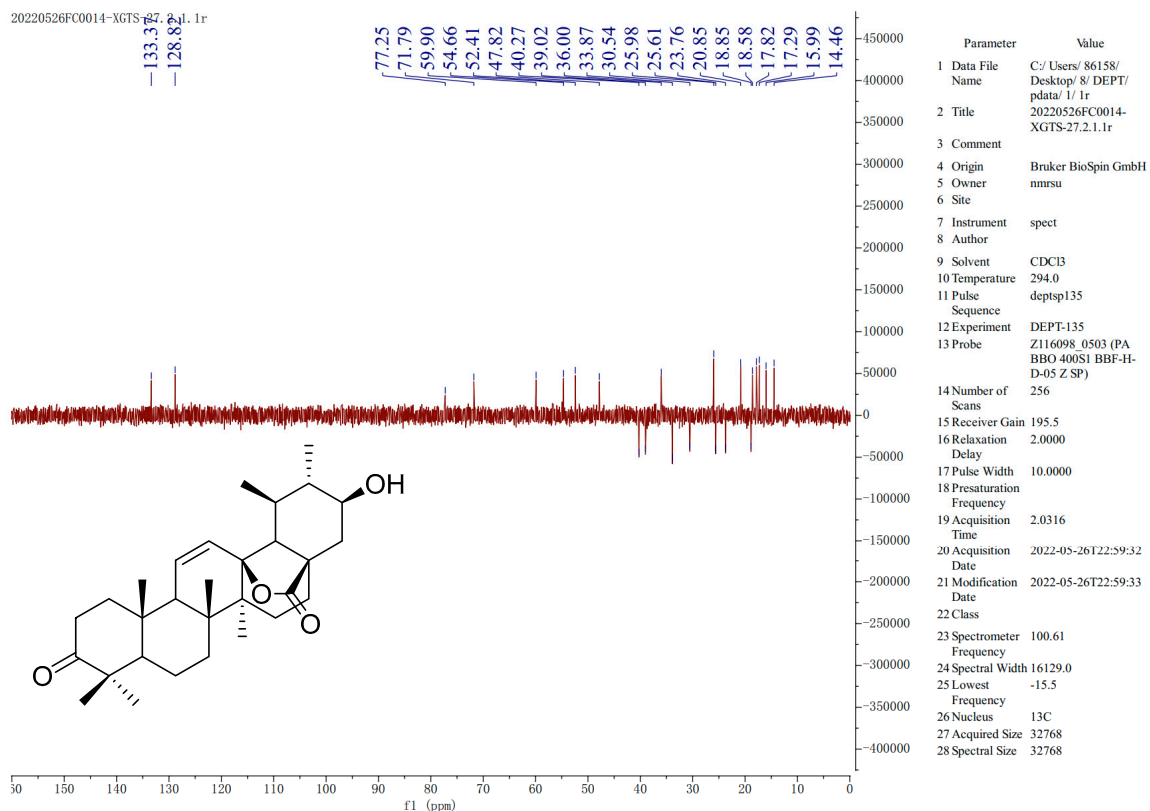


Figure S27 DEPT-135 spectrum (100 MHz) of compound **8** in CDCl<sub>3</sub>

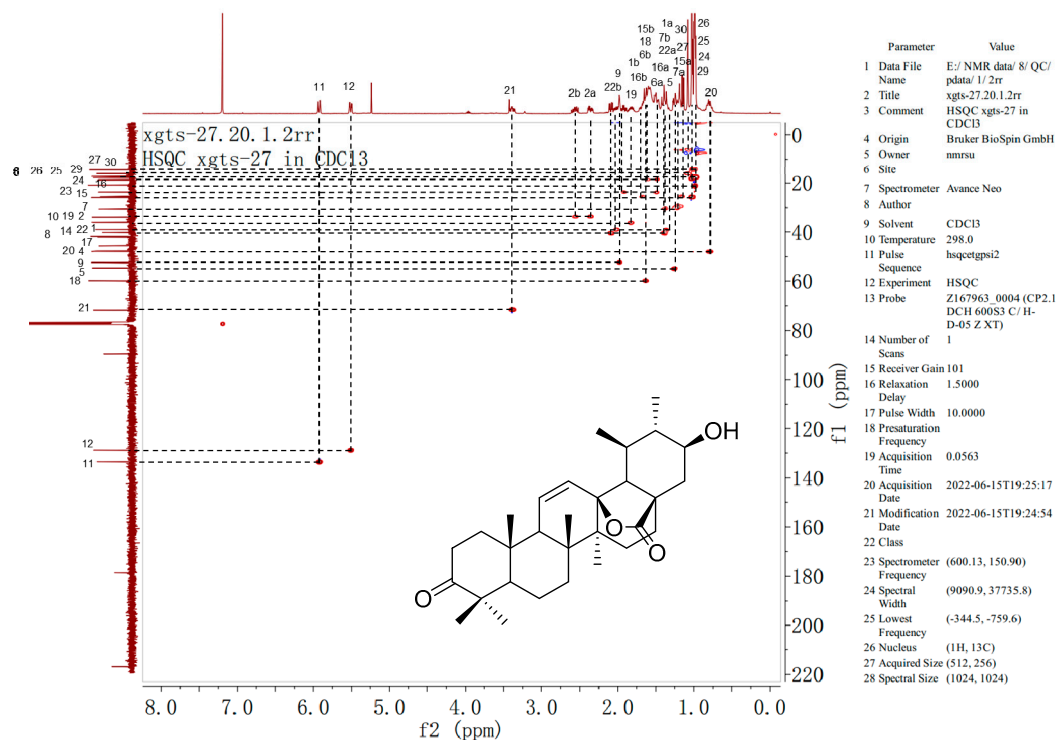
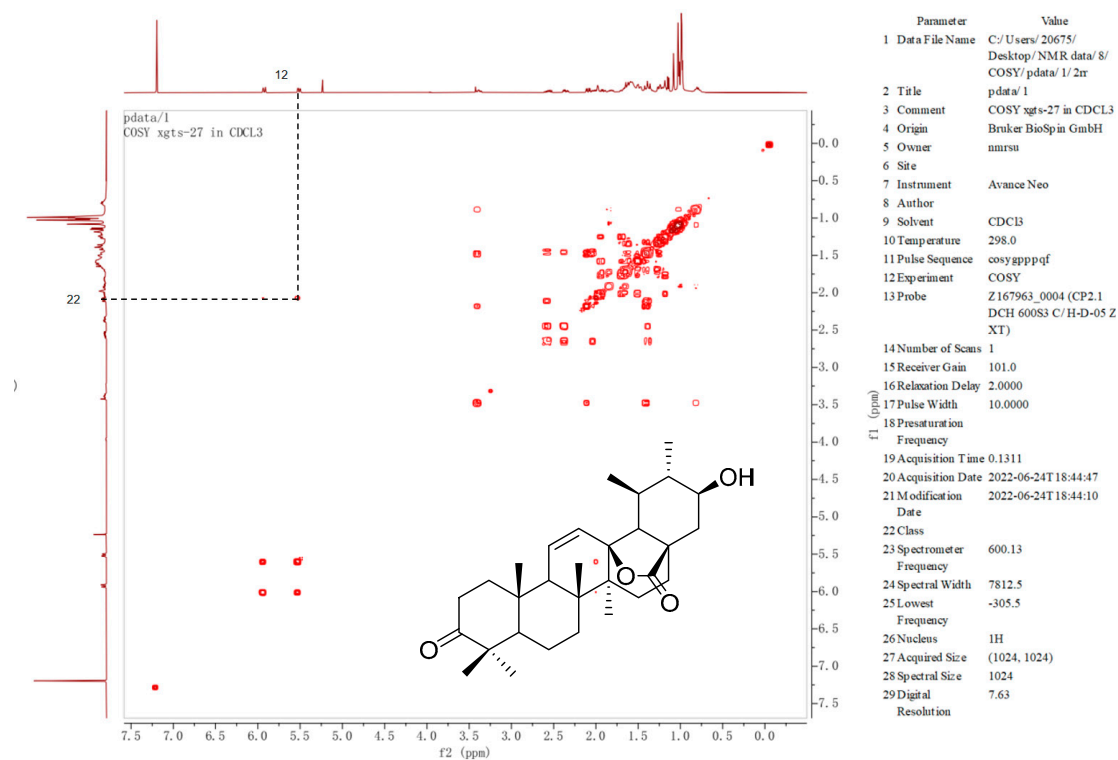
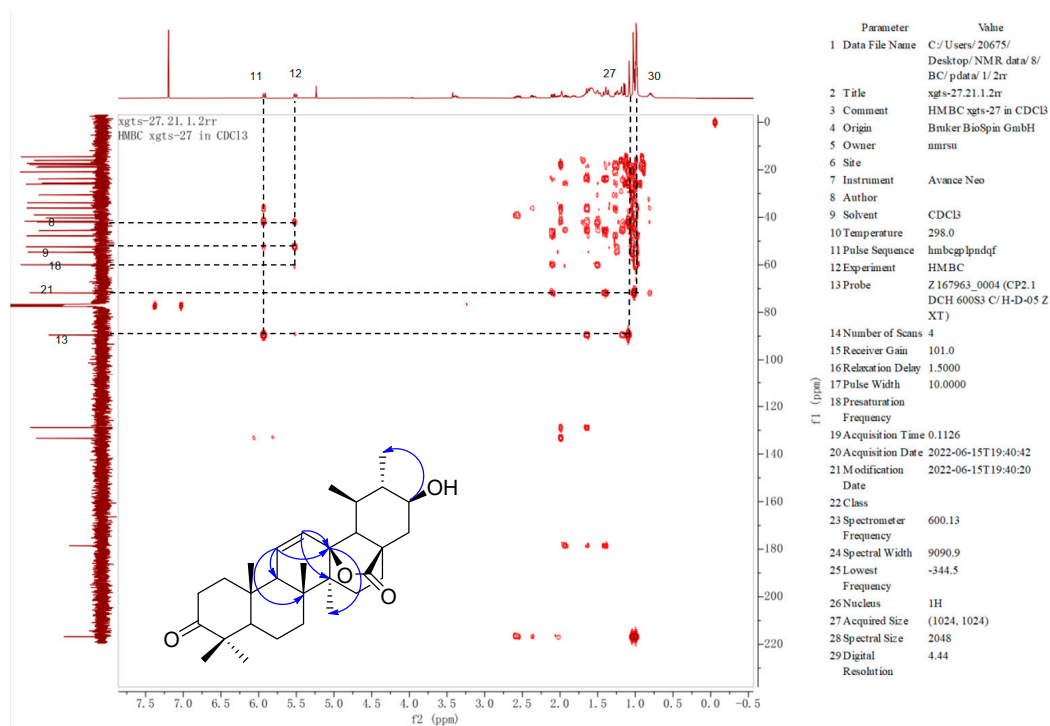


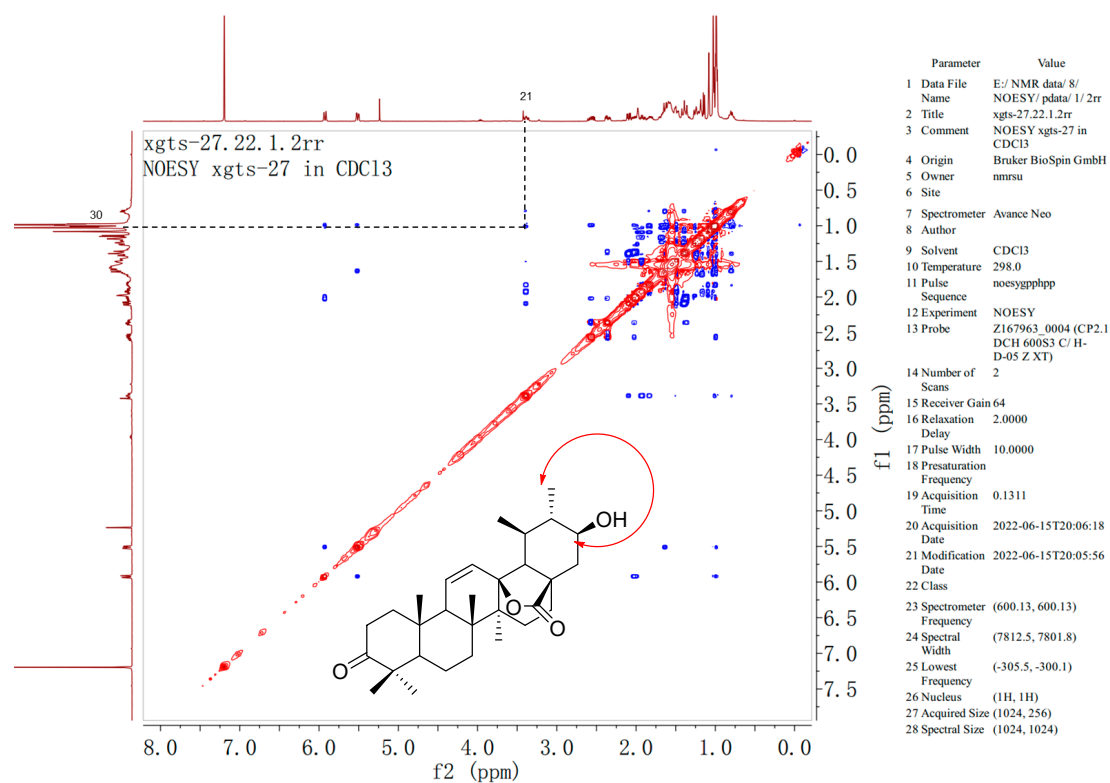
Figure S28 HSQC spectrum (100 MHz) of compound **8** in CDCl<sub>3</sub>



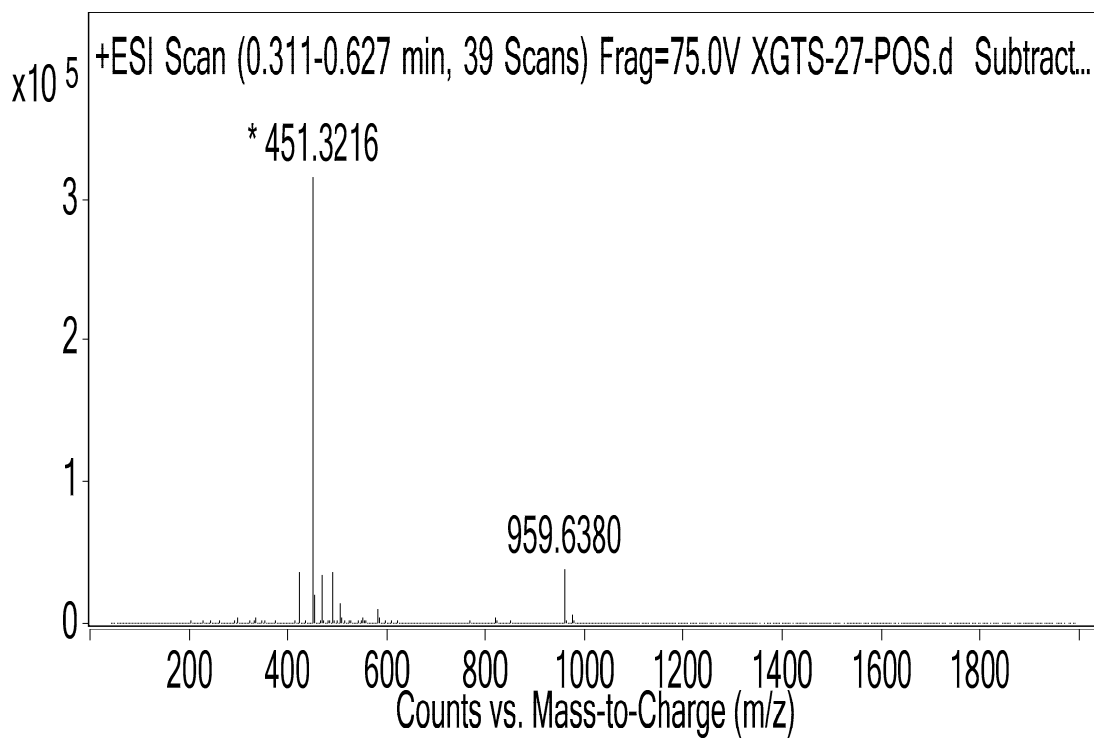
**Figure S29**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **8** in  $\text{CDCl}_3$



**Figure S30** HMBC spectrum (100 MHz) of compound **8** in  $\text{CDCl}_3$



**Figure S31** NOESY spectrum (400 MHz) of compound **8** in CDCl<sub>3</sub>



**Figure S32** HR-ESI-MS spectrum of compound **8**

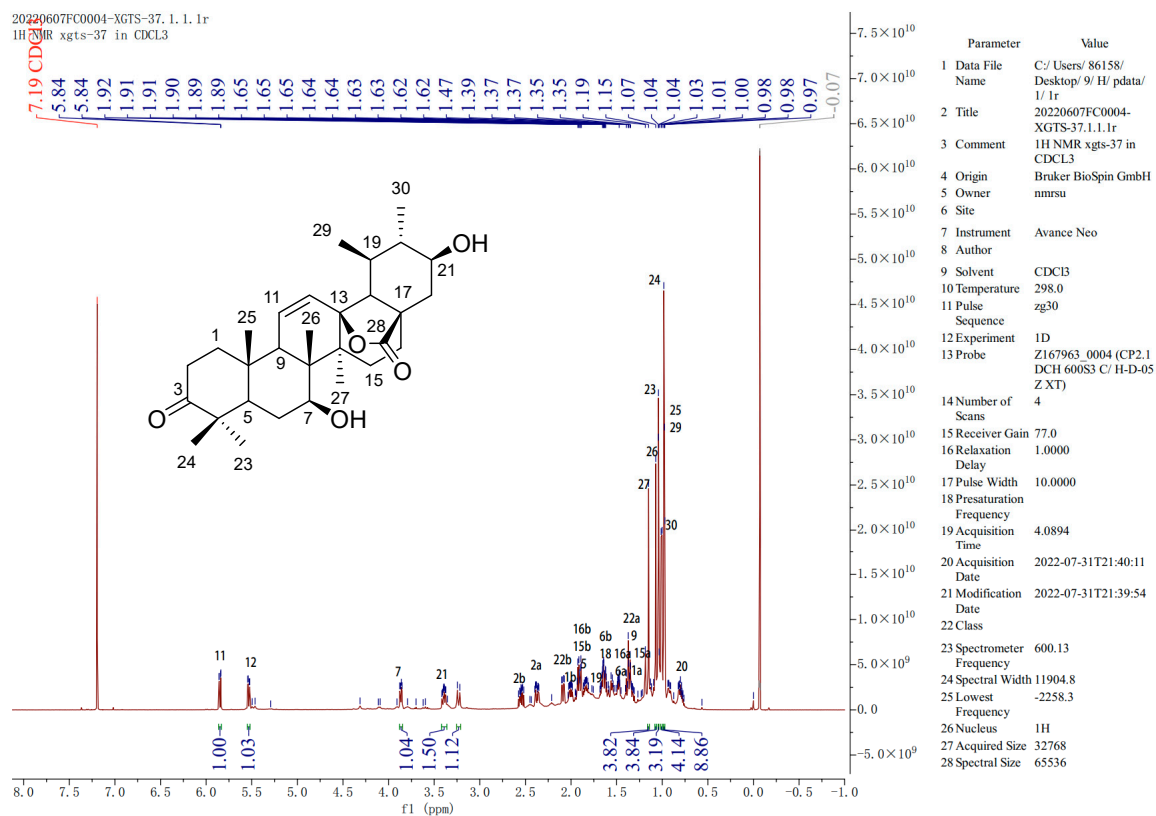


Figure S33 <sup>1</sup>H NMR spectrum (400 MHz) of compound **9** in CDCl<sub>3</sub>

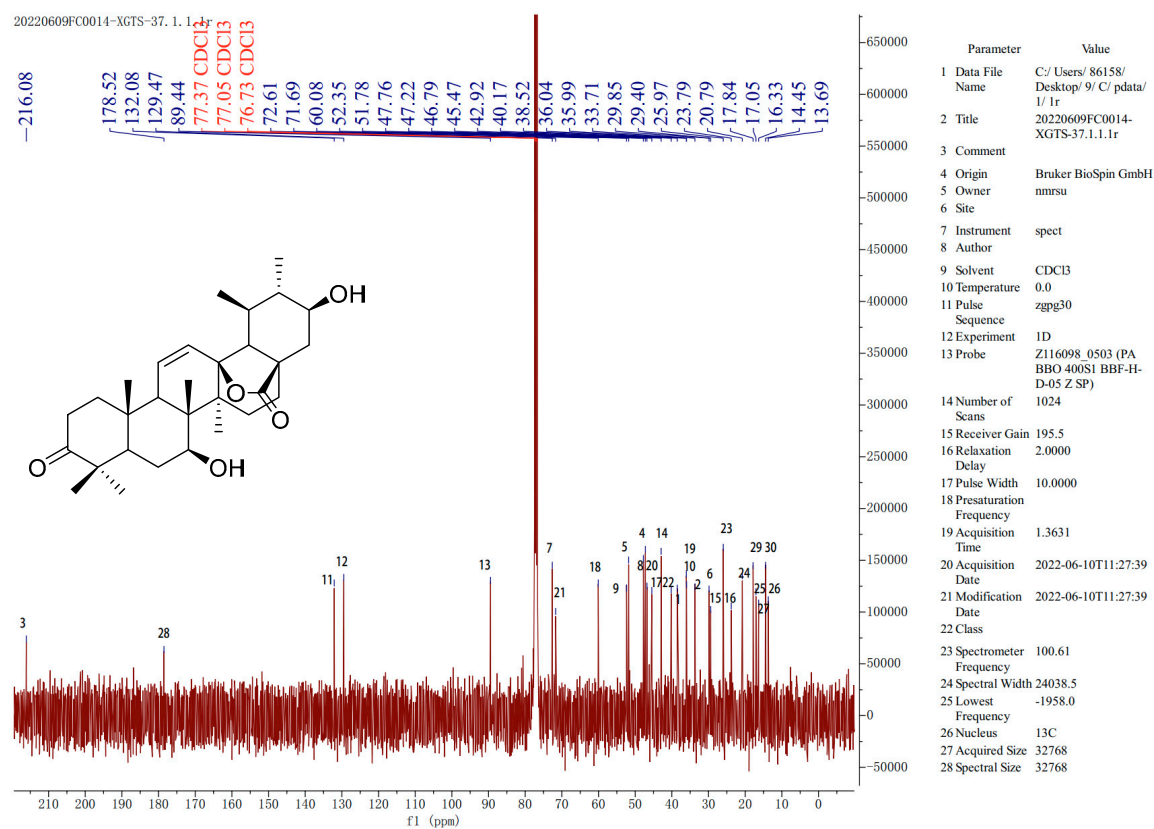


Figure S34 <sup>13</sup>C NMR spectrum (100 MHz) of compound **9** in CDCl<sub>3</sub>

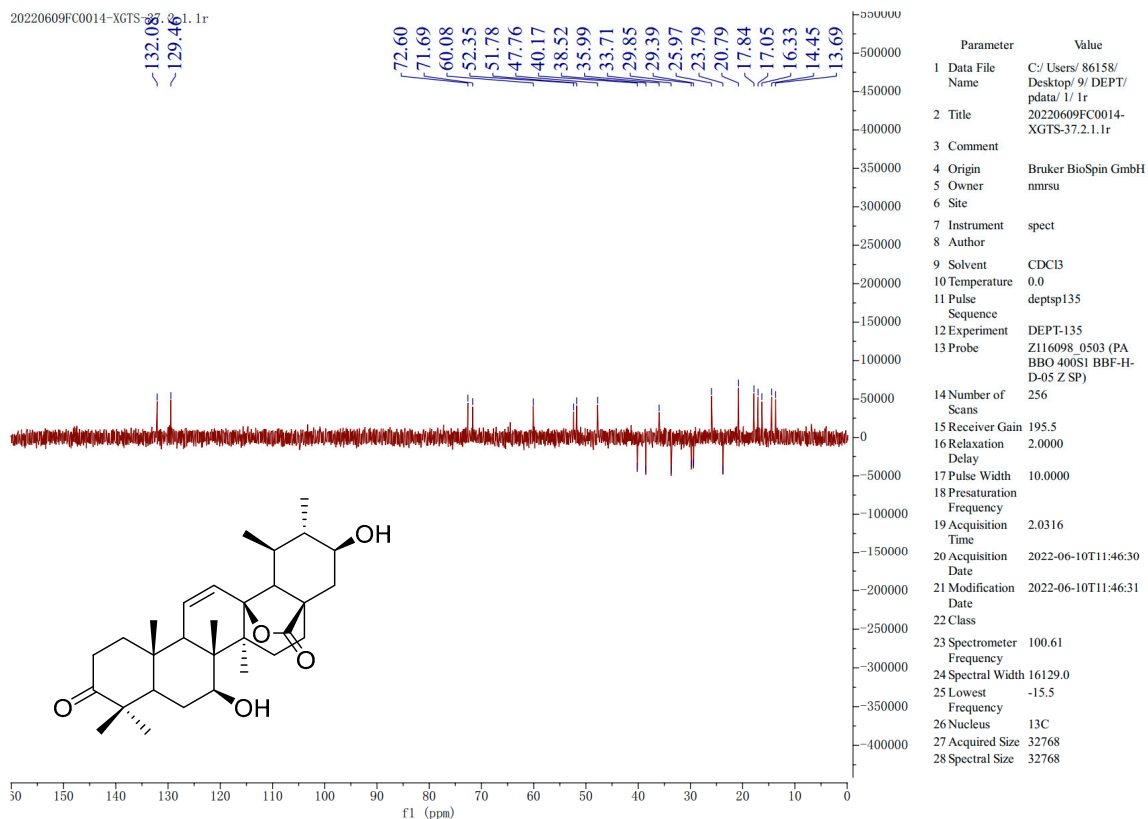


Figure S35 DEPT-135 spectrum (100 MHz) of compound 9 in CDCl<sub>3</sub>

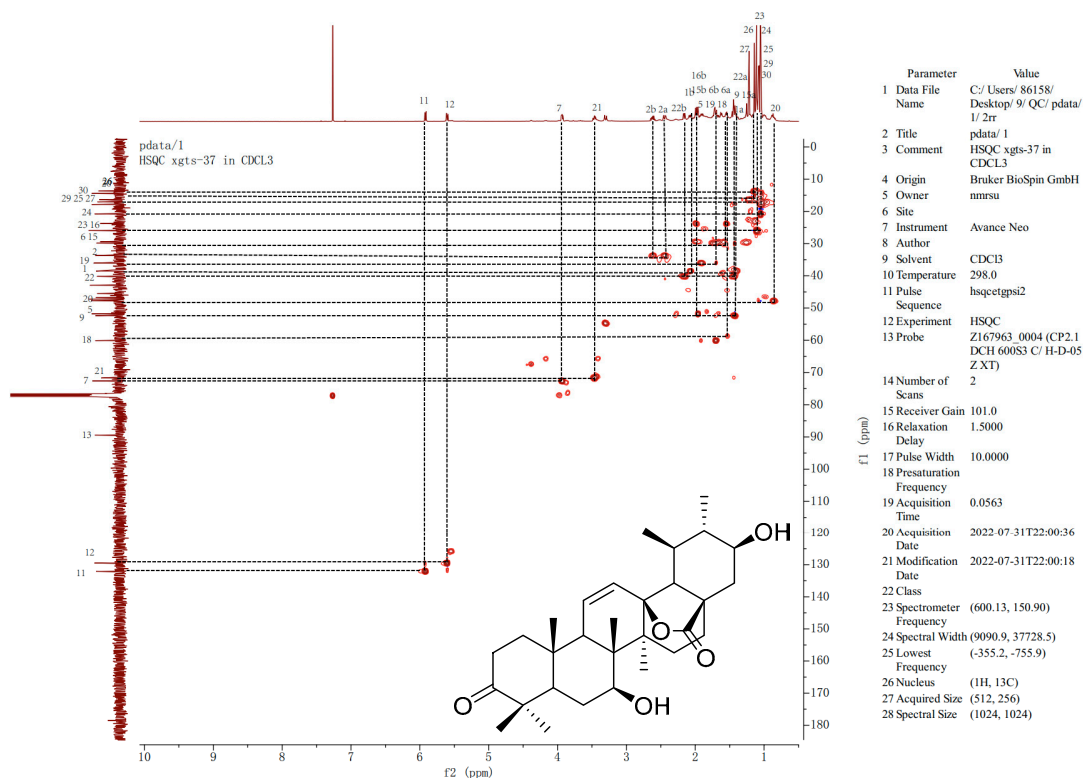
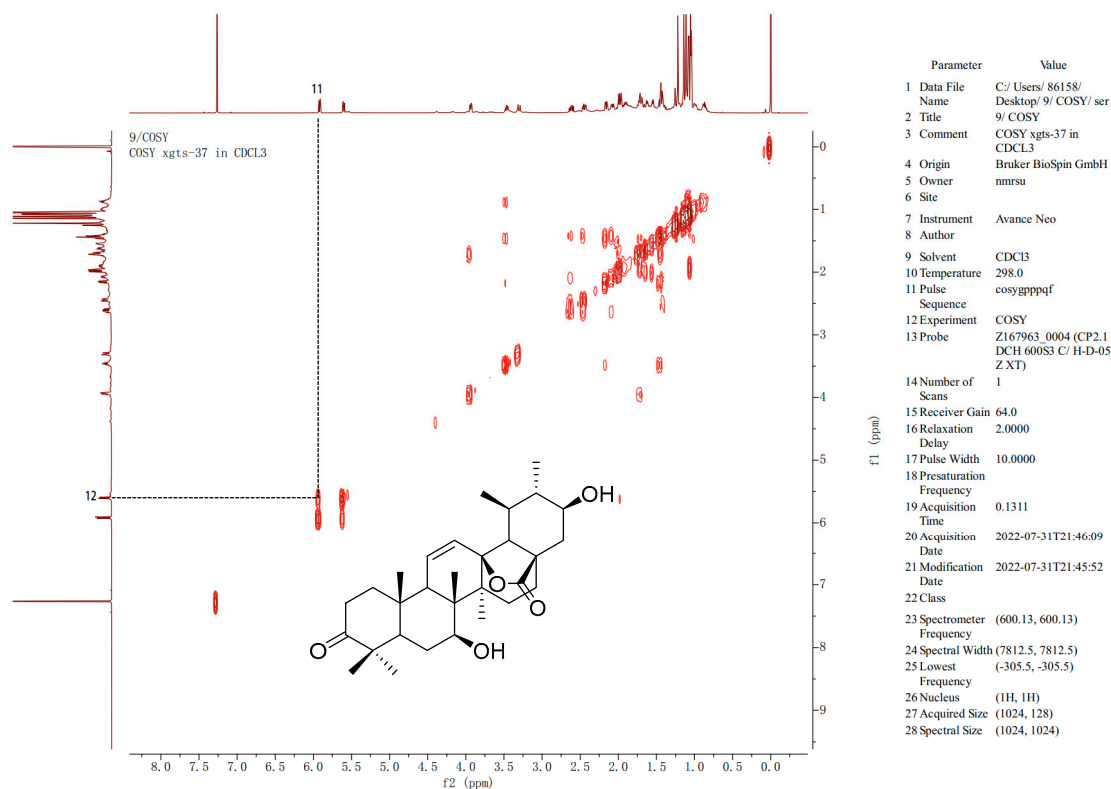
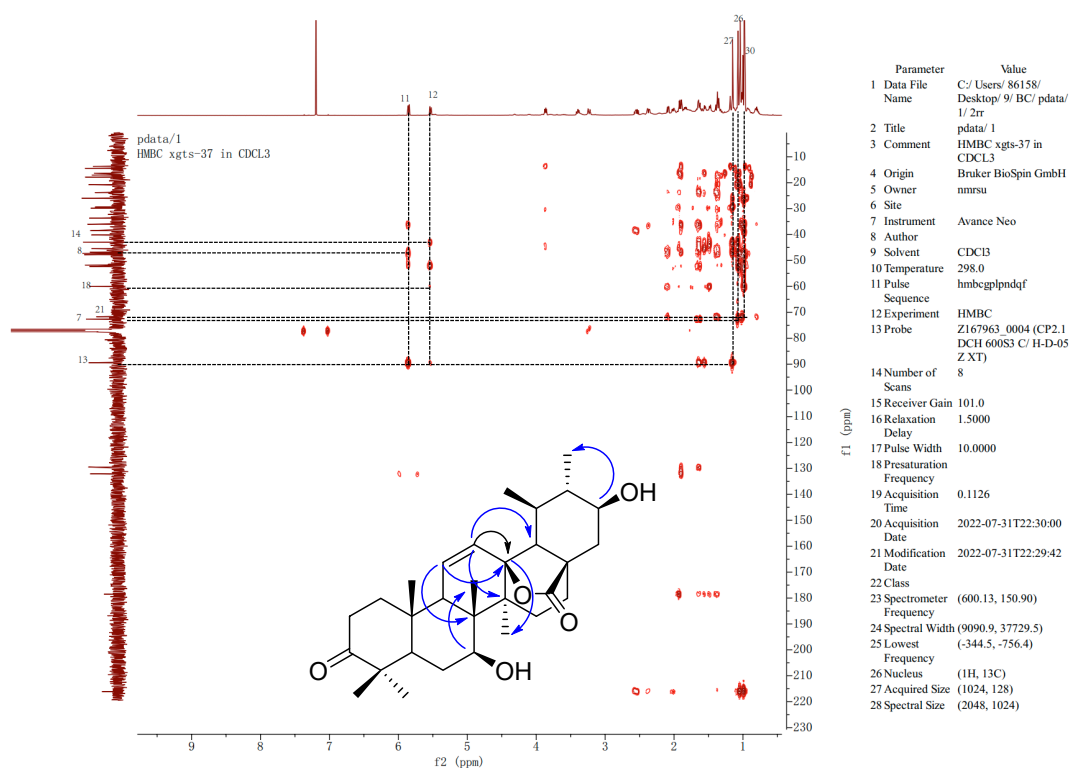


Figure S36 HSQC spectrum (100 MHz) of compound 9 in CDCl<sub>3</sub>

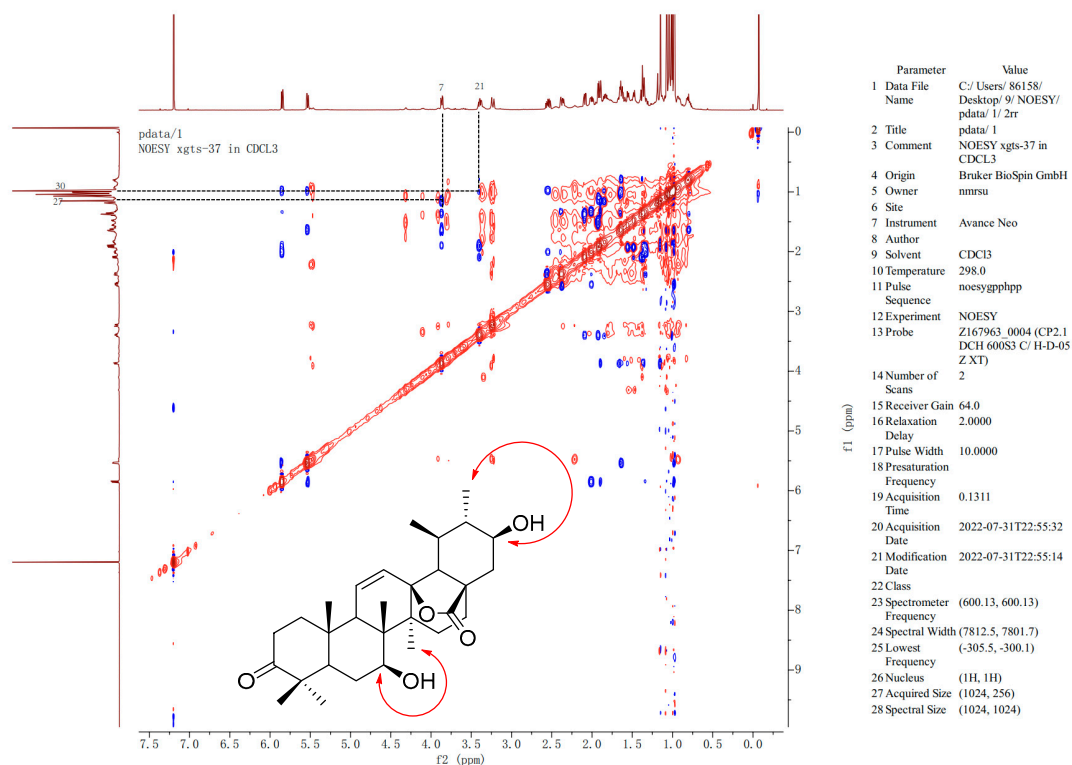




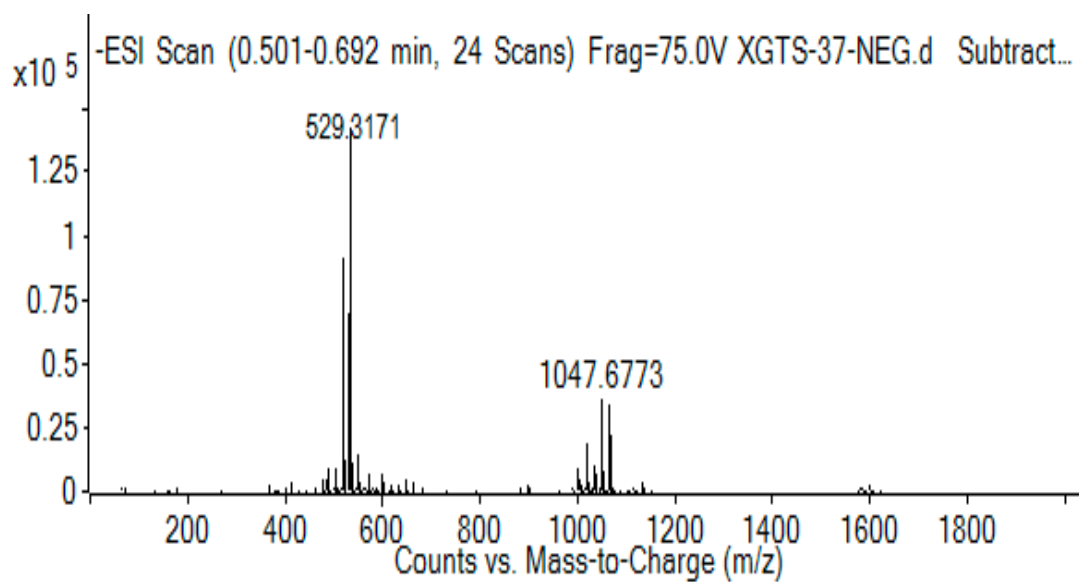
**Figure S37**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **9** in  $\text{CDCl}_3$



**Figure S38** HMBC spectrum (100 MHz) of compound **9** in  $\text{CDCl}_3$



**Figure S39** NOESY spectrum (400 MHz) of compound **9** in CDCl<sub>3</sub>



**Figure S40** HR-ESI-MS spectrum of compound **9**



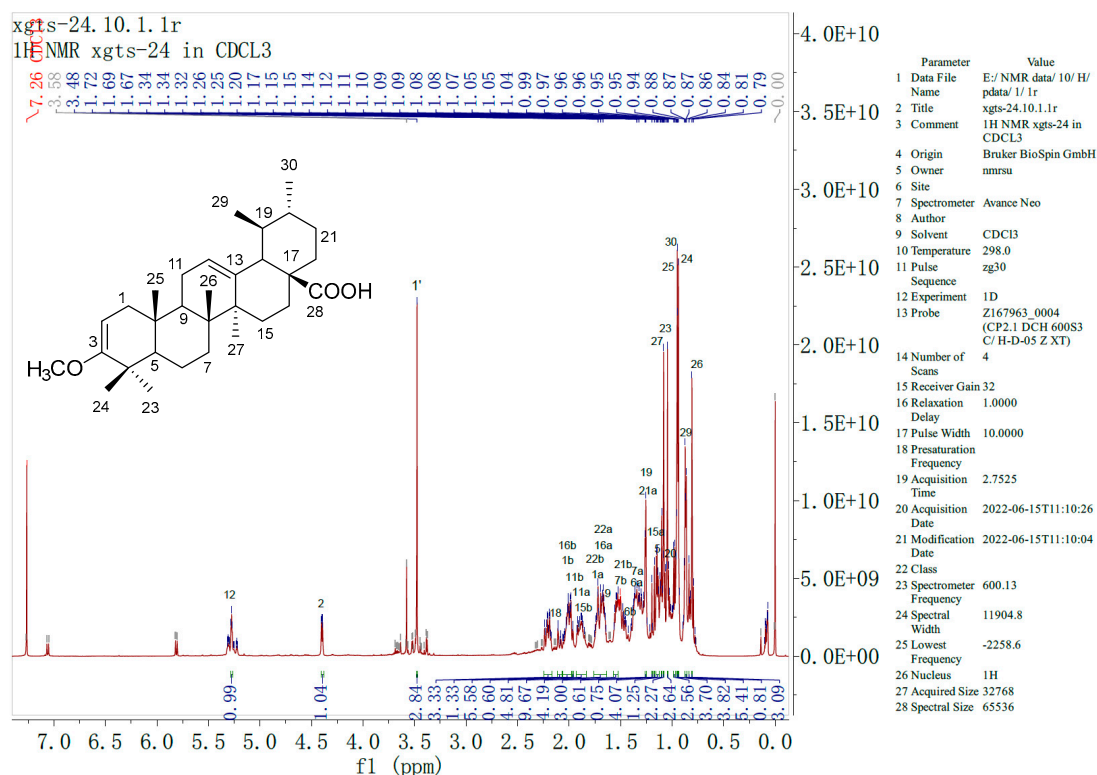


Figure S41 <sup>1</sup>H NMR spectrum (400 MHz) of compound **10** in CDCl<sub>3</sub>

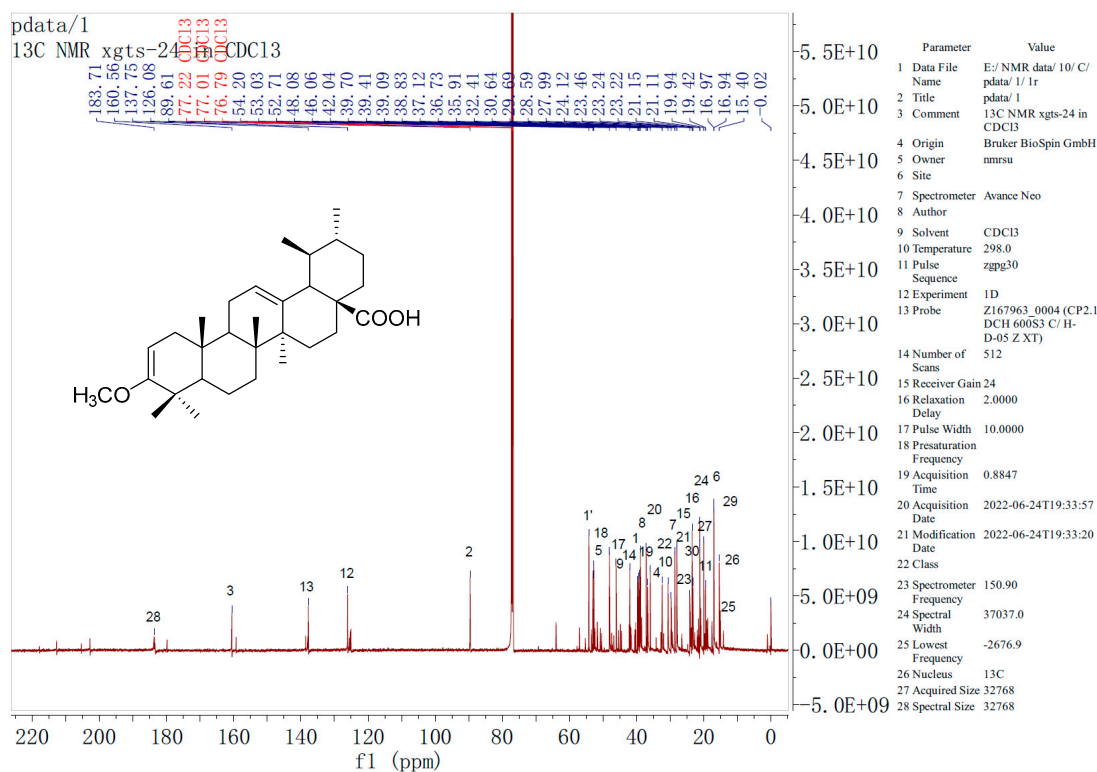


Figure S42 <sup>13</sup>C NMR spectrum (100 MHz) of compound **10** in CDCl<sub>3</sub>

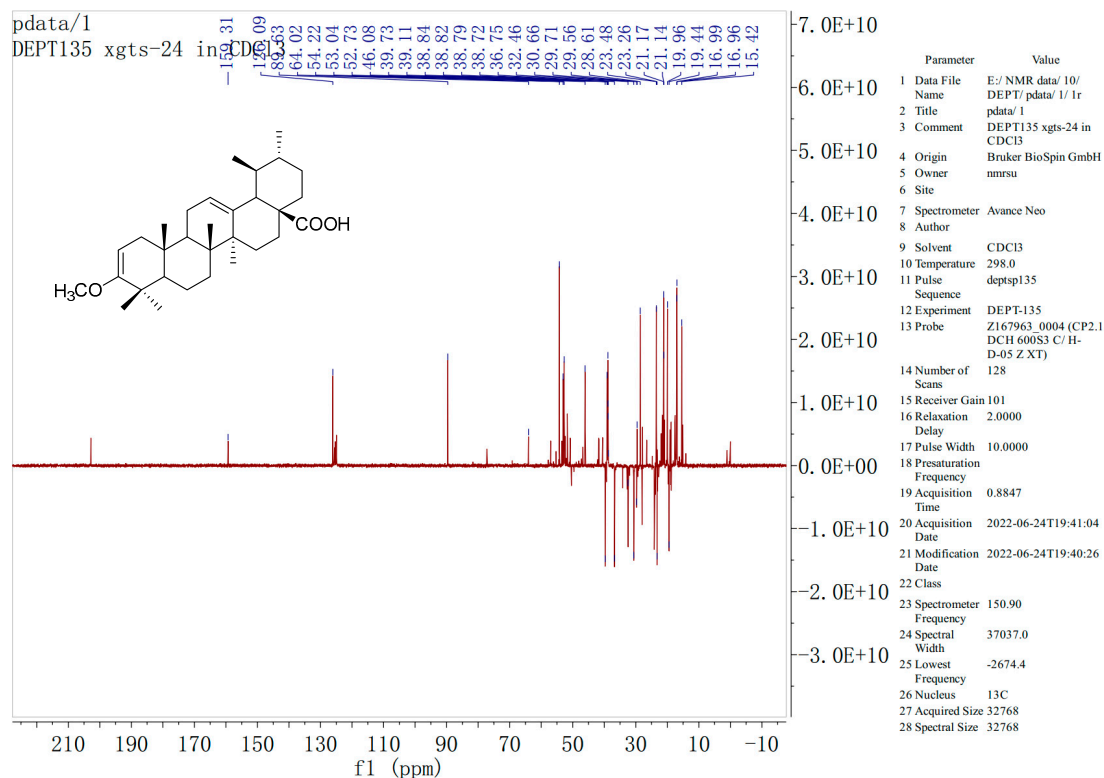


Figure S43 DEPT-135 spectrum (100 MHz) of compound **10** in CDCl<sub>3</sub>

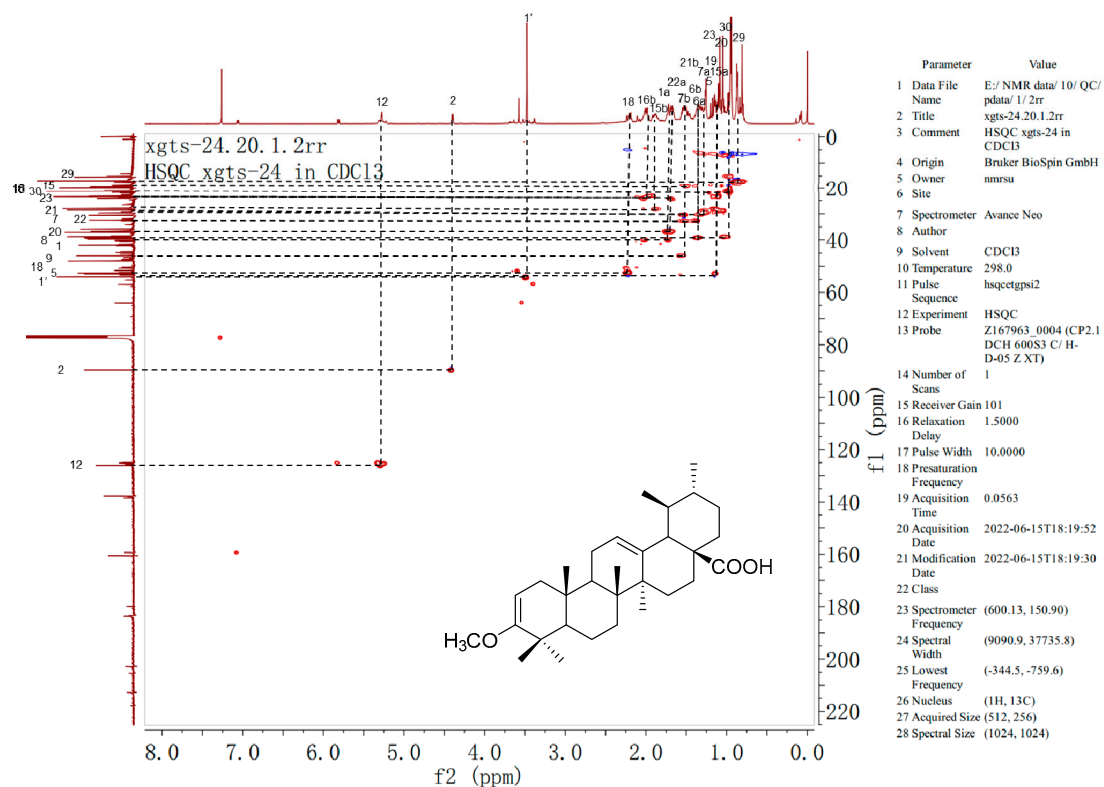
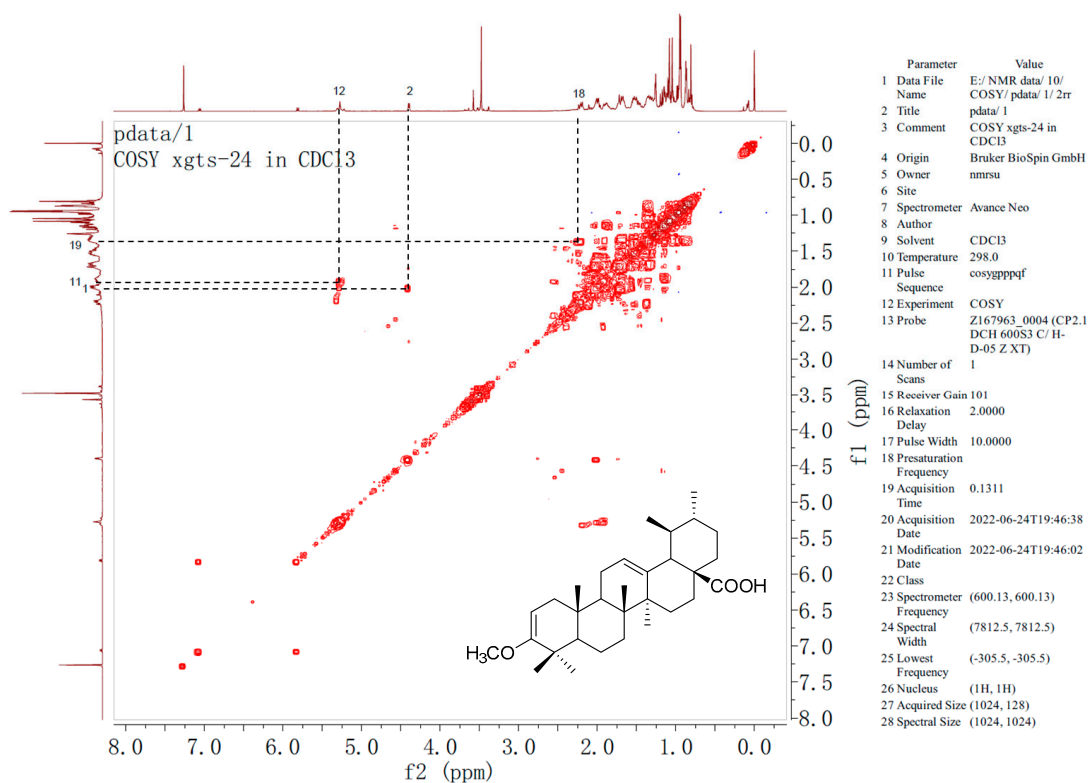
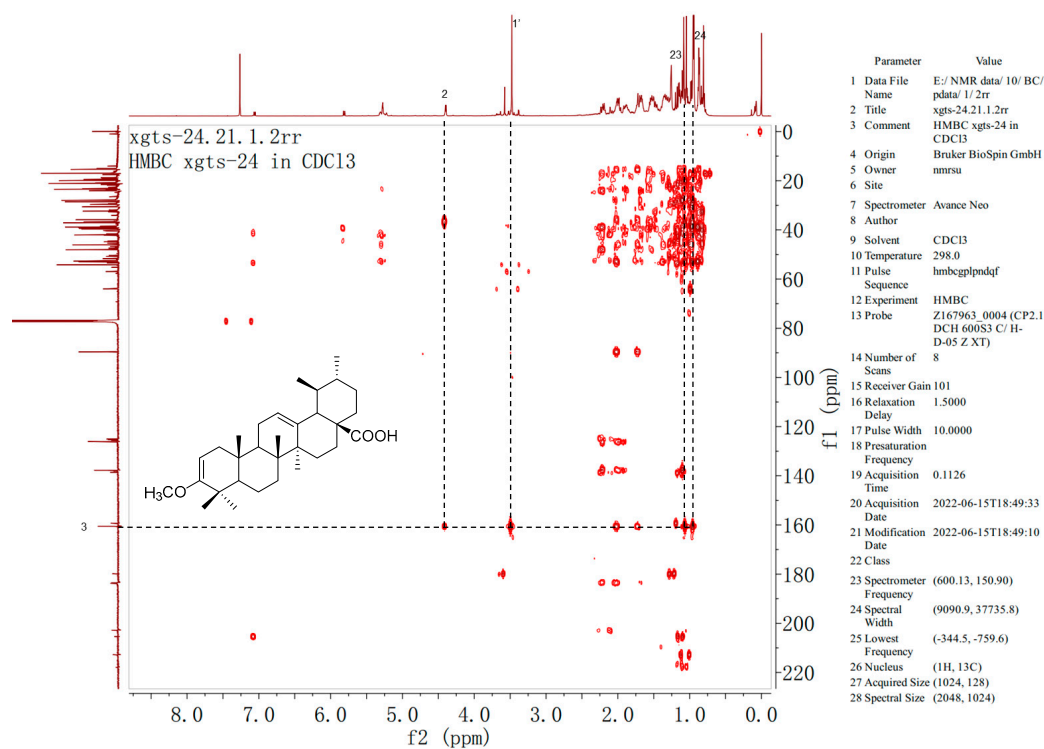


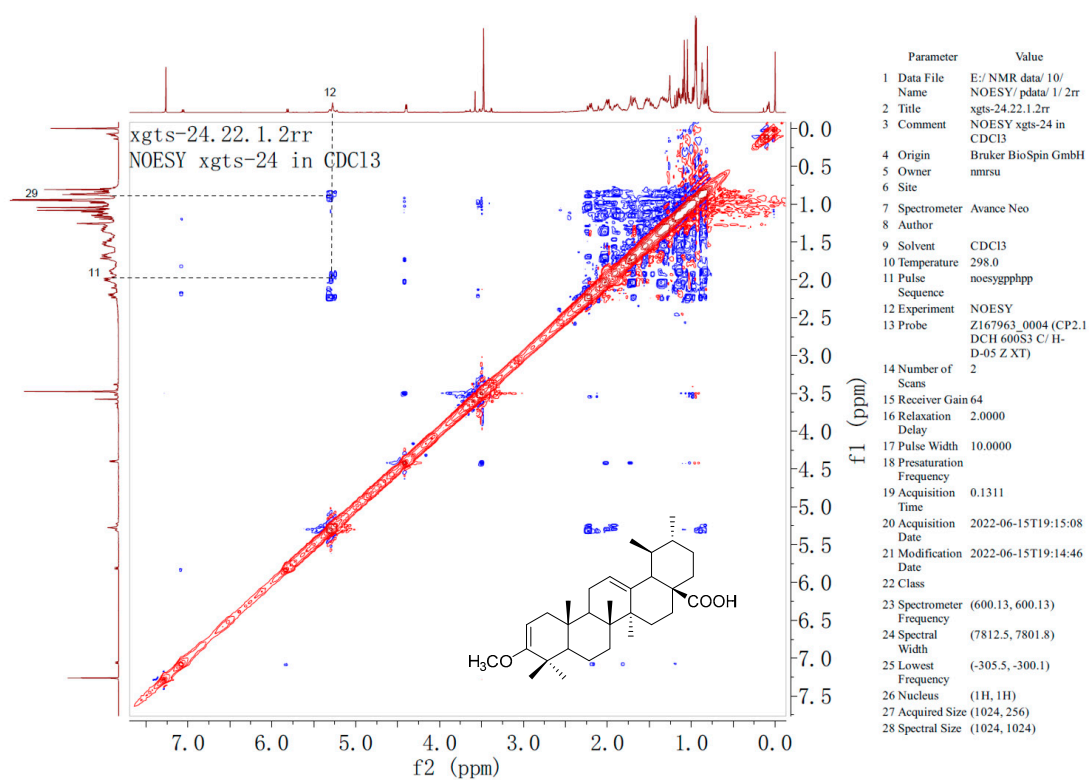
Figure S44 HSQC spectrum (100 MHz) of compound **10** in CDCl<sub>3</sub>



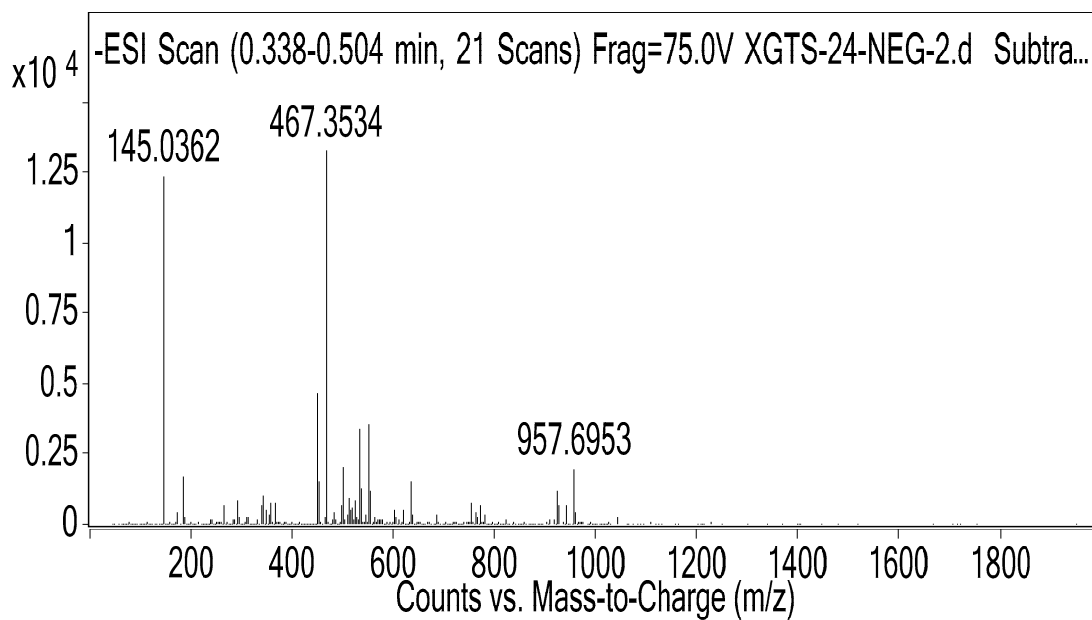
**Figure S45** <sup>1</sup>H-<sup>1</sup>H COSY spectrum (400 MHz) of compound **10** in CDCl<sub>3</sub>



**Figure S46** HMBC spectrum (100 MHz) of compound **10** in CDCl<sub>3</sub>



**Figure S47** NOESY spectrum (400 MHz) of compound **10** in CDCl<sub>3</sub>



**Figure S48** HR-ESI-MS spectrum of compound **10**





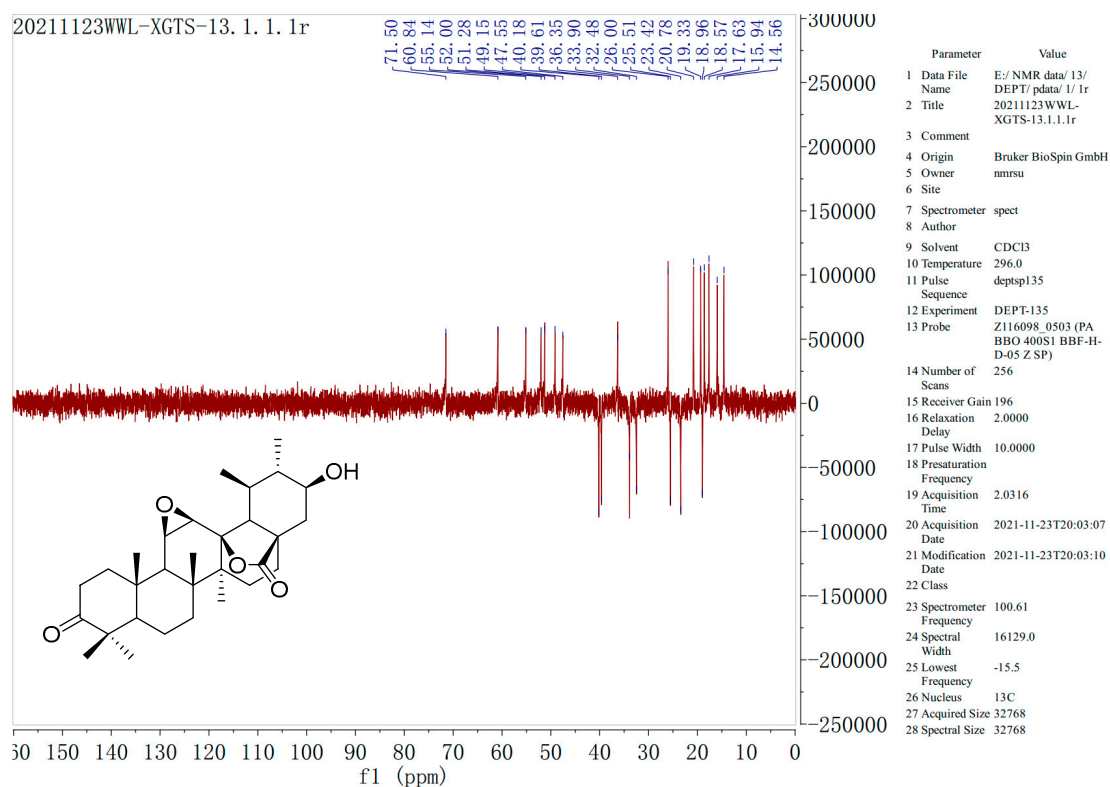


Figure S51 DEPT-135 spectrum (100 MHz) of compound **13** in CDCl<sub>3</sub>

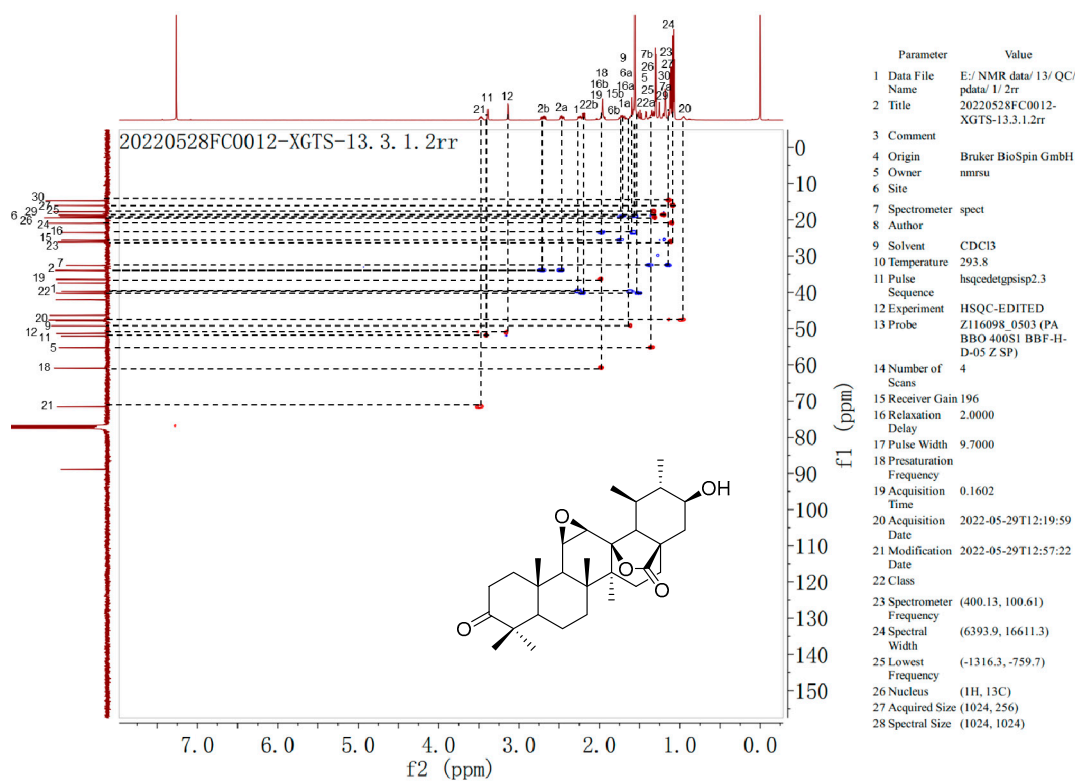


Figure S52 HSQC spectrum (100 MHz) of compound **13** in CDCl<sub>3</sub>

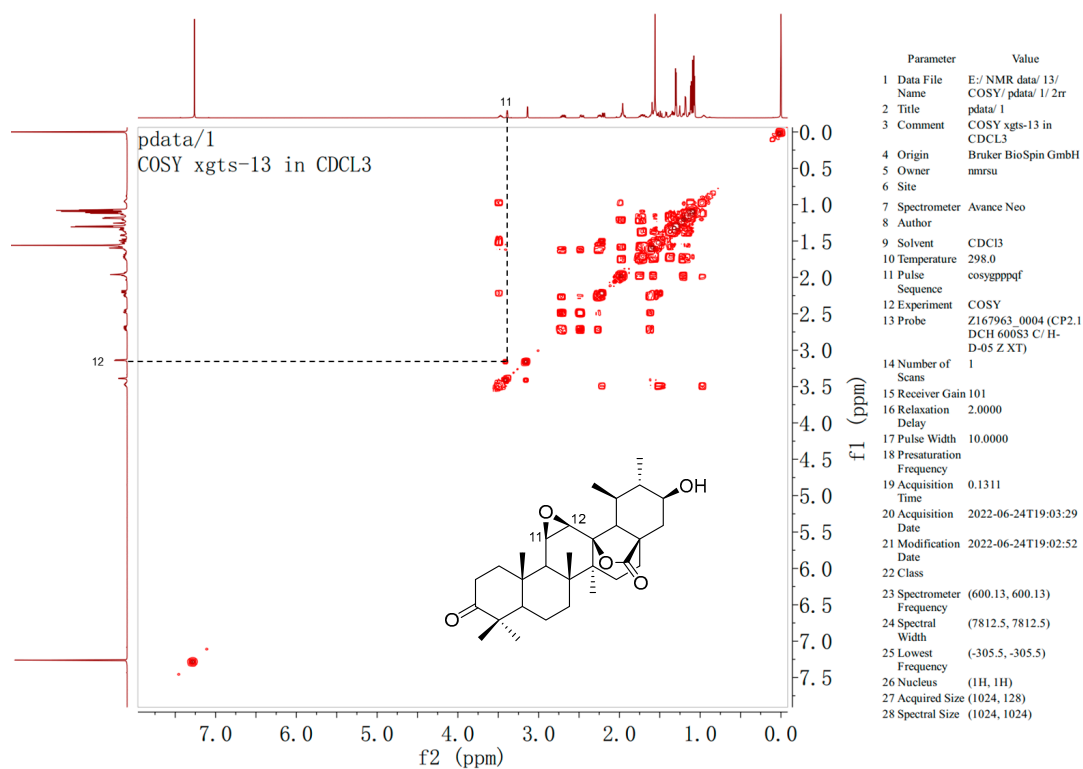


Figure S53  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **13** in  $\text{CDCl}_3$

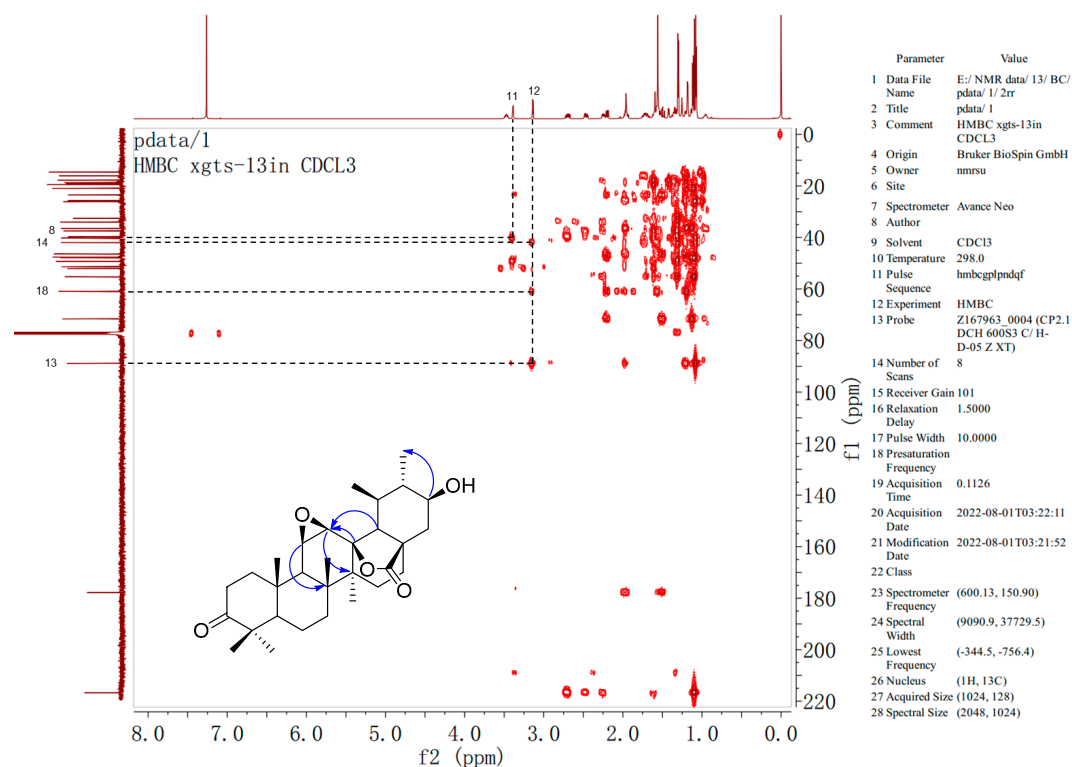
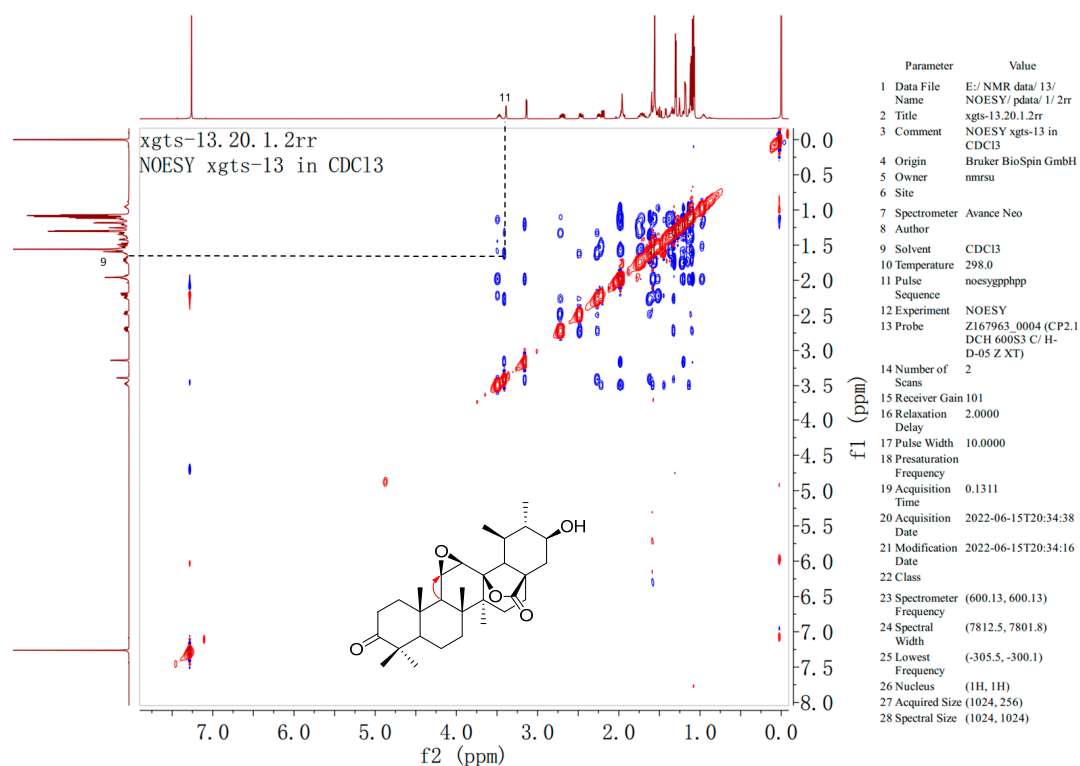
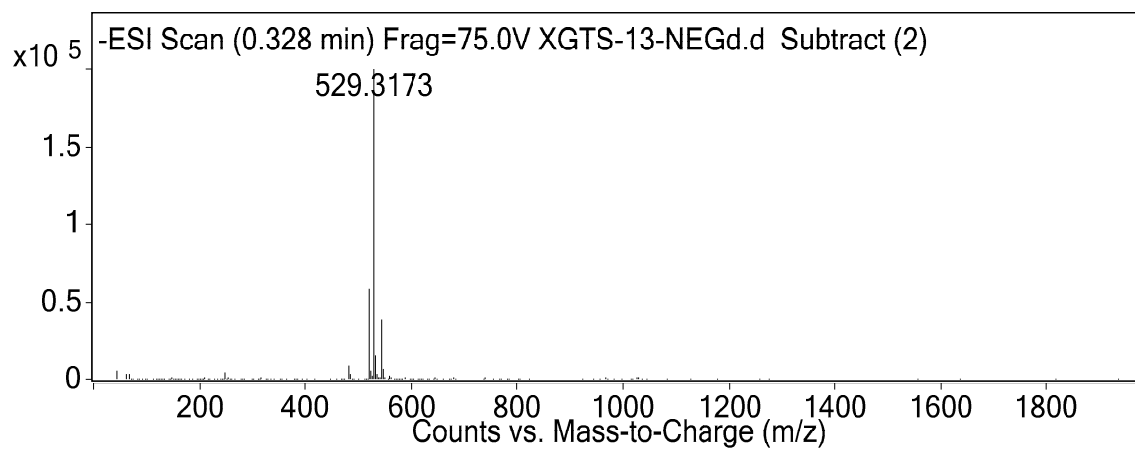


Figure S54 HMBC spectrum (100 MHz) of compound **13** in  $\text{CDCl}_3$

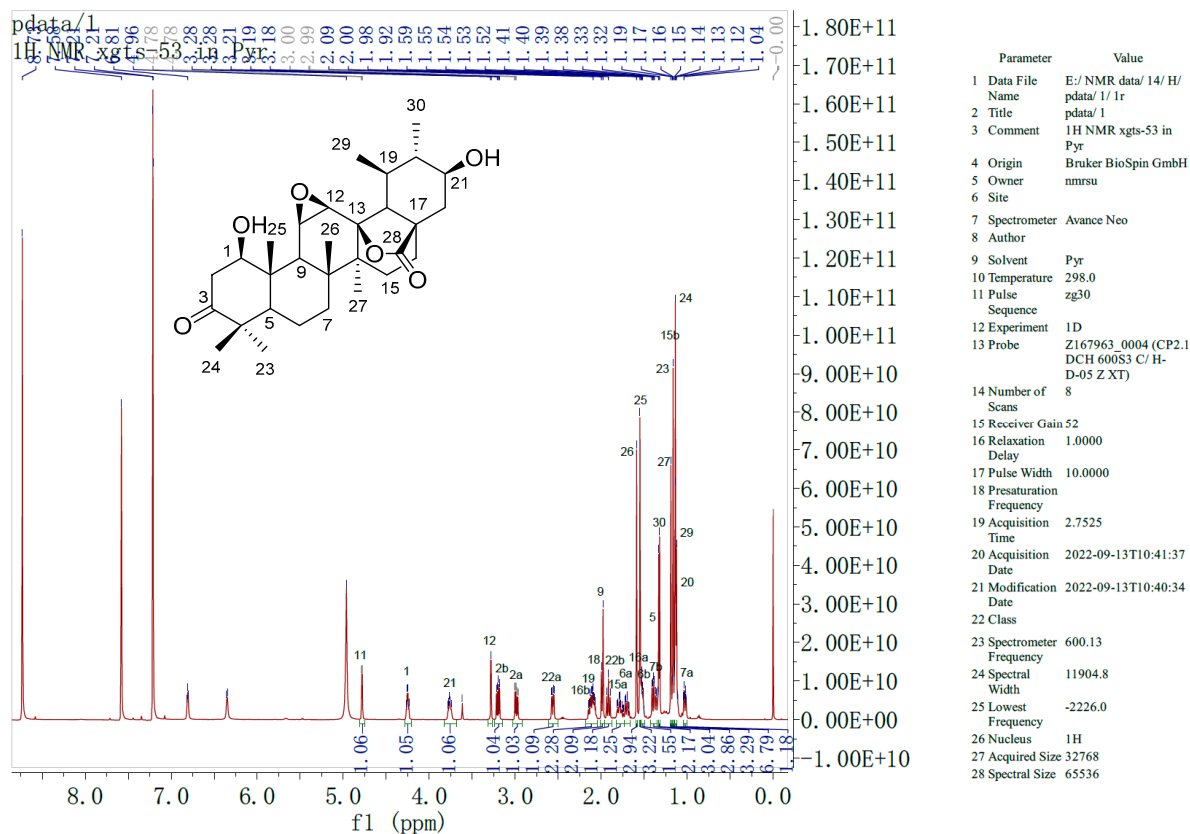


**Figure S55** NOESY spectrum (400 MHz) of compound 13 in CDCl<sub>3</sub>

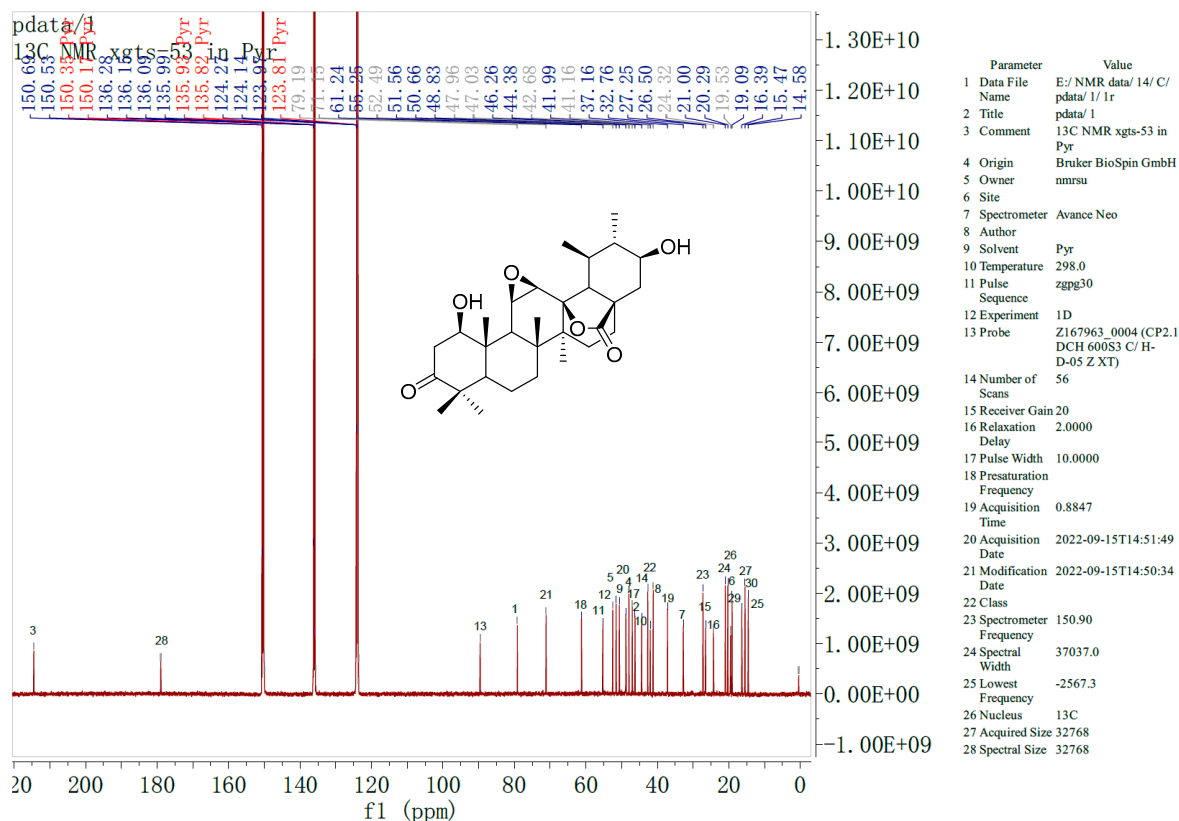


**Figure S56** HR-ESI-MS spectrum of compound 13

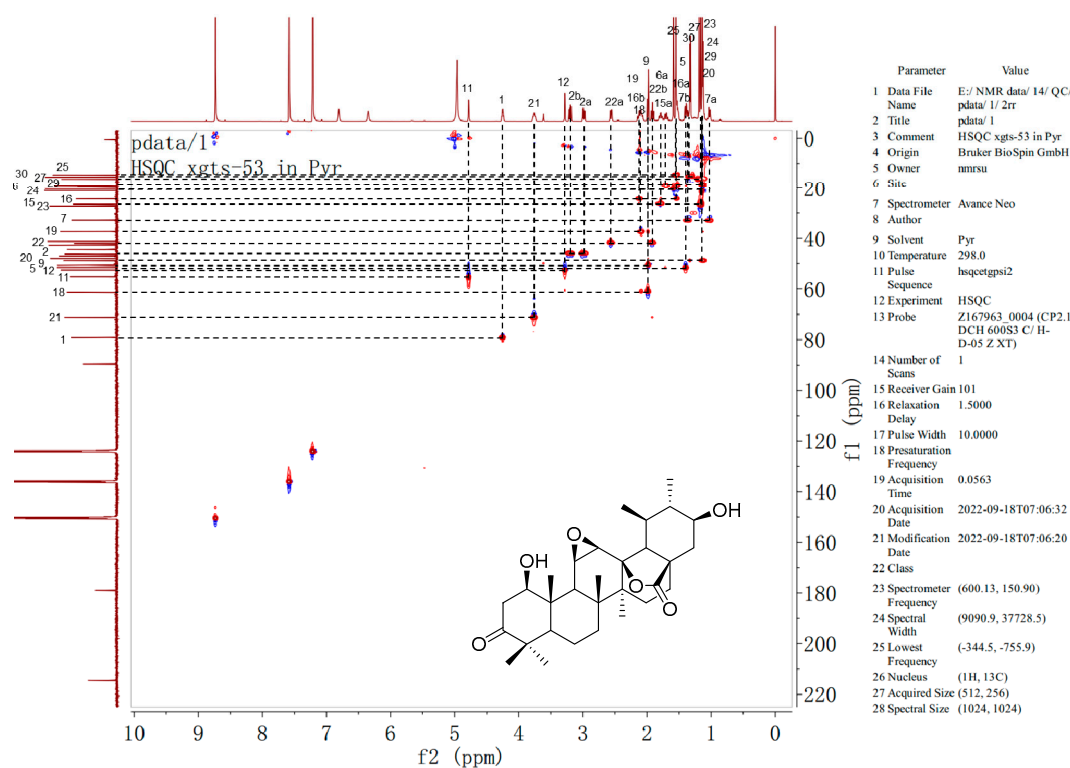
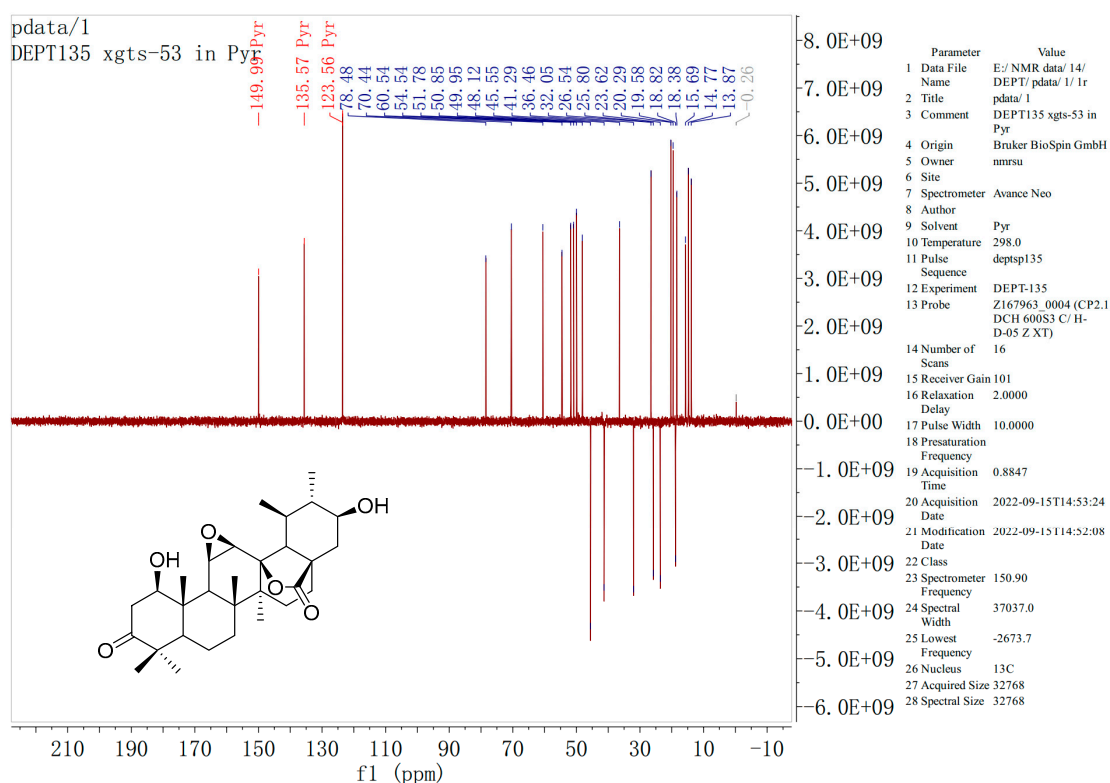


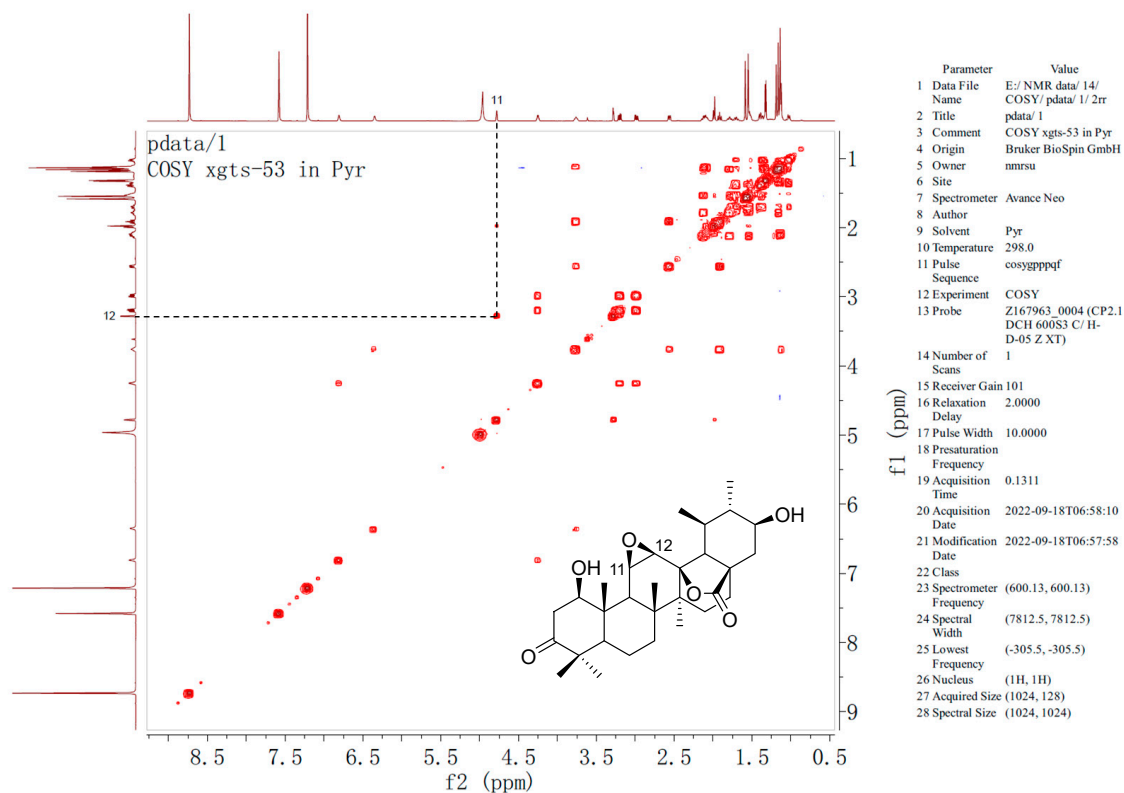


**Figure S57**  $^1\text{H}$  NMR spectrum (600 MHz) of compound **14** in Pyridine- $d_5$

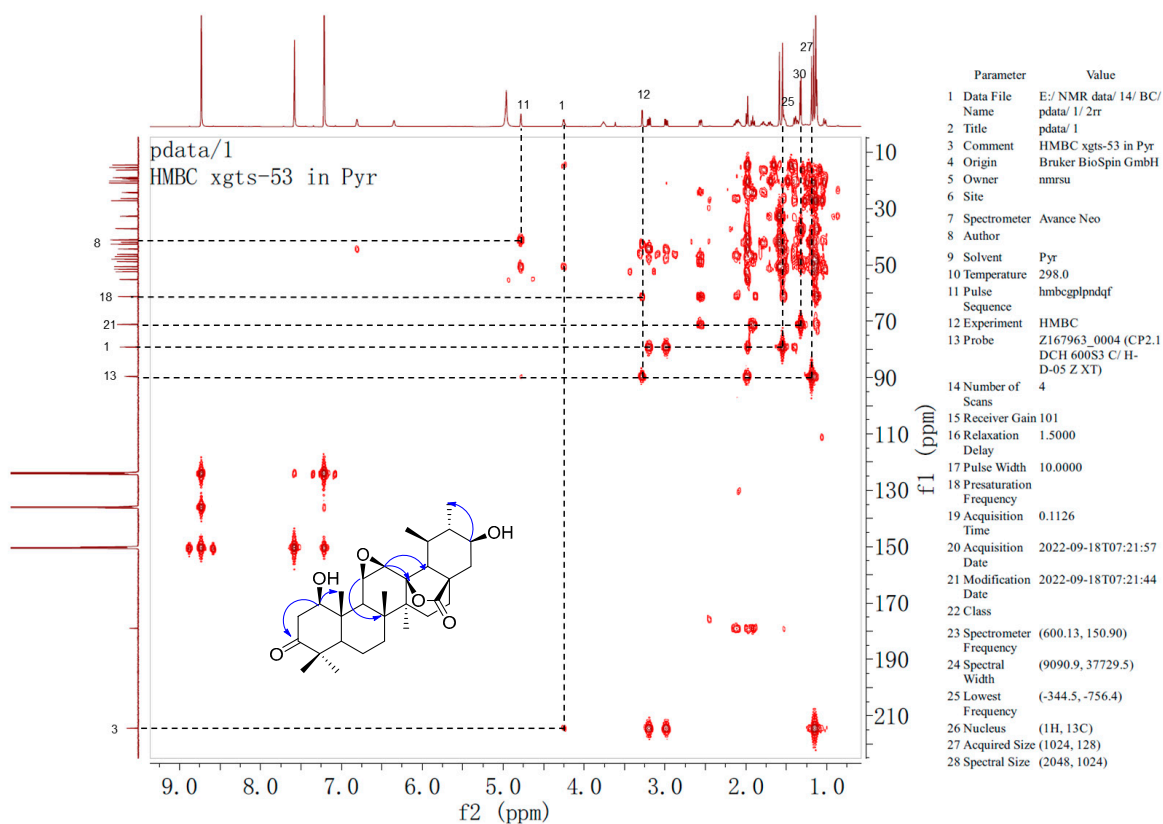


**Figure S58**  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **14** in Pyridine- $d_5$

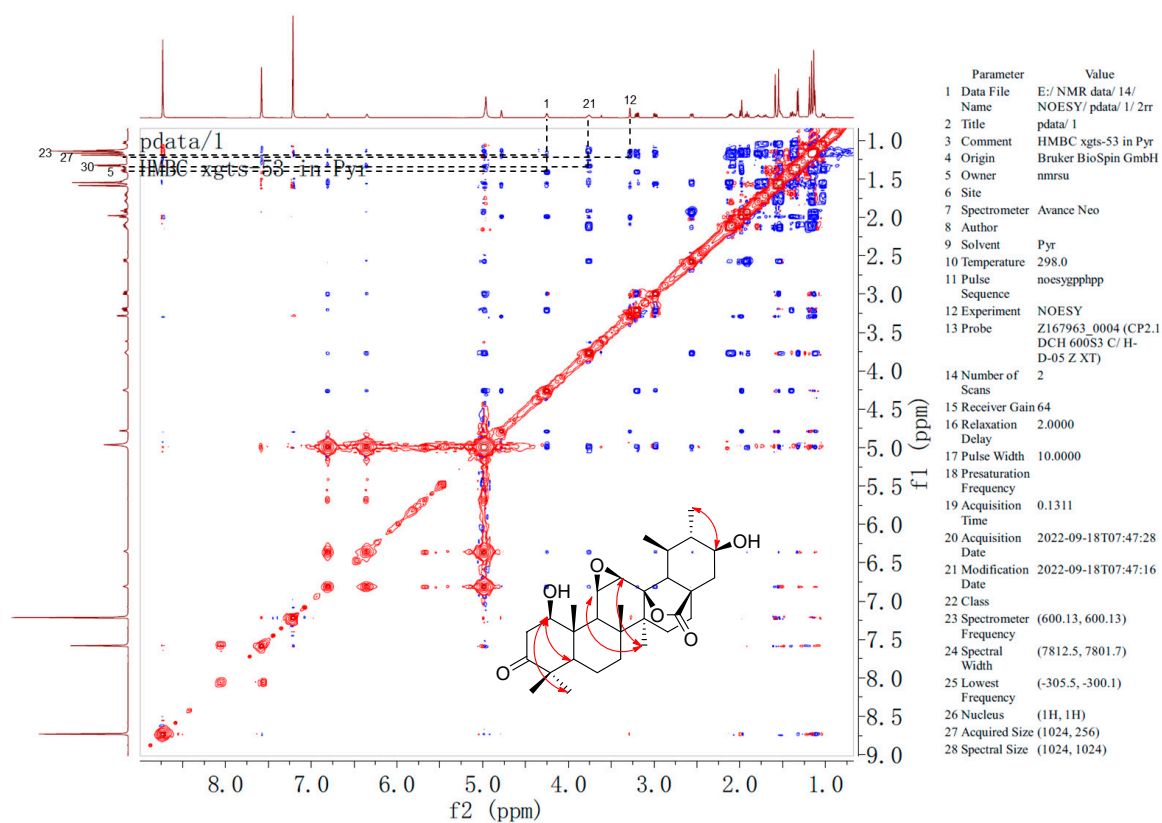




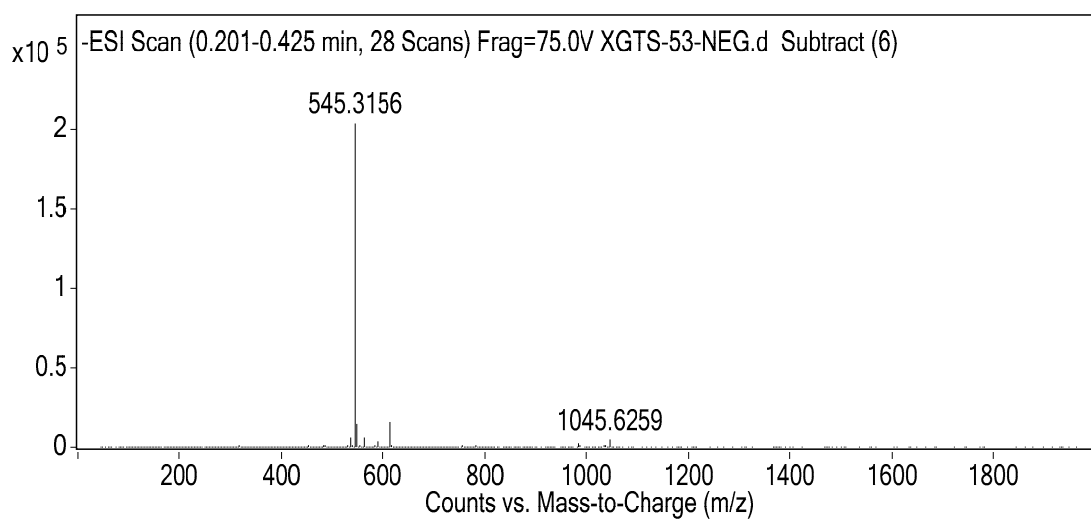
**Figure S61**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz) of compound **14** in Pyridine- $d_5$



**Figure S62** HMBC spectrum (150 MHz) of compound **14** in Pyridine- $d_5$



**Figure S63** NOESY spectrum (600 MHz) of compound **14** in Pyridine-*d*<sub>5</sub>



**Figure S64** HR-ESI-MS spectrum of compound **14**

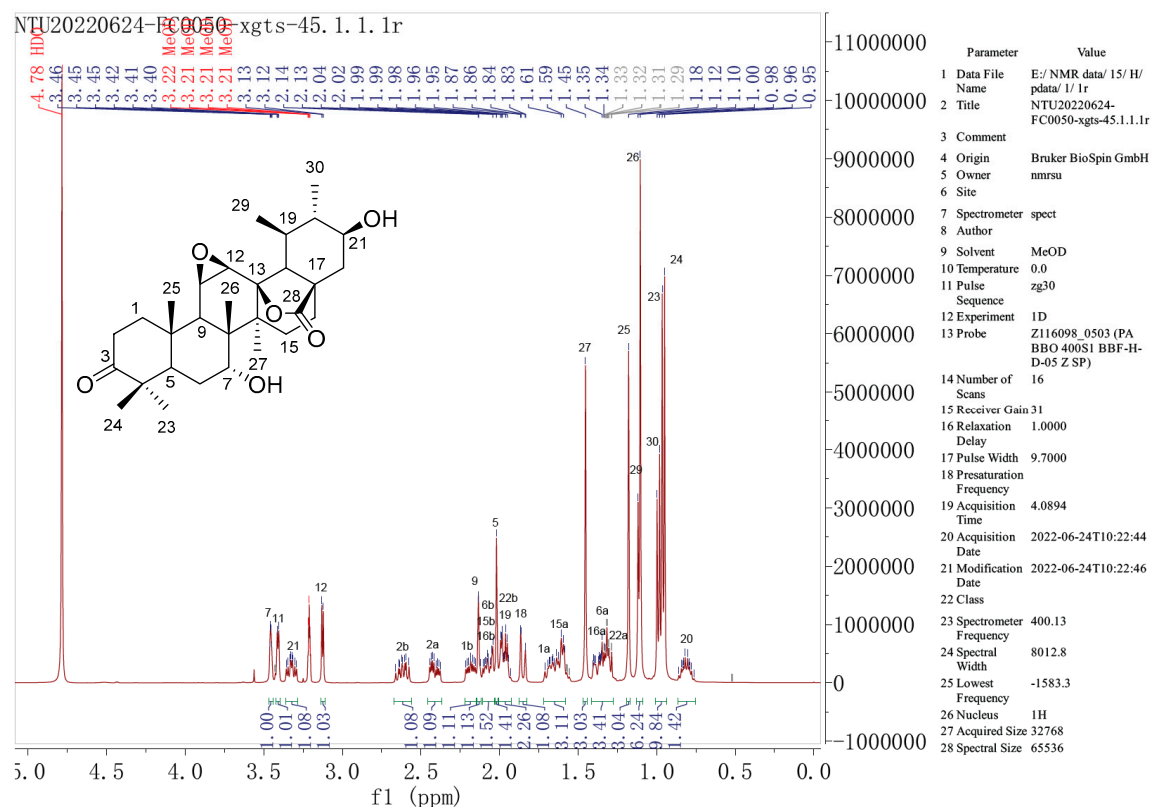


Figure S65  $^1\text{H}$  NMR spectrum (400 MHz) of compound **15** in  $\text{CD}_3\text{OD}$

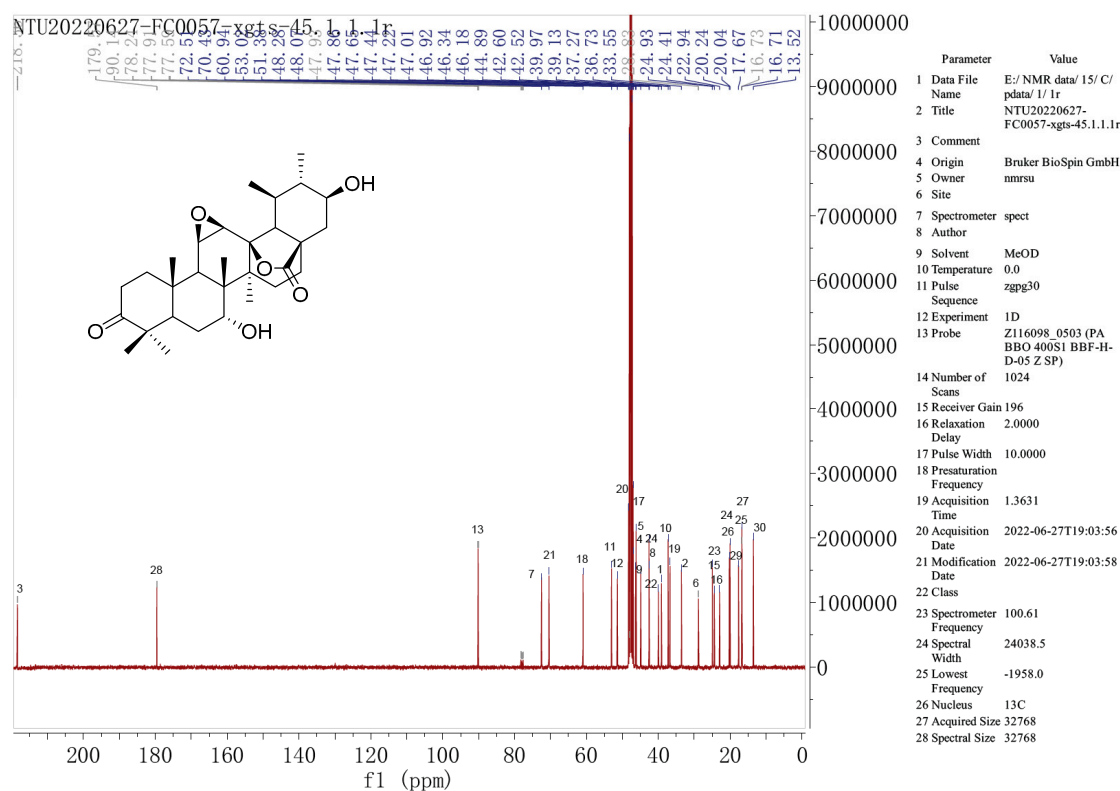


Figure S66  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **15** in  $\text{CD}_3\text{OD}$

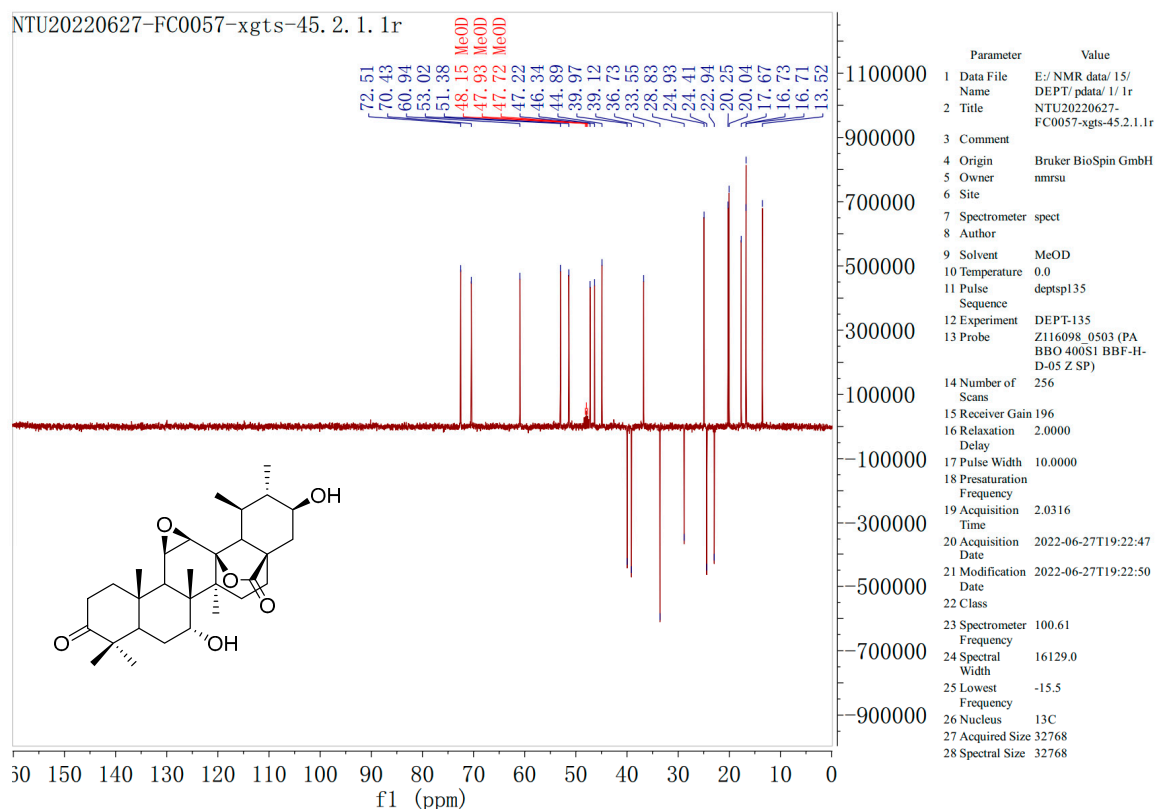


Figure S67 DEPT-135 spectrum (100 MHz) of compound **15** in CD<sub>3</sub>OD

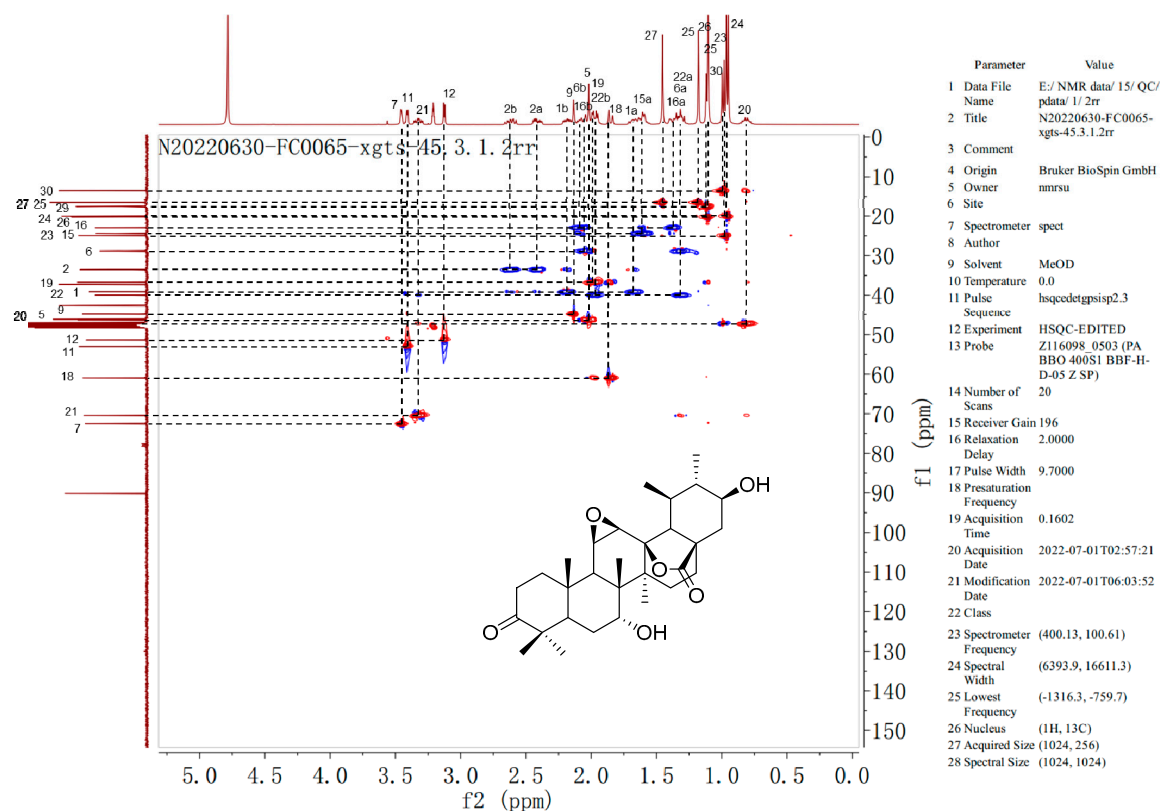
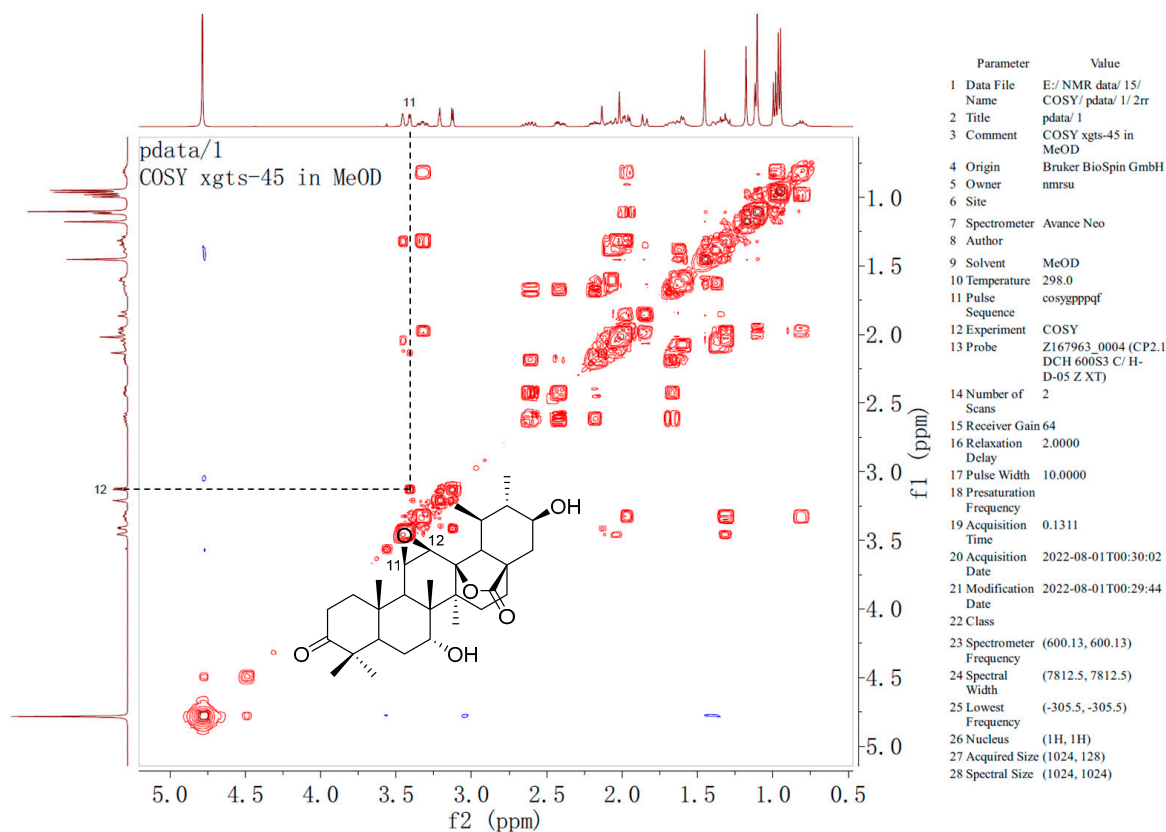
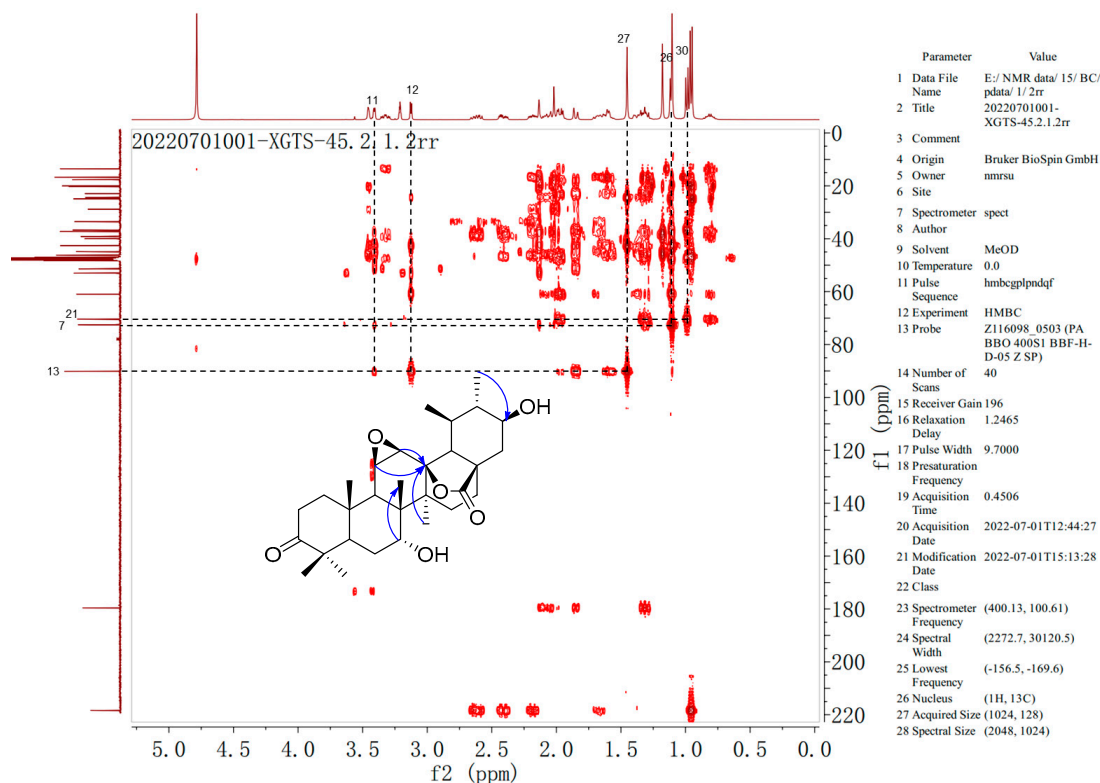


Figure S68 HSQC spectrum (100 MHz) of compound **15** in CD<sub>3</sub>OD

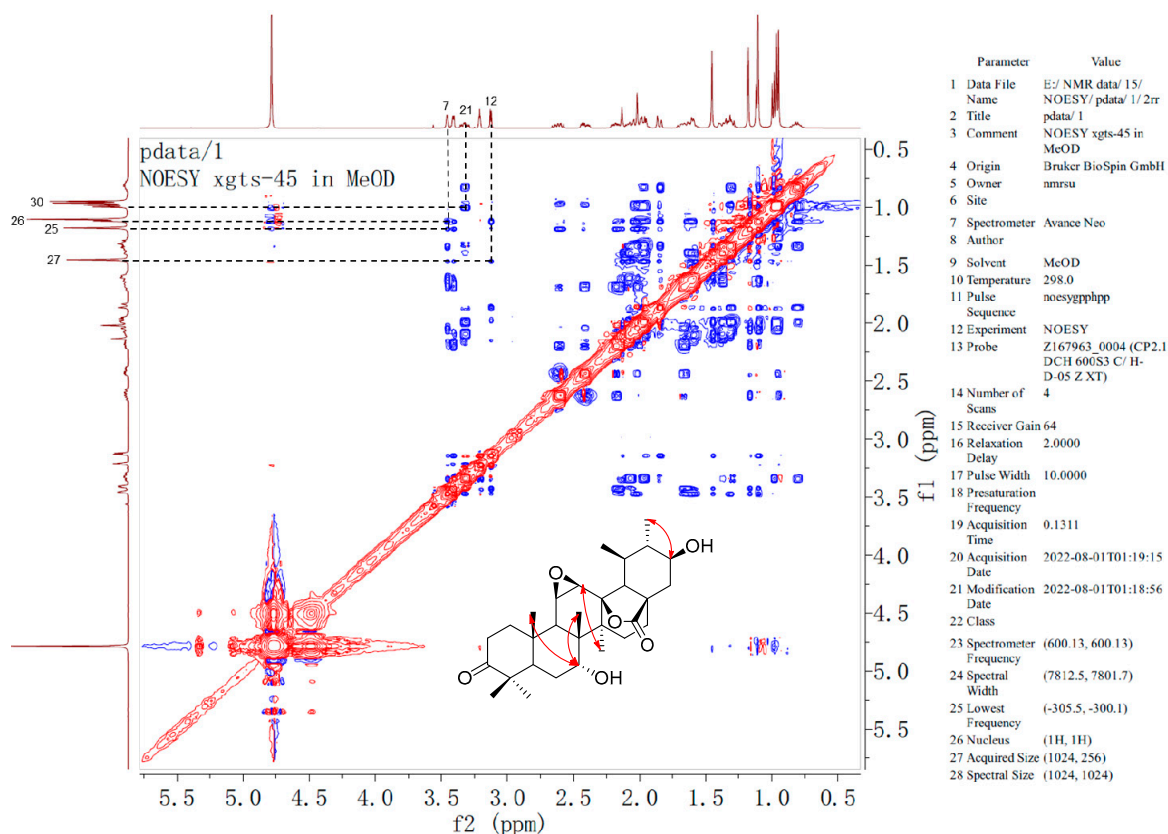




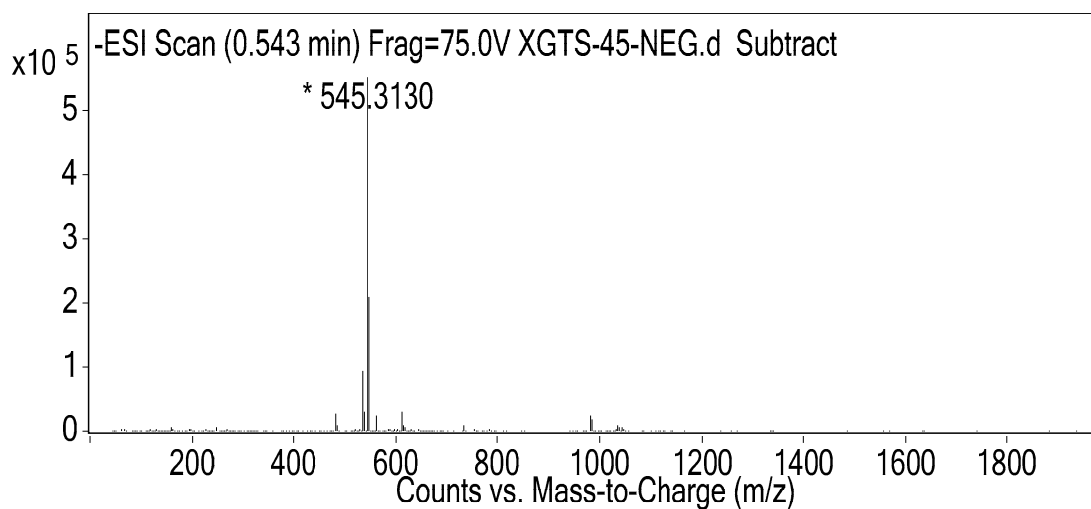
**Figure S69**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **15** in  $\text{CD}_3\text{OD}$



**Figure S70** HMBC spectrum (100 MHz) of compound **15** in  $\text{CD}_3\text{OD}$

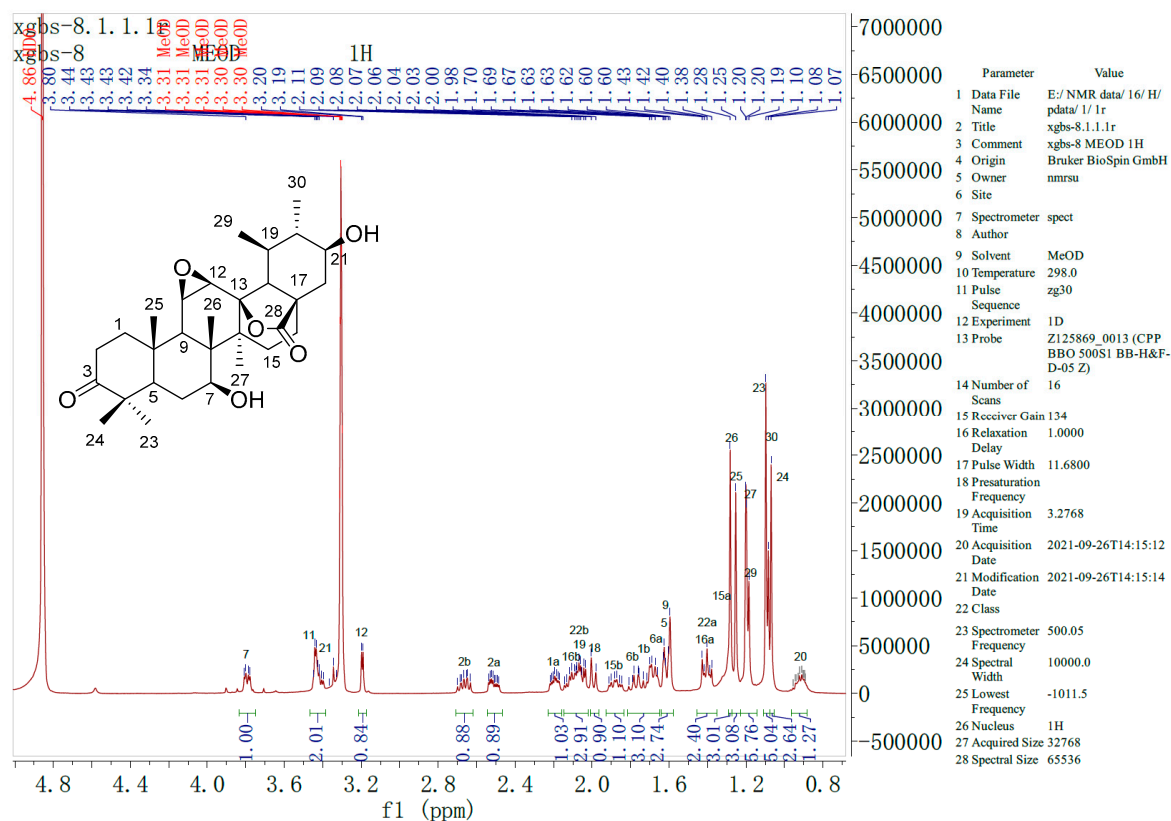


**Figure S71** NOESY spectrum (400 MHz) of compound **15** in CD<sub>3</sub>OD

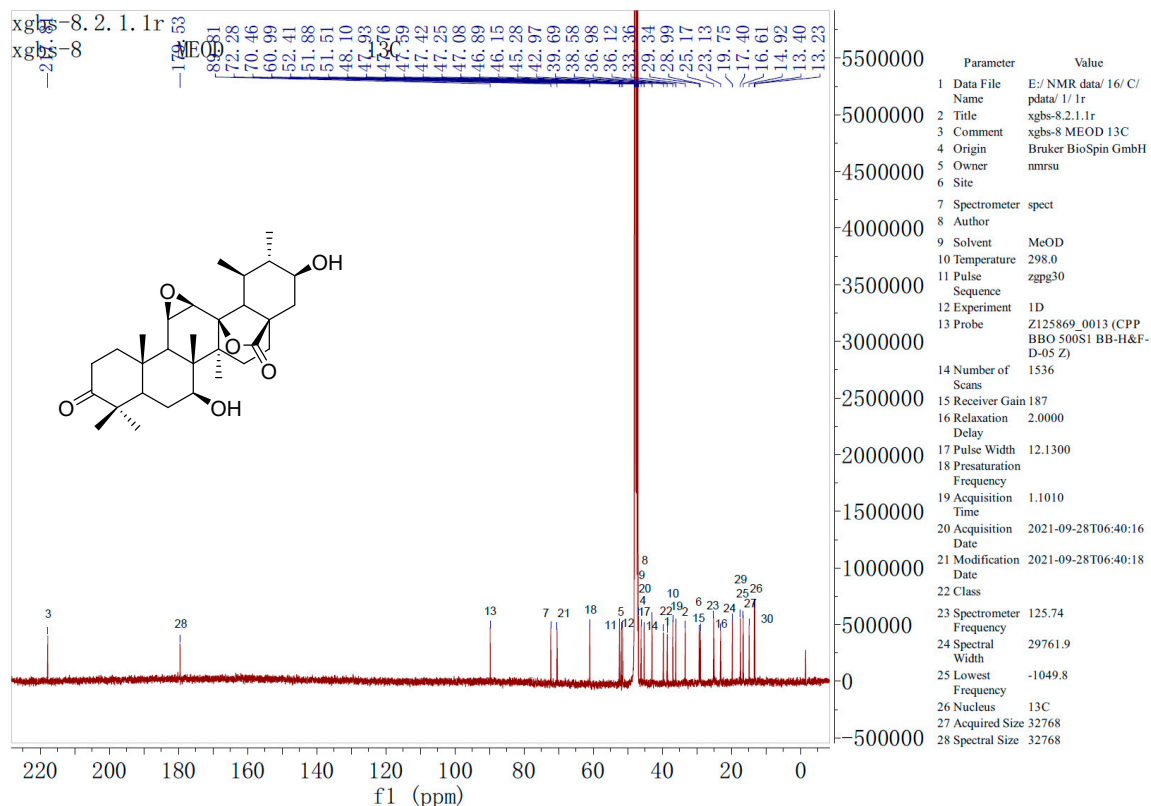


**Figure S72** HR-ESI-MS spectrum of compound **15**





**Figure S73**  $^1\text{H}$  NMR spectrum (500 MHz) of compound **16** in  $\text{CD}_3\text{OD}$



**Figure S74**  $^{13}\text{C}$  NMR spectrum (125 MHz) of compound **16** in  $\text{CD}_3\text{OD}$

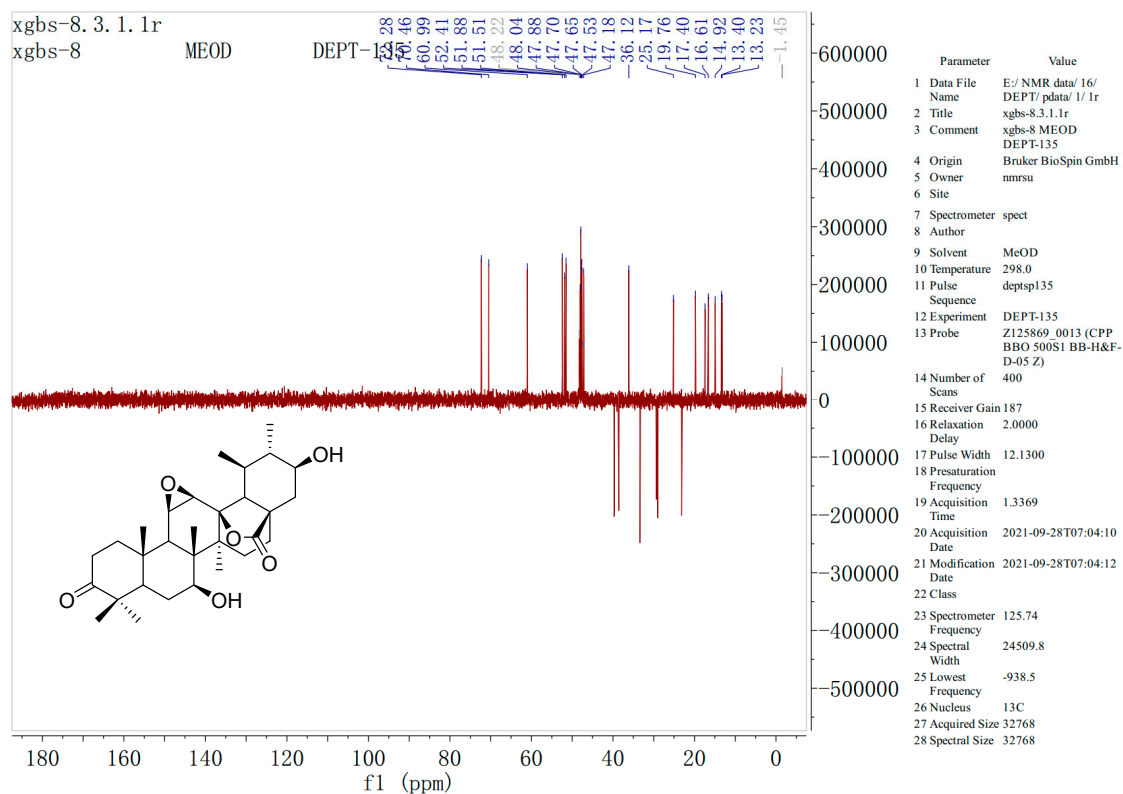


Figure S75 DEPT-135 spectrum (125 MHz) of compound 16 in CD<sub>3</sub>OD

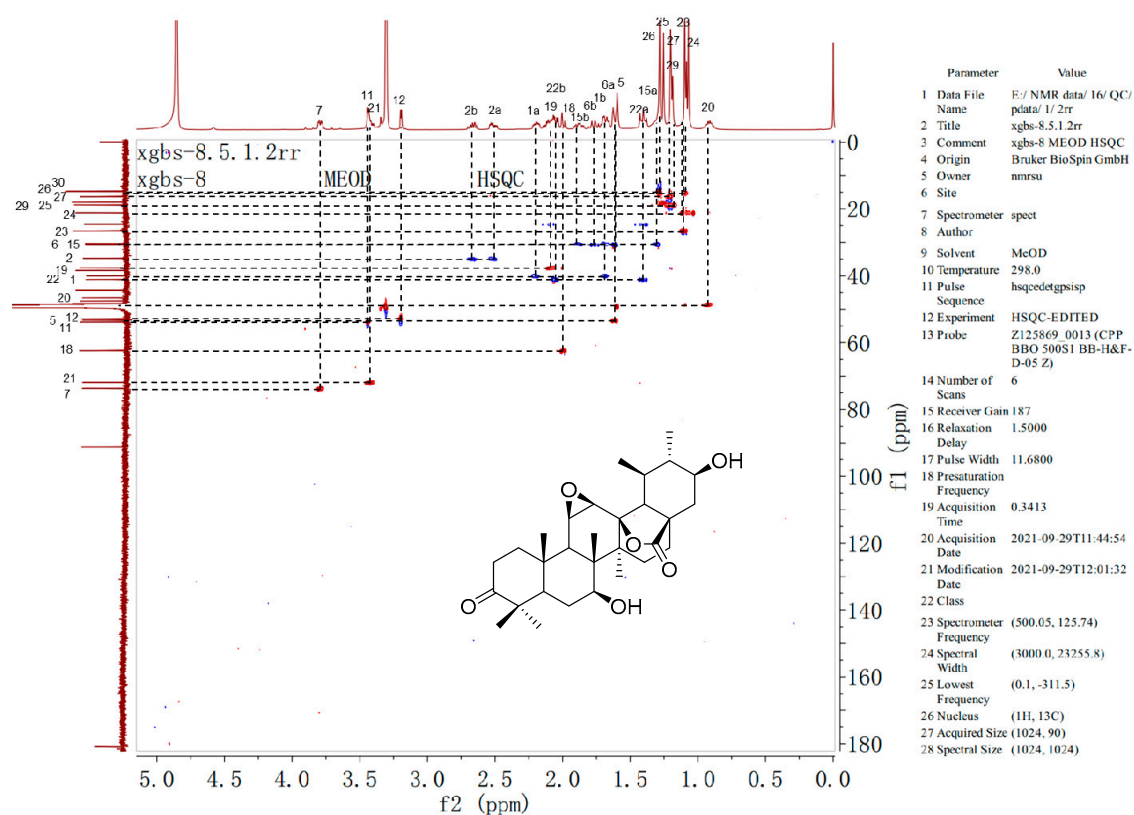
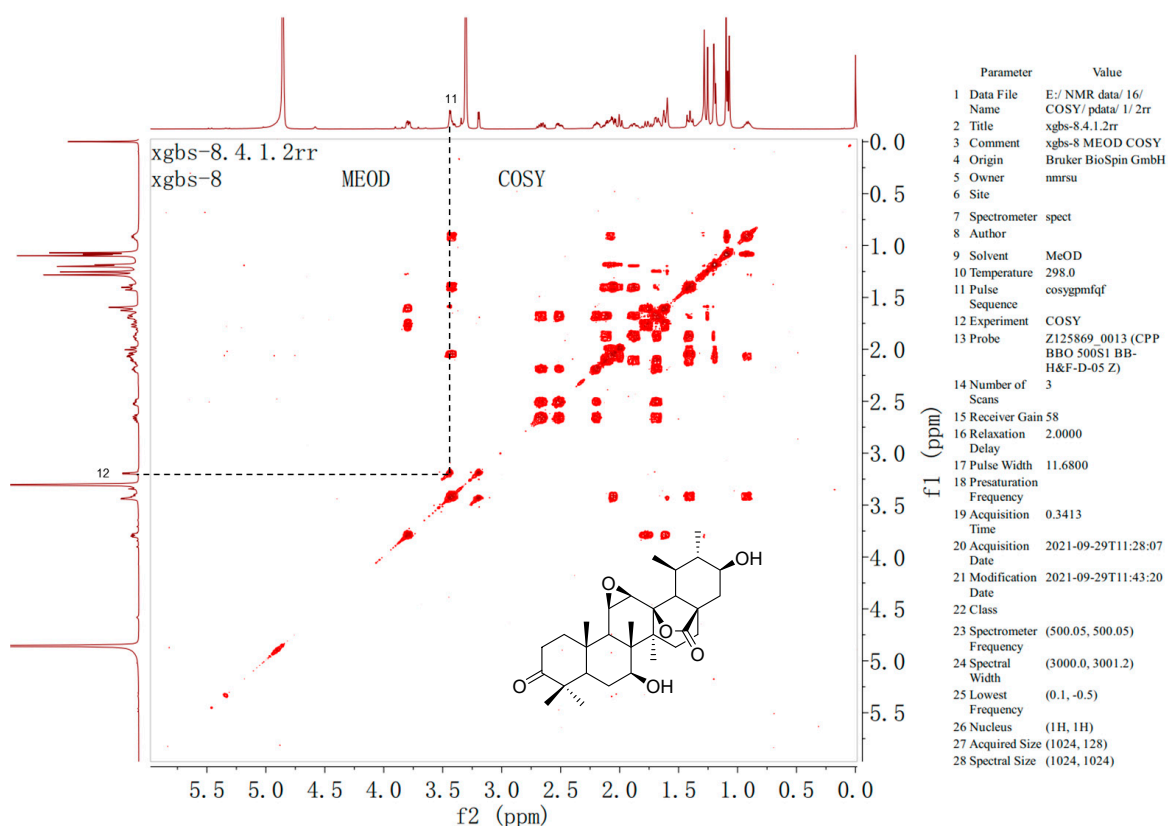
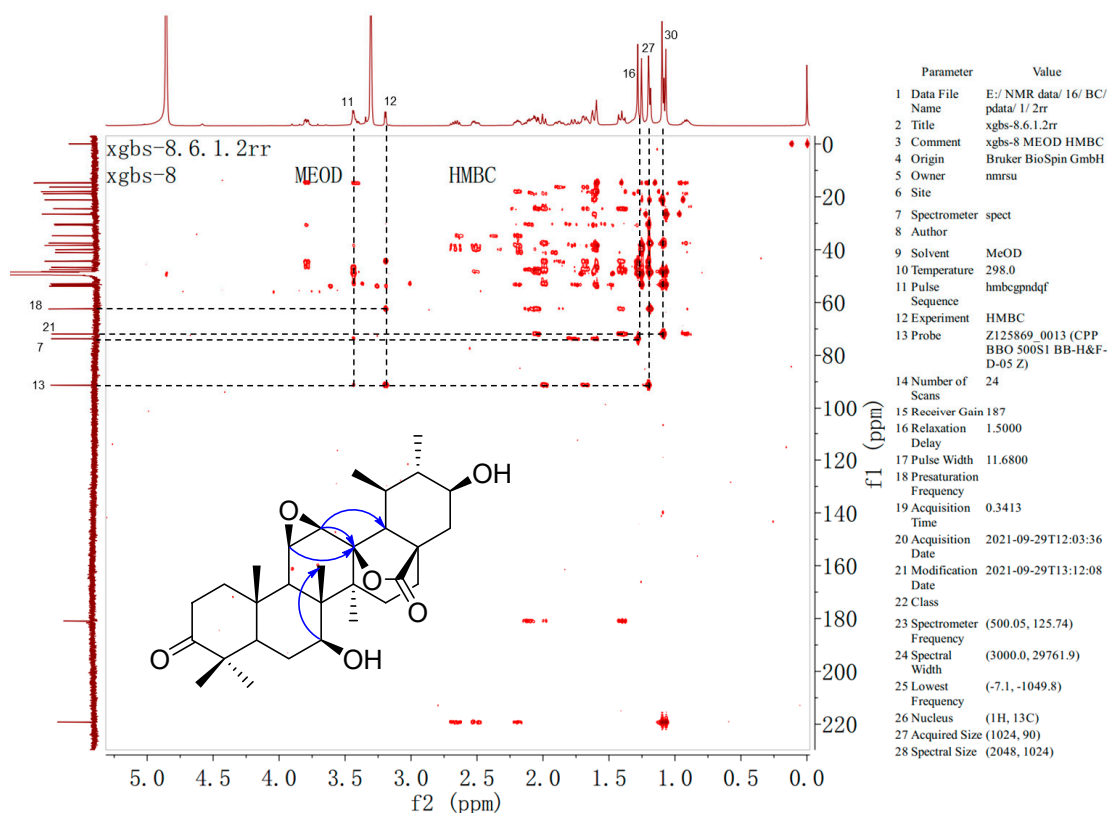


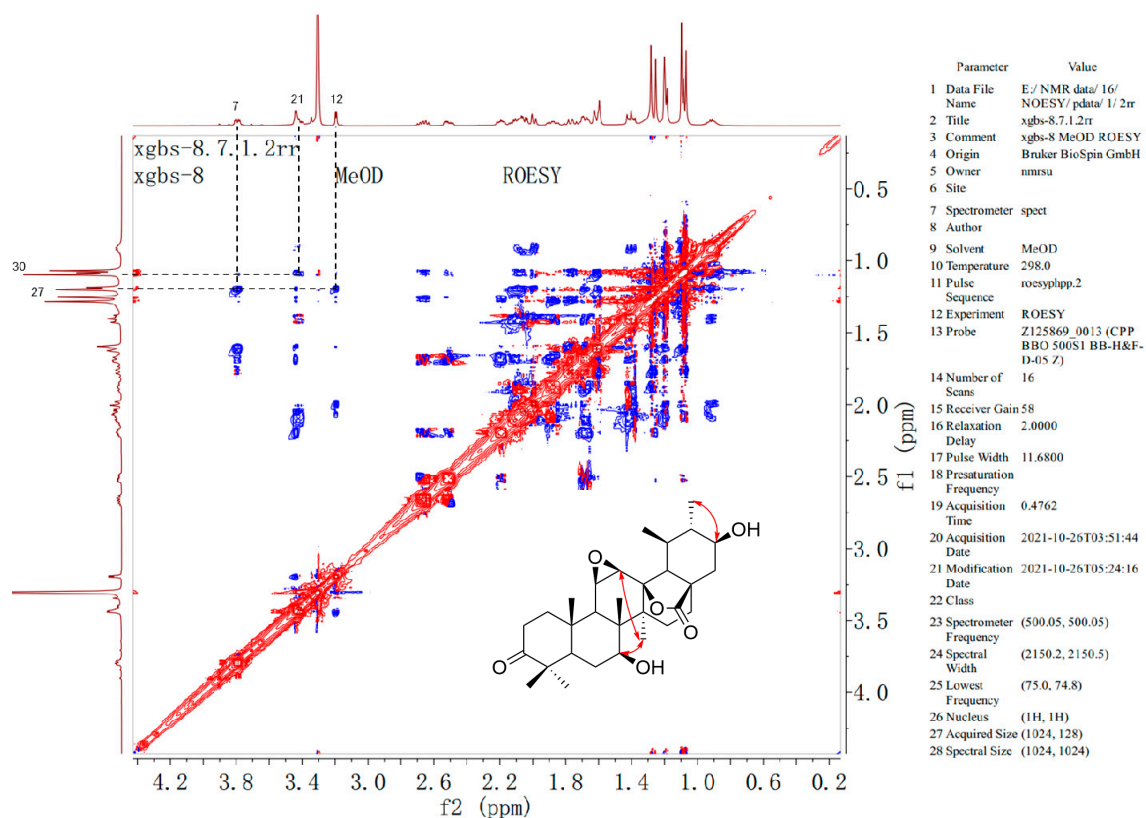
Figure S76 HSQC spectrum (125 Mz) of compound 16 in CD<sub>3</sub>OD



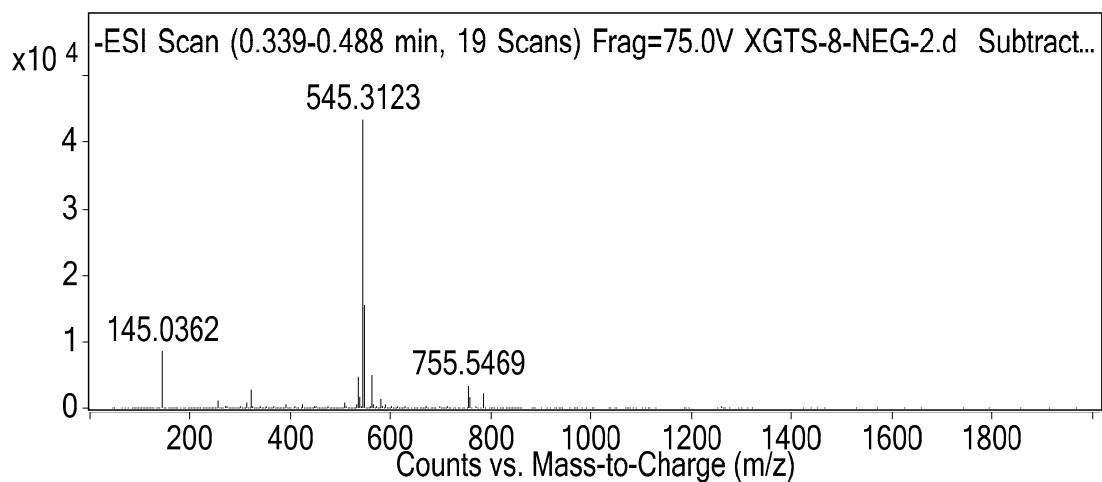
**Figure S77**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **16** in  $\text{CD}_3\text{OD}$



**Figure S78** HMBC spectrum (125 MHz) of compound **16** in  $\text{CD}_3\text{OD}$



**Figure S79** NOESY spectrum (500 MHz) of compound **16** in CD<sub>3</sub>OD



**Figure S80** HR-ESI-MS spectrum of compound **16**

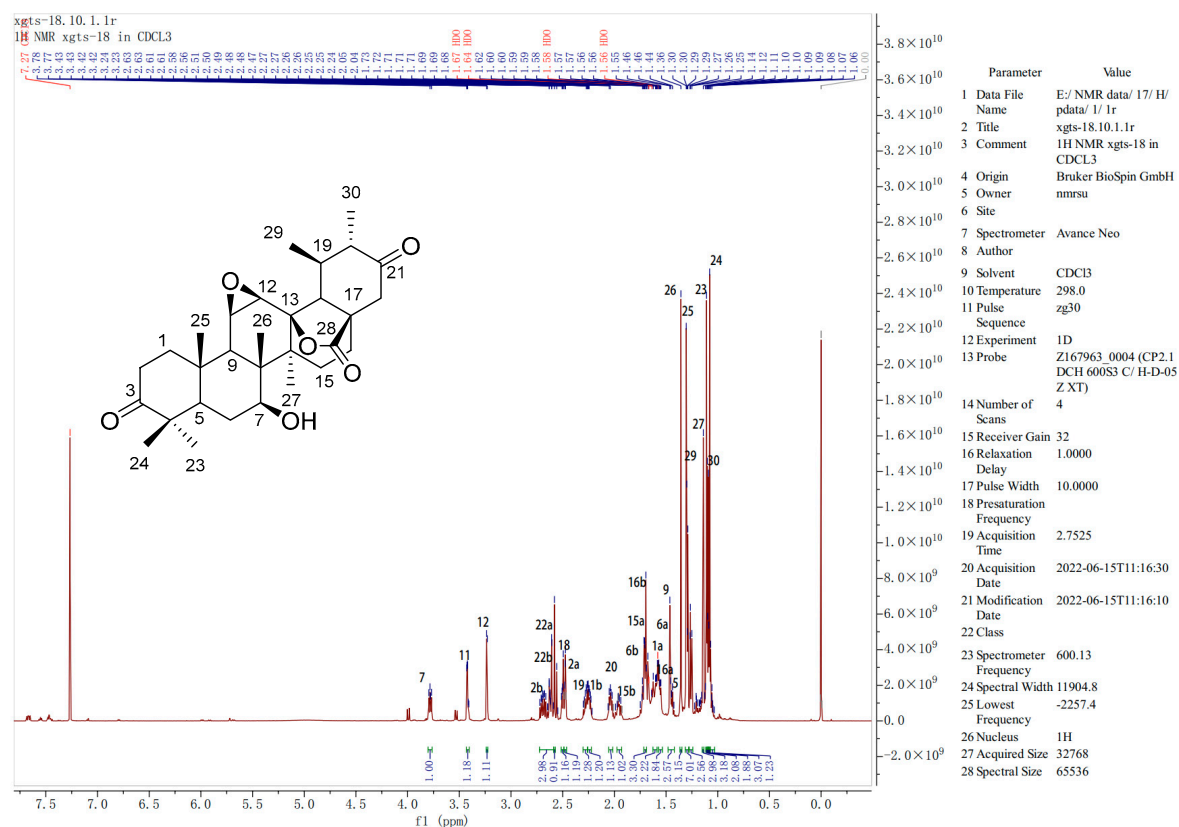


Figure S81  $^1\text{H}$  NMR spectrum (400 MHz) of compound **17** in  $\text{CDCl}_3$

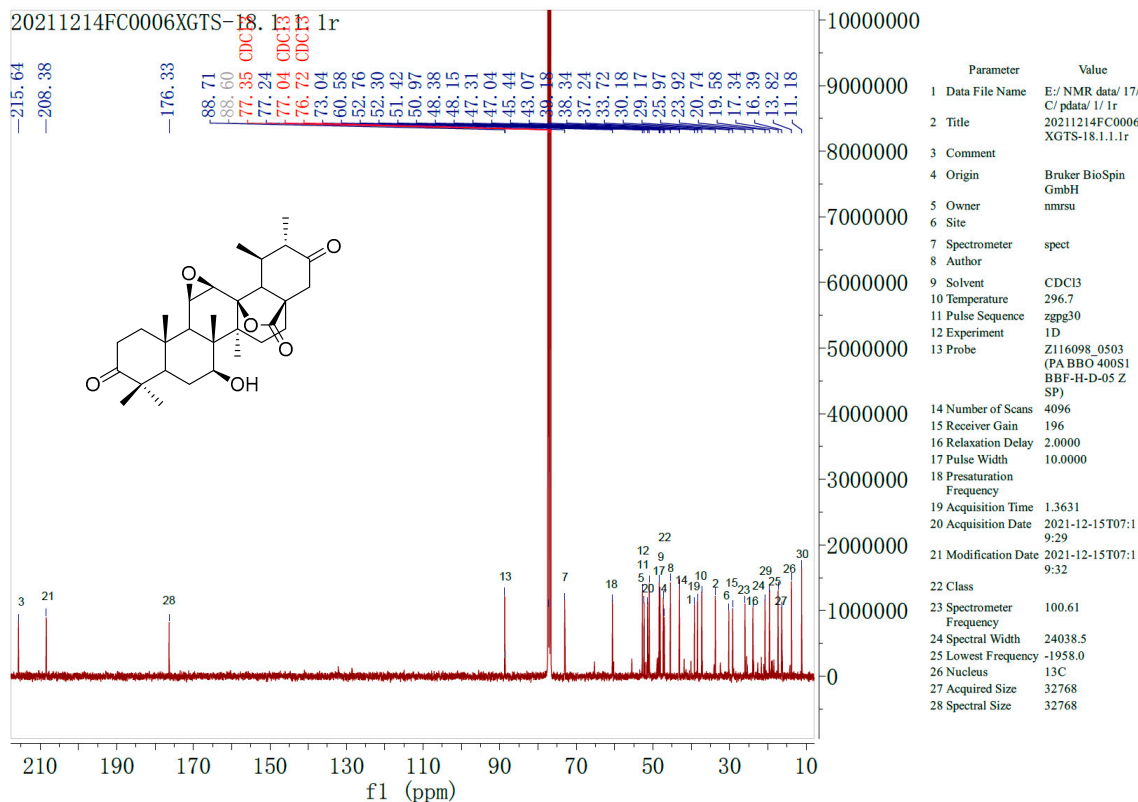
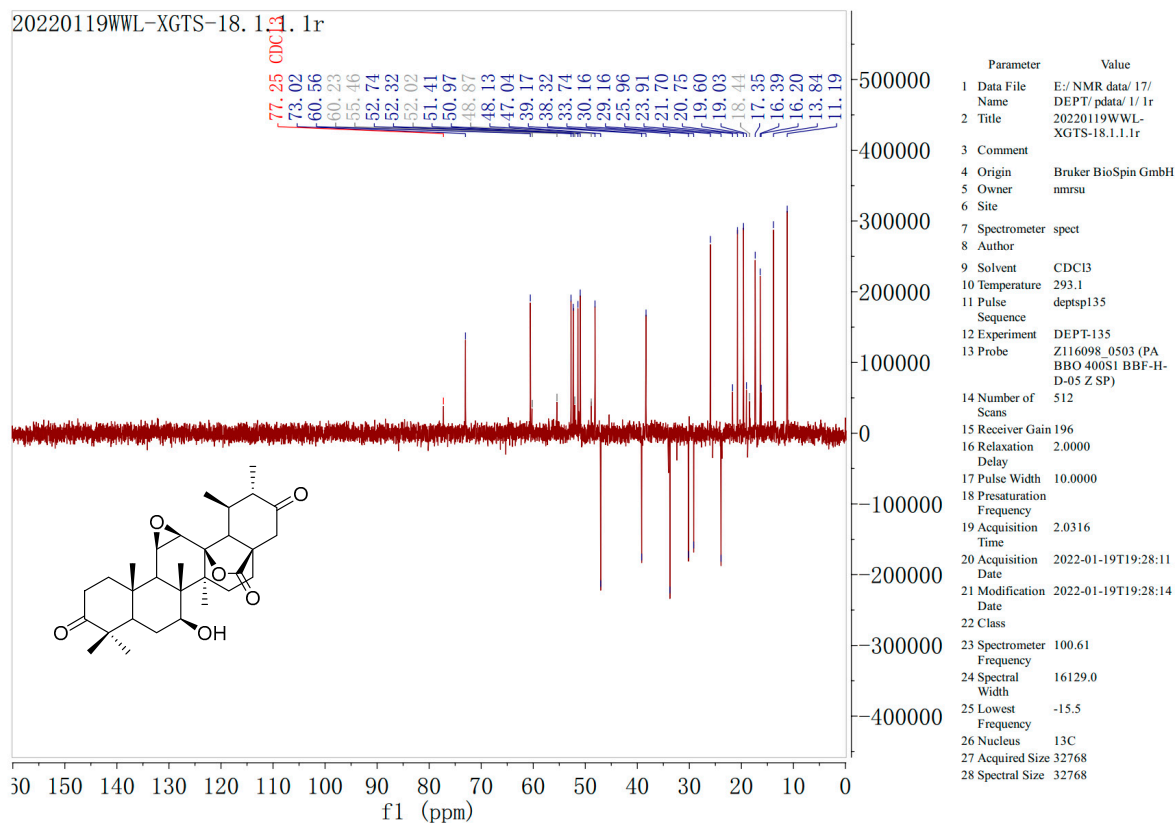
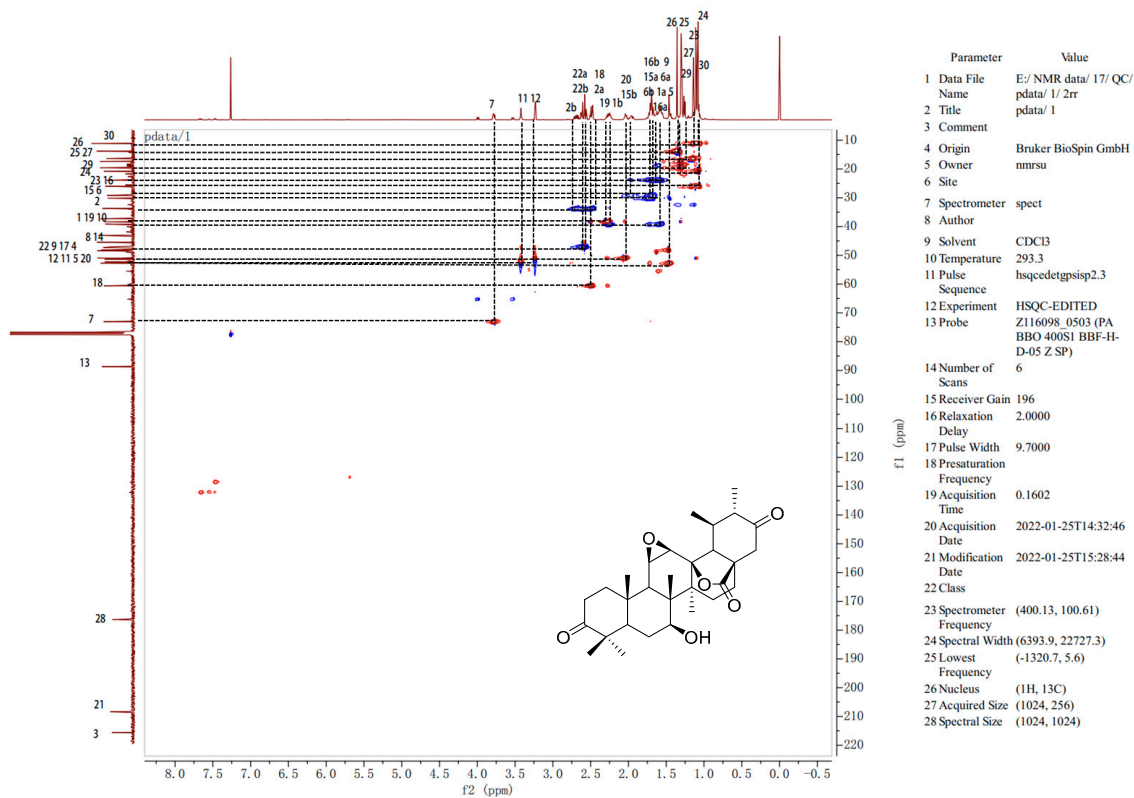


Figure S82  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound **17** in  $\text{CDCl}_3$





**Figure S83** DEPT-135 spectrum (100 MHz) of compound **17** in CDCl<sub>3</sub>



**Figure S84** HSQC spectrum (100 MHz) of compound **17** in CDCl<sub>3</sub>

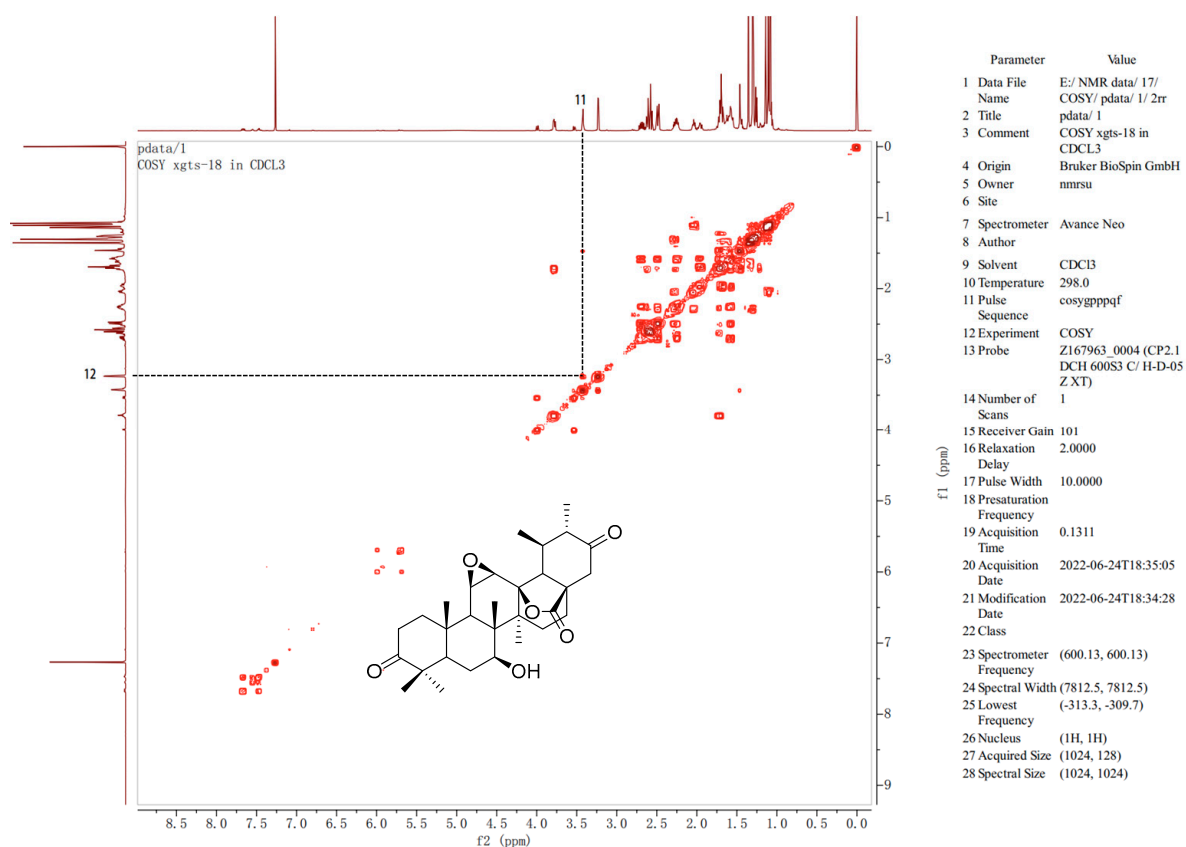


Figure S85  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **17** in  $\text{CDCl}_3$

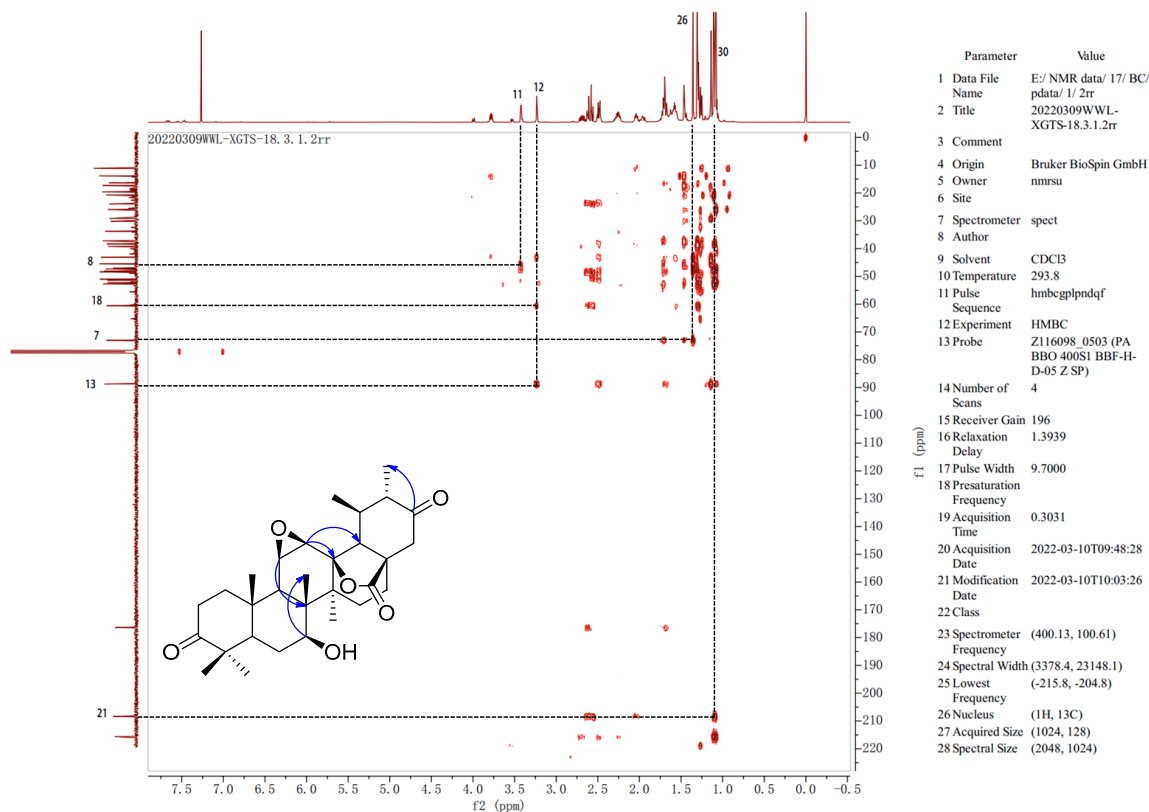
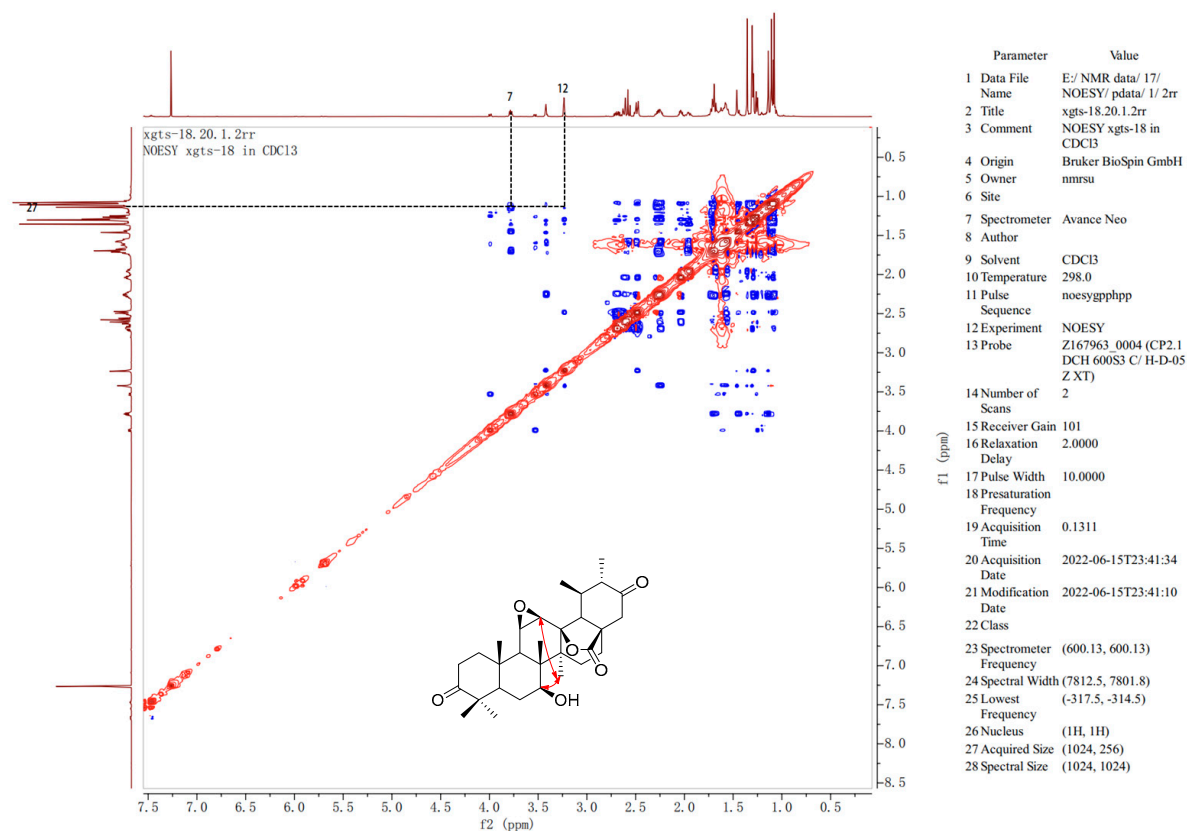
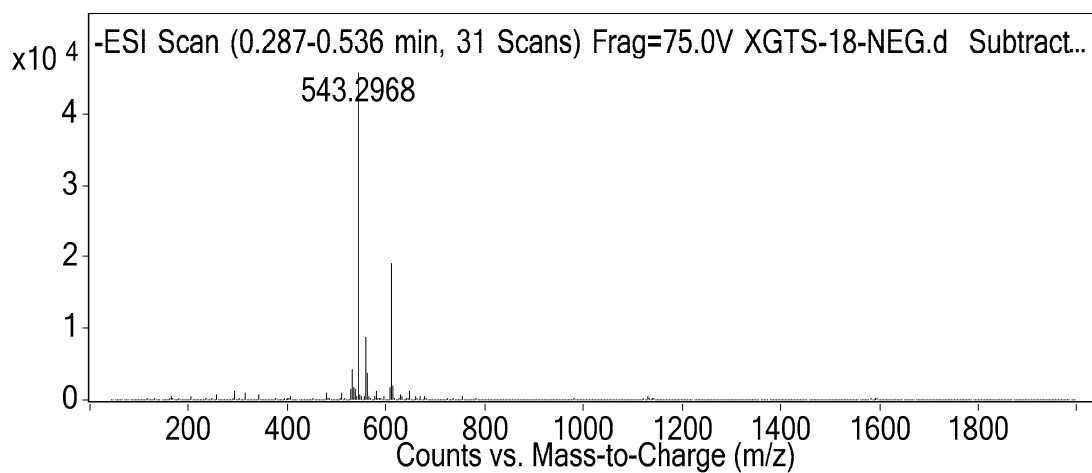


Figure S86 HMBC spectrum (100 MHz) of compound **17** in  $\text{CDCl}_3$



**Figure S87** NOESY spectrum (400 MHz) of compound **17** in CDCl<sub>3</sub>



**Figure S88** HR-ESI-MS spectrum of compound **17**



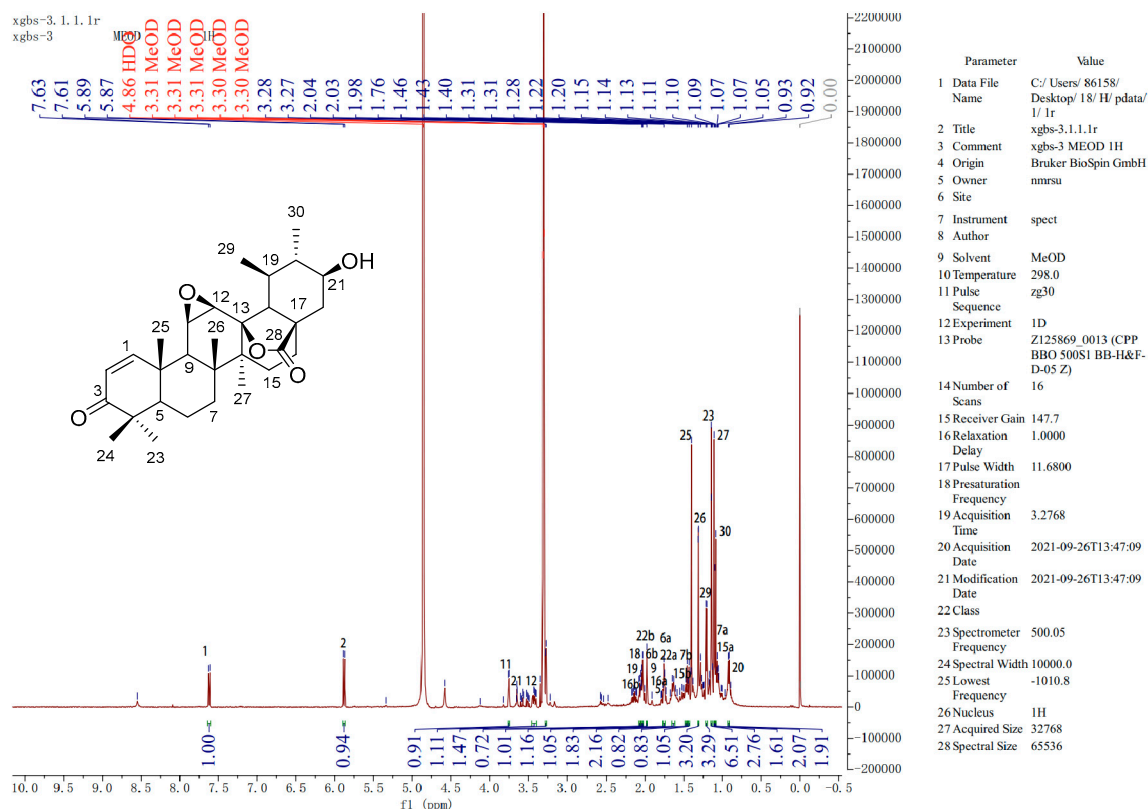


Figure S89  $^1\text{H}$  NMR spectrum (500 MHz) of compound **18** in  $\text{CD}_3\text{OD}$

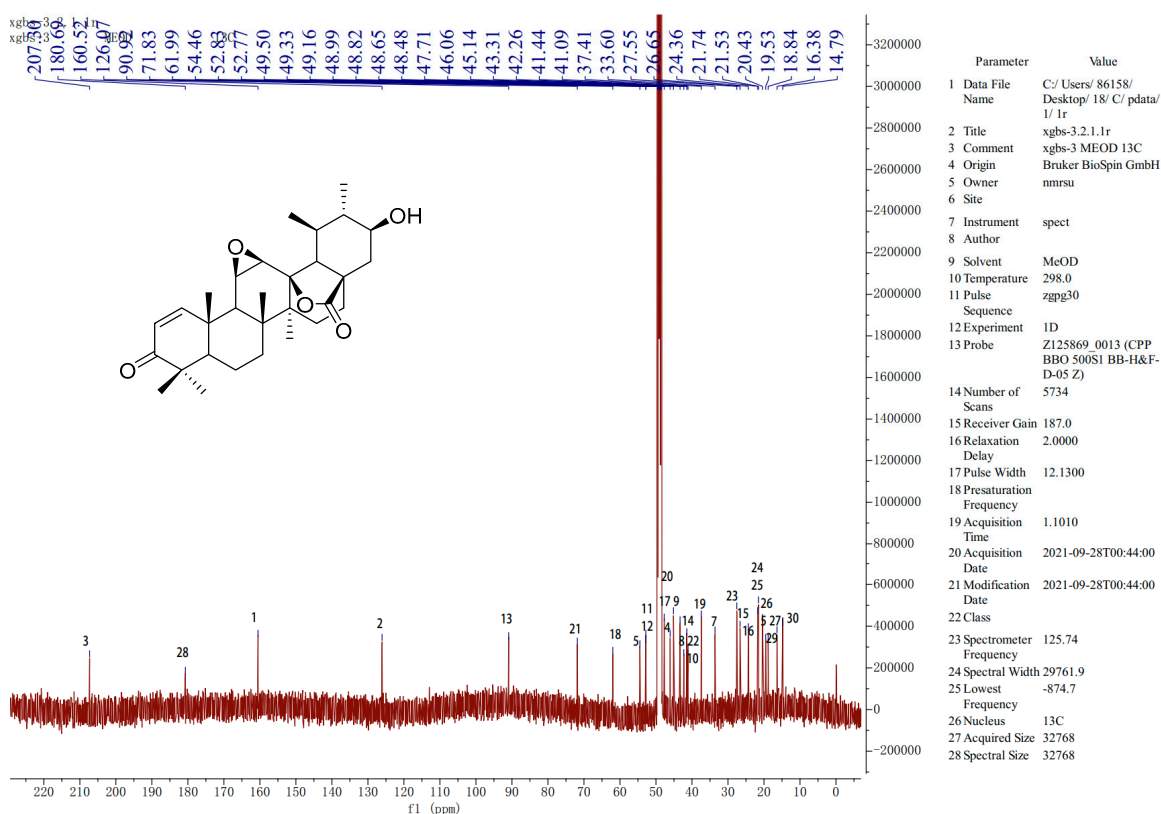


Figure S90  $^{13}\text{C}$  NMR spectrum (125 MHz) of compound **18** in  $\text{CD}_3\text{OD}$

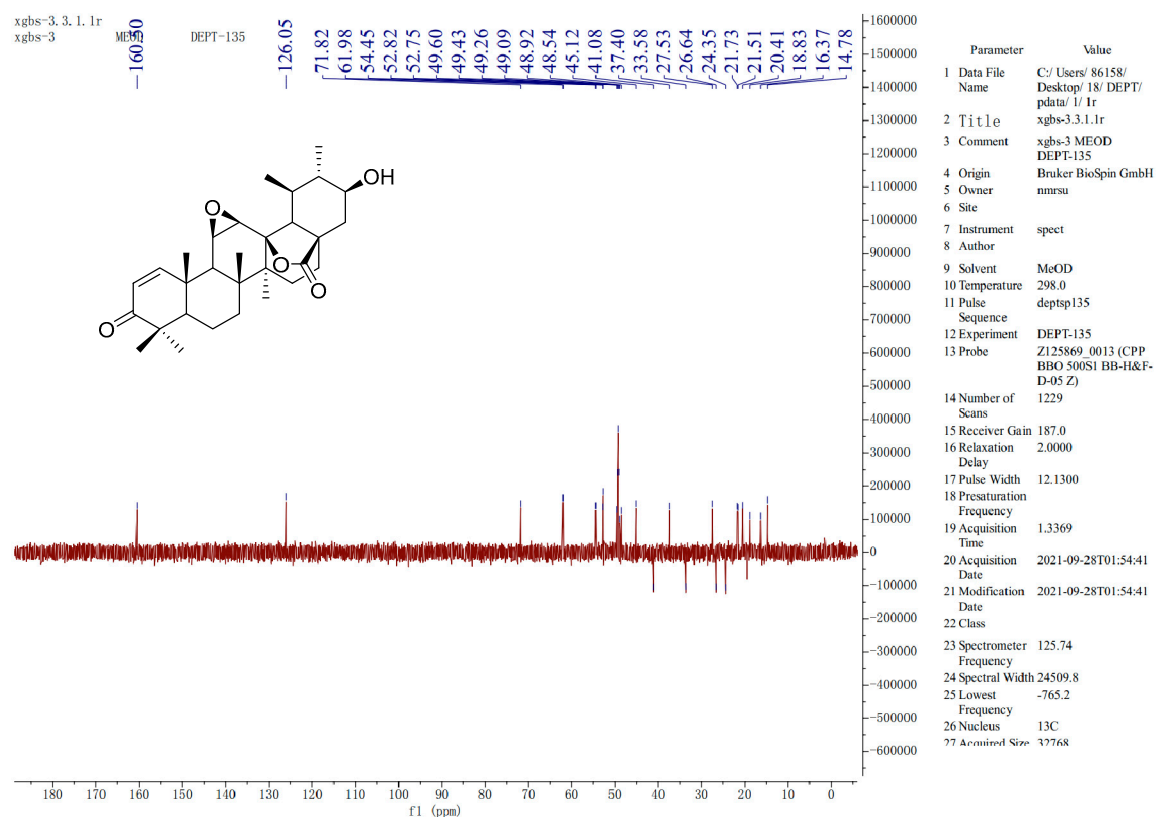


Figure S91 DEPT-135 spectrum (125 MHz) of compound 18 in CD<sub>3</sub>OD

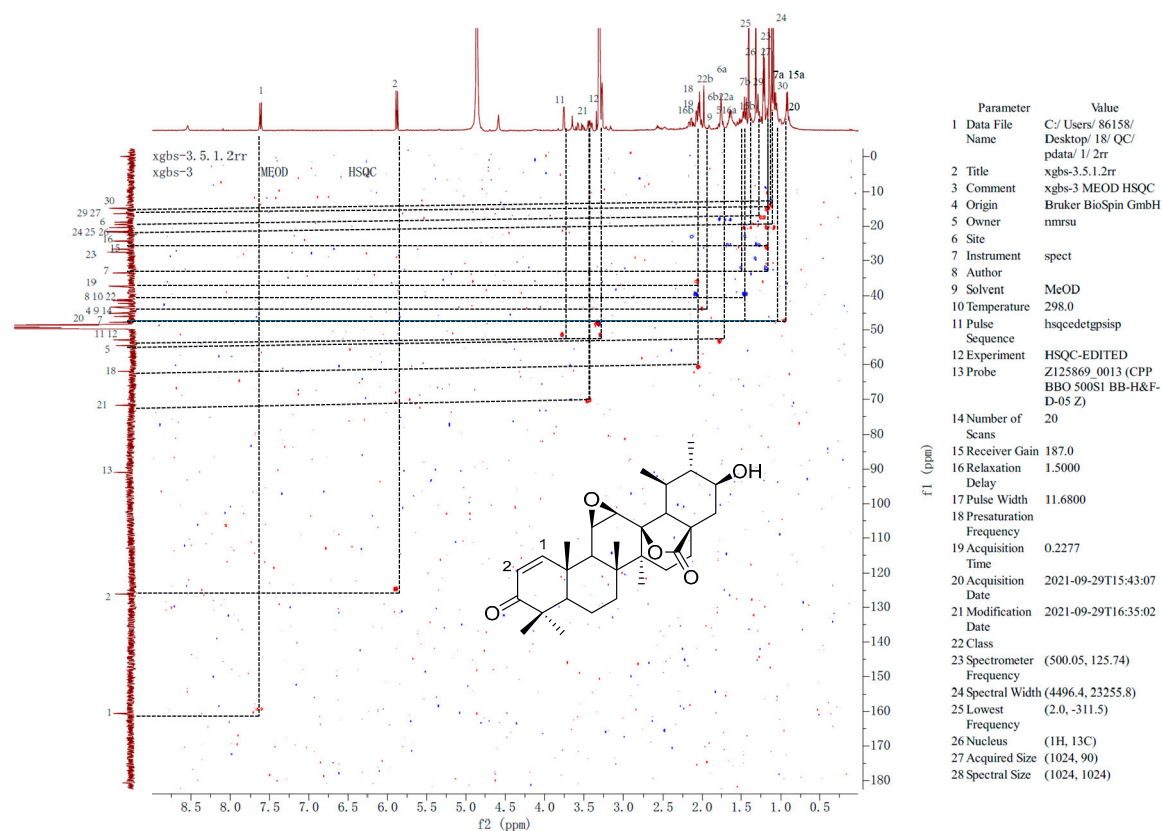
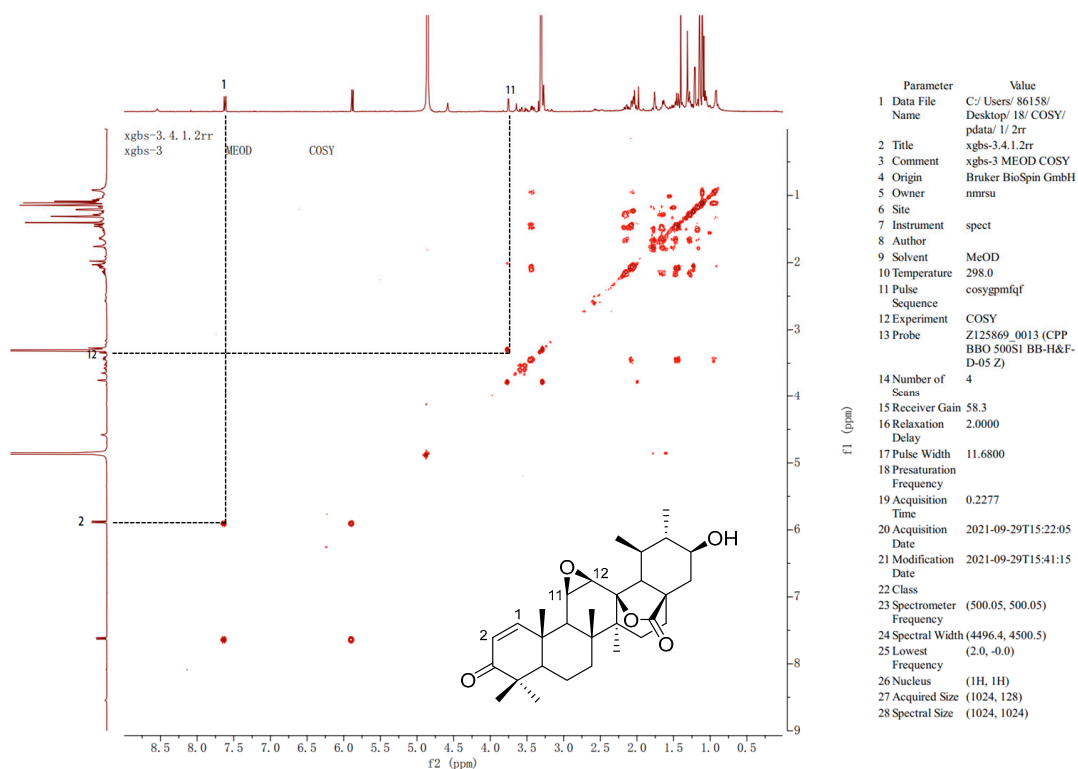
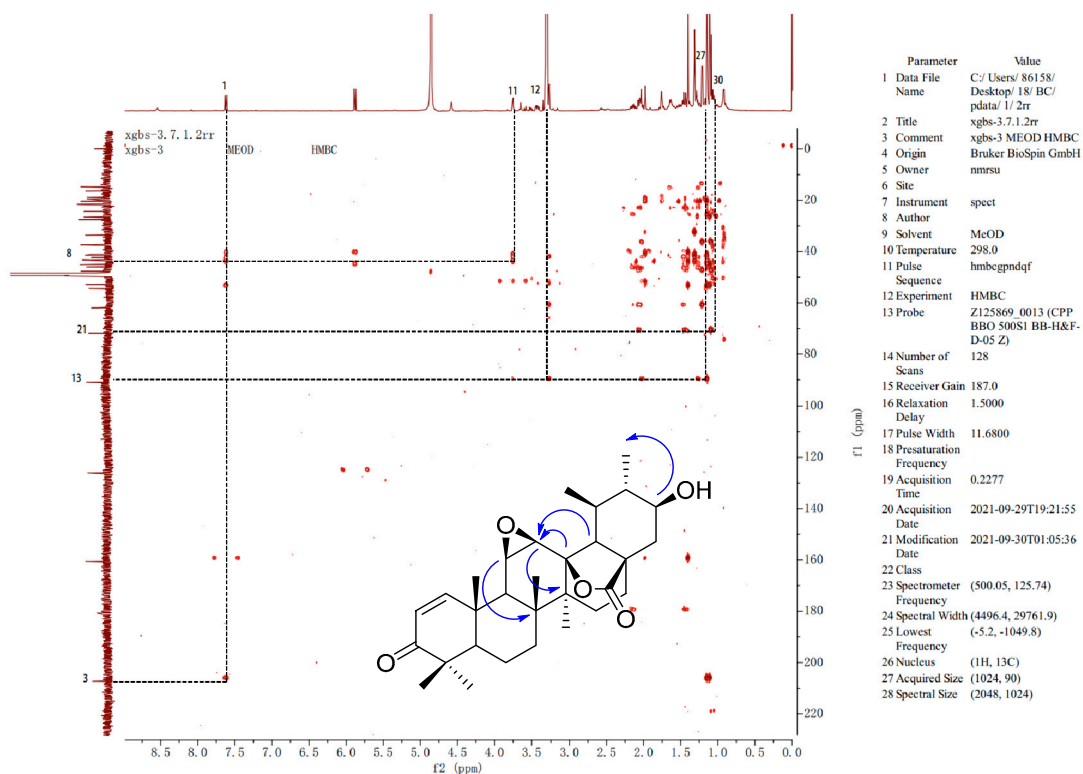


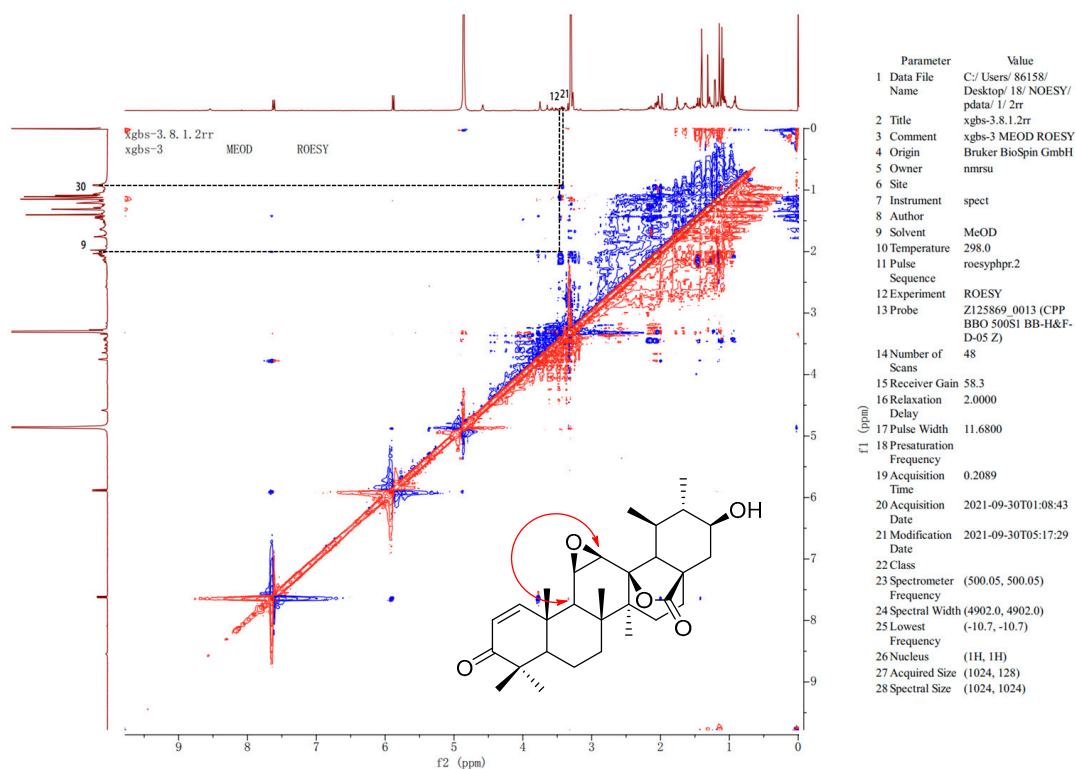
Figure S92 HSQC spectrum (125 MHz) of compound 18 in CD<sub>3</sub>OD



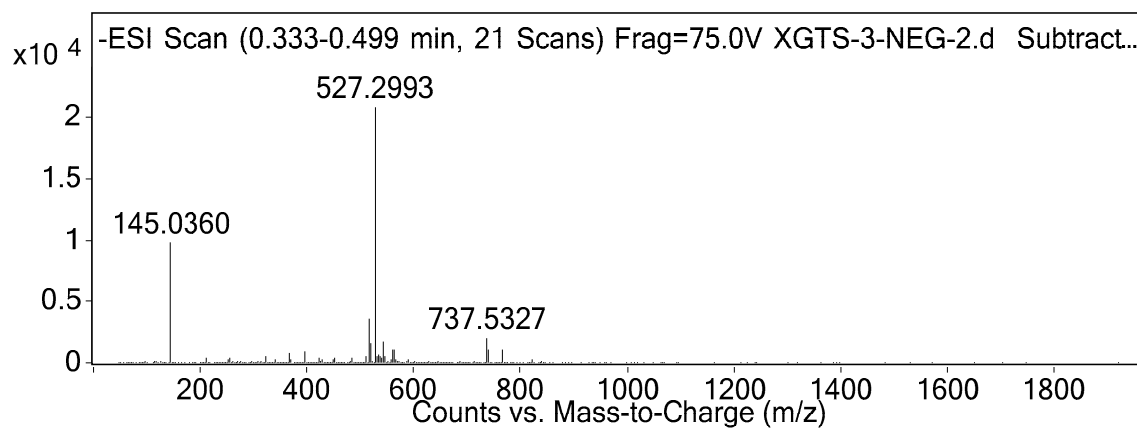
**Figure S93**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz) of compound **18** in  $\text{CD}_3\text{OD}$



**Figure S94** HMBC spectrum (125 MHz) of compound **18** in  $\text{CD}_3\text{OD}$



**Figure S95** NOESY spectrum (500 MHz) of compound **18** in CD<sub>3</sub>OD



**Figure S96** HR-ESI-MS spectrum of compound **18**

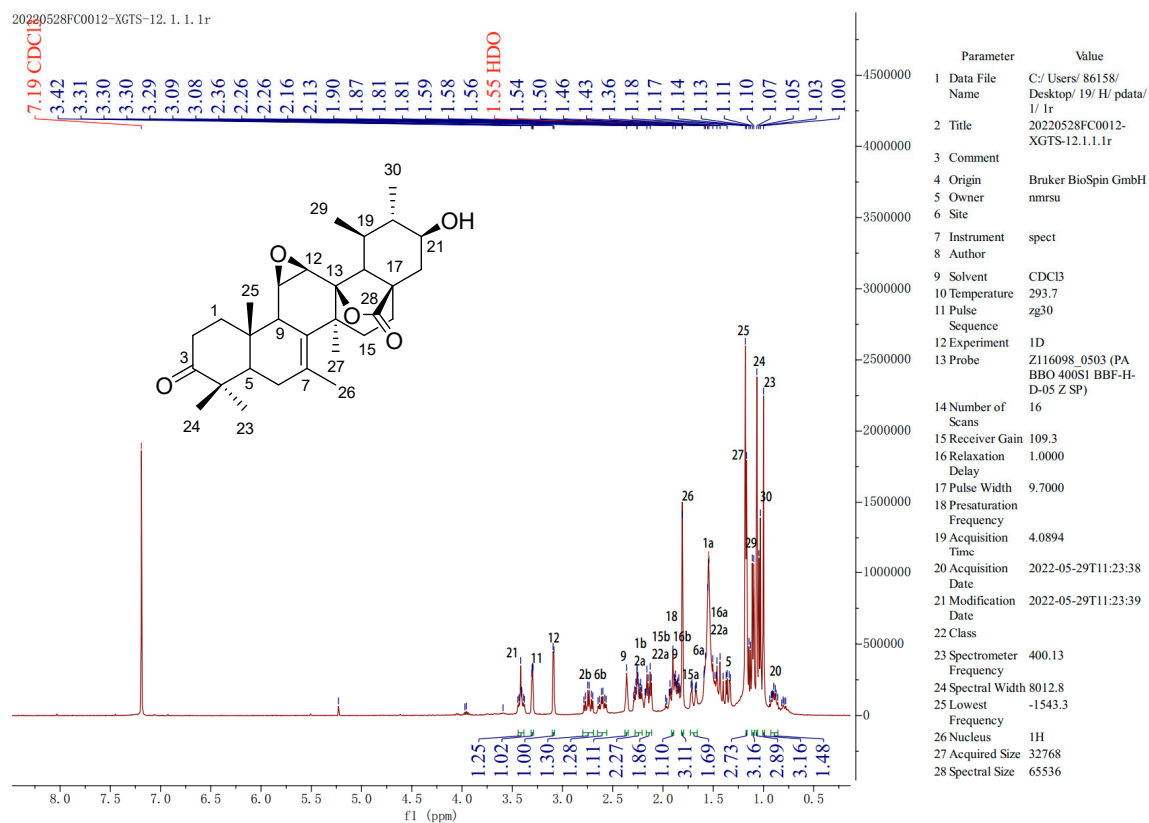


Figure S97  $^1\text{H}$  NMR spectrum (400 MHz) of compound 19 in  $\text{CDCl}_3$

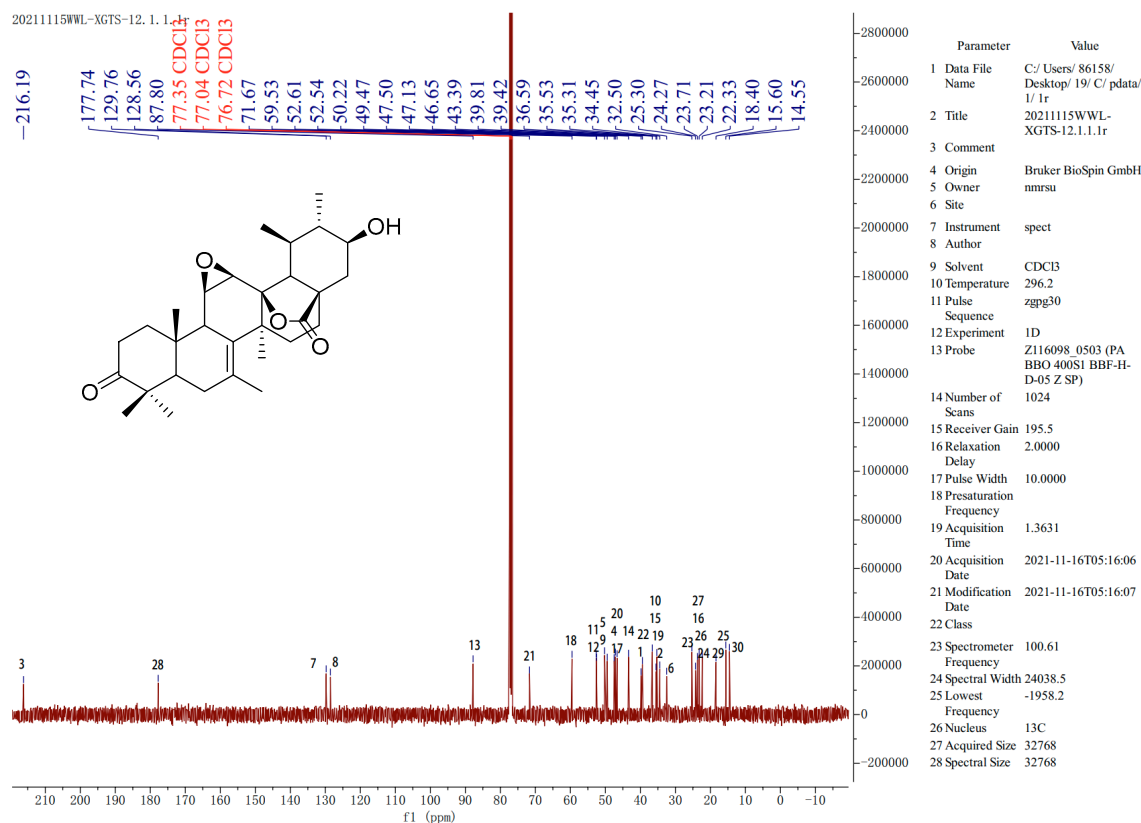
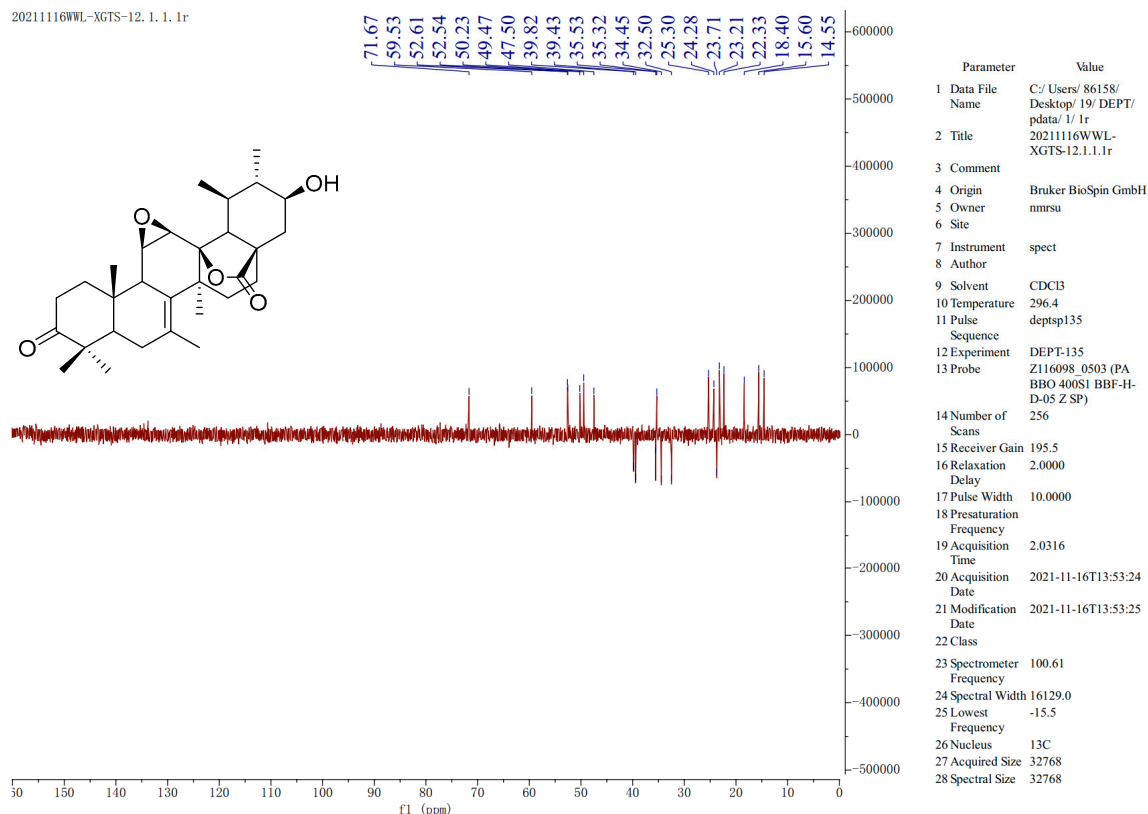
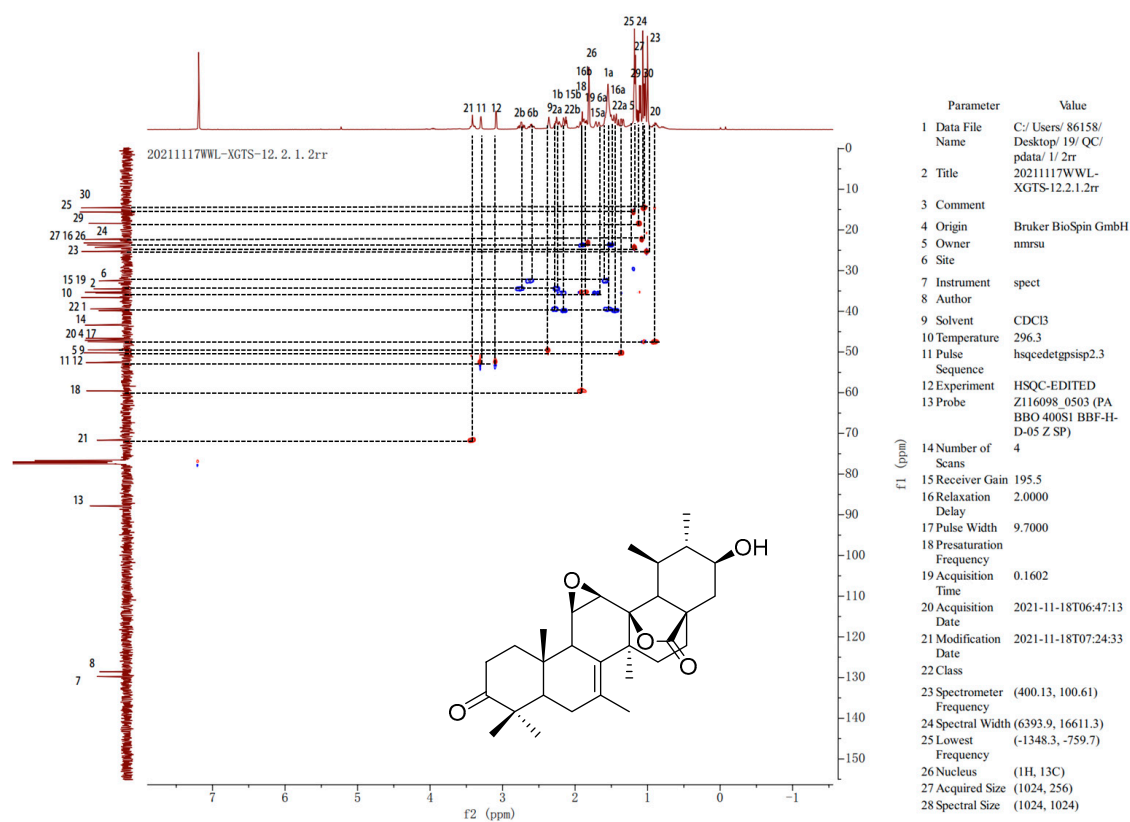
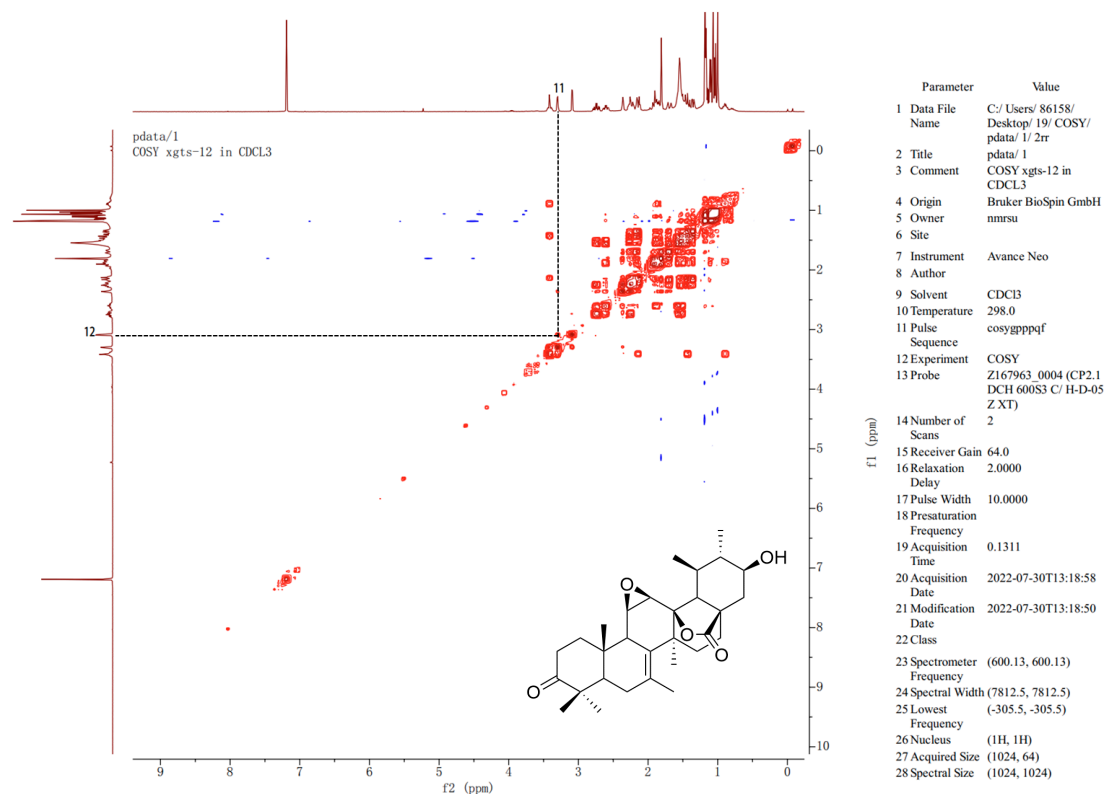


Figure S98  $^{13}\text{C}$  NMR spectrum (100 MHz) of compound 19 in  $\text{CDCl}_3$

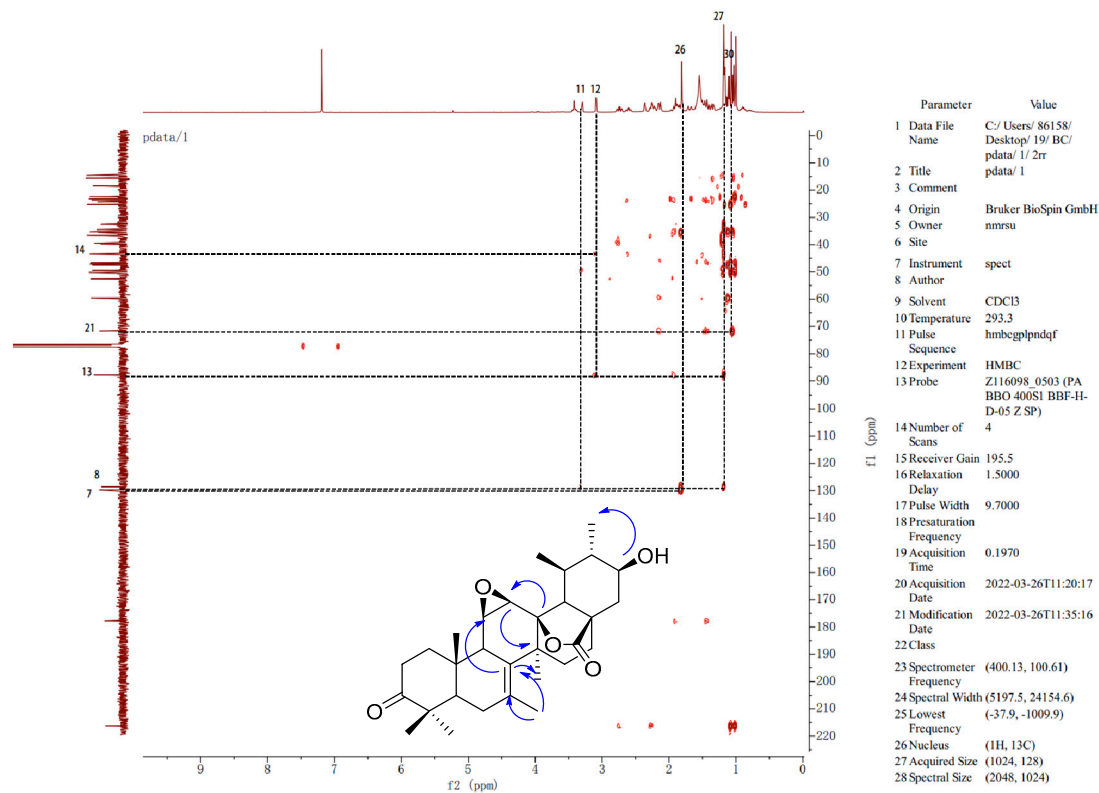


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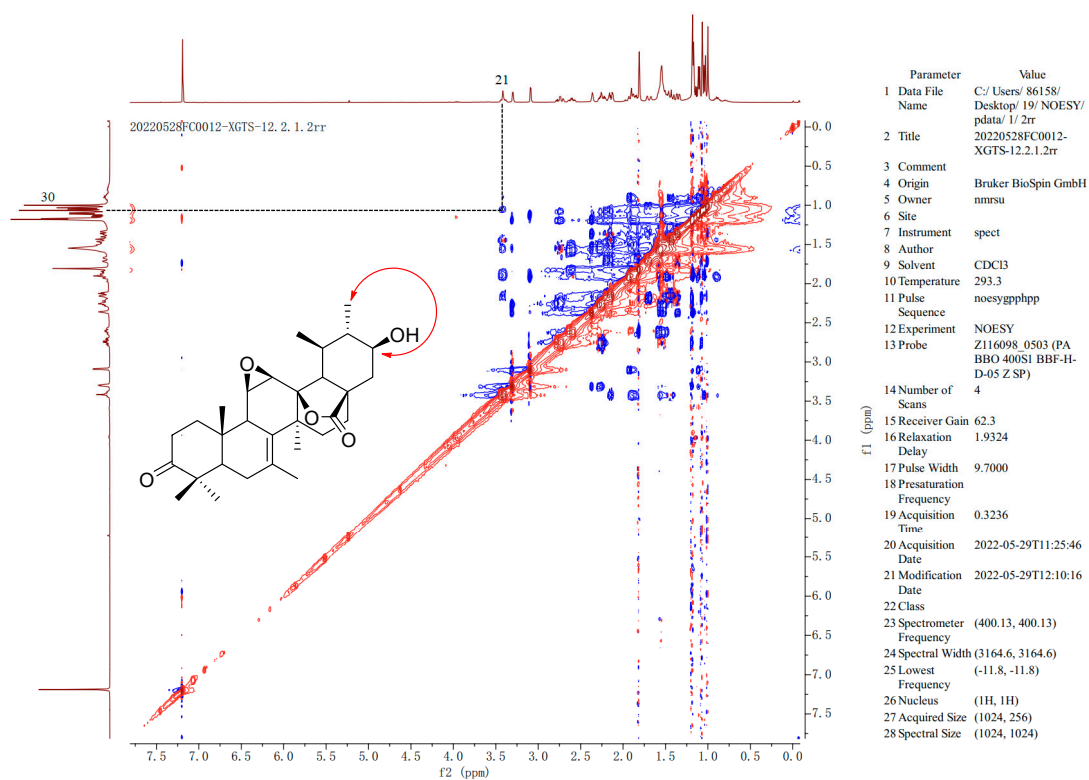
Figure S99 DEPT-135 spectrum (100 MHz) of compound 19 in CDCl<sub>3</sub>Figure S100 HSQC spectrum (100 MHz) of compound 19 in CDCl<sub>3</sub>



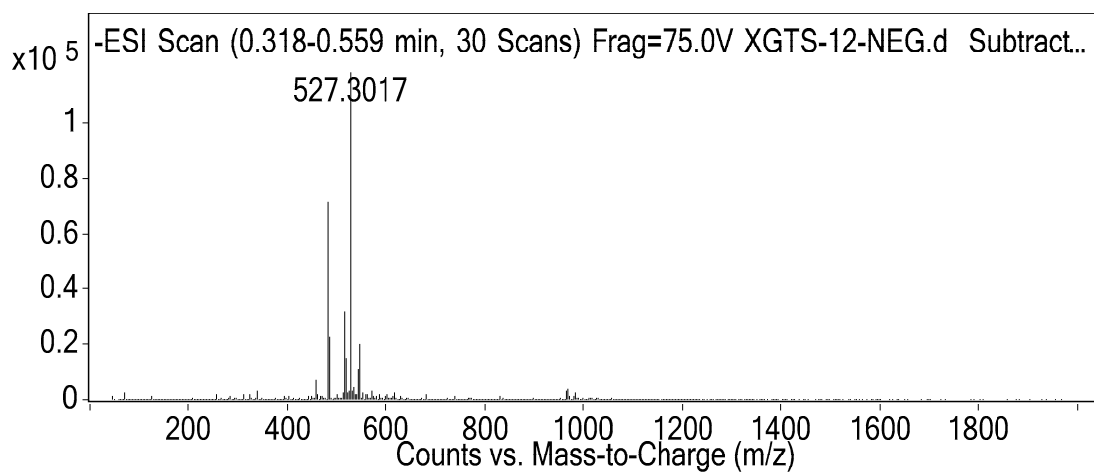
**Figure S101**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (400 MHz) of compound **19** in  $\text{CDCl}_3$



**Figure S102** HMBC spectrum (100 MHz) of compound **19** in  $\text{CDCl}_3$



**Figure S103** NOESY spectrum (400 MHz) of compound **19** in CDCl<sub>3</sub>



**Figure S104** HR-ESI-MS spectrum of compound **19**