Biocatalytic oxidation of flavone analogues mediated by general biocatalysts: horseradish peroxidase and laccase

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Supporting Information

List of Supporting Information

Table S1. The ^{1}H and ^{13}C NMR spectroscopic data of transformed products 1a, 5a, 8a and 8b (δ in ppm, J in Hz)

No.	1a[a]		5a[a]		8a[a]		8b[b]	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
I-2		159.3		191.7	5.41 dd (13.0, 2.5)	80.4	5.53 dd (13.0, 2.5)	77.9
3		132.5		105.8	3.16 dd (17.0, 13.0) 2.77 dd (17.0, 2.5)	40.5	3.23-3.27 m	42.0
4		182.8		193.3		197.8		196.0
5		164.8		171.3		165.5		163.4
6	6.13 s	94.9	5.95 d (1.5)	97.9	5.92 d (1.5)	97.1	5.90 m	95.8
7		166.0		174.0		168.3		166.7
8	6.41 s	100.16	5.98 d (1.5)	92.1	5.88 d (1.5)	96.2	5.90 m	95.0
9		160.9		160.4		164.9		162.7
10		105.1		102.1		103.4		101.7
1'		122.4		126.3		131.3		132.1
2'	7.32 d (8.0)	131.8	8.04 d (9.0)	134.2	7.37 s	128.2	7.19 d (1.5)	124.4
3'	6.66 d (8.0)	116.1	6.81 d (9.0)	116.0		131.8		120.9
4'		163.2		164.4		155.8		157.7
5'	6.66 d (8.0)	116.1	6.81 d (9.0)	116.0	6.97 d (8.5)	117.4	7.03 d (8.5)	115.8
6'	7.32 d (8.0)	131.8	8.04 d (9.0)	134.2	7.36 d (8.5)	131.2	7.23 dd (8.15, 1.5)	128.3
II-2		159.4			5.41 dd (13.0, 2.5)	80.4	5.47 dd (13.0, 3.0)	18.0
3	6.41 s	117.6			3.16 dd (17.0, 13.0) 2.77 dd (17.0, 2.5)	40.5	2.70-2.72 m	42.0
4		183.8				197.8		196.1
5		165.8				165.5		163.4
6	6.22 s	95.2			5.92 d (1.5)	97.1	5.90 m	95.8
7		166.1				168.3		166.7
8	6.34 s	100.2			5.88 d (1.5)	96.2		113.7
9		161.2				164.9		162.7
10		105.3				103.4		101.7
1'		123.7				131.3		130.1
2'	7.73 s	129.3			7.37 s	128.2	7.46 d (8.5)	128.3
3'		117.6				131.8	6.89 d (8.5)	116.1
4'		163.4				155.8		157.9
5'	6.94 d (7.0)	165.8			6.97 d (8.5)	117.4	7.46 d (8.5)	116.1
6'	7.77 d (7.0)	125.0			7.36 d (8.5)	131.2	6.89 d (8.5)	128.3

[a] The ^{1}H-NMR (500 MHz) and ^{13}C-NMR (125 MHz) spectroscopic data of compounds **1a**, **5a**, **8a** were measured in methanol-d_4. [b] The ^{1}H-NMR (500 MHz) and ^{13}C-NMR (125 MHz) spectroscopic data of compound **8b** was measured in DMSO-d_6.

Table S2. The ^{1}H and ^{13}C NMR spectroscopic data of transformed products 10a, 10b, 10c, 12a and 12b (δ in ppm, J in Hz)

No.	10a		10b		10c		12a		12b	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
I-2	8.19 s	155.1	8.15 s	155.2	8.31 s	155.6	5.86 d (11.5)	85.5	5.29 d (10.0)	84.6
3		125.5		125.4		120.1	2.67 d (11.5)	52.5	3.17 dd (10.0, 3.0)	52.2
4		177.9		177.9		174.43		193.6		192.6
5	8.06 d (9.0)	128.5	8.04 d (8.5)	128.3	7.92 d (8.5)	126.9	7.68 d(9.0)	130.0	7.43 d (8.5)	129.9
6	6.96 dd (9.0, 2.5)	116.6	6.93 dd (8.5, 2.5)	116.54	6.91 m	115.2	6.49 d (9.0)	111.7	6.39 dd (8.5, 2.0)	111.6
7		164.7		164.7		162.9		166.6		166.6
8	6.87 d (2.5)	103.3	6.85 d (2.5)	103.3	6.88 d (2.0)	102.0	6.26 brs	103.6	6.22 d (2.0)	103.5
9		159.8		159.8		157.3		165.0		164.2
10		118.2		118.1		146.5		115.2		115.5
1'		128.3		127.7		49.9		129.5		129.4
2'	7.51 d (8.5)	131.5	77.62 d (2.0)	127.3	7.40 brs	83.8	6.90 brd (8.5)	130.2	6.92 d (8.5)	130.3
3'	7.21 d (8.5)	118.2		126.9		38.0	6.76 brd (8.5)	116.4	6.67 d (8.5)	116.2
4'		158.1		160.2		195.5		159.4		159.0
5'	7.21 d (8.5)	118.2	7.07 d (8.0)	111.6	6.90 m	126.5	6.76 brd (8.5)	116.4	6.67 d (8.5)	116.2
6'	7.51 d (8.5)	131.5	7.48 dd (8.0, 2.0)	133.3	7.40 dd (8.0, 1.5)	145.2	6.90 brd (8.5)	130.2	6.92 d (8.5)	130.3
II-2	6.25 s	104.9	6.32 s	87.5	8.16 s	155.6	5.86 d (11.5)	85.5	5.55 d (5.0)	82.4
3	7.37 s	78.4		90.0		120.1	2.67 d (11.5)	52.5	2.94 dd (5.0, 3.0)	50.5
4		189.6		189.1		174.43		193.6		194.9
5	7.79 d (8.5)	129.5	7.66 d (8.5)	130.7	7.82 d (8.5)	126.9	7.68 d (9.0)	130.0	7.61 d (8.5)	130.0
6	6.56 d (8.5, 2.5)	112.3	6.53 dd (8.5, 2.5)	113.0	6.91 m	115.2	6.49 d (9.0)	111.7	6.49 dd (8.5, 2.0)	111.7
7	7.79	167.1		167.9		162.9		166.6		166.3
8	6.247 d (2.5)	104.5	6.46 d (2.5)	104.3	6.84 d (2.0)	102.0	6.26 brs	103.6	6.45 d (2.0)	103.9
9	7.79	159.7		163.1		157.3		165.0		166.0
10		115.3		114.3		146.5		115.2		116.9
1'	6.75	130.0		129.8		49.9		129.5		129.3
2'	7.37 d (8.5)	129.3	7.39 d (9.0)	128.0	5.44 m	83.8	6.90 brd (8.5)	130.2	7.09 d (8.5)	128.4
3'	6.75 d (8.5)	116.3	6.79 d (9.0)	116.46	3.08 dd (17.5, 4.0) 2.79 dd (17.5, 2.5)	38.0	6.76 brd (8.5)	116.4	6.79 d (8.5)	116.4
4'		159.1		159.1		195.5		159.4		158.5
5'	6.75 d (8.5)	116.3	6.79 d (9.0)	116.46	6.04 d (10.0)	126.5	6.76 brd (8.5)	116.4	6.79 d (8.5)	116.4
6'	7.37 d (8.5)	129.3	7.39 d (9.0)	128.0	6.80 dd (10.0, 2.0)	145.2	6.90 brd (8.5)	130.2	7.09 d (8.5)	128.4

[a] The ^{1}H-NMR (500 MHz) and ^{13}C-NMR (125 MHz) spectroscopic data of compounds **10a**, **10b**, **10c** were measured in DMSO-d_6. [b] The ^{1}H-NMR (500 MHz) and ^{13}C-NMR (125 MHz) spectroscopic data of compound **12a**, **12b** was measured in methanol-d_4.

Figure S1.The ^{1}H NMR spectrum of 1a

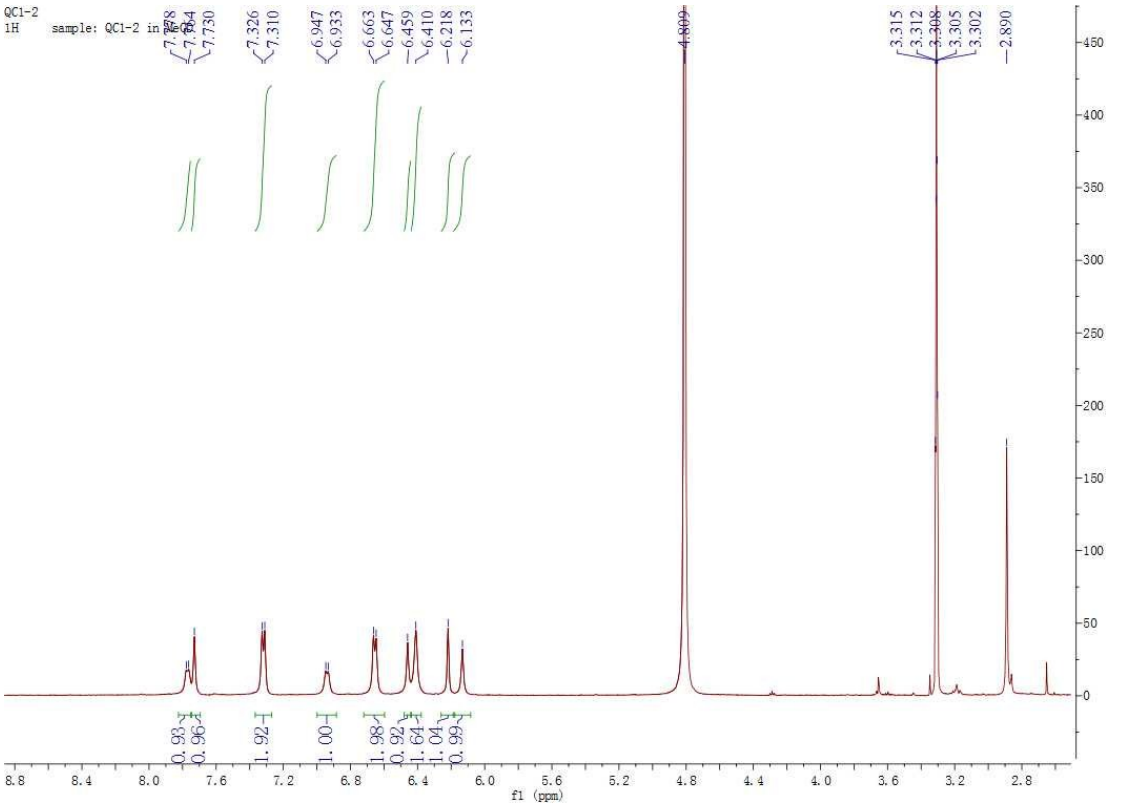

Figure S2. The ^{13}C NMR spectrum of 1a

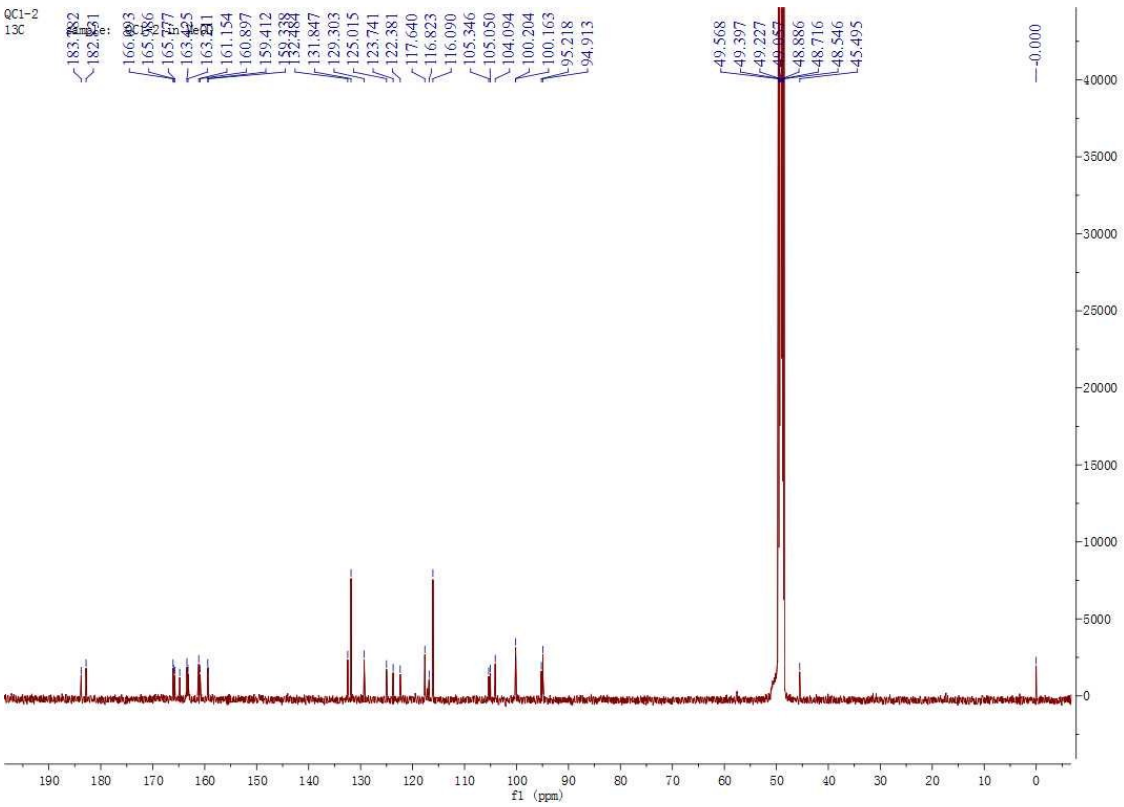

Figure S3. The HR-MS of 1a

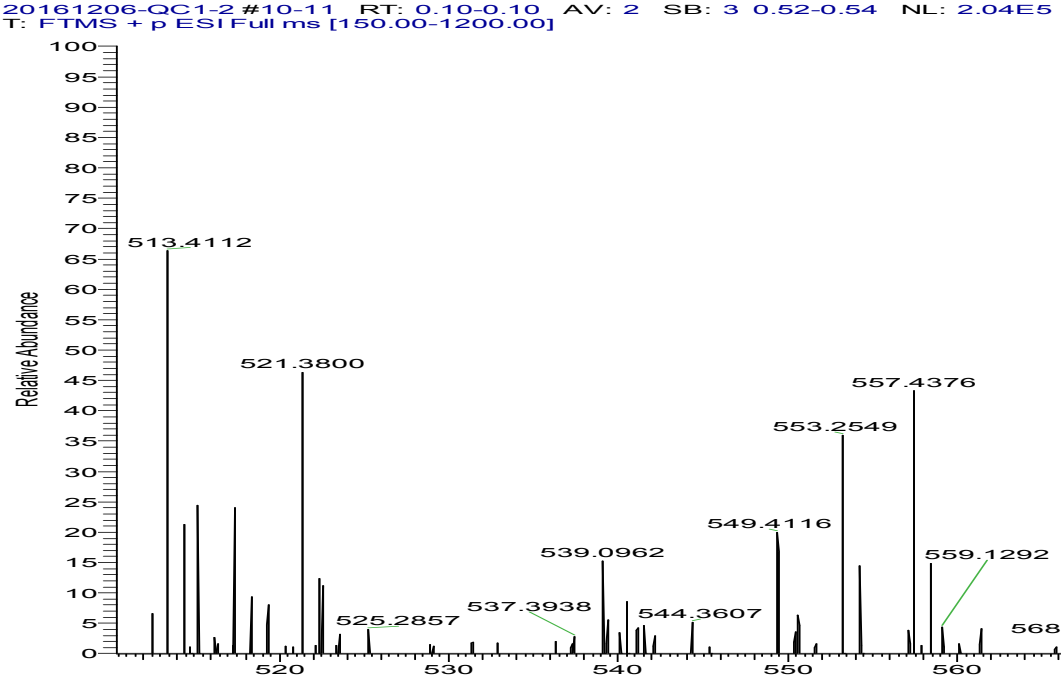

Figure S4. The ^{1}H NMR spectrum of 5a

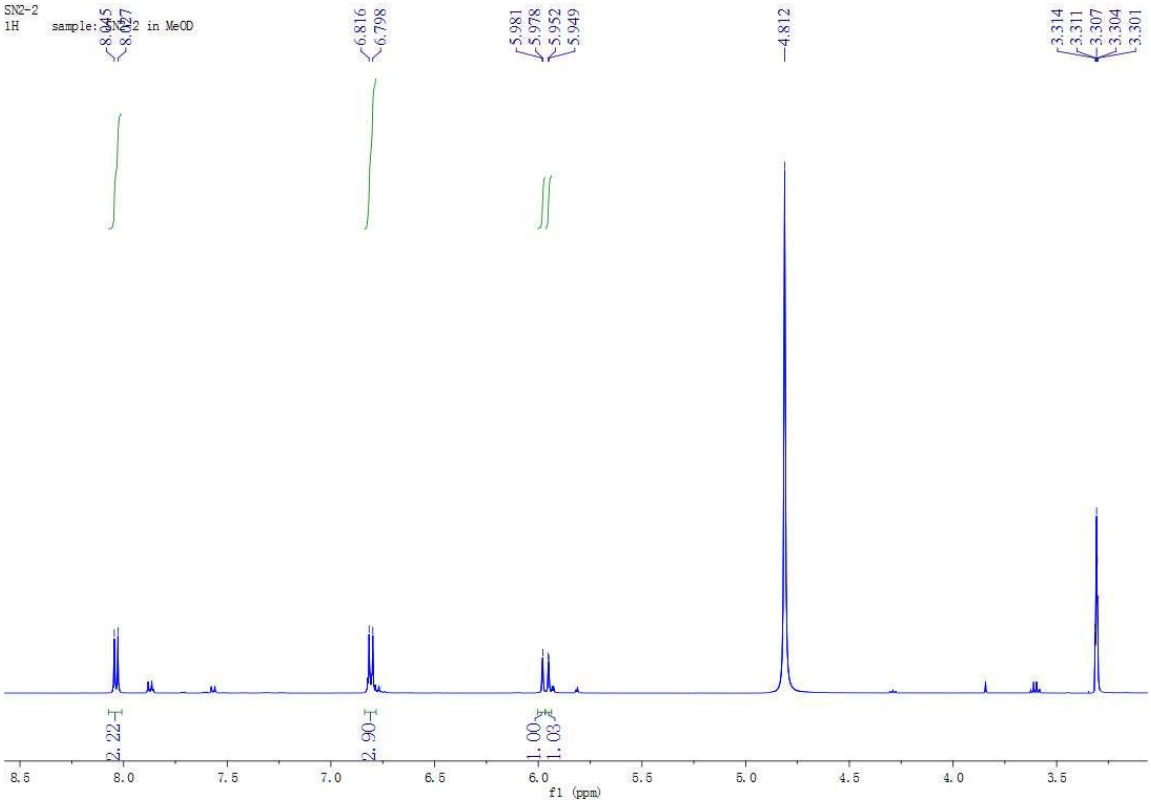

Figure S5. The ^{13}C NMR spectrum of 5a

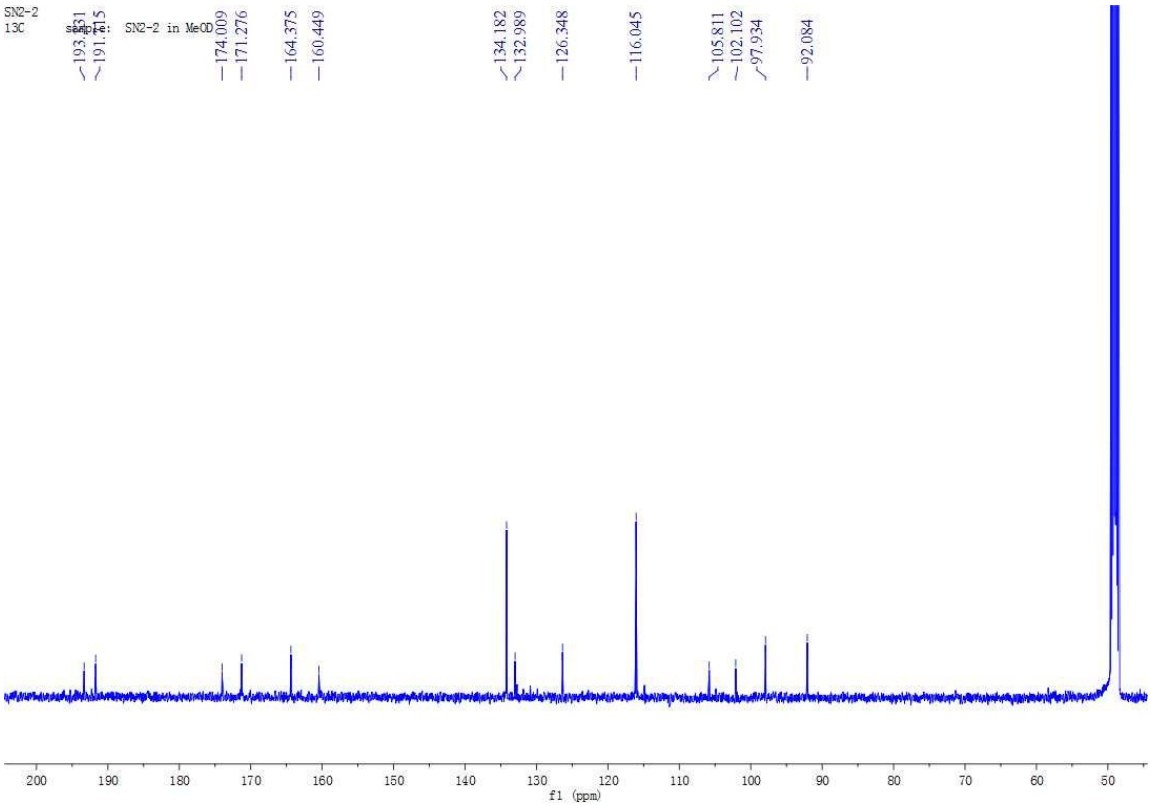

Figure S6. The HR-MS of 5a

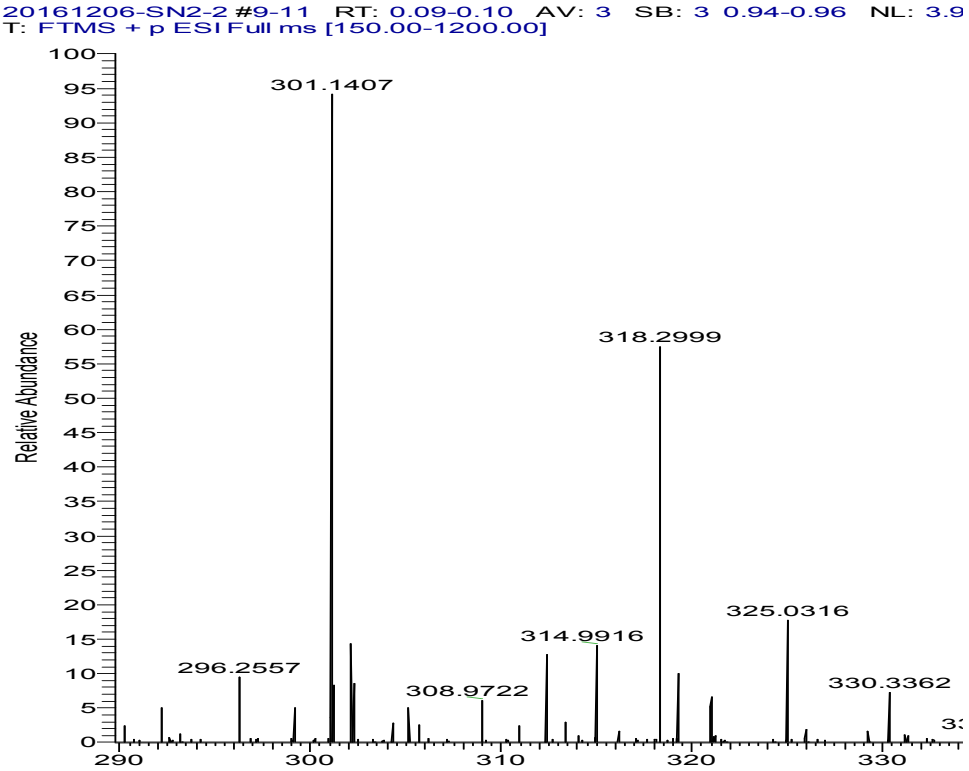

Figure S7. The ^{1}H NMR spectrum of 8a

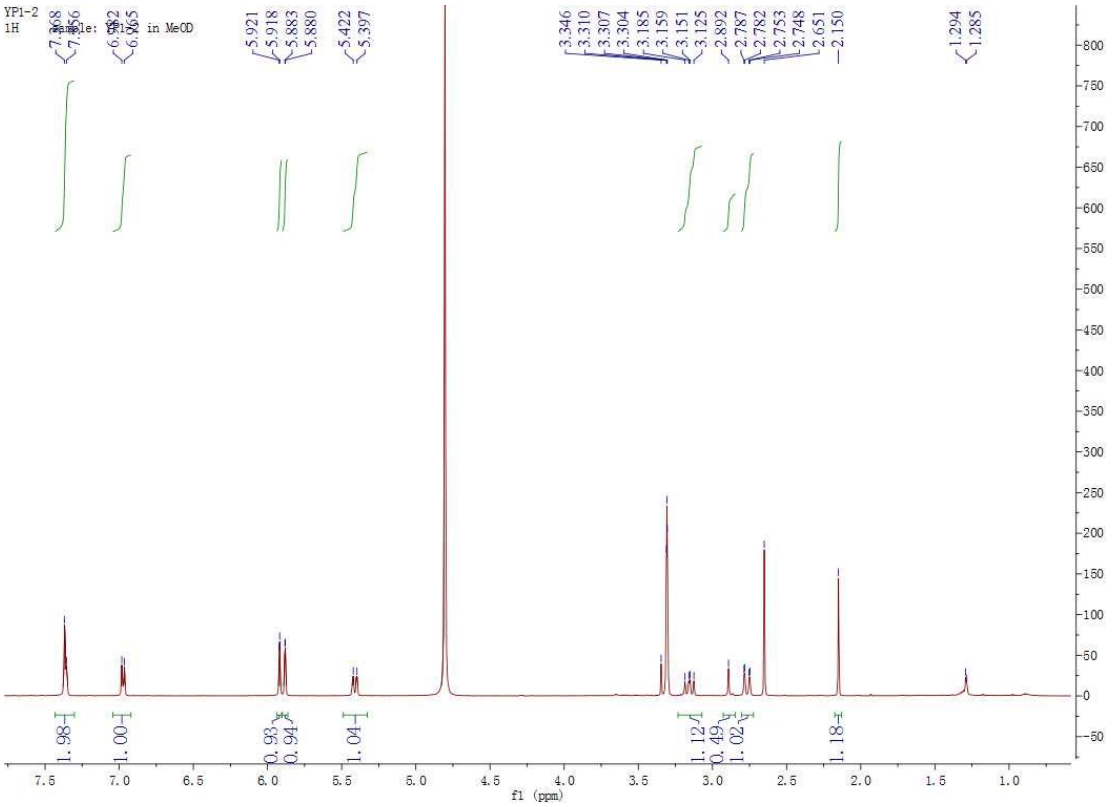

Figure S8. The ^{13}C NMR spectrum of 8a

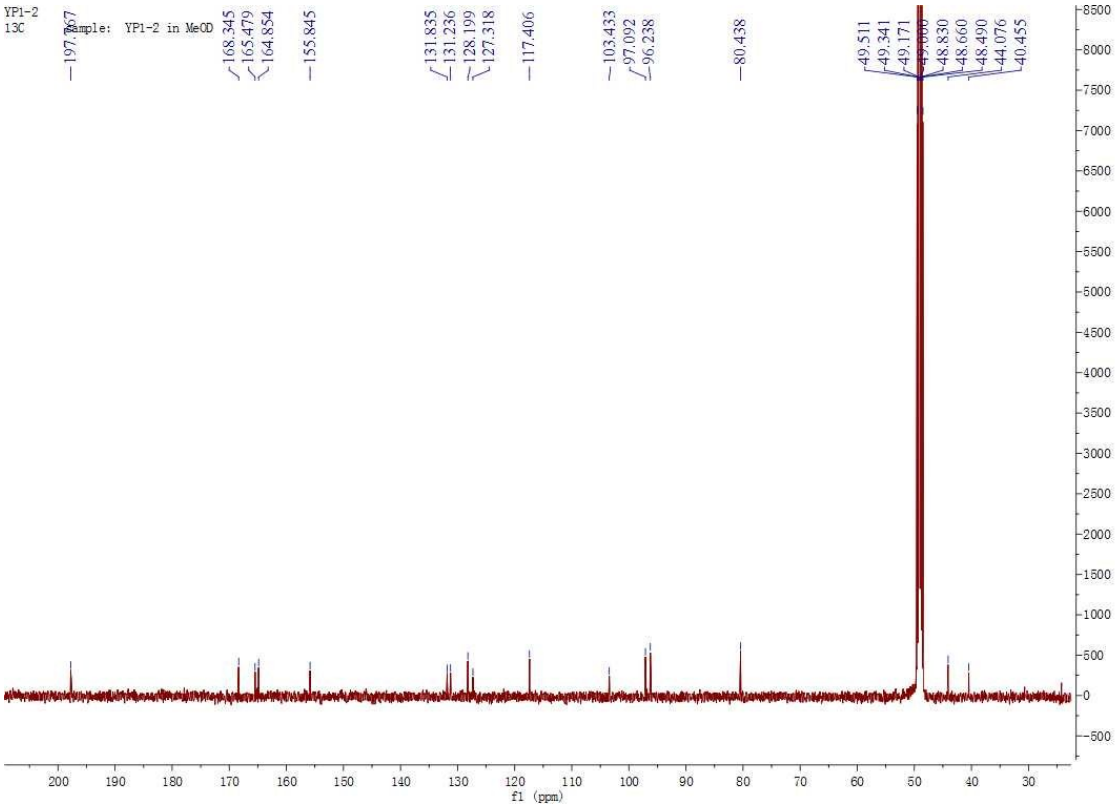

Figure S9. The ^{1}H NMR spectrum of 8b

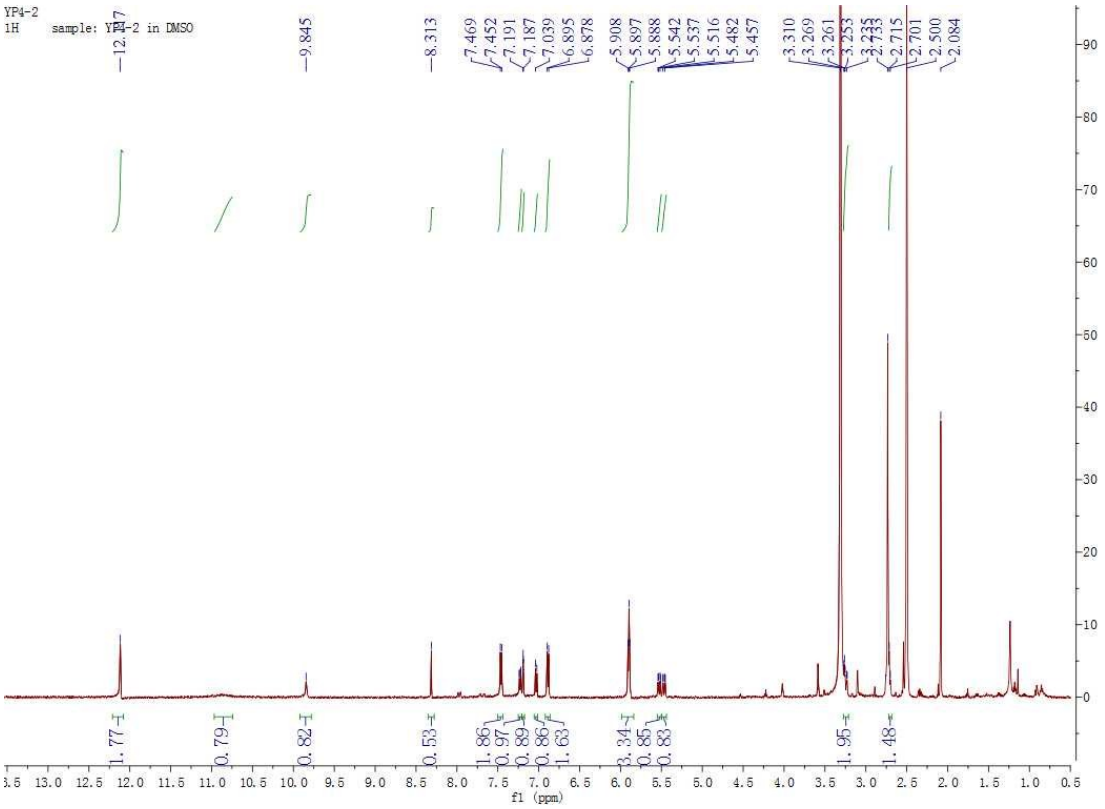

Figure S10. The ^{13}C NMR spectrum of 8b

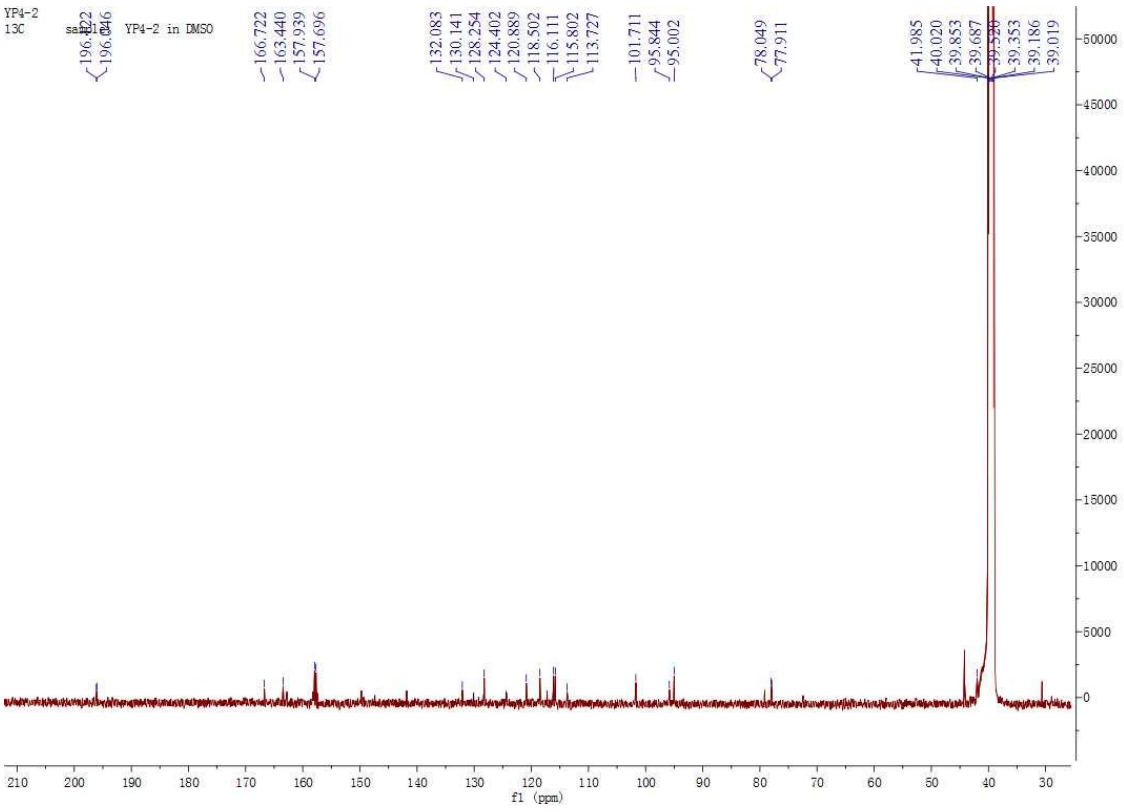

Figure S11. The ^{1}H NMR spectrum of 10a

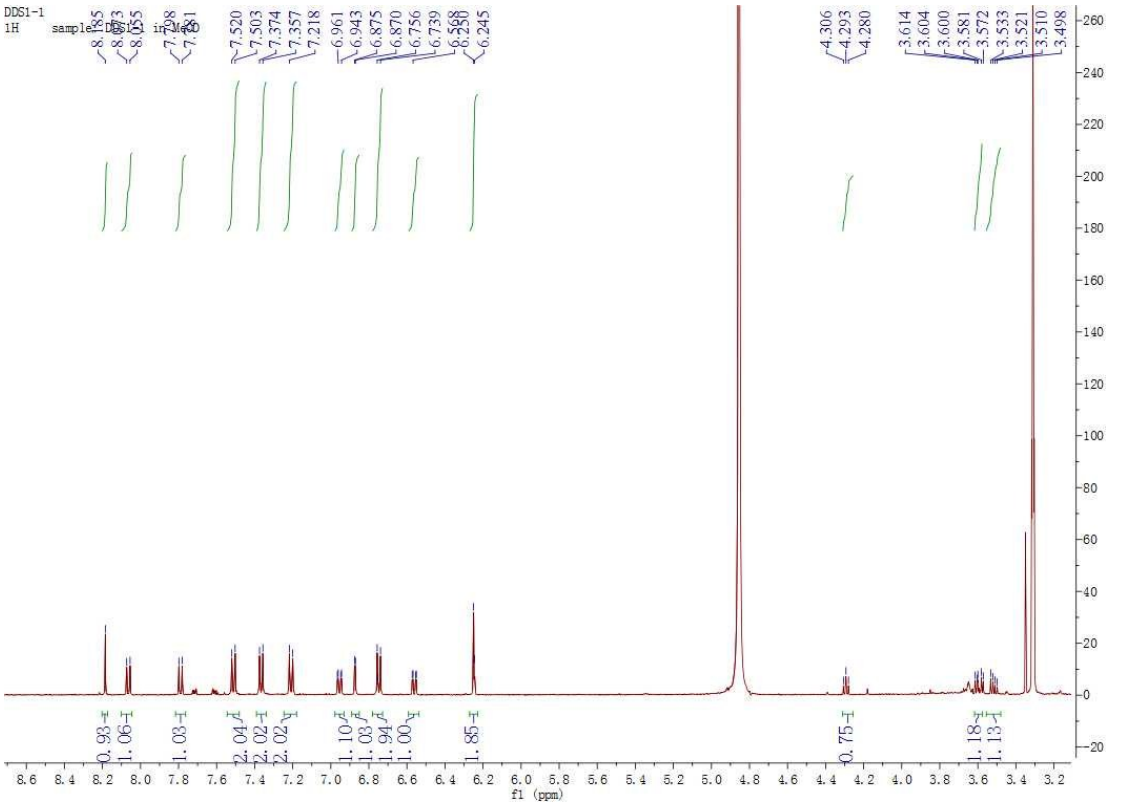

Figure S12. The ^{13}C NMR spectrum of 10a

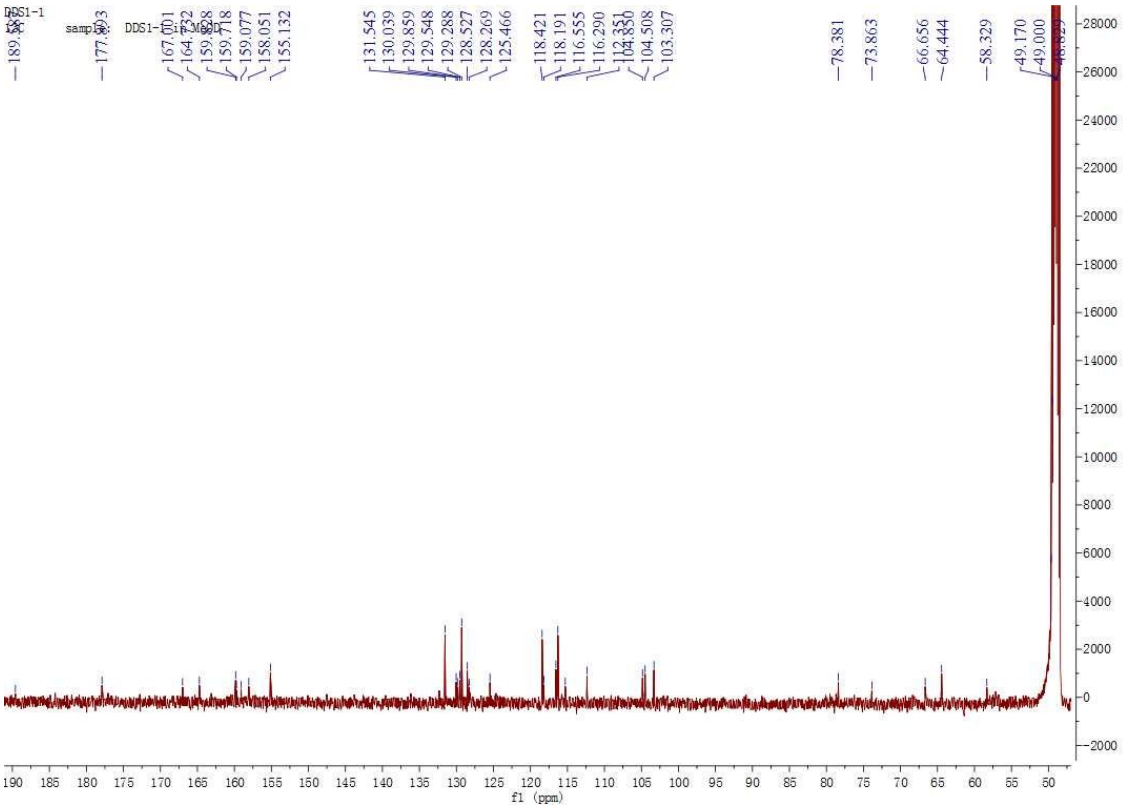

Figure S13. The HSQC spectrum of 10a

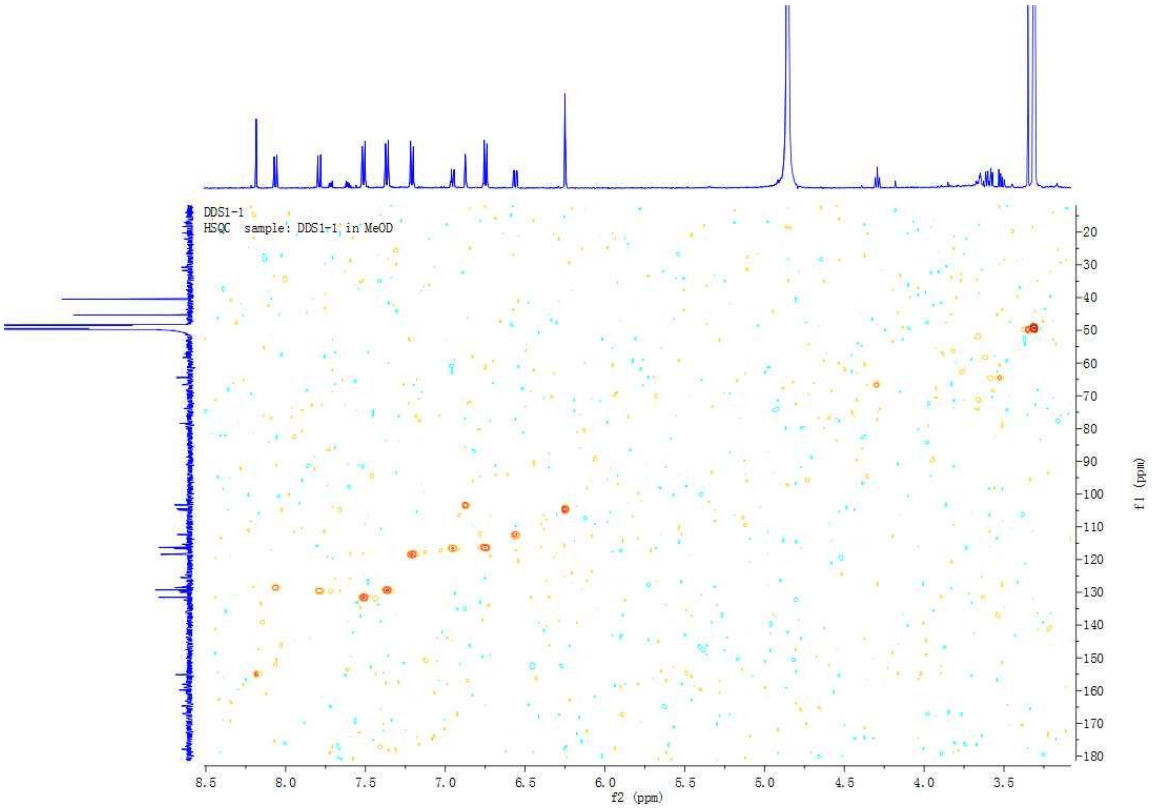

Figure S14. The HMBC spectrum of 10a

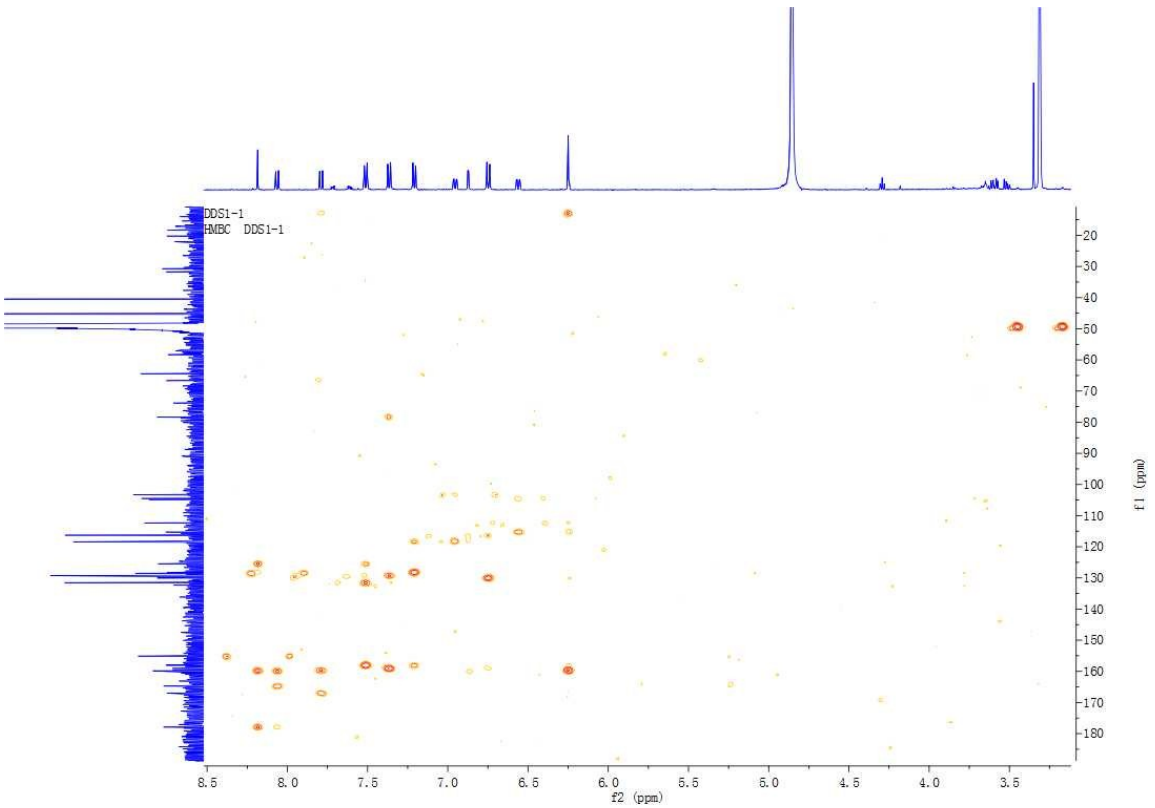

Figure S15. The ^{1}H-^{1}H COSY spectrum of 10a

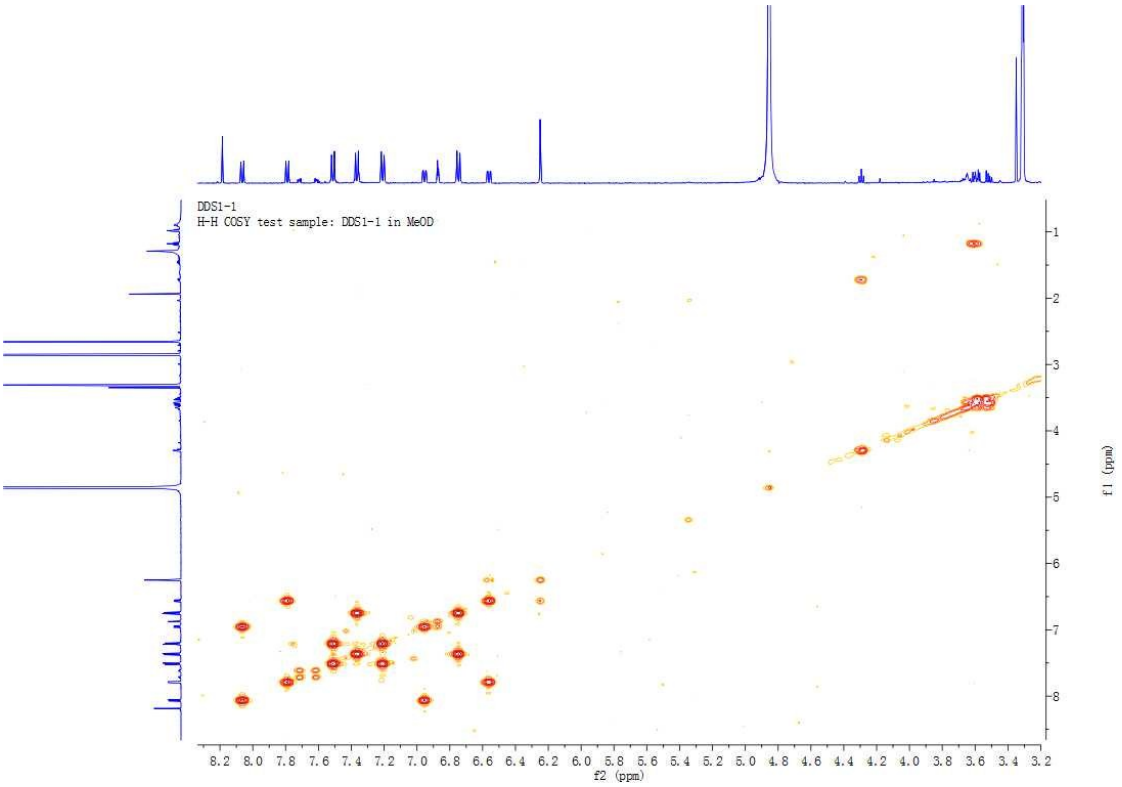

Figure S16. The NOESY spectrum of 10a

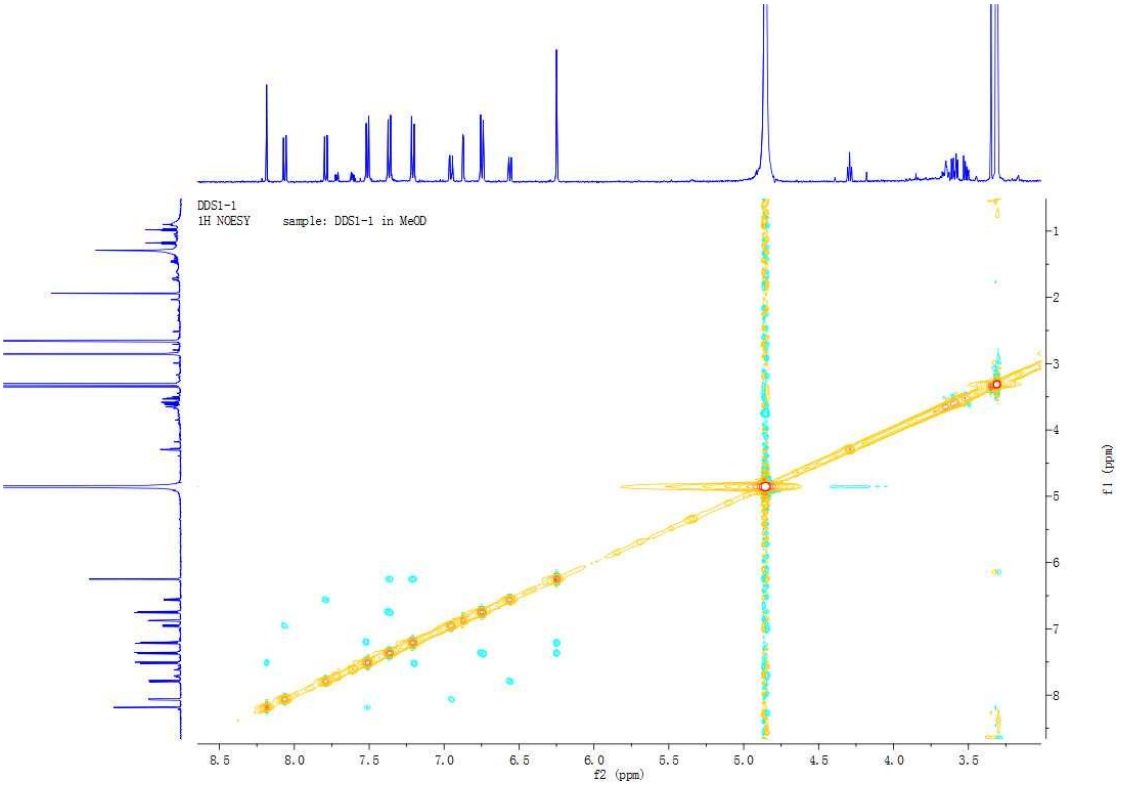

Figure S17. The HR-MS of 10a

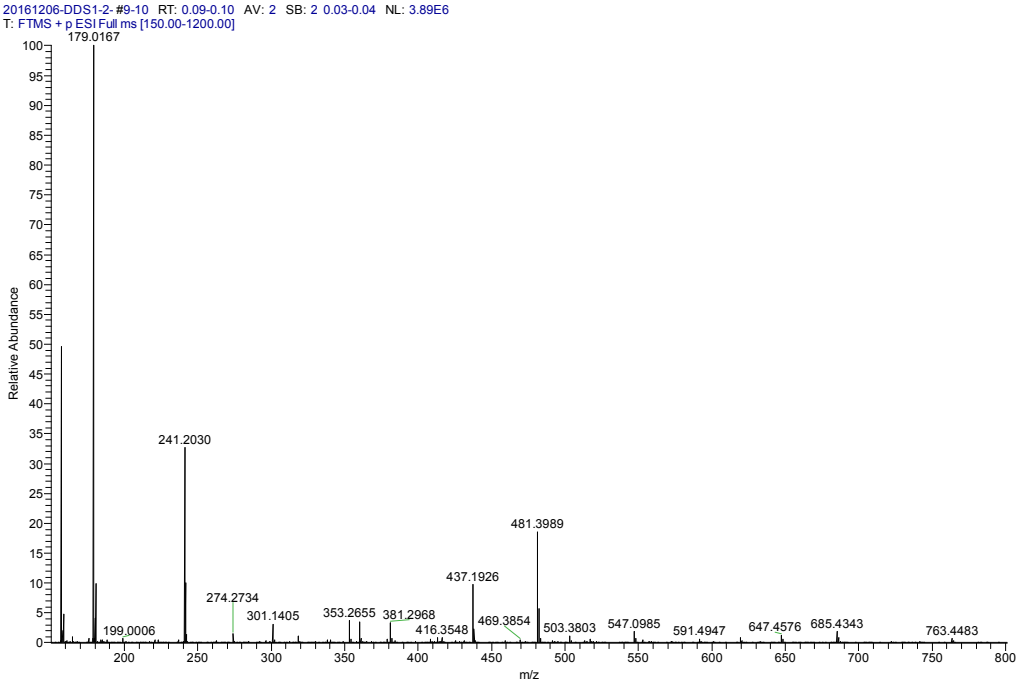

Figure S18. The ^{1}H NMR spectrum of 10b

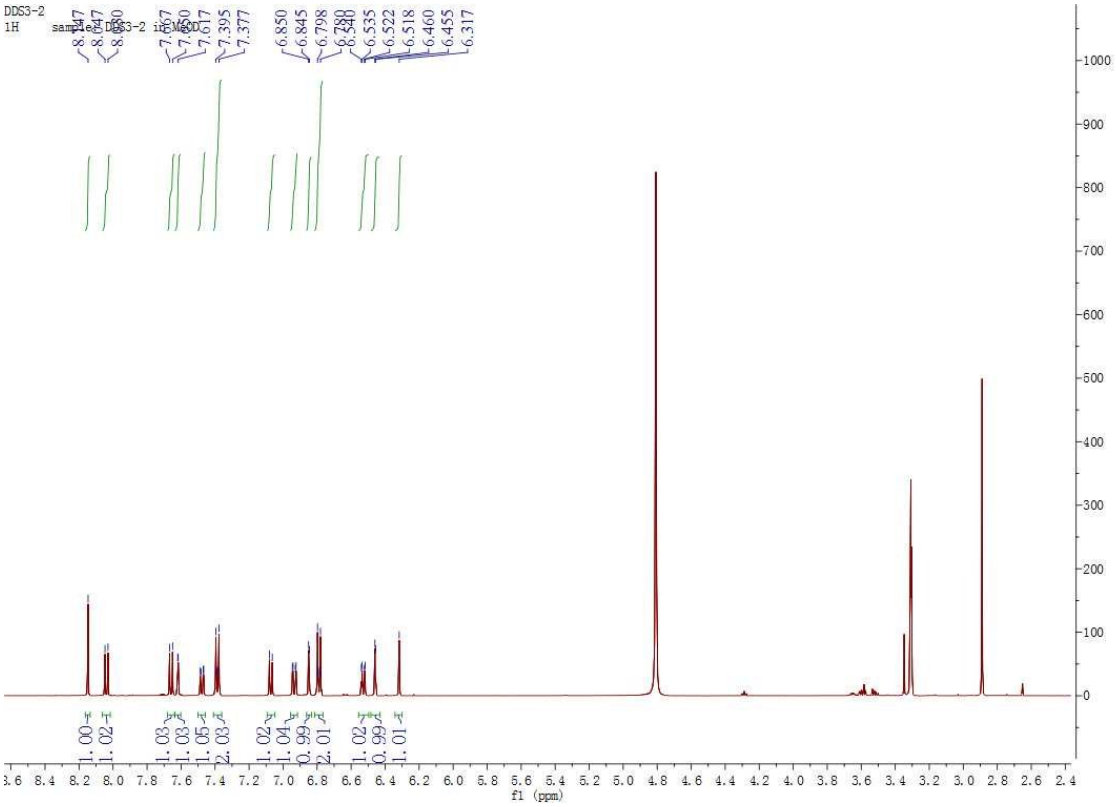

Figure S19. The ^{13}C NMR spectrum of 10b

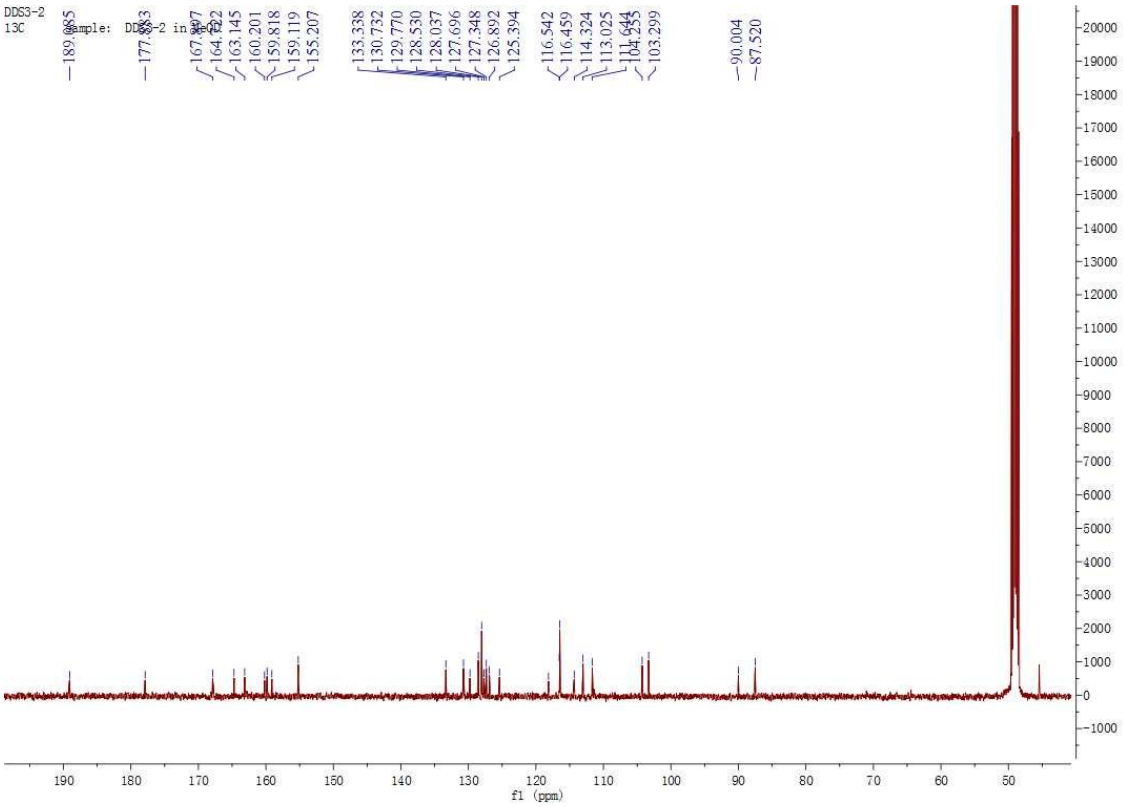

Figure S20. The HSQC spectrum of 10b

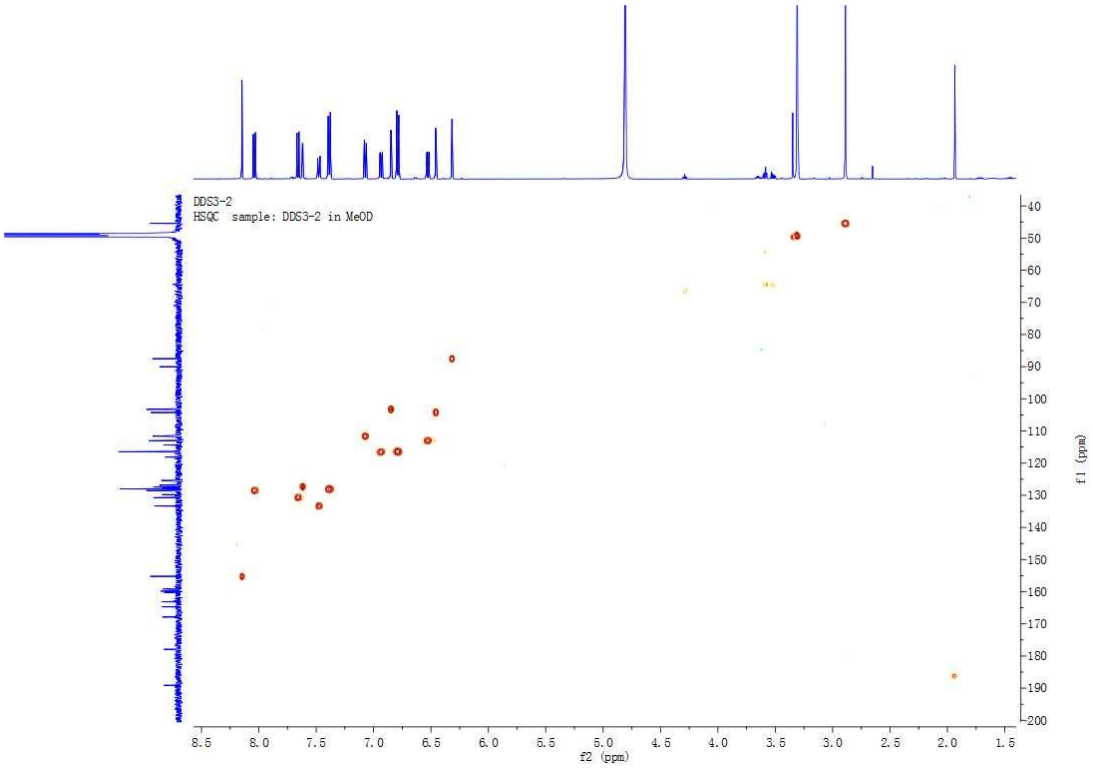

Figure S21. The HMBC spectrum of 10b

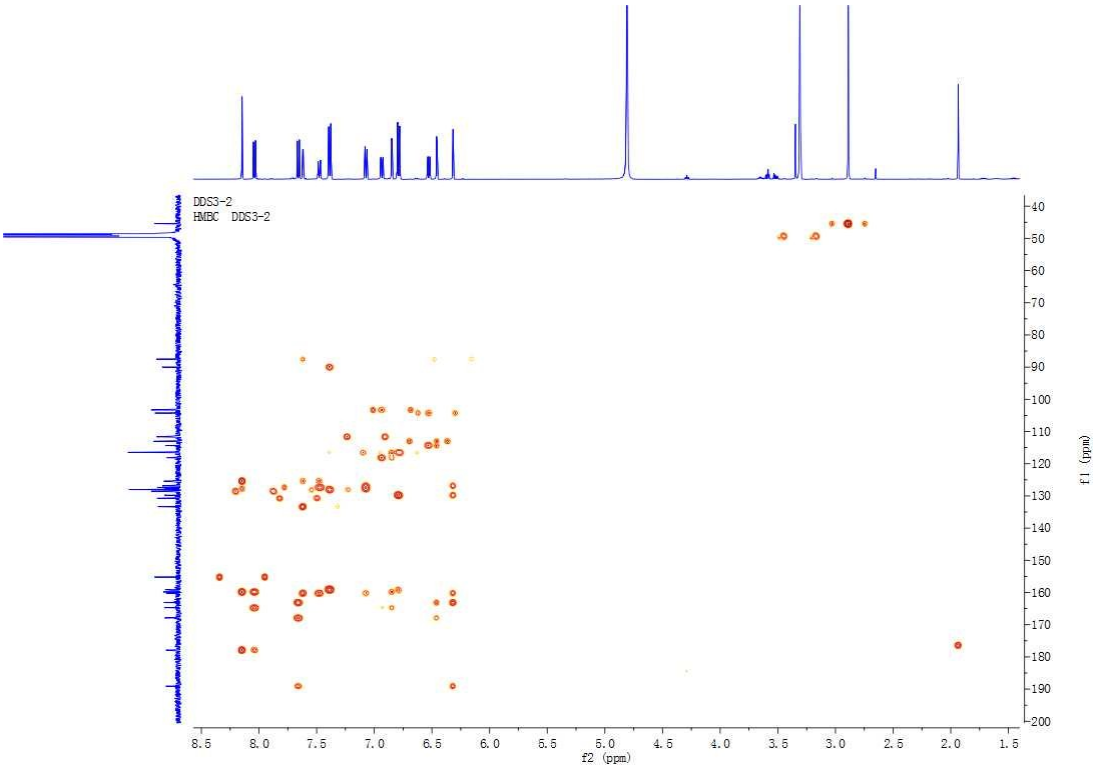

Figure S22. The ^{1}H-^{1}H COSY spectrum of 10b

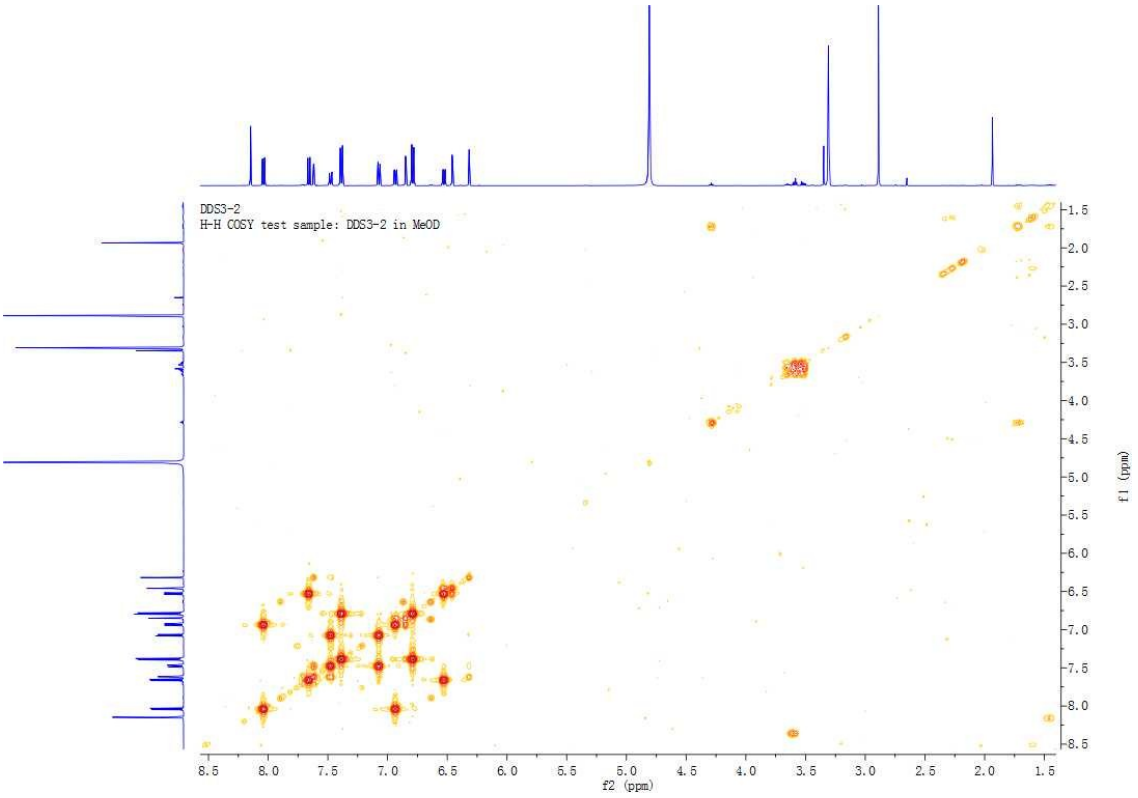

Figure S23. The NOESY spectrum of 10b

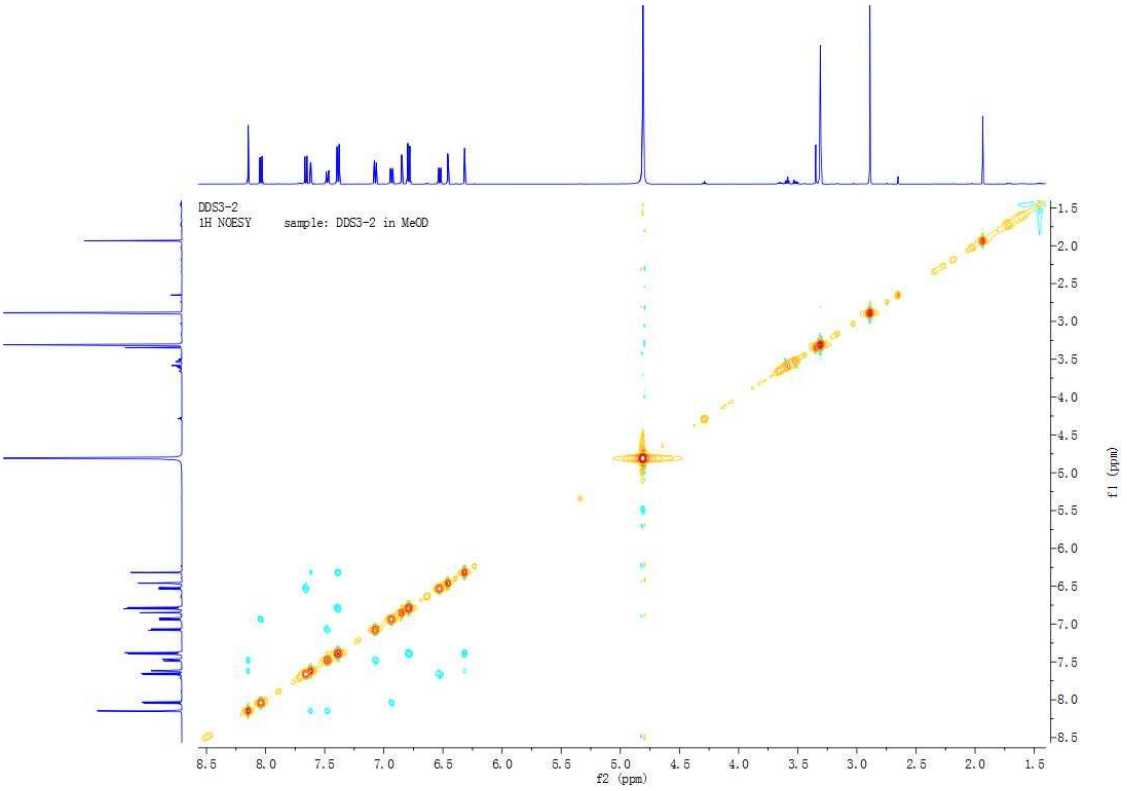

Figure S24. The ^{1}H NMR spectrum of 10c

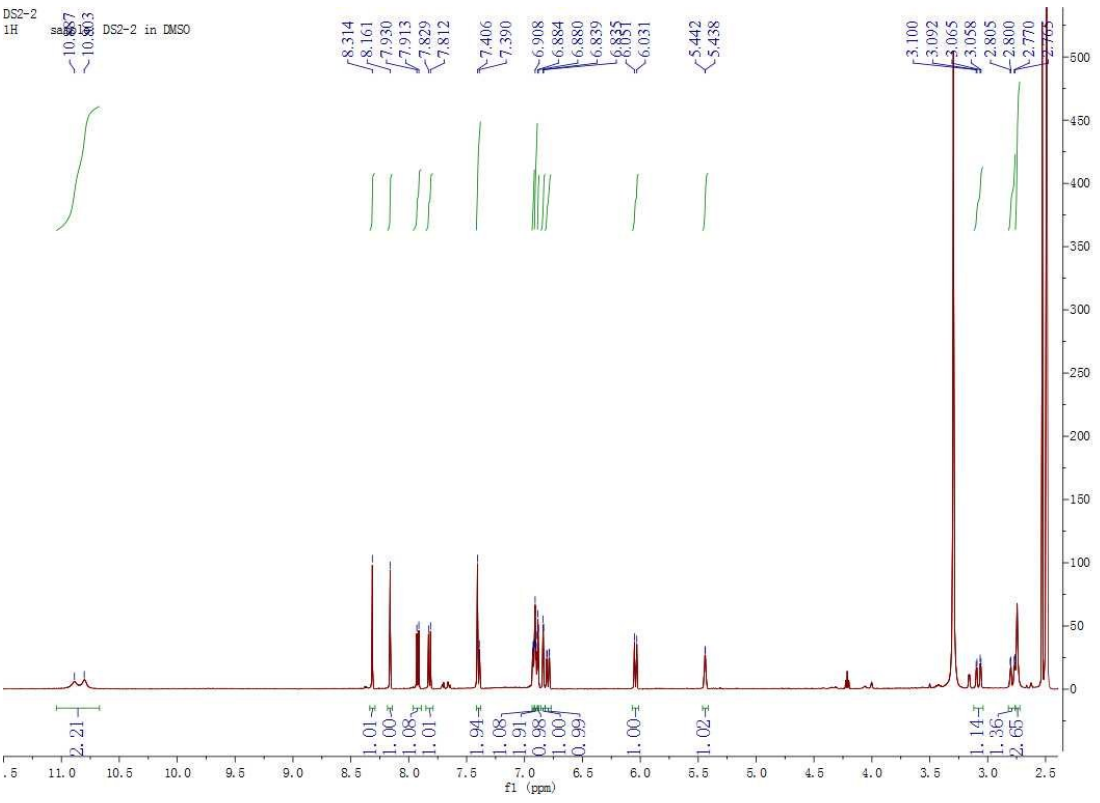

Figure S25. The ^{13}C NMR spectrum of 10c

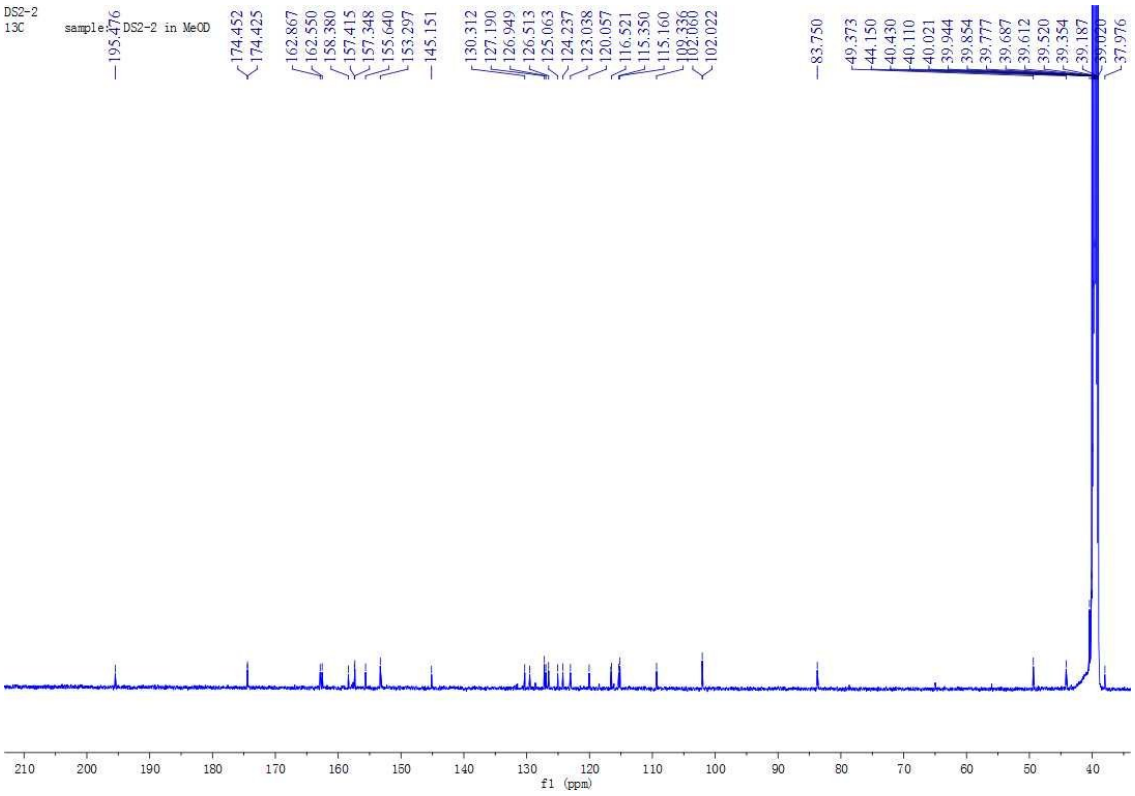

Figure S26. The HSQC spectrum of 10c

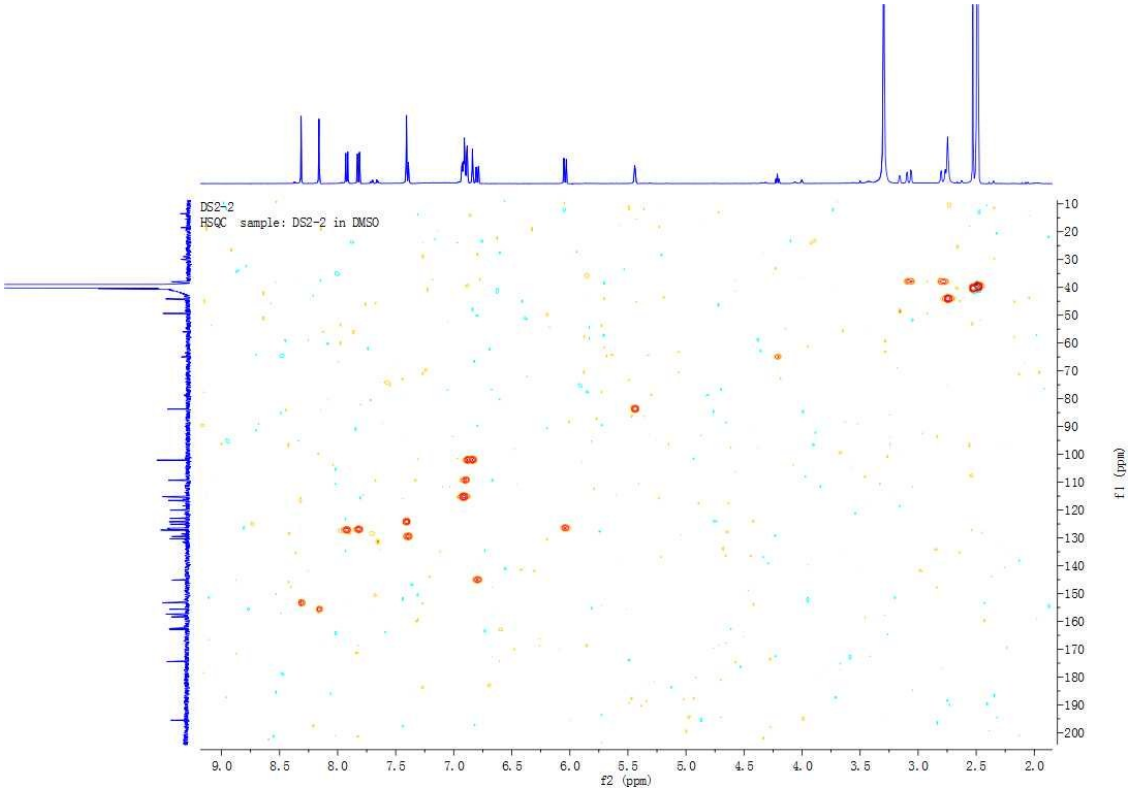

Figure S27. The HMBC spectrum of 10c

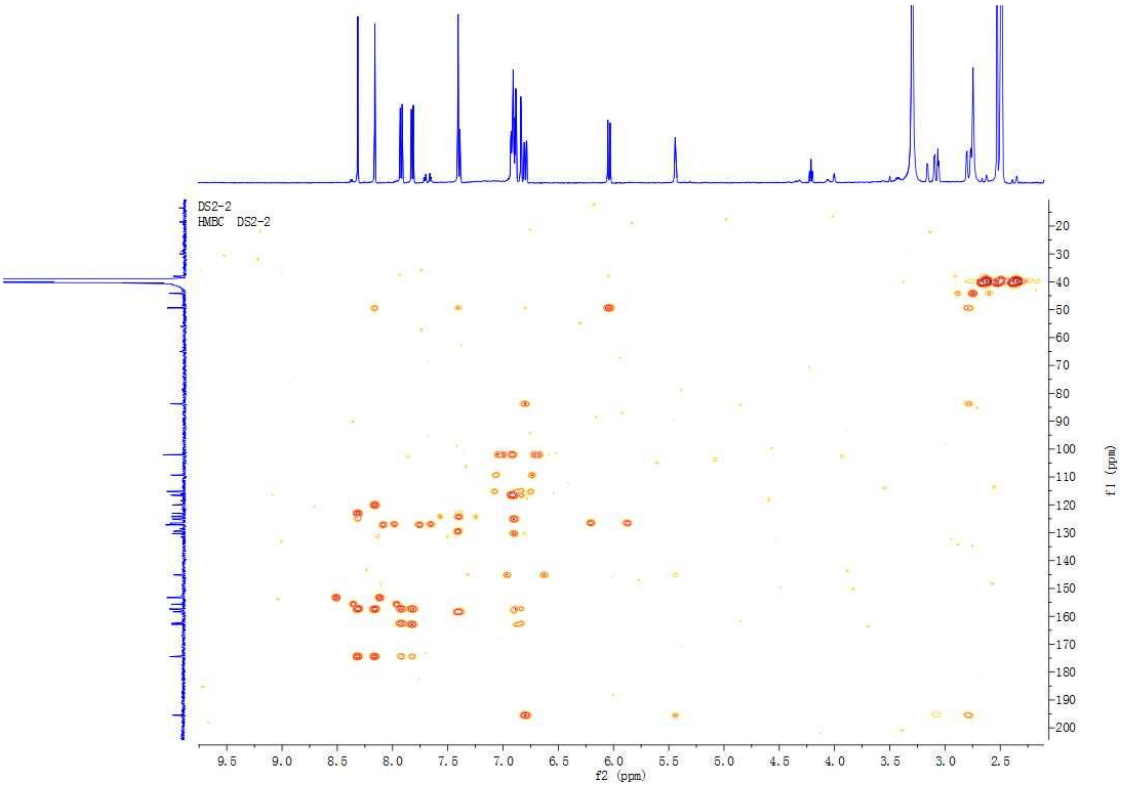

Figure S28. The ^{1}H-^{1}H COSY spectrum of 10c

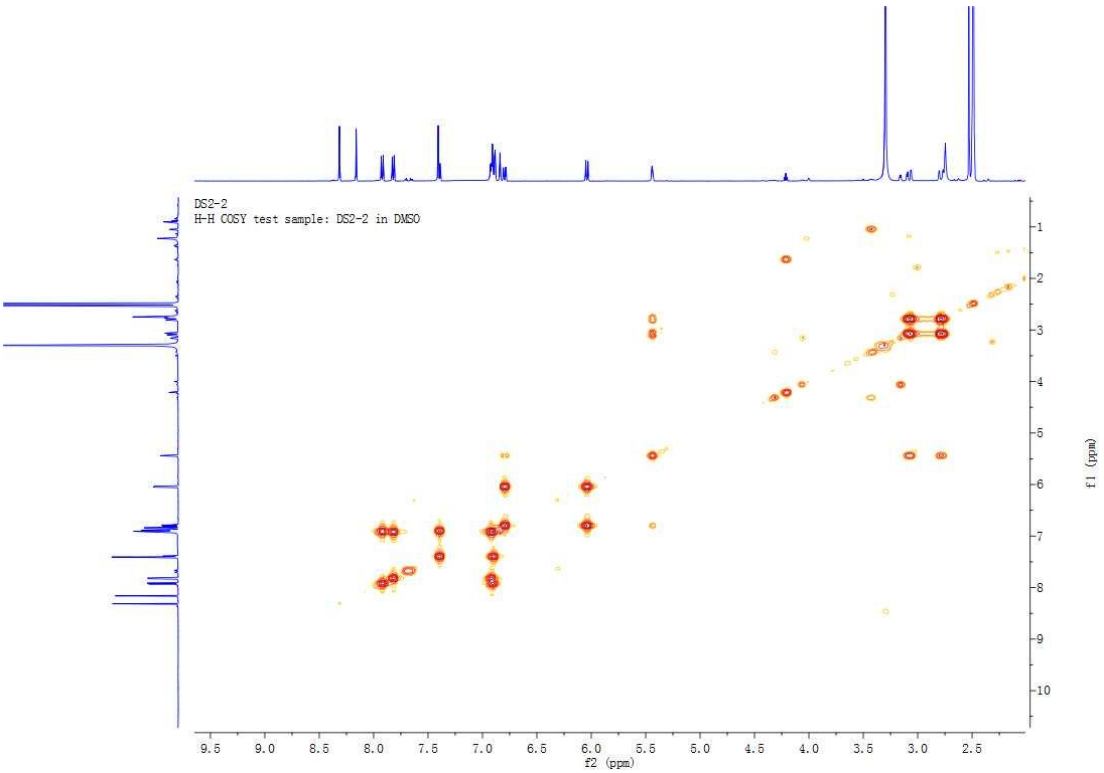

Figure S29. The NOESY spectrum of 10c

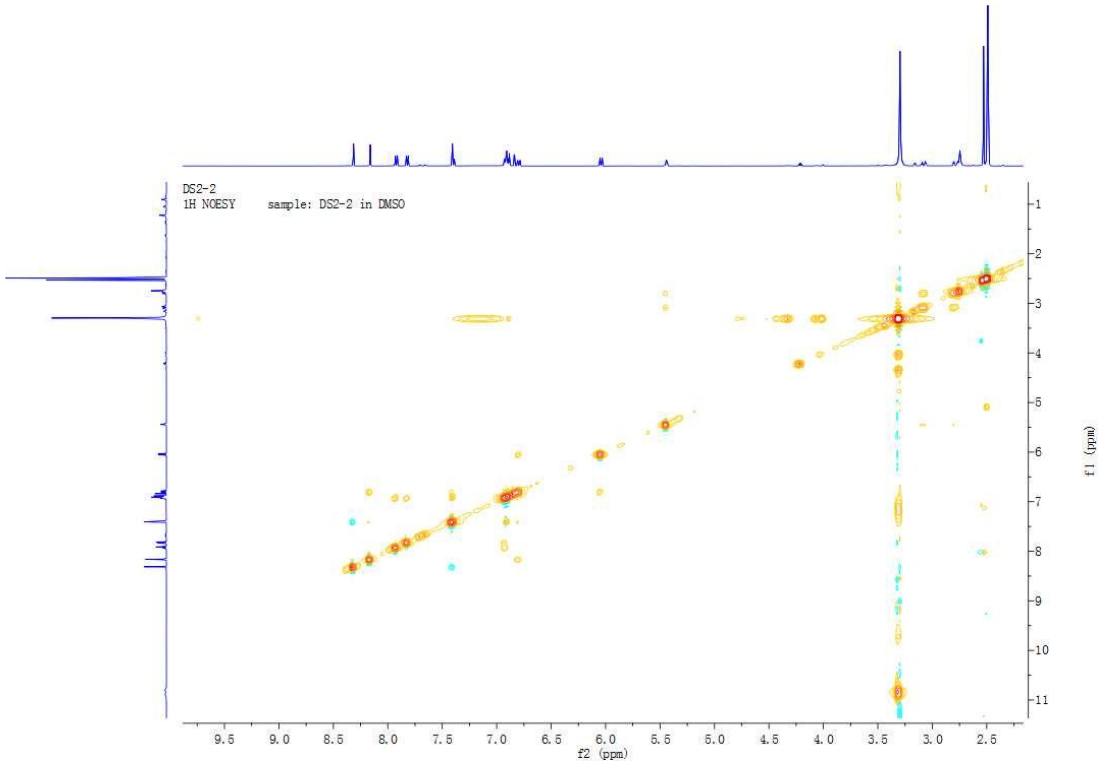

Figure S30. The HR-MS of 10c.

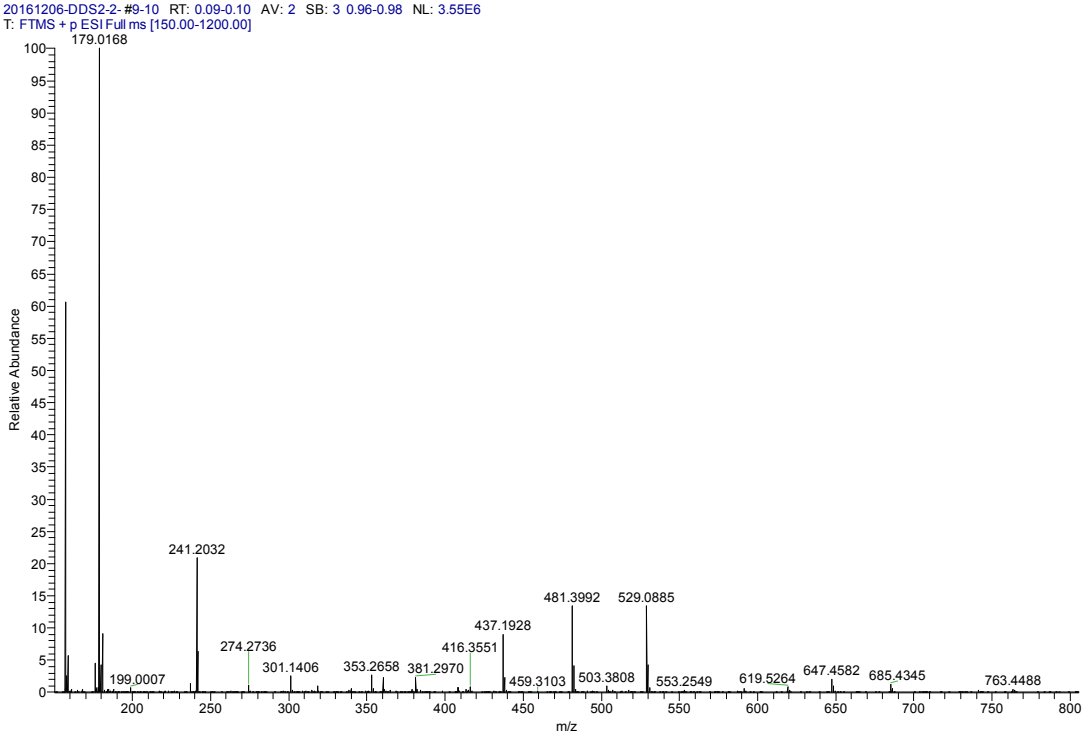

Figure S31. The ^{1}H-NMR spectrum of 12a

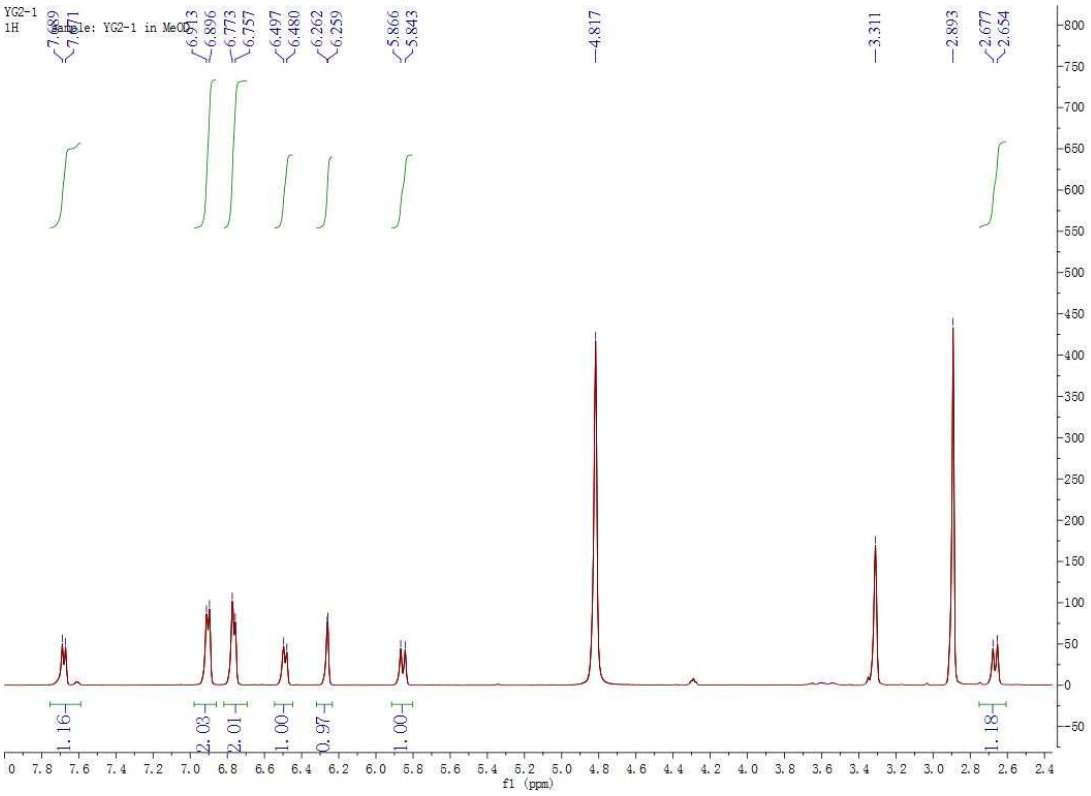

Figure S32. The ^{13}C NMR spectrum of 12a

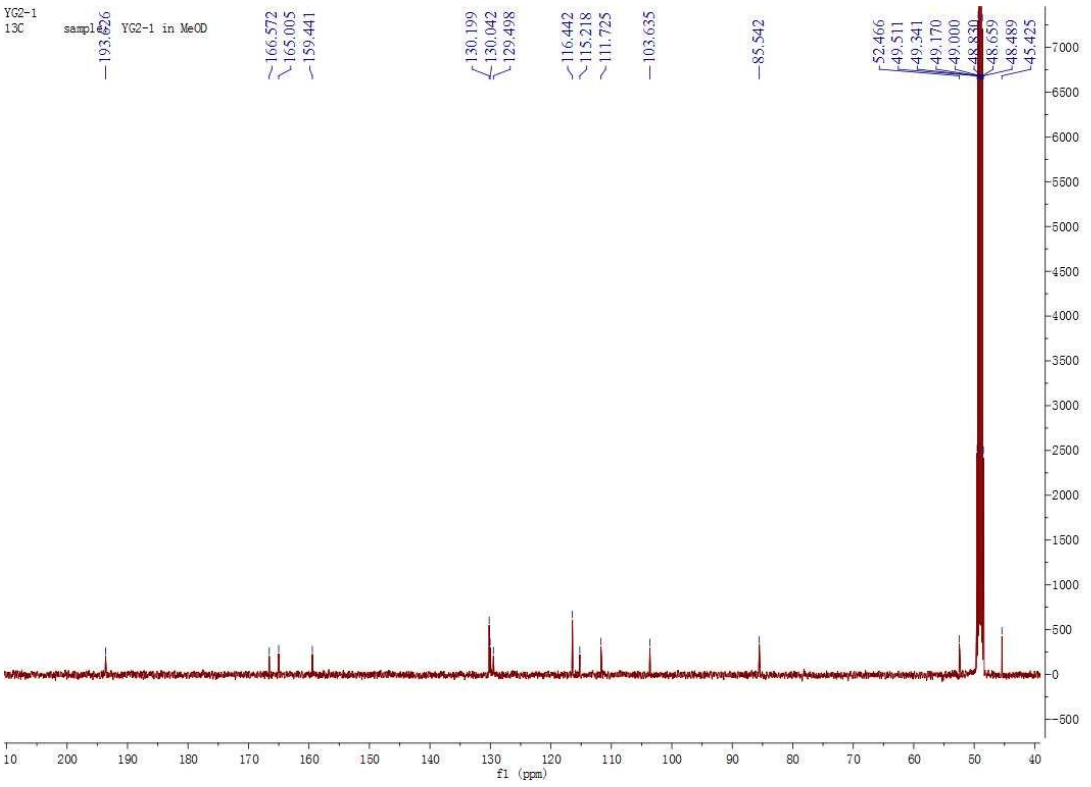

Figure S33. The HR-MS of 12a

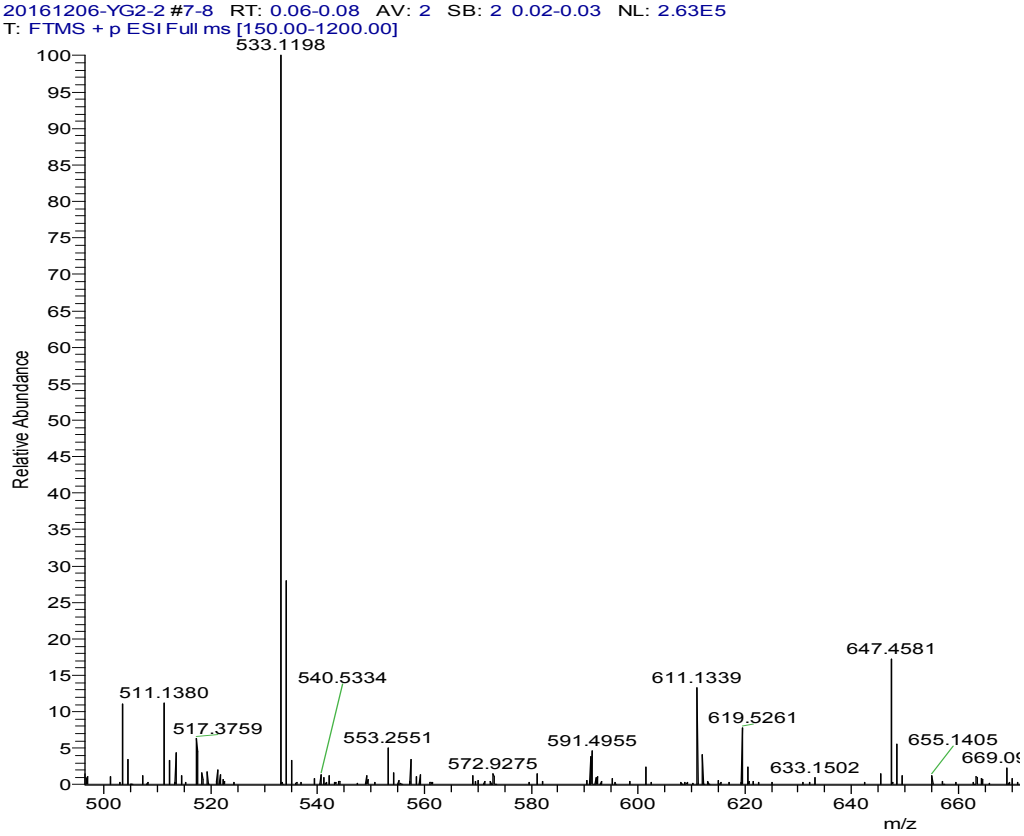

Figure S34.[1]H NMR spectrum of 12b

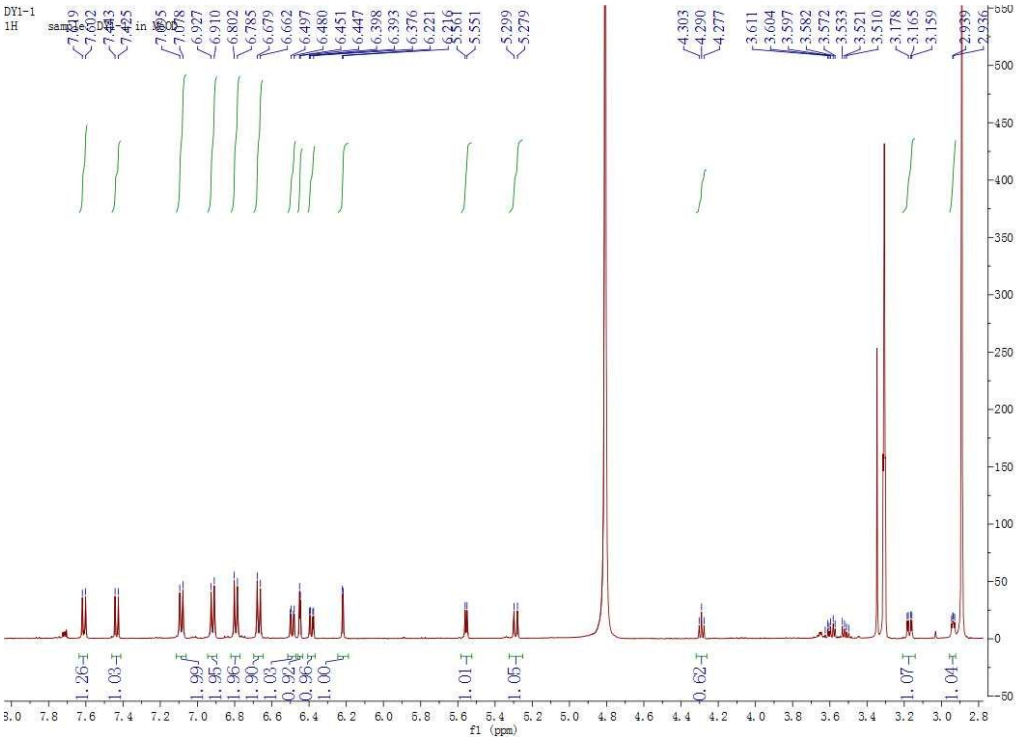

Figure S35. The ^{13}C NMR spectrum of 12b

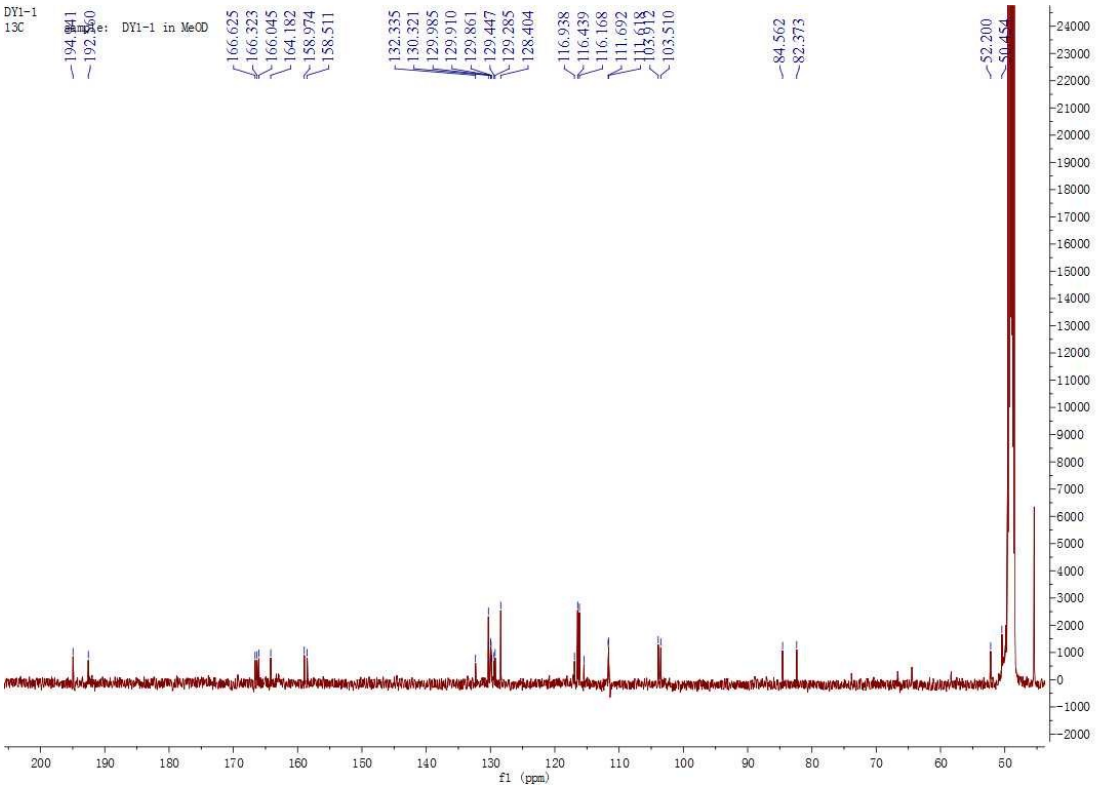

Figure S36. The HSQC spectrum of 12b

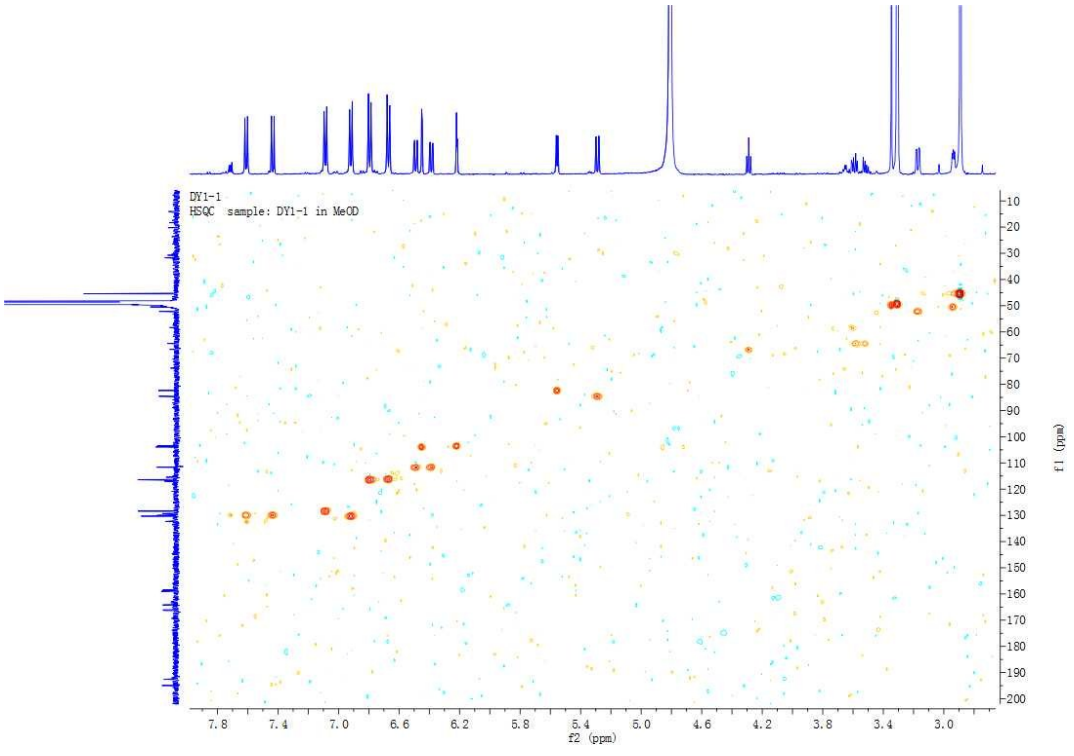

Figure S37. The HMBC spectrum of 12b

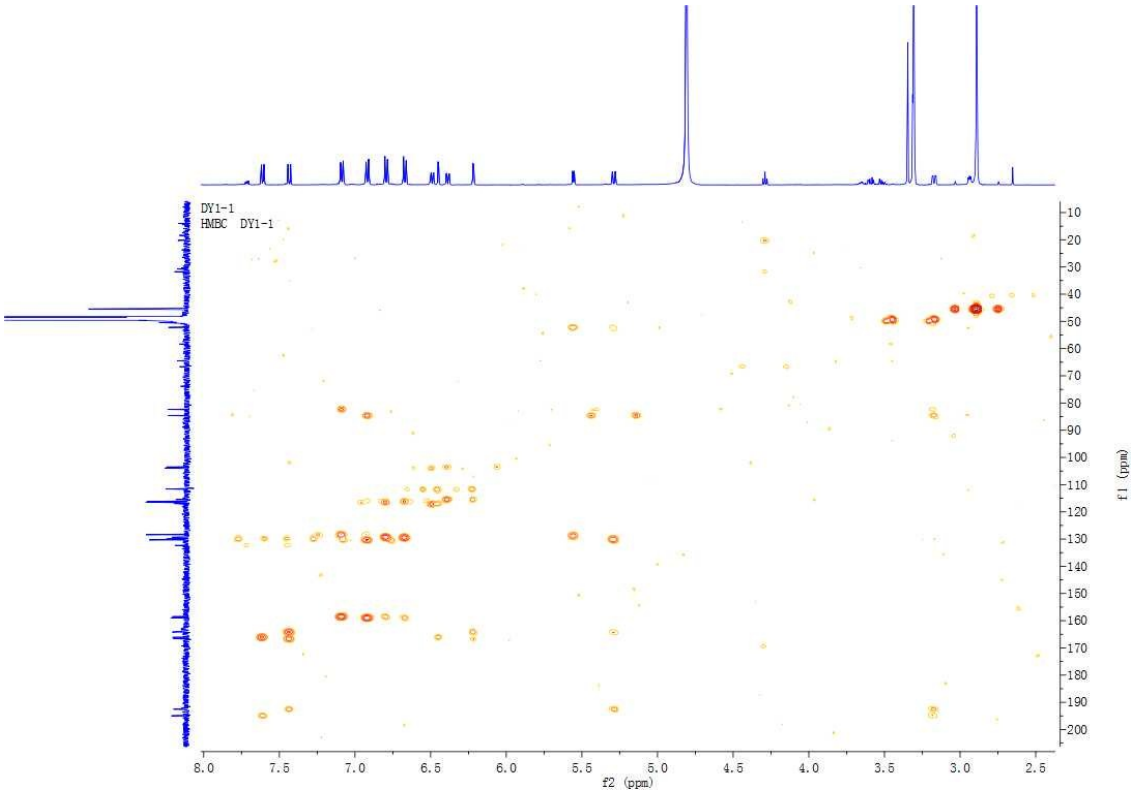

Figure S38. The ^{1}H-^{1}H COSY spectrum of 12b

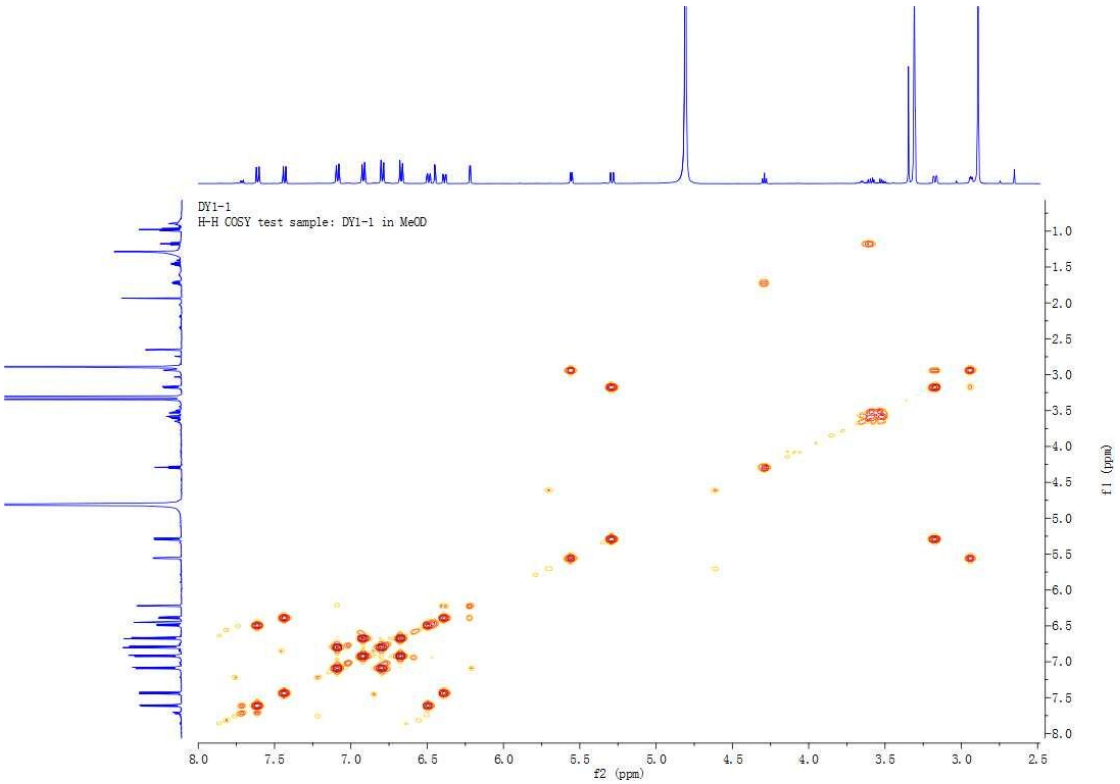

Figure S39. The NOESY spectrum of 12b

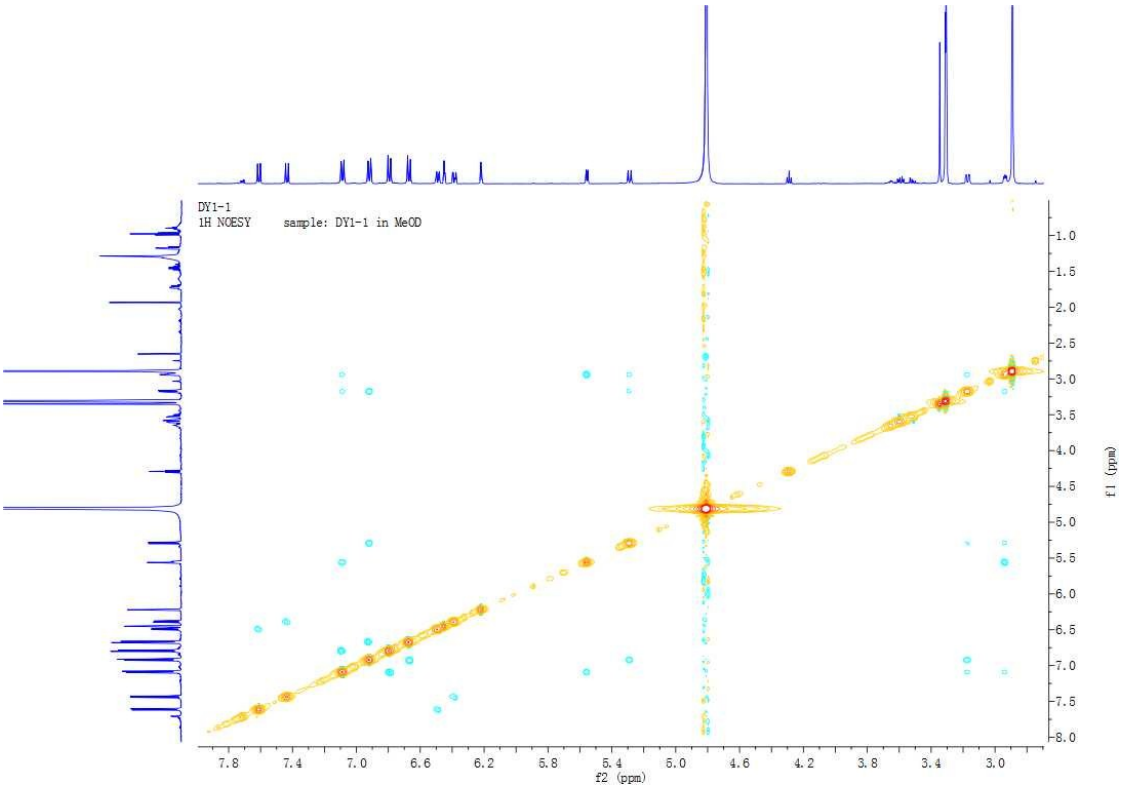

Figure S40. The HR-MS of 12b