

Supplementary Information:

Structurally diverse diterpenoid alkaloids from the lateral roots of *Aconitum carmichaelii* Debx. and their anti-tumor activities based on *in vitro* systematic evaluation and network pharmacology analysis

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Table S1 The 1D and 2D NMR data of compound **26** in CDCl₃.

No.	δ_H (ppm) (<i>J</i> in Hz)	δ_C (ppm)	¹ H- ¹ H COSY	HMBC	NOESY
1	3.35-3.38 (1H, m)	81.5	H-2a; H-2b	C-10	H-10
2a	1.96-2.09 (1H, m)	23.1	H-1; H-2b; H-3	-	H-2b
2b	1.39-1.51 (1H, m)		H-1; H-2a; H-3	-	H-2a; H-5; H-12b
3	1.80-1.93 (2H, m)	28.9	H-2a; H-2b	-	-
4	-	38.4	-	-	-
5	2.31 (1H, d, <i>J</i> =6.6 Hz)	42.1	H-6	C-4; C-7; C-11; C-17; C-18; C-19	H-2b; H-6; H-18a
6	4.10 (1H, d, <i>J</i> =6.6 Hz)	82.2	H-5	C-4; C-7; C-8; C-17; 6-OMe	H-5; H-9; 6-OMe
7	2.82-2.91 (1H, m)	43.5	-	C-8; C-9; C-11; C-17	8-OCH ₂ CH ₃
8	-	82.5	-	-	-
9	2.63 (1H, t, <i>J</i> =6.2 Hz)	44.3	H-10; H-14	C-8; C-10; C-12; C-13	H-6; H-10; H-14
10	2.14-2.22 (1H, m)	40.7	H-9	-	H-1; H-9
11	-	50.9	-	-	-
12a	2.22-2.29 (1H, m)	35.9	H-12b	C-10; C-13; C-16	H-14
12b	1.96-2.09 (1H, m)		H-12a	-	H-2b
13	-	74.7	-	-	-
14	4.83 (1H, d, <i>J</i> =5.1 Hz)	79.1	H-9	C-8; C-13; C-16; 14-OCOPh	H-9; H-12a
15	4.59 (1H, d, <i>J</i> =4.7 Hz)	77.5	H-16	C-8; C-16	8-OCH ₂ CH ₃ ; 8-OCH ₂ CH ₃ ; H-2', 6'
16	3.48-3.50 (1H, m)	92.4	H-15	-	-
17	3.25-3.30 (1H, m)	65.6	-	-	-
18a	3.55 (1H, d, <i>J</i> =8.0 Hz)	78.5	H-18b	C-3; C-4; C-19	H-18b
18b	3.11 (1H, d, <i>J</i> =8.0 Hz)		H-18a	C-3; C-4; C-5; 18-OMe	H-18a
19a	3.13-3.19 (1H, m)	57.9	-	-	-
19b	3.02-3.09 (1H, m)		-	-	-
NCH ₃	2.97 (3H, s)	43.0	-	-	-
1-OMe	3.35 (3H, s)	56.2	-	C-1	-
6-OMe	3.28 (3H, s)	59.0	-	C-6	H-6
8-OCH ₂ CH ₃	3.38-3.50 (2H, m)	57.6	8-OCH ₂ CH ₃	8-OCH ₂ CH ₃	H-7; H-15; 8-OCH ₂ CH ₃
8-OCH ₂ CH ₃	0.56 (3H, t, <i>J</i> =6.9 Hz)	15.3	8-OCH ₂ CH ₃	8-OCH ₂ CH ₃	H-15; 8-OCH ₂ CH ₃
16-OMe	3.82 (3H, s)	62.0	-	C-16	-
18-OMe	3.32 (3H, s)	59.3	-	C-18	H-5
14-OCOC ₆ H ₅	-	166.3	-	-	-
1'	-	130.1	-	-	-
2'	8.05 (1H, d, <i>J</i> =7.7 Hz)	129.8	H-3', H-5'	14-OCOC ₆ H ₅ ; C-4'; C-2'; H-6'	H-15; H-3'; H-5'
3'	7.45 (1H, t, <i>J</i> =7.6 Hz)	128.6	H-2'; H-6'; H-4'	C-2'; C-6'	H-2'; H-6'
4'	7.56 (1H, t, <i>J</i> =7.4 Hz)	133.2	H-3'; H-5'	C-2' C-6'	-
5'	7.45 (1H, t, <i>J</i> =7.6 Hz)	128.6	H-2'; H-6'; H-4'	C-2'; C-6'	H-2'; H-6'
6'	8.05 (1H, d, <i>J</i> =7.7 Hz)	129.8	H-3'; H-5'	14-OCOC ₆ H ₅ ; C-4'; C-2'; C-6'	H-15; H-3'; H-5'

NMR spectra were acquired on a Bruker Avance III HD 600 MHz spectrometer.

Table S2 The 1D and 2D NMR data of compound **37** in CDCl₃

No.	δ_H (ppm) (<i>J</i> in Hz)	δ_C (ppm)	HMBC	¹ H- ¹ H COSY	NOESY
1	2.96 (1H, dd, <i>J</i> = 10.2, 6.2 Hz)	86.3	1-OMe, C-10, C-11, C-17	H-2a, H-2b	H-10
2a	2.10-2.17 (1H, m)	25.8	-	H-1, H-2b	H-2b
2b	1.85-1.94 (1H, m)	-	-	H-1, H-2a	H-2a
3a	1.61-1.70 (1H, m)	34.7	-	H-3b	H-3b
3b	1.48-1.57 (1H, m)	-	-	H-2a, H-3a	H-3a
4	-	39.8	-	-	-
5	2.04-2.06 (1H, m)	48.8	C-7, C-10, C-11, C-17, C-18, C-19	H-6	H-16
6	3.87-3.90 (1H, m)	84.2	6-OMe, C-4, C-8	H-5	H-9
7	2.83 (1H, d, <i>J</i> = 5.7 Hz)	40.8	C-6, C-9, C-17	-	-
8	2.79-2.80 (1H, m)	48.9	C-7, C-9, C-10, C-15, C-17	H-9	H-16, H-9
9	2.50 (1H, q, <i>J</i> = 5.6 Hz)	40.8	C-12, C-13, C-14, C-15	H-14, H-8, H-10	H-6, H-8, H-14
10	2.06-2.11 (1H, m)	45.3	-	H-9, H-12a, H-12b	H-1, H-14
11	-	51.4	-	-	-
12a	2.74-2.78 (1H, m)	33.4	C-11, C-13, C-14, C-16	H-10	H-12b
12b	1.69-1.74 (1H, m)	-	C-10, C-13	H-10	H-12a
13	-	78.6	-	-	-
14	4.24 (1H, d, <i>J</i> = 5.0 Hz)	76.6	C-8, C-13, C-16	H-9	H-9, H-10
15	-	212.4	-	-	-
16	3.89-3.92 (1H, m)	86.0	16-OMe, C-12, C-13, C-15	-	H-5, H-8
17	2.89(1H, s)	63.6	C-6, C-8, C-10, C-11, C-19, NCH ₃	-	NCH ₃
18a	3.67 (1H, d, <i>J</i> = 8.4 Hz)	80.4	18-OMe, C-3, C-4, C-19	H-18b	H-18b
18b	3.21(1H, d, <i>J</i> = 8.4 Hz)	-	18-OMe, C-3, C-4, C-5	H-18a	H-18a
19a	2.72 (1H, d, <i>J</i> = 10.8 Hz)	56.6	C-3, C-7, C-18	H-19b	H-19b
19b	2.43(1H, d, <i>J</i> = 10.8 Hz)	-	C-17	H-19a	H-19a
NCH ₃	2.32 (3H, s)	42.4	C-17, C-19	-	H-17
1-OMe	3.23(3H, s)	56.6	C-1	-	-
6-OMe	3.27 (3H, s)	58.0	C-6	-	-
16-OMe	3.74 (3H, s)	62.2	C-16	-	-
18-OMe	3.28 (3H, s)	59.4	C-18	-	-

NMR spectra were acquired on a Bruker Avance III HD 600 MHz spectrometer.

Table S3 Top 21 target genes with degree values not less than 45

Target genes	Name	Degree value
AKT1	RAC-alpha serine/threonine-protein kinase	100
VEGFA	Vascular endothelial growth factor A	82
EGFR	Epidermal growth factor receptor	81
STAT3	Signal transducer and activator of transcription 3	73
SRC	Proto-oncogene tyrosine-protein kinase Src	73
ESR1	Estrogen receptor	72
TNF	Tumor necrosis factor	71
MAPK1	Mitogen-activated protein kinase 1	68
JUN	Transcription factor AP-1	67
HSP90AA1	Heat shock protein HSP 90-alpha	66
MTOR	Serine/threonine-protein kinase mTOR	65
CXCL8	Interleukin-8	64
PTGS2	Prostaglandin G/H synthase 2	56
AR	Androgen receptor	48
PIK3CA	Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	48
MAPK14	Mitogen-activated protein kinase 14	46
NFKB1	Nuclear factor NF-kappa-B p105 subunit	46
IL2	Interleukin-2	46
HIF1A	Hypoxia-inducible factor 1-alpha	46
ATM	Serine-protein kinase ATM	45
KDR	Vascular endothelial growth factor receptor 2	45

Table S4 Enrichment analysis results of 173 target genes

SampleGroup	GeneRatio	Qvalue	Count	Description	Target genes
KEGG Pathway	44/576	-34.63	44	Pathways in cancer	AKT1, ALK, BIRC2, XIAP, AR, BCL2L1, EGFR, EPAS1, ESR1, ESR2, FGF2, FLT3, MTOR, GNAS, GSK3B, HDAC1, HDAC2, HIF1A, HSP90AA1, IKBKB, IL2, CXCL8, JUN, SMAD3, MMP2, NFKB1, NOS2, PDGFRA, PIK3CA, PIK3CB, PIM1, PIK3CD, PPARG, PRKCA, PRKCB, MAPK1, PTGS2, RAF1, SLC2A1, STAT3, TERT, TGFB1, VEGFA, NCOA3, ATM, CYP24A1, DNMT1, MCL1, ABCC1, ABCB1, MAPK7
Reactome Gene Sets	38/461	-30.97	38	Signaling by Interleukins	AKT1, BCL2L1, CA1, CCR1, MAPK14, PTK2B, FGF2, HIF1A, HSP90AA1, IKBKB, IL2, CXCL8, JUN, LCK, LGALS9, SMAD3, MAOA, MCL1, MMP2, MTAP, NFKB1, NOS2, OPRM1, PIK3CA, PIK3CB, PIM1, PIK3CD, MAPK1, MAPK7, PTAFR, PTGS2, RORA, RORC, STAT3, SYK, TNF, VEGFA, CCR2, BIRC2, EIF4A1, FLT3, PIN1, PRKCD, PTPN1
GO Biological Processes	44/740	-30.00	44	regulation of MAPK cascade	ADRA1A, ADRA2B, AKT1, ALK, AR, CASR, CDK1, CCR1, MAPK14, DRD2, EGFR, ELANE, PTK2B, FGF2, FLT3, GPER1, IGFBP3, IGFBP4, KDR, LGALS9, OPRM1, PAK1, PDGFRA, PIK3CB, PIK3CG, PIN1, PLA2G1B, PLA2G2A, PRKCA, PRKCD, MAPK1, PTPN1, RAF1, REN, RGS4, SRC, SYK, TGFB1, TNF, VEGFA, HDAC3, TLR9, HRH4, GPBAR1, ACE, MTOR, HSP90AA1, IL2, MAPT, PDPK1, PIK3CA, PLK1, STK11, MERTK, IKBKB, NFKB1
WikiPathways	23/114	-27.86	23	Gastrin Signaling Pathway	AKT1, BIRC2, BCL2L1, MAPK14, EGFR, MTOR, GSK3B, IKBKB, IL2, CXCL8, JUN, NFKB1, PAK1, PIK3CA, PPARG, PRKCA, PRKCD, MAPK1, PTGS2, RAF1, SRC, STAT3, VEGFA, FGF2, KDR, PDGFRA, PDPK1, PIK3CB, PIK3CD, PRKCB, MYLK, PIK3CG, PLA2G2A, MAPK7, TNF, CCR1, PTK2B, GNAS, NCOA3, SMAD3, MMP2, PIM1, TGFB1, CYP2D6, ESR1, ESR2, GPER1, HIF1A, SYK, ACE, NOS2, TLR9, HDAC1, HDAC2, SLC2A1, HDAC3, HSP90AA1, OPRM1, PGR, CXCR1, CCR2, PPARA, PTPN1, NR1H2, NR1H3, XBP1, NOS1, ERG, IGFBP3, FLT3, LCK, MCL1, STK11, EPAS1, PPP5C, XIAP, ATM, ATR, TERT, CDK1, KCNA5, G6PD, CYP19A1, AR, SLC22A1, CYP17A1, PLA2G1B, PARP1, DRD2, MERTK, CYP3A4, CNR1, PLK1, BTK, ALK, PIN1, ALDH1A1, NR5A2, PLG, ABCC1, PTGS1, GHSR, PDE10A, PTAFR, ABCB1, IGFBP1, HSD11B2, ACHE, CHRM3, CHRNA4, MAPT, AURKA
GO Biological Processes	41/701	-27.59	41	response to wounding	ADRA2B, KLF5, CCR1, DRD2, EGFR, FAP, FGF2, MTOR, GNAS, HDAC1, HDAC2, HIF1A, IGFBP1, KDR, LCK, LGALS1, SMAD3, MYLK, OPRM1, PAK1, PDGFRA, PDPK1, PIK3CA, PIK3CB, PIK3CG, PLG, PPARA, PRKCA, PRKCB, PRKCD, MAPK1, RAF1, SRC, AURKA, SYK, TGFB1, TNF, VEGFA, XBP1, MERTK, CCR2, CHRM3, HSD11B2, OPRK1, SLC6A3, UGCG, NR1H2, NR1H3, AKT1, MAPK14, KIF11, NOS1, NOS2, PTPN1, PDE5A, PDE10A
GO Biological Processes	37/565	-26.54	37	cellular response to	PARP1, AKT1, AR, ATM, CASR, MAPK14, CYP24A1, EGFR, ESR1, ESR2, PTK2B, FLT3, GHSR, GPER1, NR3C1,

				lipid	HDAC1, HDAC2, CXCL8, NFKB1, NOS2, PAK1, PGR, PIM1, PPARA, PPARG, PPP5C, PRKCA, MAPK1, PTAFR, RORA, RORC, SRC, TNF, XBP1, NCOA3, NR1H3, GPBAR1, KLF5, LGALS1, OPRM1, PIK3CG, AGL, HSD11B2, NR5A2, REN
GO Biological Processes	35/538	-24.97	35	regulation of hormone levels	ACHE, ADRA2B, ALDH1A1, BTK, CASR, CNR1, CYP1A2, CYP2C9, CYP2D6, CYP3A4, CYP17A1, CYP19A1, ACE, DPP4, DRD2, EGFR, ESR1, GHSR, GNAS, GPER1, HIF1A, HSD11B2, HSD17B1, KCNA5, MME, NFKB1, NOS2, PDGFRA, PRKCA, RAF1, REN, SLC2A1, SLC22A1, TNF, TARDBP, STS, CYP2C19, CYP24A1, NR5A2, G6PD, RORA, RORC, SOAT1, NR1I2, PPARA, SLC10A2, SLCO1B1, SLCO1B3, PTGS2
WikiPathways	29/317	-24.81	29	Nuclear Receptors Meta-Pathway	BIRC2, CDK1, CYP1A2, CYP2C19, CYP2C9, CYP3A4, EGFR, ESR1, G6PD, NR3C1, HSP90AA1, IGFBP1, IL2, JUN, ABCB1, PPARA, PTGS2, SLC2A1, SLC5A1, SLC5A2, SLC6A2, SLC6A3, SRC, STAT3, TNF, NCOA3, NR1I2, NR1H3, SLCO1B1
GO Biological Processes	36/597	-24.57	36	positive regulation of cellular component movement	AKT1, ATM, CCR1, MAPK14, EGFR, ELANE, PTK2B, FGF2, MTOR, GPER1, HIF1A, CXCL8, KDR, LGALS3, LGALS9, SMAD3, MYLK, PAK1, PDGFRA, PDPK1, PIK3CB, PIK3CD, PIK3CG, PRKCA, MAPK1, PTAFR, PTGS2, SRC, STAT3, STK11, TERT, TGFBR1, TNF, VEGFA, XBP1, CCR2, CASR, KLF5, DNMT1, EPAS1, FAP, GHSR, JUN, MMP2, PIK3CA, PPARG, PRKCB, MAPK7, RORA, SYK, ALK, AR, FLT3, GSK3B, HSP90AA1, IGFBP1, IGFBP3, IGFBP4, LCK, PRKCD, PTPN1, RAF1, MERTK, ESR1, PGR, PLG, TLR9, GPBAR1, DPP4
WikiPathways	18/66	-24.47	18	AGE/RAGE pathway	AKT1, MAPK14, EGFR, HIF1A, IKBKB, JUN, LGALS3, SMAD3, MMP2, NFKB1, NOS2, PRKCA, PRKCB, PRKCD, MAPK1, RAF1, SRC, STAT3, PARP1, ATM, ATR, CDK1, DYRK1A, MTOR, GSK3B, HSP90AA1, NOS1, PAK1, PDPK1, PIK3CA, PLK1, MAPK7, AURKA, SYK, TGFBR1, TNF, VEGFA, PTK2B, NCOA3, CNR1, MAPT, BTK, LCK, PIK3CG, FGF2, FLT3, KDR, PDGFRA, PPP5C, GNAS, IL2, CXCL8, OPRM1, CYP19A1, PIN1, PPARG, BCL2L1, PIM1, AR, MYLK, HDAC1, TERT, PTGS2
GO Biological Processes	36/623	-23.93	36	regulation of secretion	ACHE, ADRA1A, ADRA2B, CASR, CHRNA4, CNR1, CYP19A1, DPP4, DRD2, EGFR, GHSR, GNAS, GPER1, GSK3B, HIF1A, KCNA5, LGALS9, NOS2, OPRK1, OPRM1, PDPK1, PLA2G1B, PRKCA, PRKCB, PTAFR, REN, SLC2A1, SYK, TNF, NR1H2, XBP1, PTGES, NR1H3, TARDBP, BACE1, CCR2, MAPK14, SMAD3, MAPT, PAK1, PRKCD, MAPK1, PTPN1, SRC, HDAC3, BTK, RAF1, SLC22A1
GO Biological Processes	30/385	-23.62	30	response to oxygen levels	AKT1, BIRC2, ATM, CA9, CASR, CHRNA4, DPP4, DRD2, EPAS1, PTK2B, MTOR, HDAC2, HIF1A, HSD11B2, KCNA5, SMAD3, MMP2, NOS1, NOS2, PAK1, PIN1, PPARA, PPARG, PTGS2, RAF1, RORA, SLC2A1, SRC, TERT, VEGFA, IGFBP1, JUN, MCL1, ABCB1, BCL2L1, IGFBP3
GO Biological Processes	35/597	-23.46	35	regulation of system process	PARP1, ADRA1A, ADRA2B, AKT1, CASR, CHRM3, ACE, DRD2, EGFR, EPAS1, PTK2B, MTOR, G6PD, GHSR, GLRA1, GNAS, GPER1, GPR35, IL2, KCNA5, SMAD3, NOS1, OPRK1, OPRM1, PAK1, PIK3CG, PIN1, PPARA,

GO Biological Processes	36/665	-22.97	36	cellular response to hormone stimulus	PRKCA, PTAFR, REN, RGS4, SRC, NR1H2, NR1H3, AR, CNR1, HSD11B2, MME, NOS2, PIK3CA, PPARG, PTGS1, PTGS2, VEGFA, HDAC2, MYLK, GSK3B, MAPT, PRKCD, BTK, MAPK1, MAPK7, HRH4 ACHE, PARP1, AKT1, AR, CHRM3, EGFR, ESR1, ESR2, FLT3, NR5A2, GHSR, GPER1, NR3C1, GSK3B, HDAC1, IGFBP1, NFKB1, OPRM1, PAK1, PDPK1, PGR, PIK3CA, PLA2G1B, PPARA, PPARG, PPP5C, PRKCB, PRKCD, PTPN1, REN, SRC, STAT3, UGCG, XBP1, NCOA3, HRH4, KLF5, CASR, MTOR, GLRA1, HDAC2, MMP2, ABCC1, PDGFRA, PIK3CG, MAPK1, PTAFR, TNF, BACE1, MAPK14, HSD11B2, SLC2A1
GO Biological Processes	29/444	-20.68	29	second-messenger-mediated signaling	ADRA1A, ADRA2B, BTK, CHRM3, CCR1, CNR1, DRD2, EGFR, PTK2B, MTOR, NR5A2, GNAS, GPER1, GSK3B, CXCL8, CXCR1, KDR, MAPT, NOS1, NOS2, OPRM1, PDPK1, PRKCA, MAPK7, SYK, TNF, VEGFA, PDE10A, CCR2
GO Biological Processes	26/331	-20.54	26	positive regulation of response to external stimulus	BTK, CASR, CCR1, CNR1, EGFR, PTK2B, FGF2, GHSR, IL2, CXCL8, KDR, LGALS9, SMAD3, ABCC1, OPRM1, PIK3CG, PLA2G2A, PLG, PRKCA, MAPK1, PTGS2, STAT3, TNF, VEGFA, TLR9, CCR2, CDK1, LGALS3, NOS1, NOS2
GO Biological Processes	35/736	-20.49	35	response to growth factor	PARP1, AKT1, XIAP, CASR, MAPK14, EGFR, FGF2, FLT3, NR3C1, HDAC2, HIF1A, CXCL8, JUN, KDR, SMAD3, MAPT, NOS1, OPRM1, PDGFRA, PDPK1, PIK3CA, PIK3CB, PIK3CD, PIN1, PPARA, PPARG, PRKCB, MAPK1, MAPK7, PTPN1, RAF1, SRC, STK11, TGFBR1, VEGFA
GO Biological Processes	23/236	-20.31	23	protein autophosphorylation	AKT1, ALK, ATM, ATR, BTK, ACE, DYRK1A, EGFR, PTK2B, FLT3, MTOR, GSK3B, KDR, LCK, PAK1, PDGFRA, PDPK1, PIM1, SRC, AURKA, STK11, SYK, VEGFA, PARP1, BCL2L1, HIF1A, HSP90AA1, LGALS9, MAPT, MCL1, MGMT, OPRM1, PRKCD, MAPK1, MAPK7, PTPN1, TERT, TNF, NR1H2, USP1, XBP1, HDAC3, NR1H3, TLR9, ESR1, JUN, LGALS3, BIRC2, RAF1, SMAD3, PIK3CA, PRKCA, TGFBR1, DNMT1, GPER1, KMT2A, NOS1, PLK1
GO Biological Processes	24/277	-19.97	24	intracellular receptor signaling pathway	PARP1, BIRC2, XIAP, AR, CYP24A1, ESR1, ESR2, NR5A2, GPER1, NR3C1, HDAC1, PAK1, PGR, PIM1, PPARA, PPARG, PPP5C, RORA, RORC, SRC, STAT3, NR1H2, NR1I2, NR1H3, DNMT1, HDAC2, AURKA, CDK1, JUN, CYP3A4
GO Biological Processes	30/526	-19.72	30	leukocyte differentiation	PARP1, ATM, BTK, CCR1, MAPK14, PTK2B, FLT3, MTOR, GNAS, IL2, JUN, LCK, LGALS1, LGALS3, LGALS9, PIK3CD, PPARG, PRKCA, RORA, RORC, SRC, STAT3, STK11, SYK, TNF, VEGFA, XBP1, MERTK, TLR9, CCR2, AKT1, DPP4, ELANE, GSK3B, CXCL8, KDR, SMAD3, PAK1, PDPK1, PIK3CA, PIK3CB, PIK3CG, PLG, PPARA, PRKCD, MAPK7, PTAFR, CHRNA4, PRKCB, CNR1, GPER1, PDGFRA, PLA2G2A, NR1H3, DRD2, NR1H2, ACE, MAPK1

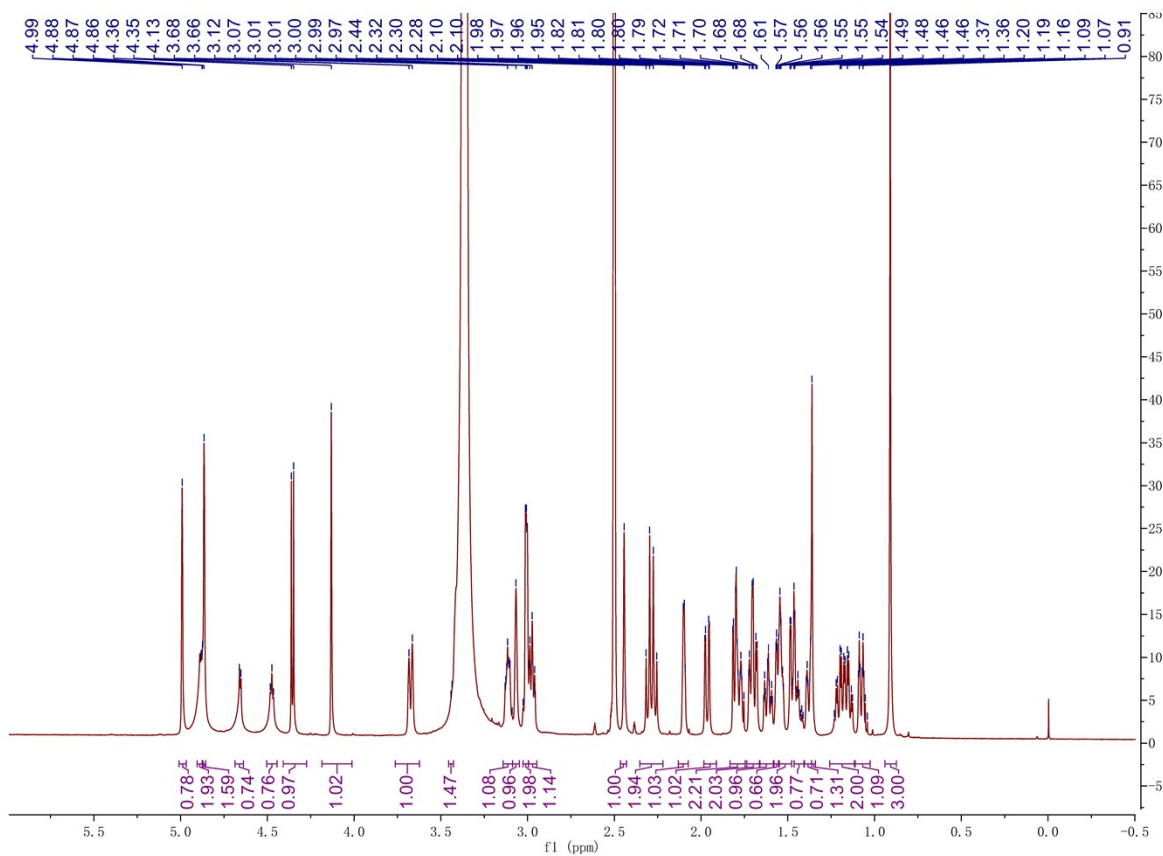


Figure S1 The ^1H NMR spectrum of compound **1** in DMSO-d_6 (500 MHz)

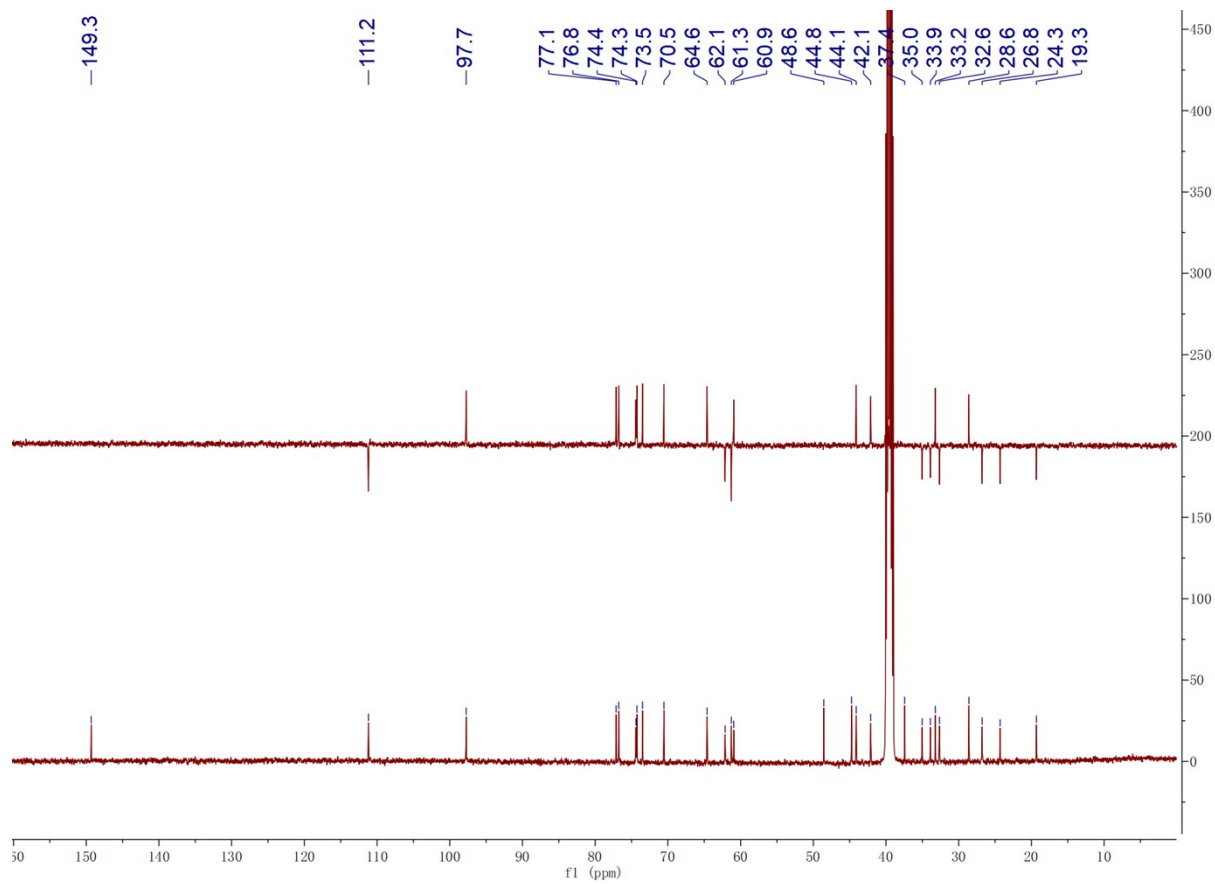


Figure S2 The ^{13}C NMR spectrum of compound **1** in DMSO-d_6 (125 MHz)

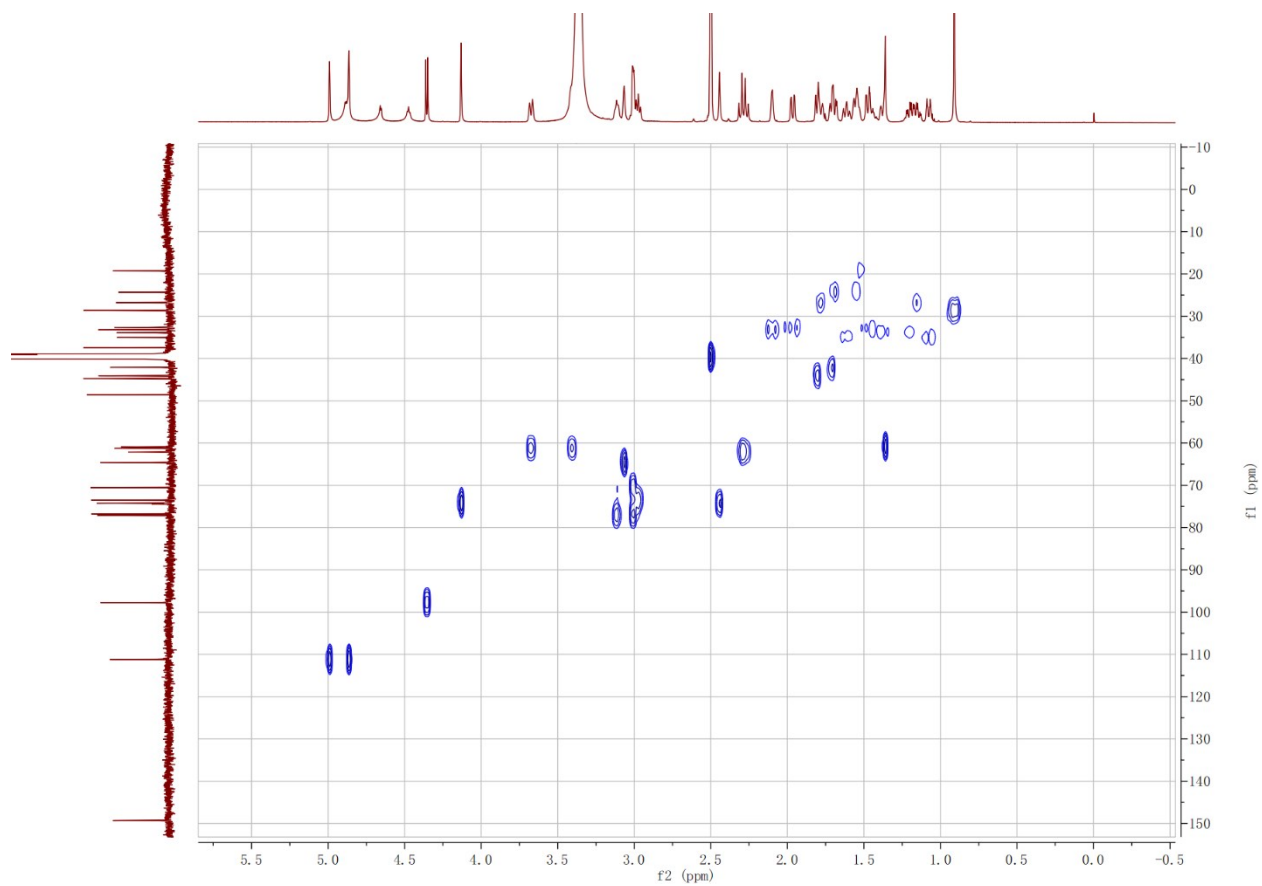


Figure S3 The HSQC spectrum of compound **1** in DMSO-d_6

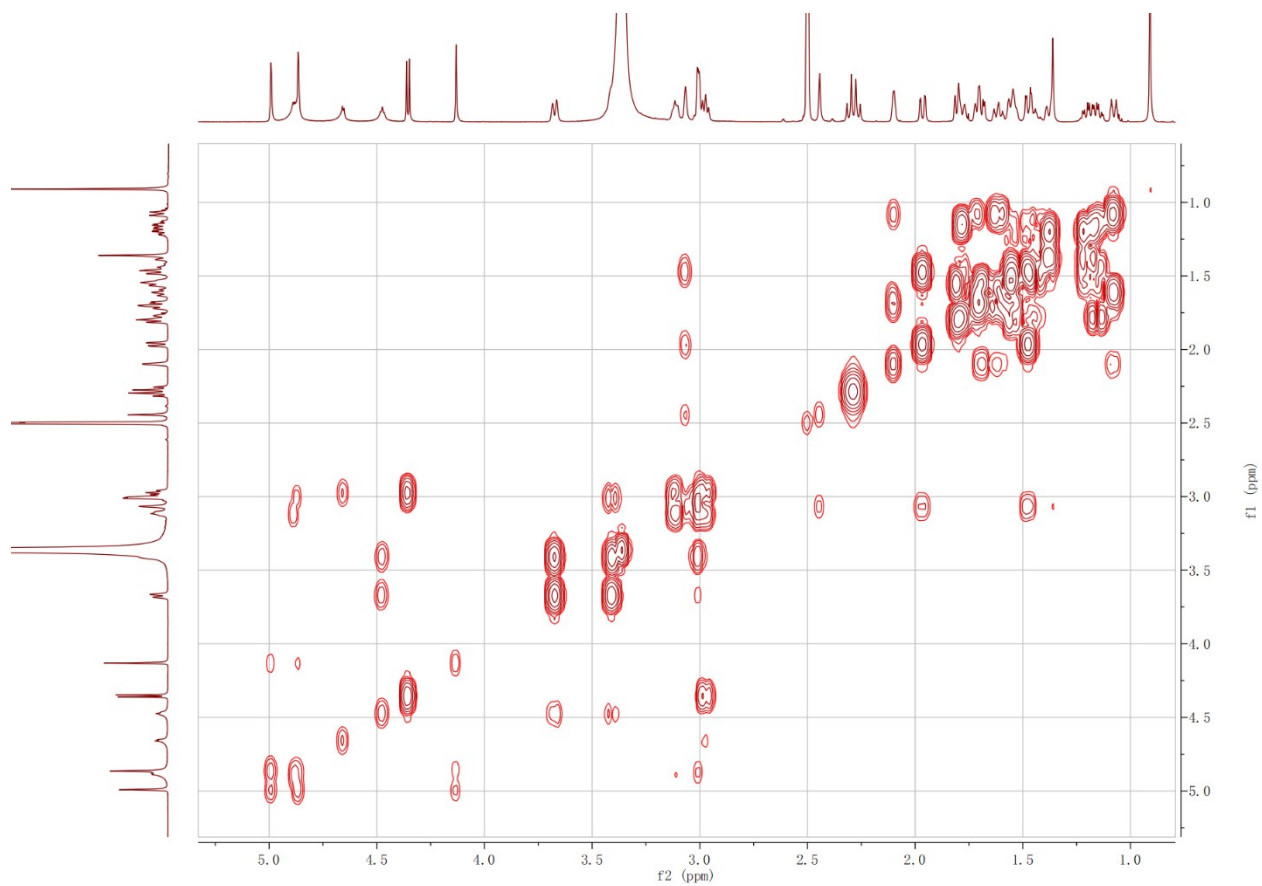


Figure S4 The ^1H - ^1H COSY spectrum of compound **1** in DMSO-d_6

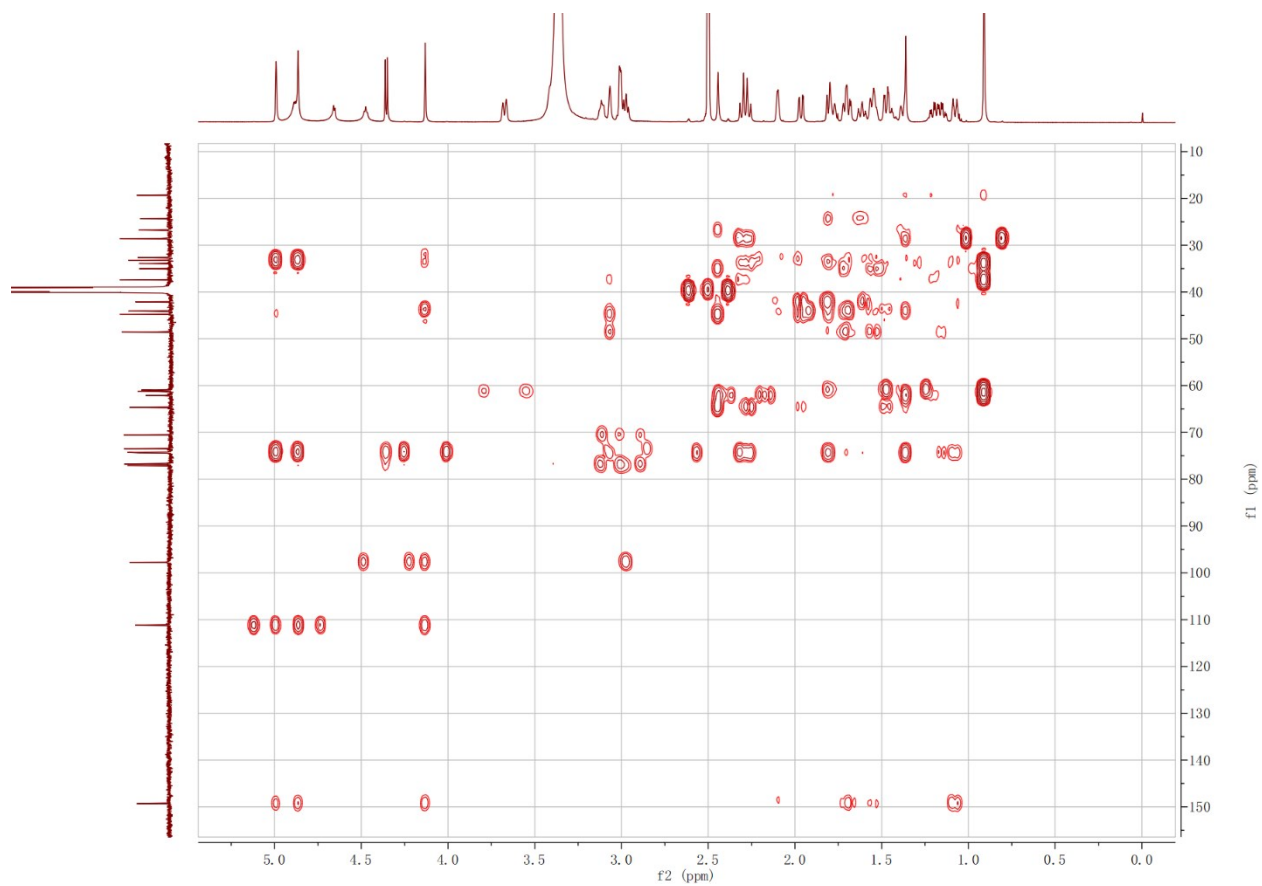


Figure S5 The HMBC spectrum of compound **1** in DMSO-d₆

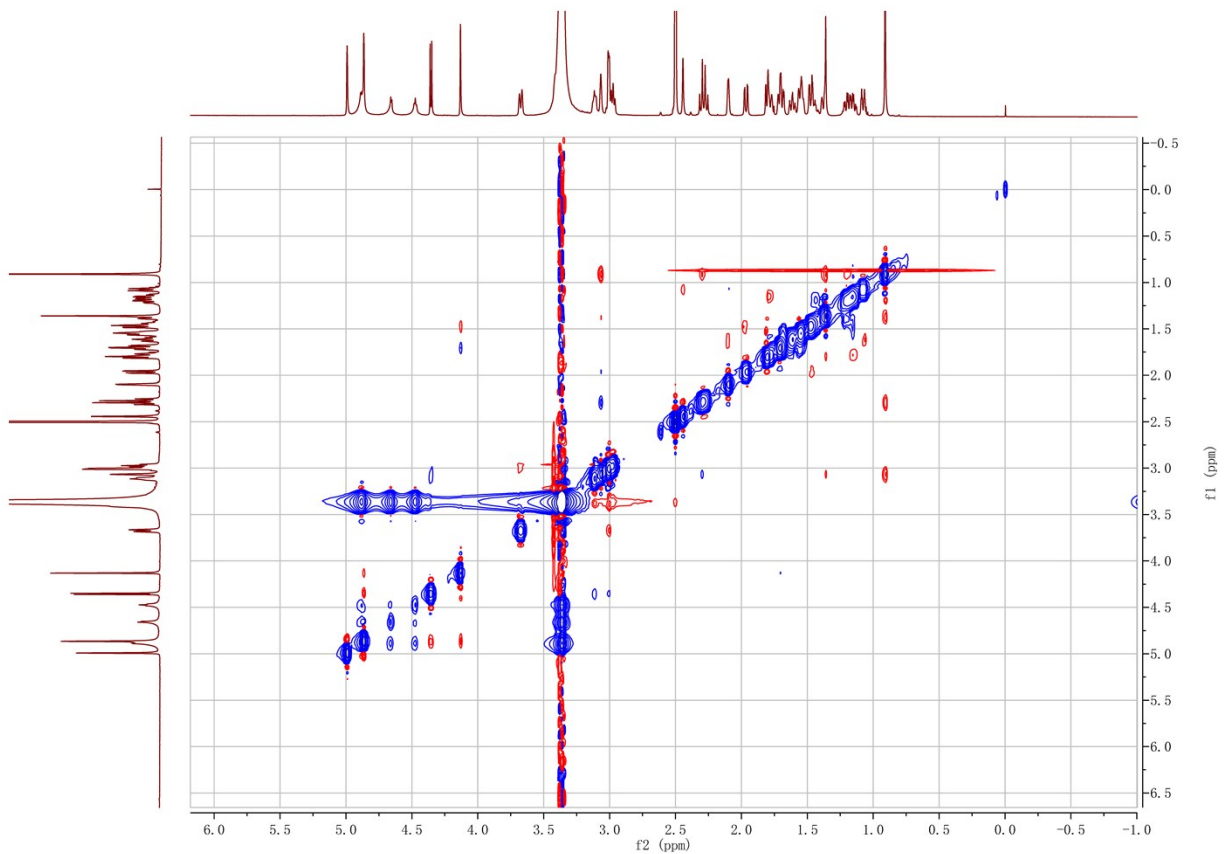


Figure S6 The NOESY spectrum of compound **1** in DMSO-d₆

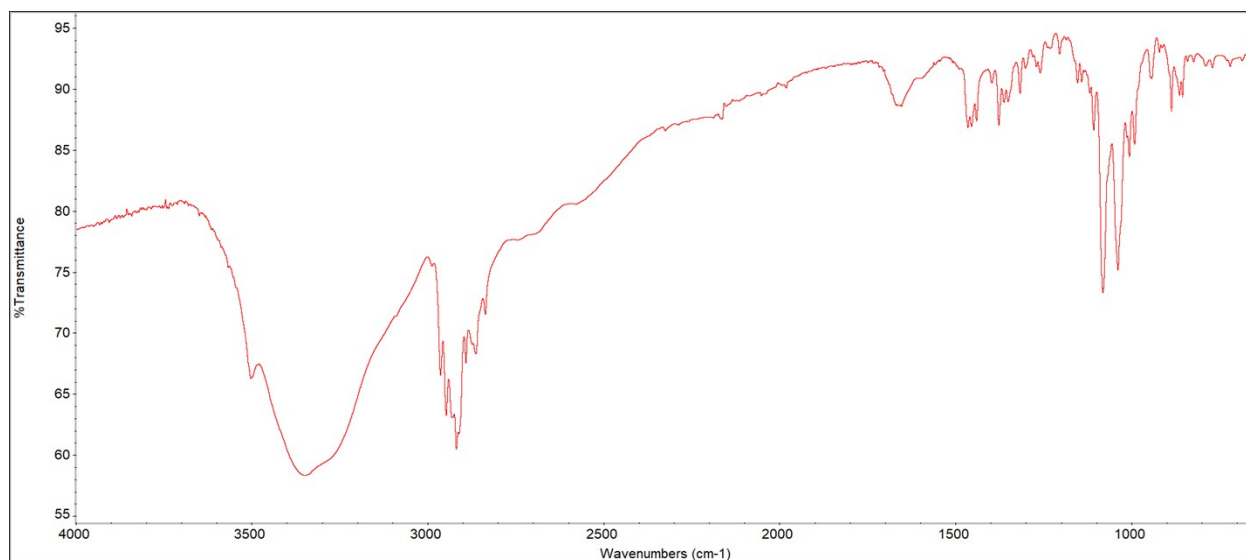


Figure S7 The IR spectrum of compound 1

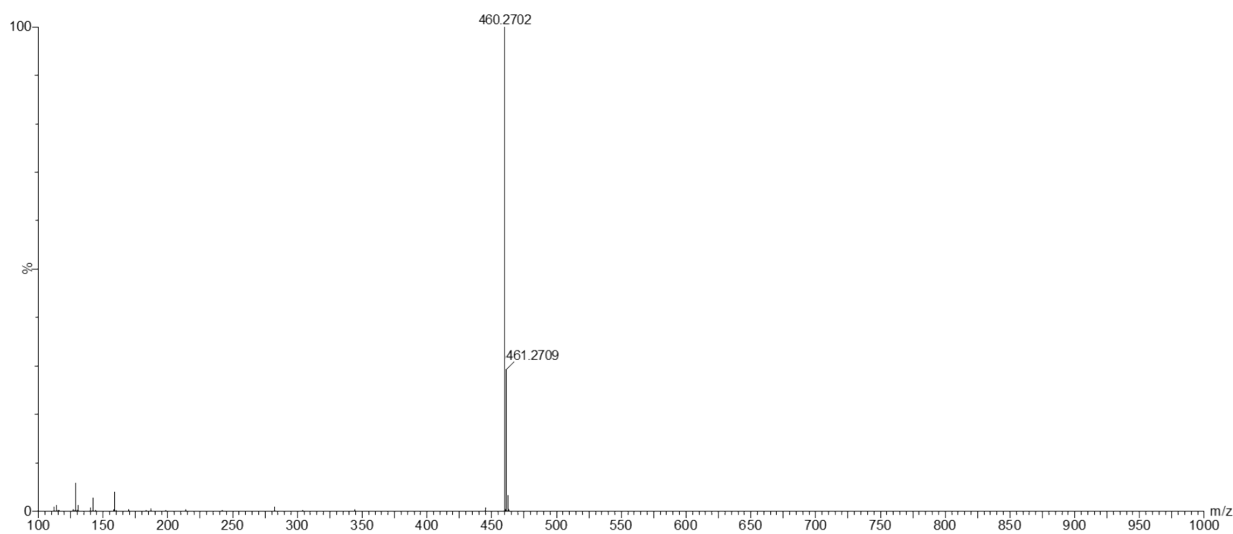
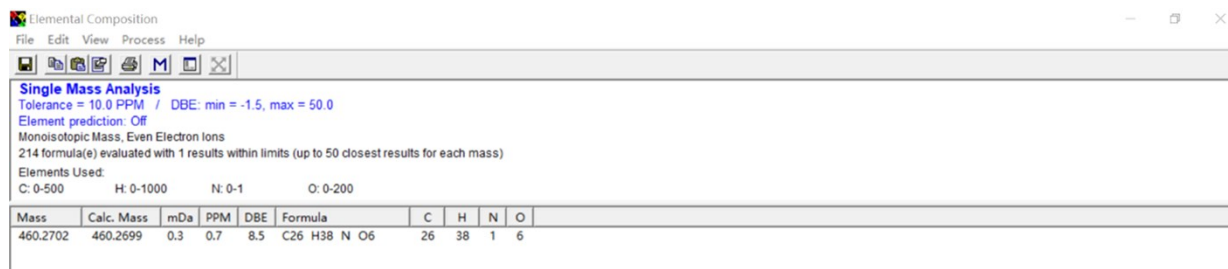


Figure S8 The HR-ESI-MS data of compound 1

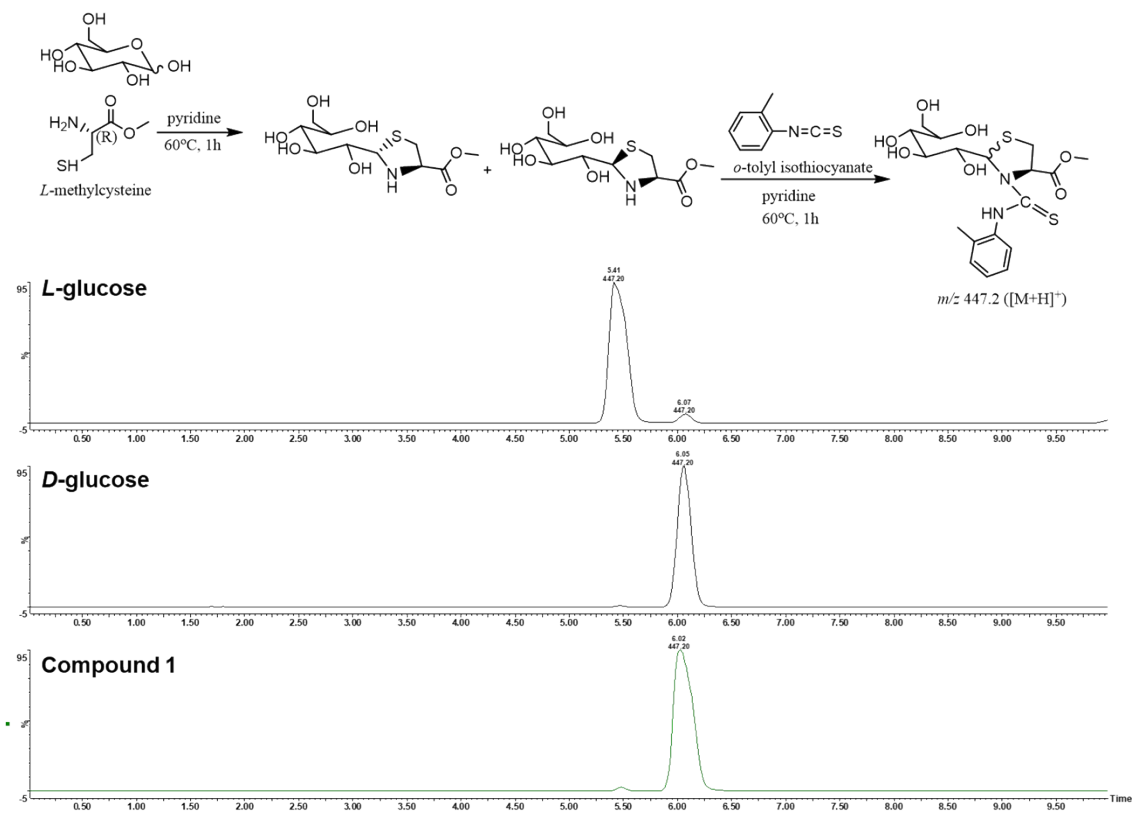


Figure S9 The UHPLC-MS single ion recording (SIR) chromatograms of m/z 447.2 for sugar configuration confirmation of compound **1**

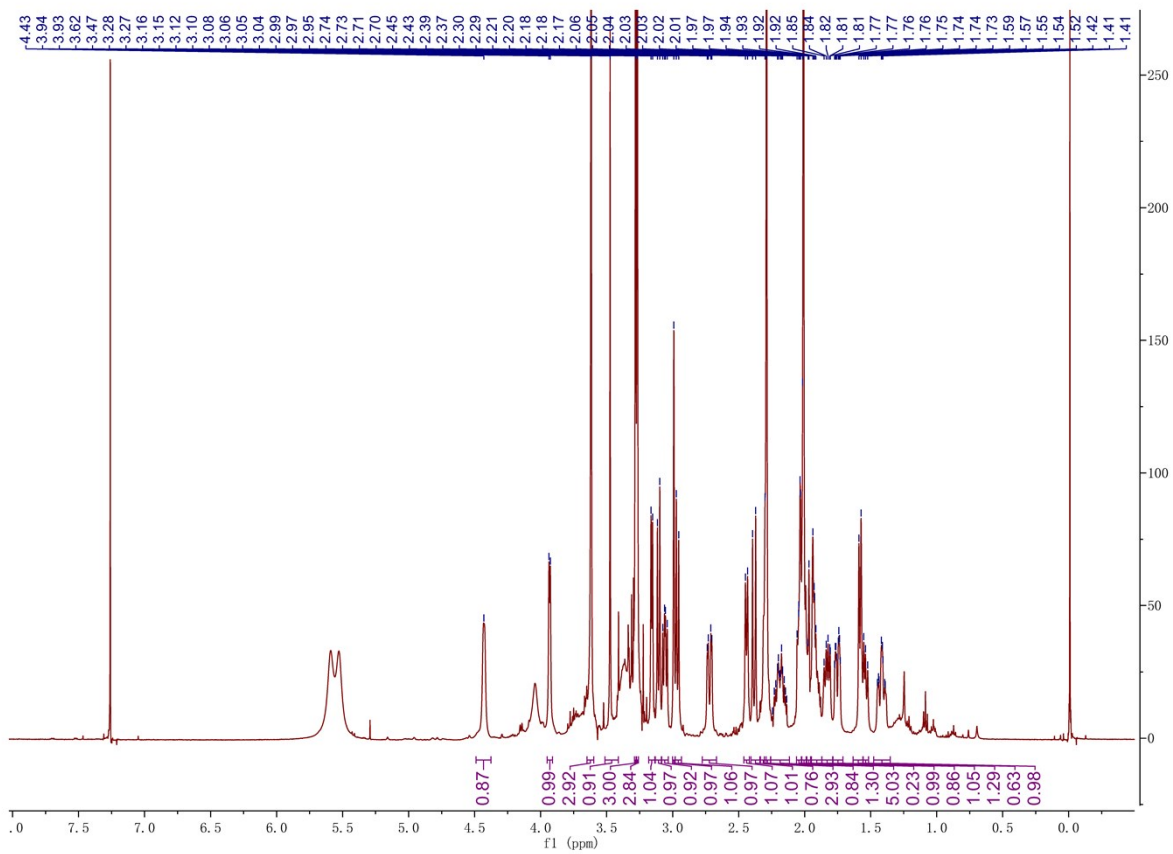


Figure S10 The ^1H NMR spectrum of compound **14a** in CDCl_3 (500 MHz)

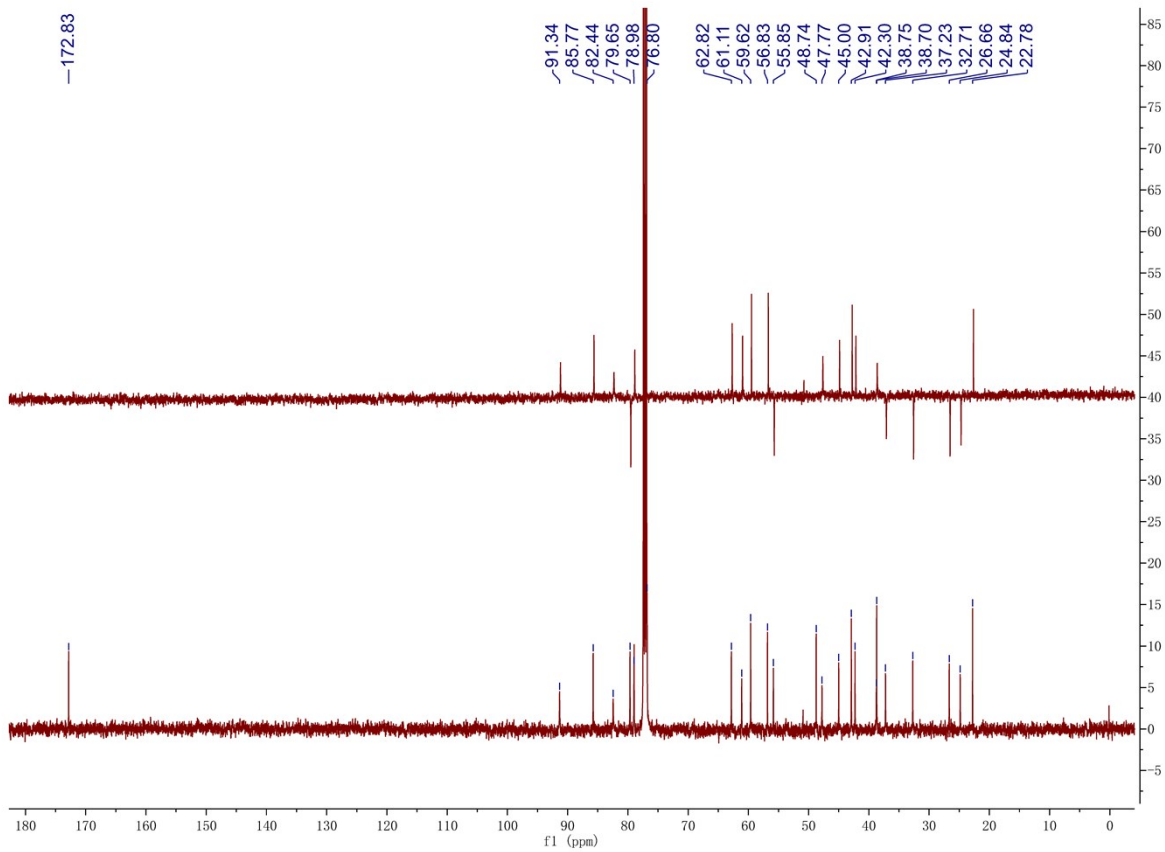


Figure S11 The ^{13}C NMR spectrum of compound **14a** in CDCl_3 (125 MHz)

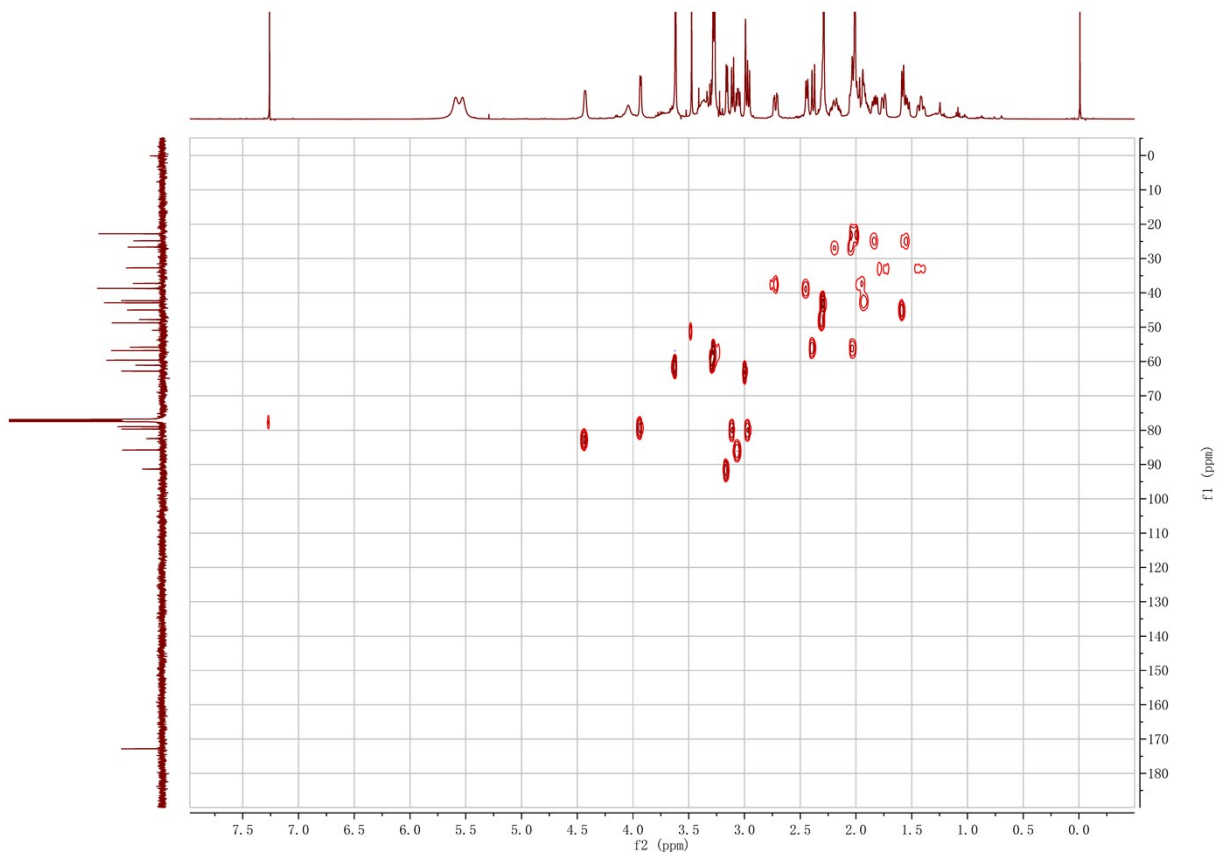


Figure S12 The HSQC spectrum of compound **14a** in CDCl_3

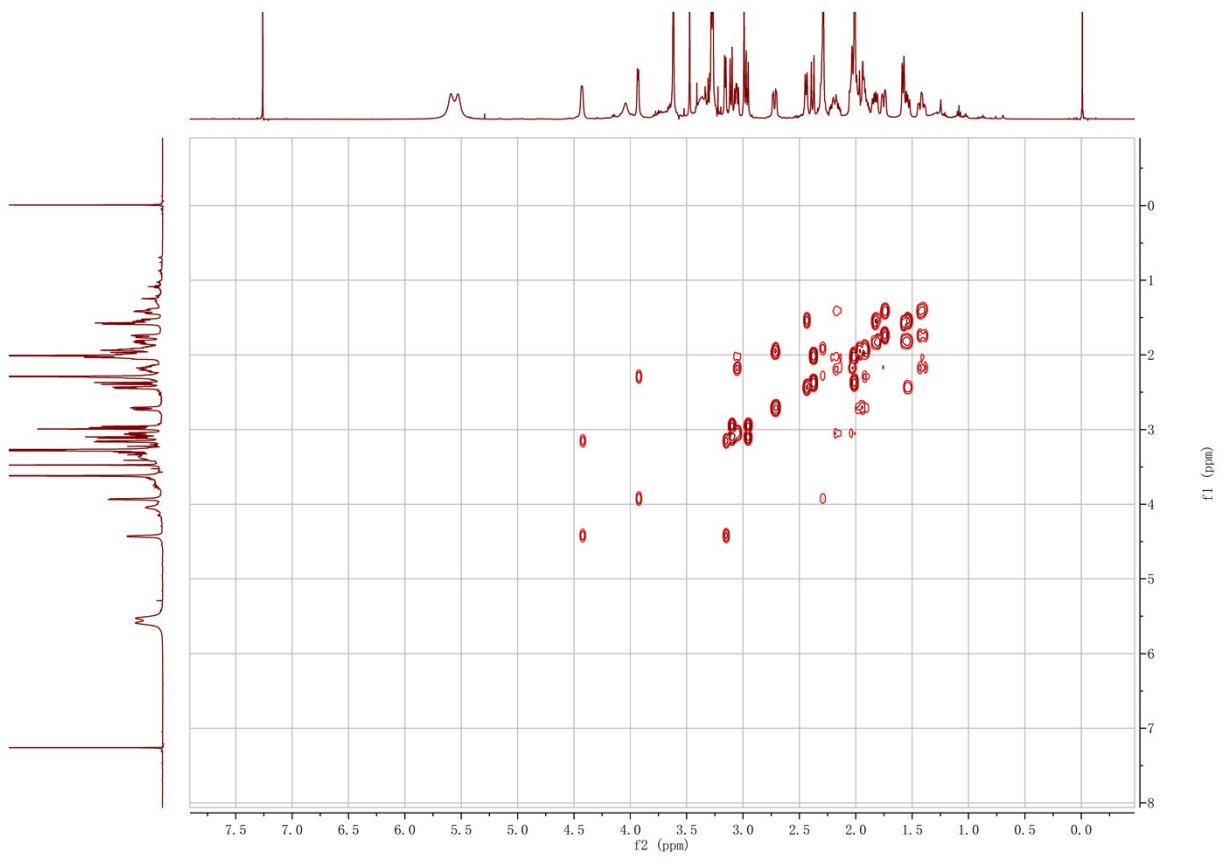


Figure S13 The ^1H - ^1H COSY spectrum of compound **14a** in CDCl_3

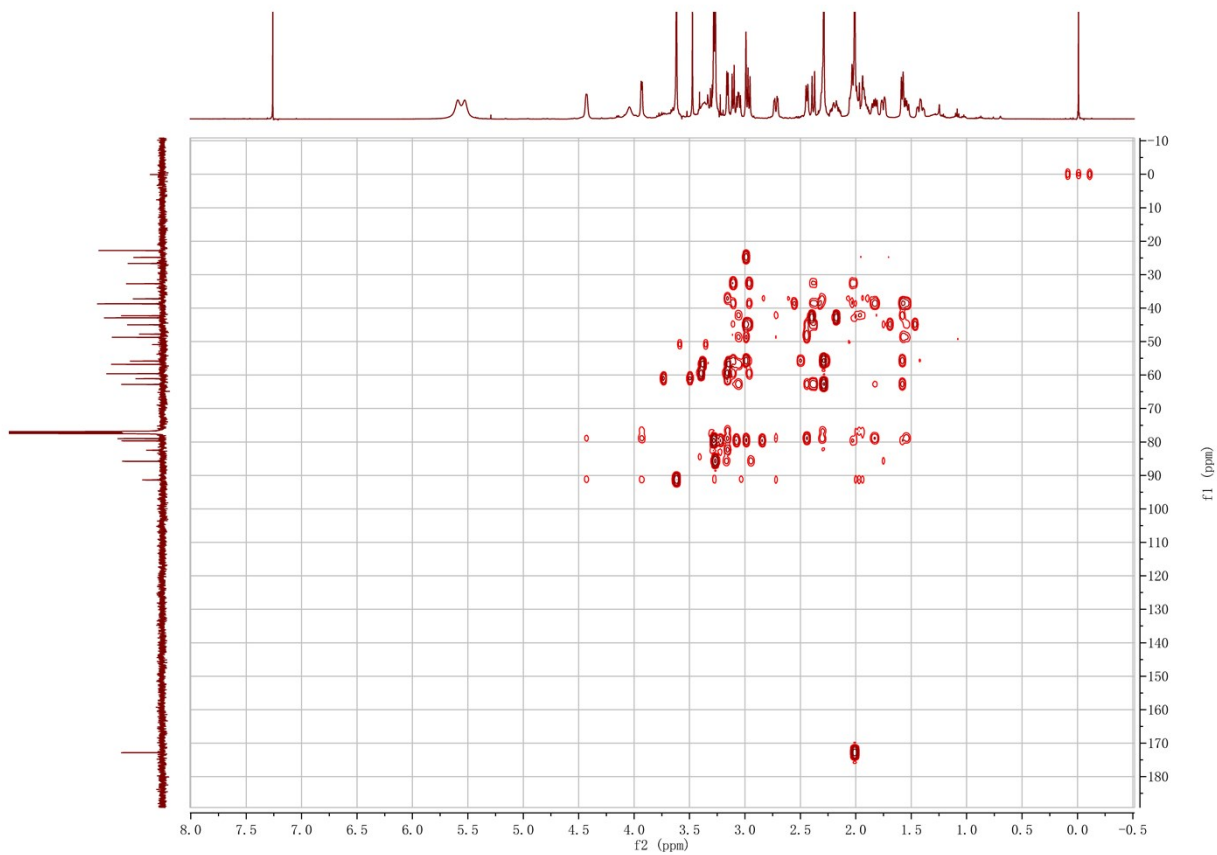


Figure S14 The HMBC spectrum of compound **14a** in CDCl_3

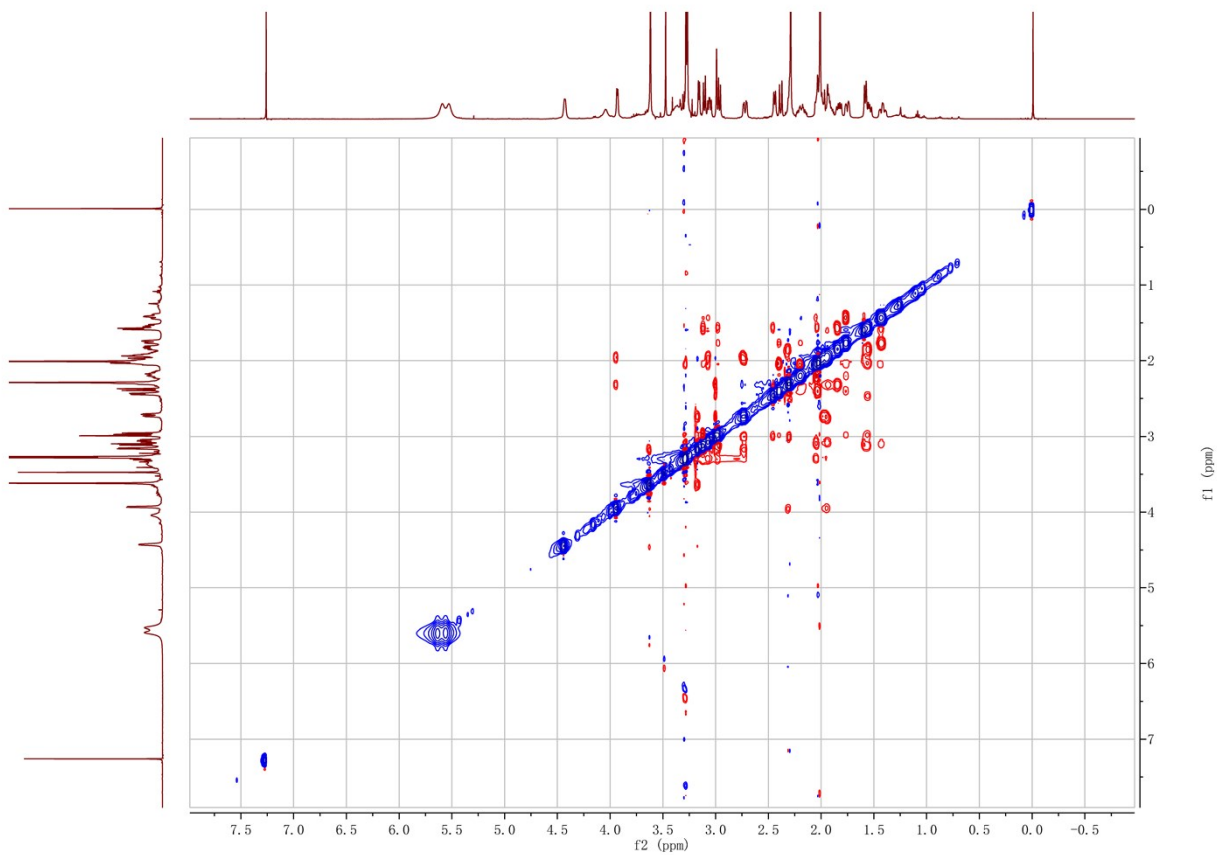


Figure S15 The NOESY spectrum of compound **14a** in CDCl₃

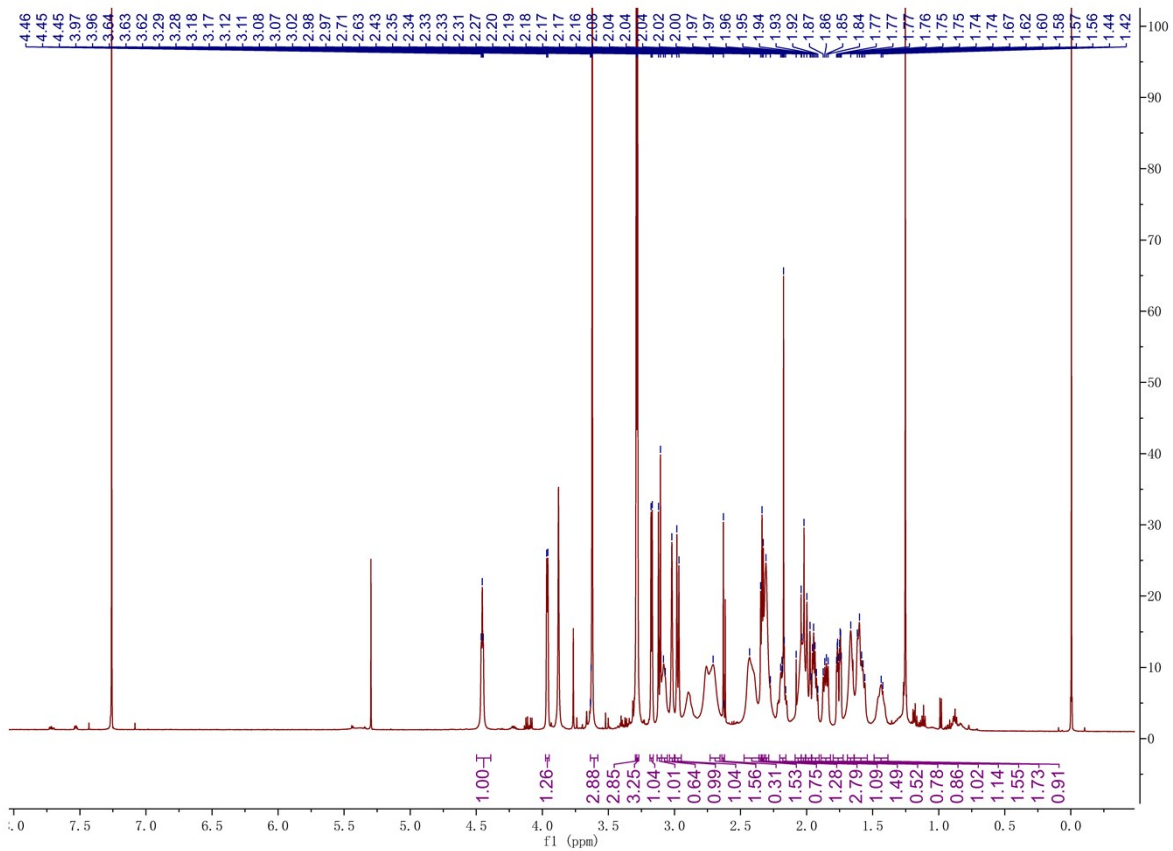


Figure S16 The ¹H NMR spectrum of compound **14** in CDCl₃ (600 MHz)

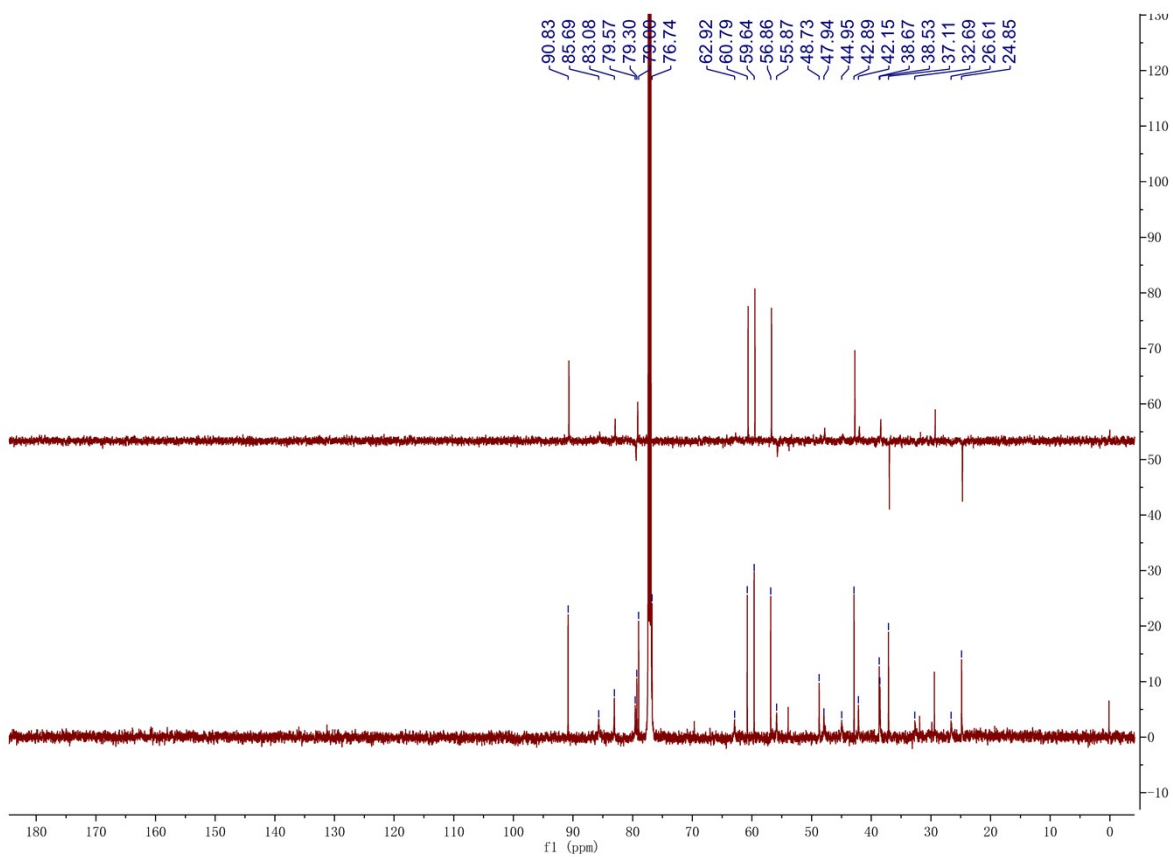


Figure S17 The ^{13}C NMR spectrum of compound **14** in CDCl_3 (150 MHz)

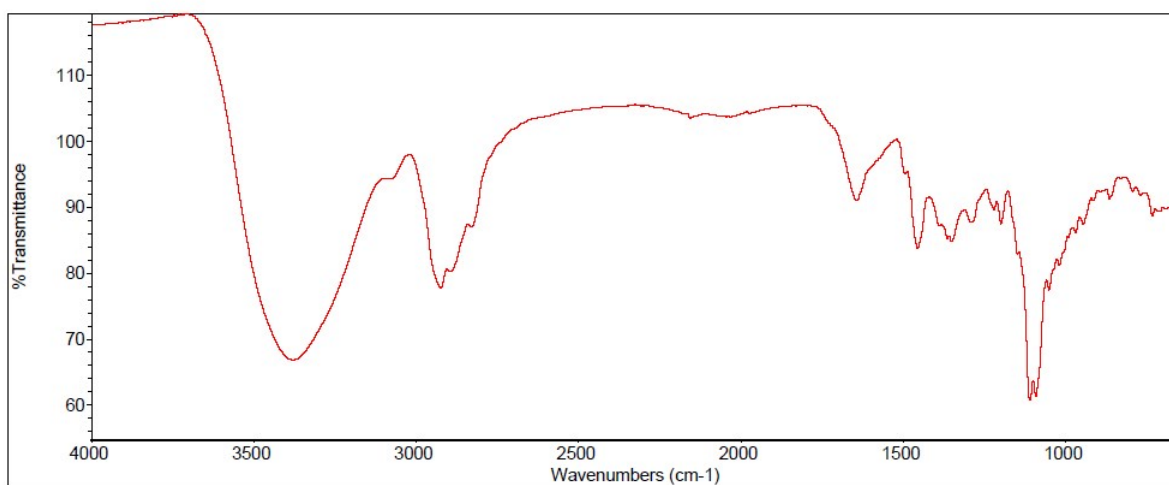


Figure S18 The IR spectrum of compound **14**

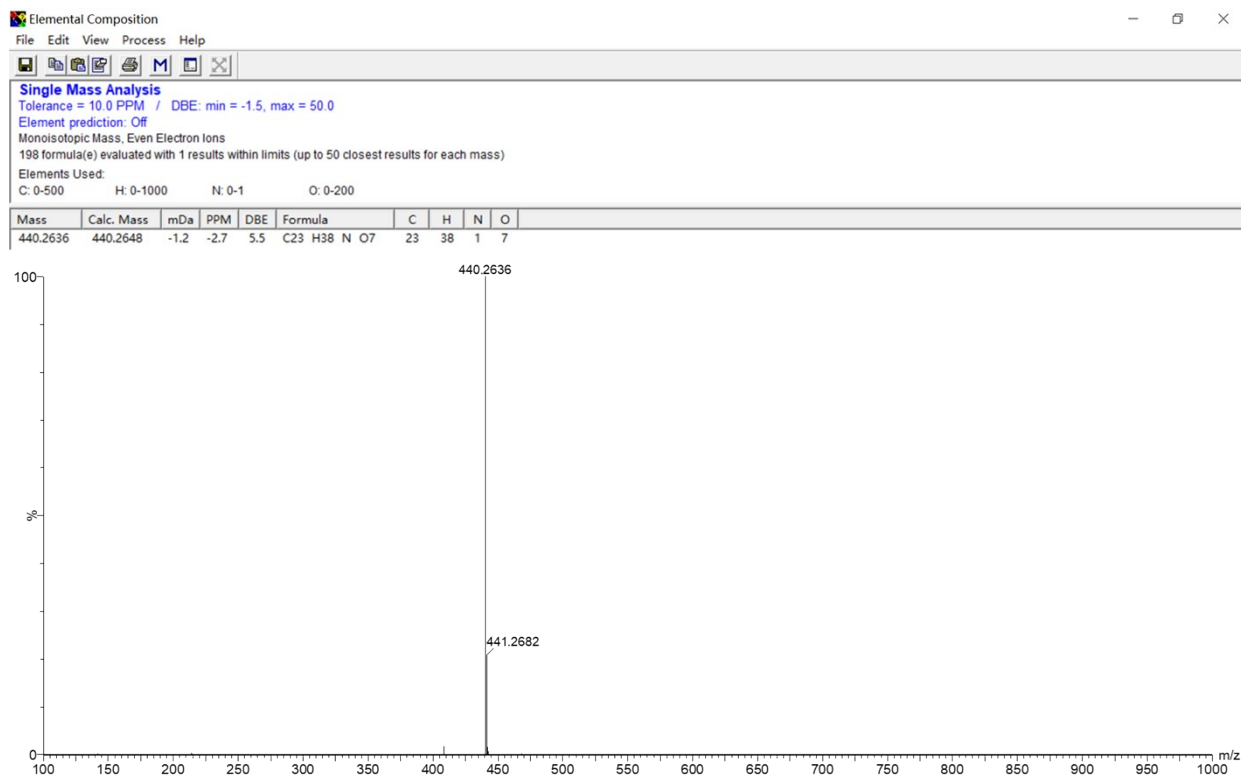


Figure S19 The HR-ESI-MS data of compound 14a

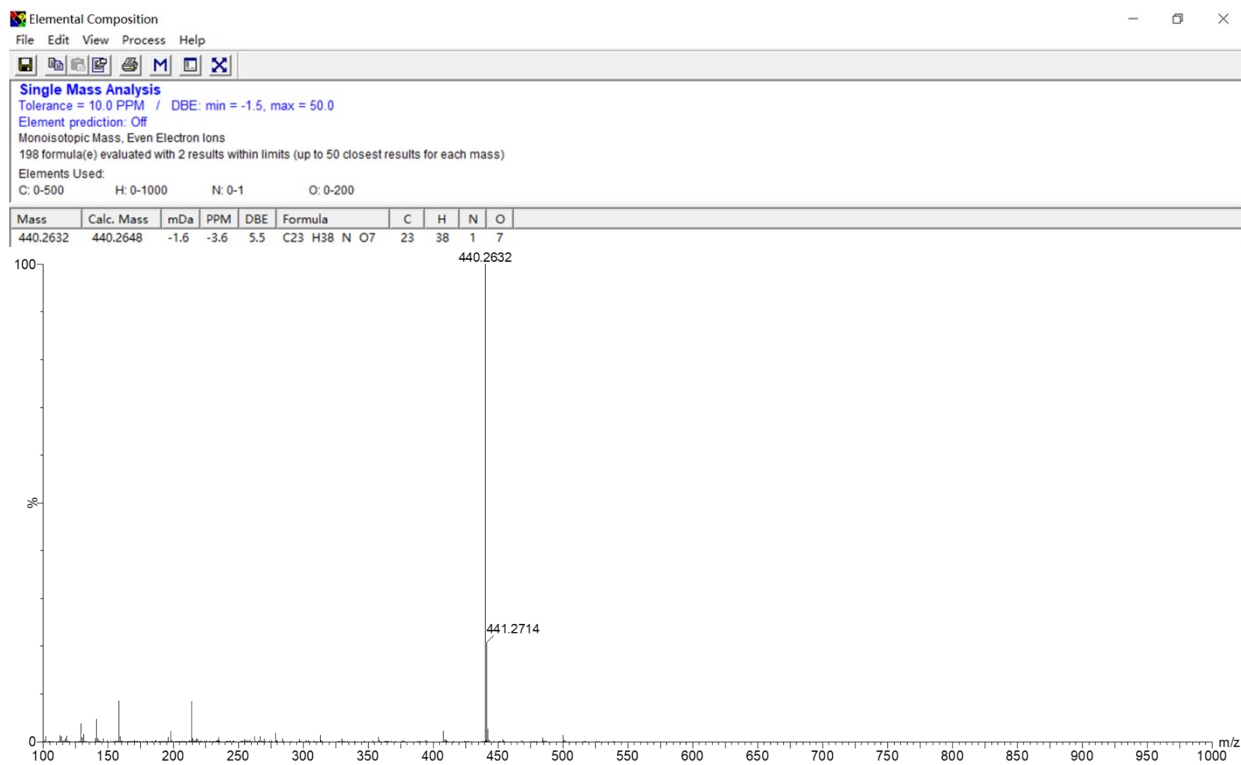


Figure S20 The HR-ESI-MS data of compound 14

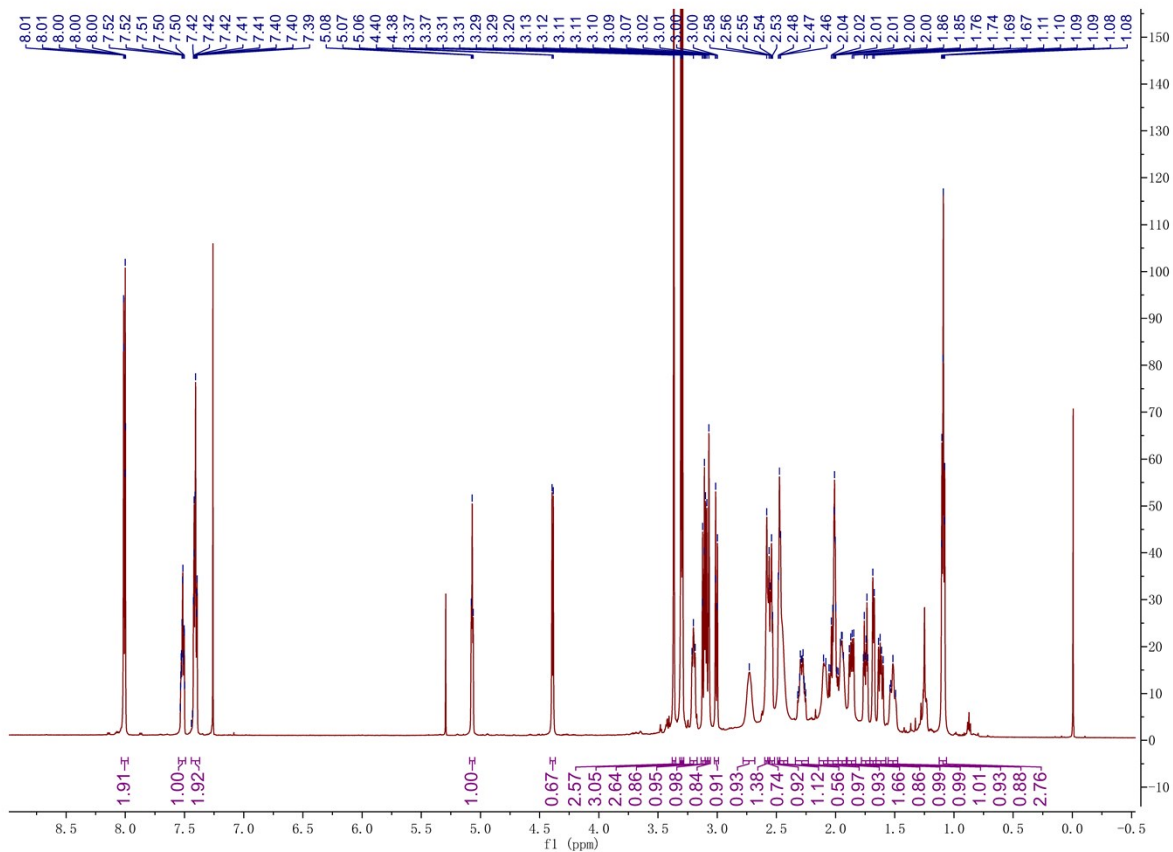


Figure S21 The ^1H NMR spectrum of compound **17** in CDCl_3 (600 MHz)

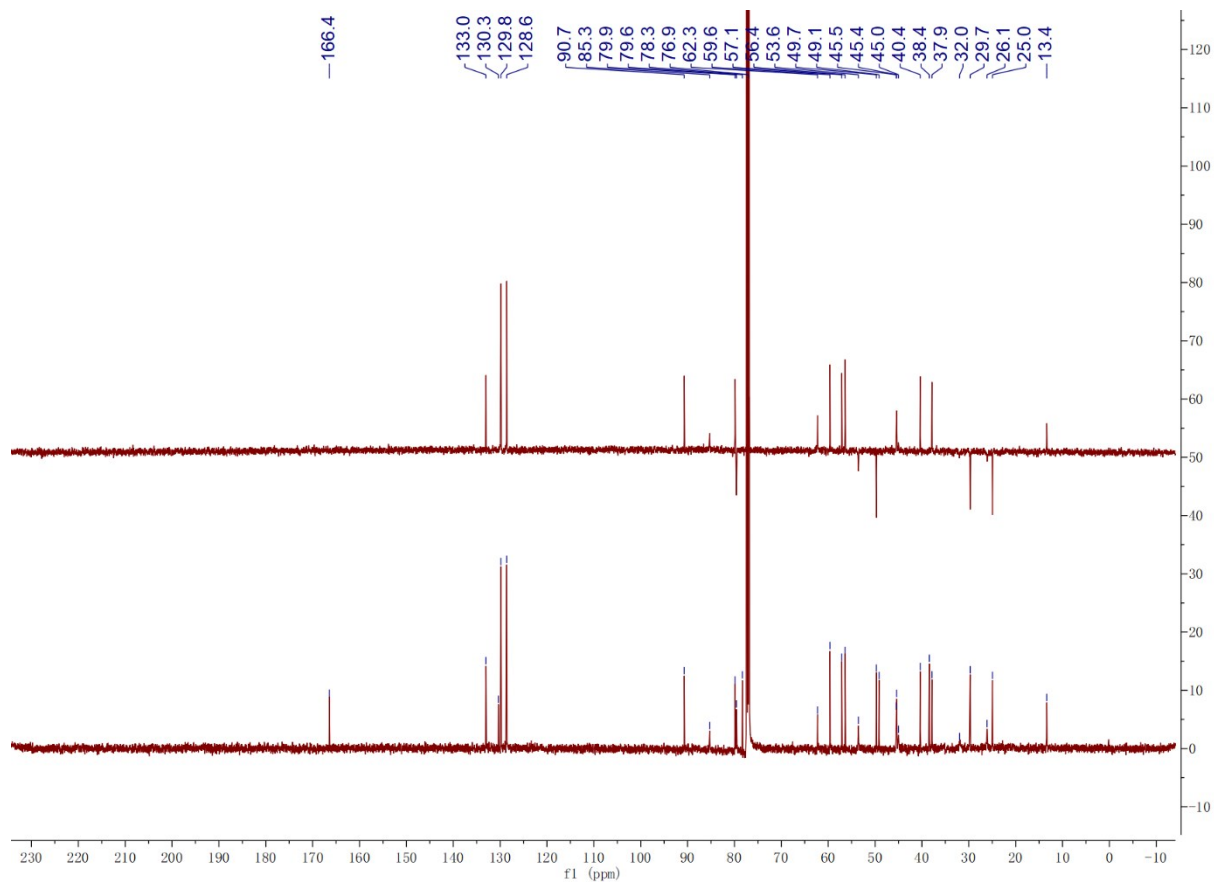


Figure S22 The ^{13}C NMR spectrum of compound **17** in CDCl_3 (150 MHz)

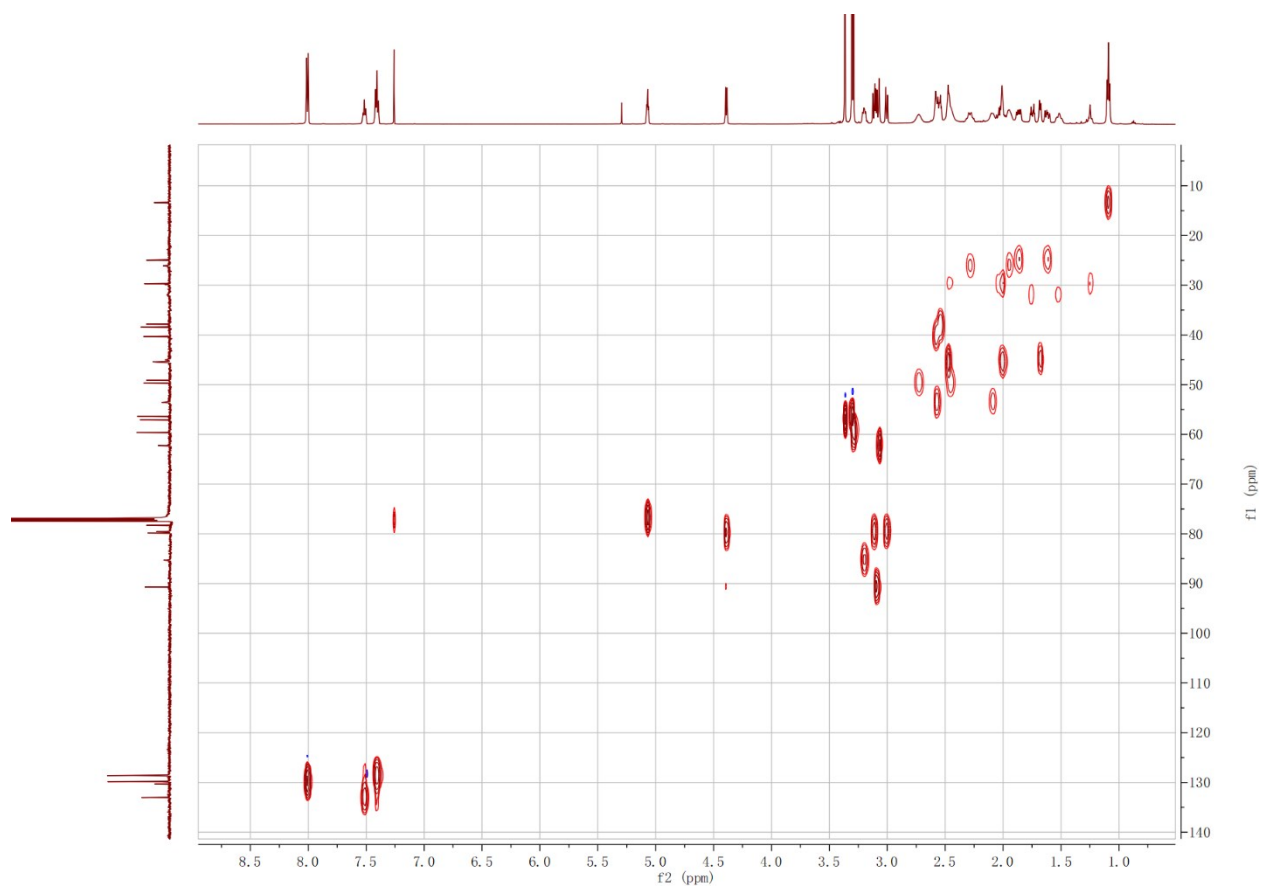


Figure S23 The HSQC spectrum of compound **17** in CDCl_3

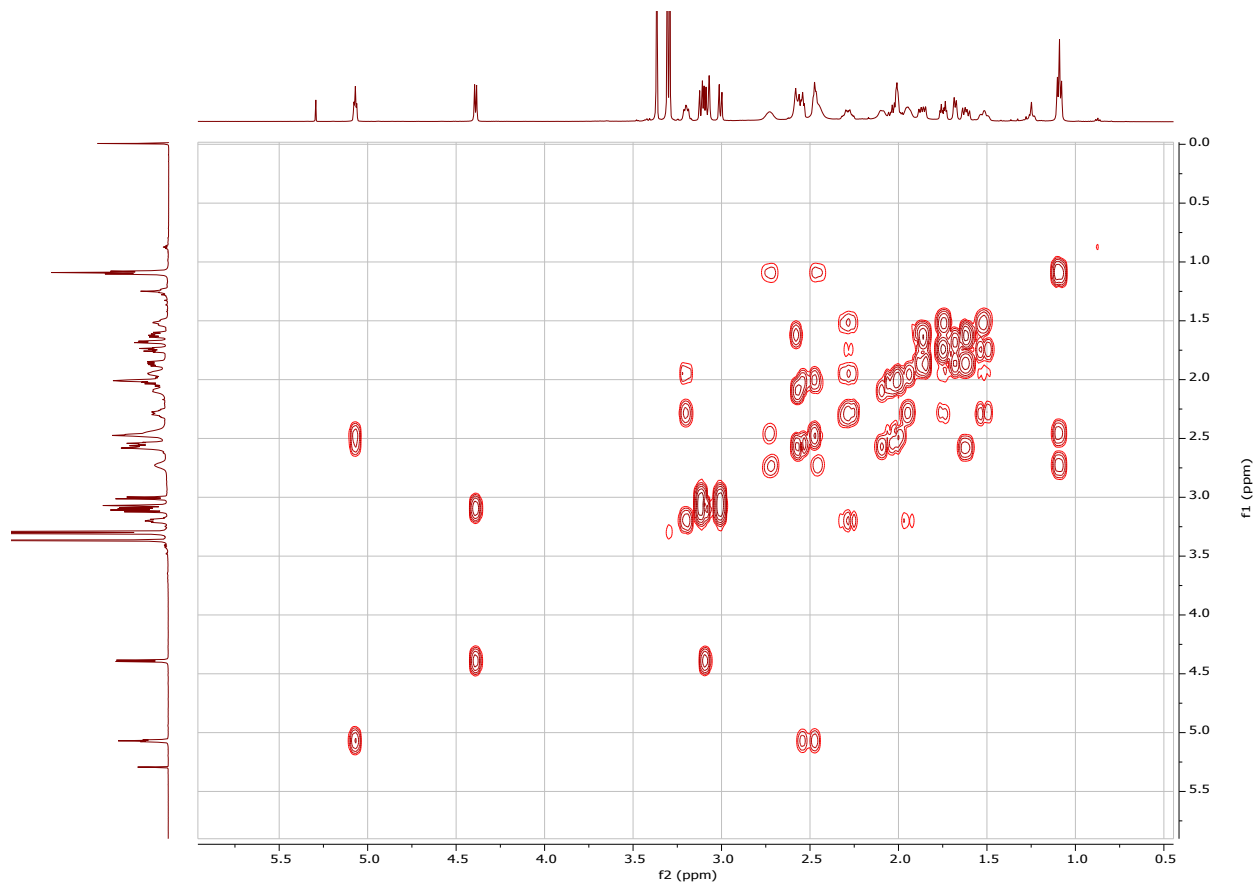


Figure S24 The ^1H - ^1H COSY spectrum of compound **17** in CDCl_3

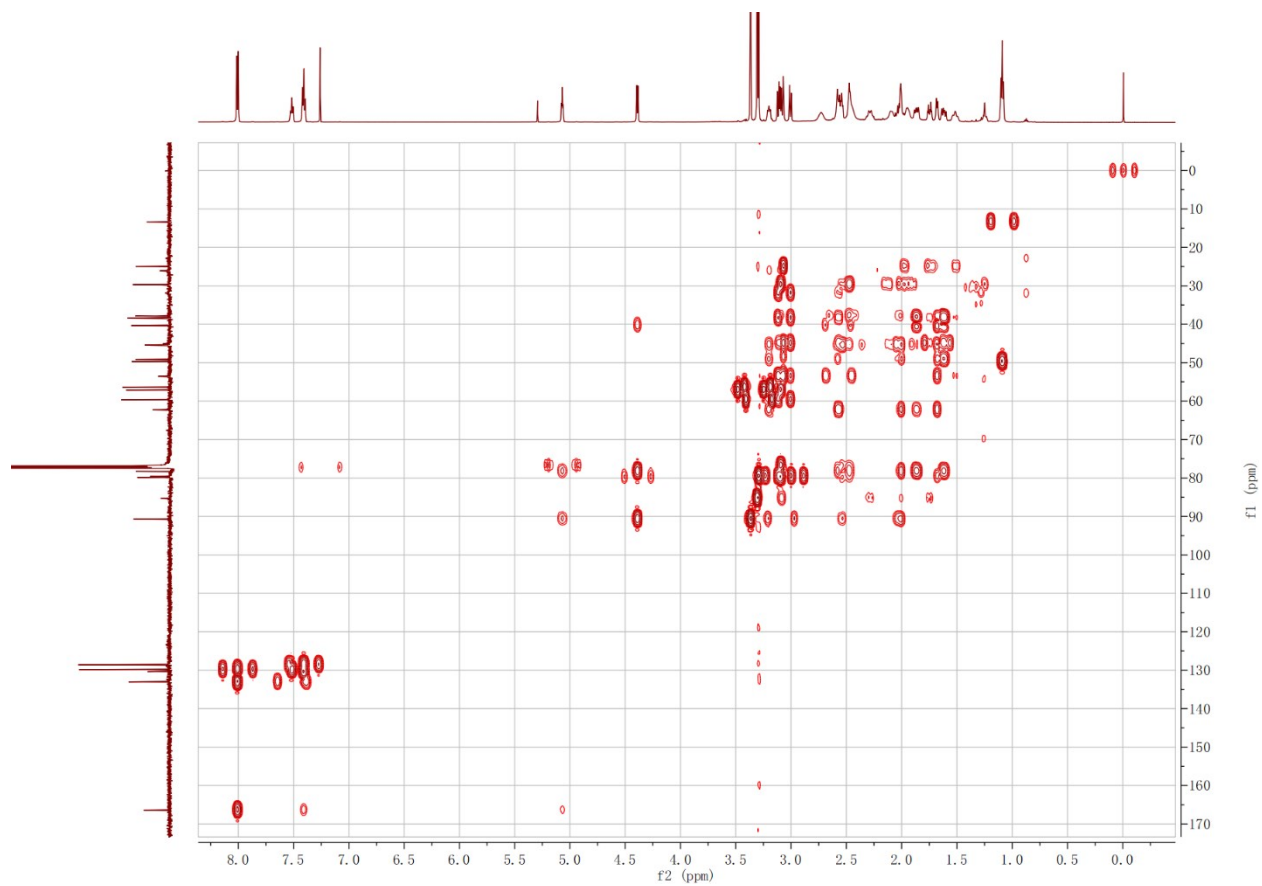


Figure S25 The HMBC spectrum of compound **17** in CDCl₃

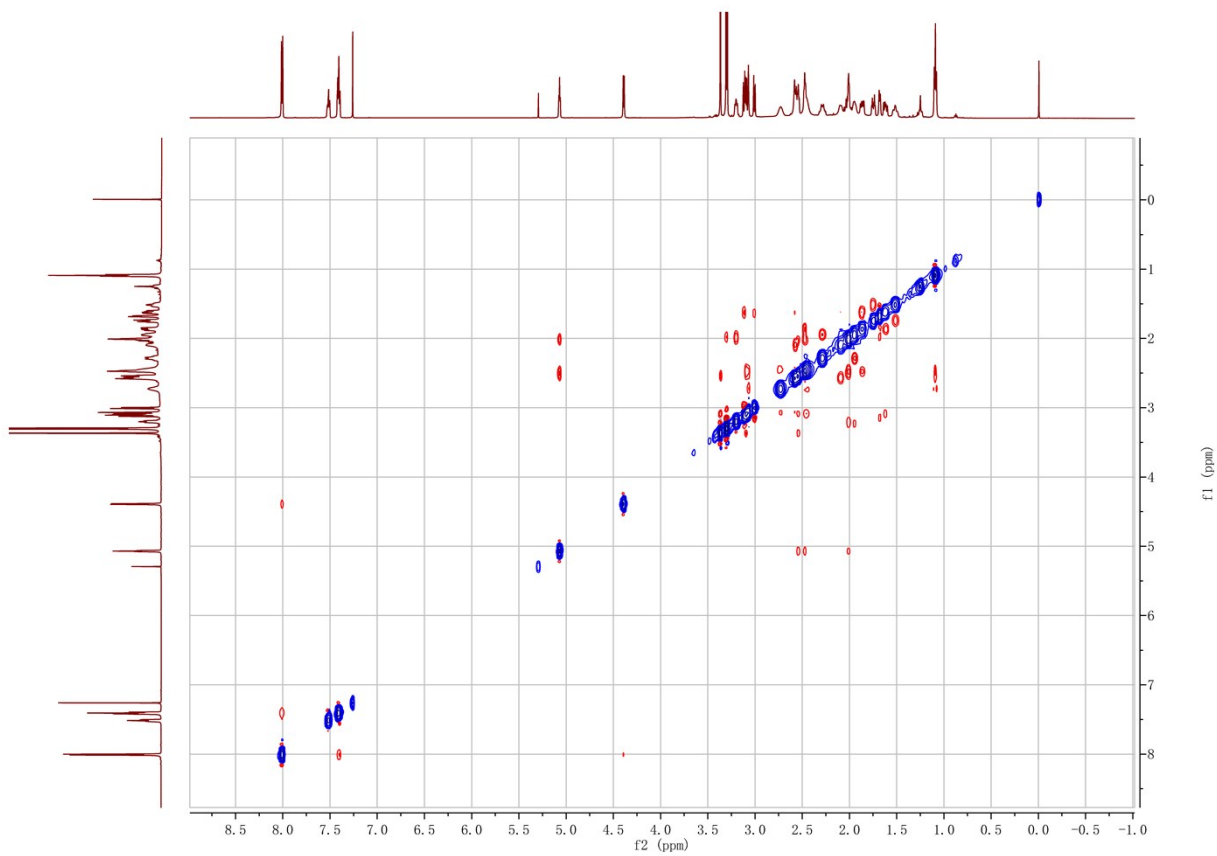


Figure S26 The NOESY spectrum of compound **17** in CDCl₃

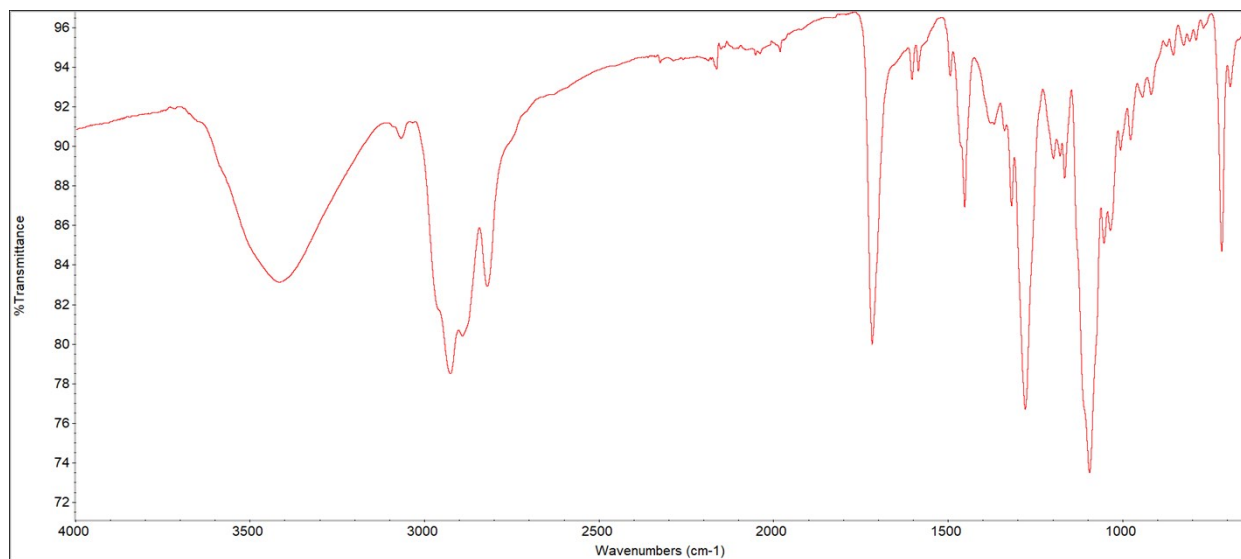


Figure S27 The IR spectrum of compound **17**

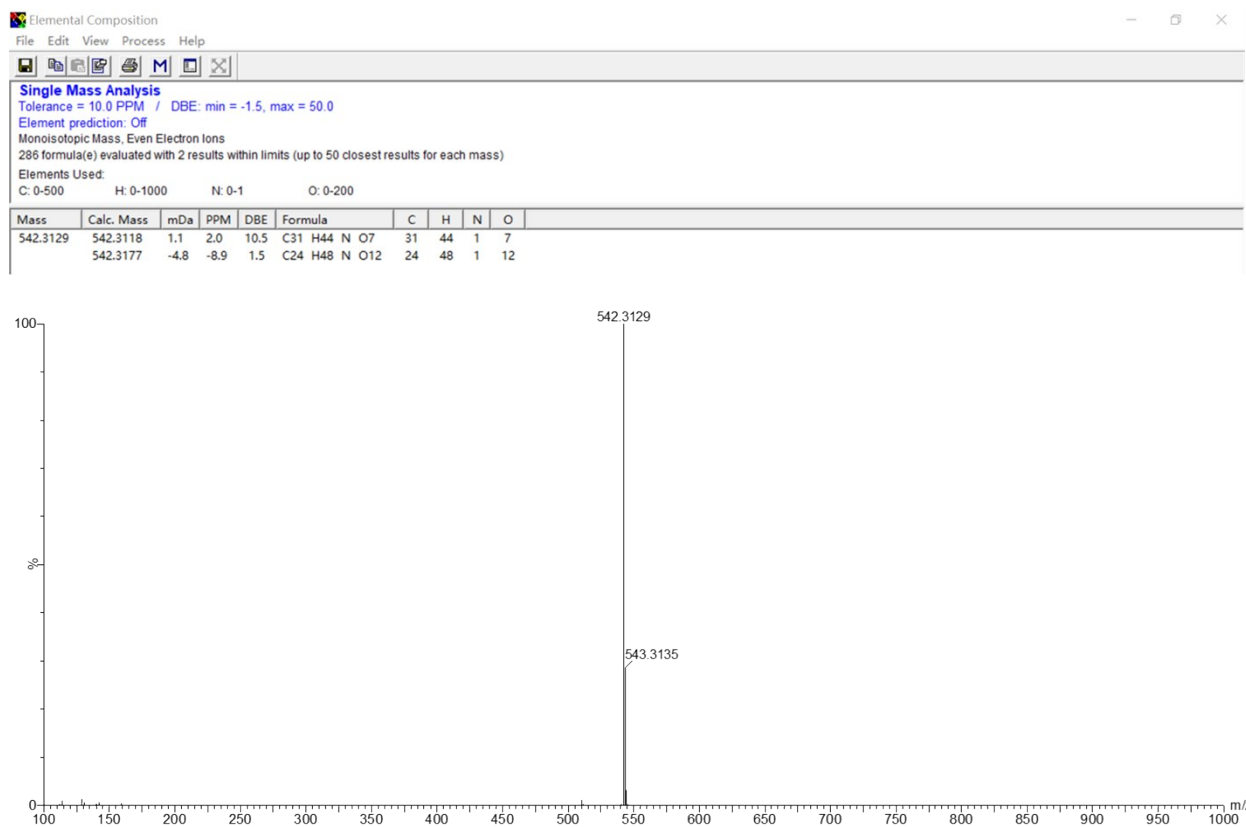


Figure S28 The HR-ESI-MS data of compound **17**

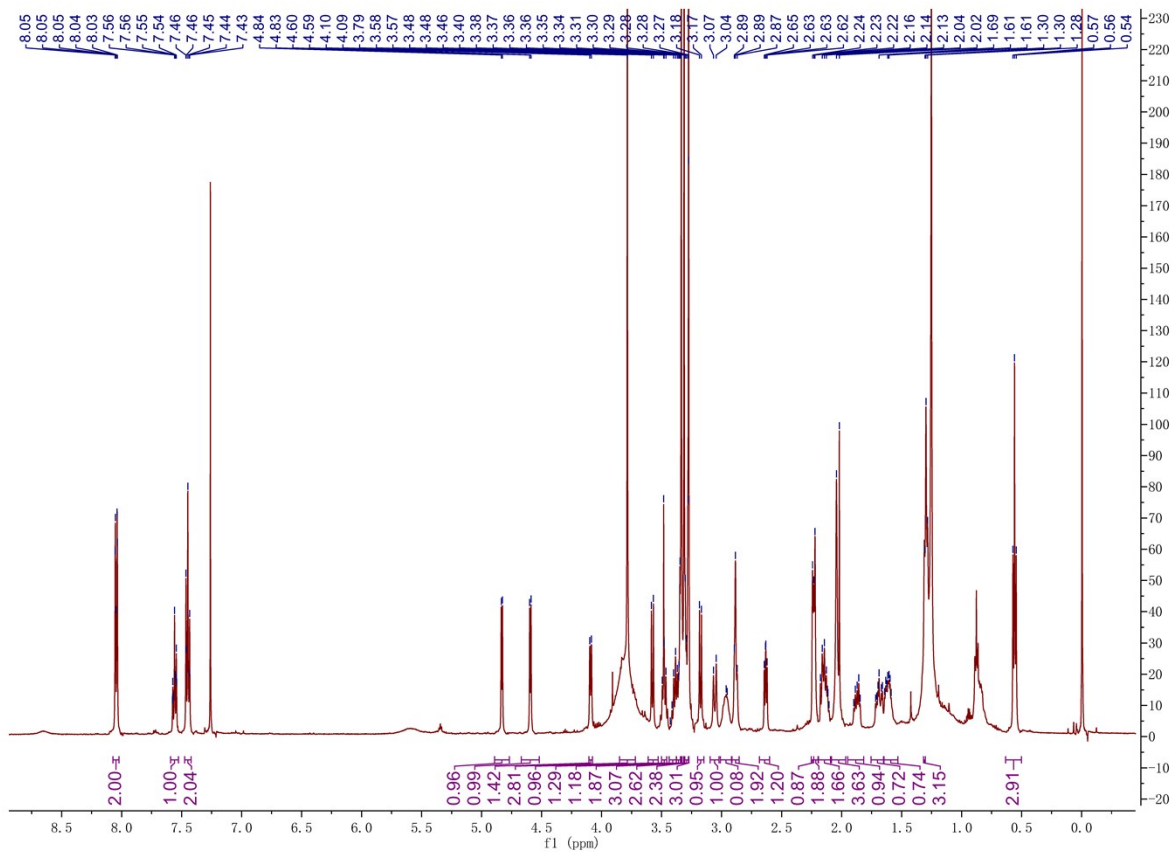


Figure S29 The ^1H NMR spectrum of compound **25** in CDCl_3 (500 MHz)

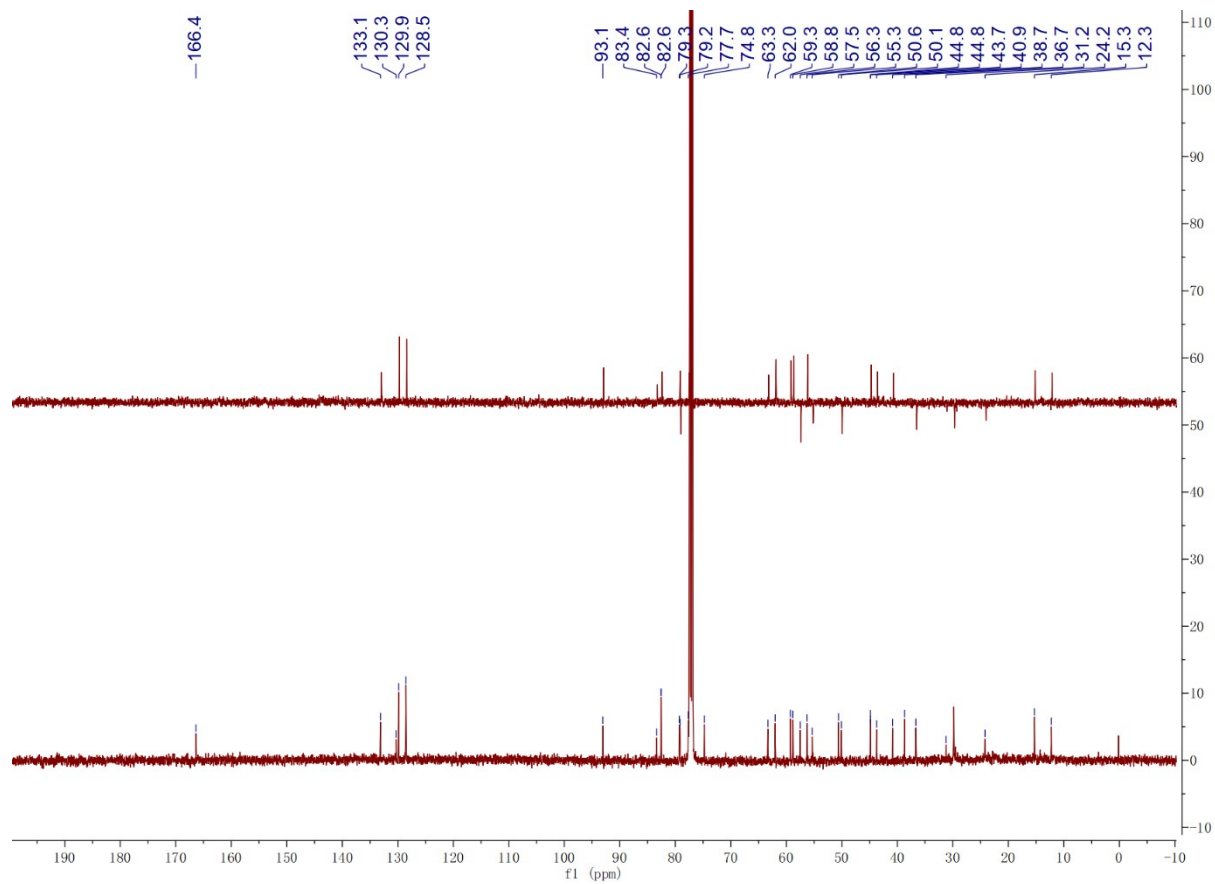


Figure S30 The ^{13}C NMR spectrum of compound **25** in CDCl_3 (125 MHz)

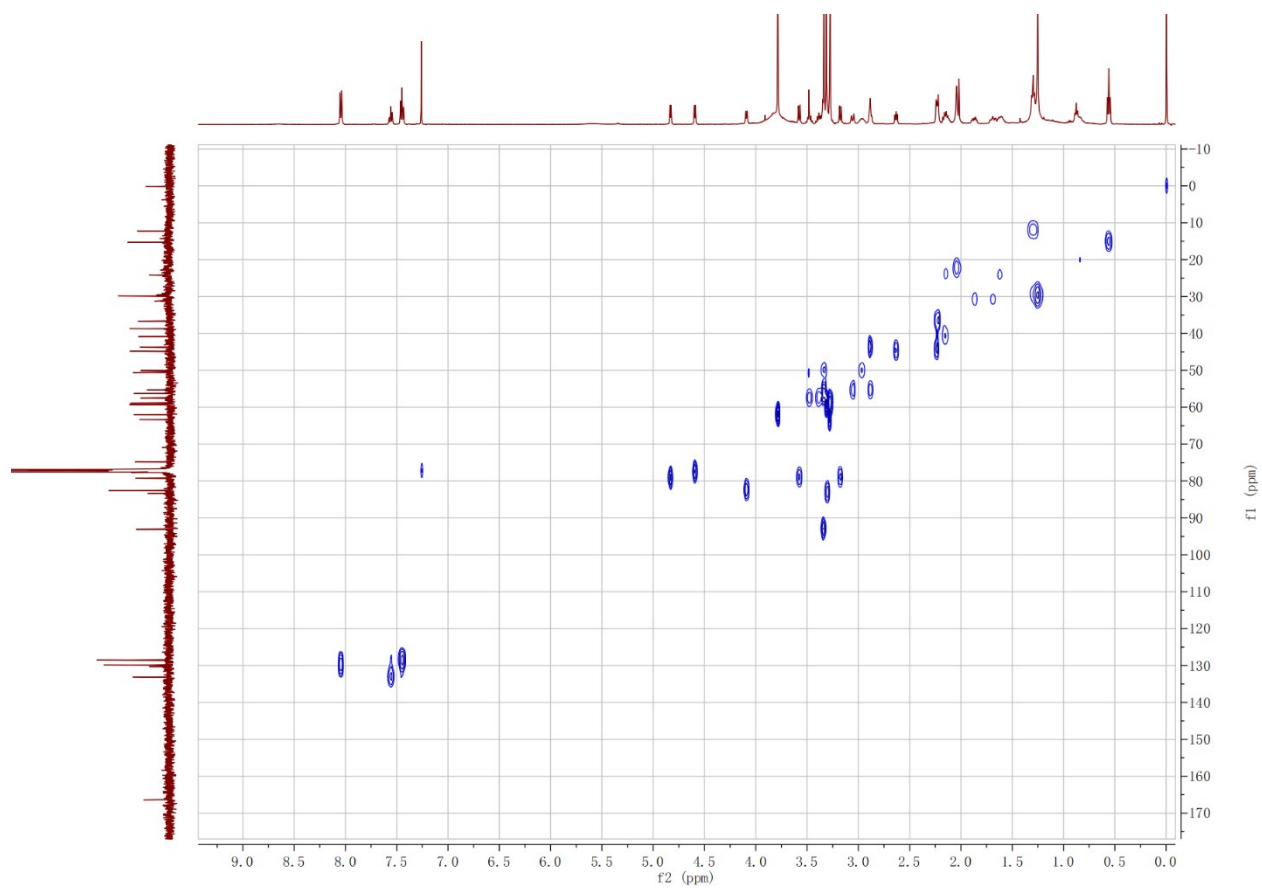


Figure S31 The HSQC spectrum of compound **25** in CDCl₃

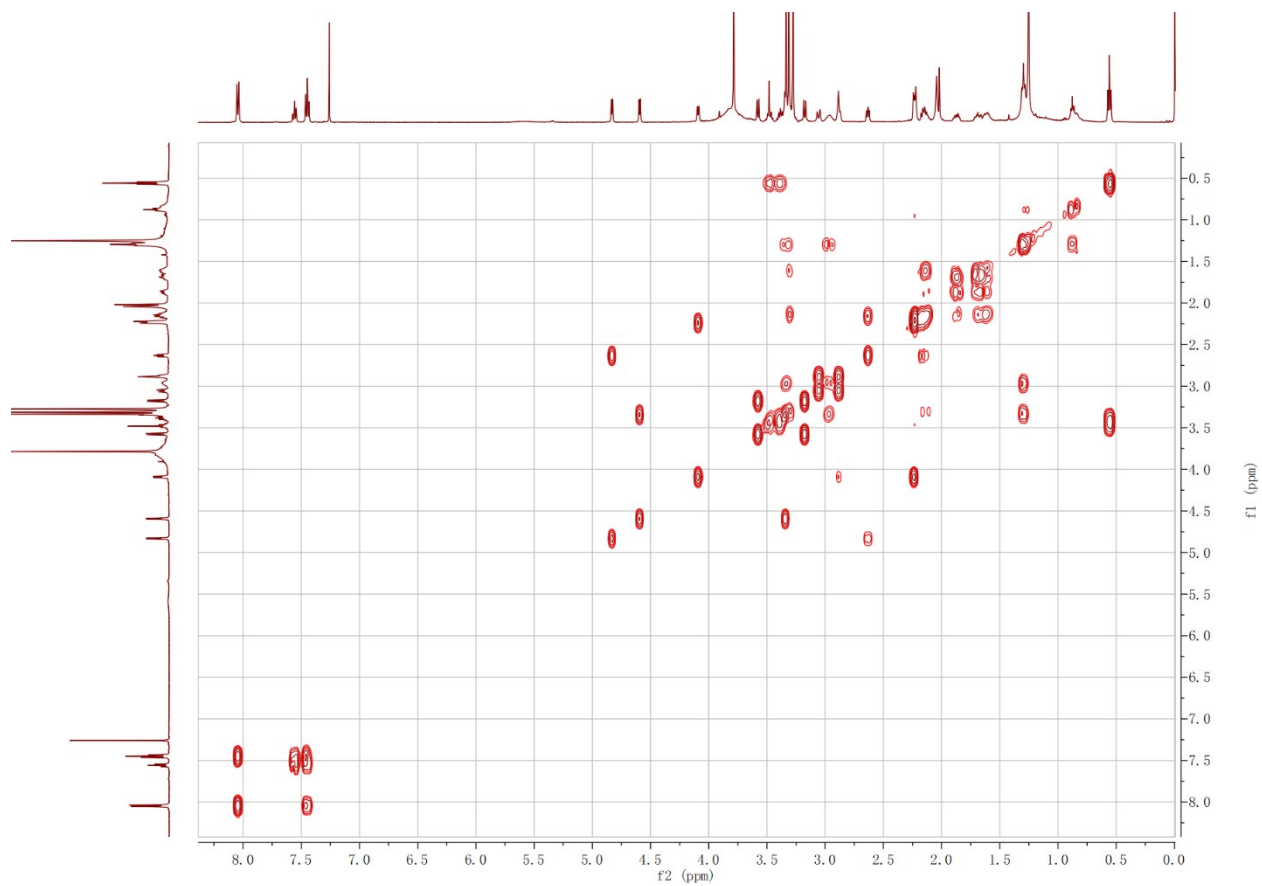


Figure S32 The ^1H - ^1H COSY spectrum of compound **25** in CDCl_3

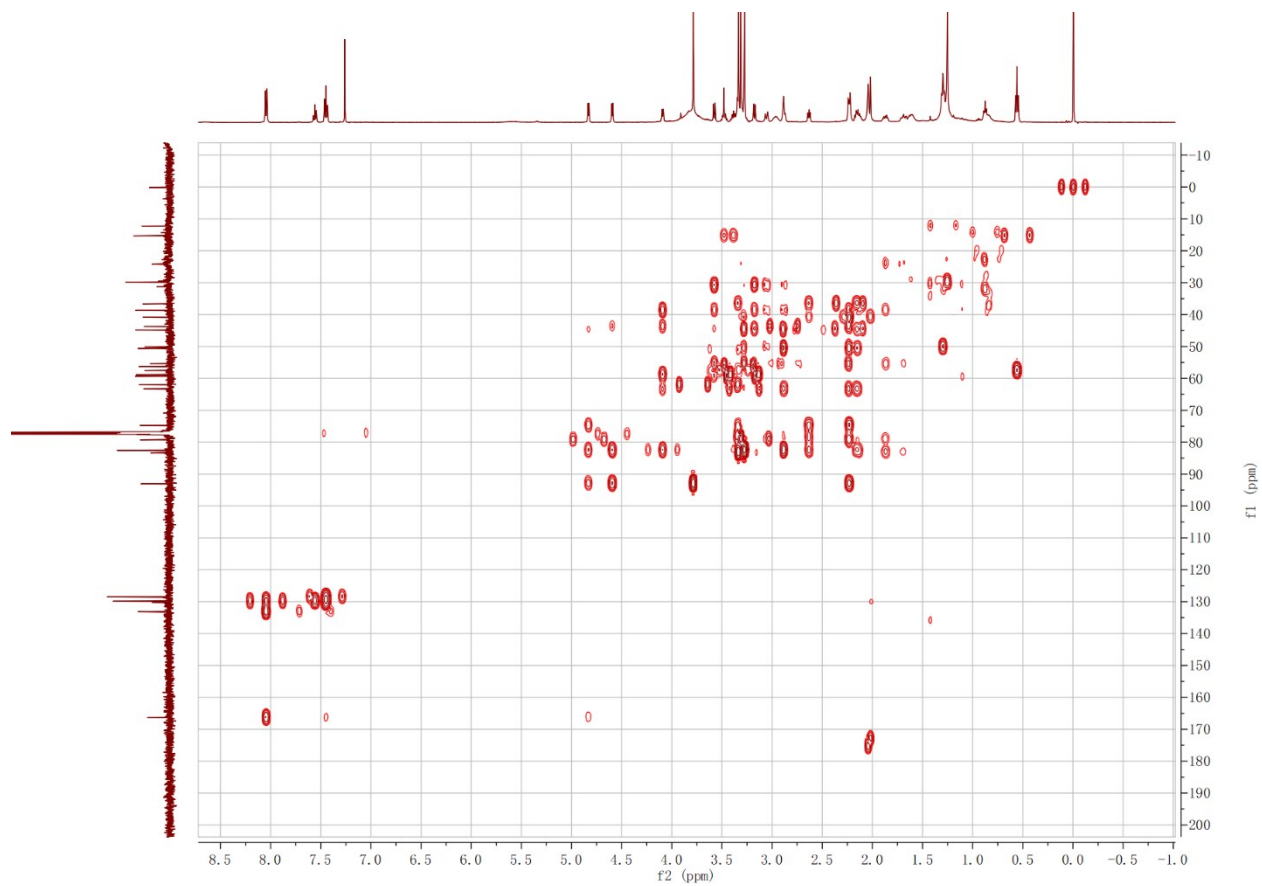


Figure S33 The HMBC spectrum of compound **25** in CDCl_3

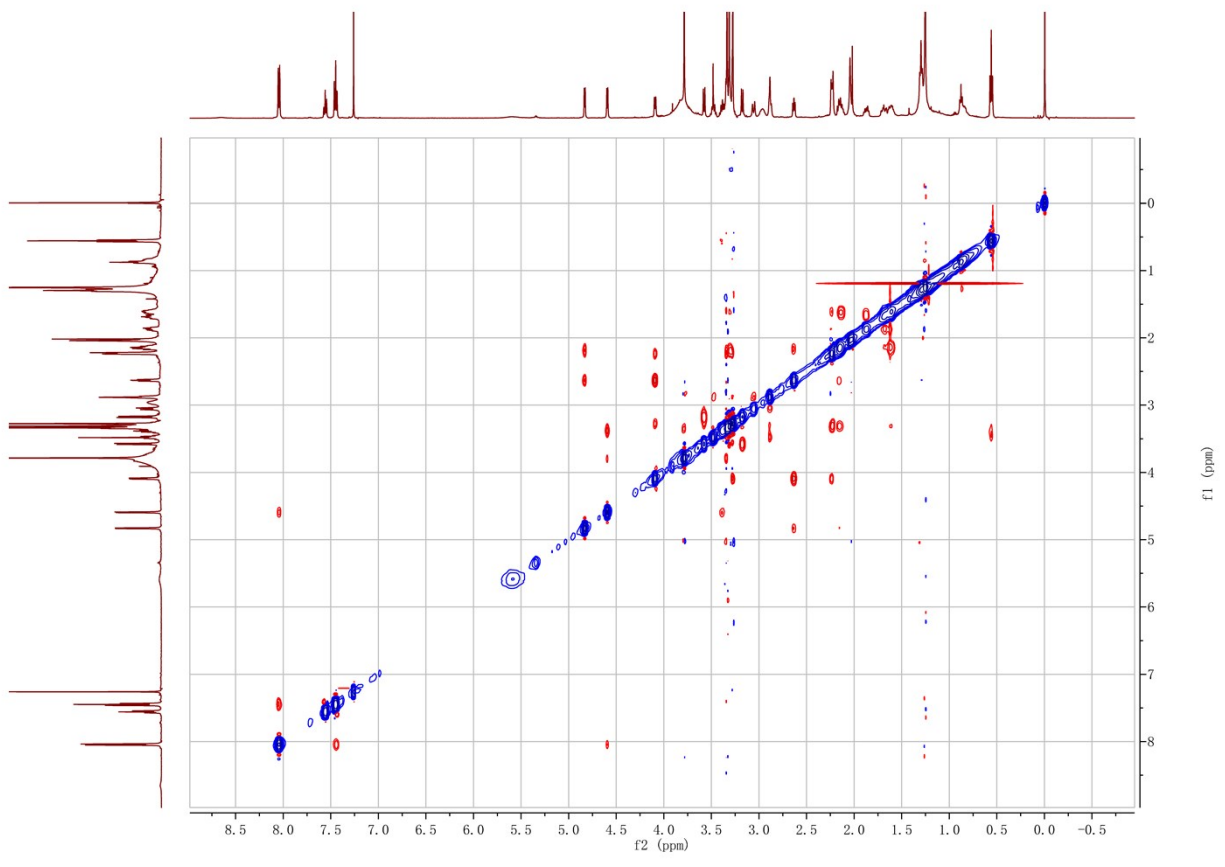


Figure S34 The NOESY spectrum of compound **25** in CDCl₃

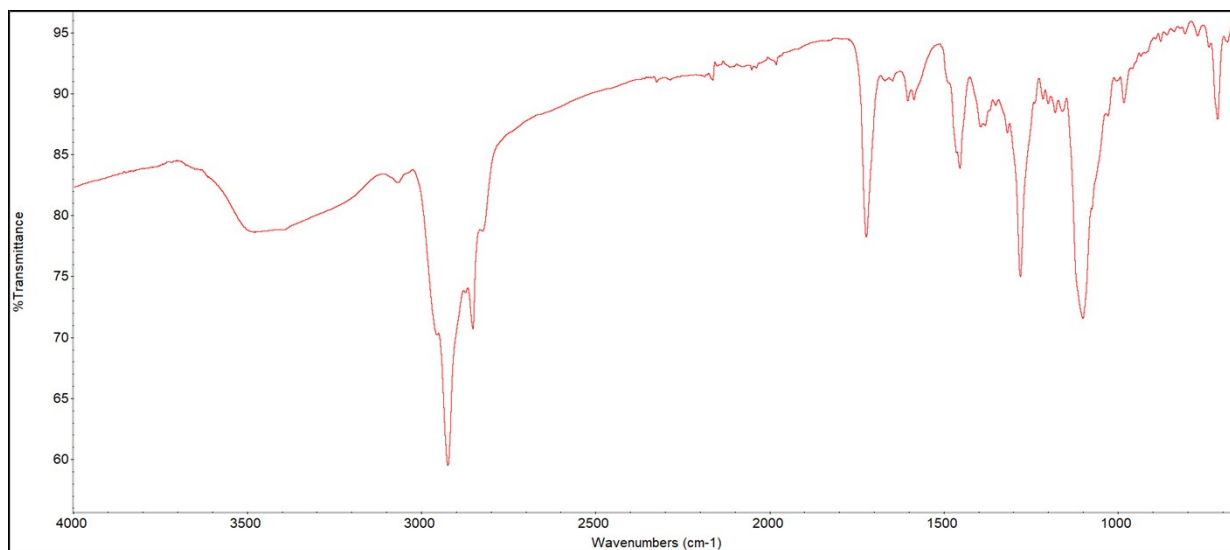


Figure S35 The IR spectrum of compound 25

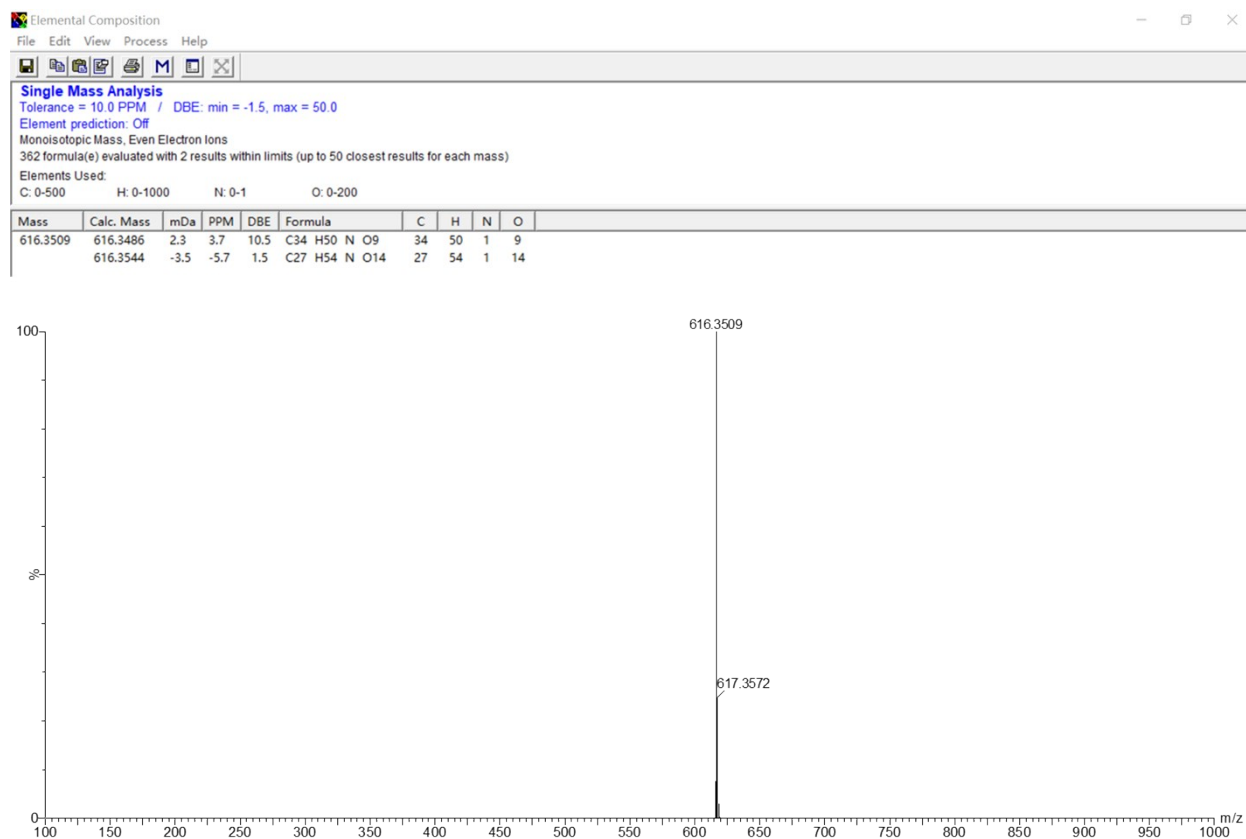


Figure S36 The HR-ESI-MS data of compound 25

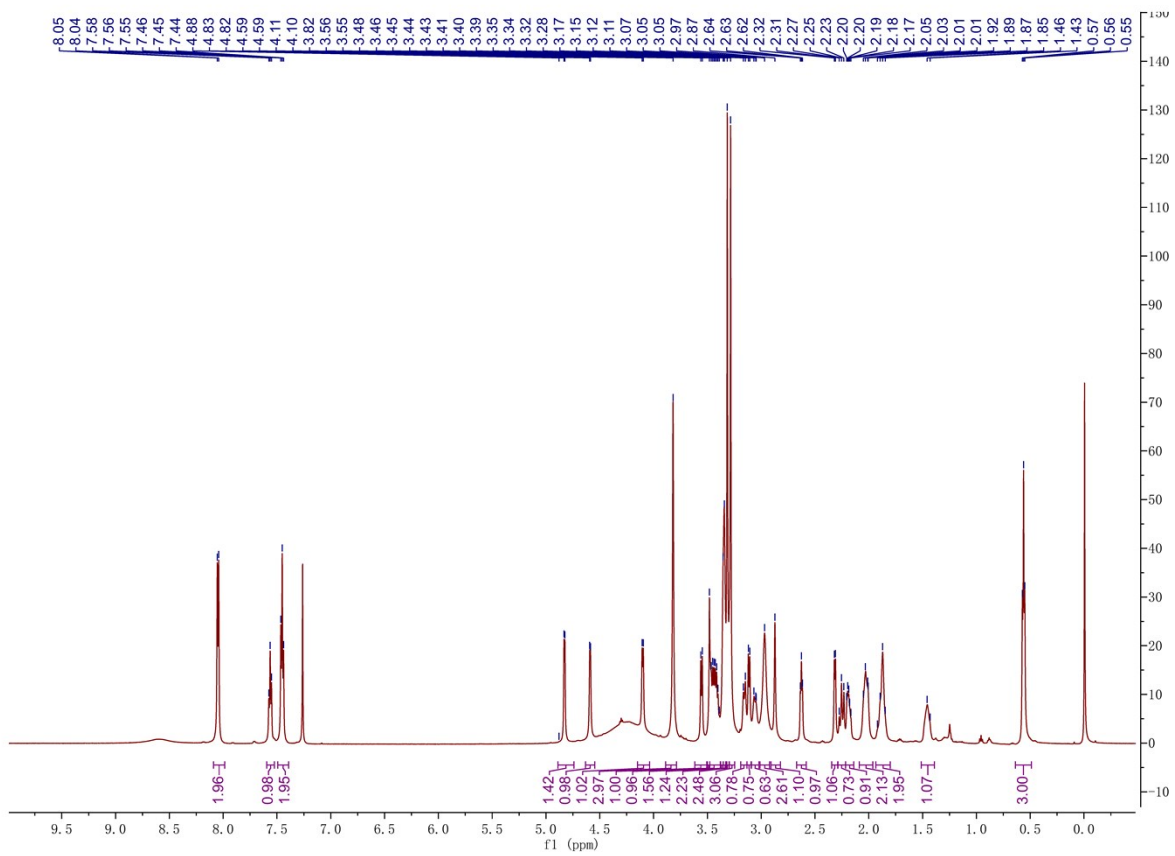


Figure S37 The ^1H NMR spectrum of compound **26** in CDCl_3 (600 MHz)

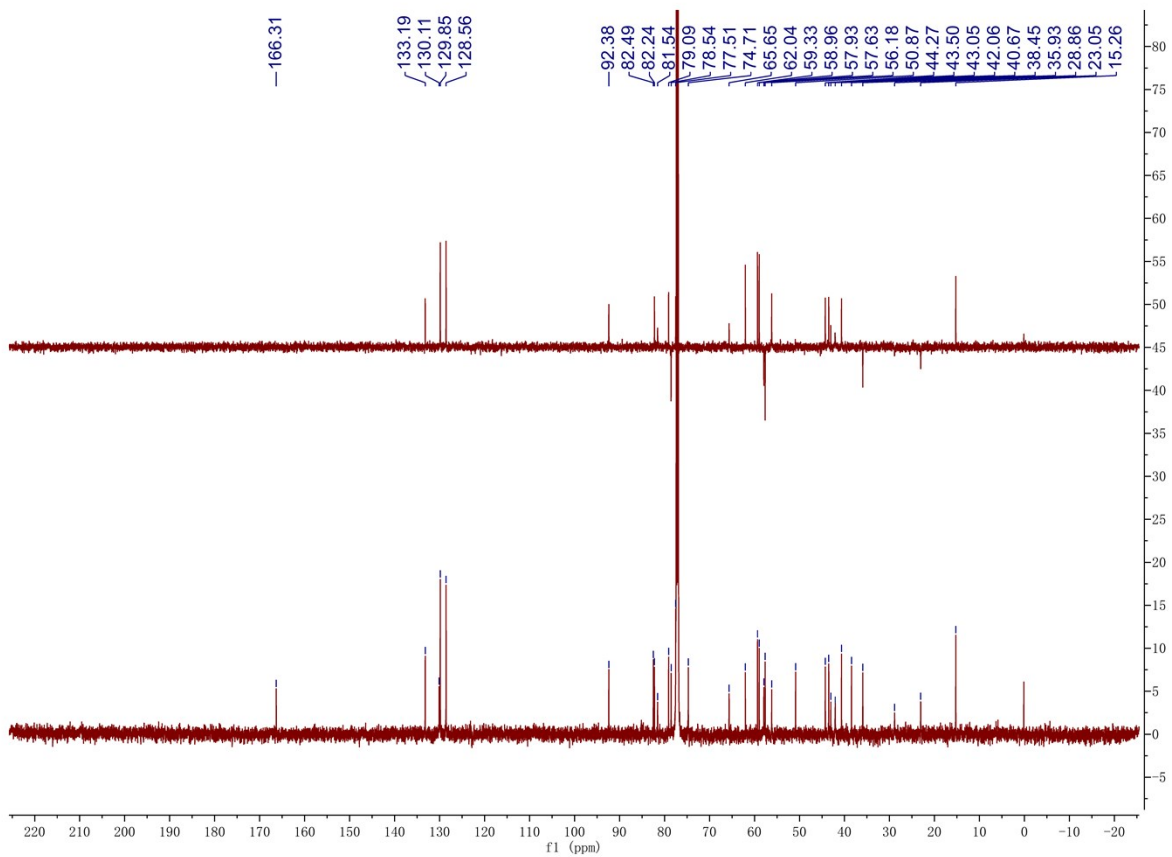


Figure S38 The ^{13}C NMR spectrum of compound **26** in CDCl_3 (150 MHz)

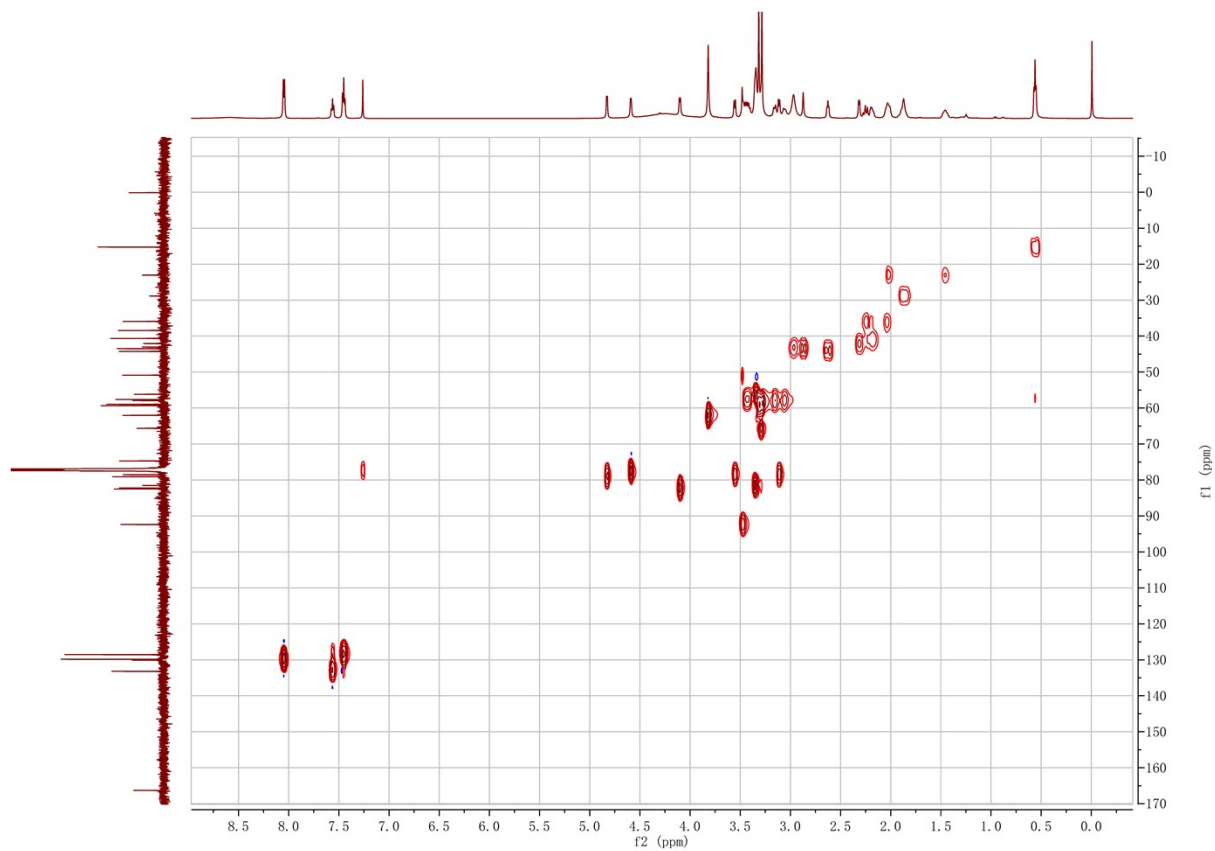


Figure S39 The HSQC spectrum of compound **26** in CDCl₃

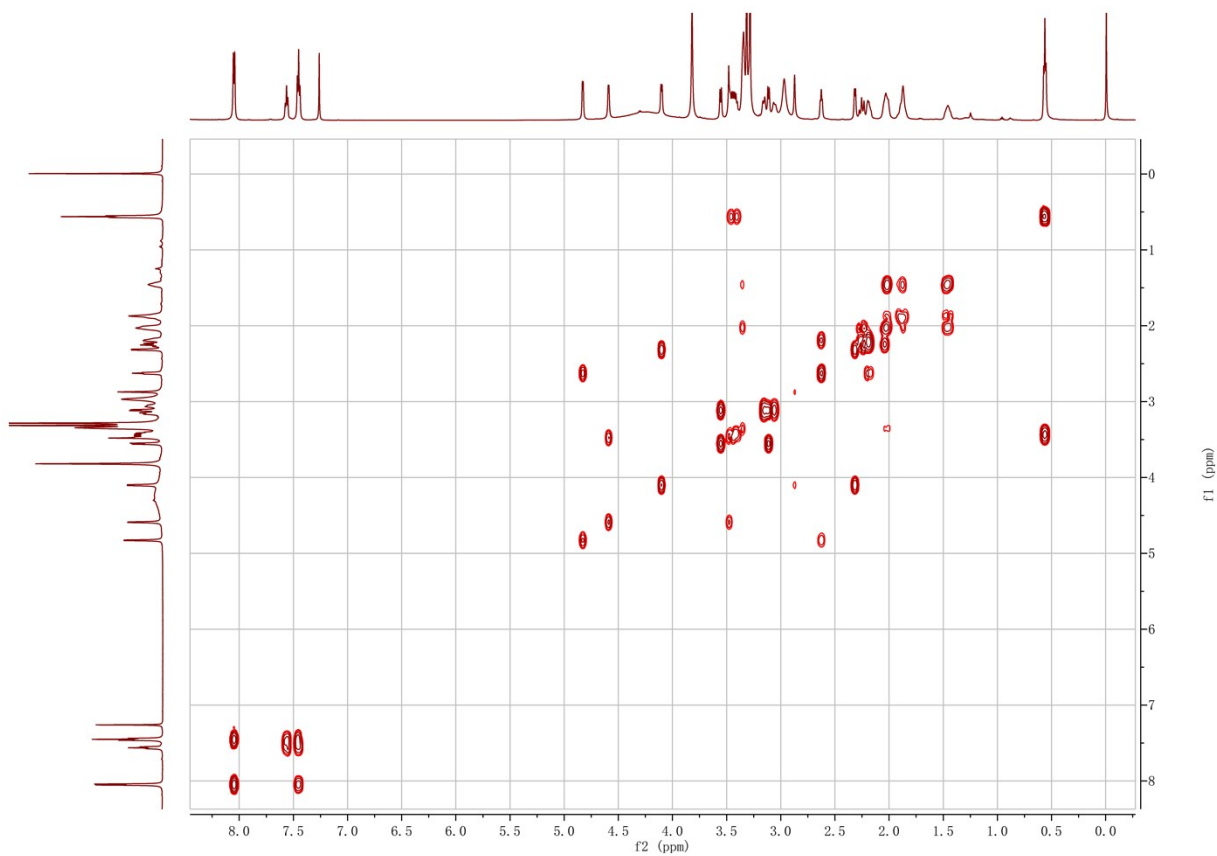


Figure S40 The ^1H - ^1H COSY spectrum of compound **26** in CDCl_3

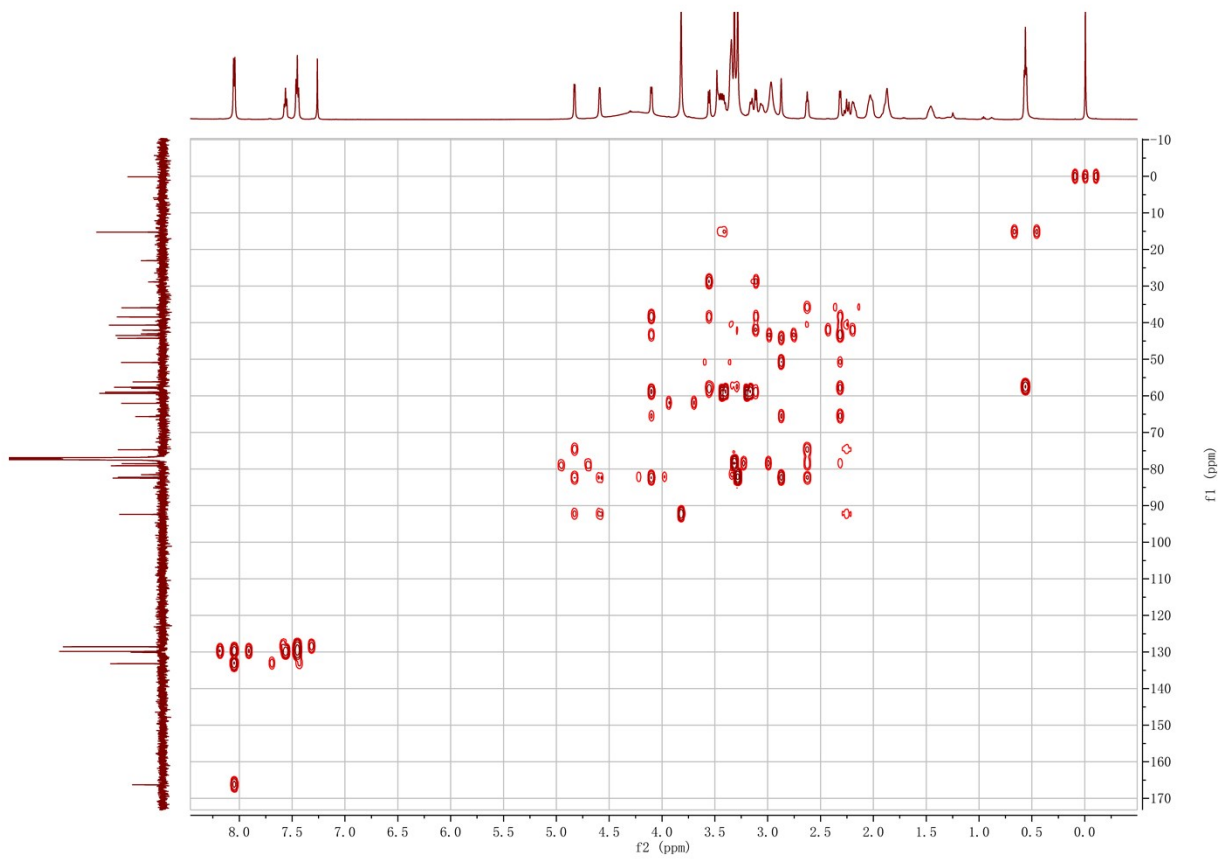


Figure S41 The HMBC spectrum of compound **26** in CDCl_3

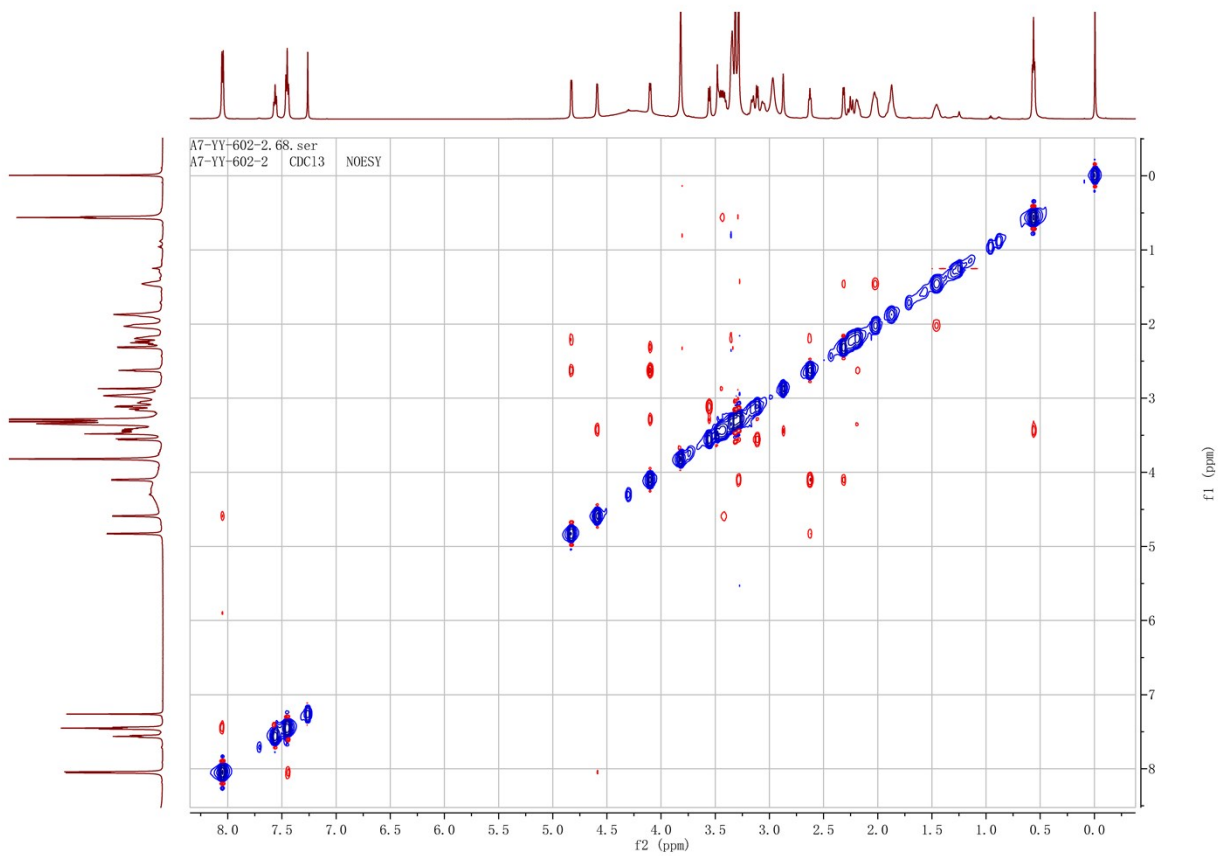


Figure S42 The NOESY spectrum of compound **26** in CDCl₃

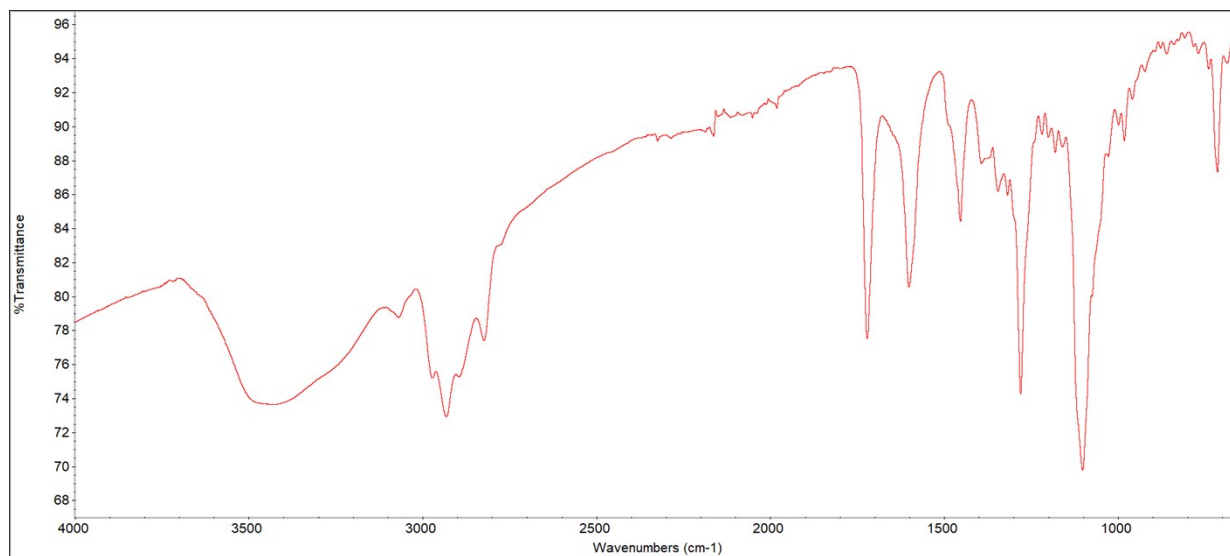


Figure S43 The IR spectrum of compound 26

Elemental Composition

File Edit View Process Help

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
346 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-1 O: 0-200

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	N	O
602.3336	602.3329	0.7	1.2	10.5	C33 H48 N O9	33	48	1	9
	602.3388	-5.2	-8.6	1.5	C26 H52 N O14	26	52	1	14

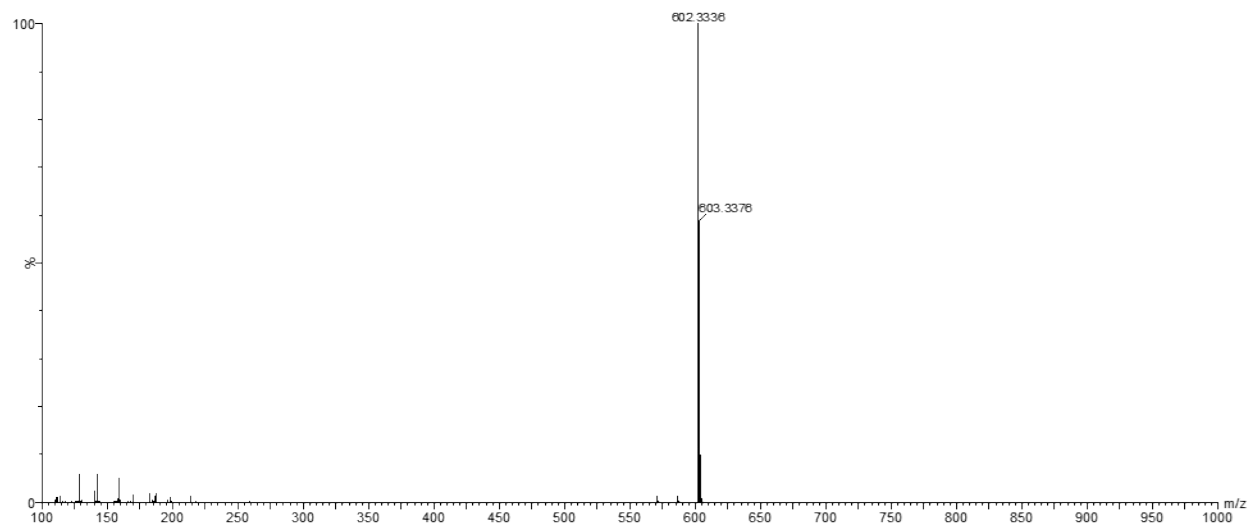


Figure S44 The HR-ESI-MS data of compound 26

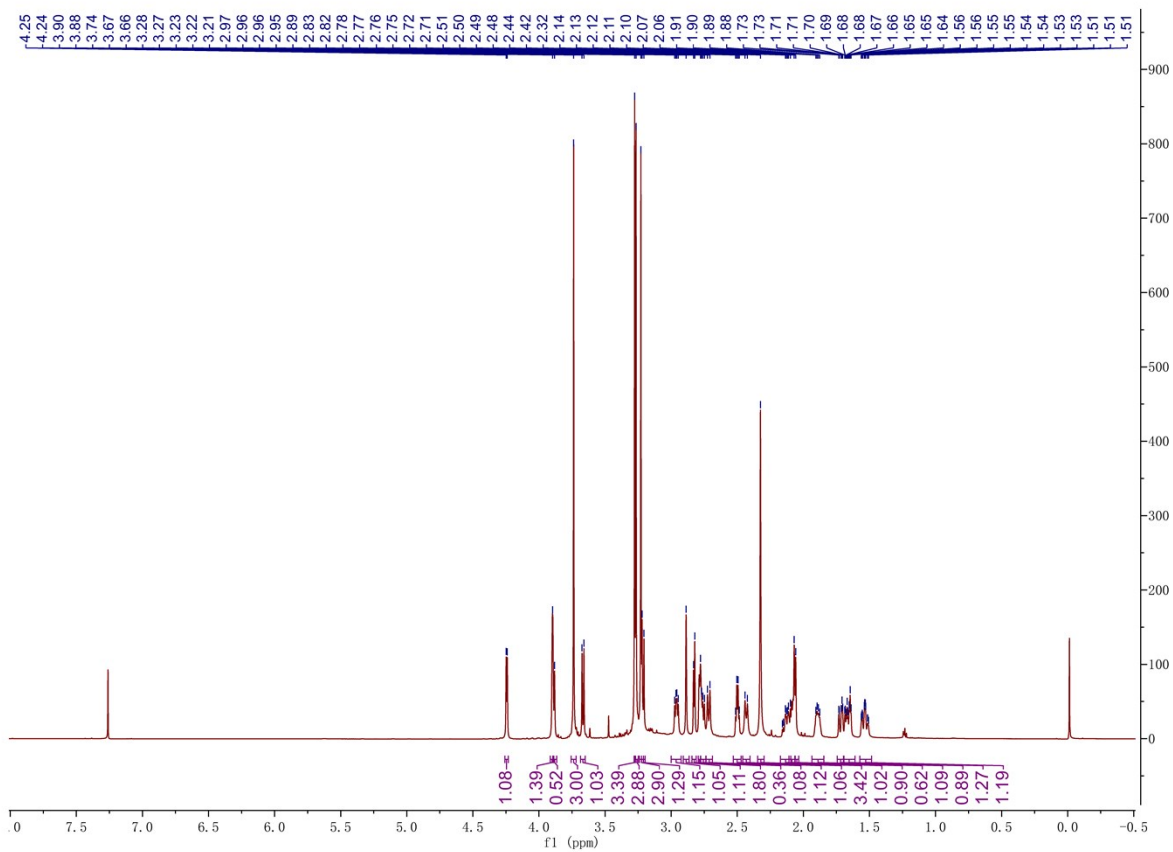


Figure S45 The ^1H NMR spectrum of compound **37** in CDCl_3 (600 MHz)

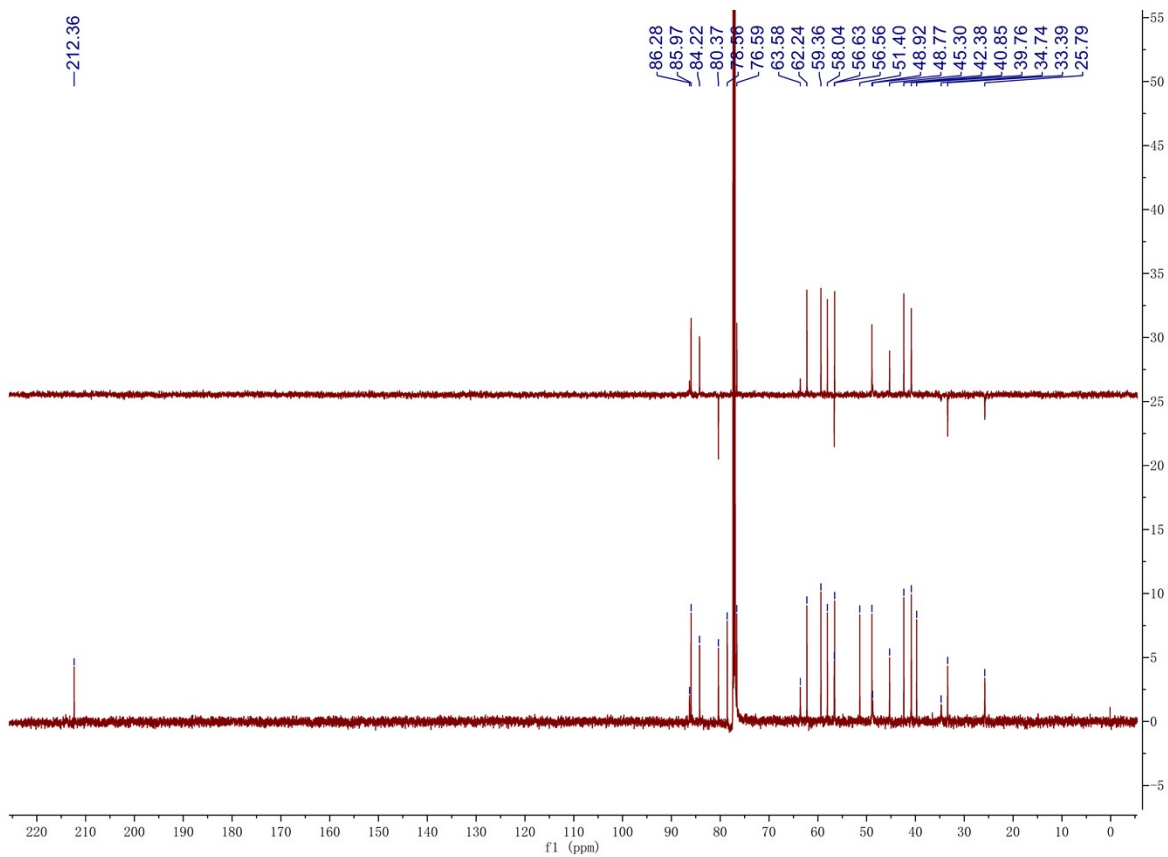


Figure S46 The ^{13}C NMR spectrum of compound **37** in CDCl_3 (150 MHz)

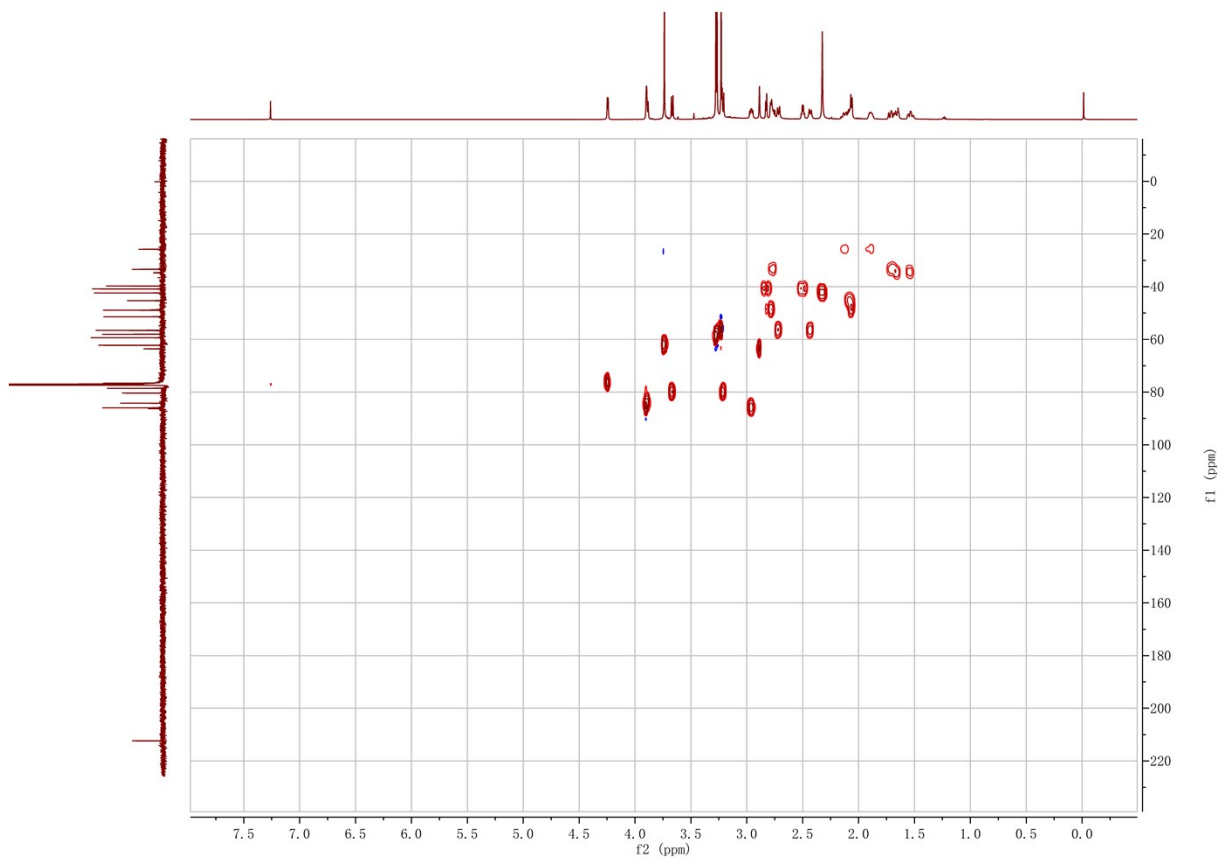


Figure S47 The HSQC spectrum of compound **37** in CDCl₃

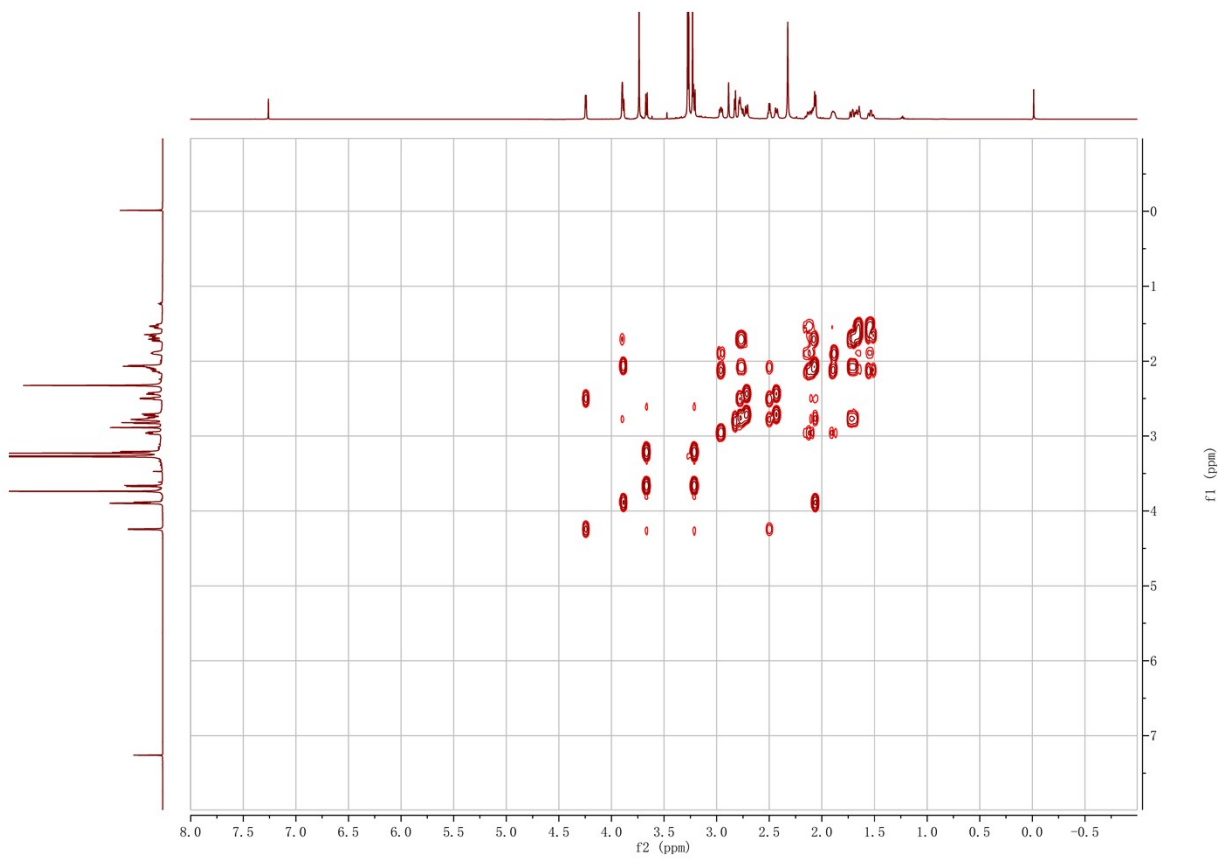


Figure S48 The ^1H - ^1H COSY spectrum of compound **37** in CDCl_3

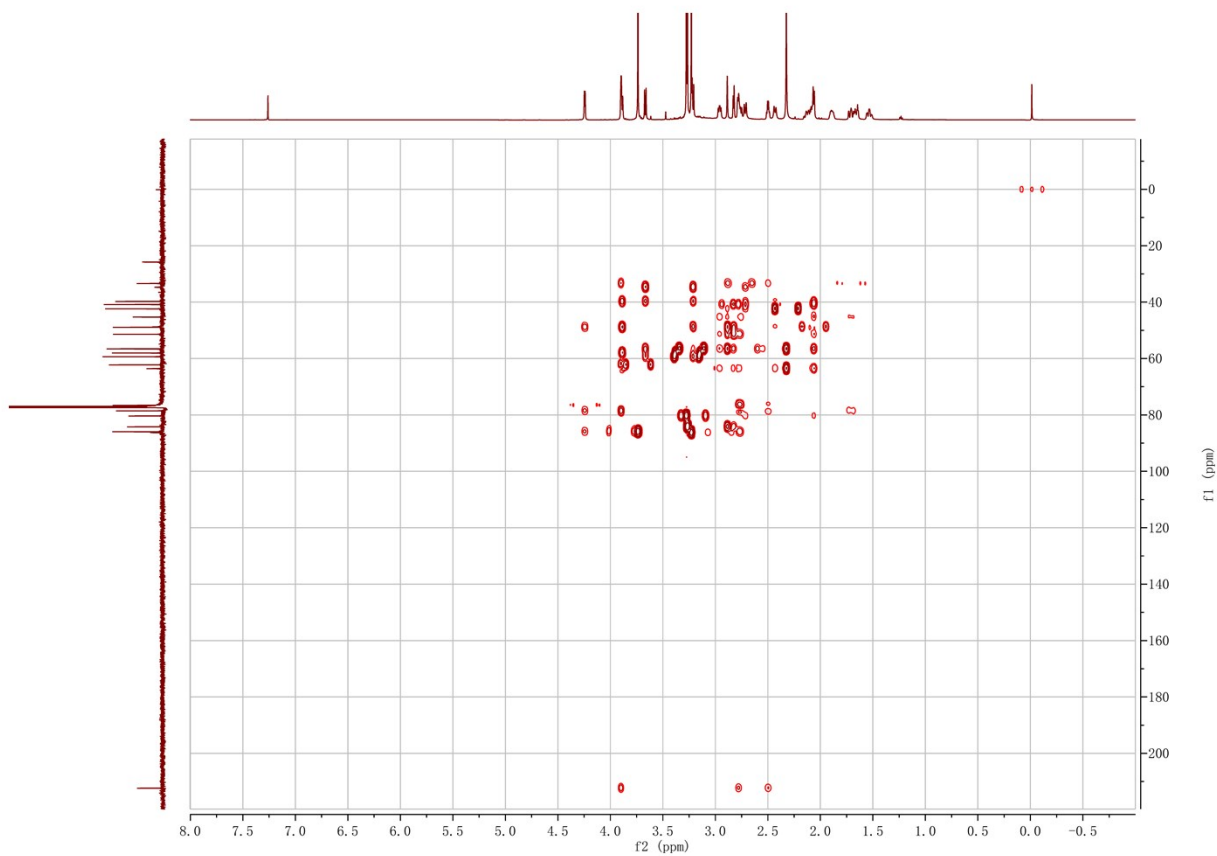


Figure S49 The HMBC spectrum of compound **37** in CDCl_3

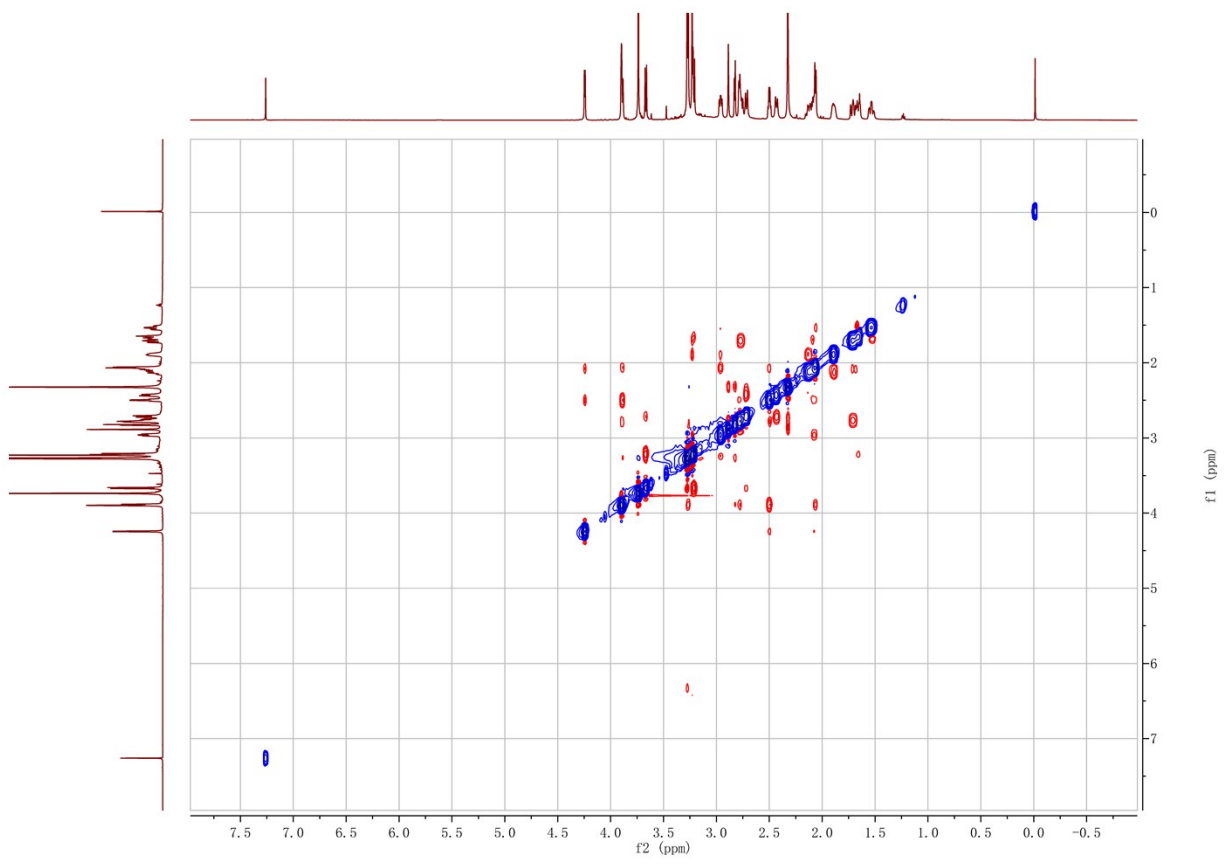


Figure S50 The NOESY spectrum of compound **37** in CDCl₃

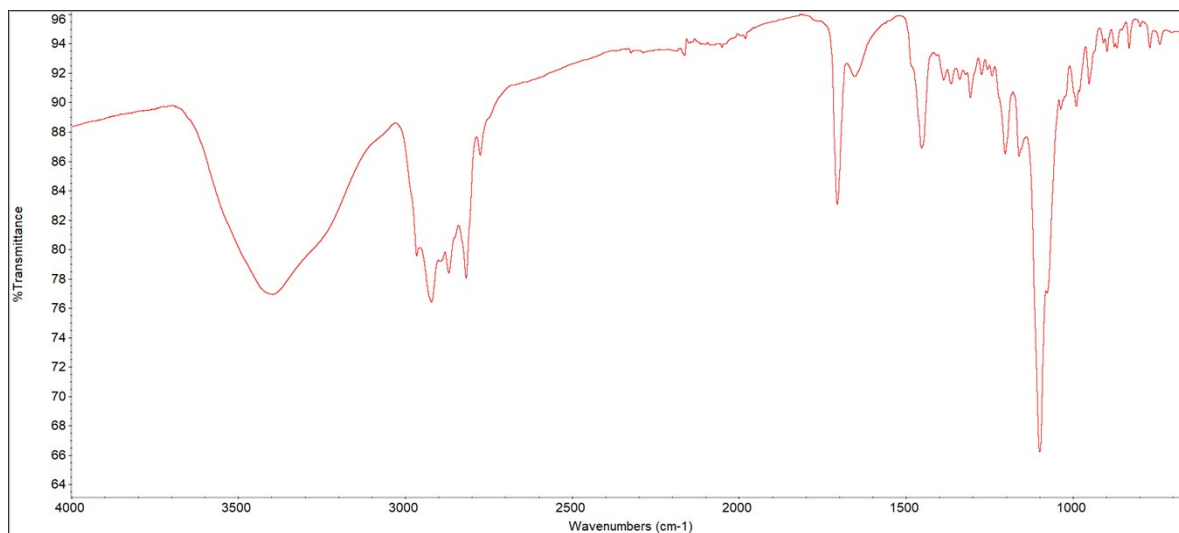


Figure S51 The IR spectrum of compound 37

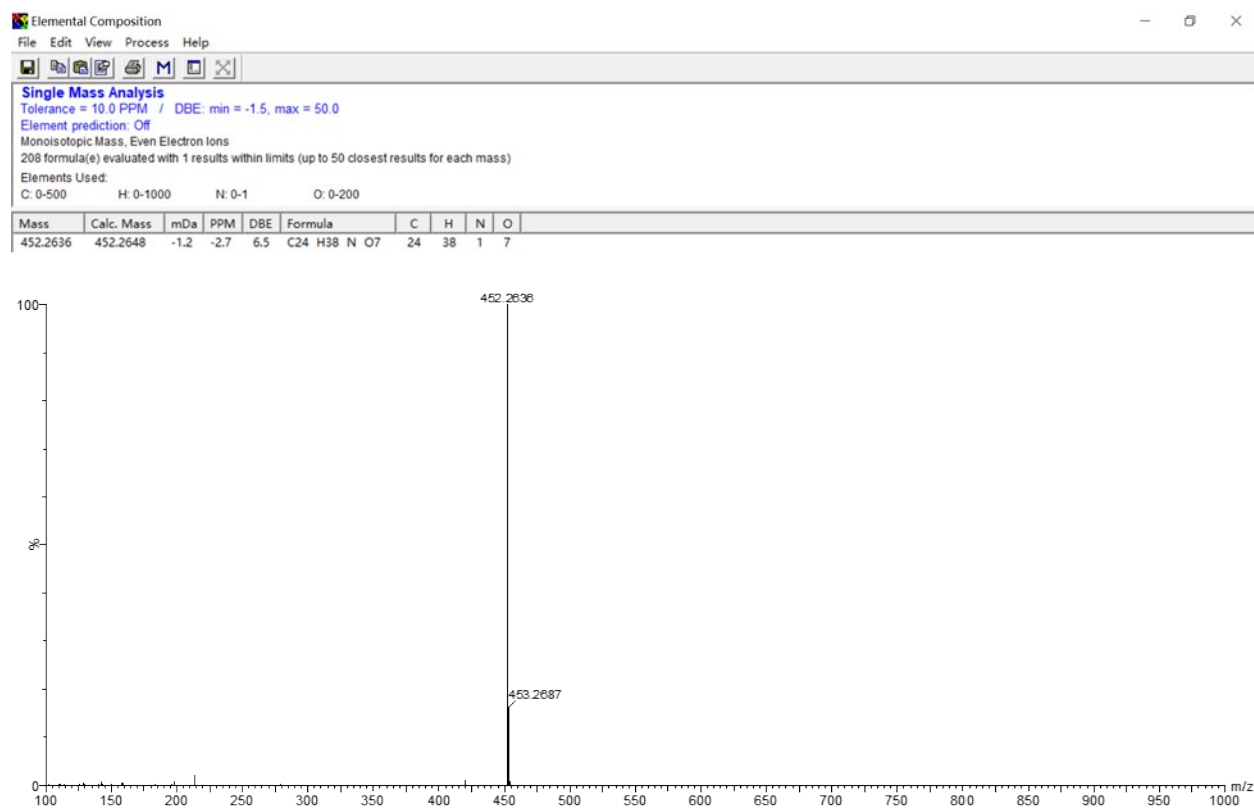


Figure S52 The HR-ESI-MS data of compound 37

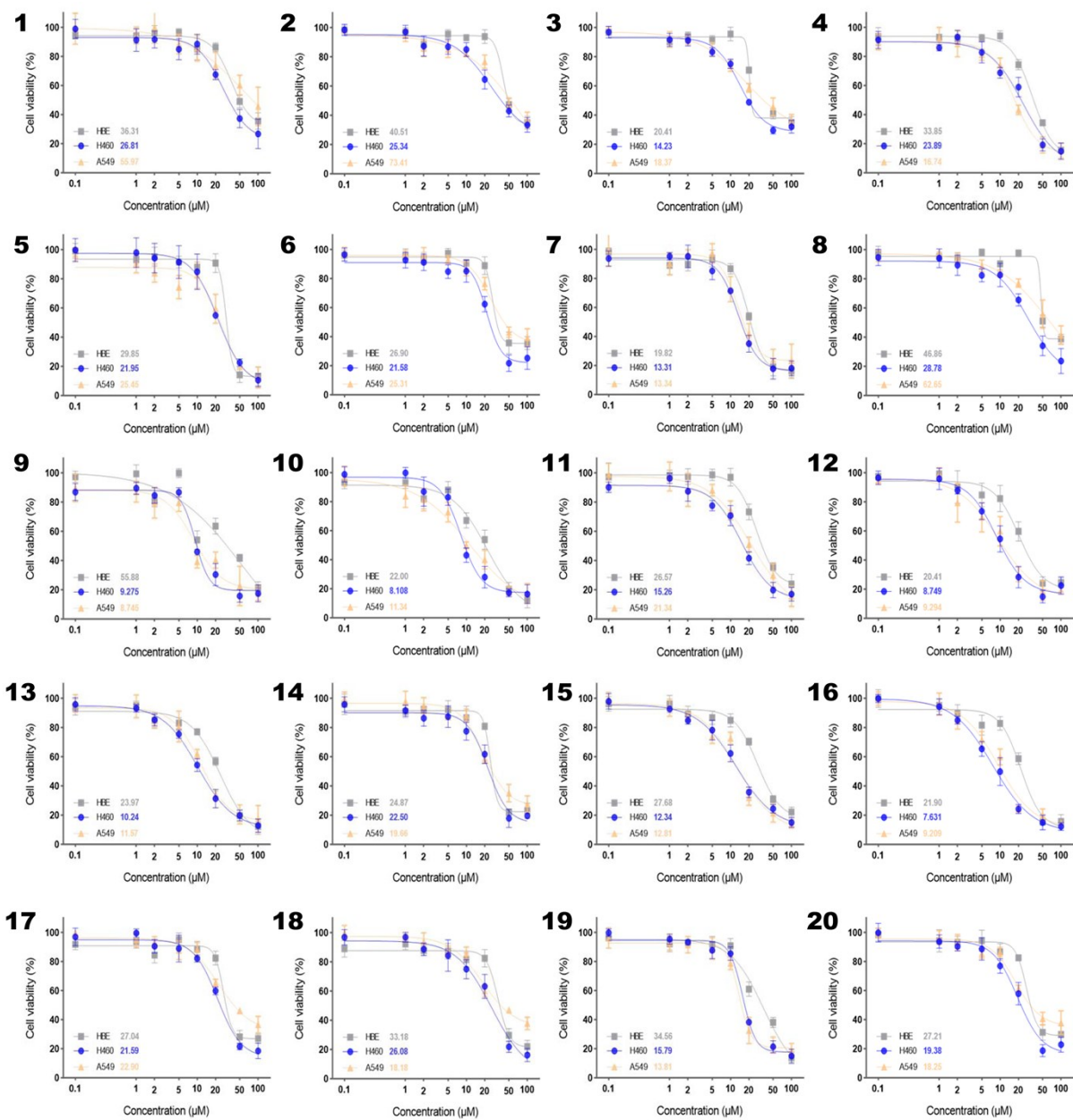


Figure S53 The representative IC₅₀ curves of compounds 1-20

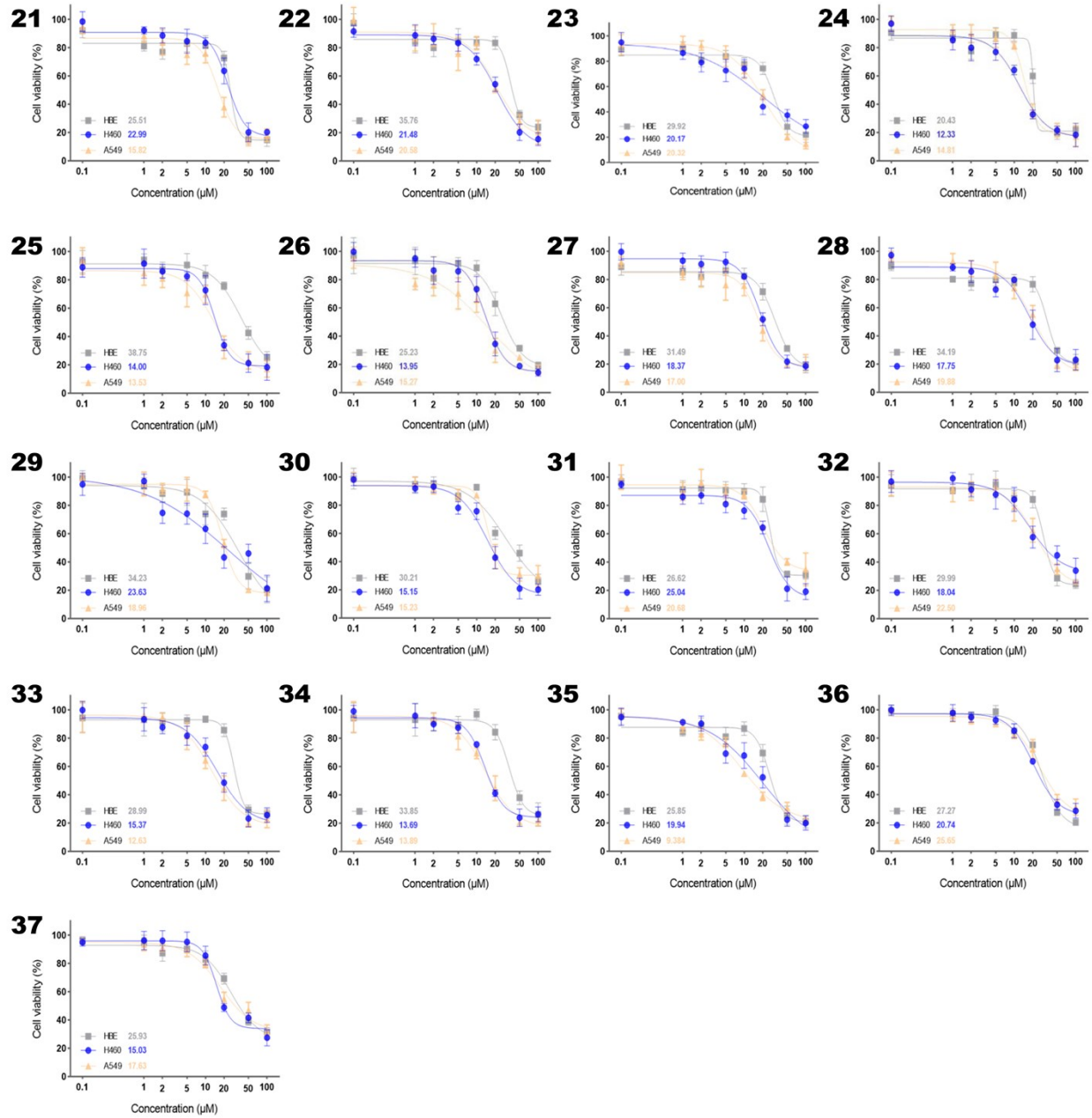


Figure S54 The representative IC₅₀ curves of compounds 21-37