

A novel adduct of ECG fused to piceid and four new dimeric stilbene glycosides from *Polygonum cuspidatum*†

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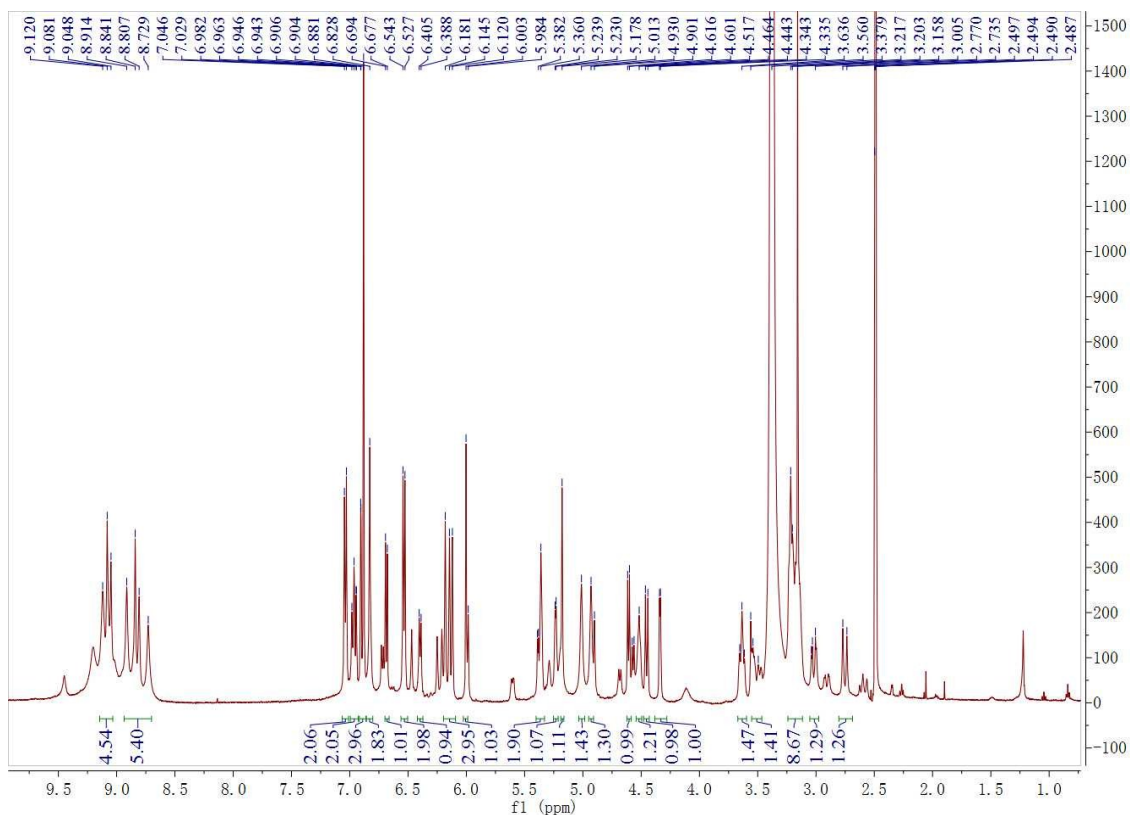


Figure S1. The ^1H NMR spectrum of compound **1** in $\text{DMSO}-d_6$.

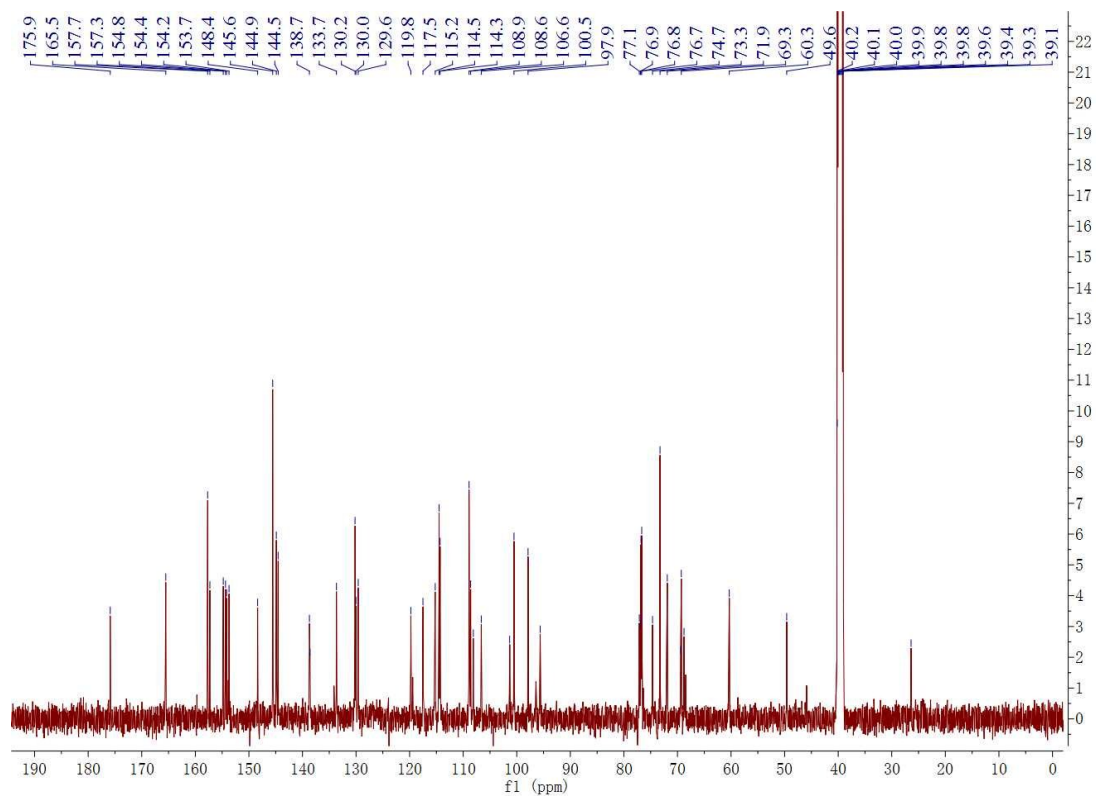


Figure S2. The ^{13}C NMR spectrum of compound **1** in $\text{DMSO}-d_6$.

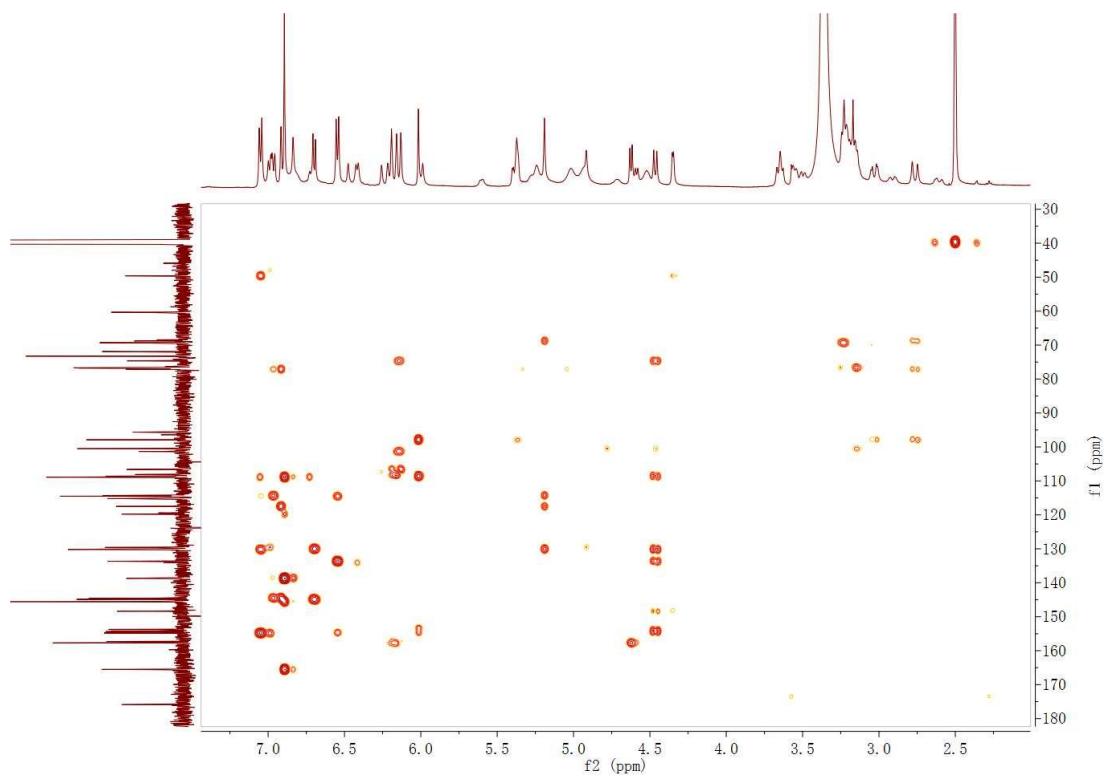


Figure S3. The HMBC spectrum of compound **1** in DMSO- d_6 .

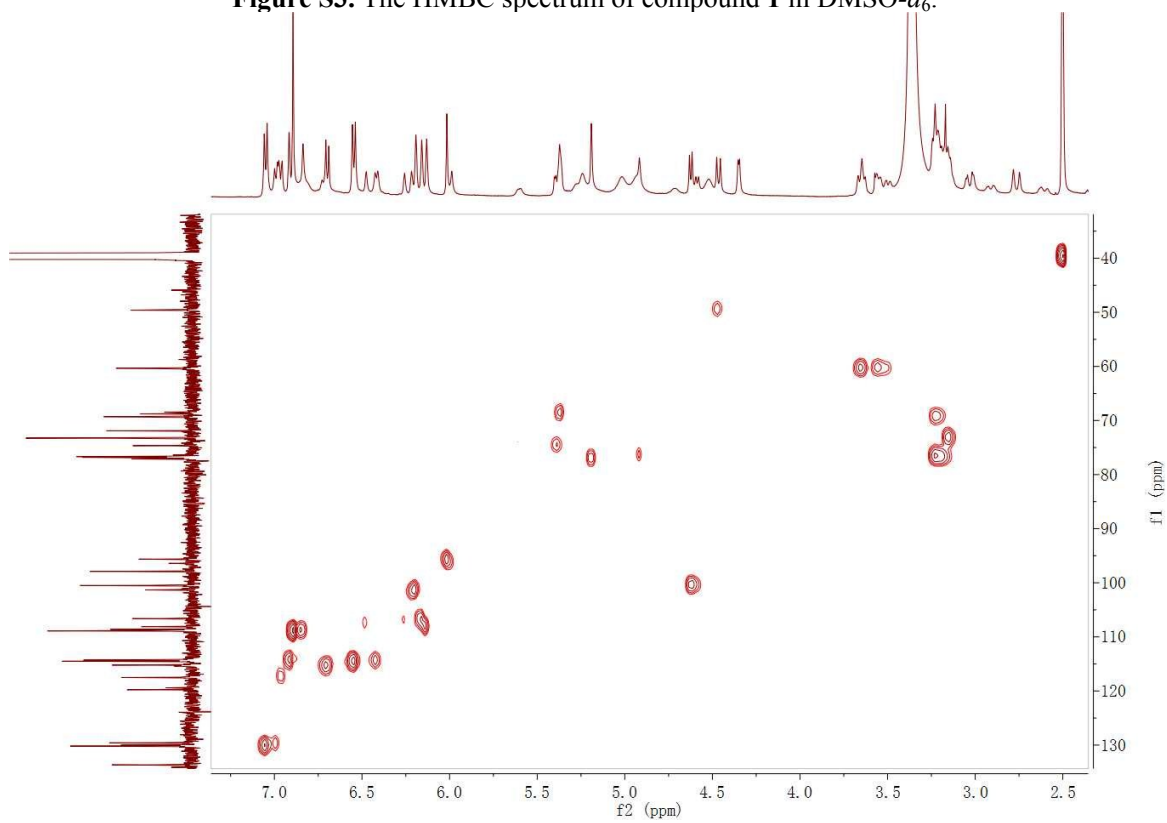


Figure S4. The HSQC spectrum of compound **1** in DMSO- d_6 .

m/z	Ion	Formula	Abundance											
847.2094	(M+H) ⁺	C42 H39 O19	570946.1											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C42 H40 O19	C42 H39 O19	847.2091	99.95		848.2166	848.2164	-0.29	0.29	99.88	99.94	100	847.2094	23
☐	C39 H44 O19 S	C39 H43 O19 S	847.2125	99.01		848.2166	848.2197	3.67	3.67	97.41	99.95	99.51	847.2094	18
☐	C46 H40 O14 S	C46 H39 O14 S	847.2066	98.9		848.2166	848.2139	-3.25	3.25	96.82	99.97	99.61	847.2094	27
☐	C35 H44 O24	C35 H43 O24	847.215	98.72		848.2166	848.2223	6.64	6.64	98.23	99.95	98.4	847.2094	14
☐	C49 H36 O14	C49 H35 O14	847.2032	98.39		848.2166	848.2105	-7.21	7.21	97.55	99.93	98.12	847.2094	32
☐	C60 H32 O6	C60 H31 O6	847.2126	96.68		848.2166	848.2199	3.85	3.85	89.34	99.91	99.46	847.2094	45
☐	C57 H36 O6 S	C57 H35 O6 S	847.216	96.2		848.2166	848.2233	7.81	7.81	90.39	99.98	97.79	847.2094	40
☐	C28 H48 O27 S	C28 H47 O27 S	847.2031	95.86		848.2166	848.2104	-7.39	7.39	88.9	99.9	98.02	847.2094	5
☐	C64 H32 O S	C64 H31 O S	847.2101	95.57		848.2166	848.2174	0.89	0.89	84.55	99.98	99.97	847.2094	49
☐	C67 H28 O	C67 H27 O	847.2067	94.92		848.2166	848.214	-3.08	3.08	82.88	99.9	99.65	847.2094	54

Figure S5. The HRESIMS of compound **1**.

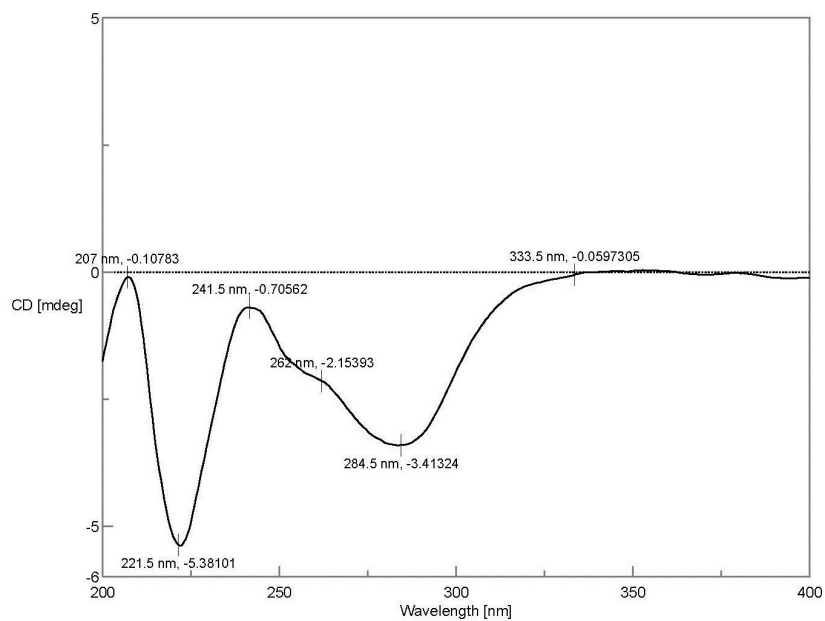


Figure S6. The CD spectrum of **1** in MeOH

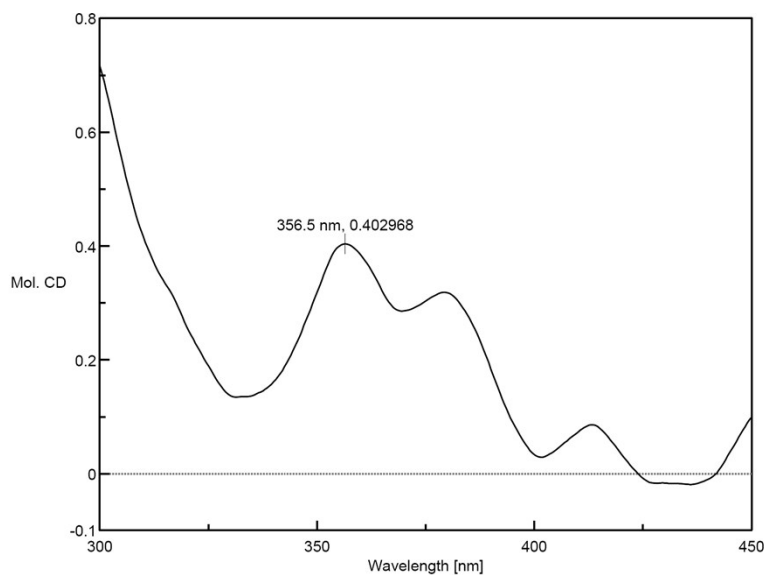


Figure S7. The $\text{Rh}_2(\text{OCOCF}_3)_4$ induced CD spectrum of **1a** in CHCl_3 .

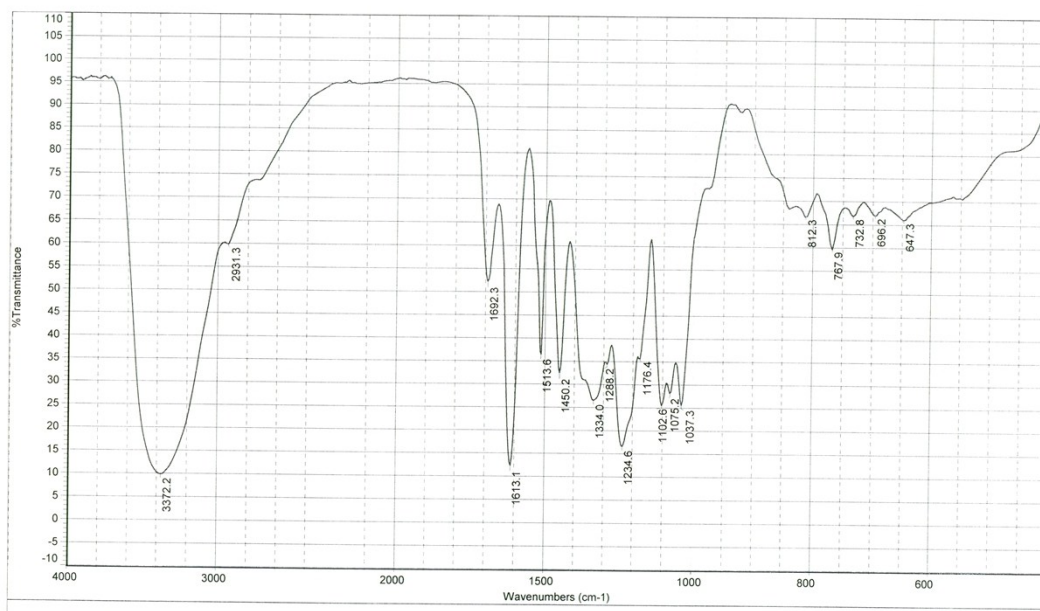


Figure S8. The IR spectrum of compound **1**.

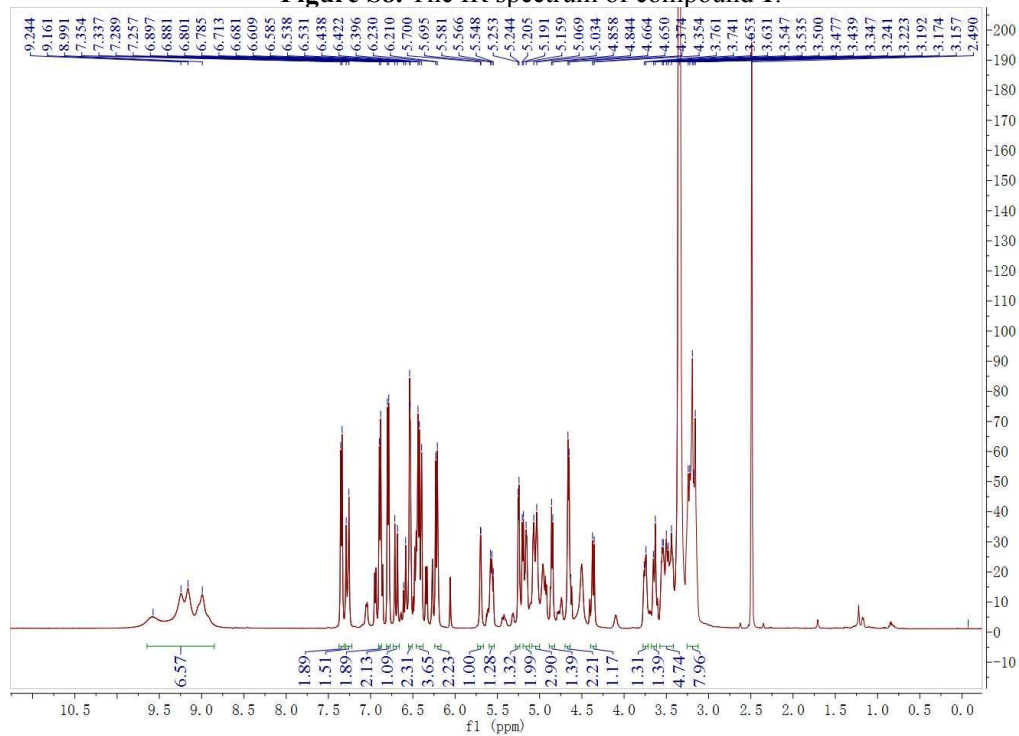


Figure S9. The ¹H NMR spectrum of compound **2** in DMSO-*d*₆.

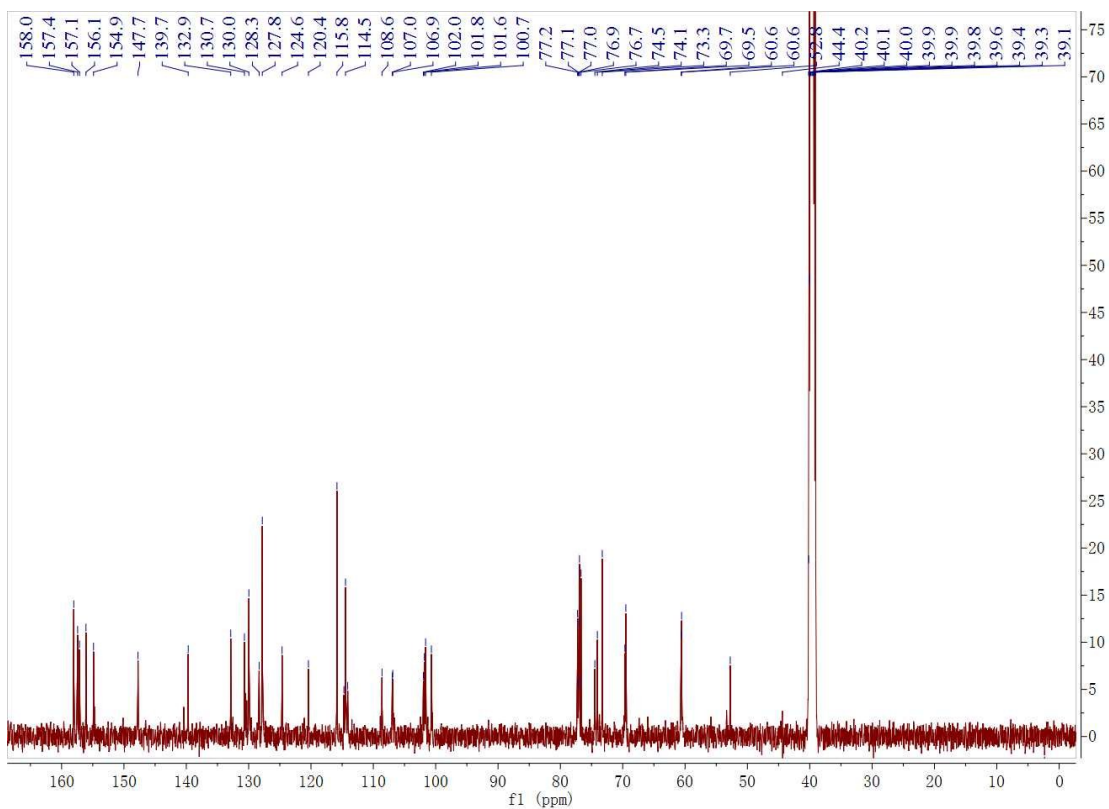


Figure S10. The ^{13}C NMR spectrum of compound **2** in $\text{DMSO}-d_6$.

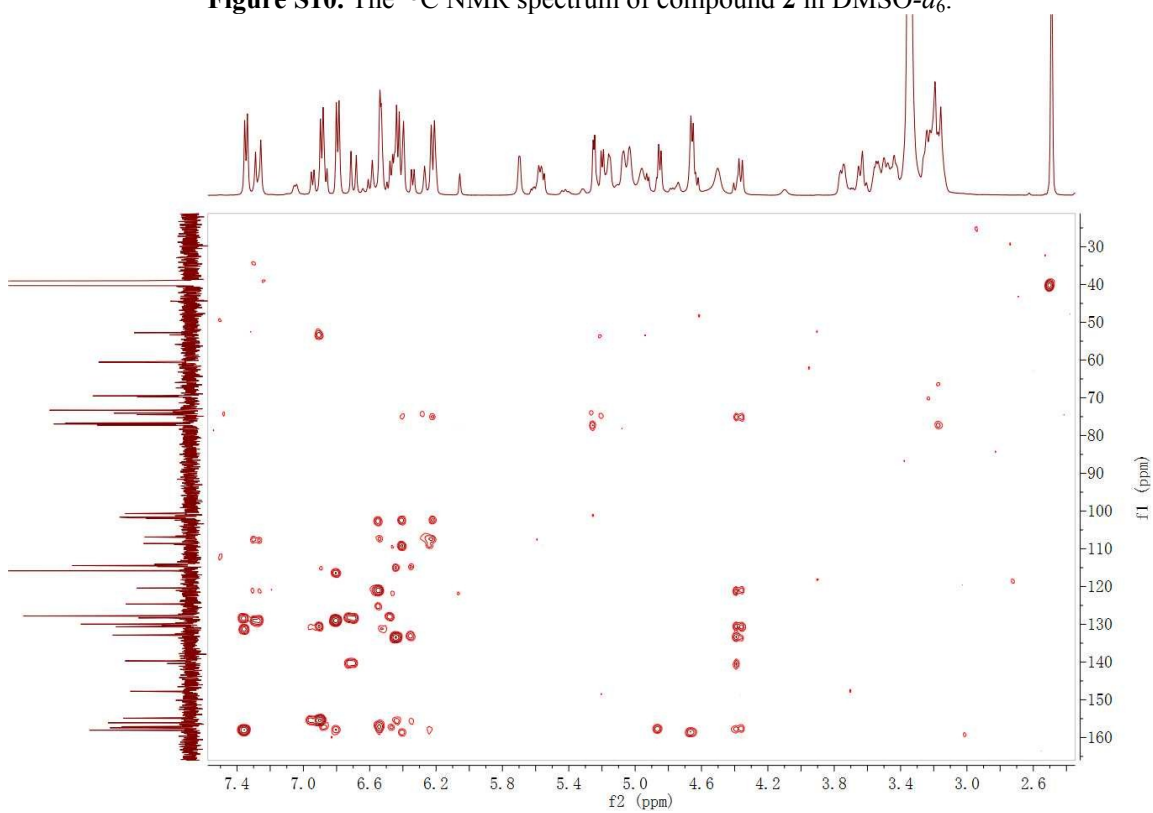


Figure S11. The HMBC spectrum of compound **2** in $\text{DMSO}-d_6$.

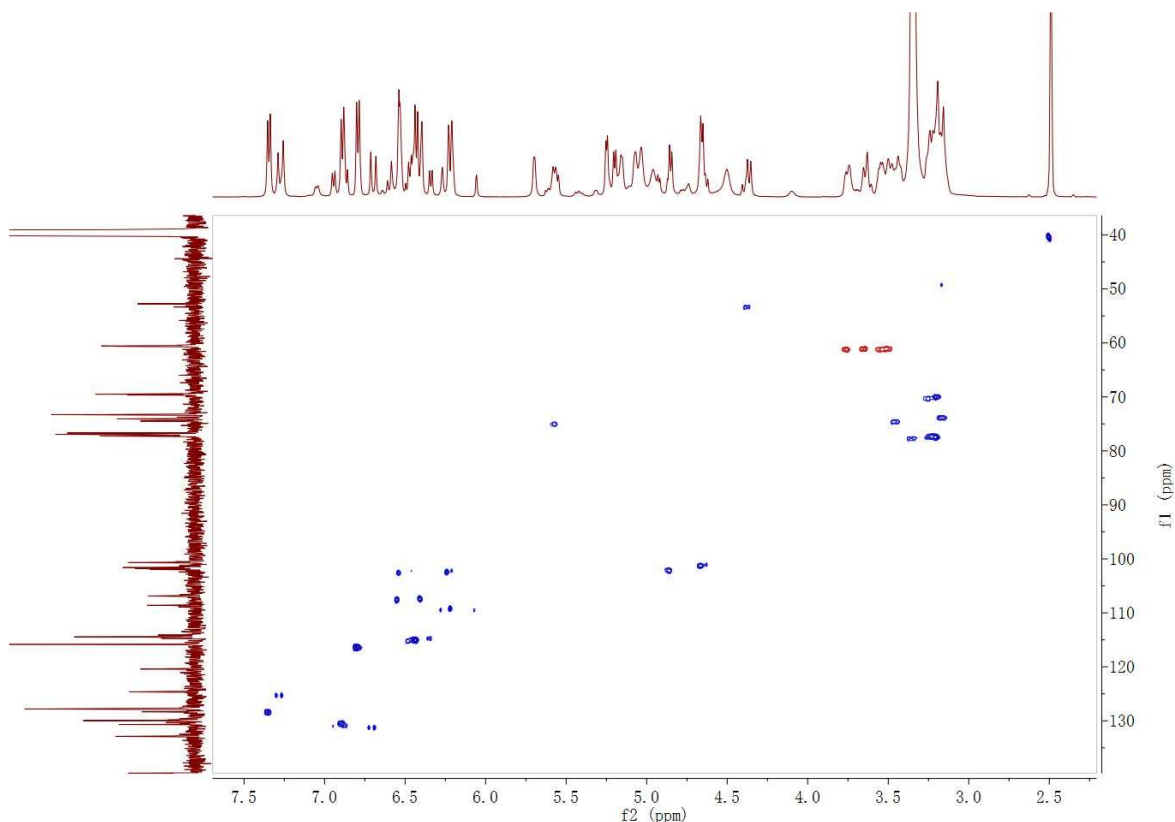


Figure S12. The HSQC spectrum of compound **2** in DMSO-*d*₆.

m/z	Ion	Formula	Abundance
819.2478	(M+Na) ⁺	C40 H44 Na O17	192430.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C40 H44 O17	C40 H44 Na O17	819.2471	99.98		796.2585	796.2578	-0.82	0.82	99.99	99.97	99.98	819.2478	19
✓	C41 H40 N4 O13	C41 H40 Na O13	819.2484	99.91		796.2585	796.2592	0.84	0.84	99.74	99.99	99.98	819.2478	24
✓	C38 H44 N4 O13 S	C38 H44 Na O13 S	819.2518	99.2		796.2585	796.2626	5.05	5.05	98.76	99.88	99.13	819.2478	19
✓	C37 H48 O17 S	C37 H48 Na O17 S	819.2504	99.2		796.2585	796.2612	3.4	3.4	97.96	99.87	99.6	819.2478	14
✓	C45 H40 N4 O8 S	C45 H40 Na O8 S	819.2459	99.17		796.2585	796.2567	-2.32	2.32	97.46	99.92	99.62	819.2478	28
✓	C35 H44 N2 O19	C35 H44 Na O19	819.243	99.15		796.2585	796.2538	-5.89	5.89	99.03	99.99	99.82	819.2478	15
✓	C44 H44 O12 S	C44 H44 Na O12 S	819.2446	99.14		796.2585	796.2553	-3.98	3.98	97.96	99.92	99.46	819.2478	23
✓	C46 H40 N2 O11	C46 H40 Na O11	819.2524	98.94		796.2585	796.2632	5.9	5.9	98.3	99.98	98.81	819.2478	28
✓	C32 H48 N2 O19 S	C32 H48 Na O19 S	819.2464	98.71		796.2585	796.2572	-1.67	1.67	98.3	99.83	99.9	819.2478	10
✓	C34 H44 N4 O18	C34 H44 Na O18	819.2543	98.58		796.2585	796.2651	8.21	8.21	98.85	99.99	97.71	819.2478	15
✓	C33 H48 O22	C33 H48 Na O22	819.2529	98.57		796.2585	796.2637	6.56	6.56	97.46	99.98	98.53	819.2478	10
✓	C50 H40 N2 O6 S	C50 H40 Na O6 S	819.2499	98.44		796.2585	796.2607	2.75	2.75	95.02	99.95	99.74	819.2478	32
✓	C48 H36 N4 O8	C48 H36 Na O8	819.2425	98.39		796.2585	796.2533	-6.54	6.54	96.82	99.98	98.54	819.2478	33
✓	C47 H40 O12	C47 H40 Na O12	819.2412	98.38		796.2585	796.252	-8.2	8.2	98.17	99.97	97.72	819.2478	28
✓	C42 H44 N4 O8 S2	C42 H44 Na O8 S2	819.2483	98.34		796.2585	796.2601	1.9	1.9	94.62	99.73	99.88	819.2478	23
✓	C41 H48 O12 S2	C41 H48 Na O12 S2	819.2479	98.29		796.2585	796.2587	0.24	0.24	94.23	99.73	100	819.2478	18
✓	C39 H44 N2 O14 S	C39 H44 Na O14 S	819.2405	98.26		796.2585	796.2513	-9.04	9.04	98.61	99.89	97.23	819.2478	19
✓	C53 H36 N2 O6	C53 H36 Na O6	819.2466	98.19		796.2585	796.2573	-1.48	1.48	93.8	99.97	99.93	819.2478	37
✓	C28 H48 N2 O24	C28 H48 Na O24	819.2489	97.96		796.2585	796.2597	1.49	1.49	92.98	99.99	99.92	819.2478	6
✓	C36 H48 N2 O14 S2	C36 H48 Na O14 S2	819.2439	97.76		796.2585	796.2547	-4.82	4.82	93.78	99.66	99.2	819.2478	14
✓	C49 H40 N4 O3 S2	C49 H40 Na O3 S2	819.2434	97.18		796.2585	796.2542	-5.47	5.47	91.99	99.8	98.98	819.2478	32
✓	C47 H44 N2 O6 S2	C47 H44 Na O6 S2	819.2533	97.17		796.2585	796.2641	6.97	6.97	93.03	99.79	98.35	819.2478	27
✓	C48 H44 O7 S2	C48 H44 Na O7 S2	819.2421	97.01		796.2585	796.2528	-7.13	7.13	92.59	99.81	98.27	819.2478	27
✓	C58 H36 O4	C58 H36 Na O4	819.2506	96.98		796.2585	796.2614	3.58	3.58	90.2	99.96	99.56	819.2478	41
✓	C54 H40 N2 O S2	C54 H40 Na O S2	819.2474	96.83		796.2585	796.2582	-0.4	0.4	89.05	99.85	99.99	819.2478	36
✓	C35 H48 N4 O13 S2	C35 H48 Na O13 S2	819.2552	96.81		796.2585	796.2659	9.27	9.27	93.99	99.63	97.09	819.2478	14
✓	C27 H48 N4 O21 S	C27 H48 Na O21 S	819.2424	96.76		796.2585	796.2532	-6.74	6.74	91.43	99.78	98.45	819.2478	6
✓	C34 H52 O17 S2	C34 H52 Na O17 S2	819.2538	96.74		796.2585	796.2646	7.62	7.62	92.19	99.64	98.03	819.2478	9
✓	C57 H36 N2 O S	C57 H36 Na O S	819.2441	96.73		796.2585	796.2548	-4.63	4.63	89.81	99.97	99.27	819.2478	41
✓	C55 H40 O4 S	C55 H40 Na O4 S	819.254	96.67		796.2585	796.2647	7.81	7.81	91.82	99.96	97.93	819.2478	36
✓	C29 H52 N2 O19 S2	C29 H52 Na O19 S2	819.2498	96.58		796.2585	796.2606	2.55	2.55	88.78	99.56	99.78	819.2478	5
✓	C52 H36 N4 O3 S	C52 H36 Na O3 S	819.24	96.57		796.2585	796.2508	-9.69	9.69	93.33	99.95	96.83	819.2478	37
✓	C59 H32 N4	C59 H32 Na O	819.2519	96.12		796.2585	796.2627	5.25	5.25	88	99.97	99.06	819.2478	46
✓	C31 H48 N4 O16 S2	C31 H48 Na O16 S2	819.2399	95.92		796.2585	796.2507	-9.89	9.89	91.58	99.57	96.7	819.2478	10
✓	C25 H52 N2 O24 S	C25 H52 Na O24 S	819.2523	95.8		796.2585	796.2631	5.7	5.7	87.35	99.76	98.89	819.2478	1
✓	C56 H36 N4 S	C56 H36 Na O	819.2553	95.74		796.2585	796.2661	9.47	9.47	90.19	99.96	96.97	819.2478	41
✓	C26 H52 O25 S	C26 H52 Na O25 S	819.2411	95.3		796.2585	796.2518	-8.39	8.39	87.71	99.78	97.61	819.2478	1
✓	C60 H32 N2 O	C60 H32 Na O	819.2407	95.23		796.2585	796.2515	-8.85	8.85	87.76	99.97	97.34	819.2478	46
✓	C24 H52 N4 O21 S2	C24 H52 Na O21 S2	819.2458	94.96		796.2586	796.2565	-2.52	2.52	83.18	99.47	99.78	819.2478	1

Figure S13. The HRESIMS spectrum of compound **2**.

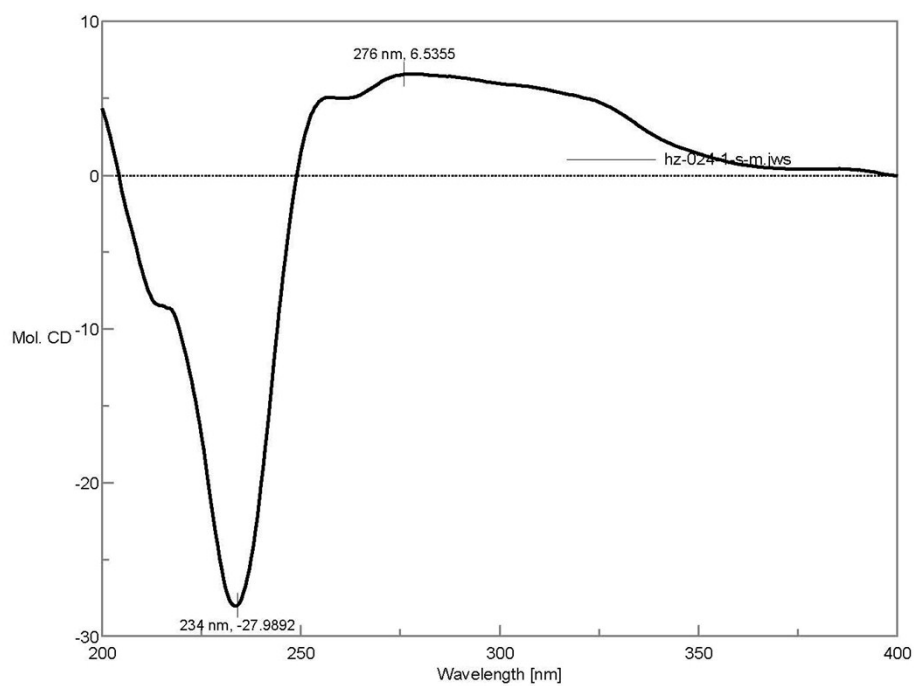


Figure S14. The CD spectrum of **2** in MeOH.

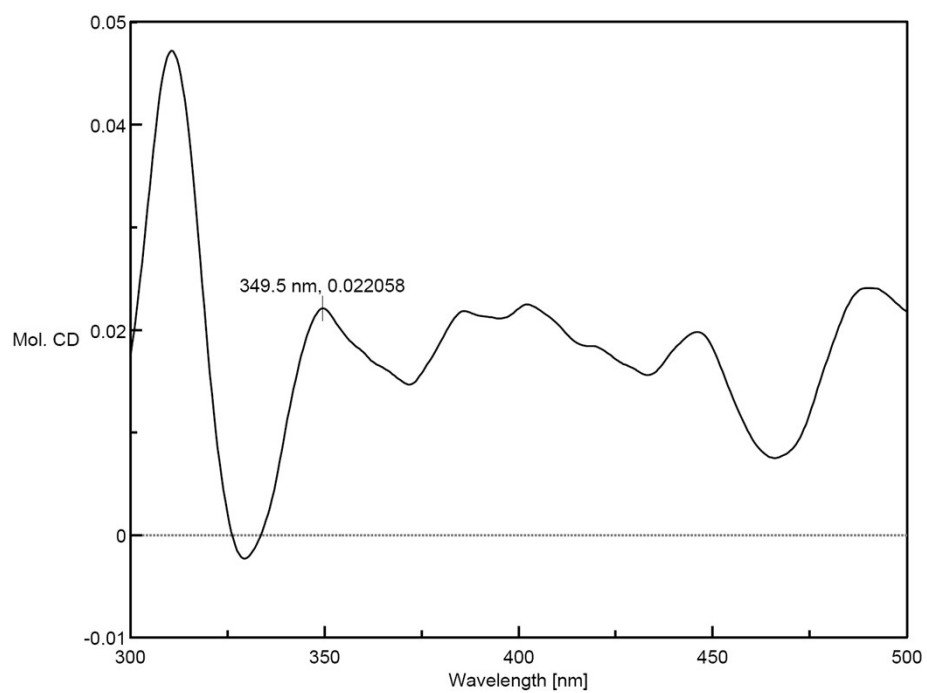


Figure S15. The $\text{Rh}_2(\text{OCOCF}_3)_4$ induced CD spectrum of **2a** in CHCl_3 .

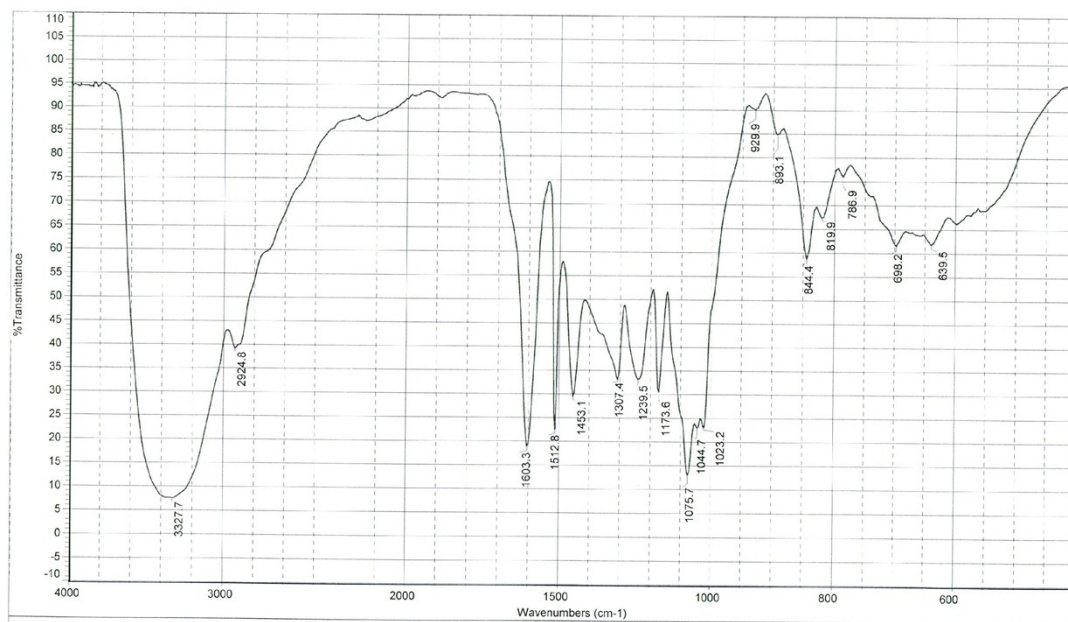


Figure S16. The IR spectrum of compound **2**.

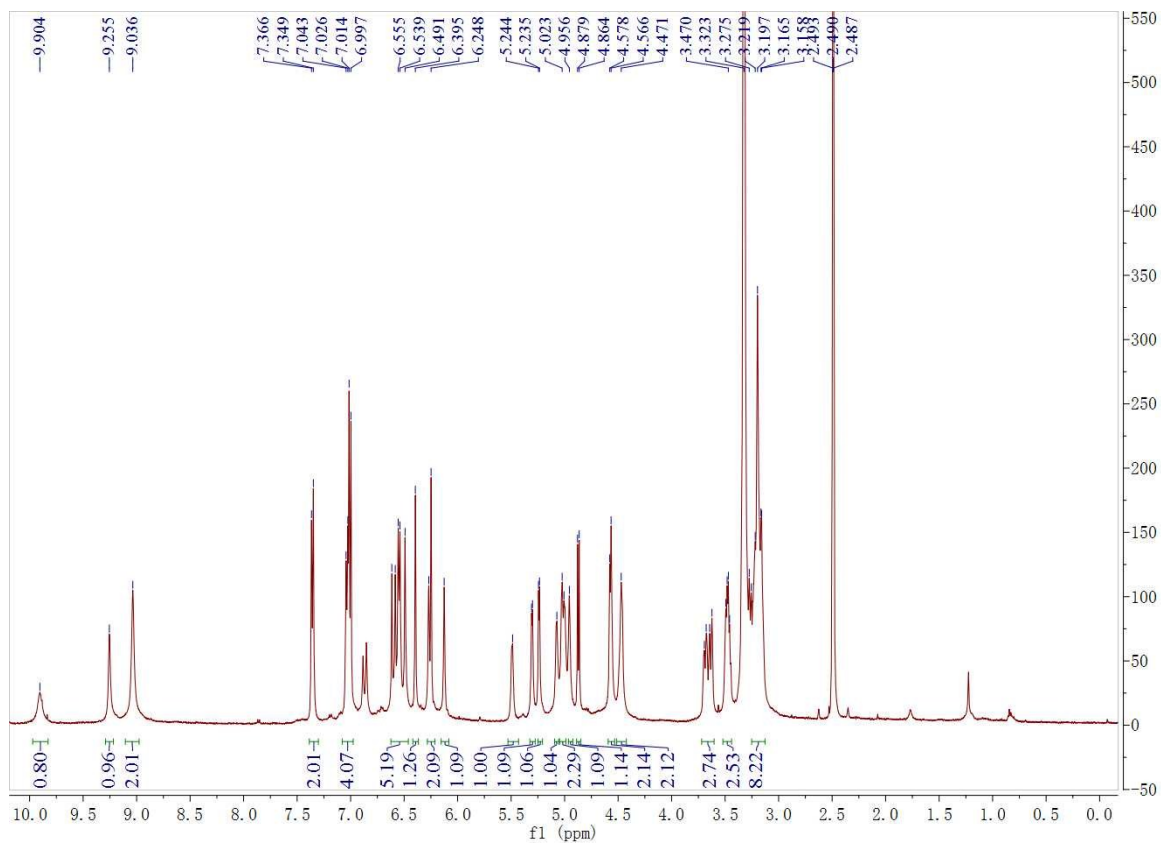


Figure S17. The ¹H NMR spectrum of compound **3** in DMSO-*d*₆.

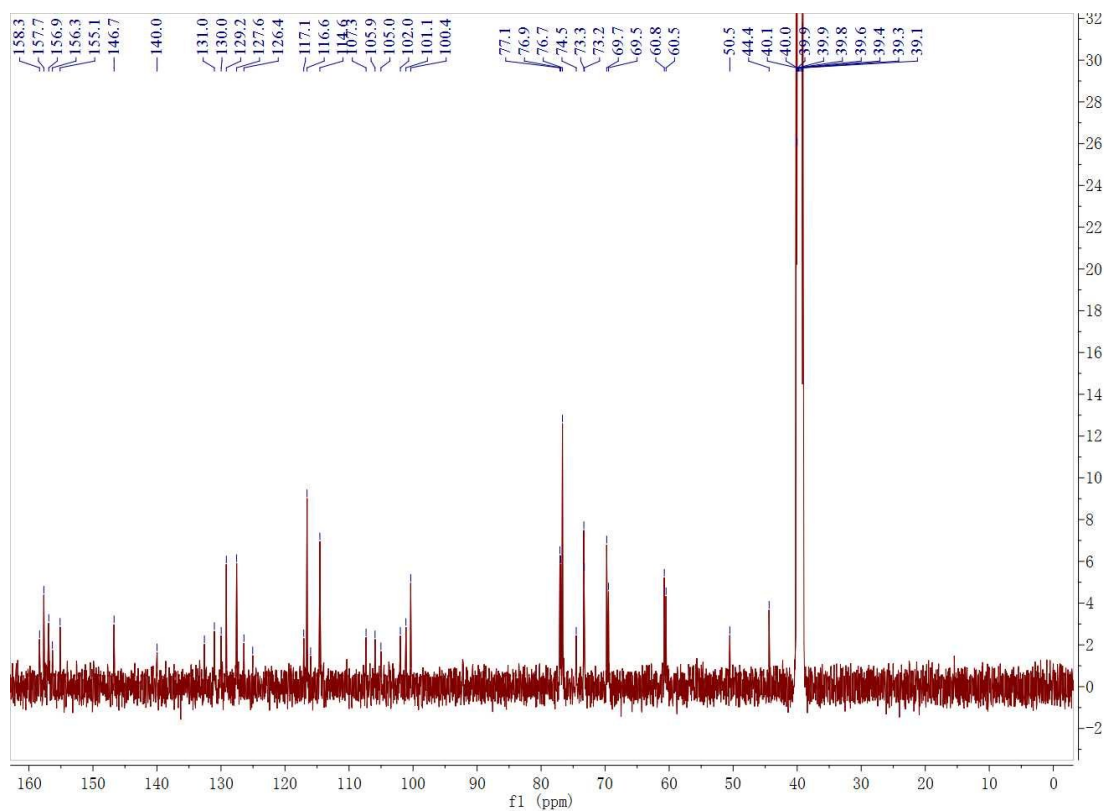


Figure S18. The ^{13}C NMR spectrum of compound **3** in $\text{DMSO-}d_6$.

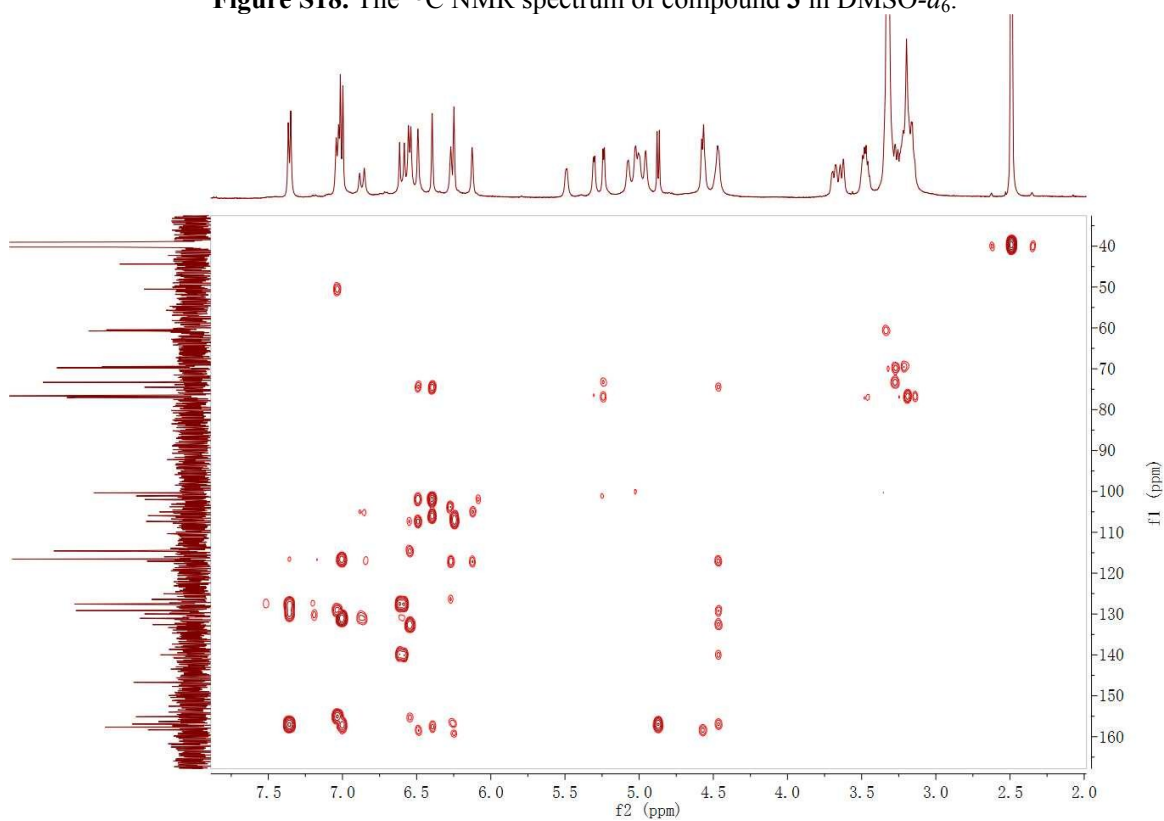


Figure S19. The HMBC spectrum of compound **3** in $\text{DMSO-}d_6$.

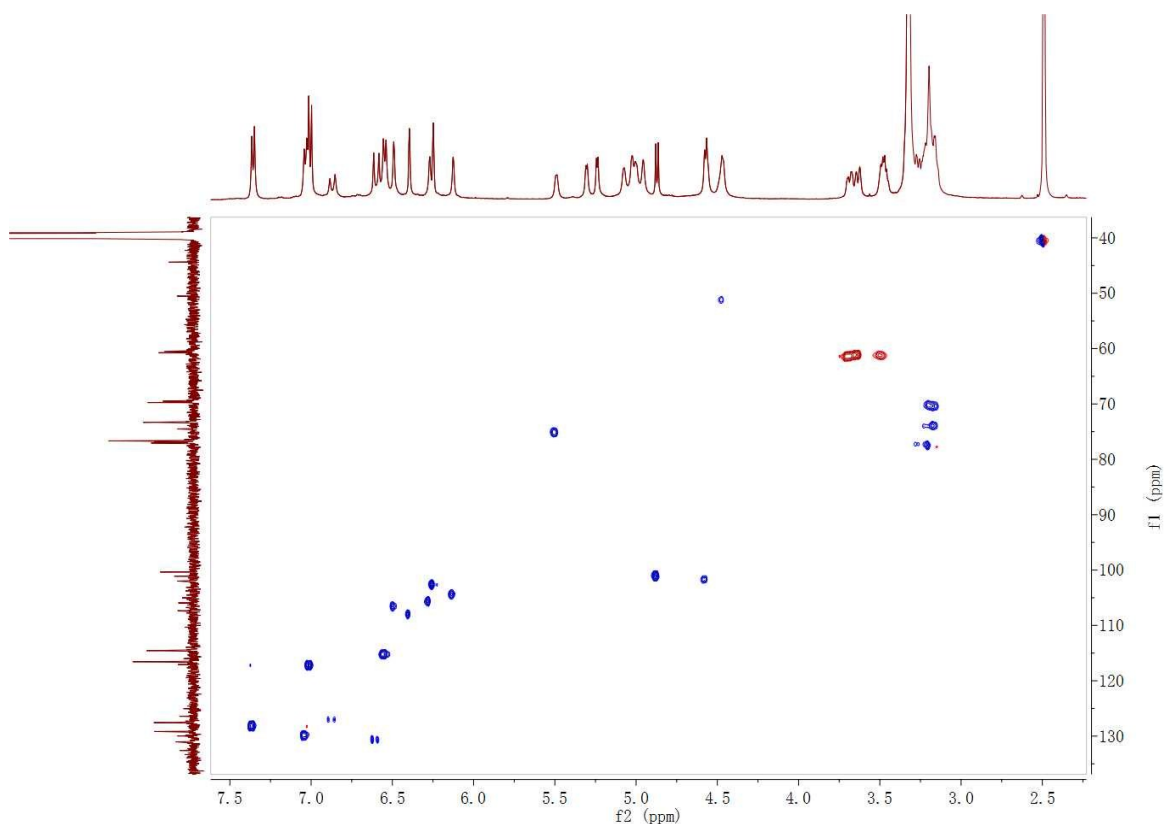


Figure S20. The HSQC spectrum of compound **3** in DMSO- d_6 .

m/z	Ion	Formula	Abundance
819.2464	(M+Na) ⁺	C40 H44 Na O17	246252.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C40 H44 O17	C40 H44 Na O17	819.2471	99.96		796.2572	796.2578	0.86	0.86	99.94	99.95	99.97	819.2464	19
+	C35 H44 N2 O19	C35 H44 N2 Na O19	819.243	99.55		796.2572	796.2538	-4.2	4.2	95.47	99.97	99.39	819.2454	15
+	C47 H40 O12	C47 H40 Na O12	819.2412	98.55		796.2572	796.252	-6.52	6.52	97.39	99.93	98.55	819.2454	26
+	C33 H48 O22	C33 H48 Na O22	819.2529	98.38		796.2572	796.2637	8.24	8.24	98.18	99.97	97.7	819.2454	10
+	C46 H40 N2 O11	C46 H40 N2 Na O11	819.2524	98.36		796.2572	796.2632	7.58	7.58	97.58	99.94	98.04	819.2454	26
+	C28 H48 N2 O24	C28 H48 N2 Na O24	819.2489	98.17		796.2572	796.2597	3.17	3.17	94.18	99.98	99.66	819.2454	6
+	C53 H35 N2 O6	C53 H35 N2 Na O6	819.2466	97.83		796.2572	796.2573	0.21	0.21	92.46	99.93	100	819.2454	37
+	C58 H36 O4	C58 H36 Na O4	819.2506	96.26		796.2572	796.2614	5.27	5.27	85.55	99.91	99.05	819.2454	41
+	C60 H32 N2 O	C60 H32 N2 Na O	819.2407	95.14		796.2572	796.2515	-7.17	7.17	85.97	99.92	98.25	819.2454	46
+	C47 H41 Cl N2 O8	C47 H41 Cl N2 Na O8	819.2444	86.94		796.2572	796.2551	-2.56	2.56	55	99.6	99.77	819.2454	26
+	C52 H41 Cl O6	C52 H41 Cl Na O6	819.2484	86.89		796.2572	796.2592	2.5	2.5	54.74	99.66	99.79	819.2454	32
+	C59 H37 Cl O	C59 H37 Cl Na O	819.2425	86.32		796.2572	796.2533	-4.88	4.88	53.7	99.73	99.19	819.2454	41
+	C40 H45 Cl N2 O13	C40 H45 Cl N2 Na O13	819.2502	86.17		796.2572	796.261	4.81	4.81	53.32	99.52	99.21	819.2454	19
+	C58 H37 Cl N2	C58 H37 Cl N2 Na	819.2537	85.45		796.2572	796.2645	9.22	9.22	54.11	99.72	97.12	819.2454	41
+	C54 H37 Cl N2 O3	C54 H37 Cl N2 Na O3	819.2385	85.43		796.2572	796.2493	-9.94	9.94	54.82	99.68	96.66	819.2454	37
+	C34 H49 Cl O19	C34 H49 Cl Na O19	819.2449	85.27		796.2572	796.2557	-1.91	1.91	49.11	99.46	99.87	819.2454	10
+	C45 H45 Cl O11	C45 H45 Cl Na O11	819.2543	85.27		796.2572	796.265	9.87	9.87	54.27	99.58	96.71	819.2454	23
+	C41 H45 Cl O14	C41 H45 Cl Na O14	819.239	85.09		796.2572	796.2498	-9.29	9.29	53.05	99.54	97.08	819.2454	19

Figure S21. The HRESIMS of compound **3**.

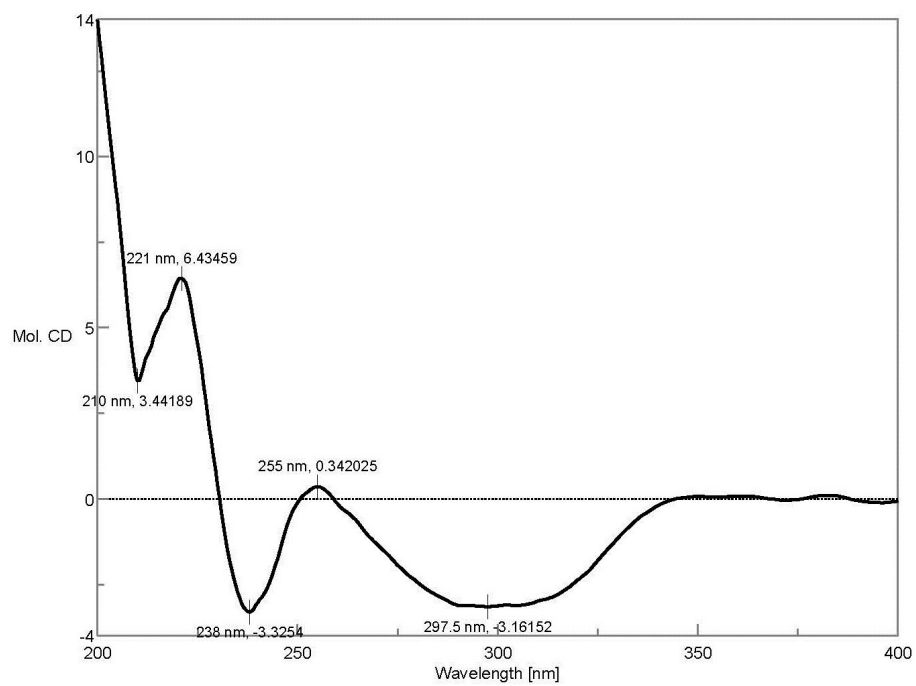


Figure S22. The CD spectrum of **3** in MeOH.

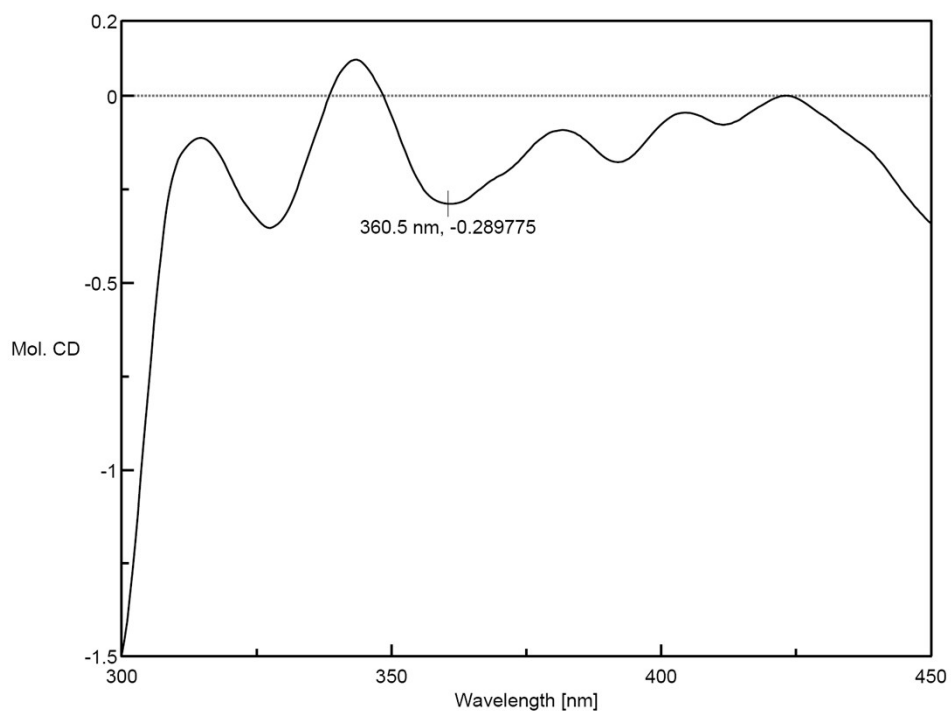


Figure S23. The $\text{Rh}_2(\text{OCOCF}_3)_4$ induced CD spectrum of **3a** in CHCl_3 .

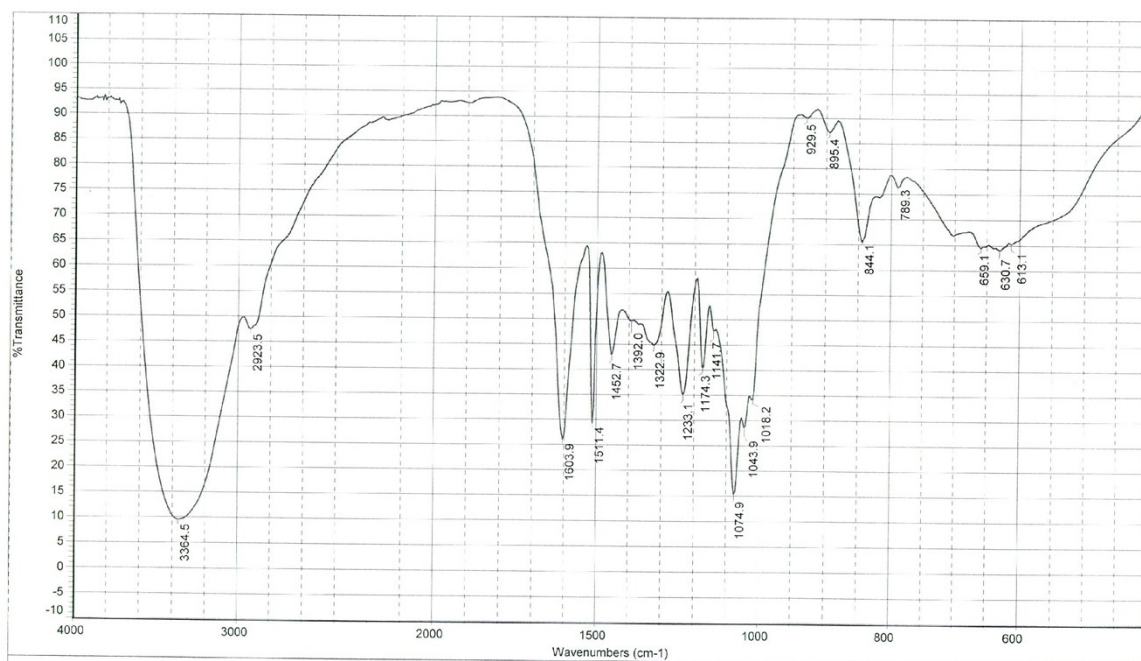


Figure S24. The IR spectrum of compound 3.

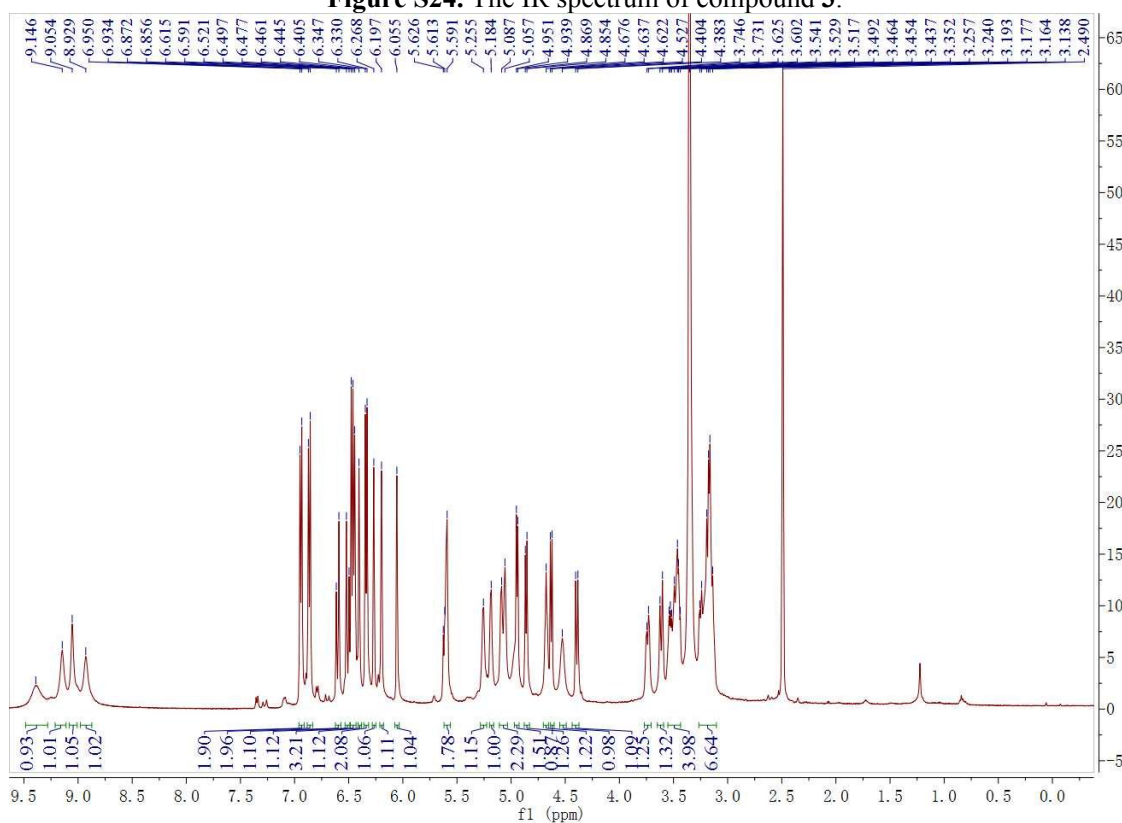


Figure S25. The ¹H NMR spectrum of compound 4 in DMSO-d₆.

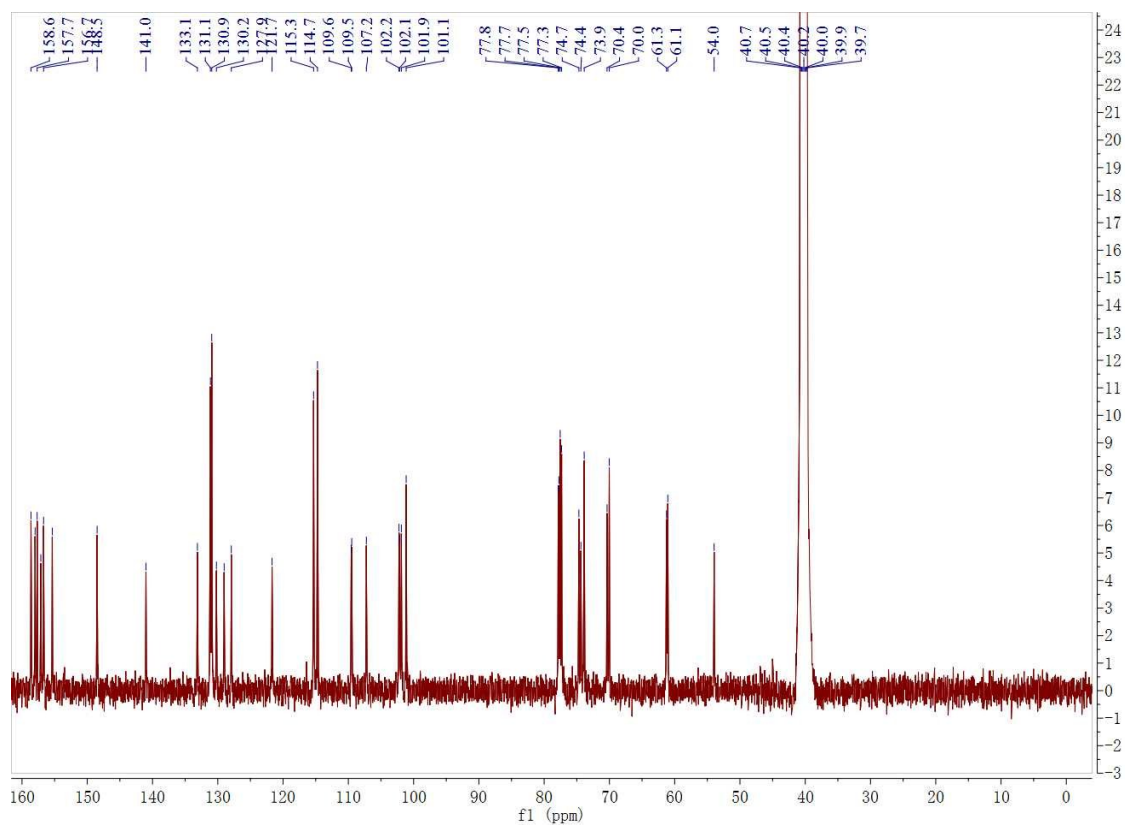


Figure S26. The ^{13}C NMR spectrum of compound **4** in $\text{DMSO}-d_6$.

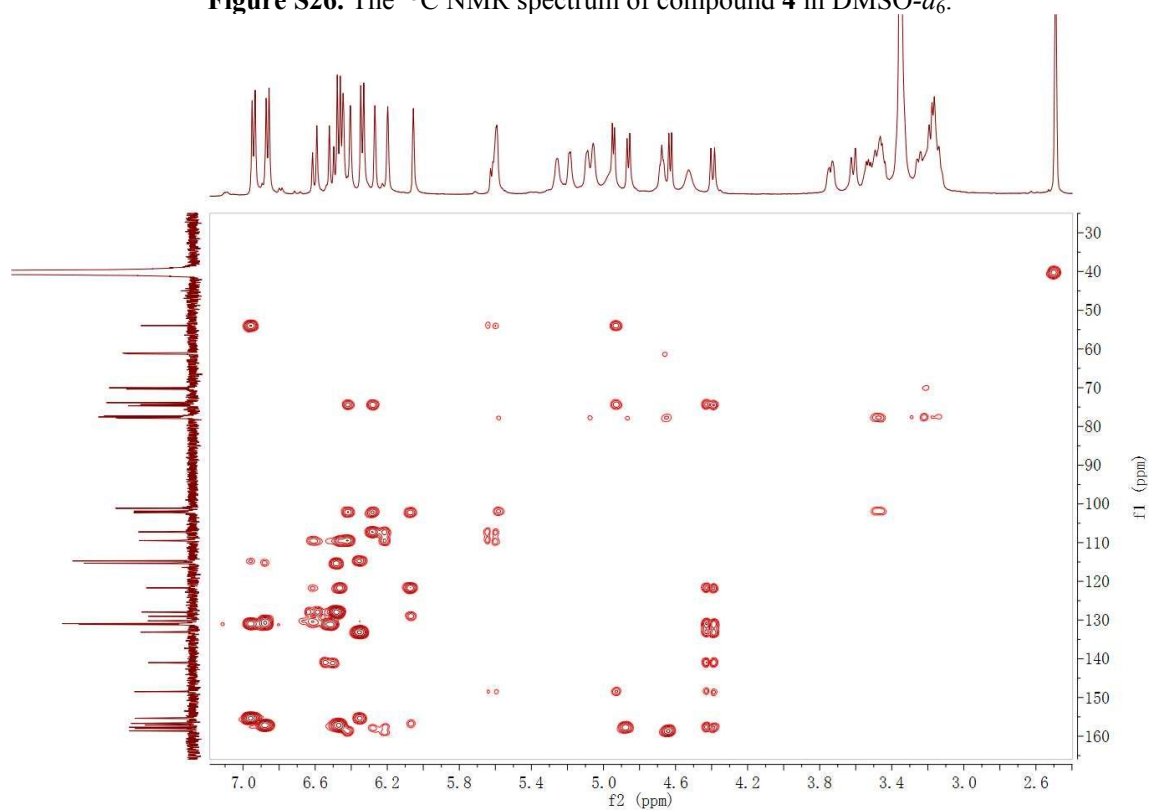


Figure S27. The HMBC spectrum of compound **4** in $\text{DMSO}-d_6$.

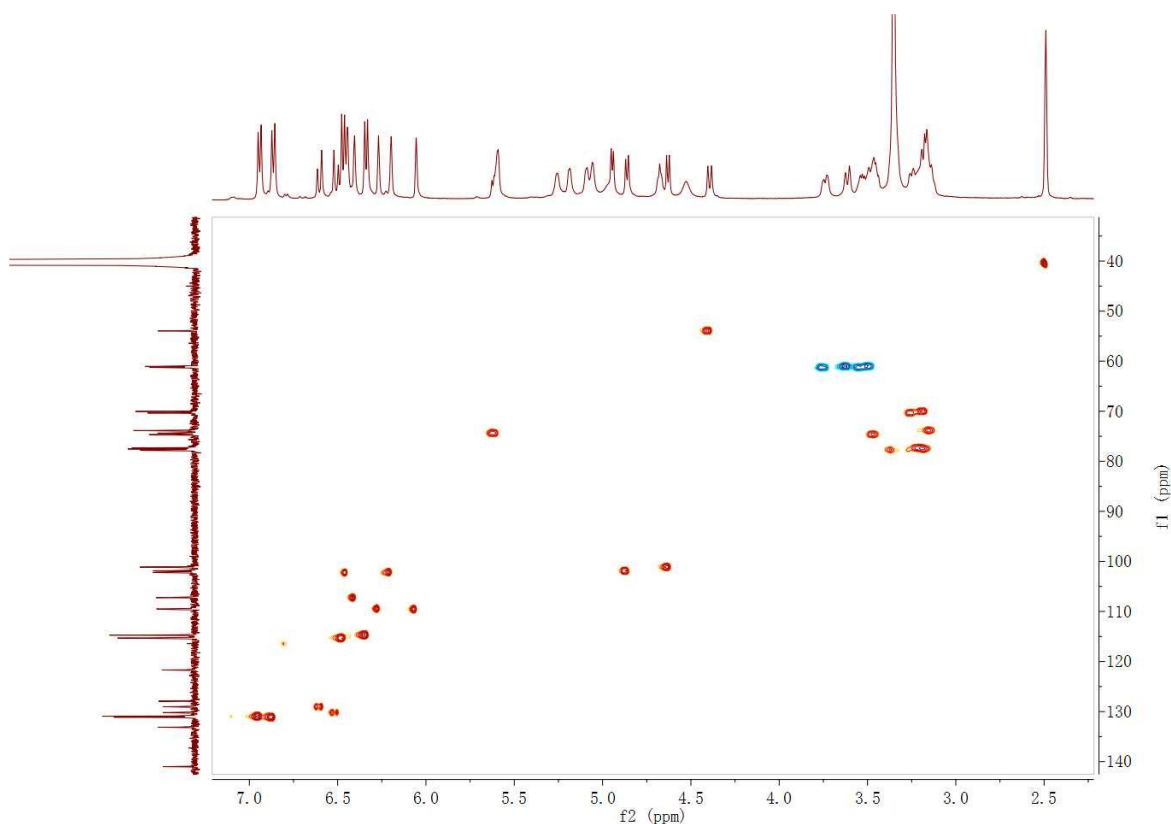


Figure S28. The HSQC spectrum of compound **4** in DMSO- d_6 .

m/z	Ion	Formula	Abundance
819.2463	(M+Na) ⁺	C40 H44 Na O12	199275.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C40 H44 O12	C40 H44 Na O12	819.2471	99.94		796.257	796.2578	1.01	1.01	99.87	99.98	99.97	819.2463	19
+	C35 H44 N2 O19	C35 H44 Na O19	819.243	99.61		796.2571	796.2538	-4.06	4.06	99.59	99.99	99.44	819.2463	15
+	C47 H40 O12	C47 H40 Na O12	819.2412	98.49		796.257	796.252	-6.37	6.37	97.05	99.98	96.62	819.2463	28
+	C33 H48 O22	C33 H48 Na O22	819.2529	98.41		796.257	796.2637	8.38	8.38	98.41	99.99	97.61	819.2463	10
+	C28 H48 N2 O24	C28 H48 Na O24	819.2469	98.27		796.2571	796.2597	3.32	3.32	94.59	99.99	99.62	819.2463	6
+	C46 H40 N2 O11	C46 H40 Na O11	819.2524	98.24		796.2571	796.2632	7.73	7.73	97.24	99.99	97.57	819.2463	28
+	C53 H36 N2 O6	C53 H36 Na O6	819.2466	97.68		796.2571	796.2573	0.35	0.35	91.91	99.98	100	819.2463	37
+	C58 H26 O4	C58 H26 Na O4	819.2506	96.06		796.257	796.2614	5.41	5.41	87.9	99.97	99	819.2463	41
+	C60 H32 N2 O	C60 H32 Na O	819.2407	94.98		796.2571	796.2515	-7.02	7.02	85.76	99.98	98.32	819.2463	46
+	C47 H41 Cl N2 O8	C47 H41 Cl Na O8	819.2444	86.9		796.2571	796.2561	-2.41	2.41	95.01	99.36	99.8	819.2463	28
+	C52 H41 Cl O6	C52 H41 Cl Na O6	819.2484	86.82		796.2571	796.2562	-2.65	2.65	94.73	99.43	99.76	819.2463	32
+	C59 H37 Cl O	C59 H37 Cl Na O	819.2425	86.28		796.2571	796.2533	-4.73	4.73	93.66	99.52	99.23	819.2463	41
+	C40 H45 Cl N2 O13	C40 H45 Cl Na O13	819.2522	86.09		796.2571	796.261	4.96	4.96	93.35	99.25	99.16	819.2463	19
+	C54 H37 Cl N2 O3	C54 H37 Cl Na O3	819.2385	85.41		796.2571	796.2493	-6.79	6.79	94.8	99.45	96.76	819.2463	37
+	C58 H37 Cl N2	C58 H37 Cl Na	819.2637	85.35		796.2571	796.2645	9.37	9.37	94.08	99.51	97.03	819.2463	41
+	C34 H49 Cl O19	C34 H49 Cl Na O19	819.2649	85.23		796.2571	796.2557	-1.76	1.76	49.17	99.19	99.89	819.2463	10
+	C41 H45 Cl O14	C41 H45 Cl Na O14	819.239	85.08		796.2571	796.2498	-9.14	9.14	53.09	99.28	97.17	819.2463	19

Figure S29. The HRESIMS of compound **4**.

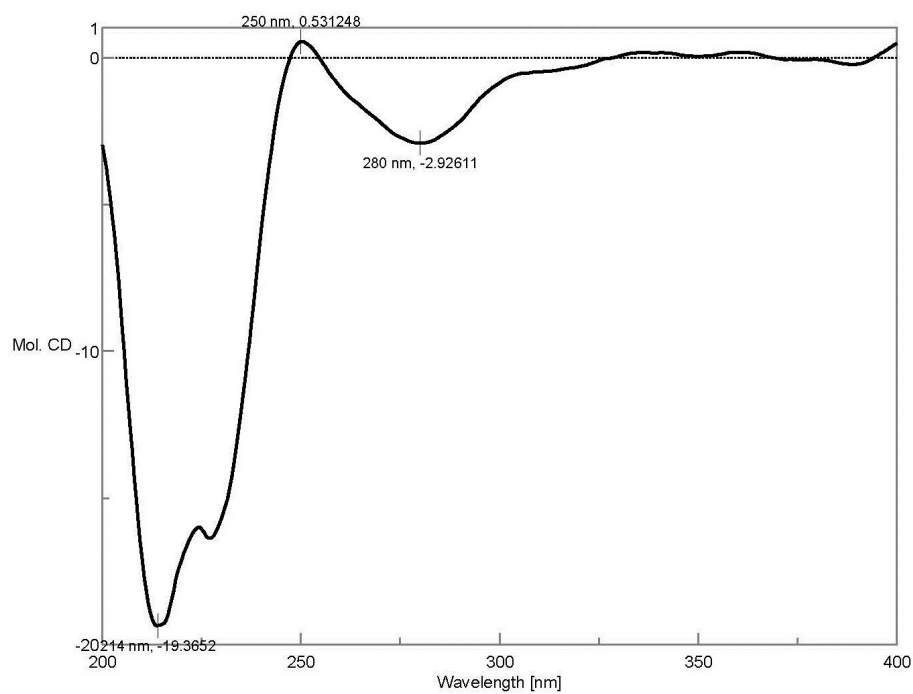


Figure S30. The CD spectrum of **4** in MeOH.

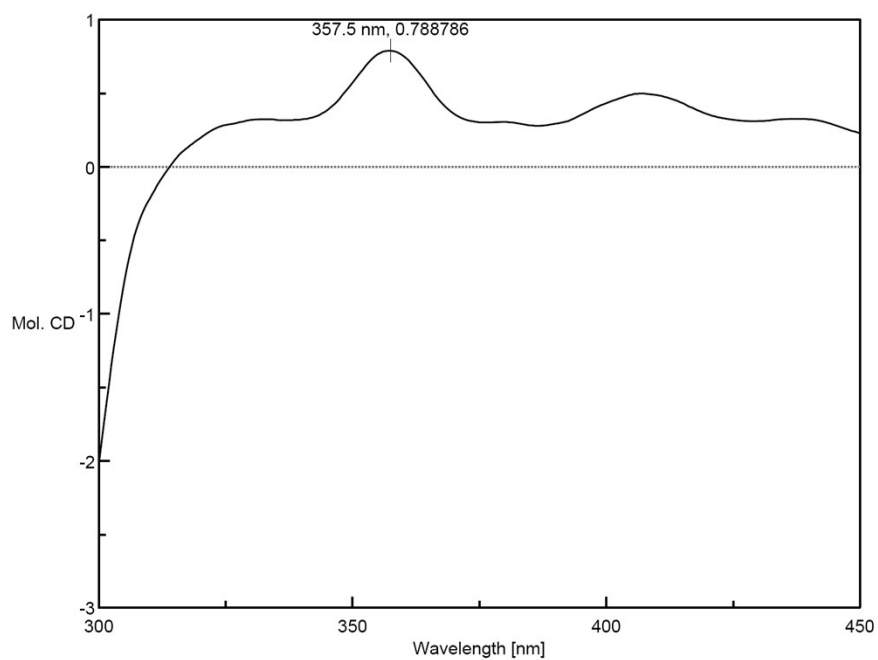


Figure S31. The $\text{Rh}_2(\text{OCOCF}_3)_4$ induced CD spectrum of **4a** in CHCl_3 .

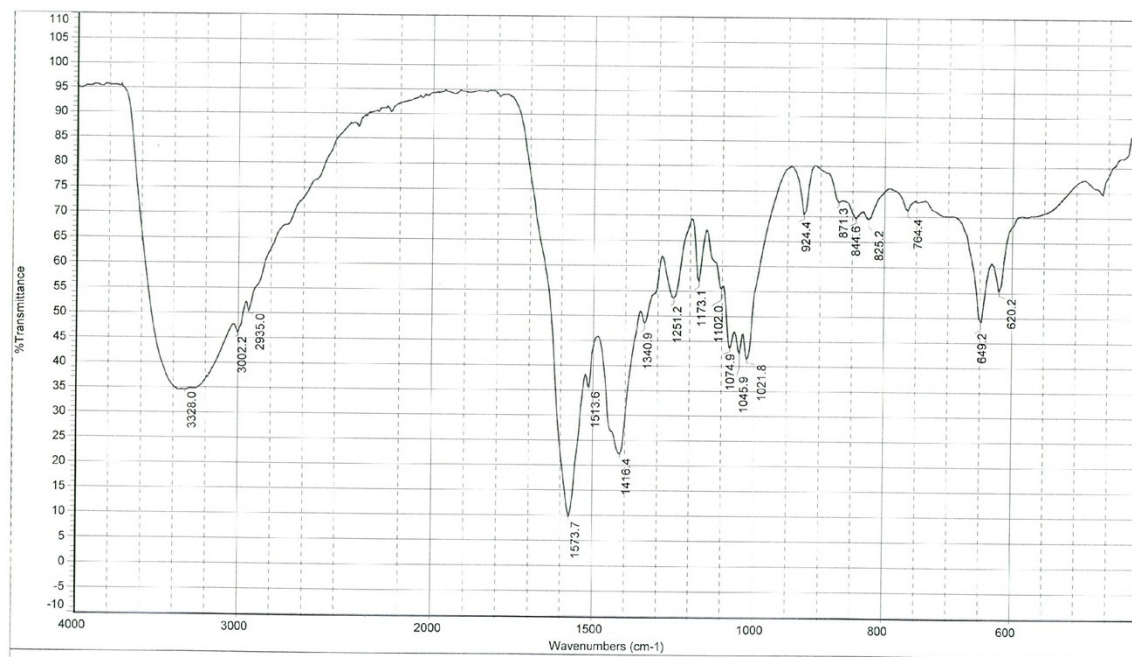


Figure S32. The IR spectrum of compound 4.

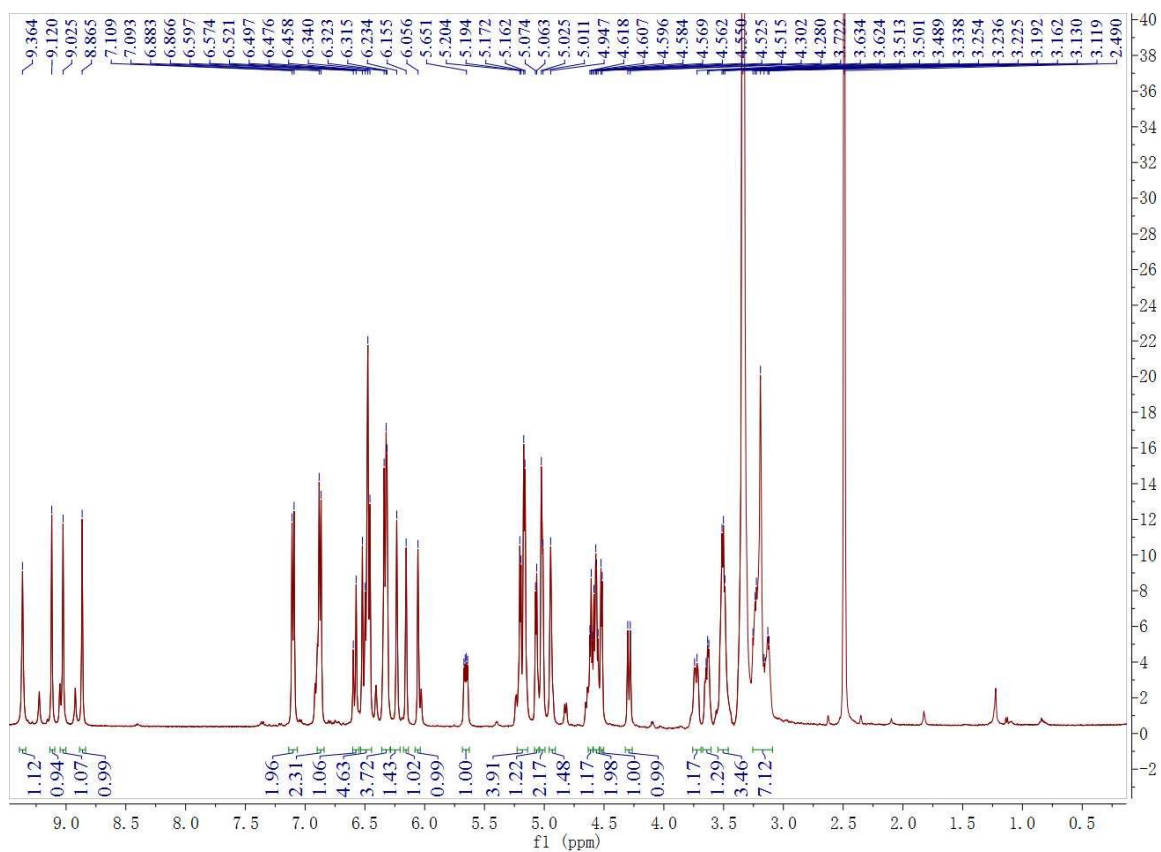


Figure S33. The ¹H NMR spectrum of compound 5 in DMSO-d₆.

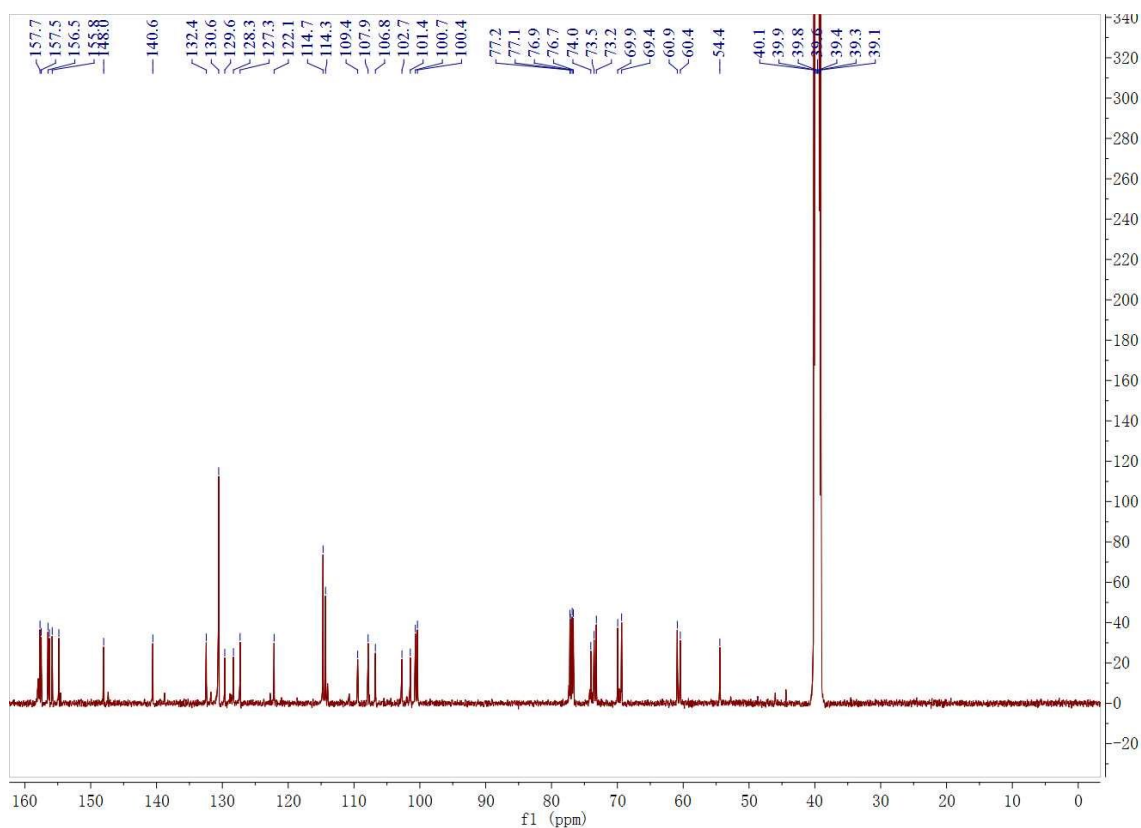


Figure S34. The ^{13}C NMR spectrum of compound **5** in $\text{DMSO-}d_6$.

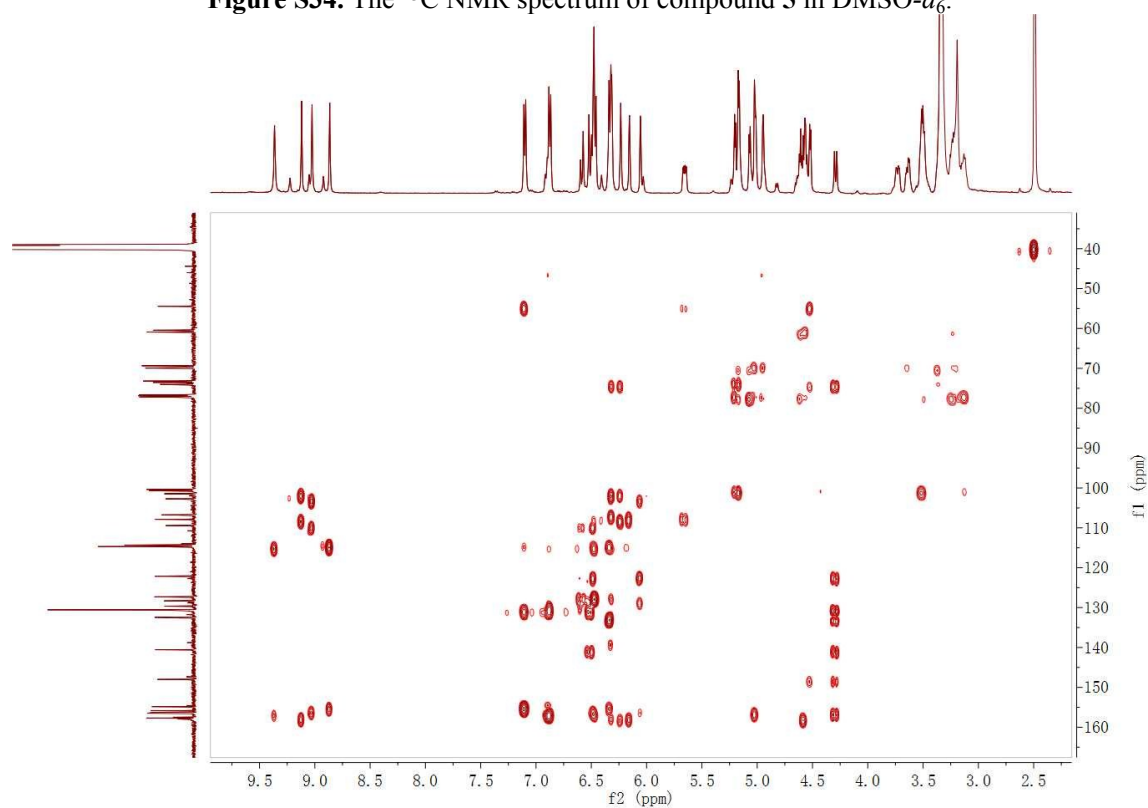


Figure S35. The HMBC spectrum of compound **5** in $\text{DMSO-}d_6$.

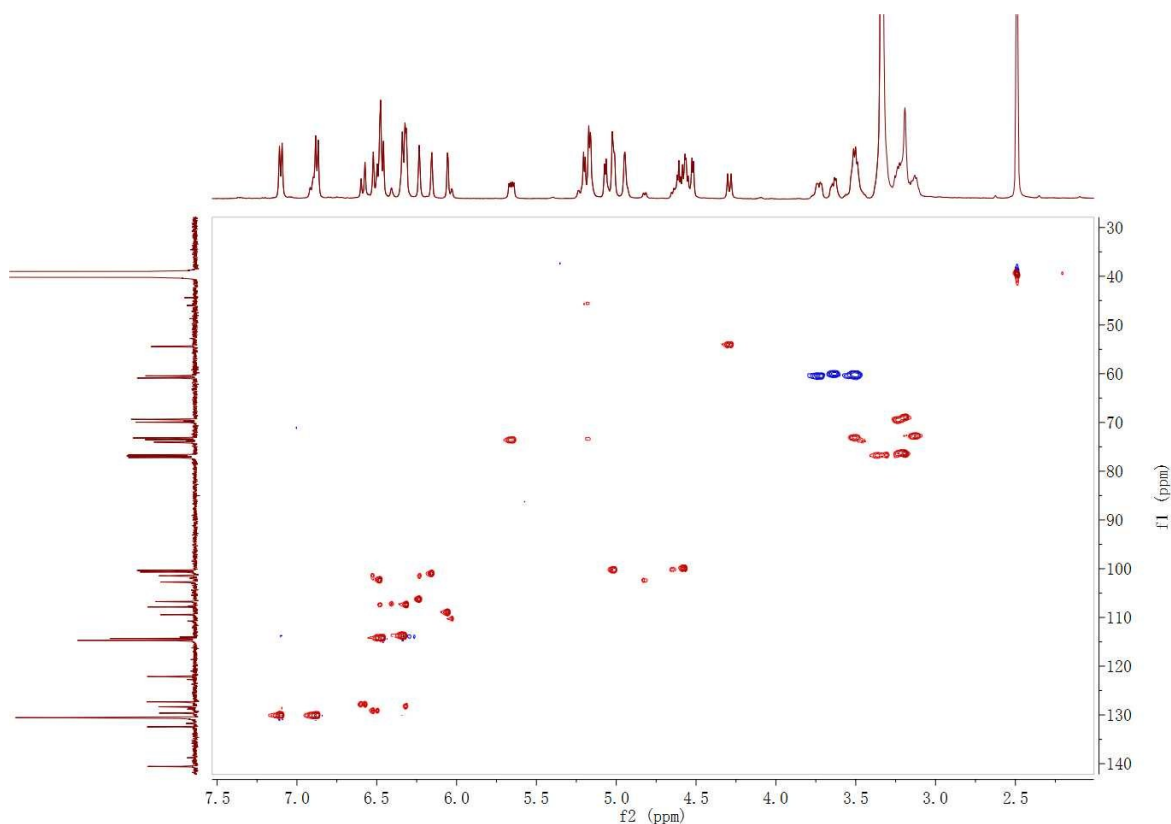


Figure S36. The HSQC spectrum of compound **5** in DMSO- d_6 .

m/z	Ion	Formula	Abundance
819.2468	(M+Na) ⁺	C40 H44 Na O17	295589.7

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spicing Mat	Mass Match	m/z	DBE
✓	C40 H44 O17	C40 H44 Na O17	819.2471	99.97		796.2576	796.2578	0.36	0.36	99.96	99.94	100	819.2468	19
	C41 H40 N4 O13	C41 H40 N4 Na O13	819.2484	99.79		796.2576	796.2592	2.02	2.02	99.52	99.96	99.86	819.2468	24
	C35 H44 N2 O19	C35 H44 N2 Na O19	819.2453	99.47		796.2576	796.2538	-4.7	4.7	99.42	99.96	99.24	819.2468	15
	C44 H44 O12 S	C44 H44 Na O12 S	819.2446	99.12		796.2576	796.2553	-2.79	2.79	97.41	99.97	99.73	819.2468	23
	C37 H48 O17 S	C37 H48 Na O17 S	819.2504	99.07		796.2576	796.2512	-4.58	4.58	97.99	99.94	99.28	819.2468	14
	C45 H40 N4 O8 S	C45 H40 N4 Na O8 S	819.2450	99.04		796.2576	796.2567	-1.13	1.13	96.75	99.97	99.96	819.2468	28
	C38 H44 N4 O13 S	C38 H44 N4 Na O13 S	819.2518	98.96		796.2576	796.2526	-6.24	6.24	98.61	99.94	98.67	819.2468	19
	C32 H48 N2 O19 S	C32 H48 N2 Na O19 S	819.2464	98.9		796.2576	796.2572	-0.48	0.48	96.23	99.91	96.99	819.2468	10
	C39 H44 N2 O14 S	C39 H44 N2 Na O14 S	819.2405	98.54		796.2576	796.2513	-7.85	7.85	98.42	99.95	97.9	819.2468	19
	C46 H40 N2 O11	C46 H40 N2 Na O11	819.2524	98.51		796.2576	796.2532	-7.09	7.09	97.69	99.94	98.29	819.2468	28
	C47 H40 O12	C47 H40 Na O12	819.2412	98.48		796.2576	796.252	-7.61	7.61	97.52	99.93	98.32	819.2468	28
	C33 H48 O22	C33 H48 Na O22	819.2529	98.48		796.2576	796.2537	-7.74	7.74	98.1	99.96	97.96	819.2468	10
	C48 H36 N4 O8	C48 H36 N4 Na O8	819.2425	98.38		796.2576	796.2533	-5.35	5.35	96.01	99.95	96.02	819.2468	33
	C34 H44 N4 O18	C34 H44 N4 Na O18	819.2543	98.37		796.2576	796.2551	-9.4	9.4	99.28	99.97	97.01	819.2468	15
	C28 H48 N2 O24	C28 H48 N2 Na O24	819.2489	98.17		796.2576	796.2597	2.67	2.67	94.03	99.98	96.75	819.2468	6
	C50 H40 N2 O6 S	C50 H40 N2 Na O6 S	819.2499	98.03		796.2576	796.2607	3.93	3.93	94	99.98	96.47	819.2468	32
	C53 H36 N2 O6	C53 H36 N2 Na O6	819.2466	97.89		796.2576	796.2573	-0.29	0.29	92.68	99.93	100	819.2468	37
	C30 H44 N4 O21	C30 H44 N4 Na O21	819.239	97.54		796.2576	796.2496	-9.77	9.77	96.79	99.98	96.78	819.2468	11
	C27 H48 N4 O21 S	C27 H48 N4 Na O21 S	819.2424	97.25		796.2576	796.2532	-5.55	5.55	92.25	99.87	96.95	819.2468	6
	C52 H36 N4 O3 S	C52 H36 N4 Na O3 S	819.24	96.59		796.2576	796.2508	-8.5	8.5	92.16	99.98	97.55	819.2468	37
	C57 H36 N2 O S	C57 H36 N2 Na O S	819.2441	96.49		796.2576	796.2548	-3.44	3.44	88.41	99.99	99.59	819.2468	41
	C58 H36 O4	C58 H36 Na O4	819.2506	96.42		796.2576	796.2614	4.77	4.77	88.83	99.91	99.22	819.2468	41
	C55 H40 O4 S	C55 H40 Na O4 S	819.254	95.99		796.2576	796.2647	8.99	8.99	90.56	99.98	97.26	819.2468	36
	C26 H52 O25 S	C26 H52 Na O25 S	819.2411	95.89		796.2576	796.2518	-7.2	7.2	88.67	99.87	96.23	819.2468	1
	C25 H52 N2 O24 S	C25 H52 N2 Na O24 S	819.2523	95.87		796.2576	796.2631	6.89	6.89	88.36	99.86	96.38	819.2468	1
	C59 H32 N4	C59 H32 N4 Na	819.2519	95.46		796.2576	796.2627	6.44	6.44	86.53	99.93	96.59	819.2468	46
	C60 H32 N2 O	C60 H32 N2 Na O	819.2407	95.1		796.2576	796.2515	-7.67	7.67	86.26	99.92	98	819.2468	46

Figure S37. The HRESIMS of compound **5**.

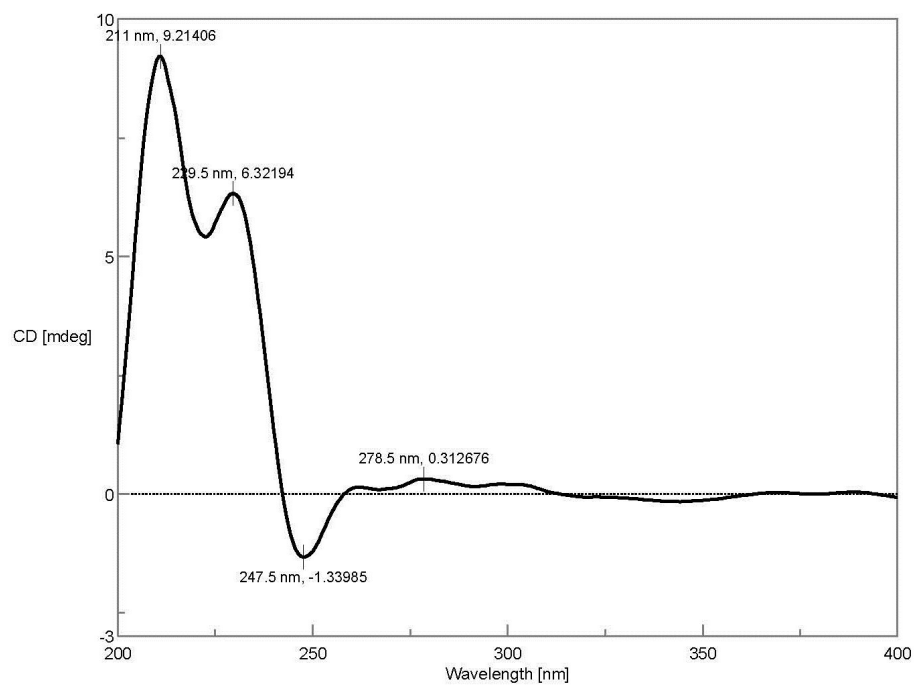


Figure S38. The CD spectrum of **5** in MeOH.

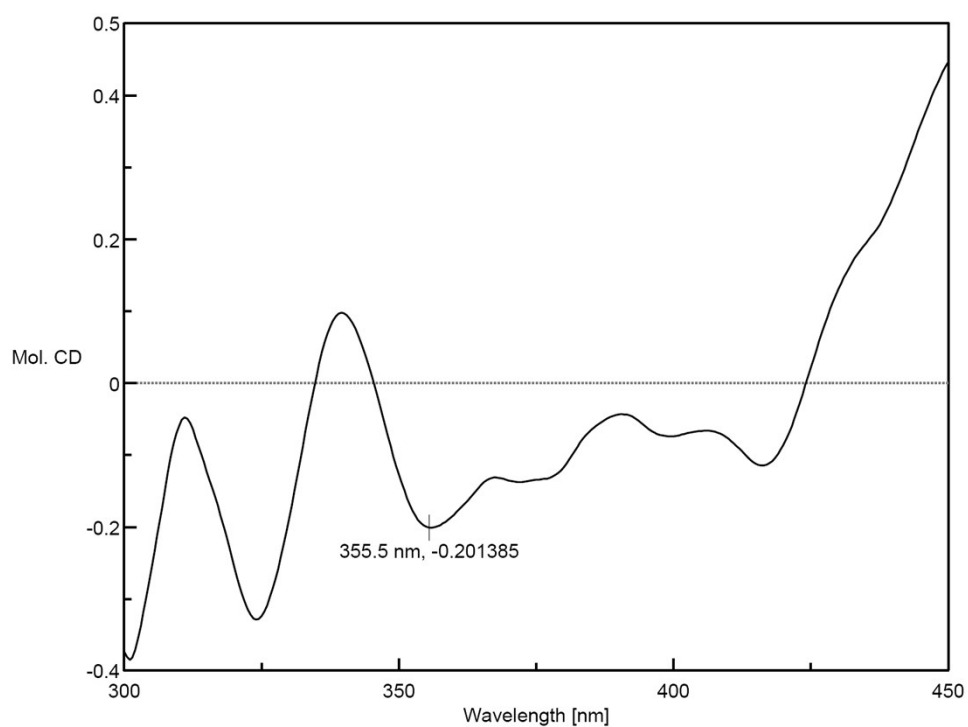


Figure S39. The $\text{Rh}_2(\text{OCOCF}_3)_4$ induced CD spectrum of **5a** in CHCl_3 .

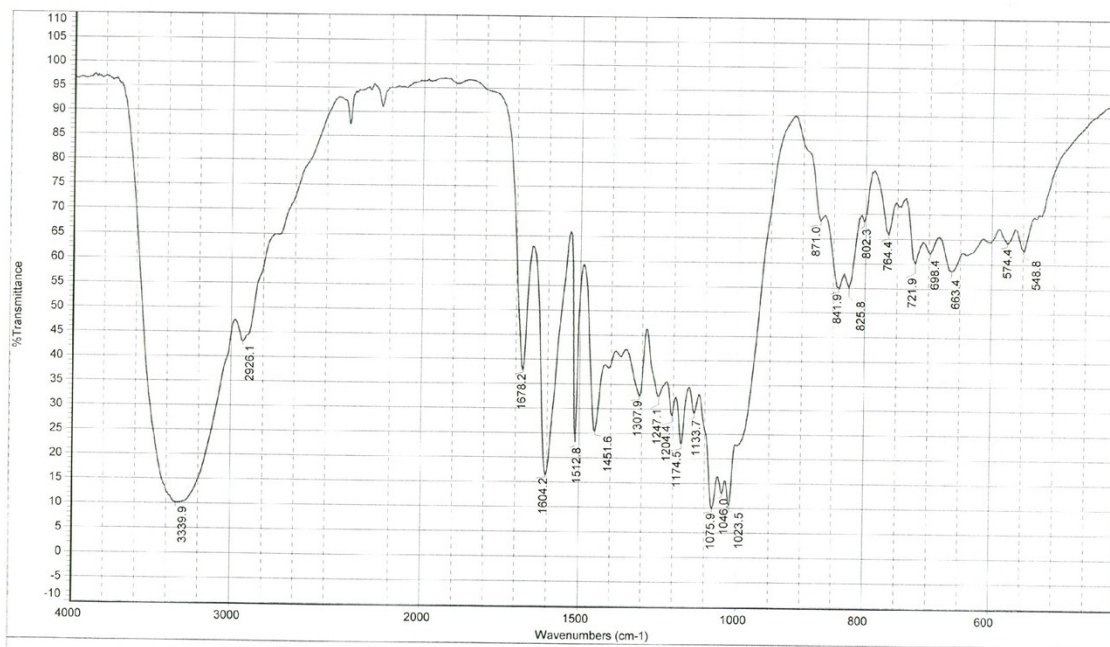


Figure S40. The IR spectrum of compound **5**

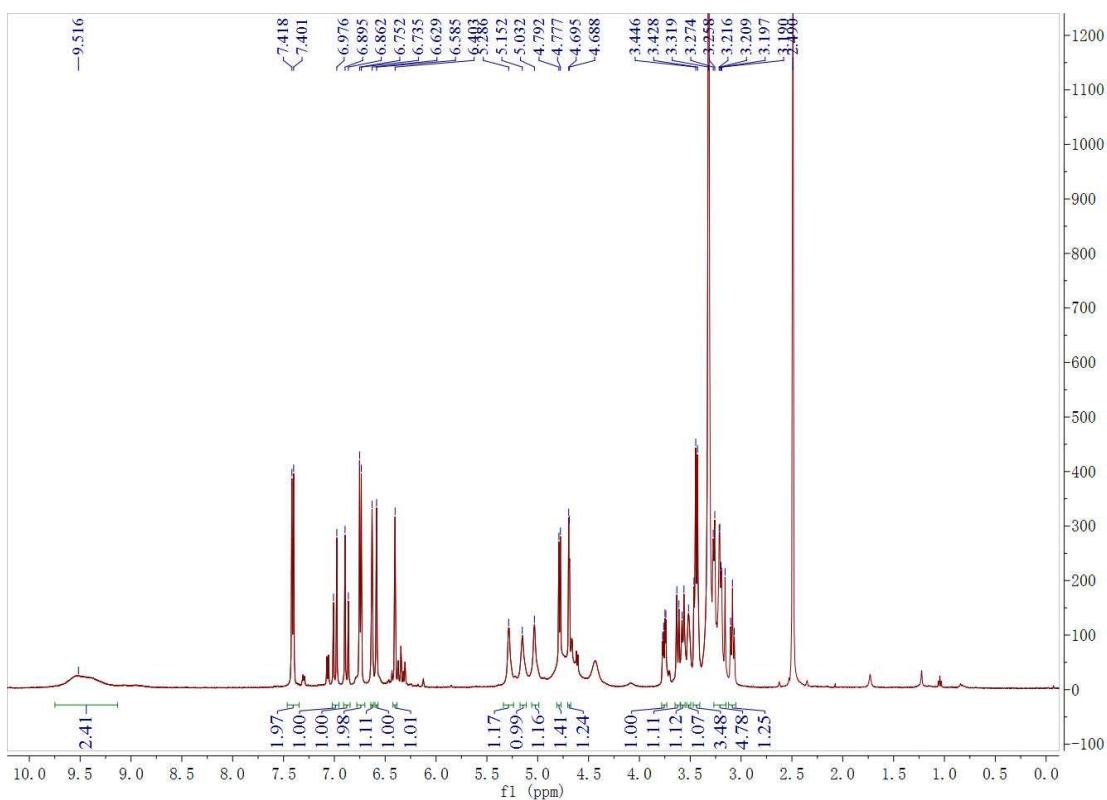


Figure S41. The ¹H NMR spectrum of compound **6** in DMSO-d₆.

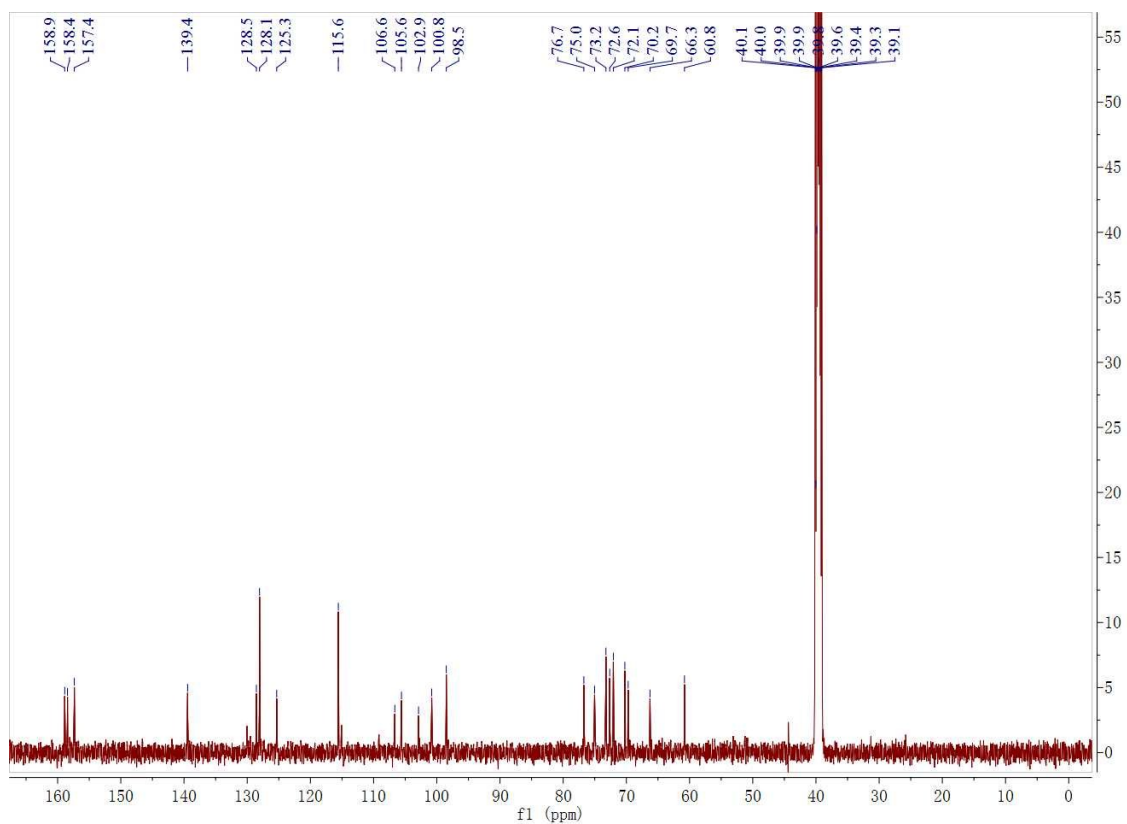


Figure S42. The ^{13}C NMR spectrum of compound **6** in $\text{DMSO}-d_6$.

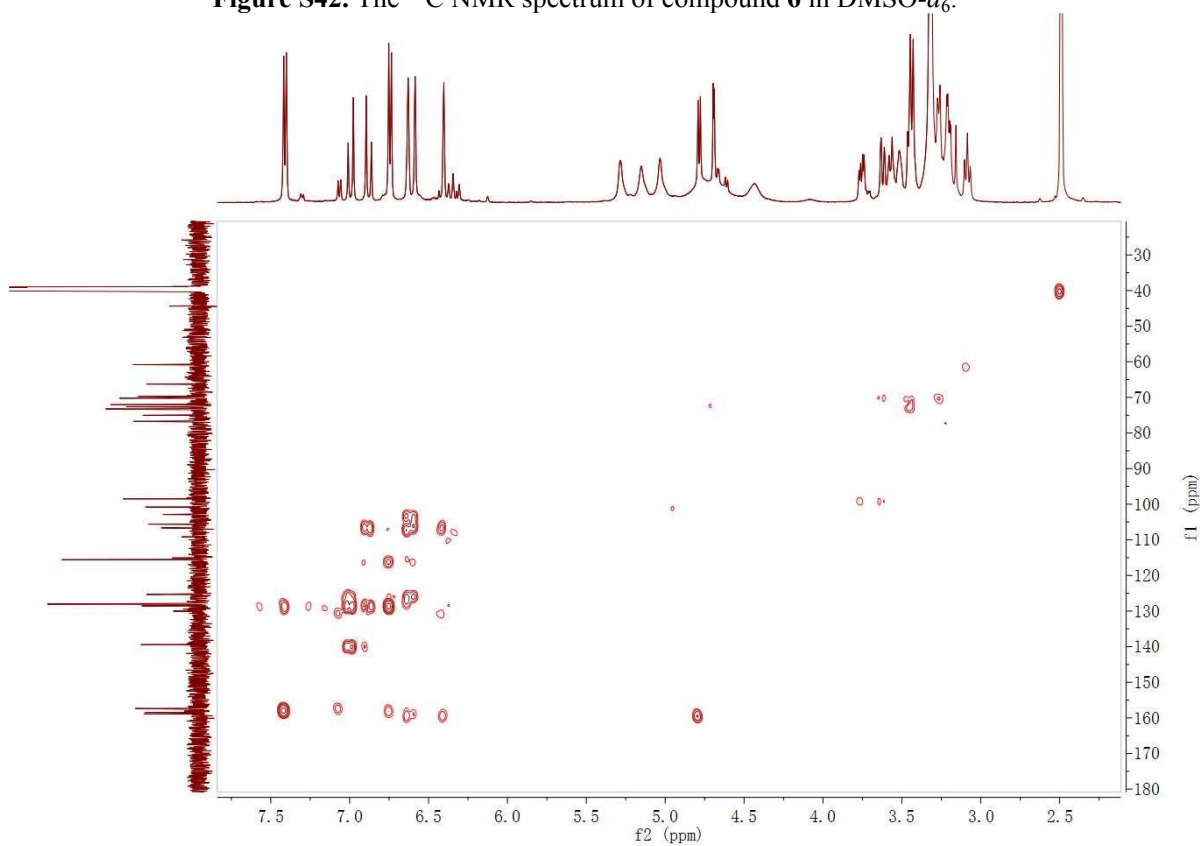


Figure S43. The HMBC spectrum of compound **6** in $\text{DMSO}-d_6$.

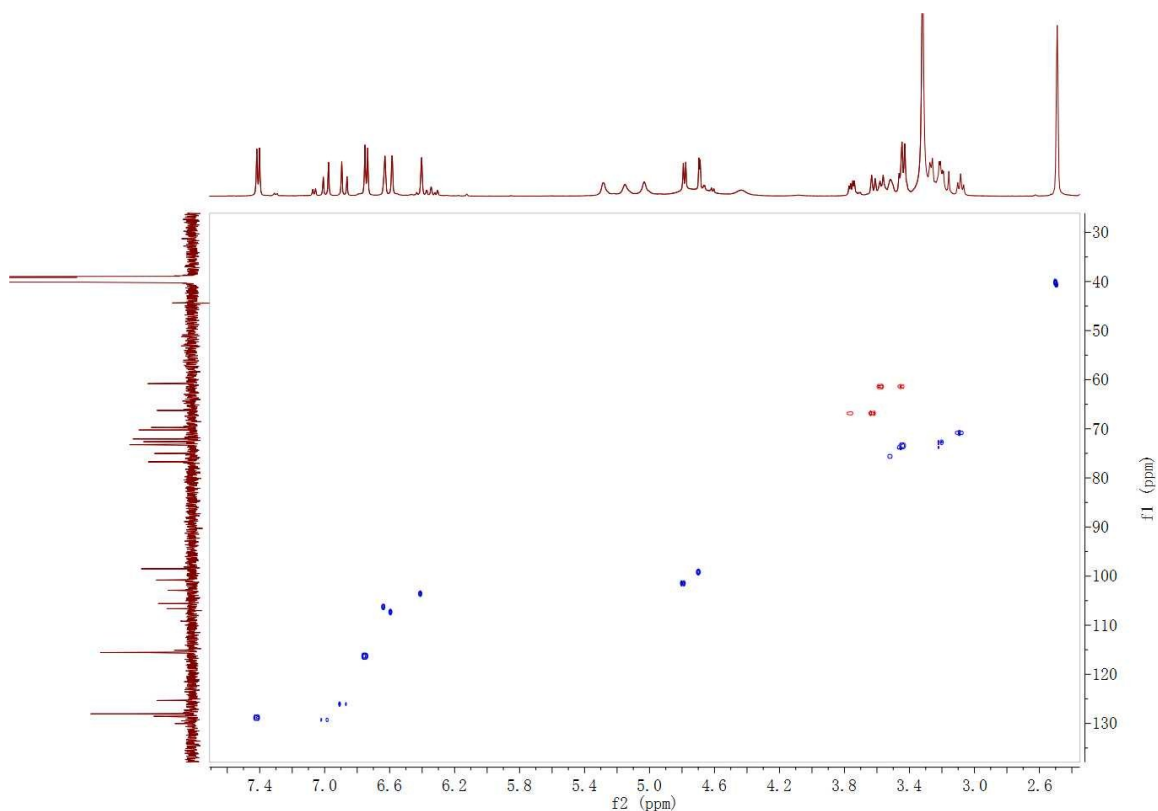


Figure S44. The HSQC spectrum of compound **6** in DMSO-*d*₆.

m/z	Ion	Formula	Abundance											
553.192	(M+H) ⁺	C ₂₆ H ₃₃ O ₁₃	262311.5											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C ₂₆ H ₃₂ O ₁₃	C ₂₆ H ₃₃ O ₁₃	553.1916	99.94		552.1847	552.1843	-0.82	0.82	99.85	99.97	99.98	553.192	11
☐	C ₂₁ H ₃₂ N ₂ O ₁₅	C ₂₁ H ₃₃ N ₂ O ₁₅	553.1875	98.07		552.1847	552.1803	-8.11	8.11	99.11	99.99	97.74	553.192	7
☐	C ₁₉ H ₃₆ O ₁₈	C ₁₉ H ₃₇ O ₁₈	553.1974	97.52		552.1847	552.1902	9.82	9.82	96.83	99.97	96.71	553.192	2
☐	C ₃₂ H ₂₈ N ₂ O ₇	C ₃₂ H ₂₉ N ₂ O ₇	553.1969	97.36		552.1847	552.1897	8.88	8.88	95.28	99.97	97.3	553.192	20
☐	C ₃₉ H ₂₄ N ₂ O ₂	C ₃₉ H ₂₅ N ₂ O ₂	553.1911	95.98		552.1847	552.1838	-1.75	1.75	86.14	99.96	99.89	553.192	29
☐	C ₄₄ H ₂₄	C ₄₄ H ₂₅	553.1951	93.65		552.1847	552.1878	5.53	5.53	79.57	99.94	98.94	553.192	33
☐	C ₃₈ H ₂₉ Cl ₂	C ₃₈ H ₃₀ Cl ₂ O ₂	553.1929	85.26		552.1847	552.1856	1.56	1.56	49.14	99.28	99.92	553.192	24
m/z	Ion	Formula	Abundance											
575.1743	(M+Na) ⁺	C ₂₆ H ₃₂ NaO ₁₃	383658.3											
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C ₂₆ H ₃₂ O ₁₃	C ₂₆ H ₃₂ NaO ₁₃	575.1735	99.96		552.1851	552.1843	-1.4	1.4	99.96	99.99	99.94	575.1743	11
☐	C ₂₁ H ₃₂ N ₂ O ₁₅	C ₂₁ H ₃₂ N ₂ NaO ₁₅	575.1695	98.23		552.1851	552.1803	-8.69	8.69	97.82	100	97.59	575.1743	7
☐	C ₃₂ H ₂₈ N ₂ O ₇	C ₃₂ H ₂₈ N ₂ NaO ₇	575.1789	98.18		552.1851	552.1897	8.3	8.3	97.28	99.99	97.8	575.1743	20
☐	C ₁₉ H ₃₆ O ₁₈	C ₁₉ H ₃₆ NaO ₁₈	575.1794	97.18		552.1851	552.1902	9.24	9.24	94.66	99.99	97.29	575.1743	2
☐	C ₃₉ H ₂₄ N ₂ O ₂	C ₃₉ H ₂₄ N ₂ NaO ₂	575.173	96.91		552.1851	552.1838	-2.33	2.33	89.49	99.98	99.82	575.1743	29
☐	C ₄₄ H ₂₄	C ₄₄ H ₂₄ Na	575.177	94.88		552.1851	552.1878	4.96	4.96	83.43	99.96	99.21	575.1743	33
☐	C ₃₈ H ₂₉ Cl ₂	C ₃₈ H ₂₉ Cl ₂ NaO ₂	575.1748	85.29		552.1851	552.1856	0.98	0.98	49.14	99.33	99.97	575.1743	24

Figure S45. The HRESIMS of compound **6**.

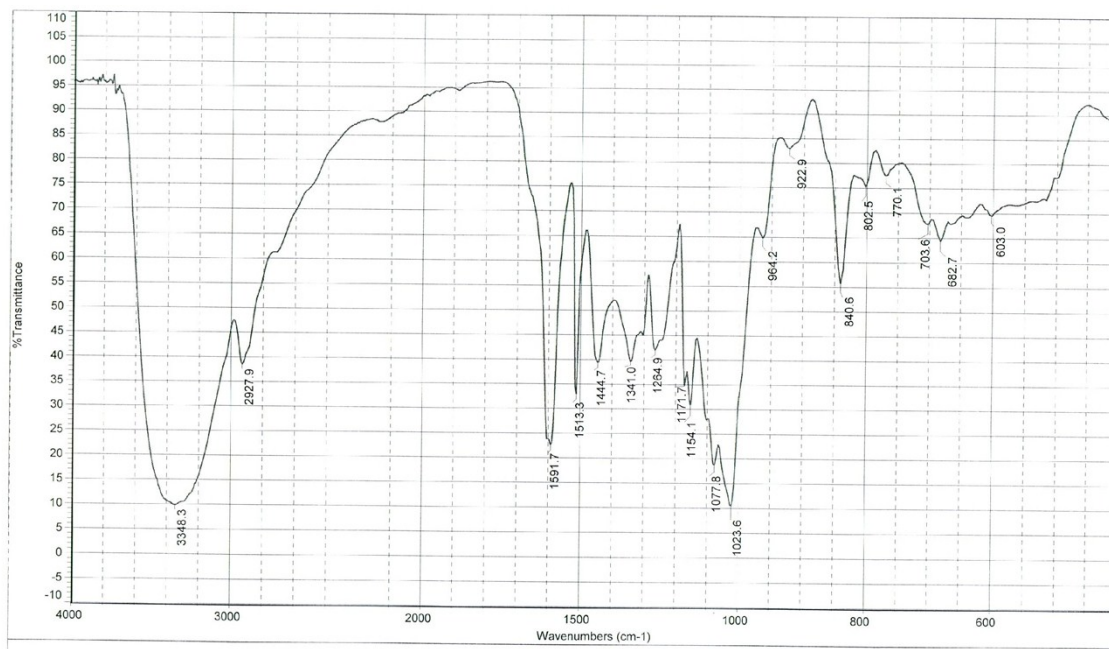


Figure S46. The IR spectrum of compound **6**.

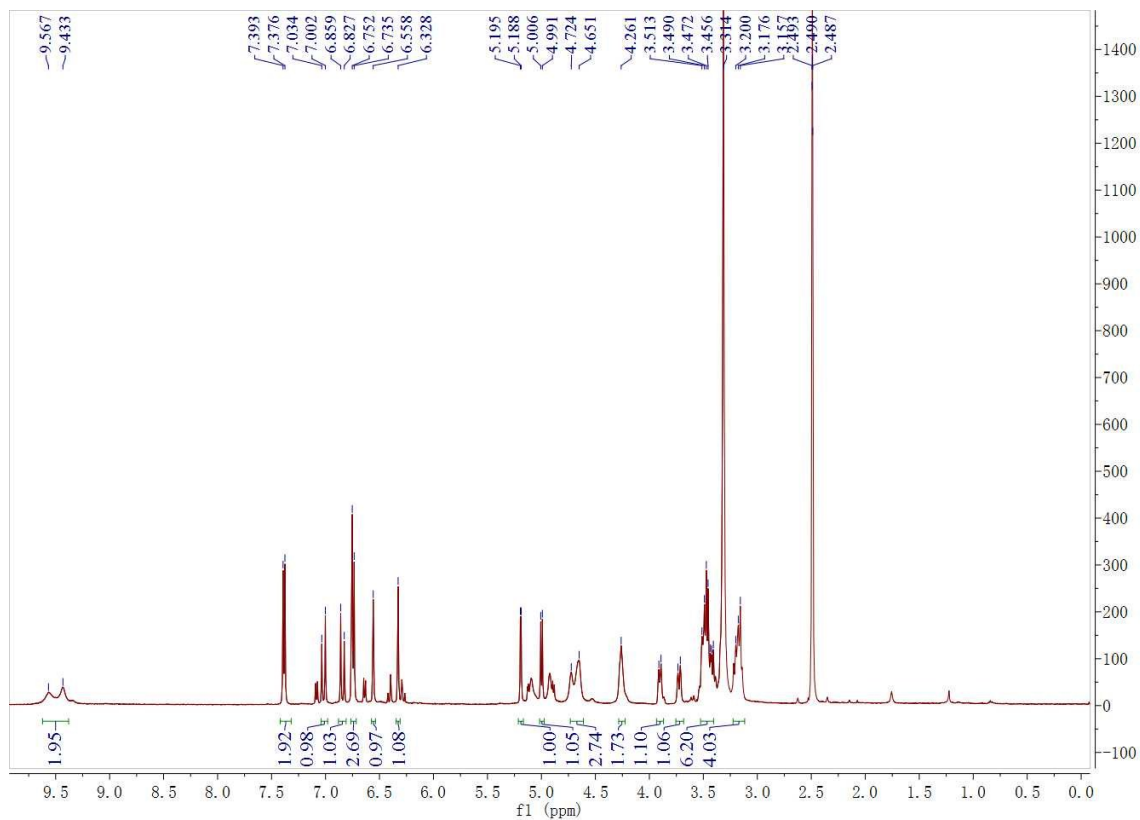


Figure S47. The ¹H NMR spectrum of compound **7** in DMSO-*d*₆.

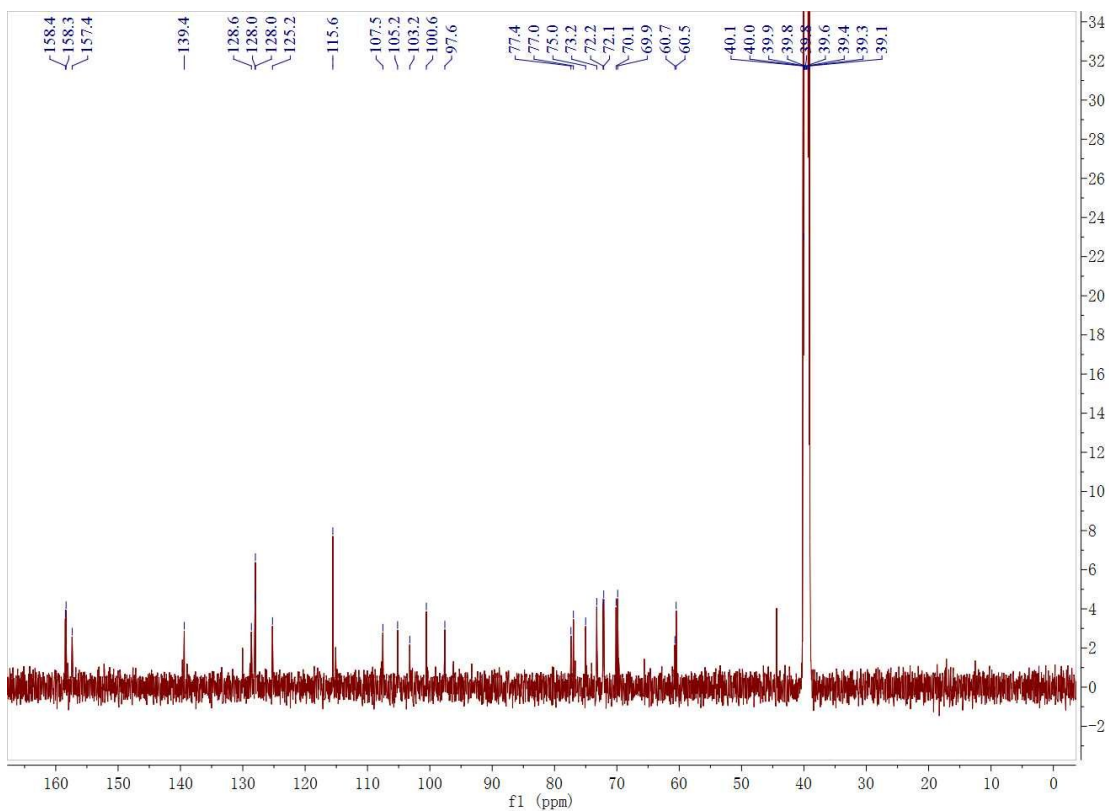


Figure S48. The ^{13}C NMR spectrum of compound **7** in $\text{DMSO}-d_6$.

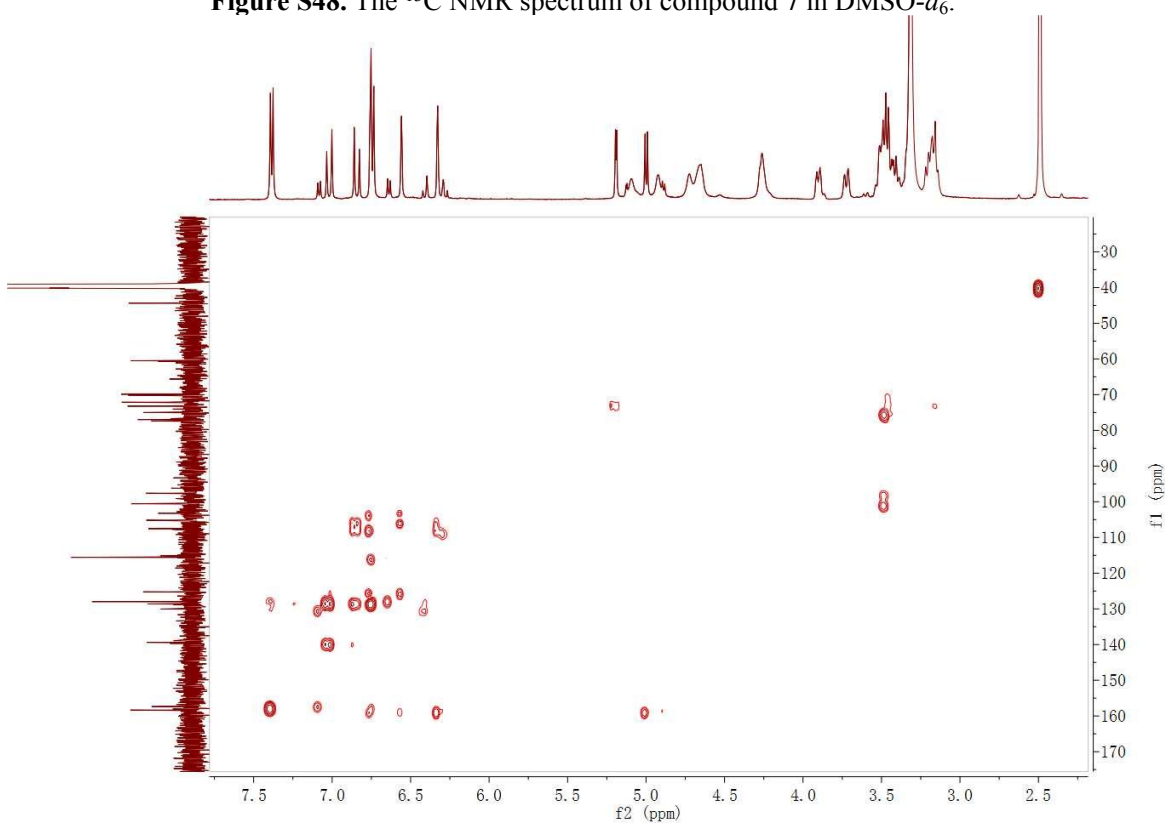


Figure S49. The HMBC spectrum of compound **7** in $\text{DMSO}-d_6$.

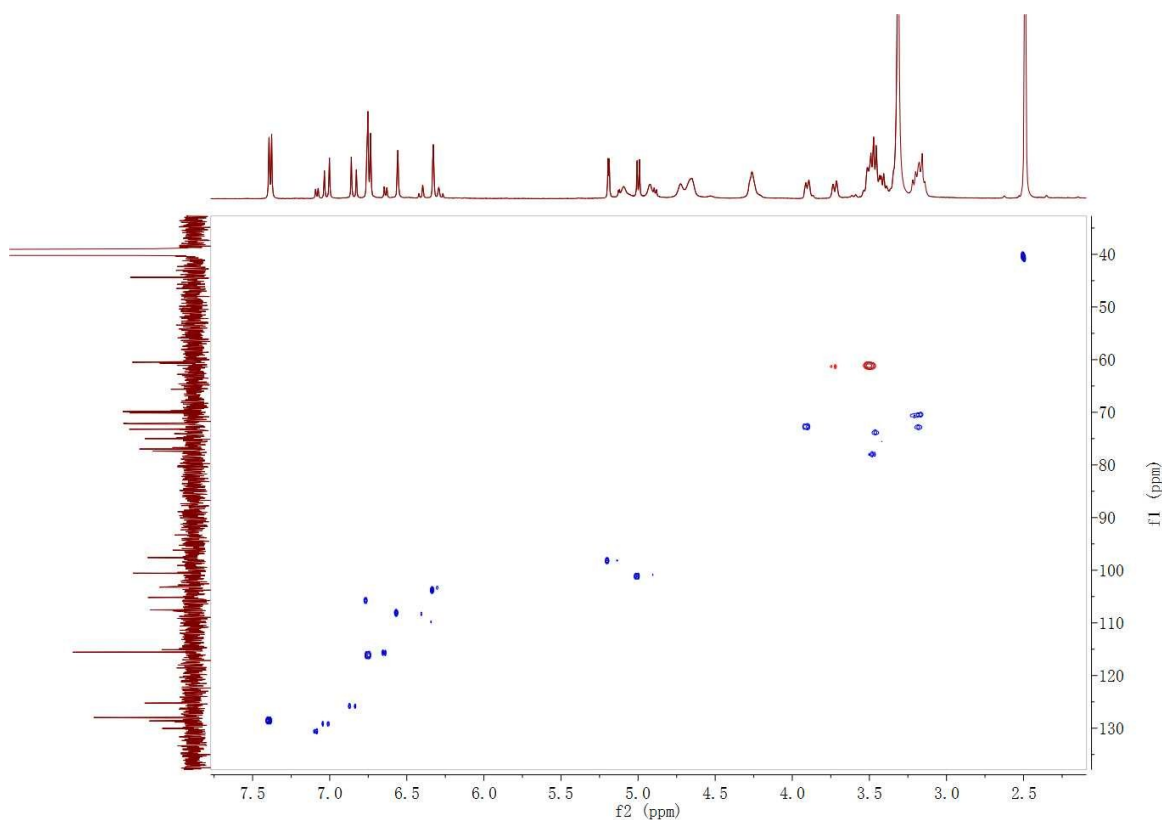


Figure S50. The HSQC spectrum of compound **7** in DMSO-*d*₆.

m/z	Ion	Formula	Abundance
553.1911	(M+H) ⁺	C ₂₆ H ₃₃ O ₁₃	211946
Best	Formula (M)	Ion Formula	Calc m/z
✓	C ₂₆ H ₃₂ O ₁₃	C ₂₆ H ₃₃ O ₁₃	553.1916
✗	C ₂₁ H ₃₂ N ₂ O ₁₅	C ₂₁ H ₃₃ N ₂ O ₁₅	553.1875
✗	C ₃₃ H ₂₈ O ₈	C ₃₃ H ₂₉ O ₈	553.1857
✗	C ₃₉ H ₂₄ N ₂ O ₂	C ₃₉ H ₂₅ N ₂ O ₂	553.1911
✗	C ₄₄ H ₂₄	C ₄₄ H ₂₅	553.1951
✗	C ₃₈ H ₂₉ Cl ₂ O ₂	C ₃₈ H ₃₀ Cl ₂ O ₂	553.1929
✗	C ₃₃ H ₂₉ Cl ₂ N ₂ O ₄	C ₃₃ H ₃₀ Cl ₂ N ₂ O ₄	553.1889
Score	Cross S	Mass	Calc Mass
99.98		552.1838	552.1843
98.81		552.1838	552.1803
97.47		552.1838	552.1784
96.77		552.1838	552.1838
94.15		552.1838	552.1878
85.38		552.1838	552.1856
85.23		552.1838	552.1816
Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat
0.89	0.89	99.99	99.98
-6.4	6.4	98.18	100
-9.75	9.75	96.59	99.96
-0.05	0.05	98.75	99.95
7.24	7.24	82.6	99.93
3.27	3.27	50.01	99.33
4.02	4.02	49.86	99.26
Mass Match	m/z	DBE	
99.97	553.1911	11	
98.59	553.1911	7	
96.76	553.1911	20	
100	553.1911	29	
98.2	553.1911	33	
99.63	553.1911	24	
99.44	553.1911	20	

m/z	Ion	Formula	Abundance
575.1735	(M+Na) ⁺	C ₂₆ H ₃₂ Na ₂ O ₁₃	372538.8
Best	Formula (M)	Ion Formula	Calc m/z
✓	C ₂₆ H ₃₂ O ₁₃	C ₂₆ H ₃₂ Na ₂ O ₁₃	575.1735
✗	C ₂₁ H ₃₂ N ₂ O ₁₅	C ₂₁ H ₃₂ N ₂ Na ₂ O ₁₅	575.1695
✗	C ₃₂ H ₂₈ N ₂ O ₇	C ₃₂ H ₂₈ N ₂ Na ₂ O ₇	575.1789
✗	C ₃₉ H ₂₄ N ₂ O ₂	C ₃₉ H ₂₄ N ₂ Na ₂ O ₂	575.173
✗	C ₄₄ H ₂₄	C ₄₄ H ₂₄ Na	575.177
✗	C ₃₈ H ₂₉ Cl ₂ O ₂	C ₃₈ H ₂₉ Cl ₂ Na ₂ O ₂	575.1748
Score	Cross S	Mass	Calc Mass
99.95		552.1842	552.1843
98.96		552.1843	552.1803
97.19		552.1843	552.1897
95.99		552.1843	552.1838
93.47		552.1843	552.1878
85.14		552.1843	552.1856
Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat
0.08	0.08	99.85	99.96
-7.22	7.22	99.14	99.98
9.78	9.78	95.24	99.96
-0.86	0.86	86.03	99.95
6.43	6.43	79.43	99.92
2.46	2.46	48.8	99.44
Mass Match	m/z	DBE	
100	575.1735	11	
98.34	575.1735	7	
96.97	575.1735	20	
99.95	575.1735	29	
98.68	575.1735	33	
99.81	575.1735	24	

Figure S51. The HRESIMS of compound **7**.

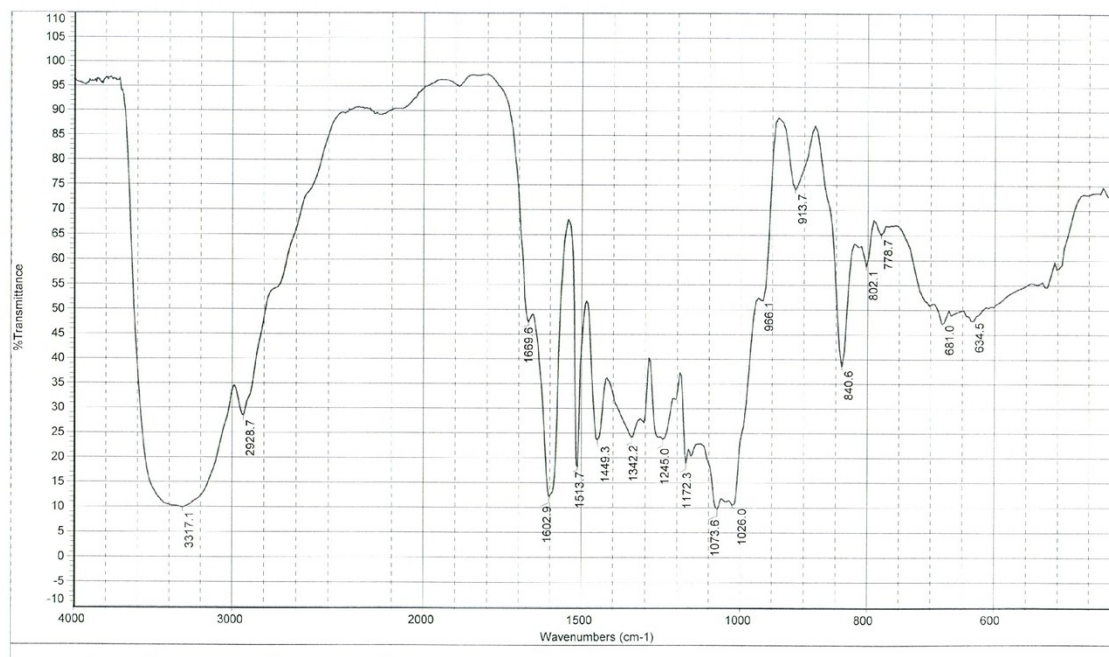


Figure S52. The IR spectrum of compound **7**.

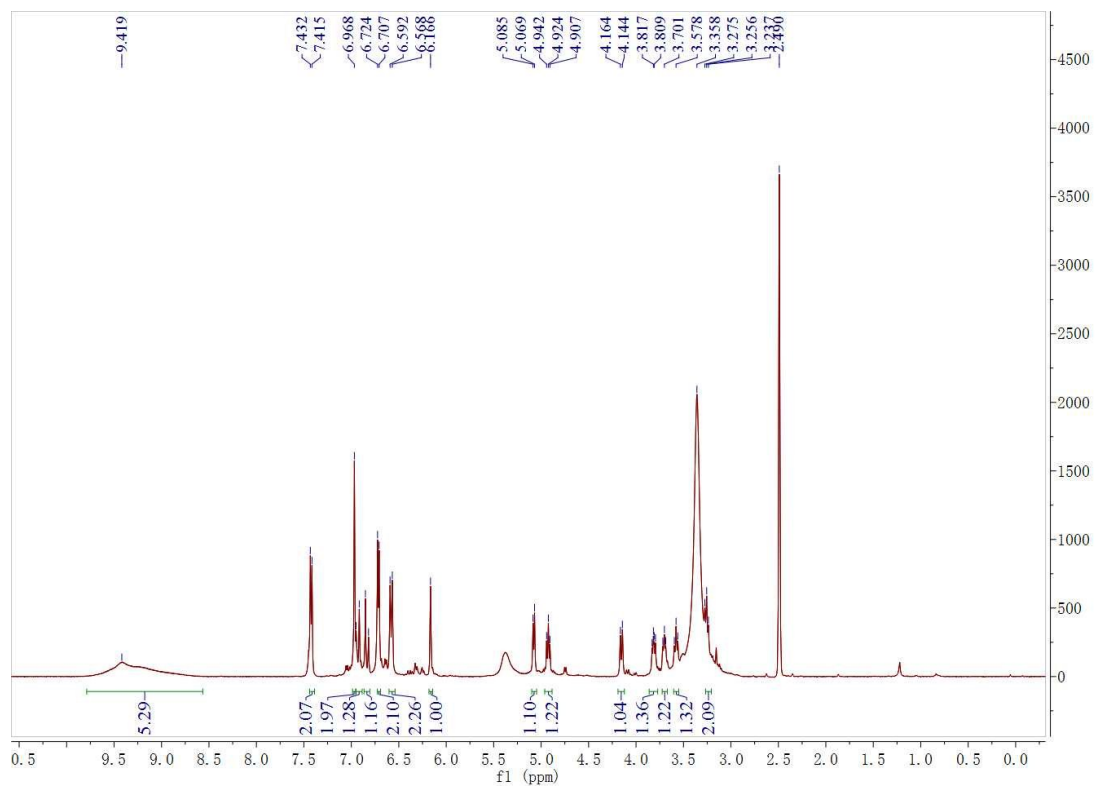


Figure S53. The ¹H NMR spectrum of compound **8** in DMSO-d₆.

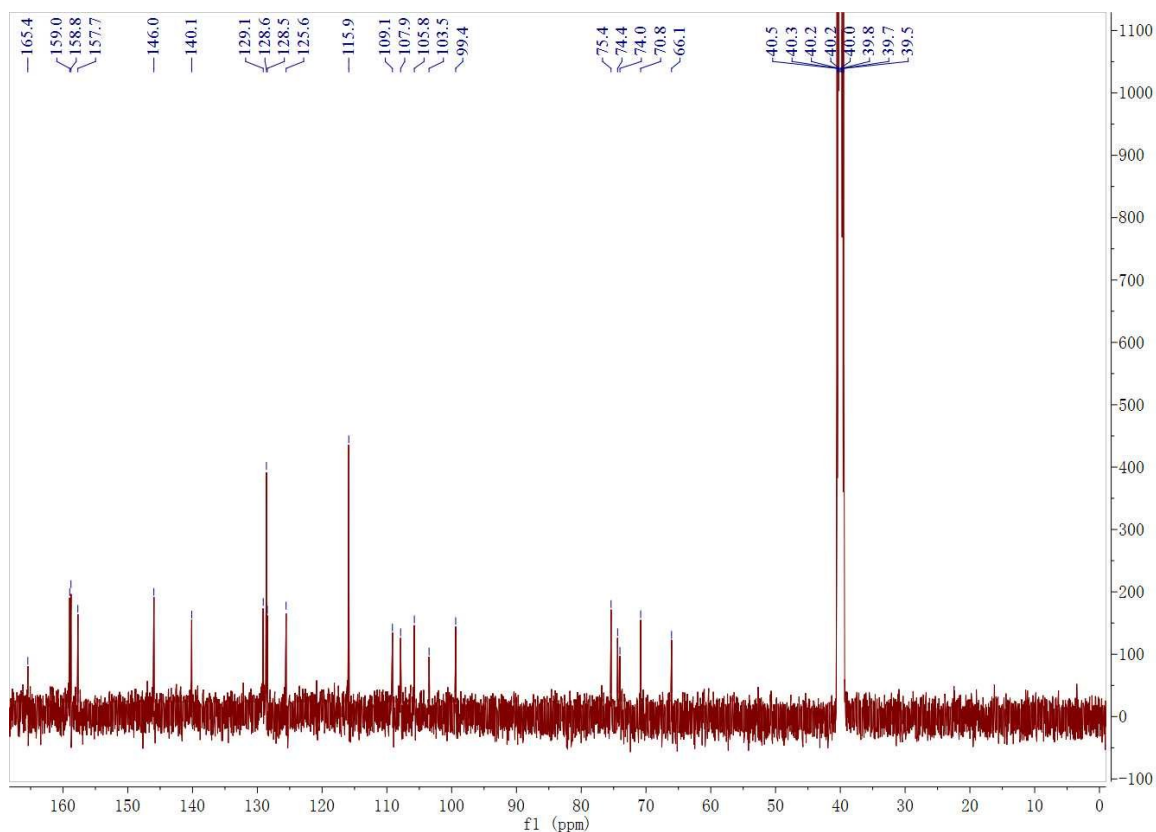


Figure S54. The ^{13}C NMR spectrum of compound **8** in $\text{DMSO}-d_6$.

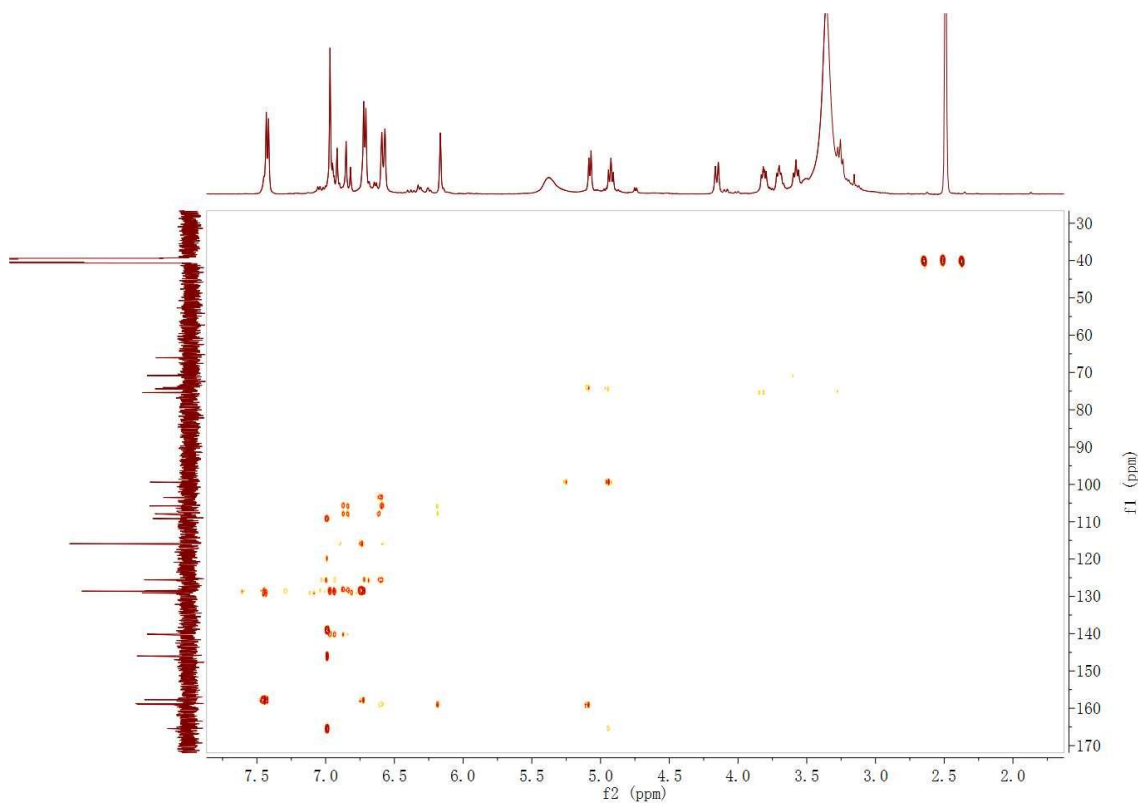


Figure S55. The HMBC spectrum of compound **8** in $\text{DMSO}-d_6$.

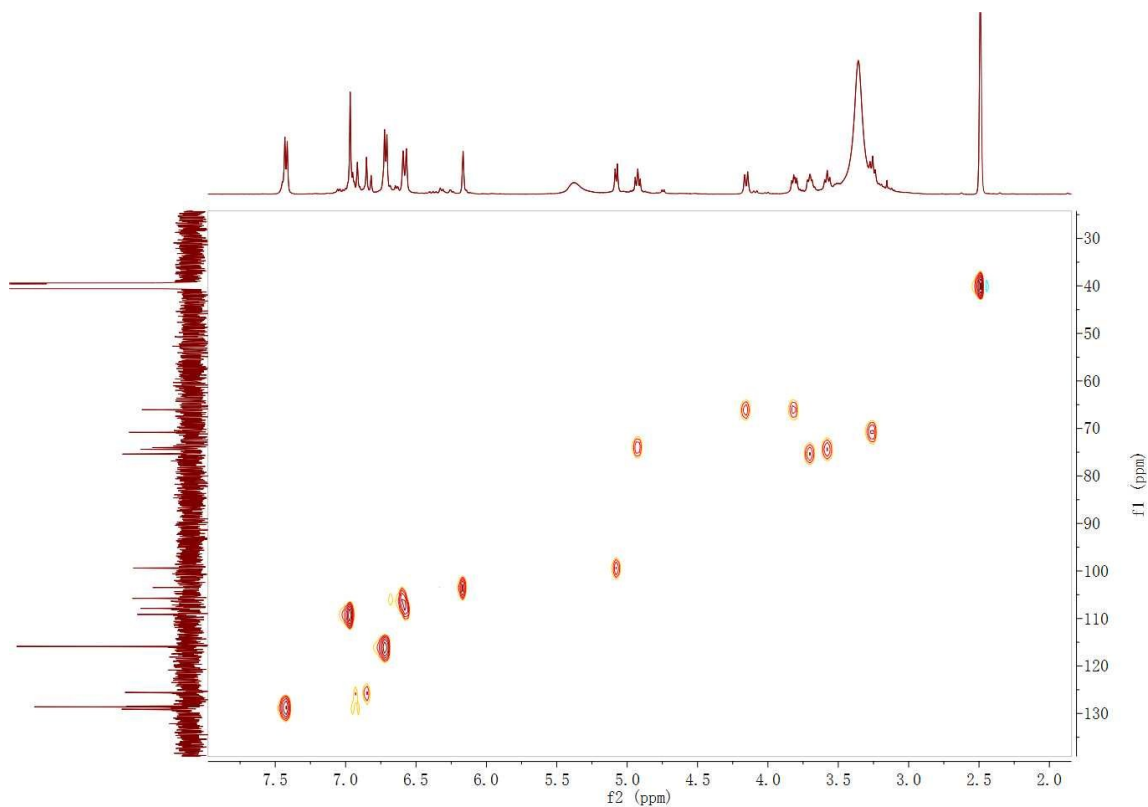


Figure S56. The HSQC spectrum of compound **8** in DMSO- d_6 .

m/z	Ion	Formula	Abundance
621.0929	[M+H] ⁺	C27H25O15S	909449.3

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mot	Mass Match	m/z	DBE
☒	C27H26O15S	C27H25O15S	621.092	99.92		622.1001	622.0992	-1.4	1.4	99.9	99.91	99.93	621.0929	15
☐	C23H25O20	C23H25O20	521.0545	96.92		622.1001	622.1017	2.53	2.63	97.25	99.26	99.76	621.0929	11
☐	C30H22O15	C30H21O15	521.0686	96.51		622.1001	622.0959	-6.81	5.81	98.23	99.11	98.37	621.0929	20
☐	C20H30O20S	C20H29O20S	521.0578	97.59		622.1001	622.1051	8.03	8.03	95.36	99.94	97.74	621.0929	5
☐	C45H18O2S	C45H17O2S	521.0555	95.5		622.1001	622.1028	4.24	4.24	85.92	99.68	99.36	621.0929	37
☐	C41H18O7	C41H17O7	621.098	95.4		622.1001	622.1053	8.27	8.27	88.8	98.92	97.6	621.0929	33
☐	C48H14O2	C48H13O2	521.0521	93.95		622.1001	622.0994	-1.17	1.17	79.87	98.83	99.55	621.0929	42

Figure S57. The HRESIMS of compound **8**.

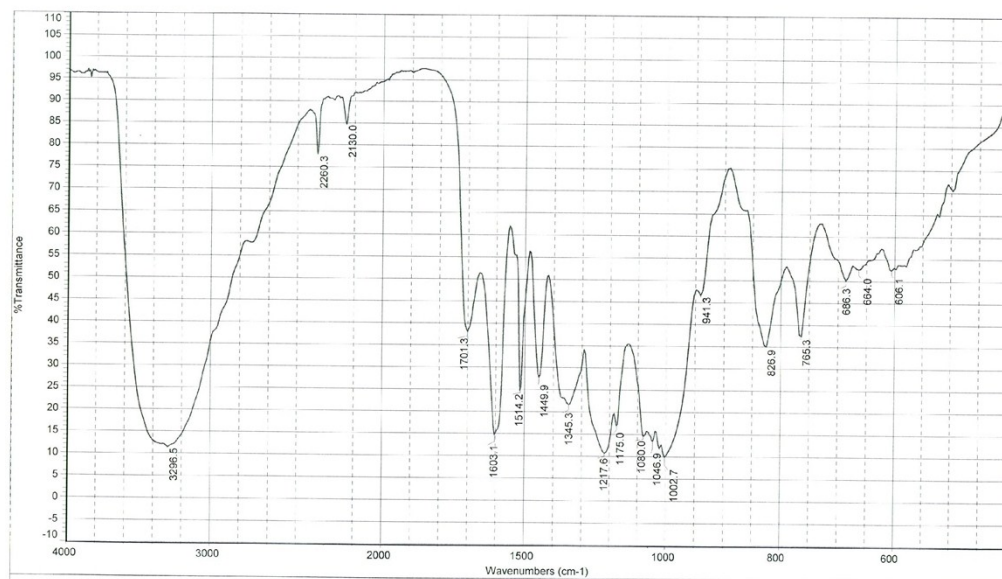


Figure S58. The IR spectrum of compound **8**.

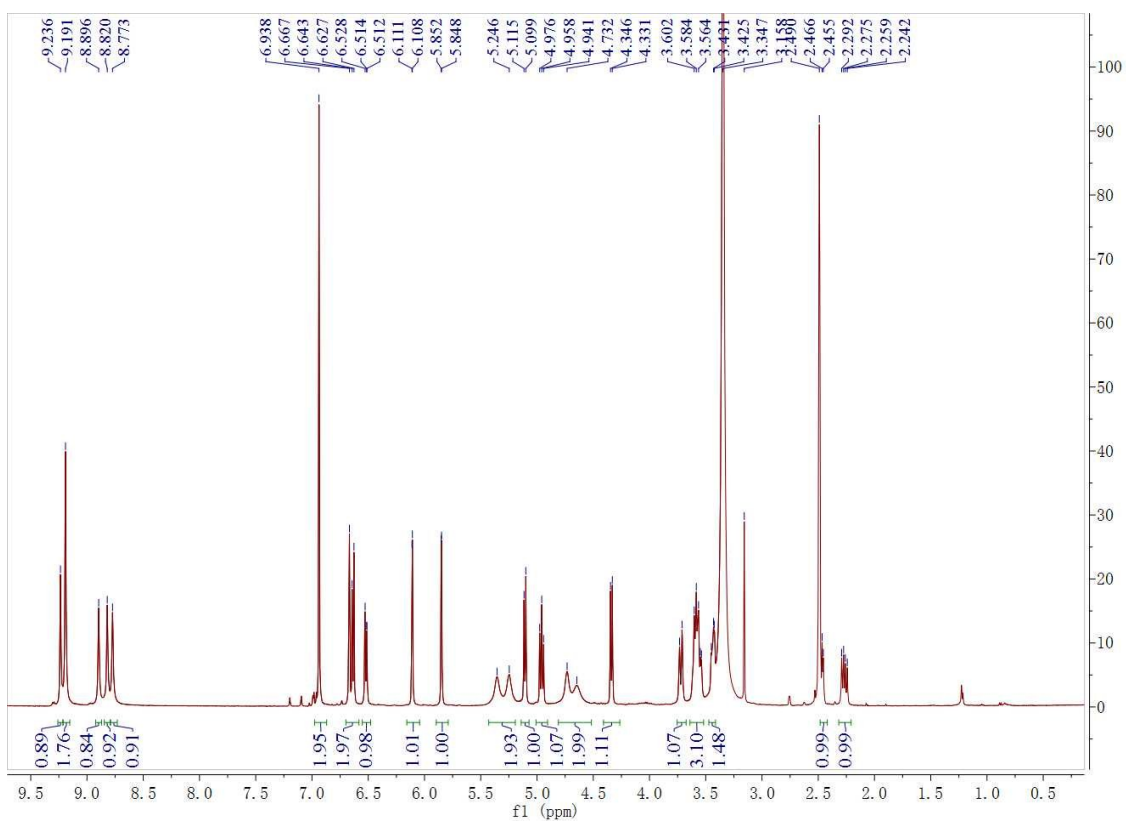


Figure S59. The ¹H NMR spectrum of compound **9** in DMSO-*d*₆.

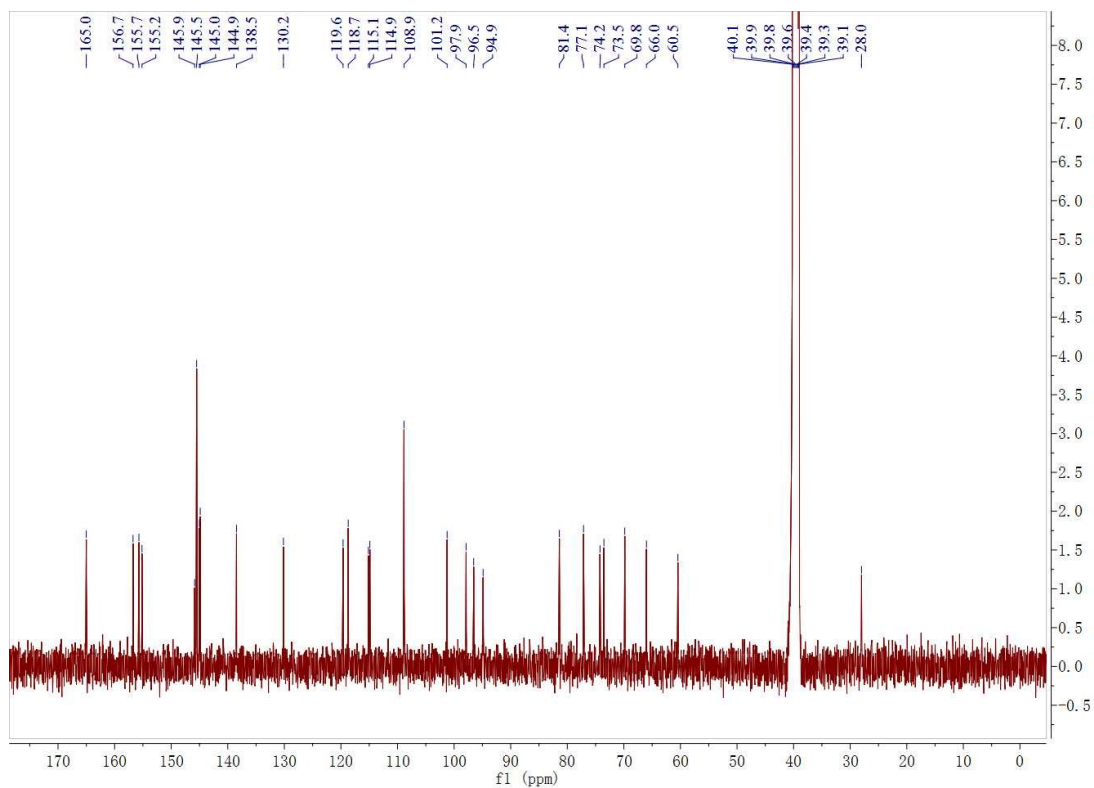


Figure S60. The ^{13}C NMR spectrum of compound **9** in $\text{DMSO-}d_6$.

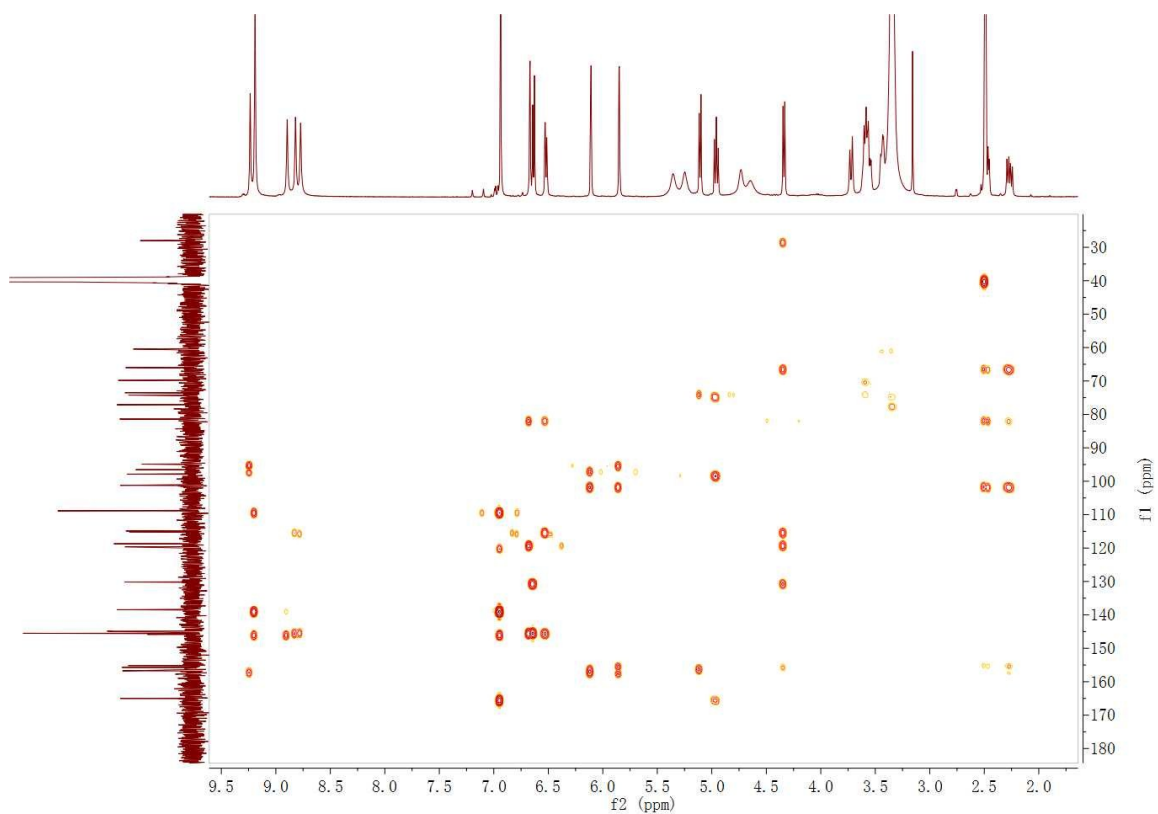


Figure S61. The HMBC spectrum of compound **9** in $\text{DMSO-}d_6$.



Figure S62. The HSQC spectrum of compound **9** in DMSO-*d*₆.

m/z	Ion	Formula	Abundance
627.1316	[M+Na] ⁺	C28H28NaO15	31596.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C28H28O15	C28H28NaO15	627.132	99.93		604.1424	604.1428	0.08	0.68	99.9	99.85	99.98	627.1316	15
+	C29H24N4O11	C29H24N4NaO11	627.1334	99.7		604.1424	604.1442	2.88	2.88	99.52	99.84	99.73	627.1316	20
+	C32H28O10S	C32H28NaO10S	627.1295	99.21		604.1424	604.1403	-3.47	3.47	97.93	99.96	99.61	627.1316	19
+	C33H24N4O6S	C33H24N4NaO6S	627.1309	99.1		604.1424	604.1417	-1.27	1.27	96.98	99.94	99.95	627.1316	24
+	C23H28N2O17	C23H28N2NaO17	627.128	98.86		604.1424	604.1388	-5.99	5.99	98.05	99.88	98.83	627.1316	11
+	C25H32O15S	C25H32NaO15S	627.1354	98.69		604.1424	604.1462	6.25	6.25	97.6	99.92	98.73	627.1316	10
+	C26H28N4O11S	C26H28N4NaO11S	627.1367	98.54		604.1424	604.1475	8.45	8.45	98.84	99.88	97.69	627.1316	15
+	C29H32O10S2	C29H32NaO10S2	627.1329	98.19		604.1424	604.1437	2.1	2.1	94.11	99.77	99.86	627.1316	14
+	C20H32N2O17S	C20H32N2NaO17S	627.1314	98.15		604.1424	604.1422	-0.42	0.42	93.66	99.86	99.99	627.1316	6
+	C30H28N4O6S2	C30H28N4NaO6S2	627.1342	98.08		604.1424	604.145	4.3	4.3	94.51	99.73	99.39	627.1316	19
+	C35H24O10	C35H24NaO10	627.1262	97.86		604.1424	604.1369	-9.04	9.04	97.1	99.8	97.35	627.1316	24
+	C34H24N2O9	C34H24N2NaO9	627.1374	97.78		604.1424	604.1482	9.55	9.55	97.28	99.81	97.06	627.1316	24
+	C36H20N4O6	C36H20N4NaO6	627.1275	97.77		604.1424	604.1383	-6.84	6.84	94.88	99.8	98.48	627.1316	29
+	C38H24N2O4S	C38H24N2NaO4S	627.1349	97.61		604.1424	604.1457	5.4	5.4	93.24	99.97	99.05	627.1316	28
+	C24H32N2O12S2	C24H32N2NaO12S2	627.1289	97.59		604.1424	604.1397	-4.57	4.57	92.99	99.67	99.32	627.1316	10
+	C41H20N2O4	C41H20N2NaO4	627.1315	97.13		604.1424	604.1423	-0.18	0.18	90.14	99.77	100	627.1316	33
+	C37H24N4O5S2	C37H24N4NaO5S2	627.1284	96.79		604.1424	604.1392	-5.41	5.41	90.5	99.83	99.04	627.1316	28
+	C36H28O5S2	C36H28NaO5S2	627.127	96.7		604.1424	604.1378	-7.62	7.62	91.71	99.85	98.11	627.1316	23
+	C17H36N2O17S2	C17H36N2NaO17S2	627.1348	96.05		604.1424	604.1455	5.15	5.15	84.46	99.57	99.13	627.1316	1
+	C46H20O2	C46H20NaO2	627.1356	94.89		604.1424	604.1463	6.49	6.49	84.64	99.73	98.63	627.1316	37

Figure S63. The HRESIMS of compound **9**.

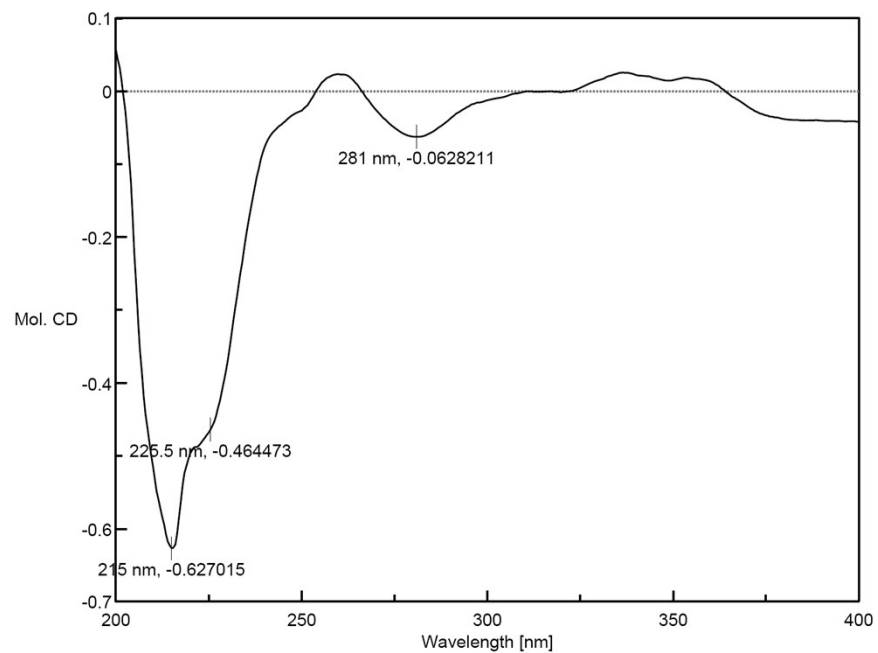


Figure S64. The CD spectrum of compound **9a**.

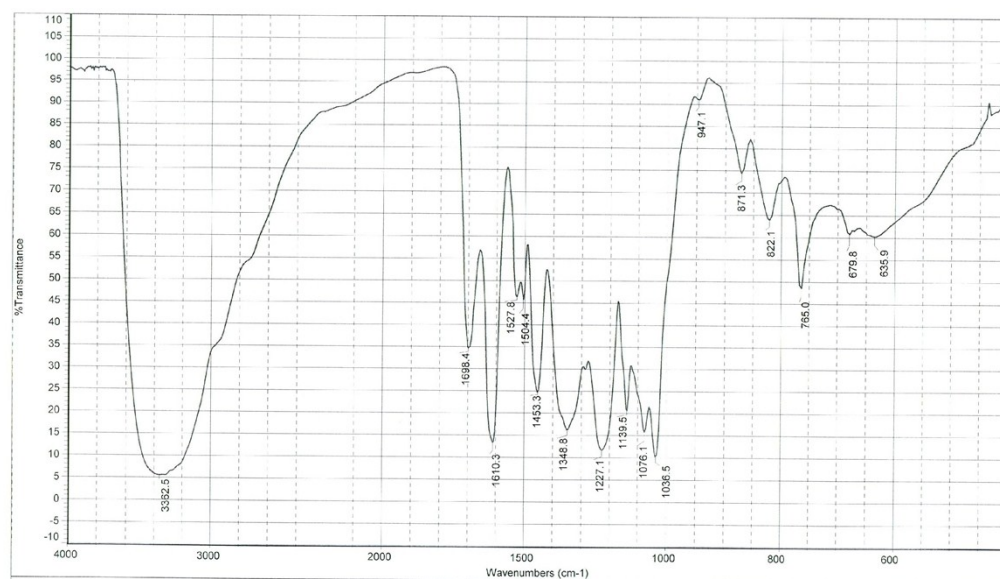


Figure S65. The IR spectrum of compound **9**.