

Supplementary Information

Structural Transformation of Methasterone with *Cunninghamella blakesleeana* and *Macrophomina phaseolina*

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2/26/2019 2:57:34 PM

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Ionization mode: EI+

Run By: HEJ-104

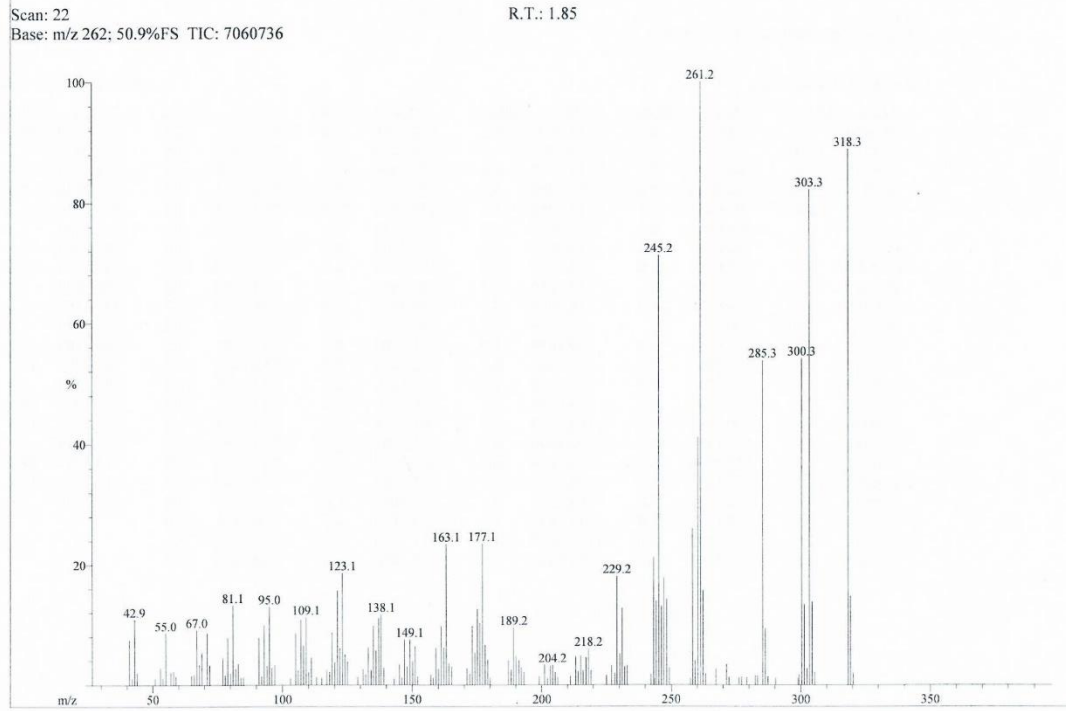
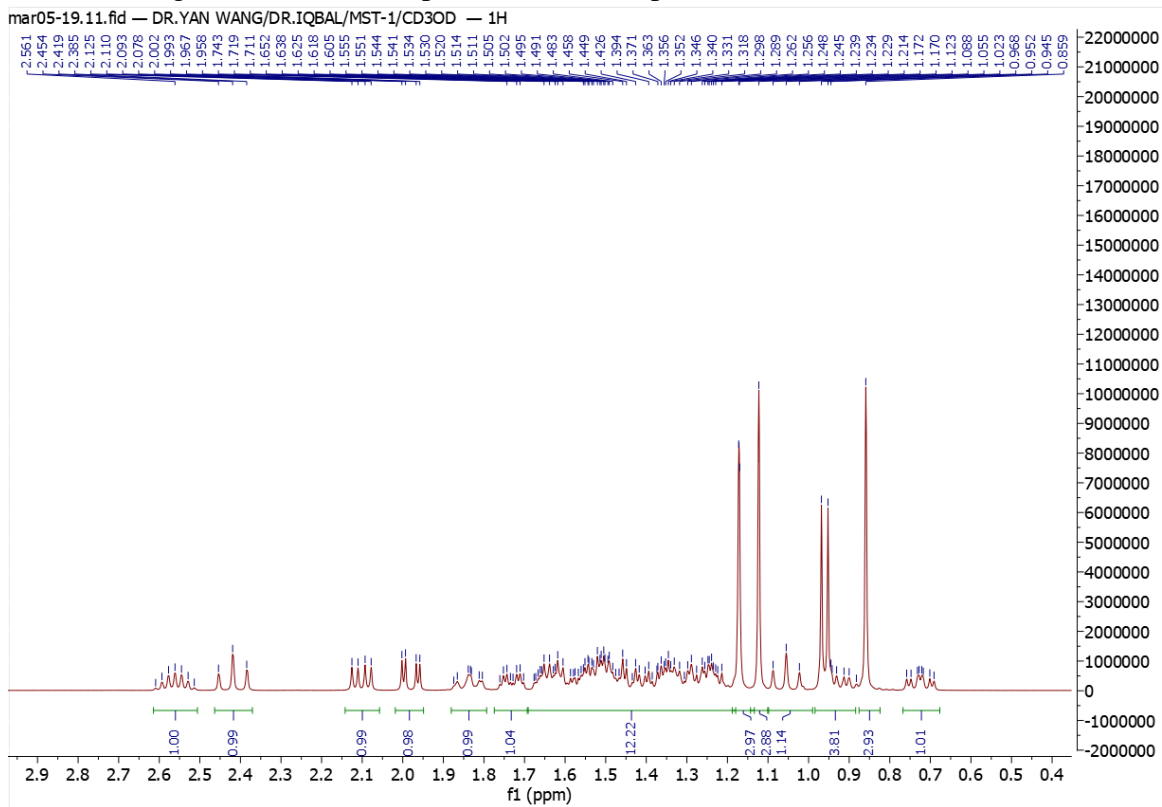
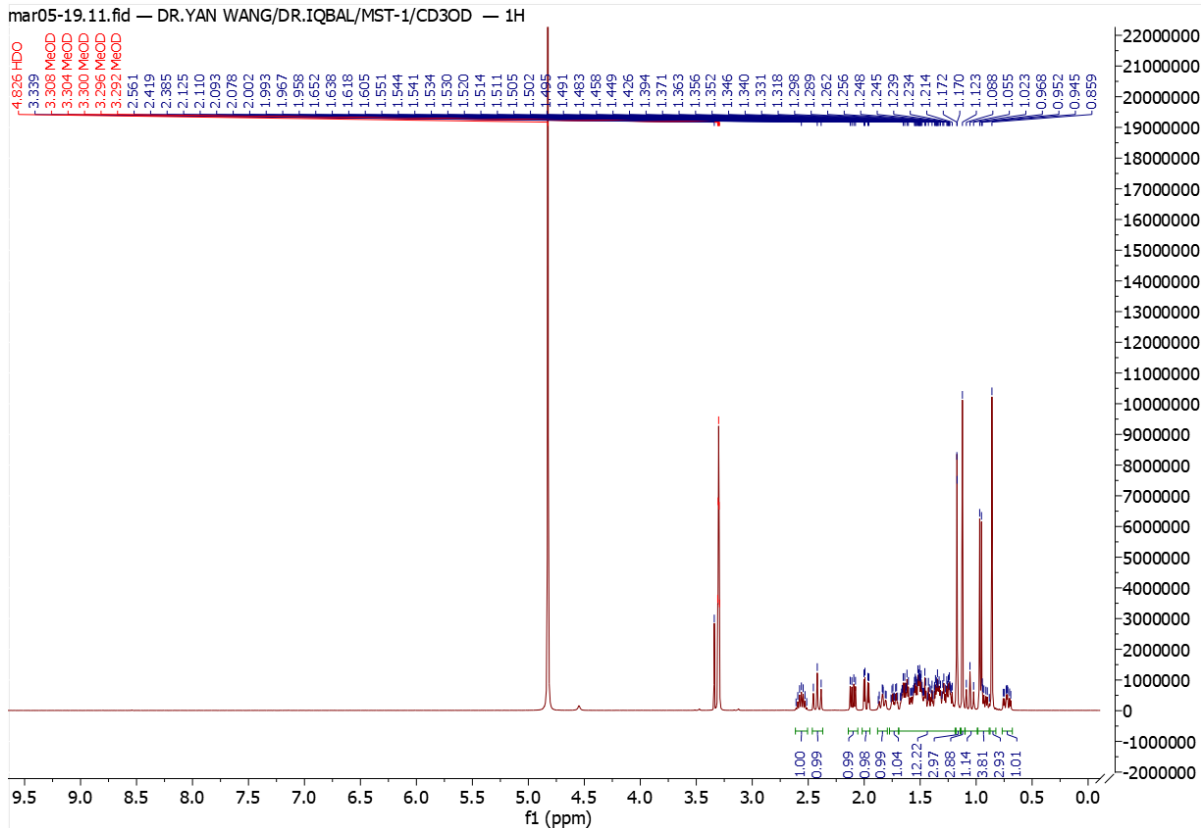


Figure S1. EI-MS spectrum of compound **1**



mar06-19.5.fid — DR.YAN WANG/DR.IQBAL/MST-1/CD3OD — BB/

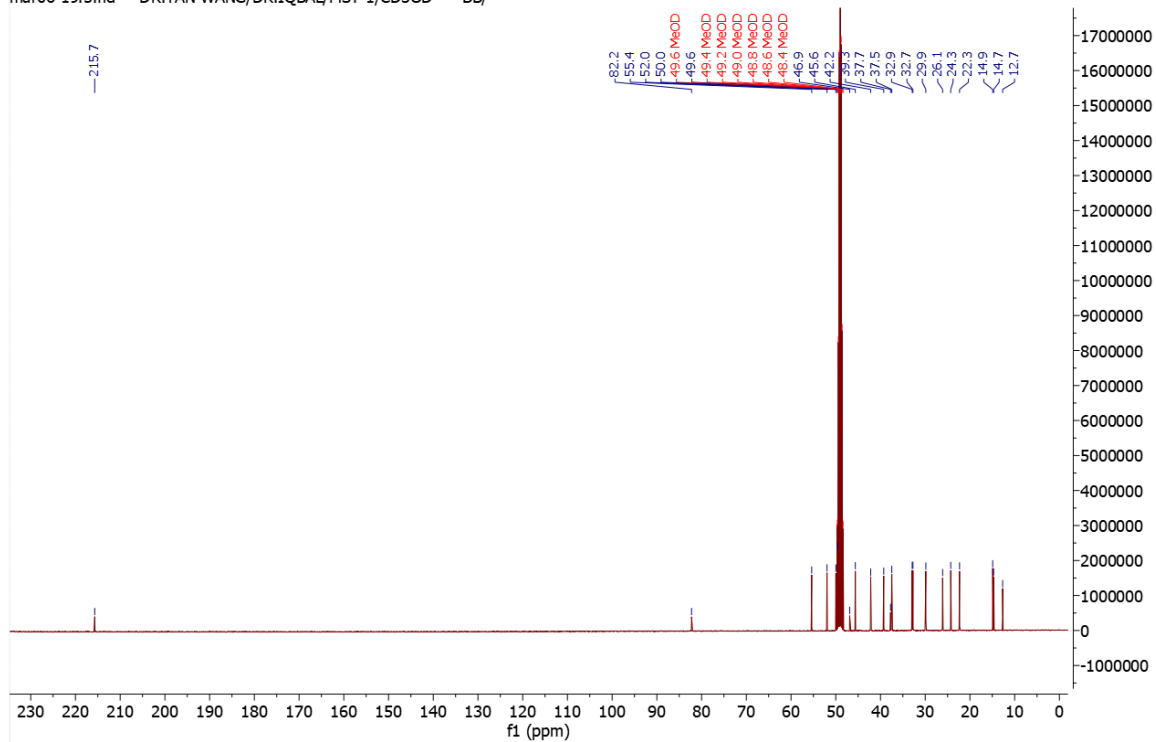


Figure S4. ^{13}C NMR spectrum-1 of compound **1** (100 MHz, CD_3OD)

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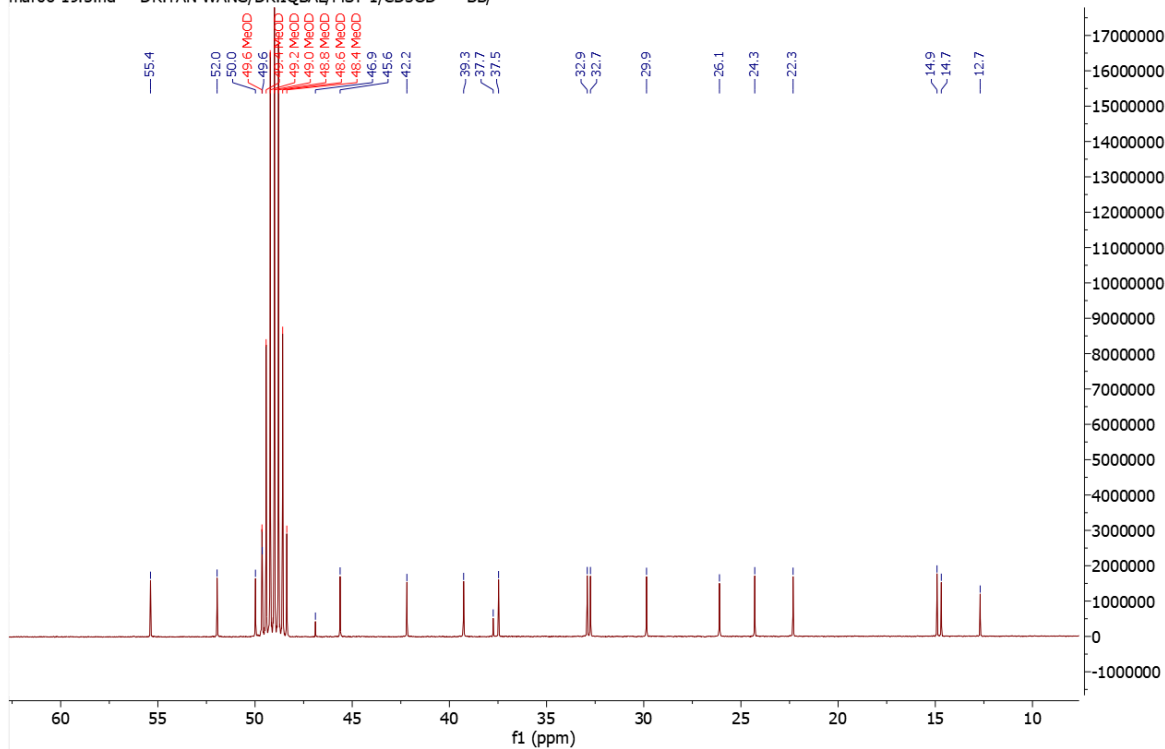


Figure S5. ^{13}C NMR spectrum-2 of compound **1** (100 MHz, CD_3OD)

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Instrument: JEOL 600H-1
Inlet: Direct Probe

Date Run: 11-16-2020 (Time Run: 10:13:59)

Ionization mode: EI+

Run By: MASS LAB-104

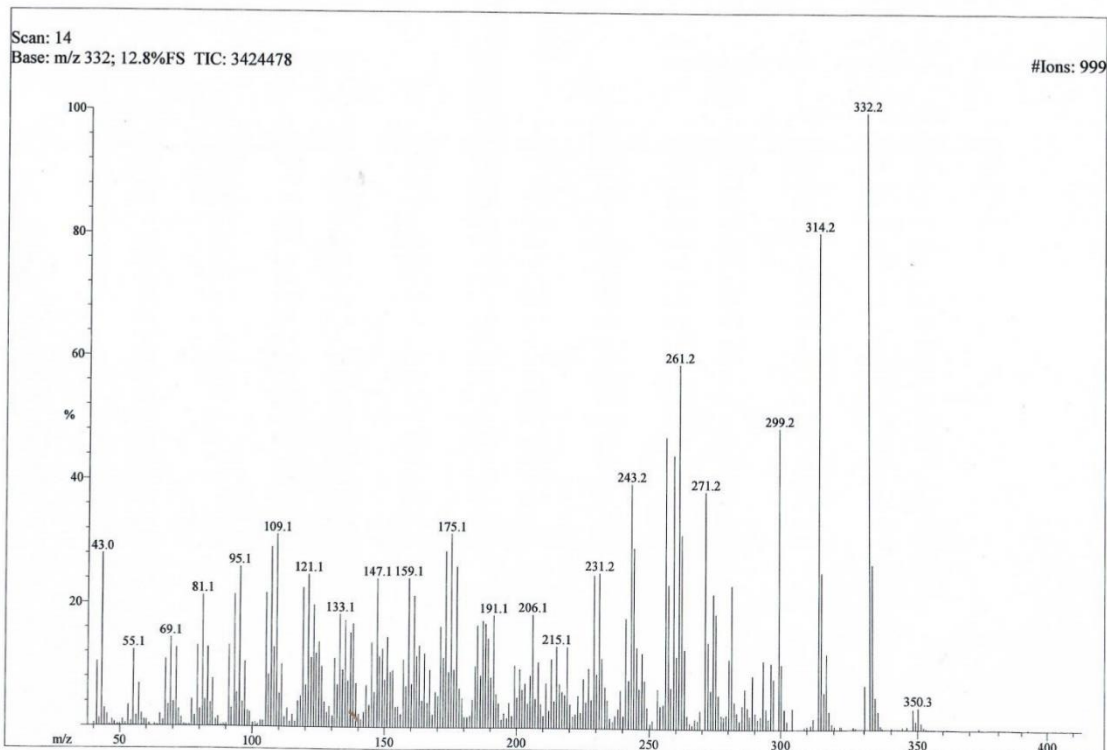


Figure S6. EI-MS spectrum of compound 2

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		317.2328	-32.5	-10.3	1.5	C ₁₇ H ₃₃ O ₇
		317.2117	34.1	10.8	6.5	C ₂₀ H ₂₉ O ₃
318.2226	5.8	318.2195	9.9	3.1	6.0	C ₂₀ H ₃₀ O ₃
319.2213	1.4	319.2273	-18.8	-6.0	5.5	C ₂₀ H ₃₁ O ₃
		319.2121	29.0	9.2	1.5	C ₁₆ H ₃₁ O ₆
328.2129	0.4	328.2191	-18.9	-6.2	12.0	C ₂₅ H ₂₉
		328.2038	27.6	9.0	8.0	C ₂₅ H ₂₈ O ₃
330.2158	3.3	330.2195	-11.2	-3.7	7.0	C ₂₁ H ₃₀ O ₃
		330.2042	35.0	11.6	3.0	C ₁₇ H ₃₀ O ₆
331.2244	1.4	331.2273	-8.6	-2.9	6.5	C ₂₁ H ₃₁ O ₃
332.2309	100.0	332.2351	-12.7	-4.2	6.0	C ₂₁ H ₃₂ O ₃
		332.2199	33.3	11.1	2.0	C ₁₇ H ₃₂ O ₆
333.2349	25.4	333.2277	21.6	7.2	1.5	C ₁₇ H ₃₃ O ₆
		333.2430	-24.2	-8.1	5.5	C ₂₁ H ₃₃ O ₃
333.3495	0.3	333.3521	-8.0	-2.7	2.5	C ₂₄ H ₁₅
333.3630	0.3	333.3521	32.6	10.9	2.5	C ₂₄ H ₁₅
334.2415	3.6	334.2355	17.9	6.0	1.0	C ₂₄ H ₁₅ O ₆
		334.2508	-27.8	-9.3	5.0	C ₁₇ H ₃₄ O ₃
335.2239	2.8	335.2222	4.9	1.6	5.5	C ₂₀ H ₃₁ O ₄
336.2248	0.7	336.2301	-15.7	-5.3	5.0	C ₂₀ H ₃₂ O ₄
		336.2148	29.7	10.0	1.0	C ₁₆ H ₃₂ O ₇
346.2202	0.5	346.2144	16.6	5.7	7.0	C ₂₁ H ₃₀ O ₄
		346.2297	-27.5	-9.5	11.0	C ₂₅ H ₃₀ O ₁
348.2285	1.3	348.2301	-4.6	-1.6	6.0	C ₂₁ H ₃₂ O ₄
349.2216	0.6	349.2226	-3.1	-1.1	1.5	C ₁₇ H ₃₃ O ₇
		349.2168	13.8	4.8	10.5	C ₂₄ H ₂₉ O ₂
350.2458	2.2	350.2457	0.4	0.1	5.0	C ₂₁ H ₃₄ O ₁
351.2543	0.5	351.2535	2.1	0.7	4.5	C ₂₁ H ₃₅ O ₁

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Figure S7. HREI-MS spectrum of compound 2

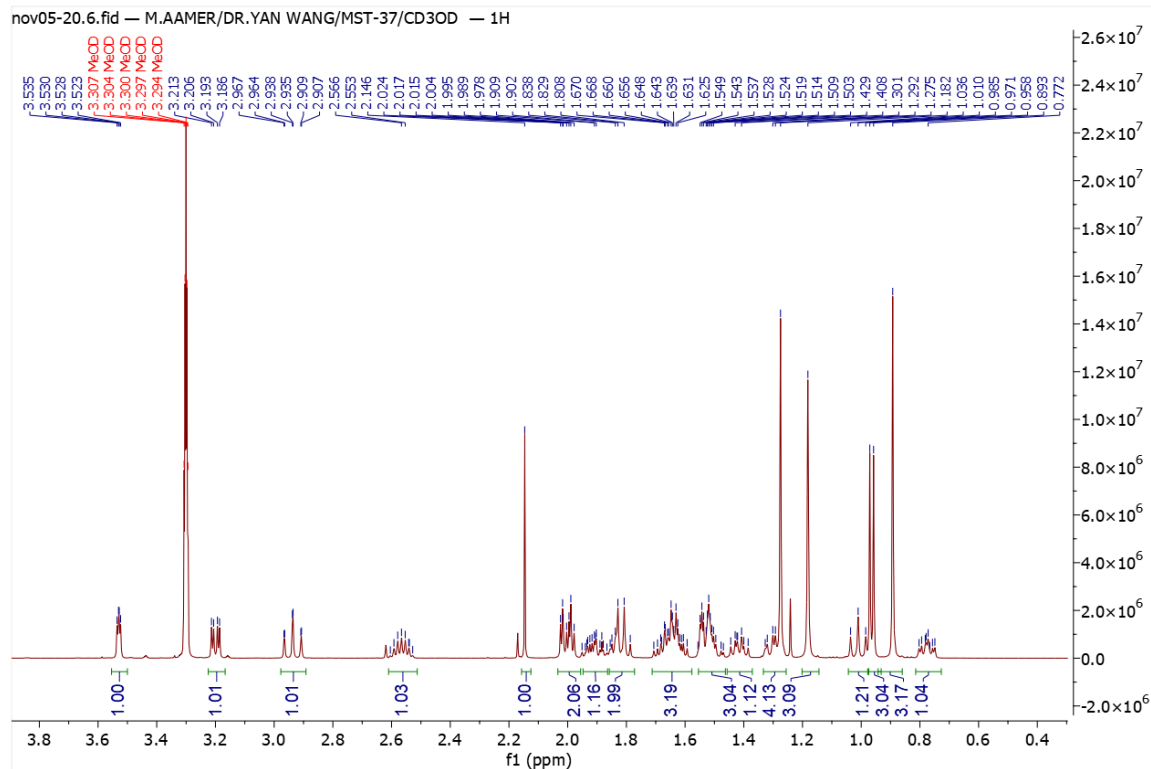


Figure S10. ^1H NMR spectrum-2 of compound **2** (500 MHz, CD_3OD)

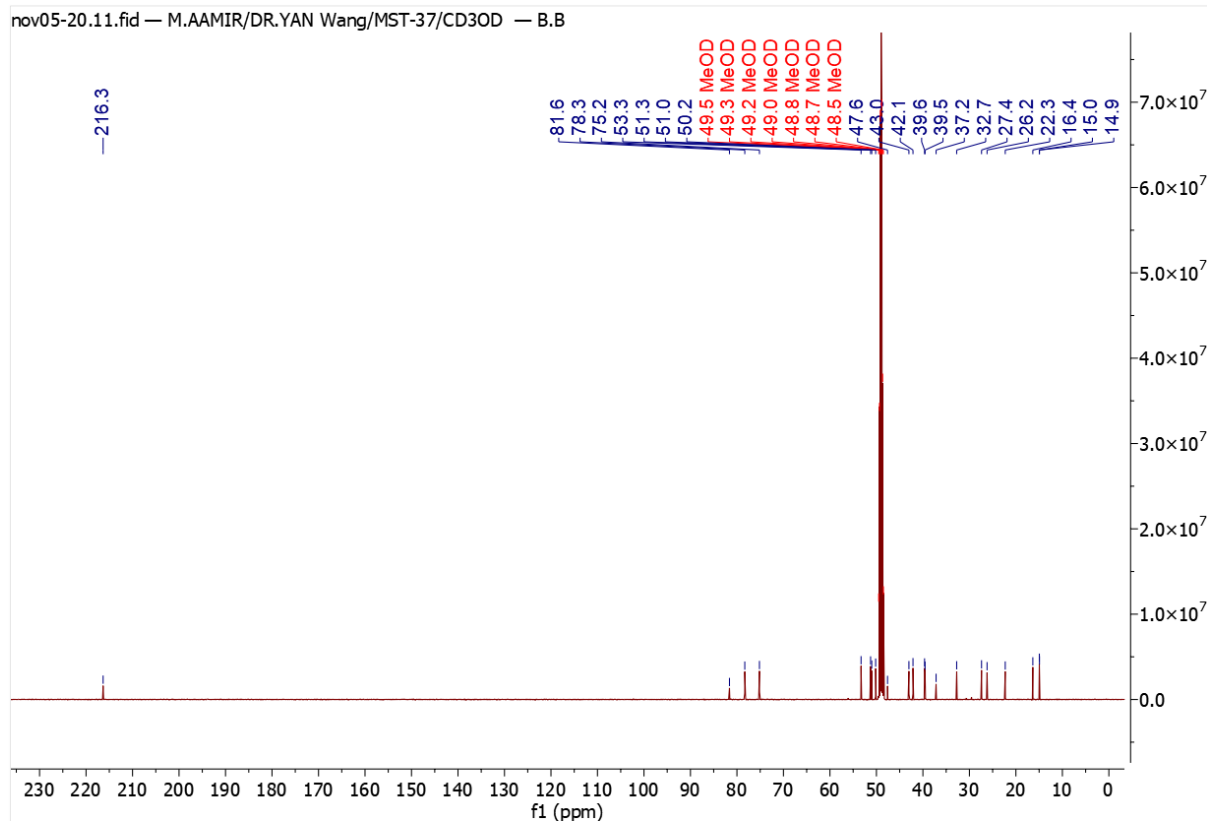


Figure S11. ^{13}C NMR spectrum-1 of compound **2** (125 MHz, CD_3OD)

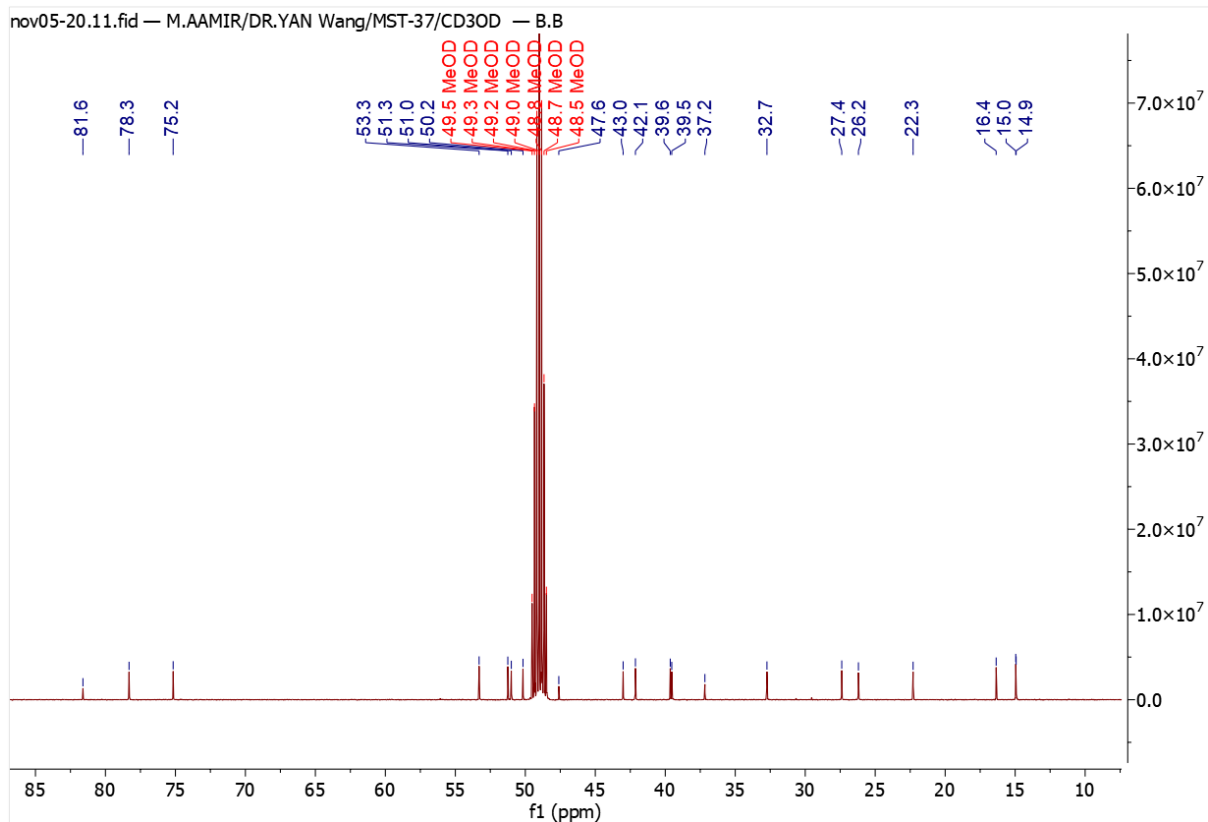


Figure S12. ^{13}C NMR spectrum-2 of compound **2** (125 MHz, CD_3OD)

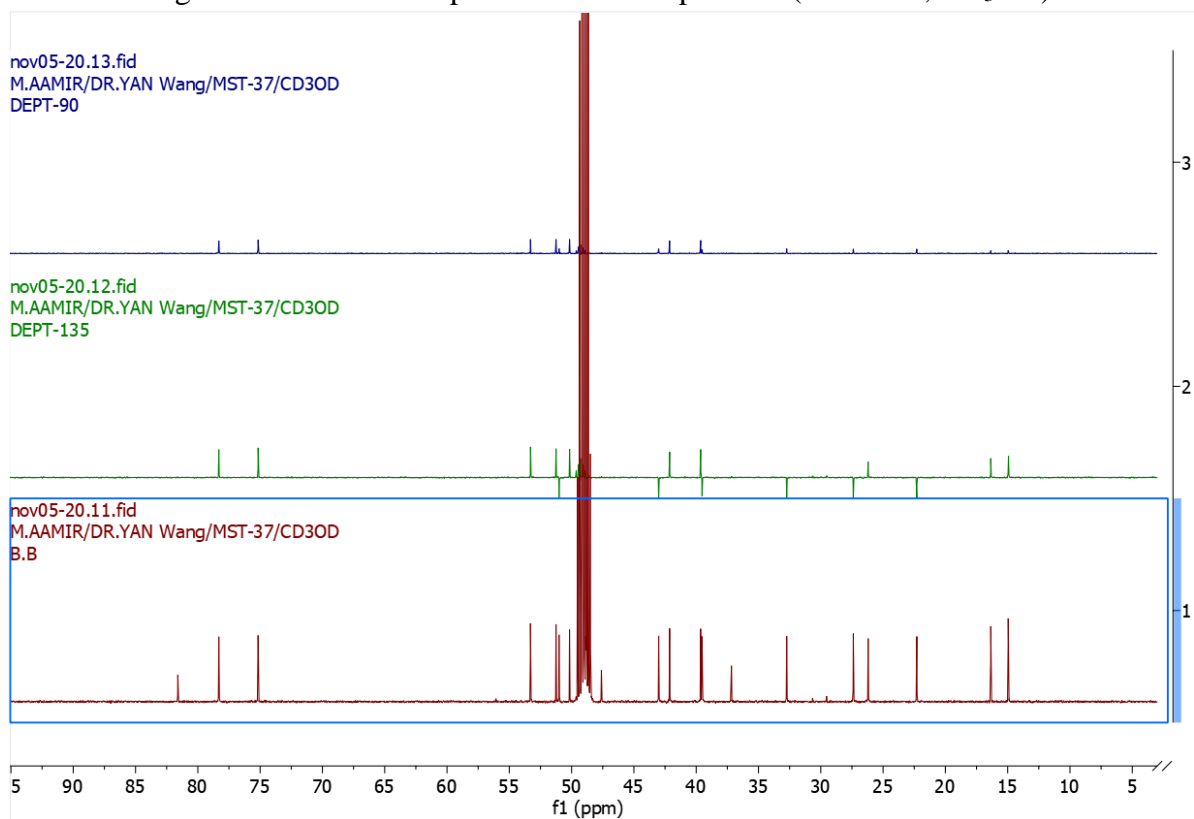


Figure S13. DEPT spectrum of compound **2**

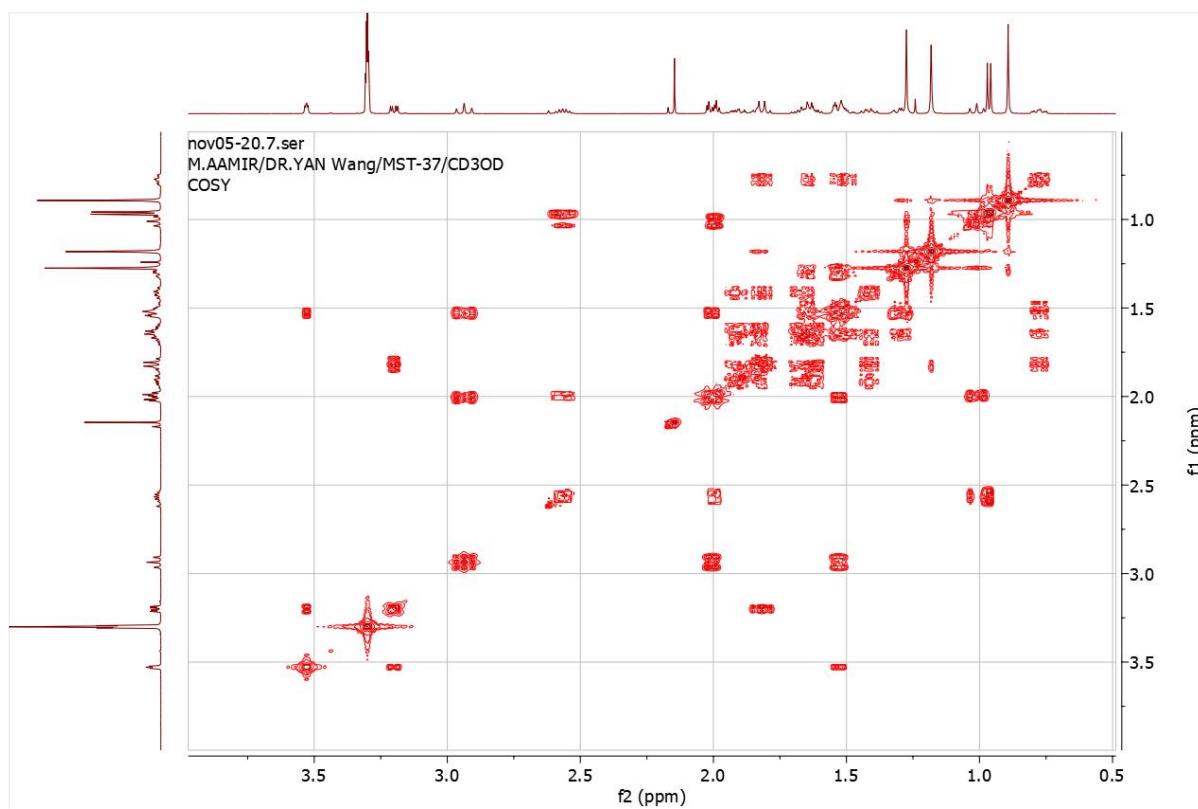


Figure S14. ¹H-¹H COSY spectrum of compound **2**

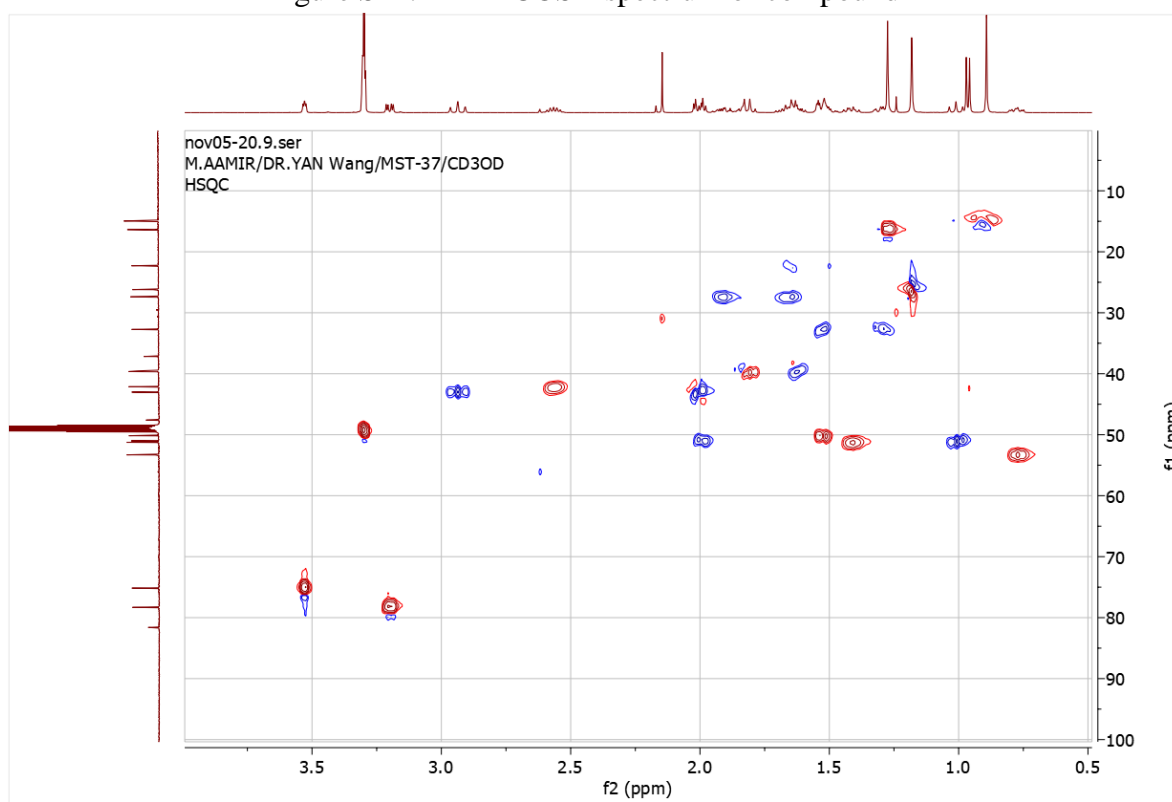


Figure S15. HSQC spectrum of compound **2**

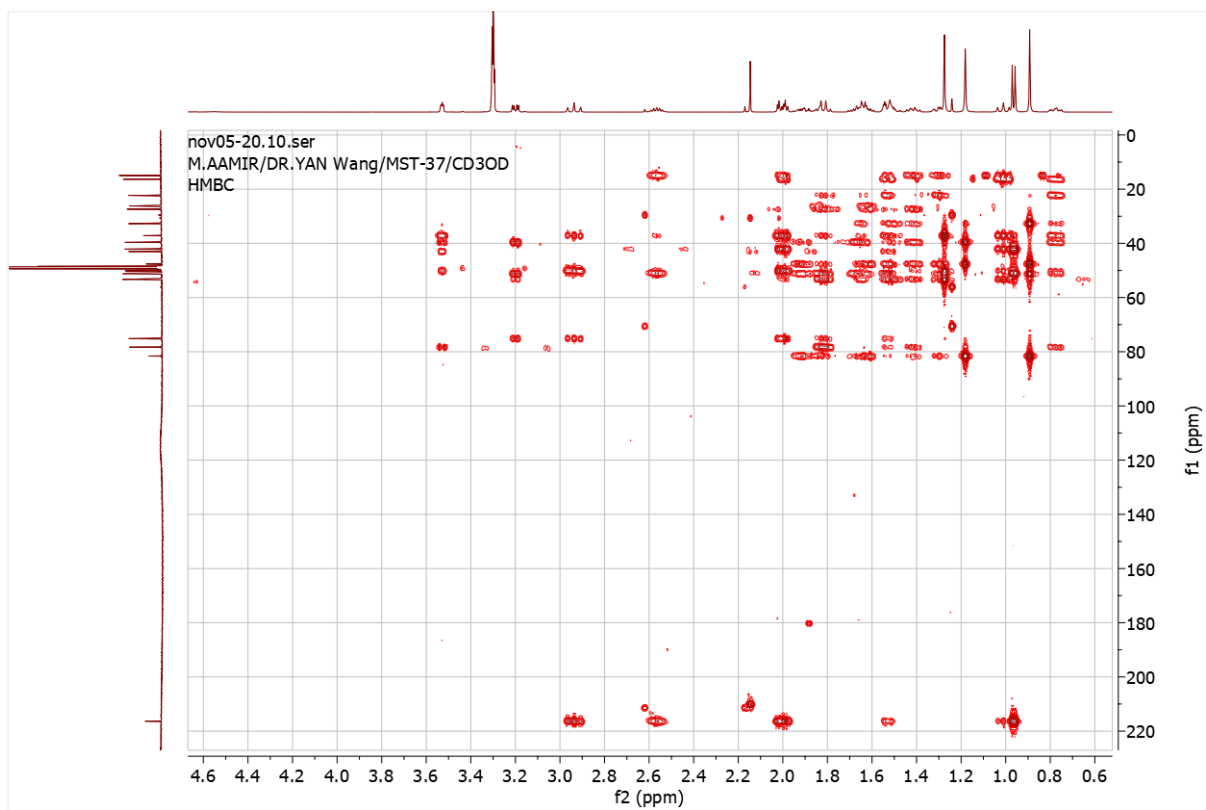


Figure S16. HMBC spectrum-1 of compound 2

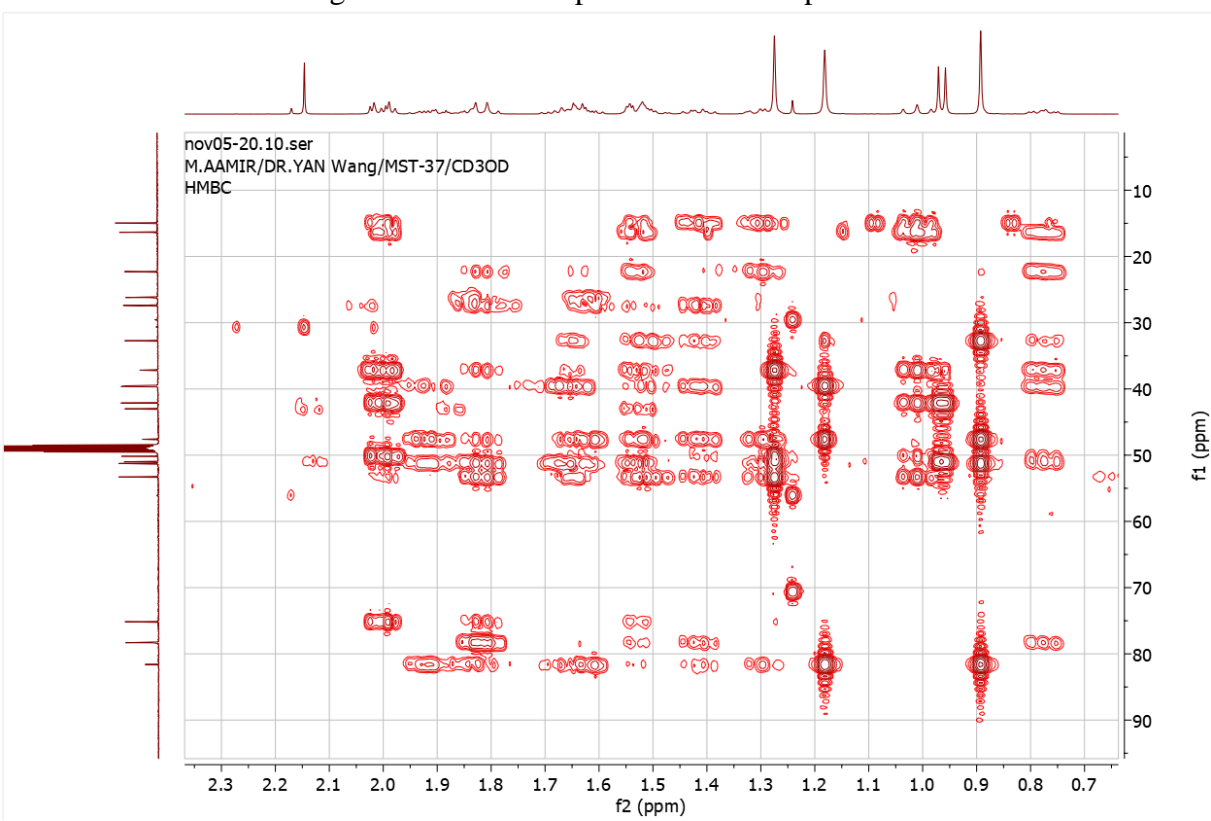


Figure S17. HMBC spectrum-2 of compound 2

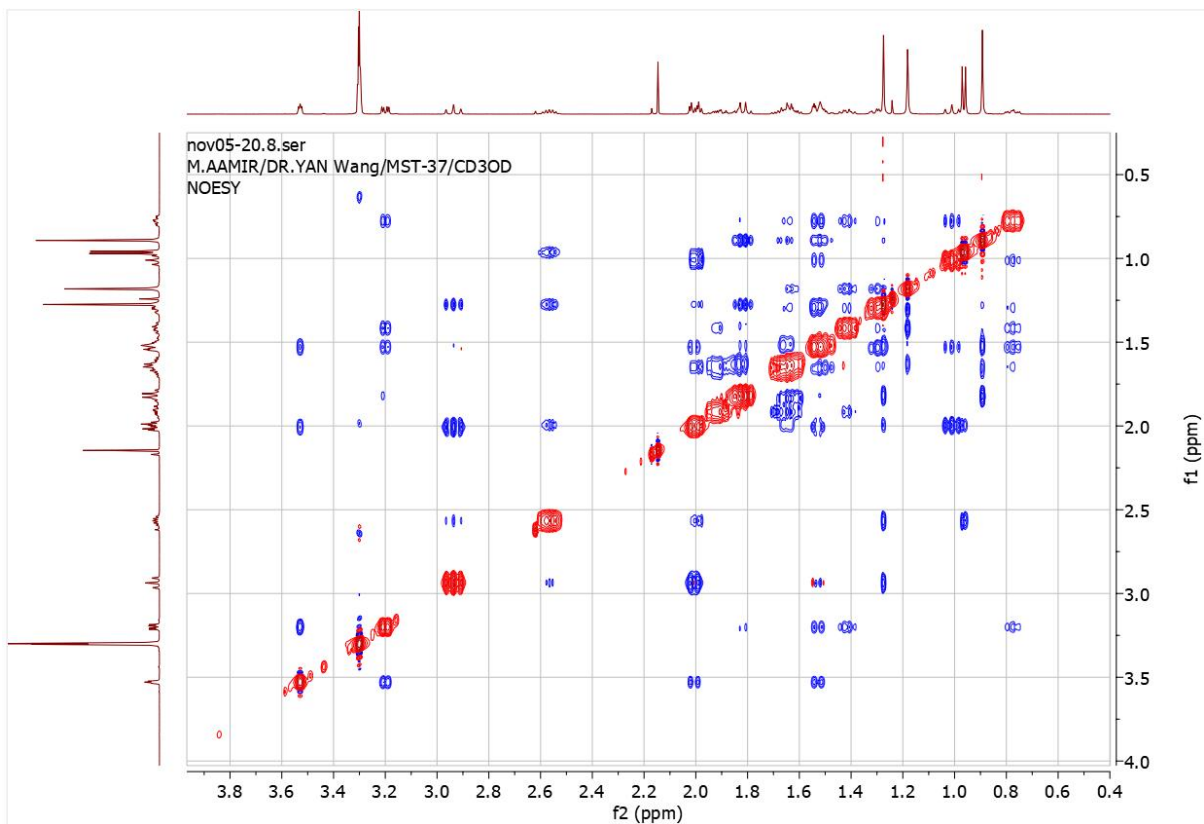


Figure S18. NOESY spectrum of compound 2

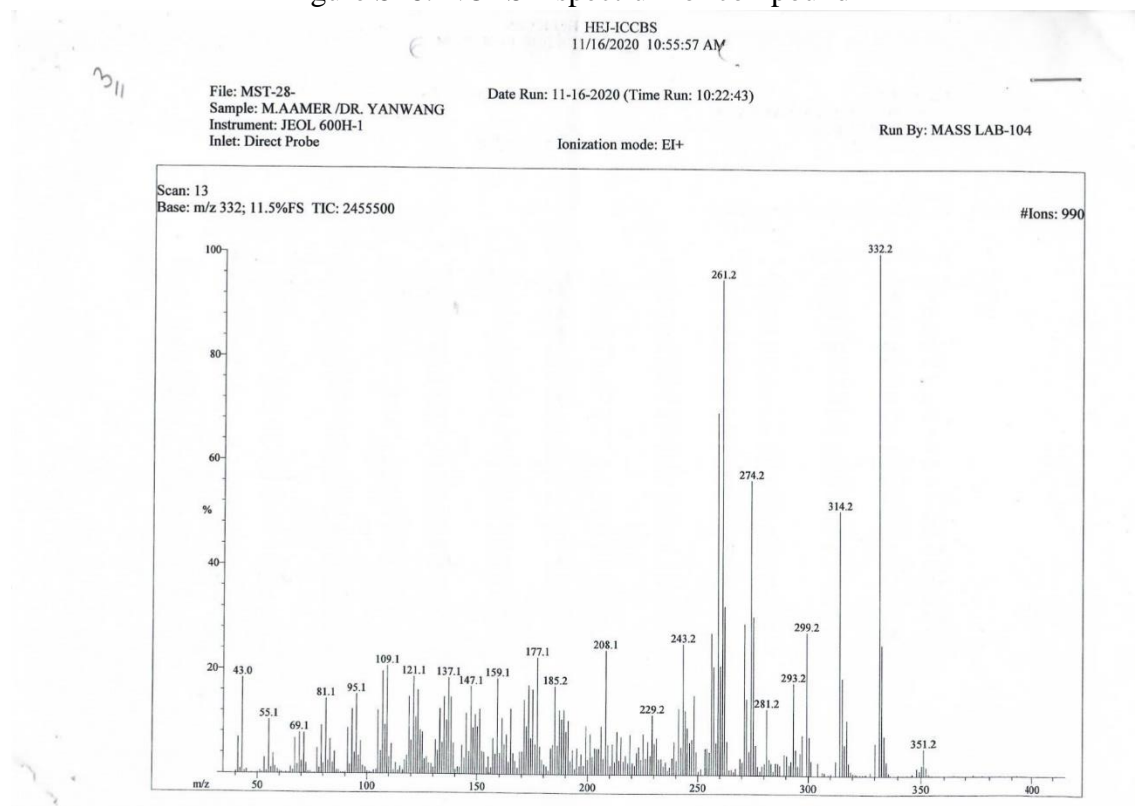


Figure S19. EI-MS spectrum of compound 3

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
311.1819	0.3	310.1780	37.6	11.7	5.0	C ₁₇ H ₂₆ O ₅
		311.1800	6.1	1.9	13.5	C ₂₄ H ₂₃
		311.1858	-12.8	-4.0	4.5	C ₁₇ H ₂₇ O ₅
		311.1706	36.2	11.3	0.5	C ₁₃ H ₂₇ O ₈
312.2176	5.2	312.2089	27.6	8.6	8.0	C ₂₁ H ₂₈ O ₂
313.2085	3.3	313.2015	22.2	7.0	3.5	C ₁₇ H ₂₉ O ₅
		313.2168	-26.5	-8.3	7.5	C ₂₁ H ₂₅ O ₂
314.2246	72.9	314.2246	0.2	0.1	7.0	C ₂₁ H ₃₀ O ₂
315.2306	24.2	315.2324	-5.6	-1.8	6.5	C ₂₁ H ₃₁ O ₂
316.2345	6.8	316.2402	-18.0	-5.7	6.0	C ₂₁ H ₃₂ O ₂
		316.2250	30.3	9.6	2.0	C ₁₇ H ₃₂ O ₃
317.2109	51.1	317.2117	-2.4	-0.8	6.5	C ₂₀ H ₂₉ O ₃
318.2160	12.0	318.2195	-11.0	-3.5	6.0	C ₂₀ H ₃₀ O ₃
		318.2042	37.0	11.8	2.0	C ₂₀ H ₃₀ O ₆
319.2259	1.8	319.2273	-4.6	-1.5	5.5	C ₁₆ H ₃₀ O ₅
328.2148	0.8	328.2191	-13.2	-4.3	12.0	C ₂₅ H ₂₈
		328.2250	-31.1	-10.2	3.0	C ₁₈ H ₃₂ O ₅
		328.2038	33.3	10.9	8.0	C ₂₁ H ₂₈ O ₃
330.2241	7.6	330.2195	14.0	4.6	7.0	C ₂₁ H ₃₀ O ₃
		330.2348	-32.2	-10.6	11.0	C ₂₅ H ₃₀
331.2283	3.2	331.2273	2.9	1.0	6.5	C ₂₁ H ₃₁ O ₃
332.2345	61.6	332.2351	-1.9	-0.6	6.0	C ₂₁ H ₃₁ O ₃
333.2370	15.7	333.2430	-17.8	-5.9	5.5	C ₂₁ H ₃₃ O ₃
		333.2277	28.0	9.3	1.5	C ₁₇ H ₃₃ O ₆
334.2527	4.0	334.2508	5.6	1.9	5.0	C ₂₁ H ₃₄ O ₂
335.2445	1.0	335.2434	3.5	1.2	0.5	C ₁₇ H ₃₅ O ₇
		335.2375	21.0	7.0	9.5	C ₁₇ H ₃₅ O ₇
348.2103	1.0	348.2089	3.9	1.4	11.0	C ₂₄ H ₃₁ O ₁
		348.2148	-13.0	-4.5	2.0	C ₂₄ H ₃₁ O ₂
350.2439	0.5	350.2457	-5.2	-1.8	5.0	C ₁₇ H ₃₁ O ₇
		350.2305	38.3	13.4	1.0	C ₂₁ H ₃₄ O ₄
351.2530	0.3	351.2535	-1.5	-0.5	4.5	C ₂₁ H ₃₅ O ₄

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Figure S20. HREI-MS spectrum of compound 3

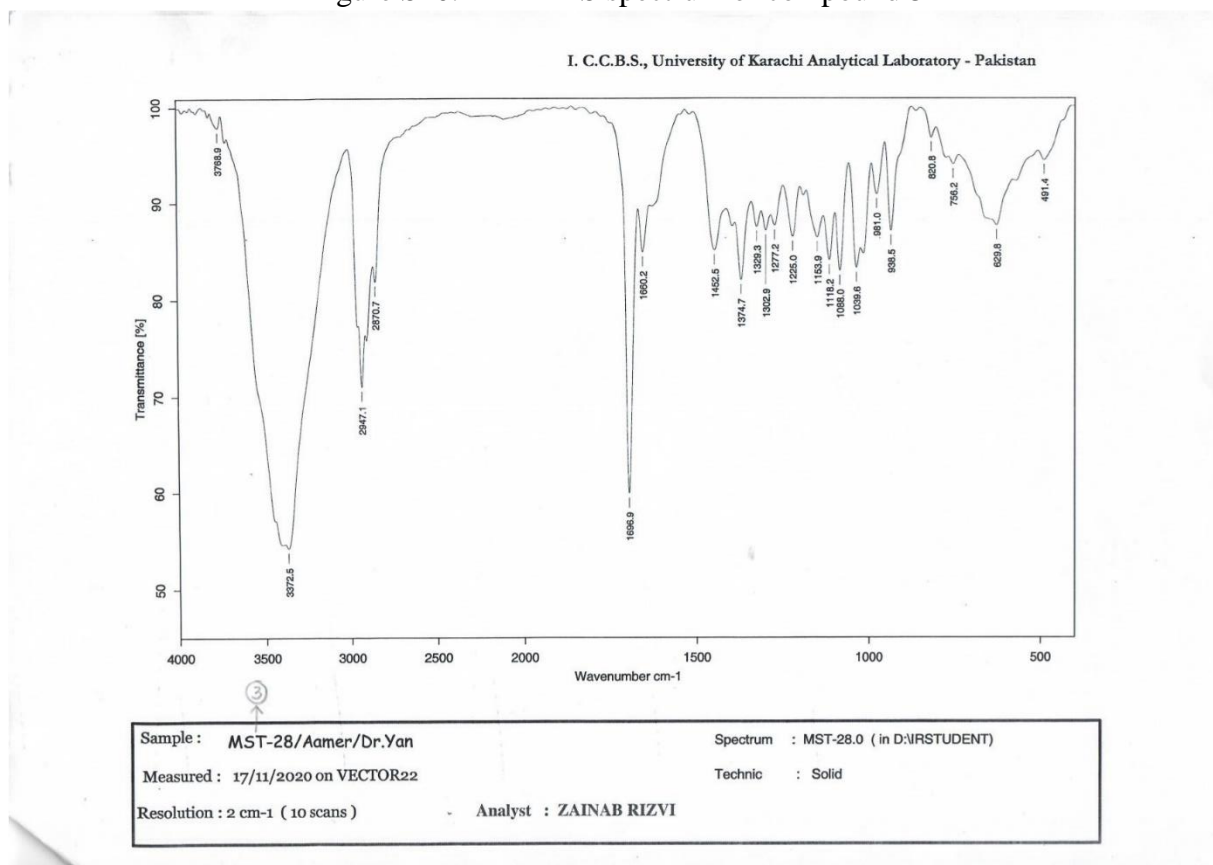


Figure S21. IR spectrum of compound 3

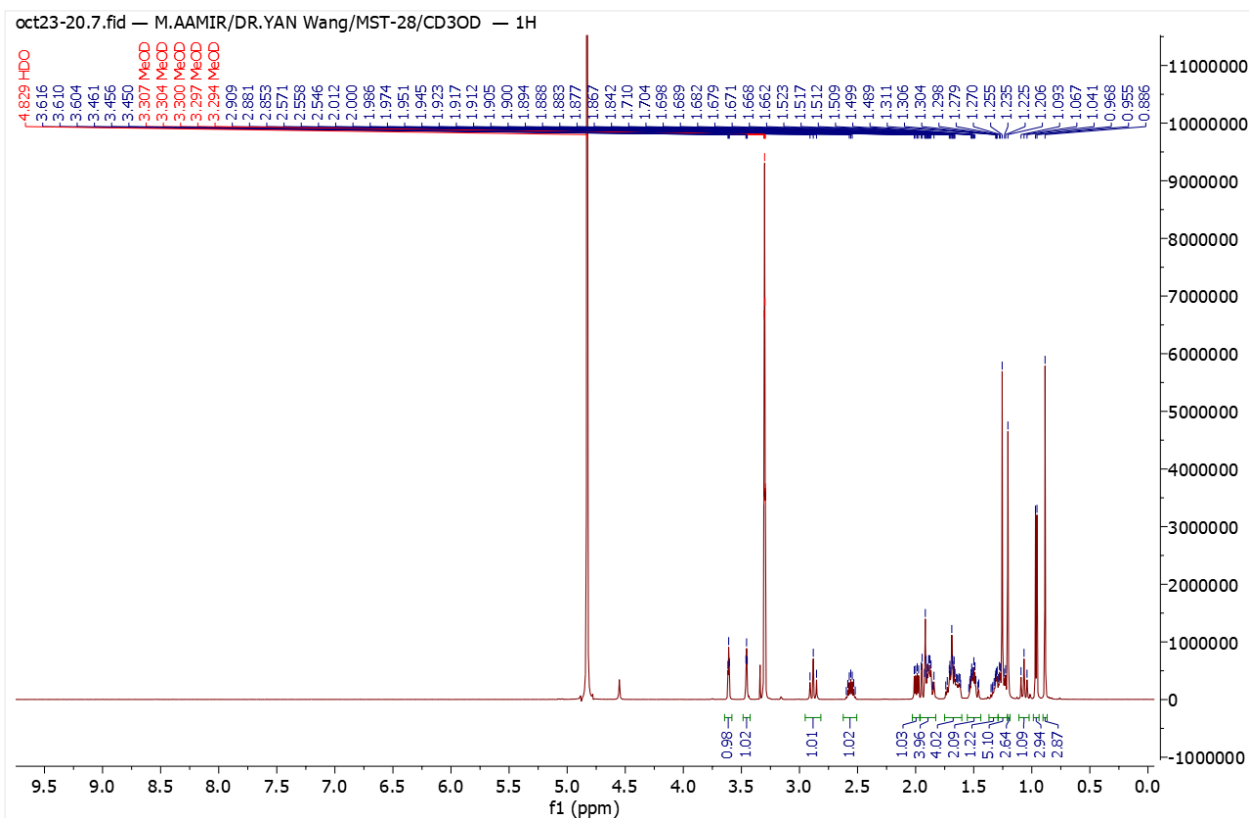


Figure S22. ¹H NMR spectrum-1 of compound **3** (500 MHz, CD₃OD)

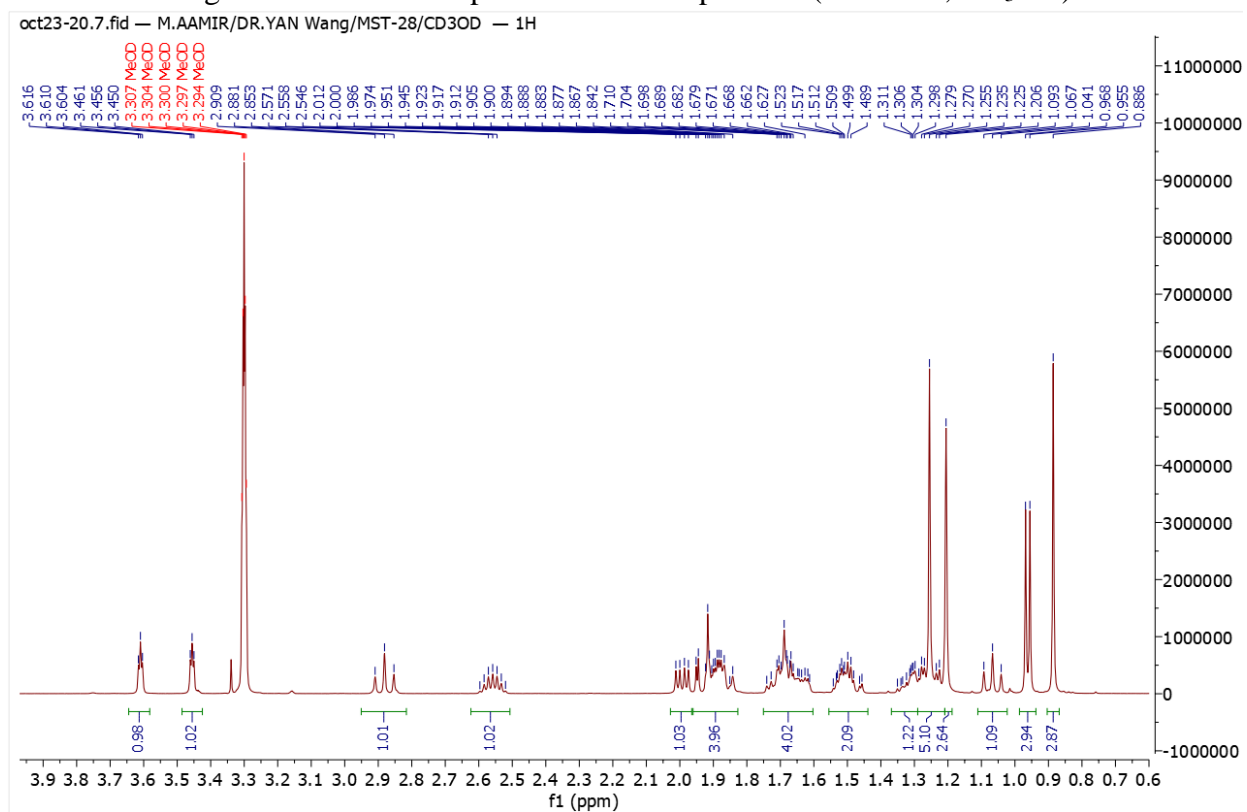
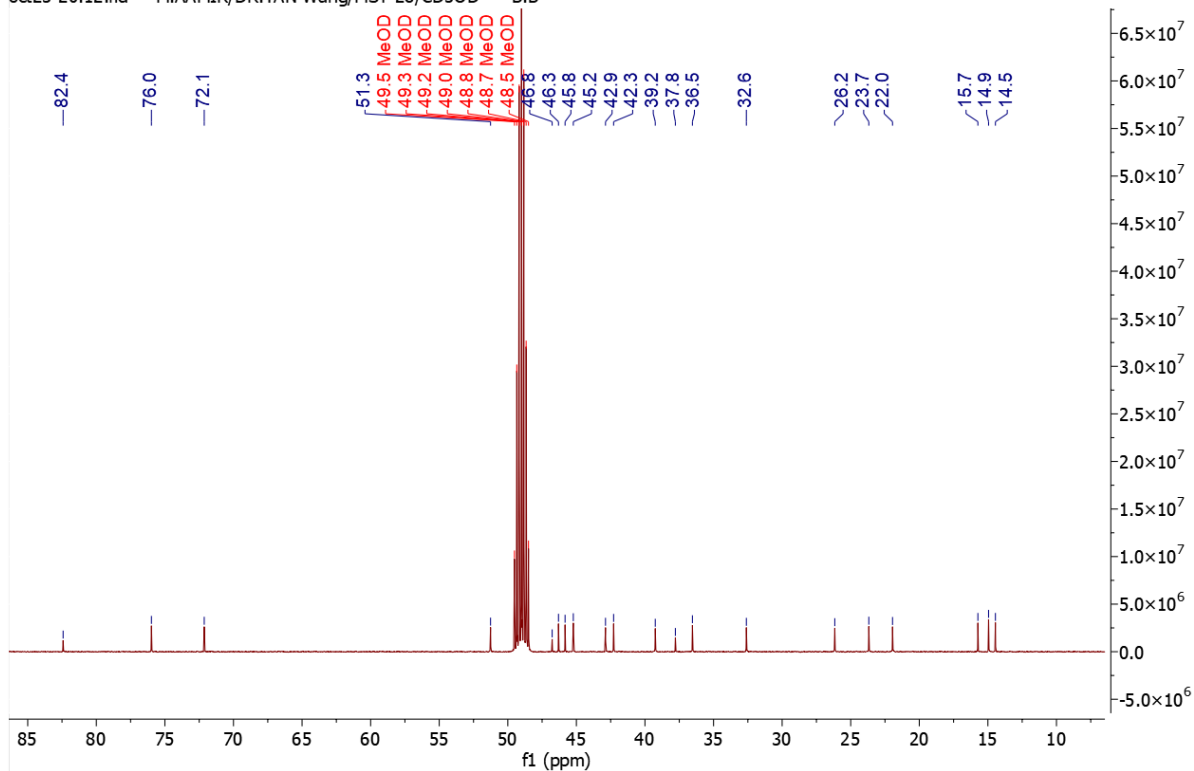
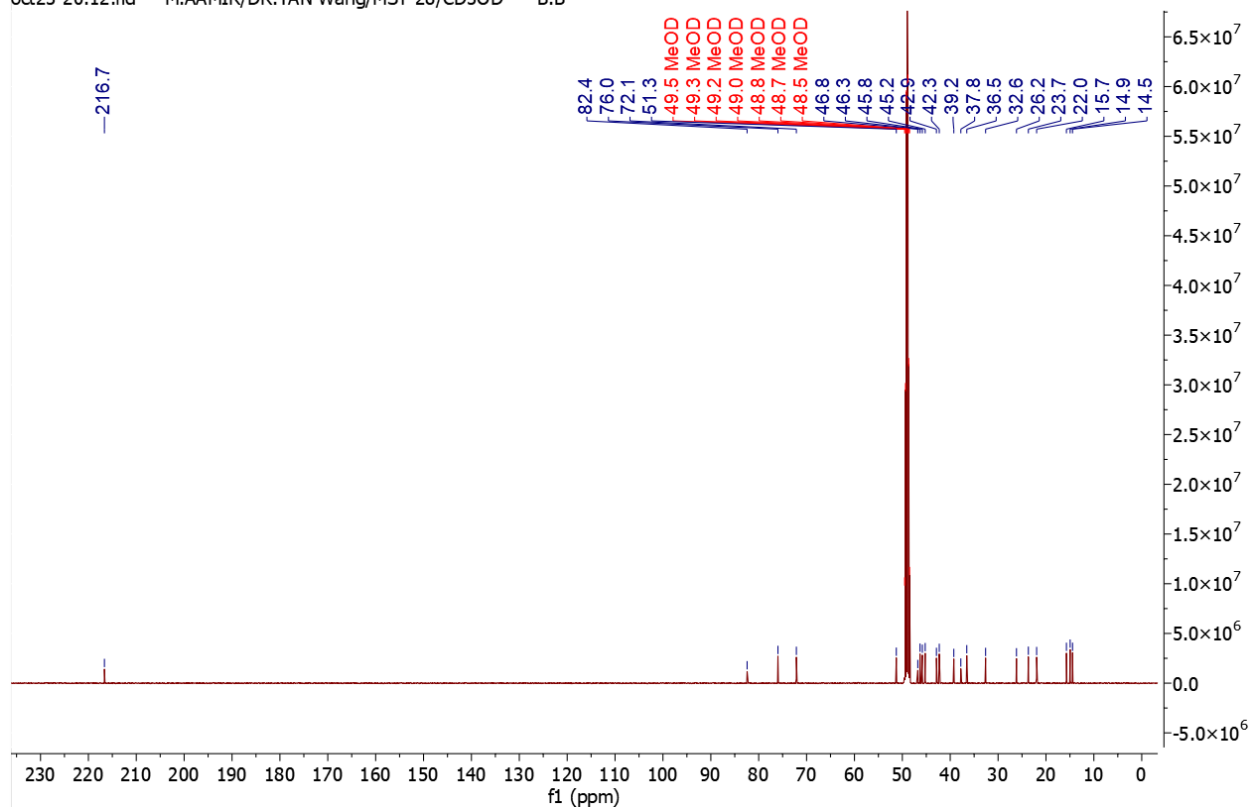


Figure S23. ¹H NMR spectrum-2 of compound **3** (500 MHz, CD₃OD)



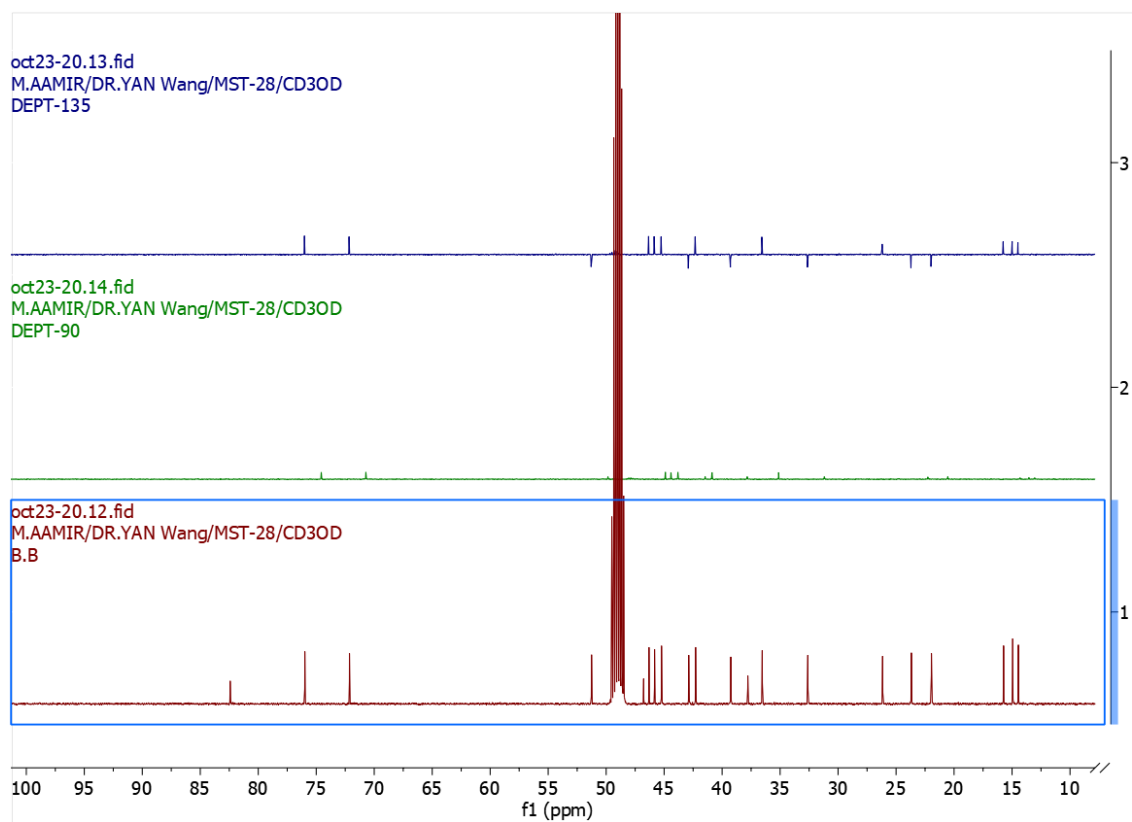


Figure S26. DEPT spectrum of compound **3**

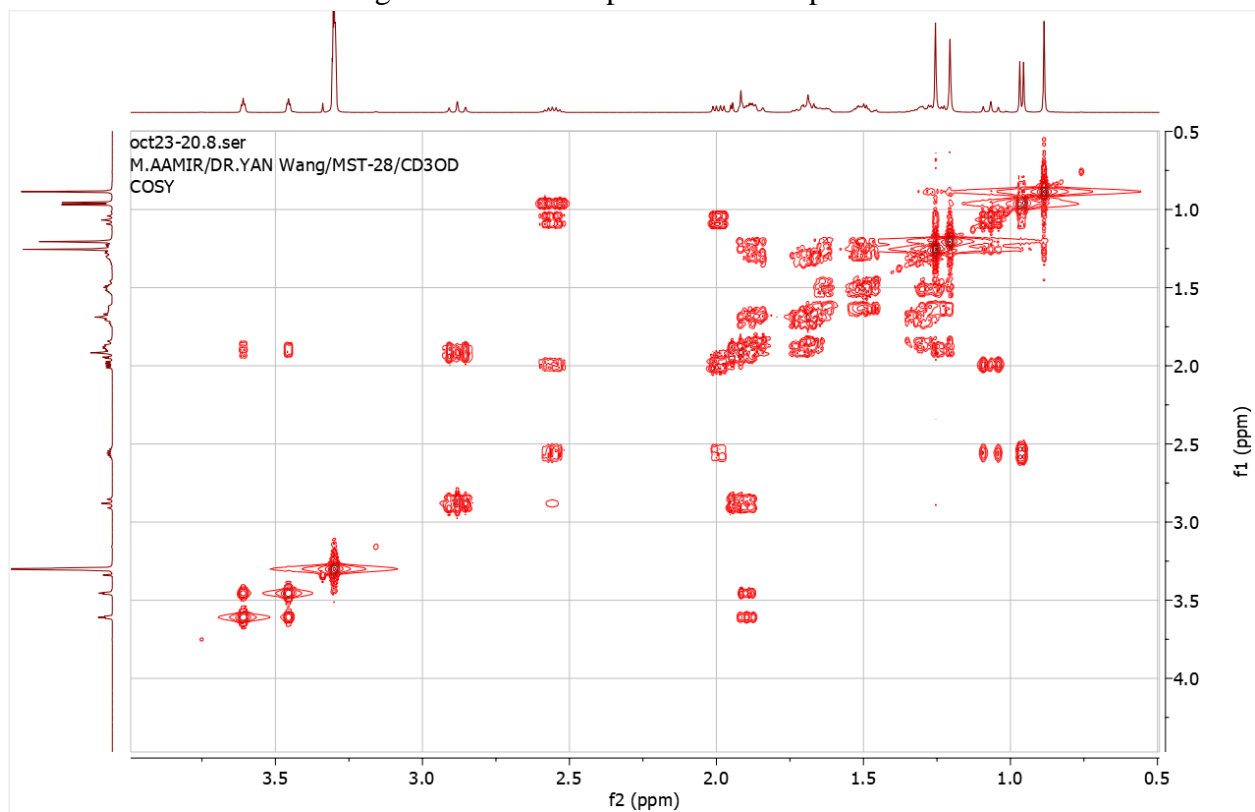


Figure S27. ^1H - ^1H COSY spectrum of compound **3**

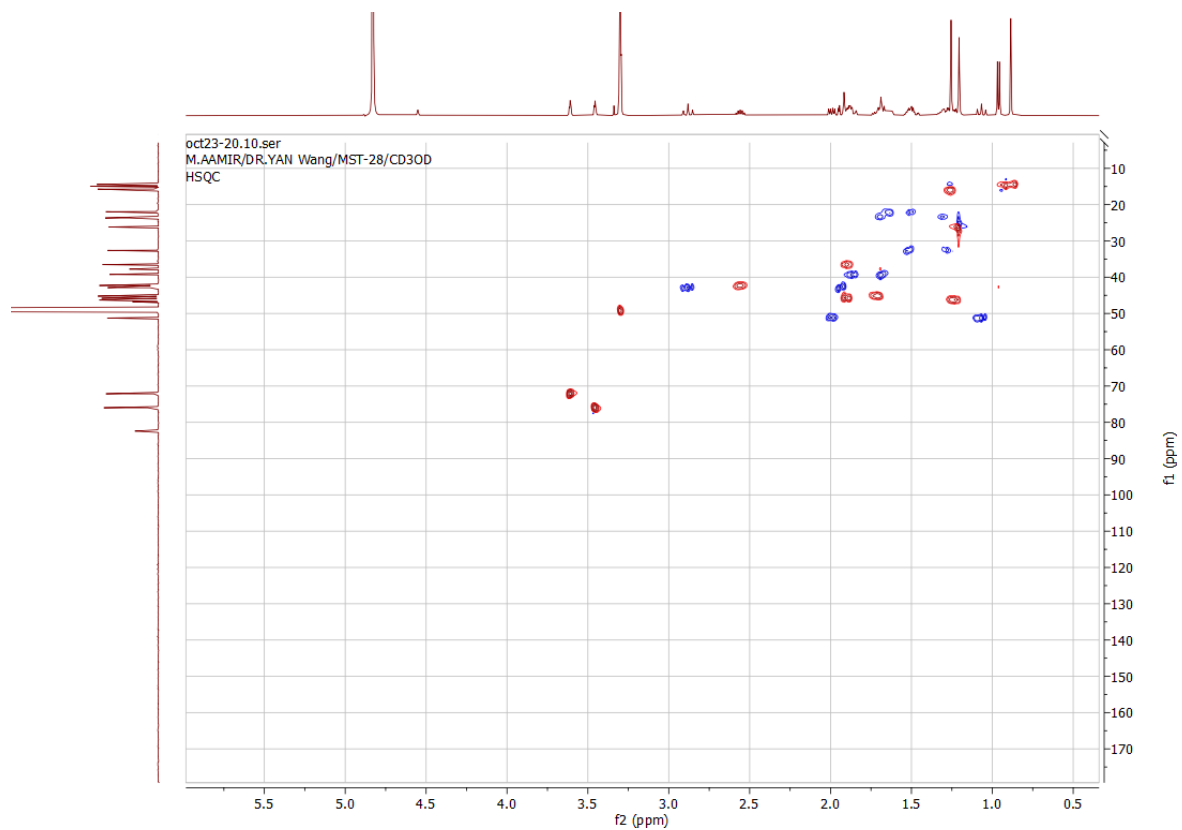


Figure S28. HSQC spectrum-1 of compound 3

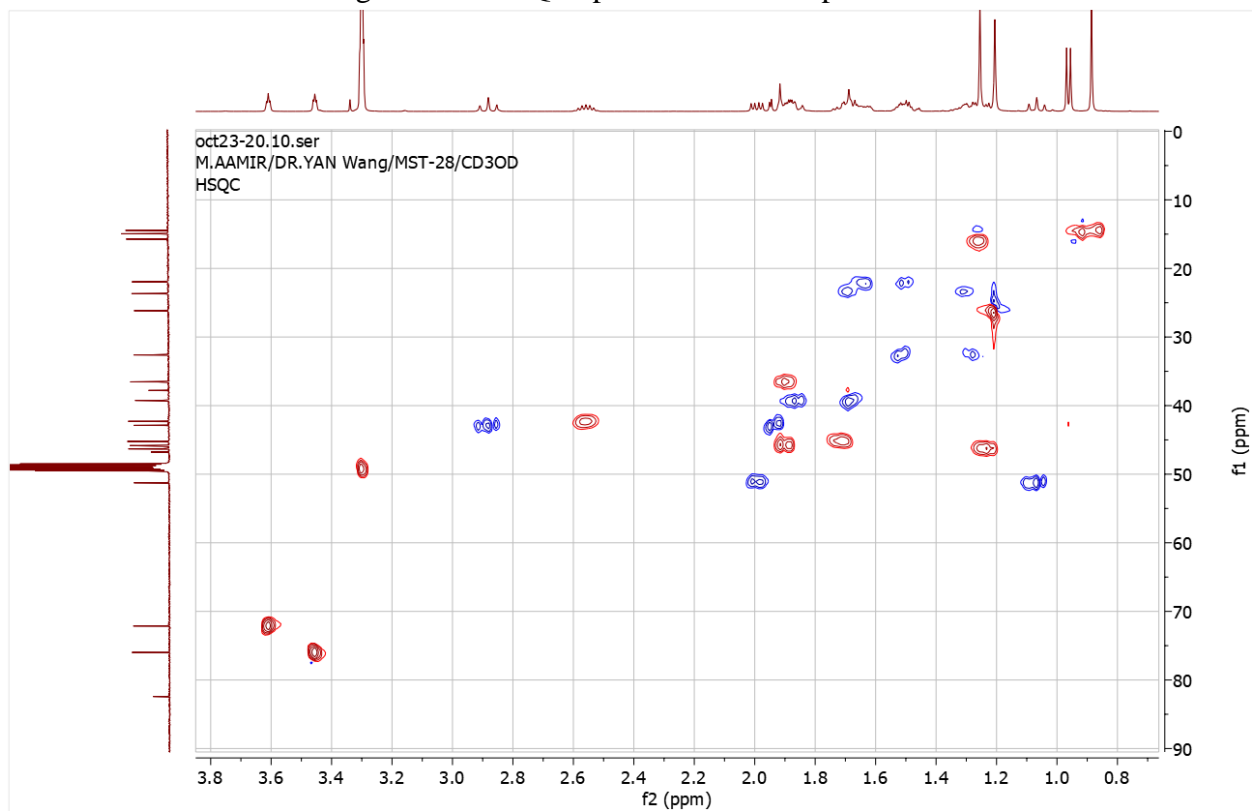


Figure S29. HSQC spectrum-2 of compound 3

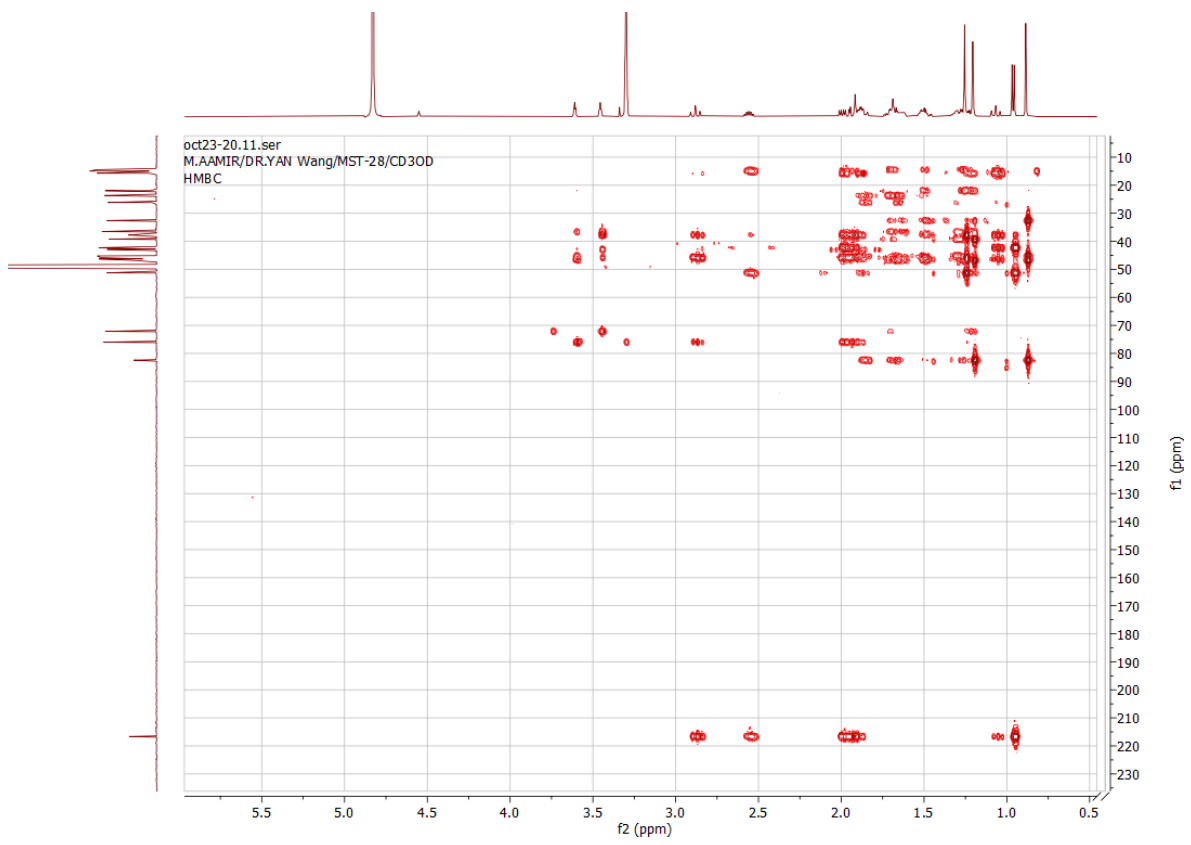


Figure S30. HMBC spectrum-1 of compound **3**

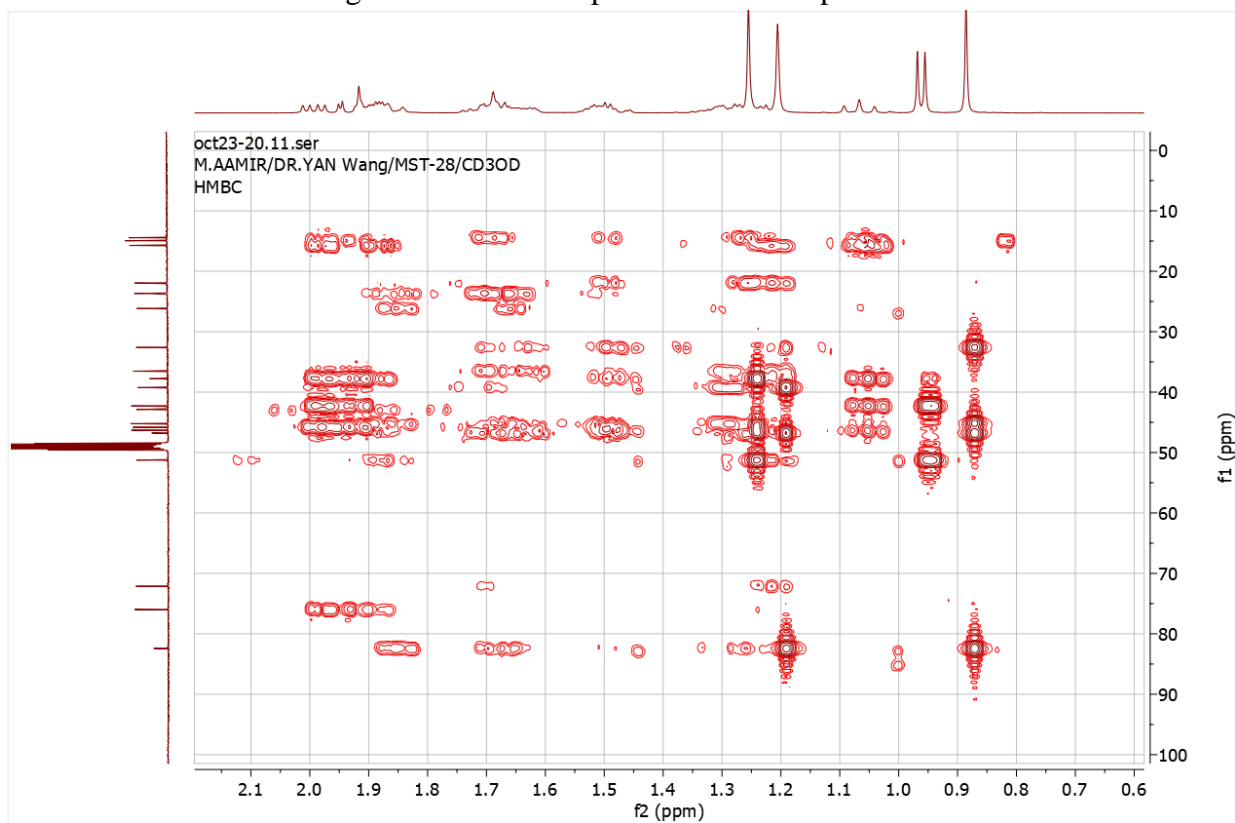


Figure S31. HMBC spectrum-2 of compound **3**

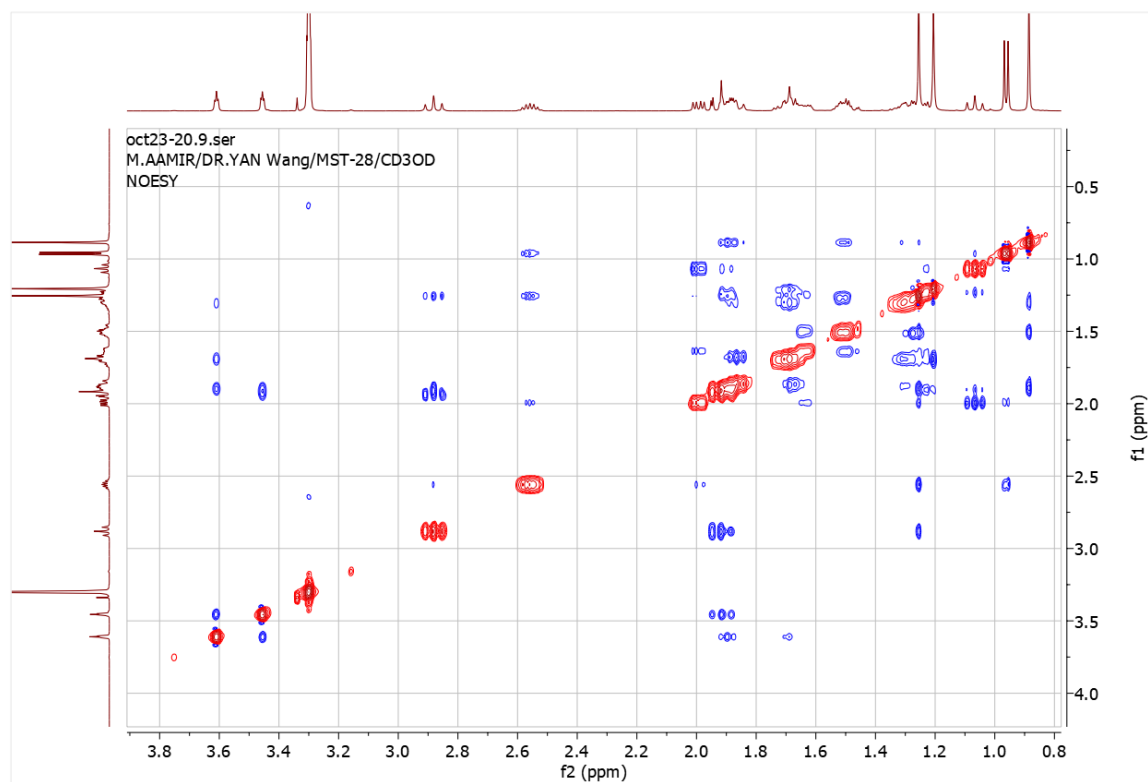


Figure S32. NOESY spectrum of compound **3**

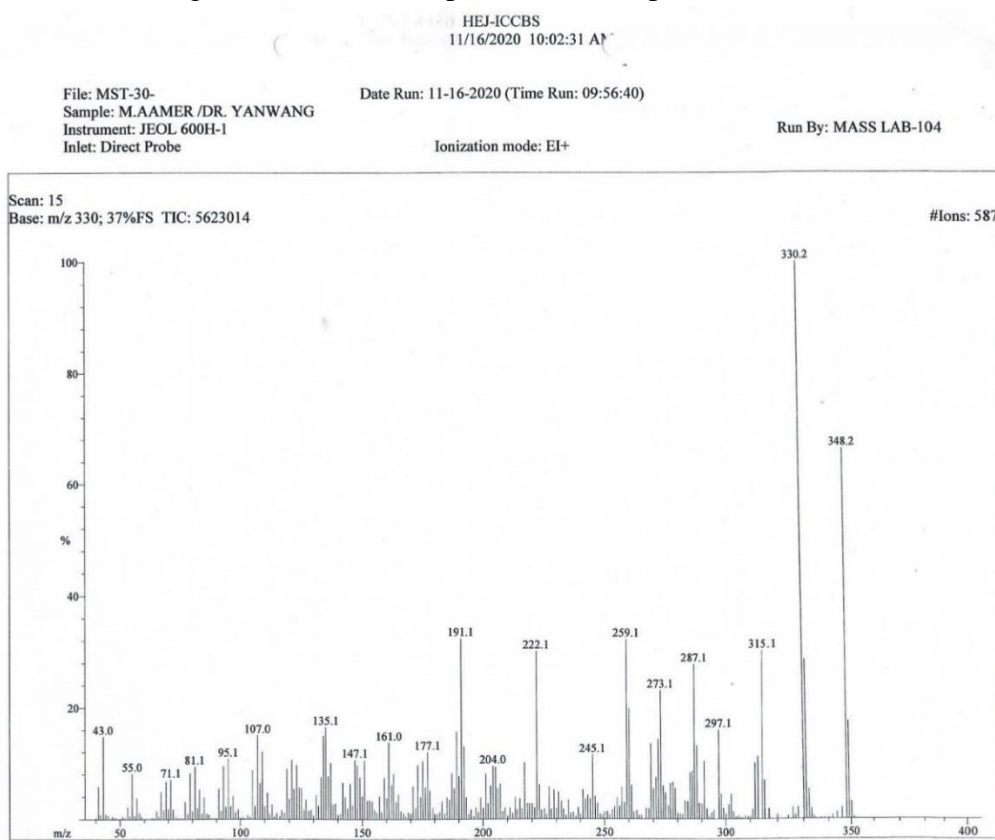


Figure S33. EI-MS spectrum of compound **4**

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
287.2024	9.0	287.2011	4.4	1.3	6.5	C ₁₉ H ₂₇ O ₂
288.1905	4.5	288.1878	9.5	2.7	11.0	C ₂₂ H ₂₄
		288.1937	-10.9	-3.1	2.0	C ₁₅ H ₂₈ O ₅
289.1816	1.2	289.1804	4.3	1.2	6.5	C ₁₈ H ₂₅ O ₃
290.1845	1.0	290.1882	-12.7	-3.7	6.0	C ₁₈ H ₂₆ O ₃
291.1963	3.3	291.1960	1.1	0.3	5.5	C ₁₈ H ₂₇ O ₃
295.1946	1.1	295.1909	12.3	3.6	4.5	C ₁₇ H ₂₇ O ₄
297.1851	10.7	297.1855	-1.4	-0.4	8.5	C ₂₀ H ₂₅ O ₂
298.1926	2.6	298.1933	-2.2	-0.7	8.0	C ₂₀ H ₂₆ O ₂
299.2004	2.2	299.2011	-2.3	-0.7	7.5	C ₂₀ H ₂₇ O ₂
302.2079	1.3	302.2093	-4.7	-1.4	2.0	C ₁₆ H ₃₀ O ₅
		302.2035	14.7	4.5	11.0	C ₂₃ H ₂₆
312.2023	5.9	312.2089	-21.2	-6.6	8.0	C ₂₁ H ₂₀ O ₂
		312.1937	27.6	8.6	4.0	C ₁₇ H ₂₈ O ₅
313.2092	4.0	313.2168	-24.1	-7.5	7.5	C ₂₁ H ₂₉ O ₂
		313.2015	24.6	7.7	3.5	C ₁₇ H ₂₉ O ₅
314.2201	1.7	314.2246	-14.3	-4.5	7.0	C ₂₁ H ₃₀ O ₂
		314.2093	34.3	10.8	3.0	C ₁₇ H ₃₀ O ₅
315.1947	18.0	315.1960	-4.2	-1.3	7.5	C ₂₀ H ₂₇ O ₃
316.2022	3.9	316.2038	-5.3	-1.7	7.0	C ₂₀ H ₂₈ O ₃
328.2081	1.0	328.2038	12.9	4.2	8.0	C ₂₁ H ₂₈ O ₃
		328.2191	-33.6	-11.0	12.0	C ₂₅ H ₂₈
330.2218	25.4	330.2195	7.1	2.3	7.0	C ₂₁ H ₃₀ O ₃
331.2249	6.9	331.2273	-7.4	-2.5	6.5	C ₂₁ H ₃₁ O ₃
332.2369	2.4	332.2351	5.4	1.8	6.0	C ₂₁ H ₃₂ O ₃
348.2305	11.4	348.2301	1.3	0.5	6.0	C ₂₁ H ₃₂ O ₄
349.2318	2.6	349.2379	-17.4	-6.1	5.5	C ₂₁ H ₃₃ O ₄
		349.2226	26.3	9.2	1.5	C ₁₇ H ₃₃ O ₇

MST-30

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Figure S34. HREI-MS spectrum of compound 4

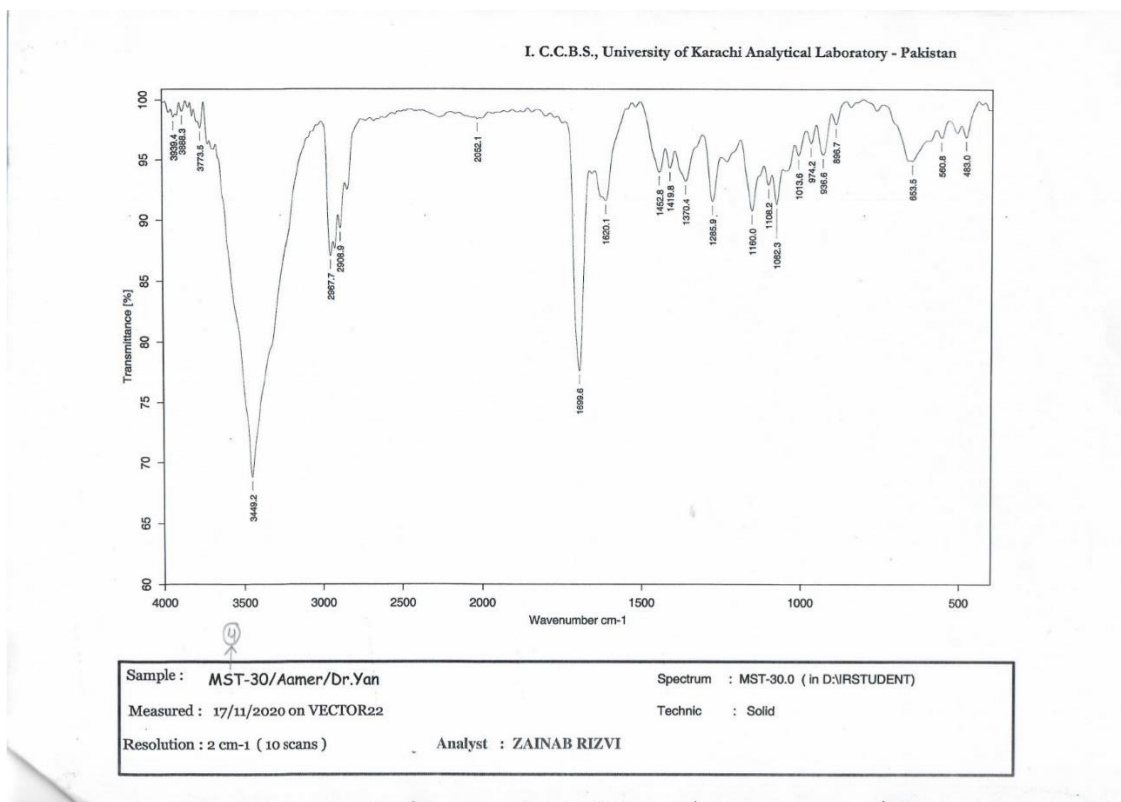


Figure S35. IR spectrum of compound 4

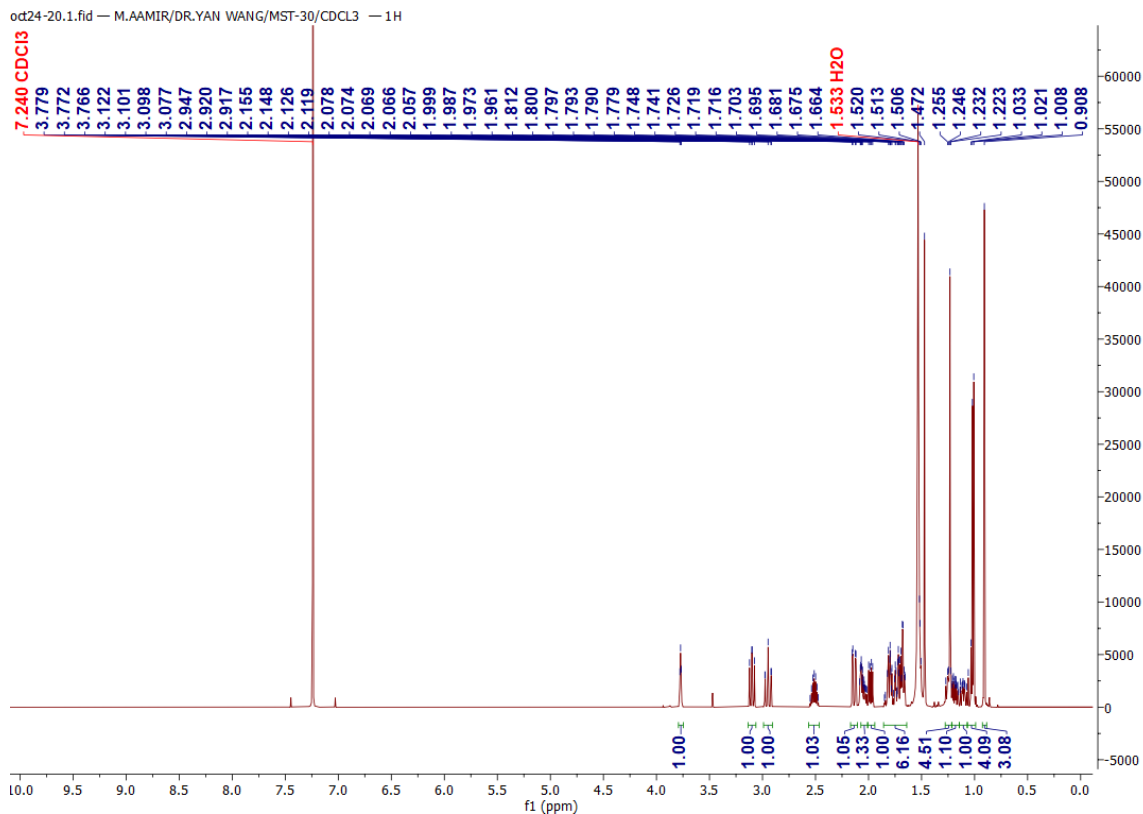


Figure S36. ¹H NMR spectrum-1 of compound **4** (500 MHz, CD₃OD)

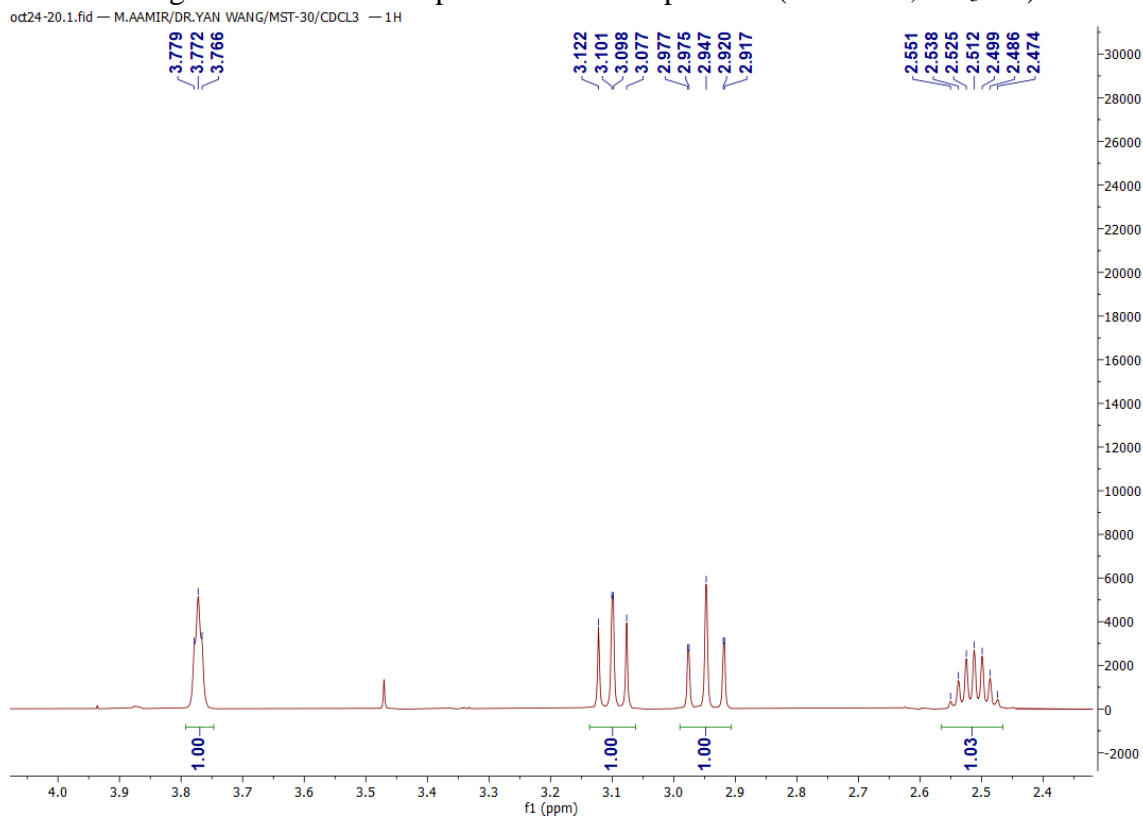


Figure S37. ¹H NMR spectrum-2 of compound **4** (500 MHz, CD₃OD)

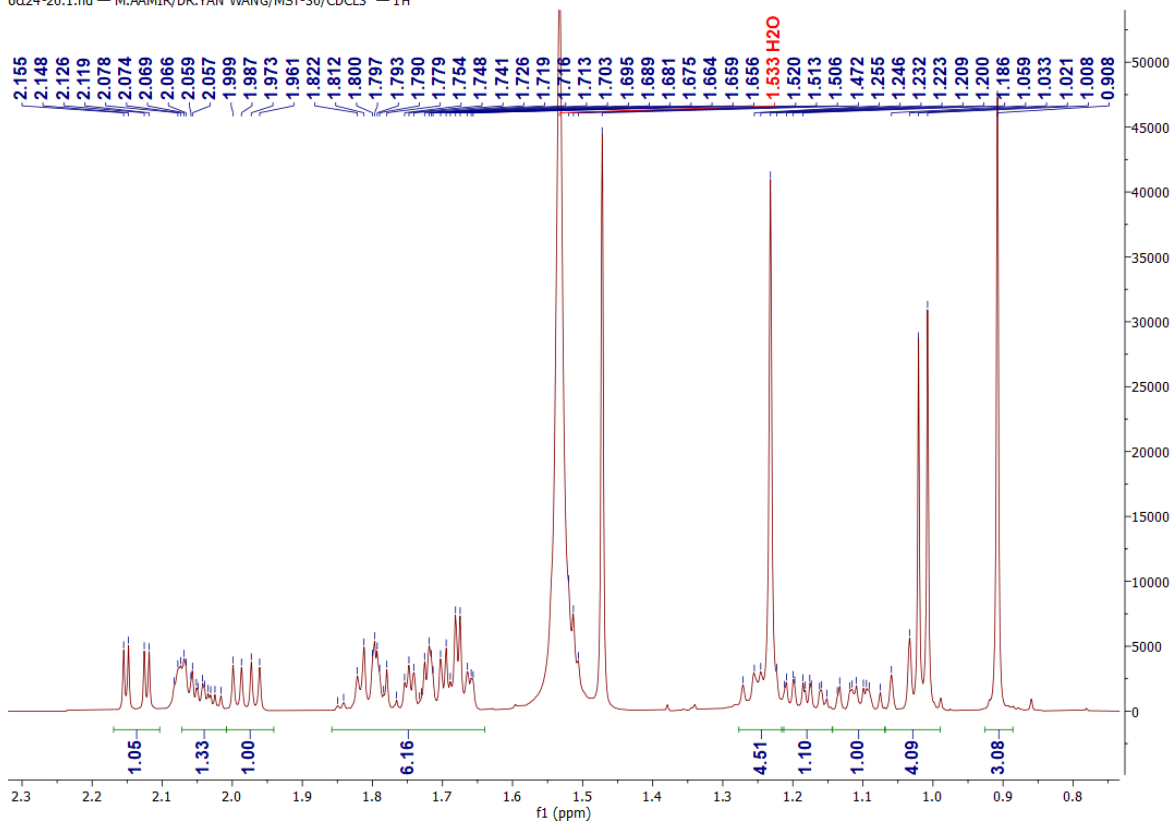


Figure S38. ^1H NMR spectrum-3 of compound **4** (500 MHz, CD_3OD)

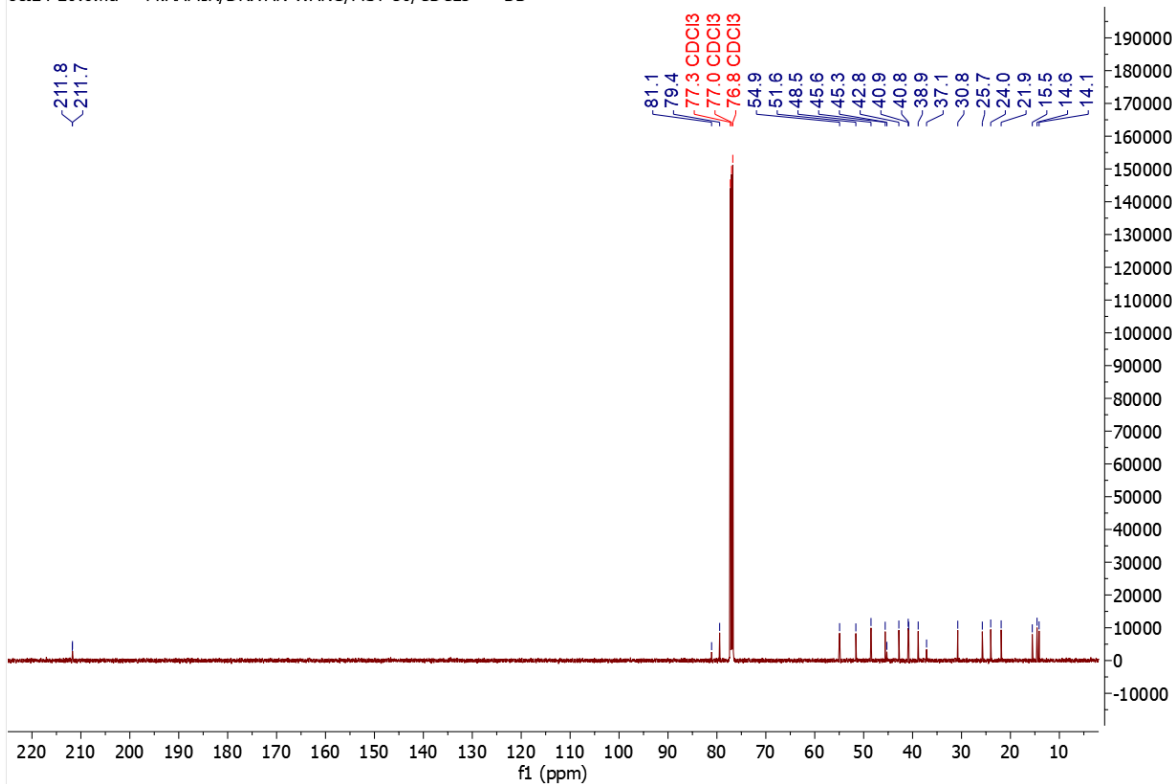


Figure S39. ^{13}C NMR spectrum-1 of compound **4** (125 MHz, CD_3OD)

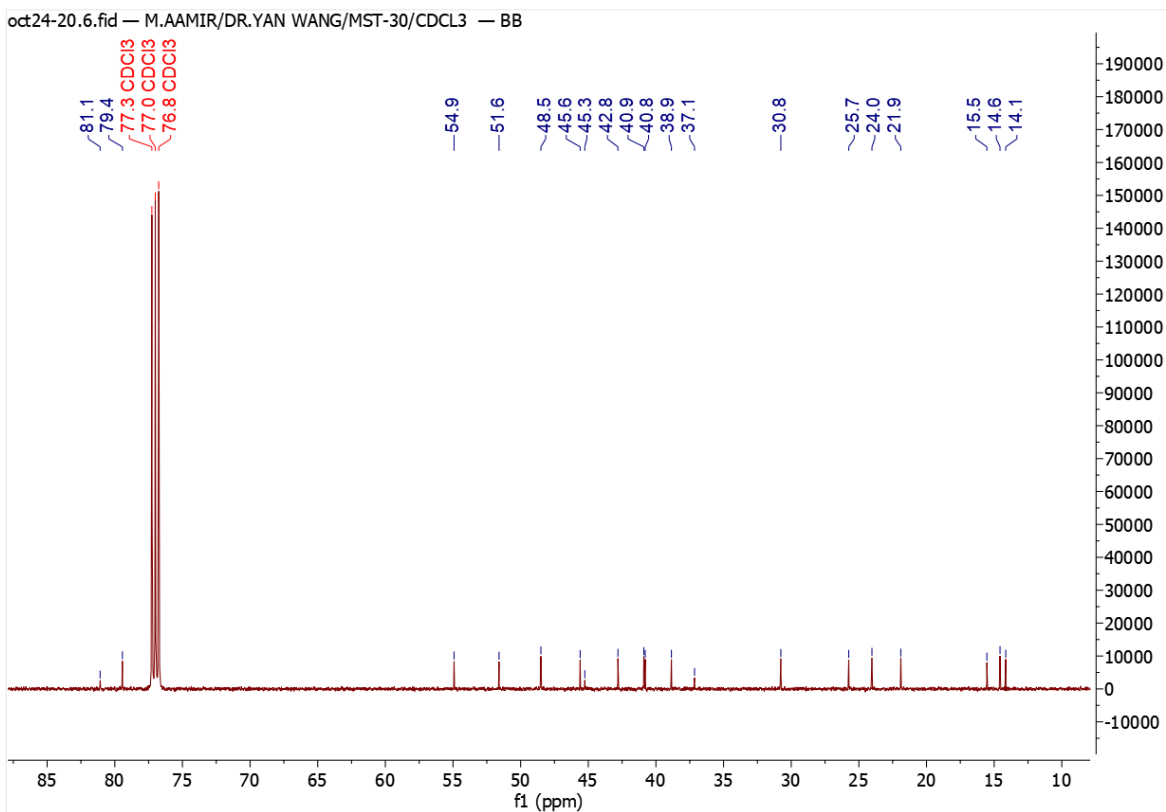


Figure S40. ¹³C NMR spectrum-2 of compound **4** (125 MHz, CD₃OD)

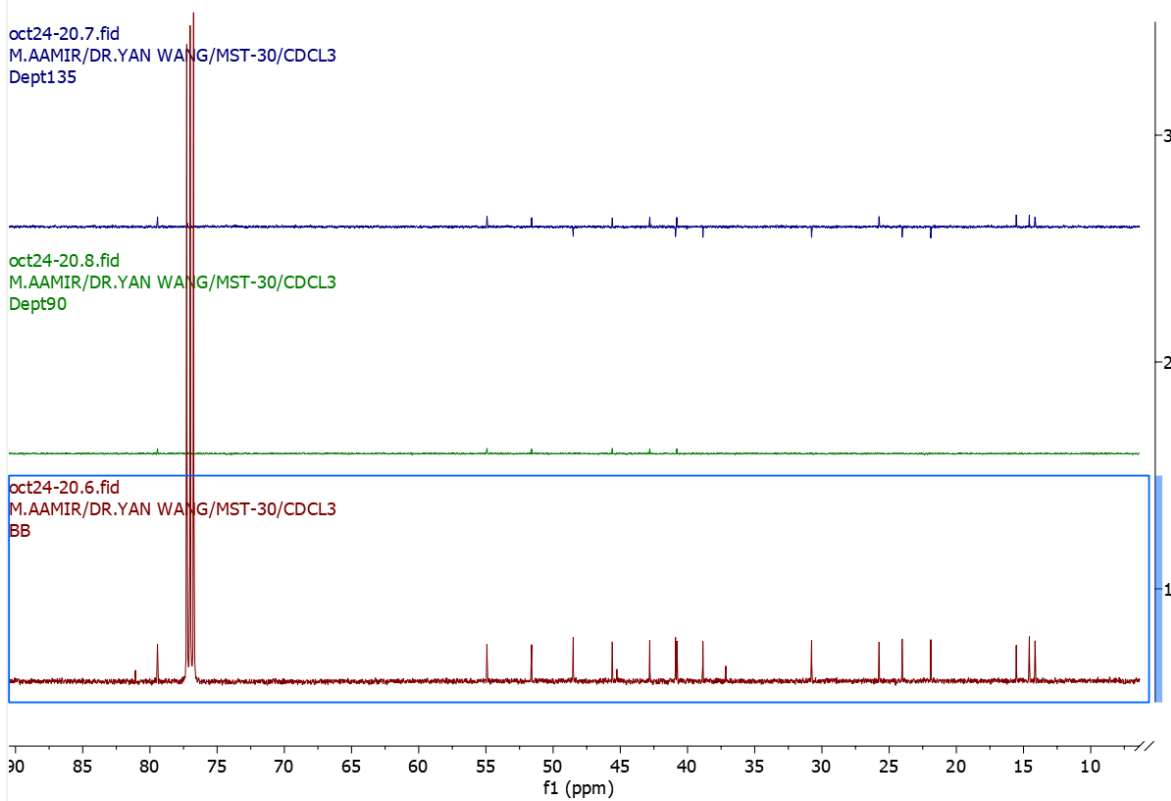


Figure S41. DEPT spectrum of compound **4**

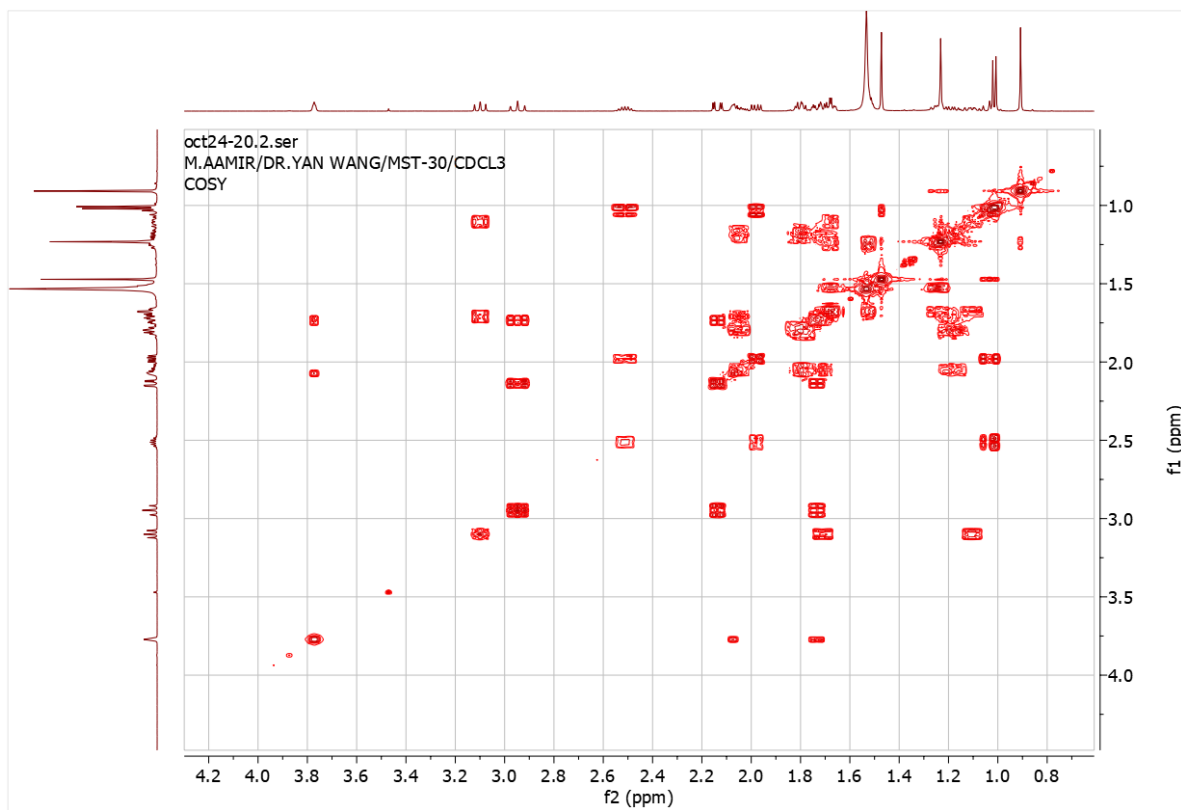


Figure S42. ^1H - ^1H COSY spectrum of compound **4**

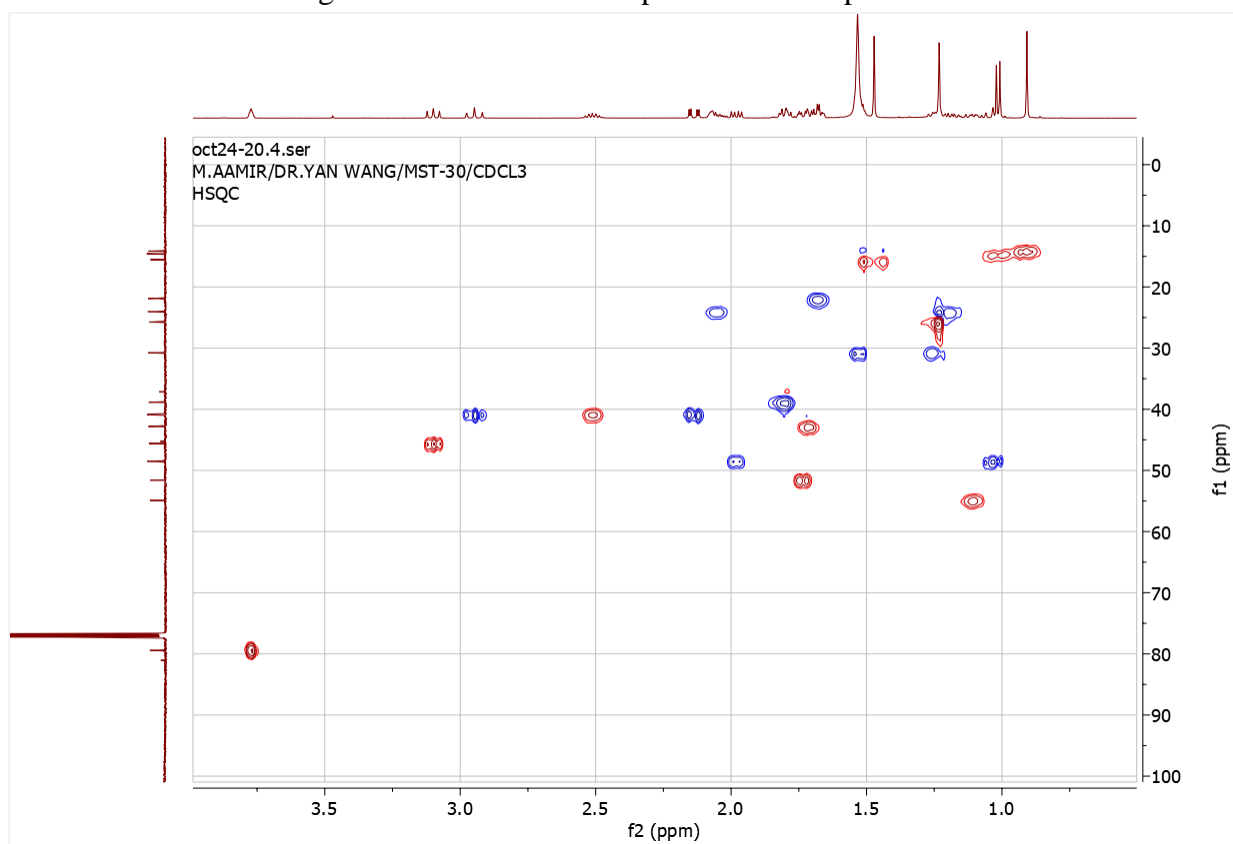


Figure S43. HSQC spectrum of compound **4**

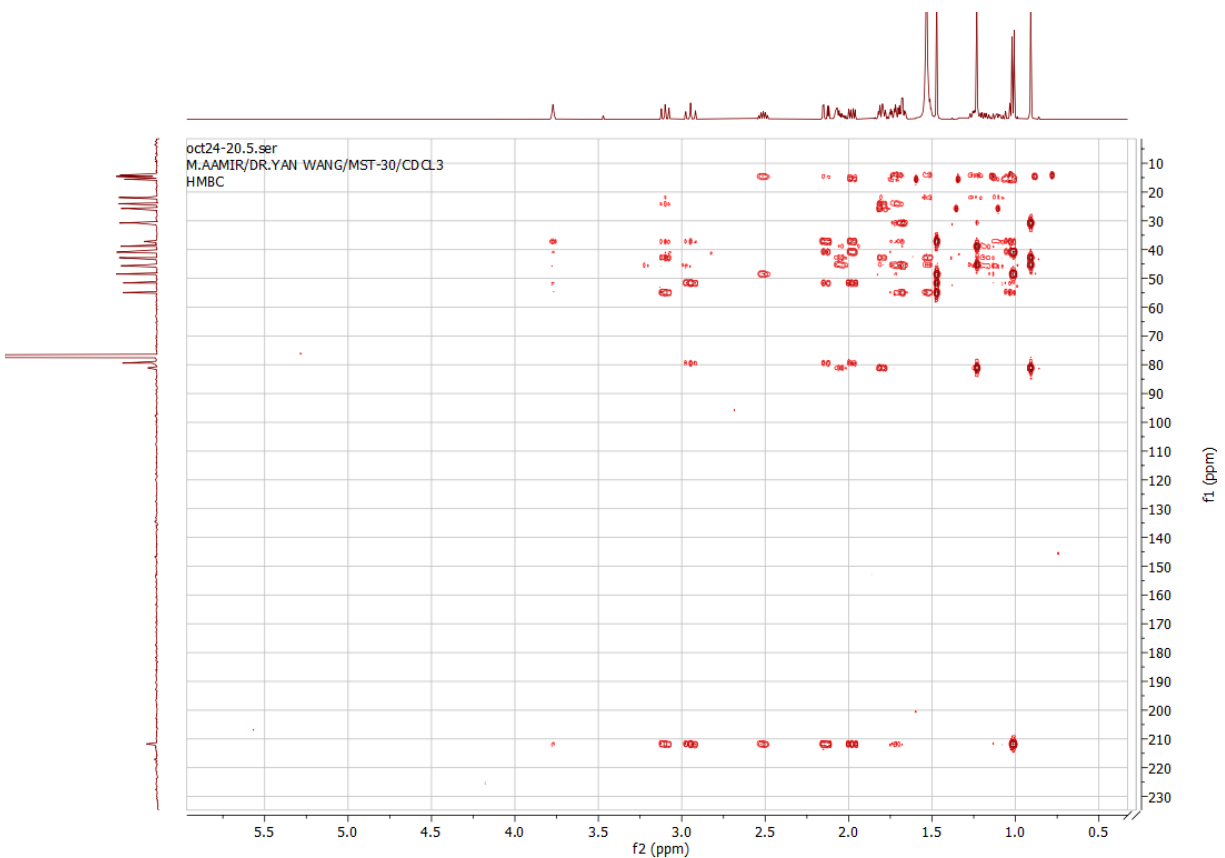


Figure S44. HMBC spectrum-1 of compound **4**

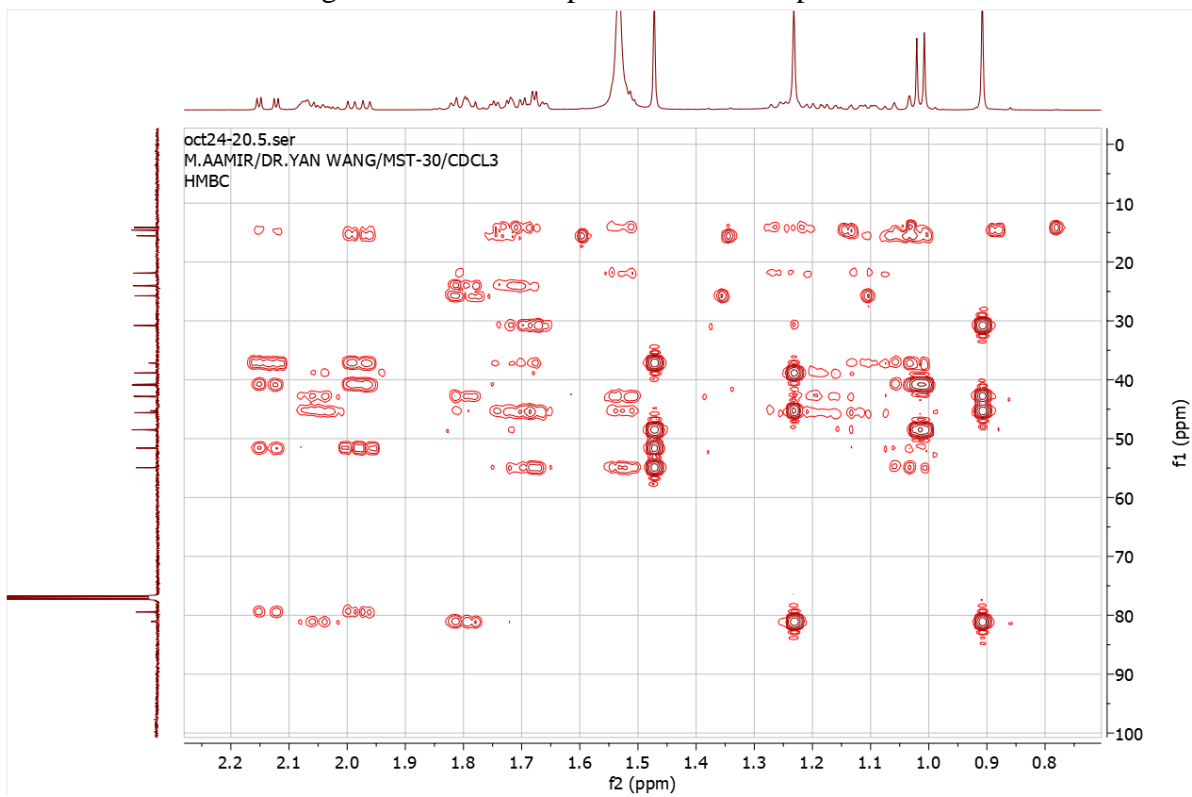


Figure S45. HMBC spectrum-2 of compound **4**

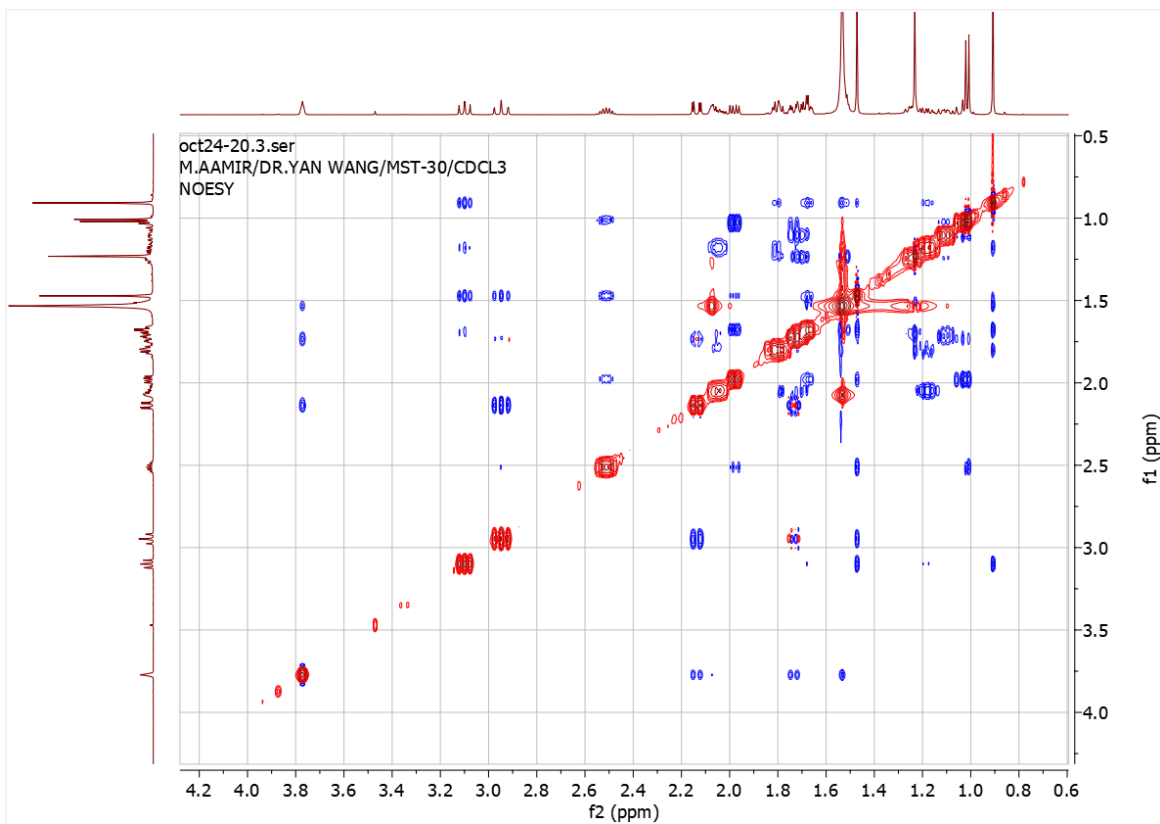


Figure S46. NOESY spectrum of compound 4

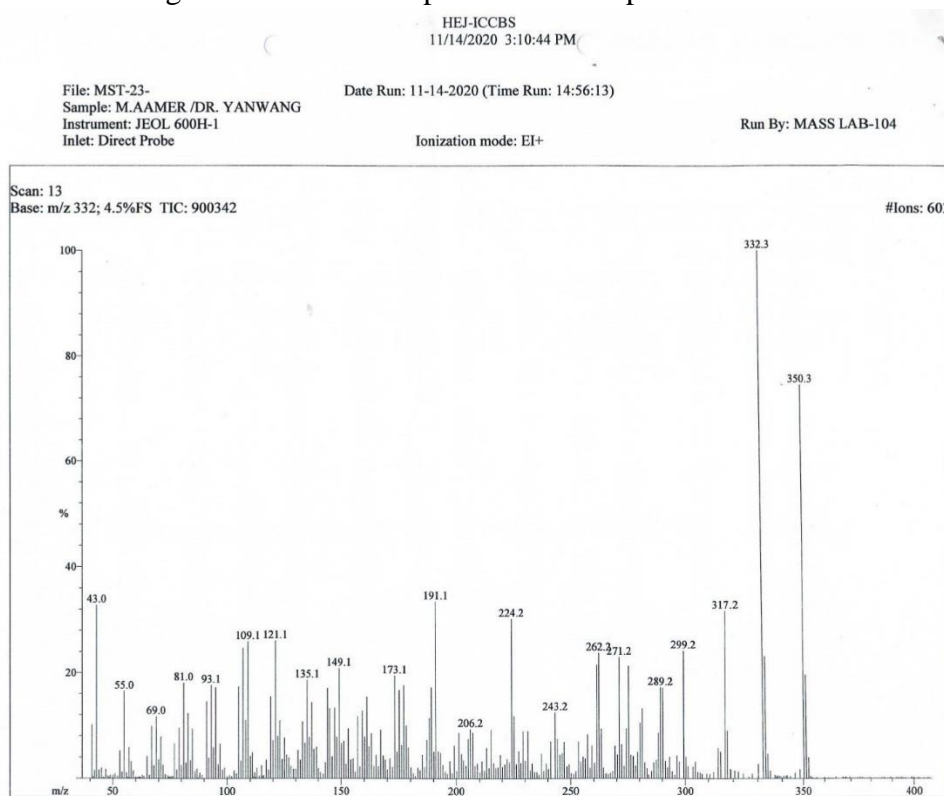


Figure S47. EI-MS spectrum of compound 5

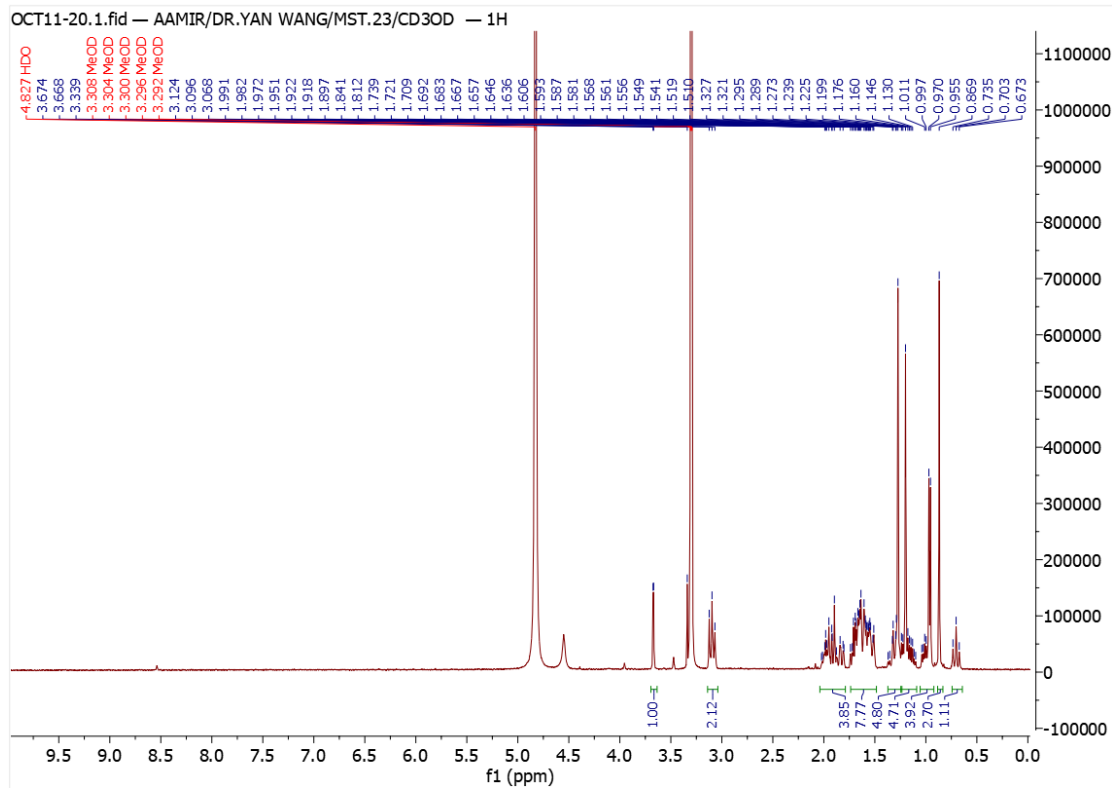


Figure S50. ^1H NMR spectrum-1 of compound **5** (400 MHz, CD_3OD)

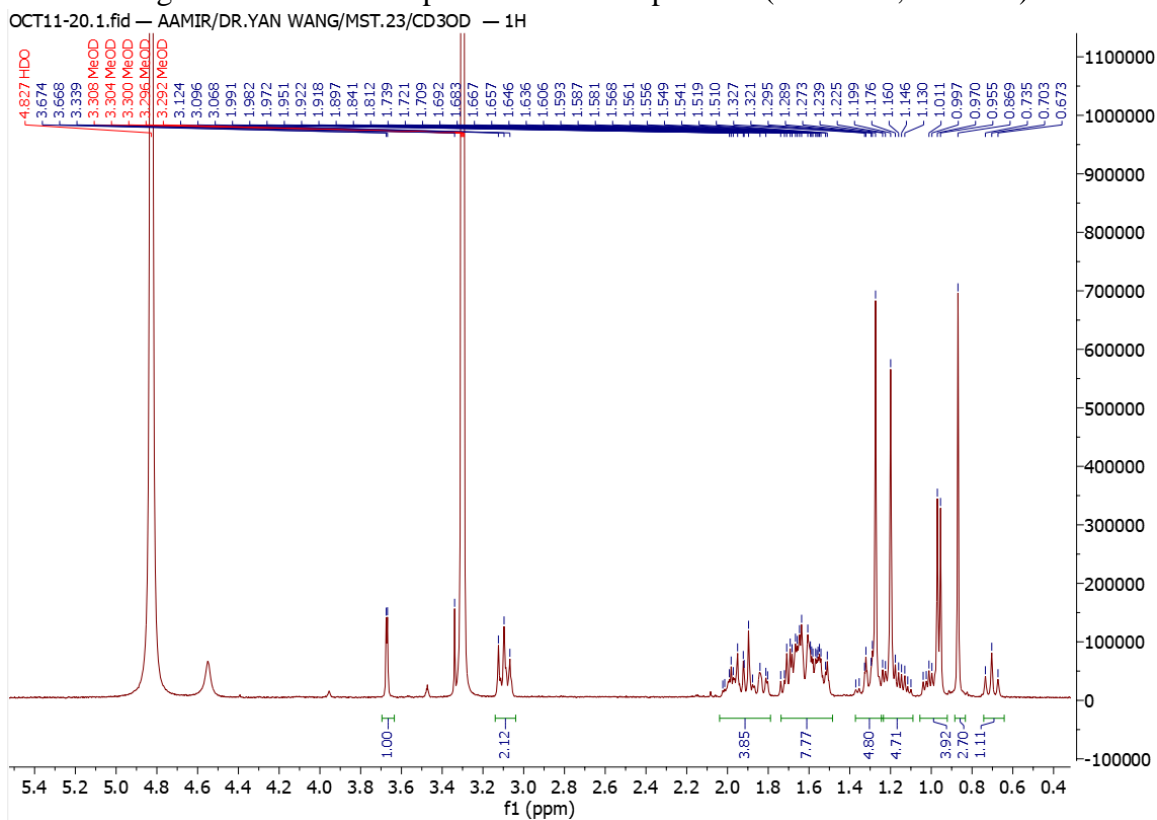
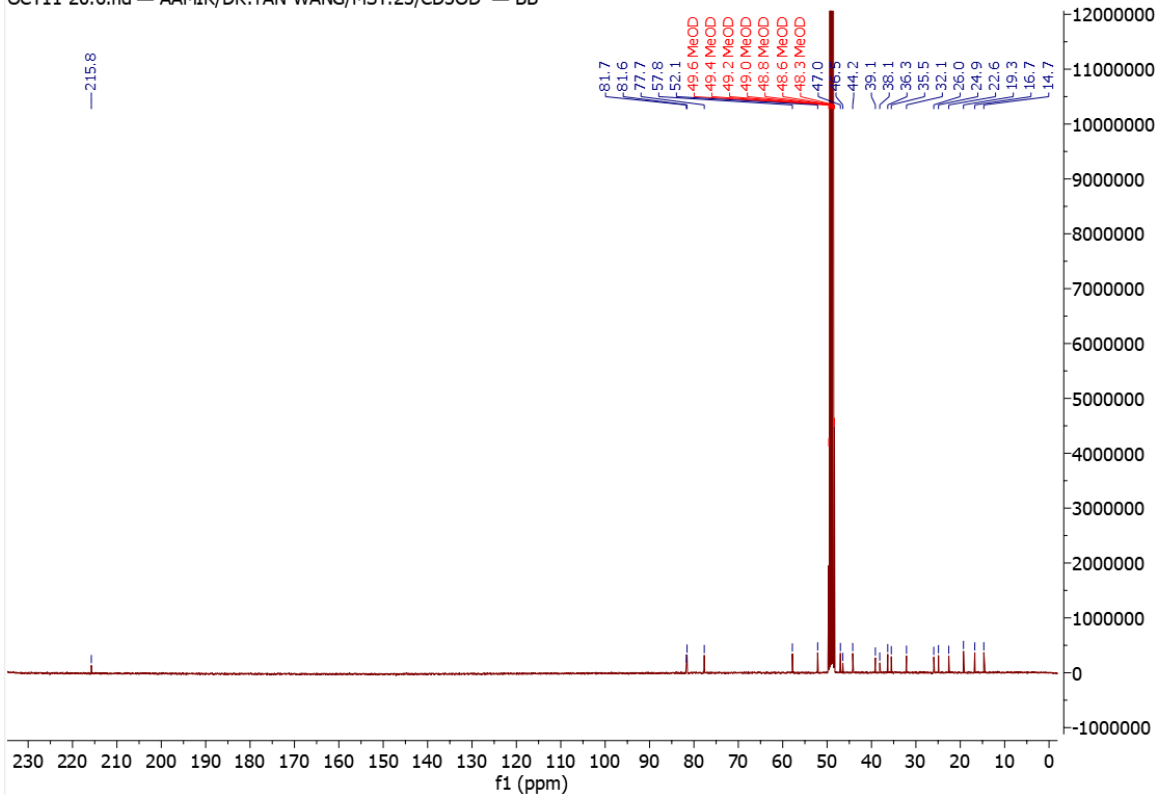
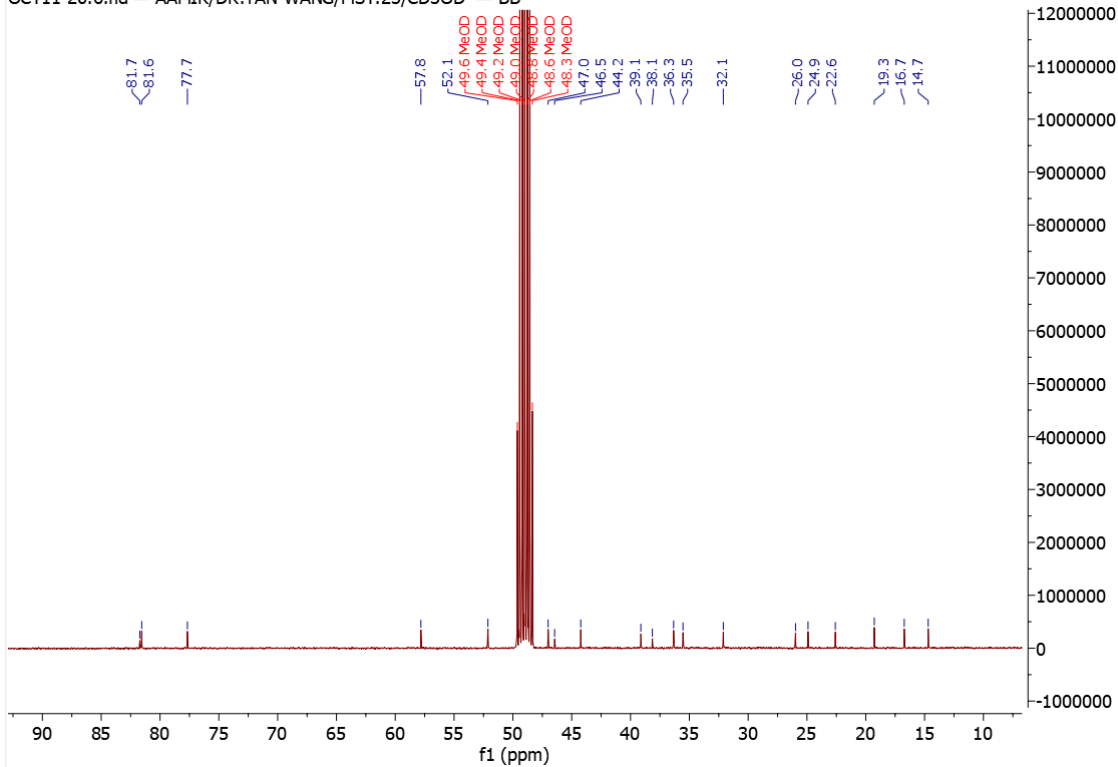


Figure S51. ^1H NMR spectrum-2 of compound **5** (400 MHz, CD_3OD)

OCT11-20.6.fid — AAMIR/DR.YAN WANG/MST.23/CD3OD — BB



OCT11-20.6.fid — AAMIR/DR.YAN WANG/MST.23/CD3OD — BB



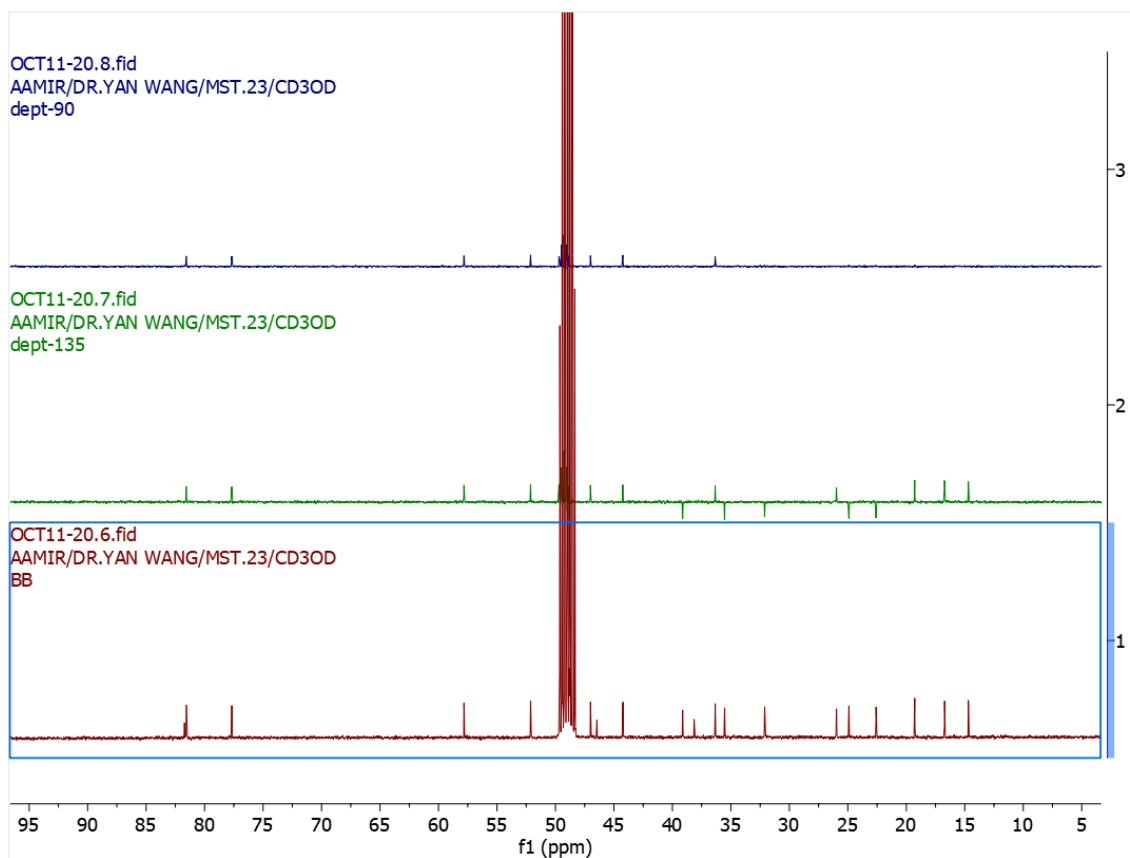


Figure S54. DEPT spectrum of compound **5**

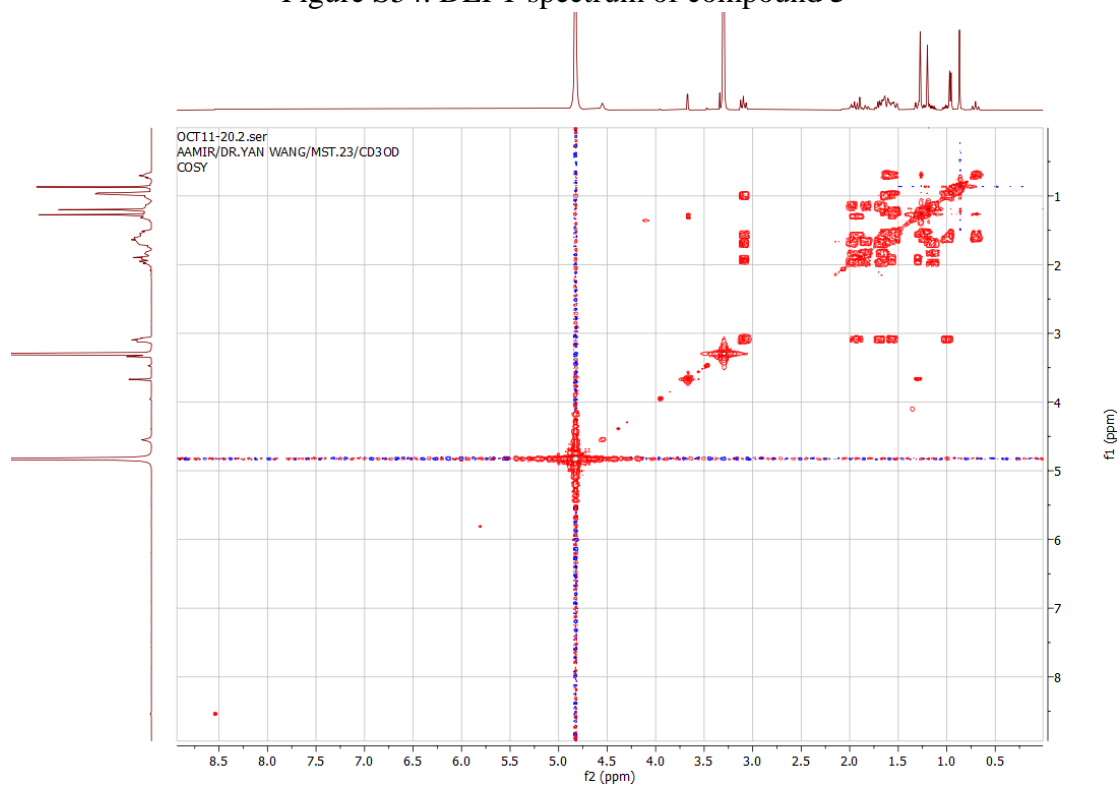


Figure S55. ^1H - ^1H COSY spectrum-1 of compound **5**

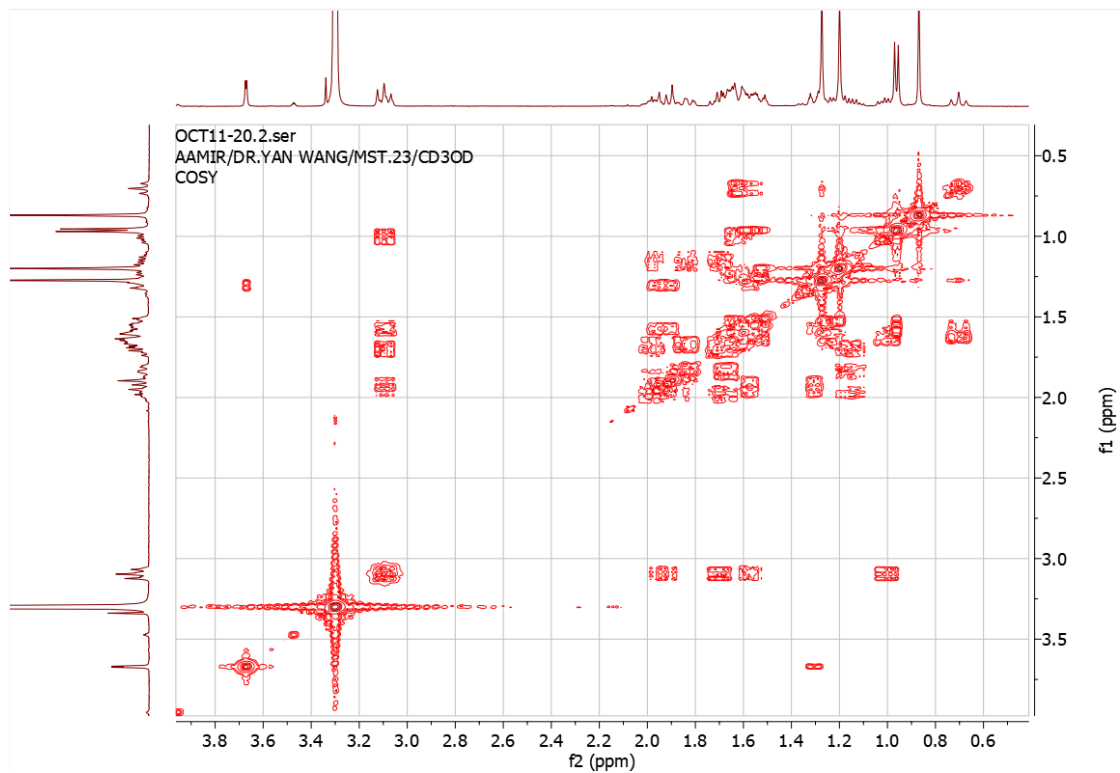


Figure S56. ^1H - ^1H COSY spectrum-2 of compound **5**

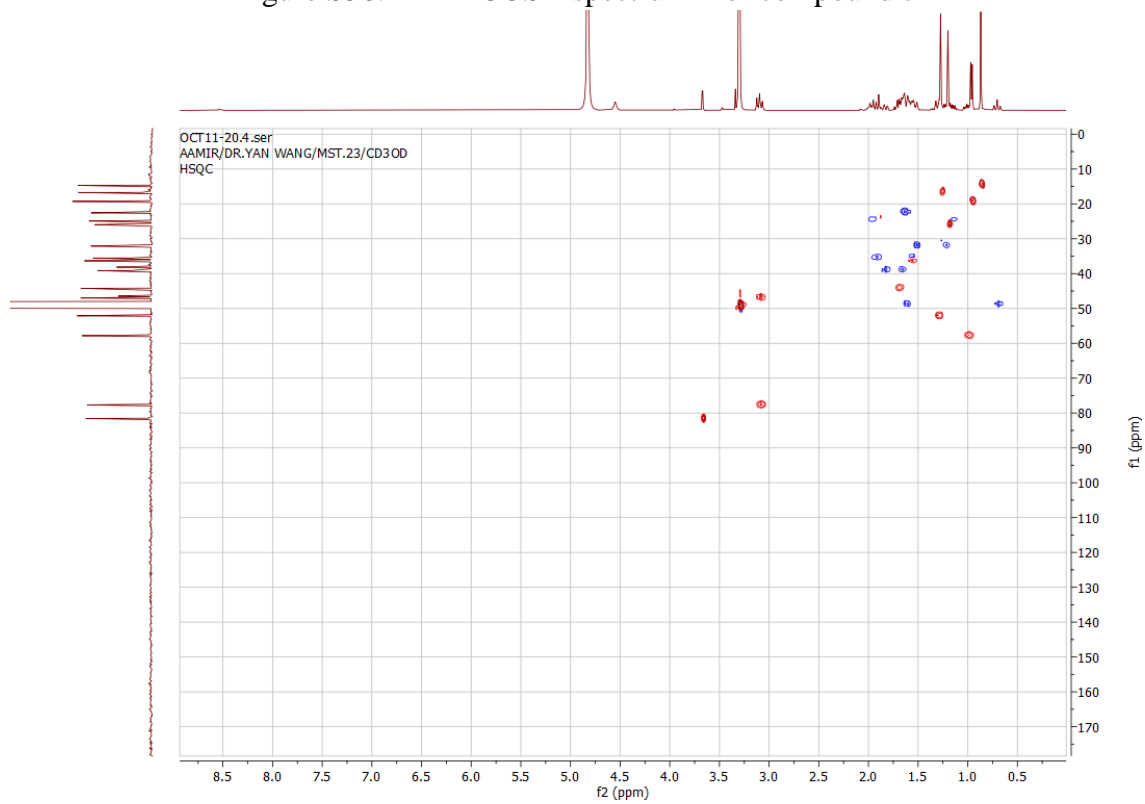


Figure S57. HSQC spectrum-1 of compound **5**

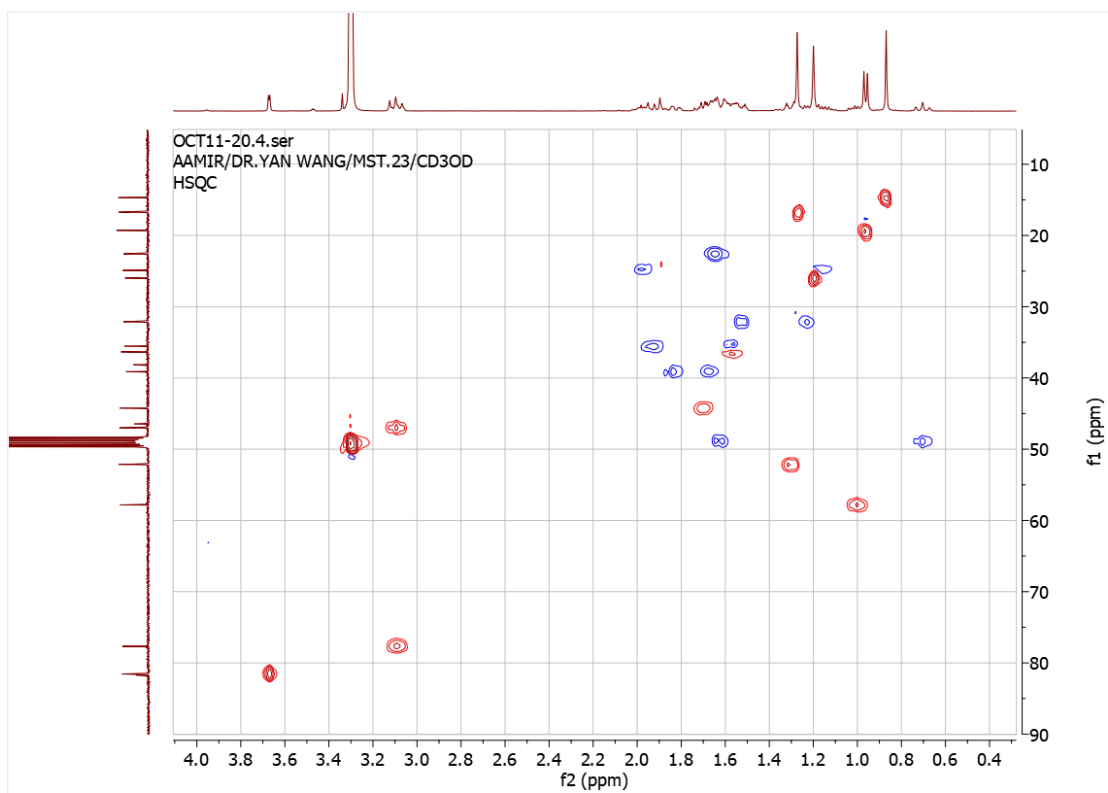


Figure S58. HSQC spectrum-2 of compound **5**

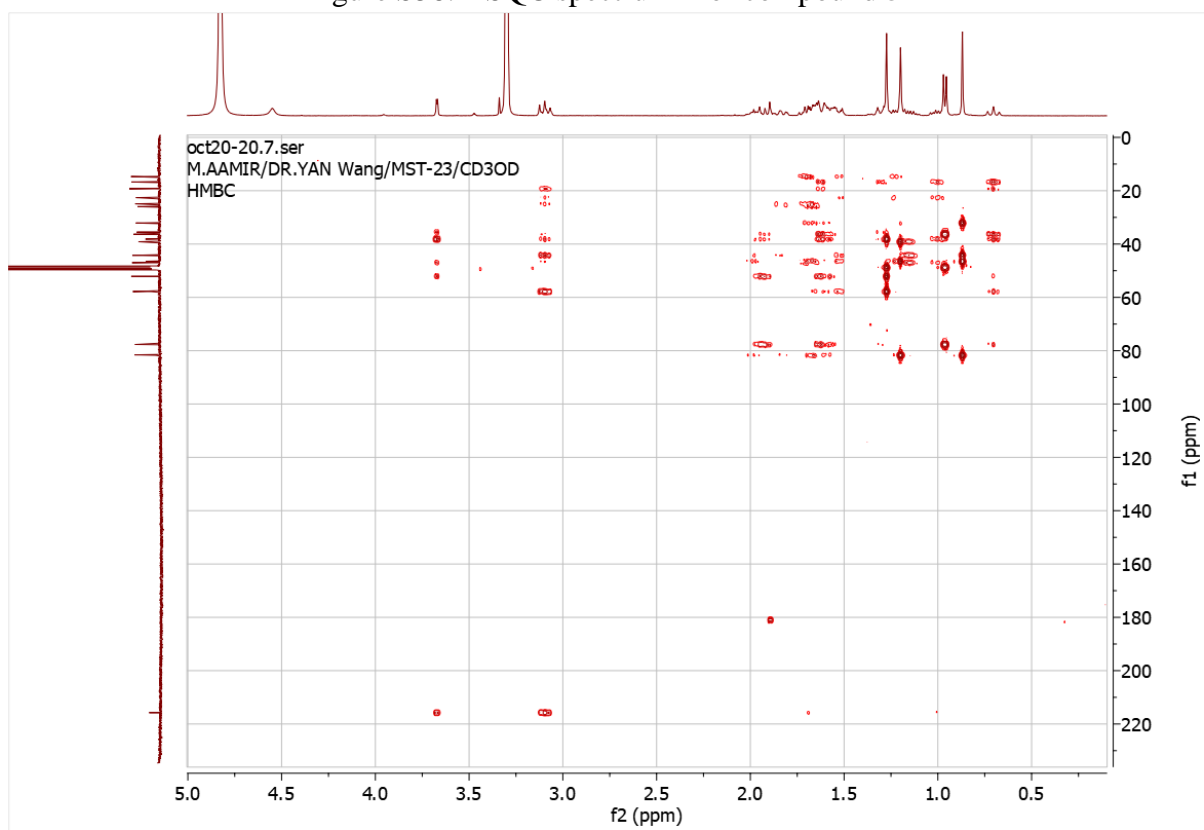


Figure S59. HMBC spectrum-1 of compound **5**

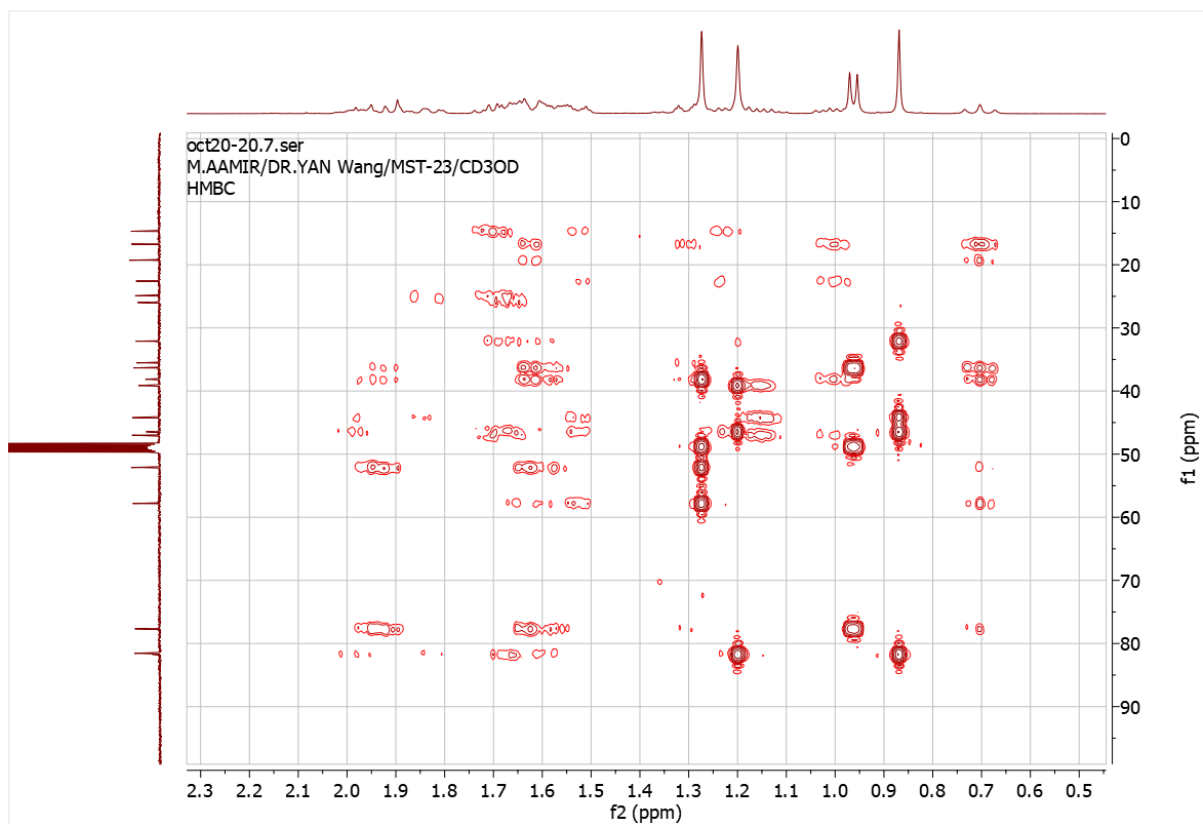


Figure S60. HMBC spectrum-2 of compound **5**

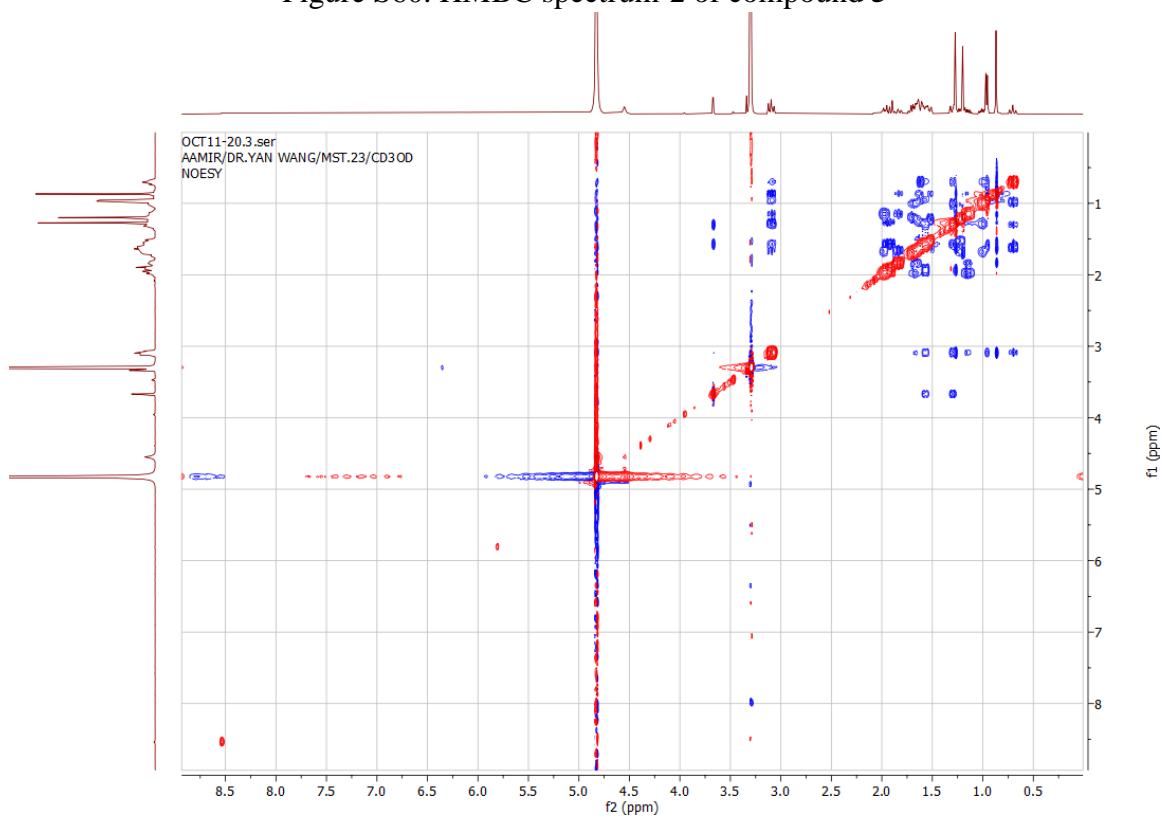


Figure S61. NOESY spectrum-1 of compound **5**

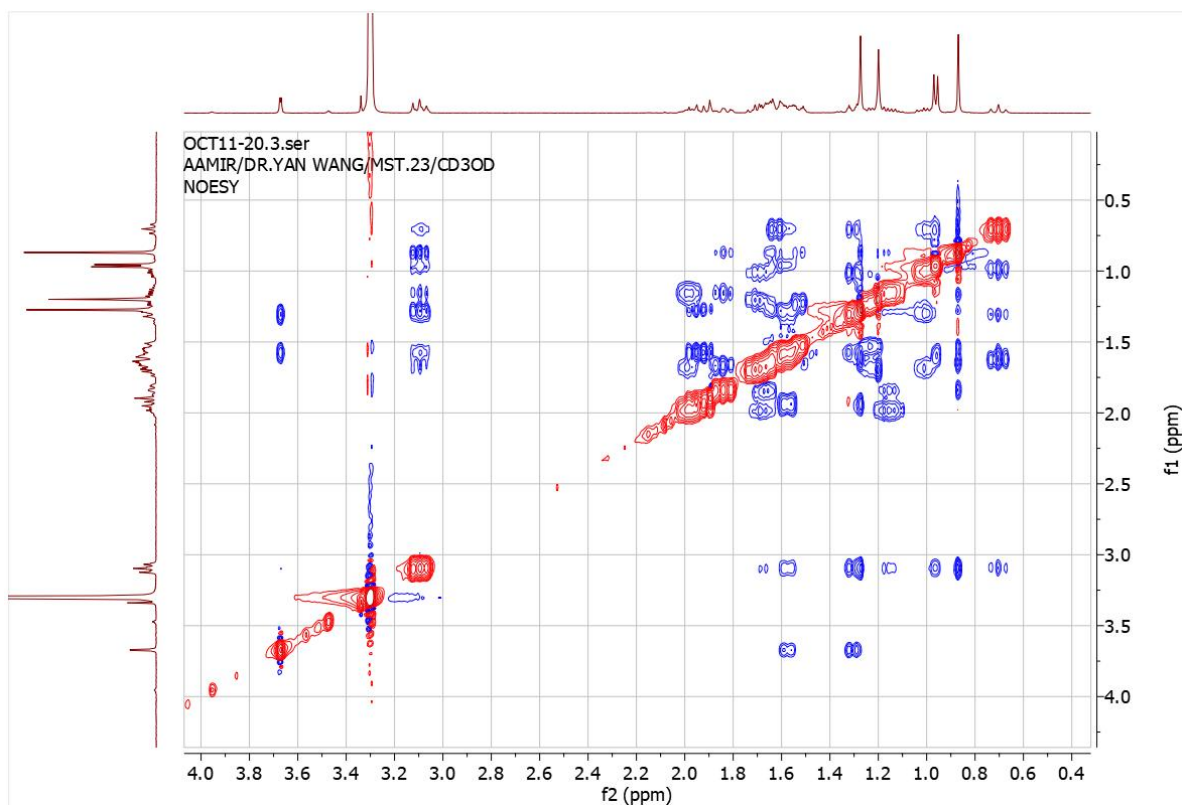


Figure S62. NOESY spectrum-2 of compound **5**

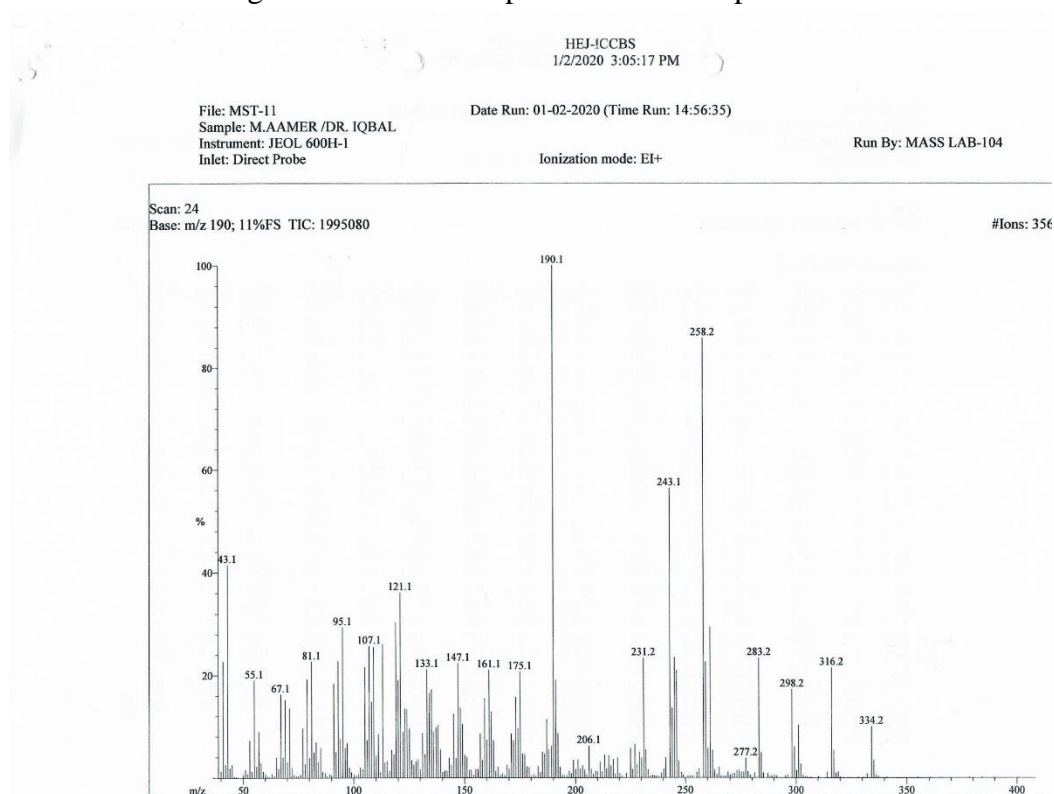


Figure S63. EI-MS spectrum of compound **6**

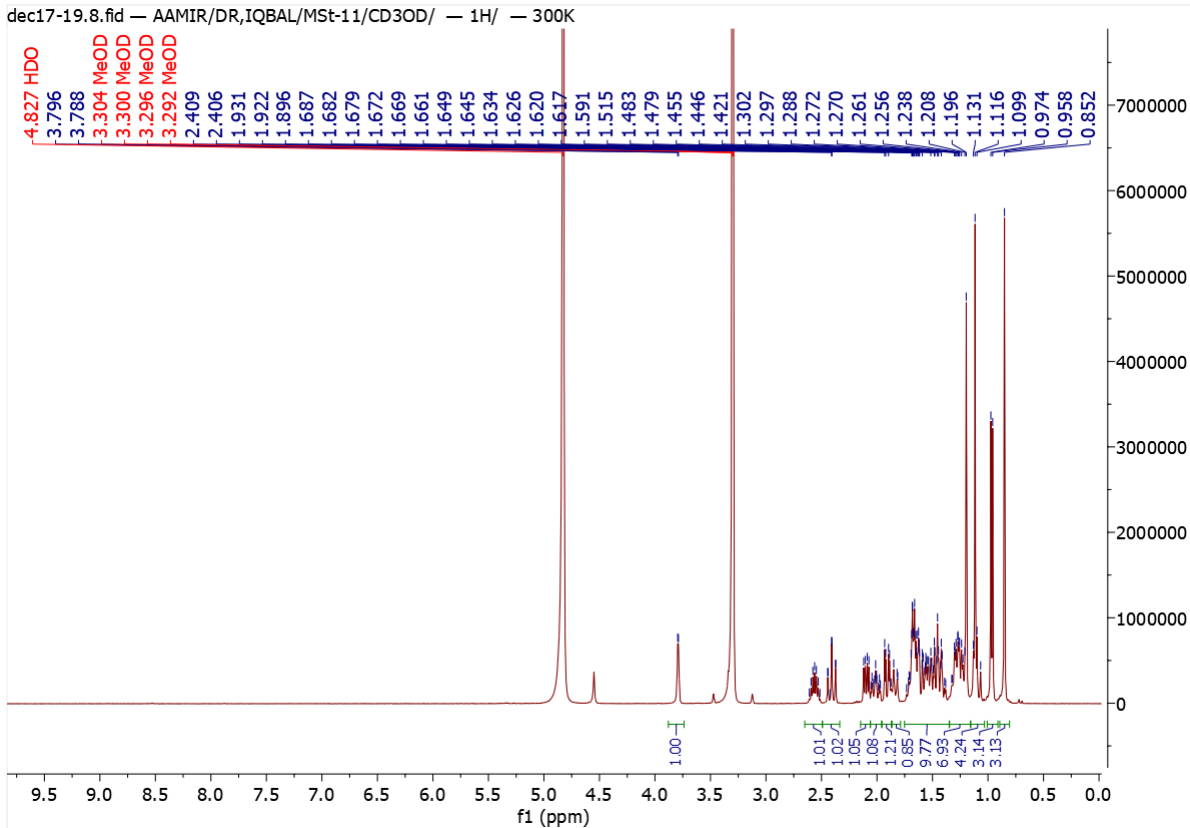


Figure S64. ¹H NMR spectrum-1 of compound **6** (400 MHz, CD₃OD)

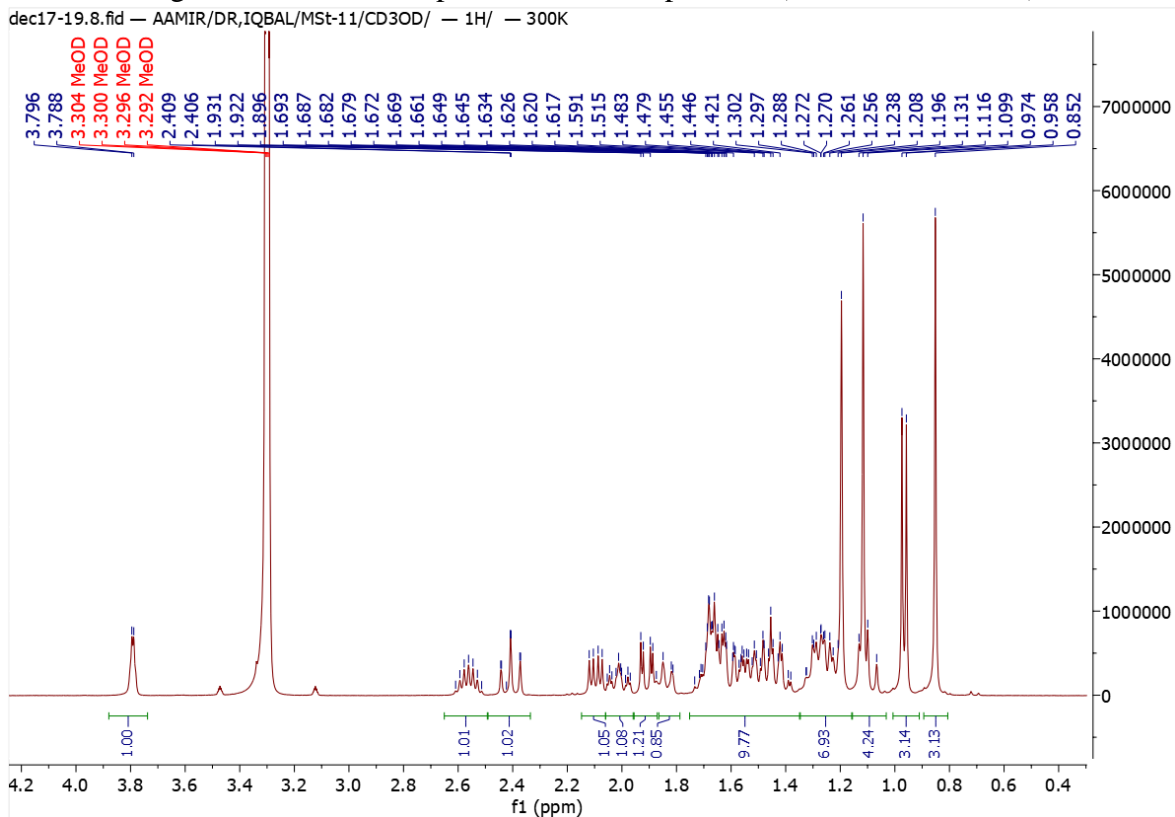


Figure S65. ¹H NMR spectrum-2 of compound **6** (400 MHz, CD₃OD)

MST-11 (C13, AND 2D).14.fid — AAMIR/DR.WANG YAN/MST-11/CD3OD — B.B

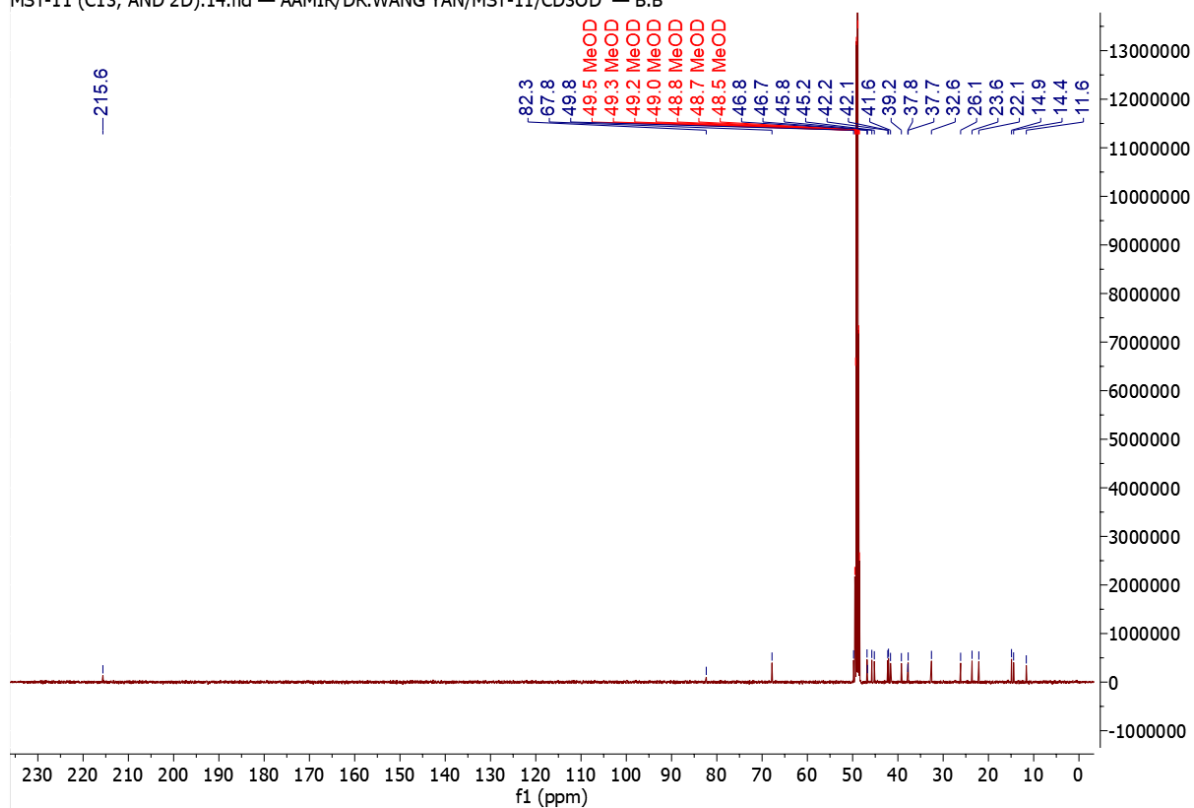


Figure S66. ^{13}C NMR spectrum-1 of compound **6** (125 MHz, CD_3OD)

MST-11 (C13, AND 2D).14.fid — AAMIR/DR.WANG YAN/MST-11/CD3OD — B.B

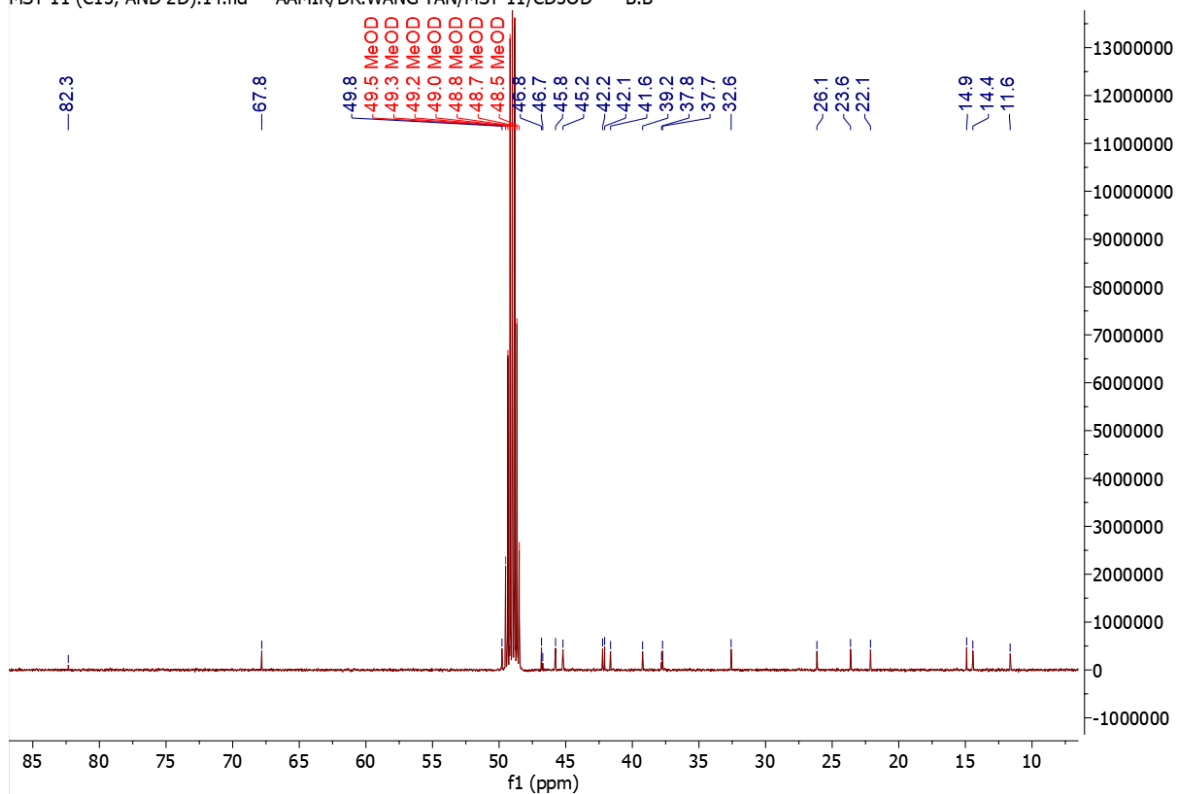


Figure S67. ^{13}C NMR spectrum-2 of compound **6** (125 MHz, CD_3OD)

HEJ-ICCBS
2/26/2019 4:09:32 PM

File: 14-ST-CB
Sample: DR. YAN WANG /DR. IQBAL
Instrument: JEOL JMS600H-1

Date Run: 02-26-2019 (Time Run: 16:00:23)

Run By: HEJ-104

Ionization mode: EI+

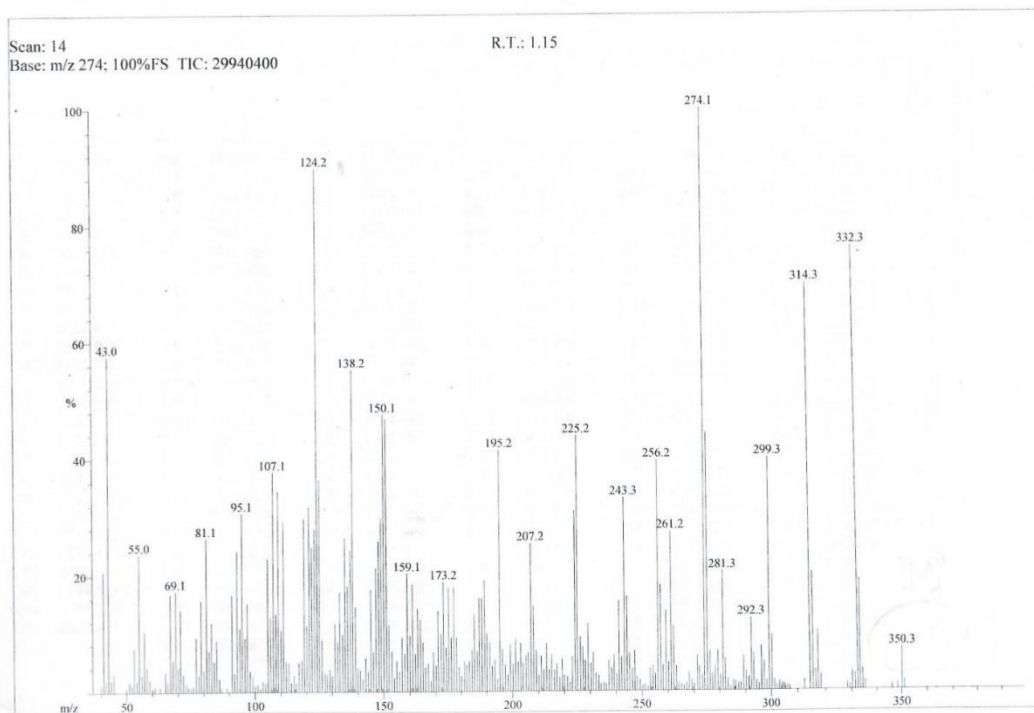
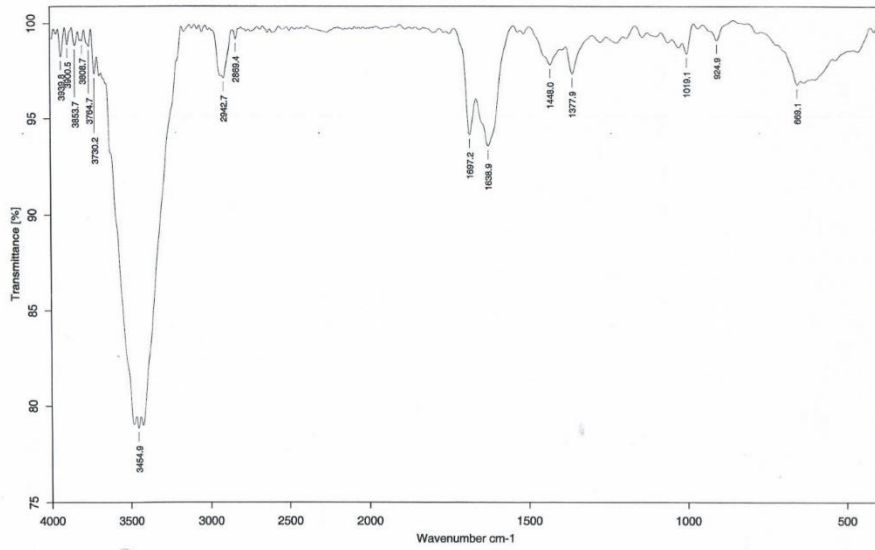


Figure S68. EI-MS spectrum of compound 7

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
		288.2089	-35.8	-10.3	6.0	C ₁₈ H ₂₈ O ₂
		288.1878	37.5	10.8	11.0	C ₂₂ H ₂₄
289.2036	2.8	289.2015	7.4	2.1	1.5	C ₁₅ H ₂₉ O ₅
		289.1956	27.7	8.0	10.5	C ₂₂ H ₂₅
290.1837	2.5	290.1882	-15.5	-4.5	6.0	C ₁₈ H ₂₆ O ₃
		290.1729	37.1	10.8	2.0	C ₁₄ H ₂₆ O ₆
291.1950	1.0	291.1960	-3.4	-1.0	5.5	C ₁₈ H ₂₇ O ₃
292.1998	5.5	292.2038	-13.8	-4.0	5.0	C ₁₈ H ₂₈ O ₃
		292.1886	38.5	11.2	1.0	C ₁₄ H ₂₈ O ₆
293.2016	2.5	293.1964	17.7	5.2	0.5	C ₁₄ H ₂₉ O ₆
		293.2117	-34.4	-10.1	4.5	C ₁₈ H ₂₉ O ₃
		293.1905	37.7	11.1	9.5	C ₂₁ H ₂₅ O ₁
294.1993	3.6	294.1984	3.3	1.0	9.0	C ₂₁ H ₂₆ O ₁
		294.2042	-16.6	-4.9	0.0	C ₁₄ H ₂₆ O ₆
295.1953	2.4	295.1909	14.9	4.4	4.5	C ₁₇ H ₂₇ O ₄
		295.2062	-36.8	-10.9	8.5	C ₂₁ H ₂₇ O ₁
296.2178	44.8	296.2140	12.9	3.8	8.0	C ₂₁ H ₂₈ O ₁
297.2143	15.1	297.2218	-25.3	-7.5	7.5	C ₂₁ H ₂₉ O ₁
		297.2066	26.0	7.7	3.5	C ₁₇ H ₂₉ O ₄
298.2207	5.9	298.2144	21.2	6.3	3.0	C ₁₇ H ₃₀ O ₄
		298.2297	-30.0	-8.9	7.0	C ₂₁ H ₃₀ O ₁
299.2063	59.2	299.2011	17.4	5.2	7.5	C ₂₀ H ₂₇ O ₂
300.2086	13.1	300.2089	-1.2	-0.4	7.0	C ₂₀ H ₂₈ O ₂
301.2115	2.9	301.2168	-17.3	-5.2	6.5	C ₂₀ H ₂₈ O ₂
		301.2015	33.3	10.0	2.5	C ₂₀ H ₂₉ O ₂
302.2045	0.9	302.2035	3.5	1.1	11.0	C ₁₆ H ₂₉ O ₅
		302.2093	-15.9	-4.8	2.0	C ₂₃ H ₂₆
303.2086	1.1	303.2113	-8.9	-2.7	10.5	C ₁₆ H ₃₀ O ₅
		303.2171	-28.3	-8.6	1.5	C ₂₃ H ₂₇
310.1874	1.5	310.1933	-18.9	-5.9	9.0	C ₁₆ H ₃₁ O ₅
		310.1780	30.3	9.4	5.0	C ₂₁ H ₂₆ O ₂
		310.1992	-37.8	-11.7	0.0	C ₁₇ H ₂₆ O ₅
311.2007	1.0	311.2011	-1.3	-0.4	8.5	C ₁₄ H ₃₀ O ₂
312.2026	5.9	312.2089	-20.4	-6.4	8.0	C ₂₁ H ₂₇ O ₂
		312.1937	28.5	8.9	4.0	C ₂₁ H ₂₈ O ₂
313.2052	2.5	313.2015	11.7	3.7	3.5	C ₁₇ H ₂₈ O ₅
		313.1956	30.5	9.5	12.5	C ₁₇ H ₂₉ O ₅
		313.2168	-37.0	-11.6	7.5	C ₂₄ H ₂₅
314.2219	75.0	314.2246	-8.4	-2.6	7.0	C ₂₁ H ₂₉ O ₃
315.2170	19.4	315.2171	-0.6	-0.2	2.5	C ₂₁ H ₃₀ O ₂
		315.2113	18.0	5.7	11.5	C ₁₇ H ₃₁ O ₅
316.2283	4.4	316.2250	10.4	3.3	2.0	C ₂₄ H ₂₇
		316.2191	29.0	9.2	11.0	C ₁₇ H ₃₂ O ₅
		316.2402	-37.8	-12.0	6.0	C ₂₄ H ₂₈
317.2079	8.1	317.2117	-12.0	-3.8	6.5	C ₂₁ H ₃₂ O ₂
		317.1964	36.1	11.5	2.5	C ₂₀ H ₂₉ O ₃
318.2078	1.6	318.2042	11.3	3.6	2.0	C ₁₆ H ₂₉ O ₆
		318.1984	29.8	9.5	11.0	C ₁₆ H ₃₀ O ₆
		318.2195	-36.6	-11.7	6.0	C ₂₃ H ₂₆ O ₁
328.2041	1.9	328.2038	0.7	0.2	8.0	C ₂₀ H ₃₀ O ₃
328.9966	0.9	328.9934	9.8	3.2	13.5	C ₂₁ H ₂₈ O ₃
		329.0027	-18.7	-6.1	26.5	C ₁₅ H ₅ O ₉
		328.9875	27.7	9.1	22.5	C ₂₆ H ₁ O ₁
		329.0086	-36.5	-12.0	17.5	C ₂₂ H ₁ O ₄
330.2260	3.4	330.2195	19.6	6.5	7.0	C ₁₉ H ₅ O ₆
		330.2348	-26.6	-8.8	11.0	C ₂₁ H ₃₀ O ₃
331.2197	1.1	331.2121	23.0	7.6	2.5	C ₂₅ H ₃₀
		331.2273	-23.1	-7.6	6.5	C ₁₇ H ₃₁ O ₆
332.2392	36.0	332.2351	12.2	4.1	6.0	C ₂₁ H ₃₁ O ₃
		332.2504	-33.7	-11.2	10.0	C ₂₁ H ₃₂ O ₃
333.2412	8.6	333.2430	-5.3	-1.8	5.5	C ₂₅ H ₃₂
334.2512	1.4	334.2508	1.3	0.4	5.0	C ₂₁ H ₃₃ O ₃
350.2434	2.1	350.2457	-6.7	-2.4	5.0	C ₂₁ H ₃₄ O ₃
						C ₂₁ H ₃₄ O ₄

Figure S69. HREI-MS spectrum of compound 7



Sample : MST-14-ST-CB/Aamer/Dr.Yan Spectrum : 14-ST-CB.0 (in D:\IRSTUDENT)
 Measured : 17/11/2020 on VECTOR22 Technic : Liquid
 Resolution : 2 cm-1 (10 scans) Analyst : ZAINAB RIZVI

Figure S70. IR spectrum of compound 7

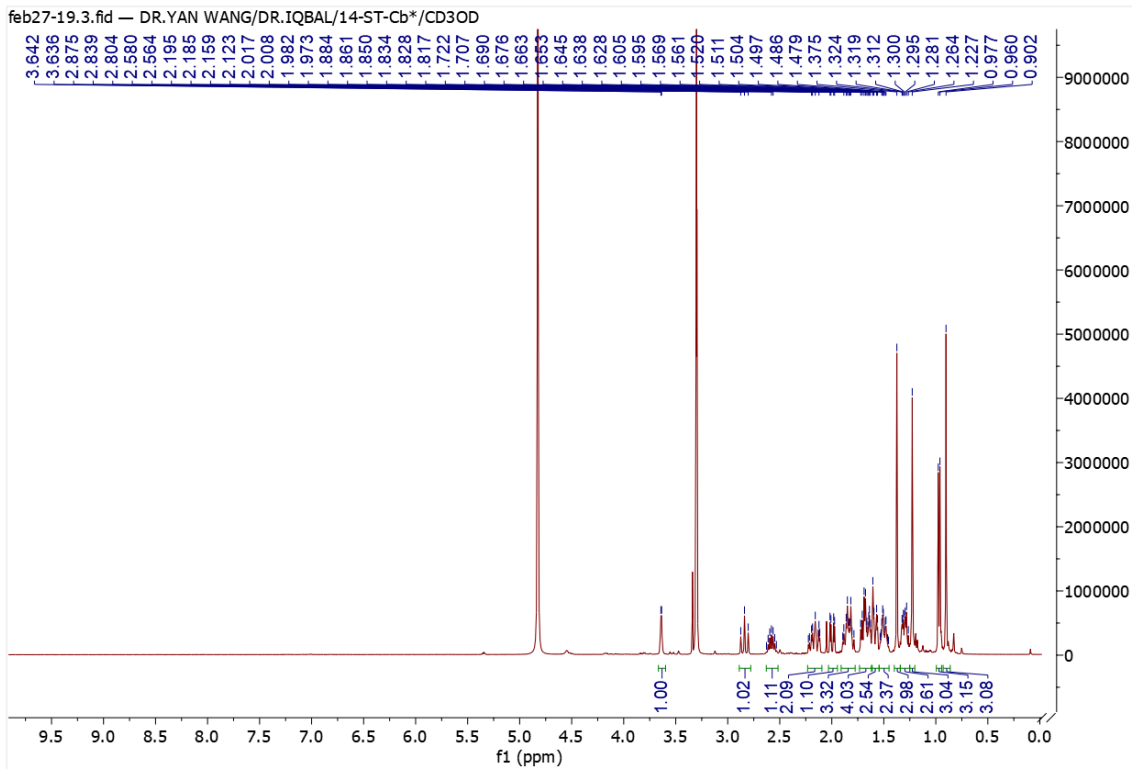
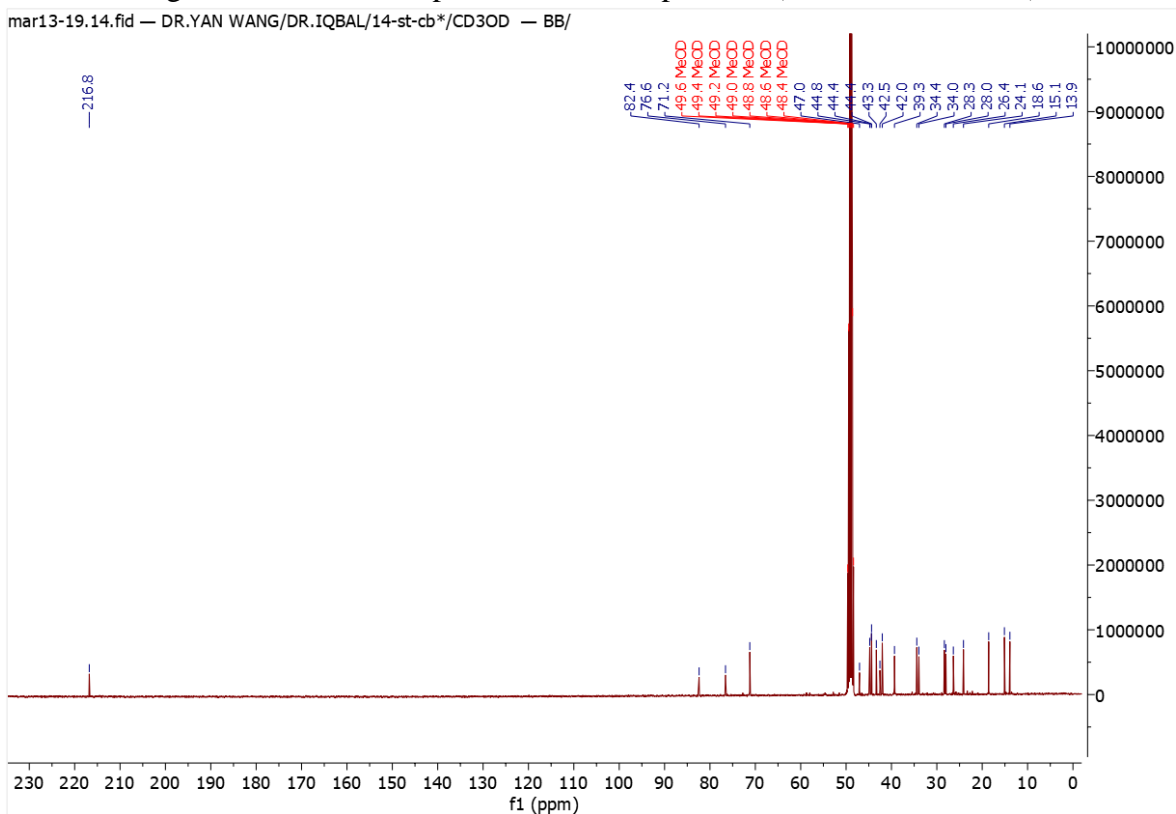
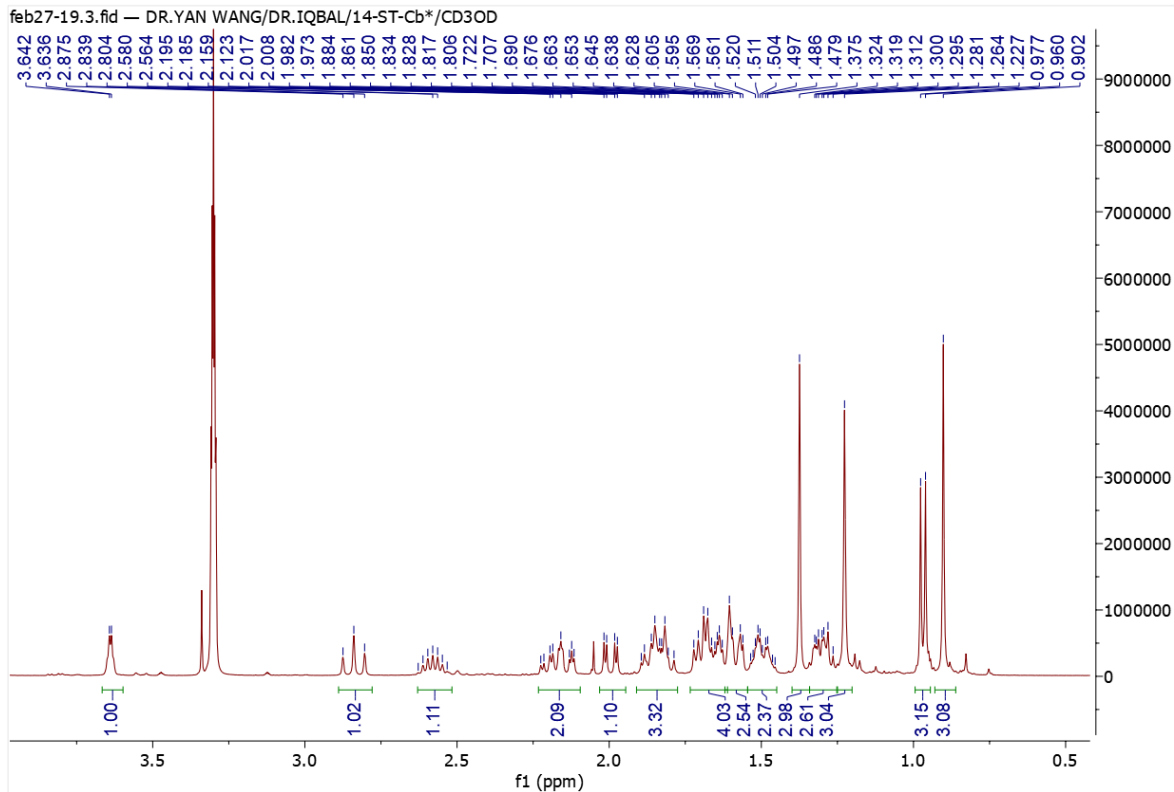


Figure S71. ¹H NMR spectrum-1 of compound 7 (400 MHz, CD₃OD)



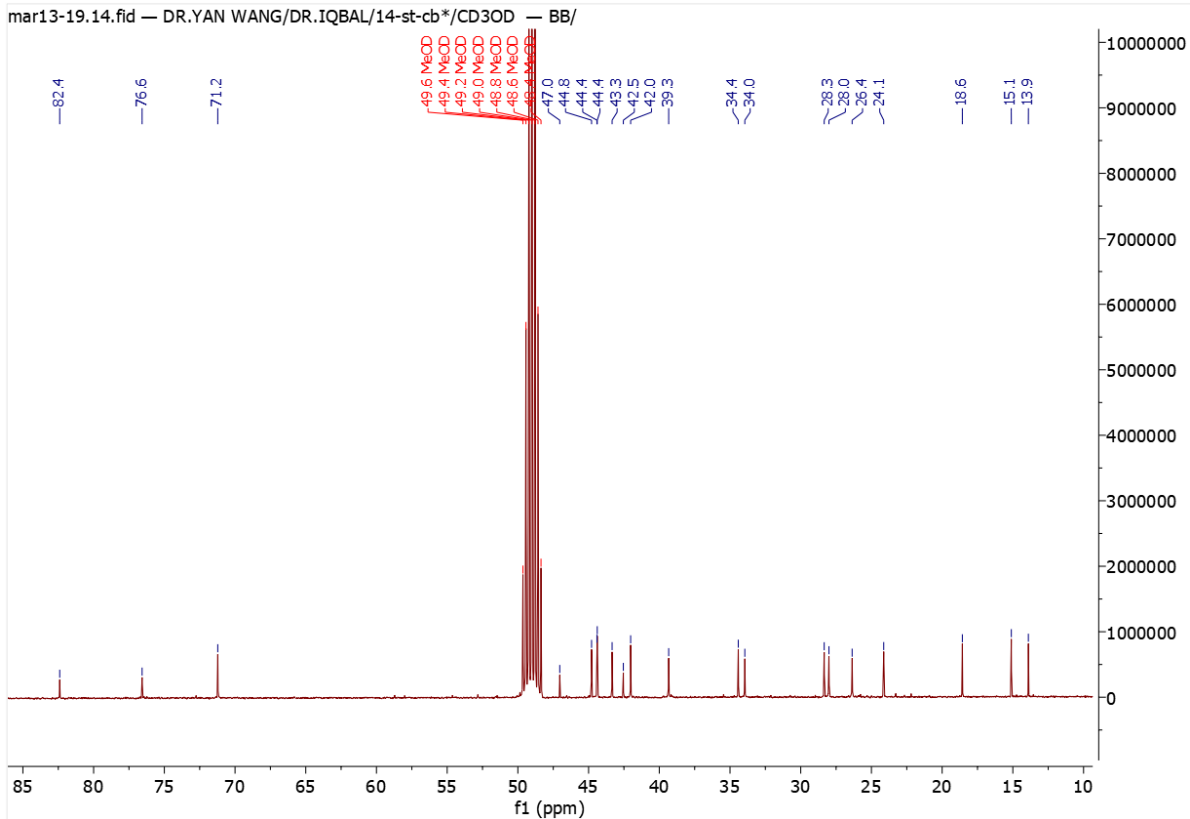


Figure S74. ^{13}C NMR spectrum-2 of compound **7** (100 MHz, CD_3OD)

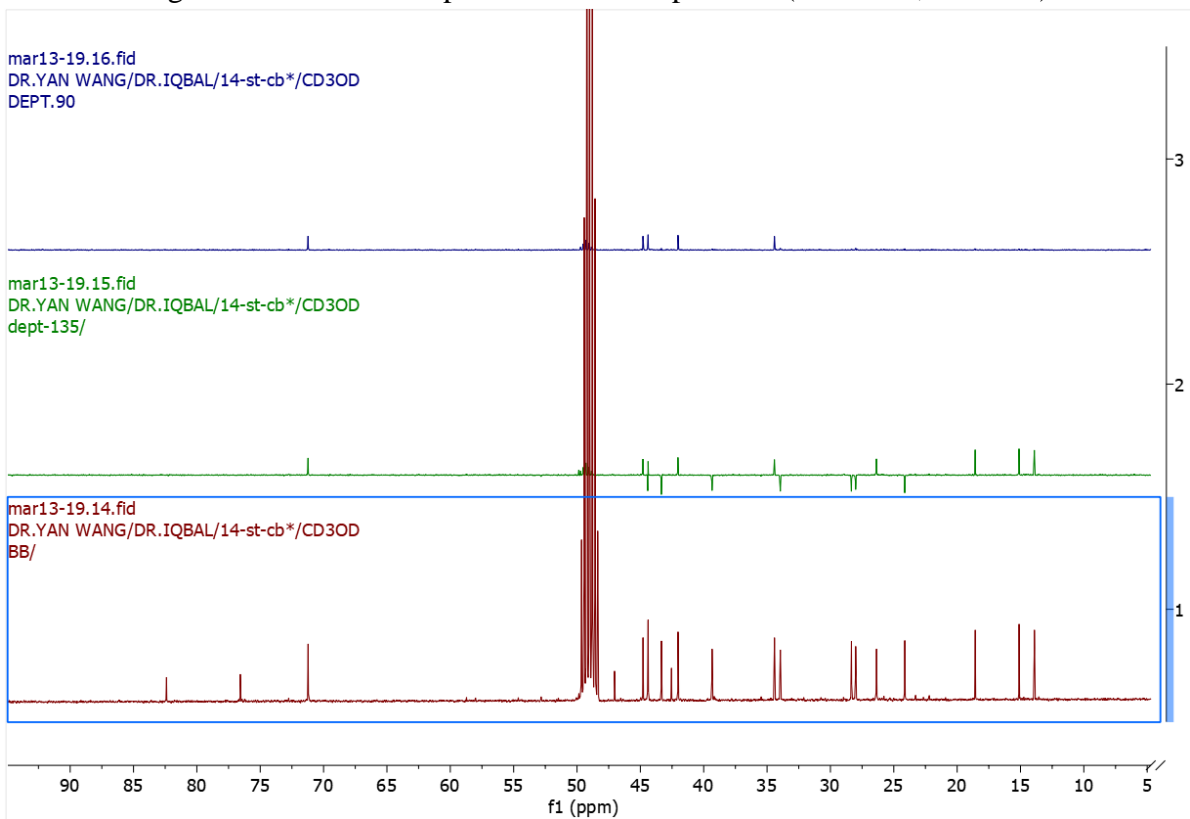


Figure S75. DEPT spectrum of compound **7**

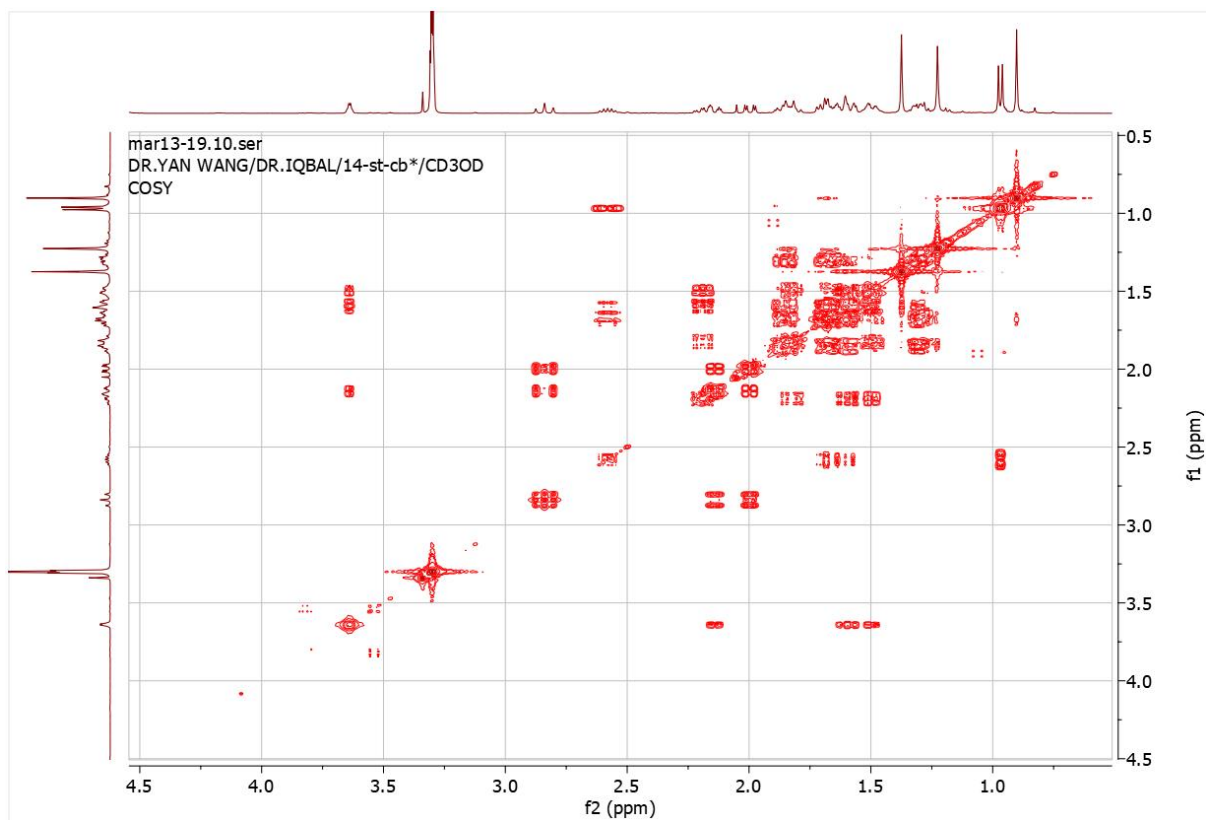


Figure S76. ^1H - ^1H COSY spectrum of compound **7**

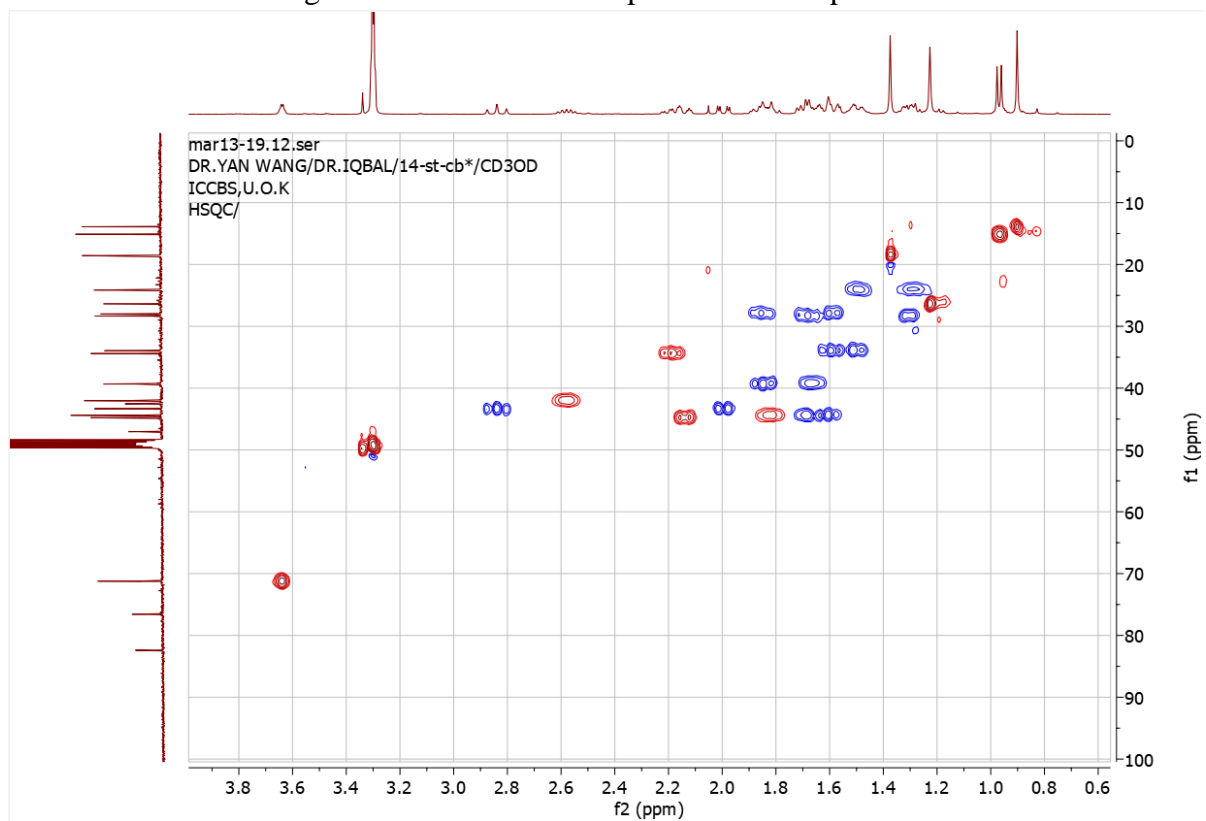


Figure S77. HSQC spectrum of compound **7**

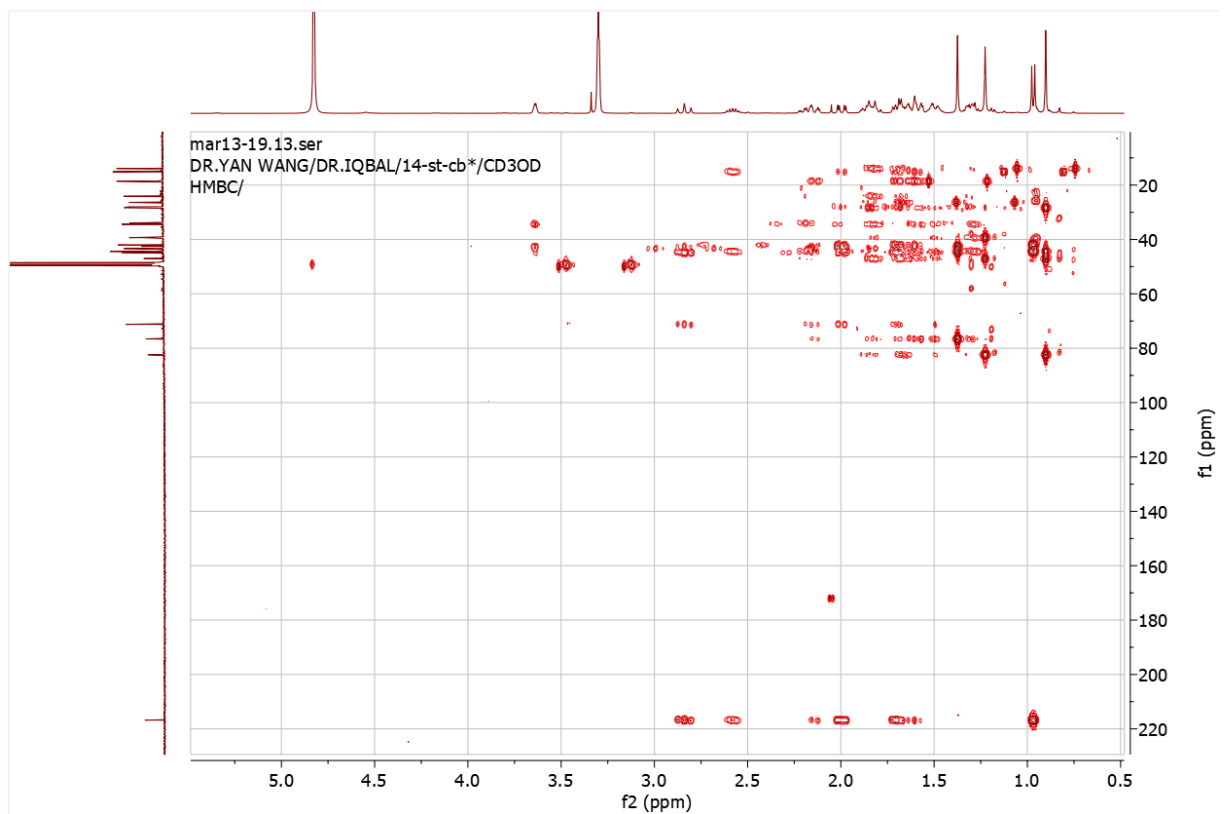


Figure S78. HMBC spectrum-1 of compound 7

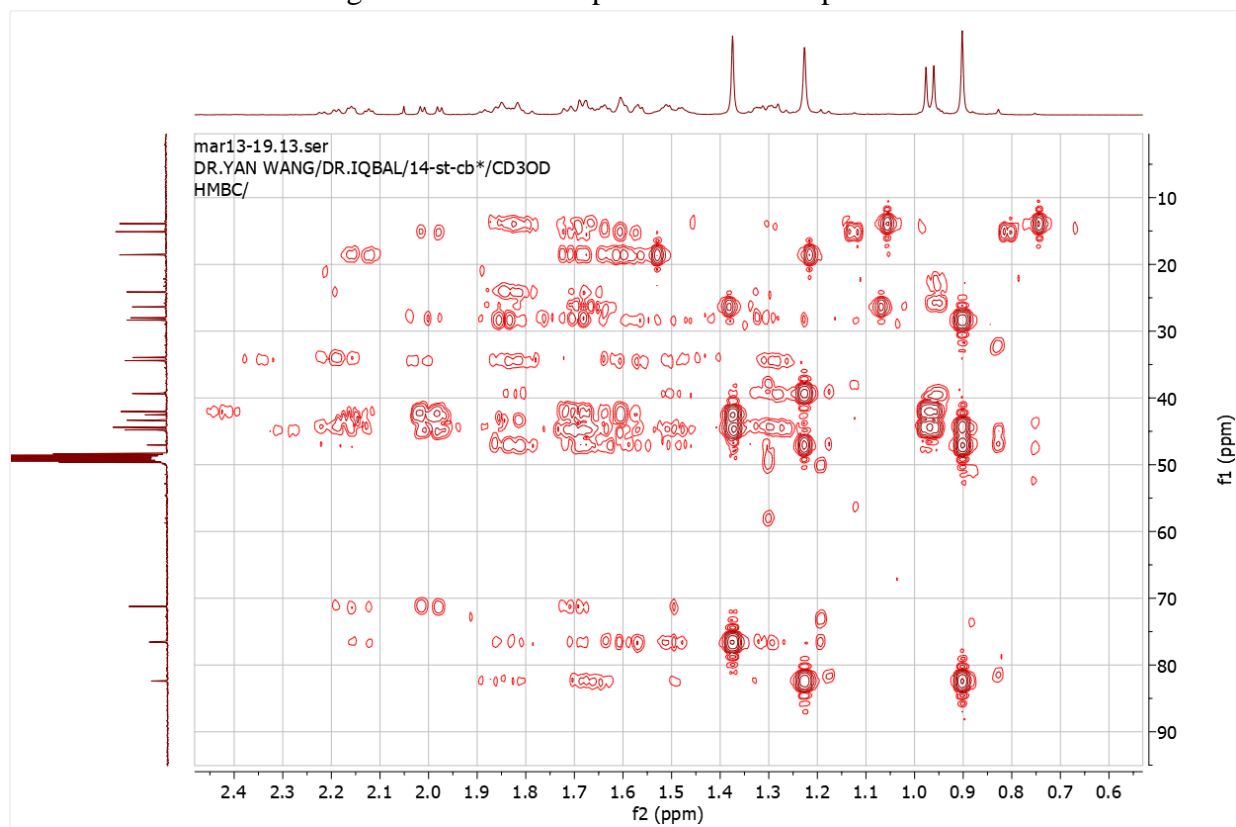


Figure S79. HMBC spectrum-2 of compound 7

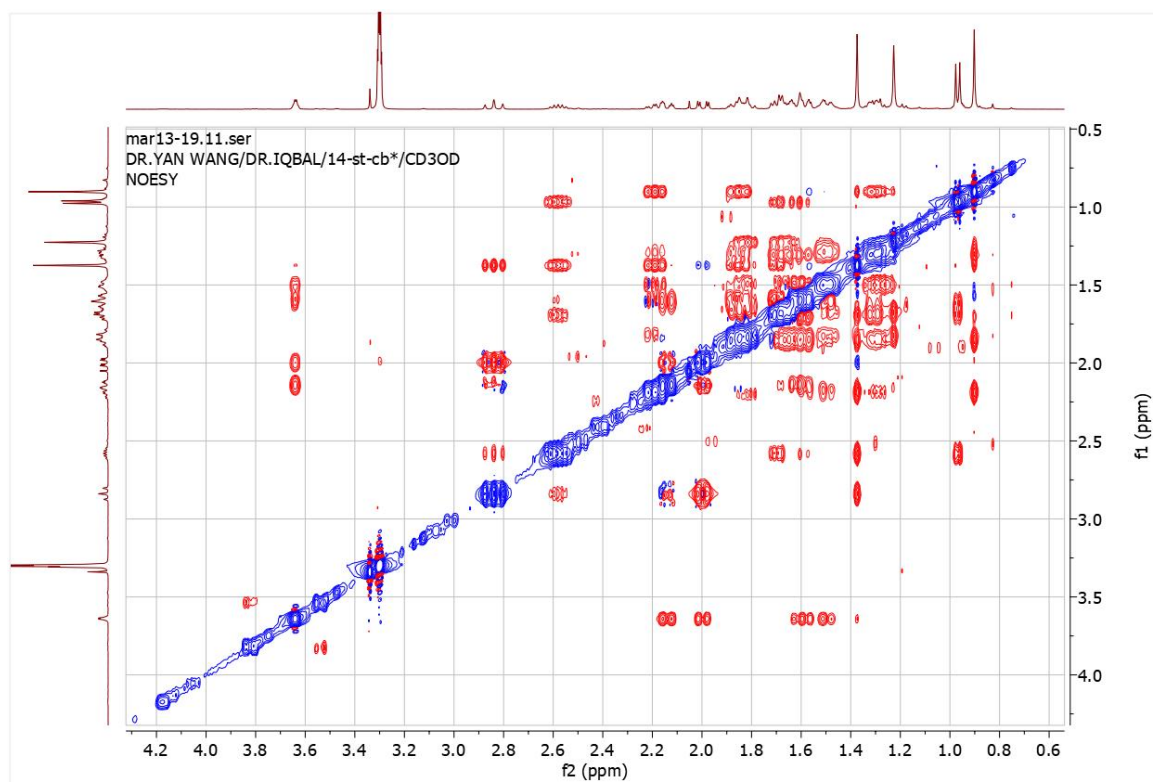


Figure S80. NOESY spectrum of compound **7**