

Supporting Information

Anti-inflammatory Diterpenoids from the Root Bark of *Acanthopanax gracilistylus*

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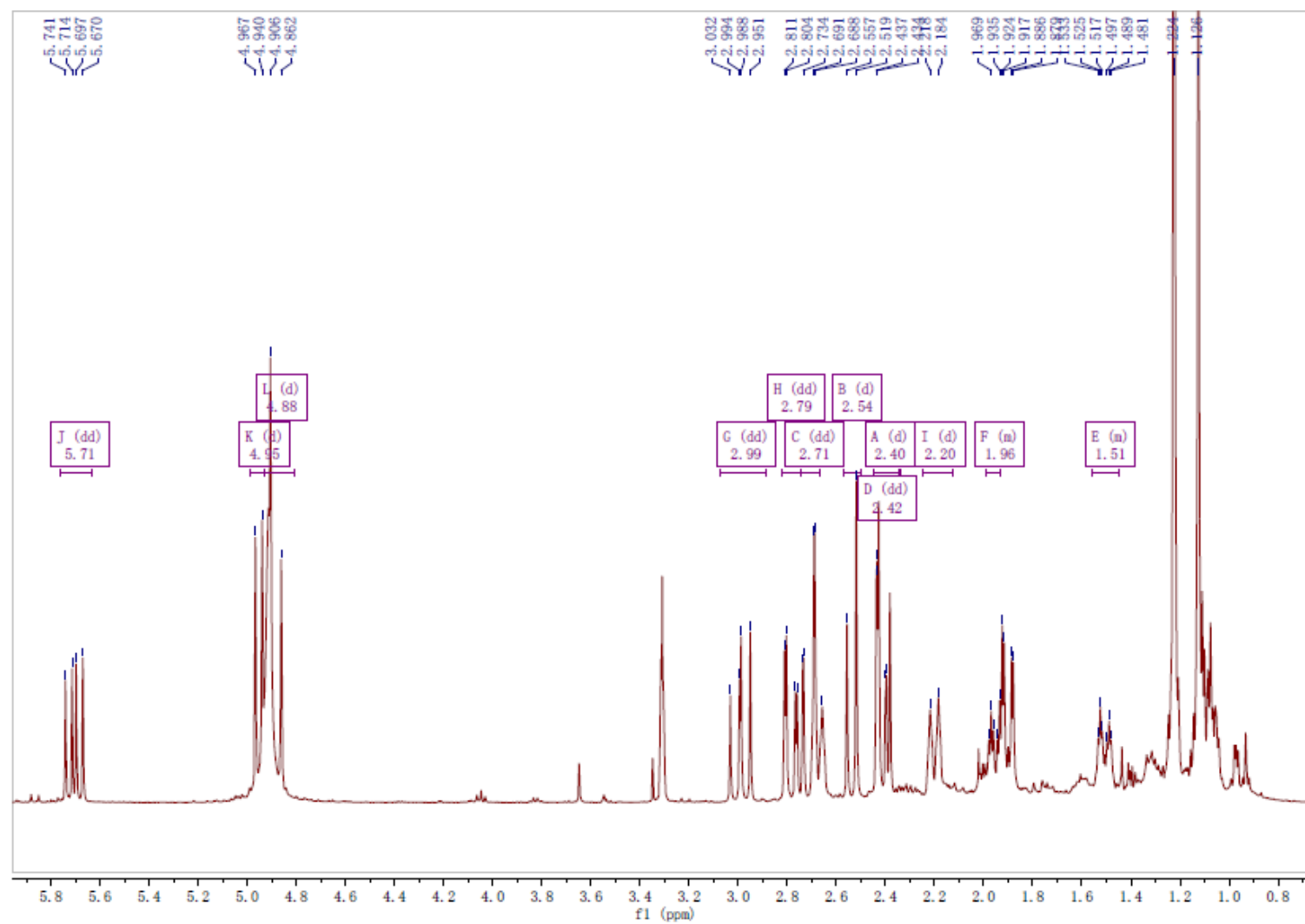
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[§]These authors contributed equally to this study.

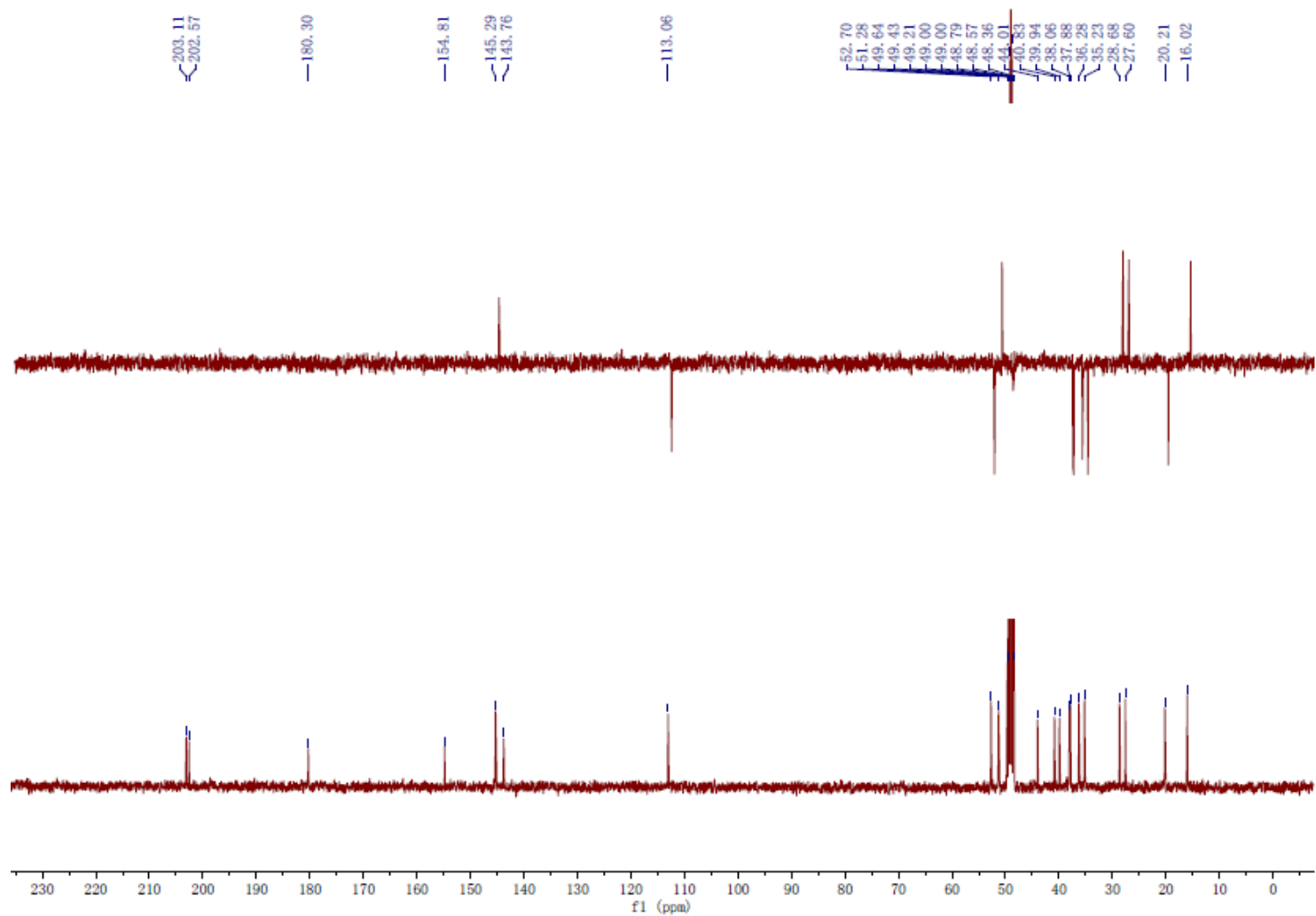
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List of Supporting Information

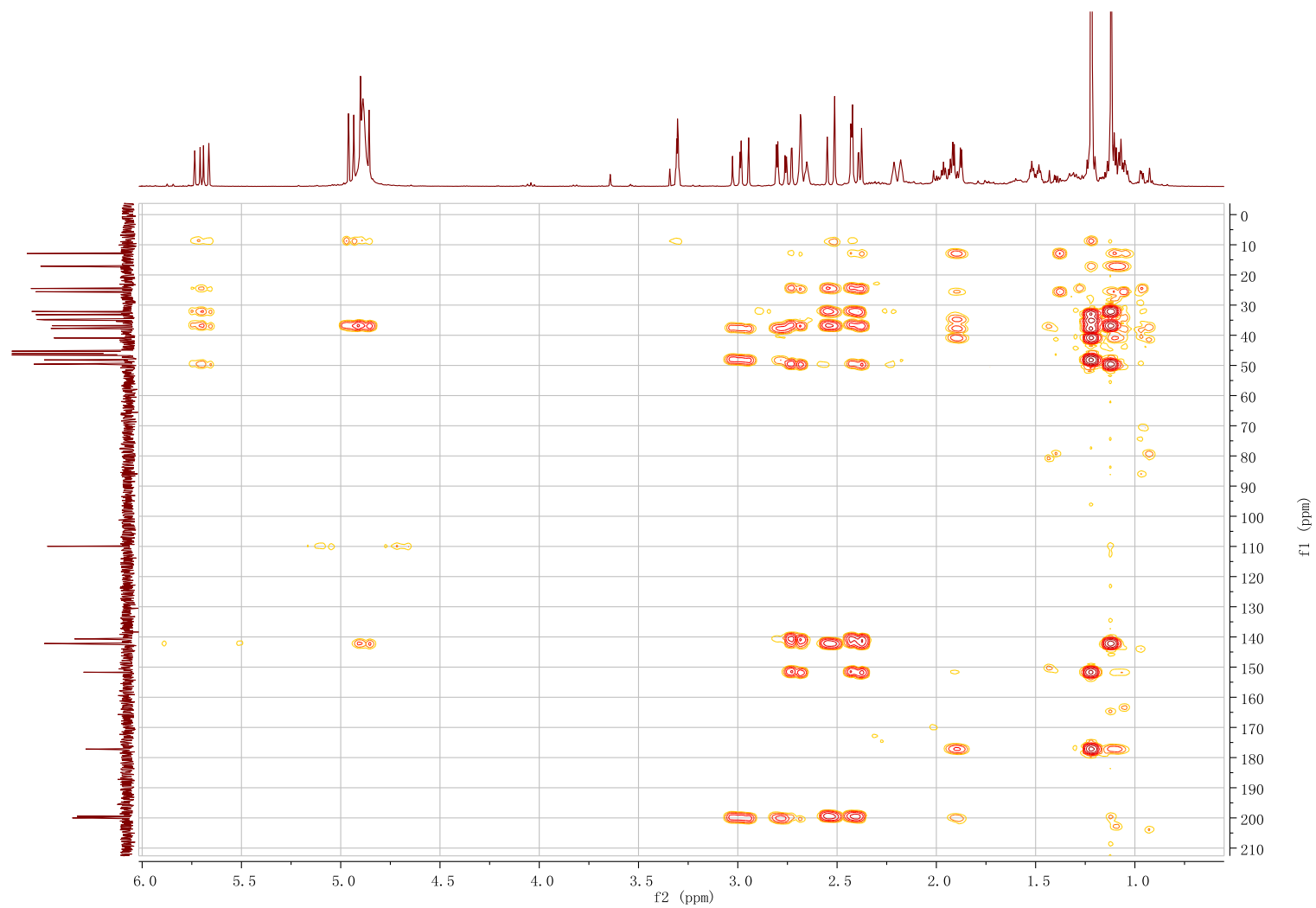
- S1-S6. ^1H NMR, ^{13}C NMR, DEPT, HMBC, HSQC, IR and HR-EI-MS spectra of the new compound **1**
- S7-S12. ^1H NMR, ^{13}C NMR, DEPT, HMBC, HSQC, ^1H - ^1H COSY, IR and HR-EI-MS spectra of the new compound **2**
- S13-18. ^1H NMR, ^{13}C NMR, DEPT, HMBC, HSQC, IR and HR-EI-MS spectra of the new compound **3**
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- S52-S53. CD spectra of compound **7** and **11** measured in methanol
- S54. Assurance document from Shanghai Blood Administration Office
- S55. Blood donor statement of healthy donator



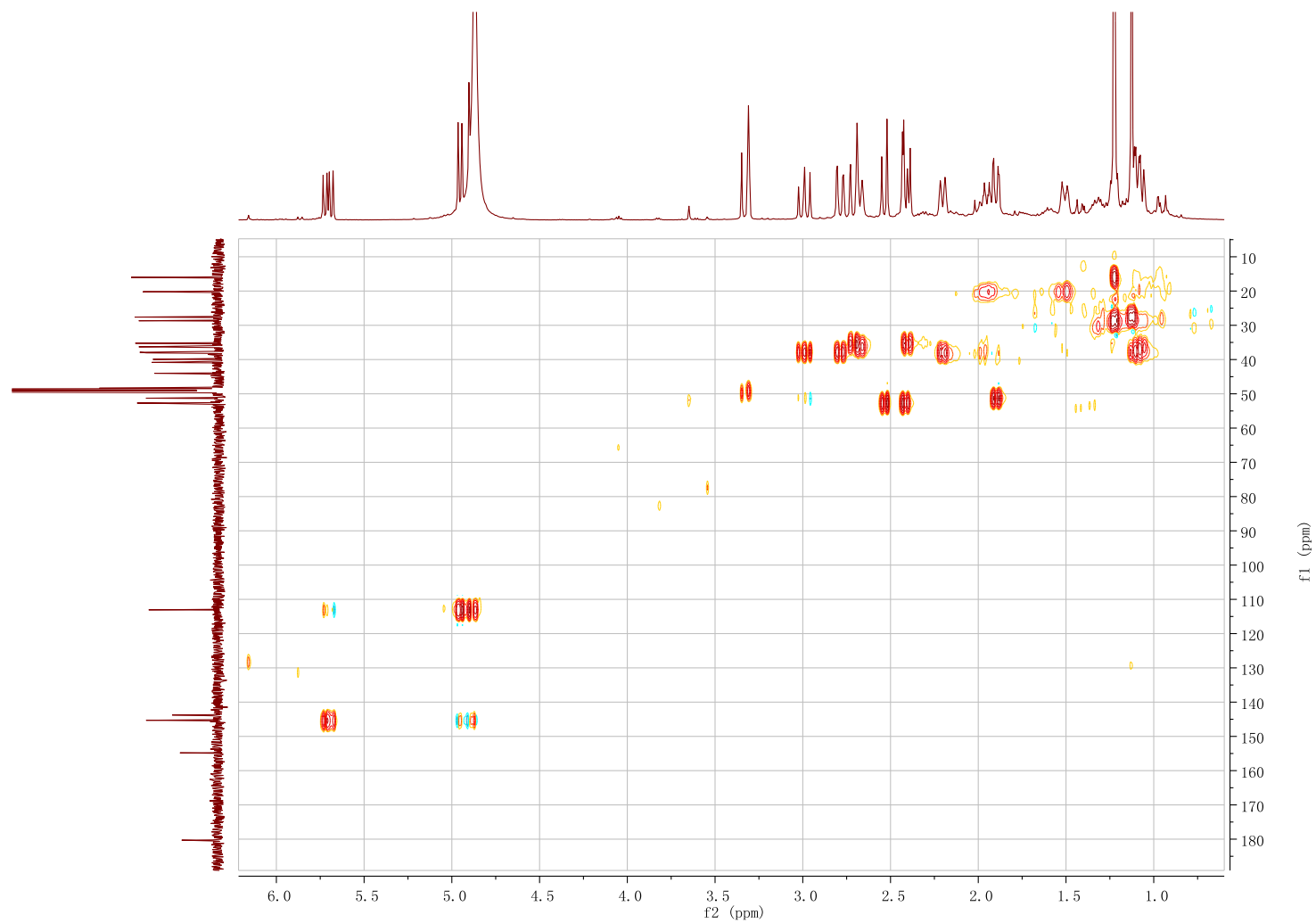
S1. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **1**



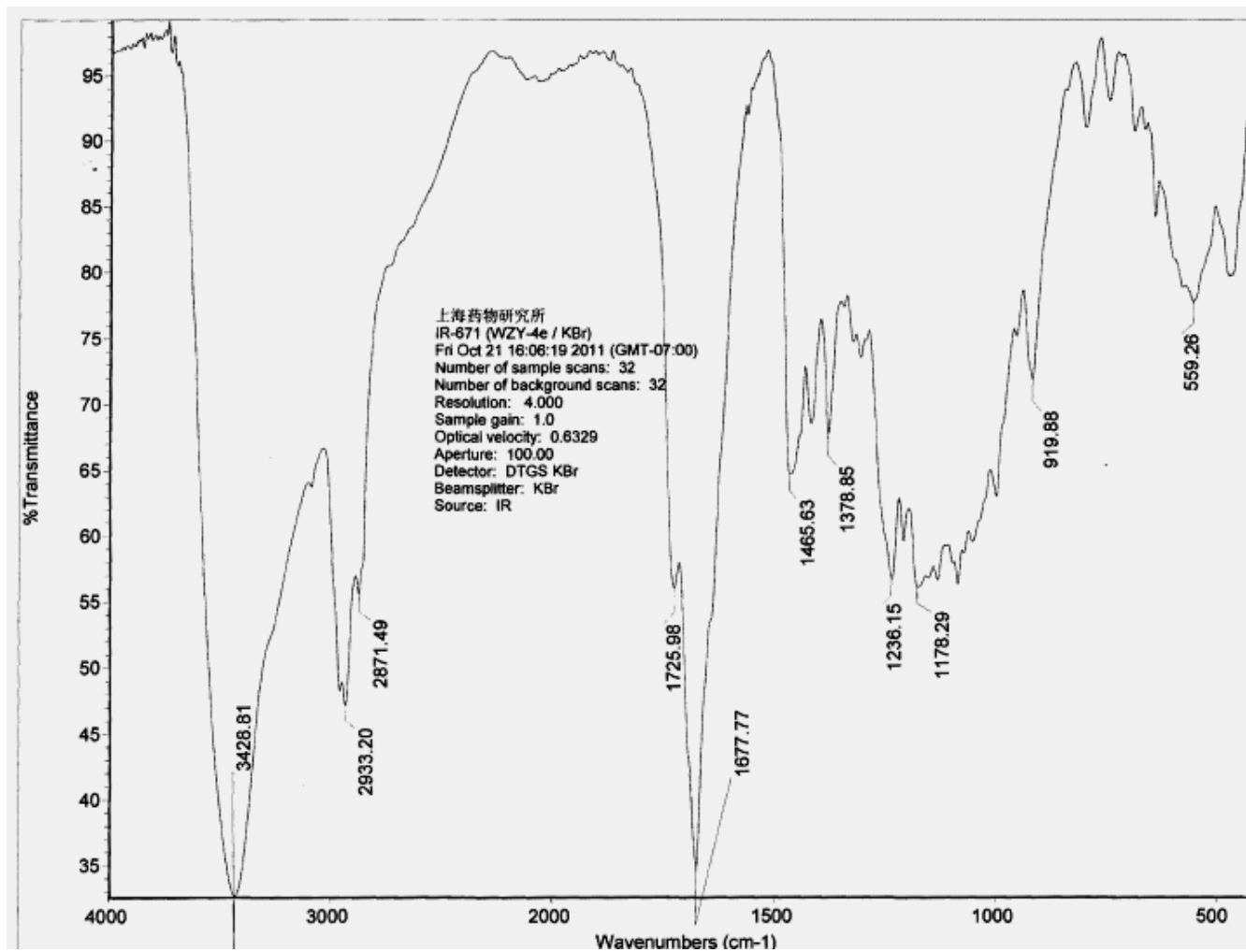
S2. ^{13}C NMR (400MHz, CD_3OD) spectrum of the new compound **1**



S3. HMBC (400MHz, CD₃OD) spectrum of the new compound **1**



S4. HSQC (400MHz, CD₃OD) spectrum of the new compound **1**

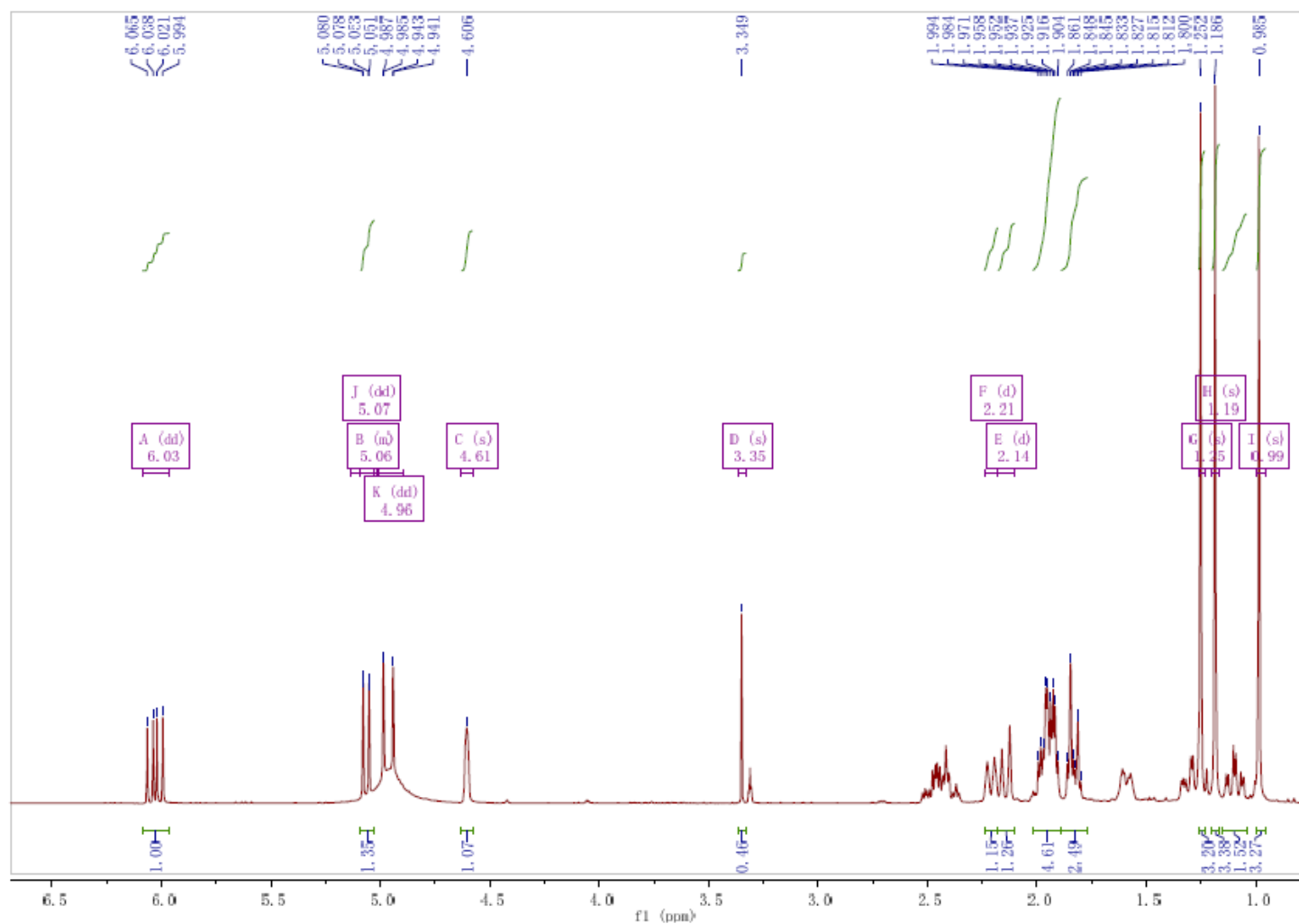


S5. IR (KBr) spectrum of the new compound **1**

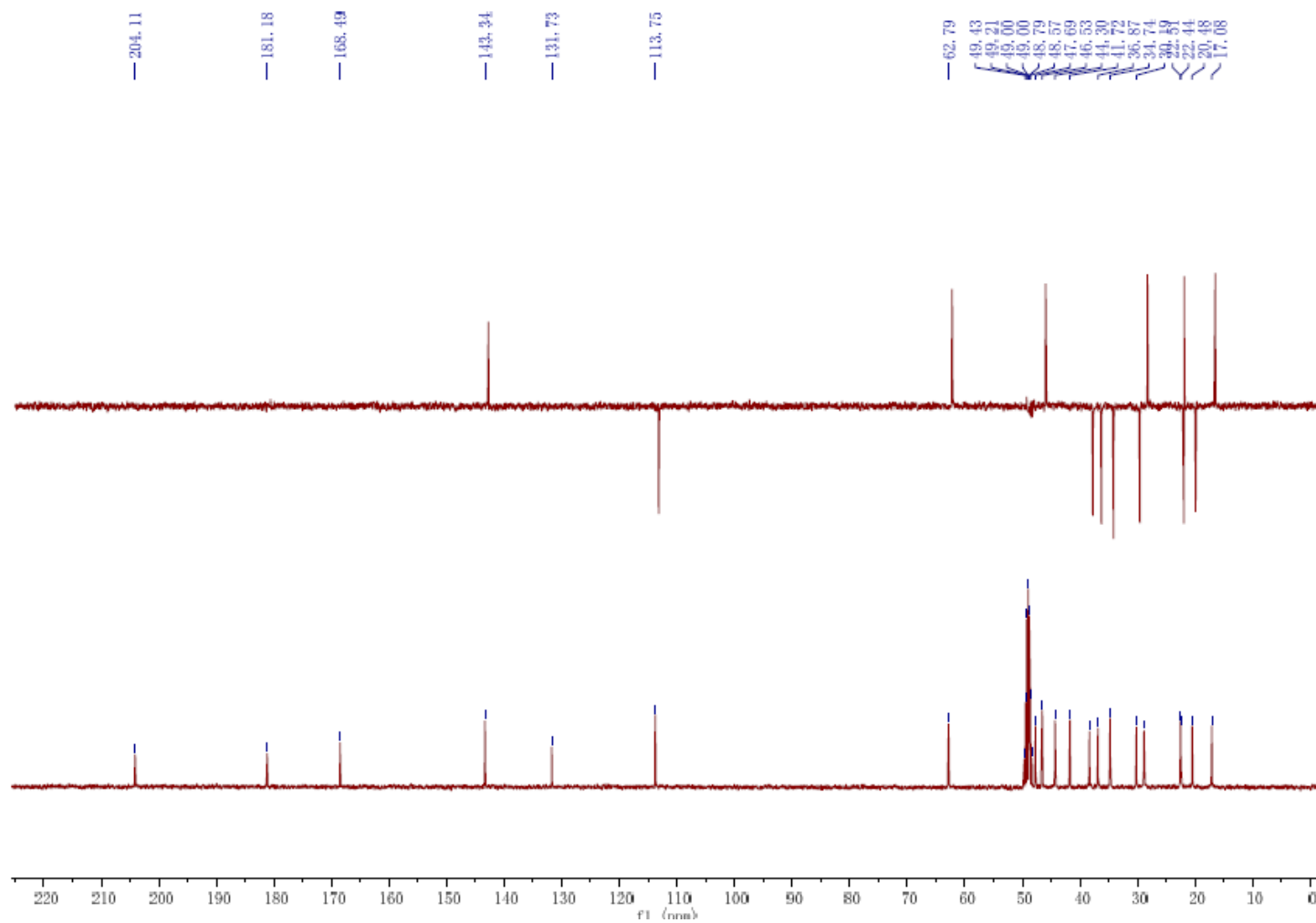
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 : (429) C22.H100.O4
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
53.05542	* 73725	6.25	0.33			
55.06747	* 160130	13.58	0.71			
67.06535	* 144031	12.21	0.64			
69.07086	* 89254	7.57	0.40	-0.4	1.5	C5.H9
77.04534	* 145385	12.33	0.65			
79.05939	* 161982	13.74	0.72			
81.07018	* 122519	10.39	0.55	0.2	2.5	C6.H9
91.01277	* 281937	23.91	1.26			
93.03109	* 129500	10.98	0.58	2.9	4.5	C6.H5.O
95.02459	* 241477	20.48	1.08			
95.06102	* 74366	6.31	0.33			
96.03765	* 70377	5.97	0.31			
105.0685	* 201088	17.05	0.90	2.0	4.5	C8.H9
107.0848	* 102431	8.69	0.46	1.3	3.5	C8.H11
109.1004	* 72941	6.19	0.33	1.3	2.5	C8.H13
115.0545	* 82914	7.03	0.37	0.3	6.5	C9.H7
117.0704	* 85834	7.28	0.38	0.0	5.5	C9.H9
119.0863	* 101221	8.58	0.45	-0.2	4.5	C9.H11
121.0649	* 79993	6.78	0.36	0.4	4.5	C8.H9.O
128.0616	* 69593	5.90	0.31	1.0	7.0	C10.H8
129.0694	* 79495	6.74	0.35	1.0	6.5	C10.H9
131.0857	* 82130	6.97	0.37	0.4	5.5	C10.H11
133.0645	* 64750	5.49	0.29	0.9	5.5	C9.H9.O
133.1008	* 67528	5.73	0.30	0.9	4.5	C10.H13
145.1008	* 86048	7.30	0.38	0.9	5.5	C11.H13
147.0788	* 66032	5.60	0.29	2.2	5.5	C10.H11.O
148.0858	* 79708	6.76	0.36	3.0	5.0	C10.H12.O
159.0789	* 77928	6.61	0.35	2.1	6.5	C11.H11.O
159.1150	* 65106	5.52	0.29	2.4	5.5	C12.H15
161.0948	* 67884	5.76	0.30	1.8	5.5	C11.H13.O
173.0972	* 155571	13.19	0.69	-0.5	6.5	C12.H13.O
175.1122	* 101007	8.57	0.45	0.1	5.5	C12.H15.O
187.1121	* 111692	9.47	0.50	0.2	6.5	C13.H15.O
188.1199	* 126935	10.76	0.57	0.2	6.0	C13.H16.O
189.1281	* 372829	31.62	1.66	-0.2	5.5	C13.H17.O
201.0916	* 73084	6.20	0.33	0.0	7.5	C13.H13.O2
201.1280	* 69665	5.91	0.31	-0.1	6.5	C14.H17.O
216.1148	* 62541	5.30	0.28	0.2	7.0	C14.H16.O2
217.1232	* 76289	6.47	0.34	-0.4	6.5	C14.H17.O2
219.1017	* 59407	5.04	0.26	0.4	6.5	C13.H15.O3
227.1430	* 96163	8.16	0.43	0.6	7.5	C16.H19.O
229.1223	* 67813	5.75	0.30	0.5	7.5	C15.H17.O2
241.1593	* 68667	5.82	0.31	0.0	7.5	C17.H21.O
242.1308	* 69736	5.91	0.31	-0.2	8.0	C16.H18.O2
243.1743	* 92744	7.87	0.41	0.6	6.5	C17.H23.O
247.0962	* 64963	5.51	0.29	0.9	7.5	C14.H15.O4
256.1835	* 73796	6.26	0.33	-0.8	7.0	C18.H24.O
262.1206	* 192896	16.36	0.86	-0.1	7.0	C15.H18.O4
269.1547	* 123160	10.44	0.55	-0.6	8.5	C18.H21.O2
284.1769	* 230436	19.54	1.03	0.7	8.0	C19.H24.O2
285.1833	* 67955	5.76	0.30	2.2	7.5	C19.H25.O2
287.1686	* 65961	5.59	0.29			
288.1729	* 323893	27.47	1.44	-0.3	7.0	C18.H24.O3
289.1756	* 67741	5.74	0.30			
330.1831	* 1179178	100.00	5.25	0.0	8.0	C20.H26.O4
331.1883	* 274244	23.26	1.22	2.6	7.5	C20.H27.O4
332.1941	* 61829	5.24	0.28			

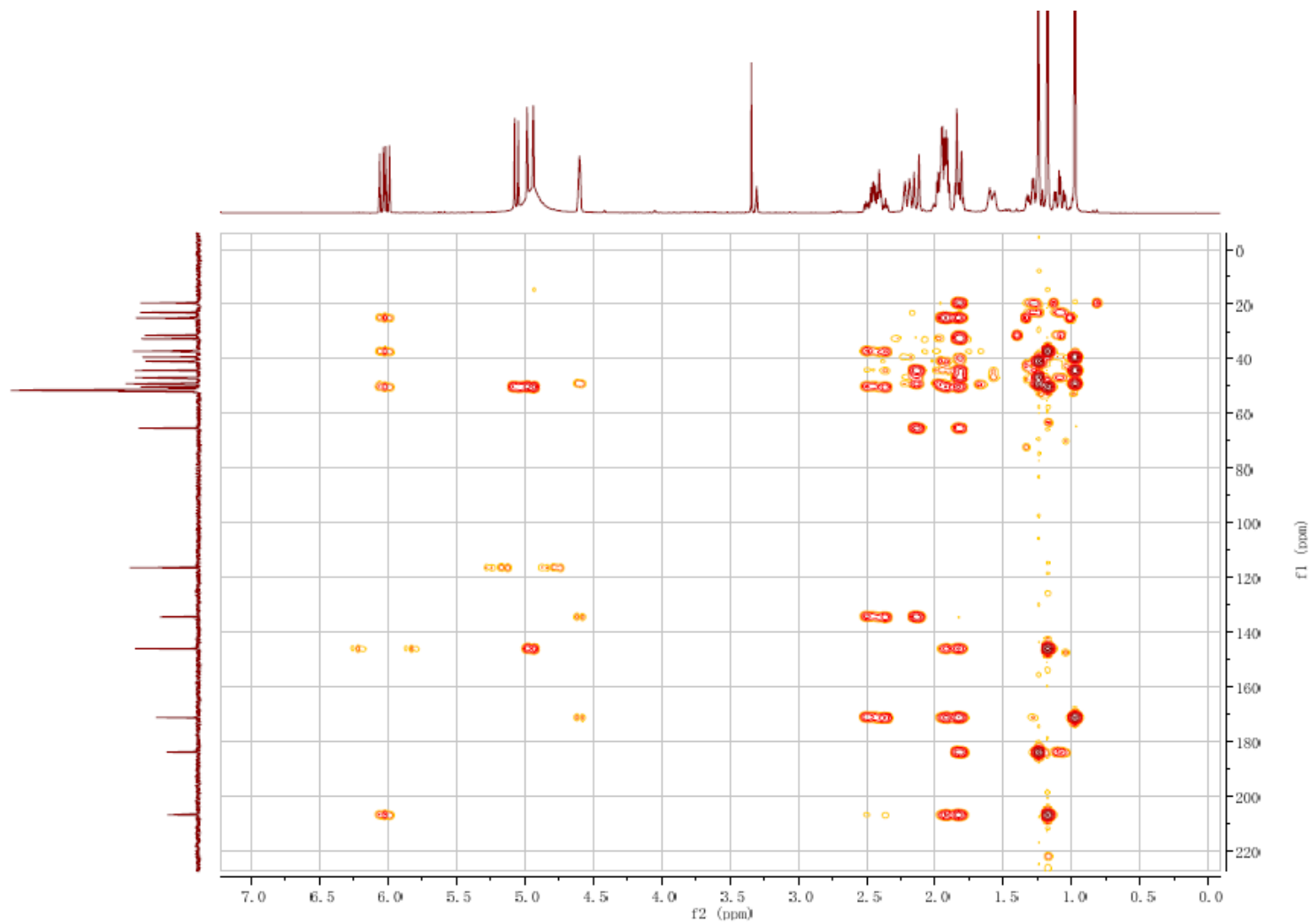
S6. HR-EI-MS data of the new compound 1



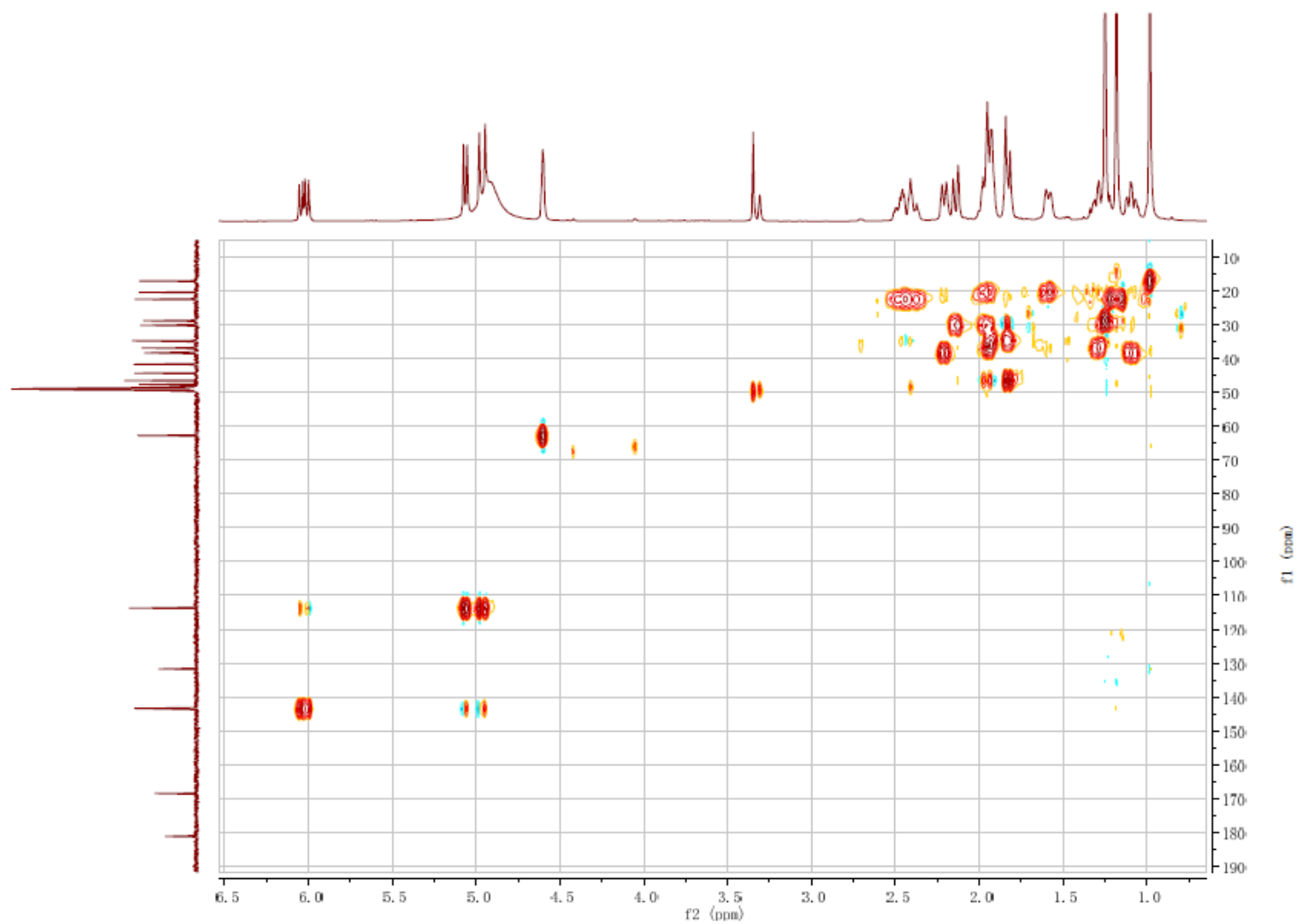
S7. ¹H NMR (400MHz, CD₃OD) spectrum of the new compound **2**



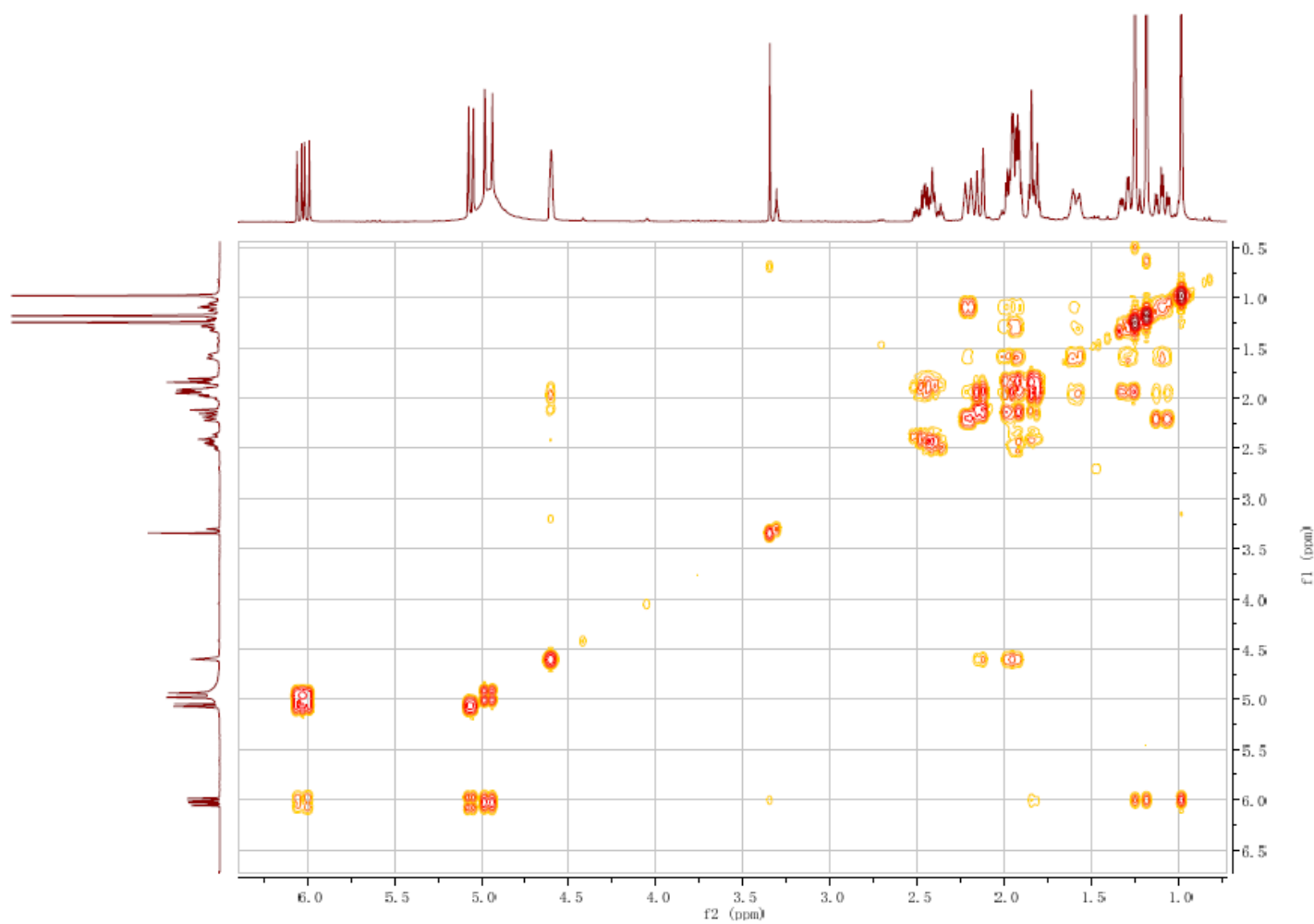
S8. ^{13}C NMR (400MHz, CD_3OD) spectrum of the new compound **2**



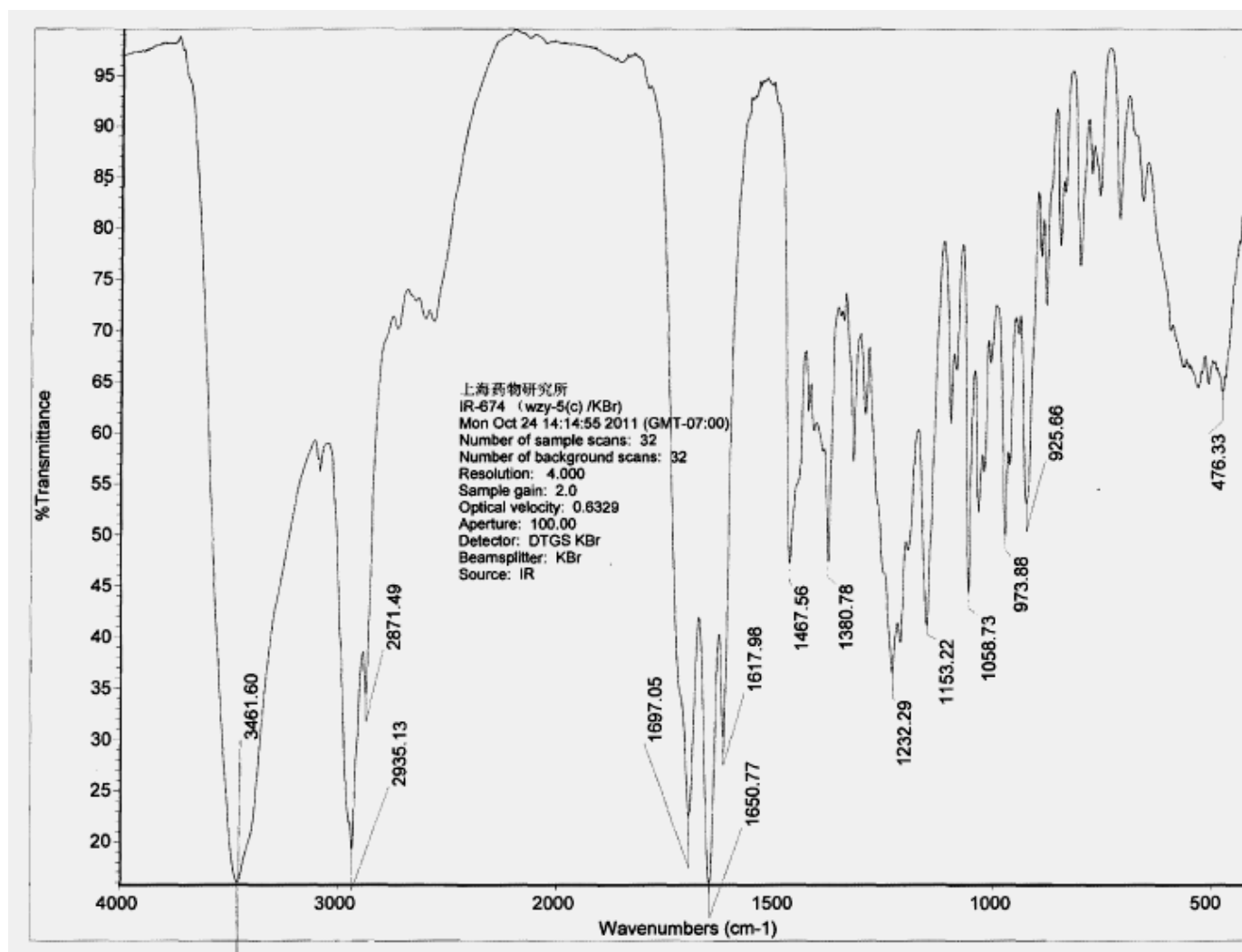
S9. HMBC (400MHz, CD₃OD) spectrum of the new compound **2**



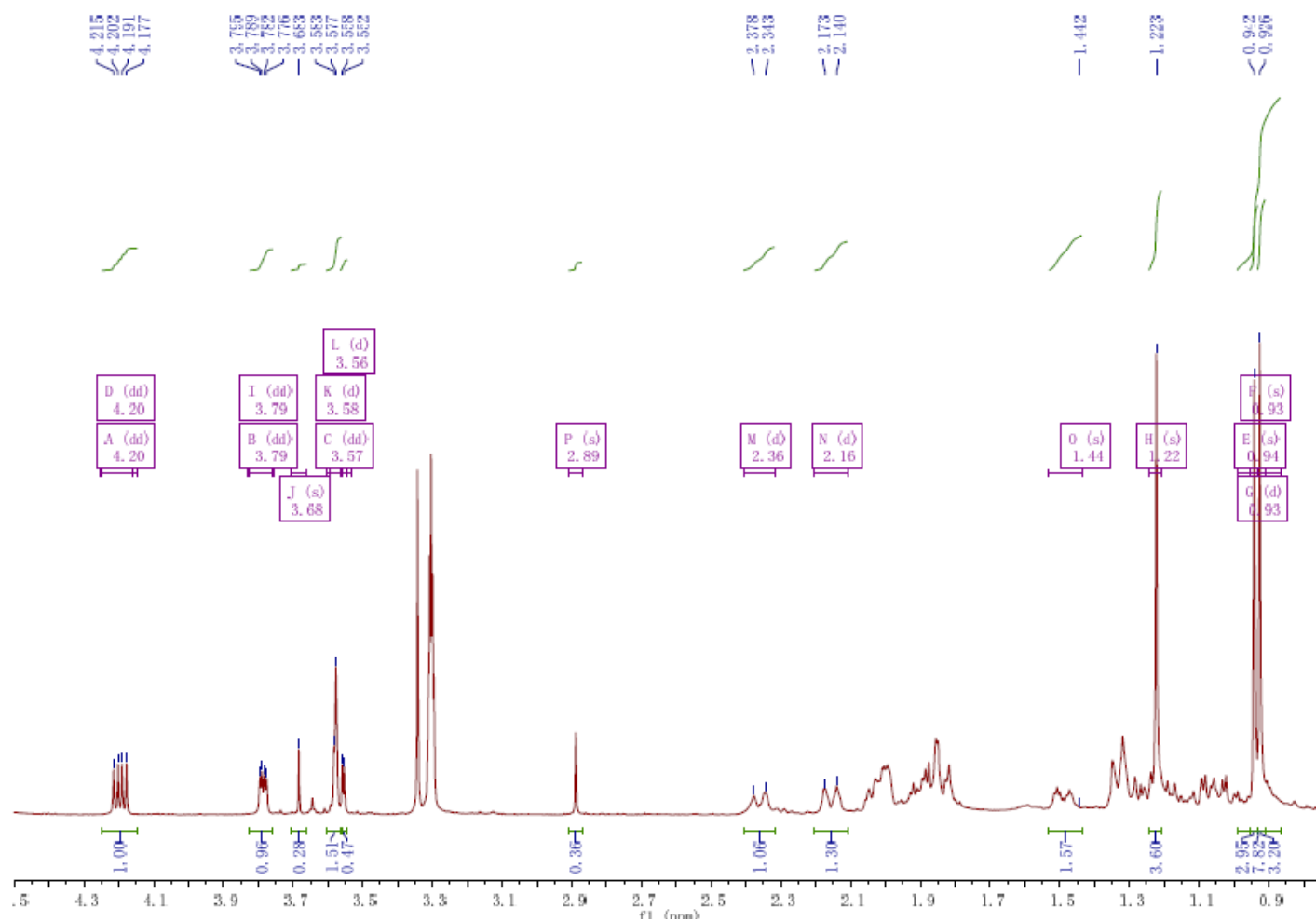
S10. HSQC (400MHz, CD₃OD) spectrum of the new compound **2**



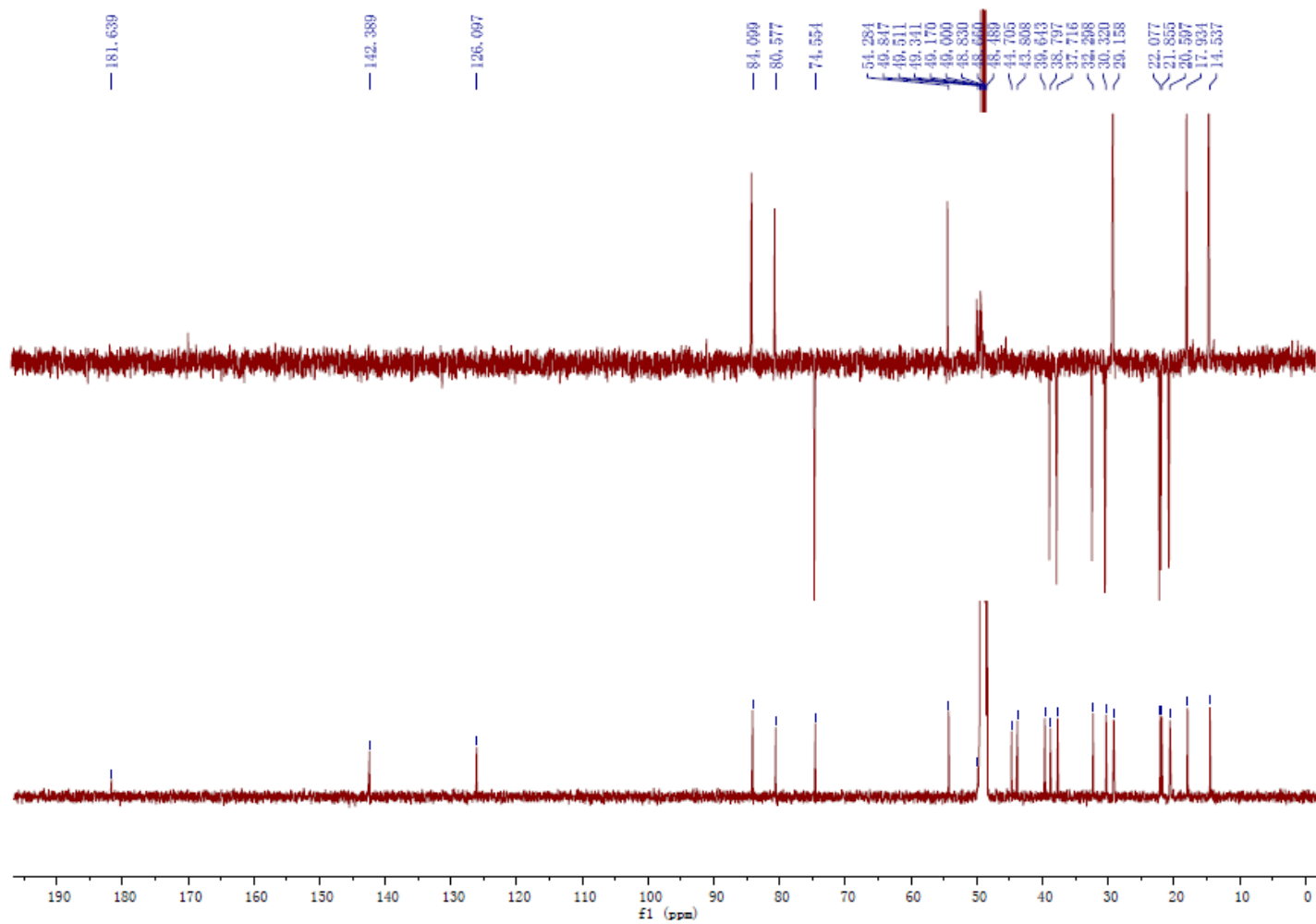
S11. ^1H - ^1H COSY (400MHz, CD_3OD) spectrum of the new compound **2**



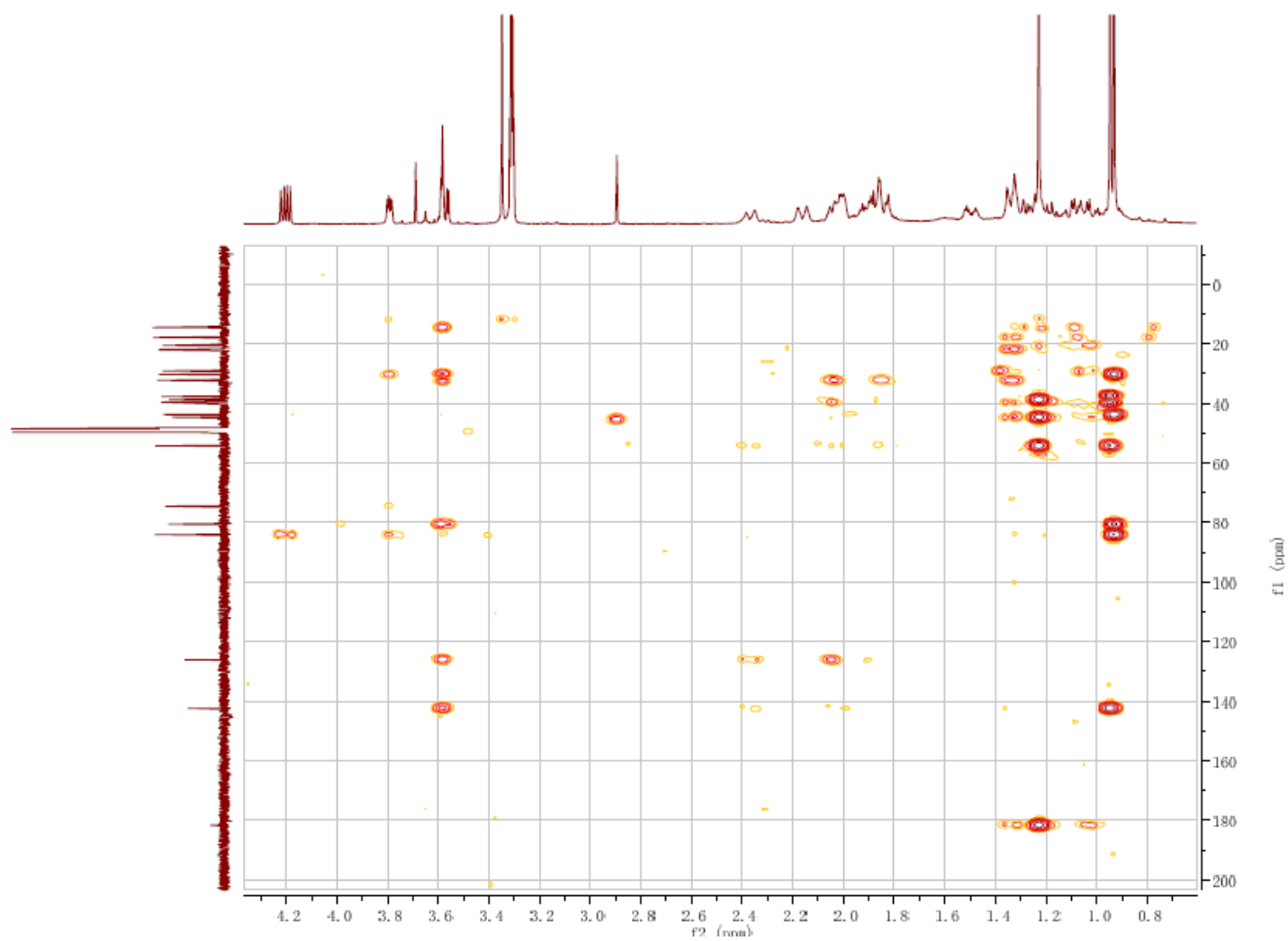
S12.IR (KBr) spectrum of the new compound 2



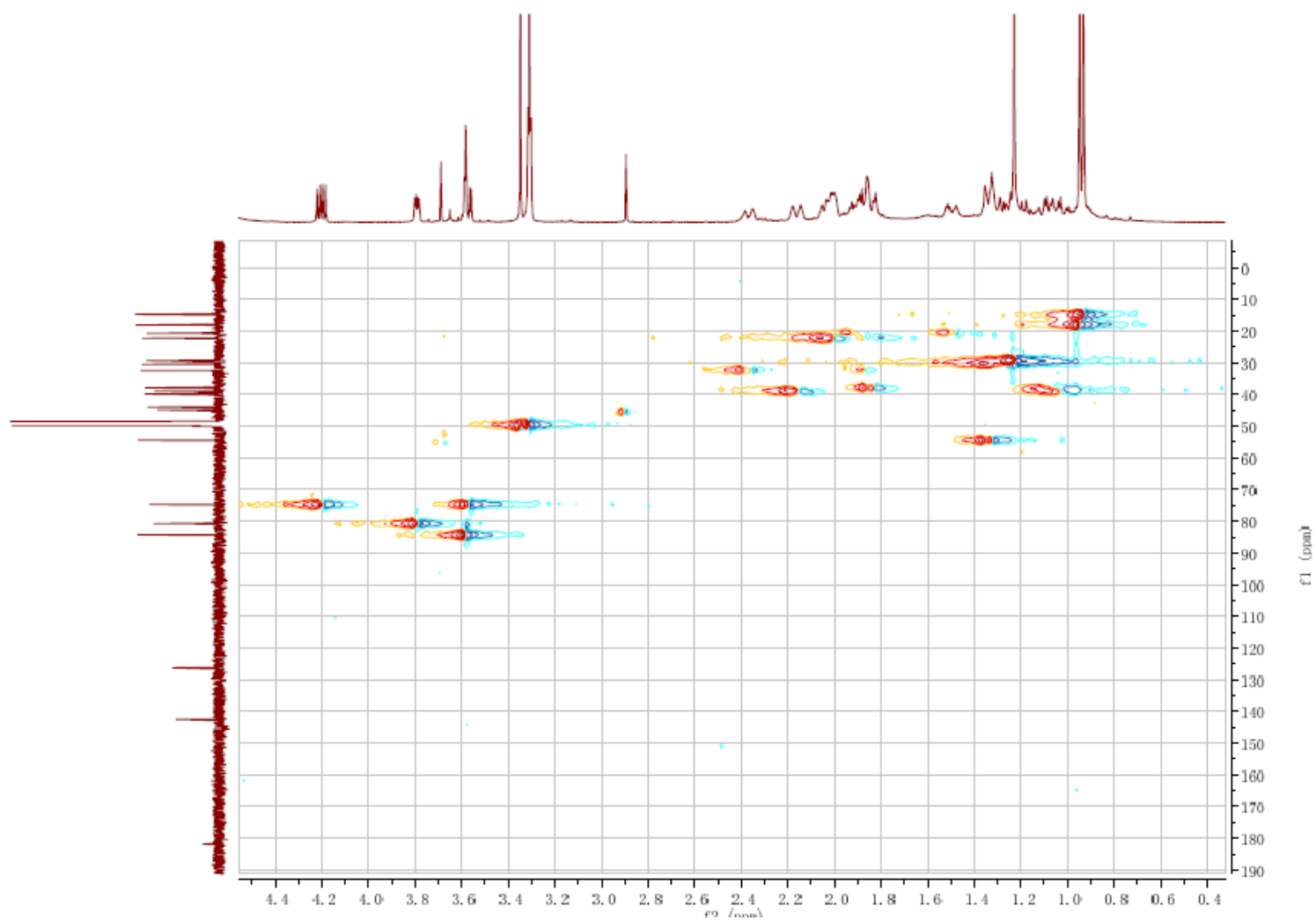
S13. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **3**



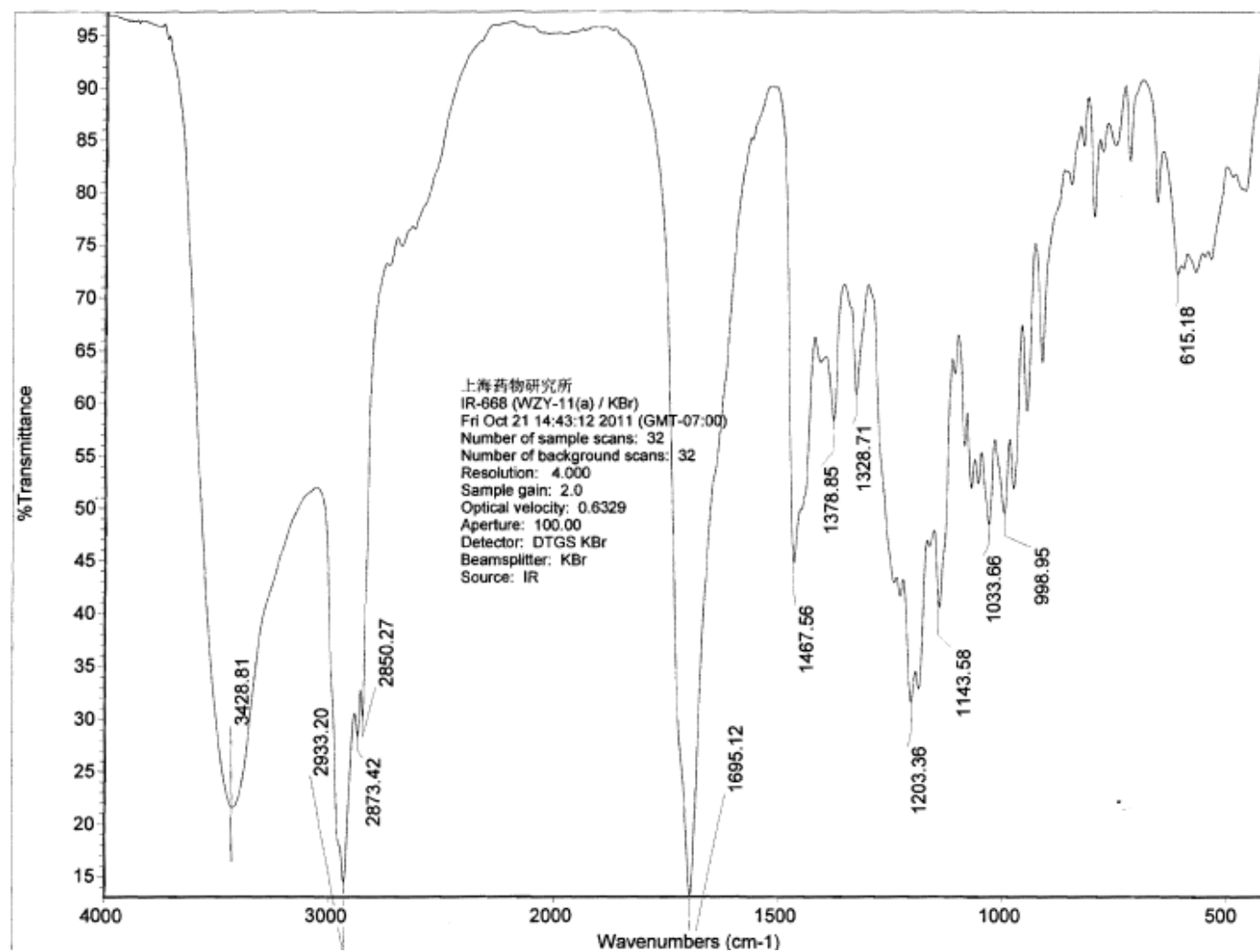
S14. ¹³C NMR (400MHz, CD₃OD) spectrum of the new compound **3**



S15. HMBC (400MHz, CD₃OD) spectrum of the new compound **3**



S16. HSQC (400MHz, CD₃OD) spectrum of the new compound **3**

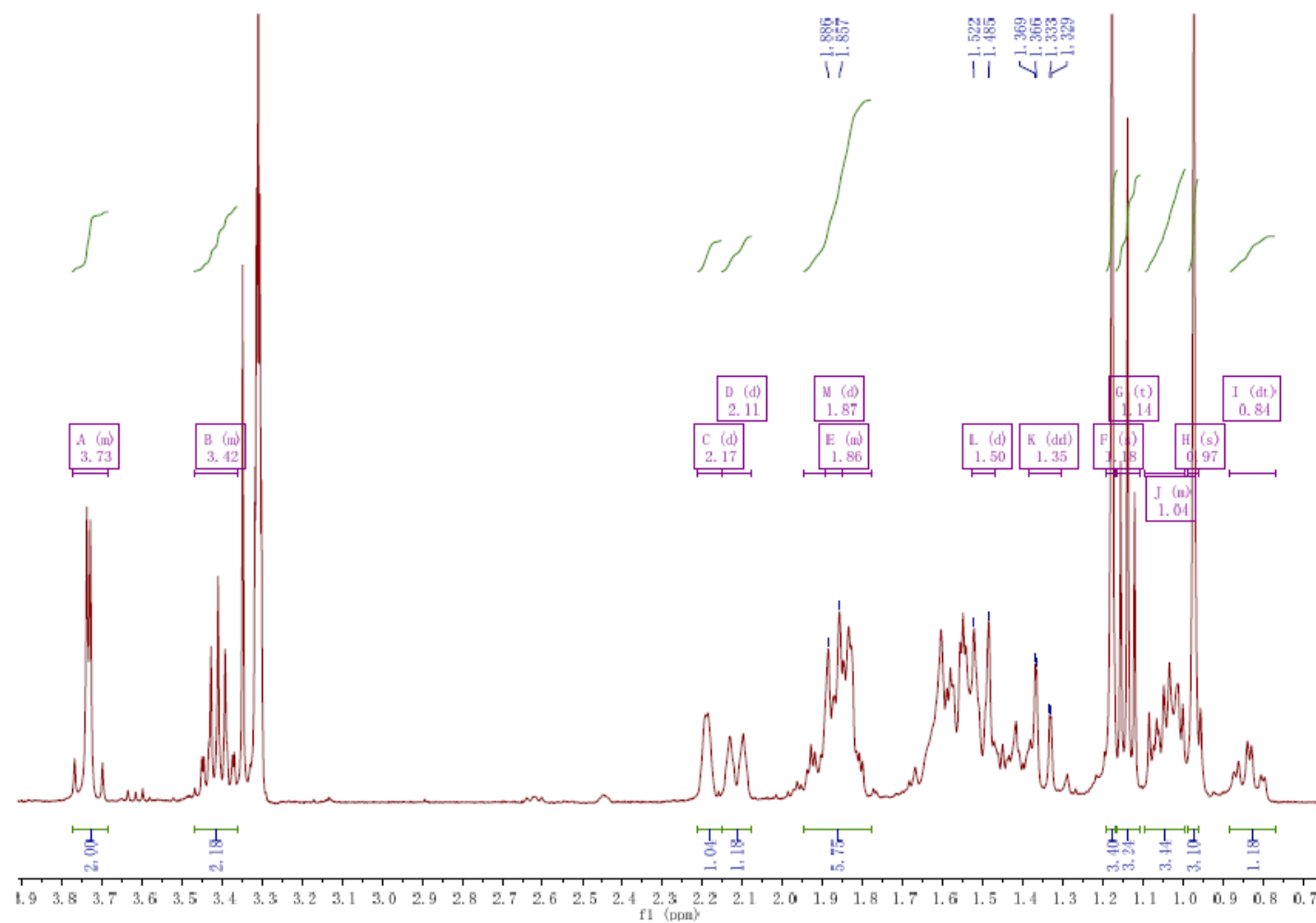


S17. IR (KBr) spectrum of the new compound 3

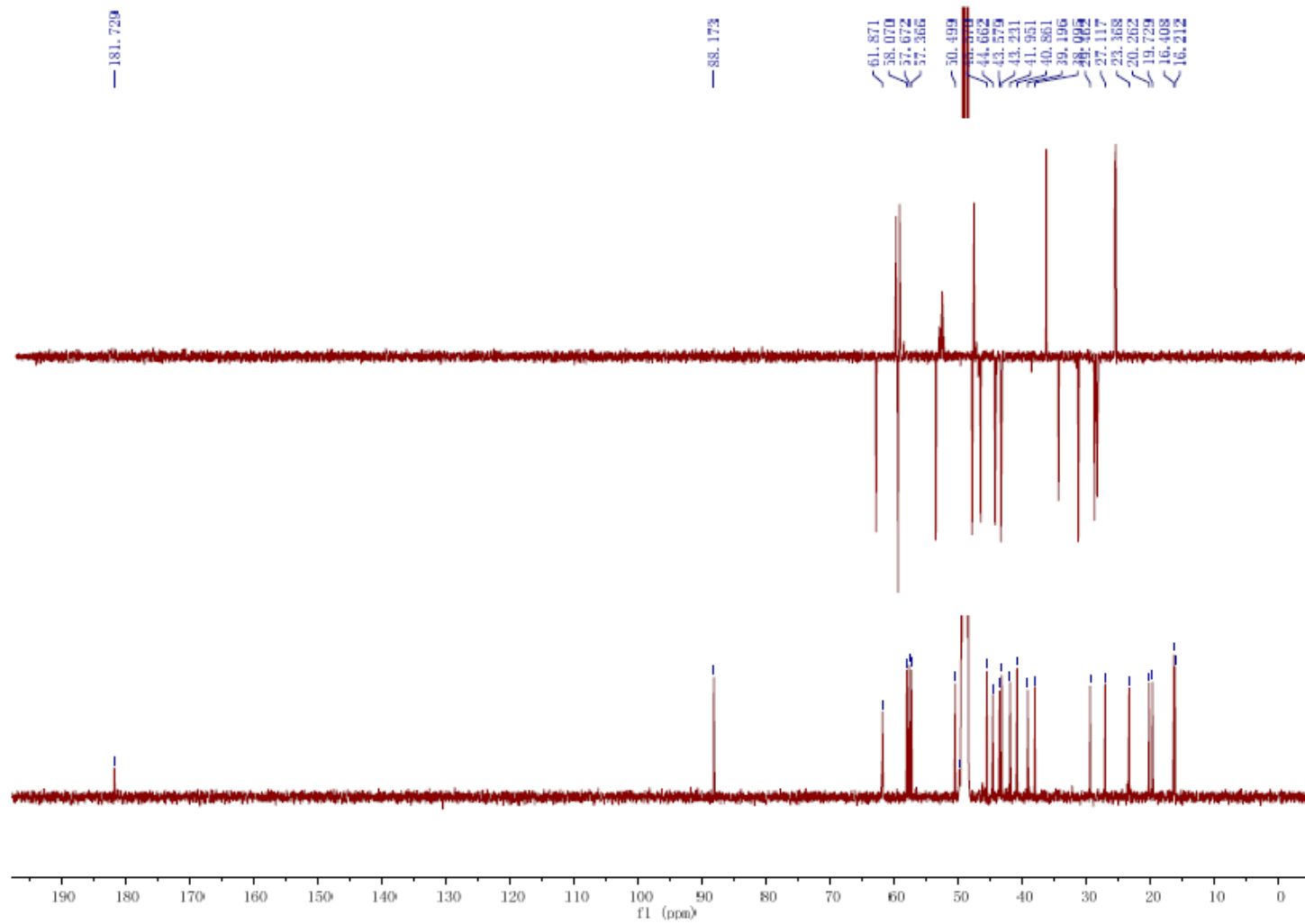
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 Oper: WANG_J@SIMM.CAS Inlet :
 Limit: (0)
 : (429) C22.H100.O4
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

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Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
55.06802	* 14175	10.16	0.12			
57.08171	* 10756	7.71	0.09			
58.07675	* 5983	4.29	0.05	1.5	0.0	C4.H10
67.06575	* 5983	4.29	0.05			
69.07019	* 9331	6.69	0.08	0.2	1.5	C5.H9
77.04040	* 7835	5.62	0.07	-1.3	4.5	C6.H5
79.05532	* 8262	5.92	0.07	-0.5	3.5	C6.H7
81.07012	* 10827	7.76	0.09	0.3	2.5	C6.H9
91.05396	* 13676	9.81	0.12	0.8	4.5	C7.H7
95.08498	* 12465	8.94	0.11	1.1	2.5	C7.H11
105.0717	* 27709	19.87	0.24	-1.3	4.5	C8.H9
107.0874	* 8547	6.13	0.07	-1.4	3.5	C8.H11
109.1026	* 7336	5.26	0.06	-0.9	2.5	C8.H13
119.0867	* 13177	9.45	0.12	-0.7	4.5	C9.H11
120.0932	* 7835	5.62	0.07	0.7	4.0	C9.H12
121.1020	* 11895	8.53	0.10	-0.3	3.5	C9.H13
129.0679	* 8975	6.43	0.08	2.5	6.5	C10.H9
131.0876	* 12251	8.78	0.11	-1.5	5.5	C10.H11
133.1019	* 9616	6.89	0.08	-0.1	4.5	C10.H13
143.0851	* 6695	4.80	0.06	1.0	6.5	C11.H11
145.1005	* 16810	12.05	0.15	1.2	5.5	C11.H13
149.0230	* 6553	4.70	0.06	0.8	6.5	C8.H5.O3
155.0867	* 5698	4.09	0.05	-0.6	7.5	C12.H11
157.1009	* 17309	12.41	0.15	0.8	6.5	C12.H13
159.1165	* 9687	6.95	0.08	0.9	5.5	C12.H15
166.0988	* 8761	6.28	0.08	0.6	4.0	C10.H14.O2
167.1065	* 139472	100.00	1.22	0.7	3.5	C10.H15.O2
168.1091	* 11895	8.53	0.10			
173.1311	* 5983	4.29	0.05	1.9	5.5	C13.H17
180.1144	* 31912	22.88	0.28	0.6	4.0	C11.H16.O2
211.1468	* 11610	8.32	0.10	1.9	7.5	C16.H19
213.1635	* 10399	7.46	0.09	0.9	6.5	C16.H21
219.1396	* 7621	5.46	0.07	-1.1	5.5	C14.H19.O2
227.1798	* 16525	11.85	0.14	0.2	6.5	C17.H23
257.1525	* 15172	10.88	0.13	1.6	7.5	C17.H21.O2
259.1699	* 20229	14.50	0.18	0.0	6.5	C17.H23.O2
272.1805	* 12180	8.73	0.11	-2.8	7.0	C18.H24.O2
273.1874	* 18662	13.38	0.16	-1.9	6.5	C18.H25.O2
274.1942	* 17166	12.31	0.15	-0.9	6.0	C18.H26.O2
334.2147	* 25358	18.18	0.22	-0.3	6.0	C20.H30.O4
335.9757	* 10542	7.56	0.09			

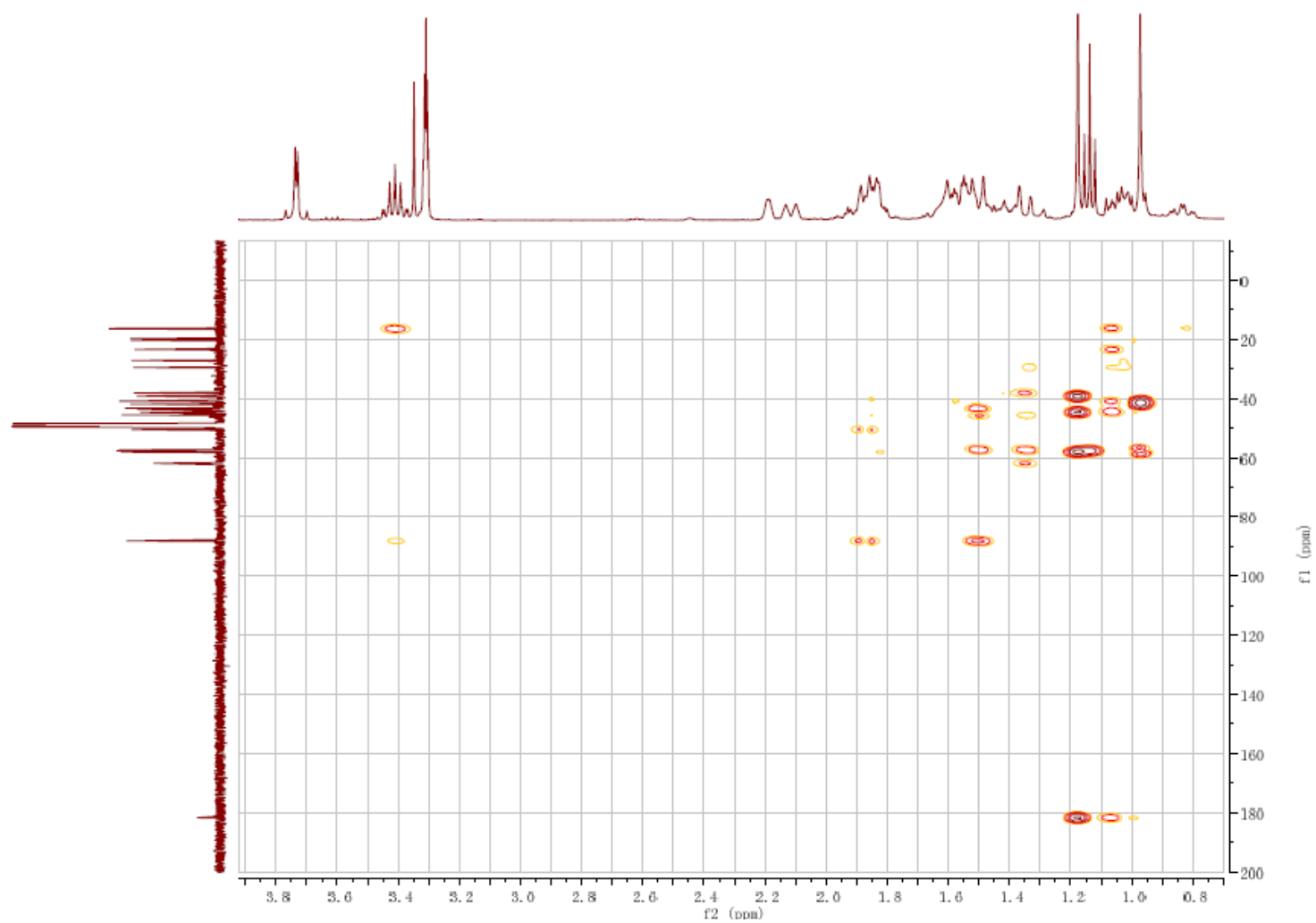
S18. HR-EI-MS data of the new compound 3



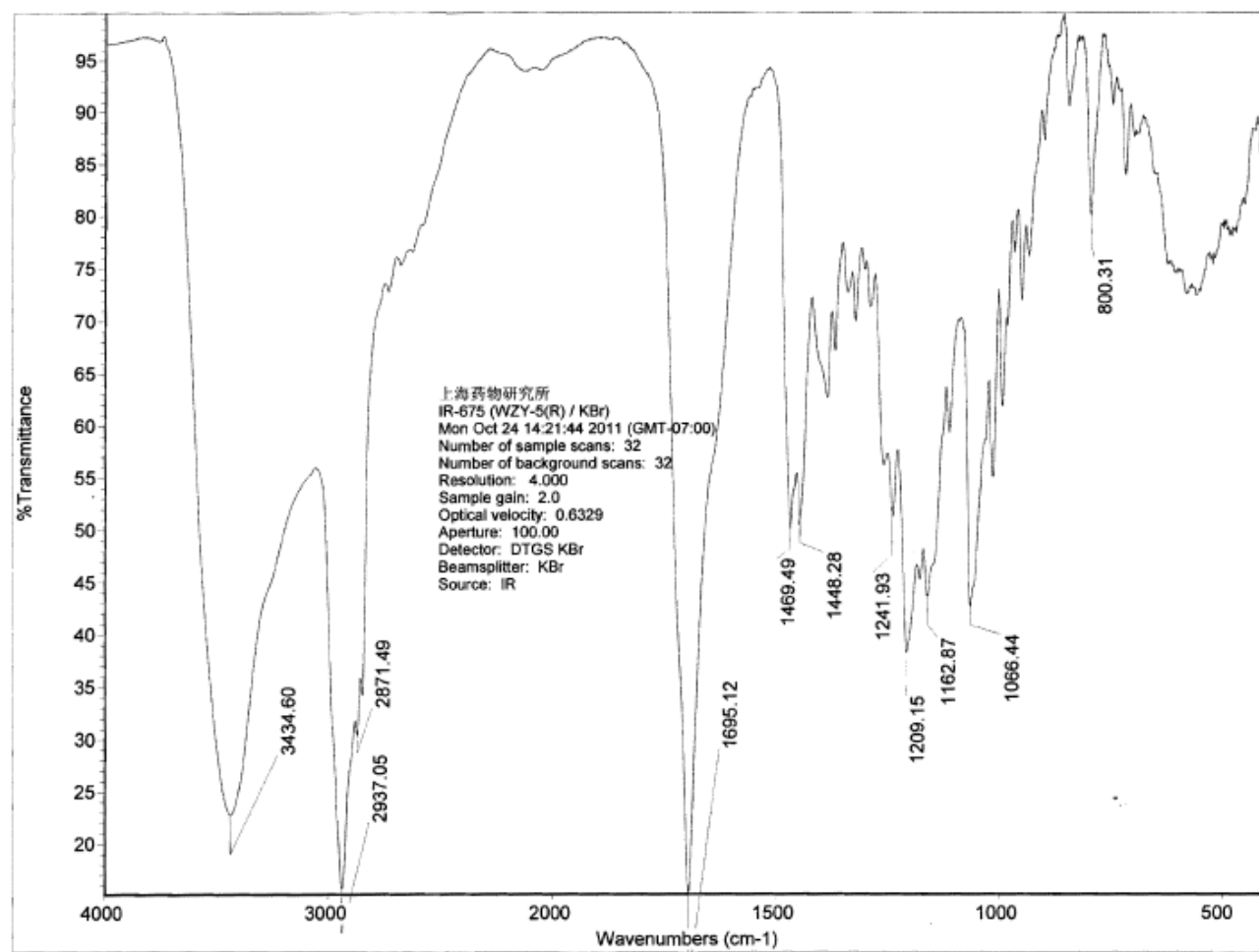
S19. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **4**



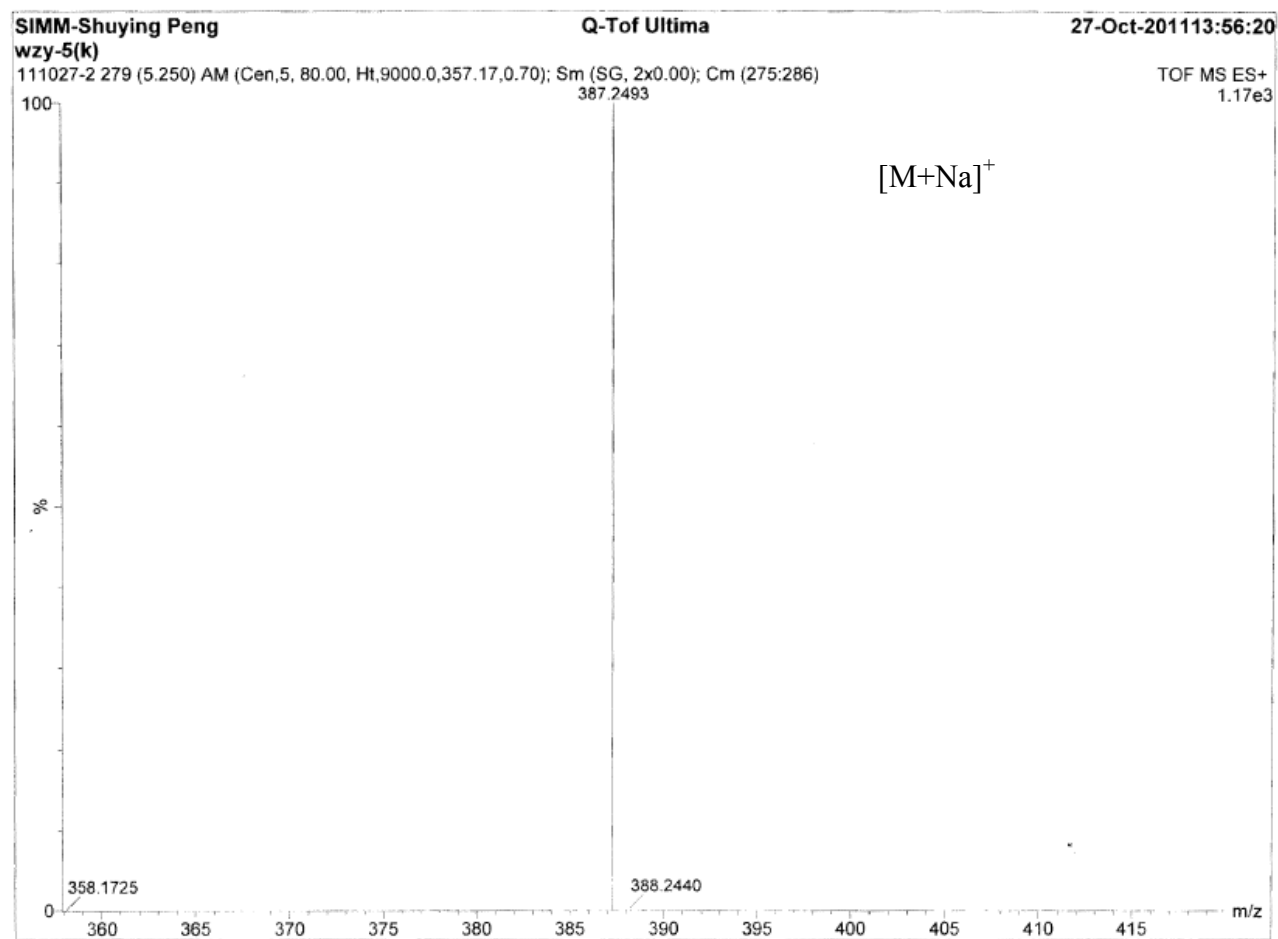
S20. ¹³C NMR (400MHz, CD₃OD) spectrum of the new compound **4**



S21. HMBC (400MHz, CD₃OD) spectrum of the new compound **4**



S22. IR (KBr) spectrum of the new compound 4



S23. HR-ESI-MS spectrum of the new compound 4

Elemental Composition Report

Page 1

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Shuying Peng

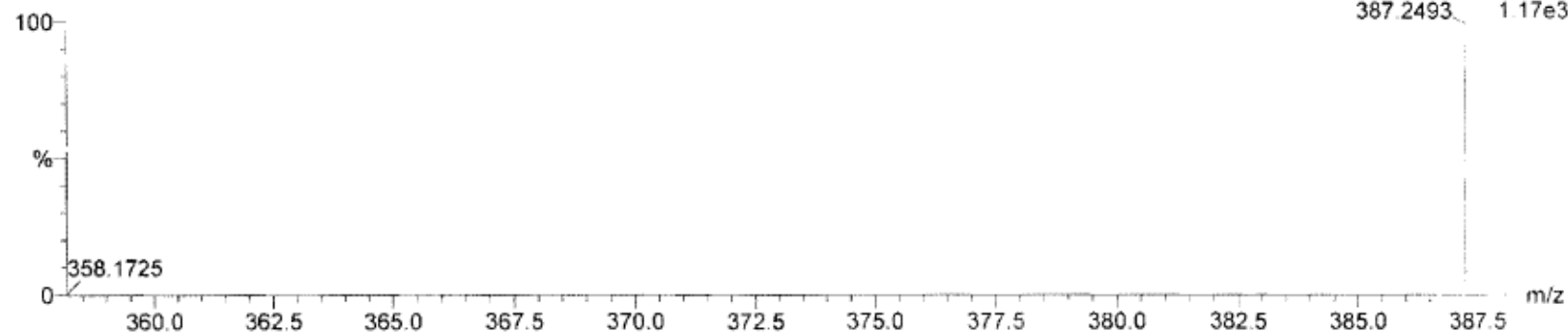
Q-Tof Ultima

27-Oct-2011 13:56:20

wzy-5(k)

111027-2 279 (5.250) AM (Cen,5, 80.00, Ht,9000.0,357.17,0.70); Sm (SG, 2x0.00); Cm (275:286)

TOF MS ES+
387.2493 1.17e3

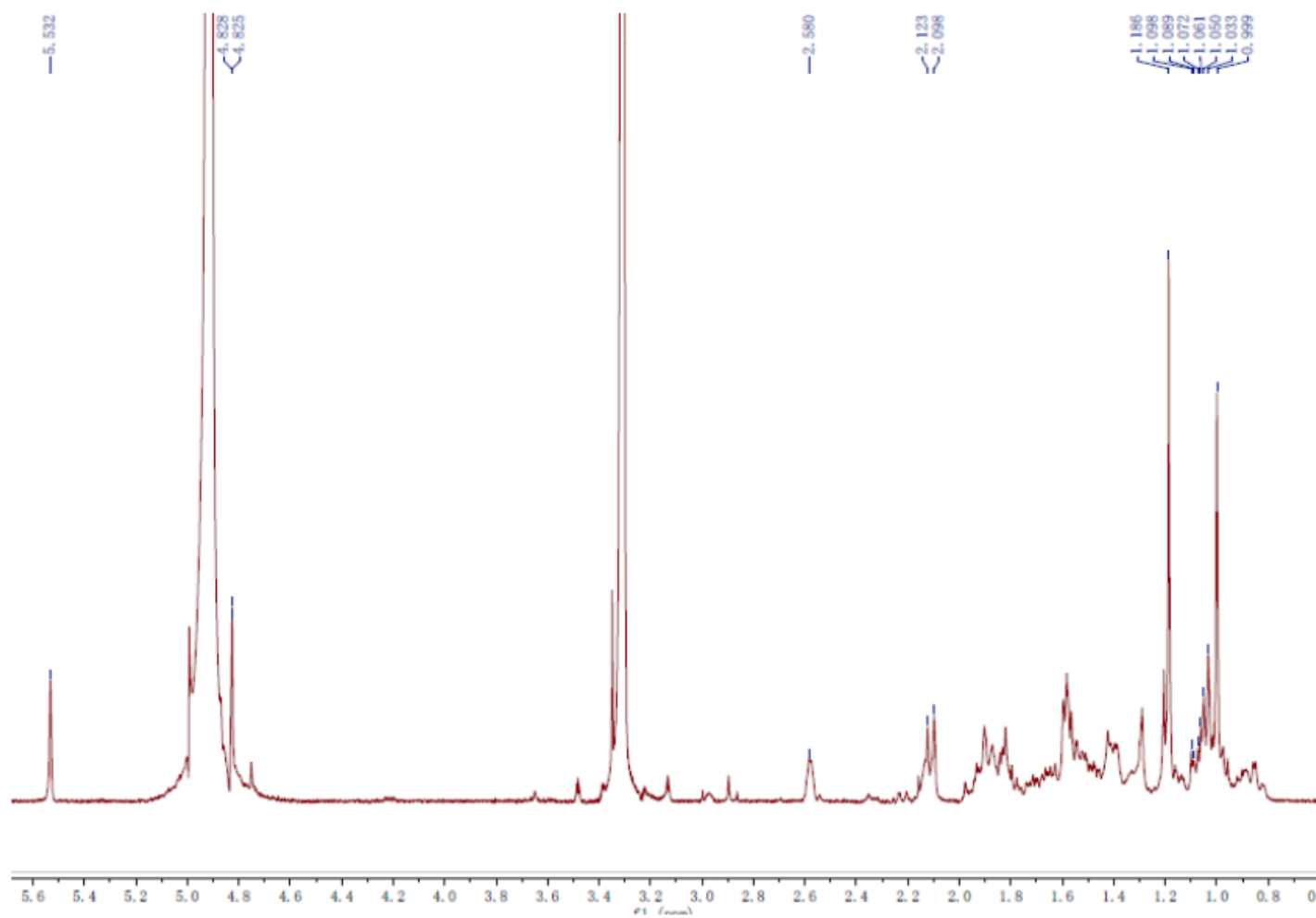


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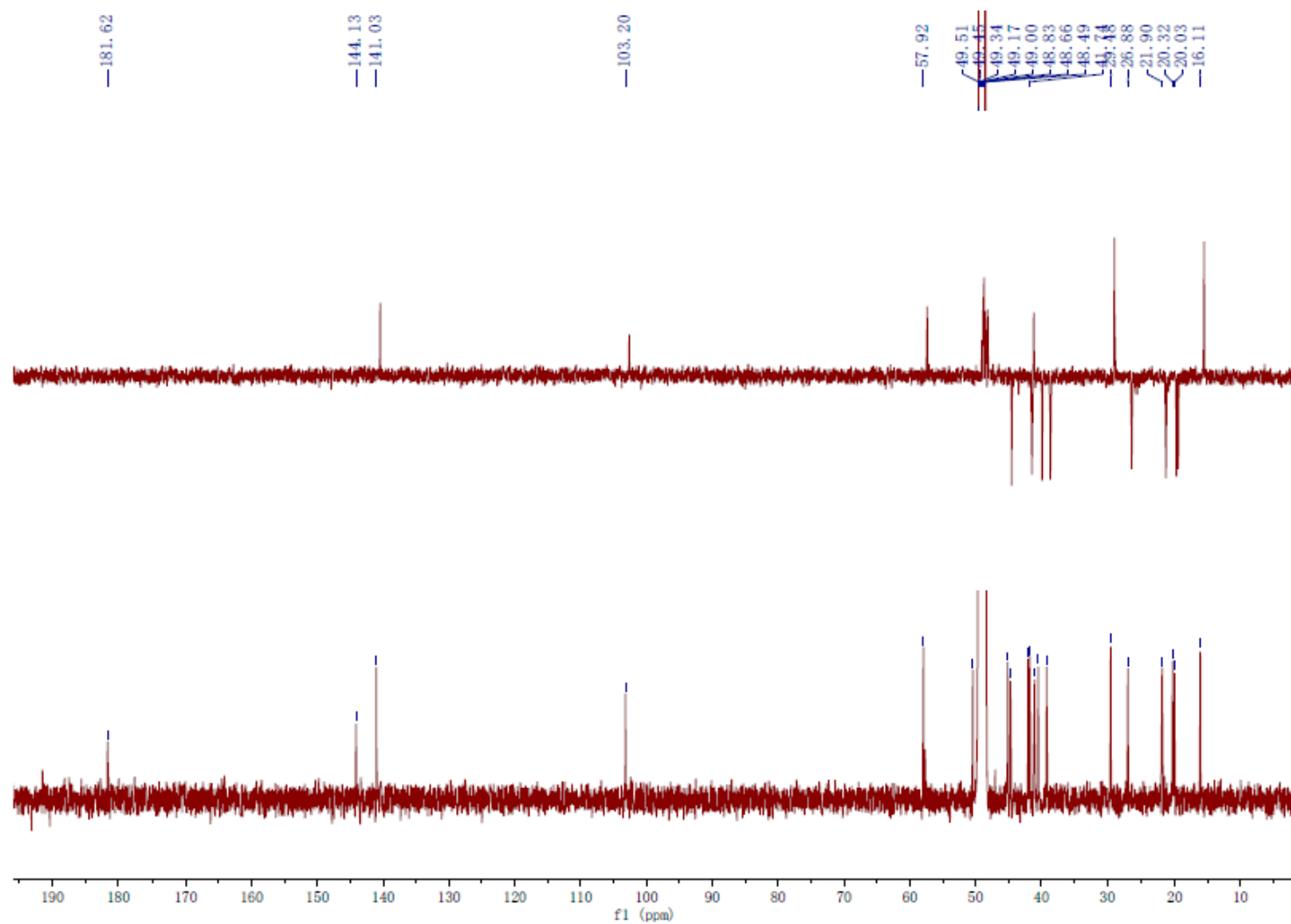
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
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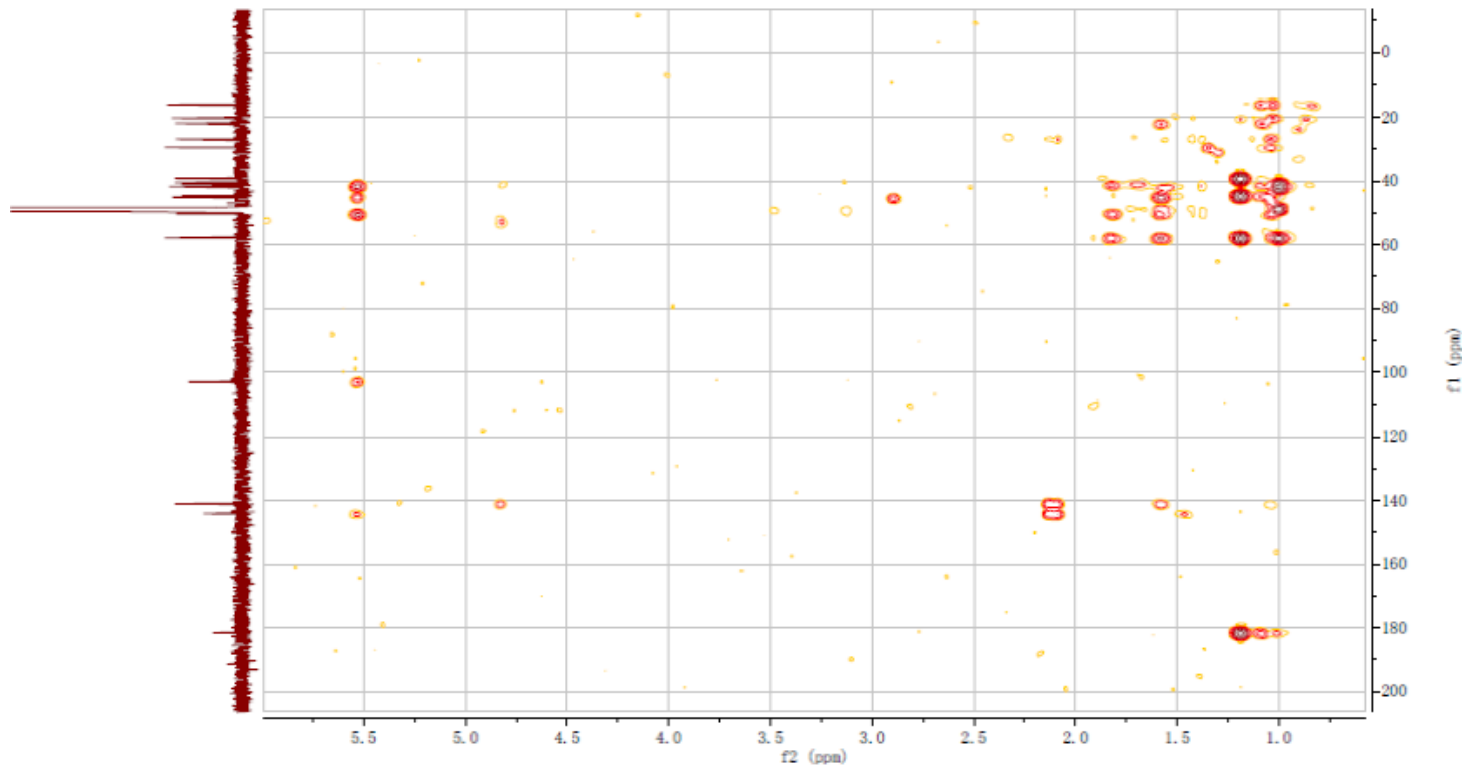
S24. HR-ESI-MS spectrum of the new compound 4



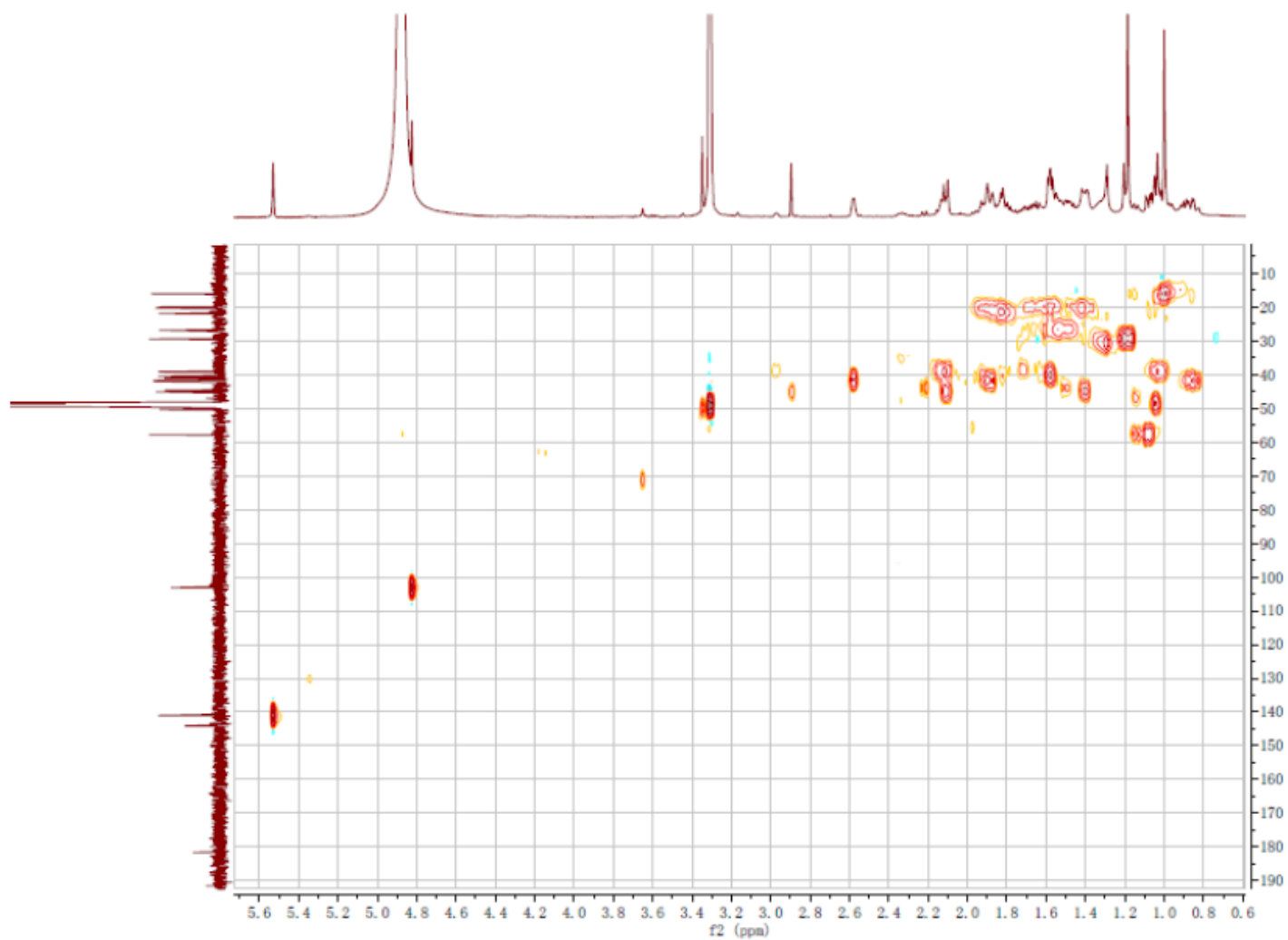
S25. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **5**



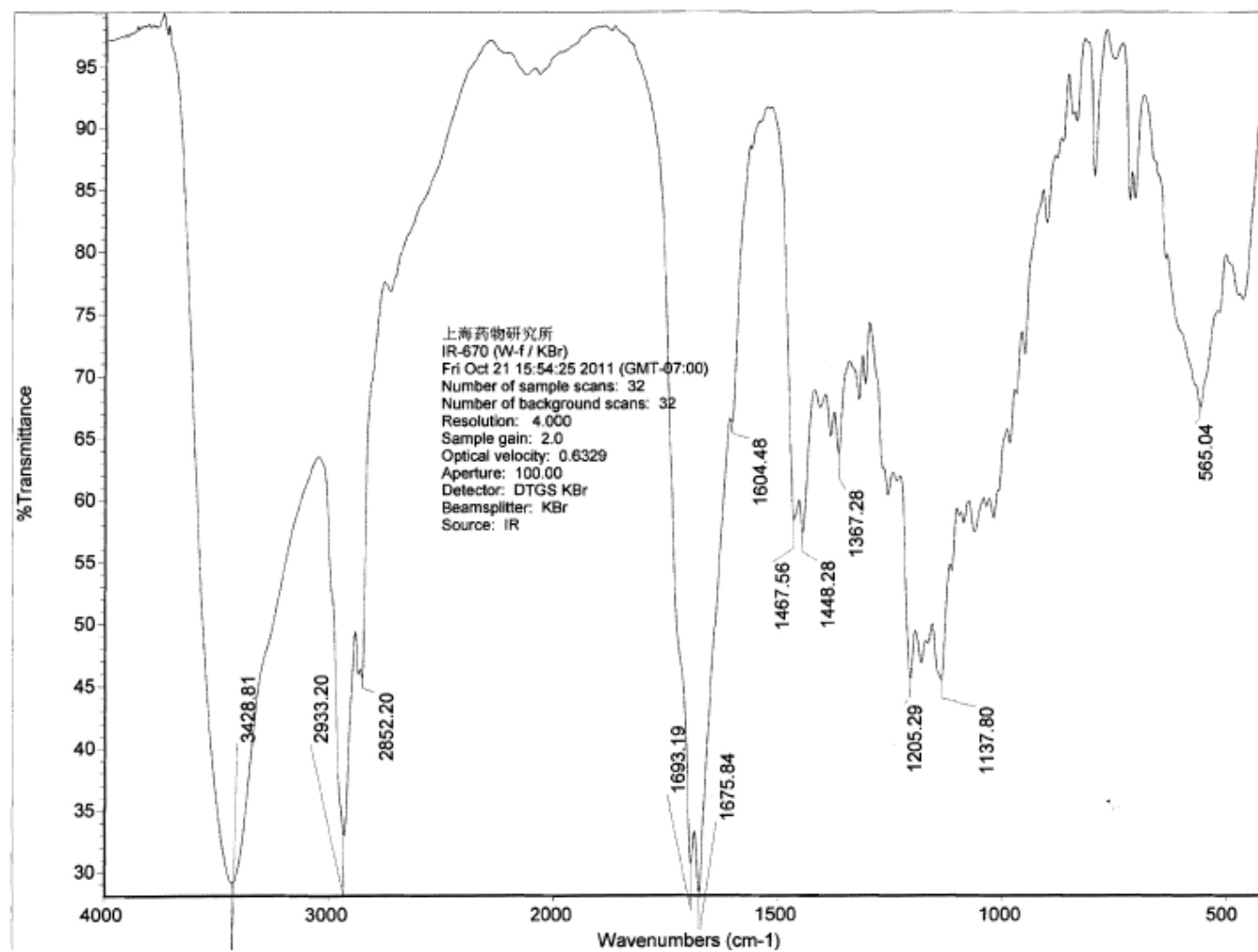
S26. ^{13}C NMR (400MHz, CD_3OD) spectrum of the new compound **5**



S27. HMBC (400MHz, CD₃OD) spectrum of the new compound **5**



S28. HSQC (400MHz, CD_3OD) spectrum of the new compound **5**

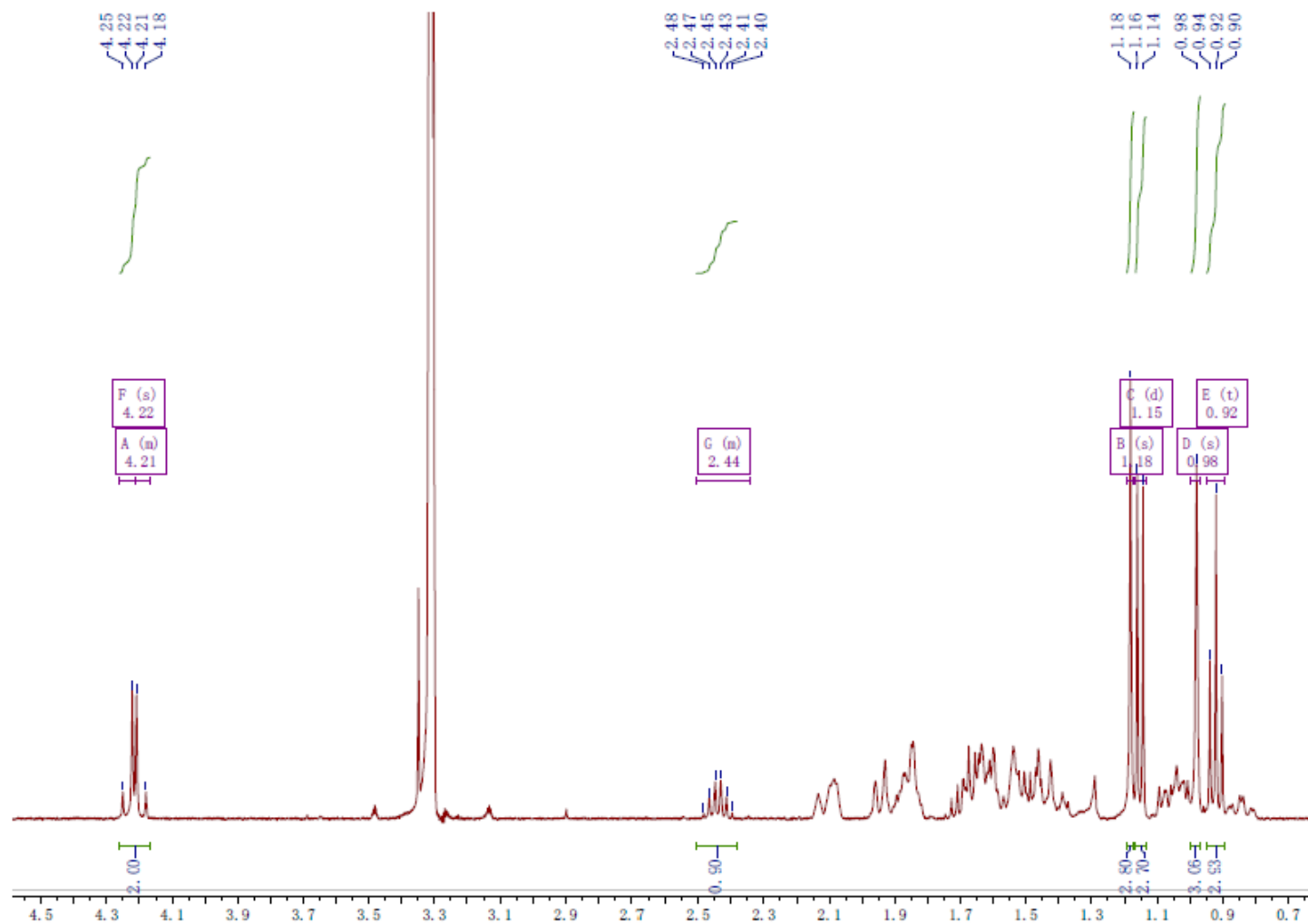


S29. IR (KBr) spectrum of the new compound **5**

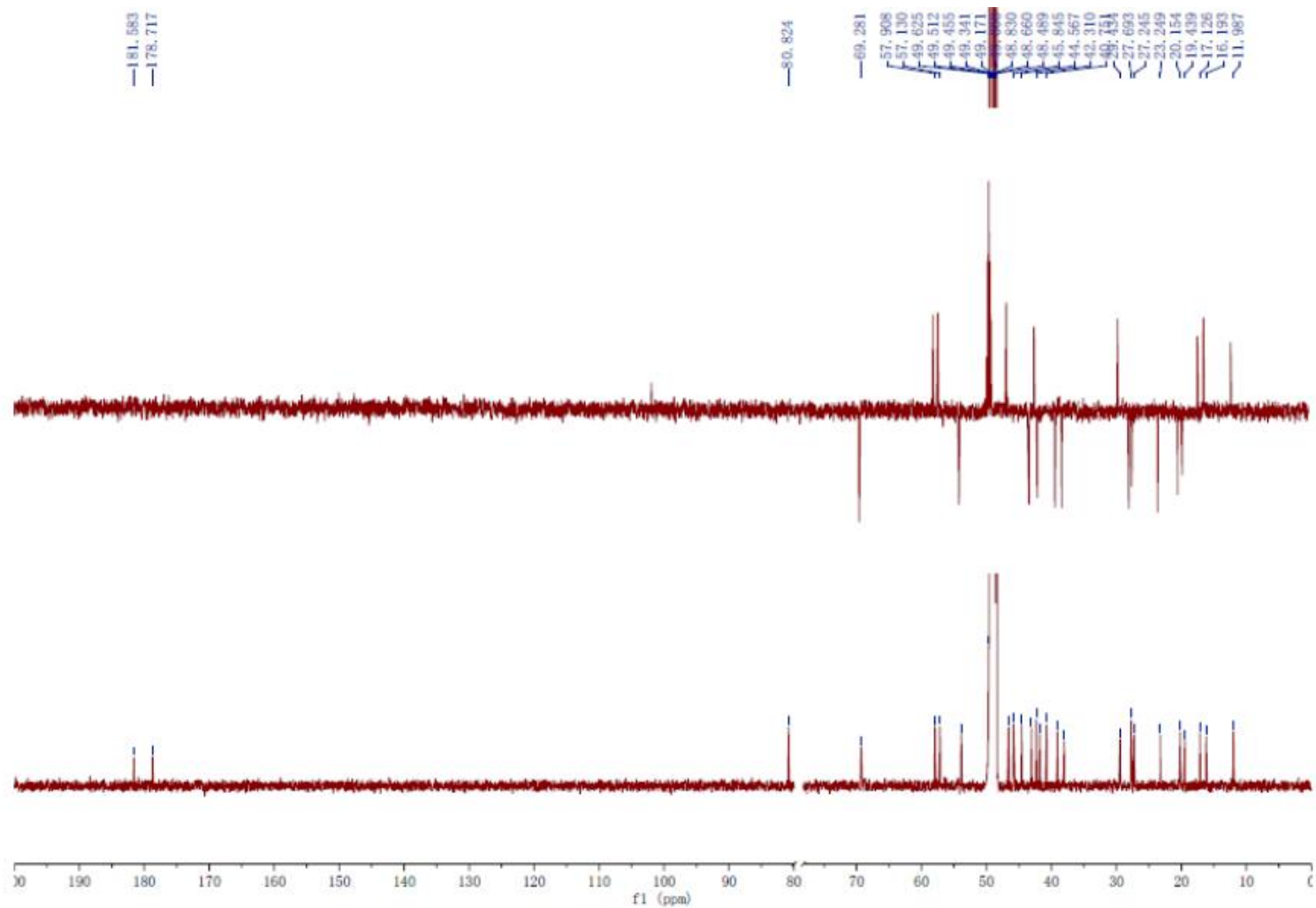
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 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-0
 Oper: WANG_J@SIMM.CAS Inlet :
 Limit: (0)
 : (429) C22.H100.O4
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
71.08597	* 26718	29.31	0.13	0.1	0.5	C5.H11
77.03971	* 38858	42.62	0.19	-0.6	4.5	C6.H5
79.05575	* 69742	76.50	0.34	-1.0	3.5	C6.H7
81.06985	* 64684	70.95	0.32	0.6	2.5	C6.H9
82.07741	* 15174	16.64	0.07	0.8	2.0	C6.H10
83.08546	* 19994	21.93	0.10	0.6	1.5	C6.H11
85.10129	* 14936	16.38	0.07	0.4	0.5	C6.H13
91.05450	* 91165	100.00	0.45	0.3	4.5	C7.H7
92.06136	* 31300	34.33	0.15	1.2	4.0	C7.H8
93.07052	* 52723	57.83	0.26	-0.1	3.5	C7.H9
95.08592	* 40822	44.78	0.20	0.2	2.5	C7.H11
97.10153	* 18744	20.56	0.09	0.2	1.5	C7.H13
105.0682	* 53973	59.20	0.26	2.2	4.5	C8.H9
106.0753	* 18030	19.78	0.09	3.0	4.0	C8.H10
107.0478	* 16305	17.89	0.08	1.9	4.5	C7.H7.O
107.0844	* 43499	47.71	0.21	1.6	3.5	C8.H11
108.0915	* 16602	18.21	0.08	2.4	3.0	C8.H12
109.0995	* 43916	48.17	0.21	2.2	2.5	C8.H13
117.0699	* 28027	30.74	0.14	0.6	5.5	C9.H9
119.0856	* 32431	35.57	0.16	0.5	4.5	C9.H11
120.0568	* 19577	21.47	0.10	0.7	5.0	C8.H8.O
121.1007	* 38679	42.43	0.19	1.0	3.5	C9.H13
123.1172	* 32788	35.97	0.16	0.2	2.5	C9.H15
129.0703	* 15174	16.64	0.07	0.1	6.5	C10.H9
130.0768	* 15828	17.36	0.08	1.4	6.0	C10.H10
131.0848	* 28325	31.07	0.14	1.2	5.5	C10.H11
133.0657	* 13805	15.14	0.07	-0.4	5.5	C9.H9.O
133.1025	* 27016	29.63	0.13	-0.8	4.5	C10.H13
143.0862	* 21541	23.63	0.11	-0.1	6.5	C11.H11
145.1027	* 27611	30.29	0.13	-1.0	5.5	C11.H13
147.1174	* 15590	17.10	0.08	0.0	4.5	C11.H15
148.0887	* 14162	15.53	0.07	0.1	5.0	C10.H12.O
149.0239	* 20173	22.13	0.10	0.0	6.5	C8.H5.O3
159.1176	* 13805	15.14	0.07	-0.2	5.5	C12.H15
162.1054	* 21660	23.76	0.11	-0.9	5.0	C11.H14.O
163.1123	* 50402	55.29	0.25	0.0	4.5	C11.H15.O
200.0657	* 38025	41.71	0.19			
224.0545	* 14817	16.25	0.07			
225.0595	* 31776	34.86	0.16			
226.0680	* 17852	19.58	0.09			
227.0753	* 25052	27.48	0.12			
237.1636	* 26659	29.24	0.13	0.8	8.5	C18.H21
255.1735	* 35704	39.16	0.17	1.4	7.5	C18.H23.O
270.1988	* 32848	36.03	0.16	-0.4	7.0	C19.H26.O
271.2075	* 23386	25.65	0.11	-1.3	6.5	C19.H27.O
283.1681	* 17852	19.58	0.09	1.7	8.5	C19.H23.O2
298.1921	* 26480	29.05	0.13	1.1	8.0	C20.H26.O2
301.1794	* 32967	36.16	0.16	0.9	7.5	C19.H25.O3
316.2029	* 73075	80.16	0.36	0.9	7.0	C20.H28.O3
317.2067	* 14936	16.38	0.07			

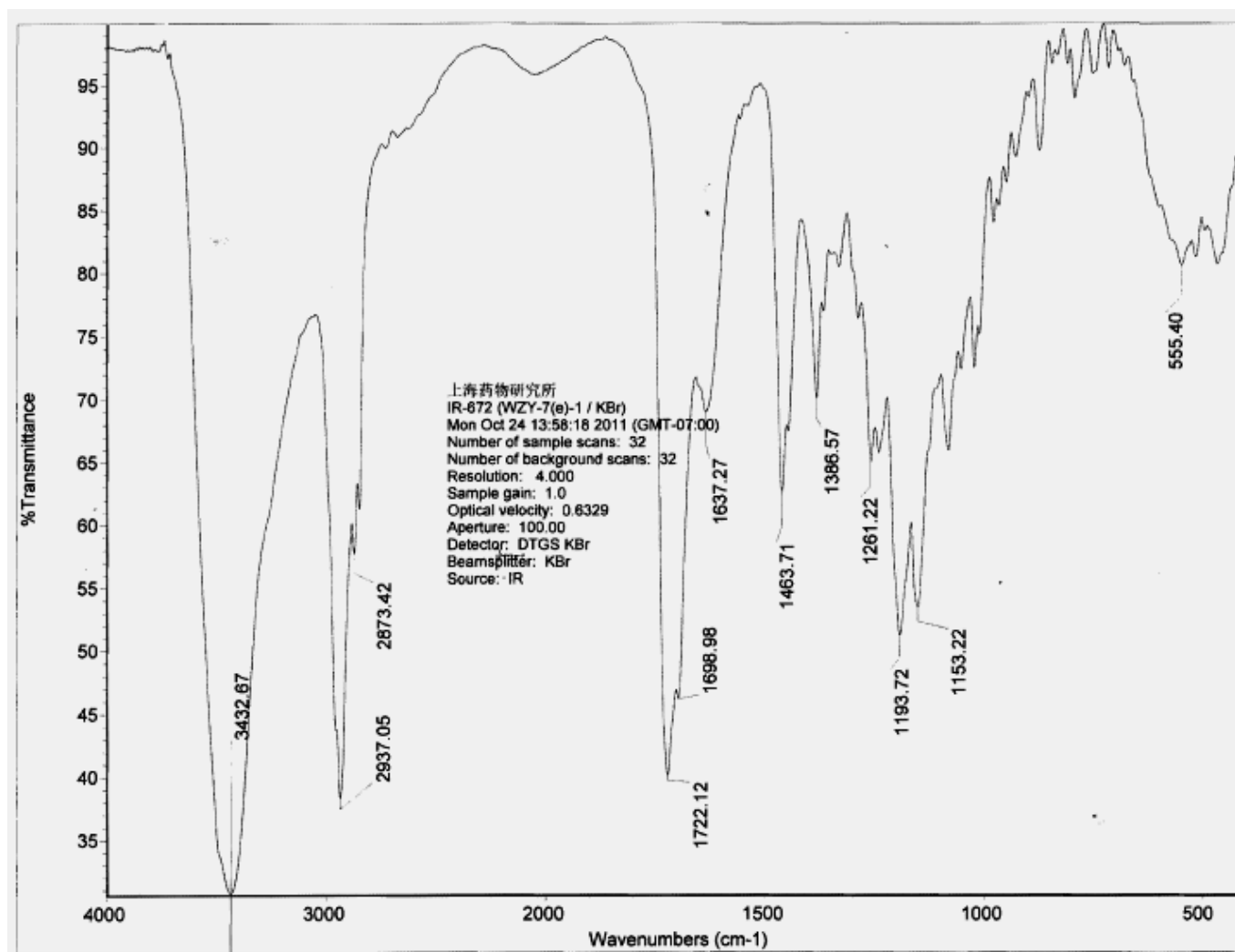
S30. HR-EI-MS data of the new compound 5



S31. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **6**



S32. ^{13}C NMR (400MHz, CD_3OD) spectrum of the new compound **6**

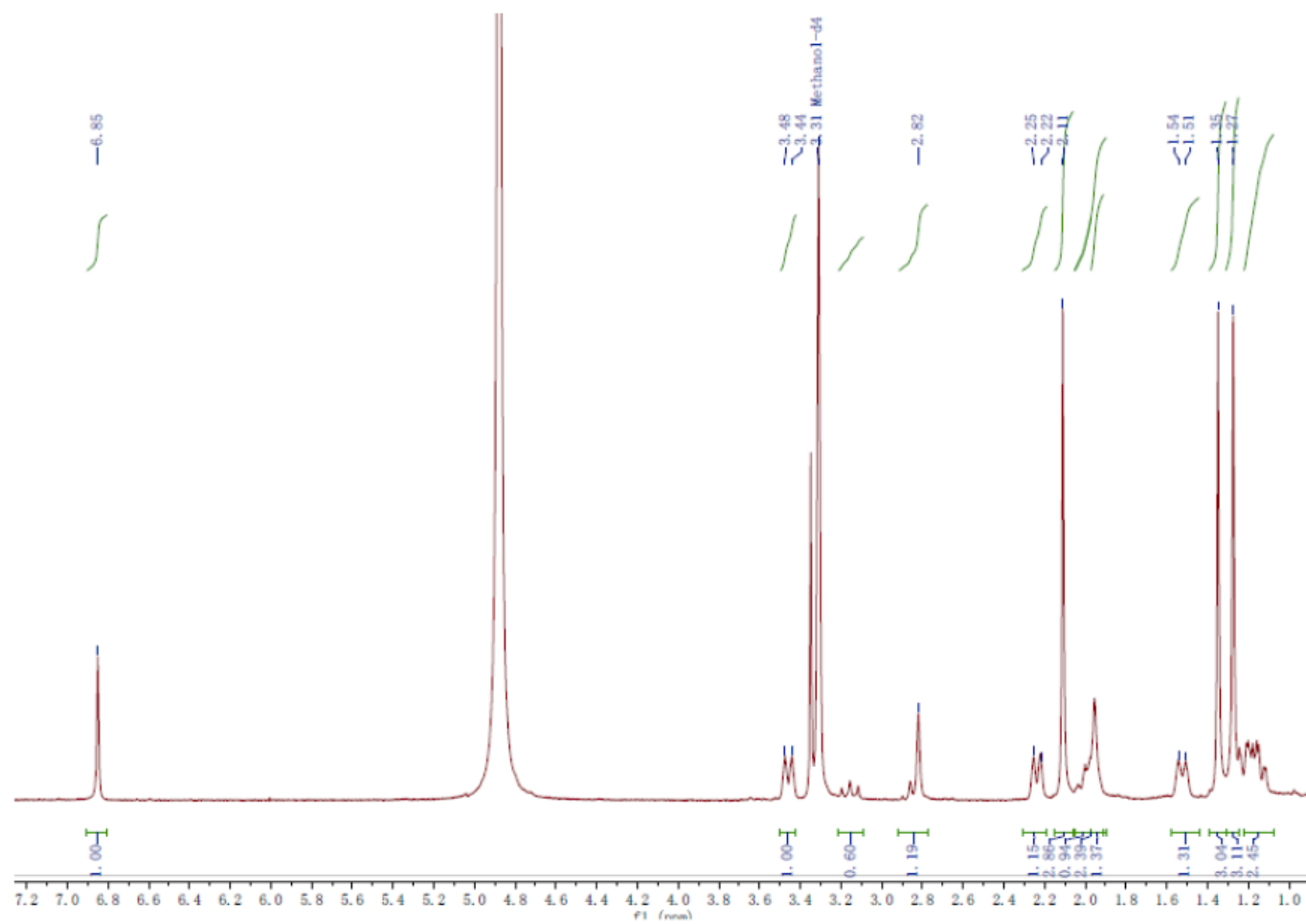


S33. IR (KBr) spectrum of the new compound **6**

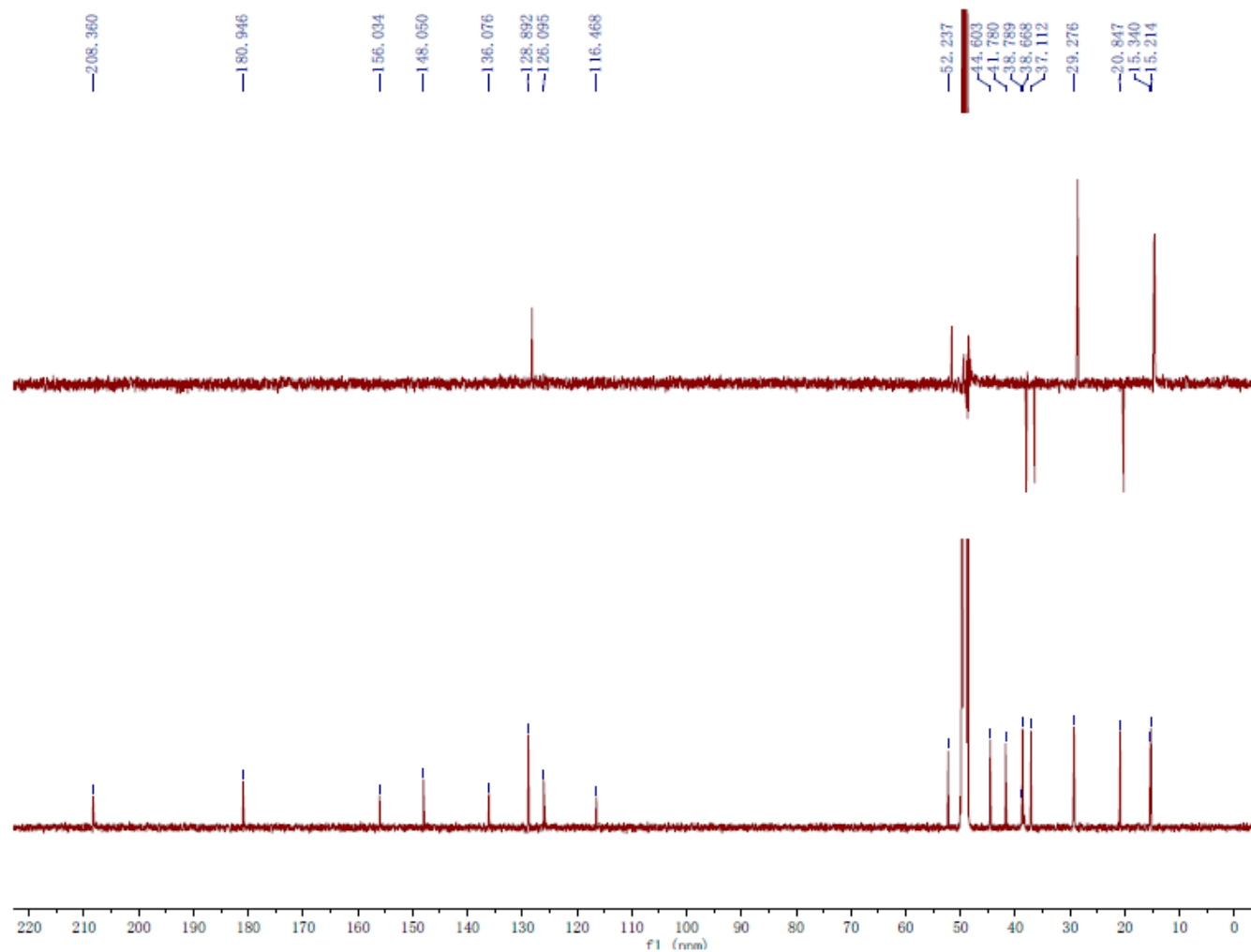
LIST: h110758-c1 28-Oct-11 Elapse: 06:39.9 32
 Samp: wzy-7(e)-1 Start : 16:08:03 41
 Comm: Finnigan/MAT95//70eV/Tsou:220c/R:10000
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-01
 Oper: WANG_J@SIMM.CAS Inlet :
 Limt: (0)
 : (493) C26.H100.O5
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
258.1630	*	30986	0.55	0.05	-1.0	7.0 C17.H22.O2
258.1973	*	27780	0.49	0.04	1.0	6.0 C18.H26.O
259.1690	*	94169	1.66	0.15	0.8	6.5 C17.H23.O2
259.2066	*	2722568	48.13	4.39	-0.4	5.5 C18.H27.O
260.1778	*	343909	6.08	0.55	-0.1	6.0 C17.H24.O2
260.2104	*	523913	9.26	0.84		
261.1851	*	324890	5.74	0.52	0.4	5.5 C17.H25.O2
261.2163	*	45802	0.81	0.07		
262.1926	*	583463	10.32	0.94	0.7	5.0 C17.H26.O2
263.1983	*	244041	4.31	0.39	2.9	4.5 C17.H27.O2
264.2039	*	41314	0.73	0.07		
267.1756	*	14175	0.25	0.02	-0.7	8.5 C19.H23.O
269.1909	*	144743	2.56	0.23	-0.4	7.5 C19.H25.O
270.1945	*	31270	0.55	0.05		
271.1681	*	38251	0.68	0.06	1.7	7.5 C18.H23.O2
271.2068	*	34333	0.61	0.06	-0.6	6.5 C19.H27.O
272.1778	*	89254	1.58	0.14	-0.1	7.0 C18.H24.O2
272.2142	*	181571	3.21	0.29	-0.2	6.0 C19.H28.O
273.1791	*	20871	0.37	0.03		
273.2212	*	138048	2.44	0.22	0.7	5.5 C19.H29.O
274.1934	*	15172	0.27	0.02	-0.1	6.0 C18.H26.O2
274.2273	*	32553	0.58	0.05	2.4	5.0 C19.H30.O
275.2024	*	15528	0.27	0.03	-1.3	5.5 C18.H27.O2
277.2173	*	14673	0.26	0.02	-0.5	4.5 C18.H29.O2
282.1992	*	95807	1.69	0.15	-0.8	8.0 C20.H26.O
283.1986	*	27424	0.48	0.04		
285.1852	*	585814	10.36	0.94	0.3	7.5 C19.H25.O2
286.1915	*	157067	2.78	0.25	1.8	7.0 C19.H26.O2
287.2010	*	1845343	32.62	2.97	0.1	6.5 C19.H27.O2
288.2042	*	359081	6.35	0.58		
289.2095	*	53994	0.95	0.09		
290.2219	*	24503	0.43	0.04	2.7	5.0 C19.H30.O2
299.2003	*	27994	0.49	0.05	0.8	7.5 C20.H27.O2
300.2090	*	1285457	22.73	2.07	-0.1	7.0 C20.H28.O2
301.2143	*	316128	5.59	0.51	2.4	6.5 C20.H29.O2
302.2187	*	48936	0.87	0.08		
303.1989	*	59478	1.05	0.10	-2.9	6.5 C19.H27.O3
304.2047	*	748294	13.23	1.21	-0.9	6.0 C19.H28.O3
305.2125	*	5656269	100.00	9.12	-0.8	5.5 C19.H29.O3
306.2167	*	1165573	20.61	1.88	2.7	5.0 C19.H30.O3
307.2194	*	130426	2.31	0.21		
308.2189	*	11183	0.20	0.02		
317.2130	*	17594	0.31	0.03	-1.3	6.5 C20.H29.O3
318.2192	*	288775	5.11	0.47	0.3	6.0 C20.H30.O3
319.2224	*	63681	1.13	0.10		
336.2332	*	11753	0.21	0.02		
341.2493	*	13534	0.24	0.02	-1.3	7.5 C23.H33.O2
343.2641	*	19375	0.34	0.03	-0.4	6.5 C23.H35.O2
356.2725	*	40816	0.72	0.07	-1.0	7.0 C24.H36.O2
357.2786	*	24503	0.43	0.04	0.8	6.5 C24.H37.O2
358.2875	*	21369	0.38	0.03	-0.3	6.0 C24.H38.O2
374.2841	*	20016	0.35	0.03	-2.0	6.0 C24.H38.O3
387.2539	*	20942	0.37	0.03	-0.3	7.5 C24.H35.O4
389.2659	*	11397	0.20	0.02		
402.2723	*	134700	2.38	0.22		
403.2761	*	41314	0.73	0.07		
420.2875	*	11183	0.20	0.02	0.1	6.0 C25.H40.O5

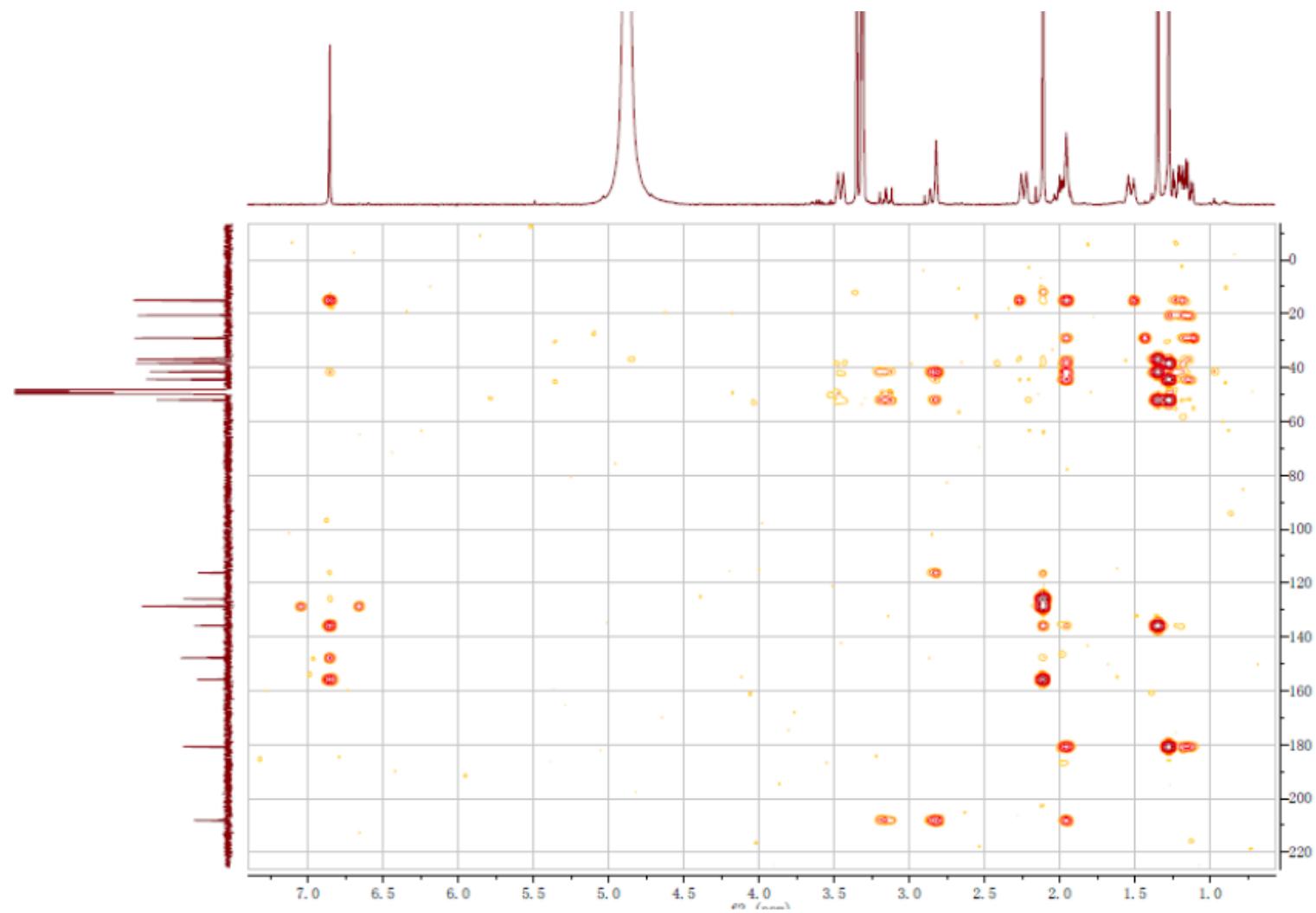
S34. HR-EI-MS data of the new compound 6

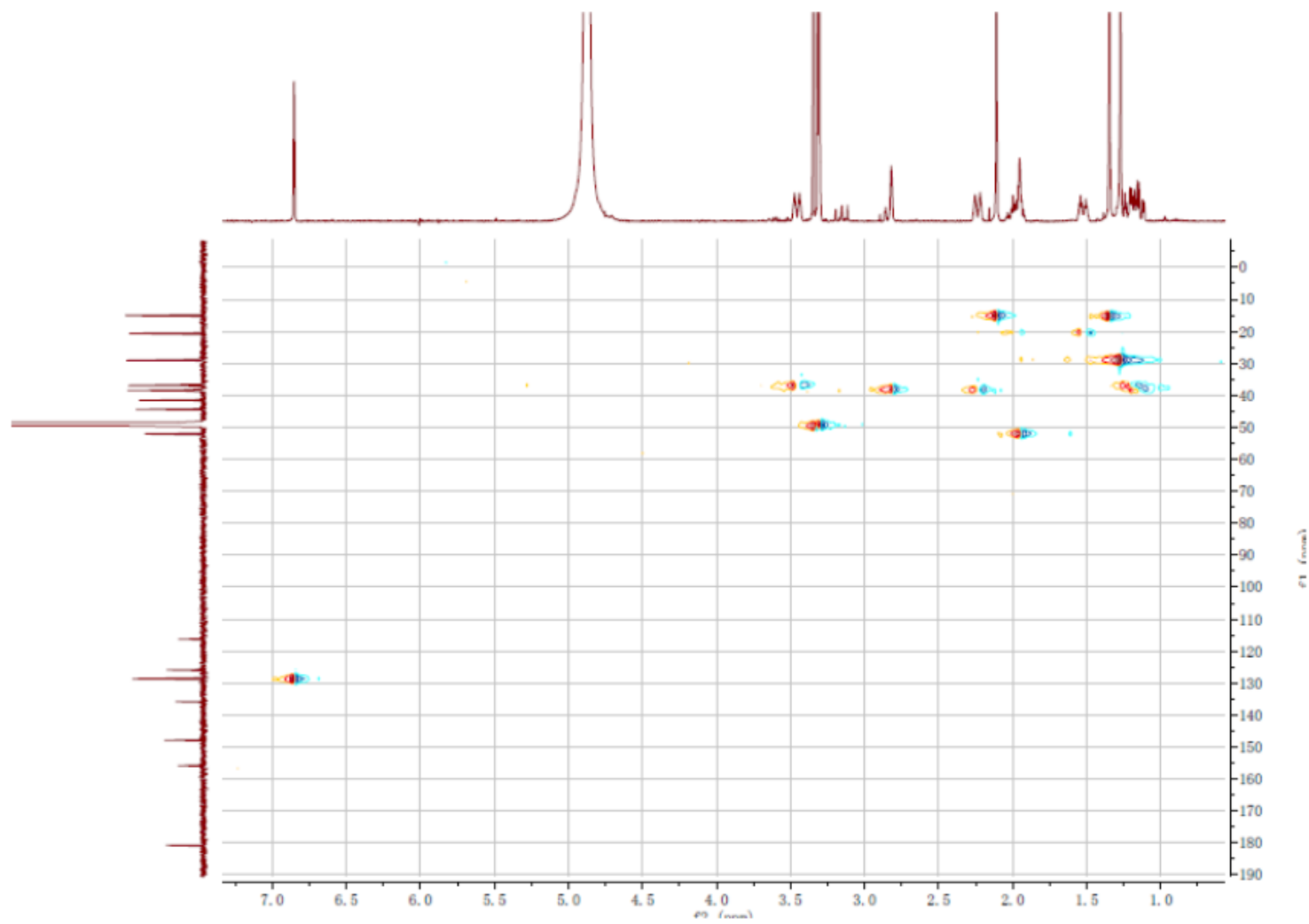


S35. ¹H NMR (400MHz, CD₃OD) spectrum of the new compound 7

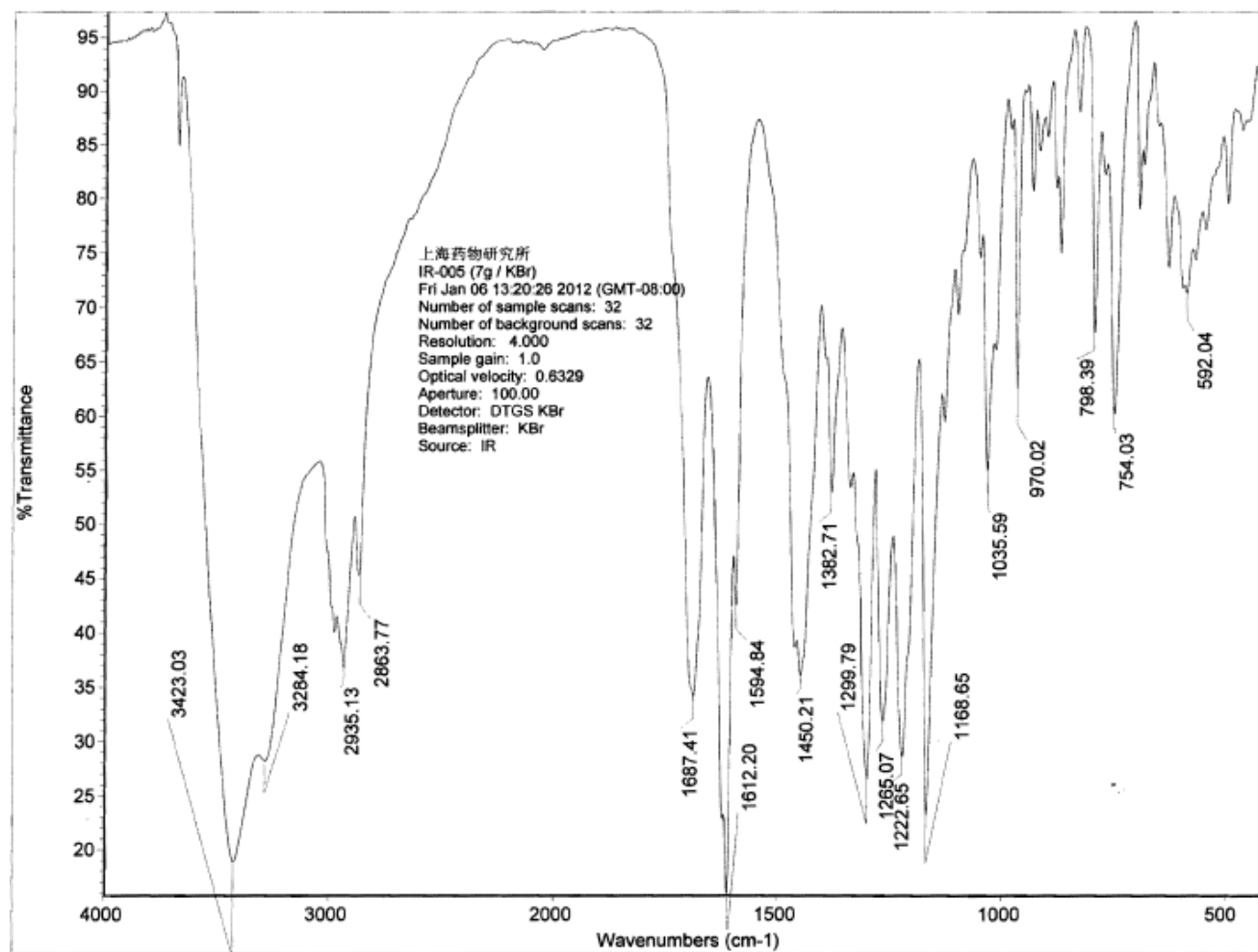


S36. ¹³C NMR (400MHz, CD₃OD) spectrum of the new compound 7





S38. HSQC (400MHz, CD_3OD) spectrum of the new compound 7

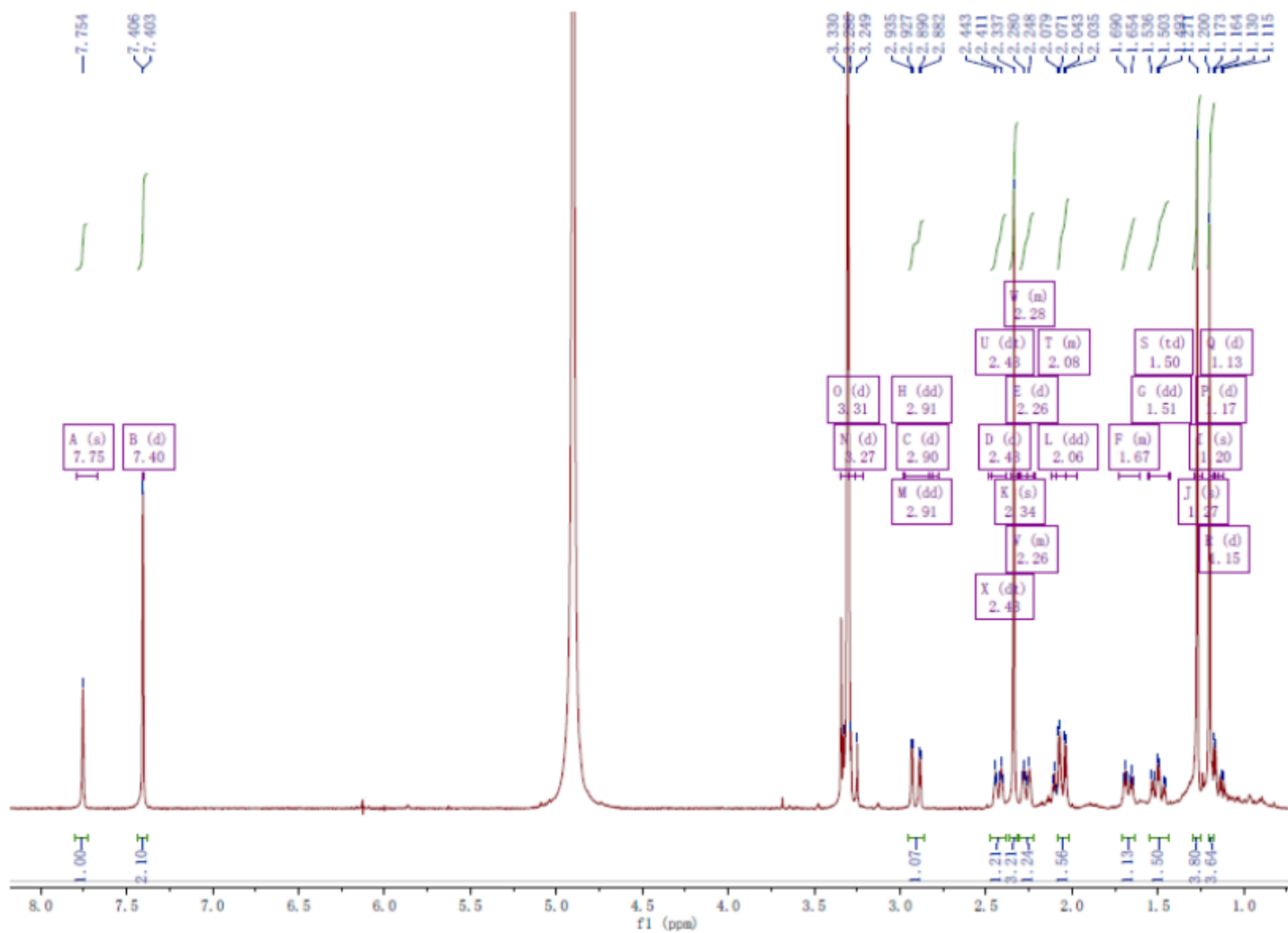


S39. IR (KBr) spectrum of the new compound 7

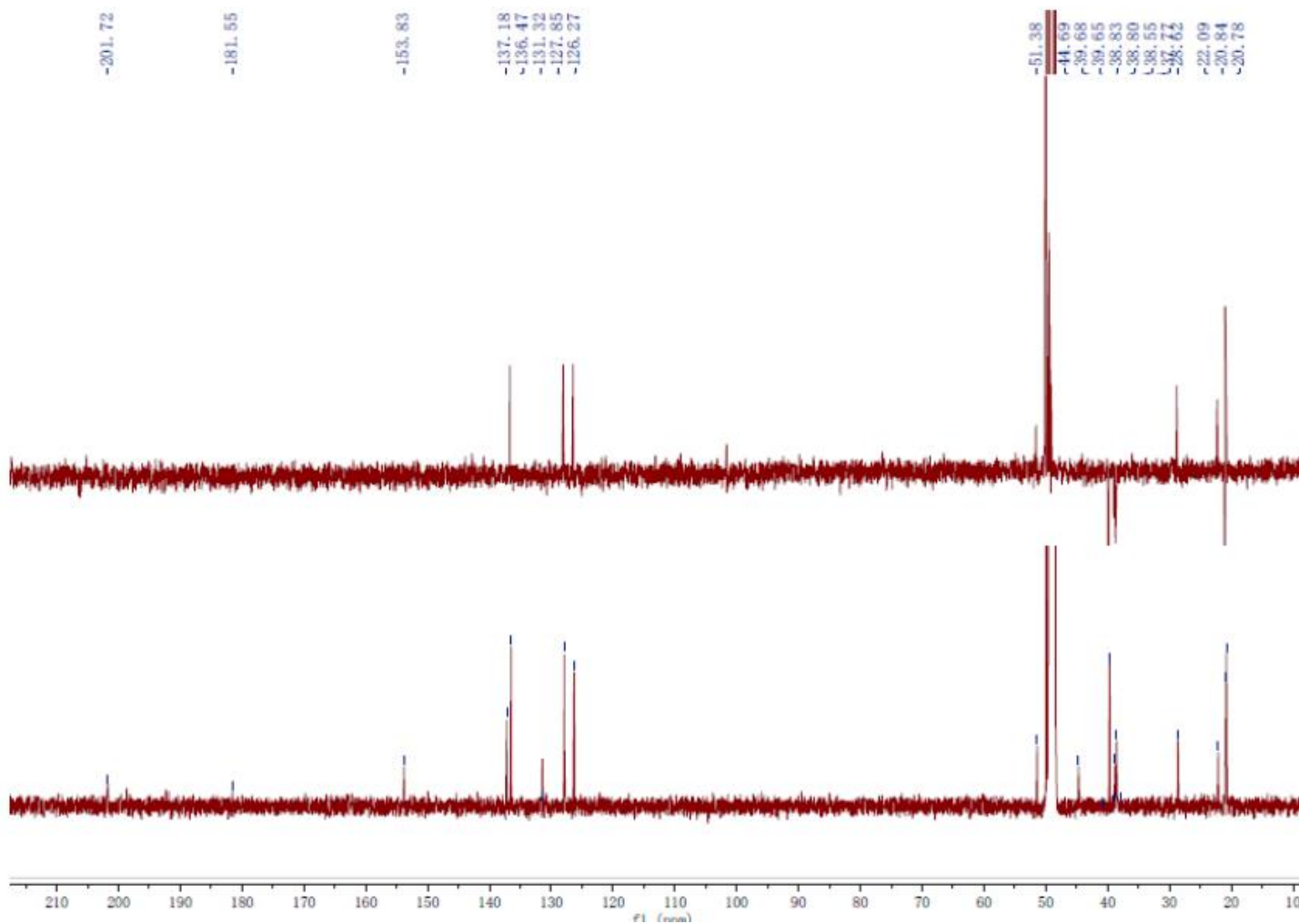
LIST: h120004-c1 09-Jan-12 Elapse: 06:01.6 29
 Samp: WZY-7(g) Start : 10:58:03 31
 Comm: Finnigan/MAT95//70eV/Tsou:220c/R:1000
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-01
 Oper: WANG_J@SIMM.CAS Inlet :
 Limt: (0)
 : (421) C20.H100.05
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
71.08657	* 103455	5.17	0.25	-0.5	0.5	C5.H11
73.02950	* 112242	5.61	0.28	-0.5	1.5	C3.H5.O2
74.06167	* 77024	3.85	0.19			
77.04044	* 107423	5.37	0.26	-1.3	4.5	C6.H5
79.05631	* 102534	5.13	0.25	-1.5	3.5	C6.H7
81.07033	* 83614	4.18	0.21	0.1	2.5	C6.H9
83.08575	* 74190	3.71	0.18	0.3	1.5	C6.H11
87.04400	* 90558	4.53	0.22	0.6	1.5	C4.H7.O2
88.07576	* 194864	9.74	0.48			
89.05966	* 81843	4.09	0.20	0.6	0.5	C4.H9.O2
91.05487	* 153695	7.69	0.38	-0.1	4.5	C7.H7
98.07350	* 87724	4.39	0.22	-0.3	2.0	C6.H10.O
105.0376	* 69159	3.46	0.17			
109.0603	* 69442	3.47	0.17			
115.0336	* 70222	3.51	0.17			
118.0827	* 85598	4.28	0.21			
161.0604	* 73481	3.67	0.18	-0.2	6.5	C10.H9.O2
165.0593	* 64057	3.20	0.16			
175.0749	* 67033	3.35	0.16	1.0	6.5	C11.H11.O2
177.0556	* 122871	6.14	0.30	-0.4	6.5	C10.H9.O3
189.0540	* 67883	3.39	0.17	1.2	7.5	C11.H9.O3
190.0620	* 73056	3.65	0.18	1.0	7.0	C11.H10.O3
191.0698	* 94810	4.74	0.23	1.0	6.5	C11.H11.O3
201.0548	* 60585	3.03	0.15	0.3	8.5	C12.H9.O3
203.0710	* 224342	11.22	0.55	-0.2	7.5	C12.H11.O3
204.0776	* 74473	3.72	0.18	1.0	7.0	C12.H12.O3
215.1071	* 190684	9.54	0.47	0.1	7.5	C14.H15.O2
217.0863	* 238727	11.94	0.59	0.2	7.5	C13.H13.O3
229.0858	* 82268	4.11	0.20	0.6	8.5	C14.H13.O3
229.1224	* 66112	3.31	0.16	0.4	7.5	C15.H17.O2
230.1293	* 72985	3.65	0.18	1.4	7.0	C15.H18.O2
239.1065	* 74544	3.73	0.18	0.7	9.5	C16.H15.O2
242.2477	* 373219	18.66	0.92			
243.1017	* 74261	3.71	0.18	0.4	8.5	C15.H15.O3
243.2528	* 64695	3.24	0.16			
245.1183	* 375770	18.79	0.92	-0.5	7.5	C15.H17.O3
255.1020	* 69017	3.45	0.17	0.1	9.5	C16.H15.O3
257.1184	* 1449935	72.50	3.56	-0.6	8.5	C16.H17.O3
258.1216	* 275857	13.79	0.68			
270.2791	* 137680	6.88	0.34			
301.1078	* 94031	4.70	0.23	-0.2	9.5	C17.H17.O5
303.1232	* 206698	10.34	0.51	0.0	8.5	C17.H19.O5
316.1304	* 406169	20.31	1.00	0.6	9.0	C18.H20.O5
317.1345	* 90700	4.54	0.22			
<u>318.1459</u>	* 1999808	100.00	4.91	<u>0.8</u>	<u>8.0</u>	<u>C18.H22.O5</u>
319.1493	* 476249	23.81	1.17			
320.1535	* 62002	3.10	0.15			

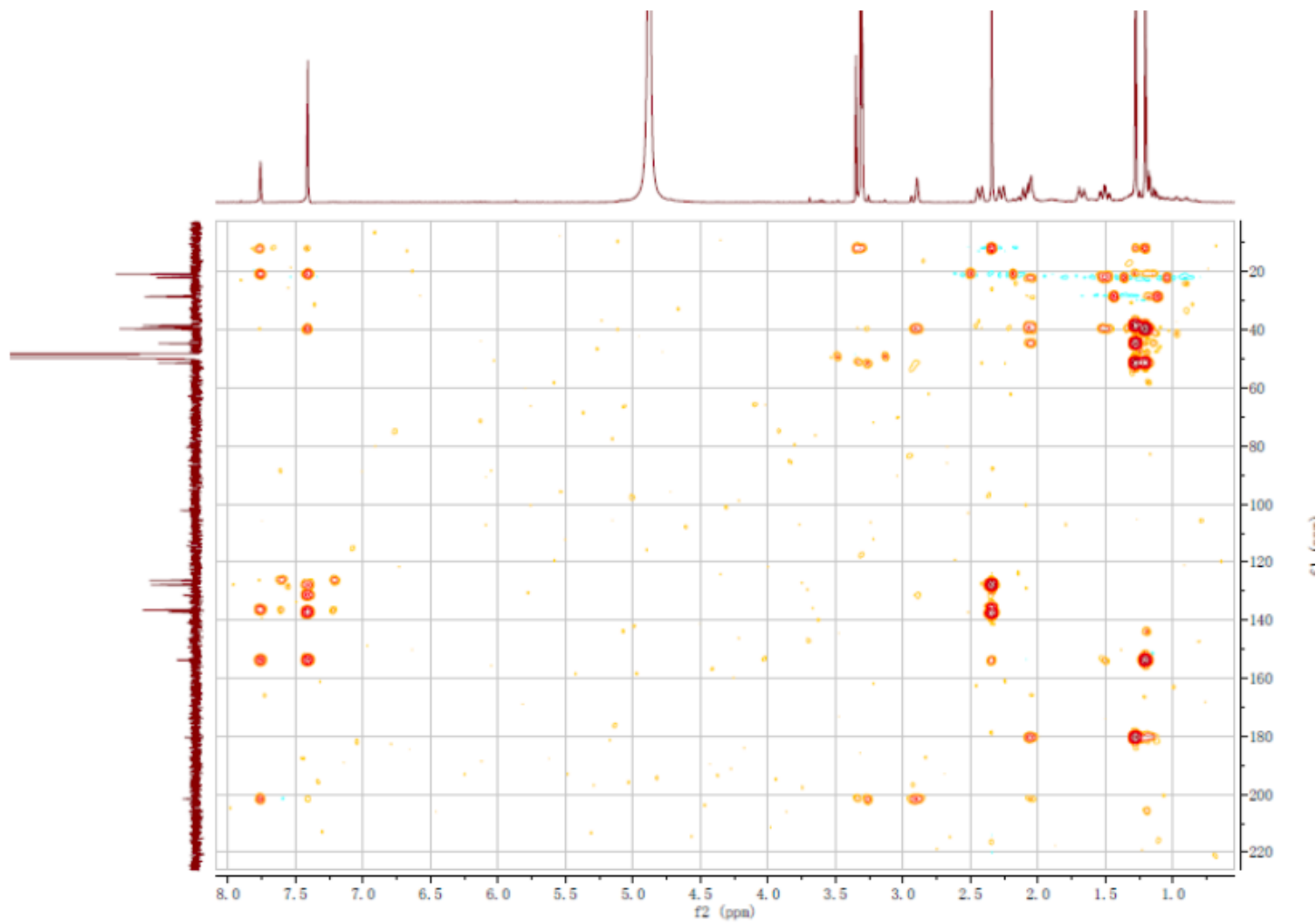
S40. HR-EI-MS data of the new compound 7



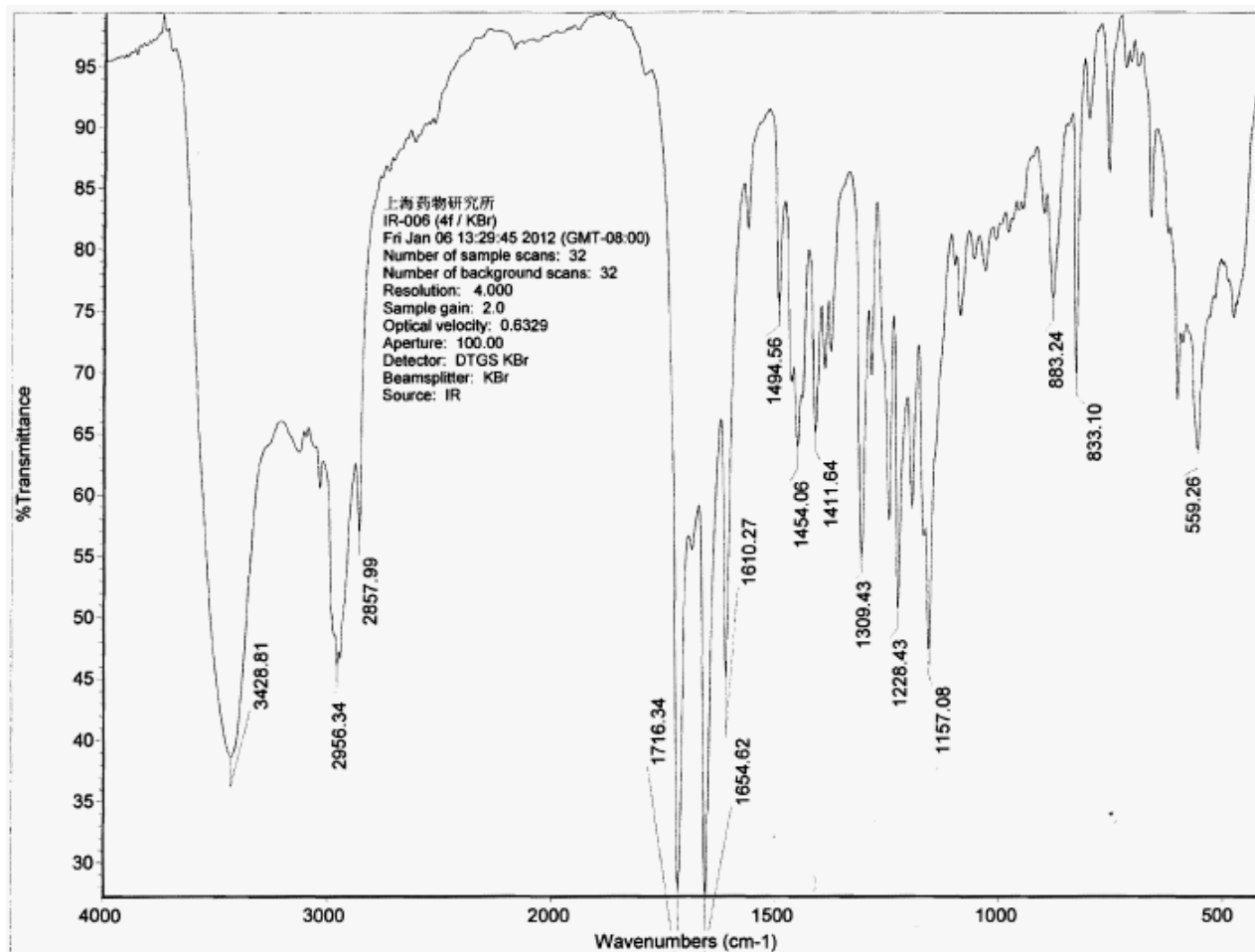
S41. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **8**



S42. ^{13}C NMR (400MHz, CD_3OD) spectrum of the new compound **8**



S43. HMBC (400MHz, CD₃OD) spectrum of the new compound **8**

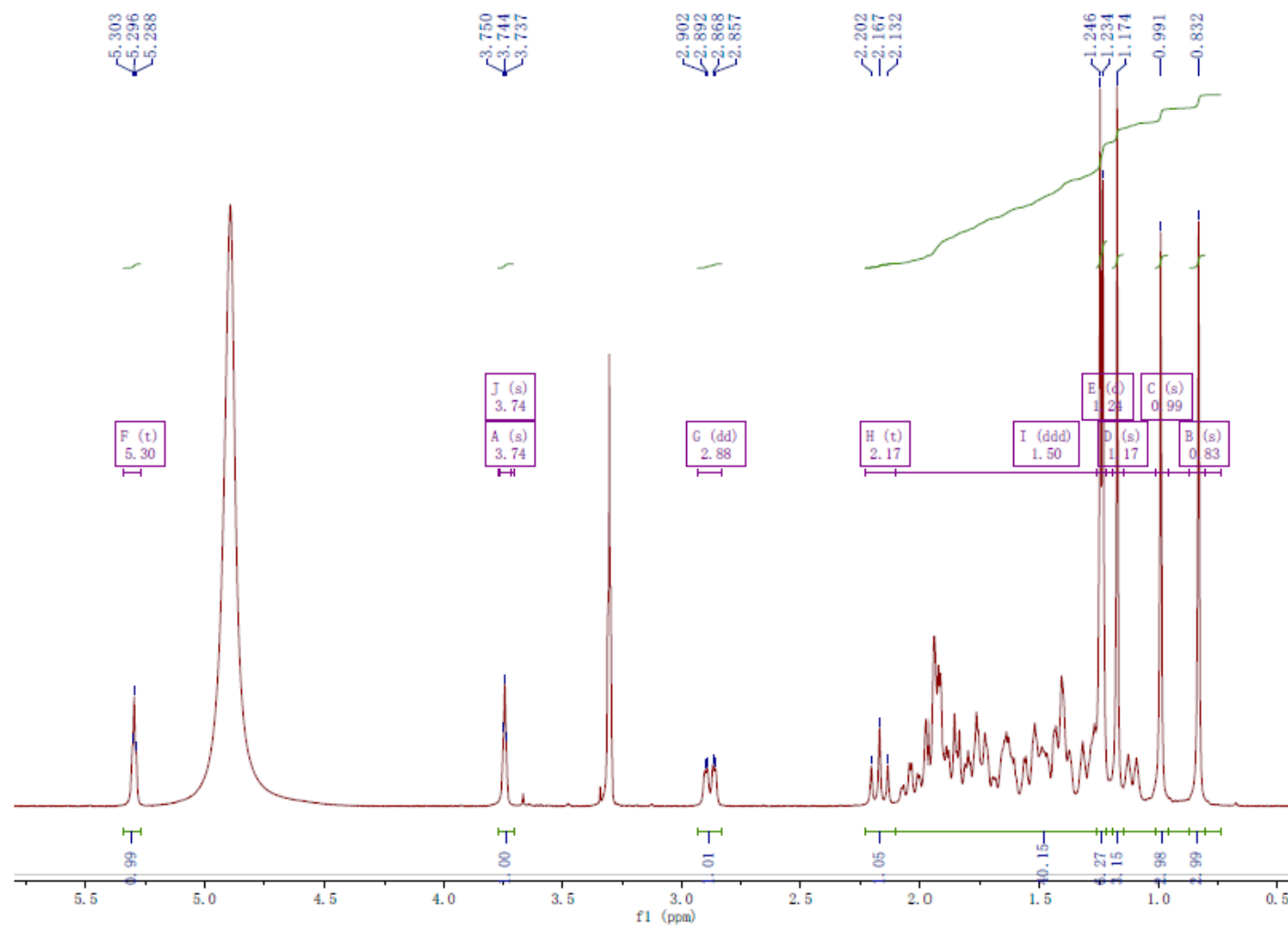


S44. IR (KBr) spectrum of the new compound **8**

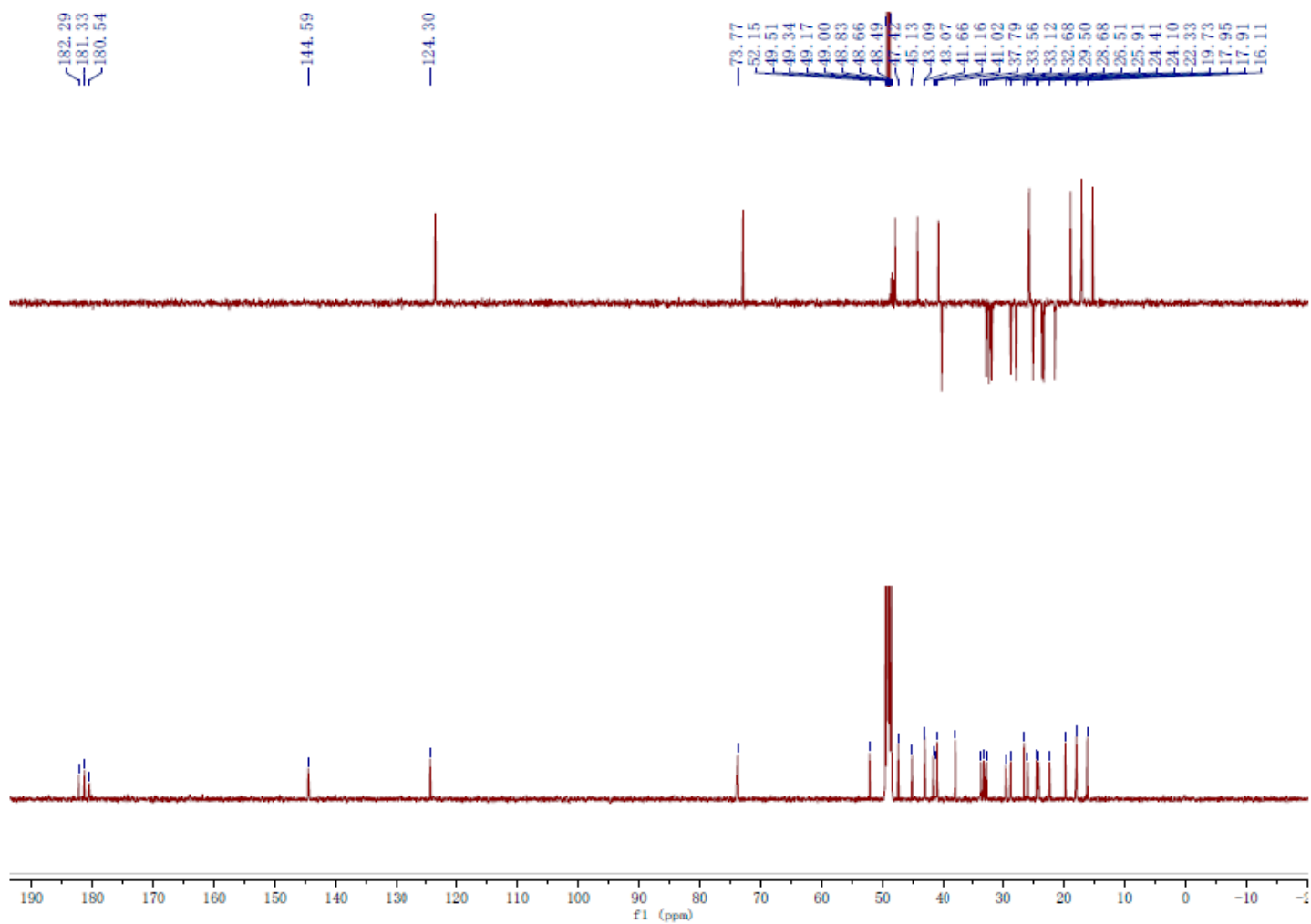
LIST: h120003-c1 09-Jan-12 Elapse: 04:08.7 19
 Samp: WZY-4(f) Start : 10:48:57 25
 Comm: Finnigan/MAT95//70eV/Tsou:220c/R:1000
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-0
 Oper: WANG_J@SIMM.CAS Inlet :
 Limit: (0)
 : (389) C20.H100.03
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
91.05427	* 135271	10.51	0.35	0.5	4.5	C7.H7
93.07025	* 49814	3.87	0.13	0.2	3.5	C7.H9
95.08591	* 38902	3.02	0.10	0.2	2.5	C7.H11
105.0742	* 92543	7.19	0.24			
107.0902	* 58530	4.55	0.15			
115.0574	* 103809	8.06	0.27	-2.6	6.5	C9.H7
116.0630	* 60089	4.67	0.15	-0.4	6.0	C9.H8
117.0712	* 51586	4.01	0.13	-0.8	5.5	C9.H9
119.0864	* 53924	4.19	0.14	-0.3	4.5	C9.H11
124.0877	* 52790	4.10	0.14	1.1	3.0	C8.H12.O
128.0621	* 120036	9.33	0.31	0.5	7.0	C10.H8
129.0693	* 150010	11.65	0.39	1.2	6.5	C10.H9
130.0762	* 56262	4.37	0.14	2.1	6.0	C10.H10
131.0851	* 49176	3.82	0.13	1.0	5.5	C10.H11
133.0657	* 48184	3.74	0.12	-0.3	5.5	C9.H9.O
141.0705	* 63703	4.95	0.16	-0.1	7.5	C11.H9
142.0781	* 78725	6.12	0.20	0.2	7.0	C11.H10
143.0851	* 84606	6.57	0.22	1.0	6.5	C11.H11
144.0929	* 45208	3.51	0.12	1.0	6.0	C11.H12
145.0655	* 62215	4.83	0.16	-0.2	6.5	C10.H9.O
145.1016	* 50097	3.89	0.13	0.2	5.5	C11.H13
146.0718	* 75040	5.83	0.19	1.4	6.0	C10.H10.O
147.0797	* 38689	3.01	0.10	1.3	5.5	C10.H11.O
149.0234	* 100621	7.82	0.26	0.4	6.5	C8.H5.O3
155.0854	* 49814	3.87	0.13	0.7	7.5	C12.H11
156.0924	* 40461	3.14	0.10	1.5	7.0	C12.H12
157.1012	* 49247	3.83	0.13	0.5	6.5	C12.H13
159.0792	* 97361	7.56	0.25	1.8	6.5	C11.H11.O
160.0866	* 41949	3.26	0.11	2.2	6.0	C11.H12.O
171.0760	* 124004	9.63	0.32			
172.0876	* 178779	13.89	0.46	1.2	7.0	C12.H12.O
173.0599	* 65120	5.06	0.17	0.4	7.5	C11.H9.O2
173.0948	* 98424	7.65	0.25	1.8	6.5	C12.H13.O
174.1026	* 59380	4.61	0.15	1.8	6.0	C12.H14.O
183.1164	* 45988	3.57	0.12	1.0	7.5	C14.H15
185.0962	* 294281	22.86	0.76	0.5	7.5	C13.H13.O
186.1027	* 234475	18.22	0.60	1.8	7.0	C13.H14.O
187.1081	* 45562	3.54	0.12			
191.0717	* 57042	4.43	0.15	-0.9	6.5	C11.H11.O3
197.0951	* 41027	3.19	0.11	1.6	8.5	C14.H13.O
199.1478	* 119398	9.28	0.31	0.9	6.5	C15.H19
200.1193	* 42941	3.34	0.11	0.8	7.0	C14.H16.O
201.1260	* 60089	4.67	0.15	2.0	6.5	C14.H17.O
225.1271	* 1138152	88.42	2.93	0.8	8.5	C16.H17.O
226.1330	* 1287241	100.00	3.31	2.8	8.0	C16.H18.O
227.1379	* 239719	18.62	0.62			
228.1457	* 42161	3.28	0.11			
244.1468	* 59947	4.66	0.15	-0.5	7.0	C16.H20.O2
244.1838	* 58884	4.57	0.15	-1.1	6.0	C17.H24.O
248.1414	* 51940	4.03	0.13	-0.2	6.0	C15.H20.O3
271.1352	* 224838	17.47	0.58	-1.7	8.5	C17.H19.O3
272.1402	* 472848	36.73	1.22	1.0	8.0	C17.H20.O3
273.1446	* 83331	6.47	0.21			
286.1571	* 355787	27.64	0.92	-0.2	8.0	C18.H22.O3
286.1943	81914	6.36	0.21	-1.0	7.0	C19.H26.O2
287.1639	* 673310	52.31	1.73	0.9	7.5	C18.H23.O3
288.1678	* 135625	10.54	0.35			

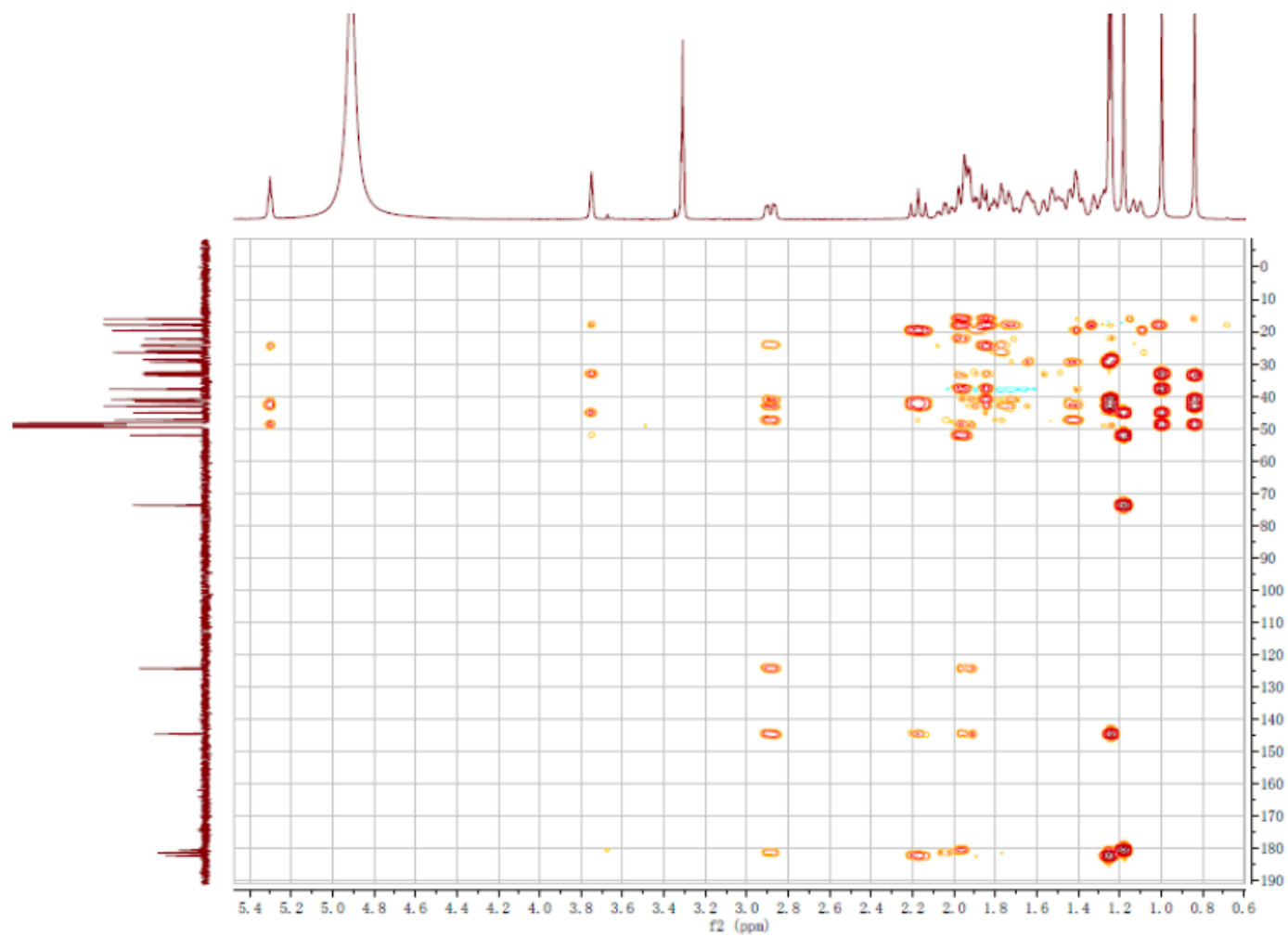
S45. HR-EI-MS data of the new compound 8



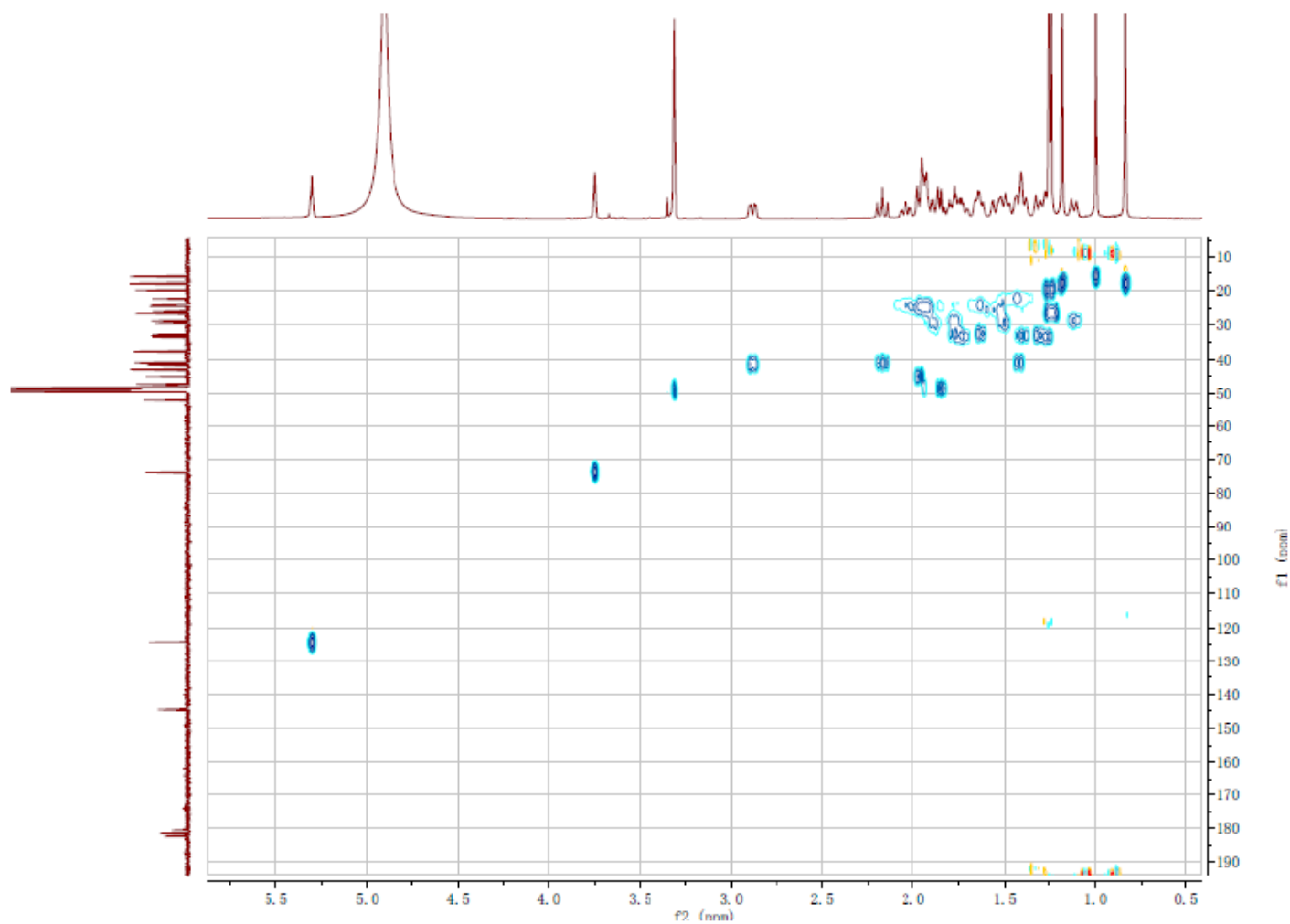
S46. ^1H NMR (400MHz, CD_3OD) spectrum of the new compound **9**



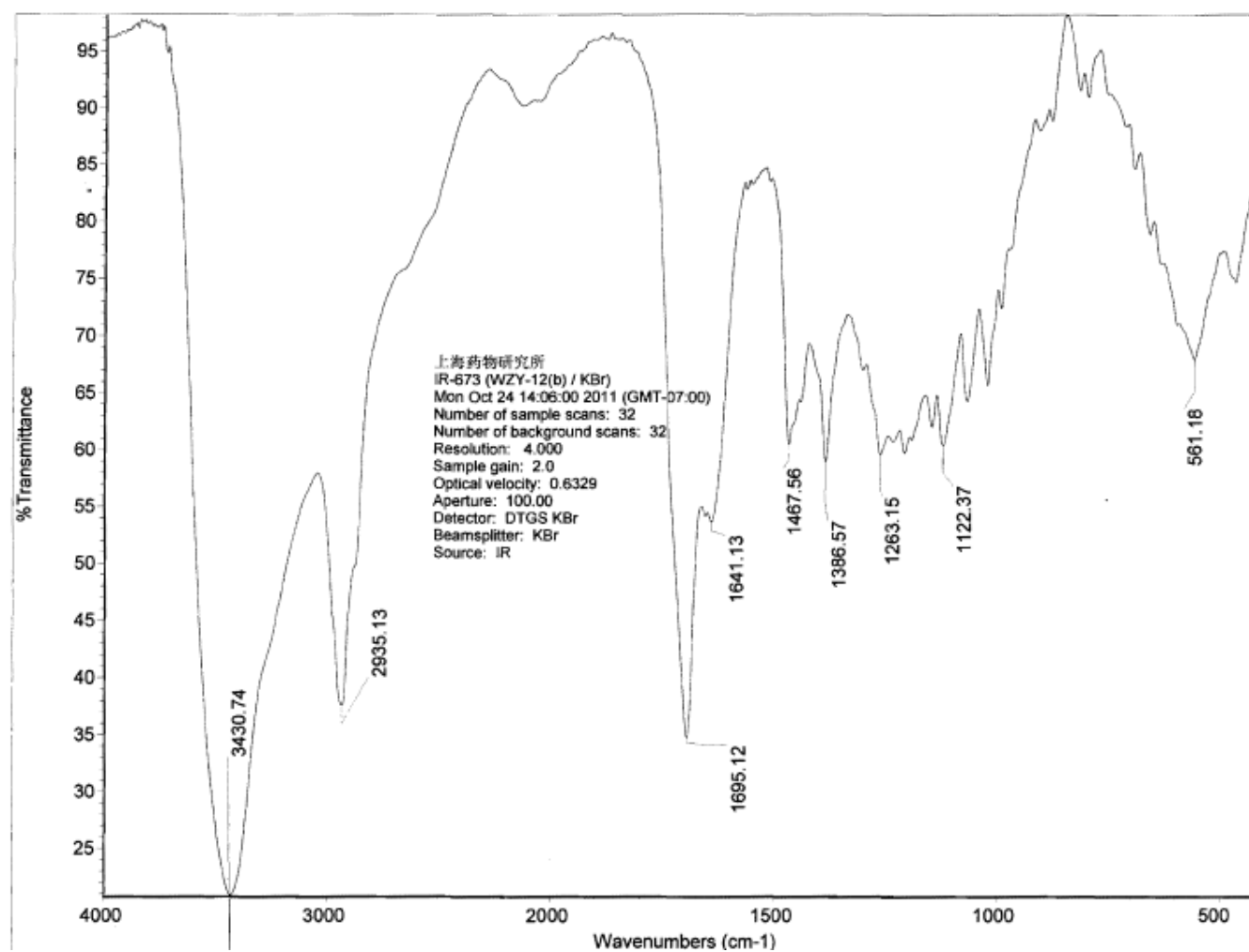
S47. ¹³C NMR (400MHz, CD₃OD) spectrum of the new compound **9**



S48. HMBC (400MHz, CD_3OD) spectrum of the new compound **9**



S49. HSQC (400MHz, CD_3OD) spectrum of the new compound **9**

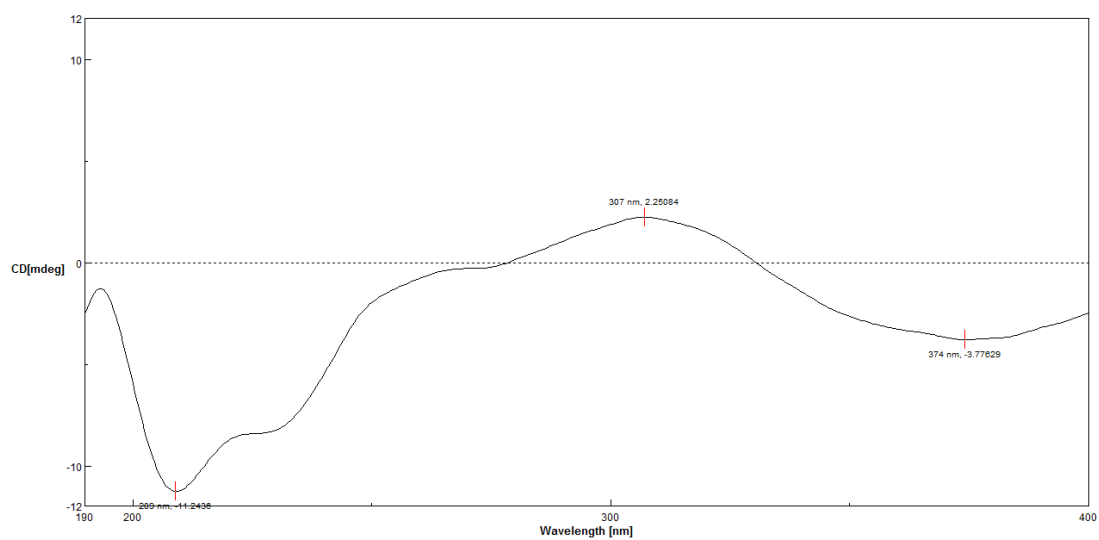


S50. IR (KBr) spectrum of the new compound 9

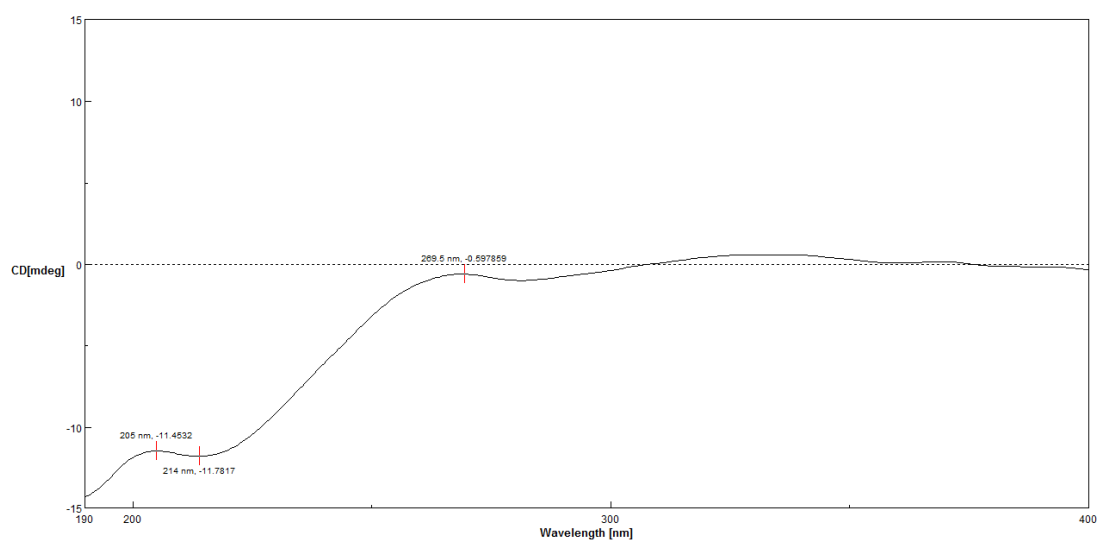
LIST: h1107031-c3 14-Oct-11 Elapse: 04:43.8 22
 Samp: wzy-12(b) Start : 17:13:17 37
 Comm: Finnigan/MAT95//70eV/Tsou:220c/R:10000
 Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-01
 Oper: WANG_J@SIMM.CAS Inlet :
 Limt: (0)
 : (585) C31.H100.07
 Peak: 1000.00 mmu R+D: -2.0 > 60.0
 Data: CMASS : converted

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
402.9795	* 5732	0.36	0.01			
405.9771	* 14124	0.90	0.04			
406.2784	* 6205	0.39	0.02			
407.2859	* 8391	0.53	0.02			
408.3028	* 20979	1.33	0.05	0.1	9.0	C28.H40.02
408.9740	* 7741	0.49	0.02	3.3	26.5	C26.H.06
409.2642	* 7505	0.48	0.02			
409.3094	* 21629	1.38	0.06	1.2	8.5	C28.H41.02
410.3135	* 6914	0.44	0.02	5.0	8.0	C28.H42.02
411.9848	* 4668	0.30	0.01			
417.9850	* 5614	0.36	0.01			
420.9698	* 9573	0.61	0.02			
421.9792	* 4195	0.27	0.01			
422.2931	* 4905	0.31	0.01			
423.2884	* 5200	0.33	0.01	1.5	9.5	C28.H39.03
423.9769	* 7387	0.47	0.02	2.7	31.0	C30.04
424.3030	* 13769	0.88	0.04			
425.3047	* 3959	0.25	0.01	0.9	8.5	C28.H41.03
426.3100	* 18615	1.18	0.05	3.4	8.0	C28.H42.03
428.3329	* 7268	0.46	0.02	-3.9	7.0	C28.H44.03
429.0953	* 8628	0.55	0.02	2.1	17.5	C25.H17.07
436.2597	* 3959	0.25	0.01	1.6	11.0	C28.H36.04
437.2665	* 10046	0.64	0.03	2.7	10.5	C28.H37.04
438.2688	* 3486	0.22	0.01			
439.2836	* 27125	1.73	0.07	1.2	9.5	C28.H39.04
440.2926	* 5318	0.34	0.01	0.1	9.0	C28.H40.04
443.9814	* 13119	0.83	0.03			
447.9680	* 5614	0.36	0.01	-3.6	29.0	C28.07
451.2736	* 3663	0.23	0.01	-4.0	6.5	C25.H39.07
452.2950	* 19088	1.21	0.05	-2.4	10.0	C29.H40.04
452.9719	* 5141	0.33	0.01			
453.3059	* 5200	0.33	0.01			
454.3063	* 39358	2.50	0.10	2.0	9.0	C29.H42.04
455.2827	* 6736	0.43	0.02	-3.0	9.5	C28.H39.05
455.3172	* 12883	0.82	0.03	-1.0	8.5	C29.H43.04
458.9633	* 7800	0.50	0.02			
459.9721	* 8805	0.56	0.02			
461.9687	* 4727	0.30	0.01			
465.2710	* 4314	0.27	0.01			
466.2839	* 3604	0.23	0.01			
468.2811	* 4136	0.26	0.01			
468.9581	* 4018	0.26	0.01			
470.3029	* 11169	0.71	0.03	0.3	9.0	C29.H42.05
470.9670	* 8450	0.54	0.02			
471.3062	* 5082	0.32	0.01	4.9	8.5	C29.H43.05
471.9756	* 3900	0.25	0.01			
473.9693	* 5318	0.34	0.01			
479.9706	* 3368	0.21	0.01			
482.3103	* 5495	0.35	0.01			
482.9671	* 4727	0.30	0.01			
483.3138	* 3486	0.22	0.01	-2.7	9.5	C30.H43.05
490.9878	* 4018	0.26	0.01			
498.2993	* 3368	0.21	0.01	-1.1	10.0	C30.H42.06
502.9700	* 5377	0.34	0.01			
508.9633	* 4254	0.27	0.01			
509.9691	* 5200	0.33	0.01			
516.3119	* 5850	0.37	0.02	-3.2	9.0	C30.H44.07

S51. HR-EI-MS data of the new compound 9



S52.CD spectrum of compound **7** in methanol



S53.CD spectrum of compound **7** in methanol

上海市血液管理办公室()

关于同意上海药物研究所 申请科研用血的函

上海市血液中心:

上海药物研究所因科研需要, 13 年度申请单核细胞 1 单位。
请贵中心在确保医疗临床用血前提下, 协调供应。具体由你们和
该单位商定协议, 按相关程序办理, 协议签定后生效执行, 并报
我办备案。

特此函告。



抄送: 上海药物研究所

Agreement on the Application of Using Blood for Science Research of Shanghai Institute of Materia Medica


To Shanghai Blood Center:

Shanghai Institute of Materia Medica applicates for 1 units of monocytes for science research in 2013. Please coordinate the blood supply on the premise of meeting the clinical use firstly. Detail processes can be discussed between your center and this institute according to the regulation. The agreement will be implemented after both signed and please inform us to keep the record.

Shanghai Blood Management Office

05/05/2013

Cc to: Shanghai Institute of Materia Medica



再次感谢您的爱心和奉献，谢谢您的合作！

献血者声明

我已知晓献血者的权利和义务，本人自愿献血并同意采供血机构将所献血液用于临床救治。为了用血者的安全，同意采供血机构按照国家《献血者健康检查标准》对我的血样进行检验和部分血样可能被匿名用于安全输血的相关研究，检验结果储存于献血档案中。本人理解献血液体和检验结果只是安全输血的需要，不能用于保险、疾病的诊断或其它目的。

本人对上述“征询表”中所提供信息的真实性负责，愿意承担由于信息虚假所造成一切后果。特此声明。

献血者签名：张静娴

日期：2013年4月21日

Blood Donors Statement

I have been aware of the rights and obligations of donors. I volunteer to donate blood and authorize the center to use the blood for clinical treatments. I agree with the blood center to check my blood in accordance with the prescriptive “donors health-check standards” and the result should be recorded in the blood donation records detaily. I understand that the physical examination and blood inspection is the just for the safety of blood transfusion , not for insurance, the disease diagnosis or other purposes. I am responsible for the information provided in “consultation table” above, willing to bear any consequences caused by any false information.

Jing-xian Zhang

S55. Blood donor statement of healthy donator