Supplementary Materials

Contents

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

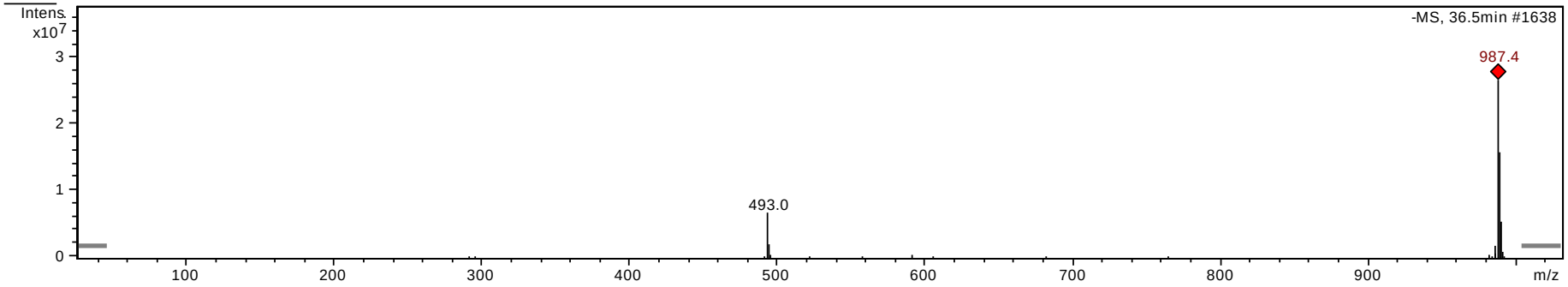
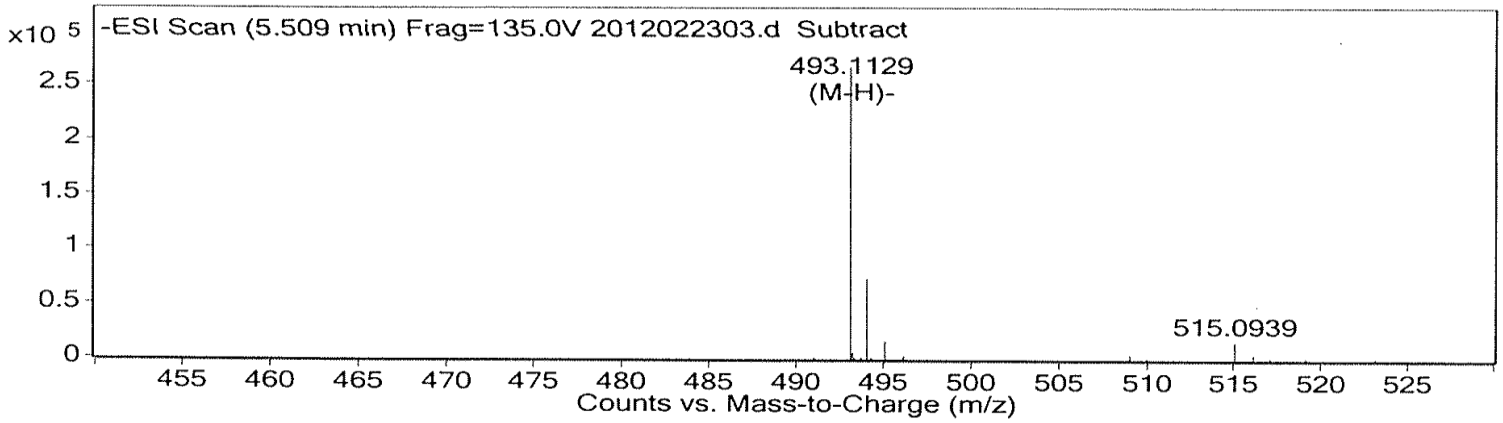


Figure S2. HR ESI-MS spectrum of compound **1**.



MS Formula Results: - Scan (5.509 min) Sub (2012022303.d)

m/z	Ion	Formula	Abundance
493.1129	(M-H)-	C26 H21 O10	265700.4

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
☑	C26 H22 O10	C26 H21 O10	493.114	99.89		494.1202	494.1213	2.23	2.23	99.92	99.95	99.83	493.1129	16
☐	C27 H18 N4 O6	C27 H17 N4 O6	493.1154	99.34		494.1202	494.1226	4.93	4.93	99.07	99.99	99.17	493.1129	21
☐	C21 H22 N2 O12	C21 H21 N2 O12	493.11	99.11		494.1202	494.1173	-5.92	5.92	98.9	99.97	98.8	493.1129	12
☐	C30 H22 O5 S	C30 H21 O5 S	493.1115	98.71		494.1202	494.1188	-2.84	2.84	96.2	99.72	99.72	493.1129	20
☐	C31 H18 N4 O S	C31 H17 N4 O S	493.1129	98.43		494.1202	494.1201	-0.14	0.14	94.75	99.72	100	493.1129	25
☐	C18 H26 N2 O12 S	C18 H25 N2 O12 S	493.1134	98.14		494.1202	494.1206	0.9	0.9	93.94	99.52	99.97	493.1129	7
☐	C23 H26 O10 S	C23 H25 O10 S	493.1174	97.82		494.1202	494.1247	9.05	9.05	97.34	99.6	97.23	493.1129	11
☐	C27 H26 O5 S2	C27 H25 O5 S2	493.1149	97.36		494.1202	494.1222	3.98	3.98	92.22	99.36	99.46	493.1129	15
☐	C22 H26 N2 O7 S2	C22 H25 N2 O7 S2	493.1109	97.21		494.1202	494.1181	-4.17	4.17	91.87	99.24	99.4	493.1129	11
☐	C33 H18 O5	C33 H17 O5	493.1081	97.14		494.1202	494.1154	-9.65	9.65	95.28	99.95	96.85	493.1129	25
☐	C34 H14 N4 O	C34 H13 N4 O	493.1095	97.06		494.1202	494.1168	-6.96	6.96	92.46	99.98	98.35	493.1129	30
☐	C28 H22 N4 O S2	C28 H21 N4 O S2	493.1162	96.91		494.1202	494.1235	6.67	6.67	92.24	99.35	98.48	493.1129	20
☐	C14 H26 N2 O17	C14 H25 N2 O17	493.1159	96.22		494.1202	494.1231	5.97	5.97	88.81	99.96	98.78	493.1129	3
☐	C34 H22 S2	C34 H21 S2	493.109	95.54		494.1202	494.1163	-7.91	7.91	88.33	99.5	97.87	493.1129	24
☐	C13 H26 N4 O14 S	C13 H25 N4 O14 S	493.1093	95.17		494.1202	494.1166	-7.26	7.26	86.55	99.44	98.21	493.1129	3

Figure S3. UV spectrum of compound **1**.

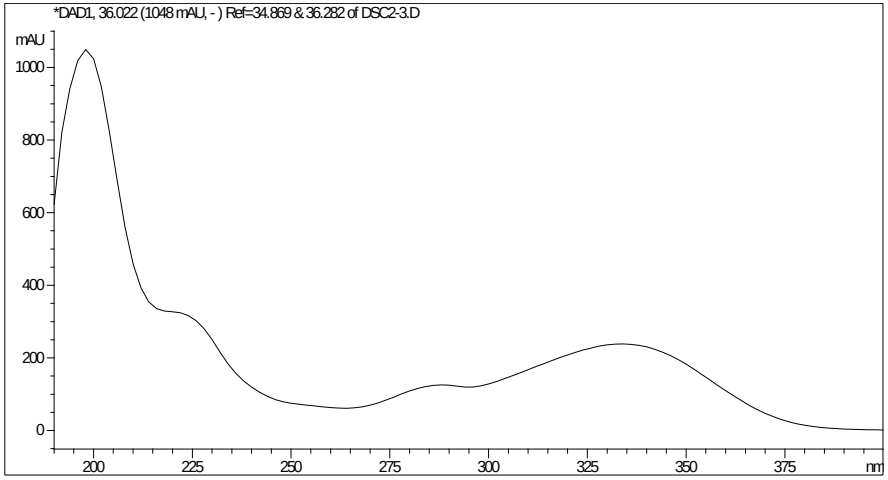
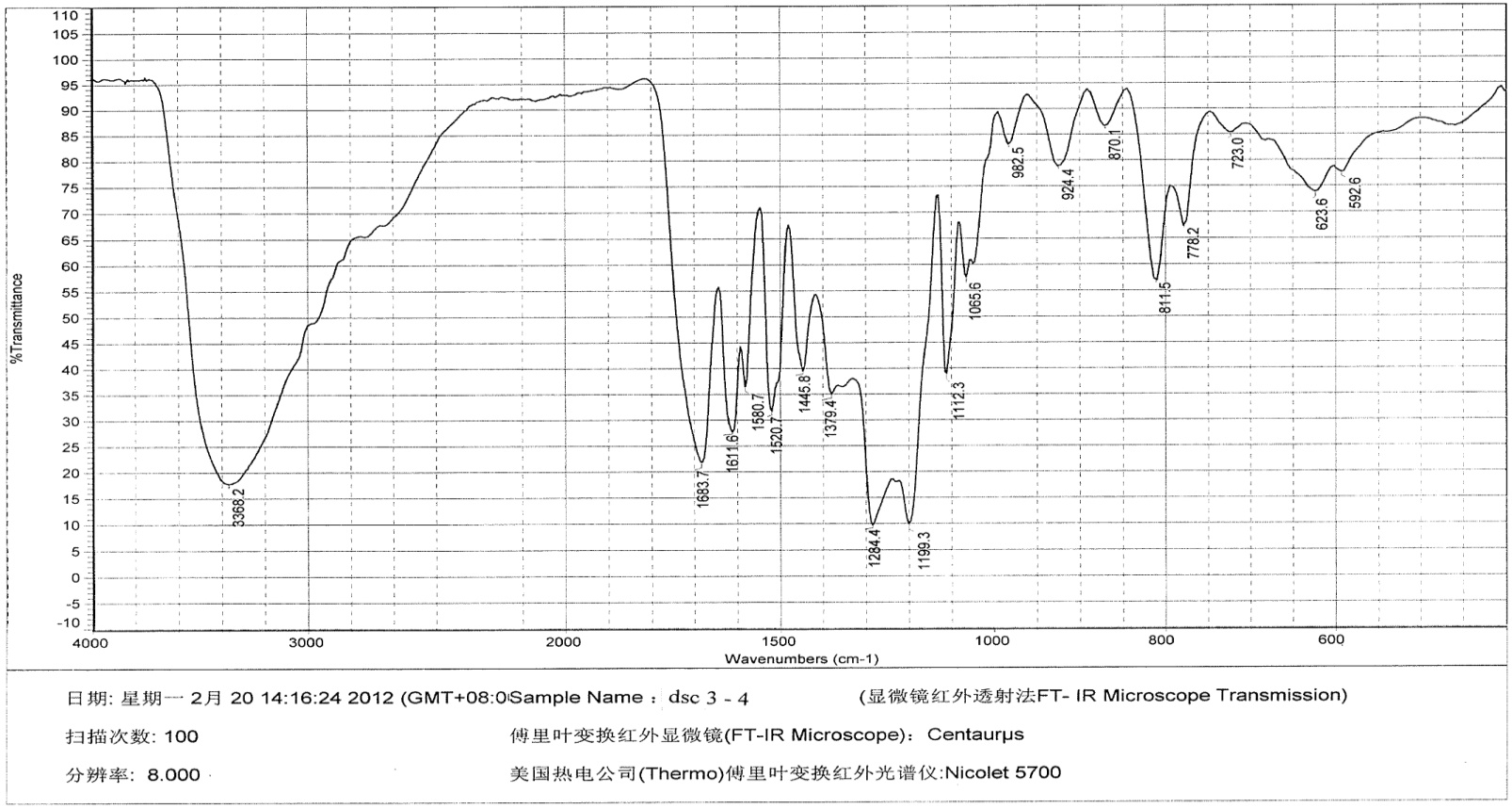


Figure S4. IR spectrum of compound **1**.



Date: Monday, Feb 20th, 14:16:24 2012 (GMT+08:0Sample Name: dsc 3-4) (Microscopy infrared transmission method FT-IR Microscope Transmission)
Numbers of scan: 100 Fourier transform infrared spectroscopy (FT-IR Microscope): Centaurus
Resolution ratio: 8,000 America Thermo Electron Corporation (Thermo) Fourier transform infrared spectrometer: Nicolet 5700.

Figure S5. ^{1}H NMR spectrum (acetone-d_6, 500 MHz) of compound **1**.

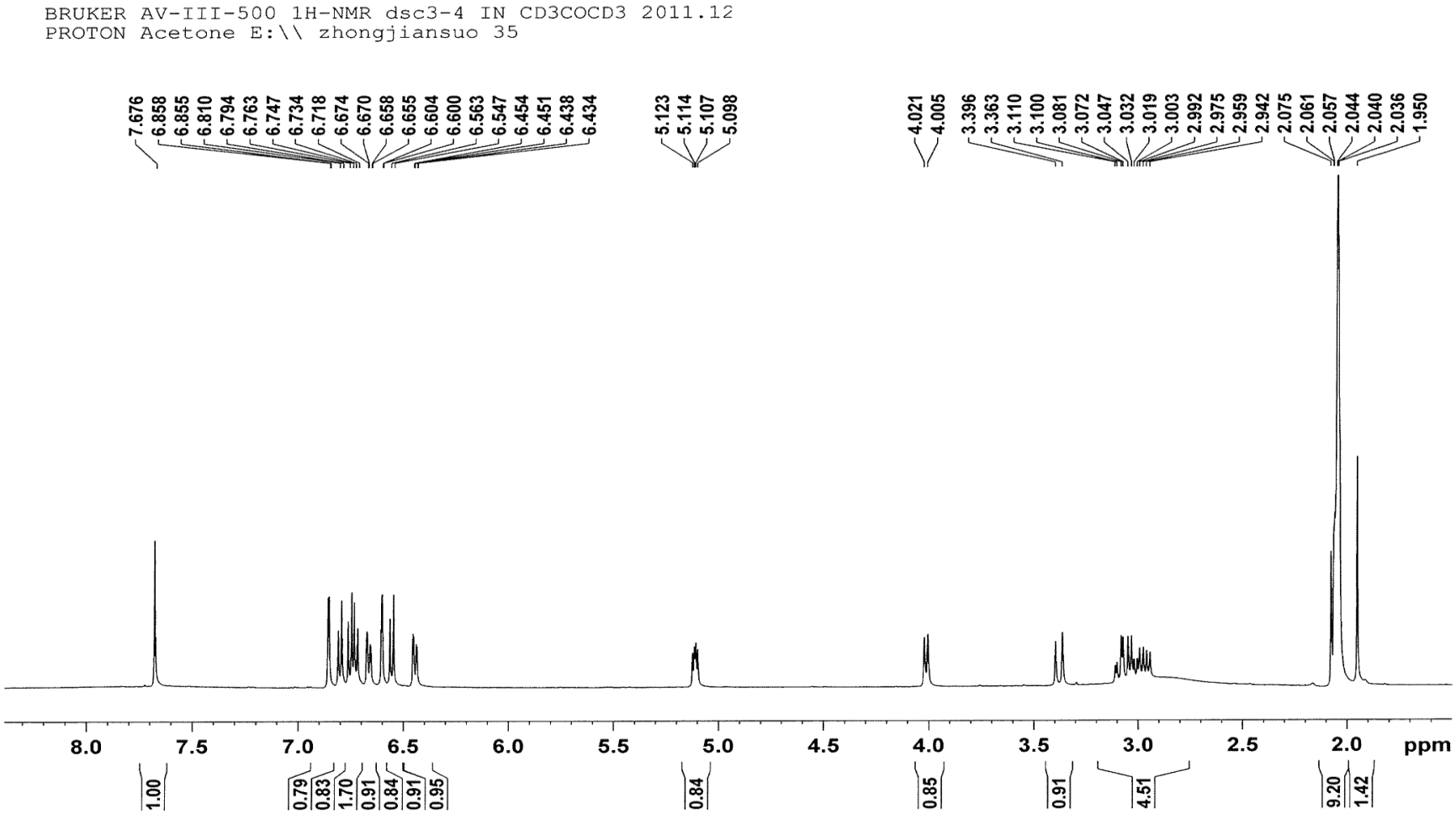


Figure S6. ^{13}C NMR spectrum (acetone-d_6, 125 MHz) of compound **1**.

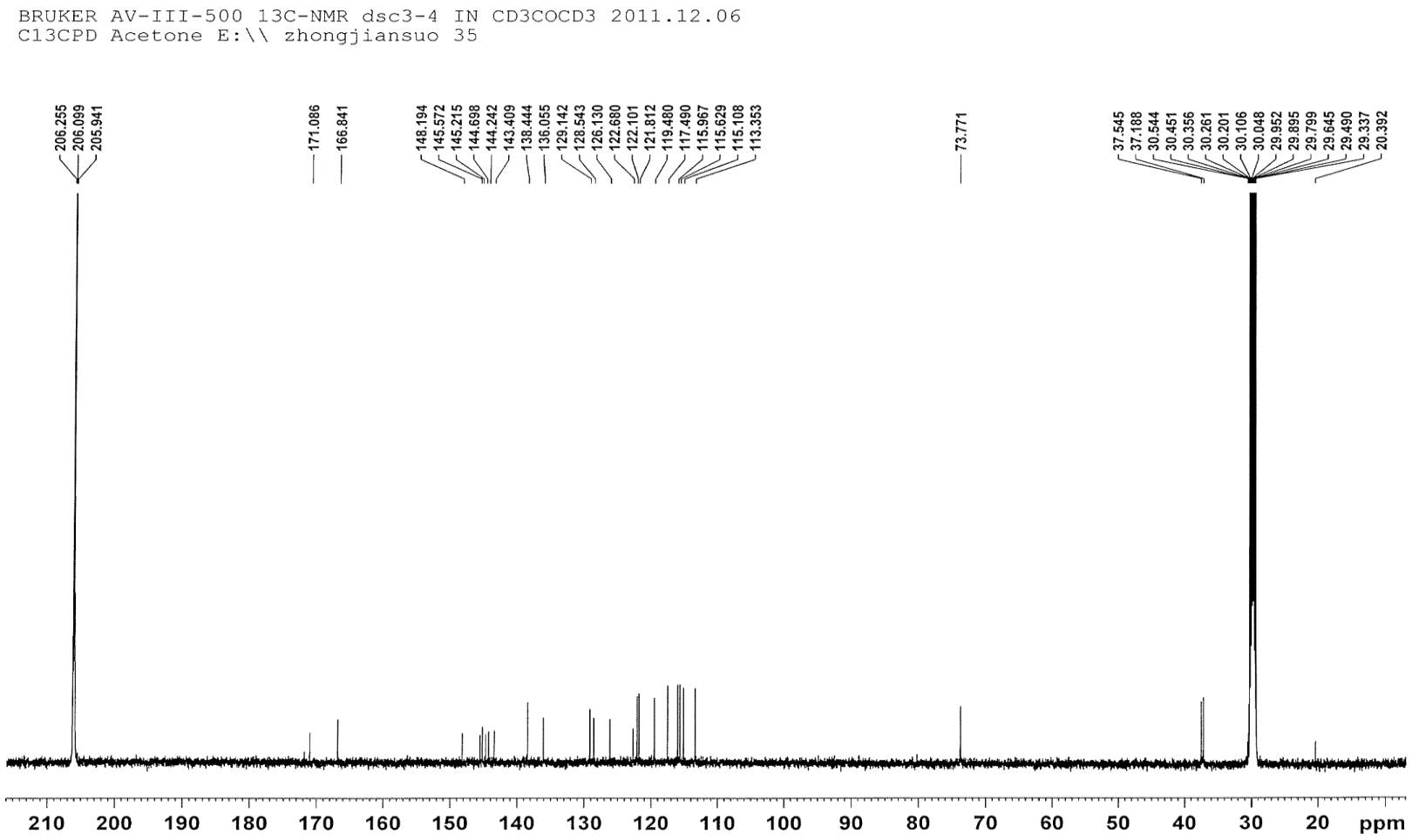


Figure S7. DEPT spectrum of compound **1**.

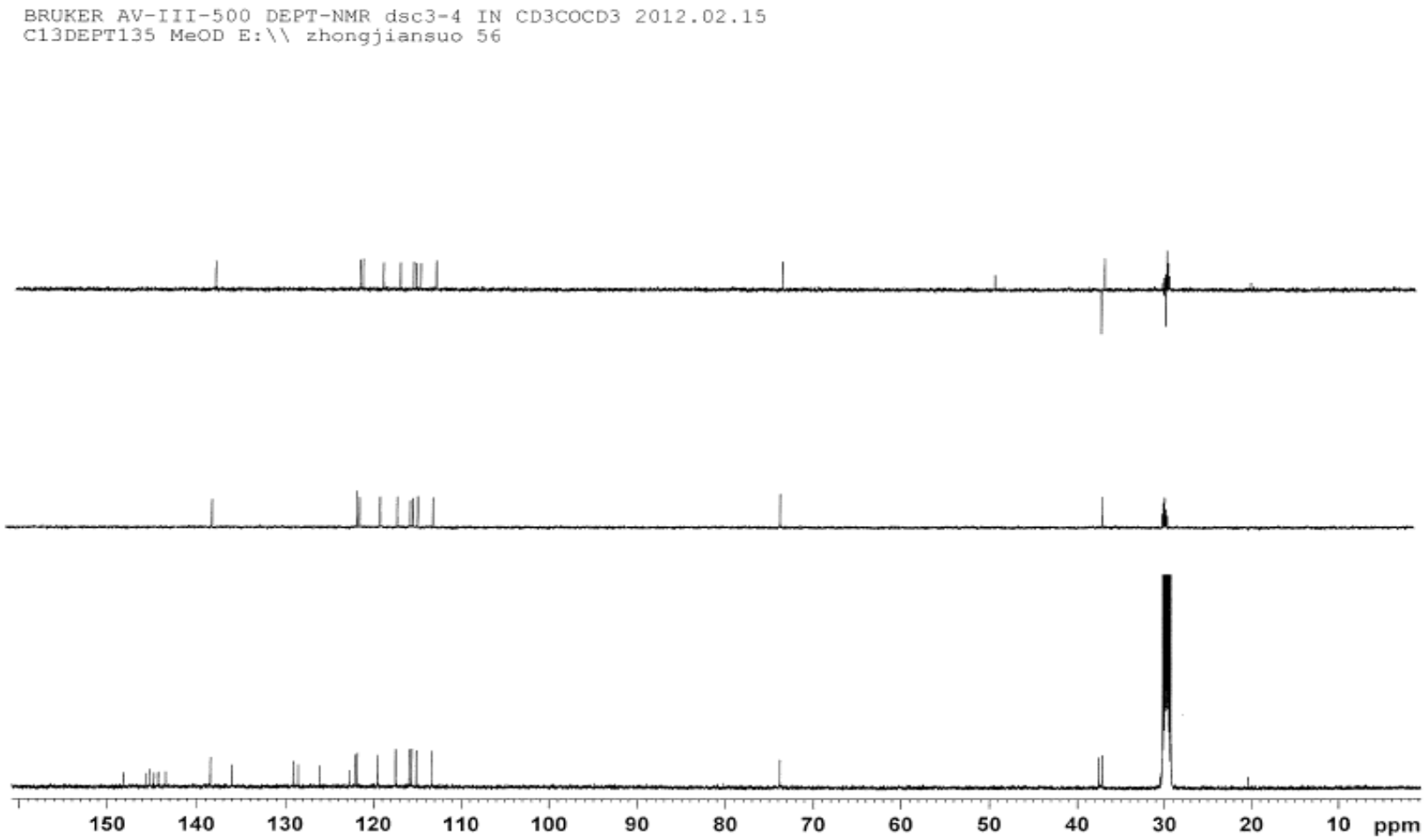


Figure S8. HSQC spectrum of compound **1**.

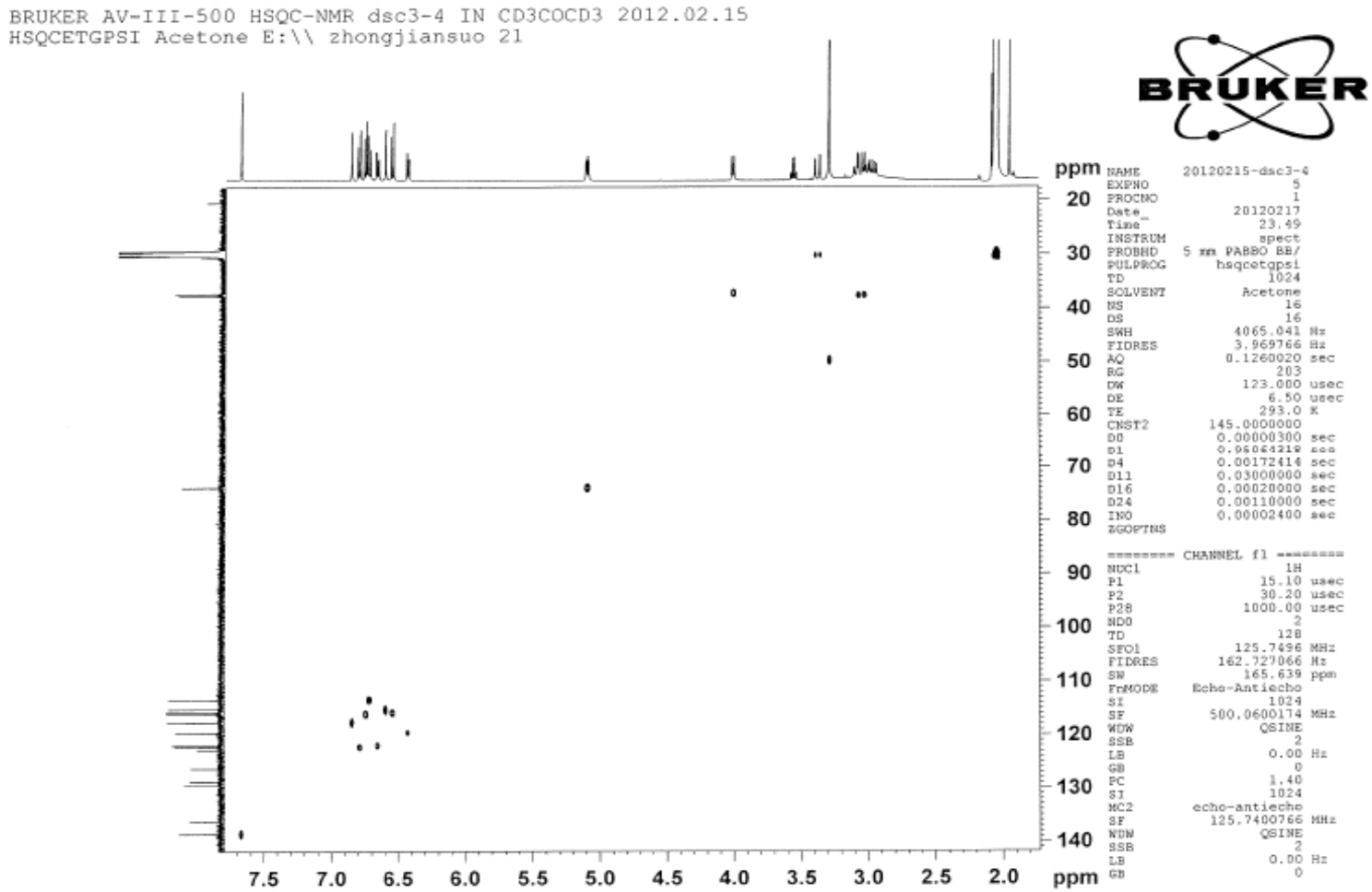


Figure S9. HMBC spectrum of compound **1**.

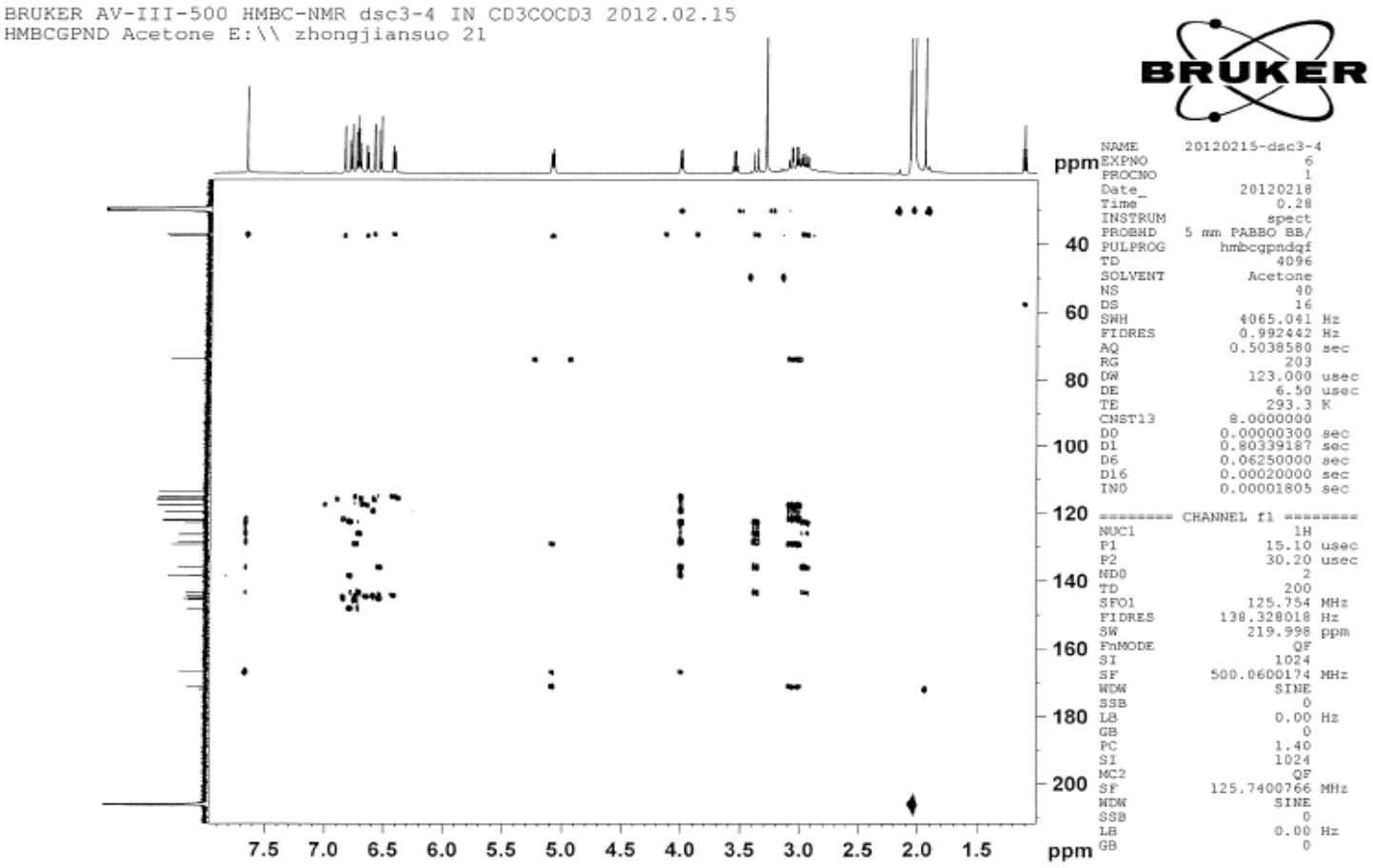


Figure S10. ^{1}H-^{1}H COSY spectrum of compound **1**.

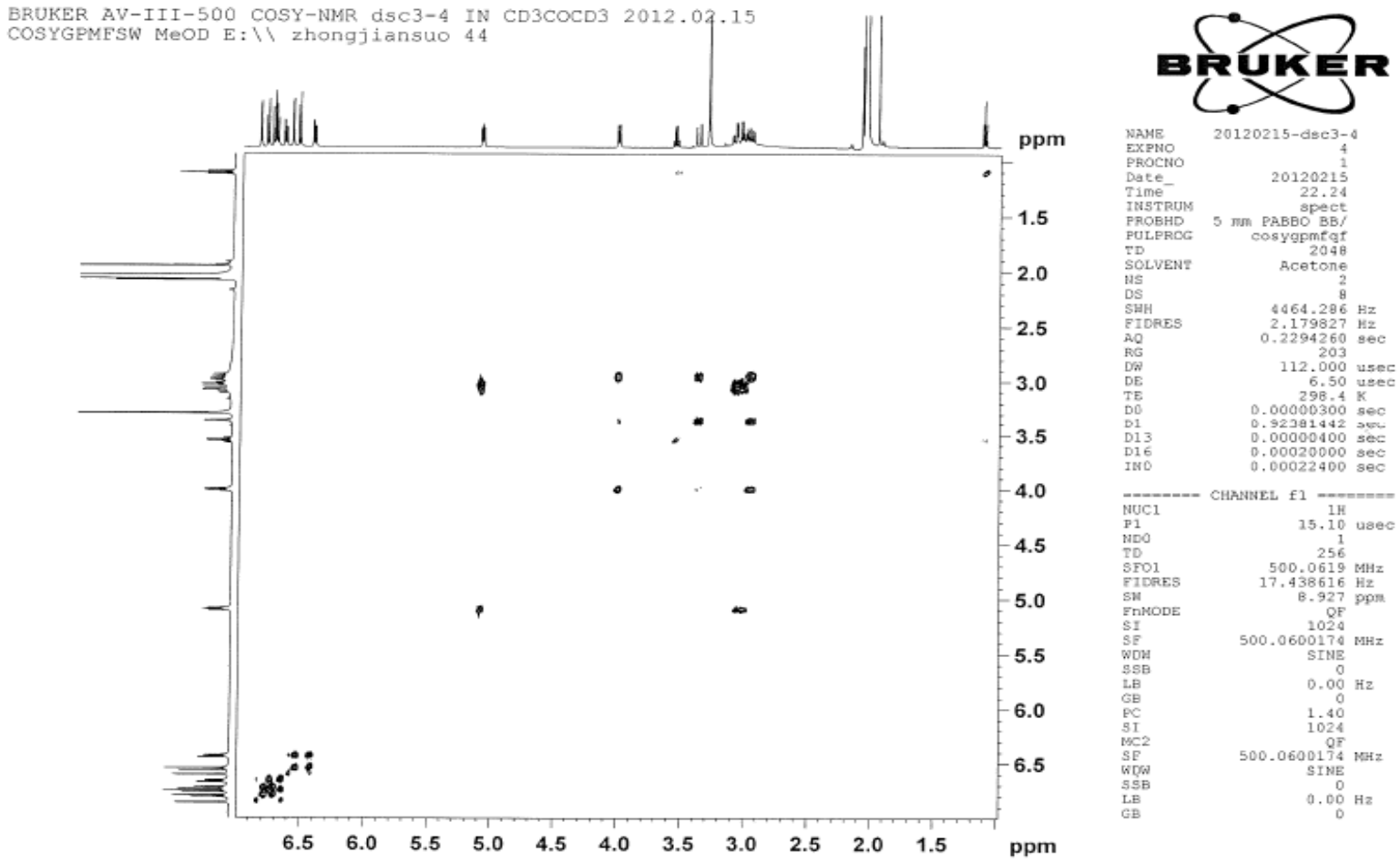


Figure S11. ESI-MS spectrum of compound **2**.

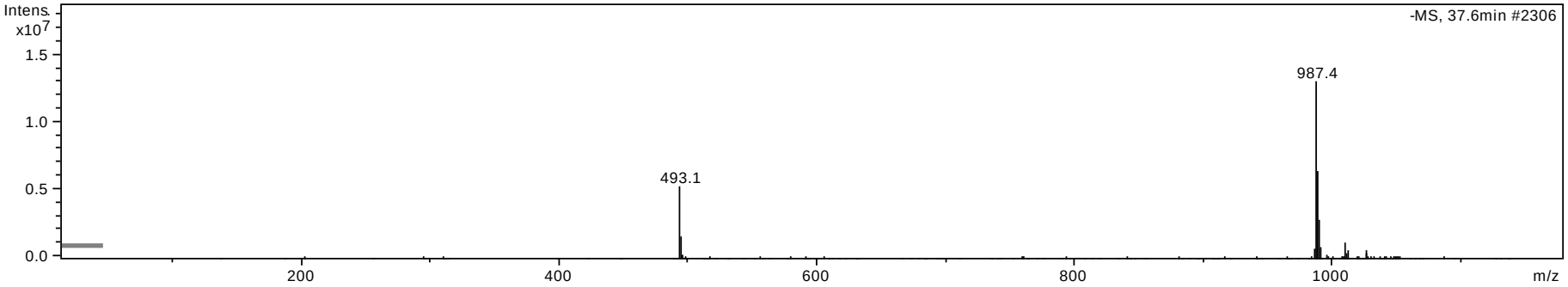
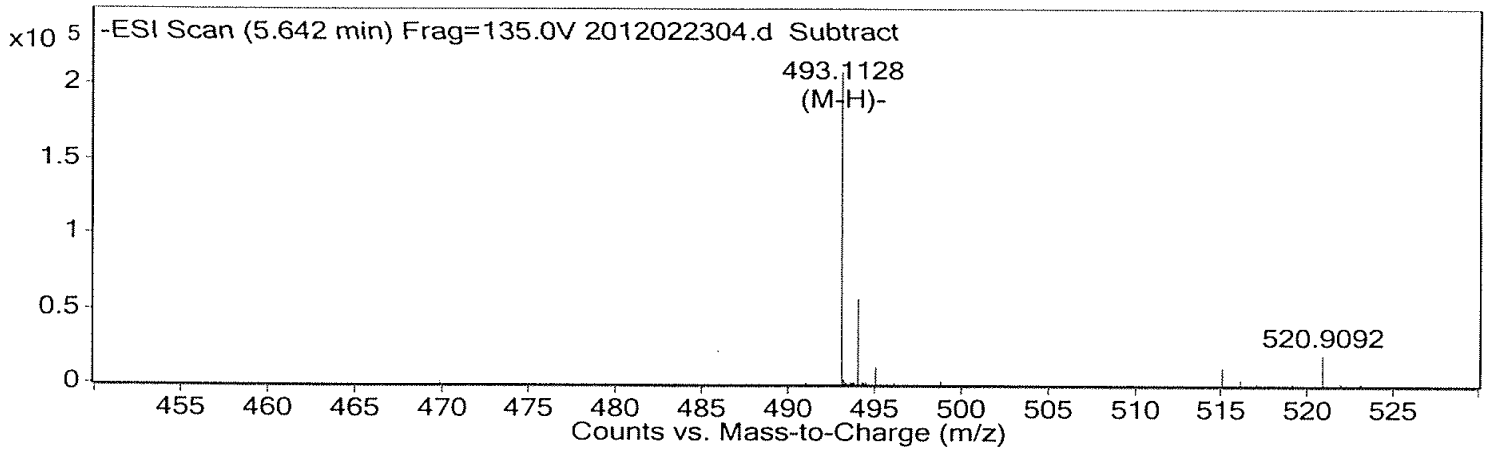


Figure S12. HR ESI-MS spectrum of compound **2**.



MS Formula Results: - Scan (5.642 min) Sub (2012022304.d)

m/z	Ion	Formula	Abundance
493.1128	(M-H)-	C26 H21 O10	207723.4

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
☑	C26 H22 O10	C26 H21 O10	493.114	99.86		494.12	494.1213	2.56	2.56	99.89	99.98	99.77	493.1128	16
☐	C27 H18 N4 O6	C27 H17 N4 O6	493.1154	99.29		494.12	494.1226	5.26	5.26	99.11	99.99	99.05	493.1128	21
☐	C21 H22 N2 O12	C21 H21 N2 O12	493.11	99.16		494.12	494.1173	-5.59	5.59	98.85	100	98.93	493.1128	12
☐	C30 H22 O5 S	C30 H21 O5 S	493.1115	98.62		494.12	494.1188	-2.51	2.51	95.65	99.86	99.78	493.1128	20
☐	C31 H18 N4 O S	C31 H17 N4 O S	493.1129	98.33		494.12	494.1201	0.19	0.19	94.27	99.85	100	493.1128	25
☐	C18 H26 N2 O12 S	C18 H25 N2 O12 S	493.1134	97.99		494.12	494.1206	1.23	1.23	93.3	99.71	99.95	493.1128	7
☐	C23 H26 O10 S	C23 H25 O10 S	493.1174	97.59		494.12	494.1247	9.38	9.38	96.72	99.78	97.02	493.1128	11
☐	C33 H18 O5	C33 H17 O5	493.1081	97.24		494.12	494.1154	-9.32	9.32	95.26	99.97	97.06	493.1128	25
☐	C34 H14 N4 O	C34 H13 N4 O	493.1095	97.14		494.12	494.1168	-6.63	6.63	92.49	99.98	98.5	493.1128	30
☐	C27 H26 O5 S2	C27 H25 O5 S2	493.1149	97.09		494.12	494.1222	4.31	4.31	91.21	99.6	99.36	493.1128	15
☐	C22 H26 N2 O7 S2	C22 H25 N2 O7 S2	493.1109	97.02		494.12	494.1181	-3.84	3.84	90.84	99.5	99.49	493.1128	11
☐	C28 H22 N4 O S2	C28 H21 N4 O S2	493.1162	96.62		494.12	494.1235	7.01	7.01	91.3	99.58	98.33	493.1128	20
☐	C14 H26 N2 O17	C14 H25 N2 O17	493.1159	96.11		494.12	494.1231	6.3	6.3	88.64	100	98.65	493.1128	3
☐	C34 H22 S2	C34 H21 S2	493.109	95.4		494.12	494.1163	-7.57	7.57	87.4	99.71	98.05	493.1128	24
☐	C13 H26 N4 O14 S	C13 H25 N4 O14 S	493.1093	95.1		494.12	494.1166	-6.93	6.93	85.89	99.62	98.36	493.1128	3

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

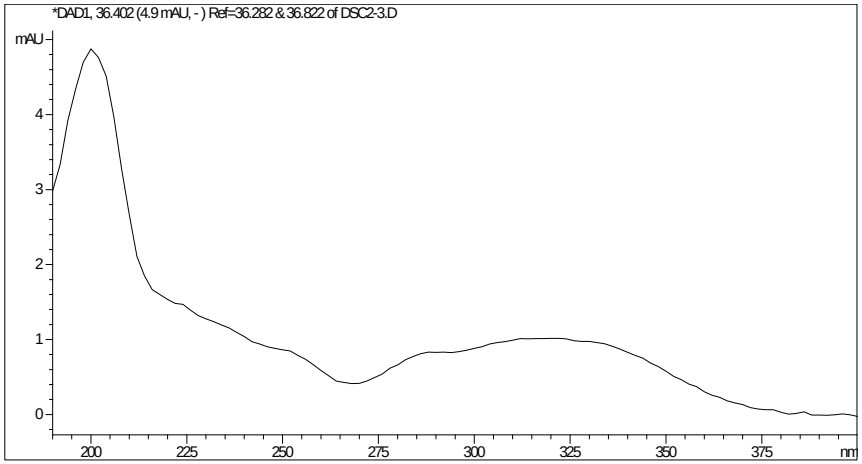
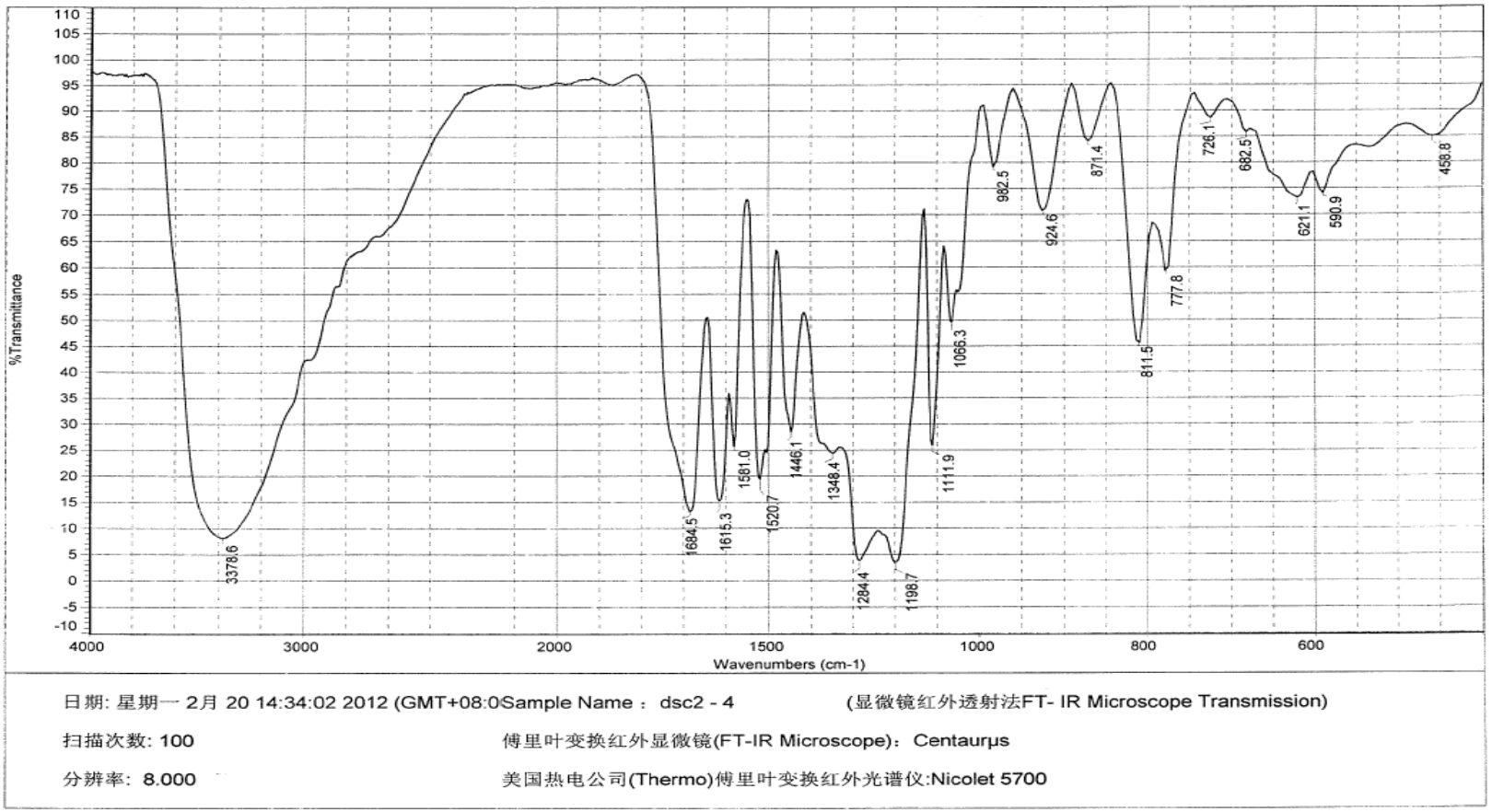


Figure S14. IR spectrum of compound **2**.



Date: Monday, Feb 20th, 14:34:02 2012 (GMT+08:0Sample Name: dsc 2-4) (Microscopy infrared transmission method FT-IR Microscope Transmission)
Numbers of scan: 100 Fourier transform infrared spectroscopy (FT-IR Microscope): Centaurus
Resolution ratio: 8,000 America Thermo Electron Corporation (Thermo) Fourier transform infrared spectrometer: Nicolet 5700

Figure S15. ^{1}H NMR spectrum (acetone-d_6, 500 MHz) of compound **2**.

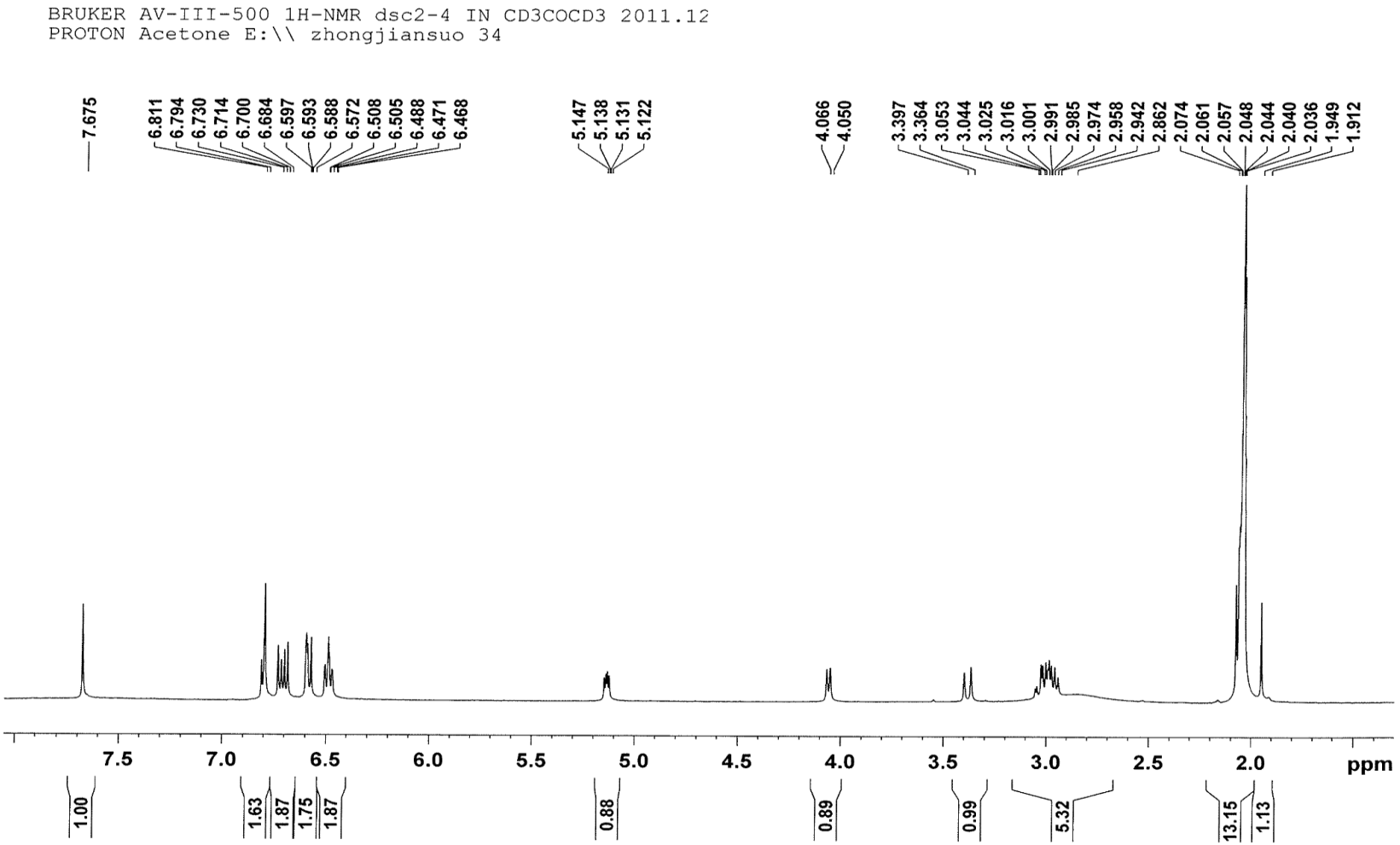


Figure S16. ^{13}C NMR spectrum (acetone-d_6, 125 MHz) of compound **2**.

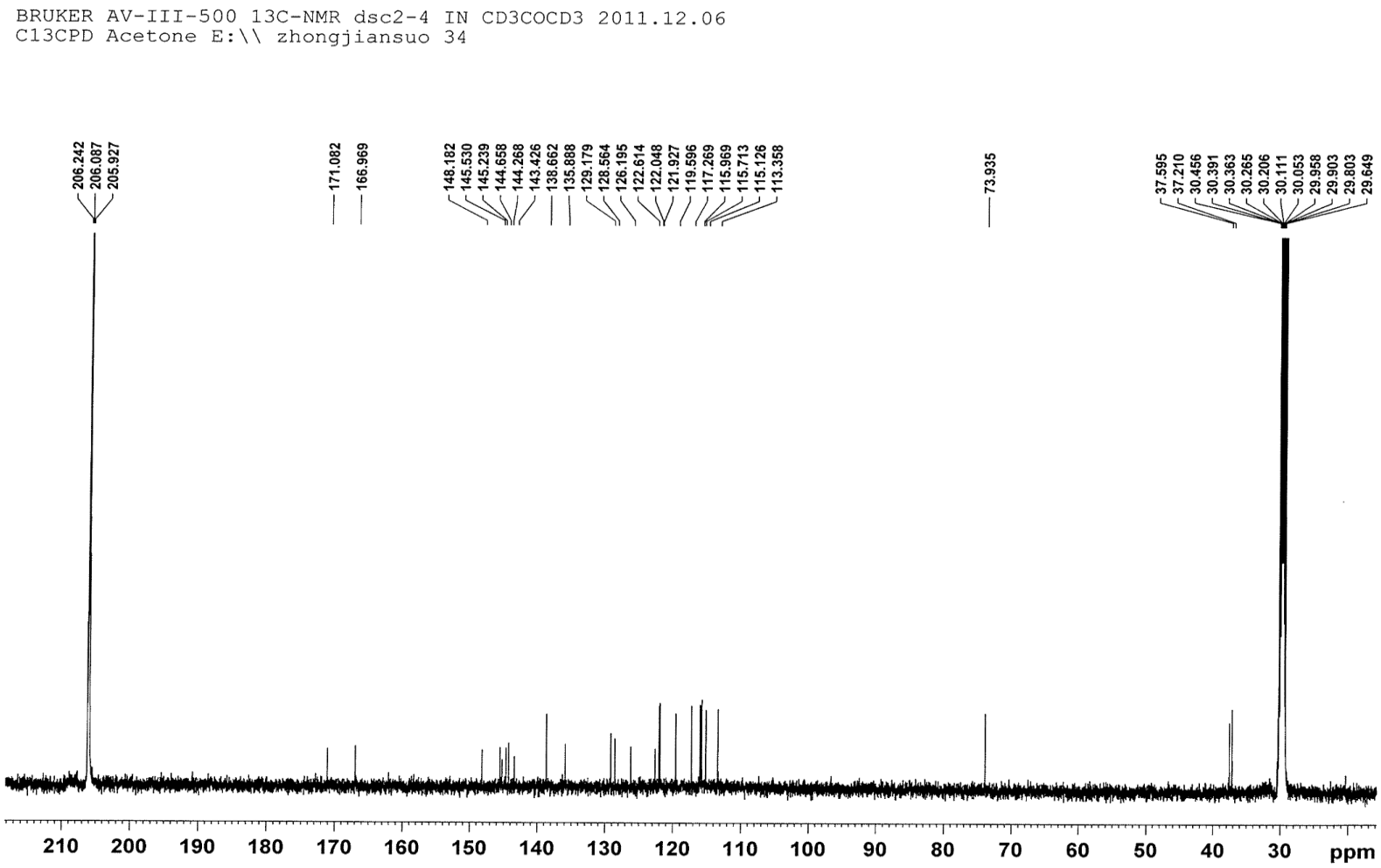


Figure S17. DEPT spectrum of compound **2.**

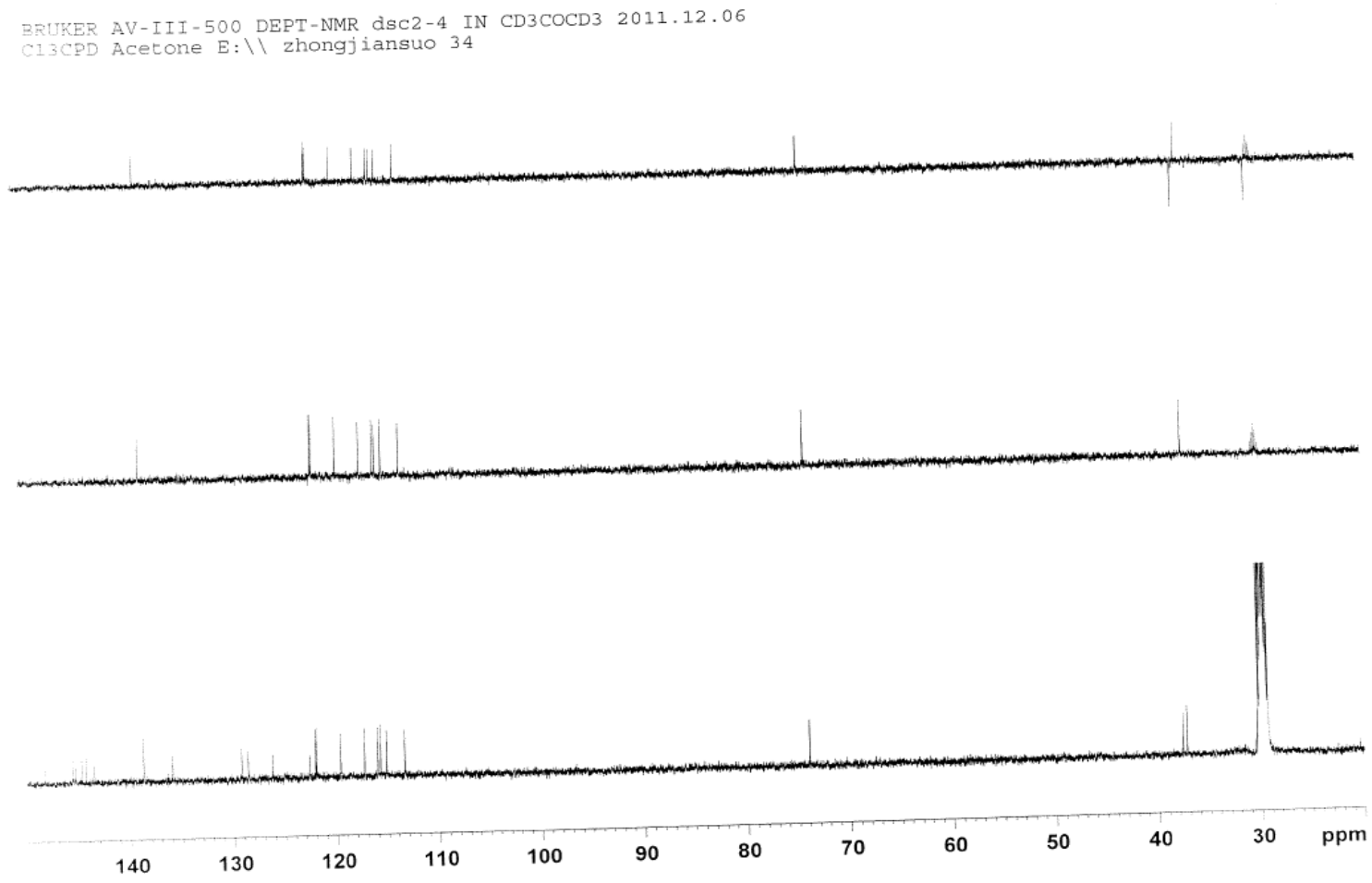


Figure S18. HSQC spectrum of compound **2**.

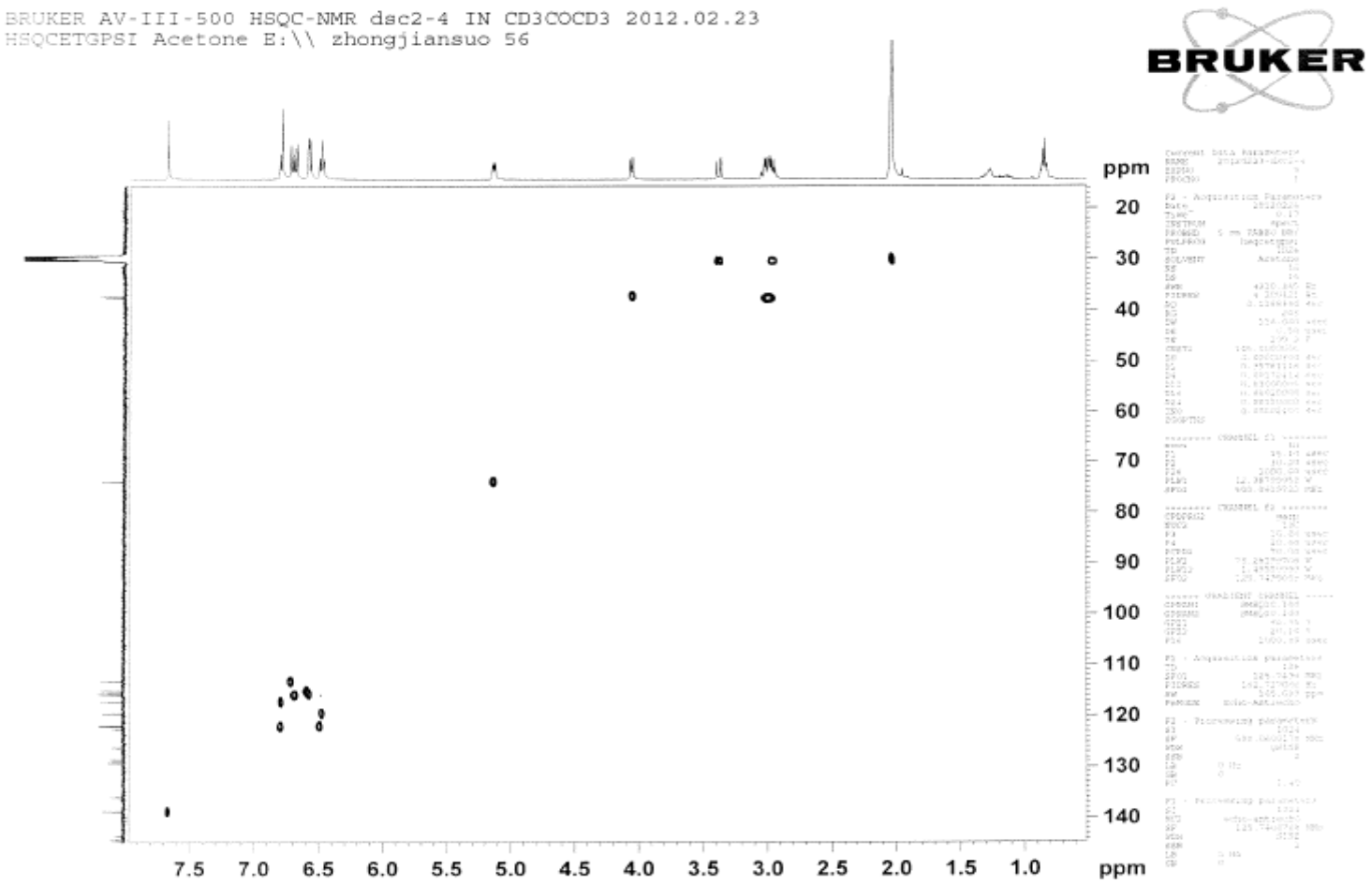


Figure S19. HMBC spectrum of compound **2**.

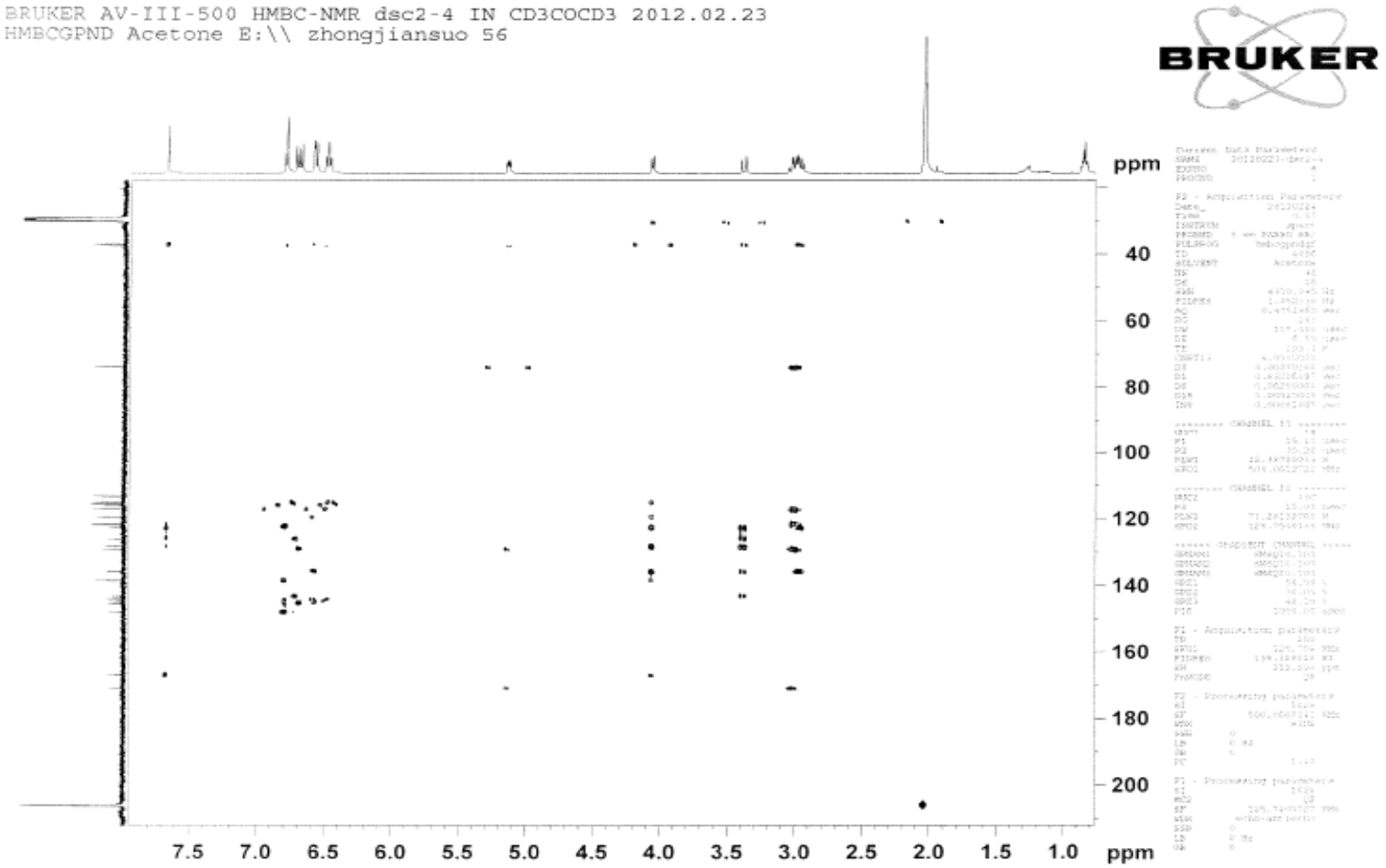


Figure S20. ^{1}H-^{1}H COSY spectrum of compound **2**.

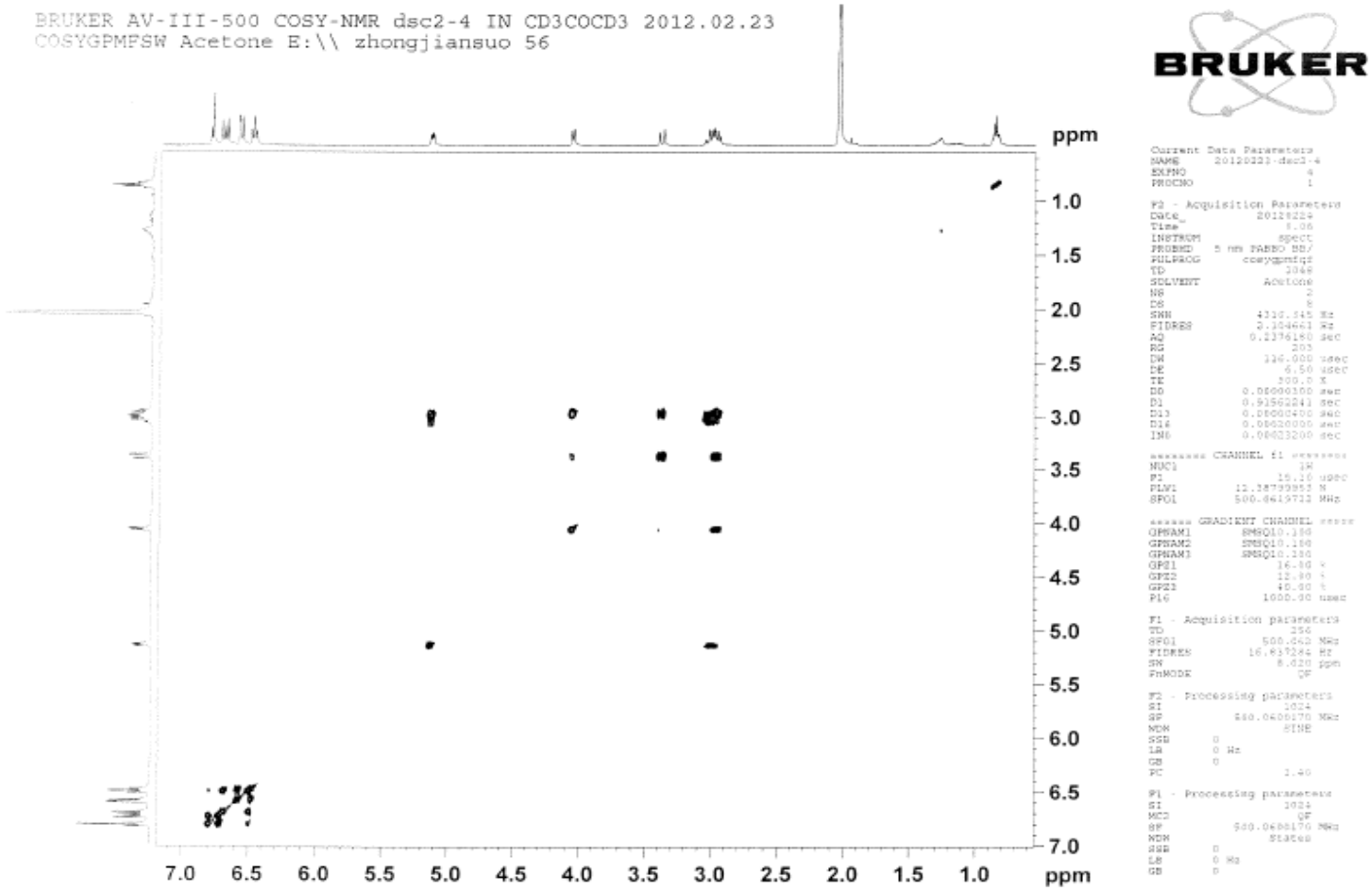
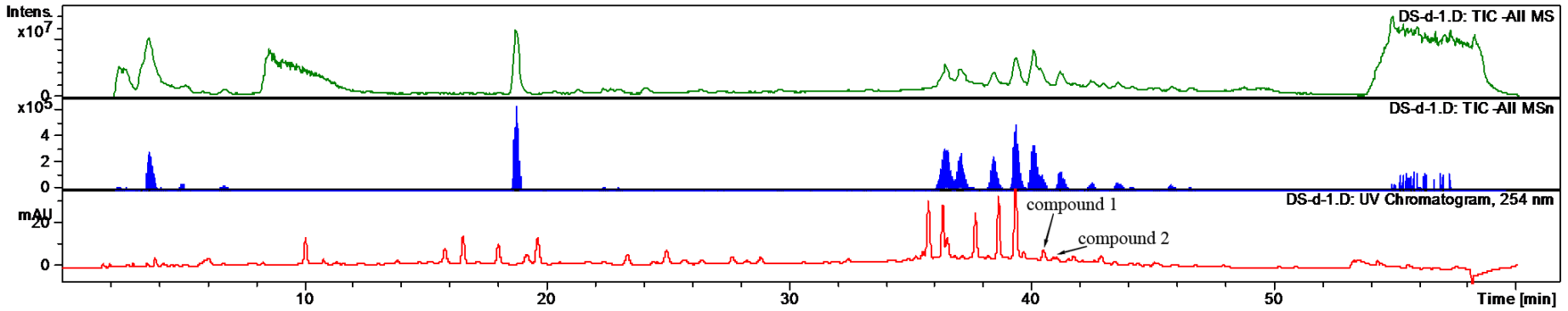


Figure S21. HPLC-UV-ESI-MS^n Chromatograms of Danshen Injection (lyophilized powder).



TIC-MS, TIC-MS^n and HPLC chromatograms (from top to bottom) (HPLC: Compound **1**, t_R = 40.5 min; Compound **2**, t_R = 41.1 min).

Apparatus and Chromatographic condition

HPLC: Agilent 6320 LC/MSD mass spectrometer; Column: Germany MACHEREY-NAGEL NUCLEODUR C_{18} Pyramid (4.6 mm × 250 mm, 5 μm); Mobile phase: gradient elution by 0.1% formic acid (HCOOH)-acetonitrile (CH_3CN), see table below; Wavelength: 254 nm; Flow: 1.0 mL min^{-1} (Split ratio, 4:1); Column temperature: 30 ℃; Concentration: 0.2 mg/mL; Injection volume: 5 μL.

Time (min)	0	8	30	45	50	51	55	56	60
A. 0.1%HCOOH (%)	100	97	80	55	55	10	10	100	100
B. CH_3CN (%)	0	3	20	45	45	90	90	0	0

MS: Nebulizer: 30.0 psi; Gas flow: 9.0 L/min; Temperature of drying gas: 350 ℃; Capillary voltage: 3500 V; Ionization mode: negative ESI; scan: *m/z* 100–1000.