

New *Abeo*-abietanoids from *Tripterygium wilfordii*

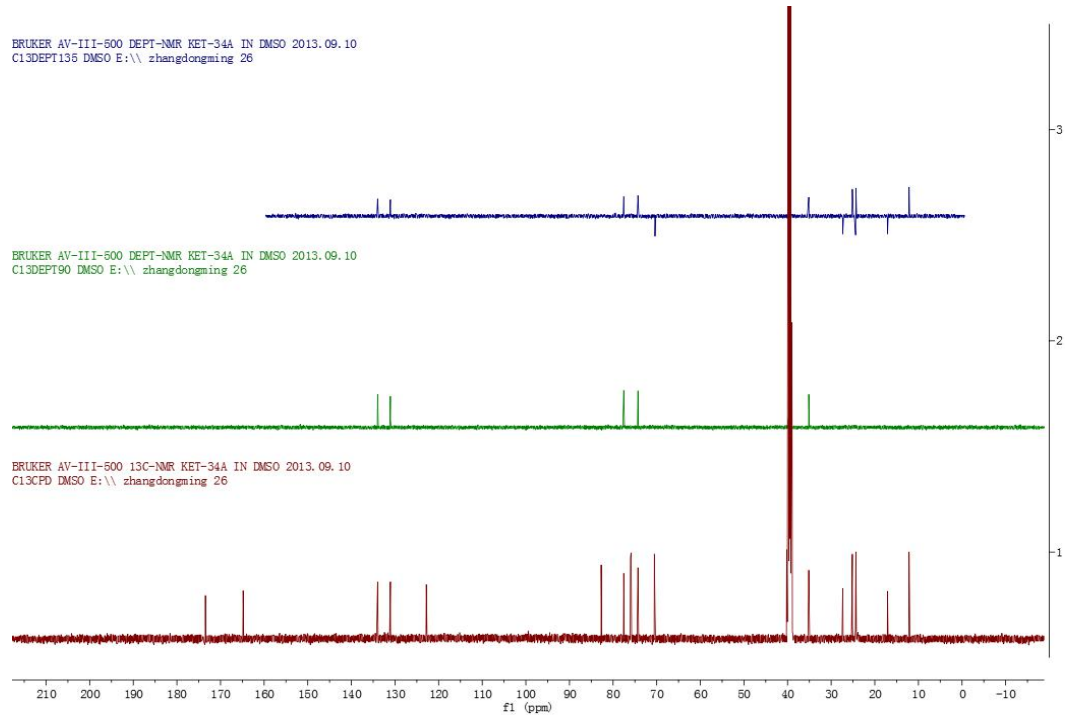
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Supplementary Materials

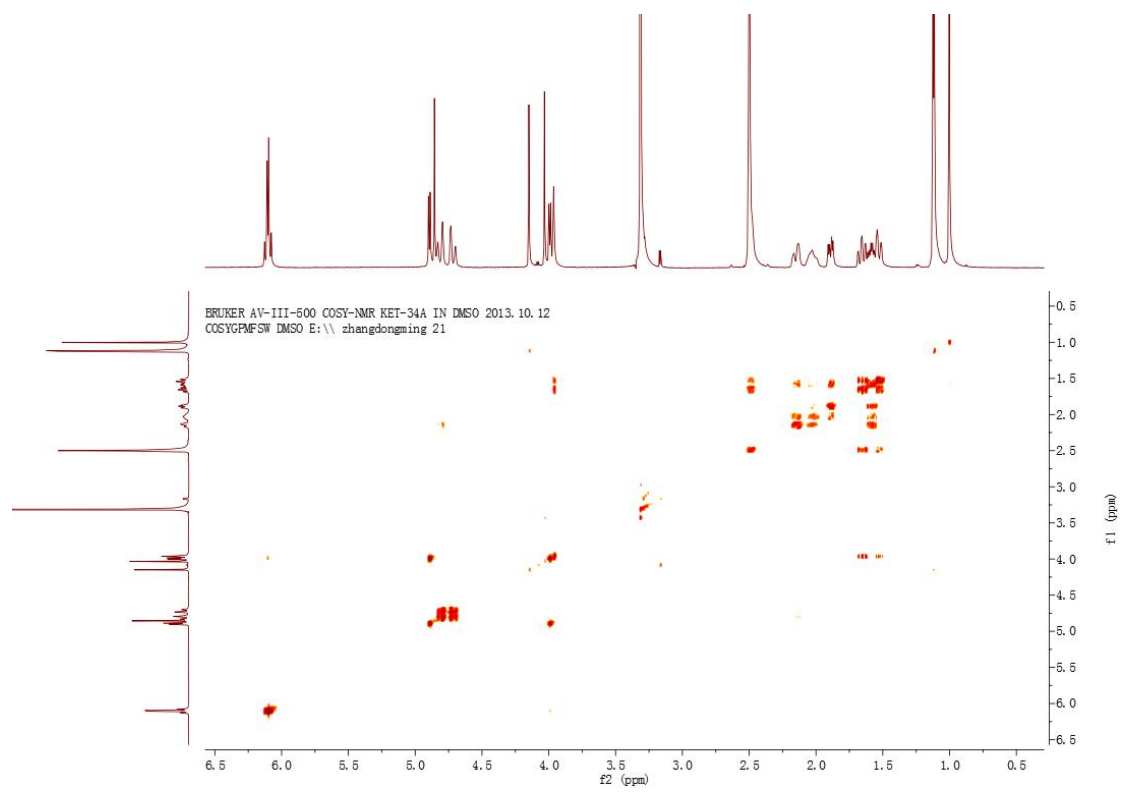
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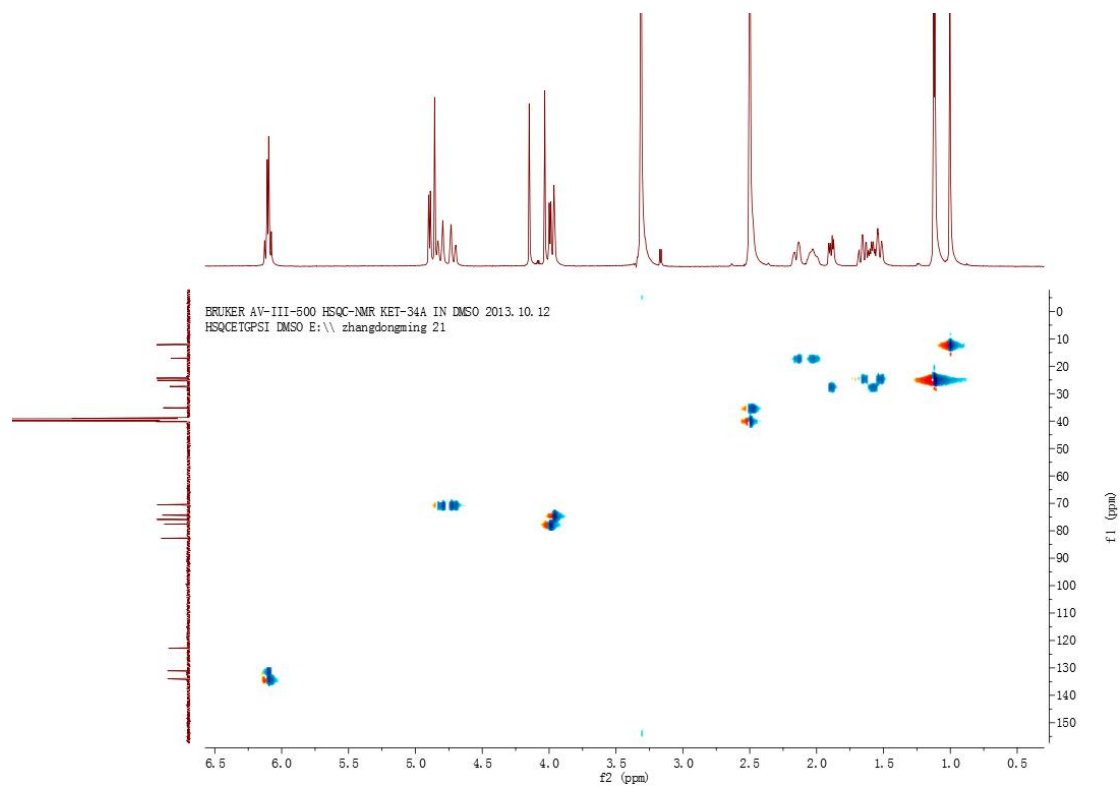
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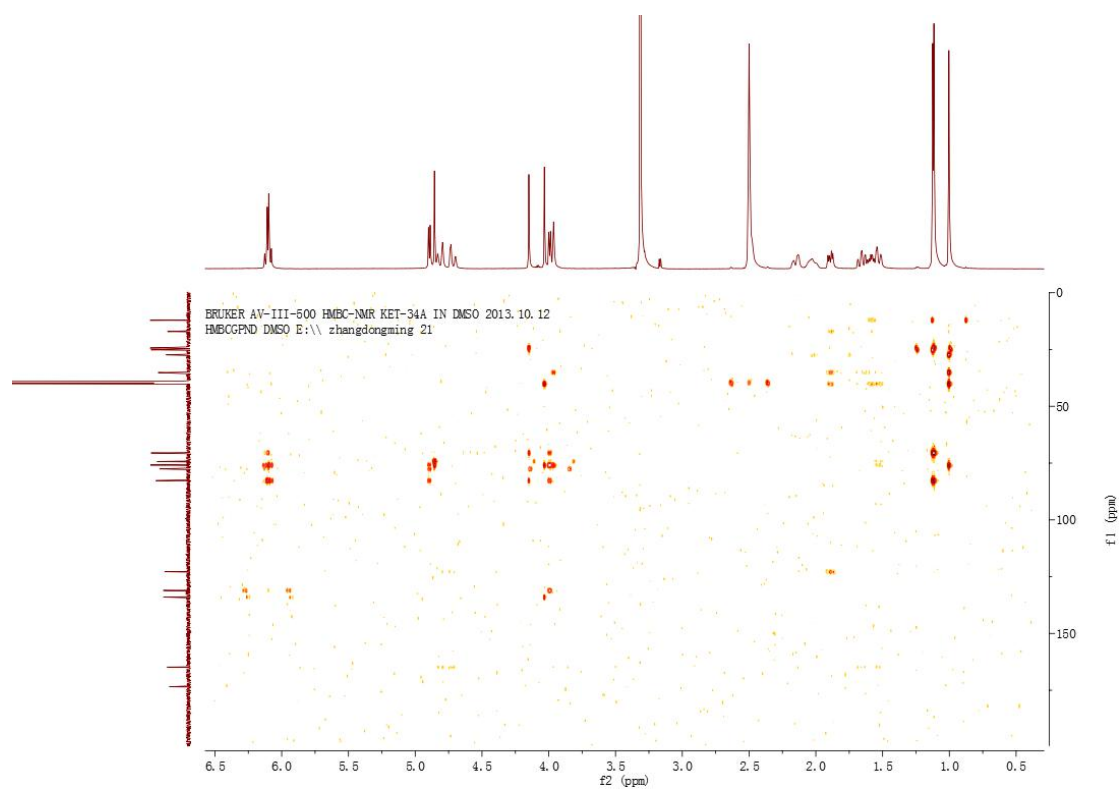
DEPT spectrum of compound 1



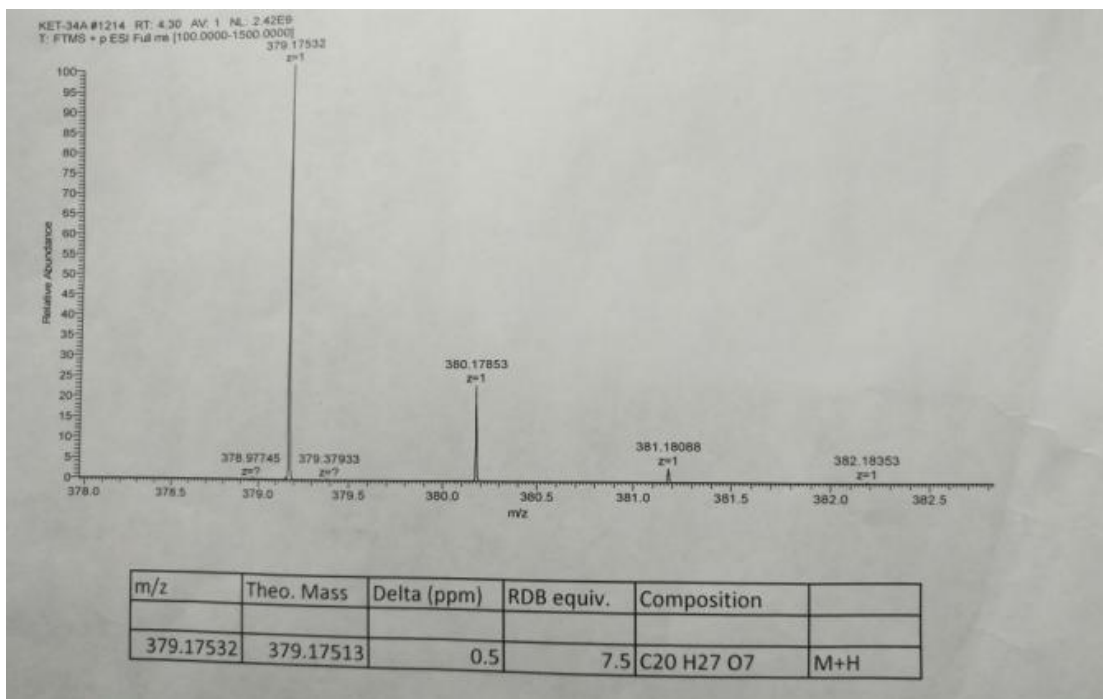
¹H, ¹H COSY spectrum of compound 1



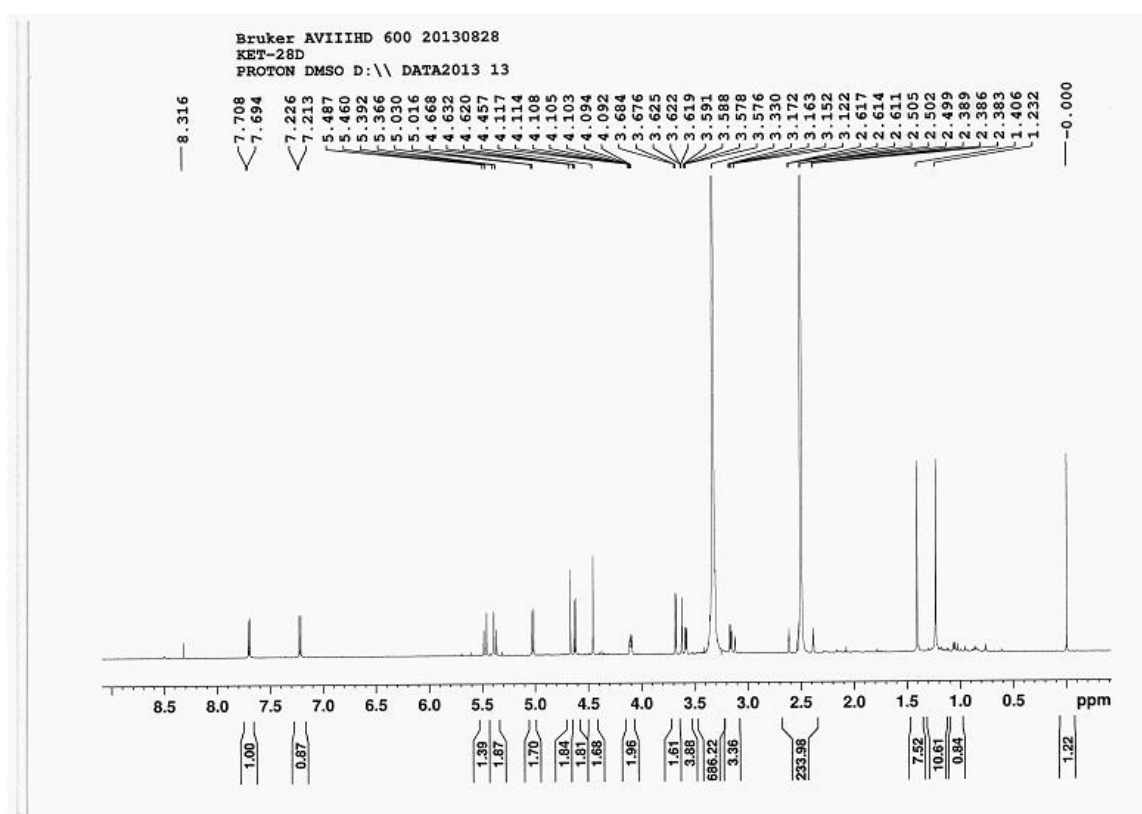
HSQC spectrum of compound **1**



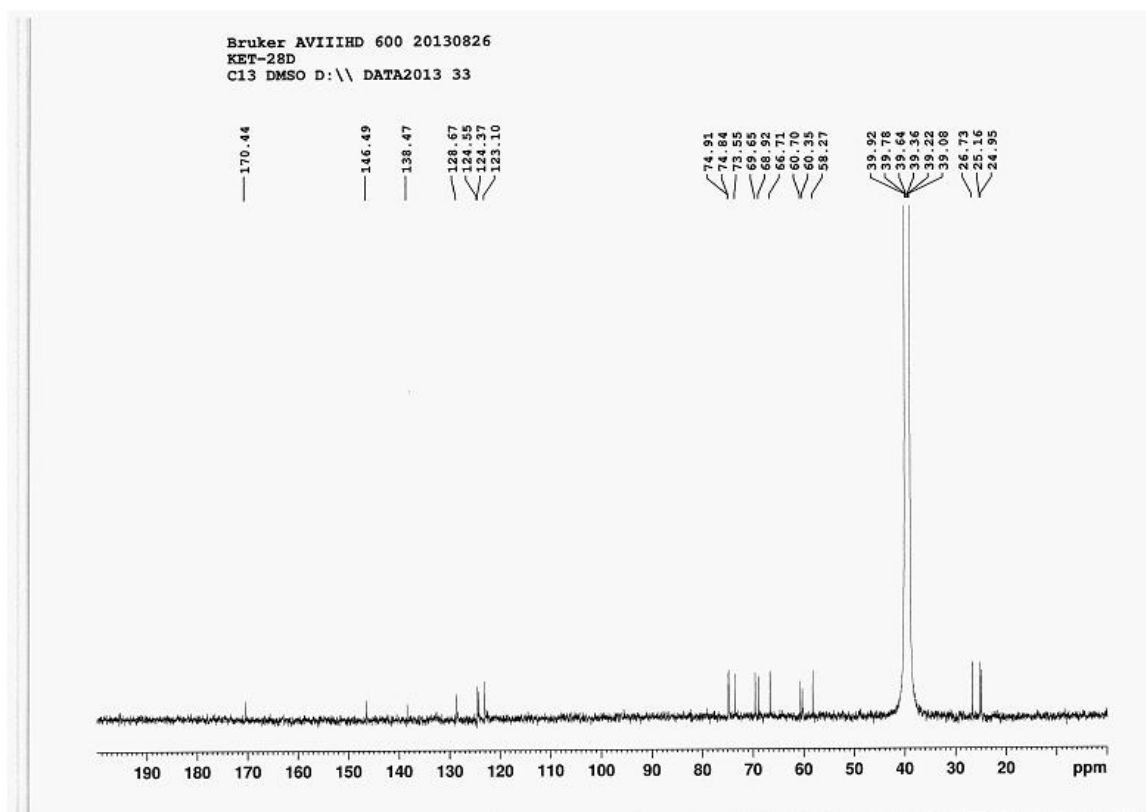
HMBC spectrum of compound **1**



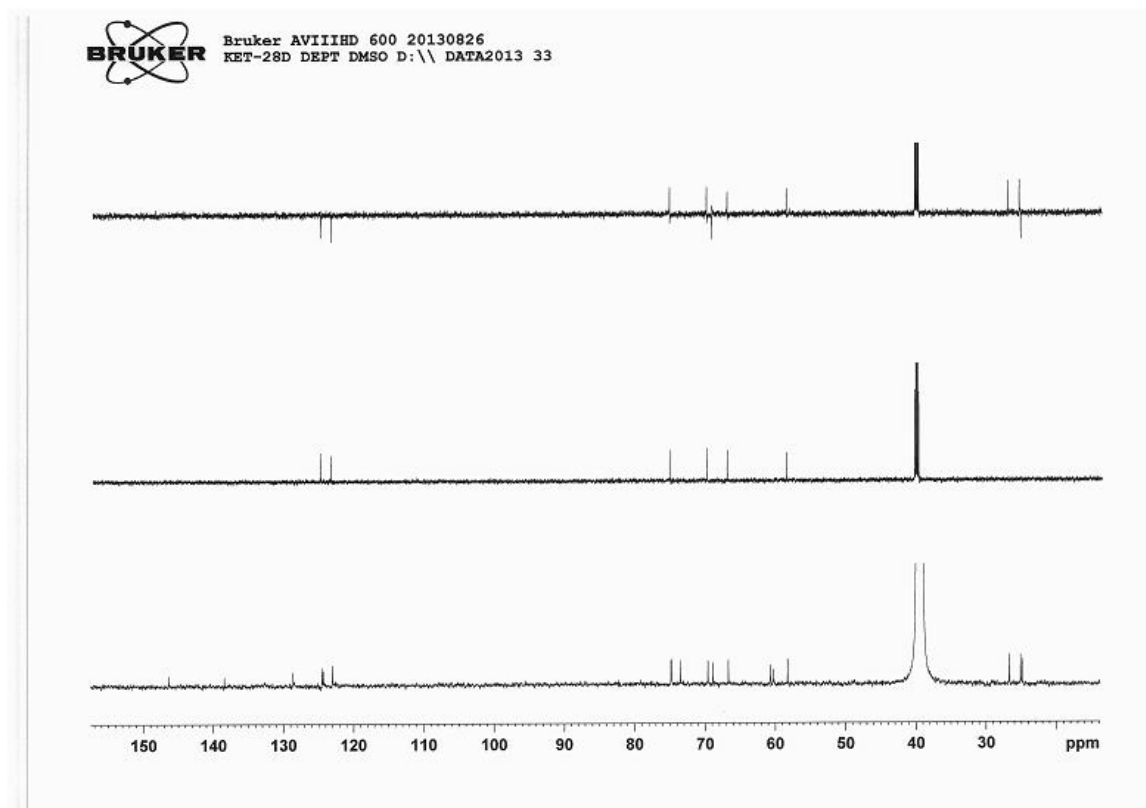
HRESIMS spectrum of compound 1



¹H NMR spectrum of compound 2 (600 MHz, DMSO-d₆)



^{13}C NMR spectrum of compound **2** (150 MHz, DMSO- d_6)



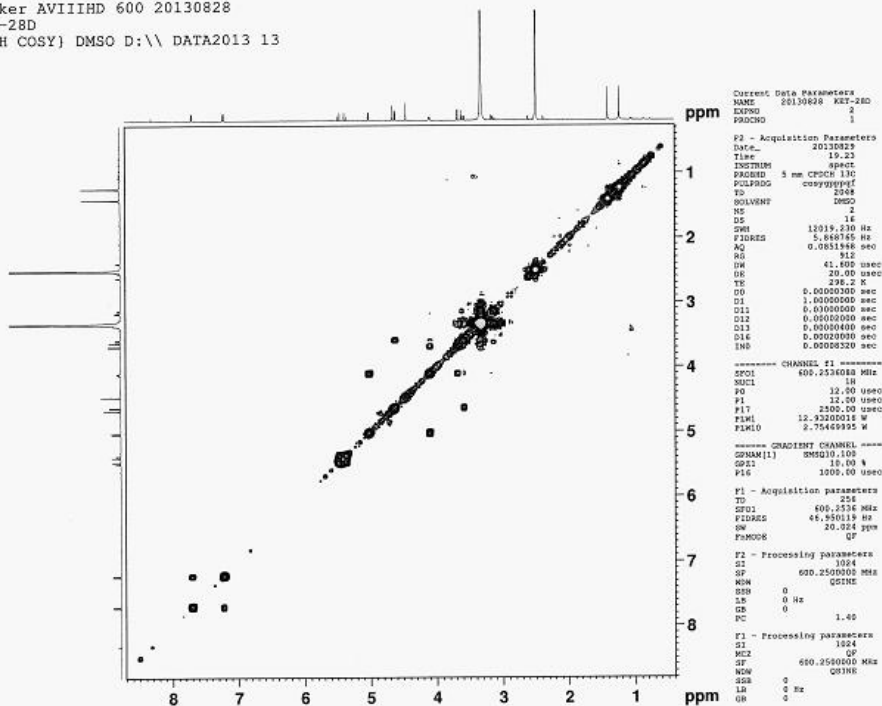
DEPT spectrum of compound **2** (150 MHz, DMSO- d_6)

MS Formula Results: + Scan (4.094 min) Sub (2013090202.d)

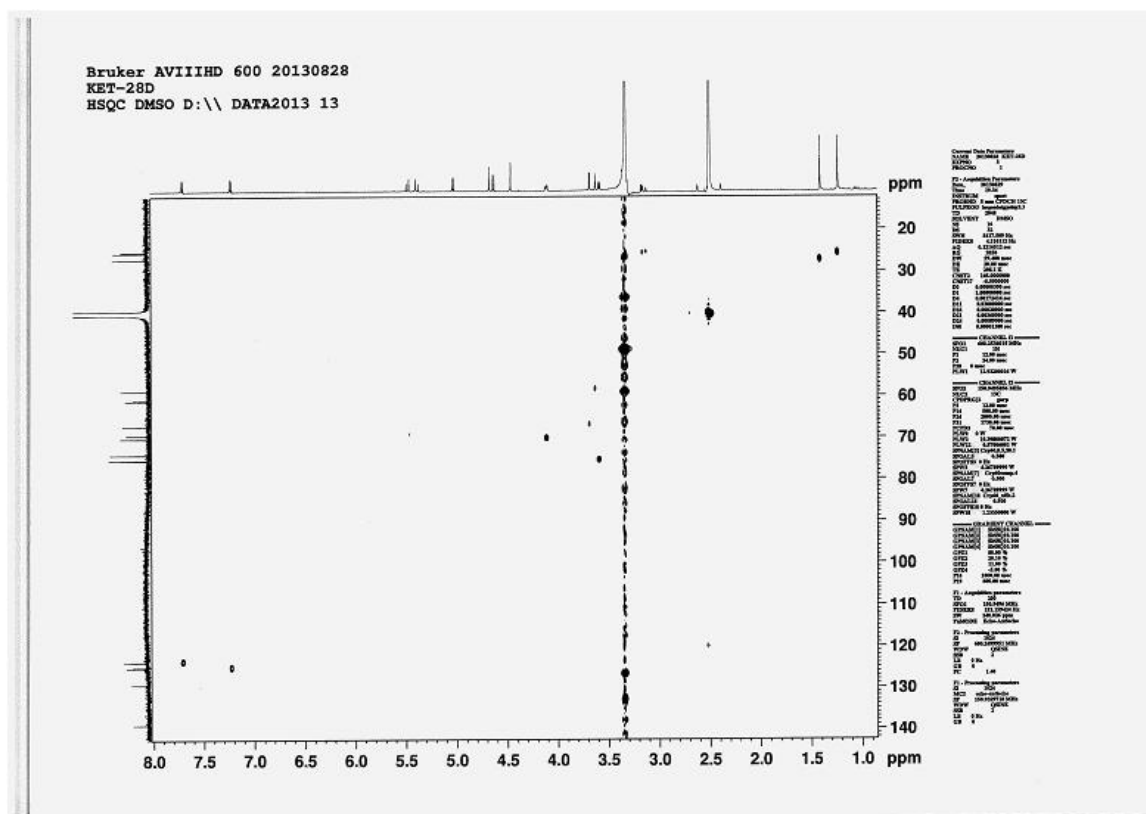
m/z	Ion	Formula	Abundance											
377.1249	(M+H) ⁺	C19 H21 O3	8952.4											
m/z	Formula (M)	Ion Formula	Calc. m/z	Score	± Cross S	Mass	Calc. Mass	Diff (ppm)	Abn. Diff (ppm)	Abund. Match	Spacing (m/z)	Mass Match	m/z	DBE
377.1248	C20 H18 N1 O4	C20 H17 N1 O4	377.1244	85.38		376.1177	376.1172	-1.44	1.44	98.17	40.51	99.93	377.1249	15
377.1249	C17 H17 F N4 O5	C17 H18 F N4 O5	377.1259	83.37		376.1177	376.1180	1.6	1.6	97.95	40.39	99.92	377.1249	11
377.1250	C19 H20 O3	C19 H20 O3	377.1251	84.89		376.1177	376.1178	-0.68	-0.68	97.76	40.28	99.92	377.1249	12
377.1251	C18 H21 F O4	C18 H22 F O4	377.1262	84.92		376.1177	376.1177	-1.94	1.94	94.83	41.41	99.88	377.1249	8
377.1252	C20 H18 N2 O2	C20 H17 N2 O2	377.1283	83.4		376.1177	376.1212	9.37	9.37	95.87	40.98	97.35	377.1249	18
377.1253	C21 H21 F N4 S	C21 H20 F N4 S	377.1231	83.17		376.1177	376.1158	-5.05	5.05	92.33	40.28	96.17	377.1249	13
377.1254	C20 H21 F O4 S	C20 H22 F O4 S	377.1217	82.35		376.1177	376.1148	-8.6	8.6	91.29	41.08	97.62	377.1249	15
377.1255	C17 H20 N4 O4 S	C17 H21 N4 O4 S	377.1236	82.31		376.1177	376.1056	-7.02	7.02	91.95	40.11	96.18	377.1249	10
377.1256	C18 H24 O3 S	C18 H25 O3 S	377.1286	82.29		376.1177	376.1190	3.98	3.98	87.99	41.06	96.49	377.1249	5
377.1257	C18 H21 F N4 S2	C18 H22 F N4 S2	377.1284	82.93		376.1177	376.1190	3.8	3.8	82.87	39.88	96.61	377.1249	10
377.1258	C19 H26 F O4 S	C19 H27 F O4 S	377.1236	88.57		376.1177	376.1203	7.02	7.02	83.78	41.09	96.41	377.1249	1
377.1259	C20 H24 O3 S2	C20 H25 O3 S2	377.124	88.49		376.1177	376.1187	-2.88	2.88	81.43	40.81	96.77	377.1249	3
377.1260	C17 H25 F O4 S2	C17 H26 F O4 S2	377.1251	88.25		376.1177	376.1178	0.36	0.36	85.25	40.74	100	377.1249	5
m/z	Ion	Formula	Abundance											
382.1052	(M+H) ⁺	C19 H20 N1 O3	33813.3											
m/z	Formula (M)	Ion Formula	Calc. m/z	Score	± Cross S	Mass	Calc. Mass	Diff (ppm)	Abn. Diff (ppm)	Abund. Match	Spacing (m/z)	Mass Match	m/z	DBE
382.1051	C20 H18 N1 O4	C20 H18 N1 O4	382.1054	87.41		378.116	378.1172	3.05	3.05	98.12	46.73	98.95	382.1052	15
382.1052	C17 H17 F N4 O5	C17 H18 F N4 O5	382.1076	88.71		378.116	378.1160	0.99	0.99	97	46.94	98.63	382.1052	11
382.1053	C19 H21 F O4	C19 H22 F O4	382.1087	88.21		378.116	378.117	2.96	2.96	93.89	44.3	96.61	382.1052	8
382.1054	C24 H13 F N4	C24 H13 F N4	382.1076	85.95		378.116	378.1104	-6.52	6.52	97.54	49.91	97.33	382.1052	20
382.1055	C21 H21 F N4 S	C21 H20 F N4 S	382.105	85.88		378.116	378.1158	-0.57	0.57	82.3	46.95	96.98	382.1052	18
382.1056	C20 H21 F O4 S	C20 H22 F O4 S	382.1027	85.20		378.116	378.1148	-4.11	4.11	91.52	49.85	96.61	382.1052	15
382.1057	C23 H20 N1 O3 S	C23 H20 N1 O3 S	382.1028	84.76		378.116	378.1153	-7.15	7.15	86.79	46.62	96.31	382.1052	14
382.1058	C19 H24 N1 O4 S	C19 H25 N1 O4 S	382.1084	83.39		378.116	378.1190	8.41	8.41	81.32	49.28	97.62	382.1052	2
382.1059	C11 H21 F N2 O11	C11 H22 F N2 O11	382.1022	82.95		378.116	378.1159	-0.16	0.16	85.3	48.1	96.67	382.1052	2
382.1060	C20 H24 O3 S2	C20 H25 O3 S2	382.1069	84.84		378.116	378.1167	1.81	1.81	81.55	46.88	98.1	382.1052	9
382.1061	C11 H24 N2 O10 S	C11 H25 N2 O10 S	382.1044	82.15		378.116	378.1152	-2.34	2.34	78.49	49.05	96.85	382.1052	1
382.1062	C18 H21 F N4 S2	C18 H22 F N4 S2	382.1084	82.10		378.116	378.1196	8.36	8.36	82.41	49.98	97.66	382.1052	10
382.1063	C17 H25 F O4 S2	C17 H26 F O4 S2	382.1071	81.91		378.116	378.1178	4.05	4.05	76.6	48.1	96.31	382.1052	5
382.1064	C18 H24 N2 O3 S2	C18 H25 N2 O3 S2	382.1079	83.71		378.116	378.1127	-6.4	6.4	75	49.98	97.7	382.1052	5
382.1065	C12 H25 F N2 O8 S2	C12 H26 F N2 O8 S2	382.103	83.09		378.116	378.1158	-0.86	0.86	73.88	46.67	96	382.1052	1

HRESIMS spectrum of compound 2

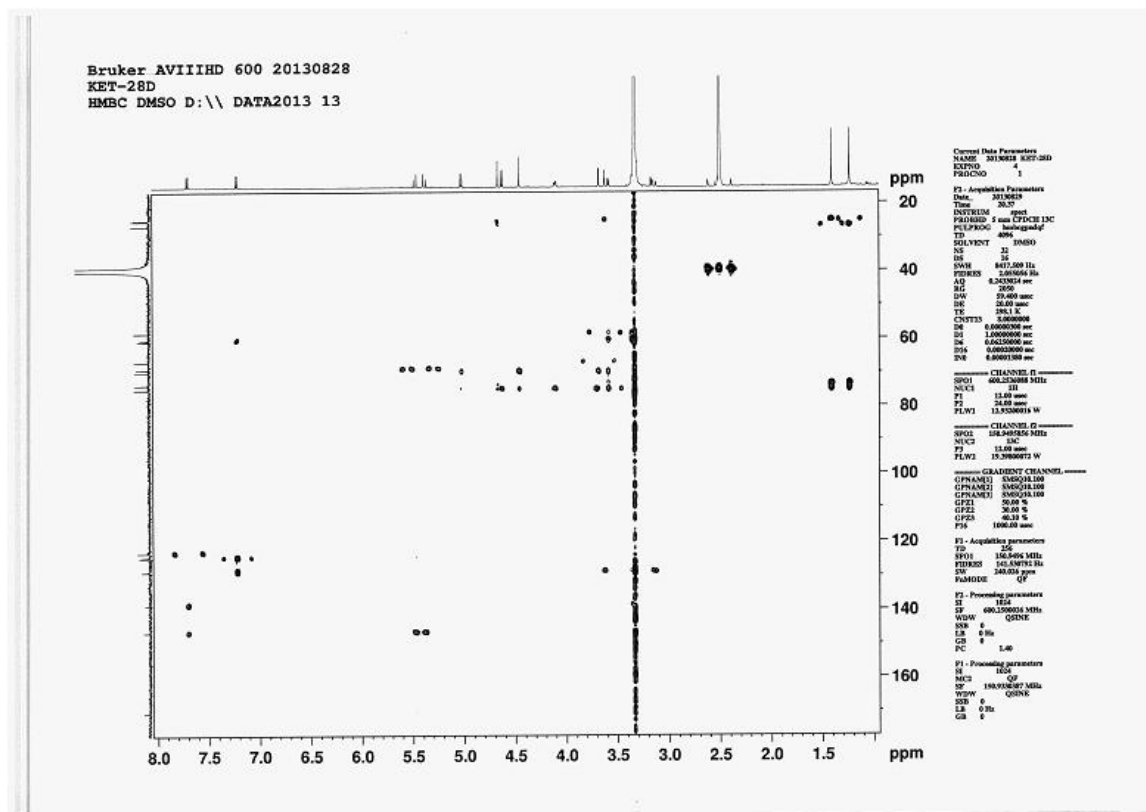
Bruker AVIIIHD 600 20130828
KET-28D
{H-H COSY} DMSO D:\ \ DATA2013 13



¹H,¹H COSY spectrum of compound 2

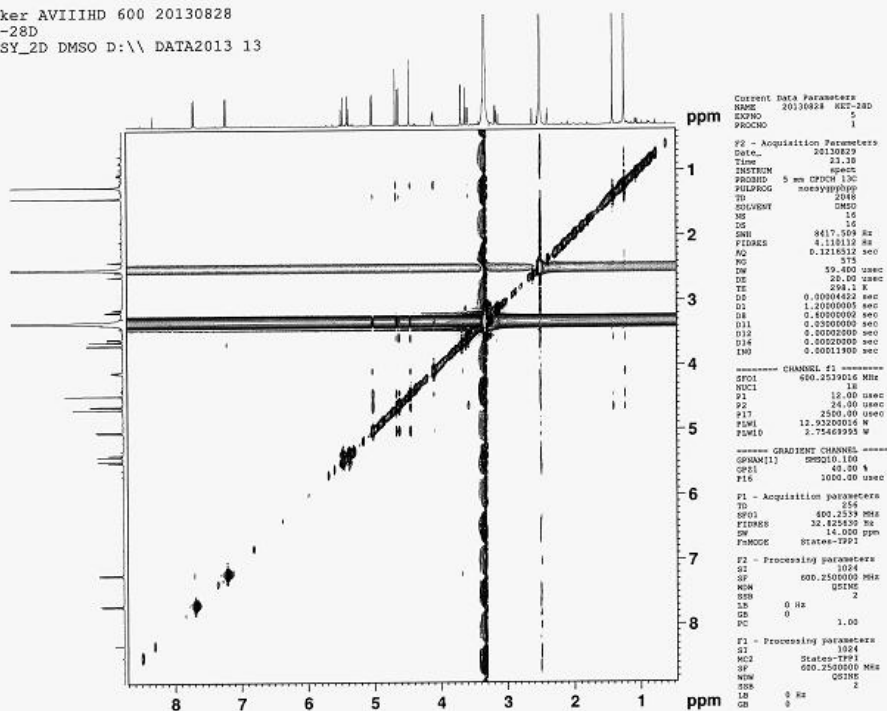


HSQC spectrum of compound 2

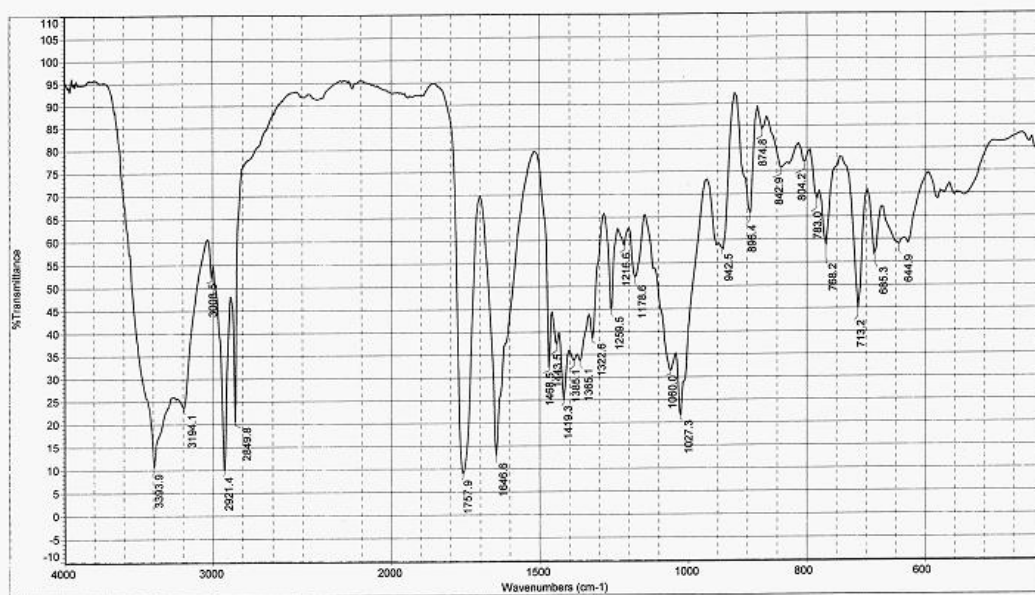


HMBC spectrum of compound 2

Bruker AVIIIHD 600 20130828
 KET-28D
 NOESY_2D DMSO D:\ DATA2013 13



NOESY spectrum of compound 2



日期: 星期五 1月 03 12:43:51 2014 (GMT+08:00) Sample Name: KET - 28D (显微镜透射法FT-IR Microscope Transmission)

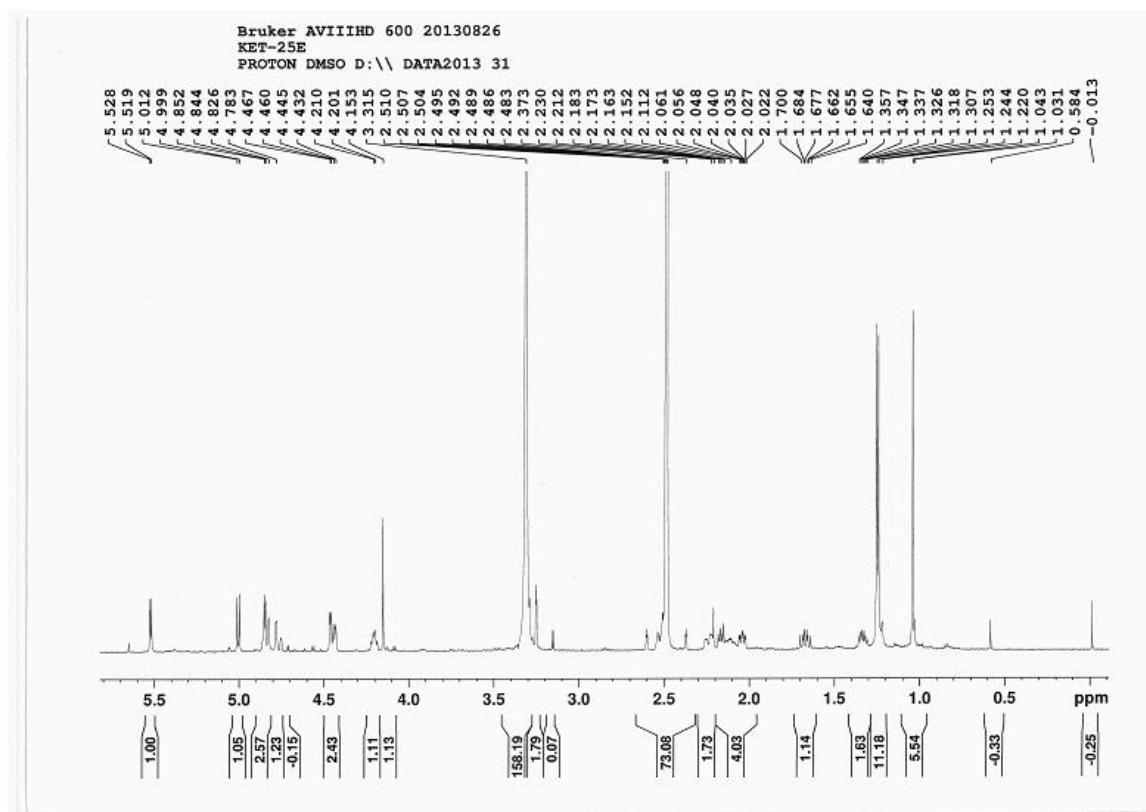
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傅里叶变换显微镜红外 (FT-IR Microscope): Centaurus

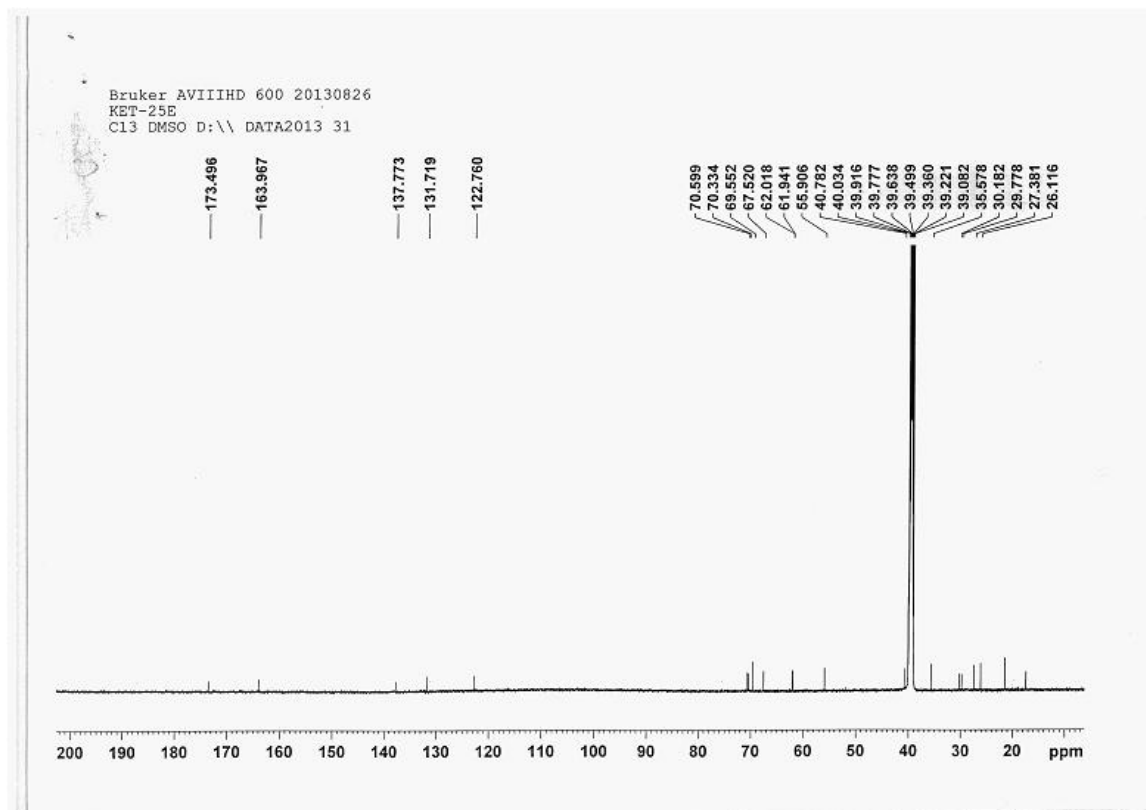
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美国热电公司 (Thermo) 傅里叶变换红外光谱仪: Nicolet 5700

IR spectrum of compound 2



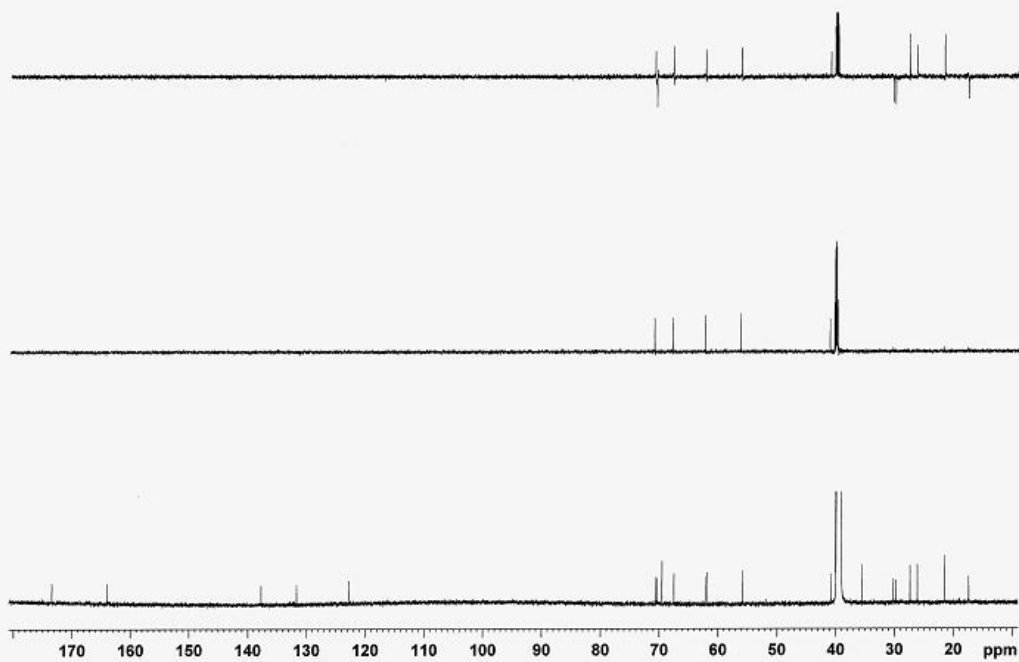
^1H NMR spectrum of compound **3** (600 MHz, $\text{DMSO-}d_6$)



^{13}C NMR spectrum of compound **3** (150 MHz, $\text{DMSO-}d_6$)



Bruker AVIHD 600 20130826
KET-25E DEPT DMSO D:\ DATA2013 31

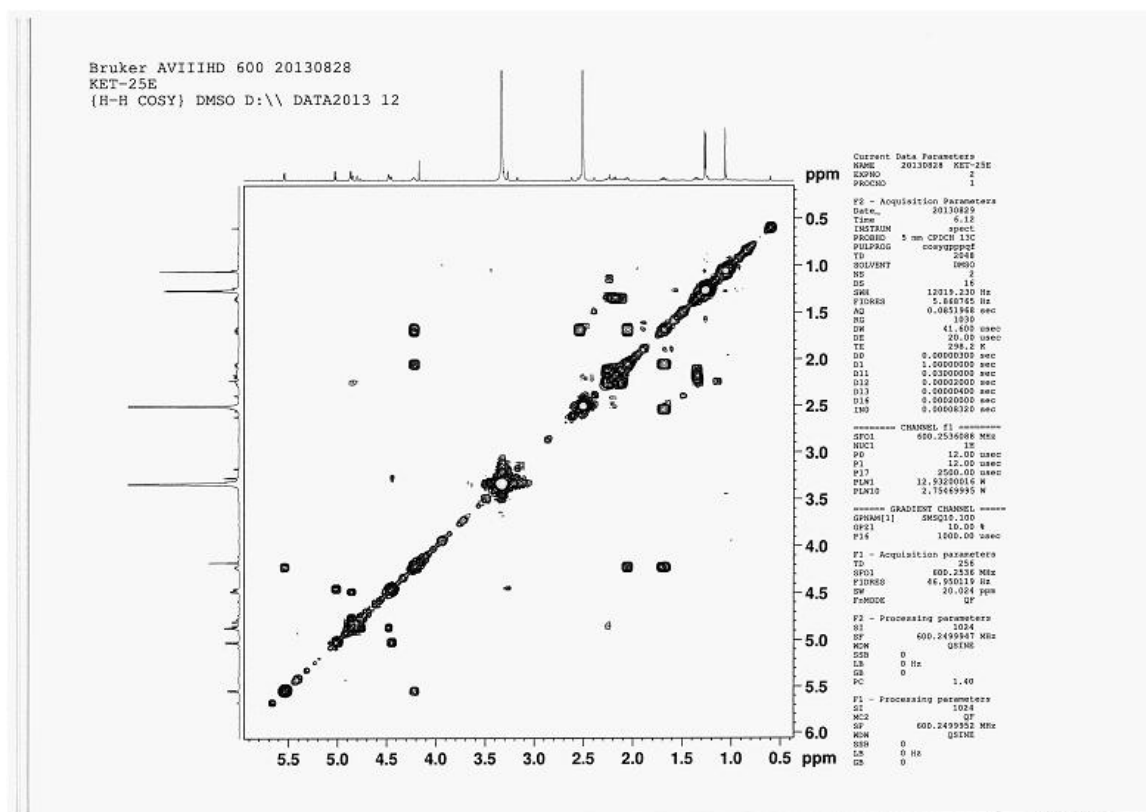


DEPT spectrum of compound 3 (150 MHz, DMSO-*d*₆)

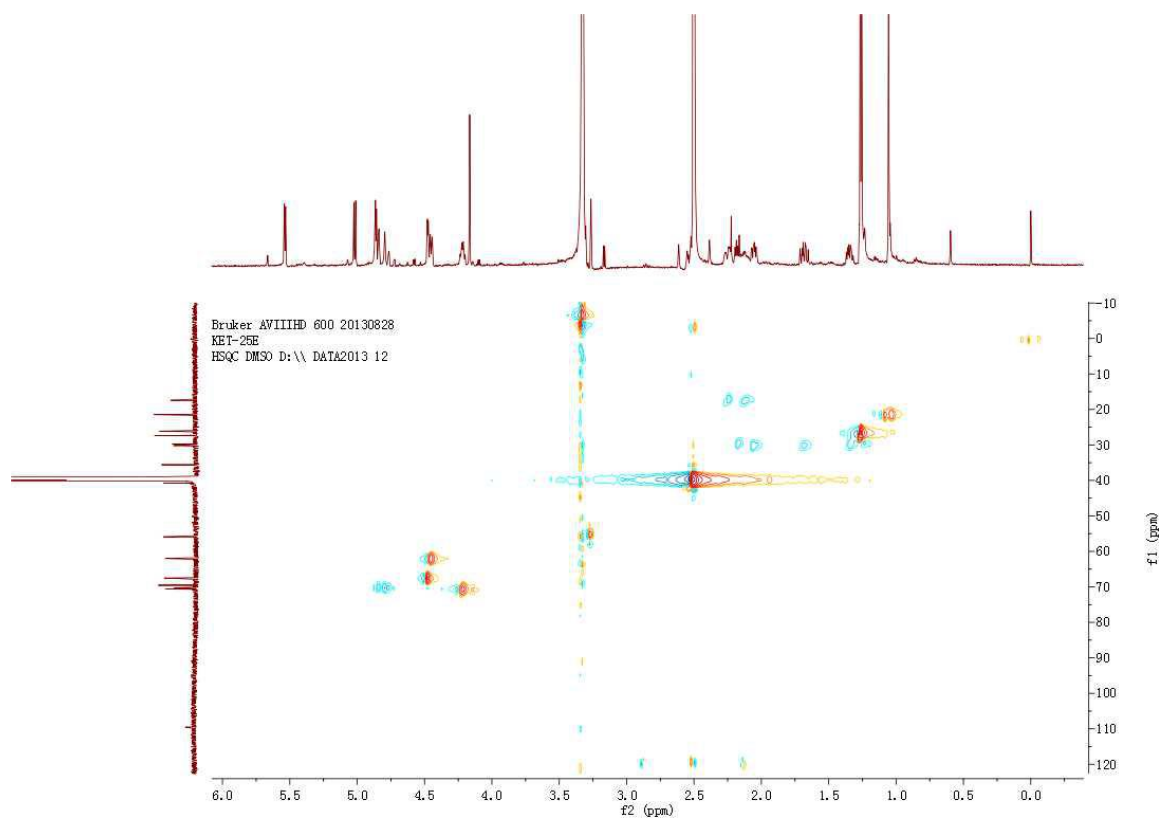
MS Formula Results: + Scan (4.699 min) Sub (2013090201.d)

m/z	Ion	Formula	Abundance											
378.1557	(M+H) ⁺	C28 H27 O7	36895.2											
Best	Formula (M)	Ion Formula	Calc. m/z	Score	Cross S	Mass	Calc. Mass	Diff (ppm)	Abs. Diff (ppm)	Abund. Match	Spiking Int.	Mass Match	m/z	DEC
[*]	C27 H22 Na O8	C27 H22 Na O8	378.1583	98.41		378.1684	378.1682	2.11	2.11	85.77	90.5	98.85	378.1557	11
[*]	C28 H26 O7	C28 H26 O7	378.1761	98.15		378.1684	378.1679	-1.4	-1.4	91.18	89.92	98.84	378.1557	8
[*]	C28 H26 O7 S	C28 H26 O7 S	379.1729	98.07		378.1684	378.1694	-8.93	8.03	90.18	87.95	87.82	378.1557	12
m/z	Ion	Formula	Abundance											
431.1574	(M+Na) ⁺	C28 H26 Na O7	43665.8											
Best	Formula (M)	Ion Formula	Calc. m/z	Score	Cross S	Mass	Calc. Mass	Diff (ppm)	Abs. Diff (ppm)	Abund. Match	Spiking Int.	Mass Match	m/z	DEC
[*]	C28 H26 O7	C28 H26 Na O7	431.1521	99.07		378.1682	378.1575	-0.8	-0.8	90.95	84.90	99.80	431.1574	8
[*]	C27 H22 Na O8	C27 H22 Na O8	431.1594	98.83		378.1682	378.1596	-2.73	2.73	82.2	90	88.78	431.1574	11
[*]	C28 H26 O7 S	C28 H26 Na O7 S	431.1594	98.89		378.1682	378.1654	-7.42	7.42	97.14	85.85	98.99	431.1574	12

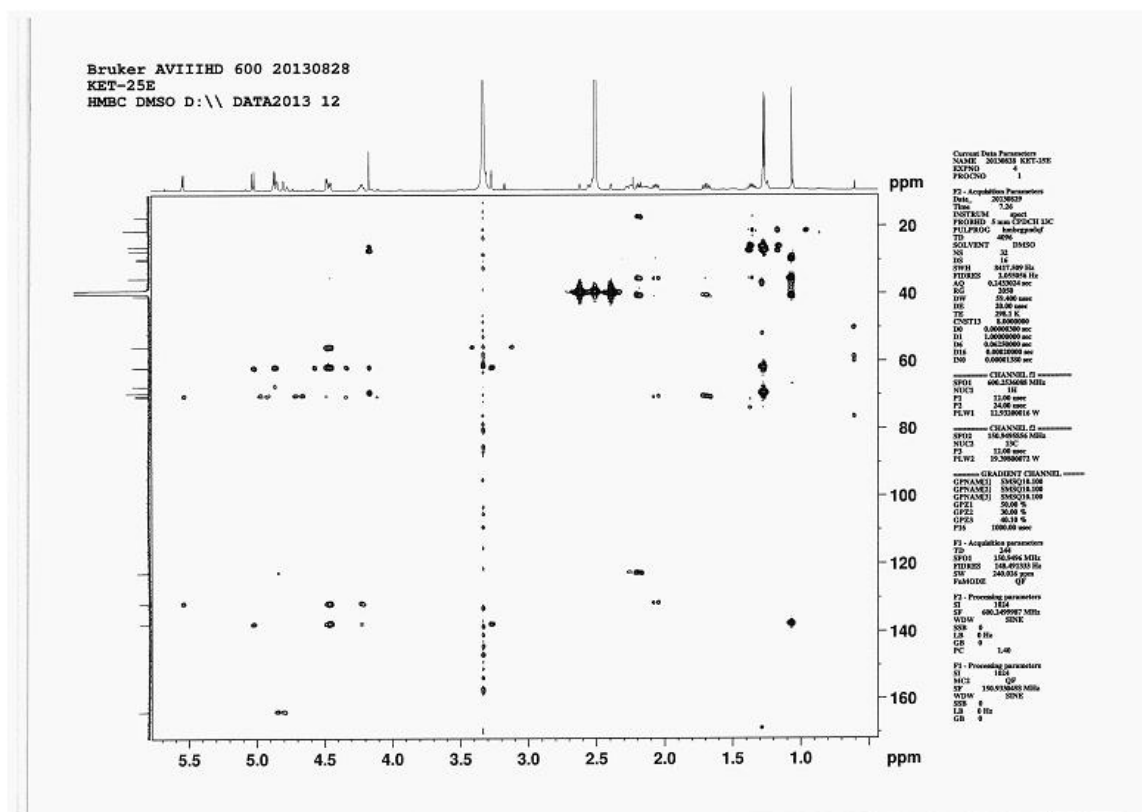
HRESIMS spectrum of compound 3



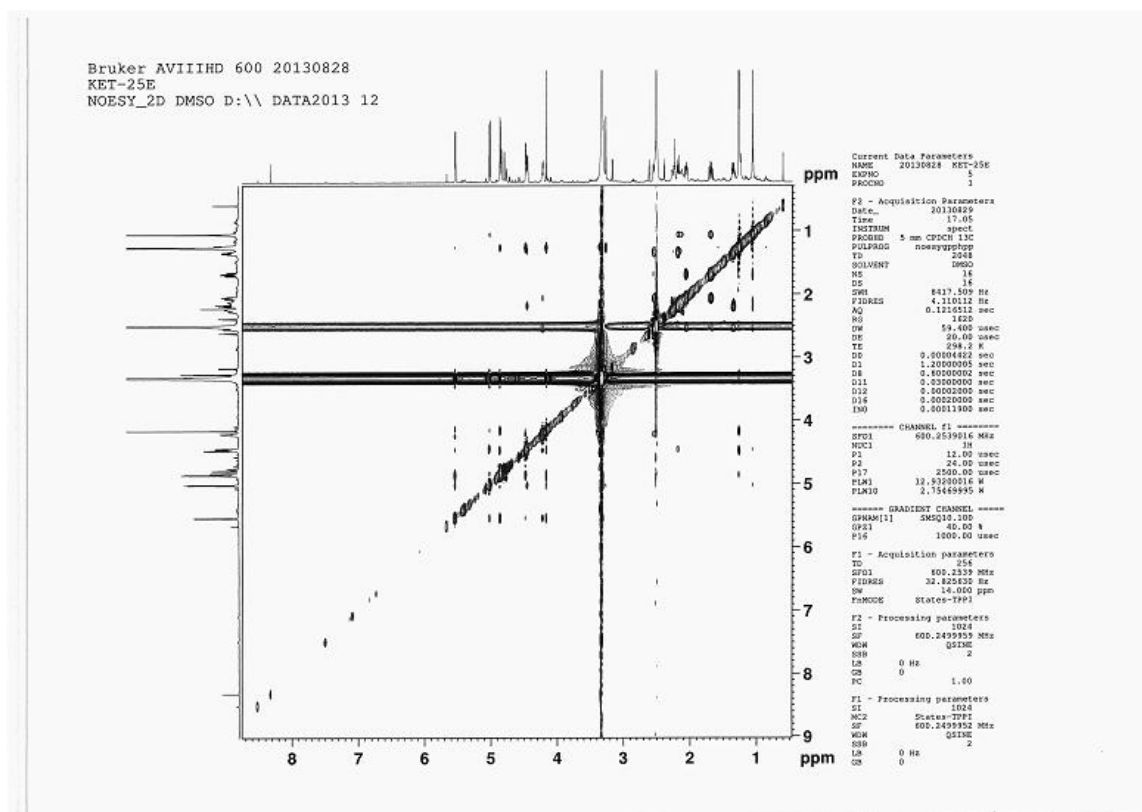
$^1\text{H}, ^1\text{H}$ COSY spectrum of compound 3



HSQC spectrum of compound 3



HMBC spectrum of compound 3



NOESY spectrum of compound 3