Rings A,D-*seco* Limonoids from the Stems of *Clausena emarginata*

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Supporting Information

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For Compound 3:

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For Compound 6:

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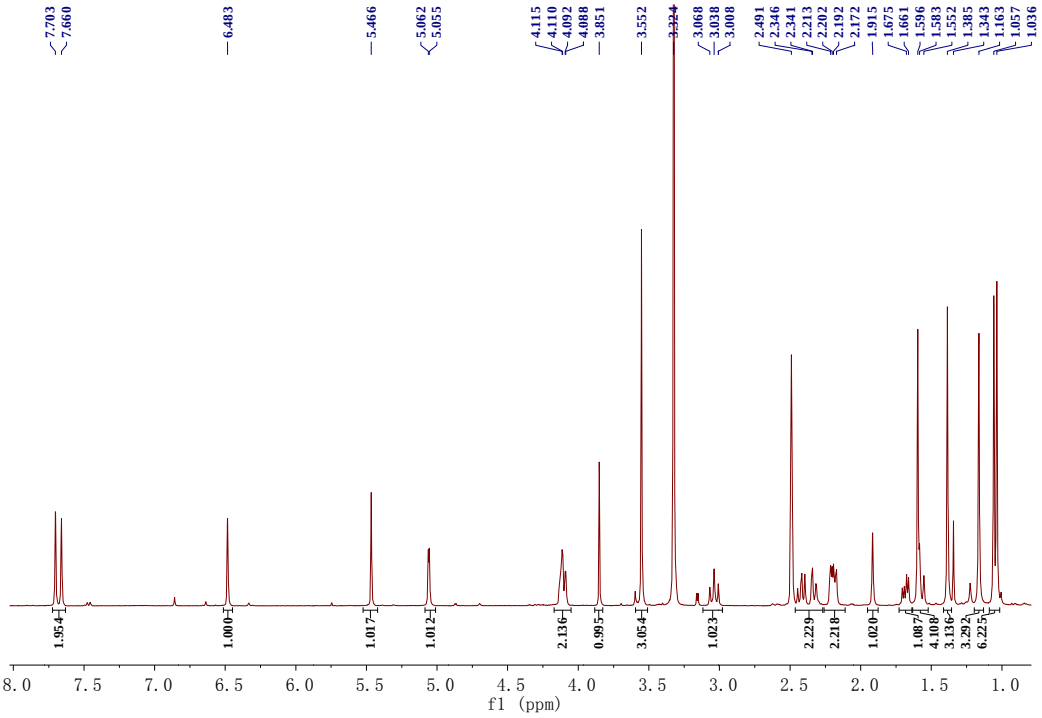
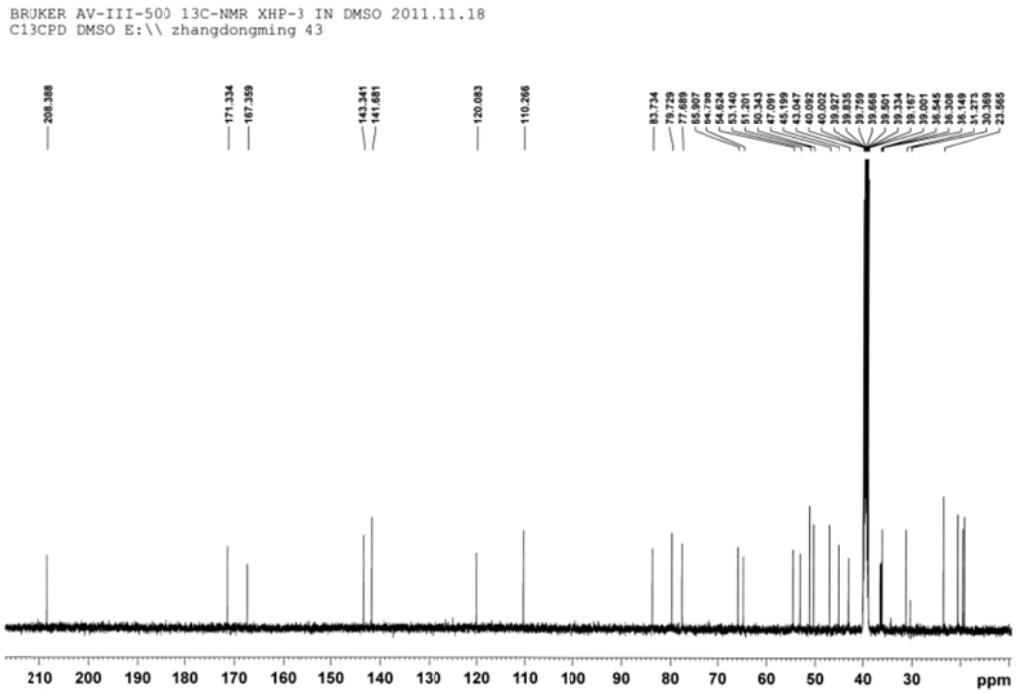
For Compound 11:

For Compound 12:

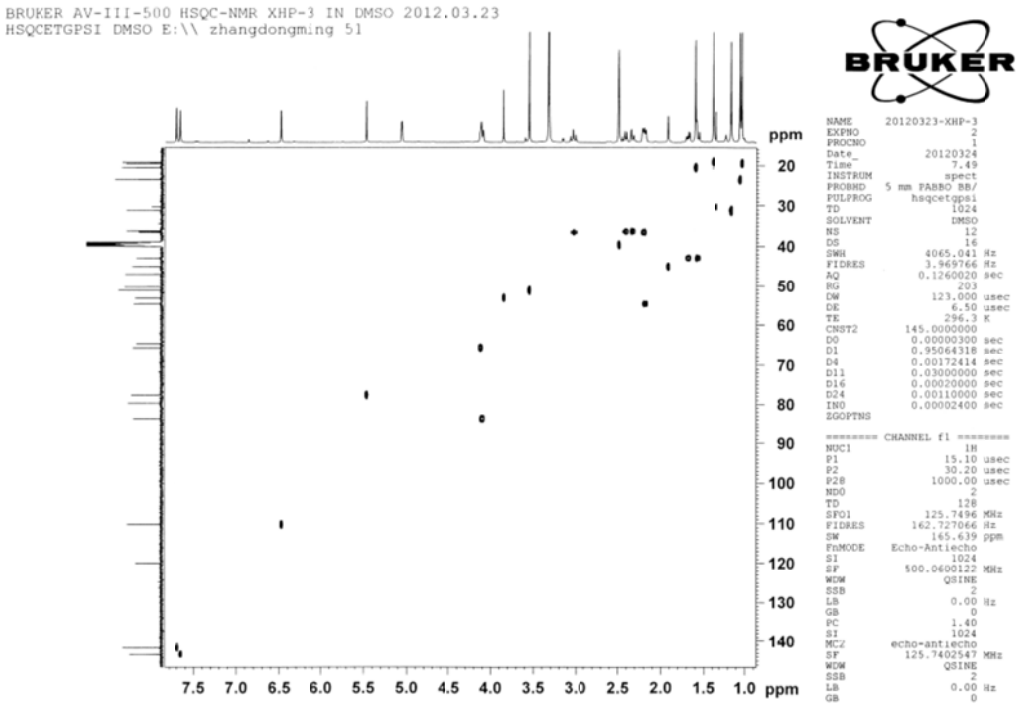
S1. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **1**



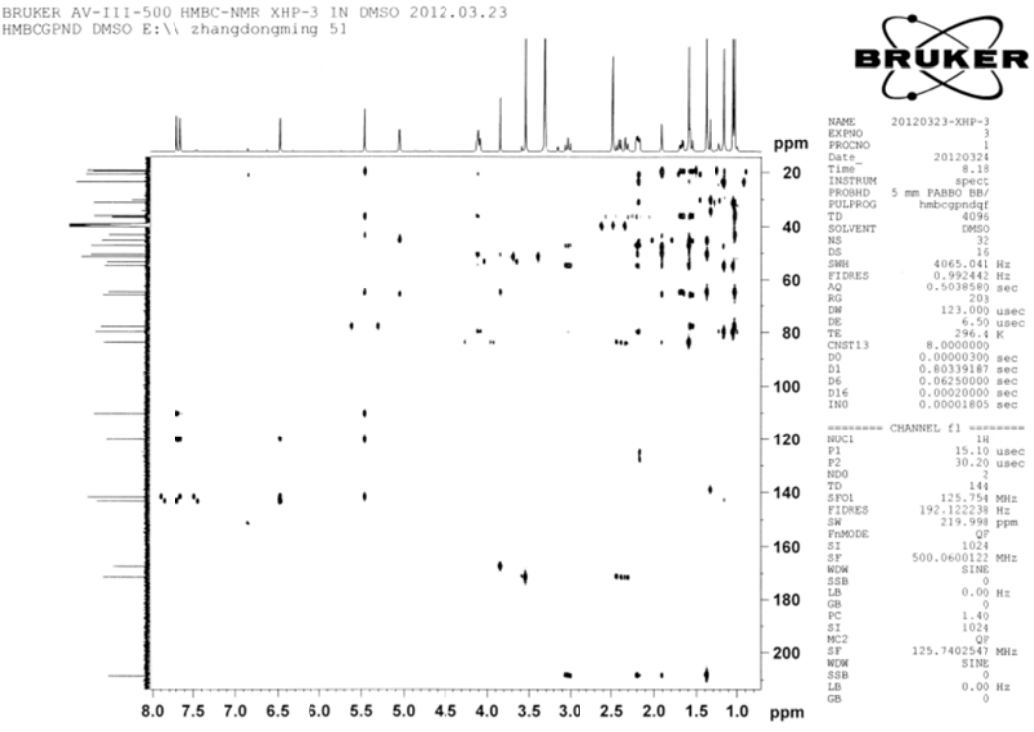
S2. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **1**



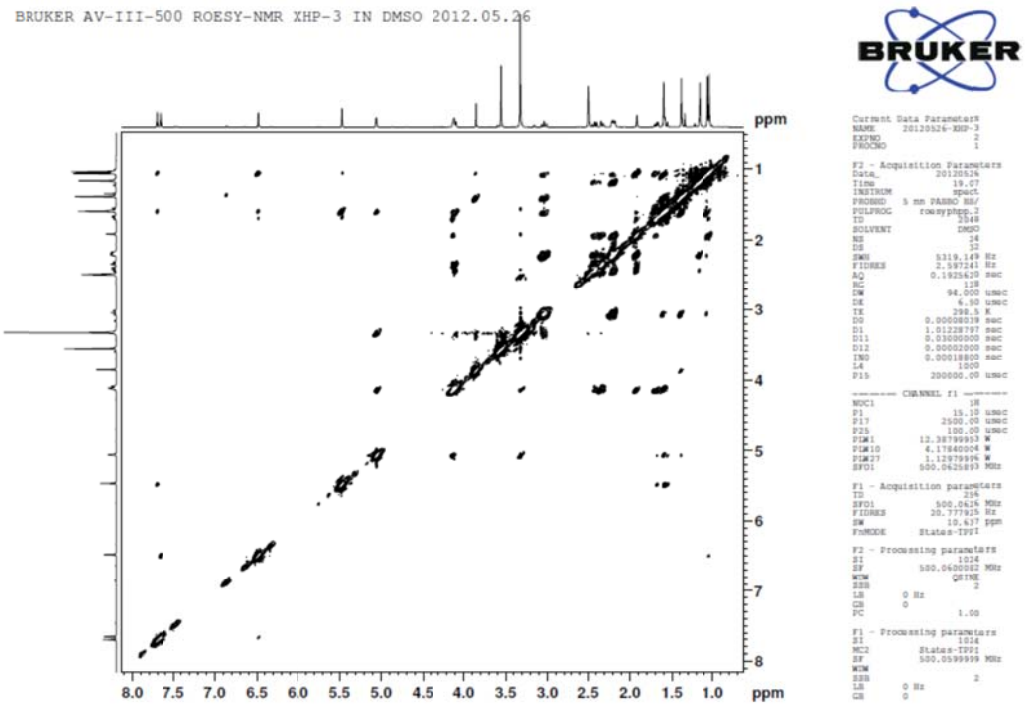
S3. HSQC Spectrum of Compound **1**



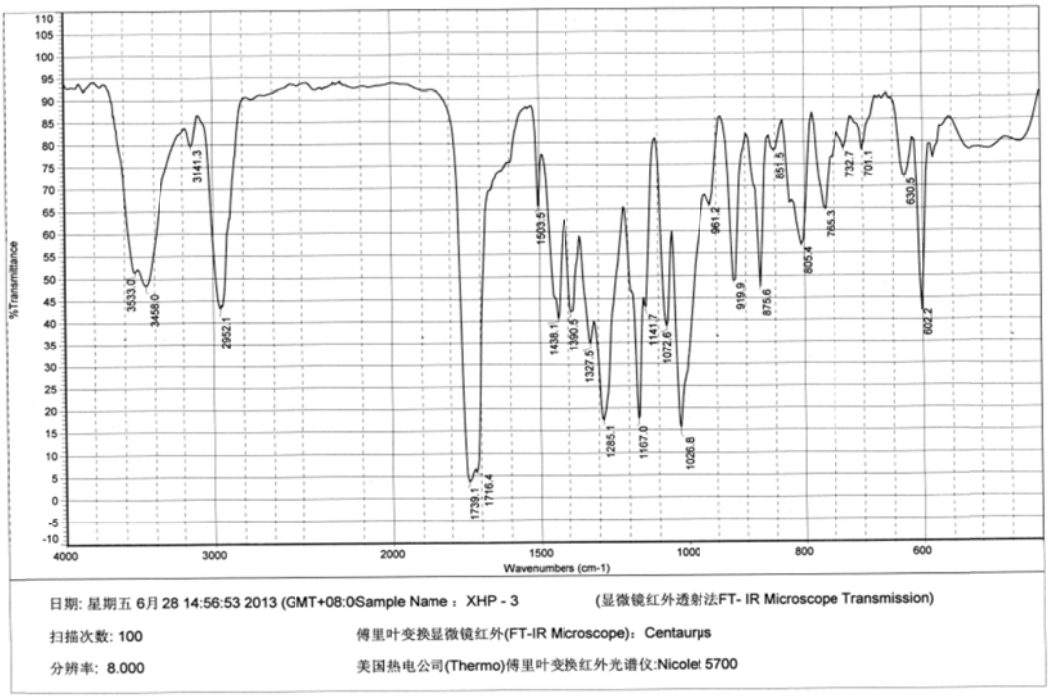
S4. HMBC Spectrum of Compound **1**



S5. ROESY Spectrum of Compound **1**



S6. IR Spectrum of Compound **1**



S7. HRESIMS Spectrum of Compound **1**

MS Formula Results: + Scan (6.775 min) Sub (2012040902.d)

m/z	Ion	Formula	Abundance
503.2285	(M+H)+	C27 H35 O9	4986615

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
☑	**C27 H34 O9**	**C27 H35 O9**	**503.2276**	**99.29**		**502.2212**	**502.2203**	**-1.8**	**1.8**	**97.73**	**99.94**	**99.89**	**503.2285**	11
☐	C31 H34 O4 S	C31H35 O4 S	503.2251	98.72		502.2212	502.2178	-6.8	6.8	98.55	99.51	98.43	503.2285	15
☐	C33 H30 N2 O3	C33 H31 N2 O3	503.2329	98.66		502.2212	502.2256	8.86	8.86	99.75	99.96	97.35	503.2285	20
☐	C28 H38 O4 S2	C28 H39 O4 S2	503.2284	97.61		502.2212	502.2212	-0.1	0.1	92.59	98.85	100	503.2285	10
☐	C24 H38 O9 S	C24H39 O9 S	503.2309	97.56		502.2212	502.2237	4.89	4.89	93.39	99.31	99.18	503.2285	6
☐	C22 H34 N2 O11	C22 H35 N2 O11	503.2235	96.28		502.2212	502.2163	-9.83	9.83	92.44	99.96	96.75	503.2285	7
☐	C19 H38 N2 O11 S	C19 H39N2 O11 S	503.2269	95.72		502.2212	502.2196	-3.14	3.14	86.3	99.13	99.66	503.2285	2
☐	C23 H38 N2 O6 S2	C23 H39N2 O6 S2	503.2244	95.38		502.2212	502.2171	-8.13	8.13	88.71	98.63	97.77	503.2285	6
☐	C20 H38 O14	C20 H39 O14	503.2334	94.9		502.2212	502.2262	9.89	9.89	87.68	99.93	96.71	503.2285	2

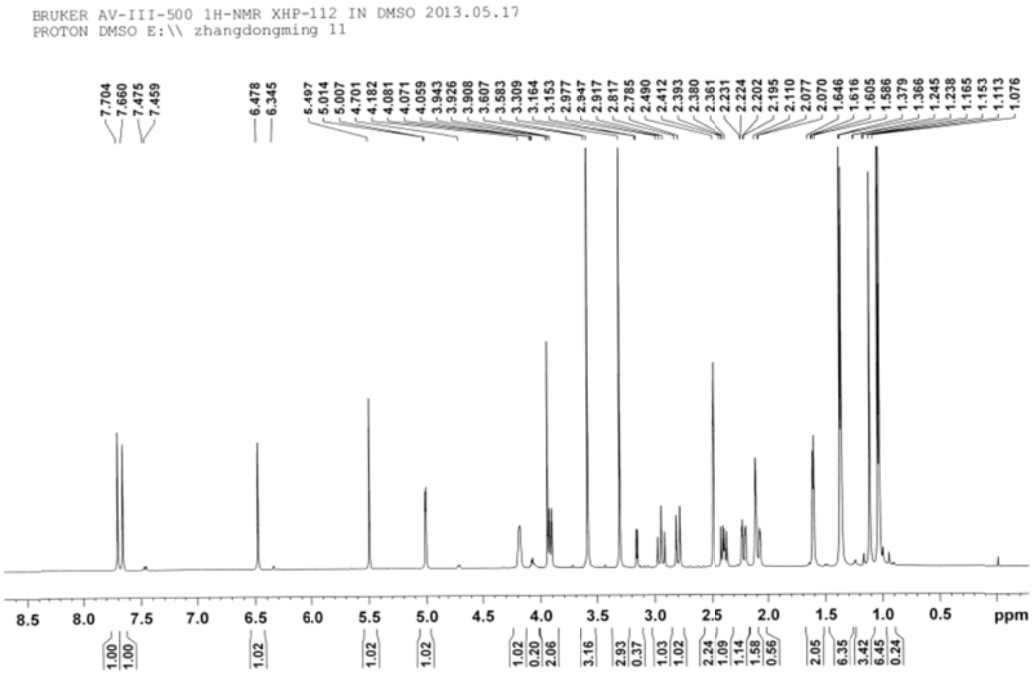
m/z	Ion	Formula	Abundance
520.2551	(M+NH4)+	C27H38 N O9	5463927

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
☑	**C27 H34 O9**	**C27H38 N O9**	**520.2541**	**99.17**		**502.2212**	**502.2203**	**-1.87**	**1.87**	**97.34**	**99.91**	**99.89**	**520.2551**	11
☐	C33 H30 N2 O3	C33 H34 N3 O3	520.2595	98.75		502.2212	502.2256	8.79	8.79	99.77	99.93	97.54	520.2551	20
☐	C31 H34 O4 S	C31 H38 N O4 S	520.2516	98.75		502.2212	502.2178	-6.86	6.86	98.56	99.47	98.5	520.2551	15
☐	C28 H38 O4 S2	C28 H42 N O4 S2	520.255	97.6		502.2212	502.2212	-0.16	0.16	92.6	98.79	100	520.2551	10
☐	C24 H38 O9 S	C24 H42 N O9 S	520.2575	97.48		502.2212	502.2237	4.83	4.83	93.04	99.26	99.25	520.2551	6
☐	C22 H34 N2 O11	C22 H38 N3 O11	520.2501	96.18		502.2212	502.2163	-9.89	9.89	91.84	99.94	96.9	520.2551	7
☐	C19 H38 N2 O11 S	C19 H42 N3 O11 S	520.2535	95.57		502.2212	502.2196	-3.2	3.2	85.81	99.09	99.67	520.2551	2
☐	C23 H38 N2 O6 S2	C23 H42 N3 O6 S2	520.251	95.37		502.2212	502.2171	-8.19	8.19	88.53	98.57	97.87	520.2551	6
☐	C20 H38 O14	C20 H42 N O14	520.26	94.81		502.2212	502.2262	9.83	9.83	87.02	99.91	96.94	520.2551	2

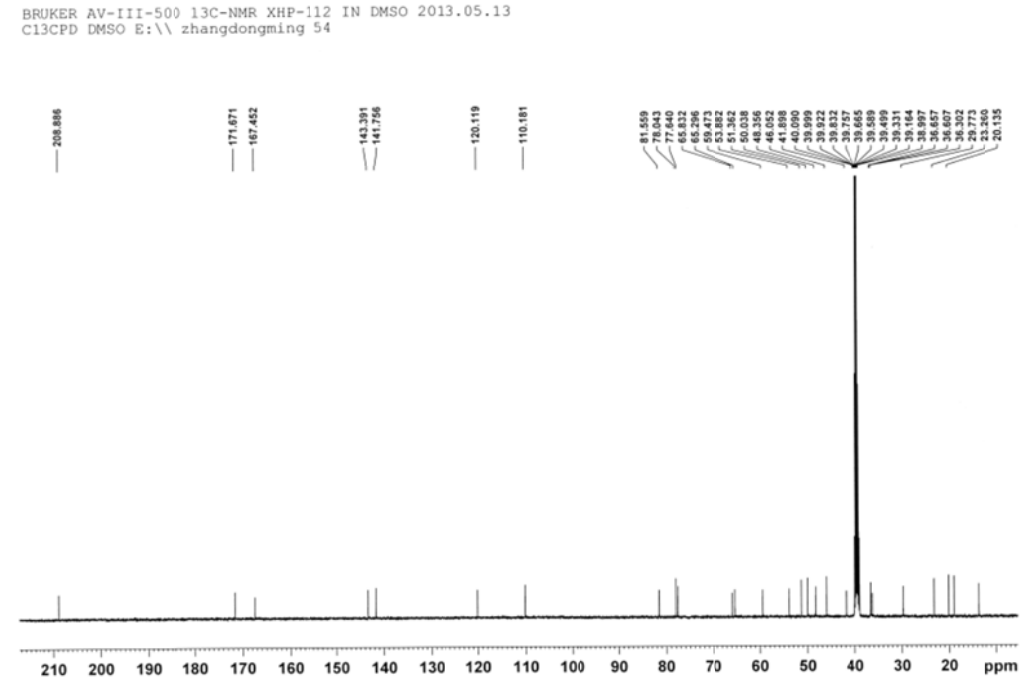
m/z	Ion	Formula	Abundance
525.2103	(M+Na)+	C27 H34 Na O9	1098874

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
☑	**C27 H34 O9**	**C27 H34 Na O9**	**525.2095**	**99.93**		**502.2211**	**502.2203**	**-1.55**	**1.55**	**99.89**	**100**	**99.92**	**525.2103**	11
☐	C31 H34 O4 S	C31 H34 Na O4 S	525.207	98.61		502.2211	502.2178	-6.54	6.54	97.61	99.73	98.66	525.2103	15
☐	C24 H38 O9 S	C24 H38 Na O9 S	525.2129	98.52		502.2211	502.2237	5.16	5.16	96.54	99.6	99.16	525.2103	6
☐	C33 H30 N2 O3	C33 H30N2 Na O3	525.2149	98.14		502.2211	502.2256	9.12	9.12	97.82	100	97.41	525.2103	20
☐	C22 H34 N2 O11	C22 H34 N2 Na O11	525.2055	97.89		502.2211	502.2163	-9.57	9.57	97.38	100	97.15	525.2103	7
☐	C28 H38 O4 S2	C28 H38 Na O4 S2	525.2104	97.78		502.2211	502.2212	0.17	0.17	92.79	99.31	100	525.2103	10
☐	C19 H38 N2 O11 S	C19 H38 NJ Na O11 S	525.2089	97.43		502.2211	502.2196	-2.87	2.87	91.89	99.47	99.74	525.2103	2
☐	C23 H38 N2 O6 S2	C23 H38 NJ Na O6 S2	525.2063	96.38		502.2211	502.2171	-7.85	7.85	91.24	99.16	98.07	525.2103	6

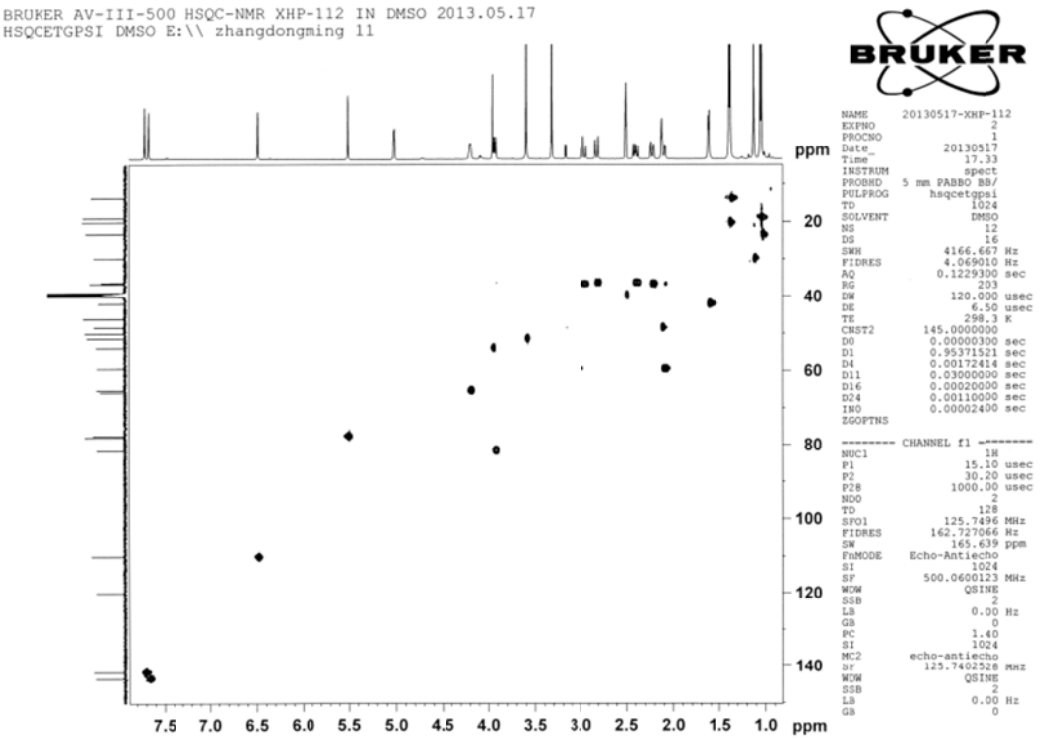
S8. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **2**



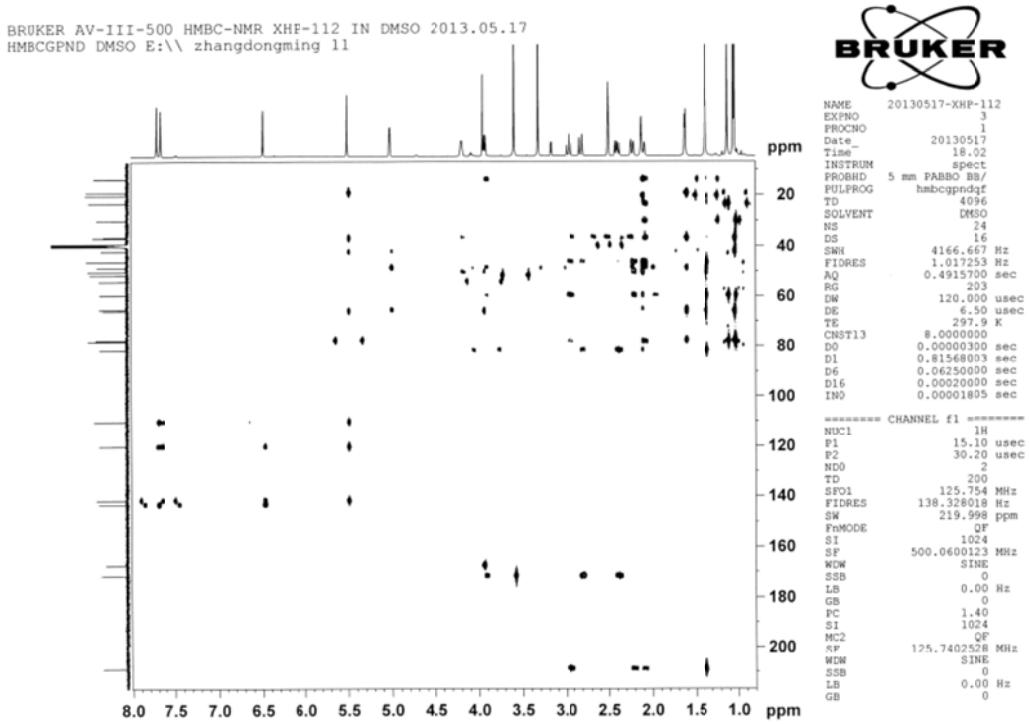
S9. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **2**



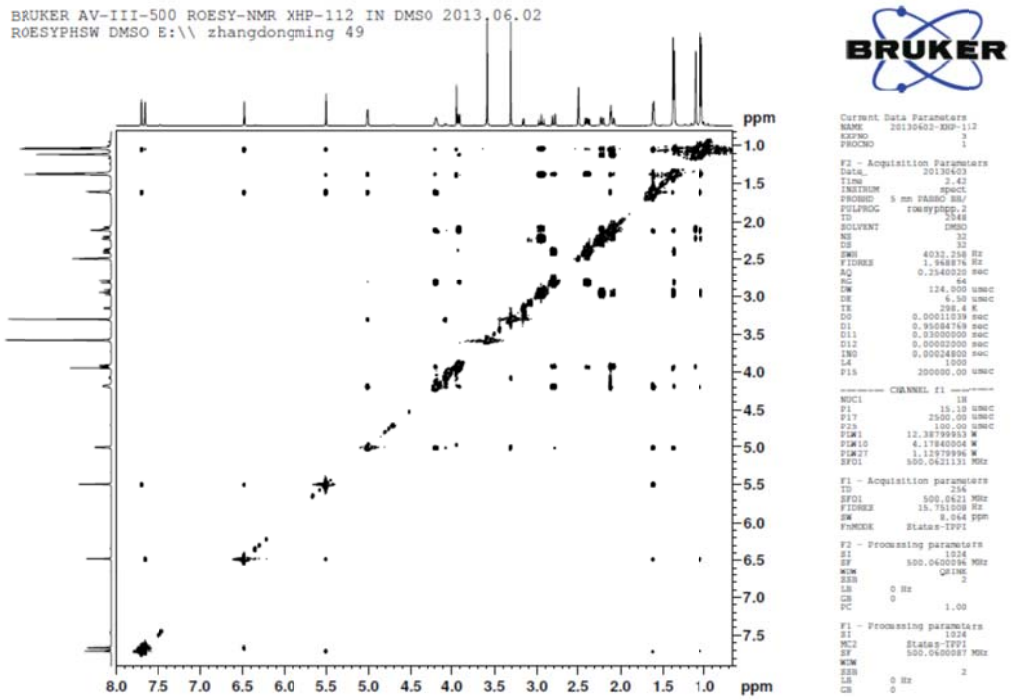
S10. HSQC Spectrum of Compound **2**



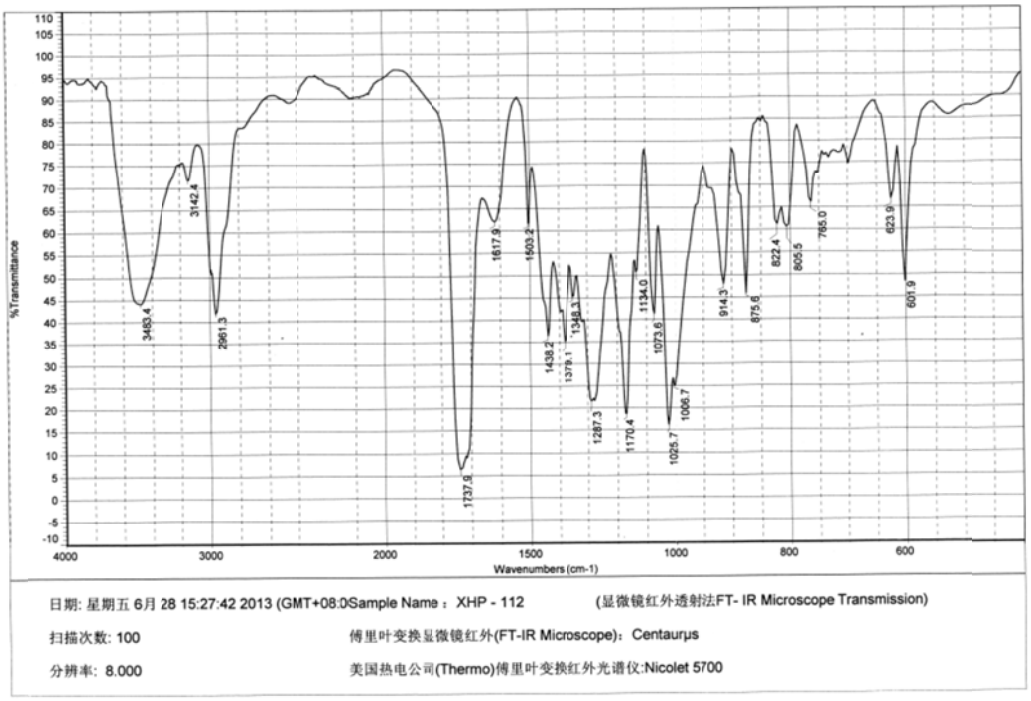
S11. HMBC Spectrum of Compound **2**



S12. ROESY Spectrum of Compound **2**



S13. IR Spectrum of Compound **2**



S14. HRESIMS Spectrum of Compound **2**

MS Formula Results: + Scan (6.836 min) Sub (2013050202.d)

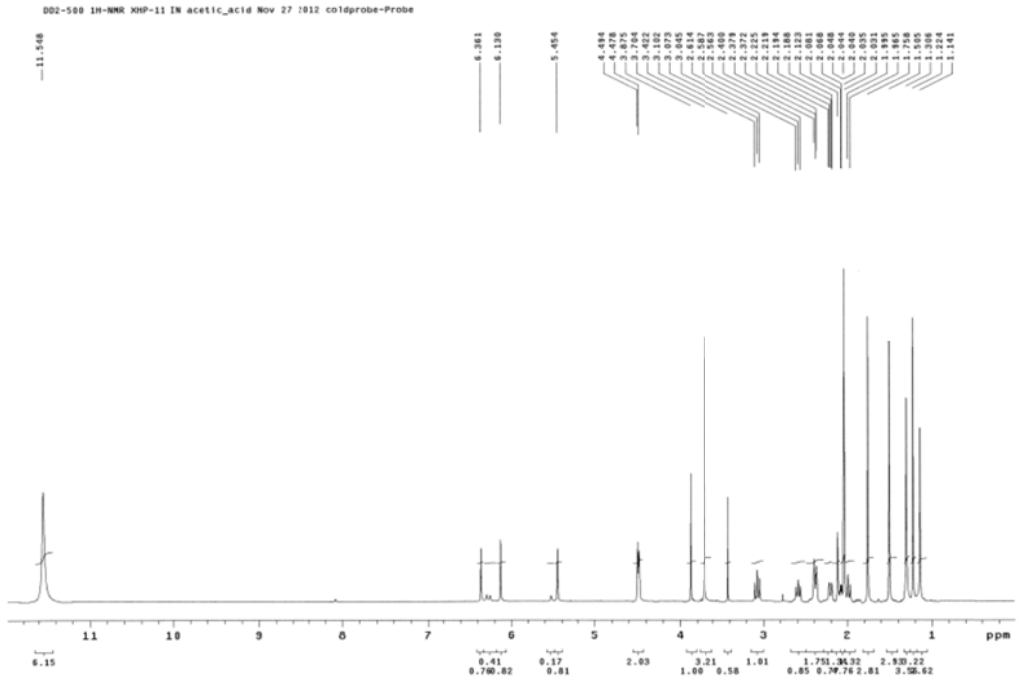
	m/z	Ion	Formula	Abundance
+	503.2277	(M+H)+	C27 H35 O9	2439140.5

	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
+	☑	C27 H34 O9	C27 H35 O9	503.2276	99.89		502.2204	502.2203	-0.29	0.29	99.72	99.87	100	503.2277	11
+	☐	C31 H34 O4 S	C31H35 O4 S	503.2251	98.8		502.2204	502.2178	-5.28	5.28	97.83	99.47	99.05	503.2277	15
+	☐	C24 H38 O9 S	C24H39 O9 S	503.2309	98.04		502.2204	502.2237	6.42	6.42	96.04	99.32	98.8	503.2277	6

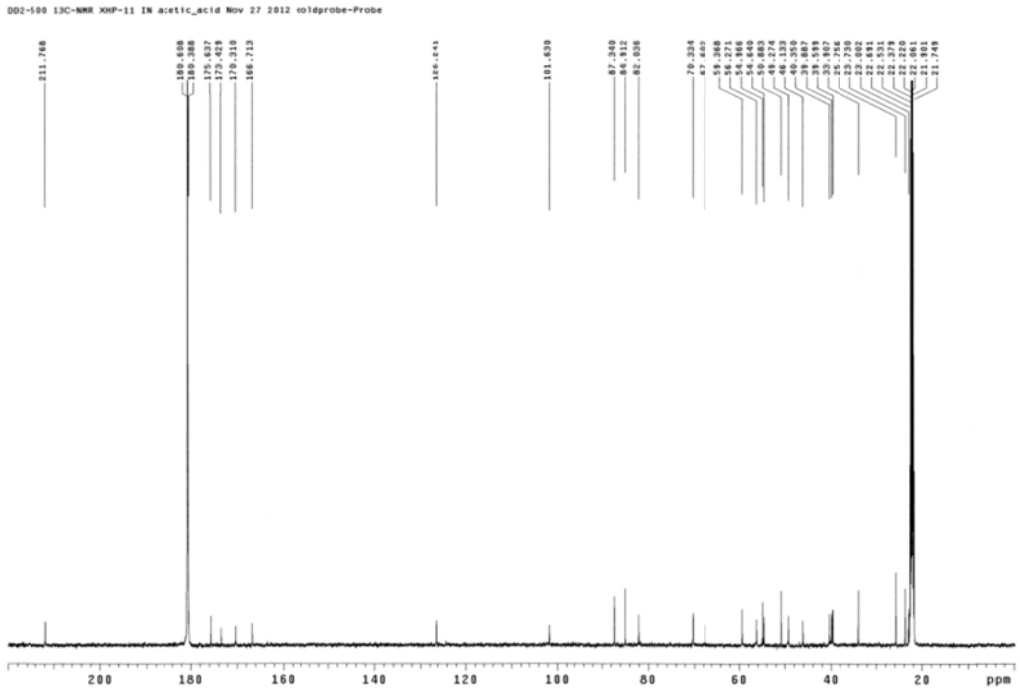
	m/z	Ion	Formula	Abundance
+	525.2096	(M+Na)+	C27 H34 Na O9	1782246.8

	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
+	☑	C27 H34 O9	C27 H34 Na O9	525.2095	99.89		502.2204	502.2203	-0.29	0.29	99.72	99.89	100	525.2096	11
+	☐	C31 H34 O4 S	C31 H34 Na O4 S	525.207	98.76		502.2204	502.2178	-5.28	5.28	97.57	99.56	99.12	525.2096	15
+	☐	C24 H38 O9 S	C24 H38 Na O9 S	525.2129	98.04		502.2204	502.2237	6.41	6.41	95.75	99.43	98.71	525.2096	6

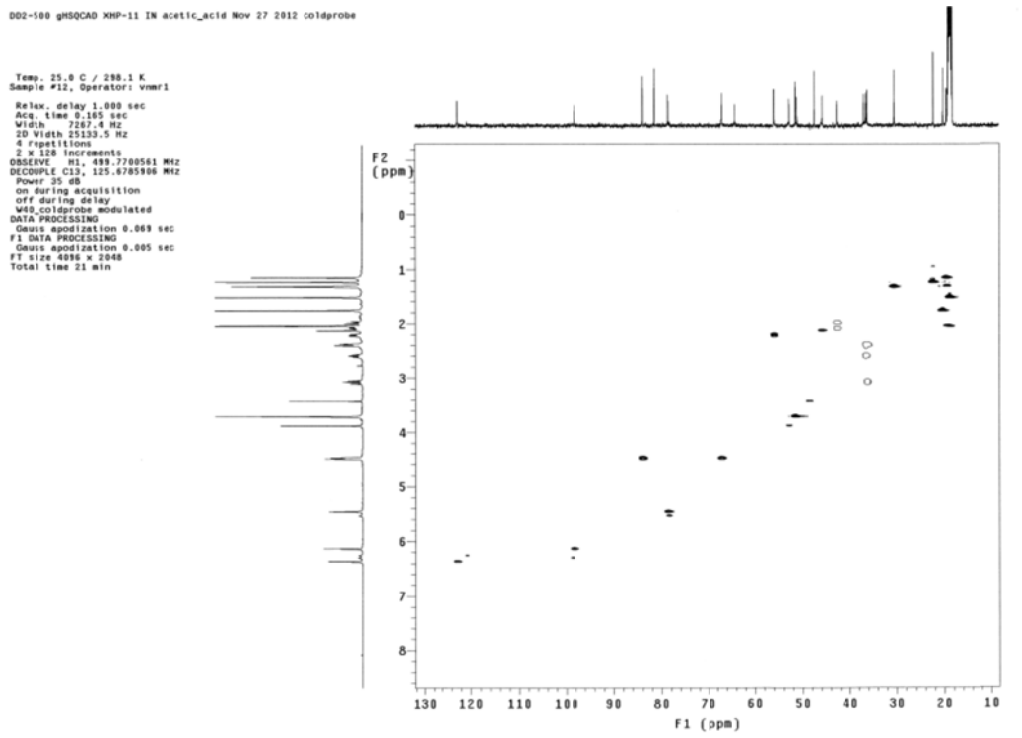
S15. ^{1}H NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **3**



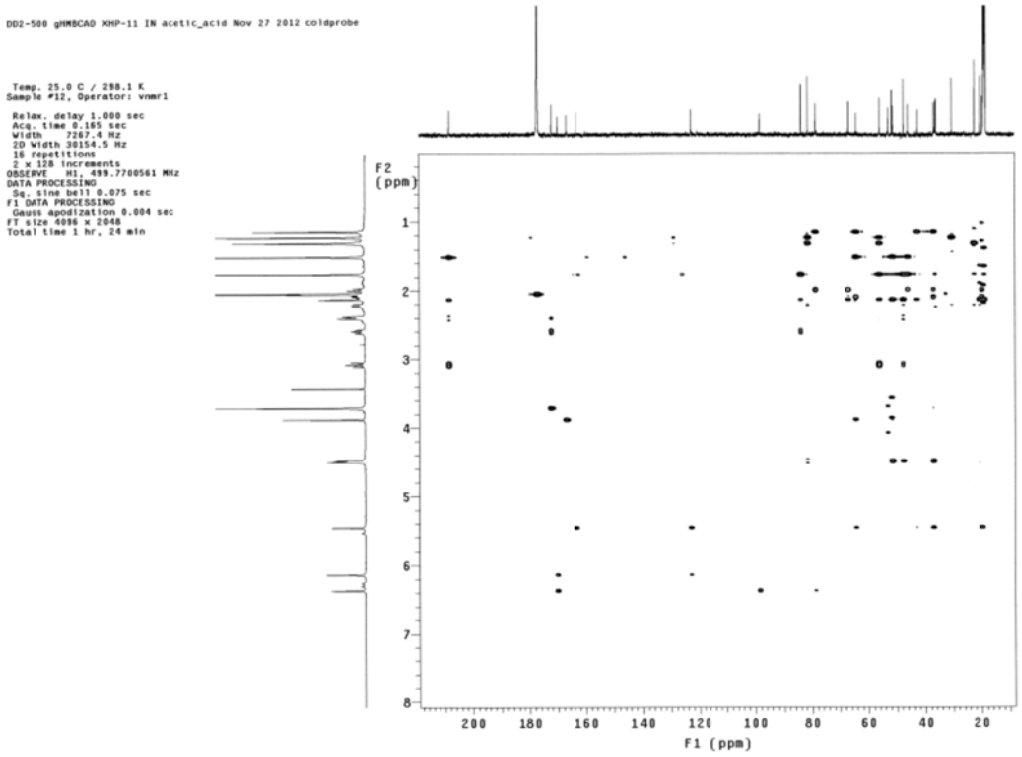
S16. ^{13}C NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **3**



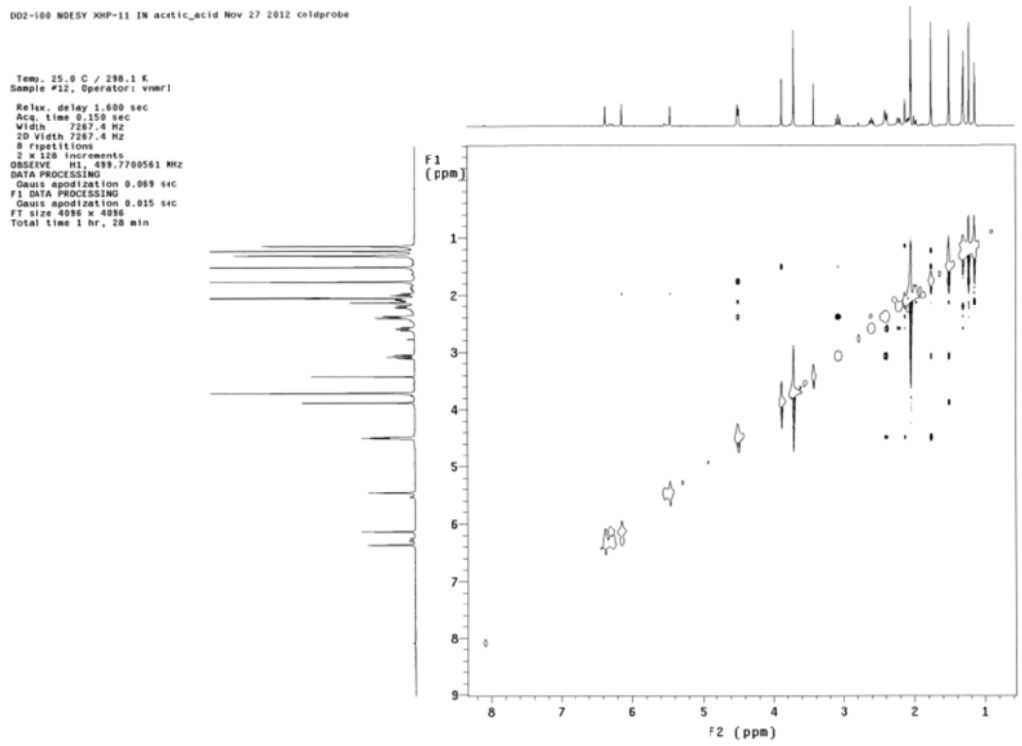
S17. HSQC Spectrum of Compound **3**



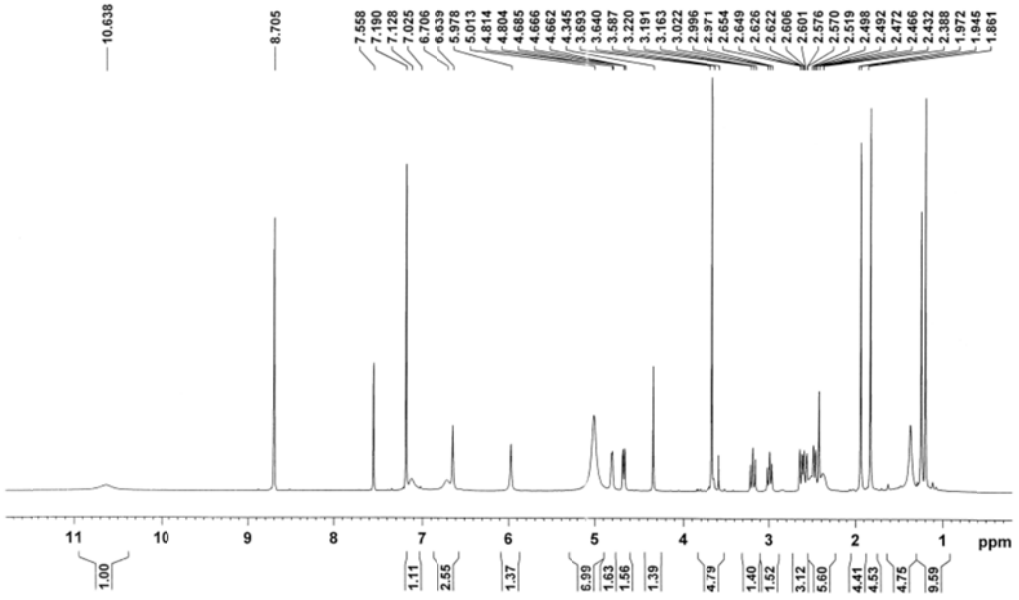
S18. HMBC Spectrum of Compound **3**



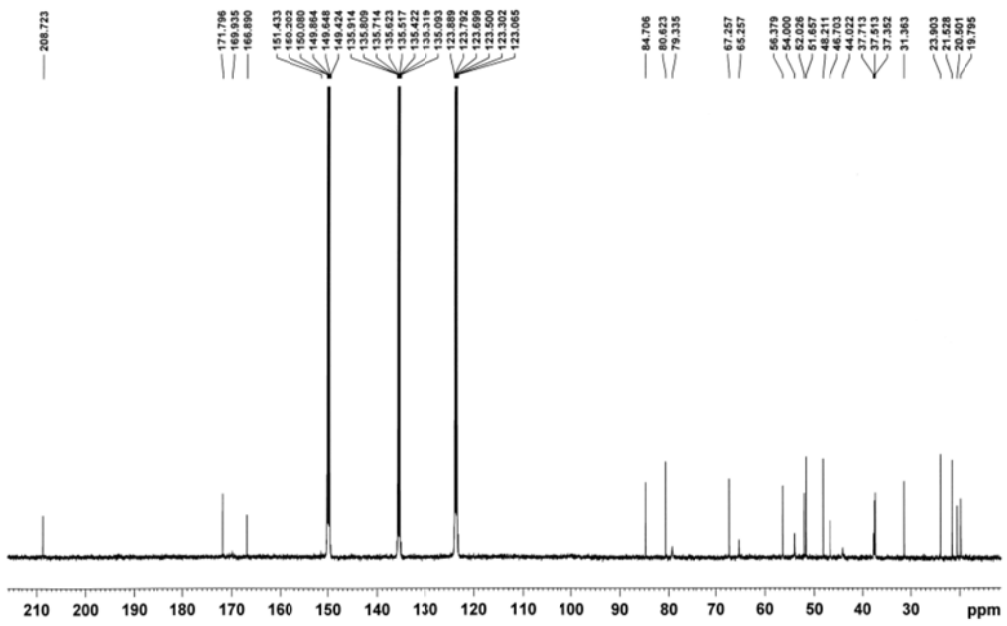
S19. NOESY Spectrum (in acetic acid-d_4) of Compound **3**



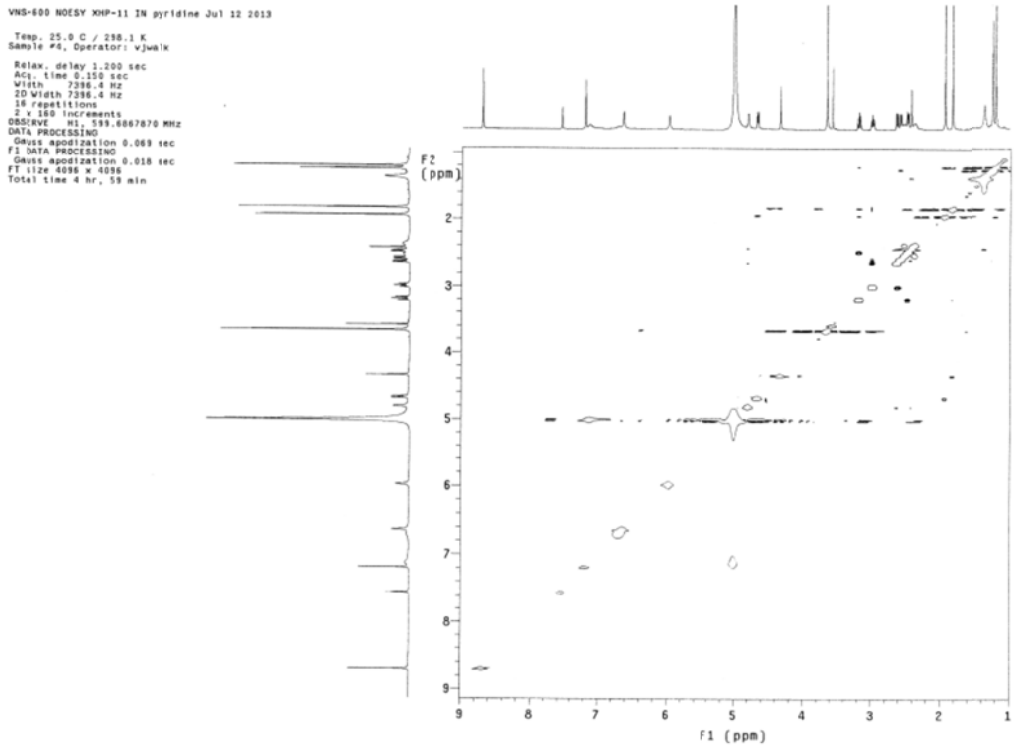
S20. ^{1}H NMR Spectrum (500 MHz, pyridine-d_5) of Compound **3**



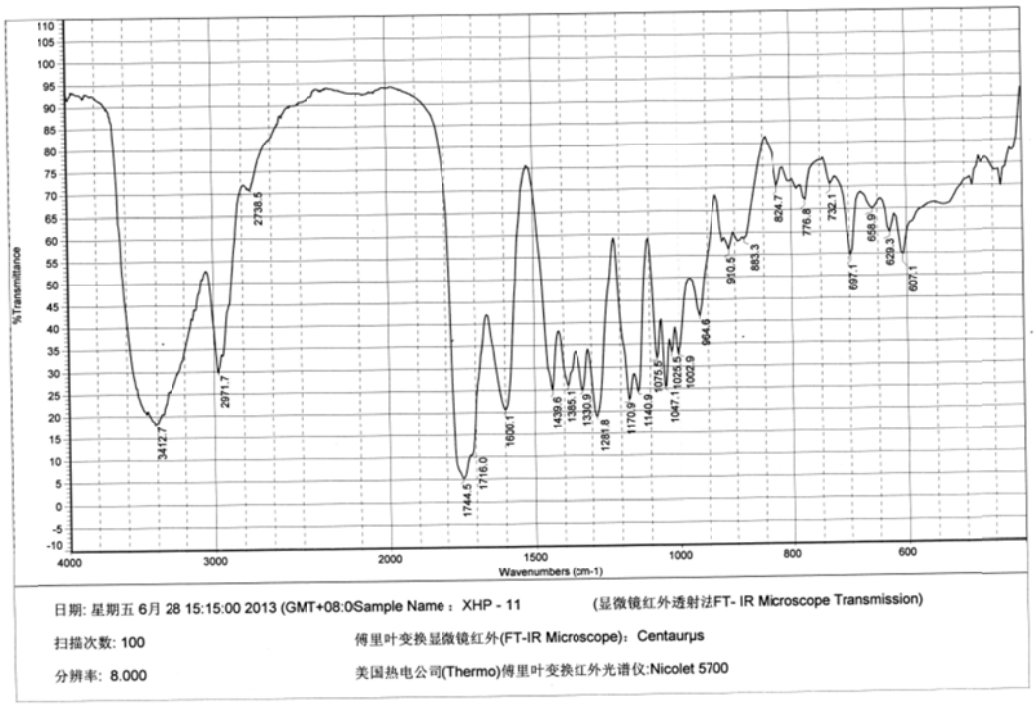
S21. ^{13}C NMR Spectrum (125 MHz, pyridine-d_5) of Compound **3**



S22. NOESY Spectrum (in pyridine-d_5) of Compound **3**



S23. IR Spectrum of Compound **3**



S24. HRESIMS Spectrum of Compound **3**

MS Formula Results: + Scan (6.136 min) Sub (2012050301.d)

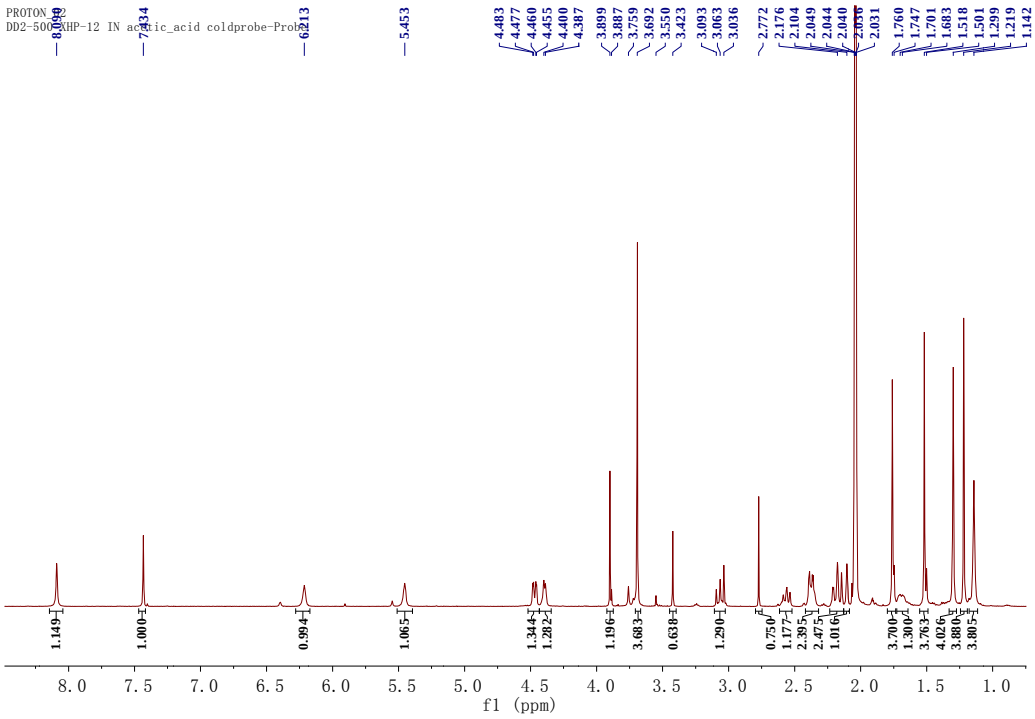
m/z	Ion	Formula	Abundance
535.2182	(M+H)+	C27 H35 O11	3308701.3

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
	C28 H30 N4 O7	C28 H31 N4 O7	535.2187	99.93		534.2109	534.2114	1.03	1.03	99.88	99.94	99.96	535.2182	16
☑	C27 H34 O11	C27 H35 O11	535.2174	99.82		534.2109	534.2101	-1.45	1.45	99.51	99.98	99.93	535.2182	11
	C32H30 N4 O2 S	C32 H31 N4 O2 S	535.2162	99.08		534.2109	534.2089	-3.66	3.66	97.94	99.52	99.54	535.2182	20
	C31 H34 O6 S	C31 H35 O6 S	535.2149	98.8		534.2109	534.2076	-6.15	6.15	98.31	99.58	98.7	535.2182	15
	C33 H30 N2 O5	C33 H31 N2 O5	535.2227	98.44		534.2109	534.2155	8.57	8.57	98.73	99.97	97.5	535.2182	20
	C25H34 N4 O7 S	C25 H35 N4 O7 S	535.2221	98.39		534.2109	534.2148	7.33	7.33	97.97	99.34	98.16	535.2182	11
	C34 H38 O11 S	C34 H39 O11 S	535.2208	98.32		534.2109	534.2135	4.85	4.85	95.95	99.42	99.19	535.2182	6
	C37 H30 N2 S	C37 H31 N2 S	535.2202	98.23		534.2109	534.213	3.88	3.88	94.93	99.67	99.48	535.2182	24
	C29 H34 N4 O2 S2	C29 H35 N4 O2 S2	535.2196	98		534.2109	534.2123	2.64	2.64	94.28	98.96	99.76	535.2182	15
	C28 H38 O6 S2	C28 H39 O6 S2	535.2183	97.84		534.2109	534.211	0.16	0.16	93.26	99.03	100	535.2182	10
	C40 H26 N2	C40 H27 N2	535.2169	97.61		534.2109	534.2096	-2.42	2.42	92.7	99.97	99.8	535.2182	29
	C22 H34 N2 O13	C22 H35 N2 O13	535.2134	97.57		534.2109	534.2061	-8.99	8.99	96.13	99.95	97.25	535.2182	7
	C35 H26 N4 O2	C35 H27 N4 O2	535.2129	97.49		534.2109	534.2056	-9.96	9.96	96.86	99.95	96.64	535.2182	25
	C19 H38 N2 O13 S	C19 H39 N2 O13 S	535.2167	97		534.2109	534.2095	-2.7	2.7	90.54	99.24	99.75	535.2182	2
	C20 H38 O16	C20 H39 O16	535.2233	96.35		534.2109	534.216	9.54	9.54	92.4	99.97	96.91	535.2182	2
	C23 H38 N2 O8 S2	C23 H39 N2 O8 S2	535.2142	96.25		534.2109	534.207	-7.39	7.39	90.96	98.82	98.14	535.2182	6

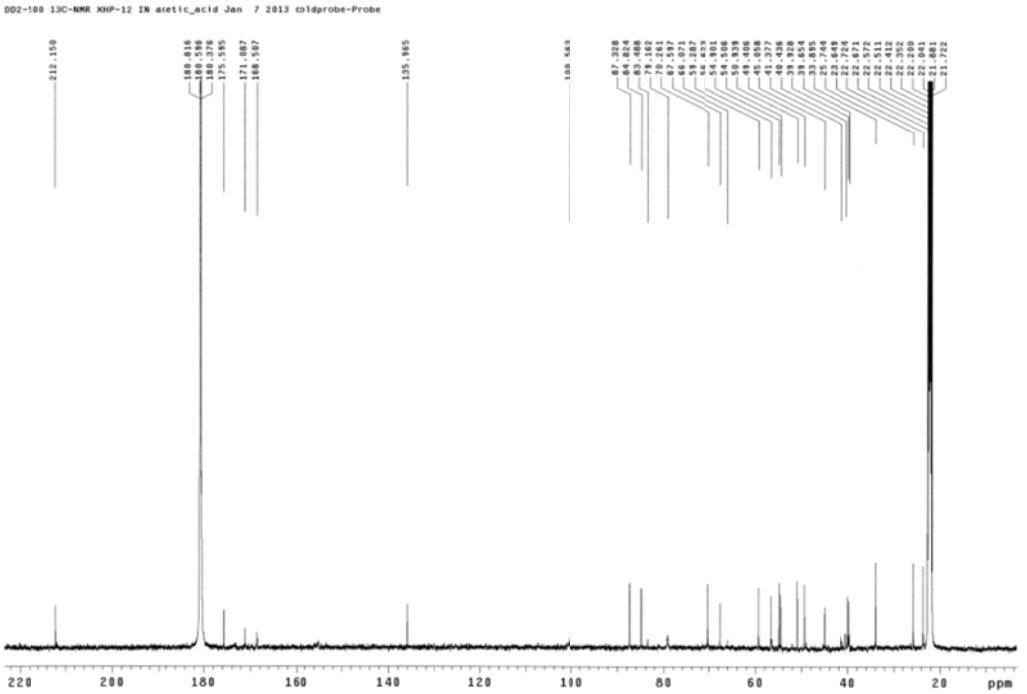
m/z	Ion	Formula	Abundance
552.2457	(M+NH4)+	C27 H38 N O11	802751.6

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
	C28 H30 N4 O7	C28 H34 N5 O7	552.2453	99.77		534.2119	534.2114	-0.82	0.82	99.72	99.41	99.98	552.2457	16
☑	C27 H34 O11	C27H38 N O11	552.2439	99.6		534.2119	534.2101	-3.31	3.31	99.77	99.32	99.64	552.2457	11
	C25H34 N4 O7 S	C25 H38 N5 O7 S	552.2486	99.13		534.2119	534.2148	5.48	5.48	98.6	99.96	99.03	552.2457	11
	C24 H38 O11 S	C24 H42 N O11 S	552.2473	98.98		534.2119	534.2135	2.99	2.99	96.99	99.91	99.71	552.2457	6
	C32H30 N4 O2 S	C32 H34 N5 O2 S	552.2428	98.82		534.2119	534.2089	-5.51	5.51	97.56	99.93	99.02	552.2457	20
	C33 H30 N2 O5	C33 H34 N3 O5	552.2493	98.55		534.2119	534.2155	6.72	6.72	97.97	99.28	98.54	552.2457	20
	C31 H34 O6 S	C31 H38 N O6 S	552.2414	98.5		534.2119	534.2076	-8	8	98.27	99.88	97.94	552.2457	15
	C29 H34 N4 O2 S2	C29 H38 N5 O2 S2	552.2461	98.44		534.2119	534.2123	0.79	0.79	94.61	99.94	99.98	552.2457	15
	C37 H30 N2 S	C37 H34 N3 S	552.2468	98.22		534.2119	534.213	2.03	2.03	94.11	99.86	99.87	552.2457	24
	C28 H38 O6 S2	C28 H42 N O6 S2	552.2448	98.2		534.2119	534.211	-1.7	1.7	93.92	99.91	99.91	552.2457	10
	C19 H38 N2 O13 S	C19 H42 N3 O13 S	552.2433	97.46		534.2119	534.2095	-4.55	4.55	92.28	99.95	99.33	552.2457	2
	C20 H38 O16	C20 H42 N O16	552.2498	97.22		534.2119	534.216	7.69	7.69	93.92	99.44	98.09	552.2457	2
	C40 H26 N2	C40 H30 N3	552.2434	97.02		534.2119	534.2096	-4.27	4.27	91.24	99.2	99.41	552.2457	29
	C34 H34 N2 S2	C3 H38 N3 S2	552.2502	96.84		534.2119	534.2163	8.33	8.33	92.69	99.94	97.77	552.2457	19
	C23 H38 N2 O8 S2	C23 H42 N3 O8 S2	552.2408	96.45		534.2119	534.207	-9.24	9.24	92.23	99.9	97.26	552.2457	6
	C21 H42 O11 S2	C21 H46 N O11 S2	552.2507	95.57		534.2119	534.2169	9.29	9.29	89.22	99.88	97.23	552.2457	1

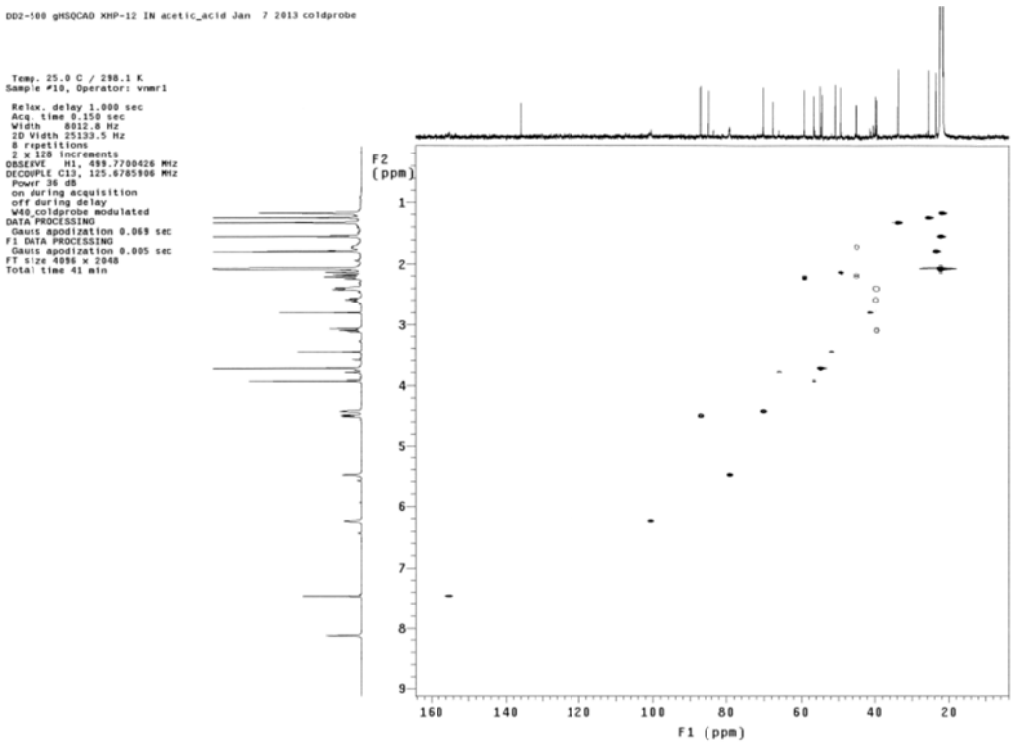
S25. ^{1}H NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **4**



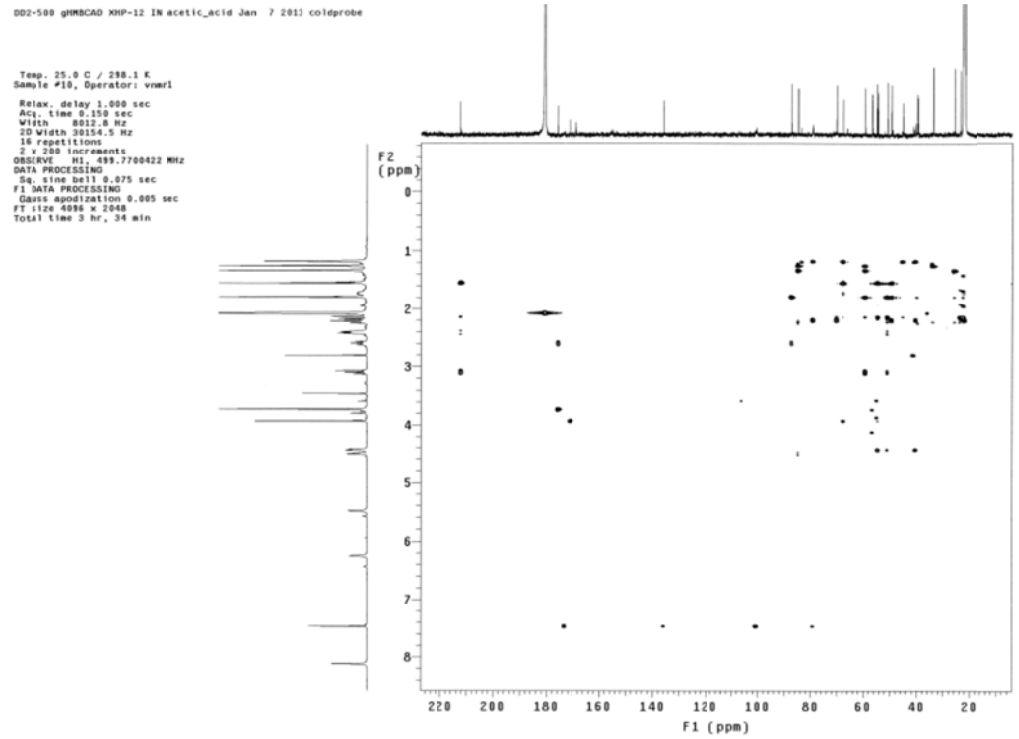
S26. ^{13}C NMR Spectrum (125 MHz, acetic acid-d_4) of Compound **4**



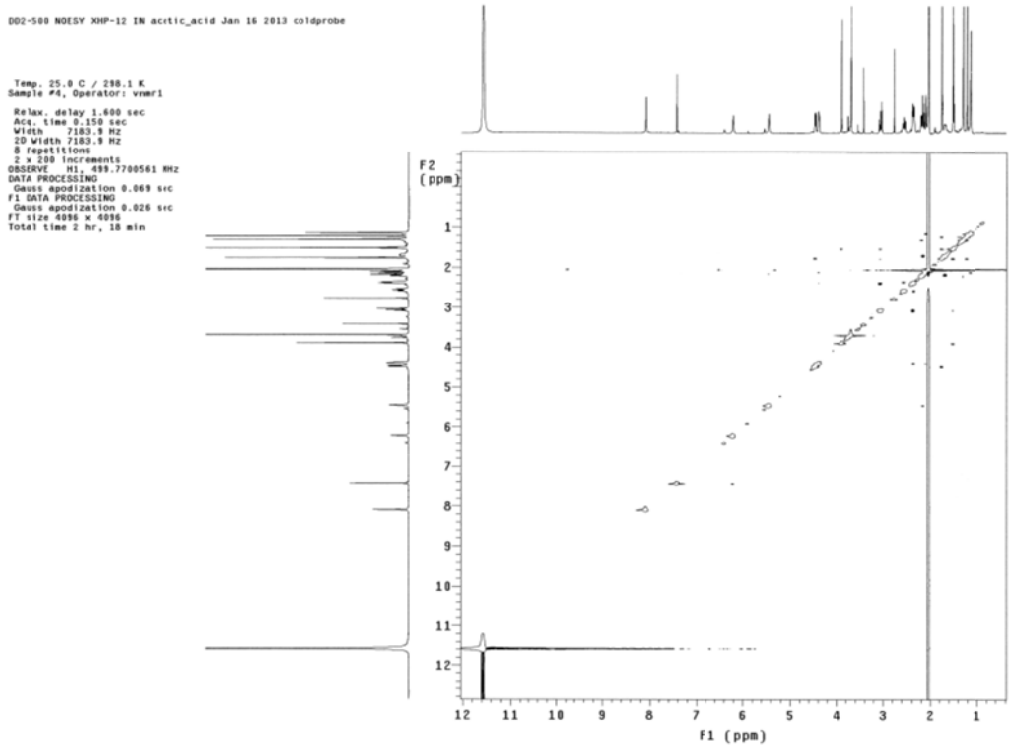
S27. HSQC Spectrum of Compound **4**



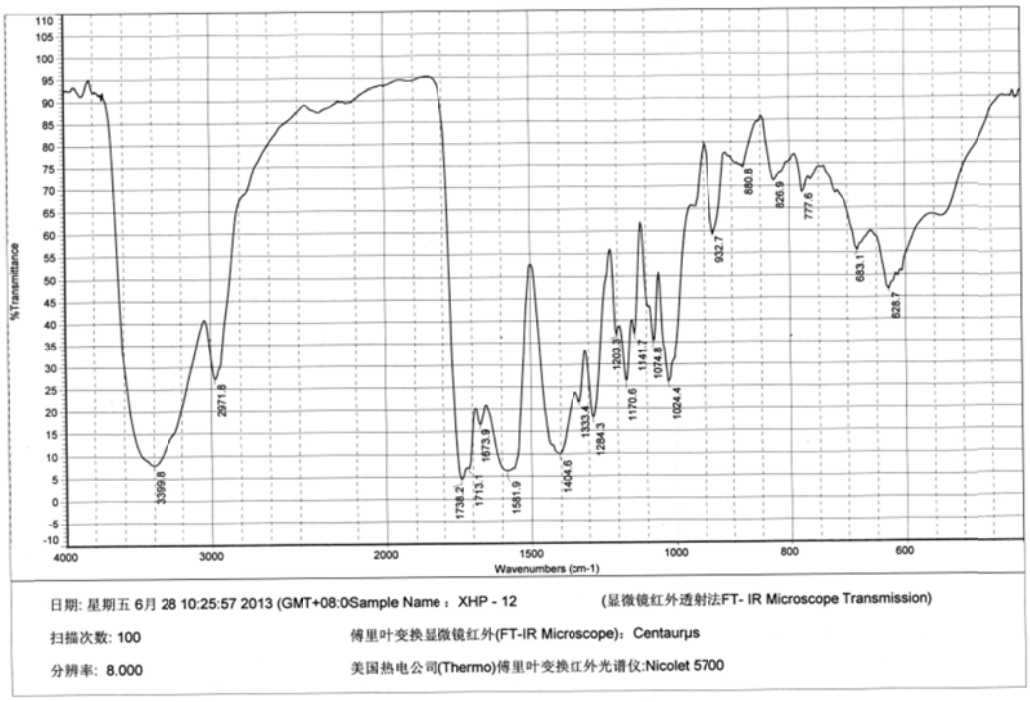
S28. HMBC Spectrum of Compound **4**



S29. NOESY Spectrum of Compound **4**



S30. IR Spectrum of Compound **4**



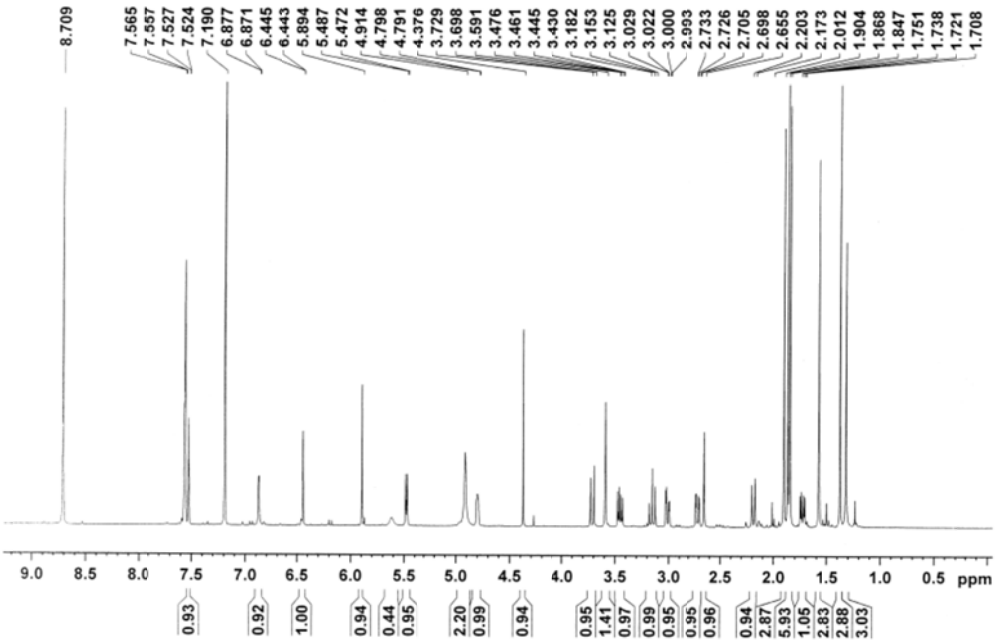
S31. HRESIMS Spectrum of Compound **4**

MS Formula Results: + Scan (6.045 min) Sub (2013011001.d)

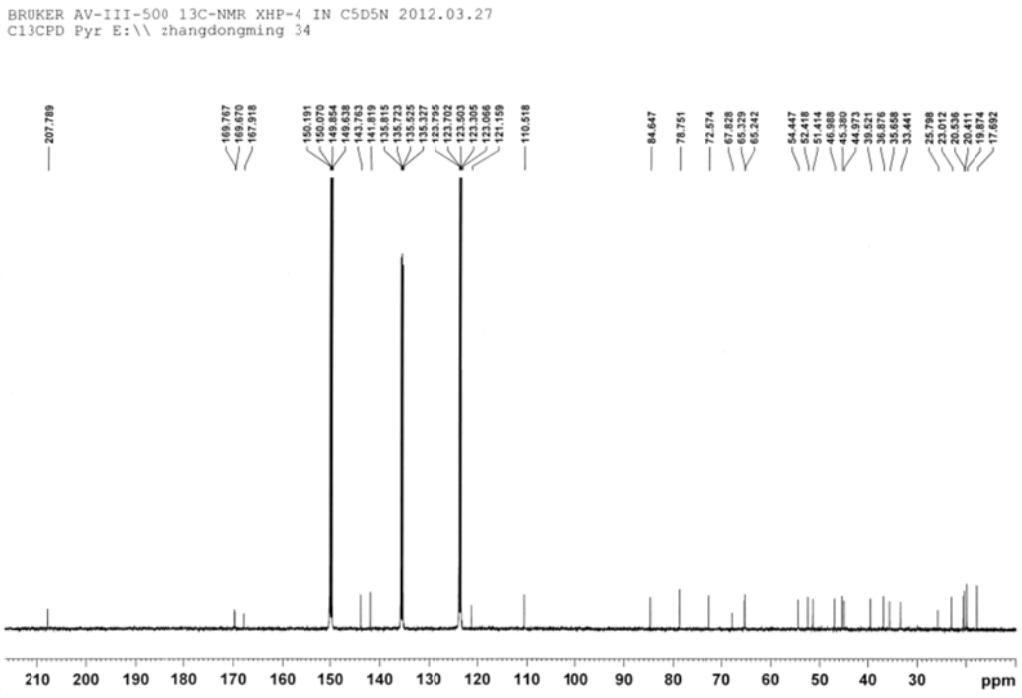
	m/z	Ion	Formula	Abundance
-	557.1991	(M+Na)+	C27 H34 Na O11	72299

	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
+	☑	C7 H34 O11	C27 H34 Na O11	557.1993	99.92		534.2098	534.2101	0.51	0.51	99.75	99.97	99.99	557.1991	11
+	☐	C3 H34 O6 S	C31 H34 Na O6 S	557.1968	98.85		534.2098	534.2076	-4.19	4.19	97.32	99.51	99.44	557.1991	15
+	☐	C22 H34 N2 O13	C22 H34 N2 Na O13	557.1953	98.55		534.2098	534.2061	-7.03	7.03	97.59	99.95	98.43	557.1991	7
+	☐	C24 H38 O11 S	C24 H38 Na O11 S	557.2027	98.25		534.2098	534.2135	6.81	6.81	96.87	99.34	98.53	557.1991	6

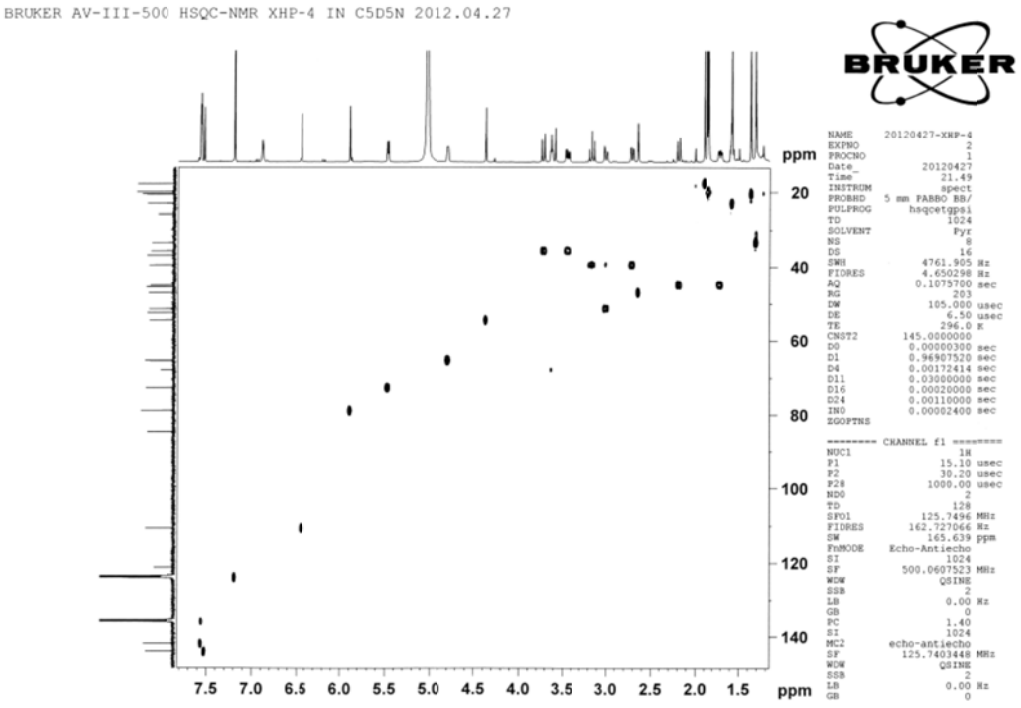
S32. ^{1}H NMR Spectrum (500 MHz, pyridine-d_5) of Compound **5**



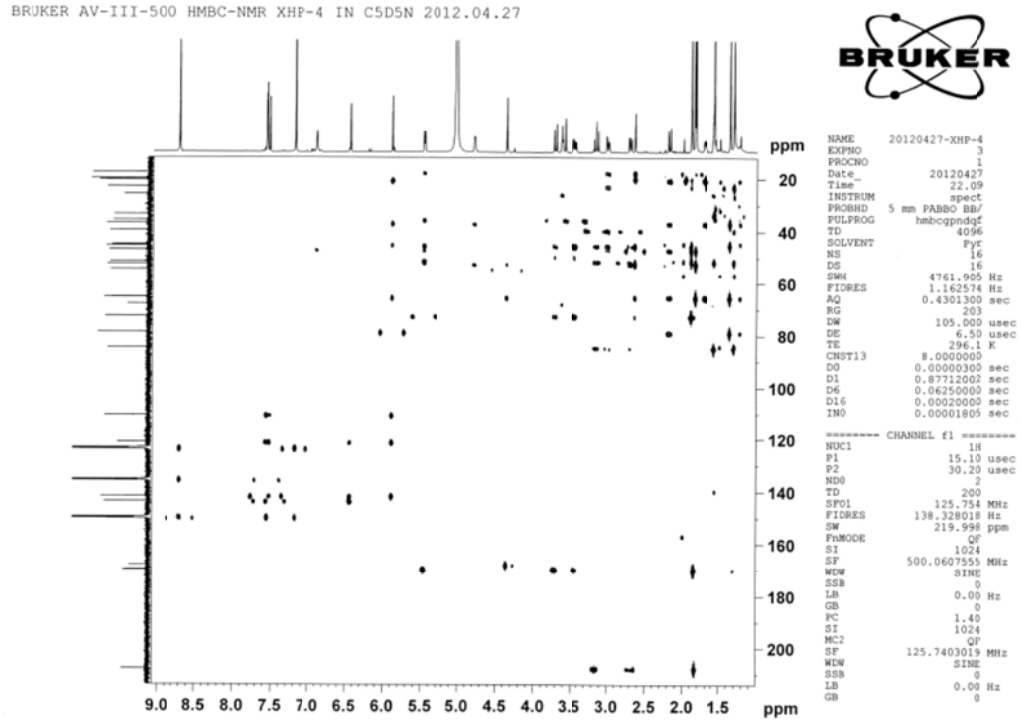
S33. ^{13}C NMR Spectrum (125 MHz, pyridine-d_5) of Compound **5**



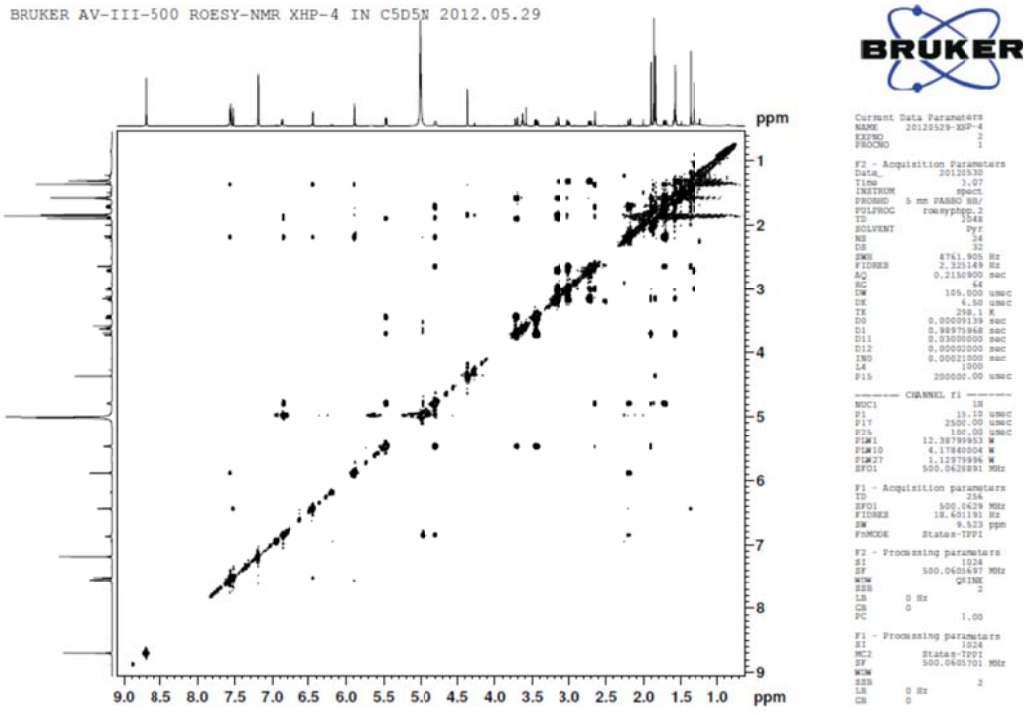
S34. HSQC Spectrum of Compound **5**



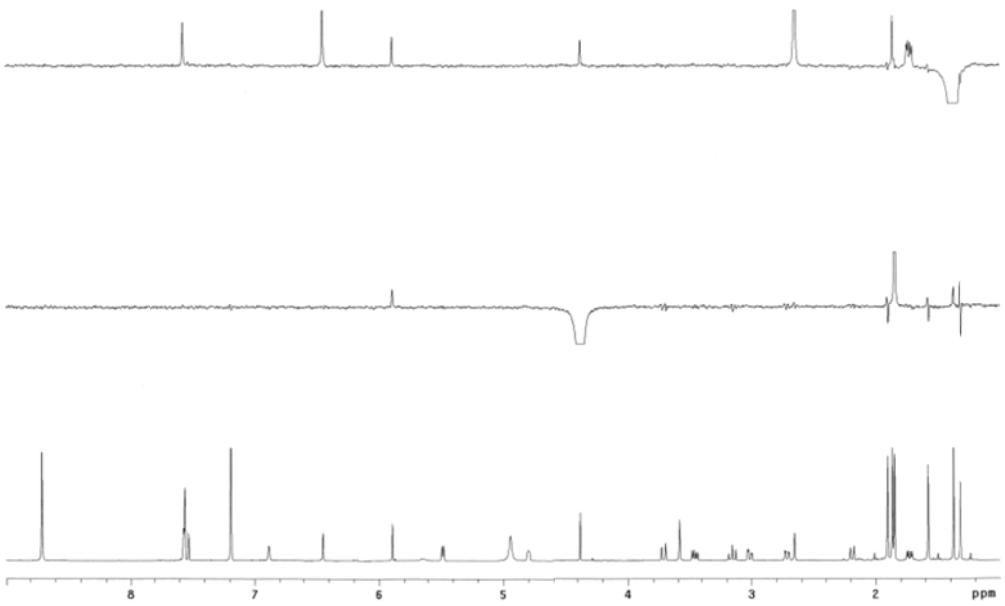
S35. HMBC Spectrum of Compound **5**



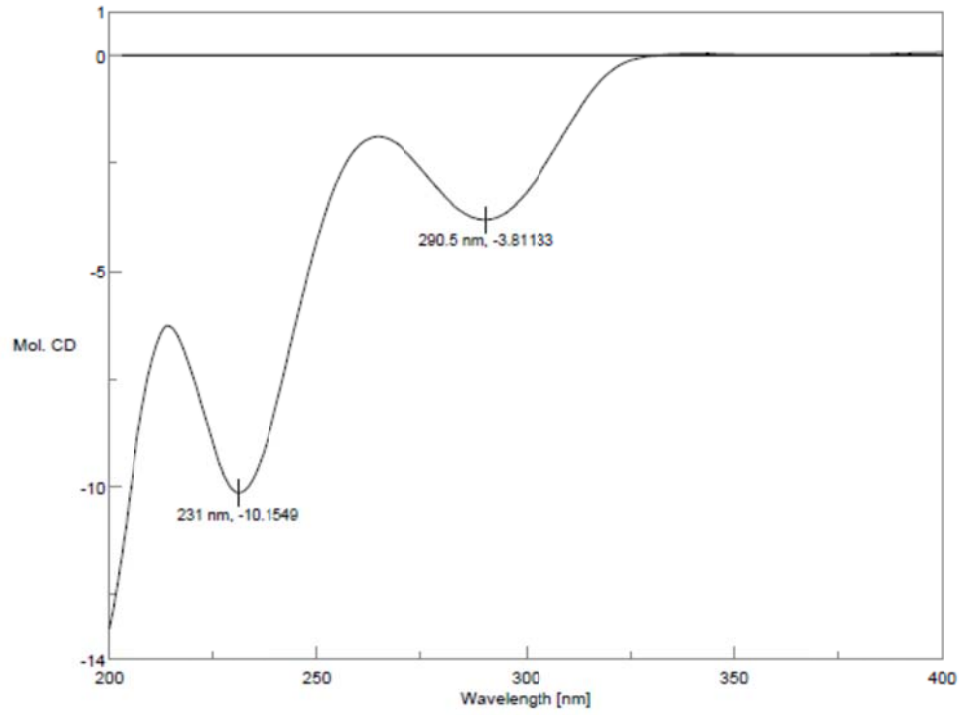
S36. ROESY Spectrum of Compound **5**



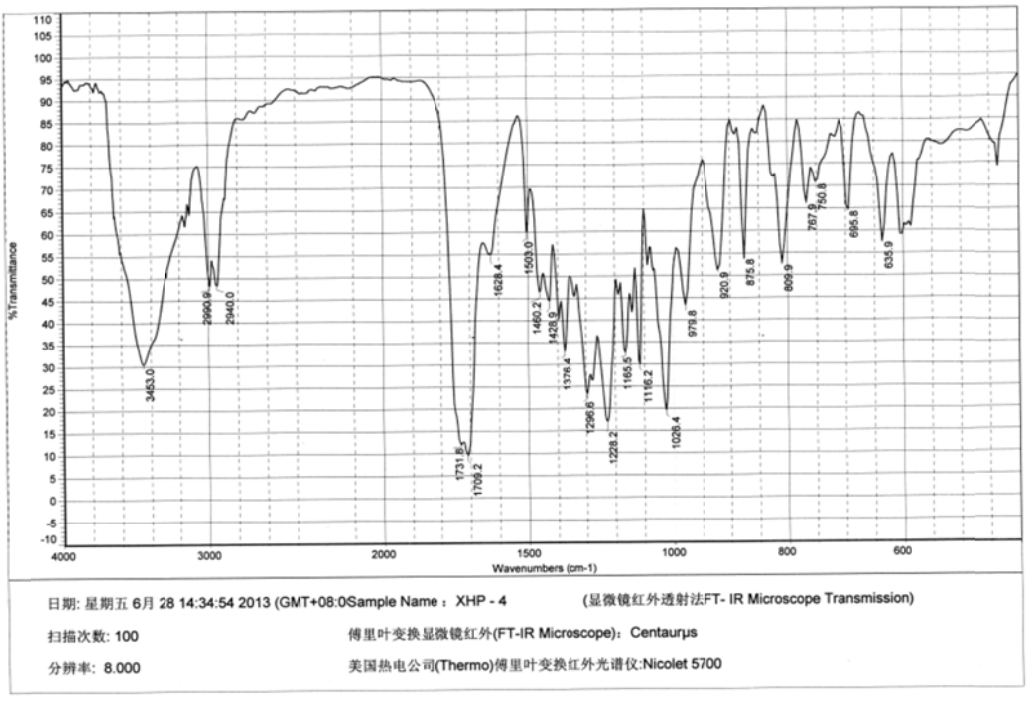
S37. NOE Difference Spectrum of Compound **5**



S38. CD Spectrum (in MeOH) of Compound **5**



S39. IR Spectrum of Compound **5**



S40. HRESIMS Spectrum of Compound **5**

MS Formula Results: + Scan (6.177 min) Sub (2012042501.d)

m/z	Ion	Formula	Abundance
531.2238	(M+H)+	C28H35 O10	509380.2

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
☑	C28 H34 O10	C28 H35 O10	531.2225	99.9		530.2165	530.2152	-2.42	2.42	99.99	99.99	99.8	531.2238	12
☐	C29 H30 N4 O6	C29 H31 N4 O6	531.2238	99.85		530.2165	530.2165	0.09	0.09	99.49	99.98	100	531.2238	17
☐	C25 H38 O10 S	C25 H39 O10 S	531.2258	98.92		530.2165	530.2186	3.93	3.93	97.36	99.7	99.47	531.2238	7
☐	C26 H34 N4 O6 S	C26 H35 N4 O6 S	531.2272	98.82		530.2165	530.2199	6.44	6.44	98.52	99.98	98.58	531.2238	12
☐	C33 H30 N4 O S	C33 H31 N4 O S	531.2213	98.49		530.2165	530.214	-4.64	4.64	96.13	99.78	99.26	531.2238	21
☐	C32 H34 O6 S	C32 H35 O6 S	531.22	98.32		530.2165	530.2127	-7.15	7.15	97.2	99.81	98.26	531.2238	16
☐	C34 H30 N2 O4	C34 H31 N2 O4	531.2278	98.14		530.2165	530.2206	7.68	7.68	96.87	99.98	97.99	531.2238	21
☐	C30 H34 N4 O S2	C30 H35 N4 O S2	531.2247	97.91		530.2165	530.2174	1.71	1.71	93.35	99.39	99.9	531.2238	16
☐	C26 H38 N2 O12 S	C26 H39 N2 O12 S	531.2218	97.87		530.2165	530.2145	-3.67	3.67	93.67	99.58	99.54	531.2238	3
☐	C29 H38 O5 S2	C29 H39 O5 S2	531.2233	97.87		530.2165	530.2161	-0.79	0.79	93.04	99.43	99.98	531.2238	11
☐	C21 H38 O15	C21 H39 O15	531.2283	97.58		530.2165	530.2211	8.66	8.66	95.77	100	97.45	531.2238	3
☐	C24 H36 N2 O7 S2	C24 H39 N2 O7 S2	531.2193	96.47		530.2165	530.212	-8.39	8.39	92.24	99.28	97.6	531.2238	7

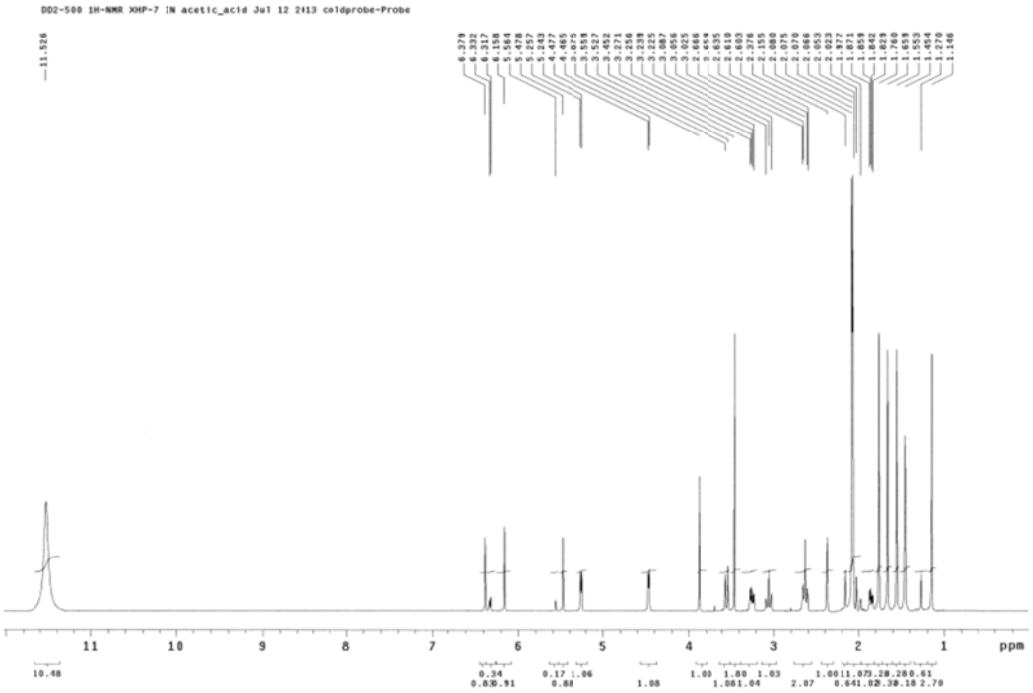
m/z	Ion	Formula	Abundance
548.2509	(M+NH4)+	C28 H38 N O10	1118052

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
☐	C29 H30 N4 O6	C29 H34 N5 O6	548.2504	99.94		530.217	530.2165	-0.9	0.9	99.91	99.92	99.97	548.2509	17
☑	C28 H34 O10	C28 H38 N O10	548.249	99.72		530.217	530.2152	-3.41	3.41	99.74	99.87	99.62	548.2509	12
☐	C26 H34 N4 O6 S	C26 H38 N5 O6 S	548.2537	98.93		530.217	530.2199	5.44	5.44	98.04	99.77	99.04	548.2509	12
☐	C34 H30 N2 O4	C34 H34 N3 O4	548.2544	98.83		530.217	530.2206	6.7	6.7	98.43	99.87	98.55	548.2509	21
☐	C33 H30 N4 O S	C33 H34 N5 O S	548.2479	98.75		530.217	530.214	-5.63	5.63	97.44	99.86	98.98	548.2509	21
☐	C25 H38 O10 S	C25 H42 N O10 S	548.2524	98.74		530.217	530.2186	2.94	2.94	96.27	99.76	99.72	548.2509	7
☐	C32 H34 O6 S	C32 H38 N O6 S	548.2465	98.36		530.217	530.2127	-8.13	8.13	97.93	99.84	97.87	548.2509	16
☐	C30 H34 N4 O S2	C30 H38 N5 O S2	548.2512	98.11		530.217	530.2174	0.72	0.72	93.8	99.55	99.98	548.2509	16
☐	C29 H38 O5 S2	C29 H42 N O5 S2	548.2499	97.83		530.217	530.2161	-1.78	1.78	92.94	99.54	99.9	548.2509	11
☐	C21 H38 O15	C21 H42 N O15	548.2549	97.24		530.217	530.2211	7.67	7.67	93.57	99.9	98.11	548.2509	3
☐	C26 H38 N2 O12 S	C26 H42 N3 O12 S	548.2484	97.16		530.217	530.2145	-4.66	4.66	91.48	99.7	99.3	548.2509	3
☐	C24 H38 N2 O7 S2	C24 H42 N3 O7 S2	548.2459	95.99		530.217	530.212	-9.38	9.38	91.12	99.64	97.18	548.2509	7
☐	C22 H42 O10 S2	C22 H46 N O10 S2	548.2558	95.13		530.217	530.2219	9.29	9.29	88.04	99.41	97.23	548.2509	2

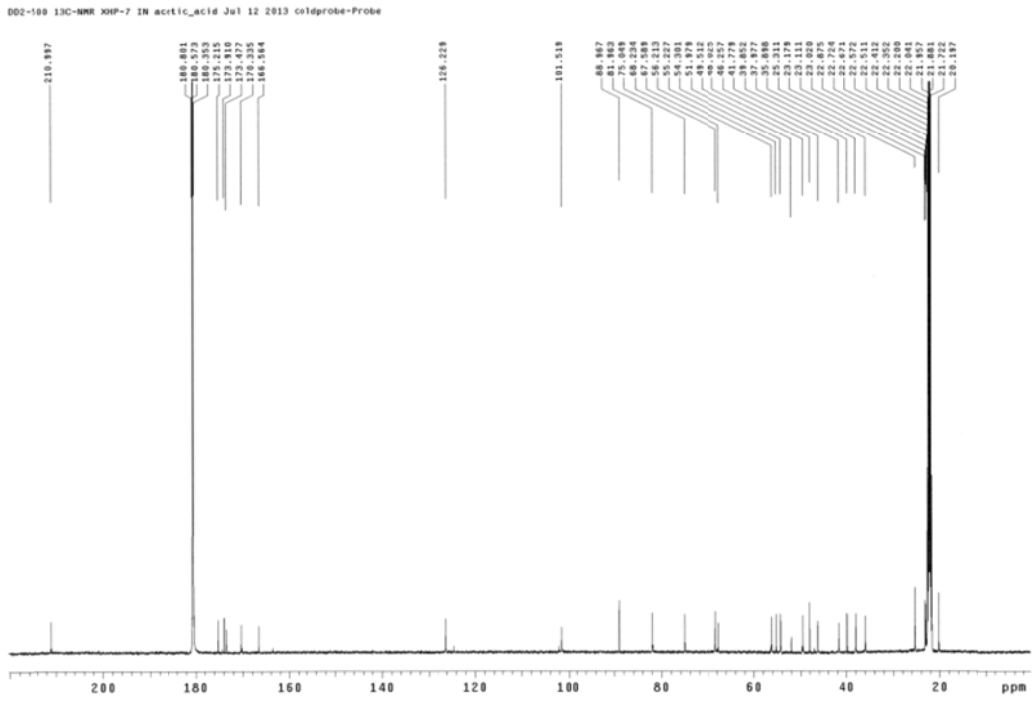
m/z	Ion	Formula	Abundance
553.2065	(M+Na)+	C28 H34 Na O10	325282.8

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
☑	C28 H34 O10	C28 H34 Na O10	553.2044	99.66		530.2173	530.2152	-3.96	3.96	99.77	99.84	99.5	553.2065	12
☐	C29 H30 N4 O6	C29 H30 N4 Na O6	553.2058	99.58		530.2173	530.2165	-1.45	1.45	98.71	99.9	99.93	553.2065	17
☐	C25 H38 O10 S	C25 H38 Na O10 S	553.2078	99.23		530.2173	530.2186	2.39	2.39	97.87	99.69	99.82	553.2065	7
☐	C26 H34 N4 O6 S	C26 H34 N4 Na O6 S	553.2091	99.13		530.2173	530.2199	4.9	4.9	98.47	99.72	99.24	553.2065	12
☐	C21 H38 O15	C21 H38 Na O15	553.2103	98.45		530.2173	530.2211	7.12	7.12	97.38	99.85	98.39	553.2065	3
☐	C22 H34 N4 O11	C22 H34 N4 Na O11	553.2116	98.35		530.2173	530.2224	9.63	9.63	99.14	99.92	97.08	553.2065	8
☐	C26 H38 N2 O12 S	C26 H38 N2 Na O12 S	553.2038	98.15		530.2173	530.2145	-5.2	5.2	95.25	99.64	99.14	553.2065	3
☐	C34 H30 N2 O4	C34 H30 N2 Na O4	553.2098	98.01		530.2173	530.2206	6.15	6.15	95.14	99.85	98.8	553.2065	21

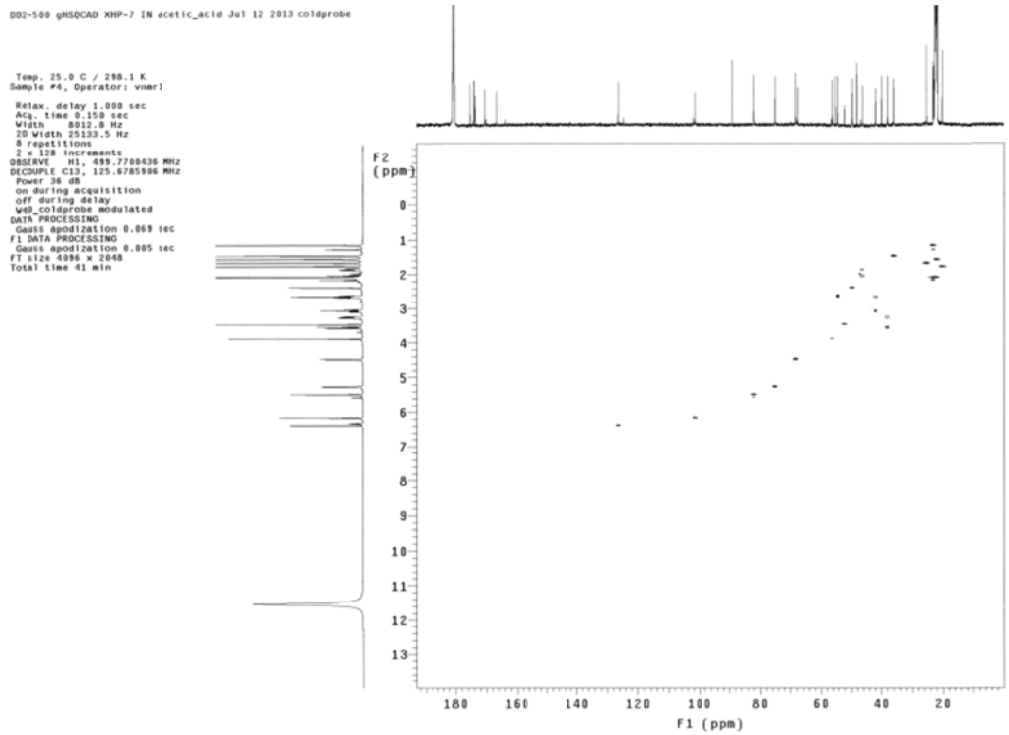
S41. ^{1}H NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **6**



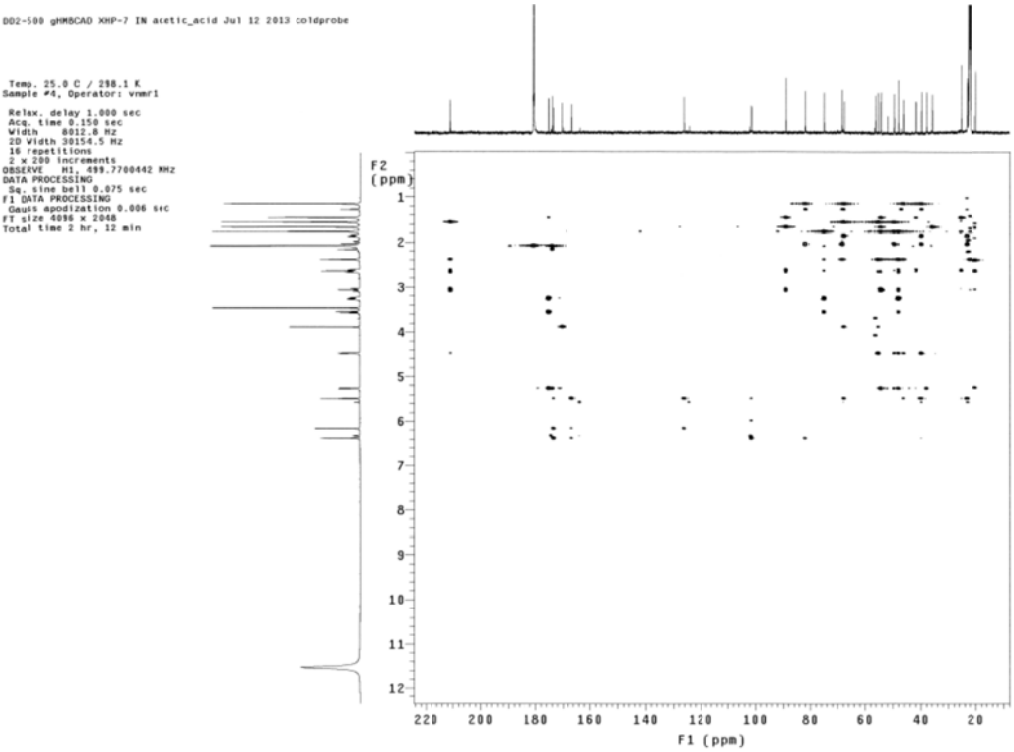
S42. ^{13}C NMR Spectrum (125 MHz, acetic acid-d_4) of Compound **6**



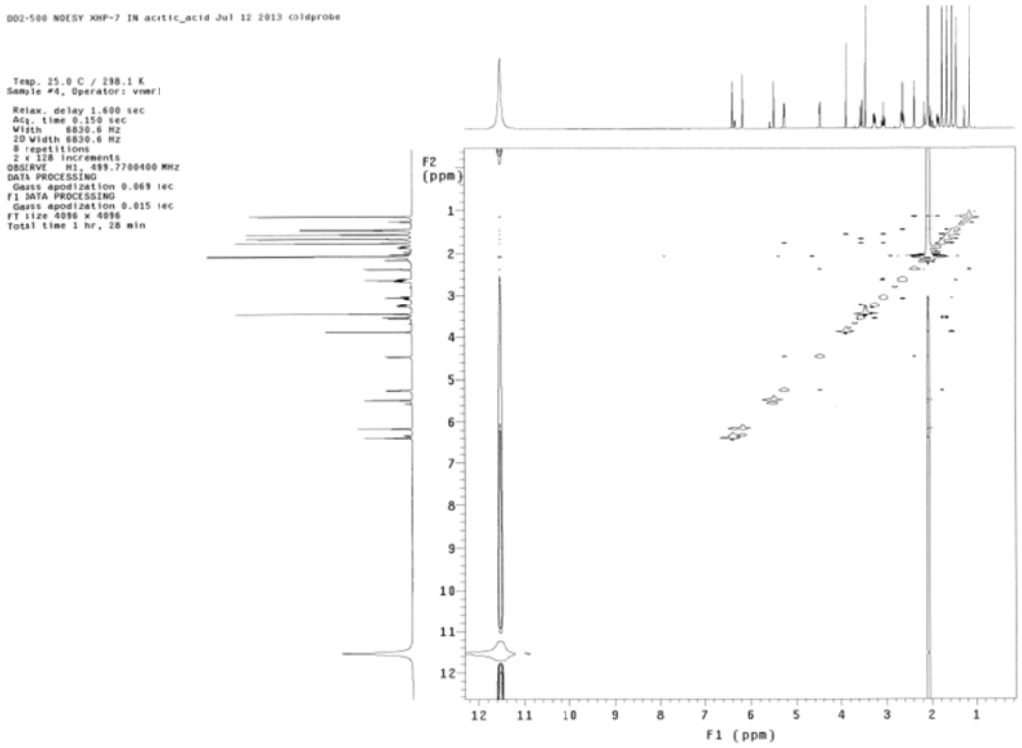
S43. HSQC Spectrum of Compound **6**



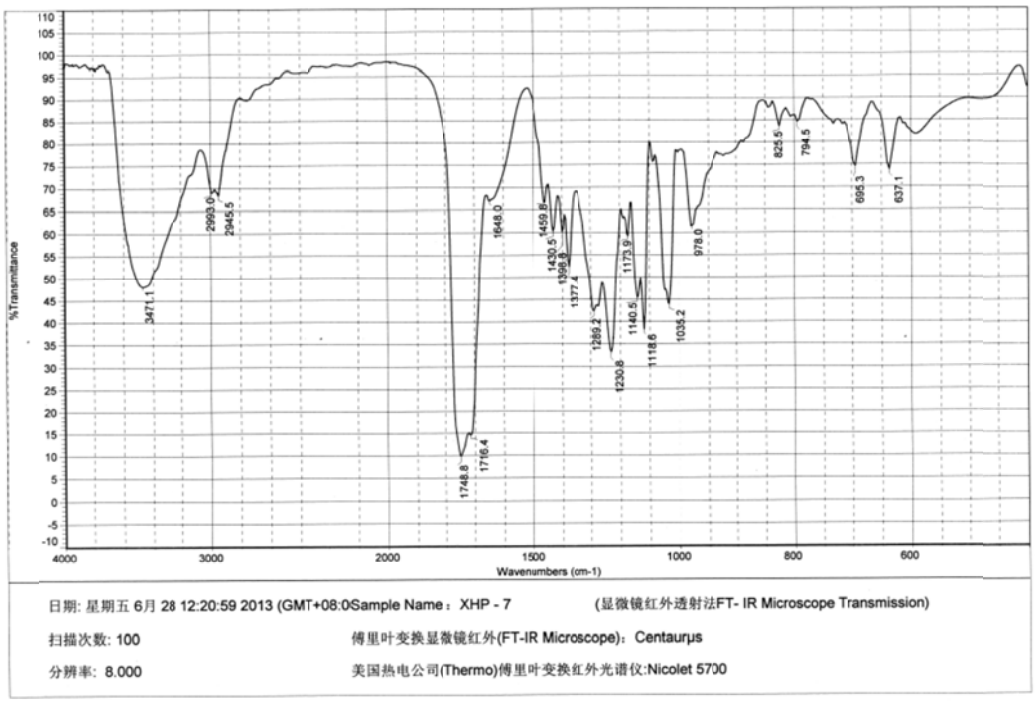
S44. HMBC Spectrum of Compound **6**



S45. NOESY Spectrum of Compound **6**



S46. IR Spectrum of Compound **6**



S47. HRESIMS Spectrum of Compound **6**

MS Formula Results: + Scan (5.459 min) Sub (2012050901.d)

m/z	Ion	Formula	Abundance
563.2131	(M+H)+	C28 H35 O12	436091.8

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
✓	C28 H34 O12	C28 H35 O12	563.2123	99.95		562.2058	562.205	-1.41	1.41	99.96	99.96	99.93	563.2131	12
	C25 H38 O12 S	C25 H39 O12 S	563.2157	98.6		562.2058	562.2084	4.58	4.58	96.52	99.76	99.27	563.2131	7
	C32 H34 O7 S	C32 H35 O7 S	563.2098	98.51		562.2058	562.2025	-5.87	5.87	96.9	99.84	98.81	563.2131	16
	C21 H34 N2 O14	C21 H35 N2 O14	563.2083	98.25		562.2058	562.201	-8.57	8.57	98.08	99.99	97.48	563.2131	8
	C34 H30 N2 O6	C34 H31 N2 O6	563.2177	98.16		562.2058	562.2104	8.12	8.12	97.36	99.97	97.74	563.2131	21
	C20 H38 N2 O14 S	C20 H39 N2 O14 S	563.2117	97.69		562.2058	562.2044	-2.59	2.59	92.55	99.69	99.77	563.2131	3
	C38 H30 N2 O S	C38 +31 N2 O S	563.2152	97.53		562.2058	562.2079	3.66	3.66	92.2	99.9	99.54	563.2131	25
	C21 H38 O17	C21 H39 O17	563.2182	97.29		562.2058	562.2109	9.04	9.04	95.2	99.97	97.2	563.2131	3
	C41 H26 N2 O	C41 H27 N2 O	563.2118	97.04		562.2058	562.2045	-2.33	2.33	89.98	99.95	99.81	563.2131	30

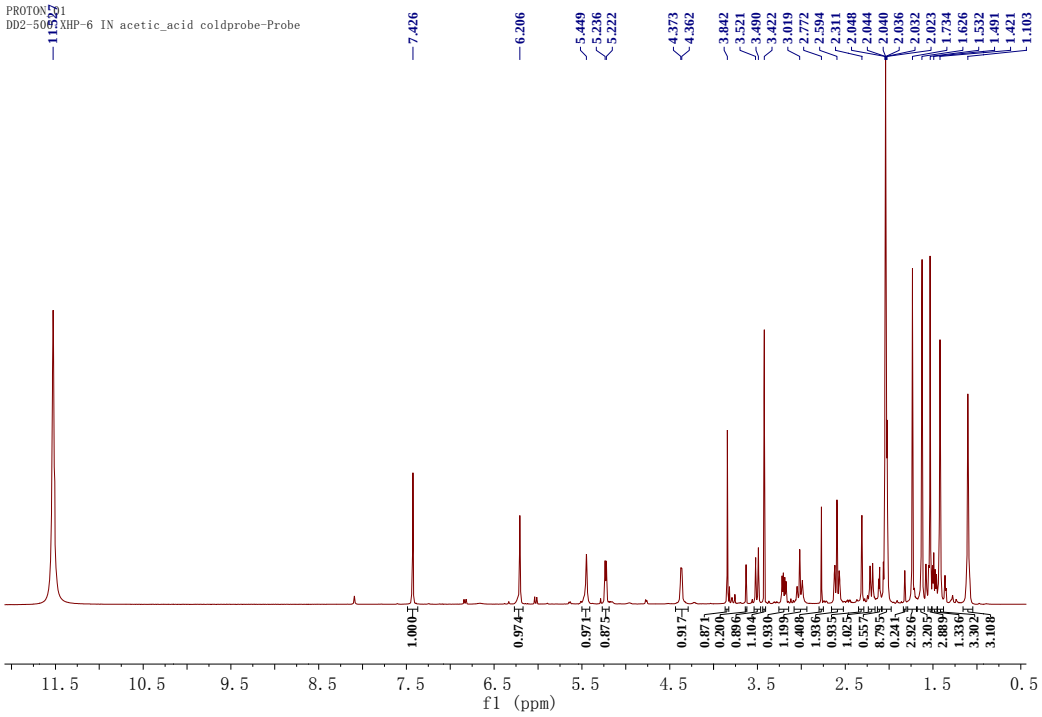
m/z	Ion	Formula	Abundance
580.2399	(M+NH4)+	C28 H38 N O12	531438

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
✓	C28 H34 O12	C28 H38 N O12	580.2389	99.66		562.2061	562.205	-1.82	1.82	99.9	98.91	99.89	580.2399	12
	C25 H38 O12 S	C25 H42 N O12 S	580.2422	99.14		562.2061	562.2084	4.16	4.16	98.08	99.82	99.43	580.2399	7
	C32 H34 O7 S	C32 +38 N O7 S	580.2363	98.56		562.2061	562.2025	-6.28	6.28	97.34	99.72	98.71	580.2399	16
	C20 H38 N2 O14 S	C20 H42 N3 O14 S	580.2382	98.37		562.2061	562.2044	-3	3	94.87	99.9	99.7	580.2399	3
	C21 H34 N2 O14	C23 H38 N3 O14	580.2348	98.18		562.2061	562.201	-8.99	8.99	98.79	99.06	97.38	580.2399	8
	C34 H30 N2 O6	C34 H34 N3 O6	580.2442	97.74		562.2061	562.2104	7.7	7.7	96.28	98.84	98.07	580.2399	21
	C21 H38 O17	C21 H42 N O17	580.2447	97.63		562.2061	562.2109	8.62	8.62	96.52	99.06	97.59	580.2399	3
	C38 H30 N2 O S	C38 H34 N3 O S	580.2417	97.42		562.2061	562.2079	3.25	3.25	91.84	99.64	99.65	580.2399	25
	C41 H26 N2 O	C41 H30 N3 O	580.2383	96.26		562.2061	562.2045	-2.74	2.74	88.37	98.74	99.75	580.2399	30

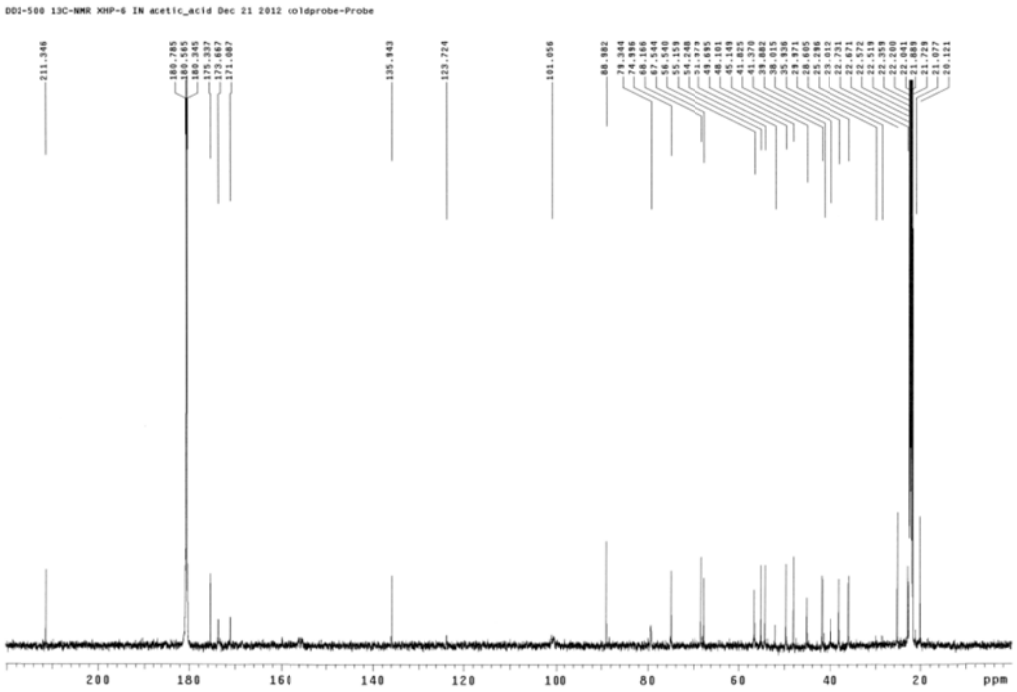
m/z	Ion	Formula	Abundance
585.1946	(M+Na)+	C28 +34 Na O12	1991230.6

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
✓	C28 H34 O12	C28 +34 Na O12	585.1942	99.9		562.2054	562.205	-0.72	0.72	99.74	99.92	99.98	585.1946	12
	C32 H34 O7 S	C32 H34 Na O7 S	585.1917	98.86		562.2054	562.2025	-5.18	5.18	97.81	99.58	99.13	585.1946	16
	C34 H30 N2 O6	C34 H30 N2 Na O6	585.1996	98.36		562.2054	562.2104	8.8	8.8	98.47	99.89	97.53	585.1946	21
	C25 H38 O12 S	C25 H38 Na O12 S	585.1976	98.33		562.2054	562.2084	5.26	5.26	96.09	99.45	99.11	585.1946	7
	C21 H34 N2 O14	C23 H34 N2 Na O14	585.1902	98.14		562.2054	562.201	-7.89	7.89	96.91	99.87	98.01	585.1946	8
	C38 H30 N2 O S	C38 H34 N2 Na O S	585.1971	97.96		562.2054	562.2079	4.34	4.34	94.17	99.64	99.39	585.1946	25
	C41 H26 N2 O	C41 H26 N2 Na O	585.1937	97.71		562.2054	562.2045	-1.64	1.64	92.21	99.89	99.91	585.1946	30
	C20 H38 N2 O14 S	C20 H38 N2 Na O14 S	585.1936	97.27		562.2054	562.2044	-1.91	1.91	91.25	99.29	99.88	585.1946	3
	C21 H38 O17	C21 H38 Na O17	585.2001	96.69		562.2054	562.2109	9.72	9.72	93.5	99.9	96.99	585.1946	3

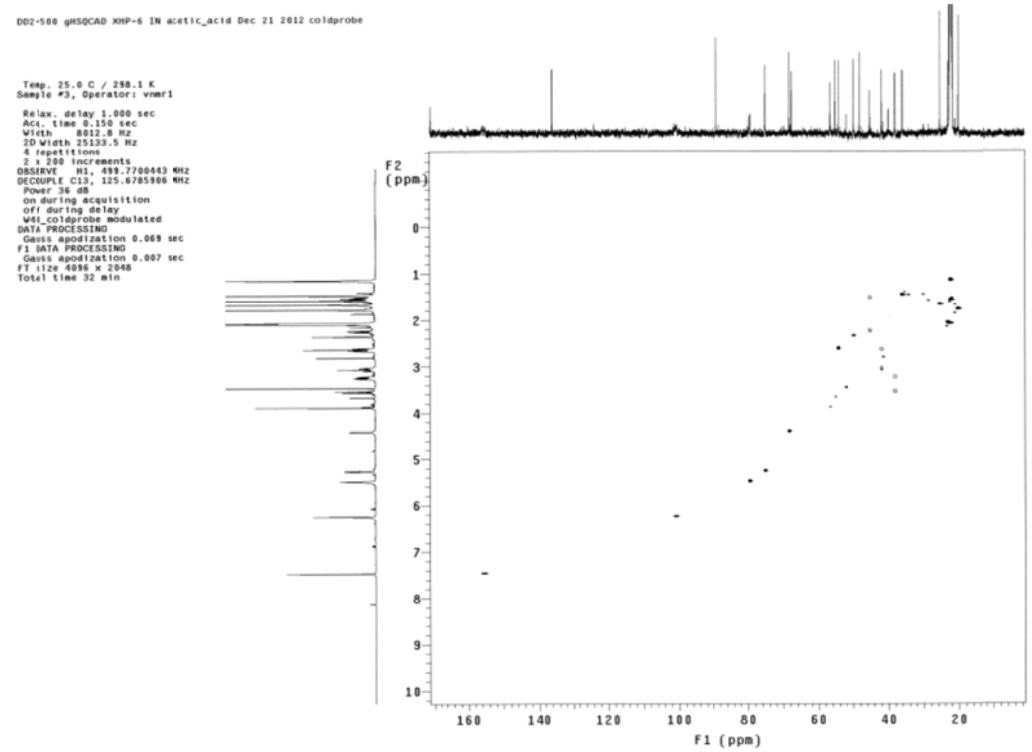
S48. ^{1}H NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **7**



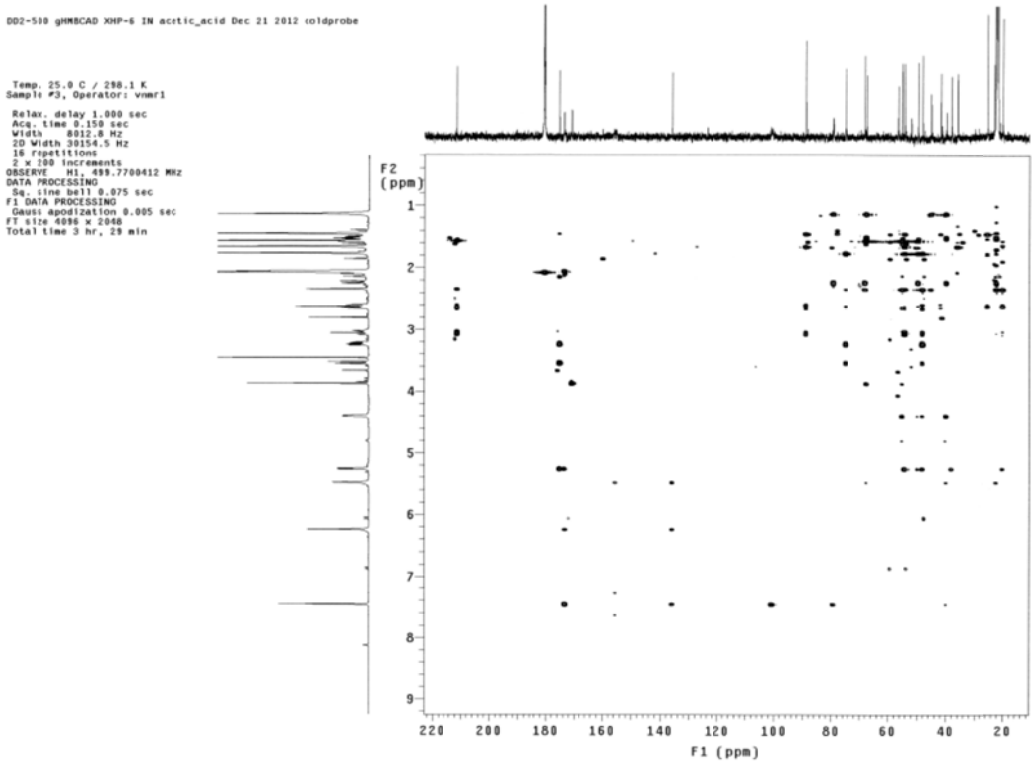
S49. ^{13}C NMR Spectrum (125 MHz, acetic acid-d_4) of Compound **7**



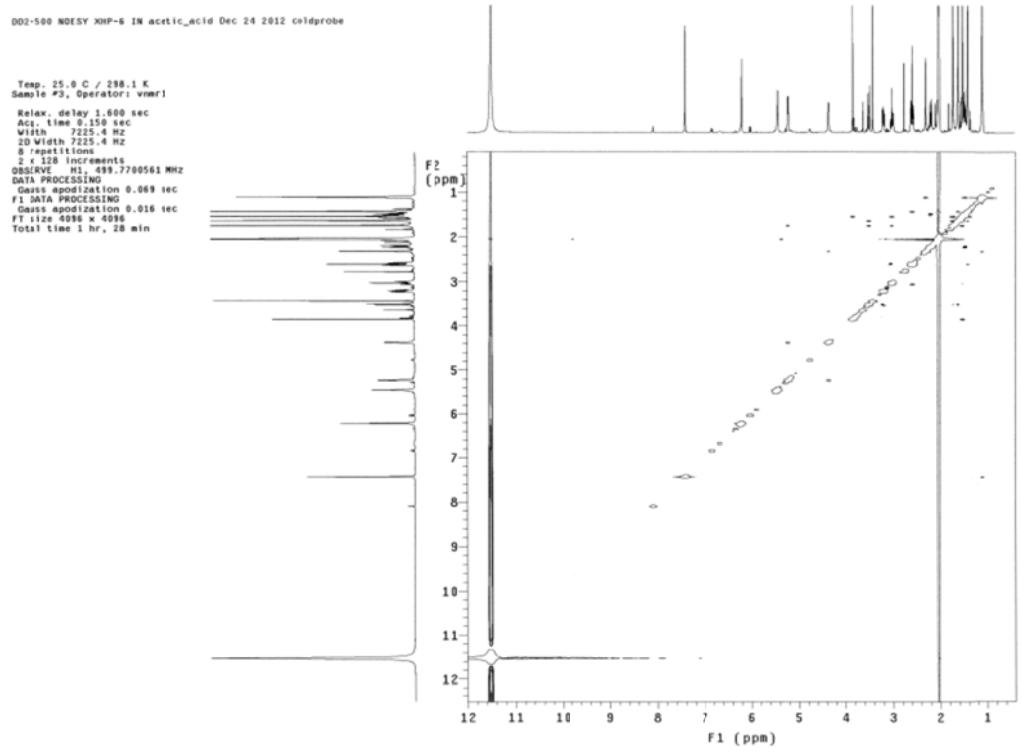
S50. HSQC Spectrum of Compound **7**



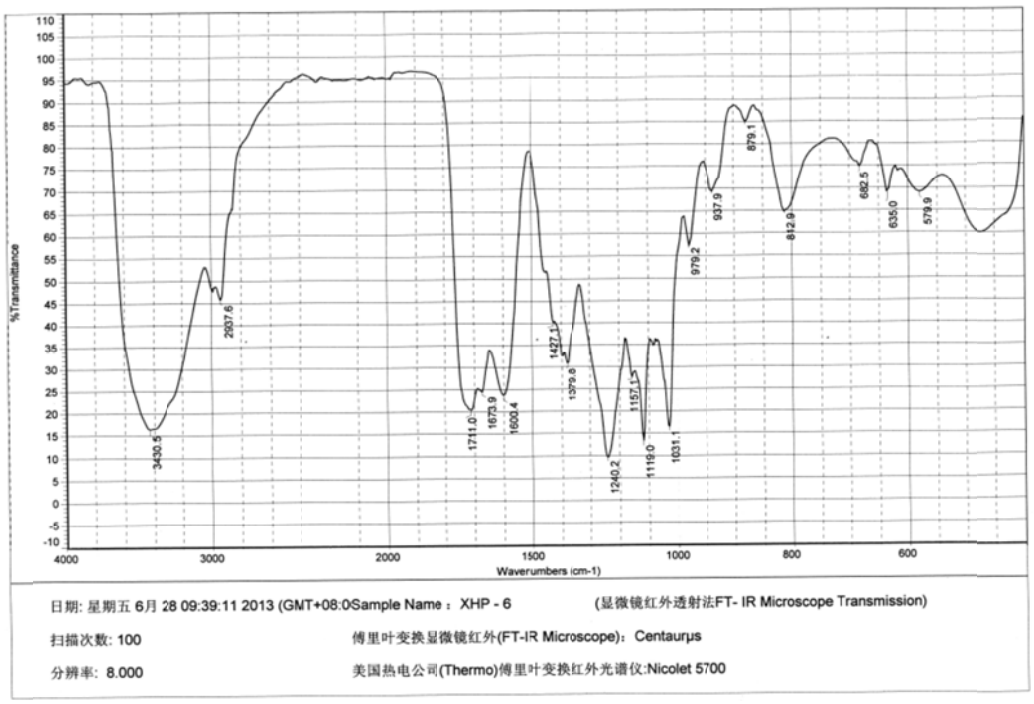
S51. HMBC Spectrum of Compound **7**



S52. NOESY Spectrum of Compound **7**



S53. IR Spectrum of Compound **7**



S54. HRESIMS Spectrum of Compound **7**

MS Formula Results: + Scan (5.339 min) Sub (2012122401.d)

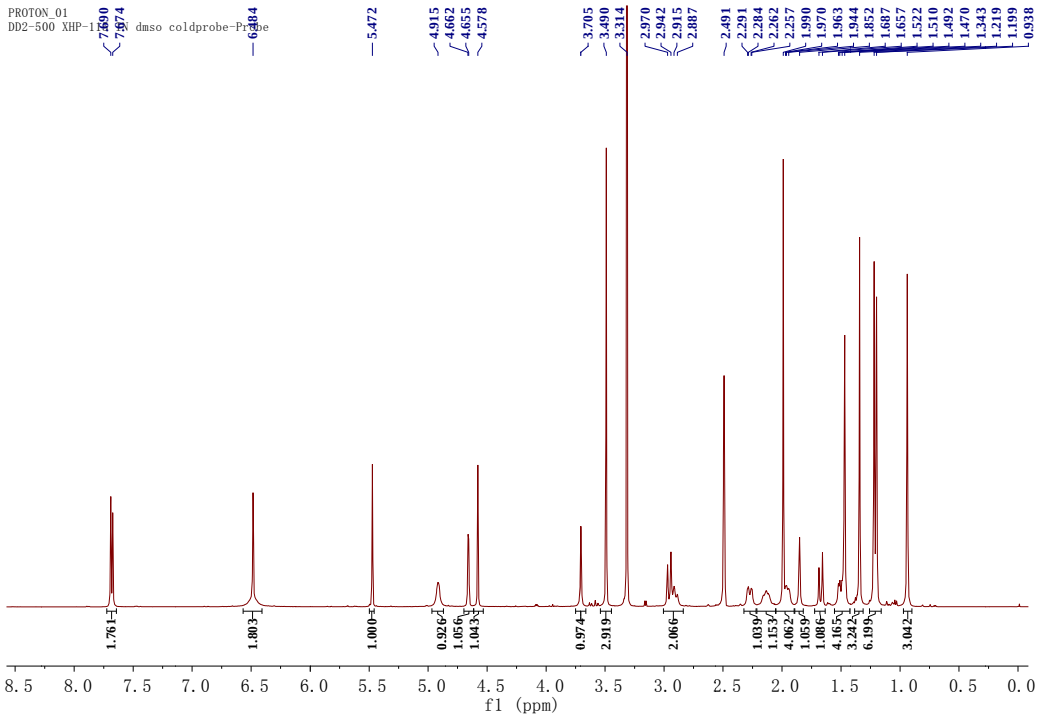
m/z	Ion	Formula	Abundance
563.2128	(M+H)+	C28 H35 O12	49768.7

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
☑	C28 H34 O12	C28 H35 O12	563.2123	99.64		562.2055	562.205	-0.83	0.83	98.89	99.85	99.98	563.2128	12
☐	C19 H38 N2 O15 Si	C19 H39 N2 O15 Si	563.2114	99.58		562.2055	562.2041	-2.43	2.43	99.17	99.65	99.79	563.2128	3
☐	C24 H38 O13 Si	C24 H39 O13 Si	563.2154	99.12		562.2055	562.2082	4.73	4.73	98.42	99.76	99.23	563.2128	7
☐	C23 K34 N2 O14	C23 H35 N2 O14	563.2083	98.78		562.2055	562.201	-7.99	7.99	99.52	99.86	97.8	563.2128	8
☐	C21 H38 O17	C21 H39 O17	563.2182	98		562.2055	562.2109	9.62	9.62	98.38	99.89	96.84	563.2128	3

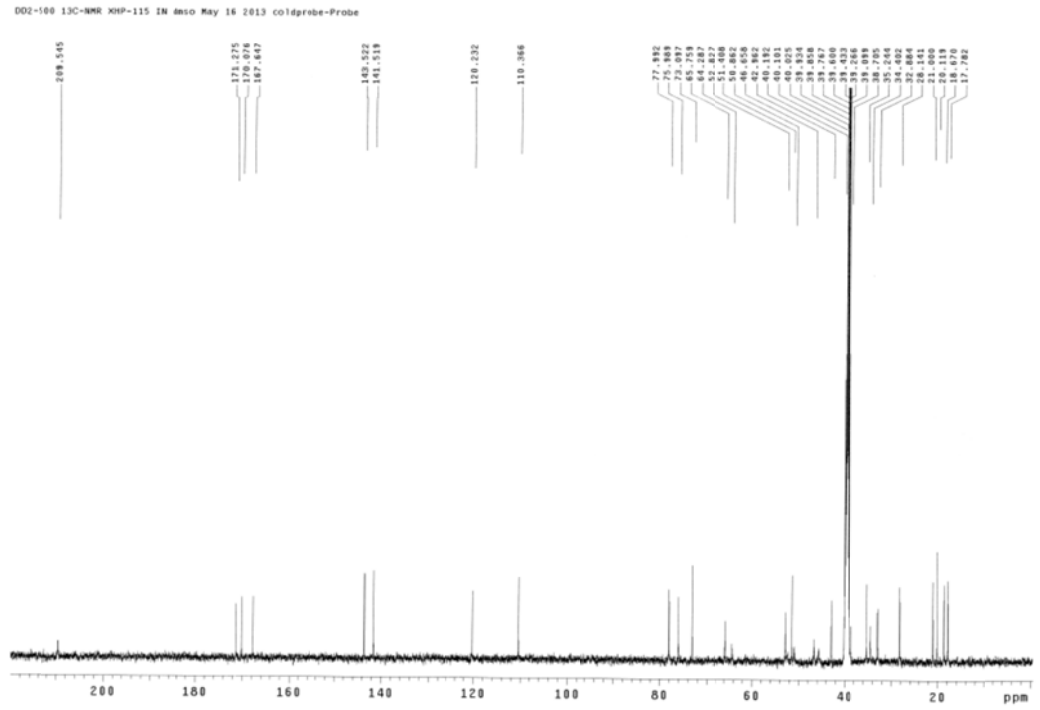
m/z	Ion	Formula	Abundance
585.1943	(M+Na)+	C28 H34 Na O12	168405.4

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
☑	C28 H34 O12	C28 H34 Na O12	585.1942	99.93		562.2051	562.205	-0.1	0.1	99.77	99.98	100	585.1943	12
☐	C24 H38 O13 Si	C24 H38 Na O13 Si	585.1974	99.05		562.2051	562.2082	5.45	5.45	98.61	99.57	99.05	585.1943	7
☐	C19 H38 N2 O15 Si	C19 H38 N2 Na O15 Si	585.1934	98.75		562.2051	562.2041	-1.73	1.73	98.25	99.42	99.9	585.1943	3
☐	C31 H34 O8 Si	C31 H34 Na O8 Si	585.1915	98.7		562.2051	562.2023	-5	5	97.05	99.68	99.2	585.1943	16
☐	C23 K34 N2 O14	C23 H34 K2 Na O14	585.1902	98.34		562.2051	562.201	-7.27	7.27	97.07	99.95	98.31	585.1943	8
☐	C34 H30 N2 O6	C34 H30 N2 Na O6	585.1996	98.16		562.2051	562.2104	9.42	9.42	98.29	99.98	97.17	585.1943	21

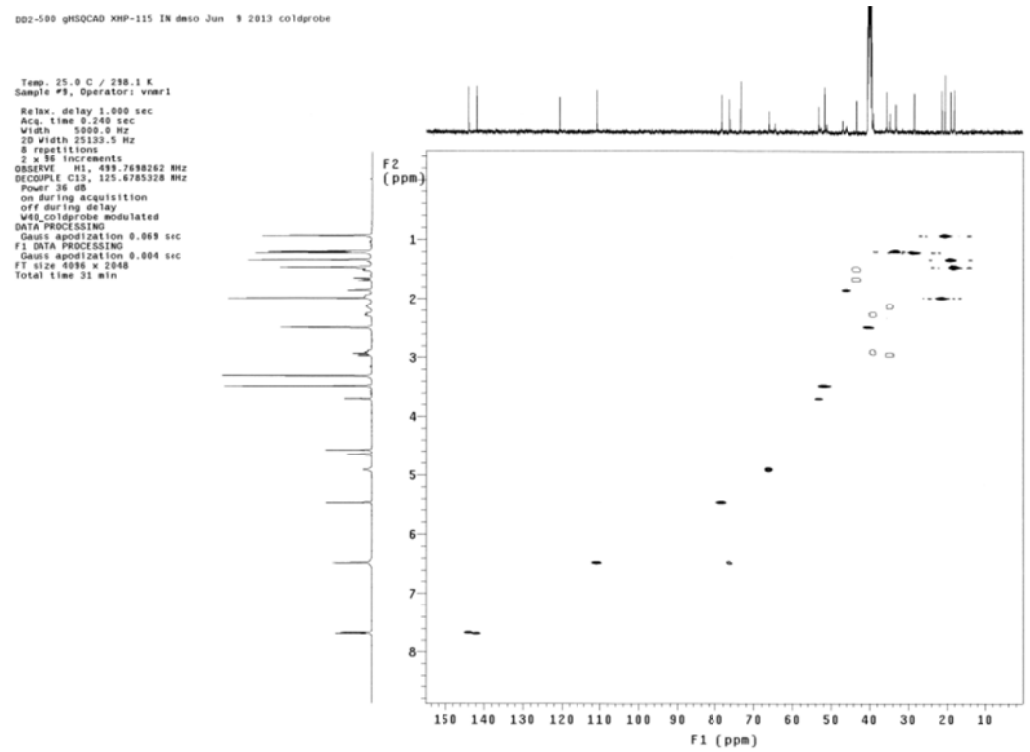
S55. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **8**



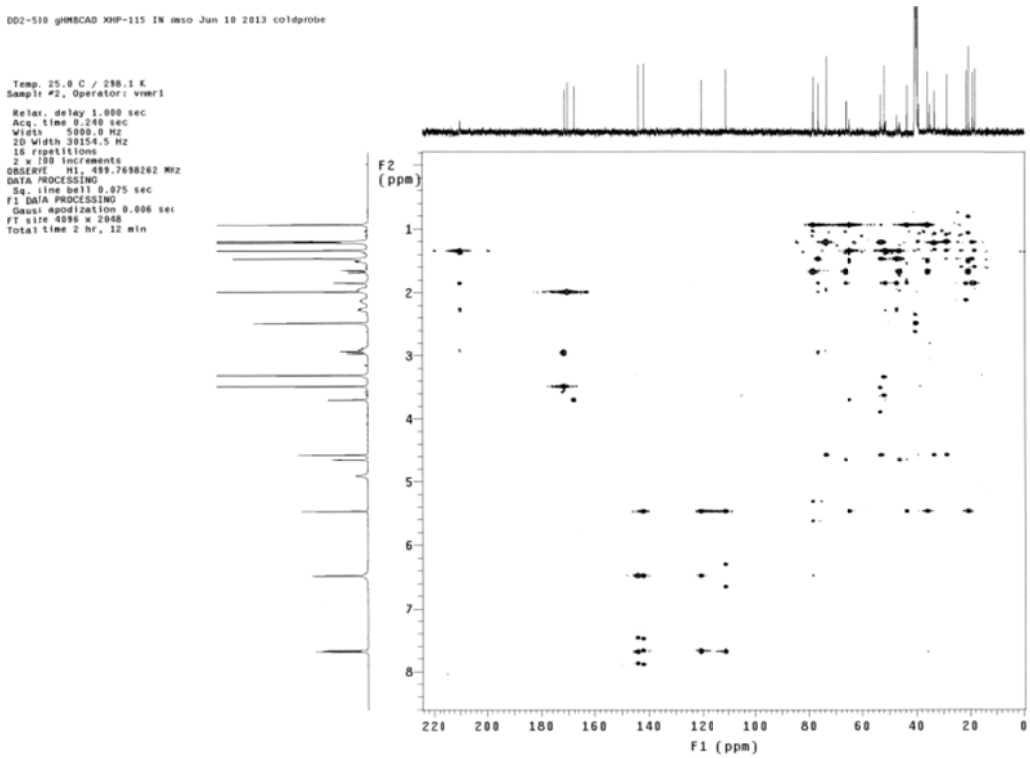
S56. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **8**



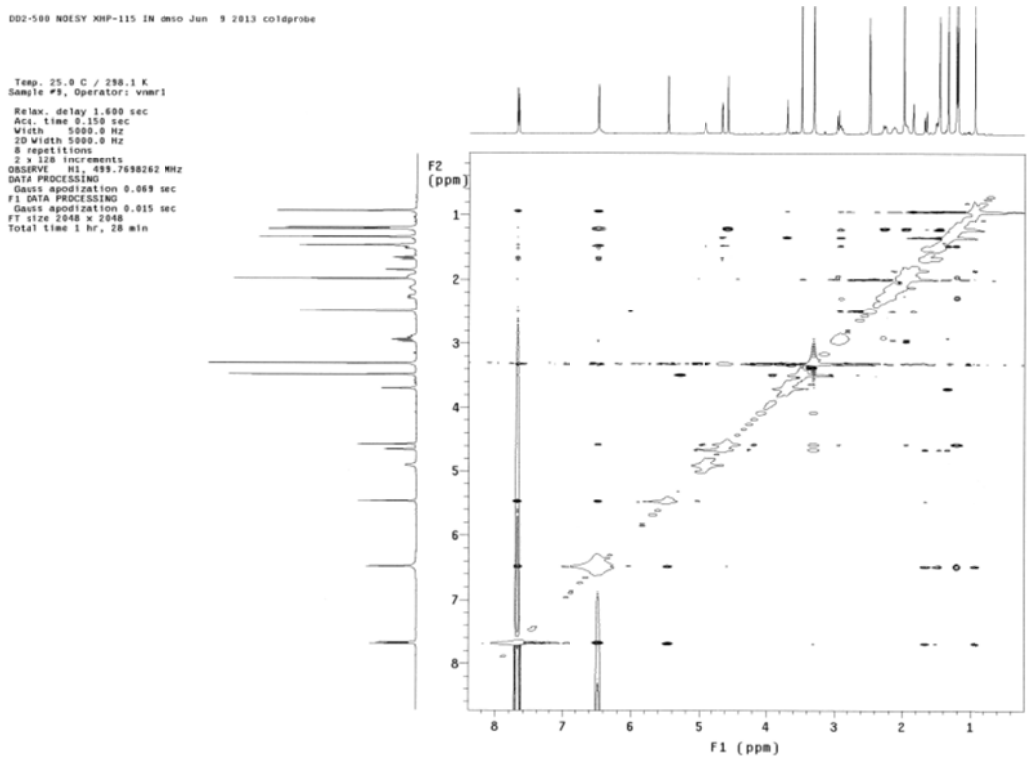
S57. HSQC Spectrum of Compound **8**



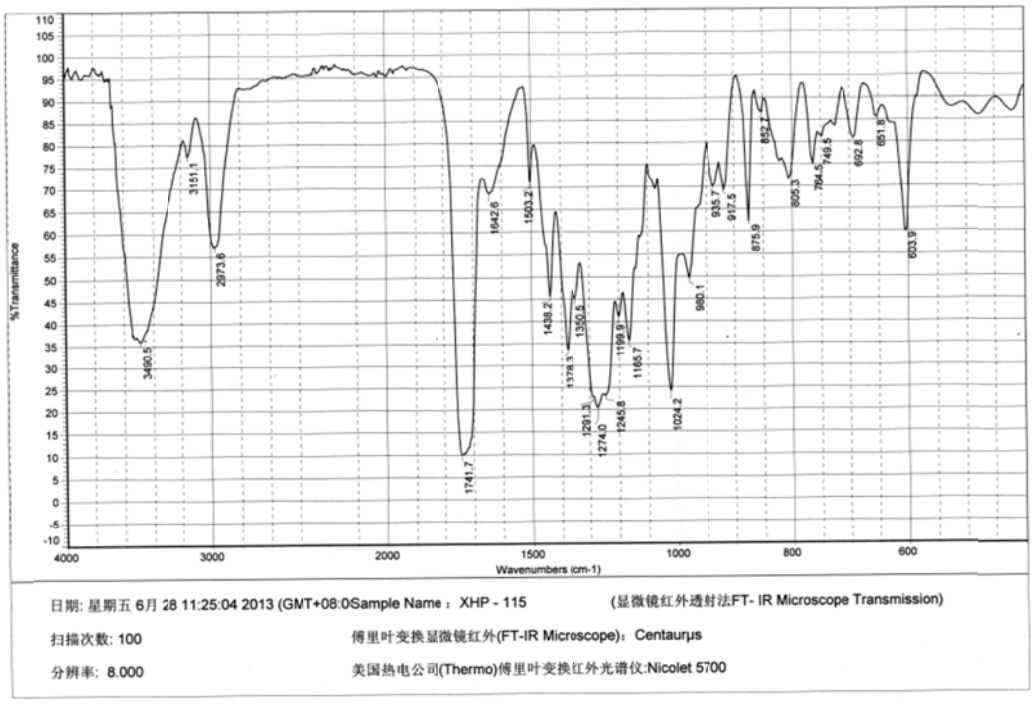
S58. HMBC Spectrum of Compound **8**



S59. NOESY Spectrum of Compound **8**



S60. IR Spectrum of Compound **8**



S61. HRESIMS Spectrum of Compound **8**

MS Formula Results: + Scan (6.426 min) Sub (2013053003.d)

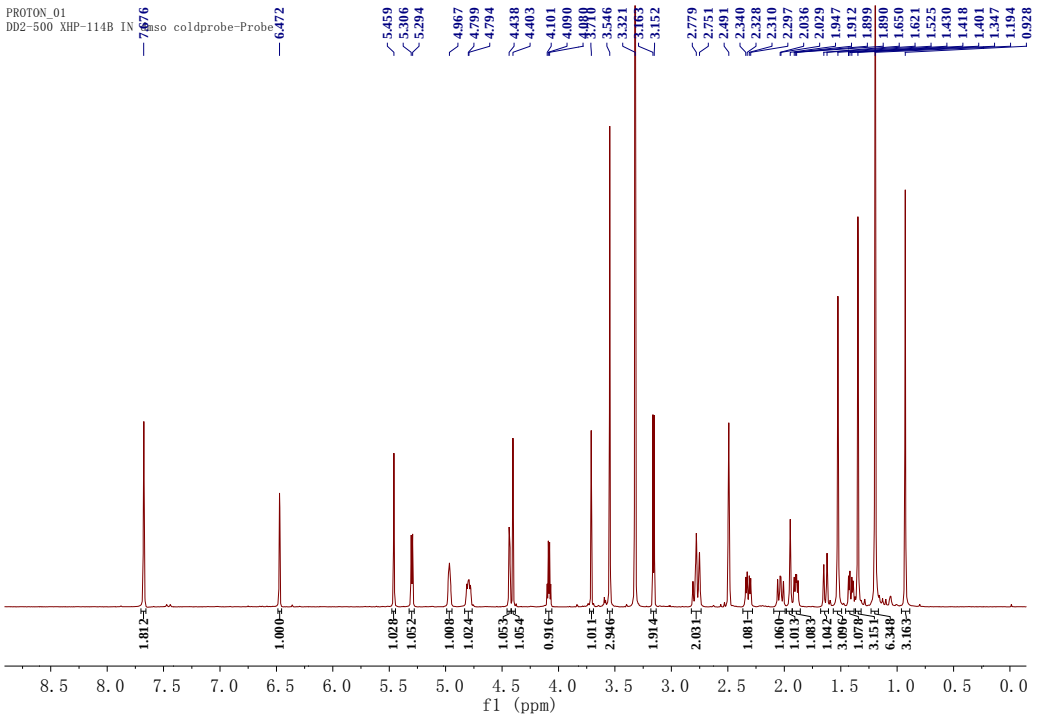
m/z	Ion	Formula	Abundance
563.2488	(M+H)+	C29 H39 O11	448555.2

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
☑	C29 H38 O11	C29 H39 O11	563.2487	99.99		562.2415	562.2414	-0.2	0.2	99.99	99.96	100	563.2488	11
☐	C26 H30 N10 O5	C26 H31 N10 O5	563.2473	99.81		562.2415	562.2401	-2.64	2.64	99.75	99.97	99.76	563.2488	17
☐	C30 H34 N4 O7	C30 H35 N4 O7	563.25	99.8		562.2415	562.2427	2.16	2.16	99.61	99.97	99.84	563.2488	16
☐	C25 H34 N6 O9	C25 H35 N6 O9	563.246	99.45		562.2415	562.2387	-5	5	99.53	99.98	99.13	563.2488	12
☐	C23 H3(N10 O5 S	C23 H35 N10 O5 S	563.2507	99.26		562.2416	562.2434	3.34	3.34	98.38	99.6	99.61	563.2488	12
☐	C31 H30 N8 O3	C31 H31 N8 O3	563.2514	99.21		562.2415	562.2441	4.53	4.53	98.46	99.97	99.29	563.2488	21

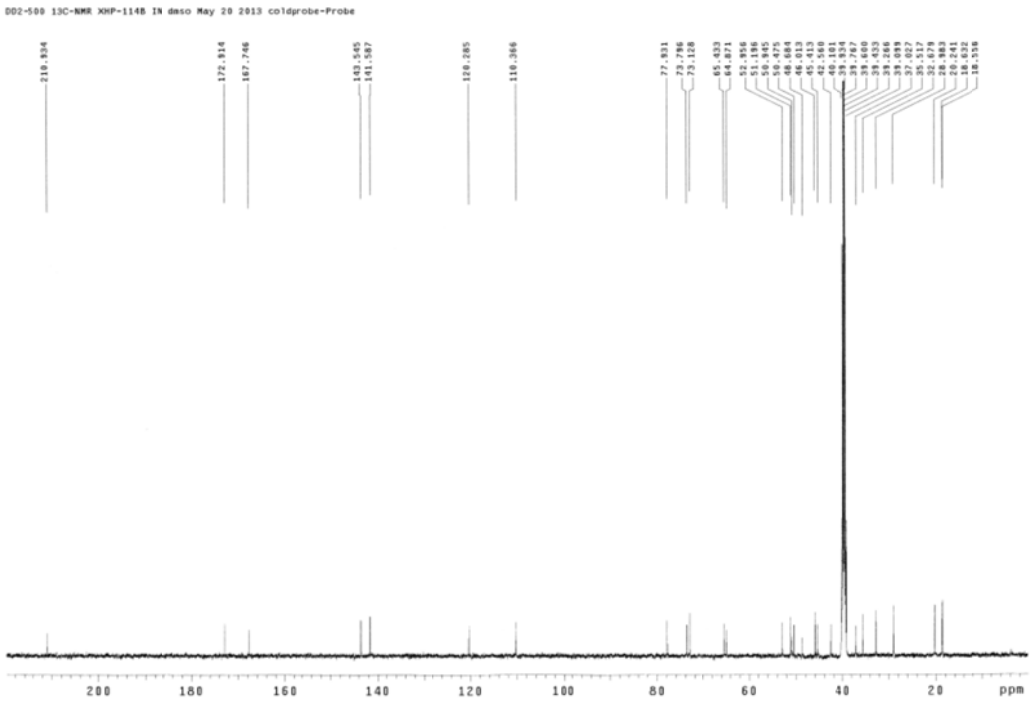
m/z	Ion	Formula	Abundance
585.2313	(M+Na)+	C29 H38 Na O11	714373.1

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
☑	C29 H38 O11	C29 H38 Na O11	585.2306	99.96		562.2421	562.2414	-1.25	1.25	99.95	99.98	99.95	585.2313	11
☐	C30 H34 N4 O7	C30 H34 N4 Na O7	585.232	99.78		562.2421	562.2427	1.11	1.11	99.31	100	99.96	585.2313	16
☐	C26 H30 N10 O5	C26 H30 N10 Na O5	585.2293	99.72		562.2421	562.2401	-3.69	3.69	99.77	99.99	99.56	585.2313	17
☐	C25 H34 N6 O9	C25 H34 N6 Na O9	585.2279	99.39		562.2421	562.2387	-6.05	6.05	99.82	100	98.82	585.2313	12
☐	C23 H3(N10 O5 S	C23 H3(N10 Na O5 S	585.2327	99.37		562.2421	562.2434	2.3	2.3	98.43	99.6	99.83	585.2313	12
☐	C31 H30 N8 O3	C31 H30 N8 Na O3	585.2333	99.21		562.2421	562.2441	3.48	3.48	97.91	100	99.61	585.2313	21
☐	C22 H28 N6 O9 S	C22 H28 N6 Na O9 S	585.2313	99		562.2421	562.2421	-0.07	0.07	96.78	99.65	100	585.2313	7

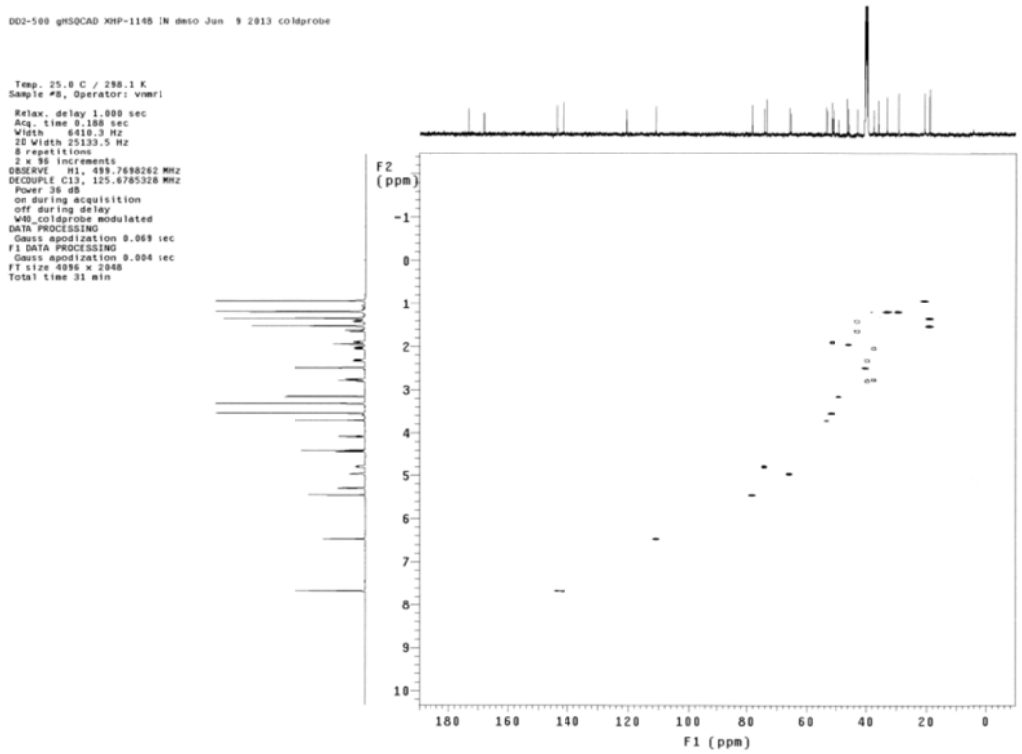
S62. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **9**



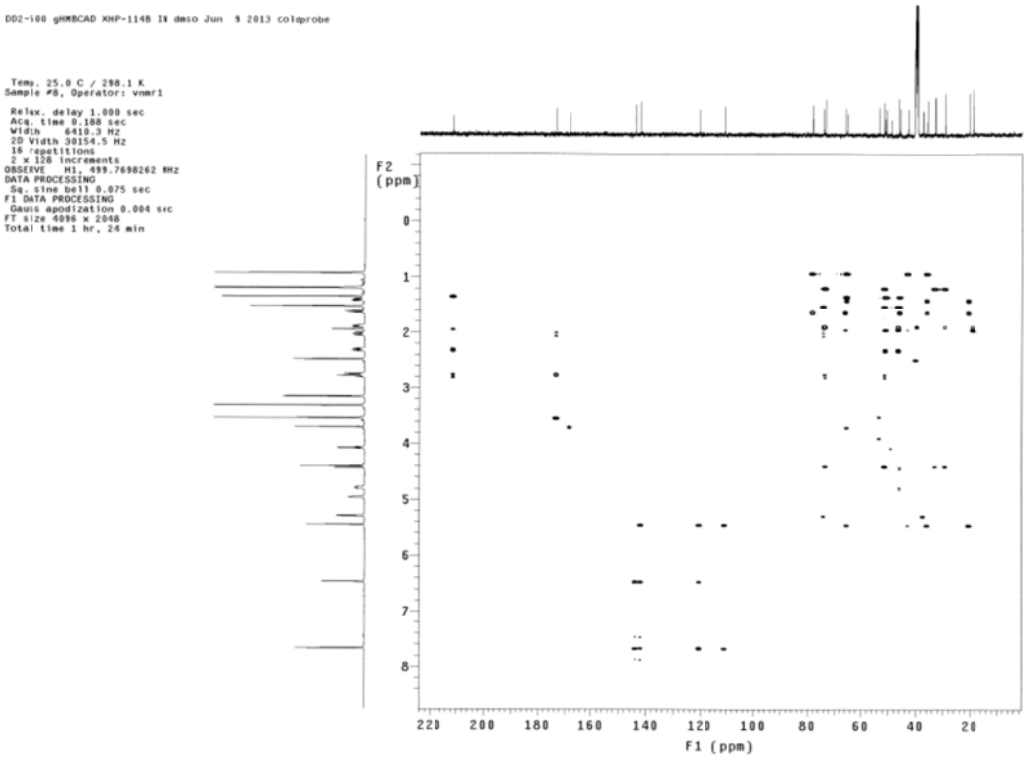
S63. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **9**



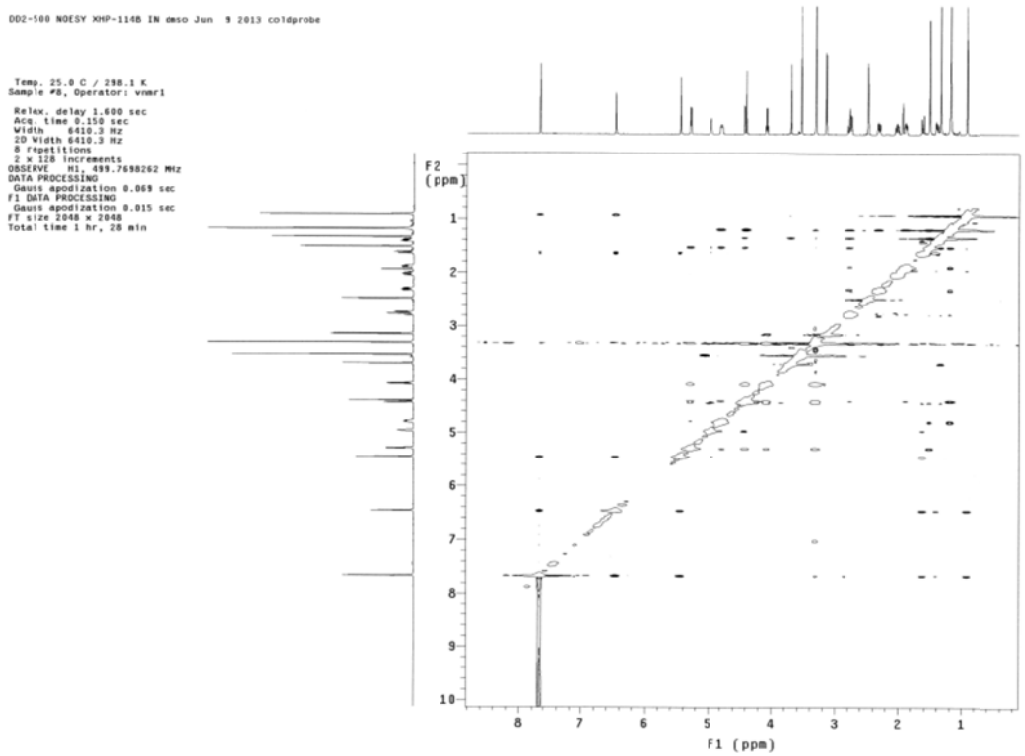
S64. HSQC Spectrum of Compound **9**



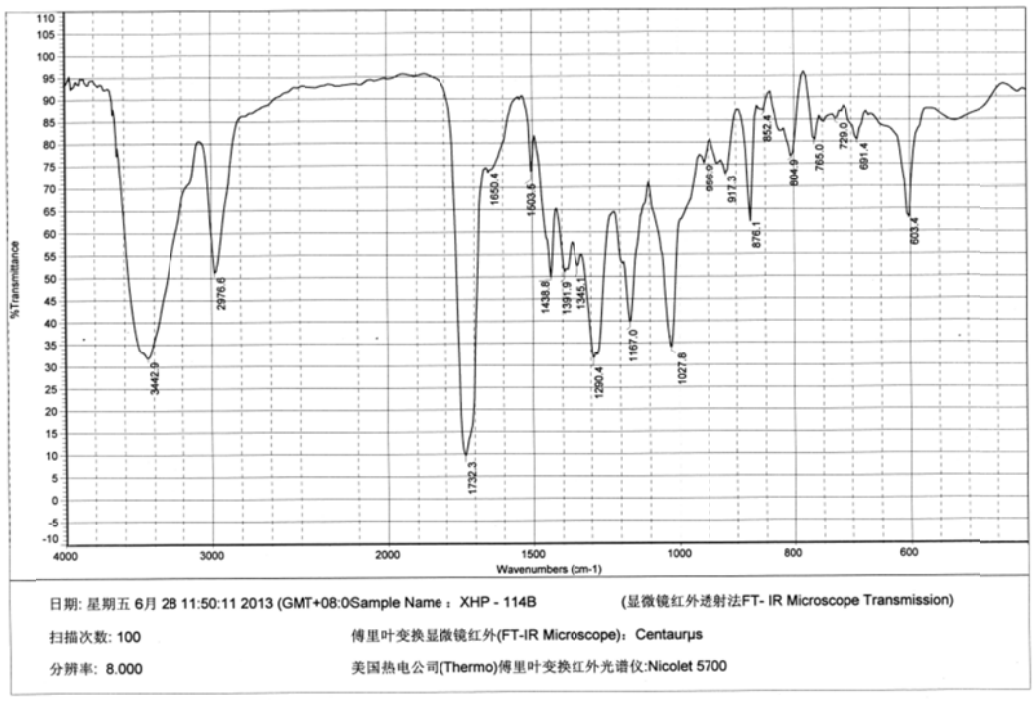
S65. HMBC Spectrum of Compound **9**



S66. NOESY Spectrum of Compound **9**



S67. IR Spectrum of Compound **9**



S68. HRESIMS Spectrum of Compound **9**

MS Formula Results: + Scan (6.252 min) Sub (2013053002.d)

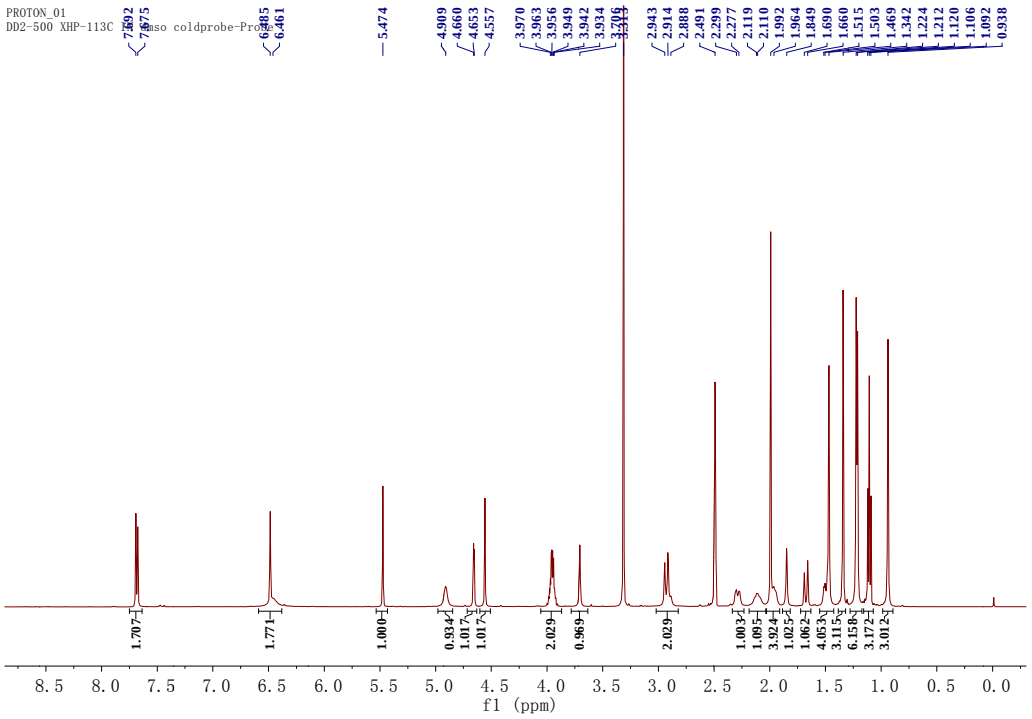
m/z	Ion	Formula	Abundance
521.2377	(M+H)+	C27 H37 O10	89392.2

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
☑	C27 H36 O10	C27 H37 O10	521.2381	99.97		520.2304	520.2308	0.86	0.86	99.99	99.92	99.97	521.2377	10
☐	C24 H38 N10 O4	C24 H39 N10 O4	521.2368	99.86		520.2304	520.2295	-1.77	1.77	99.81	99.87	99.89	521.2377	16
☐	C28 H32 N4 O6	C28 H33 N4 O6	521.2395	99.65		520.2304	520.2322	3.41	3.41	99.51	99.93	99.6	521.2377	15
☐	C23 H32 N6 O8	C23 H33 N6 O8	521.2354	99.56		520.2304	520.2282	-4.33	4.33	99.62	99.9	99.36	521.2377	11

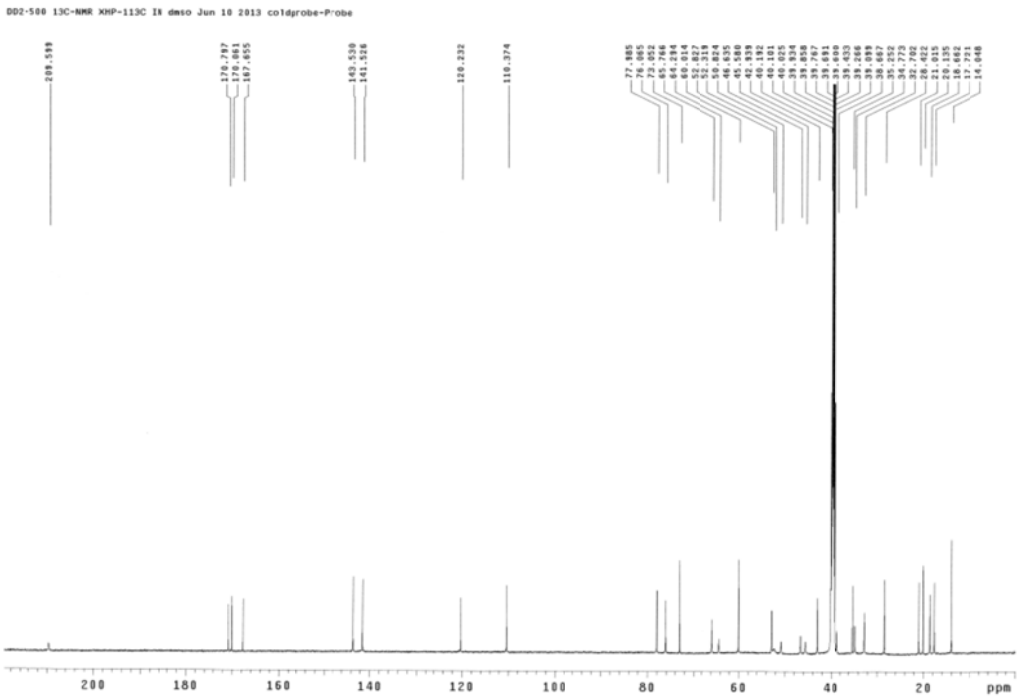
m/z	Ion	Formula	Abundance
543.2194	(M+Na)+	C27 H36 Na O10	82444.1

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
☑	C27 H36 O10	C27 H36 Na O10	543.2201	99.93		520.2302	520.2308	1.17	1.17	99.9	99.9	99.96	543.2194	10
☐	C24 H38 N10 O4	C24 H28 N10 Na O4	543.2187	99.8		520.2303	520.2295	-1.45	1.45	99.61	99.75	99.93	543.2194	16
☐	C23 H32 N6 O8	C23 H32 N6 Na O8	543.2174	99.67		520.2302	520.2282	-4.01	4.01	99.84	99.82	99.49	543.2194	11
☐	C28 H32 N4 O6	C28 H32 N4 Na O6	543.2214	99.47		520.2302	520.2322	3.73	3.73	99.02	99.85	99.56	543.2194	15
☐	C21 H32N10 O4 S	C21 H32N10 Na O4 S	543.2221	99.11		520.2303	520.2329	5.02	5.02	98.69	99.42	99.2	543.2194	11
☐	C22 H36 N2 O12	C22 H36 N2 Na O12	543.216	99.05		520.2302	520.2268	-6.57	6.57	99.02	99.89	98.64	543.2194	6

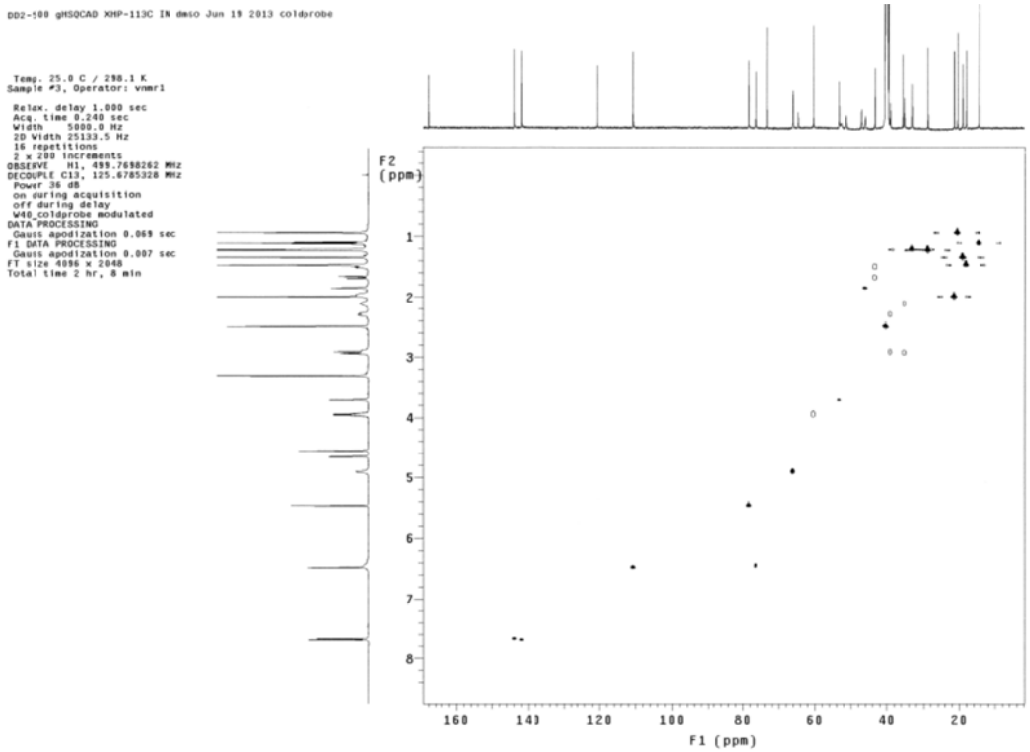
S69. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **10**



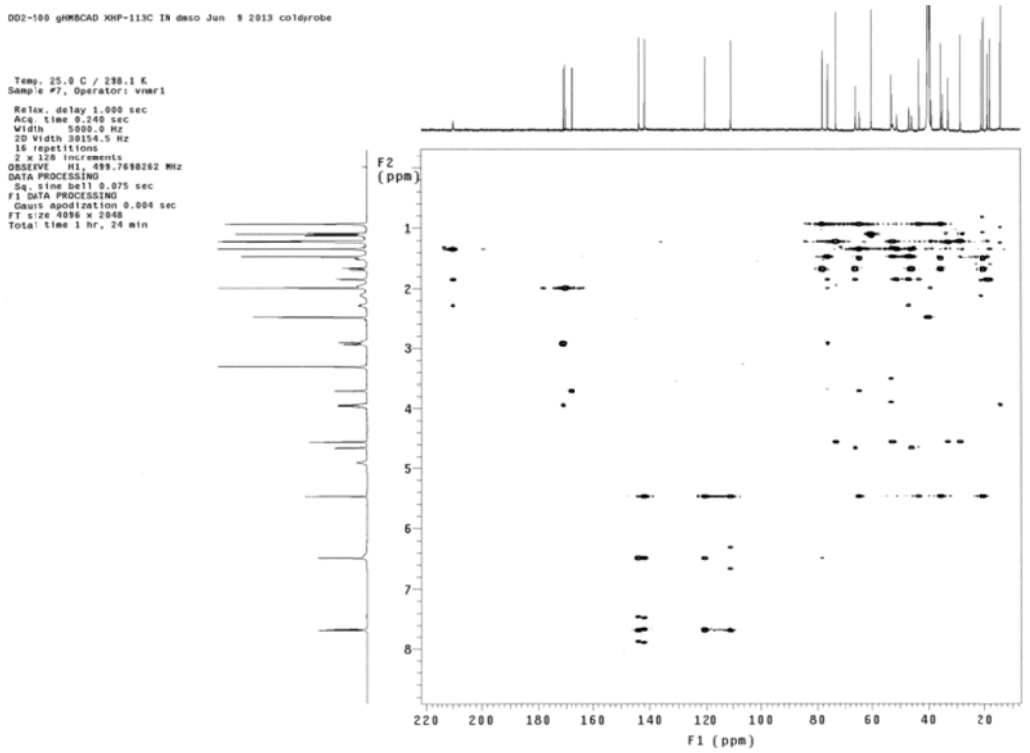
S70. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **10**



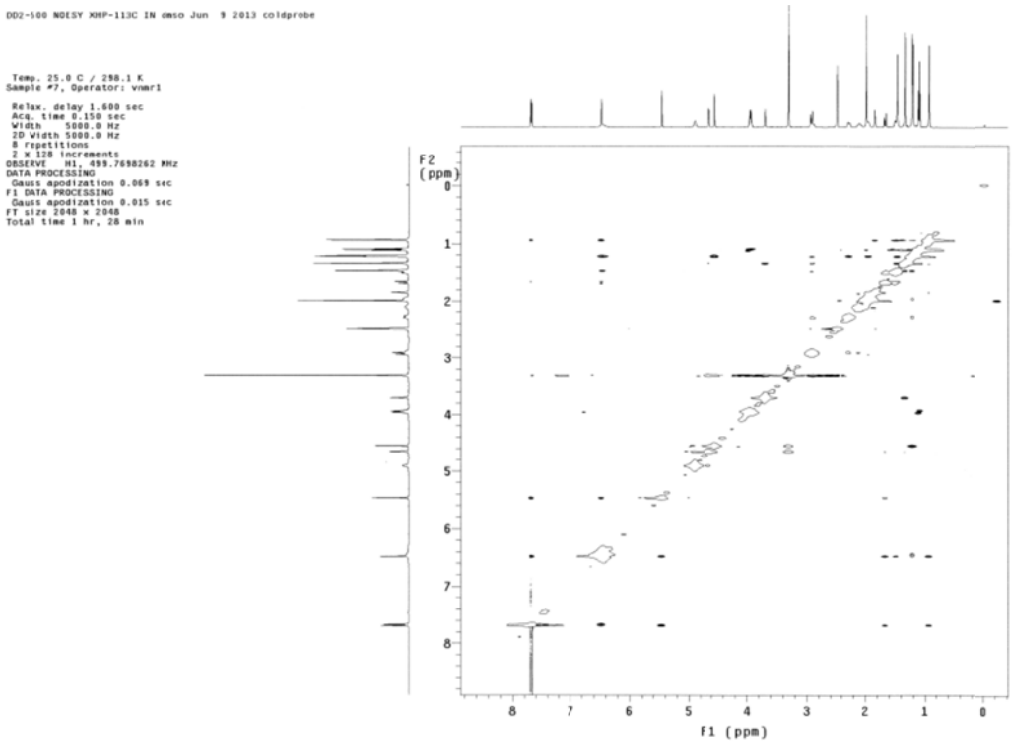
S71. HSQC Spectrum of Compound **10**



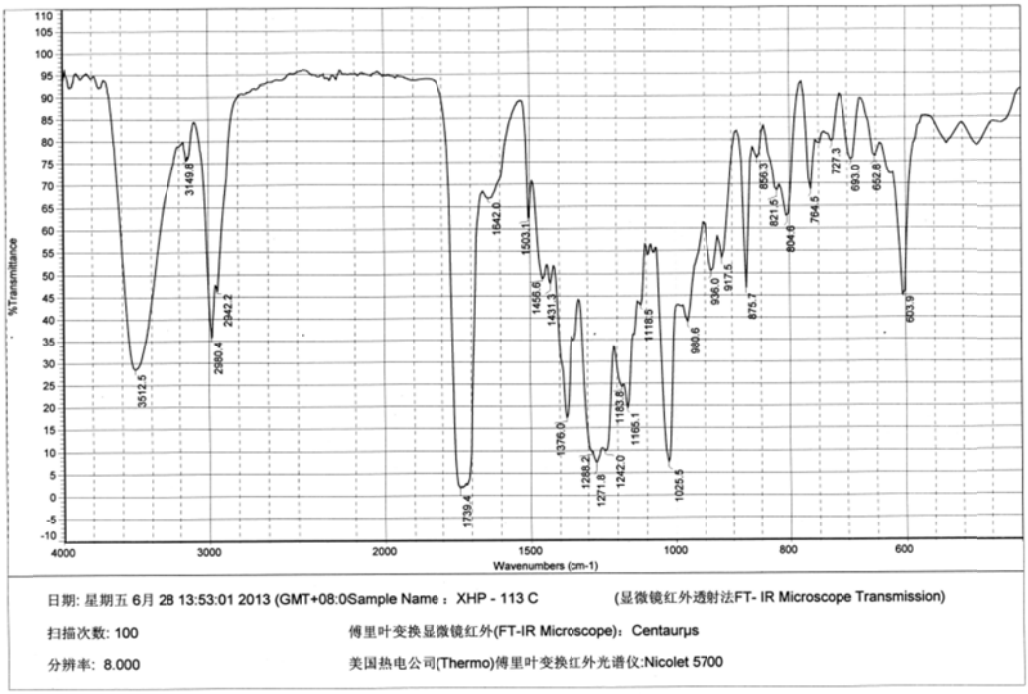
S72. HMBC Spectrum of Compound **10**



S73. NOESY Spectrum of Compound **10**



S74. IR Spectrum of Compound **10**



S75. HRESIMS Spectrum of Compound **10**

MS Formula Results: + Scan (6.704 min) Sub (2013053001.d)

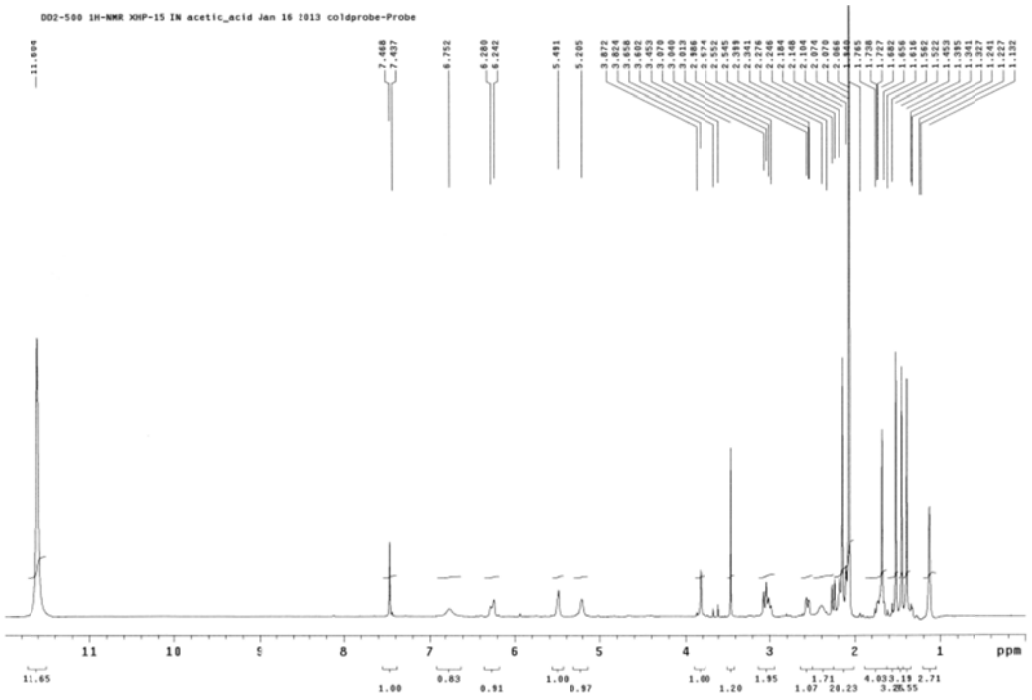
	m/z	Ion	Formula	Abundance
-	577.2642	(M+H)+	C30 H41 O11	113818.4

	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
*	☑	C30 H40 O11	C30 H41 O11	577.2643	99.94		576.2569	576.2571	0.22	0.22	99.85	99.93	100	577.2642	11
*	☐	C31 H36 N4 O7	C31 H37 N4 O7	577.2657	99.83		576.2569	576.2584	2.52	2.52	99.86	99.88	99.78	577.2642	16
*	☐	C27 H32 N10 O5	C27 H33 N10 O5	577.263	99.75		576.257	576.2557	-2.17	2.17	99.63	99.74	99.84	577.2642	17
*	☐	C26 H36 N6 O9	C26 H37 N6 O9	577.2617	99.35		576.257	576.2544	-4.48	4.48	99.03	99.81	99.3	577.2642	12
*	☐	C32 H32 N8 O3	C32 H33 N8 O3	577.267	99.32		576.257	576.2597	4.82	4.82	99.12	99.82	99.19	577.2642	21
*	☐	C35 H36 N4 O2 S	C35H37 N4 O2 S	577.2632	99.05		576.257	576.2559	-1.83	1.83	97.39	99.36	99.88	577.2642	20

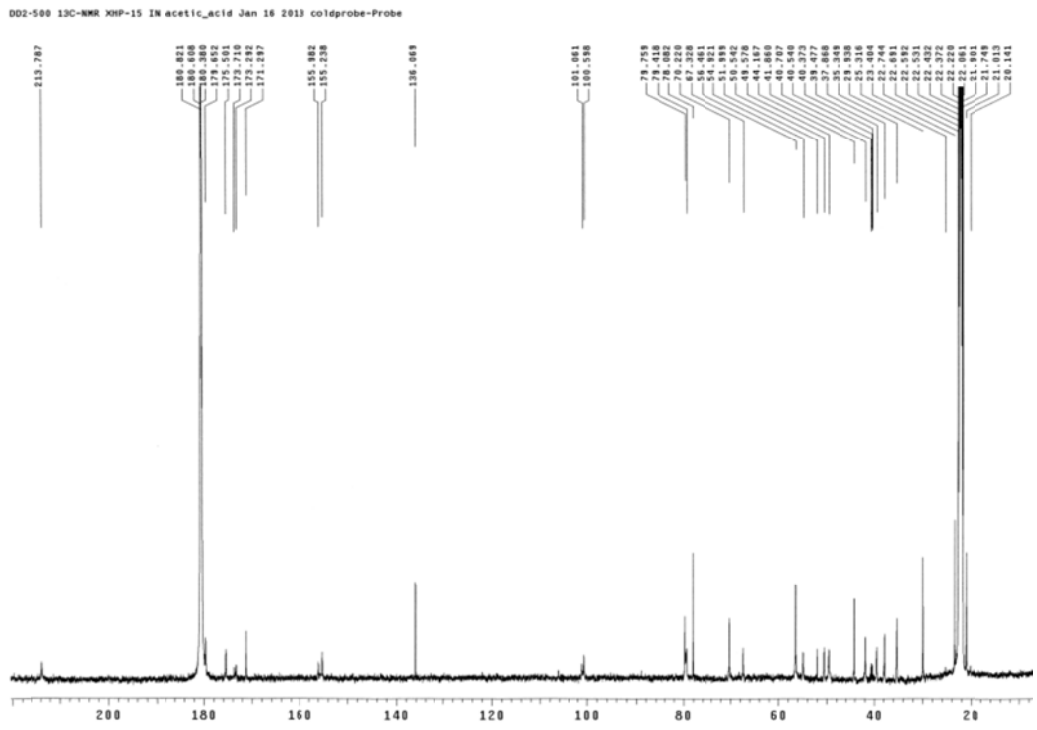
	m/z	Ion	Formula	Abundance
-	599.2468	(M+Na)+	C30 H40 Na O11	489349.7

	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
*	☑	C30 H40 O11	C30 H40 Na O11	599.2463	99.96		576.2576	576.2571	-0.94	0.94	99.96	99.93	99.97	599.2468	11
*	☐	C31 H36 N4 O7	C31 H36 N4 Na O7	599.2476	99.77		576.2576	576.2584	1.37	1.37	99.32	99.96	99.94	599.2468	16
*	☐	C27 H32 N10 O5	C27 H32 N10 Na O5	599.2449	99.76		576.2576	576.2557	-3.32	3.32	99.76	99.99	99.64	599.2468	17
*	☐	C26 H36 N6 O9	C26 H36 N6 Na O9	599.2436	99.46		576.2576	576.2544	-5.62	5.62	99.83	99.99	98.98	599.2468	12
*	☐	C24 H36 N10 O5 S	C24 H36N10 Na O5 S	599.2483	99.42		576.2576	576.2591	2.52	2.52	98.52	99.74	99.79	599.2468	12
*	☐	C32 H32 N8 O3	C32 H32 N8 Na O3	599.249	99.2		576.2576	576.2597	3.67	3.67	97.95	99.98	99.56	599.2468	21
*	☐	C23 H40 N6 O9 S	C23 H40 N6 Na O9 S	599.247	99.07		576.2576	576.2577	0.21	0.21	96.96	99.77	100	599.2468	7

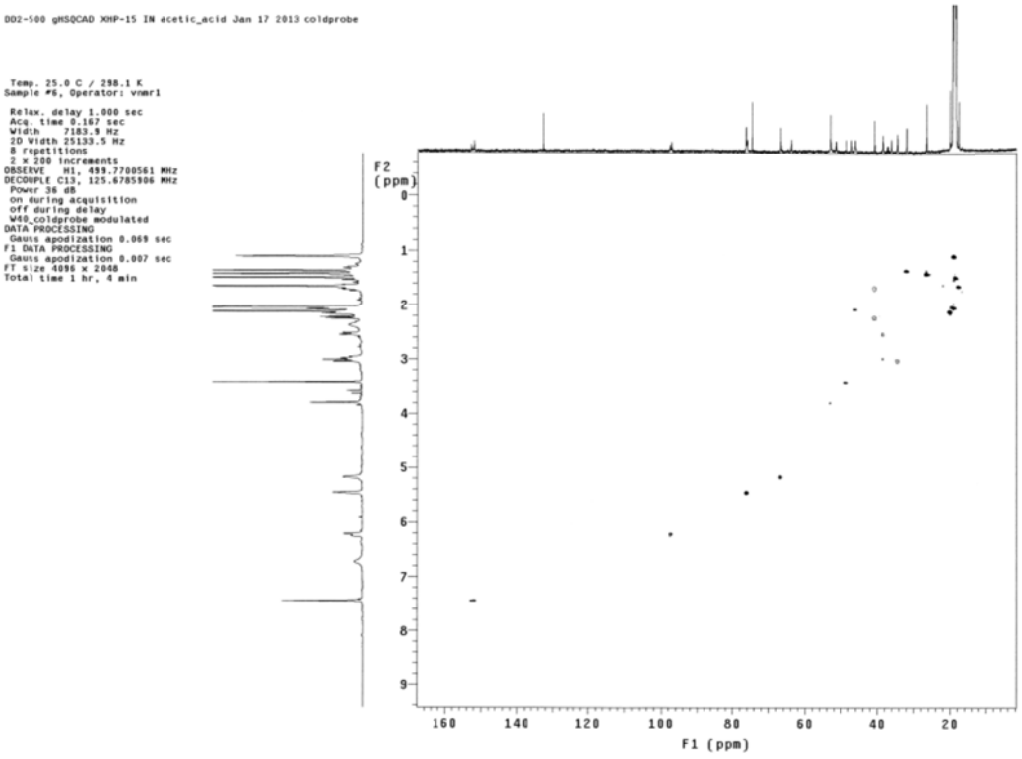
S76. ^{1}H NMR Spectrum (500 MHz, acetic acid-d_4) of Compound **11**



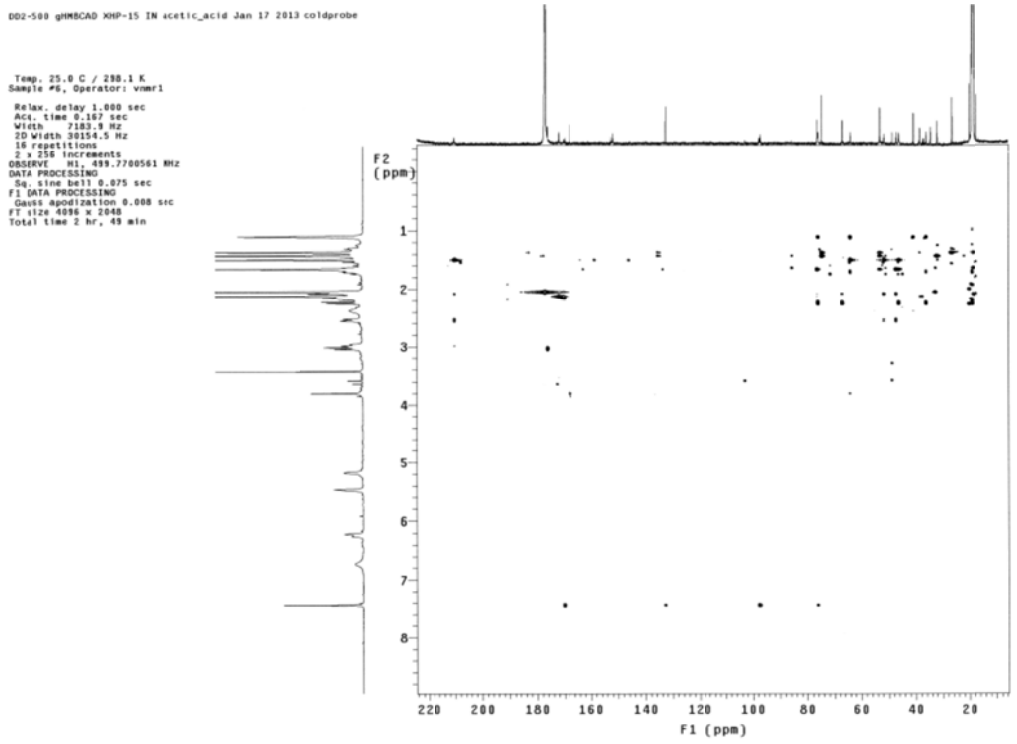
S77. ^{13}C NMR Spectrum (125 MHz, acetic acid-d_4) of Compound **11**



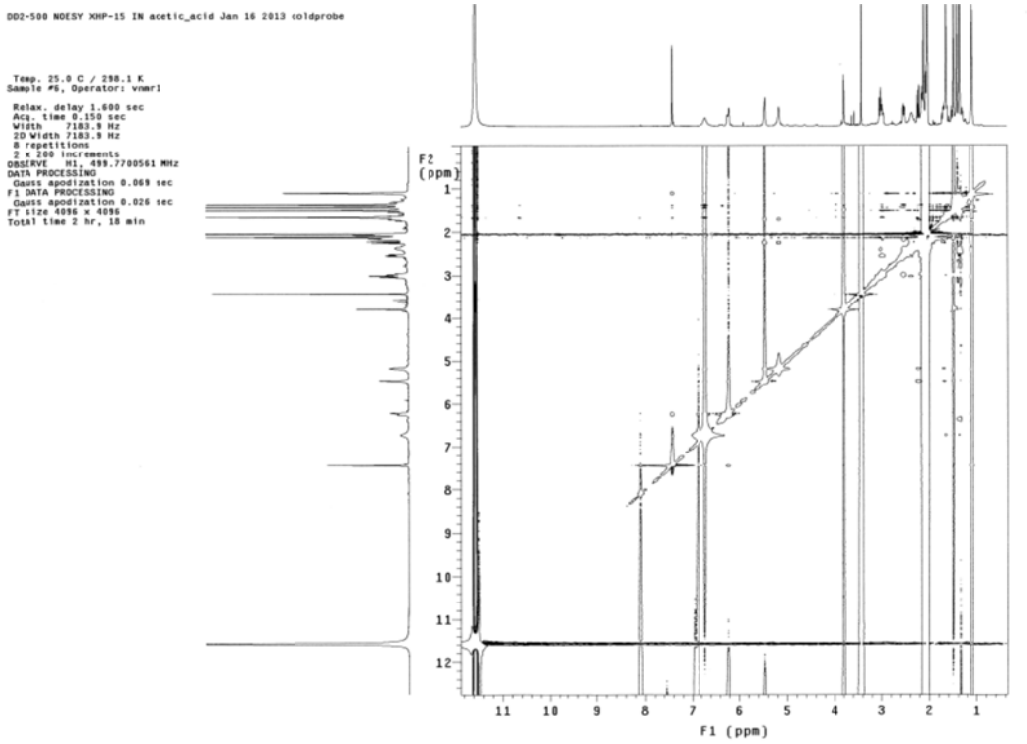
S78. HSQC Spectrum of Compound **11**



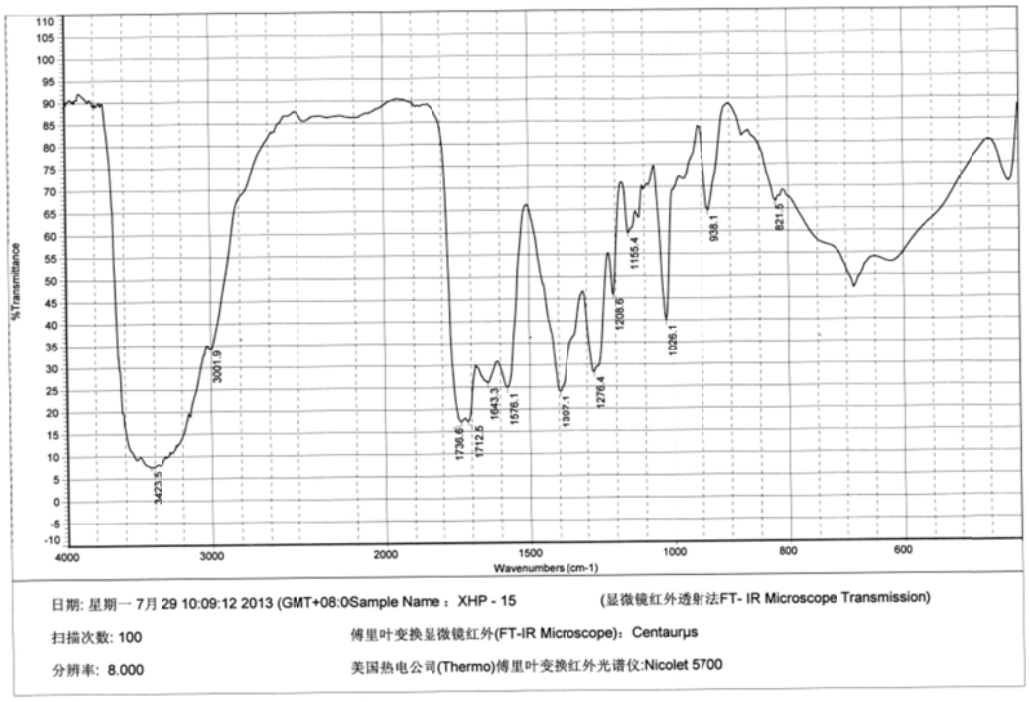
S79. HMBC Spectrum of Compound **11**



S80. NOESY Spectrum of Compound **11**



S81. IR Spectrum of Compound **11**



S82. HRESIMS Spectrum of Compound **11**

MS Formula Results: + Scan (5.705 min) Sub (2012052901.d)

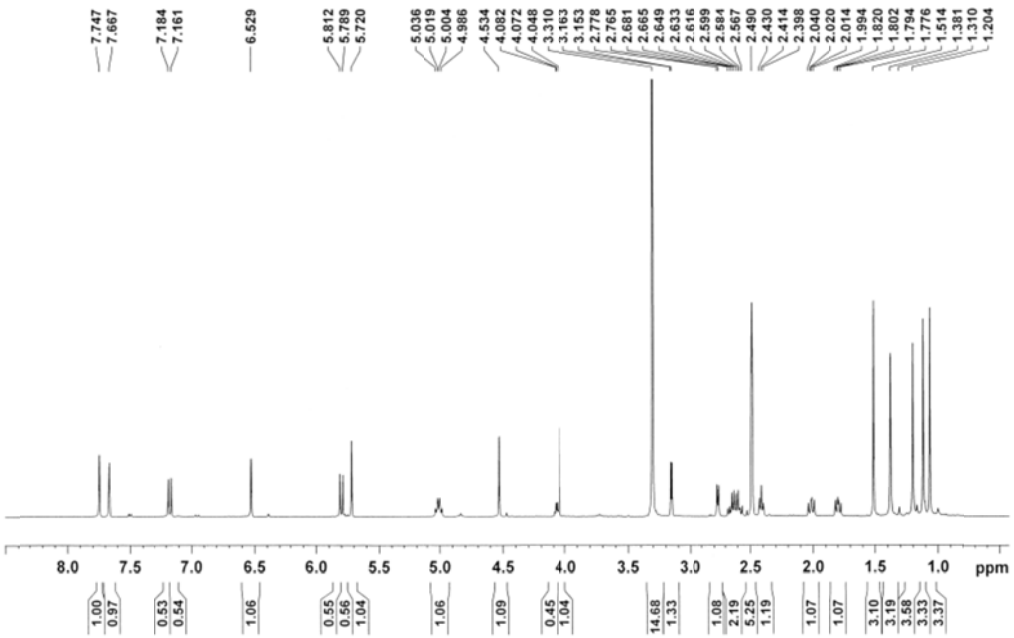
m/z	Ion	Formula	Abundance
598.2494	(M+NH4)+	C28 H40 N O13	1265923.9

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
✓	C28 H36 O13	C28 H40 N O13	598.2494	99.89		580.2156	580.2156	-0.09	0.09	99.66	99.95	100	598.2494	11
	C29 H32 N4 O9	C29 H36 N5 O9	598.2508	99.88		580.2157	580.2169	2.19	2.19	99.91	99.93	99.84	598.2494	16
	C33 H32 N4 O4 S	C33 H36 N5 O4 S	598.2483	99.24		580.2157	580.2144	-2.12	2.12	97.77	99.77	99.85	598.2494	20
	C32 H36 O8 S	C32 H40 N O8 S	598.2469	99.13		580.2156	580.2131	-4.41	4.41	98.17	99.82	99.36	598.2494	15
	C26 H36 N4 O9 S	C26 H40 N5 O9 S	598.2541	98.37		580.2157	580.2203	7.99	7.99	98.07	99.66	97.91	598.2494	11
	C25 H40 O13 S	C25 H44 N O13 S	598.2528	98.35		580.2157	580.219	5.71	5.71	96.25	99.72	98.93	598.2494	6
	C34 H32 N2 O7	C34 H36 N3 O7	598.2548	98.3		580.2156	580.221	9.14	9.14	98.64	99.93	97.28	598.2494	20
	C23 H36 N2 O15	C23 H40 N3 O15	598.2454	98.28		580.2157	580.2116	-7.04	7.04	95.72	99.95	98.38	598.2494	7
	C38 H32 N2 O2 S	C38 H36 N3 O2 S	598.2523	98.12		580.2157	580.2184	4.82	4.82	94.8	99.86	99.24	598.2494	24
	C36 H28 N4 O4	C36 H32 N5 O4	598.2449	98.09		580.2157	580.2111	-7.92	7.92	96.81	99.92	97.95	598.2494	25
	C30 H36 N4 O4 S2	C30 H40 N5 O4 S2	598.2516	97.99		580.2157	580.2178	3.68	3.68	94.2	99.39	99.55	598.2494	15
	C29 H40 O8 S2	C29 H44 N O8 S2	598.2503	97.92		580.2157	580.2165	1.39	1.39	93.28	99.45	99.94	598.2494	10
	C41 H28 N2 O2	C41 H32 N3 O2	598.2489	97.89		580.2156	580.2151	-0.98	0.98	92.76	99.91	99.97	598.2494	29
	C20 H40 N2 O15 S	C20 H44 N3 O15 S	598.2488	97.42		580.2157	580.2149	-1.24	1.24	91.38	99.8	99.95	598.2494	2
	C21 H40 N2 O10 S2	C24 H44 N3 O10 S2	598.2463	96.86		580.2157	580.2124	-5.56	5.56	91.31	99.29	98.98	598.2494	6
	C36 H36 O3 S2	C36 H40 N O3 S2	598.2444	96.5		580.2157	580.2106	-8.73	8.73	92.22	99.6	97.51	598.2494	19
	C46 H28	C46 H32 N	598.2529	95.92		580.2156	580.2191	5.96	5.96	87.76	99.9	98.83	598.2494	33

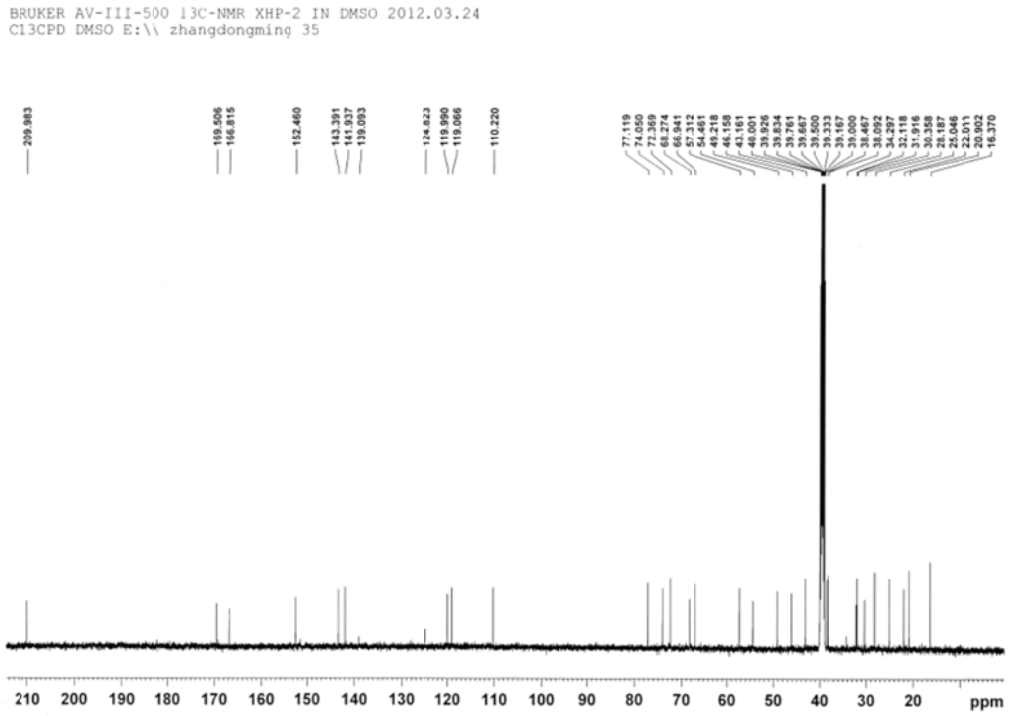
m/z	Ion	Formula	Abundance
603.2053	(M+Na)+	C28 H36 Na O13	1178295.5

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
✓	C28 H36 O13	C28 H36 Na O13	603.2048	99.97		580.2161	580.2156	-0.84	0.84	99.96	99.99	99.98	603.2053	11
	C29 H32 N4 O9	C29 H32 N4 Na O9	603.2061	99.9		580.2161	580.2169	1.45	1.45	99.79	99.98	99.93	603.2053	16
	C33 H32 N4 O4 S	C33 H32 N4 Na O4 S	603.2036	98.85		580.2161	580.2144	-2.86	2.86	96.6	99.8	99.73	603.2053	20
	C32 H36 O8 S	C32 H36 Na O8 S	603.2023	98.8		580.2161	580.2131	-5.16	5.16	97.38	99.83	99.14	603.2053	15
	C25 H40 O13 S	C25 H40 Na O13 S	603.2082	98.62		580.2161	580.219	4.97	4.97	96.73	99.74	99.2	603.2053	6
	C26 H36 N4 O9 S	C26 H36 N4 Na O9 S	603.2095	98.6		580.2161	580.2203	7.25	7.25	98.17	99.7	98.3	603.2053	11
	C23 H36 N2 O15	C23 H36 N2 Na O15	603.2008	98.47		580.2161	580.2116	-7.78	7.78	97.89	99.99	98.05	603.2053	7
	C34 H32 N2 O7	C34 H32 N2 Na O7	603.2102	98.24		580.2161	580.221	8.4	8.4	97.65	99.98	97.73	603.2053	20
	C30 H36 N4 O4 S2	C30 H36 N4 Na O4 S2	603.207	97.83		580.2161	580.2178	2.94	2.94	93.32	99.46	99.72	603.2053	15
	C29 H40 O8 S2	C29 H40 Na O8 S2	603.2057	97.8		580.2161	580.2165	0.65	0.65	92.75	99.5	99.99	603.2053	10
	C20 H40 N2 O15 S	C20 H40 N2 Na O15 S	603.2042	97.74		580.2161	580.2149	-1.98	1.98	92.59	99.64	99.87	603.2053	2
	C38 H32 N2 O2 S	C38 H32 N2 Na O2 S	603.2077	97.69		580.2161	580.2184	4.08	4.08	92.92	99.88	99.46	603.2053	24
	C36 H28 N4 O4	C36 H28 N4 Na O4	603.2003	97.51		580.2161	580.2111	-8.67	8.67	95.34	99.97	97.59	603.2053	25
	C41 H28 N2 O2	C41 H28 N2 Na O2	603.2043	97.26		580.2161	580.2151	-1.73	1.73	90.59	99.97	99.9	603.2053	29
	C21 H40 O18	C21 H40 Na O18	603.2107	97.23		580.2161	580.2215	9.29	9.29	94.94	100	97.23	603.2053	2
	C24 H40 N2 O10 S2	C24 H40 N2 Na O10 S2	603.2017	96.81		580.2161	580.2124	-6.3	6.3	91.48	99.37	98.72	603.2053	6
	C35 H36 N2 O2 S2	C35 H36 N2 Na O2 S2	603.211	95.89		580.2161	580.2218	9.88	9.88	91.16	99.59	96.87	603.2053	19
	C36 H36 O3 S2	C36 H36 Na O3 S2	603.1998	95.86		580.2161	580.2106	-9.47	9.47	90.61	99.63	97.12	603.2053	19
	C46 H28	C46 H28 Na	603.2083	95.29		580.2161	580.2191	5.21	5.21	85.01	99.96	99.12	603.2053	33

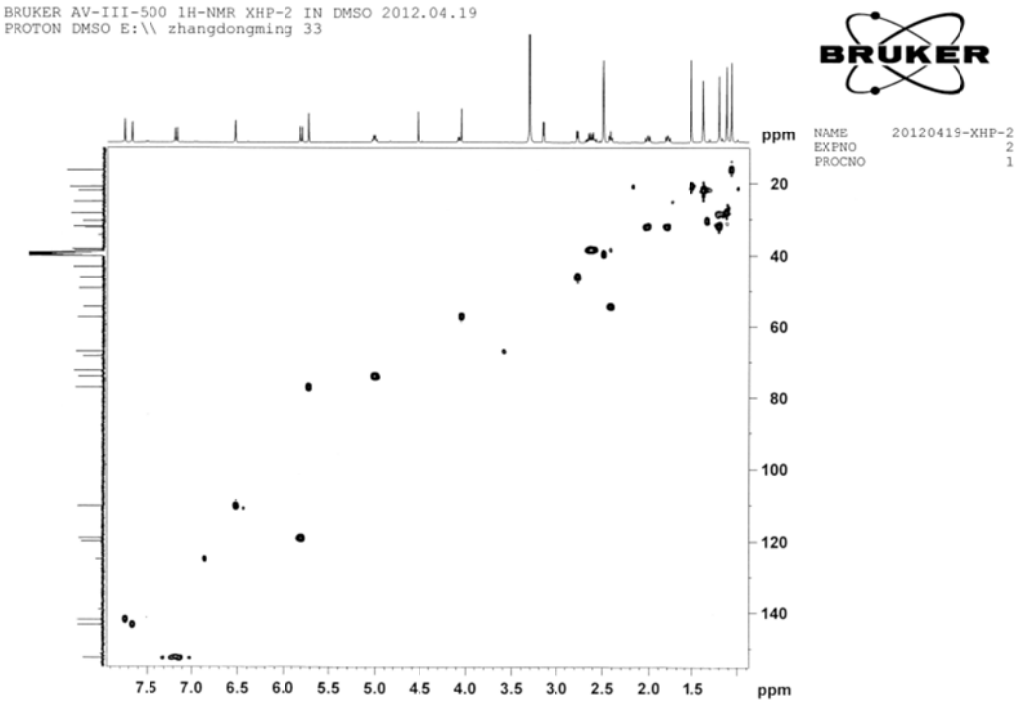
S83. ^{1}H NMR Spectrum (500 MHz, DMSO-d_6) of Compound **12**



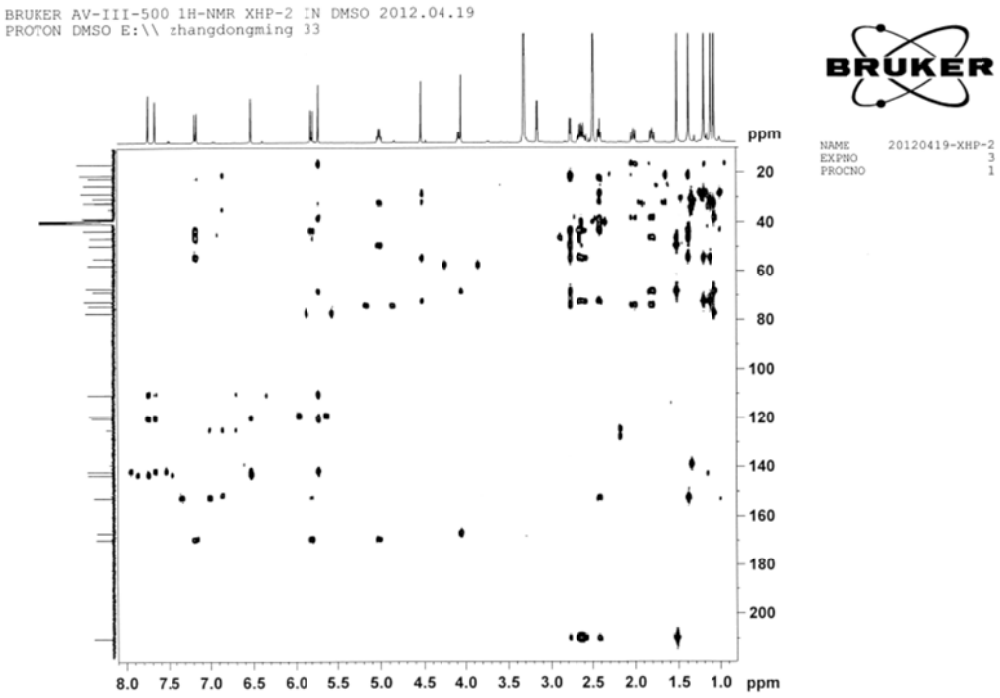
S84. ^{13}C NMR Spectrum (125 MHz, DMSO-d_6) of Compound **12**



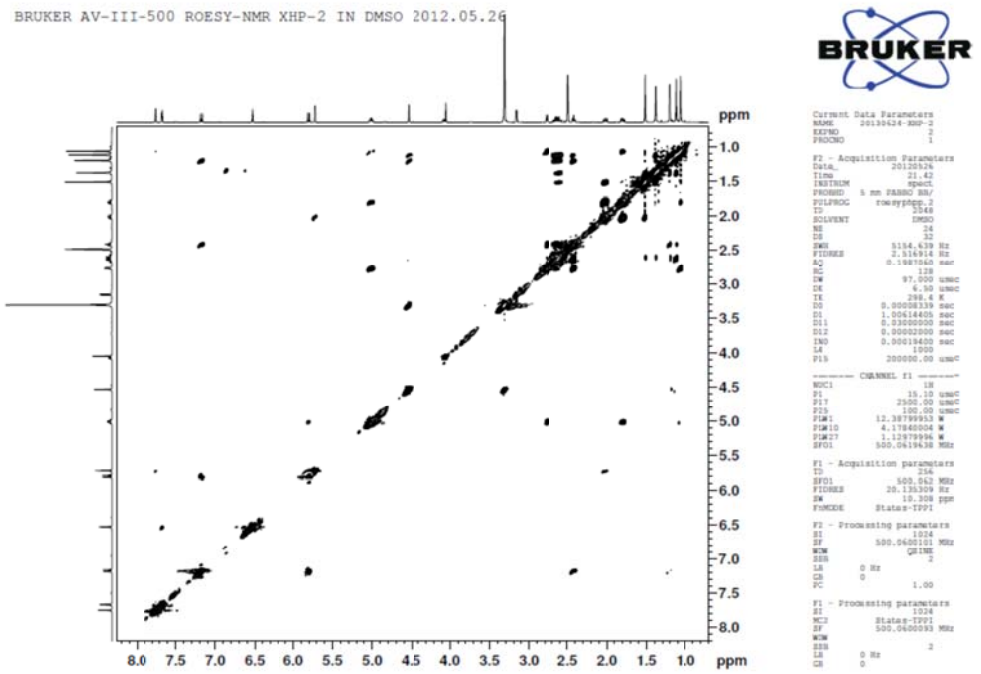
S85. HSQC Spectrum of Compound **12**



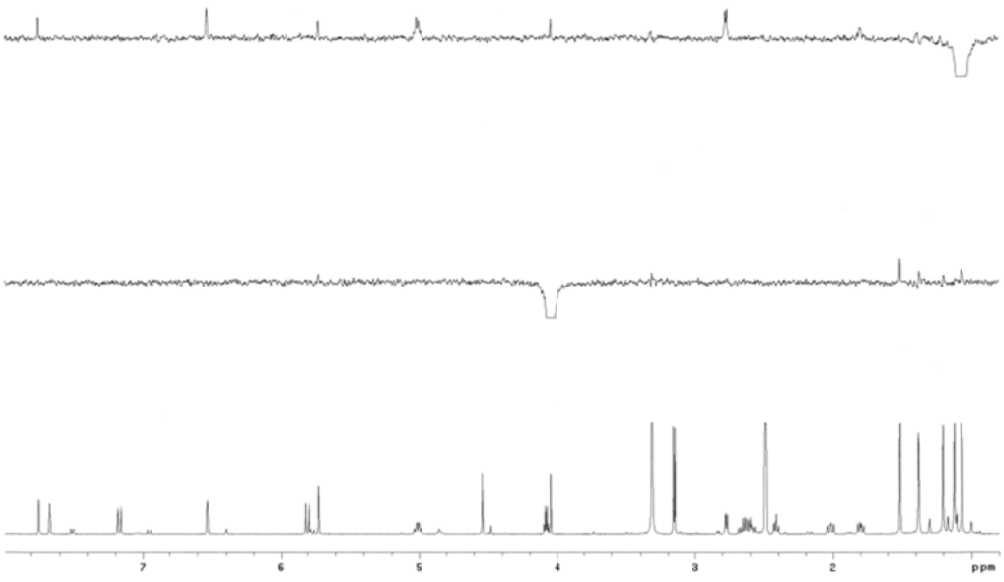
S86. HMBC Spectrum of Compound **12**



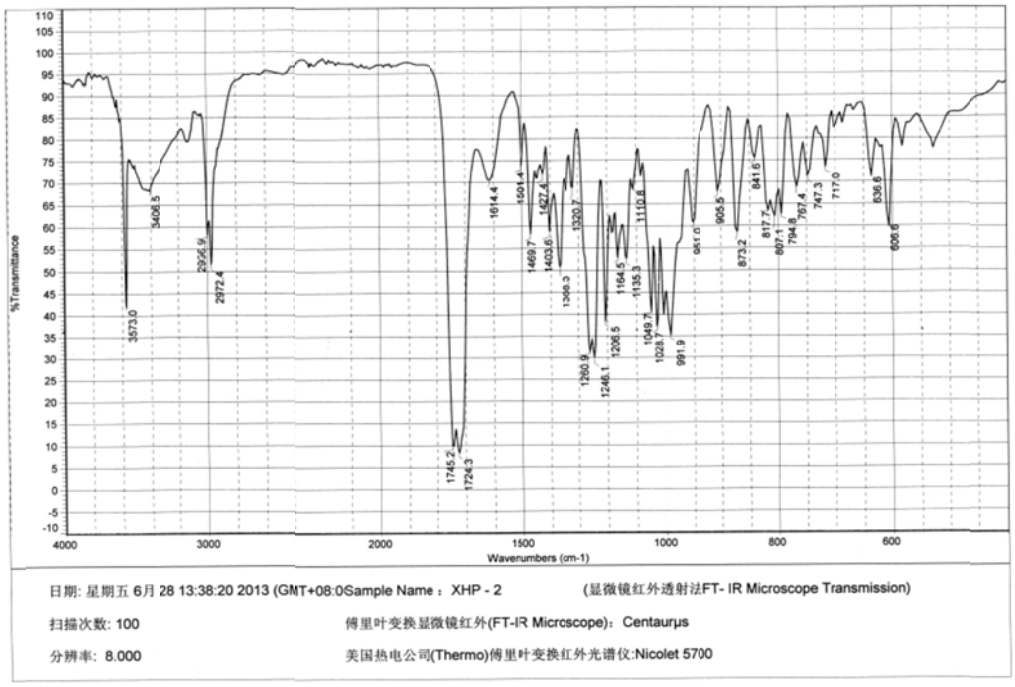
S87. ROESY Spectrum of Compound **12**



S88. NOE Difference Spectrum of Compound **12**



S89. IR Spectrum of Compound **12**



S90. HRESIMS Spectrum of Compound **12**

MS Formula Results: + Scan (6.575 min) Sub (2012040901.d)

	m/z	Ion	Formula	Abundance
+	471.2018	(M+H)+	C26 H31 O8	2072629.3

	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
+	☐	C27 H26 N4 O4	C27 H27 N4 O4	471.2027	99.92		470.1946	470.1954	1.73	1.73	99.96	99.9	99.9	471.2018	17
+	☑	C26 H30 O8	C26 H31 O8	471.2013	99.8		470.1946	470.1941	-1.1	1.1	99.4	99.96	99.96	471.2018	12
+	☐	C30 H30 O3 S	C30 H31 O3 S	471.1988	98.62		470.1946	470.1916	-6.43	6.43	97.75	99.56	98.61	471.2018	16
+	☐	C23 H34 O8 S	C23 H35 O8 S	471.2047	97.87		470.1946	470.1974	6.06	6.06	94.99	99.52	98.76	471.2018	7
+	☐	C24 H30 N4 O4 S	C24 H31 N4 O4 S	471.2061	97.83		470.1946	470.1988	8.89	8.89	97.28	99.42	97.36	471.2018	12
+	☐	C27 H34 O3 S2	C27 H35 O3 S2	471.2022	97.5		470.1946	470.1949	0.73	0.73	91.95	99.21	99.98	471.2018	11
+	☐	C21 H30 N2 O10	C21 H31 N2 O10	471.1973	97.25		470.1946	470.19	-9.66	9.66	95.62	99.93	95.89	471.2018	8
+	☐	C11 H34 N2 O10 S	C18 H35 N2 O10 S	471.2067	96.63		470.1946	470.1934	-2.51	2.51	89.1	99.35	99.79	471.2018	3
+	☐	C21 H34 N2 O5 S2	C22 H35 N2 O5 S2	471.1982	95.76		470.1946	470.1909	-7.84	7.84	89.39	99.01	97.94	471.2018	7

	m/z	Ion	Formula	Abundance
+	488.2289	(M+NH4)+	C26 H34 N O8	4926334.5

	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
+	☐	C27 H26 N4 O4	C17 H30 N5 O4	488.2292	99.77		470.195	470.1954	0.81	0.81	99.24	99.99	99.98	488.2289	17
+	☑	C26 H30 O8	C26 H34 N O8	488.2279	99.37		470.195	470.1941	-2.01	2.01	98.04	99.95	99.87	488.2289	12
+	☐	C30 H30 O3 S	C31 H34 N O3 S	488.2254	98.69		470.195	470.1916	-7.35	7.35	96.65	99.49	98.3	488.2289	16
+	☐	C32 H26 N2 O2	C32 H30 N3 O2	488.2333	98.58		470.195	470.1994	9.38	9.38	99.63	99.97	97.25	488.2289	21
+	☐	C24 H30 N4 O4 S	C24H34 N5 O4 S	488.2326	97.92		470.195	470.1988	7.96	7.96	96.64	99.26	98.01	488.2289	12
+	☐	C27 H34 O3 S2	C27H38 N O3 S2	488.2288	97.67		470.195	470.1949	-0.19	0.19	92.79	98.85	100	488.2289	11
+	☐	C23 H34 O8 S	C23 H38 N O8 S	488.2313	97.66		470.195	470.1974	5.14	5.14	93.8	99.29	99.17	488.2289	7
+	☐	C18 H34 N2 O10 S	C18 H38 N3 O10 S	488.2272	95.83		470.195	470.1934	-3.43	3.43	86.75	99.12	99.63	488.2289	3
+	☐	C22 H34 N2 O5 S2	C22 H38 N3 O5 S2	488.2247	95.4		470.195	470.1909	-8.76	8.76	89.05	98.64	97.6	488.2289	7

	m/z	Ion	Formula	Abundance
+	493.1844	(M+Na)+	C26 H30 Na O8	525470

	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
+	☐	C27 H26 N4 O4	C27 H26 N4 Na O4	493.1846	99.88		470.1952	470.1954	0.5	0.5	99.63	99.97	99.99	493.1844	17
+	☑	C26 H30 O8	C26 H30 Na O8	493.1833	99.86		470.1952	470.1941	-2.32	2.32	99.86	99.92	99.83	493.1844	12
+	☐	C23 H34 O8 S	C23H34 Na O8 S	493.1867	98.58		470.1952	470.1974	4.84	4.84	96.53	99.65	99.27	493.1844	7
+	☐	C24 H30 N4 O4 S	C24 H32 N4 Na O4 S	493.188	98.49		470.1952	470.1988	7.66	7.66	98.03	99.86	98.19	493.1844	12
+	☐	C30 H30 O3 S	C30H30 Na O3 S	493.1808	98.22		470.1952	470.1916	-7.65	7.65	96.97	99.76	98.19	493.1844	16
+	☐	C32 H26 N2 O2	C32 H26 N2 Na O2	493.1886	97.98		470.1952	470.1994	9.07	9.07	97.19	99.83	97.47	493.1844	21
+	☐	C27 H34 O3 S2	C27 H34 Na O3 S2	493.1842	97.62		470.1952	470.1949	-0.49	0.49	92.15	99.43	99.99	493.1844	11
+	☐	C18 H34 N2 O10 S	C18 H34N2 Na O10 S	493.1826	97.43		470.1952	470.1934	-3.73	3.73	92.07	99.58	99.57	493.1844	3
+	☐	C22 H34 N2 O5 S2	C22 H34N2 Na O5 S2	493.1801	96.07		470.1952	470.1909	-9.06	9.06	91.01	99.32	97.48	493.1844	7