Supplemental Information

Supplemental Information List

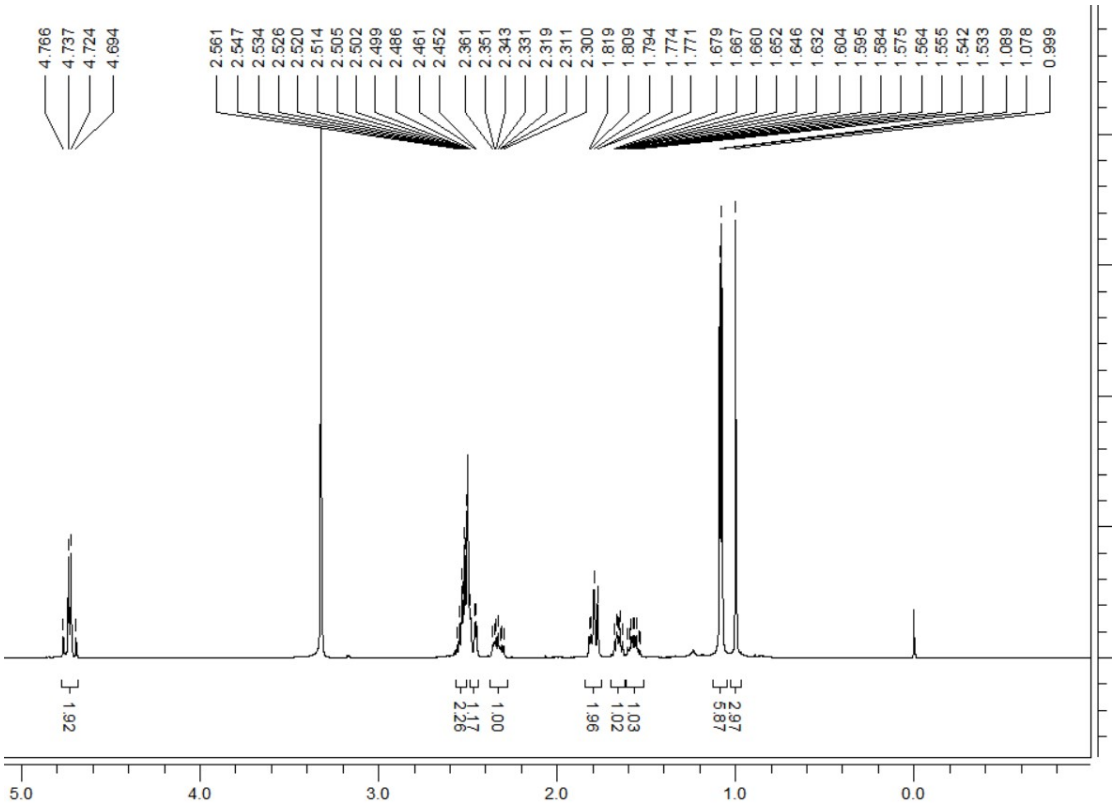

Fig S1 ^{1}H-NMR spectrum of compound **1** (DMSO-d_6, 600 MHz)

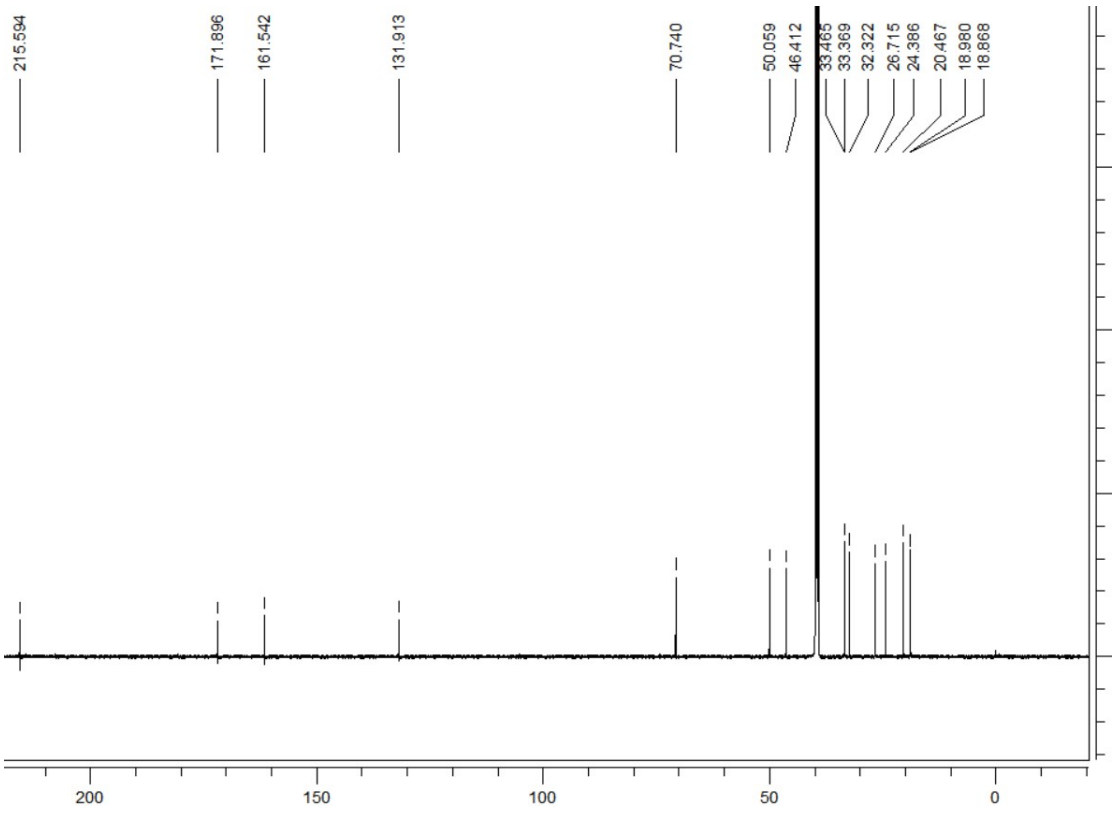

Fig S2 ^{13}C-NMR spectrum of compound **1** (DMSO-d_6, 150 MHz)

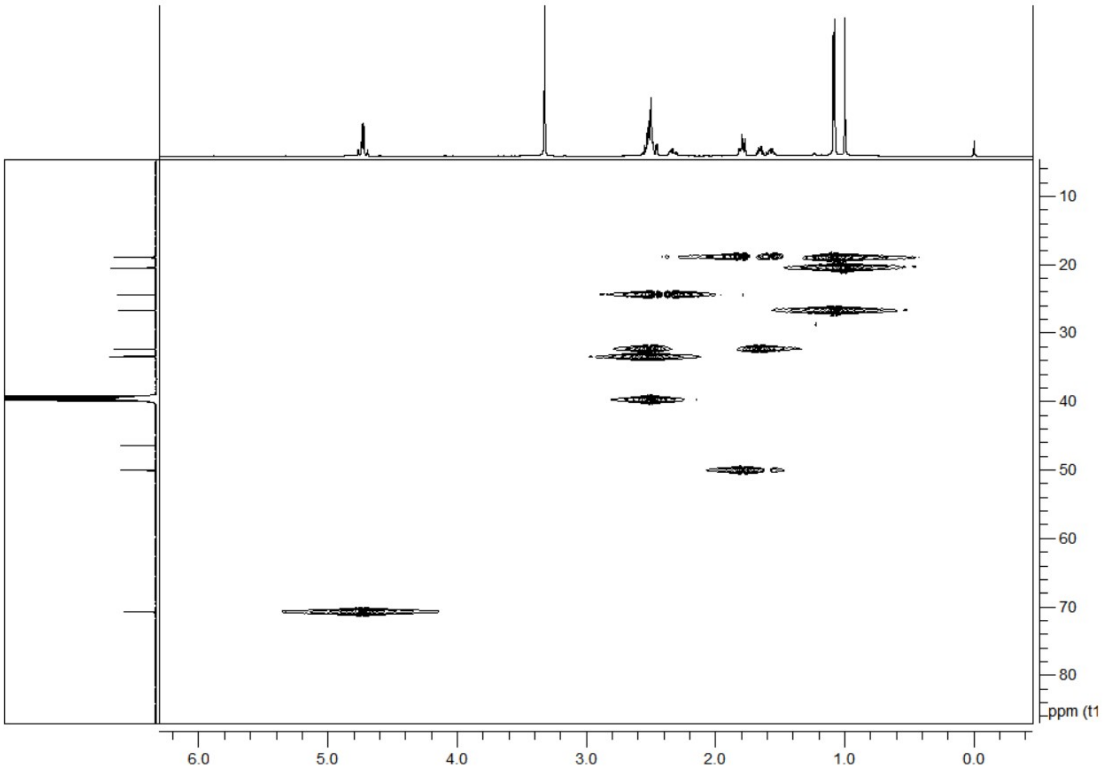

Fig S3 HSQC spectrum of compound **1** (DMSO-d_6)

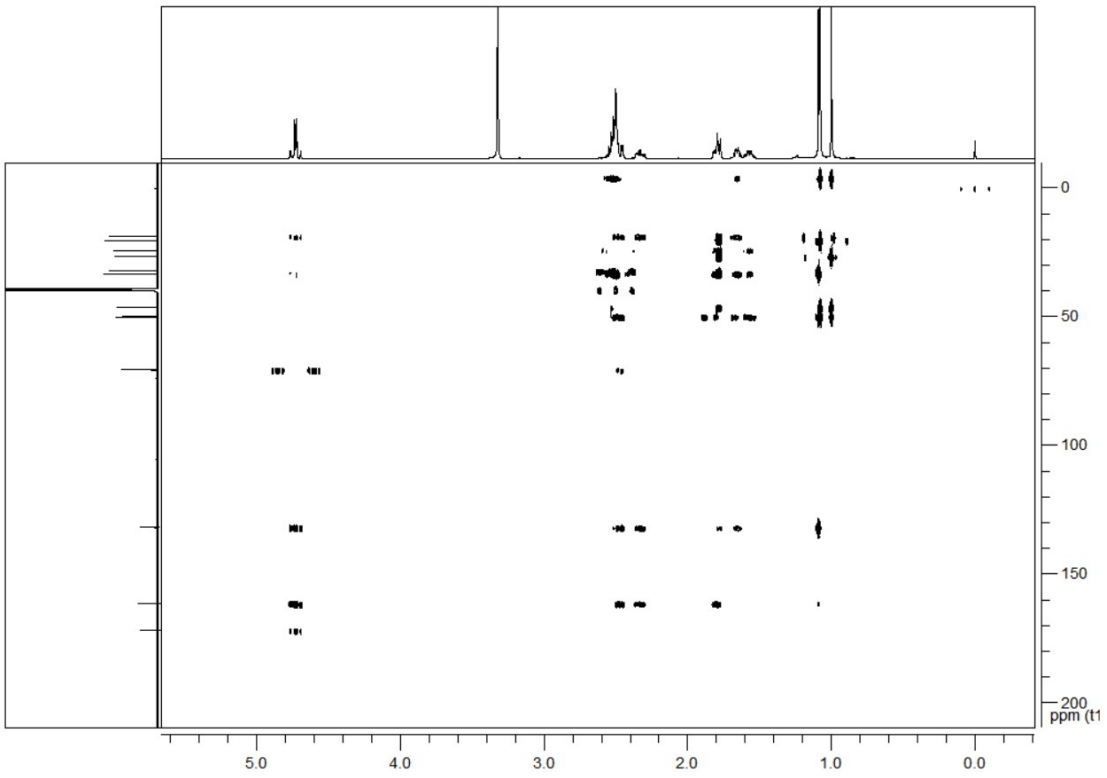

Fig S4 HMBC spectrum of compound **1** (DMSO-d_6)

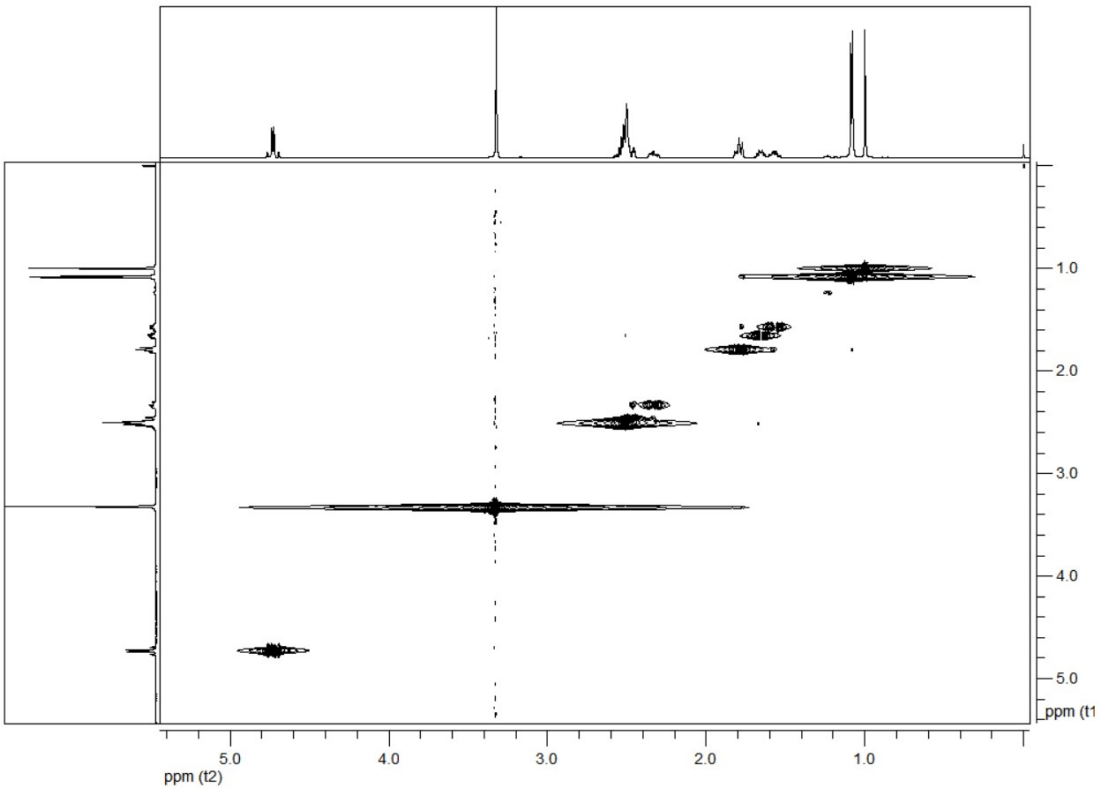

Fig S5 NOESY spectrum of compound **1** (DMSO-d_6)

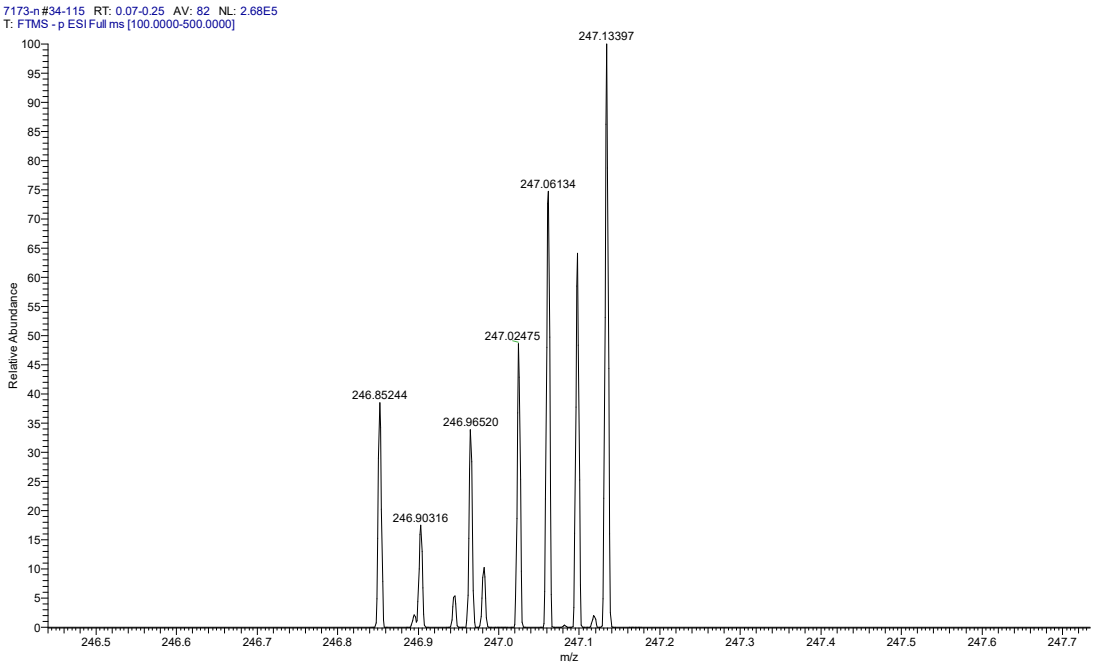

Fig S6 HRESIMS spectrum of compound **1** (MeOH)

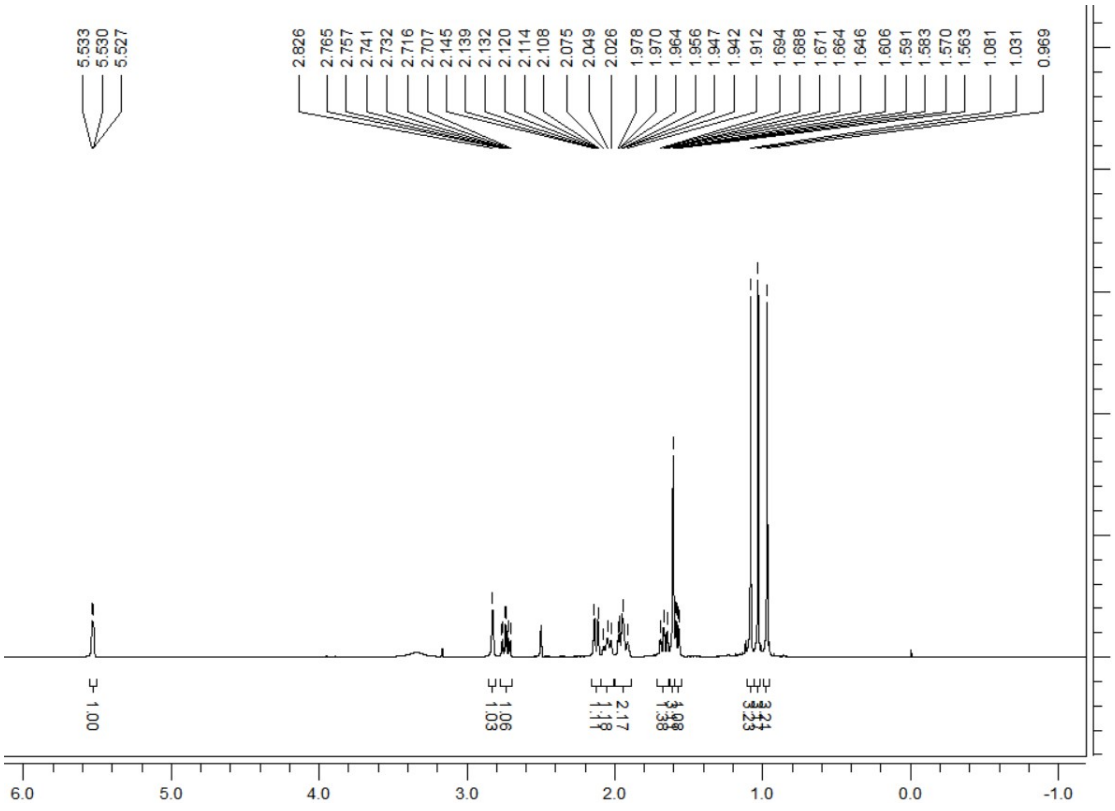

Fig S7 ^{1}H-NMR spectrum of compound **2** (DMSO-d_6, 600 MHz)

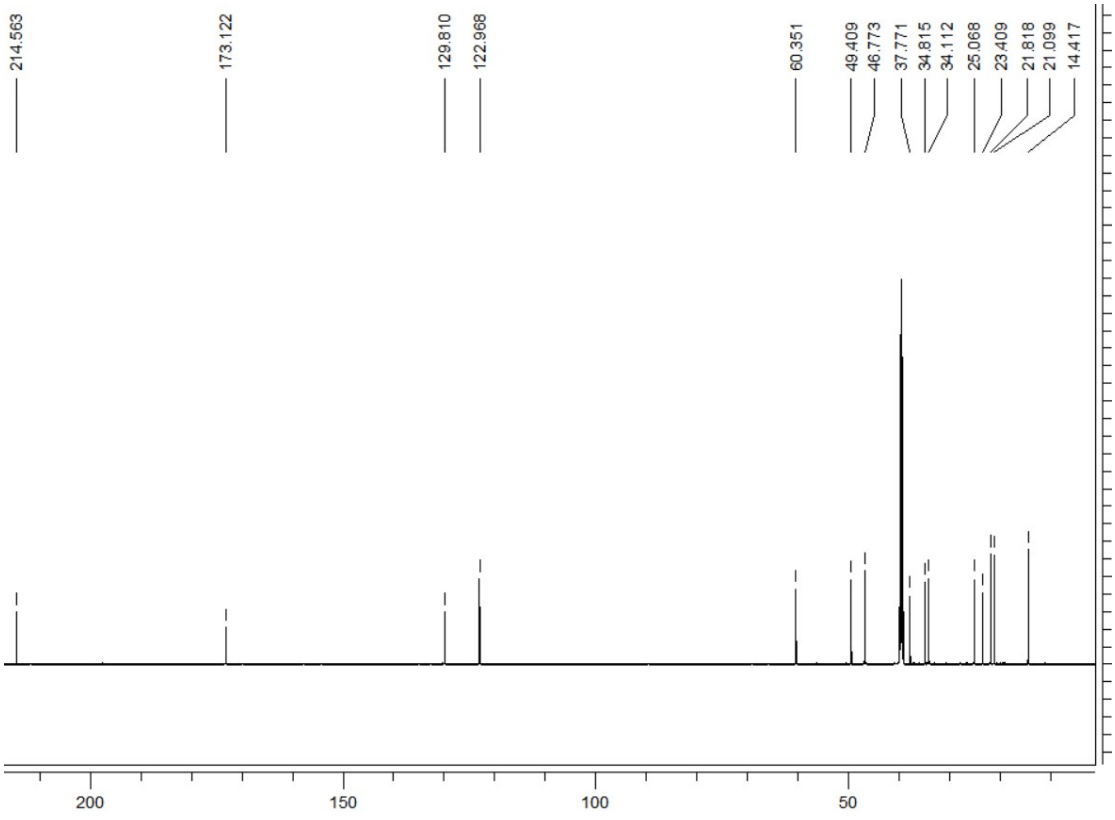

Fig S8 ^{13}C-NMR spectrum of compound **2** (DMSO-d_6, 150 MHz)

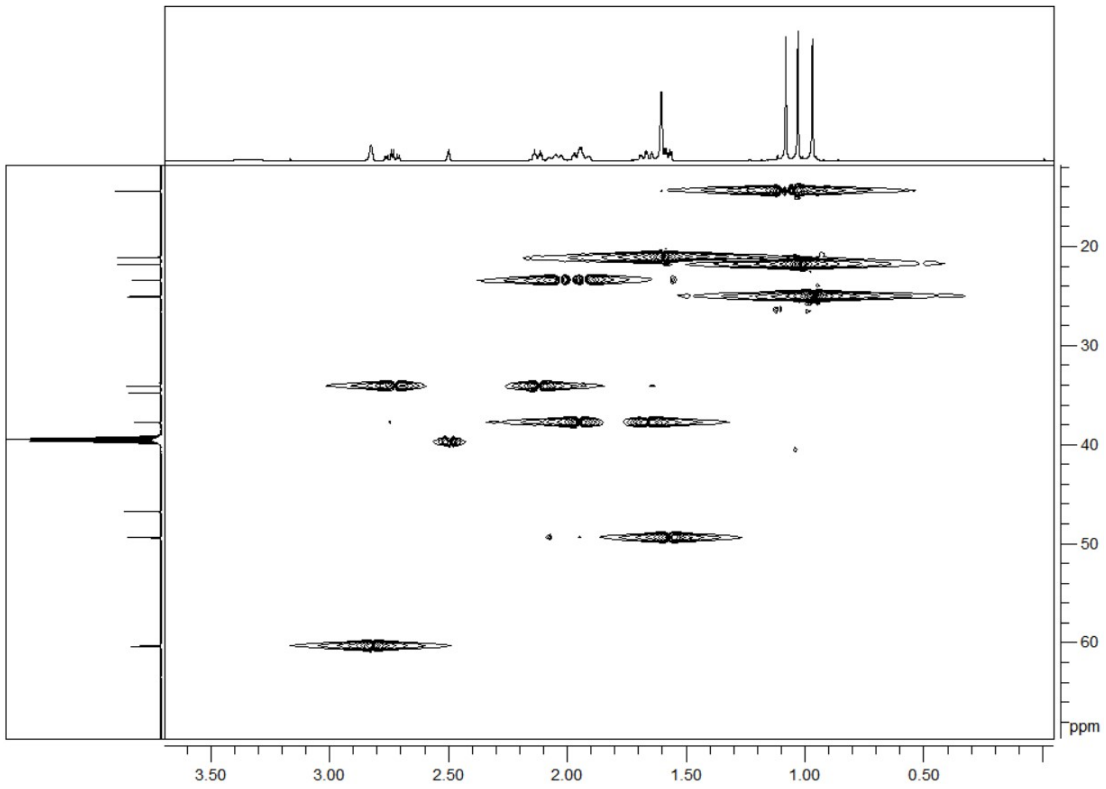

Fig S9 HSQC spectrum of compound **2** (DMSO-d_6)

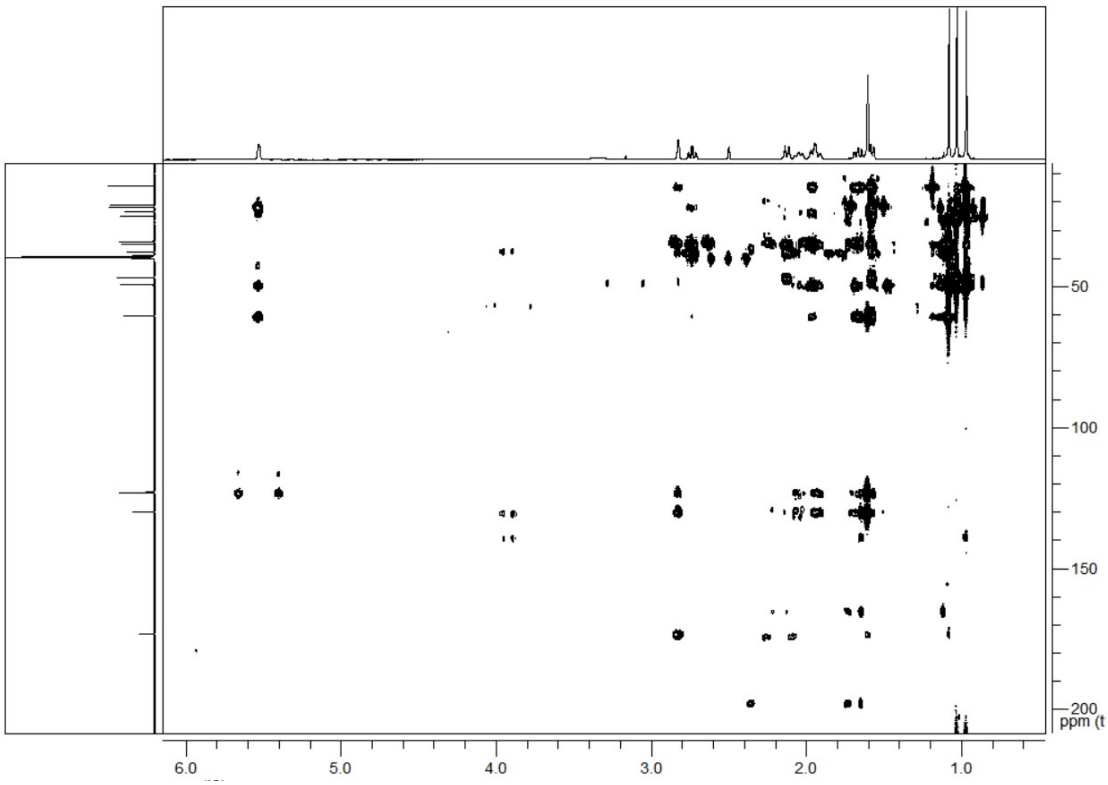

Fig S10 HMBC spectrum of compound **2** (DMSO-d_6)

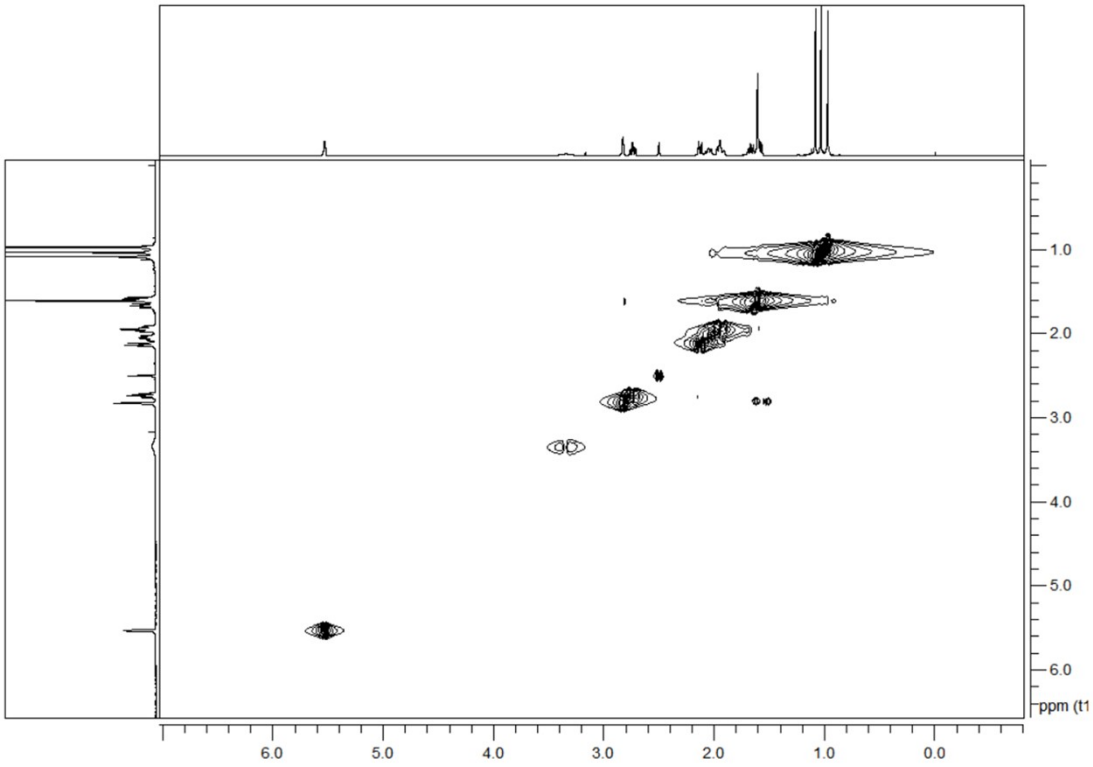

Fig S11 NOESY spectrum of compound **2** (DMSO-d_6)

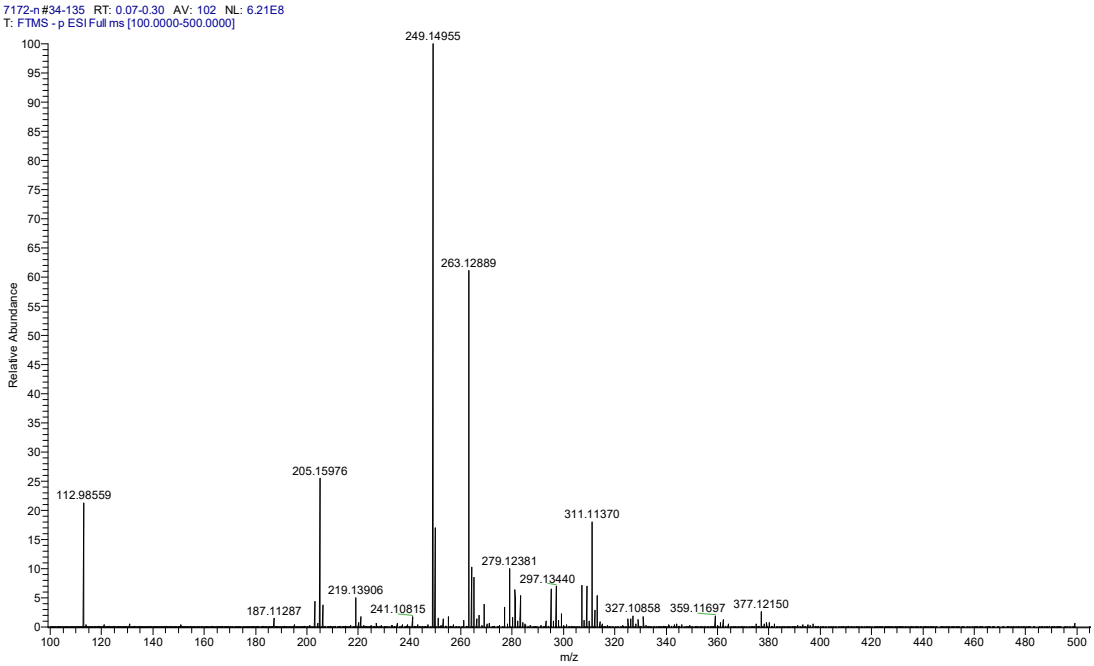

Fig S12 HRESIMS spectrum of compound **2** (MeOH)

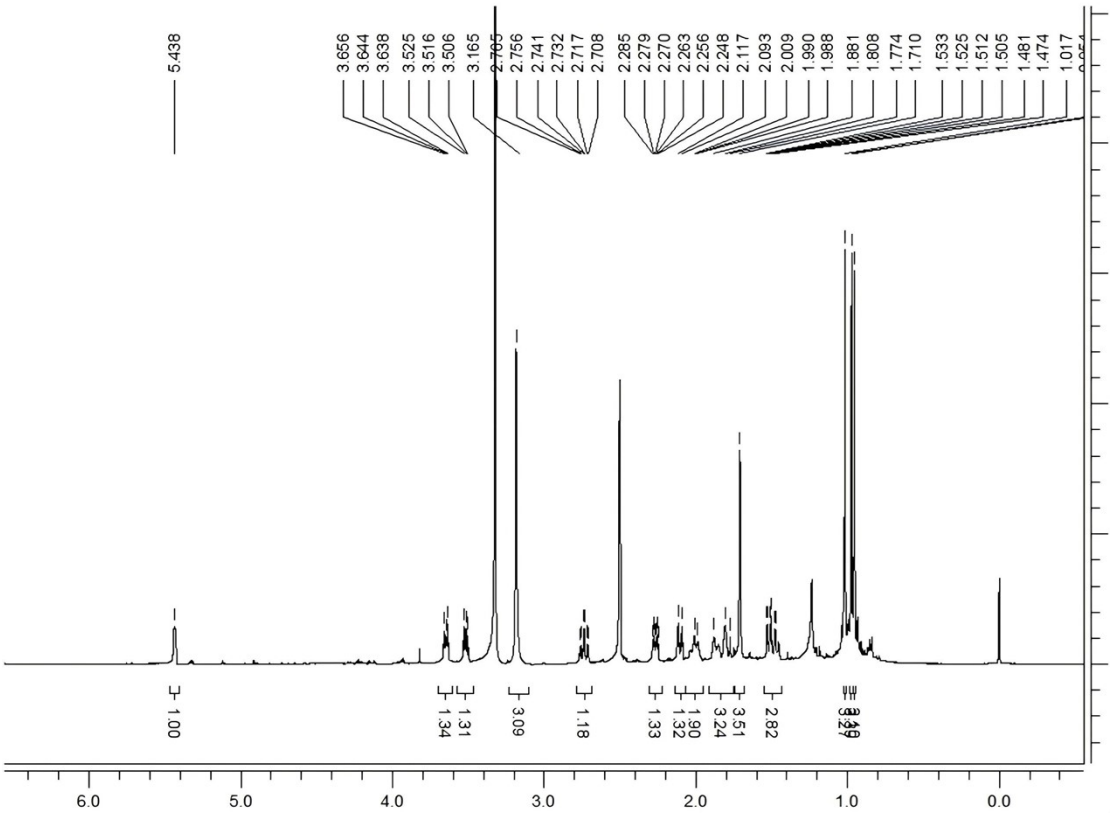

Fig S13 ^{1}H-NMR spectrum of compound **3** (DMSO-d_6, 600 MHz)

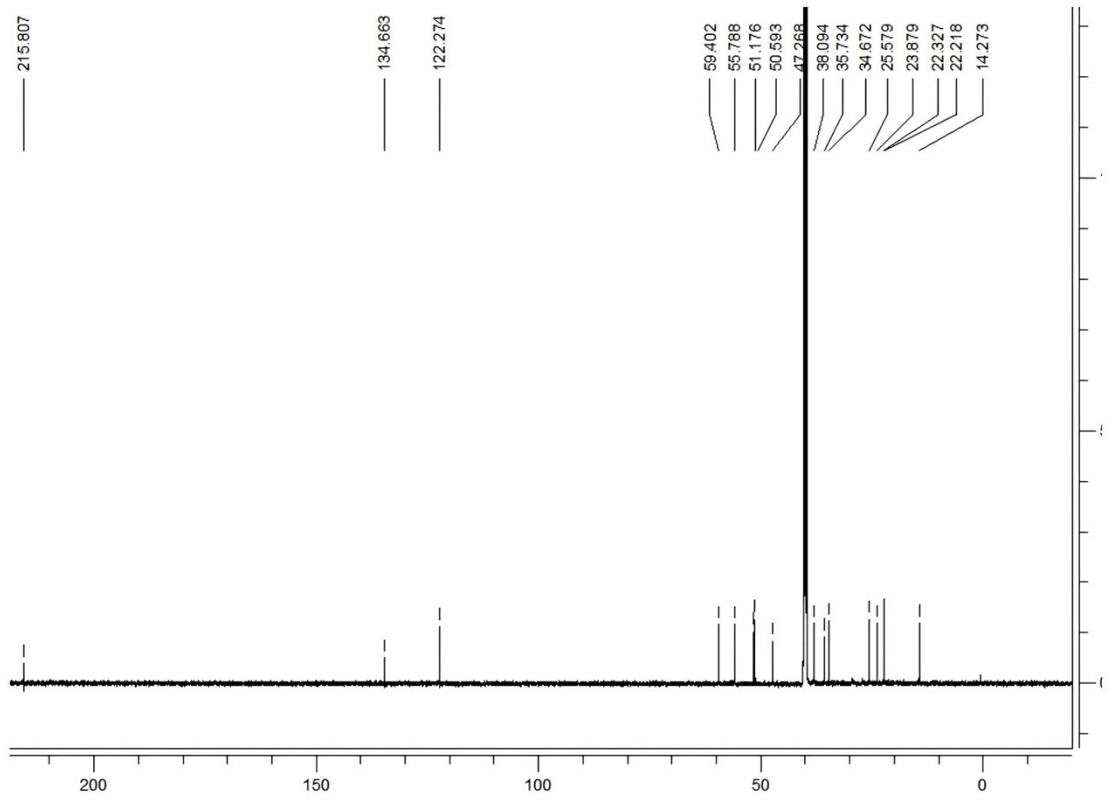

Fig S14 ^{13}C-NMR spectrum of compound **3** (DMSO-d_6, 150 MHz)

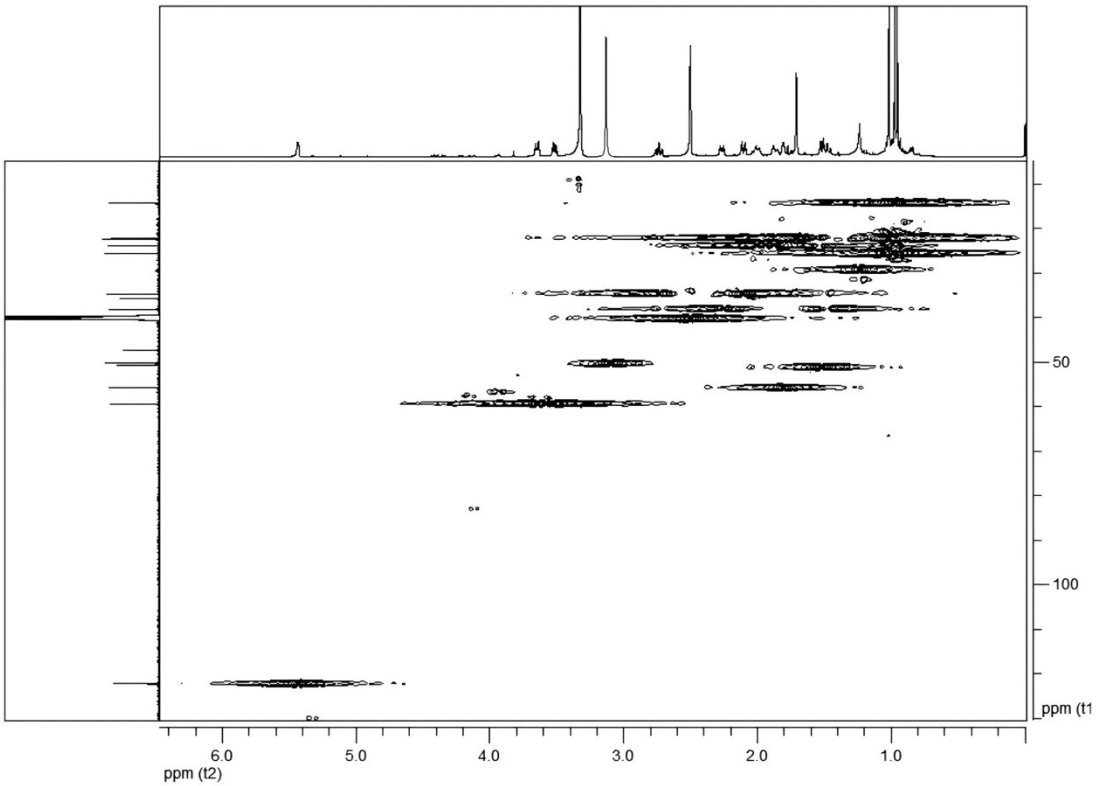

Fig S15 HSQC spectrum of compound **3** (DMSO-d_6)

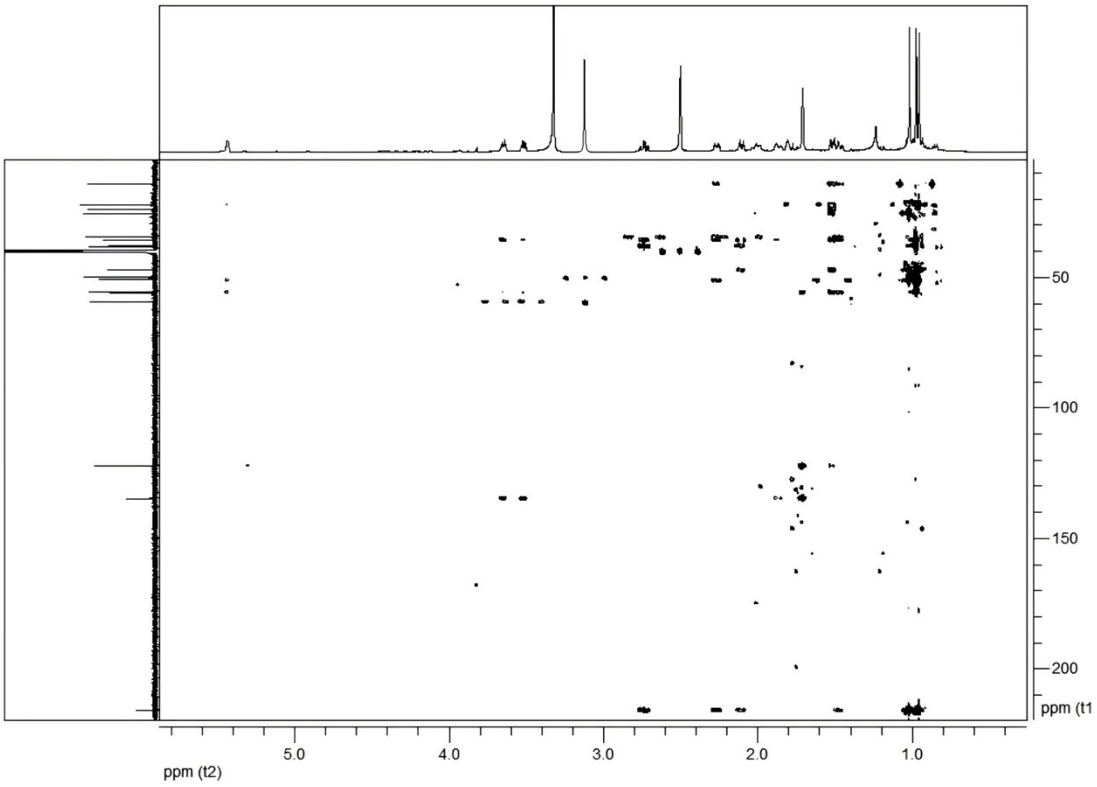

Fig S16 HMBC spectrum of compound **3** (DMSO-d_6)

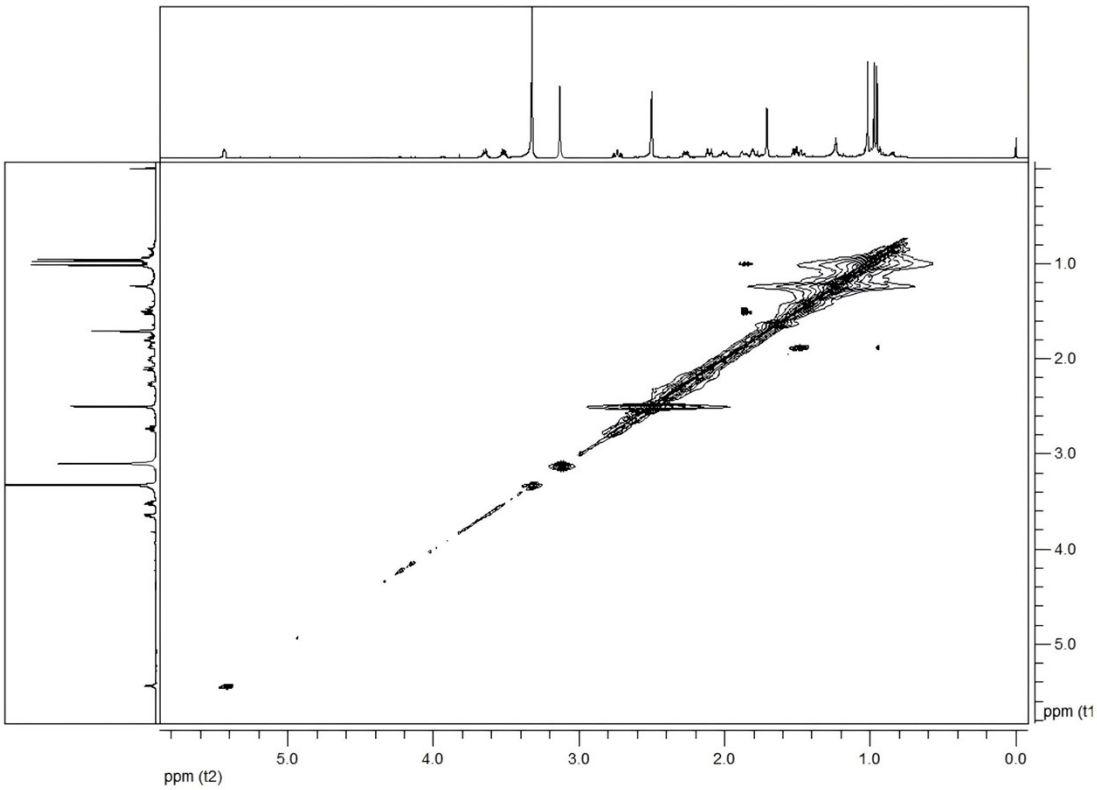

Fig S17 NOESY spectrum of compound **3** (DMSO-d_6)

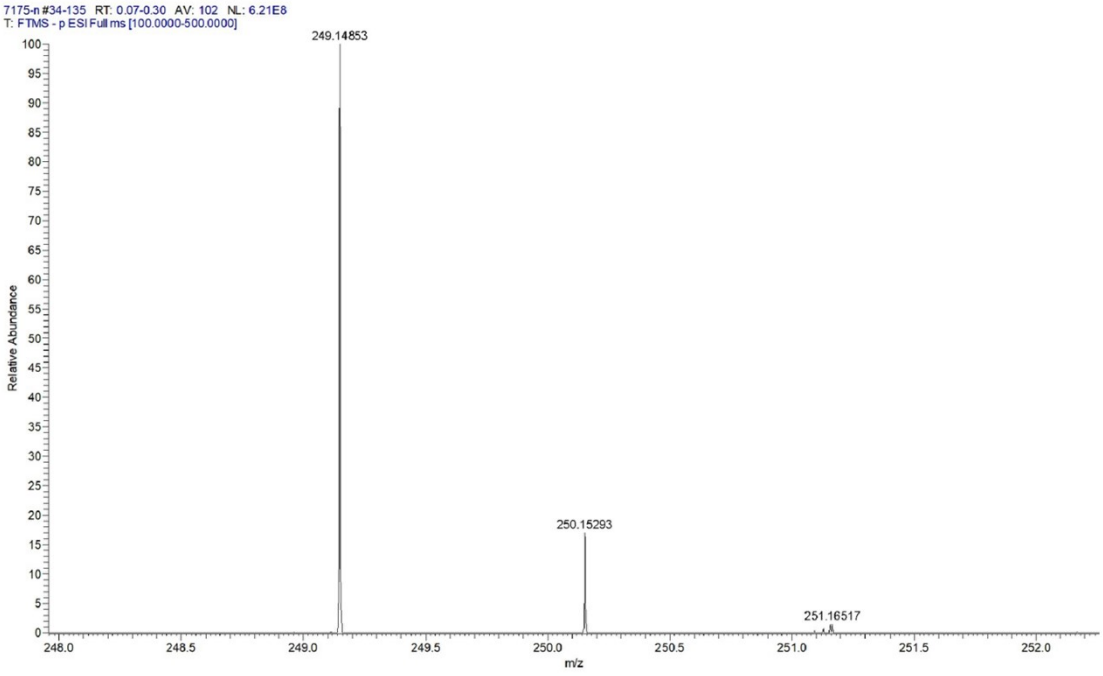

Fig S18 HRESIMS spectrum of compound **3** (MeOH)

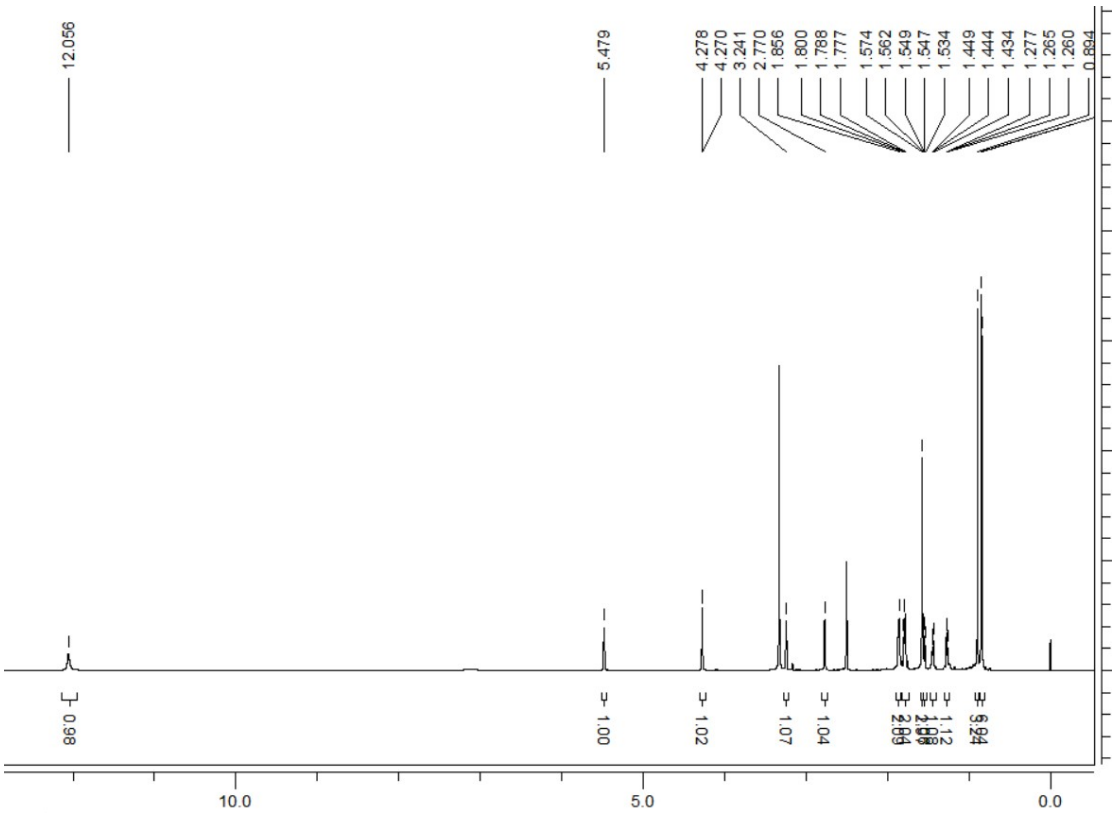

Fig S19 [1]H-NMR spectrum of compound **4** (DMSO-d_6, 600 MHz)

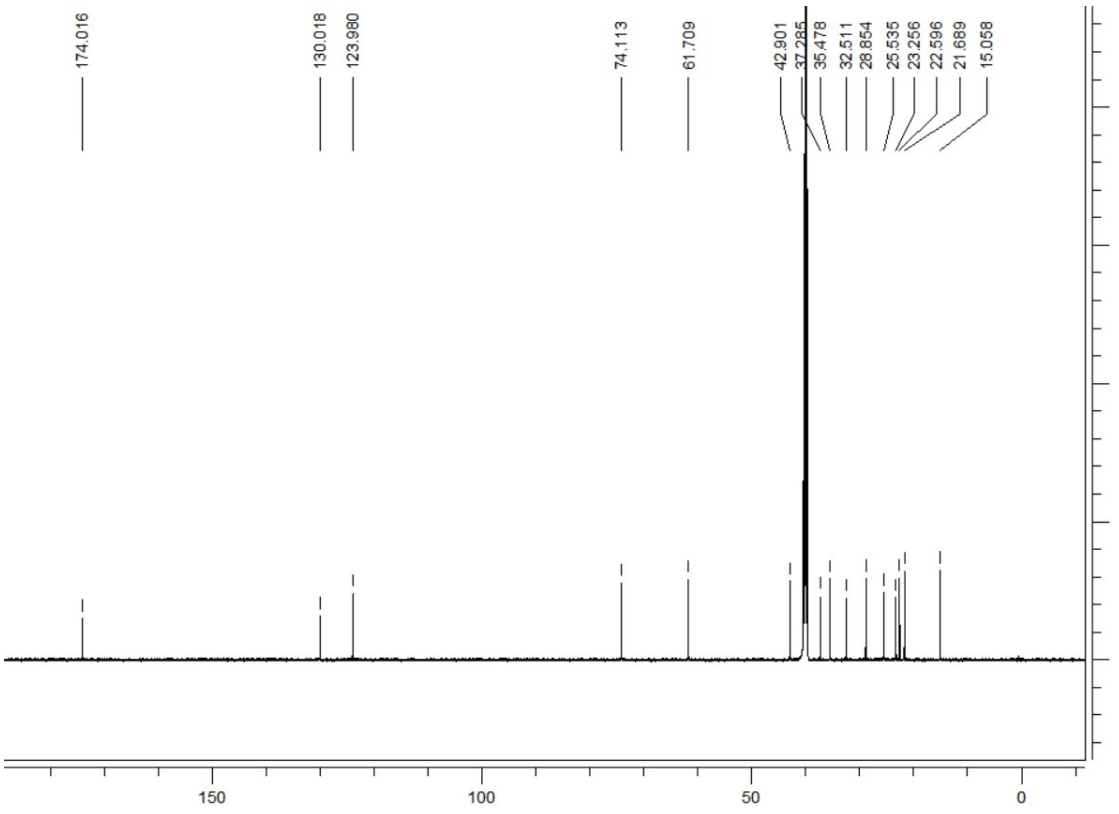

Fig S20 [13]C-NMR spectrum of compound **4** (DMSO-d_6, 150 MHz)

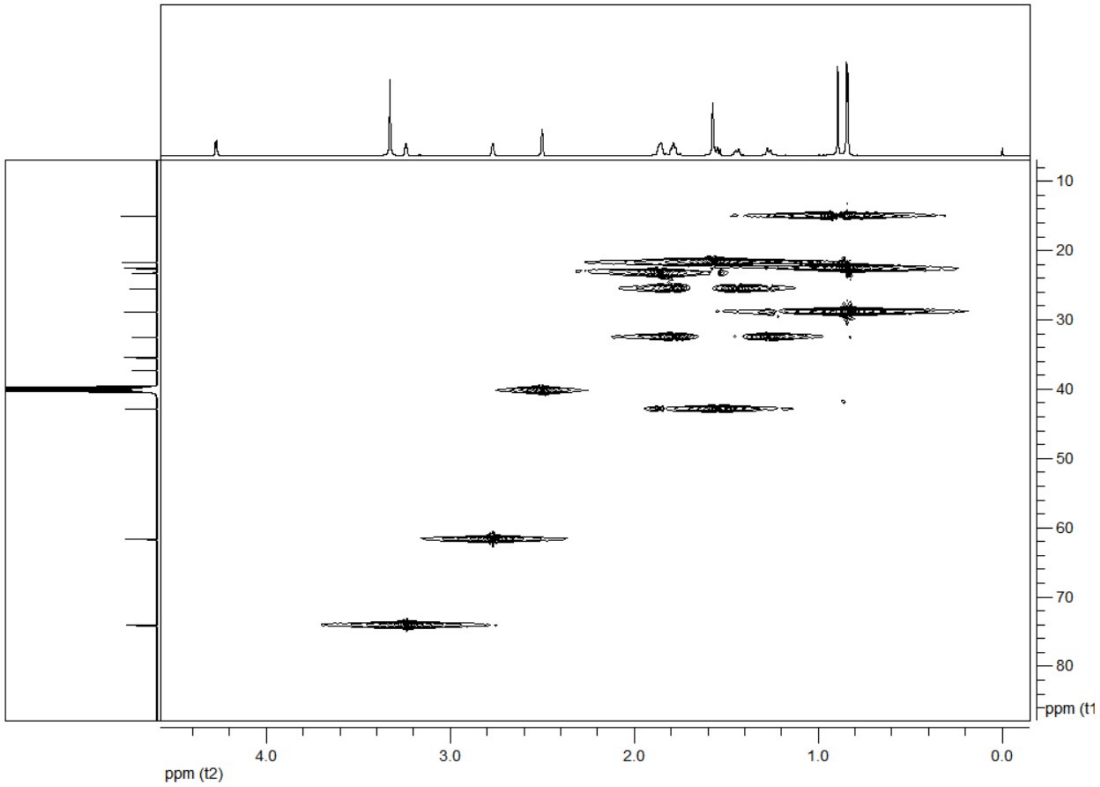

Fig S21 HSQC spectrum of compound **4** (DMSO-d_6)

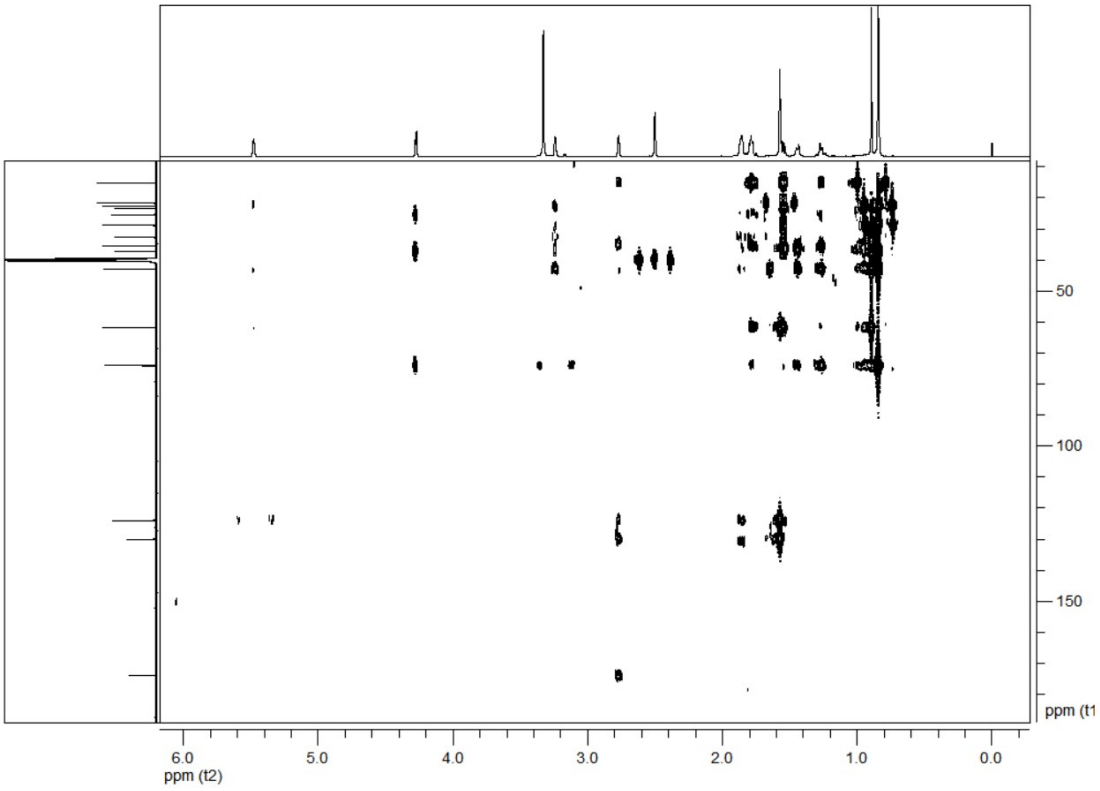

Fig S22 HMBC spectrum of compound **4** (DMSO-d_6)

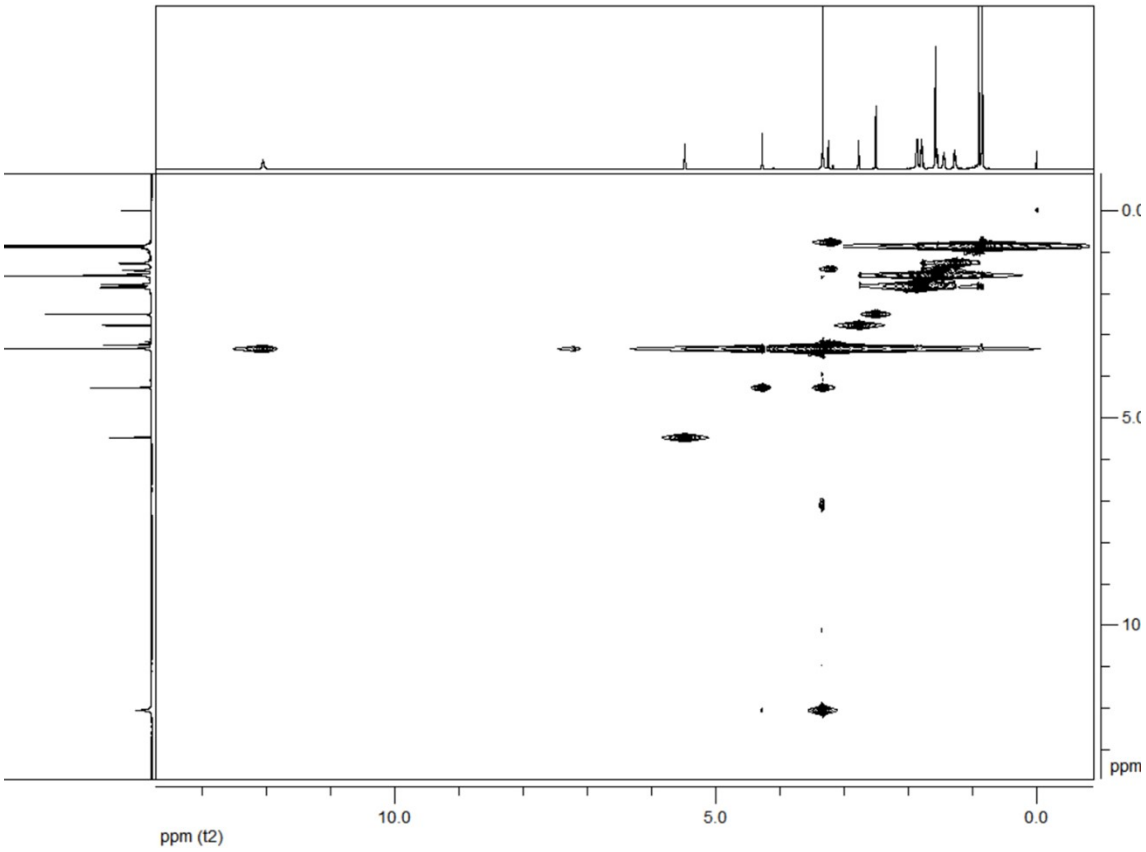

Fig S23 NOESY spectrum of compound **4** (DMSO-d_6)

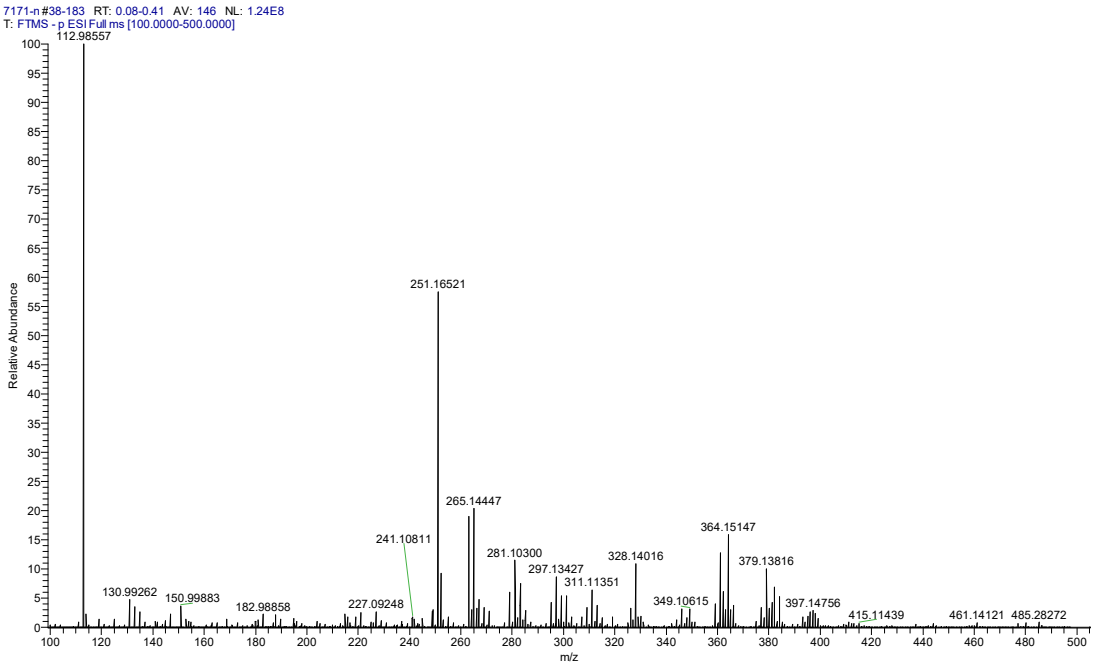

Fig S24 HRESIMS spectrum of compound **4** (MeOH)

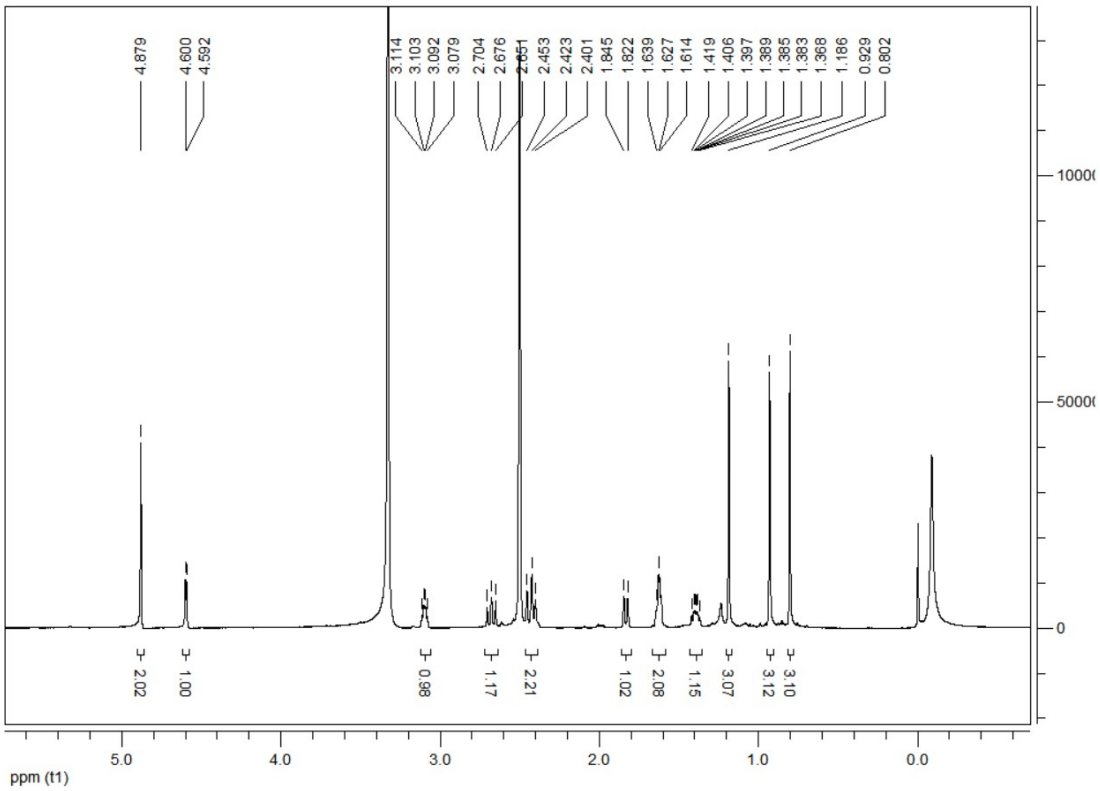

Fig S25 ^{1}H-NMR spectrum of compound **5** (DMSO-d_6, 600 MHz)

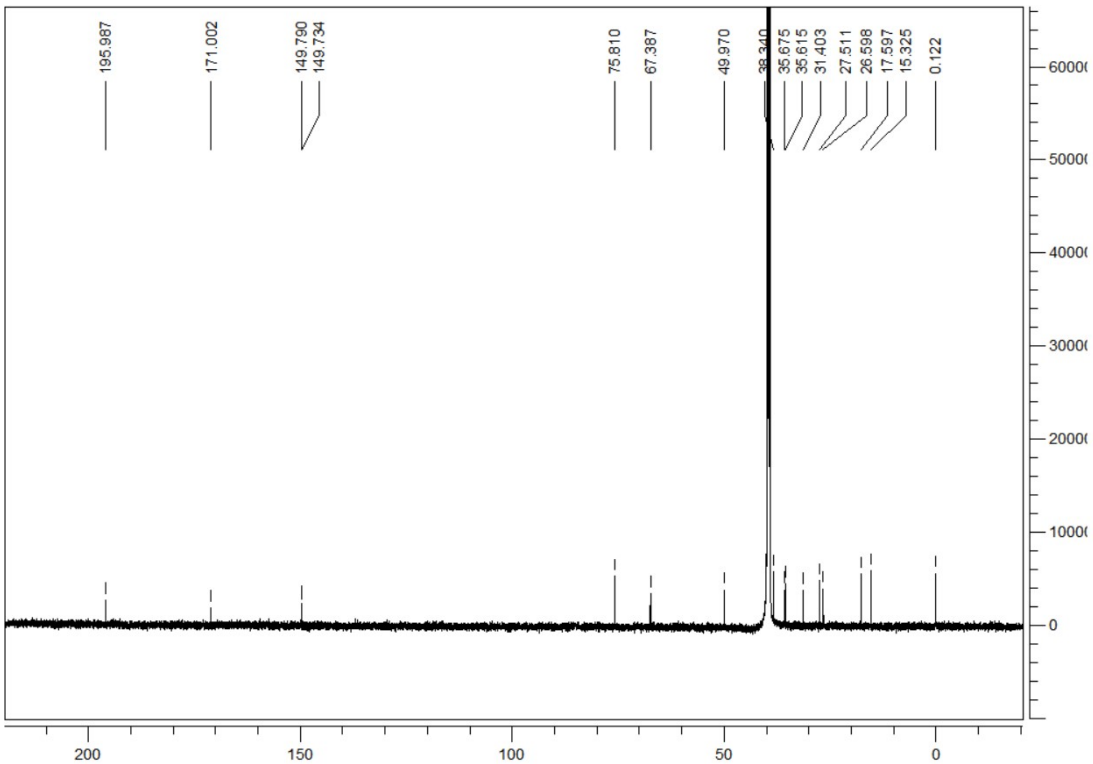

Fig S26 ^{13}C-NMR spectrum of compound **5** (DMSO-d_6, 150 MHz)

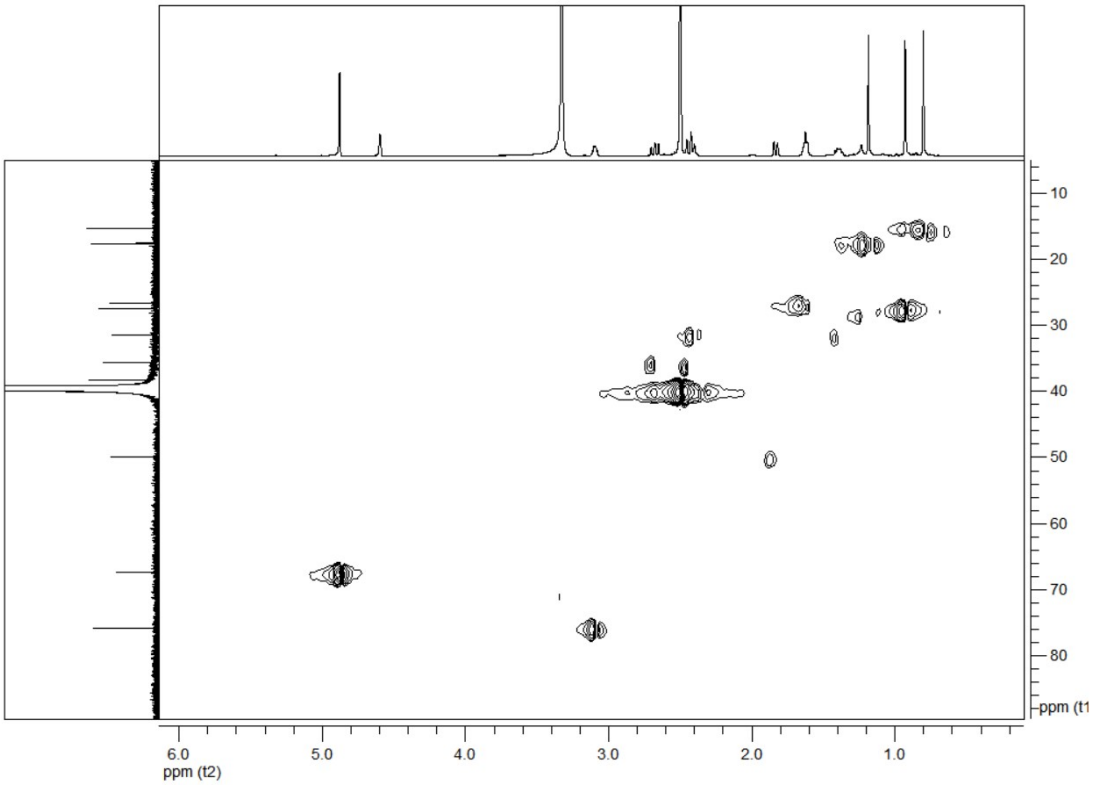

Fig S27 HSQC spectrum of compound **5** (DMSO-d_6)

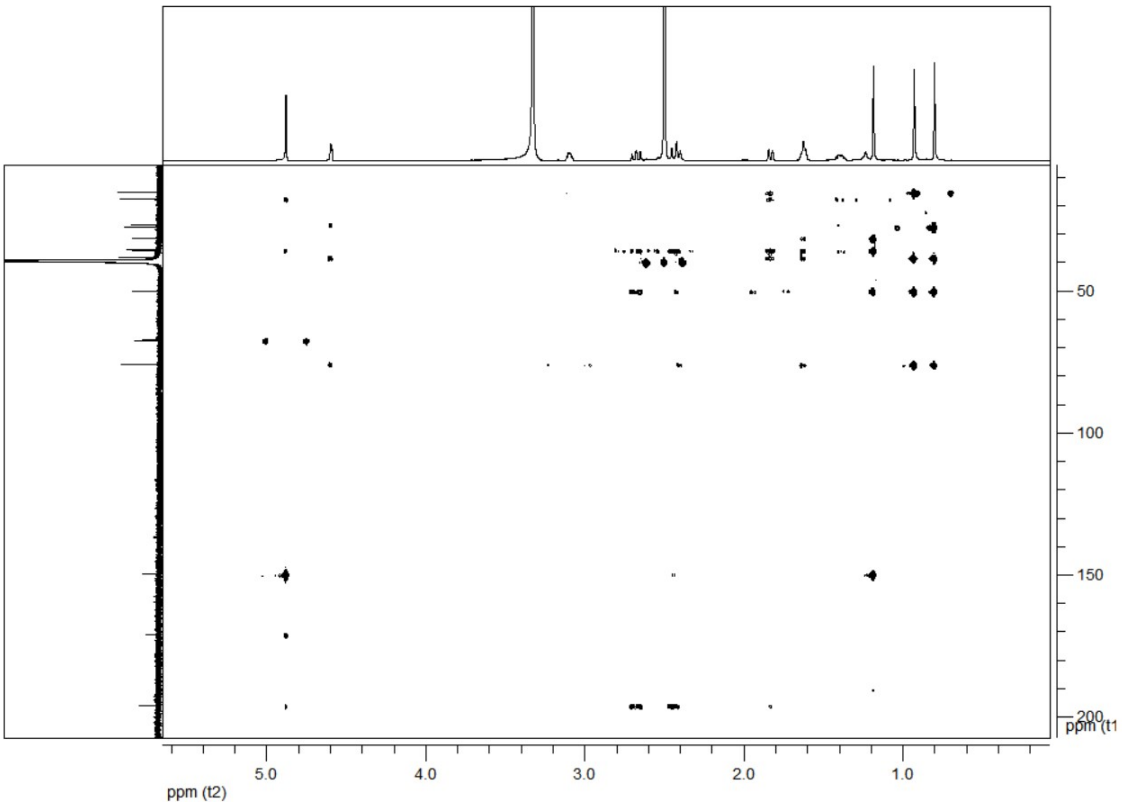

Fig S28 HMBC spectrum of compound **5** (DMSO-d_6)

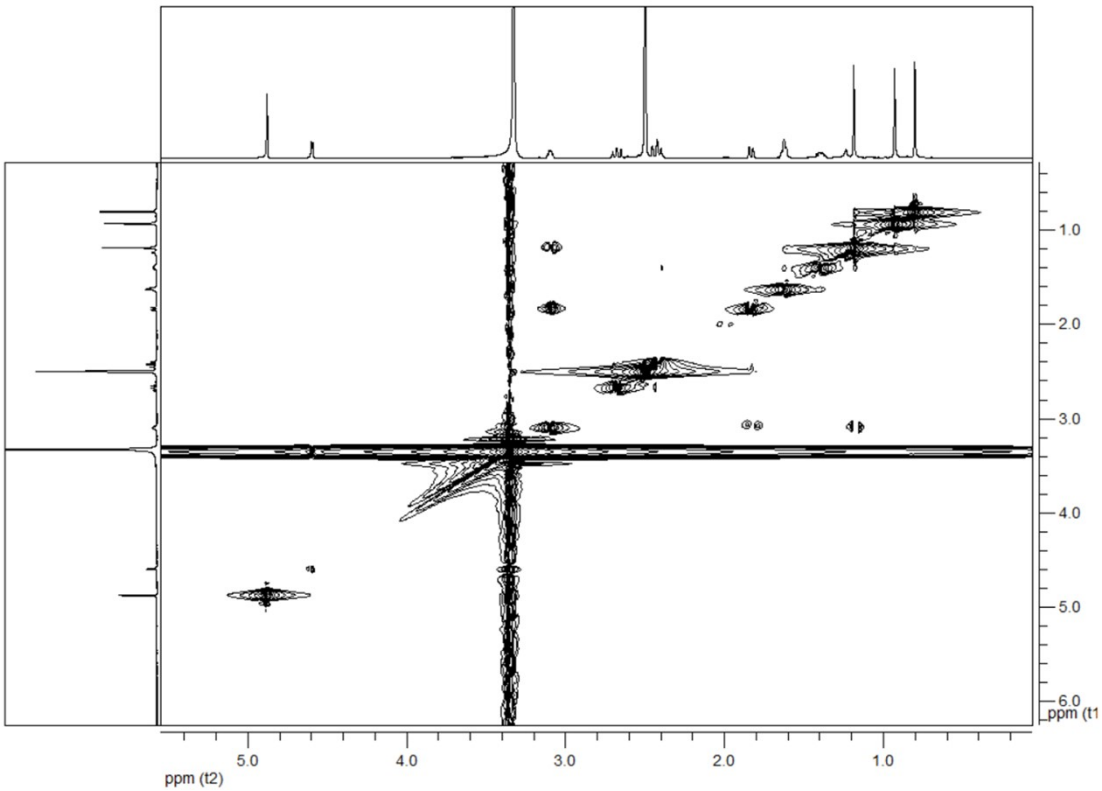

Fig S29 NOESY spectrum of compound **5** (DMSO-d_6)

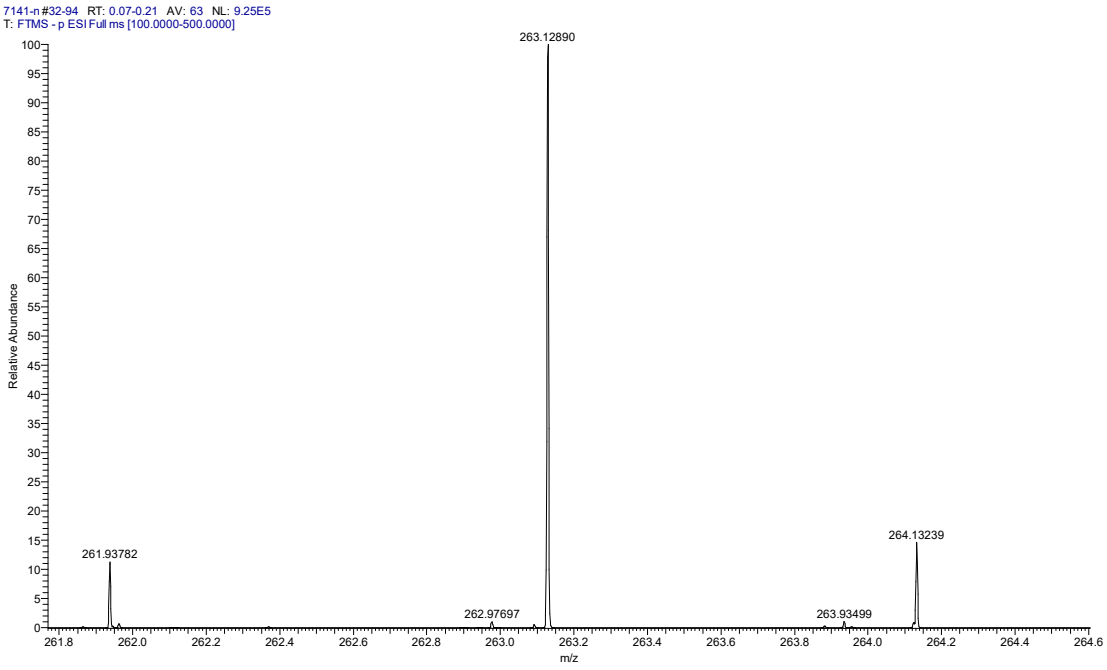

Fig S30 HRESIMS spectrum of compound **5** (MeOH)

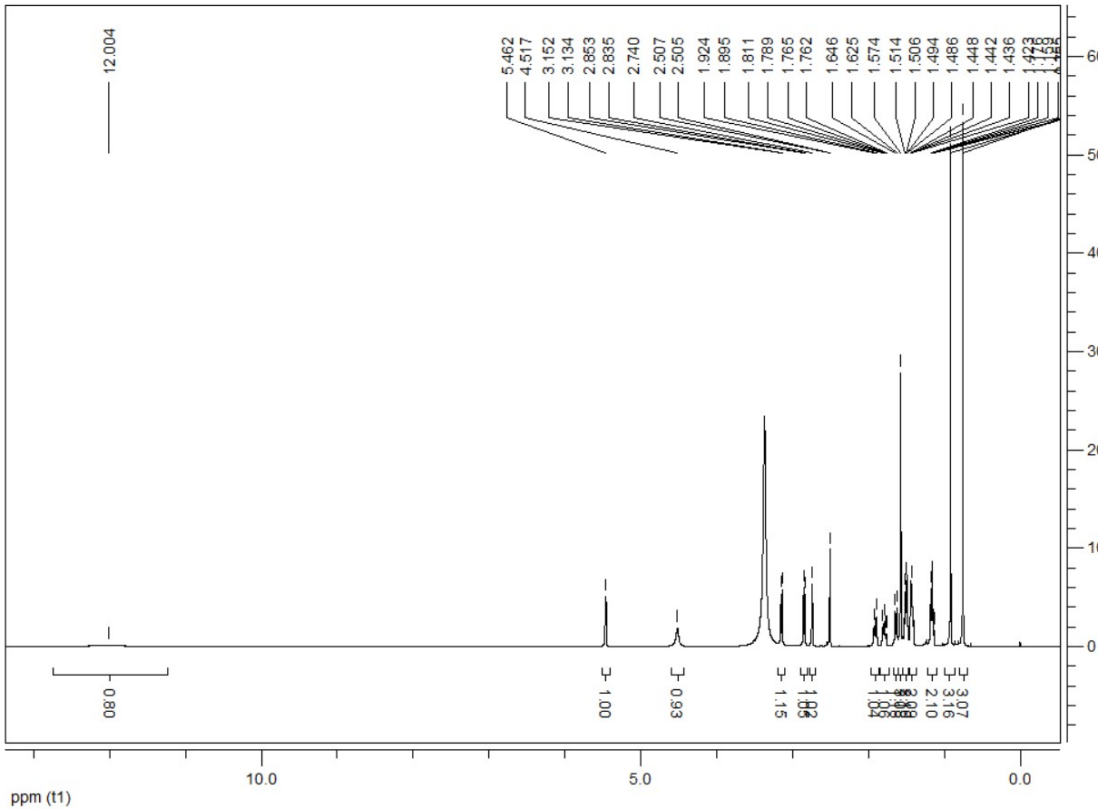

Fig S31 ^{1}H-NMR spectrum of compound **6** (DMSO-d_6, 600 MHz)

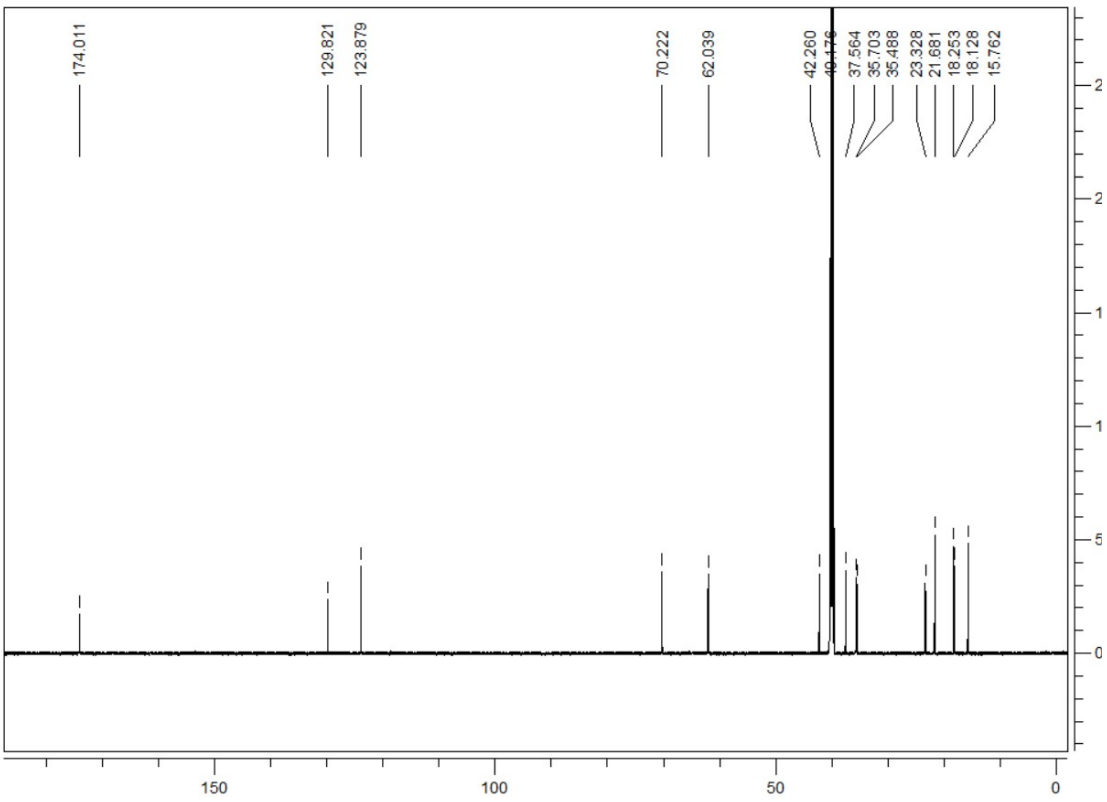

Fig S32 ^{13}C-NMR spectrum of compound **6** (DMSO-d_6, 150 MHz)

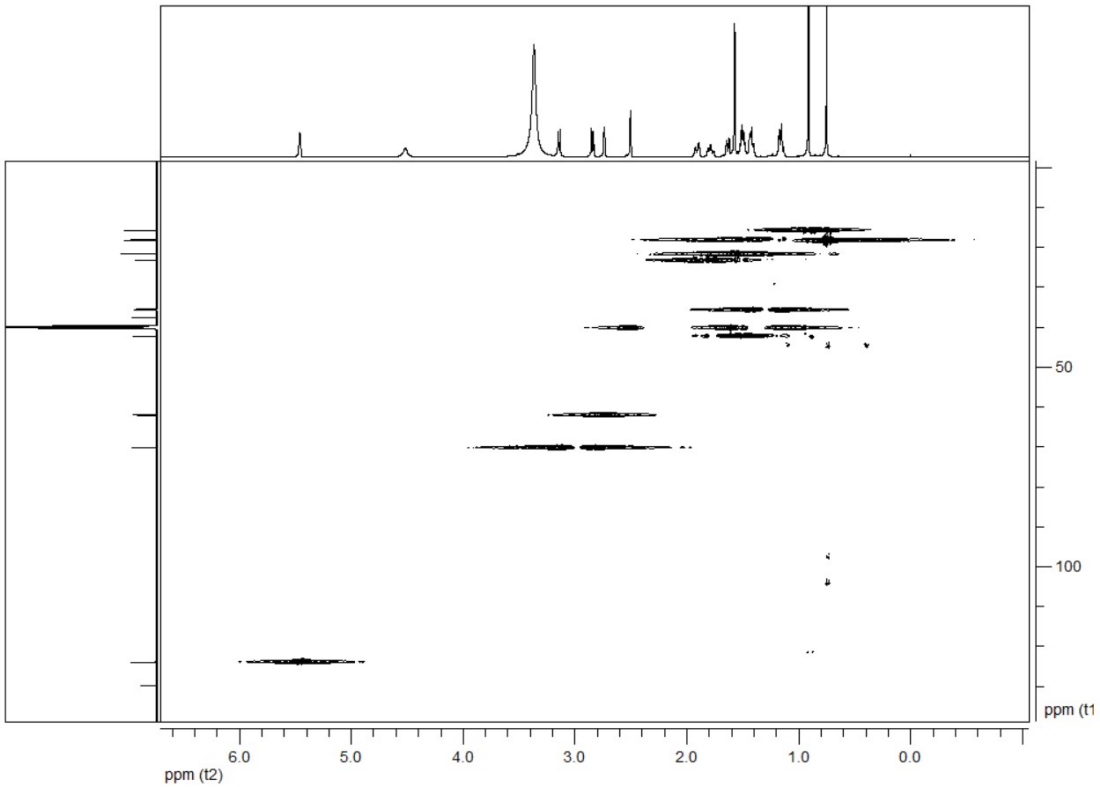

Fig S33 HSQC spectrum of compound **6** (DMSO-d_6)

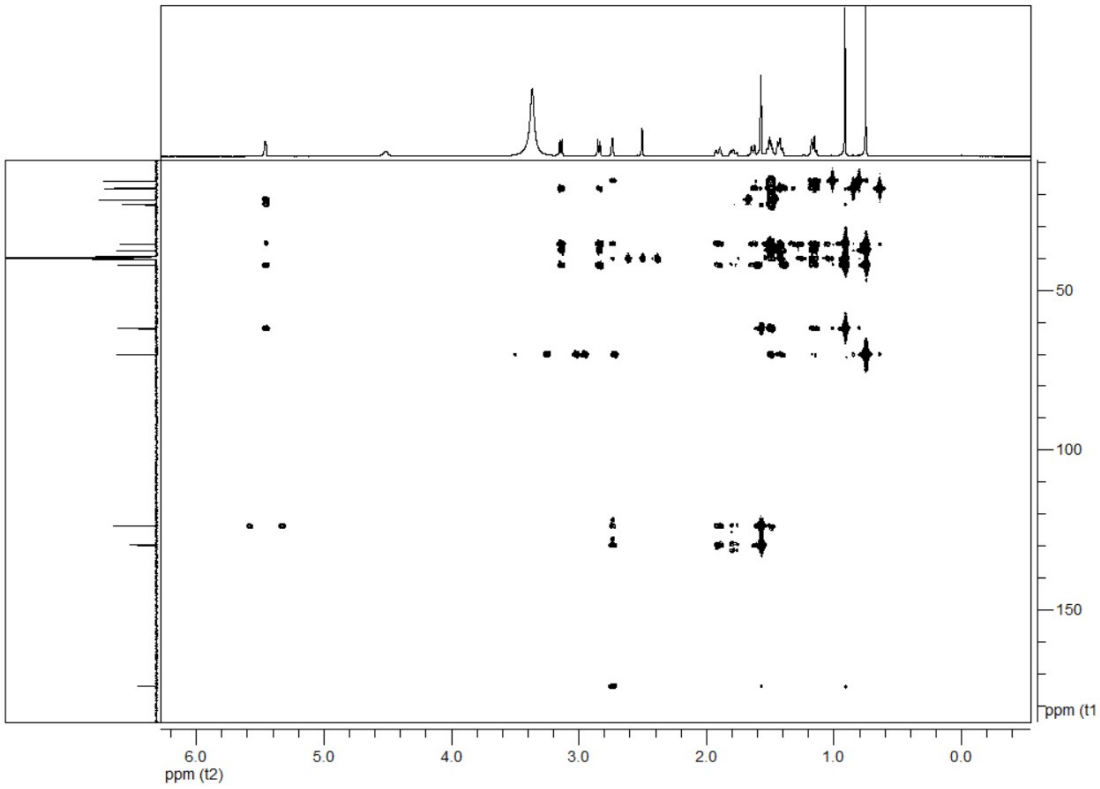

Fig S34 HMBC spectrum of compound **6** (DMSO-d_6)

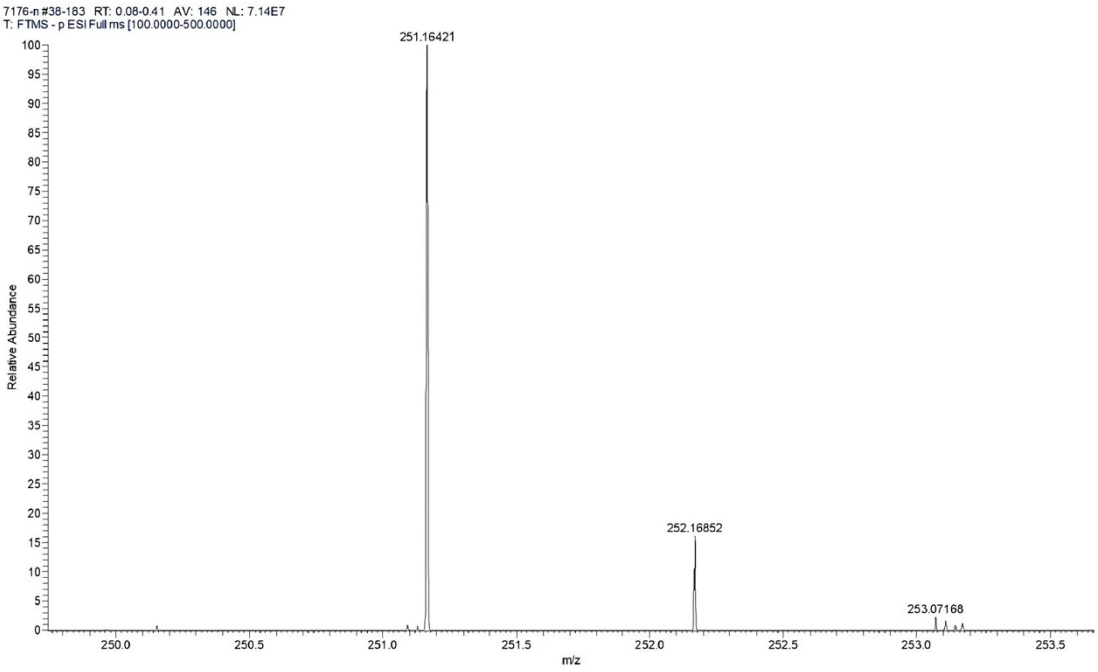

Fig S35 HRESIMS spectrum of compound **6** (MeOH)

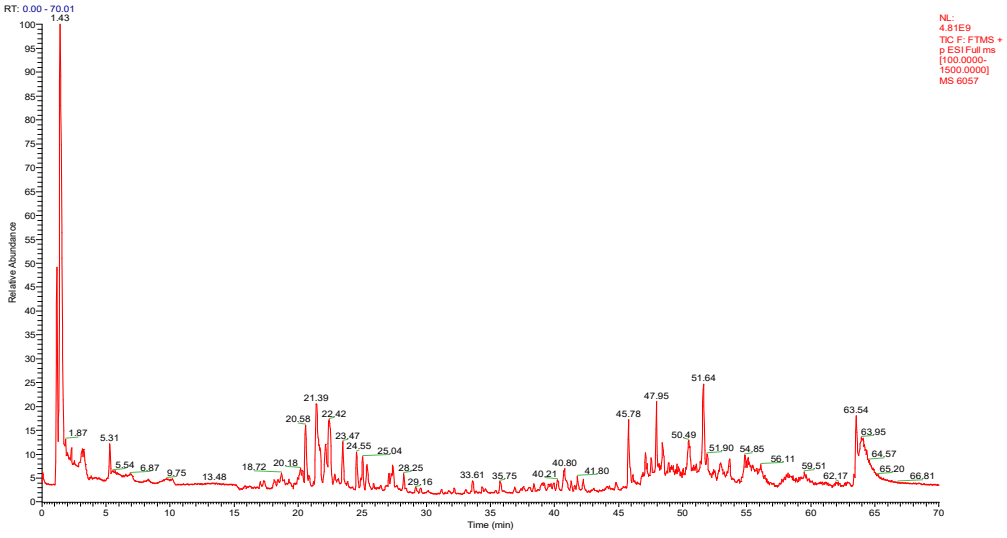

Fig S36 TIC scan of positive ion mode.

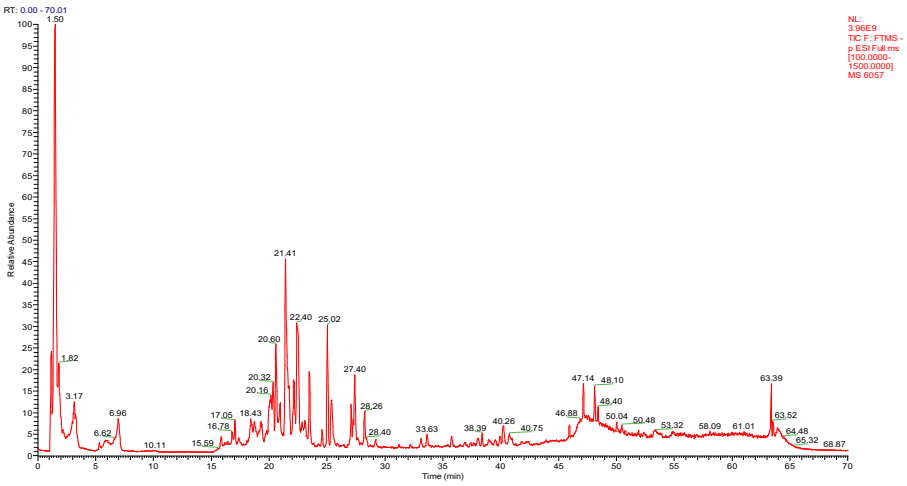

Fig S37 TIC scan of negative ion mode.

Table S1 Qualitative study of chemical constituents (terpenes are marked in red) in *L. sinense*

No.	Name of Compounds	Molecular Formula	Molecular Weight	Retention Time（min）	Matching Score	Peak Area	Relative Amount（%）
1	Astragalin	$C_{21}H_{20}O_{11}$	448.10057	22.43	89.8	9274917989	14.689
2	Eriodictyol	$C_{15}H_{12}O_6$	288.06323	25.025	90.3	5254255258	8.321
3	2-Pyrrolidinecarboxylic acid	$C_5H_9NO_2$	115.06343	1.504	83	4474868465	7.087
4	Citric acid	$C_6H_8O_7$	192.02703	1.596	89.3	3662073133	5.800
5	Luteolin	$C_{15}H_{10}O_6$	286.04771	25.381	90.6	3530575938	5.592
6	Hesperetin	$C_{16}H_{14}O_6$	302.07892	27.408	82.3	3381200185	5.355
7	Myricetin	$C_{15}H_{10}O_8$	318.03761	21.422	90.7	3293405865	5.216
8	Morin	$C_{15}H_{10}O_7$	302.04277	21.535	88.4	2313117979	3.663
9	Kaempferol	$C_{15}H_{10}O_6$	286.04787	22.41	89.6	2296853392	3.638
10	Ethyl gallate	$C_9H_{10}O_5$	198.05277	20.959	93.4	2253928305	3.570
11	Quercetin	$C_{15}H_{10}O_7$	302.04277	22.51	86.3	2222657047	3.520
12	(-)-Epigallocatechin gallate	$C_{22}H_{18}O_{11}$	458.08494	20.137	92.8	2007546045	3.179
13	Apigenin	$C_{15}H_{10}O_5$	270.05281	27.264	90.1	1690845337	2.678
14	Pyrogallol	$C_6H_6O_3$	126.0316	6.974	87.1	1193484071	1.890
15	Trigonelline HCl	$C_7H_7NO_2$	137.04781	1.502	88.1	1178497981	1.866
16	Naringenin	$C_{15}H_{12}O_5$	272.06836	27.084	91.1	1001919566	1.587
17	α-Linolenic acid	$C_{18}H_{30}O_2$	278.22466	40.24	89.2	768354265.9	1.217
18	Ellagic acid	$C_{14}H_6O_8$	302.00606	21.582	85.6	734884837.4	1.164
19	Pinoresinol 4-O-glucoside	$C_{26}H_{32}O_{11}$	520.1946	22.07	89	496203609.2	0.786
20	Cynaroside	$C_{21}H_{20}O_{11}$	448.10065	23.086	84.4	365955756.8	0.580
21	Corilagin	$C_{27}H_{22}O_{18}$	634.08082	19.388	87.5	341722987.1	0.541
22	Adenosine	$C_{10}H_{13}N_5O_4$	267.09696	8.296	83.8	340554208.2	0.539
23	Epigallocatechin	$C_{15}H_{14}O_7$	306.07397	18.247	95.6	333056807	0.527
24	Diosmetin	$C_{16}H_{12}O_6$	300.06348	27.7	83.6	285743375.4	0.453
25	Protocatechualdehyde	$C_7H_6O_3$	138.03172	20.133	75.1	258279191	0.409
26	Phloridzin	$C_{21}H_{24}O_{10}$	436.13706	23.119	86.1	257846820.2	0.408
27	Azelaic acid	$C_9H_{16}O_4$	188.10489	23.033	88.6	193768242.5	0.307
28	p-Coumaric acid	$C_9H_8O_3$	164.04739	18.712	85.8	172539163.1	0.273
29	2-Hydroxy-4-methoxybenzaldehyde	$C_8H_8O_3$	152.04748	18.855	70.7	169143183.8	0.268
30	Shikimic acid	$C_7H_{10}O_5$	174.05275	2.175	89.4	163931100.3	0.260
31	Vitamin D3	$C_{27}H_{44}O$	384.33943	59.871	74	160475705.1	0.254
32	Apigenin-7-O-β-D-glucoside	$C_{21}H_{20}O_{10}$	432.1057	22.646	89.2	116342998.3	0.184
33	Kaempferitrin	$C_{27}H_{30}O_{14}$	578.16372	21.658	92	109319156.8	0.173
34	Rutin	$C_{27}H_{30}O_{16}$	610.15376	21.195	91.6	107165711	0.170
35	Coumarin	$C_9H_6O_2$	164.04746	19.947	73.1	105877889.6	0.168

36	Gallic acid	$C_7H_6O_5$	170.02147	20.155	86.8	99387372.38	0.157
37	Phloretin	$C_{15}H_{14}O_5$	274.08423	23.122	84.1	95235391.34	0.151
38	5-Hydroxymethylfurfural	$C_6H_6O_3$	126.03182	15.969	71.4	95060414.35	0.151
39	L-Tryptophan	$C_{11}H_{12}N_2O_2$	204.08983	21.742	87.2	94047657.32	0.149
40	Esculetin	$C_9H_6O_4$	178.02656	19.309	87.1	93364990.18	0.148
41	(+)-Pinoresinol	$C_{20}H_{22}O_6$	358.14149	22.073	84.7	81607289.87	0.129
42	Vitamin D2	$C_{28}H_{44}O$	396.33945	48.824	84.5	77920375.75	0.123
43	Isoalantolactone	$C_{15}H_{20}O_2$	232.14644	33.902	82.5	75275400.69	0.119
44	Manninotriose	$C_{18}H_{32}O_{16}$	504.16934	2.246	84.7	68428426.9	0.108
45	Trilobatin	$C_{21}H_{24}O_{10}$	436.13693	22.081	74.5	63881223.32	0.101
46	5,7-Dihydroxychromone	$C_9H_6O_4$	178.02656	20.686	86.5	63557573.85	0.101
47	Uridine	$C_9H_{12}N_2O_6$	244.06947	5.185	92.3	58343649.69	0.092
48	α-Cyperone	$C_{15}H_{22}O$	218.1672	39.249	81.6	54641995.31	0.087
49	Kaempferol-3-O-rutinoside	$C_{27}H_{30}O_{15}$	594.15908	21.948	89	48757353.43	0.077
50	4-Methoxysalicylic acid	$C_8H_8O_4$	168.04221	16.781	76.9	48630984.23	0.077
51	**Pachymic acid**	**$C_{33}H_{52}O_5$**	**264.19068**	**47.802**	**72.7**	**46340797.96**	**0.073**
52	Linolenic acid ethyl ester	$C_{20}H_{34}O_2$	306.25603	46.344	85.1	44293009.83	0.070
53	7-Methoxycoumarin	$C_{10}H_8O_3$	144.02123	24.893	77.4	40985346.95	0.065
54	Ferulaldehyde	$C_{10}H_{10}O_3$	178.0631	19.885	78	40078685.81	0.063
55	Ferulic acid	$C_{10}H_{10}O_4$	194.05788	18.384	88.1	39761883.67	0.063
56	Salicylic acid	$C_7H_6O_3$	138.03168	18.022	81.9	39648498.38	0.063
57	Methyl hexadecanoate	$C_{17}H_{34}O_2$	316.26118	37.926	73.1	39120315.91	0.062
58	Protocatechuic acid	$C_7H_6O_4$	154.02668	20.793	84.8	38712119.18	0.061
59	Narcissoside	$C_{28}H_{32}O_{16}$	624.16951	21.111	86.6	37880777.16	0.060
60	Adenine	$C_5H_5N_5$	135.05453	2.587	71.8	37820565.56	0.060
61	Taxifolin	$C_{15}H_{12}O_7$	304.05818	22.019	87.6	37387743.06	0.059
62	Hydroprotopine	$C_{20}H_{19}NO_5$	353.12651	22.73	89.4	35137134.98	0.056
63	**Dehydrocostus lactone**	**$C_{15}H_{18}O_2$**	**230.13075**	**20.042**	**85.6**	**34342464.54**	**0.054**
64	Methyl 4-hydroxy-3-methoxycinnamate	$C_{11}H_{12}O_4$	208.07363	23.104	73	34233805.94	0.054
65	Atractylenolide I	$C_{15}H_{18}O_2$	248.1413	20.309	79.6	33929756.92	0.054
66	Ethyl 3,4-dihydroxybenzoate	$C_9H_{10}O_4$	182.05795	23.555	83.9	30622405.94	0.048
67	Brevifolincarboxylic acid	$C_{13}H_8O_8$	309.04844	19.022	85.8	29323143.34	0.046
68	Sinapic acid	$C_{11}H_{12}O_5$	224.06844	18.787	90.7	28919203.61	0.046
69	p-Hydroxybenzaldehyde	$C_7H_6O_2$	122.03675	19.569	78.9	28446664.11	0.045
70	Homoorientin	$C_{21}H_{20}O_{11}$	448.10076	20.437	85	27928781.29	0.044
71	Tryptamine	$C_{10}H_{12}N_2$	160.1001	18.153	73.8	27557365.16	0.044
72	S-Isocorydine(+)	$C_{20}H_{23}NO_4$	341.16283	21.293	79.6	26924803.43	0.043
73	Iristectorigenin B	$C_{17}H_{14}O_7$	330.07403	27.566	74.1	26624821.88	0.042
74	Emodin-3-methyl ether/Physcion	$C_{16}H_{12}O_5$	284.06868	23.867	71.8	26018465.16	0.041
75	Genistein	$C_{15}H_{10}O_5$	270.05297	19.84	85.5	25120275.24	0.040
76	L-Tyrosine	$C_9H_{11}NO_3$	181.07394	5.124	78.5	25069448.47	0.040

77	Isorhamnetin	$C_{16}H_{12}O_7$	316.05846	21.109	80.4	21703541.95	0.034
78	Artemisinic acid	$C_{15}H_{22}O_2$	234.16214	27.446	83.2	19242063.7	0.030
79	Orsellinic acid	$C_8H_8O_4$	168.04228	18.919	73.2	19108302.15	0.030
80	Panaxtriol	$C_{30}H_{52}O_4$	476.38695	51.684	77.6	18374228.23	0.029
81	Epiberberine	$C_{20}H_{17}NO_4$	335.11583	25.289	84.6	18268870.59	0.029
82	Methyl 4-hydroxycinnamate	$C_{10}H_{10}O_3$	178.06308	6.255	78.8	18228538.23	0.029
83	Methyl gallate	$C_8H_8O_5$	184.03715	17.449	71.3	16699997.6	0.026
84	Deoxyandrographolide	$C_{20}H_{30}O_4$	334.21202	35.787	74.4	15465572.1	0.024
85	**Abietic Acid**	**$C_{20}H_{30}O_2$**	**302.2246**	**44.909**	**71.4**	**15452228.88**	**0.024**
86	Isoquercitrin	$C_{21}H_{20}O_{12}$	464.09544	20.526	70.3	15283476.22	0.024
87	Vicenin III	$C_{26}H_{28}O_{14}$	564.14823	20.209	83.8	13950759.81	0.022
88	Indigo	$C_{16}H_{10}N_2O_2$	262.07427	33.075	85.6	13540631.87	0.021
89	Pinocembrin	$C_{15}H_{12}O_4$	256.07362	32.394	83.2	12595571.74	0.020
90	**Nardosinone**	**$C_{15}H_{22}O_3$**	**250.157**	**24.335**	**70.1**	**12337122.68**	**0.020**
91	Amentoflavone	$C_{30}H_{18}O_{10}$	538.09055	29.522	85.4	11991375.82	0.019
92	Vicenin II	$C_{27}H_{30}O_{15}$	594.15919	19.517	83.7	10983855.74	0.017
93	Quercitrin	$C_{21}H_{20}O_{11}$	448.10088	20.948	84.8	10948781.34	0.017
94	Lonicerin	$C_{27}H_{30}O_{15}$	594.15898	19.935	73.8	9921065.343	0.016
95	**Atractylenolide II**	**$C_{15}H_{20}O_2$**	**232.14644**	**34.708**	**78.9**	**9199087.463**	**0.015**
96	Gentisic acid	$C_7H_6O_4$	154.02664	17.984	83.7	8698650.883	0.014
97	Baicalin	$C_{21}H_{18}O_{11}$	446.08529	23.718	80.8	8664899.096	0.014
98	Arteannuin	$C_{15}H_{20}O_3$	248.14129	27.945	77	8641092.281	0.014
99	Orcinol gentiobioside	$C_{19}H_{28}O_{12}$	448.15828	16.738	77.3	8347273.665	0.013
100	**Germacrone**	**$C_{15}H_{22}O$**	**218.16721**	**36.55**	**70.2**	**8090186.028**	**0.013**
101	3,5-Dimethoxy-4-hydroxybenzaldehyde	$C_9H_{10}O_4$	182.05799	19.304	75	7988630.882	0.013
102	Steviol	$C_{20}H_{30}O_3$	318.21907	45.53	74.2	7900744.225	0.013
103	Senkyunolide A	$C_{12}H_{16}O_2$	192.11521	39.291	76.9	7817087.243	0.012
104	**Curdione**	**$C_{15}H_{24}O_2$**	**236.17768**	**33.123**	**78.8**	**7464166.212**	**0.012**
105	Cinnamic acid	$C_9H_8O_2$	148.05251	21.766	79.4	7048511.731	0.011
106	**Sclareolide**	**$C_{16}H_{26}O_2$**	**250.19336**	**30.131**	**88.6**	**6197688.179**	**0.010**
107	Cinnamaldehyde	C_9H_8O	132.05766	20.978	72.3	3211857.556	0.005
108	Taxifolin 7-rhamnoside	$C_{21}H_{22}O_{11}$	450.11503	17.319	72.1	1830755.843	0.003
109	Parthenolide	$C_{15}H_{20}O_3$	248.14127	32.302	72	1653947.96	0.003

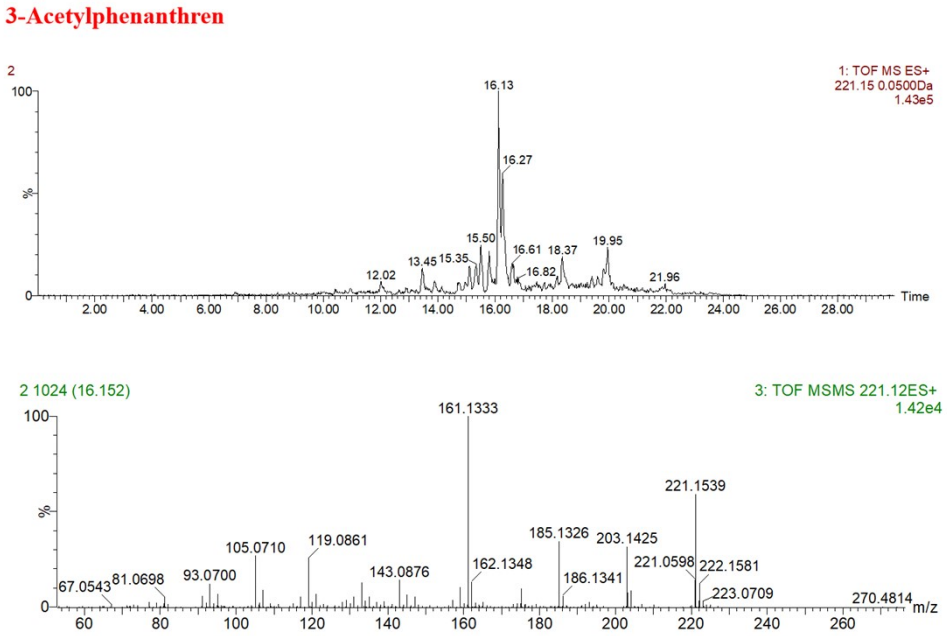

Fig S38 The HPLC-MS/MS spectrum of 3-acetylphenanthren

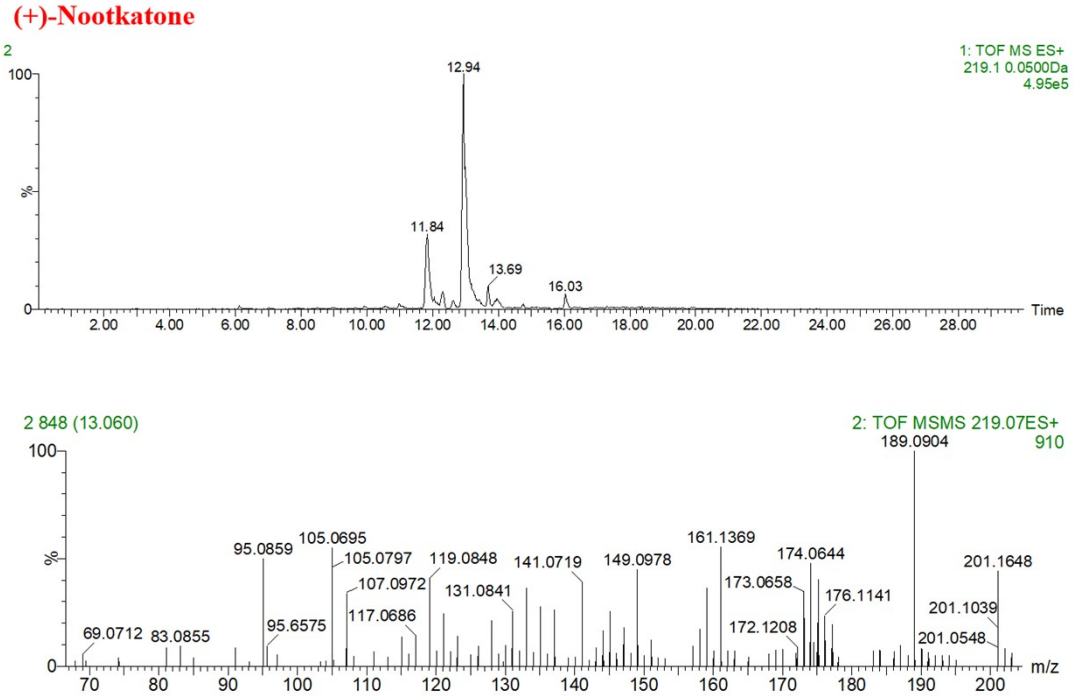

Fig S39 The HPLC-MS/MS spectrum of (+)-nootkatone

7α-hydroxy-3-desoxyzaluzanin C

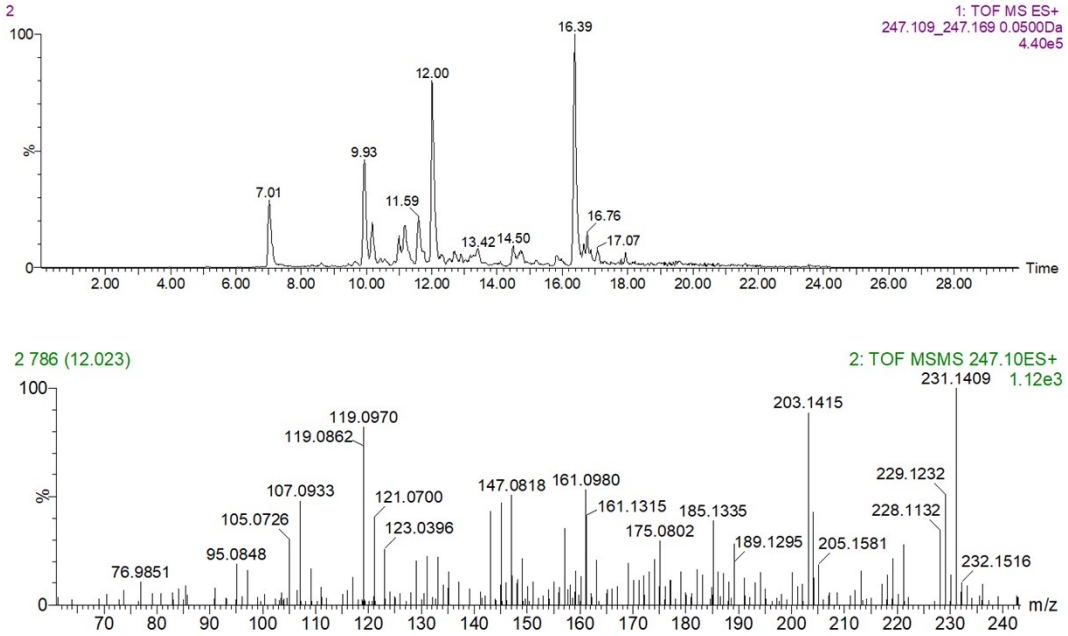

Fig S40 The HPLC-MS/MS spectrum of 7α-hydroxy-3-desoxyzaluzanin C

Dehydrocostus lactone

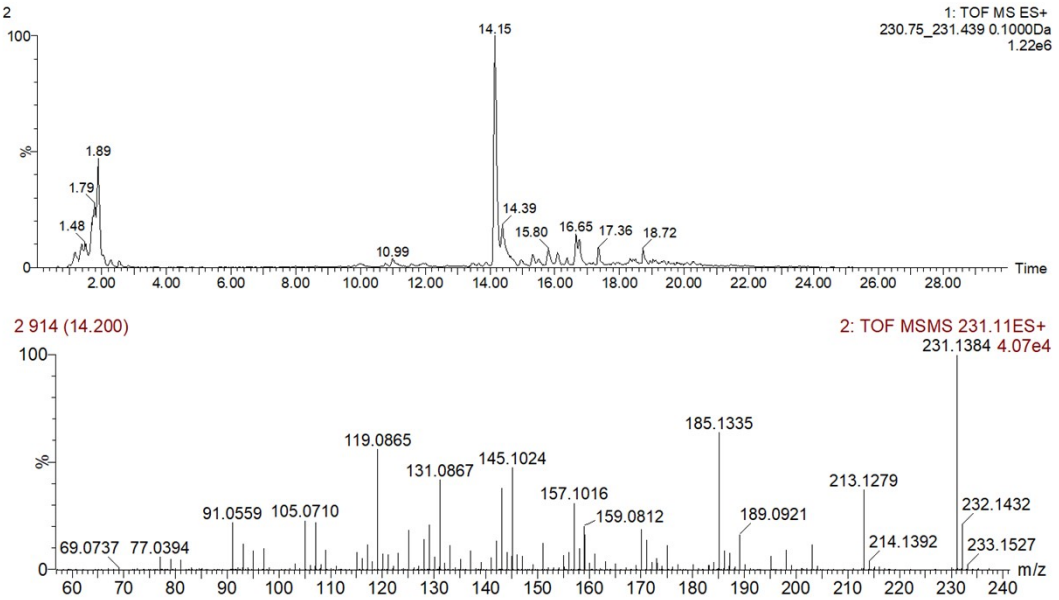

Fig S41 The HPLC-MS/MS spectrum of dehydrocostus lactone

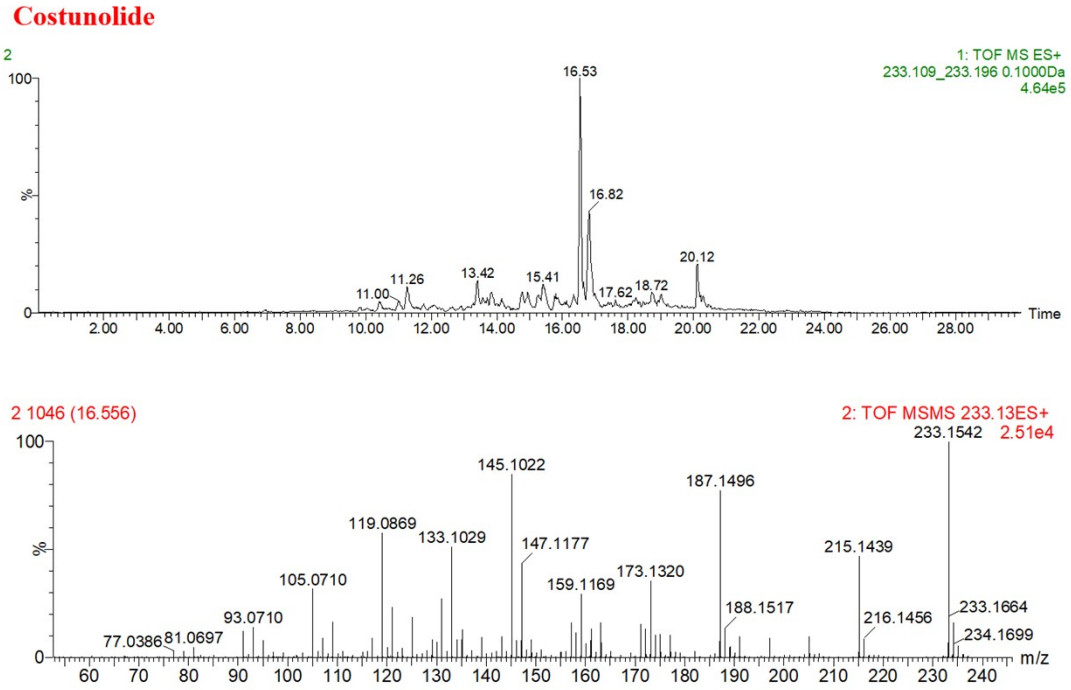

Fig S42 The HPLC-MS/MS spectrum of costunolide