Supplementary Materials

New benzothiazole-monoterpenoid hybrids as multifunctional molecules with potential applications in cosmetics

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Figure S1 ^{1}H-NMR spectrum of **4a** - DMSO-d$_6$, 80 °C, 600 MHz

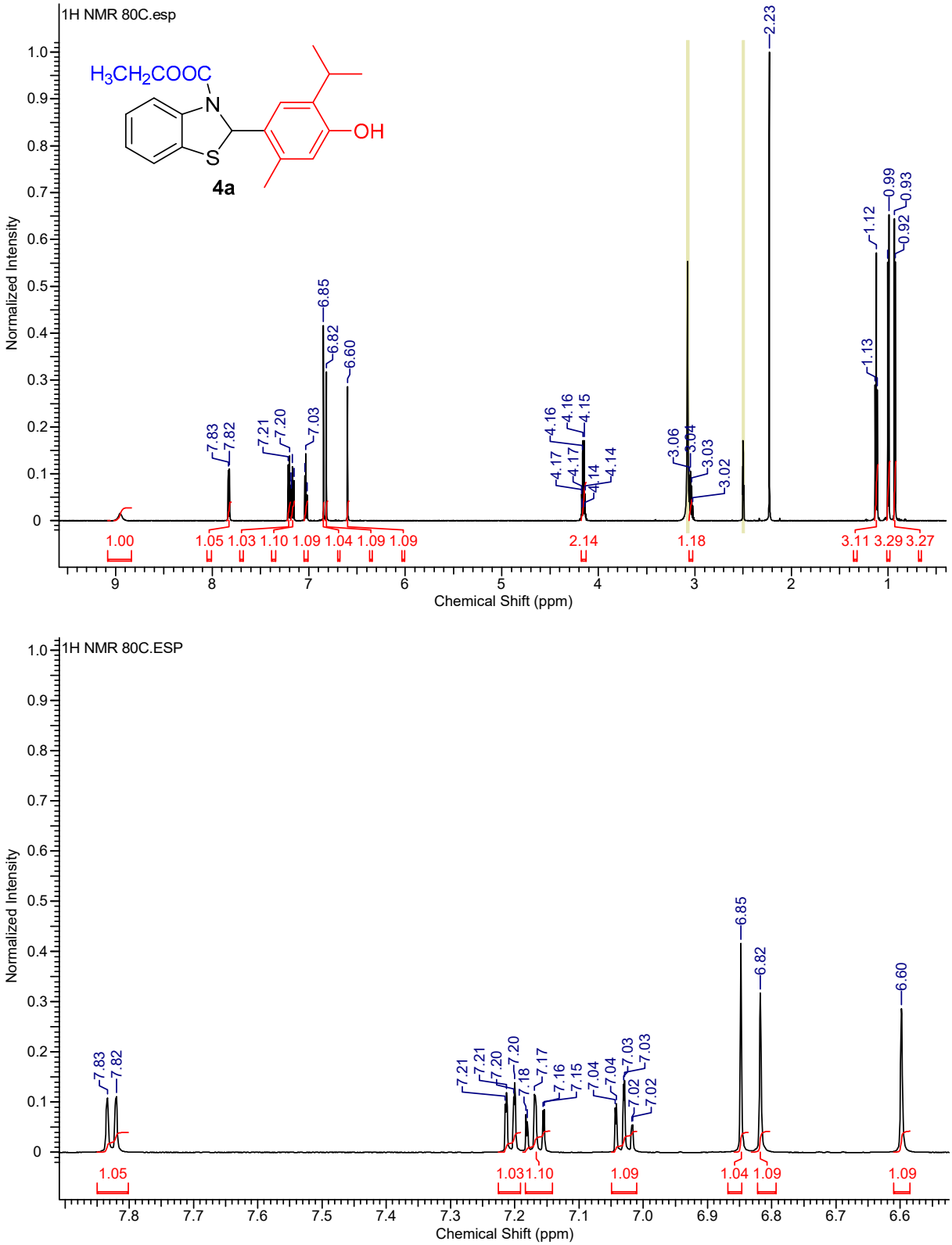


Figure S2 ^{13}C-NMR spectrum of **4a** - DMSO-d$_6$, 80 ºC, 150 MHz

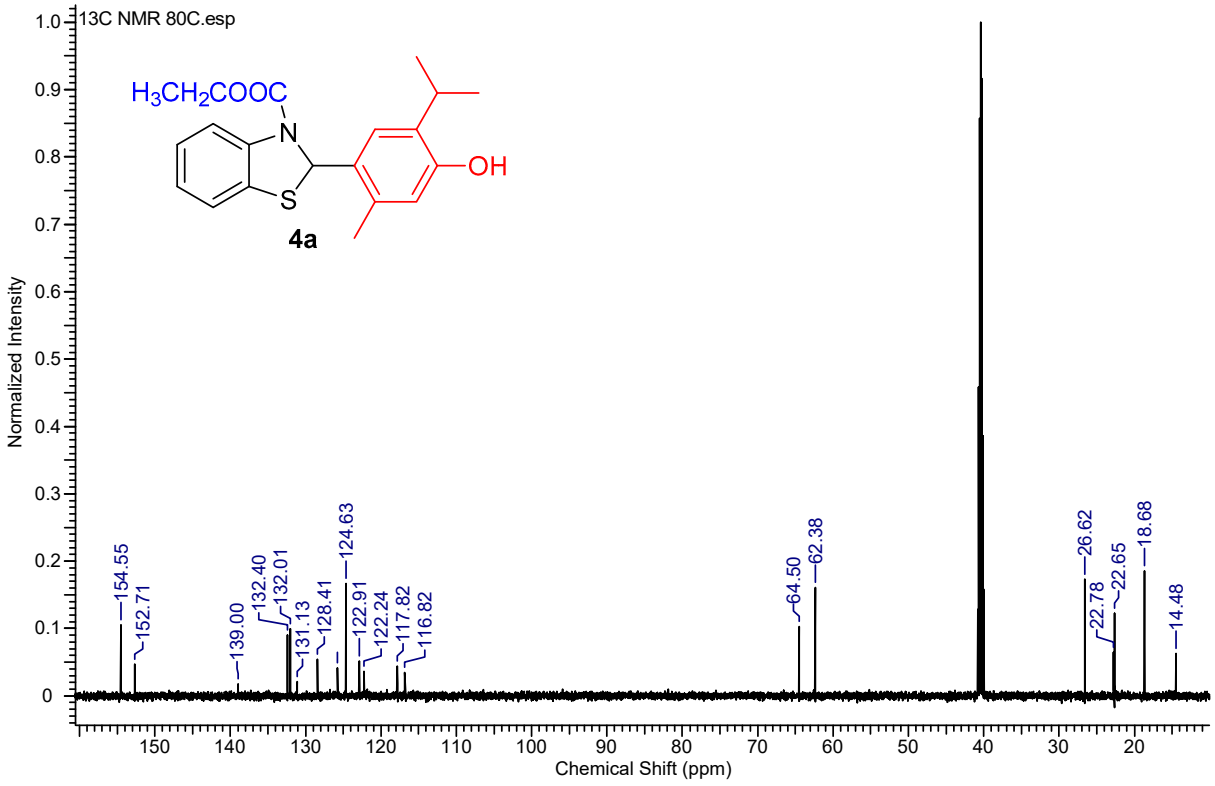


Figure S3 FT-IR spectrum of compound **4a**, KBr tablet, cm^{-1}

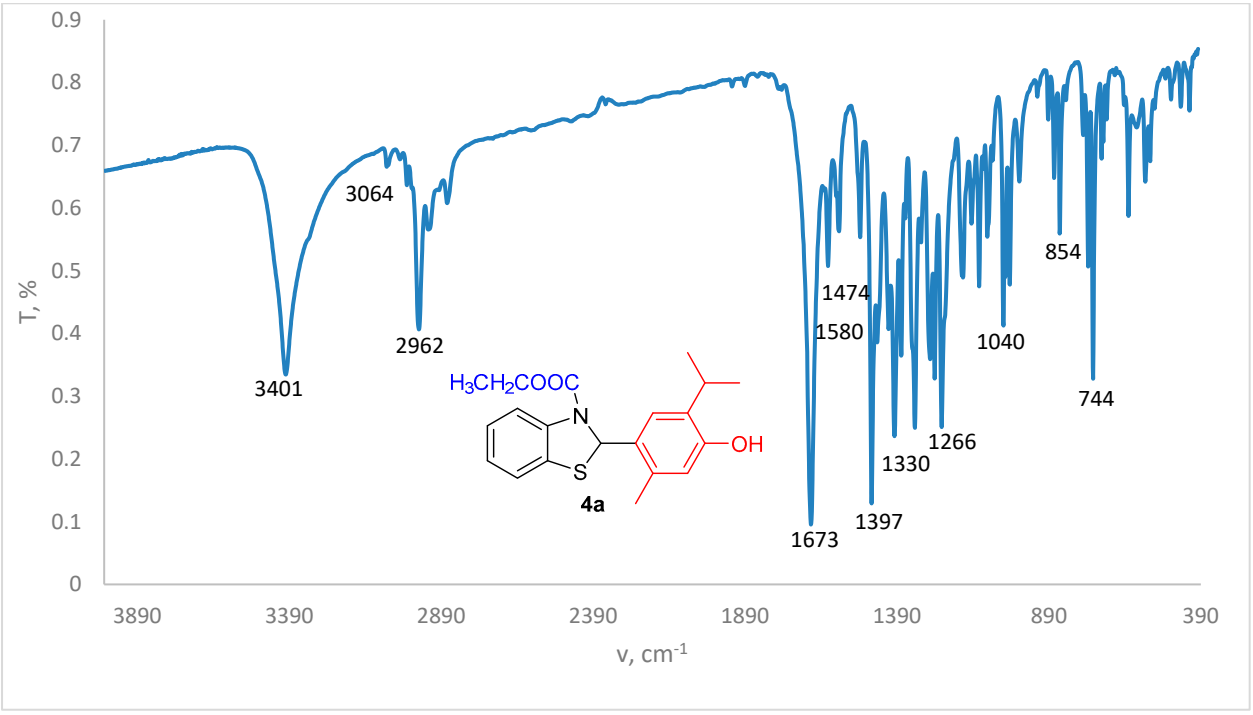


Figure S4 ESI-HRMS spectrum of compound **4a**

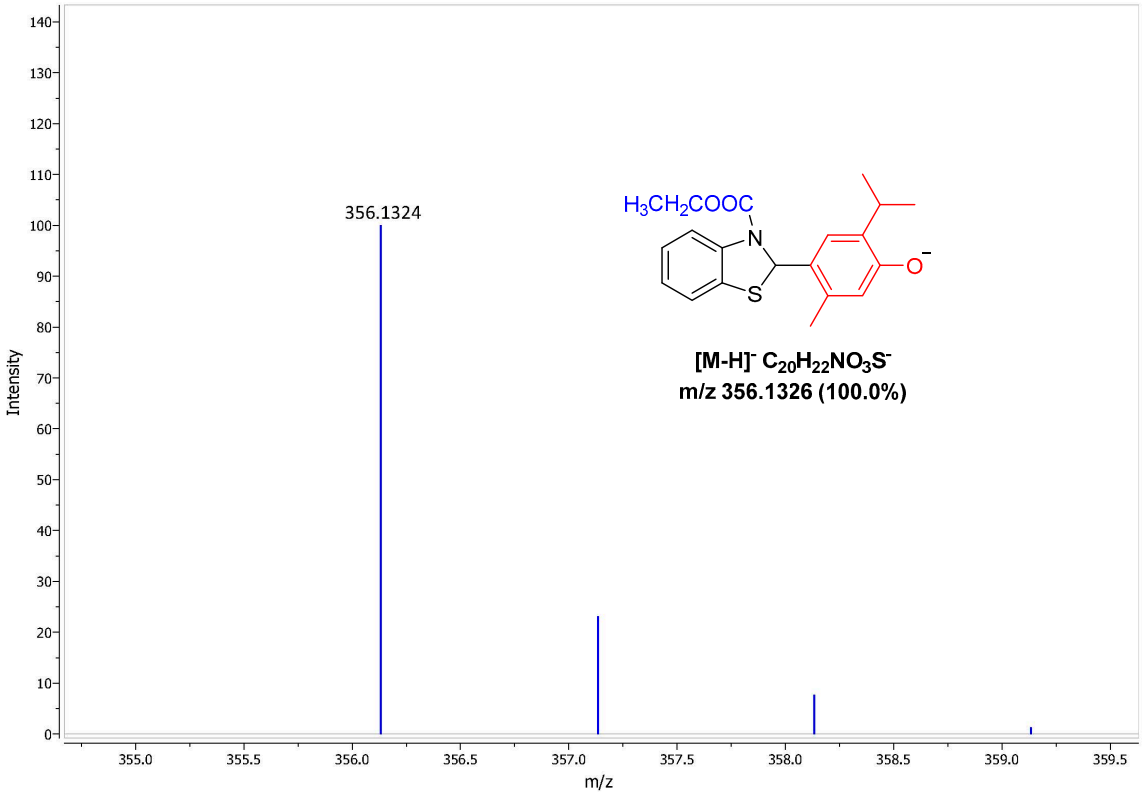
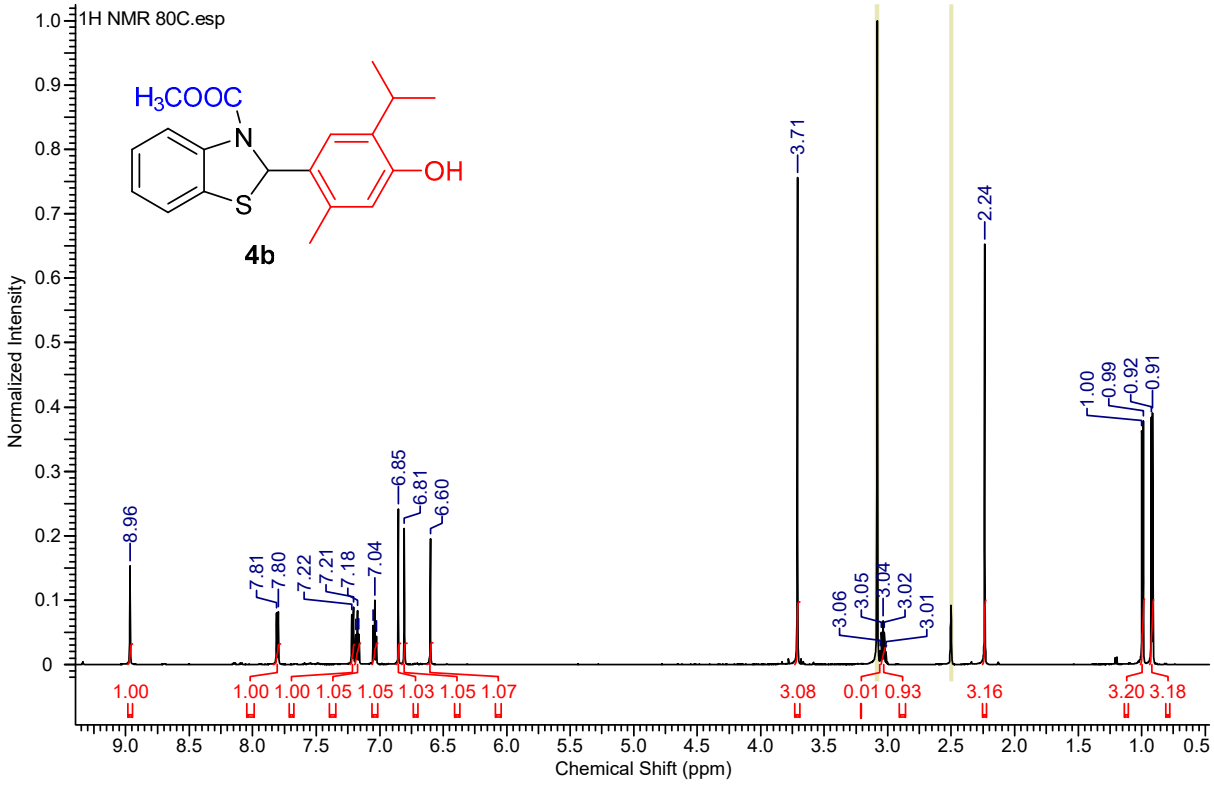


Figure S5 ^{1}H-NMR spectrum of **4b** - DMSO-d$_6$, 80 ºC, 600 MHz



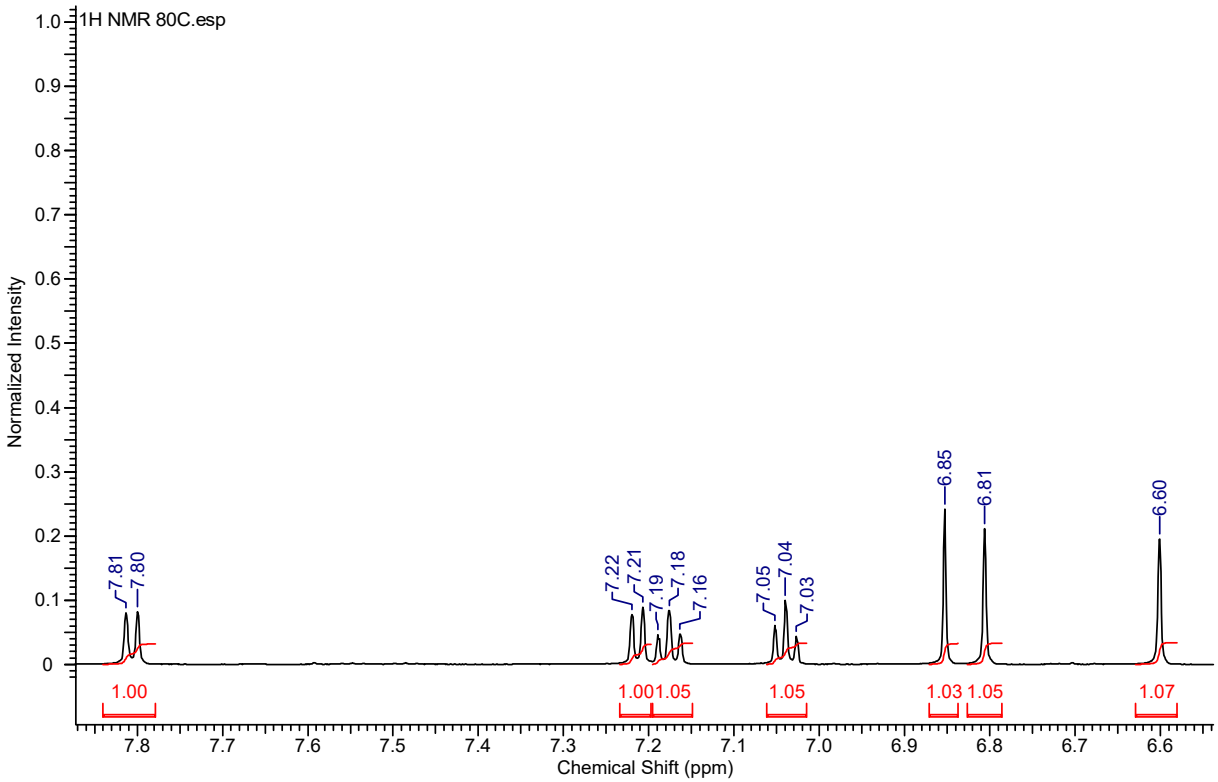


Figure S6 ^{13}C-NMR spectrum of **4b -** DMSO-d_6, 80 ºC, 150 MHz

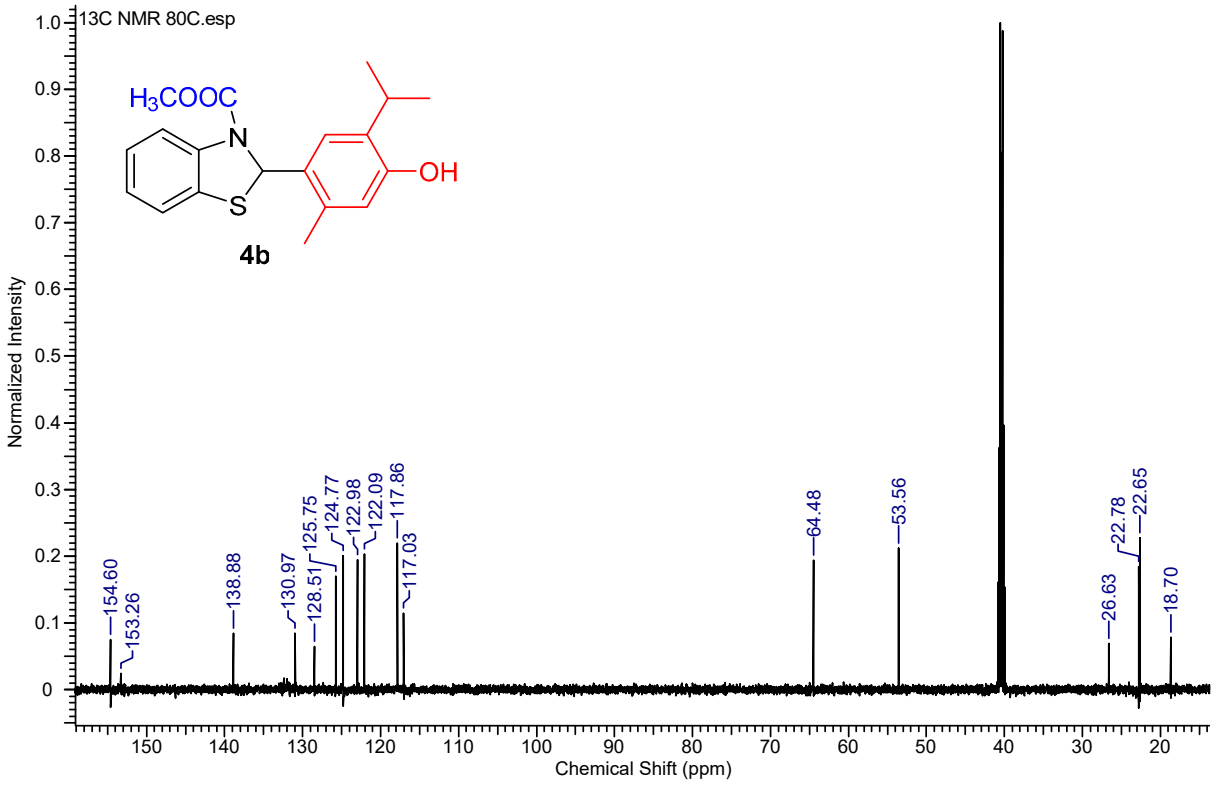


Figure S7 FT-IR spectrum of compound **4b**, KBr tablet, cm^{-1}

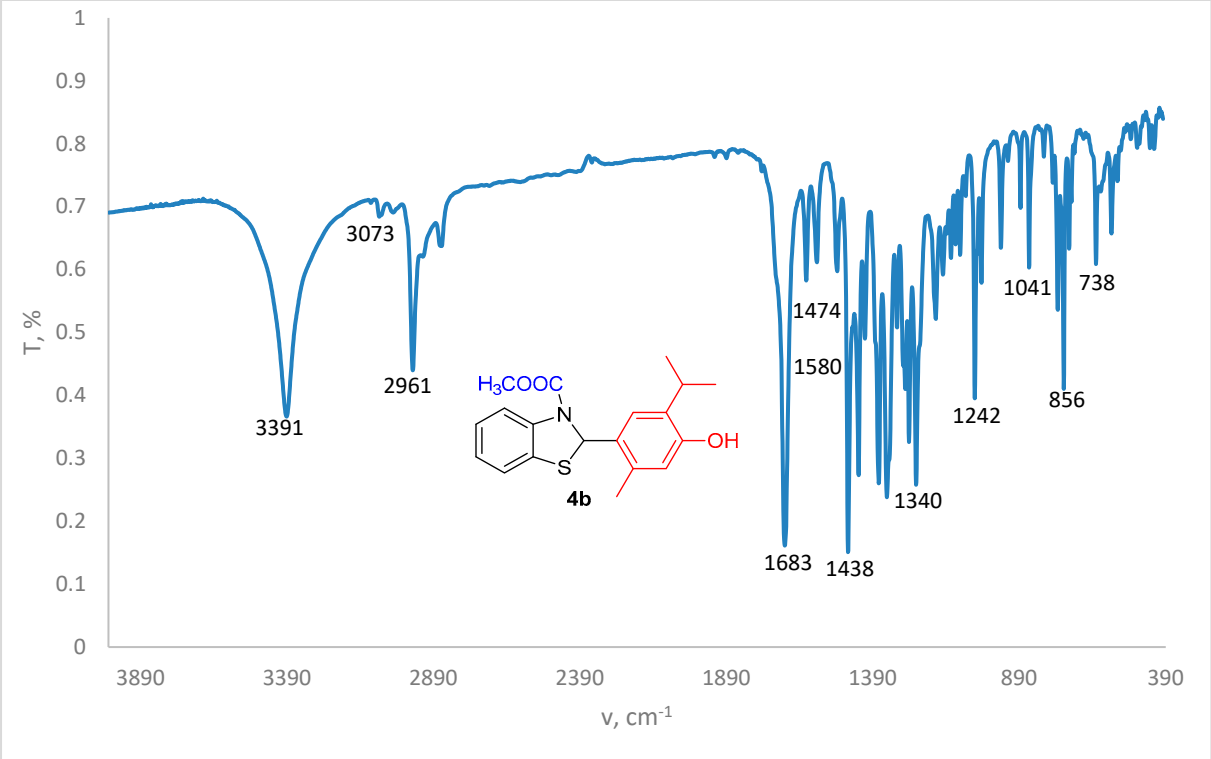


Figure S8 ESI-HRMS spectrum of compound **4b**

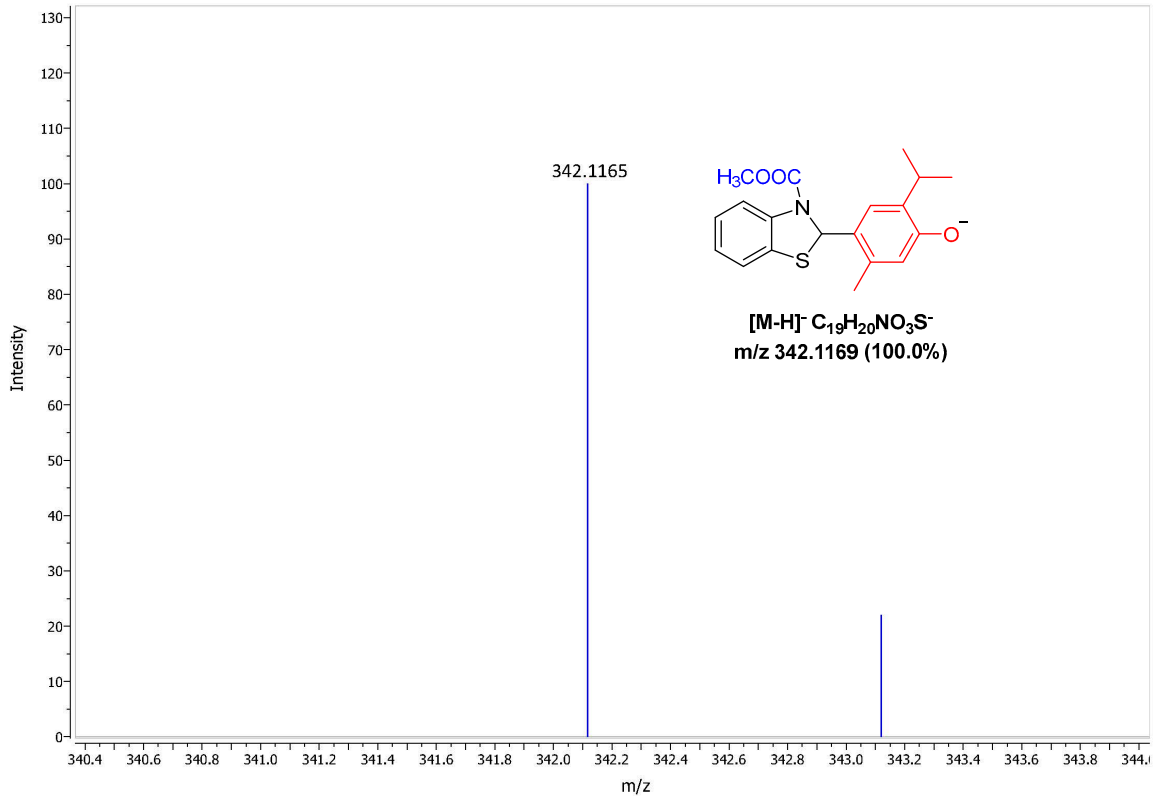


Figure S9 ^{1}H-NMR spectrum of **4c** - DMSO-d$_6$, 80 ^{o}C, 600 MHz

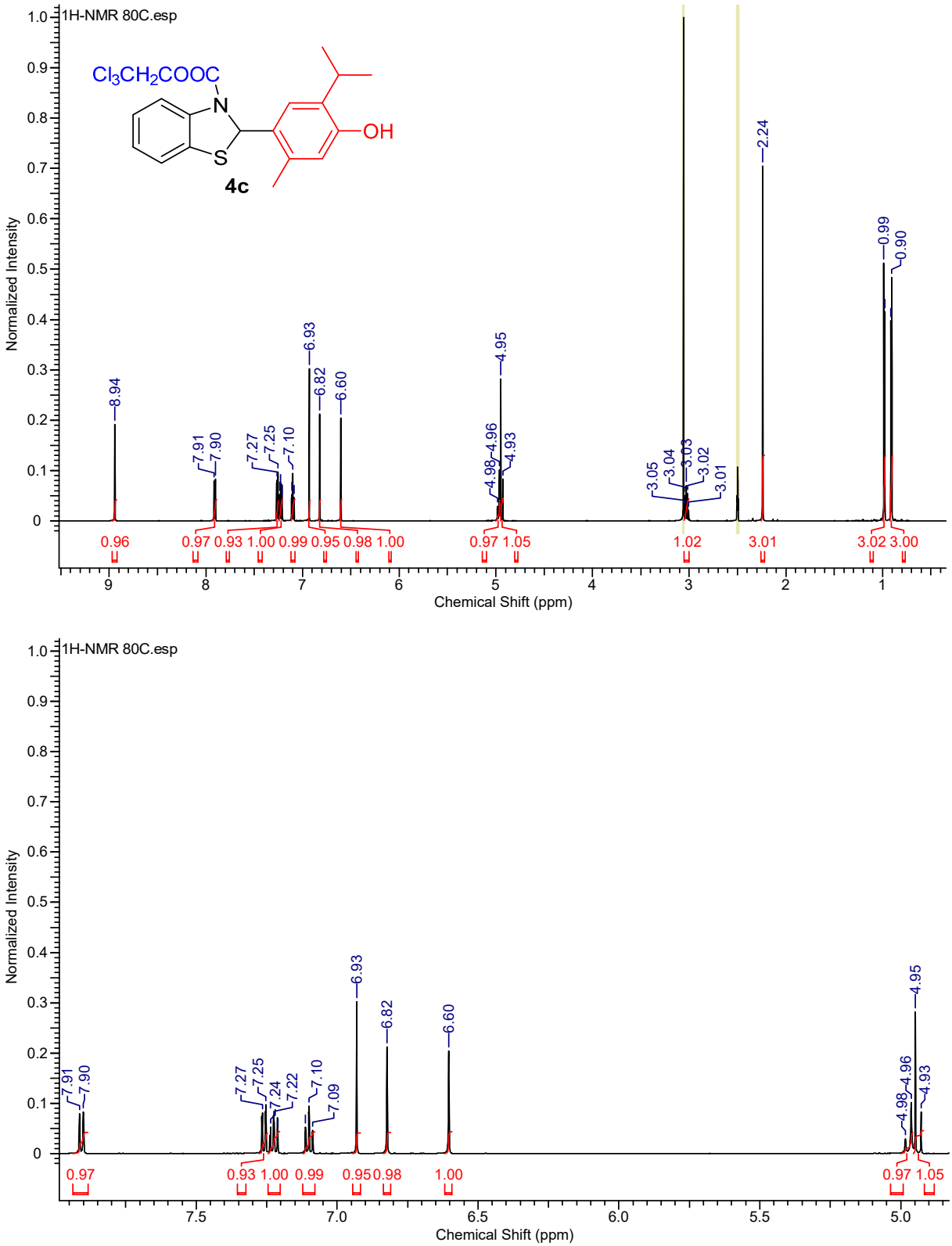


Figure S10 ^{13}C-NMR spectrum of **4c** - DMSO-d$_6$, 80 ºC, 150 MHz

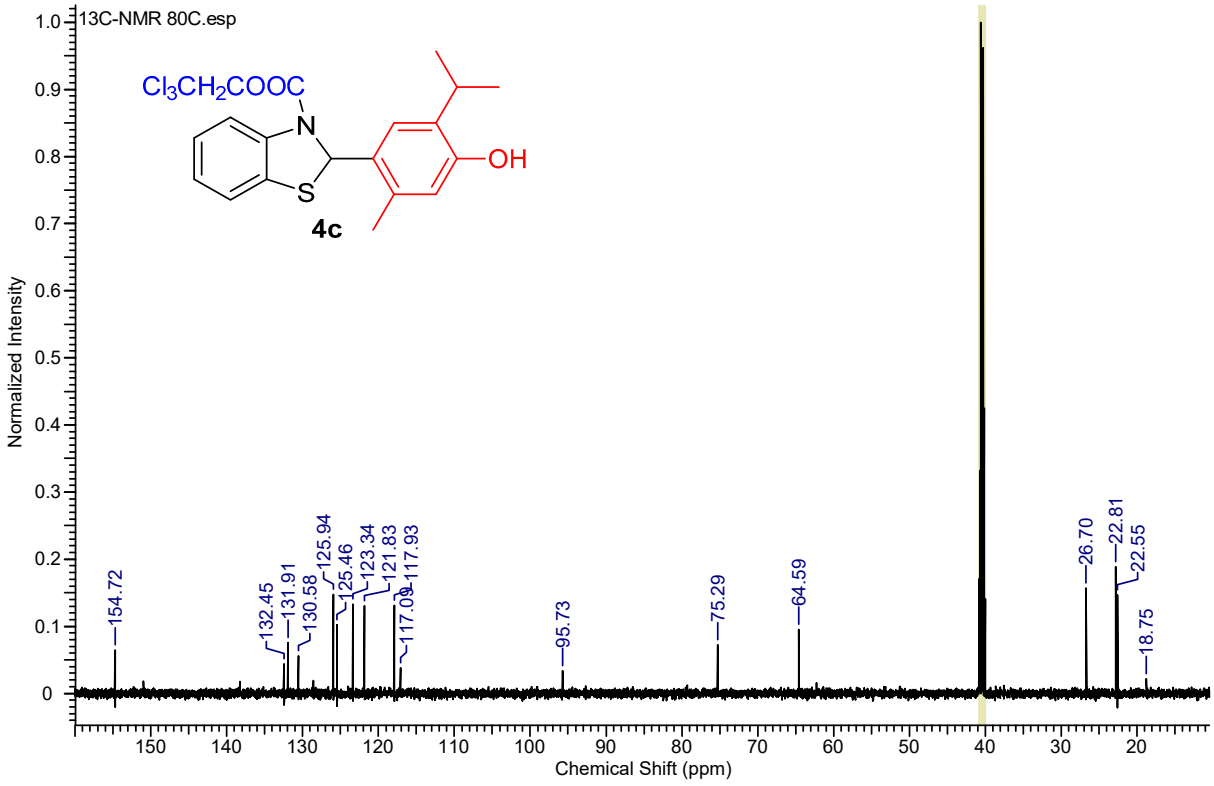


Figure S11 FT-IR spectrum of compound **4c**, KBr tablet, cm^{-1}

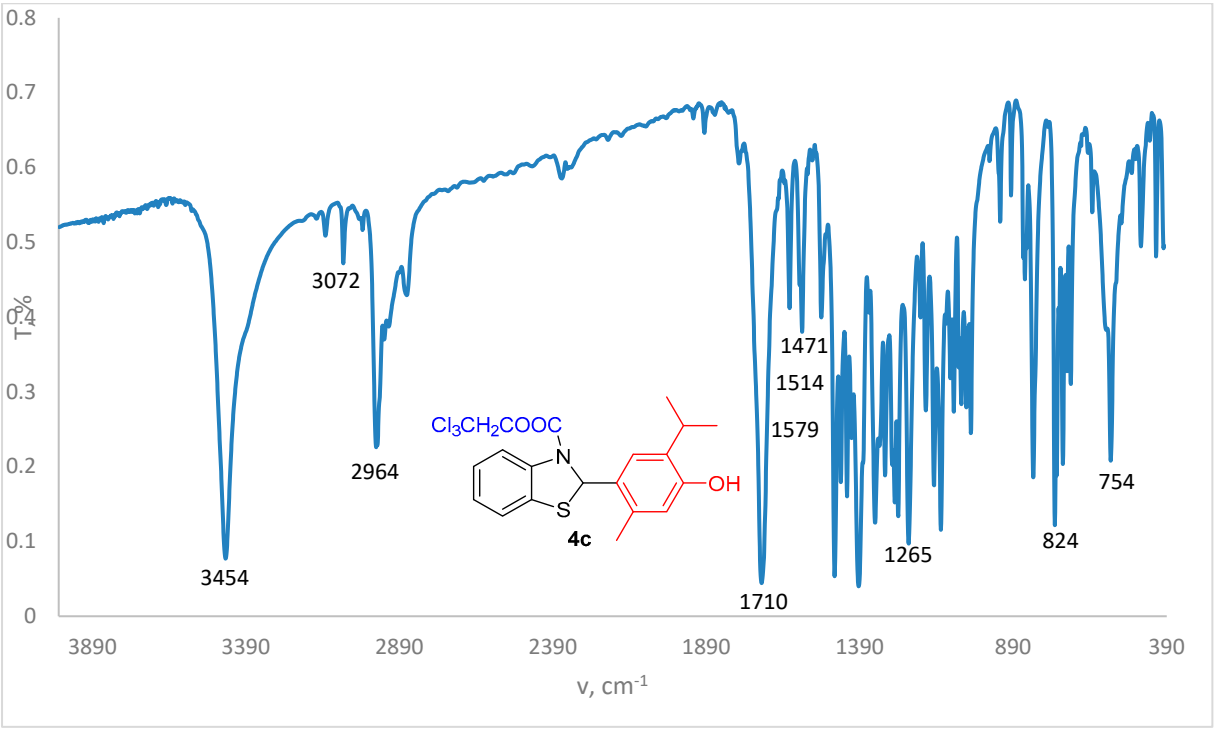


Figure S12 ESI-HRMS spectrum of compound **4c**

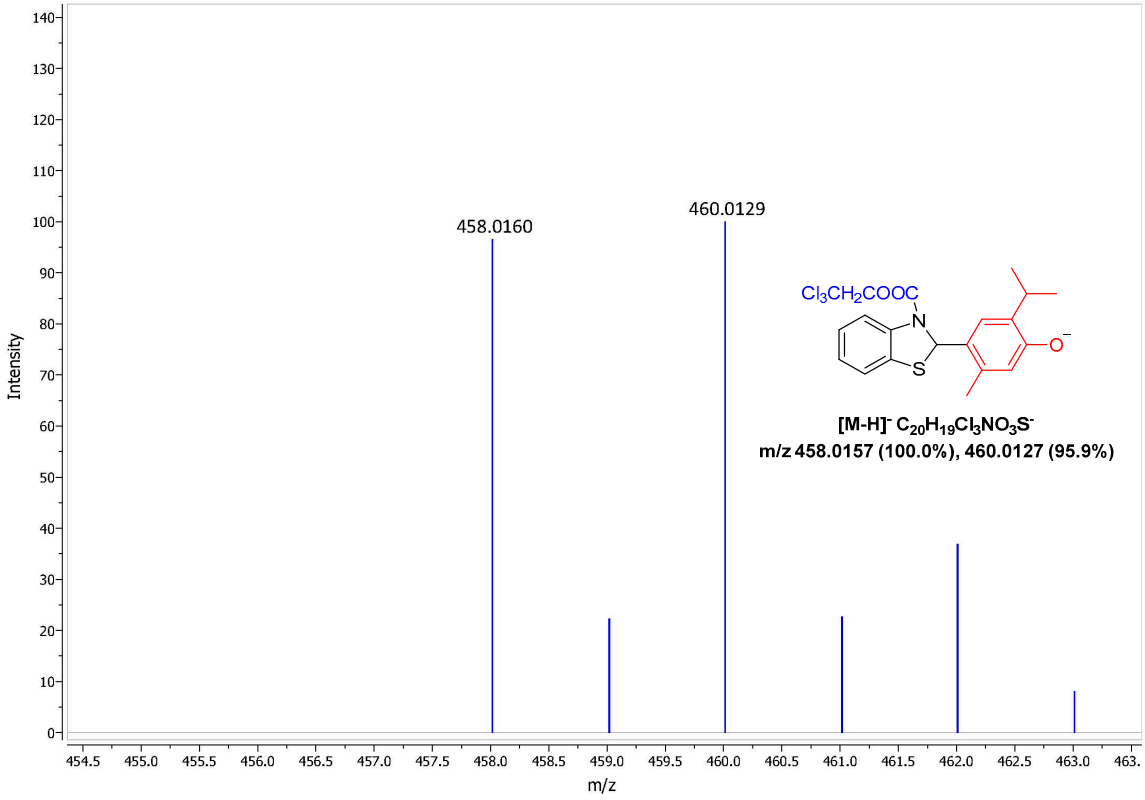
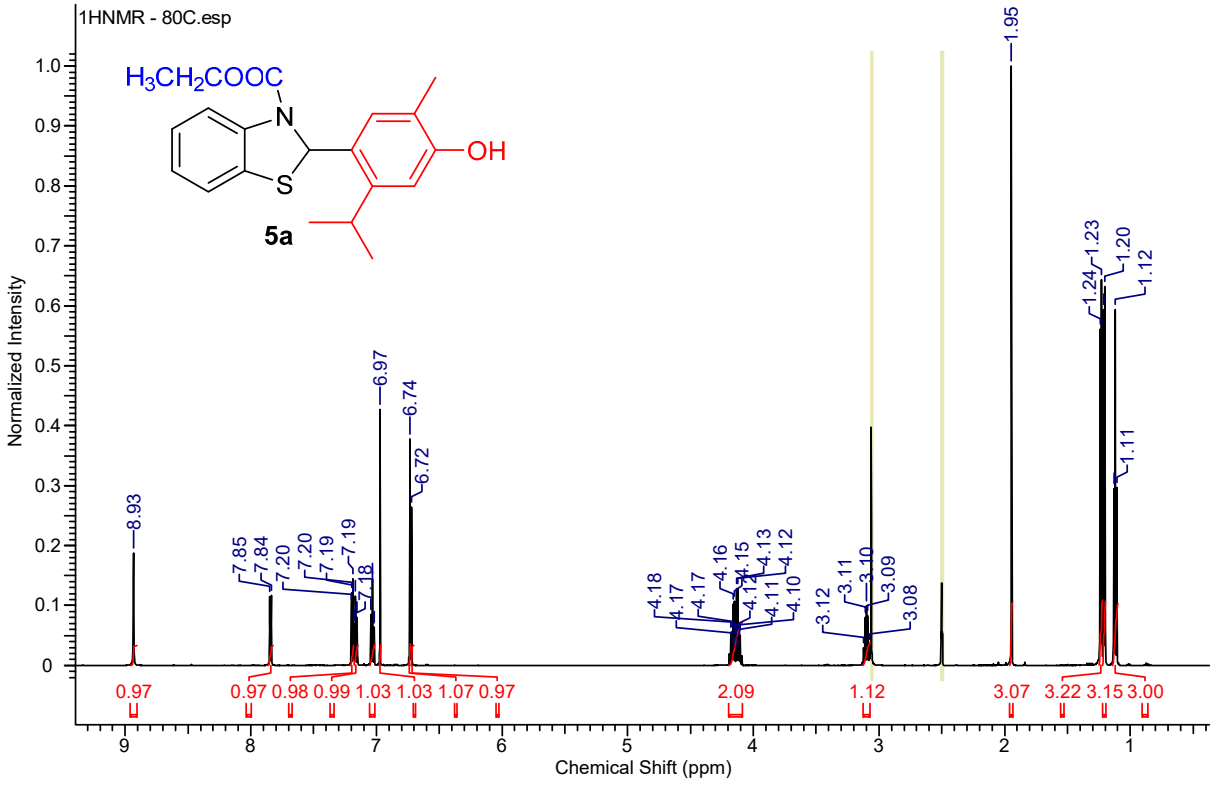


Figure S13 ^{1}H-NMR spectrum of **5a** - DMSO-d$_6$, 80 ºC, 600 MHz



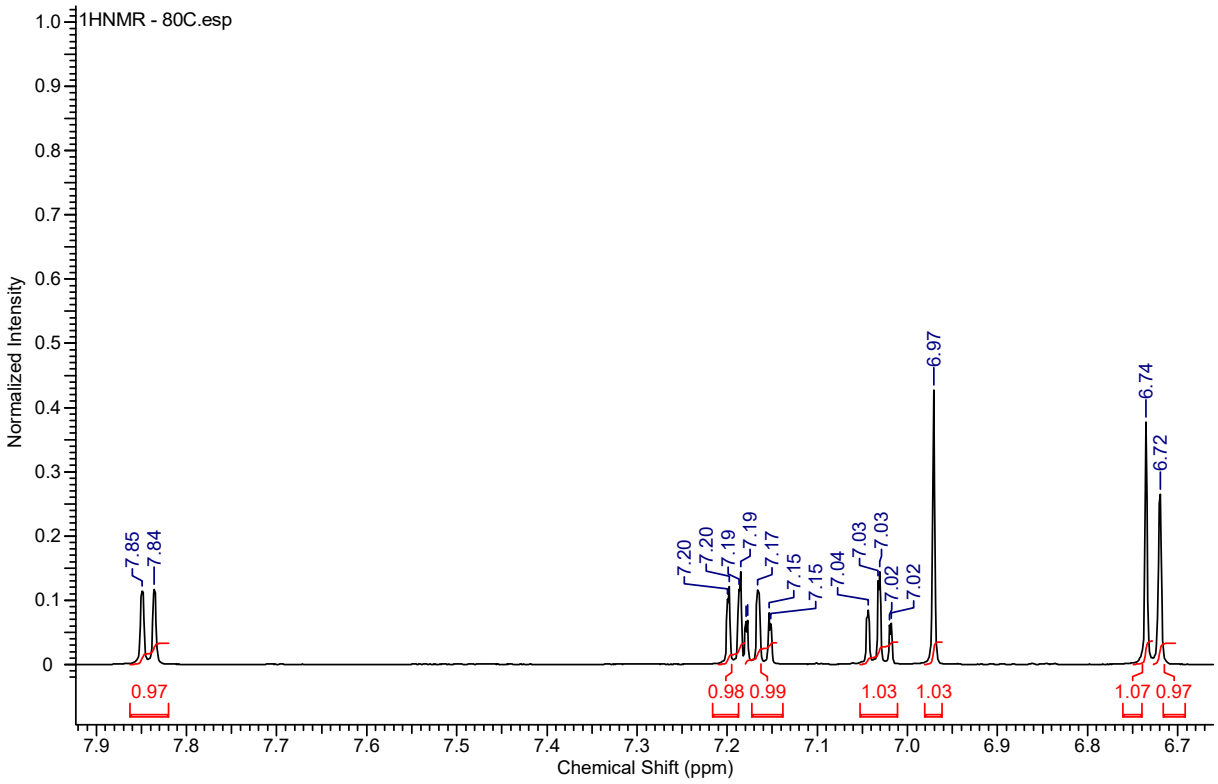


Figure S14 ^{13}C-NMR spectrum of **5a -** DMSO-d_6, 80 ºC, 150 MHz

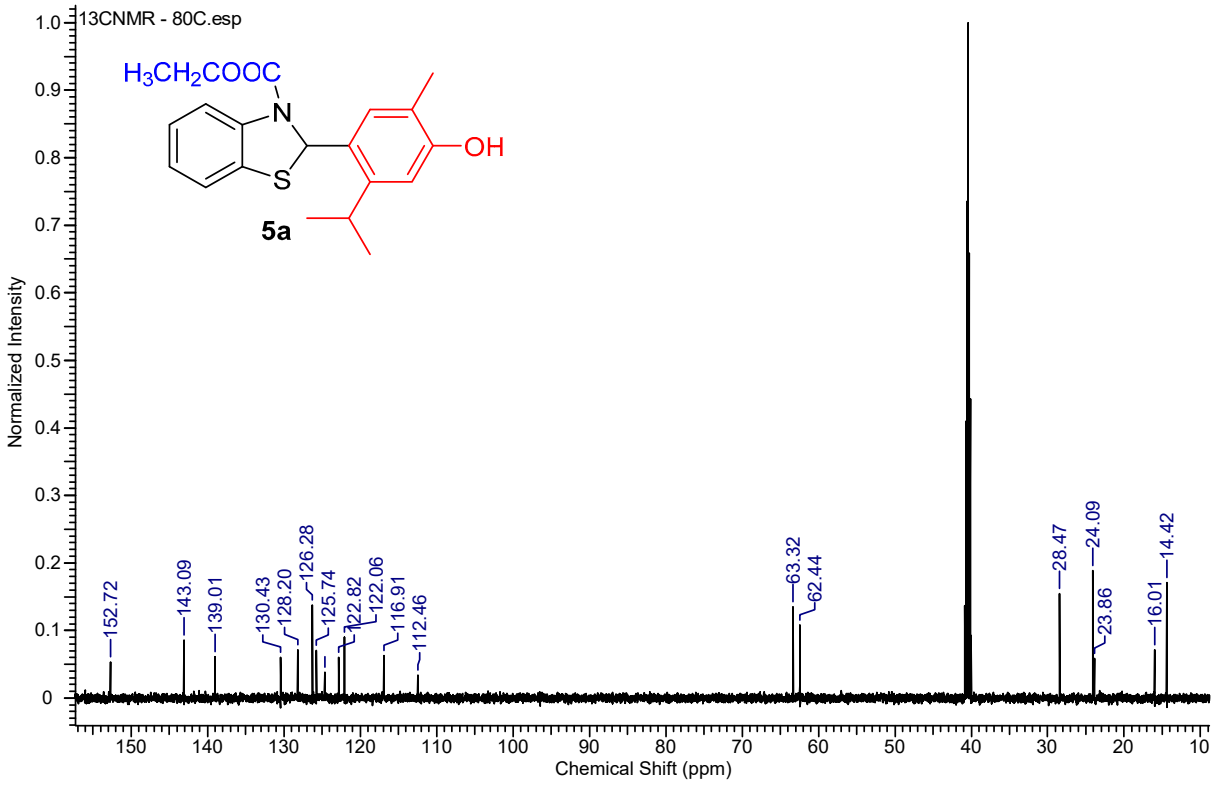


Figure S15 FT-IR spectrum of compound **5a**, KBr tablet, cm^{-1}

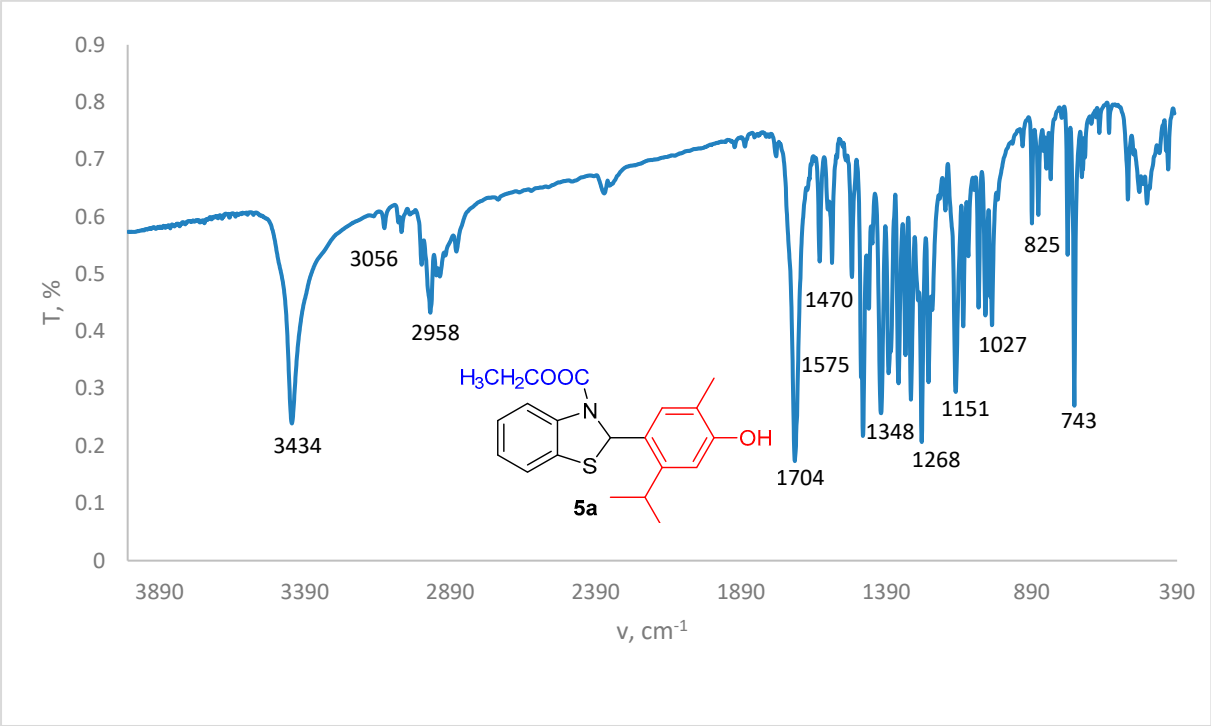


Figure S16 ESI-HRMS spectrum of compound **5a**

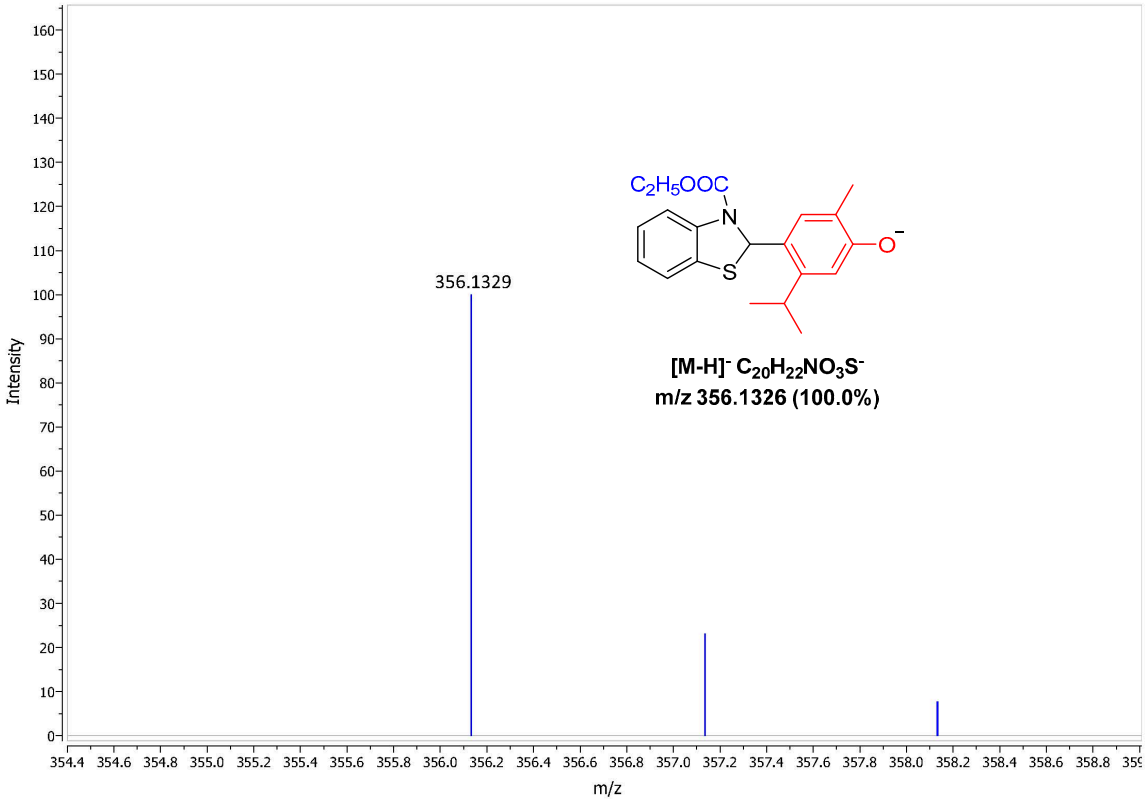


Figure S17 ^{1}H-NMR spectrum of **5b** - DMSO-d$_6$, 80 ºC, 600 MHz

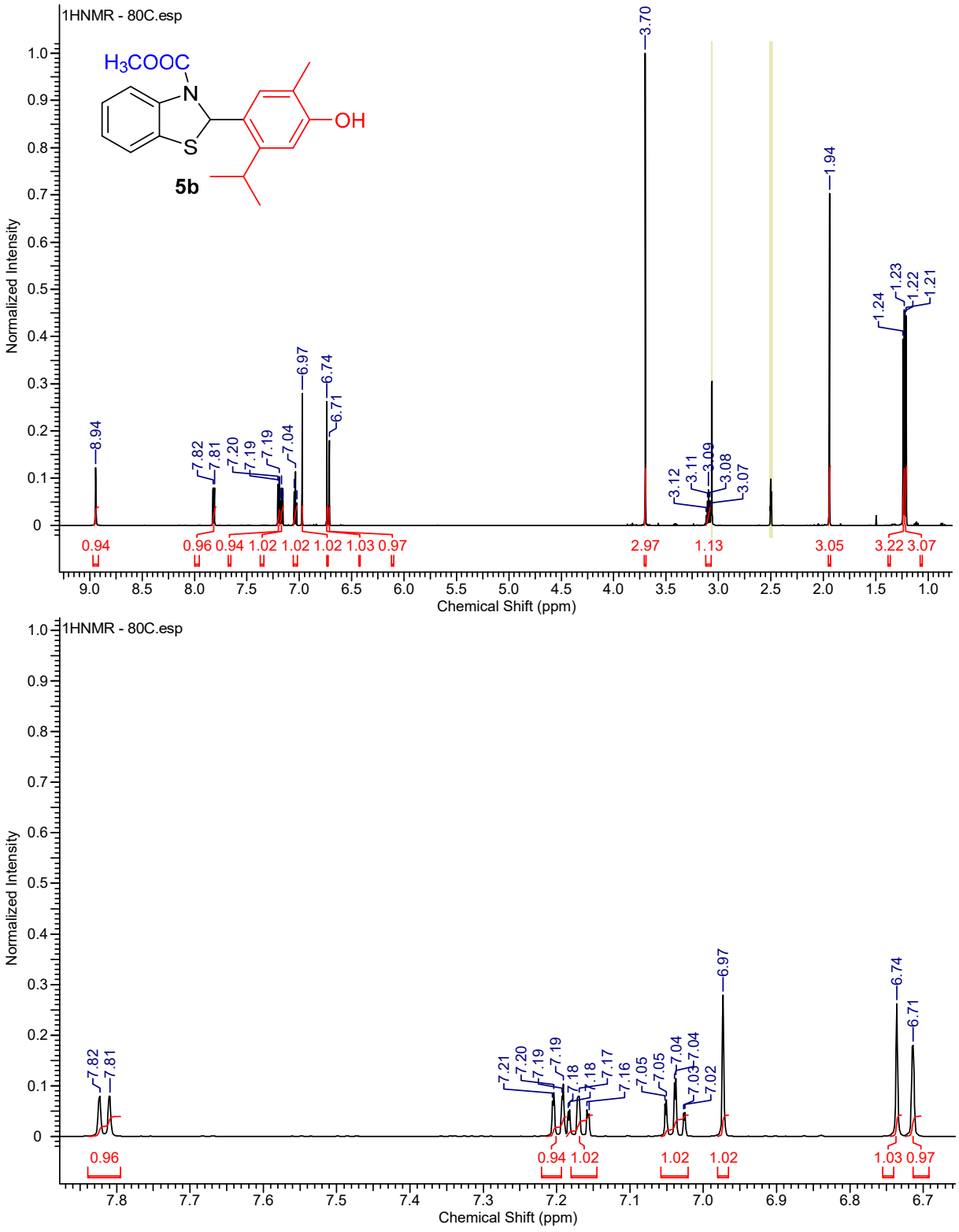


Figure S18 ^{13}C-NMR spectrum of **5b** - DMSO-d$_6$, 80 ºC, 150 MHz

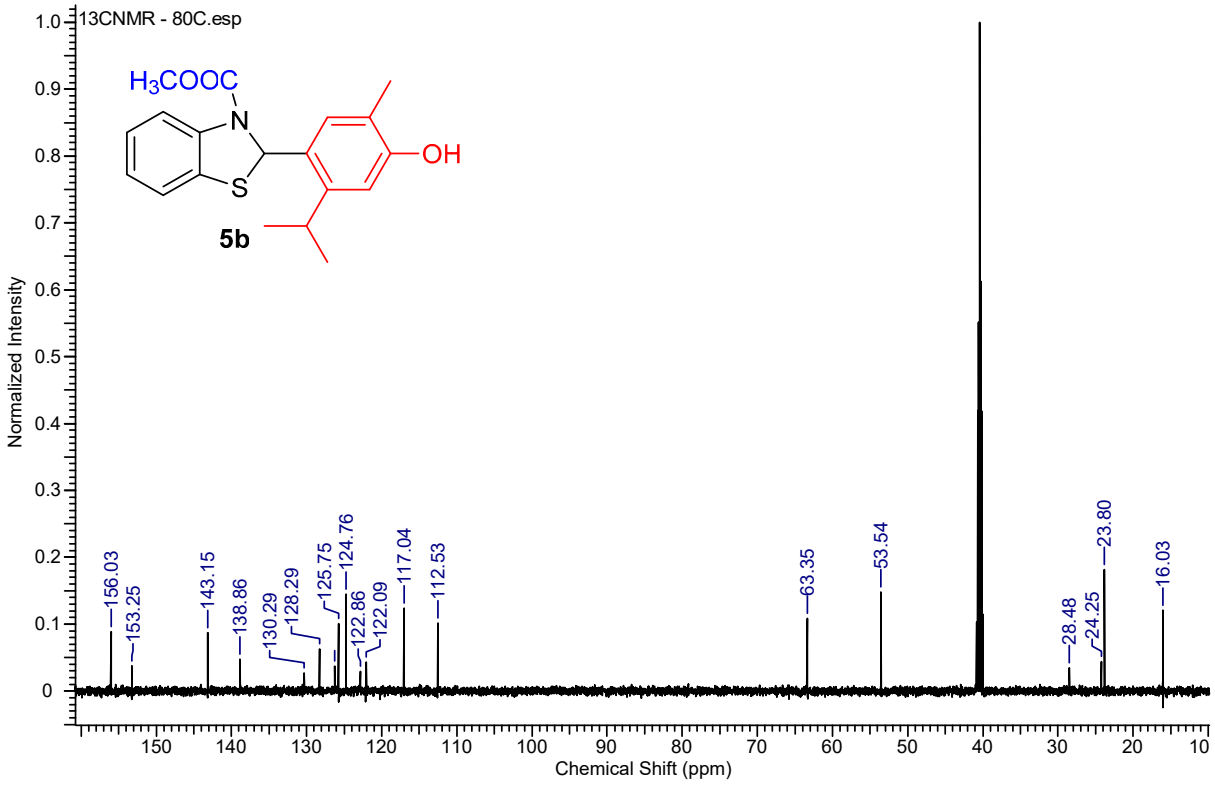


Figure S19 FT-IR spectrum of compound **5b**, KBr tablet, cm^{-1}

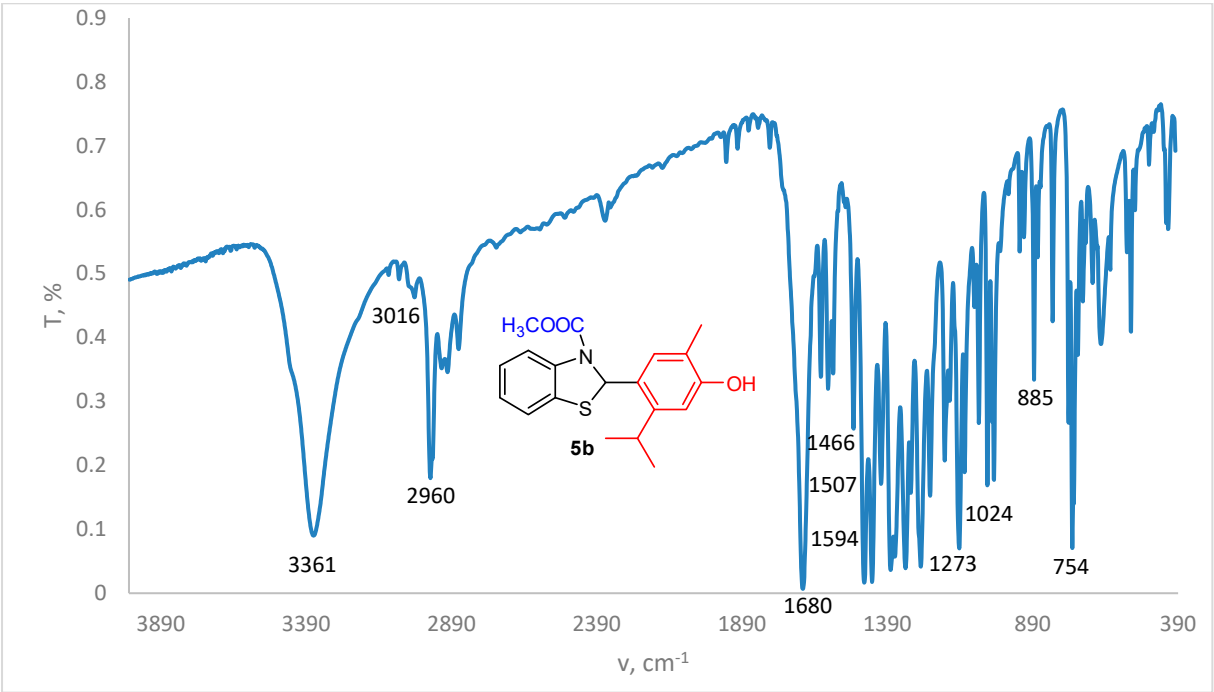


Figure S20 ESI-HRMS spectrum of compound **5b**

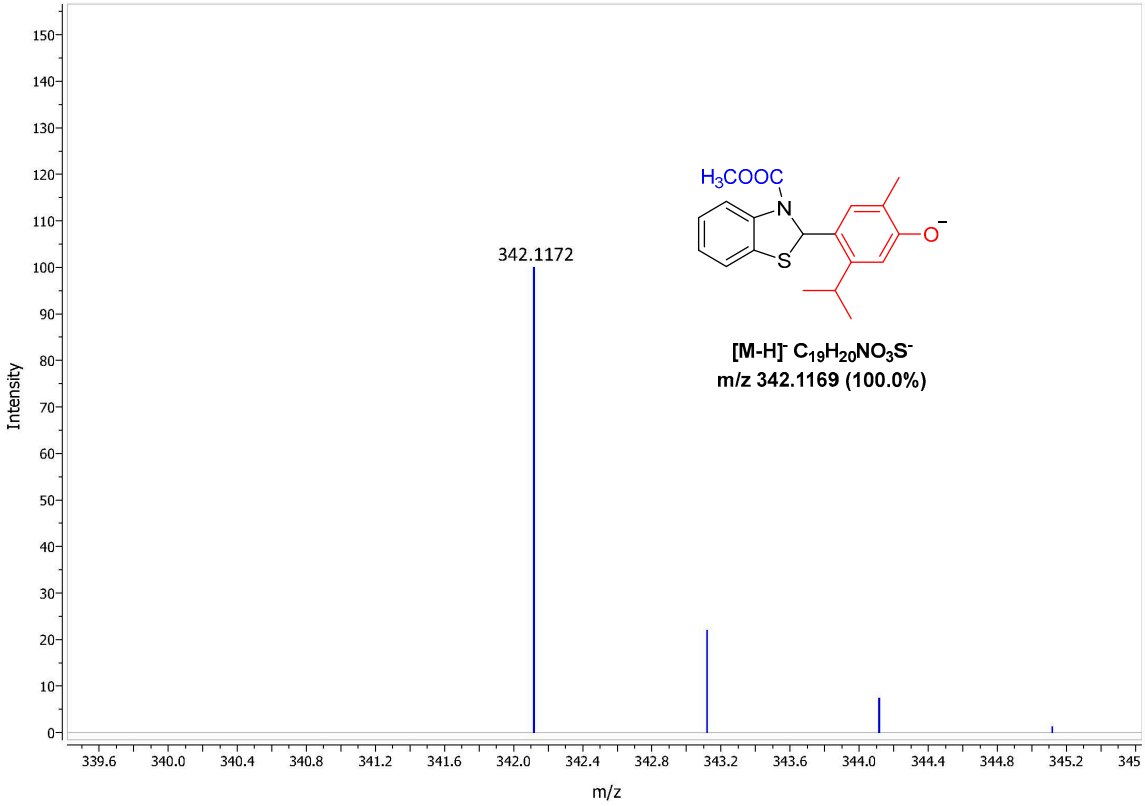
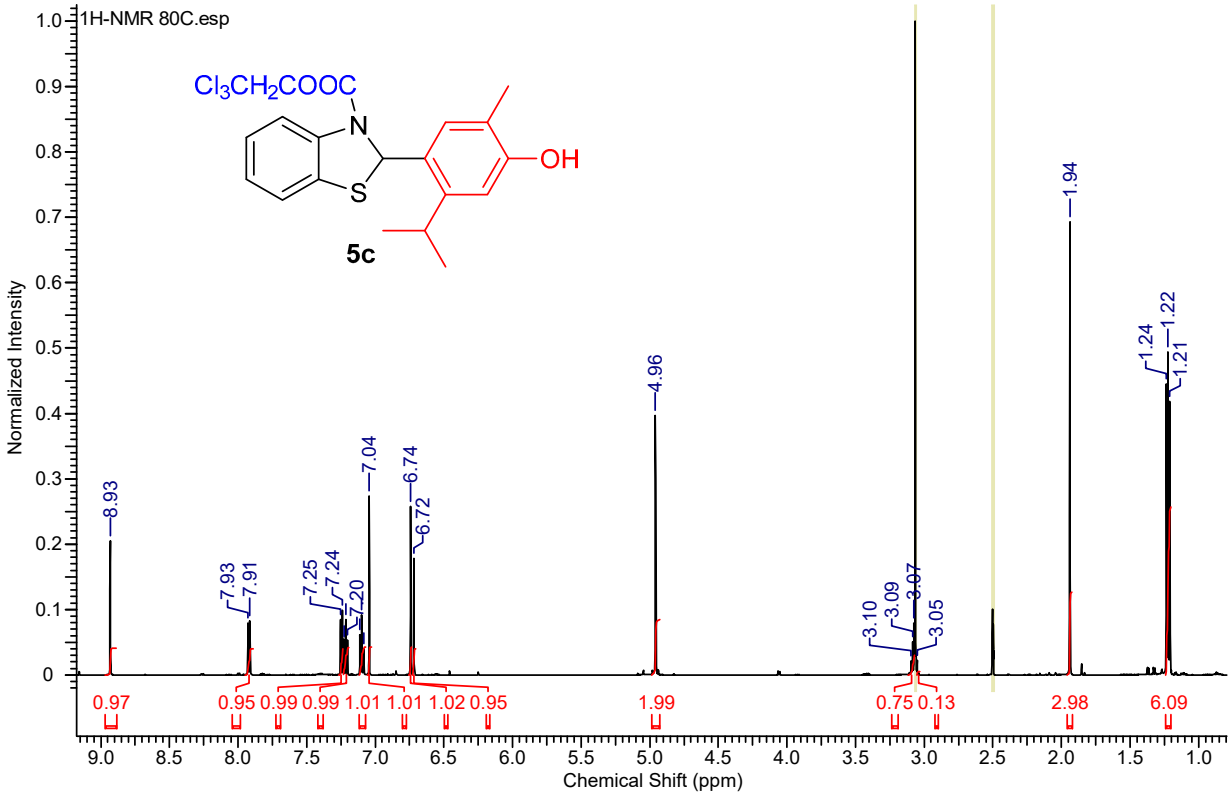


Figure S21 ^{1}H-NMR spectrum of **5c** - DMSO-d_6, 80 °C, 600 MHz



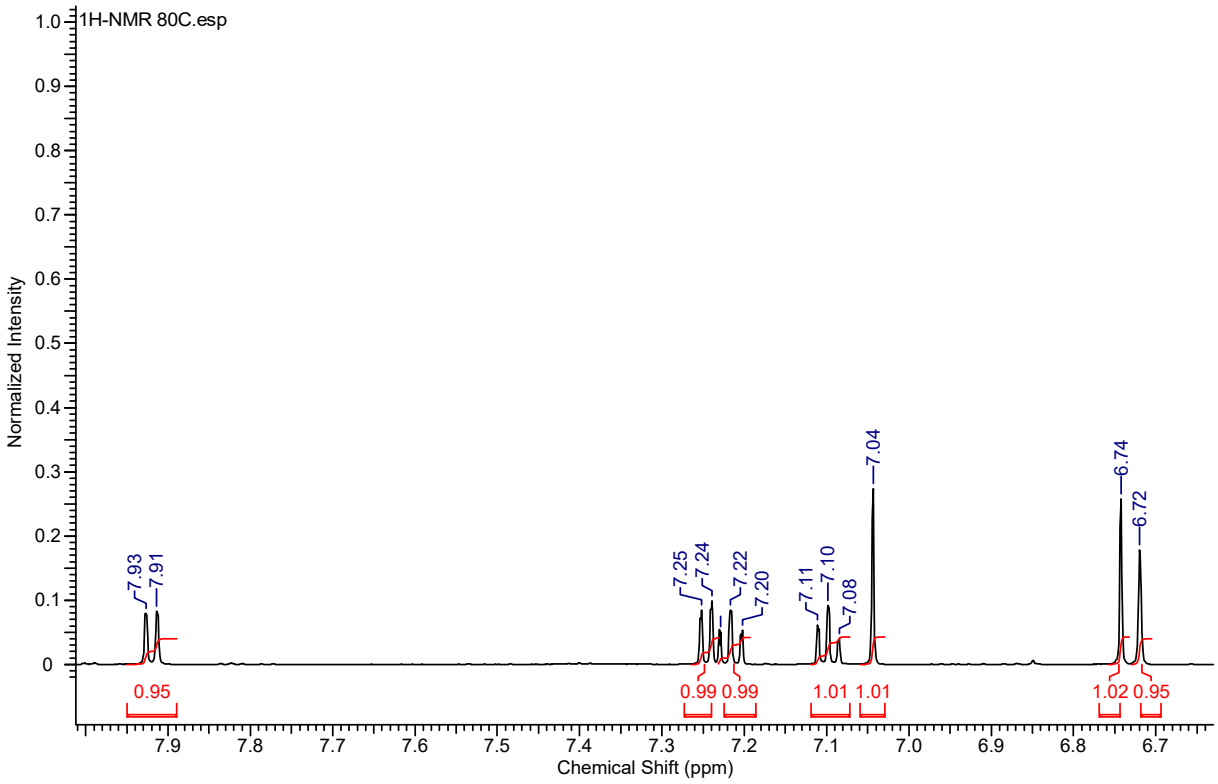


Figure S22 ^{13}C-NMR spectrum of **5c** - DMSO-d$_6$, 80 ºC, 150 MHz

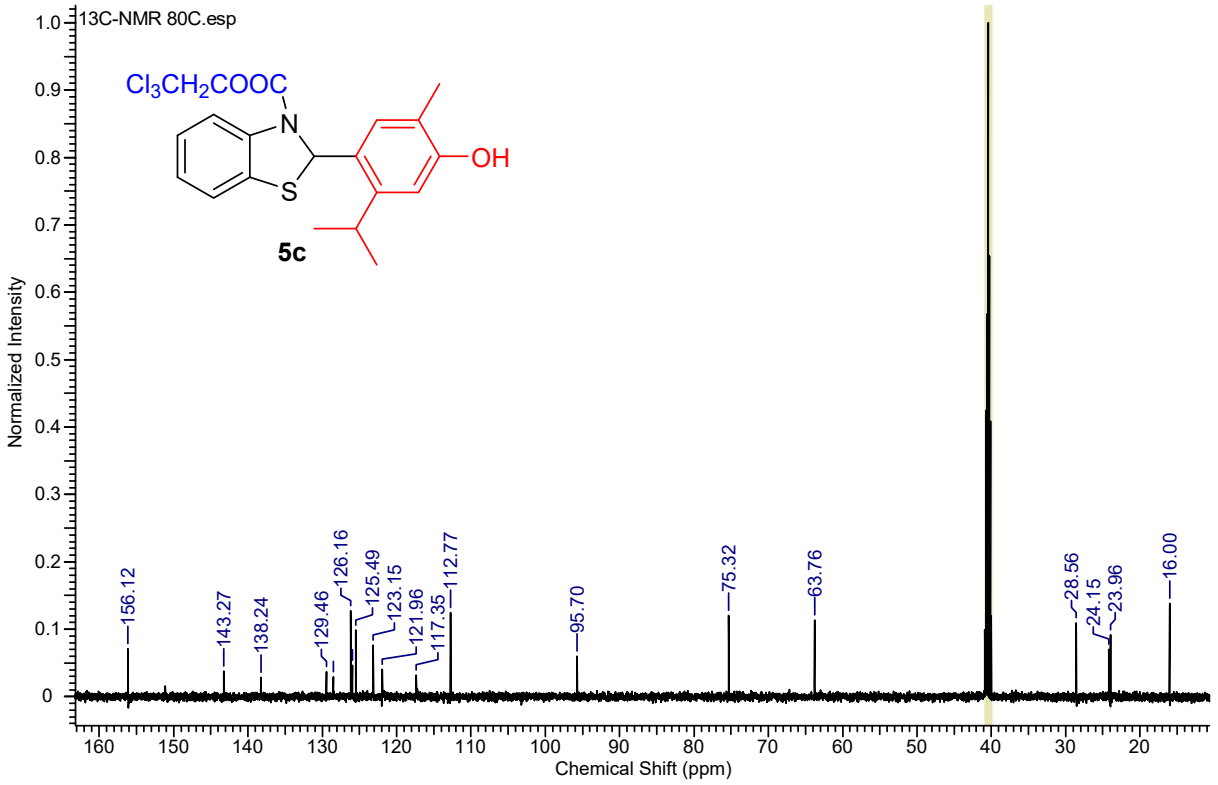


Figure S23 FT-IR spectrum of compound **5c**, KBr tablet, cm^{-1}

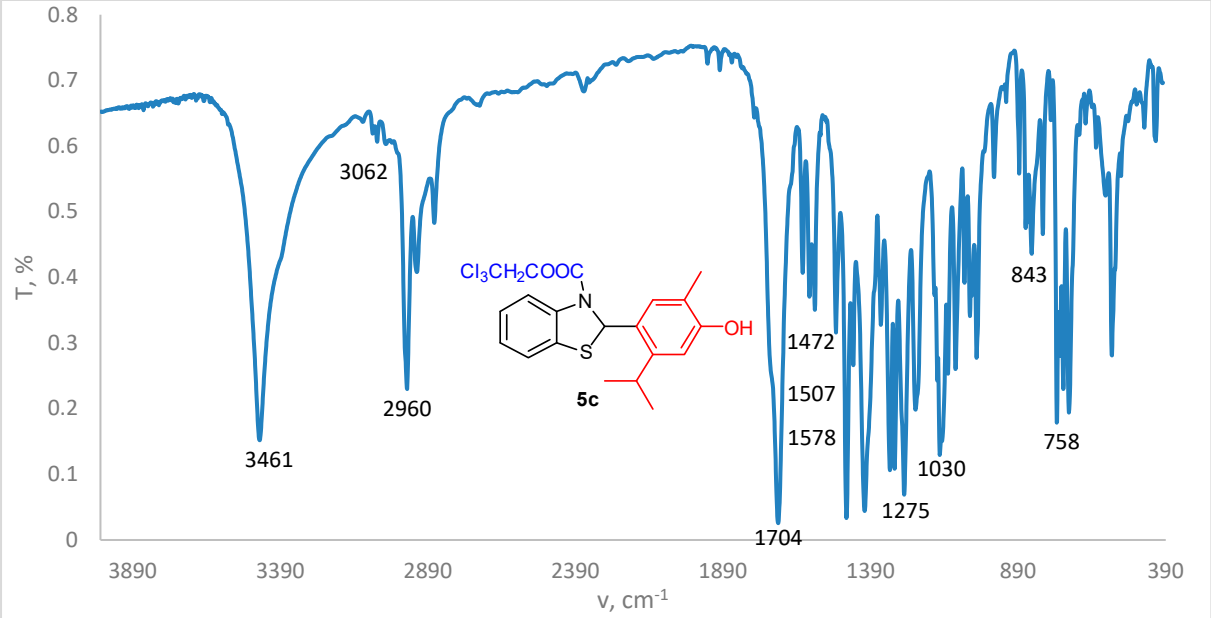


Figure S24 HRMS spectrum of compound **5c**

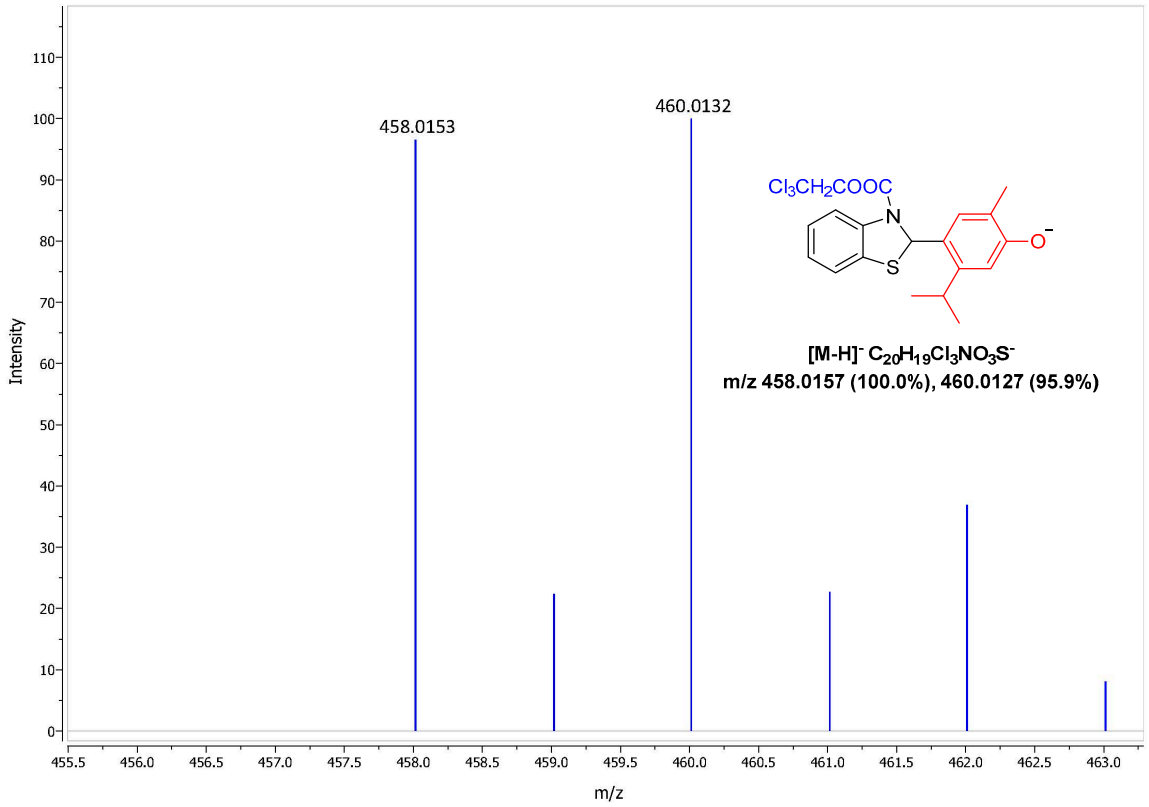


Figure S25 ^{1}H-NMR spectrum of **6** - DMSO-d$_6$, 80 ^{o}C, 600 MHz

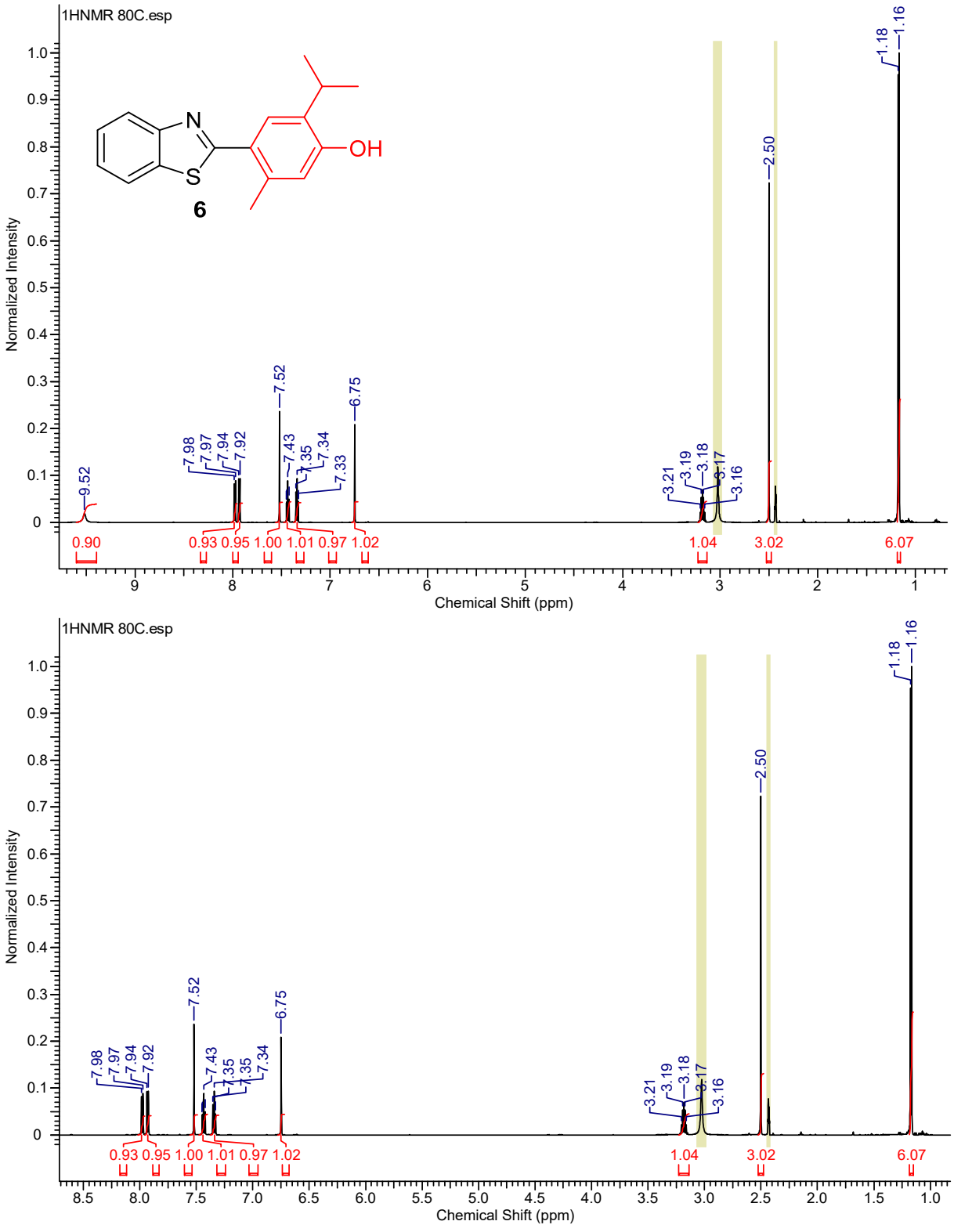


Figure S26 ^{13}C-NMR spectrum of **6** - DMSO-d$_6$, 80 ºC, 150 MHz

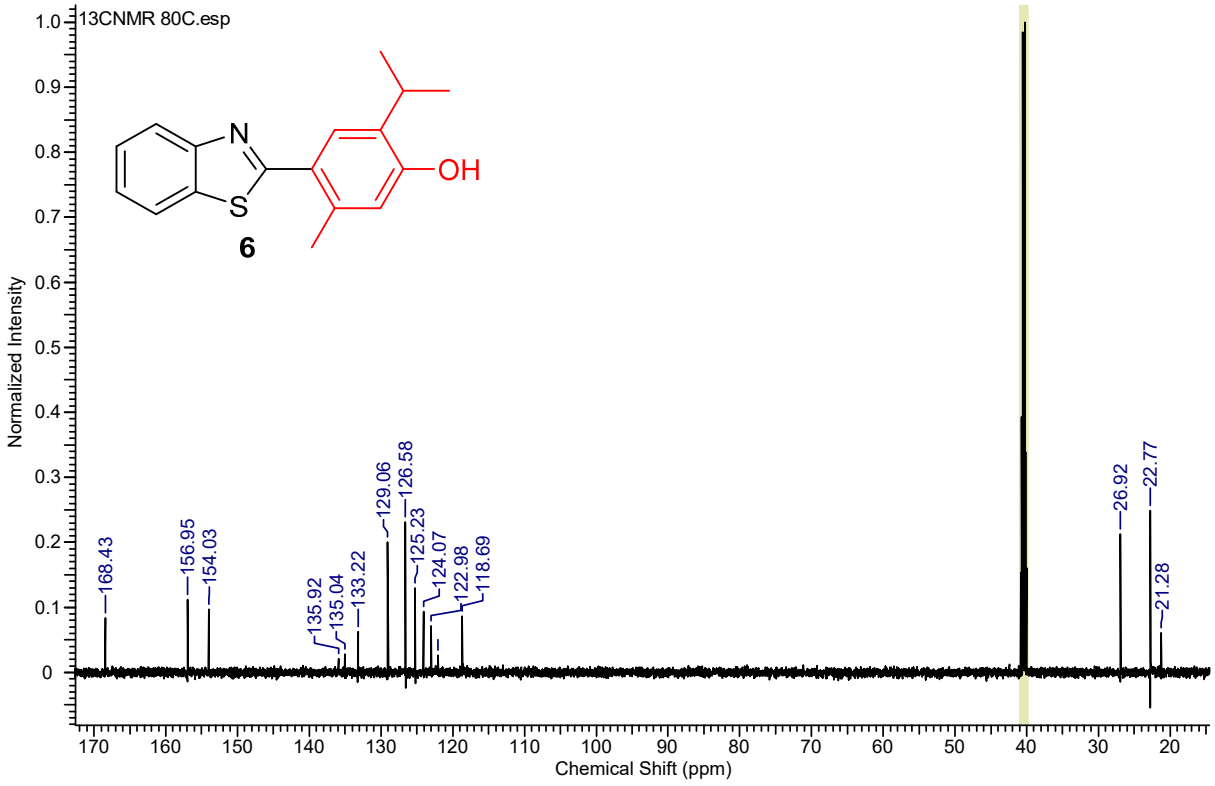


Figure S27 FT-IR spectrum of compound **6**, KBr tablet, cm^{-1}

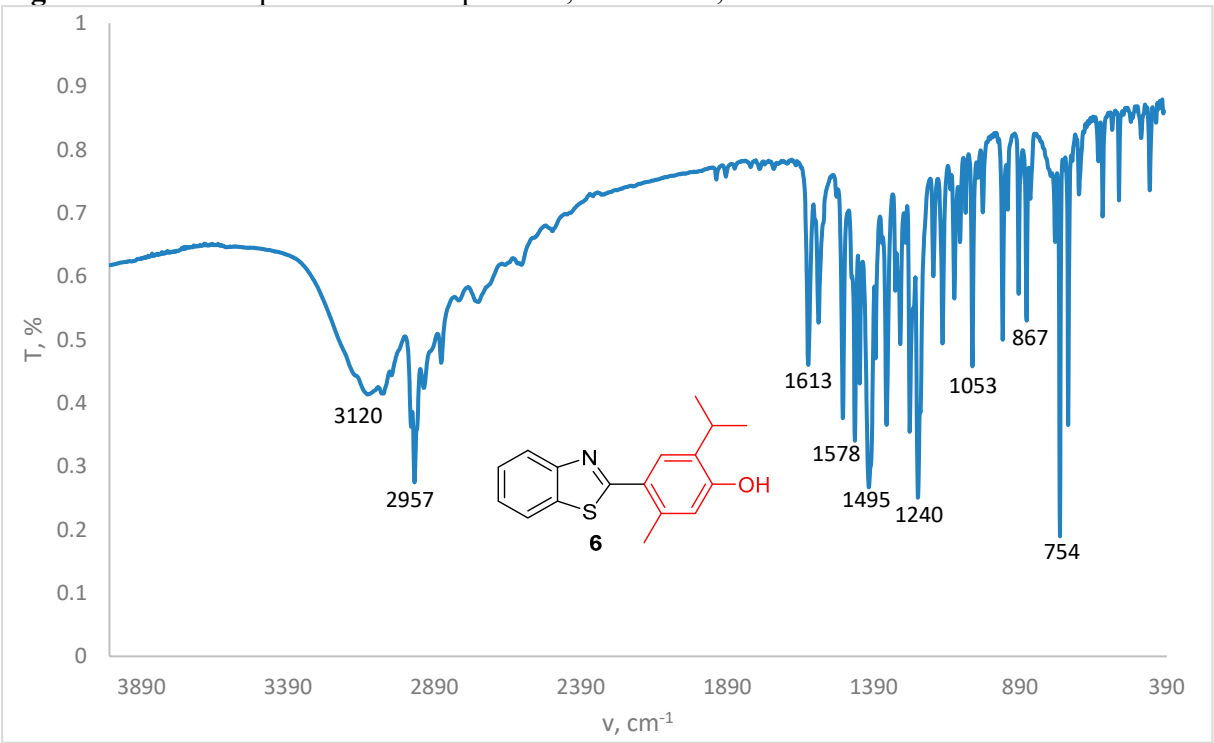


Figure S28 ESI-HRMS spectrum of compound **6**

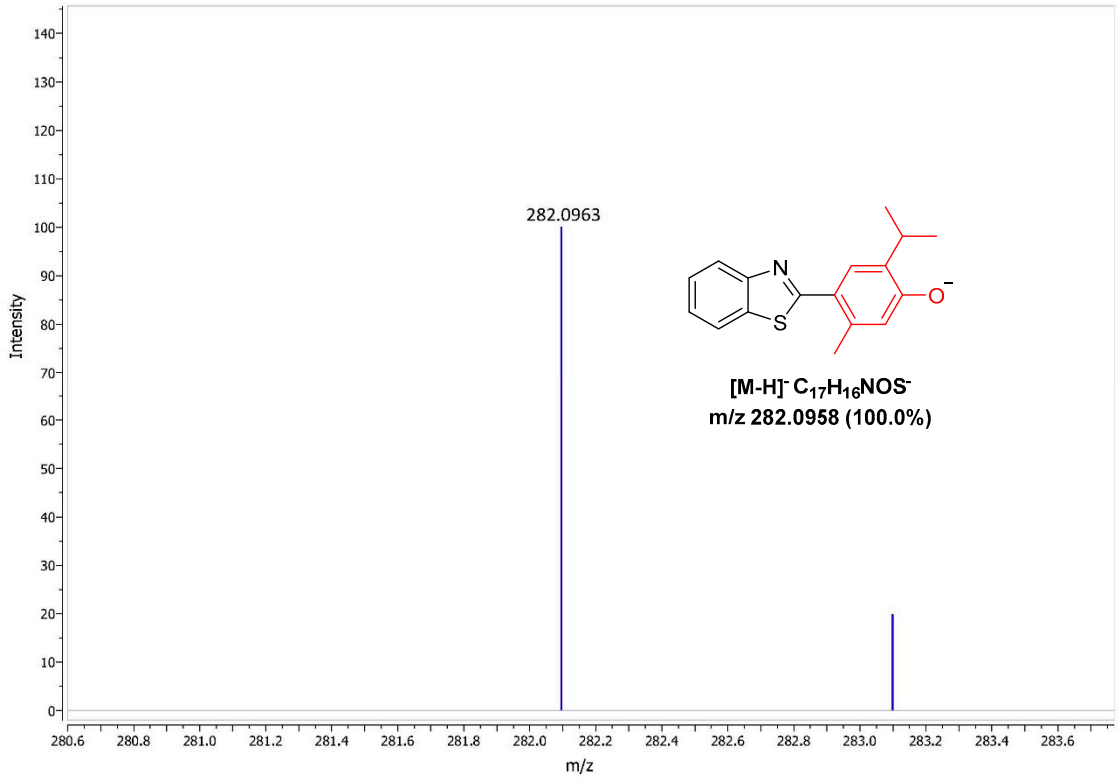
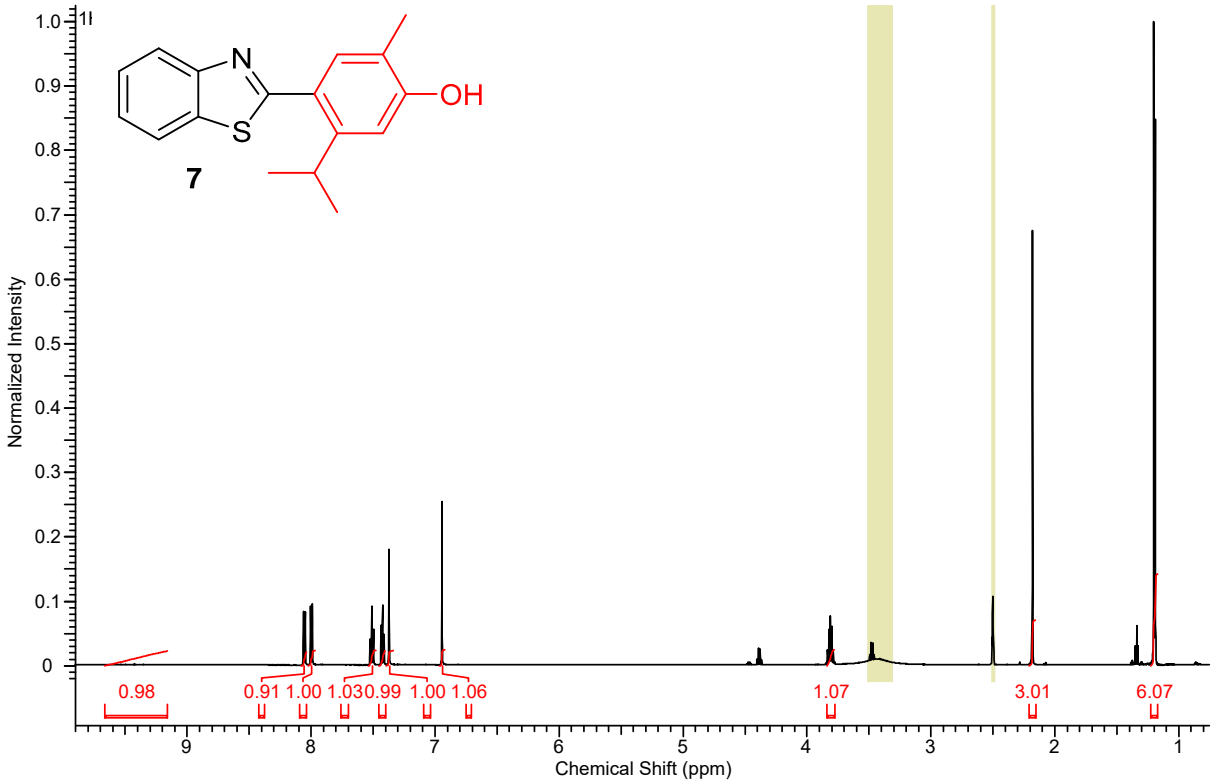


Figure S29 ^{1}H-NMR spectrum of **7** - DMSO-d$_6$, 80 °C, 600 MHz



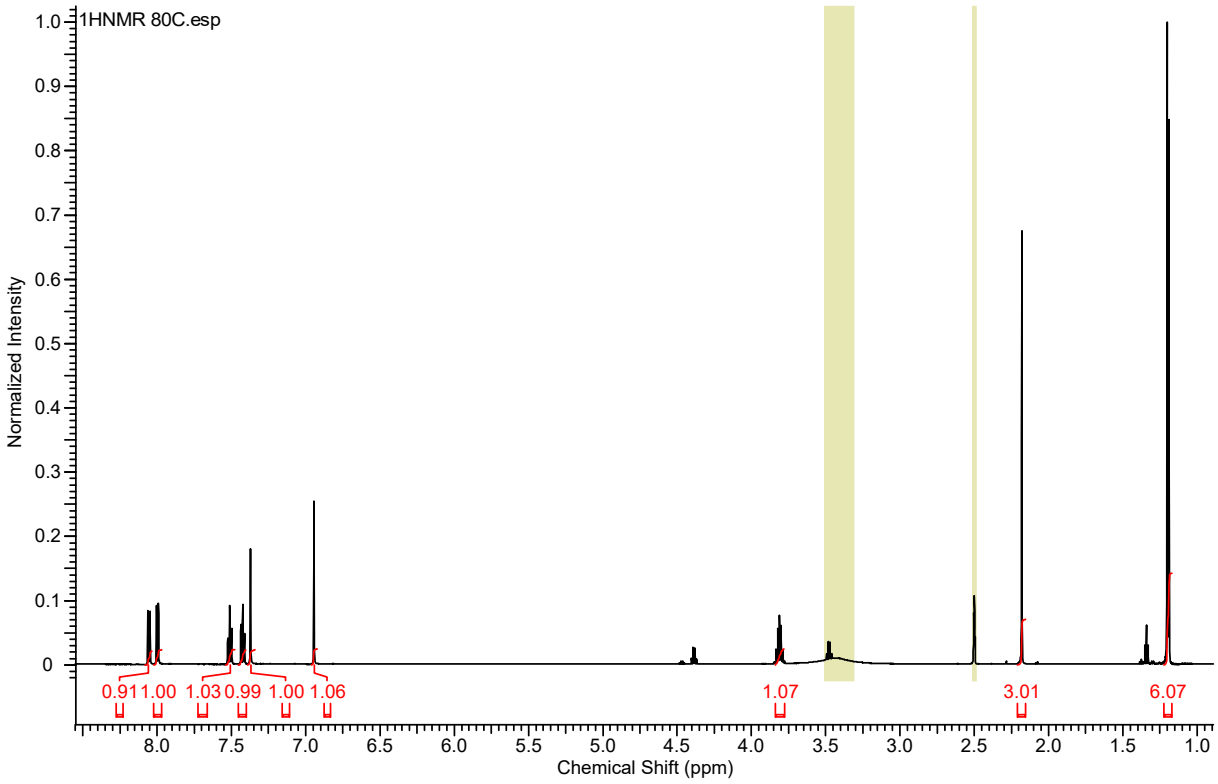


Figure S30 ^{13}C-NMR spectrum of **7** - DMSO-d$_6$, 80 ºC, 150 MHz

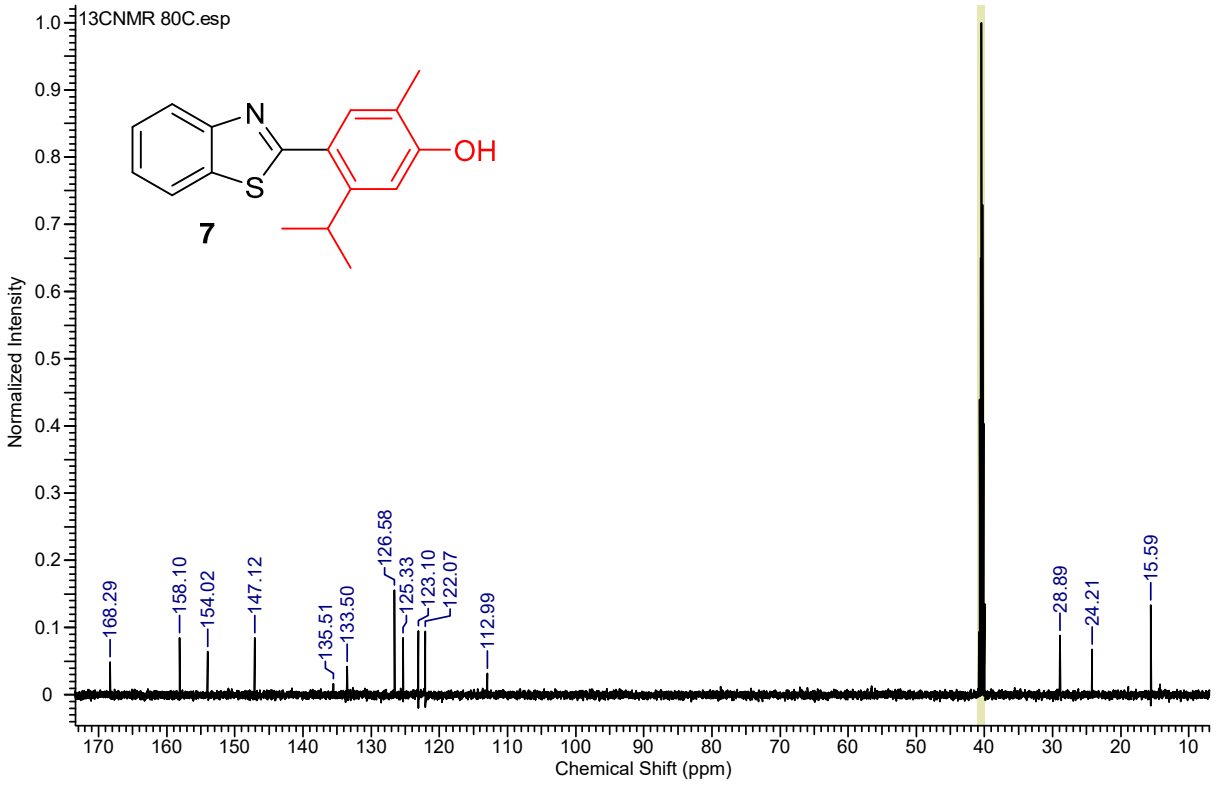


Figure S31 FT-IR spectrum of compound **7**, KBr tablet, cm^{-1}

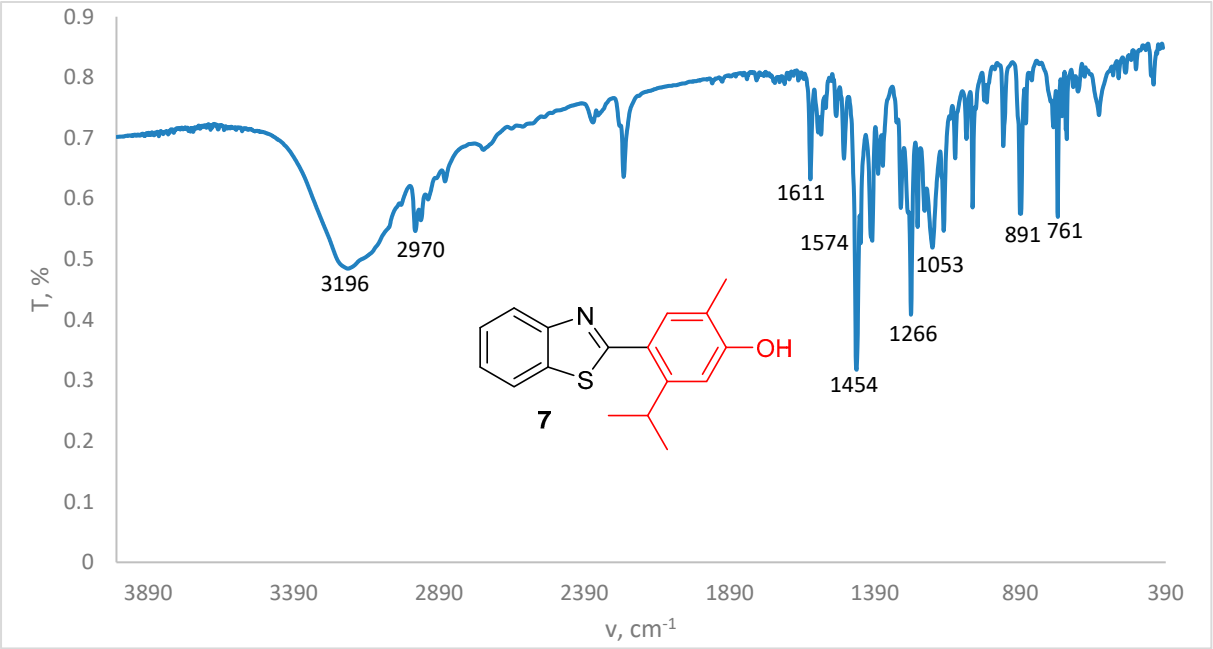


Figure S32 ESI-HRMS spectrum of compound **7**

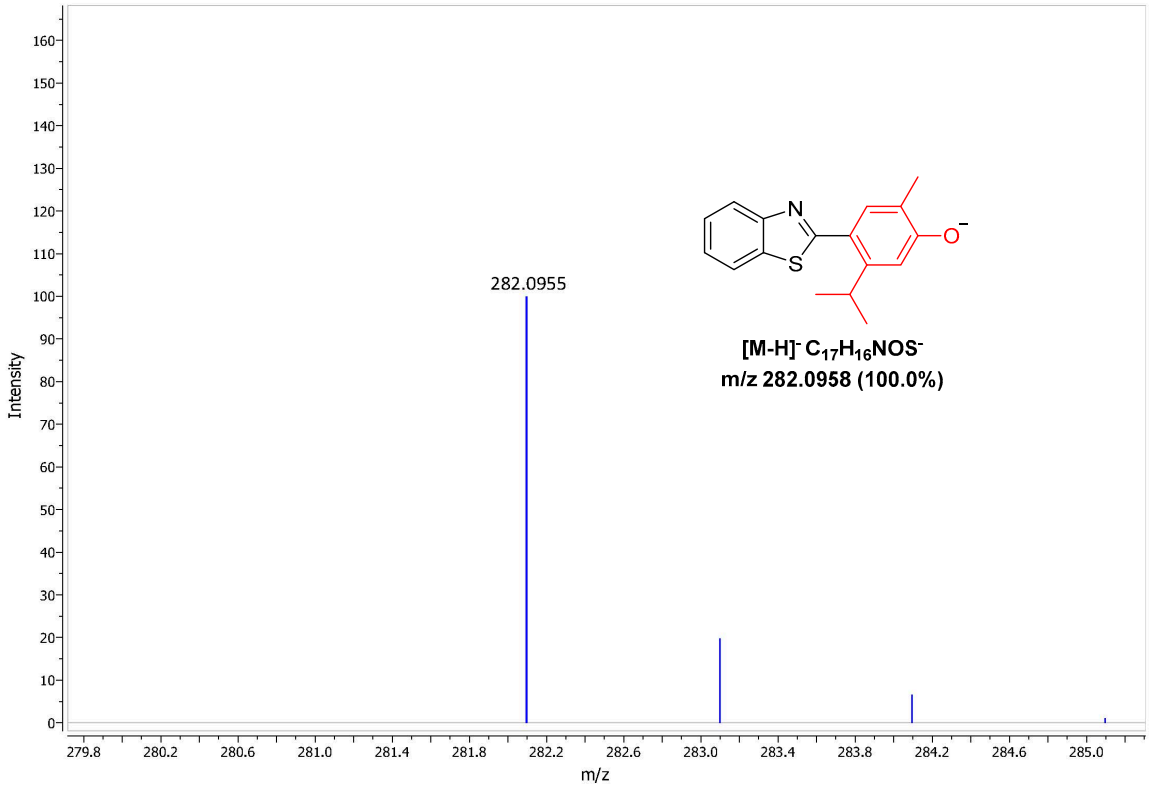


Figure S33. GC-MS/MS analysis - full scan 25-500 m/z, dwell time: 0.2 sec

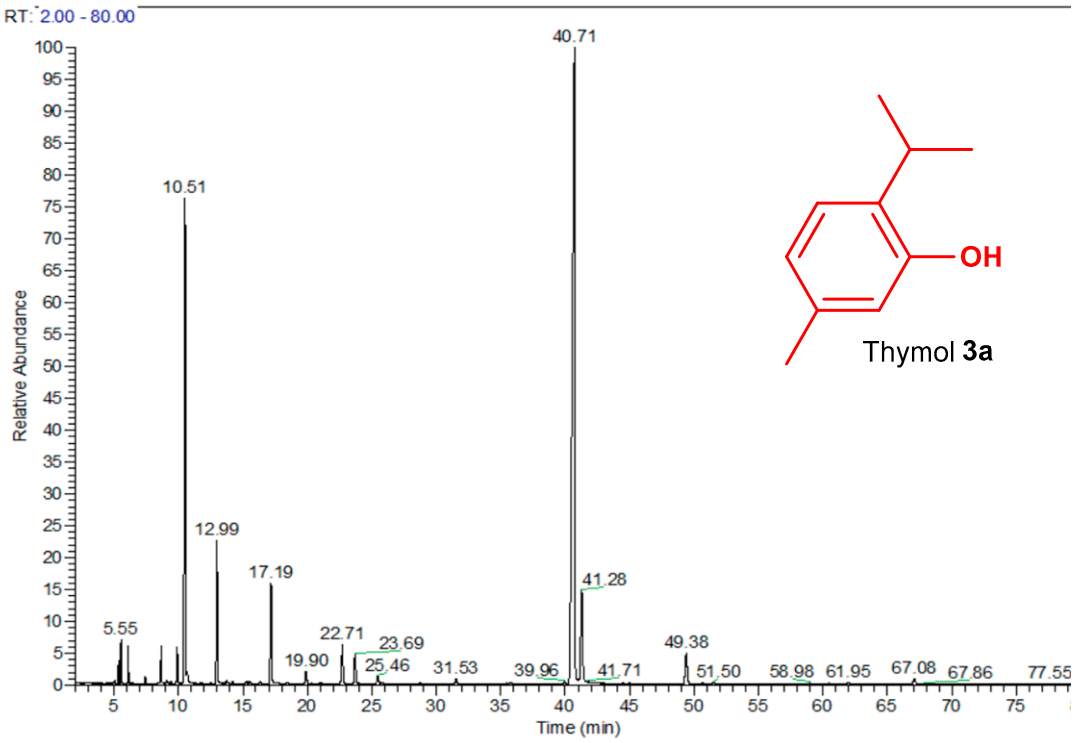


Table S1. Component composition of thyme essential oil (*Thymus vulgaris*) obtained by GC-MS/MS analysis

Apex RT	Compound	RI	Area	Area, %
5.36	*α*-Thujene	929	104434816	0.45
5.55	*α*-Pinene	929	202877822	0.87
6.11	Camphene	952	194880519	0.84
7.43	Sabinene	974	39760315	0.17
8.65	*β*-Myrcene	991	248247929	1.07
9.10	*α*-Phellandrene	1005	23801823	0.10
9.42	3-Carene	1011	13420274	0.06
9.90	*α*-Terpinene	1017	259788308	1.12
10.51	p-Cymene	1025	4084754060	17.61
10.68	Limonene	1030	137940130	0.59
12.99	*γ*-Terpinene	1060	1270342619	5.48
13.74	4-Thujanol	1075	35007920	0.15
15.29	Terpinolene	1088	18834109	0.08
17.19	Linalool	1099	1086102774	4.68
19.90	Camphor	1145	137948452	0.59
22.71	endo-Borneol	1167	475572950	2.05

23.69	Terpinen-4-ol	1177	351648334	1.52
25.46	α-Terpineol	1189	90410362	0.39
31.53	Thymol methyl ether	1235	62694657	0.27
40.71	**Thymol**	**1291**	**12421001540**	**53.54**
41.28	Carvacrol	1299	1392669846	6.00
49.39	Caryophyllene	1419	463930841	2.00
67.08	Caryophyllene oxide	1581	82353730	0.35

Figure S34. GC-MS/MS analysis - full scan 25-500 m/z, dwell time: 0.2 sec

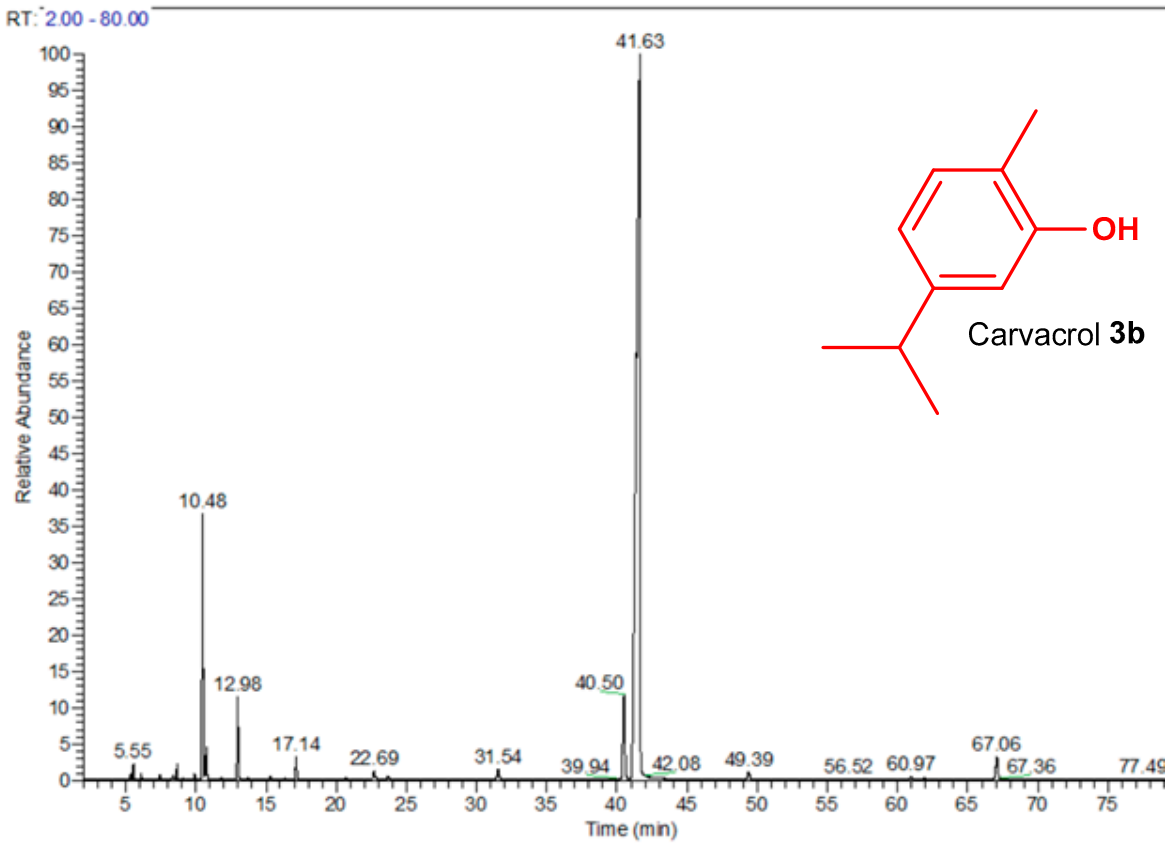


Table S2. Component composition of oregano essential oil (*Origanum vulgare*) obtained by GC-MS/MS analysis

Apex RT	Compound	RI	Area	Area, %
5.36	α-Thujene	5.44	24699853	0.10
5.55	α-Pinene	5.65	68092605	0.26
6.11	Camphene	6.23	30148082	0.12
7.43	Sabinene	7.56	30041469	0.12

8.38	1-Octen-3-ol	8.54	35187901	0.14
8.65	*β*-Myrcene	8.82	94947297	0.37
9.07	Pseudolimonen	9.2	7639584	0.03
9.89	*α*-Terpinene	10	38440427	0.15
10.48	*p*-Cymene	10.6	2067346229	8.01
10.75	Limonene	10.95	323258829	1.25
11.83	*β*-cis-Ocimene	11.97	10214706	0.04
12.98	*γ*-Terpinene	13.2	712755284	2.76
13.74	4-Thujanol	13.99	14044344	0.05
15.29	Terpinolene	15.42	25147367	0.10
17.14	Linalool	17.37	221496870	0.86
22.69	endo-Borneol	22.89	96326065	0.37
23.68	Terpinen-4-ol	23.89	33753936	0.13
31.54	Thymol methyl ether	31.77	134547185	0.52
40.50	Thymol	40.88	1246171282	4.83
41.63	**Carvacrol**	**42.32**	**20072626547**	**77.78**
49.39	Caryophyllene	49.63	110131374	0.43
60.97	*β*-Bisabolene	61.17	31943716	0.12
61.93	*β*-Cadinene	62.14	17936082	0.07
67.06	Caryophyllene oxide	67.39	359908069	1.39