



## Supporting Information

for

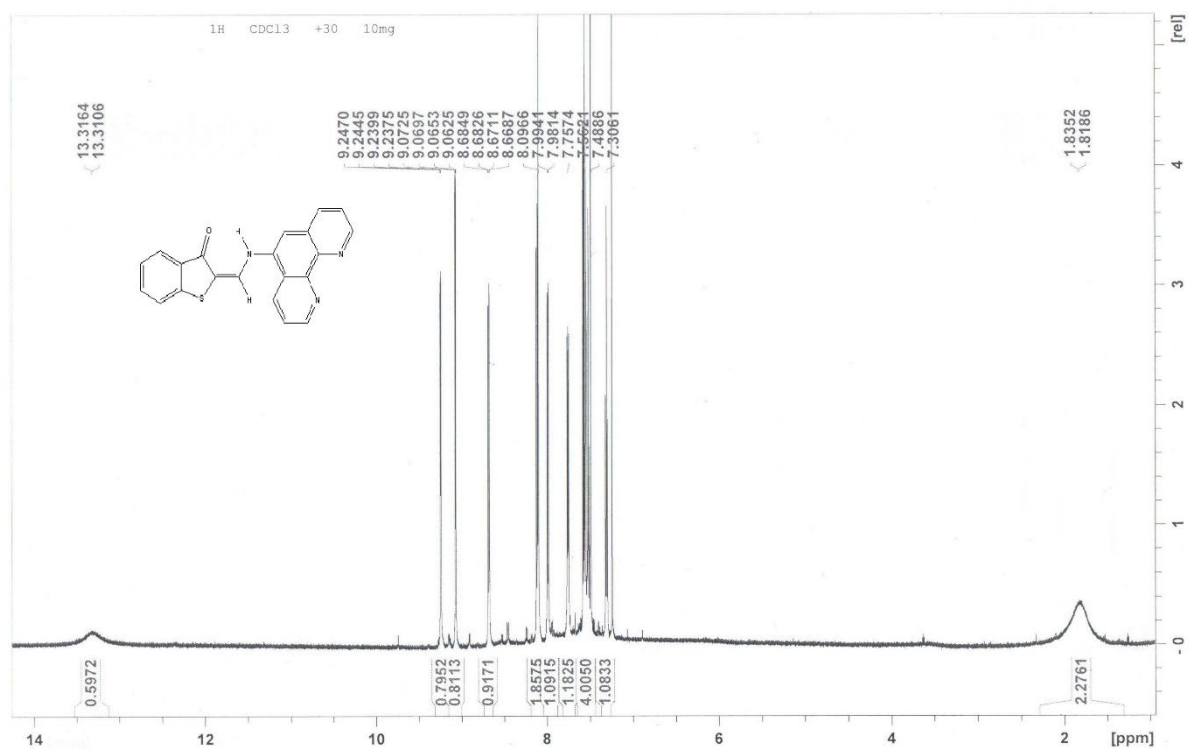
### **Synthesis of photo- and ionochromic N-acylated 2-(aminomethylene)benzo[*b*]thiophene-3(2*H*)-ones with a terminal phenanthroline group**

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### **$^1\text{H}$ and $^{13}\text{C}$ NMR, IR and HRMS spectra of all novel compounds**

**Figure S1:**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$ .



**Figure S2:**  $^1\text{H}$  NMR spectrum of compound **2a** in  $\text{CDCl}_3$ .

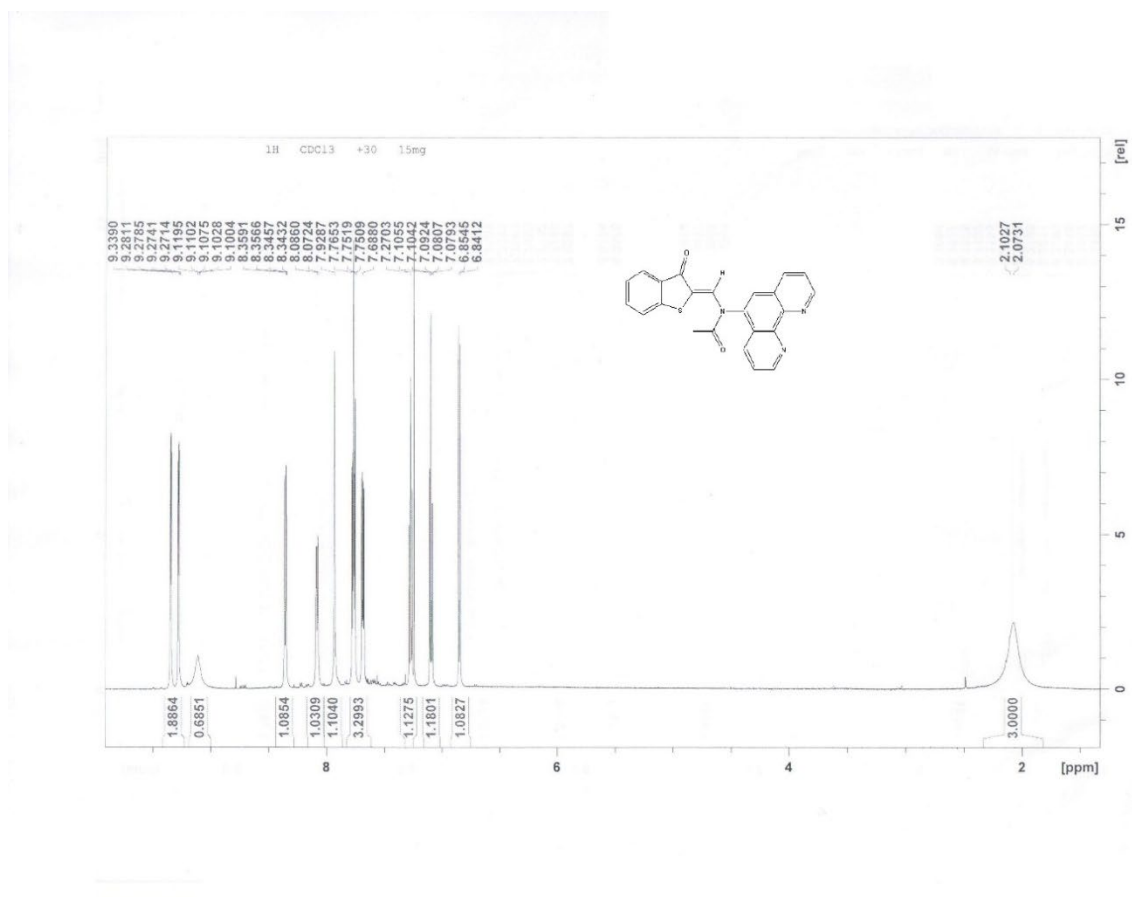


Figure S3:  $^1\text{H}$  NMR spectrum of compound **2b** in  $\text{CDCl}_3$ .

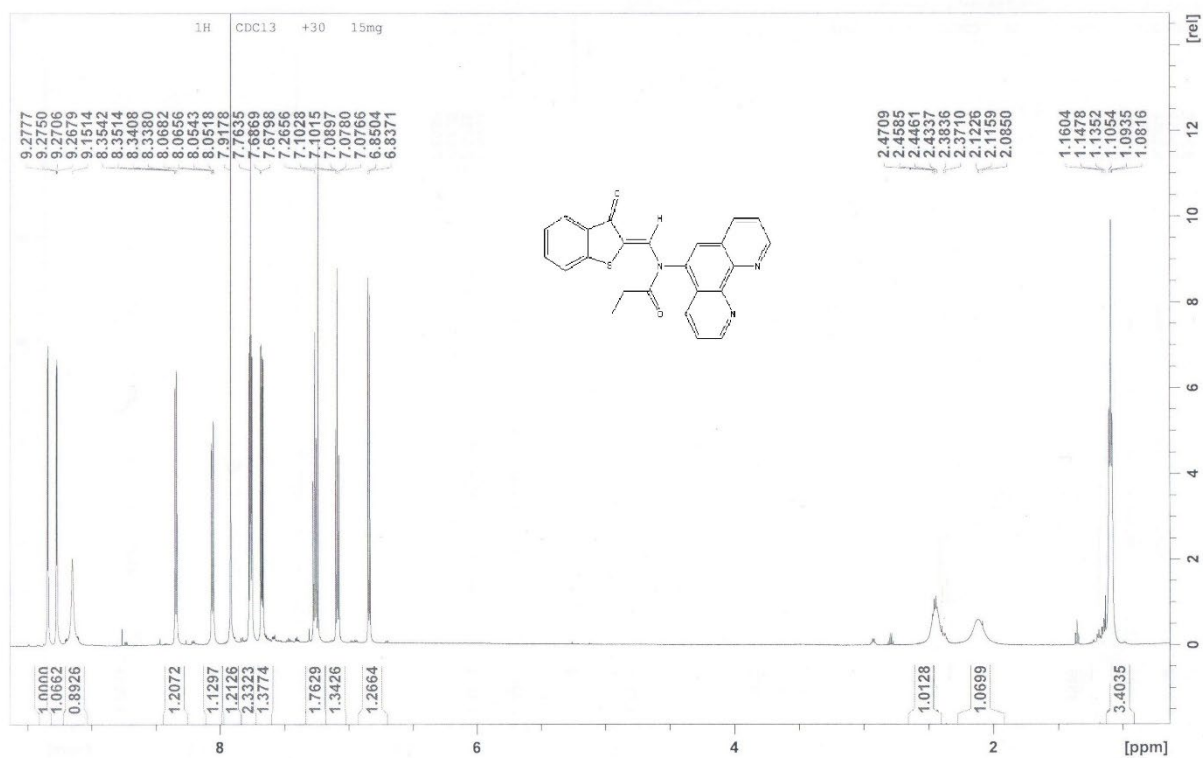


Figure S4:  $^1\text{H}$  NMR spectrum of compound **2c** in  $\text{CDCl}_3$ .

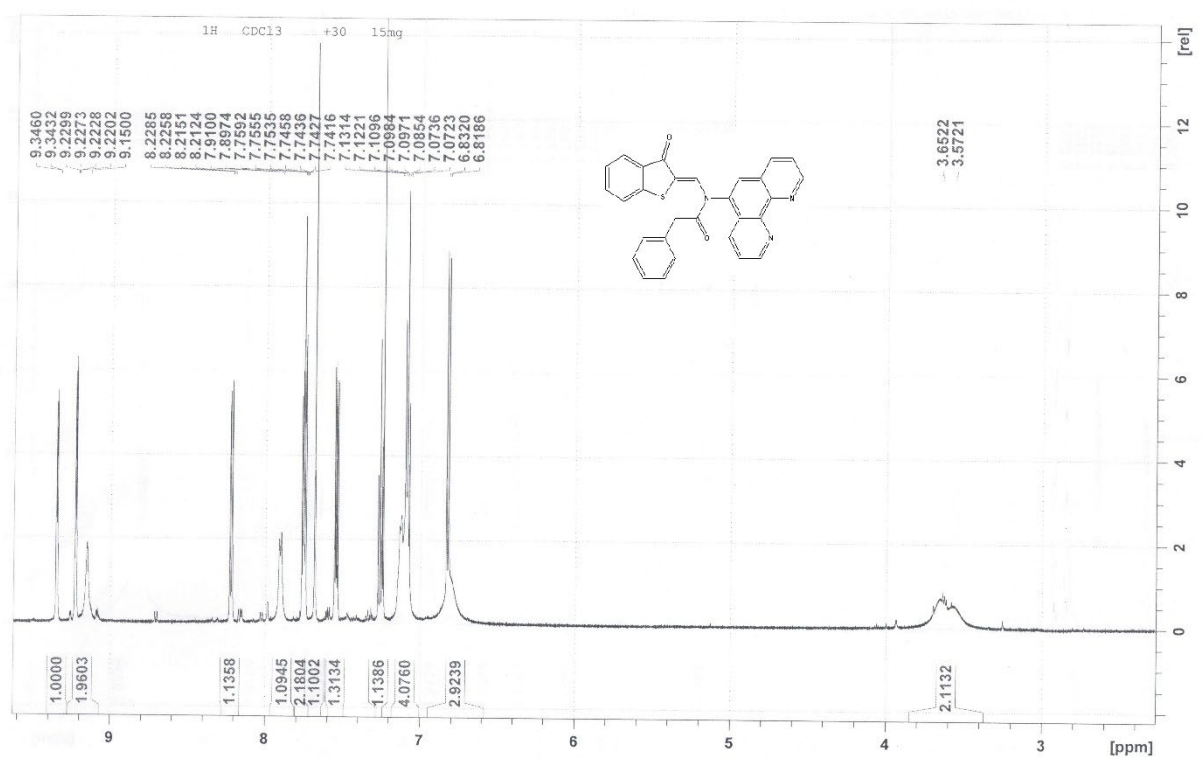


Figure S5:  $^1\text{H}$  NMR spectrum of compound **3a** in  $\text{CDCl}_3$ .

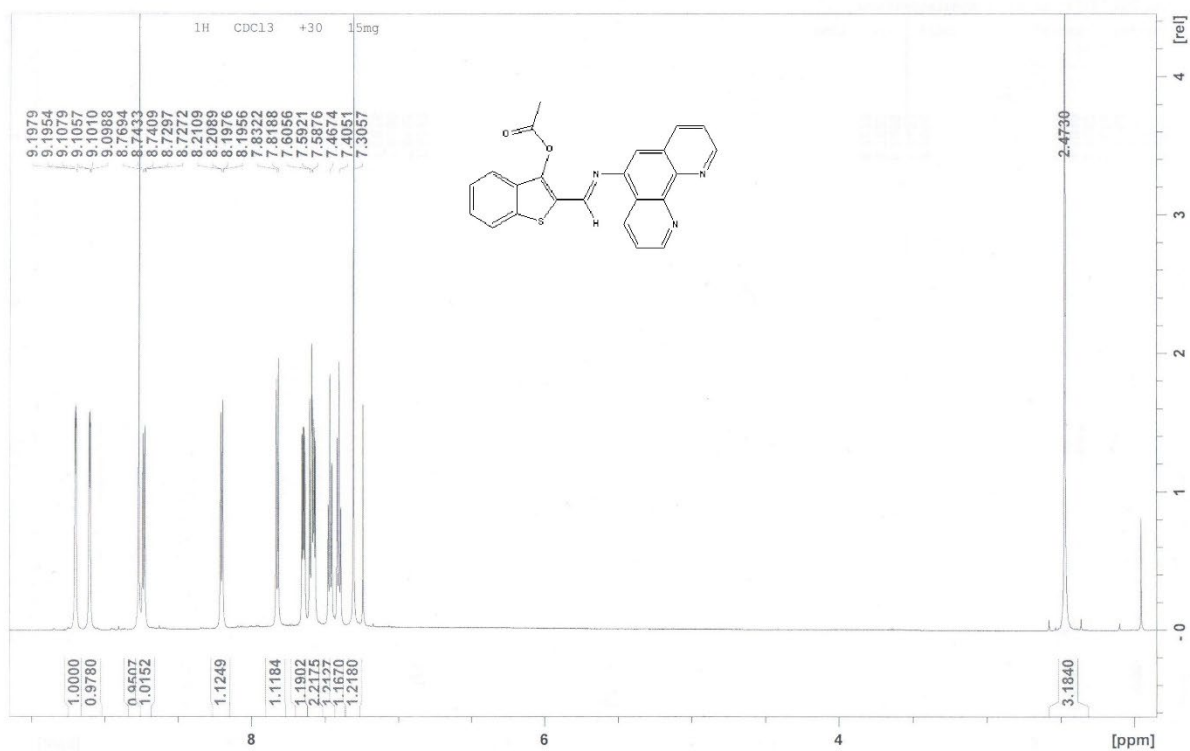
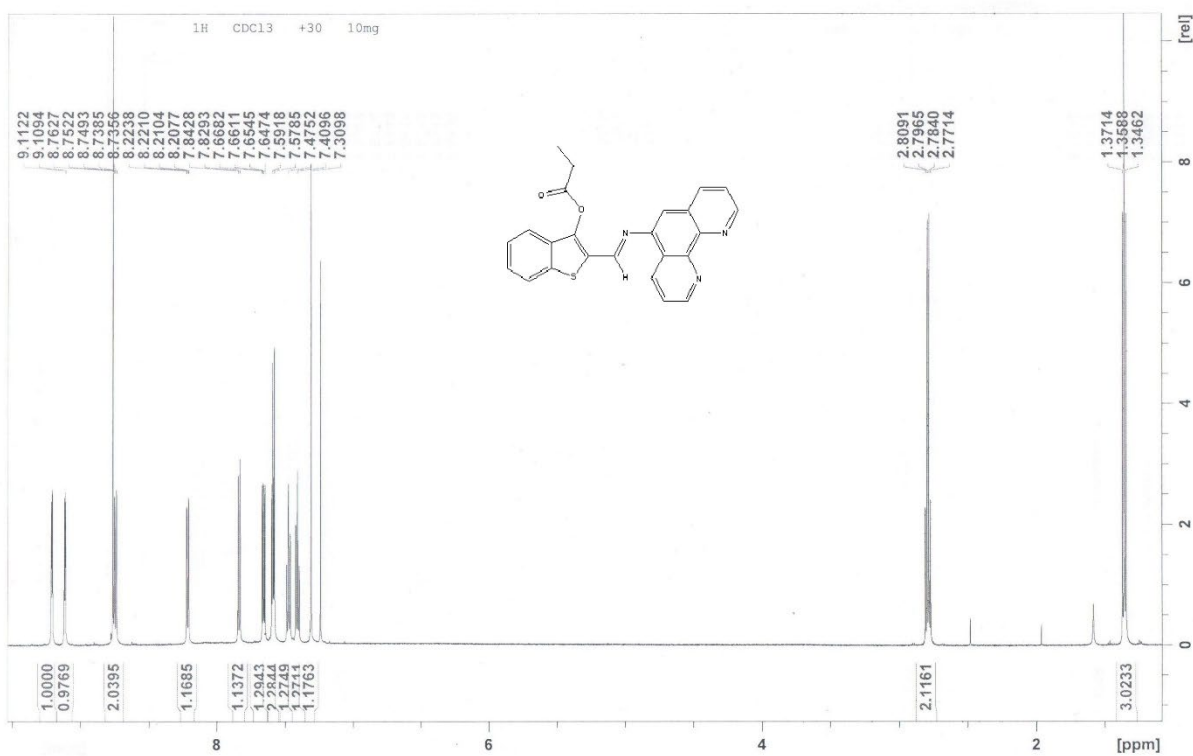
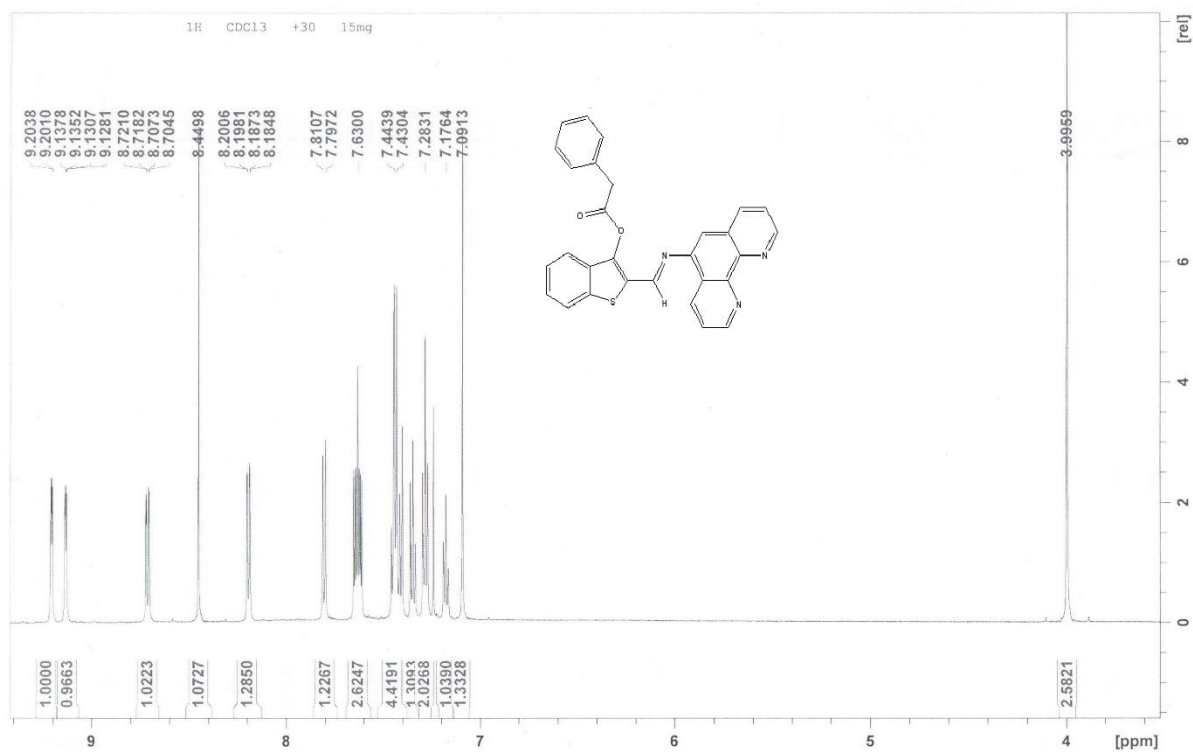


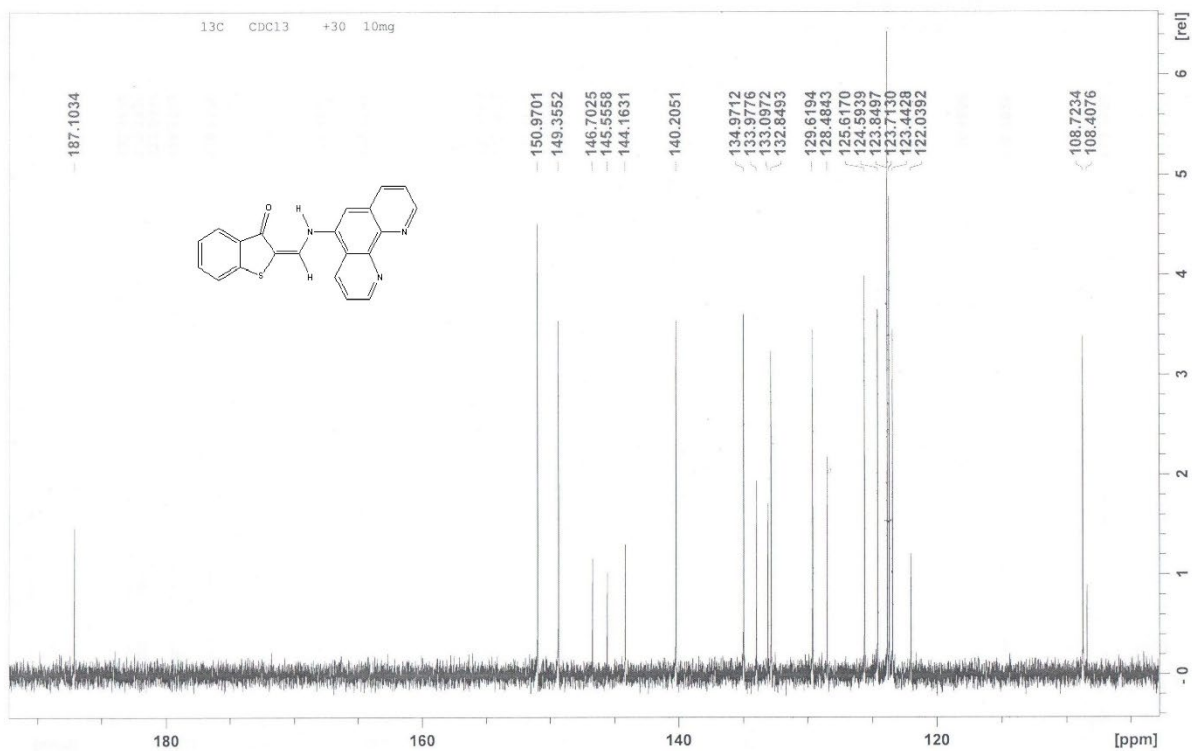
Figure S6:  $^1\text{H}$  NMR spectrum of compound **3b** in  $\text{CDCl}_3$ .



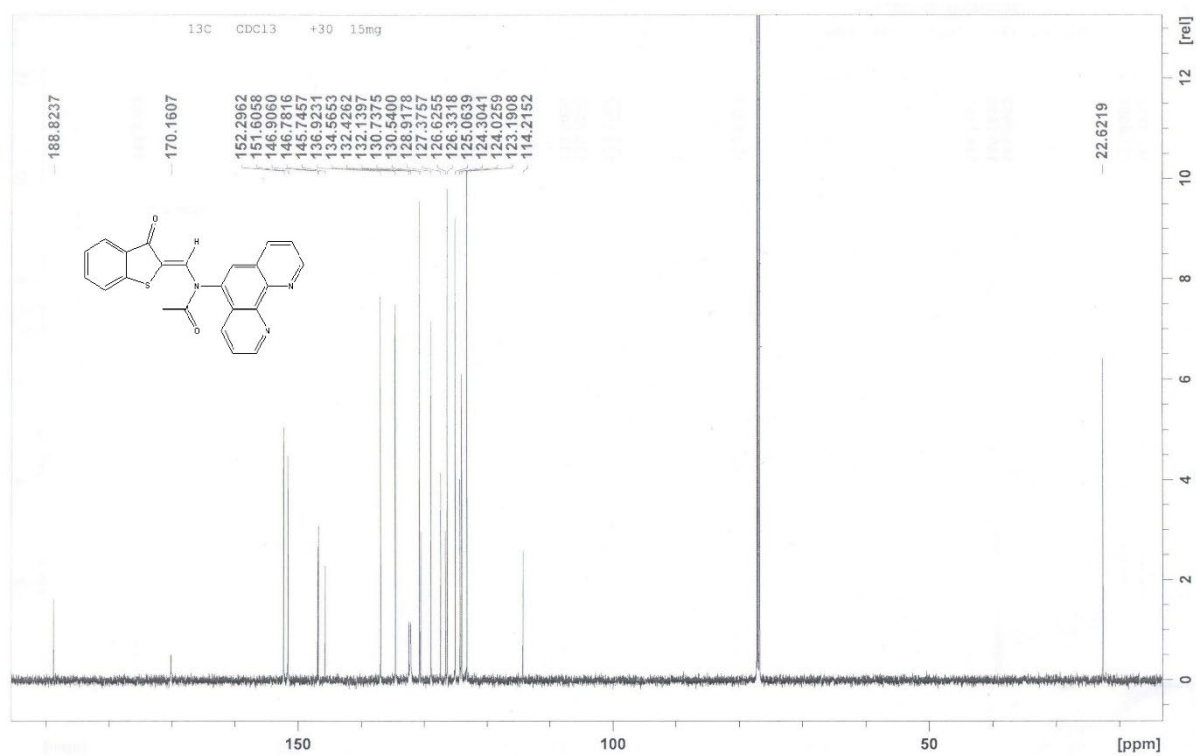
**Figure S7:**  $^1\text{H}$  NMR spectrum of compound **3c** in  $\text{CDCl}_3$ .



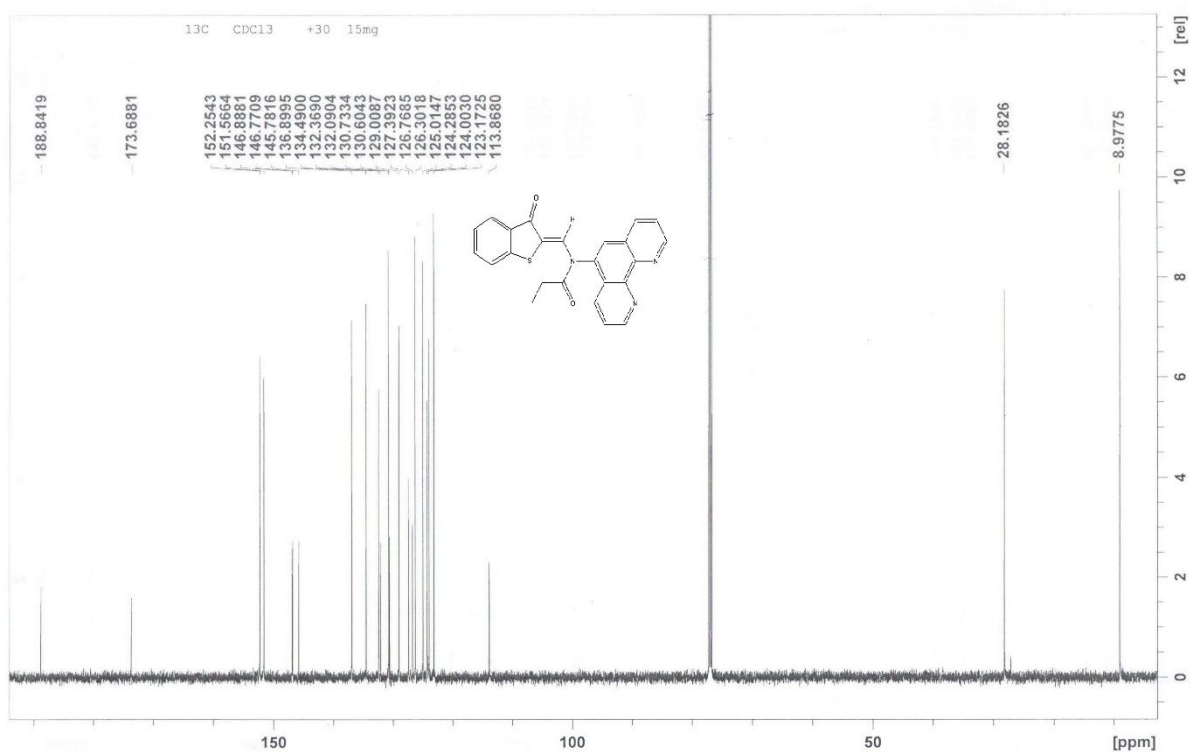
**Figure S8:**  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$ .



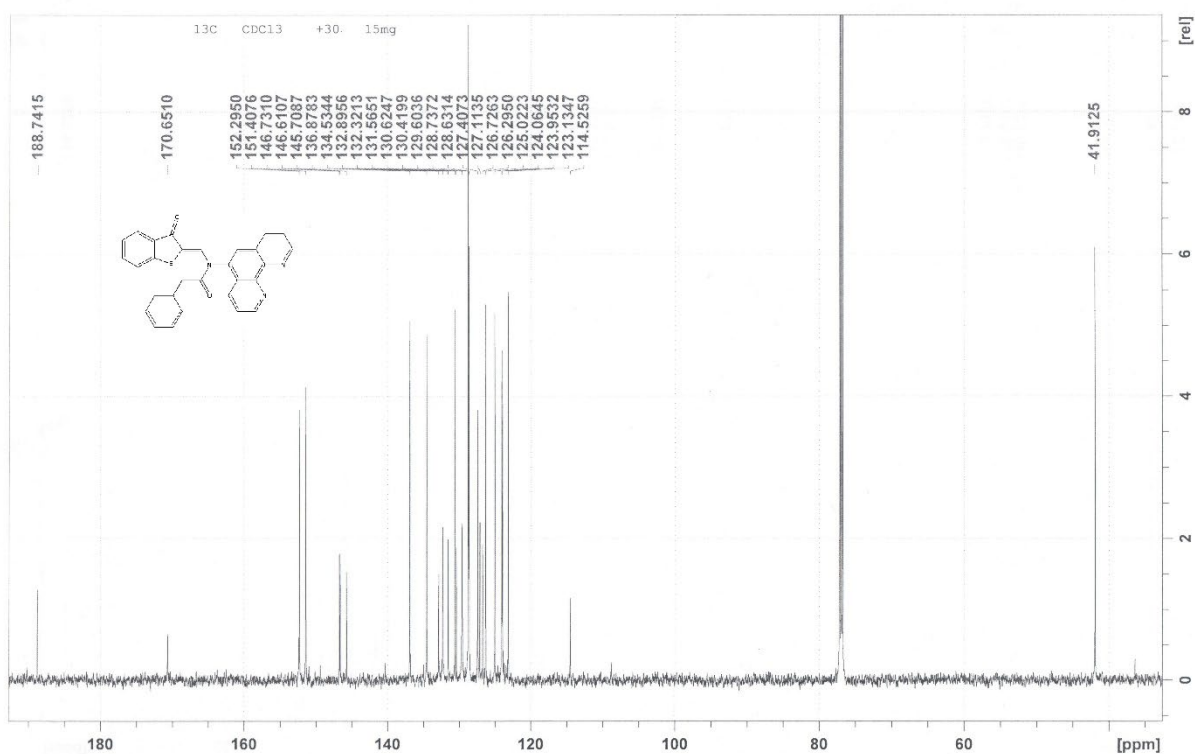
**Figure S9:**  $^{13}\text{C}$  NMR spectrum of compound **2a** in  $\text{CDCl}_3$ .



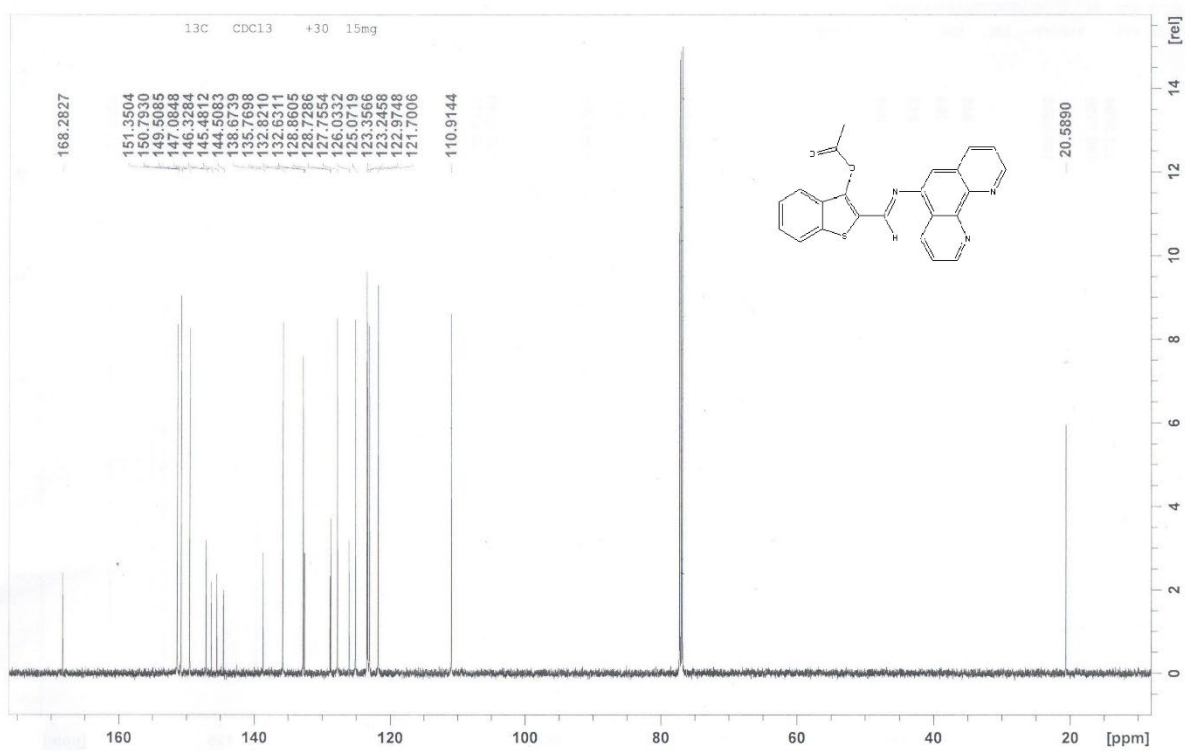
**Figure S10:**  $^{13}\text{C}$  NMR spectrum of compound **2b** in  $\text{CDCl}_3$ .



**Figure S11:**  $^{13}\text{C}$  NMR spectrum of compound **2c** in  $\text{CDCl}_3$ .

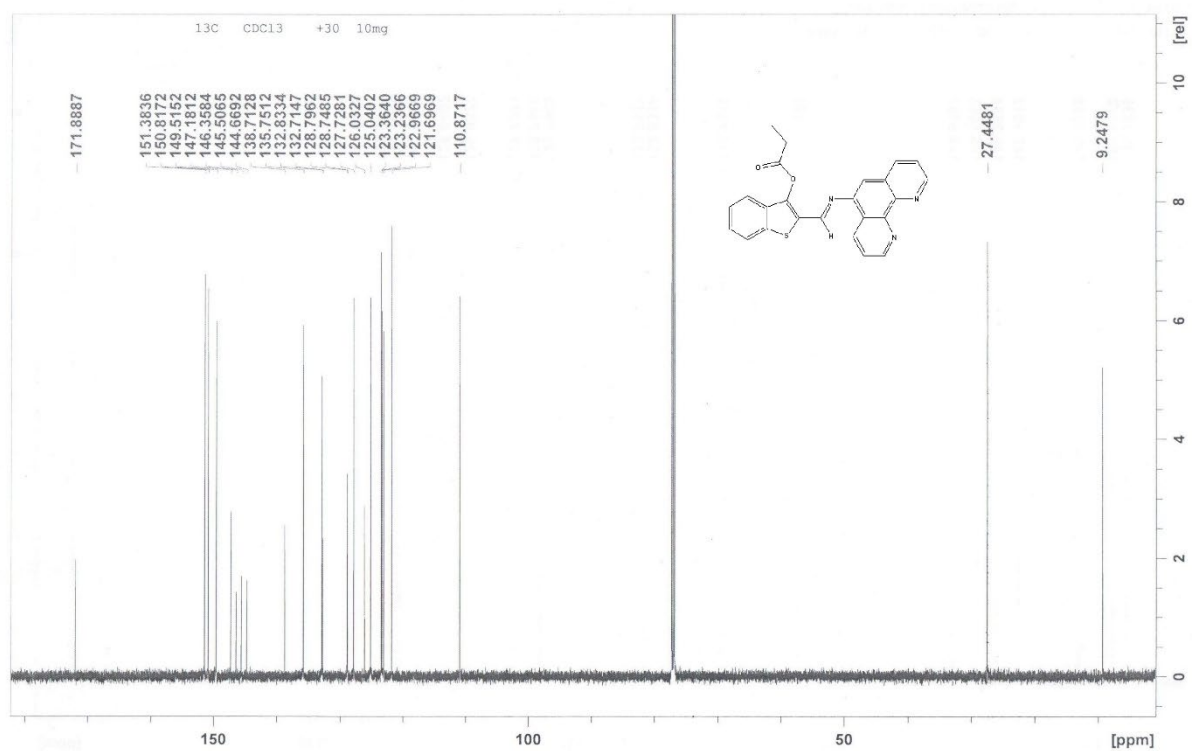


**Figure S12:**  $^{13}\text{C}$  NMR spectrum of compound **3a** in  $\text{CDCl}_3$ .





**Figure S13:**  $^{13}\text{C}$  NMR spectrum of compound **3b** in  $\text{CDCl}_3$ .



**Figure S14:**  $^{13}\text{C}$  NMR spectrum of compound **3c** in  $\text{CDCl}_3$ .

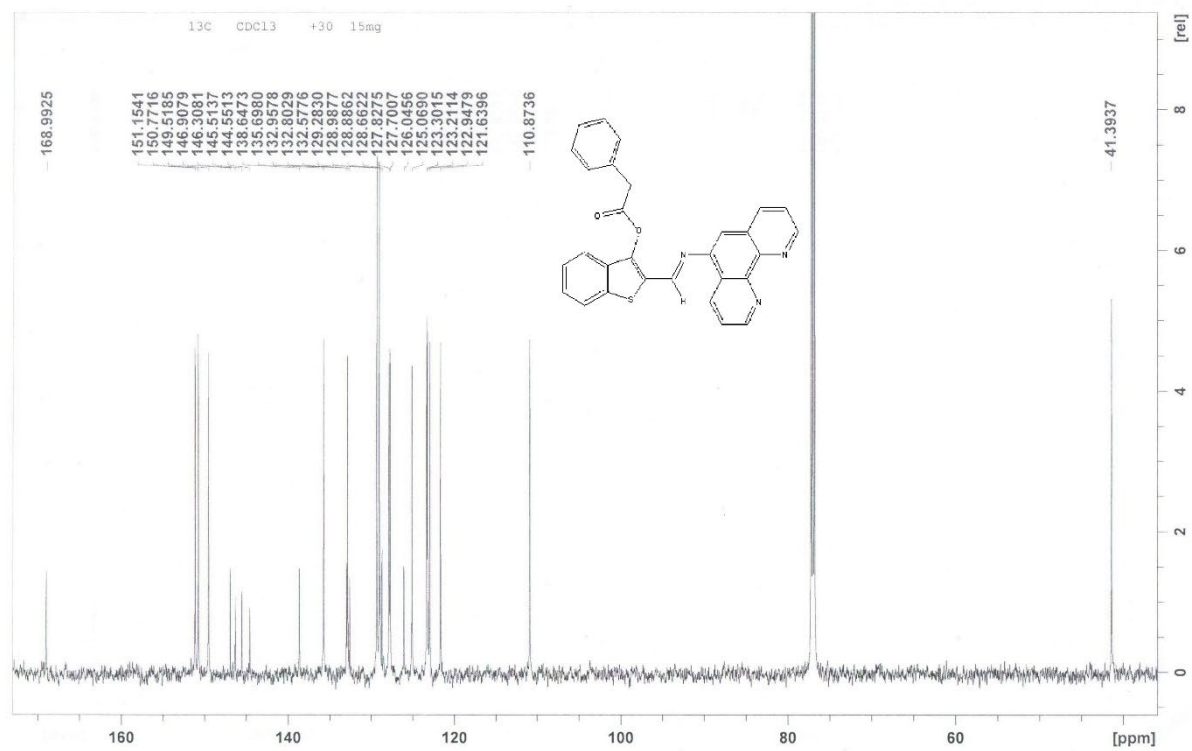




Figure S15: IR spectrum of compound 1.

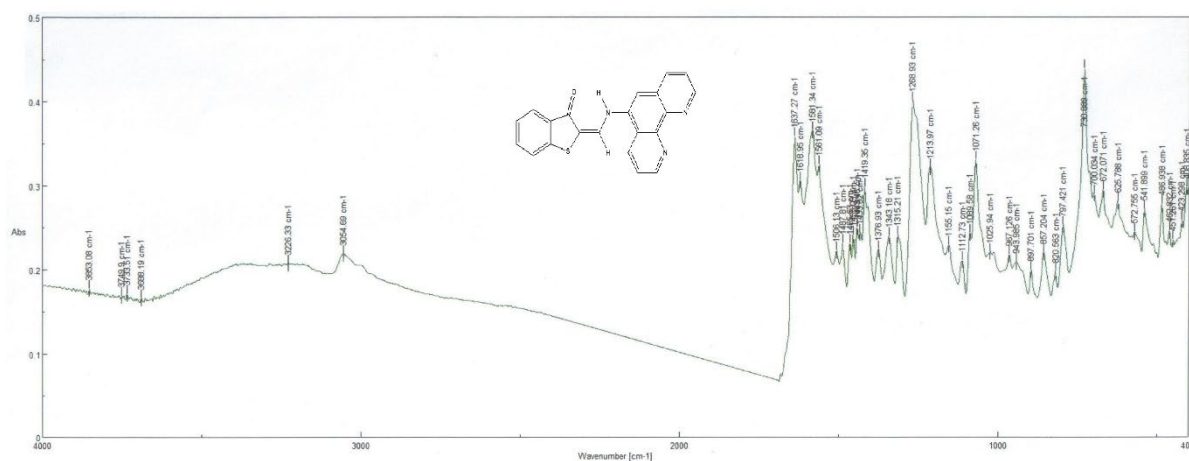


Figure S16: IR spectrum of compound 2a.

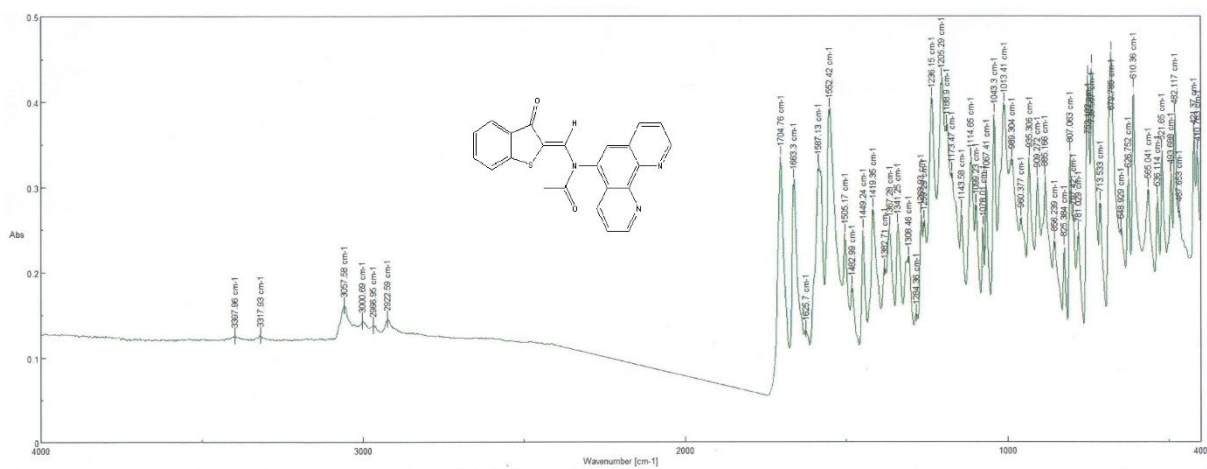


Figure S17: IR spectrum of compound 2b.

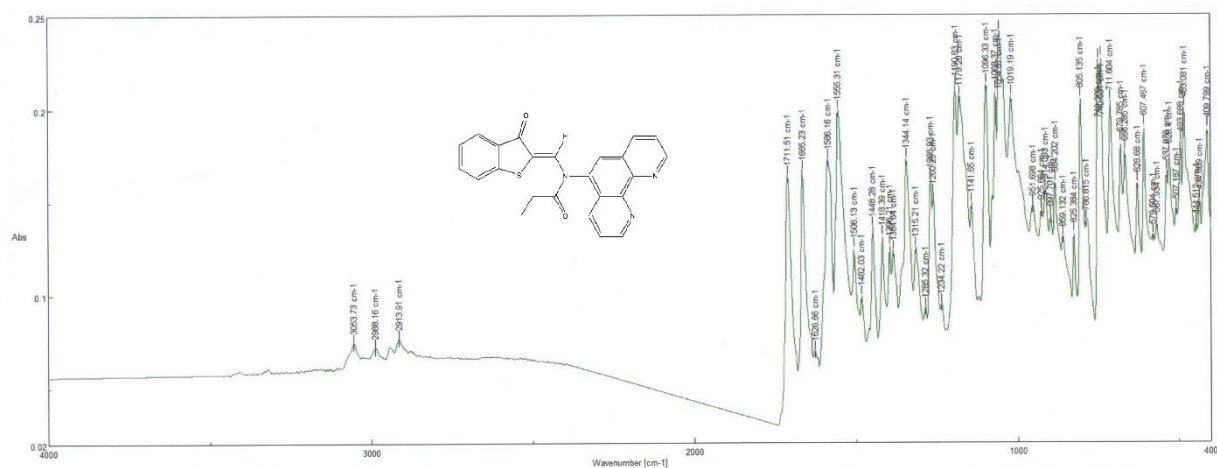


Figure S18: IR spectrum of compound 2c.

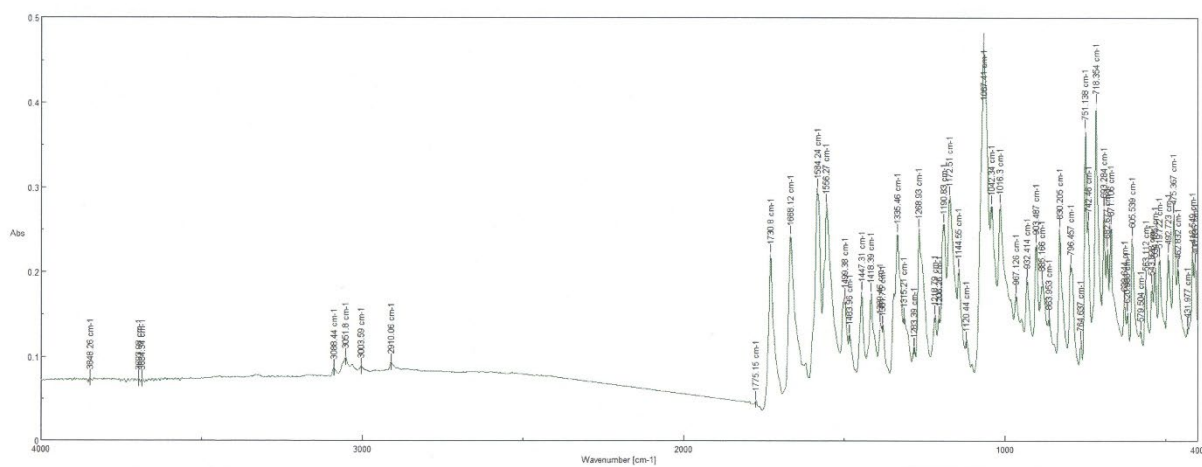


Figure S19: IR spectrum of compound 3a.

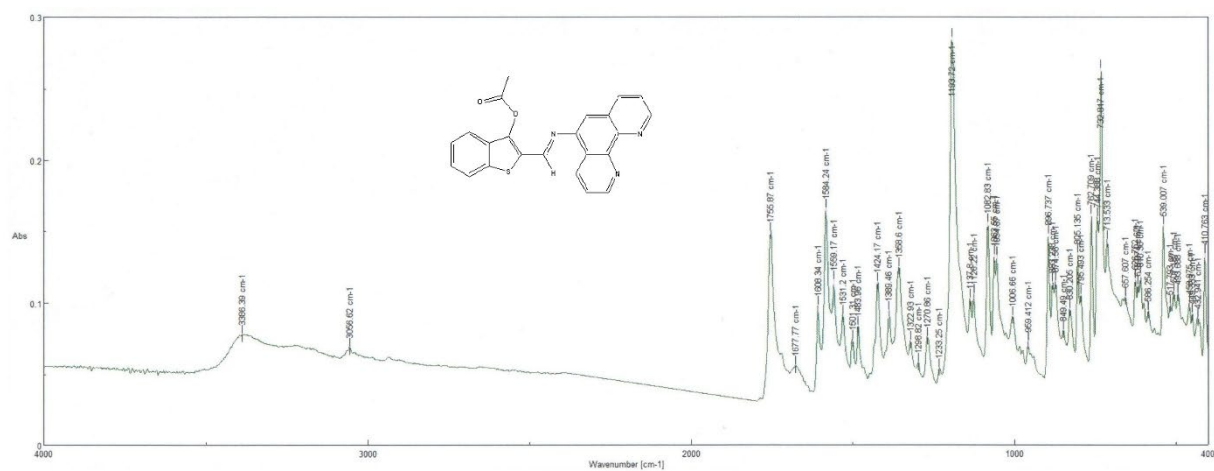


Figure S20: IR spectrum of compound 3b.

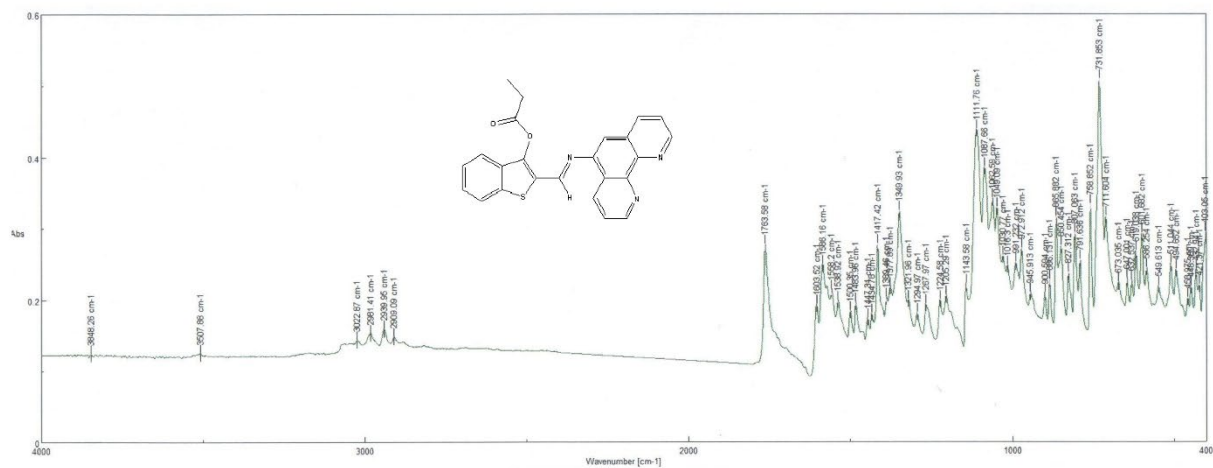
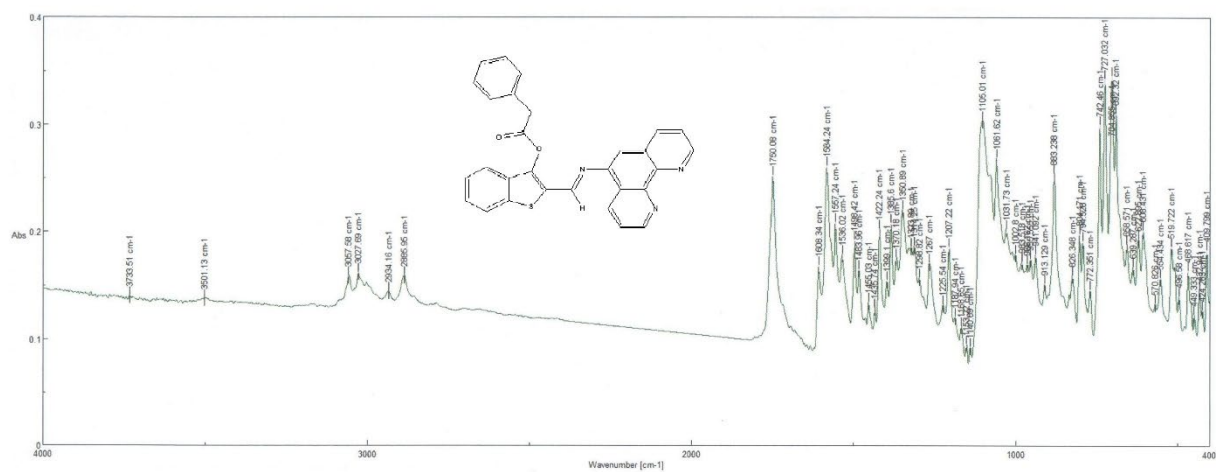
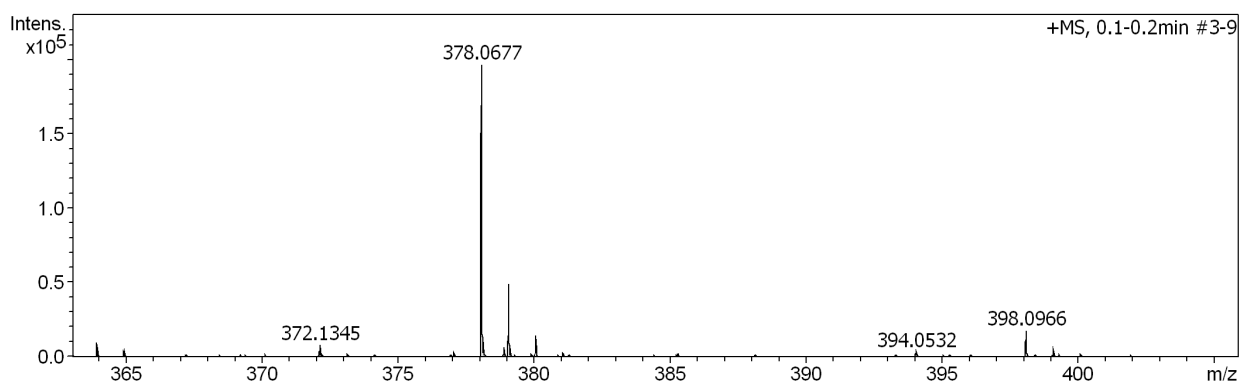
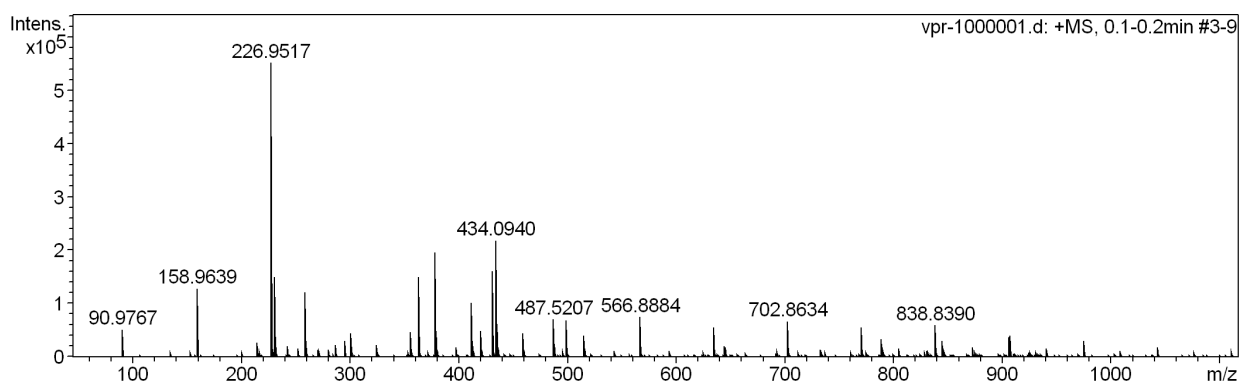
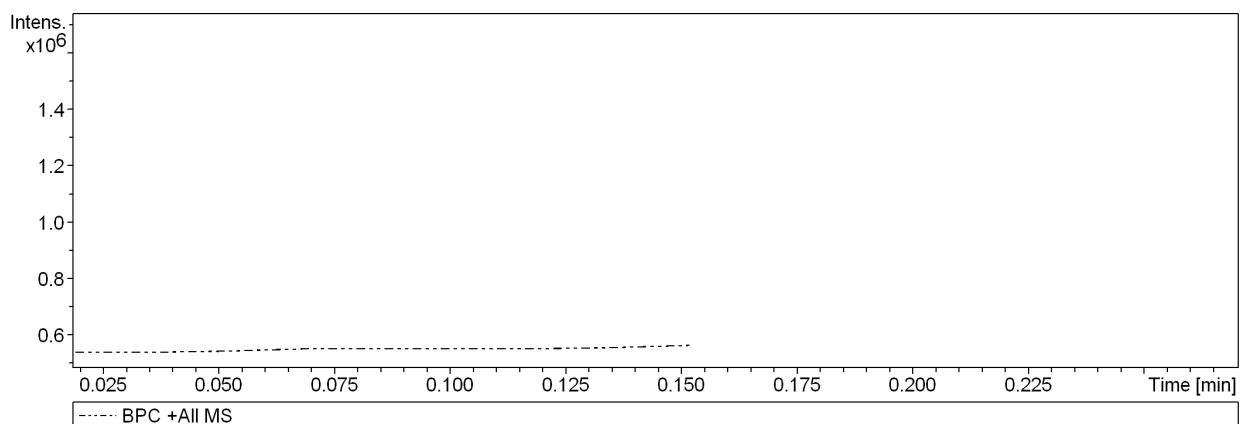


Figure S21: IR spectrum of compound 3c.



**Figure S22: Mass spectrum of compound 1.**

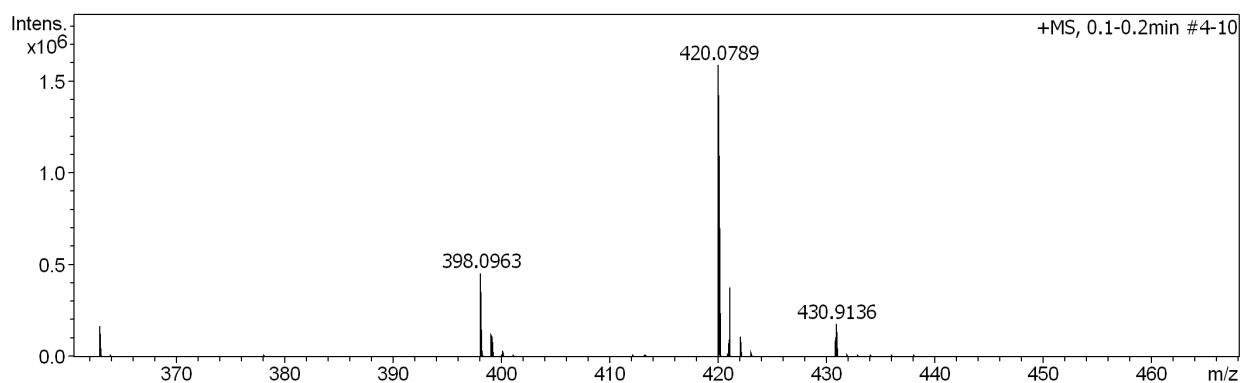
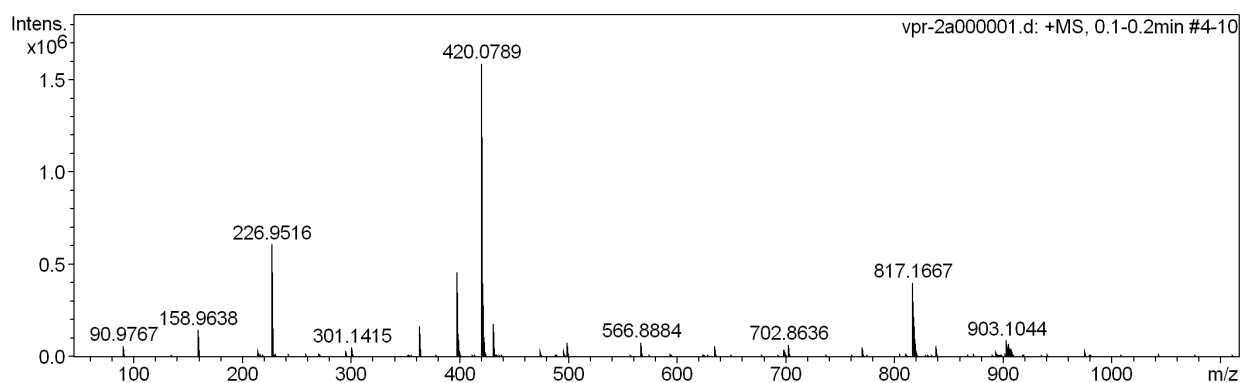
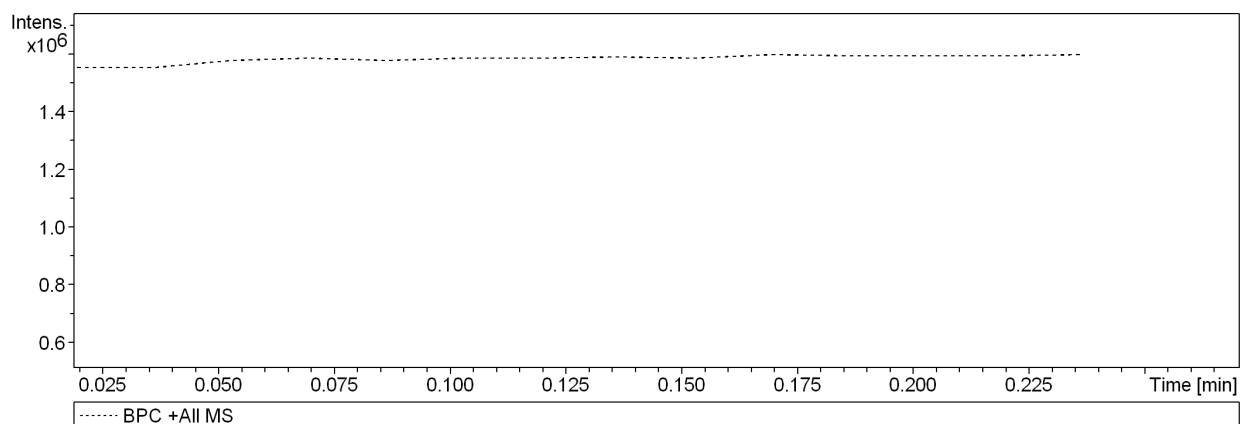


### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	
378.0677	1	C <sub>23</sub> H <sub>12</sub> N <sub>3</sub> OS	378.0696	4.8	10.7	1	100.00	19.5	even	ok
	1	C <sub>21</sub> H <sub>13</sub> N <sub>3</sub> NaOS	378.0672	-1.5	1.6	1	100.00	16.5	even	ok

**+MS, 0.1-0.2min #3-9**

**Figure S23: Mass spectrum of compound 2a.**

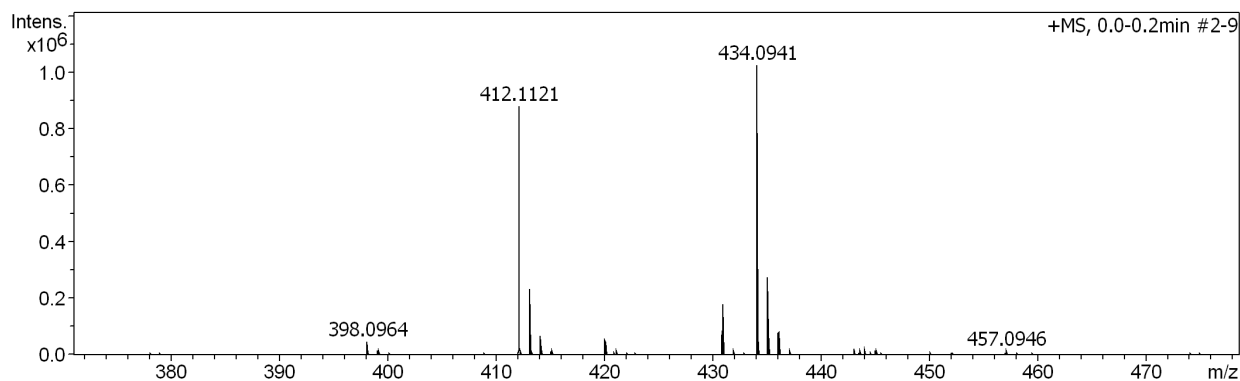
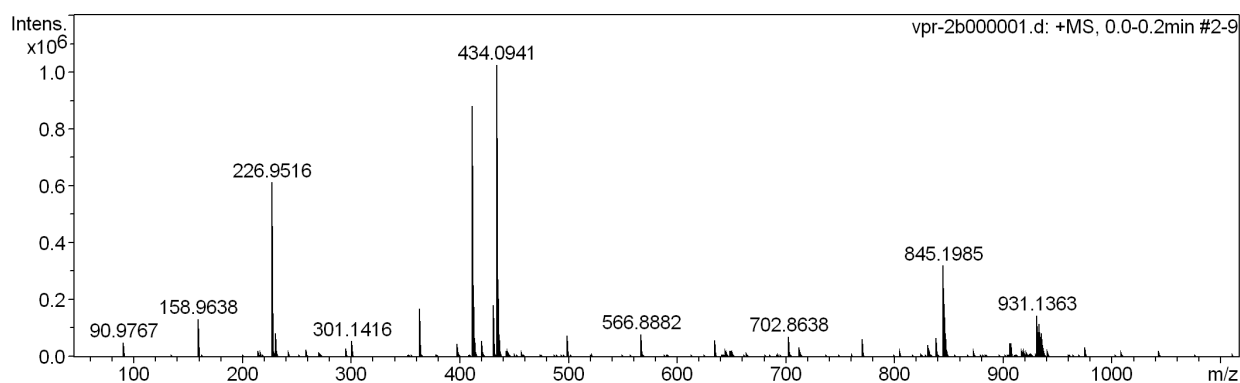
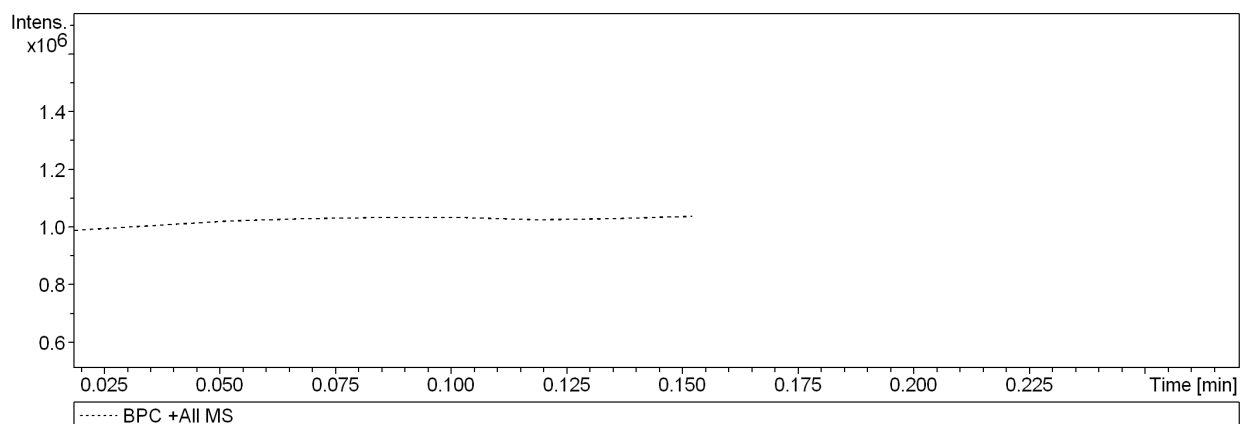


### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule	
398.0963	1	C23H16N3O2S	398.0958	-1.4	3.4	1	100.00	17.5	even	ok
420.0789	1	C25H14N3O2S	420.0801	3.0	28.6	1	100.00	20.5	even	ok
	1	C23H15N3NaO2S	420.0777	-2.8	17.5	1	100.00	17.5	even	ok

**+MS, 0.1-0.2min #4-10**

**Figure S24:** Mass spectrum of compound **2b**.



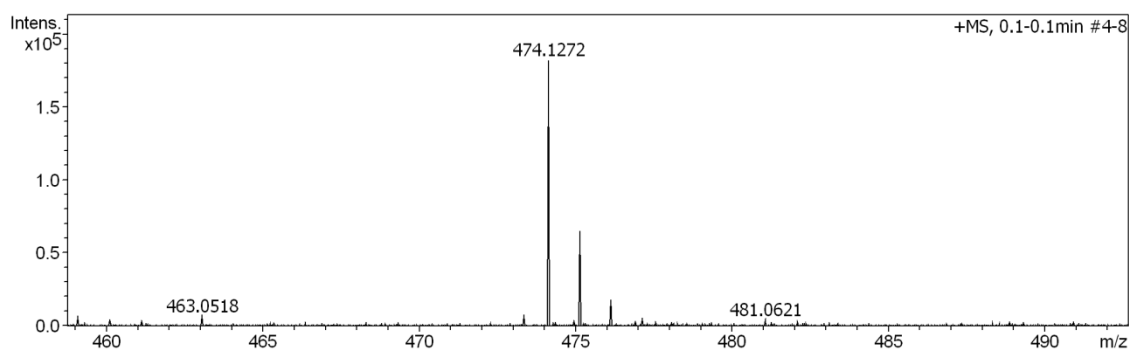
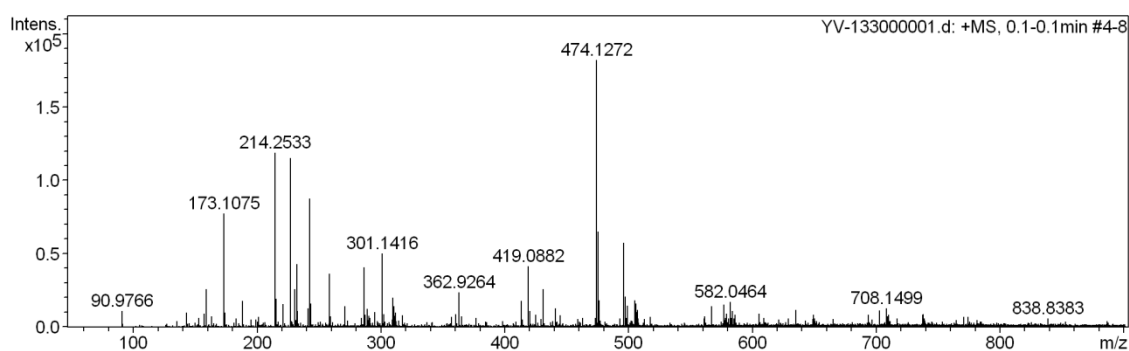
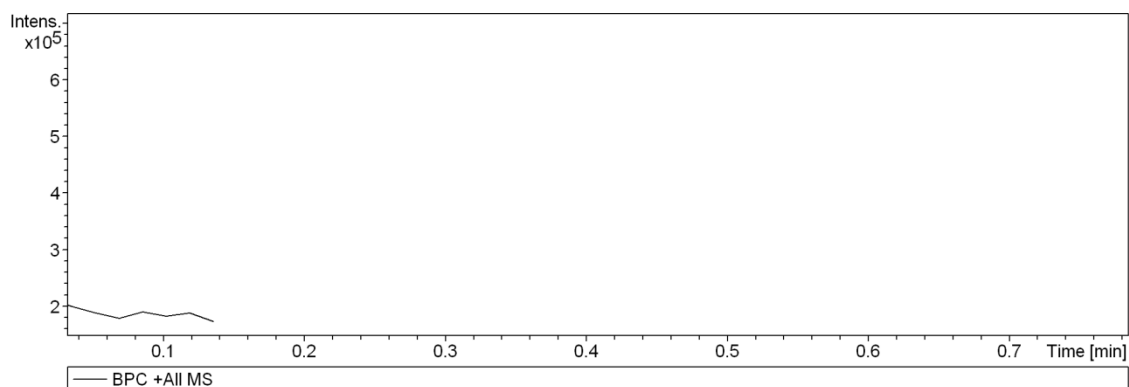
### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
412.1121	1	C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> O <sub>2</sub> S	412.1114	-1.8	8.6	1	100.00	17.5	even ok
434.0941	1	C <sub>26</sub> H <sub>16</sub> N <sub>3</sub> O <sub>2</sub> S	434.0958	3.8	20.2	1	100.00	20.5	even ok
	1	C <sub>24</sub> H <sub>17</sub> N <sub>3</sub> NaO <sub>2</sub> S	434.0934	-1.7	9.2	1	100.00	17.5	even ok

+MS, 0.0-0.2min #2-9



**Figure S25:** Mass spectrum of compound **2c**.

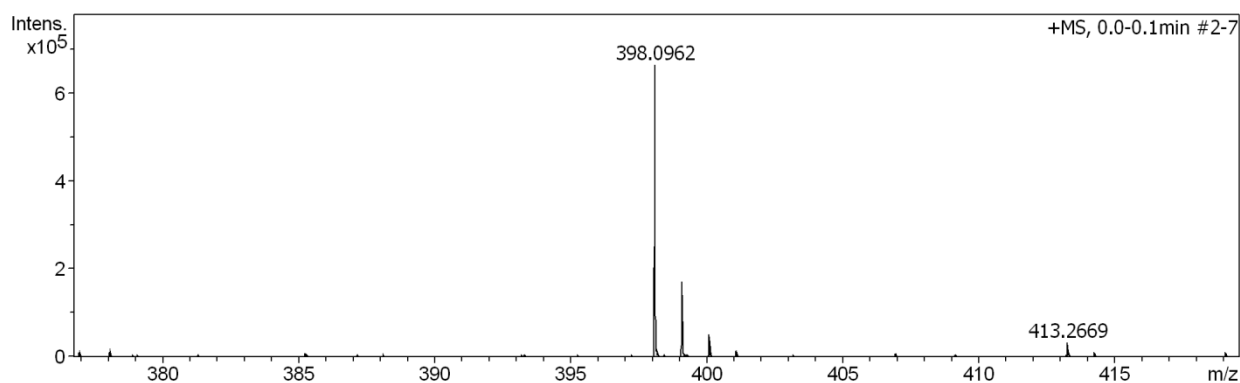
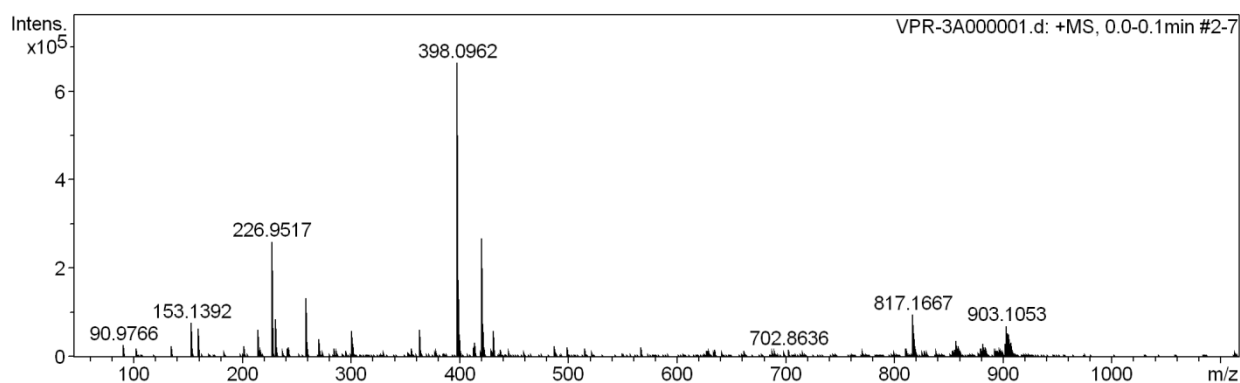
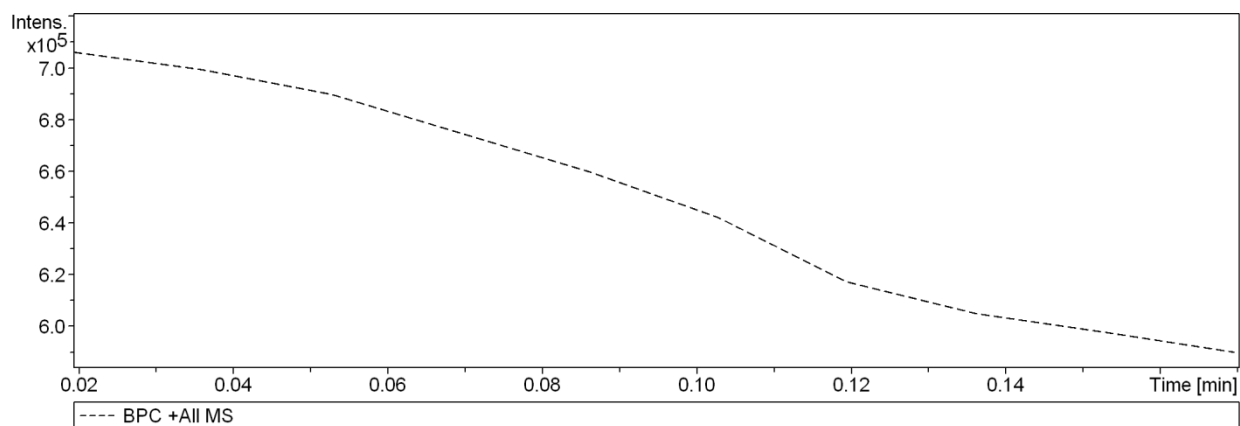


### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
474.1272	1	C <sub>29</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub> S	474.1271	-0.2	11.5	1	100.00	21.5	even ok
	1	C <sub>32</sub> H <sub>21</sub> NNaS	474.1287	3.2	4.4	1	100.00	22.5	even ok
	1	C <sub>29</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub> S	474.1271	-0.2	11.5	1	100.00	21.5	even ok

**+MS, 0.1-0.1min #4-8**

**Figure S26:** Mass spectrum of compound **3a**.

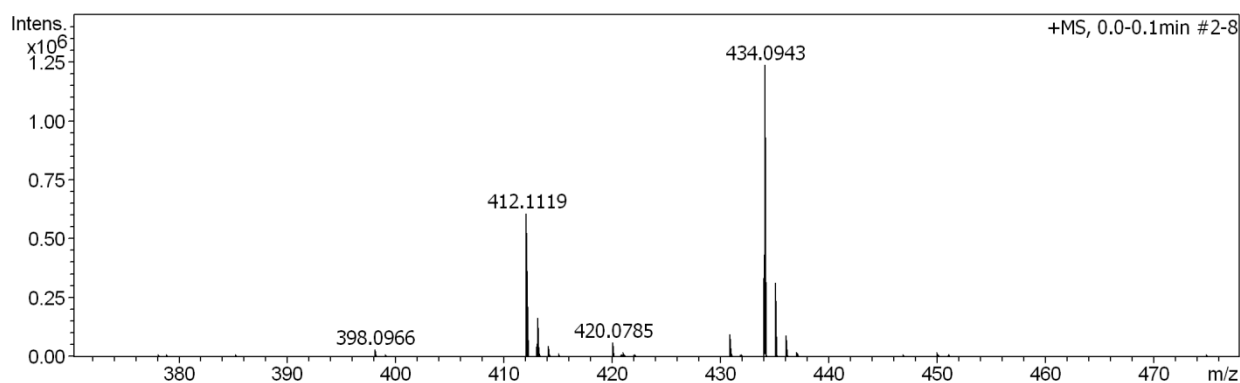
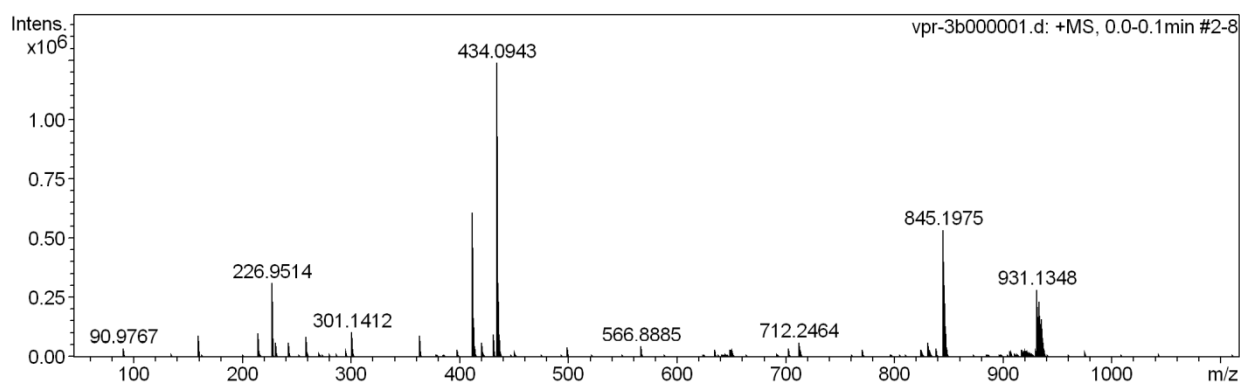
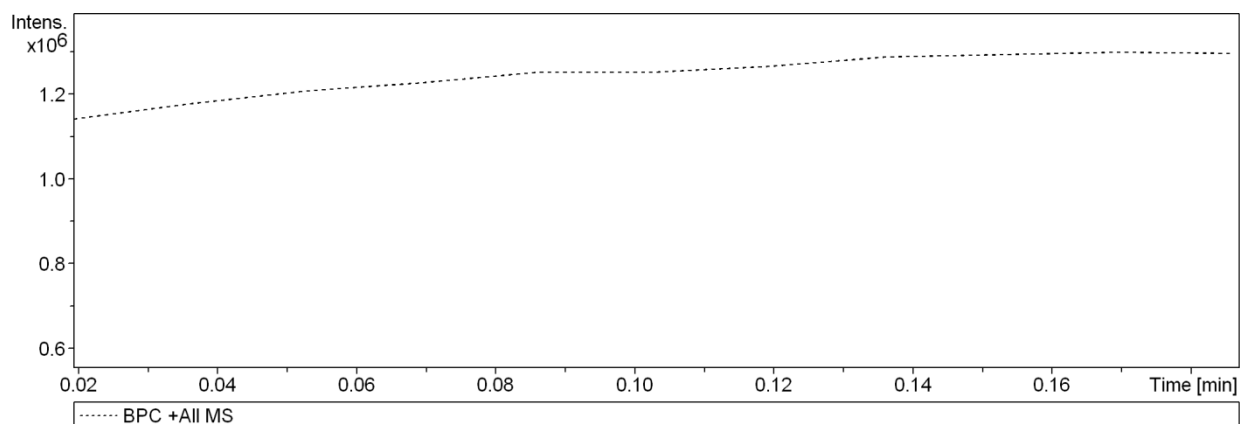


### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
398.0962	1	C <sub>23</sub> H <sub>16</sub> N <sub>3</sub> O <sub>2</sub> S	398.0958	-1.1	6.3	100.00	17.5	even	ok

+MS, 0.0-0.1min #2-7

**Figure S27:** Mass spectrum of compound **3b**.

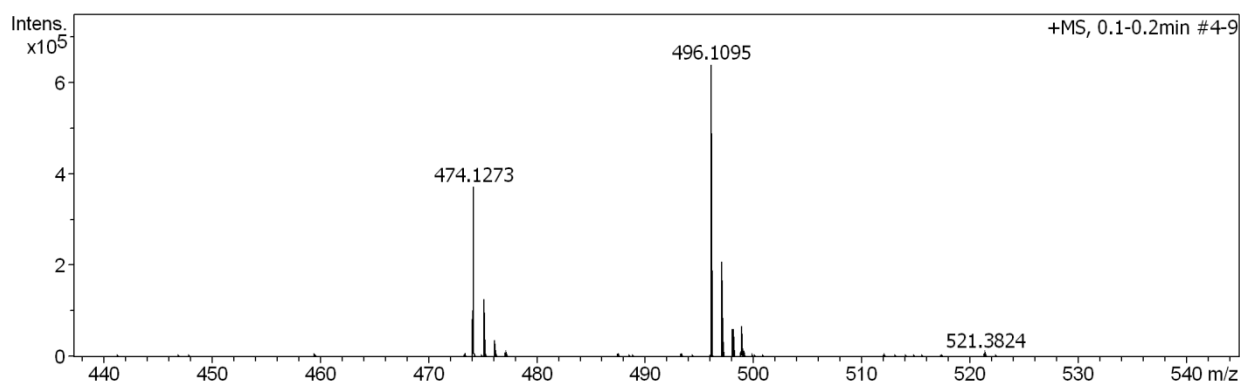
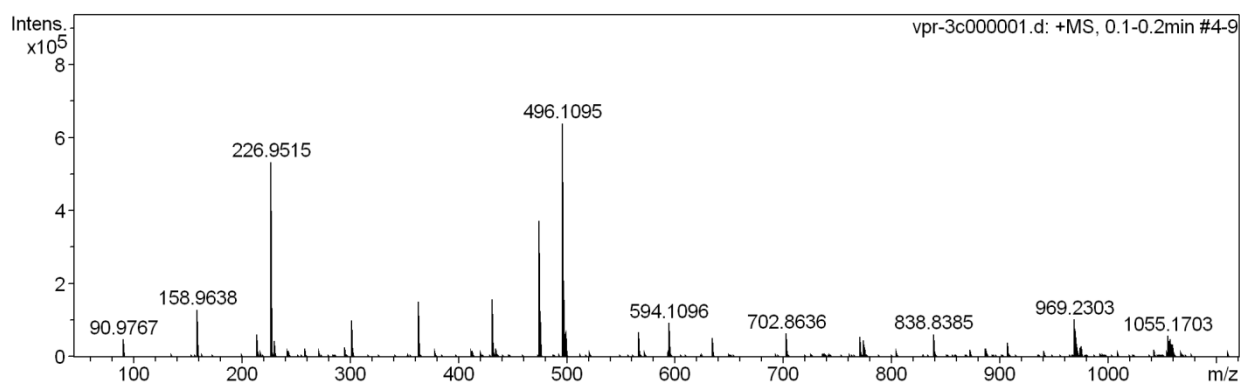
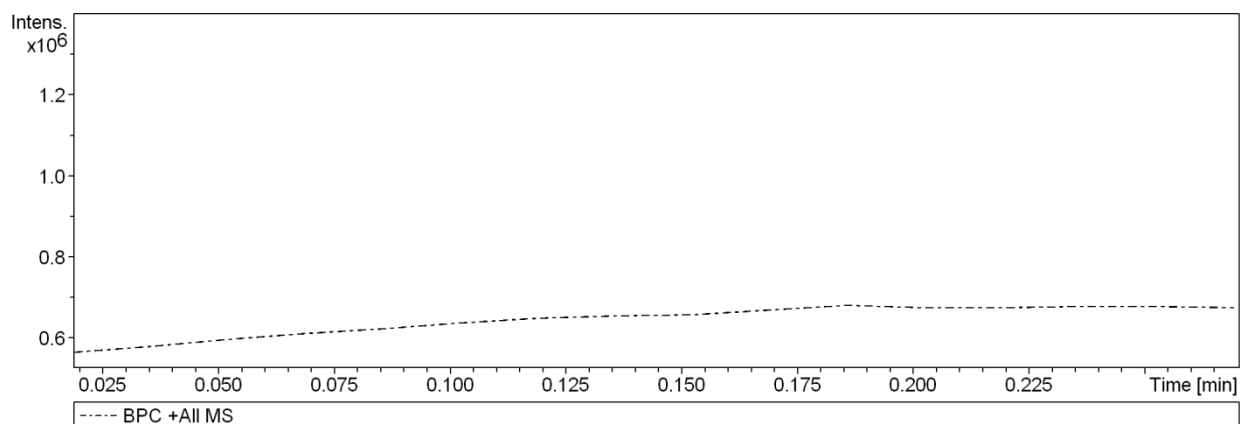


### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
412.1119	1	C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> O <sub>2</sub> S	412.1114	-1.3	8.0	100.00	17.5	even	ok
434.0943	1	C <sub>26</sub> H <sub>16</sub> N <sub>3</sub> O <sub>2</sub> S	434.0958	3.3	26.7	100.00	20.5	even	ok
	1	C <sub>24</sub> H <sub>17</sub> N <sub>3</sub> NaO <sub>2</sub> S	434.0934	-2.2	15.5	100.00	17.5	even	ok

**+MS, 0.0-0.1min #2-8**

**Figure S28:** Mass spectrum of compound **3c**.



### Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
474.1273	1	C <sub>29</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub> S	474.1271	-0.6	4.1	100.00	21.5	even	ok
	1	C <sub>24</sub> H <sub>25</sub> N <sub>3</sub> NaO <sub>2</sub> S <sub>2</sub>	474.1280	1.5	28.5	100.00	13.5	even	ok
496.1095	1	C <sub>31</sub> H <sub>18</sub> N <sub>3</sub> O <sub>2</sub> S	496.1114	3.9	16.1	100.00	24.5	even	ok
	1	C <sub>29</sub> H <sub>19</sub> N <sub>3</sub> NaO <sub>2</sub> S	496.1090	-0.9	7.0	100.00	21.5	even	ok

+MS, 0.1-0.2min #4-9