

# Supplementary Information

## Induction of cryptic antifungal pulicatin derivatives from *Pantoea agglomerans* by microbial co-culture

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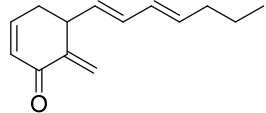
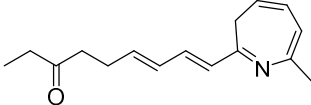
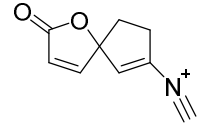
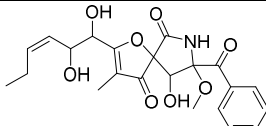
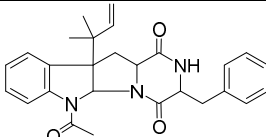
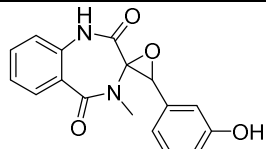
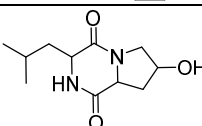
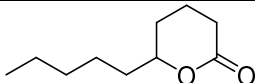
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Table S1. Pc LC-HRMS dereplication

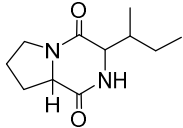
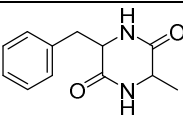
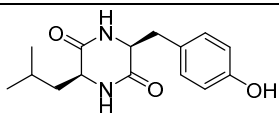
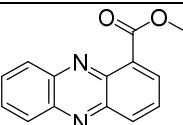
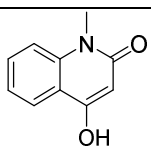
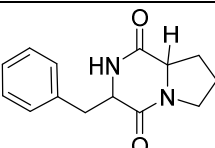
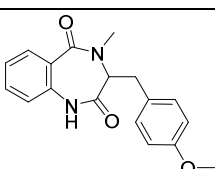
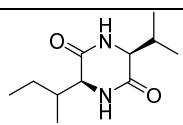
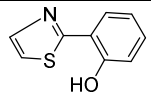
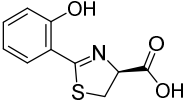
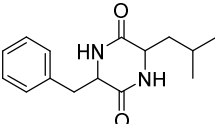
Retention time (min)	m/z [M+H] <sup>+</sup>	Molecular formula	Tentative Identification	structure
3.46	197.1293	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclo(pro-val)	
4.28	279.1159	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	dehydrocyclopeptin	
5.48	197.1285	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclo(Pro-Val)	
5.75	166.0865	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	p-dimethylamino-benzoic acid	
6.57	225.0880	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	N-{3-Nitro-4-hydroxyphenylethyl} acetamide	

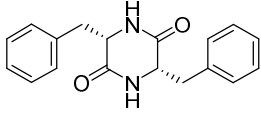
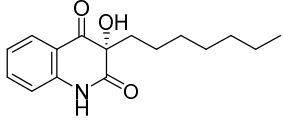
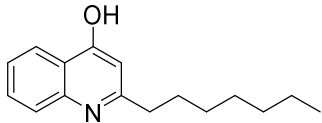
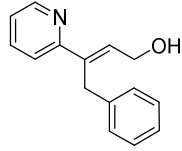
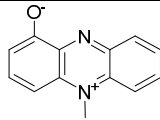
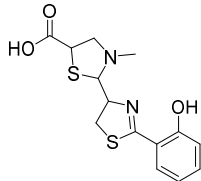
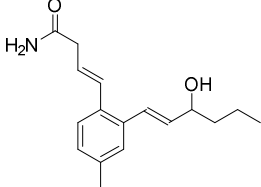
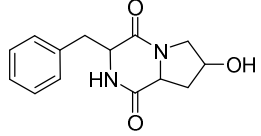
6.57	324.1566	C <sub>17</sub> H <sub>24</sub> O <sub>7</sub>	AF toxin 11A	
6.59	324.1566	C <sub>20</sub> H <sub>22</sub> NO	New hit	
8.17	254.0763	C <sub>15</sub> H <sub>11</sub> NO <sub>3</sub>	phomopsin A	
8.39	235.1446	C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	Fungerin	
9.10	281.1289	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclopeptin	
9.12	628.3254	C <sub>22</sub> H <sub>45</sub> O <sub>12</sub> N <sub>9</sub>	desferrichrome	
9.64	221.8219	C <sub>12</sub> H <sub>12</sub> O <sub>4</sub>	Hispolon	
9.69	211.14454	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	Cyclo(Pro-leu)	
9.88	172.0427	C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S	4-methylbenzene sulfonamide	
9.69	311.1394958	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	4'-Methoxycyclopeptin	
9.88	190.0323	C <sub>10</sub> H <sub>7</sub> NOS	New hit	

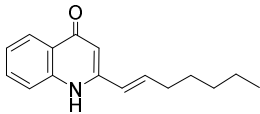
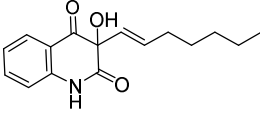
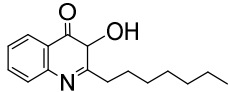
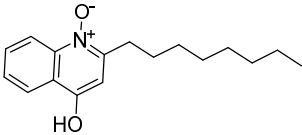
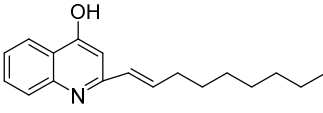
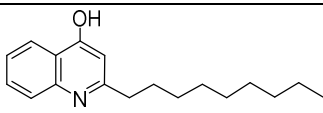
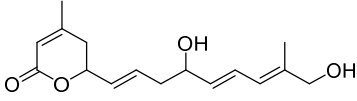
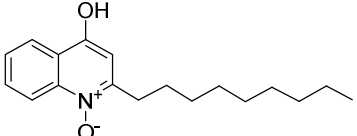
10.19	203.1433	C <sub>14</sub> H <sub>18</sub> O	Penidienone	
10.95	244.1701	C <sub>16</sub> H <sub>21</sub> NO	Isochalciporon	
11.43	162.0549	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>	7-isocyano-1-oxaspiro[4.4]nona-3,6-dien-2-one	
12.05	432.1598	C <sub>22</sub> H <sub>25</sub> NO <sub>8</sub>	Pseurotin A	
12.53	444.22818	C <sub>27</sub> H <sub>29</sub> N <sub>3</sub> O <sub>3</sub>	Fructigenine	
15.87	311.0954	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	cyclopeniol	
13.00	227.1018	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	Cyclo(4-OH-pro-Leu)	
13.18	171.1380	C <sub>10</sub> H <sub>18</sub> O <sub>2</sub>	5-Decanolide	
16.50	673.3775	C <sub>30</sub> H <sub>52</sub> O <sub>11</sub> N <sub>6</sub>	New hit	
17.81	1038.6356	C <sub>68</sub> H <sub>83</sub> O <sub>6</sub> N <sub>3</sub>	New hit	

**Table S2. Pa LC-HRMS dereplication (Cherif-Silini *et al.*, 2019)**

Rt (min)	m/z [M+H] <sup>+</sup>	Molecular formula	Tentative Identification	Structure
5.02	235.1082	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	Cyclo(Phe-Ser)	
5.02	247.1083	C <sub>13</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	N-Acetyltryptophan	
5.10	261.18533	C <sub>14</sub> H <sub>16</sub> O <sub>3</sub> N <sub>2</sub>	cyclo(Pro-Tyr)	
5.11	205.0976	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	Cyclo(Gly-Phe)	
5.20	217.0977	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	Sannanine	
5.40	197.12887	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclo(Pro-Val)	
5.58	185.1287537	C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclo(Ala-Leu)	
5.80	227.1395645	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	cyclo-4-hydroxyPro-Leu	

5.94	211.1446	C <sub>11</sub> H <sub>18</sub> O <sub>2</sub> N <sub>2</sub>	Cyclo(Ile-Pro)	
6.90	219.1133	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	Cyclo(Ala-Phe)	
6.90	277.1551	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	cyclo(Leu-Tyr)	
7.12	239.0820	C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	6-Carboxymethyl-phenazine	
7.76	176.0708	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>	4-Hydroxy-N-methylcarbostyryl	
8.74	245.1289	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	cyclo-(Pro-phe)	
9.69	311.1394	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	4'-Methoxycyclopeptin	
10.22	213.1602	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	cyclo(L-Ile-L-Valine)	
11.48	178.0324	C <sub>9</sub> H <sub>7</sub> NOS	2-(2-Hydroxyphenyl)thiazole	
11.52	224.0381	C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub> S	(+)-(S)-dihydroaeruginic acid	
12.61	218.1182	C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>	New quinoline derivative	
12.65	261.1603	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	Cyclo(Leu-Phe)	

13.18	214.1232	C <sub>14</sub> H <sub>15</sub> NO	New quinoline derivative	
13.40	295.1448	C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>	cyclo-(L-Phe-L-Phe)	
13.51	276.1602	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>	3-n-Heptyl-3-hydroxy-(1H,3H)-quinoline-2,4-dione	
13.62	284.1651	C <sub>18</sub> H <sub>21</sub> NO <sub>2</sub>	New quinoline derivative	
13.98	244.1713	C <sub>16</sub> H <sub>21</sub> NO	2-heptyl-4-hydroxy-quinolone	
14.01	226.1231	C <sub>15</sub> H <sub>15</sub> NO	(E)-4-Phenyl-3-(pyridine-2-yl)but-2-en-1-ol	
14.06	228.1389	C <sub>15</sub> H <sub>17</sub> NO	New quinoline derivative	
14.49	211.0872	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O	Cyanomycin	
14.79	228.1389	C <sub>15</sub> H <sub>17</sub> NO	New quinoline derivative	
14.88	274.1444	C <sub>16</sub> H <sub>19</sub> NO <sub>3</sub>	New quinoline derivative	
14.88	323.0530	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> S <sub>2</sub>	Pyochelin	
15.70	274.1809	C <sub>17</sub> H <sub>23</sub> NO <sub>2</sub>	Lorneamide A	
15.81	325.0679	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	cyclo(4-OH-Pro-Phe)	
16.07	246.1494	C <sub>15</sub> H <sub>19</sub> NO <sub>2</sub>	New quinoline derivative	

16.33	244.1338	$C_{15}H_{17}NO_2$	New quinoline derivative	
16.54	242.1548	$C_{16}H_{19}NO$	2-Heptenyl-4-quinolinone	
16.87	274.1444	$C_{16}H_{19}NO_3$	ε-3-(hept-1-en-1-yl)-3-hydroxyquinoline-2,4(1H,3H)-dione	
17.01	651.2722	$C_{30}H_{41}O_{13}N_3$	New hit	
18.32	260.1654	$C_{16}H_{21}NO_2$	2-Heptyl-3-hydroxy-4(3H)-quinolone	
19.43	272.1645	$C_{17}H_{21}NO_2$	New quinoline derivative	
19.14	272.1647	$C_{17}H_{21}NO_2$	New quinoline derivative	
19.19	274.1805	$C_{17}H_{23}NO_2$	4-hydroxy-2-octylquinoline 1-oxide	
19.63	270.1861	$C_{18}H_{23}NO$	2-(n-delta(1)-Nonyl)-4-oxyquinoline	
19.84	272.2017	$C_{18}H_{25}NO$	1. 2-Nonyl-quinonyl-4-ol	
19.7	358.2380	$C_{22}H_{31}NO_3$	New quinoline derivative	
19.93	356.2224	$C_{22}H_{29}NO_3$	New quinoline derivative	
20.15	277.1172	$C_{16}H_{22}O_4$	Oncorhyncolide	
20.16	286.1809	$C_{18}H_{23}NO_2$	New quinoline derivative	
20.89	288.1965	$C_{18}H_{25}NO_2$	4-Hydroxy-2-n-nonyl-quinoline N-oxide	

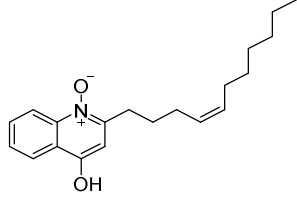
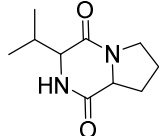
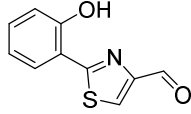
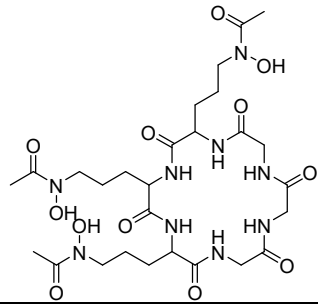
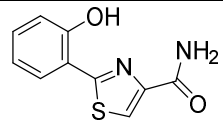
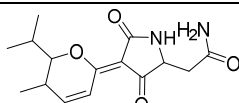
21.67	314.2118	C <sub>20</sub> H <sub>27</sub> NO <sub>2</sub>	(Z)-4-hydroxy-2-(undec-4-en-1-yl)quinoline 1-oxide	
22.53	340.22730	C <sub>22</sub> H <sub>29</sub> NO <sub>2</sub>	New quinoline derivative	

Table S3. Pa-Pc LC-HRMS dereplication

Retention time (min)	m/z [M+H] <sup>+</sup>	Molecular formula	Tentative Identification	structure
5.41	197.1274	C <sub>10</sub> H <sub>16</sub> O <sub>2</sub> N <sub>2</sub>	cyclo( pro-Val)	
7.31	684.3877	C <sub>30</sub> H <sub>53</sub> N <sub>9</sub> O <sub>7</sub> S	New hit	
7.35	206.993	C <sub>10</sub> H <sub>7</sub> NO <sub>2</sub> S	Aeruginaldehyde	
8.06	560.26715	C <sub>22</sub> H <sub>37</sub> O <sub>10</sub> N <sub>7</sub>	New hit	
9.15	628.3254	C <sub>22</sub> H <sub>45</sub> O <sub>12</sub> N <sub>9</sub>	Desferrichrome	
9.32	221.0385	C <sub>10</sub> H <sub>8</sub> O <sub>2</sub> N <sub>2</sub> S	Pulicatin F	
9.41	264.0695	C <sub>13</sub> H <sub>13</sub> NO <sub>5</sub> S	New hit	
9.45	293.14984	C <sub>15</sub> H <sub>20</sub> O <sub>4</sub> N <sub>2</sub>	5Z-Bripiodionen	



11.74	229.1552	C <sub>11</sub> H <sub>20</sub> O <sub>3</sub> N <sub>2</sub>	Libramycin A	
12.86	246.0519	C <sub>13</sub> H <sub>11</sub> NO <sub>2</sub> S	New hit	
13.12	227.1018	C <sub>11</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	Cyclo(4-OH-pro-Leu)	
13.87	244.1713	C <sub>16</sub> H <sub>21</sub> NO	2-heptyl-4-hydroxy-quinolone	

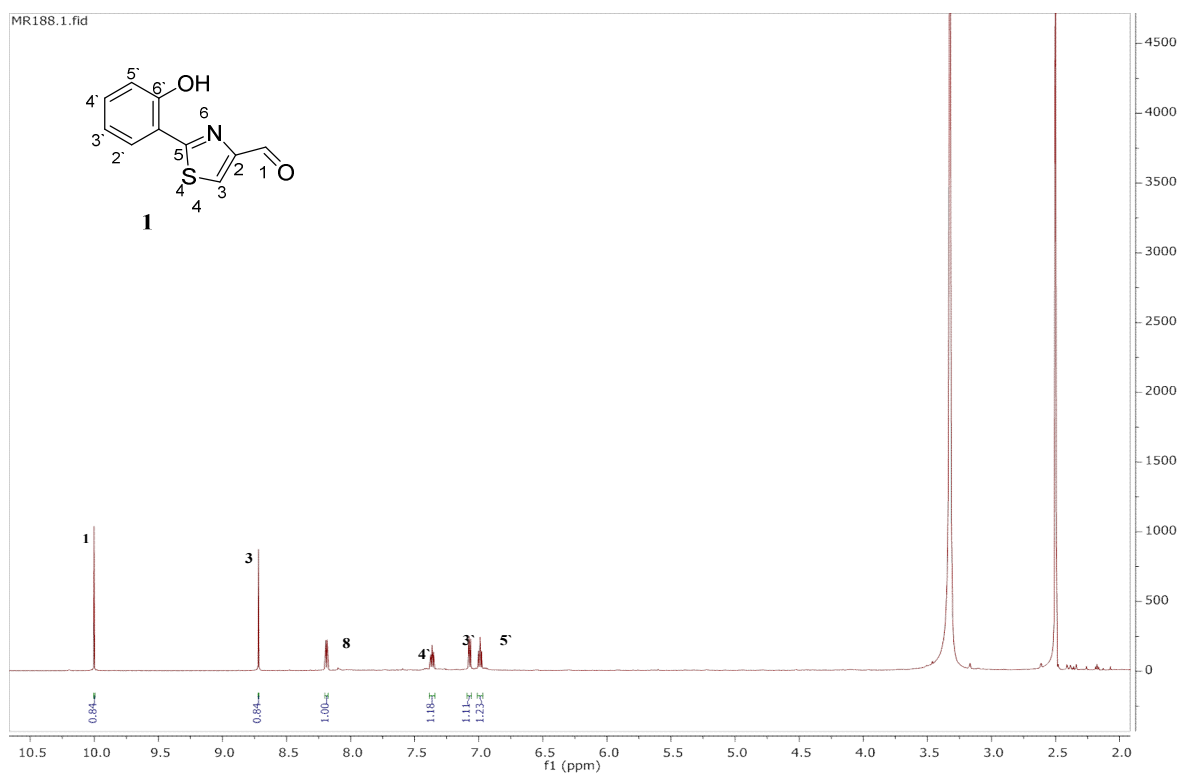


Figure S1. <sup>1</sup>H NMR spectrum of compound **1**.

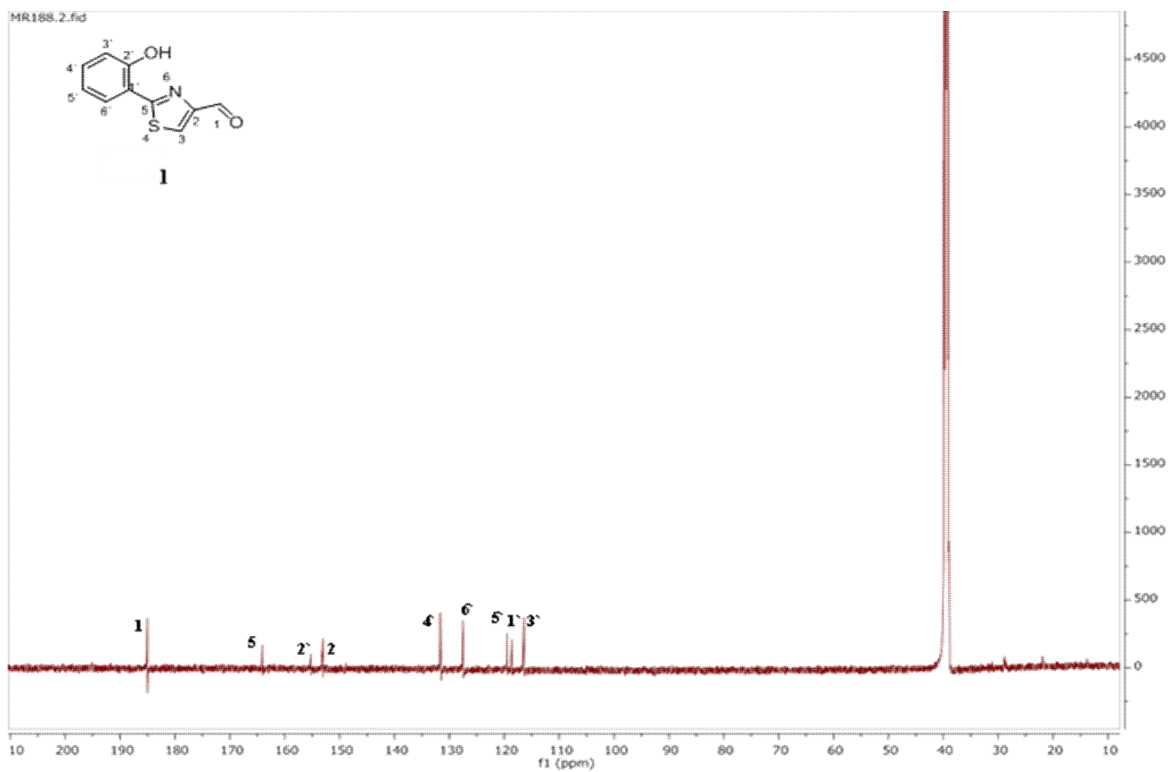


Figure S 2.  $^{13}\text{C}$  NMR spectrum of Compound 1.

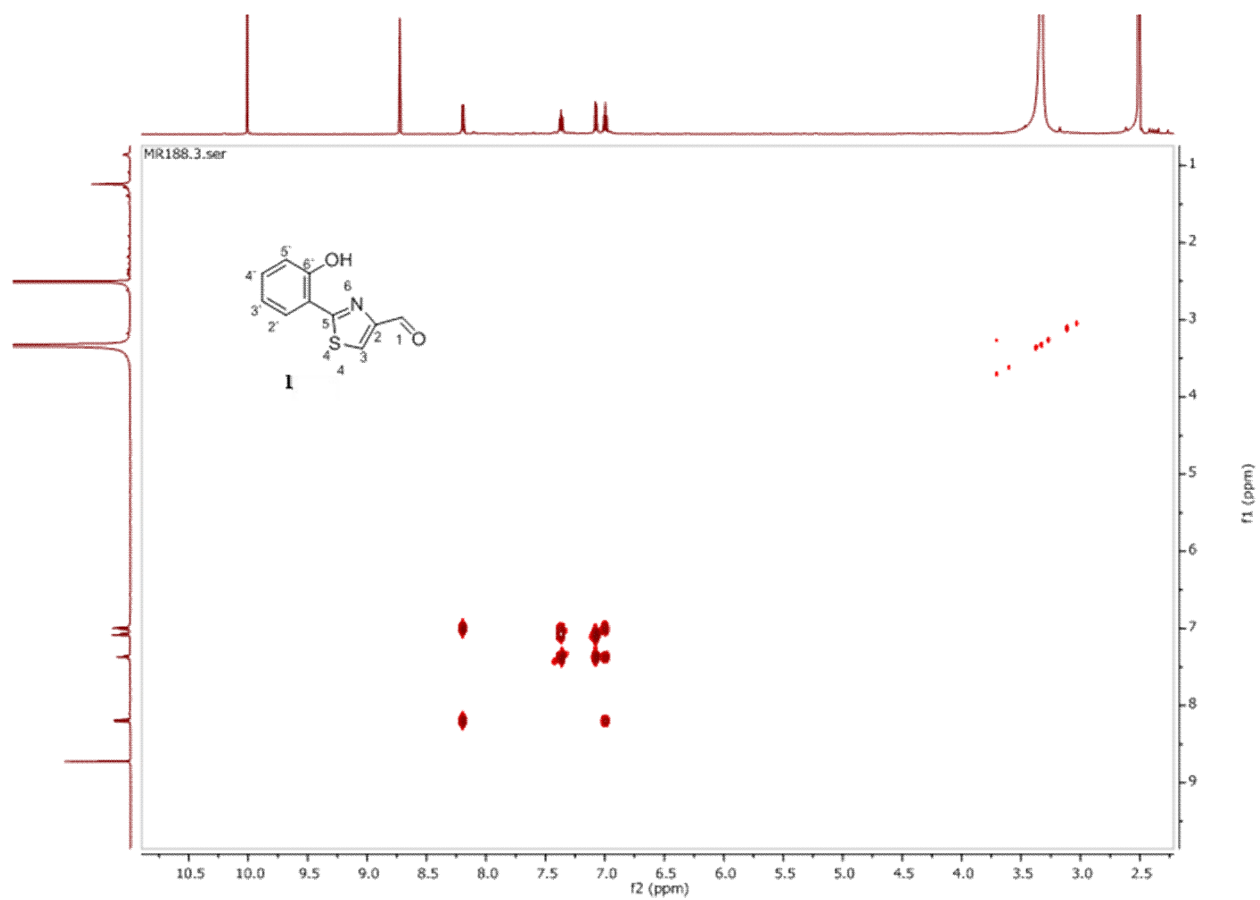


Figure S3. COSY spectrum of compound 1

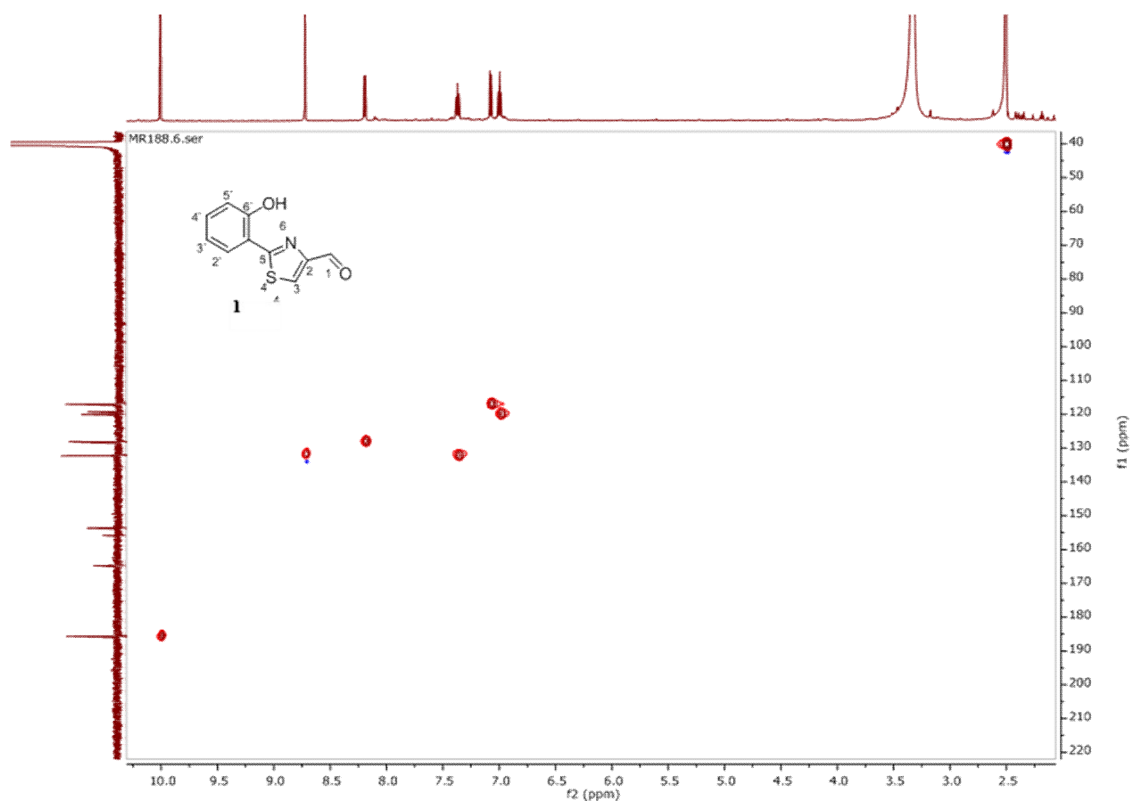


Figure S4. HSQC spectrum of compound 1

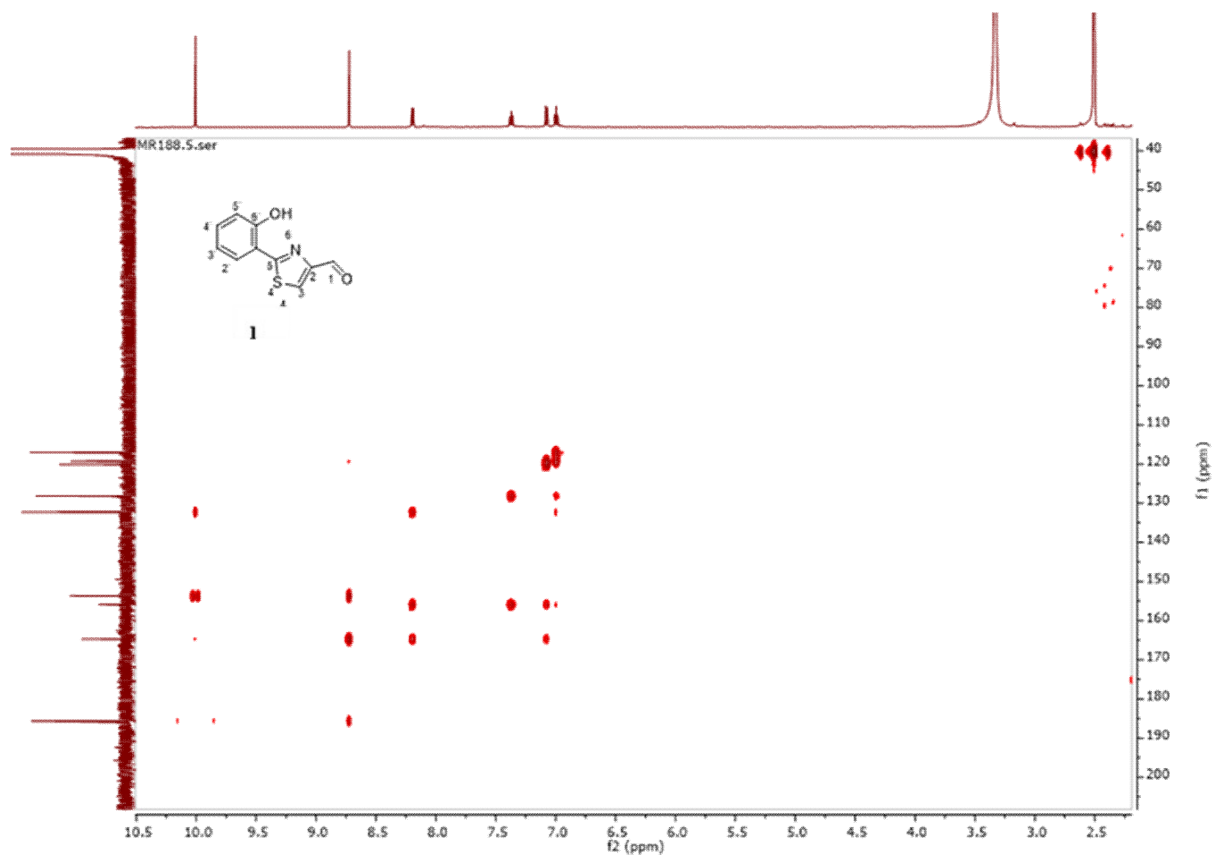


Figure S5. HMBC spectrum of compound 1

MR188 #682 RT: 13.12 AV: 1 NL: 5.98E3  
T: FTMS + p ESI Full ms [150.00-2000.00]

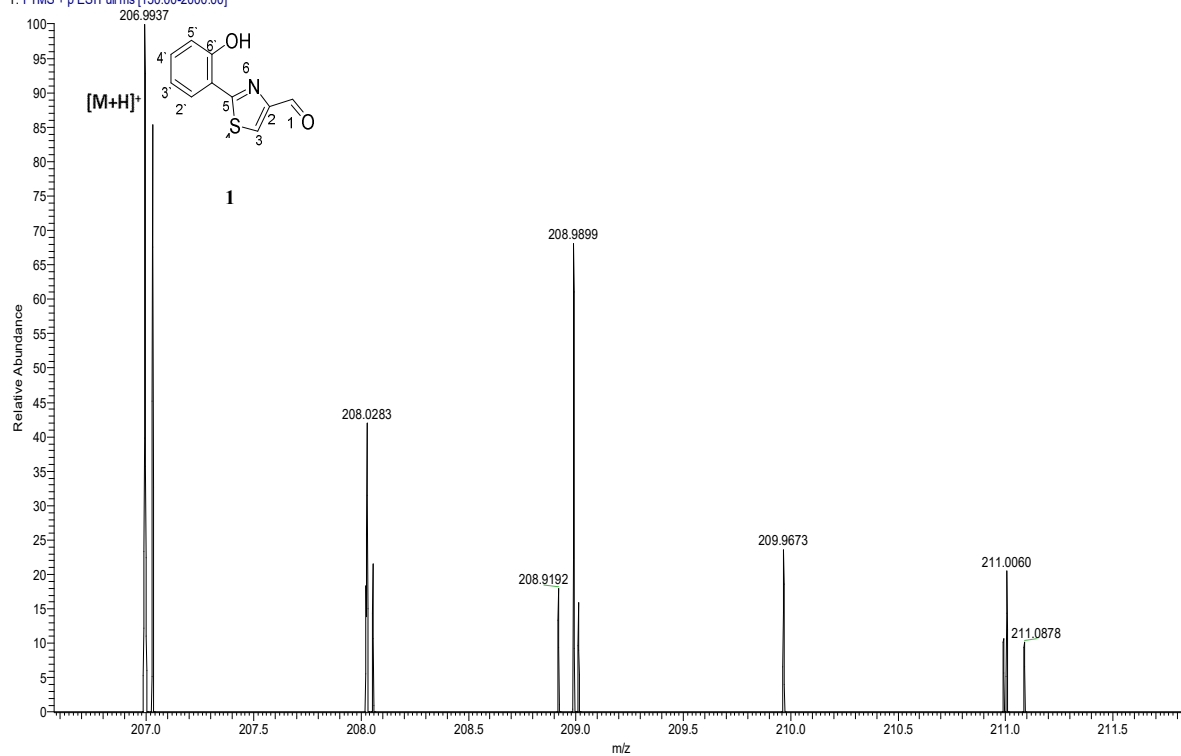


Figure S6. HRESIMS spectrum of compound 1

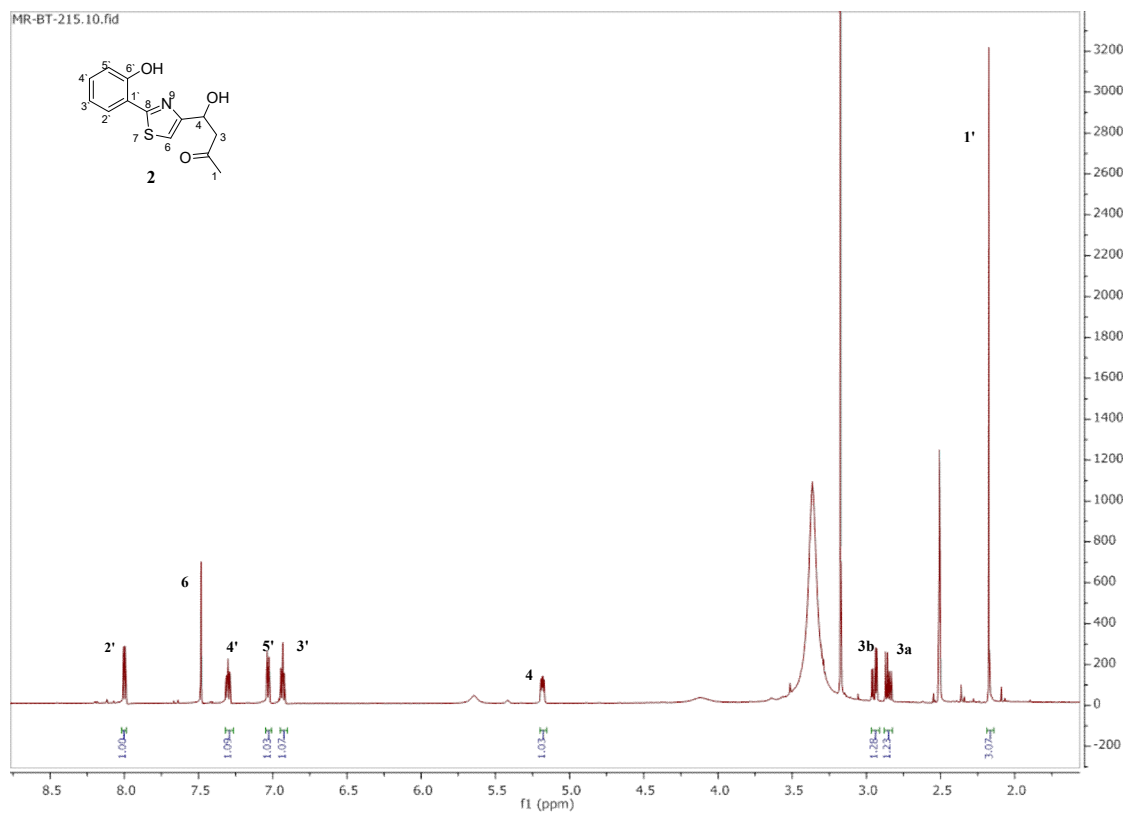


Figure S7. <sup>1</sup>H NMR spectrum of compound 2.

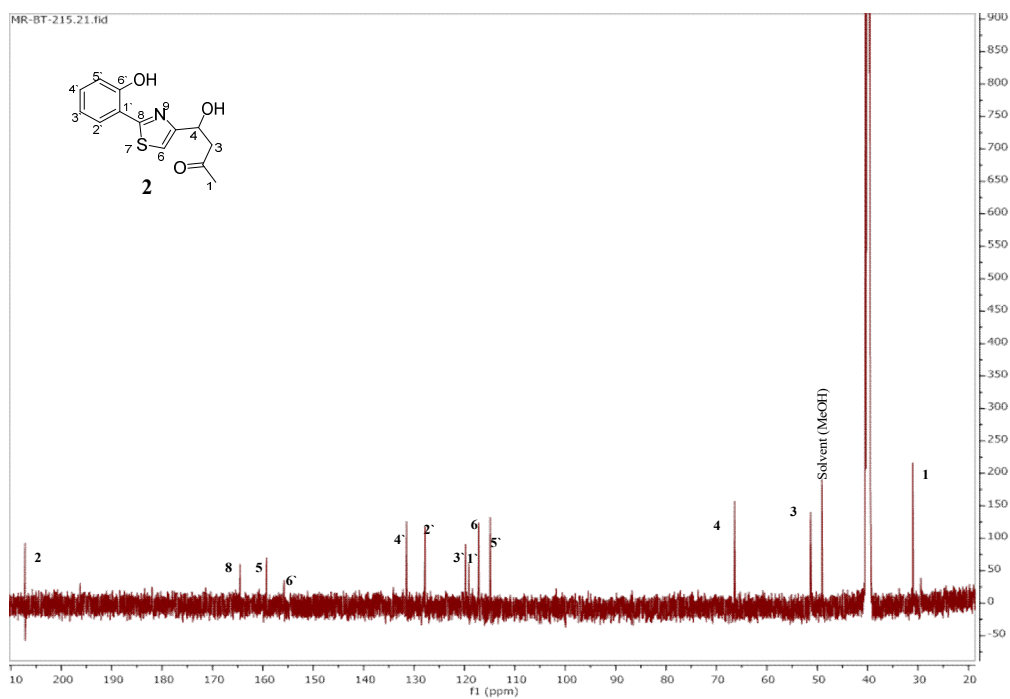


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound 2.

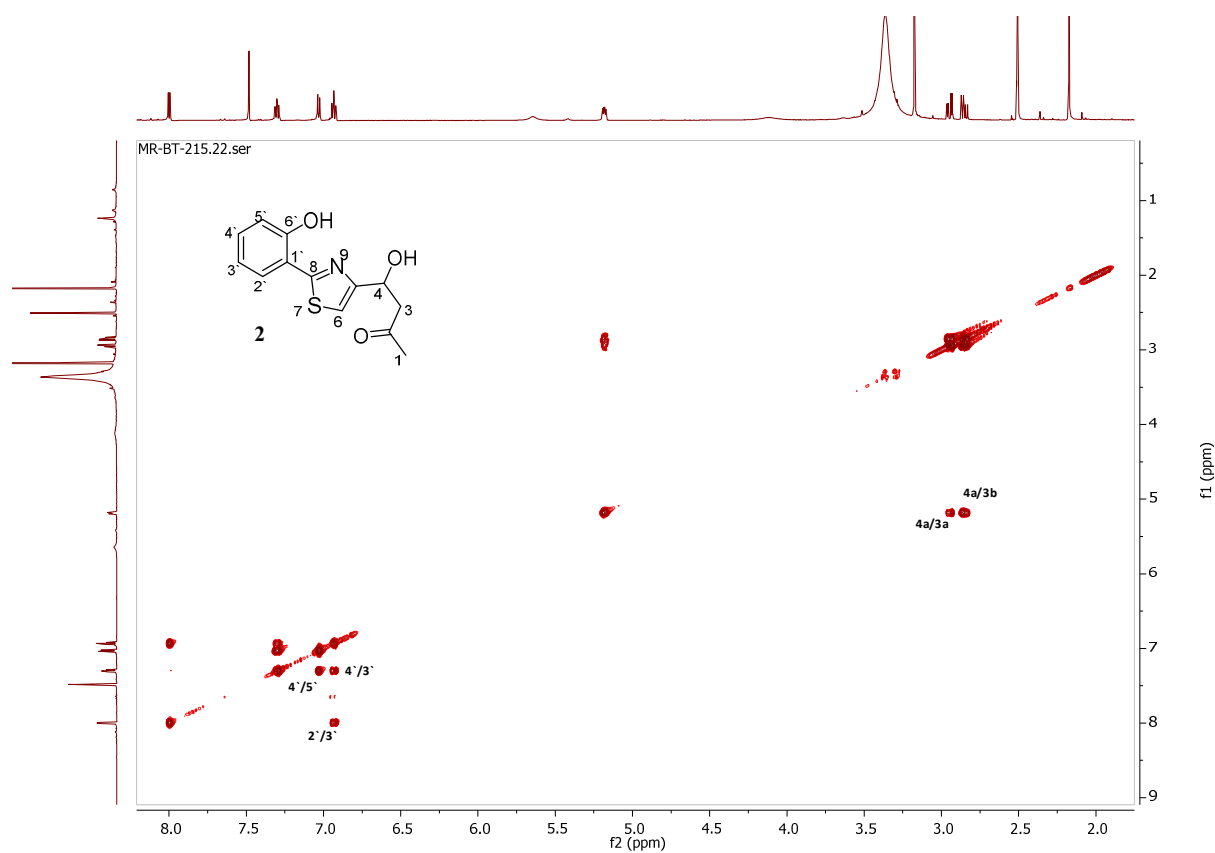


Figure S9. COSY spectrum of compound 2

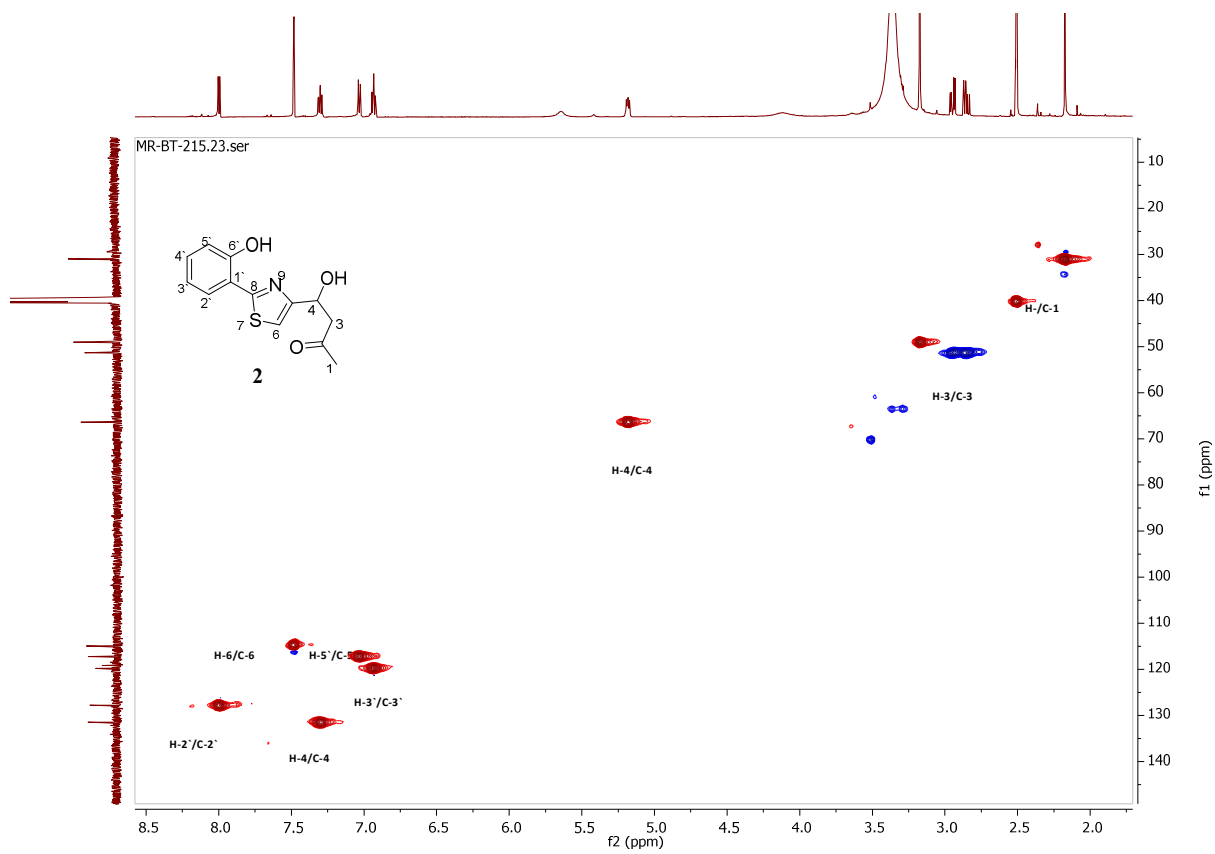


Figure S10. HSQC spectrum of compound 2

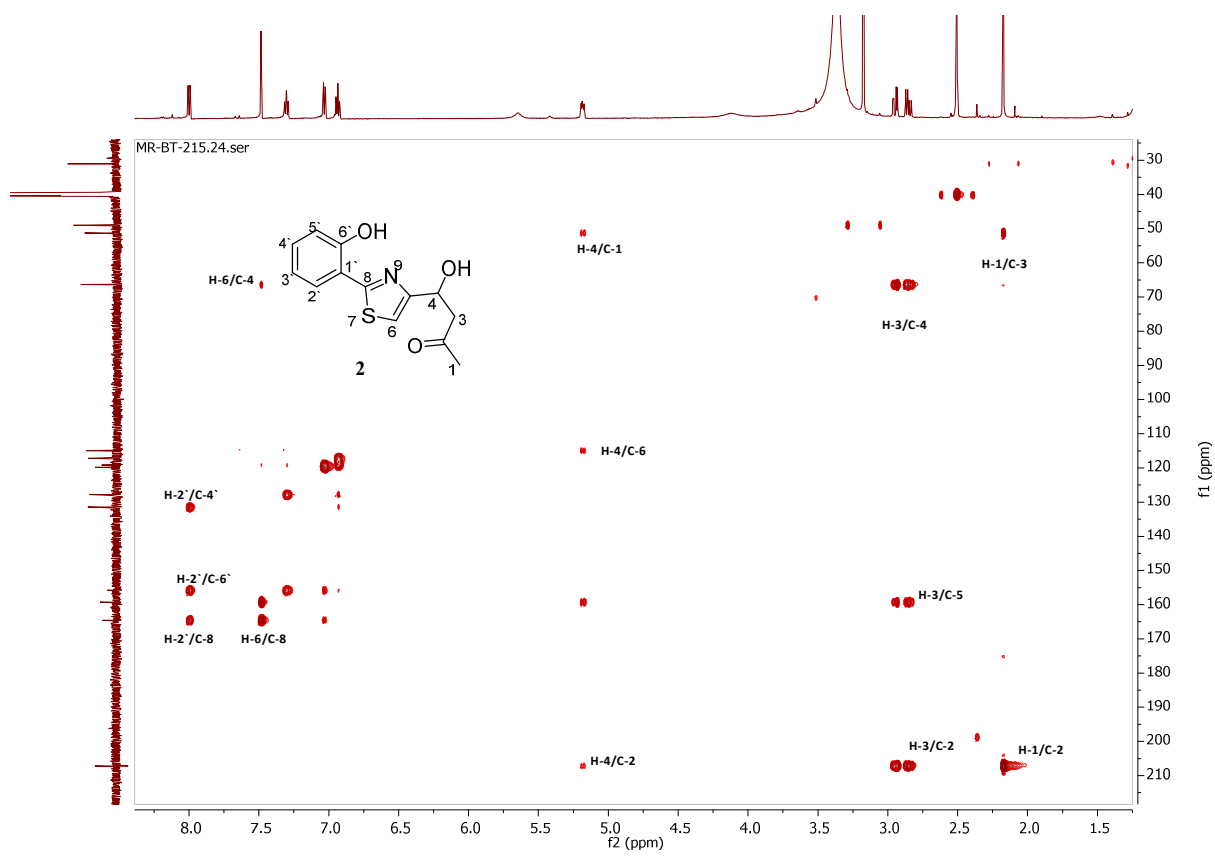


Figure S11. HMBC spectrum of compound 2.

MR484 #1025 RT: 9.82 AV: 1 NL: 4.13E6  
T: FTMS + p ESI Full ms [230.00-2000.00]

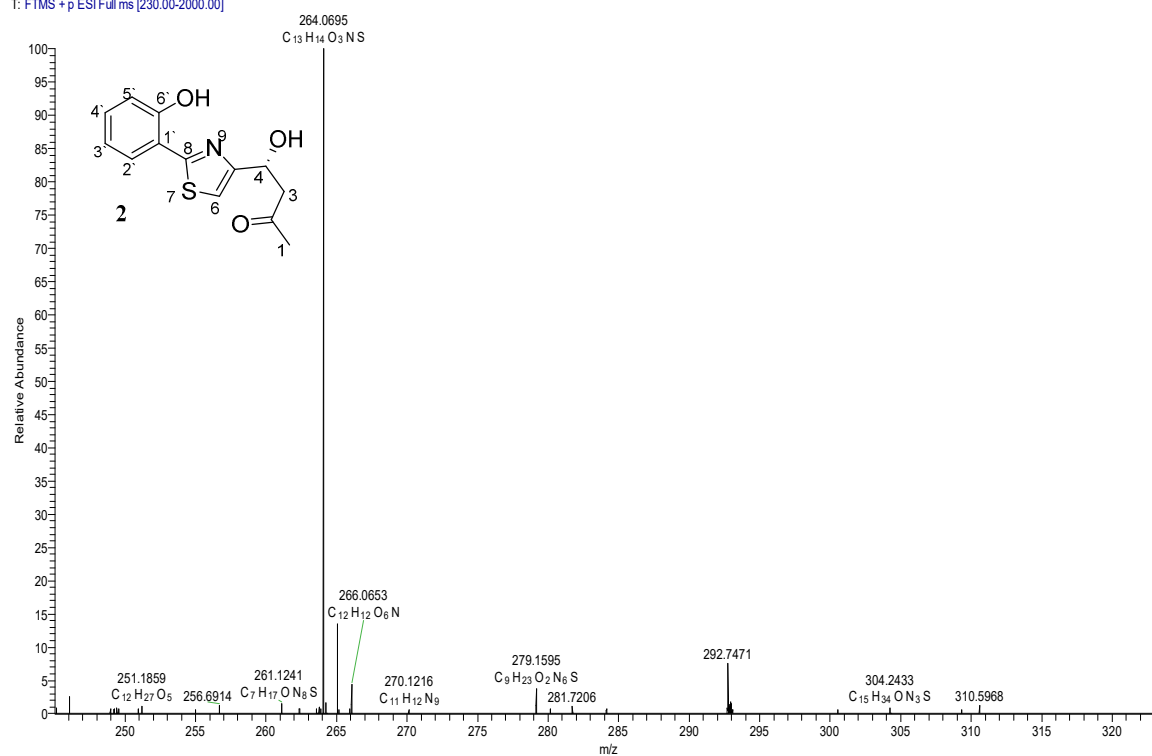


Figure S12. HRMS spectrum of compound 2.

MR-BT-225.20.fid

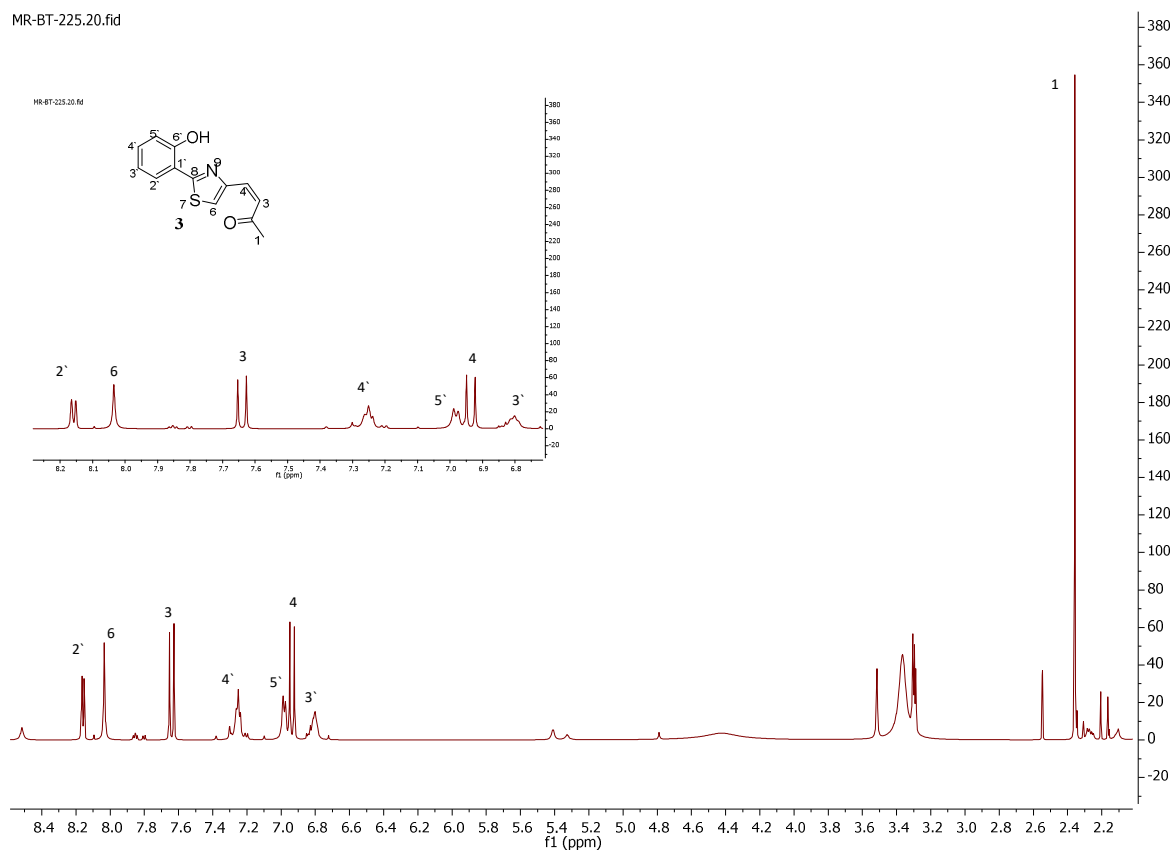


Figure S13. <sup>1</sup>H NMR spectrum of compound 3.

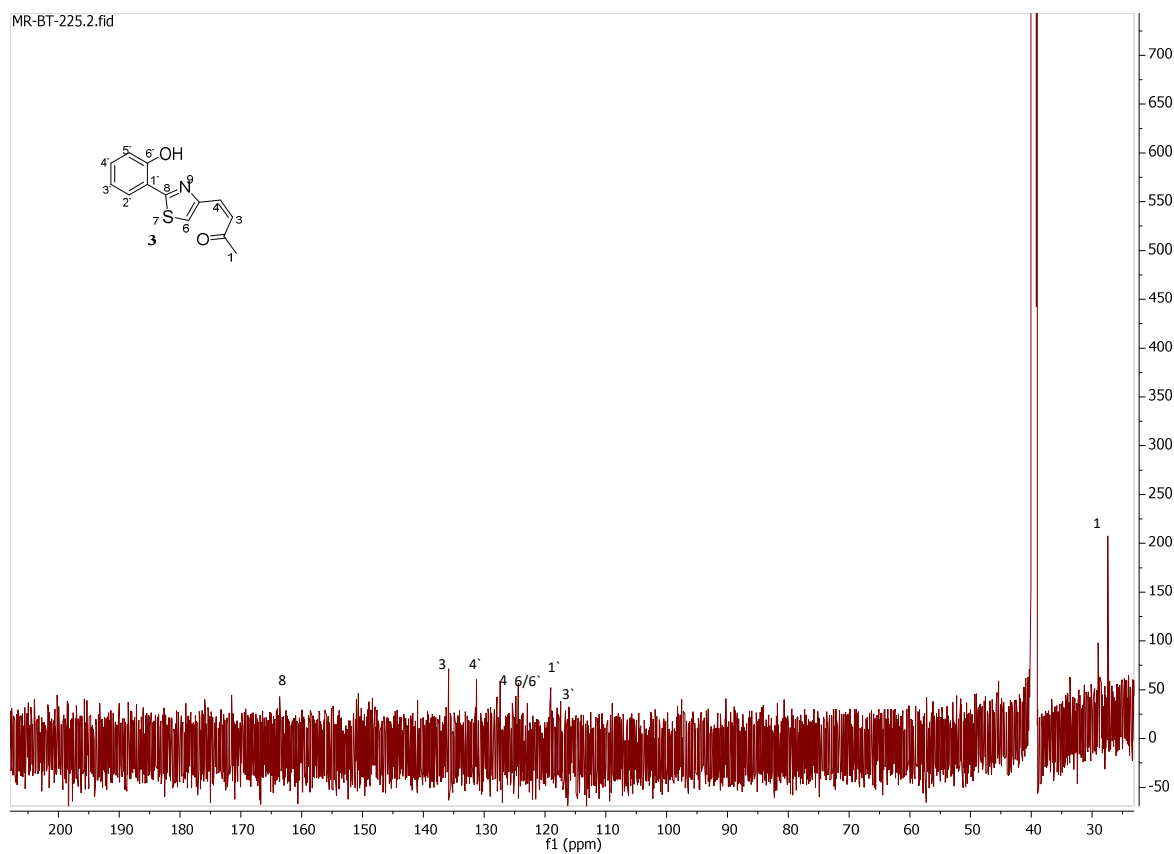


Figure S14.  $^{13}\text{C}$  NMR spectrum of compound 3.

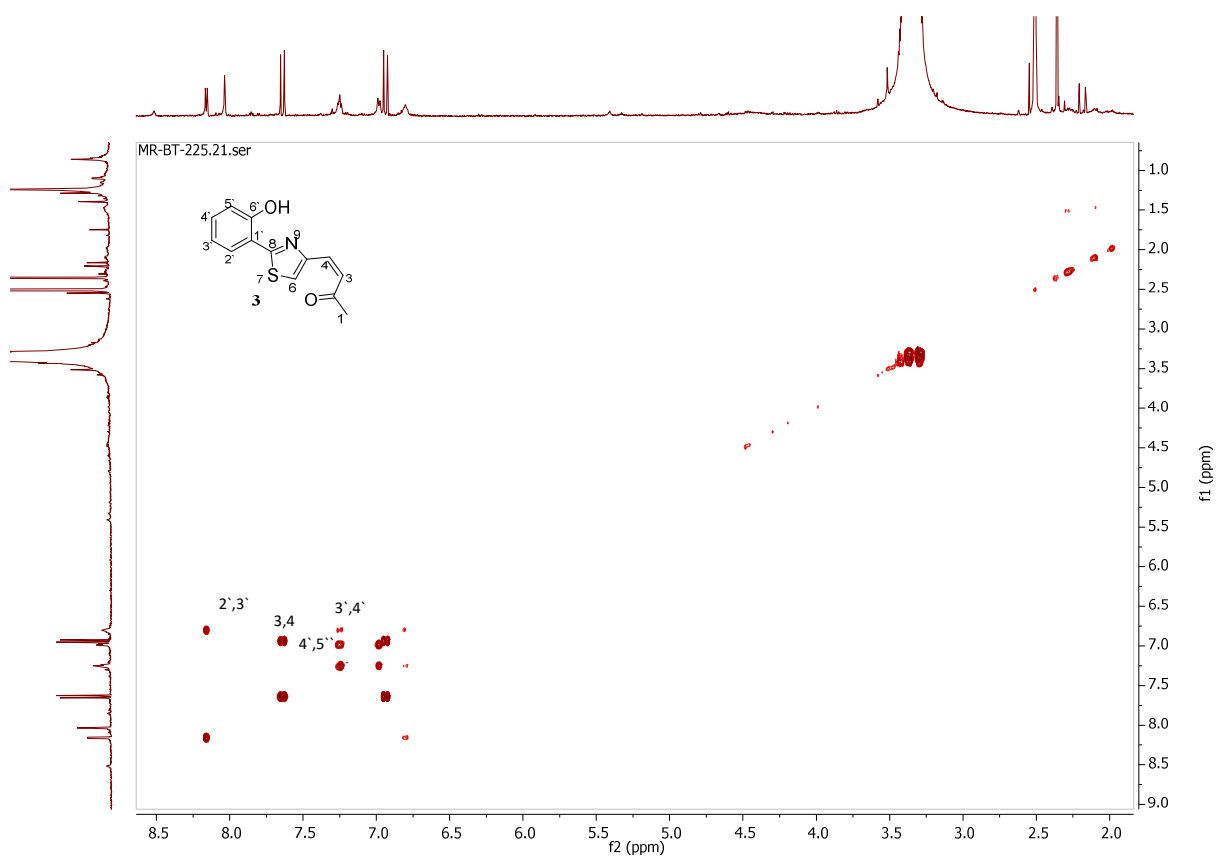


Figure S15. COSY spectrum of compound 3.



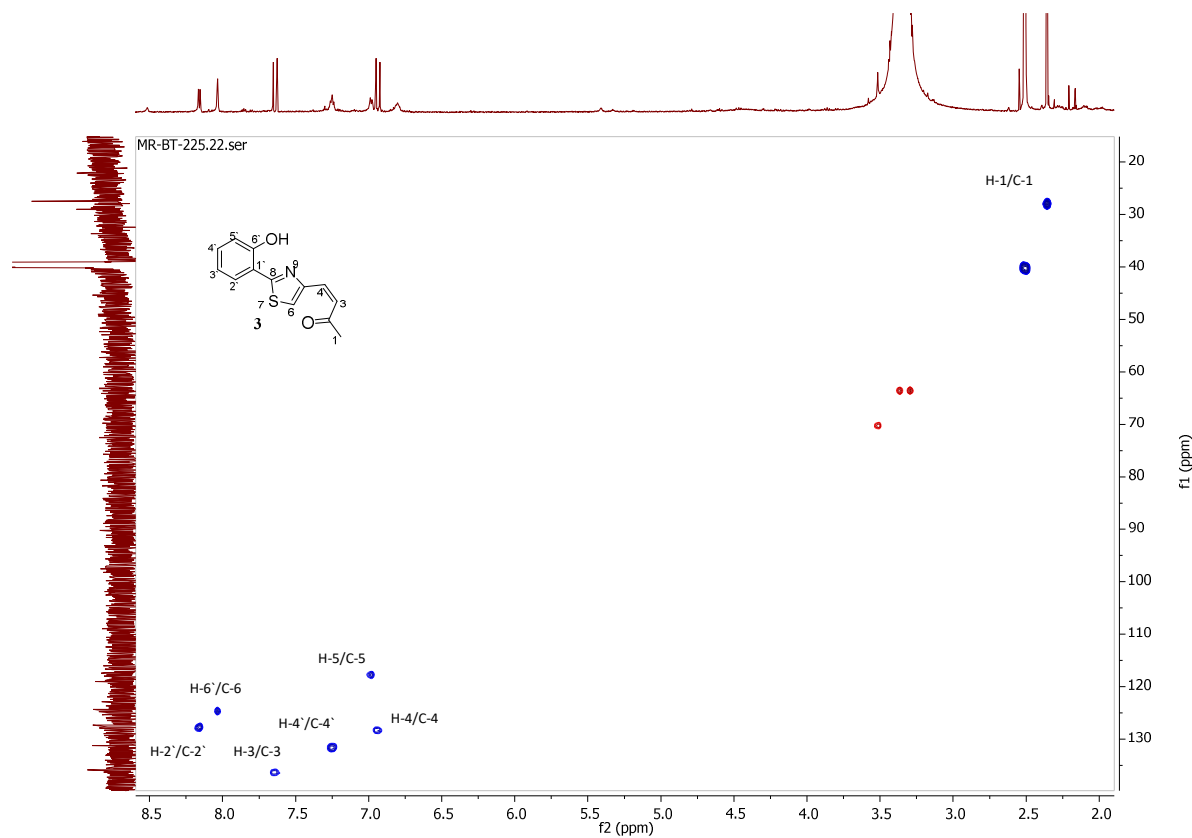


Figure S16. HSQC spectrum of compound 3.

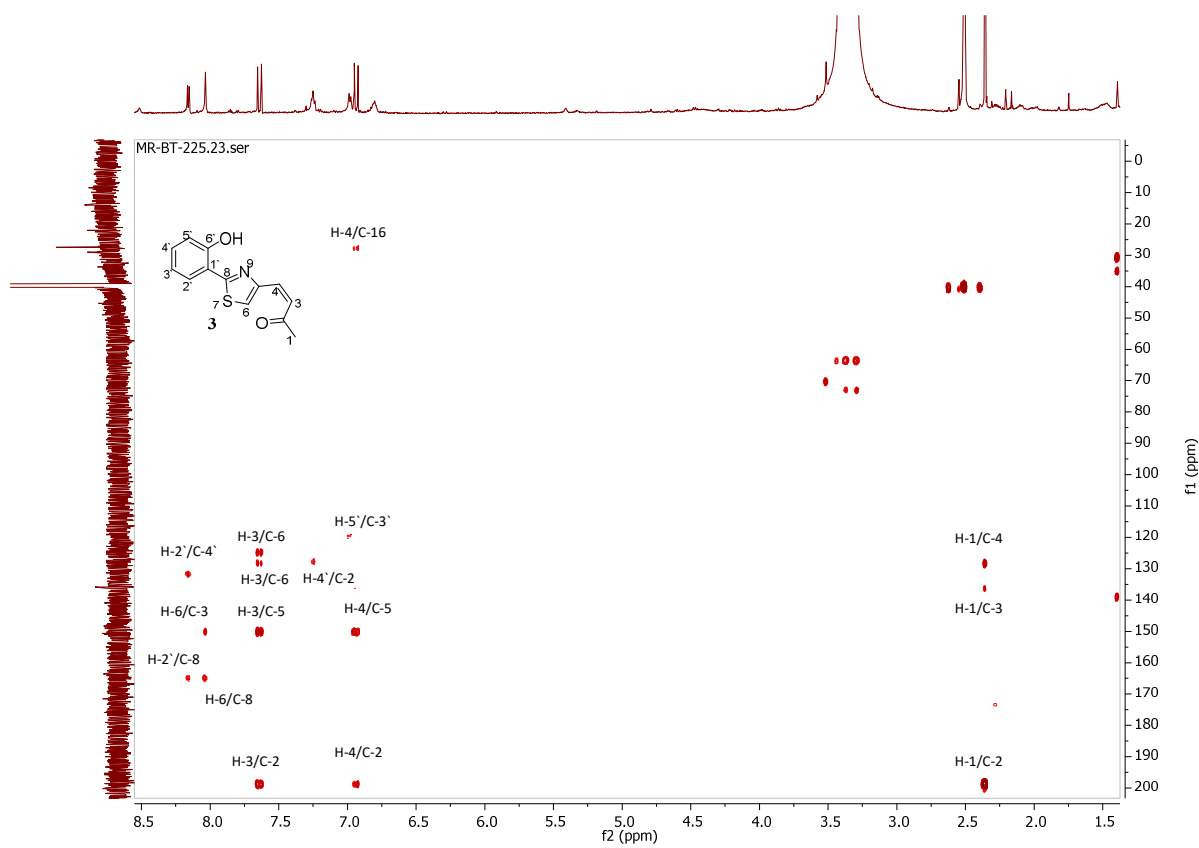


Figure S17. HMBC spectrum of compound 3.

MR485 #1505 RT: 13.14 AV: 1 NL: 2.20E5  
F: FTMS + p ESI Full ms [230.00-2000.00]

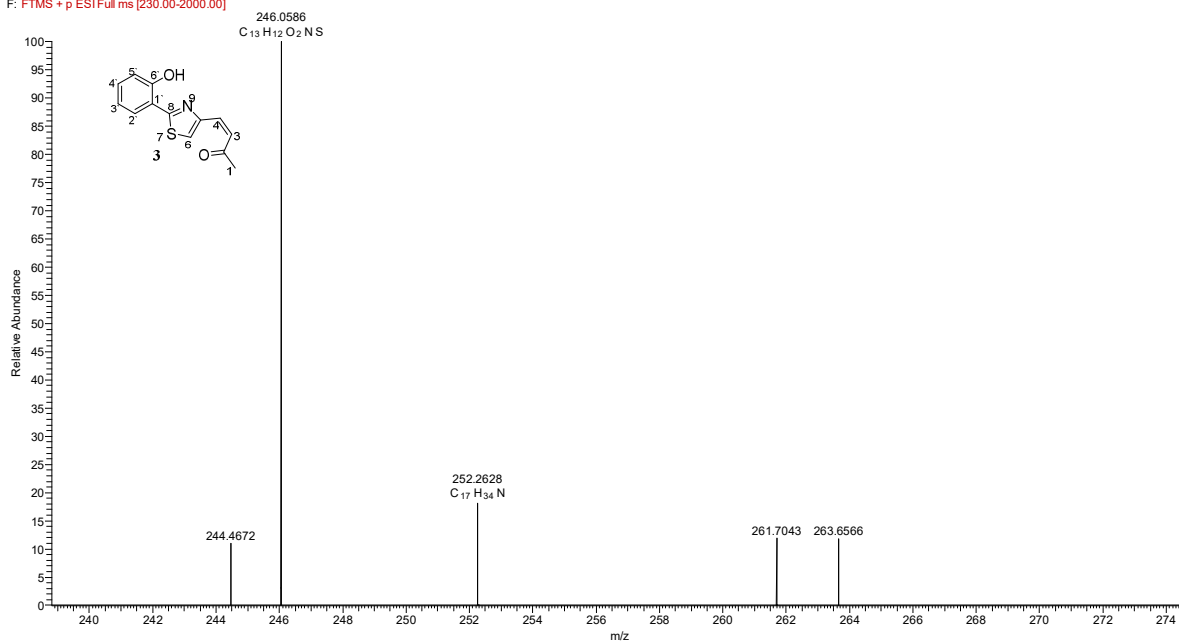


Figure S18. HRMS of compound 3.

Pulicatin cpd 2  
single\_pulse

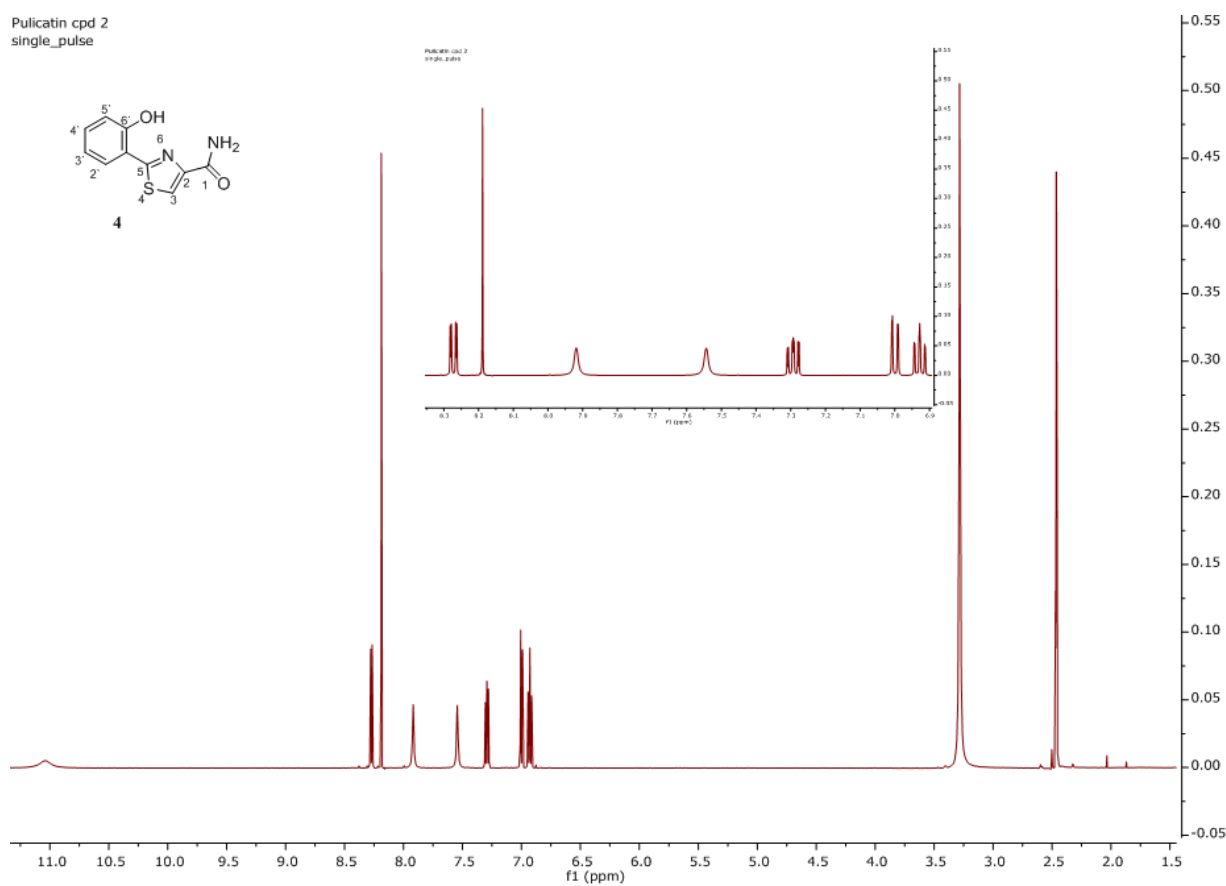


Figure S19. <sup>1</sup>H NMR spectrum of compound 4.

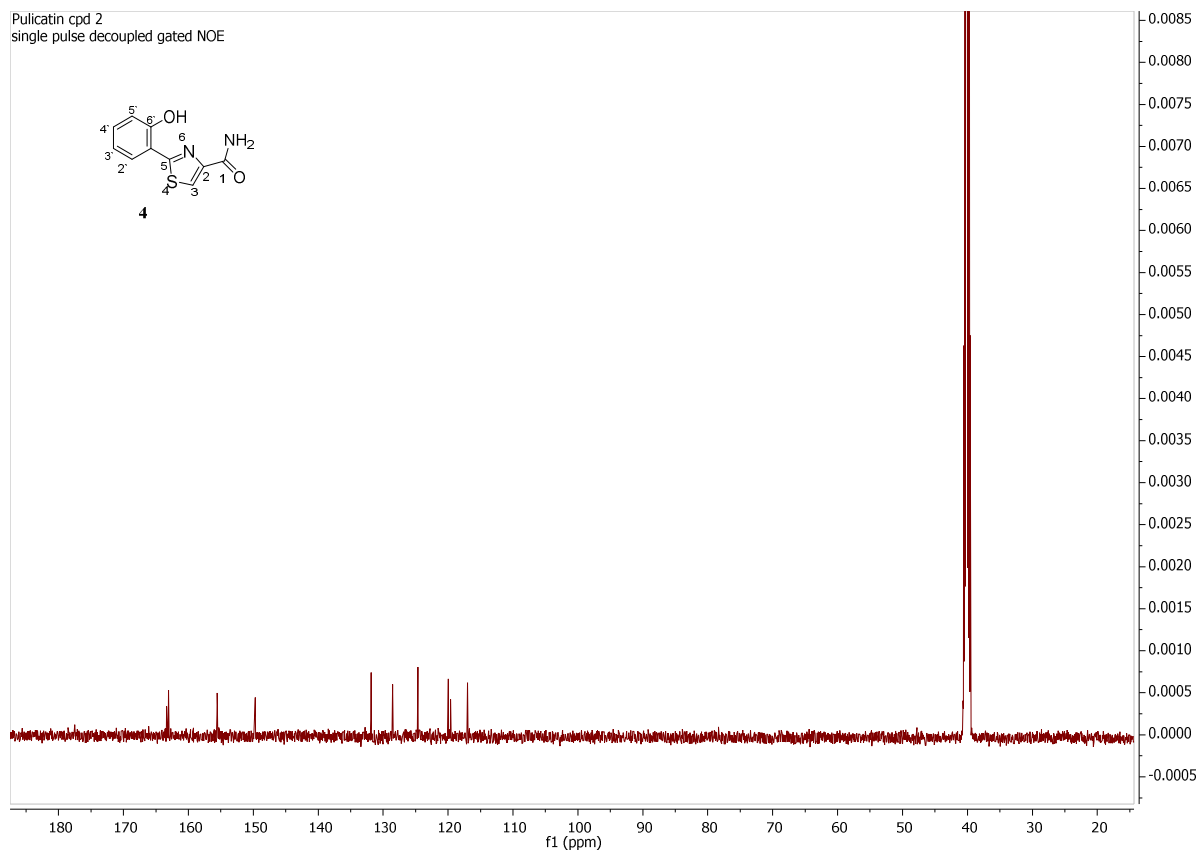


Figure S20.  $^{13}\text{C}$  NMR spectrum of compound 4.

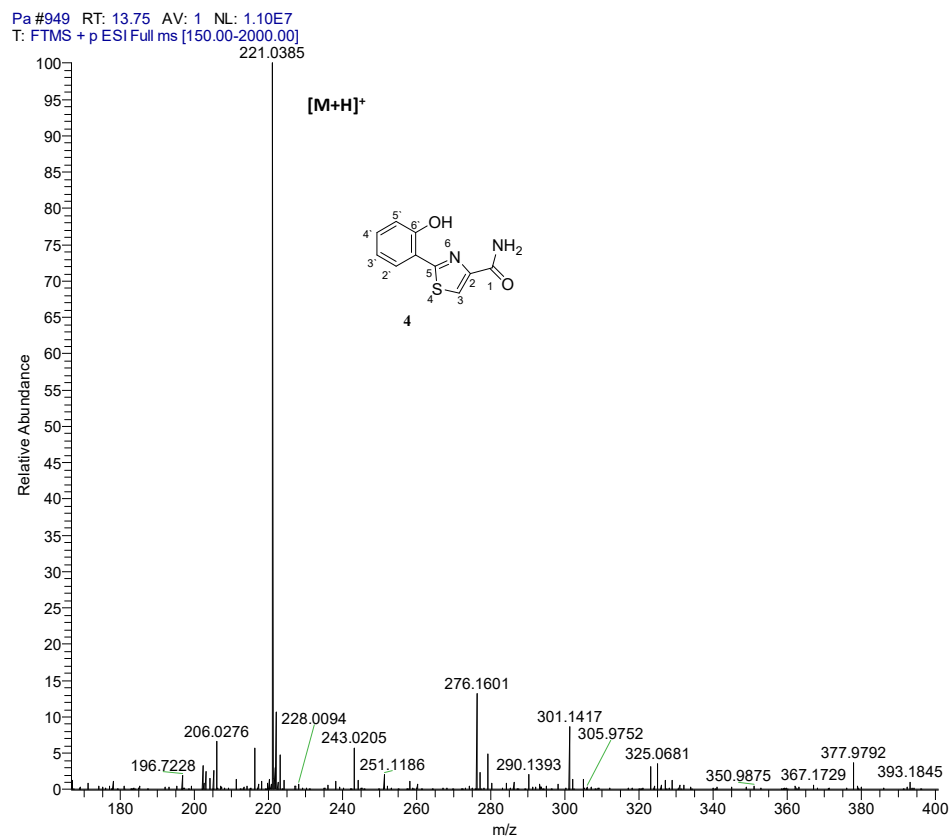


Figure S21. HRMS of compound 4.