Electronic Supplementary Information

HBr-Promoted Sulfenylation of Pyrazolones and 4-Hydroxylcoumarins with *N*-(organothio)succinimides

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1. General methods

^{1}H and ^{13}C NMR spectra were recorded on Bruker Ascend™ 400(400 MHz) using tetramethylsilane as an internal reference. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, m = multiplet, br = broad signal. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz. HRMS date were obtained

by ESI on a TOF mass analyser. The substrates, reagents and solvents were purchased from the Sinopharm Chemical Reagent Co., Adamas, Aladdin and TCI, and used as received.

2. General Procedure for 3

HBr (40% wt HBr aqueous solution, 84 μL, 0.6 mmol) and *N*-(organothio)succinimide (**1**, 0.6 mmol) were added to a solution of pyrazolone (**2**, 0.3 mmol) in 1,4-dioxane (3 mL). The reaction mixture was stirred in a sealed tube at 100 °C for 2 h. After completion of the reaction, the reaction mixture was diluted with water (15 mL), and was extracted for three times with ethyl acetate (3×10 mL). The organic layer was washed with water and dried over anhydrous sodium sulfate. The solvent was evaporated in vacuo, and the residue was subjected to column chromatography using ethyl acetate in petroleum ether as the eluent to afford the pure target product **3**.

3. General Procedure for 5

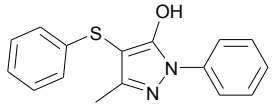
HBr (40% wt HBr aqueous solution, 84 μL, 0.6 mmol) and *N*-(organothio)succinimide (**1**, 0.6 mmol) were added to a solution of 4-hydroxycoumarins (**4**, 0.3 mmol) in 1,4-dioxane (3 mL). The reaction mixture was stirred in a sealed tube at 100 °C for 2 h. After completion of the reaction, the reaction mixture was diluted with water (10 mL), and extracted three times with ethyl acetate (3×10 mL). The organic layer was washed with water and dried over anhydrous sodium sulfate. The solvent was evaporated in vacuo, and the residue was subjected to column chromatography using ethyl acetate in petroleum ether as the eluent to afford the pure target product **5**.

4. Characterization Data for All products

The following compounds have all previously been reported in the literatures[1,2,3,4,5,6]: **3a, 3b, 3c, 3d, 3f, 3g, 3h, 3i, 3j, 3k, 3l, 3m, 3n, 3o, 5a, 5b, 5c, 5d** in the following six reference papers.

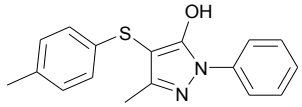
Reference 1: Purohit, V. B.; Karad, S. C.; Patel, K. H.; Raval, D. K. *Tetrahedron*. **2016**, *72*, 1114.
Reference 2: Zhao, X.; Lu, X. Y.; Wei, A. Q.; Jia, X. L.; Chen, J.; Lu, K. *Tetrahedron Lett.* **2016**, *57*, 5330.
Reference 3: Liu, X.; Cui, H.; Yang, D.; Dai, S.; Zhang, T.; Sun, J.; Wei, W.; Wang, H. *RSC Adv.*, **2016**, *6,* 51830.
Reference 4: Sun, P.; Yang, D.; Wei, W.; Sun, X.; Zhang, W.; Zhang, H.; Wang, Y.; Wang, H. *Tetrahedron* **2017**, *73*, 2022.
Reference 5: Gao, T.; Wei, X.-N. *Synlett* **2017**, *28*, 2499.
Reference 6: Parumala, S. K. R.; Peddinti, R. K. *Green Chem*. **2015**, *17*, 4068.

3-methyl-1-phenyl-4-(phenylthio)-*1H*-pyrazol-5-ol (3a)



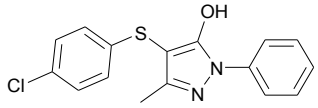
Compound **3a** was obtained in 90% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.08 (s, 1H), 7.73 (d, J = 7.8 Hz, 2H), 7.45 (t, J = 7.9 Hz, 2H), 7.25 (t, J = 7.5 Hz, 3H), 7.08 (dd, J = 14.8, 7.4 Hz, 3H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 156.91, 152.45, 138.80, 138.55, 129.48, 129.40, 126.18, 125.37, 125.29, 121.18, 87.75, 12.76.

3-methyl-1-phenyl-4-(p-tolylthio)-1H-pyrazol-5-ol (3b)



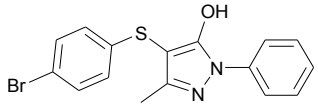
Compound **3b** was obtained in 92% yield according to general procedure. Colorless Solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.11 (s, 1H), 7.72 (d, J = 7.9 Hz, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.25 (t, J = 7.2 Hz, 1H), 6.96 (d, J = 7.9 Hz, 2H), 2.20 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.13, 152.41, 138.59, 135.19, 134.74, 130.09, 129.37, 126.12, 125.71, 121.13, 88.44, 20. 85, 12.76.

4-(4-chlorophenylthio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (3c)



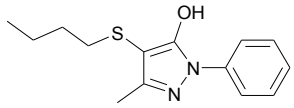
Compound **3c** was obtained in 85% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.18 (s, 1H), 7.74 (d, J = 7.8 Hz, 2H), 7.45 (t, J = 7.9 Hz, 2H), 7.30 (d, J = 8.6 Hz, 2H), 7.25 (t, J = 7.4 Hz, 1H), 7.07 (d, J = 8.5 Hz, 2H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.11, 152.33, 138.49, 138.02, 129.98, 129.38, 129.36, 126.99, 126.22, 121.20, 87.27, 12.71.

4-(4-bromophenylthio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (3d)



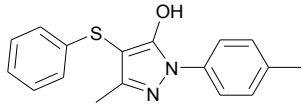
Compound **3d** was obtained in 82% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.22 (s, 1H), 7.73 (d, J = 6.9 Hz, 2H), 7.44 (s, 4H), 7.26 (d, J = 5.9 Hz, 1H), 7.01 (d, J = 7.3 Hz, 2H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.00, 152.37, 138.60, 138.46, 132.22, 129.40, 127.31, 126.24, 121.20, 118.12, 87.20, 12.71.

4-(*n*-butylthio)-3-methyl-1-phenyl-1H-pyrazol-5-ol (3e)



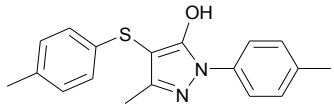
Compound **3e** was obtained in 73% yield according to general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 7.8 Hz, 2H), 7.15 (t, J = 7.7 Hz, 2H), 7.06 (t, J = 7.3 Hz, 1H), 2.33 (t, J = 7.2 Hz, 2H), 2.22 (s, 3H), 1.30 (m,5H), 0.81 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.50, 151.98, 136.15, 128.67, 125.82, 120.95, 95.02, 34.93, 31.71, 21.75, 13.72, 11.59. HRMS (ESI) m/z: calcd for $C_{14}H_{19}N_2OS$: 263.1218 $[M+H]^+$; found: 263.1220.

3-methyl-4-(phenylthio)-1-p-tolyl-1H-pyrazol-5-ol (**3f**)



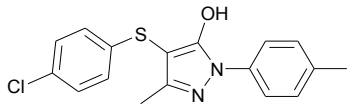
Compound **3f** was obtained in 90% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 11.86 (s, 1H), 7.61 (d, J = 8.3 Hz, 2H), 7.27 – 7.21 (m, 4H), 7.08 (t, J = 9.0 Hz, 3H), 2.29 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 156.87, 152.09, 147.52, 138.89, 136.23, 135.49, 129.77, 129.45, 125.32, 125.28, 121.25, 87.54, 20.94, 12.73.

3-methyl-1-p-tolyl-4-(p-tolylthio)-1H-pyrazol-5-ol (**3g**)



Compound **3g** was obtained in 90% yield according to general procedure. Colorless solid. ^{1} H NMR (400 MHz, d_6-DMSO) δ 11.86 (s, 1H), 7.61 (d, J = 8.3 Hz, 2H), 7.27 – 7.21 (m, 4H), 7.08 (t, J = 9.0 Hz, 3H), 2.29 (s, 3H), 2.11 (s, 3H); ^{13} C NMR (101 MHz, d_6-DMSO) δ 156.87, 152.09, 147.52, 138.89, 136.23, 135.49, 129.77, 129.45, 125.32, 125.28, 121.25, 87.54, 20.94, 12.73.

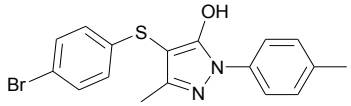
4-(4-chlorophenylthio)-3-methyl-1-p-tolyl-1H-pyrazol-5-ol (**3h**)



Compound **3h** was obtained in 86% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.05 (s, 1H), 7.60 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8. 1 Hz, 2H), 7.06 (d, J = 8.4 Hz, 2H), 2.28 (s, 3H),

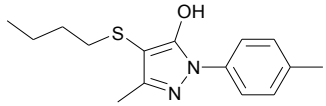
2.10 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.19, 152.00, 147.51, 138.09, 135.57, 129.96, 129.76, 129.32, 126.97, 121.27, 87.14, 20.93, 12.65.

4-(4-bromophenylthio)-3-methyl-1-p-tolyl-1H-pyrazol-5-ol (**3i**)



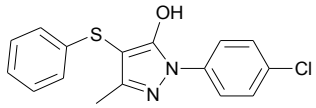
Compound **3i** was obtained in 85% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.14 (s, 1H), 7.60 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.2 Hz, 2H), 7.24 (d, J = 7.9 Hz, 2H), 7. 00 (d, J = 8.2 Hz, 2H), 2.29 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.30, 152.41, 138.59, 135.19, 134.74, 130.09, 129.37, 126.12, 125.71, 121.13, 88.59, 20.85, 12.76.

4-(butylthio)-3-methyl-1-p-tolyl-1H-pyrazol-5-ol (**3j**)



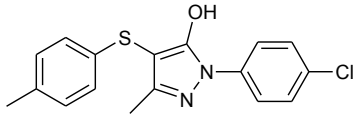
Compound **3j** was obtained in 76% yield according to general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 8.2 Hz, 2H), 6.93 (s, 2H), 2.32 (s, 2H), 2.20 (t, J = 12.6 Hz, 5H), 1.36 – 1.23 (m, 5H), 0.79 (d, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.02, 151.46, 135.61, 133.80, 129.20, 121.14, 94.66, 34.99, 31.71, 21.76, 20.94, 13.70, 11.59.

1-(4-chlorophenyl)-3-methyl-4-(phenylthio)-1H-pyrazol-5-ol (**3k**)



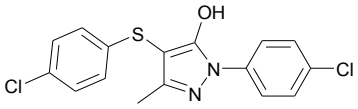
Compound **3k** was obtained in 85% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.24 (s, 1H), 7.78 (s, 2H), 7.49 (s, 2H), 7.23 (s, 2H), 7.06 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.41, 152.90, 138.65, 137.43, 130.15, 129.46, 129.34, 125.39, 125.33, 122.42, 88.01, 12.76.

1-(4-chlorophenyl)-3-methyl-4-(p-tolylthio)-1H-pyrazol-5-ol (**3l**)



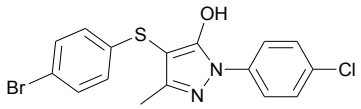
Compound **3l** was obtained in 88% yield according to general procedure. White solid, ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.19 (s, 1H), 7.77 (s, 2H), 7.48 (d, J = 5.4 Hz, 2H), 7.00 (d, J = 20.3 Hz, 4H), 2.18 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.32, 152.84, 137.48, 135.04, 134.77, 130.08, 129.32, 125.74, 122.35, 88.56, 20.84, 12.77.

1-(4-chlorophenyl)-4-(4-chlorophenylthio)-3-methyl-1H-pyrazol-5-ol (**3m**)



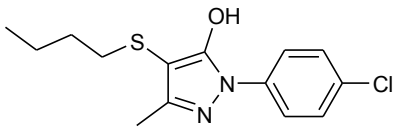
Compound **3m** was obtained in 85% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 7.76 (d, J = 8.7 Hz, 2H), 7.46 (d, J = 8.7 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 7.05 (d, J = 8.4 Hz, 2H), 2.09 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.65, 152.86, 137.81, 137.25, 130.25, 130.06, 129.31, 127.03, 122.43, 87.78, 12.63.

4-(4-bromophenylthio)-1-(4-chlorophenyl)-3-methyl-1H-pyrazol-5-ol (**3n**)



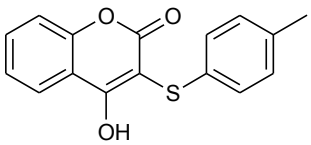
Compound **3n** was obtained in 81% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 11.91 (s, 1H), 7.77 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 8.6 Hz, 2H), 7.41 (d, J = 8.3 Hz, 2H), 7.00 (d, J = 8.3 Hz, 2H), 2.09 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 157.45, 152.79, 138.44, 137.35, 132.21, 130.20, 129.35, 127.33, 122.43, 118.17, 87.49, 12.73.

4-(butylthio)-1-(4-chlorophenyl)-3-methyl-1H-pyrazol-5-ol (**3o**)



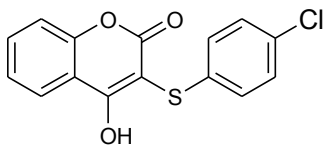
Compound **3o** was obtained in 70% yield according to general procedure. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.07 (s, 1H), 7.43 (d, J = 8.6 Hz, 2H), 7.12 (d, J = 8.6 Hz, 2H), 2.33 (t, J = 7.1 Hz, 2H), 2.26 (s, 3H), 1.36 – 1.26 (m, 4H), 0.81 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.85, 152.76, 134.58, 131.24, 128.74, 121.96, 95.40, 34.98, 31.72, 21.75, 13.70, 11.68.

4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (**5a**)



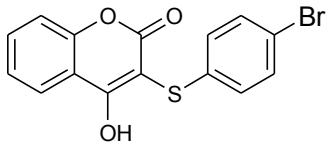
Compound **5a** was obtained in 89% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.61 (t, J = 7.6 Hz, 1H), 7.32 (t, J = 8.0 Hz, 2H), 7.25 (d, J = 7.7 Hz, 2H), 7.06 (d, J = 7.5 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.55, 160.79, 153.58, 137.62, 133.79, 130.12, 129.15, 124.37, 124.24, 116.93, 113.85, 105.77, 97.98, 20.97.

3-(4-chlorophenylthio)-4-hydroxy-2H-chromen-2-one (**5b**)



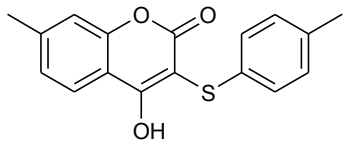
Compound **5b** was obtained in 87% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, DMSO) δ 7.93 (d, J = 7.8 Hz, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.45 – 7.22 (m, 4H), 7.20 (d, J = 8.4 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 168.97, 161.22, 153.48, 135.56, 134.13, 130.62, 129.35, 128.51, 124.81, 124.66, 116.91, 116.14, 94.60.

3-**(4-bromophenylthio)-4-hydroxy-2H-chromen-2-one** (**5c**)



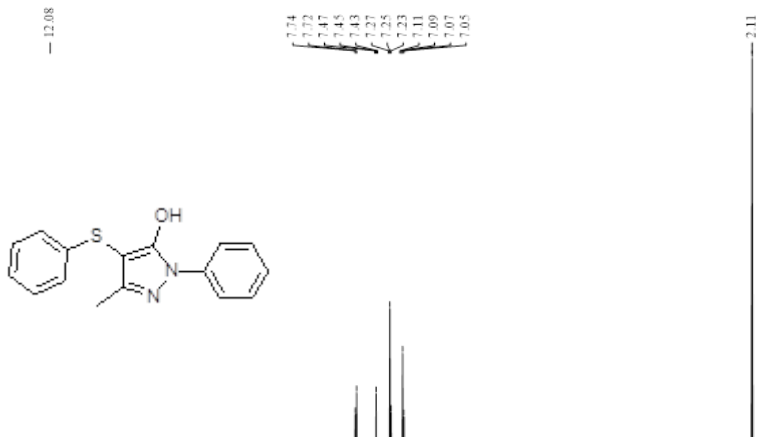
Compound **5c** was obtained in 84% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 7.93 (d, J = 7.7 Hz, 1H), 7.69 (t, J = 7.5 Hz, 1H), 7.47 – 7.35 (m, 4H) , 7.12 (d, J = 8.3 Hz, 2H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 169.09, 161.25, 153.49, 136.20, 134.18, 132.22, 128.71, 124.83, 124. 70, 118.73, 116.95, 116.21, 94.30.

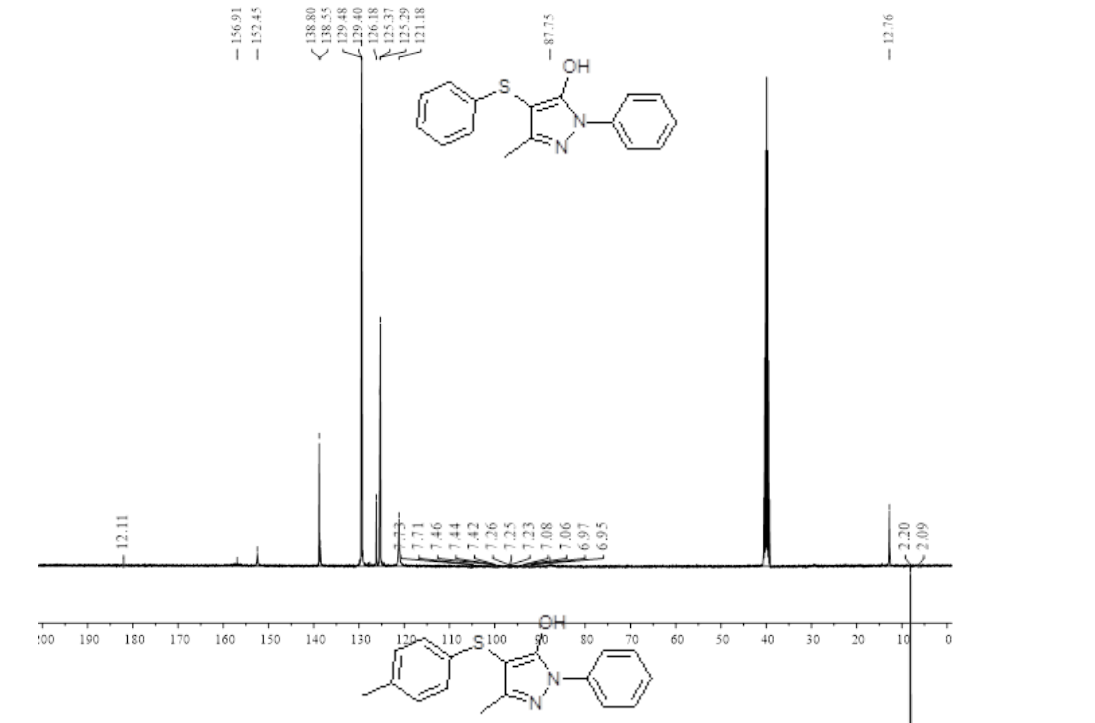
4-hydroxy-7-methyl-3-(p-tolylthio)-2H-chromen-2-one (**5d**)



Compound **5d** was obtained in 91% yield according to general procedure. Colorless solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ 7.69 (s, 1H), 7.45 (d, J = 7.8 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 7.11 – 7.04 (m, 4H), 2.35 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (101 MHz, d_6-DMSO) δ 168.33, 161.33, 151.52, 135.58, 134.81, 133.98, 132.68, 130.10, 127.36, 124.23, 116.64, 115.64, 95.63, 20.89, 20.77.

5. ^{1}H and ^{13}C NMR spectra of all the products




156.91
152.45
138.80
138.55
129.48
129.40
126.18
125.37
125.29
121.18
87.75
12.76
12.11
7.71
7.46
7.44
7.42
7.26
7.25
7.23
7.08
7.06
6.97
6.95
2.20
2.09
OH
S
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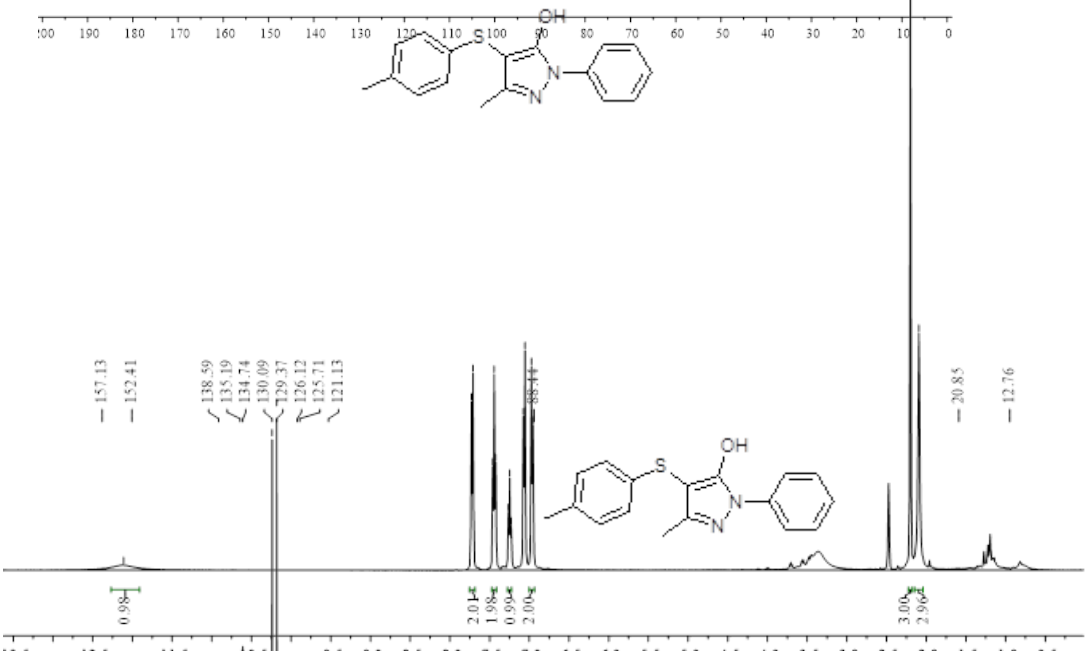
N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121.13
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S
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1.98
0.99
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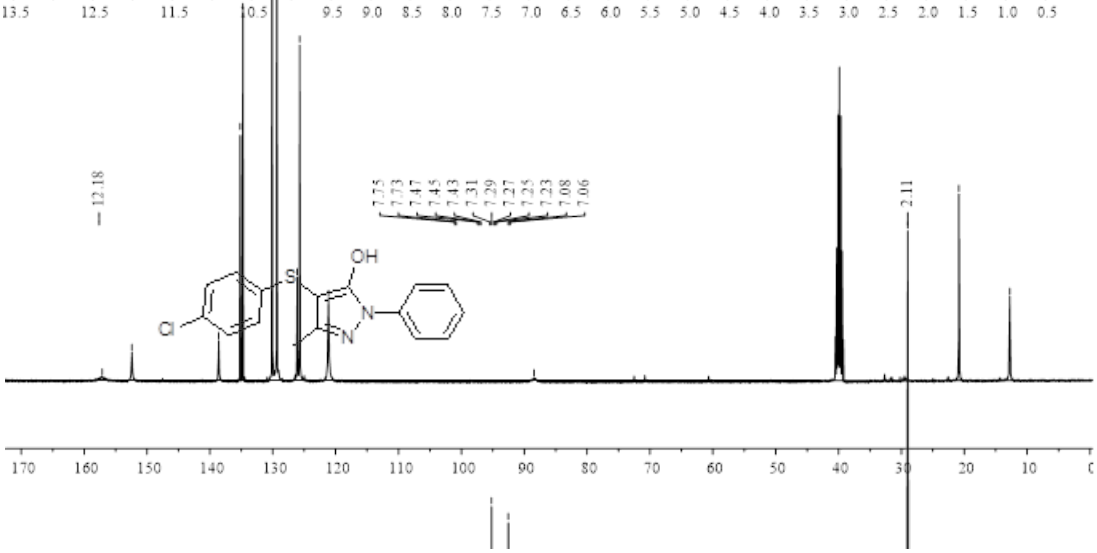
2.96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7.73
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7.29
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7.25
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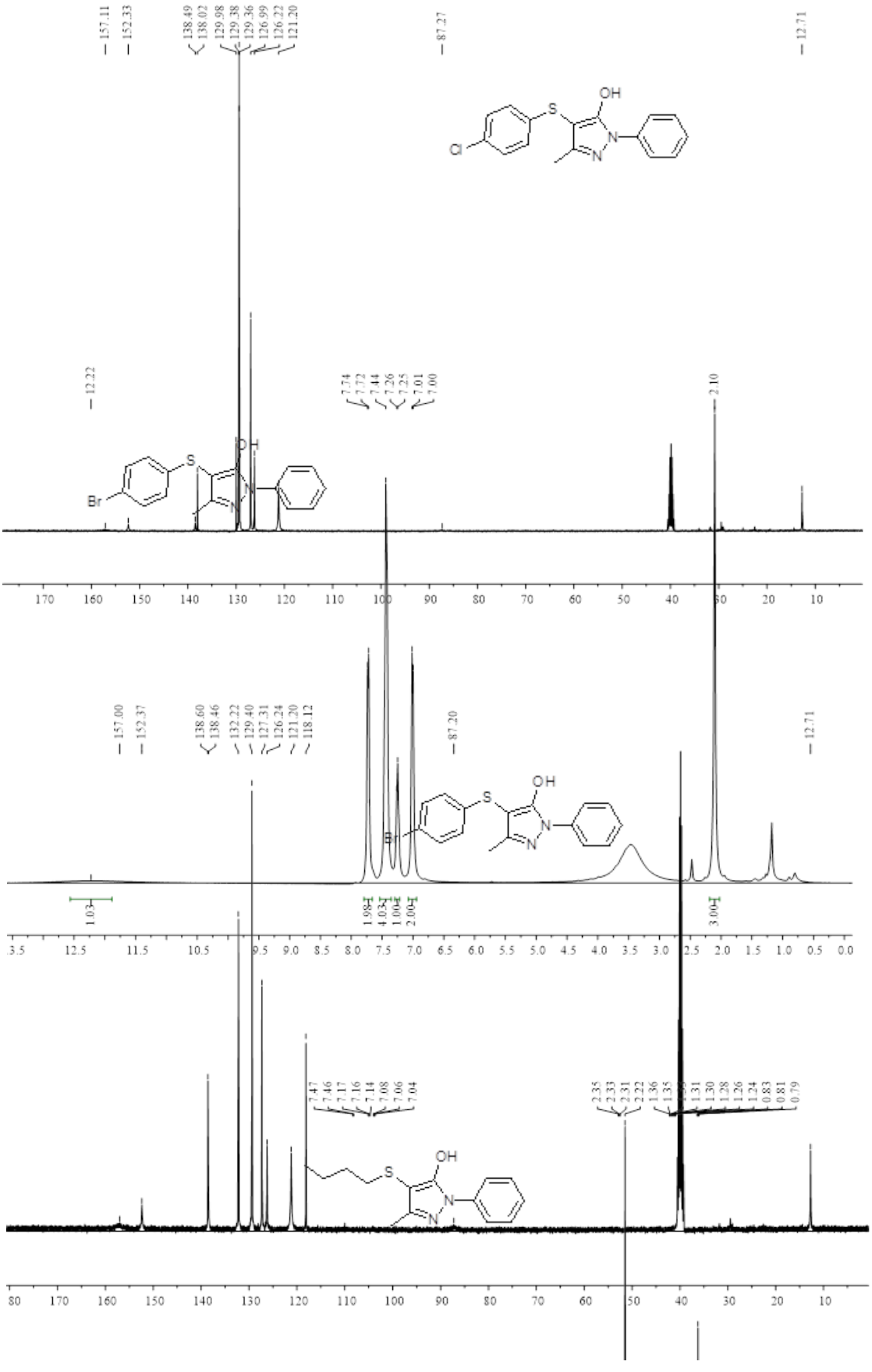
7.06
2.11
OH
Cl
Cl
N
N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126.99
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12.71
OH
S
Cl
N
12.22
7.74
7.72
7.44
7.26
7.25
7.01
7.00
2.10
Br
157.00
152.37
138.60
138.46
132.22
129.40
127.31
126.24
121.20
118.12
87.20
12.71
1.03
1.98
4.03
1.00
2.00
3.00
7.47
7.46
7.17
7.16
7.14
7.08
7.06
7.04
2.35
2.33
2.31
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1.35
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1.30
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1.26
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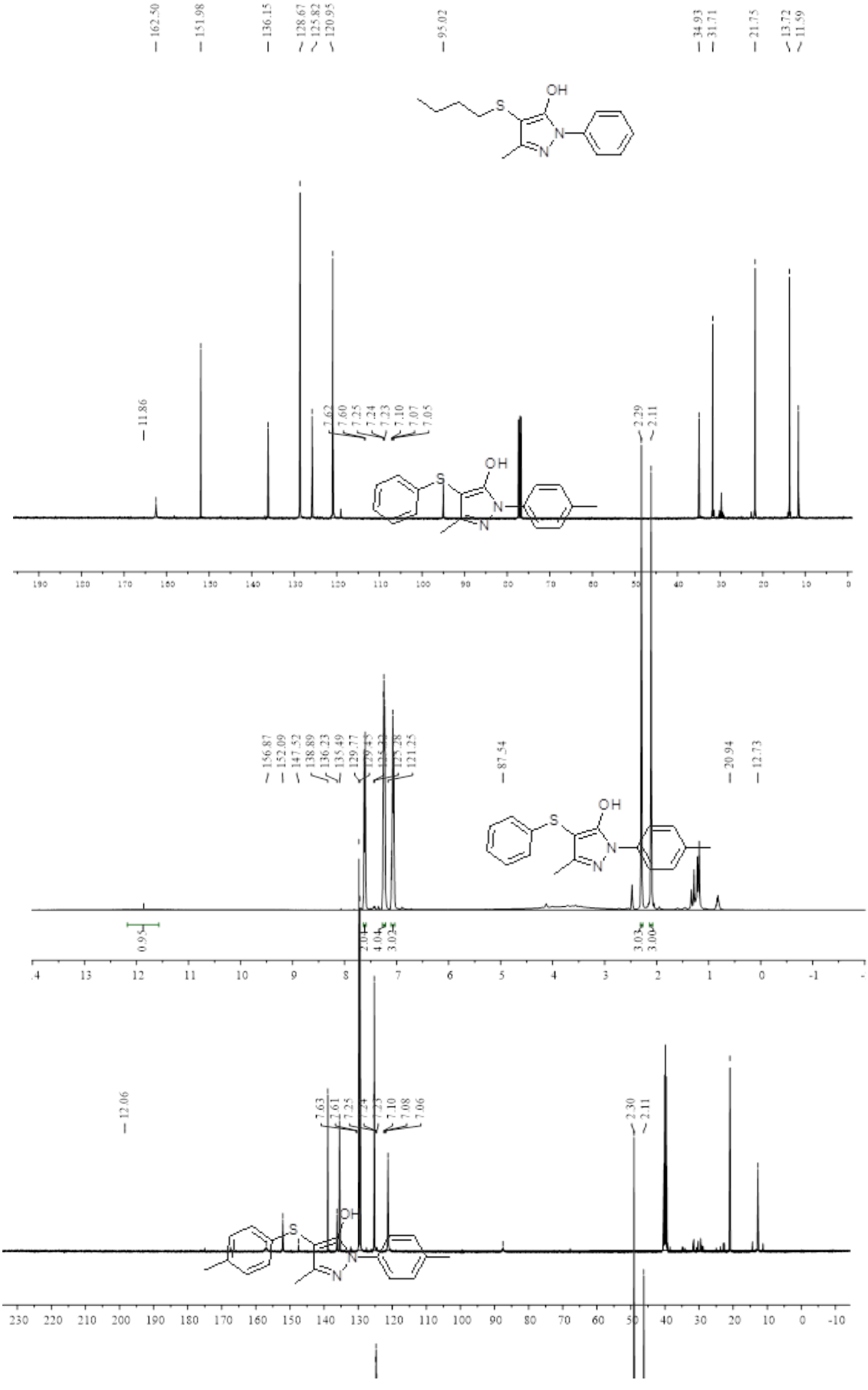
0.79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34.93
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21.75
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S
N
N
11.86
7.62
7.60
7.25
7.24
7.23
7.10
7.07
7.05
2.29
2.11
156.87
152.09
147.52
138.89
136.23
135.49
129.77
129.45
125.28
121.25
87.54
20.94
12.73
0.95
2.04
4.04
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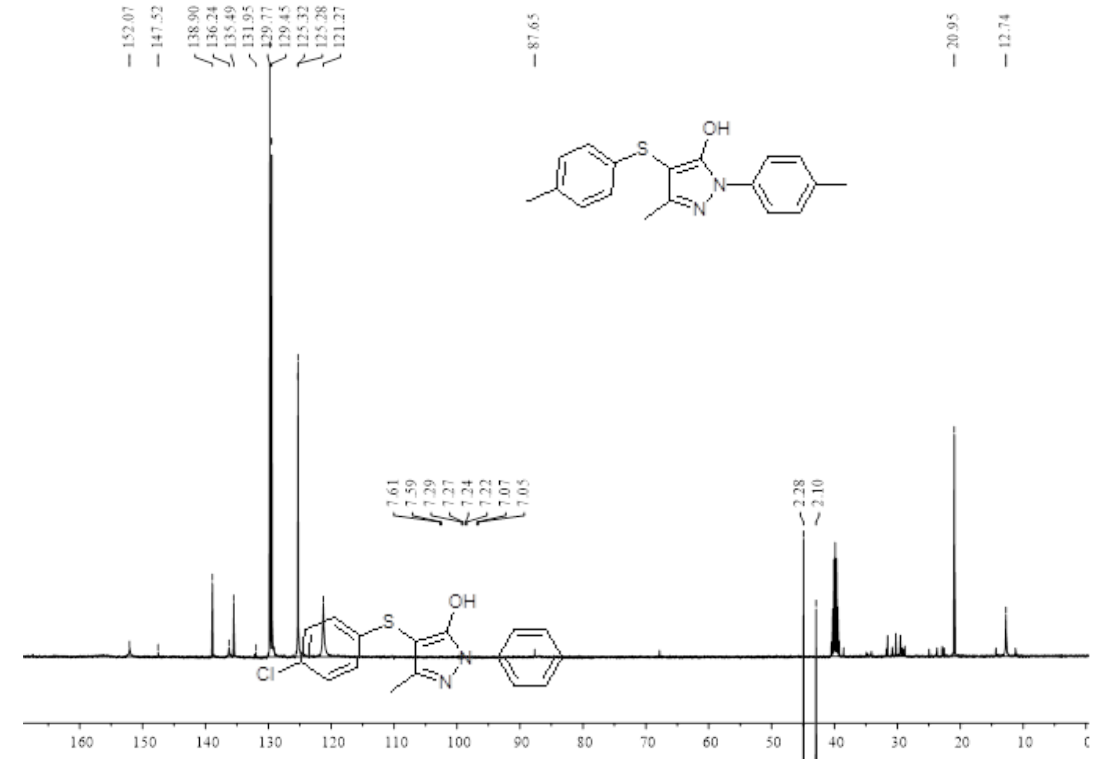
7.10
7.08
7.06
2.30
2.11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87.65
20.95
12.74
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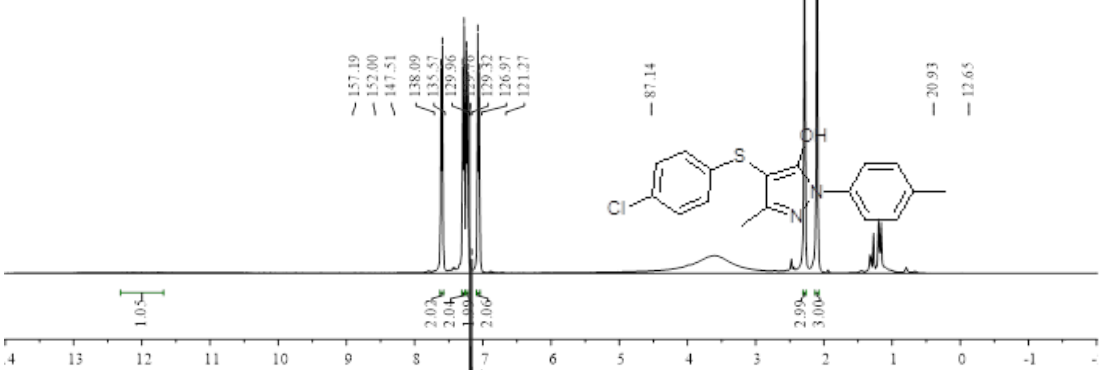
7.27
7.24
7.22
7.07
7.05
2.28
2.10
OH
S
N
Cl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2.04
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2.06
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3.00
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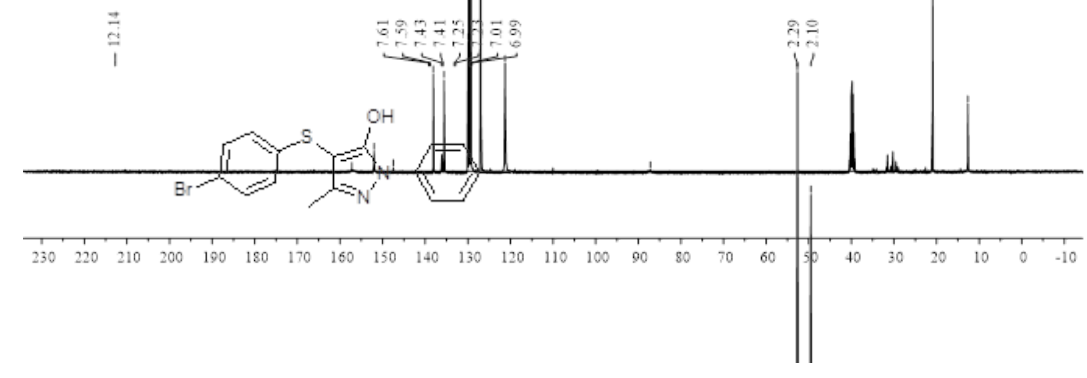
Cl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6.99
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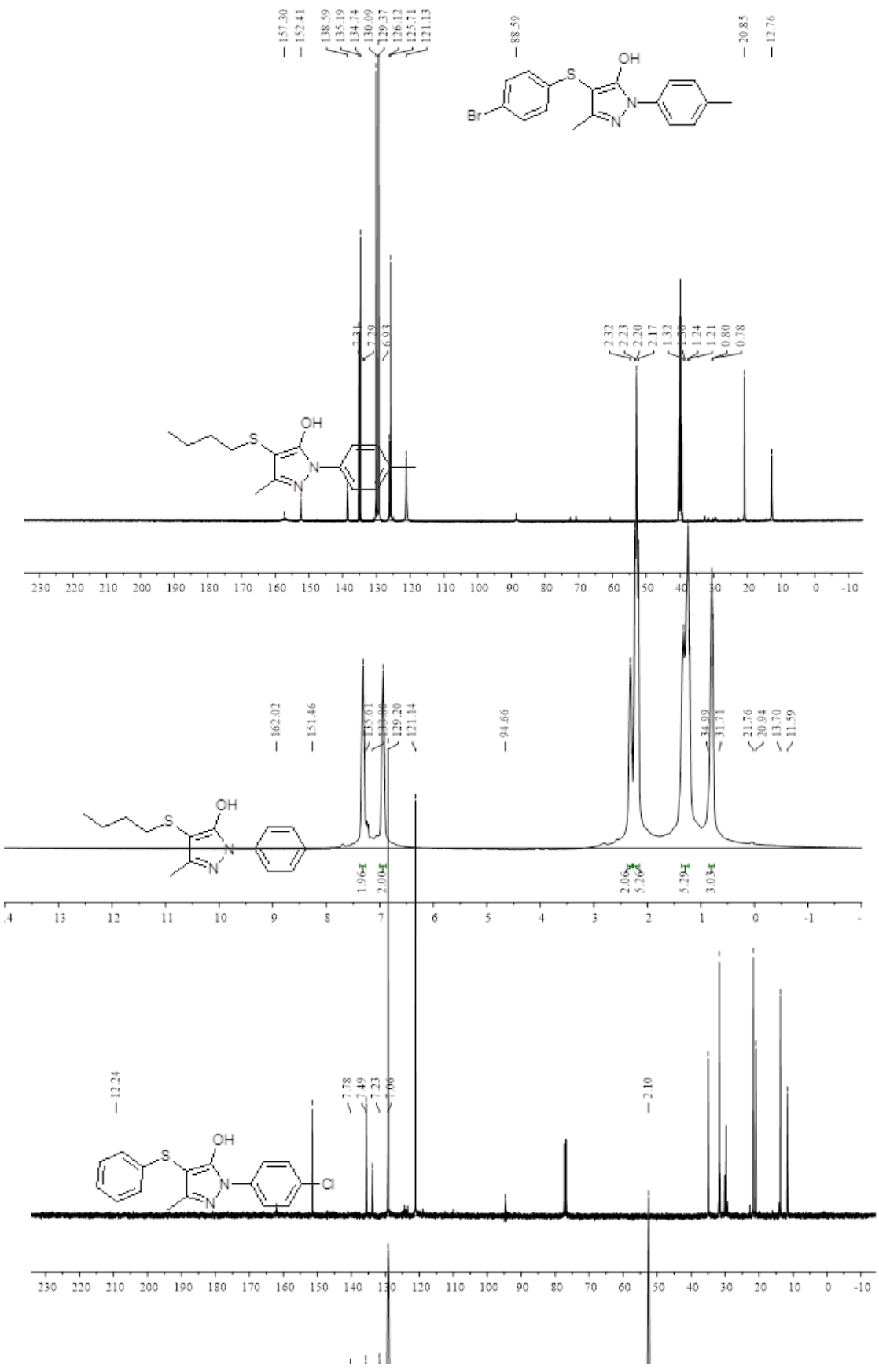
N
Br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12.76
OH
S
Br
N
N
7.31
7.29
6.93
2.32
2.23
2.20
2.17
1.32
1.30
1.24
1.21
0.80
0.78
OH
S
N
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
162.02
151.46
135.61
133.86
129.20
121.14
94.66
34.99
31.71
21.76
20.94
13.70
11.59
OH
S
N
N
1.96
2.00
2.06
5.96
5.29
3.03
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
12.24
7.78
7.49
7.23
7.06
2.10
OH
S
N
N
Cl
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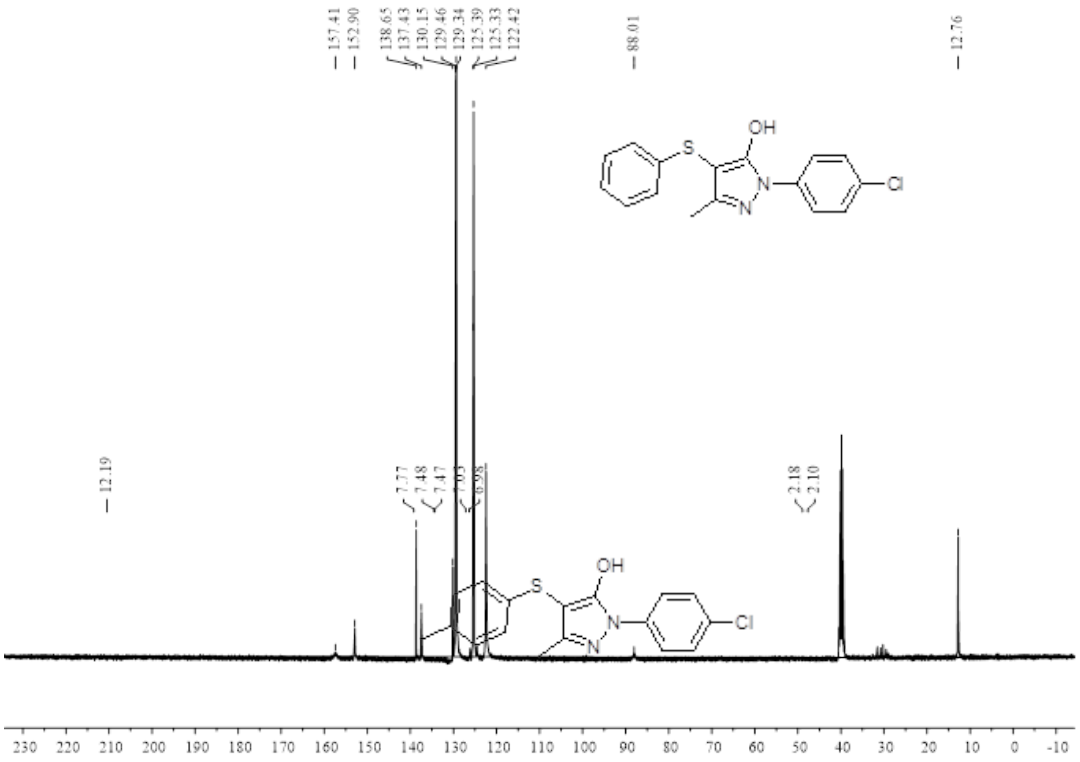
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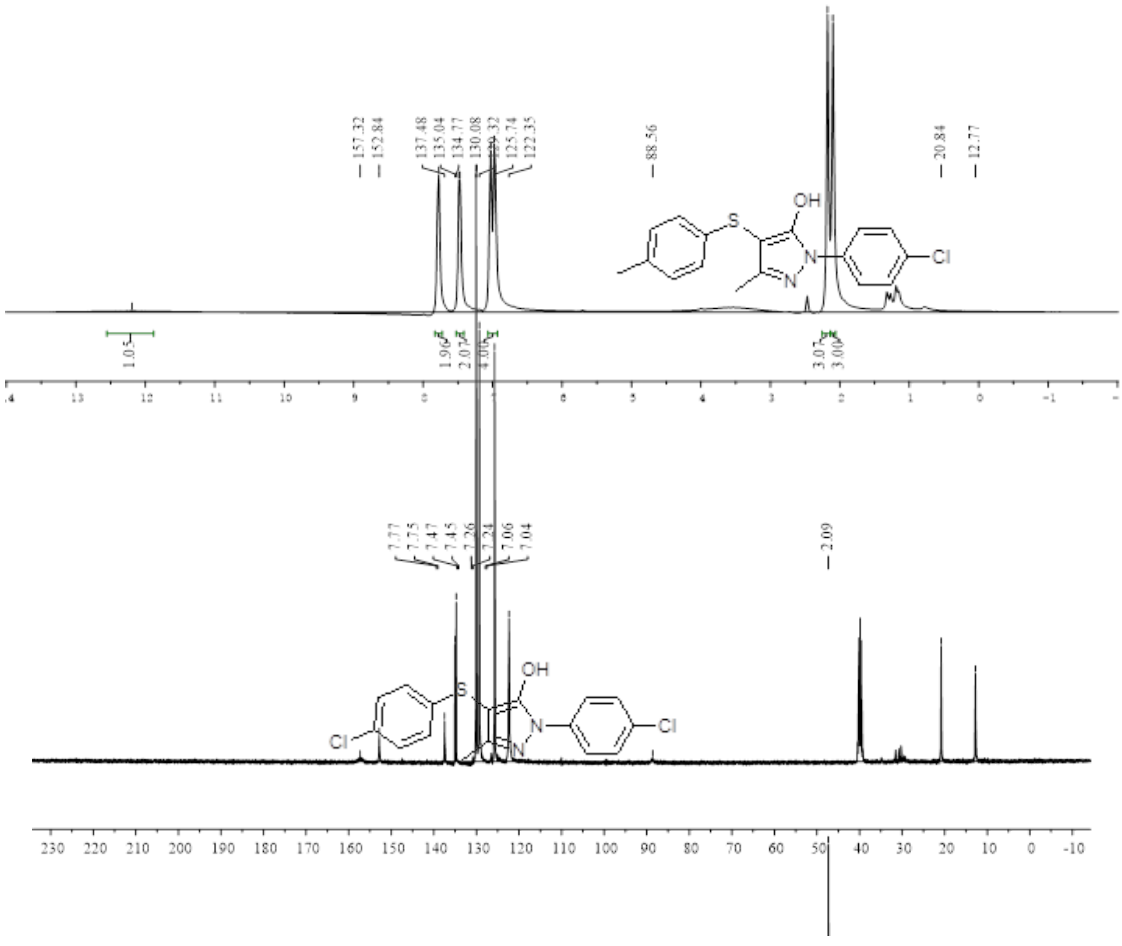
Cl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12.77
OH
S
N
N
Cl
1.05
1.96
2.07
4.08
3.07
3.00
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7.45
7.26
7.24
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2.09
OH
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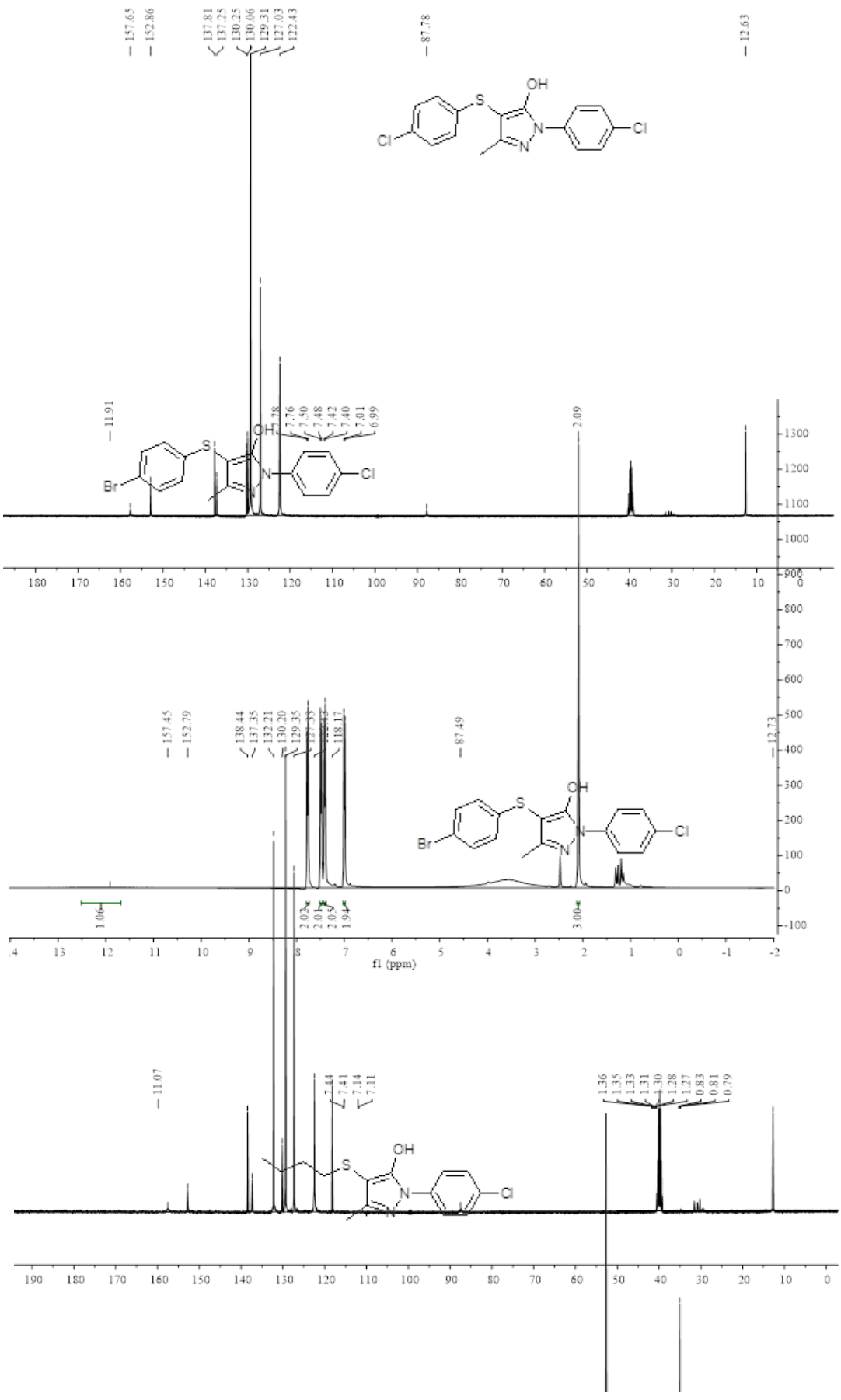
N
N
Cl
Cl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137.25
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130.06
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127.03
122.43
87.78
12.63
OH
S
Cl
N
N
Cl
11.91
7.78
7.76
7.50
7.48
7.42
7.40
7.01
6.99
2.09
Br
1.06
2.03
2.01
2.03
1.94
3.00
f1 (ppm)
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138.44
137.35
132.21
130.20
129.35
118.17
87.49
12.73
11.07
7.44
7.41
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1.28
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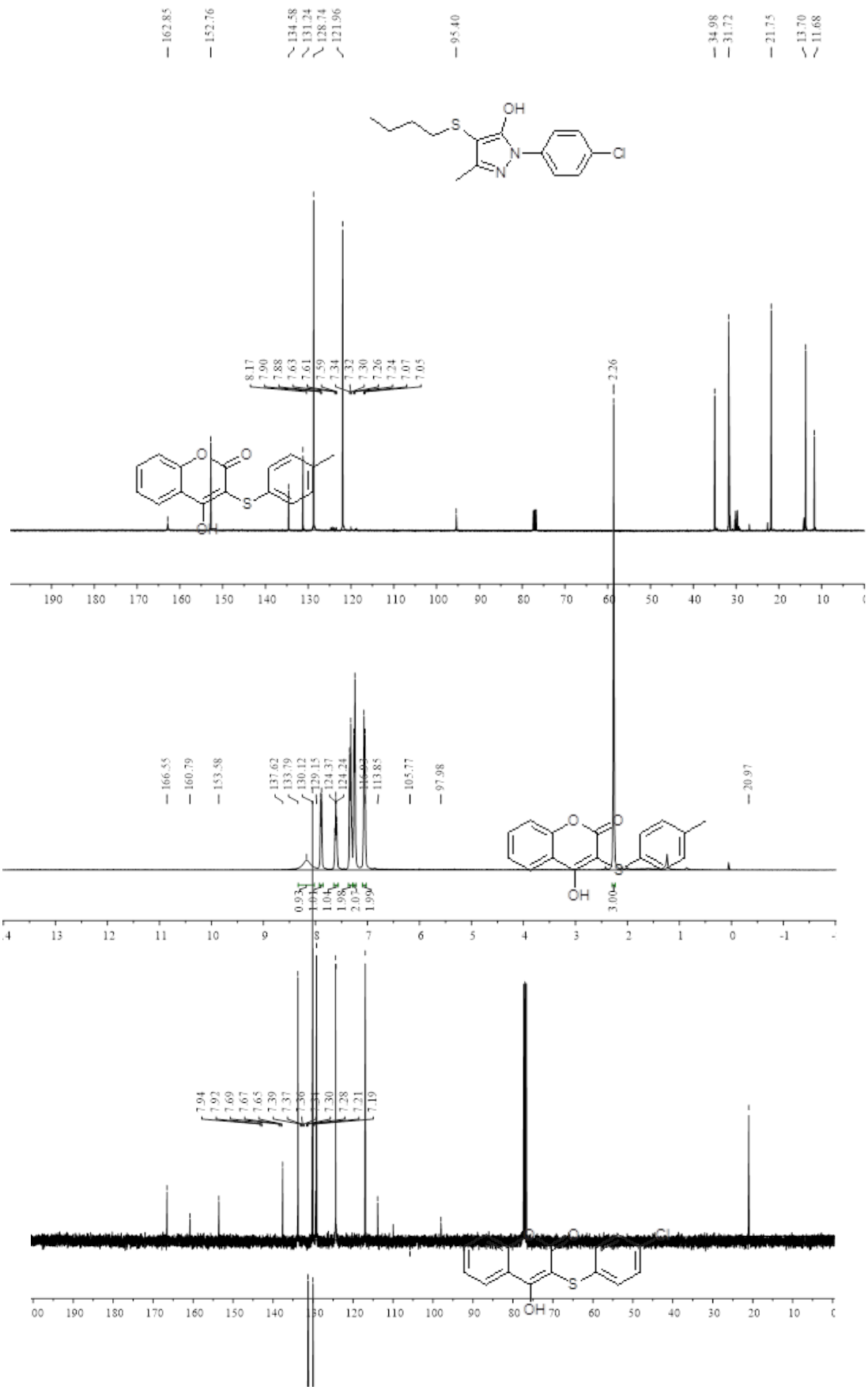
0.79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N
Cl
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7.88
7.63
7.61
7.59
7.34
7.32
7.30
7.26
7.24
7.07
7.05
2.26
O
O
S
OH
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
166.55
160.79
153.58
137.62
133.79
130.12
129.15
124.37
124.24
116.93
113.85
105.77
97.98
20.97
0.93
1.01
1.04
1.98
2.05
1.99
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
7.94
7.92
7.69
7.67
7.65
7.39
7.37
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7.28
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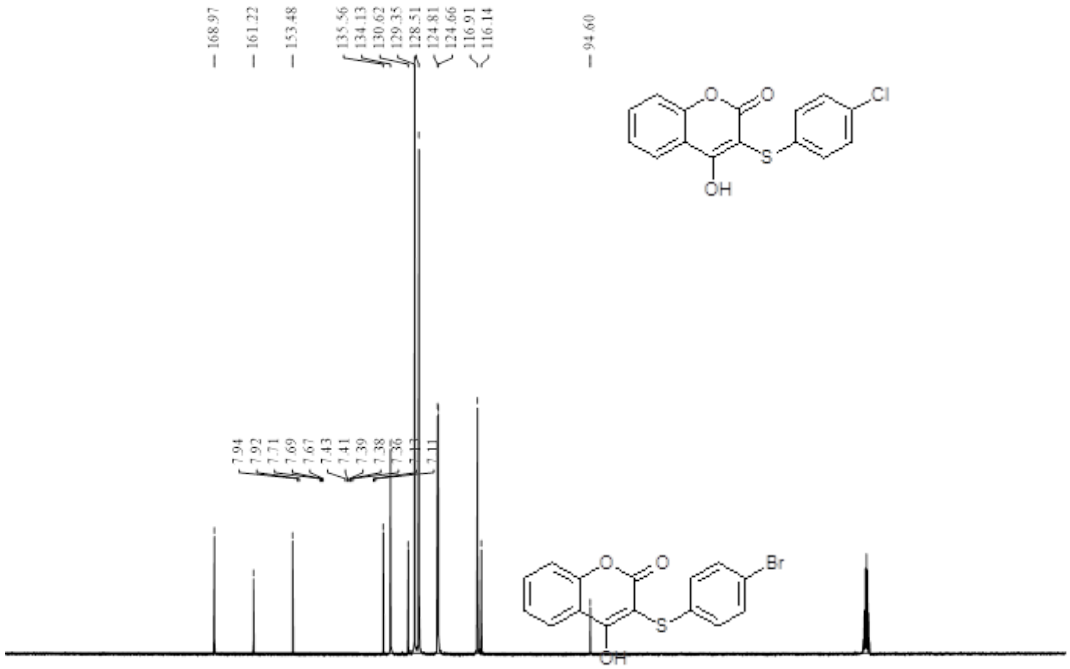
7.19
Cl
S
OH
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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94.60
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7.92
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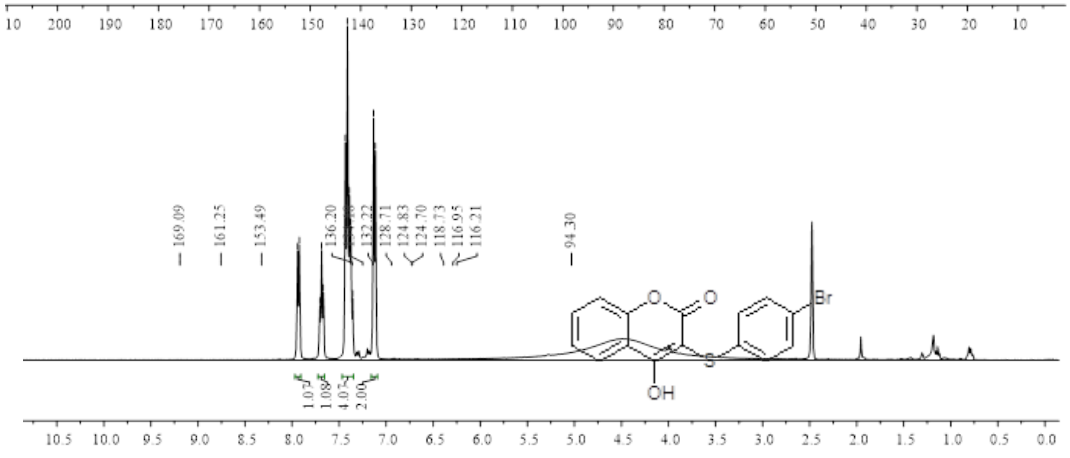
7.41
7.39
7.38
7.36
7.11
O
O
S
Cl
OH
Br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124.83
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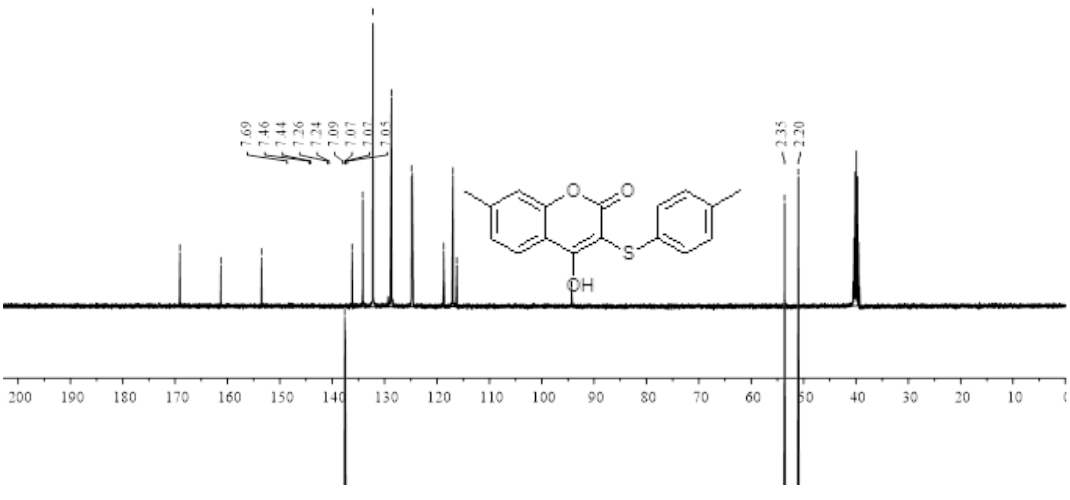
116.21
94.30
1.07
1.08
4.07
2.00
O
O
S
Br
OH


7.69
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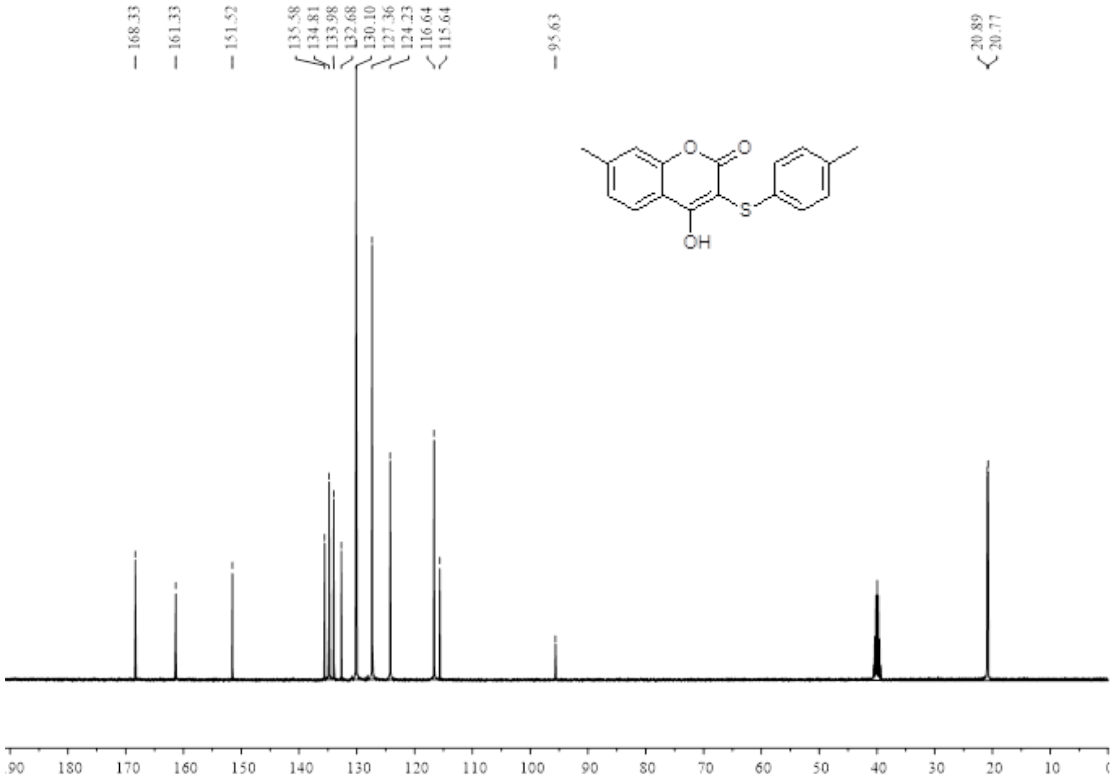
7.24
7.09
7.07
7.02
7.04
2.35
2.20
O
O
S
OH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O
O
S
OH
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10