

Supplementary Information

Synthesis and Antifungal Activity Against *Candida* Strains of Mesoionic System Derived From 1,3-Thiazolium-5-thiolate

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N-Methyl-C-p-isopropylphenylglycine **2**

Yield: 70%; m.p.: 164-166 °C; IR (KBr) ν_{\max} / cm⁻¹ 3210 (NH₂⁺), 3056, 3029 (CH_{Ar}), 2971 (CH_{Alif}), 1740 (C=O), 1588 (NH of NH₂⁺), 1550, 1425 (C=C_{Ar}), 1462 (C–O of C–O–H); ¹H NMR (200 MHz, CDCl₃) δ 1.14 (d, 6H, CH₃), 2.39 (s, 3H, CH₃–N), 2.86 (sept, 1H, CH), 4.96 (s, 1H, CH), 7.27 (d, 2H, CH_{Ar}), 7.42 (d, 2H, CH_{Ar}), 9.67 (s, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 169.21, 150.57, 129.13, 128.44, 127.38, 63.26, 33.43, 31.08, 23.90.

N-p-Chlorobenzoyl-N-methyl-C-p-isopropylphenylglycine **3**

Yield: 75%; m.p.: 145-147 °C; IR (KBr) ν_{\max} / cm⁻¹ 3113, 3019 (CH_{Ar}), 2987, 2932 (CH_{Alif}), 1721 (C=O, acid), 1633 (C=O, amide), 1609, 1587, 1483 (C=C), 1413 (C–O of C–O–H), 1087 (C–Cl); ¹H NMR (200 MHz, CDCl₃) δ 1.25 (d, 6H, CH₃), 2.74 (s, 3H, CH₃ of CH₃–N), 2.93 (sept, 1H, CH of isopropyl group), 6.39 (s, 1H, CH), 7.21 (d, 2H, CH_{Ar}), 7.34 (d, 2H, CH_{Ar}), 7.49 (d, 2H, CH_{Ar}), 7.78 (d, 2H, CH_{Ar}), 9.31 (s, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 171.12, 169.43, 148.79, 138.90, 136.38, 130.79, 130.02, 129.72, 128.17, 127.18, 58.87, 34.57, 33.71, 23.68.

Mesoionic 2-(p-chlorophenyl)-3-methyl-4-(p-isopropylphenyl)-1,3-thiazolium-5-thiolate **5**

Yield: 44%; m.p.: 173-175 °C; IR (KBr) ν_{\max} / cm⁻¹ 3008 (CH_{Ar}), 1643, 1590, 1484 (C=C and C=N of aromatic and mesoionic rings), 1431 (C–N), 1291 (C–S[–]), 1096 (C–Cl); ¹H NMR (200 MHz, CDCl₃) δ 1.22 (d, 6H, CH₃), 2.89 (sept, 1H, CH), 3.60 (s, 3H, CH₃), 7.26 (d, 2H, CH_{Ar}), 7.45 (d, 2H, CH_{Ar}), 7.48 (d, 2H, CH_{Ar}), 7.55 (d, 2H, CH_{Ar}); ¹³C NMR (50 MHz, CDCl₃) δ 160.30, 152.18, 149.65, 141.29, 137.63, 130.93, 130.72, 129.98, 129.66, 126.74, 125.14, 40.52, 33.78, 23.60.

2-Chloro-N-phenylacetamide **6a**

Yield: 93%; m.p.: 133-135 °C; IR (KBr) ν_{\max} / cm⁻¹

3267, 3205, 3143 (NH), 3098, 3049 (CH_{Ar}), 2947, 2862 (CH_{Alif}), 1672 (C=O), 1604, 1496 (C=C), 1290, 1250 (C–Cl), 1078, 858 (CH_{Ar}), 750 (NH), 557, 499 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 4.16 (s, 2H, CH₂), 7.15 (t, 1H, J 7.3 Hz, CH_{Ar}), 7.33 (t, 2H, J 7.8 Hz, CH_{Ar}), 7.52 (d, 2H, J 8.0 Hz, CH_{Ar}), 8.28 (s, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 164.01, 136.77, 129.22, 125.35, 120.27, 43.00.

2-Chloro-N-(p-nitrophenyl)acetamide **6b**

Yield: 80%; m.p.: 188-190 °C; IR (KBr) ν_{\max} / cm⁻¹ 3277, 3227, 3163 (NH), 3109, 3070 (CH_{Ar}), 2939, 2825 (CH_{Alif}), 1688 (C=O), 1624, 1506 (C=C), 1597, 1570, 1338 (NO₂), 1294, 1255 (C–Cl), 1172, 869, 850 (C–N of ArNO₂), 1111, 829 (CH_{Ar}), 748 (NH), 526 (C–C); ¹H NMR (200 MHz, DMSO-d₆) δ 4.36 (d, 2H, J 2.3 Hz, CH₂), 7.85 (dt, 2H, J 10.2, 2.7 Hz, CH_{Ar}), 8.26 (dt, 2H, CH_{Ar}), 10.93 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-d₆) δ 165.62, 144.61, 142.62, 125.07, 119.10, 43.62.

2-Chloro-N-(p-ethylphenyl)acetamide **6c**

Yield: 95%; m.p.: 140-142 °C; IR (KBr) ν_{\max} / cm⁻¹ 3308, 3273, 3201 (NH), 3088, 2965 (CH_{Ar}), 2964, 2868 (CH_{Alif}), 1668 (C=O), 1614, 1512 (C=C), 1292, 1254 (C–Cl), 1118, 864 (CH_{Ar}), 740 (NH), 540, 487 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.22 (t, 3H, CH₃), 2.63 (m, 2H, CH₂), 4.17 (s, 2H, CH₂), 7.18 (d, 2H, CH_{Ar}), 7.44 (d, 2H, CH_{Ar}), 8.23 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-d₆) δ 163.89, 141.53, 134.37, 128.56, 120.45, 43.00, 28.45, 15.72.

2-Chloro-N-(p-methylphenyl)acetamide **6d**

Yield: 95%; m.p.: 182-184 °C; IR (KBr) ν_{\max} / cm⁻¹ 3307, 3273, 3203 (NH), 3134, 3089 (CH_{Ar}), 2953 (CH_{Alif}), 1674 (C=O), 1616, 1552 (C=C), 1292, 1252 (C–Cl), 114, 864 (CH_{Ar}), 748 (NH), 505 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 2.33 (s, 3H, CH₃), 4.17 (s, 2H, CH₂), 7.15 (d, 2H, CH_{Ar}), 7.42 (d, 2H, CH_{Ar}), 8.21 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-d₆) δ 163.86, 135.11, 134.21, 129.73, 120.35, 42.66, 21.02.

2-Chloro-N-(*p*-bromophenyl)acetamide **6e**

Yield: 84%; m.p.: 184-186 °C; IR (KBr) ν_{max} / cm⁻¹ 3263, 3194 (NH), 3124, 3076 (CH_{Ar}), 2999, 2953 (CH_{Alif}), 1670 (C=O), 1610, 1550 (C=C), 1281, 1246 (C-Cl), 1188 (C-Br), 1072, 860 (CH_{Ar}), 736 (NH), 497 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.27 (s, 2H, CH₂), 7.55 (m, 4H, CH_{Ar}), 10.45 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 164.83, 137.85, 131.71, 121.28, 115.51, 43.56.

2-Chloro-N-(*p*-chlorophenyl)acetamide **6f**

Yield: 76%; m.p.: 170-172 °C; IR (KBr) ν_{max} / cm⁻¹ 3264, 3198 (NH), 3128, 3080 (CH_{Ar}), 3003, 2951 (CH_{Alif}), 1668 (C=O), 1612, 1551 (C=C), 1281, 1246 (C-Cl), 1095 (C-Cl of ArCl), 1010, 862 (CH_{Ar}), 737 (NH), 567, 501 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.27 (s, 2H, CH₂), 7.40 (d, 2H, CH_{Ar}), 7.63 (dd, 2H, CH_{Ar}), 10.45 (2, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 164.81, 137.44, 128.81, 127.45, 120.92, 43.54.

2-Chloro-N-(*p*-isopropylphenyl)acetamide **6g**

Yield: 78%; m.p.: 141-143 °C; IR (KBr) ν_{max} / cm⁻¹ 3271, 3199 (NH), 3130 (CH_{Ar}), 2960, 2870 (CH_{Alif}), 1674 (C=O), 1612, 1548 (C=C), 1282, 1250 (C-Cl), 1300, 1282 (*i*CH_{Alif}), 1016, 837 (CH_{Ar}), 779 (NH), 534 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 1.24 (d, 3H, CH₃), 2.90 (dt, 1H, CH₂), 4.17 (s, 2H, CH₂), 7.23 (t, 2H, CH_{Ar}), 7.45 (d, 2H, CH_{Ar}), 8.21 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 163.87, 146.19, 134.42, 127.16, 120.47, 43.01, 33.76, 24.12.

2-Chloro-N-(*p*-methoxyphenyl)acetamide **6h**

Yield: 80%; m.p.: 119-120 °C; IR (KBr) ν_{max} / cm⁻¹ 3296, 3199 (NH), 3136, 3072 (CH_{Ar}), 2956, 2835 (CH_{Alif}), 1666 (C=O), 1605, 1548 (C=C), 1346, 1301 (C-Cl), 1248, 1113 (C-O-C), 1029, 831 (CH_{Ar}), 788 (NH), 582, 532 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.79 (s, 3H, CH₃), 4.17 (s, 2H, CH₂), 6.88 (d, 2H, CH_{Ar}), 7.43 (d, 2H, CH_{Ar}), 8.20 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 163.89, 157.16, 129.79, 122.22, 114.34, 55.61, 42.97.

2-Chloro-N-(*m*-nitro-*p*-fluorophenyl)acetamide **6i**

Yield: 70%; m.p.: 90-92 °C; IR (KBr) ν_{max} / cm⁻¹ 3337, 3211 (NH), 3130, 3074 (CH_{Ar}), 2943, 2860 (CH_{Alif}), 1678 (C=O), 1608, 1552 (C=C), 1495, 1438, 1344 (NO₂), 1306, 1259 (C-Cl), 1080, 810 (CH_{Ar}), 885 (C-N of ArNO₂), 779 (NH), 596, 559 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.33 (s, 2H, CH₂), 7.53 (dd, 1H, CH_{Ar}), 7.89 (m, 1H, CH_{Ar}), 8.51 (dd, 1H, CH_{Ar}), 10.81 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 165.36, 150.81 (J 257.5 Hz), 135.82 (J 8.0 Hz), 135.30 (J 3.5 Hz), 126.73 (J 8.0 Hz), 118.94 (J 22.0 Hz), 115.88 (J 3.0 Hz), 43.45.

2-Chloro-N-(*m*-nitro-*p*-chlorophenyl)acetamide **6j**

Yield: 78%; m.p.: 120-122 °C; IR (KBr) ν_{max} / cm⁻¹ 3313, 3269 (NH), 3122, 3094 (CH_{Ar}), 2945, 2881 (CH_{Alif}), 1691 (C=O), 1605, 1544 (C=C), 1483, 1404, 1344 (NO₂), 1300, 1265 (C-Cl), 1131 (C-Cl of ArCl), 1045, 831 (CH_{Ar}), 895 (C-N of ArNO₂), 785 (NH), 559 (C-C); ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.32 (s, 2H, CH₂), 7.74 (d, 1H, CH_{Ar}), 7.81 (dd, 1H, CH_{Ar}), 8.40 (d, 1H, CH_{Ar}), 10.87 (s, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 165.54, 147.28, 138.33, 132.20, 124.27, 119.16, 115.76, 43.42.

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*-phenylacetamide)thio chloridate **7a**

Yield: 92.13%; m.p.: 130-132 °C; anal. calcd.: C, 60.58; H, 4.69; N, 5.43; S, 12.44; found: C, 60.60; H, 4.70; N, 5.42; S, 12.42; IR (KBr) ν_{max} / cm⁻¹ 3181 (NH), 3003 (CH_{Ar}), 2958 (CH_{Alif}), 1680 (C=O), 1599, 1551, 1491 (C=C and C=N of aromatic and heterocyclic rings), 1442 (C-N of N-CH₃), 1404 (C-N), 1092 (C-Cl), 1001, 922 (CH_{Ar}), 756 (NH), 557, 537 (C-C); ¹H NMR (200 MHz, CDCl₃) δ 1.30 (d, 6H, J 6.9 Hz, H-16, H-16'), 2.98 (sept, 1H, H-15), 3.79 (s, 2H, H-17), 3.84 (s, 3H, H-10), 7.09 (t, 2H, J 7.3 Hz, H-23), 7.28-7.34 (m, 4H, H-13, H-13', H-21, H-25), 7.60 (d, 2H, J 8.1 Hz, H-8, H-8'), 7.73 (d, 2H, J 7.9 Hz, H-12, H-12'), 7.86-7.93 (t, 4H, J 7.3 Hz, H-7, H-7', H-22, H-24), 11.02 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.21 (C-2), 166.81 (C-18), 152.68 (C-14), 140.28 (C-4), 138.93 (C-9), 132.04 (C-20), 131.64 (C-7, C-7'), 130.89 (C-12, C-12'), 130.27 (C-8, C-8'), 128.69 (C-22, C-24), 127.54 (C-13, C-13'), 124.09 (C-23), 123.79 (C-11), 123.59 (C-6), 120.28 (C-21, C-25), 42.24 (C-17), 40.92 (C-10), 34.21 (C-15), 23.76 (C-16, 16').

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*-(*p*-nitrophenyl)acetamide)thio chloridate **7b**

Yield: 94.97%; m.p.: 135-136 °C; anal. calcd.: C, 59.47; H, 4.42; N, 8.00; S, 12.21; found: C, 59.46; H, 4.40; N, 7.99; S, 12.22; IR (KBr) ν_{max} / cm⁻¹ 3317, 3277 (NH), 3071, 3028 (CH_{Ar}), 2939 (CH_{Alif}), 1688 (C=O), 1624, 1294 (NO₂), 1597, 1506 (C=C and C=N of aromatic and heterocyclic rings), 1408 (C-N of N-CH₃), 1338 (C-N), 1111 (C-Cl), 1009, 922 (CH_{Ar}), 850 (C-N of ArNO₂), 773 (NH), 567, 526 (C-C); ¹H NMR (200 MHz, CDCl₃) δ 1.26 (d, 6H, J 6.9 Hz, H-16, H-16'), 2.94 (sept, 1H, J 13.8, 6.9 Hz, H-15), 3.70 (s, 2H, H-17), 3.81 (s, 3H, H-10), 7.29 (d, 2H, J 3.6 Hz, H-13, H-13'), 7.66 (dd, 4H, J 10.7, 8.3 Hz, H-8, H-8', H-12, H-12'), 7.87 (d, 2H, J 8.4 Hz, H-7, H-7'), 8.11 (s, 4H, H-21, H-22, H-24, H-25), 11.58 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.82 (C-2), 167.69 (C-18), 155.01 (C-14), 153.02 (C-4), 145.09 (C-20), 143.34 (C-23), 140.65 (C-9), 131.45 (C-7, C-7'), 130.88 (C-12, C-12'), 130.40

(C-8, C-8'), 127.59 (C-13, C-13'), 124.69 (C-22, C-24), 123.52 (C-11), 123.41 (C-6), 119.96 (C-21, C-25), 42.34 (C-17), 40.90 (C-10), 34.21 (C-15), 23.75 (C-16, C-16').

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*(*p*-ethylphenyl)acetamide)thio chloride **7c**

Yield: 93.14%; m.p.: 127–129 °C; anal. calcd.: C, 61.87; H, 5.19; N, 5.15; S, 11.80; found: C, 61.85; H, 5.20; N, 5.14; S, 11.82; IR (KBr) ν_{max} / cm⁻¹ 3306, 3273 (NH), 3088, 3034 (CH_{Ar}), 2965 (CH_{Alif}), 1668 (C=O), 1553, 1512 (C=C and C=N of aromatic and heterocyclic rings), 1450 (C–N of N–CH₃), 1404 (C–N), 1118 (C–Cl), 962, 920 (CH_{Ar}), 743 (NH), 542 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.23 (dd, 9H, *J* 10.3, 6.9 Hz, H-16, H-16', CH₃), 2.74–3.00 (m, 3H, H-15, CH₂), 3.72 (s, 2H, H-17), 3.80 (s, 3H, H-10), 7.09 (d, 2H, *J* 8.4 Hz, H-22, H-24), 7.29 (d, 2H, *J* 3.8 Hz, H-13, H-13'), 7.55 (d, *J* 8.2 Hz, 2H, H-8, H-8'), 7.71 (t, 4H, *J* 7.1 Hz, H-12, H-12', H-21, H-25), 7.87 (d, *J* 8.3 Hz, 2H, H-7, H-7'), 10.83 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.21 (C-2), 166.53 (C-18), 154.00 (C-14), 152.65 (C-4), 144.61 (C-23), 140.26 (C-9), 136.62 (C-5), 132.12 (C-20), 131.68 (C-7, C-7'), 130.92 (C-12, C-12'), 130.26 (C-8, C-8'), 127.55 (C-22, C-24), 126.55 (C-13, C-13'), 123.84 (C-11), 123.64 (C-6), 120.35 (C-21, C-25), 42.32 (C-17), 40.88 (C-10), 34.20 (C-15), 33.68 (CH₂), 24.17 (C-16, C-16'), 23.77 (CH₃).

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*(*p*-methylphenyl)acetamide)thio chloride **7d**

Yield: 98.00%; m.p.: 170–172 °C; anal. calcd.: C, 61.87; H, 5.19; N, 5.15; S, 11.80; found: C, 61.89; H, 5.18; N, 5.13; S, 11.78; IR (KBr) ν_{max} / cm⁻¹ 3427, 3221 (NH), 3170, 3098 (CH_{Ar}), 2961 (CH_{Alif}), 1672 (C=O), 1545, 1512 (C=C and C=N of aromatic and heterocyclic rings), 1458 (C–N of N–CH₃), 1406 (C–N), 1091 (C–Cl), 1016, 928 (CH_{Ar}), 729 (NH), 557, 511 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.20 (d, 6H, *J* 6.9 Hz, H-16, H-16'), 2.22 (s, 3H, CH₃), 2.88 (sept, 1H, *J* 13.8, 6.8 Hz, H-15), 3.68 (s, 2H, H-17), 3.73 (s, 3H, H-10), 6.98 (d, 2H, *J* 8.1 Hz, H-22, H-24), 7.22 (d, 2H, *J* 7.1 Hz, H-13, H-13'), 7.50 (d, 4H, *J* 6.1 Hz, H-8, H-8', H-21, H-25), 7.65 (d, 2H, *J* 8.2 Hz, H-12, H-12'), 7.79 (d, 2H, *J* 6.2 Hz, H-7, H-7'), 10.92 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.34 (C-2), 166.90 (C-16), 154.24 (C-14), 152.63 (C-4), 140.24 (C-9), 136.18 (C-20), 133.84 (C-5), 131.97 (C-23), 131.68 (C-7, C-7'), 130.92 (C-12, C-12'), 130.30 (C-22, C-24), 129.14 (C-8, C-8'), 127.60 (C-13, C-13'), 123.83 (C-11), 123.61 (C-6), 120.30 (C-21, C-25) 42.09 (C-17), 40.96 (C-10), 34.20 (C-15), 23.78 (C-16, C-16'), 21.09 (CH₃).

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*(*p*-bromophenyl)acetamide)thio chloride **7e**

Yield: 92.73%; m.p.: 134–137 °C; anal. calcd.: C, 56.60; H, 4.40; N, 4.89; S, 11.19; found: C, 56.61; H, 4.42; N, 4.87; S, 11.18; IR (KBr) ν_{max} / cm⁻¹ 3262, 3194 (NH), 3111, 3076 (CH_{Ar}), 2999, 2953 (CH_{Alif}), 1670 (C=O), 1589, 1548, 1489 (C=C and C=N of aromatic and heterocyclic rings), 1433 (C–N of N–CH₃), 1394 (C–N), 1112 (C–Br), 1072 (C–Cl), 1011 (CH_{Ar}), 737 (NH), 694, 499 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.27 (d, 6H, *J* 6.9 Hz, H-16, H-16'), 2.95 (sept, 1H, H-15), 3.66 (s, 2H, H-17), 3.80 (s, 3H, H-10), 7.28 (d, 2H, *J* 8.8 Hz, H-13, H-13'), 7.34 (d, 2H, *J* 8.7 Hz, H-22, H-24), 7.59 (m, 2H, *J* 8.3 Hz, H-8, H-8'), 7.68 (d, 2H, *J* 8.1 Hz, H-12, H-12'), 7.79 (m, 2H, H-21, H-25), 7.86 (m, 2H, *J* 8.3 Hz, H-7, H-7'), 11.06 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.36 (C-2), 166.70 (C-18), 154.37 (C-4), 152.69 (C-14), 140.31 (C-9), 138.04 (C-20), 131.70 (C-5), 131.43 (C-7, C-7'), 131.40 (C-22, C-24), 130.73 (C-12, C-12'), 130.22 (C-8, C-8'), 127.42 (C-13, C-13'), 123.54 (C-11), 123.38 (C-6), 121.75 (C-21, C-25), 116.47 (C-23), 42.22 (C-17), 40.69 (C-10), 34.05 (C-15), 23.59 (C-16, C-16').

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*(*p*-chlorophenyl)acetamide)thio chloride **7f**

Yield: 97.20%; m.p.: 137–139 °C; anal. calcd.: C, 57.50; H, 4.47; N, 4.97; S, 11.37; found: C, 57.51; H, 4.48; N, 4.95; S, 11.36; IR (KBr) ν_{max} / cm⁻¹ 3263, 3198 (NH), 3130, 3080 (CH_{Ar}), 2951 (CH_{Alif}), 1668 (C=O), 1612, 1551, 1489 (C=C and C=N of aromatic and mesoionic rings), 1440 (C–N of N–CH₃), 1401 (C–N), 1095 (C–Cl), 1012, 920 (CH_{Ar}), 738 (NH), 501 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.27 (d, 6H, *J* 6.9 Hz, H-16, H-16'), 2.26 (s, 3H, CH₃), 2.95 (sept, 1H, *J* 13.8, 6.8 Hz, H-15), 3.68 (s, 2H, H-17), 3.80 (s, 3H, H-10), 7.19 (d, 2H, *J* 8.8 Hz, H-22, H-24), 7.29 (d, 2H, *J* 6.7 Hz, H-21, H-25), 7.58–7.69 (dd, 4H, *J* 15.1, 8.0 Hz, H-8, H-8', H-13, H-13'), 7.81–7.87 (dd, 4H, *J* 8.5, 3.6 Hz, H-7, H-7', H-12, H-12'), 11.00 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.53 (C-2), 166.83 (C-18), 154.57 (C-14), 152.87 (C-4), 140.50 (C-9), 137.62 (C-20), 131.84 (C-5), 131.53 (C-7, C-7'), 130.88 (C-12, C-12'), 130.40 (C-8, C-8'), 128.94 (C-23), 128.66 (C-22, C-24), 127.60 (C-13, C-13'), 123.64 (C-11), 123.50 (C-6), 121.54 (C-21, C-25), 42.38 (C-17), 40.91 (C-10), 34.20 (C-15), 23.76 (C-16, C-16').

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*(*p*-isopropylphenyl)acetamide)thio chloride **7g**

Yield: 92.93%; m.p.: 135–137 °C; anal. calcd.: C, 63.03; H, 5.64; N, 4.90; S, 11.22; found: C, 63.01; H, 5.63; N, 4.89;

S, 11.24; IR (KBr) ν_{max} / cm⁻¹ 3308, 3271 (NH), 3130, 3105 (CH_{Ar}), 2926 (CH_{Alif.}), 1674 (C=O), 1612, 1549, 1512 (C=C and C=N of aromatic and heterocyclic rings), 1446 (C–N of N–CH₃), 1408 (C–N), 1053 (C–Cl), 1018, 921 (CH_{Ar}), 740 (NH), 534 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.23 (dd, 12H, J 9.8, 7.0 Hz, H-16, H-16'), 2CH₃, 2.89 (sept, 2H, J 20.6, 13.7, 6.9 Hz, H-15, CH), 3.73 (s, 2H, H-17), 3.80 (s, 3H, H-10), 7.09 (d, 2H, J 8.3 Hz, H-22, H-24), 7.27 (d, 2H, J 6.6 Hz, H-13, H-13'), 7.55 (d, 2H, J 7.9 Hz, H-8, H-8'), 7.67-7.74 (t, 4H, J 6.8 Hz, H-12, H-12', H-21, H-25), 7.87 (d, 2H, J 8.0 Hz, H-7, H-7'), 10.85 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.13 (C-2), 166.53 (C-18), 153.77 (C-14), 152.62 (C-4), 144.66 (C-23), 140.22 (C-9), 136.58 (C-5), 132.15 (C-20), 131.69 (C-7, C-7'), 130.91 (C-12, C-12'), 130.24 (C-8, C-8'), 127.52 (C-22, C-24), 126.54 (C-13, C-13'), 123.83 (C-11), 123.62 (C-6), 42.23 (C-17), 40.95 (C-10), 34.17 (CH), 33.67 (C-15), 24.15 (2CH₃), 27.76 (C-16, C-16').

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*-(*p*-methoxyphenyl)acetamide)thiochloridate 7h

Yield: 95.48%; m.p.: 132-135 °C; anal. calcd.: C, 64.17; H, 5.38; N, 5.34; S, 12.24; found: C, 64.18; H, 5.36; N, 5.33; S, 12.23; IR (KBr) ν_{max} / cm⁻¹ 3231, 3180 (NH), 3119, 3038 (CH_{Ar}), 2958 (CH_{Alif.}), 1668 (C=O), 1606, 1548, 1510 (C=C and C=N of aromatic and heterocyclic rings), 1492 (C–N of N–CH₃), 1410 (C–N), 1240, 1091 (C–O–C), 1063 (C–Cl), 1018, 958 (CH_{Ar}), 744 (NH), 559 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.23 (d, 6H, J 6.9 Hz, H-16, H-16'), 2.92 (sept, 1H, J 13.8, 6.9 Hz, H-15), 3.65 (s, 2H, H-17), 3.72 (s, 3H, CH₃), 3.76 (s, 3H, H-10), 6.73 (d, 2H, H-22, H-24), 7.26 (d, 2H, H-13, H-13'), 7.53 (d, 2H, H-12, H-12'), 7.63-7.74 (dd, 4H, H-8, H-8', H-21, H-25), 7.82 (d, 2H, J 8.4 Hz, H-7, H-7'), 10.77 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.23 (C-2), 166.21 (C-18), 156.24 (C-23), 154.08 (C-14), 152.65 (C-4), 140.33 (C-9), 132.32 (C-5), 132.09 (C-20), 131.65 (C-7, C-7'), 130.91 (C-8, C-8'), 130.24 (C-12, C-12'), 127.60 (C-13, C-13'), 123.84 (C-11), 123.60 (C-6), 121.72 (C-21), 113.84 (C-22), 55.53 (CH₃ of O–CH₃), 42.34 (C-17), 40.91 (C-10), 34.18 (C-15), 23.82 (C-16, C-16').

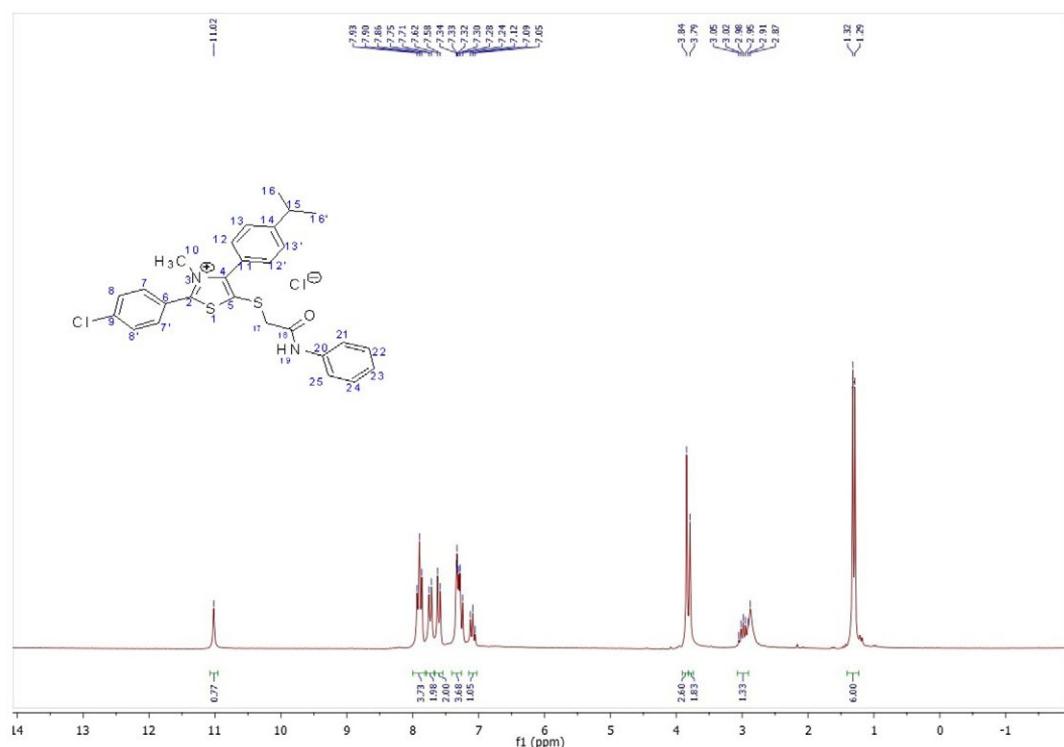
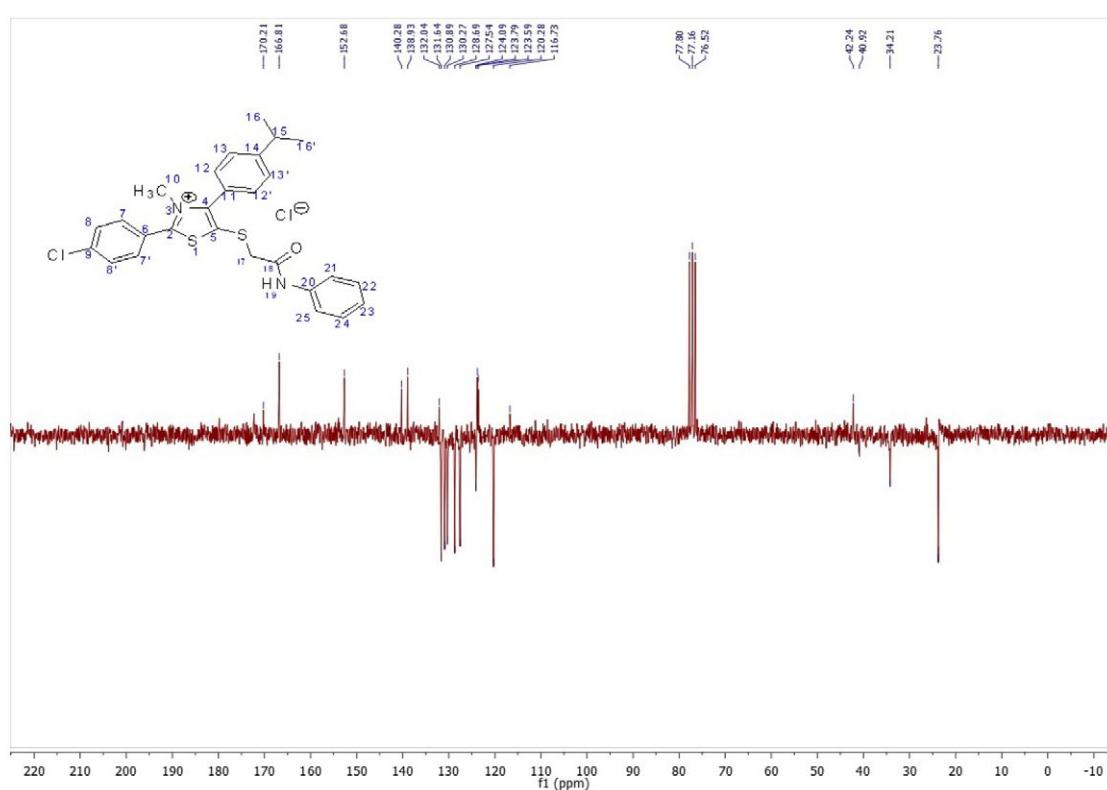
2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*-(*m*-nitro-*p*-fluorophenyl)acetamide)thiochloridate 7i

Yield: 96.98%; m.p.: 129-132 °C; anal. calcd.: C, 58.21; H, 4.34; N, 7.54; S, 11.51; found: C, 58.22; H, 4.32; N, 7.56; S, 11.52; IR (KBr) ν_{max} / cm⁻¹ 3335, 3207 (NH), 3128, 3072 (CH_{Ar}), 2943, 2860 (CH_{Alif.}), 1678 (C=O), 1624, 1257 (NO₂), 1608, 1535, 1492 (C=C and C=N of aromatic and

heterocyclic rings), 1439 (C–N of N–CH₃), 1402 (C–N), 1078 (C–Cl), 960, 901 (CH_{Ar}), 885 (C–N of ArNO₂), 754 (NH), 505 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.27 (d, 6H, J 6.9 Hz, H-16, H-16'), 2.96 (sept, 1H, J 13.7, 6.8 Hz, H-15,), 3.67 (s, 2H, H-17), 3.82 (s, 3H, H-10), 7.14 (t, 1H, H-24), 7.33 (d, 2H, H-13, H-13'), 7.60-7.71 (dd, 4H, J 8.5 Hz, H-8, H-8', H-12, H-12'), 7.89 (d, 2H, J 8.5 Hz, H-7, H-7'), 8.14 (m, 1H, H-24), 8.73 (dd, 1H, J 6.8, 2.5 Hz, H-21), 11.55 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.77 (C-2), 167.21 (C-18), 154.69 (C-14), 153.03 (C-4), 151.48 (C-23, J 260 Hz), 140.57 (C-9), 137.03 (C-22), 136.87 (C-5), 135.69 (C-20, J 3.5 Hz), 131.48 (C-7, C-7'), 130.84 (C-12, C-12'), 130.46 (C-8, C-8'), 127.60 (C-13, C-13'), 127.24 (C-25, J 7.5 Hz), 123.60 (C-11), 123.38 (C-6), 118.18 (C-24, J 22 Hz), 116.95 (C-21), 42.09 (C-17), 40.91 (C-10), 34.20 (C-15), 23.74 (C-16).

2-(*p*-Chlorophenyl)-3-methyl-4-(*p*-isopropylphenyl)-1,3-thiazolium-5-(*N*-(*m*-nitro-*p*-chlorophenyl)acetamide)thiochloridate 7j

Yield: 91.14%; m.p.: 138-140°C; anal. calcd.: C, 56.54; H, 4.22; N, 7.33; S, 11.18; found: C, 56.55; H, 4.24; N, 7.32; S, 11.19; IR (KBr) ν_{max} / cm⁻¹ 3396, 3224 (NH), 3155, 3082 (CH_{Ar}), 2958, 2866 (CH_{Alif.}), 1683 (C=O), 1599, 1271 (NO₂), 1535, 1483 (C=C and C=N of aromatic and heterocyclic rings), 1402 (C–N of N–CH₃), 1327 (C–N), 1091 (C–Cl), 1008, 956 (CH_{Ar}), 887 (C–N of ArNO₂), 750 (NH), 509 (C–C); ¹H NMR (200 MHz, CDCl₃) δ 1.28 (d, 6H, J 6.9 Hz, H-16, H-16'), 2.97 (sept, 1H, J 13.8, 6.9 Hz, H-15), 3.64 (s, 2H, H-17), 3.81 (s, 3H, H-10), 7.33 (d, 2H, J 8.1 Hz, H-13, H-13'), 7.37 (d, 1H, H-24), 7.64 (d, 2H, J 8.4 Hz, H-8, H-8'), 7.69 (d, 2H, J 8.3 Hz, H-12, H-12'), 7.87 (d, 2H, J 8.6 Hz, H-7, H-7'), 8.08 (dd, 1H, J 8.8, 2.5 Hz, H-25), 8.60 (d, 1H, J 2.5 Hz, H-21), 11.61 (s, 1H, H-19); ¹³C NMR (50 MHz, CDCl₃) δ 170.97 (C-2), 167.31 (C-18), 155.14 (C-4), 153.15 (C-14), 148.08 (C-22), 140.66 (C-9), 138.84 (C-20), 131.52 (C-24), 131.46 (C-12, C-12'), 131.36 (C-5), 130.88 (C-7, C-7'), 130.53 (C-8, C-8'), 127.62 (C-13, C-13'), 124.71 (C-25), 123.59 (C-11), 123.38 (C-6), 120.77 (C-23), 116.37 (C-21), 42.26 (C-17), 40.86 (C-10), 34.24 (C-15), 23.76 (C-16, C-16').

**Figure S1.** ^1H NMR spectrum (200 MHz, CDCl_3) of compound 7a.**Figure S2.** ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 7a.

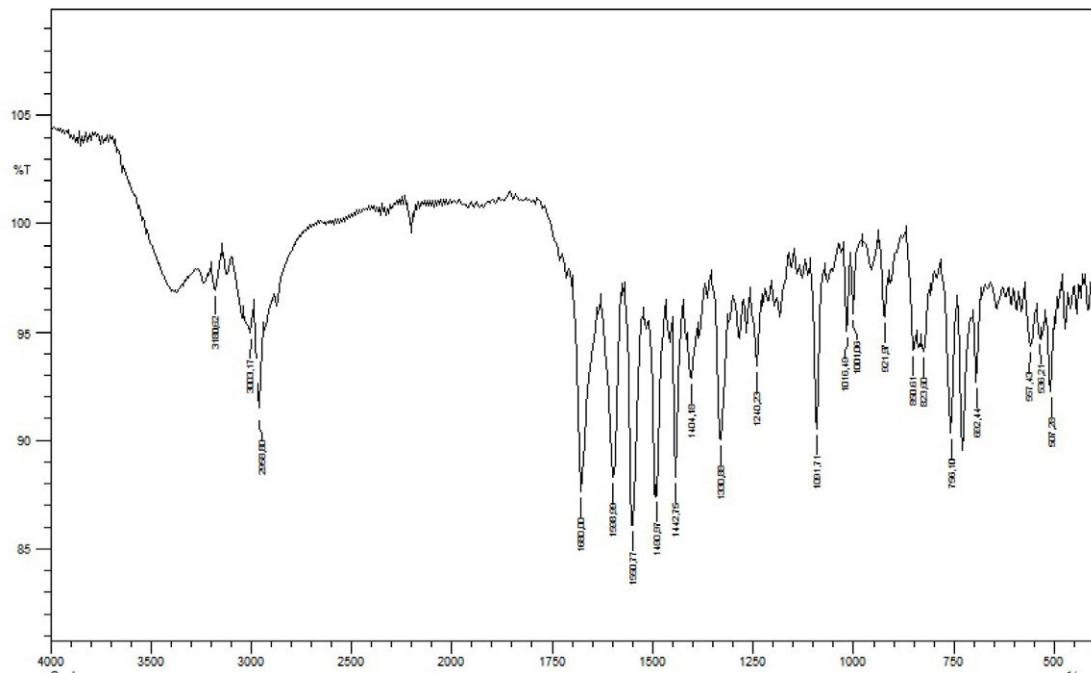


Figure S3. FTIR (KBr) spectrum of compound 7a.

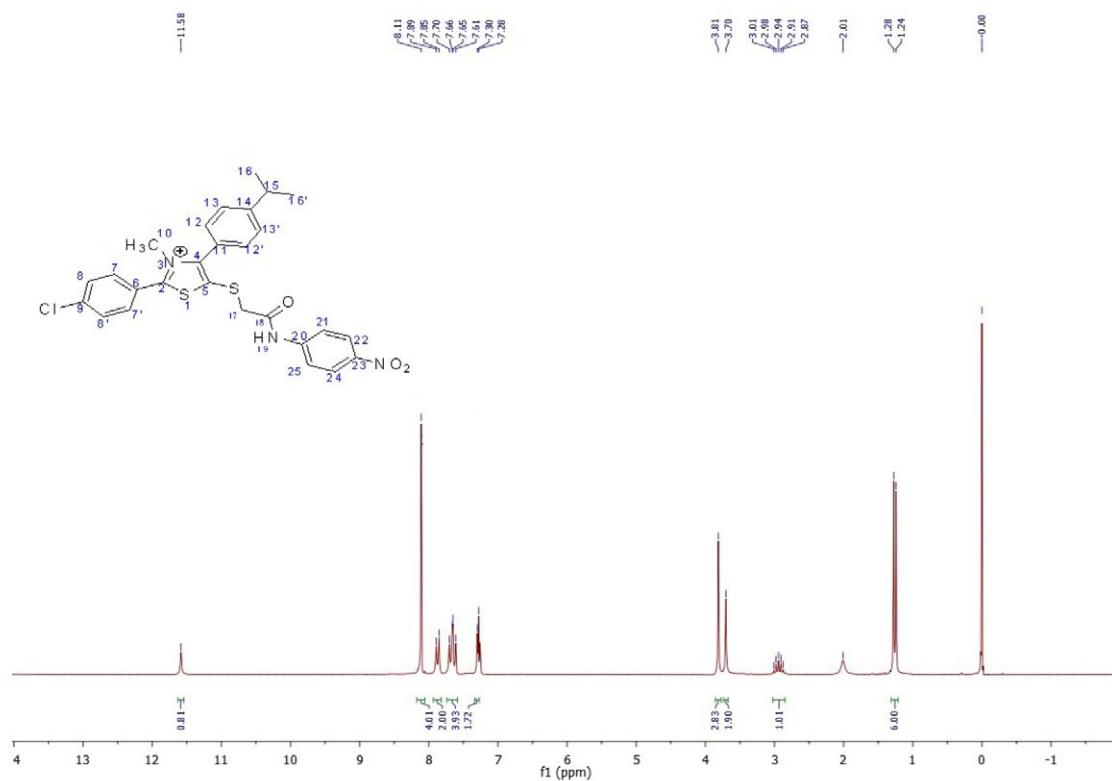


Figure S4. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 7b.

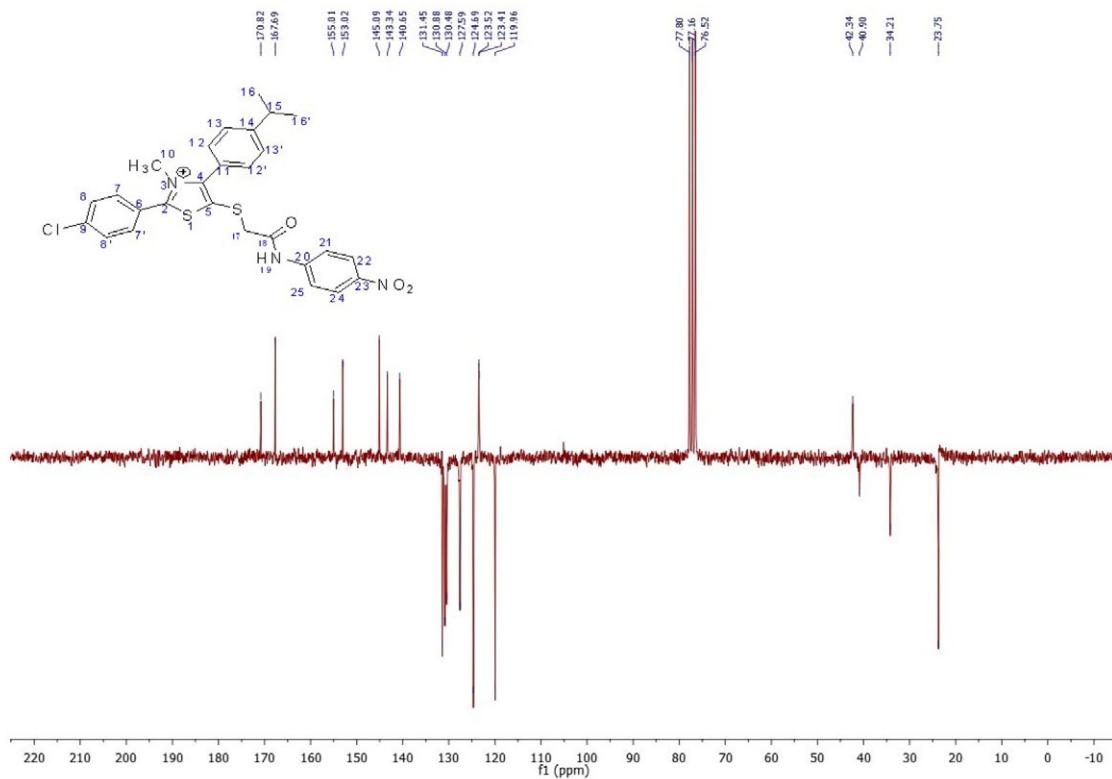


Figure S5. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound **7b**.

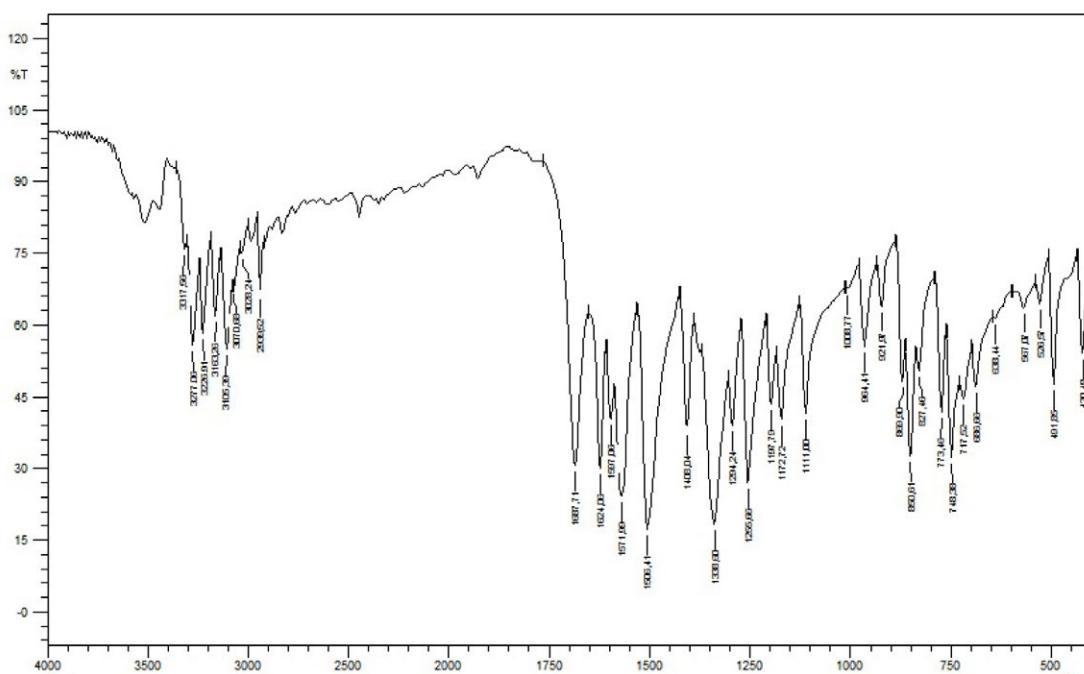


Figure S6. FTIR (KBr) spectrum of compound **7b**.

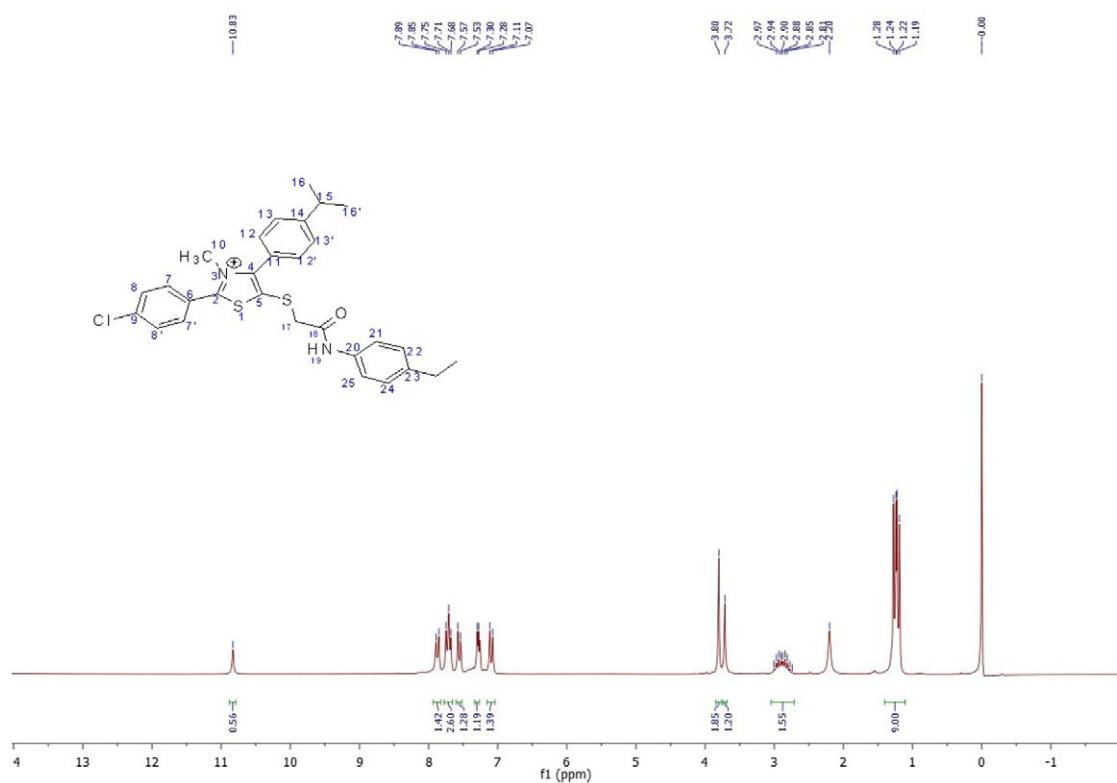


Figure S7. ^1H NMR spectrum (200 MHz, CDCl_3) of compound 7c.

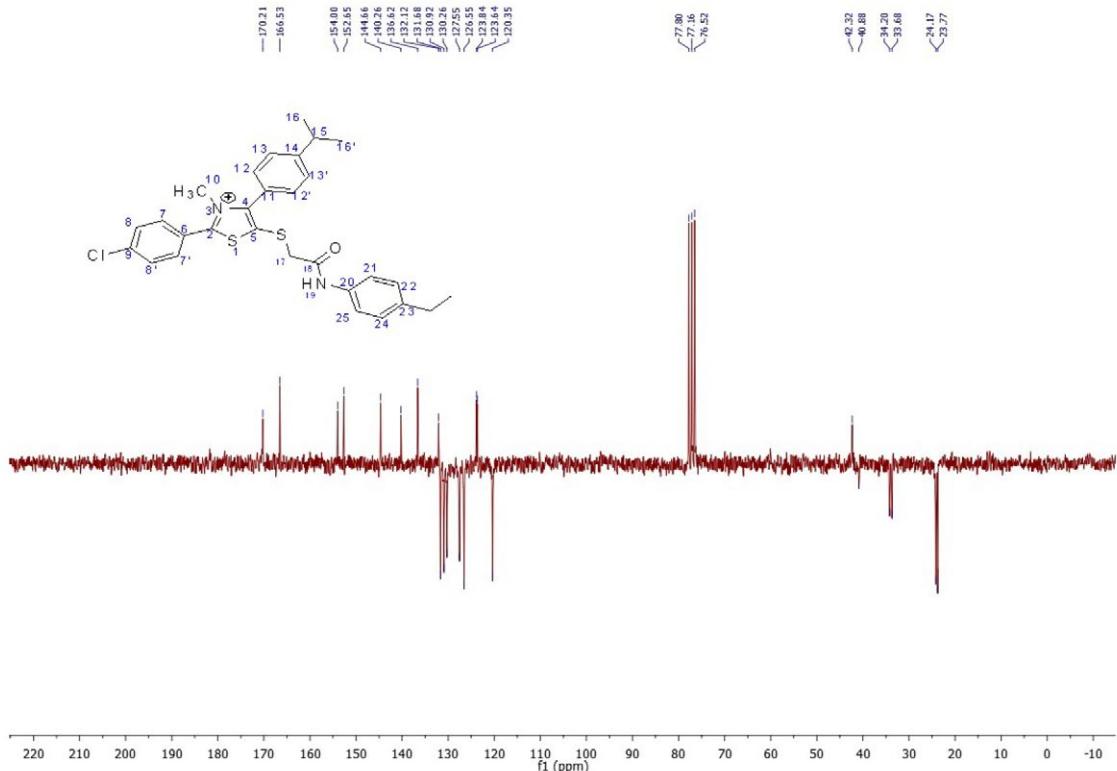
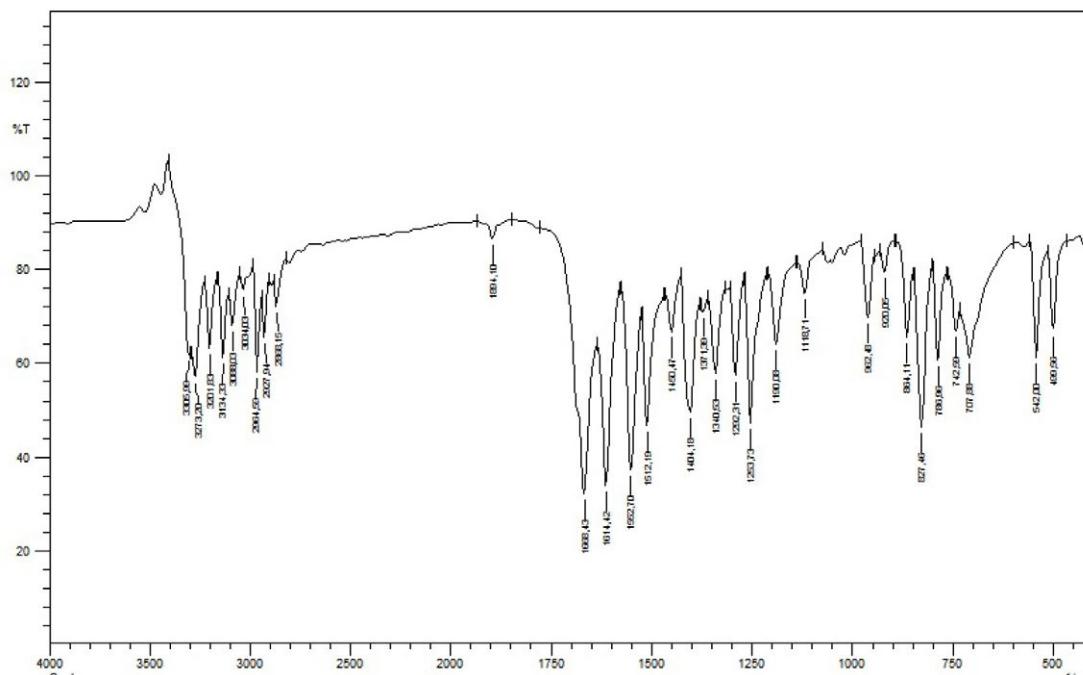
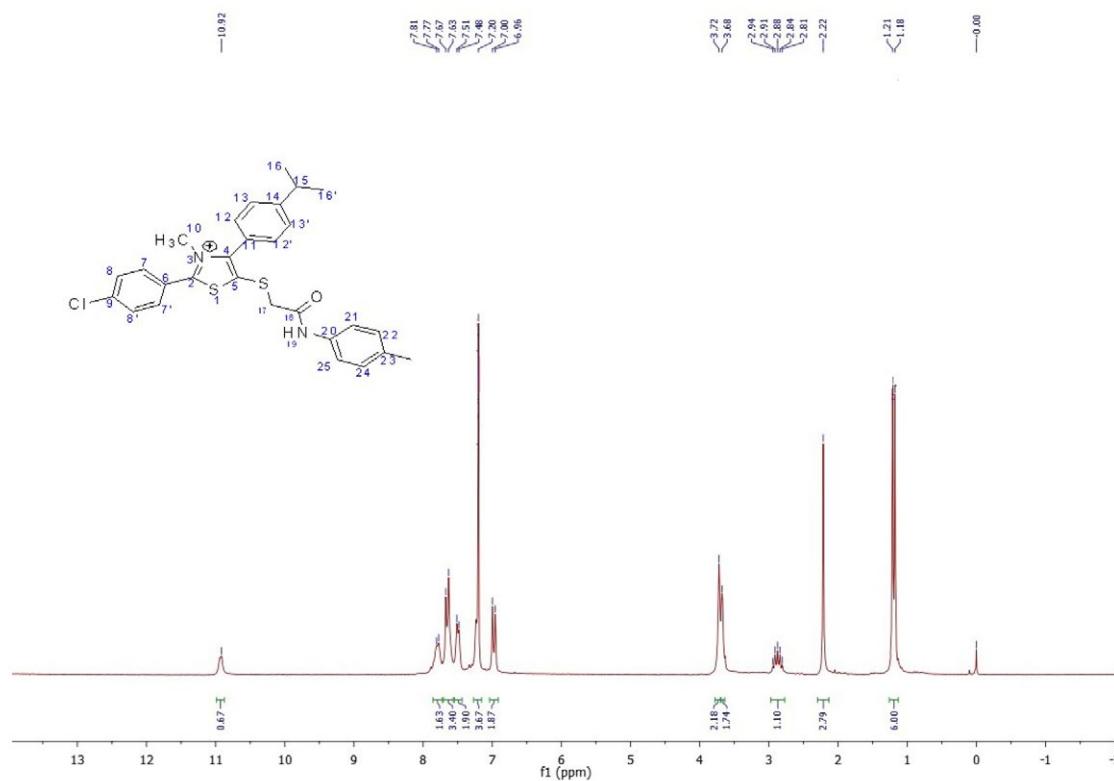


Figure S8. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 7c.

**Figure S9.** FTIR (KBr) spectrum of compound **7c**.**Figure S10.** ^1H NMR spectrum (200 MHz, CDCl_3) of compound **7d**.

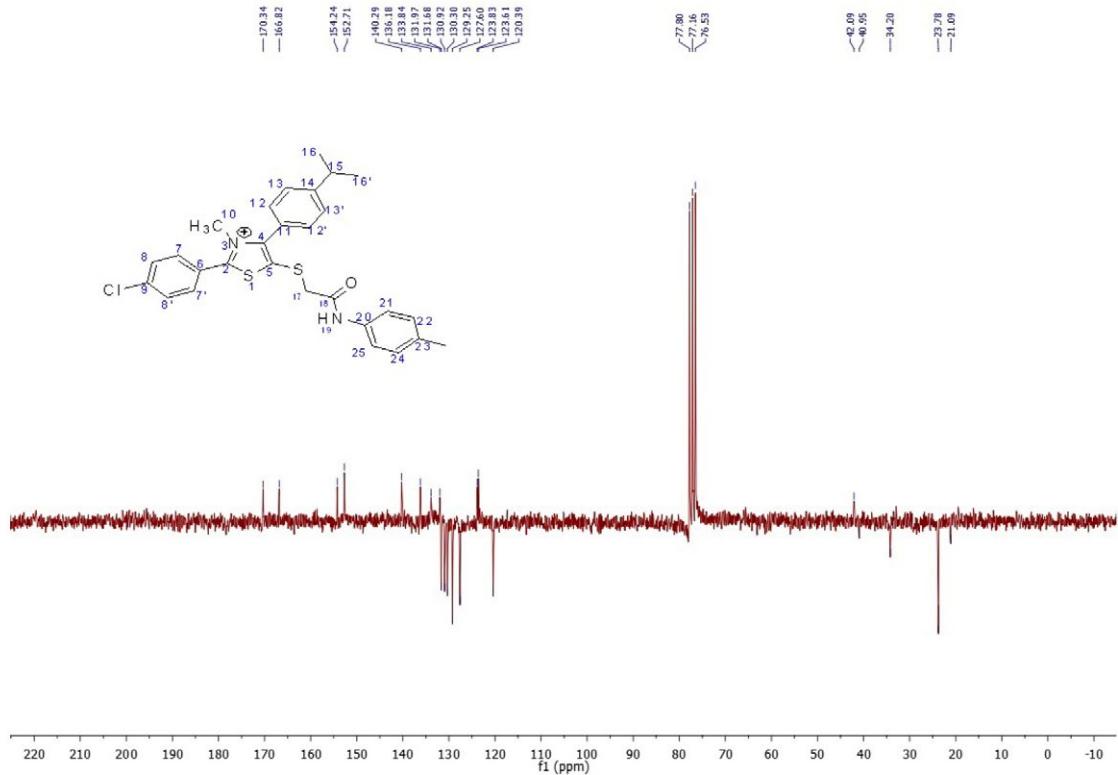


Figure S11. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound **7d**.

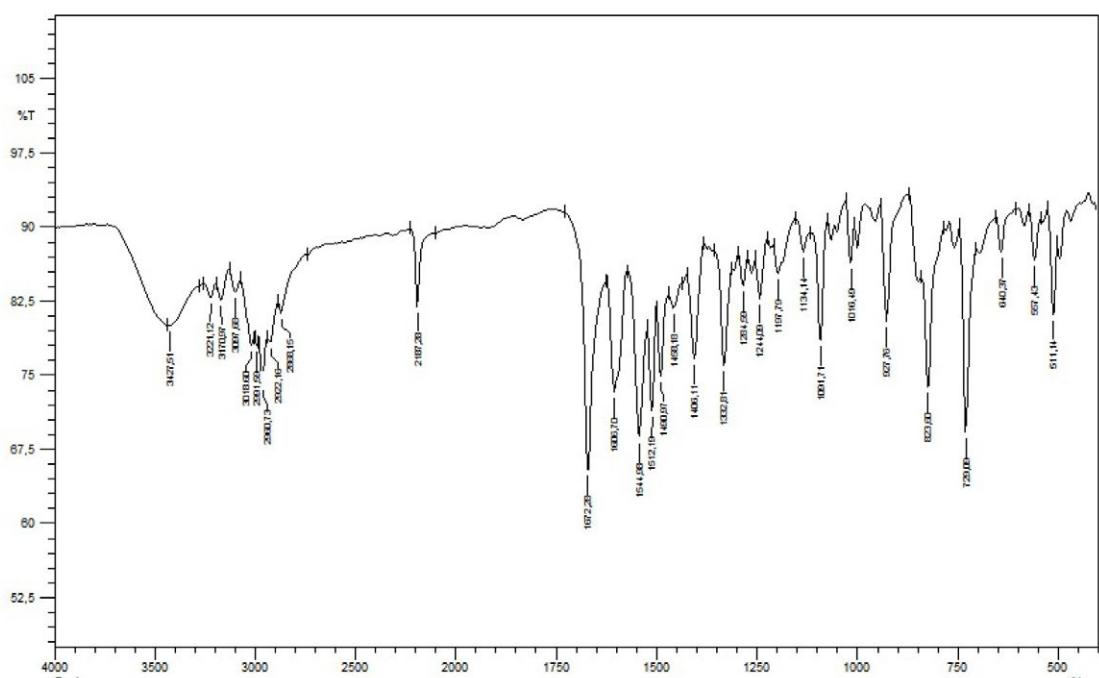
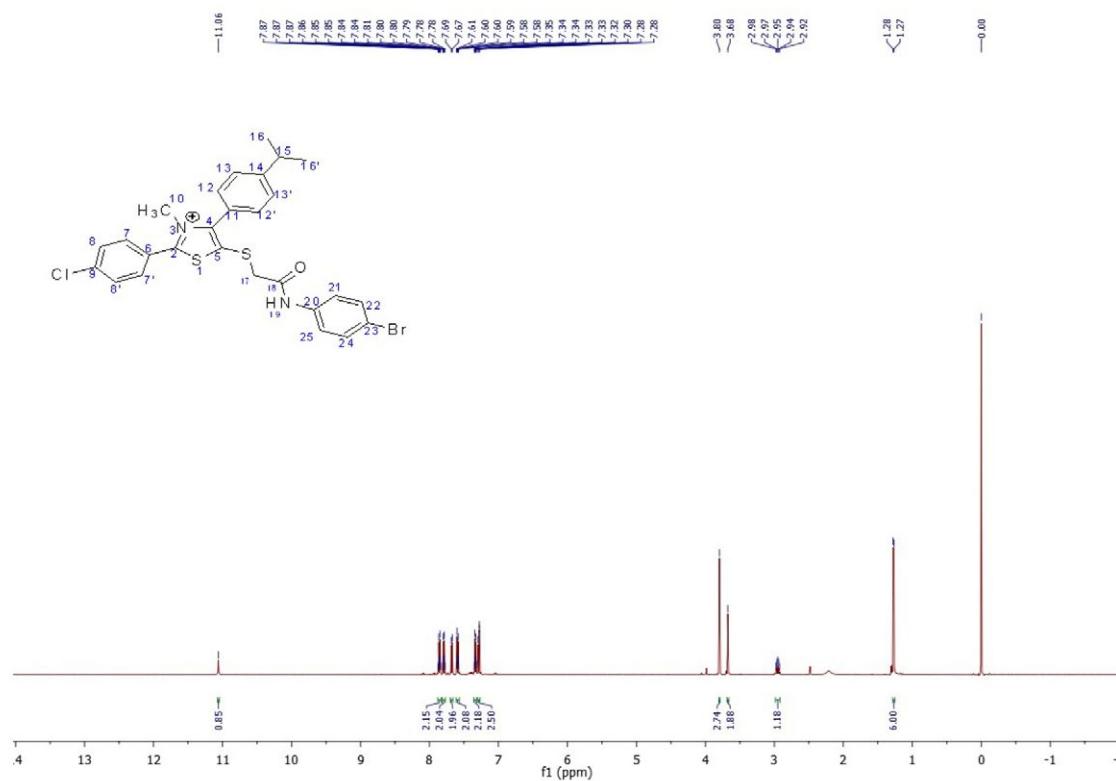
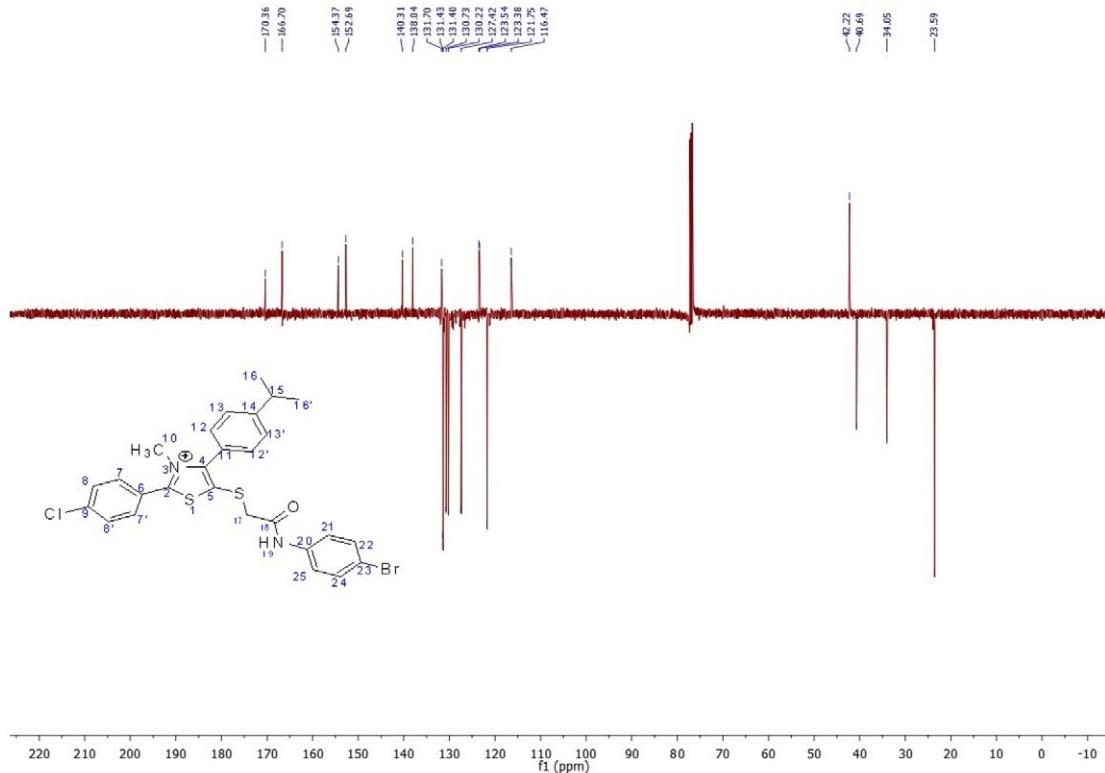


Figure S12. FTIR (KBr) spectrum of compound **7d**.

**Figure S13.** ¹H NMR spectrum (200 MHz, CDCl₃) of compound 7e.**Figure S14.** ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 7e.

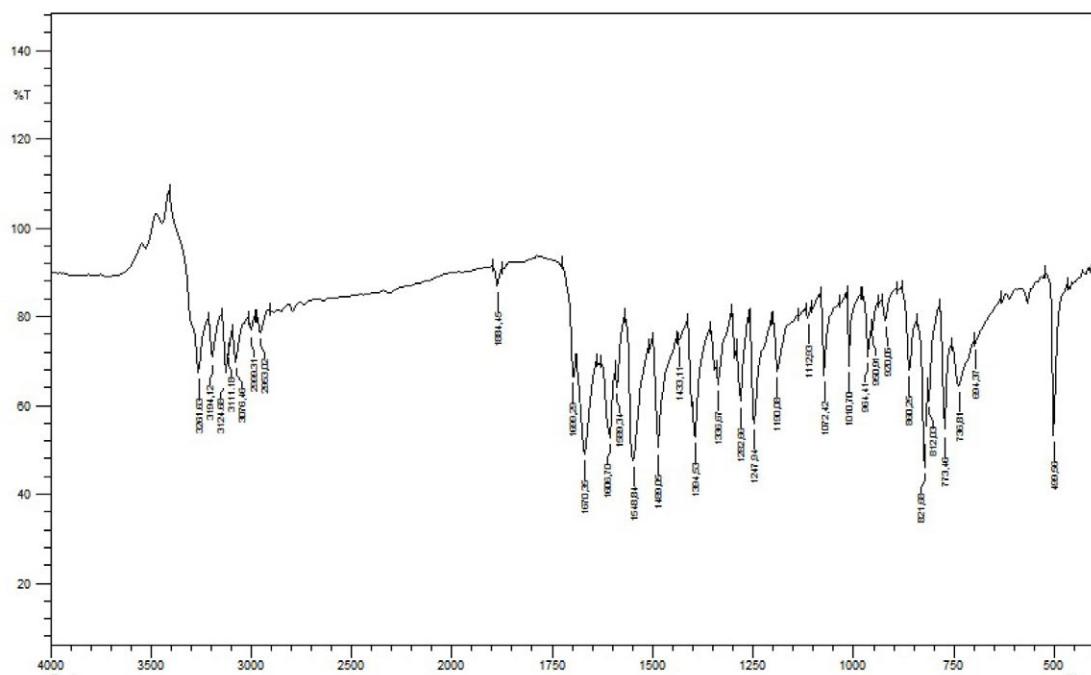


Figure S15. FTIR (KBr) spectrum of compound 7e.

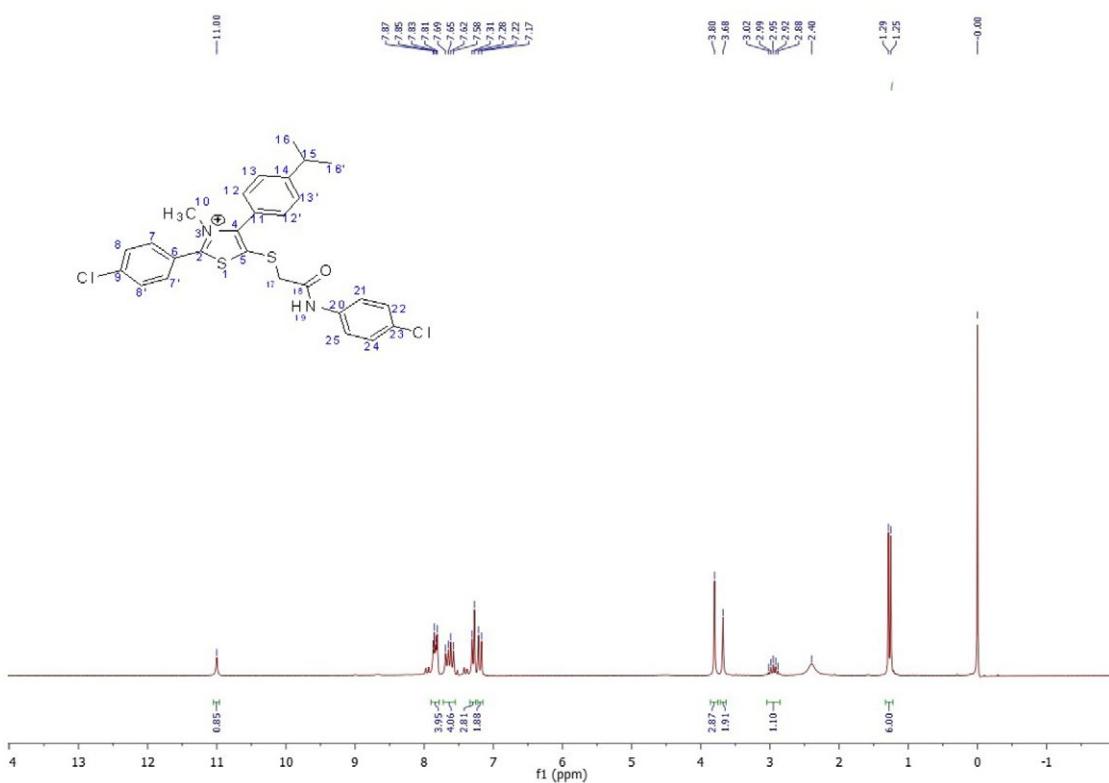


Figure S16. ^1H NMR spectrum (200 MHz, CDCl_3) of compound 7f.

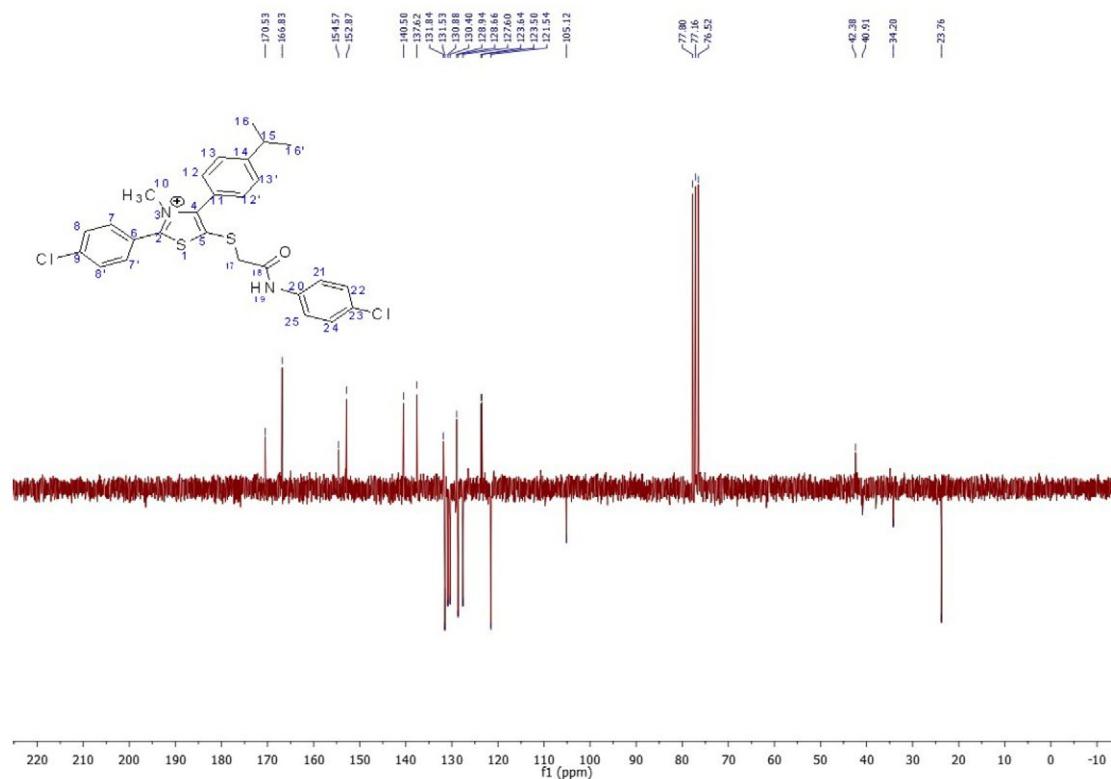


Figure S17. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 7f.

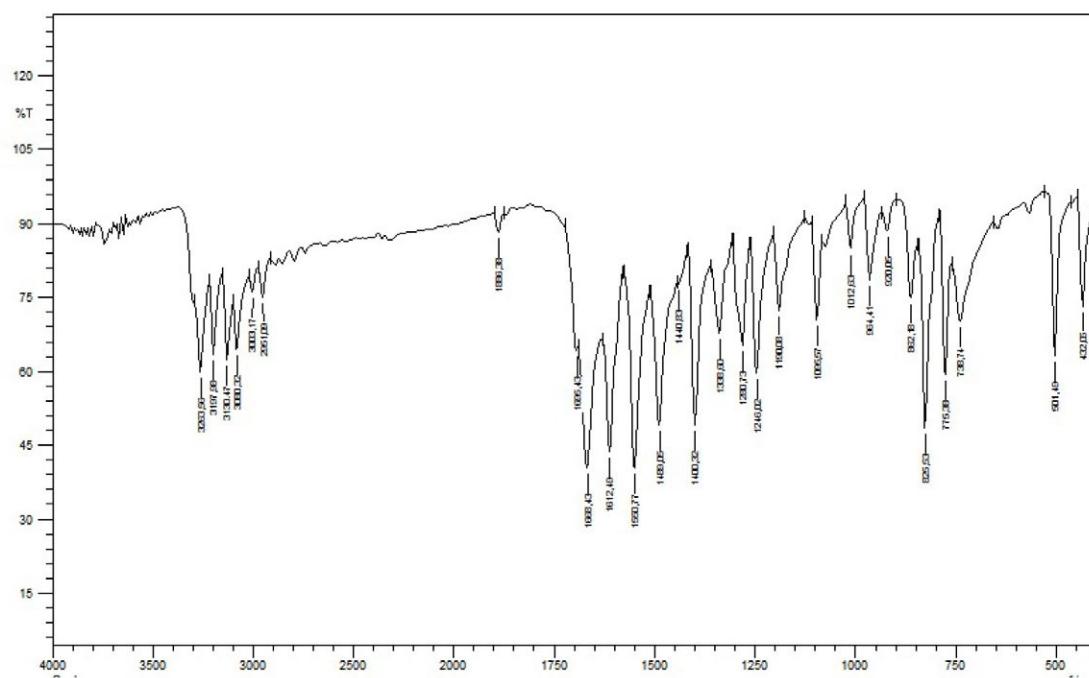


Figure S18. FTIR (KBr) spectrum of compound 7f.

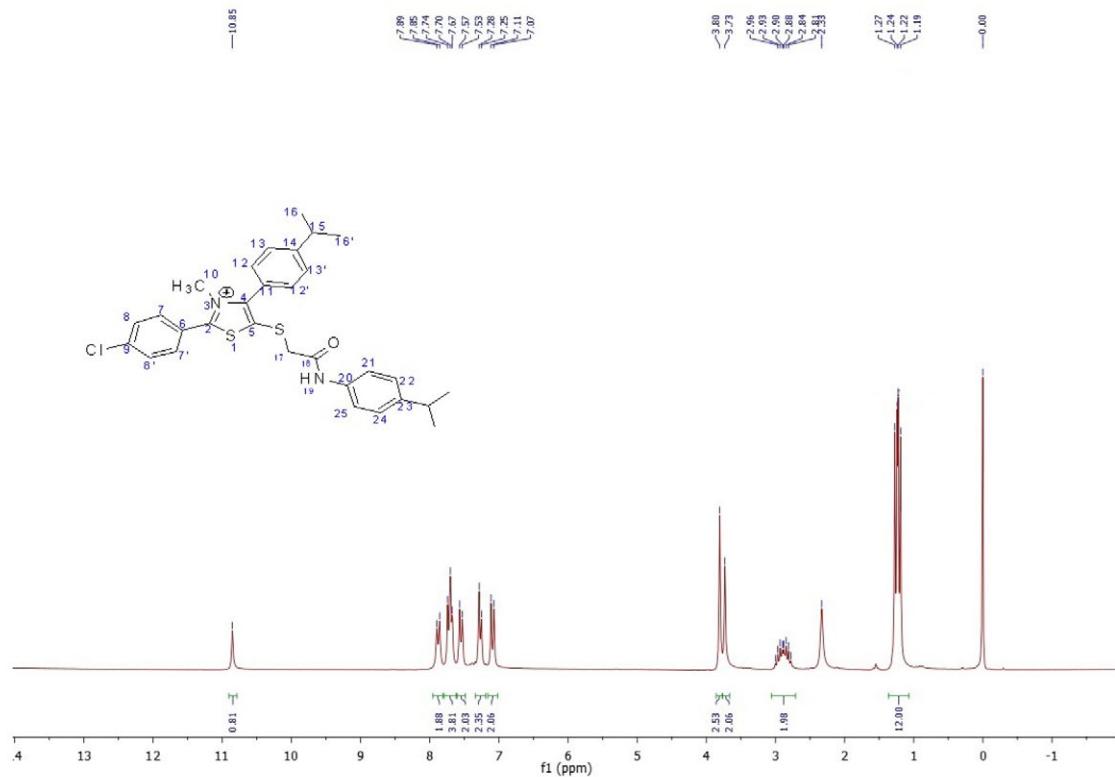


Figure S19. ^1H NMR spectrum (200 MHz, CDCl_3) of compound 7g.

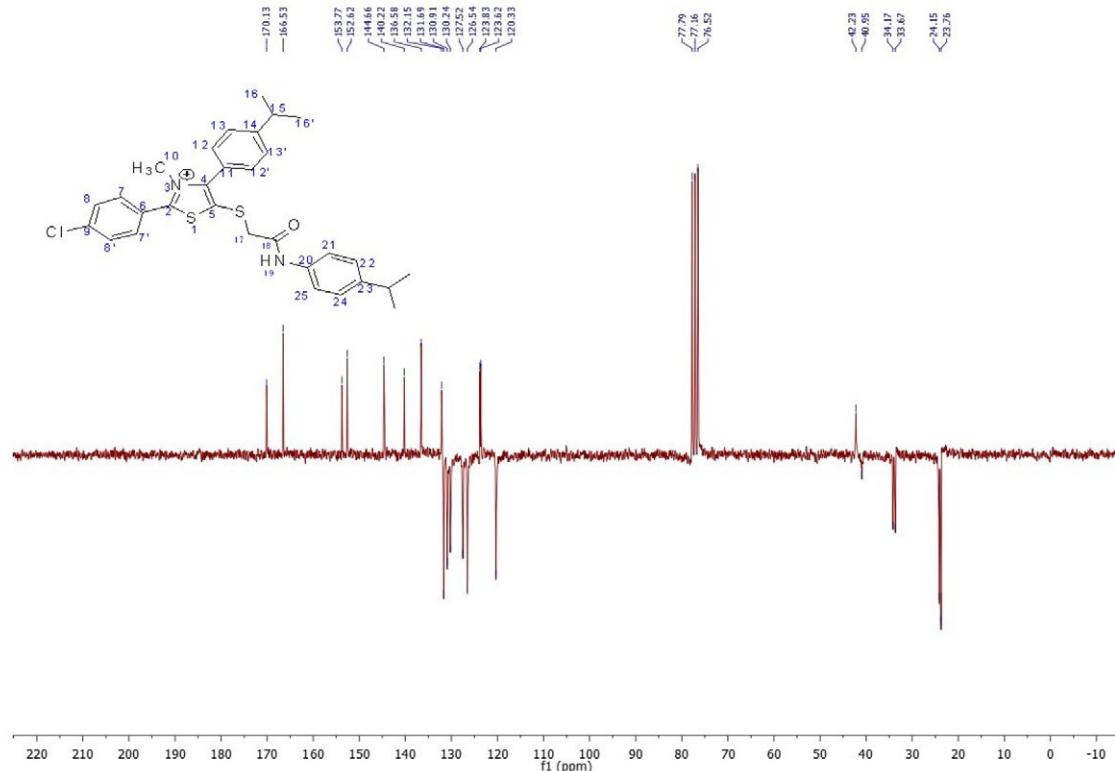
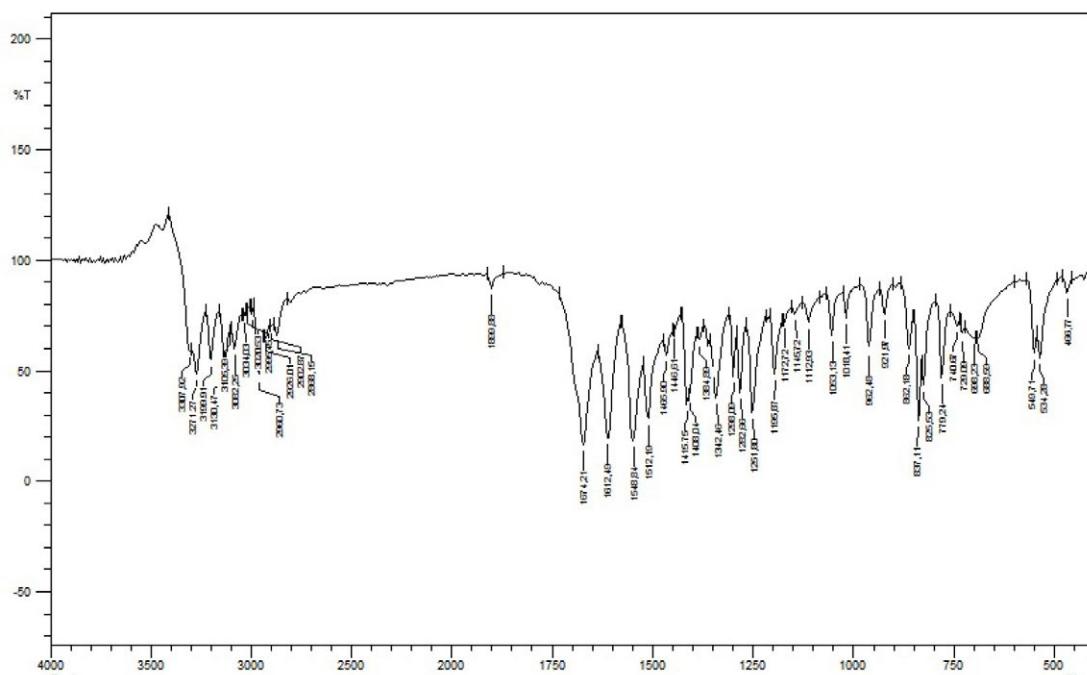
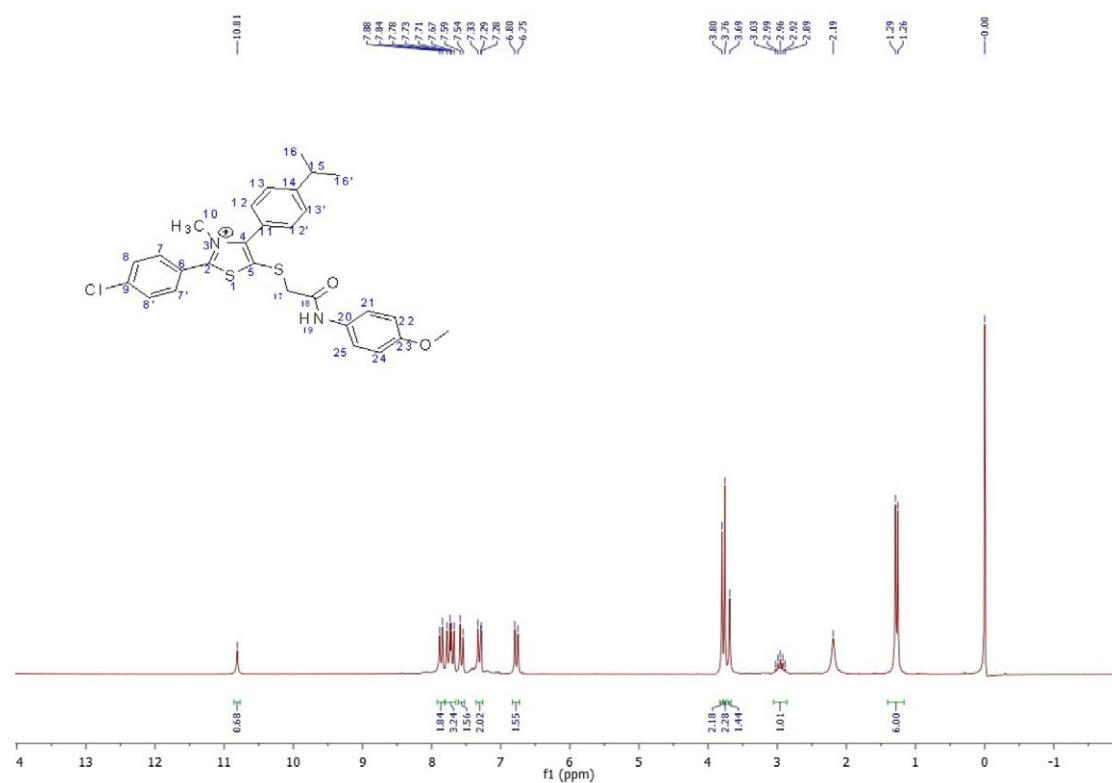


Figure S20. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 7g.

**Figure S21.** FTIR (KBr) spectrum of compound 7g.**Figure S22.** ^1H NMR spectrum (200 MHz, CDCl_3) of compound 7h.

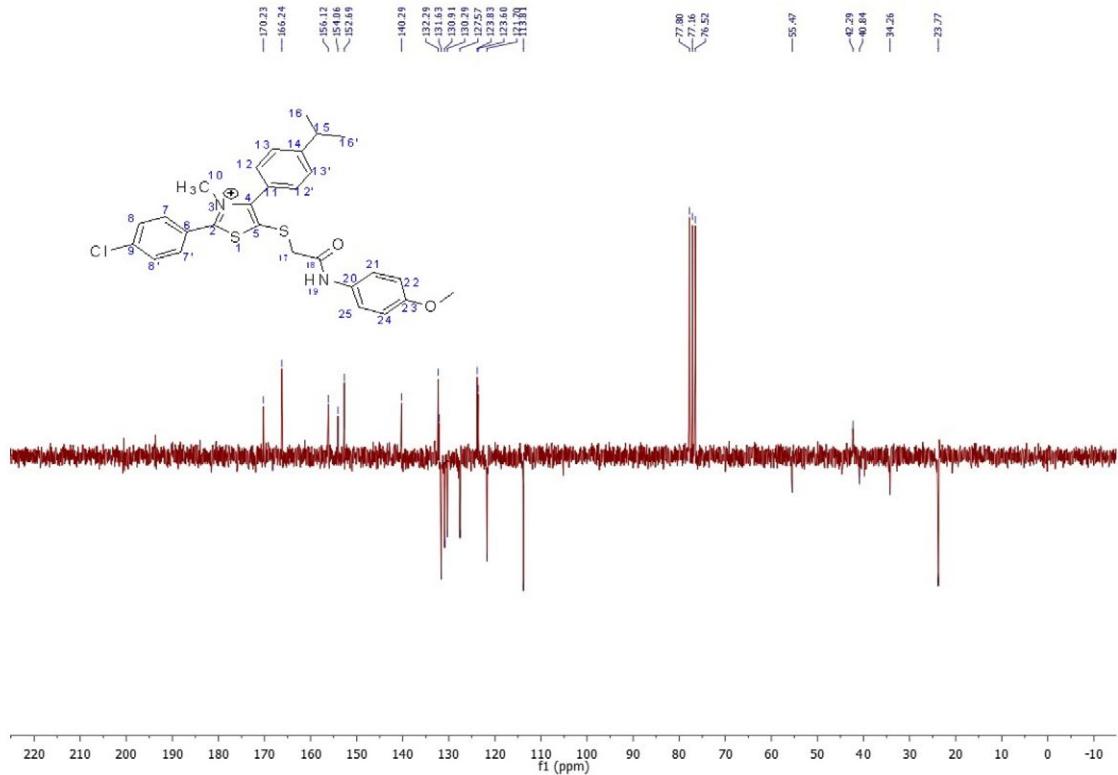


Figure S23. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 7h.

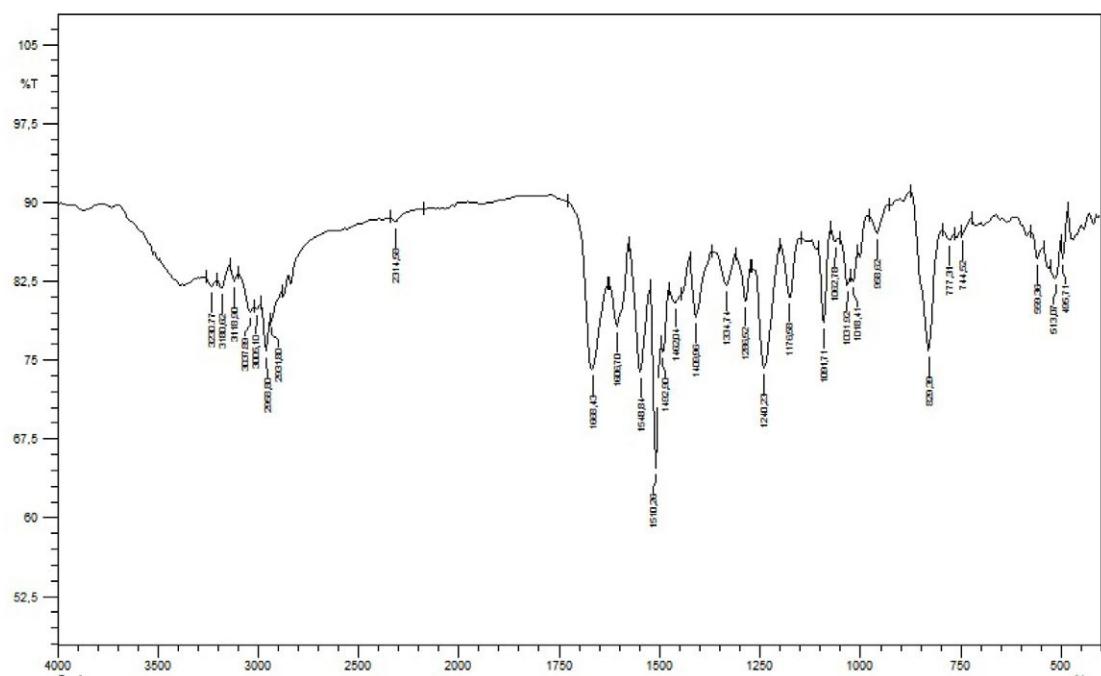


Figure S24. FTIR (KBr) spectrum of compound 7h.

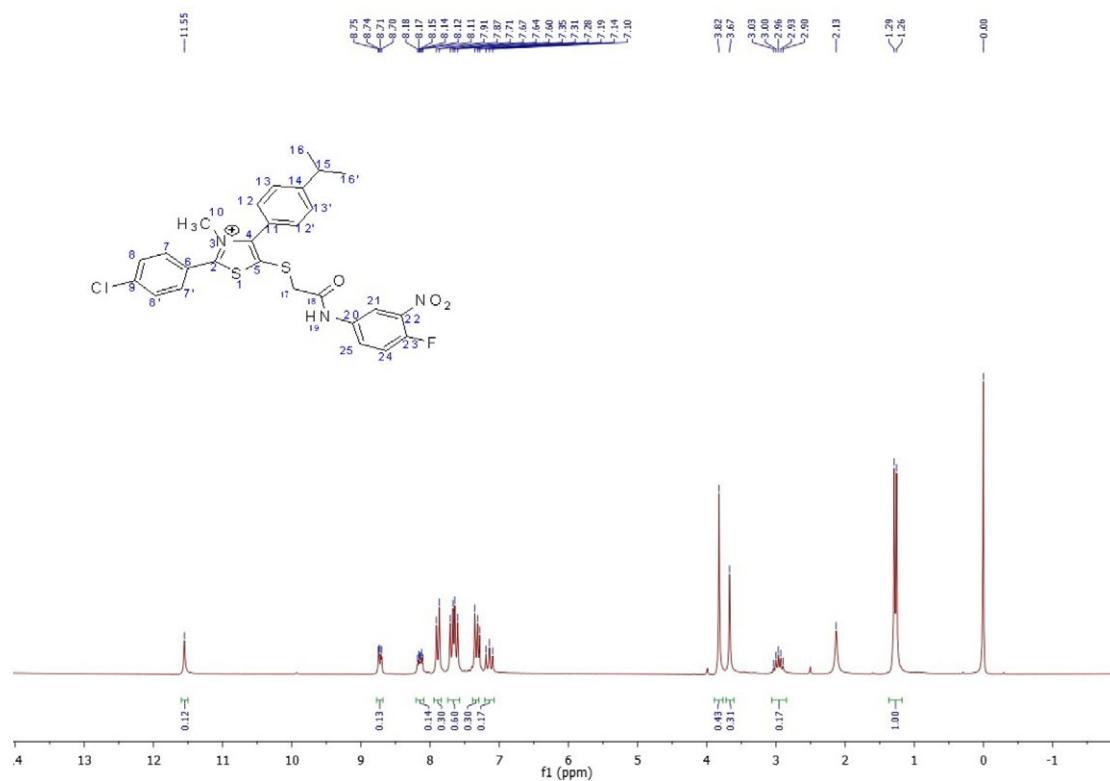


Figure S25. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 7i.

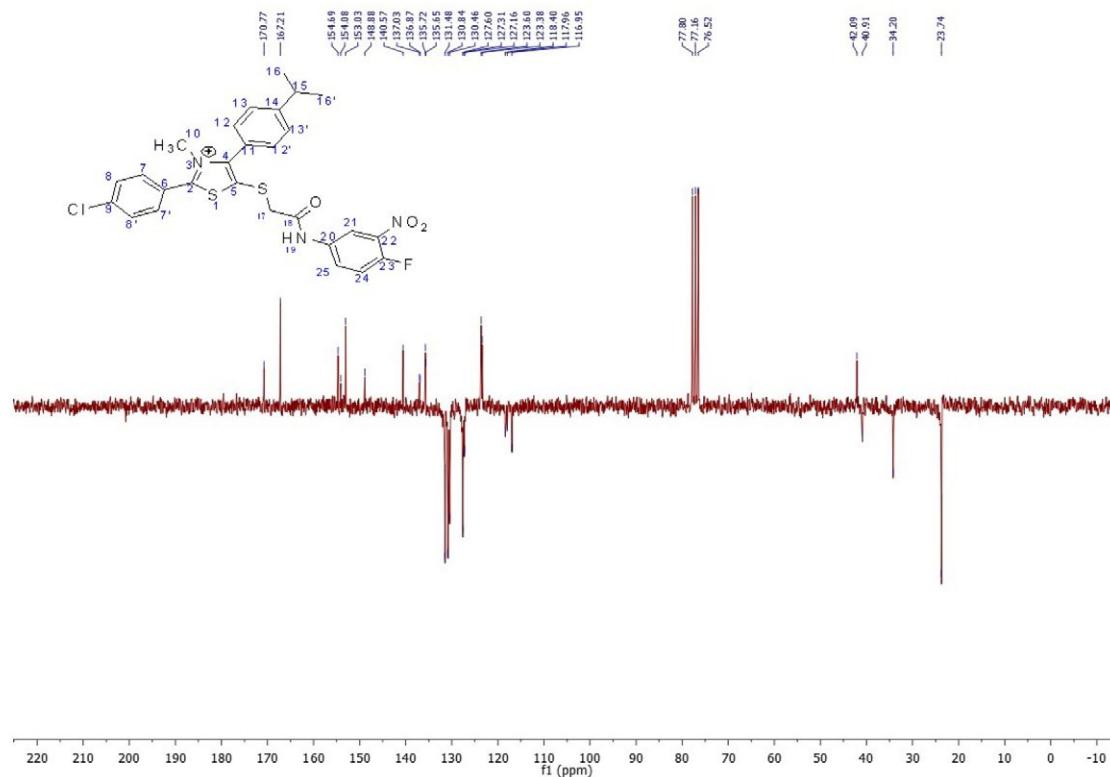


Figure S26. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 7i.

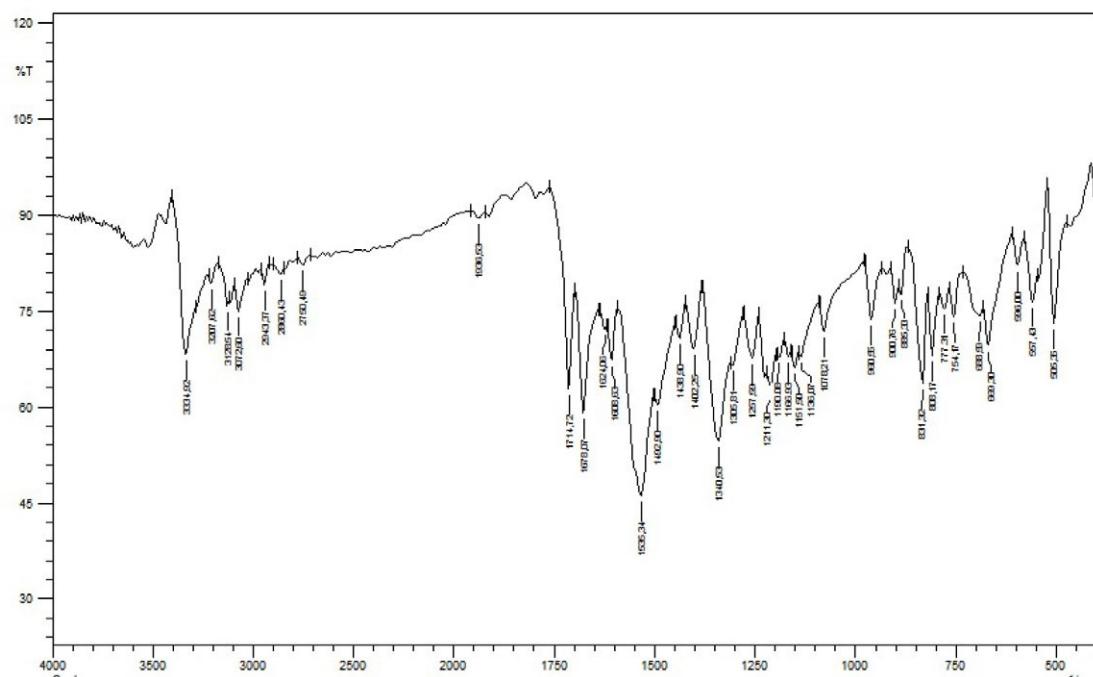


Figure S27. FTIR (KBr) spectrum of compound 7i.

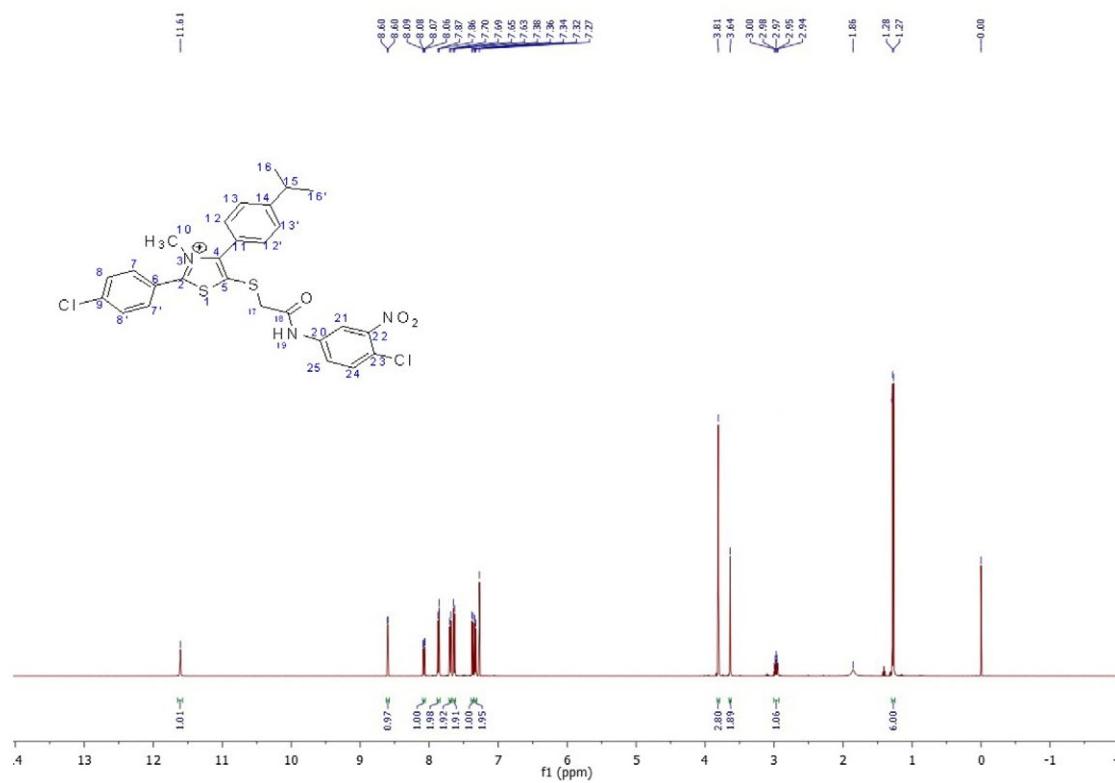
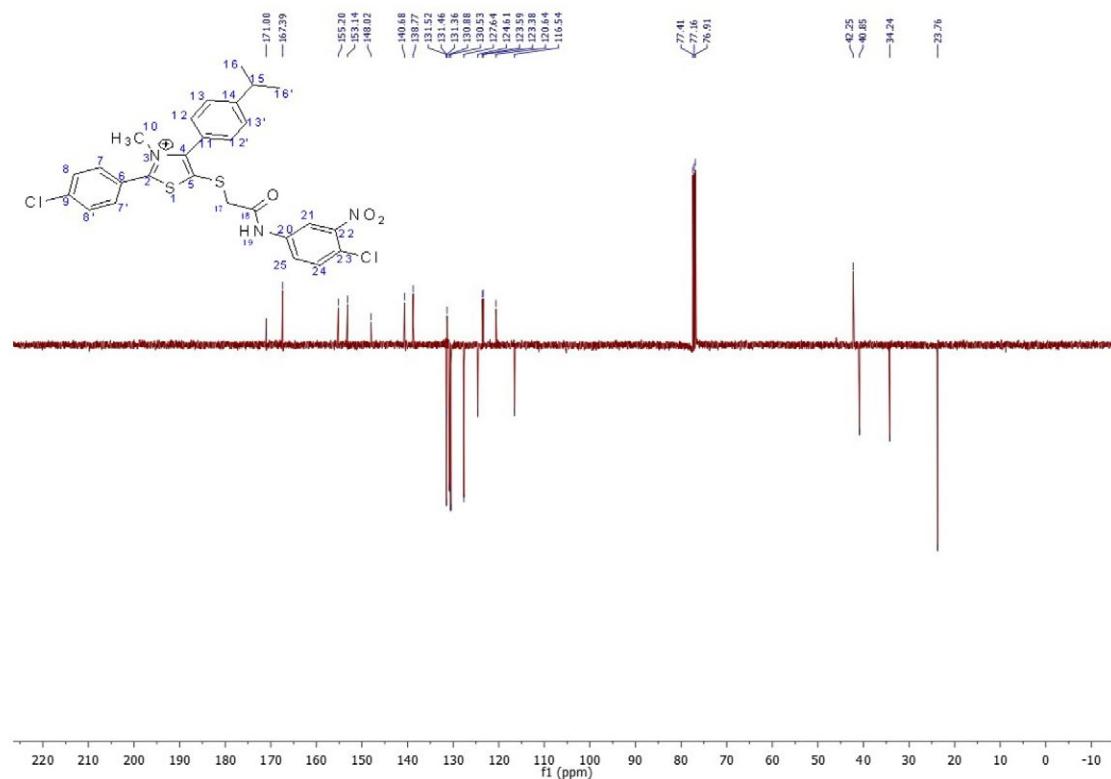
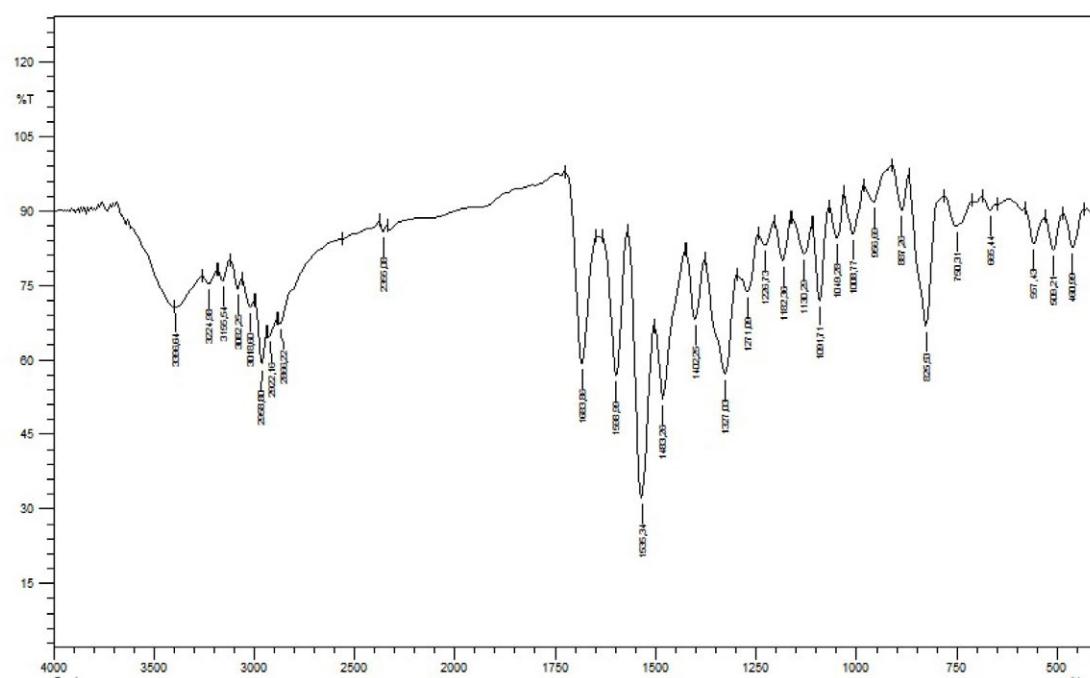


Figure S28. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 7j.

**Figure S29.** ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 7j.**Figure S30.** FTIR (KBr) spectrum of compound 7j.