

Supporting Information

Iodine-Catalyzed Oxidative Cyclisation for the Synthesis of Sarisan Analogues Containing 1,3,4-Oxadiazole as Insecticidal Agents

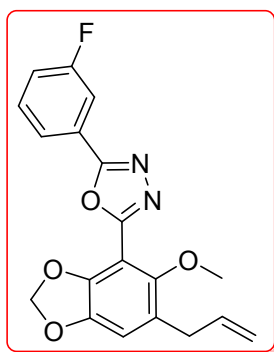
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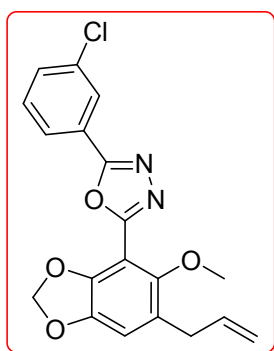
Research and Safety Evaluation, Henan Province, No. 100, KeXue DaDao, Zhengzhou, 450001, PR China

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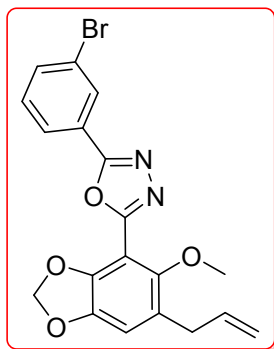
Spectra data for 8f-u



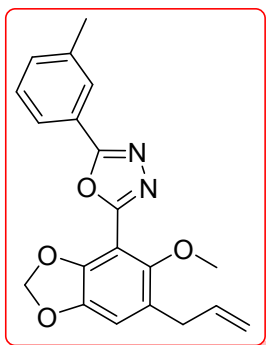
Data for 8f: White solid, yield: 68%, m.p. 151-153 °C; IR cm⁻¹ (KBr): 3077, 2974, 2921, 1639, 1473, 995, 933; ¹H NMR (400 MHz, CDCl₃) δ: 7.94 (d, *J* = 8.0 Hz, 1H, -Ar), 7.82-7.85 (m, 1H, -Ar), 7.48-7.54 (m, 1H, -Ar), 7.22-7.28 (m, 1H, -Ar), 6.84 (s, 1H, H-6), 6.13 (s, 2H, -OCH₂O-), 5.91-6.00 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.81 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ: 164.1, 163.5, 161.6, 159.9, 150.1, 146.1, 144.4, 136.6, 130.9, 130.9, 126.7, 125.7, 122.8, 122.8, 118.9, 118.7, 116.4, 114.1, 113.9, 112.3, 102.4, 101.8, 62.6, 33.5. HRMS (ESI): Calcd for C₁₉H₁₆O₄N₂F ([M+H]⁺), 355.1089; Found, 355.1089.



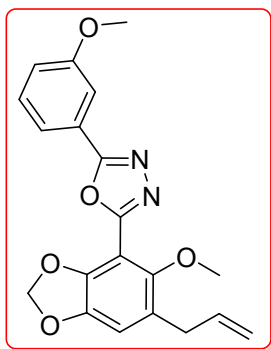
Data for 8g: White solid, yield: 84%, m.p. 115-116 °C; IR cm⁻¹ (KBr): 3080, 2941, 1640, 1479, 997, 926; ¹H NMR (400 MHz, CDCl₃) δ: 8.13 (d, *J* = 1.6 Hz, 1H, -Ar), 8.03 (dt, *J* = 7.6, 1.6 Hz, 1H, -Ar), 7.45-7.54 (m, 2H, -Ar), 6.84 (s, 1H, H-6), 6.13 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.80 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ: 163.4, 159.9, 150.1, 146.1, 144.4, 136.6, 135.2, 131.7, 130.4, 126.9, 126.7, 125.5, 125.1, 116.5, 112.3, 102.5, 101.7, 62.6, 33.5. HRMS (ESI): Calcd for C₁₉H₁₆O₄N₂Cl ([M+H]⁺), 371.0792; Found, 371.0793.



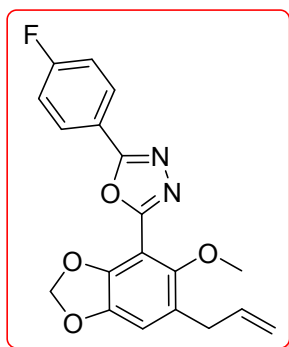
Data for 8h: White solid, yield: 69%, m.p. 119-120 °C; IR cm^{-1} (KBr): 3079, 2937, 1640, 1478, 996, 930; ^1H NMR (400 MHz, CDCl_3) δ : 8.28 (d, $J = 2.0$ Hz, 1H, -Ar), 8.08 (d, $J = 8.0$ Hz, 1H, -Ar), 7.69 (dt, $J = 8.0, 0.8$ Hz, 1H, -Ar), 7.39 (t, $J = 8.0$ Hz, 1H, -Ar), 6.84 (s, 1H, H-6), 6.13 (s, 2H, $-\text{OCH}_2\text{O}-$), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.80 (s, 3H, $-\text{OCH}_3$), 3.42 (d, $J = 6.4$ Hz, 2H, H-1'). ^{13}C NMR (100 MHz, CDCl_3) δ : 163.3, 159.9, 150.1, 146.1, 144.4, 136.6, 134.7, 130.6, 129.8, 126.7, 125.7, 125.5, 123.1, 116.5, 112.3, 102.5, 101.7, 62.6, 33.5. HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_4\text{N}_2\text{Br}$ ($[\text{M}+\text{H}]^+$), 415.0287; Found, 415.0288.



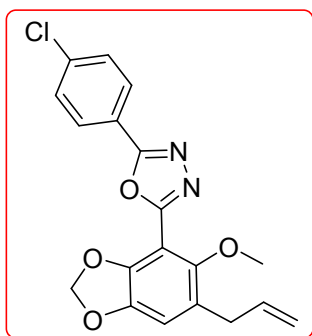
Data for 8i: White solid, yield: 81%, m.p. 105-106 °C; IR cm^{-1} (KBr): 3005, 2907, 2846, 1640, 1470, 993, 931; ^1H NMR (400 MHz, CDCl_3) δ : 7.98 (s, 1H, -Ar), 7.92 (d, $J = 6.8$ Hz, 1H, -Ar), 7.35-7.43 (m, 2H, -Ar), 6.84 (s, 1H, H-6), 6.12 (s, 2H, $-\text{OCH}_2\text{O}-$), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.79 (s, 3H, $-\text{OCH}_3$), 3.42 (d, $J = 6.4$ Hz, 2H, H-1'), 2.45 (s, 3H, $-\text{CH}_3$). ^{13}C NMR (100 MHz, CDCl_3) δ : 164.8, 159.4, 150.1, 146.0, 144.4, 138.9, 136.7, 132.5, 128.9, 127.5, 126.6, 124.2, 123.8, 116.4, 112.1, 102.4, 102.0, 62.6, 33.5, 21.3. HRMS (ESI): Calcd for $\text{C}_{20}\text{H}_{19}\text{O}_4\text{N}_2$ ($[\text{M}+\text{H}]^+$), 351.1338; Found, 351.1339.



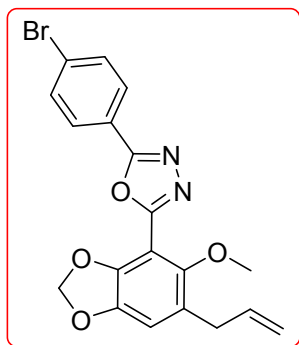
Data for 8j: White solid, yield: 30%, m.p. 93-94 °C; IR cm⁻¹ (KBr): 3003, 2976, 2944, 2841, 1630, 1476, 995, 928; ¹H NMR (400 MHz, CDCl₃) δ: 7.69-7.73 (m, 2H, -Ar), 7.41 (t, *J* = 8.0 Hz, 1H, -Ar), 7.08 (t, *J* = 8.4, 2.4 Hz, 1H, -Ar), 6.83 (s, 1H, H-6), 6.12 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.90 (s, 3H, -OCH₃), 3.81 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ: 164.5, 160.0, 159.6, 150.1, 146.0, 144.4, 136.7, 130.2, 126.6, 125.0, 119.4, 118.1, 116.4, 112.1, 111.7, 102.4, 102.0, 62.6, 55.5, 33.5. HRMS (ESI): Calcd for C₂₀H₁₉O₅N₂ ([M+H]⁺), 367.1288; Found, 367.1288.



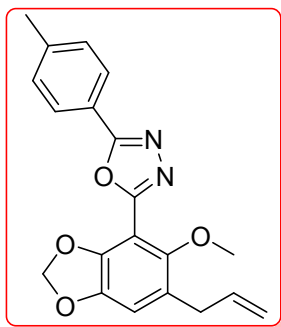
Data for 8k: Pale yellow solid, yield: 53%, m.p. 101-103 °C; IR cm⁻¹ (KBr): 3063, 2911, 1607, 1496, 1002, 925; ¹H NMR (400 MHz, CDCl₃) δ: 8.13-8.17 (m, 2H, H-6), 7.20-7.26 (m, 2H, H-6), 6.84 (s, 1H, H-6), 6.12 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.80 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ: 166.1, 163.8, 163.5, 159.6, 150.1, 146.0, 144.4, 136.6, 129.3, 129.2, 126.7, 120.3, 120.2, 116.5, 116.4, 116.3, 112.2, 102.4, 101.9, 62.5, 33.5. HRMS (ESI): Calcd for C₁₉H₁₆O₄N₂F ([M+H]⁺), 355.1087; Found, 355.1089.



Data for 8f: White solid, yield: 83%, m.p. 111-113 °C; IR cm^{-1} (KBr): 3089, 3000, 2934, 1603, 1483, 994, 936; ^1H NMR (400 MHz, CDCl_3) δ : 8.07 (d, $J = 8.4$ Hz, 2H, -Ar), 7.50 (d, $J = 8.4$ Hz, 2H, -Ar), 6.84 (s, 1H, H-6), 6.12 (s, 2H, - OCH_2O -), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.79 (s, 3H, - OCH_3), 3.42 (d, $J = 6.8$ Hz, 2H, H-1'). ^{13}C NMR (100 MHz, CDCl_3) δ : 163.8, 159.7, 150.1, 146.0, 144.4, 138.0, 136.6, 129.4, 128.3, 126.7, 122.4, 116.4, 112.3, 102.4, 101.8, 62.6, 33.5. HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_4\text{N}_2\text{Cl}$ ($[\text{M}+\text{H}]^+$), 371.0800; Found, 371.0800.

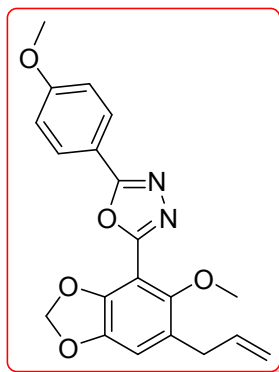


Data for 8m: White solid, yield: 51%, m.p. 128-129 °C; IR cm^{-1} (KBr): 3087, 3070, 2974, 2931, 1599, 1458, 993, 934; ^1H NMR (400 MHz, CDCl_3) δ : 8.00 (d, $J = 8.4$ Hz, 2H, -Ar), 7.66 (d, $J = 8.4$ Hz, 2H, -Ar), 6.84 (s, 1H, H-6), 6.12 (s, 2H, - OCH_2O -), 5.91-6.01 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.79 (s, 3H, - OCH_3), 3.42 (d, $J = 6.8$ Hz, 2H, H-1'). ^{13}C NMR (100 MHz, CDCl_3) δ : 163.9, 159.7, 150.1, 146.0, 144.4, 136.6, 132.4, 128.4, 126.7, 126.4, 122.8, 116.4, 112.3, 102.4, 101.8, 62.6, 33.5. HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_4\text{N}_2\text{Br}$ ($[\text{M}+\text{H}]^+$), 415.0286; Found, 415.0288.

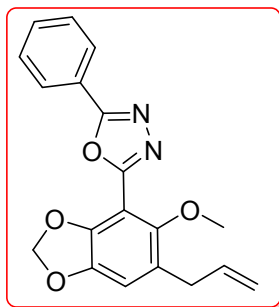


Data for 8n: White solid, yield: 55%, m.p. 113-114 °C; IR cm^{-1} (KBr): 3082, 3002, 2940, 2909, 1640, 1470, 993, 925; ^1H NMR (400 MHz, CDCl_3) δ : 8.02 (d, $J = 8.0$ Hz, 2H, -Ar), 7.31 (d, $J = 8.0$ Hz, 2H, -Ar), 7.18-7.20 (m, 1H, -Ar), 6.82 (s,

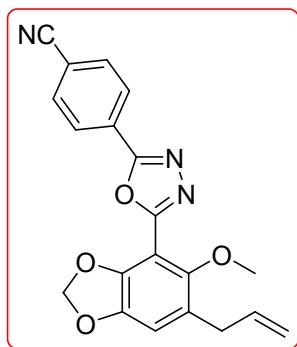
1H, H-6), 6.12 (s, 2H, -OCH₂O-), 5.89-6.01 (m, 1H, H-2'), 5.09-5.13 (m, 2H, H-3'), 3.79 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'), 2.44 (s, 3H, -CH₃). ¹³C NMR (100 MHz, CDCl₃) δ : 164.7, 159.3, 150.1, 146.0, 144.4, 136.7, 129.7, 127.0, 126.6, 121.1, 116.4, 112.0, 102.4, 102.1, 62.5, 33.5, 21.6. HRMS (ESI): Calcd for C₂₀H₁₉O₄N₂ ([M+H]⁺), 351.1340; Found, 351.1339.



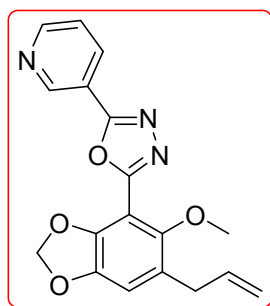
Data for 8o: White solid, yield: 70%, m.p. 123-124 °C; IR cm⁻¹ (KBr): 3068, 3004, 2981, 2948, 2902, 2845, 1612, 1497, 989, 949; ¹H NMR (400 MHz, CDCl₃) δ : 8.07 (d, *J* = 8.8 Hz, 2H, -Ar), 7.01 (d, *J* = 8.8 Hz, 2H, -Ar), 6.82 (s, 1H, H-6), 6.11 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.13 (m, 2H, H-3'), 3.89 (s, 3H, -OCH₃), 3.79 (s, 3H, -OCH₃), 3.41 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ : 164.5, 162.3, 159.0, 150.1, 145.9, 144.4, 136.7, 128.8, 126.6, 116.4, 116.4, 114.5, 112.0, 102.3, 102.1, 62.5, 55.4, 33.5. HRMS (ESI): Calcd for C₂₀H₁₉O₅N₂ ([M+H]⁺), 367.1288; Found, 367.1288.



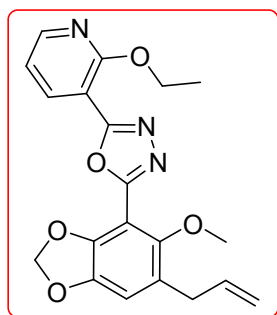
Data for 8p: White solid, yield: 89%, m.p. 76-78 °C; IR cm⁻¹ (KBr): 3006, 2976, 2905, 1640, 1532, 952, 936; ¹H NMR (400 MHz, CDCl₃) δ : 8.14-8.16 (m, 2H, -Ar), 7.52-7.56 (m, 3H, -Ar), 6.83 (s, 1H, H-6), 6.10 (s, 2H, -OCH₂O-), 5.91-6.12 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.80 (s, 3H, -OCH₃), 3.42 (d, *J* = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ : 164.3, 159.5, 150.2, 146.0, 144.4, 136.6, 131.6, 129.0, 126.9, 126.5, 123.9, 116.4, 112.1, 105.0, 102.2, 62.6, 33.5. HRMS (ESI): Calcd for C₁₉H₁₇O₄N₂ ([M+H]⁺), 337.1183; Found, 337.1183.



Data for 8q: Yellow solid, yield: 17%, m.p. 178-180 °C; IR cm^{-1} (KBr): 3077, 2980, 2947, 2225, 1631, 1468, 992, 935; ^1H NMR (400 MHz, CDCl_3) δ : 8.25 (d, $J = 8.4$ Hz, 2H, -Ar), 7.82 (d, $J = 8.4$ Hz, 2H, -Ar), 7.38-7.49 (m, 2H, -Ar), 6.86 (s, 1H, H-6), 6.13 (s, 2H, $-\text{OCH}_2\text{O}-$), 5.91-5.99 (m, 1H, H-2'), 5.09-5.14 (m, 2H, H-3'), 3.81 (s, 3H, $-\text{OCH}_3$), 3.42 (d, $J = 6.8$ Hz, 2H, H-1'). ^{13}C NMR (100 MHz, CDCl_3) δ : 163.0, 160.4, 150.1, 146.2, 144.5, 136.5, 132.9, 127.8, 127.4, 126.9, 117.9, 116.5, 115.2, 112.6, 102.5, 101.5, 62.6, 33.5. HRMS (ESI): Calcd for $\text{C}_{20}\text{H}_{16}\text{O}_4\text{N}_3$ ($[\text{M}+\text{H}]^+$), 362.1135; Found, 362.1135.

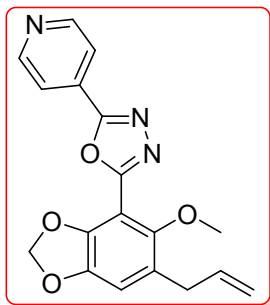


Data for 8r: White solid, yield: 29%, m.p. 125-126 °C; IR cm^{-1} (KBr): 3074, 2974, 2941, 2908, 1641, 1476, 983, 932; ^1H NMR (400 MHz, CDCl_3) δ : 9.36 (s, 1H, -Ar), 8.79 (d, $J = 4.8$ Hz, 1H, -Ar), 8.46 (d, $J = 8.0$ Hz, 1H, -Ar), 7.49-7.52 (m, 1H, -Ar), 6.86 (s, 1H, H-6), 6.13 (s, 2H, $-\text{OCH}_2\text{O}-$), 5.91-6.01 (m, 1H, H-2'), 5.10-5.14 (m, 2H, H-3'), 3.82 (s, 3H, $-\text{OCH}_3$), 3.42 (d, $J = 6.4$ Hz, 2H, H-1'). ^{13}C NMR (100 MHz, CDCl_3) δ : 162.3, 160.2, 152.1, 150.1, 147.7, 146.1, 144.5, 136.5, 134.5, 126.8, 123.9, 120.6, 116.5, 112.5, 102.5, 101.6, 62.6, 33.5. HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{16}\text{O}_4\text{N}_3$ ($[\text{M}+\text{H}]^+$), 338.1135; Found, 338.1135.

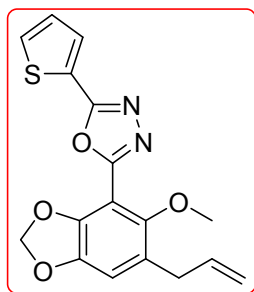


Data for 8s: Pale yellow solid, yield: 36%, m.p. 89-90 °C; IR cm^{-1} (KBr): 3004, 2980, 2940, 1630, 1469, 993, 920; ^1H

NMR (400 MHz, CDCl₃) δ : 8.32-8.36 (m, 2H, -Ar), 7.01 (d, J = 7.6 Hz, 1H, -Ar), 6.83 (s, 1H, H-6), 6.11 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.13 (m, 2H, H-3'), 4.54 (q, J = 6.8 Hz, 2H, -CH₂CH₃), 3.81 (s, 3H, -OCH₃), 3.41 (d, J = 6.4 Hz, 2H, H-1'), 1.44 (t, J = 7.2 Hz, 2H, -CH₂CH₃). ¹³C NMR (100 MHz, CDCl₃) δ : 162.4, 160.7, 159.8, 150.3, 150.1, 146.0, 144.3, 139.4, 136.7, 126.7, 116.5, 116.4, 112.1, 107.9, 102.3, 102.1, 62.7, 62.6, 33.5, 14.5. HRMS (ESI): Calcd for C₂₀H₂₀O₅N₃ ([M+H]⁺), 382.1396; Found, 382.1397.



Data for **8t**: White solid, yield: 20%, m.p. 125-127 °C; IR cm⁻¹ (KBr): 3002, 2973, 2935, 1643, 1460, 991, 927; ¹H NMR (400 MHz, CDCl₃) δ : 8.84 (d, J = 5.2 Hz, 2H, -Ar), 8.01 (d, J = 6.0 Hz, 1H, -Ar), 7.49-7.52 (m, 1H, -Ar), 6.87 (s, 1H, H-6), 6.14 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.10-5.14 (m, 2H, H-3'), 3.81 (s, 3H, -OCH₃), 3.42 (d, J = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ : 162.6, 160.6, 150.6, 150.2, 146.2, 144.5, 136.5, 131.2, 126.9, 120.5, 116.5, 112.7, 102.5, 101.5, 62.6, 33.5. HRMS (ESI): Calcd for C₁₈H₁₆O₄N₃ ([M+H]⁺), 338.1135; Found, 338.1135.



Data for **8u**: White solid, yield: 58%, m.p. 92-93 °C; IR cm⁻¹ (KBr): 3119, 2976, 2943, 1639, 1497, 997, 923; ¹H NMR (400 MHz, CDCl₃) δ : 7.84 (dd, J = 3.6, 0.8 Hz, 1H, -Ar), 7.56 (dd, J = 4.8, 0.8 Hz, 1H, -Ar), 7.18-7.20 (m, 1H, -Ar), 6.82 (s, 1H, H-6), 6.11 (s, 2H, -OCH₂O-), 5.91-6.01 (m, 1H, H-2'), 5.09-5.13 (m, 2H, H-3'), 3.79 (s, 3H, -OCH₃), 3.41 (d, J = 6.4 Hz, 2H, H-1'). ¹³C NMR (100 MHz, CDCl₃) δ : 160.9, 158.9, 150.1, 146.0, 144.4, 136.6, 130.2, 129.9, 128.2, 126.6, 125.2, 116.4, 112.2, 102.4, 101.8, 62.6, 33.5. HRMS (ESI): Calcd for C₁₇H₁₅O₄N₂S ([M+H]⁺), 343.0746; Found, 343.0747.