Supporting information

Novel one-pot synthesis, characterization, and antifungal and antibacterial activity of a small library of 2-aryloxy-1,4-naphthoquinone derivatives

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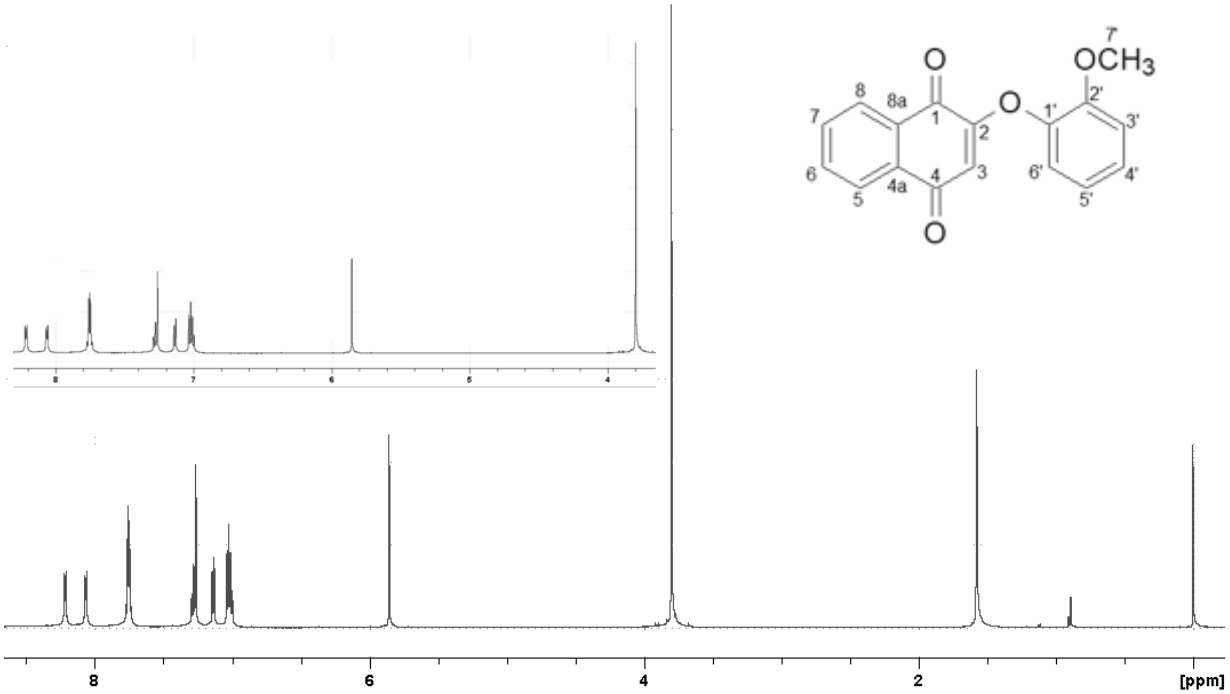
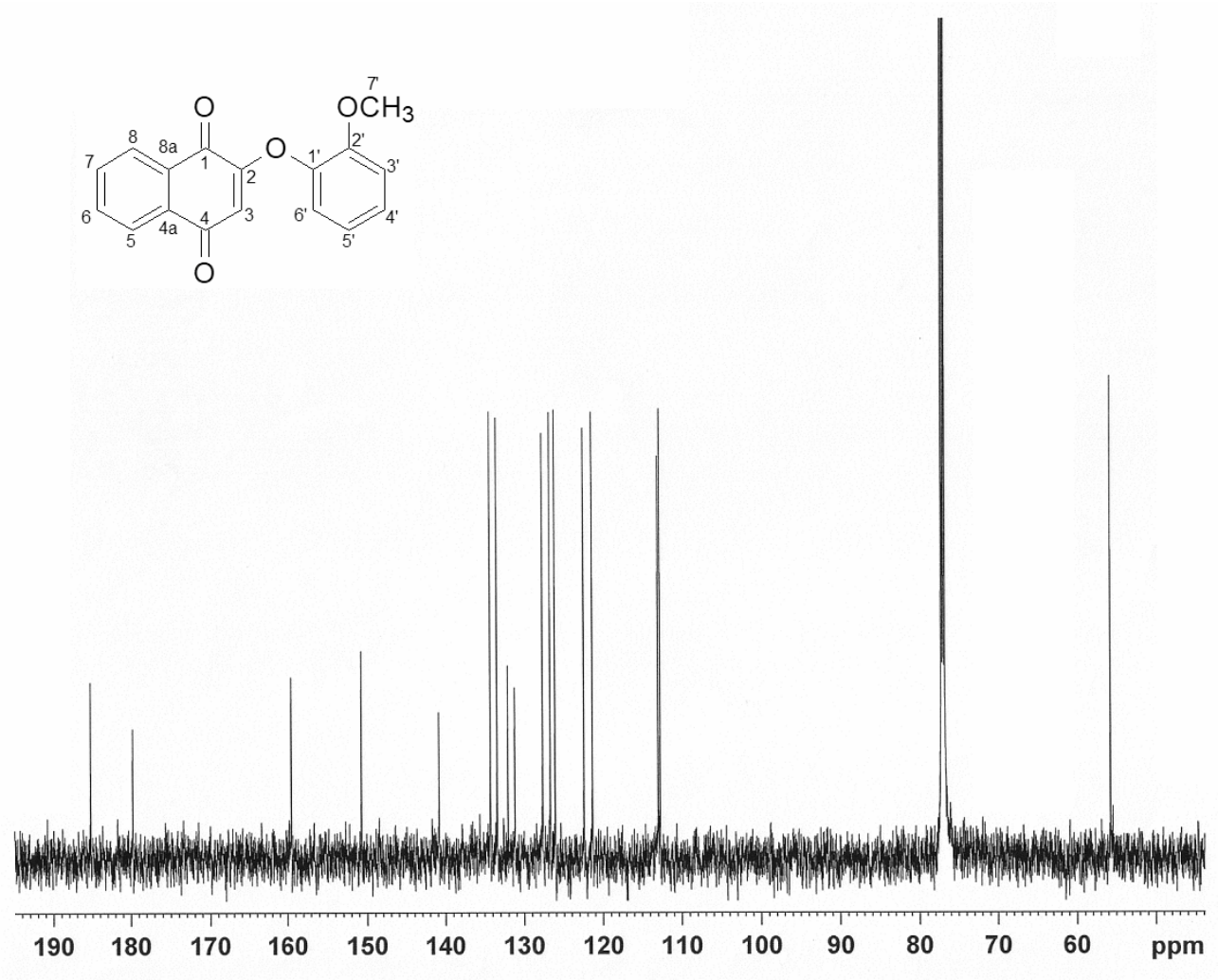
34 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, cold base wash (MTBE as solvent and NaOH 0.5 mol/L as base) and recrystallization with isooctane. Yield 141 mg (68%), yellow crystals, mp = (151.0 – 153.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.21 (1H, d, *J* = 9 Hz, ArH), 8.06 (1H, d, *J* = 9 Hz, ArH), 7.75 (2H, m, ArH), 7.28 (1H, t, J_{ortho} = 8 Hz, ArH), 7.13 (1H, d, J_{ortho} = 9 Hz, ArH), 7.03 (1H, t, J_{ortho} = 8 Hz, ArH), 7.00 (1H, d, J_{ortho} = 8 Hz, ArH), 5.85 (1H, s, ArH, 3.80 (3H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.2, 179.7, 159.5, 150.7, 140.9, 134.2, 133.4, 132.1, 131.2, 127.7, 126.7, 126.1, 122.4, 121.4, 113.0, 112.7, 55.7. IR (KBr pellet) cm^{-1}: 3068, 2958, 1683, 1652, 1611, 1499, 1261, 1205. UV-Vis (MeOH) nm: 201, 243 (max), 271, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_4$: 281.0814; found: 281.0819. Purity: 99.9%. MIC (μM): 892 (*s. aureus),* > 3000 (*E. coli, C. albicans).*

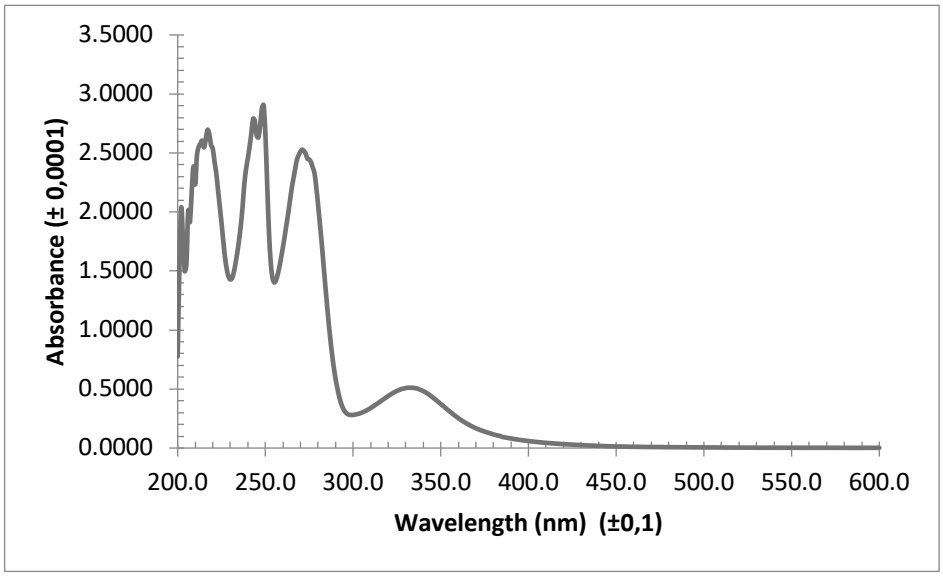
2-(2-methoxyphenoxy)-1,4-naphthoquinone **34** ^{1}H-NMR



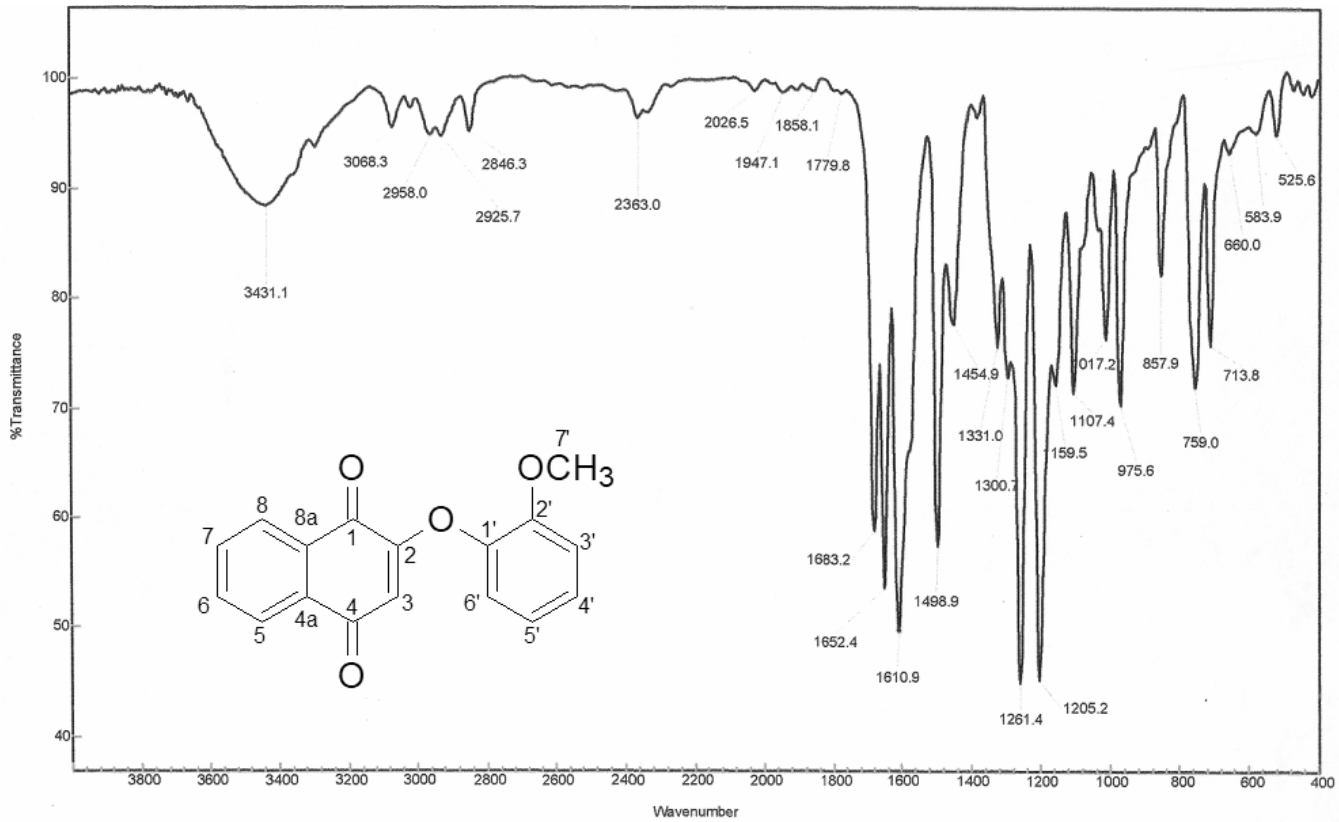
2-(2-methoxyphenoxy)-1,4-naphthoquinone **34** ^{13}C-NMR



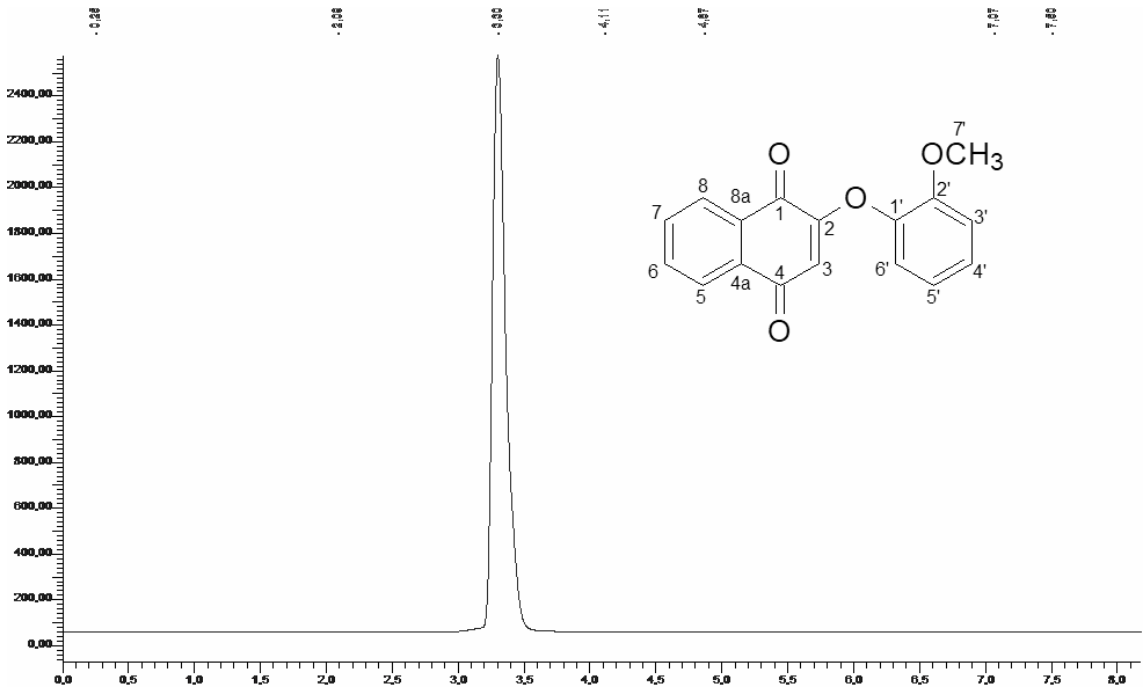
2-(2-methoxyphenoxy)-1,4-naphthoquinone **34** UV-Vis (MeOH)



2-(2-methoxyphenoxy)-1,4-naphthoquinone **34** IR (KBr pellet)



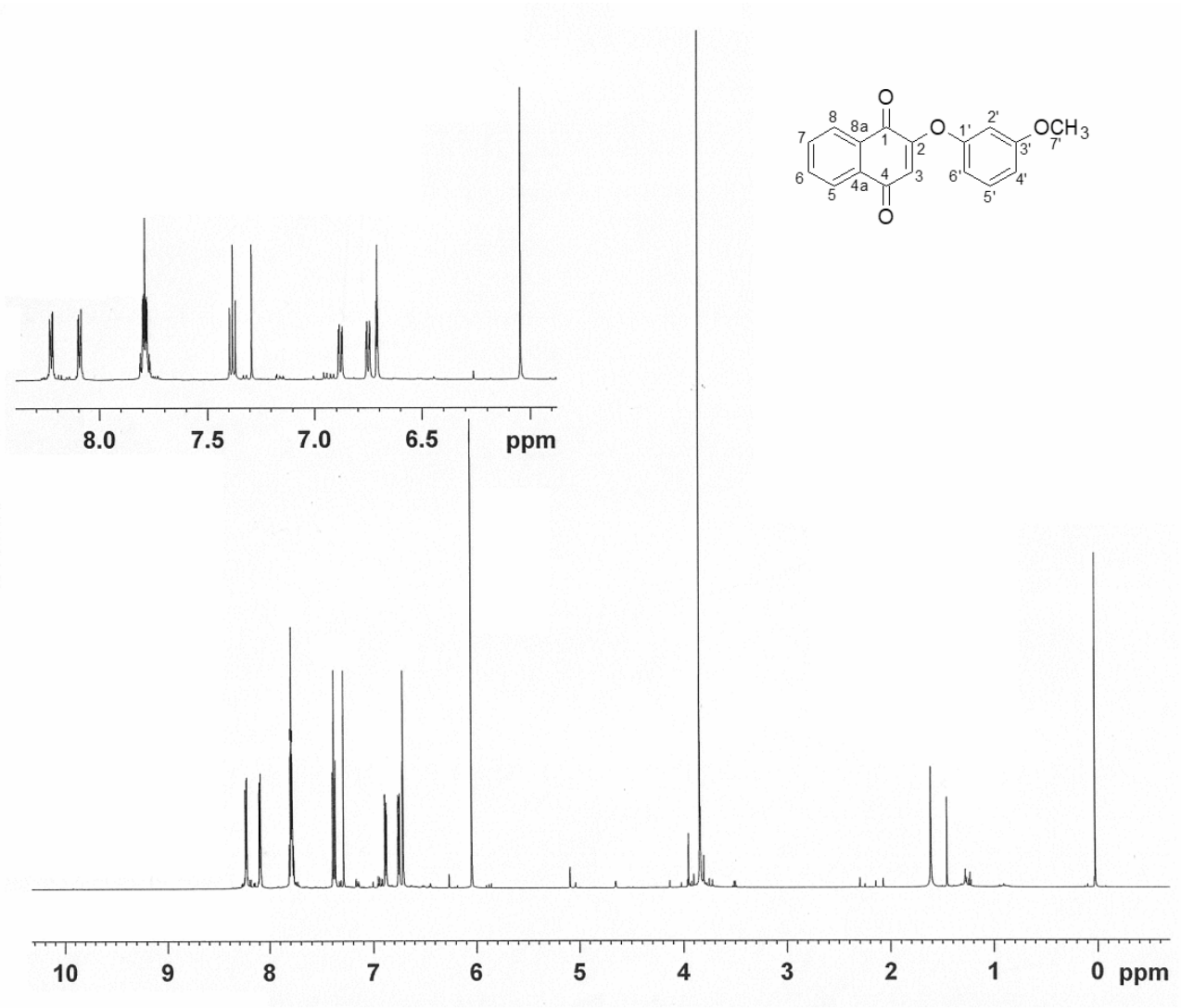
2-(2-methoxyphenoxy)-1,4-naphthoquinone **34** HPLC chromatogram (274 nm, 100% MeCN)



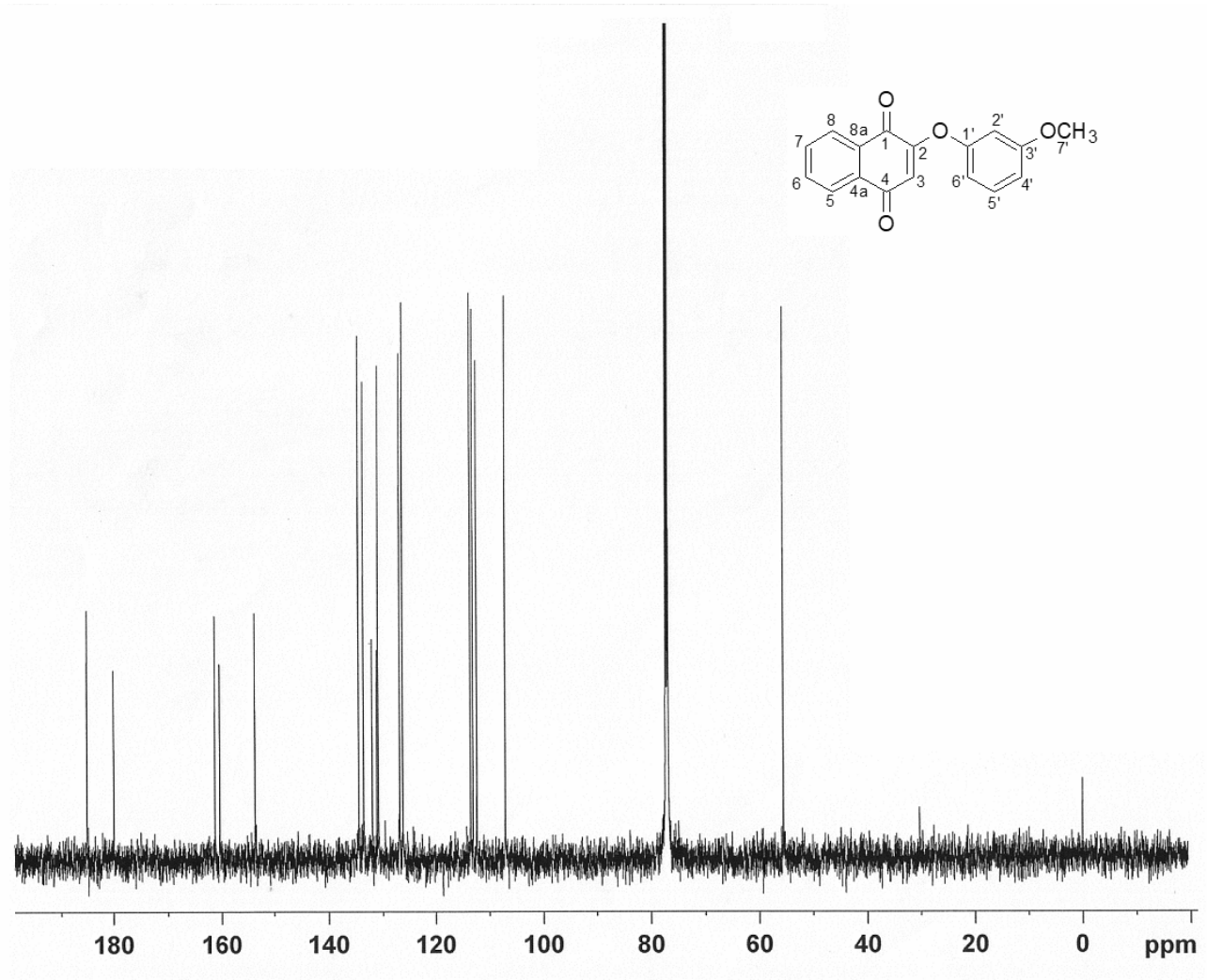
2-(3-methoxyphenoxy)-1,4-naphthoquinone 35

35 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, cold base wash (MTBE as solvent and NaOH 0.5 mol/L as base) and recrystallization with isooctane. Yield 109 mg (52%), orange crystals, mp = (84.0 – 87.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.23 (1H, d, J = 7.5 Hz, ArH), 8.09 (1H, d, J = 7.5 Hz, ArH), 7.80 (2H, m, ArH), 7.38 (1H, t, J_{ortho} = 7.5 Hz, ArH), 6.88 (1H, d, J_{ortho} = 9 Hz, ArH), 6.76 (1H, d, J_{ortho} = 8 Hz, ArH), 6.71 (1H, s, ArH), 6.05 (1H, s, ArH), 3.84 (3H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.0, 179.9, 161.2, 160.4, 153.6, 134.4, 133.5, 132.0, 131.1, 130.8, 126.8, 126.2, 113.5, 113.0, 112.3, 55.5. UV-Vis (MeOH) nm: 211, 244 (max), 270, 331. IR (KBr pellet) cm^{-1}: 3053, 2960, 1678, 1653, 1611, 1584, 1264, 1204. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_4$: 281.0814; found: 281.0812. Purity: 95.9%. MIC (µM): 223 (*S. aureus*), 446 (*C. albicans*), >3000 (*E. coli*).

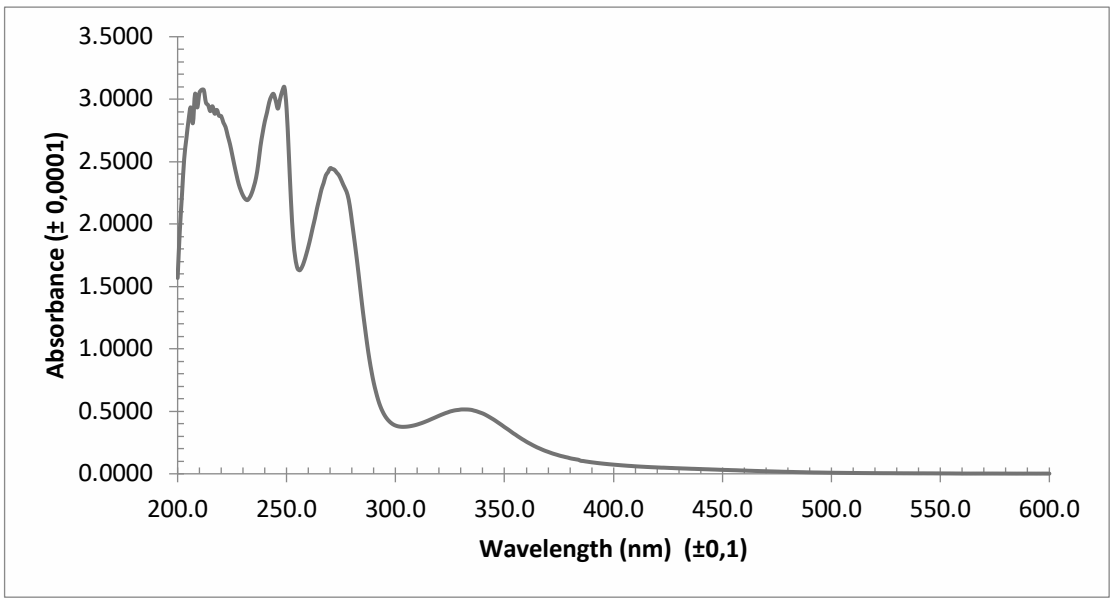
2-(3-methoxyphenoxy)-1,4-naphthoquinone **35** ^{1}H NMR



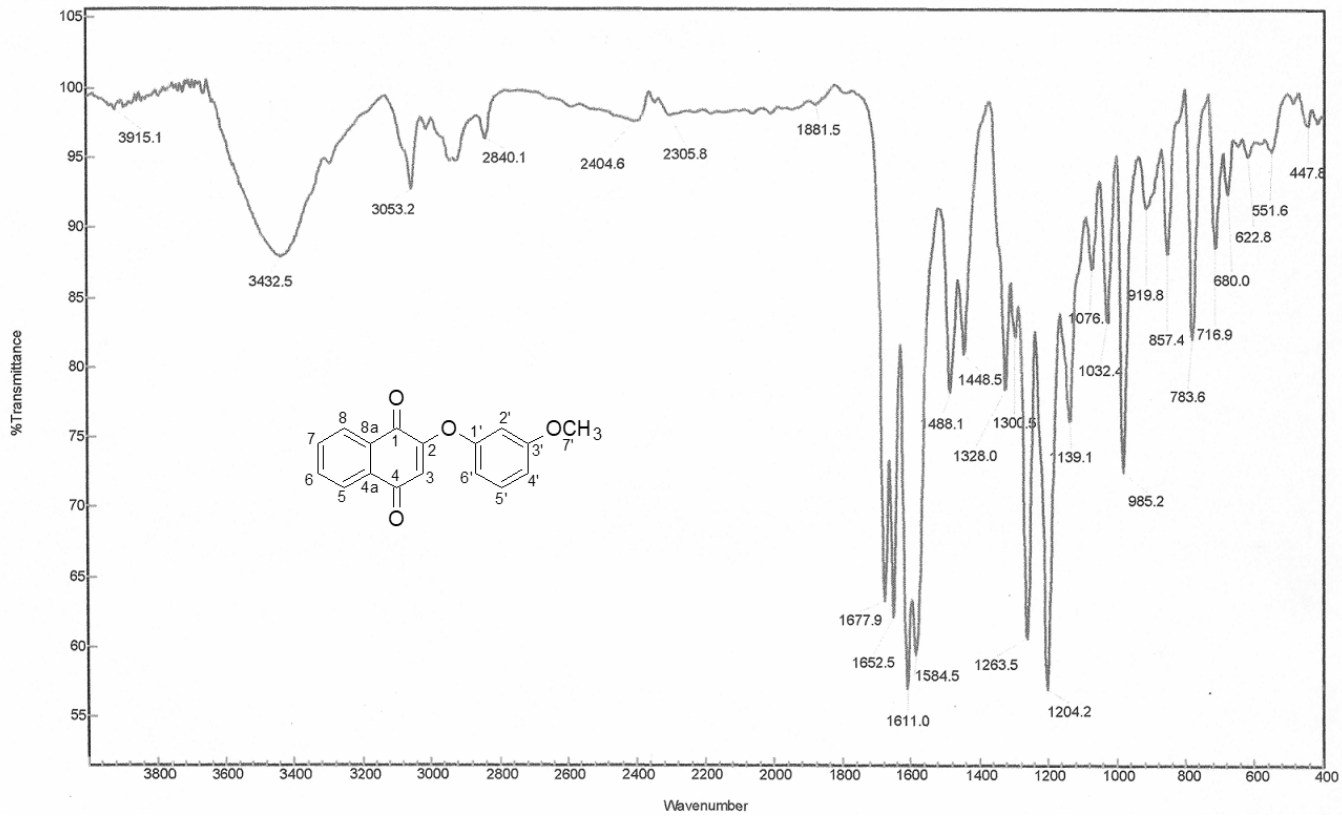
2-(3-methoxyphenoxy)-1,4-naphthoquinone **35** ^{13}C RMN



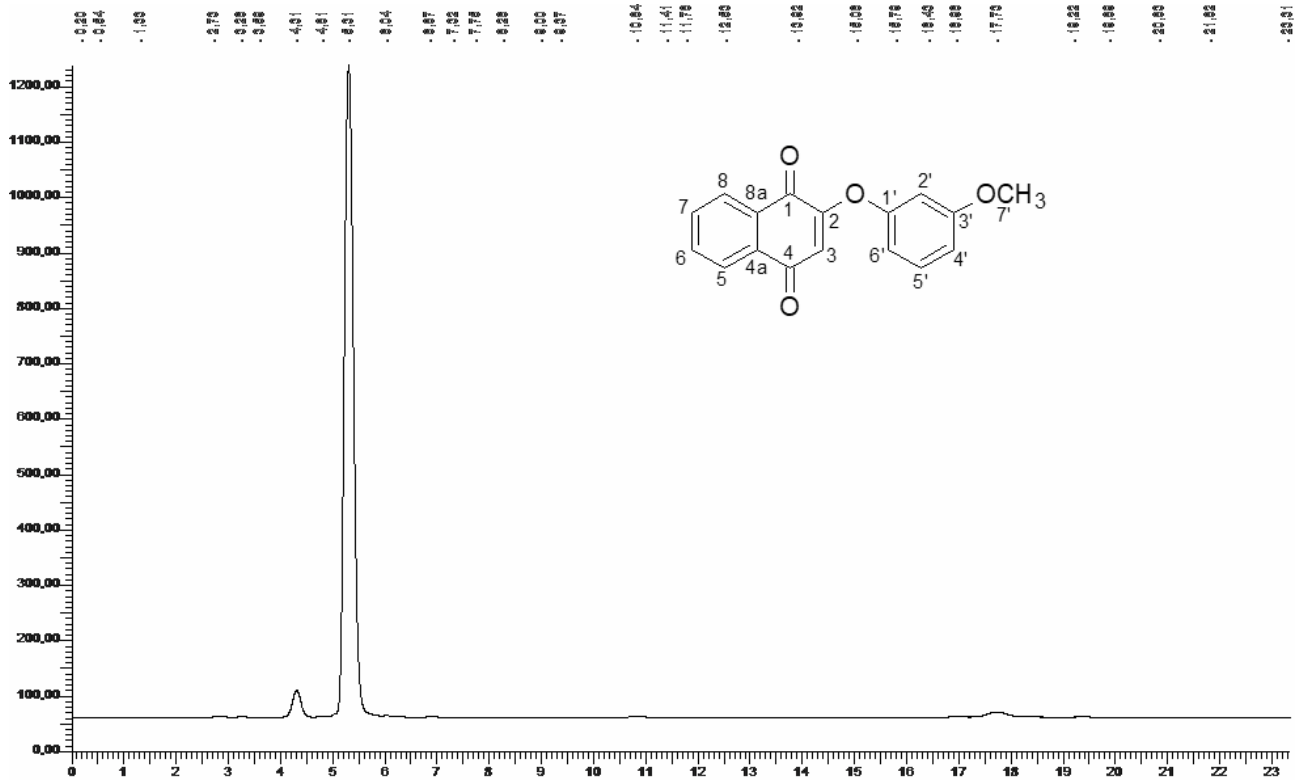
2-(3-methoxyphenoxy)-1,4-naphthoquinone **35** UV-Vis (MeOH)



2-(3-methoxyphenoxy)-1,4-naphthoquinone **35** IR (KBr pellet)



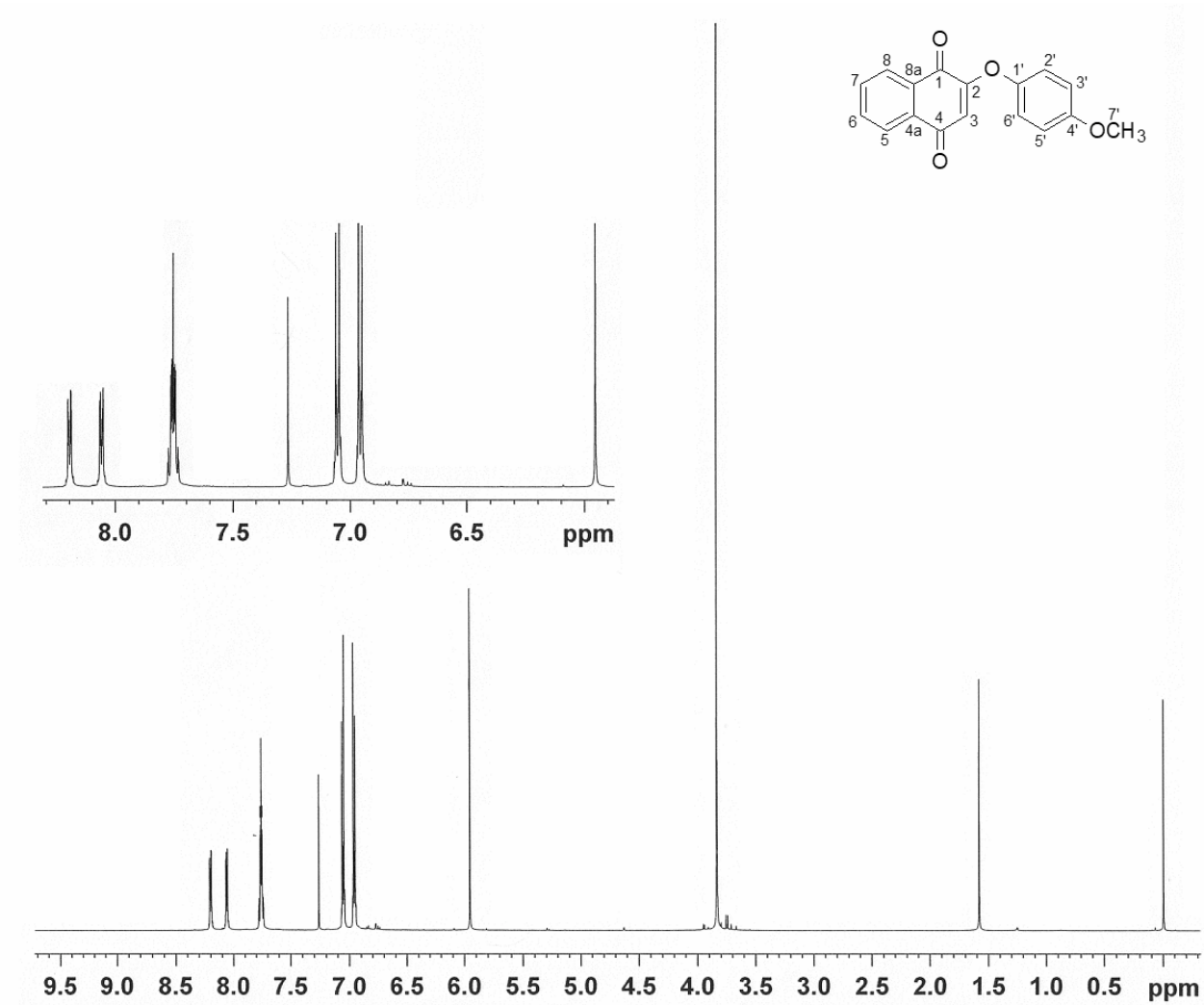
2-(3-methoxyphenoxy)-1,4-naphthoquinone **35** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



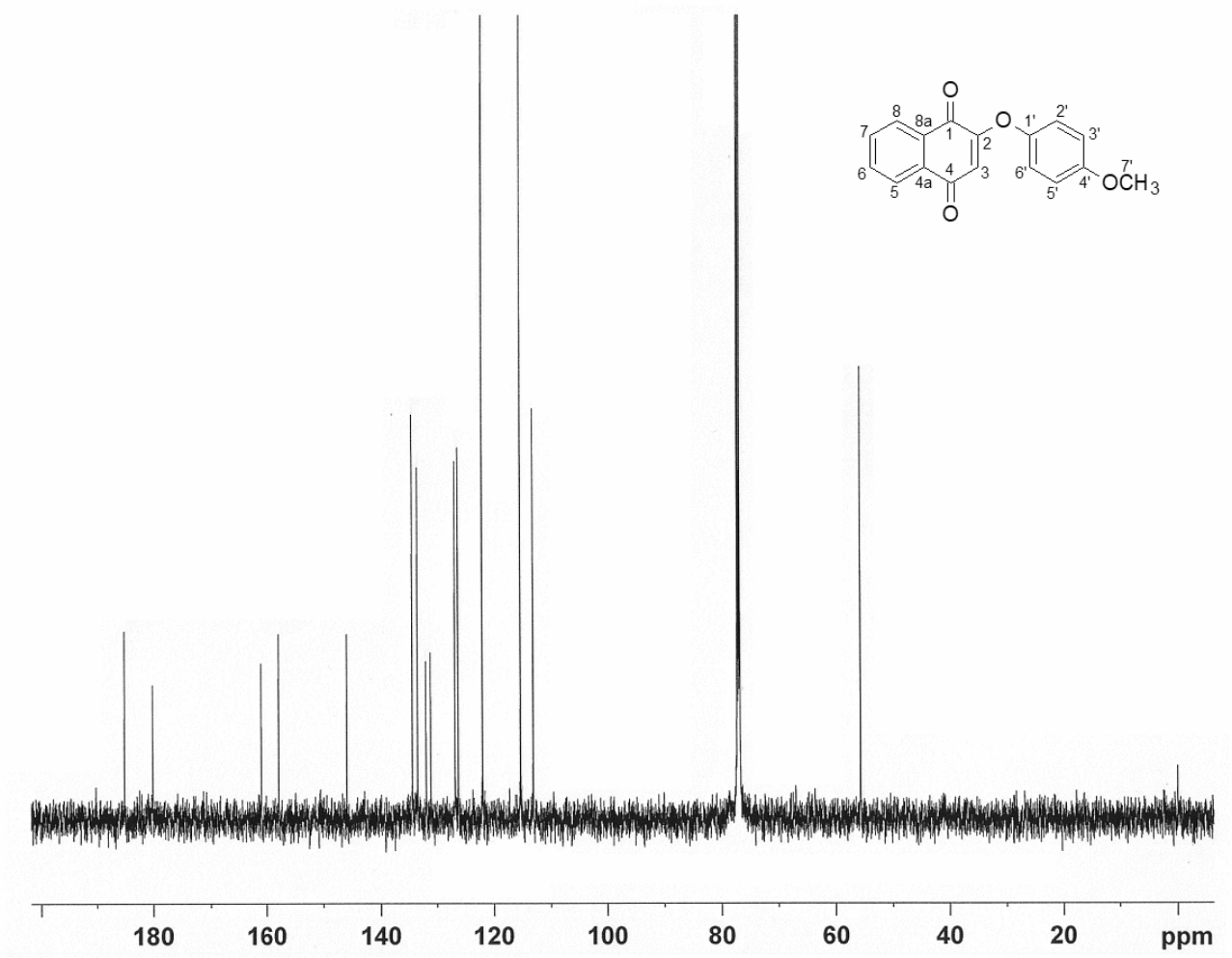
2-(4-methoxyphenoxy)-1,4-naphthoquinone **36**

36 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, chromatography column (CH_2Cl_2 as eluent, isocratically) and recrystallization with isooctane. Yield 201 mg (96%), yellow crystals, mp = (133.0 – 134.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, d, *J* = 8 Hz, ArH), 8.06 (1H, d, *J* = 8 Hz, ArH), 7.76 (2H, m, ArH), 7.05 (2H, d, J_{ortho} = 8 Hz, ArH), 6.96 (2H, d, J_{ortho} = 8 Hz, ArH), 5.95 (1H, s, ArH), 3.83 (3H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.0, 179.9, 161.2, 160.4, 153.6, 132.0, 131.1, 126.8, 126.2, 121.1, 117.6, 113.0, 55.5. IR (KBr pellet) cm^{-1}: 3073, 2923, 1680, 1650, 1619, 1503, 1259, 1219. UV-Vis (MeOH) nm: 204, 243 (max), 274, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_4$: 281.0814; found: 281.0817. Purity: 99.3%. MIC (μM): 1784 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

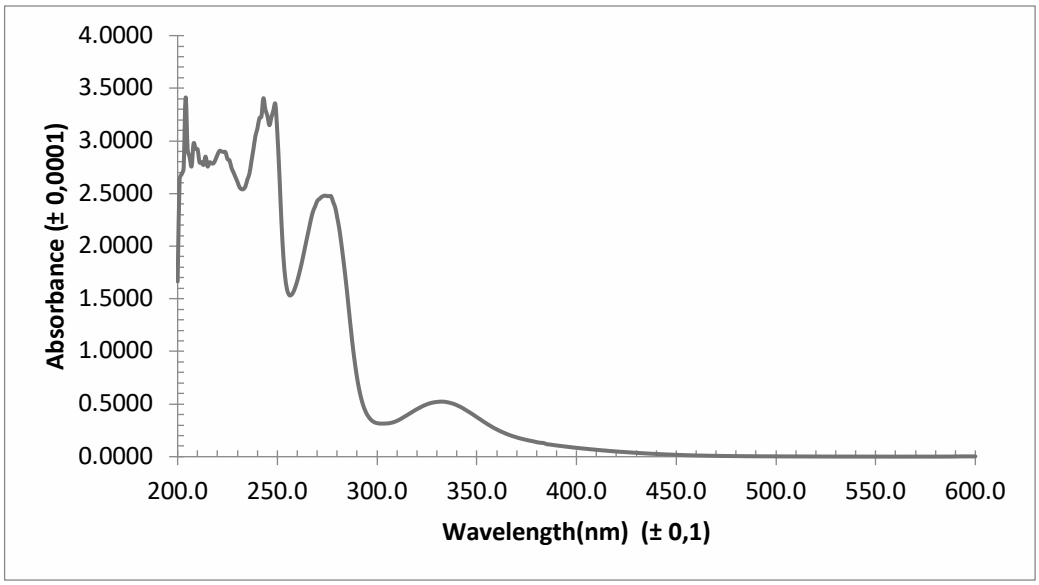
2-(4-methoxyphenoxy)-1,4-naphthoquinone **36** ^{1}H NMR



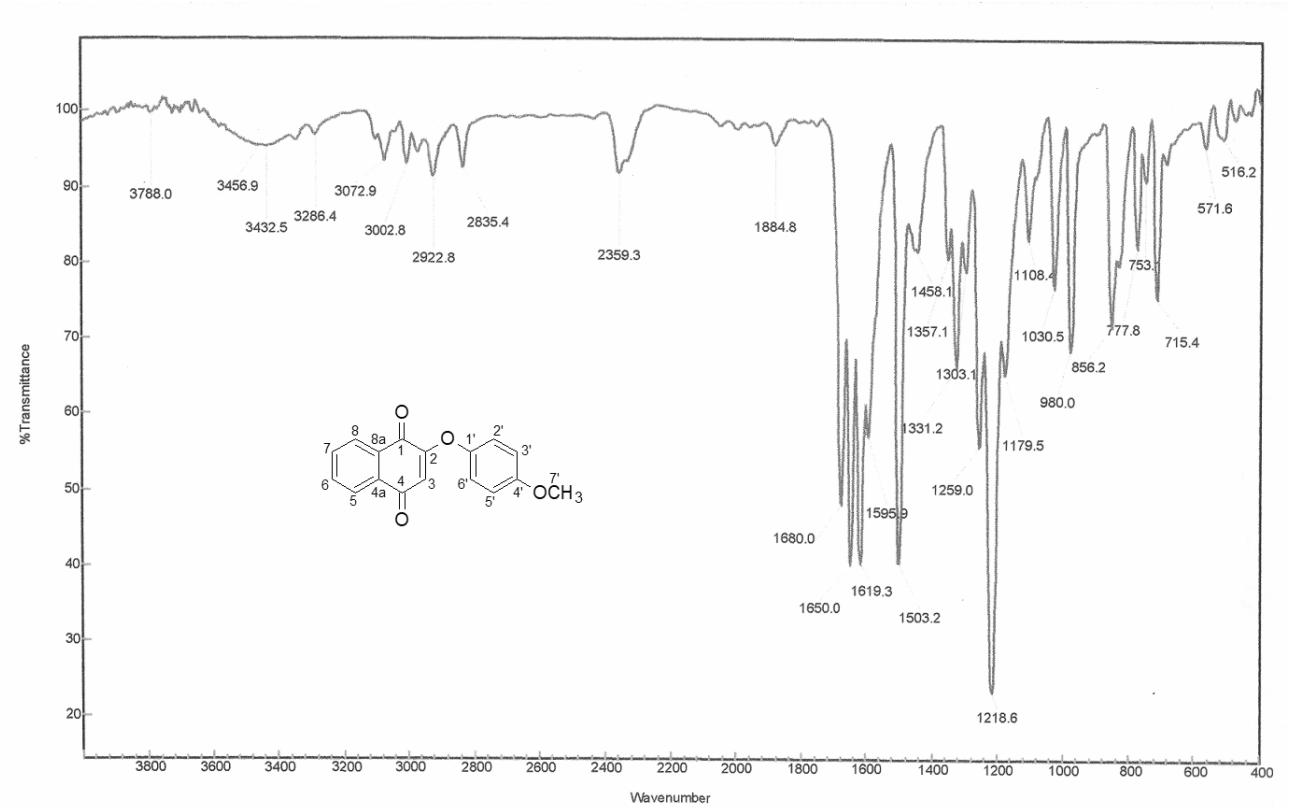
2-(4-methoxyphenoxy)-1,4-naphthoquinone **36** ^{13}C NMR



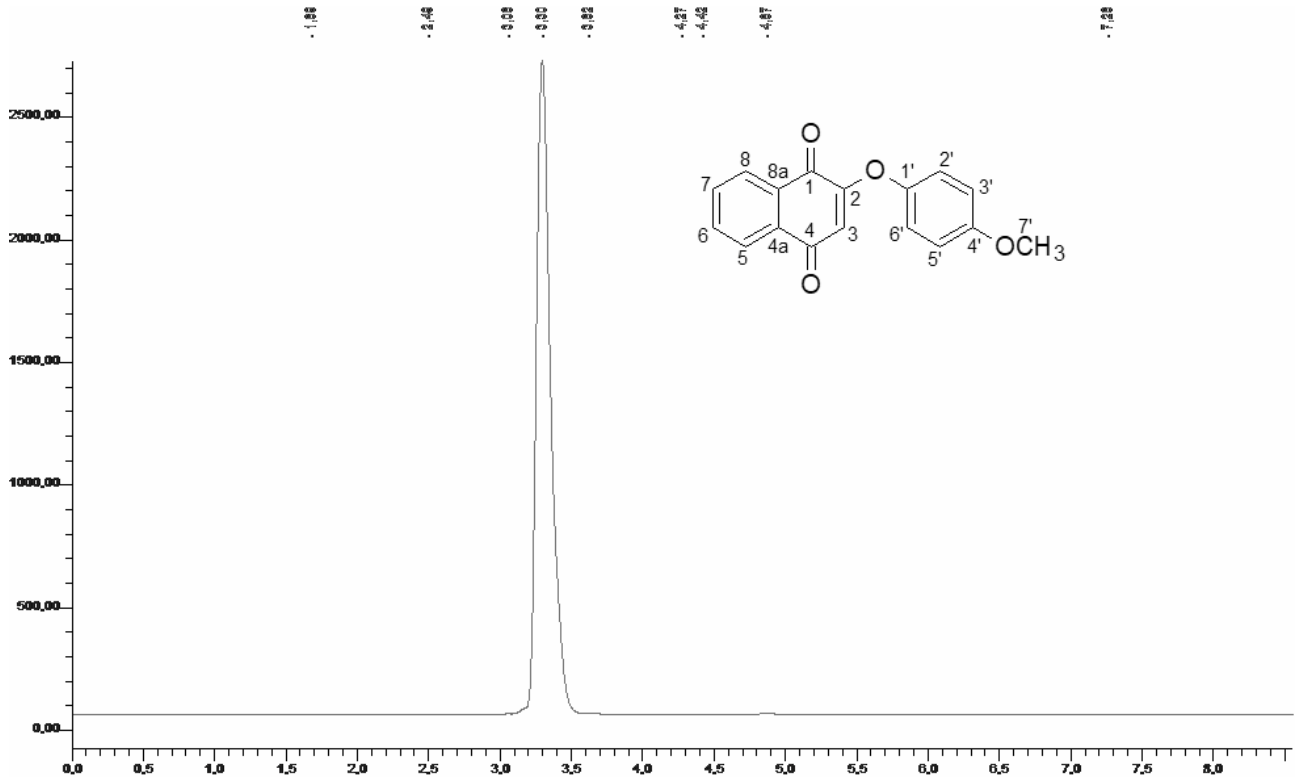
2-(4-methoxyphenoxy)-1,4-naphthoquinone **36** UV-Vis (MeOH)



2-(4-methoxyphenoxy)-1,4-naphthoquinone **36** IR (KBr pellet)



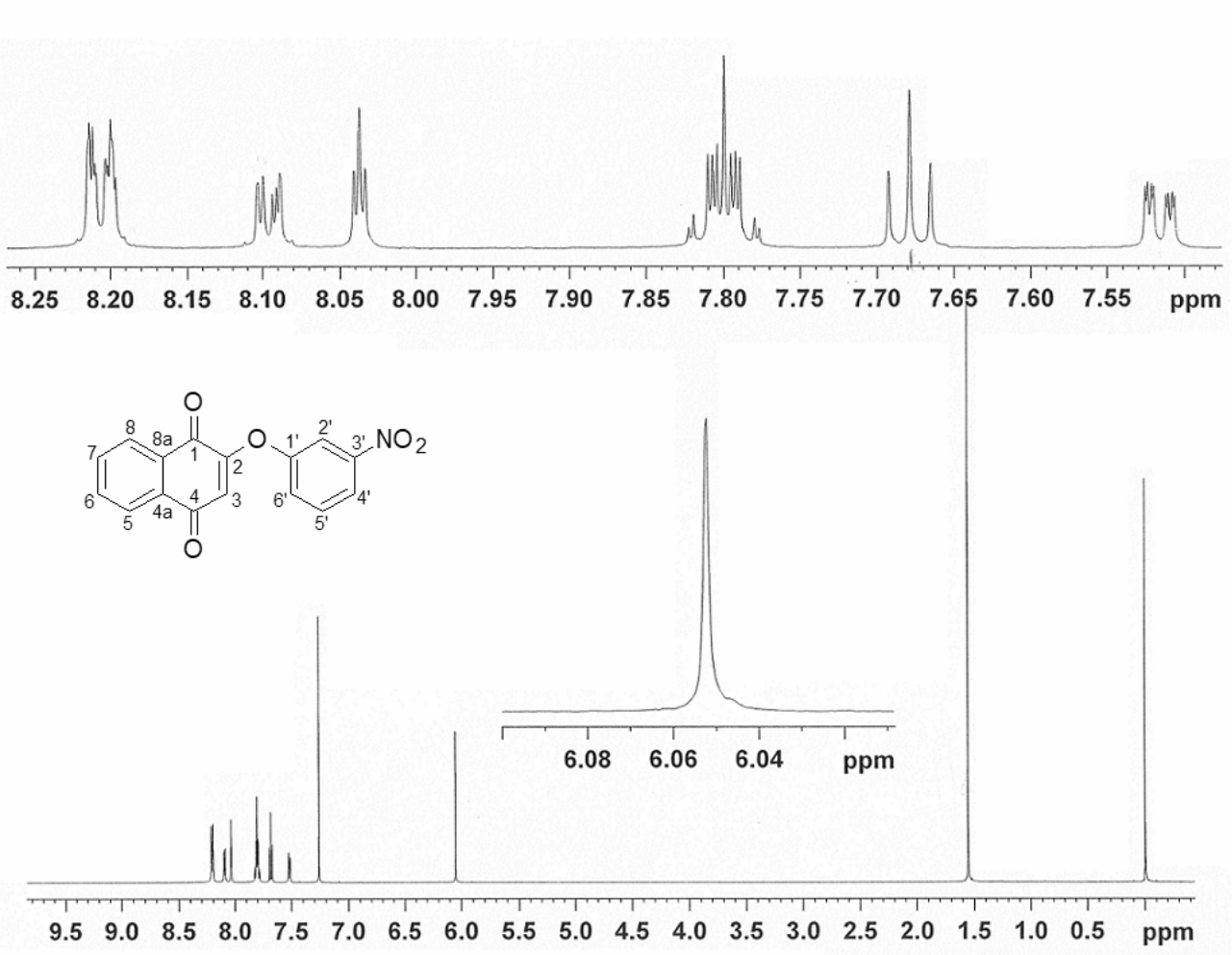
2-(4-methoxyphenoxy)-1,4-naphthoquinone **36** HPLC chromatogram (270 nm, 100% MeCN)



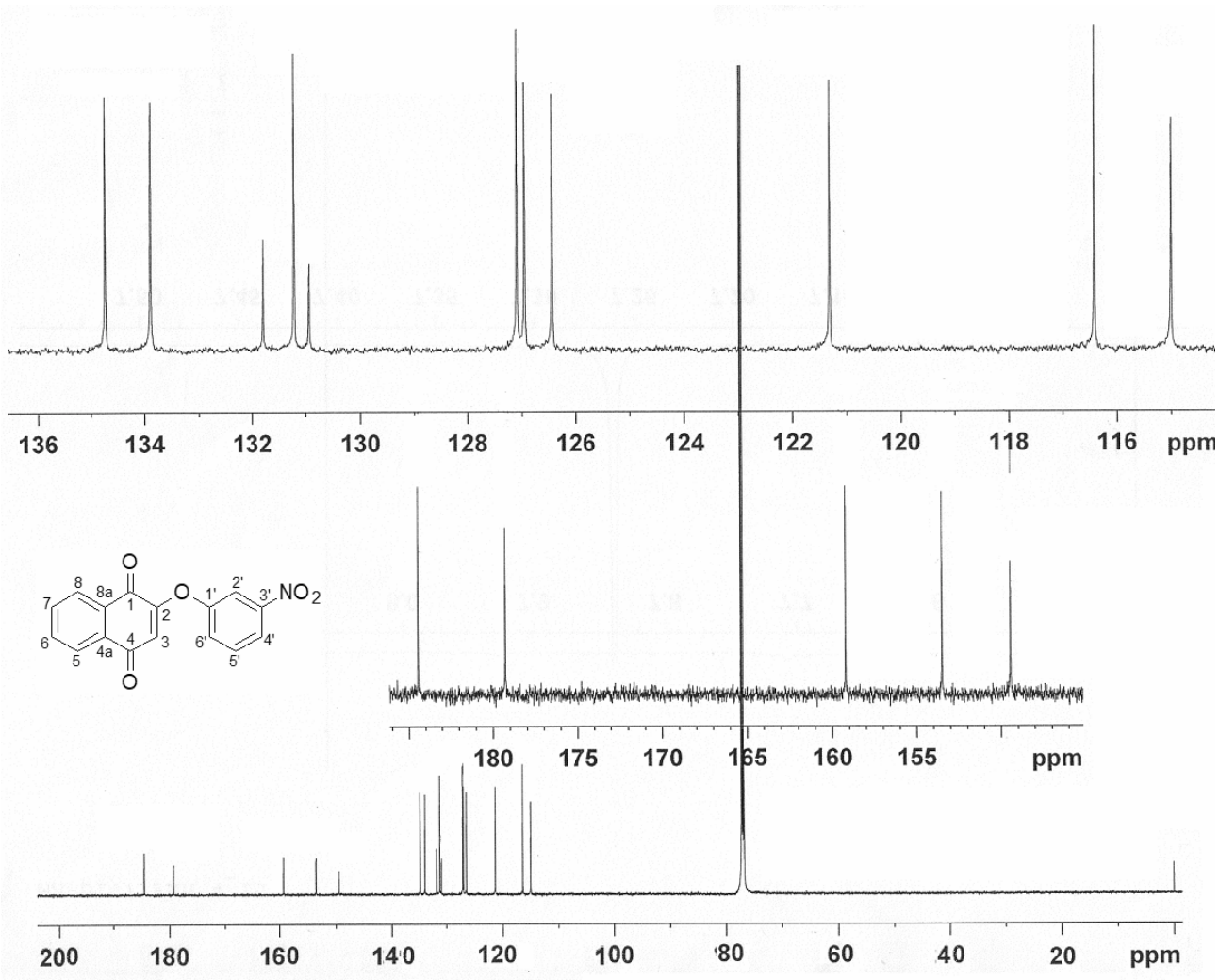
2-(3-nitrophenoxy)-1,4-naphthoquinone **37**

37 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with 50% n-heptane/toluene and recrystallization with n-heptane. Yield 173 mg (58%), yellow crystals, mp = (166.0 – 167.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) =8.21 (2H, d, *J* = 6 Hz, ArH), 8.10 (1H, dd, *J* = 1.2 Hz, *J* = 6.9 Hz, ArH), 8.04 (1H, t, J_{meta} = 1.2 Hz, ArH), 7.80 (2H, m, ArH), 7.68 (1H, t, J_{ortho} = 8.1 Hz, ArH), 7.52 (1H, ddd, J_{meta} = 1.2 Hz, J_{meta} = 2.3 Hz, J_{ortho} = 8.1 Hz, ArH), 6.05 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.4, 179.3, 159.2, 153.5, 149.4, 134.7, 133.9, 131.8, 131.2, 130.9, 127.1, 127.0, 126.4, 121.3, 116.4, 115.0. IR (KBr pellet) cm^{-1}: 3085, 1676, 1654, 1608, 1527, 1353, 1261, 1222. UV-Vis (MeOH) nm: 209 (max), 241, 272, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}NO_5$: 296.0559; found: 296.0558. Purity: 99.0%. MIC (µM): 21.2 (*S. aureus*), > 3000 (*C. albicans*), > 3000 (*E. coli*).

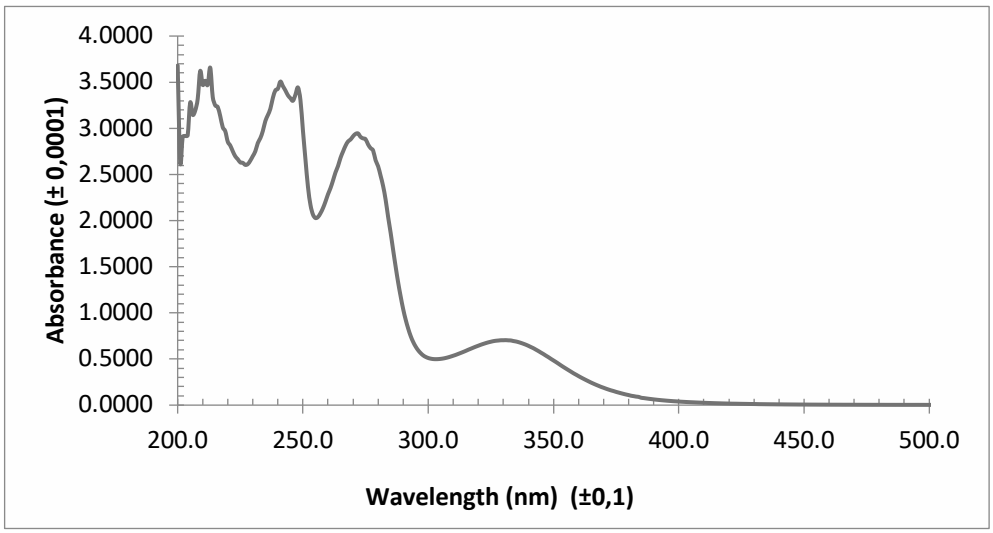
2-(3-nitrophenoxy)-1,4-naphthoquinone **37** ^{1}H NMR



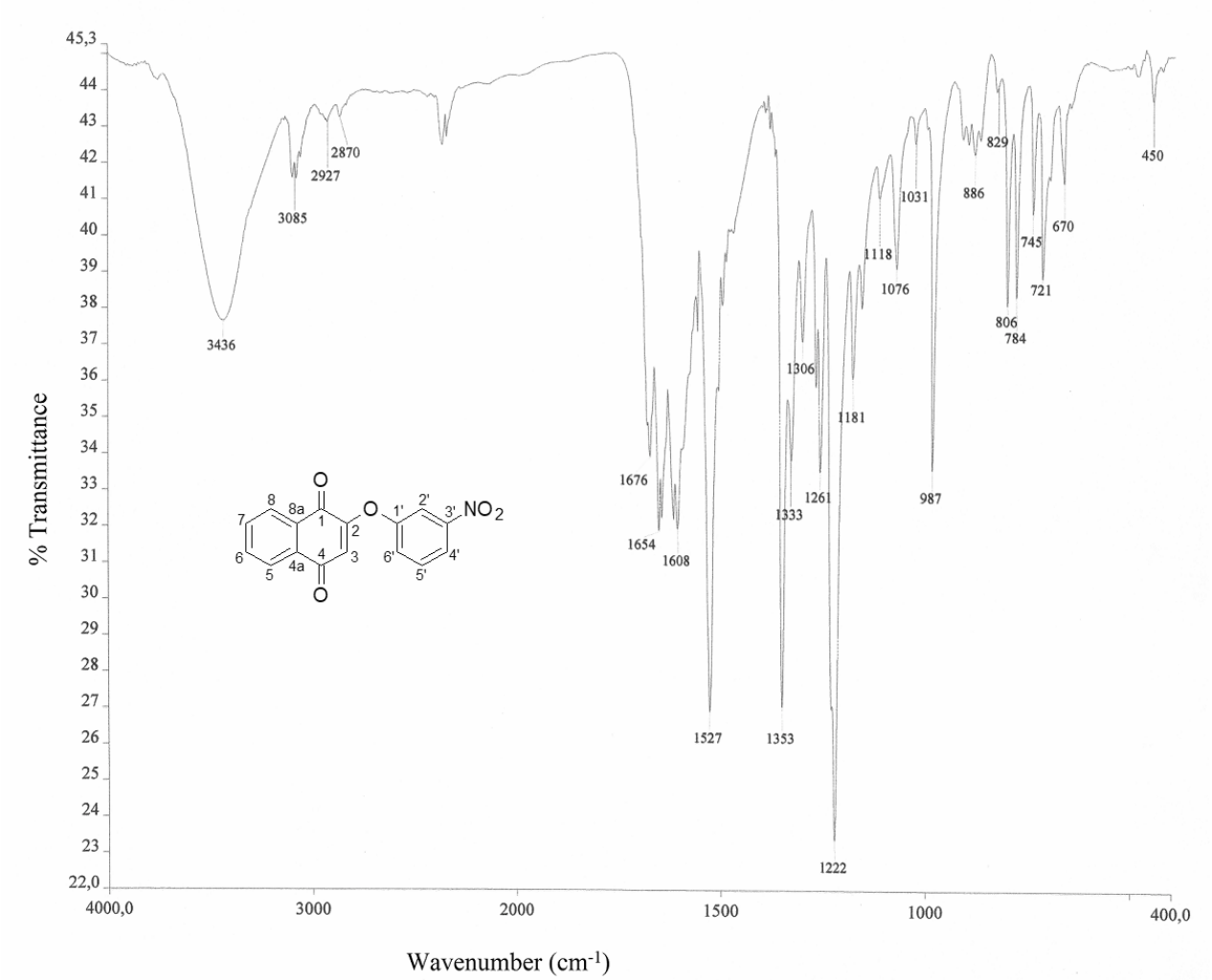
2-(3-nitrophenoxy)-1,4-naphthoquinone **37** ^{13}C NMR



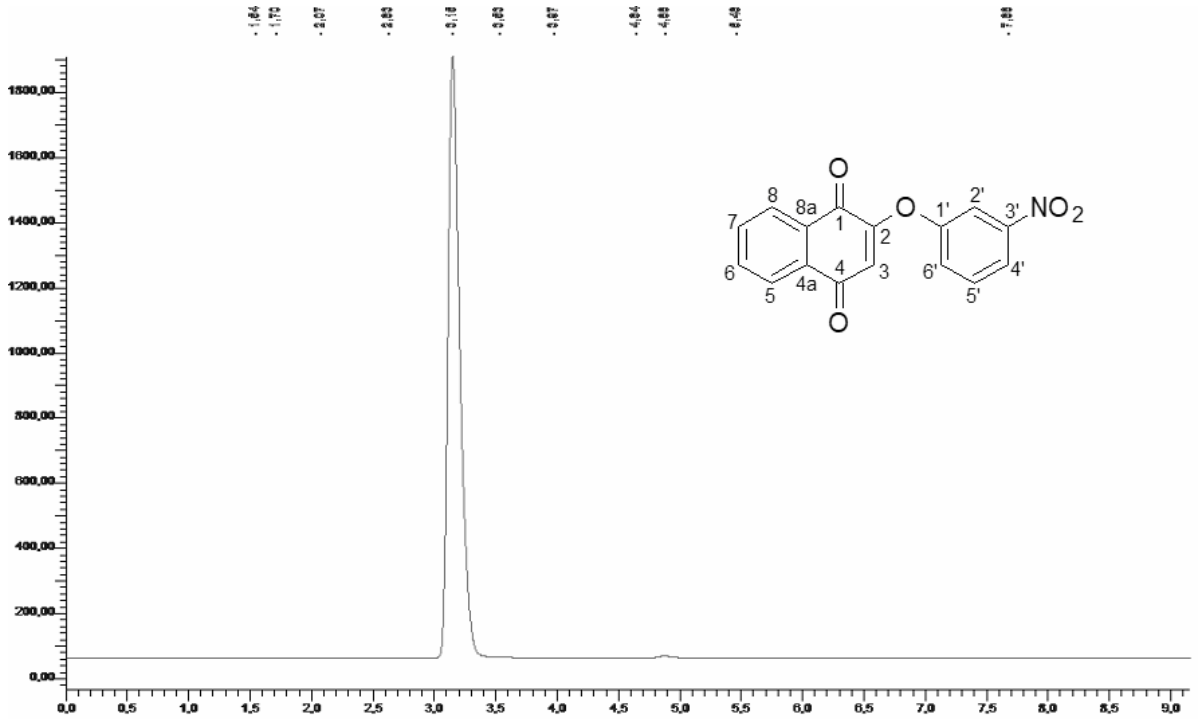
2-(3-nitrophenoxy)-1,4-naphthoquinone **37** UV-Vis (MeOH)



2-(3-nitrophenoxy)-1,4-naphthoquinone **37** IR (KBr pellet)



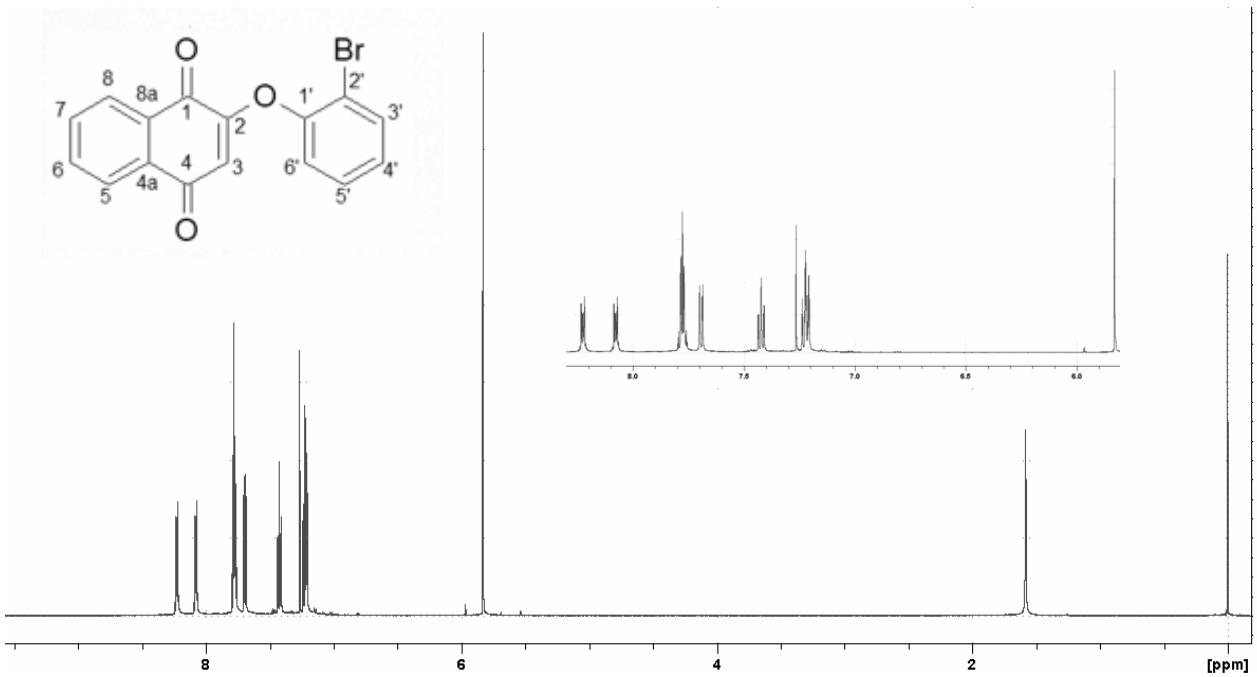
2-(3-nitrophenoxy)-1,4-naphthoquinone **37** HPLC chromatogram (268 nm, 100% MeCN)



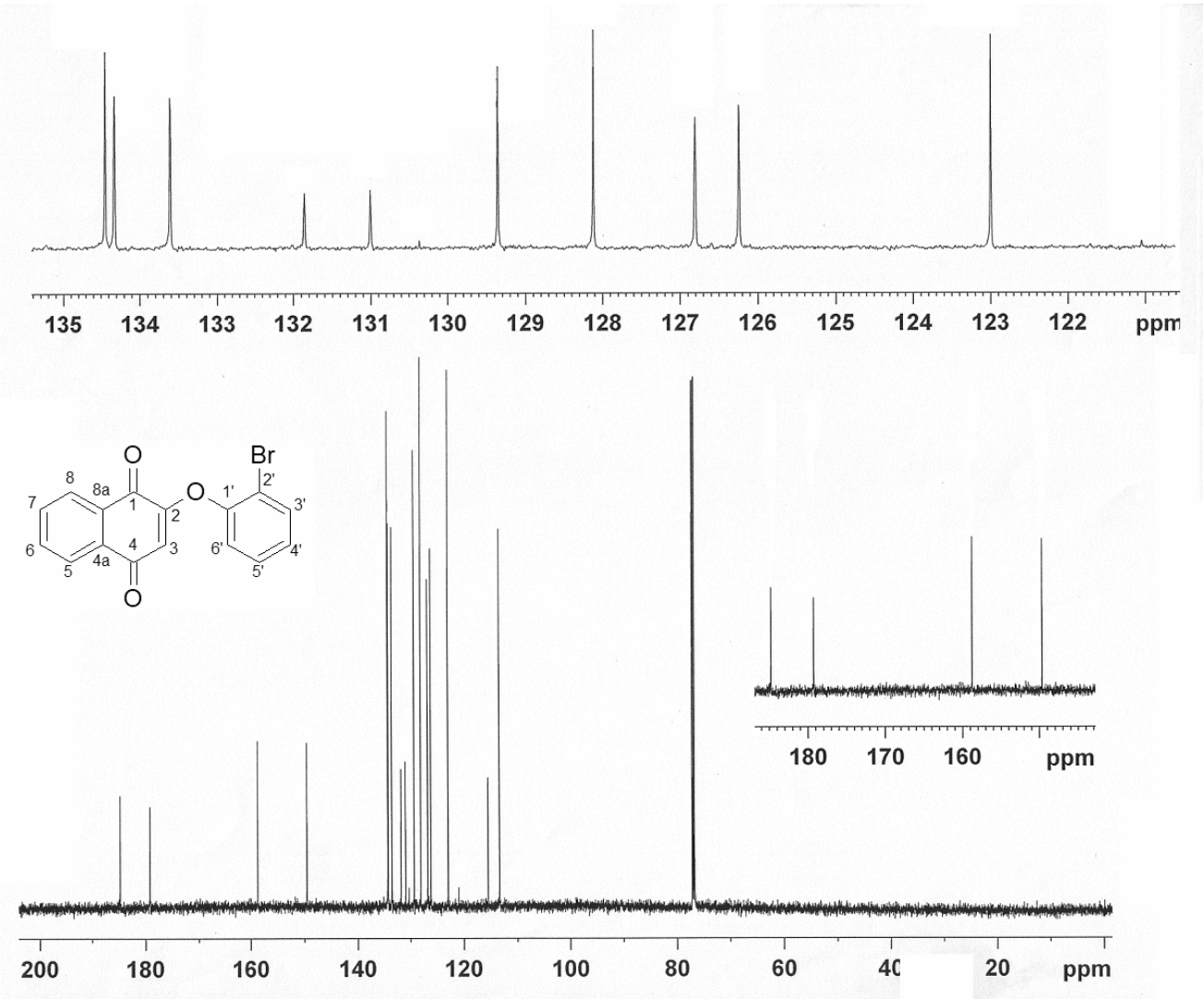
2-(2-bromophenoxy)-1,4-naphthoquinone 38

38 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, column chromatography (1% triethylamine/benzene as eluent, isocratically) and recrystallization with isooctane. Yield 287 mg (87%), yellow crystals, mp = (119.0 – 121.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.23 (1H, d, *J* = 6.4 Hz, ArH), 8.08 (1H, d, *J* = 6.4 Hz, ArH), 7.78 (2H, m, ArH), 7.69 (1H, d, J_{ortho} = 8.6 Hz, ArH), 7.42 (1H, t, J_{ortho} = 8.6 Hz, ArH), 7.22 (1H, t, J_{ortho} = 8.6 Hz, ArH), 7.21 (1H, d, J_{ortho} = 6.4 Hz, ArH), 5.83 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.8, 179.3, 158.7, 149.6, 134.4, 134.3, 133.6, 131.9, 131.0, 129.4, 128.1, 126.8, 126.2, 123.0, 115.6, 113.5. IR (KBr pellet) cm^{-1}: 3068, 1684, 1654, 1612, 1595, 1263, 1225, 660. UV-Vis (MeOH) nm: 203, 209 (max), 215, 249, 271, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}O_3Br$: 328.9813; found: 328.9806. Purity: 99.7%. MIC (μM): 760 (*S. aureus*), 190 (*C. albicans*), >3000 (*E. coli*).

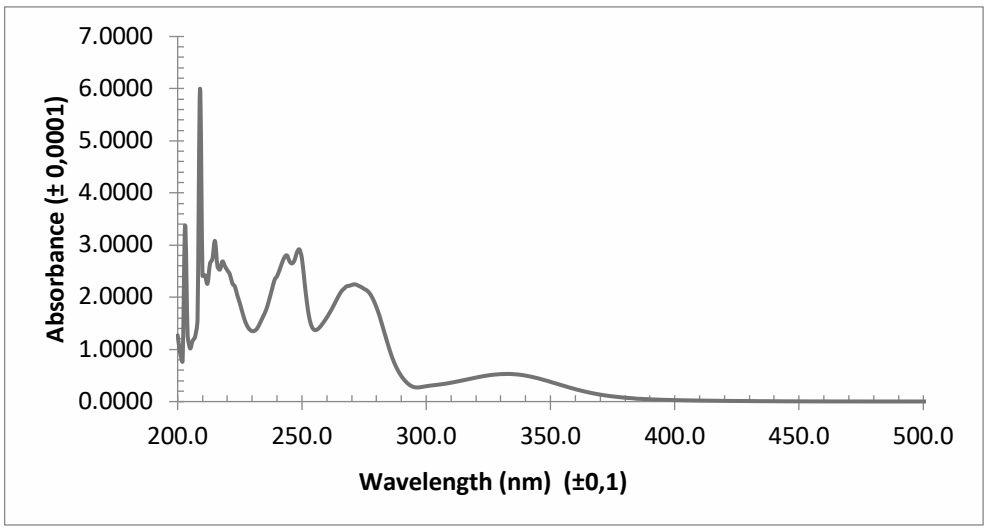
2-(2-bromophenoxy)-1,4-naphthoquinone **38** ^{1}H NMR



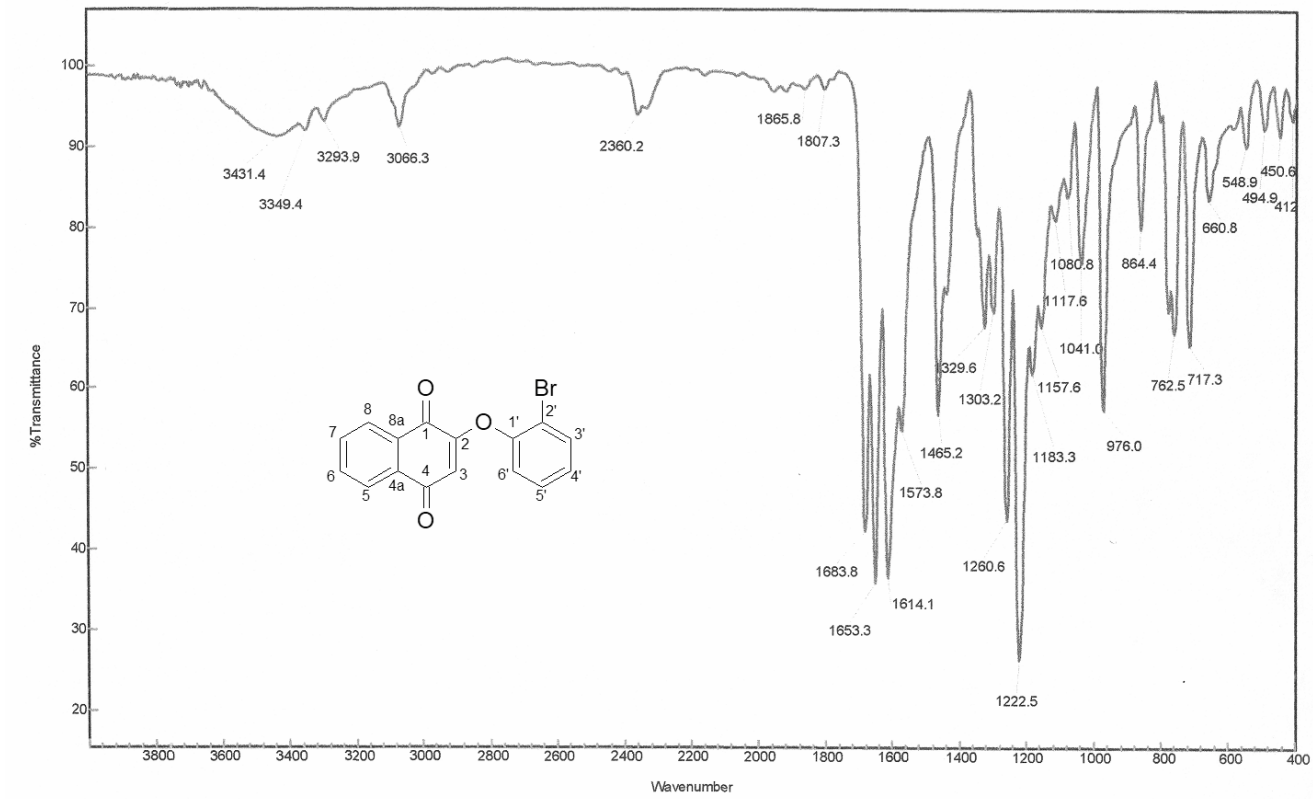
2-(2-bromophenoxy)-1,4-naphthoquinone **38** ^{13}C NMR



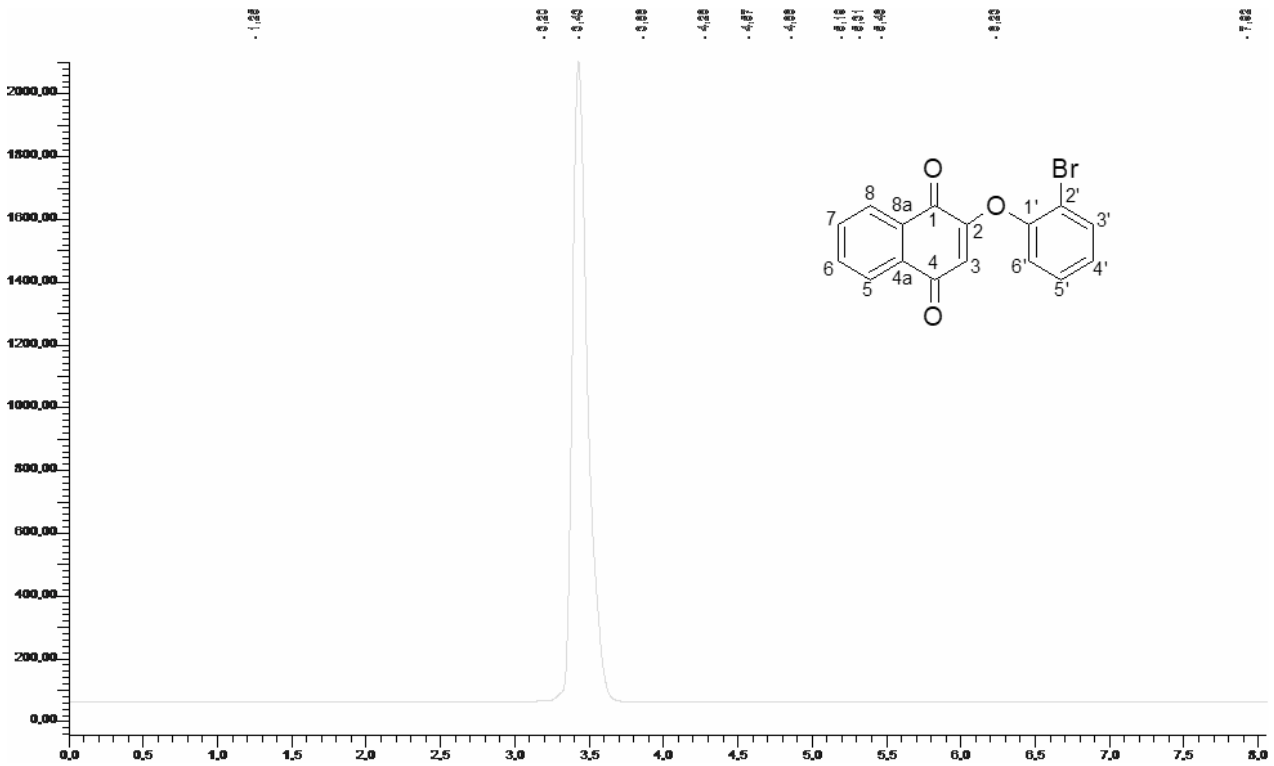
2-(2-bromophenoxy)-1,4-naphthoquinone **38** UV-Vis (MeOH)



2-(2-bromophenoxy)-1,4-naphthoquinone **38** IR (KBr pellet)



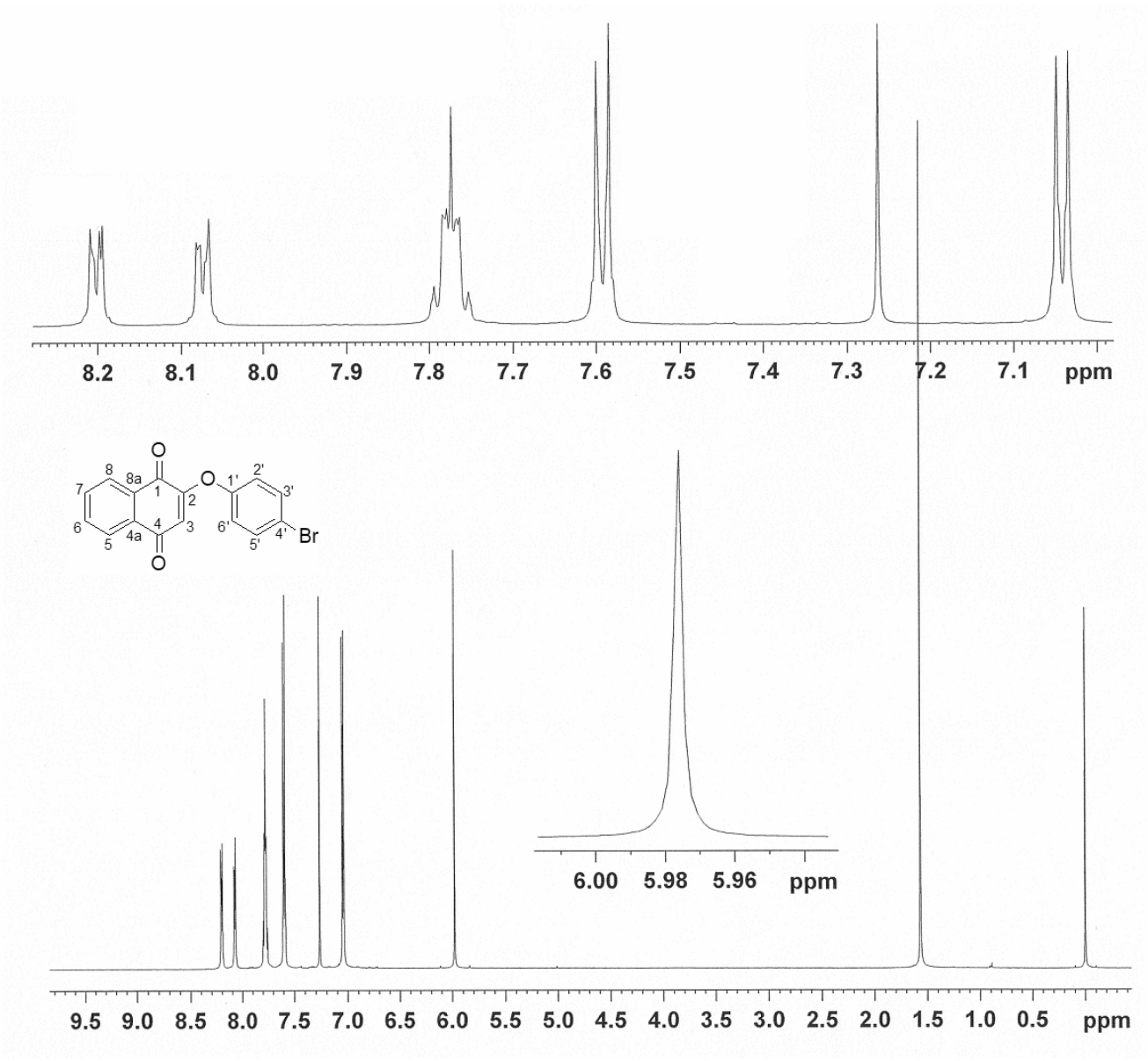
2-(2-bromophenoxy)-1,4-naphthoquinone **38** HPLC chromatogram (270 nm, 100% MeCN)



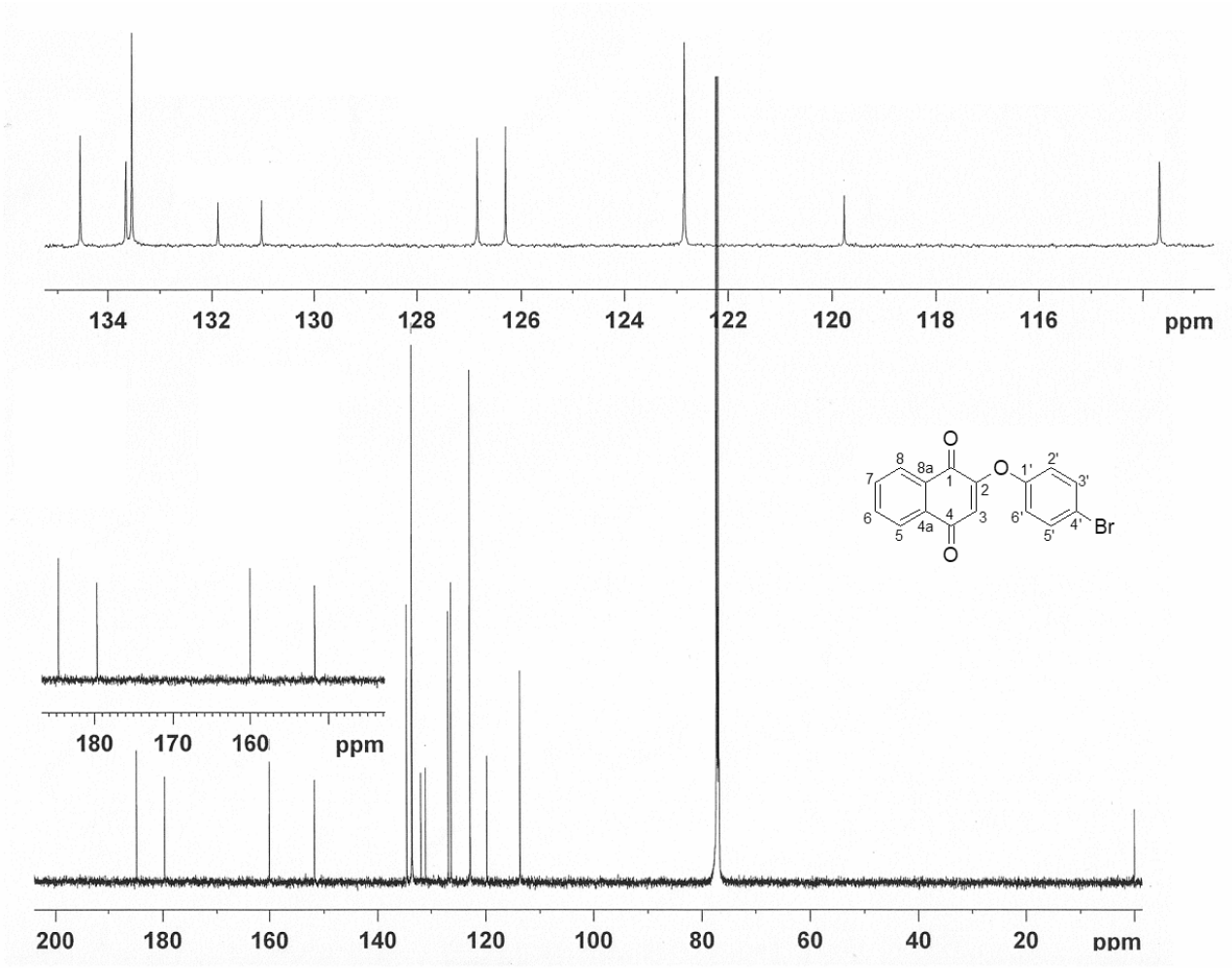
2-(4-bromophenoxy)-1,4-naphthoquinone 39

39 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE and recrystallization with isooctane. Yield 246 mg (75%), yellow needles, mp = (134.0 – 135.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, dd, *J* = 2 Hz, *J* = 6 Hz, ArH), 8.07 (1H, dd, *J* = 6 Hz, ArH), 7.77 (2H, m, ArH), 7.59 (2H, d, J_{ortho} = 8 Hz, ArH), 7.04 (2H, d, J_{ortho} = 8 Hz, ArH), 5.98 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.7, 179.7, 160.0, 151.8, 134.6, 133.7, 133.5, 131.9, 131.0, 126.8, 126.3, 122.9, 119.8, 113.7. IR (KBr pellet) cm^{-1}: 3095, 1684, 1652, 1612, 1479, 1263, 1232, 717. UV-Vis (MeOH) nm: 221, 249 (max), 269, 335. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}O_3Br$: 328.9813; found: 328.9814. Purity: 99.7%. MIC (µM): >3000 (*S. aureus*), > 3000 (*C. albicans*), >3000 (*E. coli*).

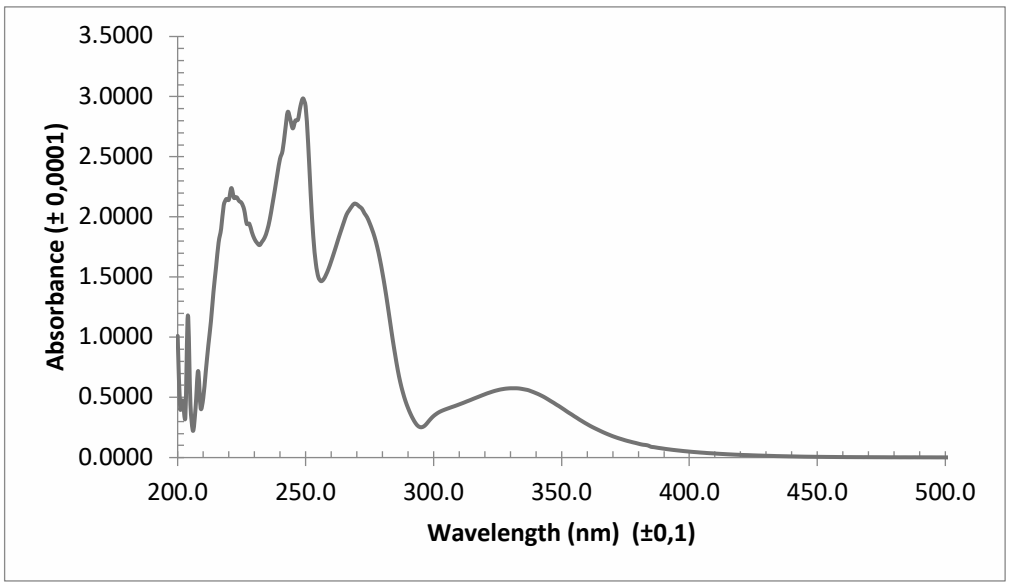
2-(4-bromophenoxy)-1,4-naphthoquinone **39** ^{1}H NMR



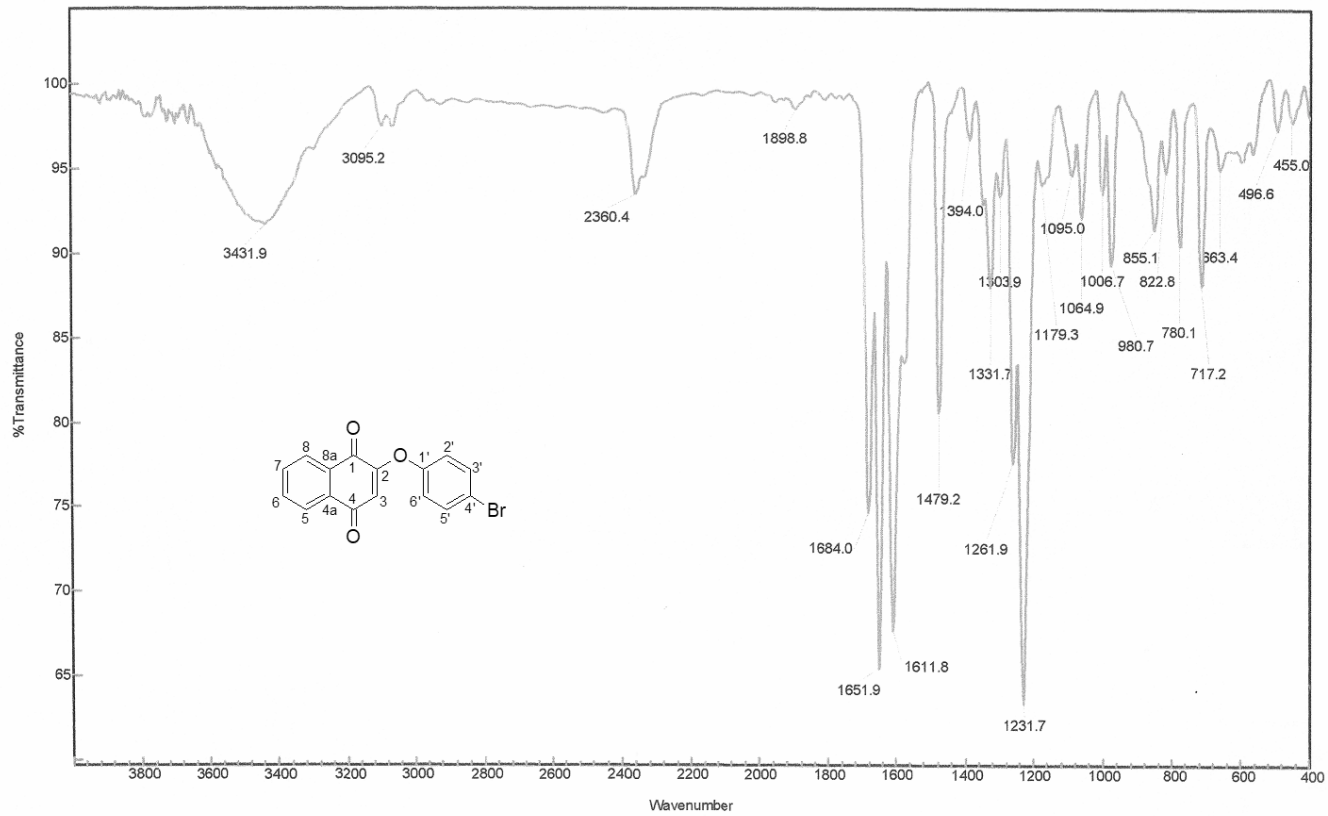
2-(4-bromophenoxy)-1,4-naphthoquinone **39** ^{13}C NMR



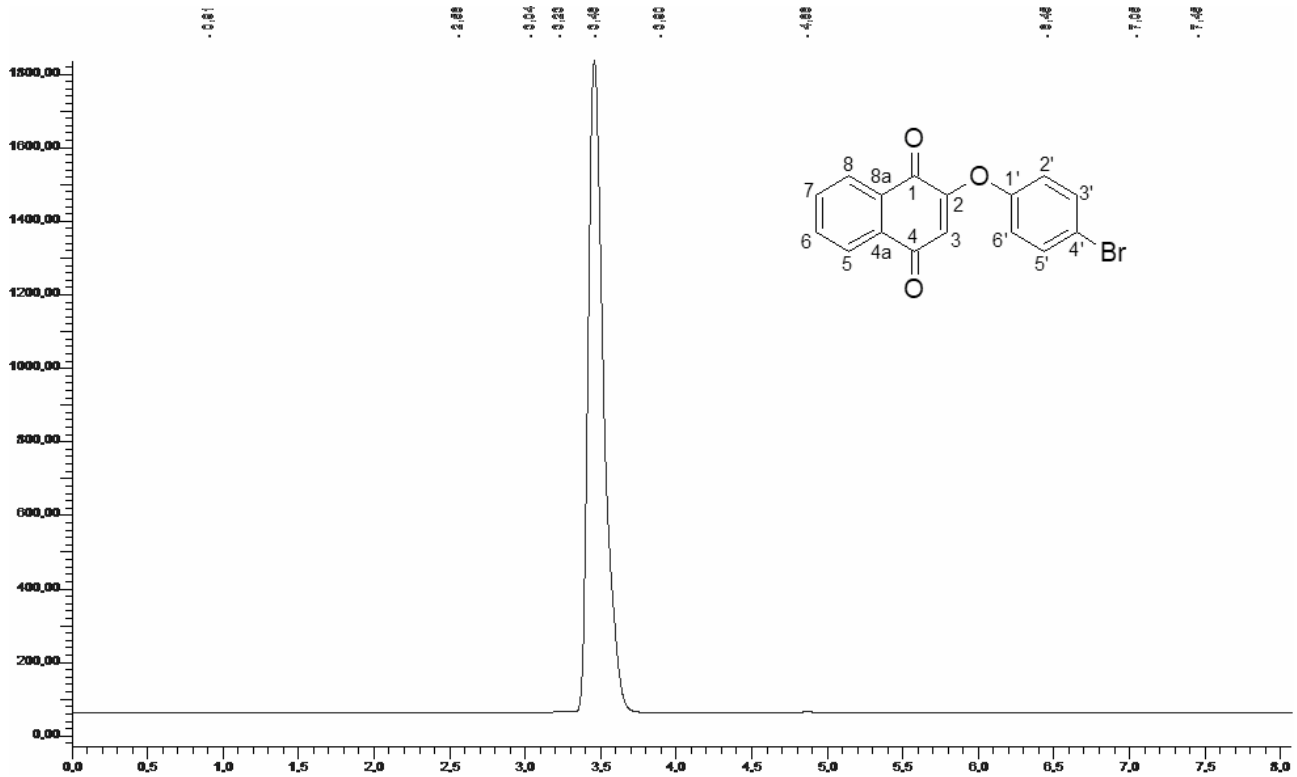
2-(4-bromophenoxy)-1,4-naphthoquinone **39** UV-Vis (MeOH)



2-(4-bromophenoxy)-1,4-naphthoquinone **39** IR (KBr pellet)



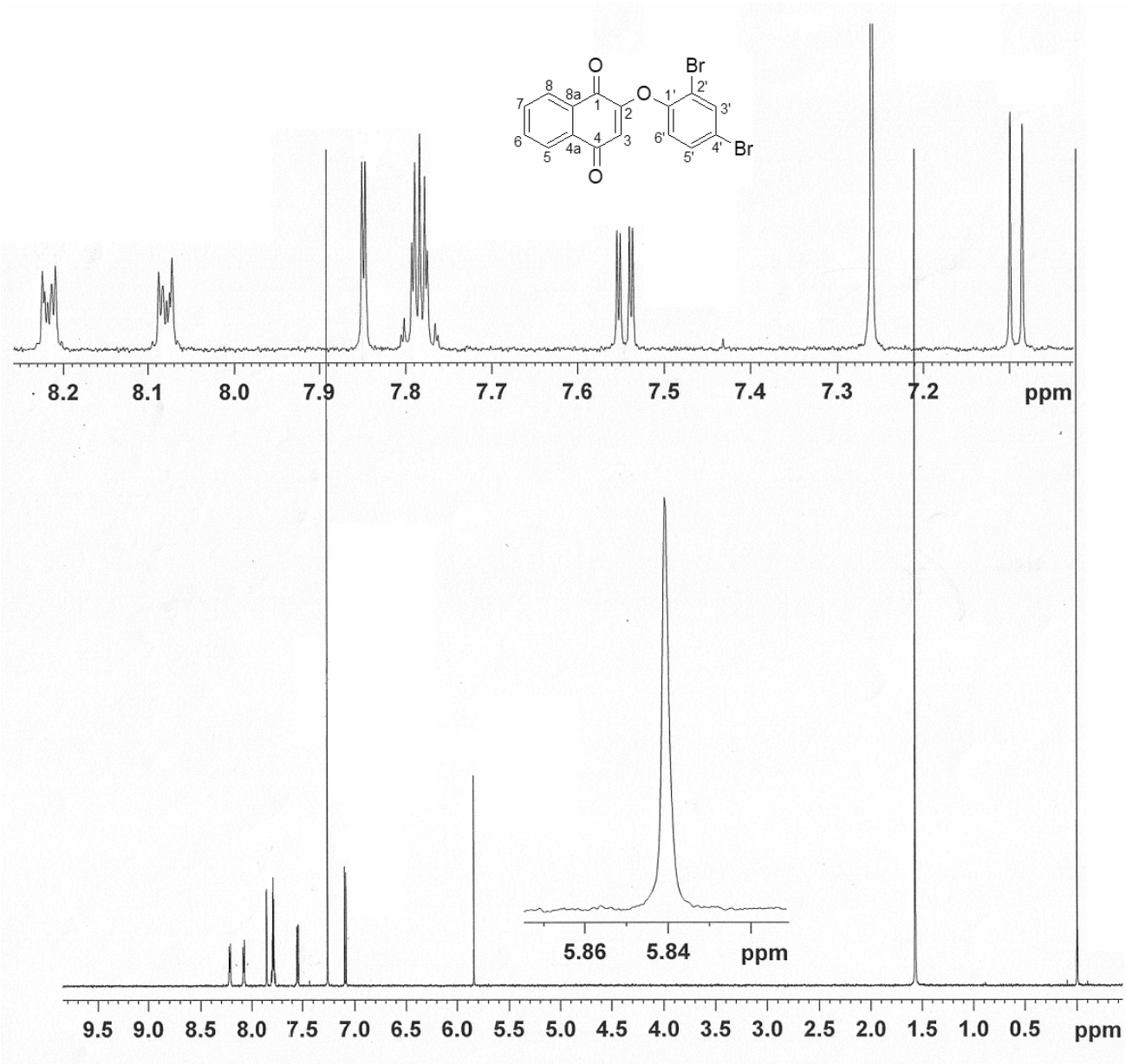
2-(4-bromophenoxy)-1,4-naphthoquinone **39** HPLC chromatogram (270 nm, 100% MeCN)



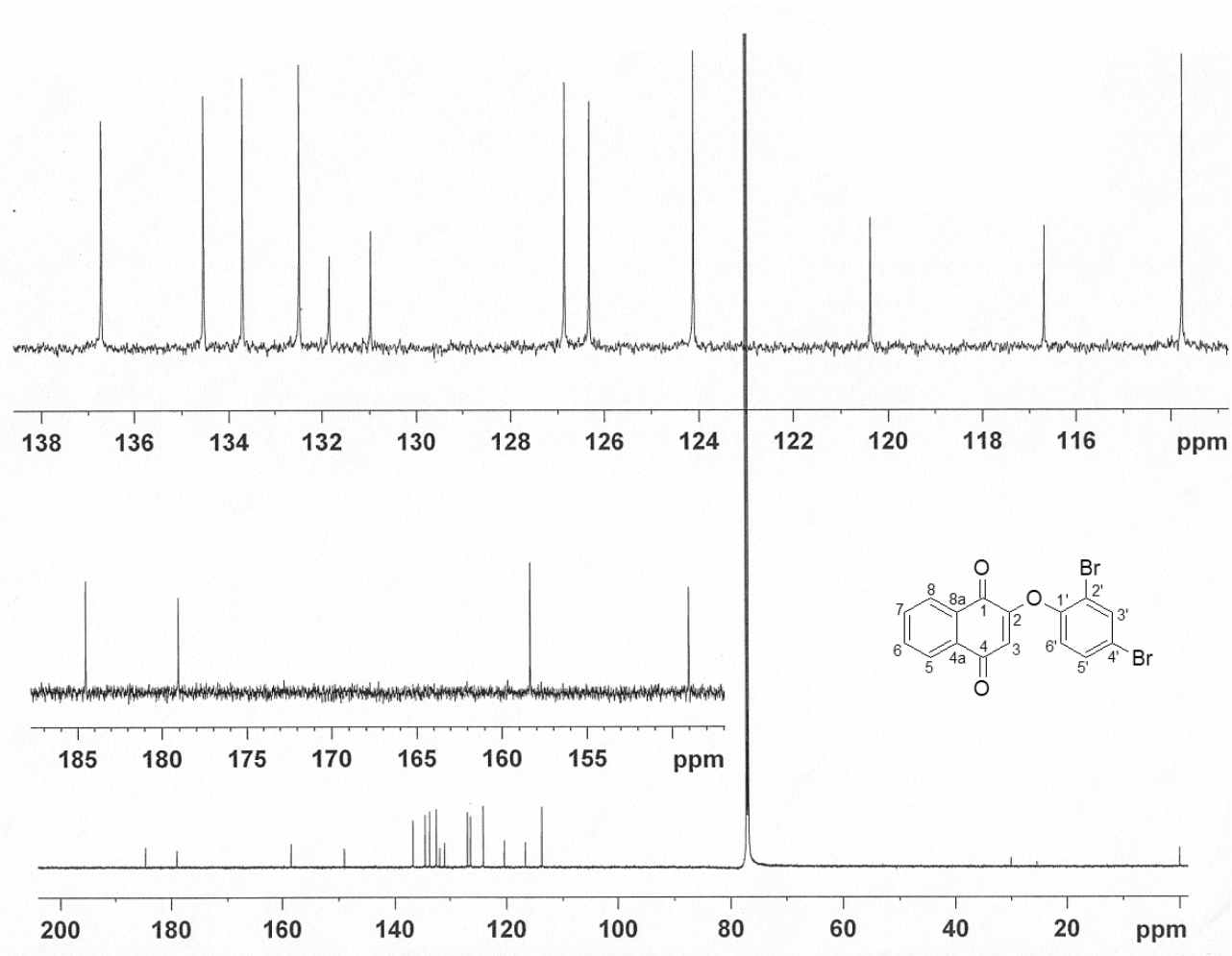
2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40**

40 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE and recrystallization with isooctane. Yield 251 mg (62%), yellow solid, mp = (133.0 – 134.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.21 (1H, dd, J_{ortho} = 7.5 Hz, ArH), 8.08 (1H, dd, J_{ortho} = 7.5 Hz, ArH), 7.84 (1H, d, J_{meta} = 1.9 Hz, ArH), 7.78 (2H, m, ArH), 7.54 (1H, dd, J_{meta} = 1.9 Hz, J_{ortho} = 9.4 Hz, ArH), 7.09 (1H, d, J_{orto} = 7.5 Hz, ArH), 5.84 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.5, 179.1, 158.4, 149.0, 136.7, 134.6, 133.7, 132.5, 131.9, 131.0, 126.9, 126.3, 124.1, 120.4, 116.7, 113.8. IR (KBr pellet) cm^{-1}: 3086, 1686, 1652, 1612, 1465, 1260, 1236, 783, 717. UV-Vis (MeOH) nm: 221, 249 (max), 270, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_9O_3Br_2$: 406.8918; found: 406.8923. Purity: 98.9%. MIC (μM): >2000 (*S. aureus*), >2000 (*C. albicans*), >2000 (*E. coli*).

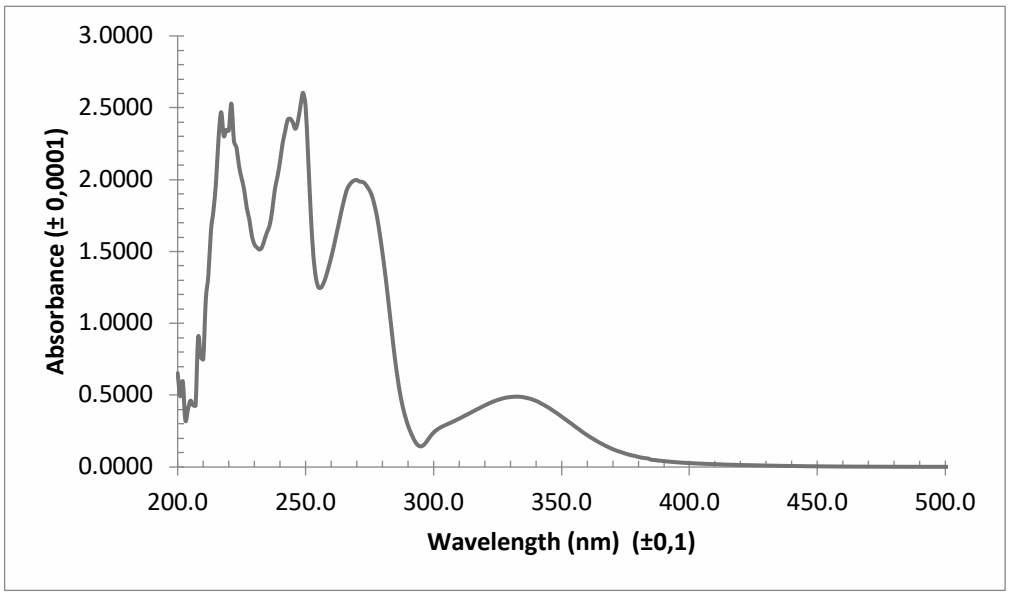
2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40** ^{1}H NMR



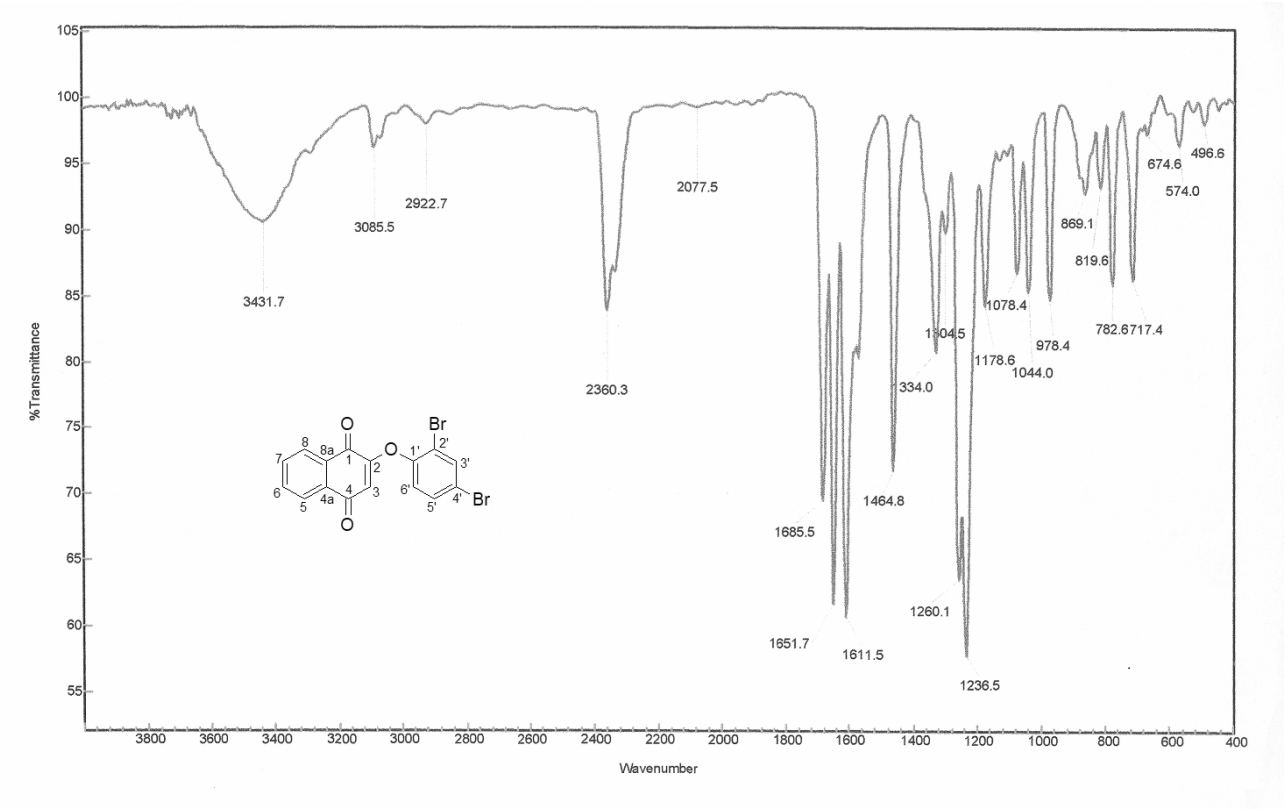
2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40** ^{13}C NMR



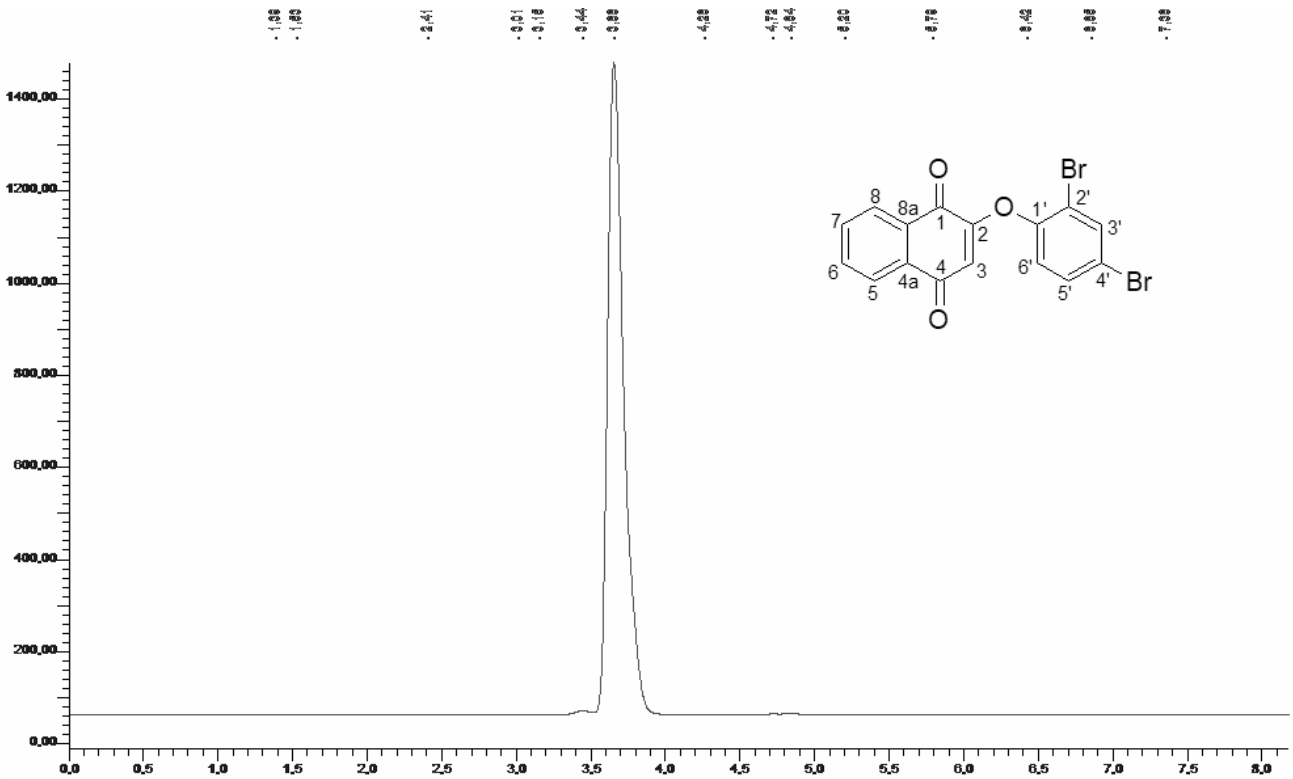
2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40** UV-Vis (MeOH)



2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40** IR (KBr pellet)



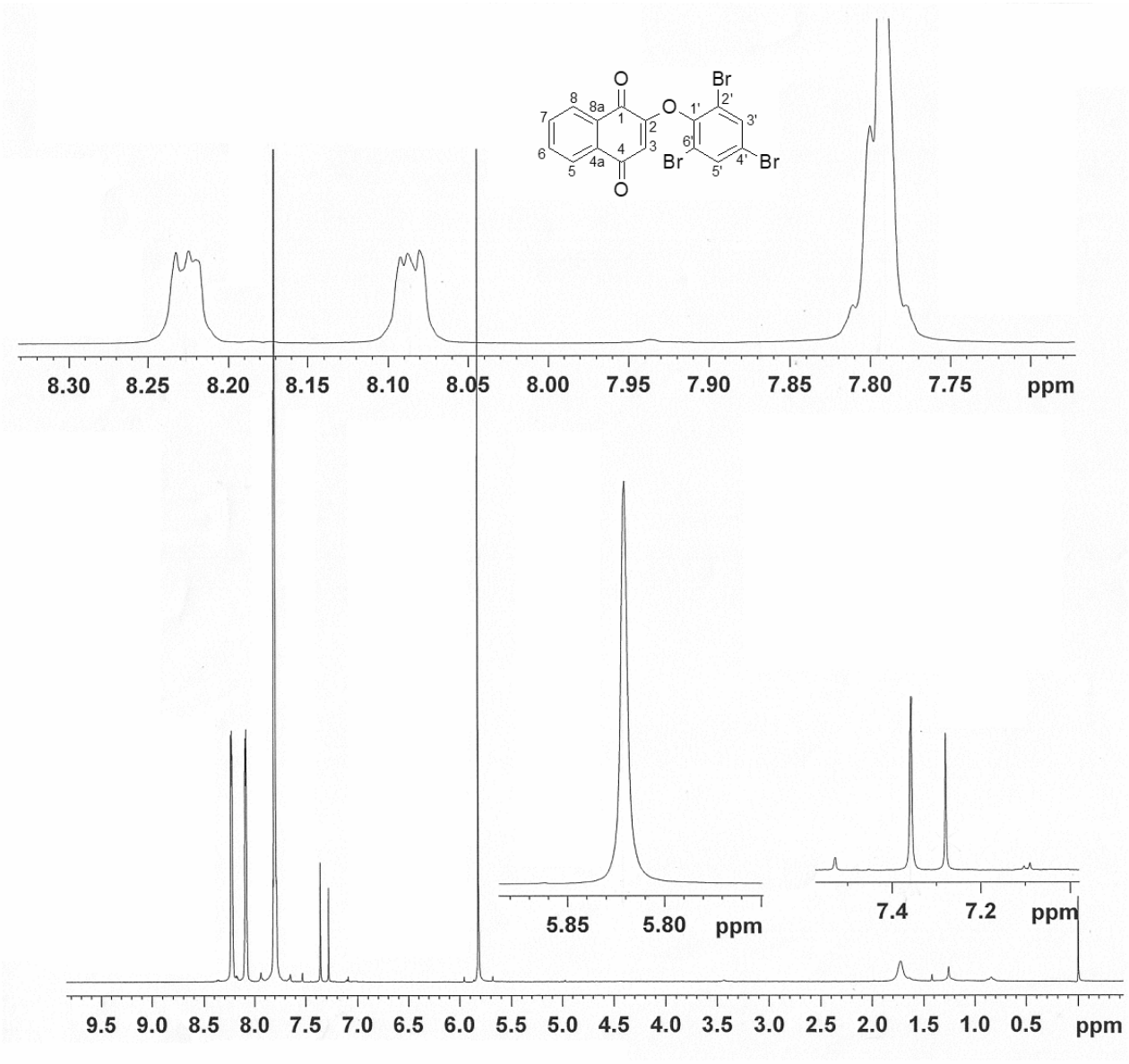
2-(2,4-dibromophenoxy)-1,4-naphthoquinone **40** HPLC chromatogram (270 nm, 100% MeCN)



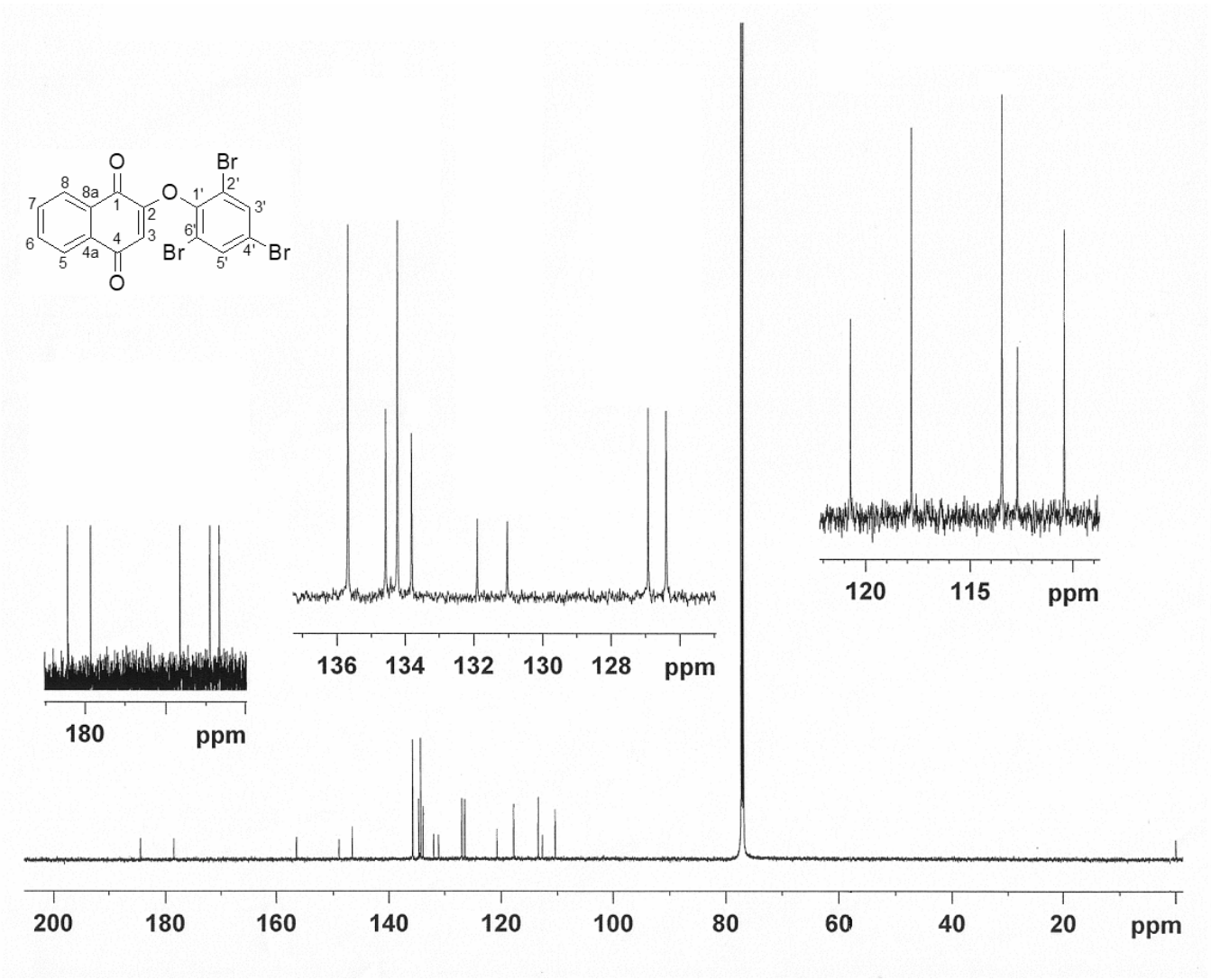
2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41**

41 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with CH_2Cl_2, column chromatography (50% benzene/cyclohexane to dissolve the solid and benzene as eluent, isocratically) and recrystallization with methanol. Yield 316 mg (65%), yellow solid, mp = (170.0 – 172.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.23 (1H, m, ArH), 8.09 (1H, m, ArH), 7.79 (2H, m, ArH), 7.36 (2H, s, ArH), 5.82 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.4, 178.5, 156.4, 148.9, 134.6, 134.2, 133.8, 131.9, 131.0, 126.9, 126.4, 117.8, 113.4, 112.7. IR (KBr pellet) cm^{-1}: 3067, 1684, 1654, 1618, 1593, 1237, 1176, 714. UV-Vis (MeCN) nm: 231, 271 (max). TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_8O_3Br_3$: 484.8024; found: 484.8034. Purity: 97.3%. MIC (μM): >2000 (*S. aureus*), >2000 (*C. albicans*), >2000 (*E. coli*).

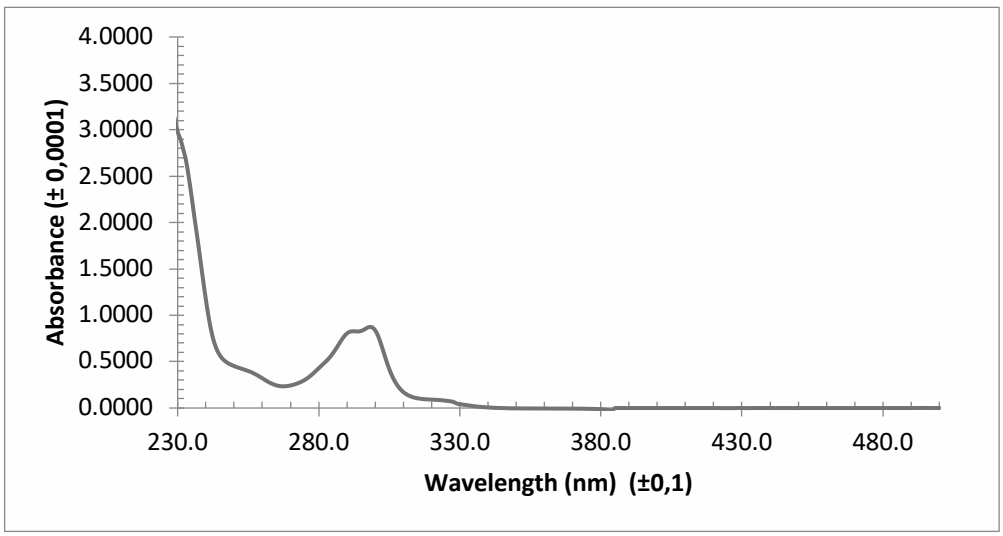
2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41** ^{1}H NMR



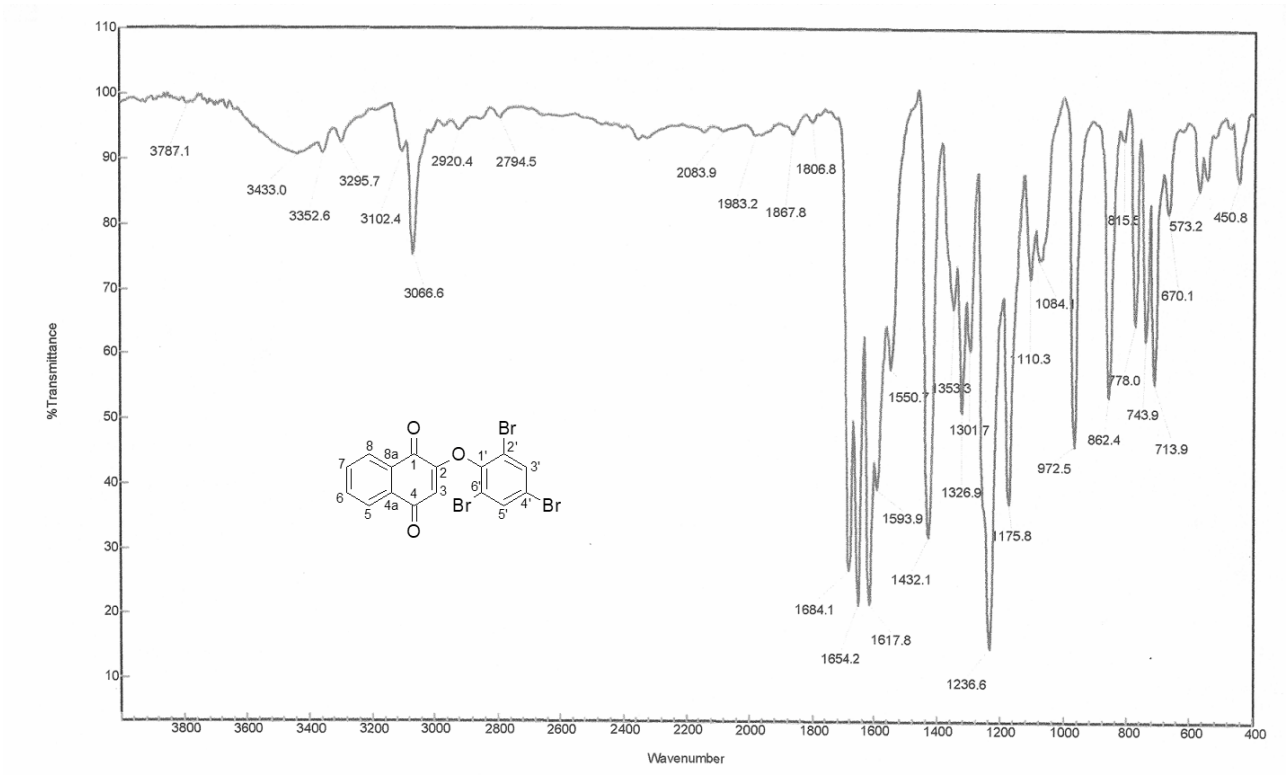
2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41** ^{13}C NMR



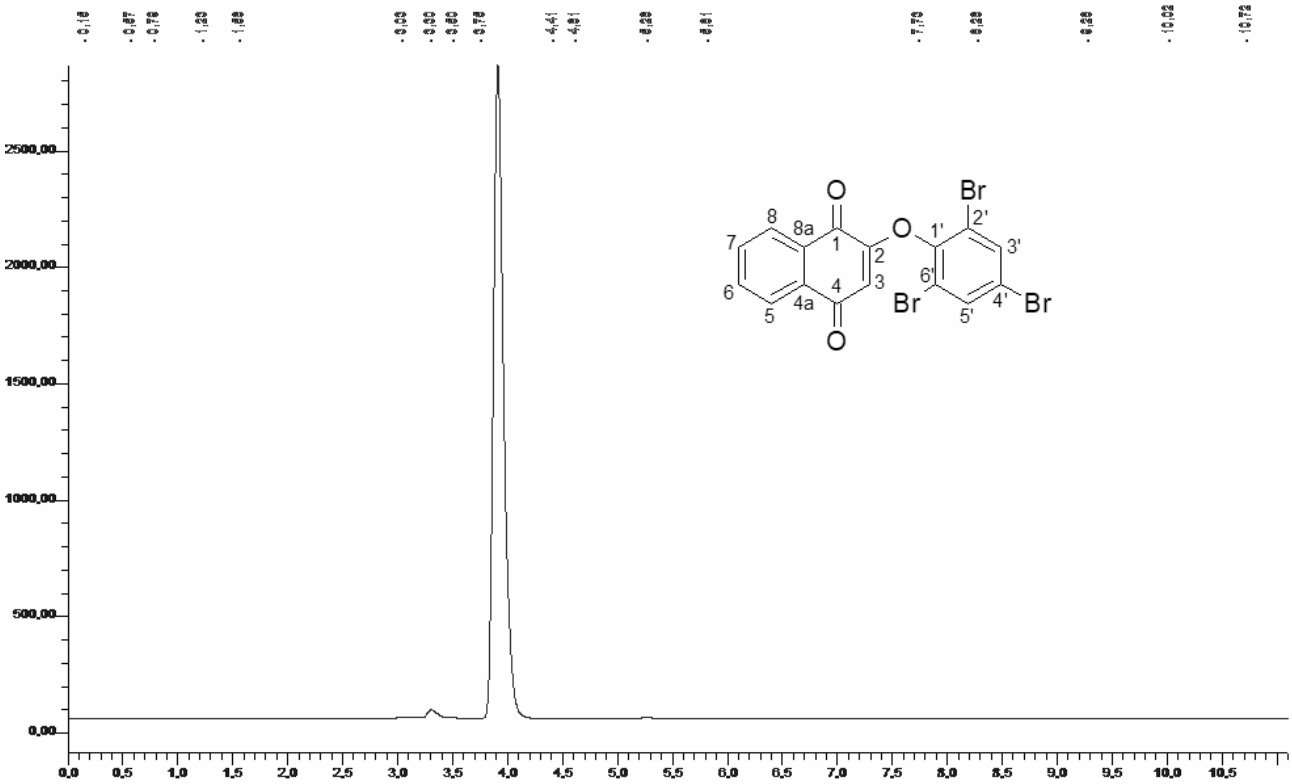
2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41** UV-Vis (MeCN)



2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41** IR (KBr pellet)



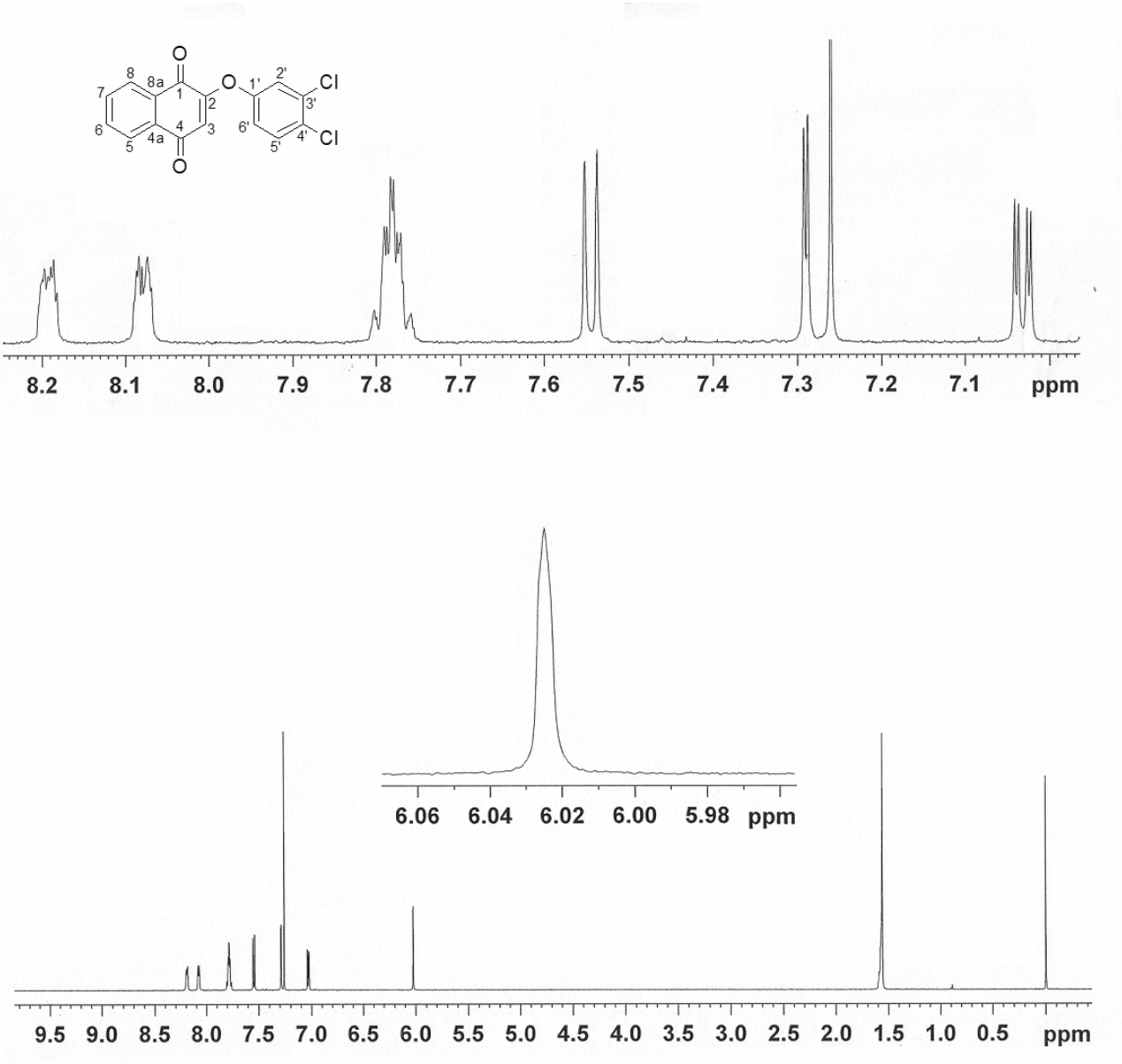
2-(2,4,6-tribromophenoxy)-1,4-naphthoquinone **41** HPLC chromatogram (270 nm, 100% MeCN)



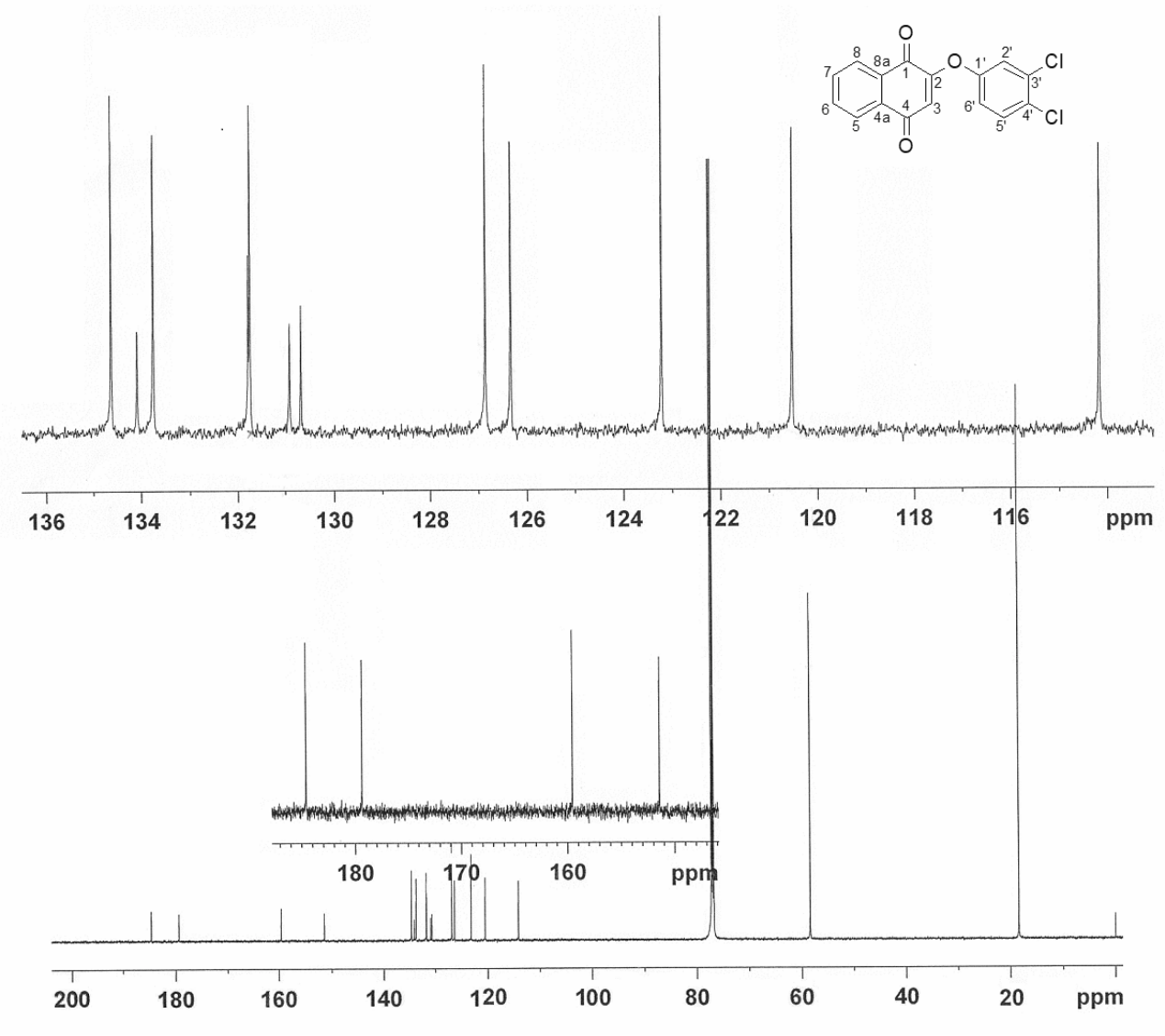
2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42**

42 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE and recrystallization with isooctane. Yield 160 mg (50%), yellow needles, mp = (162.0 – 163.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.19 (1H, m, ArH), 8.08 (1H, m, ArH), 7.78 (2H, m, ArH), 7.54 (1H, d, J_{ortho} = 8 Hz, ArH), 7.29 (1H, d, J_{meta} = 2 Hz, ArH), 7.03 (1H, dd, J_{meta} = 2 Hz, J_{ortho} = 8 Hz, ArH), 6.03 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.6, 179.4, 159.5, 151.5, 134.6, 134.1, 133.8, 131.8, 131.8, 130.9, 130.7, 126.9, 126.3, 123.2, 120.5, 114.6. IR (KBr pellet) cm^{-1}: 3069, 1683, 1643, 1624, 1595, 1466, 1265, 1216, 986. UV-Vis (MeOH) nm: 207 (max), 241, 276, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_9O_3Cl_2$: 318.9929; found: 318.9930. Purity: 98.7%. MIC (μM): >3000 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

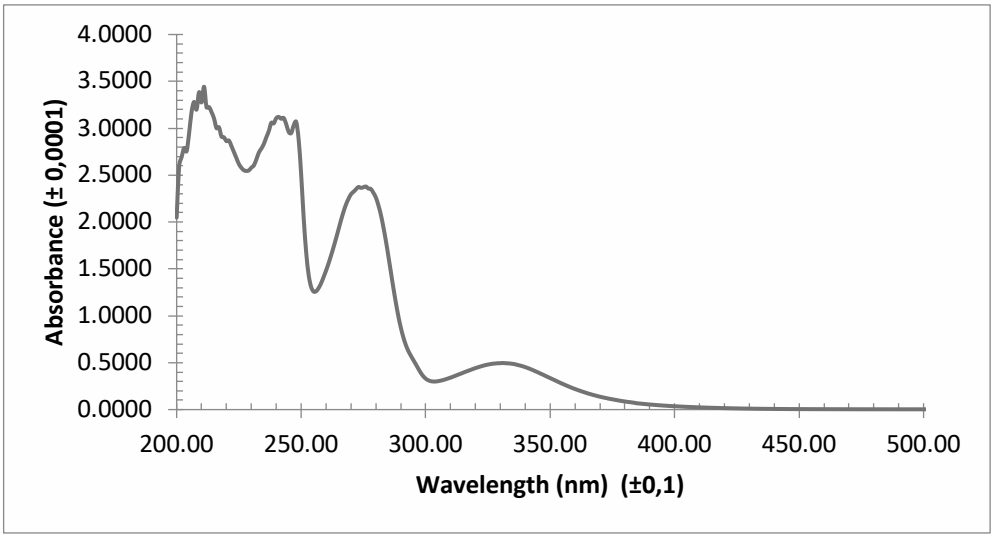
2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42** ^{1}H NMR



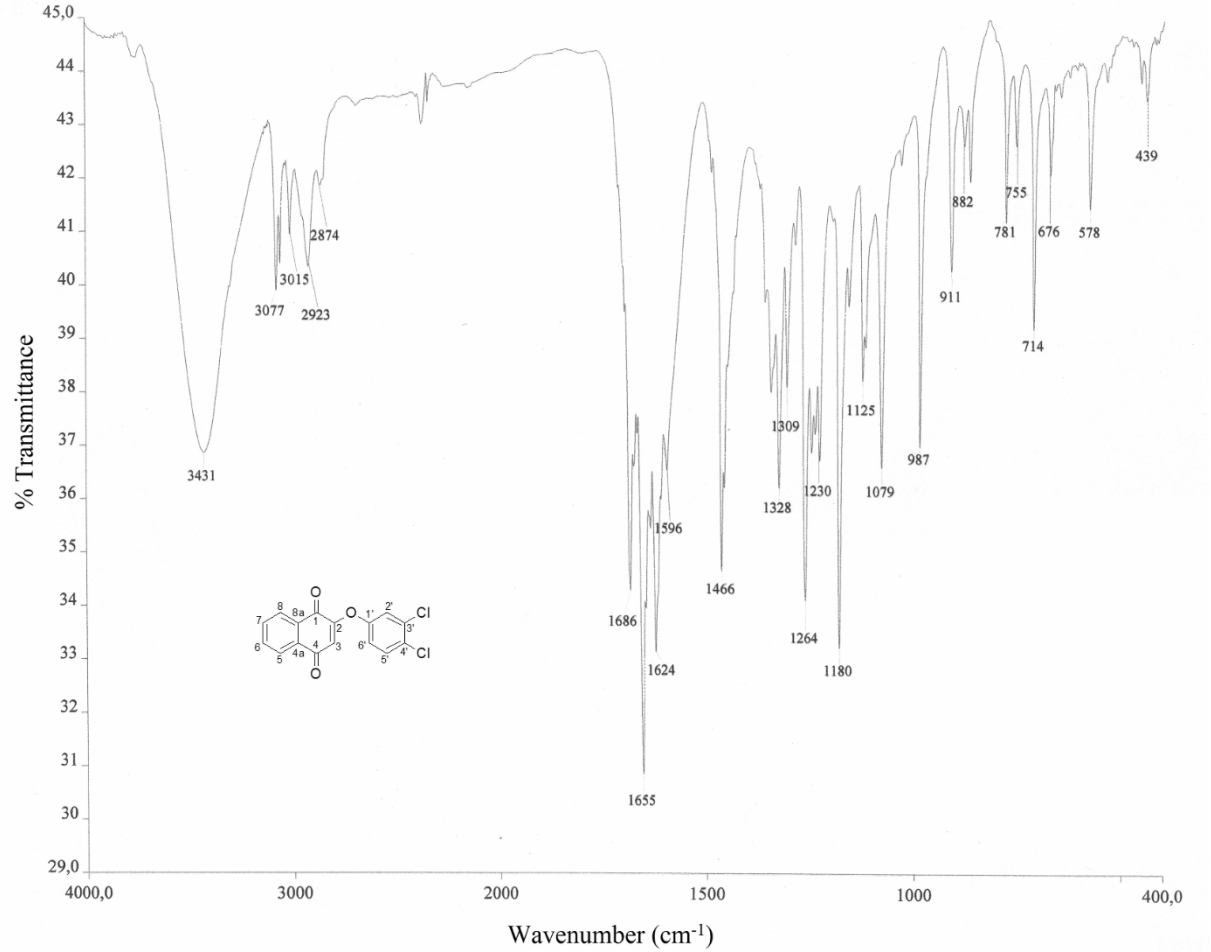
2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42** ^{13}C NMR



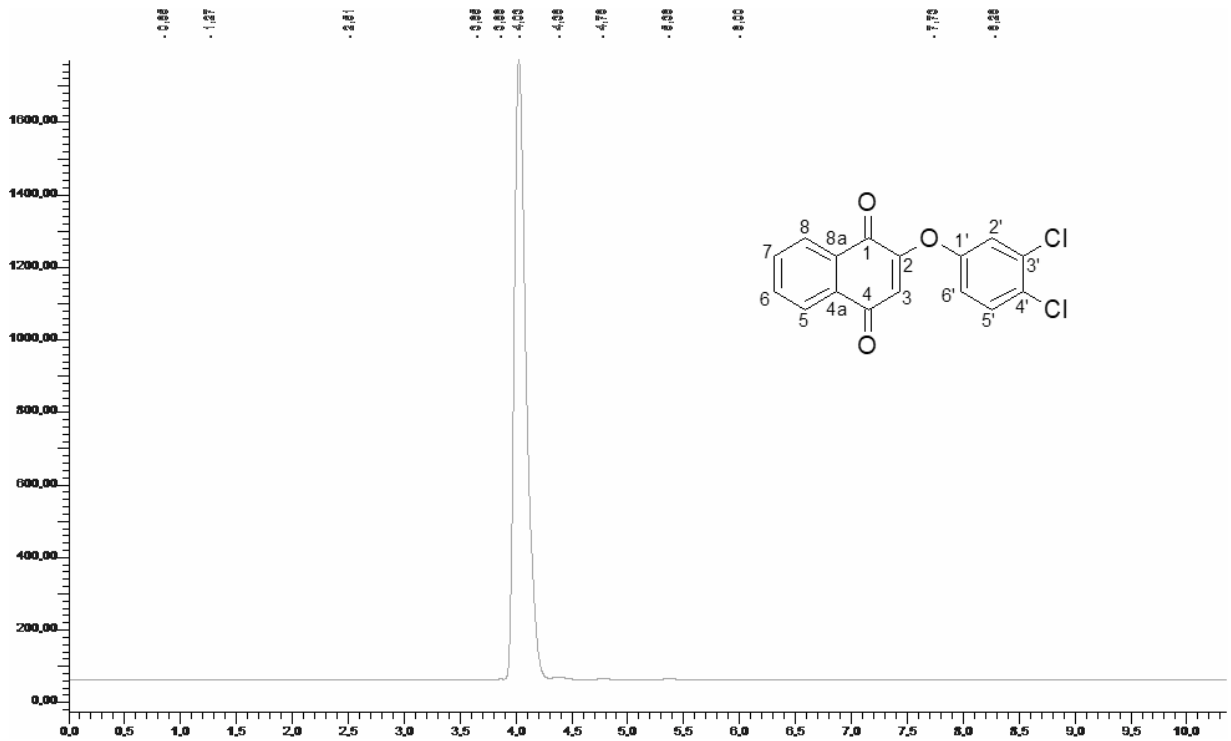
2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42** UV-Vis (MeOH)



2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42** IR (KBr pellet)



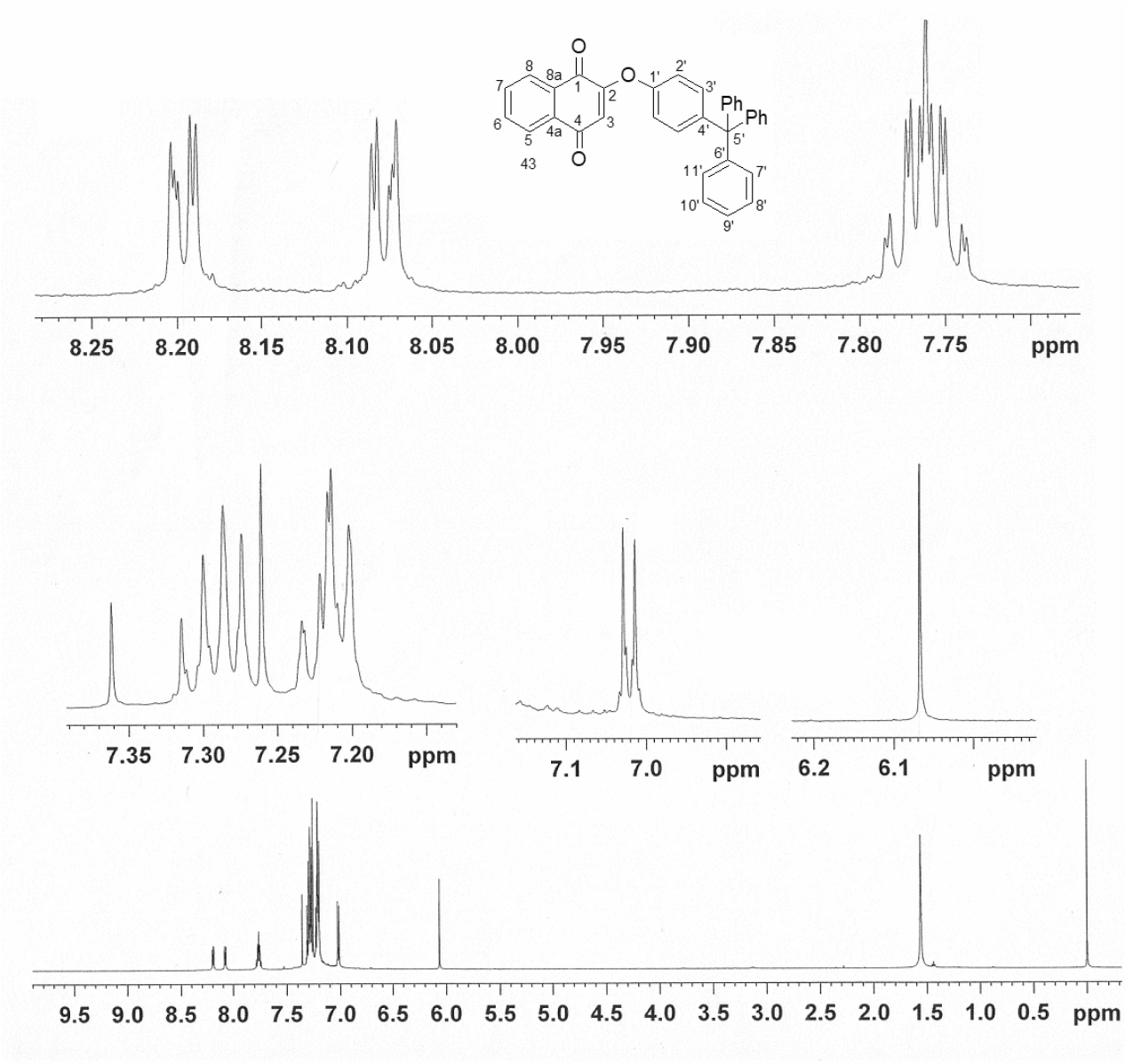
2-(3,4-dichlorophenoxy)-1,4-naphthoquinone **42** HPLC chromatogram (270 nm, 100% MeCN)



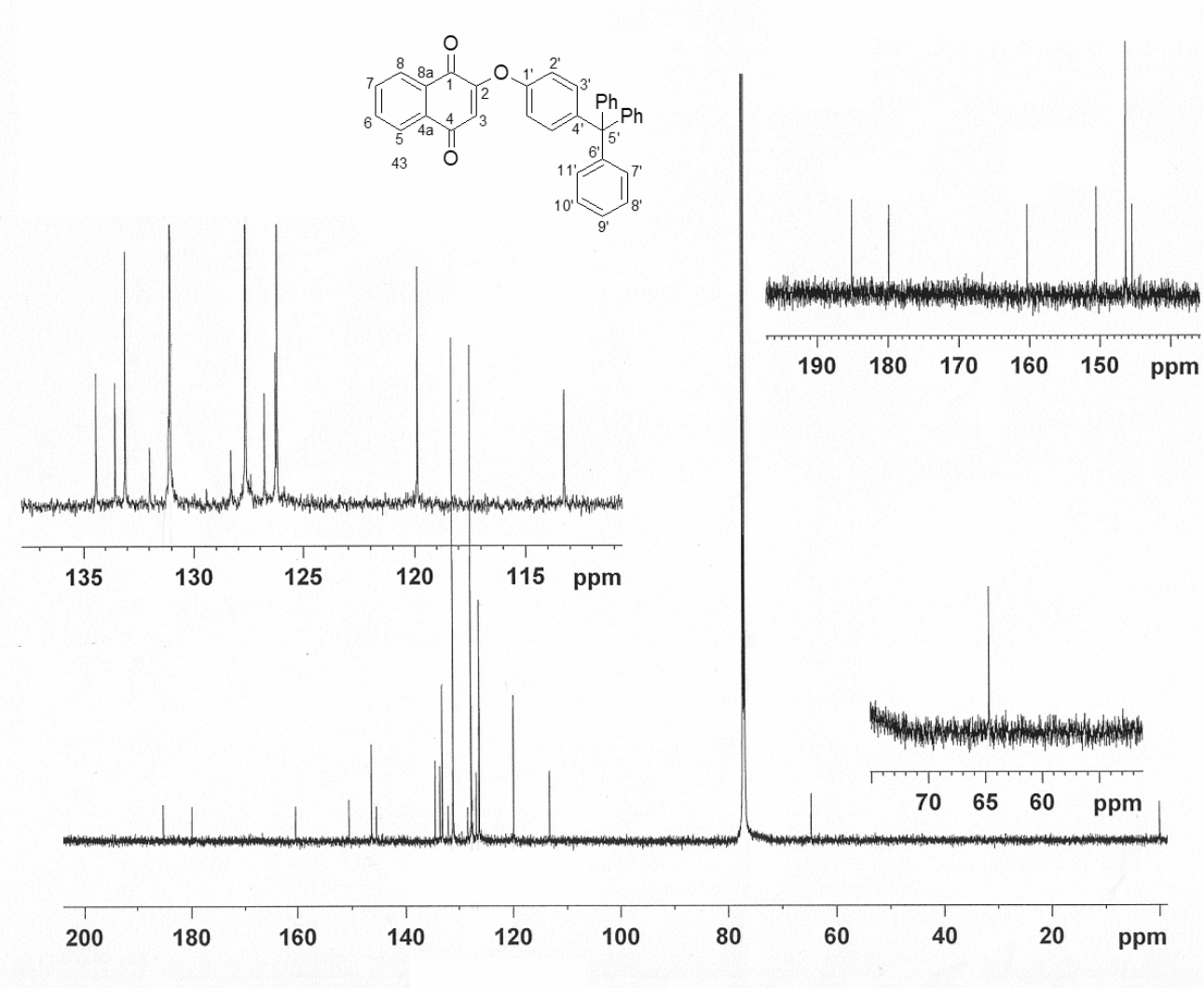
2-(4-tritylphenoxy)-1,4-naphthoquinone **43**

43 was obtained according to general procedure I 2.1.1, but with lesser amount of reagents (0.40 mmol of 2-bromo-1,4-naphthoquinone, 0.40 mmol of 4-tritylphenol and 0.60 mmol of dried Cs_2CO_3), and purified by hot extraction-filtration with CH_2Cl_2 and column chromatography (1% triethylamine/benzene as eluent, isocratically). Yield 163 mg (82%), beige solid, mp = (256.0 – 257.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.20 (1H, dd, *J* = 2.0 Hz, *J* = 7.7 Hz, ArH), 8.08 (1H, dd, *J* = 2.0 Hz, *J* = 7.7 Hz, ArH), 7.76 (2H, m, ArH), 7.30 (6H, t, ArH), 7.28 (3H, d, ArH), 7.22 (6H, t, ArH), 7.21 (2H, d, ArH), 7.02 (2H, d, J_{ortho} = 8.3 Hz, ArH), 6.07 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.1, 179.9, 160.3, 150.5, 146.3, 145.4, 134.4, 133.5, 133.2, 132.0, 131.1, 131.0, 127.4, 126.8, 126.3, 126.3, 120.0, 113.3, 64.7. IR (KBr pellet) cm^{-1}: 3059, 1681, 1655, 1600, 1496, 1261, 1225. UV-Vis (MeCN) nm: 218 (max), 245, 269, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{35}H_{25}O_3$: 493.1804; found: 493.1801. Purity: 96.0%. MIC (μM): >2000 (*S. aureus*), >2000 (*C. albicans*), >2000 (*E. coli*).

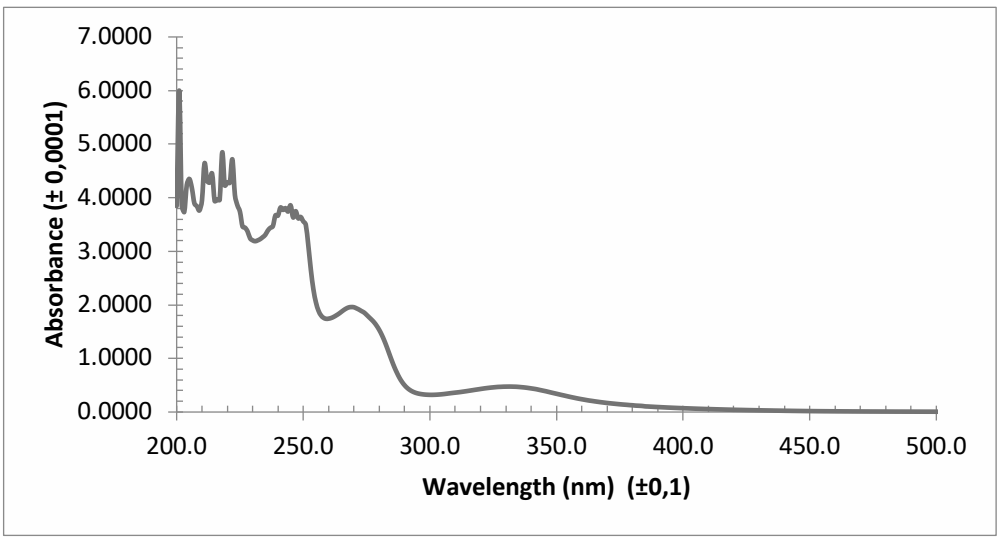
2-(4-tritylphenoxy)-1,4-naphthoquinone **43** ^{1}H NMR



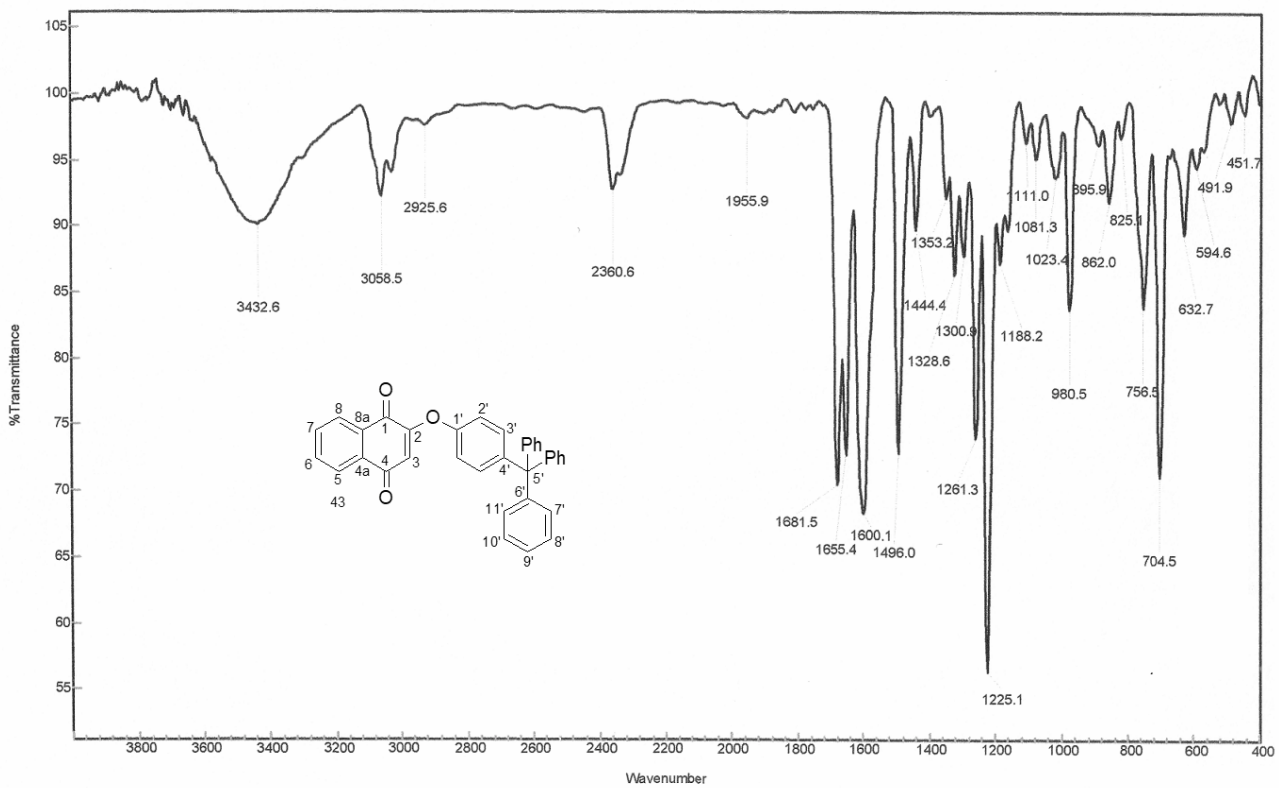
2-(4-tritylphenoxy)-1,4-naphthoquinone **43** ^{13}C NMR



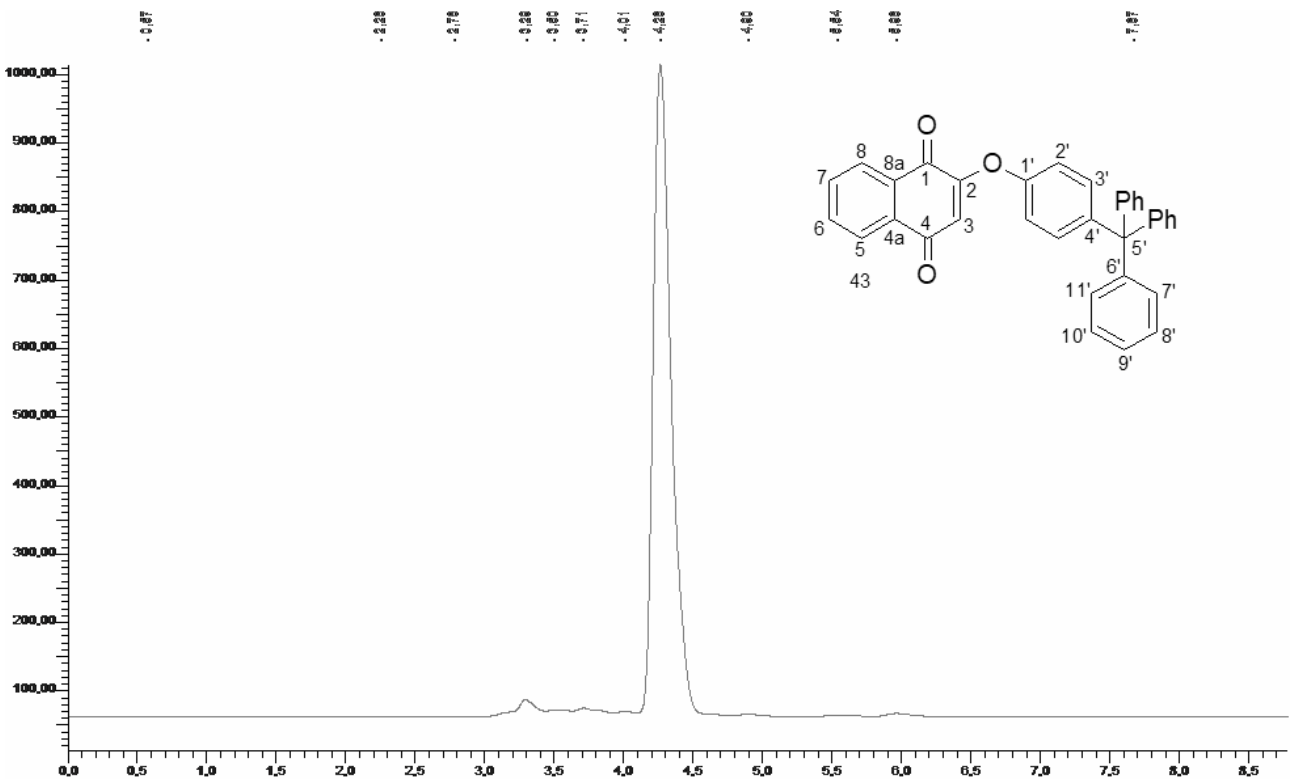
2-(4-tritylphenoxy)-1,4-naphthoquinone **43** UV-Vis (MeCN)



2-(4-tritylphenoxy)-1,4-naphthoquinone **43** IR (KBr pellet)



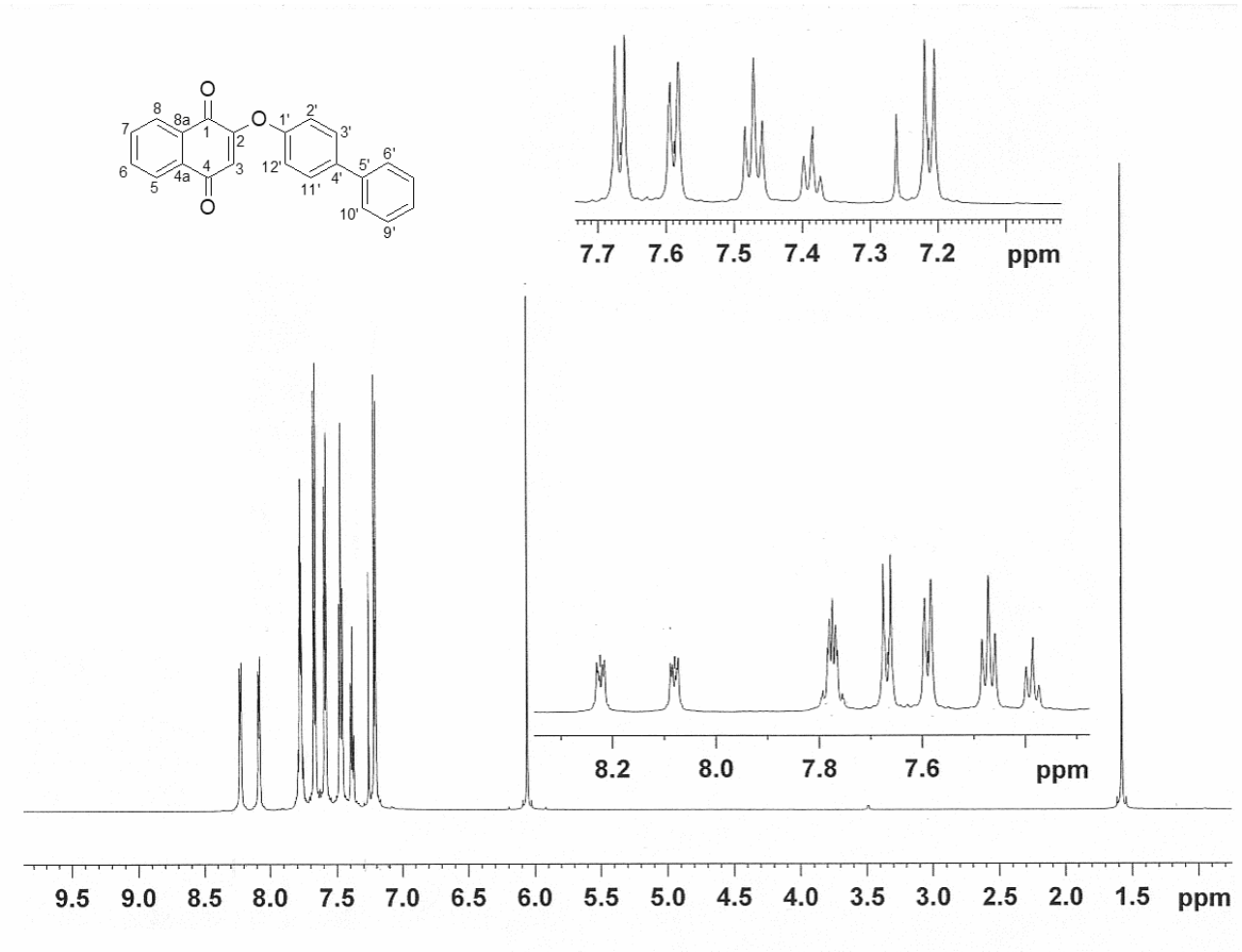
2-(4-tritylphenoxy)-1,4-naphthoquinone **43** HPLC chromatogram (270 nm, 100% MeCN)



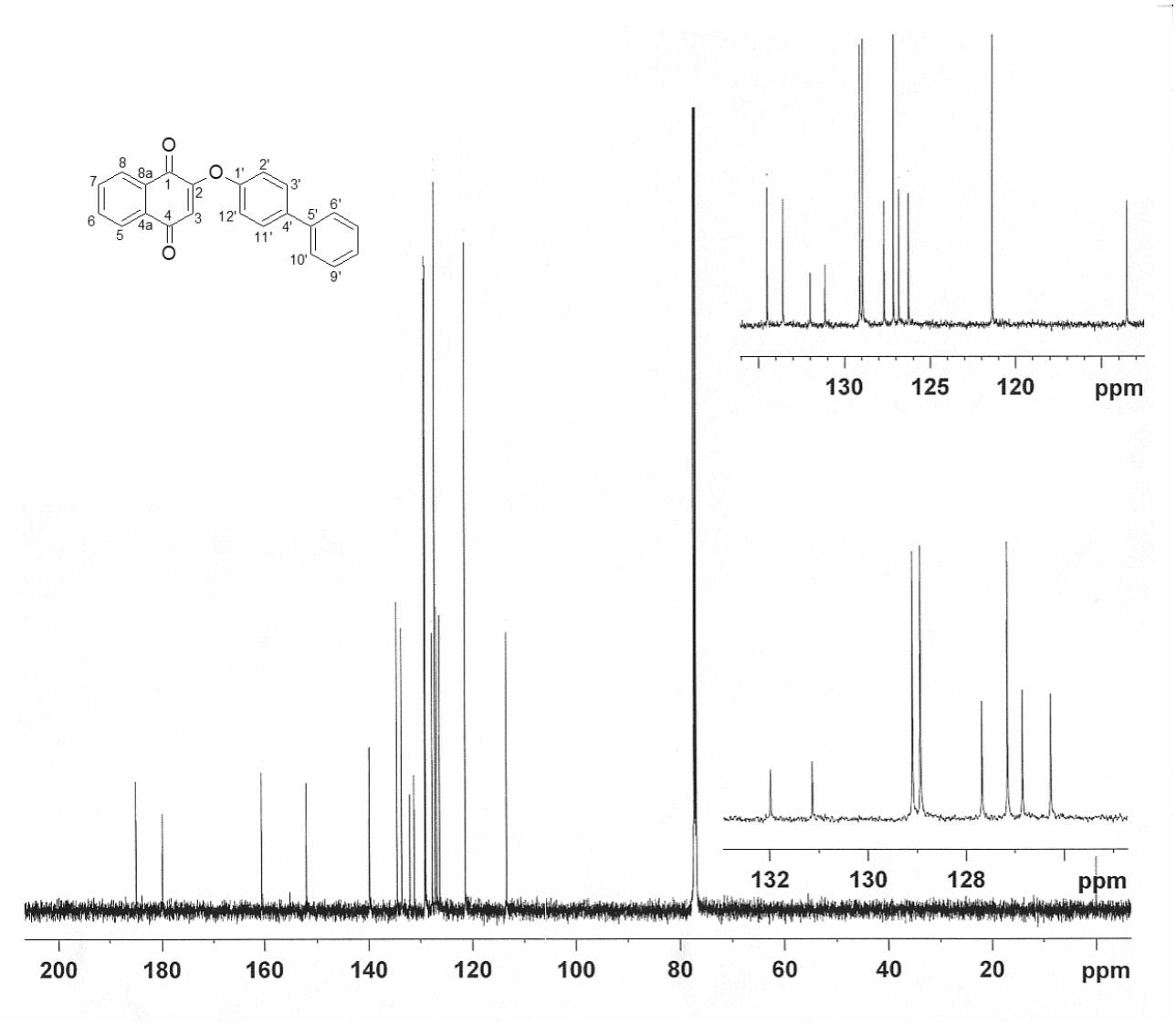
2-(4-phenylphenoxy)-1,4-naphthoquinone **44**

44 was obtained according to general procedure I 2.1.1 and purified by column chromatography (benzene as eluent, isocratically) and recrystallization with methanol. Yield 53 mg (16%), beige needles, mp = (199.0 – 200.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.22 (1H, d, *J* = 8 Hz, ArH), 8.08 (1H, d, *J* = 8 Hz, ArH), 7.77 (2H, m, ArH), 7.67 (2H, d, J_{ortho} = 8 Hz, ArH), 7.59 (2H, d, J_{ortho} = 8 Hz, ArH), 7.47 (2H, t, J_{ortho} = 8 Hz, ArH), 7.38 (1H, t, J_{ortho} = 8 Hz, ArH), 7.21 (2H, d, J_{ortho} = 8 Hz, ArH), 6.06 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 185.0, 179.9, 160.5, 152.0, 139.9, 134.5, 133.6, 132.0, 131.1, 129.1, 128.9, 127.7, 127.2, 126.8, 126.3, 121.4, 113.5. IR (KBr pellet) cm^{-1}: 3036, 1683, 1651, 1615, 1593, 1263, 1226. UV-Vis (MeOH) nm: 212, 247 (max), 332. TOF-MS: m/z $[M+H]^+$ calc for $C_{22}H_{15}O_3$: 327.1021; found: 327.1021. Purity: 99.4%. MIC (µM): >3000 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

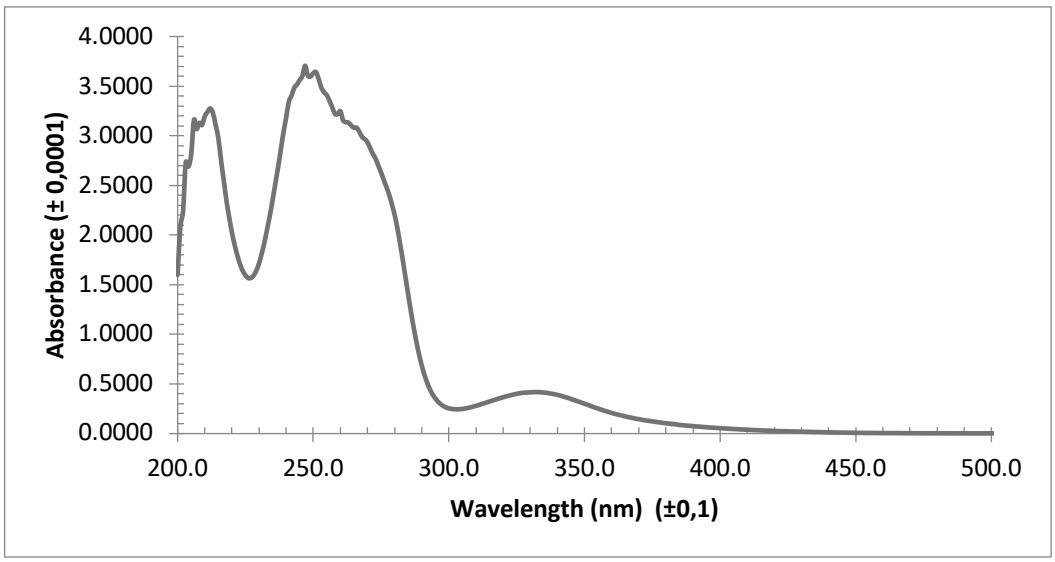
2-(4-phenylphenoxy)-1,4-naphthoquinone **44** ^{1}H NMR



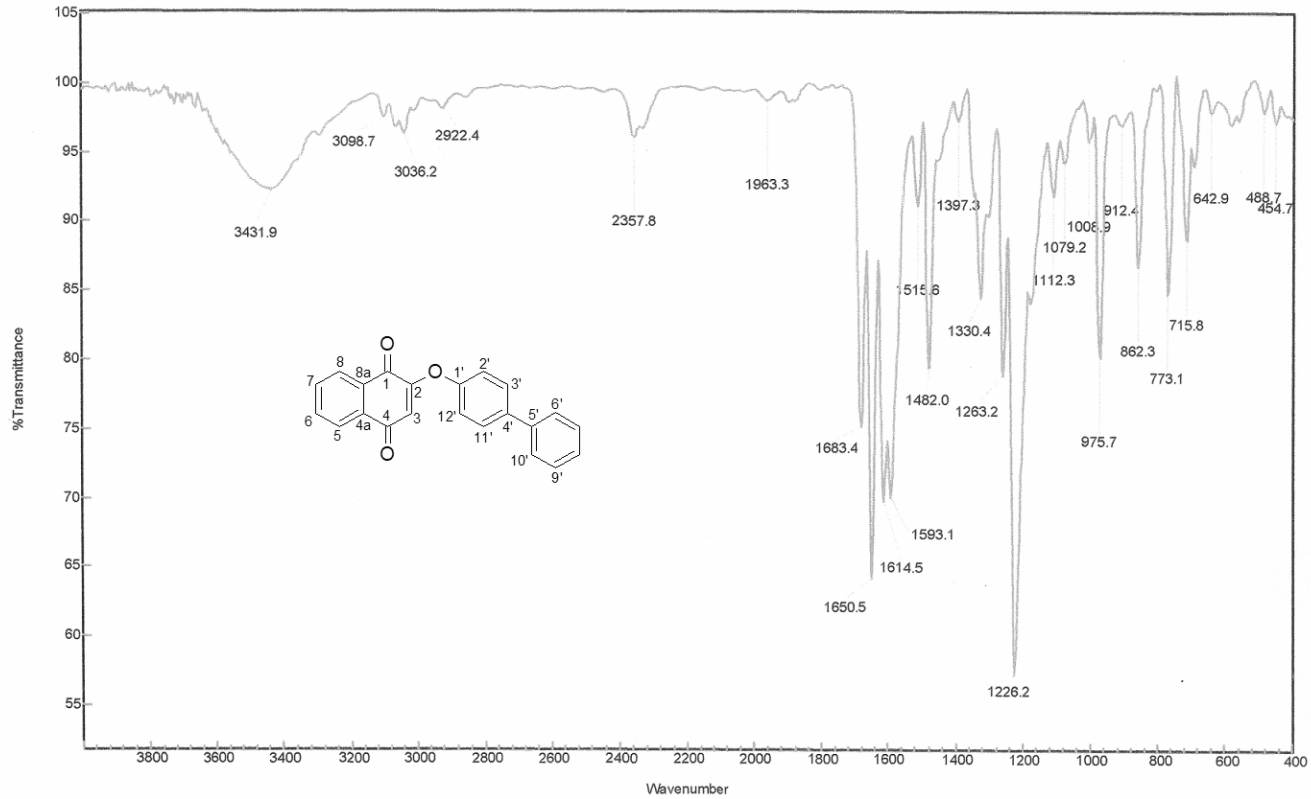
2-(4-phenylphenoxy)-1,4-naphthoquinone **44** ^{13}C NMR



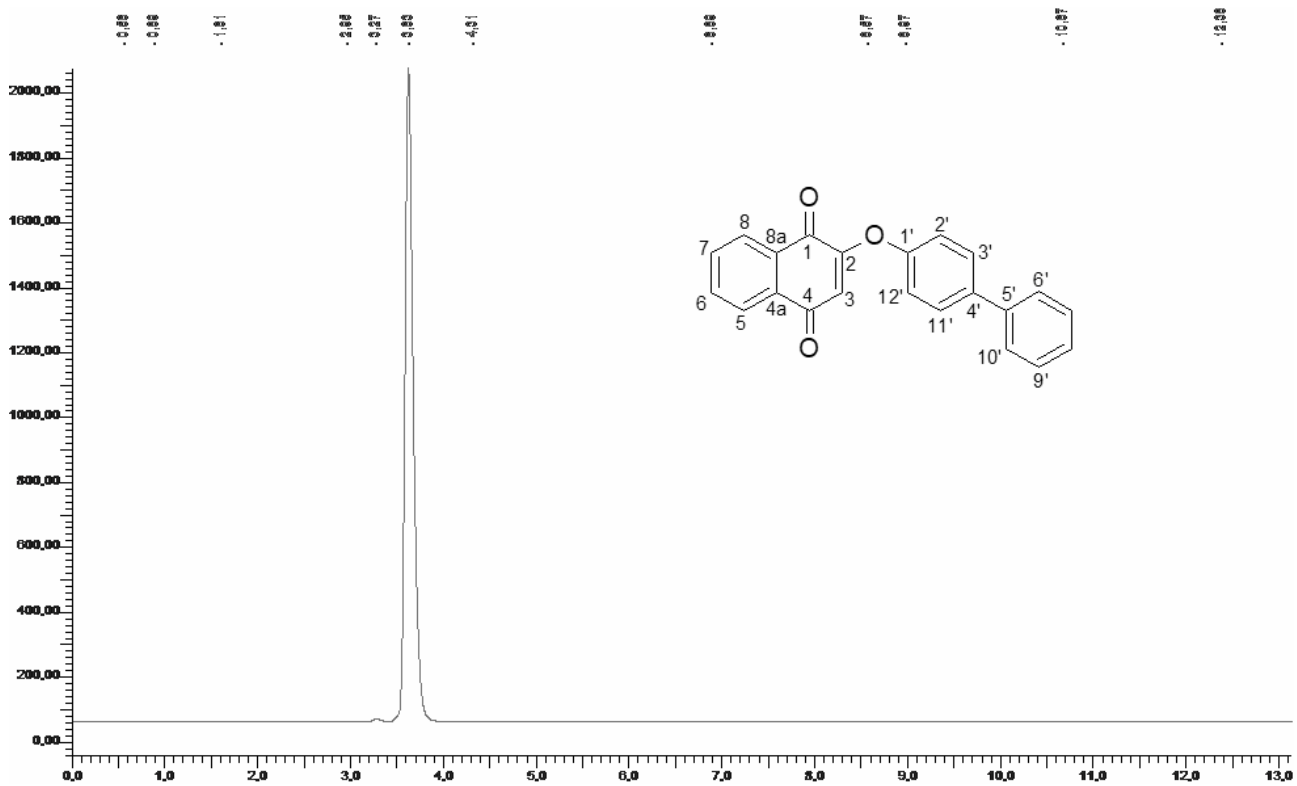
2-(4-phenylphenoxy)-1,4-naphthoquinone **44** UV-Vis (MeOH)



2-(4-phenylphenoxy)-1,4-naphthoquinone **44** IR (KBr pellet)



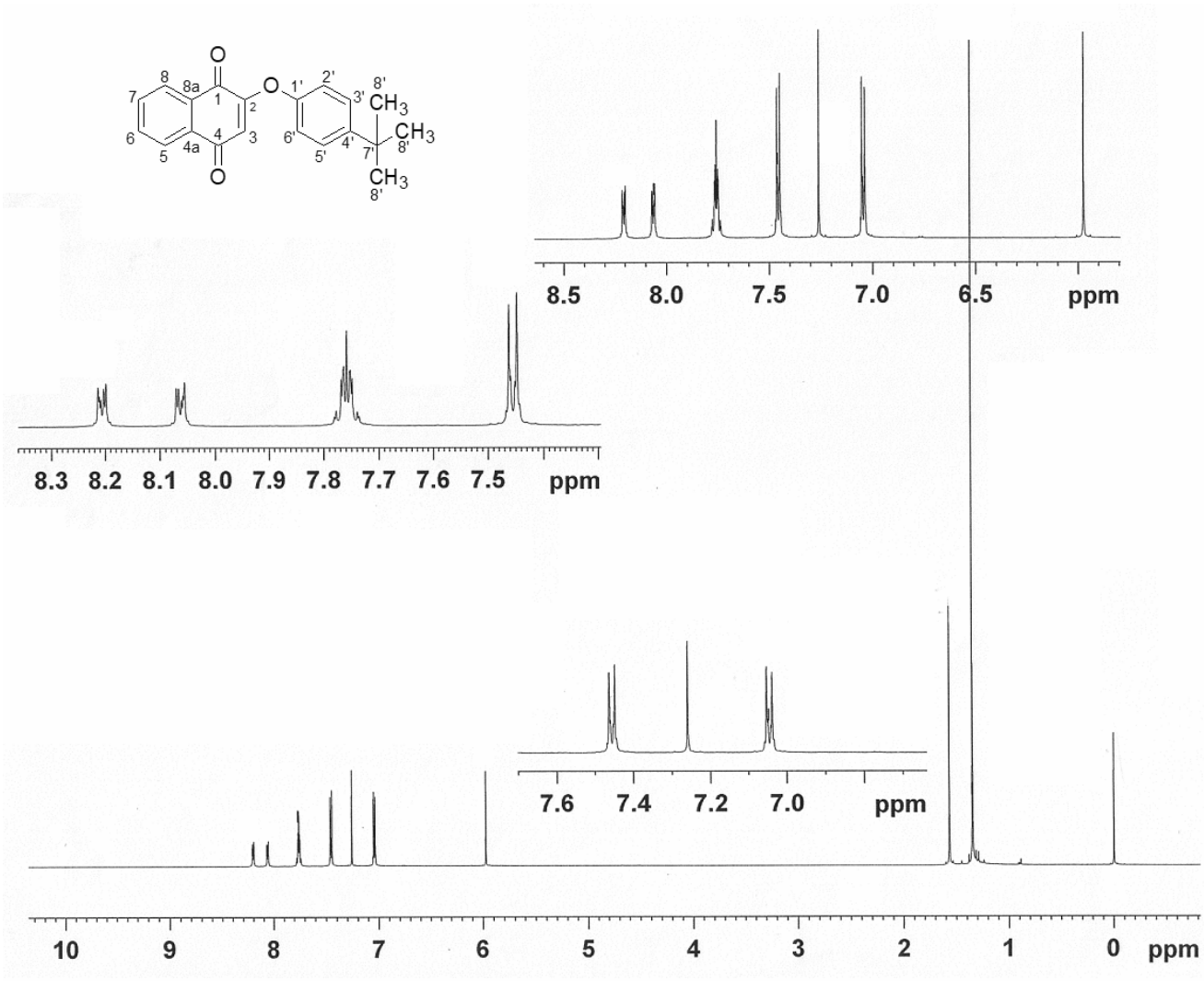
2-(4-phenylphenoxy)-1,4-naphthoquinone **44** HPLC chromatogram (270 nm, 100% MeCN)



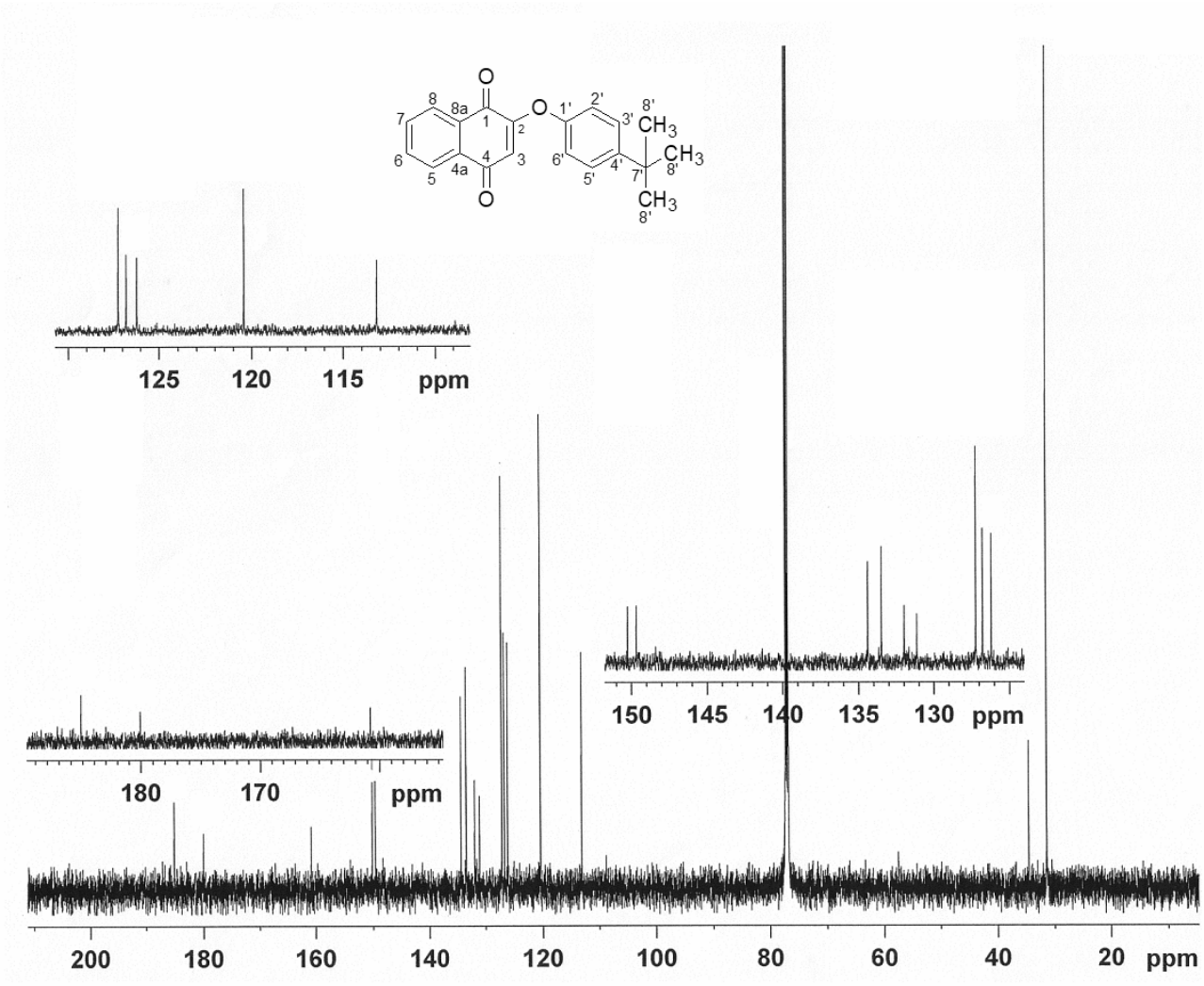
2-(4-tert-butylphenoxy)-1,4-naphthoquinone **45**

45 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, column chromatography (benzene as eluent, isocratically) and recrystallization with isooctane. Yield 171 mg (56%), yellow needles, mp = (151.0 – 152.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.22 (1H, d, *J* = 6 Hz, ArH), 8.06 (1H, d, *J* = 6 Hz, ArH), 7.77 (2H, m, ArH), 7.46 (2H, d, J_{ortho} = 7 Hz, ArH), 7.05 (2H, d, J_{ortho} = 9 Hz, ArH), 5.97 (1H, s, ArH), 1.35 (9H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 185.1, 180.0, 160.8, 150.2, 149.7, 134.4, 133.5, 132.0, 131.1, 127.2, 126.8, 126.2, 120.4, 113.2, 34.6, 31.4. IR (KBr pellet) cm^{-1}: 3061, 2958, 1678, 1657, 1598, 1504, 1262, 1213. UV-Vis (MeCN) nm: 201, 249 (max), 270, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{20}H_{19}O_3$: 307.1334; found: 307.1335. Purity: 98.8%. MIC (μM): >3000 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

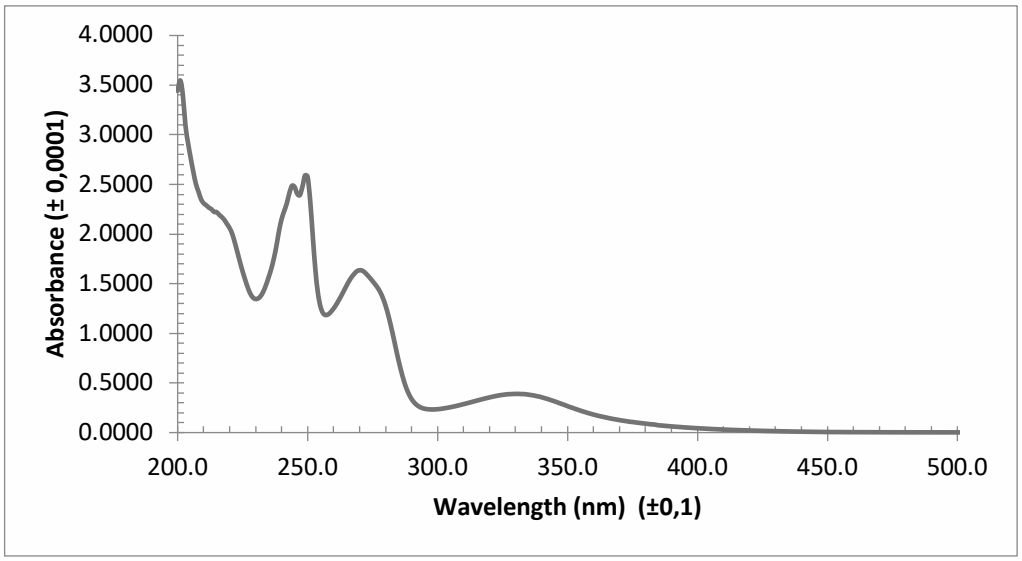
2-(4- tert-butylphenoxy)-1,4-naphthoquinone **45** ^{1}H NMR



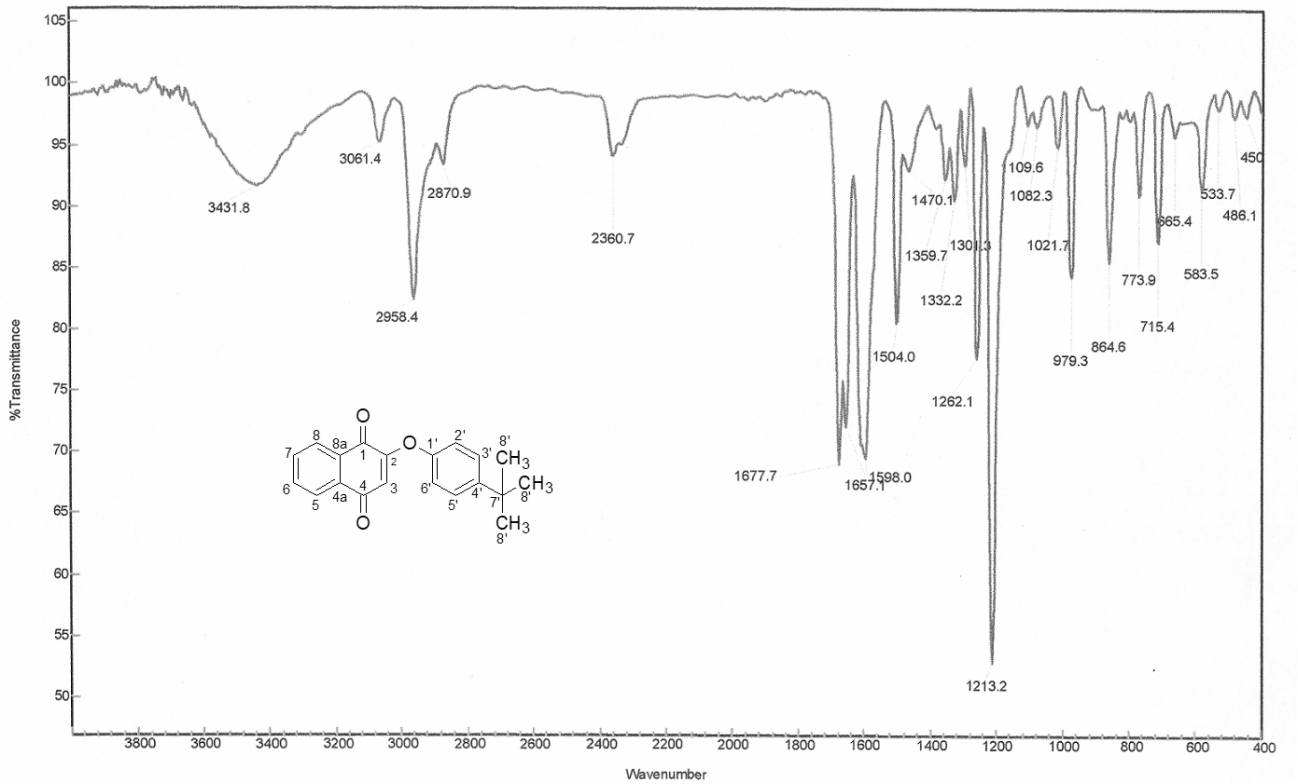
2-(4- tert-butylphenoxy)-1,4-naphthoquinone **45** ^{13}C NMR



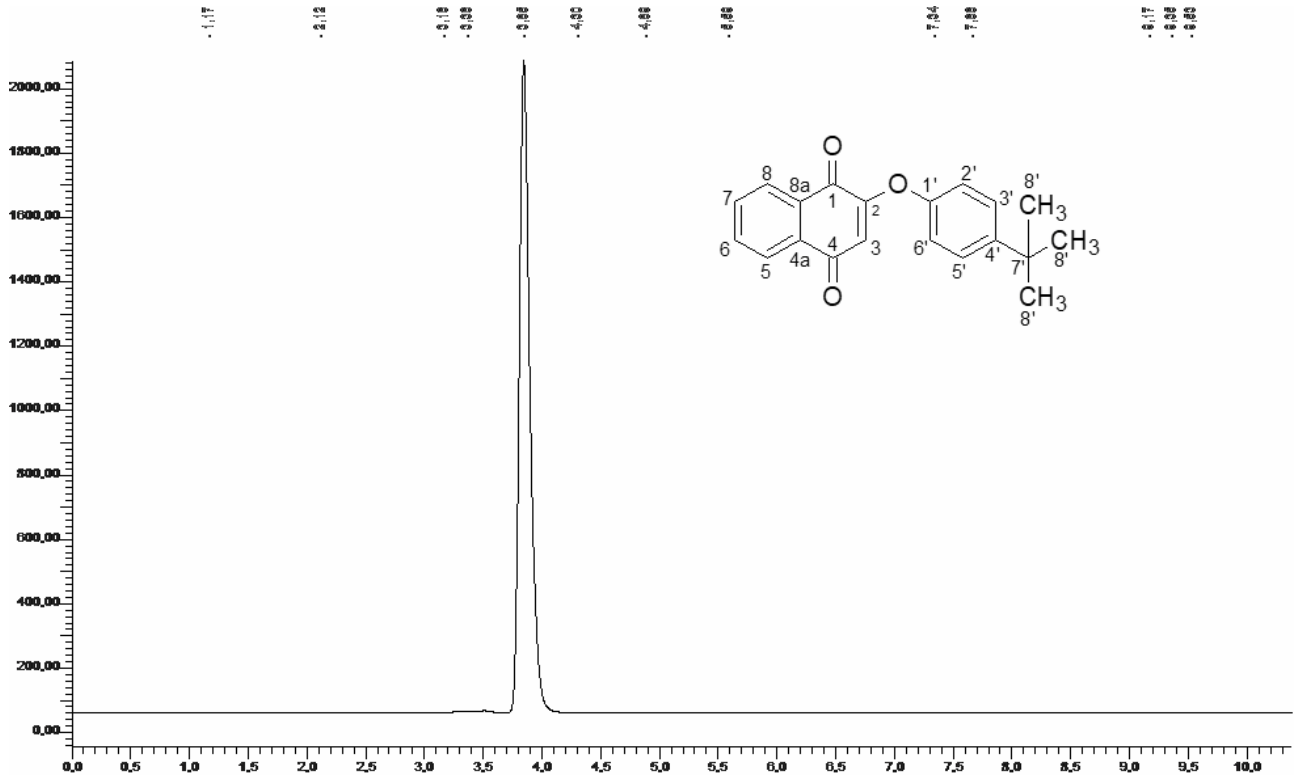
2-(4- tert-butylphenoxy)-1,4-naphthoquinone **45** UV-Vis (MeCN)



2-(4- tert-butylphenoxy)-1,4-naphthoquinone **45** IR (KBr pellet)



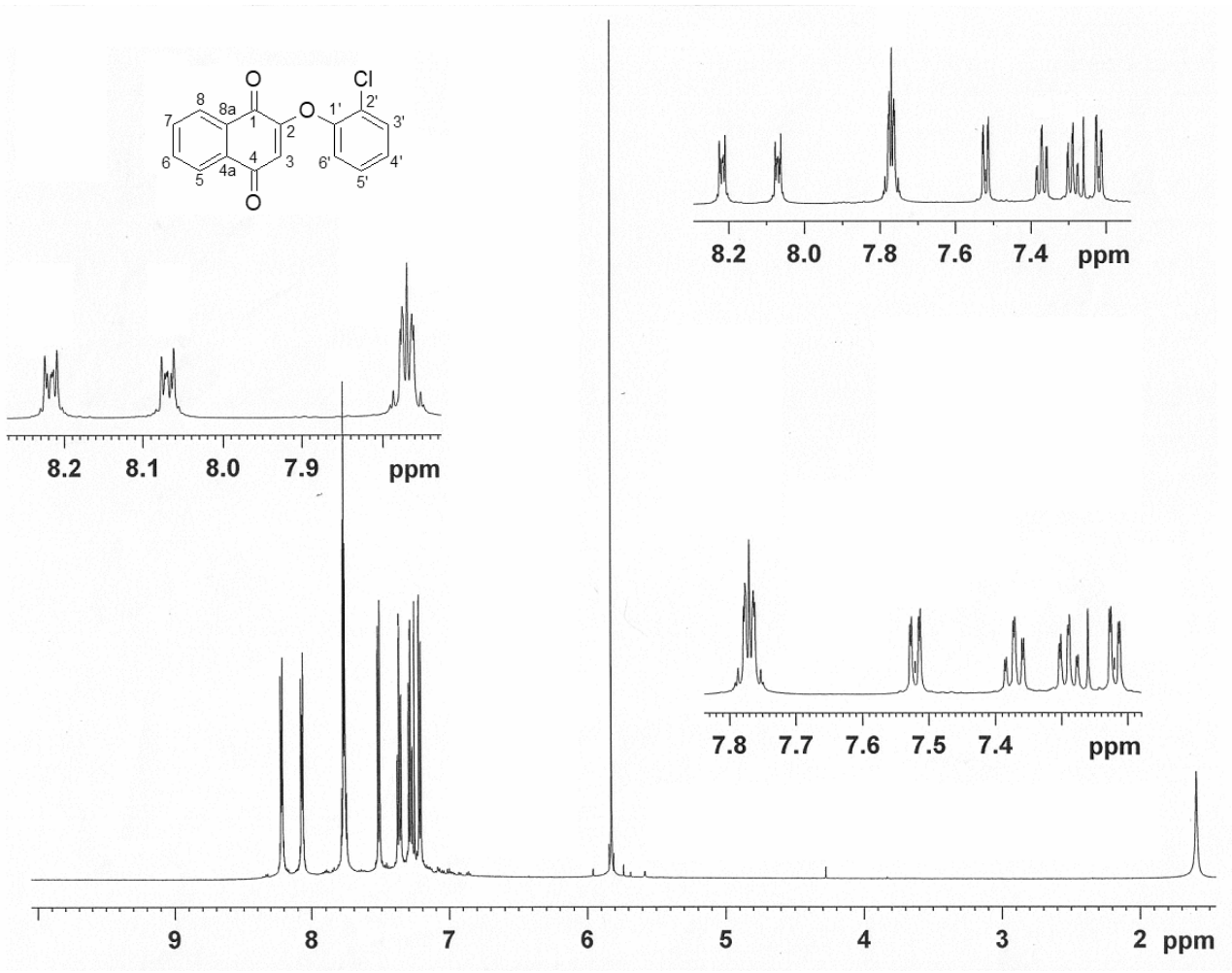
2-(4- tert-butylphenoxy)-1,4-naphthoquinone **45** HPLC chromatogram (270 nm, 100% MeCN)



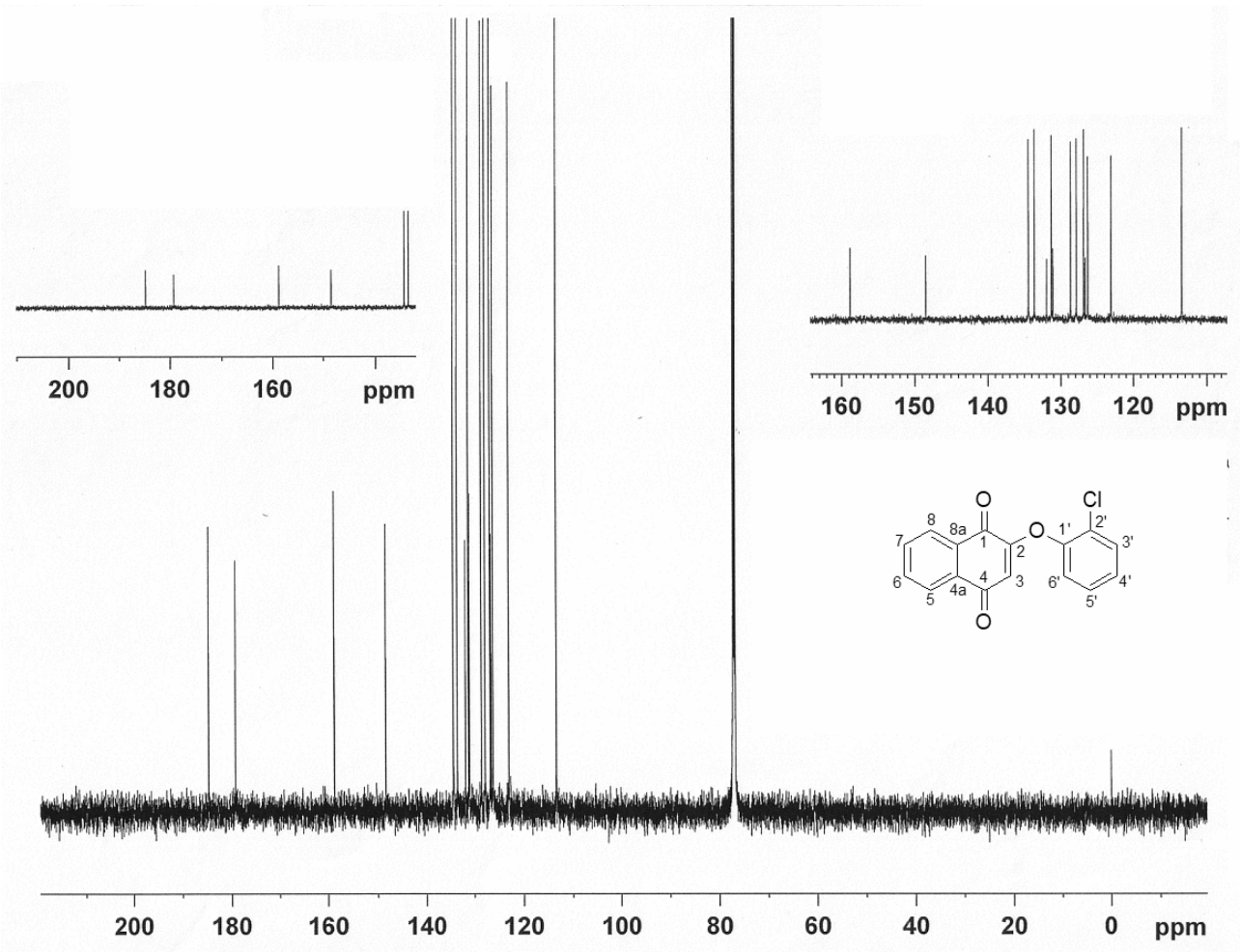
2-(2-chlorophenoxy)-1,4-naphthoquinone **46**

46 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, column chromatography (gradient elution starting with 15% MTBE/cyclohexane to 50% MTBE/cyclohexane) and recrystallization with isooctane. Yield 124 mg (58%), yellow solid, mp = (95.0 – 96.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.22 (1H, d, J = 7 Hz, ArH), 8.07 (1H, d, J = 7 Hz, ArH), 7.77 (2H, m, ArH), 7.52 (1H, dd, J_{meta} = 3 Hz, J_{ortho} = 8 Hz, ArH), 7.37 (1H, td, J_{meta} = 3 Hz, J_{ortho} = 8 Hz, ArH), 7.29 (1H, td, J_{meta} = 3 Hz, J_{ortho} = 8 Hz, ArH), 7.22 (1H, dd, J_{meta} = 3 Hz, J_{ortho} = 8 Hz, ArH), 5.83 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.8, 179.3, 158.8, 148.5, 134.5, 133.7, 132.0, 131.3, 131.1, 128.7, 127.9, 126.9, 126.7, 126.3, 123.1, 113.4. IR (KBr pellet) cm^{-1}: 3068, 1683, 1653, 1611, 1499, 1261, 1205, 976. UV-Vis (MeOH) nm: 203 (max), 243, 270, 332. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}O_3Cl$: 285.0318; found: 285.0320. Purity: 97.9%. MIC (µM): 220 (*S. aureus*), 220 (*C. albicans*), >3000 (*E. coli*).

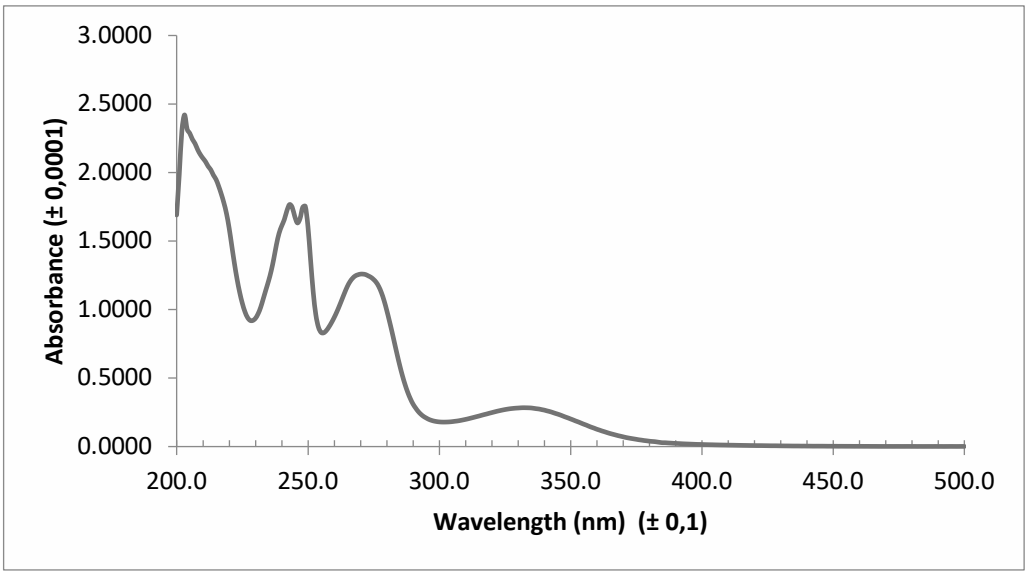
2-(2-chlorophenoxy)-1,4-naphthoquinone **46** ^{1}H NMR



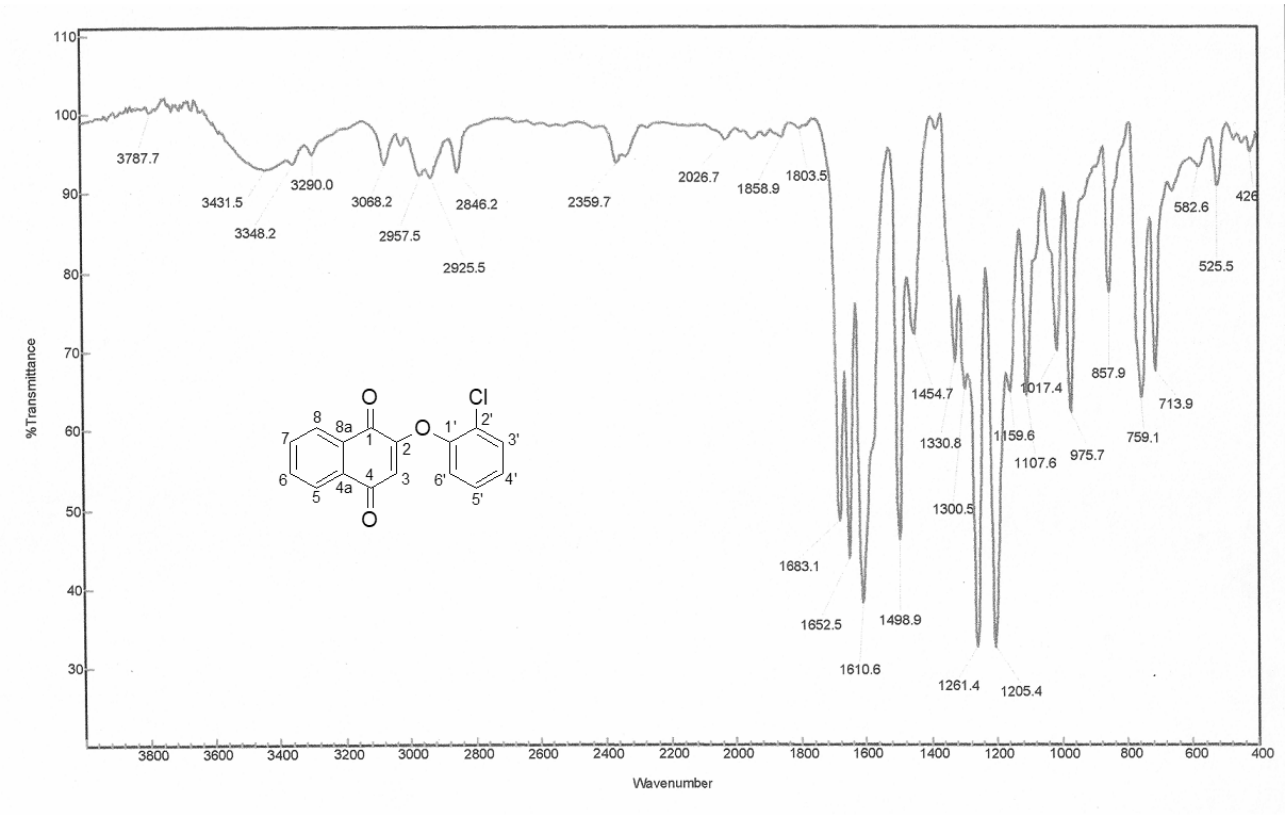
2-(2-chlorophenoxy)-1,4-naphthoquinone **46** ^{13}C NMR



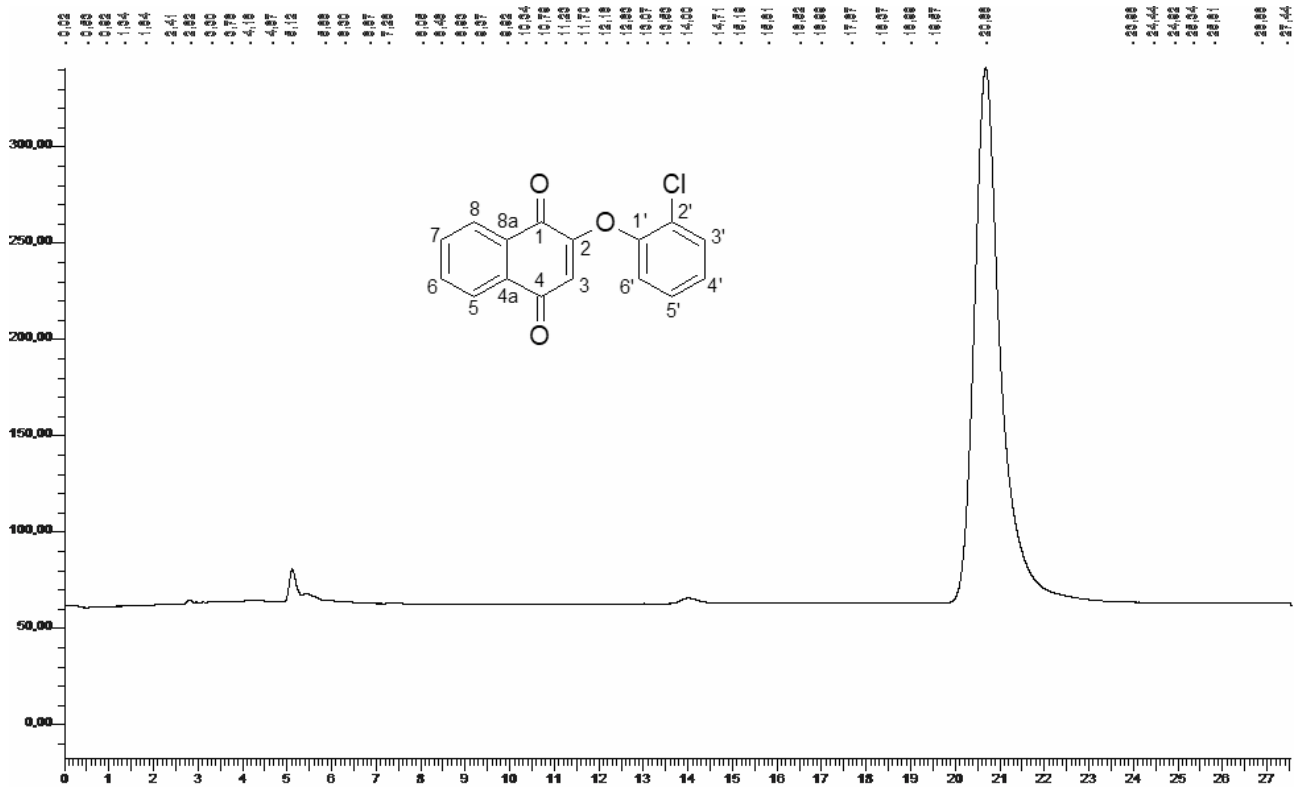
2-(2-chlorophenoxy)-1,4-naphthoquinone **46** UV-Vis (MeOH)



2-(2-chlorophenoxy)-1,4-naphthoquinone **46** IR (KBr pellet)



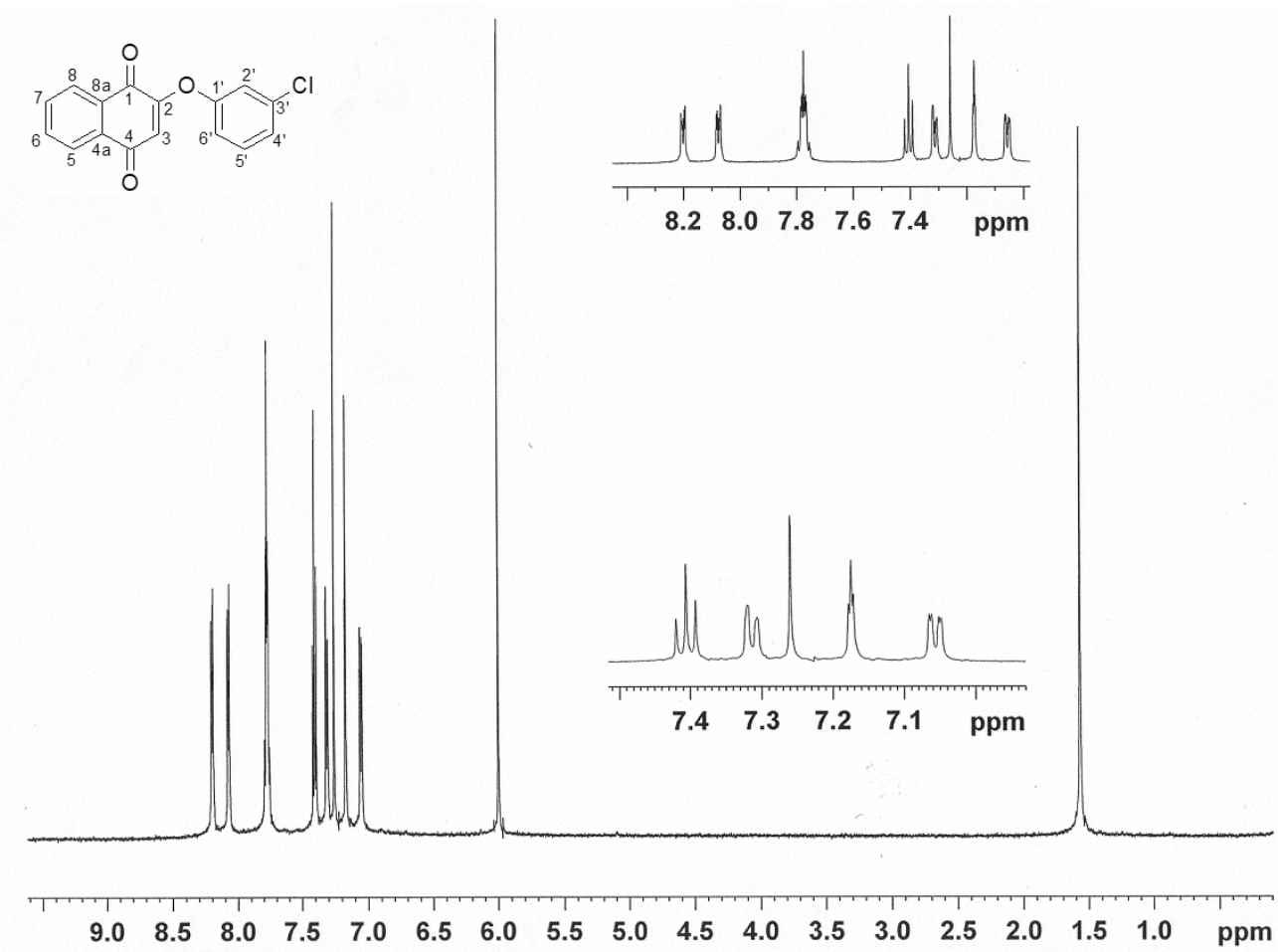
2-(2-chlorophenoxy)-1,4-naphthoquinone **46** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



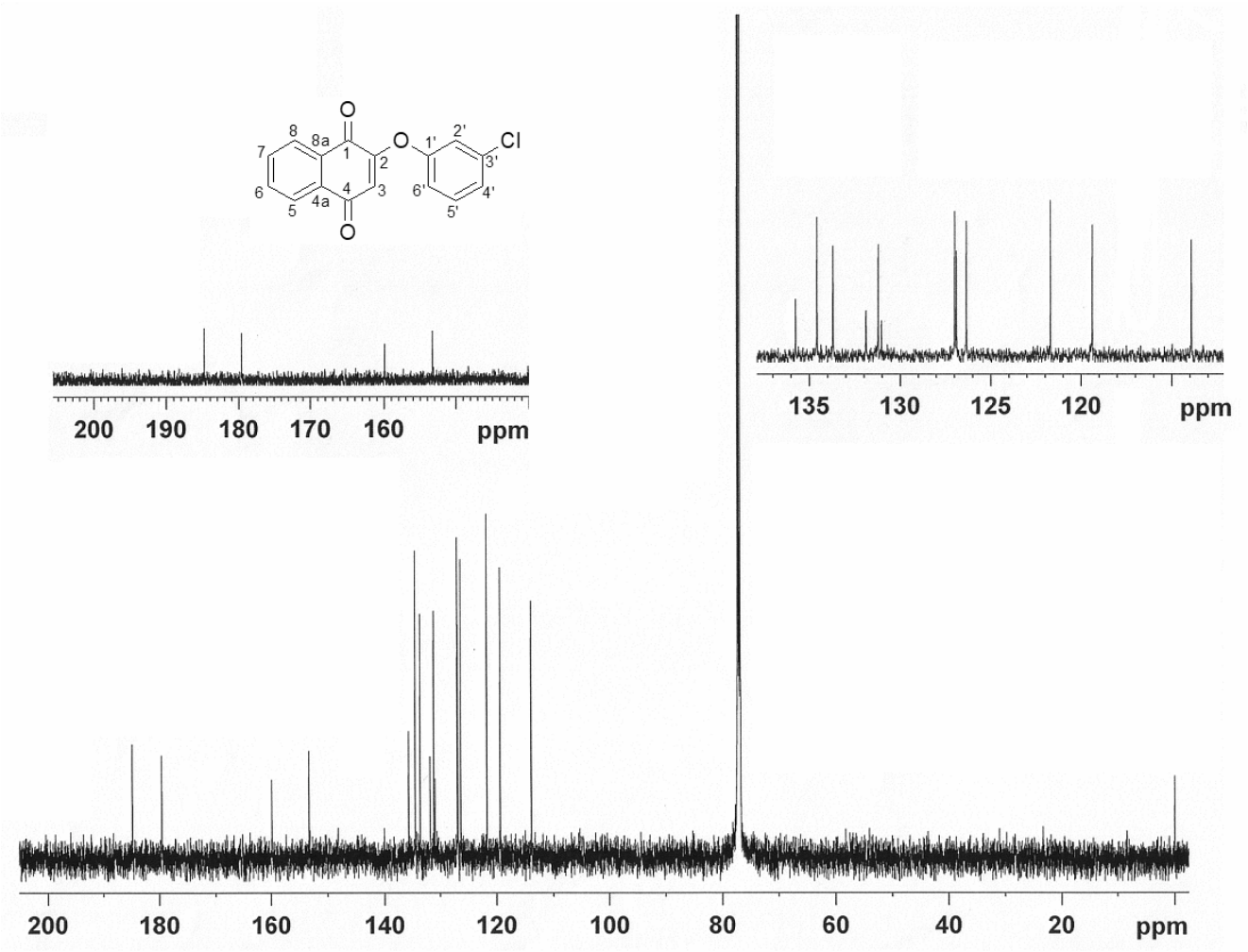
2-(3-chlorophenoxy)-1,4-naphthoquinone **47**

47 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, column chromatography (gradient elution starting with 10% MTBE/cyclohexane to 20% MTBE/cyclohexane) and recrystallization with isooctane. Yield 103 mg (48%), yellow solid, mp = (103.0 – 105.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.20 (1H, d, *J* = 7 Hz, ArH), 8.08 (1H, d, *J* = 7 Hz, ArH), 7.78 (2H, m, ArH), 7.40 (1H, t, J_{ortho} = 8 Hz, ArH), 7.31 (1H, d, J_{ortho} = 8 Hz, ArH), 7.17 (1H, s, ArH), 7.06 (1H, d, J_{ortho} = 8 Hz, ArH), 6.00 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.8, 179.6, 159.9, 153.3, 135.7, 134.6, 133.7, 131.9, 131.9, 131.0, 127.0, 126.9, 126.3, 121.7, 119.4, 113.9. IR (KBr pellet) cm^{-1}: 3071, 1681, 1651, 1614, 1585, 1262, 1222, 982. UV-Vis (MeOH) nm: 204 (max), 248, 273, 332. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}O_3Cl$: 285.0318; found: 285.0323. Purity: 92.3%. MIC (µM): 878 (*S. aureus*), 220 (*C. albicans*), >3000 (*E. coli*).

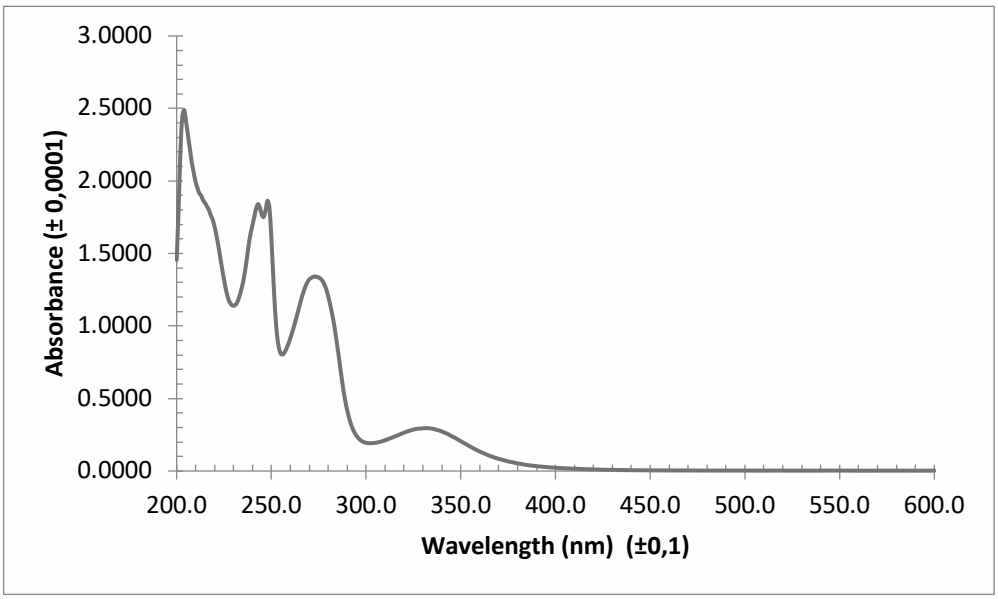
2-(3-chlorophenoxy)-1,4-naphthoquinone **47** ^{1}H NMR



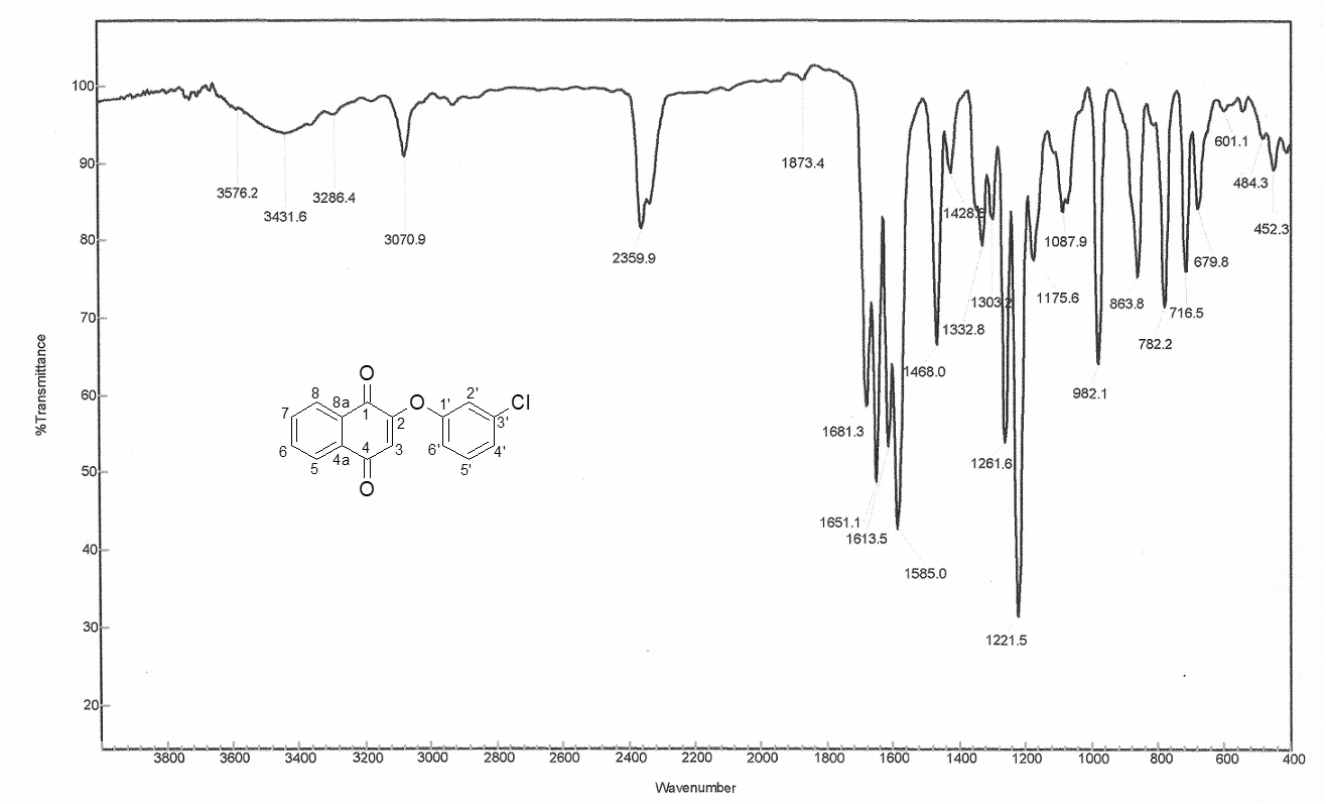
2-(3-chlorophenoxy)-1,4-naphthoquinone **47** ^{13}C NMR



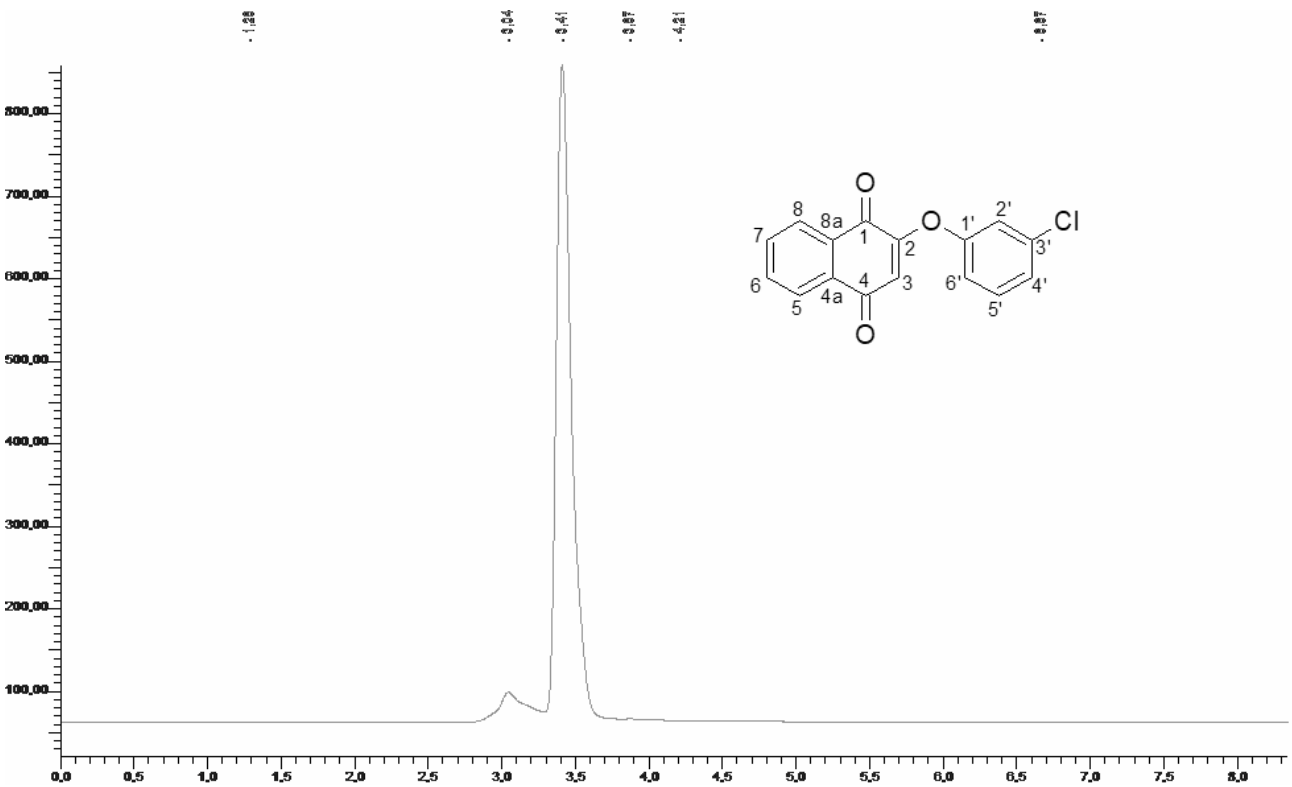
2-(3-chlorophenoxy)-1,4-naphthoquinone **47** UV-Vis (MeOH)



2-(3-chlorophenoxy)-1,4-naphthoquinone **47** IR (KBr pellet)



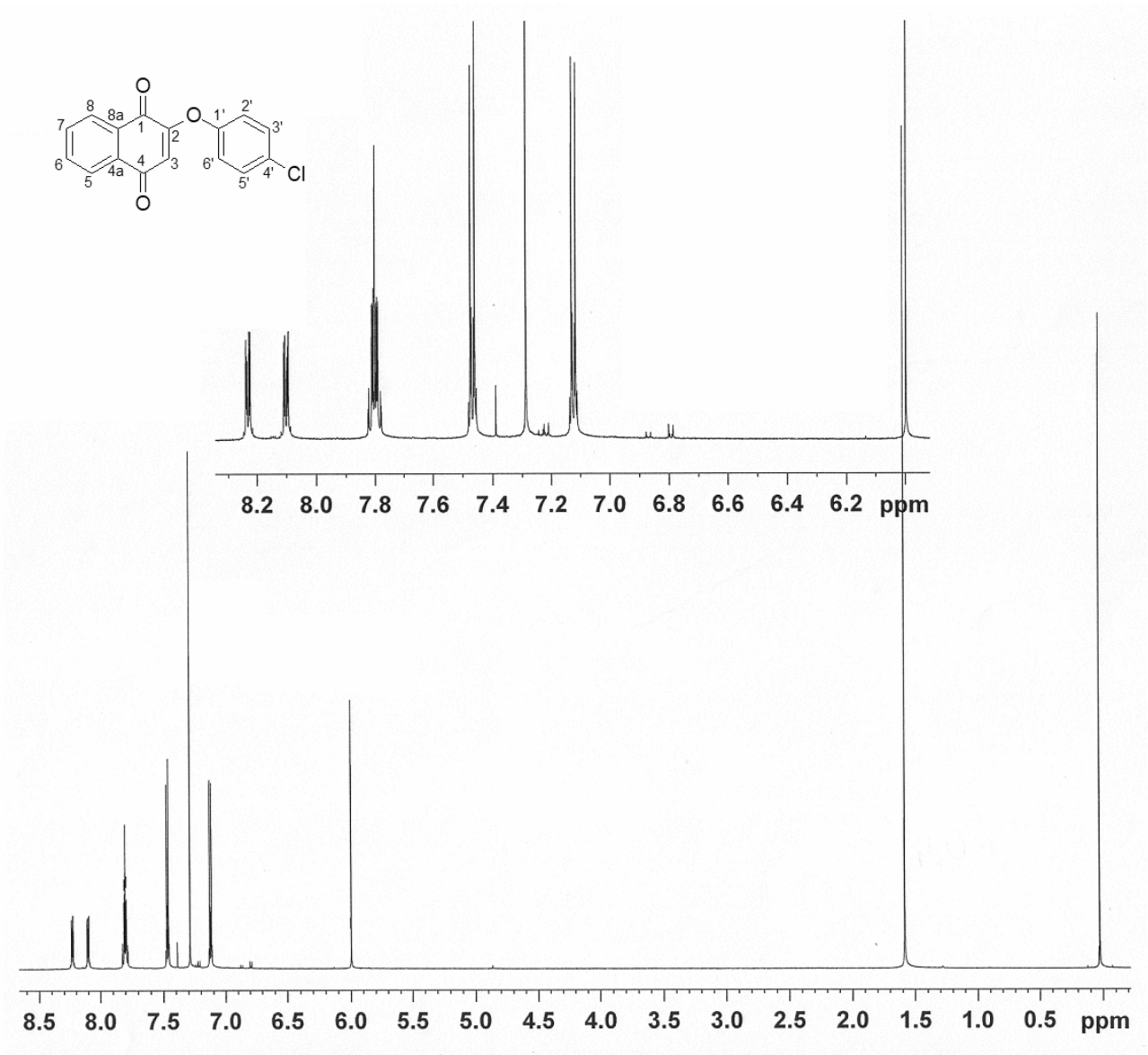
2-(3-chlorophenoxy)-1,4-naphthoquinone **47** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



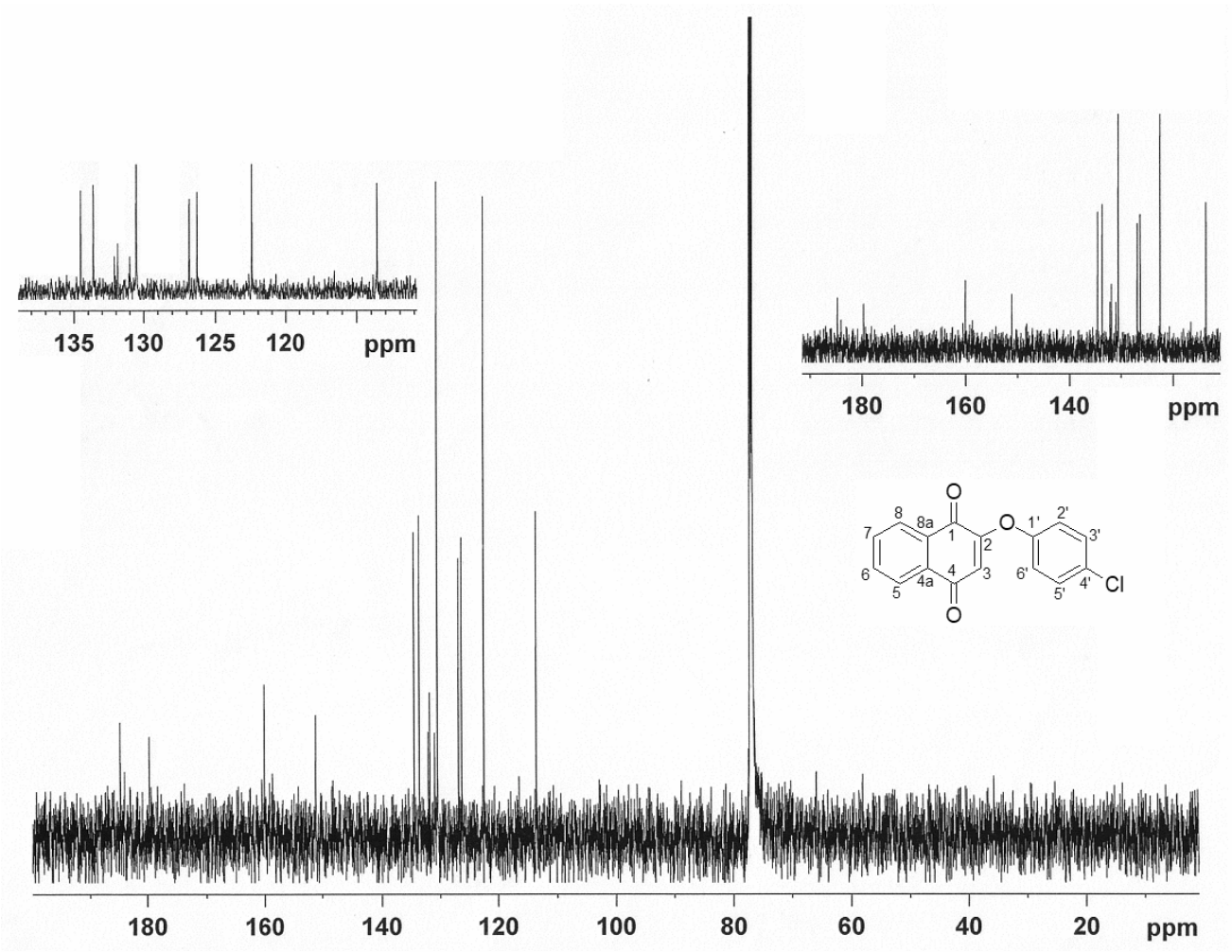
2-(4-chlorophenoxy)-1,4-naphthoquinone **48**

48 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, column chromatography (benzene as eluent, isocratically) and recrystallization with isooctane. Yield 162 mg (76%), yellow solid, mp = (131.0 – 133.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.23 (1H, dd, *J* = 2 Hz, *J* = 7 Hz, ArH), 8.11 (1H, dd, *J* = 2 Hz, *J* = 7 Hz, ArH), 7.81 (2H, m, ArH), 7.47 (2H, d, J_{ortho} = 6 Hz, ArH), 7.12 (2H, d, J_{ortho} = 6 Hz, ArH), 6.00 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.7, 179.7, 160.1, 151.2, 134.6, 133.6, 132.1, 131.9, 131.1, 130.5, 126.8, 126.3, 122.5, 113.6. IR (KBr pellet) cm^{-1}: 3049, 1684, 1654, 1625, 1482, 1238, 981. UV-Vis (MeOH) nm: 204, 221, 243 (max), 271, 330. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}O_3Cl$: 285.0318; found: 285.0321. Purity: 99.6%. MIC (µM): 439 (*S. aureus*), 439 (*C. albicans*), >3000 (*E. coli*).

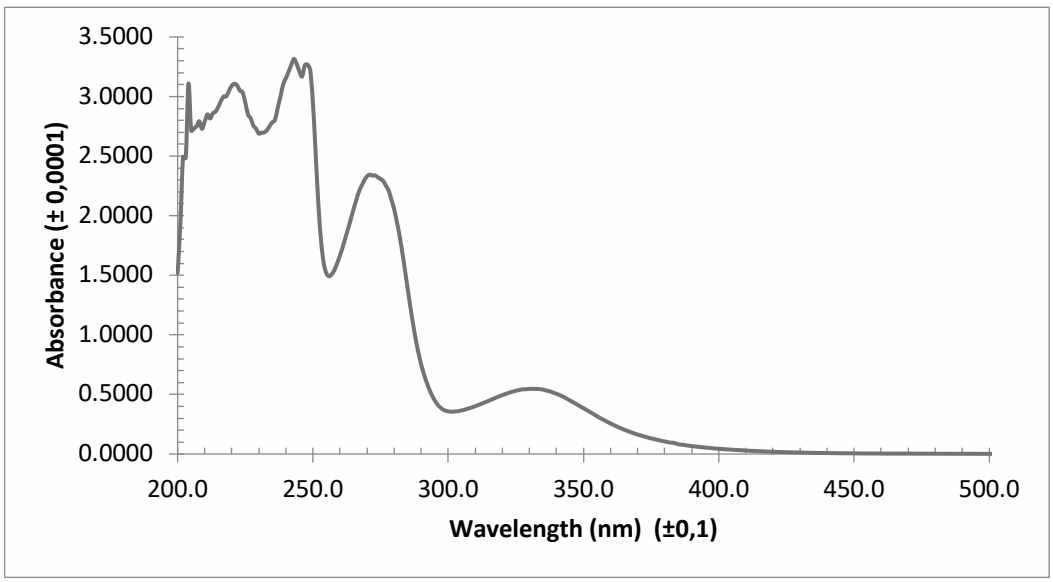
2-(4-chlorophenoxy)-1,4-naphthoquinone **48** ^{1}H NMR



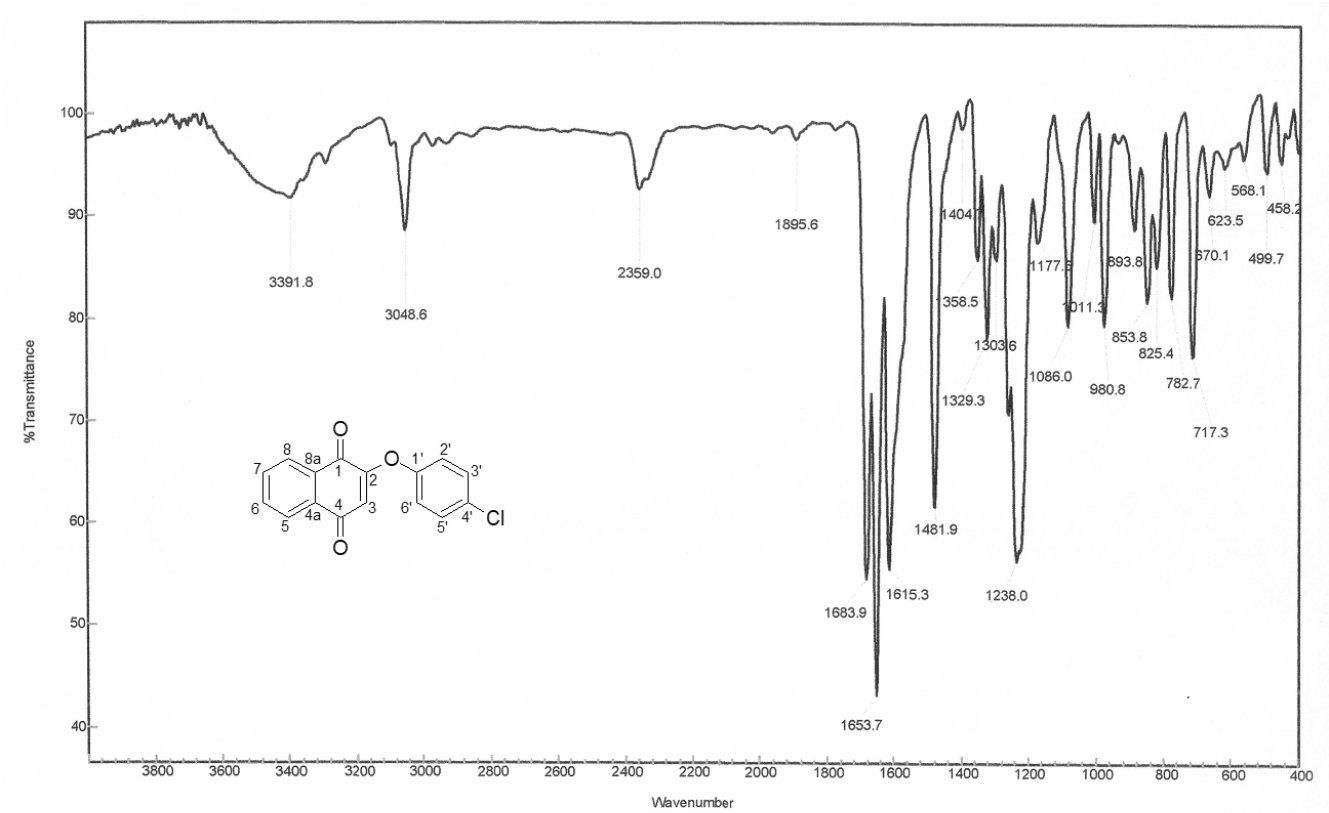
2-(4-chlorophenoxy)-1,4-naphthoquinone **48** ^{13}C NMR



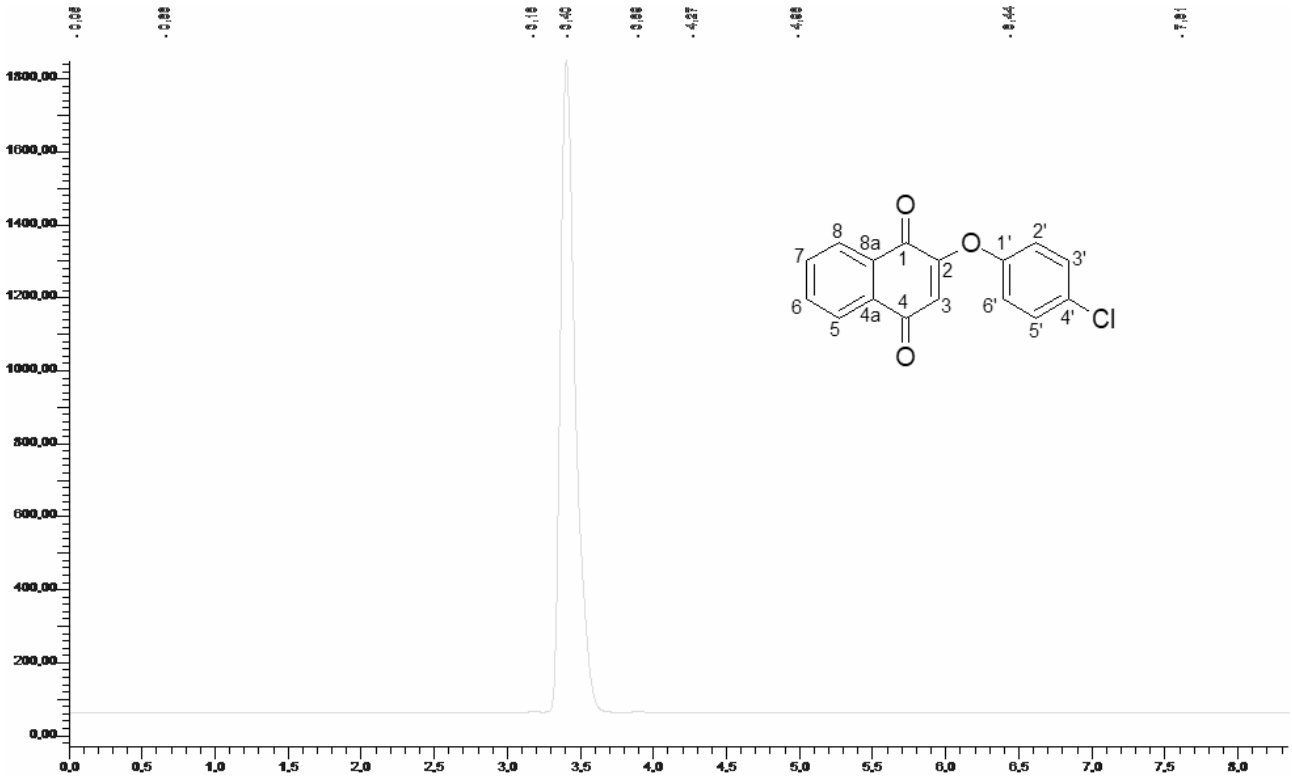
2-(4-chlorophenoxy)-1,4-naphthoquinone **48** UV-Vis (MeOH)



2-(4-chlorophenoxy)-1,4-naphthoquinone **48** IR (KBr pellet)



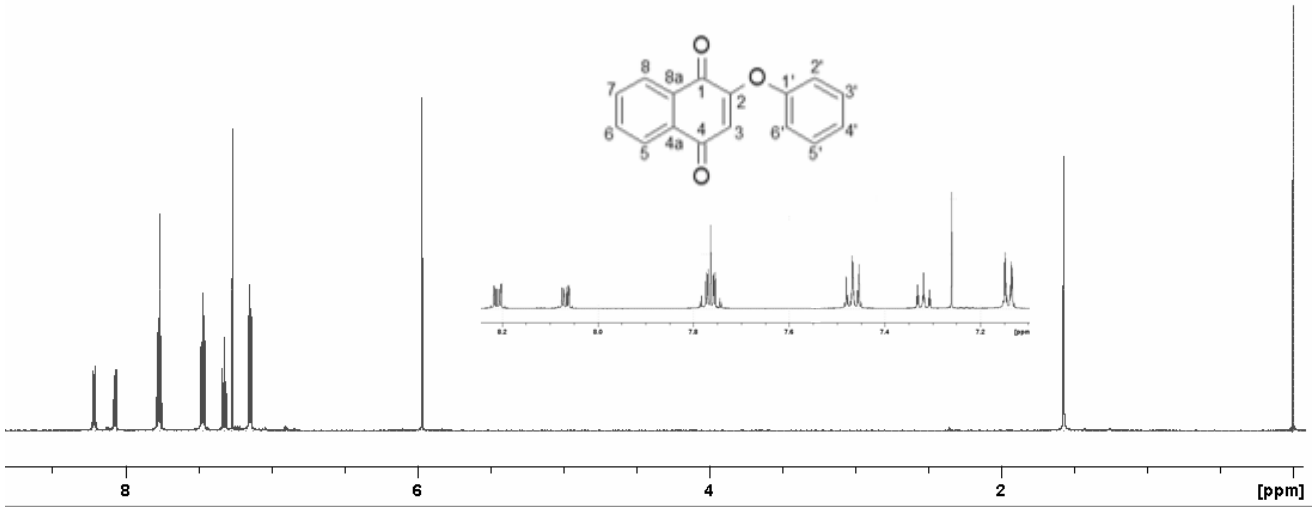
2-(4-chlorophenoxy)-1,4-naphthoquinone **48** HPLC chromatogram (270 nm, 100% MeCN)



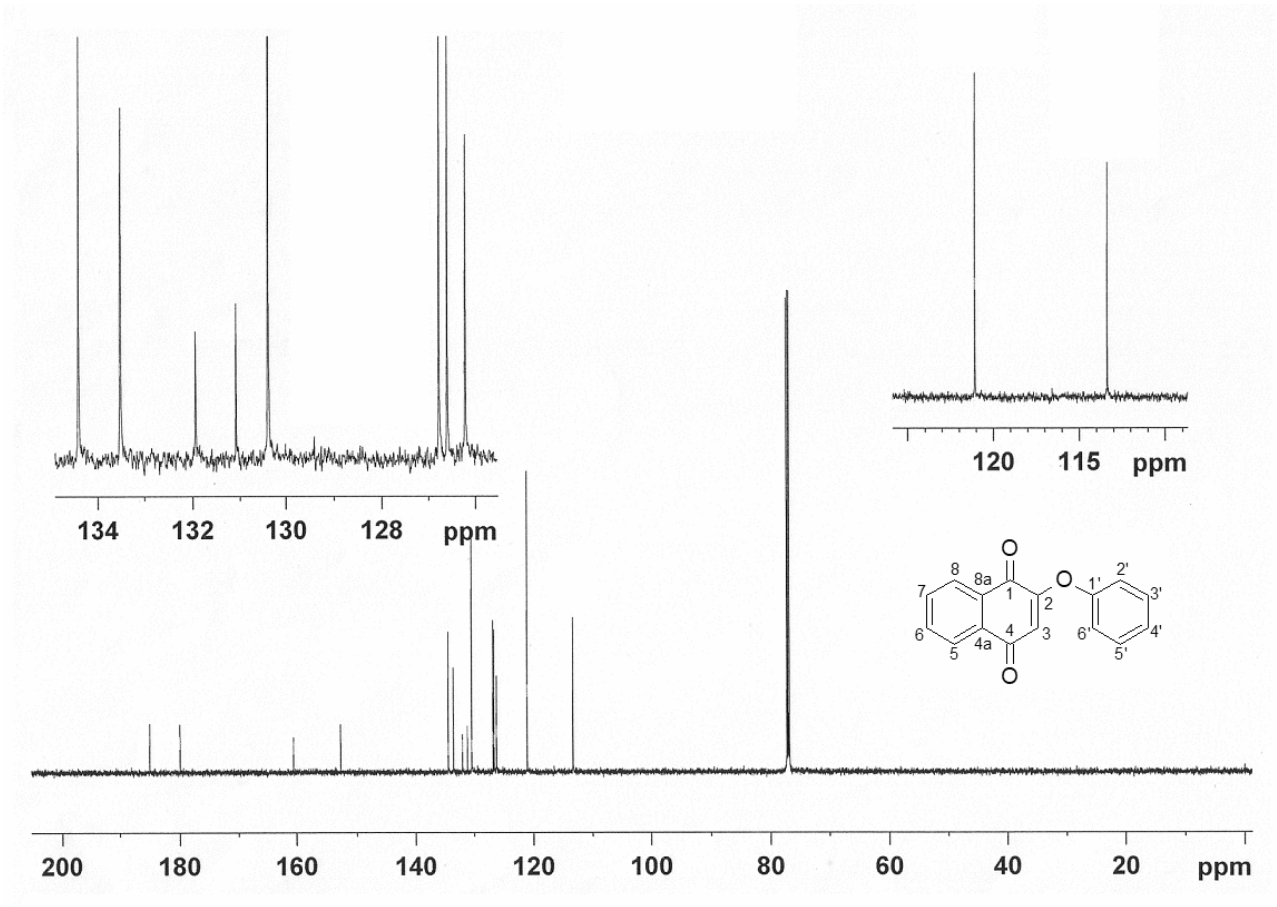
2-phenoxy-1,4-naphthoquinone 49

49 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE, cold base wash with MTBE as solvent and NaOH 0.5 mol/L and recrystallization with isooctane. Yield 144 mg (77%), yellow-orange crystals, mp = (94.0 – 102.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, dd, *J* = 3.4 Hz, *J* = 6.8 Hz, ArH), 8.07 (1H, dd, *J* = 3.4 Hz, *J* = 6.8 Hz, ArH), 7.76 (2H, m, ArH), 7.47 (2H, t, ArH), 7.32 (1H, tt, J_{meta} = 1.3 Hz, J_{ortho} = 7.5 Hz, ArH), 7.14 (2H, d, J_{ortho} = 8.8 Hz, ArH), 5.96 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.0, 179.9, 160.5, 152.7, 134.5, 133.5, 132.0, 131.1, 130.4, 126.8, 126.6, 126.2, 121.1, 113.4. IR (KBr pellet) cm^{-1}: 3067, 1684, 1654, 1614, 1586, 1262, 1213. UV-Vis (MeOH) nm: 210, 244 (max), 270, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{11}O_3$: 251.0708; found: 251.0703. Purity: 98.6%. MIC (µM): 250 (*S. aureus*), 250 (*C. albicans*), >3000 (*E. coli*).

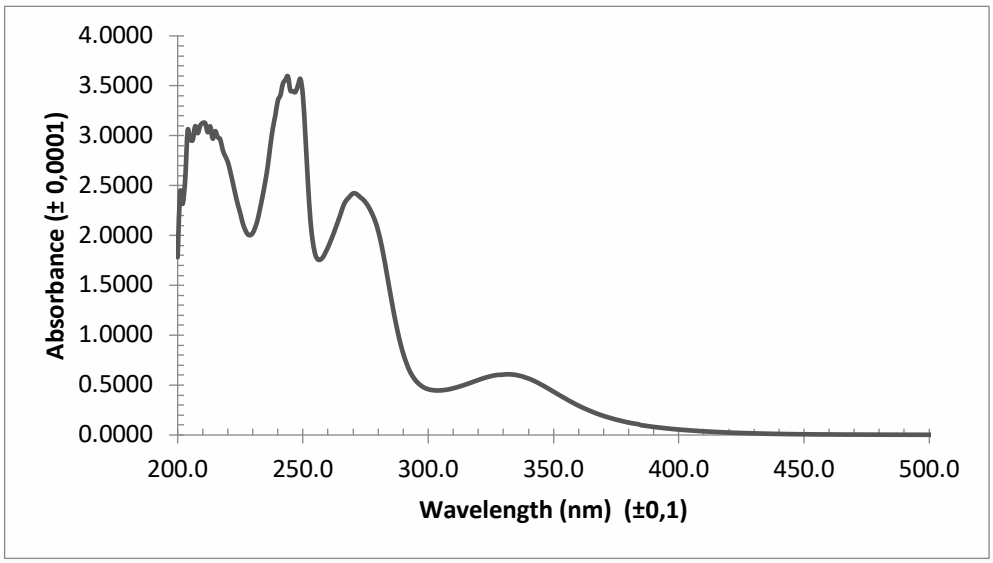
2-phenoxy-1,4-naphthoquinone **49** ^{1}H NMR



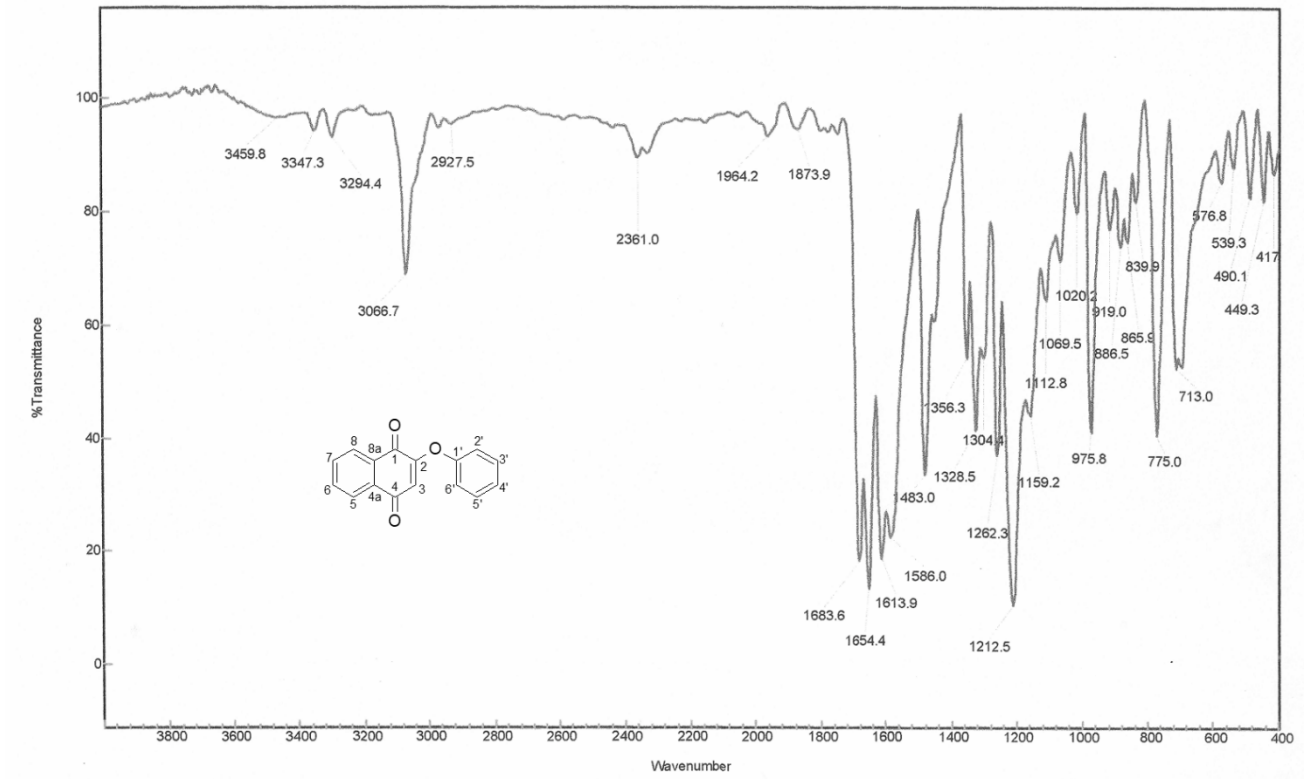
2-phenoxy-1,4-naphthoquinone **49** ^{13}C NMR



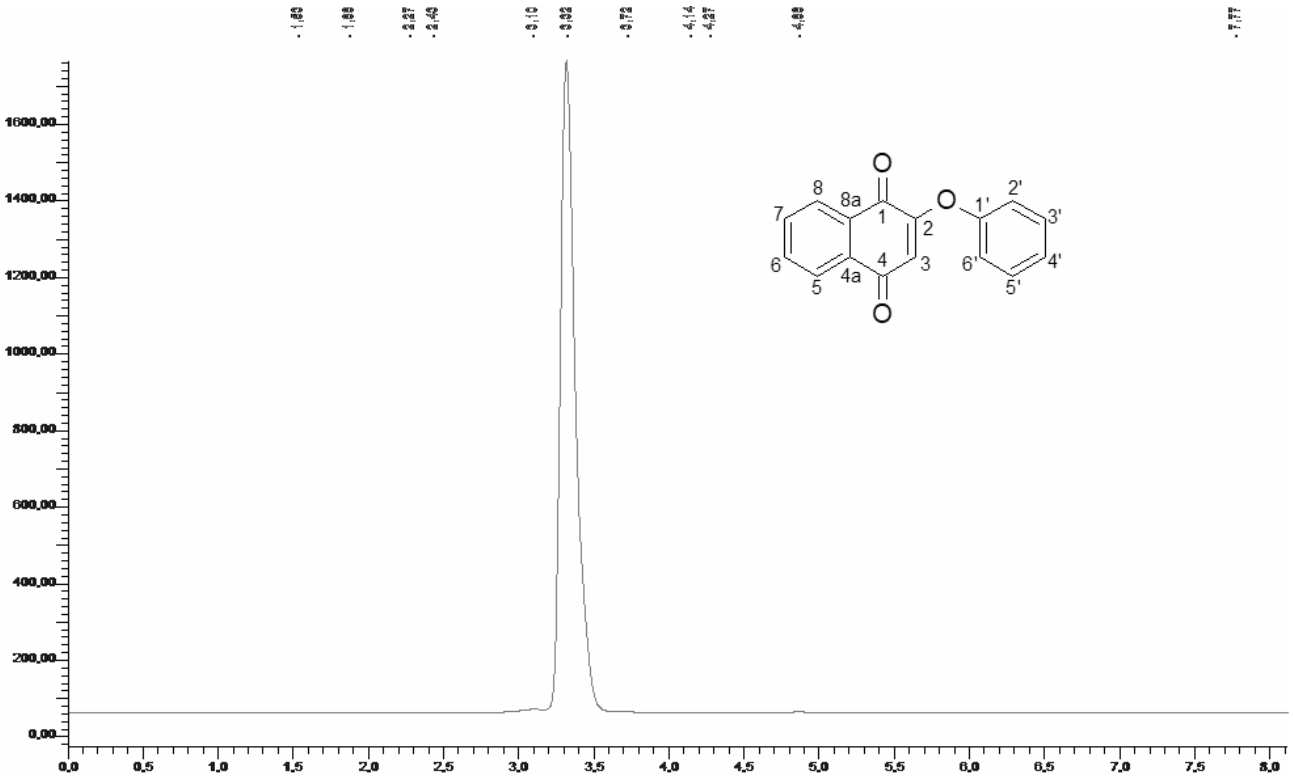
2-phenoxy -1,4-naphthoquinone **49** UV-Vis (MeOH)



2-phenoxy -1,4-naphthoquinone **49** IR (KBr pellet)



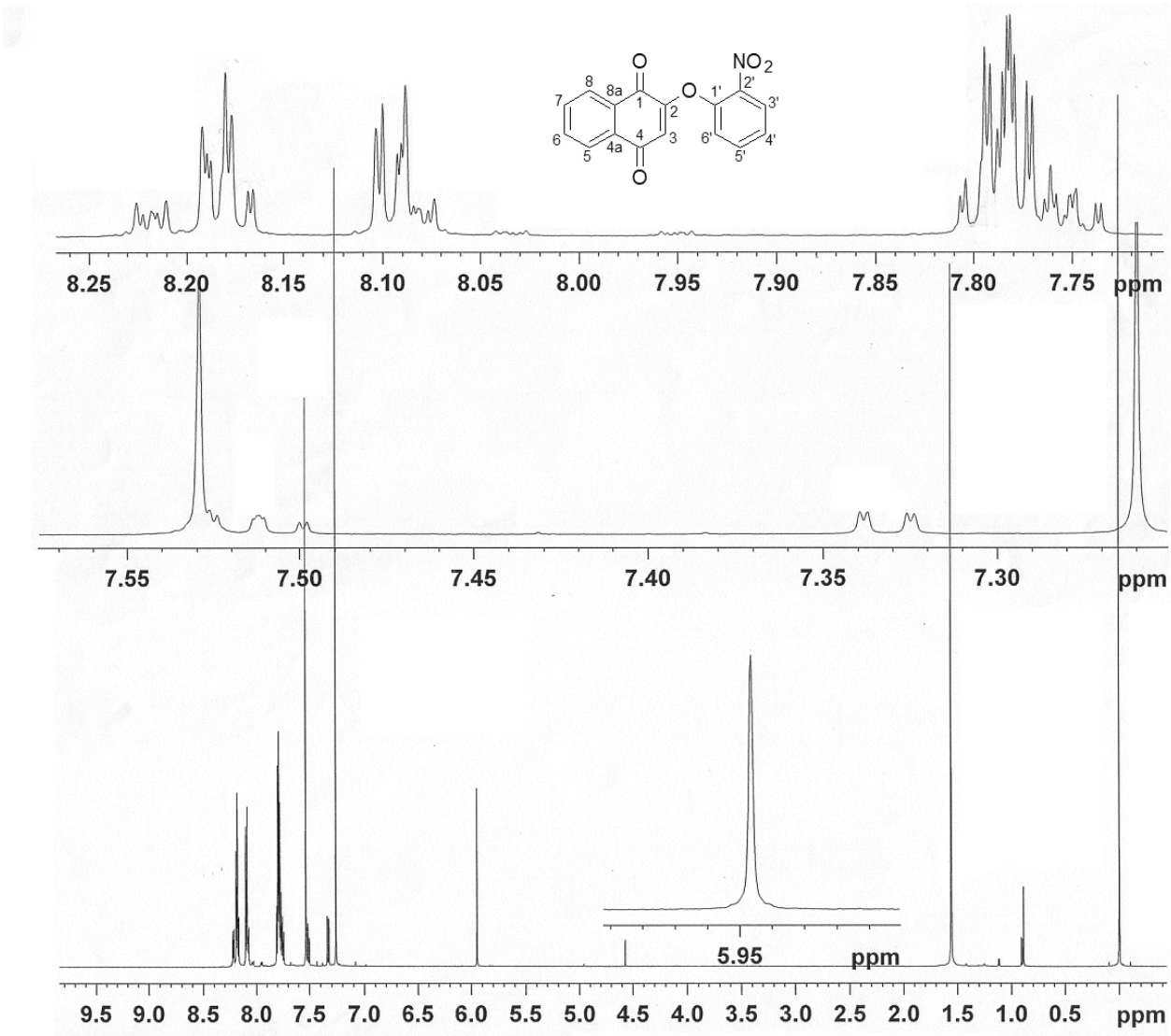
2-phenoxy -1,4-naphthoquinone **49** HPLC chromatogram (270 nm, 100% MeCN)



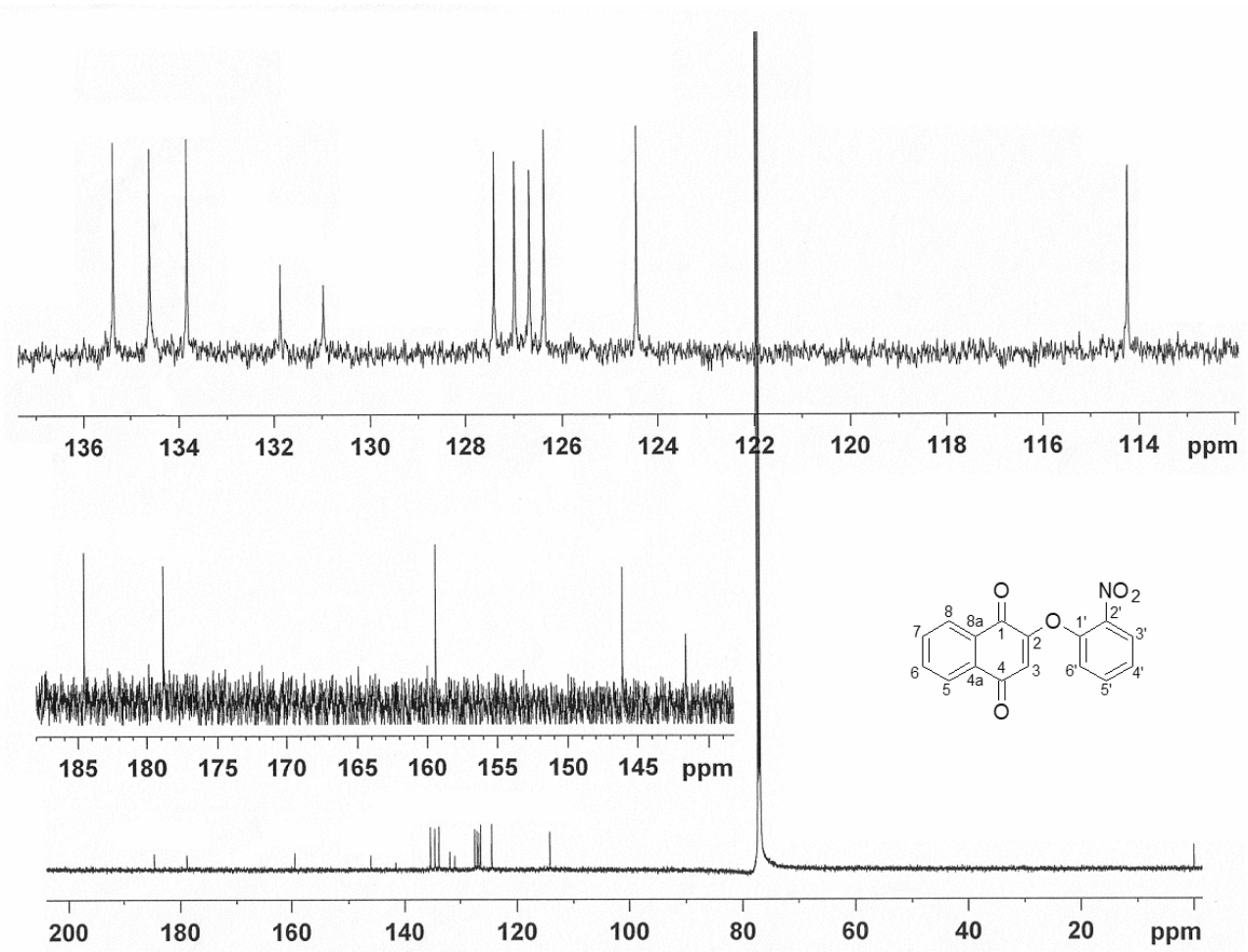
2-(2-nitrophenoxy)-1,4-naphthoquinone **50**

50 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with 25% n-heptane/isooctane and recrystallization with isooctane. Yield 89 mg (30%), yellow crystals, mp = (115.0 – 118.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.22 (1H, m, ArH), 8.18 (1H, dd, *J* = 2.6 Hz, *J* = 6.9 Hz, ArH), 8.08 (1H, m, ArH), 7.78 (2H, m, ArH), 7.75 (1H, m, ArH), 7.51 (1H, m, ArH), 7.33 (1H, dd, J_{meta} = 1.4 Hz, J_{ortho} = 8.2 Hz, ArH), 5.95 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.5, 178.8, 159.4, 146.1, 141.6, 135.4, 134.6, 133.8, 131.9, 131.0, 127.4, 127.0, 126.7, 126.4, 124.4, 114.2. IR (KBr pellet) cm^{-1}: 3072, 1677, 1655, 1602, 1529, 1349, 1264, 1231. UV-Vis (MeOH) nm: 204, 218, 252 (max), 273, 334. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}NO_5$: 296.0559; found: 296.0562. Purity: non measured. MIC (µM): 13 (*S. aureus*), 85 (*C. albicans*), 1693 (*E. coli*).

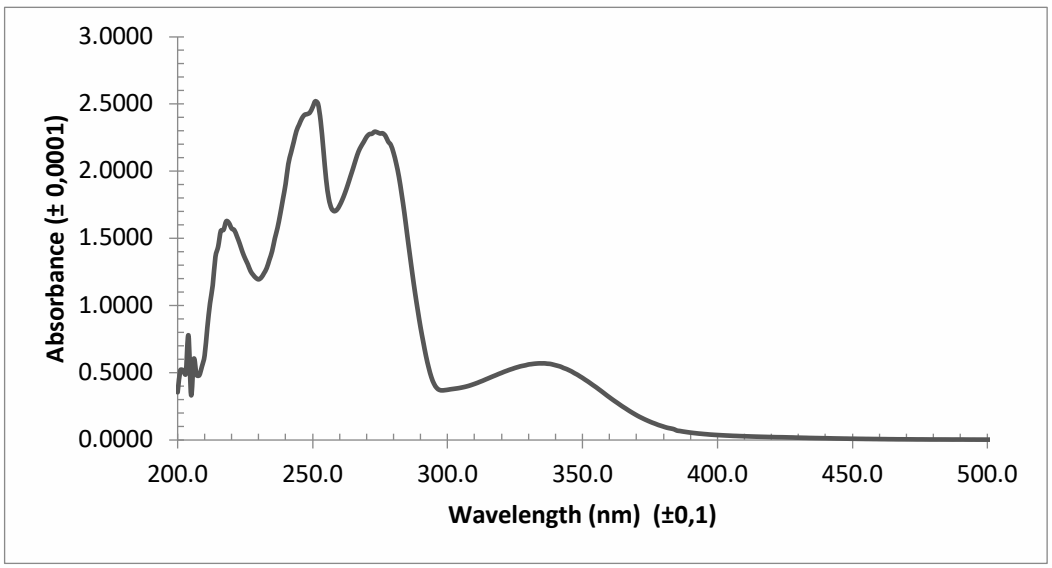
2-(2-nitrophenoxy)-1,4-naphthoquinone **50** ^{1}H NMR



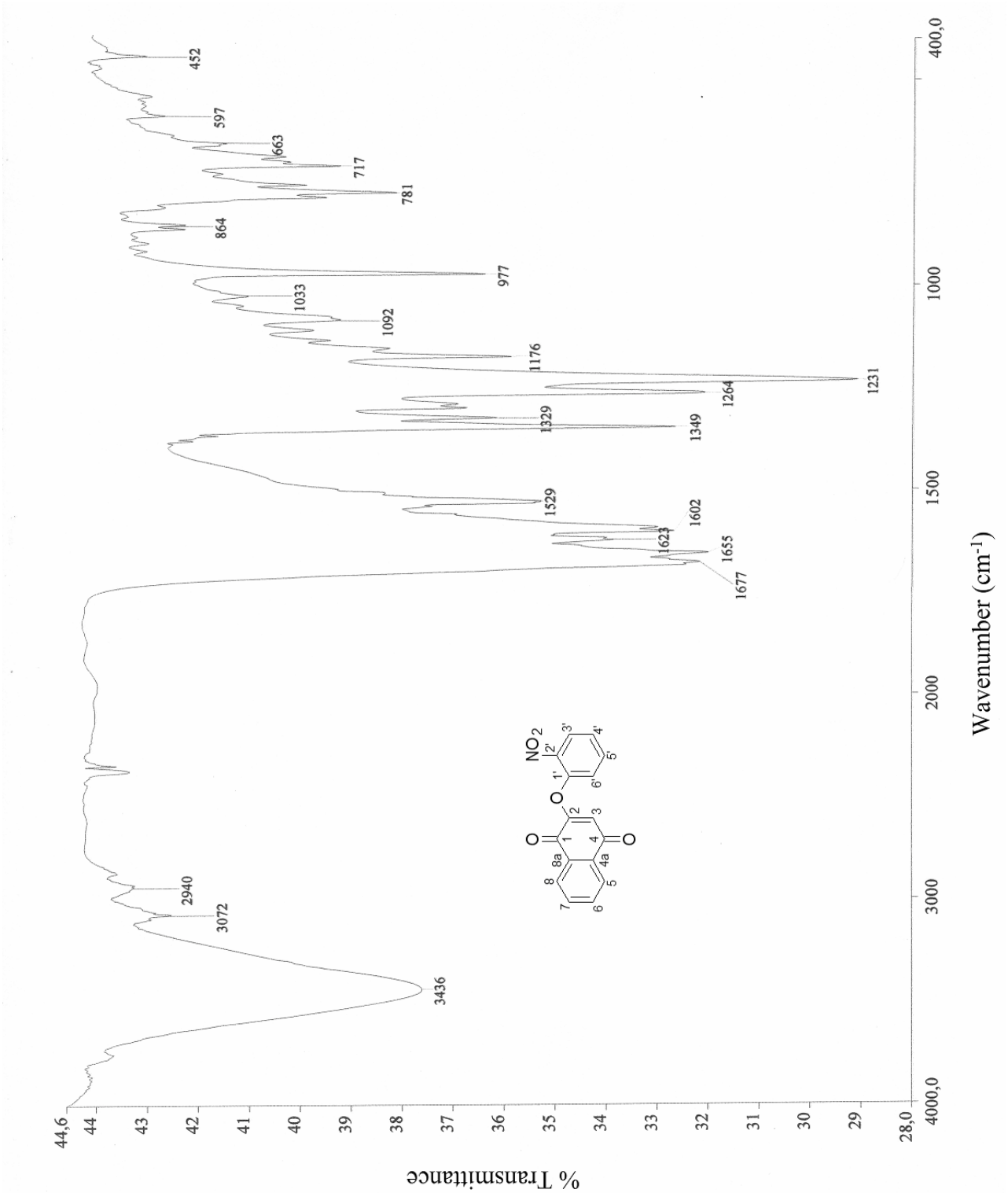
2-(2-nitrophenoxy)-1,4-naphthoquinone **50** ^{13}C NMR



2-(2-nitrophenoxy)-1,4-naphthoquinone **50** UV-Vis (MeOH)



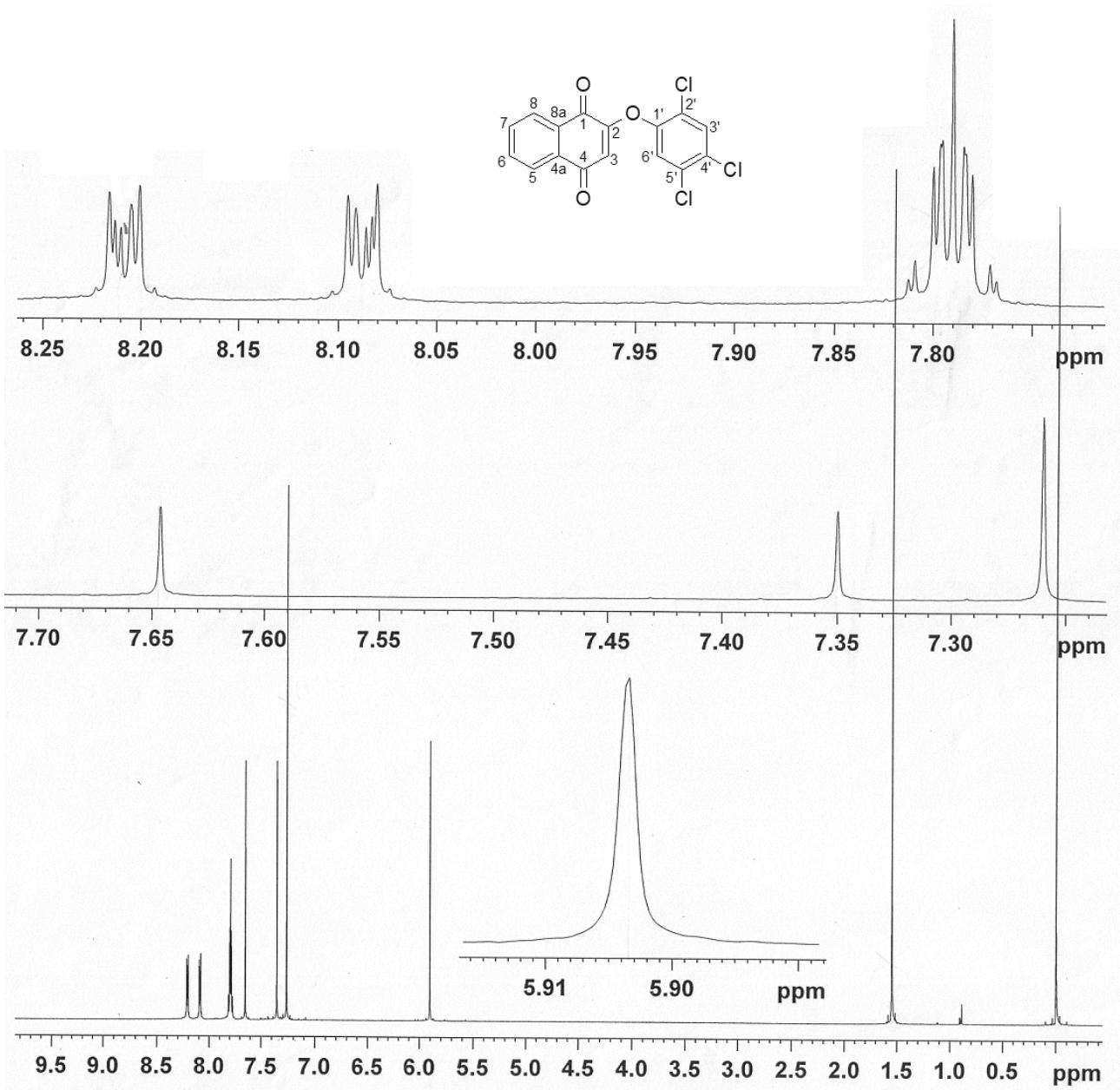
2-(2-nitrophenoxy)-1,4-naphthoquinone **50** IR (KBr pellet)



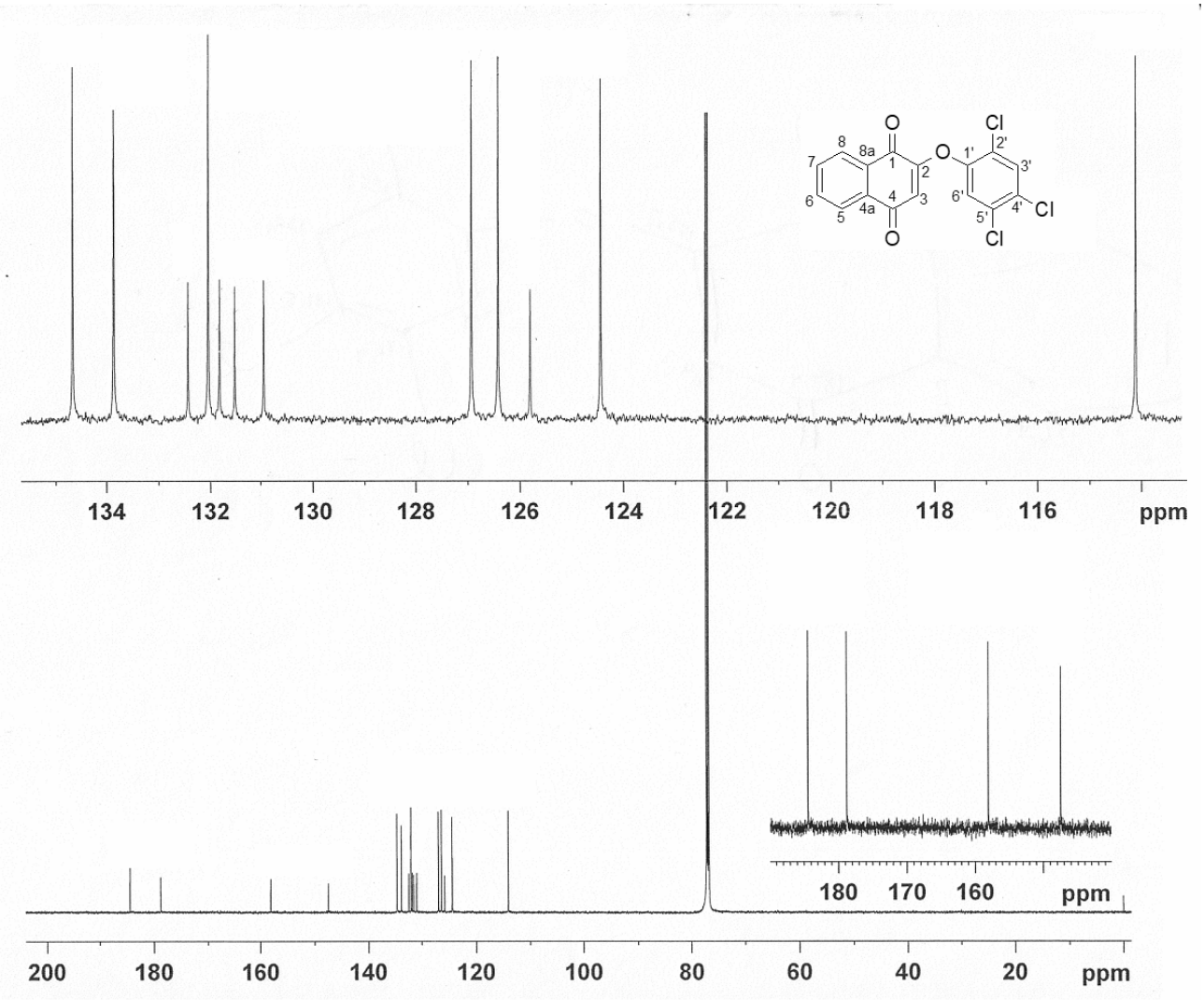
2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51**

51 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration and recrystallization, both with n-heptane. Yield 92 mg (26%), yellow needles, mp = (158.0 – 159.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.21 (1H, dd, *J* = 2.5 Hz, *J* = 7.6 Hz, ArH), 8.09 (1H, dd, *J* = 2.5 Hz, *J* = 7.6 Hz, ArH), 7.79 (2H, m, ArH), 7.65 (1H, s, ArH), 7.35 (1H, s, ArH), 5.93 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.4, 178.8, 158.1, 147.5, 134.7, 133.9, 132.4, 132.0, 131.8, 131.5, 131.0, 126.9, 126.4, 125.8, 124.4, 114.1. IR (KBr pellet) cm^{-1}: 3077, 1686, 1655, 1624, 1466, 1264, 1180, 755. UV-Vis (MeOH) nm: 217, 249 (max), 269, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_8O_3Cl_3$: 352.9539; found: 352.9547. Purity: 98.7%. MIC (µM): >2000 (*S. aureus*), >2000 (*C. albicans*), >2000 (*E. coli*).

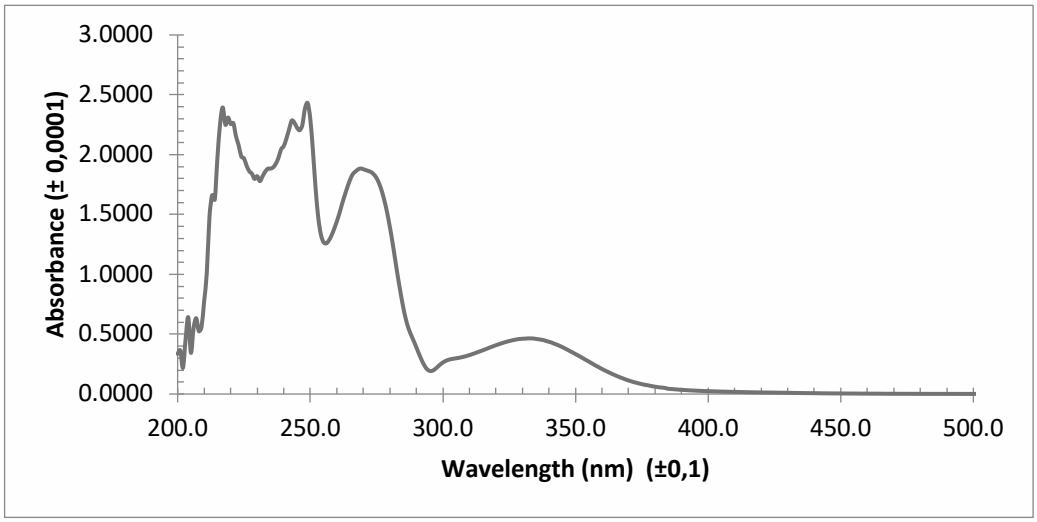
2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51** ^{1}H NMR



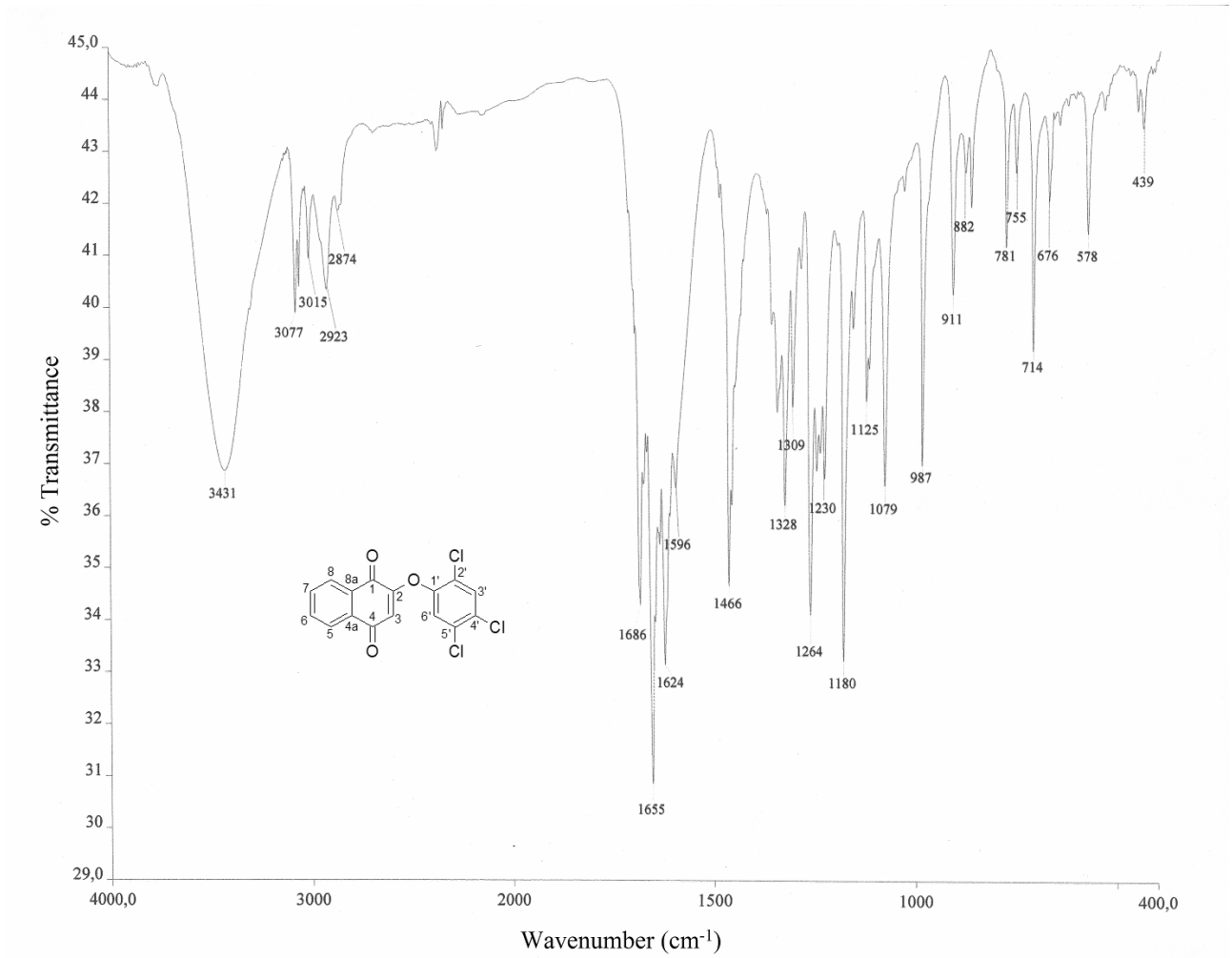
2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51** ^{13}C NMR



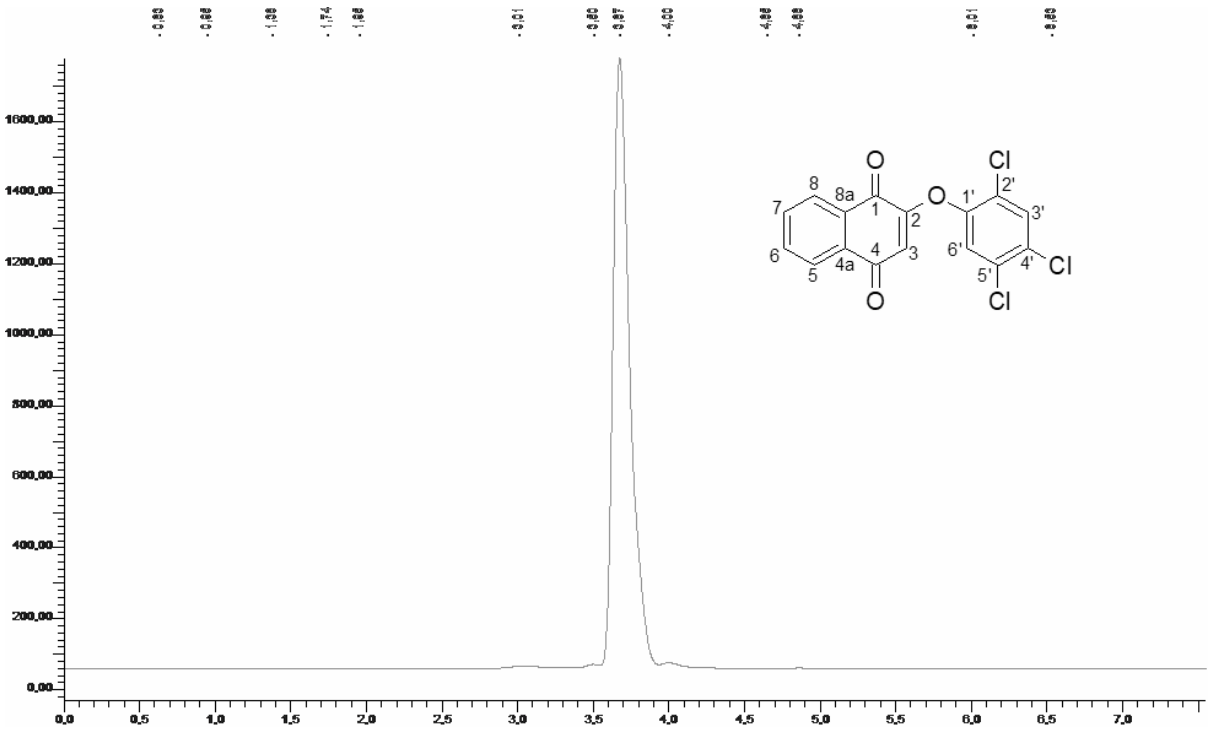
2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51** UV-Vis (MeOH)



2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51** IR (KBr pellet)



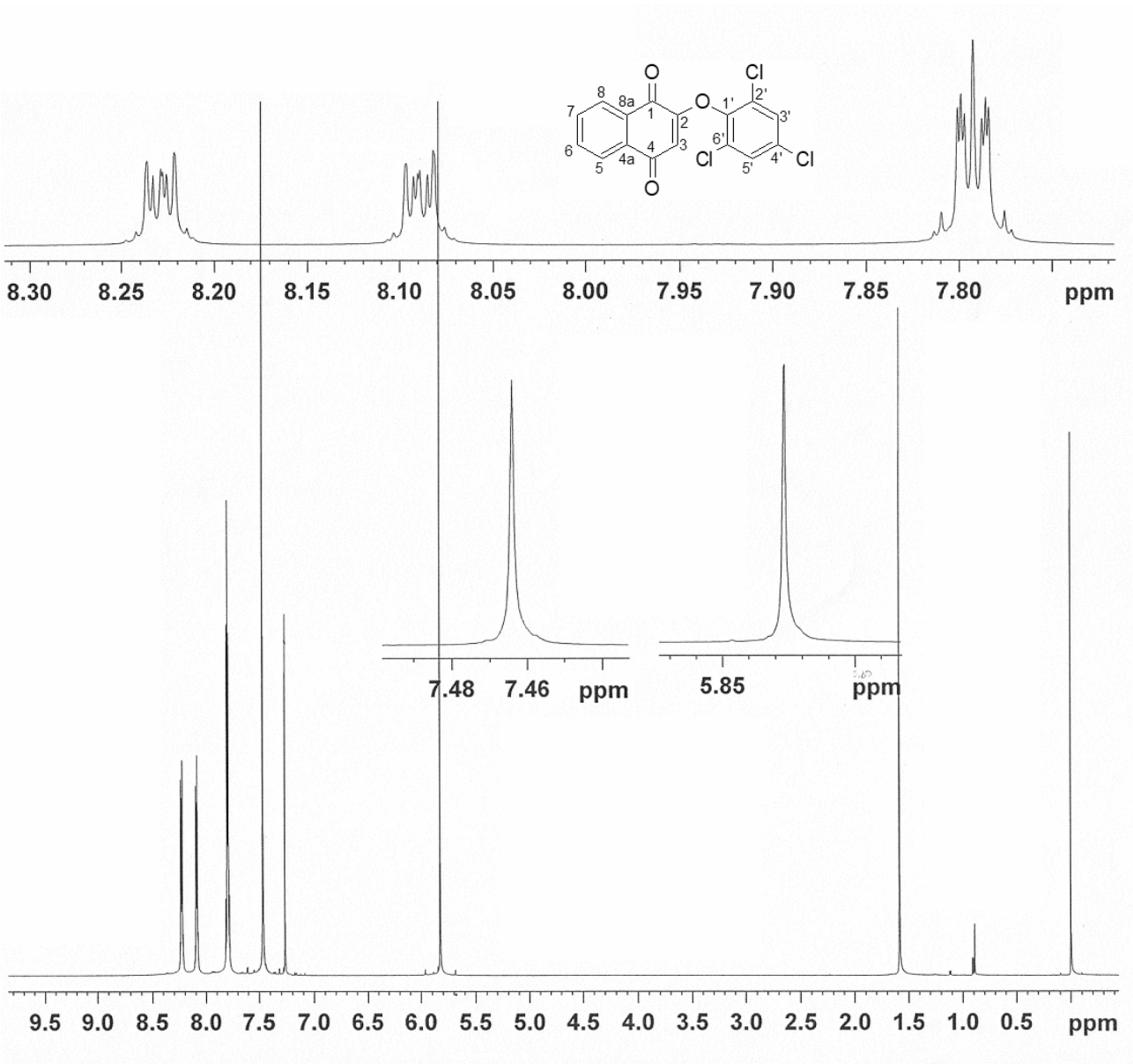
2-(2,4,5-trichlorophenoxy)-1,4-naphthoquinone **51** HPLC chromatogram (274 nm, 100% MeCN)



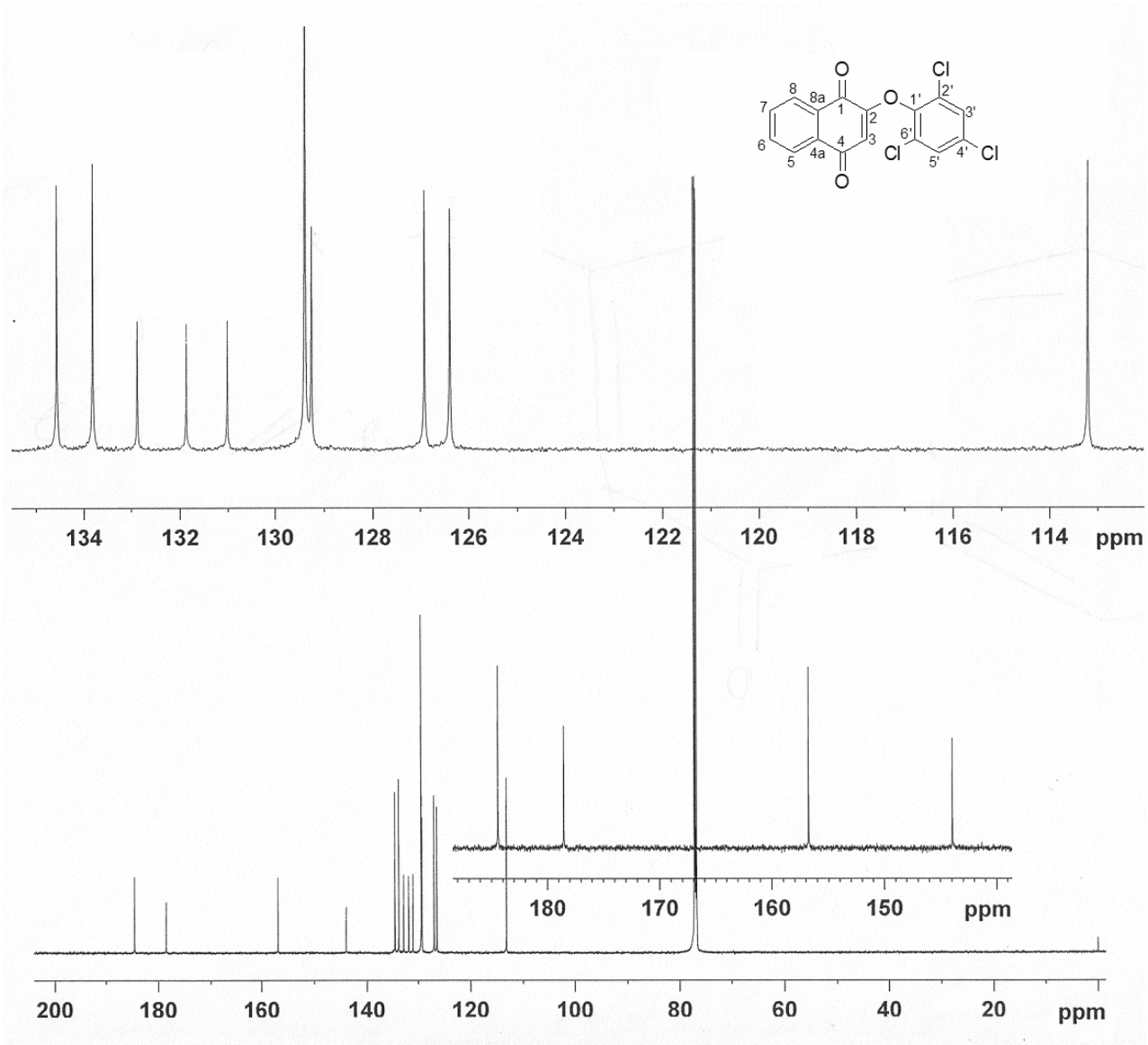
2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52**

52 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with MTBE and recrystallization with isooctane. Yield 155 mg (44%), yellow needles, mp = (163.0 – 164.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 8.23 (1H, m, ArH), 8.08 (1H, m, ArH), 7.78 (2H, m, ArH), 7.46 (2H, s, ArH), 5.82 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.4, 178.5, 156.8, 143.9, 134.6, 133.8, 132.9, 131.9, 131.0, 129.4, 129.3, 126.9, 126.4, 113.2. IR (KBr pellet) cm^{-1}: 3070, 1684, 1654, 1618, 1444, 1260, 1243, 972. UV-Vis (MeCN) nm: 246 (max), 270, 335. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_8O_3Cl_3$: 352.9537; found: 352.9539. Purity: 99.3%. MIC (µM): >2000 (*S. aureus*), >2000 (*C. albicans*), >2000 (*E. coli*).

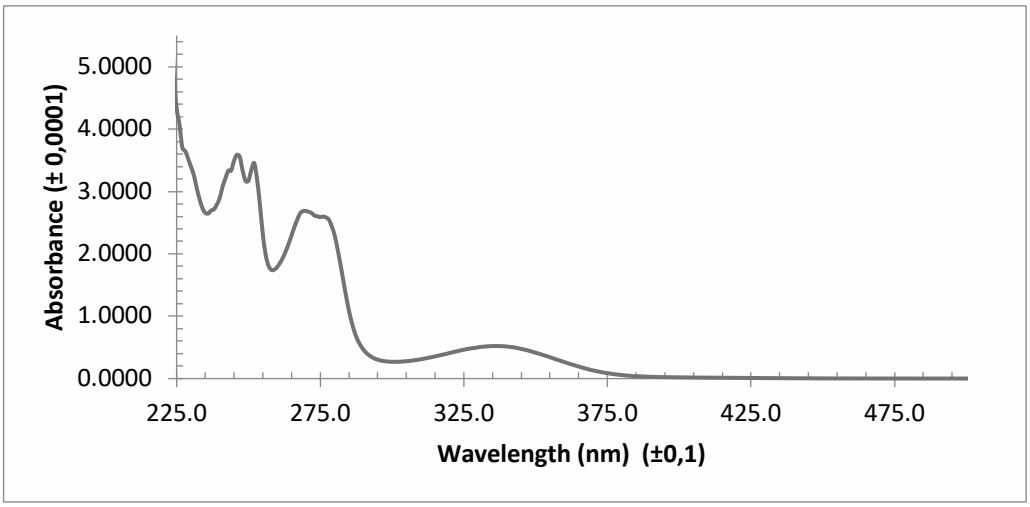
2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52** ^{1}H NMR



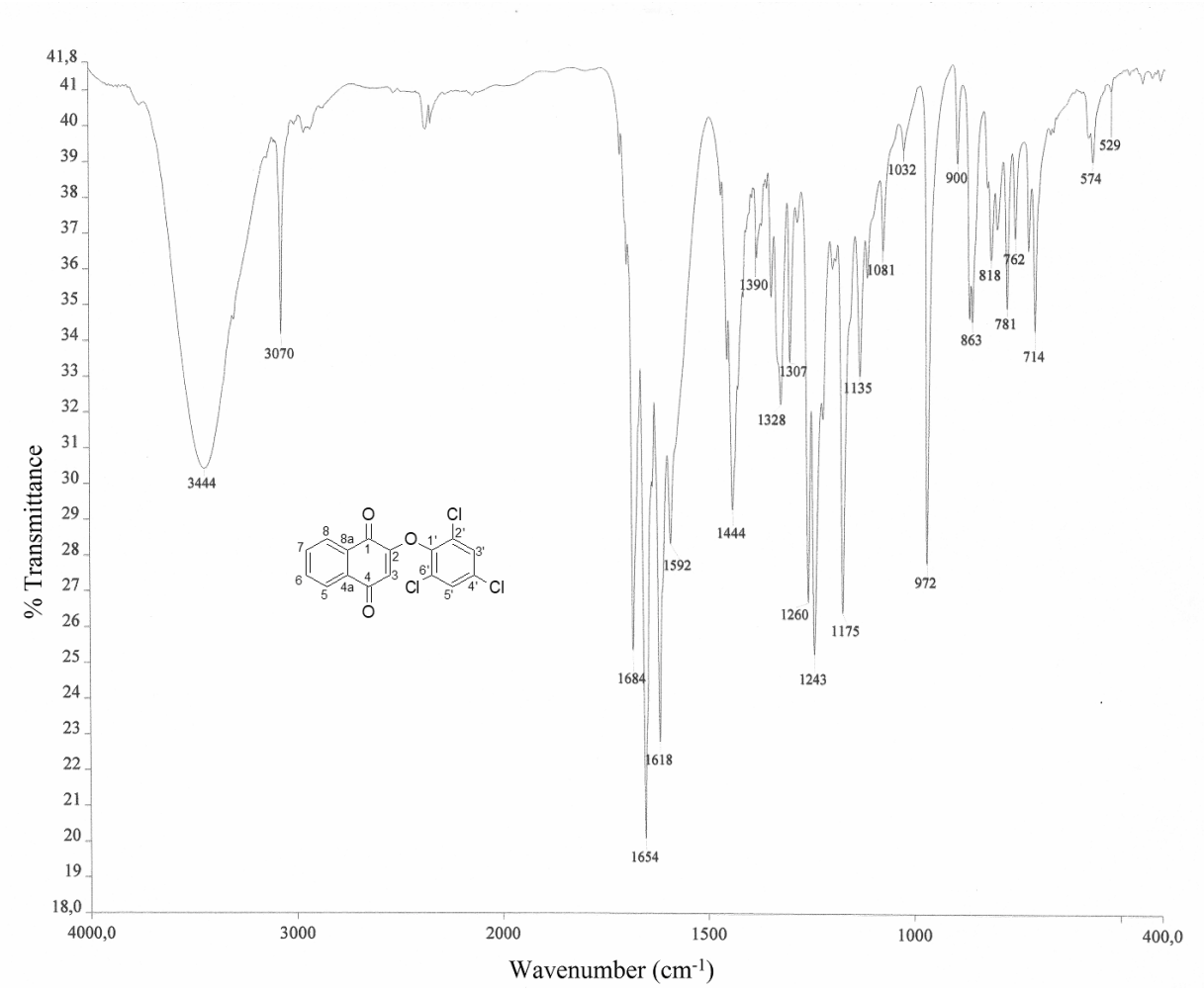
2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52** ^{13}C NMR



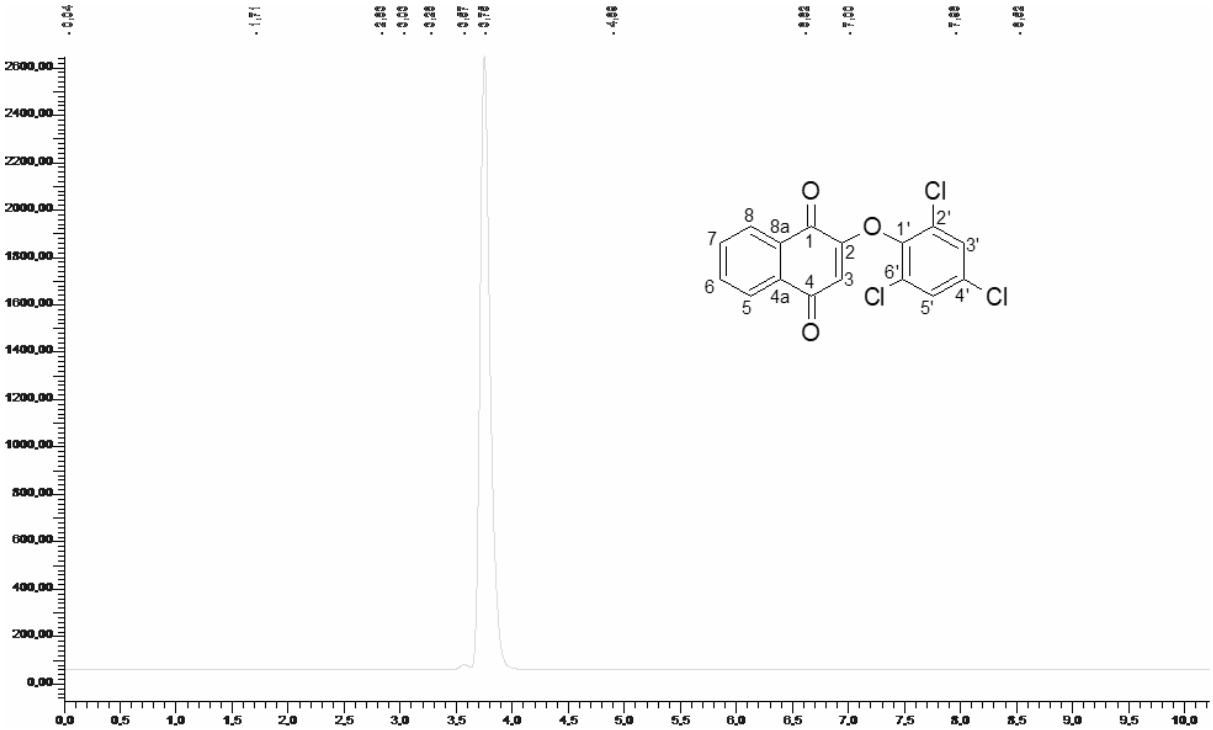
2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52** UV-Vis (MeCN)



2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52** IR (KBr pellet)



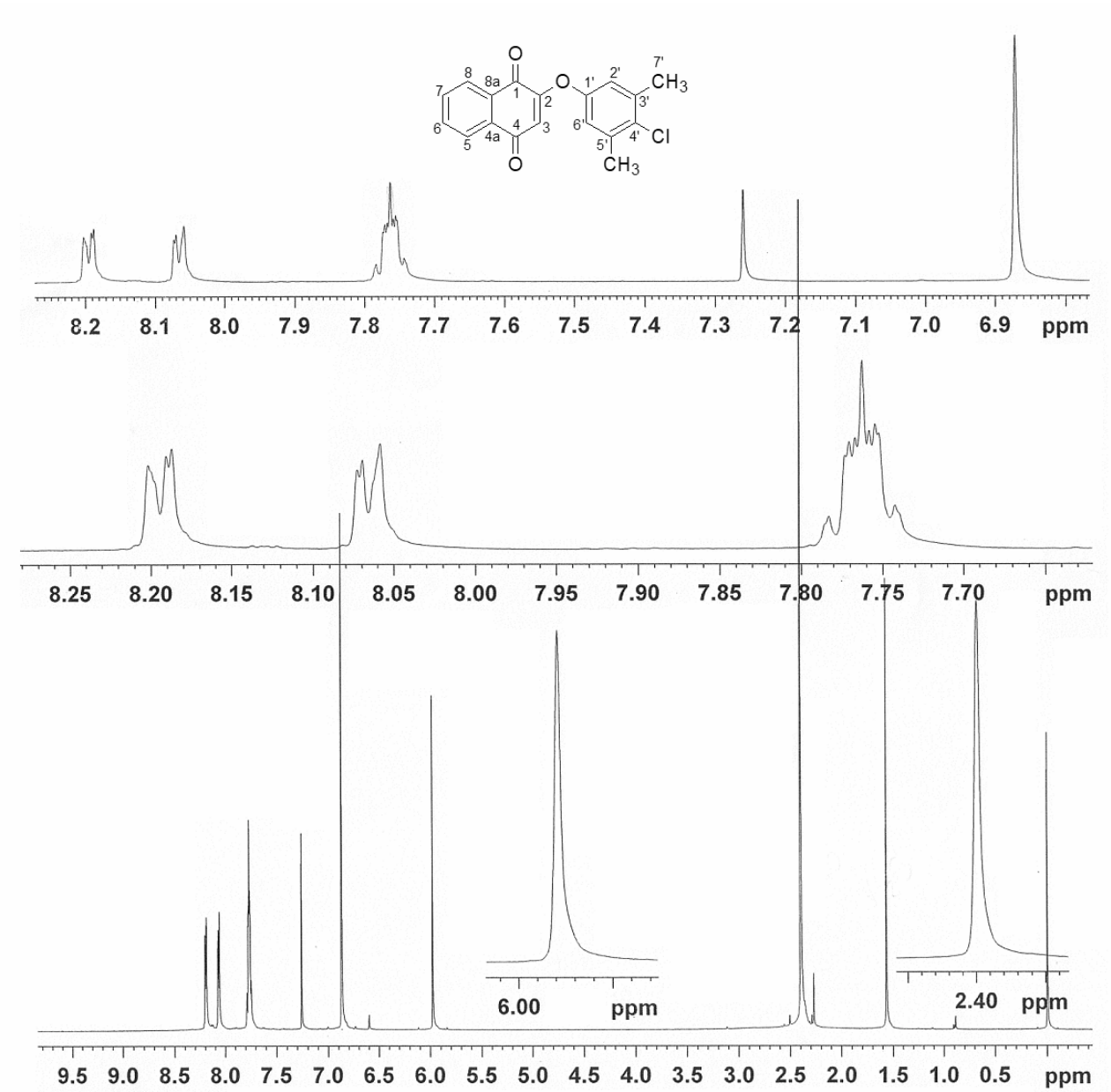
2-(2,4,6-trichlorophenoxy)-1,4-naphthoquinone **52** HPLC chromatogram (270 nm, 100% MeCN)



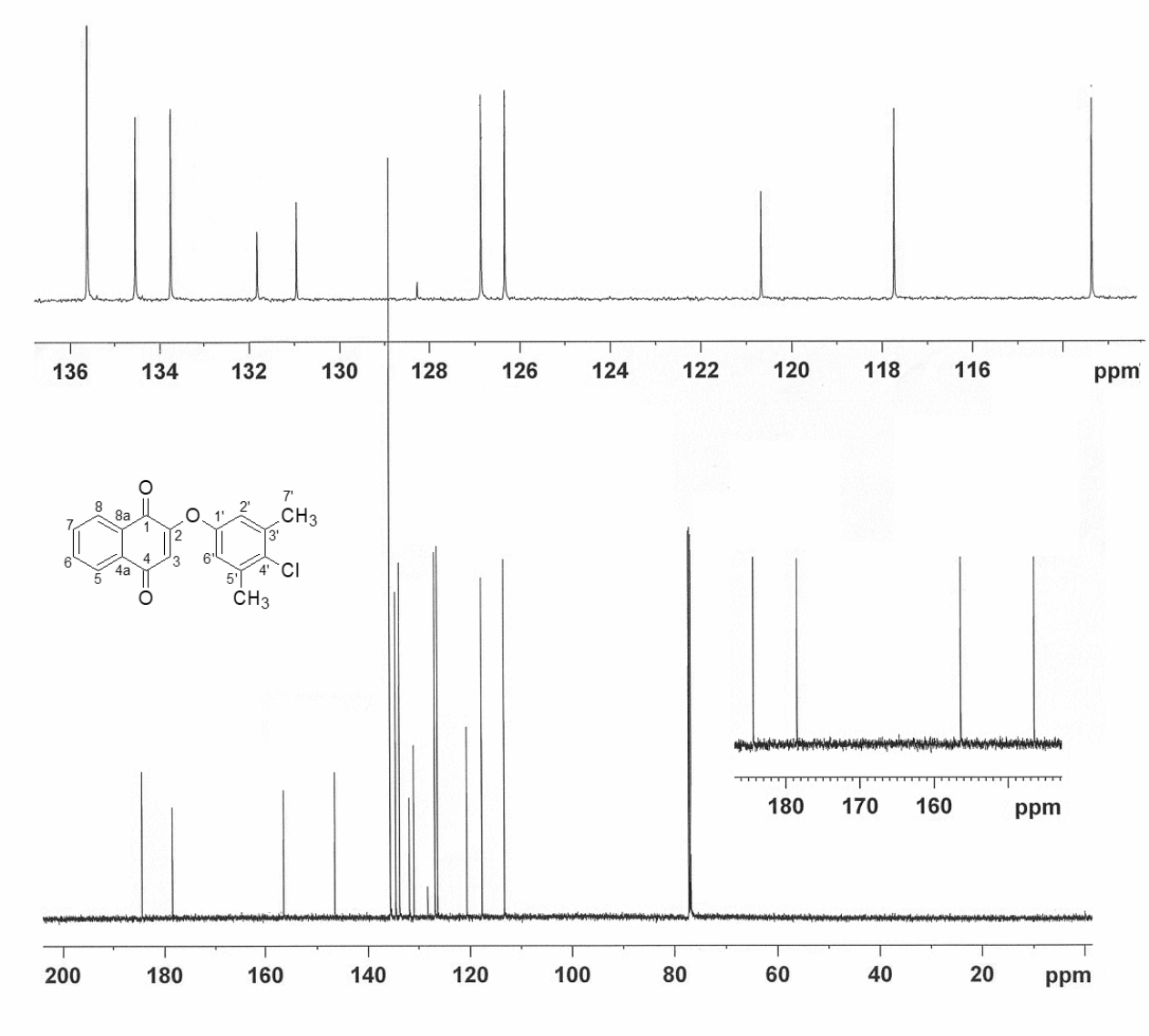
2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone 53

53 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with isooctane, cold base wash with NaOH 0.5 mol/L and CCl_4 as solvent, and recrystallization with isooctane. Yield 164 mg (53%), yellow-orange crystals, mp = (144.0 – 145.5) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, dd, J_{ortho} = 7.3 Hz, ArH), 8.07 (1H, dd, J_{ortho} = 7.3 Hz, ArH), 7.76 (2H, m, ArH), 6.88 (2H, s, ArH), 5.98 (1H, s, ArH), 2.40 (6H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.0, 179.8, 160.4, 150.3, 138.7, 134.5, 133.6, 132.4, 131.9, 131.1, 126.8, 126.2, 120.7, 113.5, 20.9. IR (KBr pellet) cm^{-1}: 3068, 2953, 2931, 1686, 1648, 1615, 1596, 1259, 1200, 777. UV-Vis (MeOH) nm: 201, 210 (max), 248, 273, 331. TOF-MS: m/z $[M+H]^+$ calc for $C_{18}H_{14}O_3Cl$: 313.0631; found: 313.0631. Purity: 98.0%. MIC (µM): >3000 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

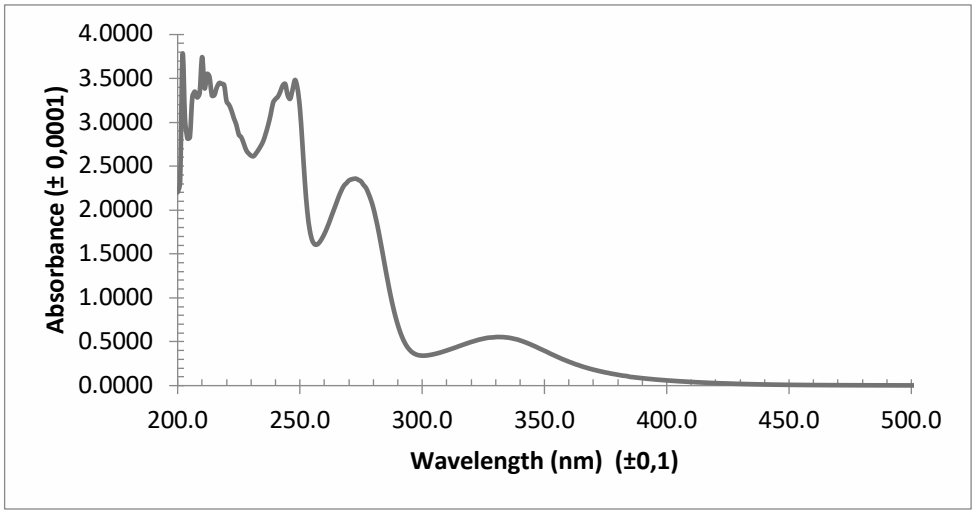
2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone **53** ^{1}H NMR



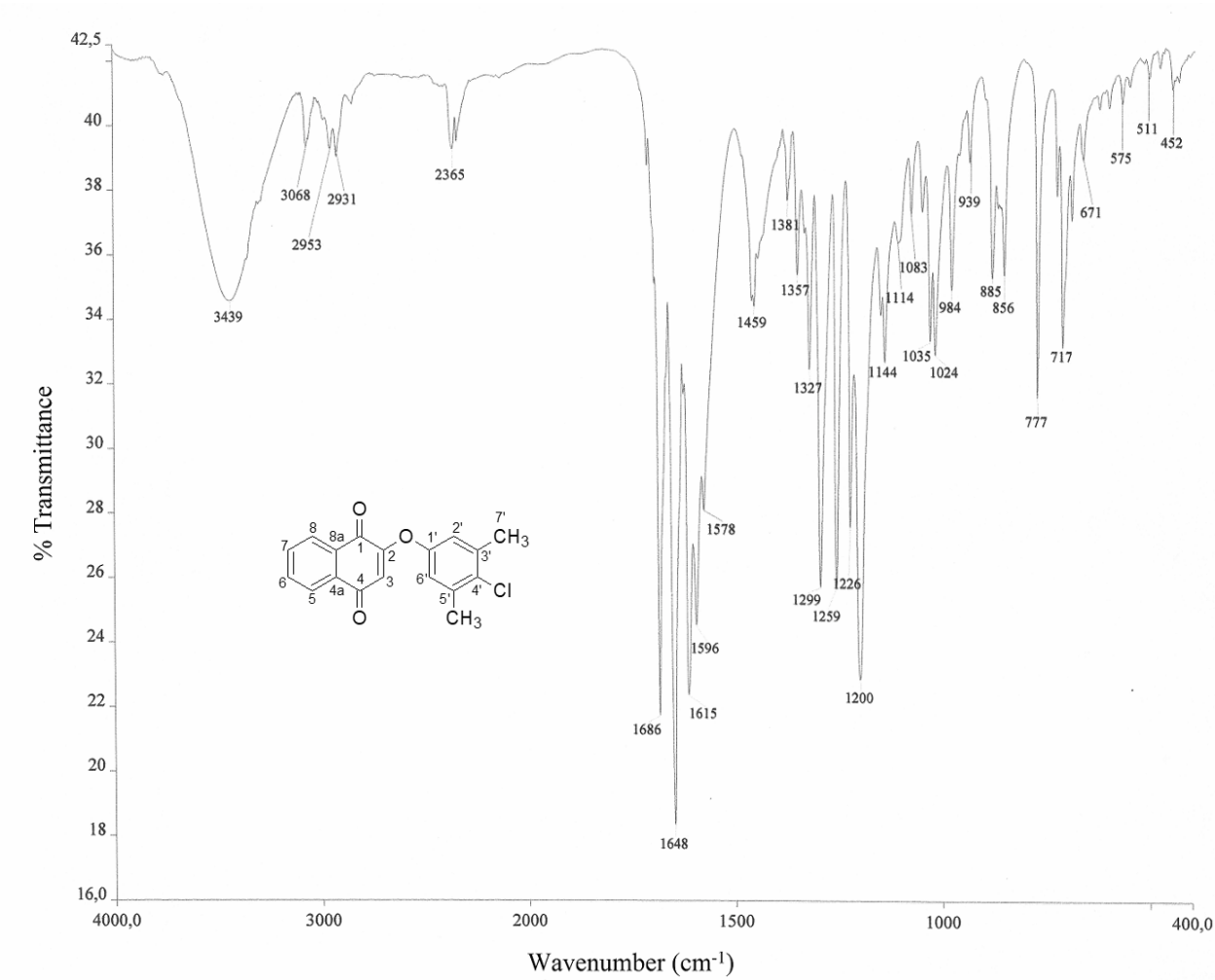
2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone **53** ^{13}C NMR



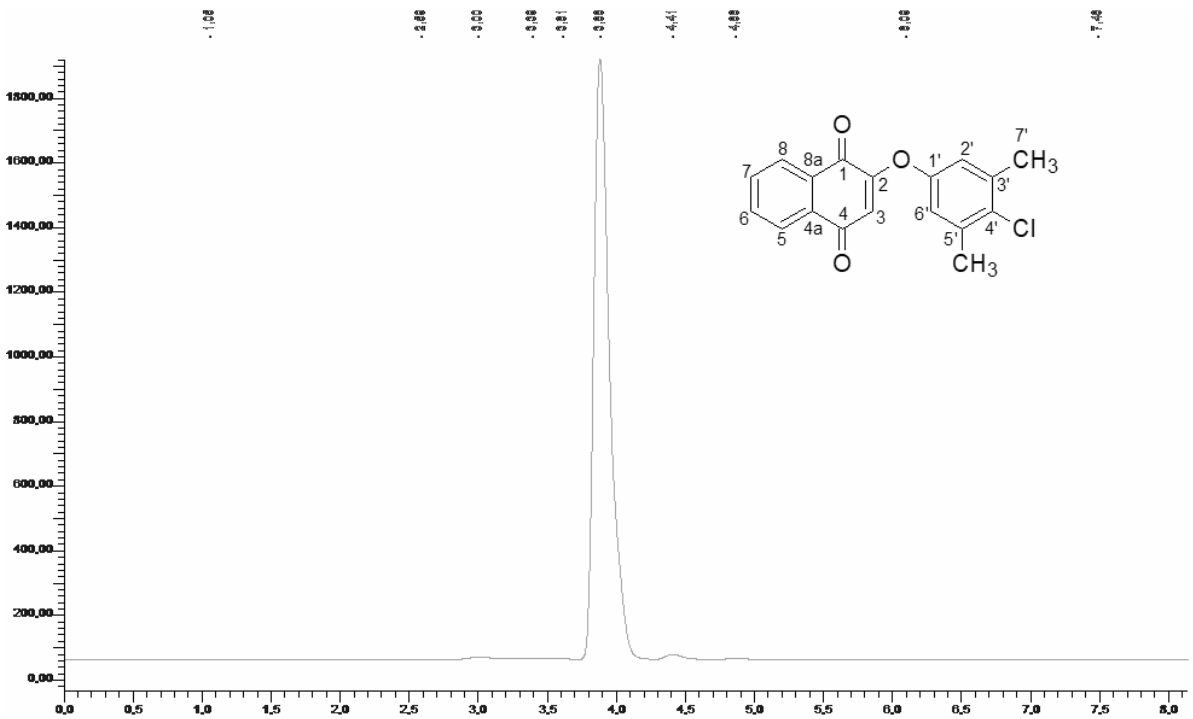
2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone **53** UV-Vis (MeOH)



2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone **53** IR (KBr pellet)



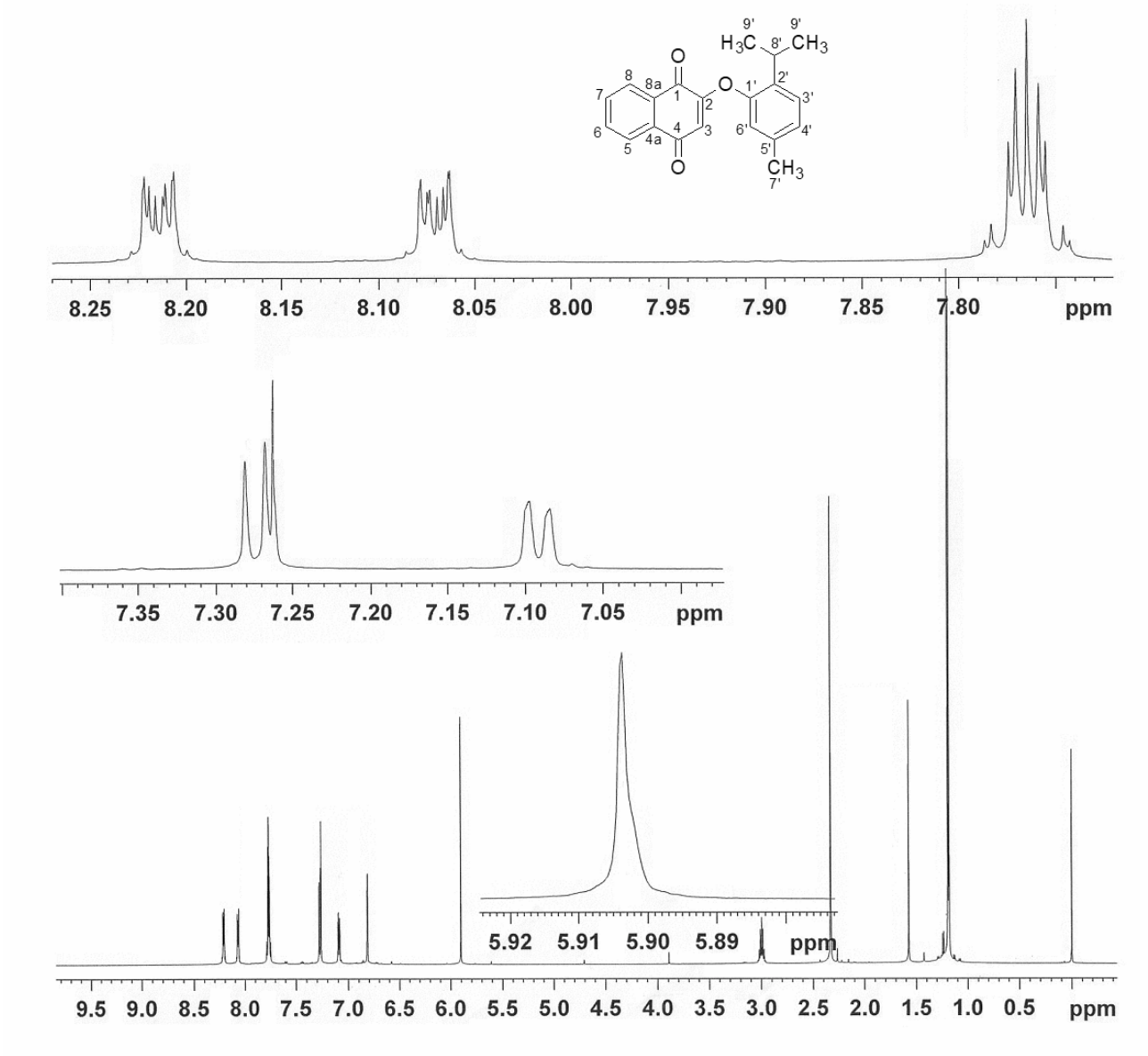
2-(4-chloro-3,5-dimethylphenoxy)-1,4-naphthoquinone **53** HPLC chromatogram (270 nm, 100% MeCN)



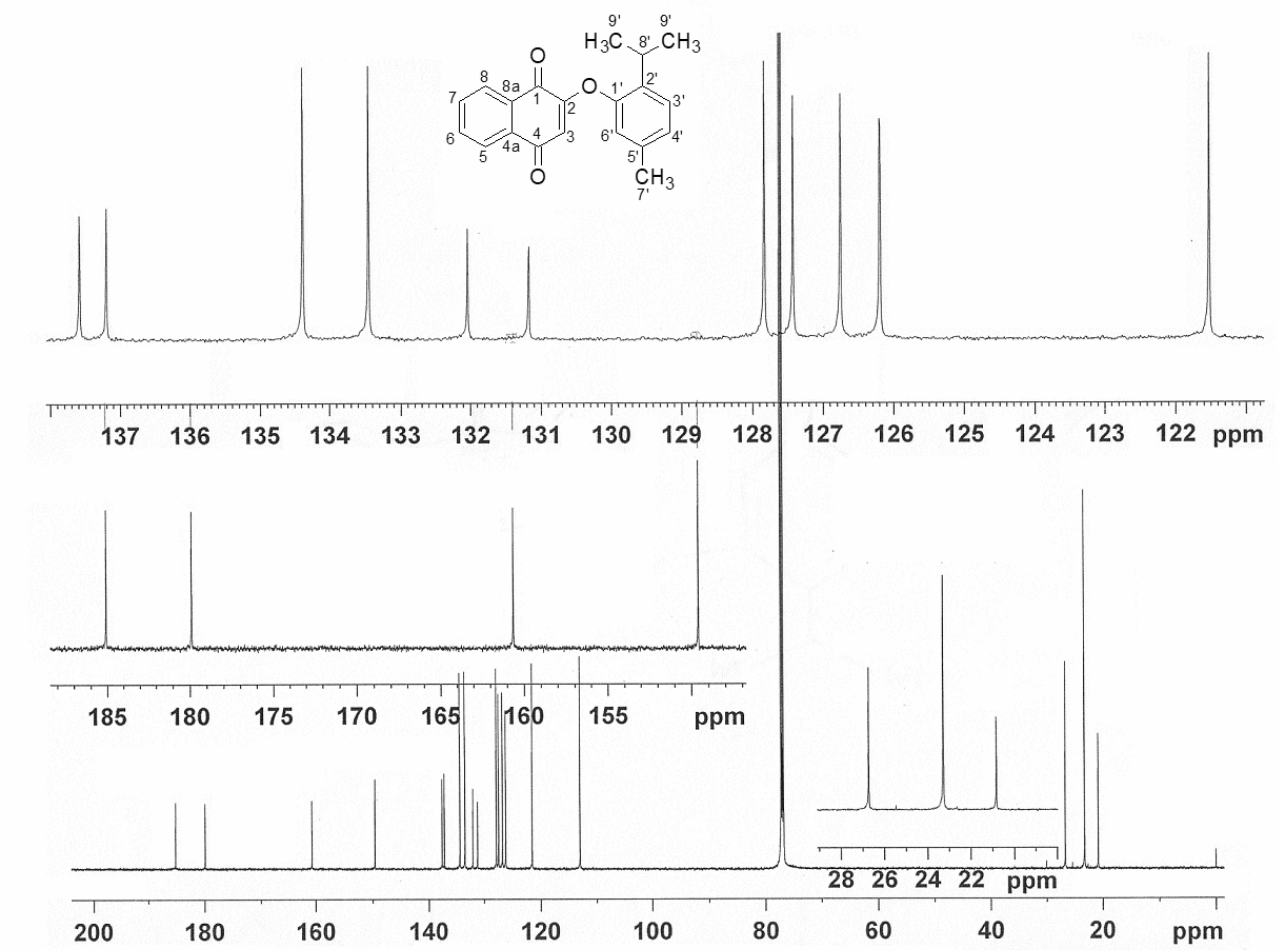
2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone 54

54 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with isooctane, cold base wash with NaOH 0.5 mol/L and CCl_4 as solvent, and recrystallization with isooctane. Yield 178 mg (58%), yellow-orange pellets, mp = (97.0 – 99.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.21 (1H, m, ArH), 8.07 (1H, m, ArH), 7.76 (2H, m, ArH), 7.27 (1H, d, J_{ortho} = 7.4 Hz, ArH), 7.09 (1H, d, J_{ortho} = 8.4 Hz, ArH), 6.81 (1H, d, ArH), 5.93 (1H, s, ArH), 3.00 (1H, m, CH), 2.35 (3H, s, CH_3), 1.20 (6H, d, -CH(C**H₃**)$_2$). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.1, 179.9, 160.6, 149.6, 137.6, 137.2, 134.4, 133.5, 132.0, 131.2, 127.8, 127.4, 126.0, 126.2, 121.5, 113.0, 26.7, 23.3, 20.8. IR (KBr pellet) cm^{-1}: 3071, 2953, 1685, 1654, 1607, 1577, 1262, 1194. UV-Vis (MeOH) nm: 218, 249 (max), 272, 332. TOF-MS: m/z [M+H]$^+$ calc for $C_{20}H_{19}O_3$: 307.1334; found: 307.1339. Purity: 96.2%. MIC (µM): >3000 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

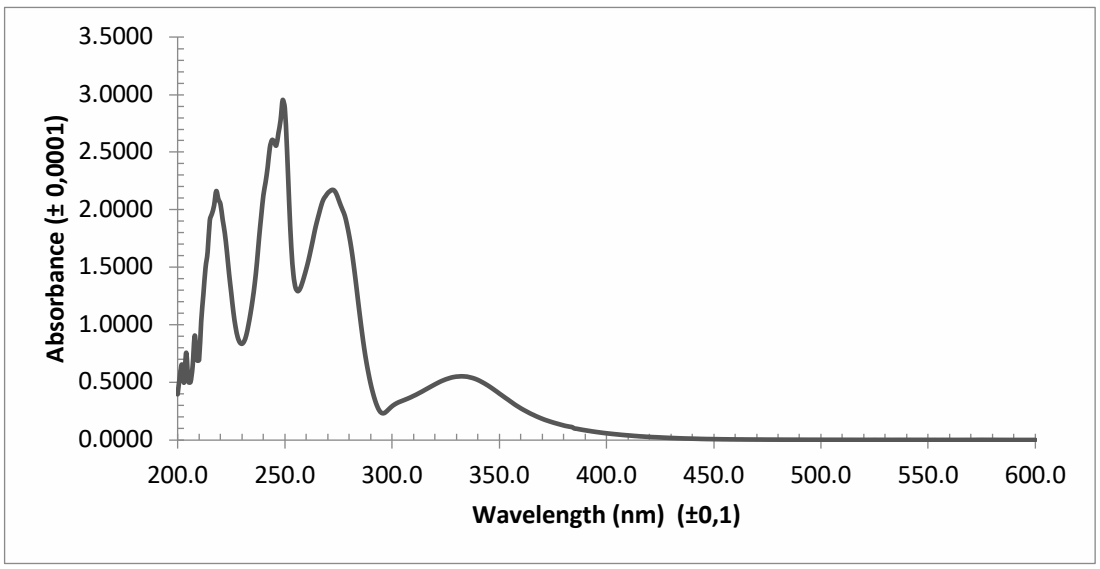
2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone **54** ^{1}H NMR



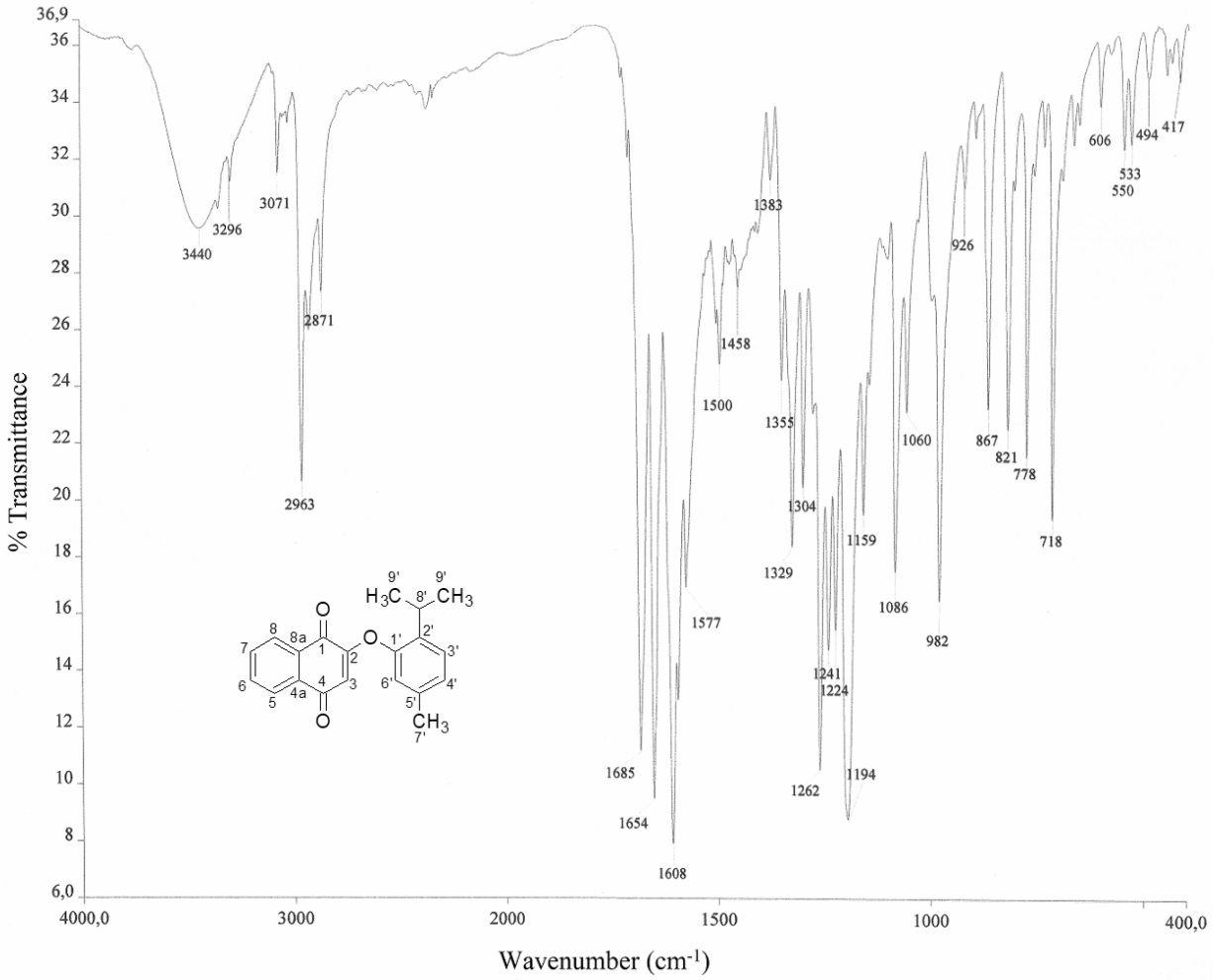
2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone **54** ^{13}C NMR



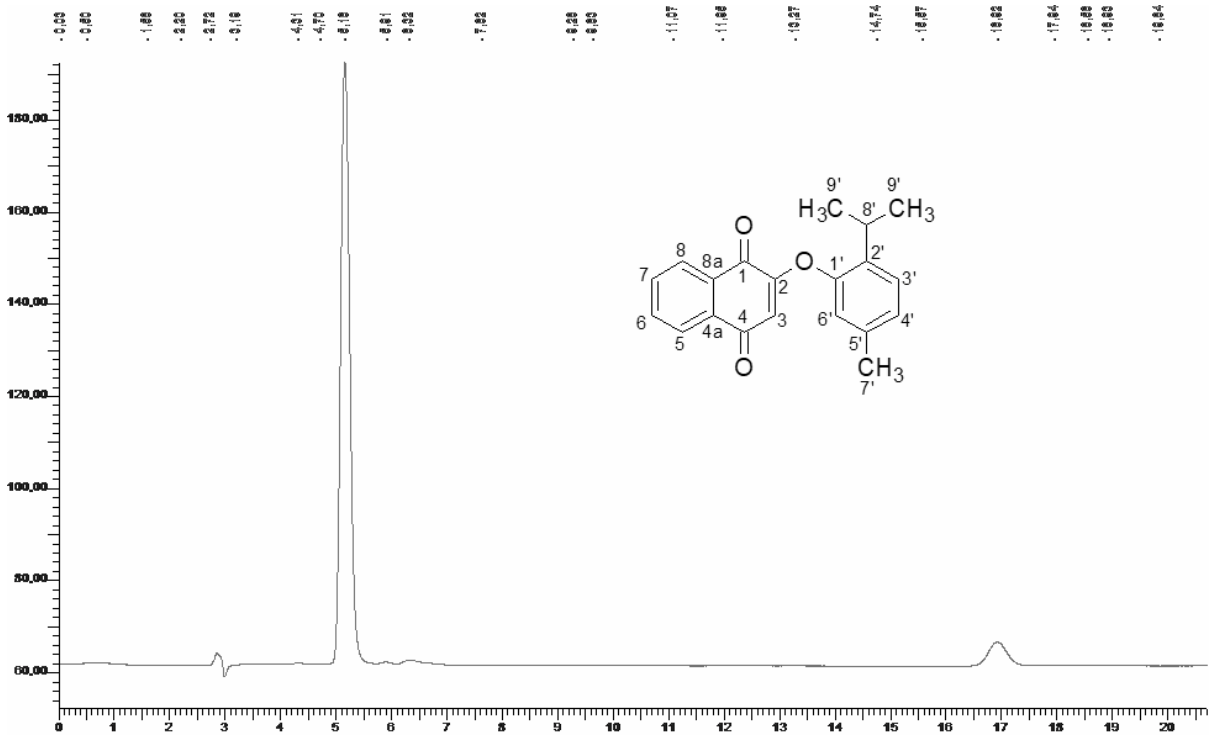
2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone **54** UV-Vis (MeOH)



2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone **54** IR (KBr pellet)



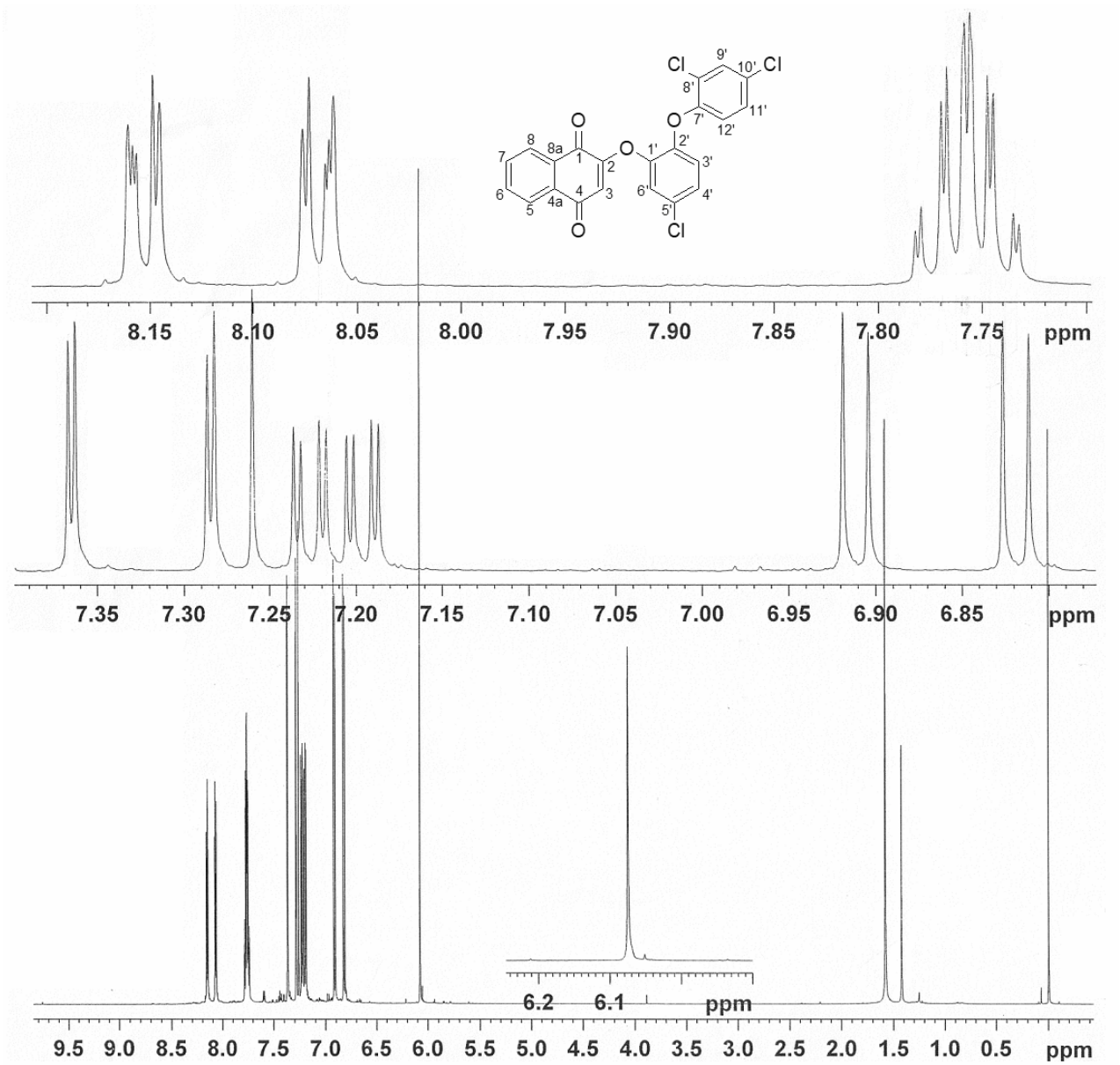
2-(2-isopropyl-5-methylphenoxy)-1,4-naphthoquinone **54** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



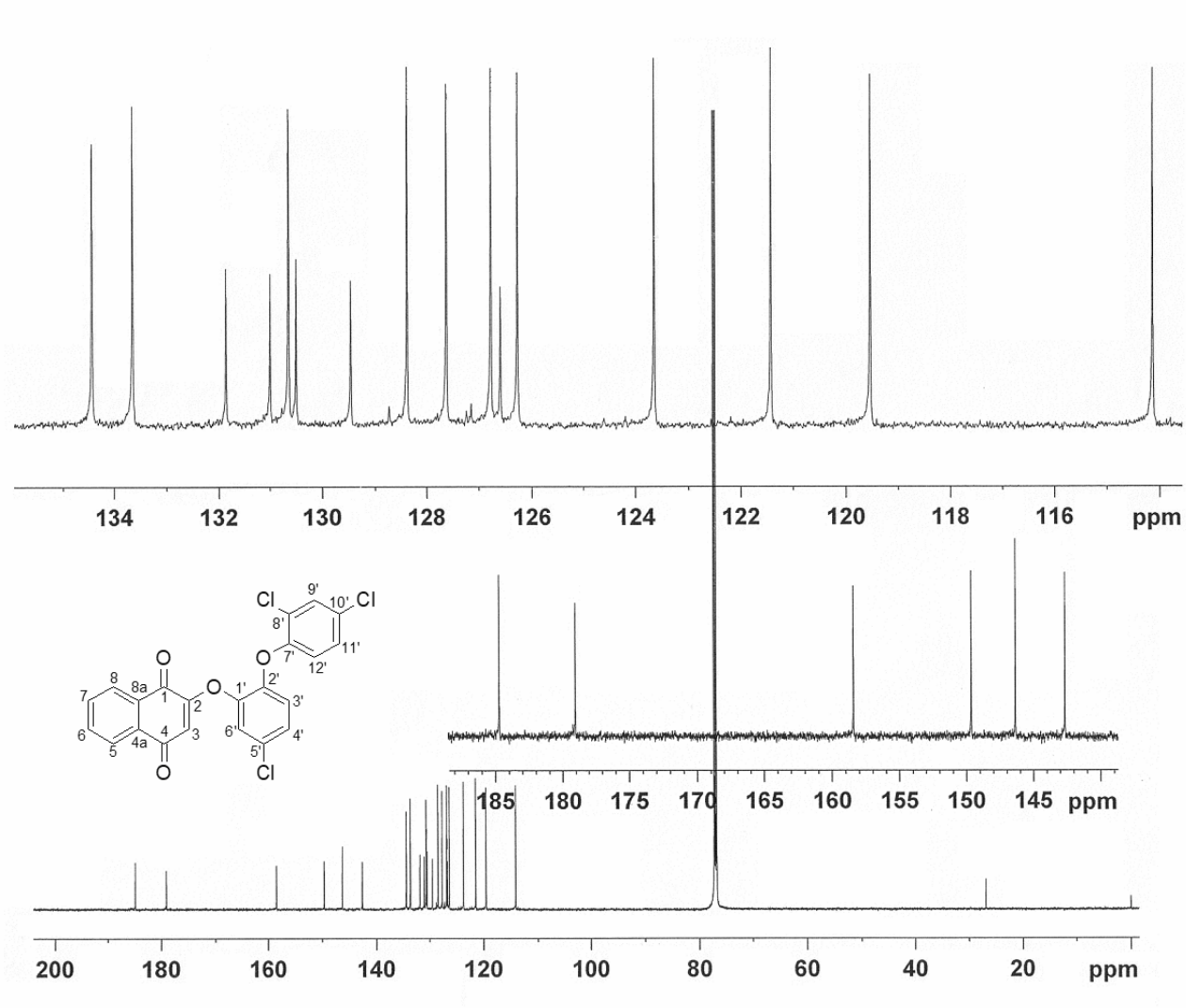
2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55**

55 was obtained according to general procedure I 2.1.1 and purified by hot extraction-filtration with CH_2Cl_2, column chromatography (gradient elution from 100% benzene to 15% diethyl ether/benzene) and cold base wash with NaOH 0.5 mol/L and CH_2Cl_2 as solvent. Yield 178 mg (40%), ochre solid, mp = (116.0 – 119.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.15 (1H, dd, *J* = 1.6 Hz, *J* = 7.1 Hz, ArH), 8.07 (1H, dd, *J* = 1.6 Hz, *J* = 7.1 Hz, ArH), 7.76 (2H, ddd, J_{meta} = 1.6 Hz, J_{ortho} = 7.9 Hz, J_{ortho} = 7.9 Hz, ArH), 7.36 (1H, d, J_{meta} = 1.9 Hz, ArH), 7.28 (1H, d, J_{meta} = 1.9 Hz, ArH), 7.22 (1H, dd, J_{meta} = 1.9 Hz, J_{ortho} = 8.4 Hz, ArH), 7.19 (1H, dd, J_{meta} = 1.9 Hz, J_{ortho} = 8.4 Hz, ArH), 6.91 (1H, d, J_{ortho} = 8.4 Hz, ArH), 6.82 (1H, d, J_{ortho} = 8.4 Hz, ArH), 6.07 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.7, 179.0, 158.4, 149.6, 146.4, 142.6, 134.4, 133.6, 131.9, 131.0, 130.6, 130.5, 129.5, 128.4, 127.6, 126.8, 126.6, 126.3, 123.7, 121.4, 119.5, 114.1. IR (KBr pellet) cm^{-1}: 3067, 1684, 1655, 1619, 1595, 1472, 1260, 1218, 980. UV-Vis (MeCN) nm: 271 (max), 335. TOF-MS: m/z $[M+H]^+$ calc for $C_{22}H_{12}O_4Cl_3$: 444.9801; found: 444.9804. Purity: 99.1%. MIC (μM): 0.34 (*S. aureus*), >2000 (*C. albicans*), 0.56 (*E. coli*).

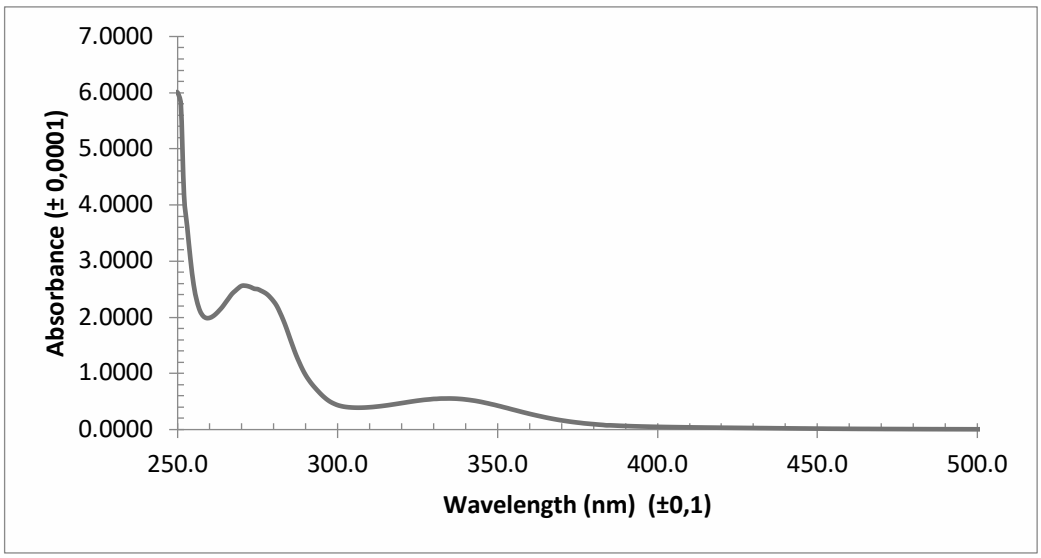
2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55** ^{1}H NMR



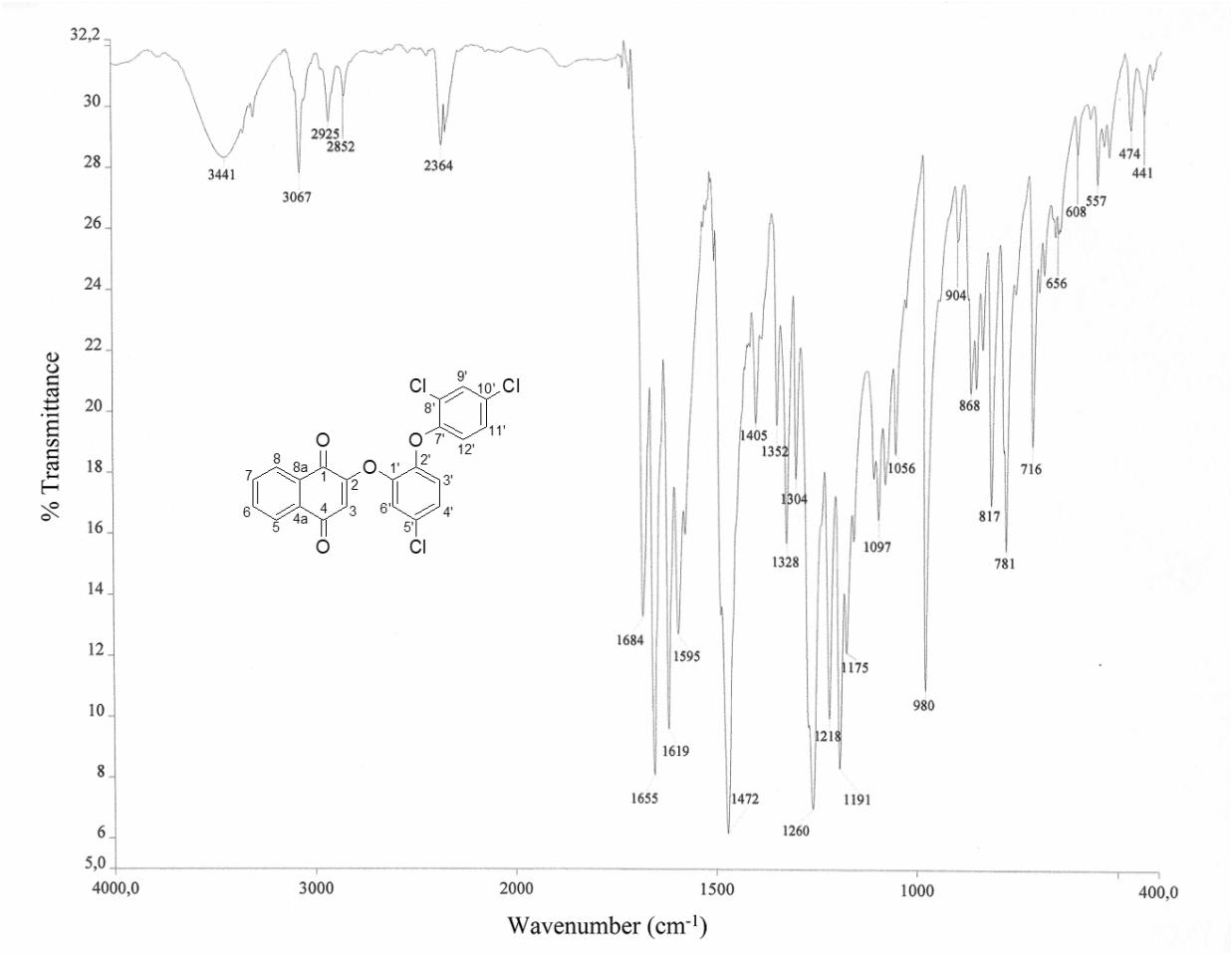
2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55** ^{13}C NMR



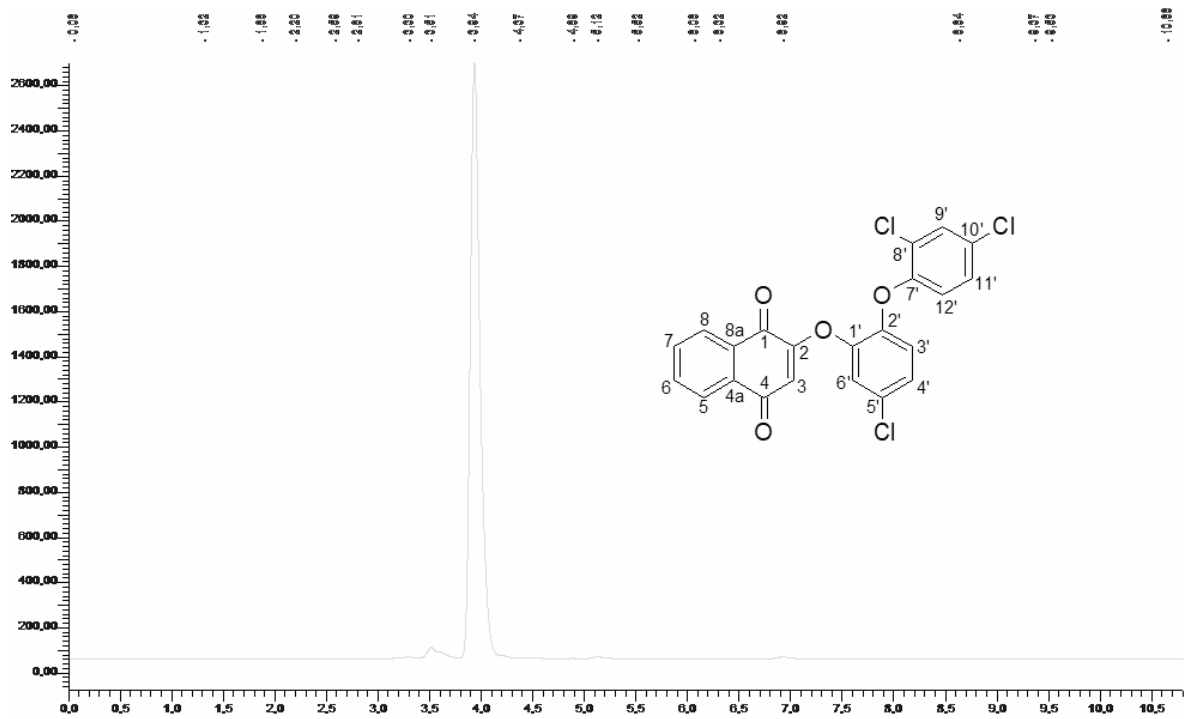
2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55** UV-Vis (MeCN)



2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55** IR (KBr pellet)



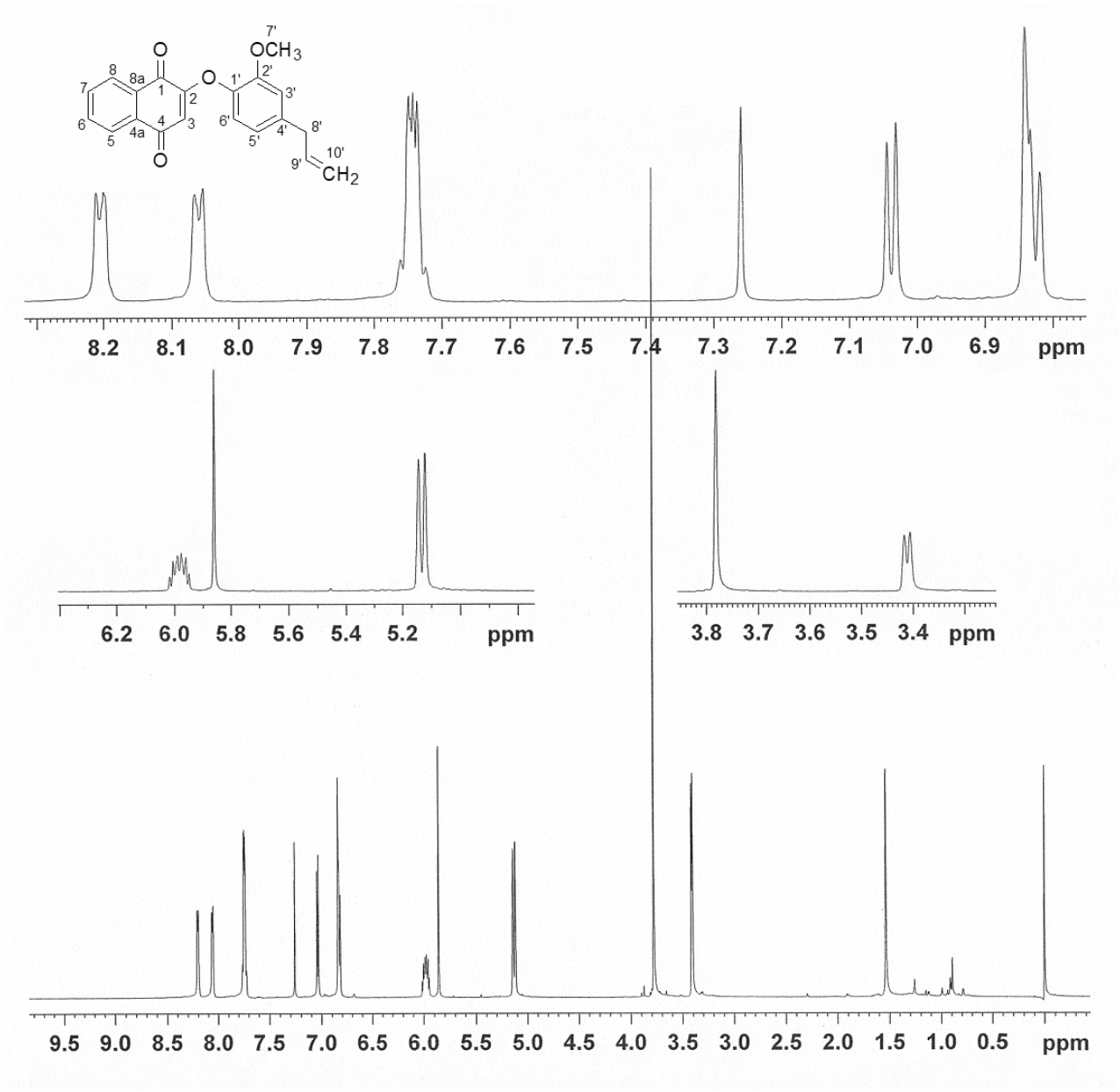
2-(5-chloro-2-(2,4-dichlorophenoxy)phenoxy)-1,4-naphthoquinone **55** HPLC chromatogram (270 nm, 100% MeCN)



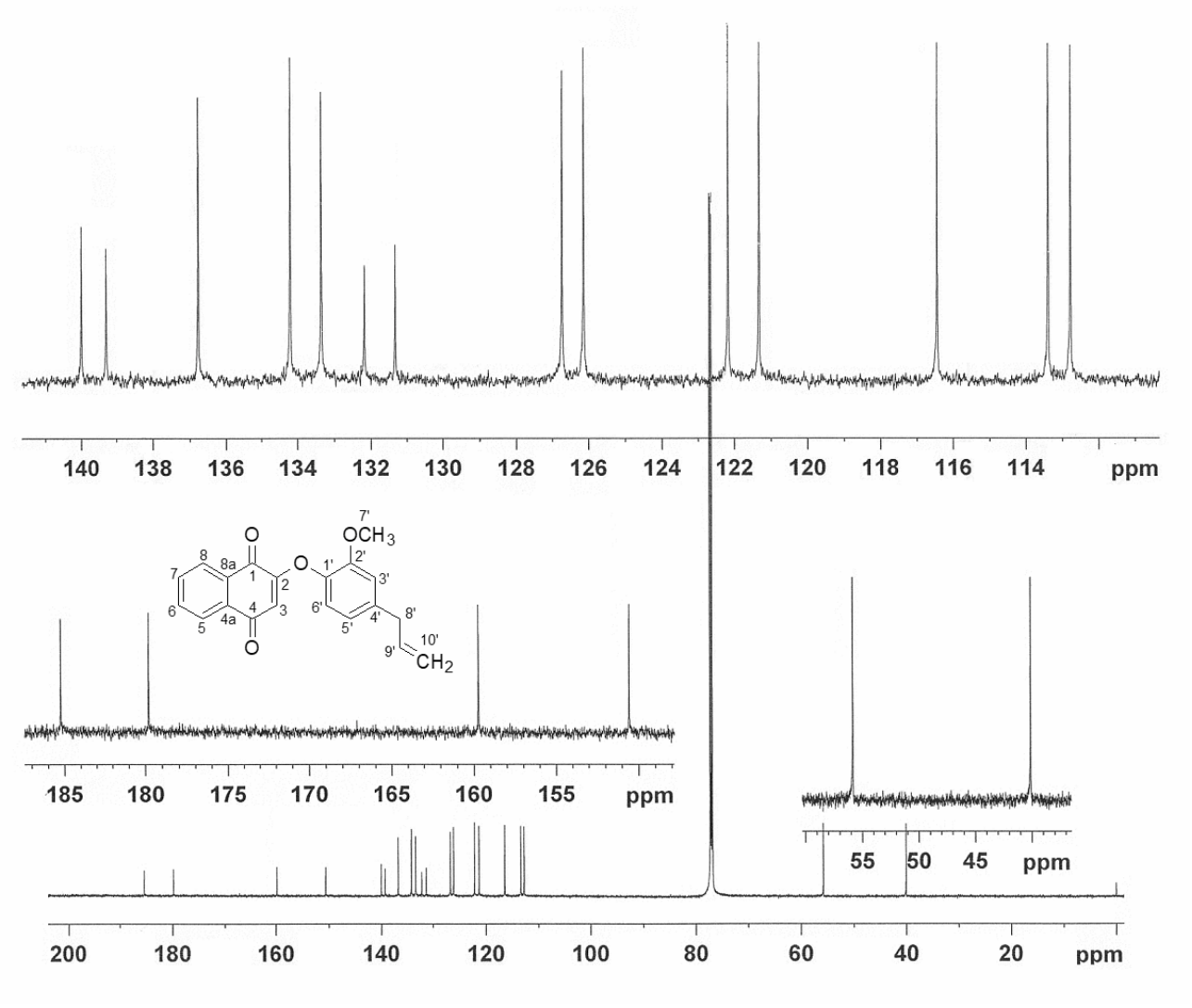
2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56**

56 was obtained according to general procedure I 2.1.1, except that 3.0 g of whole cloves (*Syzygium aromaticum)* were used to give approx. 1.25 mmol of eugenol. The purification included hot extraction-filtration with diethyl ether and recrystallization with isooctane. Yield 35 mg (11%), ochre solid, mp = (75.0 – 77.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, d, *J* = 4.8 Hz, ArH), 8.10 (1H, d, *J* = 4.8 Hz, ArH), 7.80 (2H, m, ArH), 7.04 (1H, d, J_{ortho} = 4.8 Hz, ArH), 6.85 (1H, s, ArH), 6.82 (1H, dd, J_{ortho} = 4.8 Hz , ArH), 5.98 (1H, m, CH), 5.85 (1H, s, ArH), 5.14 (2H, d, *J* = 5.7 Hz, =CH_2), 3.78 (3H, s, CH_3), 3.41 (2H, d, *J* = 6.3 Hz, -CH_2). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.3, 179.8, 159.8, 150.6, 140.0, 139.3, 136.8, 134.2, 133.4, 132.2, 131.3, 126.7, 126.1, 122.2, 121.3, 116.4, 113.4, 112.8, 55.8, 40.1. IR (KBr pellet) cm^{-1}: 3068, 2938, 1683, 1650, 1617, 1596, 1503, 1262, 1210. UV-Vis (MeOH) nm: 219, 249 (max), 271, 332. TOF-MS: m/z $[M+H]^+$ calc for $C_{20}H_{17}O_4$: 321.1127; found: 321.1122. Purity: 97.1%. MIC (µM): 1561 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

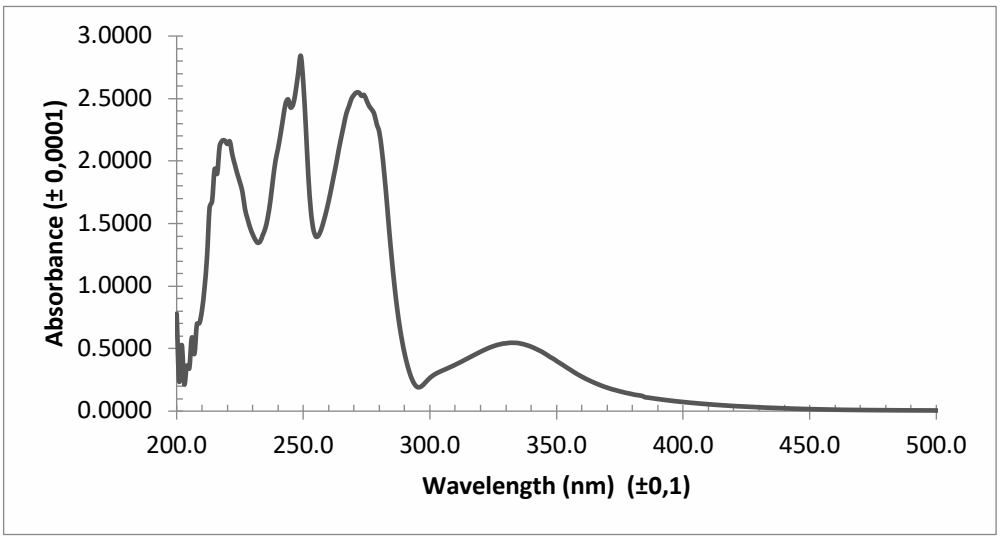
2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56** ^{1}H NMR



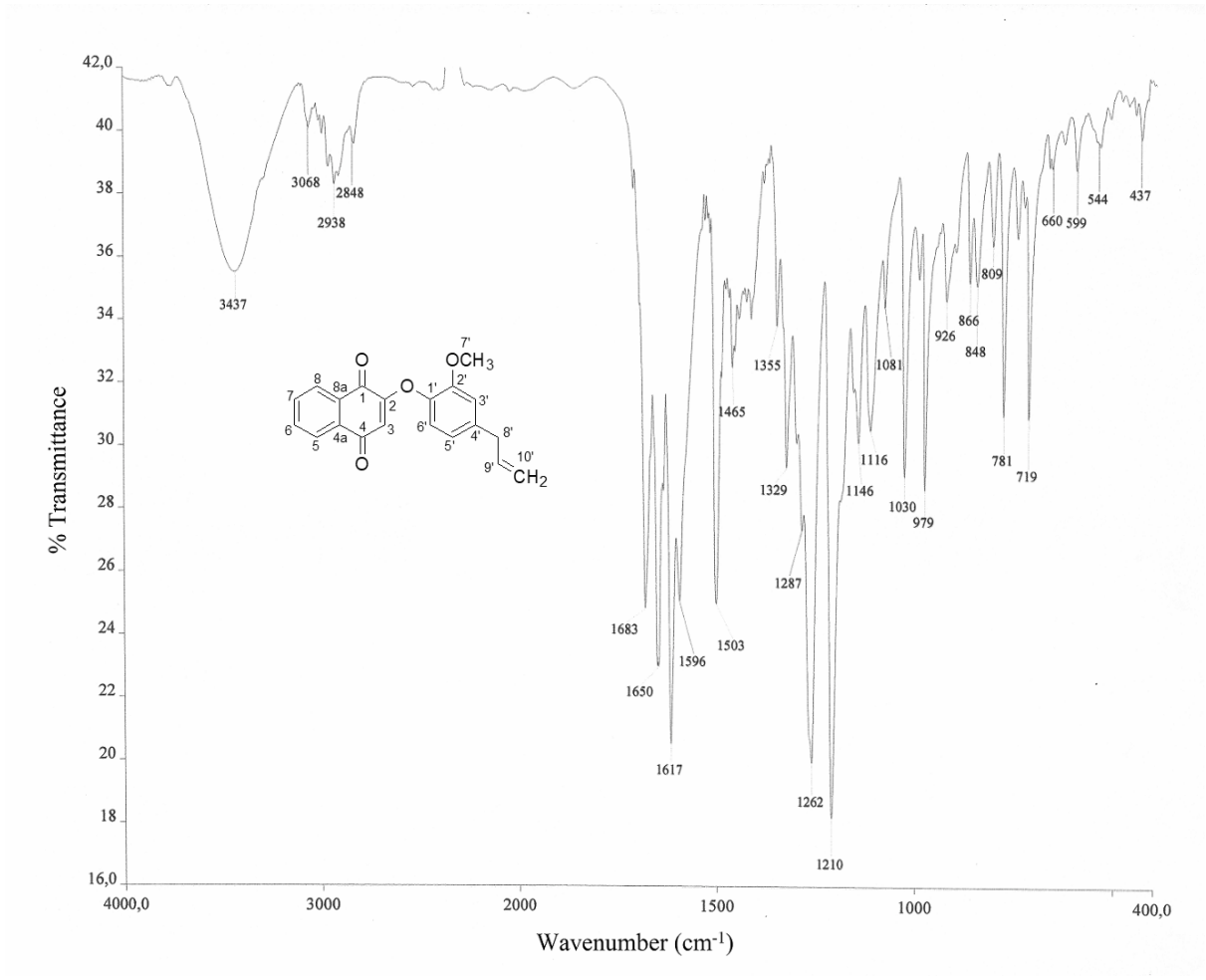
2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56** ^{13}C NMR



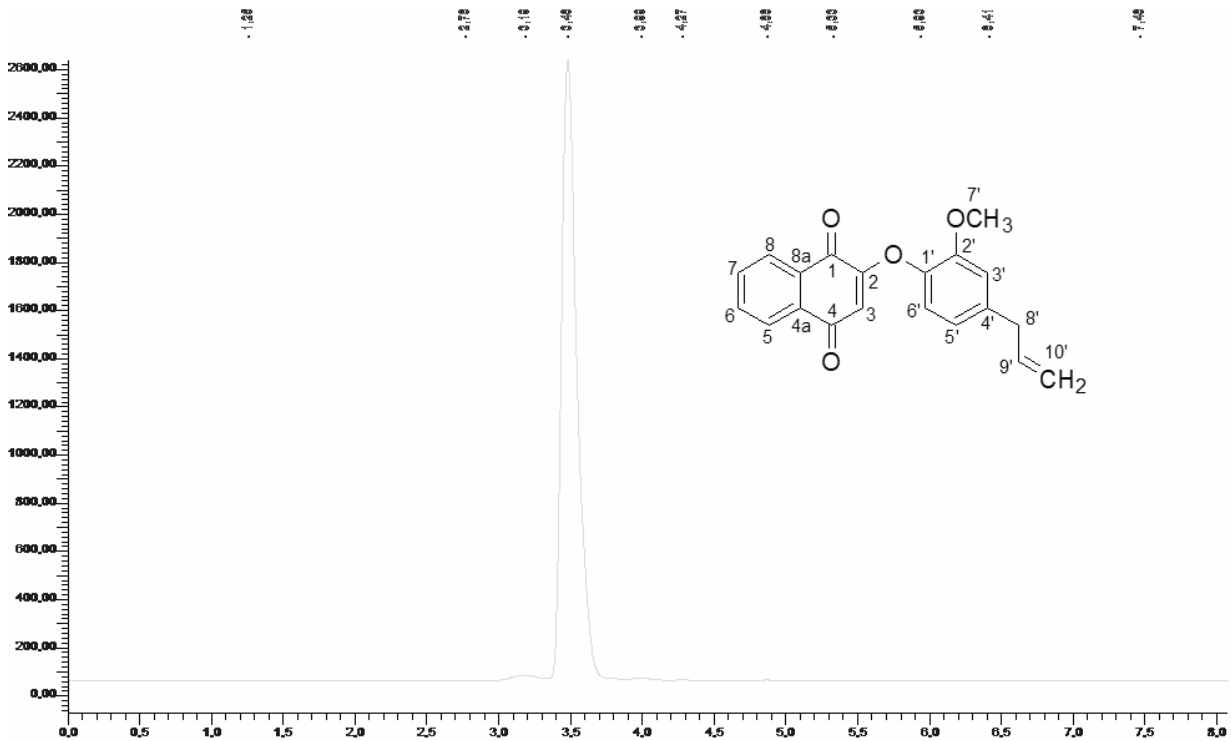
2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56** UV-Vis (MeOH)



2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56** IR (KBr pellet)



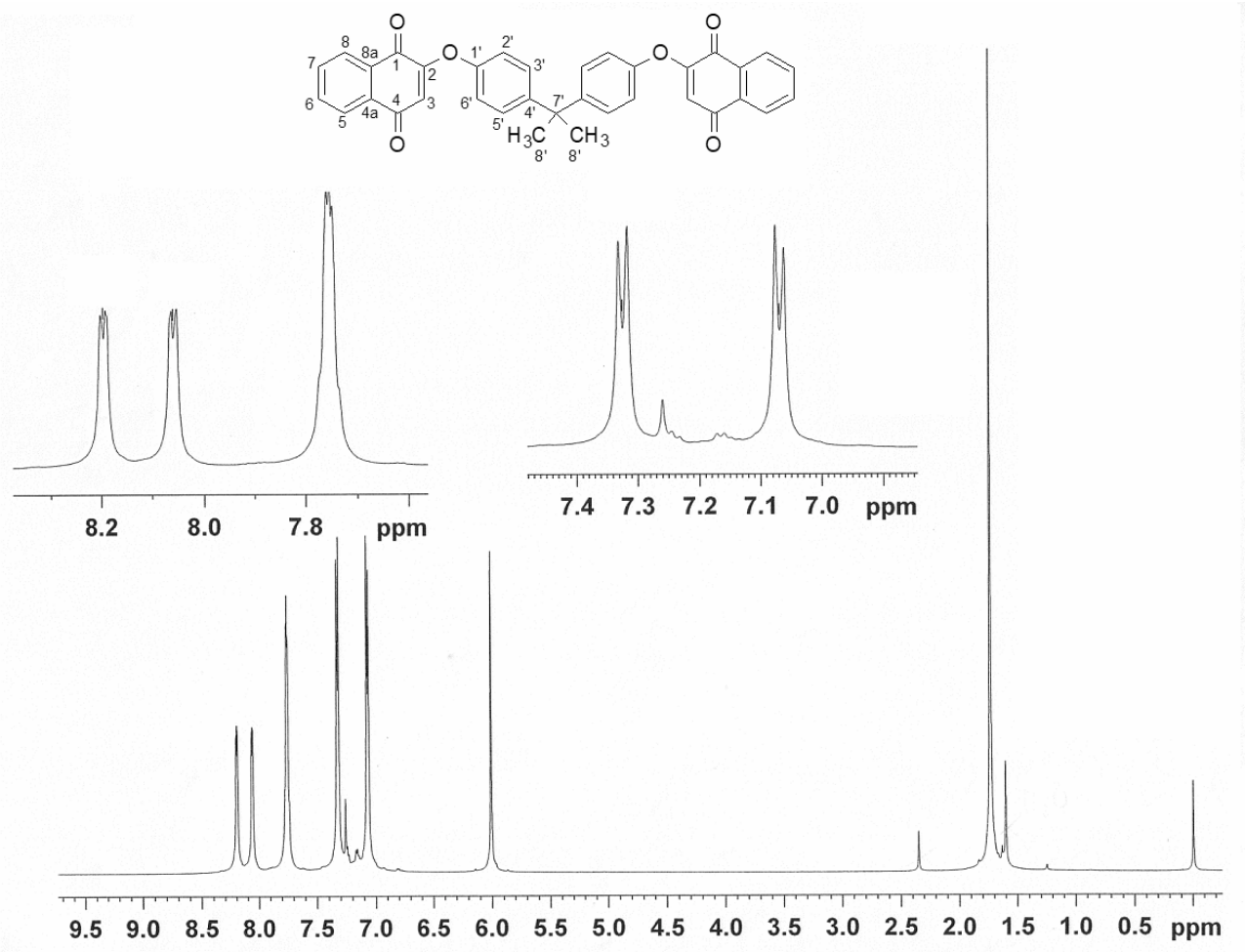
2-(4-allyl-2-methoxyphenoxy)-1,4-naphthoquinone **56** HPLC chromatogram (270 nm, 100% MeCN)



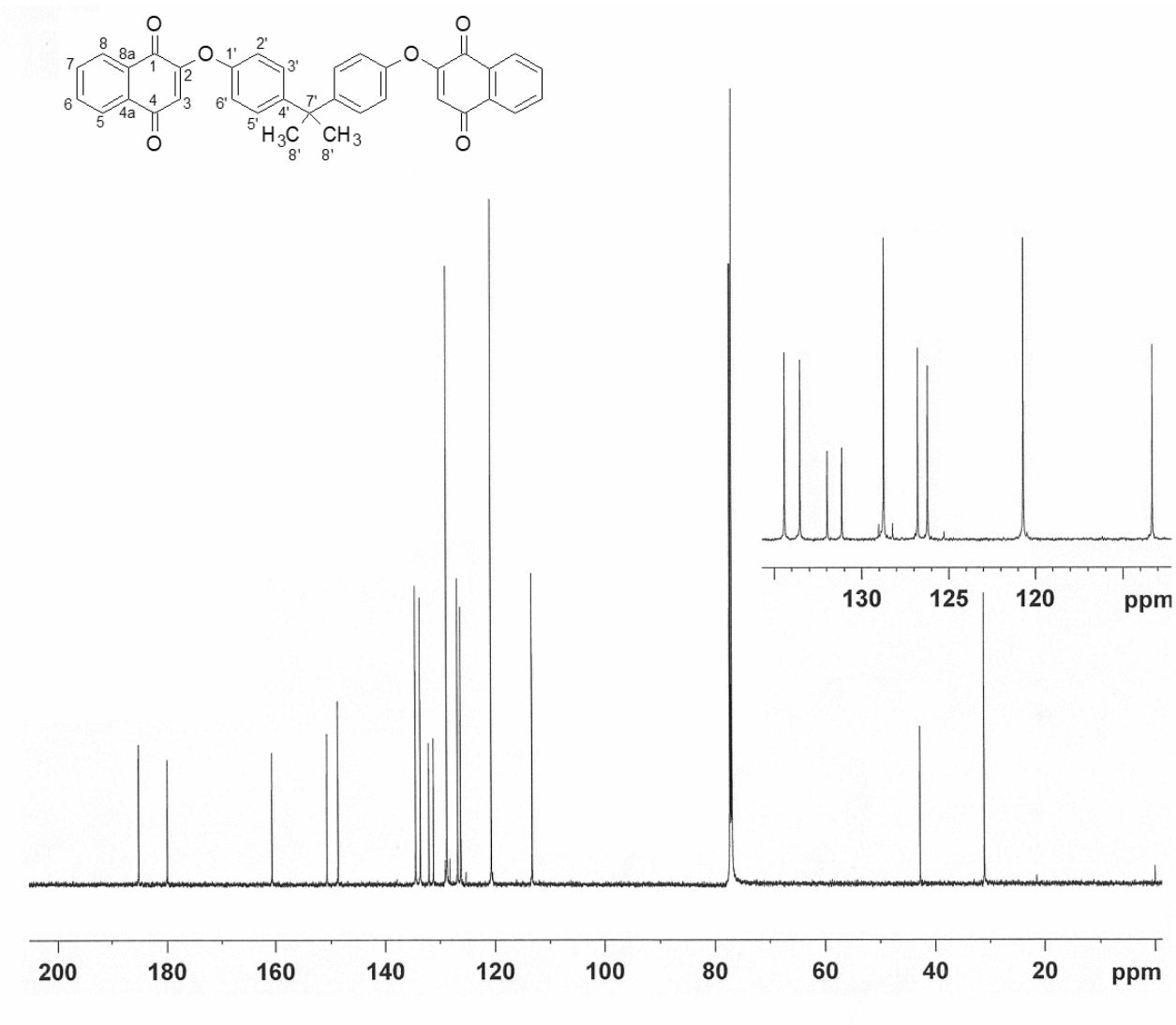
2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone 57

57 was obtained according to general procedure I 2.1.1, but using 474 mg (2.0 mmol) of 2-bromo-1,4-naphthoquinone, 228 mg (1.0 mmol) of bisphenol A and 975 mg (3.0 mmol) of dried Cs_2CO_3. The product was purified by hot extraction-filtration with MTBE and recrystallization with toluene. Yield 304 mg (56%), yellow-to-orange solid, mp = (199.0 – 201.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (2H, d, *J* = 7 Hz, ArH), 8.06 (2H, d, *J* = 7 Hz, ArH), 7.76 (4H, m, ArH), 7.33 (4H, d, J_{ortho} = 9 Hz, ArH), 7.07 (4H, d, J_{ortho} = 9 Hz, ArH), 6.01 (2H, s, ArH), 1.73 (6H, s, CH_3). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.1, 179.7, 160.5, 150.6, 148.6, 134.4, 133.5, 131.9, 131.1, 128.7, 126.8, 126.2, 120.7, 113.3, 42.7, 31.0. IR (KBr pellet) cm^{-1}: 3066, 2974, 1684, 1650, 1597, 1498, 1263, 1216. UV-Vis (MeCN) nm: 251 (max), 271, 334. TOF-MS: m/z $[M+H]^+$ calc for $C_{35}H_{25}O_6$: 541.1651; found: 541.1664. Purity: 95.1%. MIC (µM): 925 (*S. aureus*), >1850 (*C. albicans*), >1850 (*E. coli*).

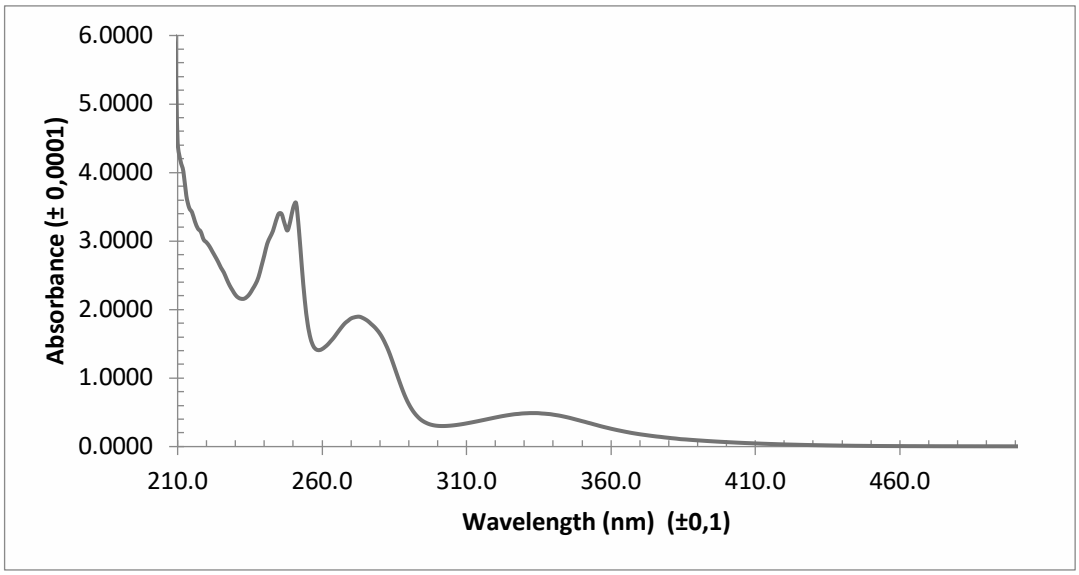
2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone **57** ^{1}H NMR



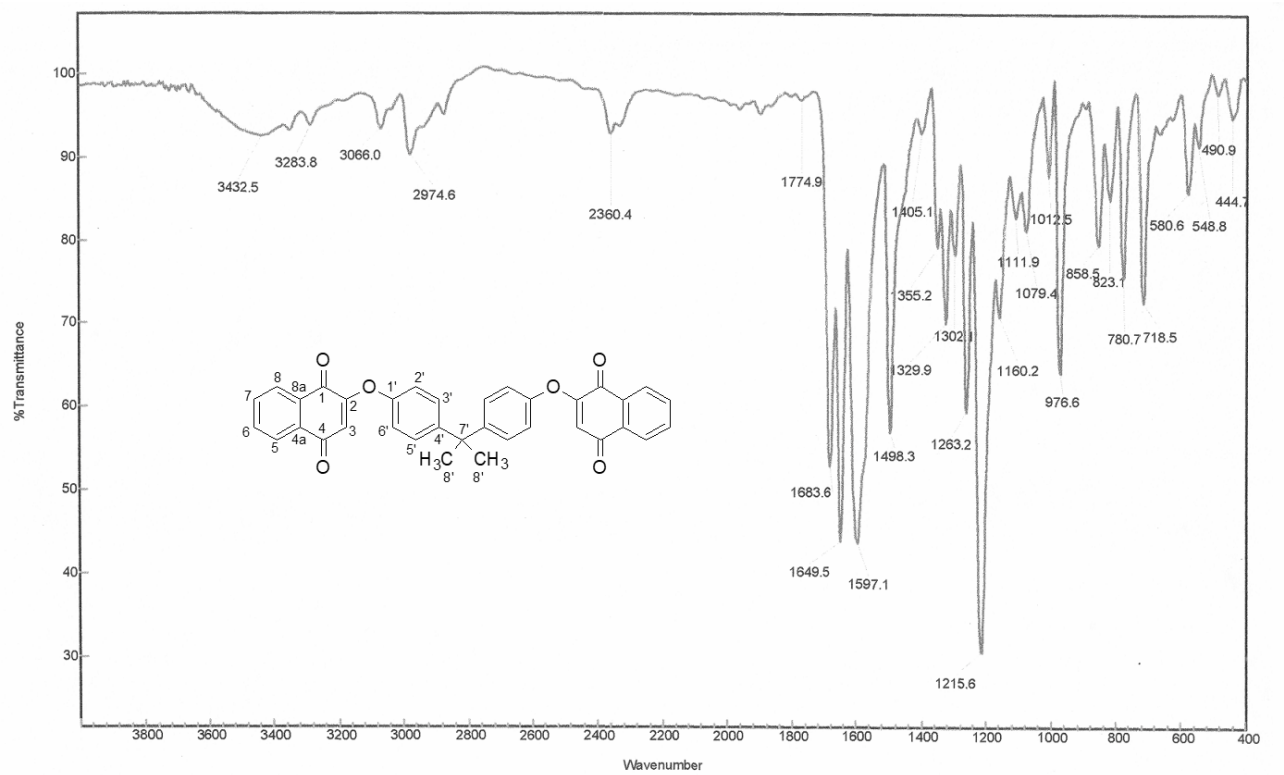
2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone **57** ^{13}C NMR



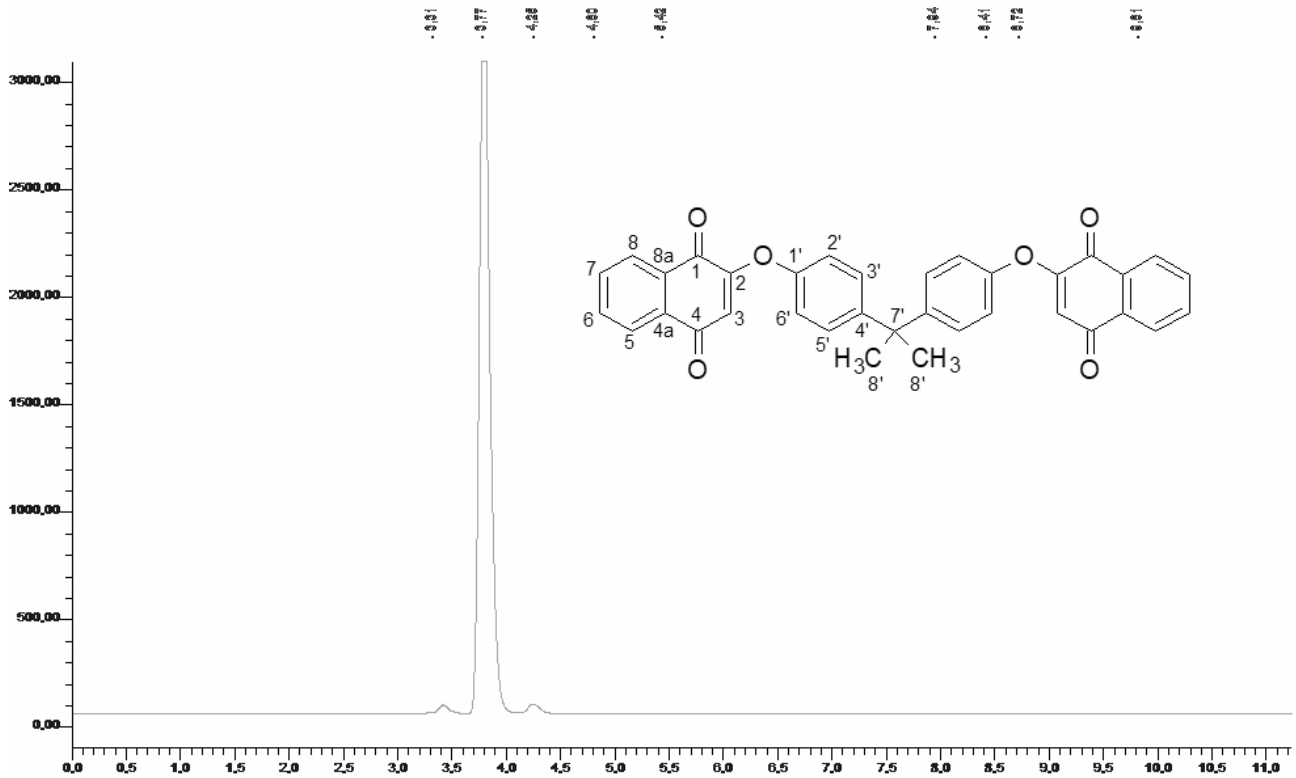
2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone **57** UV-Vis (MeCN)



2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone **57** IR (KBr pellet)



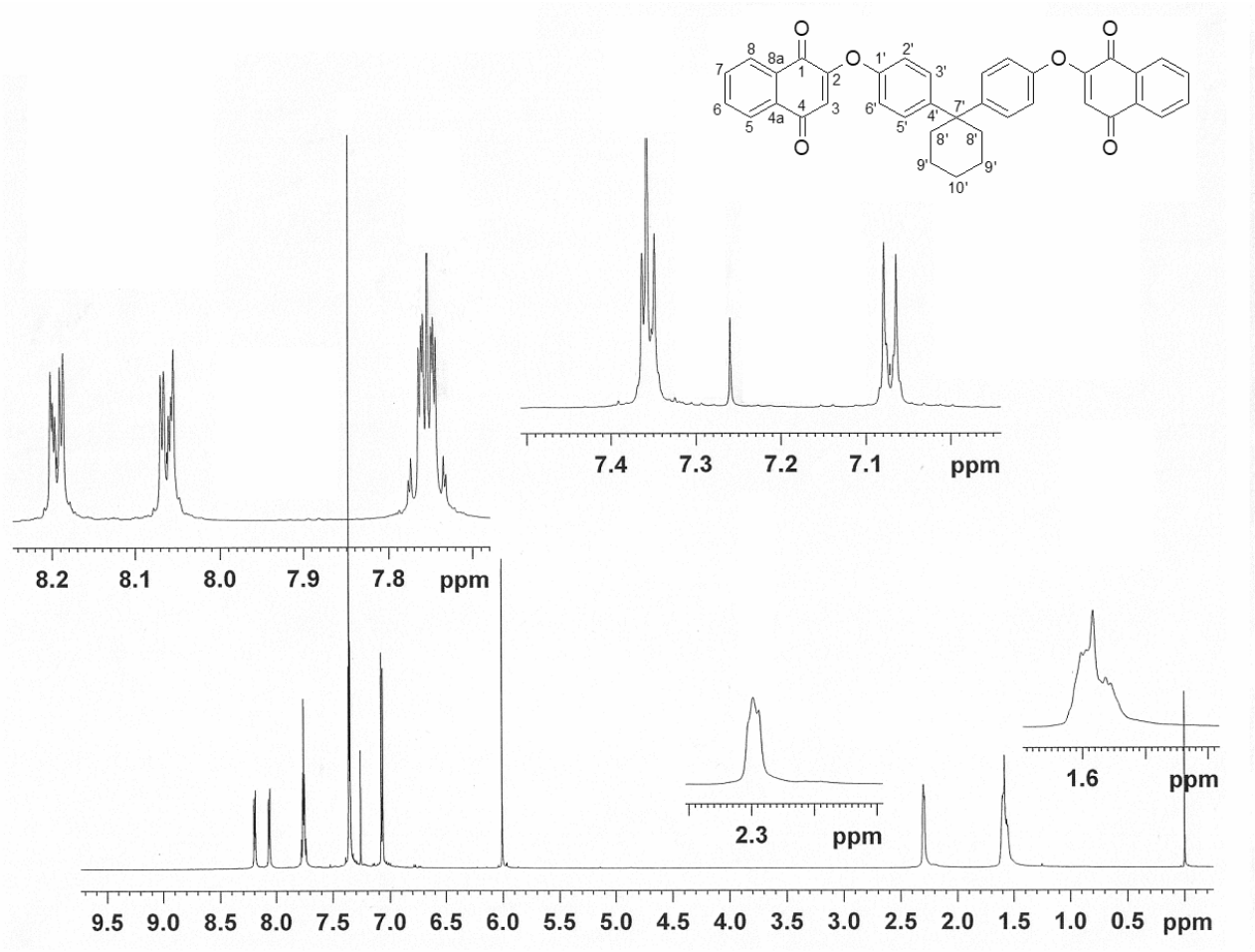
2-(4-[2-(4-hydroxyphenyl)propan-2-yl]phenoxy)-1,4-naphthoquinone **57** HPLC chromatogram (270 nm, 100% MeCN)



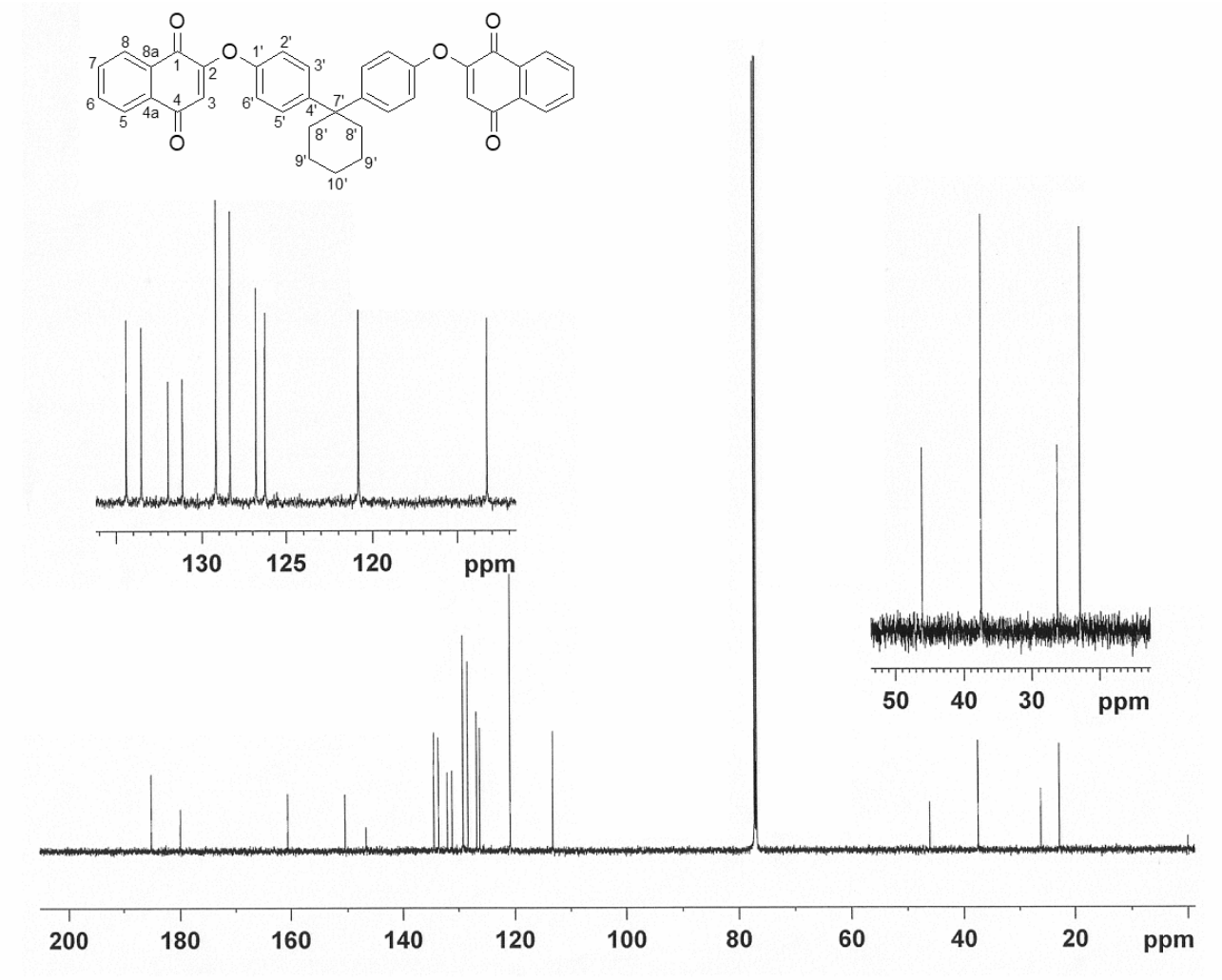
2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58**

58 was obtained according to general procedure I 2.1.1, but using 237 mg (1.0 mmol) of 2-bromo-1,4-naphthoquinone, 200 mg (0.75 mmol) of bisphenol Z and 590 mg (1.6 mmol) of dried Cs_2CO_3. The product was purified by hot extraction-filtration with MTBE and recrystallization with benzene. Yield 251 mg (92%), yellow solid, mp = (248.0 – 250.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (2H, d, *J* = 7 Hz, ArH), 8.06 (2H, d, *J* = 7 Hz, ArH), 7.76 (4H, m, ArH), 7.36 (4H, d, J_{ortho} = 6 Hz; ArH), 7.07 (4H, d, J_{ortho} = 8 Hz, ArH), 6.01 (2H, s, ArH), 2.30 (4H, s, -C(C**H₂**CH₂)₂CH₂), 1.59 (2H, m, -C(CH₂CH₂)₂C**H₂**), 1.56 (4H, m, -C(CH₂C**H₂**)₂CH₂). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.1, 179.9, 160.5, 150.4, 146.6, 134.4, 133.5, 132.0, 131.1, 128.3, 126.8, 126.2, 120.8, 113.3, 46.1, 37.5, 26.2, 22.8. IR (KBr pellet) cm^{-1}: 3058, 2931, 1681, 1652, 1597, 1501, 1262, 1225. UV-Vis (MeCN) nm: 270 (max), 330. TOF-MS: m/z $[M+H]^+$ calc for $C_{38}H_{29}O_6$: 581.1964; found: 581.1965. Purity: 93.6%. MIC (μM): (*S. aureus*), (*C. albicans*), (*E. coli*).

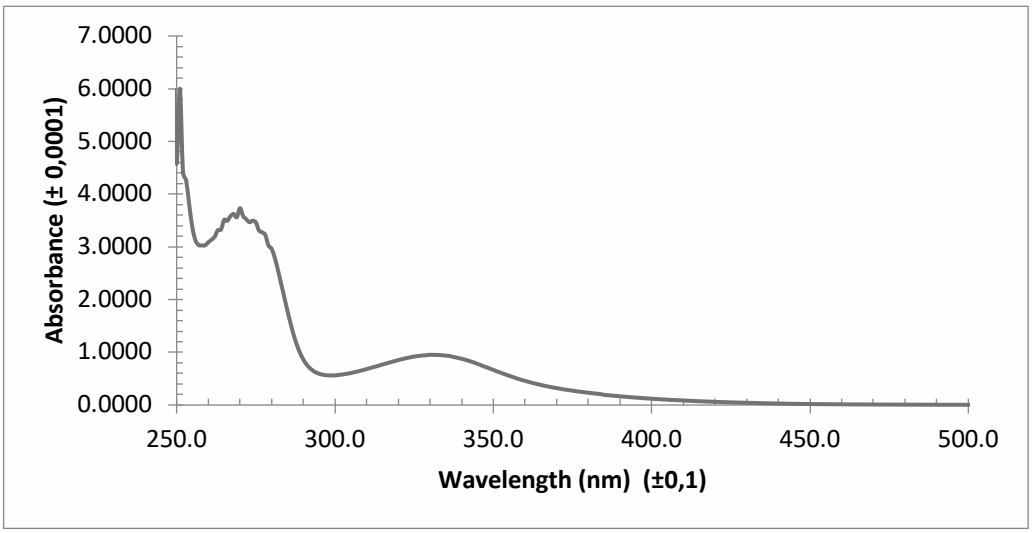
2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58** ^{1}H NMR



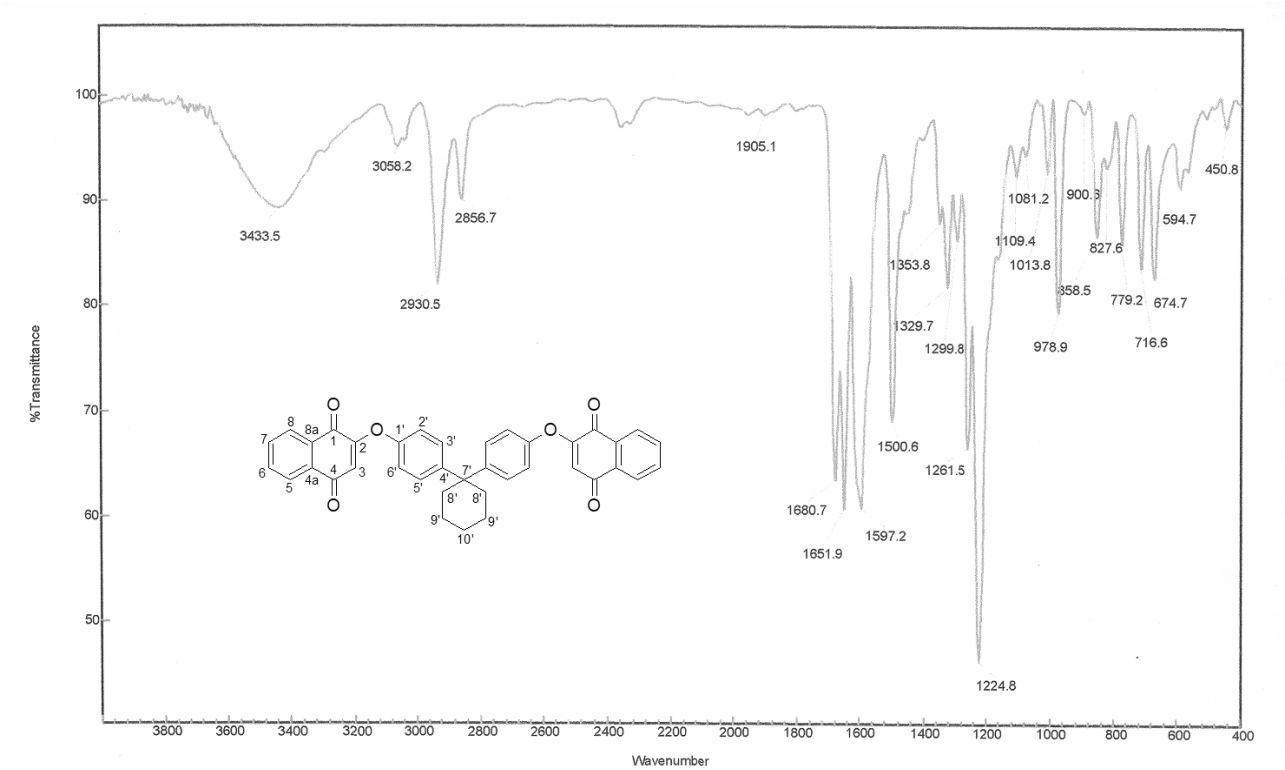
2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58** ^{13}C NMR



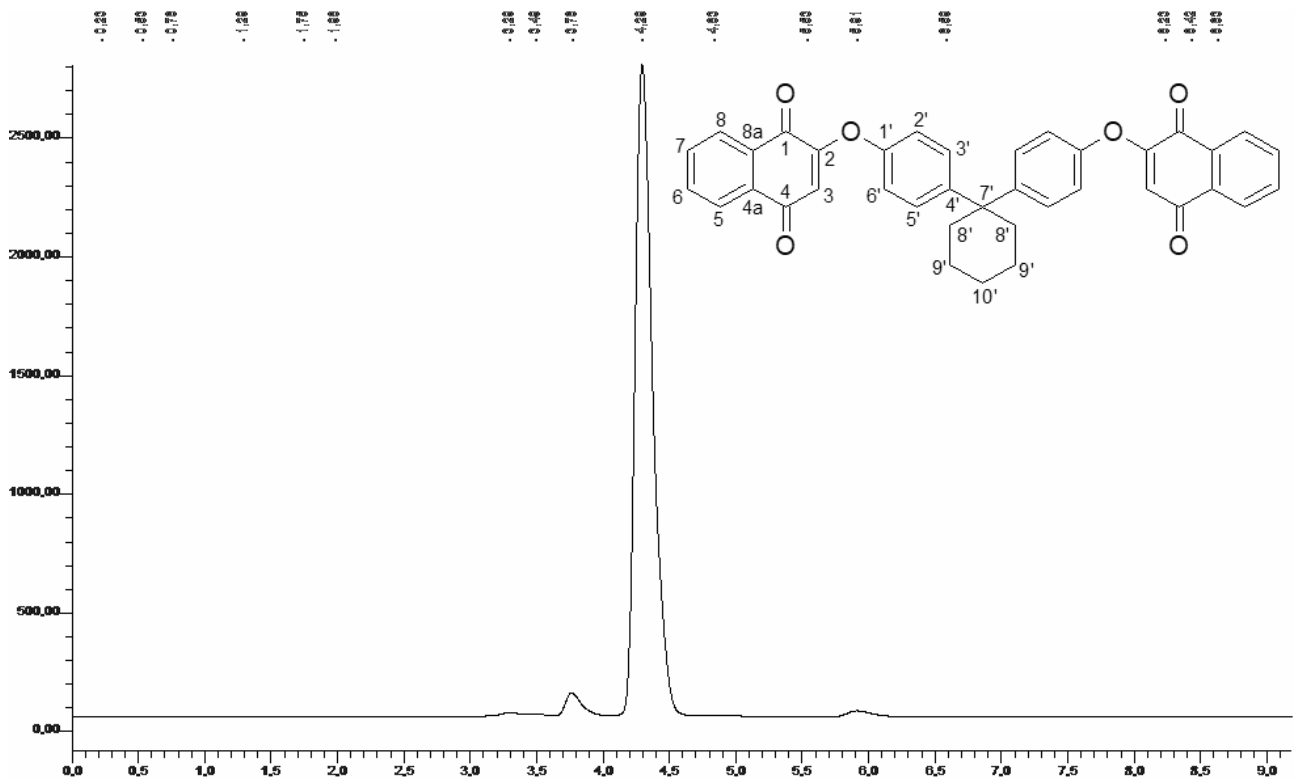
2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58** UV-Vis (MeCN)



2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58** IR (KBr pellet)



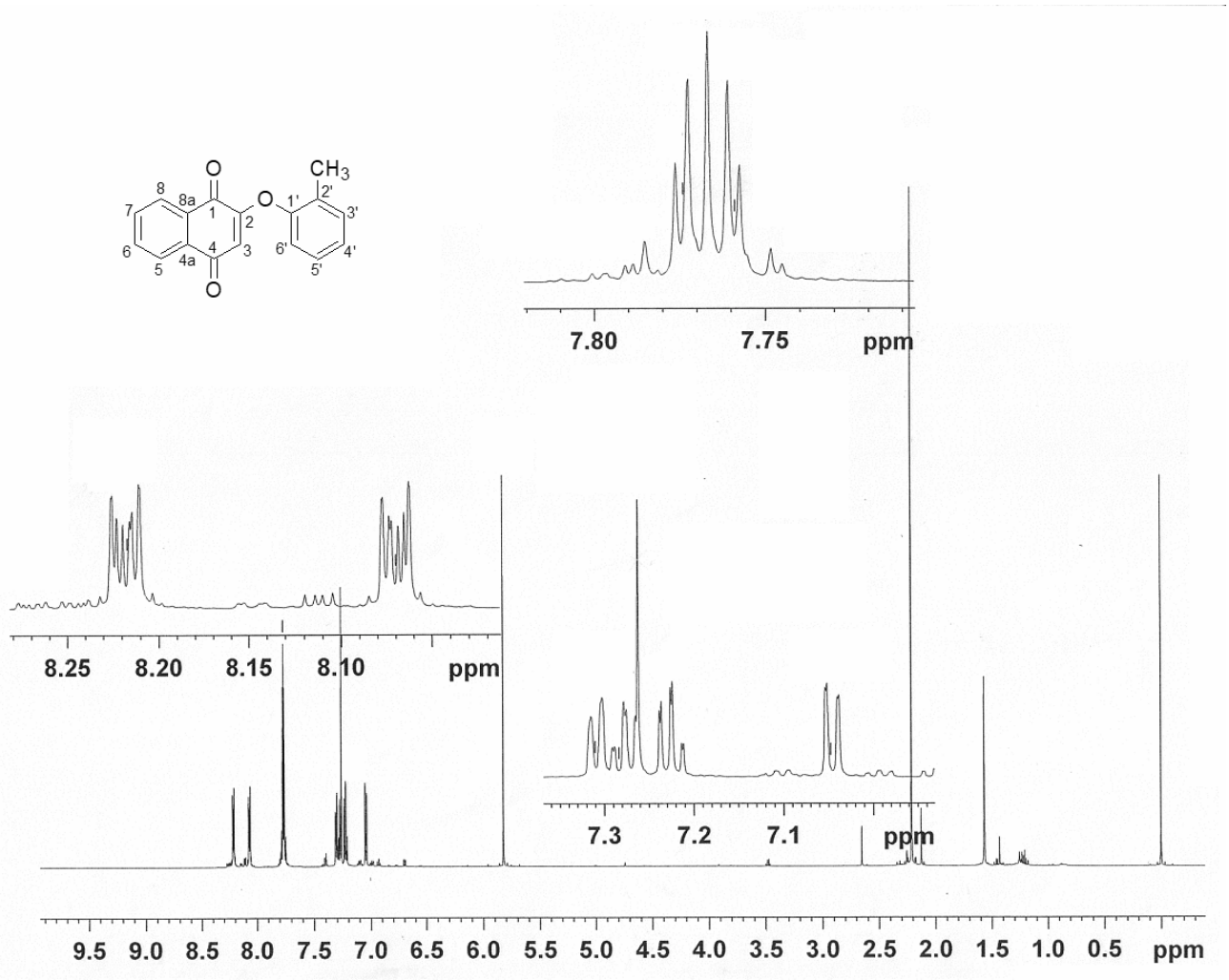
2-(4-[2-(4-hydroxyphenyl)cyclohexyl]phenoxy)-1,4-naphthoquinone **58** HPLC chromatogram (270 nm, 100% MeCN)



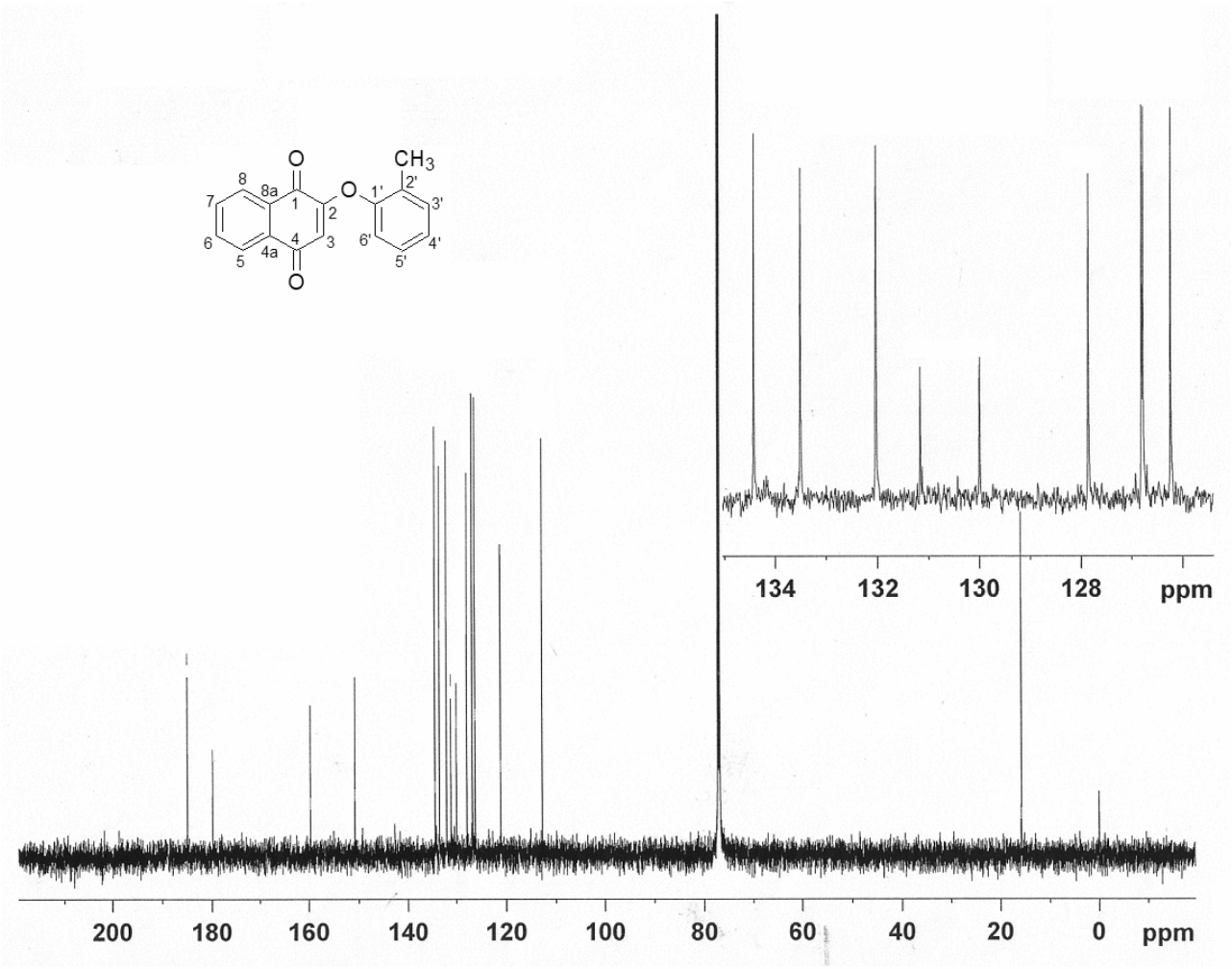
2-(2-methylphenoxy)-1,4-naphthoquinone **59**

59 was obtained according to general procedure II 2.1.2 and purified by hot extraction-filtration with MTBE and column chromatography (1% triethylamine/benzene as eluent, isocratically). Yield 70 mg (27%), reddish-brown solid, mp = (79.0 – 83.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.22 (1H, d, J = 6.8 Hz, ArH), 8.07 (1H, d, J = 6.8 Hz, ArH), 7.77 (2H, m, ArH), 7.31 (1H, d, J_{ortho} = 8 Hz, ArH), 7.28 (1H, td, J_{meta} = 2 Hz, J_{ortho} = 8 Hz, ArH), 7.22 (1H, td, J_{meta} = 2 Hz, J_{ortho} = 8 Hz, ArH), 7.05 (1H, d, J_{ortho} = 8 Hz, ArH), 5.83 (1H, s, ArH), 2.21 (3H, s, $-CH_3$). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.0, 179.9, 159.7, 150.8, 134.4, 133.5, 132.0, 131.2, 130.0, 127.9, 126.8, 126.8, 126.2, 121.2, 112.8, 15.8. IR (KBr pellet) cm^{-1}: 3068, 2927, 1685, 1655, 1613, 1595, 1260, 1226. UV-Vis (MeOH) nm: 213, 249 (max), 268, 332. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_3$: 265.0865; found: 265.0865. Purity: 96.6%.

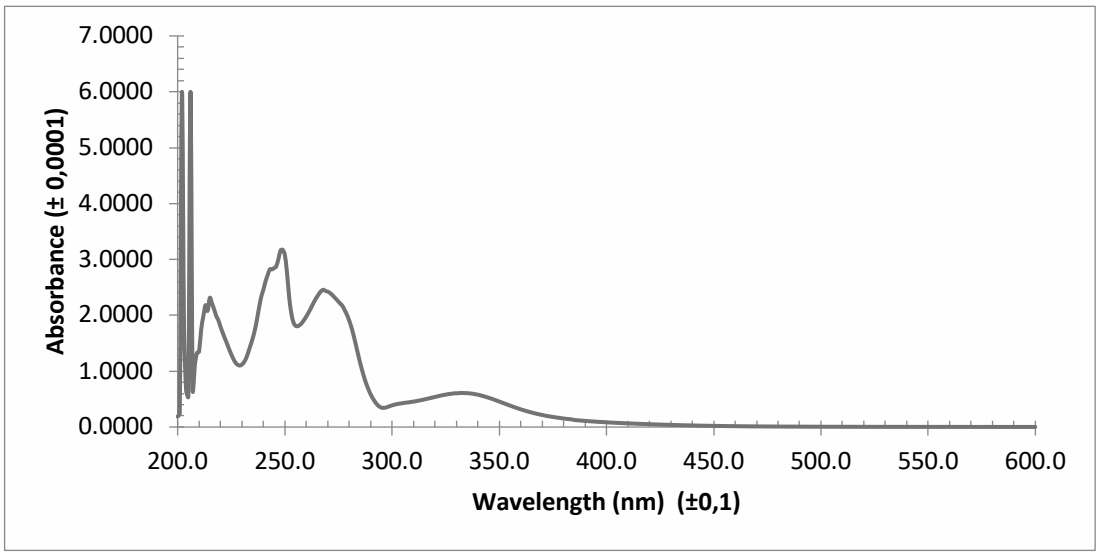
2-(2-methylphenoxy)-1,4-naphthoquinone **59** ^{1}H NMR



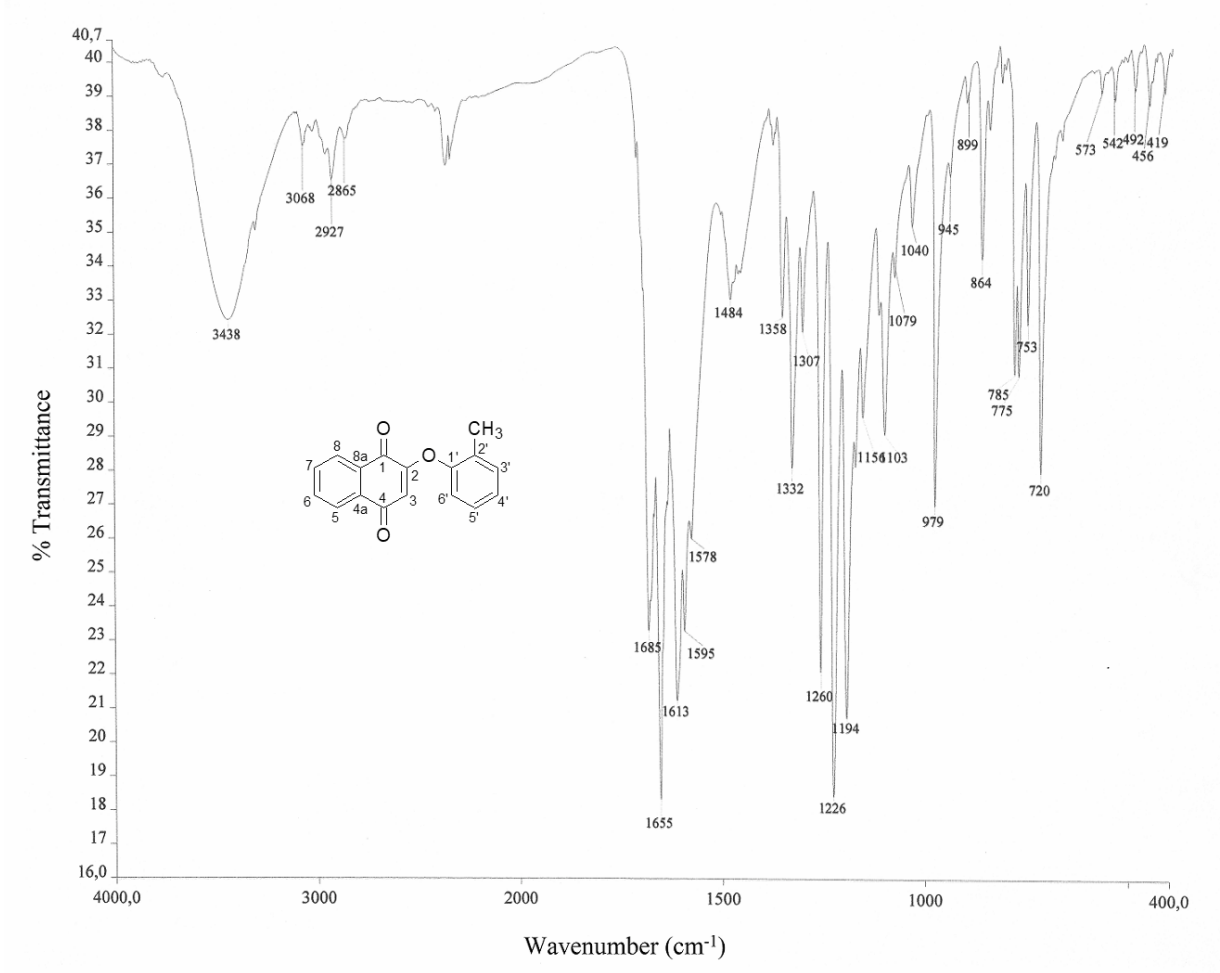
2-(2-methylphenoxy)-1,4-naphthoquinone **59** ^{13}C NMR



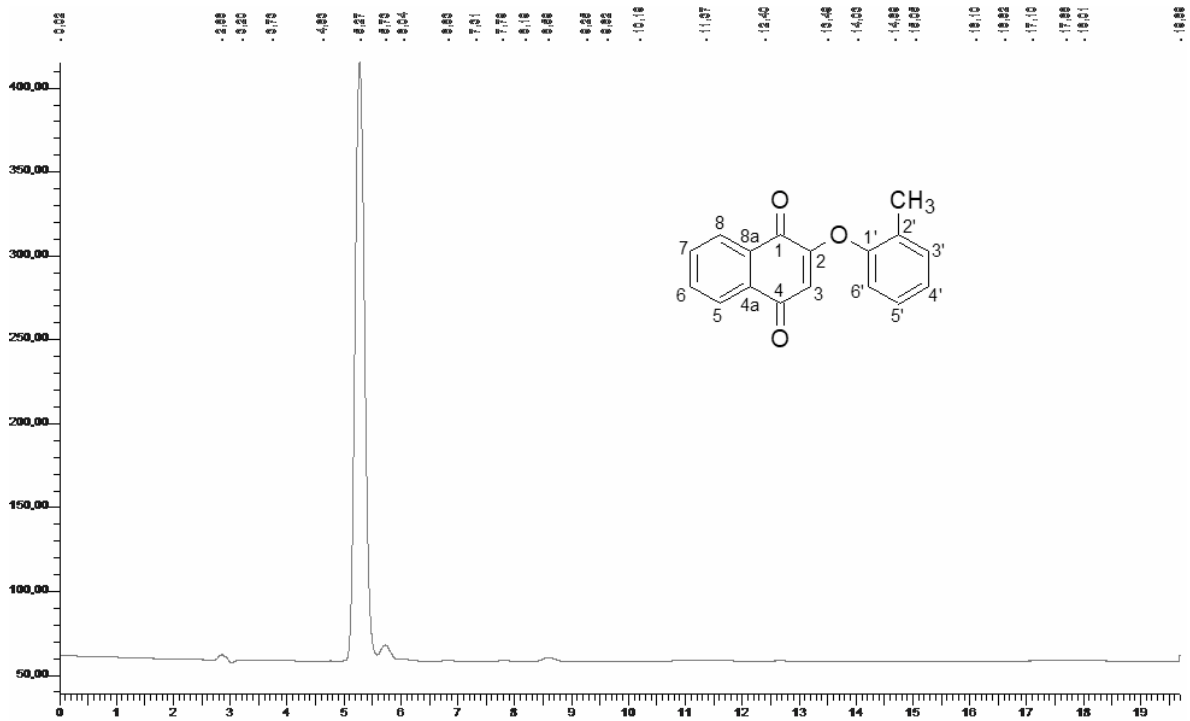
2-(2-methylphenoxy)-1,4-naphthoquinone **59** UV-Vis (MeOH)



2-(2-methylphenoxy)-1,4-naphthoquinone **59** IR (KBr pellet)



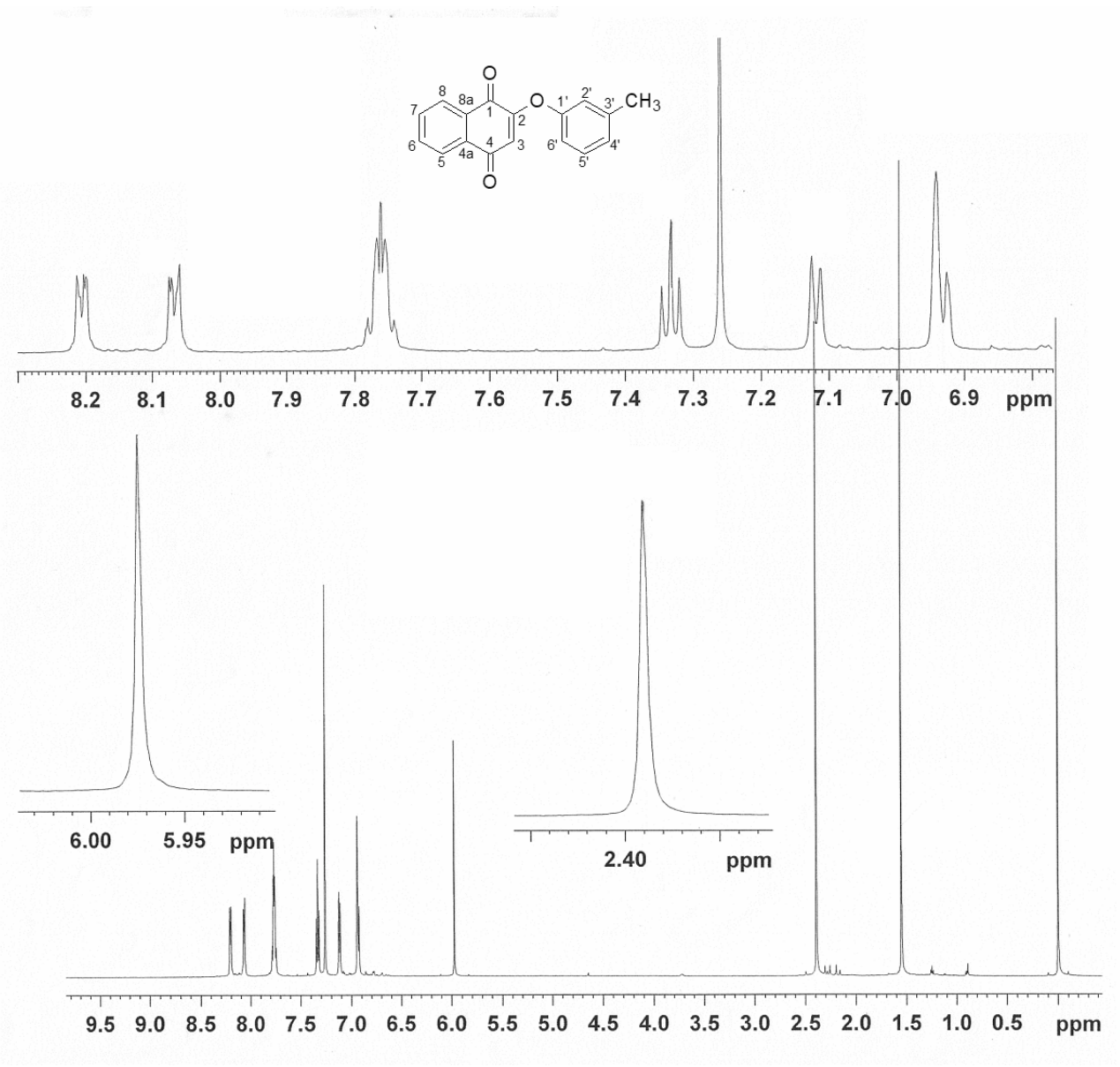
2-(2-methylphenoxy)-1,4-naphthoquinone **59** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



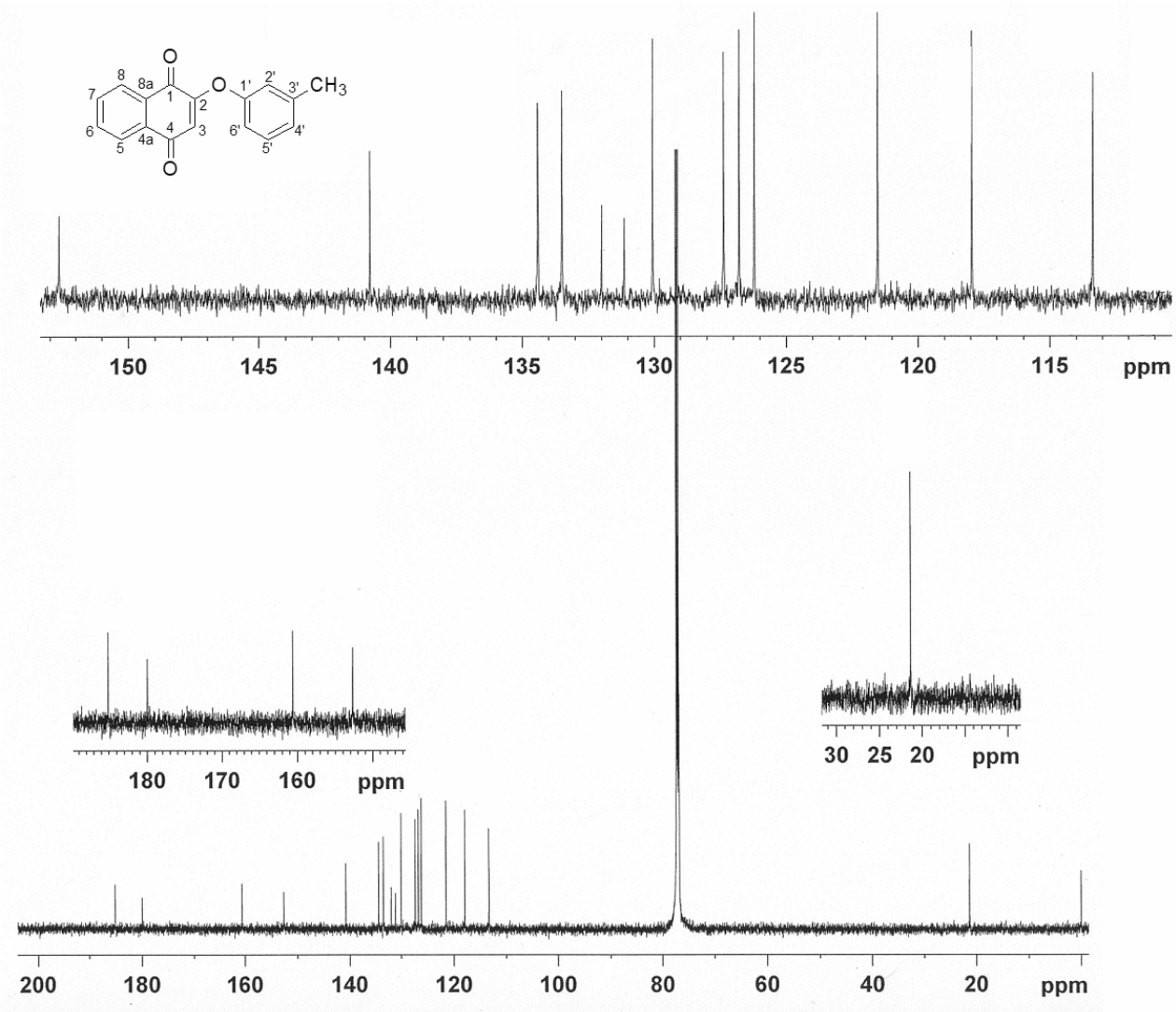
2-(3-methylphenoxy)-1,4-naphthoquinone 60

60 was obtained according to general procedure II 2.1.2 and purified by hot extraction-filtration with MTBE and column chromatography (1% triethylamine/benzene as eluent, isocratically). Yield 181 mg (69%), yellow solid, mp = (97.0 – 102.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.21 (1H, dd, *J* = 2.1 Hz, *J* = 6.4 Hz, ArH), 8.07 (1H, dd, *J* = 2.1 Hz, *J* = 6.4 Hz, ArH), 7.77 (2H, m, ArH), 7.33 (1H, t, J_{ortho} = 6.4 Hz, ArH), 7.12 (1H, d, J_{ortho} = 6.4 Hz, ArH), 6.95 (1H, d, ArH), 6.93 (2H, d, J_{ortho} = 8.6 Hz, ArH), 5.97 (1H, s, ArH), 2.39 (3H, s, $-CH_3$). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.1, 180.0, 160.6, 152.7, 140.8, 134.4, 133.5, 132.0, 131.2, 130.1, 127.4, 126.8, 126.2, 121.6, 118.0, 113.4, 21.3. IR (KBr pellet) cm^{-1}: 3068, 2927, 1685, 1648, 1607, 1594, 1261, 1245. UV-Vis (MeOH) nm: 212, 248 (max), 270, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_3$: 265.0865; found: 265.0863. Purity: 98.7%. MIC (μM): 473 (*S. aureus*), 237 (*C. albicans*), >3000 (*E. coli*).

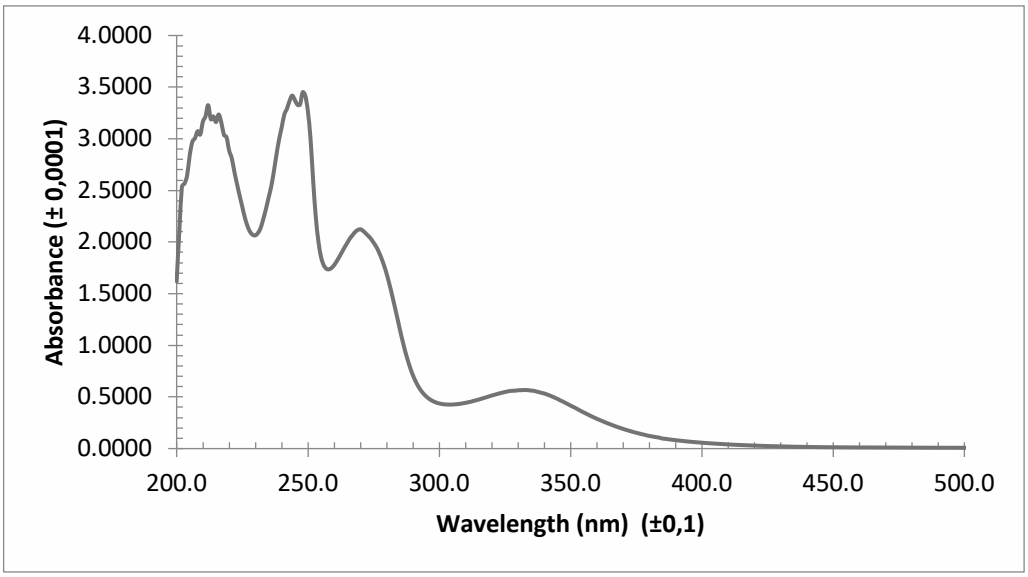
2-(3-methylphenoxy)-1,4-naphthoquinone **60** ^{1}H NMR



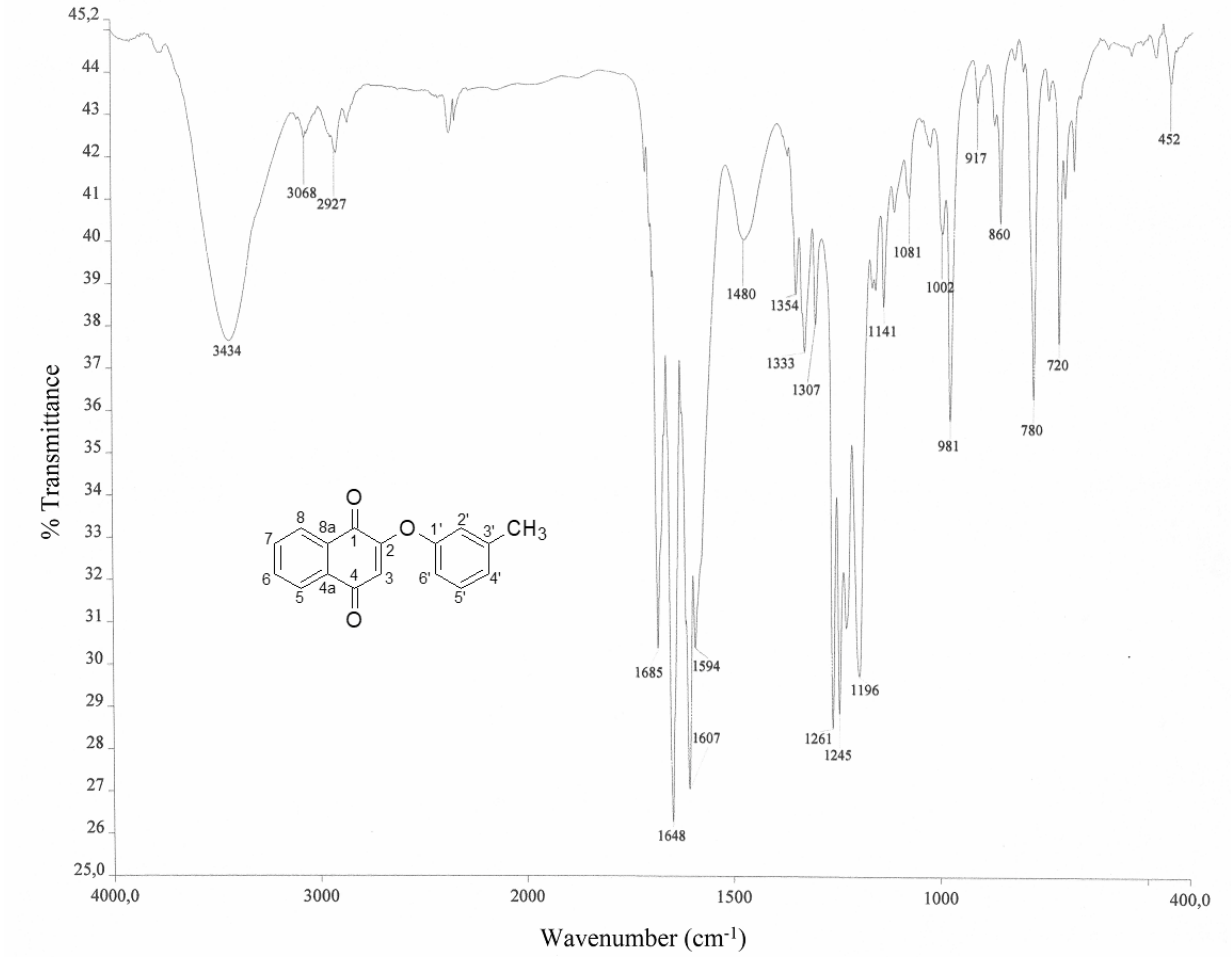
2-(3-methylphenoxy)-1,4-naphthoquinone **60** ^{13}C NMR



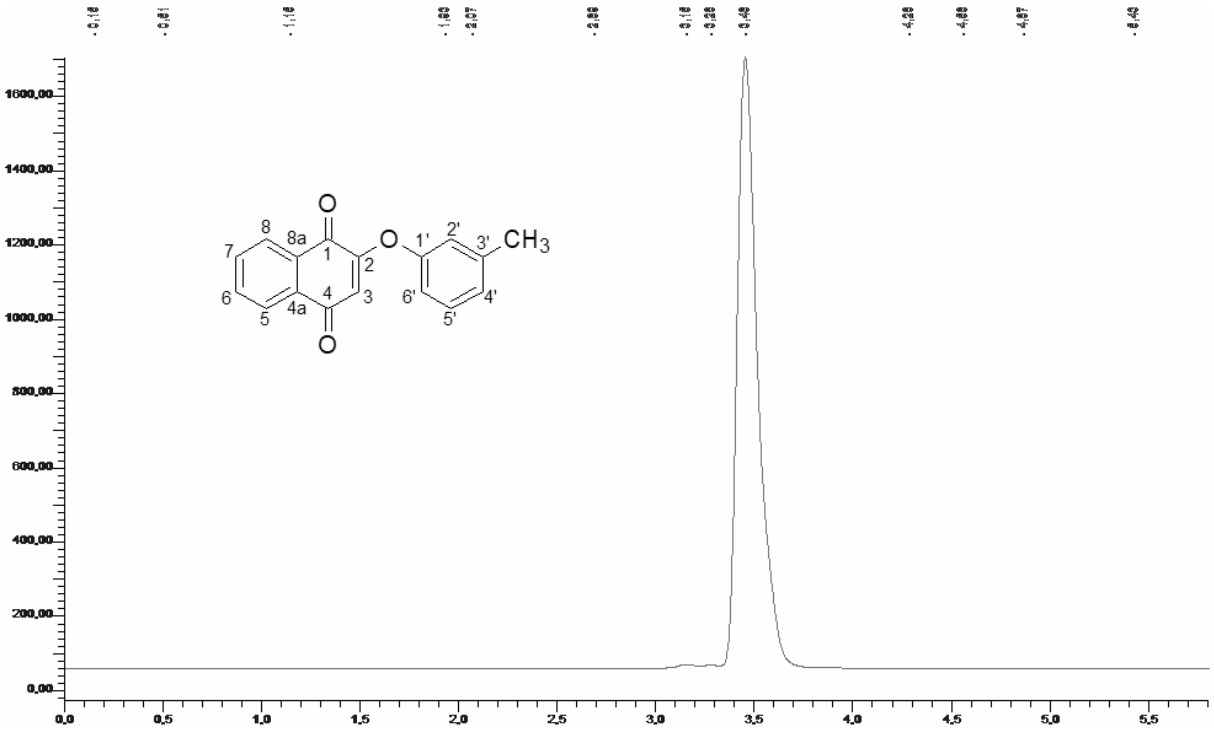
2-(3-methylphenoxy)-1,4-naphthoquinone **60** UV-Vis (MeOH)



2-(3-methylphenoxy)-1,4-naphthoquinone **60** IR (KBr pellet)



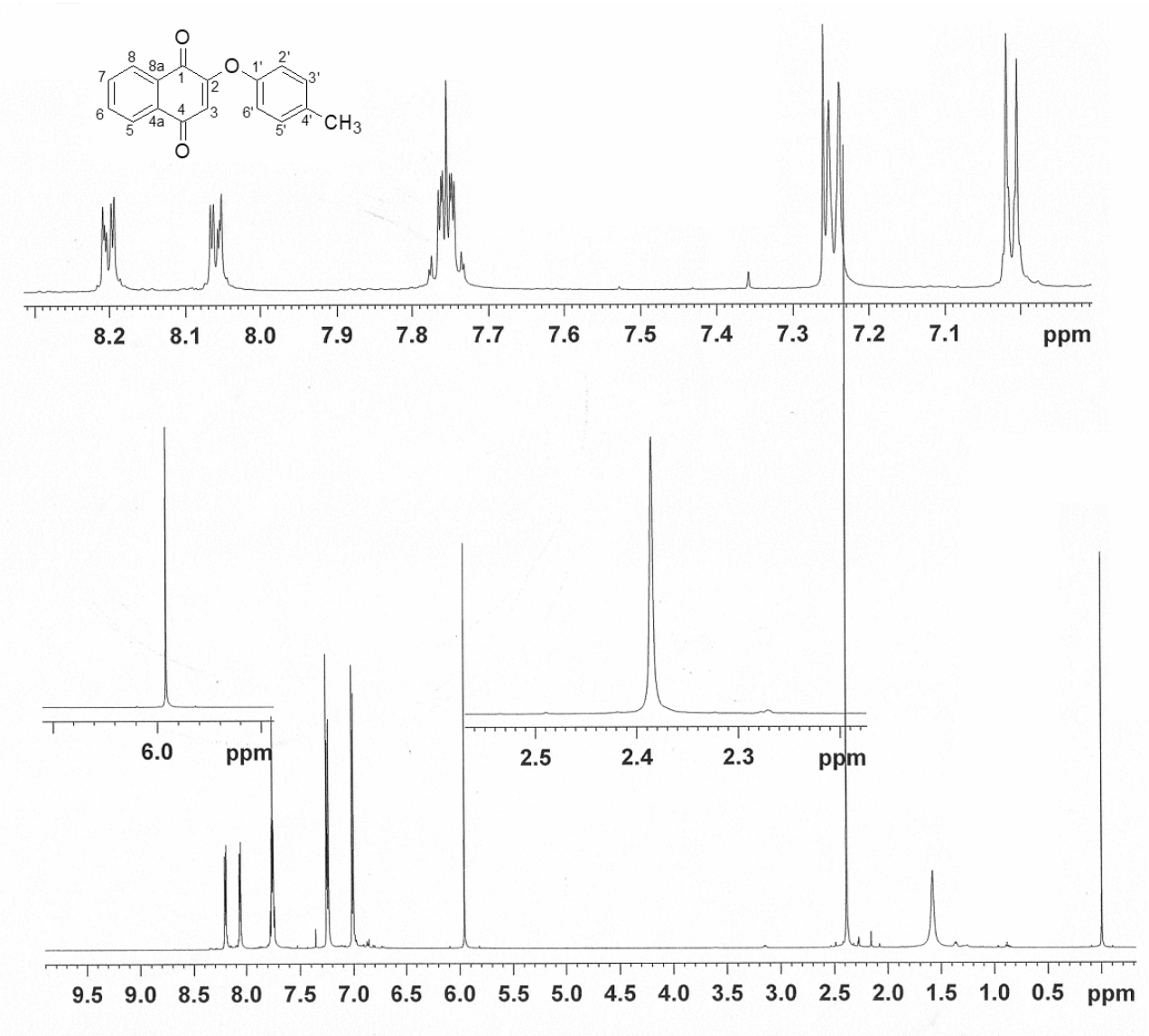
2-(3-methylphenoxy)-1,4-naphthoquinone **60** HPLC chromatogram (274 nm, 100% MeCN)



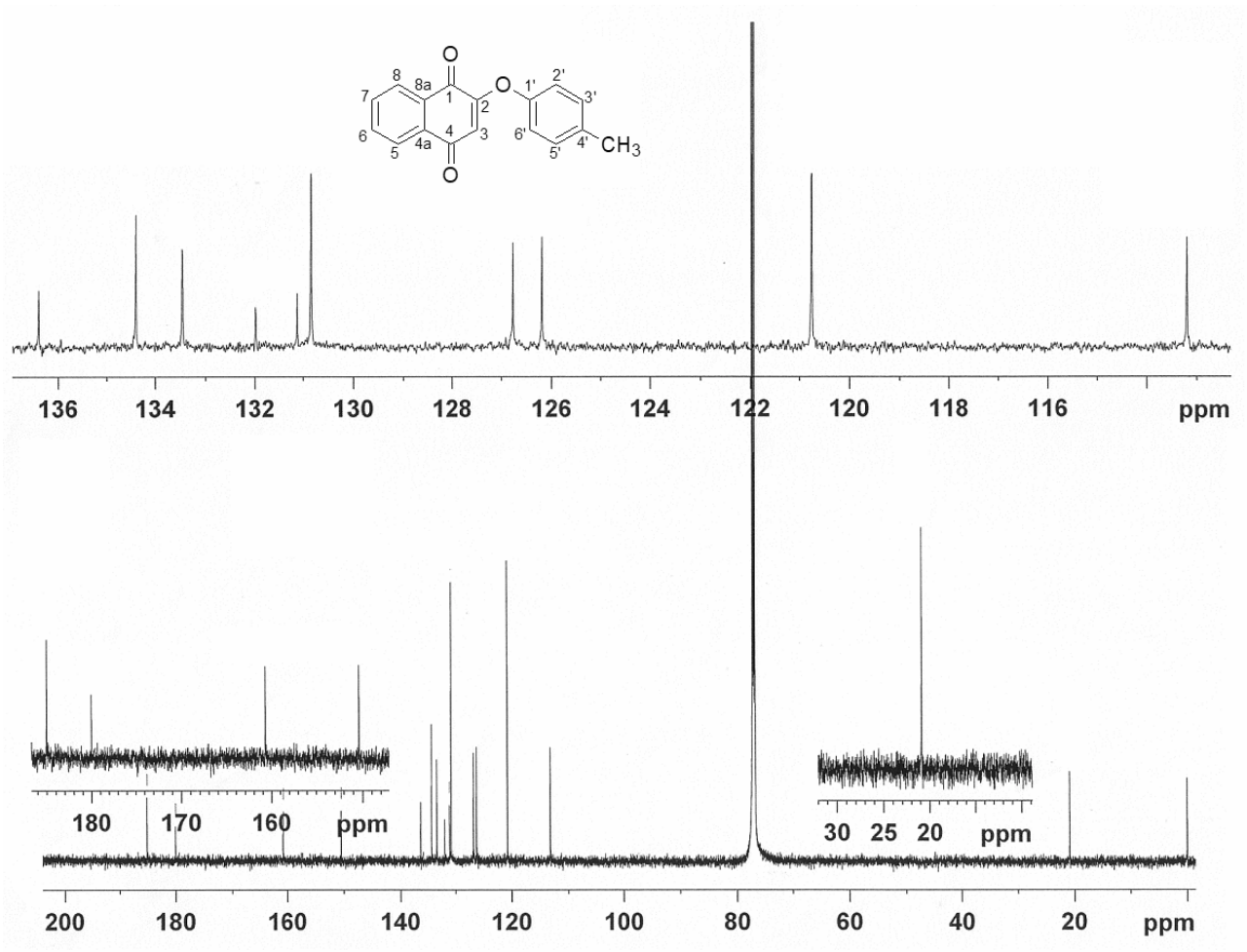
2-(4-methylphenoxy)-1,4-naphthoquinone **61**

61 was obtained according to general procedure II 2.1.2 and purified by hot extraction-filtration with MTBE and column chromatography (1% triethylamine/benzene as eluent, isocratically). Yield 155 mg (59%), yellow solid, mp = (100.0 – 102.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.20 (1H, d, J = 5 Hz, ArH), 8.06 (1H, d, J = 5 Hz, ArH), 7.76 (2H, m, ArH), 7.25 (2H, d, J_{ortho} = 7.5 Hz, ArH), 7.01 (2H, d, J_{ortho} = 7.5 Hz, ArH), 5.98 (1H, s, ArH), 2.40 (3H, s, $-CH_3$). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 185.4, 180.0, 160.7, 150.4, 136.4, 134.4, 133.5, 132.0, 131.2, 130.8, 126.8, 126.2, 120.8, 113.2, 20.9. IR (KBr pellet) cm^{-1}: 3072, 2922, 2865, 1679, 1651, 1618, 1506, 1261, 1231. UV-Vis (MeOH) nm: 205, 249 (max), 271, 330. TOF-MS: m/z $[M+H]^+$ calc for $C_{17}H_{13}O_3$: 265.0865; found: 265.0866. Purity: 97.9%. MIC (μM): 237 (*S. aureus*), 473 (*C. albicans*), >3000 (*E. coli*).

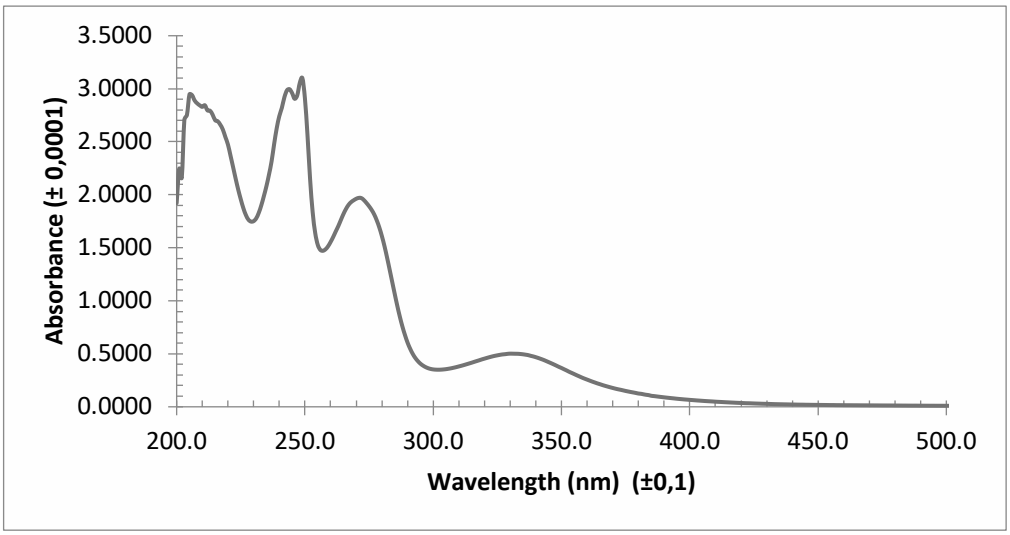
2-(4-methylphenoxy)-1,4-naphthoquinone **61** ^{1}H NMR



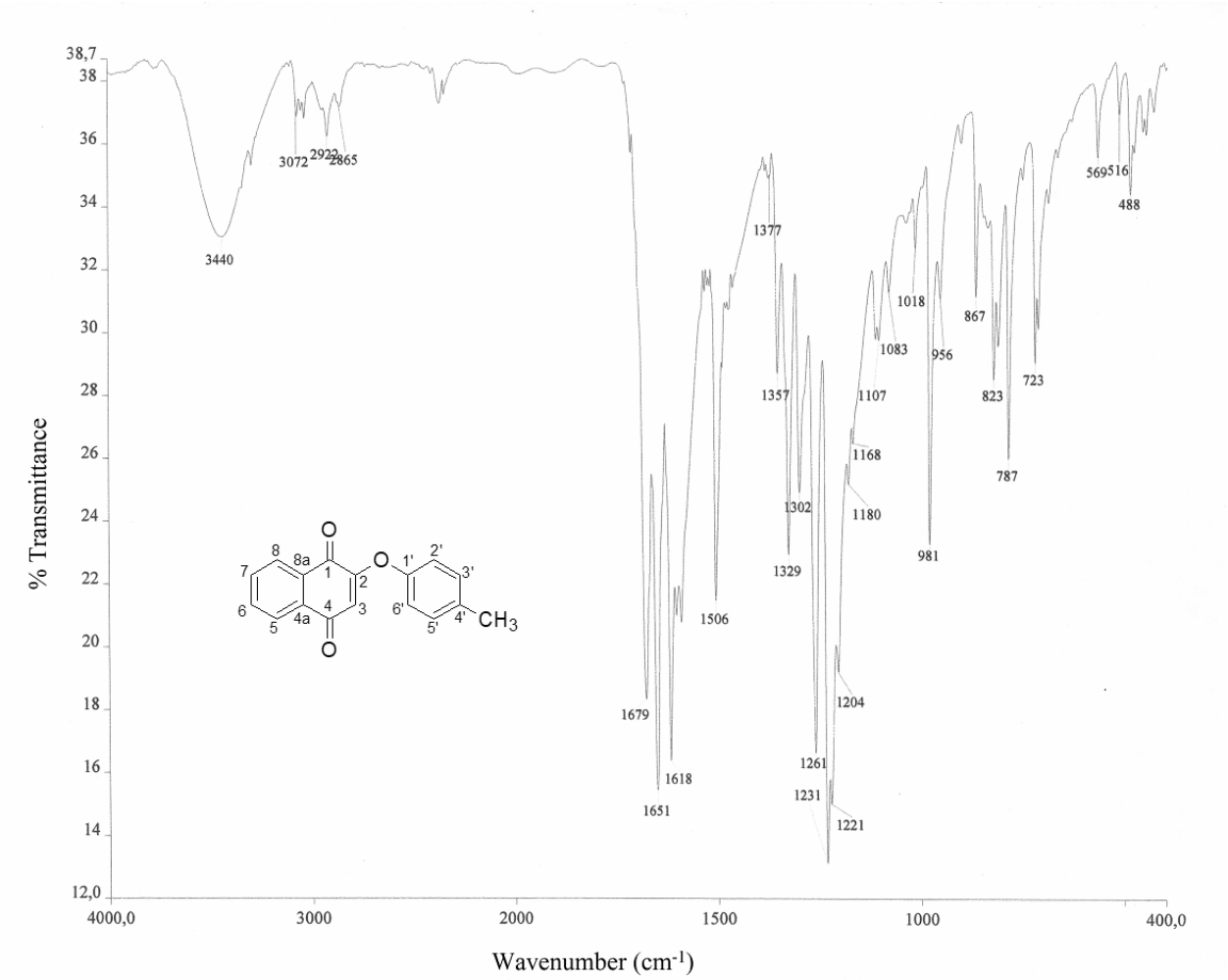
2-(4-methylphenoxy)-1,4-naphthoquinone **61** ^{13}C NMR



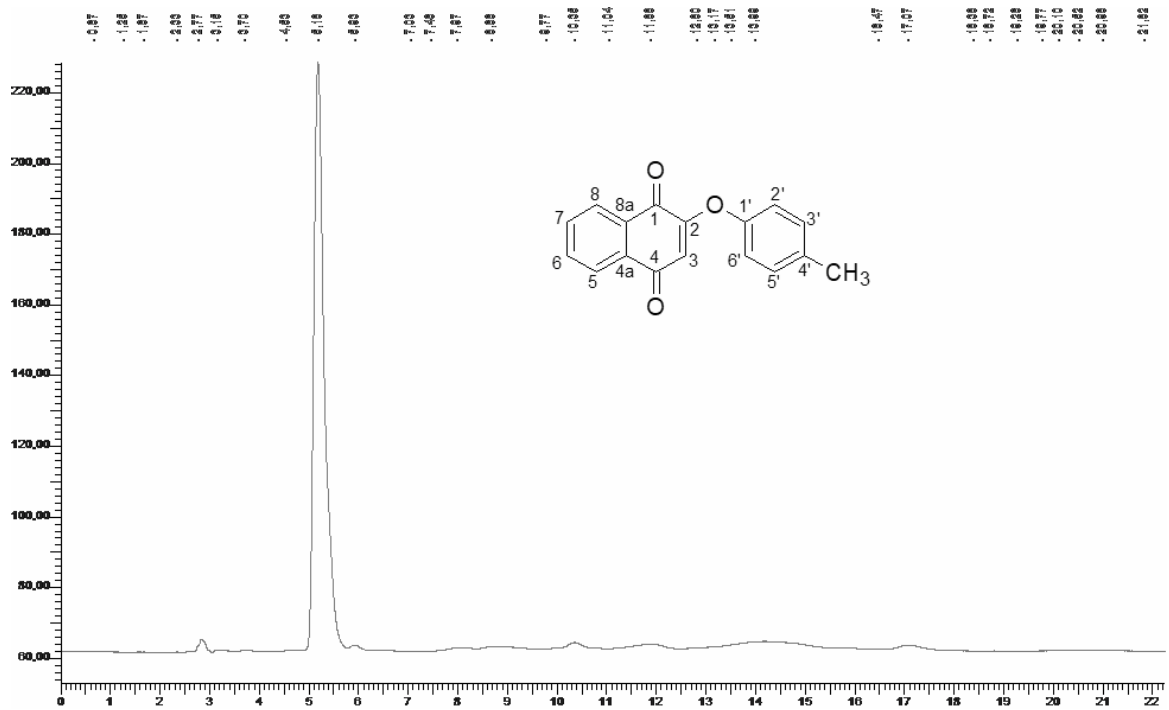
2-(4-methylphenoxy)-1,4-naphthoquinone **61** UV-Vis (MeOH)



2-(4-methylphenoxy)-1,4-naphthoquinone **61** IR (KBr pellet)



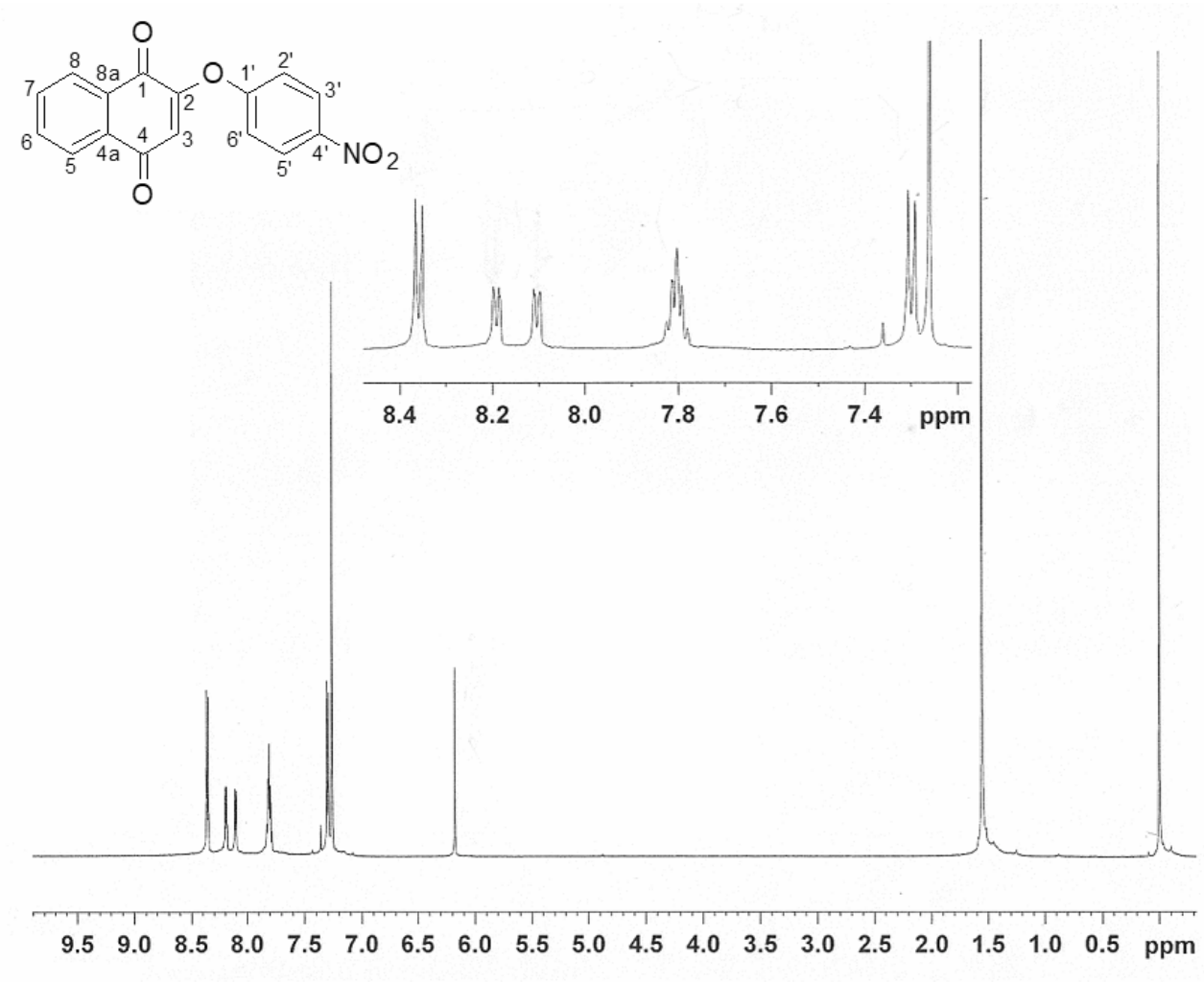
2-(4-methylphenoxy)-1,4-naphthoquinone **61** HPLC chromatogram (286 nm, 40% H_2O/MeOH)



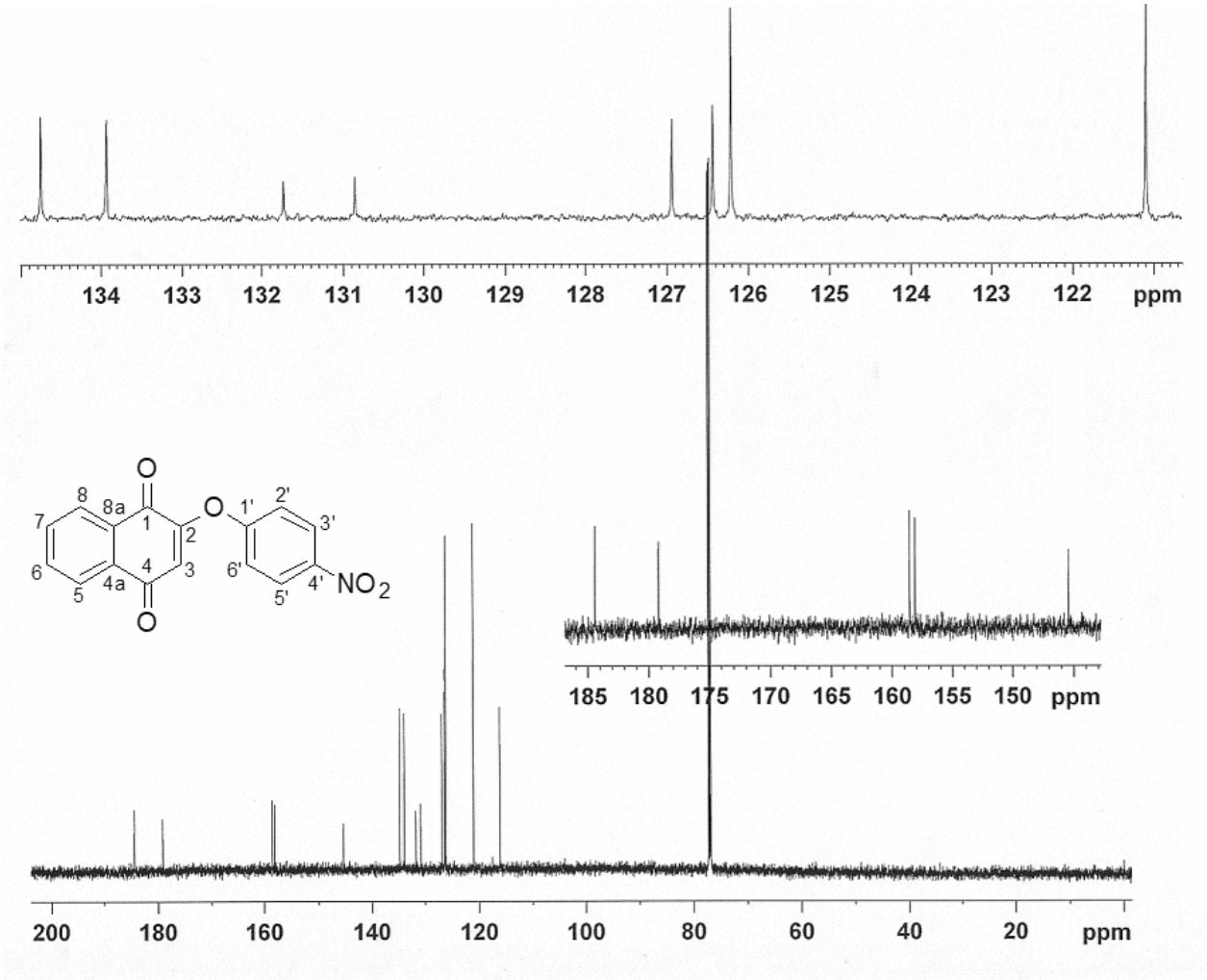
2-(4-nitrophenoxy)-1,4-naphthoquinone 62

62 was obtained according to general procedure III 2.1.3 and purified by cold base wash (MTBE as solvent and K_2CO_3 sat as base), column chromatography (benzene as eluent, isocratically) and recrystallization with isooctane. Yield 71 mg (24%), brown to yellow crystals, mp = (190.0 – 192.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.36 (2H, d J_{orto} = 7.5 Hz, ArH), 8.20 (1H, d, $J_{8\text{-}7}$ = 7.5 Hz, ArH), 8.11 (1H, d, $J_{5\text{-}6}$ = 7.5 Hz, ArH), 7.81 (2H, m, ArH), 7.30 (2H, d, J_{orto} = 7.5 Hz, ArH), 6.18 (1H, s, ArH). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.4, 179.2, 158.6, 158.1, 145.4, 134.8, 133.9, 131.7, 130.9, 126.9, 126.4, 126.2, 121.1, 116.2. IR (KBr pellet) cm^{-1}: 3050, 1686, 1646, 1616, 1587, 1514, 1340, 1229, 886. UV-Vis (MeOH) nm: 203, 250, 269 (max). TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_{10}NO_5$: 296.0559; found: 296.0592. Purity: 97.1%. MIC (µM): 212 (*S. aureus*), 3387 (*C. albicans*), >3000 (*E. coli*).

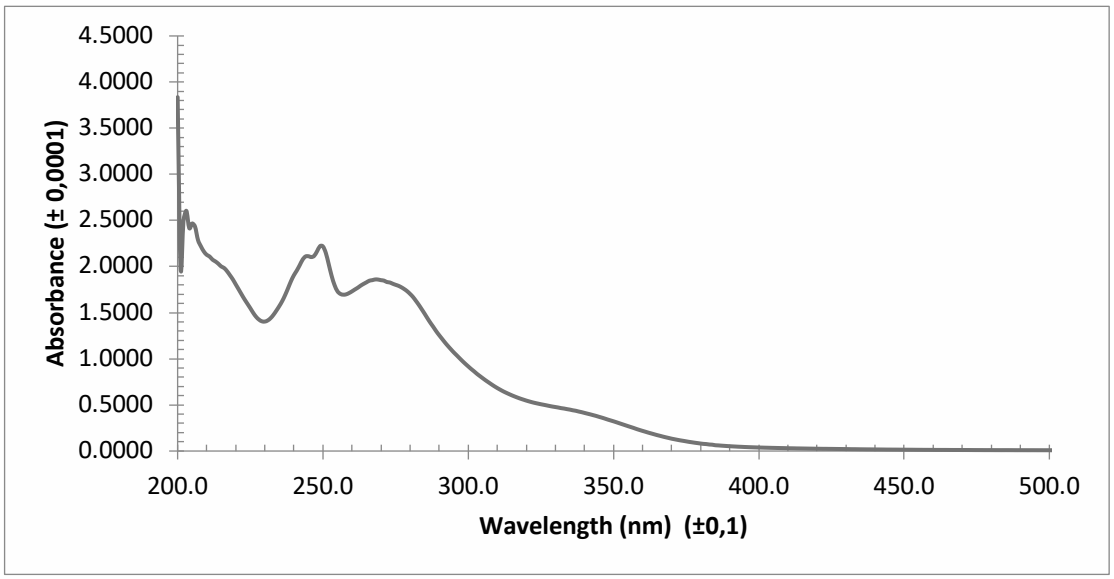
2-(4-nitrophenoxy)-1,4-naphthoquinone **62** ^{1}H NMR



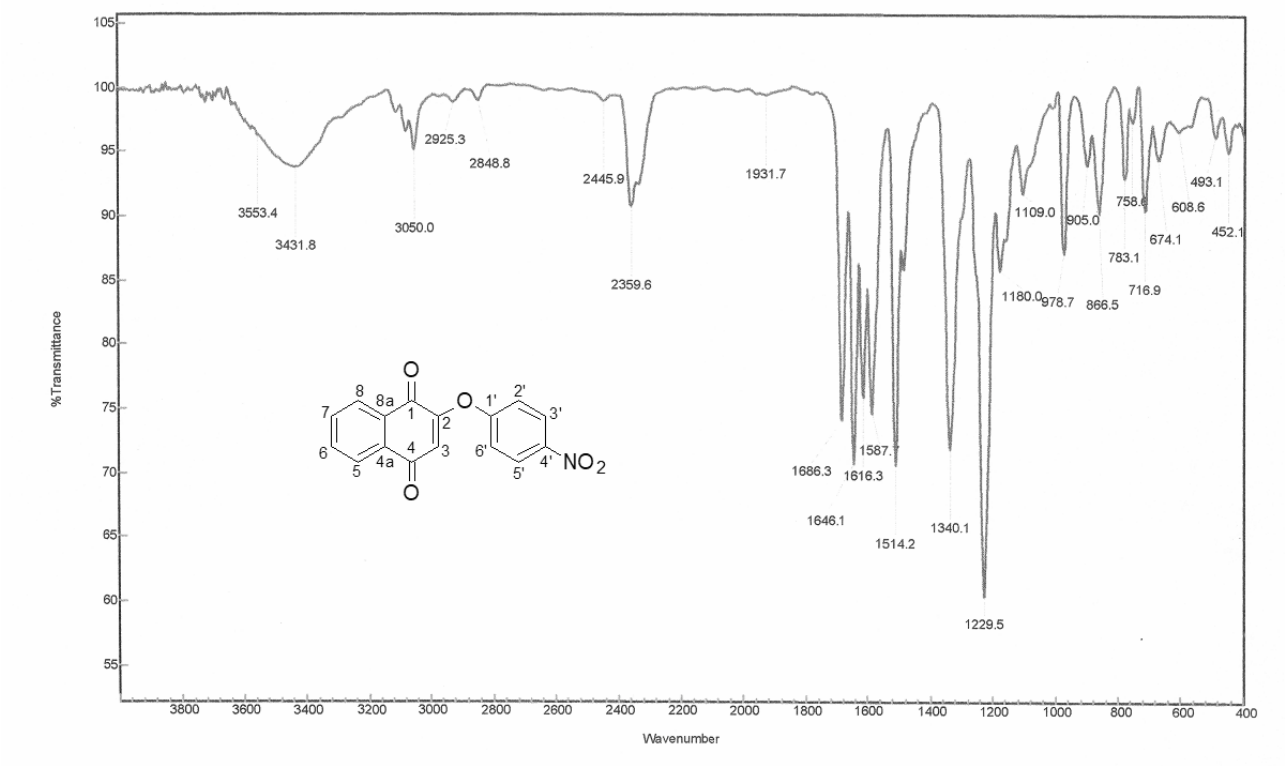
2-(4-nitrophenoxy)-1,4-naphthoquinone **62** ^{13}C NMR



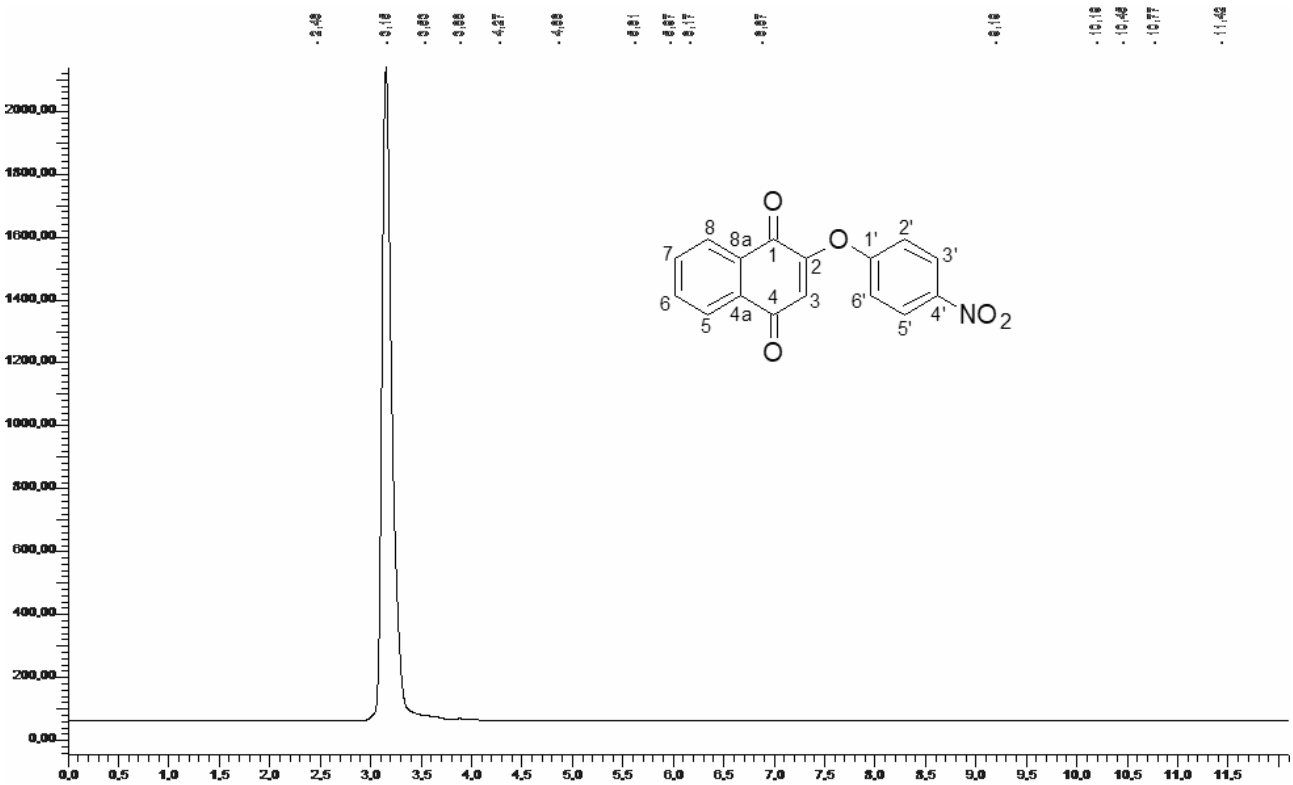
2-(4-nitrophenoxy)-1,4-naphthoquinone **62** UV-Vis (MeOH)



2-(4-nitrophenoxy)-1,4-naphthoquinone **62** IR (KBr pellet)



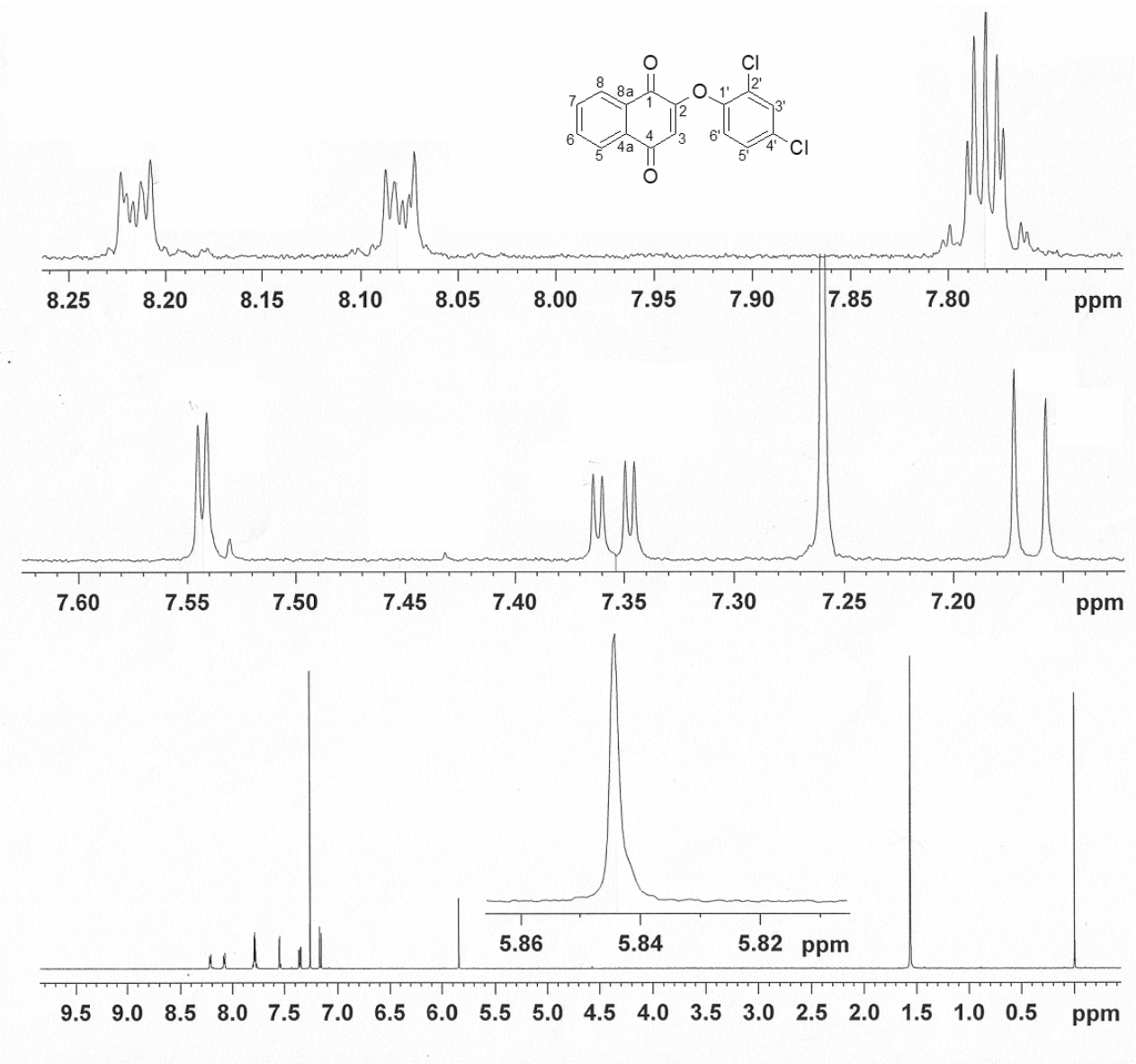
2-(4-nitrophenoxy)-1,4-naphthoquinone **62** HPLC chromatogram (270 nm, 100% MeCN)



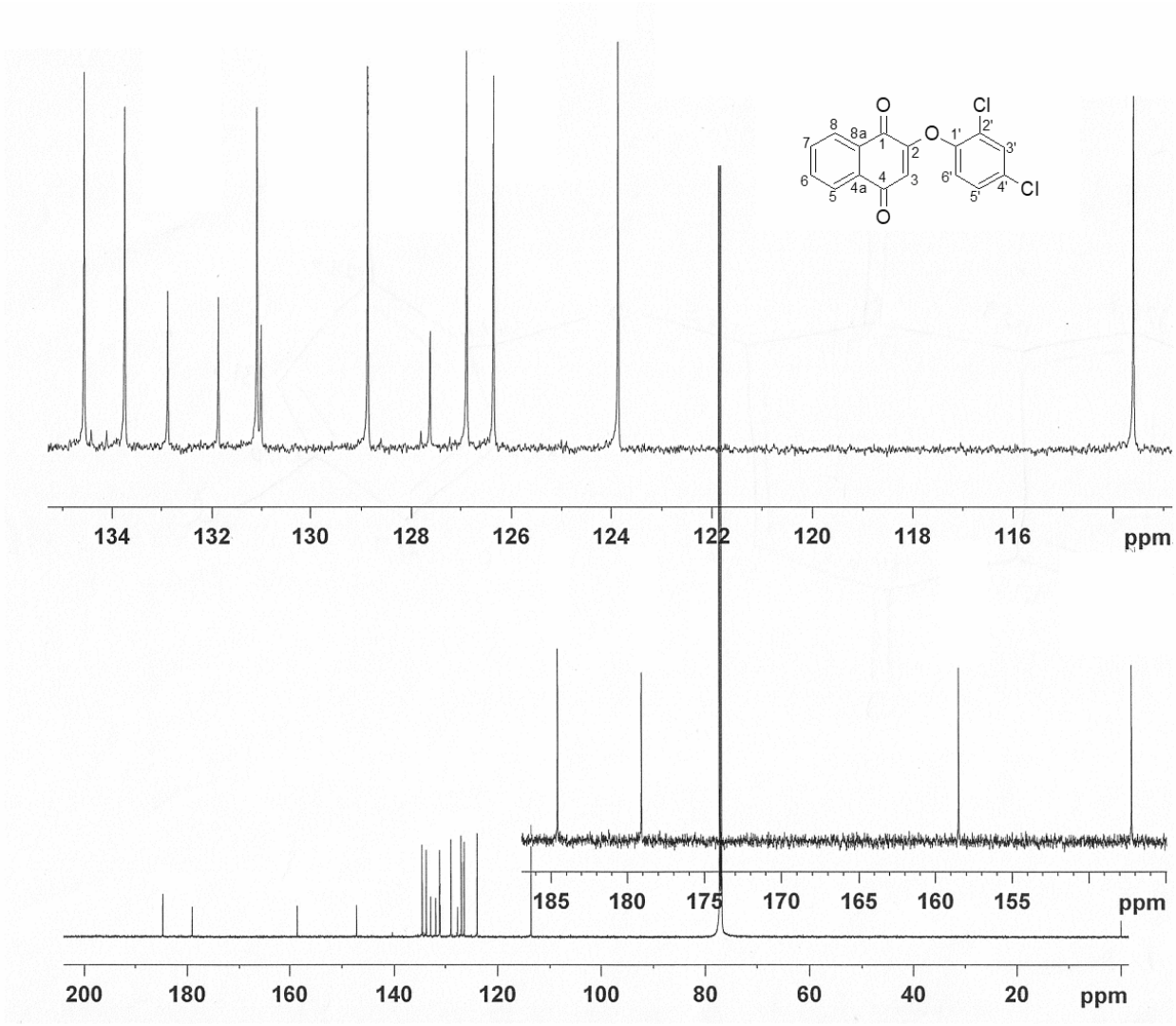
2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63**

63 was obtained according to general procedure III 2.1.3 and purified by hot extraction-filtration and recrystallization, both with isooctane. Yield 177 mg (56%), yellow needle crystals, mp = (127.0 – 130.0) °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 8.21 (1H, dd, *J* = 2.5 Hz, *J* = 6.7 Hz, ArH), 8.08 (1H, dd, *J* = 2.5 Hz, *J* = 6.7 Hz, ArH), 7.78 (2H, m, ArH), 7.54 (1H, d, J_{meta} = 2.3 Hz, ArH), 7.35 (1H, dd, J_{meta} = 3.0 Hz, J_{ortho} = 8.3 Hz, ArH), 7.16 (1H, d, J_{ortho} = 8.3 Hz, ArH), 5.84 (1H, s, ArH),. ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) = 184.6, 179.1, 158.5, 147.2, 134.6, 133.7, 132.9, 131.9, 131.1, 131.0, 128.9, 127.6, 126.9, 126.4, 123.9, 113.6. IR (KBr pellet) cm^{-1}: 3094, 1685, 1653, 1613, 1474, 1262, 1242, 982. UV-Vis (MeOH) nm: 219, 249(max), 268, 333. TOF-MS: m/z $[M+H]^+$ calc for $C_{16}H_9O_3Cl_2$: 318.9929; found: 318.9928. Purity: 98.3%. MIC (µM): 49 (*S. aureus*), >3000 (*C. albicans*), >3000 (*E. coli*).

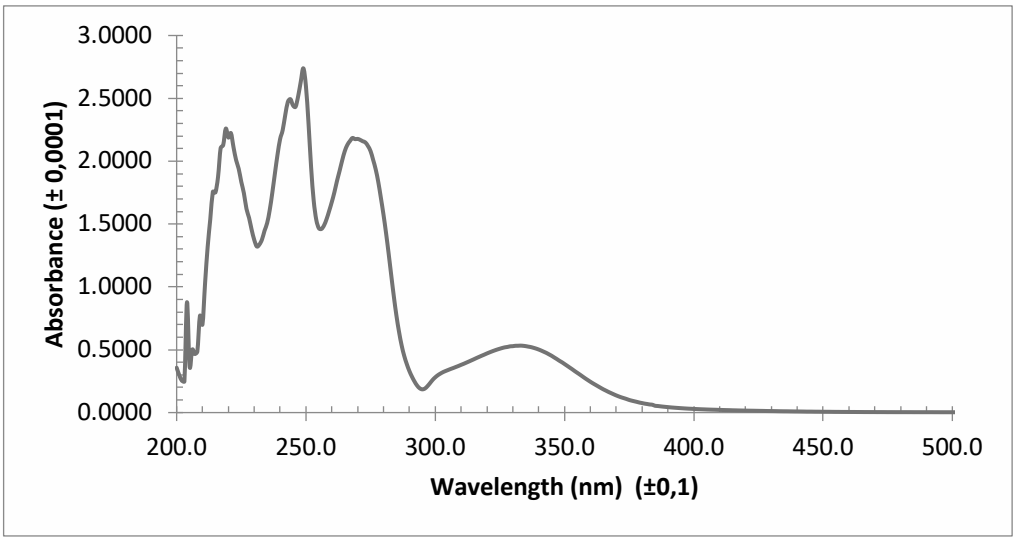
2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63** ^{1}H NMR



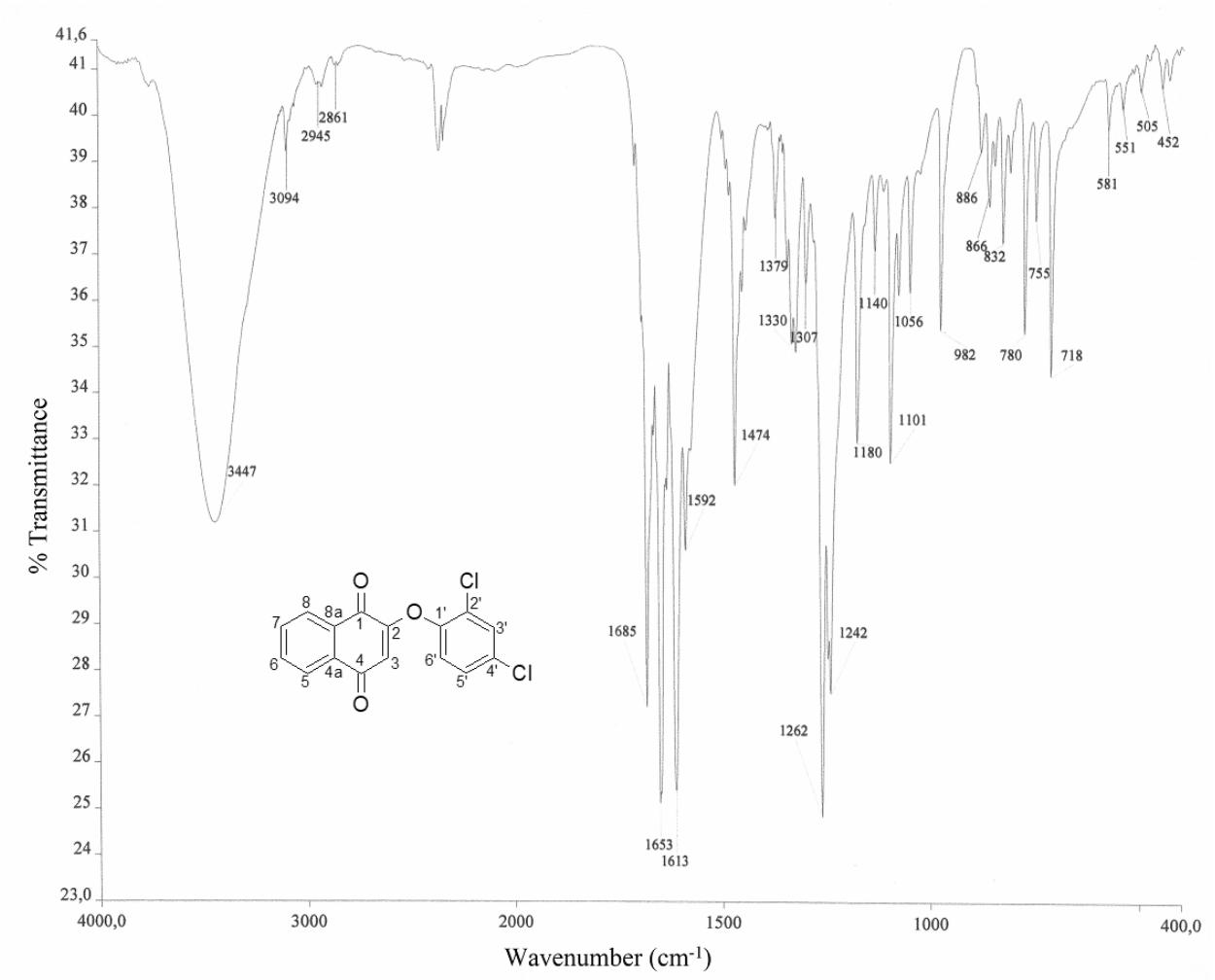
2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63** ^{13}C NMR



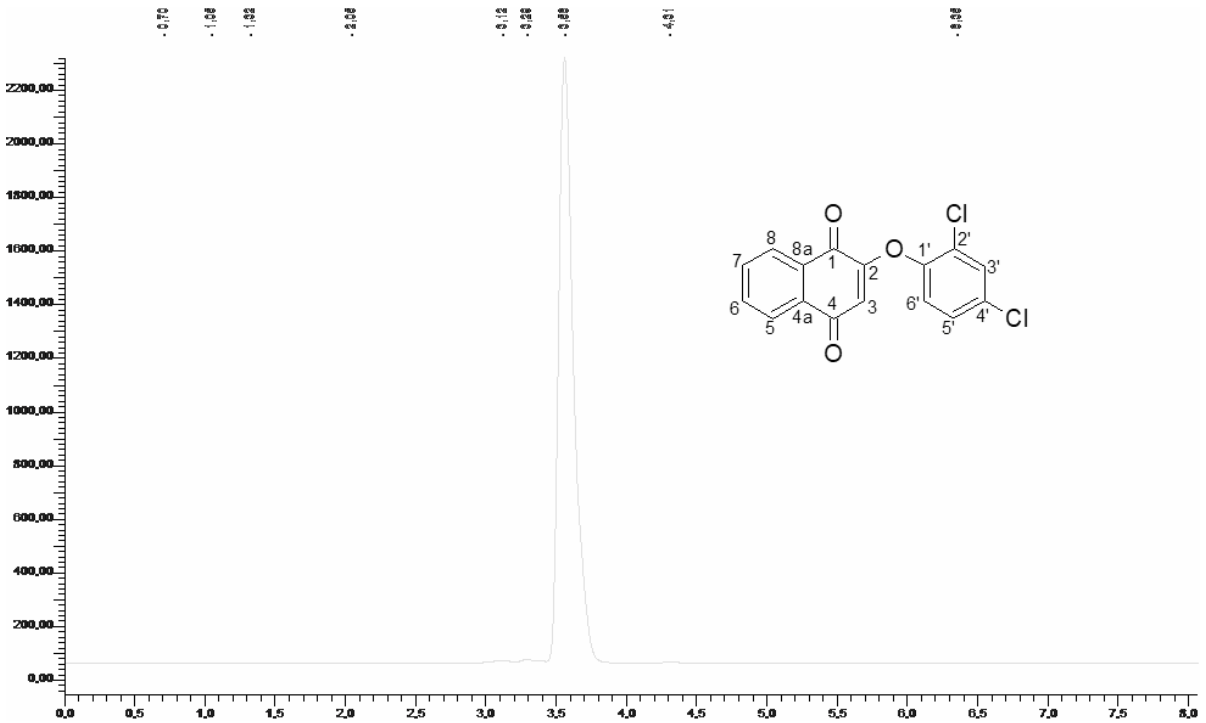
2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63** UV-Vis (MeOH)



2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63** IR (KBr pellet)



2-(2,4-dichlorophenoxy)-1,4-naphthoquinone **63** HPLC chromatogram (270 nm, 100% MeCN)



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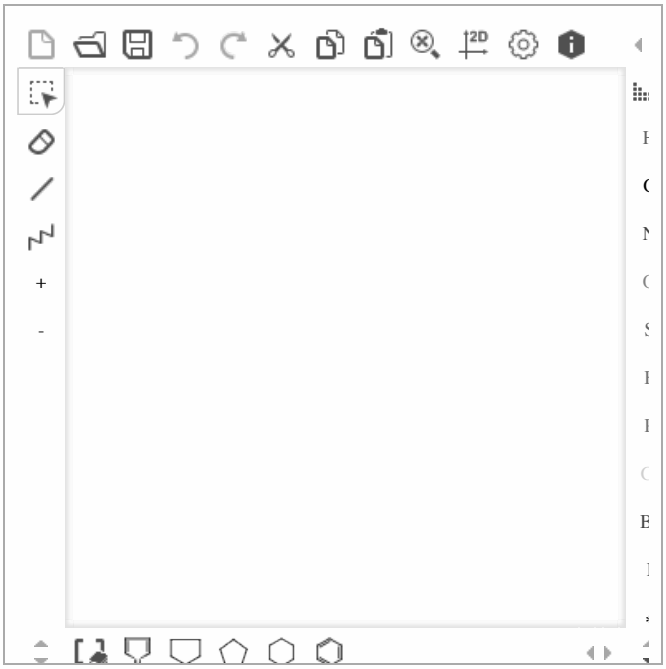
The main article describing the web service and its underlying methodologies is SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* (2017) 7:42717.
For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
For details about development and validation of the BOILED-Egg, please refer to this article: A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* (2016) 11(11):1117-1121.

Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.



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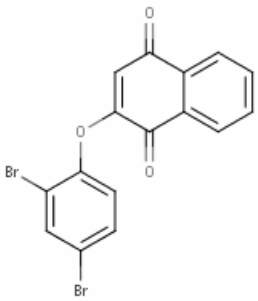
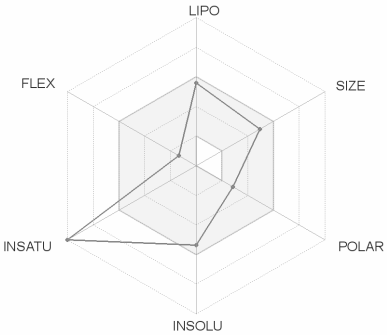
Molecule 1





SMILES Brc1ccc(c(c1)Br)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H8Br2O3
Molecular weight	408.04 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	85.66
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-5.36
Solubility	1.77e-03 mg/ml ; 4.33e-06 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.91
Solubility	4.98e-03 mg/ml ; 1.22e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.89
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.29
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.55
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.93
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.68
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.91
Solubility	5.01e-05 mg/ml ; 1.23e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.87	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.74 cm/s

Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

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SwissADME

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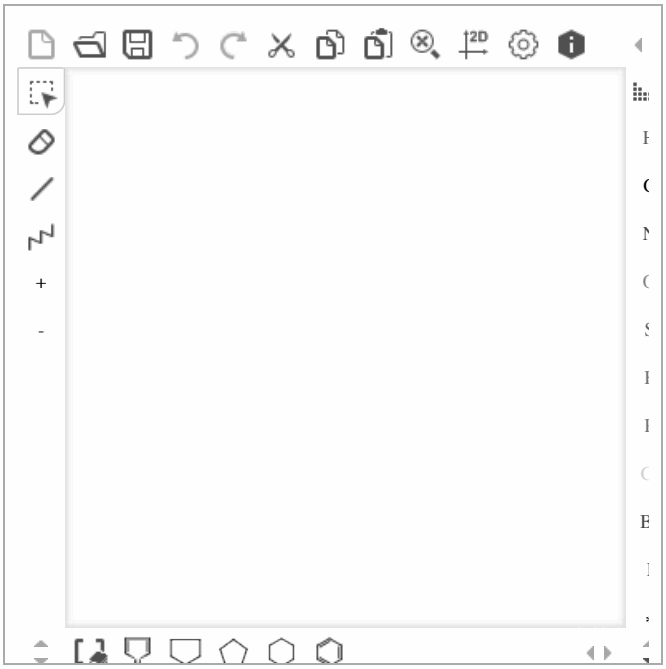

Enter a list of SMILES here:

Clc3ccc(OC2=CC(=O)c1ccccc1C2=O)c(Cl)c3

Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

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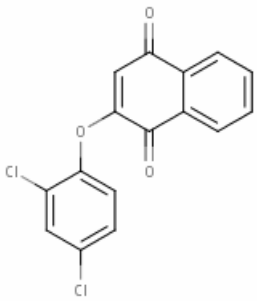
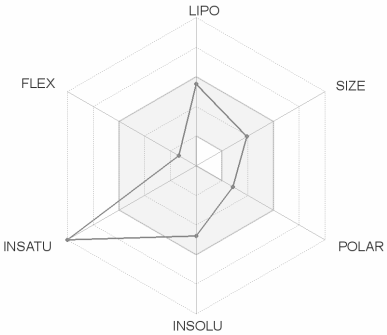
Molecule 1





SMILES Clc1ccc(c(c1)Cl)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H8Cl2O3
Molecular weight	319.14 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	80.28
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.73
Solubility	5.94e-03 mg/ml ; 1.86e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.78
Solubility	5.31e-03 mg/ml ; 1.66e-05 mol/l
Class	
Solubility class: Log *S*	

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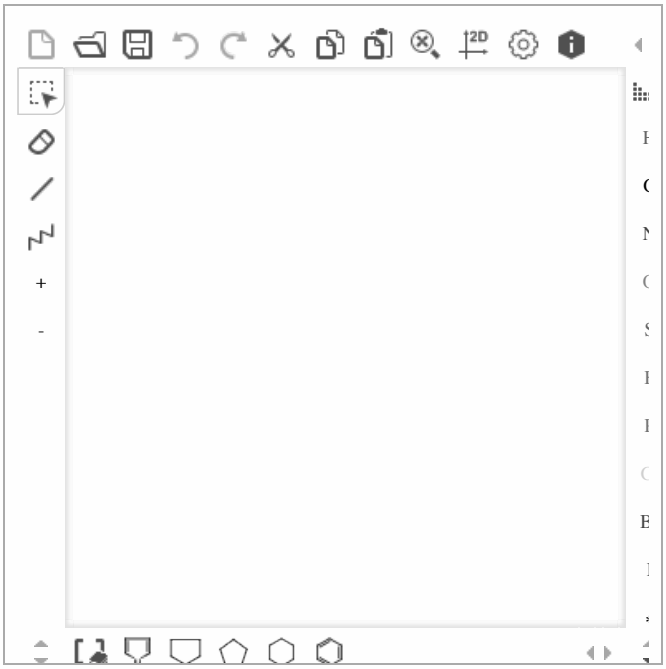

Enter a list of SMILES here:

Brc3cc(Br)cc(Br)c3OC2=CC(=O)c1ccccc1C2=O

Fill with an example | Clear | Run!

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Retrieve data: CSV

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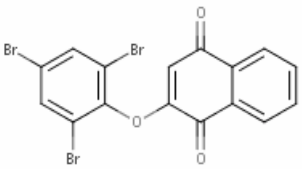
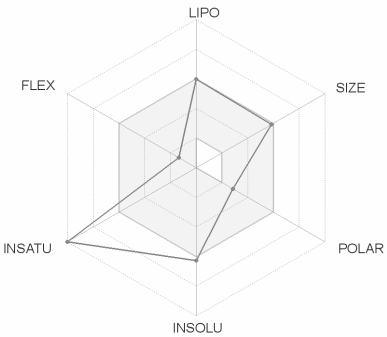
Molecule 1





SMILES Brc1cc(Br)c(c(c1)Br)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H7Br3O3
Molecular weight	486.94 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	93.36
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-6.27
Solubility	2.63e-04 mg/ml ; 5.39e-07 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.63
Solubility	1.14e-03 mg/ml ; 2.35e-06 mol/l
Class	
Solubility class: Log *S*	

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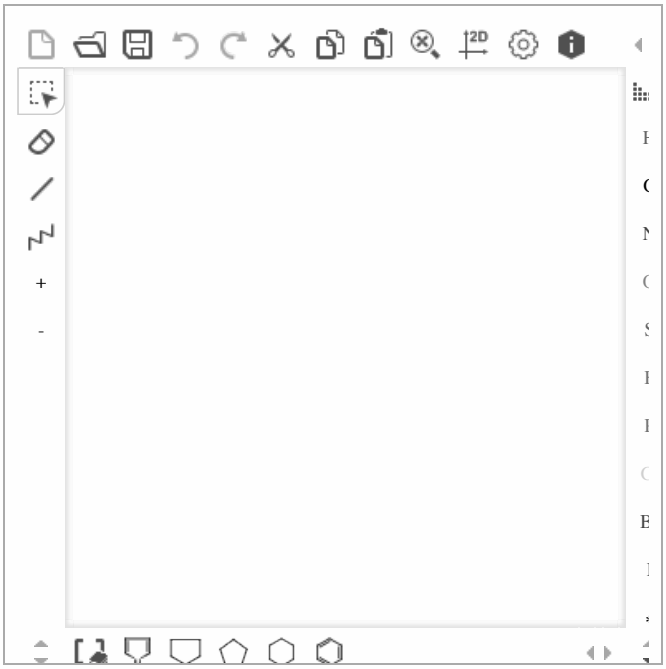

Enter a list of SMILES here:

Clc1ccc(cc1Cl)OC3=CC(=O)c2ccccc2C3=O

Fill with an example | Clear | Run!

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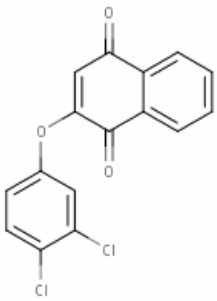
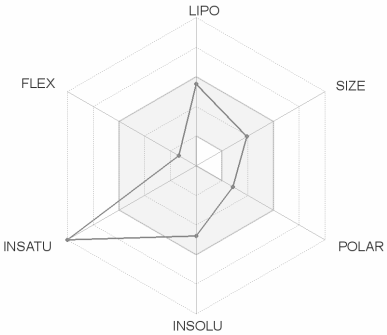
Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccc(c(c1)Cl)Cl

Physicochemical Properties

Formula	C16H8Cl2O3
Molecular weight	319.14 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	80.28
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.73
Solubility	5.94e-03 mg/ml ; 1.86e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.78
Solubility	5.31e-03 mg/ml ; 1.66e-05 mol/l
Class	
Solubility class: Log *S*	

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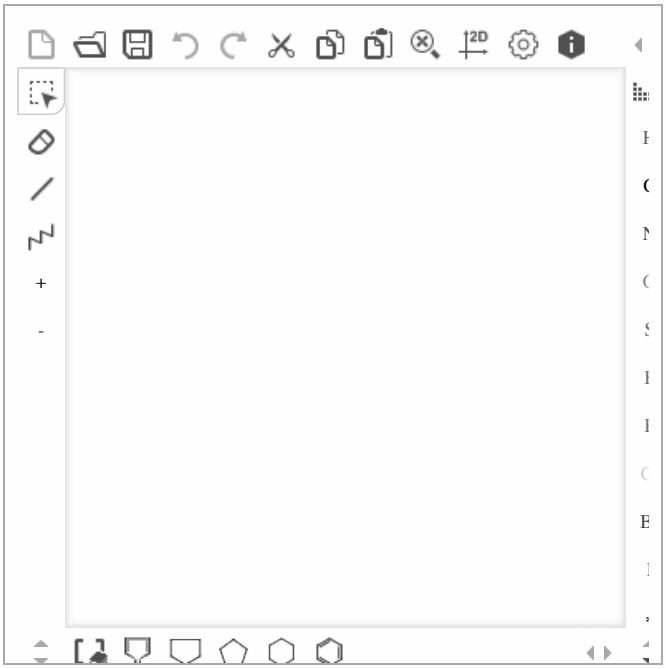


Enter a list of SMILES here:

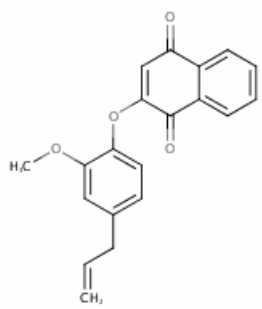
C=CCc3ccc(OC2=CC(=O)c1ccccc1C2=O)c(OC)c3

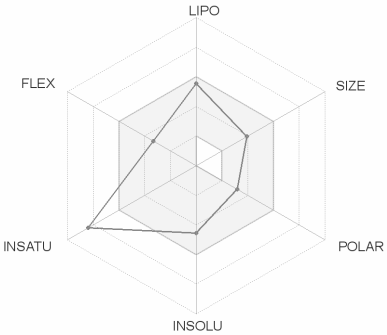
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES C=CCc1ccc(c(c1)OC)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C20H16O4
Molecular weight	320.34 g/mol
Num. heavy atoms	24
Num. arom. heavy atoms	12
Fraction Csp3	0.10
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Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	90.85
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.53
Solubility	9.43e-03 mg/ml ; 2.94e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.05
Solubility	2.89e-03 mg/ml ; 9.01e-06 mol/l
Class	
Solubility class: Log *S*	

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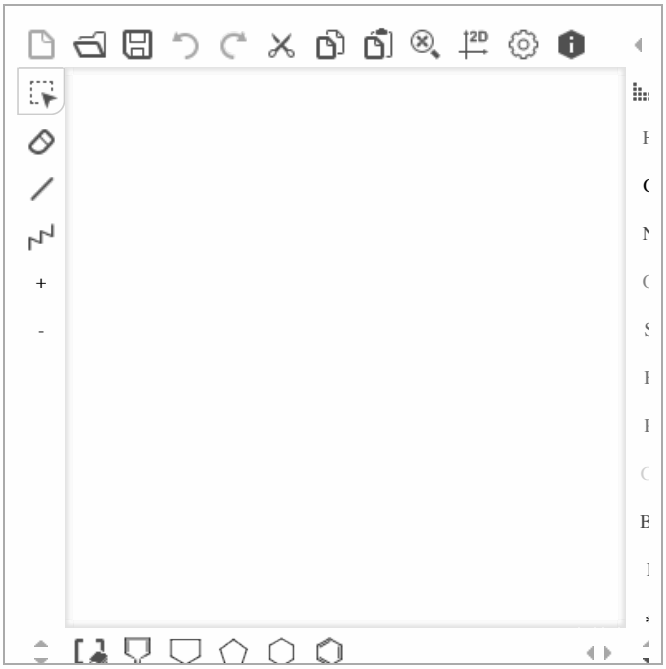


Enter a list of SMILES here:

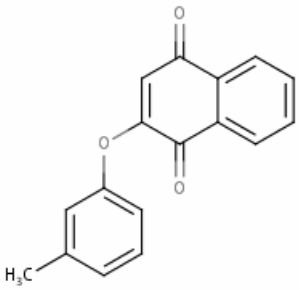
Cc1cc(ccc1)OC3=CC(=O)c2ccccc2C3=O

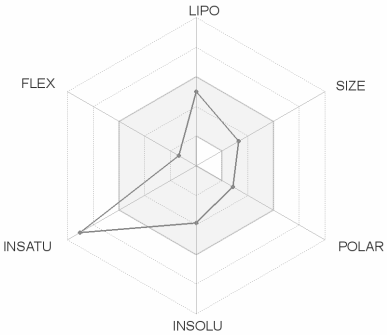
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





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Physicochemical Properties

Formula	C17H12O3
Molecular weight	264.28 g/mol
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Num. arom. heavy atoms	12
Fraction Csp3	0.06
Num. rotatable bonds	2
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Molar Refractivity	75.22
TPSA	

Water Solubility

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Solubility 3.73e-02 mg/ml ; 1.41e-04 mol/l

Class

Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly Soluble

Log *S* (Ali)

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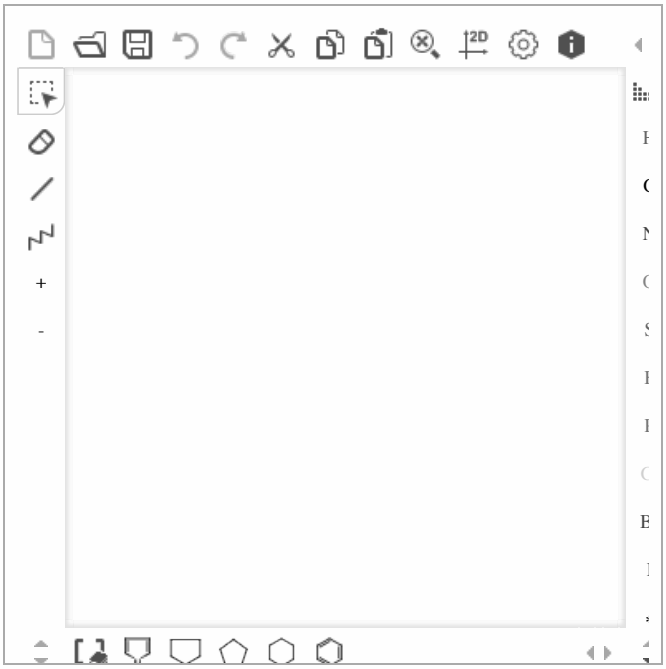

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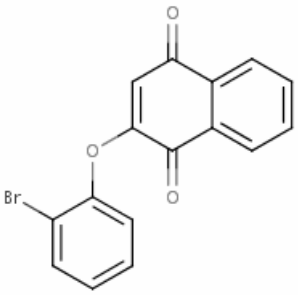
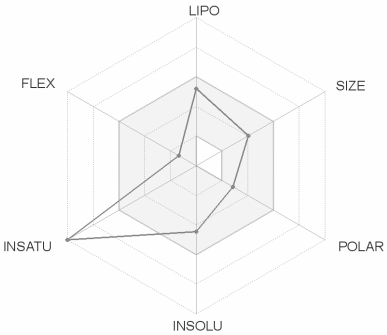
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





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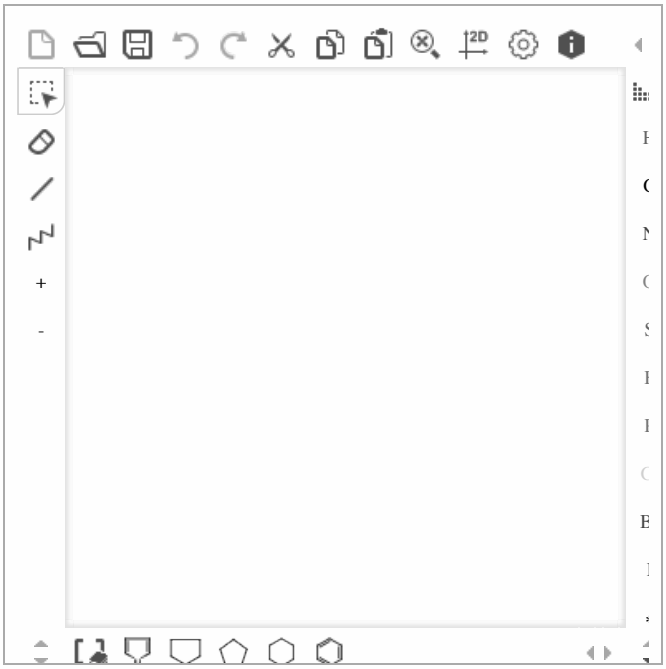

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Cc3ccccc3OC2=CC(=O)c1ccccc1C2=O

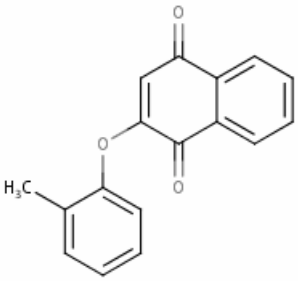
Fill with an example | Clear | Run!

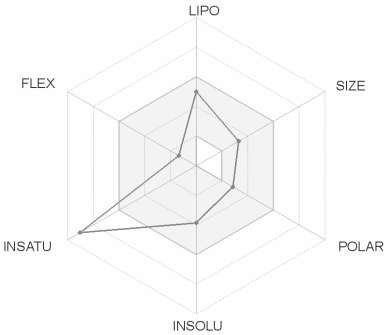
Show BOILED-Egg

Retrieve data:

Powered by ChemAxon

Molecule 1





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TPSA	

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Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-3.85
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Class	
Solubility class: Log *S*	

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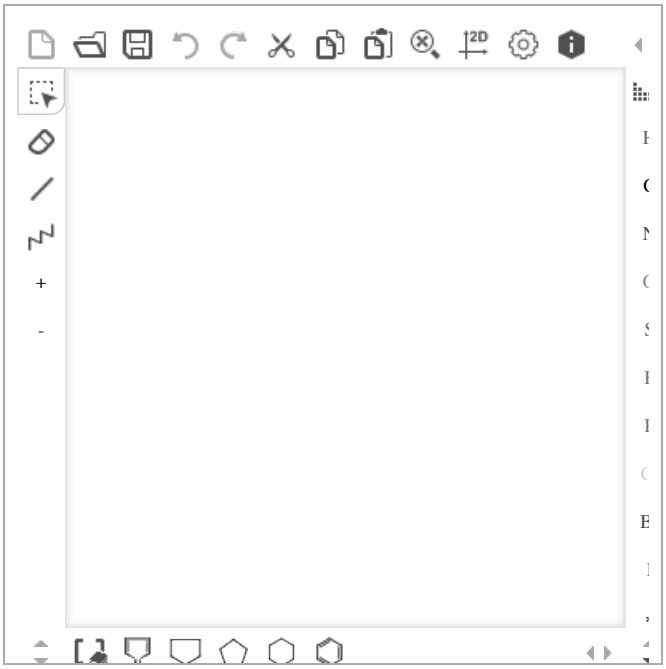


Enter a list of SMILES here:

COc3ccccc3OC2=CC(=O)c1ccccc1C2=O

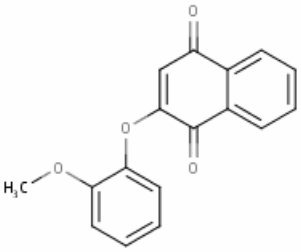
Fill with an example | Clear | Run!

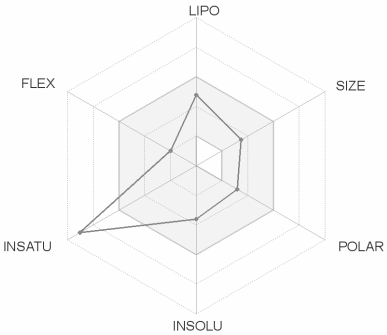
Show BOILED-Egg

Retrieve data:

Powered by ChemAxon

Molecule 1





SMILES COc1ccccc1OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C17H12O4
Molecular weight	280.27 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.06
Num. rotatable bonds	3
Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	76.75
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model. -3.62

Solubility 6.77e-02 mg/ml ; 2.42e-04 mol/l

Class

Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model. -3.64

Solubility 6.36e-02 mg/ml ; 2.27e-04 mol/l

Class

Solubility class: Log *S*

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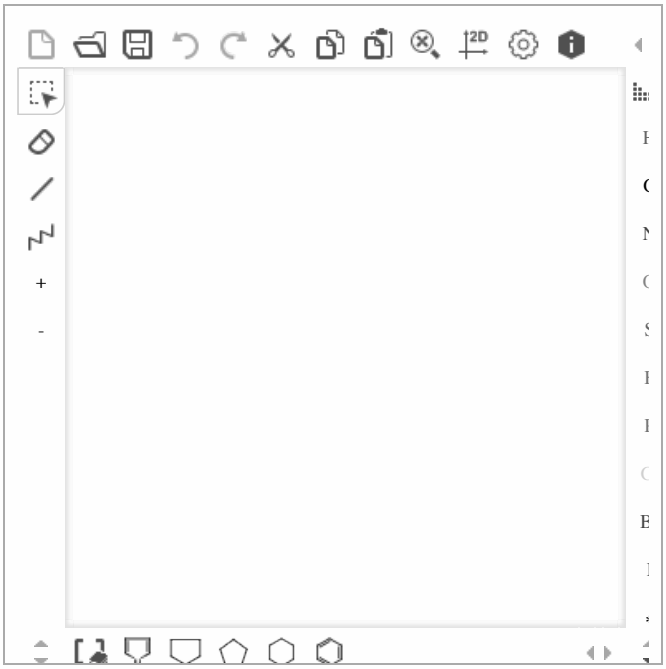

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Fill with an example | Clear | Run!

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Powered by ChemAxon

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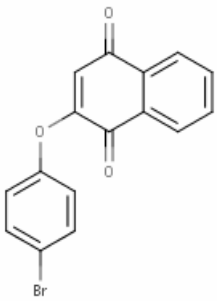

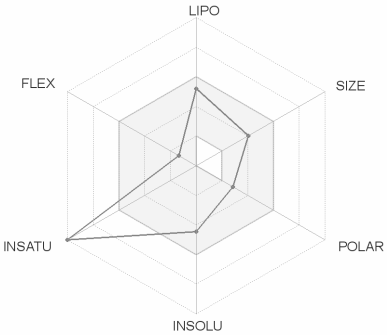

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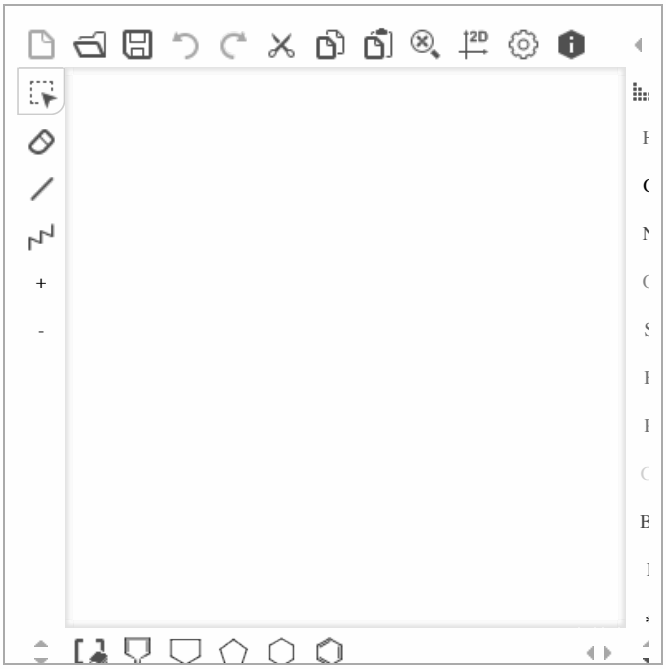

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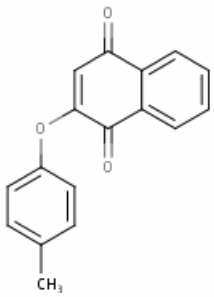

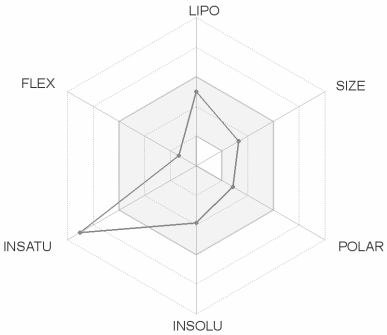

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Click here to proceed.

SwissADME

This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.

The main article describing the web service and its underlying methodologies is SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* (2017) 7:42717.
For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
For details about development and validation of the BOILED-Egg, please refer to this article: A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* (2016) 11(11):1117-1121.

Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.

In order to avoid security-related warning messages when switching to secured connection, you may want either to:

- confirm the exception on the next page, or
- import our CA key in your web browser

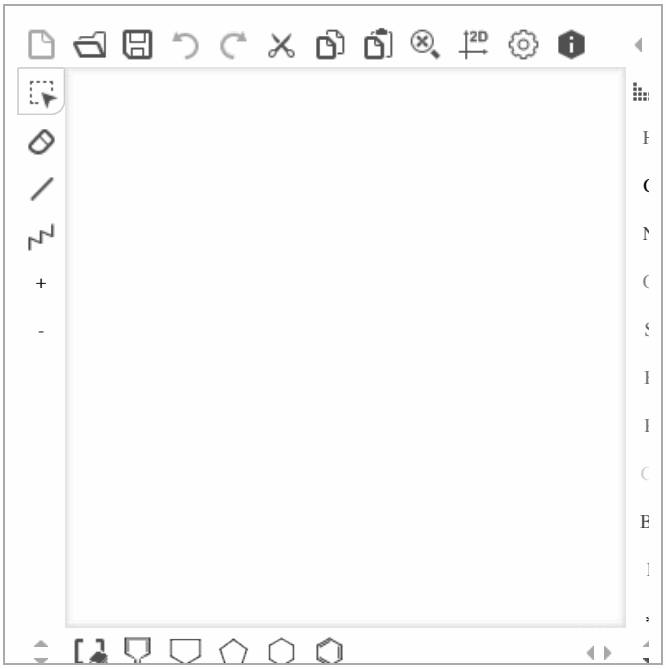
Click here to proceed.

SwissADME

This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.

The main article describing the web service and its underlying methodologies is SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* (2017) 7:42717.
For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
For details about development and validation of the BOILED-Egg, please refer to this article: A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* (2016) 11(11):1117-1121.

Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.



Enter a list of SMILES here:

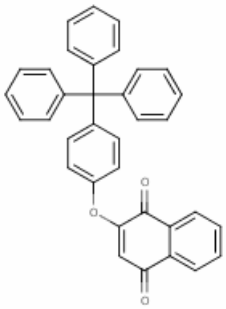
O=C6C=C(Oc1ccc(cc1)C(c2ccccc2)(c3ccccc3)c4ccccc4)C(=O)c5ccccc56

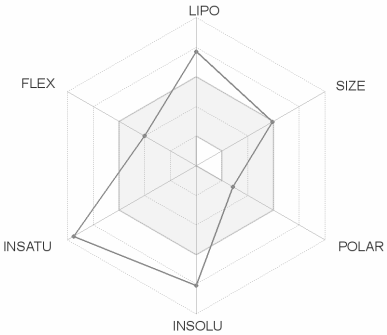
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccc(cc1)C(c1ccccc1)(c1ccccc1)c1ccccc1

Physicochemical Properties

Formula	C35H24O3
Molecular weight	492.56 g/mol
Num. heavy atoms	38
Num. arom. heavy atoms	30
Fraction Csp3	0.03
Num. rotatable bonds	6
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	148.57
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-8.09
Solubility	4.00e-06 mg/ml ; 8.12e-09 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-8.71
Solubility	9.57e-07 mg/ml ; 1.94e-09 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	4.29
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	7.95
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	7.41
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	4.99
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	7.82
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-12.72
Solubility	9.36e-11 mg/ml ; 1.90e-13 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Insoluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	Low
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	No
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	6.49	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	No
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	No
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-3.66 cm/s

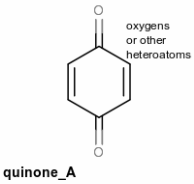
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 1 violation: MLOGP>4.15
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	No; 3 violations: MW>480, WLOGP>5.6, MR>130
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	No; 1 violation: WLOGP>5.88
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	No; 1 violation: XLOGP3>5

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

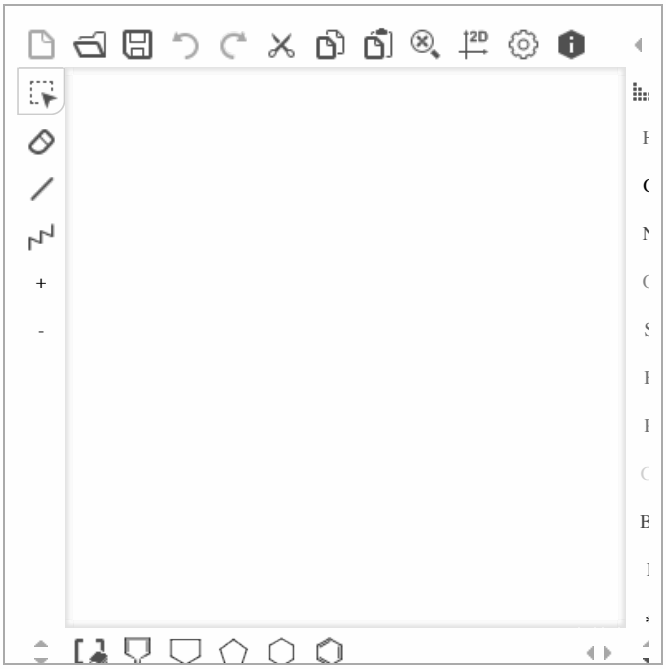
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	4.50



Enter a list of SMILES here:

CC(C)(C)c1ccc(cc1)OC3=CC(=O)c2ccccc2C3=O

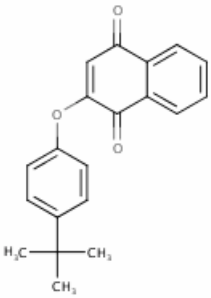
Fill with an example | Clear | Run!

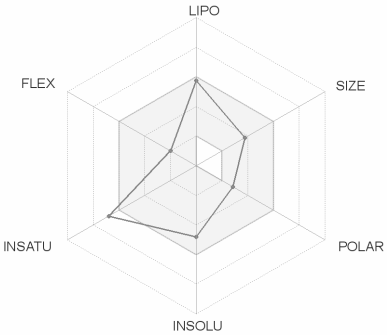
Show BOILED-Egg

Retrieve data:

Powered by ChemAxon

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccc(cc1)C(C)(C)C

Physicochemical Properties

Formula	C20H18O3
Molecular weight	306.36 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	12
Fraction Csp3	0.20
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	89.53
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.81
Solubility	4.71e-03 mg/ml ; 1.54e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.21
Solubility	1.87e-03 mg/ml ; 6.10e-06 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.10
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.58
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.33
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.62
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.66
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.49
Solubility	9.94e-05 mg/ml ; 3.24e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.86	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-4.92 cm/s

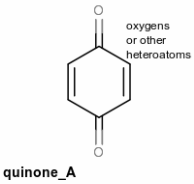
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.22

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.50
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.27
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.34
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.92
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.85
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.68
Solubility	5.50e-04 mg/ml ; 2.08e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.98	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.59 cm/s

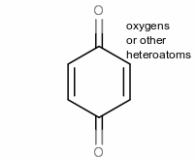
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A

Brenk

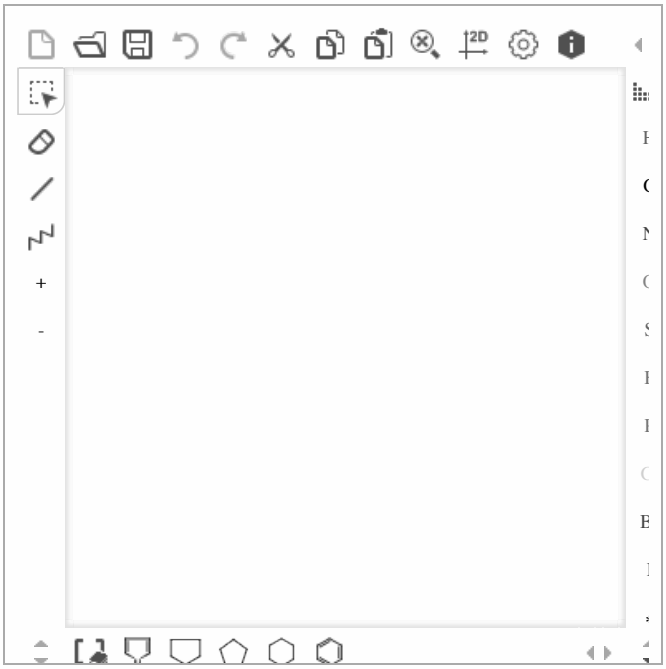
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.91



Enter a list of SMILES here:

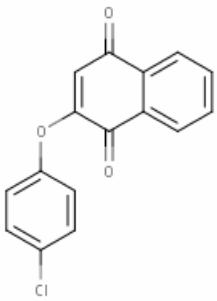
Clc1ccc(cc1)OC3=CC(=O)c2ccccc2C3=O

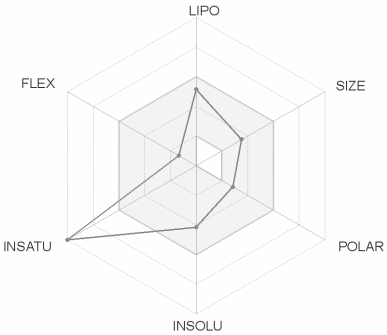
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES Clc1ccc(cc1)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H9ClO3
Molecular weight	284.69 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	75.27
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.15
Solubility	2.03e-02 mg/ml ; 7.12e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.14
Solubility	2.08e-02 mg/ml ; 7.32e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.54
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.54
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.68
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.19
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.98
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.90
Solubility	3.55e-04 mg/ml ; 1.25e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.19	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.52 cm/s

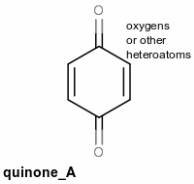
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.79

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.65
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.60
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.79
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.31
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.01
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.12
Solubility	2.51e-04 mg/ml ; 7.62e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.27	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.75 cm/s

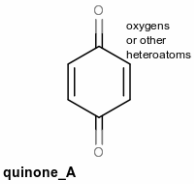
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

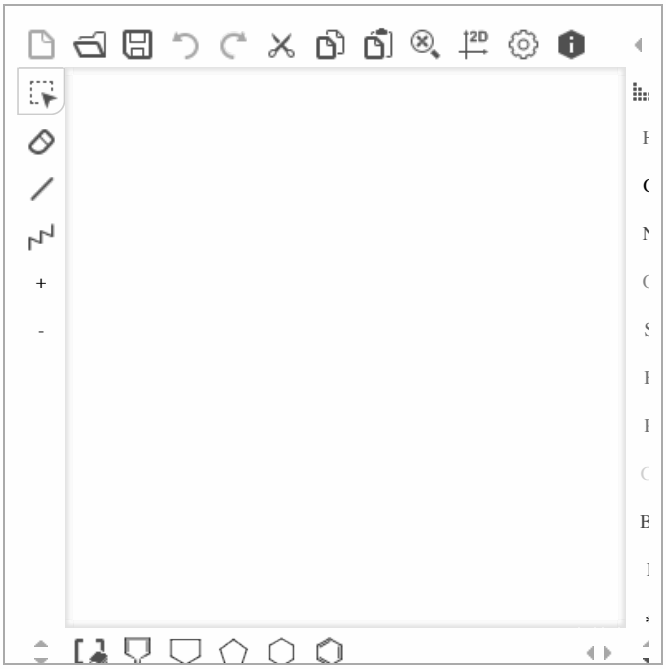
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.80



Enter a list of SMILES here:

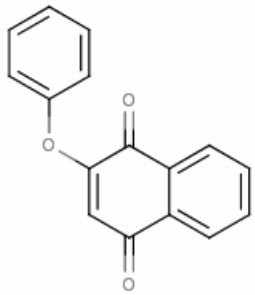
O=C3C=C(Oc1ccccc1)C(=O)c2ccccc23

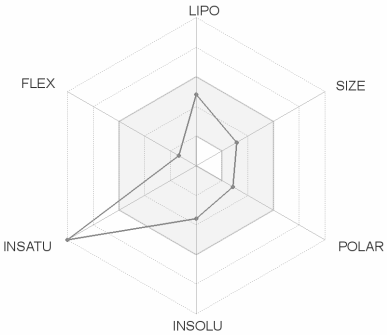
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccccc1

Physicochemical Properties

Formula	C16H10O3
Molecular weight	250.25 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	70.26
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model. -3.56

Solubility 6.89e-02 mg/ml ; 2.75e-04 mol/l

Class

Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model. -3.48

Solubility 8.25e-02 mg/ml ; 3.30e-04 mol/l

Class

Solubility class: Log *S*

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.25
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.91
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.03
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.68
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.36
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.30
Solubility	1.26e-03 mg/ml ; 5.05e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.65	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	No
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.76 cm/s

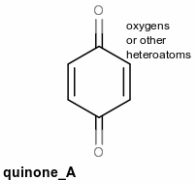
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.81

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	52.60 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.45
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.88
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.04
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.34
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.38
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.42
Solubility	1.07e-03 mg/ml ; 3.83e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.62	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.96 cm/s

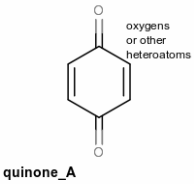
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

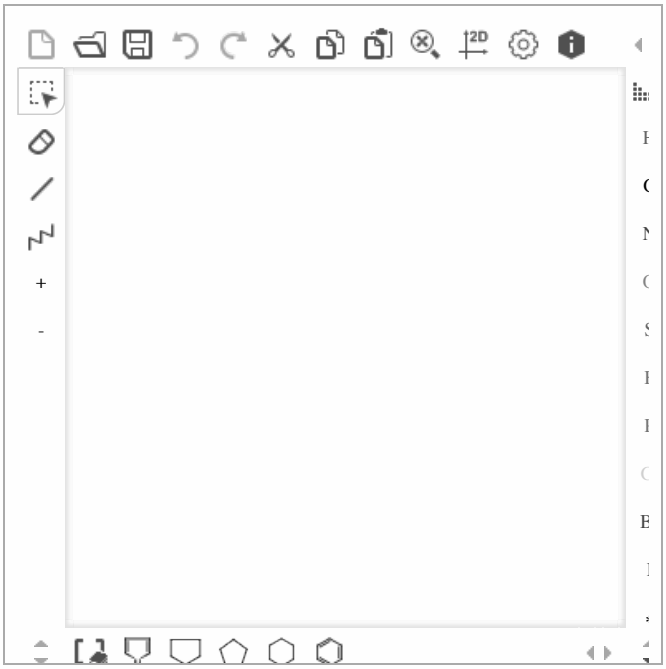
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.96



Enter a list of SMILES here:

[O-][N+](=O)c3ccccc3OC2=CC(=O)c1ccccc1C2=O

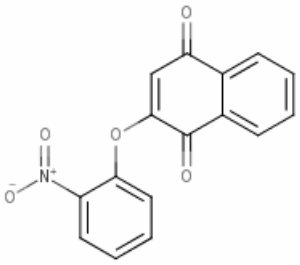
Fill with an example | Clear | Run!

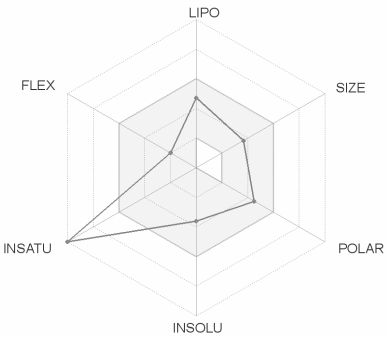
Show BOILED-Egg

Retrieve data: CSV

Powered by ChemAxon

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccccc1[N+](=O)[O-]

Physicochemical Properties

Formula	C16H9NO5
Molecular weight	295.25 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	5
Num. H-bond donors	0
Molar Refractivity	79.08
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-3.60
Solubility	7.38e-02 mg/ml ; 2.50e-04 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.27
Solubility	1.59e-02 mg/ml ; 5.40e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	89.19 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	1.73
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.74
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	2.94
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.48
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	1.15
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-4.66
Solubility	6.40e-03 mg/ml ; 2.17e-05 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	No
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	No

Average of all five predictions	2.01	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-6.16 cm/s

Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

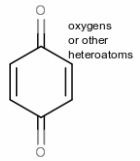
Abbott Bioavailability Score: Probability of F ≥ 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.

1 alert: quinone_A

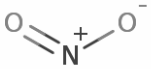


quinone_A

2 alerts: nitro_group, oxygen-nitrogen_single_bond

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem



nitro_group

oxygen-nitrogen_single_bon

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules (r^2 = 0.94)	2.99

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.49
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.27
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.34
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.92
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.85
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.68
Solubility	5.50e-04 mg/ml ; 2.08e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.97	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.59 cm/s

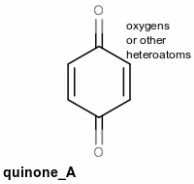
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

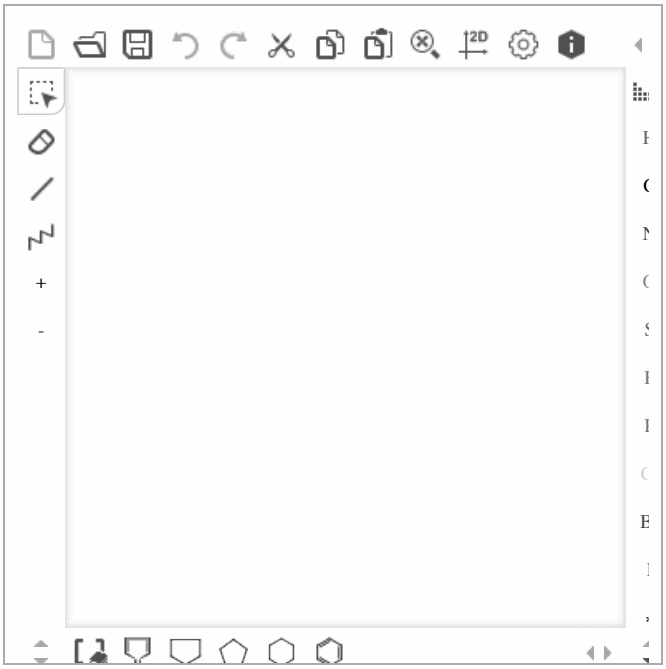
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.99



Enter a list of SMILES here:

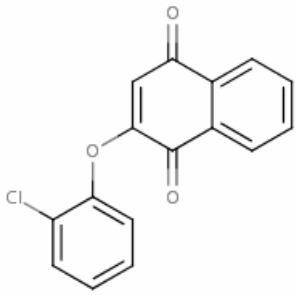
Clc3ccccc3OC2=CC(=O)c1ccccc1C2=O

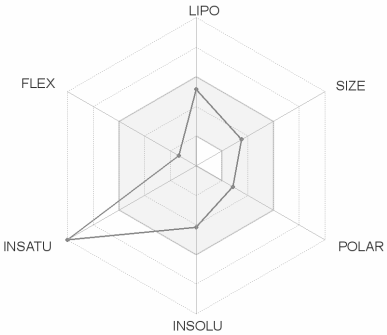
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES Clc1ccccc1OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H9ClO3
Molecular weight	284.69 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	75.27
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.15
Solubility	2.03e-02 mg/ml ; 7.12e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.14
Solubility	2.08e-02 mg/ml ; 7.32e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.45
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.54
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.68
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.19
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.98
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.90
Solubility	3.55e-04 mg/ml ; 1.25e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.17	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.52 cm/s

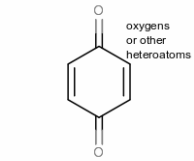
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.82

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.56
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.60
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.79
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.31
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.01
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.12
Solubility Class	2.51e-04 mg/ml ; 7.62e-07 mol/l
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.26	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.75 cm/s

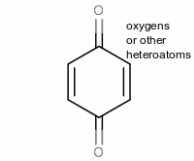
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A

Brenk

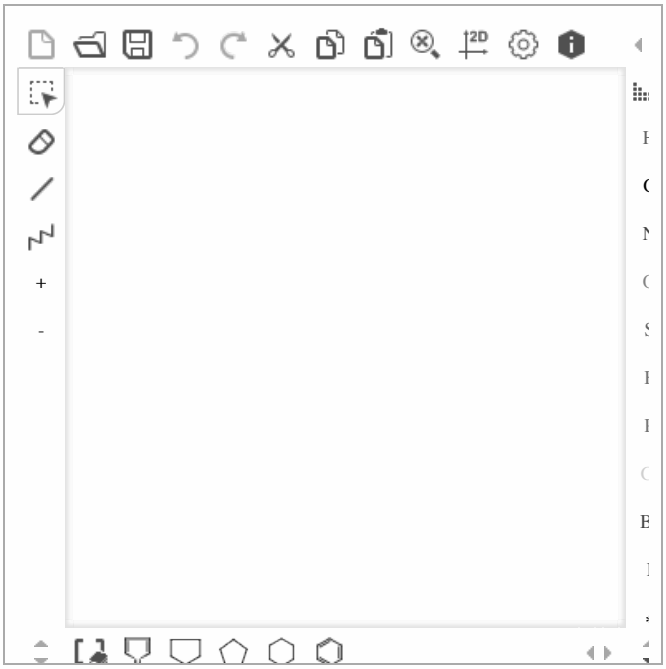
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.81



Enter a list of SMILES here:

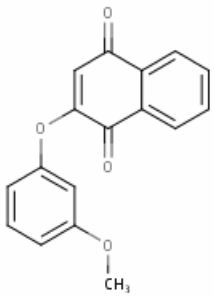
COc1cccc(c1)OC3=CC(=O)c2ccccc2C3=O

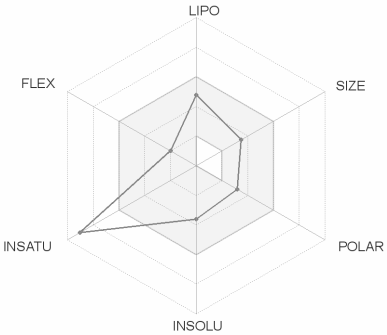
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES COc1cccc(c1)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C17H12O4
Molecular weight	280.27 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.06
Num. rotatable bonds	3
Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	76.75
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model. -3.62

Solubility 6.77e-02 mg/ml ; 2.42e-04 mol/l

Class

Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model. -3.64

Solubility 6.36e-02 mg/ml ; 2.27e-04 mol/l

Class

Solubility class: Log *S*

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	52.60 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.56
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.88
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.04
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.34
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.38
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.42
Solubility	1.07e-03 mg/ml ; 3.83e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.64	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.96 cm/s

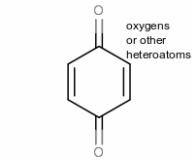
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A

Brenk

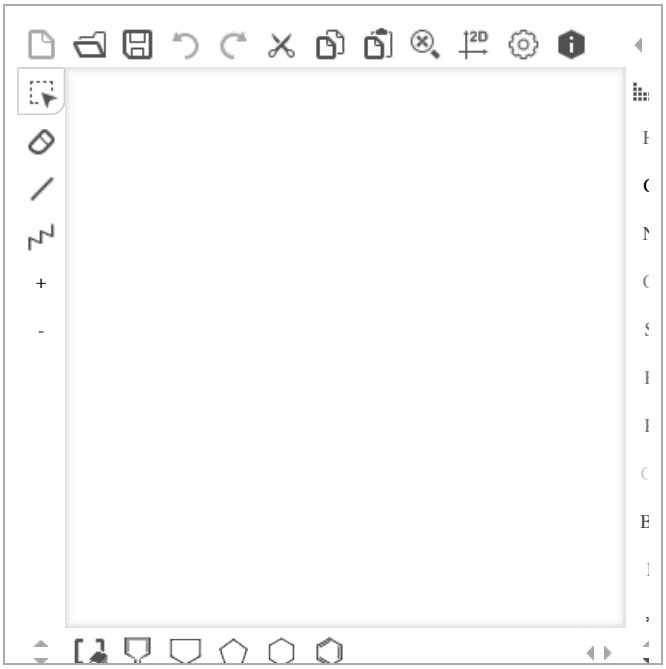
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.01



Enter a list of SMILES here:

[O-][N+](=O)c1cccc(c1)OC3=CC(=O)c2ccccc2C3=O

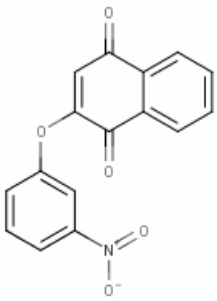
Fill with an example | Clear | Run!

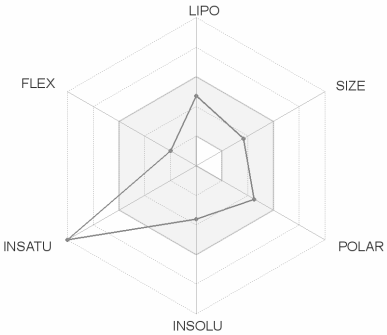
Show BOILED-Egg

Retrieve data:

Powered by ChemAxon

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1cccc(c1)[N+](=O)[O-]

Physicochemical Properties

Formula	C16H9NO5
Molecular weight	295.25 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	5
Num. H-bond donors	0
Molar Refractivity	79.08
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-3.60
Solubility	7.38e-02 mg/ml ; 2.50e-04 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.27
Solubility	1.59e-02 mg/ml ; 5.40e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	89.19 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.01
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.74
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	2.94
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.48
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	1.15
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-4.66
Solubility	6.40e-03 mg/ml ; 2.17e-05 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	No
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.06	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-6.16 cm/s

Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

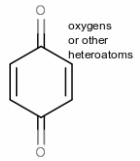
Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.

1 alert: quinone_A

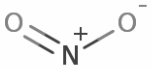


quinone_A

2 alerts: nitro_group, oxygen-nitrogen_single_bond

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem



nitro_group

oxygen-nitrogen_single_bon

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.01

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.52
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.27
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.34
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.92
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.85
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.68
Solubility	5.50e-04 mg/ml ; 2.08e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.98	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.59 cm/s

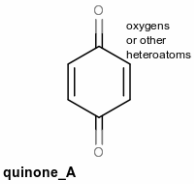
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

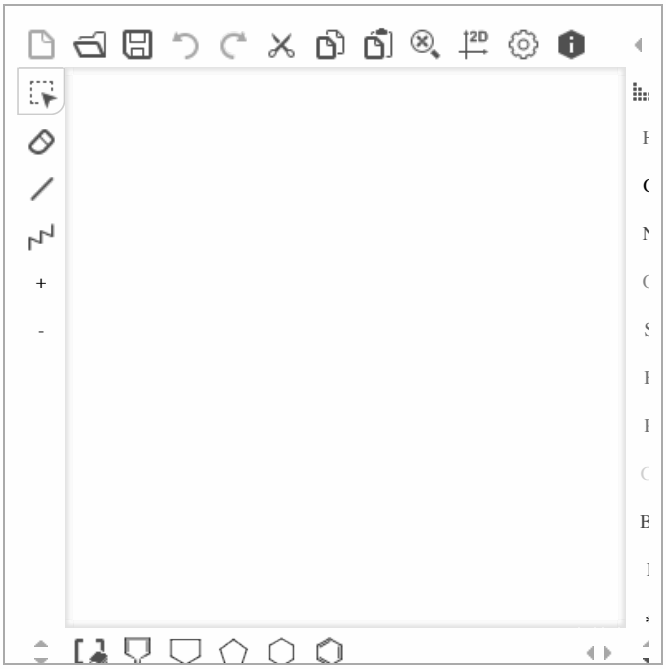
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.90



Enter a list of SMILES here:

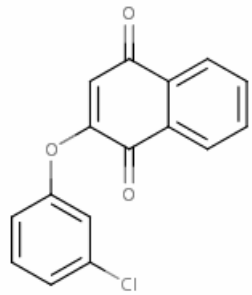
Clc1cccc(c1)OC3=CC(=O)c2ccccc2C3=O

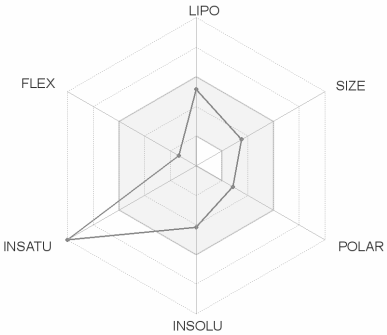
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES Clc1cccc(c1)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H9ClO3
Molecular weight	284.69 g/mol
Num. heavy atoms	20
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	75.27
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.15
Solubility	2.03e-02 mg/ml ; 7.12e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.14
Solubility	2.08e-02 mg/ml ; 7.32e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.53
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	3.54
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.68
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.19
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.98
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.90
Solubility	3.55e-04 mg/ml ; 1.25e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.18	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.52 cm/s

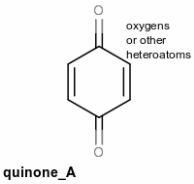
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.83

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	52.60 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.05
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.23
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.77
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.97
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.64
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.25
Solubility	1.80e-04 mg/ml ; 5.62e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

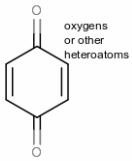
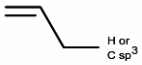
Average of all five predictions	3.53	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.25 cm/s

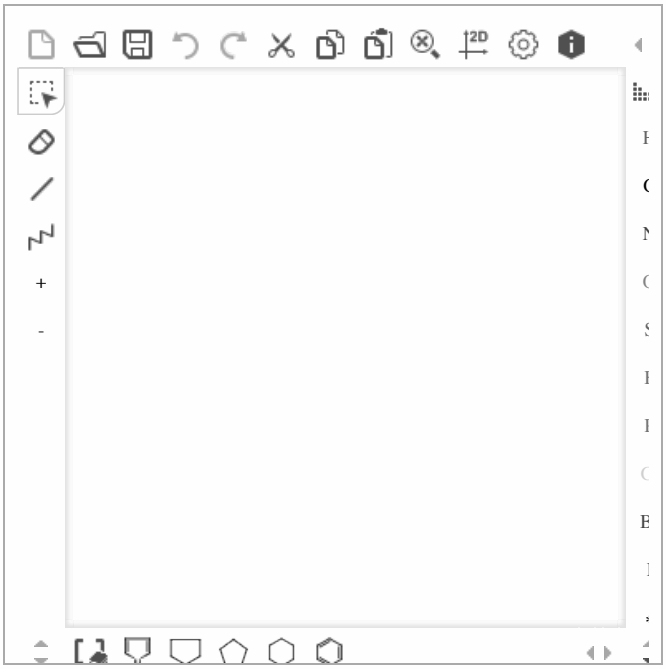
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS **Pan Assay Interference Structures:** implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A
Brenk **Structural Alert:** implemented from Brenk R. et al. 2008 ChemMedChem	1 alert: isolated_alkene  isolated_alkene
Leadlikeness **Leadlikeness:** implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5
Synthetic accessibility **Synthetic accessibility score:** from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.21



Enter a list of SMILES here:

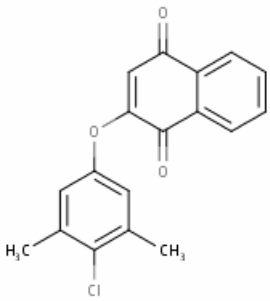
Cc1cc(cc(C)c1Cl)OC3=CC(=O)c2ccccc2C3=O

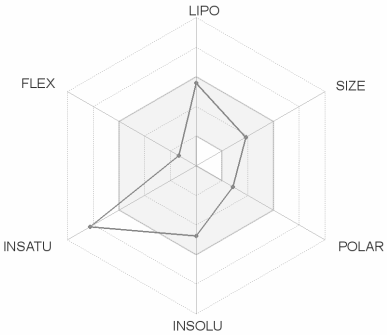
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1cc(C)c(c(c1)C)Cl

Physicochemical Properties

Formula	C18H13ClO3
Molecular weight	312.75 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.11
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	85.20
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.73
Solubility	5.76e-03 mg/ml ; 1.84e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.88
Solubility	4.10e-03 mg/ml ; 1.31e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.96
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.26
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.30
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.66
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.99
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.67
Solubility	6.75e-05 mg/ml ; 2.16e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.83	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.18 cm/s

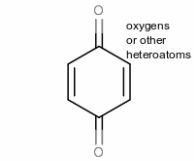
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A  quinone_A

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.99

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.70
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.16
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.34
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.70
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.60
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.50
Solubility	1.00e-04 mg/ml ; 3.13e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.70	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.29 cm/s

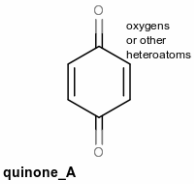
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

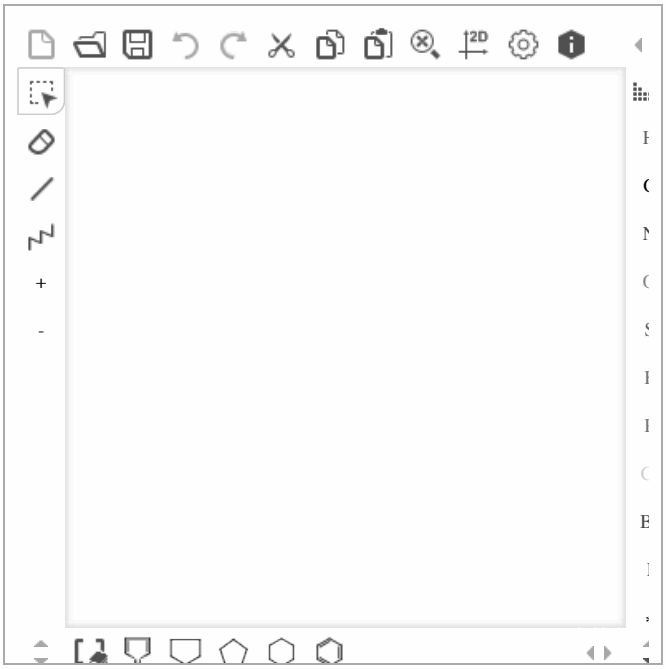
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.85



Enter a list of SMILES here:

Clc3cc(Cl)cc(Cl)c3OC2=CC(=O)c1ccccc1C2=O

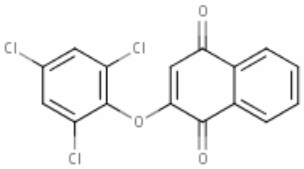
Fill with an example | Clear | Run!

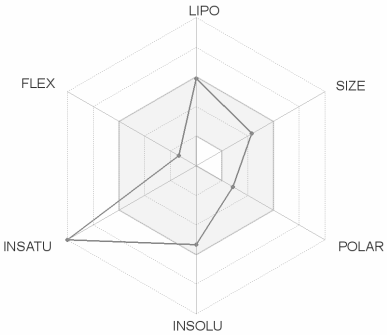
Show BOILED-Egg

Retrieve data: CSV

Powered by ChemAxon

Molecule 1





SMILES Clc1cc(Cl)c(c(c1)Cl)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C16H7Cl3O3
Molecular weight	353.58 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	85.29
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-5.32
Solubility	1.69e-03 mg/ml ; 4.77e-06 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.43
Solubility	1.31e-03 mg/ml ; 3.69e-06 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.77
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.79
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.99
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	3.20
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	5.24
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-7.10
Solubility	2.82e-05 mg/ml ; 7.96e-08 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	4.20	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.06 cm/s

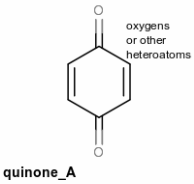
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.87

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.11
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.98
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	5.32
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	3.54
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	5.35
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-7.68
Solubility	1.01e-05 mg/ml ; 2.07e-08 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	4.46	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.73 cm/s

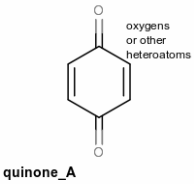
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	No; 1 violation: MW>480
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

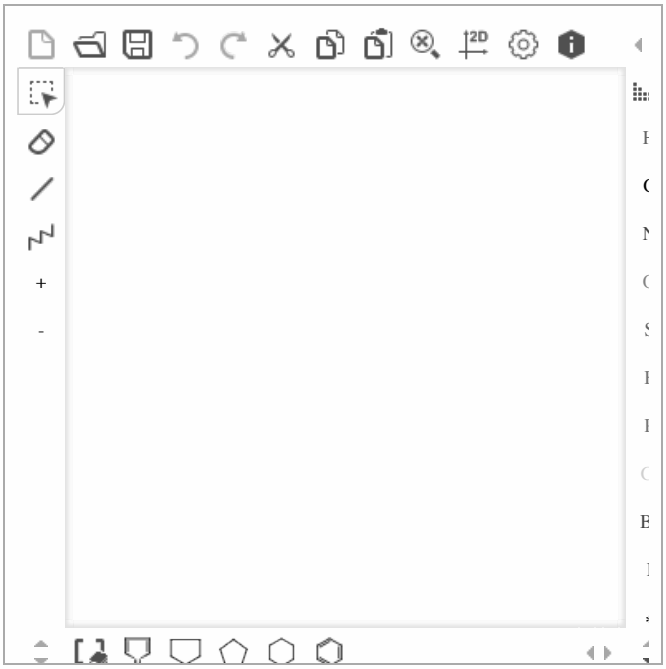
Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.85



Enter a list of SMILES here:

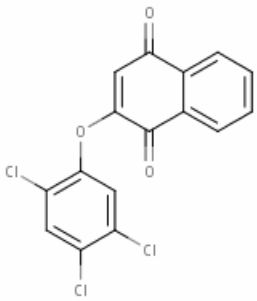
Clc3cc(OC2=CC(=O)c1ccccc1C2=O)c(Cl)cc3Cl

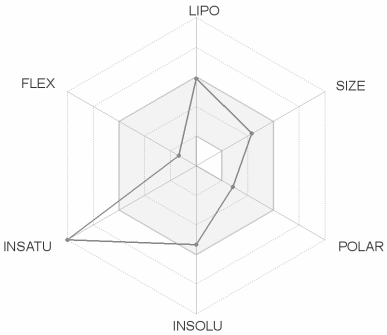
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES Clc1cc(Cl)c(cc1OC1=CC(=O)c2c(C1=O)cccc2)Cl

Physicochemical Properties

Formula	C16H7Cl3O3
Molecular weight	353.58 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	2
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	85.29
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-5.32
Solubility	1.69e-03 mg/ml ; 4.77e-06 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.43
Solubility	1.31e-03 mg/ml ; 3.69e-06 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.93
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.79
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.99
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	3.20
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	5.24
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-7.10
Solubility	2.82e-05 mg/ml ; 7.96e-08 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	4.23	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.06 cm/s

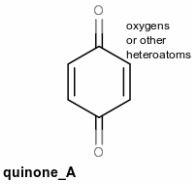
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

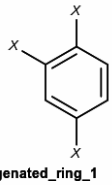
Abbott Bioavailability Score: Probability of F ≥ 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	1 alert: halogenated_ring_1 

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.93

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.66
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.16
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.34
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.70
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.60
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.50
Solubility	1.00e-04 mg/ml ; 3.13e-07 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.69	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.29 cm/s

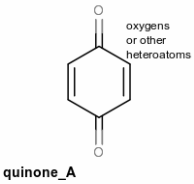
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

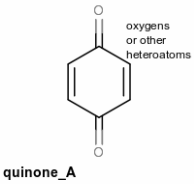
Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.87

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.85

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- confirm the exception on the next page, or
- import our CA key in your web browser

Click here to proceed.

SwissADME

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For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
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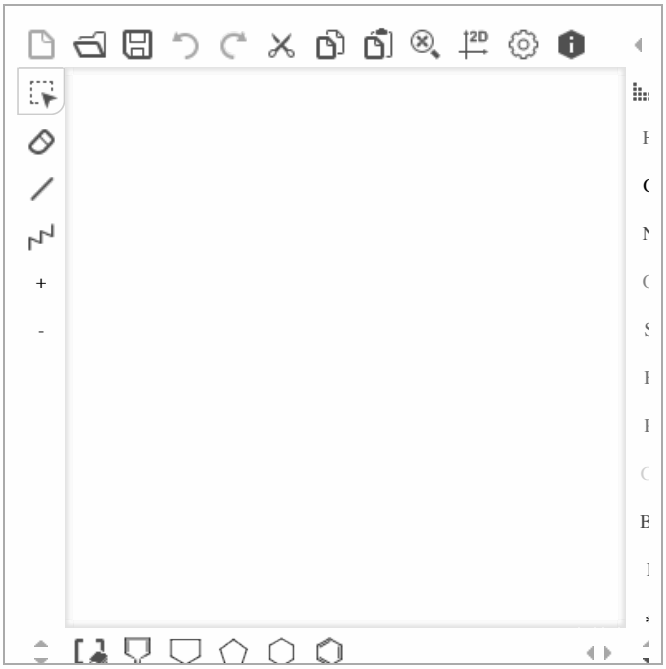
Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.



Enter a list of SMILES here:

[O-][N+](=O)c1ccc(cc1)OC3=CC(=O)c2ccccc2C3=O

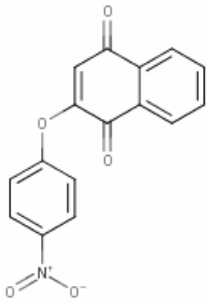
Fill with an example | Clear | Run!

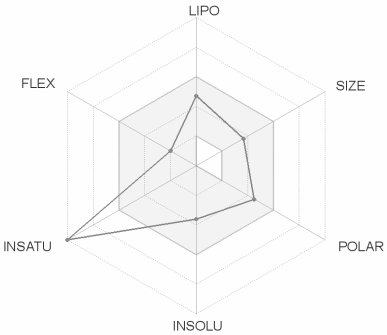
Show BOILED-Egg

Retrieve data:

Powered by ChemAxon

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccc(cc1)[N+](=O)[O-]

Physicochemical Properties

Formula	C16H9NO5
Molecular weight	295.25 g/mol
Num. heavy atoms	22
Num. arom. heavy atoms	12
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	5
Num. H-bond donors	0
Molar Refractivity	79.08
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-3.60
Solubility	7.38e-02 mg/ml ; 2.50e-04 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-4.27
Solubility	1.59e-02 mg/ml ; 5.40e-05 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	89.19 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.01
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.74
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	2.94
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.48
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	1.15
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-4.66
Solubility	6.40e-03 mg/ml ; 2.17e-05 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	No
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.06	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-6.16 cm/s

Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

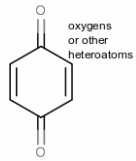
Abbott Bioavailability Score: Probability of F ≥ 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.

1 alert: quinone_A

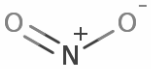


quinone_A

2 alerts: nitro_group, oxygen-nitrogen_single_bond

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem



nitro_group

oxygen-nitrogen_single_bon

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	2.82

In order to avoid security-related warning messages when switching to secured connection, you may want either to:

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SwissADME

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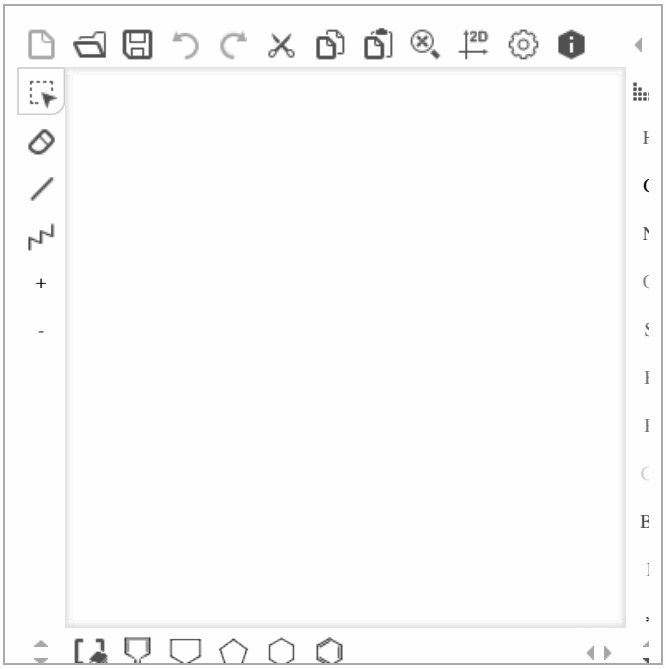
The main article describing the web service and its underlying methodologies is SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* (2017) 7:42717.
For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
For details about development and validation of the BOILED-Egg, please refer to this article: A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* (2016) 11(11):1117-1121.

Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.



Enter a list of SMILES here:

COc1ccc(cc1)OC3=CC(=O)c2ccccc2C3=O

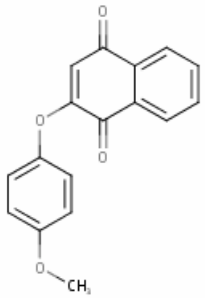
Fill with an example | Clear | Run!

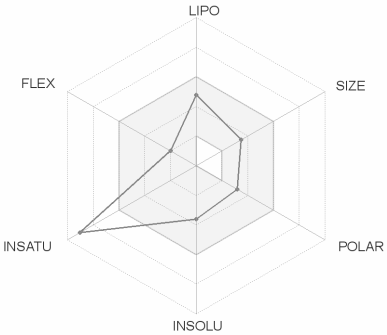
Show BOILED-Egg

Retrieve data: CSV

Powered by ChemAxon

Molecule 1





SMILES COc1ccc(cc1)OC1=CC(=O)c2c(C1=O)cccc2

Physicochemical Properties

Formula	C17H12O4
Molecular weight	280.27 g/mol
Num. heavy atoms	21
Num. arom. heavy atoms	12
Fraction Csp3	0.06
Num. rotatable bonds	3
Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	76.75
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model. -3.62

Solubility 6.77e-02 mg/ml ; 2.42e-04 mol/l

Class

Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly Soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model. -3.64

Solubility 6.36e-02 mg/ml ; 2.27e-04 mol/l

Class

Solubility class: Log *S*

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	52.60 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.57
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	2.88
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	3.04
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	1.34
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	3.38
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-5.42
Solubility	1.07e-03 mg/ml ; 3.83e-06 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	2.64	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.96 cm/s

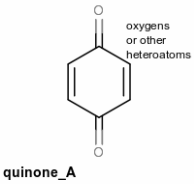
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	Yes

Synthetic accessibility

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For details about development and validation of iLOG, please refer to this article: iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* (2014) 54(12):3284-3301.
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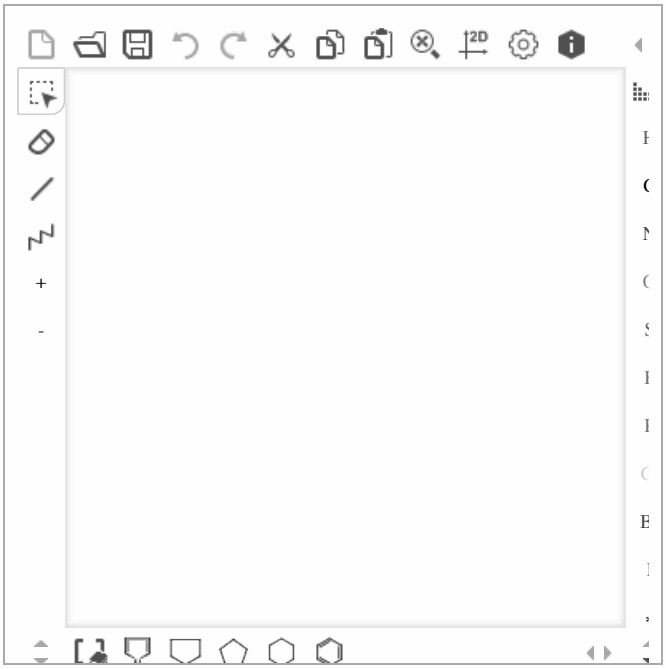
Developed and maintained by the Molecular Modeling Group of the SIB | Swiss Institute of Bioinformatics.



Enter a list of SMILES here:

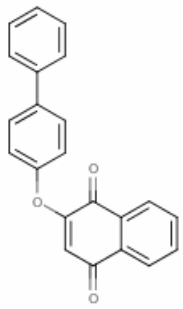
O=C4C=C(Oc1ccc(cc1)c2ccccc2)C(=O)c3ccccc34

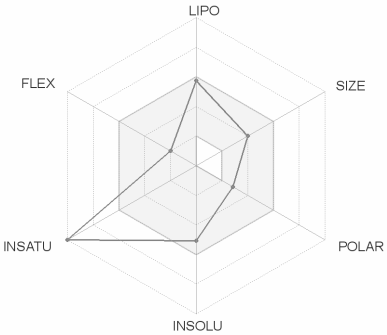
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES O=C1C(=CC(=O)c2c1cccc2)Oc1ccc(cc1)c1ccccc1

Physicochemical Properties

Formula	C22H14O3
Molecular weight	326.34 g/mol
Num. heavy atoms	25
Num. arom. heavy atoms	18
Fraction Csp3	0.00
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	95.69
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-5.05
Solubility	2.89e-03 mg/ml ; 8.87e-06 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.16
Solubility	2.24e-03 mg/ml ; 6.87e-06 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.89
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.53
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.70
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.85
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.92
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-7.79
Solubility	5.35e-06 mg/ml ; 1.64e-08 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.98	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-5.07 cm/s

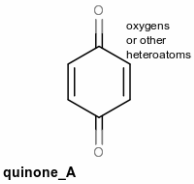
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.14

In order to avoid security-related warning messages when switching to secured connection, you may want either to:

- confirm the exception on the next page, or
- import our CA key in your web browser

Click here to proceed.

SwissADME

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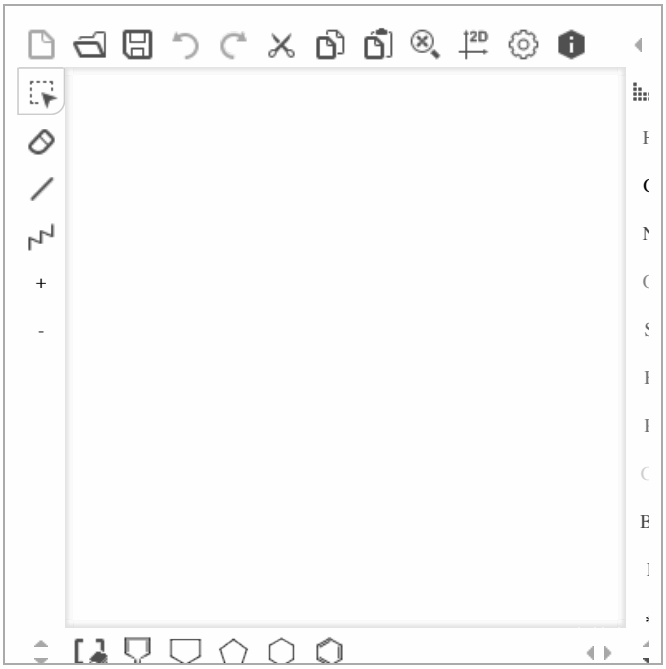


Enter a list of SMILES here:

CC(C)c3ccc(C)cc3OC2=CC(=O)c1ccccc1C2=O

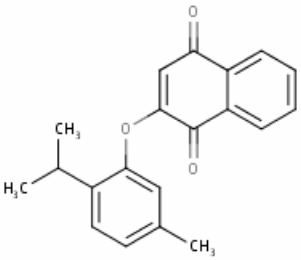
Fill with an example | Clear | Run!

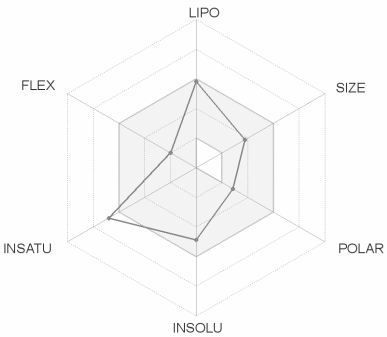
Show BOILED-Egg

Retrieve data: CSV

Powered by ChemAxon

Molecule 1





SMILES Cc1ccc(c(c1)OC1=CC(=O)c2c(C1=O)cccc2)C(C)C

Physicochemical Properties

Formula	C20H18O3
Molecular weight	306.36 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	12
Fraction Csp3	0.20
Num. rotatable bonds	3
Num. H-bond acceptors	3
Num. H-bond donors	0
Molar Refractivity	89.80
TPSA	

Water Solubility

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-4.88
Solubility	4.08e-03 mg/ml ; 1.33e-05 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-5.32
Solubility	1.47e-03 mg/ml ; 4.80e-06 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	43.37 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.06
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	4.68
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	4.46
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	2.62
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	4.95
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Moderately soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-6.49
Solubility Class	9.94e-05 mg/ml ; 3.24e-07 mol/l
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	Yes
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	Yes

Average of all five predictions	3.95	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
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		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	Yes
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-4.85 cm/s

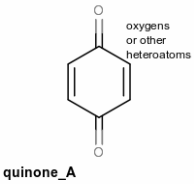
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	Yes
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	Yes
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	Yes

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 1 violation: XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.31

In order to avoid security-related warning messages when switching to secured connection, you may want either to:

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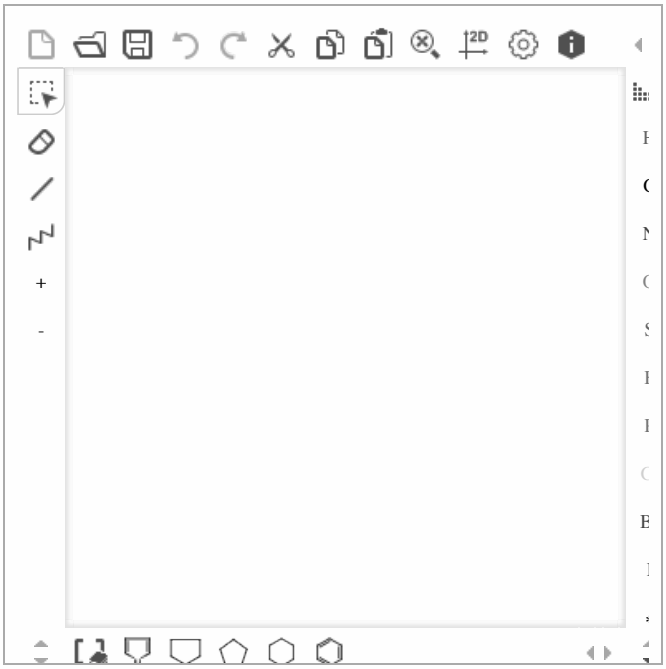


Enter a list of SMILES here:

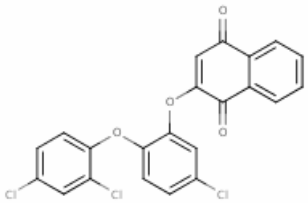
Clc4ccc(Oc3ccc(Cl)cc3OC2=CC(=O)c1ccccc1C2=O)c(Cl)c4

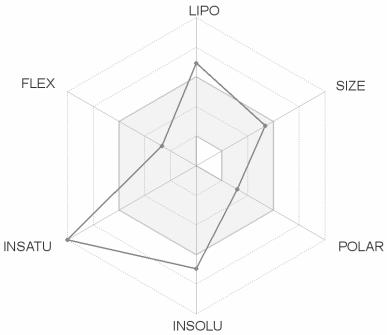
Fill with an example | Clear | Run!

Show BOILED-Egg

Retrieve data:

Molecule 1





SMILES Clc1ccc(c(c1)OC1=CC(=O)c2c(C1=O)cccc2)Oc1ccc(cc1Cl)Cl

Physicochemical Properties

Formula	C22H11Cl3O4
Molecular weight	445.68 g/mol
Num. heavy atoms	29
Num. arom. heavy atoms	18
Fraction Csp3	0.00
Num. rotatable bonds	4
Num. H-bond acceptors	4
Num. H-bond donors	0
Molar Refractivity	111.80
TPSA	

Water Solubility

Log *S* (ESOL)	
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.	-6.96
Solubility	4.93e-05 mg/ml ; 1.11e-07 mol/l
Class	
Solubility class: Log *S* scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble
Log *S* (Ali)	
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-7.50
Solubility	1.39e-05 mg/ml ; 3.13e-08 mol/l
Class	
Solubility class: Log *S*	

Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	52.60 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.66
Log $P_{o/w}$ (XLOGP3)	
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry	6.60
Log $P_{o/w}$ (WLOGP)	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	6.78
Log $P_{o/w}$ (MLOGP)	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	3.97
Log $P_{o/w}$ (SILICOS-IT)	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	6.34
Consensus Log $P_{o/w}$	
Consensus Log $P_{o/w}$: scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble
Log S (SILICOS-IT)	
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-9.28
Solubility	2.36e-07 mg/ml ; 5.28e-10 mol/l
Class	
Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Poorly soluble

Pharmacokinetics

GI absorption	
Gatrointestinal absorption: according to the white of the BOILED-Egg	High
BBB permeant	
BBB permeation: according to the yolk of the BOILED-Egg	No
P-gp substrate	
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
CYP1A2 inhibitor	
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set)	No

Average of all five predictions	5.47	10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	Yes
		CYP2C9 inhibitor	
		Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81	Yes
		CYP2D6 inhibitor	
		Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87	No
		CYP3A4 inhibitor	
		Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) 10-fold CV: ACC=0.77 / AUC=0.85 External: ACC=0.78 / AUC=0.86	No
		Log K_p (skin permeation)	
		Skin permeation: QSPR model implemented from	-4.33 cm/s

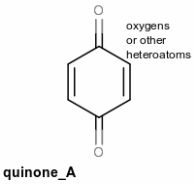
Potts RO and Guy RH. 1992 Pharm. Res.	
	Druglikeness
Lipinski	
Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. MW ≤ 500 MLOGP ≤ 4.15 N or O ≤ 10 NH or OH ≤ 5	Yes; 0 violation
Ghose	
Ghose filter: implemented from Ghose AK. et al. 1999 J. Comb. Chem. 160 ≤ MW ≤ 480 -0.4 ≤ WLOGP ≤ 5.6 40 ≤ MR ≤ 130 20 ≤ atoms ≤ 70	No; 1 violation: WLOGP>5.6
Veber	
Veber (GSK) filter: implemented from Veber DF. et al. 2002 J. Med. Chem. Rotatable bonds ≤ 10 TPSA ≤ 140	Yes
Egan	
Egan (Pharmacia) filter: implemented from Egan WJ. et al. 2000 J. Med. Chem. WLOGP ≤ 5.88 TPSA ≤ 131.6	No; 1 violation: WLOGP>5.88
Muegge	
Muegge (Bayer) filter: implemented from Muegge I. et al. 2001 J. Med. Chem. 200 ≤ MW ≤ 600 -2 ≤ XLOGP ≤ 5 TPSA ≤ 150 Num. rings ≤ 7 Num. carbon > 4 Num. heteroatoms > 1 Num. rotatable bonds ≤ 15 H-bond acc. ≤ 10 H-bond don. ≤ 5	No; 1 violation: XLOGP3>5

Bioavailability Score

Abbott Bioavailability Score: Probability of F > 10% in rat implemented from Martin YC. 2005 J. Med. Chem.	0.56

Medicinal Chemistry

PAINS

Pan Assay Interference Structures: implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.	1 alert: quinone_A 

Brenk

Structural Alert: implemented from Brenk R. et al. 2008 ChemMedChem	0 alert

Leadlikeness

Leadlikeness: implemented from Teague SJ. 1999 Angew. Chem. Int. Ed. 250 ≤ MW ≤ 350 XLOGP ≤ 3.5 Num. rotatable bonds ≤ 7	No; 2 violations: MW>350, XLOGP3>3.5

Synthetic accessibility

Synthetic accessibility score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penaties, trained on 12’782’590 molecules and tested on 40 external molecules ($r^2 = 0.94$)	3.34