Supplementary Information

A greener route for the synthesis of Pyrrolo[2,3-d]pyrimidine derivatives catalyzed by β-cyclodextrin

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Experimental Section

Materials and methods

All chemical were reagent grade purchased from Aldrich and Alfa Aesar and were utilized without purification. IR spectra were recorded in KBr on a Perkin-Elmer 993 IR spectrophotometer. NMR spectra were recorded on a BRUKER AVANCE II-400FT. Spectrometer (400 MHz for 1H NMR, 100 MHz for 13C NMR) taking DMSO-d_6, as solvent and TMS as an internal reference. Mass spectra were recorded on a JEOL SX-102 (FAB) mass spectrometer at 70eV. Elemental analyses were carried out in a Coleman automatic carbon, hydrogen and nitrogen analyzer. All the reactions were monitored by TLC using precoated sheets of silica gel G/UV-254 of 0.25 mm thickness (Merck 60F254). Melting points were determined by open glass capillary method and were uncorrected.

General Experimental Procedure for the synthesis of compound 4 and 6:

β-Cyclodextrin (1 mmol) was dissolved in 5 ML water to a round bottom flask and then respective arylglyoxal monohydrate 1 (1mmol), 6-amino-1,3-dimethyluracil 2 (1mmol) and malononitrile/thiols 3 (1mmol), were added under stirring at 65ºC. It was allowed to stir till reaction was completed, as indicated on (TLC). After that corresponding solid product was isolated by simple filtration and filtrate was utilised for next cycle. The solid product was recrystallized from ethanol.

Spectral data of all synthesised compounds:

2-cyano-2-(6-(4-methoxyphenyl)-1,3-dimethyl-2,4-dioxo-2,3,4,7-tetrahydro-1H-pyrrolo[2,3-d]pyrimidin-5-yl)acetamide [4a]: Mp. 259-261 ^{o}C; IR (KBr): 3622, 3500, 3385, 3193, 2226, 1692, 1672, 1638, 1583, 1512, 1429, 1364, 1279, 1251, 1220, 1168, 1018,

959, 730 cm^{-1}; ^1H NMR (DMSO-d_6, 400 MHz): δ = 11.98 (s, 1H, NH), 7.58 (s, 2H, NH_2), 7.56 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.08 (d, *J* = 8.7 Hz, 2H, Ar-H), 5.12 (s, 1H, CH), 3.80 (s, 3H, OCH_3), 3.53 (s, 3H, NCH_3), 3.31 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 164.7, 158.4, 157.8, 149.8, 139.2, 131.5, 129.2, 123.0, 115.9, 112.7, 106.3, 98.3, 55.6, 34.7, 31.2, 29.1; HRMS m/z Calc. for $C_{18}H_{17}N_5O_4$ $[M+H]^+$ 368.13; Found: 368.14, Elemental Analysis: Calc. C, 58.85; H, 4.66; N, 19.06; O, 17.42; Found: C, 58.62; H, 4.54; N, 19.12; O, 17.30.

2-cyano-2-(1,3-dimethyl-2,4-dioxo-6-phenyl-2,3,4,7-tetrahydro-1H-pyrrolo[2,3-d]pyrimidin-5-yl)acetamide [4b]: Mp. 235-237 ^oC; IR (KBr): 3346, 3224, 2216, 1656, 1609, 1568, 1506, 1475, 1429, 1262, 1163, 1018, 831 cm^{-1}; ^1H NMR (DMSO-d_6, 400 MHz): δ = 12.04 (s, 1H, NH), 7.58 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.54 (s, 2H, NH_2), 7.44 (t, *J* = 7.3 Hz, 2H, Ar-H), 7.36 (t, *J* = 7.3 Hz, 1H, Ar-H), 5.23 (s, 1H, CH), 3.44 (s, 3H, NCH_3), 3.25 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 166.3, 157.4, 149.8, 139.1, 130.8, 129.9, 129.1, 128.4, 127.7, 115.9, 104.7, 98.2, 33.6, 31.5, 29.2; HRMS m/z Calc. for $C_{17}H_{15}N_5O_3$ $[M+H]^+$ 338.12 ; Found: 338.11 Elemental Analysis: Calc. C, 60.53; H, 4.48; N, 20.76; O, 14.23; Found: C, 60.38; H, 4.33; N, 20.61; O, 14.35.

2-cyano-2-(6-(6-methoxynaphthalen-2-yl)-1,3-dimethyl-2,4-dioxo-2,3,4,7-tetrahydro-1H-pyrrolo[2,3-d]pyrimidin-5-yl)acetamide [4c]: Mp. 270-272 ^oC; IR (KBr): 3458, 3354, 2364, 1682, 1640, 1610, 1558, 1472, 1371, 1256, 1226, 1172, 1031, 958, 862, 731 cm^{-1}; ^1H NMR (DMSO-d_6, 400 MHz): δ = 12.10 (s, 1H, NH), 8.06 (s, 1H, Ar-H), 7.74 (d, *J* = 8.5 Hz, 1H, Ar-H), 7.82 (d, *J* = 9.0 Hz, 1H, Ar-H), 7.65 (dd, *J* = 8.5, 1.7 Hz, 1H, Ar-H), 7.57-7.53 (b, 2H, NH_2), 7.36 (m, 1H, Ar-H), 7.21 (dd, *J* = 8.9, 2.5 Hz, 1H, Ar-H), 5.36 (s, 1H, CH), 3.94 (s, 3H, OCH_3), 3.56 (s, 3H, NCH_3), 3.25 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ

= 165.1, 157.8, 156.9, 149.5, 139.2, 133.2, 131.1, 129.2, 128.1, 127.2, 126.9, 125.8, 123.7, 118.5, 115.3, 106.4, 98.5, 55.8, 34.2, 31.5, 29.2; HRMS m/z Calc. for $C_{22}H_{19}N_5O_4$ $[M+H]^+$ 418.15; Found: 418.16. Elemental Analysis: Calc. C, 63.30; H, 4.59; N, 16.78; O, 15.33; Found: C, 63.39; H, 4.47; N, 16.71; O, 15.42.

6-(4-methoxyphenyl)-1,3-dimethyl-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6a]: Mp. 303-305 ^oC; IR (KBr): 3350, 3120, 1690, 1623, 1540, 1480, 1355, 1240, 1165, 1040, 885, 775 cm^{-1}; ^1H NMR (DMSO-d_6 400 MHz): δ = 12.14 (s, 1H, NH), 8.55 (d, *J* = 4.8 Hz, 2H, Ar-H), 7.53 (d, *J* = 8.7 Hz, 2H, Ar-H), 7.11 (t, *J* = 4.8 Hz, 1H, Ar-H), 6.96 (d, *J* = 8.8 Hz, 2H, Ar-H), 3.81 (s, 3H, OCH_3), 3.58 (s, 3H, NCH_3), 3.16 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 174.5, 156.3, 154.6, 154.3, 148.9, 148.2, 133.2, 127.5, 122.0, 118.1, 114.5, 99.3, 98.2, 57.8, 31.4, 29.2; HRMS m/z Calc. for $C_{19}H_{17}N_5O_3S$ $[M+H]^+$ 396.11; Found: 396.12; Elemental Analysis: Calc. C, 57.71; H, 4.33; N, 17.71; O, 12.14; S, 8.11; Found: C, 57.80; H, 4.38; N, 17.62; O, 12.22; S, 8.04.

1,3-dimethyl-6-phenyl-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H) dione [6b]: Mp. 311-313 ^oC; IR (KBr): 3447, 3376, 1687, 1642, 1571, 1422, 1355, 1325, 1285, 1180, 970, 820, 755, 685 cm^{-1}; ^1H NMR (DMSO d_6, 400 MHz): δ = 12.16 (s, 1H, NH), 8.45 (d, *J* = 4.8 Hz, 2H, Ar-H), 7.56 (dd, *J* = 8.5 and 1.5 Hz, 2H, Ar-H), 7.37 (t, *J* = 7.0 Hz, 2H, Ar-H), 7.30 (t, *J* = 7.2 Hz, 1H, Ar-H), 7.05 (t, *J* = 4.8 Hz, 1H, Ar-H), 3.52 (s, 3H, NCH_3), 3.21 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 174.1, 155.7, 155.4, 148.8, 138.6, 133.2, 130.6, 127.9, 127.4, 126.8, 118.6, 102.7, 97.6, 31.2, 26.5; HRMS m/z Calc. for $C_{18}H_{15}N_5O_2S$ $[M+H]^+$ 366.10; Found: 366.11; Elemental Analysis: Calc. C, 59.17; H, 4.14; N, 19.17; O, 8.76; S, 8.77; Found: C, 59.12; H, 4.19; N, 19.25; O, 8.64; S, 8.70.

6-(6-methoxynaphthalen-2-yl)-1,3-dimethyl-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6c]: Mp. 280-282 ^oC; IR (KBr): 3210, 1692, 1625, 1610,

1525, 1445, 1385, 1255, 1192, 1135, 1022, 970, 855, 735 cm^{-1}; ^1H NMR (DMSO-d_6, 400 MHz): δ = 12.20 (s, 1H, NH), 8.54 (d, *J* = 4.8 Hz, 2H, Ar-H), 8.05 (s, 1H, Ar-H), 7.86 (d, *J* = 8.6 Hz, 1H, Ar-H), 7.75 (d, *J* = 9.0 Hz, 1H, Ar-H), 7.74 (dd, *J* = 8.5 and 1.7 Hz, 1H, Ar-H), 7.25 (m, 1H, Ar-H), 7.19-7.14 (m, 2H, Ar-H), 3.85 (s, 3H, OCH_3), 3.56 (s, 3H, NCH_3), 3.15 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 174.1, 157.2, 156.1, 149.6, 139.7, 134.7, 133.2, 128.8, 127.5, 127.0, 125.8, 125.1, 124.4, 120.1, 118.6, 106.0, 101.2, 98.7, 54.8, 31.2, 29.1; HRMS m/z Calc. for $C_{23}H_{19}N_5O_3S$ $[M+H]^+$ 446.12; Found: 446.13; Elemental Analysis: Calc. C, 62.01; H, 4.30; N, 15.72; O, 10.77; S, 7.20; Found: C, 62.08; H, 4.23; N, 15.64; O, 10.71; S, 7.28.

1,3-dimethyl-6-phenyl-5-(pyridin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6d]: Mp.285-287 ^oC, IR 3338, 3146, 3041, 2810, 1704, 1659, 1626, 1589, 1565, 1418, 1158, 958, 751, 721, 680 cm^{-1}. ^1H-NMR (400 MHz, DMSO-d_6) δ 12.30 (s, 1H, NH), 8.31 (d, *J* = 5.8 Hz, 1H, ArH), 7.57 (t, *J* = 7.2 Hz, 2H, ArH), 7.52 (td, *J* = 7.8 Hz, *J* = 2.0 Hz, 1H, ArH), 7.47 (d, *J* = 7.6 Hz, 2H, ArH), 7.38-7.33 (m, 1H, ArH), 7.57 (t, *J* = 7.6 Hz, 1H, ArH), 6.94 (d, *J* = 8.2 Hz, 1H, ArH), 3.58 (s, 3H, NCH_3), 3.12 (s, 3H, NCH_3). ^{13}C-NMR(100MHz, DMSO-d_6) 161.3, 155.3, 149.4, 147.7, 139.4, 136.6, 134.2, 130.2, 128.1, 127.6, 127.2, 120.3, 119.8, 100.8, 99.2, 31.4, 29.3. HRMS m/z: calc. for $C_{19}H_{16}N_4O_2S$ $[M + H]^+$ 365.10; Found: 365.11. Elemental Analysis: Calc. C, 62.62; H, 4.43; N, 15.37; O, 8.78; S, 8.80; Found: C, 62.71; H, 4.32; N, 15.31; O, 8.59; S, 8.68.

6-(4-methoxyphenyl)-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6e]: Mp. 269-271 ^oC; IR (KBr): 3320, 3155, 3032, 2831, 1714, 1635, 1625, 1473, 1436, 1373, 1225, 1157, 1120, 1022, 825, 775, 712 cm^{-1}; ^1H NMR (DMSO-d_6 +$CDCl_3$, 400 MHz): δ = 11.98 (s, 1H, NH), 11.43 (s, 1H, NH), 10.38 (s, 1H, NH), 8.52 (d, *J*= 4.7 Hz, 2H, Ar-H), 7.51 (d, *J* = 8.6 Hz, 2H, Ar-H), 7.12 (t, *J* = 4.7 Hz, 1H, Ar-H) 6.94 (d, *J* = 8.4 Hz, 2H, Ar-H), 3.74 (s, 3H, OMe); ^{13}C NMR (DMSO-d_6 , 100 MHz): δ = 174.3, 157.8, 156.3, 155.6,

149.7, 139.3, 133.8, 129.5 123.4, 118.1, 114.3, 99.2, 98.4, 55.7; HRMS m/z Calc. for $C_{17}H_{13}N_5O_3S$ $[M+H]^+$ 368.08; Found: 368.09; Elemental Analysis: Calc. C, 55.58; H, 3.57; N, 19.06; O, 13.06; S, 8.73; Found: C, 55.46; H, 3.50; N, 19.15; O, 13.12; S, 8.81.

6-phenyl-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6f]: Mp. 291-293 ^oC; IR (KBr): 3325, 3245, 3155, 3045, 1715, 1640, 1612, 1540, 1425, 1370, 1232, 992, 667 cm^{-1}; ^1H NMR (DMSO-d_6+$CDCl_3$, 400 MHz): δ = 12.08 (s, 1H, NH), 11.42 (s, 1H, NH), 10.39 (s, 1H, NH), 8.52 (d, *J* = 4.8 Hz, 2H, Ar-H), 7.56 (dd, *J* = 7.1 and 1.6 Hz, 2H, Ar-H), 7.39 (dt, *J* = 7.1 and 1.7 Hz, 2H, Ar-H), 7.31-7.25 (m, 1H, Ar-H), 7.06 (t, *J* = 4.8 Hz, 1H, Ar-H); ^{13}C NMR (DMSO-d_6,100 MHz): δ = 174.2, 157.8, 156.8, 149.7, 139.7, 134.5, 133.4, 129.2, 126.9, 126.1, 125.8, 125.2, 124.5, 120.4, 118.3, 106.4, 101.8, 99.6, 54.6, 31.3, 29.3; HRMS m/z Calc. for $C_{16}H_{11}N_5O_2S$ $[M+H]^+$ 338.07; Found: 338.06; Elemental Analysis: Calc. C, 56.97; H, 3.29; N, 20.76; O, 9.48; S, 9.50; Found: C, 56.85; H, 3.41; N, 20.59; O, 9.35; S, 9.42.

6-(4-fluorophenyl)-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6g]: Mp. 297-299 ^oC; IR (KBr): 3365, 3132, 2974, 2832, 1692, 1652, 1642, 1540, 1485, 1425, 1357, 1243, 1168, 1028, 985 882, 830, 742, 679 cm^{-1}; ^1H NMR (DMSO-d_6 + $CDCl_3$, 400 MHz): δ = 12.15 (s, 1H, NH), 11.56 (bs, 1H, NH), 10.42 (s, 1H, NH), 8.54 (d, *J* = 4.7 Hz, 2H, Ar-H), 7.56 (t, *J* = 5.6 Hz, 2H, Ar-H), 7.23 (t, *J* = 8.8 Hz, 2H, Ar-H) 7.11 (t, *J* = 4.6 Hz, 1H, Ar-H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 174.1, 168.6, 158.5, 157.2, 155.6, 149.8, 139.5, 133.6, 131.0, 129.7, 127.7, 126.5, 118.4, 115.8, 115.5, 101.3, 99.3; HRMS m/z Calc. for $C_{16}H_{10}FN_5O_2S$ $[M+H]^+$ 356.06; Found: 356.06; Elemental Analysis: Calc. C, 54.08; H, 2.84; F, 5.35; N, 19.71; O, 9.00; S, 9.02; Found: C, 54.15; H, 2.65; F, 5.44; N, 19.52; O, 9.08; S, 9.11.

6-(6-methoxynaphthalen-2-yl)-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6h]: Mp. 273-275 ^{o}C; IR (KBr): 3335, 3148, 3026, 2843, 1710, 1640, 1619, 1475, 1442, 1372, 1238, 1149, 1102, 1015, 822, 735, 712 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz): δ = 12.18 (s, 1H, NH), 11.62 (s, 1H, NH), 10.50 (s, 1H, NH), 8.52 (d, *J* = 4.4 Hz, 2H, Ar-H), 8.02 (s, 1H, Ar-H), 7.83-7.70 (m, 3H, Ar-H), 7.34 (s, 1H, Ar-H), 7.15 (d, *J* = 10.1 Hz, 2H, Ar-H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 174.6, 157.8, 155.4, 155.1, 149.4, 139.2, 133.8, 132.5, 130.1, 127.2, 126.5, 126.1, 125.8, 125.1, 120.2, 118.5, 106.3, 100.6, 99.5, 55.8; HRMS m/z Calc. for $C_{21}H_{15}N_5O_3S$ $[M+H]^+$ 418.09; Found: 418.10; Elemental Analysis: Calc. C, 60.42; H, 3.62; N, 16.78; O, 11.50; S, 7.68; Found: C, 60.31; H, 3.56; N, 16.54; O, 11.68; S, 7.46.

1,3-dimethyl-6-phenyl-5-(phenylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6i]: Mp. 310-312 ^{o}C; IR (KBr): 3258, 3221, 1694, 1639, 1610, 1588, 1552, 1458, 1353, 1272, 1233, 956, 716 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz): δ = 12.25 (s, 1H, NH), 7.65-7.12 (m, 10H), 3.56 (s, 3H, NCH_3), 3.14 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 157.1, 149.7, 139.8, 138.2, 135.1, 130.6, 129.6, 128.3, 127.8, 127.4, 126.1, 124.2, 123.5, 102.4, 99.4, 31.1, 29.4; HRMS m/z Calc. for $C_{20}H_{17}N_3O_2S$ $[M+H]^+$ 364.11; Found: 364.12; Elemental Analysis: Calc. C, 66.10; H, 4.72; N, 11.56; O, 8.80; S, 8.82; Found: C, 66.03; H, 4.63; N, 11.59; O, 8.65; S, 8.71.

5-(4-methoxyphenylthio)-1,3-dimethyl-6-phenyl-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6j]: Mp. 276-278 ^{o}C; IR(ATR): 3255, 1678, 1624, 1542, 1521, 1484, 1434, 1362, 1296, 1232, 1162, 1025, 995 cm^{-1}; ^{1}H-NMR (400MHz, DMSO-d_6) δ 12.19 (s, 1H, NH), 7.61 (d, *J* = 7.2 Hz, 2H, ArH), 7.42 (t, *J* = 7.2 Hz, 2H, ArH), 7.43 (t, *J* = 7.2 Hz,

1H, ArH), 7.03 (d, *J* = 8.8 Hz, 2H, ArH), 6.79 (d, *J* = 8.8 Hz, 2H, ArH), 3.63 (s, 3H, OMe), 3.55 (s, 3H, NCH_3), 3.15 (s, 3H, NCH_3); ^{13}C-NMR(100MHz, DMSO-d_6) δ 157.8, 149.8, 139.3, 135.7, 131.0, 129.2, 128.8, 128.0, 127.5, 126.8, 115.4, 102.3, 99.5, 55.7, 31.8, 29.5; HRMS m/z: calcd for $C_{21}H_{19}N_3O_3S$ $[M + H]^+$ 394.12; Found: 394.11; Elemental Analysis: Calc. C, 64.11; H, 4.87; N, 10.68; O, 12.20; S, 8.15 Found: C, 64.02; H, 4.80; N, 10.72; O, 12.28; S, 8.24.

1,3-dimethyl-6-phenyl-5-(p-tolylthio)-1H-pyrrolo[2,3-d]pyrimidine-2,4(3H,7H)-dione [6k] Mp. 255-257 ^{o}C; IR (KBr): 3254, 3225, 1691, 1657, 1595, 1542, 1489, 1441, 1362, 1258, 956, 725 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz): δ = 12.16 (s, 1H, NH), 7.65 (dd, *J* = 8.5, 1.4 Hz, 2H, Ar-H), 7.41 (t, *J* = 7.72, 7.12 Hz, 2H, Ar-H), 7.39 (t, *J* = 7.28 Hz, 1H, Ar-H), 7.08 (d, *J* = 8.16 Hz, 2H, Ar-H), 6.91 (d, *J* = 8.24 Hz, 2H, Ar-H), 3.57 (s, 3H, NCH_3), 3.12 (s, 3H, NCH_3), 2.26 (s, 3H, CH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 157.8, 149.8, 139.4, 134.5, 134.3, 133.6, 129.8, 129.7, 128.9, 128.1, 127.6, 124.7, 101.8, 99.6, 31.4, 29.2, 22.6; HRMS m/z Calc. for $C_{21}H_{19}N_3O_2S$ $[M+H]^+$ 378.12; Found: 378.13; Elemental Analysis:Calc. C, 66.82; H, 5.07; N, 11.13; O, 8.48; S, 8.49; Found: C, 66.67; H, 5.12; N, 11.26; O, 8.57; S, 8.62.

1,3-dimethyl-6-(4-nitrophenyl)-5-(pyrimidin-2-ylthio)-1H-pyrrolo[2,3-d]pyrimidine 2,4(3H,7H)-dione [6l]: Mp. 297-299 ^{o}C; IR (KBr): 3355, 3120, 1691, 1625, 1542, 1482, 1365, 1246, 1162, 1043, 882, 767cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz): δ = 12.26 (s, 1H, NH), 8.42 (d, *J* = 4.8 Hz, 2H, Ar-H), 8.26 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.84 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.14 (t, *J* = 4.8 Hz, 1H, Ar-H), 3.43 (s, 3H, NCH_3), 3.08 (s, 3H, NCH_3); ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 173.8, 156.4, 155.7, 149.1, 145.2, 139.2, 135.5, 131.7, 128.8, 122.6, 118.2, 102.9, 101.2, 31.4, 29.3; HRMS m/z Calc. for $C_{18}H_{14}N_6O_4S$ $[M+H]^+$ 411.08;

Found: 411.09; Elemental Analysis: Calc. C, 52.68; H, 3.44; N, 20.48; O, 15.59; S, 7.81; Found: C, 52.49; H, 3.38; N, 20.26; O, 15.42; S, 7.53.