Electronic Supplementary Information

Application of quinazoline and pyrido[3,2-*d*]pyrimidine templates to design multi-targeting agents in Alzheimer's disease

Tarek Mohamed [a, b], Mandeep K. Mann [a] and Praveen P. N. Rao [a,*]

[a]*School of Pharmacy, Health Sciences Campus and* [b]*Department of Chemistry, University of Waterloo, 200 University Ave. West., Waterloo, Ontario, Canada N2L 3G1*

***Corresponding author**

Praveen P. N. Rao, B'Phm., M'Phm., PhD
Associate Professor - Pharmaceutical Sciences
PHR 5002, School of Pharmacy
Health Sciences Campus, 200 University Ave W
University of Waterloo, Waterloo, Ontario, CANADA, N2L 3G1
Tel: 519-888-4567 ext: 21317
Email: praopera@uwaterloo.ca

Table of Contents

1. Analytical data for compounds 3a–d.

2,4,6-Trichloroquinazoline (3a). White solid; yield 75% (4.43 g, 19.12 mmol); mp 126–128 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.31 (s, 1H), δ 8.15 (d, J = 9.0 Hz, 1H), δ 8.04 (d, J = 8.9 Hz, 1H). LRMS (ESI) m/z calcd for $C_8H_4Cl_3N_2$ $[M + H]^+$ 232.93, found 232.92.

2,4,7-Trichloroquinazoline (3b). Yellow solid; yield 80% (4.73 g, 20.41 mmol); mp 137–139 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.30 (d, J = 9.0 Hz, 1H), δ 8.20 (s, 1H), δ 7.88 (d, J = 8.7 Hz, 1H). LRMS (ESI) m/z calcd for $C_8H_4Cl_3N_2$ $[M + H]^+$ 232.93, found 232.92.

2,4,8-Trichloroquinazoline (3c). Yellow solid; yield 65% (3.84 g, 16.56 mmol); mp 135–137 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.31 (d, J = 7.7 Hz, 1H), δ 8.25 (d, J = 8.5 Hz, 1H), δ 7.78 (t, J = 7.4 Hz, 1H). LRMS (ESI) m/z calcd for $C_8H_4Cl_3N_2$ $[M + H]^+$ 232.93, found 232.92.

2,4-Dichloropyrido[3,2-*d*]pyrimidine (3d). Brownish solid; yield 65% (3.97 g, 19.94 mmol); mp 197–199 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.17 (d, J = 4.1 Hz, 1H), δ 8.44 (d, J = 8.4 Hz, 1H), δ 8.10 (dd, J = 8.6, 4.1 Hz, 1H). LRMS (ESI) m/z calcd for $C_7H_4Cl_2N_3$ $[M + H]^+$ 199.97, found 199.96.

2. Analytical data for compounds 4a–c, 5a–c, 6a and 7a.

2,6-Dichloro-*N*-phenethylquinazolin-4-amine (4a). Yellow solid; yield 75% (1.03 g, 3.25 mmol); mp 133–135 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.88 (br s, 1H), δ 8.38 (d, J = 2.2 Hz, 1H), δ 7.77 (dd, J = 8.9, 2.2 Hz, 1H), δ 7.59 (d, J = 8.9 Hz, 1H), δ 7.30–7.16 (m, 5H), δ 3.65 (q, J = 6.1 Hz, 2H), δ 2.90 (t, J = 7.2 Hz, 2H). LRMS (ESI) m/z calcd for $C_{16}H_{14}Cl_2N_3$ $[M + H]^+$ 318.04, found 318.00.

2,7-Dichloro-*N*-phenethylquinazolin-4-amine (4b). Yellow solid; yield 75% (1.03 g, 3.25 mmol); mp 137–139 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.94 (br s, 1H), δ 8.22 (d, J = 8.8 Hz, 1H), δ 7.68–7.65 (m, 1H), δ 7.58 (d, J = 8.7 Hz, 1H), δ 7.28–7.17 (m, 5H), δ 3.65 (q, J = 6.1 Hz, 2H), δ 2.90 (t, J = 7.2 Hz, 2H). LRMS (ESI) m/z calcd for $C_{16}H_{14}Cl_2N_3$ $[M + H]^+$ 318.04, found 318.06.

2,8-Dichloro-*N*-phenethylquinazolin-4-amine (4c). Yellow solid; yield 90% (1.24 g, 3.90 mmol); mp 136–138 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.01 (br s, 1H), δ 8.16 (d, J = 8.8 Hz, 1H), δ 7.91 (d, J = 8.7 Hz, 1H), δ 7.45 (t, J = 8.0 Hz, 1H), δ 7.29–7.15 (m, 5H), δ 3.68 (q, J = 6.1 Hz, 2H), δ 2.92 (t, J = 7.2 Hz, 2H). LRMS (ESI) m/z calcd for $C_{16}H_{14}Cl_2N_3$ $[M + H]^+$ 318.04, found 318.03.

2,6-Dichloro-*N*-(3,4-dimethoxyphenethyl)quinazolin-4-amine (5a). Yellow solid; yield 80% (1.31 g, 3.45 mmol); mp 143–145 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.82 (br s, 1H), δ 8.39 (d, J = 2.2 Hz, 1H), δ 7.77 (d, J = 8.9 Hz, 1H), δ 7.60 (d, J = 8.7 Hz, 1H), δ 6.85–6.73 (m, 3H), δ 3.71–3.65 (m, 8H), δ 2.83 (t, J = 7.4 Hz, 2H). LRMS (ESI) m/z calcd for $C_{18}H_{18}Cl_2N_3O_2$ $[M + H]^+$ 378.06, found 378.09.

2,7-Dichloro-*N*-(3,4-dimethoxyphenethyl)quinazolin-4-amine (5b). Yellow solid; yield 77% (1.26 g, 3.34 mmol); mp 147–149 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.92 (br s, 1H), δ 8.24 (d, J = 8.6 Hz, 1H), δ 7.66 (s, 1H), δ 7.57 (d, J = 8.9 Hz, 1H), δ 6.85–6.72 (m, 3H), δ 3.71–3.65 (m, 8H), δ 2.83 (t, J = 7.4 Hz, 2H). LRMS (ESI) m/z calcd for $C_{18}H_{18}Cl_2N_3O_2$ $[M + H]^+$ 378.06, found 378.10.

2,8-Dichloro-*N*-(3,4-dimethoxyphenethyl)quinazolin-4-amine (5c). Yellow solid; yield 87% (1.39 g, 3.67 mmol); mp 145–147 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.97 (br s, 1H), δ 8.18 (d, J = 8.6 Hz, 1H), δ 7.92 (d, J = 8.9 Hz, 1H), δ 7.45 (t, J = 8.4 Hz, 1H), δ 6.85–6.71 (m, 3H), δ 3.71–3.65 (m, 8H), δ 2.83 (t, J = 7.4 Hz, 2H). LRMS (ESI) m/z calcd for $C_{18}H_{18}Cl_2N_3O_2$ $[M + H]^+$ 378.06, found 378.04.

2-Chloro-*N*-phenethylpyrido[3,2-*d*]pyrimidin-4-amine (6a). Brown oil; yield 82% (1.17 g, 4.12 mmol). ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.02 (br s, 1H), δ 8.77–8.74 (m, 1H), δ 7.99 (d, J = 8.8 Hz, 1H), δ 7.78 (d, J = 8.5 Hz, 1H), δ 7.28–7.13 (m, 5H), δ 3.68 (q, J = 6.1 Hz, 2H), δ 2.91 (t, J = 7.2 Hz, 2H). LRMS (ESI) m/z calcd for $C_{15}H_{14}ClN_4$ $[M + H]^+$ 285.08, found 285.09.

2-Chloro-*N*-(3,4-dimethoxyphenethyl)pyrido[3,2-*d*]pyrimidin-4-amine (7a). Pale brown solid; yield 84% (1.45 g, 4.22 mmol); mp 156–158 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.96 (br s, 1H), δ 8.77–8.73 (m, 1H), δ 7.99 (d, J = 8.6 Hz, 1H), δ 7.78 (dd, J = 8.6 Hz, 1H), δ 6.83–6.71 (m, 3H), δ 3.74–3.67

(m, 8H), δ 2.84 (t, *J* = 7.4 Hz, 2H). LRMS (ESI) m/z calcd for $C_{17}H_{18}ClN_4O_2$ $[M + H]^+$ 345.10, found 345.11.

3. Analytical data for compounds 8a–i, 9a–i, 10a–c, 11a–c, 12a–c, 13a–c, 14a and 15a.

6-Chloro-*N*^{4}-phenethyl-*N*^{2}-propylquinazoline-2,4-diamine (8a). Yellow solid; yield 71% (0.38 g, 1.12 mmol); mp 107–109 °C. ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.09–8.02 (m, 2H), δ 7.41 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 7.30–7.14 (m, 6H), δ 6.72 (br s, 1H), δ 3.60 (q, *J* = 7.5 Hz, 2H), δ 3.23–3.20 (m, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 1.47 (sextet, *J* = 7.2 Hz, 2H), δ 0.84 (t, *J* = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1527. Purity: 99.7%

6-Chloro-*N*^{2}-isopropyl-*N*^{4}-phenethylquinazoline-2,4-diamine (8b). Yellow solid; yield 75% (0.40 g, 1.18 mmol); mp 104–106 °C. ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.10–8.04 (m, 2H), δ 7.44 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 7.30–7.15 (m, 6H), δ 6.65 (br s, 1H), δ 4.18–4.07 (m, 1H), δ 3.60 (q, *J* = 7.5 Hz, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 1.13 (d, *J* = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1527. Purity: 98.6%

6-Chloro-*N*^{2}-cyclopropyl-*N*^{4}-phenethylquinazoline-2,4-diamine (8c). Yellow solid; yield 73% (0.39 g, 1.15 mmol). mp 108–110 °C. ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.07–8.04 (m, 2H), δ 7.43 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 7.29–7.14 (m, 6H), δ 6.87 (br s, 1H), 3.67–3.60 (m, 2H), δ 2.89 (t, *J* = 7.6 Hz, 2H), δ 2.81–2.75 (m, 1H), δ 0.65–0.58 (m, 2H), δ 0.48–0.43 (m, 2H). HRMS (ESI) m/z calcd for $C_{19}H_{20}ClN_4$ $[M + H]^+$ 338.1298, found 339.1371. Purity: 99.6%

7-Chloro-*N*^{4}-phenethyl-*N*^{2}-propylquinazoline-2,4-diamine (8d). Yellow solid; yield 70% (0.37 g, 1.10 mmol); mp 105–107 °C. ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.03 (br s, 1H), δ 7.89 (d, *J* = 8.7 Hz, 1H), δ 7.30–7.15 (m, 6H), δ 6.96 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 6.71 (br s, 1H), δ 3.60 (q, *J* = 7.5 Hz, 2H), δ 3.23–3.20 (m, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 1.46 (sextet, *J* = 7.2 Hz, 2H), δ 0.84 (t, *J* = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1528. Purity: 99.4%

7-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8e). Yellow solid; yield 75% (0.40 g, 1.18 mmol); mp 106–108 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.07 (br s, 1H), δ 7.91 (d, J = 8.7 Hz, 1H), δ 7.30–7.15 (m, 6H), δ 6.98 (dd, J = 8.9, 2.3 Hz, 1H), δ 6.62 (br s, 1H), δ 4.16–4.09 (m, 1H), δ 3.60 (q, J = 7.5 Hz, 2H), δ 2.89 (t, J = 7.3 Hz, 2H), δ 1.13 (d, J = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1528. Purity: 99.6%

7-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8f). Yellow solid; yield 73% (0.39 g, 1.15 mmol). mp 111–113 °C °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.07 (br s, 1H), δ 7.92 (d, J = 8.7 Hz, 1H), δ 7.29–7.14 (m, 6H), δ 6.99 (dd, J = 8.7, 2.0 Hz, 1H), δ 6.92 (br s, 1H), δ 3.67–3.60 (m, 2H), δ 2.89 (t, J = 7.6 Hz, 2H), δ 2.85–2.77 (m, 1H), δ 0.65–0.59 (m, 2H), δ 0.48–0.45 (m, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 160.94, δ 159.43, δ 152.96, δ 139.64, δ 136.75, δ 128.65, δ 128.29, δ 126.03, δ 124.75, δ 123.14, δ 122.43, δ 119.97, δ 109.87, δ 42.14, δ 34.53, δ 23.85, δ 6.37. HRMS (ESI) m/z calcd for $C_{19}H_{20}ClN_4$ $[M + H]^+$ 338.1298, found 339.1371. Purity: 98.5%

8-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8g). White solid; yield 70% (0.37 g, 1.10 mmol); mp 102–104 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.03 (br s, 1H), δ 7.85 (d, J = 8.6 Hz, 1H), δ 7.57 (d, J = 8.6 Hz, 1H), δ 7.30–7.15 (m, 5H), δ 6.89 (t, J = 7.9 Hz, 1H), δ 6.79 (br s, 1H), δ 3.61 (q, J = 7.5 Hz, 2H), δ 3.23–3.20 (m, 2H), δ 2.89 (t, J = 7.3 Hz, 2H), δ 1.50 (sextet, J = 7.2 Hz, 2H), δ 0.84 (t, J = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1528. Purity: 98.8%

8-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8h). Yellow solid; yield 70% (0.37 g, 1.10 mmol); mp 107–109 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.99 (br s, 1H), δ 8.16 (d, J = 8.6 Hz, 1H), δ 7.88 (d, J = 8.6 Hz, 1H), δ 7.44 (t, J = 7.9 Hz, 1H), δ 7.30-7.09 (m, 5H), δ 6.97 (br s, 1H), δ 4.25-4.14 (m, 1H), δ 3.67 (q, J = 7.5 Hz, 2H), δ 2.89 (t, J = 7.3 Hz, 2H), δ 1.16 (d, J = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{19}H_{22}ClN_4$ $[M + H]^+$ 341.1455, found 341.1527. Purity: 100.0%

8-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8i). Yellow solid; yield 69% (0.37 g, 1.09 mmol); mp 111–113 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.17–8.15 (m, 1H), δ 7.92–7.87 (m,

1H), δ 7.63–7.59 (m, 1H), δ 7.31–7.04 (m, 5H), δ 6.98–6.92 (m, 2H), δ 3.75–3.64 (m, 2H), δ 2.97–2.88 (m, 3H), δ 0.65–0.59 (m, 2H), δ 0.48–0.45 (m, 2H). HRMS (ESI) m/z calcd for $C_{19}H_{20}ClN_4$ $[M + H]^+$ 338.1298, found 338.1372. Purity: 98.7%

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9a). Yellow solid; yield 71% (0.37 g, 0.93 mmol); mp 107–109 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.08–8.03 (m, 2H), δ 7.40 (dd, J = 8.9, 2.3 Hz, 1H), δ 7.17 (d, J = 8.8 Hz, 1H), δ 6.84–6.71 (m, 4H), δ 3.67–3.59 (m, 8H), δ 3.27–3.23 (m, 2H), δ 2.81 (t, J = 7.3 Hz, 2H), δ 1.48 (sextet, J = 7.2 Hz, 2H), δ 0.84 (t, J = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1740. Purity: 99.4%

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9b). White solid; yield 75% (0.40 g, 0.99 mmol); mp 109–111 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.09–8.05 (m, 2H), δ 7.43 (dd, J = 8.9, 2.2 Hz, 1H), δ 7.18 (d, J = 9.0 Hz, 1H), δ 6.84–6.72 (m, 3H), δ 6.71 (br s, 1H), δ 4.16–4.09 (m, 1H), δ 3.67–3.59 (m, 8H), δ 2.82 (t, J = 7.3 Hz, 2H), δ 1.12 (d, J = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1740. Purity: 98.3%

6-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9c). Yellow solid; yield 72% (0.38 g, 0.95 mmol); mp 104–106 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.07 (d, J = 2.2 Hz, 1H), δ 8.00 (br s, 1H), δ 7.42 (dd, J = 8.9, 2.3 Hz, 1H), δ 7.22 (d, J = 8.9 Hz, 1H), δ 6.86–6.71 (m, 4H), δ 3.67–3.59 (m, 8H), δ 2.87–2.75 (m, 3H), δ 0.64–0.58 (m, 2H), δ 0.48–0.43 (m, 2H). HRMS (ESI) m/z calcd for $C_{21}H_{24}ClN_4O_2$ $[M + H]^+$ 399.1510, found 399.1582. Purity: 98.5%

7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9d). Yellow solid; yield 71% (0.37 g, 0.93 mmol); mp 105–107 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.96–7.90 (m, 2H), δ 7.20–7.15 (m, 1H), δ 6.97 (dd, J = 8.6, 2.1 Hz, 1H), δ 6.84–6.72 (m, 4H), δ 3.67–3.59 (m, 8H), δ 2.81 (t, J = 7.3 Hz, 2H), δ 1.46 (sextet, J = 7.2 Hz, 2H), δ 0.78 (t, J = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1738. Purity: 99.6%

7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9e). White solid; yield 71% (0.37 g, 0.93 mmol); mp 111–113 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.97–7.93 (m, 2H), δ

7.19–7.14 (m, 1H), δ 6.99 (dd, *J* = 8.7, 2.1 Hz, 1H), δ 6.84–6.72 (m, 4H), δ 4.17–4.10 (m, 1H), δ 3.67–3.59 (m, 8H), δ 2.82 (t, *J* = 7.3 Hz, 2H), δ 1.12 (d, *J* = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1738. Purity: 95.2%

7-Chloro-*N*^{2}-cyclopropyl-*N*^{4}-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9f). Light brown solid; yield 72% (0.38 g, 0.95 mmol); mp 108–110 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.02 (br s, 1H), δ 7.93 (d, *J* = 8.9 Hz, 1H), δ 7.21–7.17 (m, 1H), δ 6.99 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 6.91 (br s, 1H), δ 6.80–6.71 (m, 3H), δ 3.67–3.59 (m, 8H), δ 2.88–2.78 (m, 3H), δ 0.64–0.58 (m, 2H), δ 0.48–0.43 (m, 2H). HRMS (ESI) m/z calcd for $C_{21}H_{24}ClN_4O_2$ $[M + H]^+$ 399.1510, found 399.1581. Purity: 99.2%

8-Chloro-*N*^{4}-(3,4-dimethoxyphenethyl)-*N*^{2}-propylquinazoline-2,4-diamine (9g). Yellow solid; yield 71% (0.37 g, 0.93 mmol); mp 101–103 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.92–7.86 (m, 2H), δ 7.57 (d, *J* = 7.0 Hz, 1H), δ 6.94–6.72 (m, 5H), δ 3.59–3.67 (m, 8H), δ 3.37–3.33 (m, 2H), δ 2.83 (t, *J* = 7.3 Hz, 2H), δ 1.51 (sextet, *J* = 7.2 Hz, 2H), δ 0.76 (t, *J* = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1738. Purity: 98.3%

8-Chloro-*N*^{4}-(3,4-dimethoxyphenethyl)-*N*^{2}-isopropylquinazoline-2,4-diamine (9h). Yellow solid; yield 76% (0.39 g, 0.97 mmol); mp 104–106 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.92–7.86 (m, 2H), δ 7.57 (d, *J* = 7.0 Hz, 1H), δ 6.94–6.72 (m, 5H), δ 4.19–4.08 (m, 1H), δ 3.67–3.59 (m, 8H), δ 2.82 (t, *J* = 7.3 Hz, 2H), δ 1.13 (d, *J* = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{21}H_{26}ClN_4O_2$ $[M + H]^+$ 401.1666, found 401.1737. Purity: 98.6%

8-Chloro-*N*^{2}-cyclopropyl-*N*^{4}-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9i). Yellow solid; yield 71% (0.37 g, 0.94 mmol); mp 102–104 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.92–7.86 (m, 2H), δ 7.57 (d, *J* = 7.0 Hz, 1H), δ 6.94–6.72 (m, 5H), δ 3.67–3.59 (m, 8H), δ 2.88–2.78 (m, 3H), δ 0.64–0.58 (m, 2H), δ 0.48–0.43 (m, 2H). HRMS (ESI) m/z calcd for $C_{21}H_{24}ClN_4O_2$ $[M + H]^+$ 399.1510, found 399.1581 Purity: 98.4%

***N*^{4}-Phenethyl-*N*^{2}-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10a).** Yellow solid; yield 76% (0.41 g, 1.34 mmol); mp 132–134 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.22 (dd, *J* = 4.1, 1.6 Hz, 1H), δ 7.95

(br s, 1H), δ 7.54 (br s, 1H), δ 7.44 (dd, *J* = 8.4, 4.1 Hz, 1H), δ 7.29–7.14 (m, 5H), δ 6.78 (br s, 1H), δ 3.62 (q, *J* = 7.5 Hz, 2H), δ 3.23–3.20 (m, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 1.48 (sextet, *J* = 7.2 Hz, 2H), δ 0.84 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (75 MHz, DMSO-*d*$_6$) δ 159.32, δ 146.53, δ 142.32, δ 141.98, δ 139.52, δ 131.99, δ 131.41, δ 128.60, δ 128.30, δ 127.53, δ 126.4, δ 42.67, δ 41.39, δ 34.63, δ 22.34, δ 11.53. HRMS (ESI) m/z calcd for $C_{18}H_{22}N_5$ $[M + H]^+$ 308.1797, found 308.1869. Purity: 99.4%

***N*^{2}-Isopropyl-*N*^{4}-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10b).** Brownish oil; yield 76% (0.41 g, 1.34 mmol). ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.23 (dd, *J* = 4.1, 1.6 Hz, 1H), δ 7.99 (br s, 1H), δ 7.55 (br s, 1H), δ 7.44 (dd, *J* = 8.4, 4.1 Hz, 1H), δ 7.30–7.14 (m, 5H), δ 6.60 (br s, 1H), δ 4.19–4.08 (m, 1H), δ 3.63 (q, *J* = 7.5 Hz, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 1.13 (d, *J* = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{18}H_{22}N_5$ $[M + H]^+$ 308.1797, found 308.1869. Purity: 99.7%

***N*^{2}-Cyclopropyl-*N*^{4}-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10c).** Brownish oil; yield 72% (0.39 g, 1.27 mmol). ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.26 (dd, *J* = 4.1, 1.6 Hz, 1H), δ 8.02 (br s, 1H), δ 7.55 (br s, 1H), δ 7.46 (dd, *J* = 8.4, 4.1 Hz, 1H), δ 7.27–7.16 (m, 5H), δ 6.93 (br s, 1H), δ 3.63 (q, *J* = 7.5 Hz, 2H), δ 2.89 (t, *J* = 7.3 Hz, 2H), δ 2.81–2.77 (m, 1H), δ 0.63–0.59 (m, 2H), δ 0.49–0.46 (m, 2H). HRMS (ESI) m/z calcd for $C_{18}H_{20}N_5$ $[M + H]^+$ 306.1640, found 306.1711. Purity: 99.8%

***N*^{4}-(3,4-Dimethoxyphenethyl)-*N*^{2}-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11a).** Yellow solid; yield 76% (0.40 g, 1.10 mmol); mp 121–123 °C. ^{1}H NMR (300 MHz, DMSO-*d*$_6$) δ 8.22 (dd, *J* = 4.8, 1.2 Hz, 1H), δ 7.85 (br s, 1H), δ 7.53 (br s, 1H), δ 7.43 (dd, *J* = 8.4, 4.1 Hz, 1H), δ δ 6.84–6.72 (m, 4H), δ 3.67–3.61 (m, 8H), δ 3.30–3.24 (m, 2H), δ 2.82 (t, *J* = 7.3 Hz, 2H), δ 1.46 (sextet *J* = 7.2 Hz, 2H), δ 0.84 (t, *J* = 7.4 Hz, 3H). HRMS (ESI) m/z calcd for $C_{20}H_{26}N_5O_2$ $[M + H]^+$ 368.2008, found 368.2081. Purity: 99.6%

N^4-(3,4-Dimethoxyphenethyl)-N^2-isopropylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11b). White solid; yield 73% (0.39 g, 1.06 mmol); mp 127–129 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.22 (dd, *J* = 4.8, 1.2 Hz, 1H), δ 7.86 (brs, 1H), δ 7.53 (br s, 1H), δ 7.44 (dd, *J* = 8.4, 4.1 Hz, 1H), δ 6.84–6.72 (m, 3H), δ 6.57 (br s, 1H), 4.16–4.09 (m, 1H), δ 3.67–3.61 (m, 8H), δ 2.82 (t, *J* = 7.3 Hz, 2H), δ 1.12 (d, *J* = 6.5 Hz, 6H). HRMS (ESI) m/z calcd for $C_{20}H_{26}N_5O_2$ $[M + H]^+$ 368.2008, found 368.2081. Purity: 98.4%

N^2-Cyclopropyl-N^4-(3,4-dimethoxyphenethyl)pyrido[3,2-*d*]pyrimidine-2,4-diamine (11c). Brown solid; yield 71% (0.38 g, 1.03 mmol); mp 117–119 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 4.8, 1.2 Hz, 1H), δ 7.94 (br s, 1H), δ 7.59 (br s, 1H), δ 7.45 (dd, *J* = 8.4, 4.1 Hz, 1H), δ 6.94 (br s, 1H), δ 6.84–6.72 (m, 3H), δ 3.68–3.65 (m, 8H), δ 2.88–2.80 (m, 3H), δ 0.63–0.59 (m, 2H), δ 0.48–0.46 (m, 2H). HRMS (ESI) m/z calcd for $C_{20}H_{24}N_5O_2$ $[M + H]^+$ 366.1852, found 366.1927. Purity: 99.4%

6-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12a). White solid; yield 76% (0.39 g, 1.20 mmol); mp 122–124 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.11 (br s, 1H), δ 8.04 (d, *J* = 2.3 Hz, 1H), δ 7.41 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 7.28–7.16 (m, 6H), δ 3.61 (q, *J* = 5.6 Hz, 2H), δ 3.12 (s, 6H), δ 2.90 (t, *J* = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{18}H_{20}ClN_4$ $[M + H]^+$ 327.1298, found 327.1370. Purity: 99.5%

7-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12b). Yellow solid; yield 72% (0.37 g, 1.15 mmol); mp 127–129 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.12 (br s, 1H), δ 7.90 (d, *J* = 8.7 Hz, 1H), δ 7.29–7.14 (m, 6H), δ 6.97 (dd, *J* = 8.9, 2.3 Hz, 1H), δ 3.60 (q, *J* = 5.6 Hz, 2H), δ 3.12 (s, 6H), δ 2.89 (t, *J* = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{18}H_{20}ClN_4$ $[M + H]^+$ 327.1298, found 327.1371. Purity: 94.5%

8-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12c). Yellow solid; yield 72% (0.37

g, 1.15 mmol); mp 122–124 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.15 (br s, 1H), δ 7.86 (d, J = 8.7 Hz, 1H), δ 7.60 (d, J = 8.7 Hz, 1H), δ 7.30–7.15 (m, 5H), δ 6.91 (t, J = 9.0 Hz, 1H), δ 3.63 (q, J = 5.6 Hz, 2H), δ 3.18 (s, 6H), δ 2.91 (t, J = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{18}H_{19}ClN_4$ $[M + H]^+$ 327.1298, found 327.1371. Purity: 96.3%

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13a). White solid; yield 70% (0.36 g, 0.93 mmol); mp 124–126 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.08–8.05 (m, 2H), δ 7.40 (dd, J = 8.9, 2.3 Hz, 1H), δ 7.20 (d, J = 8.9 Hz, 1H), δ 6.84–6.70 (m, 3H), δ 3.67–3.58 (m, 8H), δ 3.12 (s, 6H), δ 2.82 (t, J = 7.2 Hz, 2H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.45, δ 158.72, δ 150.76, δ 148.62, δ 147.22, δ 132.28, δ 132.06, δ 126.85, δ 123.40, δ 121.95, δ 120.43, δ 112.49, δ 111.94, δ 110.86, δ 55.47, δ 55.20, δ 42.48, δ 36.44, δ 34.00. HRMS (ESI) m/z calcd for $C_{20}H_{24}ClN_4O_2$ $[M + H]^+$ 387.1510, found 387.1581. Purity: 96.5%

7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13b). Yellow solid; yield 70% (0.36 g, 0.93 mmol); mp 128–130 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.09 (br s, 1H), δ 7.90 (d, J = 8.7 Hz, 1H), δ 7.20 (d, J = 2.1 Hz, 1H), δ 6.97 (dd, J = 8.7, 2.1 Hz, 1H), δ 6.84–6.69 (m, 3H), δ 3.71–3.58 (m, 8H), δ 3.13 (s, 6H), δ 2.82 (t, J = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{20}H_{24}ClN_4O_2$ $[M + H]^+$ 387.1510, found 387.1580. Purity: 98.4%

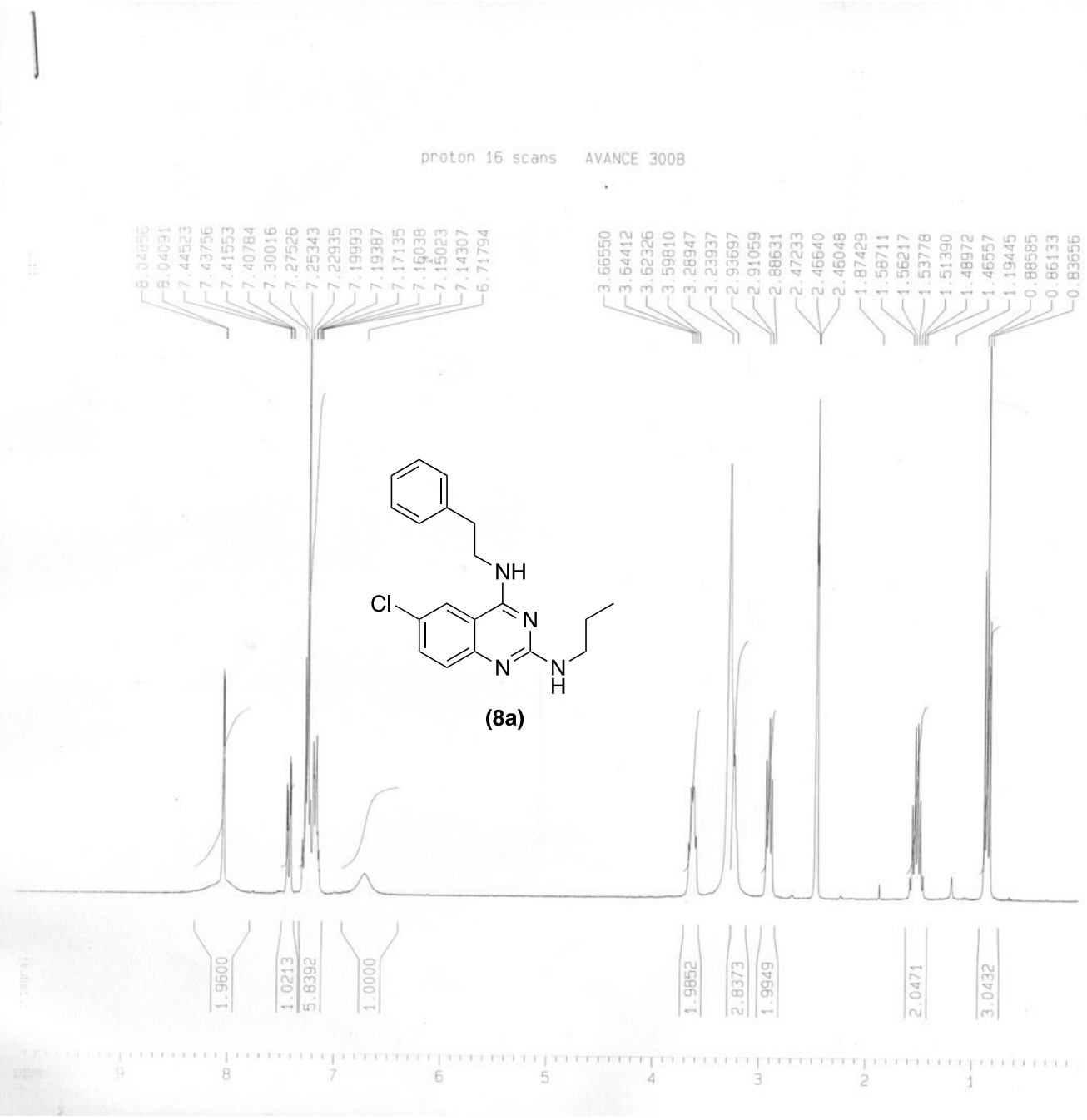
8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13c). Brown solid; yield 68% (0.35 g, 0.91 mmol); mp 121–123 °C. ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.10 (br s, 1H), δ 7.87 (d, J = 7.6 Hz, 1H), δ 7.59 (d, J = 7.5 Hz, 1H), δ 6.90 (t, J = 7.8 Hz, 1H), δ 6.84–6.70 (m, 3H), δ 3.70–3.60 (m, 8H), δ 3.17 (s, 6H), δ 2.83 (t, J = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{20}H_{24}ClN_4O_2$ $[M + H]^+$ 387.1510, found 387.1581. Purity: 99.0%

N^2,N^2-Dimethyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (14a). Brownish oil; yield 78% (0.40 g, 1.37 mmol). ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 4.2, 1.5 Hz, 1H), δ 8.09 (br s, 1H), δ 7.57 (dd, *J* = 8.5, 1.5 Hz, 1H), δ 7.44 (dd, *J* = 8.5, 4.2 Hz, 1H), δ 7.26–7.16 (m, 5H), δ 3.63 (q, *J* = 5.6 Hz, 2H), δ 3.14 (s, 6H), δ 2.90 (t, *J* = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{17}H_{20}N_5$ $[M + H]^+$ 294.1640, found 294.1712. Purity: 99.8%

N^4-(3,4-Dimethoxyphenethyl)-N^2,N^2-dimethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (15a). Brownish oil; yield 77% (0.40 g, 1.12 mmol). ^{1}H NMR (300 MHz, DMSO-d_6) δ 8.24 (dd, *J* = 4.2, 1.5 Hz, 1H), δ 8.03 (br s, 1H), δ 7.57 (dd, *J* = 8.5, 1.5 Hz, 1H), δ 7.44 (dd, *J* = 8.5, 4.2 Hz, 1H), δ 6.83–6.70 (m, 3H), δ 3.67–3.62 (m, 8H), δ 3.14 (s, 6H), δ 2.82 (t, *J* = 7.2 Hz, 2H). HRMS (ESI) m/z calcd for $C_{19}H_{24}N_5O_2$ $[M + H]^+$ 354.1852, found 354.1924. Purity: 97.3%

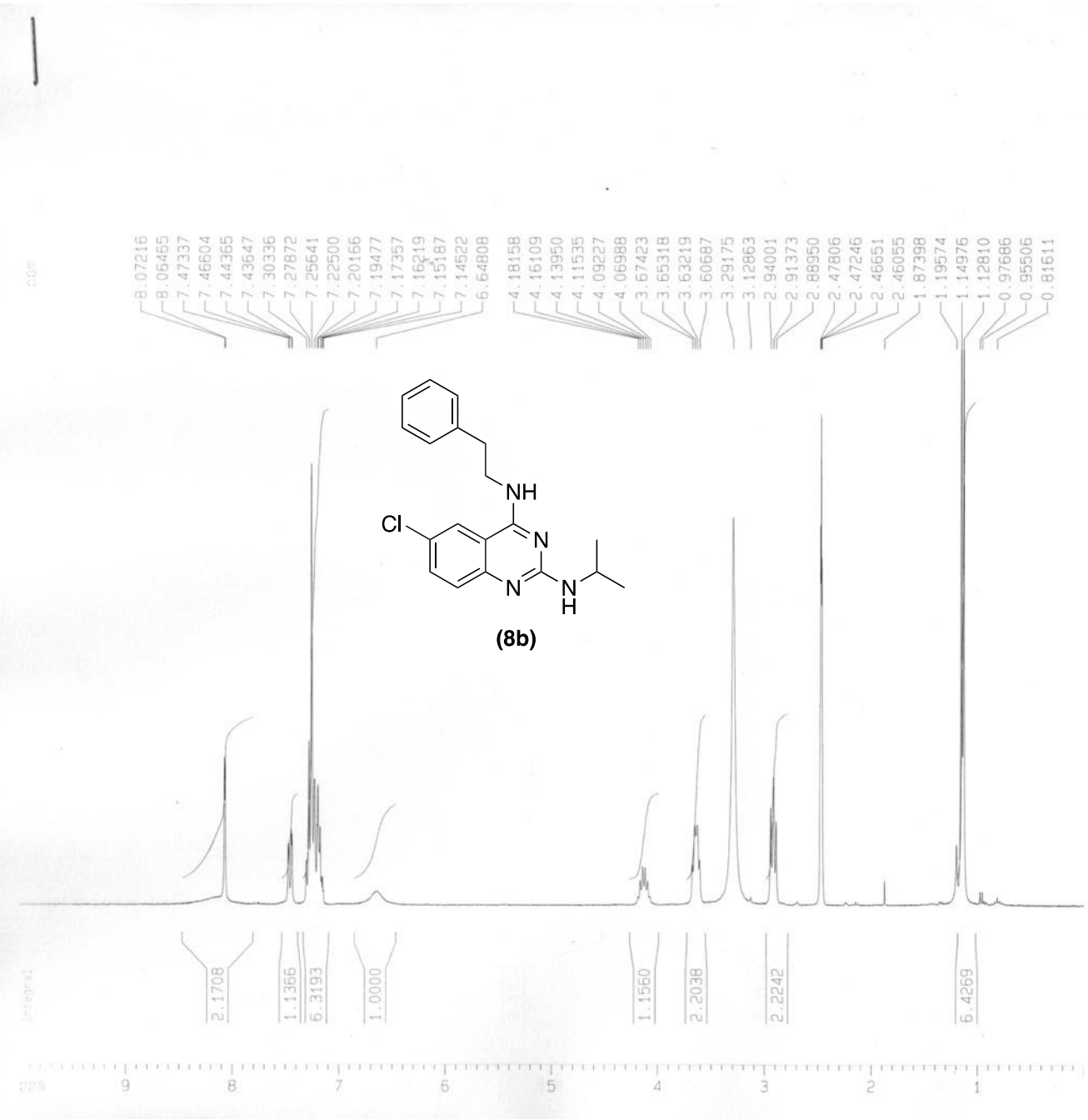
4. NMR spectra for compounds 8a–i, 9a–i, 10a–c, 11a–c, 12a–c, 13a–c, 14a and 15a

6-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (**8a**).



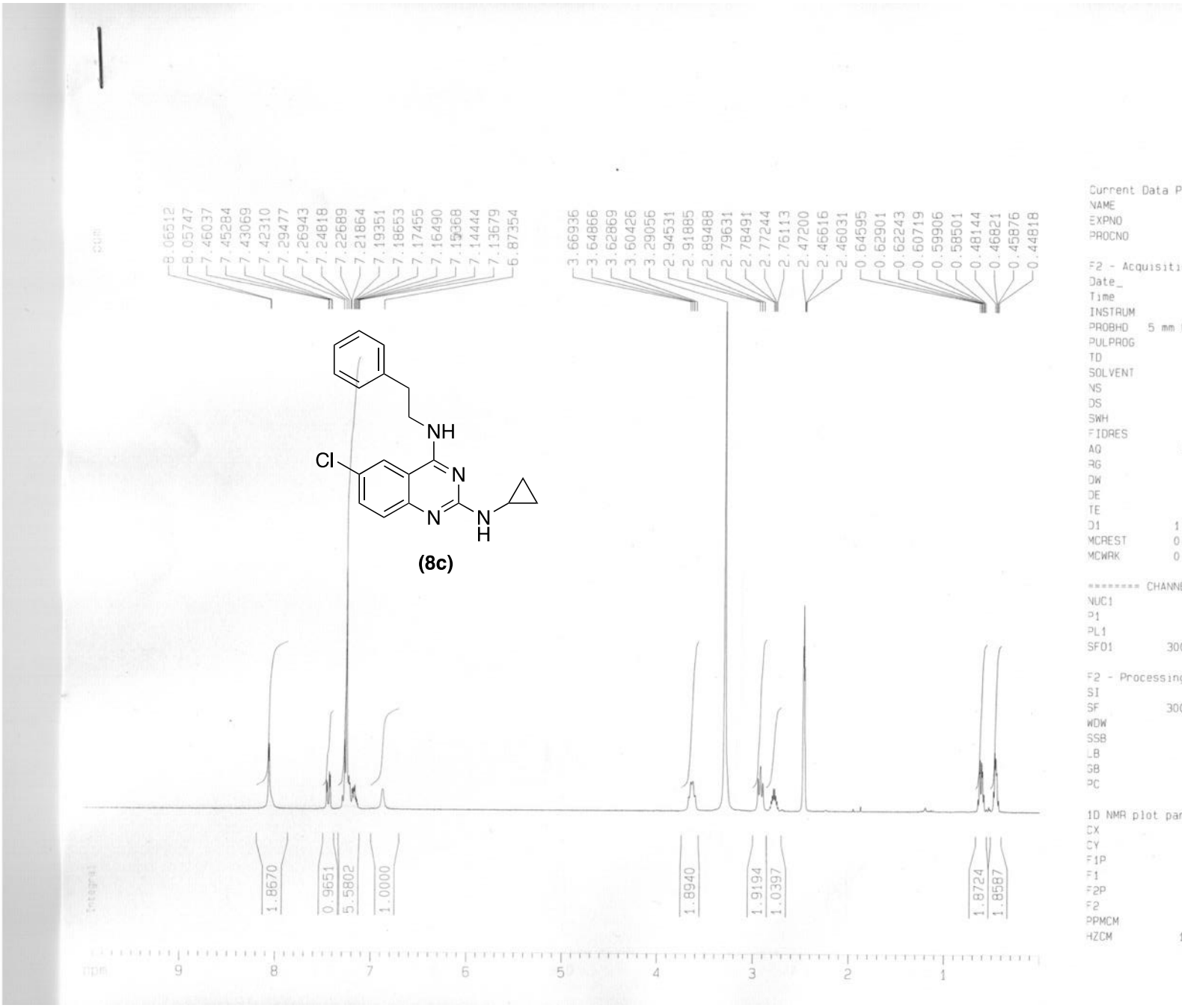

```
Current Data Parameters
NAME                  TM-Qnz286
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      21.32
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                   zg30
TD                       16384
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                   4340.278 Hz
FIDRES                0.264910 Hz
AQ                    1.8874868 sec
RG                          128
DW                    115.200 usec
DE                      6.00 usec
TE                      298.0 K
D1                    1.00000000 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                      12.00 usec
PL1                     -2.00 dB
SFO1                300.1318758 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300126 MHz
WDW                           EM
SSB                            0
LB                      0.30 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                         20.00 cm
CY                         12.50 cm
F1P                     10.000 ppm
F1                    3001.30 Hz
F2P                     0.000 ppm
F2                      0.00 Hz
PPMCM                 0.50000 ppm/cm
HZCM                150.06500 Hz/cm
```

6-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (**8b**).

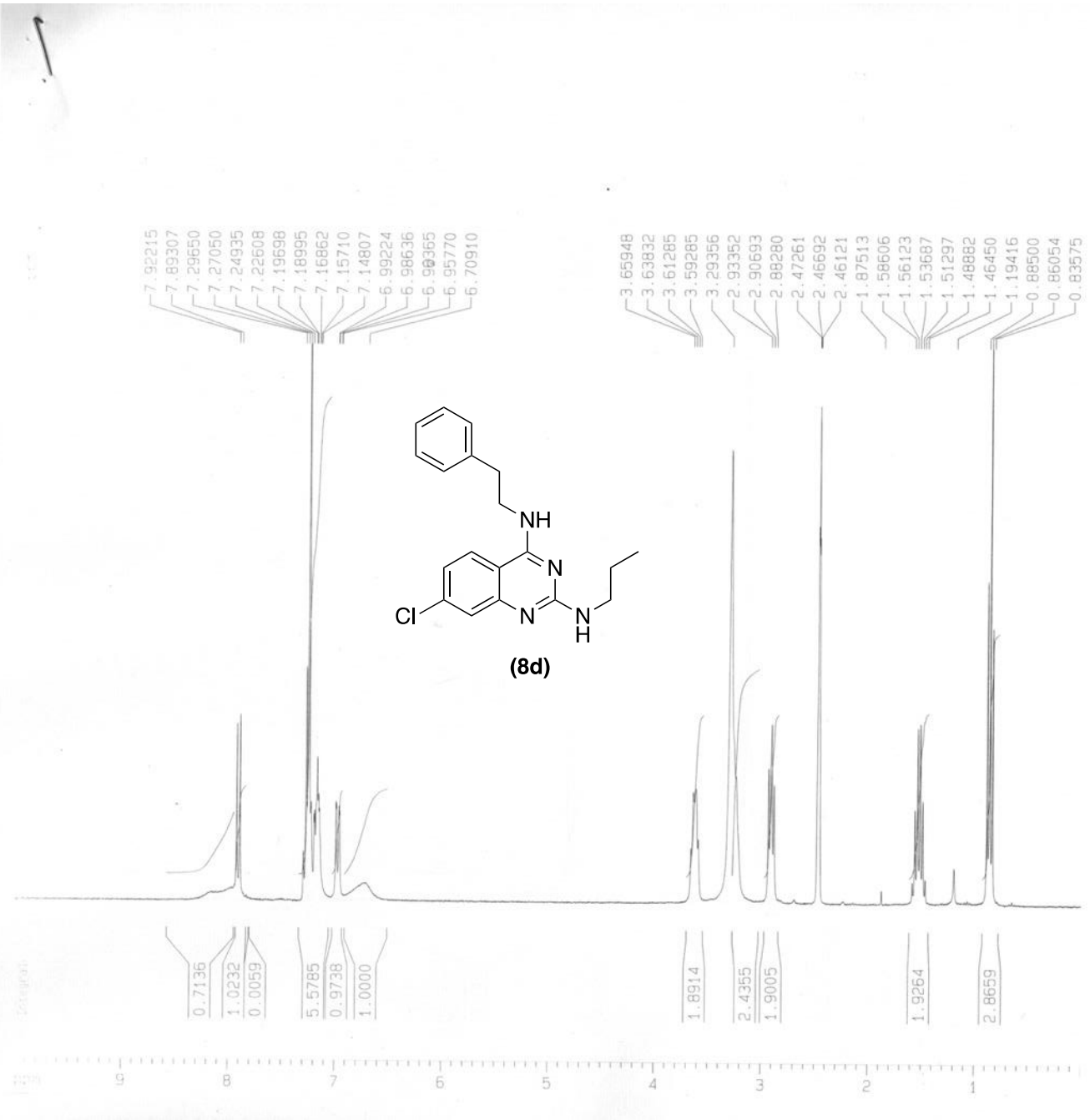



```
Current Data Parameters
NAME            TM-Qnz2B7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                21.51
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                   128
DW             115.200 usec
DE               6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -2.00 dB
SFO1         300.1318758 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300126 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          0.50000 ppm/cm
HZCM         150.06500 Hz/cm
```

6-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (**8c**).



7-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8d).

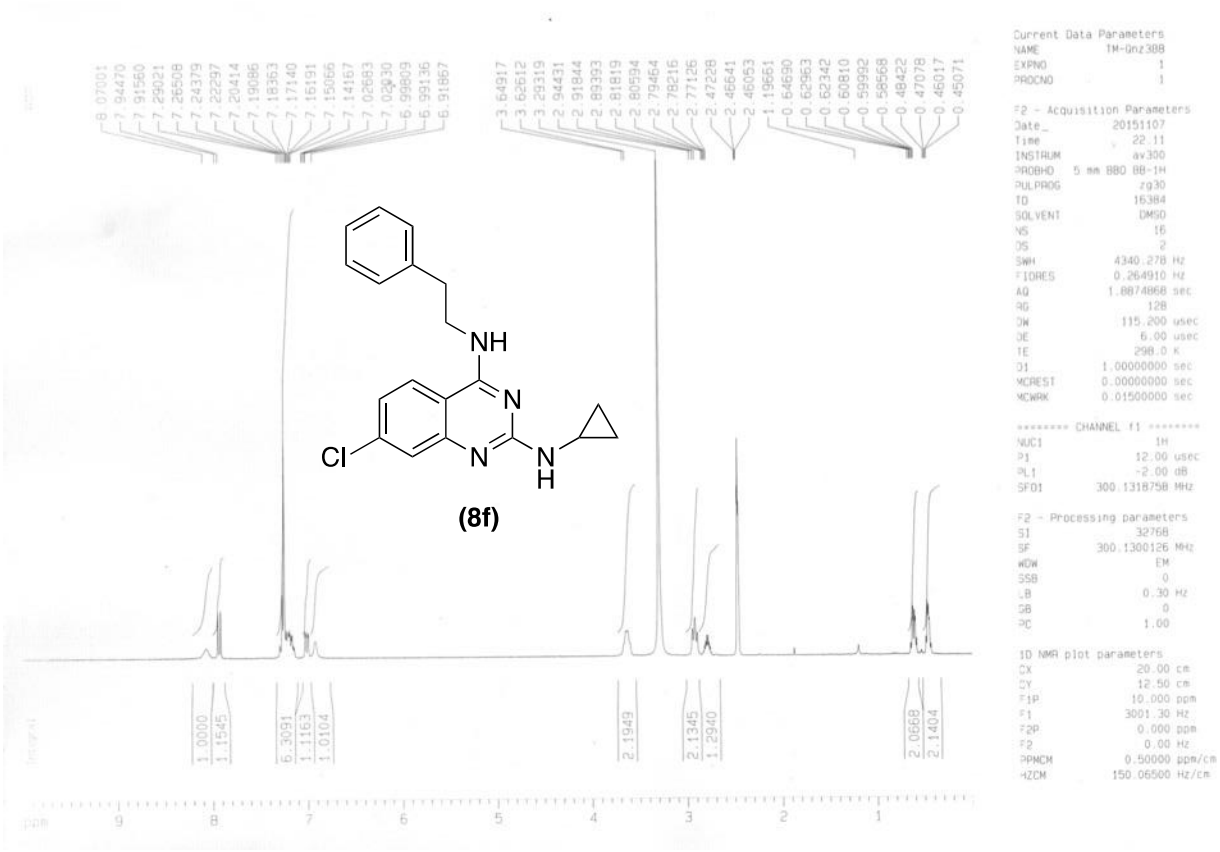


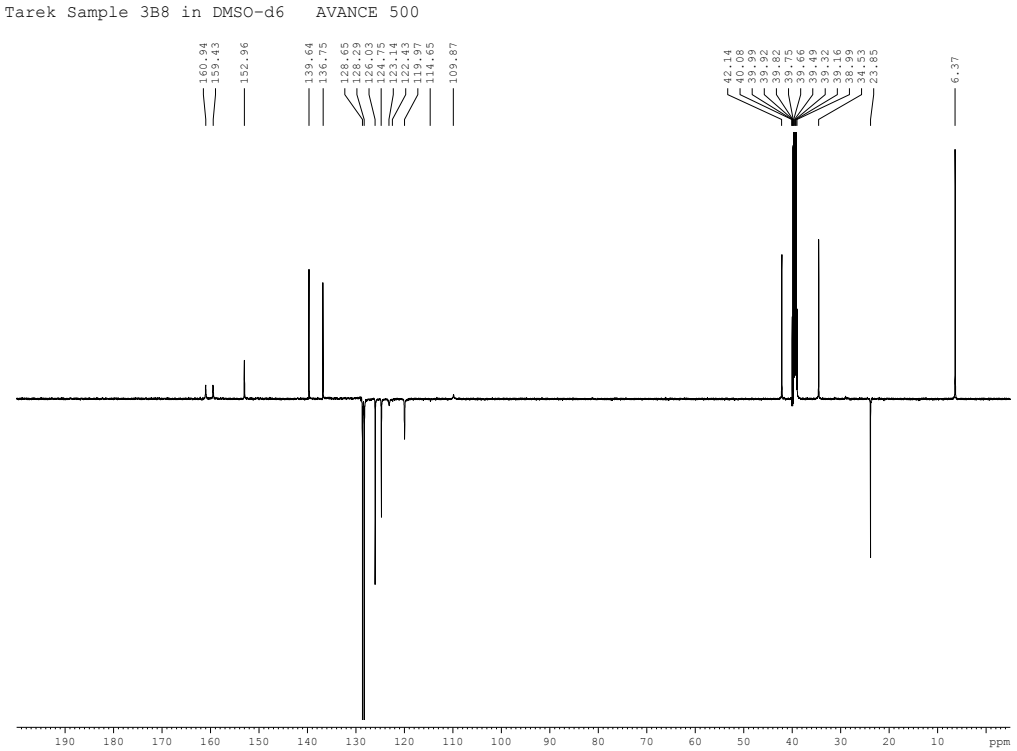

```
Current Data Parameters
NAME                  TM-Qnz3B6
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      21.37
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                   zg30
TD                       16384
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                 4340.278 Hz
FIDRES              0.264910 Hz
AQ                  1.8874868 sec
RG                          128
DW                  115.200 usec
DE                    6.00 usec
TE                    298.0 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                    12.00 usec
PL1                   -2.00 dB
SFO1           300.1318758 MHz

F2 - Processing parameters
SI                       32768
SF                 300.1300126 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    12.50 cm
F1P                  10.000 ppm
F1                  3001.30 Hz
F2P                   0.000 ppm
F2                    0.00 Hz
PPMCM                0.50000 ppm/cm
HZCM               150.06500 Hz/cm
```

7-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (**8e**).

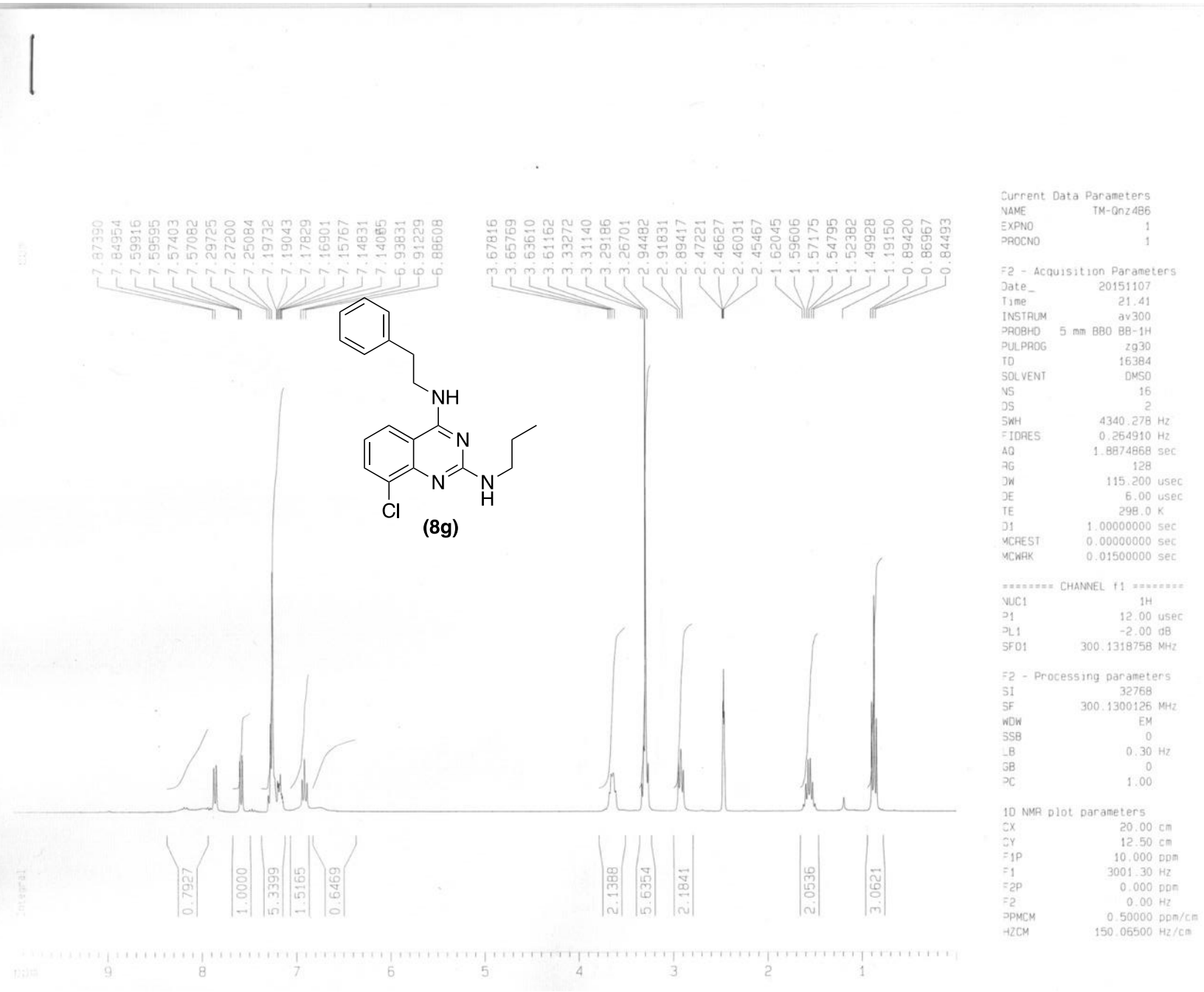

```
Current Data Parameters
NAME            TM-Qnz3B7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                21.54
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                     16
DS                      2
SWH             4340.278 Hz
FIDRES          0.264910 Hz
AQ              1.8874868 sec
RG                    128
DW               115.200 usec
DE                 6.00 usec
TE                298.0 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -2.00 dB
SFO1        300.1318758 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300126 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          0.50000 ppm/cm
HZCM         150.06500 Hz/cm
```

7-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8f).



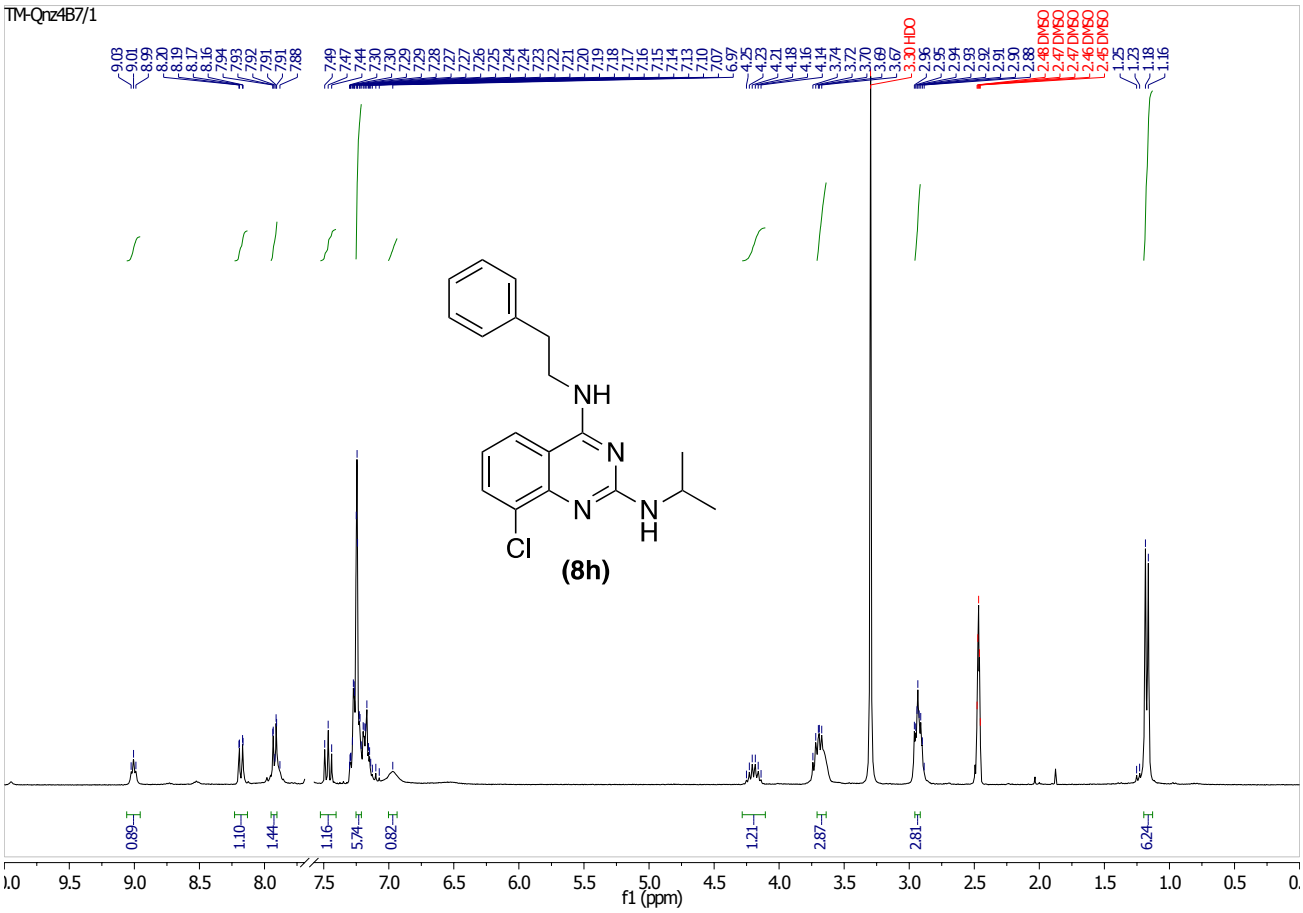


8-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8g).

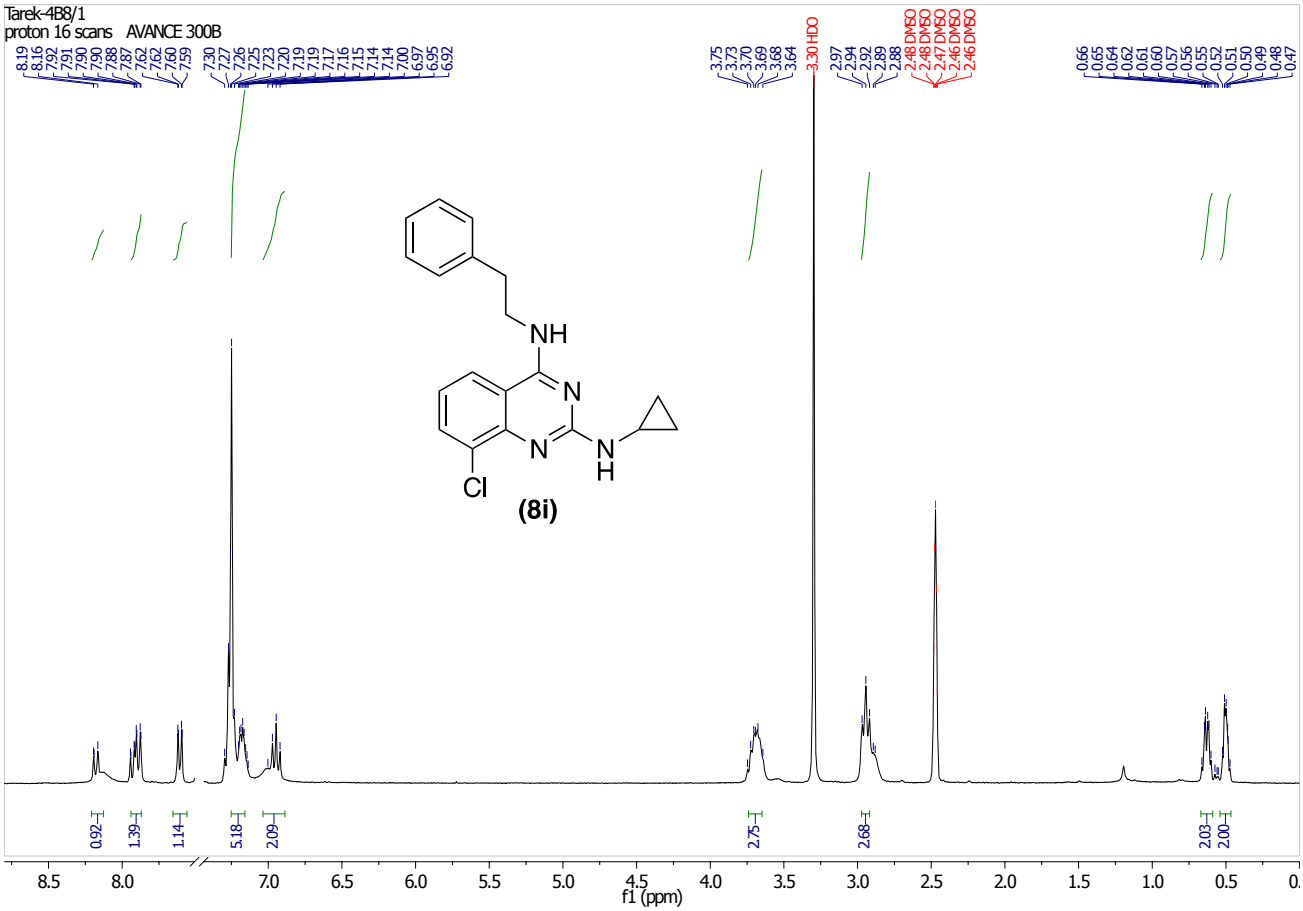



```
Current Data Parameters
NAME                  TM-Qnz4B6
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      21.41
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                    zg30
TD                        16384
SOLVENT                    DMSO
NS                           16
DS                            2
SWH                 4340.278 Hz
FIDRES              0.264910 Hz
AQ                  1.8874868 sec
RG                          128
DW                  115.200 usec
DE                    6.00 usec
TE                    298.0 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                    12.00 usec
PL1                   -2.00 dB
SFO1               300.1318758 MHz

F2 - Processing parameters
SI                         32768
SF                 300.1300126 MHz
WDW                           EM
SSB                            0
LB                     0.30 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    12.50 cm
F1P                  10.000 ppm
F1                  3001.30 Hz
F2P                   0.000 ppm
F2                    0.00 Hz
PPMCM                0.50000 ppm/cm
HZCM               150.06500 Hz/cm
```

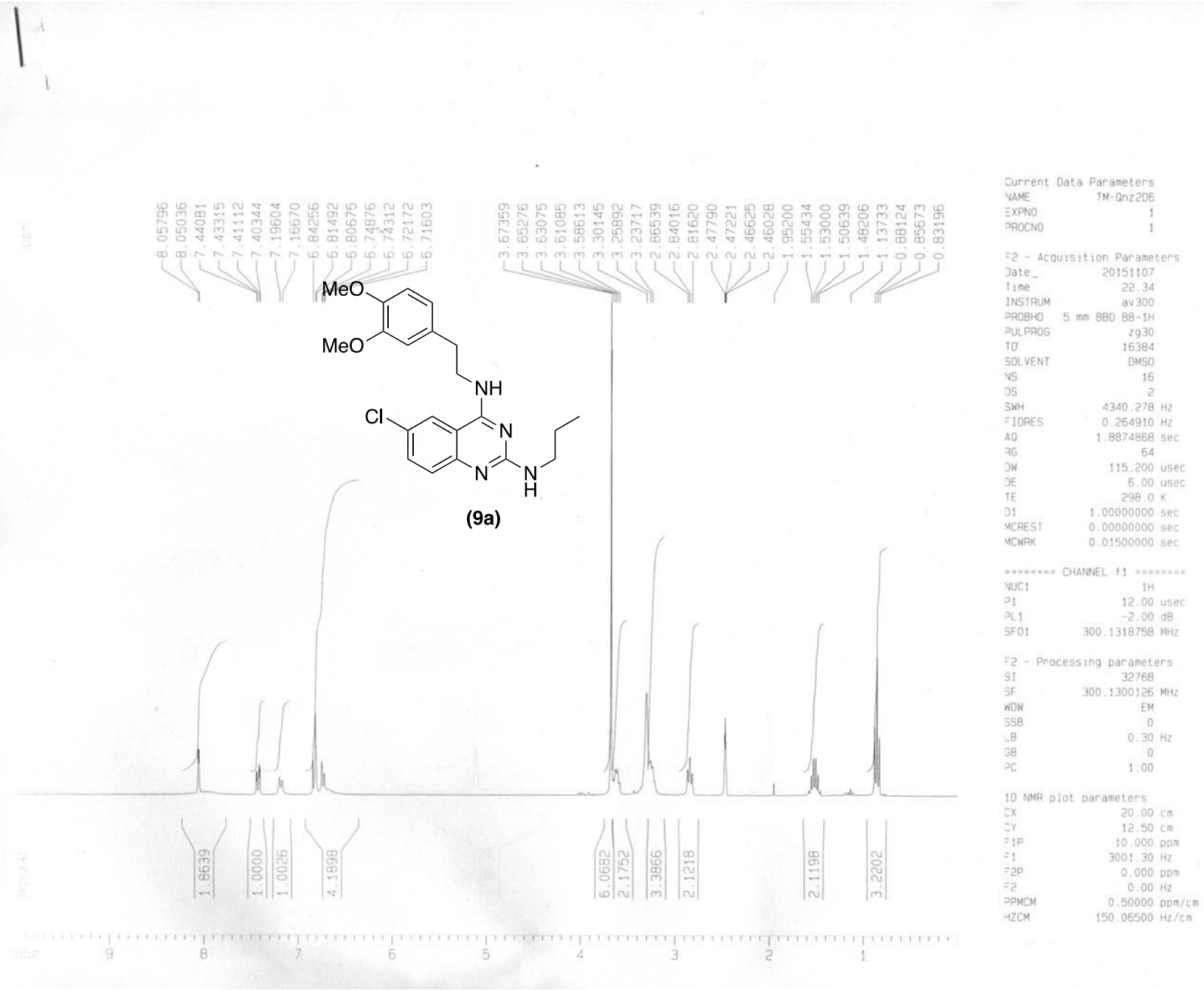
8-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8h).



8-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8i).

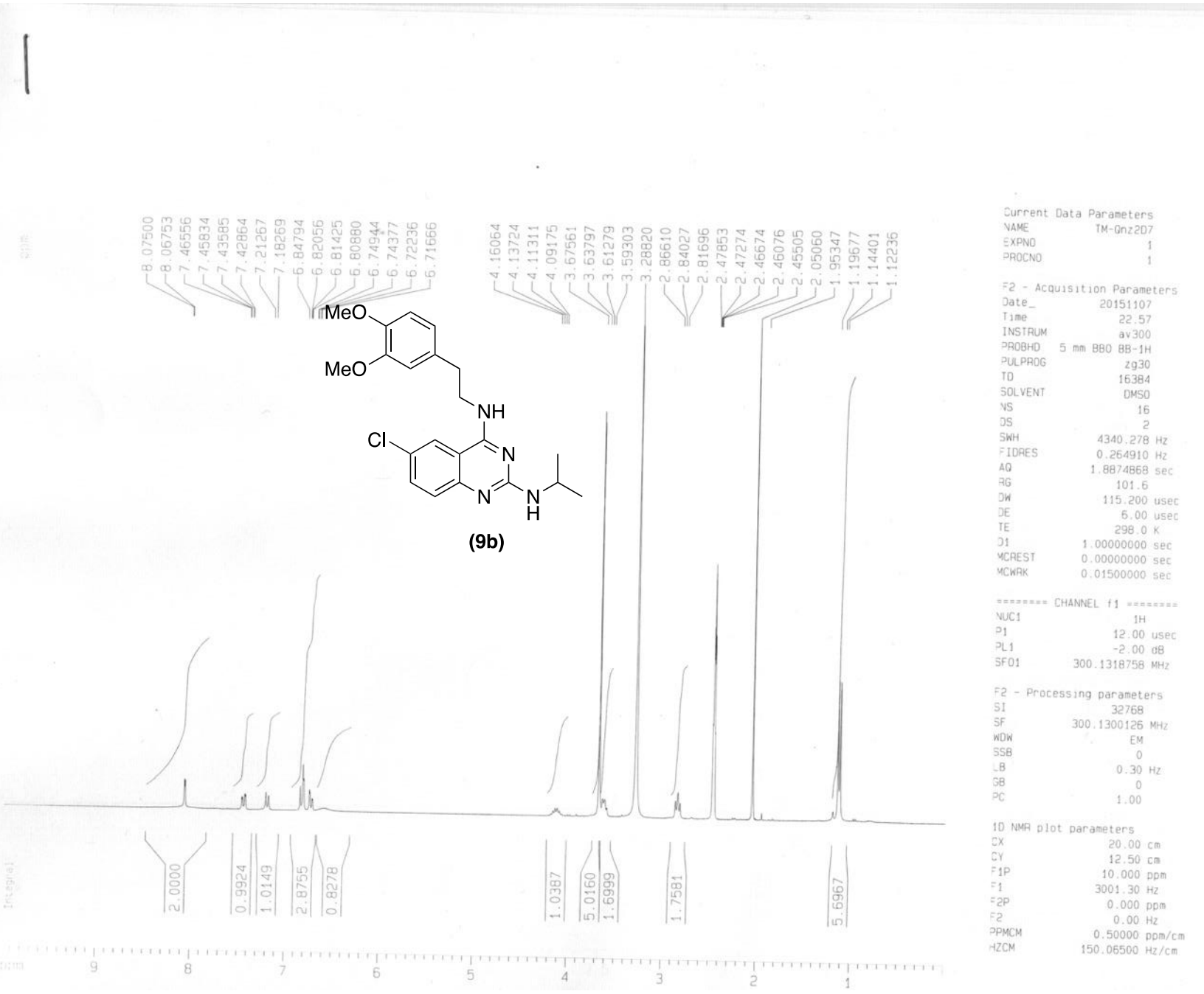


6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9a).



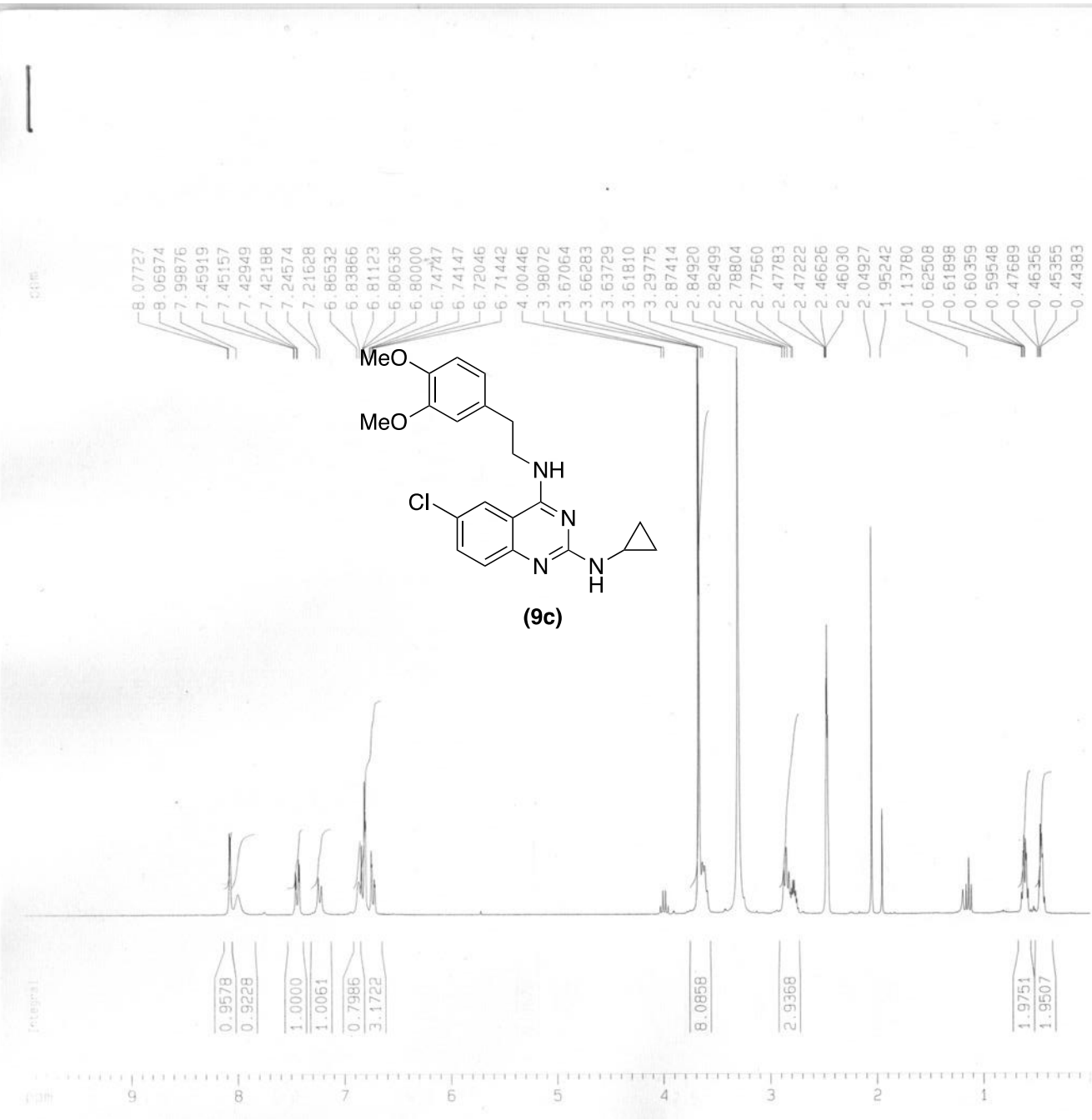

```
Current Data Parameters
NAME            TM-Qnz206
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                22.34
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                    64
DW             115.200 usec
DE               6.00 usec
TE              298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1               -2.00 dB
SFO1         300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              10.000 ppm
F1             3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM         0.50000 ppm/cm
HZCM        150.06500 Hz/cm
```

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (**9b**).



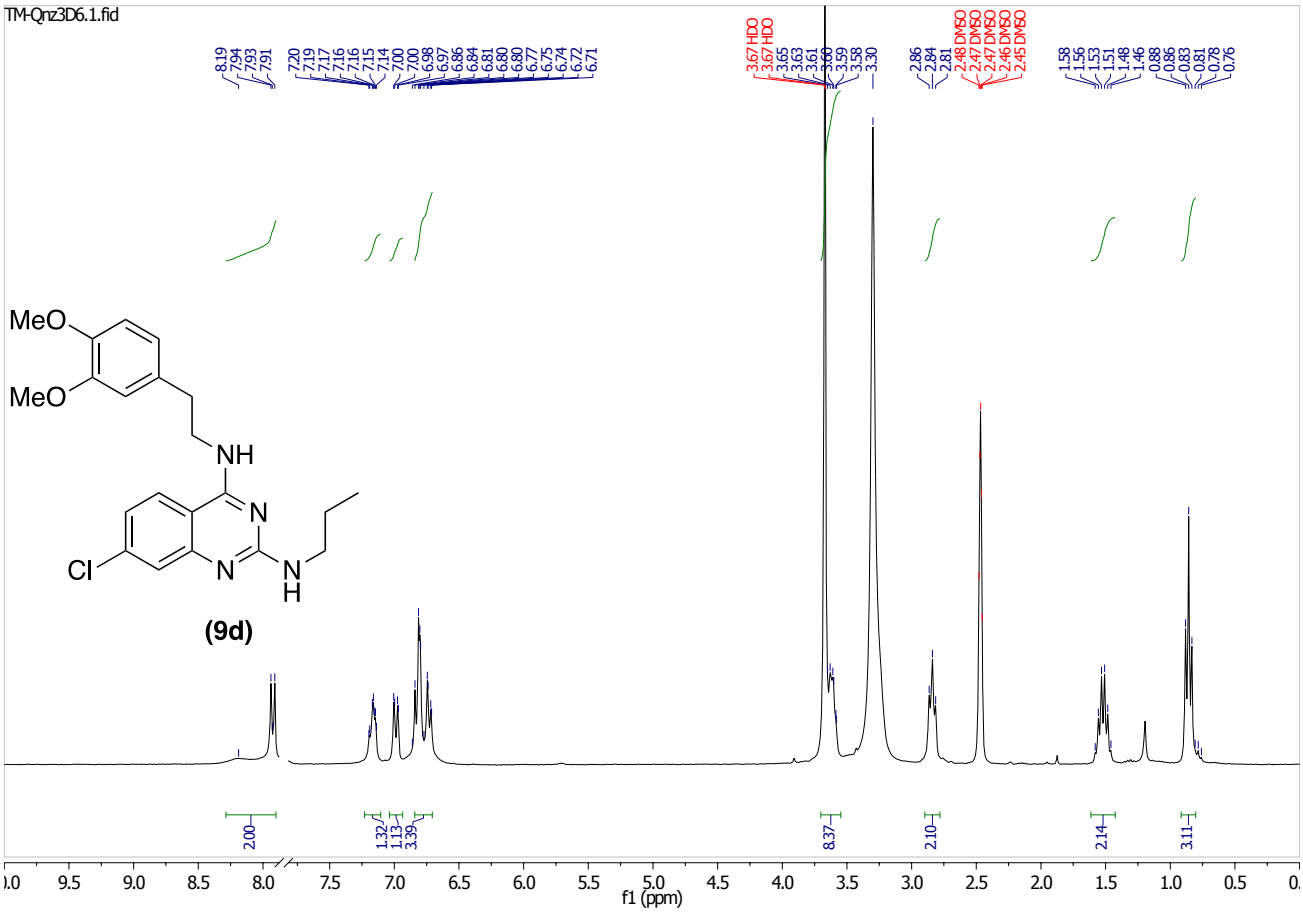

```
Current Data Parameters
NAME                  TM-Qnz2D7
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      22.57
INSTRUM                   av300
PROBHD  5 mm BBO BB-1H
PULPROG                   zg30
TD                       16384
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                 4340.278 Hz
FIDRES              0.264910 Hz
AQ                  1.8874868 sec
RG                        101.6
DW                  115.200 usec
DE                    6.00 usec
TE                    298.0 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                    12.00 usec
PL1                   -2.00 dB
SFO1                300.1318758 MHz

F2 - Processing parameters
SI                       32768
SF                  300.1300126 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    12.50 cm
F1P                  10.000 ppm
F1                  3001.30 Hz
F2P                   0.000 ppm
F2                    0.00 Hz
PPMCM               0.50000 ppm/cm
HZCM                150.06500 Hz/cm
```

6-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (**9c**).

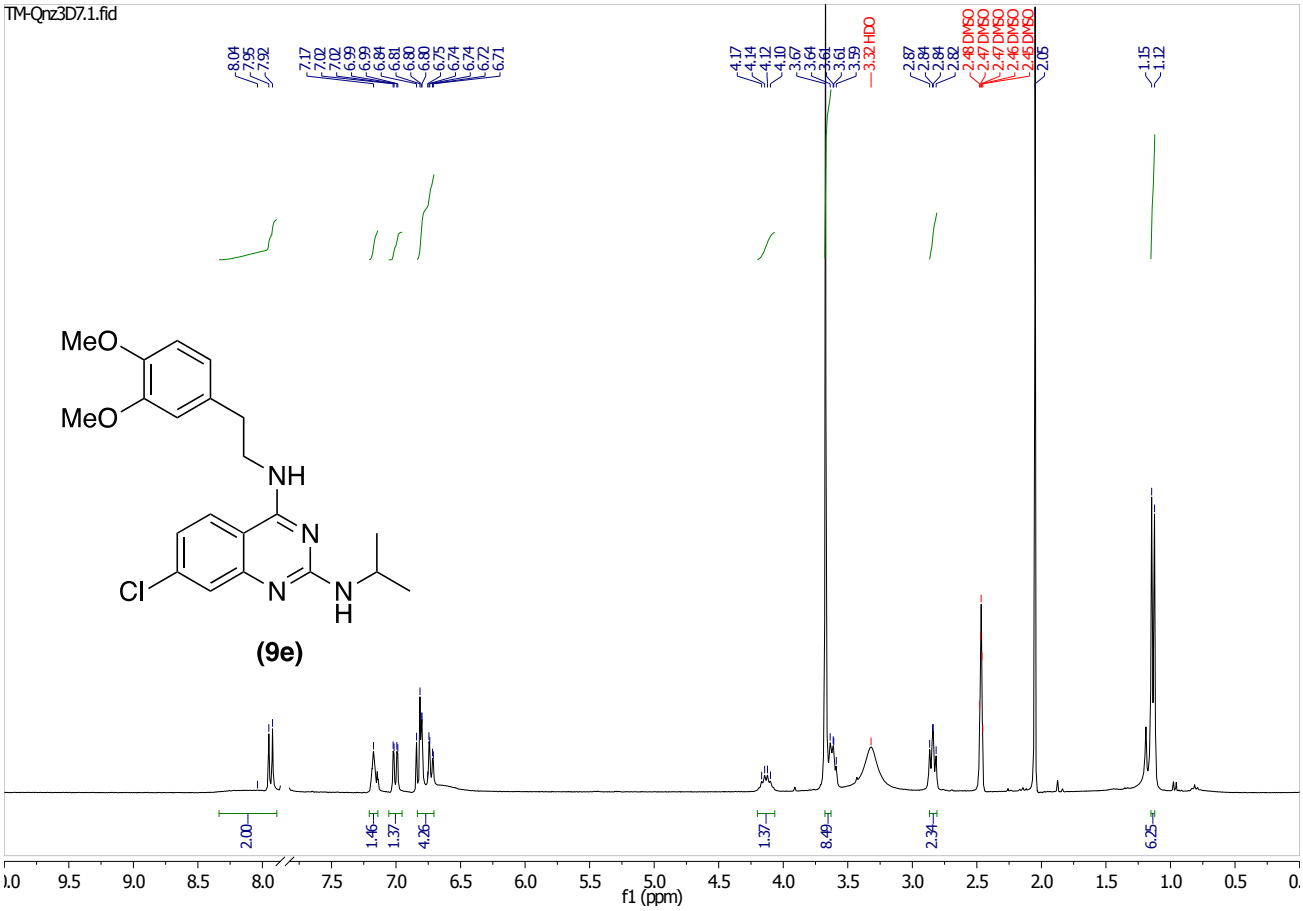



```
Current Data Parameters
NAME                  TM-Qnz208
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      23.15
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                   zg30
TD                       16384
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                 4340.278 Hz
FIDRES              0.264910 Hz
AQ                  1.8874868 sec
RG                         71.8
DW                  115.200 usec
DE                    6.00 usec
TE                    298.0 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                    12.00 usec
PL1                   -2.00 dB
SFO1               300.1318758 MHz

F2 - Processing parameters
SI                       32768
SF                 300.1300126 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       12.50 cm
F1P                     10.000 ppm
F1                    3001.30 Hz
F2P                      0.000 ppm
F2                       0.00 Hz
PPMCM                 0.50000 ppm/cm
HZCM                150.06500 Hz/cm
```

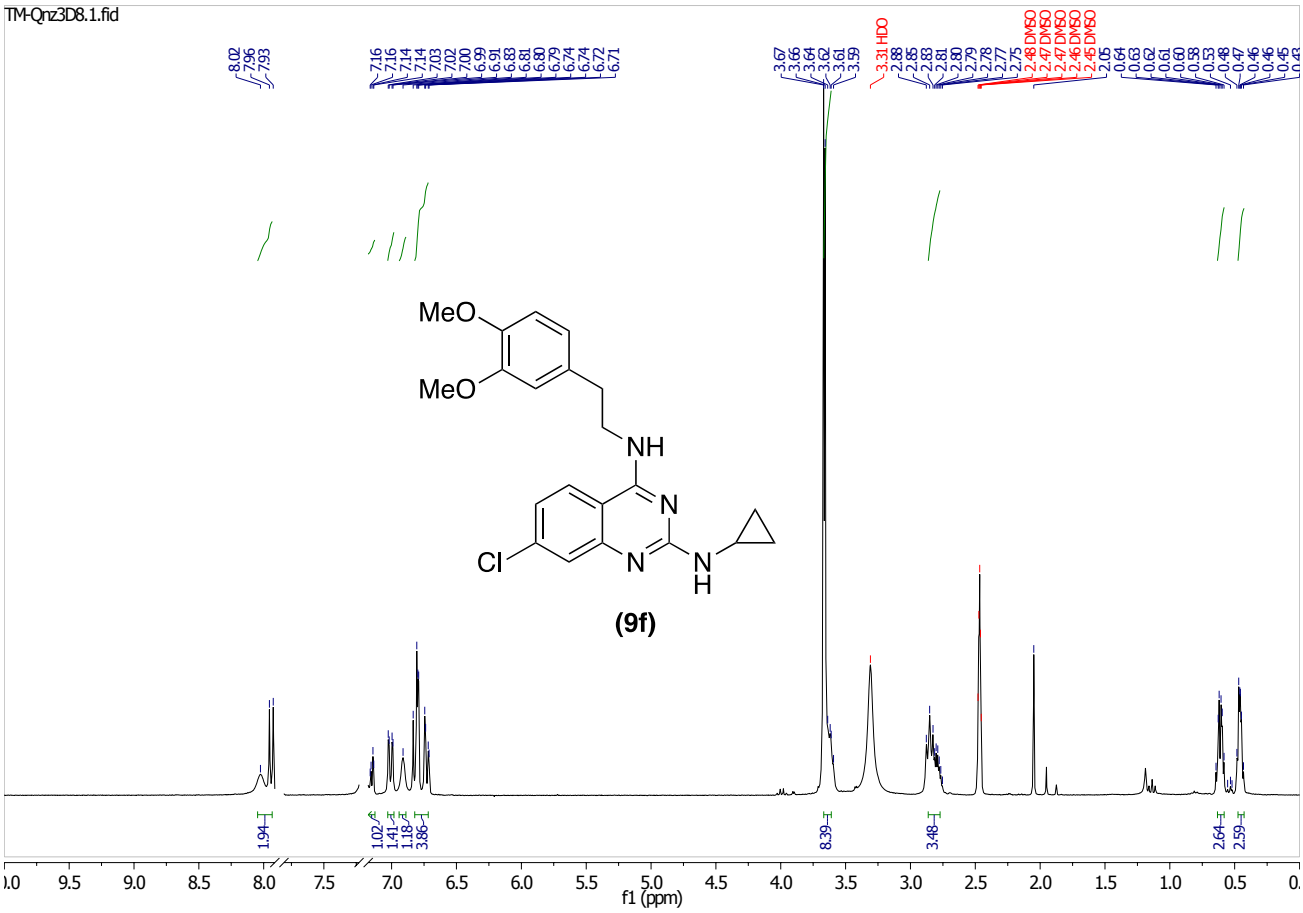
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9d).



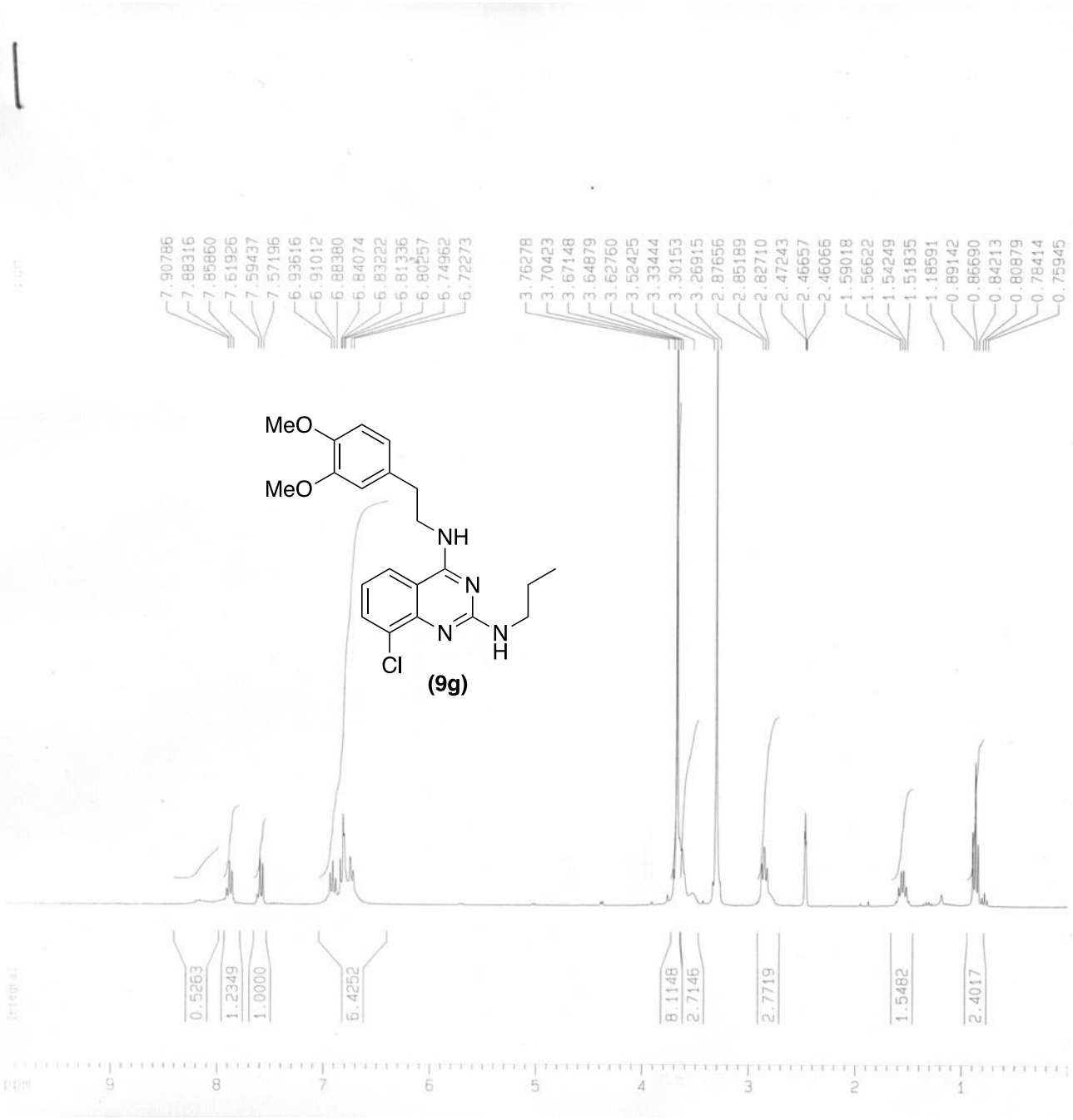
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9e).



7-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9f).

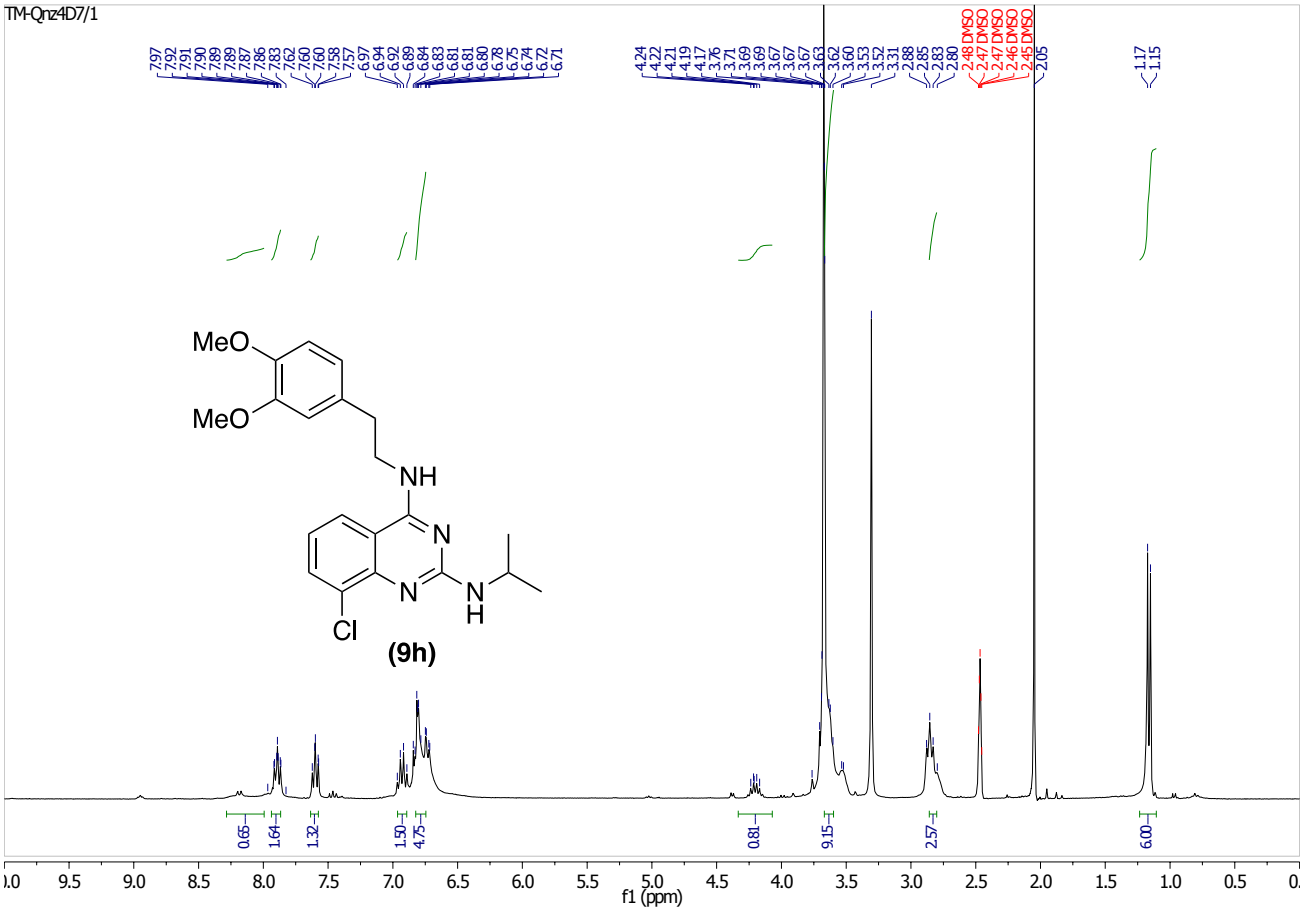


8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (**9g**).

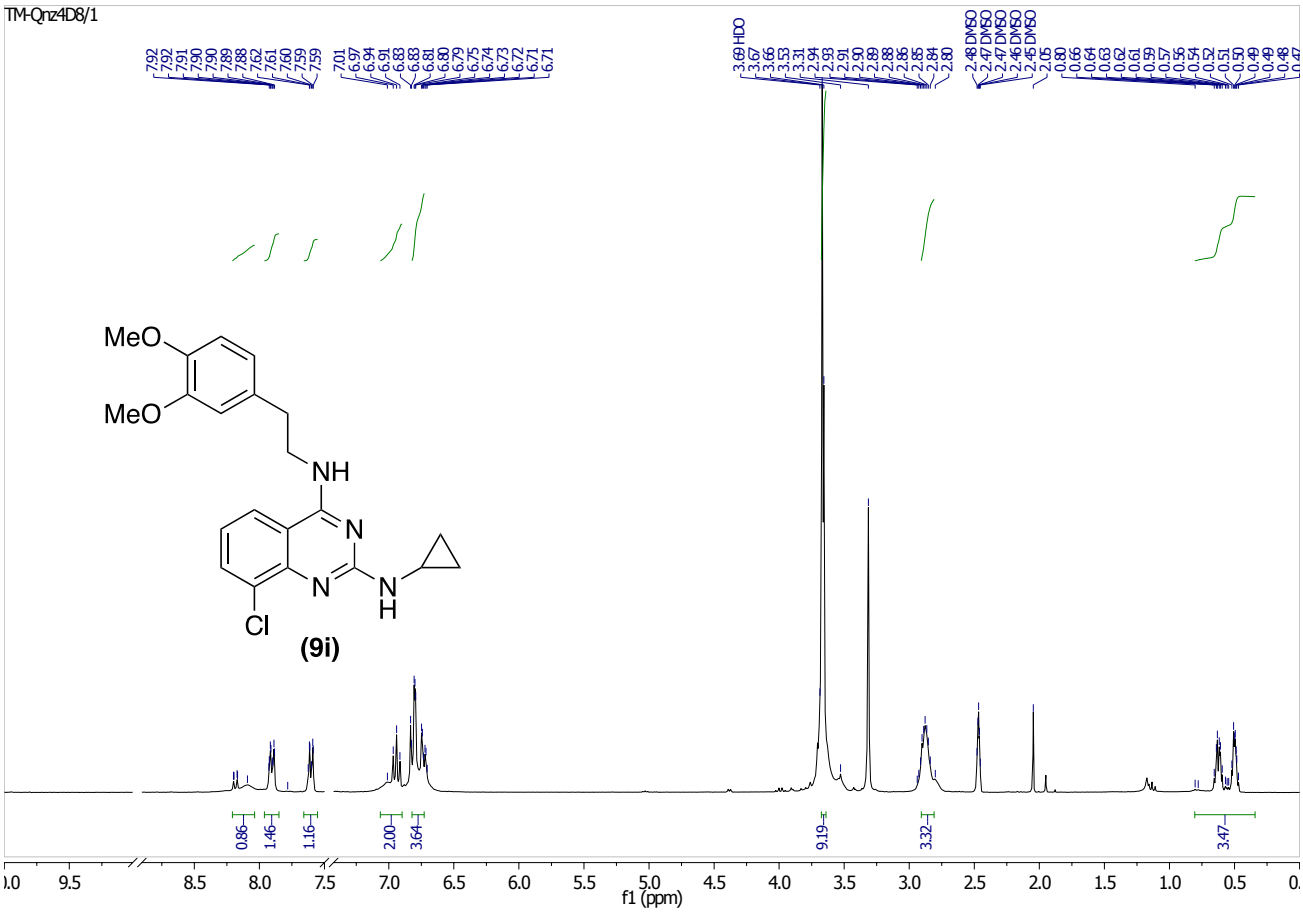



```
Current Data Parameters
NAME            TM-Qnz4D6
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                22.45
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                     16
DS                      2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                   50.8
DW             115.200 usec
DE               6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -2.00 dB
SFO1         300.1318758 MHz

F2 - Processing parameters
SI                  32768
SF           300.1300126 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                 20.00 cm
CY                 12.50 cm
F1P               10.000 ppm
F1              3001.30 Hz
F2P               0.000 ppm
F2                 0.00 Hz
PPMCM          0.50000 ppm/cm
HZCM         150.06500 Hz/cm
```

8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9h).

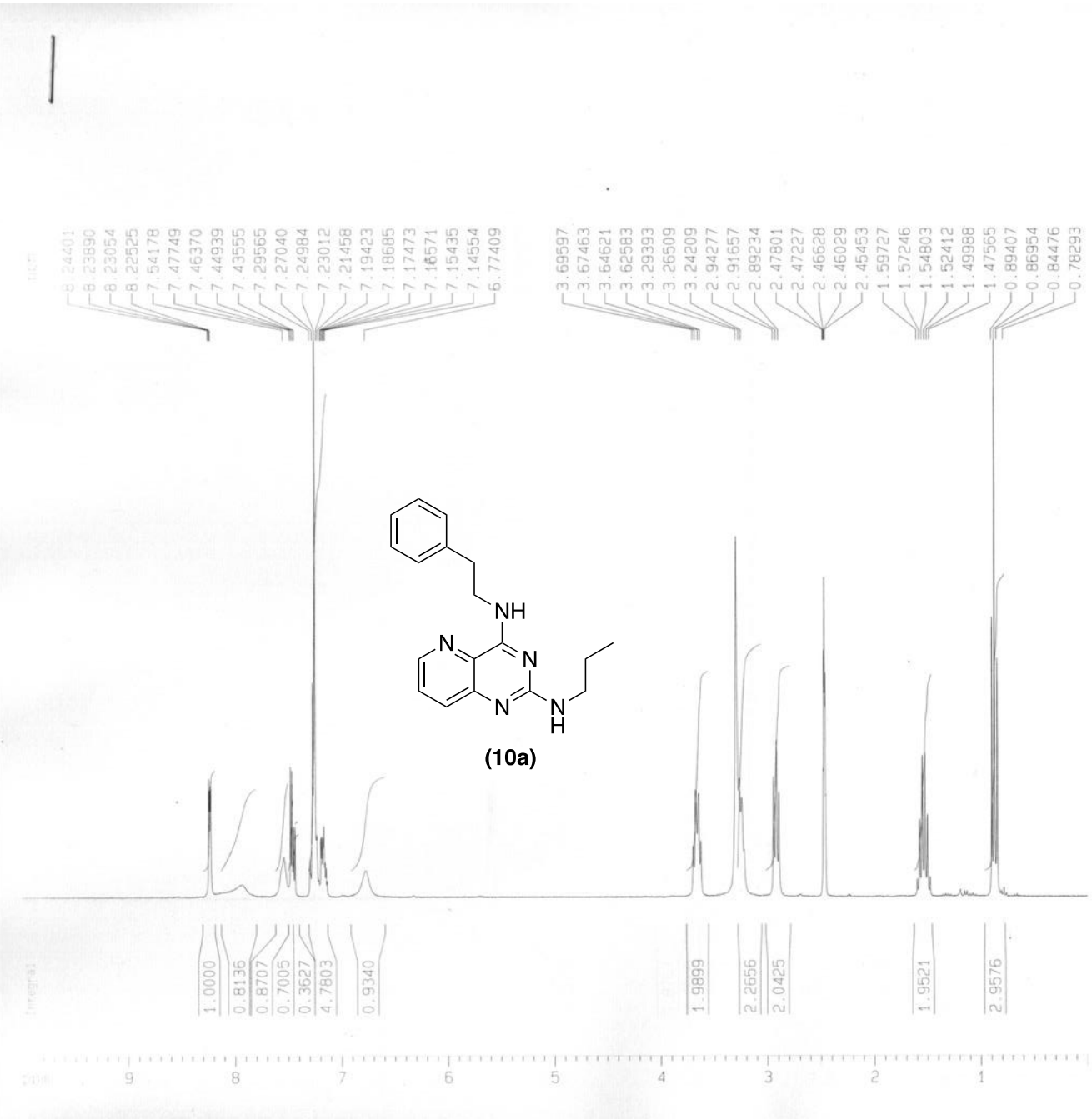


8-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9i).



***N*^{4}-Phenethyl-*N*^{2}-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10a).**

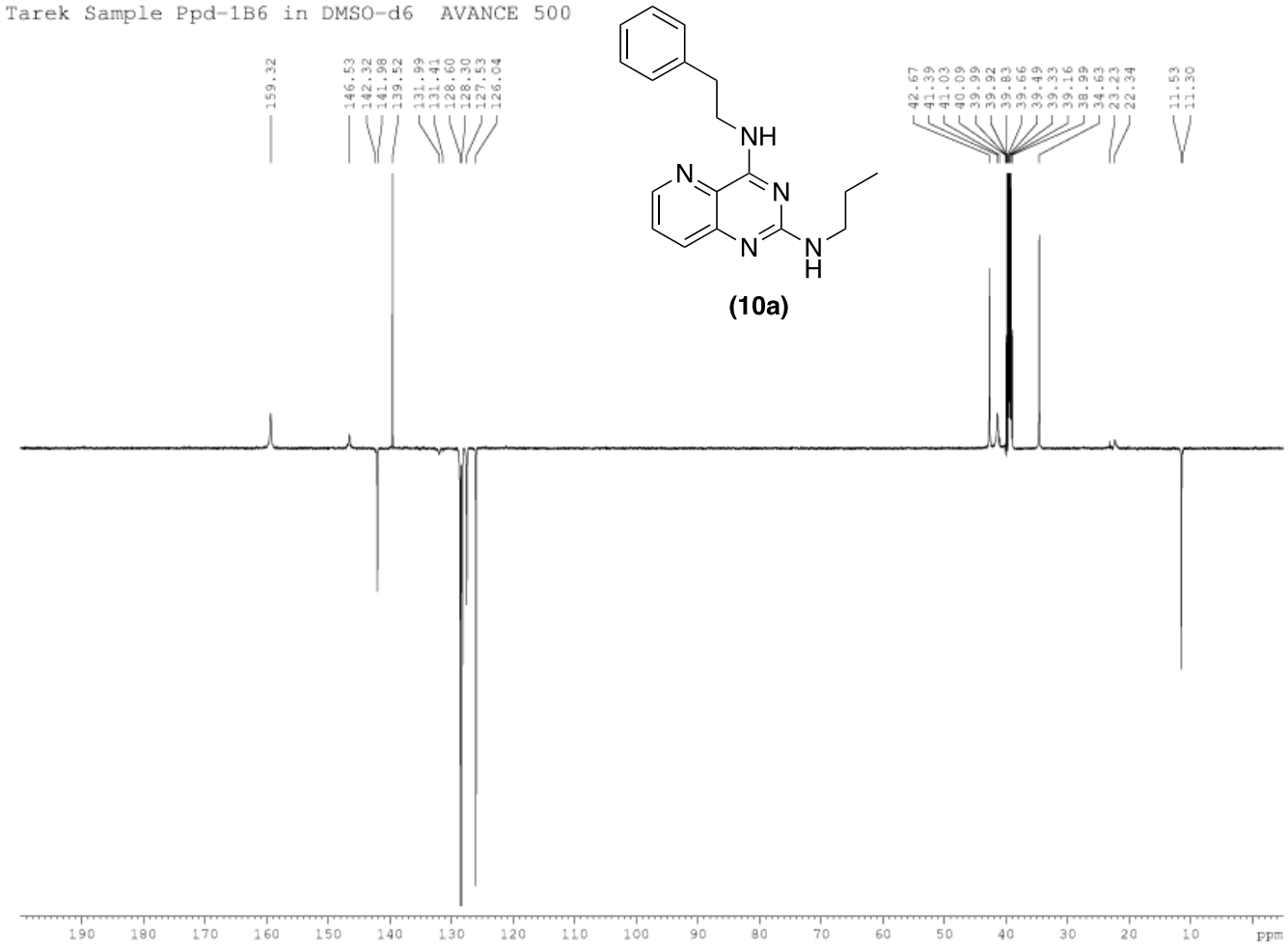
^{1}H NMR



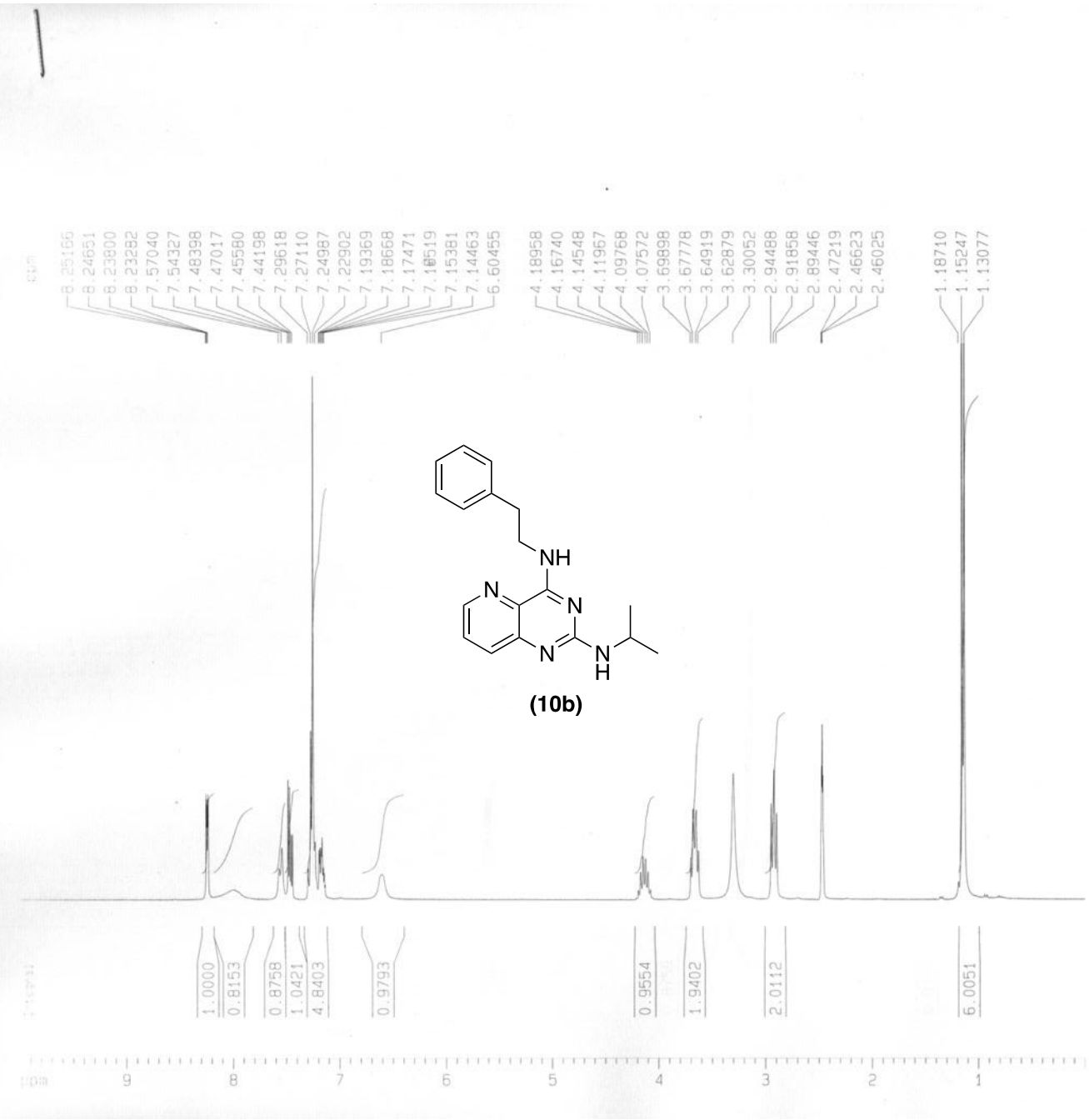

```
Current Data Parameters
NAME                  TM-Ppd1B6
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20151107
Time                      21.45
INSTRUM                   av300
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       16384
SOLVENT                   DMSO
NS                          16
DS                           2
SWH                 4340.278 Hz
FIDRES              0.264910 Hz
AQ                  1.8874868 sec
RG                          128
DW                  115.200 usec
DE                    6.00 usec
TE                    298.0 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                    12.00 usec
PL1                   -2.00 dB
SF01                300.1318758 MHz

F2 - Processing parameters
SI                       32768
SF                  300.1300126 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       12.50 cm
F1P                     10.000 ppm
F1                    3001.30 Hz
F2P                      0.000 ppm
F2                       0.00 Hz
PPMCM                 0.50000 ppm/cm
HZCM                150.06500 Hz/cm
```

N^4-Phenethyl-N^2-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10a).

^{13}C NMR

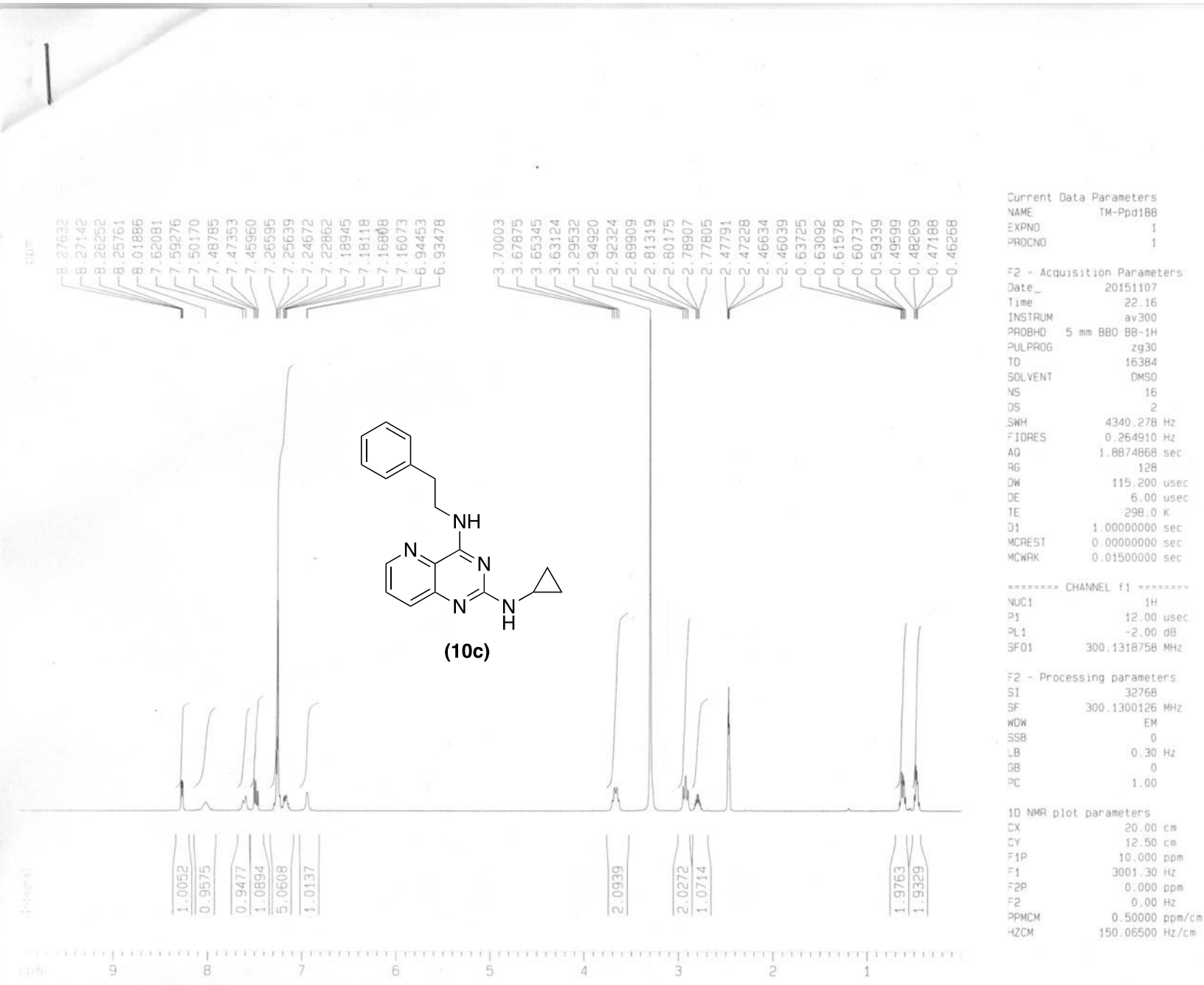


N^2-Isopropyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10b).




```
Current Data Parameters
NAME            TM-Ppd1B7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                22.02
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                      16
DS                       2
SWH              4340.278 Hz
FIDRES           0.264910 Hz
AQ               1.8874868 sec
RG                    71.8
DW                115.200 usec
DE                  6.00 usec
TE                298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                  12.00 usec
PL1                 -2.00 dB
SFO1          300.1318758 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300126 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   20.00 cm
CY                   12.50 cm
F1P                 10.000 ppm
F1                3001.30 Hz
F2P                  0.000 ppm
F2                    0.00 Hz
PPMCM             0.50000 ppm/cm
HZCM            150.06500 Hz/cm
```

N^2-Cyclopropyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10c).



Current Data Parameters
NAME TM-Ppd188
EXPNO 1
PROCNO 1

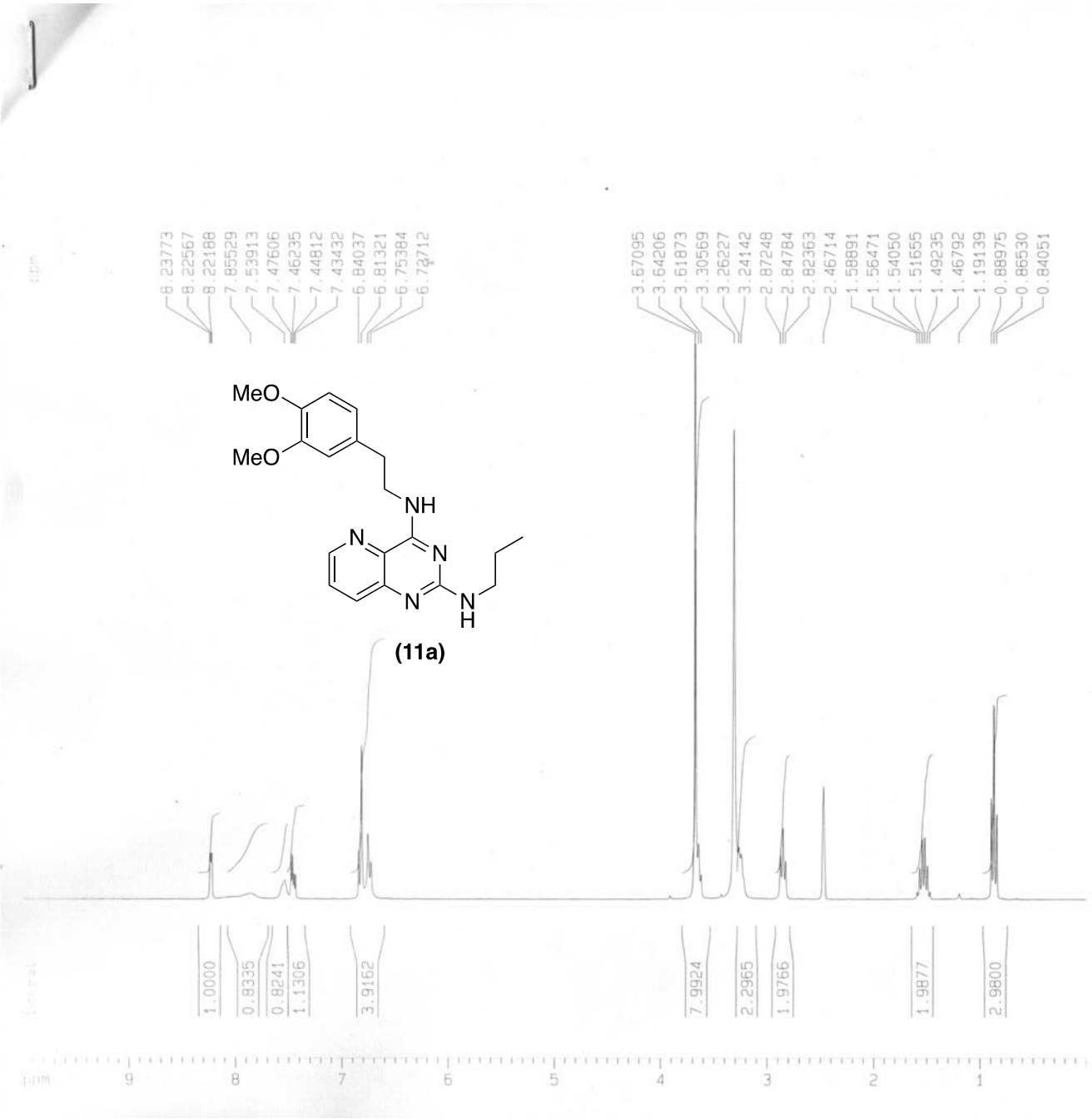
F2 - Acquisition Parameters
Date_ 20151107
Time 22.16
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT DMSO
NS 16
DS 2
SWH 4340.278 Hz
FIDRES 0.264910 Hz
AQ 1.8874868 sec
RG 128
DW 115.200 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 300.1318758 MHz

F2 - Processing parameters
SI 32768
SF 300.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

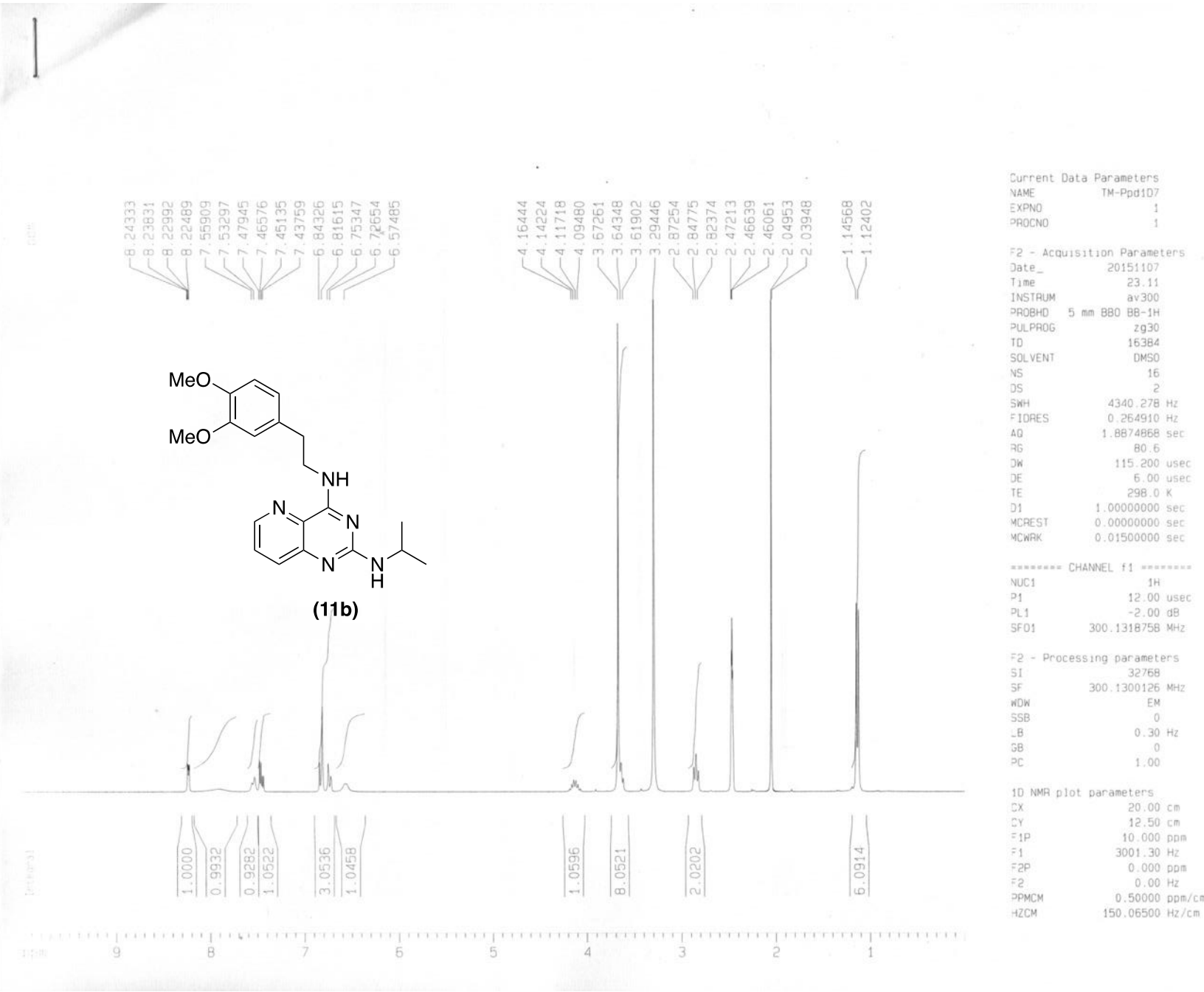
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50000 ppm/cm
HZCM 150.06500 Hz/cm

N^4-(3,4-Dimethoxyphenethyl)-N^2-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11a).



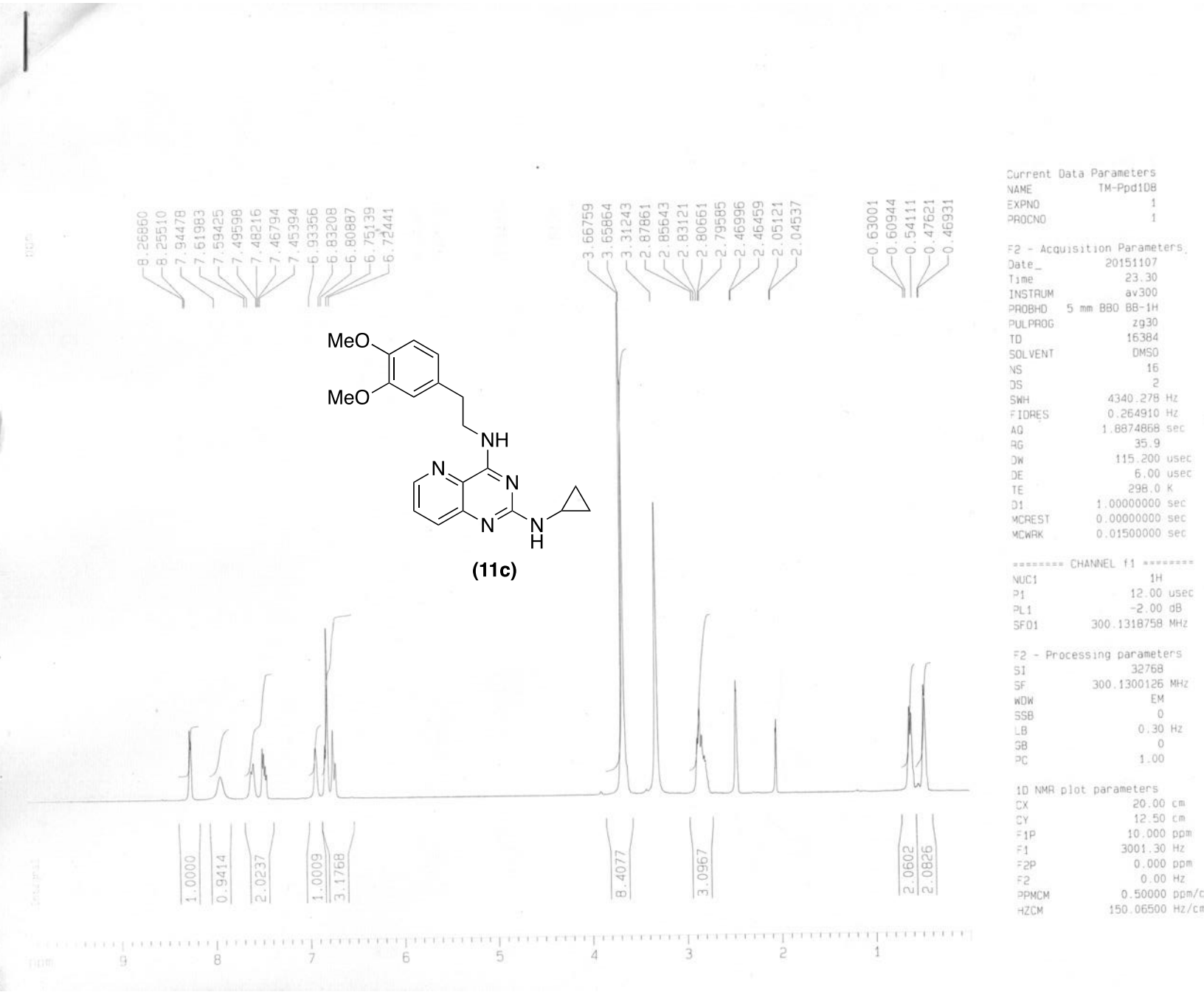

```
Current Data Parameters
NAME            TM-Ppd1D6
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                22.50
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                     16
DS                      2
SWH             4340.278 Hz
FIDRES          0.264910 Hz
AQ              1.8874868 sec
RG                   45.3
DW                115.200 usec
DE                  6.00 usec
TE                298.0 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.00 usec
PL1                 -2.00 dB
SFO1          300.1318758 MHz

F2 - Processing parameters
SI                  32768
SF            300.1300126 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                10.000 ppm
F1               3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM           0.50000 ppm/cm
HZCM          150.06500 Hz/cm
```

N^4-(3,4-Dimethoxyphenethyl)-N^2-isopropylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11b).

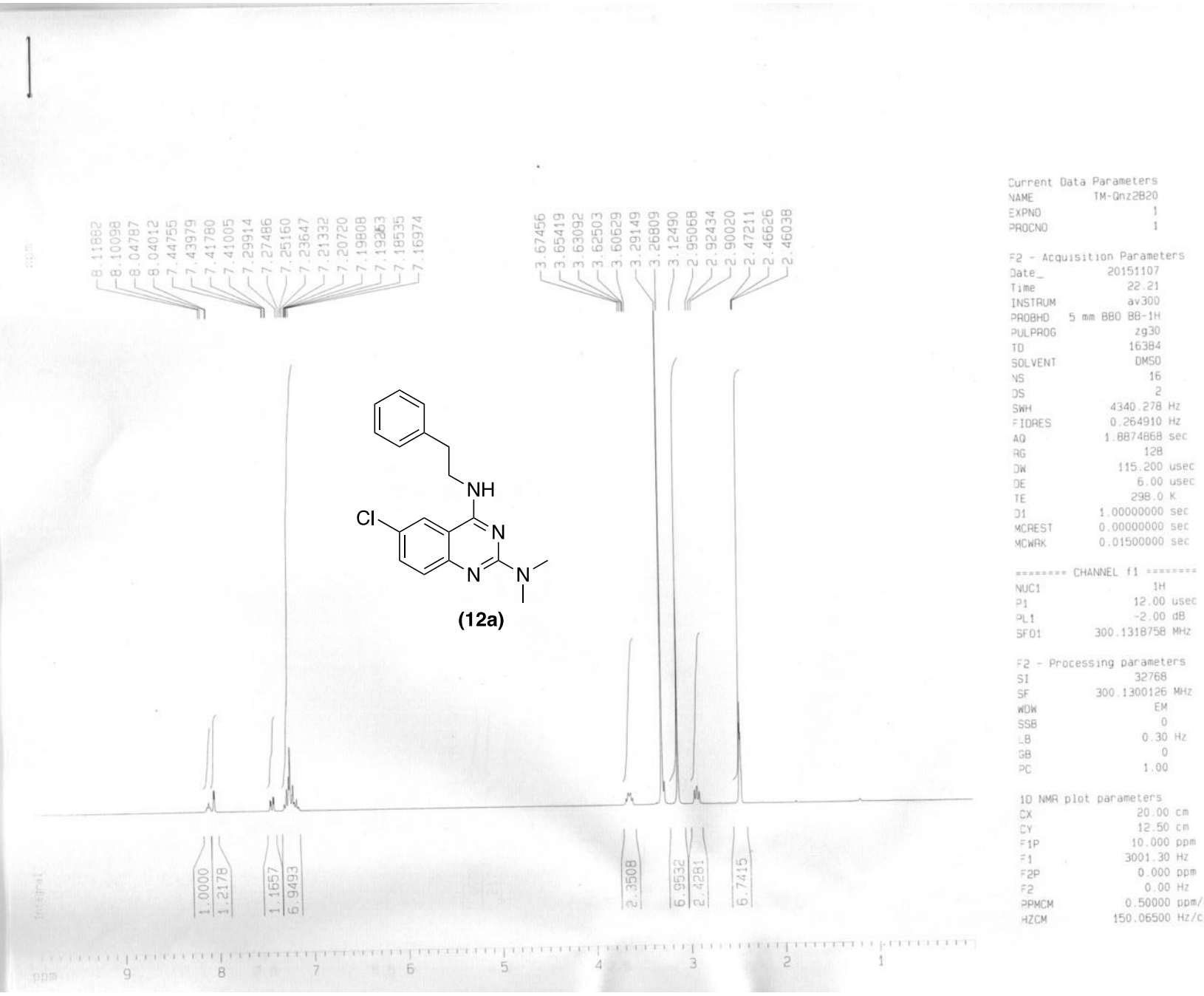



```
Current Data Parameters
NAME            TM-Ppd1D7
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151107
Time                23.11
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT              DMSO
NS                     16
DS                      2
SWH              4340.278 Hz
FIDRES           0.264910 Hz
AQ               1.8874868 sec
RG                   80.6
DW                115.200 usec
DE                  6.00 usec
TE                 298.0 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.00 usec
PL1                 -2.00 dB
SFO1           300.1318758 MHz

F2 - Processing parameters
SI                  32768
SF             300.1300126 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  12.50 cm
F1P                10.000 ppm
F1                3001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            0.50000 ppm/cm
HZCM           150.06500 Hz/cm
```

N^2-Cyclopropyl-N^4-(3,4-dimethoxyphenethyl)pyrido[3,2-*d*]pyrimidine-2,4-diamine (11c).



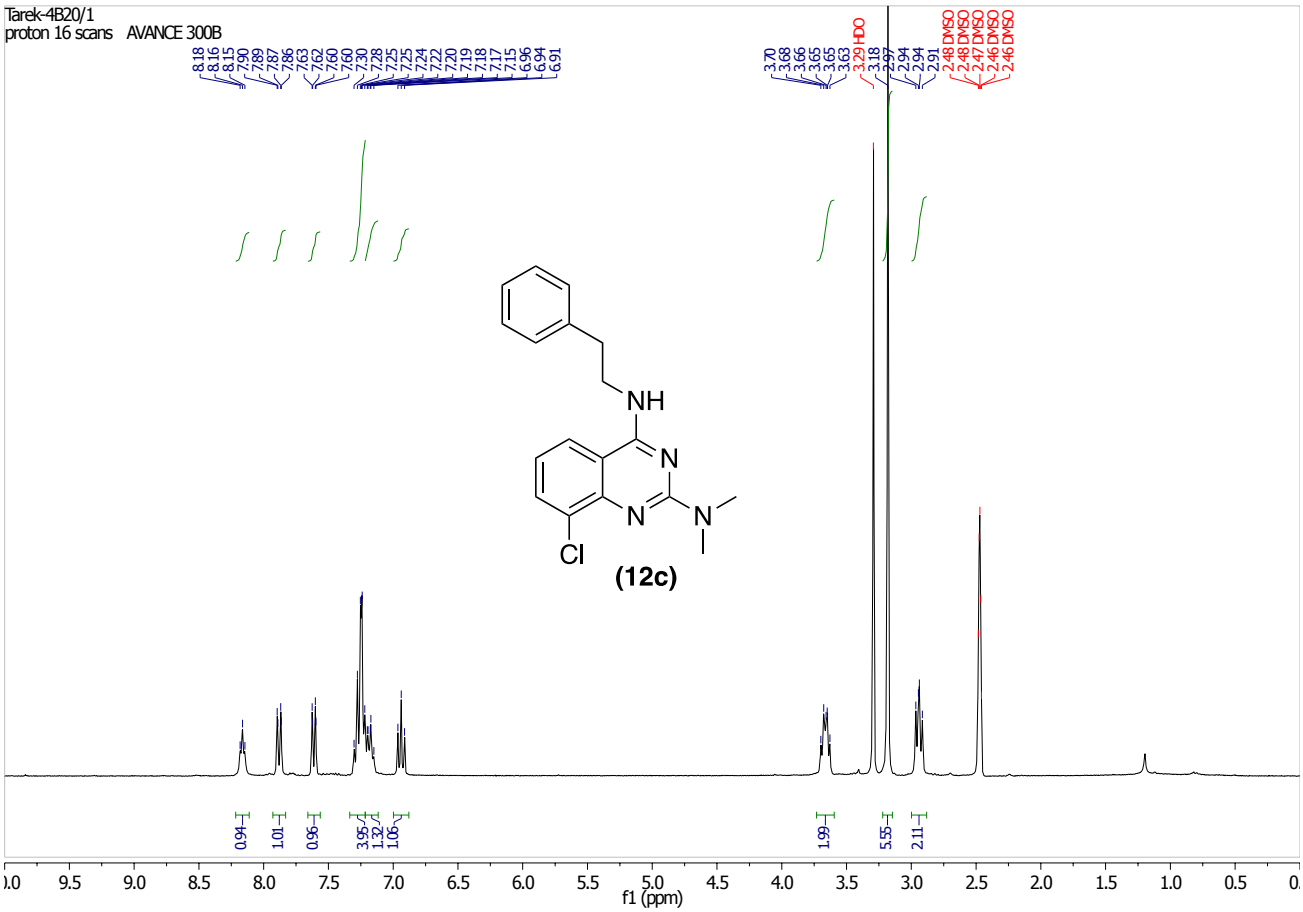
6-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12a).



7-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12b).

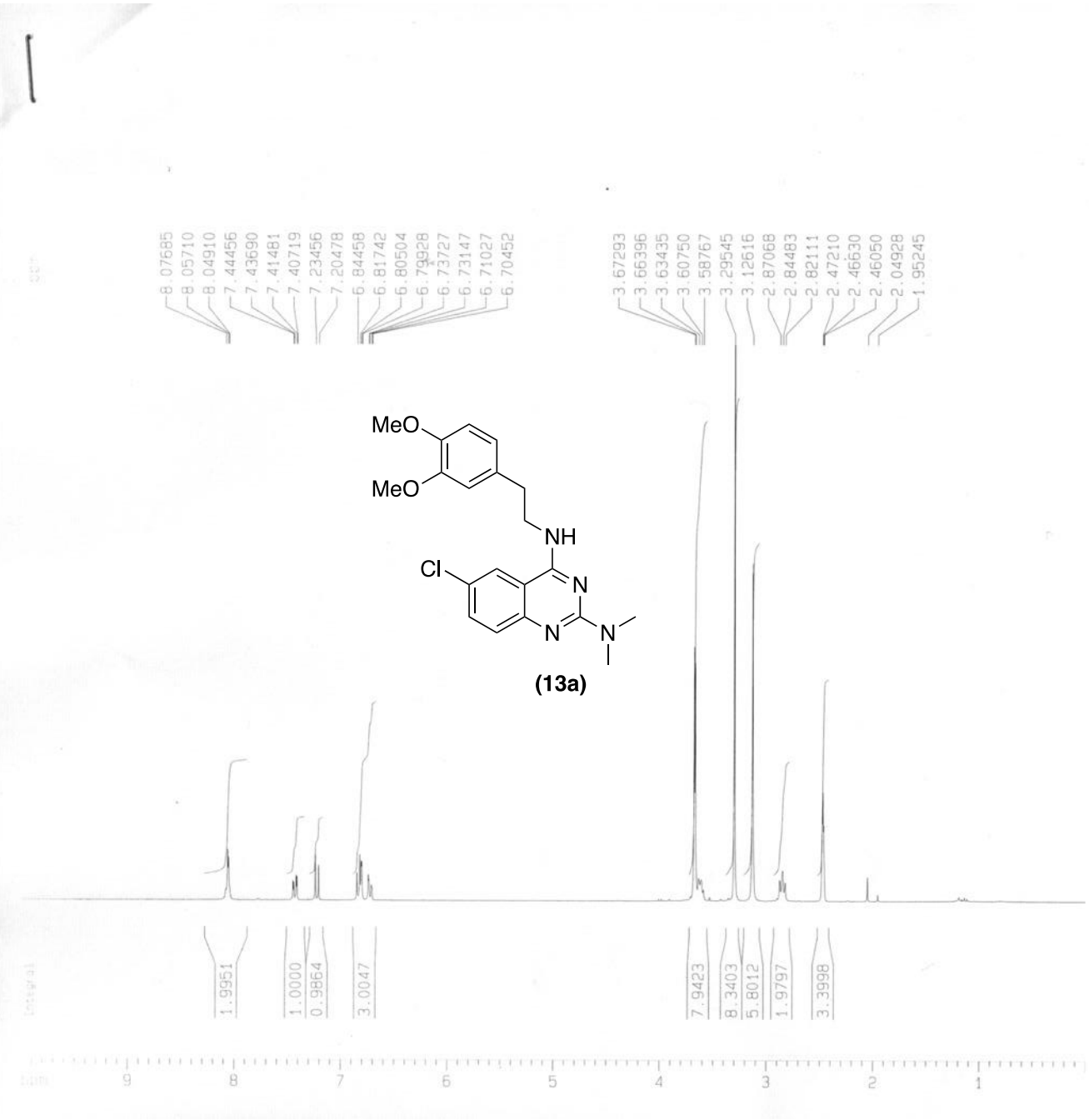

```
Current Data Parameters
NAME          TM-Qnz3B20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time               22.26
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                   128
DW             115.200 usec
DE               6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1               -2.00 dB
SF01        300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              10.000 ppm
F1              3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          0.50000 ppm/cm
HZCM         150.06500 Hz/cm
```

8-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12c).



6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13a).

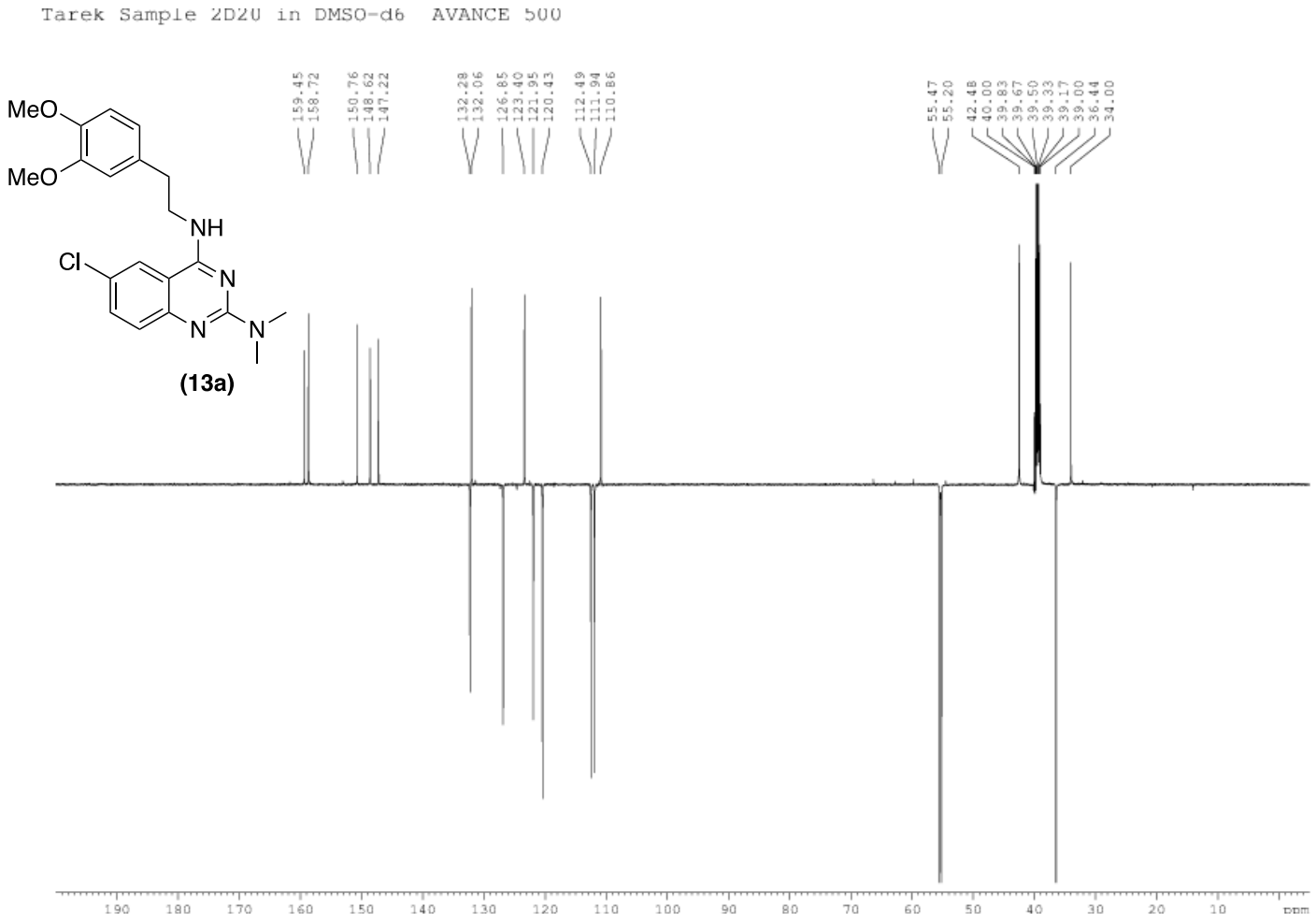
^{1}H NMR




```
Current Data Parameters
NAME          TM-Gnz2D20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time               23.33
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                  80.6
DW             115.200 usec
DE               6.00 usec
TE               298.0 K
D1          1.00000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1               -2.00 dB
SF01        300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P             10.000 ppm
F1              3001.30 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM         0.50000 ppm/cm
HZCM        150.06500 Hz/cm
```

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13a).

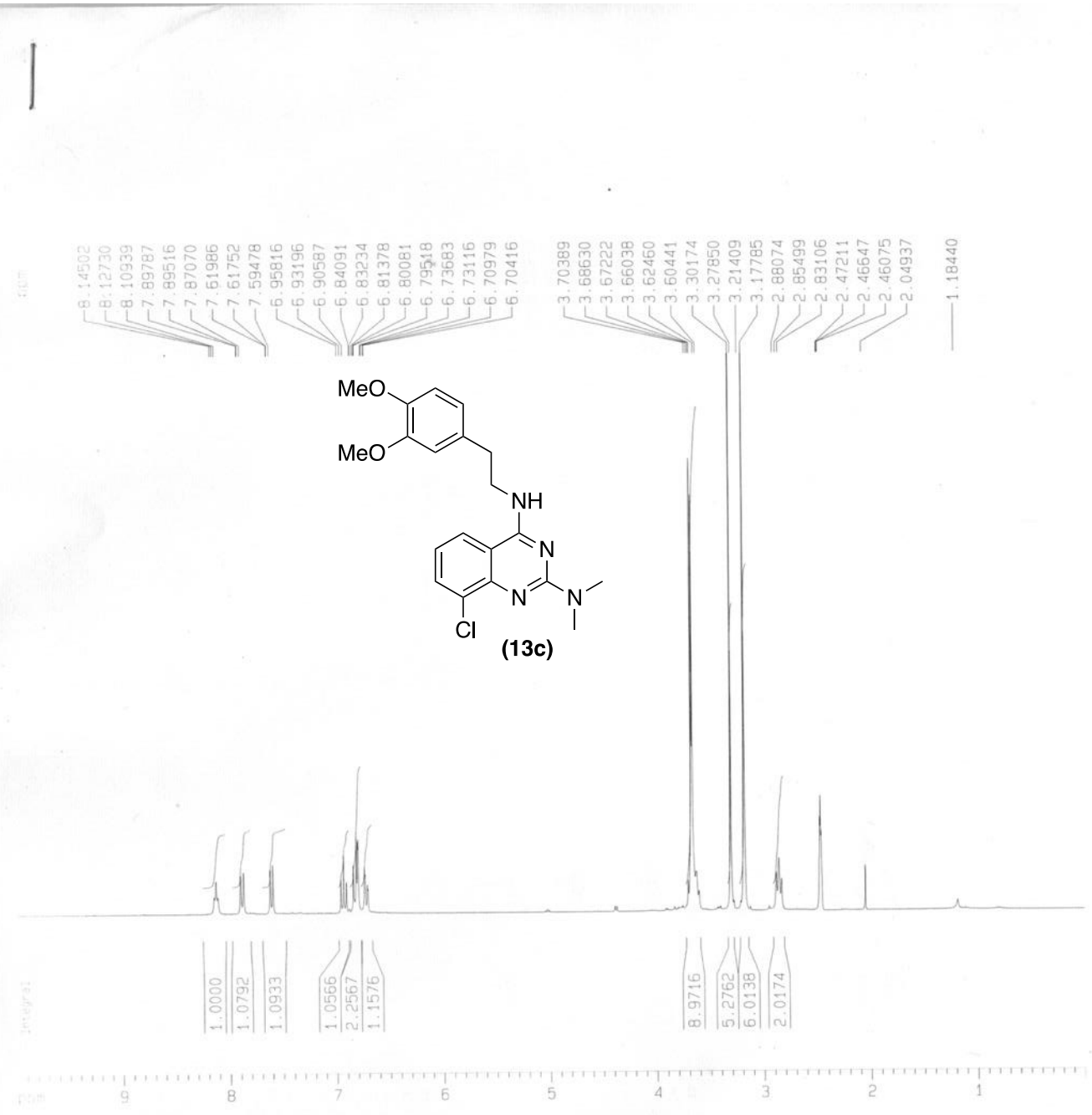
^{13}C NMR



7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13b).

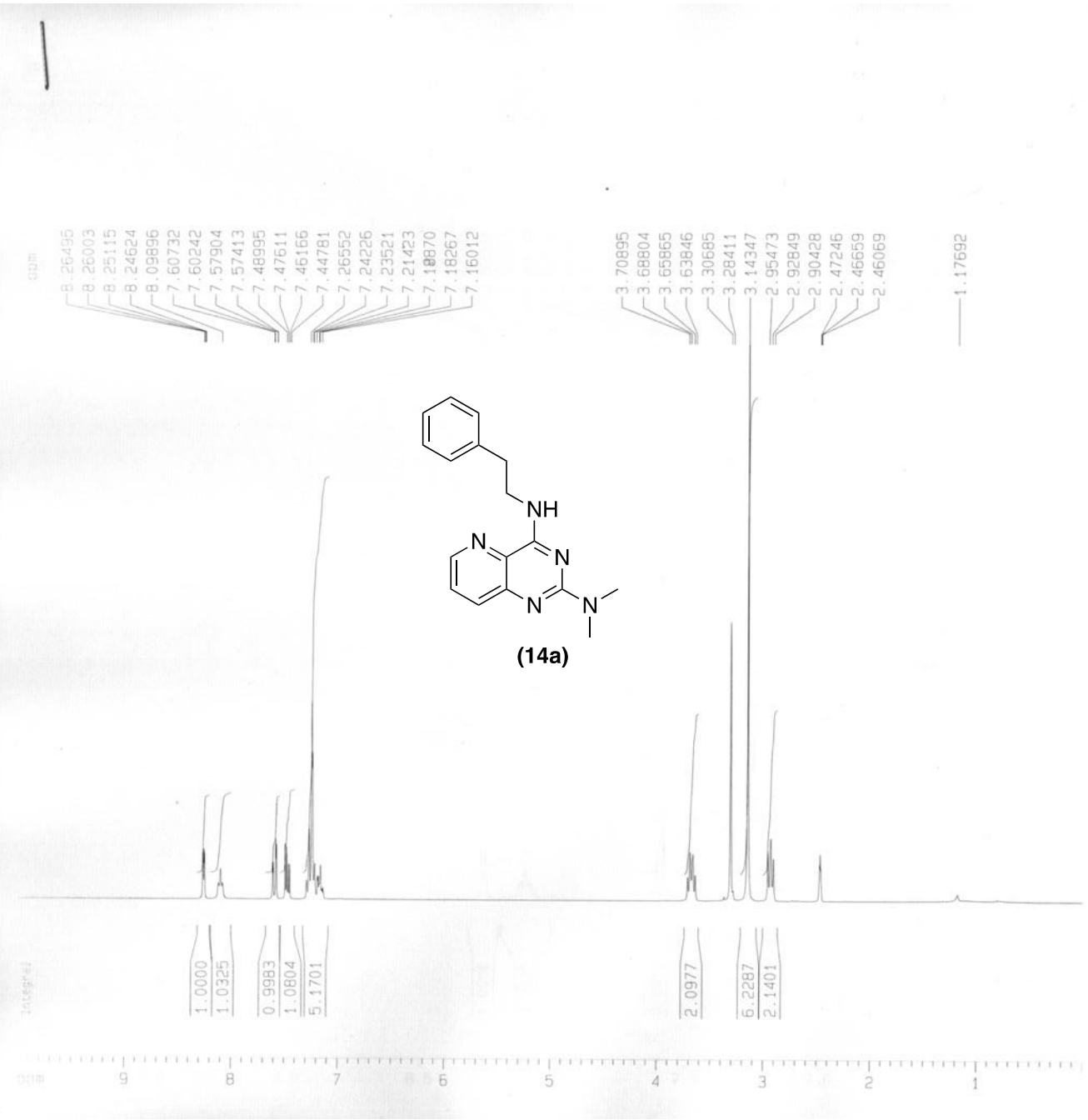

```
Current Data Parameters
NAME          TM-Qnz3D20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time               23.37
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                 71.8
DW              115.200 usec
DE                6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1               -2.00 dB
SFO1         300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              10.000 ppm
F1             3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM         0.50000 ppm/cm
HZCM        150.06500 Hz/cm
```

8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13c).



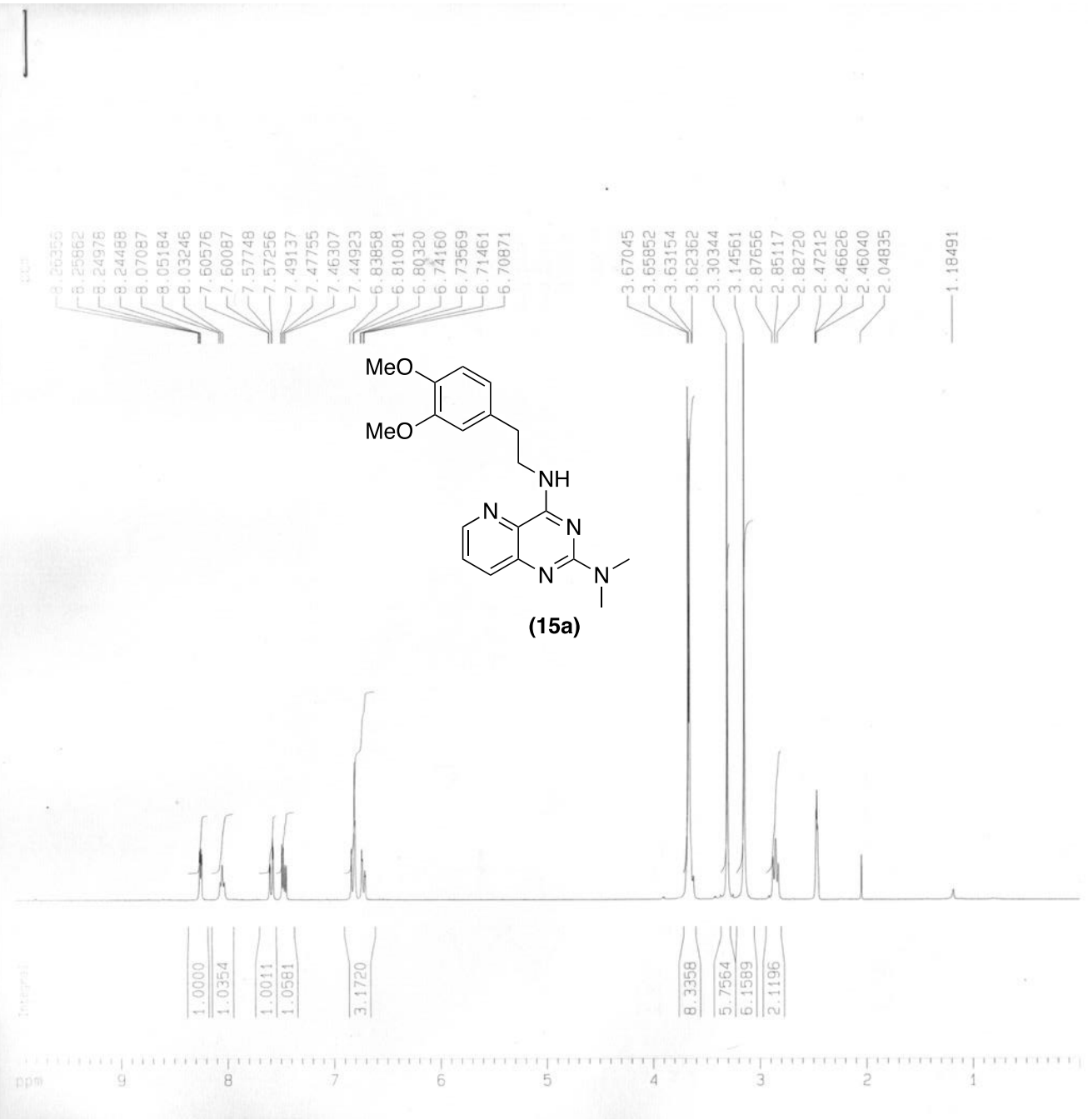

```
Current Data Parameters
NAME          TM-Qnz4D20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151107
Time              23.42
INSTRUM           av300
PROBHD  5 mm BBO BB-1H
PULPROG           zg30
TD               16384
SOLVENT           DMSO
NS                  16
DS                   2
SWH          4340.278 Hz
FIDRES       0.264910 Hz
AQ           1.8874868 sec
RG                71.8
DW           115.200 usec
DE             6.00 usec
TE            298.0 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1               12.00 usec
PL1              -2.00 dB
SFO1        300.1318758 MHz

F2 - Processing parameters
SI                32768
SF          300.1300126 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX               20.00 cm
CY               12.50 cm
F1P             10.000 ppm
F1            3001.30 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM         0.50000 ppm/cm
HZCM        150.06500 Hz/cm
```

N^2,N^2-Dimethyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (14a).




```
Current Data Parameters
NAME          TM-Ppd1B20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time               22.31
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 16384
SOLVENT             DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                  45.3
DW             115.200 usec
DE               6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1               12.00 usec
PL1              -2.00 dB
SFO1        300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX               20.00 cm
CY               12.50 cm
F1P             10.000 ppm
F1            3001.30 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM         0.50000 ppm/cm
HZCM        150.06500 Hz/cm
```

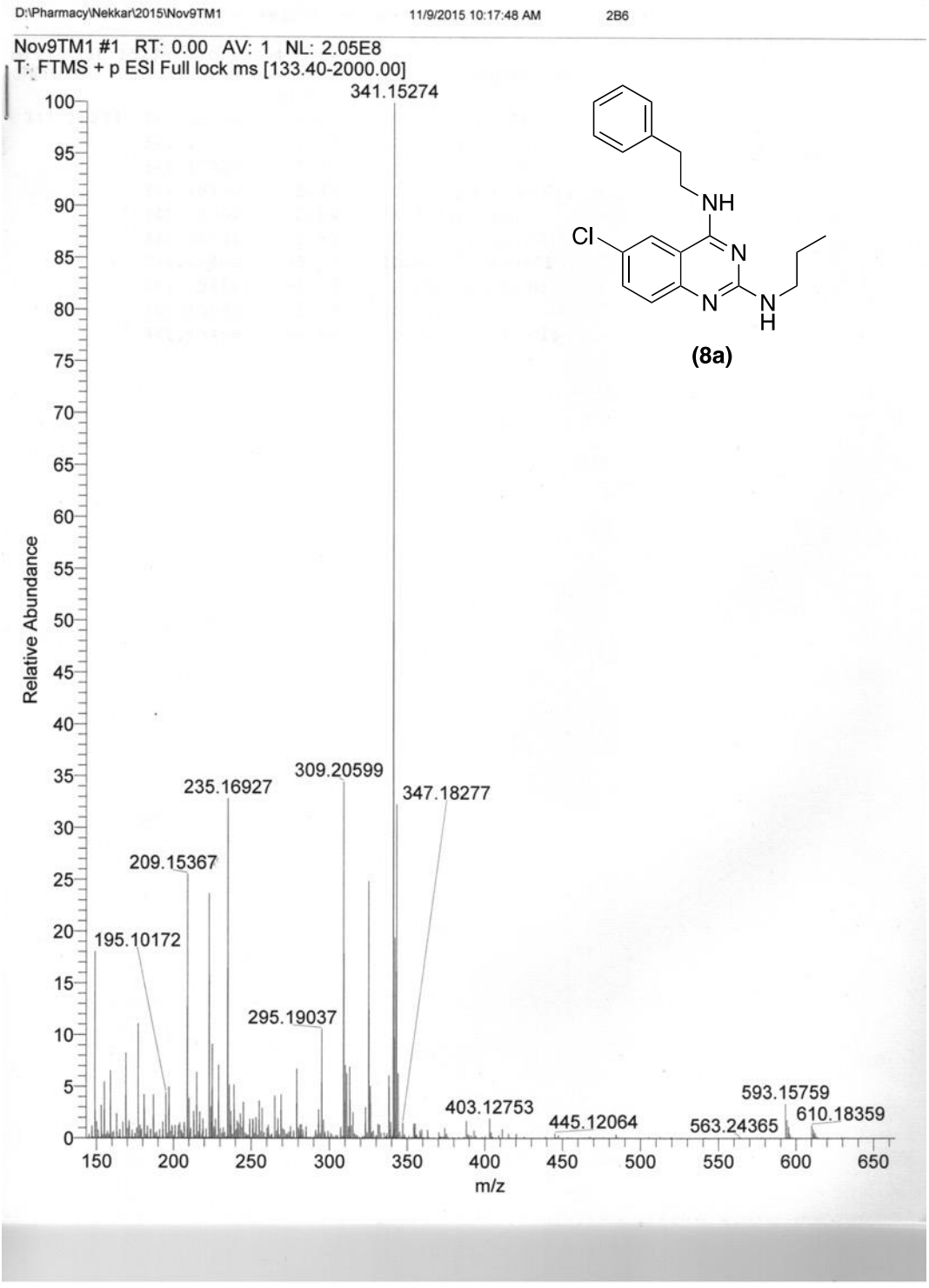
N^4-(3,4-Dimethoxyphenethyl)-N^2,N^2-dimethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (15a).




```
Current Data Parameters
NAME          TM-Ppd1D20
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151107
Time               23.49
INSTRUM          av300
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                16384
SOLVENT            DMSO
NS                    16
DS                     2
SWH           4340.278 Hz
FIDRES        0.264910 Hz
AQ            1.8874868 sec
RG                 71.8
DW              115.200 usec
DE                6.00 usec
TE               298.0 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PL1               -2.00 dB
SFO1         300.1318758 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300126 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                20.00 cm
CY                12.50 cm
F1P              10.000 ppm
F1              3001.30 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          0.50000 ppm/cm
HZCM         150.06500 Hz/cm
```

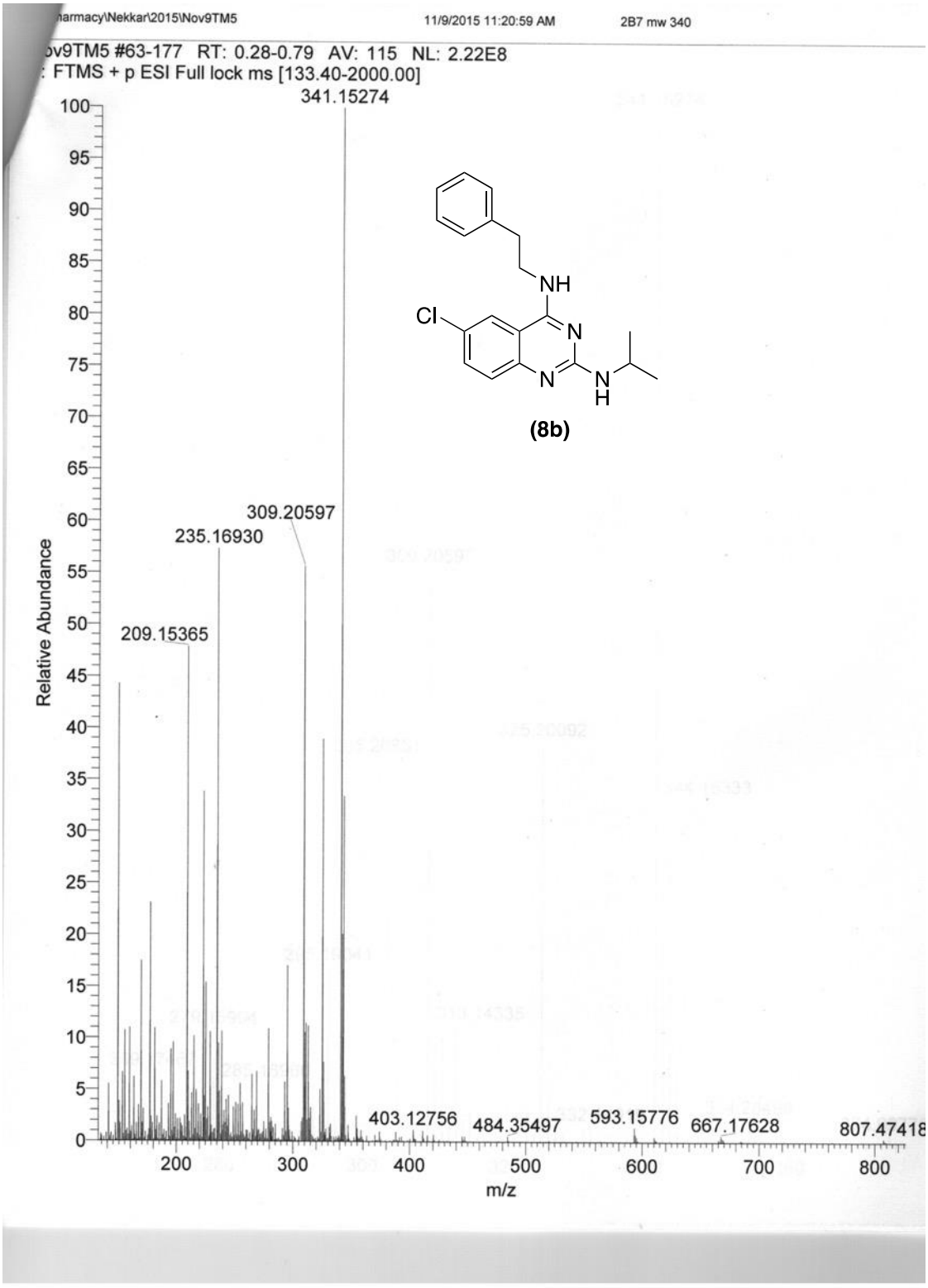
5. HRMS spectra for compounds 8a–i, 9a–i, 10a–c, 11a–c, 12a–c, 13a–c, 14a and 15a

6-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (**8a**).

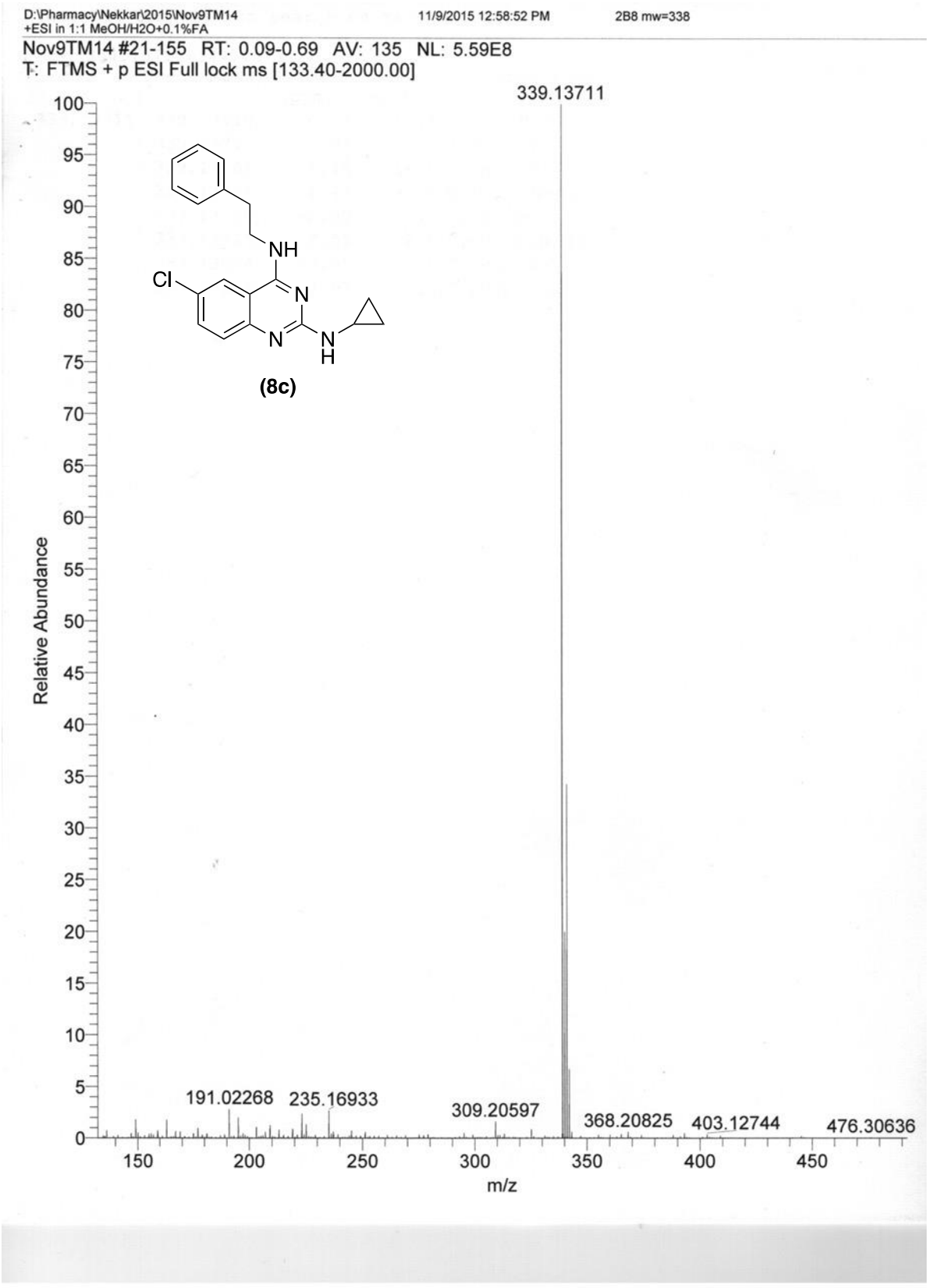


6-Chloro-

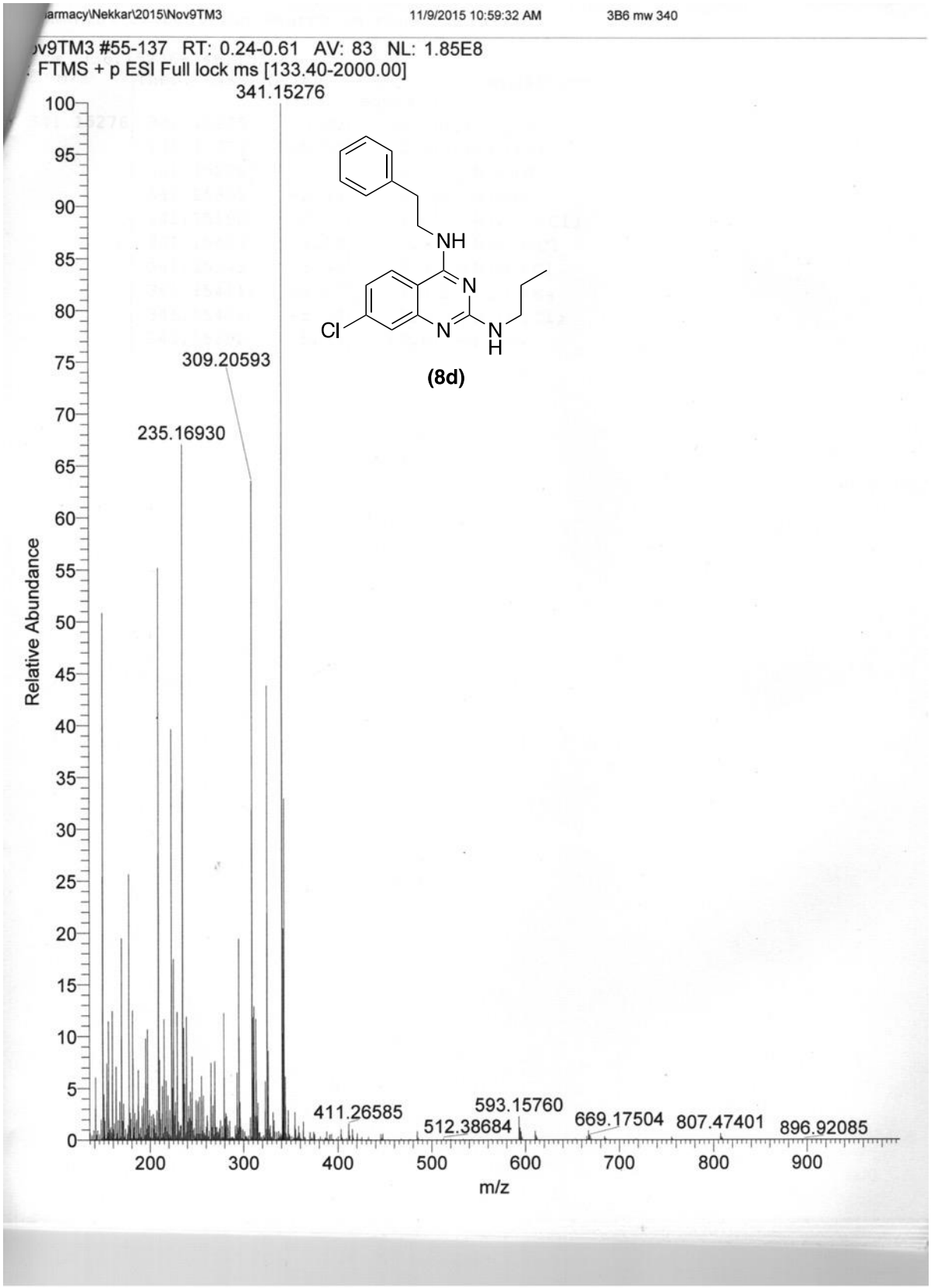
N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8b).



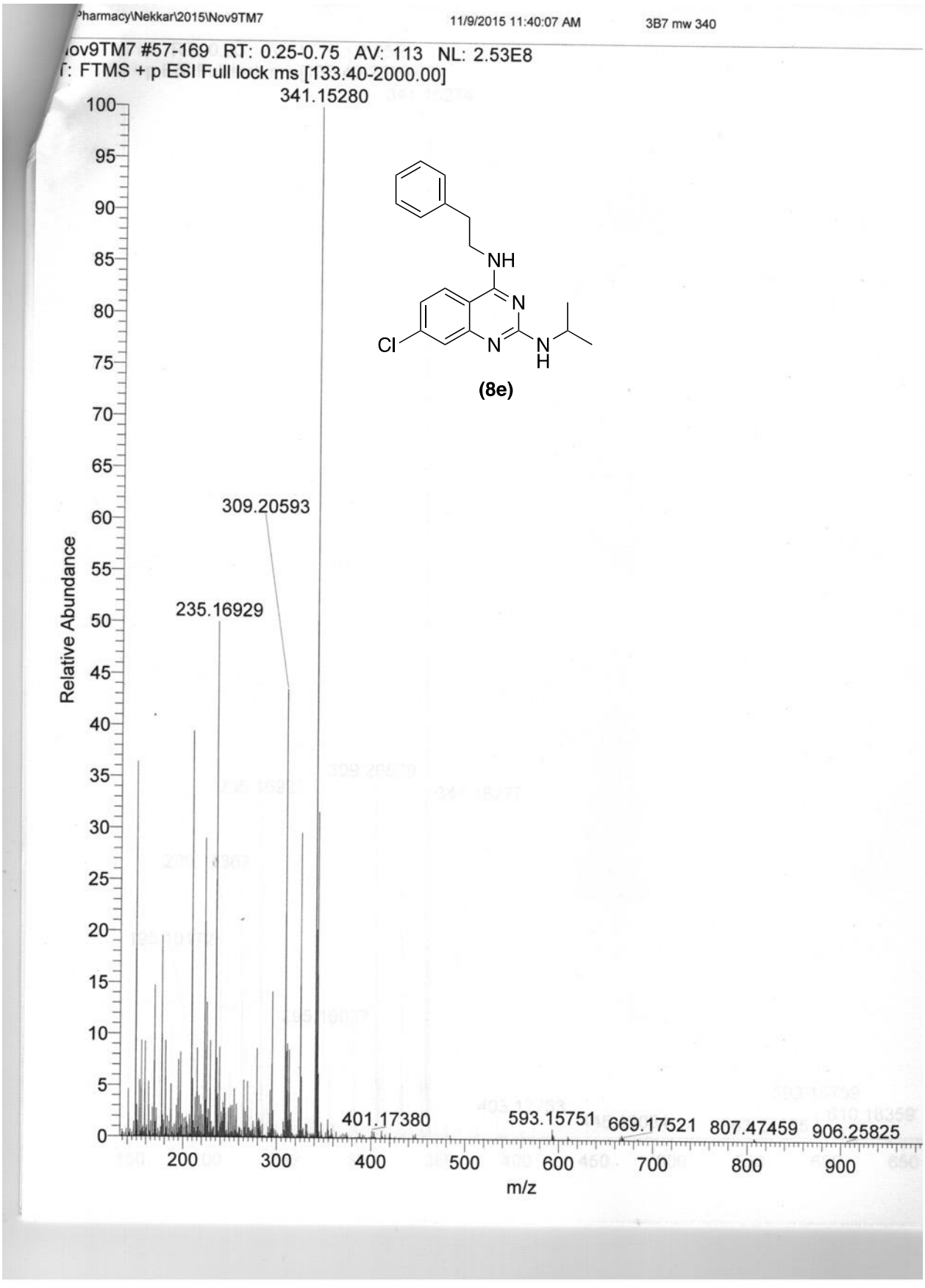
6-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8c).



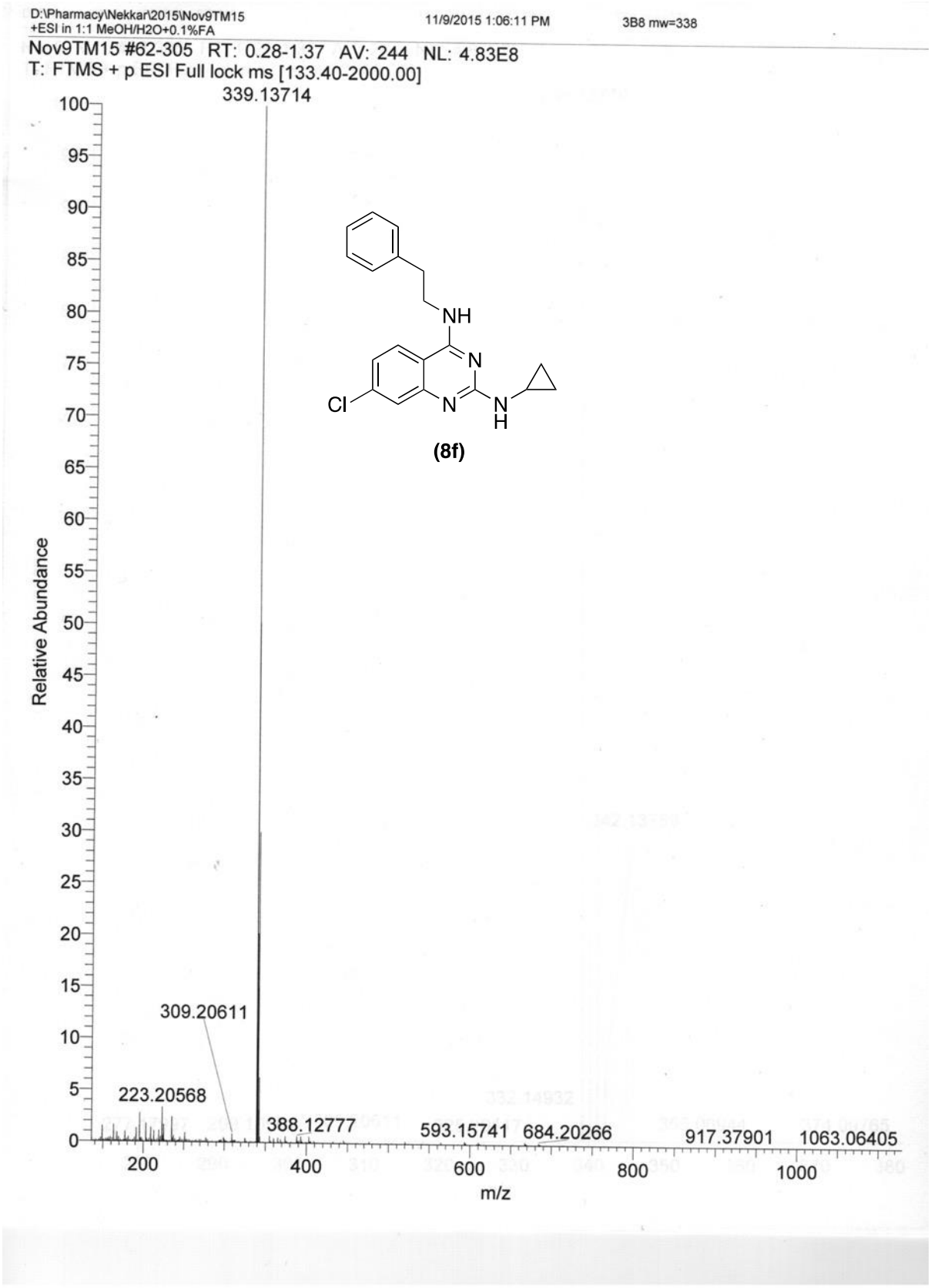
7-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8d).



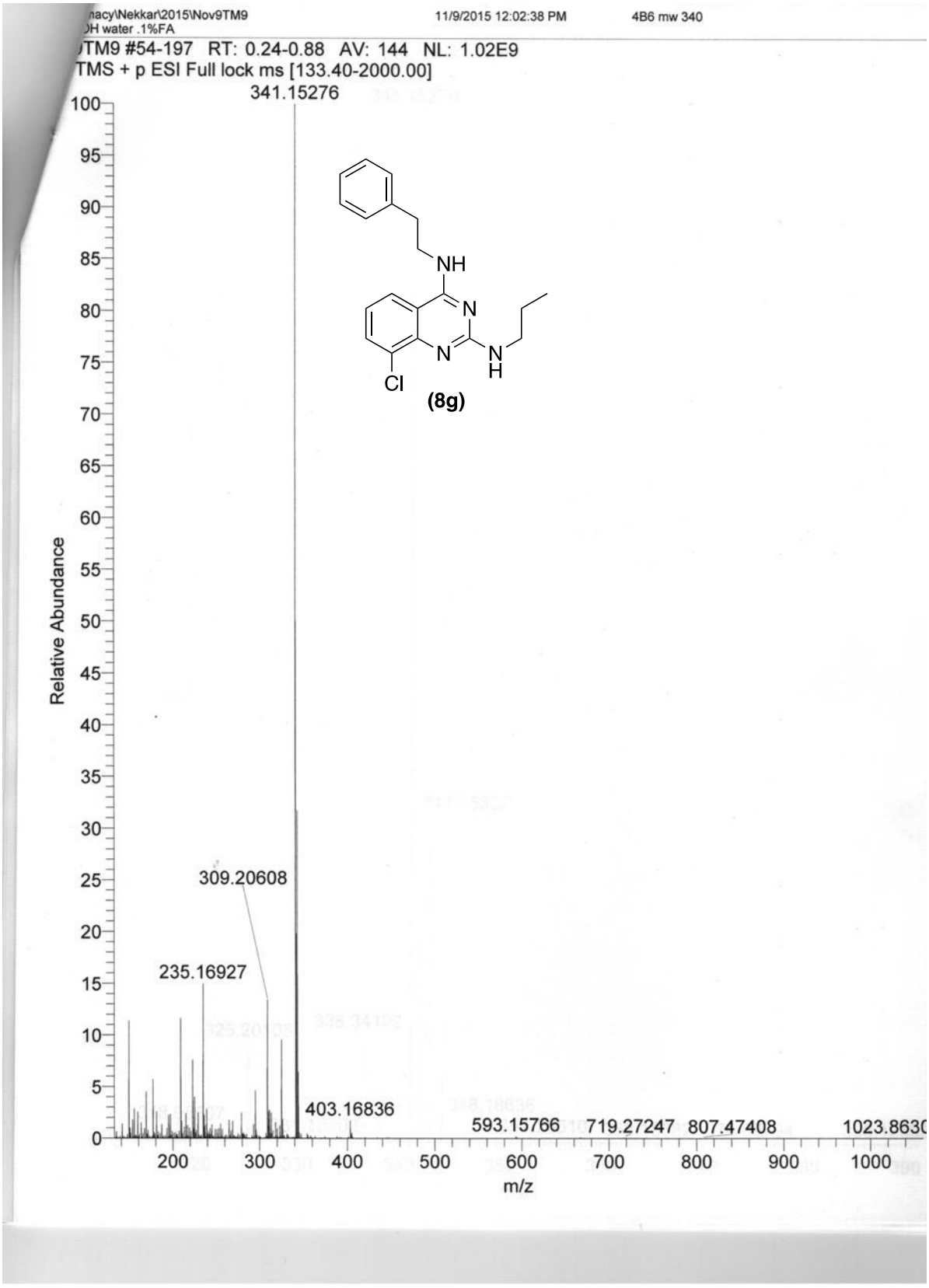
7-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8e).



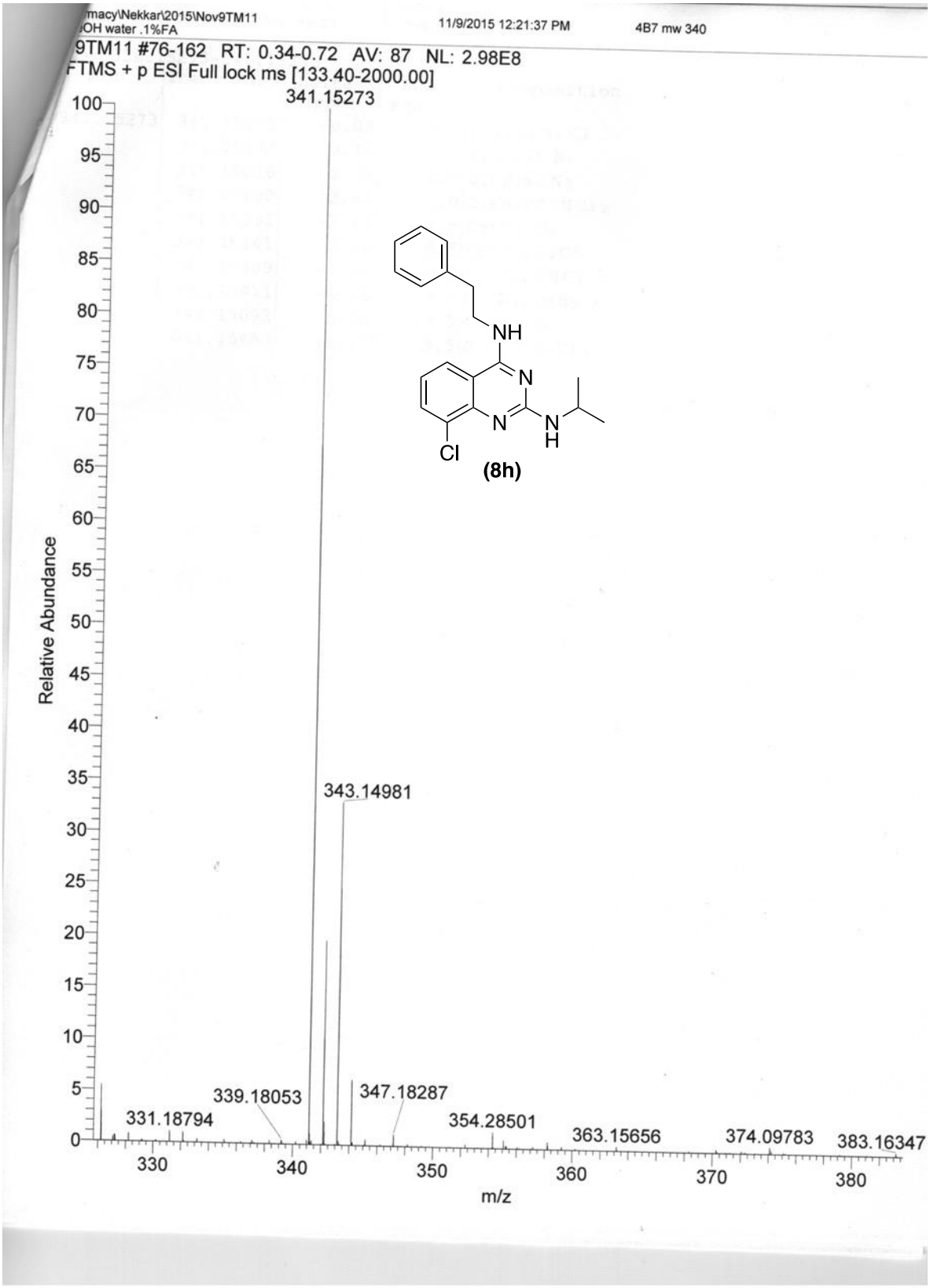
7-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8f).



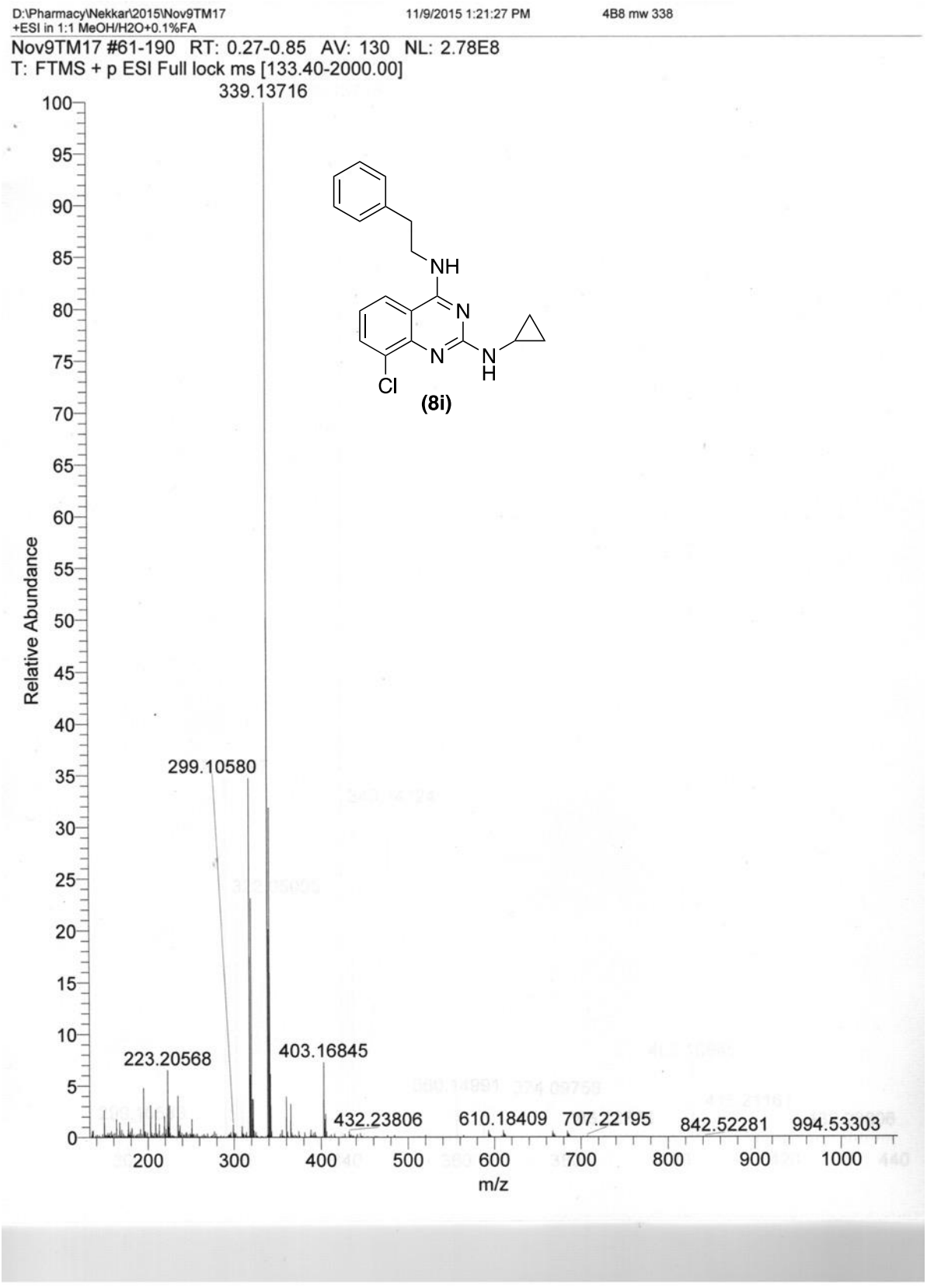
8-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8g).



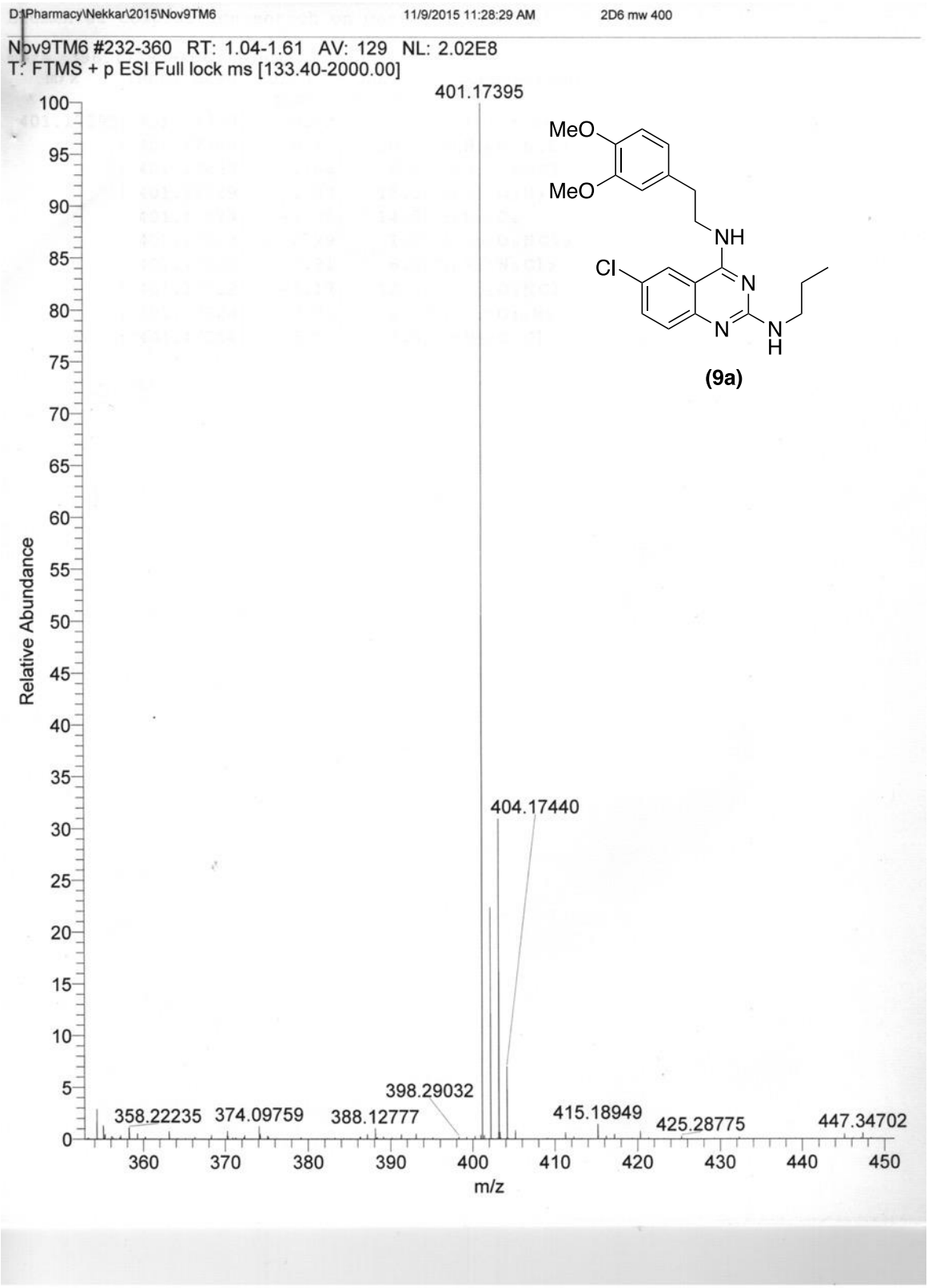
8-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8h).



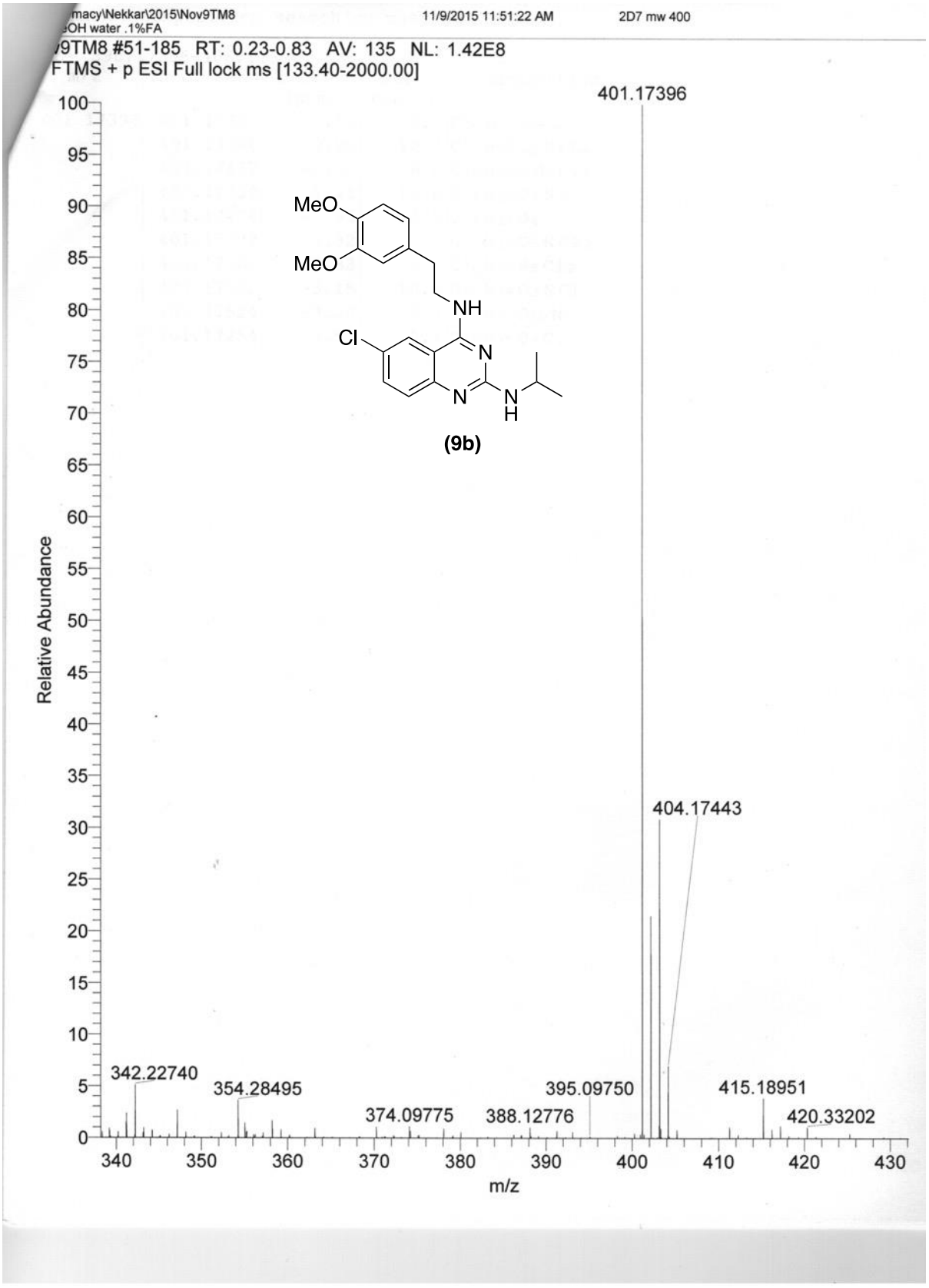
8-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8i).



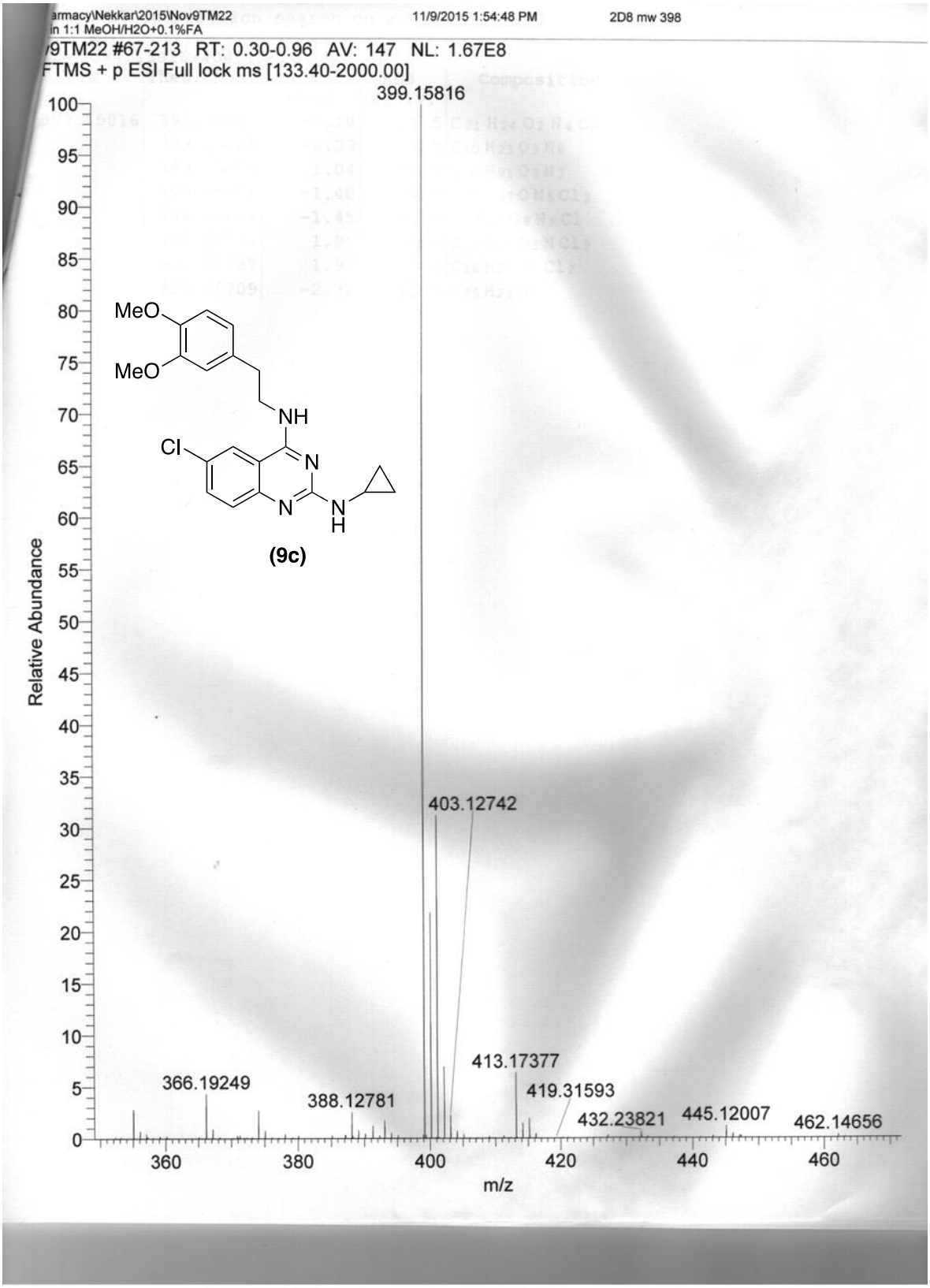
6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (**9a**).



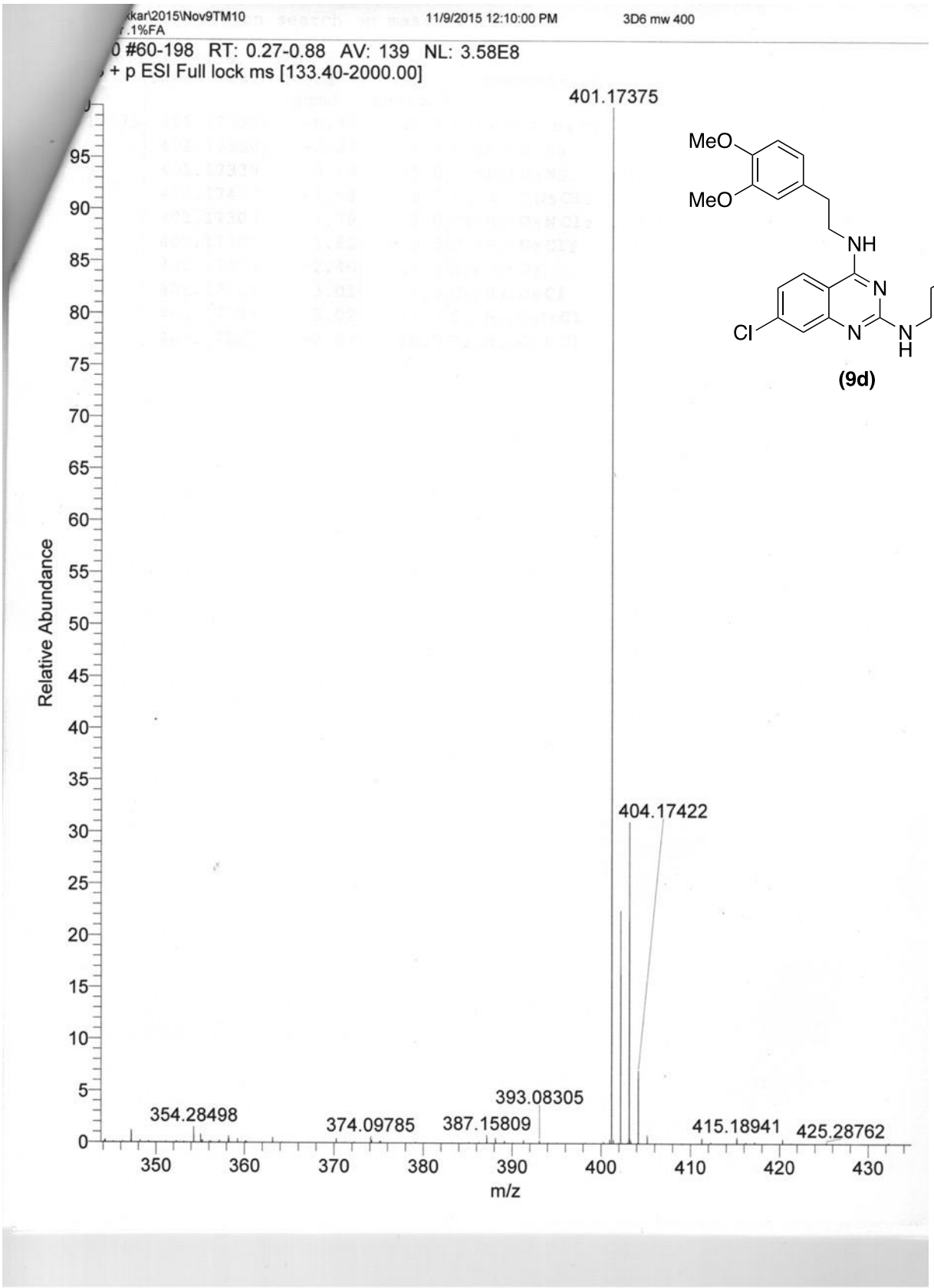
6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9b).



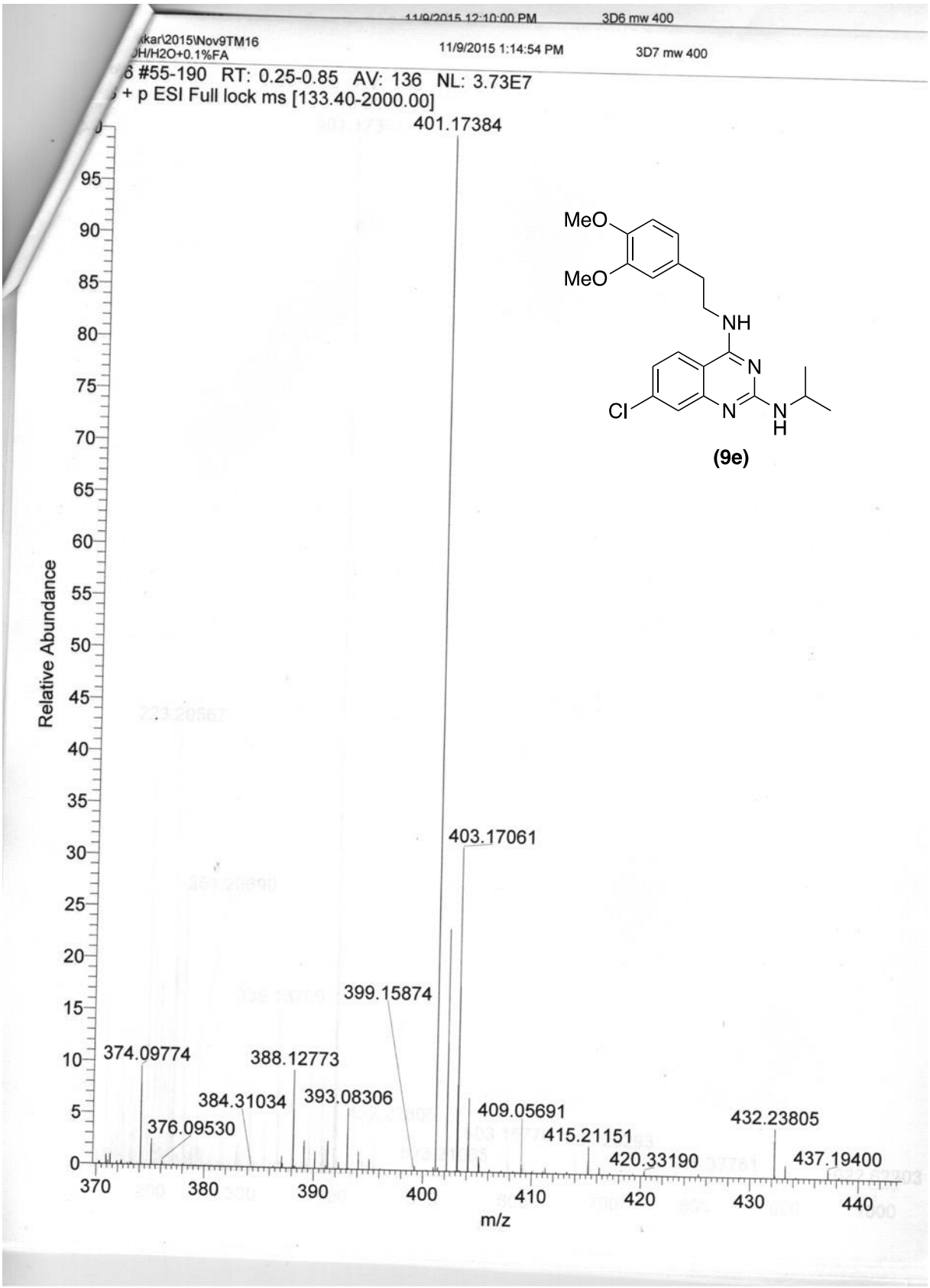
6-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9c).



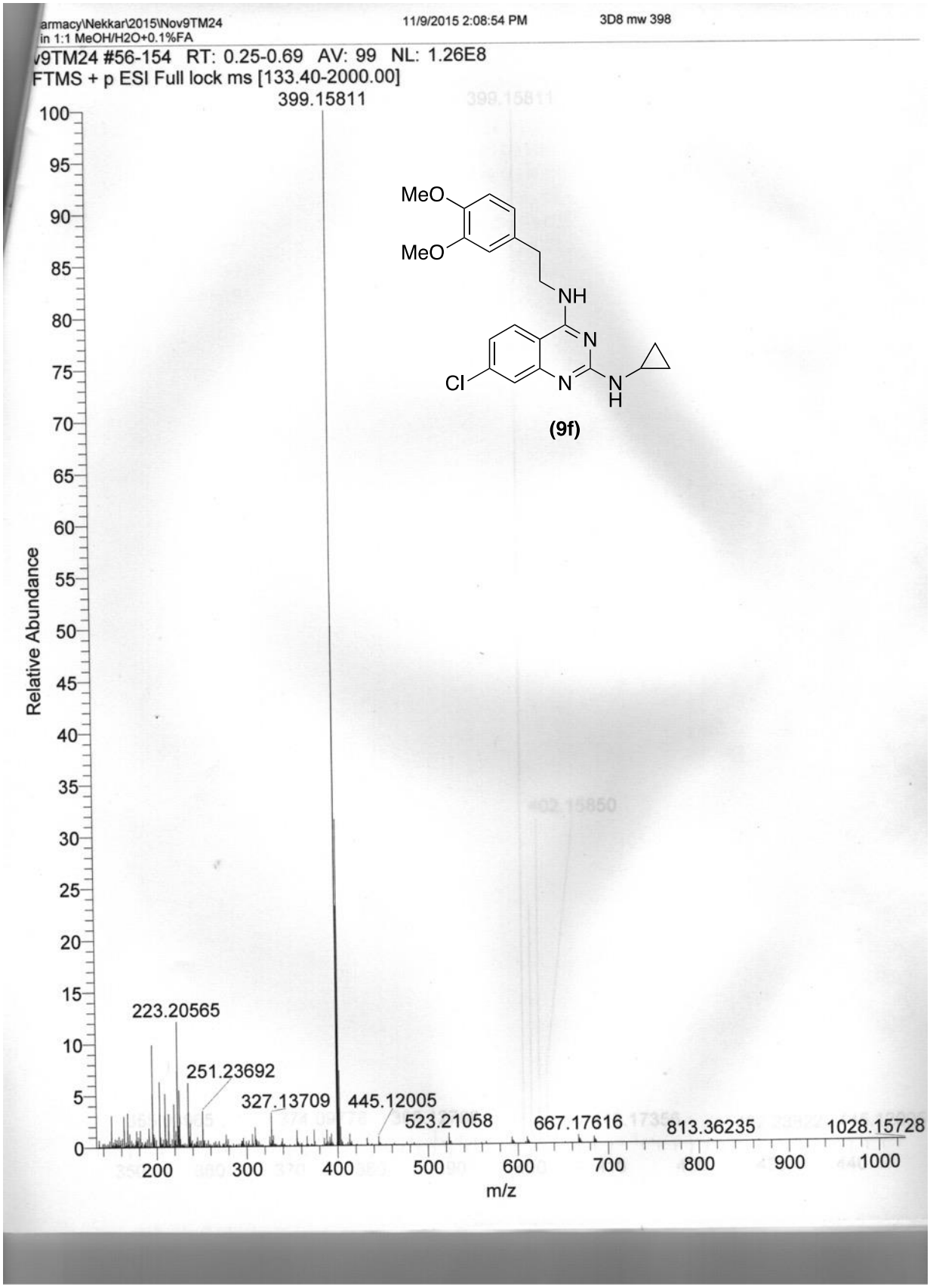
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9d).



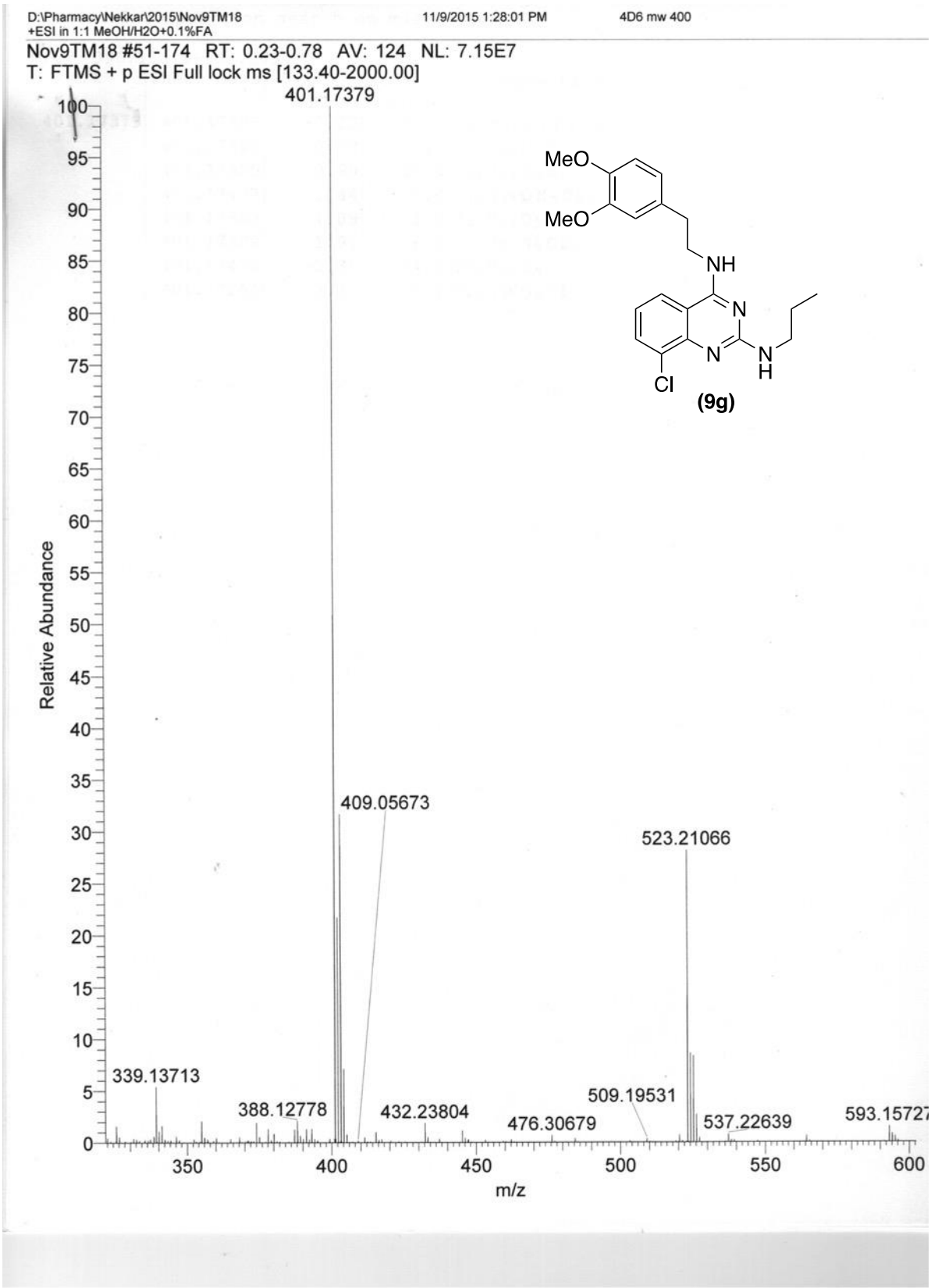
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (**9e**).



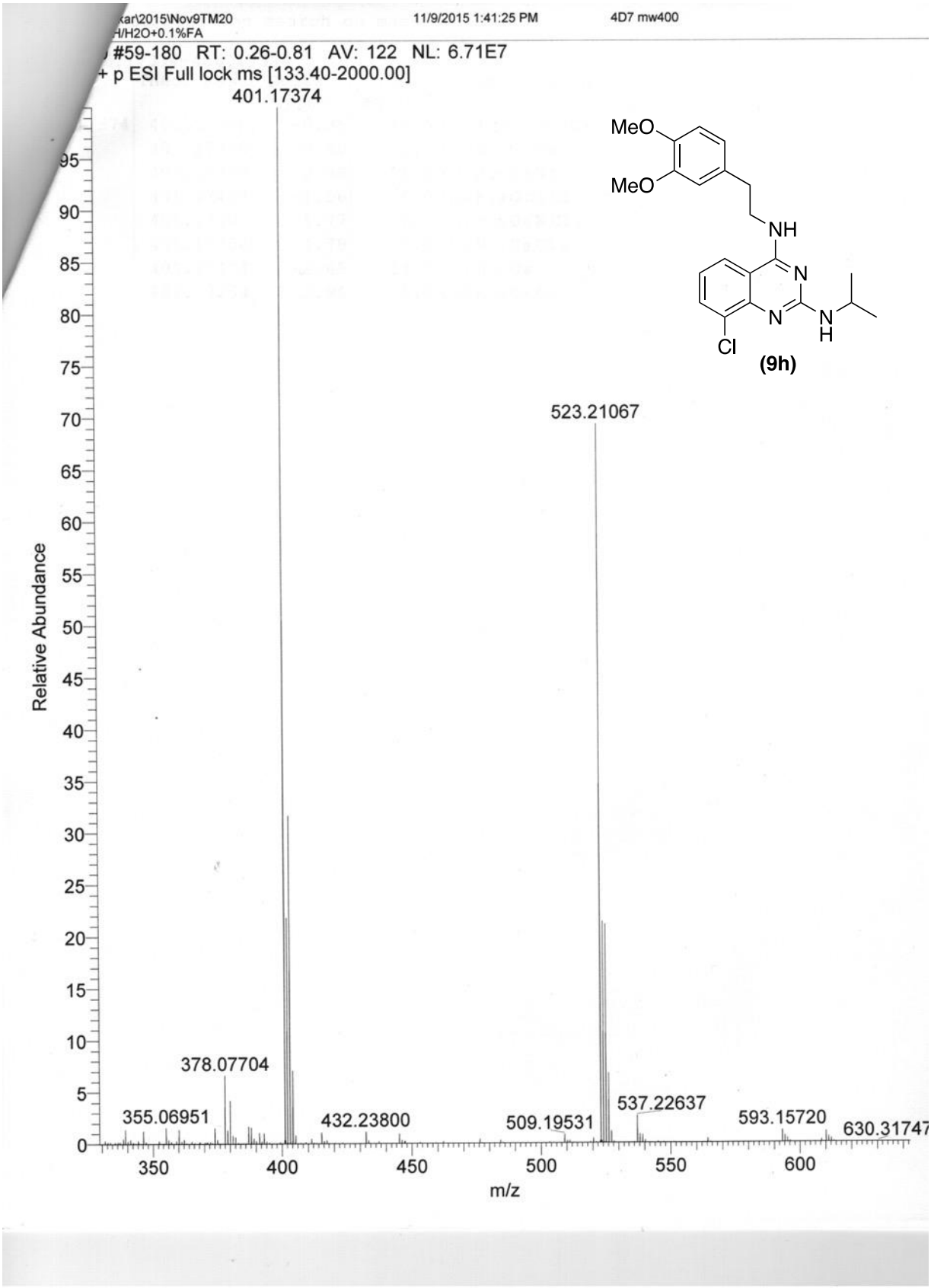
7-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9f).



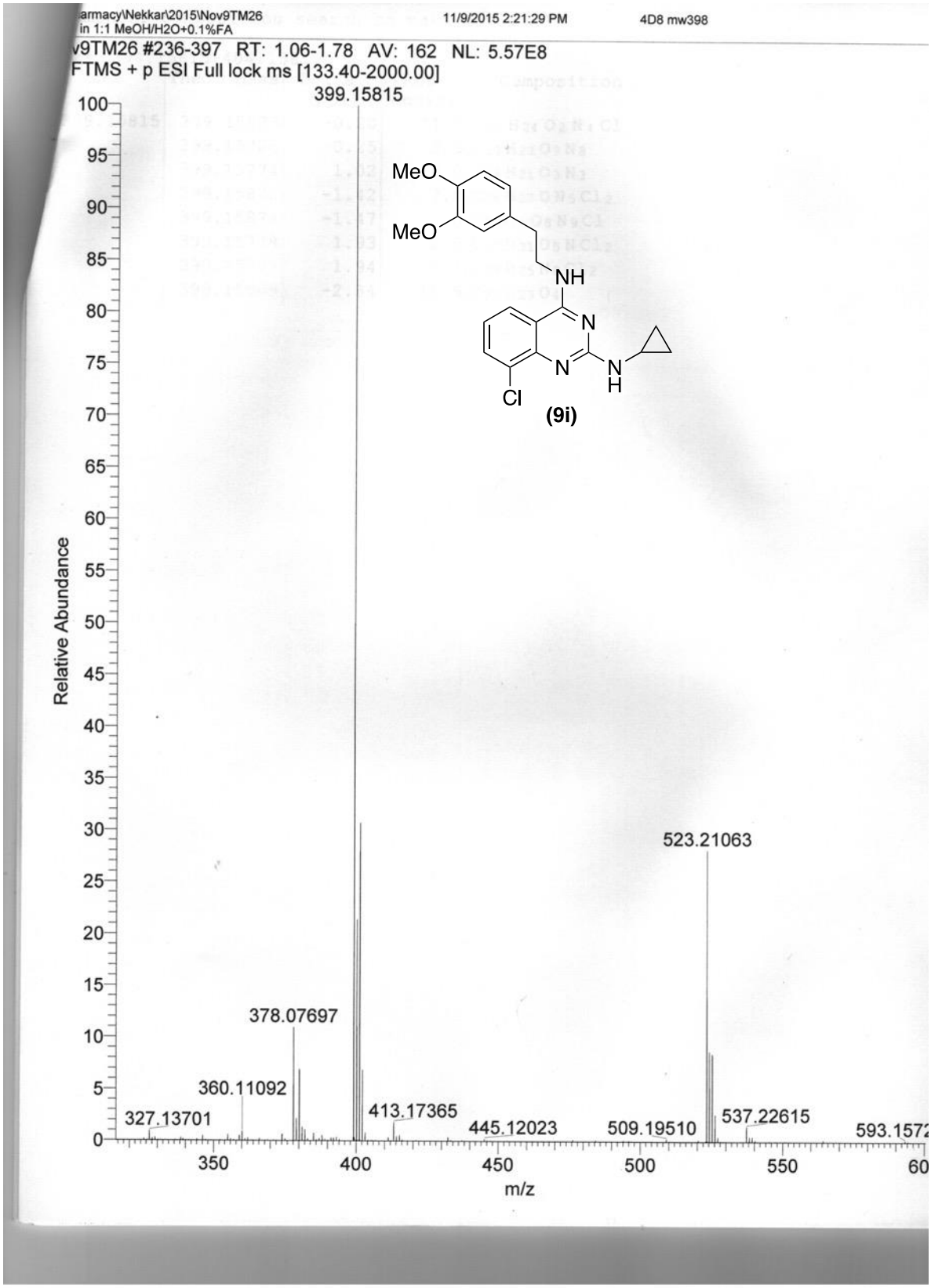
8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9g).



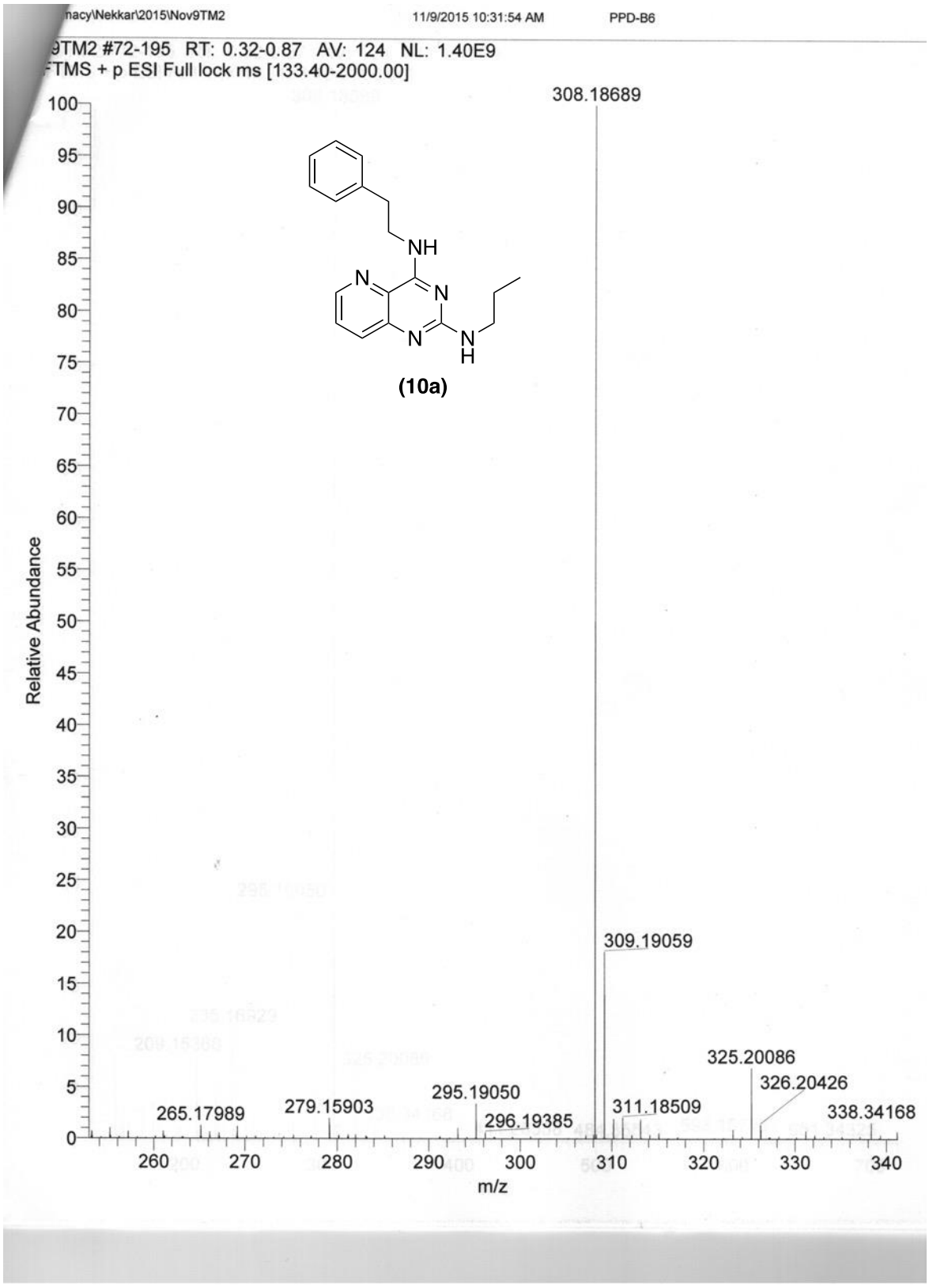
8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (**9h**).



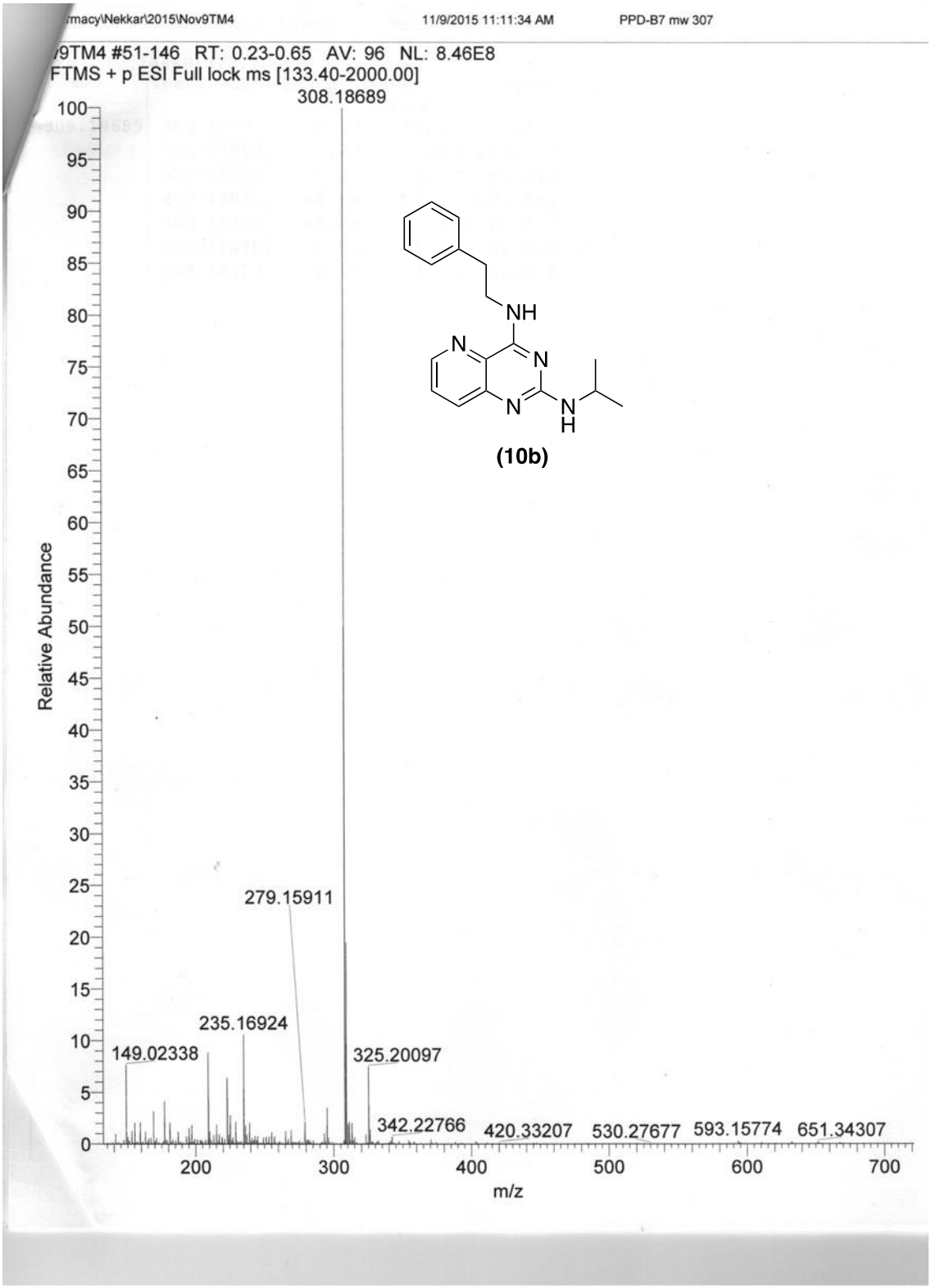
8-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (**9i**).



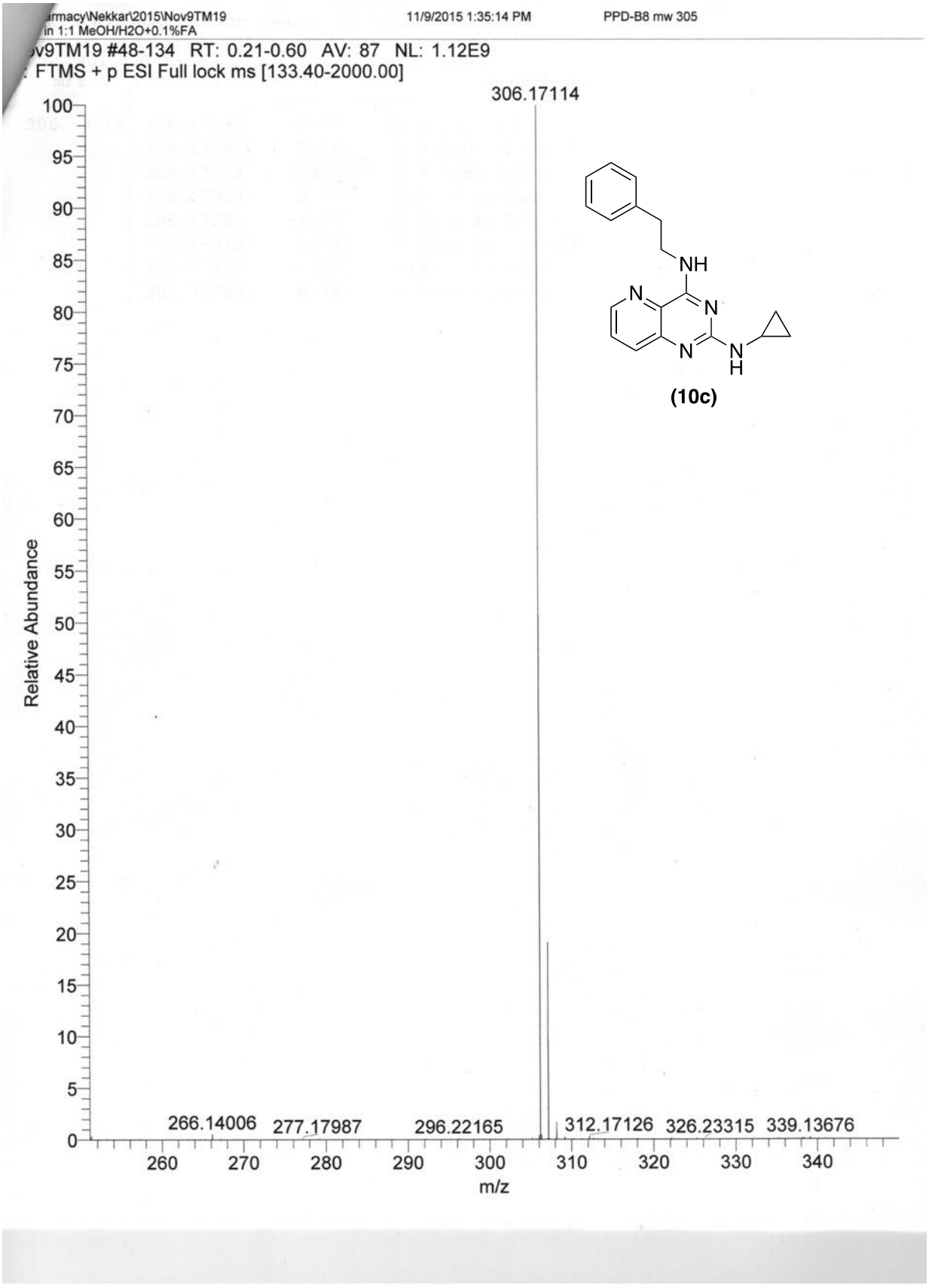
N^4-Phenethyl-N^2-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10a).



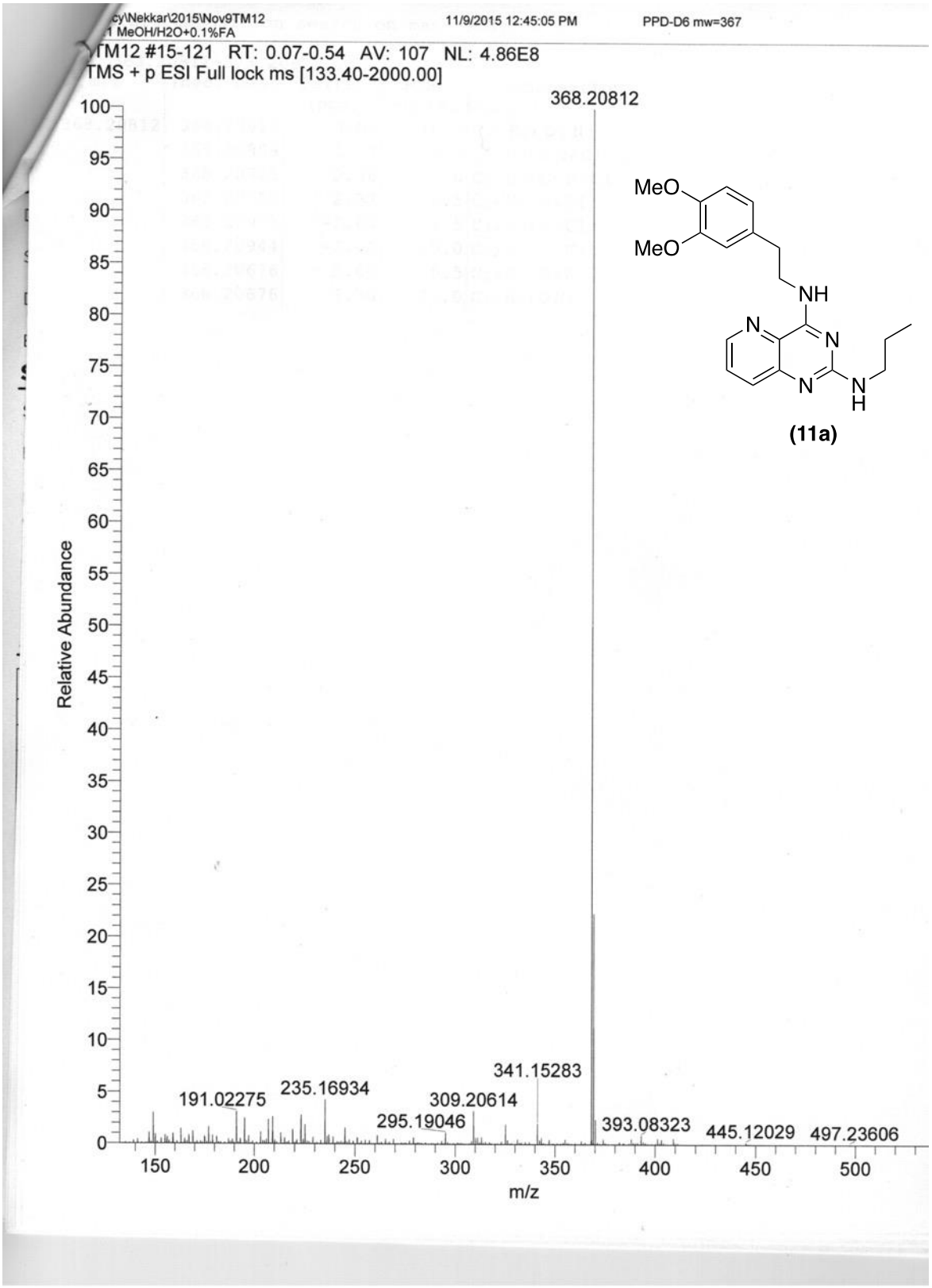
N^2-Isopropyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10b).



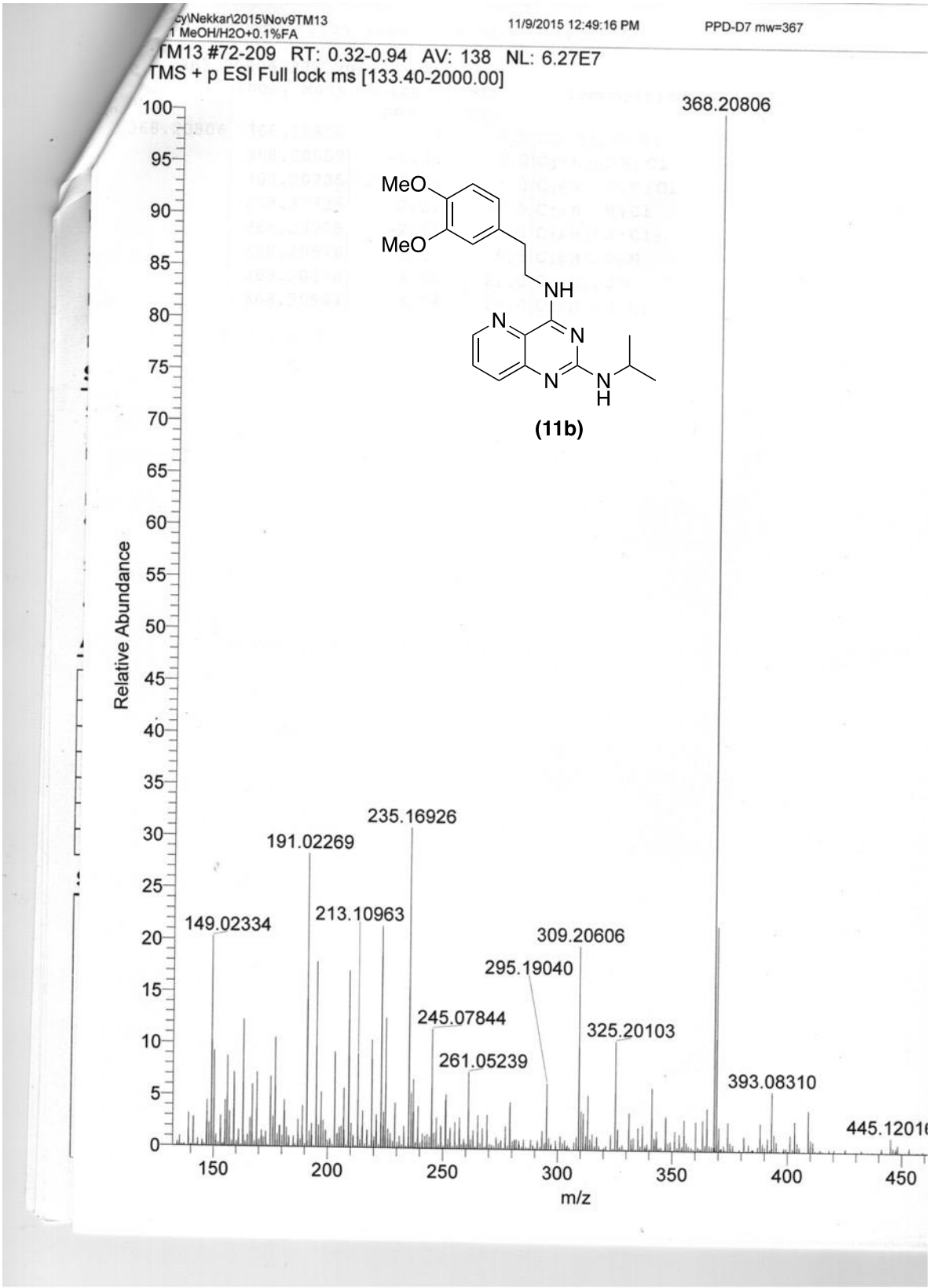
N^2-Cyclopropyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10c).



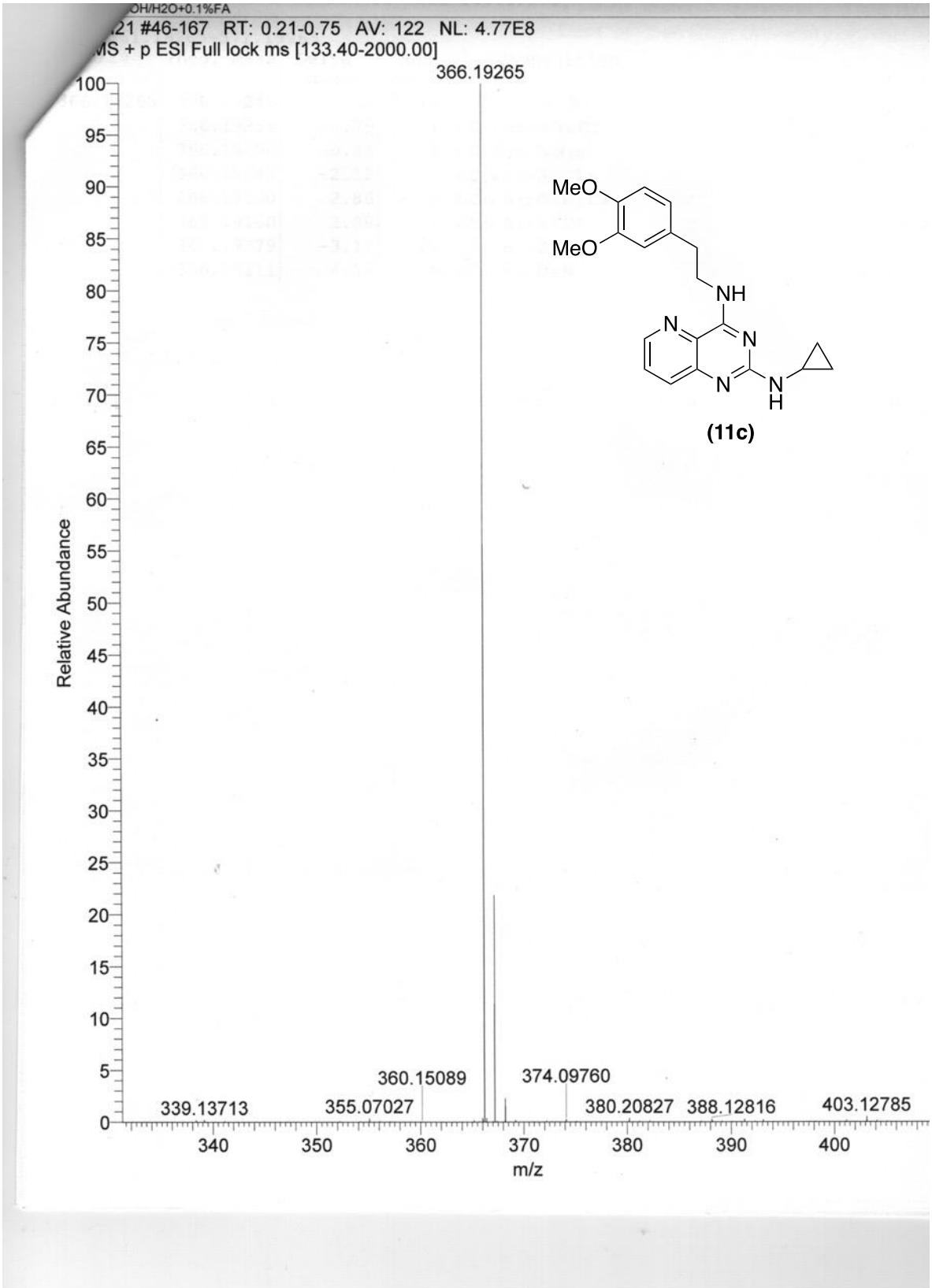
N^4-(3,4-Dimethoxyphenethyl)-N^2-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11a).



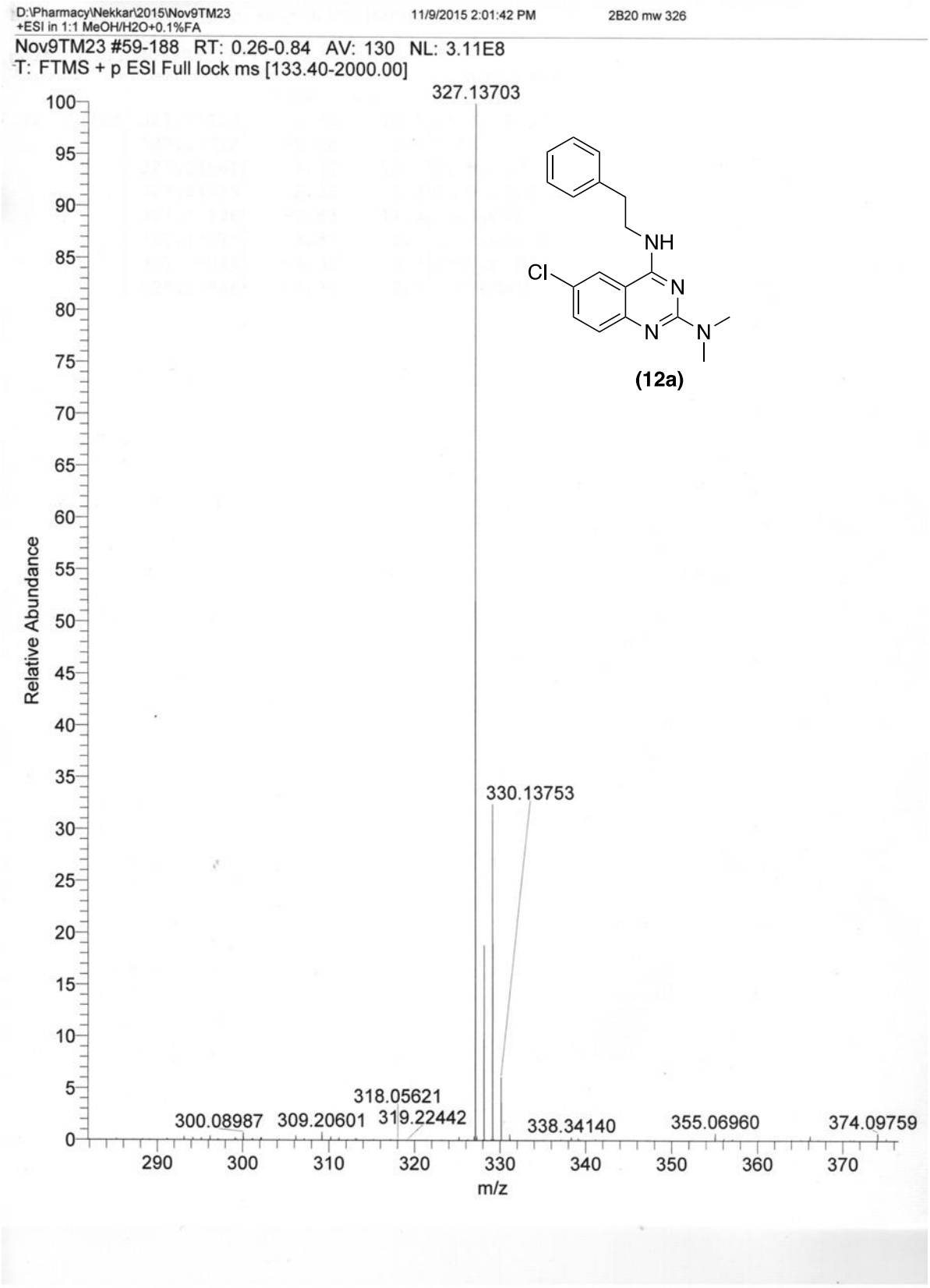
N^4-(3,4-Dimethoxyphenethyl)-N^2-isopropylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11b).



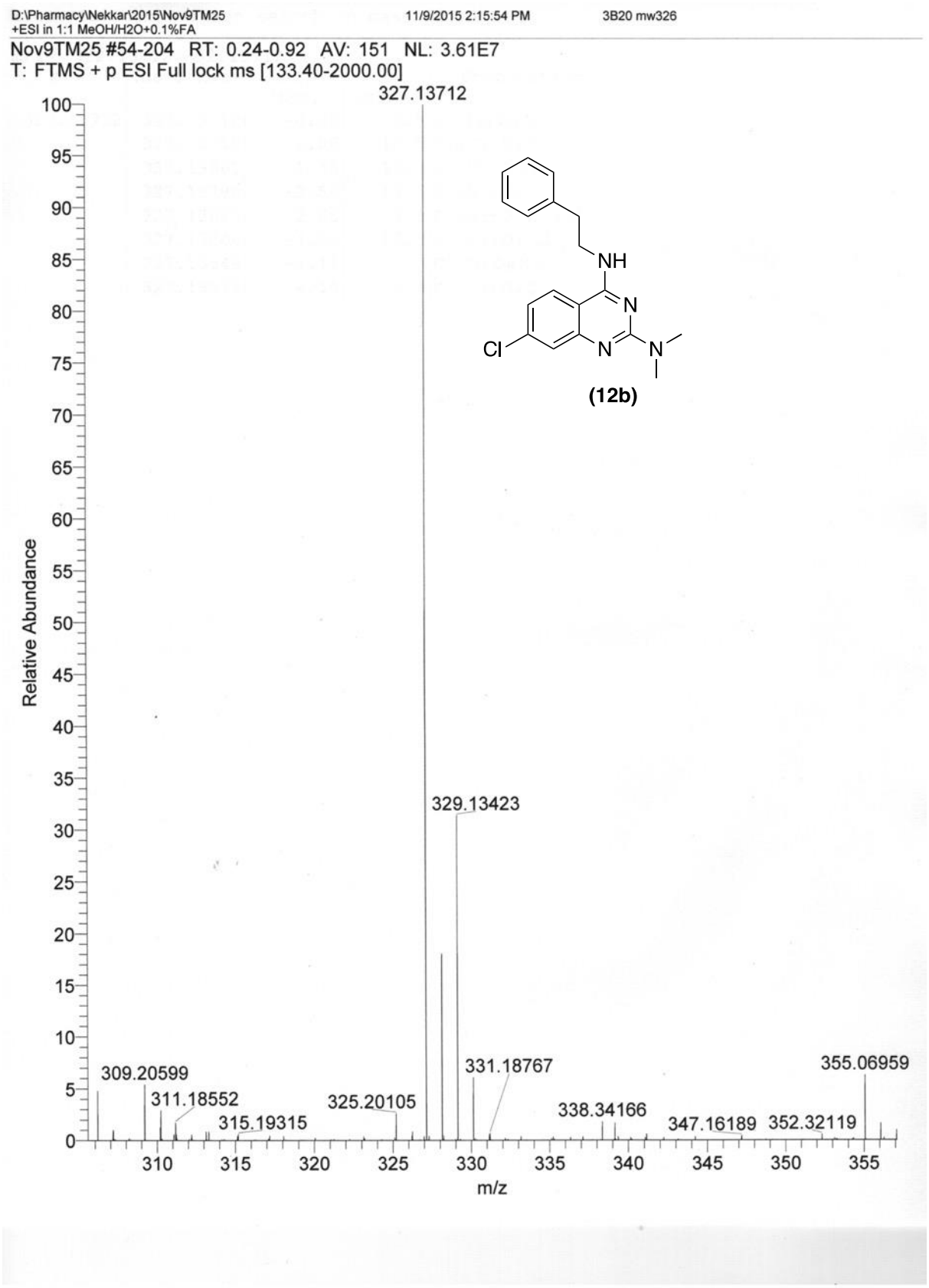
N^2-Cyclopropyl-N^4-(3,4-dimethoxyphenethyl)pyrido[3,2-*d*]pyrimidine-2,4-diamine (11c).



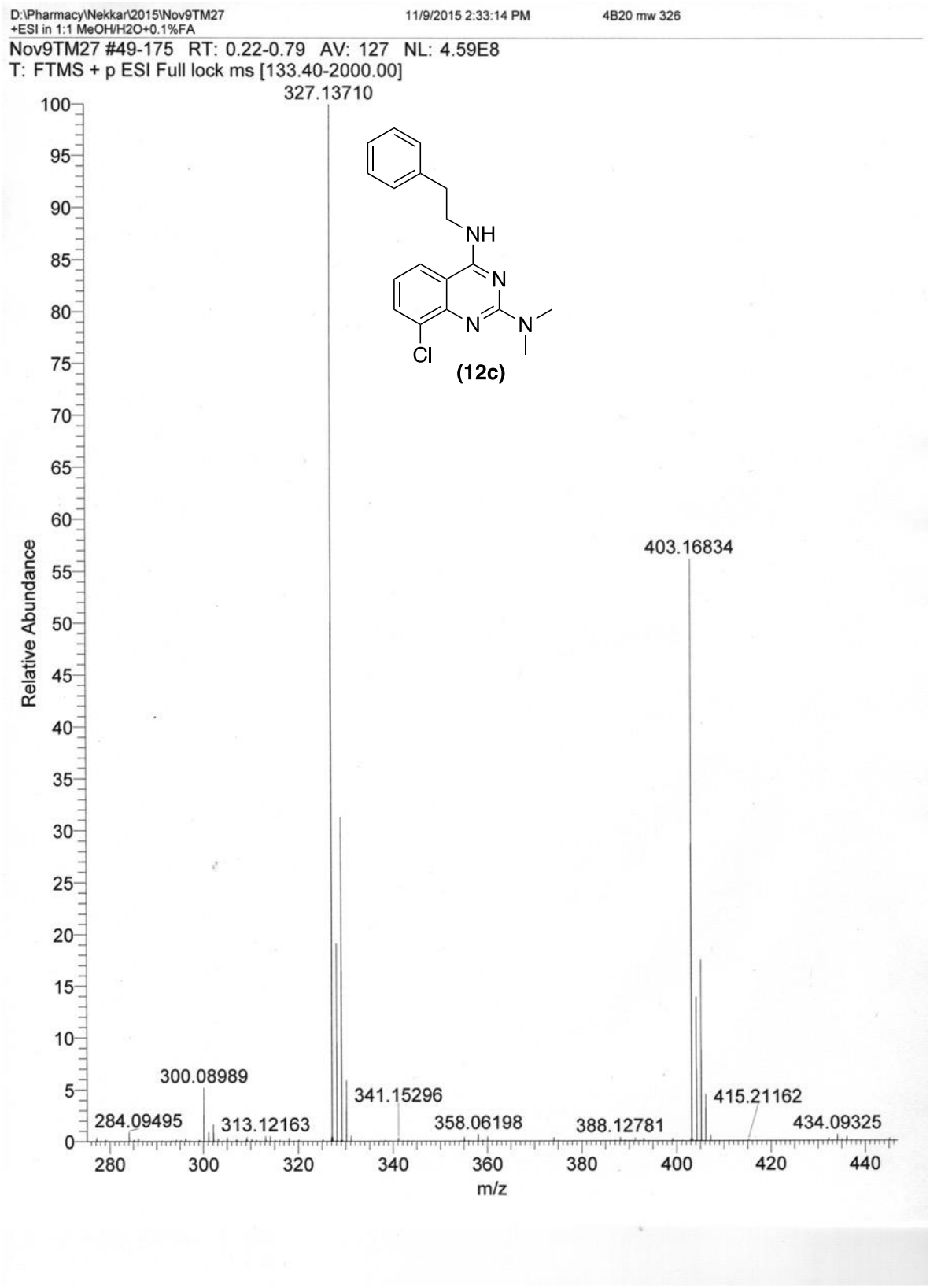
6-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12a).



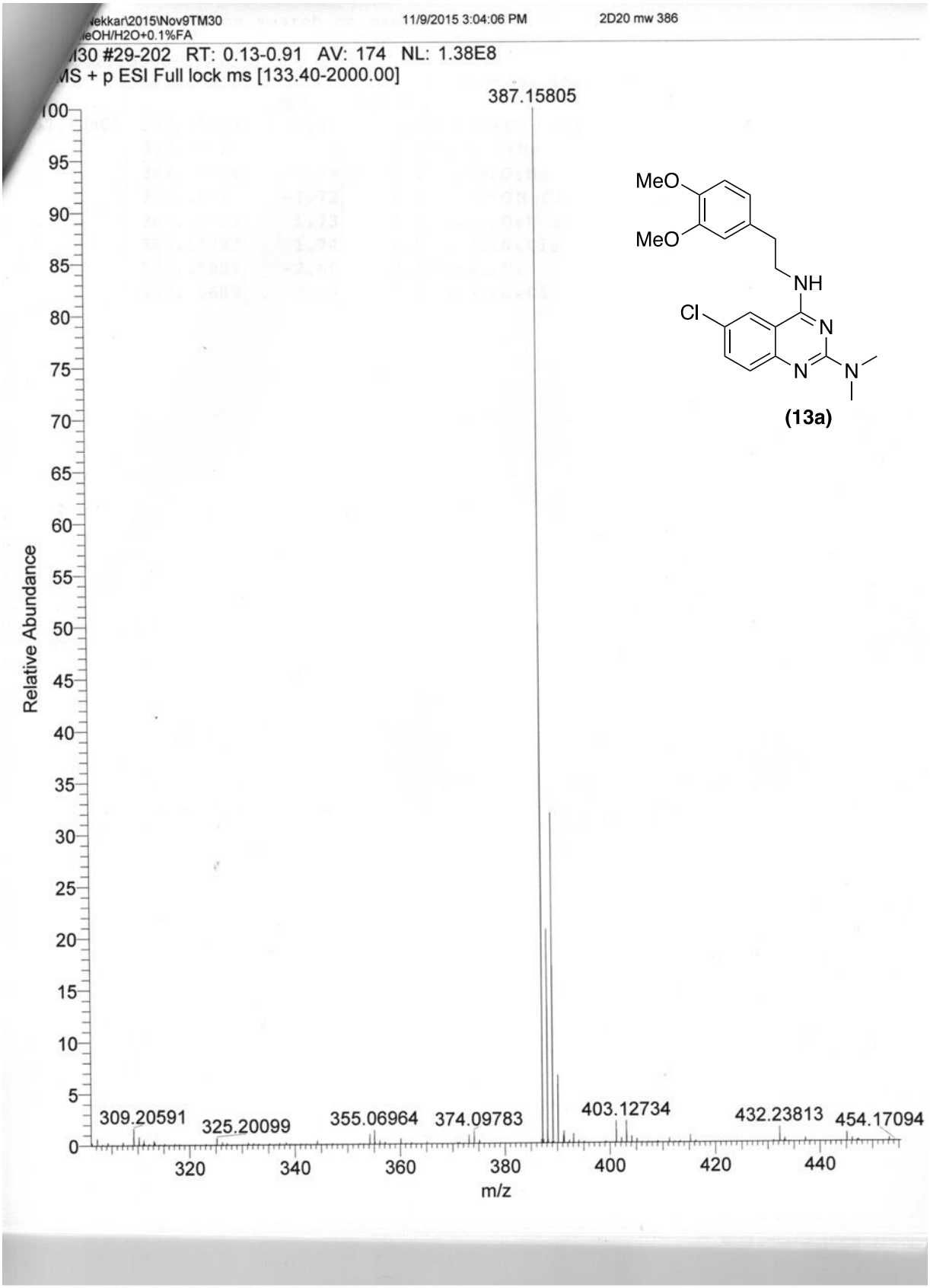
7-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12b).



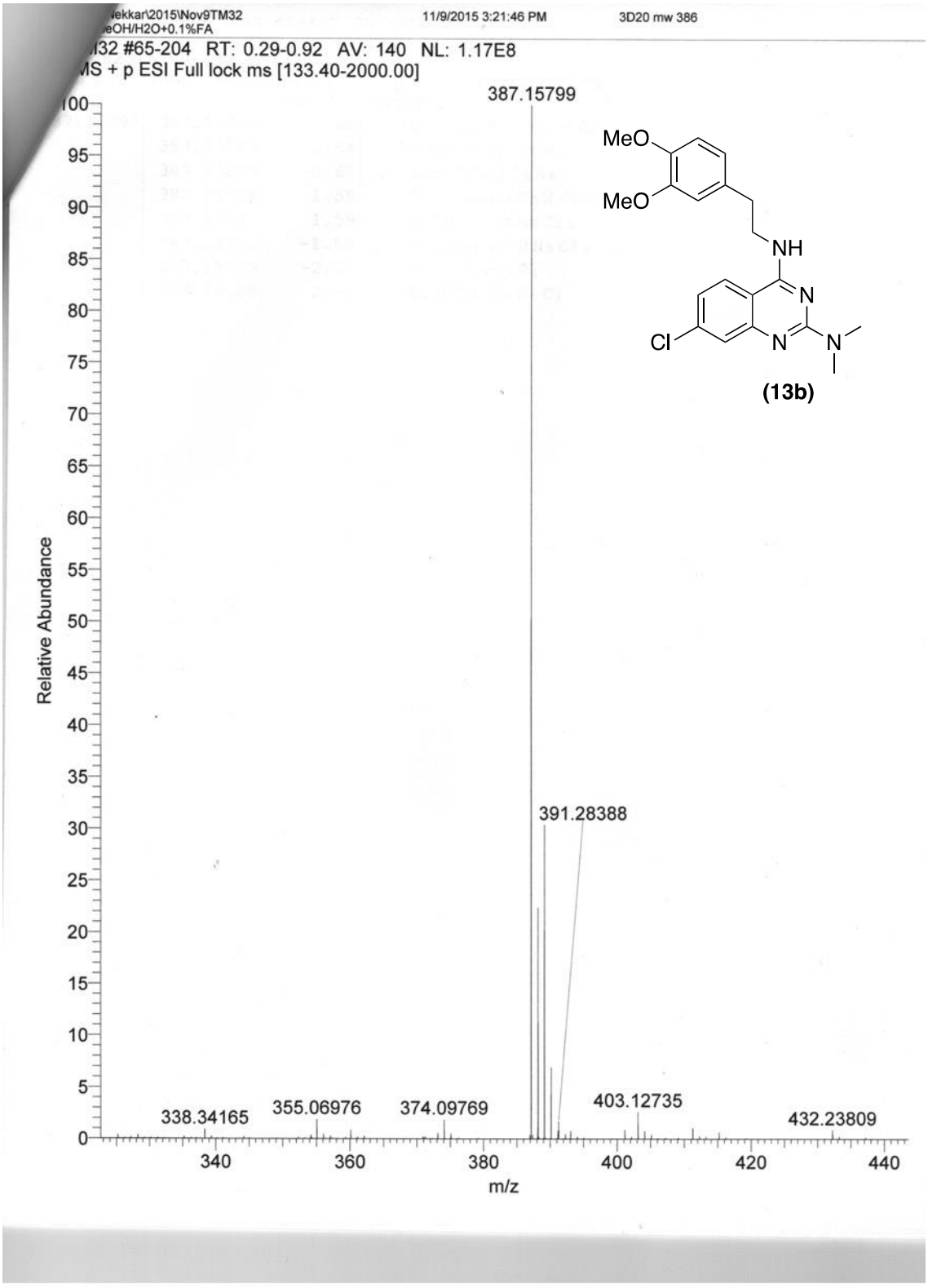
8-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12c).



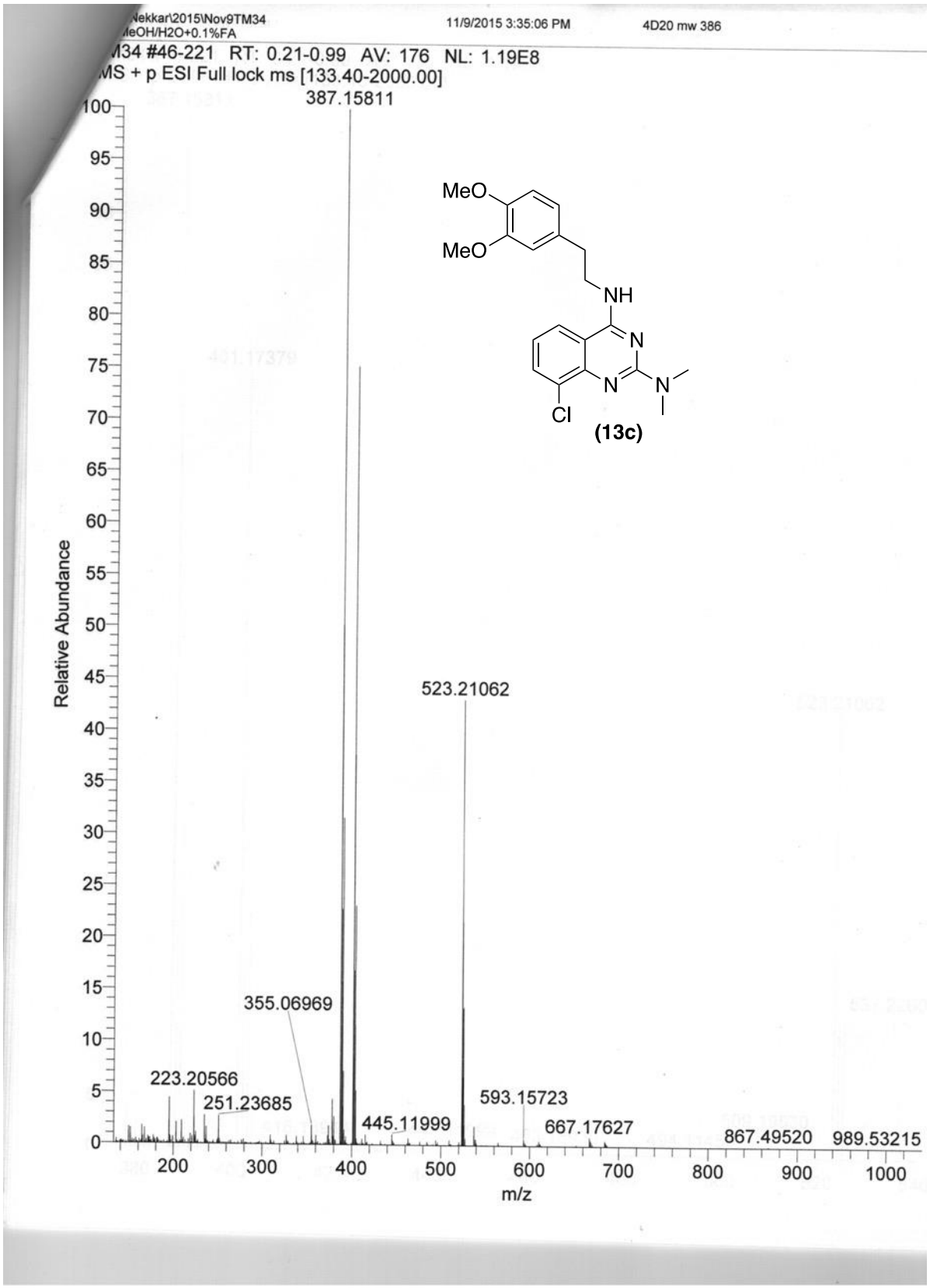
6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13a).



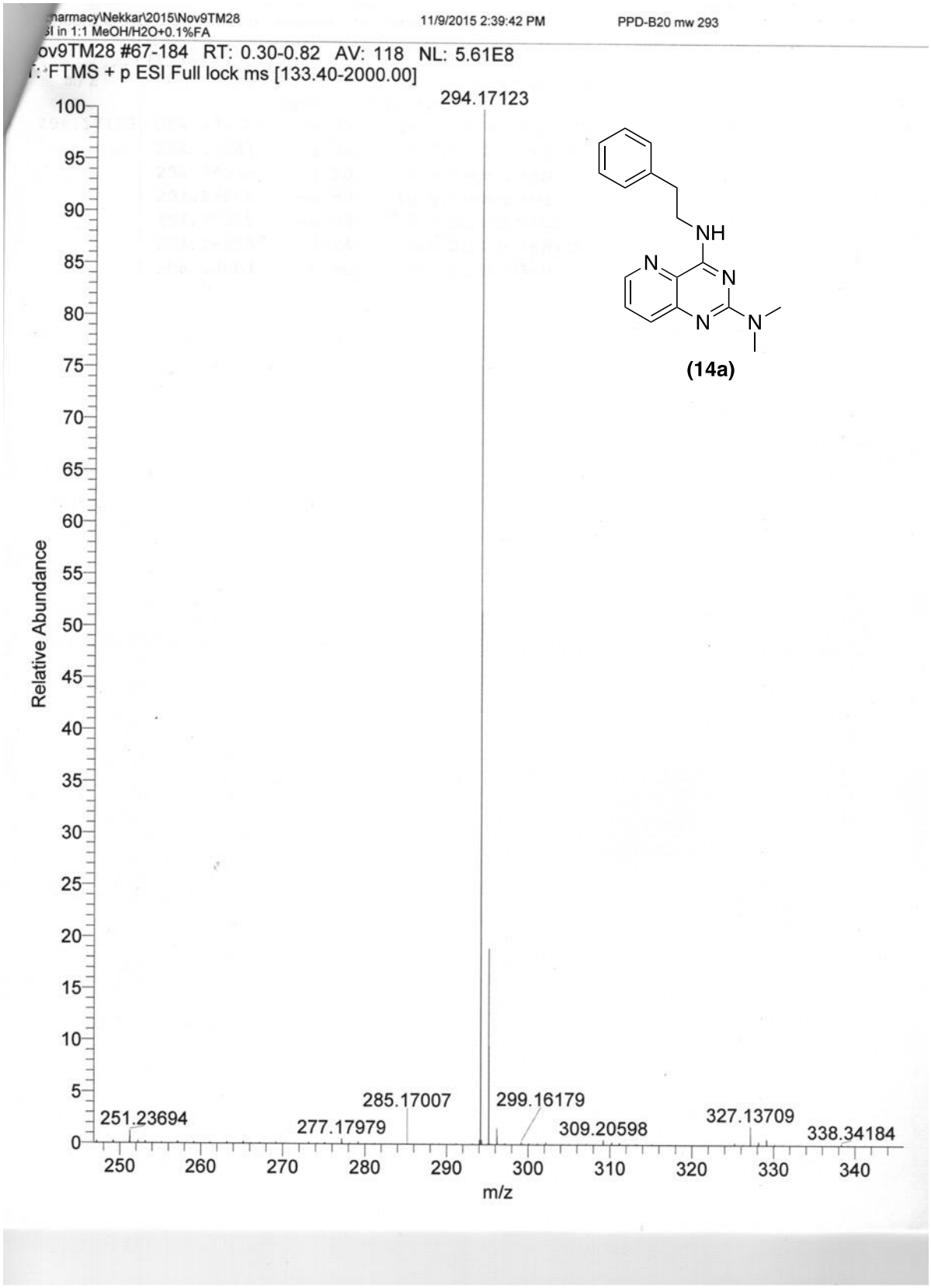
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13b).



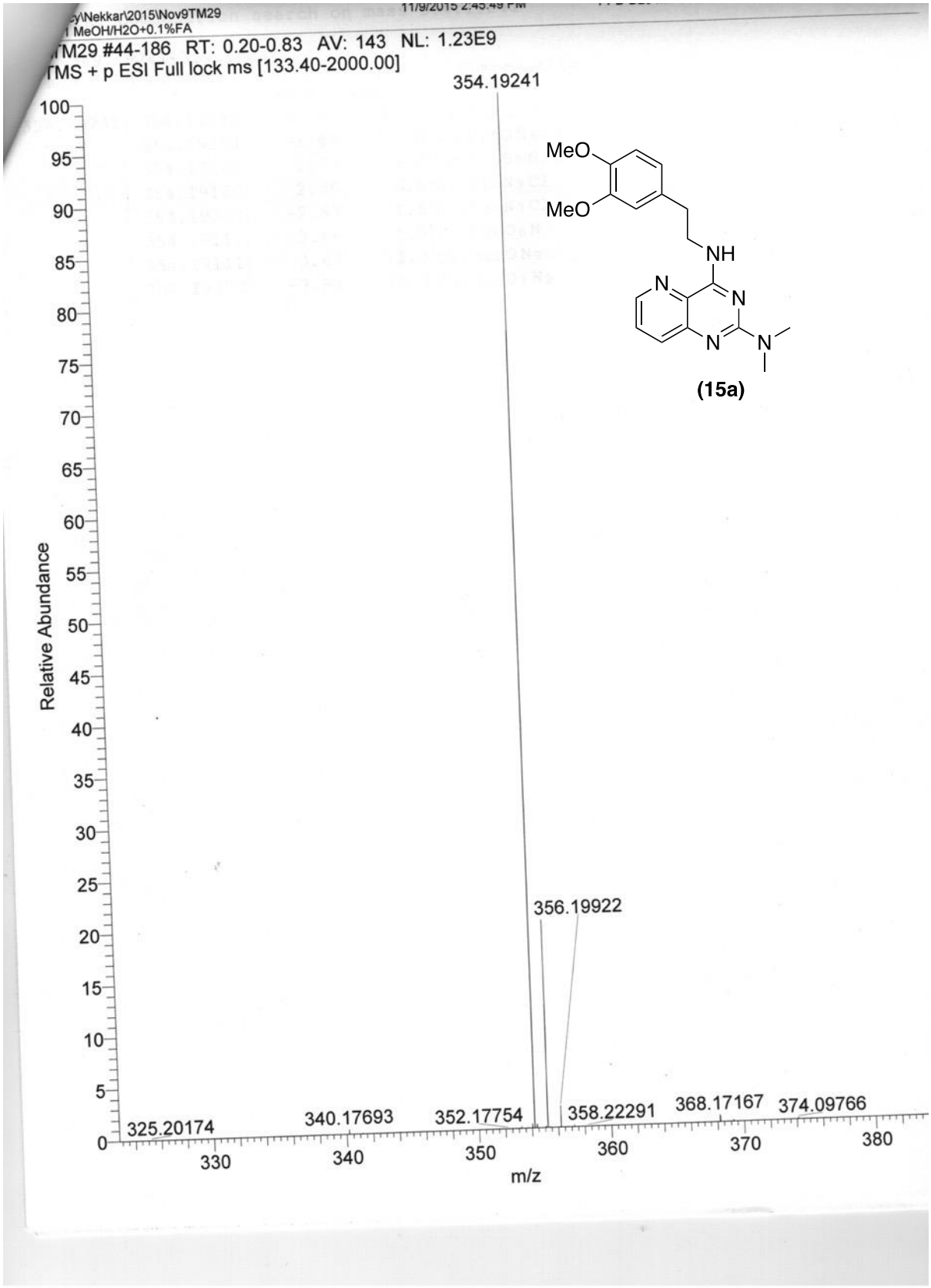
8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13c).



N^2,N^2-Dimethyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (14a).

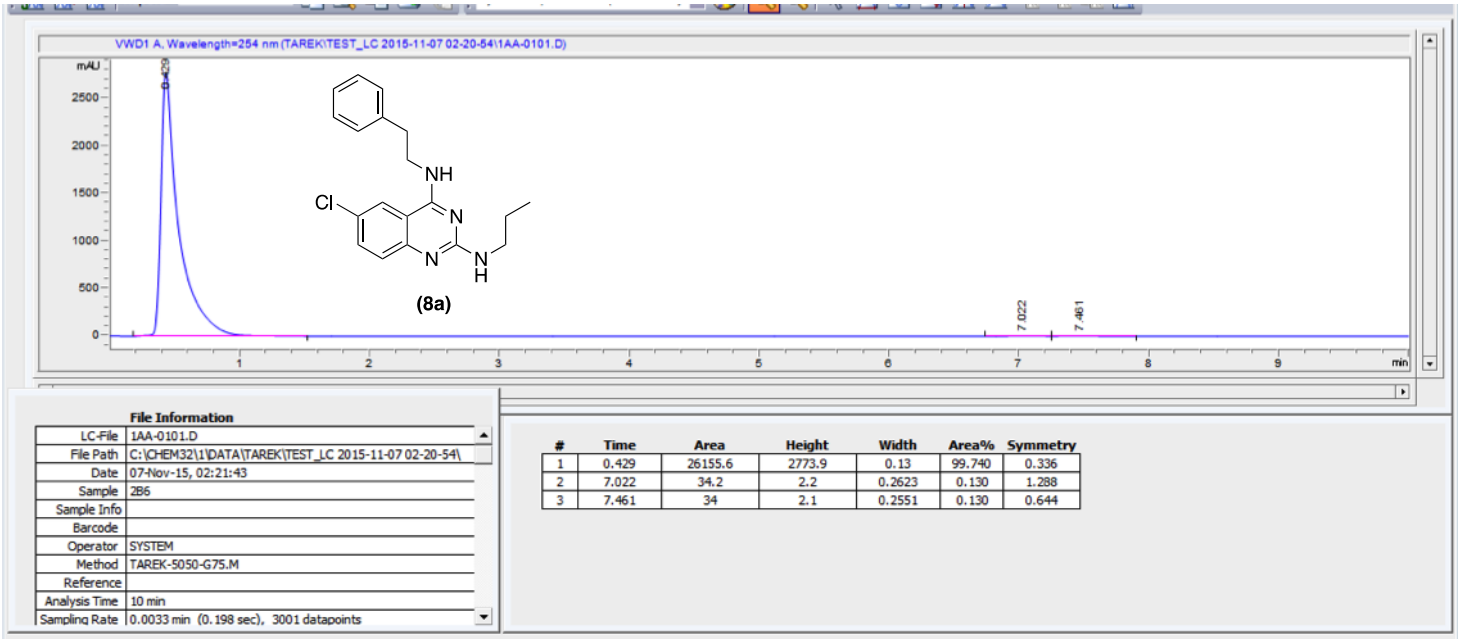


N^4-(3,4-Dimethoxyphenethyl)-N^2,N^2-dimethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (15a).



6. HPLC trace for compounds 8a–i, 9a–i, 10a–c, 11a–c, 12a–c, 13a–c, 14a and 15a

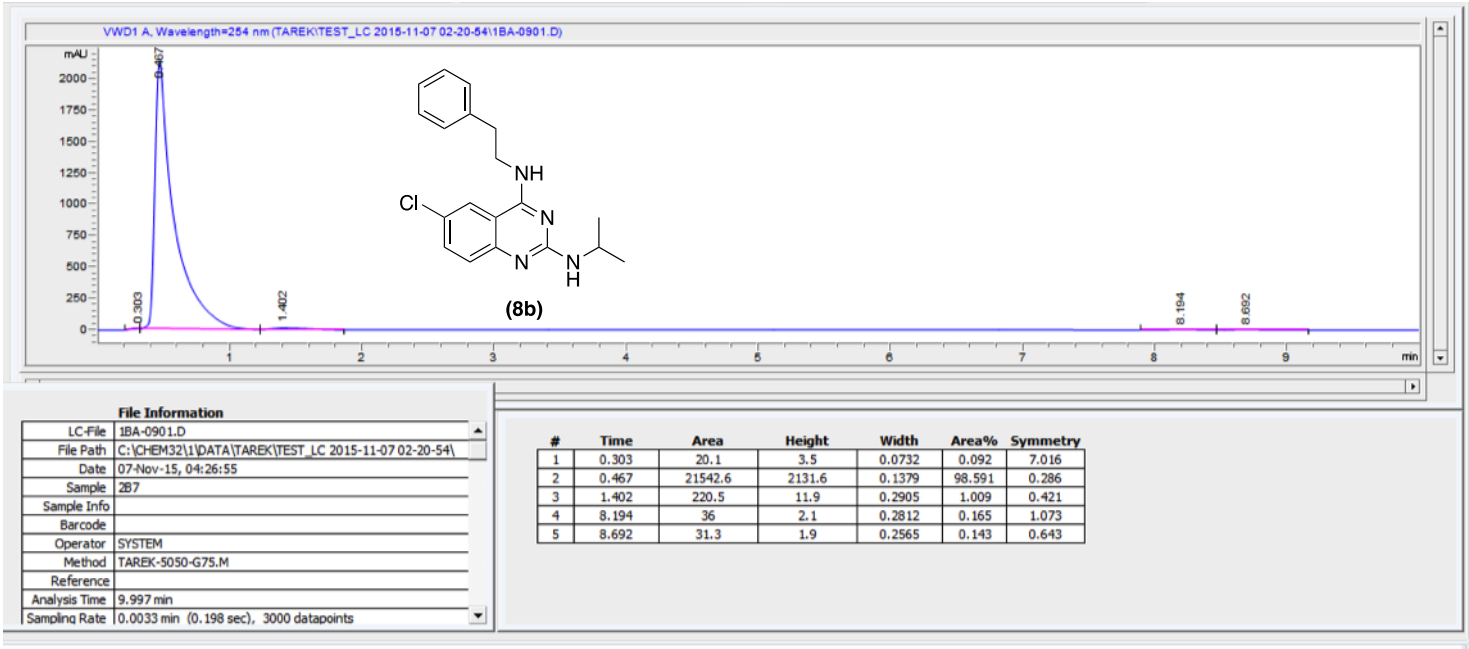
6-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8a).



File Information	
LC-File	1AA-0101.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 02:21:43
Sample	2B6
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	10 min
Sampling Rate	0.0033 min (0.198 sec), 3001 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.429	26155.6	2773.9	0.13	99.740	0.336
2	7.022	34.2	2.2	0.2623	0.130	1.288
3	7.461	34	2.1	0.2551	0.130	0.644

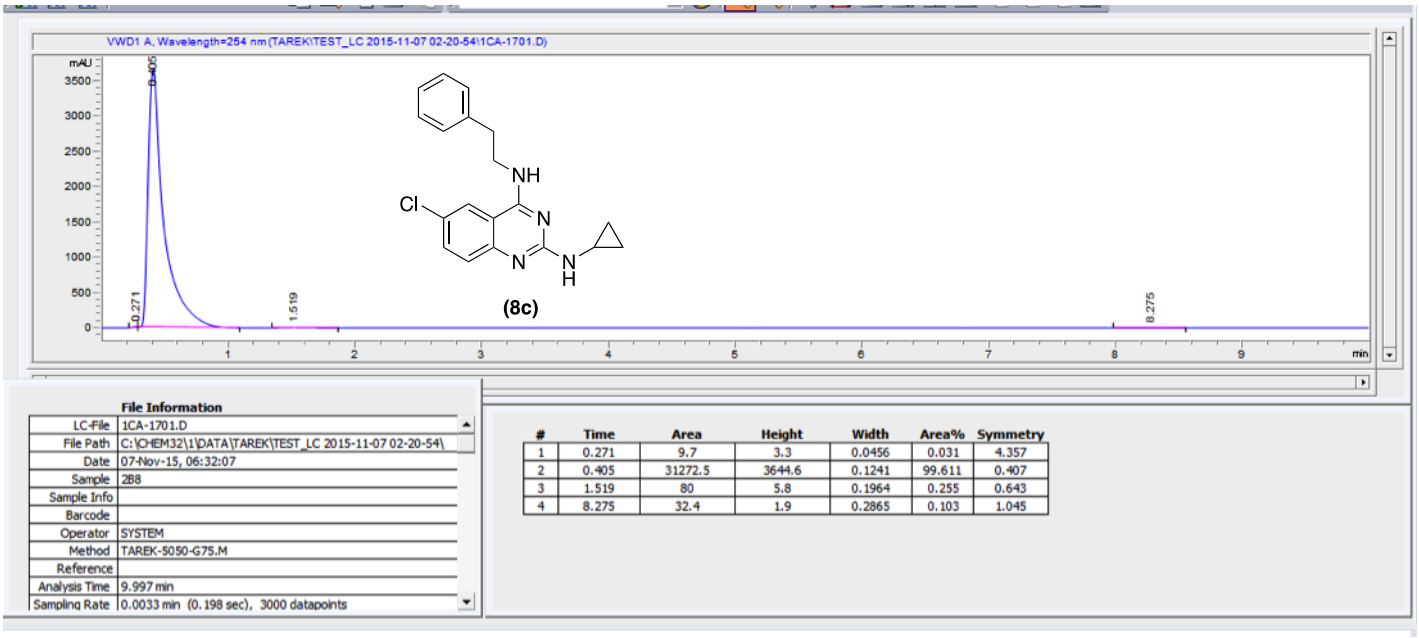
6-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8b).



File Information	
LC-File	1BA-0901.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 04:26:55
Sample	2B7
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.303	20.1	3.5	0.0732	0.092	7.016
2	0.467	21542.6	2131.6	0.1379	98.591	0.286
3	1.402	220.5	11.9	0.2905	1.009	0.421
4	8.194	36	2.1	0.2812	0.165	1.073
5	8.692	31.3	1.9	0.2565	0.143	0.643

6-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8c).

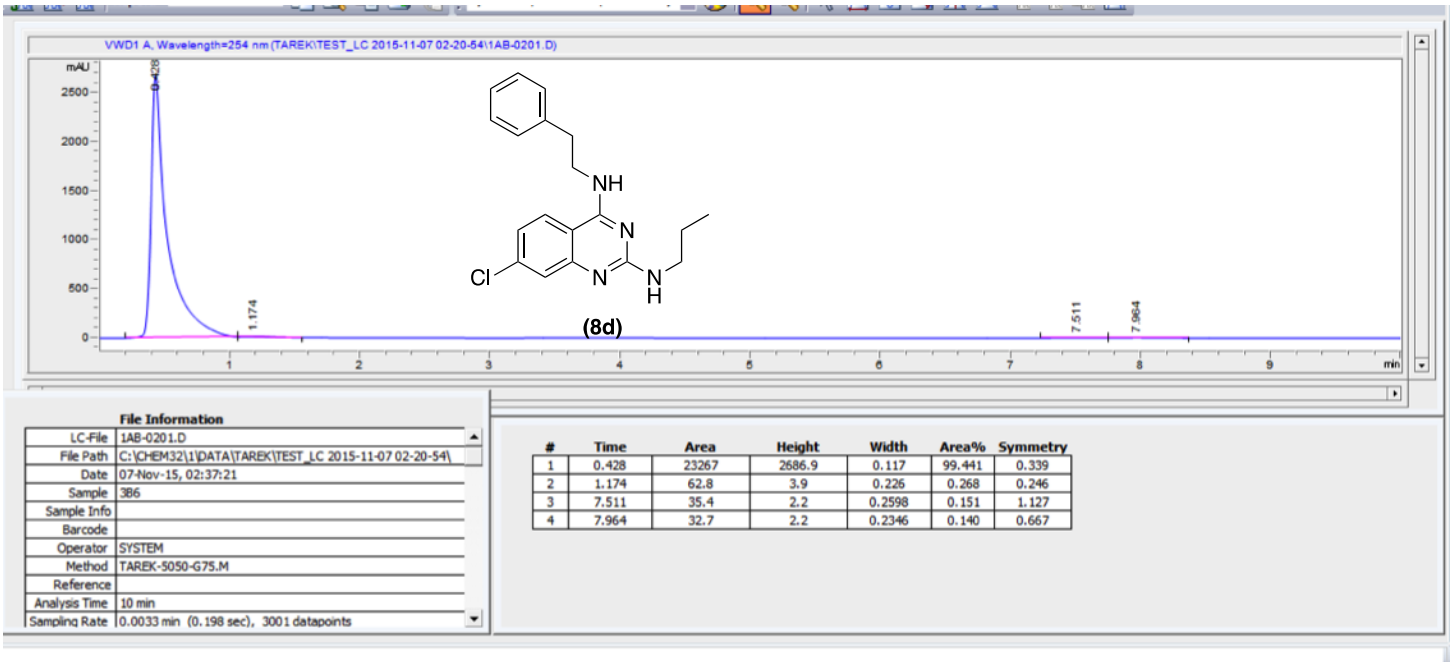


File Information

LC-File	1CA-1701.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 06:32:07
Sample	2B8
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.271	9.7	3.3	0.0456	0.031	4.357
2	0.405	31272.5	3644.6	0.1241	99.611	0.407
3	1.519	80	5.8	0.1964	0.255	0.643
4	8.275	32.4	1.9	0.2865	0.103	1.045

7-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8d).

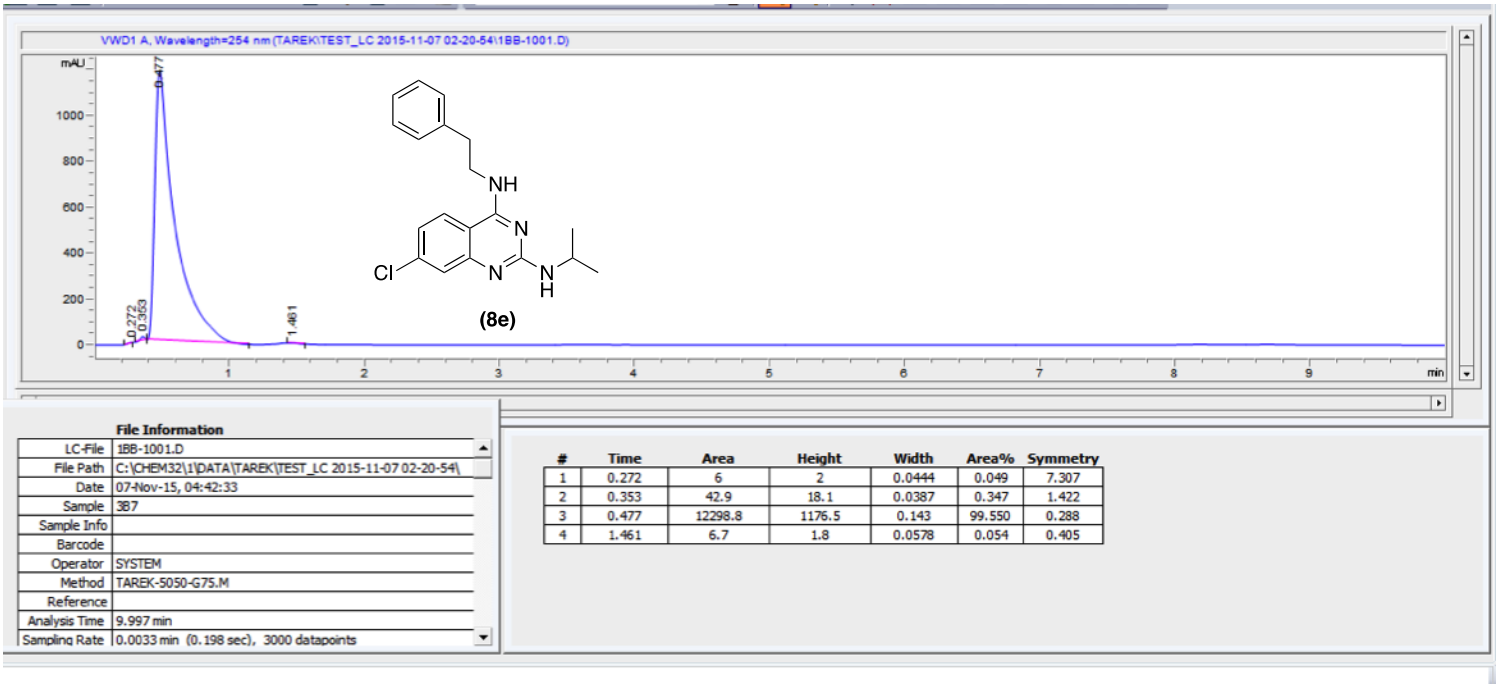


File Information

LC-File	1AB-0201.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 02:37:21
Sample	3B6
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	10 min
Sampling Rate	0.0033 min (0.198 sec), 3001 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.428	23267	2686.9	0.117	99.441	0.339
2	1.174	62.8	3.9	0.226	0.268	0.246
3	7.511	35.4	2.2	0.2598	0.151	1.127
4	7.964	32.7	2.2	0.2346	0.140	0.667

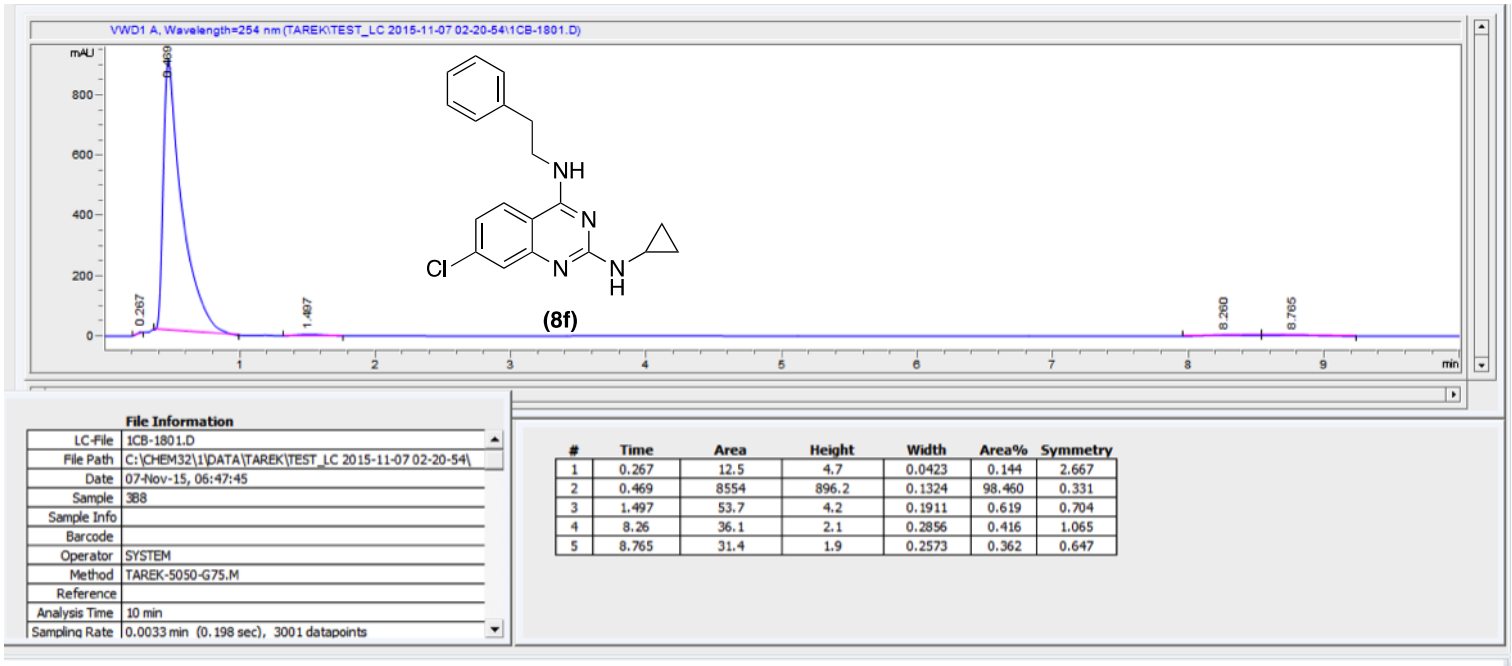
7-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8e).



File Information	
LC-File	1BB-1001.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 04:42:33
Sample	3B7
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.272	6	2	0.0444	0.049	7.307
2	0.353	42.9	18.1	0.0387	0.347	1.422
3	0.477	12298.8	1176.5	0.143	99.550	0.288
4	1.461	6.7	1.8	0.0578	0.054	0.405

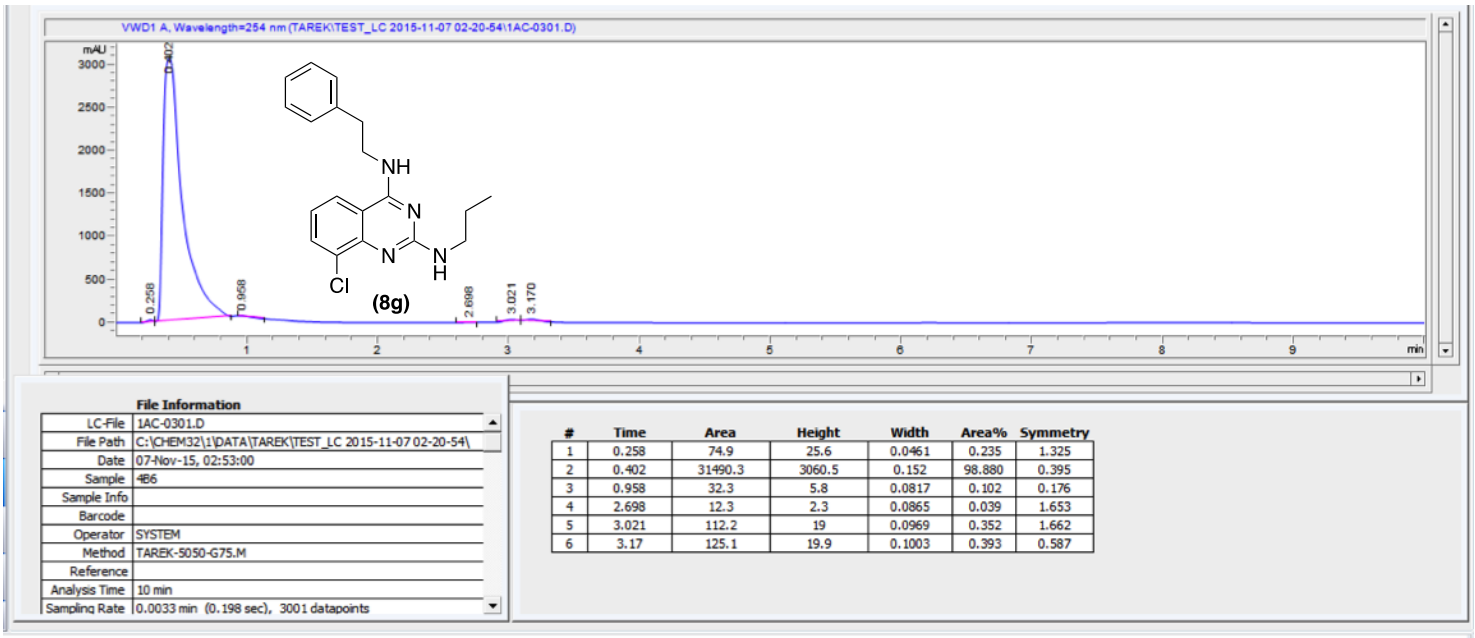
7-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8f).



File Information	
LC-File	1CB-1801.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 06:47:45
Sample	3B8
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	10 min
Sampling Rate	0.0033 min (0.198 sec), 3001 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.267	12.5	4.7	0.0423	0.144	2.667
2	0.469	8554	896.2	0.1324	98.460	0.331
3	1.497	53.7	4.2	0.1911	0.619	0.704
4	8.26	36.1	2.1	0.2856	0.416	1.065
5	8.765	31.4	1.9	0.2573	0.362	0.647

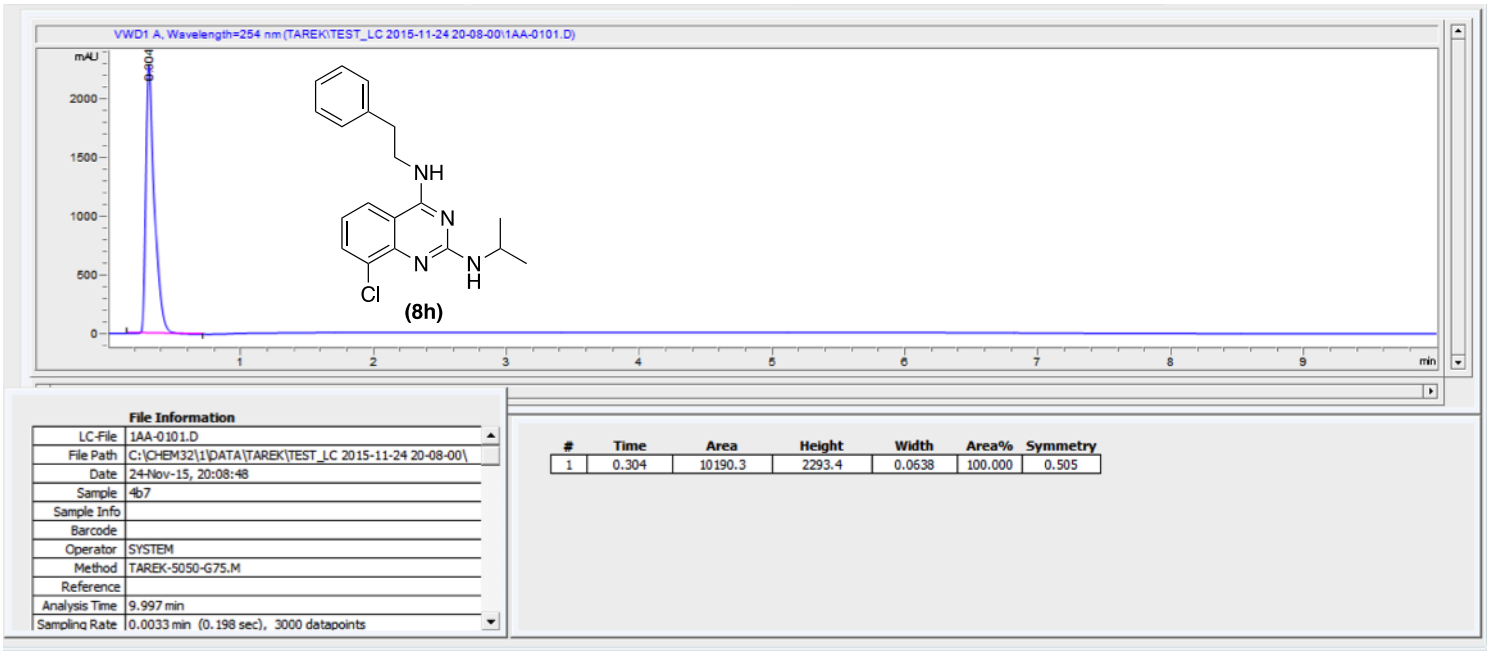
8-Chloro-N^4-phenethyl-N^2-propylquinazoline-2,4-diamine (8g).



File Information	
LC-File	1AC-0301.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 02:53:00
Sample	4B6
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	10 min
Sampling Rate	0.0033 min (0.198 sec), 3001 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.258	74.9	25.6	0.0461	0.235	1.325
2	0.402	31490.3	3060.5	0.152	98.880	0.395
3	0.958	32.3	5.8	0.0817	0.102	0.176
4	2.698	12.3	2.3	0.0865	0.039	1.653
5	3.021	112.2	19	0.0969	0.352	1.662
6	3.17	125.1	19.9	0.1003	0.393	0.587

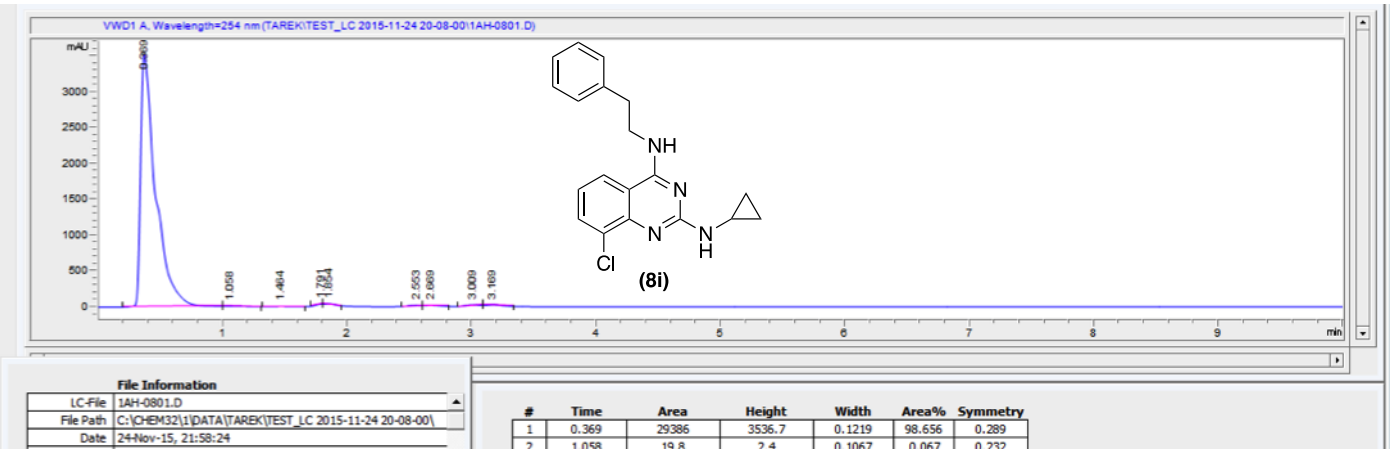
8-Chloro-N^2-isopropyl-N^4-phenethylquinazoline-2,4-diamine (8h).



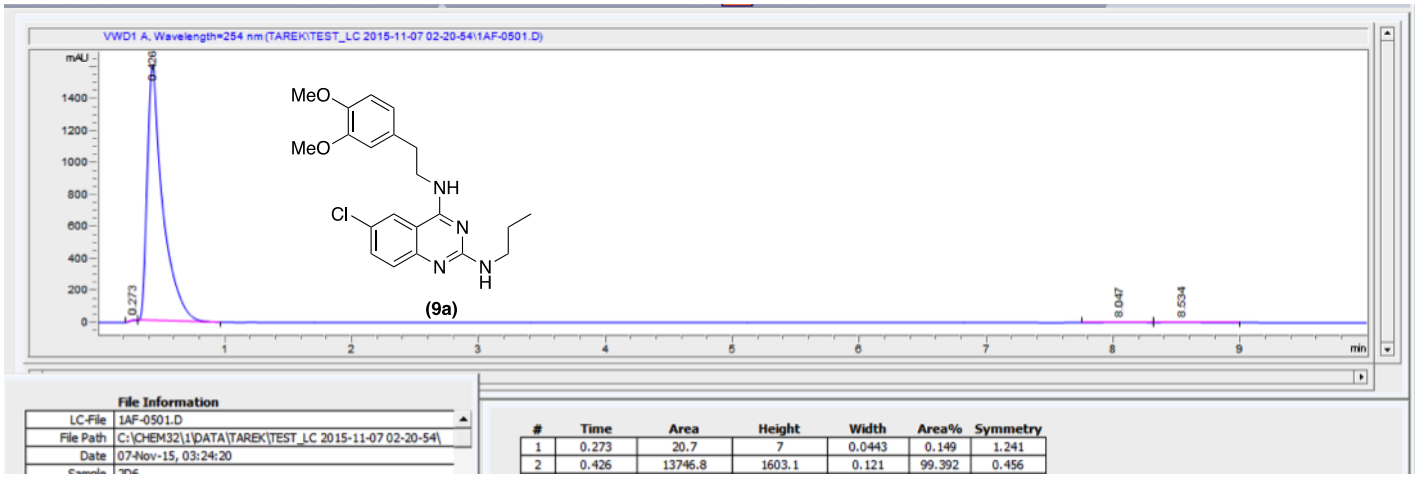
File Information	
LC-File	1AA-0101.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-24 20-08-00\
Date	24-Nov-15, 20:08:48
Sample	4b7
Sample Info	
Barcode	
Operator	SYSTEM
Method	TAREK-5050-G75.M
Reference	
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	0.304	10190.3	2293.4	0.0638	100.000	0.505

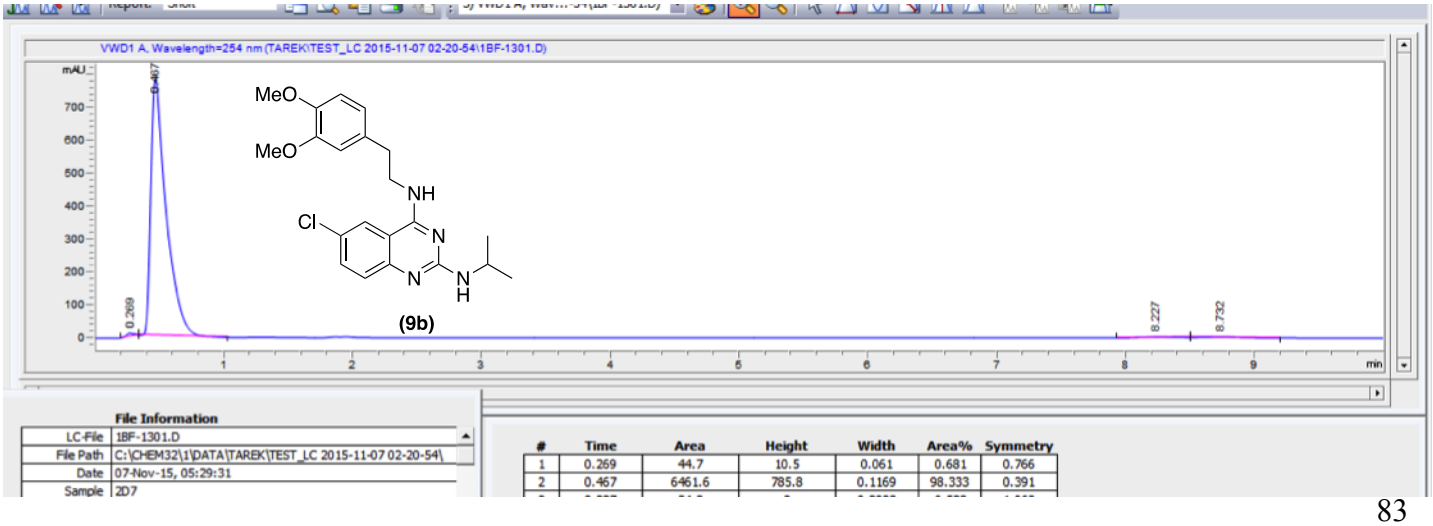
8-Chloro-N^2-cyclopropyl-N^4-phenethylquinazoline-2,4-diamine (8i).



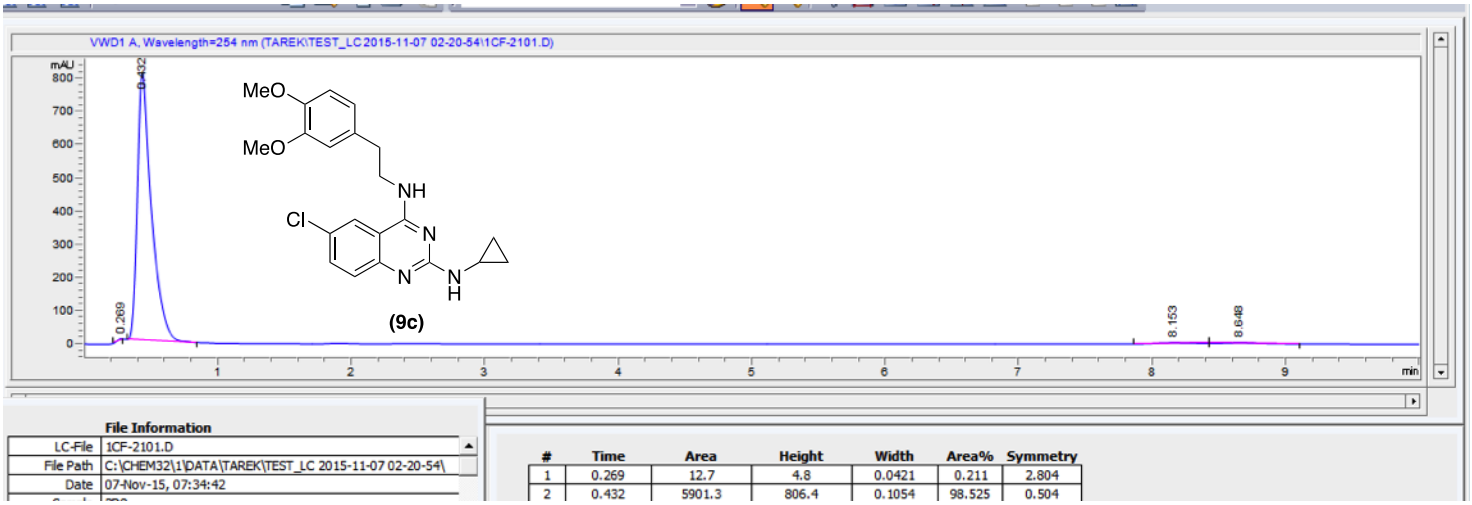
6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9a).



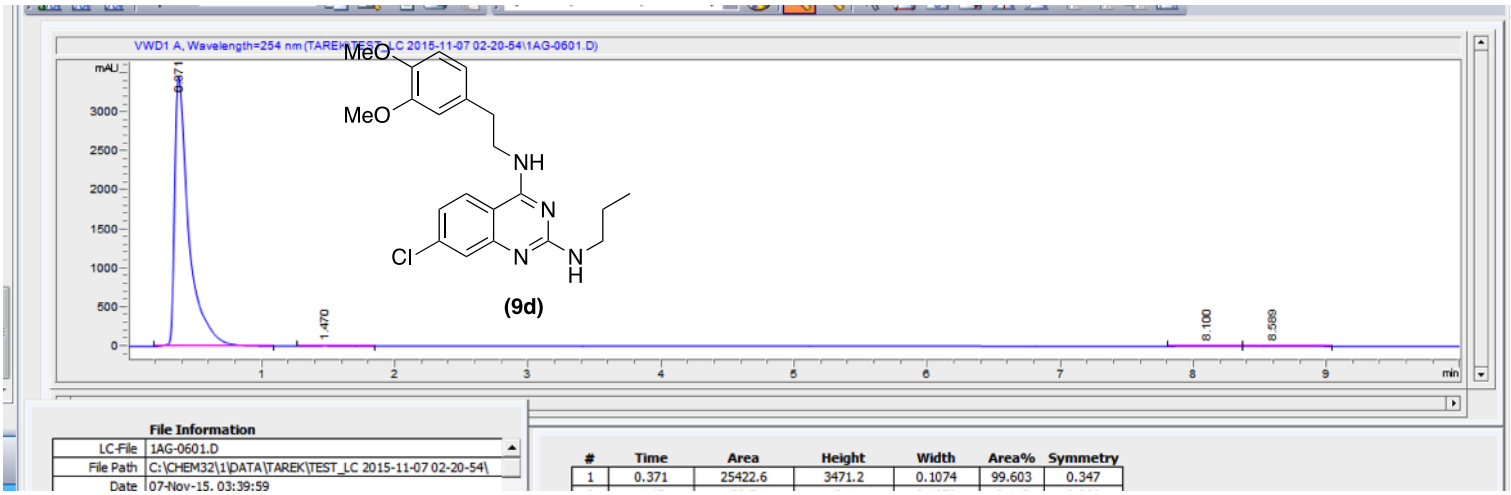
6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9b).



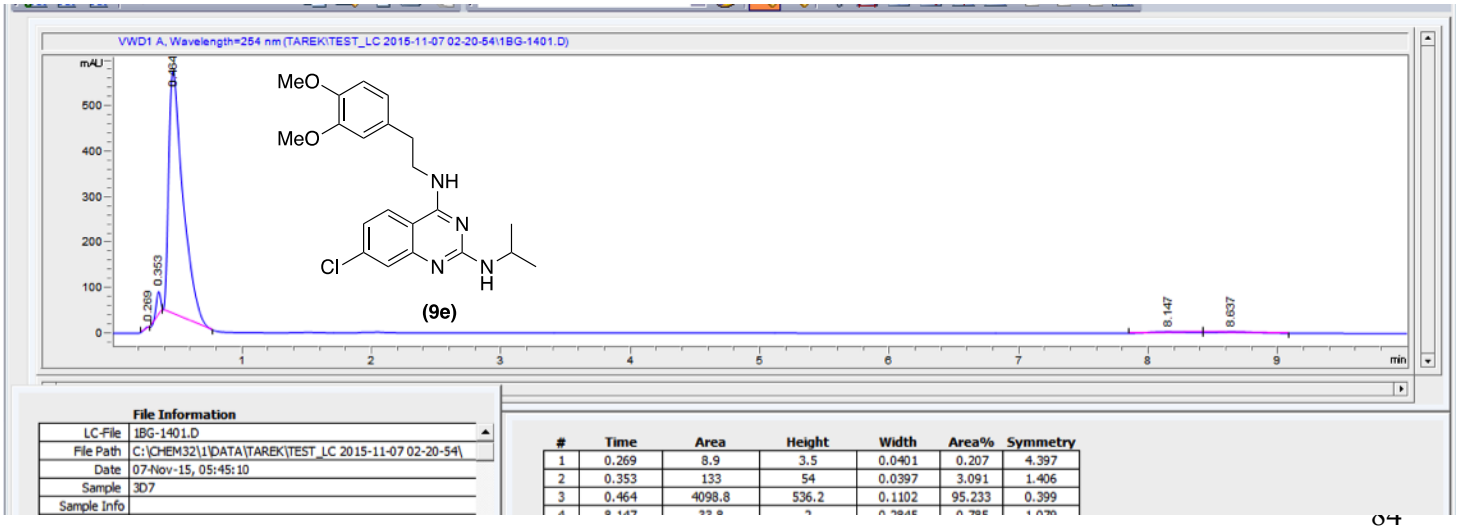
6-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9c).



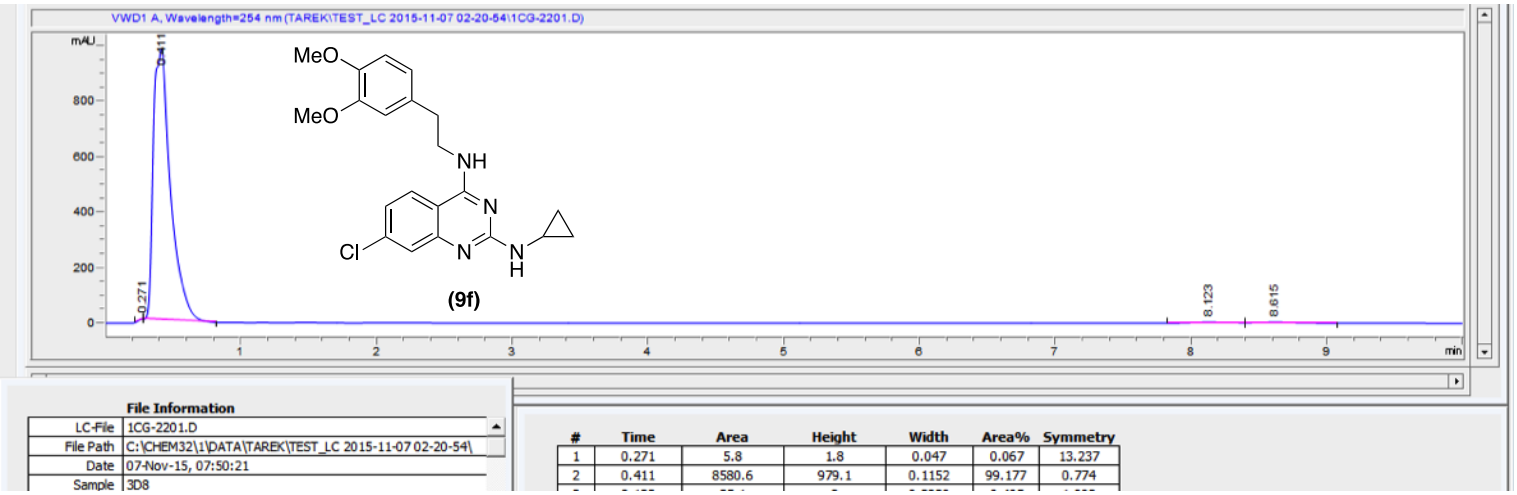
7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9d).



7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9e).

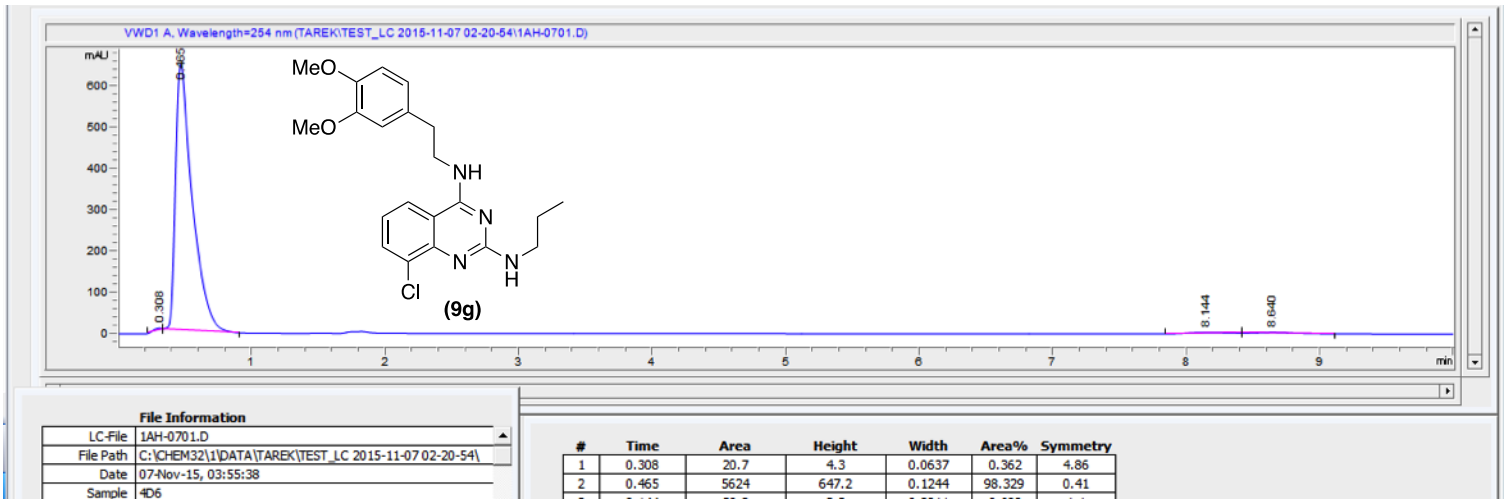


7-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9f).



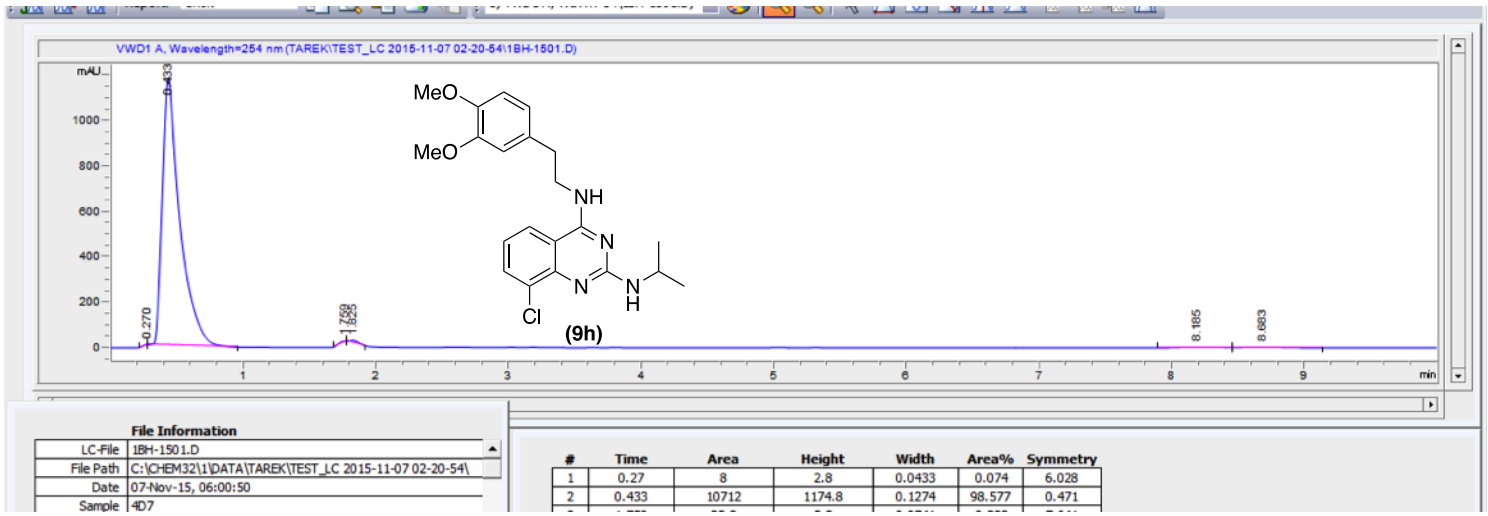
#	Time	Area	Height	Width	Area%	Symmetry
1	0.271	5.8	1.8	0.047	0.067	13.237
2	0.411	8580.6	979.1	0.1152	99.177	0.774

8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-propylquinazoline-2,4-diamine (9g).



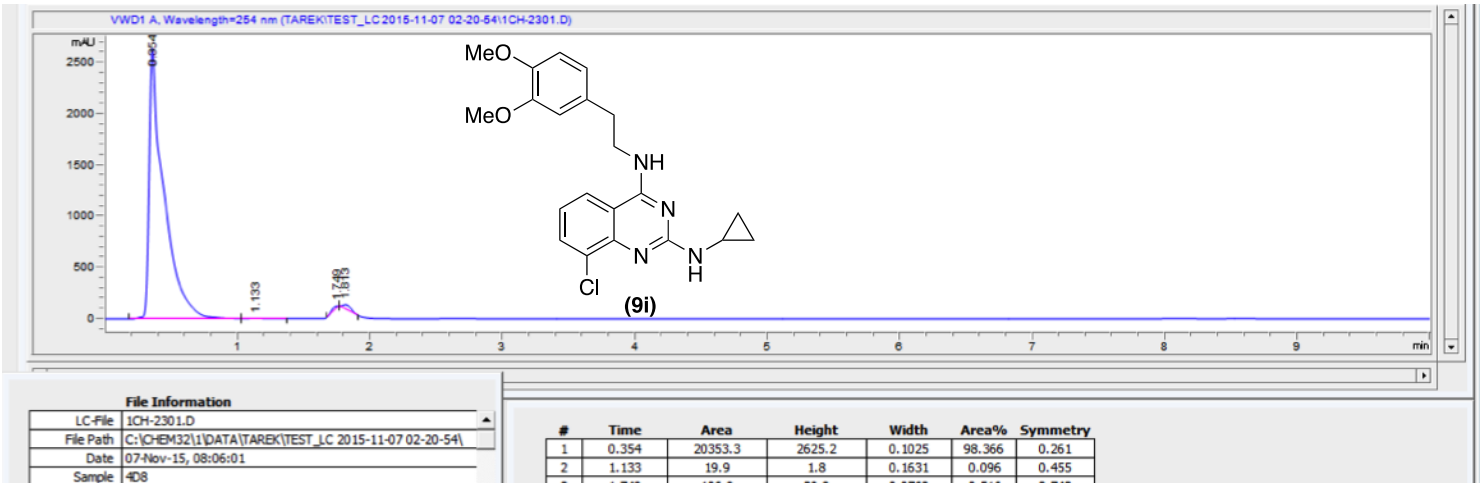
#	Time	Area	Height	Width	Area%	Symmetry
1	0.308	20.7	4.3	0.0637	0.362	4.86
2	0.465	5624	647.2	0.1244	98.329	0.41

8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2-isopropylquinazoline-2,4-diamine (9h).



#	Time	Area	Height	Width	Area%	Symmetry
1	0.27	8	2.8	0.0433	0.074	6.028
2	0.433	10712	1174.8	0.1274	98.577	0.471

8-Chloro-N^2-cyclopropyl-N^4-(3,4-dimethoxyphenethyl)quinazoline-2,4-diamine (9i).



File Information	
LC-File	1CH-2301.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 08:06:01
Sample	4D8

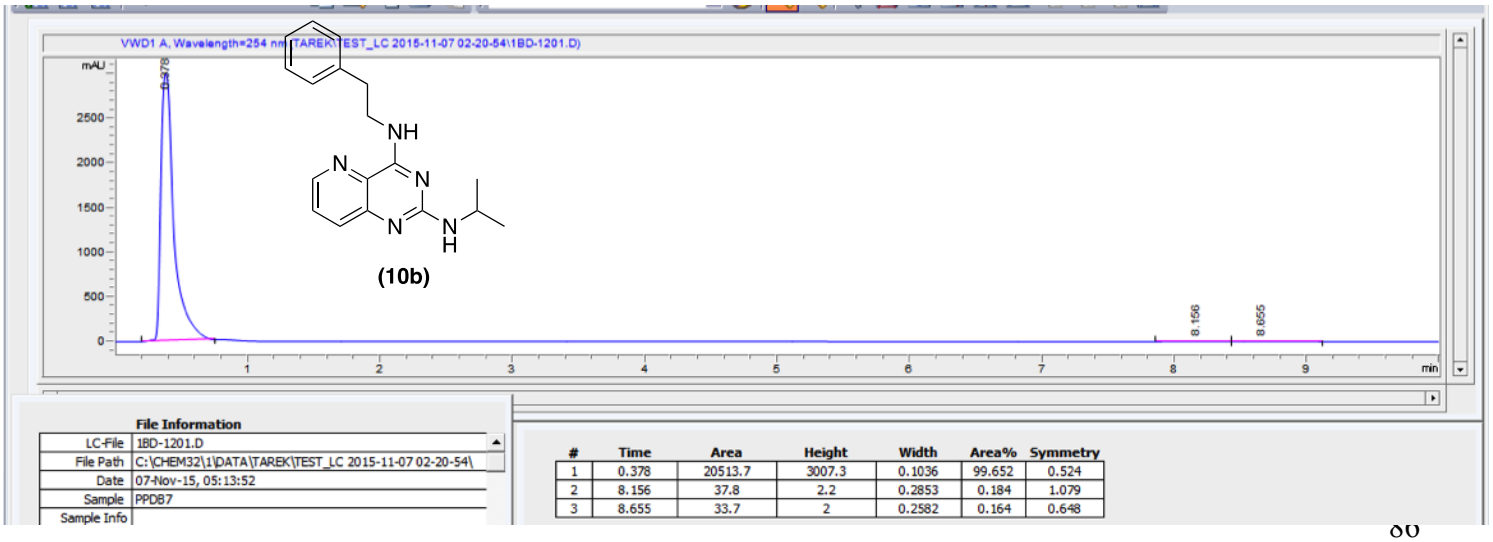
#	Time	Area	Height	Width	Area%	Symmetry
1	0.354	20353.3	2625.2	0.1025	98.366	0.261
2	1.133	19.9	1.8	0.1631	0.096	0.455

***N^4*-Phenethyl-*N^2*-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10a).**

File Information	
LC-File	1AD-0401.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 03:08:40

#	Time	Area	Height	Width	Area%	Symmetry
1	0.379	23648.2	3060.6	0.1171	99.351	0.529
2	2.645	44.2	2.4	0.2592	0.186	0.933

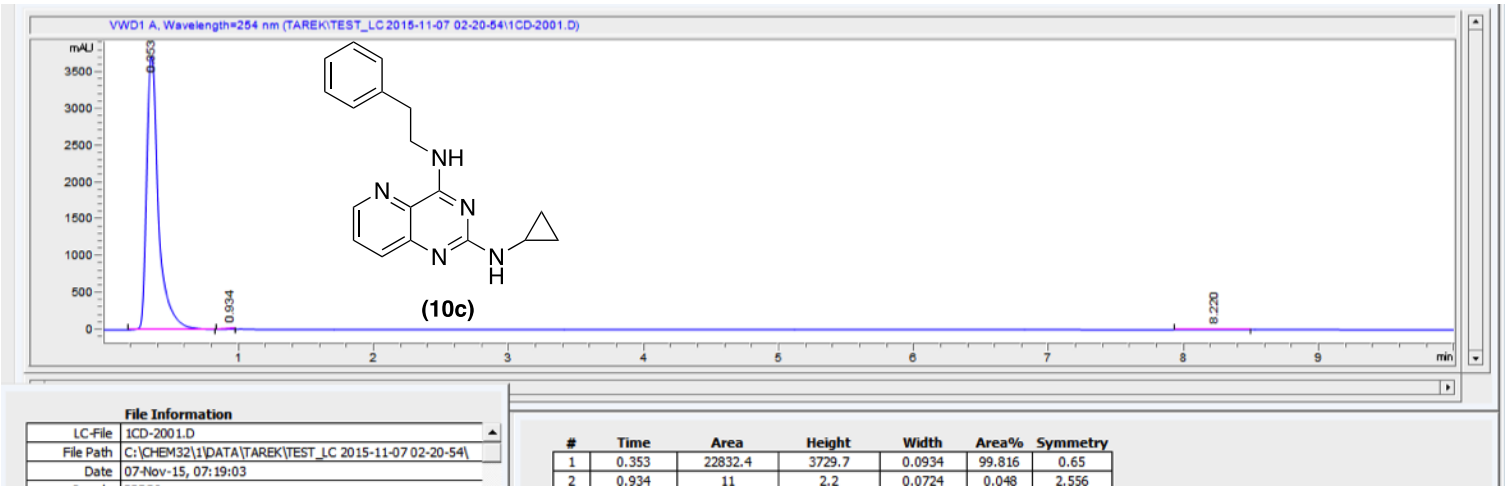
***N^2*-Isopropyl-*N^4*-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10b).**



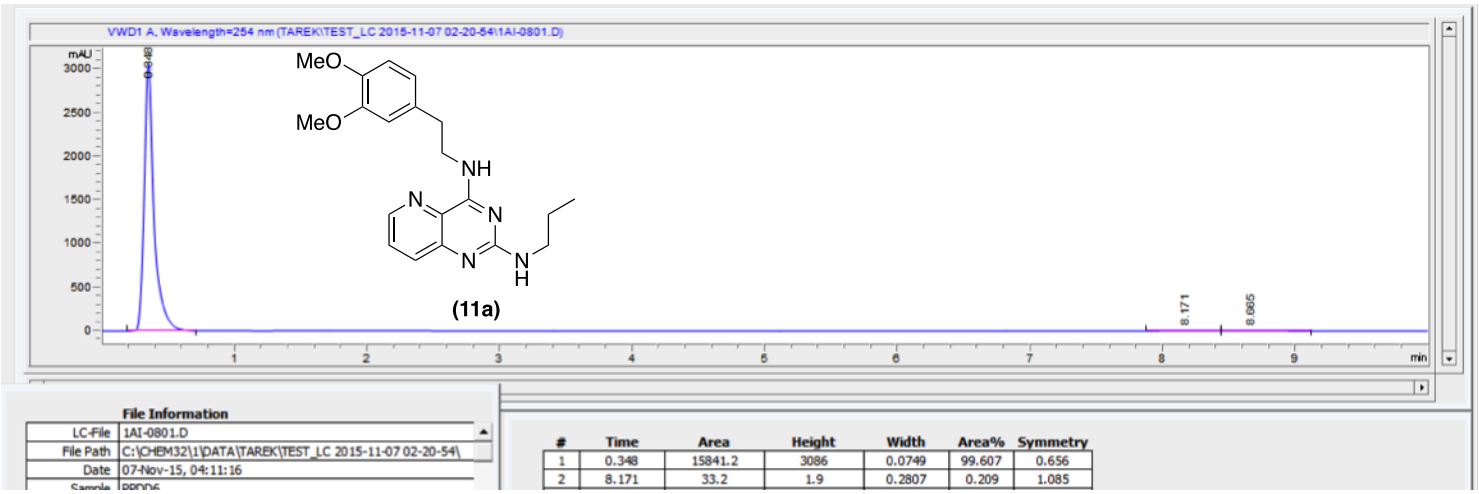
File Information	
LC-File	1BD-1201.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 05:13:52
Sample	PPDB7
Sample Info	

#	Time	Area	Height	Width	Area%	Symmetry
1	0.378	20513.7	3007.3	0.1036	99.652	0.524
2	8.156	37.8	2.2	0.2853	0.184	1.079
3	8.655	33.7	2	0.2582	0.164	0.648

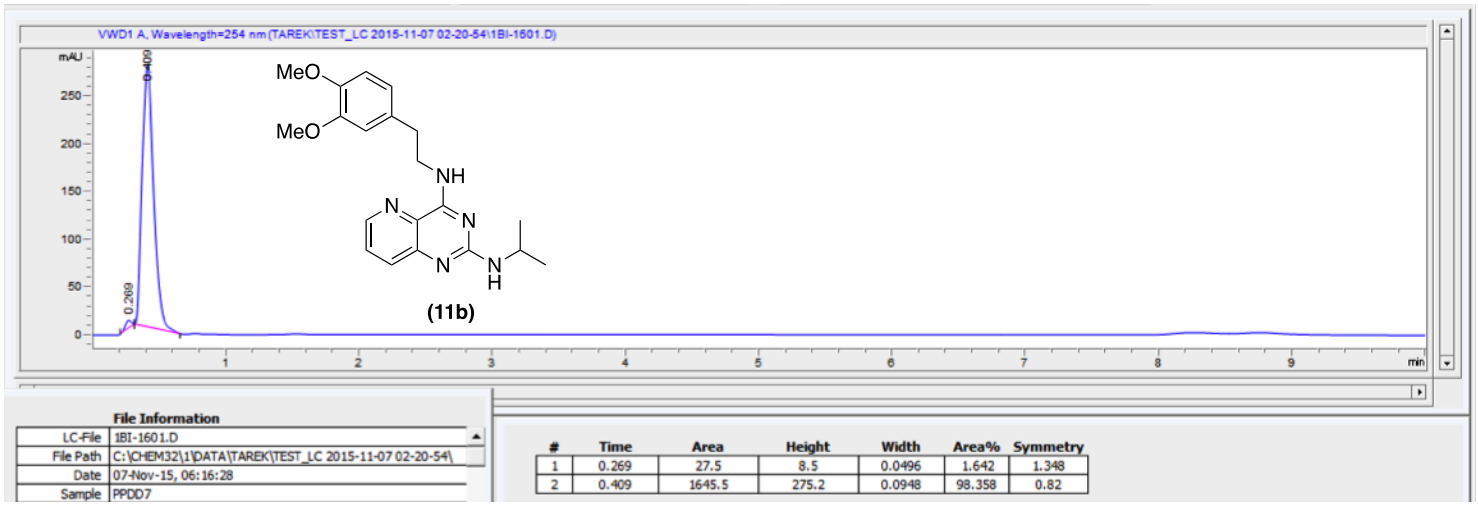
N^2-Cyclopropyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (10c).



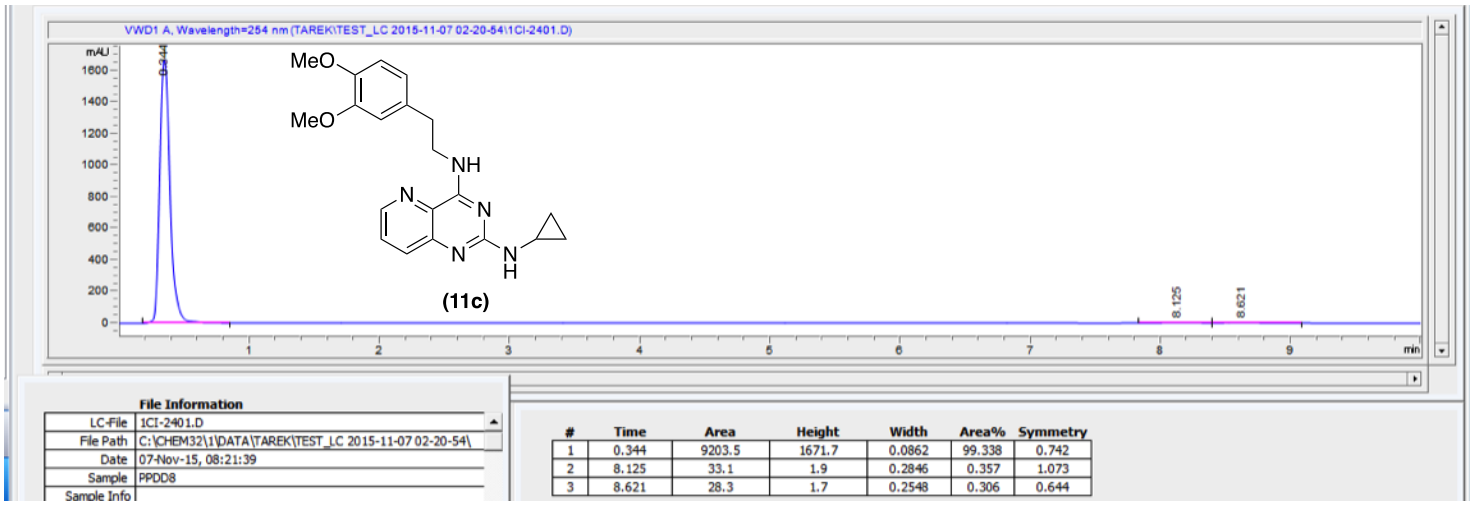
N^4-(3,4-Dimethoxyphenethyl)-N^2-propylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11a).



N^4-(3,4-Dimethoxyphenethyl)-N^2-isopropylpyrido[3,2-*d*]pyrimidine-2,4-diamine (11b).

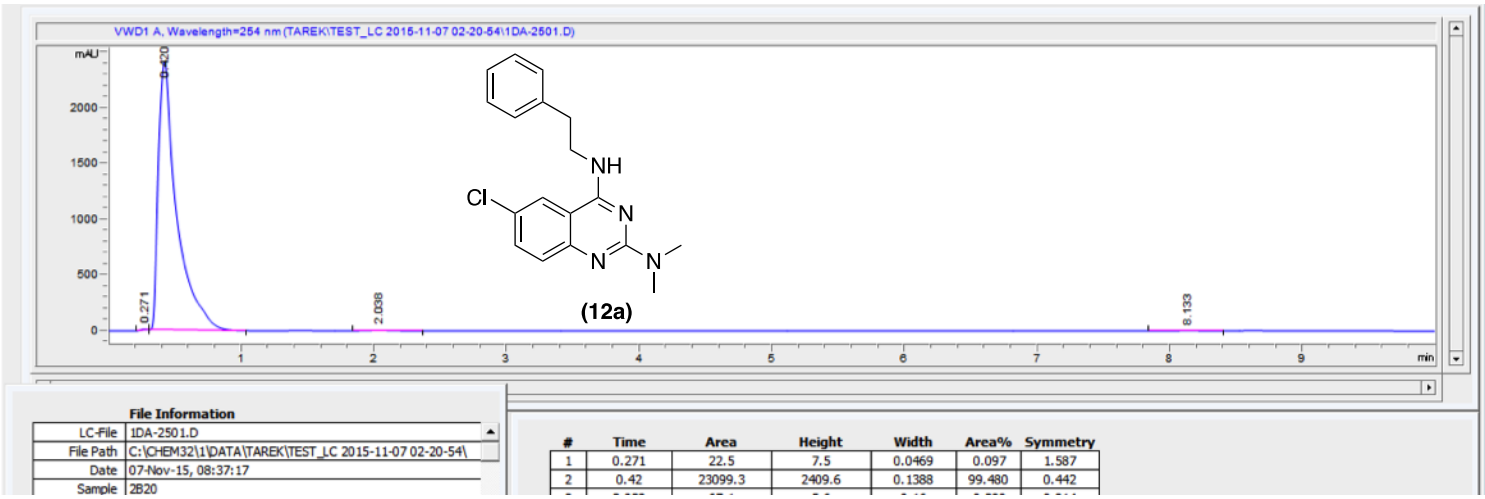


N^2-Cyclopropyl-N^4-(3,4-dimethoxyphenethyl)pyrido[3,2-*d*]pyrimidine-2,4-diamine (11c).



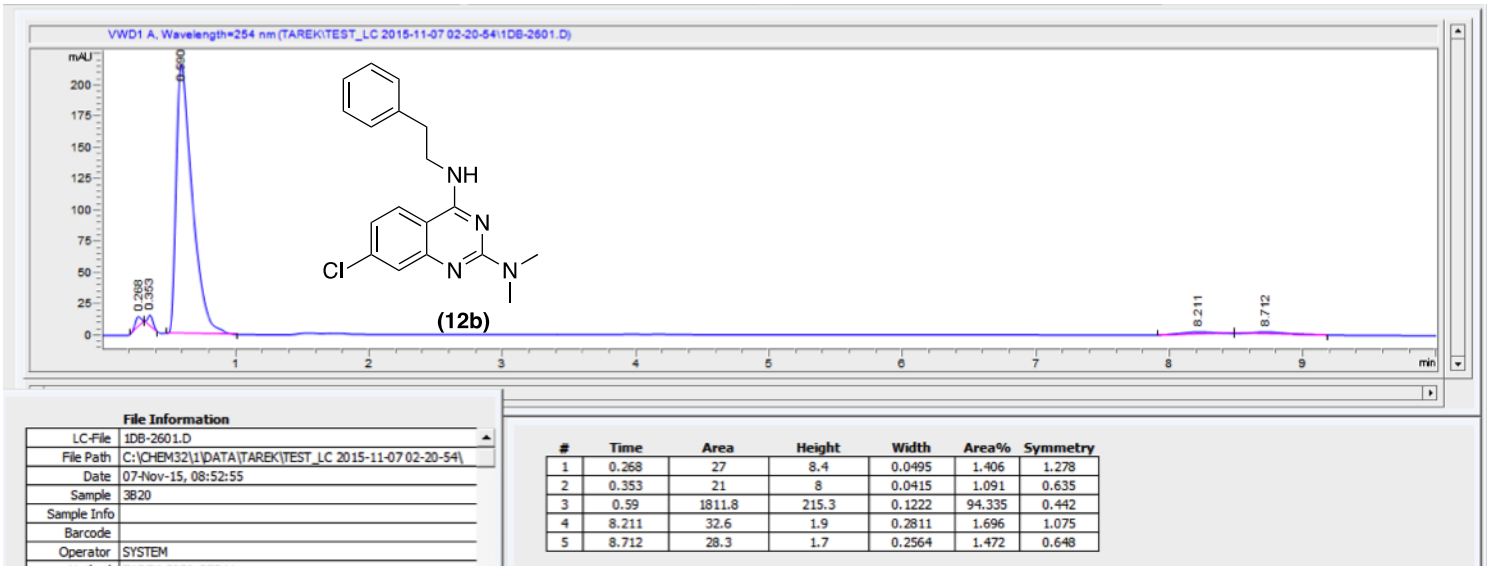
#	Time	Area	Height	Width	Area%	Symmetry
1	0.344	9203.5	1671.7	0.0862	99.338	0.742
2	8.125	33.1	1.9	0.2846	0.357	1.073
3	8.621	28.3	1.7	0.2548	0.306	0.644

6-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12a).



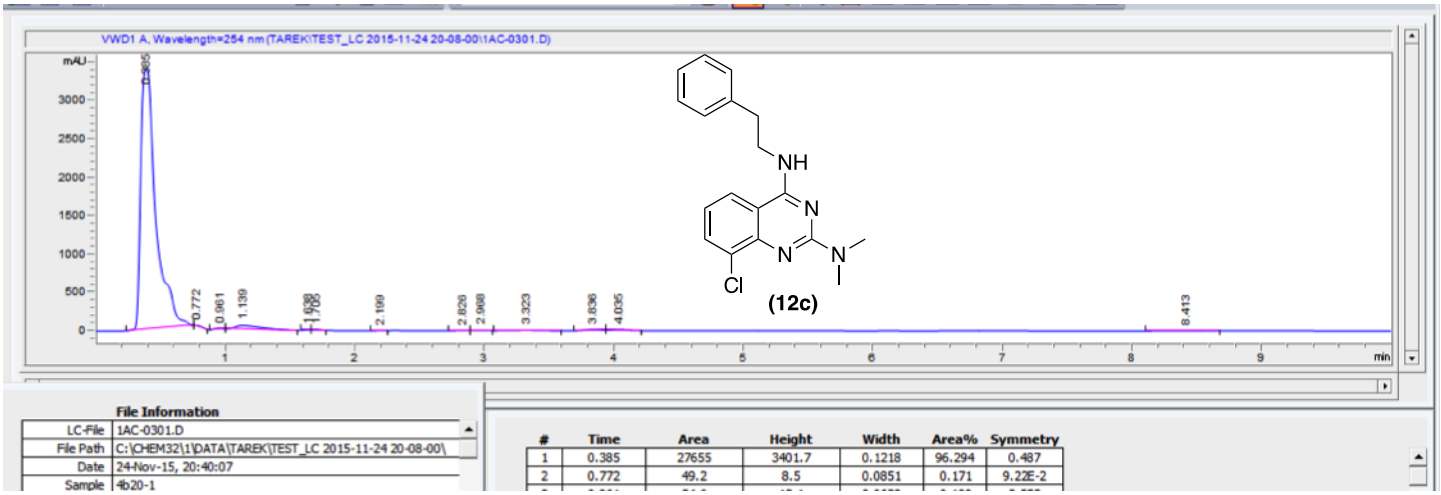
#	Time	Area	Height	Width	Area%	Symmetry
1	0.271	22.5	7.5	0.0469	0.097	1.587
2	0.42	23099.3	2409.6	0.1388	99.480	0.442

7-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12b).



#	Time	Area	Height	Width	Area%	Symmetry
1	0.268	27	8.4	0.0495	1.406	1.278
2	0.353	21	8	0.0415	1.091	0.635
3	0.59	1811.8	215.3	0.1222	94.335	0.442
4	8.211	32.6	1.9	0.2811	1.696	1.075
5	8.712	28.3	1.7	0.2564	1.472	0.648

8-Chloro-N^2,N^2-dimethyl-N^4-phenethylquinazoline-2,4-diamine (12c).

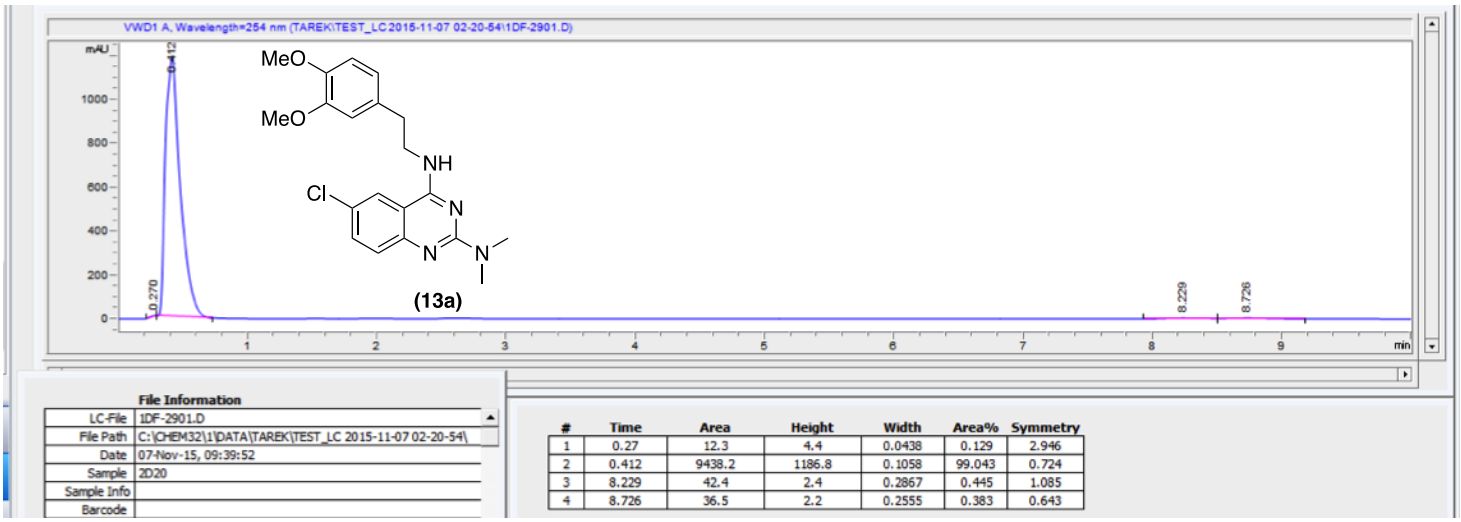


File Information

LC-File	1AC-0301.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-24 20-08-00\
Date	24-Nov-15, 20:40:07
Sample	4b20-1

#	Time	Area	Height	Width	Area%	Symmetry
1	0.385	27655	3401.7	0.1218	96.294	0.487
2	0.772	49.2	8.5	0.0851	0.171	9.22E-2

6-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13a).

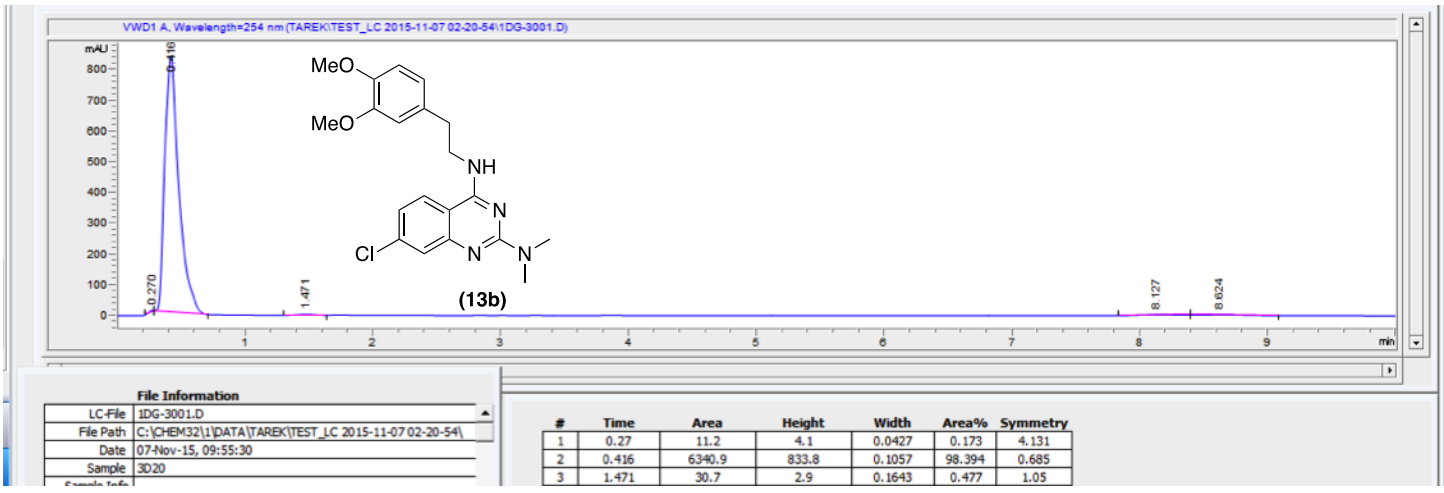


File Information

LC-File	1DF-2901.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 09:39:52
Sample	2D20
Sample Info	
Barcode	

#	Time	Area	Height	Width	Area%	Symmetry
1	0.27	12.3	4.4	0.0438	0.129	2.946
2	0.412	9438.2	1186.8	0.1058	99.043	0.724
3	8.229	42.4	2.4	0.2867	0.445	1.085
4	8.726	36.5	2.2	0.2555	0.383	0.643

7-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13b).

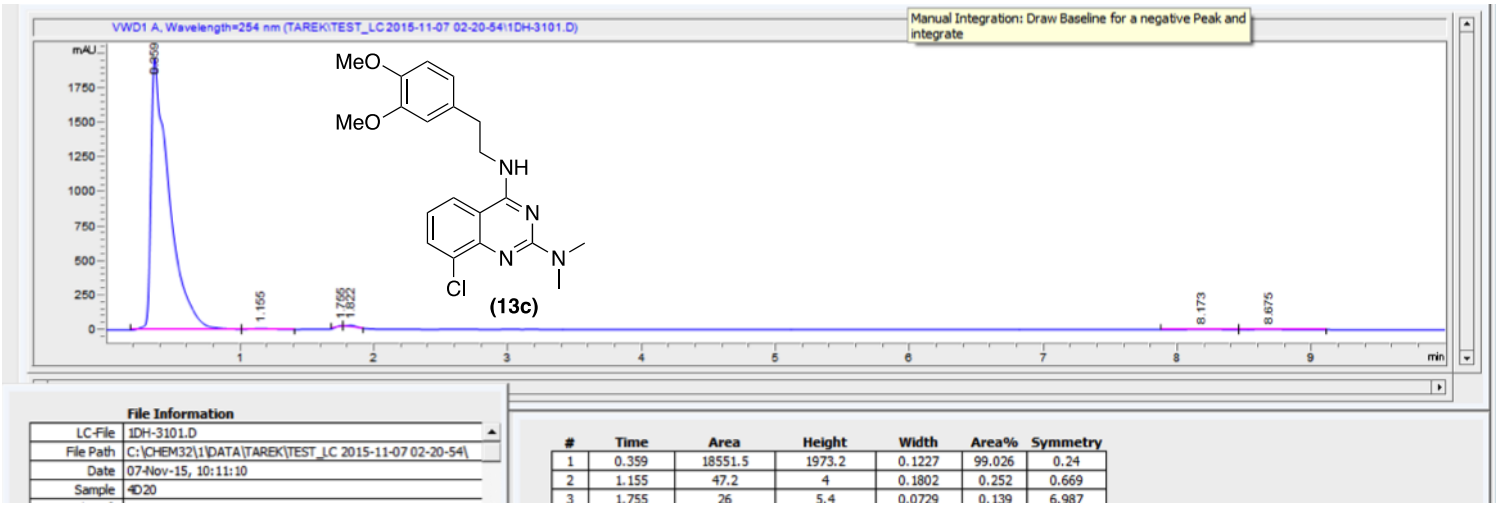


File Information

LC-File	1DG-3001.D
File Path	C:\CHEM32\1\DATA\TAREK\TEST_LC 2015-11-07 02-20-54\
Date	07-Nov-15, 09:55:30
Sample	3D20

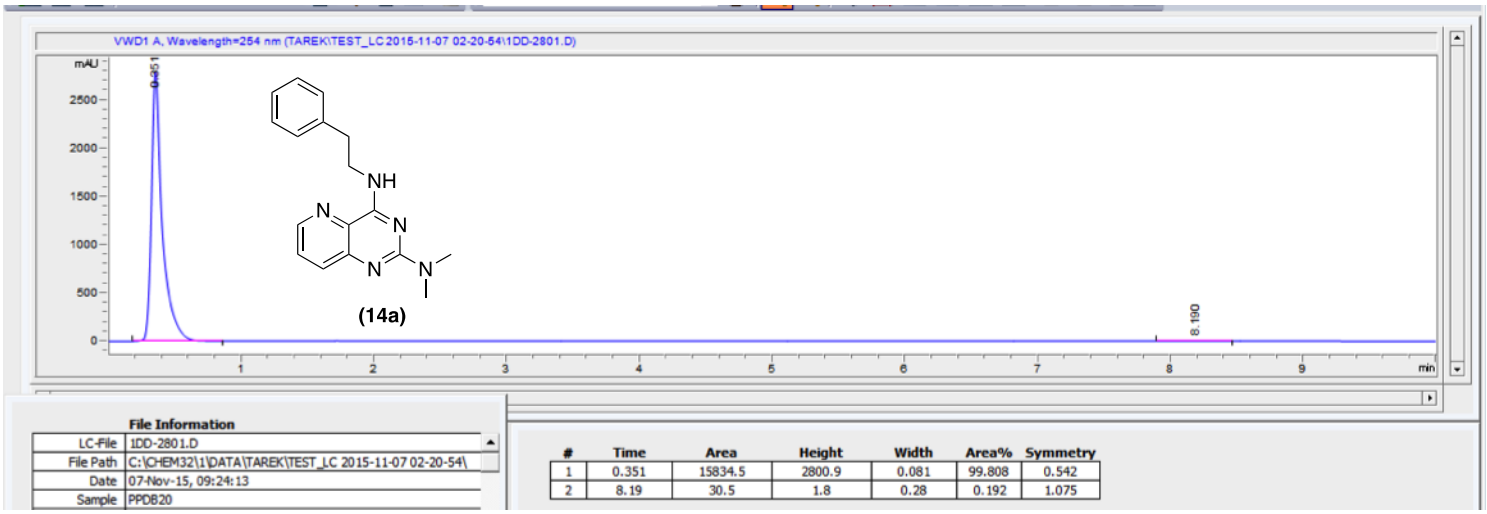
#	Time	Area	Height	Width	Area%	Symmetry
1	0.27	11.2	4.1	0.0427	0.173	4.131
2	0.416	6340.9	833.8	0.1057	98.394	0.685
3	1.471	30.7	2.9	0.1643	0.477	1.05

8-Chloro-N^4-(3,4-dimethoxyphenethyl)-N^2,N^2-dimethylquinazoline-2,4-diamine (13c).



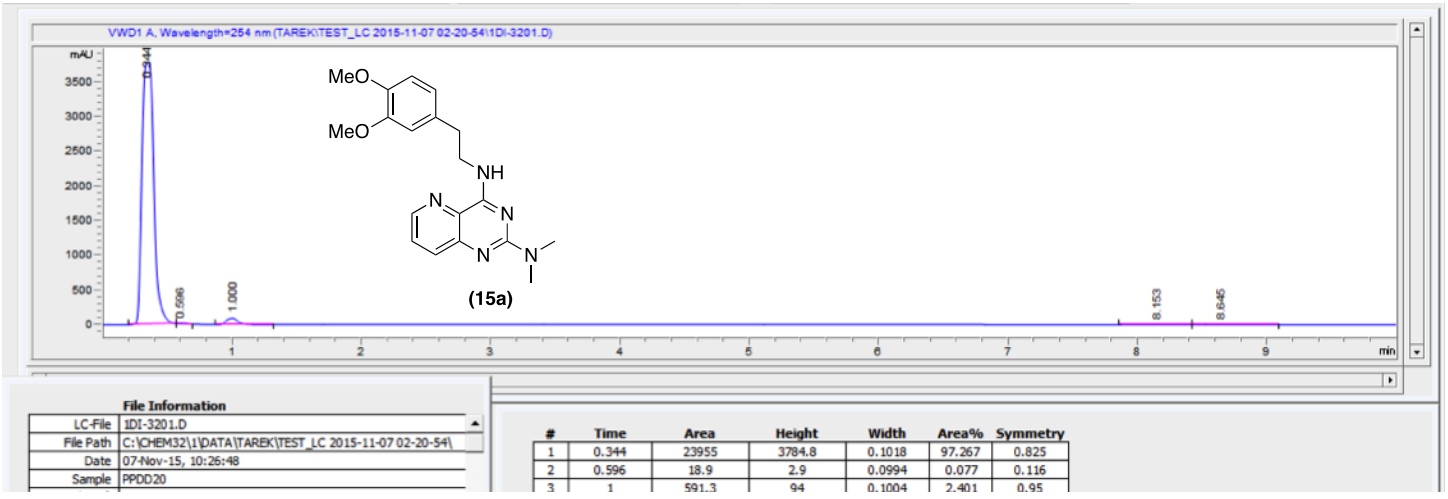
#	Time	Area	Height	Width	Area%	Symmetry
1	0.359	18551.5	1973.2	0.1227	99.026	0.24
2	1.155	47.2	4	0.1802	0.252	0.669
3	1.755	26	5.4	0.0729	0.139	6.987

***N^2,N^2*-Dimethyl-N^4-phenethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (14a).**



#	Time	Area	Height	Width	Area%	Symmetry
1	0.351	15834.5	2800.9	0.081	99.808	0.542
2	8.19	30.5	1.8	0.28	0.192	1.075

***N^4*-(3,4-Dimethoxyphenethyl)-N^2,N^2-dimethylpyrido[3,2-*d*]pyrimidine-2,4-diamine (15a).**



#	Time	Area	Height	Width	Area%	Symmetry
1	0.344	23955	3784.8	0.1018	97.267	0.825
2	0.596	18.9	2.9	0.0994	0.077	0.116
3	1	591.3	94	0.1004	2.401	0.95

7. Physicochemical properties of 8a–i, 9a–i, 10a–c, 11a–c, 12a–c, 13a–c, 14a and 15a

Compd	ClogP[a]	Molecular Volume (Å^3)[b]
8a	6.60	278.0
8b	6.38	274.4
8c	6.13	266.1
8d	6.60	271.0
8e	6.38	273.4
8f	6.13	264.1
8g	6.60	272.7
8h	6.38	275.1
8i	6.13	265.5
9a	6.26	325.8
9b	6.04	320.4
9c	5.79	320.4
9d	6.26	320.7
9e	6.04	324.5
9f	5.79	318.3
9g	6.26	324.8
9h	6.04	324.5
9i	5.79	315.2
10a	5.16	251.4
10b	4.94	255.9
10c	4.68	244.2
11a	4.81	308.3

11b	4.59	303.21
11c	4.34	299.1
12a	5.63	261.0
12b	5.63	259.0
12c	5.63	263.0
13a	5.29	311.1
13b	5.29	311.8
13c	5.29	310.4
14a	4.15	242.8
15a	3.81	290.5
Donepezil	4.59	321.7
Galantamine	1.18	>50

---

[a]ClogP values were determined using ChemDraw Professional 15.0. [b]Molecular volumes in $Å^3$ units were determined using Discovery Studio, Structure-Based Design software, BIOVIA Inc., USA.