

Supporting information

Structure -Activity Relationships of new 1*H*-Imidazo-[4,5-*c*]quinolin-4-amine Derivatives as Allosteric Enhancers of the A₃ Adenosine Receptor

Anikó Göblyös[?], Zhan-Guo Gao[†], Johannes Brussee[?], Roberto Connestari[?], Sabrina Neves Santiago[?], Kai Ye[?], Adriaan P. IJzerman*[?], Kenneth A. Jacobson*[†]

Contents:

- ¹H and ¹³C NMR data for selected compounds
- Elemental analyses

2-(2-Nitro-ethylideneamino)-benzoic acid (2).

¹H NMR (DMSO-*d*₆): d 6.76 (d, 2H, ? = 6.6 Hz, CH₂); 7.24 (t, 1H, ? = 6.6 Hz, CH); 7.54-7.82 (m, 2H, Ar); 8.02-8.12 (m, 2H, Ar); 12.09 (s, 1H, COOH).

3-Nitro-4-hydroxyquinoline (3).

¹H NMR (DMSO-*d*₆): d 7.54 (m, 1H, Ar); 7.76-7.86 (m, 2H, Ar); 8.27 (d, 1H, ? = 8.0 Hz, Ar); 9.21 (s, 1H, Ar).

3-Nitro-4-chloroquinoline (4).

¹H NMR (DMSO-*d*₆): d 7.94-8.11 (m, 2H, Ar); 8.25 (d, 1H, ? = 8.0 Hz, Ar); 8.47 (d, 1H, ? = 9.5 Hz, Ar); 9.42 (s, 1H, Ar).

3-Nitro-4-aminoquinoline (5).

¹H NMR (DMSO-*d*₆): d 7.50-7.66 (m, 1H, Ar); 7.81-7.92 (m, 2H, Ar); 8.59 (d, 1H, ? = 8.0 Hz, Ar); 9.03 (broad s, 2H, NH₂); 9.18 (s, 1H, Ar)

3,4-Diaminoquinoline (6).

¹H NMR (DMSO-*d*₆): d 4.73 (broad s, 2H, NH₂); 5.88 (s, 2H, NH₂); 7.16-7.37 (m, 2H, Ar); 7.64-7.70 (m, 1H, Ar); 7.98-8.03 (m, 1H, Ar); 8.22 (s, 1H, Ar). MS (ESI) *m/z* 161 (M + 1)⁺.

1*H*-Imidazo[4,5-*c*]quinoline (7).

¹H NMR (DMSO-*d*₆): d 7.67-7.72 (m, 2H, Ar); 8.18 (s, 1H, Ar); 8.29-8.34 (m, 1H, Ar); 8.61-8.65 (m, 1H, Ar); 8.93 (s, 1H, Ar).

2-Cyclobutyl-1*H*-imidazo[4,5-*c*]quinoline (8).

¹H NMR (CD₃OD): d 1.95-2.32 (m, 2H, CH₂); 2.44-2.66 (m, 4H, 2 × CH₂); 3.82-4.01 (m, 1H, CH); 7.58-7.71 (m, 2H, Ar); 8.01-8.11 (m, 1H, Ar); 8.32-8.38 (m, 1H, Ar); 9.01 (s, 1H, Ar).

2-Cyclopentyl-1*H*-imidazo[4,5-*c*]quinoline (9).

¹H NMR (CDCl₃): d 1.70-1.88 (m, 6H, 3 × CH₂); 2.03-2.22 (m, 2H, CH₂); 3.39-3.56 (m, 1H, CH); 7.53-7.66 (m, 2H, Ar); 8.21 (m, 2H, Ar); 9.18 (s, 1H, Ar).

2-Cyclohexyl-1*H*-imidazo[4,5-*c*]quinoline (10).

¹H NMR (CDCl₃): d 1.12-1.39 (m, 4H, 2 × CH₂); 1.66-1.77 (m, 4H, 2 × CH₂); 2.16-2.21 (m, 2H, CH₂); 3.01-3.13 (m, 1H, CH); 7.41-7.60 (m, 2H, Ar); 8.19 (d, 1H, ? = 8.0 Hz, Ar); 8.31 (d, 1H, ? = 8.0 Hz, Ar); 9.16 (s, 1H, Ar). MS (ESI) *m/z* 252 (M + 1)⁺.

2-Cycloheptyl-1*H*-imidazo[4,5-*c*]quinoline (11).

¹H NMR (CDCl₃): d 1.25-2.24 (m, 12H, 6 × CH₂); 3.20-3.32 (m, 1H, CH); 7.42-7.62 (m, 2H, Ar); 8.20 (d, 1H, ? = 8.0 Hz, Ar); 8.33 (d, 1H, ? = 8.0 Hz, Ar); 9.19 (s, 1H, Ar). MS (ESI) *m/z* 266 (M + 1)⁺.

2-(2-Furyl)-1*H*-imidazo[4,5-*c*]quinoline (12).

¹H NMR (DMSO-*d*₆): d 6.74 (s, 1H, Ar); 7.35 (d, 1H, ? = 3.7 Hz, Ar); 7.69-7.73 (m, 2H, Ar); 7.83 (s, 1H, Ar); 8.09 (s, 1H, Ar); 8.46 (s, 1H, Ar); 9.09 (s, 1H, Ar). ¹³C NMR (DMSO-*d*₆): d 111.4, 112.6, 120.7, 121.8, 126.5, 127.2, 129.5, 138.2, 143.6, 144.3, 145.1, 147.2, 155.4.

2-Pentyl-1*H*-imidazo[4,5-*c*]quinoline (13).

¹H NMR (DMSO-*d*₆): d 0.91 (t, 3H, *J* = 6, CH₃), 1.37-1.39 (m, 4H, 2 × CH₂), 1.83-1.91 (m, 2H, CH₂), 1.93-2.30 (t, 2H, *J* = 8, CH₂), 7.64-7.69 (m, 2H, Ar); 8.08-8.13 (m, 1H, Ar); 8.28-8.42 (m, 1H, Ar); 9.12 (s, 1H, Ar).

1*H*-Imidazo[4,5-*c*]quinolin-5-oxide (14).

¹H NMR (CD₃OD): d 7.41-7.61 (m, 1H, Ar); 7.87-7.96 (m, 2H, Ar); 8.45-8.53 (m, 1H, Ar); 8.75-8.80 (m, 1H, Ar); 9.16 (s, 1H, Ar).

2-Cyclobutyl-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (15).

¹H NMR (DMSO-*d*₆): d 1.95-2.22 (m, 2H, CH₂); 2.38-2.52 (m, 4H, 2 × CH₂); 3.73-3.84 (m, 1H, CH); 7.74-7.91 (m, 2H, Ar); 8.55-8.66 (m, 1H, Ar); 8.70-8.74 (m, 1H, Ar); 8.99 (s, 1H, Ar).

2-Cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (16).

¹H NMR (CD₃OD): d 1.74-2.13 (m, 6H, 3 × CH₂); 2.18-2.39 (m, 2H, CH₂); 3.38-3.54 (m, 1H, CH); 7.29-7.42 (m, 2H, Ar); 7.83-7.92 (m, 2H, Ar); 9.03 (s, 1H, Ar).

2-Cyclohexyl-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (17).

¹H NMR (CD₃OD): d 1.17-2.19 (m, 10H, 5 × CH₂); 2.97-3.12 (m, 1H, CH); 7.79-7.93 (m, 2H, Ar); 8.42-8.46 (m, 1H, Ar); 8.69-8.77 (m, 1H, Ar); 9.02 (s, 1H, Ar). ¹³C NMR (CD₃OD): d 26.6, 26.8, 32.5, 39.7, 120.8, 123.1, 128.6, 129.9, 130.1, 130.3, 132.5, 138.0, 142.6, 164.1, 166.0, 170.9, 173.8.

2-Cycloheptyl-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (18).

¹H NMR (CD₃OD): d 1.67-2.11 (m, 12H, 6 × CH₂); 3.05-3.31 (m, 1H, CH); 7.78-7.90 (m, 2H, Ar); 8.28-8.48 (m, 1H, Ar); 8.62-8.73 (m, 1H, Ar); 9.00 (s, 1H, Ar). ¹³C NMR (CD₃OD): d 25.0, 26.4, 32.1, 39.2, 117.4, 118.2, 120.6, 126.2, 127.4, 127.8, 128.2, 130.0, 130.6, 132.3, 132.6, 135.2, 162.7, 166.5.

2-(2-Furyl)-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (19).

¹H NMR (CD₃OD): d 6.74-6.77 (m, 1H, Ar); 7.37-7.47 (m, 2H, Ar); 7.87-7.96 (m, 2H, Ar); 8.55-8.60 (m, 1H, Ar); 8.74-8.79 (m, 1H, Ar); 9.07 (s, 1H, Ar).

2-Pentyl-1*H*-imidazo[4,5-*c*]quinolin-5-oxide (20).

¹H NMR (CD₃OD): d 0.88-0.94 (t, 3H, CH₃, J = 6 Hz); 1.26-1.39 (m, 4H, 2 × CH₂); 1.81-1.88 (m, 2H, CH₂); 2.88-2.95 (t, 2H, CH₂, J = 8 Hz); 7.44-7.58 (m, 2H, Ar); 7.90-8.09 (m, 2H, Ar); 9.03 (s, 1H, Ar).

4-Chloro-1*H*-imidazo[4,5-*c*]quinoline (21).

¹H NMR (CDCl₃): d 8.46-8.56 (m, 2H, Ar); 8.82-8.87 (m, 1H, Ar); 9.14-9.19 (m, 1H, Ar); 9.35 (s, 1H, Ar); 10.16 (broad s, 1H, NH). MS (ESI) *m/z* 204 (M + 1)⁺, 206 (M + 3)⁺.

4-Chloro-2-cyclobutyl-1*H*-imidazo[4,5-*c*]quinoline (22).

¹H NMR (CDCl₃): d 2.06-2.24 (m, 2H, CH₂); 2.52-2.66 (m, 4H, 2 × CH₂); 3.87-4.00 (m, 1H, CH); 7.56-7.68 (m, 2H, Ar); 8.02-8.06 (m, 1H, Ar); 8.30-8.32 (m, 1H, Ar).

4-Chloro-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinoline (23).

¹H NMR (CD₃OD): d 1.81-2.22 (m, 6H, 3 × CH₂); 2.25-2.31 (m, 2H, CH₂); 3.40-3.51 (m, 1H, CH); 7.63-7.74 (m, 2H, Ar); 8.00-8.03 (m, 1H, Ar); 8.33-8.38 (m, 1H, Ar).

4-Chloro-2-cyclohexyl-1*H*-imidazo[4,5-*c*]quinoline (24).

¹H NMR (CD₃OD): d 1.37-2.17 (m, 10H, 5 × CH₂); 3.03-3.18 (m, 1H, CH); 7.68-7.71 (m, 2H, Ar); 8.00-8.08 (m, 1H, Ar); 8.32-8.40 (m, 1H, Ar). MS (ESI) *m/z* 286 (M + 1)⁺, 288 (M + 3)⁺.

4-Chloro-2-cycloheptyl-1*H*-imidazo[4,5-*c*]quinoline (25).

¹H NMR (CD₃OD): d 1.73-2.13 (m, 12H, 6 × CH₂); 3.21-3.40 (m, 1H, CH); 7.63-7.79 (m, 2H, Ar); 7.97-8.05 (m, 1H, Ar); 8.29-8.38 (m, 1H, Ar). MS (ESI) *m/z* 300 (M + 1)⁺, 302 (M + 3)⁺.

4-Chloro-2-(2-furyl)-1*H*-imidazo[4,5-*c*]quinoline (26).

¹H NMR (CD₃OD): 6.72-6.75 (m, 1H, Ar); 7.40-7.43 (m, 1H, Ar); 7.63-7.75 (m, 2H, Ar); 7.83-7.88 (m, 1H, Ar); 7.98-8.01 (m, 1H, Ar); 8.36-8.40 (m, 1H, Ar). MS (ESI) *m/z* 270 (M + 1)⁺, 272 (M + 3)⁺.

4-Chloro-2-pentyl-1*H*-imidazo[4,5-*c*]quinoline (27).

¹H NMR (CDCl₃): d 0.65-0.72 (t, 3H, CH₃, J = 6 Hz); 1.14-1.21 (m, 4H, 2 × CH₂); 1.61-1.72 (m, 2H, CH₂); 2.76-2.84 (t, 2H, CH₂, J = 8 Hz); 7.33-7.47 (m, 2H, Ar); 7.76-7.80 (m, 1H, Ar); 7.95-8.15 (m, 1H, Ar). MS (ESI) *m/z* 274 (M + 1)⁺,

N-Phenyl-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (28).

¹H NMR (CDCl₃): d 1.80-2.27 (m, 8H, 4 × CH₂); 3.31-3.55 (m, 1H, CH); 7.00-7.09 (m, 1H, Ar); 7.15-7.29 (m, 4H, Ar); 7.49-7.56 (m, 1H, Ar); 7.78 (d, 1H, ? = 6.6 Hz, Ar); 7.96-8.09 (m, 2H, Ar). ¹³C NMR 750 MHz (CDCl₃): d 24.9, 31.7, 38.9, 114.7, 117.9, 118.1, 118.3, 119.2, 119.8, 120.9, 121.9, 123.6, 124.1, 126.1, 126.4, 126.5, 126.7, 128.1, 128.2, 128.9, 133.5, 140.5, 143.3, 146.6, 156.3, 159.1. MS (ESI) *m/z* 329 (M + 1)⁺.

N-(4-Methyl-phenyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (29).

¹H NMR (CDCl₃): d 1.55-2.15 (m, 8H, 4 × CH₂); 2.24 (s, 3H, CH₃); 3.21-3.33 (m, 1H, CH); 7.07 (d, 2H, Ar); 7.21-7.28 (m, 1H, Ar); 7.46 (m, 1H Ar); 7.74-7.87 (m, 4H, Ar). ¹³C NMR 400 MHz (CDCl₃): d 20.7, 25.4, 29.7, 32.4, 39.6, 62.5, 115.8, 120.7, 122.6, 126.7, 127.3, 129.4, 132.4, 137.1, 143.8, 147.5, 157.1. MS (ESI) *m/z* 343 (M + 1)⁺.

N-(4-Methoxy-phenyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (30).

¹H NMR (CDCl₃): d 1.71-2.29 (m, 8H, 4 × CH₂); 3.22-3.38 (m, 1H, CH); 3.65 (s, 3H, OCH₃); 6.80-6.84 (m, 2H, Ar); 7.26 (m, 1H, Ar); 7.46 (m, 1H, Ar); 7.76-7.93 (m, 4H, Ar). ¹³C NMR 400 MHz (CDCl₃): d 25.5, 32.5, 39.6, 53.4, 55.4, 114.2, 114.8, 116.5, 120.4, 122.1, 122.4, 127.0, 127.3, 133.1, 144.0, 147.8, 155.4, 156.7. MS (ESI) *m/z* 359 (M + 1)⁺.

N-(3,4-Dichloro-phenyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (31).

¹H NMR (CDCl₃): d 1.68-2.29 (m, 8H, 4 × CH₂); 3.29-3.43 (m, 1H, CH); 7.33 (m, 2H, Ar); 7.54 (m, 1H, Ar); 7.78 (m, 2H, Ar); 7.99 (d, 1H, δ = 8.0 Hz, Ar); 8.44 (s, 1H, Ar); 9.62 (broad s, 1H, NH). MS (ESI) *m/z* 397 (M + 1)⁺, 399 (M + 3)⁺, 401 (M + 5)⁺.

N-(4-Chloro-phenyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (32).

¹H NMR (CDCl₃): d 1.67-2.25 (m, 8H, 4 × CH₂); 3.28-3.43 (m, 1H, CH); 7.27-7.39 (m, 3H, Ar); 7.49-7.59 (m, 1H, Ar); 7.71-7.79 (m, 1H, Ar); 7.97 (m, 3H, Ar); 8.46 (broad s, 1H, NH). MS (ESI) *m/z* 363 (M + 1)⁺, 365 (M + 3)⁺.

N-(3-Hydroxymethyl-phenyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (33).

¹H NMR (CDCl₃/ CD₃OD): d 1.63-2.16 (m, 8H, 4 × CH₂); 3.23-3.24 (m, 1H, CH); 3.89 (s, 2H, CH₂); 6.93 (d, 1H, Ar); 7.18-7.28 (m, 3H, Ar); 7.39 (m, 1H, Ar); 7.72-7.92 (m, 3H, Ar). MS (ESI) *m/z* 359 (M + 1)⁺.

N-([3,4-*c*]Indan-5-yl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (34).

¹H NMR (CDCl₃): d 1.15-1.34 (m, 2H, CH₂); 1.65-2.19 (m, 8H, 4 × CH₂); 2.76 (t, 4H, δ = 7.3 Hz, 2 × CH₂); 3.24-3.27 (m, 1H, CH); 7.06 (d, 1H, Ar); 7.22-7.29 (m, 1H, Ar); 7.40-7.49 (m, 2H, Ar); 7.73 (s, 1H, Ar); 7.85-7.96 (m, 2H, Ar). MS (ESI) *m/z* 369 (M + 1)⁺.

N-(1*H*-indazol-6-yl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (35).

¹H NMR (CD₃OD): d 1.70-2.38 (m, 8H, 4 × CH₂); 3.23-3.50 (m, 1H, CH); 7.31-7.38 (m, 1H, Ar); 7.47-7.60 (m, 2H, Ar); 7.71-7.75 (m, 1H, Ar); 7.82-7.86 (m, 1H, Ar); 8.01-8.08 (m, 2H, Ar); 8.68 (s, 1H, Ar). MS (ESI) *m/z* 369 (M + 1)⁺.

N-(4-Methoxy-benzyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (36).

¹H NMR (CD₃OD): d 1.72-2.30 (m, 8H, 4 × CH₂); 3.26-3.41 (m, 1H, CH); 3.77 (s, 3H, OCH₃); 4.76 (s, 2H, CH₂); 6.87-6.92 (m, 2H, Ar); 7.23-7.49 (m, 4H, Ar); 7.78 (d, 1H, δ = 8.8 Hz, Ar); 8.00 (d, 1H, δ = 7.3 Hz, Ar). MS (ESI) *m/z* 373 (M + 1)⁺.

N-(1*H*-Indol-6-yl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (37).

¹H NMR (CD₃OD): d 1.79-2.29 (m, 8H, 4 × CH₂); 3.30-3.46 (m, 1H, CH); 6.45 (d, 1H, δ = 2.9 Hz, Ar); 7.23-7.50 (m, 5H, Ar); 7.77 (d, 1H, δ = 7.8 Hz, Ar); 8.01 (d, 1H, δ = 8.0 Hz, Ar); 8.20 (s, 1H, Ar). MS (ESI) *m/z* 368 (M + 1)⁺.

N-(Benzyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (38).

¹H NMR (CDCl₃): d 1.50-2.11 (m, 8H, 4 × CH₂); 3.14-3.31 (m, 1H, CH); 4.85 (s, 2H, CH₂); 6.25 (broad s, 2H, 2 × NH); 7.08-7.20 (m, 6H, Ar); 7.38 (t, 1H, δ = 8.8 Hz, Ar); 7.87 (d, 1H, δ = 8.8 Hz, Ar); 8.09 (d, 1H, δ = 8.0 Hz, Ar). ¹³C NMR (CDCl₃): d 25.3, 32.3, 39.7, 45.4, 116.1, 121.3, 122.2, 125.3, 127.0, 127.4, 128.1, 138.1, 143.3, 144.0, 149.7, 157.4, 160.6. MS (ESI) *m/z* 343 (M + 1)⁺.

N-(Phenethyl)-2-cyclopentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (39).

¹H NMR (CD₃OD): d 1.75-2.21 (m, 8H, 4 × CH₂); 3.02 (t, 2H, δ = 8.0 Hz, CH₂); 3.30-3.38 (m, 1H, CH); 3.89 (t, 2H, δ = 8.0 Hz, CH₂); 7.15-7.45 (m, 7H, Ar); 7.76 (d, 1H, δ = 8.8 Hz, Ar); 7.97 (d, 1H, δ = 6.3 Hz, Ar). ¹³C NMR (CD₃OD): d 27.6, 29.0, 34.9, 41.6, 116.8, 119.1, 121.1, 121.6, 124.2, 125.1, 128.2, 128.3, 131.2, 133.3, 141.7, 144.4, 147.3, 160.1. MS (ESI) *m/z* 357 (M + 1)⁺.

***N*-(3,4-Dichloro-phenyl)-2-cycloheptyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (40).**

¹H NMR (CDCl₃/CD₃OD 9/1, v/v): d 1.62-2.00 (m, 10H, 5 × CH₂); 2.17-2.24 (m, 2H, CH₂); 3.09-3.23 (m, 1H, CH); 7.32-7.39 (m, 2H, Ar); 7.50-7.58 (m, 1H, Ar); 7.71-7.85 (m, 2H, Ar); 7.98 (d, 1H, δ = 8.0 Hz, Ar); 8.41 (s, 1H, Ar). ¹³C NMR (DMSO-*d*₆): d 26.2, 27.7, 33.4, 40.2, 115.2, 119.3, 120.2, 121.0, 122.0, 122.9, 127.0, 128.3, 130.1, 130.6, 134.2, 141.6, 142.7, 146.8, 158.6. MS (ESI) *m/z* 425 (M + 1)⁺, 427 (M + 3)⁺.

***N*-(3,4-Dichloro-phenyl)-2-(2-furyl)-1*H*-imidazo[4,5-*c*]quinolin-4-amine (41).**

¹H NMR (CD₃OD): d 6.64-6.67 (m, 1H, Ar); 7.10 (d, 1H, δ = 3.7 Hz, Ar); 7.21-7.44 (m, 4H, Ar); 7.65-7.72 (m, 2H, Ar); 7.95 (d, 1H, δ = 8.0 Hz, Ar); 8.43-8.44 (m, 1H, Ar). ¹³C NMR (DMSO-*d*₆): d 110.6, 112.6, 115.3, 119.5, 120.4, 121.5, 122.2, 123.2, 127.1, 127.6, 128.2, 130.1, 130.3, 130.6, 134.6, 141.5, 142.3, 143.2, 144.7, 145.1, 146.9. MS (ESI) *m/z* 395 (M + 1)⁺, 397 (M + 3)⁺.

***N*-(3,4-Dichloro-phenyl)-2-cyclobutyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (42).**

¹H NMR (CD₃OD): d 2.00-2.22 (m, 2H, CH₂); 2.42-2.56 (m, 4H, 2 × CH₂); 3.72-3.89 (m, 1H, CH); 7.26-7.33 (m, 2H, Ar); 7.47-7.54 (m, 1H, Ar); 7.64-7.69 (m, 1H, Ar); 7.88-7.96 (m, 2H, Ar); 8.30 (s, 1H, Ar). MS (ESI) *m/z* 383 (M + 1)⁺, 385 (M + 3)⁺.

***N*-(3,4-Dichloro-phenyl)-2-cyclohexyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (43).**

¹H NMR (CD₃OD): d 1.40-2.00 (m, 8H, 4 × CH₂); 2.15-2.28 (m, 2H, CH₂); 2.95-3.07 (m, 1H, CH); 7.34-7.56 (m, 4H, Ar); 7.77-7.88 (m, 2H, Ar); 8.52 (s, 1H, Ar). ¹³C NMR (DMSO-*d*₆): d 25.6, 31.6, 38.2, 115.5, 119.2, 120.1, 121.1, 122.0, 123.0, 127.0, 130.1, 130.6, 134.1, 141.6, 142.7, 146.7, 153.2, 157.5. MS (ESI) *m/z* 411 (M + 1)⁺, 413 (M + 3)⁺, 415 (M + 5)⁺.

***N*-(3,4-Dichloro-phenyl)-1*H*-imidazo[4,5-*c*]quinolin-4-amine (44).**

¹H NMR (CDCl₃): d 7.23-7.36 (m, 2H, Ar); 7.39-7.43 (m, 1H, Ar); 7.62-7.72 (m, 1H, Ar); 7.65-7.95 (m, 3H, Ar); 8.32 (s, 1H, Ar). MS (ESI) *m/z* 329 (M + 1)⁺, 331 (M + 3)⁺.

***N*-(3,4-Dichloro-phenyl)-2-pentyl-1*H*-imidazo[4,5-*c*]quinolin-4-amine (45).**

¹H NMR (CDCl₃): d 0.82-0.97 (m, 3H, CH₃); 1.39-1.51 (m, 2H, CH₂); 1.86-2.01 (m, 4H, 2 × CH₂); 2.98 (t, 2H, δ = 8.0 Hz, CH₂); 7.33-7.41 (m, 2H, Ar); 7.52-7.60 (m, 1H, Ar); 7.74-7.81 (m, 2H, Ar); 7.99 (d, 1H, δ = 8.0 Hz, Ar); 8.48 (s, 1H, Ar). MS (ESI) *m/z* 399 (M + 1)⁺, 401 (M + 3)⁺.

Elemental analyses

Compounds	Theoretical in %				Experimental in %				Deviation in %				Molecular Formula
	C	H	N		C	H	N	S	C	H	N	S	
28	74.97	6.44	16.27		74.60	6.72	16.61		-0.37	0.28	0.34		$\text{C}_{21}\text{H}_{20}\text{N}_4 \bullet 0.5\text{CH}_3\text{OH}$
29	70.71	6.87	14.99		70.81	7.23	14.62		0.10	0.36	-0.37		$\text{C}_{22}\text{H}_{22}\text{N}_4 \bullet 1.7\text{H}_2\text{O}$
30	70.75	6.71	14.35		70.73	6.40	17.73		-0.02	-0.31	0.38		$\text{C}_{22}\text{H}_{22}\text{N}_4\text{O} \bullet 1\text{CH}_3\text{OH}$
31	58.21	5.12	12.93		57.97	5.36	12.90		-0.24	0.24	-0.03		$\text{C}_{21}\text{H}_{18}\text{Cl}_2\text{N}_4 \bullet 2\text{H}_2\text{O}$
32	64.69	5.69	14.37		64.67	5.42	14.23		-0.02	-0.27	-0.14		$\text{C}_{21}\text{H}_{19}\text{ClN}_4 \bullet 1.5\text{H}_2\text{O}$
33	72.17	6.46	14.96		72.21	6.72	15.32		0.04	0.26	0.36		$\text{C}_{22}\text{H}_{22}\text{N}_4\text{O} \bullet 0.5\text{CH}_3\text{OH}$
34	73.89	6.82	14.36		73.73	6.89	14.11		-0.16	0.07	-0.25		$\text{C}_{24}\text{H}_{24}\text{N}_4 \bullet 1.2\text{H}_2\text{O}$
35	66.82	5.86	21.25		67.00	5.86	21.32		0.18	0.00	0.07		$\text{C}_{22}\text{H}_{20}\text{N}_6 \bullet 1.5\text{H}_2\text{O}$
36	74.17	6.49	15.04		74.48	6.74	14.75		0.31	0.25	-0.29		$\text{C}_{23}\text{H}_{24}\text{N}_4\text{O}$
37	75.18	5.76	19.06		75.03	5.57	18.92		-0.15	-0.19	-0.14		$\text{C}_{23}\text{H}_{21}\text{N}_5$
38	77.16	6.48	16.36		77.12	6.31	16.24		-0.04	-0.17	-0.12		$\text{C}_{22}\text{H}_{22}\text{N}_4$
39	75.78	7.04	15.04		75.97	6.89	15.36		0.19	-0.15	0.32		$\text{C}_{23}\text{H}_{24}\text{N}_4 \bullet 0.5\text{CH}_3\text{OH}$
40	61.07	5.57	12.39		61.21	5.62	12.31		0.14	0.05	-0.08		$\text{C}_{23}\text{H}_{22}\text{Cl}_2\text{N}_4 \bullet 1.5\text{H}_2\text{O}$
41	59.42	3.24	13.86		59.13	3.34	13.75		-0.29	0.10	-0.11		$\text{C}_{20}\text{H}_{12}\text{Cl}_2\text{N}_4\text{O} \bullet 0.5\text{H}_2\text{O}$
42	60.73	4.85	13.49		60.77	4.81	13.83		0.04	-0.04	0.34		$\text{C}_{20}\text{H}_{16}\text{Cl}_2\text{N}_4 \bullet 1\text{CH}_3\text{OH}$
43	59.07	5.41	12.52		58.81	5.34	12.21		-0.26	-0.07	-0.31		$\text{C}_{22}\text{H}_{20}\text{Cl}_2\text{N}_4 \bullet 2\text{H}_2\text{O}$
44	55.35	3.48	16.14		54.98	3.67	16.15		-0.37	0.19	0.01		$\text{C}_{16}\text{H}_{10}\text{Cl}_2\text{N}_4 \bullet 1\text{H}_2\text{O}$
45	63.16	5.05	14.03		62.83	5.44	14.13		-0.33	0.39	0.10		$\text{C}_{21}\text{H}_{20}\text{Cl}_2\text{N}_4$