

Supporting Information

Evaluation of 3-Carboxy-4-(1H)-Quinolones as Inhibitors of Human Protein Kinase CK2

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Table 5. Atom-atom contacts between inhibitor **7** and amino acid residues of the CK2 active site at distance cut-off 4.4 Å.

#	Ligand	Atom	Residue	Atom	Distance	
1	7	C50	Trp	176	CD1	4.3149
2	7	C50	Asp	175	CA	3.7324
3	7	C00	Asp	175	CA	4.0928
4	7	C10	Asp	175	CA	4.1049
5	7	C20	Ile	174	CD	3.8378
6	7	C60	Ile	174	CD	4.0257
7	7	C80	Ile	174	CD	4.2283
8	7	C70	Ile	174	CD	4.2263
9	7	C40	Ile	174	CD	4.0125
10	7	C	Ile	174	CD	3.8114
11	7	C10	Ile	174	CD	4.2562
12	7	C00	Ile	174	CG2	4.3262
13	7	C30	Ile	174	CG2	3.4635
14	7	C20	Ile	174	CG2	3.8765
15	7	CL0	Ile	174	CG2	4.1054
16	7	C60	Ile	174	CG2	4.2396
17	7	C00	Ile	174	CB	3.9962
18	7	C30	Ile	174	CB	3.6245
19	7	C20	Ile	174	CB	4.0079
20	7	C10	Ile	174	CB	4.3634
21	7	C00	Ile	174	CA	4.3087
22	7	C30	Ile	174	CA	4.1231
23	7	CL0	Met	163	CE	4.2478
24	7	C80	Met	163	CE	4.2751
25	7	CL0	Met	163	SD	3.617
26	7	C60	Met	163	SD	4.2433
27	7	CL0	Val	116	CG1	3.7187
28	7	C50	Phe	113	CZ	3.5775
29	7	C00	Phe	113	CZ	3.6837
30	7	C30	Phe	113	CZ	3.6514
31	7	C50	Phe	113	CE2	4.106
32	7	C00	Phe	113	CE2	3.7415
33	7	C30	Phe	113	CE2	3.7182
34	7	C10	Phe	113	CE2	4.1773
35	7	C50	Phe	113	CE1	4.0754
36	7	C00	Phe	113	CE1	4.1984
37	7	C30	Phe	113	CE1	3.7538
38	7	C00	Phe	113	CD2	4.1951
39	7	C30	Phe	113	CD2	3.7532
40	7	C20	Phe	113	CD2	4.1793
41	7	C30	Phe	113	CD1	3.8152
42	7	C30	Phe	113	CG	3.8364
43	7	C50	Ile	95	CG2	4.2645
44	7	C30	Ile	95	CG2	3.6297
45	7	C30	Ile	95	CG1	3.5426

46	7	C30	Ile	95	CB	4.0755
47	7	C50	Leu	85	CD1	4.1491
48	7	C50	Glu	81	CD	4.2534
49	7	CL	Lys	68	CE	4.0706
50	7	C10	Lys	68	CD	4.2815
51	7	CL0	Val	66	CG2	4.2907
52	7	CL0	Val	66	CG1	3.9635
53	7	C60	Val	66	CG1	3.8703
54	7	C80	Val	66	CG1	3.8339
55	7	CL0	Val	66	CB	4.1486

Table 6. Atom-atom contacts between inhibitor **9** and amino acid residues of the CK2 active site at distance cut-off 4.4 Å.

#	Ligand	Atom	Residue	Atom	Distance	
1	9	C40	Asp	175	CG	3.38
2	9	C	Asp	175	CG	4.4
3	9	C40	Asp	175	CB	4.29
4	9	C40	Asp	175	CA	4.22
5	9	C40	Ile	174	CD	3.82
6	9	C	Ile	174	CD	3.56
7	9	C30	Ile	174	CD	4.1
8	9	C10	Ile	174	CD	4.17
9	9	C00	Ile	174	CD	3.6
10	9	C	Ile	174	CG2	4.25
11	9	C30	Ile	174	CG2	3.66
12	9	C	Ile	174	CG1	4.28
13	9	C30	Ile	174	CG1	4.39
14	9	C40	Ile	174	CB	3.99
15	9	C	Ile	174	CB	4
16	9	C30	Ile	174	CB	3.91
17	9	C70	Met	163	CE	3.96
18	9	C80	Met	163	CE	3.5
19	9	C60	Met	163	CE	3.64
20	9	C10	Met	163	CE	4.19
21	9	C20	Met	163	CG	4.27
22	9	C50	Met	163	CG	4.13
23	9	C70	Met	163	CG	4.4
24	9	CA0	Thr	119	CG2	4.03
25	9	CA0	Asn	118	C	4.19
26	9	CB0	Val	116	C	4.17
27	9	C90	Val	116	CG1	3.92
28	9	CB0	Val	116	CG1	4.11
29	9	C30	Phe	113	CE2	4.25
30	9	C40	Lys	68	CE	4.22
31	9	C40	Lys	68	CD	4.05
32	9	C90	Val	66	CG2	4.28
33	9	CB0	Val	66	CG2	4.35
34	9	C30	Val	66	CG1	4.29
35	9	C20	Val	66	CG1	4.38
36	9	C90	Val	66	CG1	3.85
37	9	C40	Val	53	CG2	4.06
38	9	C	Val	53	CG2	3.55
39	9	C30	Val	53	CG2	4.14
40	9	C20	Val	53	CG2	4.23
41	9	C60	Val	53	CG2	4.19
42	9	C10	Val	53	CG2	3.64
43	9	C00	Val	53	CG2	3.23
44	9	C20	Val	53	CG1	4.11
45	9	C10	Val	53	CG1	4.27

46	9	C10	Val	53	CB	4.2
47	9	C00	Val	53	CB	4.26
48	9	C60	Gly	46	CA	4.14
49	9	C70	Leu	45	C	4.19
50	9	C80	Leu	45	C	3.47
51	9	C60	Leu	45	C	3.82
52	9	CC0	Leu	45	CD2	3.97
53	9	CA0	Leu	45	CD2	4.15
54	9	C50	Leu	45	CD1	4.4
55	9	C90	Leu	45	CD1	4.12
56	9	CB0	Leu	45	CD1	3.9
57	9	CC0	Leu	45	CD1	4.04
58	9	CA0	Leu	45	CD1	4.36
59	9	CC0	Leu	45	CG	4.25
60	9	CA0	Leu	45	CG	4.24
61	9	C50	Leu	45	CB	4.06
62	9	CC0	Leu	45	CB	4.04
63	9	CA0	Leu	45	CB	3.56
64	9	C70	Leu	45	CB	3.54
65	9	C80	Leu	45	CB	3.72
66	9	C60	Leu	45	CB	4.34
67	9	CA0	Leu	45	CA	4.19
68	9	C70	Leu	45	CA	4.27
69	9	C80	Leu	45	CA	4.03

Table 7. Atom-atom contacts between IQA and amino acid residues of the CK2 active site at distance cut-off 4.4 Å.

#	Ligand	Atom	Residue	Atom	Distance	
1	IQA	C20	Asp	175	CG	3.96
2	IQA	C20	Asp	175	CB	3.64
3	IQA	C20	Asp	175	CA	3.43
4	IQA	C6	Ile	174	CD1	4.1
5	IQA	C8	Ile	174	CD1	3.5
6	IQA	C5	Ile	174	CD1	3.49
7	IQA	C18	Ile	174	CD1	3.74
8	IQA	C20	Ile	174	CD1	4.37
9	IQA	C1	Ile	174	CG2	4.14
10	IQA	C4	Ile	174	CG2	3.83
11	IQA	C6	Ile	174	CG2	3.89
12	IQA	C7	Ile	174	CG2	4.25
13	IQA	C5	Ile	174	CG1	4.39
14	IQA	C4	Ile	174	CB	4.13
15	IQA	C6	Ile	174	CB	4.1
16	IQA	C5	Ile	174	CB	4.17
17	IQA	C18	Ile	174	CB	4.37
18	IQA	C20	Ile	174	CB	4.26
19	IQA	C13	Met	163	SD	3.58
20	IQA	C14	Met	163	SD	3.79
21	IQA	C15	Met	163	SD	4.21
22	IQA	C17	Met	163	SD	4.23
23	IQA	C12	Met	163	SD	3.82
24	IQA	C13	Met	163	CG	4.4
25	IQA	C14	Asn	118	CB	4.35
26	IQA	C15	Asn	118	CB	3.7
27	IQA	C16	Asn	118	CB	4.07
28	IQA	C3	Val	116	CG2	4.11
29	IQA	C2	Val	116	CG2	3.53
30	IQA	C3	Val	116	CB	3.71
31	IQA	C2	Val	116	CB	3.69
32	IQA	C4	Phe	113	CE2	4.15
33	IQA	C1	Phe	113	CD2	3.92
34	IQA	C4	Phe	113	CD2	3.78
35	IQA	C1	Phe	113	CD1	4.27
36	IQA	C1	Phe	113	CG	3.68
37	IQA	C4	Phe	113	CG	3.99
38	IQA	C2	Phe	113	CB	4.2
39	IQA	C1	Phe	113	CB	3.53
40	IQA	C4	Phe	113	CB	4.31
41	IQA	C2	Val	95	CG2	4.08
42	IQA	C1	Val	95	CG2	3.16
43	IQA	C4	Val	95	CG2	3.94
44	IQA	C1	Val	95	CB	4.05
45	IQA	C20	Lys	68	CE	3.83

46	IQA	C18	Lys	68	CD	4.35
47	IQA	C20	Lys	68	CD	3.64
48	IQA	C3	Ile	66	CD1	3.9
49	IQA	C14	Ile	66	CD1	4.09
50	IQA	C3	Ile	66	CG2	3.82
51	IQA	C2	Ile	66	CG2	4.01
52	IQA	C1	Ile	66	CG2	4.17
53	IQA	C4	Ile	66	CG2	4.14
54	IQA	C6	Ile	66	CG2	3.94
55	IQA	C7	Ile	66	CG2	3.78
56	IQA	C3	Ile	66	CG1	3.38
57	IQA	C2	Ile	66	CG1	3.57
58	IQA	C7	Ile	66	CG1	4.17
59	IQA	C3	Ile	66	CB	3.94
60	IQA	C2	Ile	66	CB	3.85
61	IQA	C1	Ile	66	CB	4.26
62	IQA	C10	Val	53	CG2	4.22
63	IQA	C8	Val	53	CG2	4.04
64	IQA	C5	Val	53	CG2	4.2
65	IQA	C18	Val	53	CG2	3.89
66	IQA	C13	Val	53	CG1	4.26
67	IQA	C12	Val	53	CG1	4.33
68	IQA	C10	Val	53	CG1	4.09
69	IQA	C8	Val	53	CG1	3.71
70	IQA	C5	Val	53	CG1	4.14
71	IQA	C10	Val	53	CB	4.09
72	IQA	C8	Val	53	CB	4.27
73	IQA	C17	Gly	46	CA	4.4
74	IQA	C10	Gly	46	CA	4.2
75	IQA	C13	Val	45	CG2	4.19
76	IQA	C14	Val	45	CG2	4.22
77	IQA	C15	Val	45	CG2	4.06
78	IQA	C16	Val	45	CG2	3.85
79	IQA	C17	Val	45	CG2	3.8
80	IQA	C12	Val	45	CG2	3.97
81	IQA	C15	Val	45	CB	4.16
82	IQA	C16	Val	45	CB	3.7
83	IQA	C17	Val	45	CB	3.96
84	IQA	C16	Val	45	C	4.25
85	IQA	C17	Val	45	C	3.79

Spectroscopic Data:

6-Iodoquinoline-4-one-3-carboxylic acid **1**

Mp 289-291 °C: ¹H NMR (DMSO-d₆) δ 14,83 (brs,1H), 13,34 (brs,1H), 8,85 (s,1H), 8,53 (s,1H), 8,11 (d,1H, J=8,1 Hz), 7,6 (d,1H, J=8,1 Hz). Anal. (C₁₀H₆INO₃) C,H,N,I

Quinoline-4-one-3,6-dicarboxylic acid **2**

Mp >300 °C: ¹H NMR (DMSO-d₆) δ 14,08 (brs,1H), 13,95 (brs,1H), 13,36 (brs,1H), 8,91 (s,1H), 8,83 (d,1H, J=1,9 Hz), 8,34 (dd,1H, J=8,7 Hz, J=1,9 Hz), 7,95 (d,1H J=8,7 Hz). Anal. (C₁₁H₇NO₅) C,H,N

Quinoline-4-one-3,7-dicarboxylic acid **3**

Mp >300 °C: ¹H NMR (DMSO-d₆) δ 14,75 (brs,1H), 13,61 (brs,2H), 8,98 (s,1H), 8,37 (s,1H), 8,35 (d,1H, J=8,4Hz), 8,03 (d,1H, J=8,4 Hz). Anal. (C₁₁H₇NO₅) C,H,N

Quinoline-4-one-3,8-dicarboxylic acid **4**

Mp >300(295-297) °C: ¹H NMR (DMSO-d₆) δ 14,54 (brs,1H), 13,09 (d,1H, J=6,2 Hz), 8,94 (d,1H, J=6,8 Hz), 8,52 (d,2H, J=7,8 Hz), 7,68 (t,1H, J=7,8 Hz). Anal. (C₁₁H₇NO₅) C,H,N

6,7-Etylenedioxy-quinoline-4-one-3-carboxylic acid **5**

Mp 277-279 °C: ¹H NMR (DMSO-d₆) δ 13,54 (brs,1H), 8,68 (d,1H, J=6,2Hz), 7,56 (s,1H), 7,29 (s,1H), 4,40 (m,4H). Anal. (C₁₂H₉NO₅) C,H,N

6,8-Dichloroquinoline-4-one-3-carboxylic acid **6**

Mp >300 °C: ¹H NMR (DMSO-d₆) δ 14,51 (brs,1H), 13,14 (brs,1H), 8,66 (s,1H), 8,24 (d,1H, J=2,4 Hz), 8,16 (d,1H, J=2,4 Hz). Anal. (C₁₀H₅Cl₂NO₃) C,H,N,Cl

5,6,8-Trichloroquinoline-4-one-3-carboxylic acid **7**

Mp - °C: ¹H NMR (DMSO-d₆) δ 14,60 (brs,1H), 12,75 (brs,1H), 8,57 (s,1H), 8,37 (s,1H). Anal. (C₁₀H₄Cl₃NO₃) C,H,N,Cl

3-methyl-9,10-difluoro -2,3-dihydro-7-oxo-7*H*-1,4-oxazino[2,3,4-*ij*]quinoline-6-carboxylic acid **8**

Mp 298-300 °C: ¹H NMR (DMSO-d₆) δ 14,67 (brs,1H), 9,04 (s,1H), 7,79 (t,1H), 5,02 (m,1H), 4,72 (dd,2H), 1,51 (d,1H). Anal. (C₁₃H₉F₂NO₄) C,H,N

1,4-dihydro-4-oxo-benzo[*h*]quinoline-3-carboxylic acid **9**

Mp >300 °C: ¹H NMR (DMSO-d₆) δ 15,51 (brs,1H), 13,96 (brs,1H), 8,89 (m,1H), 8,73 (s,1H), 8,15 (d,1H, J=8,7 Hz), 8,09 (m,1H), 7,92 (d,1H, J=8,7 Hz), 7,83 (m,2H) Anal. (C₁₄H₉NO₃) C,H,N

6-Ethoxyquinoline-4-one-3-carboxylic acid **10**

Mp 283-285 °C: ¹H NMR (DMSO-d₆) δ 15,57 (brs,1H), 13,77 (brs,1H), 8,77 (s,1H), 7,83 (d,1H, J=9,0 Hz), 7,58 (s,1H), 7,50 (dd,1H, J=9,0 Hz, J=2,2 Hz), 4,17 (q,2H), 1,41 (t,3H). Anal. (C₁₂H₁₁NO₄) C,H,N

6-Methoxyquinoline-4-one-3-carboxylic acid **11**

Mp 279-280 °C: ¹H NMR (DMSO-d₆) δ 15,47 (brs,1H), 13,49 (brs,1H), 8,76 (s,1H), 7,80 (d,1H, J=9,0 Hz), 7,63 (d,1H, J=2,8 Hz), 7,50 (dd,1H, J=9,0 Hz, J=2,8 Hz), 3,91 (s,3H). Anal. (C₁₁H₉NO₄) C,H,N

Quinoline-4-one-3-carboxylic acid **12**

Mp 251-253 °C: ¹H NMR (DMSO-d₆) δ 15,35 (brs,1H), 13,46 (brs,1H), 8,89 (s,1H), 8,30 (d,1H, J=8,1 Hz), 7,87 (m,2H), 7,61 (dd,1, H J=7,5 Hz, J=7,8 Hz). Anal. (C₁₀H₇NO₃) C,H,N

8-Ethoxyquinoline-4-one-3-carboxylic acid 13

Mp 269-270 °C: ¹H NMR (DMSO-d₆) δ 15,26 (brs,1H), 12,90 (brd,1H,J=5,9 Hz), 8,60 (d,1H,J=6,8 Hz), 7,79 (d,1H,J=7,8 Hz), 7,48 (m,2H),4,31 (q,2H),1,50 (t,3H). Anal. (C₁₂H₁₁NO₄) C,H,N

3-methyl 9-fluoro -10-(4-methylpiperazin-1-yl) -2,3-dihydro-7-oxo-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid 14

Mp 233-234 °C: ¹H NMR (DMSO-d₆) δ 14,92 (brs,1H), 8,88 (s,1H), 7,53 (d,1H,J=12,3 Hz), 4,90 (m,1H), 4,64 (dd,2H),2,24 (s,3H),1,47(d,3H). Anal. (C₁₈H₂₀FN₃O₄) C,H,N

6-Methylquinoline-4-one-3-carboxylic acid 15

Mp 280-281 °C: ¹H NMR (DMSO-d₆) δ 15,46 (brs,1H), 13,45 (brs,1H), 8,82 (s,1H), 8,07 (s,1H), 7,73 (m,2H),2,49 (s,3H). Anal. (C₁₁H₉NO₃) C,H,N

6-Acetylquinoline-4-one-3-carboxylic acid 16

Mp 277-278 °C: ¹H NMR (DMSO-d₆) δ 14,98 (brs,1H), 13,73 (brs,1H), 8,93 (s,1H), 8,79 (d,1H,J=1,6 Hz), 8,34 (dd,1H, J=8,7 Hz, J=1,6 Hz),7,91 (d,1H, J=8,7 Hz),2,71(s,3H). Anal. (C₁₂H₉NO₄) C,H,N

6,8-Dimethoxyquinoline-4-one-3-carboxylic acid 17

Mp >300 °C: ¹H NMR (DMSO-d₆) δ 15,55 (brs,1H), 13,10 (brs,1H), 8,50 (d,1H,J=6,8 Hz), 7,21 (d,1H,1,9 Hz), 7,12 (d,1H, J=2,5 Hz),4,05 (s,3H),3,91 (s,3H). Anal. (C₁₂H₁₁NO₅) C,H,N

8-Isopropylquinoline-4-one-3-carboxylic acid 18

Mp 277-279 °C: ¹H NMR (DMSO-d₆) δ 15,35 (brs,1H), 13,01 (brs,1H), 8,67 (s,1H), 8,12 (dd,1H,J=1,0 Hz,J=8,0 Hz), 7,80 (d,1H,J=7,2 Hz),7,56 (m,1H),2,71(m,1H),1,24(d,6H). Anal. (C₁₃H₁₃NO₄) C,H,N

6-Isopropoxyquinoline-4-one-3-carboxylic acid 19

Mp 299-300 °C: ¹H NMR (DMSO-d₆) δ 15,38 (brs,1H), 13,11 (brs,1H), 8,70 (s,1H), 8,20 (dd,1H,J=1,2 Hz,J=8,4 Hz), 7,85 (d,1H,J=7,8 Hz),7,59 (dd,1H, J=7,8 Hz, J=8,4 Hz),3,71(m,1H),1,34(d,6H). Anal. (C₁₃H₁₃NO₄) C,H,N

8-Methoxyquinoline-4-one-3-carboxylic acid 20

Mp 278-280 °C: ¹H NMR (DMSO-d₆) δ 15,31 (brs,1H), 13,03 (brs,1H), 8,60 (d,1H,J=6,8Hz), 7,85 (dd,1H,J=8,1Hz,J=1,6Hz), 7,54 (m,2H),4,08 (s,3H). Anal. (C₁₁H₉NO₄) C,H,N

6-Phenoxyquinoline-4-one-3-carboxylic acid 21

Mp 267-269 °C: ¹H NMR (DMSO-d₆) δ 15,26 (brs,1H), 13,85 (brs,1H), 8,84 (s,1H), 7,96 (d,1H,9,0 Hz), 7,70 (dd,1H, J=9,0 Hz,J=2,8 Hz),7,57 (d,1H,J=2,8 Hz),7,49(m,2H),7,27(m,1H),7,16(d,2H). Anal. (C₁₆H₁₁NO₄) C,H,N

6-Butylquinoline-4-one-3-carboxylic acid 22

Mp 235-236 °C: ¹H NMR (DMSO-d₆) δ 15,46 (brs,1H), 13,42 (brd,1H), 8,87 (d,1H,J=6,2 Hz), 8,09 (s,1H), 7,76 (m,2H),2,78 (t,2H),1,63(m,2H),1,33(m,2H),0,93(t,3H). Anal. (C₁₄H₁₅NO₃) C,H,N

8-Ethylquinoline-4-one-3-carboxylic acid 23

Mp 278,5-279,5°C: ¹H NMR (DMSO-d₆) δ 15,31 (brs,1H), 12,91 (brs,1H), 8,65 (s,1H), 8,17 (dd,1H,J=7,8Hz,J=0,9Hz), 7,75 (d,1H, J=7,2 Hz),7,53 (t,1H, J=7,8 Hz),3,02(q,2H),1,28(t,3H). Anal. (C₁₂H₁₁NO₃) C,H,N

6-Propoxyquinoline-4-one-3-carboxylic acid 24

Mp 265-267 °C: ¹H NMR (DMSO-d₆) δ 15,58 (brs,1H), 13,47 (brs,1H), 8,82 (d,1H,J=6,2Hz), 7,79 (d,1H,J=9Hz), 7,63 (d,1H, J=2,8 Hz),7,53 (dd,1H,J=9 Hz, J=2,8 Hz),4,09(t,2H),1,81(m,2H),1,03(t,3H). Anal. (C₁₃H₁₃NO₄) C,H,N

7-Trifluoromethylquinoline-4-one-3-carboxylic acid 25

Mp 249-250 °C: ¹H NMR (DMSO-d₆) δ 14,89 (brs,1H), 13,62 (brs,1H), 9,05 (s,1H), 8,47 (d,1H,J=8,4Hz), 8,19 (s,1H),7,88 (dd,1H, J=1,6 Hz,J=8,4Hz). Anal. (C₁₁H₆F₃NO₃) C,H,N

6-Bromoquinoline-4-one-3-carboxylic acid 26

Mp 276-278 °C: ¹H NMR (DMSO-d₆) δ 14,96 (brs,1H), 13,51 (brs,1H), 8,93 (s,1H), 8,35 (d,1H,J=2,2Hz), 8,03 (dd,1H, J=2,2Hz, J=9,0 Hz),7,78 (d,1H,J=9,0 Hz). Anal. (C₁₀H₆BrNO₃) C,H,N,Br

6-Chloroquinoline-4-one-3-carboxylic acid 27

Mp 277-278 °C: ¹H NMR (DMSO-d₆) δ 15,03 (brs,1H), 13,62 (brs,1H), 8,96 (s,1H), 8,23 (d,1H,J=2,2Hz), 7,96 (dd,1H,J=9,0 Hz,J=2,2Hz),7,88 (d,1H,J=9,0 Hz). Anal. (C₁₀H₆ClNO₃) C,H,N,Cl

6-Dimethylaminoquinoline-4-one-3-carboxylic acid 28

Mp 258-259 °C: ¹H NMR (DMSO-d₆) δ 15,82 (brs,1H), 13,20 (brs,1H), 8,66 (s,1H), 7,67 (d,1H,J=9,0 Hz), 7,47 (dd,1H,J=9,0 Hz,J=2,8Hz),7,26 (d,1H, J=2,8Hz),3,04 (s,6H). Anal. (C₁₂H₁₂N₂O₃) C,H,N

8-Methylquinoline-4-one-3-carboxylic acid 29

Mp 271-273 °C: ¹H NMR (DMSO-d₆) δ 14,23 (brs,1H), 12,60 (brs,1H), 8,57 (s,1H), 8,10 (d,1H,J=8,4Hz), 7,69 (d,1H,J=6,7Hz),7,45(m,1H),2,45(s,3H). Anal. (C₁₁H₉NO₃) C,H,N

6-Fluoroquinoline-4-one-3-carboxylic acid 30

Mp 286-287 °C: ¹H NMR (DMSO-d₆) δ 15,06 (brs,1H), 13,60 (brs,1H), 8,89 (s,1H), 7,84 (m,3H). Anal. (C₁₀H₆FNO₃) C,H,N

8-Fluoroquinoline-4-one-3-carboxylic acid 31

Mp 275-280 °C: ¹H NMR (DMSO-d₆) δ 14,98 (brs,1H), 13,61 (brs,1H), 8,66 (s,1H), 8,10 (d,1H,J=8,4Hz), 7,85 (m,1H),7,60 (m,1H). Anal. (C₁₀H₆FNO₃) C,H,N

5,7-Dichloroquinoline-4-one-3-carboxylic acid 32

Mp 296-298 °C: ¹H NMR (DMSO-d₆) δ 14,93 (brs,1H), 13,41 (brs,1H), 8,90 (s,1H), 7,79 (d,1H,J=2,2 Hz), 7,69 (d,1H, J=2,2 Hz). Anal. (C₁₀H₅Cl₂NO₃) C,H,N,Cl

6,8-Dimethylquinoline-4-one-3-carboxylic acid 33

Mp 298-300 °C: ¹H NMR (DMSO-d₆) δ 15,36 (brs,1H), 12,75 (brs,1H), 8,59 (s,1H), 7,90 (s,1H), 7,53 (s,1H),2,57(s,3H),2,43(s,3H). Anal. (C₁₂H₁₁NO₃) C,H,N

7,8-Dimethylquinoline-4-one-3-carboxylic acid 34

Mp 272-273 °C: ¹H NMR (DMSO-d₆) δ 15,39 (brs,1H), 12,66 (brs,1H), 8,57 (s,1H), 8,02 (d,1H,J=8,4 Hz),7,40(d,1H,J=8,4 Hz),2,45 (2s,6H). Anal. (C₁₂H₁₁NO₃) C,H,N

8-Bromoquinoline-4-one-3-carboxylic acid 35

Mp 270-271 °C: ¹H NMR (DMSO-d₆) δ 14,88(brs,1H), 12,78 (brs,1H), 8,71 (s,1H), 8,24 (d,1H,J=8,1 Hz), 8,21 (d,1H,J=7,8 Hz),7,51(dd,1H, J=8,1 Hz, J=7,8 Hz). Anal. (C₁₀H₆BrNO₃) C,H,N,Br

8-Chloroquinoline-4-one-3-carboxylic acid 36

Mp 268-270°C: ¹H NMR (DMSO-d₆) δ 12,91 (brs,1H), 8,63 (s,1H), 8,25 (d,1H,J=8,1Hz), 8,06 (d,1H,J=8,1Hz), 7,59 (t,1H, J=8,1Hz). Anal. (C₁₀H₆ClNO₃) C,H,N,Cl

5,8-Dimethylquinoline-4-one-3-carboxylic acid 37

Mp 252-253 °C: ¹H NMR (DMSO-d₆) δ 12,49 (brs,1H), 8,59 (s,1H), 7,57 (d,1H,J=7,5Hz), 7,22 (d,1H,J=7,5Hz), 2,83 (s,3H),2,53(s,3H) . Anal. (C₁₂H₁₁NO₃) C,H,N

8-Methyl-7-chloroquinoline-4-one-3-carboxylic acid 38

Mp 279-281 °C: ¹H NMR (DMSO-d₆) δ 14,94 (brs,1H), 12,69 (brs,1H), 8,57 (s,1H), 8,06 (d,1H,J=8,7Hz), 7,57 (d,1H, J=8,7Hz),2,57(s,3H). Anal. (C₁₁H₈ClNO₃) C,H,N,Cl

7,8-Dichloroquinoline-4-one-3-carboxylic acid 39

Mp 270-272 °C: ¹H NMR (DMSO-d₆) δ 14,69 (brs,1H), 12,96 (brs,1H), 8,62 (s,1H), 8,21 (d,1H,J=9,0Hz), 7,79 (d,1H,J=9,0Hz). Anal. (C₁₀H₅Cl₂NO₃) C,H,N,Cl

1-Methylquinoline-4-one-3-carboxylic acid 40

Mp 255-257 °C: ¹H NMR (DMSO-d₆) δ 15,13 (brs,1H), 9,00 (s,1H), 8,39 (d,1H,J=7,8 Hz), 7,96 (m,2H), 7,68 (m,1H),4,11(s,3H). Anal. (C₁₁H₉NO₃) C,H,N

1,6,8-Trimethylquinoline-4-one-3-carboxylic acid 41

Mp 250-252 °C: ¹H NMR (DMSO-d₆) δ 15,29 (brs,1H), 8,82 (s,1H), 8,07 (s,1H), 7,59(s,1H),4,32(s,3H),2,86(s,3H),2,43(s,3H). Anal. (C₁₃H₁₃NO₃) C,H,N

1,6-Dimethylquinoline-4-one-3-carboxylic acid 42

Mp 260-262 °C: ¹H NMR (DMSO-d₆) δ 15,22 (brs,1H), 8,92 (s,1H), 8,14 (s,1H), 7,84(d,1H,J=9,0 Hz),7,77(d,1H,J=9,0 Hz),4,07(s,3H),2,50(s,3H). Anal. (C₁₂H₁₁NO₃) C,H,N

Table of elemental analyses for compounds **1–42**.

№ of compound	C%, calculated	H%, calculated	N%, calculated	Cl%, calculated	C%, found	H%, found	N%, found	Cl%, found
1	38,12	1,92	4,45	-	37,98	1,96	4,50	
2	56,66	3,03	6,01	-	56,90	2,97	5,92	
3	56,66	3,03	6,01	-	56,53	3,00	6,05	
4	56,66	3,03	6,01	-	56,45	3,09	6,09	
5	58,30	3,67	5,67	-	58,45	3,60	5,52	
6	46,54	1,95	5,43	27,48	46,33	2,01	5,51	27,59
7	41,06	1,38	4,79	36,36	41,30	1,40	4,70	36,42
8	55,52	3,23	4,98	-	55,69	3,30	4,89	
9	70,29	3,79	5,85	-	70,00	3,85	5,91	
10	61,80	4,75	6,01	-	61,66	4,71	6,10	
11	60,28	4,14	6,39	-	60,37	4,00	6,30	
12	63,49	3,73	7,40	-	63,24	3,80	7,47	
13	61,08	4,75	6,01	-	61,19	4,79	5,93	
14	59,83	5,58	11,63	-	59,70	5,50	11,79	
15	65,02	4,46	6,89	-	65,27	4,50	6,80	
16	62,34	3,92	6,06	-	62,45	3,88	5,98	
17	57,83	4,45	5,62	-	57,70	4,50	5,50	
18	67,52	5,67	6,06	-	67,45	5,59	6,13	
19	63,15	5,30	5,66	-	63,00	5,21	5,80	
20	60,28	4,14	6,39	-	60,41	4,22	6,29	
21	68,33	3,94	4,98	-	68,56	3,86	4,81	
22	68,56	6,16	5,71	-	68,31	6,05	5,60	
23	66,35	5,10	6,45	-	66,08	5,09	6,59	
24	63,15	5,30	5,66	-	63,02	5,33	5,80	
25	51,38	2,35	5,45	-	51,26	2,39	5,50	
26	44,81	2,26	5,23	-	44,95	2,30	5,18	
27	53,71	2,70	6,26	15,85	53,81	2,75	6,19	15,90
28	62,06	5,21	12,06	-	62,15	5,29	11,98	
29	65,02	4,46	6,89	-	65,19	5,19	6,76	
30	57,98	2,92	6,76	-	57,86	2,88	6,81	
31	57,98	2,92	6,76	-	58,09	2,89	6,69	
32	46,54	1,95	5,43	27,48	46,49	1,99	5,50	27,60
33	66,35	5,10	6,45	-	66,50	5,09	6,39	
34	66,35	5,10	6,45	-	66,18	5,18	6,59	
35	44,81	2,26	5,23	-	44,99	2,35	5,19	
36	53,71	2,70	6,26	15,85	53,49	2,80	6,39	15,79
37	66,35	5,10	6,45	-	66,50	5,15	6,40	
38	55,60	3,39	5,89	14,92	55,65	3,36	5,85	
39	46,54	1,95	5,43	27,48	46,70	1,99	5,38	27,44
40	65,02	4,46	6,89	-	65,29	4,40	6,78	
41	67,52	5,67	6,06	-	67,39	5,77	6,19	
42	66,35	5,10	6,45	-	66,00	5,19	6,61	