Supporting Information:

Novel Quinolinonyl Diketo Acid Derivatives as HIV-1 Integrase Inhibitors: Design, Synthesis and Biological Activities

Roberto Di Santo,[*,§] Roberta Costi,[§] Alessandra Roux,[§] Gaetano Miele,[§] Giuliana Cuzzucoli Crucitti,[§] Alberto Iacovo,[§] Federica Rosi,[§] Antonio Lavecchia,[^] Luciana Marinelli,[^] Carmen Di Giovanni,[^] Ettore Novellino,[^] Lucia Palmisano,[#] Mauro Andreotti,[#] Roberta Amici,[#] Clementina Maria Galluzzo,[#] Lucia Nencioni,[°] Anna Teresa Palamara,[°] Yves Pommier,[+] and Christophe Marchand[*,+]

Istituto Pasteur - Fondazione Cenci Bolognetti, Dipartimento di Chimica e Tecnologie del Farmaco, Università di Roma "La Sapienza", Piazzale A. Moro 5, I-00185 Roma, Italy, Dipartimento Chimica Farmaceutica e Tossicologica, Università di Napoli "Federico II", via D. Montesano 49, I-80131 Napoli, Italy, Dipartimento del Farmaco, Istituto Superiore di Sanità, Dipartimento di Sanità Pubblica, Università di Roma "La Sapienza", P.le A. Moro 5, I-00185 Roma, Italy, Laboratory of Molecular Pharmacology, Center for Cancer Research, National Cancer Institute Building 37, Room 5068, National Institute of Health, Bethesda, MD 20892-4255, USA

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1. Spectroscopic data.

3-Acetyl-4(1*H*)-quinolinone (**9a**).[17] IR ν 3420 (NH), 1644 and 1589 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.64 (s, 3H, CH_3), 7.41-7.49 (m, 1H, quinolinone C6-H), 7.51-7.76 (m, 2H, quinolinone C7-H and C8-H), 8.22-8.26 (m, 1H, quinolinone C5-H), 8.54 (s, 1H, quinolinone C2-H), 12. 54 (bs, 1H, NH).

3-Acetyl-6-fluoro-4(1*H*)-quinolinone (**9b**). IR ν 3100 (NH), 1625 and 1656 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.61 (s, 3H, CH_3), 7.61 (m, 1H, quinolinone C7-H), 7.69 (m, 1H, quinolinone C8-H), 7.85 (m, 1H, quinolinone C5-H), 8.53 (s, 1H, quinolinone C2-H), 12.05 (bs, 1H, NH).

3-Acetyl-7-fluoro-4(1*H*)-quinolinone (**9c**). IR ν 3100 (NH), 1652 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.59 (s, 3H, CH_3), 7.25-7.31 (m, 1H, quinolinone C6-H), 7.36-7.39 (m, 1H, quinolinone C8-H), 8.23-8.27 (m, 1H, quinolinone C5-H), 8.53 (s, 1H, quinolinone C2-H), 12.50 (bs, 1H, NH).

3-Acetyl-8-fluoro-4(1*H*)-quinolinone (**9d**). IR ν 3100 (NH), 1614 and 1667 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.59 (s, 3H, CH_3), 7.38-7.44 (m, 1H, quinolinone C6-H), 7.63-7.67 (m, 1H, quinolinone C7-H), 8.01 (m, 1H, quinolinone C5-H), 8.34 (s, 1H, quinolinone C2-H), 12.63 (bs, 1H, NH).

3-Acetyl-6-chloro-4(1*H*)-quinolinone (**9e**).[17] IR ν 3080 (NH), 1600 and 1650 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 7.60-7.80 (m, 2H, quinolinone C7-H and C8-H), 8.15 (m, 1H, quinolinone C5-H), 8.55 (s, 1H, quinolinone C2-H), 12.65 (bs, 1H, NH).

3-Acetyl-7-chloro-4(1*H*)-quinolinone (**9f**).[17] IR ν 3050 (NH), 1610 and 1650 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 7.48 (m, 1H, quinolinone C6-H), 7.70 (m, 1H, quinolinone C8-H), 8.22 (m, 1H, quinolinone C5-H), 8.55 (s, 1H, quinolinone C2-H), 12.50 (bs, 1H, NH).

3-Acetyl-8-chloro-4(1*H*)-quinolinone (**9g**).[17] IR ν 3183 (NH), 1637 and 1670 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.59 (s, 3H, CH_3), 7.42 (m, 1H, quinolinone C6-H), 7.89 (m, 1H, quinolinone C7-H), 8.17 (m, 1H, quinolinone C5-H), 8.37 (s, 1H, quinolinone C2-H), 12.08 (bs, 1H, NH).

3-Acetyl-6,7-dichloro-4(1*H*)-quinolinone (**9h**). IR ν 3100 (NH), 1625 and 1654 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.59 (s, 3H, CH_3), 8.21 (s, 1H, quinolinone C8-H), 8.40 (s, 1H, quinolinone C5-H), 8.63 (s, 1H, quinolinone C2-H), 12.65 (bs, 1H, NH).

3-Acetyl-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10a**). IR ν 1635 and 1660 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.86 (s, 3H, CH_3), 5.43 (s, 2H, CH_2), 7.04-7.23 (m, 4H, benzene H), 7.30-7.66 (m, 3H, quinolinone C6-H, C7-H and C8-H), 8.58 (dd, 1H, $J_{5,6}$ = 8.0 Hz, $J_{5,7}$ = 1.6 Hz, quinolinone C5-H), 8.66 (s, 1H, quinolinone C2-H).

3-Acetyl-6-fluoro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10b**). IR ν 1656 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 5.70 (s, 2H, CH_2), 7.15-7.19 (m, 2H, benzene H), 7.28-7.32 (m, 2H, benzene H), 7.59-7.64 (m, 1H, quinolinone C7-H), 7.74-7.77 (m, 1H, quinolinone C8-H), 7.93-7.96 (m, 1H, quinolinone C5-H), 8.86 (s, 1H, quinolinone C2-H).

3-Acetyl-7-fluoro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10c**). IR ν 1638 and 1660 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 5.65 (s, 2H, CH_2), 7.14-7.21 (m, 2H, benzene H), 7.28-7.35 (m, 3H, benzene H and quinolinone C6-H), 7.55 (m, 1H, quinolinone C8-H), 8.34 (m, 1H, quinolinone C5-H), 8.83 (s, 1H, quinolinone C2-H).

3-Acetyl-8-fluoro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10d**). IR ν 1640 and 1660 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 5.72 (s, 2H, CH_2), 7.13-7.20 (m, 4H, benzene H), 7.43-7.50 (m, 1H, quinolinone C6-H), 7.54-7.60 (m, 1H, quinolinone C7-H), 8.16 (m, 1H, quinolinone C5-H), 8.75 (s, 1H, quinolinone C2-H).

3-Acetyl-6-chloro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10e**). IR ν 1620 and 1650 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.67 (s, 3H, CH_3), 5.73 (s, 2H, CH_2), 7.10-7.30 (m, 4H, benzene H), 7.75-7.78 (m, 2H, quinolinone C7-H and C8-H), 8.25 (m, 1H, quinolinone C5-H), 8.90 (s, 1H, quinolinone C2-H).

3-Acetyl-7-chloro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10f**). IR ν 1635 and 1662 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 5.66 (s, 2H, CH_2), 7.16-7.21 (m, 2H, benzene H), 7.30-7.33 (m, 2H, benzene H), 7.49 (m, 1H, quinolinone C6-H), 7.78 (m, 1H, quinolinone C8-H), 8.27 (m, 1H, quinolinone C5-H), 8.82 (s, 1H, quinolinone C2-H).

3-Acetyl-8-chloro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10g**). IR ν 1640 and 1660 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 6.04 (s, 2H, CH_2), 7.13 (m, 4H, benzene H), 7.43-7.49 (m, 1H, quinolinone C6-H), 7.80 (m, 1H, quinolinone C7-H), 8.34 (m, 1H, quinolinone C5-H), 8.67 (s, 1H, quinolinone C2-H).

3-Acetyl-6,7-dichloro-1-(4-fluorophenyl)methyl-4(1*H*)-quinolinone (**10h**). IR ν 1620 and 1650 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 5.67 (s, 2H, CH_2), 7.12-7.34 (m, 4H, benzene H), 8.03 (s, 1H, quinolinone C8-H), 8.33 (m, 1H, quinolinone C5-H), 8.83 (s, 1H, quinolinone C2-H).

3-Acetyl-1-(4-fluorophenyl)methyl-7-(pyrrolidin-1-yl)-4(1*H*)-quinolinone (**10i**). IR ν 1631(C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 1.90-1.93 (m, 4H, pyrrolidine H), 2.62 (s, 3H, CH_3), 3.18-3.22 (m, 4H, pyrrolidine H), 5.60 (s, 2H, CH_2), 6.28 (m, 1H, quinolinone C8-H), 7.67 (m, 1H, quinolinone C6-H), 7.15-7.19 (m, 2H, benzene H), 7.31-7.35 (m, 2H, benzene H), 8.02 (m, 1H, quinolinone C5-H), 8.70 (s, 1H, quinolinone C2-H).

2. Analyses

Compd	Elemental Analyses Calculated/ Found				
	C	H	N	F	Cl
5a	66.82	4.59	3.53	4.81	-
	66.88	4.58	3.53	4.82	-
5b	63.91	4.15	3.39	9.20	-
	64.10	4.16	3.38	9.21	-
5c	63.91	4.15	3.39	9.20	-
	64.06	4.15	3.39	9.23	-
5d	63.91	4.15	3.39	9.20	-
	63.71	4.16	3.38	9.22	-
5e	61.48	3.99	3.26	4.42	8.25
	61.53	3.99	3.27	4.44	8.17
5f	61.48	3.99	3.26	4.42	8.25
	61.41	3.98	3.26	4.44	8.16
5g	61.48	3.99	3.26	4.42	8.25
	61.65	3.98	3.27	4.42	8.15
5h	56.91	3.47	3.02	4.09	15.27
	56.84	3.47	3.02	4.11	15.35
5i	67.22	5.43	6.03	4.09	-

	67.09	5.45	6.04	4.09	-
6a	65.40	3.84	3.81	5.17	-
	65.27	4.02	3.89	5.16	-
6b	62.34	3.40	3.64	9.86	-
	62.22	3.56	3.64	9.83	-
6c	62.34	3.40	3.64	9.86	-
	62.28	3.64	3.62	9.86	-
6d	62.34	3.40	3.64	9.86	-
	62.25	3.55	3.62	9.85	-
6e	59.79	3.26	3.49	4.73	8.82
	59.87	3.31	3.49	4.72	8.71
6f	59.79	3.26	3.49	4.73	8.82
	59.63	3.42	3.47	4.74	8.73
6g	59.79	3.26	3.49	4.73	8.82
	59.67	3.31	3.48	4.72	8.72
6h	55.07	2.77	3.21	4.36	16.25
	55.18	2.79	3.23	4.37	16.34
6i	66.03	4.85	6.42	4.36	-
	66.10	4.86	6.40	4.36	-
7a	56.00	3.76	4.35	-	11.02
	56.01	3.78	4.36	-	10.86
7b	56.00	3.76	4.35	-	11.02
	56.09	3.76	4.37	-	10.92
8a	53.17	2.75	4.77	-	12.07
	53.29	2.74	4.78	-	11.95

8b	53.17	2.75	4.77	-	12.07
	53.18	2.74	4.79	-	11.97
9a	70.58	4.85	7.48	-	-
	70.63	4.67	7.46	-	-
9b	64.39	3.93	6.83	9.26	-
	64.56	3.93	6.84	9.27	-
9c	64.39	3.93	6.83	9.26	-
	64.45	3.92	6.84	9.24	
9d	64.39	3.93	6.83	9.26	-
	64.55	3.93	6.81	9.25	
9e	59.61	3.64	6.32	-	16.00
	59.52	3.60	6.19	-	16.02
9f	59.61	3.64	6.32	-	16.00
	59.54	3.64	6.36	-	15.96
9g	59.61	3.64	6.32	-	16.00
	59.73	3.65	6.35	-	15.87
9h	51.59	2.76	5.47	-	27.69
	51.62	2.78	5.48	-	27.53
10a	73.21	4.78	4.74	6.43	-
	73.27	4.79	4.75	6.44	-
10b	69.01	4.18	4.47	12.13	-
	68.92	4.19	4.46	12.16	-
10c	69.01	4.18	4.47	12.13	-
	68.95	4.19	4.48	12.15	-
10d	69.01	4.18	4.47	12.13	-

	68.99	4.17	4.46	12.16	-
10e	65.56	3.97	4.25	5.76	10.75
	65.71	3.98	4.27	5.75	10.66
10f	65.56	3.97	4.25	5.76	10.75
	65.60	3.97	4.26	5.79	10.61
10g	65.56	3.97	4.25	5.76	10.75
	65.68	3.98	4.25	5.78	10.62
10h	59.36	3.32	3.85	5.22	19.47
	59.42	3.33	3.85	5.22	19.30
10i	72.50	5.81	7.69	5.22	-
	72.57	5.81	7.68	5.24	-