SUPPORTING INFORMATION

Contents:

1. Spectroscopic data

3-Acetyl-quinolin-4(1*H*)-one (12a). Reference [1]. White solid; 56%; IR ν 3420 (NH), 1644 and 1589 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.64 (s, 3H, CH3), 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-7-fluoroquinolin-4(1*H*)-one (12b). White solid; 52%; IR ν 3050 (NH), 1650 (C=O), 1610 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.65 (s, 3H, CH_3), 7.48 (dd, 1H, quinolinone C6-H), 7.70 (d, 1H, quinolinone C8-H), 8.22 (d, 1H, quinolinone C5-H), 8.55 (s, 1H, quinolinone C2-H), 12.50 (br s, 1H NH).

3-Acetyl-8-chloroquinolin-4(1*H*)-one (12c). Reference [1]. White solid; 58%; IR ν 3183 (NH), 1637 and 1670 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.59 (s, 3H, CH3), 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-1-[(phenyl)methyl]quinolin-4(1*H*)-one (13a). Beige solid; 56%; IR ν 1667 (C=O), 1620 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 5.70 (s, 2H, CH_2), 7.22-7.28 (m, 4H, benzene H), 7.33 (m, 1H, benzene H), 7.44 (m, 1H, quinolinone C6-H), 7.63-7.69 (m, 2H, quinolinone C7-H and C8-H), 8.30 (d, 1H, quinolinone C5-H), 8.85 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2-fluorophenyl)methyl]quinolin-4(1*H*)-one (13b). White solid; 50%; IR ν 1663 (C=O), 1634 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.63 (s, 3H, CH_3), 5.74 (s, 2H, CH_2), 7.11-7.16 (m, 2H, benzene H), 7.24 (m, 1H, benzene H), 7.35 (m, 1H, benzene H), 7.46 (m, 1H, quinolinone C6-H), 7.63-7.72 (m, 2H, quinolinone C7-H and C8-H), 8.30 (d, 1H, quinolinone C5-H), 8.84 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2-methoxyphenyl)methyl]quinolin-4(1*H*)-one (13c). White solid; 60%; IR ν 1663 (C=O), 1631 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.62 (s, 3H, CH_3), 3.81 (s, 3H, CH_3), 5.55 (s, 2H, CH_2), 6.87 (m, 1H, benzene H), 7.03-7.06 (m, 2H, benzene H), 7.29 (m, 1H, benzene H), 7.44 (m, 1H, quinolinone C6-H), 7.63-7.71 (m, 2H, quinolinone C7-H and C8-H), 8.29 (d, 1H, quinolinone C5-H), 8.77 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3-fluorophenyl)methyl]quinolin-4(1*H*)-one (13d). White solid; 52%; IR ν 1663 (C=O), 1631 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.63 (s, 3H, CH_3), 5.71 (s, 2H, CH_2), 7.01 (d, 1H, benzene H), 7.08-7.14 (m, 2H, benzene H), 7.37 (m, 1H, benzene H), 7.44 (m, 1H, quinolinone C6-H), 7.61-7.70 (m, 2H, quinolinone C7-H and C8-H), 8.31 (d, 1H, quinolinone C5-H), 8.85 (s, 1H, quinolinone C2-H).

3-acetyl-1-[(3-methoxyphenyl)methyl]quinolin-4(1H)-one (13e). Yellow solid; 68%; IR ν 1669 (C=O), 1622 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.64 (s, 3H, CH_3), 3.69 (s, 3H, CH_3), 5.65 (s, 2H, CH_2), 6.71 (d, 1H, benzene H), 6.83-6.85 (m, 2H, benzene H), 7.23 (m, 1H, benzene H), 7.44 (m, 1H, quinolinone C6-H), 7.64-7.70 (m, 2H, quinolinone C7-H and C8-H), 8.30 (d, 1H, quinolinone C5-H), 8.83 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(4-chlorophenyl)methyl]quinolin-4(1*H*)-one (13f). Yellow solid; 70%; IR ν 1660 (C=O), 1633 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.65 (s, 3H, CH_3), 3.63 (s, 3H, CH_3), 5.62 (s, 2H, CH_2), 6.88-6.92 (d, 2H, benzene H), 7.21-7.27 (d, 2H, benzene H), 7.49 (t, 1H, quinolinone C6-H), 7.70-7.79 (m, 2H, quinolinone C7-H and C8-H), 8.35 (d, 1H, quinolinone C5-H), 8.84 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(4-hydroxyphenyl)methyl]quinolin-4(1*H*)-one (13g). Yellow solid; 65%; IR ν 3067 (OH), 1646 (C=O), 1613 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 3.68 (s, 3H, CH_3), 5.60 (s, 2H, CH_2), 6.87-6.90 (d, 2H, benzene H), 7.19-7.21 (d, 2H, benzene H), 7.44 (t, 1H, quinolinone

C6-H), 7.67-7.74 (m, 2H, quinolinone C7-H and C8-H), 8.28 (d, 1H, quinolinone C5-H), 8.79 (s, 1H, quinolinone C2-H), 9.5 (br s, 1H, OH).

3-Acetyl-1-[(4-methoxyphenyl)methyl]quinolin-4(1*H*)-one (13h). Yellow solid; 75%; IR ν 1667 (C=O), 1626 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 5.54 (s, 2H, CH_2), 6.69-6.71 (d, 2H, benzene H), 7.08-7.10 (d, 2H, benzene H), 7.44 (t, 1H, quinolinone C6-H), 7.68-7.73 (m, 2H, quinolinone C7-H and C8-H), 8.29 (d, 1H, quinolinone C5-H), 8.83 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(4-nitrophenyl)methyl]quinolin-4(1*H*)-one (13i). Yellow solid; 55%; IR ν 1661 (C=O), 1631 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.65 (s, 3H, CH_3), 5.87 (s, 2H, CH_2), 7.44-7.48 (m, 3H, quinolinone C6-H and benzene H), 7.53-7.55 (d, 2H, benzene H), 7.64-7.69 (m, 2H, quinolinone C7-H and C8-H), 8.31 (d, 1H, quinolinone C5-H), 8.90 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2,4-difluorophenyl)methyl]quinolin-4(1*H*)-one (13j). Yellow solid; 62%; IR ν 1660 (C=O), 1633 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.56 (s, 3H, CH_3), 5.65 (s, 2H, CH_2), 6.97 (t, 1H, benzene H), 7.15-7.25 (m, 2H, benzene H), 7.40 (t, 1H, quinolinone C6-H), 7.59 (d, 1H, quinolinone C8-H), 7.65 (t, 1H, quinolinone C7-H), 8.24 (d, 1H, quinolinone C5-H), 8.76 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2,5-difluorophenyl)methyl]quinolin-4(1*H*)-one (13k). Yellow solid; 60%; IR ν 1663 (C=O), 1637 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.67 (s, 3H, CH_3), 5.77 (s, 2H, CH_2), 7.15 (m, 1H, benzene H), 7.26 (m, 1H, benzene H), 7.35 (m, 1H, benzene H), 7.50 (t, 1H, quinolinone C6-H), 7.67 (d, 1H, quinolinone C8-H), 7.76 (t, 1H, quinolinone C7-H), 8.35 (d, 1H, quinolinone C5-H), 8.87 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2,6-difluorophenyl)methyl]quinolin-4(1*H*)-one (13l). White solid; 65%; IR ν 1662 (C=O), 1623 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.62 (s, 3H, CH_3), 5.77 (s, 2H, CH_2), 7.13-7.17 (m, 2H, benzene H), 7.42-7.49 (m, 2H, quinolinone C6-H and benzene H), 7.63 (d, 1H, quinolinone C8-H), 7.75 (t, 1H, quinolinone C7-H), 8.29 (dd, 1H, quinolinone C5-H), 8.84 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3,4-difluorophenyl)methyl]quinolin-4(1*H*)-one (13m). Yellow solid; 54%; IR ν 1661 (C=O), 1634 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.67 (s, 3H, CH_3), 5.71 (s, 2H, CH_2), 7.09 (m, 1H, benzene H), 7.39-7.51 (m, 3H, quinolinone C6-H and benzene H), 7.67 (d, 1H, quinolinone C8-H), 7.73 (t, 1H, quinolinone C7-H), 8.34 (dd, 1H, quinolinone C5-H), 8.89 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3,5-difluorophenyl)methyl]quinolin-4(1*H*)-one (13n). Yellow solid; 62%; IR ν 1656 (C=O), 1630 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.57 (s, 3H, CH_3), 5.65 (s, 2H, CH_2), 6.93 (m, 2H, benzene H), 7.10 (t, 1H, benzene H), 7.40 (t, 1H, quinolinone C6-H), 7.53 (d, 1H, quinolinone C8-H), 7.64 (t, 1H, quinolinone C7-H), 8.25 (d, 1H, quinolinone C5-H), 8.78 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2,4-dichlorophenyl)methyl]quinolin-4(1*H*)-one (13o). Pink solid; 56%; IR ν 1664 (C=O), 1634 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.69 (s, 3H, CH_3), 5.78 (s, 2H, CH_2), 6.90 (d, 1H, benzene H), 7.38 (dd, 1H, benzene H), 7.47 (d, 1H, quinolinone C8-H), 7.54 (t, 1H, quinolinone C7-H), 7.76 (t, 1H, quinolinone C6-H), 7.82 (d, 1H, benzene H), 8.38 (dd, 1H, quinolinone C5-H), 8.87 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(2,6-dichlorophenyl)methyl]quinolin-4(1*H*)-one (13p). White solid; 54%; IR ν 1660 (C=O), 1625 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.63 (s, 3H, CH_3), 5.82 (s, 2H, CH_2), 7.58-7.63 (m, 2H, quinolinone C6-H and C7-H), 7.71-7.73 (d, 2H, benzene H), 7.89 (t, 1H, benzene H), 7.99 (d, 1H, quinolinone C8-H), 8.21 (s, 1H, quinolinone C2-H), 8.40 (d, 1H, quinolinone C5-H).

3-Acetyl-1-[(2,4-dimethylphenyl)methyl]quinolin-4(1*H*)-one (13q). White solid; 58%; IR ν 1661 (C=O), 1622 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.23 (s, 6H, CH_3), 2.71 (s, 3H, CH_3), 5.65 (s, 2H, CH_2), 6.89 (s, 2H, benzene H), 6.93 (s, 1H, benzene H), 7.53 (d, 1H, quinolinone C8-H), 7.68-7.73 (m, 2H, quinolinone C6-H and C7-H), 8.35 (d, 1H, quinolinone C5-H), 8.86 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3,5-dimethylphenyl)methyl]quinolin-4(1*H*)-one (13r). White solid; 68%; IR ν 1666 (C=O), 1625 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.24 (s, 6H, CH_3), 2.70 (s, 3H, CH_3), 5.66 (s, 2H,

CH_2), 6.88 (s, 2H, benzene H), 6.95 (s, 1H, benzene H), 7.52 (d, 1H, quinolinone C8-H), 7.67-7.74 (m, 2H, quinolinone C6-H and C7-H), 8.36 (d, 1H, quinolinone C5-H), 8.88 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3-chloro-2-fluorophenyl)methyl]quinolin-4(1*H*)-one (13s). White solid; 74%; IR ν 1667 (C=O), 1633 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.57 (s, 3H, CH_3), 5.74 (s, 2H, CH_2), 7.15-7.40 (m, 3H, benzene H and quinolinone C6-H and C7-H), 7.50-7.63 (m, 3H, benzene H and quinolinone C8-H), 8.26 (d, 1H, quinolinone C5-H), 8.77 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(3-chloro-4-fluorophenyl)methyl]quinolin-4(1*H*)-one (13t). White solid; 55%; IR ν 1662 (C=O), 1631 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.57 (s, 3H, CH_3), 5.62 (s, 2H, CH_2), 7.16-7.39 (m, 3H, benzene H and quinolinone C6-H and C7-H), 7.51-7.64 (m, 3H, benzene H and quinolinone C8-H), 8.25 (d, 1H, quinolinone C5-H), 8.79 (s, 1H, quinolinone C2-H).

3-Acetyl-8-chloro-1-[(3-chloro-4-fluorophenyl)methyl]quinolin-4(1*H*)-one (13u). White solid; 53%; IR ν 1660 (C=O), 1633 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.56 (s, 3H, CH_3), 5.96 (s, 2H, CH_2), 6.97 (t, 1H, quinolinone C6-H), 7.27-7.40 (m, 3H, benzene H and C7-H), 7.75 (d, 1H, benzene H), 8.30 (d, 1H, quinolinone C5-H), 8.58 (s, 1H, quinolinone C2-H).

3-Acetyl-8-chloro-1-[(2-fluorophenyl)methyl]quinolin-4(1*H*)-one (13v). White solid; 52%; IR ν 1665 (C=O), 1618 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.55 (s, 3H, CH_3), 5.86 (s, 2H, CH_2), 6.87-6.94 (m, 2H, benzene H and quinolinone C6-H), 7.23-7.35 (m, 3H, benzene H and quinolinone C7-H), 7.71 (d, 1H, benzene H), 8.29 (d, 1H, quinolinone C5-H), 8.56 (s, 1H, quinolinone C2-H).

3-Acetyl-7-fluoro-1-[(2-fluorophenyl)methyl]quinolin-4(1*H*)-one (13w). White solid; 62%; IR ν 1662 (C=O), 1631 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ2.55 (s, 3H, CH_3), 5.69 (s, 2H, CH_2), 7.09-7.22 (m, 3H, benzene H and quinolinone C6-H), 7.30 (m, 1H, benzene H), 7.44 (d, 1H, benzene H), 7.73 (s, 1H, quinolinone C8-H), 8.23 (d, 1H, quinolinone C5-H), 8.74 (s, 1H, quinolinone C2-H).

3-Acetyl-1-(4-phenylbutyl)quinolin-4(1*H*)-one (13x). White solid; 65%; IR ν 1672 (C=O), 1655 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 1.60 (m, 2H, CH_2), 1.75 (m, 2H, CH_2), 2.55-2.60 (m, 5H, CH_3 and CH_2), 4.41 (t, 2H, CH_2), 7.12-7.25 (m, 5H, benzene H), 7.48 (m, 1H, quinolinone C6-H), 7.74-7.79 (m, 2H, quinolinone C8-H and C7-H), 8.30 (d, 1H, quinolinone C5-H), 8.63 (s, 1H, quinolinone C2-H).

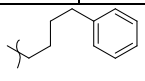
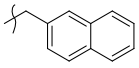
3-Acetyl-1-[(naphthalen-2-yl)methyl]quinolin-4(1*H*)-one (13y). White solid; 60%; IR ν 1668 (C=O), 1633 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.66 (s, 3H, CH_3), 5.86 (s, 2H, CH_2), 7.36-7.48 (m, 4H, naphthalene H), 7.61-7.70 (m, 2H, naphthalene H), 7.74 (s, 1H, naphthalene H), 7.82-7.90 (m, 3H, quinolinone C6-H, C7-H and C8-H), 8.31 (d, 1H, quinolinone C5-H), 8.93 (s, 1H, quinolinone C2-H).

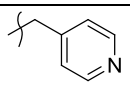
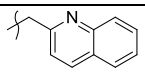
3-Acetyl-1-[(pyridin-4-yl)methyl]quinolin-4(1*H*)-one (13z). Dark solid; 55%; IR ν 1660 (C=O), 1621 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.64 (s, 3H, CH_3), 5.76 (s, 2H, CH_2), 7.17 (d, 2H, pyridine H), 7.45 (t, 1H, quinolinone C6-H), 7.51 (d, 1H, quinolinone C8-H), 7.67 (t, 1H, quinolinone C7-H), 8.31 (d, 1H, quinolinone C5-H), 8.49 (d, 2H, pyridine H), 8.86 (s, 1H, quinolinone C2-H).

3-Acetyl-1-[(quinolin-2-yl)methyl]quinolin-4(1*H*)-one (13aa). Brown solid; 52%; IR ν 1658 (C=O), 1634 (C=O) cm^{-1}; ^1H NMR (DMSO-d_6) δ 2.67 (s, 3H, CH_3), 5.98 (s, 2H, CH_2), 7.42 (m, 1H, quinoline H), 7.50 (d, 1H, quinoline H), 7.54-7.61 (m, 3H, quinoline H and quinolinone C6-H), 7.69 (t, 1H, quinolinone C7-H), 7.82 (d, 1H, quinoline H), 7.94 (d, 1H, quinolinone C8-H), 8.30 (d, 1H, quinoline H), 8.36 (d, 1H, quinolinone C5-H), 8.94 (s, 1H, quinolinone C2-H).

2. Table 1. Chemical, Physical and Analytical Data of Derivatives **13a-c** and **13a-aa.**

N°	R	R_2	R_3	R_4	R_5	R_6	mp (°C)	Recryst solvent[a]	yield (%)

12a[b]	H	-	-	-	-	-	242	a	56
12b	7-Cl	-	-	-	-	-	>300	h	95
12c[c]	8-Cl	-	-	-	-	-			
13a	-	H	H	H	H	H	212-213	b	
13b	-	F	H	H	H	H	199-201	c	79
13c	-	OCH_3	H	H	H	H	204-206	e	88
13d	-	H	F	H	H	H	247-248	d	81
13e	-	H	OCH_3	H	H	H	175-177	b	86
13f	-	H	H	Cl	H	H	242-244	d	82
13g	-	H	H	OH	H	H	203-205	i	96
13h	-	H	H	OCH_3	H	H	165-166	b	88
13i	-	H	H	NO_2	H	H	160-161	d	80
13j	-	F	H	F	H	H	234-236	c	81
13k	-	F	H	H	F	H	182-187	c	89
13l	-	F	H	H	H	F	192-193	e	
13m	-	H	F	F	H	H	256-260	f	93
13n	-	H	F	H	F	H	250-252	a	83
13o	-	Cl	H	Cl	H	H	270-273	e	98
13p	-	Cl	H	H	H	Cl	195-198	c	87
13q	-	CH_3	H	CH_3	H	H	210-212	c	100
13r	-	H	CH_3	H	CH_3	H	232-237	c	100
13s	-	F	Cl	H	H	H	132-133		
13t	-	H	Cl	F	H	H	132-133		
13u	8-Cl	H	Cl	F	H	H	197-198		
13v	8-Cl	F	H	H	H	H			
13w	7-Cl	F	H	H	H	H			
13x							99-101	b	26
13y							226-227	i	69

13z		254-256	d	73
13aa		241-242	d	100

[a] Recrystallization solvents: (a) acetone, (b) benzene/cyclohexane, (c) toluene, (d) DMF/H_2O, (e) benzene, (f) chloroform, (g) toluene/cyclohexane, (h) ethanol, (i) methanol. [b] See Mapara, R. K.; Desai, C. Synthesis of 4-hydroxyquinolines. *J. Indian. Chem. Soc.* **1954**, *31*, 951–956. [c] Reference [19b].

3. Analyses

Compd	Elemental Analyses Calculated/ Found				
	C	H	N	Cl	F
10a	70.02	5.07	3.71		
	70.29	4.97	4.01		
10b	66.83	4.59	3.54		4.81
	66.81	4.87	3.50		4.88
10c	67.80	5.20	3.44		
	68.05	5.36	3.55		
10d	66.83	4.59	3.54		4.81
	66.80	4.25	3.39		4.69
10e	67.80	5.20	3.44		
	67.78	5.21	3.41		
10f	64.16	4.41	3.40	8.61	
	63.93	4.59	3.70	8.66	
10g	67.17	4.87	3.56		
	67.21	4.93	3.80		
10h	67.80	5.20	3.44		
	67.65	5.08	3.47		

10i	62.56	4.30	6.63		
	62.50	4.20	6.99		
10j	63.92	4.15	3.39		9.19
	63.91	4.25	3.03		9.50
10k	63.92	4.15	3.39		9.19
	63.83	4.34	3.31		9.22
10l	63.92	4.15	3.39		9.19
	63.59	3.98	3.38		9.30
10m	63.92	4.15	3.39		9.19
	63.55	4.08	3.36		9.27
10n	63.92	4.15	3.39		9.19
	68.69	4.13	3.18		9.21
10o	59.21	3.84	3.14	15.89	
	59.40	3.79	3.01	15.70	
10p	59.21	3.84	3.14	15.89	
	59.49	3.71	3.18	15.78	
10q	71.10	5.72	3.45		
	71.13	5.77	3.11		
10r	71.10	5.72	3.45		
	71.21	5.79	3.63		
10s	61.48	3.99	3.26	8.25	4.42
	61.62	4.25	3.46	8.29	4.50
10t	61.48	3.99	3.26	8.25	4.42
	61.22	3.98	3.33	8.31	4.64
10u	56.91	3.47	3.02	15.27	4.09
	56.92	3.47	2.94	15.35	3.99
10v	61.48	3.99	3.26	8.25	4.42

	61.28	4.04	3.22	8.20	4.55
10w	61.48	3.99	3.26	8.25	4.42
	61.71	3.95	3.39	8.10	4.50
10x	71.58	6.01	3.34		
	71.59	6.08	3.05		
10y	73.06	4.95	3.28		
	73.13	4.91	3.34		
10z	66.66	4.79	7.40		
	66.89	4.78	7.60		
10aa	70.08	4.71	6.54		
	70.19	4.56	6.75		
11a	68.76	4.33	4.01		
	68.40	4.38	4.06		
11b	65.40	3.84	3.81		5.17
	65.59	3.86	3.87		5.11
11c	66.49	4.52	3.69		
	66.47	4.24	3.72		
11d	65.40	3.84	3.81		5.17
	65.50	3.83	3.70		5.29
11e	66.49	4.52	3.69		
	66.53	4.64	3.59		
11f	62.59	3.68	3.65	9.24	
	62.76	3.93	3.98	9.35	
11g	65.75	4.14	3.83		
	65.85	4.12	3.81		
11h	66.49	4.52	3.69		
	66.46	4.30	3.68		
11i	60.92	3.58	7.10		

	60.91	3.30	7.11		
11j	62.34	3.40	3.64		9.86
	62.30	3.51	3.49		9.99
11k	62.34	3.40	3.64		9.86
	62.40	3.57	3.51		10.00
11l	62.34	3.40	3.64		9.86
	62.38	3.23	3.33		9.72
11m	62.34	3.40	3.64		9.86
	62.70	3.33	3.41		9.66
11n	62.34	3.40	3.64		9.86
	62.10	3.40	3.71		9.88
11o	57.44	3.13	3.35	16.95	
	57.40	3.11	3.68	17.10	
11p	57.44	3.13	3.35	16.95	
	57.41	3.21	3.56	16.85	
11q	70.02	5.07	3.71		
	69.90	5.21	3.78		
11r	70.02	5.07	3.71		
	70.00	5.12	3.51		
11s	59.79	3.26	3.49	8.82	4.73
	59.54	2.98	3.22	8.70	4.60
11t	59.79	3.26	3.49	8.82	4.73
	60.01	3.13	3.52	8.80	4.99
11u	55.07	2.77	3.21	16.25	4.36
	55.10	2.90	3.29	16.30	4.38
11v	59.79	3.26	3.49	8.82	4.73
	59.87	3.20	3.57	8.80	4.77
11w	59.79	3.26	3.49	8.82	4.73
	59.70	3.04	3.23	8.75	4.70

11x	70.58	5.41	3.58
	70.51	5.22	3.40
11y	72.17	4.29	3.51
	72.18	4.18	3.50
11z	65.14	4.03	8.00
	65.14	3.99	8.32
11aa	69.00	4.03	7.00
	69.11	4.17	7.14

Molecular Modelling

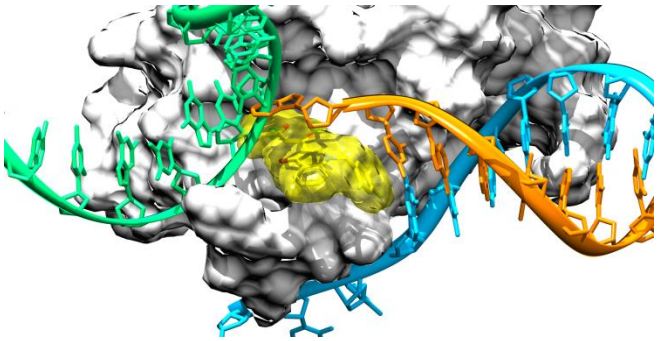


Figure S1. Superimposition between our model of the INSTI/HIV-1 IN CCD/viral DNA ternary complex and the pre-catalytic target capture complex (TCC) from PFV (PDB code 3OS1). IN enzymes are represented as light gray surfaces. The host DNA (green) and the non-transferred (cyan) and reactive (orange) viral DNA strands are shown as ribbon and sticks. Compound **11j** is depicted as yellow transparent surface and sticks.

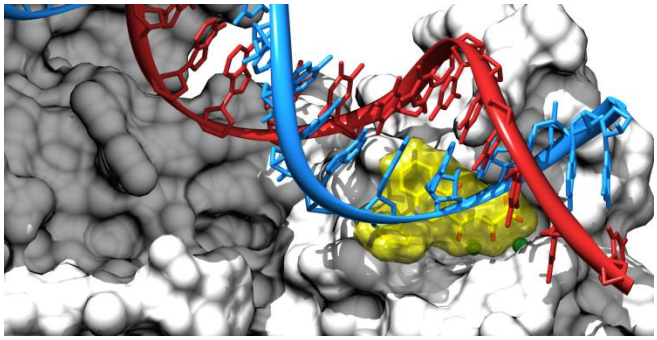


Figure S2. Superimposition between our model of the INSTI/RNase H CCD binary complex and the crystal structure of the full-length HIV-1 RT in complex with a synthetic RNA:DNA hybrid (PDB code 1HYS). RNase H enzymes are represented as white surfaces. The DNA (red) and RNA (light blue) strands are shown as ribbon and sticks. Compound **11j** is depicted as yellow transparent surface and sticks.

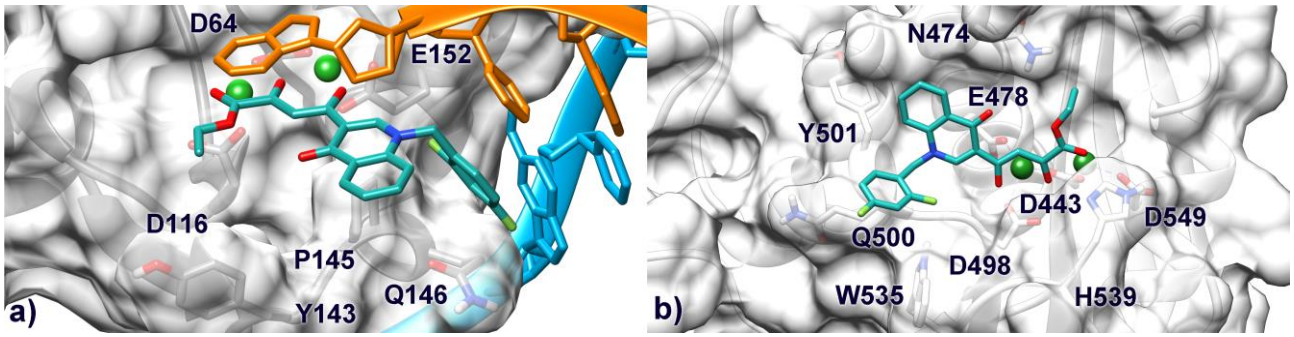


Figure S3. a) Binding mode of compound **10j** (cyan) within the HIV-1 IN/DNA model. Catalytic core domain is depicted as transparent light gray surface and ribbons. The non-transferred (blue) and reactive (orange) viral DNA strands are shown as ribbon and sticks. b) Binding mode of compound **10j** (cyan) within the HIV-1 RNase H active site. Catalytic core domain is shown as transparent white surface and ribbons. In both figures, amino acid side chains important for ligand binding are represented as sticks, while Mg^{2+} metal ions are depicted as green spheres.

References

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