Supporting Information

Design and Synthesis of New Alkenyldiarylmethane (ADAM) HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs)

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Elemental analysis data

Code	Found					Calculated				
	C	H	N	Sn(Cl)	I(F)	C	H	N	Sn(Cl)	I(F)
3	65.58	6.39	2.71			65.92	6.42	3.08		
4	66.11	6.51	3.18			65.92	6.42	3.08		
7	59.65	5.03	3.15		15.65	59.87	4.82	2.91		15.78
8	59.75	4.97	3.14		17.02	60.14	4.82	3.19		17.29
9	60.02	5.20	3.44			60.14	4.82	3.19		
10	58.99	5.34		15.01		59.11	5.18		15.17	
11	64.47	6.05		7.88		64.50	6.09		7.93	
12	61.68	5.53			15.99	61.54	5.16			16.22
13	56.70	4.56		7.03	15.23	56.51	4.33		7.25	15.55
14	64.86	6.26		7.56		64.50	6.09		7.93	
15	61.55	5.32			16.18	61.54	5.16			16.22
16	70.46	6.20	3.19			70.74	6.18	3.44		
17	64.39	5.12	3.26	8.22		64.56	5.18	3.27	8.29	
18	68.25	5.34	3.74	9.53		68.20	5.45	3.79	9.59	
19	61.32	4.89	3.07		16.65	61.20	4.69	3.10		16.83
20	70.43	5.79	7.01			70.75	5.68	7.17		
21	64.33	5.61	3.28	8.22		64.26	5.63	3.26	8.25	
22	61.39	4.88	3.06	16.59		61.20	4.69	3.10	16.83	
25	60.22	6.62	9.83			60.42	6.52	10.07		

30	64.50	6.18	4.08			64.34	6.03	4.41		
31	56.92	7.80	2.16	19.16		57.25	7.79	2.30	19.51	
32	46.03	4.45	3.40		28.69	45.86	4.53	3.15		28.50
34	65.13	6.16	4.80			65.44	6.22	5.09		
35	57.30	7.79	2.18	20.63		57.27	8.01	2.47	20.96	
36	57.02	7.74	2.49	19.38		57.25	7.79	2.30	19.51	
41	58.30	4.27		26.22		58.34	4.20			26.36
42	73.61	5.97	5.77			73.99	5.77	6.16		
43	54.18	6.99		20.36	12.87	53.91	6.96		20.49	13.12
44	60.31	7.64	2.37	22.66		60.25	7.97	2.70	22.90	
49	63.42	5.80		12.98		64.04	5.67		13.26	
51	56.17	7.67		20.88	6.14(Cl)	55.99	7.77		21.88	6.36(Cl)
56	33.05	2.68	4.73		43.01	32.79	2.75	4.78		43.30
57	35.00	2.30	4.82		46.01	34.96	2.20	5.09		46.14
58	37.52	2.84	4.55		43.53	37.39	2.79	4.85		43.90
59	37.73	2.98	4.70		44.01	37.39	2.79	4.85		43.90

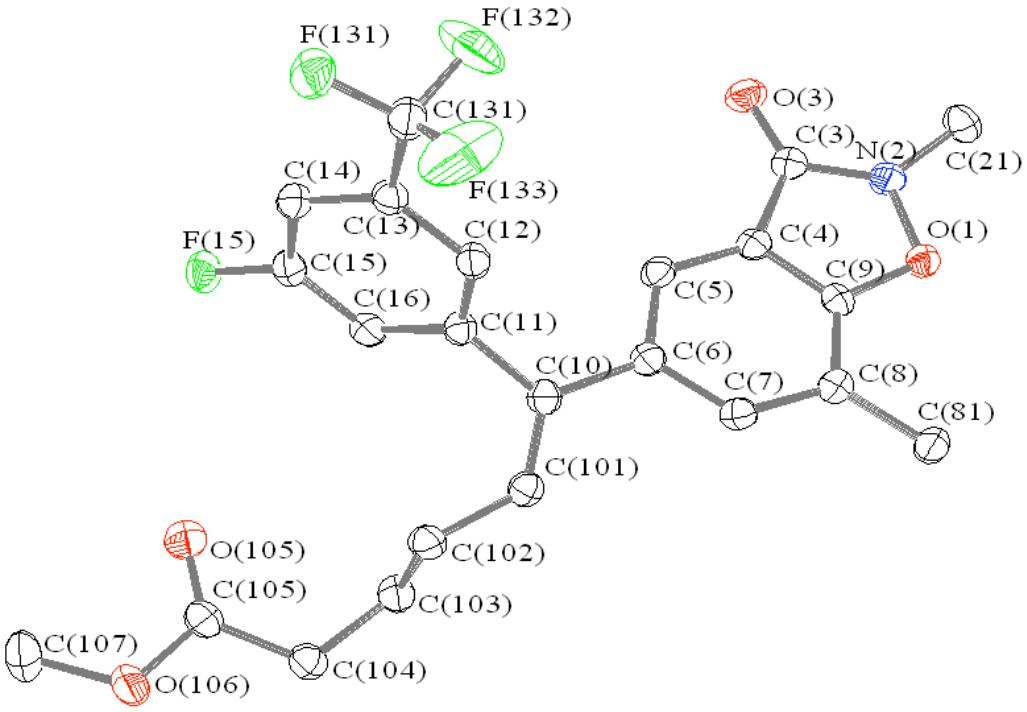

Figure 1 Structural Diagram of Compound **22**. Hydrogen atoms have been omitted for clarity.

Crystal Data and Data Collection Parameters for Compound 22

formula	$C_{23}H_{21}F_4NO_4$
formula weight	451.42
space group	P-1 (No. 2)
a, Å	8.8822(7)
b, Å	9.7444(9)
c, Å	12.9675(17)
a, deg	76.306(4)

b, deg	72.480(6)
g, deg	89.873(5)
V, $Å^3$	1036.98(19)
Z	2
d_{calc}, g cm^{-3}	1.446
crystal dimensions, mm	0.44x0.29x0.13
temperature, K	150.
radiation (wavelength, Å)	Mo K_a (0.71073)
monochromator	graphite
linear abs coef, mm^{-1}	0.115
absorption correction applied	empirical
transmission factors: min, max	0.94, 0.99
diffractometer	Nonius KappaCCD
h, k, l range	-11 to 0 -12 to 12 -17 to 15
2q range, deg	4.31-55.81
mosaicity, deg	0.39
programs used	SHELXTL
F_{000}	468.0
weighting	
$1/[\sigma^2(Fo^2)+(0.0722P)^2+0.0000P]$ where $P=(Fo^2+2Fc^2)/3$	
data collected	12884
unique data	4884
R_{int}	0.038

data used in refinement	4879
cutoff used in R-factor calculations	$F_o^2 > 2.0\sigma (F_o^2)$
data with I>2.0s(I)	3461
number of variables	292
largest shift/esd in final cycle	0.00
$R(F_o)$	0.046
$R_w(F_o^2)$	0.117
goodness of fit	1.034

Crystallographic Data for Compound 22

$C_{23}H_{21}F_4NO_4$	formula weight 451.42
a = 8.8822(7)Å	space group P-1 (No. 2)
b = 9.7444(9)Å	T = 150. K
c = 12.9675(17)Å	l = 0.71073Å
a = 76.30(4)°	r_{calc} = 1.446g cm^{-3}
b = 72.48(6)°	m = 0.115mm^{-1}
g = 89.87(5)°	transmission coeff = 0.940-0.986
V = 1036.98(19)Å ^{3}	$R(F_o)^a$ = 0.046
	$R_w(F_o^2)^b$ = 0.117

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[a] $R = \Sigma \, ||F_o| - |F_c|| / S \, |F_o|$ for $F_o^2 > 2\sigma (F_o^2)$

[b] $R_w = [\Sigma \, w \, (|F_o^2| - |F_c^2|)^2 / \Sigma \, w \, |F_o^2|^2]^{1/2}$

Table 2. Bond Distances in Angstroms for Compound **22**

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
F(15)	C(15)	1.3569(17)	C(6)	C(10)	1.491(2)
F(131)	C(131)	1.3244(18)	C(7)	C(8)	1.384(2)
F(132)	C(131)	1.328(2)	C(8)	C(9)	1.391(2)
F(133)	C(131)	1.325(2)	C(8)	C(81)	1.508(2)
O(1)	C(9)	1.3762(18)	C(10)	C(101)	1.341(2)
O(1)	N(2)	1.4192(16)	C(10)	C(11)	1.4953(19)
O(3)	C(3)	1.2366(18)	C(11)	C(16)	1.393(2)
O(105)	C(105)	1.2014(19)	C(11)	C(12)	1.395(2)
O(106)	C(105)	1.342(2)	C(12)	C(13)	1.389(2)
O(106)	C(107)	1.444(2)	C(13)	C(14)	1.390(2)
N(2)	C(3)	1.360(2)	C(13)	C(131)	1.496(2)
N(2)	C(21)	1.435(2)	C(14)	C(15)	1.379(2)
C(3)	C(4)	1.460(2)	C(15)	C(16)	1.378(2)
C(4)	C(9)	1.381(2)	C(101)	C(102)	1.495(2)
C(4)	C(5)	1.395(2)	C(102)	C(103)	1.533(2)
C(5)	C(6)	1.397(2)	C(103)	C(104)	1.522(2)
C(6)	C(7)	1.415(2)	C(104)	C(105)	1.498(2)

Numbers in parentheses are estimated standard deviations in the least significant

digits.

Table 3. Bond Angles in Degrees for Compound **22**

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(9)	O(1)	N(2)	103.74(11)	C(16)	C(11)	C(12)	118.71(13)
C(105)	O(106)	C(107)	117.08(14)	C(16)	C(11)	C(10)	120.98(13)
C(3)	N(2)	O(1)	112.95(13)	C(12)	C(11)	C(10)	120.30(13)
C(3)	N(2)	C(21)	131.58(14)	C(13)	C(12)	C(11)	120.40(13)
O(1)	N(2)	C(21)	114.93(12)	C(12)	C(13)	C(14)	121.39(13)
O(3)	C(3)	N(2)	123.66(15)	C(12)	C(13)	C(131)	118.09(13)
O(3)	C(3)	C(4)	131.74(15)	C(14)	C(13)	C(131)	120.50(13)
N(2)	C(3)	C(4)	104.59(13)	C(15)	C(14)	C(13)	116.74(13)
C(9)	C(4)	C(5)	120.47(14)	F(15)	C(15)	C(16)	118.01(13)
C(9)	C(4)	C(3)	106.62(14)	F(15)	C(15)	C(14)	118.41(13)
C(5)	C(4)	C(3)	132.91(13)	C(16)	C(15)	C(14)	123.58(14)
C(4)	C(5)	C(6)	118.34(13)	C(15)	C(16)	C(11)	119.15(13)
C(5)	C(6)	C(7)	118.48(14)	C(10)	C(101)	C(102)	129.24(14)
C(5)	C(6)	C(10)	121.20(13)	C(101)	C(102)	C(103)	110.48(13)
C(7)	C(6)	C(10)	120.31(14)	C(104)	C(103)	C(102)	113.47(14)
C(8)	C(7)	C(6)	124.41(15)	C(105)	C(104)	C(103)	115.15(14)
C(7)	C(8)	C(9)	114.35(13)	O(105)	C(105)	O(106)	123.49(15)
C(7)	C(8)	C(81)	123.62(14)	O(105)	C(105)	C(104)	126.66(15)
C(9)	C(8)	C(81)	122.02(14)	O(106)	C(105)	C(104)	109.84(13)

O(1)	C(9)	C(4)	111.98(13)	F(131)	C(131)	F(133)	106.81(15)
O(1)	C(9)	C(8)	124.11(13)	F(131)	C(131)	F(132)	106.04(14)
C(4)	C(9)	C(8)	123.91(15)	F(133)	C(131)	F(132)	105.48(15)
C(101)	C(10)	C(6)	120.93(13)	F(131)	C(131)	C(13)	113.81(13)
C(101)	C(10)	C(11)	121.54(14)	F(133)	C(131)	C(13)	112.69(14)
C(6)	C(10)	C(11)	117.53(12)	F(132)	C(131)	C(13)	111.43(15)

Numbers in parentheses are estimated standard deviations in the least significant digits.

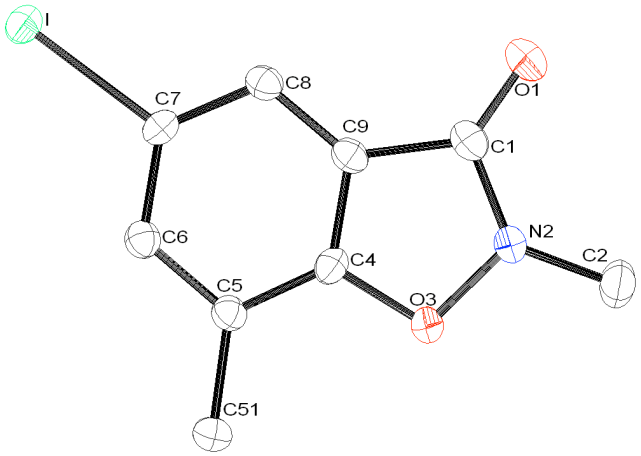

Figure 2 Structural diagram of compound **58**. Hydrogen atoms have been omitted for clarity.

Crystallographic Data for Compound 58

Formula	$C_9H_8INO_2$
Weight	289.07
a = 4.1515(5)Å	space group $P2_1/c$ (No. 14)
b = 16.0162(12)Å	T = 150. K
c = 14.1406(11)Å	l = 0.71073Å
b = 97.41(5)°	r_{calc} = 2.059g cm^{-3}
V = 932.37(15)Å ^{3}	m = 3.361mm^{-1}
	transmission coeff = 0.623-0.715
	$R(F_o)^a$ = 0.029
	$R_w(F_o^2)^b$ = 0.071

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[a] $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ for $F_o^2 > 2s(F_o^2)$

[b] $R_w = [\sum w (|F_o^2| - |F_c^2|)^2 / \sum w |F_o^2|^2]^{1/2}$

Table 4. Bond Angles in Degrees for Compound **58**

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(4)	O(3)	N(2)	103.8(2)	C(4)	C(5)	C(51)	122.9(3)
C(1)	N(2)	O(3)	113.1(3)	C(6)	C(5)	C(51)	122.7(3)
C(1)	N(2)	C(2)	130.7(3)	C(7)	C(6)	C(5)	121.5(3)
O(3)	N(2)	C(2)	114.7(3)	C(8)	C(7)	C(6)	122.5(3)
O(1)	C(1)	N(2)	123.9(3)	C(8)	C(7)	I	119.5(2)

O(1)	C(1)	C(9)	132.1(4)	C(6)	C(7)	I	118.0(2)
N(2)	C(1)	C(9)	104.0(3)	C(9)	C(8)	C(7)	116.1(3)
C(9)	C(4)	C(5)	124.6(3)	C(4)	C(9)	C(8)	120.9(3)
C(9)	C(4)	O(3)	112.2(3)	C(4)	C(9)	C(1)	106.8(3)
C(5)	C(4)	O(3)	123.2(3)	C(8)	C(9)	C(1)	132.3(3)
C(4)	C(5)	C(6)	114.4(3)				

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table 5. Bond Distances in Angstroms for Compound **58**

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
I	C(7)	2.100(3)	C(4)	C(9)	1.378(4)
O(1)	C(1)	1.218(4)	C(4)	C(5)	1.382(4)
O(3)	C(4)	1.382(4)	C(5)	C(6)	1.399(5)
O(3)	N(2)	1.420(3)	C(5)	C(51)	1.506(4)
N(2)	C(1)	1.371(5)	C(6)	C(7)	1.399(5)
N(2)	C(2)	1.427(5)	C(7)	C(8)	1.384(4)
C(1)	C(9)	1.475(4)	C(8)	C(9)	1.382(5)

Numbers in parentheses are estimated standard deviations in the least significant digits.