

Supporting Information

Diarylaniline Derivatives as a Novel Class of HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors

Bingjie Qin,[†] Xingkai Jiang,[†] Hong Lu,[§] Xingtao Tian,[†] Florent Barbault,[⊥] Li
Huang,^{||} Keduo Qian,[‡] Chin-Ho Chen,^{||} Rong Huang,[‡] Shibo Jiang,[§] Kuo-Hsiung
Lee,[‡] and Lan Xie^{†,*}

[†]*Beijing Institute of Pharmacology and Toxicology, 27 Taiping Road, Beijing, 100850, China.*

[‡]*Natural Products Research Laboratories, University of North Carolina, Chapel Hill, NC 27599,
US.*

[§]*Lindsley F. Kimball Research Institute, New York Blood Center, New York, NY 10065, US.*

[⊥]*ITODYS, Université Paris Diderot - CNRS UMR 7086, 15 rue Jean de Baïf, 75205 Paris,
France.*

^{||}*Duke University Medical Center, Box 2926, Surgical Oncology Research Facility, Durham, NC
27710, US.*

Contents.

1. HPLC conditions and summary of HPLC purity data for final compounds

HPLC analyses for purity were performed using a Grace Alltima HP C18 column (100 × 2.1 mm, 3 μm) eluting with a mixture of solvents A and B, UV wavelength, maximal absorbance at 254 nm; temperature, ambient; injection volume, 3 μL.

Condition 1: acetonitrile/water 80:20, flow rate 0.2 mL/min;

Condition 2: methanol/water 80:20, flow rate 0.2 mL/min.

Summary of HPLC purity data for final compounds

Code#	HPLC-1		HPLC-2	
	Retention time (min)	Purity %	Retention time (min)	Purity %
13	3.055	99.425	4.685	99.864
15	3.345	95.751	3.754	95.289
16	4.482	97.511	4.893	97.803
17	4.564	96.278	8.346	97.544
18	3.235	97.718	5.264	97.458
19	2.937	98.503	4.069	97.986
20	2.574	99.926	3.246	100.000
21	2.652	98.050	3.550	96.123
22	2.939	98.276	4.056	99.627
24	4.550	95.694	7.589	95.998
25	3.284	96.554	3.258	97.426
26	2.455	99.031	2.259	99.630
27	4.460	95.901	7.553	96.348
29	3.035	96.767	4.813	96.043
30	2.144	99.201	2.326	99.663
31	2.744	99.757	3.750	97.869
32	2.294	96.081	2.965	96.105
34 ^a	3.983	100.00	3.270	99.529
35 ^a	4.803	100.00	4.783	97.711
36	2.484	96.990	3.500	97.772
37	1.936	96.837	2.081	97.763
38	2.207	98.255	2.185	97.895
39 ^a	5.415	95.967	4.725	97.088
40	2.518	97.615	3.490	97.924

^a Agilent TC-C18 column (250 × 4.6 mm, 5 μm), flow rates: 1.0 mL/min (condition 1) and 1.0 mL/min (condition 2)