

**Supporting Information**

**Design, Synthesis, and Preclinical Evaluations of Novel**

**4-Substituted 1,5-Diarylanilines as Potent HIV-1**

**Non-Nucleoside Reverse Transcriptase Inhibitor (NNRTI)**

**Drug Candidates**

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**HPLC conditions:**

HPLC analyses for purity were performed using an Agilent TC-C18 column (4.6 × 250 mm, 5 μm) eluting with a mixture of solvents A and B (Condition 1: acetonitrile/water 70:30, flow rate 1.0 mL/min; Condition 2: methanol/water 70:30, flow rate 0.8 mL/min), detected under UV wavelength at 254 nm and an injection volume of 15 μL.

**Table 1.** Summary of HPLC purity data for target compounds

compounds	condition-1		condition-2	
	Retention time (min)	Purity %	Retention time (min)	Purity %
<b>13a</b>	8.346	100.00	21.905	97.91
<b>13b</b>	8.269	97.56	19.611	96.89
<b>13c</b>	8.445	99.32	18.683	100.00
<b>13d</b>	5.728	96.80	8.632	96.19
<b>13e</b>	2.801	100.00	4.524	96.42
<b>14a</b>	9.274	97.29	21.790	97.29
<b>14b</b>	3.656	100.00	5.213	100.00
<b>14c</b>	5.571	100.00	9.175	96.63
<b>14d</b>	3.786	100.00	4.353	97.03
<b>14e</b>	3.218	100.00	5.540	100.00
<b>14f</b>	4.322	100.00	7.233	100.00
<b>14h</b>	4.174	99.86	6.733	99.89
<b>15a</b>	7.329	95.47	13.276	95.80
<b>15b</b>	3.939	97.59	4.971	100.00
<b>15c</b>	4.954	100.00	7.155	100.00
<b>15d</b>	3.666	97.94	3.852	100.00
<b>15e</b>	3.785	100.00	5.338	100.00
<b>15f</b>	3.433	100.00	5.985	100.00
<b>15h</b>	4.082	96.24	5.903	99.14
<b>15i</b>	4.447	100.00	5.818	100.00
<b>16a</b>	4.388	100.00	6.741	100.00
<b>16b</b>	4.350	100.00	6.429	100.00