Supporting Information Available.

IMPROVING THE ANTIVIRAL EFFICACY AND SELECTIVITY OF HIV-1 REVERSE TRANSCRIPTASE INHIBITOR TSAO-T BY THE INTRODUCTION OF FUNCTIONAL GROUPS AT THE N-3 POSITION

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Spectroscopic data: ^{1}H and ^{13}C NMR chemical shift assignments of compounds 1-31.

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[(methoxycarbonyl)methyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (1). ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.81, 0.97 (2s, 18H, 2t-Bu), 2.00 (s, 3H, CH_3-5), 3.74 (s, 3H, OCH_3), 3.89 (dd, 1H, H-5'a, $J_{4',5'a}$ = 2.9 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.01 (dd, 1H, H-5'b, $J_{4',5'b}$ = 2.7 Hz), 4.32 (t, 1H, H-4'), 4.56 (d, 1H, H-2'), 4.62 (d, 1H, NCH_2a, J = 16.4 Hz), 4.75 (d, 1H, NCH_2b), 5.53 (bs, 2H, NH_2-4''), 5.61 (s, 1H, H-3''), 5.91 (d, 1H, H-1', $J_{1',2'}$ = 7.9 Hz), 7.24 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 12.9 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 47.3 (CH_2N), 50.1 (OCH_3), 62.1 (C-5'), 74.6 (C-2'), 85.1 (C-4'), 88.7 (C-3''), 92.1 (C-3'), 92.8 (C-1'), 111.3 (C-5), 134.6 (C-6), 150.7 (C-2), 151.6 (C-4''), 162.5 (C-4), 171.0 (CO).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(carbamoylmethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (3). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.98 (2s, 18H, 2t-Bu), 1.94 (s, 3H, CH_3-5), 4.04 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.8 Hz, $J_{5'a,5'b}$ = 12.3 Hz), 4.12 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.4 Hz), 4.32 (t, 1H, H-4'), 4.63 (d, 2H, NCH_2 , J = 15.7 Hz), 4.69 (d, 1H, H-2'), 5.74 (bs, 2H, NH_2-4''), 5.76 (s, 1H, H-3''), 6.05 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.43 (bs, 1H, CONHa), 7.04 (bs, 1H, CONHb), 7.57 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.3 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 42.6 (CH_2N), 63.1 (C-5'), 75.4 (C-2'), 85.4 (C-4'), 88.3 (C-3''), 92.1 (C-1'), 92.4 (C-3'), 110.9 (C-5), 134.7 (C-6), 152.1 (C-4''), 150.8 (C-2), 163.1 (C-4), 167.1 ($CONH_2$).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(cyclopropylmethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (4). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.48 (m, 5H, cyclopropyl),0.81, 0.97

(2s, 18H, 2t-Bu), 1.94 (s, 3H, CH_3-5), 3.78 (dd, 2H, NCH_2), 4.03 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.10 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.4 Hz), 4.33 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.76 (s, 1H, H-3''), 6.09 (d, 1H, H-1', $J_{1',2'}$ = 8.1 Hz), 6.47 (bs, 2H, NH_2-4''), 7.49 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 4.3 (CH_2-cyclopropyl), 5.7 (CH-cyclopropyl), 13.5 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 52.9 (CH_2N), 63.1 (C-5'), 75.5 (C-2'), 85.6 (C-4'), 88.5 (C-3''), 92.0 (C-1'), 92.3 (C-3'), 110.8 (C-5), 134.6 (C-6), 152.6 (C-4''), 150.8 (C-2), 163.5 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(benzyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (5). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.73, 0.96 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5), 4.00 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.10 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.4 Hz), 4.32 (t, 1H, H-4'), 4.65 (m, 2H, H-2', NCH_2), 5.09 (s, 2H, CH_2Ph), 5.76 (s, 1H, H-3''), 6.07 (d, 1H, H-1', $J_{1',2'}$ = 8.1 Hz), 6.45 (bs, 2H, NH_2-4''), 7.27-7.39 (m, 5H, Ph), 7.58 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.2 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 34.8 (CH_2Ph), 43.9 (CH_2N), 63.7 (C-5'), 75.6 (C-2'), 85.3 (C-4'), 87.6 (C-3''), 92.1 (C-1', C-3'), 111.3 (C-5), 134.2 (C-6), 150.9 (C-2), 152.4 (C-4''), 163.6 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(2-bromoethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (7). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.85, 0.99 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5), 3.59 (m, 2H, CH_2Br), 4.03 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.9 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.13 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.28 (s, 2H, NCH_2), 4.34 (t, 1H, H-4'), 4.70 (d, 1H, H-2'), 5.75 (s, 1H, H-3''), 6.04 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.40 (bs, 2H, NH_2-4''), 7.52 (s, 1H, H-6).^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 12.8 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 31.1 (CH_2Br), 47.6 (CH_2N), 62.5 (C-5'), 74.3 (C-2'), 83.6 (C-4'), 87.5

(C-3’’), 92.0 (C-3’), 92.5 (C-1’), 111.7 (C-5), 134.7 (C-6), 150.8 (C-2), 151.4 (C-4’’), 163.7 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(2-hydroxyethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (8). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.84, 0.96 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5), 3.67 (m, 2H, CH_2OH), 3.78 (t, 1H, OH, J = 2.8 Hz), 4.03 (dd, 1H, H-5’a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.06 (dd, 1H, H-5’b, $J_{4',5'b}$ = 3.4 Hz), 4.10 (s, 2H, NCH_2), 4.33 (t, 1H, H-4’), 4.64 (d, 1H, H-2’), 5.76 (s, 1H, H-3’’), 6.08 (d, 1H, H-1’, $J_{1',2'}$ = 8.2 Hz), 6.47 (bs, 2H, NH_2-4’’), 7.49 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 12.9 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 38.2 (CH_2N), 58.4 (CH_2OH), 62.3 (C-5’), 74.1 (C-2’), 83.3 (C-4’), 87.6 (C-3’’), 92.5 (C-3’), 93.0 (C-1’), 111.2 (C-5), 134.7 (C-6), 150.8 (C-2), 151.0 (C-4’’), 163.9 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(2-methoxyethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (9). ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.80, 0.96 (2s, 18H, 2t-Bu), 1.94 (s, 3H, CH_3-5), 3.27 (s, 3H, OCH_3), 3.53 (t, 2H, CH_2OCH_3), 4.03 (dd, 1H, H-5’a, $J_{4',5'a}$ = 3.8 Hz, $J_{5'a,5'b}$ = 12.0 Hz), 4.05 (dd, 1H, H-5’b, $J_{4',5'b}$ = 3.5 Hz), 4.11 (s, 2H, NCH_2), 4.32 (t, 1H, H-4’), 4.66 (d, 1H, H-2’), 5.76 (s, 1H, H-3’’), 6.07 (d, 1H, H-1’, $J_{1',2'}$ = 8.1 Hz), 6.48 (bs, 2H, NH_2-4’’), 7.49 (s, 1H, H-6). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 12.7 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 43.9 (CH_2N), 53.6 (OCH_3), 62.6 (C-5’), 70.6 (OCH_2), 74.1 (C-2’), 83.1 (C-4’), 87.2 (C-3’’), 93.0 (C-1’), 92.5 (C-3’), 111.2 (C-5), 134.7 (C-6), 151.2 (C-4’’), 150.9 (C-2), 163.5 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(2-phenylethyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (10). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.83, 0.97 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5),

2.85 (m, 2H, CH_2Ph), 4.06 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.4 Hz, $J_{5'a,5'b}$ = 9.6 Hz), 4.08 (d, 2H, NCH_2), 4.12 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.34 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.75 (s, 1H, H-3''), 6.12 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.46 (bs, 2H, NH_2-4''), 7.21-7.34 (Ph), 7.51 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.2 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 34.3 (CH_2Ph), 43.3 (CH_2N), 63.1 (C-5'), 75.3 (C-2'), 85.1 (C-4'), 87.8 (C-3''), 92.4 (C-1', C-3'), 111.6 (C-5), 127.5 (Ph), 129.5 (Ph), 134.8 (C-6), 139.5 (Ph), 152.0 (C-4''), 151.2 (C-2), 163.0 (C-4). Anal. ($C_{32}H_{51}N_3O_8SSi_2$) C, H, N, S. MS (ES+) m/z 694.3 $(M+1)^+$.

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[2-(3-indolyl)ethyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (11). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.98 (2s, 18H, 2t-Bu), 1.97 (s, 3H, CH_3-5), 3.00 (dd, 2H, CH_2-Indole), 4.05 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.4 Hz, $J_{5'a,5'b}$ = 12.3 Hz), 4.10 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.18 (t, 2H, NCH_2), 4.36 (t, 1H, H-4'), 4.70 (d, 1H, H-2'), 5.78 (s, 1H, H-3''), 6.16 (d, 1H, H-1', $J_{1',2'}$ = 8.1 Hz), 6.50 (bs, 2H, NH_2-4''), 7.22 (s, 1H, NH-Indole), 7.38 (m, 4H, Indole), 7.57 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.2 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 47.7 (CH_2N), 63.1 (C-5'), 75.4 (C-2'), 85.1 (C-4'), 87.7 (C-3'', C-1'), 92.2 (C-3'), 111.7 (C-5), 112.1-139.5 (Indole), 134.5 (C-6), 152.2 (C-4''), 152.0 (C-2), 163.2 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[(*N*'-methylcarbamoyl)methyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (12). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.83, 0.96 (2s, 18H, 2t-Bu), 1.98 (s, 3H, CH_3-5), 2.70 (d, 3H, CH_3NH, J = 4.6 Hz), 4.03 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.8 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.12 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.47 (d, 1H, NCH_2), 4.57 (d, 1H, NCH_2), 4.33 (t, 1H, H-4'), 4.67 (d, 1H, H-2'), 5.75 (s, 1H, H-3''), 6.04 (d, 1H, H-1', $J_{1',2'}$ = 8.1 Hz), 6.44 (bs, 2H, NH_2-4''), 7.52 (s, 1H, H-6), 7.18 (bs, 1H, CONH). ^{13}C

NMR [75 MHz, $(CD_3)_2CO$] δ: 13.1 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 34.2 (CH_3NH), 42.1 (CH_2N), 63.2 (C-5'), 75.3 (C-2'), 85.2 (C-4'), 88.3 (C-3''), 92.4 (C-1'), 92.9 (C-3'), 111.4 (C-5), 134.9 (C-6), 152.2 (C-4''), 150.1 (C-2), 163.1 (C-4), 167.4 (CONH).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[(*N'*,*N'*-dimethylcarbamoyl)methyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (13). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.96 (2s, 18H, 2t-Bu), 1.93 (s, 3H, CH_3-5), 2.87, 3.14 [s, 6H, $N(CH_3)_2$], 4.05 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.9 Hz, $J_{5'a,5'b}$ = 11.3 Hz), 4.09 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.6 Hz), 4.31 (t, 1H, H-4'), 4.73 (d, 1H, H-2'), 4.75 (dd, 2H, NCH_2), 5.74 (s, 1H, H-3''), 6.04 (d, 1H, H-1' , $J_{1',2'}$ = 8.5 Hz), 6.48 (bs, 2H, NH_2-4''), 7.54 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 12.6 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 34.9, 35.7 [$(CH_3)_2N$], 42.5 (CH_2N), 62.6 (C-5'), 74.3 (C-2'), 84.7 (C-4'), 87.7 (C-3''), 91.8 (C-1'), 92.0 (C-3'), 110.8 (C-5), 134.4 (C-6), 151.5 (C-4''), 151.8 (C-2), 162.6 (C-4), 165.7 (CON).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[4-(methoxycarbonyl)butyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (15). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.97 (s, 18H, 2t-Bu), 1.62 (m, 4H, CH_2), 1.93 (s, 3H, CH_3-5), 2.35 (m, 2H, CH_2CO), 3.60 (s, 3H, OCH_3), 3.92 (m, 2H, NCH_2), 4.06 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.6 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.10 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.8 Hz), 4.32 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.75 (s, 1H, H-3''), 6.06 (d, 1H, H-1', $J_{1',2'}$ = 8.1Hz), 6.44 (bs, 2H, NH_2-4''), 7.50 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.9 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 27.2 (CH_2CH_2CO), 30.7 (NCH_2CH_2), 47.4 (CH_2N), 60.0 (OCH_3), 63.9 (C-5'), 75.3 (C-2'), 85.1 (C-4'), 88.4 (C-3''), 92.2 (C-3'), 92.4 (C-1'), 111.7 (C-5), 134.4 (C-6), 152.3 (C-4''), 152.4 (C-2), 162.9 (C-4), 173.1 (CO).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[5-(ethoxycarbonyl)pentyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (16). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.97 (2s, 18H, 2t-Bu), 1.17 (t, 3H, CH_3), 1.30 (m, 2H, CH_2), 1.60 (m, 4H, CH_2), 1.94 (s, 3H, CH_3-5), 2.37 (m, 2H, CH_2CO), 3.80 (m, 2H, OCH_2), 3.99 (m, 4H, 2H-5', NCH_2), 4.36 (t, 1H, H-4'), 4.63 (d, 1H, H-2'), 5.73 (s, 1H, H-3''), 6.04 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.41 (bs, 2H, NH_2-4''), 7.53 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.3 (OCH_2), 14.7 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 26.5 (CH_2CH_2CO), 27.2 ($NCH_2CH_2CH_2$), 30.7 (NCH_2CH_2), 34.5 (CH_2CO), 47.7 (CH_2N), 60.6 (OCH_2), 63.3 (C-5'), 75.4 (C-2'), 85.3 (C-4'), 88.1 (C-3''), 92.6 (C-1'), 92.7 (C-3'), 111.6 (C-5), 134.7 (C-6), 152.1 (C-4''), 152.4 (C-2), 163.3 (C-4), 173.6 (CO).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[4-(*N'*-methylcarbamoyl)butyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (17). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.98 (2s, 18H, 2t-Bu), 1.59 (m, 2H, CH_2CH_2CO), 1.93 (s, 3H, CH_3-5), 2.66 (d, 3H, CH_3NH, J = 4.8 Hz), 3.90 (m, 2H, NCH_2), 3.91 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.6 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.09 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.9 Hz), 4.32 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.74 (s, 1H, H-3''), 6.04 (d, 1H, H-1', $J_{1',2'}$ = 7.9 Hz), 6.43 (bs, 2H, NH_2-4''), 7.49 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.1 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 29.1 (CH_3NH), 47.6 (CH_2N), 63.1 (C-5'), 75.6 (C-2'), 85.2 (C-4'), 88.3 (C-3''), 92.2 (C-1'), 92.3 (C-3'), 111.3 (C-5), 134.7 (C-6), 151.3 (C-2), 152.3 (C-4''), 163.5 (C-4), 167.1 (CONH).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[5-(*N'*-methylcarbamoyl)pentyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (18). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.98 (2s, 18H, 2t-Bu), 1.96 (s,

3H, CH_3-5), 2.69 (d, 3H, CH_3NH, J = 4.6 Hz), 2.95 (t, 2H, NCH_2, J = 4.6 Hz), 3.91 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.1 Hz, $J_{5'a,5'b}$ = 12.0 Hz), 4.05 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.9 Hz), 4.34 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.77 (s, 1H, H-3''), 6.09 (d, 1H, H-1', $J_{1',2'}$ = 8.3 Hz), 6.51 (bs, 2H, NH_2-4''), 7.50 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.5 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 29.0 (CH_3NH), 47.7 (CH_2N), 63.4 (C-5'), 75.3 (C-2'), 85.4 (C-4'), 88.6 (C-3''), 92.1 (C-1'), 92.2 (C-3'), 111.2 (C-5), 134.9 (C-6), 152.6 (C-4''), 151.3 (C-2), 163.4 (C-4), 165.1 (CONH).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-(methoxycarbonyl)-2-propenyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (19). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.98 (2s, 18H, 2t-Bu), 1.97 (s, 3H, CH_3-5), 3.69 (s, 3H, OCH_3), 4.07 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.9 Hz, $J_{5'a,5'b}$ = 13.2 Hz), 4.12 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.32 (t, 1H, H-4'), 4.70 (m, 3H, H-2', NCH_2), 5.78 (s, 1H, H-3''), 5.88 (m, 1H, CH=CH), 6.09 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.48 (bs, 2H, NH_2-4''), 6.90 (m, 1H, CH=CH), 7.56 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 14.7 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 42.3 (CH_2N), 51.6 (OCH_3), 63.2 (C-5'), 75.3 (C-2'), 85.3 (C-4'), 88.4 (C-3''), 92.6 (C-1'), 92.5 (C-3'), 111.7 (C-5), 123.4 (CH=CH), 135.2 (C-6), 142.7 (CH=CH), 152.2 (C-4''), 151.2 (C-2), 162.9 (C-4), 166.5 (CO).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(4-hydroxy-2-butenyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (20). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.82, 0.98 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5), 3.74 (s, 3H, OH), 4.03 (m, 2H, CH_2OH), 3,89 (dd, 1H, H-5'a, $J_{4',5'a}$ = 2.9 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.01 (dd, 1H, H-5'b, $J_{4',5'b}$ = 2.7 Hz), 4.32 (t, 1H, H-4'), 4.49 (d, 2H, NCH_2), 4.56 (d, 1H, H-2'), 5.61 (s, 1H, H-3''), 5.81 (m, 1H, CH=CH), 5.83 (m, 1H, CH=CH), 5.91 (d, 1H, H-1', $J_{1',2'}$ = 7.9 Hz), 5.53 (bs, 2H, NH_2-4''), 7.24 (s, 1H, H-6). ^{13}C NMR [75

MHz, $(CD_3)_2CO$] δ: 12.7 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 42.7 (CH_2N), 61.7 (CH_2OH), 62.7 (C-5'), 74.9 (C-2'), 84.8 (C-4'), 86.9 (C-3''), 91.3 (C-1'), 92.4 (C-3'), 111.2 (C-5), 123.5 (CH=CH), 134.2 (C-6), 134.7 (CH=CH), 151.7 (C-4''), 151.4 (C-2), 162.8 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(4-hydroxybutyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (21). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.80, 0.97 (2s, 18H, 2t-Bu), 1.50, 1.62 (m, 4H, 2 CH_2), 1.93 (s, 3H, CH_3-5), 3.54 (m, 2H, CH_2OH), 3.92 (t, 2H, NCH_2, J = 7.1 Hz), 3.93 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.6 Hz, $J_{5'a,5'b}$ = 12.4 Hz), 4.05 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.7 Hz), 4.32 (t, 1H, H-4'), 4.67 (d, 1H, H-2'), 5.76 (s, 1H, H-3''), 6.08 (d, 1H, H-1', $J_{1',2'}$ = 8.3 Hz), 6.47 (bs, 1H, NH_2-4''), 7.50 (s, 1H, H-6). ^{13}C NMR [75 MHz, $(CD_3)_2CO$] δ: 13.9 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 25.3, 30.3 (CH_2), 38.3 (CH_2N), 58.1 (CH_2OH), 62.3 (C-5'), 74.1 (C-2'), 83.2 (C-4'), 87.4 (C-3''), 92.6 (C-3'), 93.4 (C-1'), 111.7 (C-5), 134.4 (C-6), 151.6 (C-4''), 151.8 (C-2), 163.6 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(3-phthalimidopropyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (22). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.80, 0.96 (2s, 18H, 2t-Bu), 1.90 (s, 3H, CH_3-5), 3.72 (t, 2H, NCH_2 phthalimide), 3.98 (t, 2H, NCH_2), 4.09 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.13 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.5 Hz), 4.32 (t, 1H, H-4'), 4.65 (d, 1H, H-2'), 5.76 (s, 1H, H-3''), 6.04 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.45 (bs, 2H, NH_2-4''), 7.48 (s, 1H, H-6), 7.85 (s, 4H, Ph phthalimide).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[[3-*N*'-[benzoyl-2-(N''-methylcarbamoyl)]aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (23). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.80, 0.96 (2s, 18H, 2t-Bu), 1.90 (s, 3H, CH_3-5), 2.90 (s, 3H, NCH_3), 3.20 (t, 2H, NCH_2), 4.00 (m, 4H, 2H-

5’ and NCH_2), 4.35 (m, 1H, H-4’), 4.70 (d, 1H, H-2’), 5.60 (s, 1H, H-3’’), 6.05 (d, 1H, H-1’, $J_{1',2'}$ = 8.0 Hz), 6.60 (bs, 2H, NH_2-4’’), 7.50 (m, 4H, Ph), 7.81 (s, 1H, H-6), 8.19 (bs, 1H NHCO).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-*N*’-[(benzyloxycarbonyl)aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (24). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.80, 0.96 (2s, 18H, 2t-Bu), 1.95 (s, 3H, CH_3-5), 3.97 (t, 2H, NCH_2), 4.09 (dd, 1H, H-5’a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.1 Hz), 4.13 (dd, 1H, H-5’b, $J_{4',5'b}$ = 3.5 Hz), 4.33 (t, 1H, H-4’), 4.64 (d, 1H, H-2’), 5.05 (s, 2H, OCH_2Ph), 5.76 (s, 1H, H-3’’), 6.10 (d, 1H, H-1’, $J_{1',2'}$ = 8.0 Hz), 6.47 (bs, 2H, NH_2-4’’), 7.37 (m, 4H, Ph and H-6). ^{13}C NMR [75 MHz, DMSO-d_6] δ: 13.1 (CH_3-5), 18.2, 18.5 [$(CH_3)_3$-C-Si], 24.9, 26.2 [$(CH_3)_3$-C-Si], 28.11 (CH_2), 37.9 (CH_2N), 62.1 (C-5’), 66.9 (OCH_2Ph), 74.7 (C-2’), 83.5 (C-4’), 87.3 (C-3’’), 92.4 (C-1’), 92.9 (C-3’), 111.1 (C-5), 128.4-137.1 (NHCO, Ph), 134.2 (C-6), 151.2 (C-4’’), 150.5 (C-2), 156.6 (C-4).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-(3-aminopropyl)thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (25). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.83, 0.97 (2s, 18H, 2t-Bu), 1.85 (m, 2H, CH_2), 1.96 (s, 3H, CH_3-5), 3.20 (t, 2H, CH_2NH_2), 3.98 (t, 2H, NCH_2), 4.05 (dd, 1H, H-5’a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 12.2 Hz), 4.12 (dd, 1H, H-5’b, $J_{4',5'b}$ = 3.4 Hz), 4.32 (t, 1H, H-4’), 4.68 (d, 1H, H-2’), 5.75 (s, 1H, H-3’’), 6.09 (d, 1H, H-1’, $J_{1',2'}$ = 8.1 Hz), 6.53 (bs, 1H, NH_2-4’’), 7.52 (s, 1H, H-6). ^{13}C NMR [75 MHz, DMSO-d_6] δ: 12.8 (CH_3-5), 18.1, 18.6 [$(CH_3)_3$-C-Si], 25.0, 26.3 [$(CH_3)_3$-C-Si], 32.6 (CH_2), 39.0 (CH_2NH_2), 40.9 (CH_2N), 62.1 (C-5’), 74.5 (C-2’), 84.7 (C-4’), 87.1 (C-3’’), 91.6 (C-1’), 92.1 (C-3’), 111.3 (C-5), 135.6 (C-6), 151.3 (C-4’’), 151.6 (C-2), 161.9 (C-4).

3-[Bis(benzyloxycarbonylmethyl)amino]propyl bromide (26). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 1.85 (m, 2H, CH_2), 3.20 (t, 2H, CH_2N, J = 7.5 Hz), 3.45 (t, 2H, CH_2Br, J = 7.5 Hz), 3.68 (s, 4H, $COCH_2N$), 5.02 (s, 4H, CH_2Ph), 7.40 (s, 10H, Ph).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-[*N'*,*N'*-bis(benzyloxycarbonyl)methyl)aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (27). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.96 (2s, 18H, 2t-Bu), 1.73 (m, 2H, NCH_2CH_2),1.93 (s, 3H, CH_3-5), 2.86 (t, 2H, CH_2), 3.69 (s, 4H, NCH_2CO), 3.99 (m, 2H, NCH_2), 4.07 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 10.0 Hz), 4.12 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.7 Hz), 4.34 (t, 1H, H-4'), 4.69 (d, 1H, H-2'), 5.15 (s, 4H, CH_2Ph), 5.77 (s, 1H, H-3''), 6.10 (d, 1H, H-1', $J_{1',2'}$ = 8.1 Hz), 6.45 (bs, 2H, NH_2-4''), 7.40 (m, 10H, Ph), 7.50 (s, 1H, H-6).

[1-[2',5'-Bis-O-(tert-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-[*N'*,*N'*-bis(carboxymethyl)aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (28). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.96 (2s, 18H, 2t-Bu), 1.80 (m, 2H, NCH_2CH_2), 1.93 (s, 3H, CH_3-5), 2.89 (m, 2H, CH_2), 3.60 (s, 4H, NCH_2CO), 3.99 (m, 2H, NCH_2), 4.05 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 11.0 Hz), 4.10 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.7 Hz), 4.33 (t, 1H, H-4'), 4.66 (d, 1H, H-2'), 5.76 (s, 1H, H-3''), 6.07 (d, 1H, H-1', $J_{1',2'}$ = 8.2 Hz), 6.48 (bs, 1H, NH_2-4''), 7.51 (s, 1H, H-6).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-[*N'*,*N'*-(dimethyl)aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) (30). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.96 (2s, 18H, 2t-Bu), 1.73 (m, 2H, NCH_2CH_2),1.93 (s, 3H, CH_3-5), 2.14 [s, 6H, $N(CH_3)_2$], 2.27 (t, 2H, NCH_2, J = 6.6 Hz), 3.94 (t, 2H, NCH_2, J = 7.6 Hz), 4.04 (dd, 1H, H-5'a, $J_{4',5'a}$ = 3.7 Hz, $J_{5'a,5'b}$ = 10.0 Hz), 4.09 (dd, 1H, H-5'b, $J_{4',5'b}$ = 3.4 Hz), 4.33 (t, 1H, H-4'), 4.68 (d, 1H, H-2'), 5.75

(s, 1H, H-3''), 6.09 (d, 1H, H-1', $J_{1',2'}$ = 8.0 Hz), 6.50 (bs, 1H, NH_2-4''), 7.51 (s, 1H, H-6).

[1-[2',5'-Bis-*O*-(*tert*-butyldimethylsilyl)-β-D-ribofuranosyl]-3-*N*-[3-[*N',N',N'*-(trimethyl)aminopropyl]thymine]-3'-spiro-5"-(4"-amino-1",2"-oxathiole-2",2"-dioxide) iodide (31). ^{1}H NMR [300 MHz, $(CD_3)_2CO$] δ: 0.81, 0.93 (2s, 18H, 2t-Bu), 1.96 (s, 3H, CH_3-5), 2.20 (m, 2H, NCH_2CH_2), 3.40 [s, 9H, $N^+(CH_3)_3$], 3.71 (m, 2H, CH_2N^+), 3.95 (dd, 1H, H-5'a, $J_{4',5'a}$ = 6.7 Hz, $J_{5'a,5'b}$ = 12.3 Hz), 4.05 (dd, 1H, H-5'b, $J_{4',5'b}$ = 6.5 Hz), 4.21 (t, 1H, H-4'), 4.36 (t, 2H, NCH_2, J = 7.3 Hz), 5.16 (d, 1H, H-2'), 5.67 (s, 1H, H-3''), 6.18 (d, 1H, H-1', $J_{1',2'}$ = 8.5 Hz), 6.83 (bs, 1H, NH_2-4''), 8.28 (s, 1H, H-6).

General methods. **Chemical Procedures.** Microanalyses were obtained with a Heraeus CHN-O-RAPID instrument. Electrospray mass spectra were measured on a quadropole mass spectrometer equipped with an electrospray source (Hewlett Packard, LC/MS HP 1100). ^{1}H NMR spectra were recorded with a Varian Gemini, a Varian XL-300 and a Bruker AM-200 spectrometer operating at 300 and 200 MHz with Me_4Si as internal standard. ^{13}C NMR spectra were recorded with a Varian XL-300 and a Bruker AM-200 spectrometer operating at 75 MHz, and at 50 MHz with Me_4Si as internal standard. Analytical thin-layer chromatography (TLC) was performed on silica gel 60 F_{254} (Merck). Separations on silica gel were performed by preparative centrifugal circular thin-layer chromatography (CCTLC) on a Chromatotron^R (Kiesegel 60 PF_{254} gipshaltig; Merck), layer thickness (1 mm), flow rate (5 mL min^{-1}).

General Methods: biological evaluation

Cells and Viruses. Human immunodeficiency virus type 1 [HIV-1(III_B)] was obtained from Dr. R.C. Gallo (when at the National Cancer Institute, Bethesda, MD). HIV-2(ROD) was provided by Dr. L. Montagnier (when at the Pasteur Institute, Paris, France).

Activity Assay of Test Compounds against HIV-1 and HIV-2 in Cell Cultures. A total number of 4 x 10^6 CEM or 3 x 10^5 MT-4 cells per milliliter were infected with HIV-1(III_B) or HIV-2(ROD) or HIV-1/138K (a virus strain that was selected in the presence of TSAO-m^3T and that contained the E138K mutation in its RT) at ~ 100 $CCID_{50}$ (50% cell culture infective dose) per milliliter of cell suspension. Then an amount of 100 μL of the infected cell suspension was transferred to microtiter plate wells and mixed with 100 μL of the appropriate dilutions of the test compounds. Giant cell formation (CEM) or HIV-induced cytopathicity (MT-4) was recorded microscopically (CEM) or by trypan blue dye exclusion (MT-4) in the HIV-infected cell cultures after 4 days (CEM) or 5 days (MT-4). The 50% effective concentration (EC_{50}) of the test compounds was defined as the compound concentration required to inhibit virus-induced cytopathicity (CEM) or to reduce cell viability (MT-4) by 50%. The 50% cytostatic or cytotoxic concentration (CC_{50}) was defined as the compound concentration required to inhibit CEM cell proliferation by 50% or to reduce the number of viable MT-4 cells in mock-infected cell cultures by 50%.

Inhibitory Effect of Test Compounds against Recombinant HIV-1 RT. The assay procedure for measuring the inhibitory effects of the test compounds against HIV-1 RT used poly(rC).oligo(dG) (0.015 mM) as the template-primer, and [2,8-^{3}H]dGTP (2 μCi/assay in 50 μl; 2.5 μM) as the radiolabeled substrate. Inhibition of HIV RT activity by the different concentrations of the TSAO derivatives was determined in the presence of 5-fold dilutions of the test compounds. The 50% inhibitory concentration (IC_{50}) was

defined as the concentration of the compound required to inhibit enzyme activity by 50%.

Table 2. ANALYTICAL DATA

Comp..	Formula	Calculated (%)				Found (%)			
		C	H	N	S	C	H	N	S
1	$C_{27}H_{47}N_3O_{10}SSi_2$	48.99	7.16	6.35	4.84	48.45	7.00	6.50	4.75
3	$C_{26}H_{46}N_4O_9SSi_2$	48.27	7.17	8.66	4.96	48.33	7.06	8.11	4.70
4	$C_{28}H_{49}N_3O_8SSi_2$	52.23	7.67	6.53	4.98	52.53	7.47	6.99	4.70
5	$C_{31}H_{49}N_3O_8SSi_2$	54.76	7.26	6.18	4.72	54.60	7.45	5.99	4.60
7	$C_{26}H_{46}BrN_3O_8SSi_2$	44.82	6.65	6.03	4.60	44.50	6.49	6.10	4.65
8	$C_{26}H_{47}N_3O_9SSi_2$	49.26	7.47	6.63	5.06	49.50	7.79	6.10	5.11
9	$C_{27}H_{49}N_3O_9SSi_2$	50.05	7.62	6.49	4.95	50.50	7.79	6.10	4.80
10	$C_{32}H_{51}N_3O_8SSi_2$	55.38	7.41	6.05	4.62	55.08	7.49	5.99	4.50
11	$C_{34}H_{52}N_4O_8SSi_2$	55.71	7.15	7.64	4.37	55.15	7.50	7.55	4.20
12	$C_{27}H_{48}N_4O_9SSi_2$	49.07	7.32	8.48	4.85	49.50	7.49	8.20	4.70
13	$C_{28}H_{50}N_4O_9SSi_2$	49.83	7.47	8.30	4.75	49.50	7.35	8.20	4.60
15	$C_{30}H_{53}N_3O_{10}SSi_2$	51.18	7.59	5.97	4.55	51.45	7.79	6.20	4.30
16	$C_{32}H_{57}N_3O_{10}SSi_2$	52.20	7.85	5.74	4.38	52.60	7.45	5.99	4.20
17	$C_{30}H_{54}N_4O_9SSi_2$	51.25	7.74	7.97	4.56	51.10	7.60	7.81	4.30
18	$C_{31}H_{56}N_4O_9SSi_2$	51.93	7.87	7.81	4.47	51.60	7.45	7.99	4.30
19	$C_{29}H_{49}N_3O_{10}SSi_2$	50.63	7.18	6.11	4.66	50.20	7.35	6.65	4.50
20	$C_{28}H_{49}N_3O_9SSi_2$	50.96	7.48	6.37	4.86	50.40	7.27	6.58	4.74
21	$C_{28}H_{51}N_3O_9SSi_2$	50.80	7.77	6.35	4.84	50.36	7.28	6.51	4.60
22	$C_{35}H_{52}N_4O_{10}SSi_2$	54.10	6.75	7.21	4.13	53.90	6.50	7.10	4.03
23	$C_{36}H_{57}N_5O_{10}SSi_2$	53.51	7.11	8.67	3.97	53.80	7.00	8.50	3.65
24	$C_{35}H_{56}N_4O_9SSi_2$	53.82	7.23	7.17	4.11	53.62	7.00	7.10	4.01
25	$C_{27}H_{50}N_4O_8SSi_2$	50.13	7.79	8.66	4.96	49.83	7.69	8.42	4.66
26	$C_{21}H_{24}BrNO_4$	58.07	5.57	3.22	—	58.00	18.20	3.17	—
27	$C_{45}H_{66}N_4O_{12}SSi_2$	57.30	7.05	5.94	3.40	57.20	7.12	6.20	3.10
28	$C_{31}H_{54}N_4O_{12}SSi_2$	48.80	7.13	7.34	4.20	48.60	7.00	7.20	4.10

30	$C_{29}H_{54}N_4O_8SSi_2$	51.60	8.06	8.30	4.75	51.30	7.79	8.10	4.60
31	$C_{30}H_{57}IN_4O_8SSi_2$	44.11	6.98	6.86	3.92	44.30	6.59	6.25	3.70