

Signal intensity		Ratio (relative sensitivity)
D0A6	D2A0	D0A6/D2A0
3.60E+04	3.93E+04	0.92
D0S6	D2S0	D0S6/D2S0
5.26E+04	4.93E+04	1.07

Table S1.

Signal intensities of D0A6, D2A0, D2S0 and D0S6, and relative sensitivity of the D0A6/D2A0 and D0S6/D2S0 isomer pairs. Data were measured using direct infusion of the individual isomers in 20%A and 80%B eluent mixture, under the same mass spectrometric tuning, as in the LC-MS studies described. Values are given as the sum of singly and doubly deprotonated ion counts. Concentration of the standards were 5 μ M.