

Table S4. Precision for Lyso-Gb3 analogues.

Sample name	Lyso-Gb3(-28)				Lyso-Gb3(-12)				Lyso-Gb3(-2)				Lyso-Gb3(+14)			
	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)
Low	N.D				N.D				0.012				N.D			
	N.D				N.D				0.012	0.012	0.001	5.4	N.D			
	N.D				N.D				0.012				N.D			
	N.D				N.D				0.011				N.D			
	N.D				N.D				0.011				N.D			
Middle	0.019				N.D				0.15				0.00089			
	0.022				N.D				0.15				0.0015			
	0.017	0.019	0.002	9.0	N.D				0.15	0.15	0.01	5.5	0.0016	0.0015	0.0005	>20
	0.018				N.D				0.14				0.0013			
	0.019				N.D				0.13				0.0023			
High	0.38				0.022				2.6				0.093			
	0.44				0.024				2.8				0.12			
	0.43	0.43	0.03	6.5	0.027	0.024	0.002	8.2	3.2	2.8	0.2	7.9	0.11	0.11	0.01	9.3
	0.45				0.027				2.7				0.11			
	0.44				0.023				2.8				0.10			

Sample name	Lyso-Gb3(-16)				Lyso-Gb3(-18)				Lyso-Gb3(+34)				Lyso-Gb3(+50)			
	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)	Determined concentration (Area ratio)	Mean determined concentration (Area ratio)	S.D. (Area ratio)	Precision (%)
Low	0.00019				0.0085				0.019				0.00045			
	N.D				0.0086				0.019				0.00062			
	0.00050	0.00014	0.00022	>20	0.0067	0.0073	0.0012	17	0.023	0.020	0.002	9.2	0.00075	0.00049	0.00020	>20
	N.D				0.0072				0.018				0.00039			
	N.D				0.0057				0.020				0.00024			
Middle	0.030				0.037				0.15				0.034			
	0.028				0.045				0.14				0.031			
	0.028	0.030	0.003	8.8	0.041	0.041	0.003	7.5	0.16	0.15	0.01	6.1	0.032	0.033	0.001	4.4
	0.034				0.039				0.14				0.032			
	0.032				0.041				0.15				0.034			
High	0.46				0.82				2.8				0.62			
	0.56				0.76				2.7				0.80			
	0.68	0.58	0.08	14.4	0.63	0.71	0.08	11.0	3.1	2.8	0.2	8.5	0.76	0.73	0.07	9.4
	0.58				0.67				2.5				0.74			
	0.64				0.68				2.8				0.72			

N.D: Not detected.