

Table. Empirical formulae and calculated accurate masses for deuterated 3-ketodihydroshingo lipids.

Compound ^a	Empirical formula	exact mass ^b	Compound ^a	Empirical formula	exact mass ^b
d2Ksa	C18H35D2NO2	302.3028	d1KSo	C18H34D1NO2	299.2809
d2KsaP	C18H36D2NO5P	382.2691	d1KS1P	C18H35D1NO5P	379.2472
C16d2KdhCer	C34H65D2NO3	540.5325	C16d1KCer	C34H64D1NO3	537.5106
C18d2KdhCer	C36H69D2NO3	568.5638	C18d1KCer	C36H68D1NO3	565.5419
C20d2KdhCer	C38H73D2NO3	596.5951	C20d1KCer	C38H72D1NO3	593.5731
C22d2KdhCer	C40H77D2NO3	624.6264	C22d1KCer	C40H76D1NO3	621.6044
C24d2KdhCer	C42H81D2NO3	652.6577	C24d1KCer	C42H80D1NO3	649.6357
C16d2KdhSM	C39H78D2N2O6P	705.5880	C16d1KSM	C39H77D1N2O6P	702.5660
C18d2KdhSM	C41H82D2N2O6P	733.6193	C18d1KSM	C41H81D1N2O6P	730.5974
C20d2KdhSM	C43H86D2N2O6P	761.6506	C20d1KSM	C43H85D1N2O6P	758.6286
C22d2KdhSM	C45H90D2N2O6P	789.6819	C22d1KSM	C45H89D1N2O6P	786.6599
C24d2KdhSM	C47H94D2N2O6P	817.7131	C24d1KSM	C47H93D1N2O6P	814.6912
C16d2KdhCMH	C40H75D2NO8	702.5853	C16d1KCMH	C40H74D1NO8	699.5634
C18d2KdhCMH	C42H79D2NO8	730.6166	C18d1KCMH	C42H78D1NO8	727.5947
C20d2KdhCMH	C44H83D2NO8	758.6479	C20d1KCMH	C44H82D1NO8	755.6260
C22d2KdhCMH	C46H87D2NO8	786.6792	C22d1KCMH	C46H86D1NO8	783.6573
C24d2KdhCMH	C48H91D2NO8	814.7105	C24d1KCMH	C48H90D1NO8	811.6886
C16d2KdhLCer	C46H85D2NO13	864.6381	C16d1KLCer	C46H84D1NO13	861.6162
C18d2KdhLCer	C48H89D2NO13	892.6694	C18d1KLCer	C48H88D1NO13	889.6475
C20d2KdhLCer	C50H93D2NO13	920.7007	C20d1KLCer	C50H92D1NO13	917.6788
C22d2KdhLCer	C52H97D2NO13	948.7320	C22d1KLCer	C52H96D1NO13	945.7101
C24d2KdhLCer	C54H101D2NO13	976.7633	C24d1KLCer	C54H100D1NO13	973.7414

^a Abbreviations: d1KCer, [4-²H] ketoceramide; d1KCMH, [4-²H] ketoceramide monohexoside; d1KLCer, [4-²H] ketolactosylceramide; d1KS1P, [4-²H] ketosphingosine 1-phosphate; d1KSM, [4-²H] ketosphingomyelin; d1KSo, [4-²H] ketosphingosine; d2KdhCer, [4,4-²H₂] ketodihydroceramide; d2KdhCMH, [4,4-²H₂] ketodihydroceramide monohexoside; d2KdhLCer, [4,4-²H₂] ketolactosyldihydroceramide; d2KdhSM, [4,4-²H₂] ketodihydroshingomyelin; d2Ksa, [4,4-²H₂] ketosphinganine; d2KsaP, [4,4-²H₂] ketosphinganine 1-phosphate.

^bin ESI-positive mode.