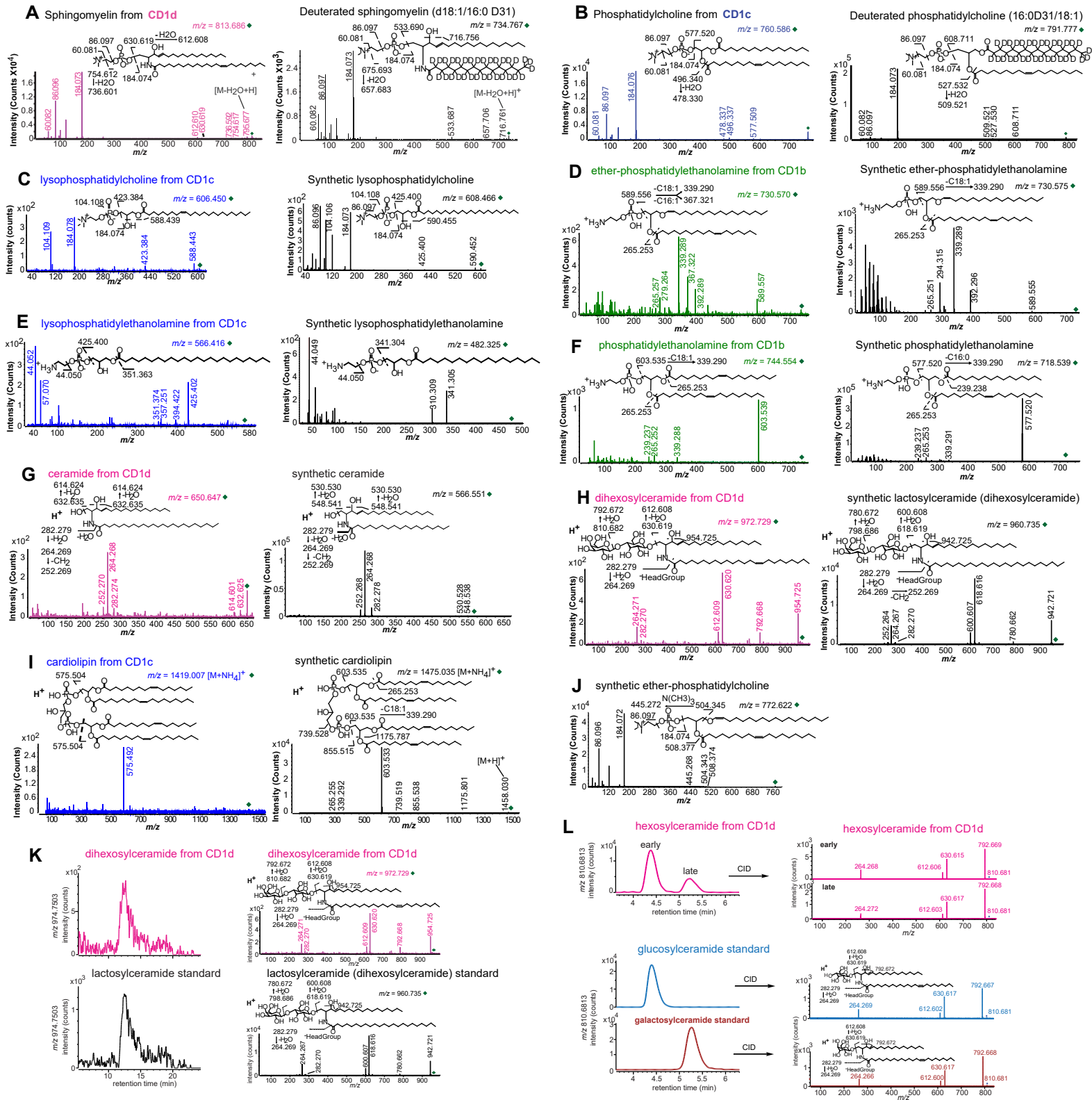


# Figure S2 related to Figures 1, 4, and 5

## Identification of CD1-associated lipids by CID-MS



(A) The molecular feature ( $m/z$  813.686) eluted from CD1d and the deuterium-labeled sphingomyelin show the expected phosphocholine ion ( $m/z$  184.07), but can be distinguished based on the altered mass of the fatty acyl unit and overall mass. (B) The molecular feature ( $m/z$  760.586) eluted from CD1c and the deuterium-labeled phosphatidylcholine show the same phosphocholine ion, but the two molecules can be distinguished based on differing masses of the fatty acyl unit and overall mass. (C-J) Synthetic lipids from commercial sources and lipids eluted from CD1 proteins were collided to generate fragmentation patterns. Positions of double bonds are not known. (K) Dihexosylceramide from CD1d had the same retention time as the standard, lactosylceramide. CID-MS of both showed the similar collisional pattern of loss carbohydrate or lipid fragment. (L) Hexosylceramides from CD1d showed early and late chromatogram peaks, which had the same retention time as the standards, glucosylceramide and galactosylceramide, respectively. The CID-MS spectra and fragmentation patterns were shown.