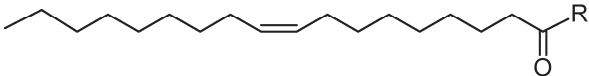

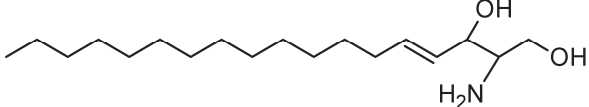
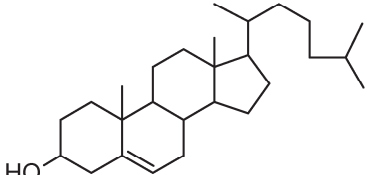
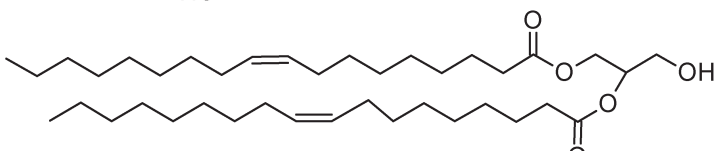
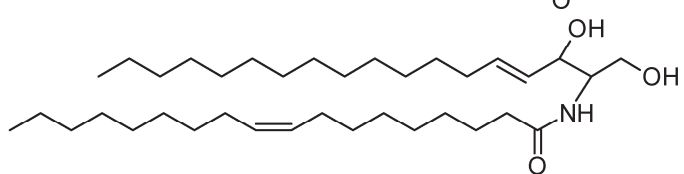
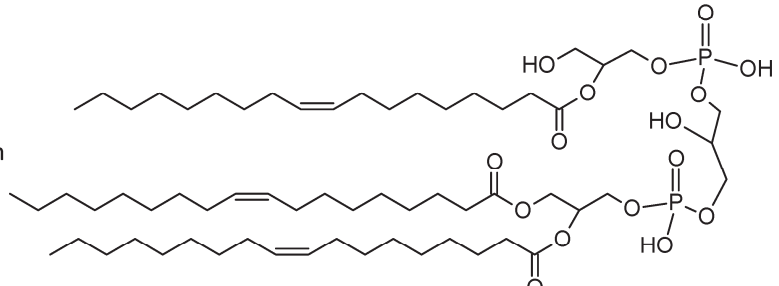


**S1 Fig**

HCA	Structure	Annotation
Fatty acyl		FA 18:1
Alkanol		O-18:1
Long-chain base		LCB 18:1;2
Sterol		ST 27:1
Diacylglycerol		DAG 36:2
Ceramide		Cer 36:1;2
Monolysocardiolipin		MLCL 54:3

**S1 Fig. Examples of minimal HCAs (hydrocarbon chain-based attributes) used for annotating neutral and charged fragment structures.** As described in the text, fragment structures containing HCAs are referenced by using the annotation of HCAs followed by chemical modifications in parentheses (e.g. “FA 18:1(+O)” denotes an acyl carboxylate anion). To eliminate possible inconsistencies due to differences in polarity, charge states and adducts, all fragment structures are annotated relative to neutral HCAs.