













Supplementary Table. Organ-specific markers for brain, kidney, lung, liver, and eye, discovered by mining the METSPACE knowledge base.

We calculated the markers by considering all datasets in METASPACE. For each molecule, we calculated its average tf-idf value for all datasets sampled from this organ ("Tf-idf"). We show only the average tf-idf values above 0.05. As an additional measure of reproducibility of each marker in each organ, we show by how many labs it was detected in data from the organ with an FDR <= 10% ("#Labs"). In order to reproduce the findings as well as show the relative intensities of the markers within the same molecular ion image, when detected we show images for a mimetic tissue model of homogenated organs from mouse. Each of the six wells represents one of the homogenated organs: liver, heart, muscle, lung, kidney, and brain.

Molecular formula	Molecule	Brain		Kidney		Lung		Liver		Eye		Mimetic organs image
		Tf-idf	# Labs	Tf-idf	# Labs	Tf-idf	# Labs	Tf-idf	# Labs	Tf-idf	# Labs	
C45H78NO8P	PE(40:6)	0.17	16	0.06	5					0.26	1	 link
C42H81NO11S	3-O-Sulfogalactosylceramide (d18:1/18:0)	0.15	9									 link
C43H82NO7P	PE(P-38:1)	0.12	12									 link
C40H80NO8P	PC(32:0)	0.11	19	0.07	7	0.10	1	0.06	6	0.18	1	 link
C39H73O8P	PA(36:2)	0.10	18					0.09	6			 link
C27H44NO7P	LysoPE(22:6)	0.09	14			0.05	1					 link
C42H80NO10P	PS(36:1)	0.09	13									 link
C75H135N3O31	Ganglioside GM1 (18:1/20:0)	0.09	2									
C73H131N3O31	Ganglioside GM1 (18:1/18:0)	0.08	2									
C39H79N2O6P	SM(d18:0/16:1) / Palmitoyl sphingomyelin	0.06	12	0.05	7	0.08	1	0.06	6	0.06	1	
C8H20NO6P	Glycerophosphocholine	0.06	9	0.18	6	0.07	1					
C43H70O3	Cholesteryl ester	0.05	5									
C7H15NO3	L-Carnitine, Malonyl-Carnitin			0.13	3							
C9H17NO4	L-Acetylcarnitine / N-lactoyl-Leucine			0.12	4	0.16	1					
C5H11NO2	Betaine / L-Valine / N-Methyl-a-aminoisobutyric acid / 5-Aminopentanoic acid			0.11	4							
C40H77NO11S	3-O-Sulfogalactosylceramide (d18:1/16:0)			0.11	5							 link
C27H46O4S	Cholesterol sulfate			0.09	5							 link
C29H47NO4	Acylcarnitine (Docosa-4,7,10,13,16-pentaenoyl carnitine / Clupanodonyl carnitine)			0.06	5	0.11	1	0.05	4	0.09	1	
C10H12N4O5	Inosine / Allopurinol riboside			0.06	6							 link
C9H12N2O6	Uridine / Pseudouridine			0.06	4							
C76H140N2O26	Ganglioside GM2 (d18:0/26:0)			0.06	2							
C40H78NO8P	PC(32:1)					0.07	1	0.05	5			
C10H26N4	Spermine					0.06	1					
C10H13N5O4	Adenosine / Deoxyguanosine					0.05	1					
C18H32O2	Linoleic acid / conjugated linoleic acid							0.07	6			 link
C37H70O5	DG(34:1)							0.07	3			
C26H45NO6S	Tauroursodeoxycholic acid / Taurodeoxycholic acid / Taurochenodesoxycholic acid							0.05	4			 link

