

Supplemental Material

NIST Lipidomics Workflow Questionnaire: An Assessment of Community-Wide Methodologies and Perspectives

Metabolomics: Short Communication

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Table of Contents

[Table S1. The survey invitations \(\$n = 322\$ \) and laboratory responses \(\$n = 125\$ \) sorted by country](#)

[Figure S1. Survey responses sorted by continent \(\$n = 5\$ \) and country \(\$n = 125\$ \)](#)

[Figure S2. How long has your laboratory been performing lipidomics?](#)

[Figure S3. Number of people in laboratory.](#)

[Figure S4. Type of institution.](#)

[Figure S5. What kind of lipid applications do you typically work on in your laboratory?](#)

[Figure S6. Approximately how many lipidomics manuscripts does your laboratory publish per year?](#)

[Figure S7. Approximately how many lipid samples does your laboratory analyze in a month?](#)

[Figure S8. For untargeted lipidomics experiments, what lipid extraction does your laboratory employ?](#)

[Figure S9. About how long does your laboratory store extracted lipidomics samples before you discard them?](#)

[Figure S10. What temperature\(s\) does your laboratory store lipid extracts at?](#)

[Figure S11. If chromatography, what type of column\(s\) does your laboratory use for lipidomics?](#)

[Figure S12. If you incorporate a high-resolution mass spectrometer, at what mass resolving power do you analyze your lipid extracts?](#)

[Figure S13. If you use LC-MS, what software does your laboratory employ for peak picking/processing?](#)

[Figure S14. What software does your laboratory employ for lipid identification?](#)

[Figure S15. What lipid databases do you use?](#)

[Figure S16. What software does your laboratory employ for lipid quality control and statistics?](#)

[Figure S17. Do you have written standard operating procedures \(SOPs\) in your laboratory, and if so, what aspects do the SOPs cover?](#)

[Figure S18. What type of quantitation do you perform in your laboratory?](#)

[Figure S19. What type of internal standards does your laboratory most often employ?](#)

[Figure S20. What lipids do you find most challenging to quantitate?](#)

[Figure S21. What software does your laboratory employ for lipid quantification?](#)

[Figure S22. How does your laboratory treat multiple adducts per lipid?](#)

[Figure S23. Does your laboratory employ relative response factors \(RRFs\) for these lipid categories?](#)

[Figure S24. How does your laboratory normalize your quantitative lipid values?](#)

[Figure S25. What types of quality control \(QC\) samples does your laboratory use in analytical measurements for lipidomics?](#)

[Figure S26. State whether the QC material you employ is commercially available or made in-house. For commercially available answers, please specify the material name.](#)

[Figure S27. What does your laboratory use QCs, SRMs, or CRMs for?](#)

[Figure S28. Do you validate your project sample measurements with...?](#)

[Figure S29. What type of reference material would be of most interest to your laboratory?](#)

[Figure S30. What types of complex biological reference materials would you like to see provided?](#)

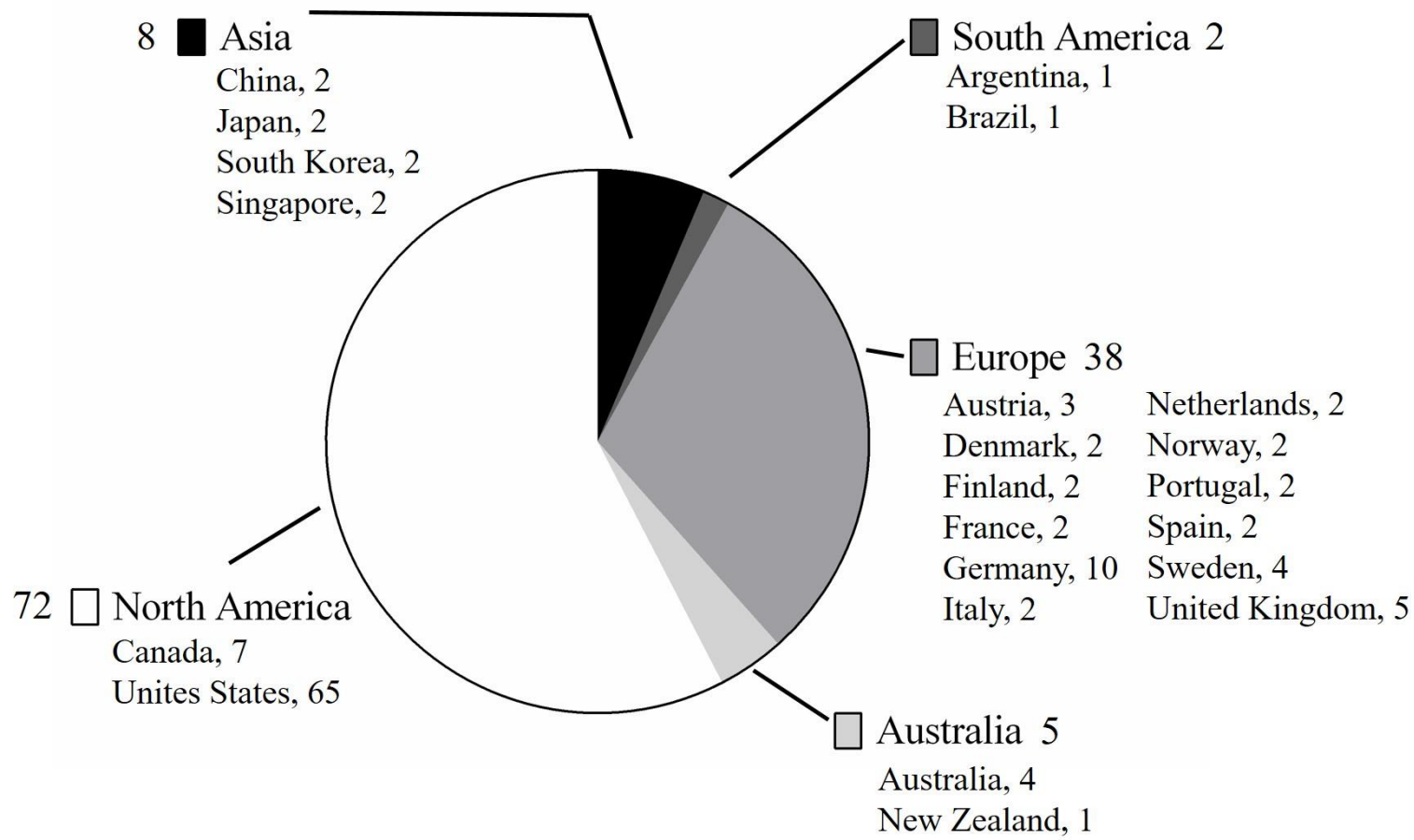
[Figure S31. If your laboratory uses commercially available QC materials, please indicate below; however, if your laboratory does not use commercially available reference materials, indicate why below?](#)

[Figure S32. Does your laboratory store your lipid data in a repository? If yes, where?](#)

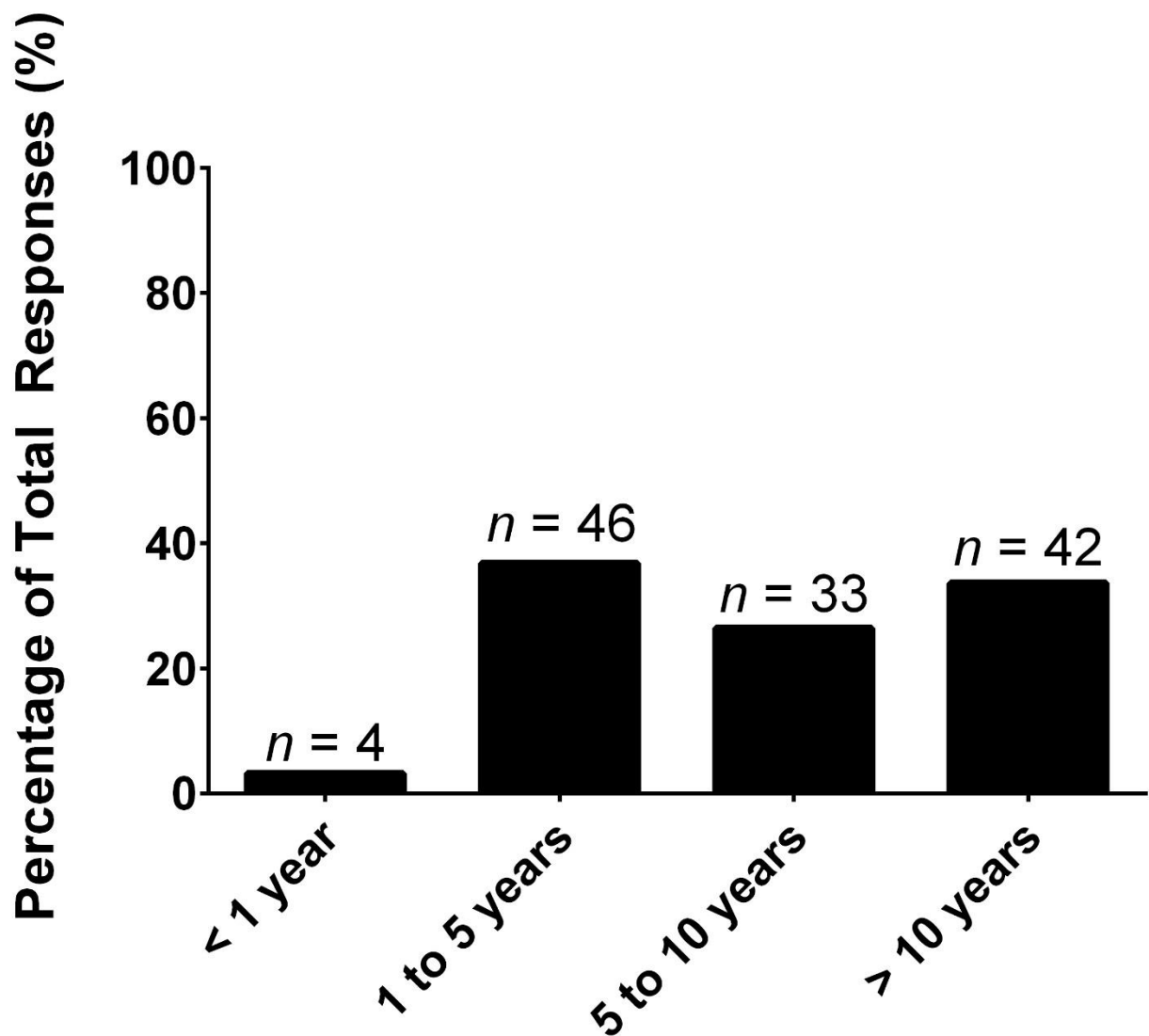
[Figure S33. What do you perceive as the biggest challenge in the lipidomics community?](#)

Table S1. The survey invitations ($n = 322$) and laboratory responses ($n = 125$) sorted by country

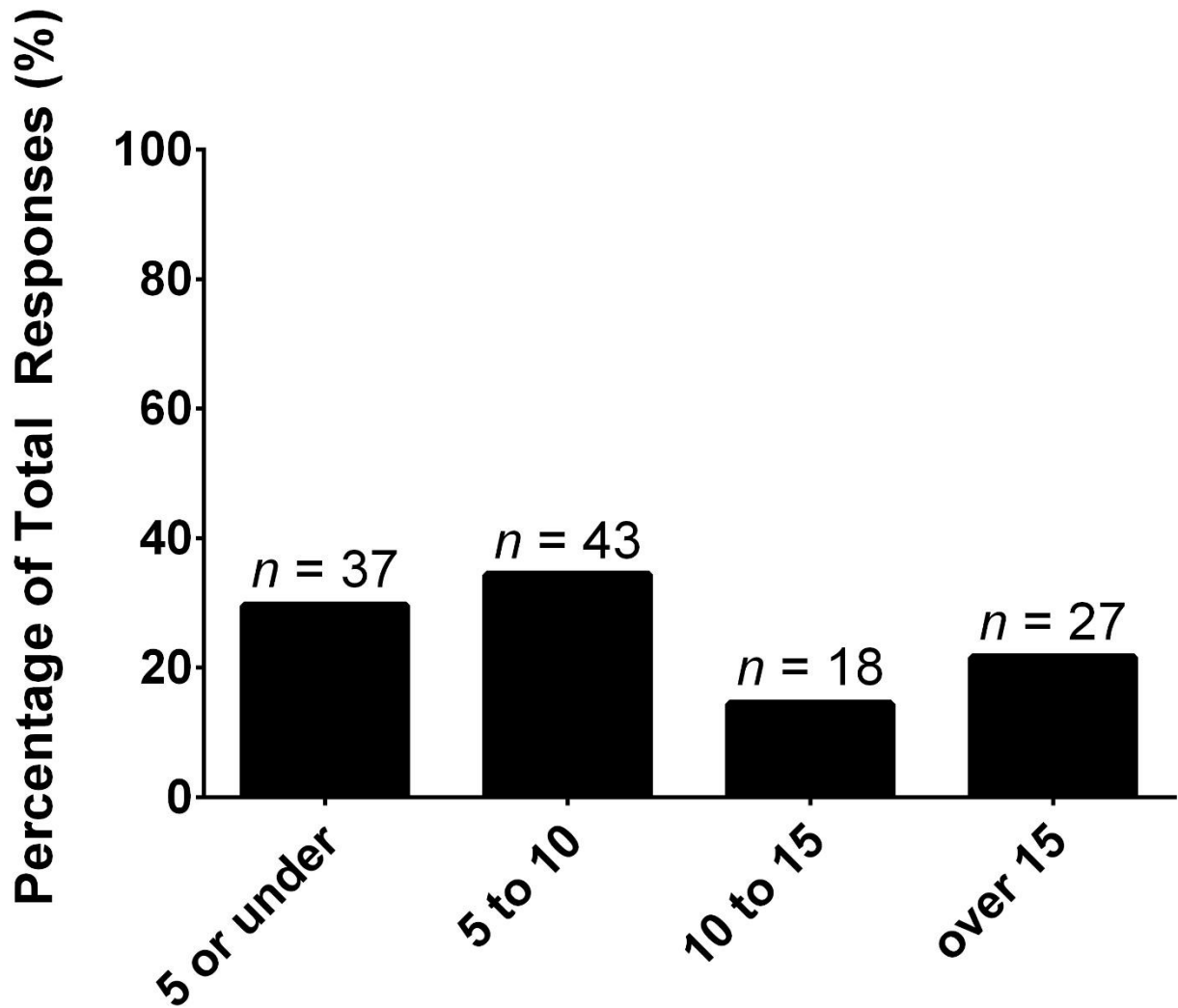
Country	Invitations	Responses
Argentina	1	1
Australia	8	4
Austria	3	3
Belgium	3	--
Brazil	6	1
Canada	13	7
China	11	2
Czech Republic	1	--
Denmark	6	2
Finland	4	2
France	12	2
Germany	27	10
Hong Kong	2	--
Hungary	1	--
India	5	--
Ireland	1	--
Israel	2	--
Italy	4	2
Japan	13	2
Luxembourg	1	--
Netherlands	8	2
New Zealand	1	1
Norway	2	2
Pakistan	1	--
Poland	1	--
Portugal	3	2
Singapore	3	2
South Korea	5	2
Spain	4	2
Sweden	6	4
Switzerland	2	--
Taiwan	2	--
United Kingdom	21	5
United States	139	65



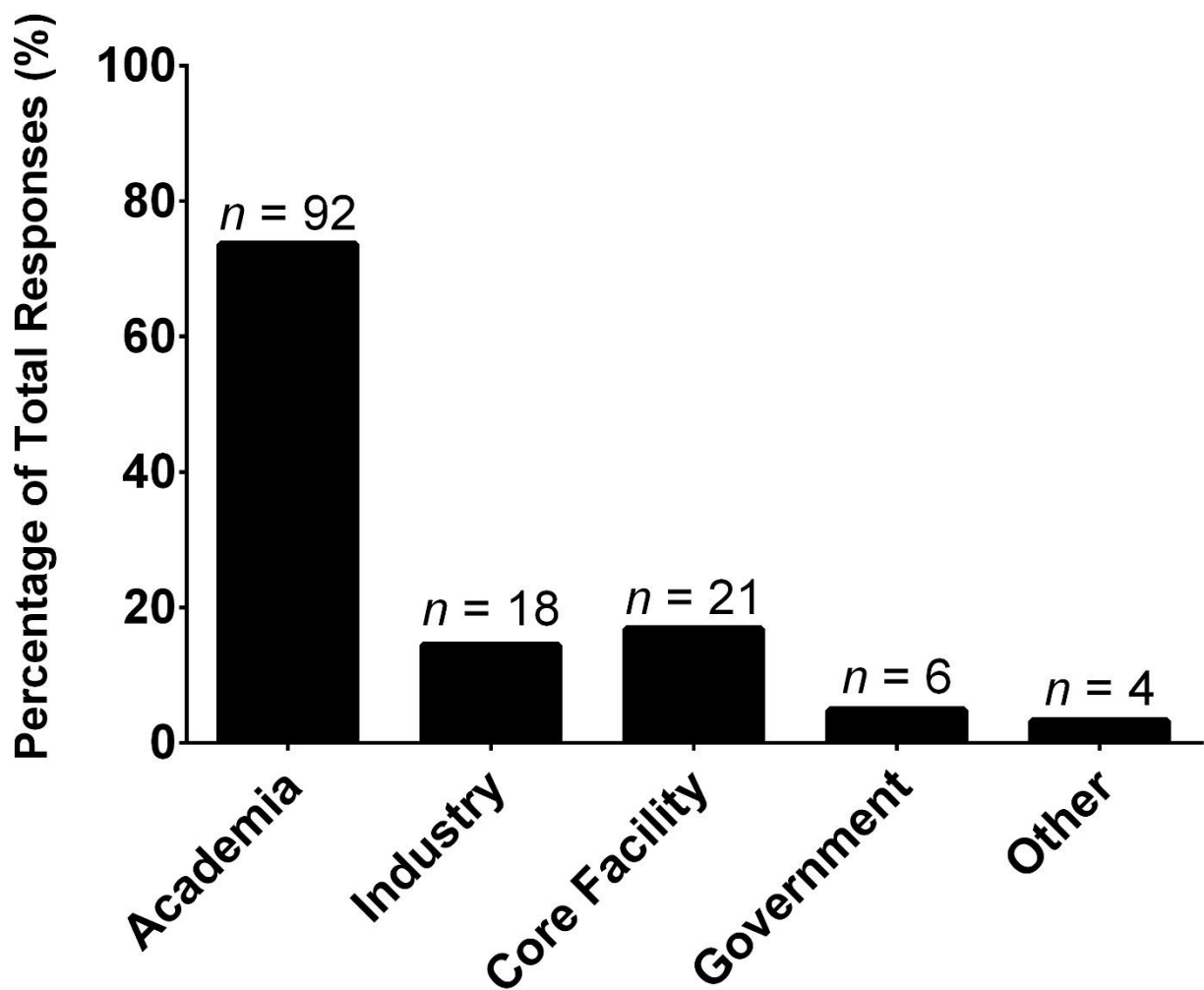
Supplemental Figure S1. Survey responses sorted by continent ($n = 5$) and country ($n = 125$)



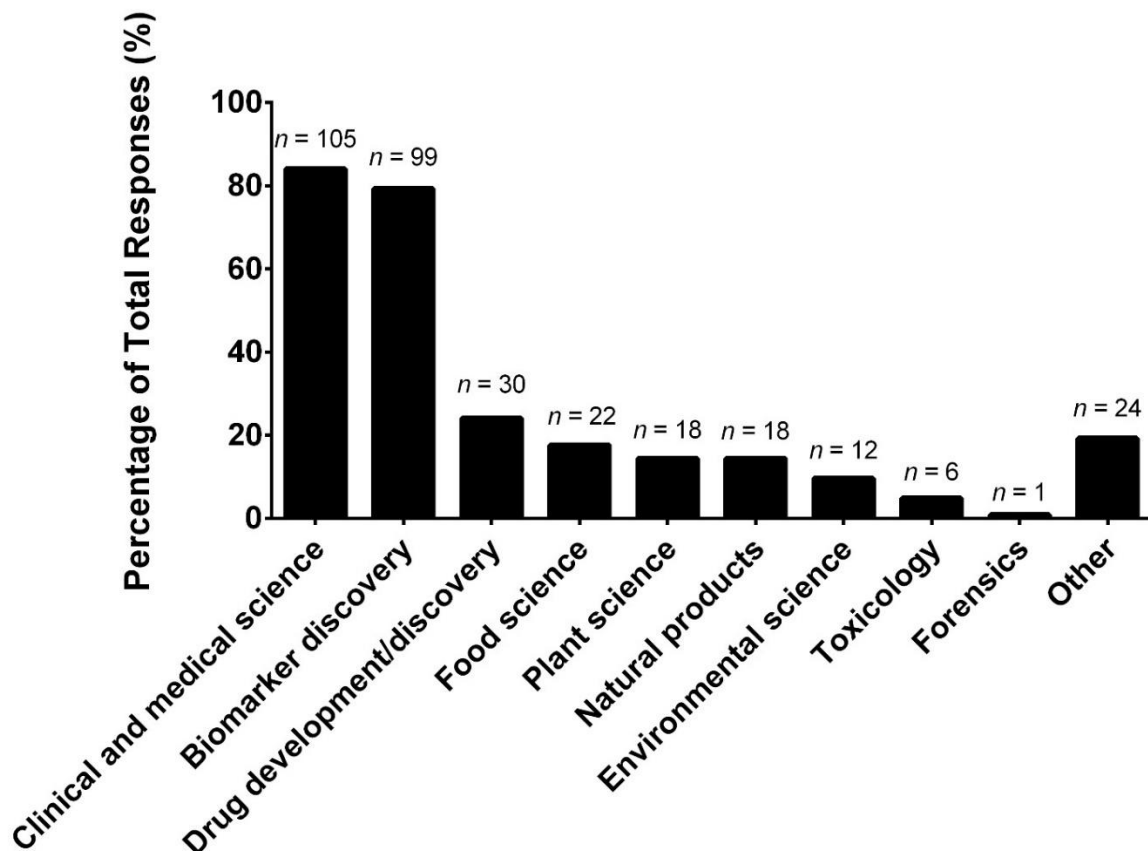
Supplemental Figure S2. “How long has your laboratory been performing lipidomics?” The values are shown as a percentage of total responses (total number of responses, $n = 125$). The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options.



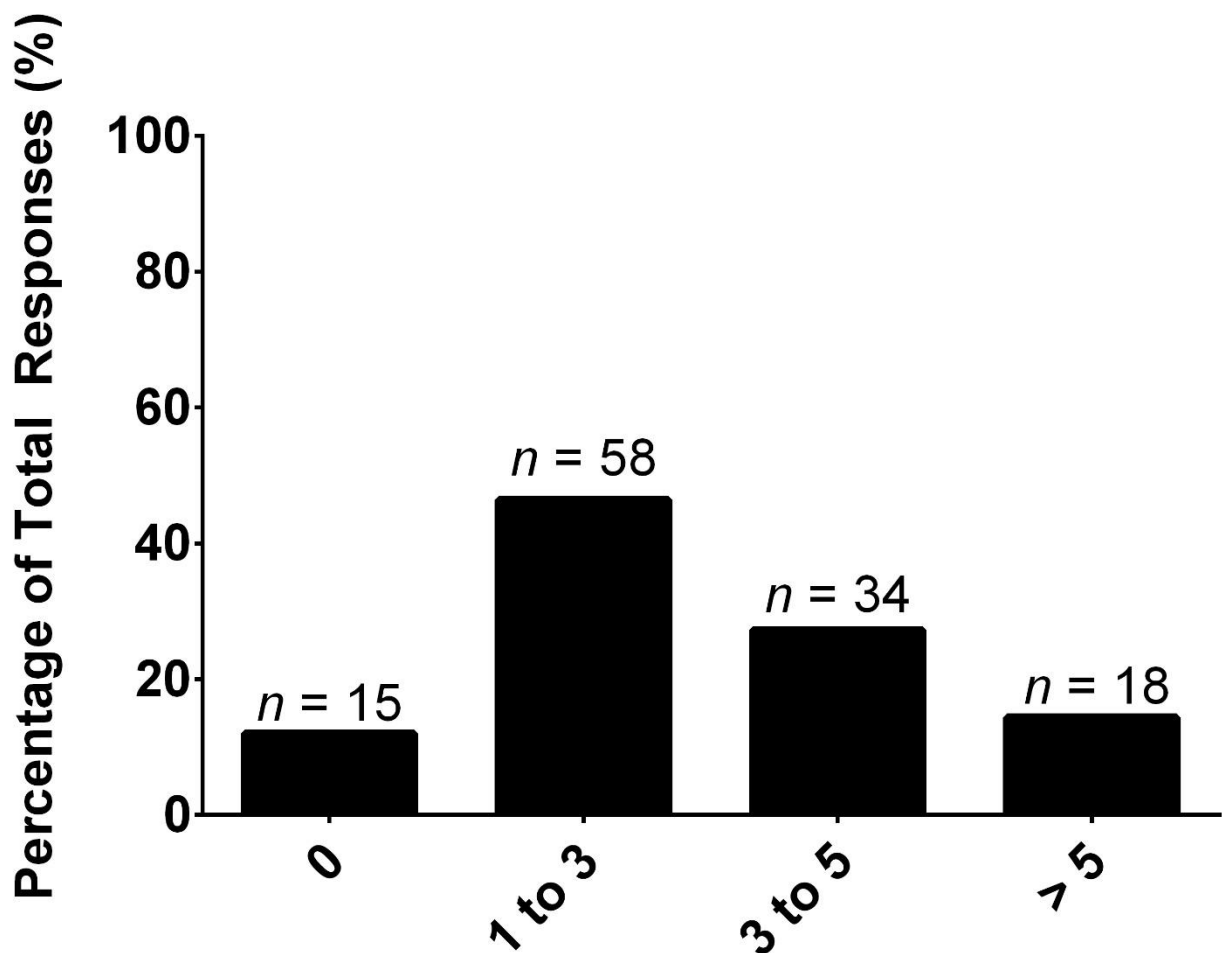
Supplemental Figure S3. “Number of people in laboratory”. The values are shown as a percentage of total responses (total number of responses, $n = 125$). The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options.



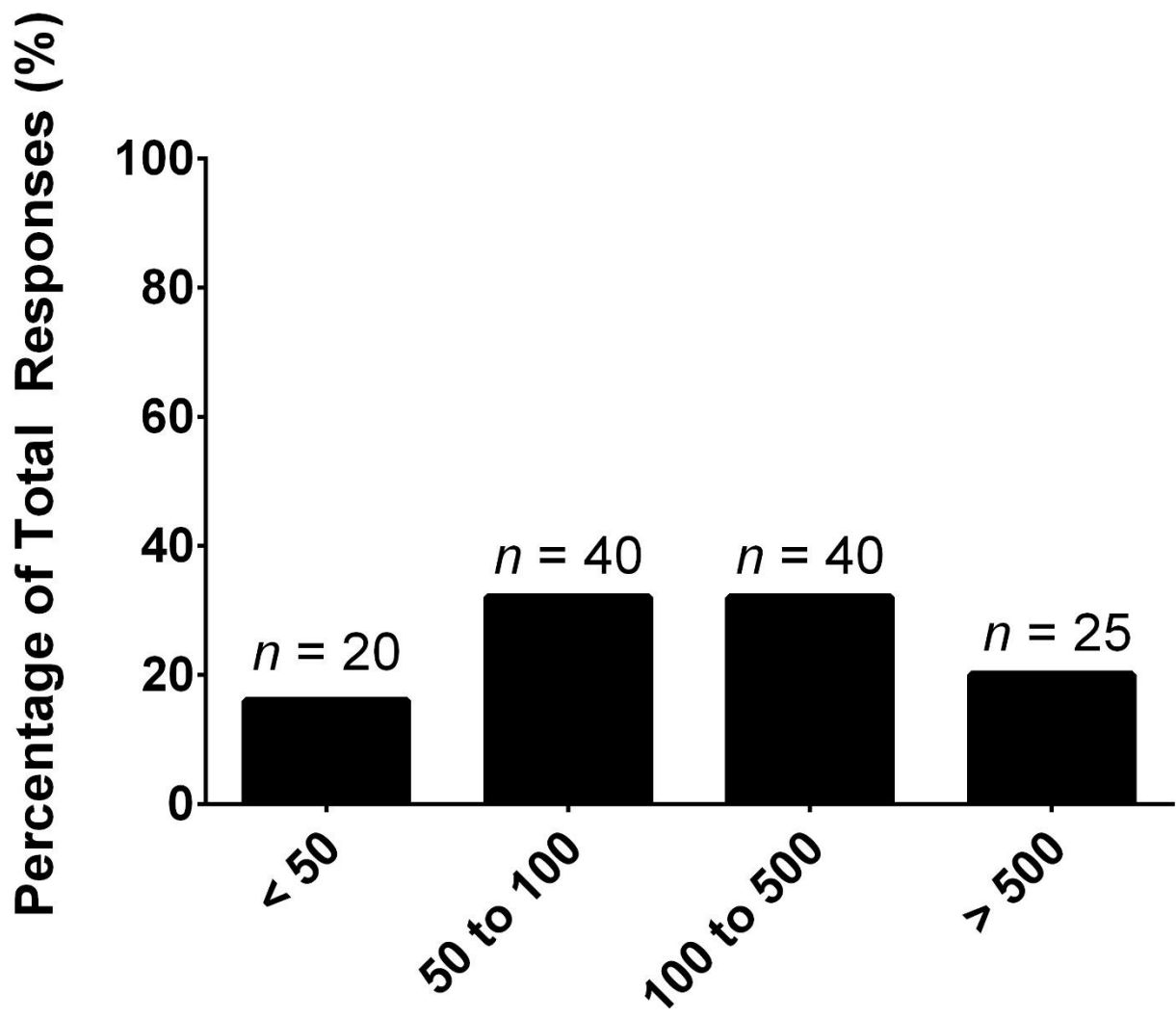
Supplemental Figure S4. “**Type of institution (select those that apply)**”. The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$; total responses, $n = 141$). The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



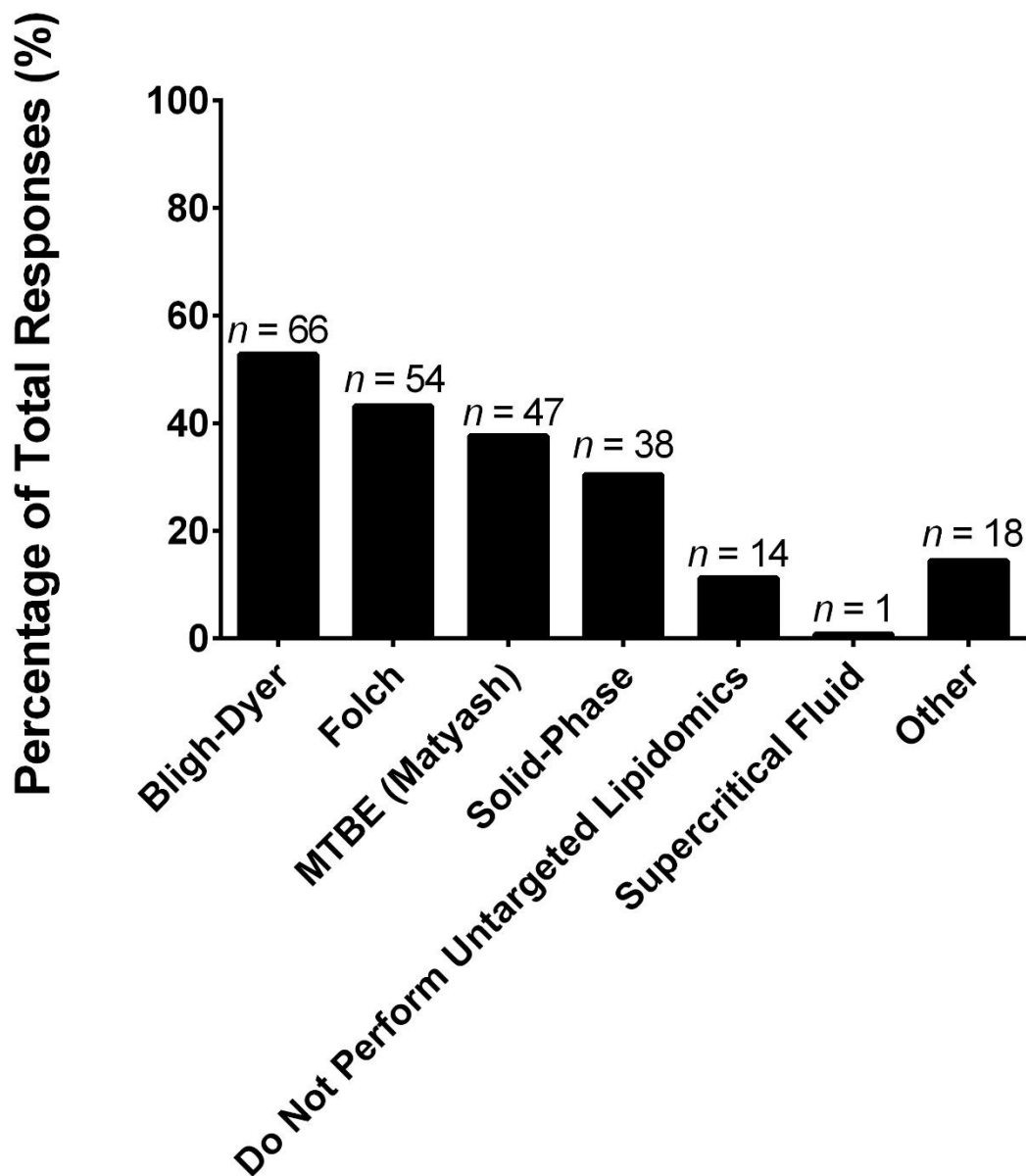
Supplemental Figure S5. “**What kind of lipid applications do you typically work on in your laboratory (select those that apply)**”. The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 335. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. Write-in responses (“other”) included basic sciences, application development, metabolism/metabolite flux, nutrition, dermatology, and yeast/fermentation research.



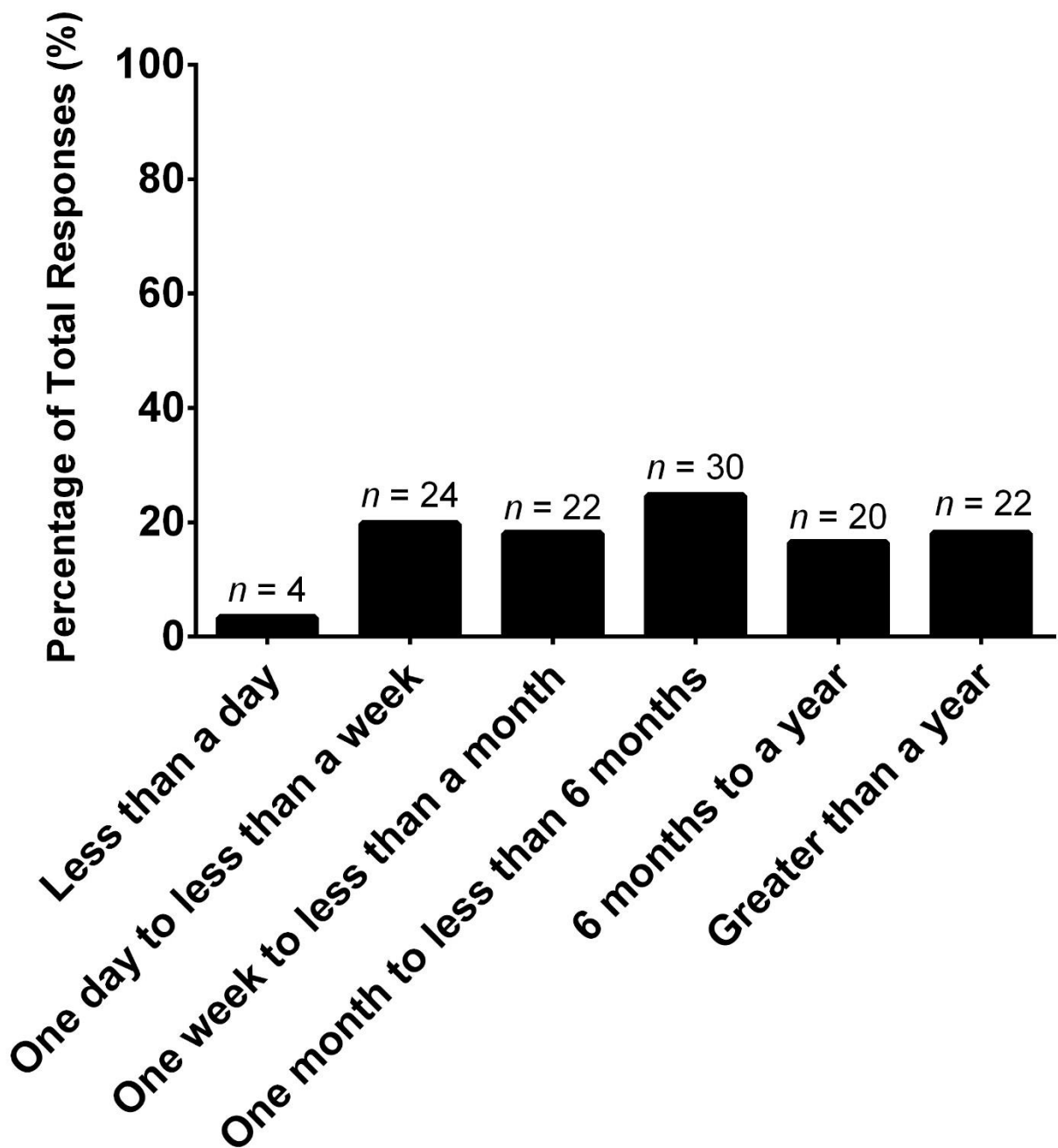
Supplemental Figure S6. “**Approximately how many lipidomics manuscripts does your laboratory publish per year**”. The values are shown as a percentage of total responses (total number of responses, $n = 125$). The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options.



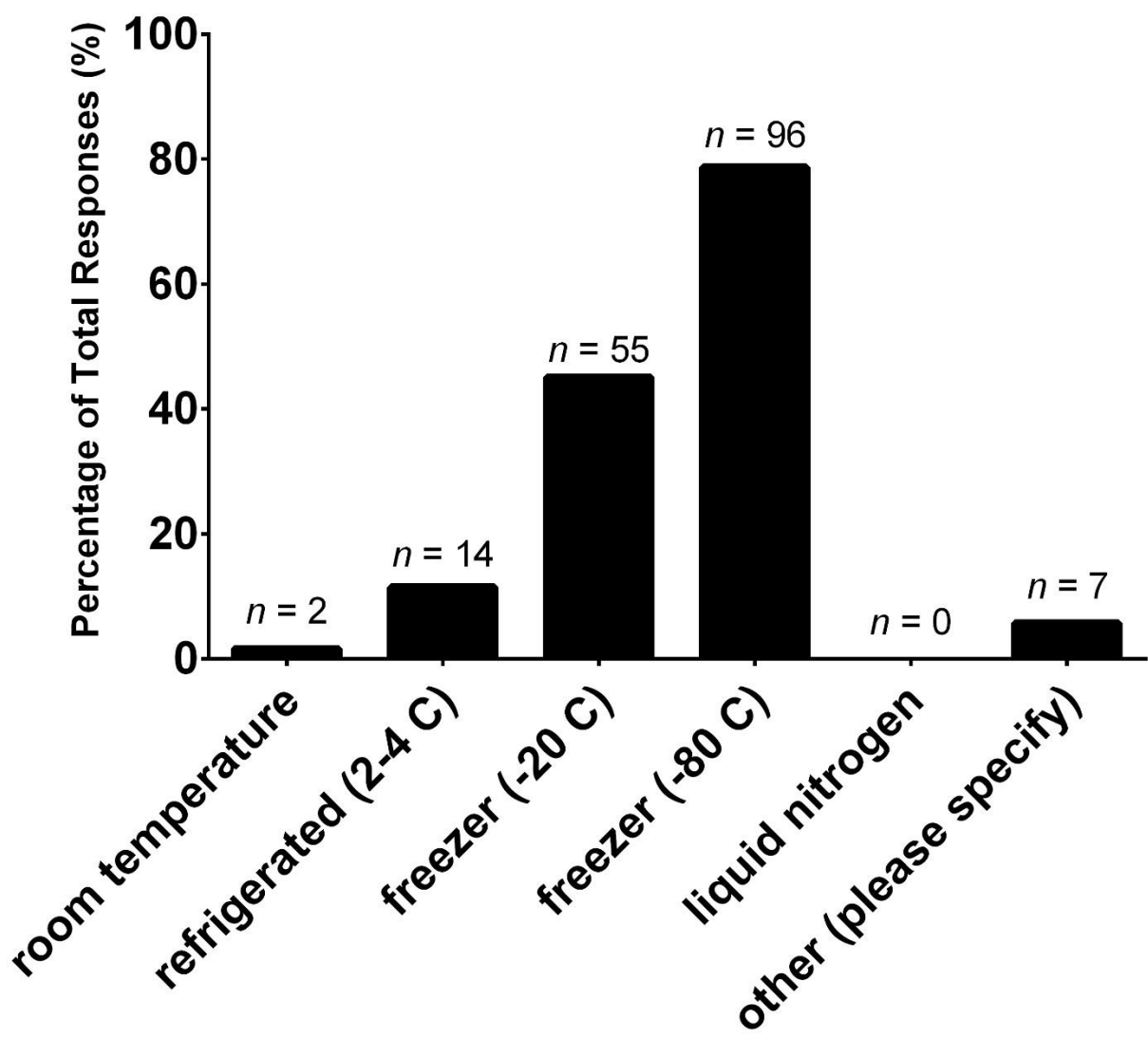
Supplemental Figure S7. “Approximately how many lipid samples does your laboratory analyze in a month”. The values are shown as a percentage of total responses (total number of responses, $n = 125$). The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options.



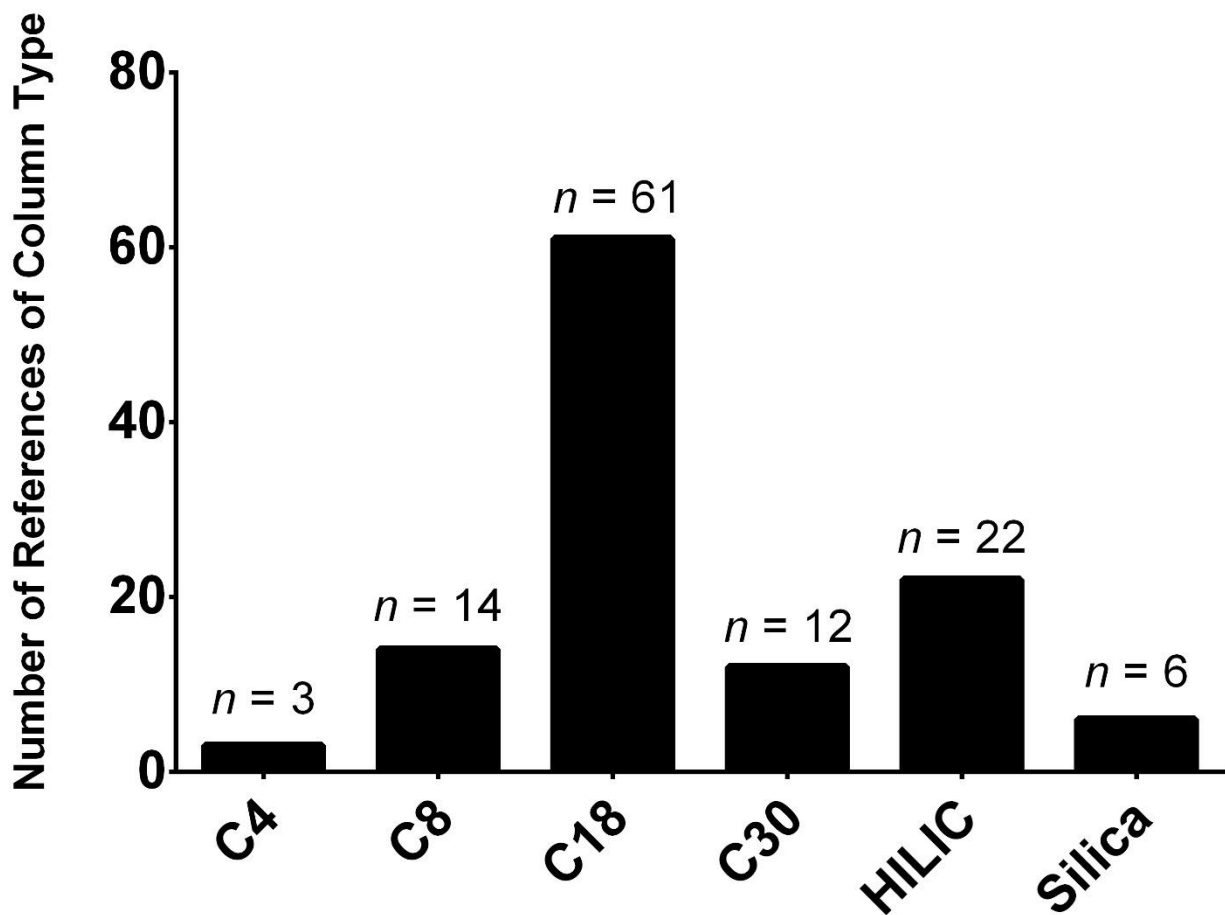
Supplemental Figure S8. “For untargeted lipidomics experiments, what lipid extraction does your laboratory employ (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 238. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



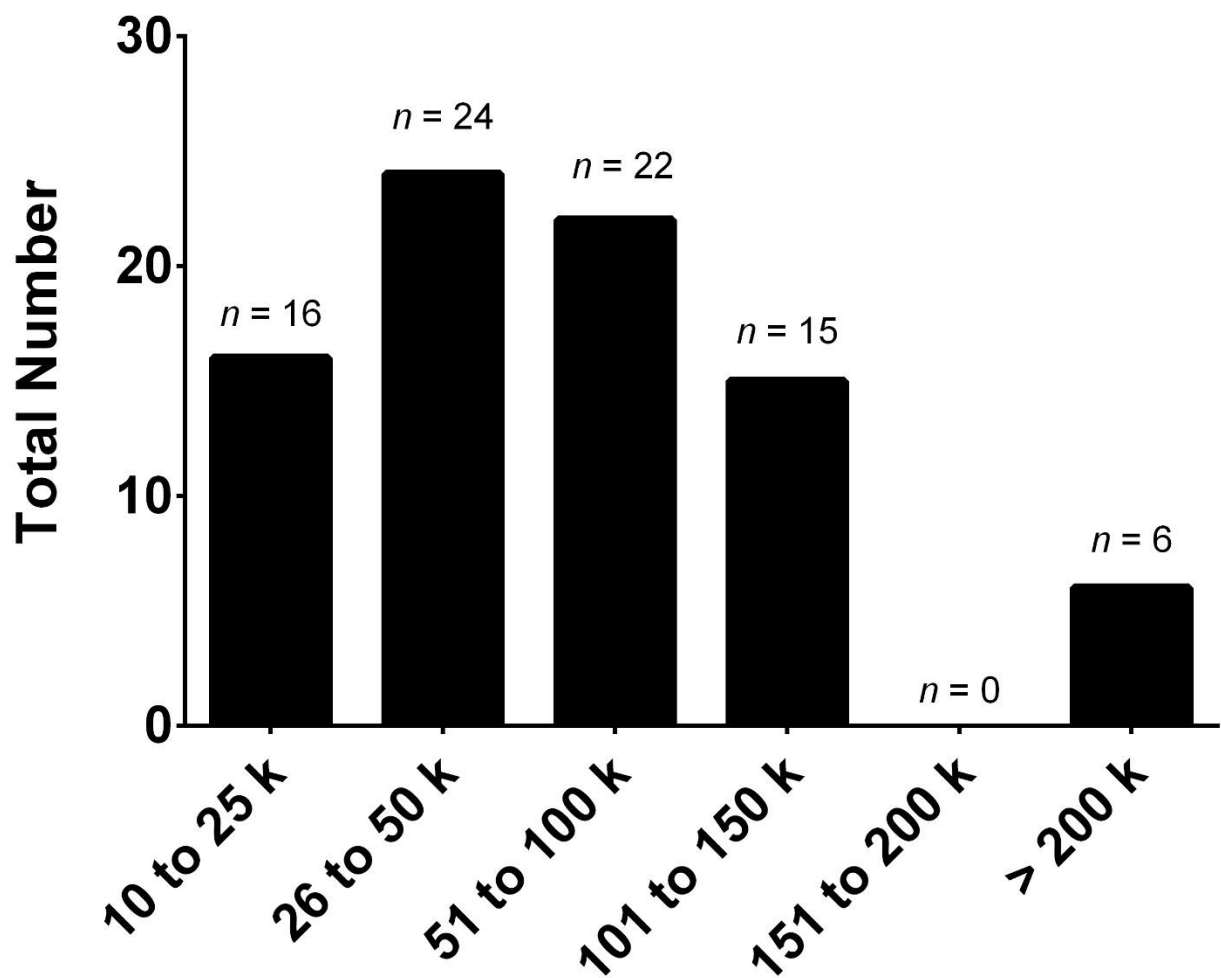
Supplemental Figure S9. “About how long does your laboratory store extracted lipidomics samples before you discard?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 122. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



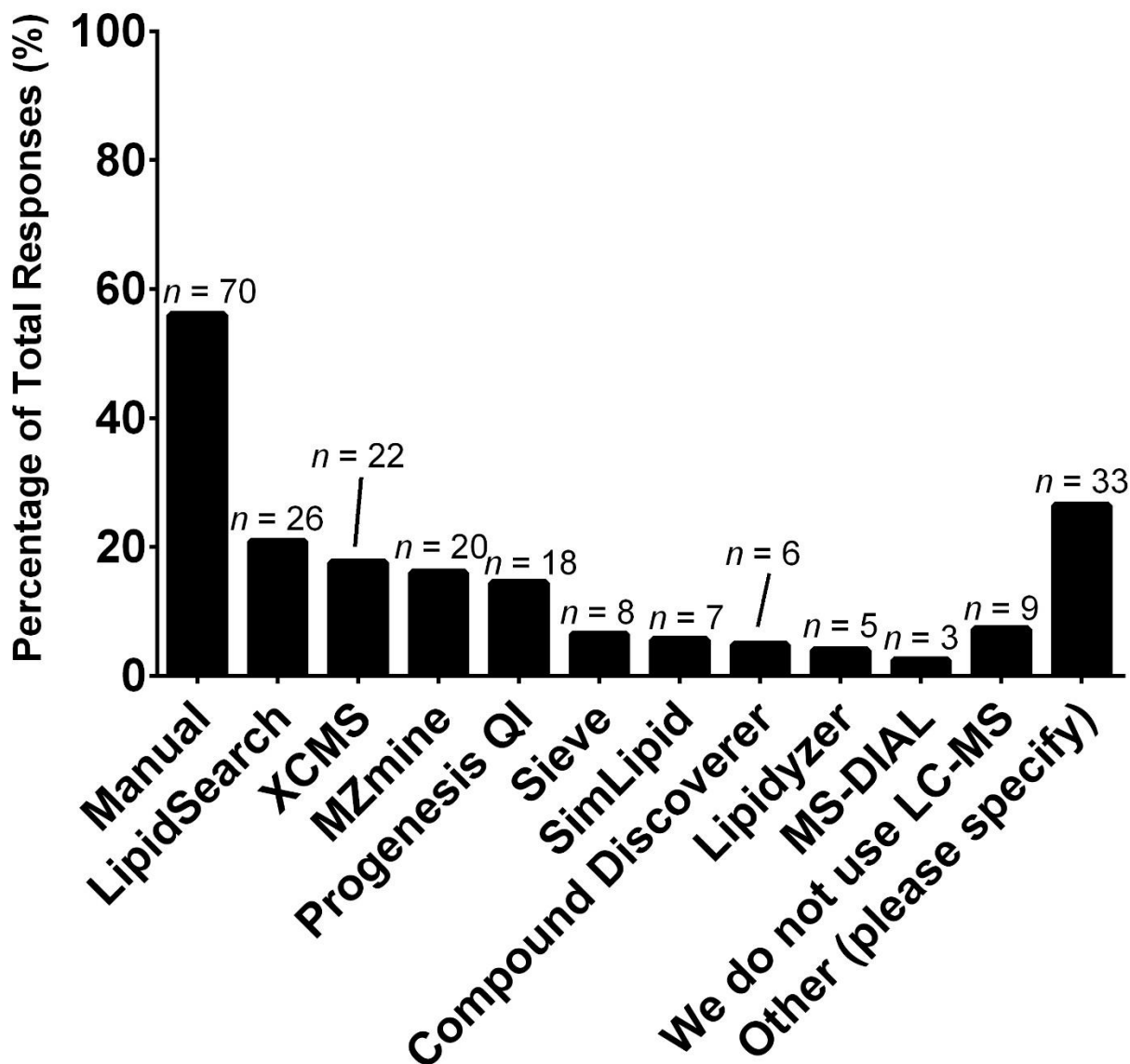
Supplemental Figure S10. “What temperature(s) does your laboratory store lipid extracts at (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 174. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



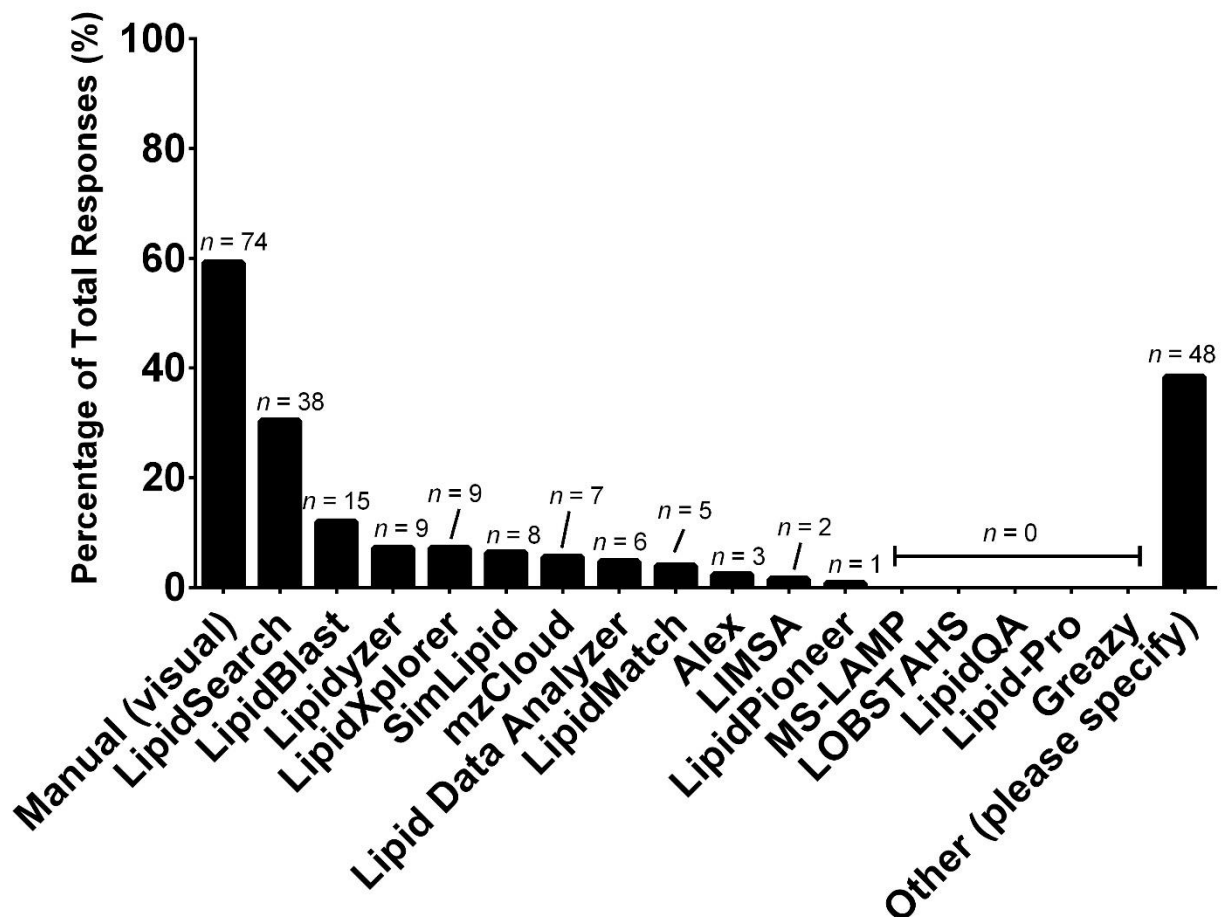
Supplemental Figure S11. “If chromatography, what type of column(s) does your laboratory use for lipidomics?” Total number of write-in responses for each column type (overall total number of responses, $n = 132$). Note that this question was optional. There were several other column types listed but had occurrences less than 3.



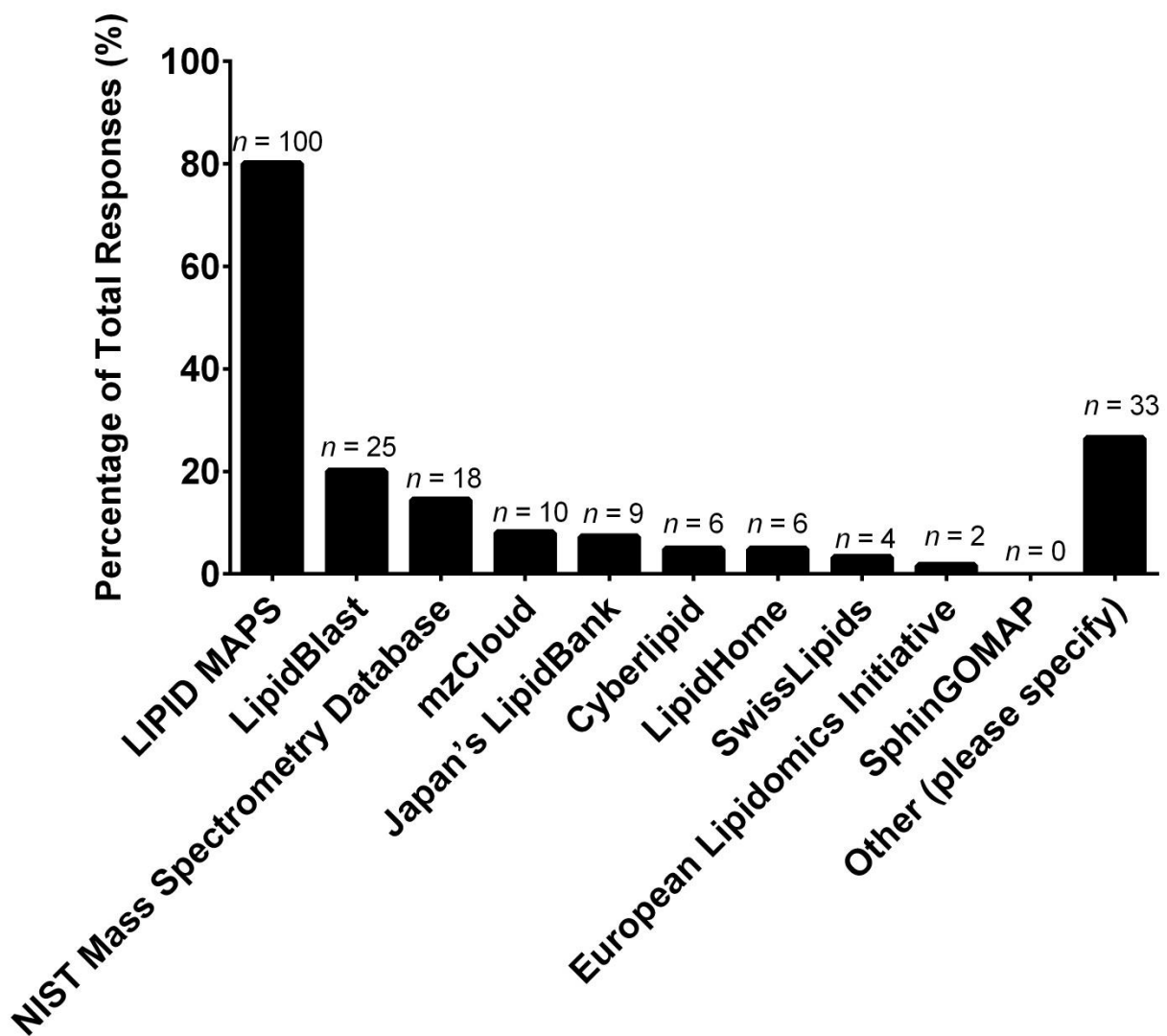
Supplemental Figure S12. “If you incorporate a high-resolution mass spectrometer, at what mass resolving power do you analyze your lipid extracts (answer N/A if you only use a low-resolution mass spectrometer)?” Total number of write-in responses for each resolution value. Note that this question was optional.



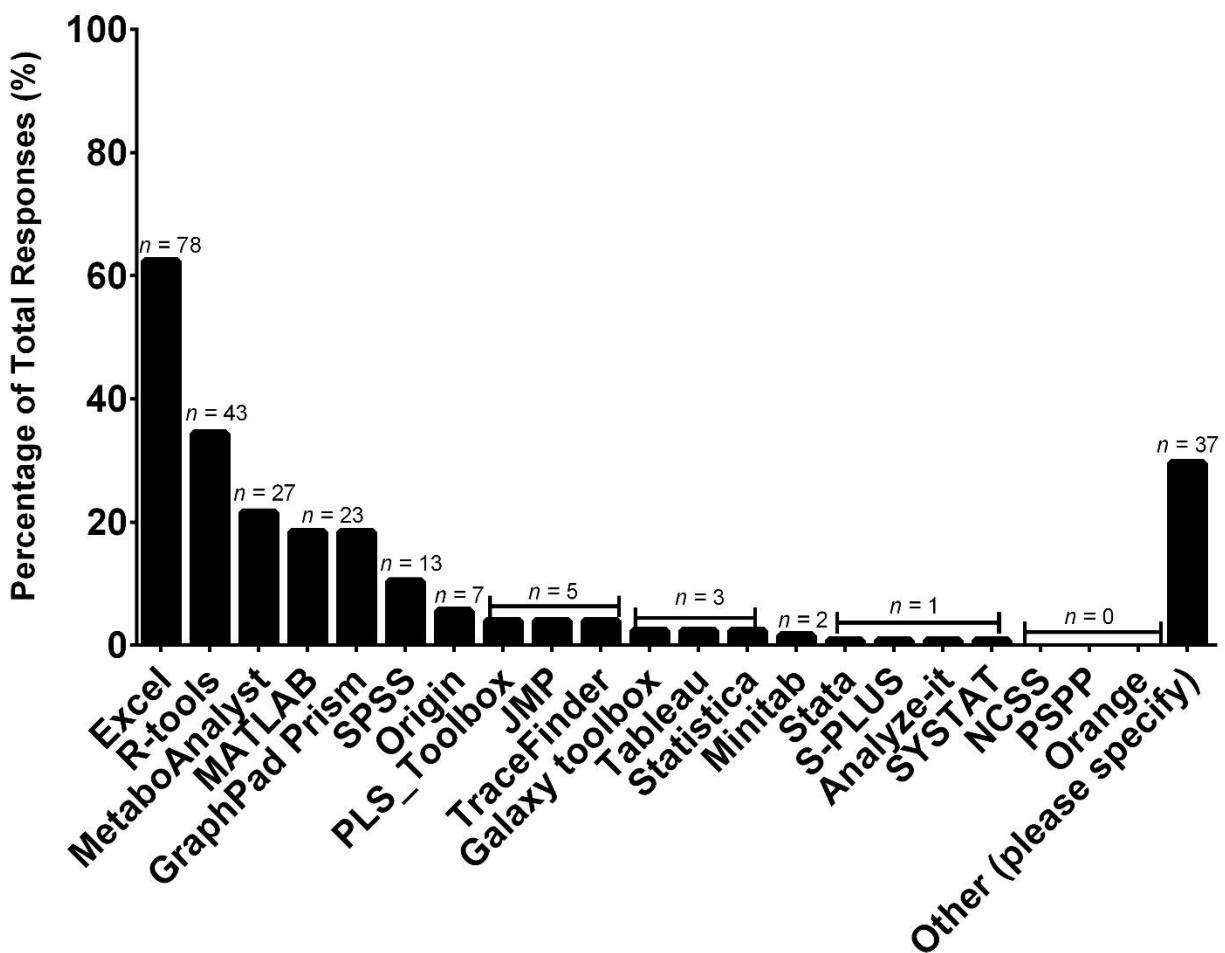
Supplemental Figure S13. “If you use LC-MS, what software does your laboratory employ for peak picking/processing (select all that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 227. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. Upon examination of the write-in responses, the most common answers included MultiQuant (7 %) and LipidView (6 %), with other responses including LipidomeDB, Skyline, LIQUID, and Elements.



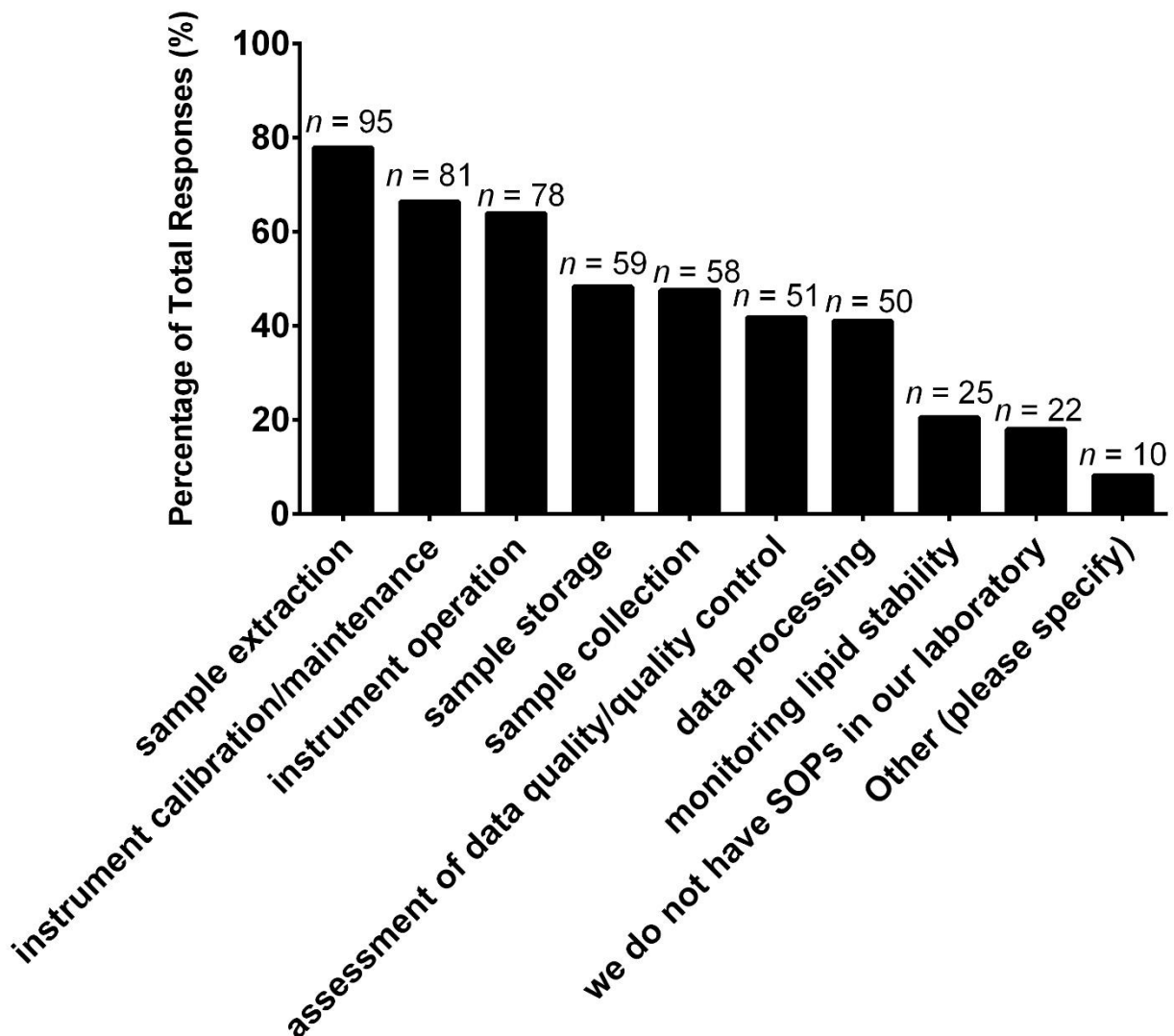
Supplemental Figure S14. “What software does your laboratory employ for lipid identification (select all that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 225. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. (%). The ‘other’ response was again large (38 %), and the most common write-in response was *in-house* strategies (14 %) and LipidView (10 %). Other write-ins included Metlin, SimLipids, MASSBANK, ChEBI, and ALEX.



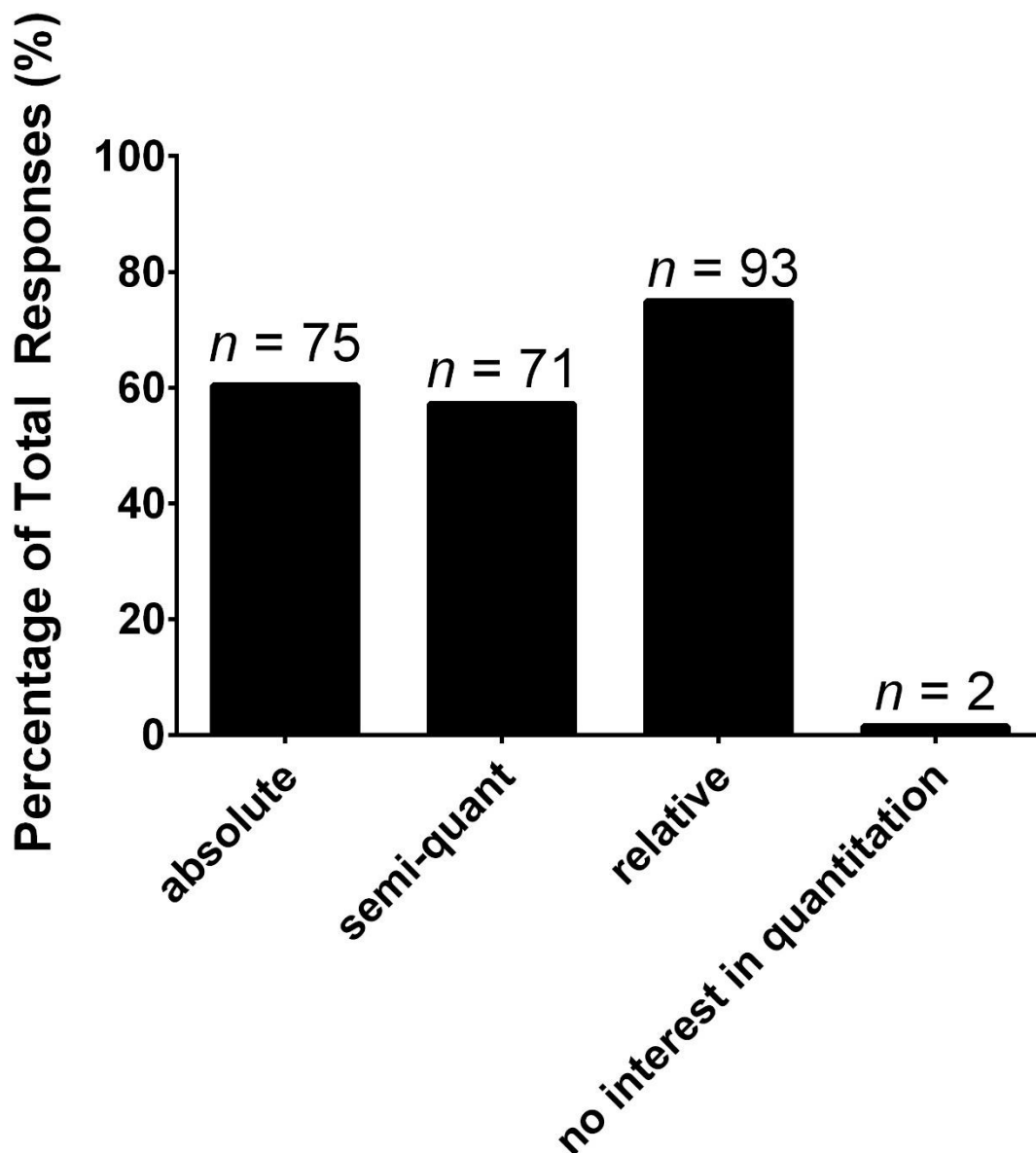
Supplemental Figure S15. “What lipid databases do you use (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 213. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. The other category (26 %) included HMDB (6 %) and *in-house* databases (6 %).



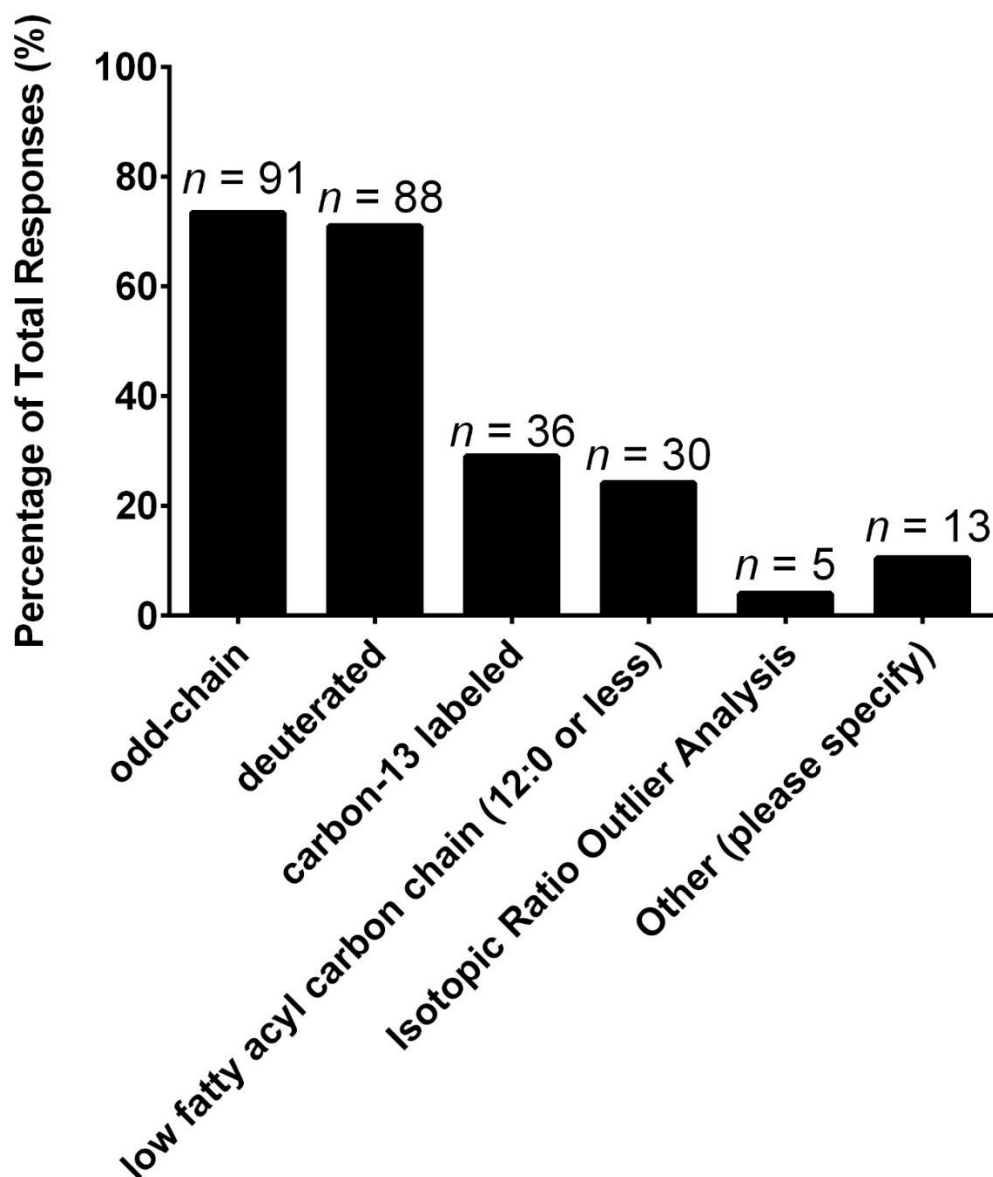
Supplemental Figure S16. “What software does your laboratory employ for lipid quality control and statistics (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 281. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. Common write-in responses included Simca (5 %) and *in-house* programs (9 %).



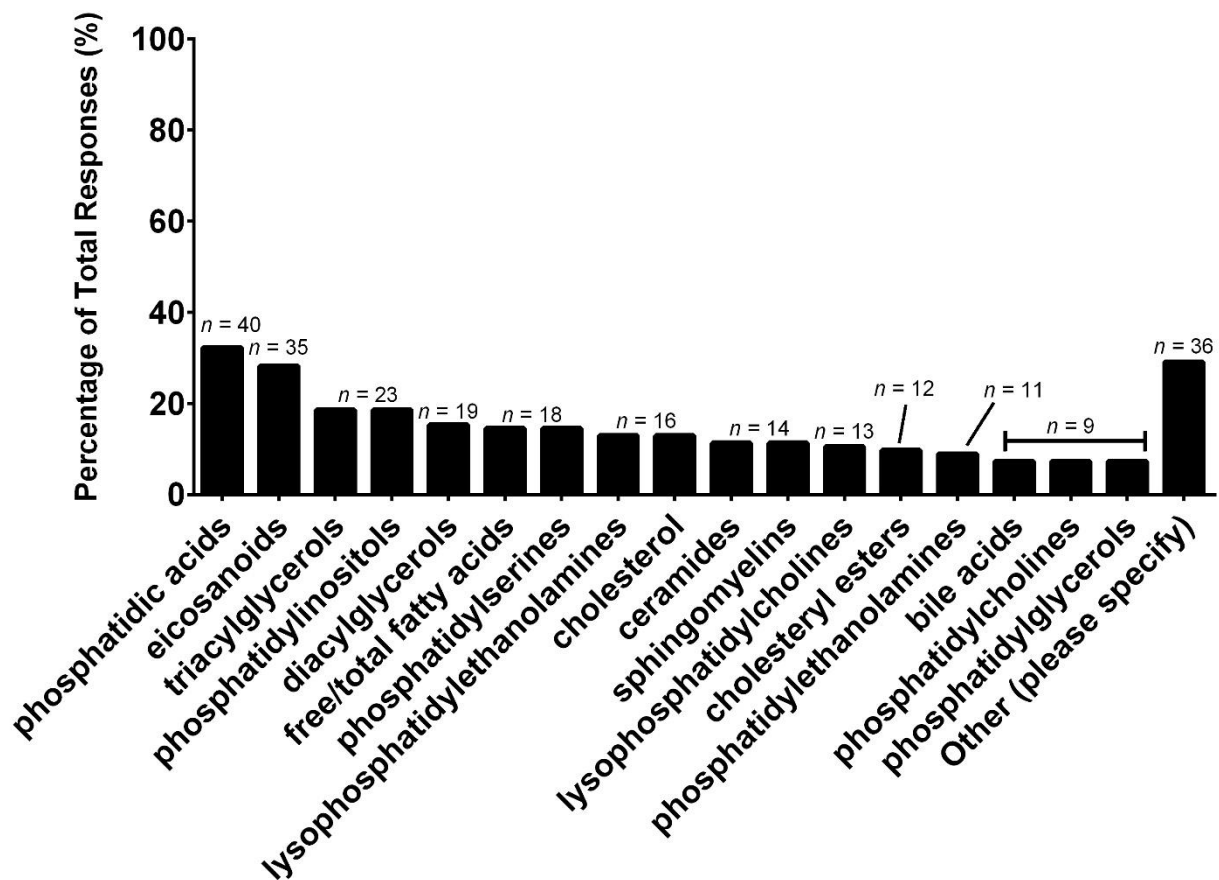
Supplemental Figure S17. “Do you have written standard operating procedures (SOPs) in your laboratory, and if so, what aspects do the SOPs cover (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 529. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. One ‘other’ write-in response was internal standard mix creation (8 %).



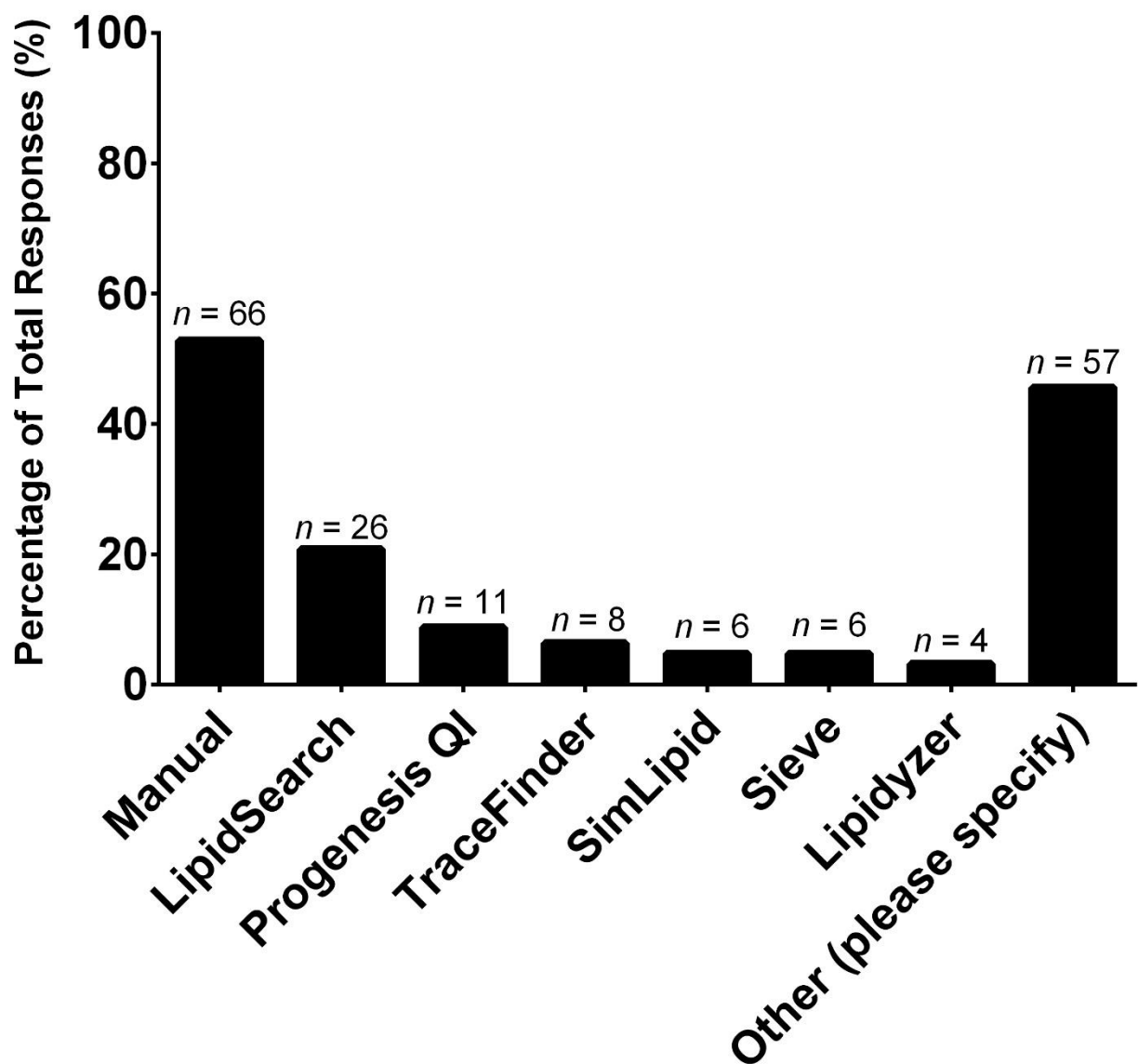
Supplemental Figure S18. “What type of quantitation do you perform in your laboratory?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 241. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



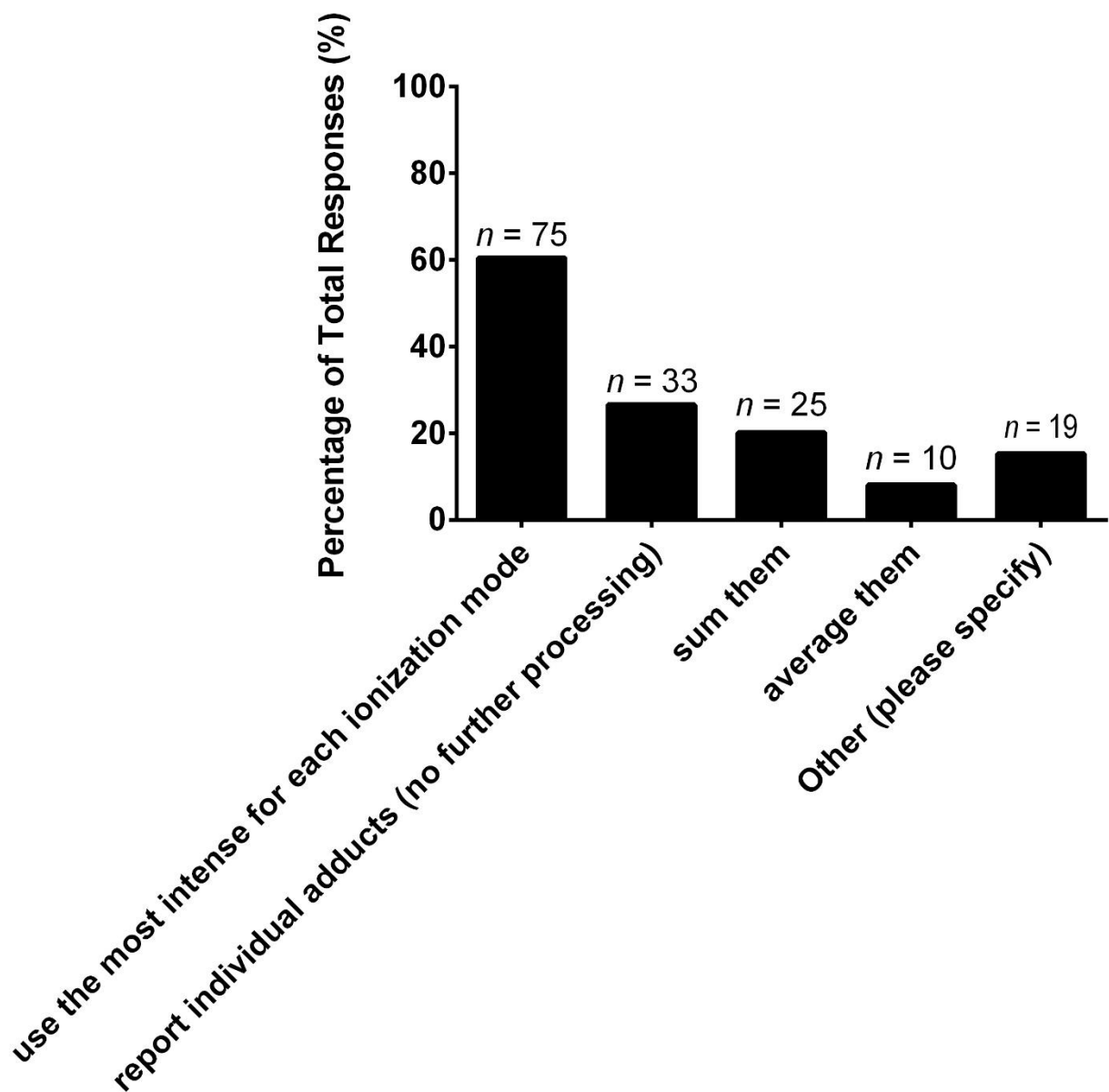
Supplemental Figure S19. “What type of internal standards does your laboratory most often employ (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 263. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



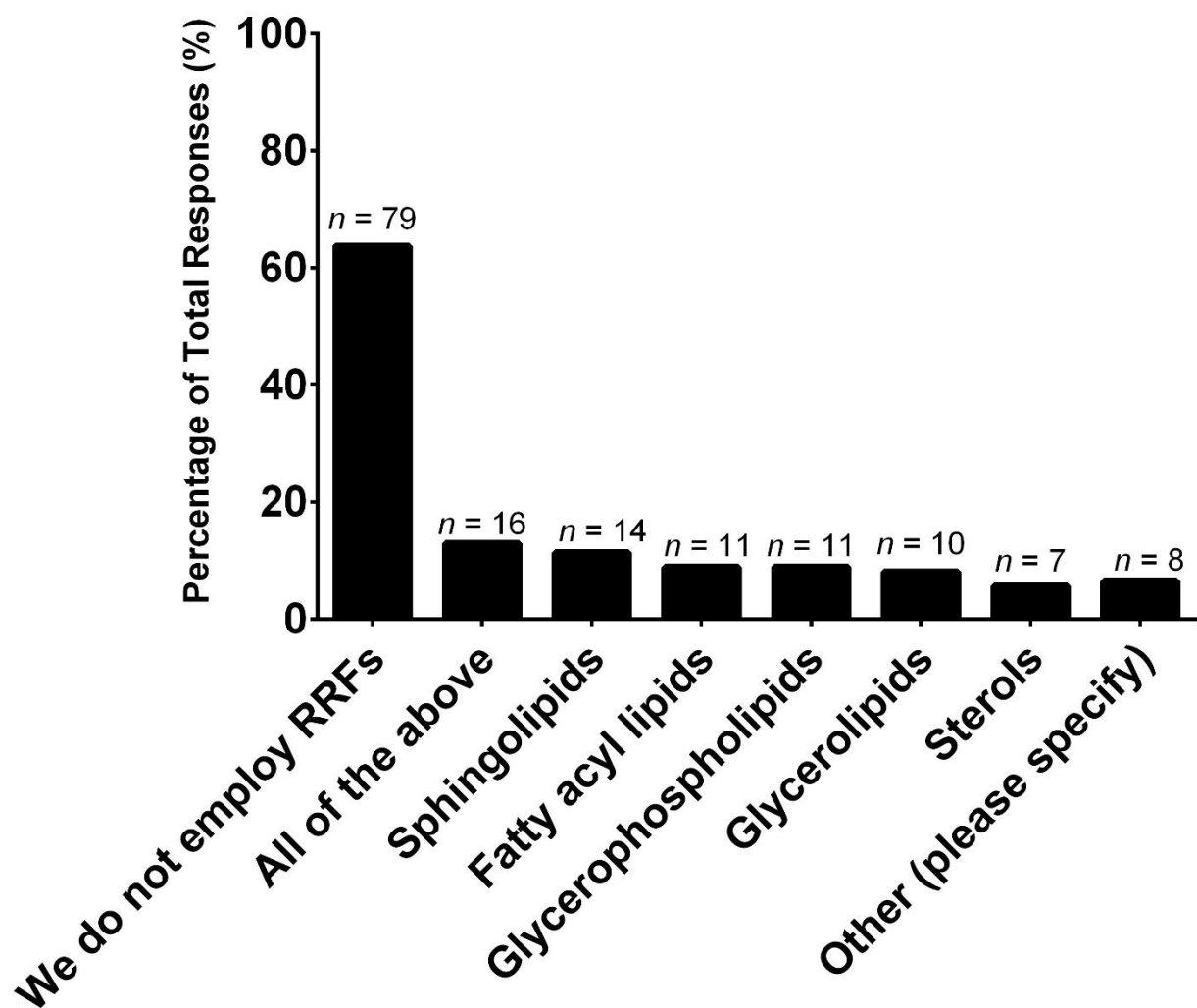
Supplemental Figure S20. “What lipids do you find most challenging to quantitate (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 335. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. The ‘other’ response had write-ins that included lysophosphatidic acids, vitamins, cardiolipins, steroids, phosphoinositides, glycosphingolipids, plasmalogens, gangliosides, endocannabinoids, monoacylglycerols, cerebroside, and oxidized lipids.



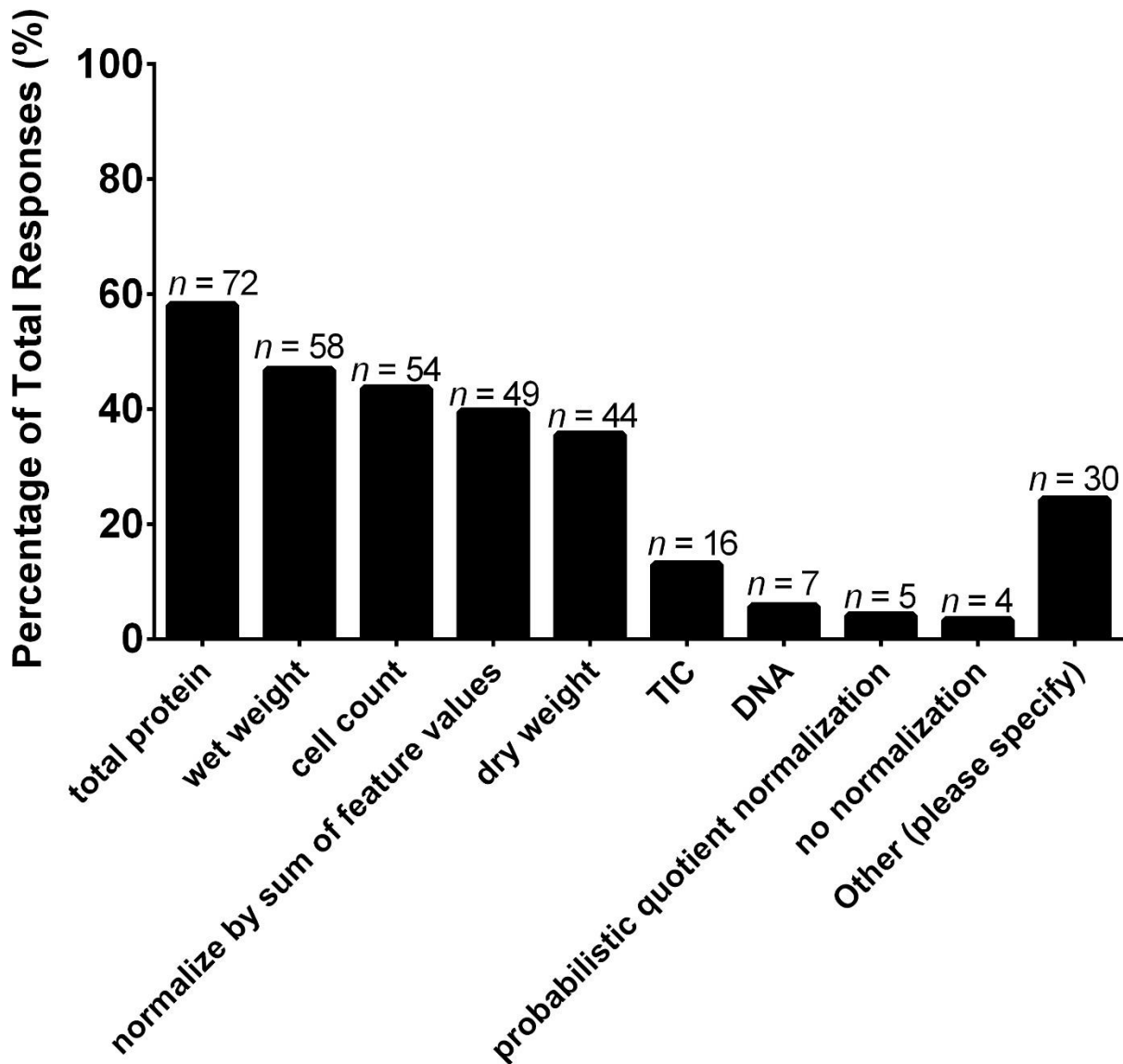
Supplemental Figure S21. “**What software does your laboratory employ for lipid quantification (select those that apply)?**” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 125$). The overall total number of responses was 184. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. The most common write-ins were MultiQuant (12 %), MassHunter (3 %), with several others briefly mentioned by only a few participants, Skyline, R-Scripts, MAVEN, LC Quan, Traverse MS, TargetLynx, MetIDQ, Elements, LipidomeDB DCE, MS-DIAL, LIMSA, and Lipid Data Analyzer.



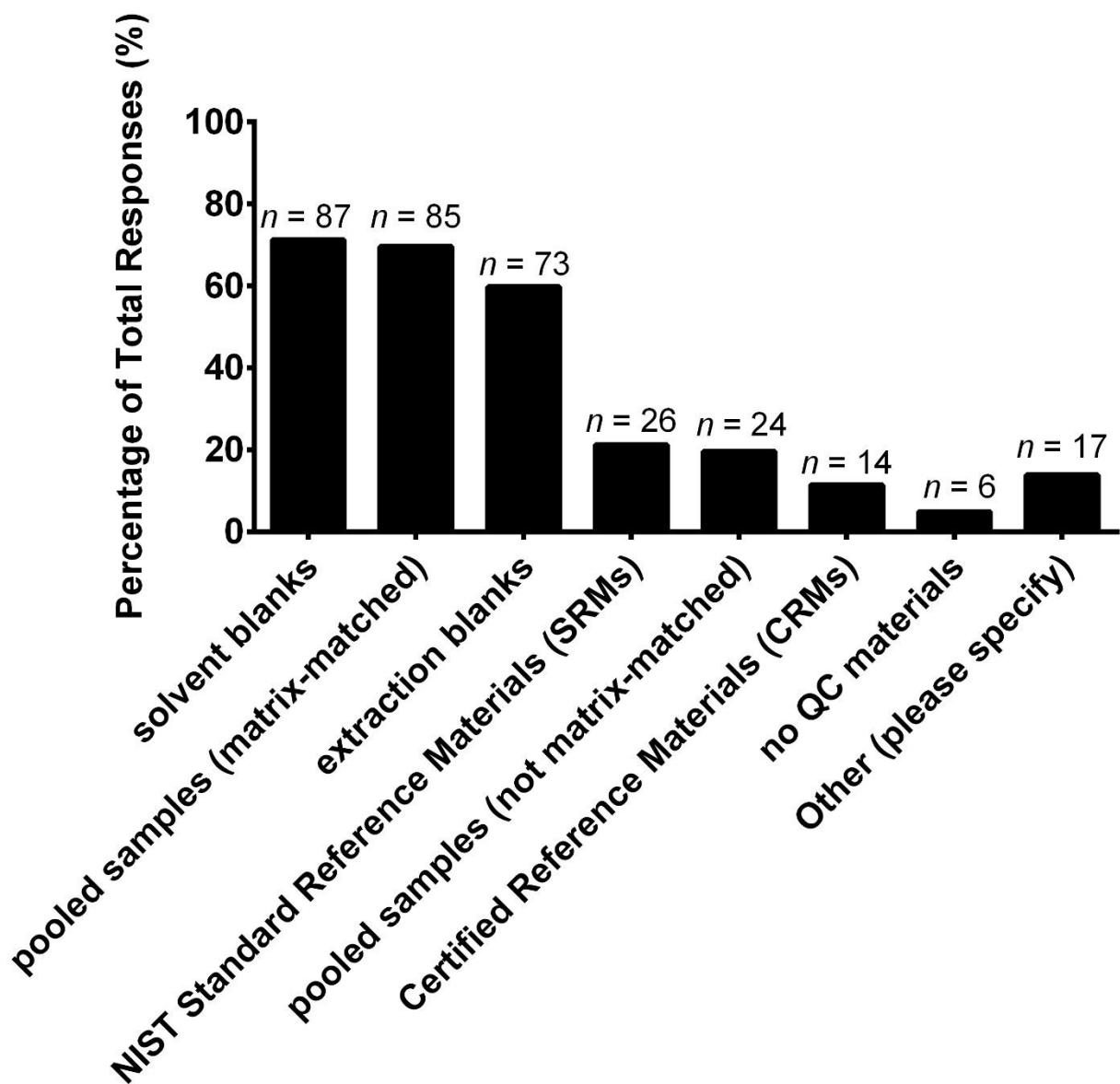
Supplemental Figure S22. “**How does your laboratory treat multiple adducts per lipid (select those that apply)?**” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 162. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



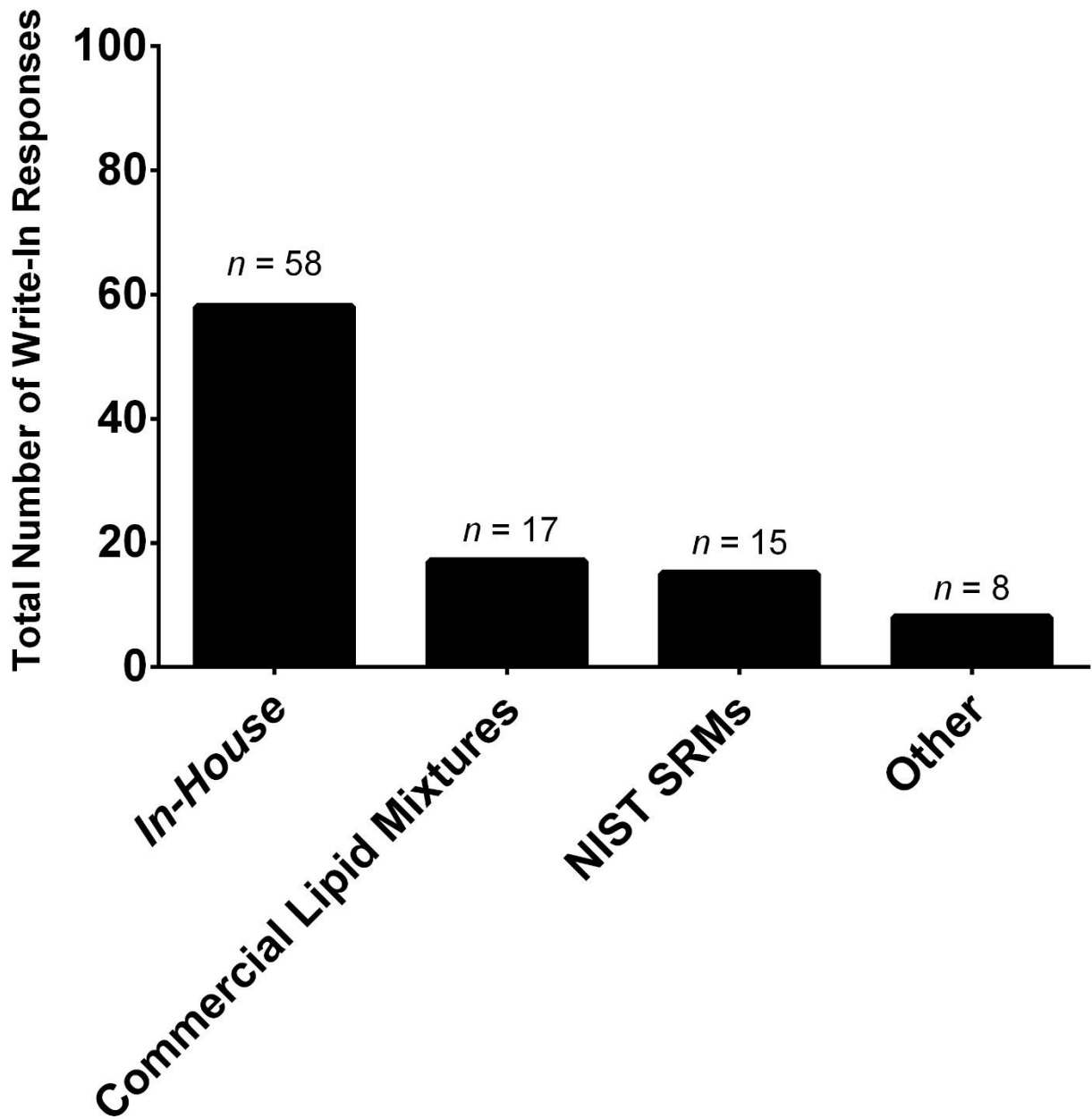
Supplemental Figure S23. “Does your laboratory employ relative response factors (RRFs) for these lipid categories (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 156. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



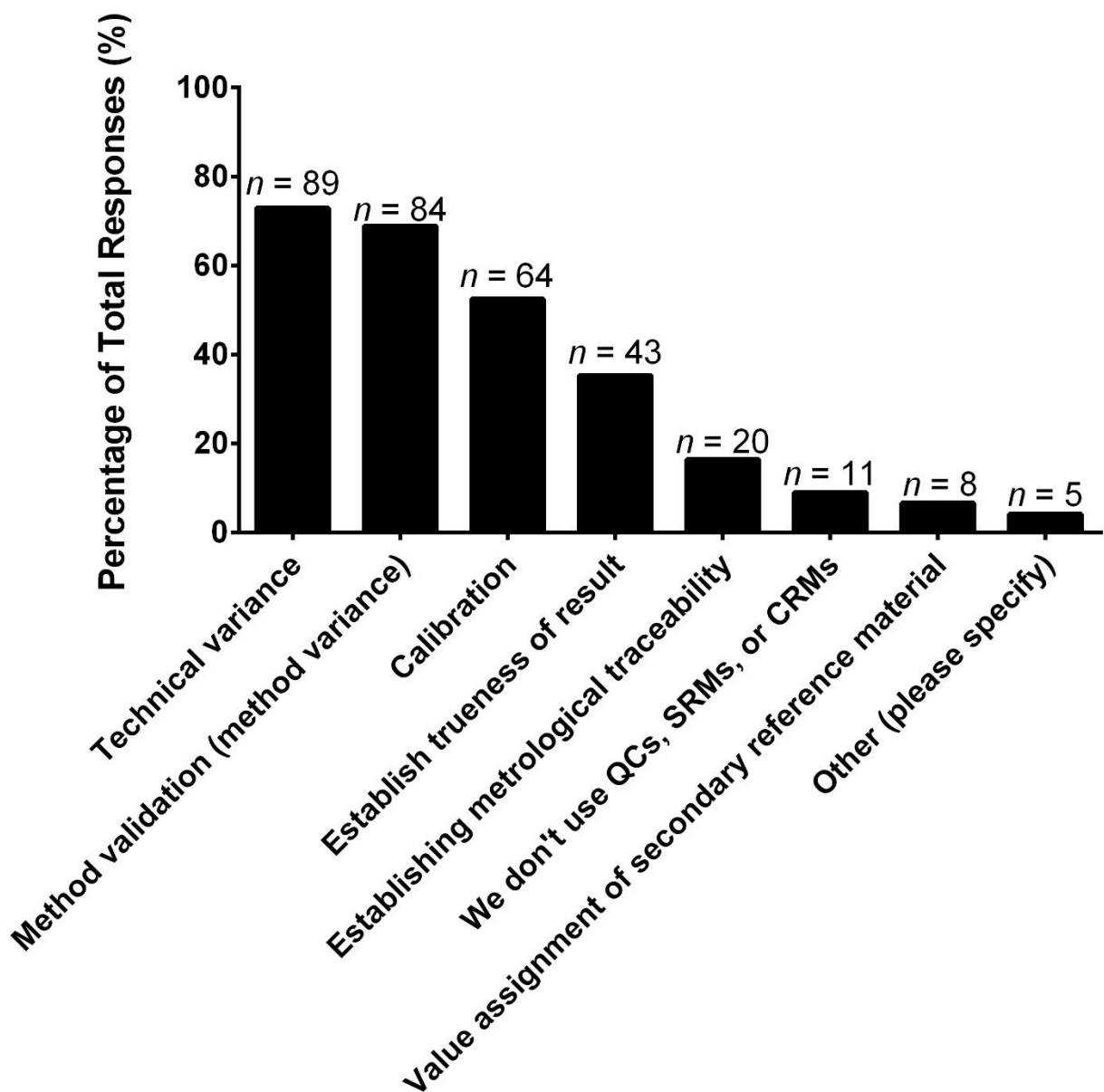
Supplemental Figure S24. “**How does your laboratory normalize your quantitative lipid values (select those that apply)?**” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 124$). The overall total number of responses was 339. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



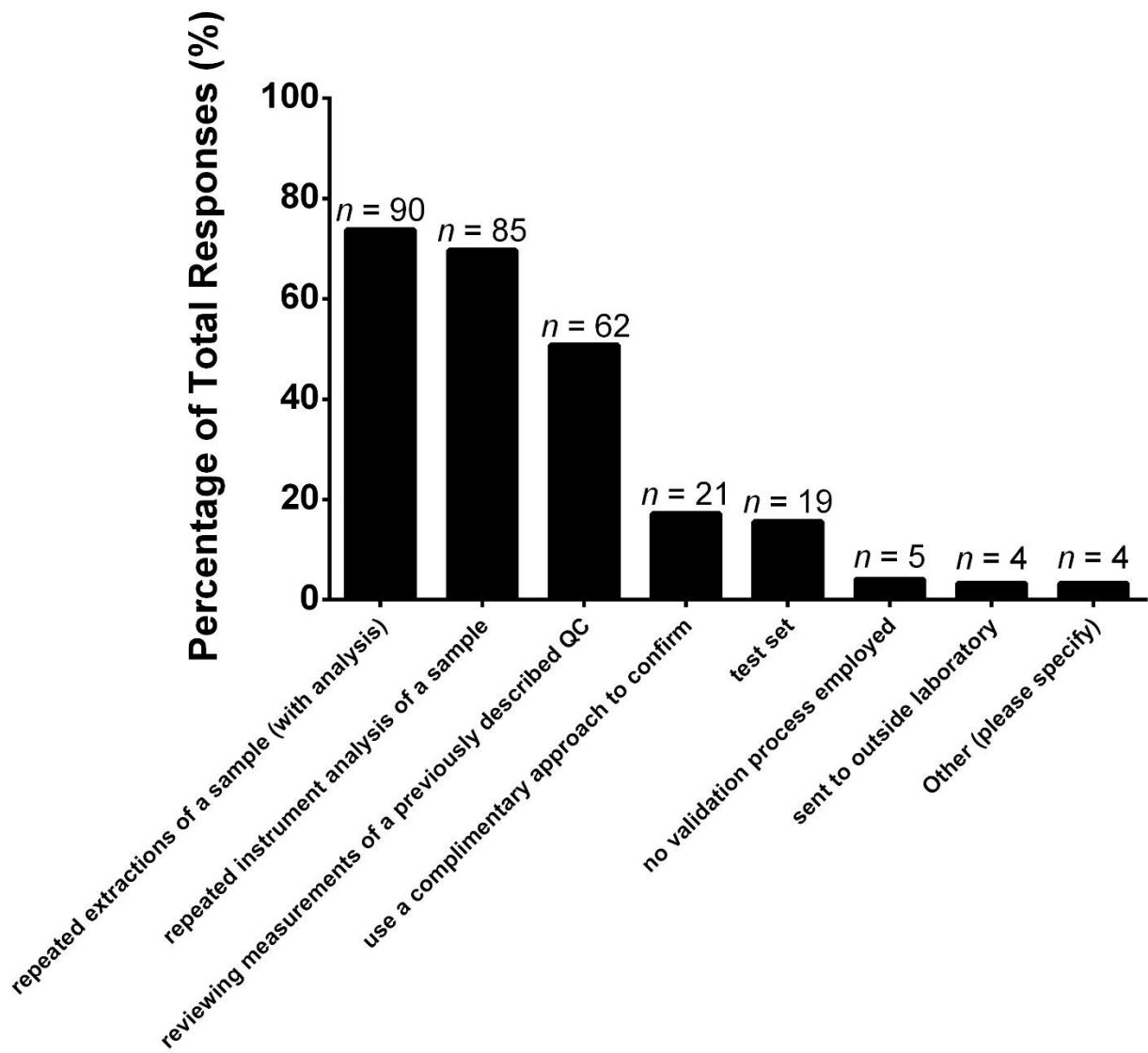
Supplemental Figure S25. “What types of quality control (QC) samples does your laboratory use in analytical measurements for lipidomics?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 332. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



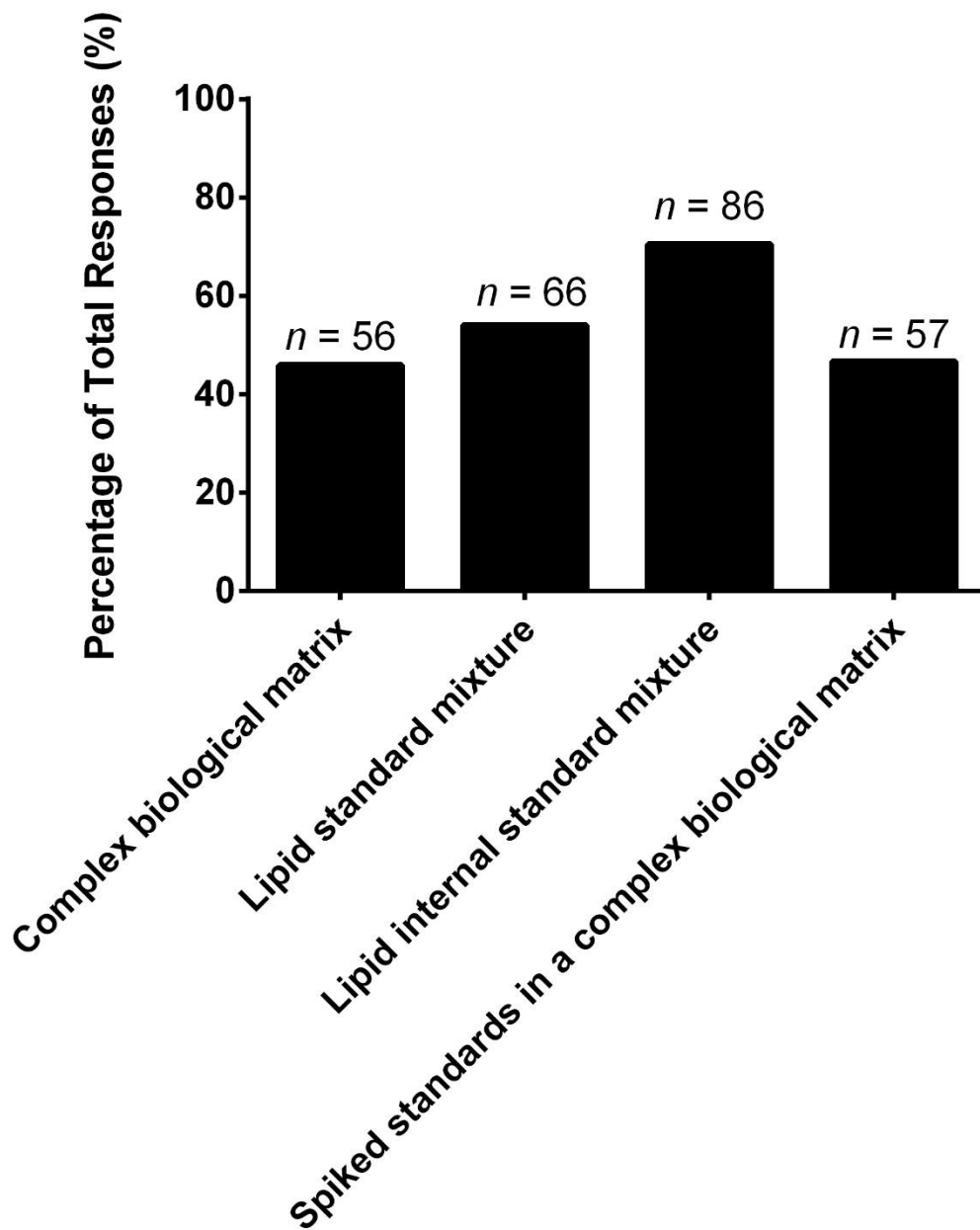
Supplemental Figure S26. “State whether the QC material you employ is commercially available or made in-house. For commercially available answers, please specify the material name.” Total number of write-in responses for each QC material. Note that this question was optional.



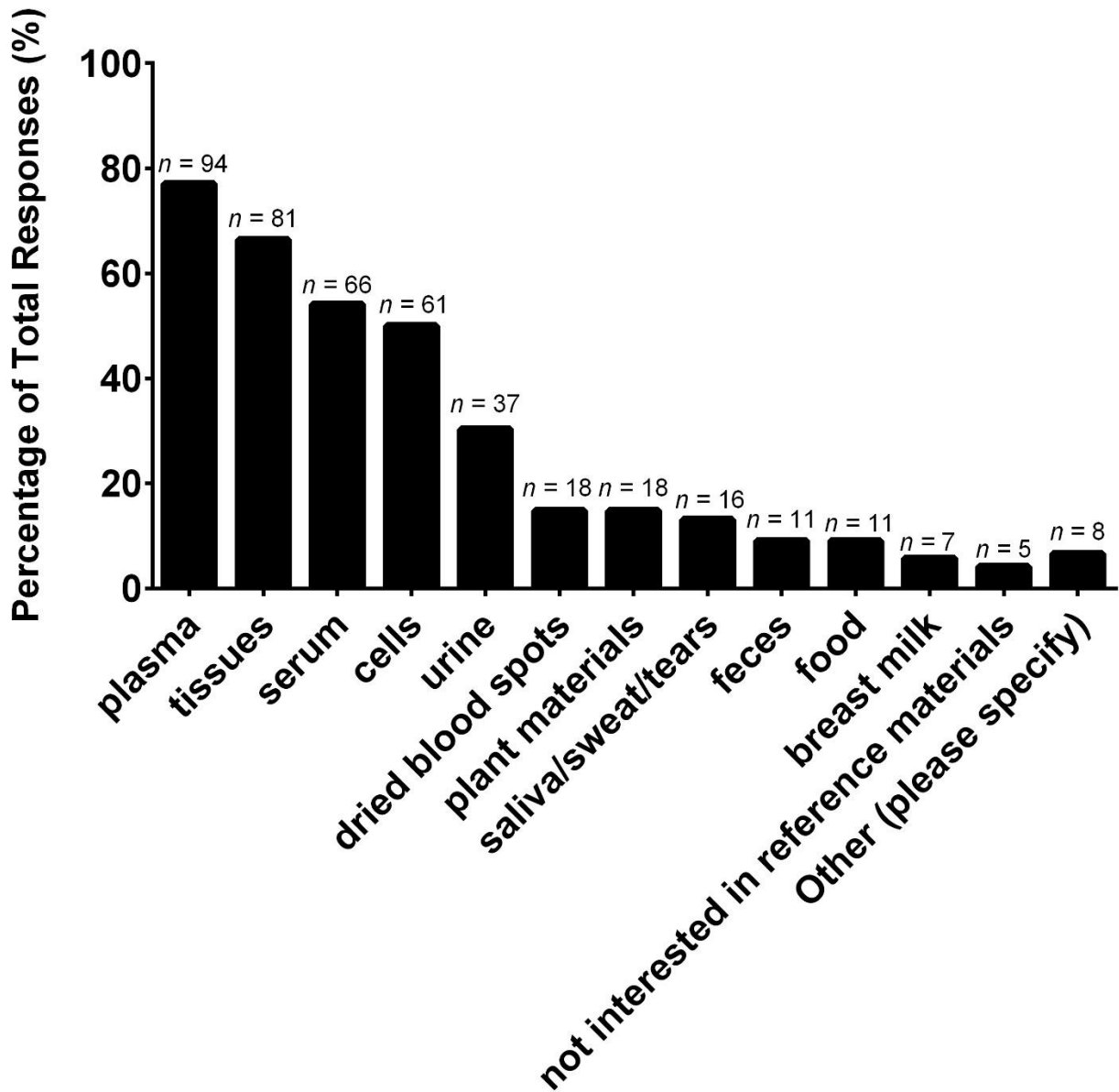
Supplemental Figure S27. “What does your laboratory use QCs, SRMs, or CRMs for (select those that apply)?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 324. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



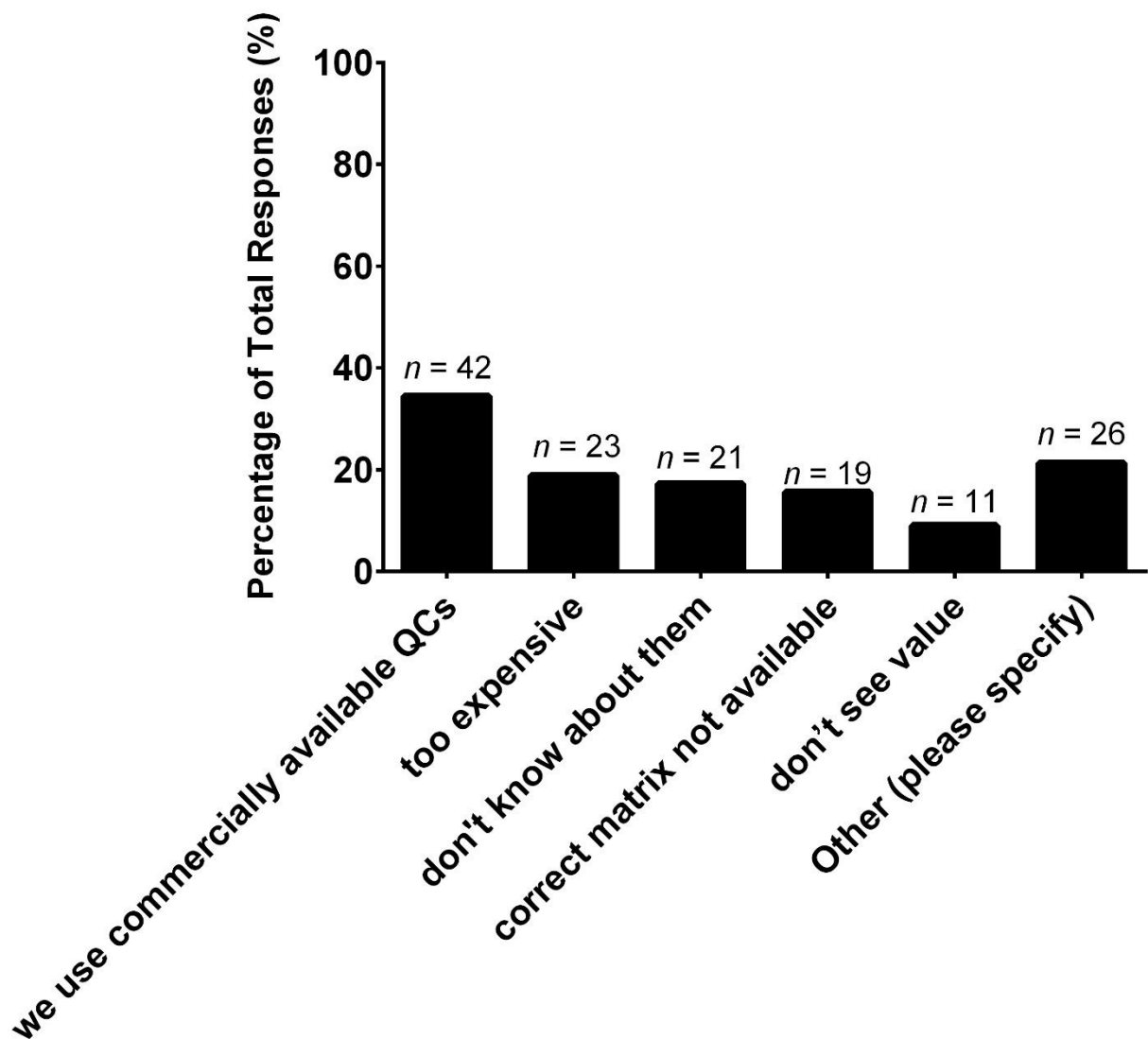
Supplemental Figure S28. **“Do you validate your project sample measurements with”**. The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 290. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



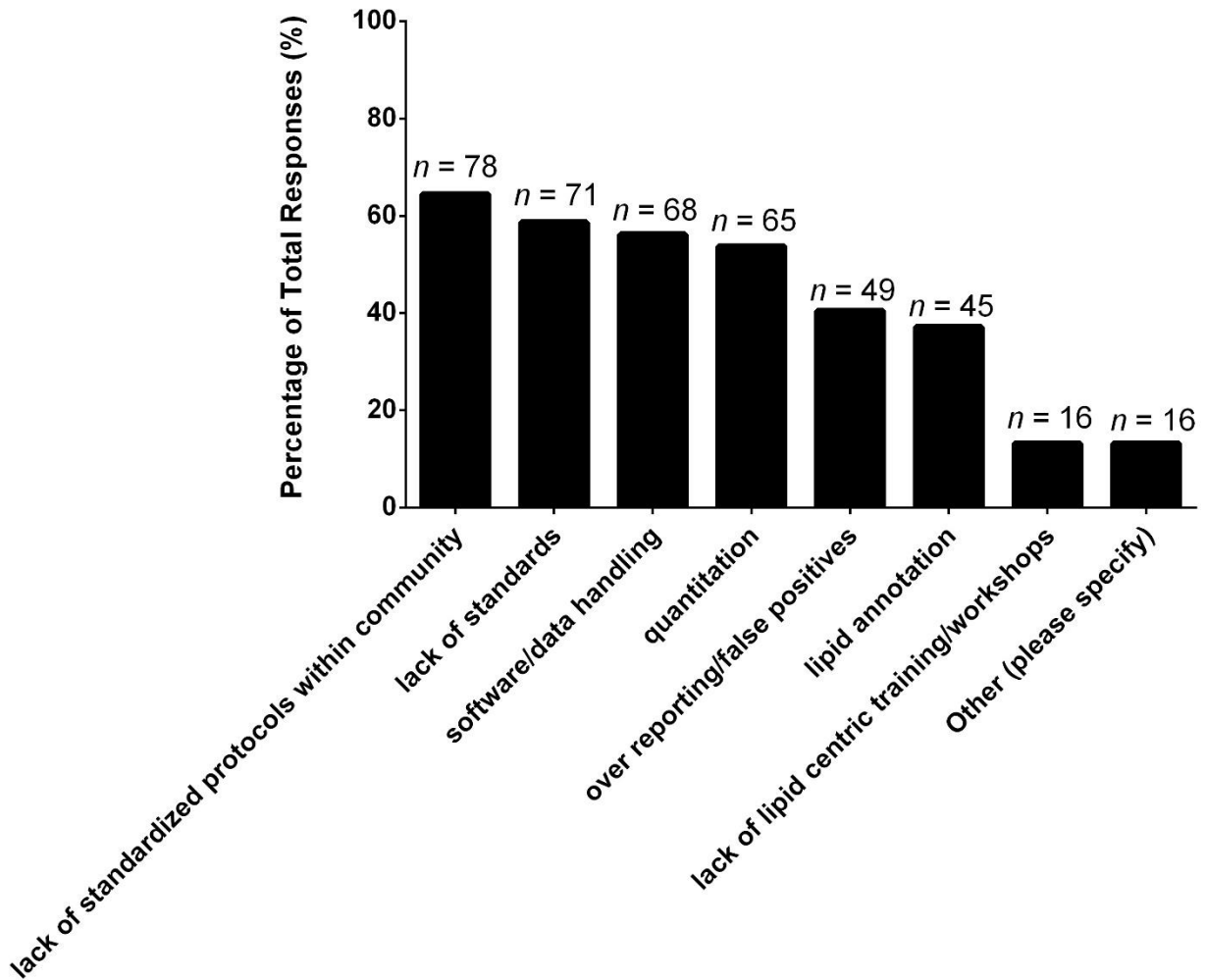
Supplemental Figure S29. “What type of reference material would be of most interest to your laboratory?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 265. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.



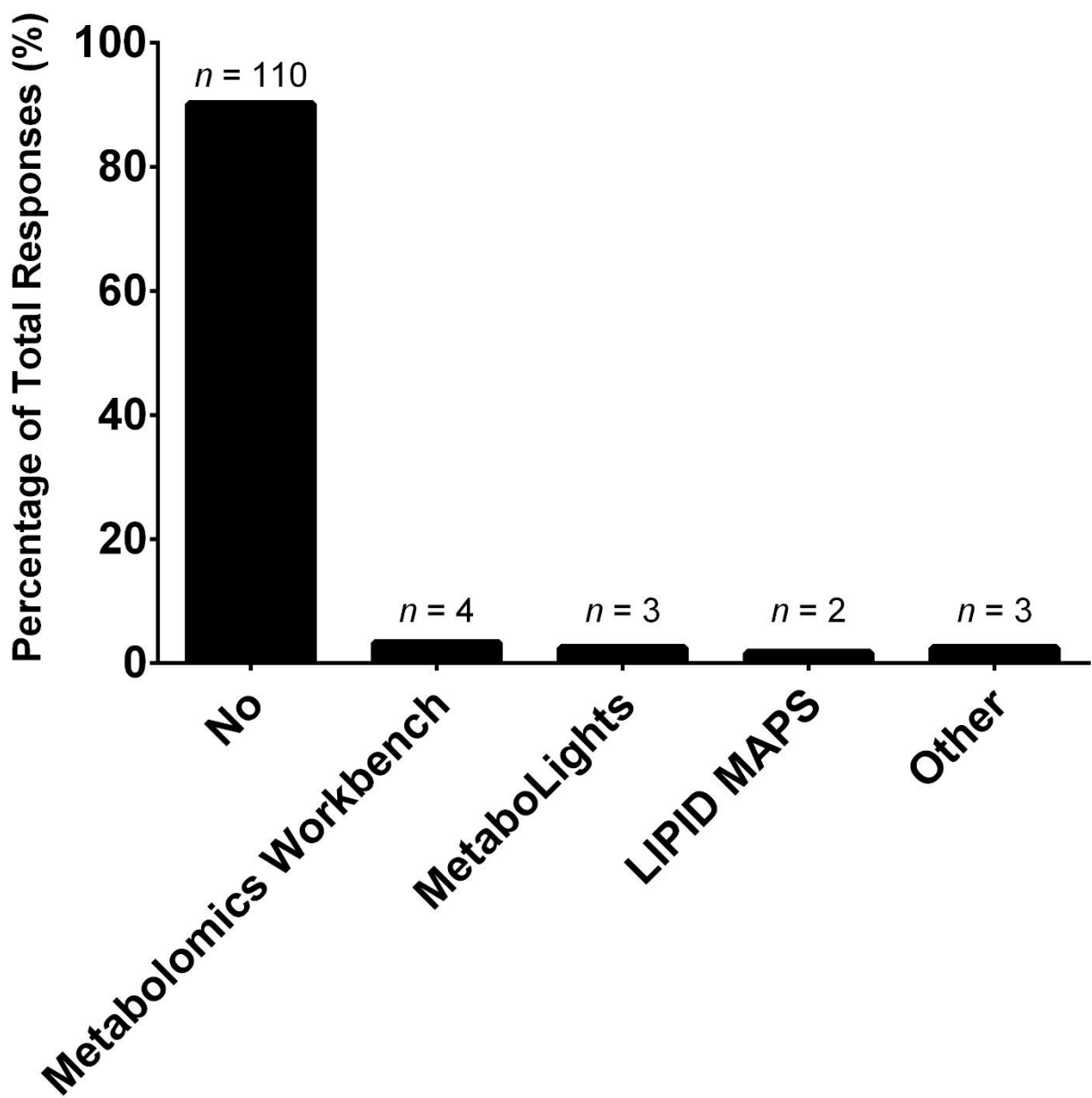
Supplemental Figure S30. “What types of complex biological reference materials would you like to see provided?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 433. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. One ‘other’ write-in response was cerebrospinal fluid, 7 %).



Supplemental Figure S31. “If your laboratory uses commercially available QC materials (e.g., NIST SRMs), please indicate below; however, if your laboratory does not use commercially available reference materials, indicate why below?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 142. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option. Other was selected 26 times (21 %) and common write-in responses included difficulties importing these materials into their country, they make their own materials, not large enough quantity per vial, and not suitable for their applications.



Supplemental Figure S32. **“What do you perceive as the biggest challenge in the lipidomics community (select those that apply)?”** The values are shown as a percentage of total responses (total number of laboratories responding, $n = 121$). The overall total number of responses was 408. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the possible survey response choices. Note that for this question, laboratories had the option to self-identify with more than one option. Write-in responses included lack of established lipid pathways, sharing of data, and lack of reference materials.



Supplemental Figure S33. “Does your laboratory store your lipid data in a repository? If yes, where?” The values are shown as a percentage of total responses (total number of laboratories responding, $n = 122$). The overall total number of responses was 122. The number of responses are indicated in the figure above the solid bars. The x-axis labels reflect the survey multiple choice response options. Note that for this question, laboratories had the option to self-identify with more than one option.