

Omics Studies

Case Report Form: 3 CRF Module – lipidomics and metabolomics.docx

CRF module: lipidomics and metabolomics

Date that this CRF was filled out:

Name of person filling out CRF:

Project name/Identifier:

Animal/ID:

| <u>CDE Name</u> | <u>Data Collected</u> |
|---|--|
| <i>Experiment type</i> | |
| Omics level | <input type="checkbox"/> Lipidomics <input type="checkbox"/> Metabolomics |
| Input type | <input type="checkbox"/> Bulk primary tissue <input type="checkbox"/> Selected cell-types from primary tissue <input type="checkbox"/> Cell-cultures <input type="checkbox"/> Single-cell/single nuclei <input type="checkbox"/> Cerebrospinal fluid <input type="checkbox"/> Whole blood <input type="checkbox"/> Plasma <input type="checkbox"/> Serum <input type="checkbox"/> Saliva <input type="checkbox"/> Sweat <input type="checkbox"/> Urine <input type="checkbox"/> Feces <input type="checkbox"/> Other |
| If other, please specify | |
| If bulk primary tissue, specify tissue type | |
| If bulk primary tissue, specify tissue localization | |
| <i>Sample preparation</i> | |
| Quality control date and time MM/DD/YYYY hh:mm: ss | |

| | |
|---|--|
| Quality assessment type | <input type="checkbox"/> Hemolytic <input type="checkbox"/> Icteric <input type="checkbox"/> Lipemic <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Sample preparation date and time MM/DD/YYYY hh:mm:ss | |
| Sample preparation | <input type="checkbox"/> Protein precipitation <input type="checkbox"/> Ultrafiltration <input type="checkbox"/> Solid phase extraction <input type="checkbox"/> Liquid-liquid extraction <input type="checkbox"/> Derivatization <input type="checkbox"/> Tissue homogenization <input type="checkbox"/> Fiber absorption <input type="checkbox"/> Tissue pulverization <input type="checkbox"/> Centrifugation <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | If other, please specify |
| Internal standards used | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| If internal standards were used, specify name(s) | |
| If internal standards were used, specify vendor(s) | |
| If internal standards were used, specify cat no | |
| If internal standards were used, specify concentration(s) | |
| External standards (calibrators) used | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| If external standards were used, specify name(s) | |
| If external standards were used, specify vendor(s) | |
| If external standards were used, specify cat no | |
| If external standards were used, specify concentration(s) | |
| Quality control samples used | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| If quality control samples were used, specify name(s) | |
| If commercially available quality control samples were used, specify vendor(s) | |
| If commercially quality control samples were used, specify cat no | |

| | |
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| If quality control samples were used, specify concentration(s) | |
| If quality control samples were used, specify matrix/solvent | |
| <i>Sample preparation method</i> | |
| Specify protein precipitation precipitant | |
| Specify volume of precipitant | |
| Specify volume of sample added to precipitant | |
| Specify ultrafiltration device | |
| Specify centrifugation speed | |
| Specify centrifugation duration | |
| Specify centrifugation temperature | |
| Specify solid phase extraction cartridge vendor | |
| Specify solid phase extraction cartridge cat no | |
| Specify liquid-liquid extraction kit vendor | |
| Specify liquid-liquid extraction kit cat no | |
| Specify liquid-liquid extraction method (not commercially available) | |
| Specify derivatization kit vendor | |
| Specify derivatization kit cat no | |
| Specify homogenizer vendor | |
| Specify homogenizer cat no | |
| Specify sample tubes vendor | |
| Specify sample tube cat no | |
| Specify beads vendor | |
| Specify beads cat no | |
| Specify commercially available homogenizing solution vendor | |
| Specify commercially available homogenizing solution cat no | |
| Specify in-house used homogenizing solution | |

| | |
|--|--|
| Specify volume of homogenizing solution | |
| Specify tissue weight that was homogenized | |
| Specify fiber absorption vendor | |
| Specify fiber absorption cat no | |
| Liquid chromatography method | |
| Instrument used, specify vendor | |
| Specify instrument used | |
| Specify instrument cat no | |
| Chromatography | <input type="checkbox"/> Reverse phase <input type="checkbox"/> HILIC <input type="checkbox"/> Ion exchange <input type="checkbox"/> Mixed-mode <input type="checkbox"/> Chiral <input type="checkbox"/> Supercritical <input type="checkbox"/> 2-D LC <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| If other, please specify | |
| Column used, specify vendor | |
| Specify column used | |
| Specify column cat no | |
| Specify column stationary phase | |
| Specify column inner diameter | |
| Specify column length | |
| Mobile phase A used | |
| Mobile phase B used | |
| Gradient used | |
| Flow rate used | |
| Column temperature used | |
| Injected sample volume used | |
| Gas chromatography method | |
| Instrument used, specify vendor | |
| Specify instrument used | |
| Specify instrument cat no | |

| | |
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| Injection mode | <input type="checkbox"/> Headspace <input type="checkbox"/> Solution <input type="checkbox"/> Fiber <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Column used, specify vendor | Column used, specify vendor |
| Specify column used | Specify column used |
| Specify column cat no | Specify column cat no |
| Specify column particle size | Specify column particle size |
| Specify column inner diameter | Specify column inner diameter |
| Specify column length | Specify column length |
| Gas used | <input type="checkbox"/> Helium <input type="checkbox"/> Nitrogen <input type="checkbox"/> Hydrogen <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Column temperature used | |
| Flow rate used | |
| Mass spectrometry method | |
| Instrument used, specify vendor | |
| Specify instrument used | |
| Specify instrument cat no | |
| Instrument type | <input type="checkbox"/> TOF <input type="checkbox"/> Q-TOF <input type="checkbox"/> Single quad <input type="checkbox"/> Triple quad <input type="checkbox"/> Ion trap <input type="checkbox"/> Fourier transform <input type="checkbox"/> TIMS-PASEF <input type="checkbox"/> IMS <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Lipidomics/Metabolomics mode | <input type="checkbox"/> Untargeted <input type="checkbox"/> Targeted <input type="checkbox"/> Unknown |
| Ionization mode | <input type="checkbox"/> ESI+ <input type="checkbox"/> ESI- <input type="checkbox"/> APCI+ <input type="checkbox"/> EI <input type="checkbox"/> CI- <input type="checkbox"/> CI+ <input type="checkbox"/> MALDI <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| MS mode | <input type="checkbox"/> Full scan <input type="checkbox"/> MS ^e <input type="checkbox"/> MRM <input type="checkbox"/> SIM <input type="checkbox"/> PASEF <input type="checkbox"/> NLS <input type="checkbox"/> PIS <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Specify peak detection and processing software | |
| Nuclear magnetic resonance method | |
| Instrument used, specify vendor | |

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|---|---|
| Specify instrument used | |
| Specify instrument cat no | |
| Metabolomics mode | <input type="checkbox"/> Untargeted <input type="checkbox"/> Targeted <input type="checkbox"/> Unknown |
| Specify peak detection and processing software | |
| Data annotation | |
| Peak/spectral identification | <input type="checkbox"/> Reference to known standards <input type="checkbox"/> Rule-based fragmentation annotation <input type="checkbox"/> Database search <input type="checkbox"/> Self-established spectral library <input type="checkbox"/> Unknown |
| If database search, specify database for lipidomics/metabolomics annotation | |
| Database version | |
| If self-established spectral library, specify availability | |
| Manual data curation | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| Database used for pathway analysis | <input type="checkbox"/> LipidMaps <input type="checkbox"/> HMDB <input type="checkbox"/> KEGG <input type="checkbox"/> METLIN <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Database version | |
| Data quantification | |
| Quantification strategy | <input type="checkbox"/> Relative quantification <input type="checkbox"/> Absolute quantification untargeted data <input type="checkbox"/> Absolute quantification targeted data <input type="checkbox"/> Label-free quantification <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |
| Class or subclass-specific lipid internal standards | |
| Pooled samples | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| Internal standards | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| Candidate identification criteria | <input type="checkbox"/> p-value <input type="checkbox"/> Log2 Fold Change <input type="checkbox"/> Unknown <input type="checkbox"/> Other |

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| If other, please specify | |
| Data validation | |
| Lipids or Metabolite confirmation by second method | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| If yes, specify method | |
| Independent biological replicates for validation | <input type="checkbox"/> Yes <input type="checkbox"/> No <input type="checkbox"/> Unknown |
| If yes, specify number | |
| Data statistical processing | |
| Statistical tests | <input type="checkbox"/> PCA <input type="checkbox"/> PLS-DA <input type="checkbox"/> T-test + FDR <input type="checkbox"/> ANOVA <input type="checkbox"/> Regression <input type="checkbox"/> Unknown <input type="checkbox"/> Other |
| If other, please specify | |

Instructions: Please check boxes where applicable. If none of the predetermined options is appropriate use the default space to specify your answer.
This form is to be filled in for one individual animal.

Abbreviations: 2-D LC, two-dimensional liquid chromatography; ANOVA, analysis of variance; APCI, atmospheric pressure chemical ionization; CI, chemical ionization; EI, electron ionization; ES, electrospray ionization; FDR, false discovery rate correction; HILIC, hydrophilic interaction liquid chromatography; IMS, Ion mobility spectrometry; MALDI, matrix-assisted laser desorption/ionization; MRM, multiple reaction monitoring; MS, mass spectrometry; NLS, Neutral Loss Scan; PASEF, Parallel Accumulation Serial Fragmentation; PCA, principal component analysis; PLS-DA, Partial least squares discriminant analysis; PIS, Precursor Ion Scan; Q-TOF, quadrupole time-of-flight; SIM, single ion monitoring; TIMS, trapped ion mobility spectrometry; TOF, time-of-flight