**NaPDI Repository Experiment Report**

**Metabolomics Experiment(s)**

**Please fill in all relevant fields to the experiment(s) performed.**

1. **General Information**

|  |  |
| --- | --- |
| **Title of experiment** |  |
| **Research organization** |  |
| **Additional information** |  |

**An example of data entered in the repository on the admin side:**

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1. **Experimental Conditions**

|  |  |
| --- | --- |
| **Material Preparation - Mass of sample material** |  |
| **Material Preparation - Volume of extraction vessel** |  |
| **Material Preparation - Solvent used** |  |
| **Material Preparation - Volume of solvent** |  |
| **Material Preparation - Temperature of storage** |  |
| **Material Preparation - Additional information** |  |
| **NMR Analysis - NMR instrument used** |  |
| **NMR Analysis - Nucleus** | 1H (proton)  13C (carbon)  15N (nitrogen) |
| **NMR Analysis – Field strength** |  |
| **NMR Analysis – Solvent used** | Methanol-d4 (CD3OD)  Chloroform-d (CDCI3)  Acetone-d6 ((CD3)3)  Dimethyl sulfoxide-d6 ((CD3)2SO)  Pyridine-d5 (C5D5N) |
| **NMR Analysis – Sample concentration** |  |
| **NMR Analysis – Additional information** |  |
| **Mass Spectrometry Analysis – Instrument used** |  |
| **Mass Spectrometry Analysis – Sample concentration** |  |
| **Mass Spectrometry Analysis – Tandem spectra** |  |
| **Mass Spectrometry Analysis – Ionization** |  |
| **Mass Spectrometry Analysis – Ionization mode** | Positive  Negative  Positive/Negative switching |
| **Mass Spectrometry Analysis – LC Instrument** |  |
| **Mass Spectrometry Analysis – Solvent system** |  |
| **Mass Spectrometry Analysis – Gradient conditions** |  |
| **Mass Spectrometry Analysis – Flow rate** |  |
| **Mass Spectrometry Analysis – Column used** |  |
| **Mass Spectrometry Analysis – Additional information** |  |
| **Metabolite Quantification – Method of quantification** |  |
| **Metabolite Quantification – Solvent used** |  |
| **Metabolite Quantification – Number of calibration points** |  |
| **Metabolite Quantification – Sample concentration range** |  |
| **Metabolite Quantification – Curve fitting method** |  |
| **Metabolite Quantification – Weighting method** |  |
| **Metabolite Quantification - Methods** |  |

**Additional information regarding experimental conditions:**

|  |  |
| --- | --- |
| **Additional information** |  |

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**3. Brief Summary of Results**

**For each experiment, please provide a brief summary of the results and conclusions**

|  |  |  |
| --- | --- | --- |
| **Experiment number and title** | **Results values and types**  **(see appendix II and III for list of parameters and value types)** | **Summary of results** |
|  |  |  |
|  |  |  |
|  |  |  |

(Add more rows if needed)

|  |  |
| --- | --- |
| **Additional Information** |  |
| **Conclusion** |  |

**Attach relevant figures and tables of results when submitting this form.**

**Appendix II: Enzyme Induction Parameters**

|  |  |  |
| --- | --- | --- |
| **Parameters** | **Preferred unit** | **Note** |
| **EC50** | µM |  |
| **Emax** | -fold |  |
| **% Increase compared with vehicle control** | % | P value can be added as needed. |
| **% Increase compared with positive control** | % | P value can be added as needed. |
| **% Decrease compared with vehicle control** | % | P value can be added as needed. |
| **% Decrease compared with positive control** | % | P value can be added as needed. |

**Appendix II: List of value types**

* Mean
* Mean ± SD
* Mean ± SEM
* Mean (range)
* Mean (CV%)
* Mean (CI)
* Median
* Median (CV%)
* Median (range)
* Median (CI)