*Suggestion of the page location Research -> MS2 libraries of suspect metabolites*

**MS2 libraries of suspect metabolites of 120 environmental chemicals in mouse urine (annotated Compound Discoverer 3.3)**

Mice were administered chemical standards by gavage and 24-hour was collected as previously described (Nomasa et al 2021, PMID:[33779022](https://pubmed.ncbi.nlm.nih.gov/33779022/)). Mice urine samples were measured using Reversed-Phase and HILIC chromatographies in negative and positive ionization modes. Compound Discoverer 3.3 was used to generate predicted/expected metabolites for each chemical and data processing. MS2 spectra of suspect metabolites present in exposed mice urine, but not in control samples were exported to MS2 libraries (manuscript in preparation).

MS2 spectra can be browsed and MS2 libraries downloaded from MoNA ([MassBank of North America](https://mona.fiehnlab.ucdavis.edu/)).

MS2 library names: CD\_annotated\_EnvCpd\_suspect\_metabolites\_NCU\_ HILIC\_NEG/HILIC\_POS/RP\_NEG/RP\_POS

[Download MS2 library HILIC negative in NIST msp format (1691 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/b231f50b-ab81-4049-8507-002356cbef3b)

[Download MS2 library HILIC positive in NIST msp format (1655 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/cb07338f-75a9-40f8-a693-906d0f39cbc9)

[Download MS2 library RP negative in NIST msp format (1261 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/cde41407-5e86-4ff3-80bf-2b340af46b90)

[Download MS2 library RP positive in NIST msp format (1308 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/4e2e8d22-62c9-47b0-9fed-37e12b8e2af9)

**MS2 libraries of suspect metabolites of 32 fungicides in mouse urine (R-scripts, MZmine 3)**

Mice were administered chemical standards by gavage and 24-hour was collected as previously described (Nomasa et al 2021, PMID:[33779022](https://pubmed.ncbi.nlm.nih.gov/33779022/)). Mice urine samples were measured using Reversed-Phase and HILIC chromatographies in negative and positive ionization modes. Data was processed in MZmine 3, suspect metabolites were selected using ratios between the control and exposed mice urine samples, and MS2 spectra of selected suspect metabolites exported to MS2 libraries (manuscript under revision).

MS2 spectra can be browsed and MS2 libraries downloaded from MoNA ([MassBank of North America](https://mona.fiehnlab.ucdavis.edu/))

MS2 library names: Fungicide\_NCU\_ HILIC\_NEG/HILIC\_POS/RP\_NEG/RP\_POS

[Download MS2 library HILIC negative in NIST msp format (1603 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/6d491933-5eb0-417b-9b92-ceb0eb3be928)

[Download MS2 library HILIC positive in NIST msp format (1533 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/55416382-e11c-4012-aa14-ecea47a2b3bd)

[Download MS2 library RP negative in NIST msp format (1705 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/77c675ba-f2e0-432a-a3fb-7ffdcbd51cf9)

[Download MS2 library RP positive in NIST msp format (2257 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/6f55c842-800d-4c36-ae50-f915d675c350)

Fungicide chemical standards

MS2 library names: Fungicide\_NCU\_ HILIC\_NEG/HILIC\_POS/RP\_NEG/RP\_POS

[Download MS2 library HILIC negative in NIST msp format (36 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/67a0bc00-4b81-401f-bc75-7926fc297c1d)

[Download MS2 library HILIC positive in NIST msp format (91 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/d98d2f6c-ee42-4bcd-b777-fdb90663fa26)

[Download MS2 library RP negative in NIST msp format (12 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/525ecc39-2f60-435c-99f0-3cd2a2f326fa)

[Download MS2 library RP positive in NIST msp format (22 MS2 spectra)](https://mona.fiehnlab.ucdavis.edu/rest/downloads/retrieve/9774aadd-de61-4eb0-96ab-b4c6af2132f4)