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Applications of the US EPA's CompTox Chemicals Dashboard to support structure identification and chemical forensics using mass spectrometry

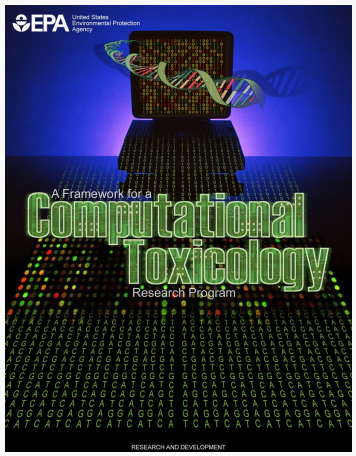
Antony Williams[1] and Andrew D. McEachran[2,3]

1) *National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC*
2) *Oak Ridge Institute of Science and Education (ORISE) Research Participant, RTP, NC*
3) *Present Address: Agilent Inc., Santa Clara, CA*

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

March 2019
Pittcon, Philadelphia

National Center for Computational Toxicology



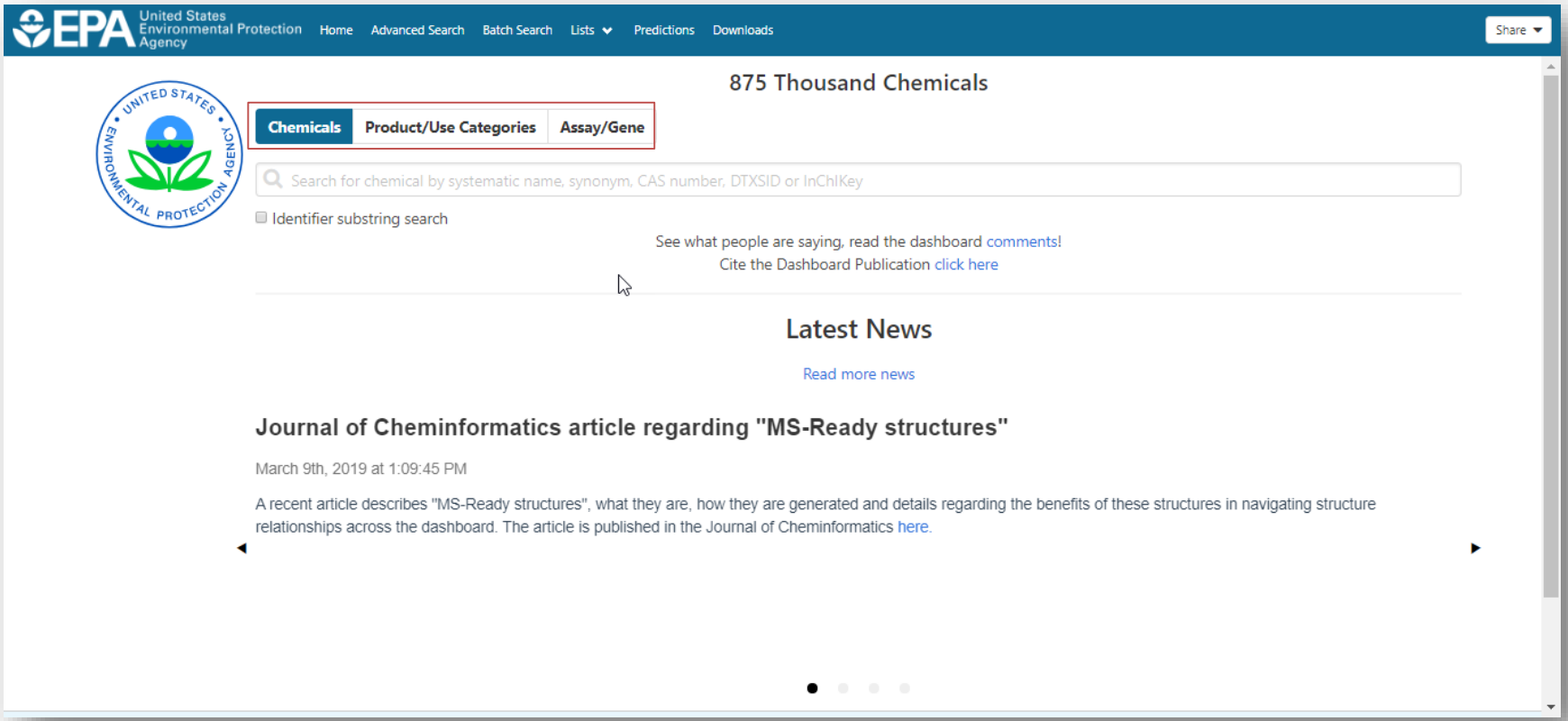
- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Researching computational approaches to quickly evaluate the safety of chemicals for potential risk.
- Outputs: a lot of data, models, algorithms and software applications

CompTox Chemicals Dashboard

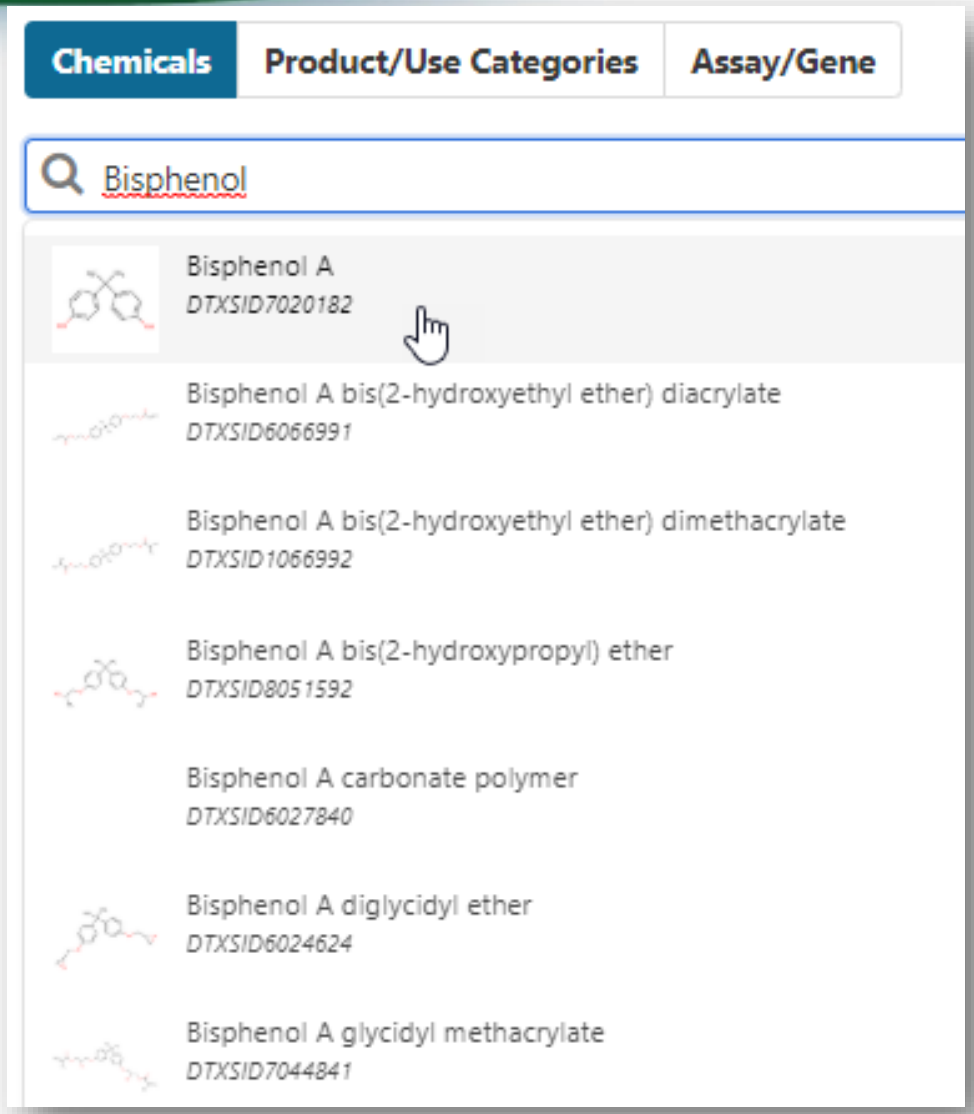
- A publicly accessible website delivering access:
  - **~875,000** chemicals with related property data
  - Searchable by chemical, product use, gene and assay (ToxCast)
  - Experimental and predicted physicochemical property data
  - “Bioactivity data” for the ToxCast/Tox21 project
  - Generalized Read-Across (GenRA) module
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - DOWNLOADABLE Open Data for reuse and repurposing

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



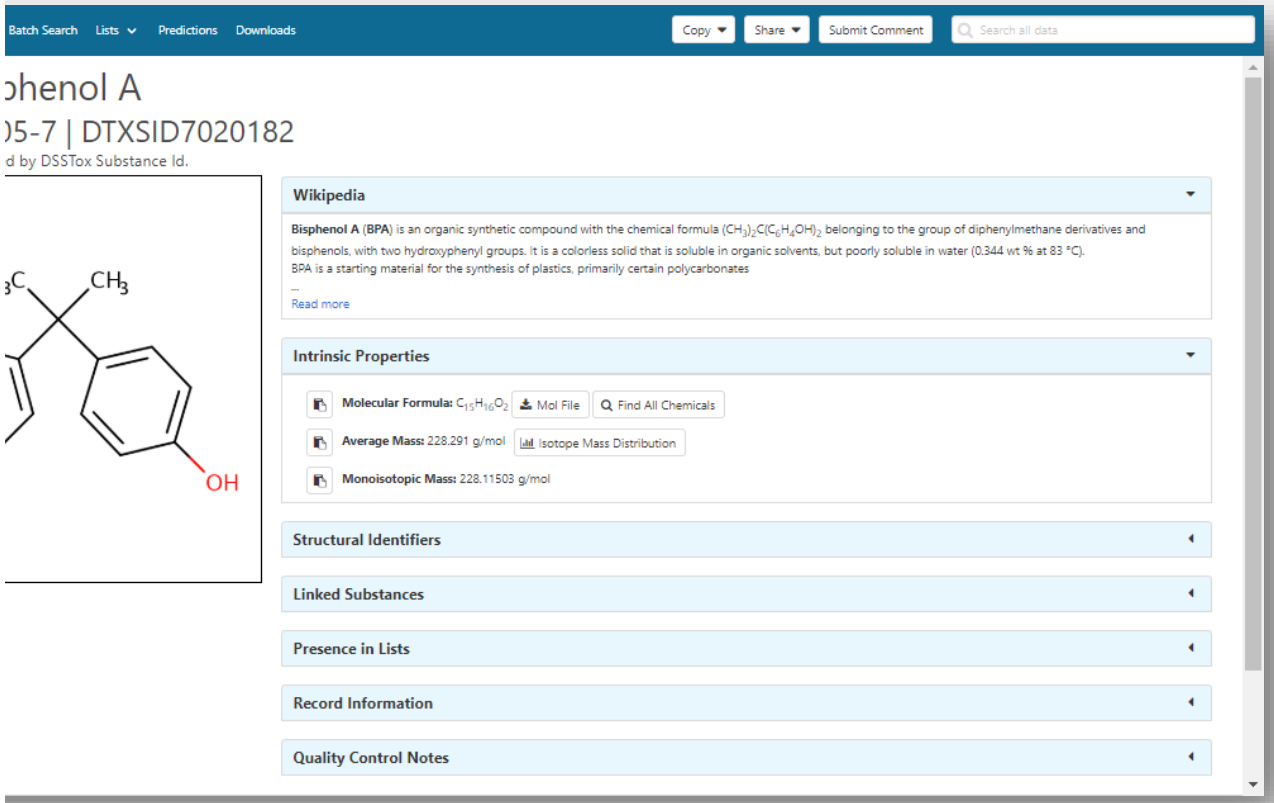
Search Chemicals



Detailed Chemical Pages

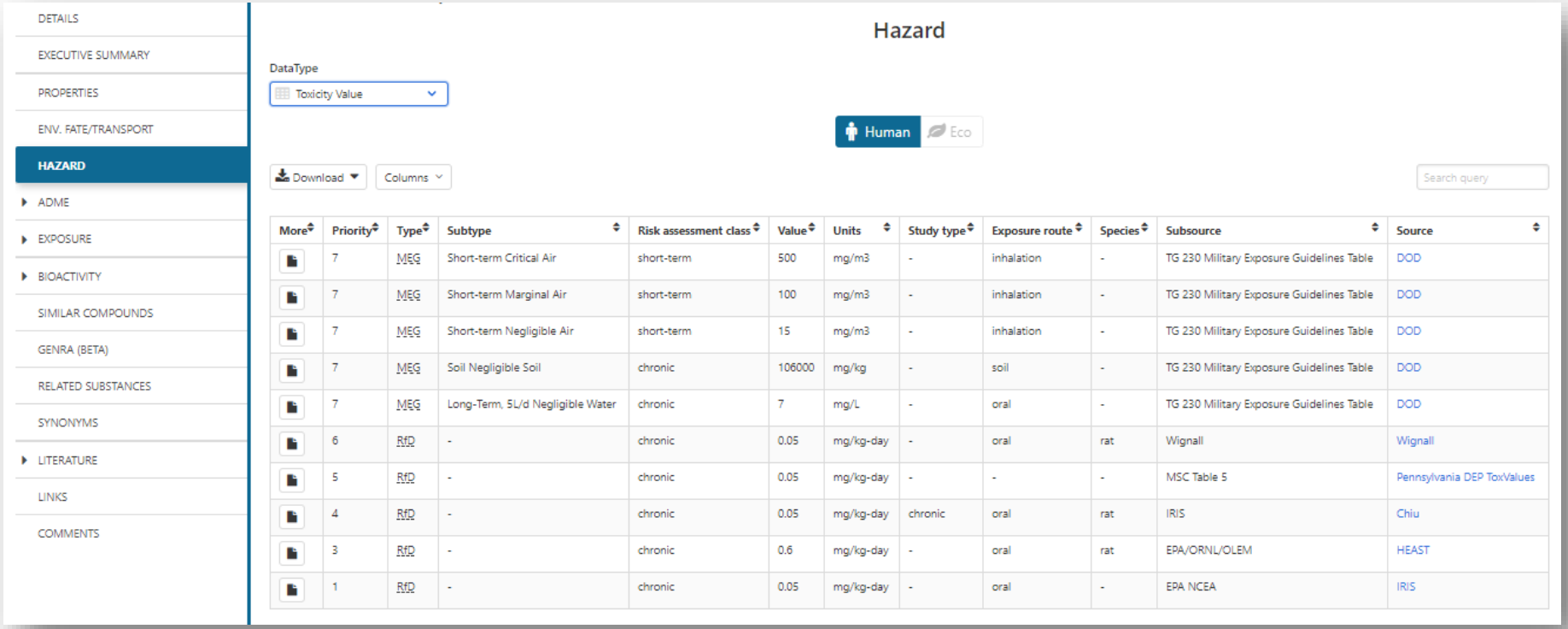
EPA United States Environmental Protection Agency

- **DETAILS**
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



Access to Chemical Hazard Data

EPA United States Environmental Protection Agency



DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES
SYNONYMS
LITERATURE
LINKS
COMMENTS

Hazard

DataType: Toxicity Value

Human | Eco

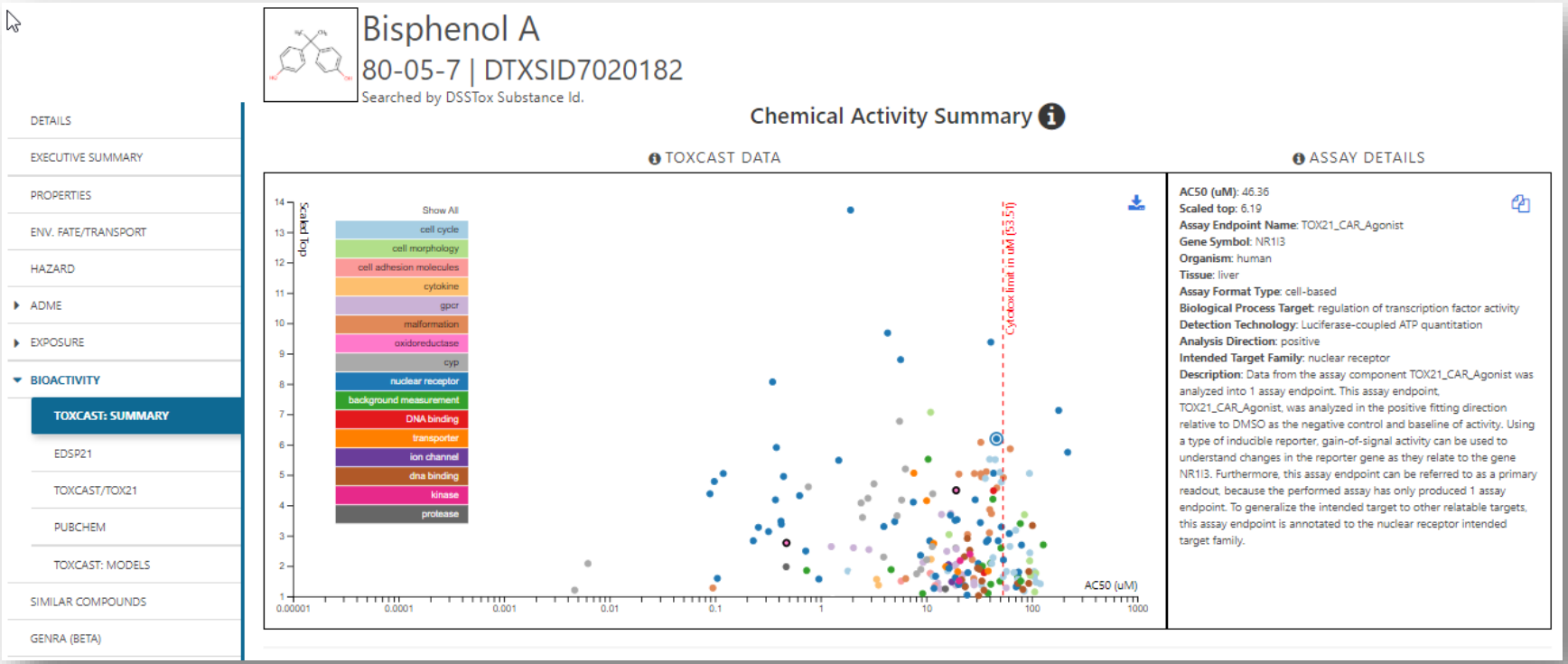
Download | Columns | Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, 5L/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RfD	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RfD	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP ToxValues
	4	RfD	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RfD	-	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

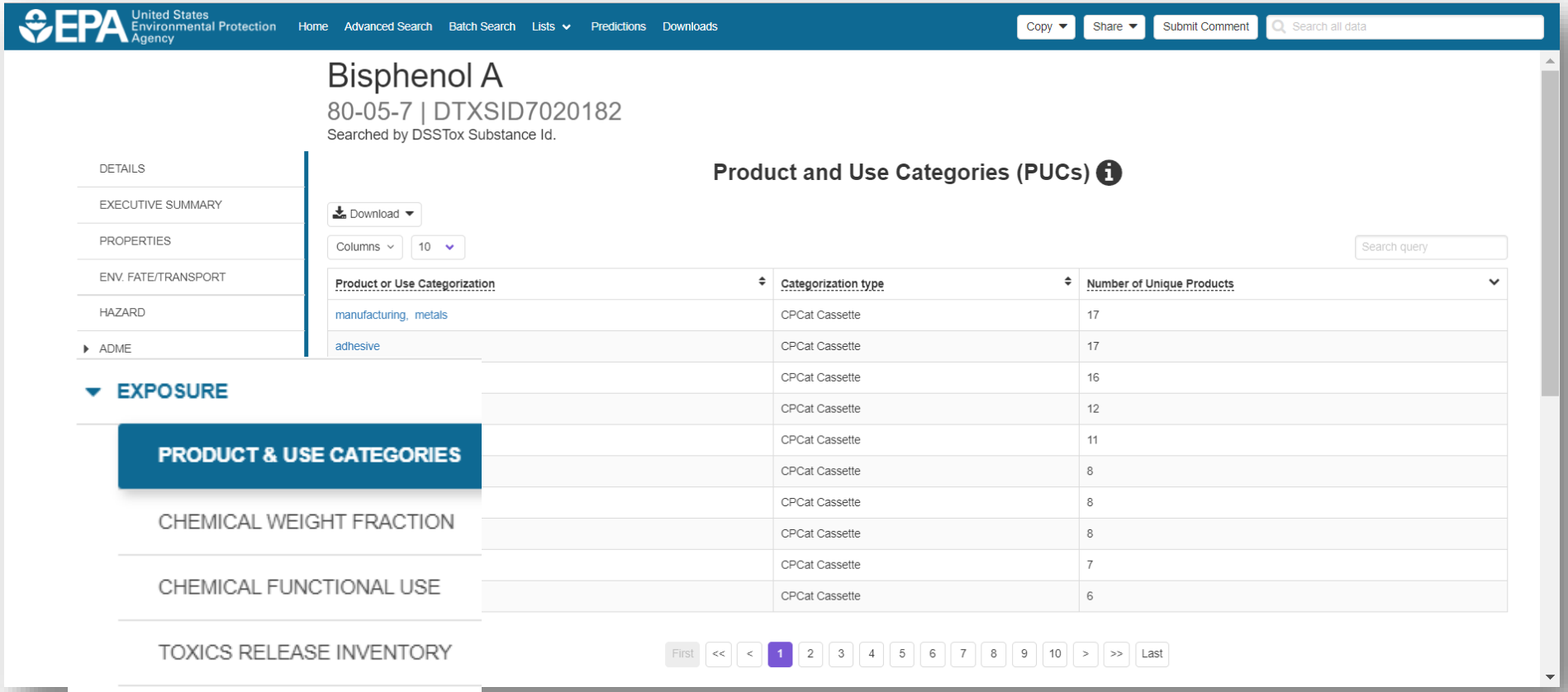
In Vitro Bioassay Screening

ToxCast and Tox21

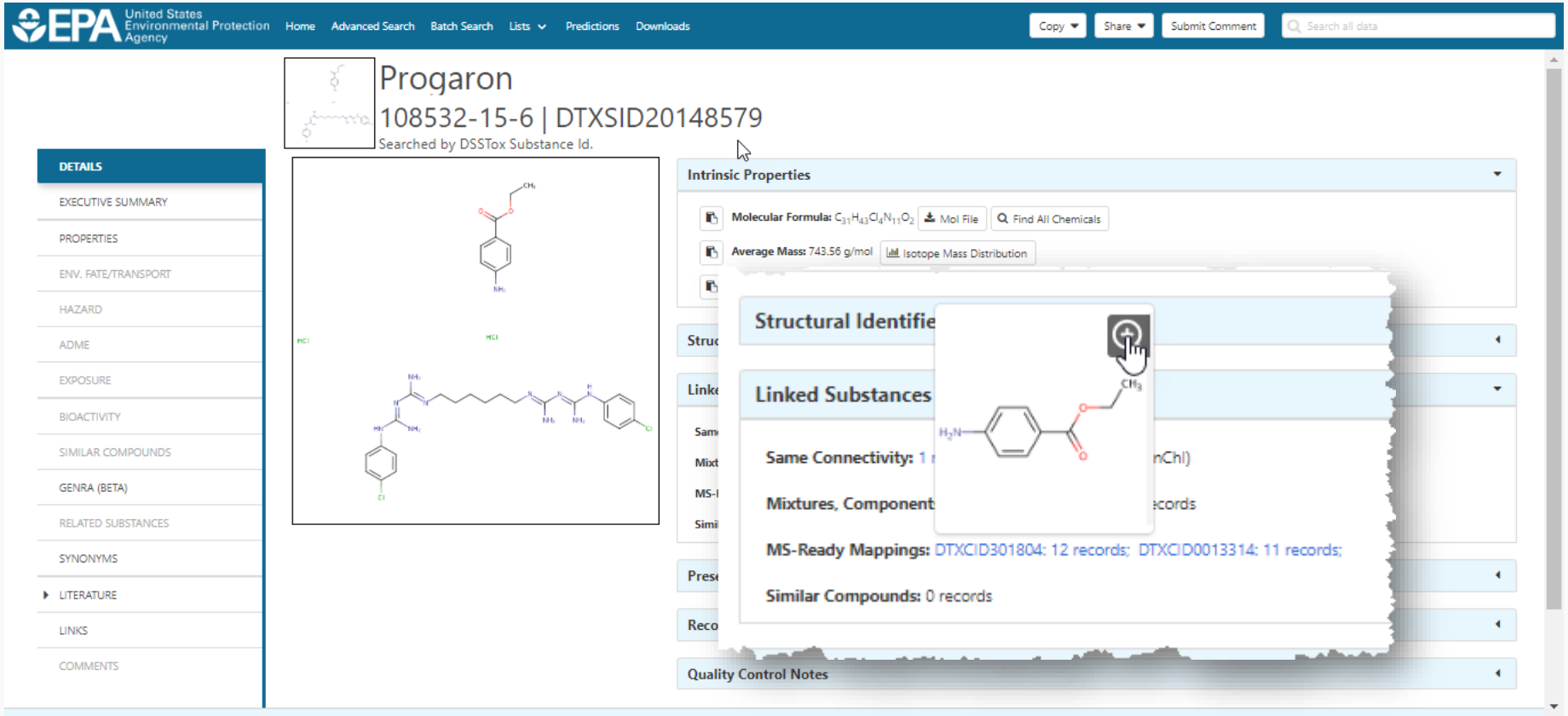
EPA United States Environmental Protection Agency



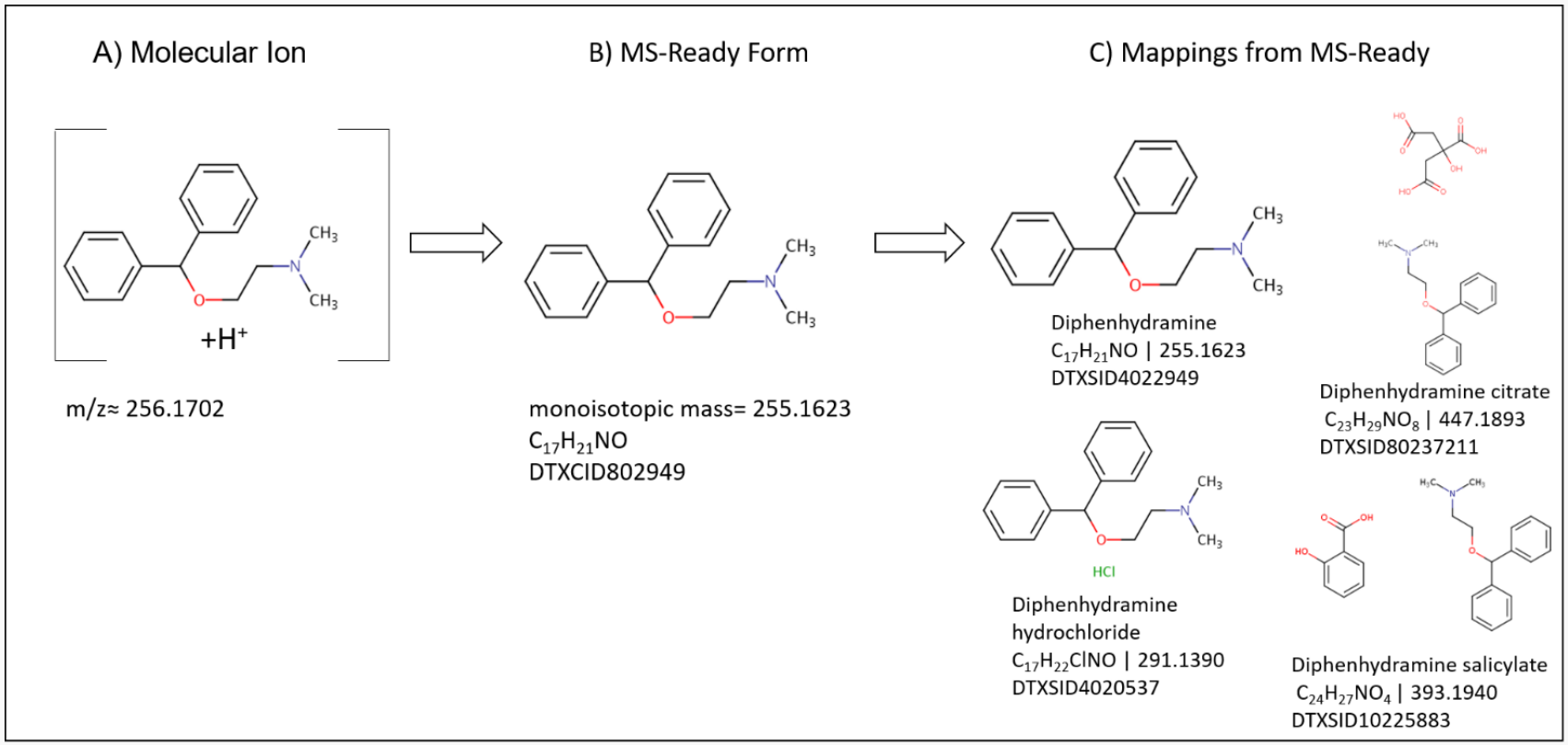
Sources of Exposure to Chemicals



MS-Ready Mappings



Specific Data-Mappings "MS-Ready Structures"



MS-Ready Publication

https://doi.org/10.1186/s13321-018-0299-2

EPA United States Environmental Protection Agency

McEachran *et al. J Cheminform (2018) 10:45*
https://doi.org/10.1186/s13321-018-0299-2

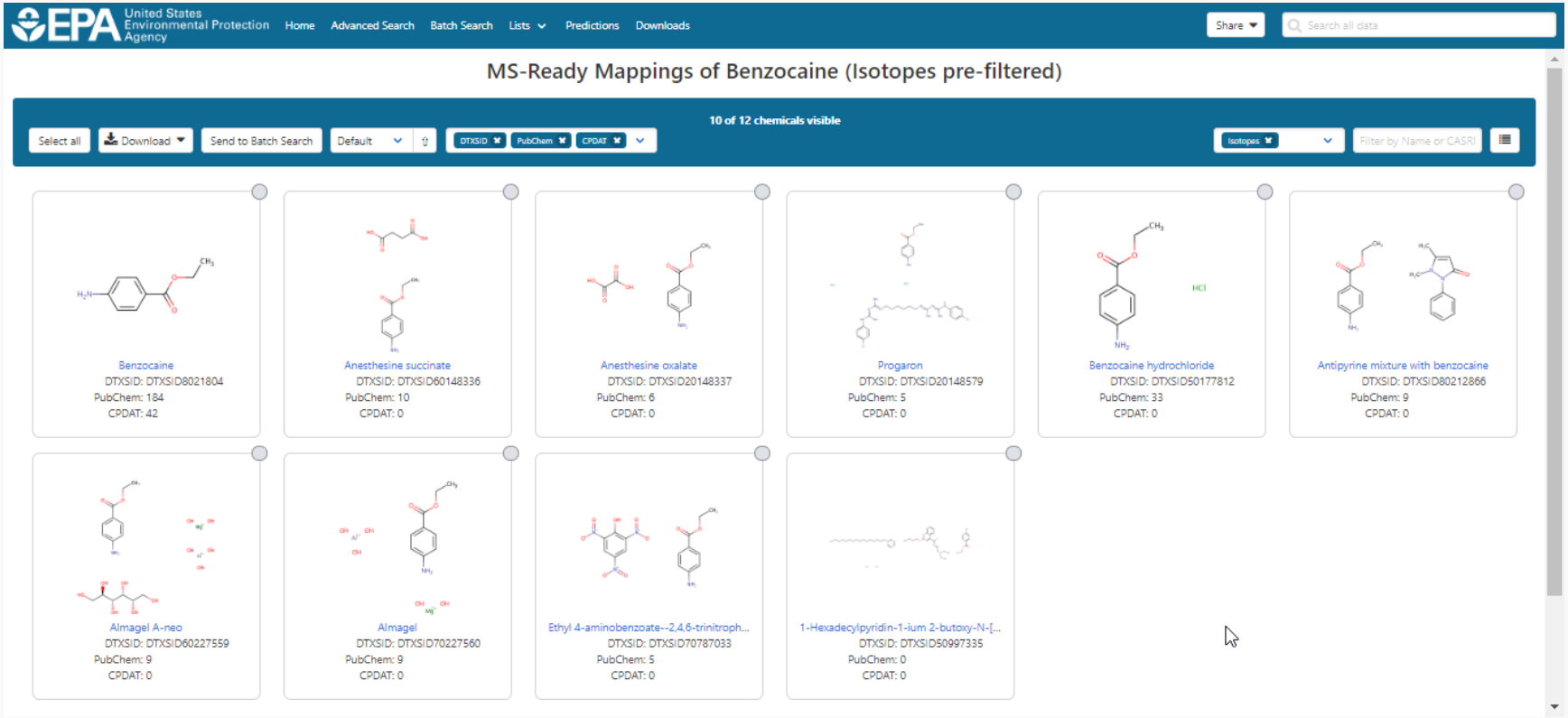
Journal of Cheminformatics

METHODOLOGY Open Access

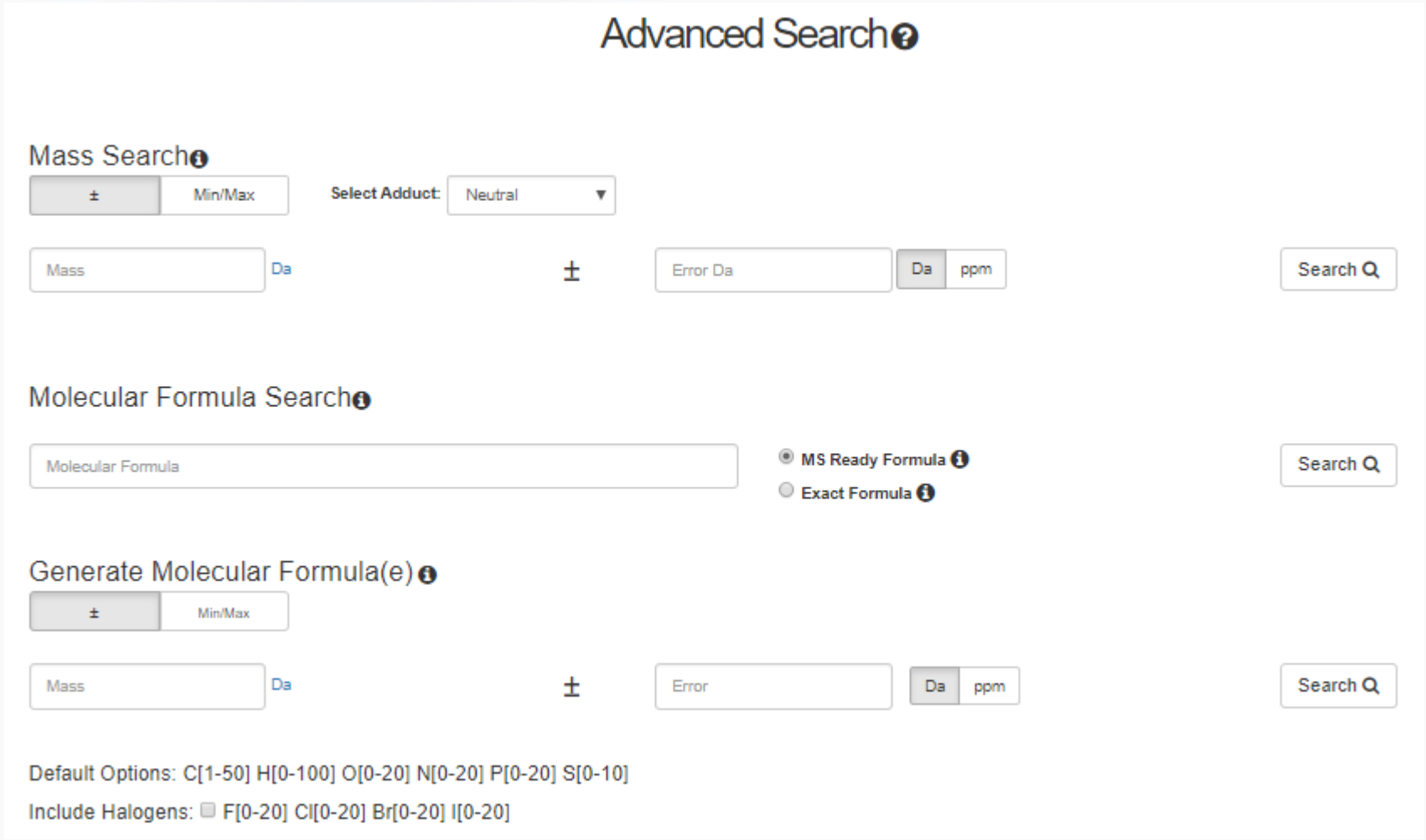
"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran[1,2*], Kamel Mansouri[1,2,3], Chris Grulke[2], Emma L. Schymanski[4], Christoph Ruttkies[5] and Antony J. Williams[2*]

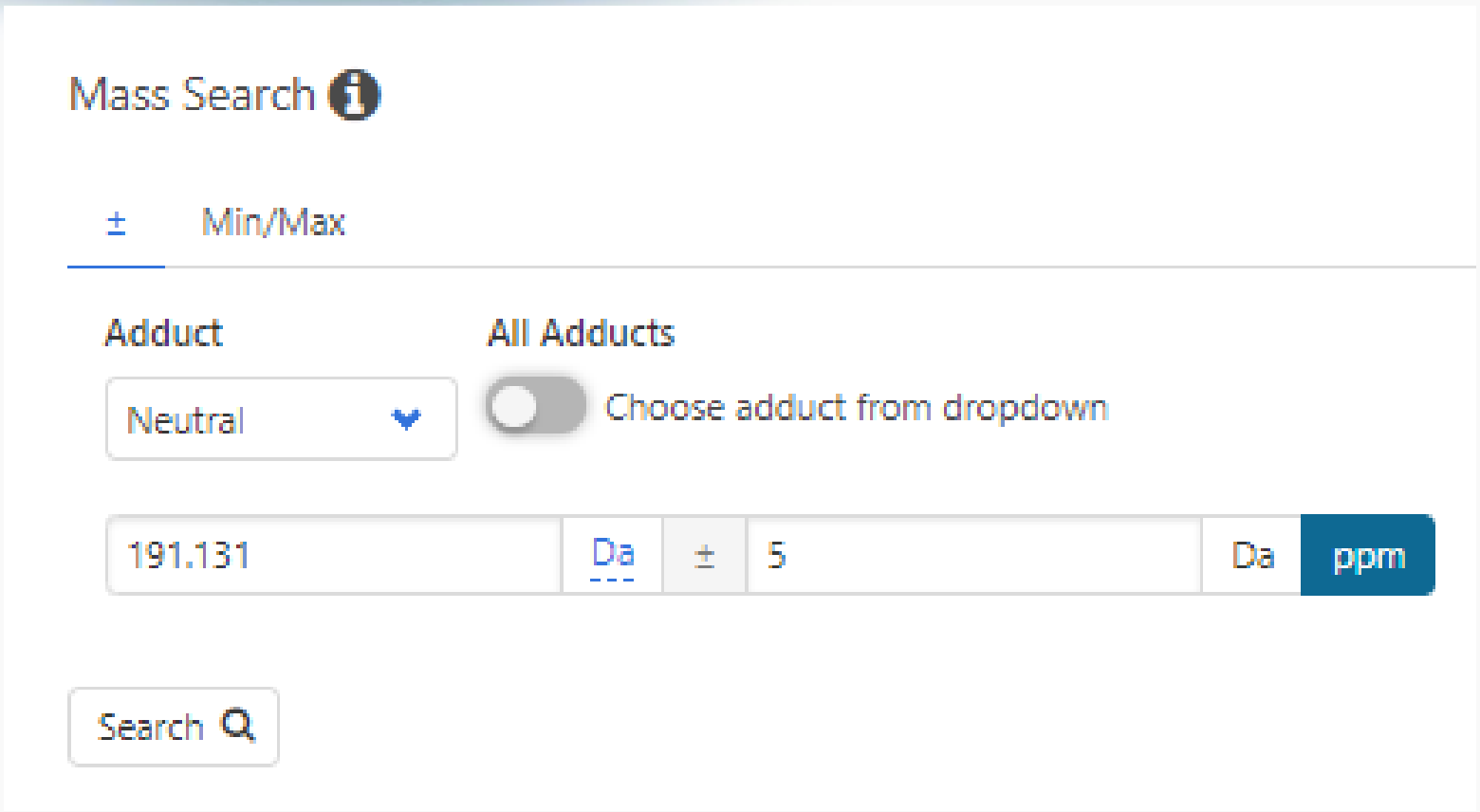
MS-Ready Mappings Set



Mass and Formula Searches Supporting Mass Spectrometry



Advanced Searches
Mass Based Search



Advanced Searches
Mass Based Search

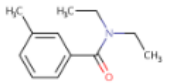
EPA United States Environmental Protection Agency

Search Results

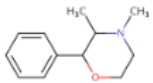
Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

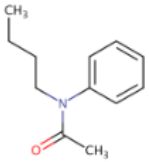
Select all | Download | Send to Batch Search | Mass Difference | DTXSID | CASRN | TOXCAST | Mass Diff | Multicomponent Chemicals | Filter by Name or CASRI



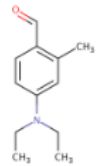
DEET
DTXSID: DTXSID2021995
CASRN: 134-62-3
TOXCAST: 12/768
Mass Diff: 0.000014



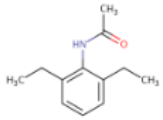
Phendimetrazine
DTXSID: DTXSID1023447
CASRN: 634-03-7
TOXCAST: -
Mass Diff: 0.000014



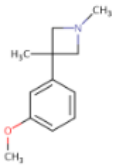
N-Butylacetanilide
DTXSID: DTXSID2042197
CASRN: 91-49-6
TOXCAST: -
Mass Diff: 0.000014



Benzaldehyde, 4-(diethylamino)-2-meth...
DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: -
Mass Diff: 0.000014



Acetanilide, 2',6'-diethyl-
DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: -
Mass Diff: 0.000014



Azetidine, 1,3-dimethyl-3-(m-methoxyp...
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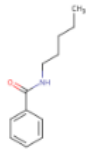
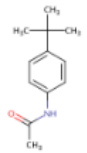
CASRN: 19832-26-9
TOXCAST: -
Mass Diff: 0.000014



Benzamide, N-pentyl-
DTXSID: DTXSID20174196
CASRN: 20308-43-4
TOXCAST: -



p-t-Butylacetanilide
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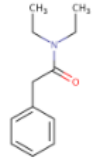
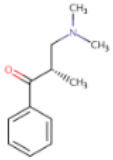
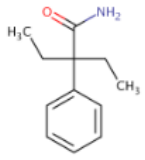
CASRN: 20330-45-4
TOXCAST: -



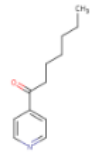
N,N-Diethylphenylacetamide
DTXSID: DTXSID00179048
CASRN: 2431-96-1
TOXCAST: -



3-(Dimethylamino)-2-methylpropiophen...
DTXSID: DTXSID60180796
CASRN: 26171-50-6
TOXCAST: -



Butyramide, 2-ethyl-2-phenyl-
DTXSID: DTXSID60184653
CASRN: 30568-39-9
TOXCAST: -



1-Heptanone, 1-(4-pyridyl)-
DTXSID: DTXSID40186594
CASRN: 32941-30-3
TOXCAST: -

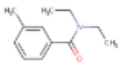
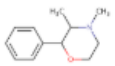
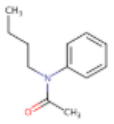
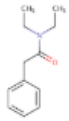
Advanced Searches
Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

Select all | Download | Send to Batch Search | Sources | Multicomponent Chemicals | Filter by Name or CASRI

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass	Mass Difference
	DTXSID2021995 ToxCast™	DEET	134-62-3	Level 1	111	135	155	753	191.131014	0.000014
	DTXSID1023447	Phendimetrazine	634-03-7	Level 2	12	34	35	50	191.131014	0.000014
	DTXSID2042197	N-Butylacetanilide	91-49-6	Level 2	1	32	50	1	191.131014	0.000014
	DTXSID00179048	N,N-Diethylphenylacetamide	2431-96-1	Level 4	0	21	52	34	191.131014	0.000014

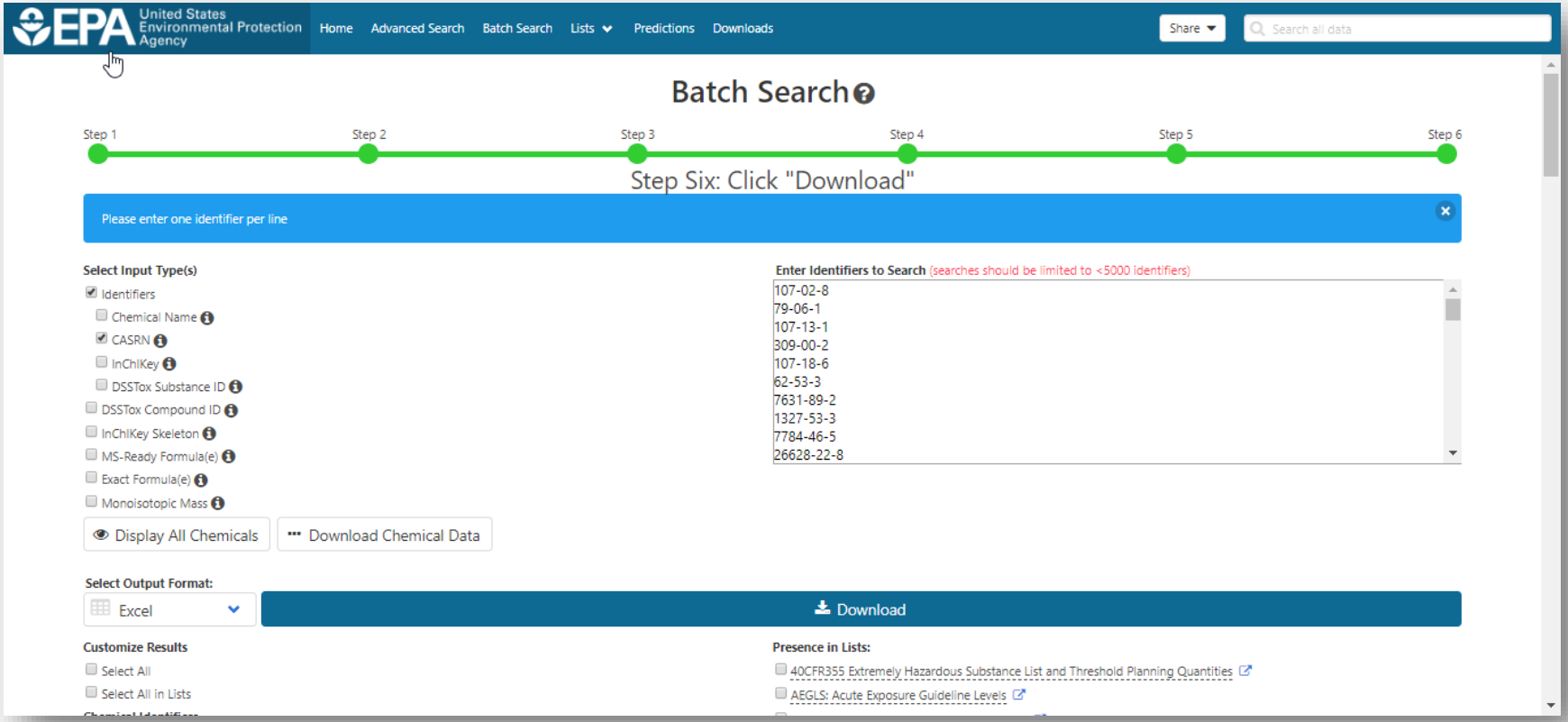
Batch Searching

- Singleton searches are useful but we work with thousands of chemicals!

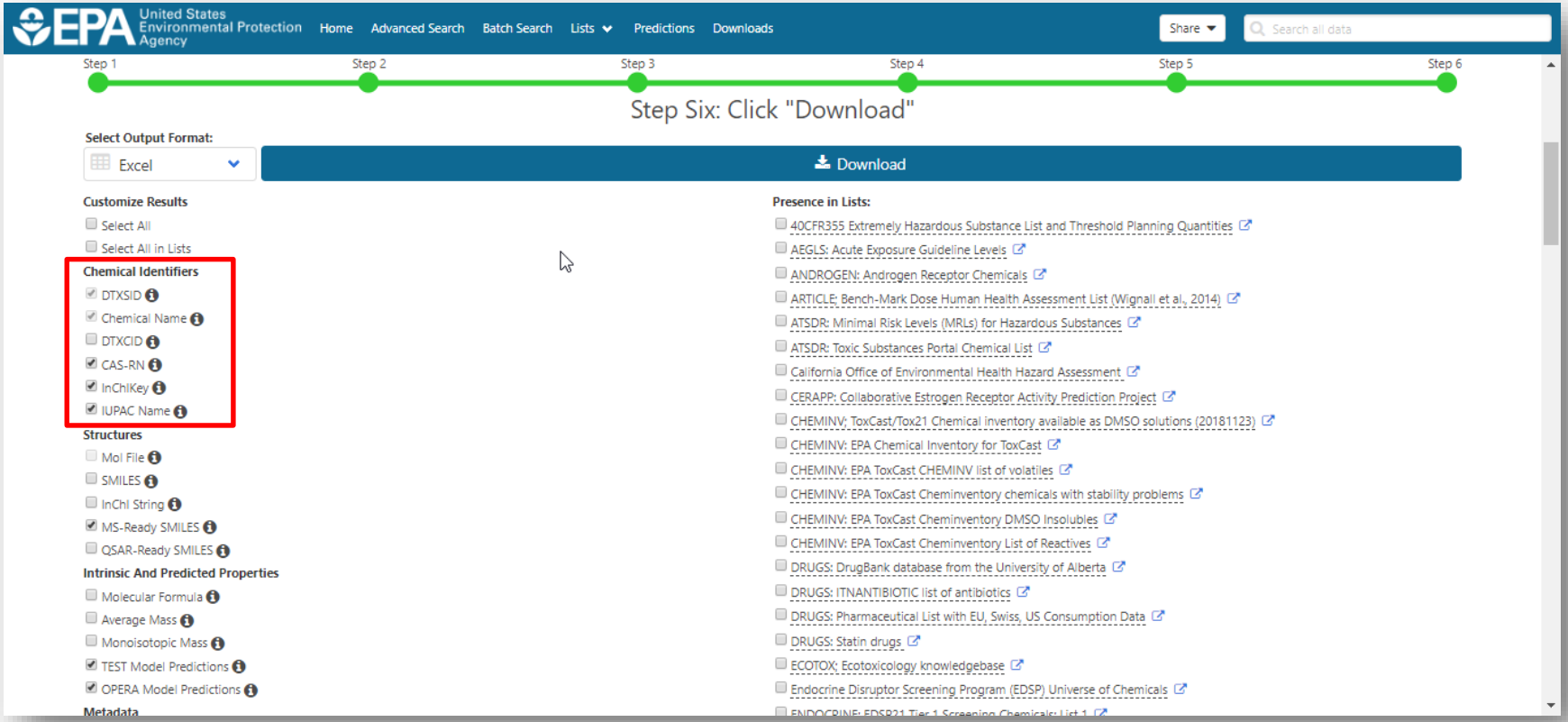
- Typical questions
  - What is the list of chemicals for the formula $C_xH_yO_z$
  - What is the list of chemicals for a mass +/- error

  - Can I get chemical lists in Excel files? In SDF files?

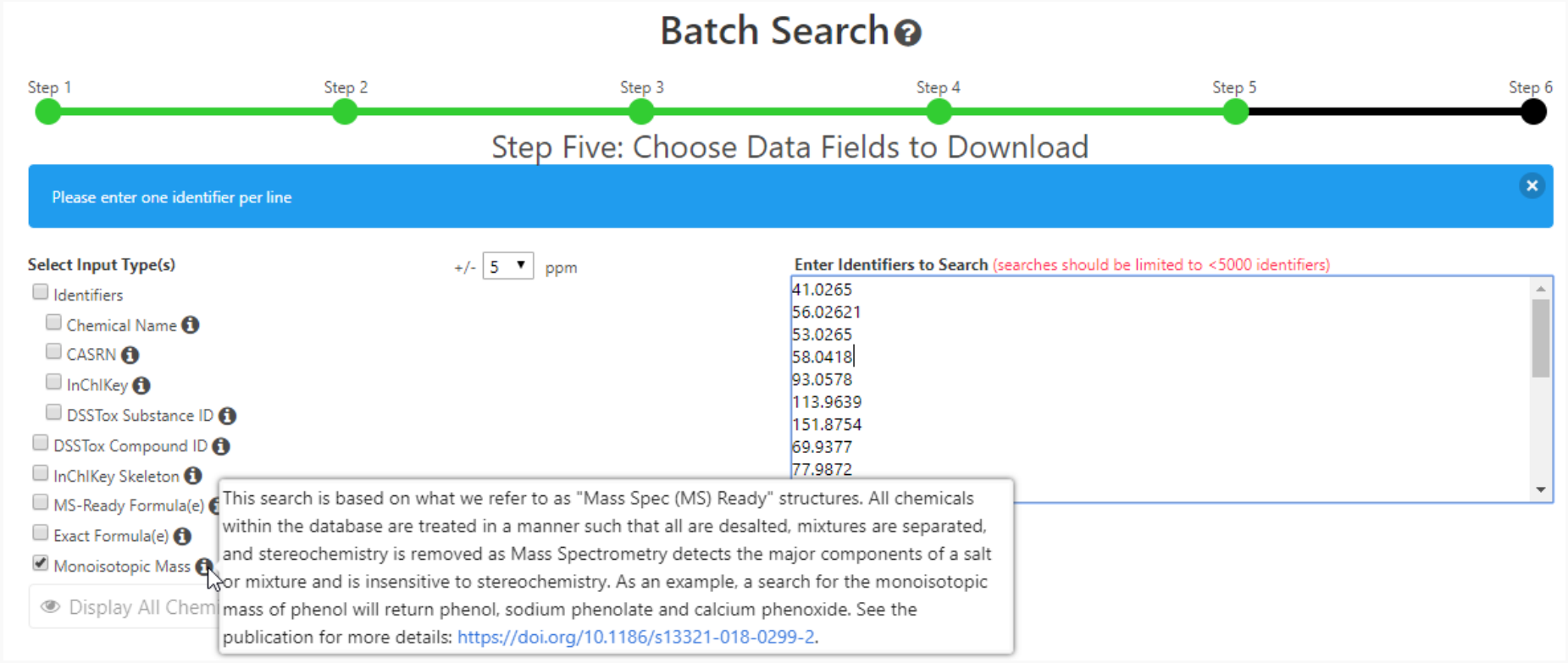
Batch Searches



Batch Searches



Batch Searching Formula/Mass



Excel Output

PREFERRE	CASRN	DATA_SOURCI	TOXVAL_D	TOXCAST_	TOXCAST_	NUMBER_OF_PUBMED	PUBCHEM_DATA_S	CPDAT_COUNT
Aniline	62-53-3	148	Y	0.47	1/211	1932	284	80
3-Methylpyr	108-99-6	93	Y	2.8	16/571	16	120	16
2-Methylpyr	109-06-8	88	Y	0.0	0/211	1395	112	12
4-Methylpyr	108-89-4	82	Y	0.52	2/381	1	118	4
Aniline hydr	142-04-1	54	Y	2.23	9/404	1932	66	5
Anilinium ni	542-15-4	13	-	2.37	5/211	1932	4	-
Benzenamii	542-16-5	13	-	-	-	-	-	5
1,3,5-Trinitr	3101-79-9	10	-	-	-	-	10	1
Di-2-propyn	6921-28-4	10	-	-	-	-	43	-
Benzenamii	542-14-3	8	-	-	-	-	15	-
Butanal--an	68411-20-1	8	-	-	-	-	-	6
Benzenamii	37832-42-1	7	-	-	-	1932	27	-
2,4-Hexadie	1516-01-4	6	-	-	-	-	25	-
Cyclobutan	15760-35-7	6	-	-	-	-	79	2
Aniline hydr	542-13-2	6	-	-	-	1932	6	-
Benzenamii	542-11-0	6	-	-	-	-	-	-
Tris(4-amin	68389-46-8	6	-	-	-	-	-	3
4-[(2-Chloro	71566-74-0	6	-	-	-	-	-	4
Heptanal--a	9003-50-3	6	-	-	-	-	-	1

Suspect Screening and Non-Targeted Analysis Workflow

EPA United States Environmental Protection Agency

Suspect Screening

- Raw Samples
- Extracted Samples
- Raw Features
- "Molecular Features"
- DSSTox Chemical Database
- Matched Formulas
- Mapped Structures
- Prioritized Structures (using ToxPi)
- Confirmed Structures (using ToxCast standards)
- Predicted Concentrations

Non-Targeted Analysis

- Processed Features
- Prioritized Features
- Predicted Formulas
- Candidate Structures
- Sorted Structures
- Predicted Retention Times
- Predicted Mass Spectra
- Predicted/Observed Functional Use
- Predicted/Observed Media Occurrence
- Methodological Concordance
- Top Candidate Structure(s)

Color Key

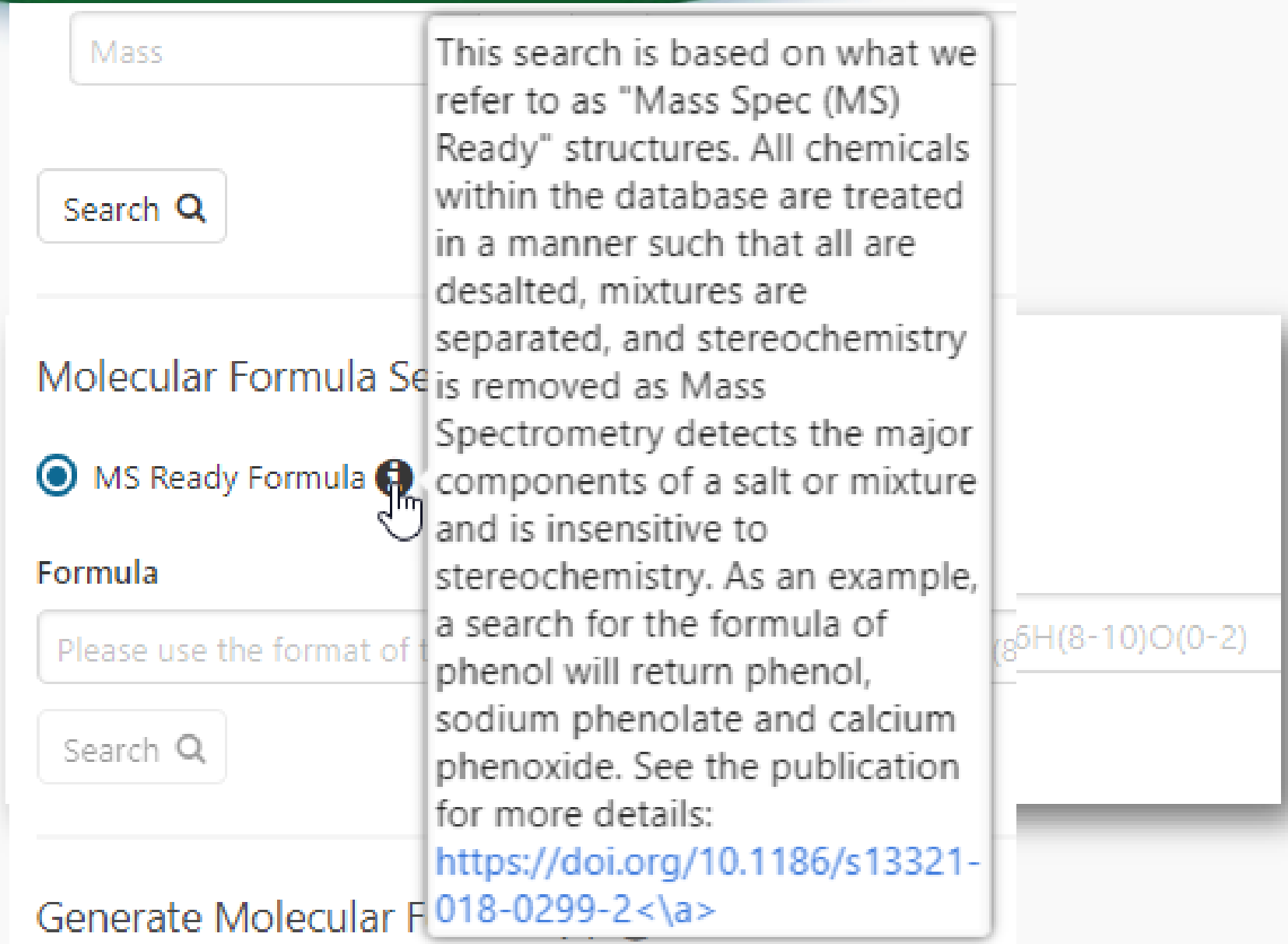
Red = Analytical Chemistry

Blue = Data Processing & Analysis

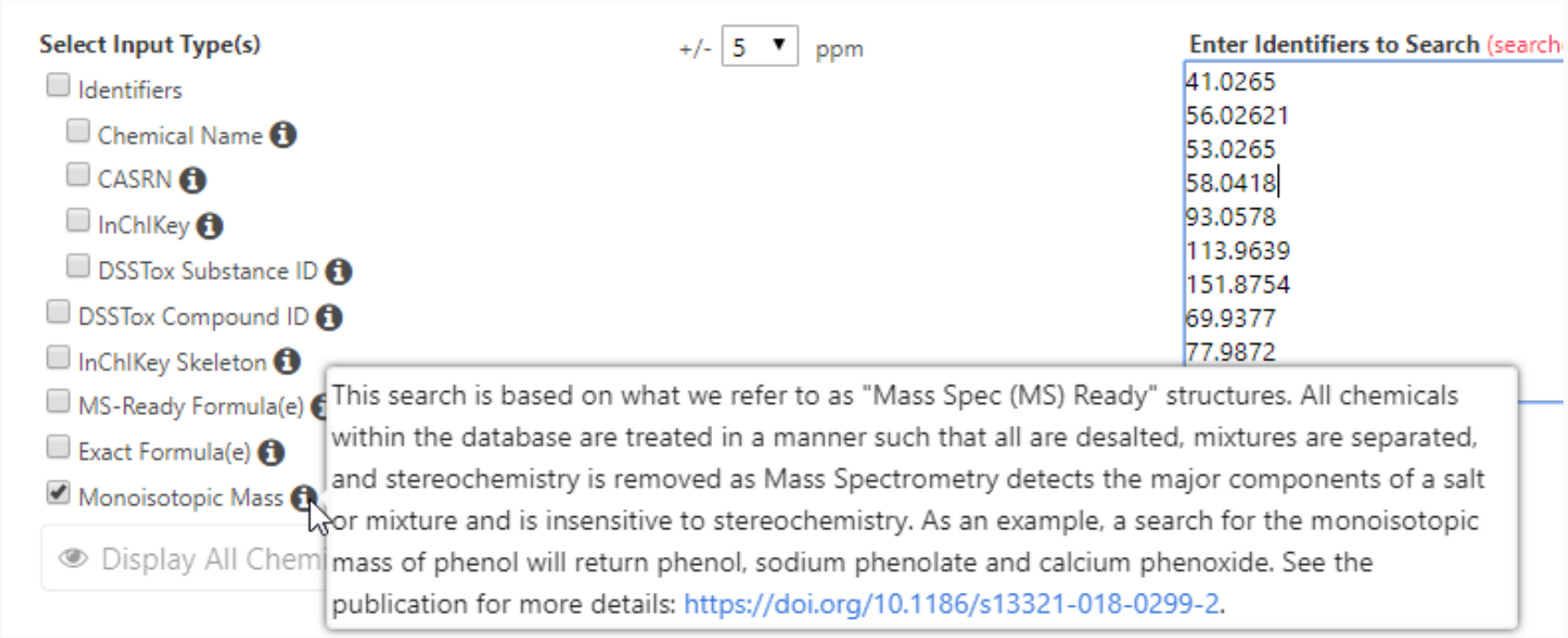
Purple = Mathematical & QSPR Modeling

Green = Informatics & Web Services

MS-Ready Structures Underpin Analysis



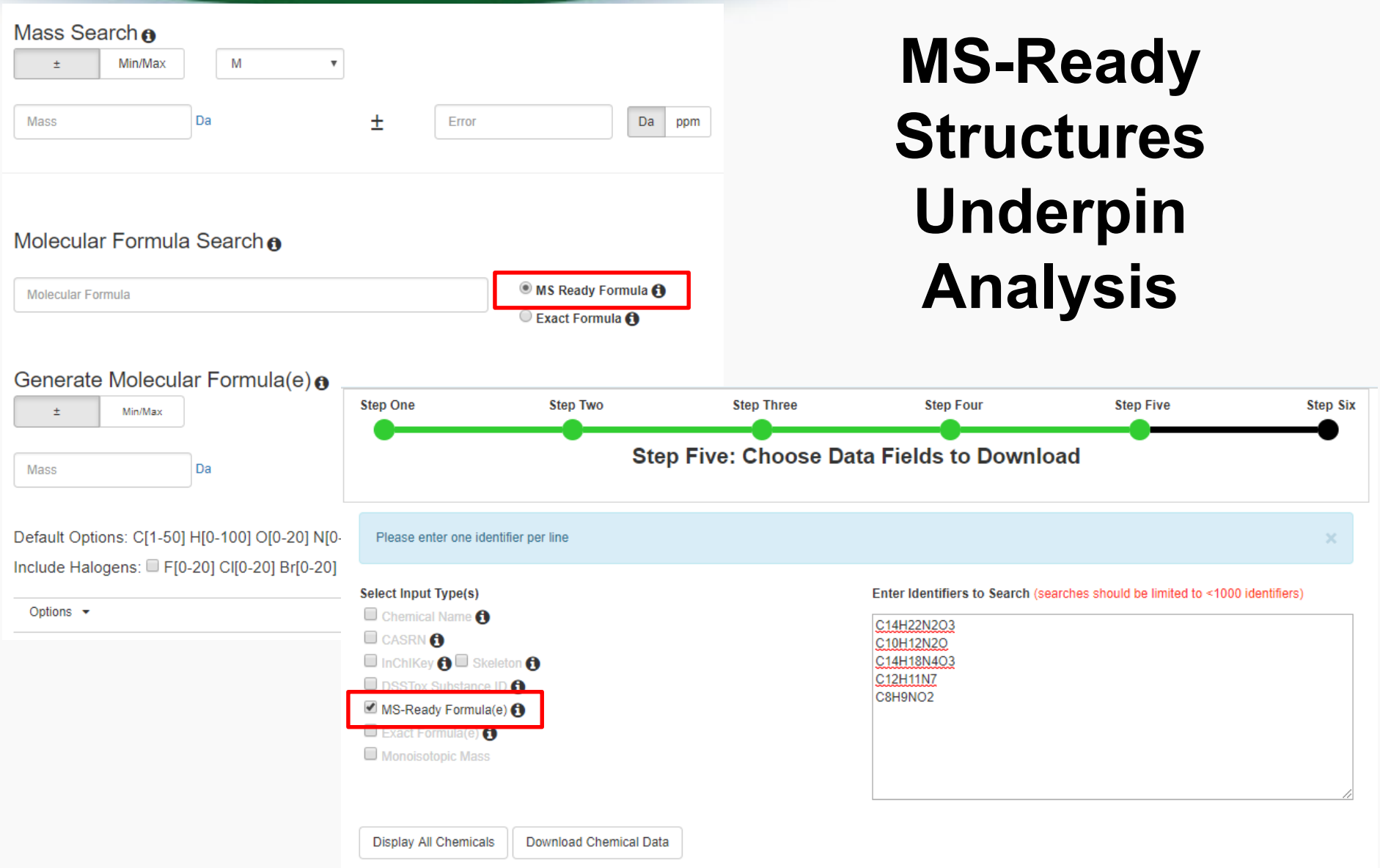
MS-Ready Structures Underpin Analysis



The Dashboard to Support MS-Analysis

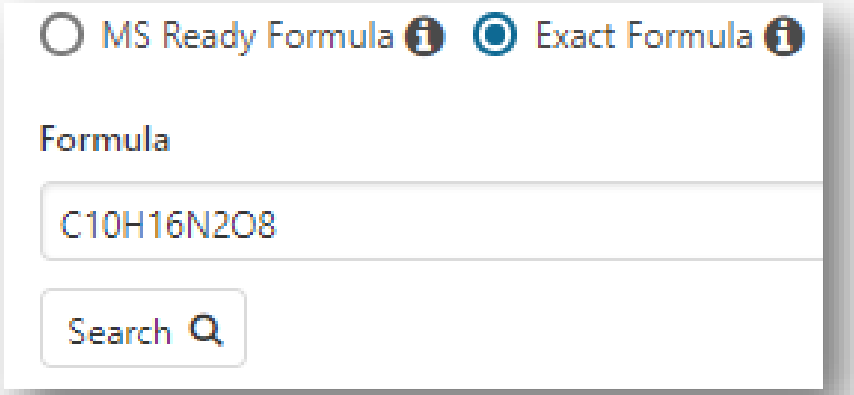
EPA United States Environmental Protection Agency

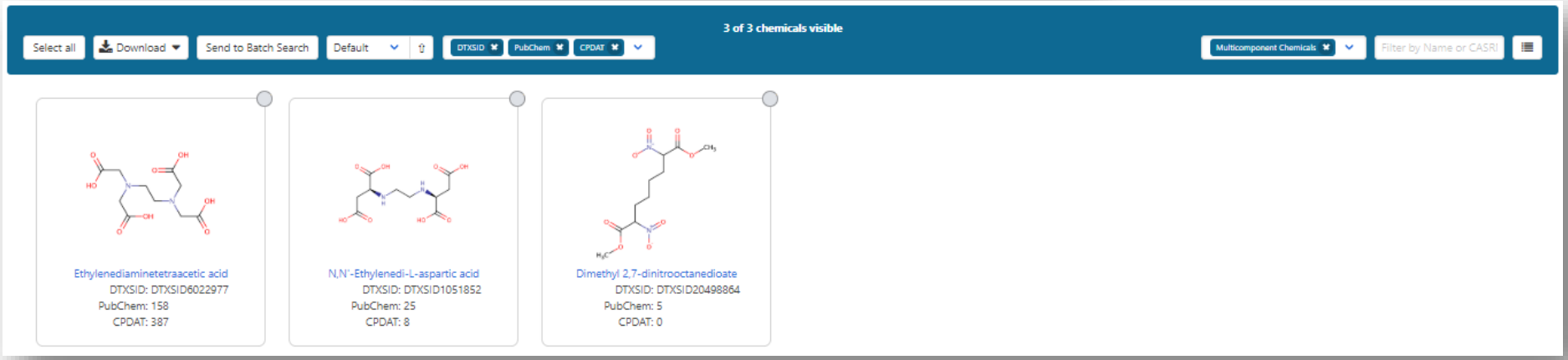
MS-Ready Structures Underpin Analysis



MS-Ready Mappings

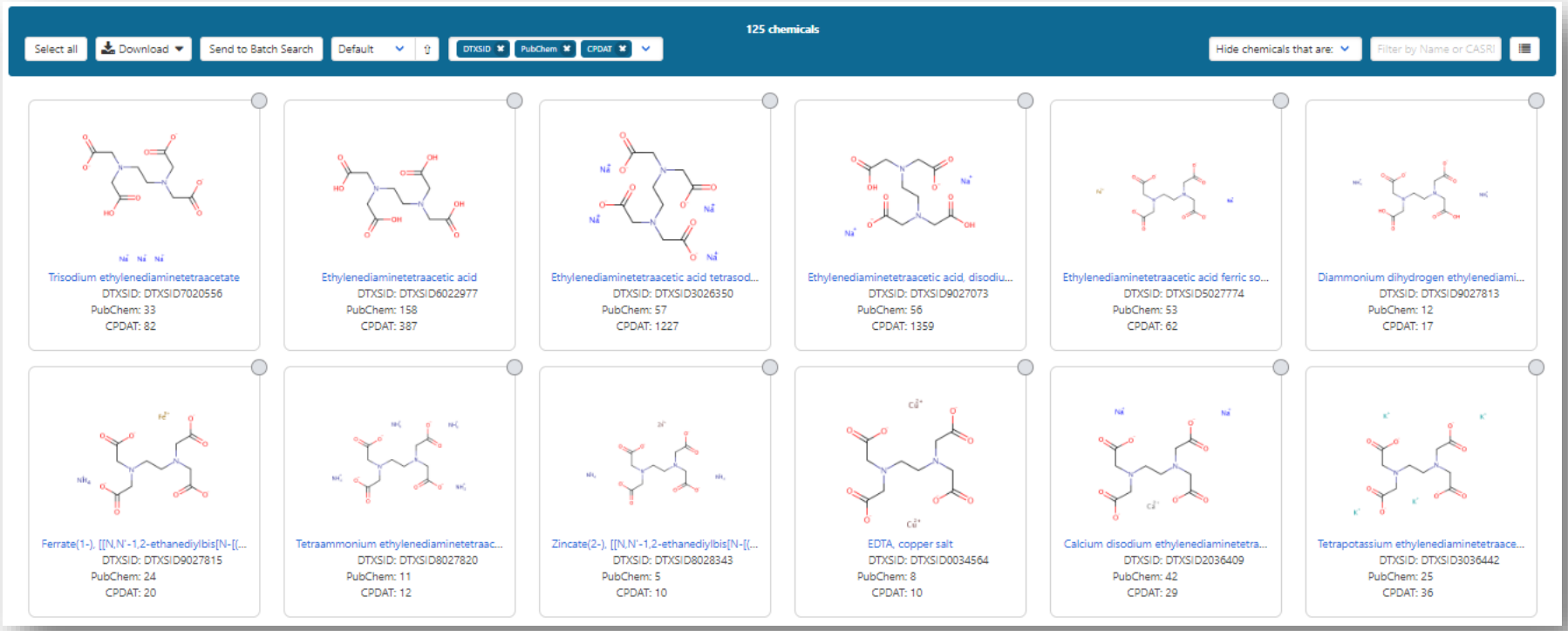
- Input Formula: C10H16N2O8: 3 Hits





MS-Ready Mappings

- **Same** Input Formula: C10H16N2O8
- MS Ready Formula Search: **125** Chemicals



MS-Ready Mappings

- 125 chemicals returned in total
  - 8 of the 125 are single component chemicals
  - 3 of the 8 are isotope-labeled
  - 3 are neutral compounds and 2 are charged

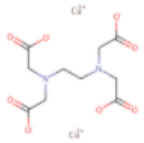
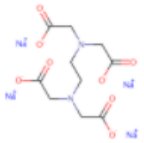
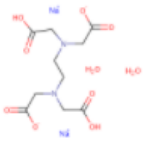
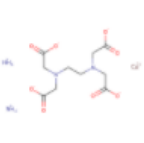
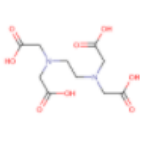
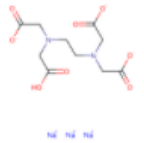
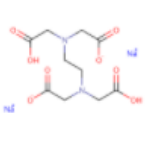
Complexity to Simplicity
93 Chemicals – 7 in EPAHFR

EPA United States Environmental Protection Agency

	INPUT	DTXCID_INDIVIDU	FORMULA	SMILES_I	DTXSID	CASRN	EXPOCAST_M	EXPOCAST	DATA_SOURCI	TOXVAL_D	TOXCAST_	TOXCAST	# OF_PUBMED	PUBCHEM	EPAHFR
2	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID6022977	60-00-4	7.96e-05	Y	71	Y	2.65	3/113	25251	158	Y
3	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID9027073	139-33-3	-	-	41	Y	-	-	25251	56	Y
4	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID3026350	64-02-8	-	-	37	Y	-	-	-	57	Y
5	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID7020556	150-38-9	-	-	30	Y	-	-	-	33	Y
6	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5049609	67989-88-2	-	-	20	Y	-	-	-	8	Y
7	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5049576	6381-92-6	-	-	19	Y	-	-	25251	31	Y
8	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID0034564	12276-01-6	-	-	11	-	-	-	-	8	Y
9	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5027774	15708-41-5	-	-	48	Y	1.98	6/303	241	53	-
10	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID2036409	62-33-9	4.64e-06	Y	37	Y	0.0	0/64	25251	42	-
11	C10H16N2O8	DTXCID00197424	C10H16N2(	OC(=O)C(	DTXSID1051852	20846-91-7	-	-	36	Y	-	-	89	25	-
12	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID6042107	15375-84-5	-	-	25	Y	-	-	97	25	-
13	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID3036442	5964-35-2	-	-	23	Y	-	-	25251	25	-
14	C10H16N2O8	DTXCID00197424	C10H16N2(	OC(=O)C(	DTXSID1051806	178949-82-1	-	-	22	Y	-	-	-	5	-
15	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID0065696	14025-21-9	-	-	22	Y	-	-	-	43	-
16	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID9027813	20824-56-0	-	-	21	Y	-	-	-	12	-
17	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID9027815	21265-50-9	-	-	20	Y	-	-	241	24	-
18	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5058272	17421-79-3	-	-	19	Y	-	-	25251	25	-
19	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID3058612	2001-94-7	-	-	18	Y	-	-	25251	19	-
20	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID8027820	22473-78-5	-	-	16	Y	-	-	-	11	-
21	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID8058324	17572-97-3	-	-	15	-	-	-	-	36	-
22	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID8028343	67859-51-2	-	-	14	Y	-	-	-	5	-
23	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID4051328	13235-36-4	-	-	14	-	-	-	-	18	-
24	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID6070980	68015-77-0	-	-	14	Y	-	-	-	13	-
25	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID9058317	15934-01-7	-	-	11	-	-	-	-	5	-
26	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID0066163	17099-81-9	-	-	11	-	-	-	241	14	-
27	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID1068988	54959-35-2	-	-	11	-	-	-	241	14	-
28	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5074266	60816-63-9	-	-	11	-	-	-	1	10	-
29	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID4048197	39208-15-6	-	-	10	-	-	-	-	28	-
30	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID2065830	14931-83-0	-	-	10	-	-	-	47	9	-
31	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID70189997	36499-65-7	-	-	10	-	-	-	25298	26	-
32	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID7051420	61916-40-3	-	-	9	-	-	-	-	4	-
33	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID2051425	73513-47-0	-	-	8	Y	-	-	-	3	-
34	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID7051426	73637-19-1	-	-	8	Y	-	-	-	5	-
35	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID2051427	73637-20-4	-	-	8	Y	-	-	-	-	-
36	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID3058741	10378-23-1	-	-	8	Y	-	-	-	31	-
37	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID6065925	15708-48-2	-	-	8	-	-	-	-	19	-
38	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID20217976	6766-87-6	-	-	8	-	-	-	-	13	-
39	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID5065807	14689-29-3	-	-	7	-	-	-	-	12	-
40	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID6069408	60544-70-9	-	-	7	-	-	-	-	12	-
41	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID00153984	123354-94-9	-	-	7	-	-	-	2	6	-
42	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID70190705	37209-61-3	-	-	7	-	-	-	6	9	-
43	C10H16N2O8	DTXCID902977	C10H16N2(	OC(=O)CI	DTXSID7051424	67401-50-7	-	-	6	-	-	-	-	4	-

Complexity to Simplicity
93 Chemicals – 7 in the list

EPA United States Environmental Protection Agency

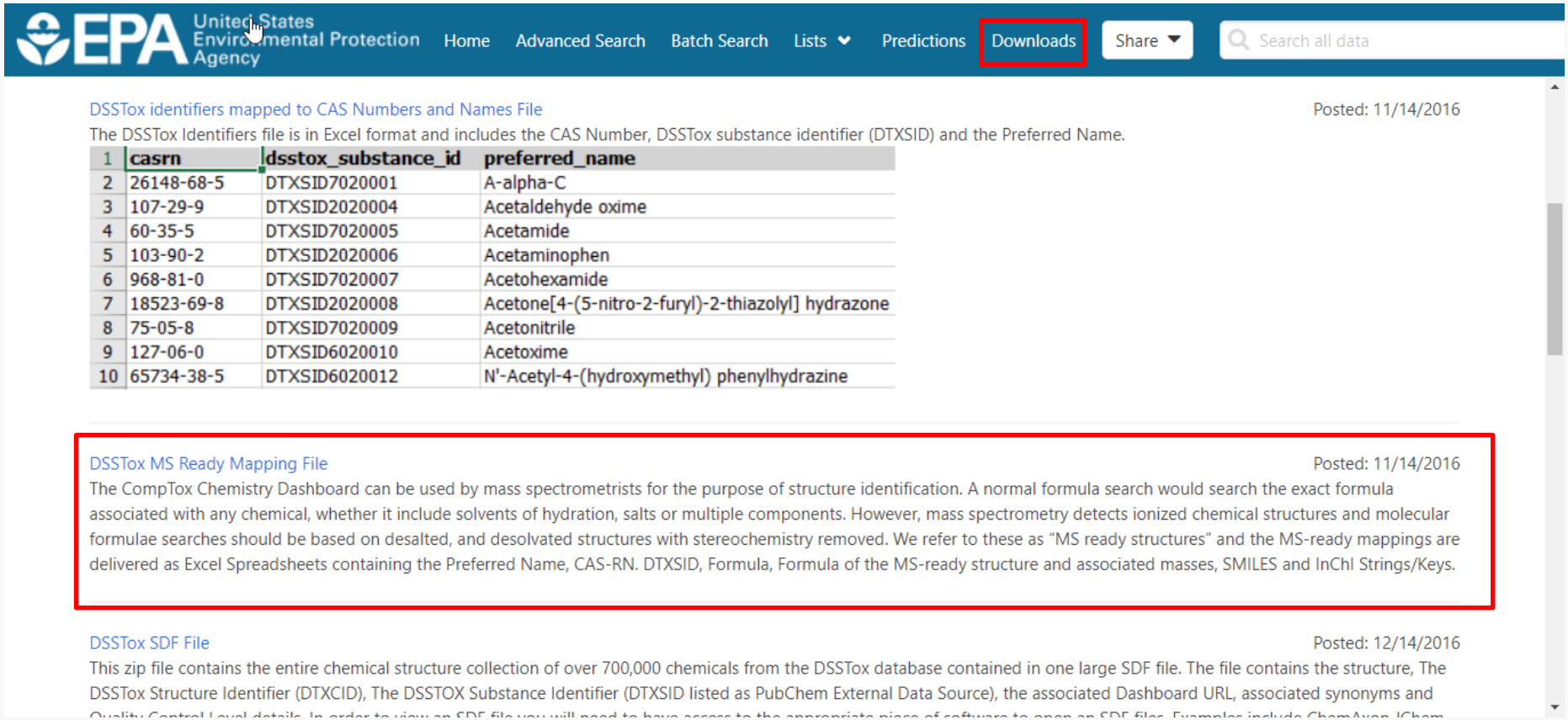
Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Source	PubMed Data Source	Monoisotopic Mass
	DTXSID0034564	EDTA, copper salt	12276-01-6	Level 1	10	11	8	0	413.918561
	DTXSID3026350	Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	Level 1	1227	37	57	0	380.018442
	DTXSID5049576	Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	Level 1	93	19	31	25251	372.075683
	DTXSID5049609	Ethylenediaminetetraacetic acid, diammonium copper salt	67989-88-2	Level 2	9	20	8	0	387.057712
	DTXSID6022977	Ethylenediaminetetraacetic acid	60-00-4	Level 1	346	71	158	25251	292.090665
	DTXSID7020556	Trisodium ethylenediaminetetraacetate	150-38-9	Level 1	85	30	33	0	358.036498
	DTXSID9027073	Ethylenediaminetetraacetic acid, disodium salt	139-33-3	Level 1	1358	41	56	25251	336.054554

Searching batches
Formula (or mass) searching

EPA United States Environmental Protection Agency

	A	B	C	D	E	F	G
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS	DATA SOURCES
2	C14H22N2O3	DTXSID2022628	29122-68-7	Atenolol	C14H22N2O3	266.163042576	46
3	C14H22N2O3	DTXSID0021179	6673-35-4	Practolol	C14H22N2O3	266.163042576	32
4	C14H22N2O3	DTXSID4048854	841-73-6	Bucolome	C14H22N2O3	266.163042576	20
5	C14H22N2O3	DTXSID1045407	13171-25-0	Trimetazidine dihydrochloride	C14H24Cl2N2O3	338.116398	19
6	C14H22N2O3	DTXSID0045753	56715-13-0	R-(+)-Atenolol	C14H22N2O3	266.163042576	19
7	C14H22N2O3	DTXSID2048531	5011-34-7	Trimetazidine	C14H22N2O3	266.163042576	14
8	C14H22N2O3	DTXSID10239405	93379-54-5	Esatenolol	C14H22N2O3	266.163042576	12
9	C14H22N2O3	DTXSID50200634	52662-27-8	N-(2-Diethylaminoethyl)-2-(4-hydroxyphenoxy)acetamide	C14H22N2O3	266.163042576	7
10	C14H22N2O3	DTXSID4020111	51706-40-2	dl-Atenolol hydrochloride	C14H23ClN2O3	302.1397203	6
11	C14H22N2O3	DTXSID1068693	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	C14H22N2O3	266.163042576	5
12	C18H34N2O6S	DTXSID3023215	154-21-2	Lincomycin	C18H34N2O6S	406.213757997	35
13	C18H34N2O6S	DTXSID7047803	859-18-7	Lincomycin hydrochloride	C18H35ClN2O6S	442.1904357	22
14	C18H34N2O6S	DTXSID20849438	1398534-62-7	PUBCHEM_71432748	C18H35ClN2O6S	442.1904357	1
15	C10H12N2O	DTXSID1047576	486-56-6	Cotinine	C10H12N2O	176.094963014	40
16	C10H12N2O	DTXSID8075330	50-67-9	Serotonin	C10H12N2O	176.094963014	22
17	C10H12N2O	DTXSID8044412	2654-57-1	4-Methyl-1-phenylpyrazolidin-3-one	C10H12N2O	176.094963014	18
18	C10H12N2O	DTXSID80165186	153-98-0	Serotonin hydrochloride	C10H13ClN2O	212.0716407	11
19	C10H12N2O	DTXSID2048870	29493-77-4	(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-amine	C10H12N2O	176.094963014	10
20	C10H12N2O	DTXSID10196105	443-31-2	6-Hydroxytryptamine	C10H12N2O	176.094963014	9
21	C10H12N2O	DTXSID90185693	31822-84-1	1,4,5,6-Tetrahydro-5-phenoxypyrimidine	C10H12N2O	176.094963014	7
22	C10H12N2O	DTXSID40178777	2403-66-9	2-Benzimidazolepropanol	C10H12N2O	176.094963014	7
23	C10H12N2O	DTXSID80157026	13140-86-8	N-Cyclopropyl-N'-phenylurea	C10H12N2O	176.094963014	6
24	C10H12N2O	DTXSID30205607	570-14-9	4-Hydroxytryptamine	C10H12N2O	176.094963014	6
25	C14H18N4O3	DTXSID5023900	17804-35-2	Benomyl	C14H18N4O3	290.137890456	68
26	C14H18N4O3	DTXSID3023712	738-70-5	Trimethoprim	C14H18N4O3	290.137890456	51
27	C14H18N4O3	DTXSID40209671	60834-30-2	Trimethoprim hydrochloride	C14H19ClN4O3	326.1145682	8
28	C14H18N4O3	DTXSID70204210	55687-49-5	Benzenemethanol, 4-((2,4-diamino-5-pyrimidinyl)methyl)-2,	C14H18N4O3	290.137890456	5
29	C14H18N4O3	DTXSID20152671	120075-57-2	6-Methoxy-4-(3-(N,N-dimethylamino)propylamino)-5,8-quin	C14H18N4O3	290.137890456	4
30	C14H18N4O3	DTXSID30213742	63931-79-3	1H-1,2,4-Benzotriazepine-3-carboxylic acid, 4,5-dihydro-4-	C14H18N4O3	290.137890456	3
31	C14H18N4O3	DTXSID30219608	69449-07-6	2,4-Pyrimidinediamine, 5-((3,4,5-trimethoxyphenyl)methyl)-	C14H20N4O4	308.14845514	3
32	C14H18N4O3	DTXSID20241155	94232-27-6	L-Aspartic acid, compound with 5-((3,4,5-trimethoxyphenyl	C18H25N5O7	423.175398165	3
33	C14H18N4O3	DTXSID80241156	94232-28-7	L-Glutamic acid, compound with 5-((3,4,5-trimethoxypheny	C19H27N5O7	437.191048229	3
34	C14H18N4O3	DTXSID20143781	101204-93-7	1H-Pyrido(2,3-e)-1,4-diazepine-2,3,5-trione, 4-(2-(diethylam	C14H18N4O3	290.137890456	3
35	C12H11N7	DTXSID6021373	396-01-0	Triamterene	C12H11N7	253.107593382	52
36	C12H11N7	DTXSID00204465	5587-93-9	Ampyrimine	C12H11N7	253.107593382	7
37	C12H11N7	DTXSID5064621	7300-26-7	Benzenamine, 4-azido-N-(4-azidophenyl)-	C12H9N7	251.091943318	4
38	C12H11N7	DTXSID00848025	90293-82-6	Sulfuric acid--6-phenylpteridine-2,4,7-triamine (1/1)	C12H13N7O4S	351.074973101	1
39	C12H11N7	DTXSID50575293	92310-83-3	(1E)-N-Phenyl-1,2-bis(1H-1,2,4-triazol-1-yl)ethan-1-imine	C12H11N7	253.107593382	1
40	C8H9NO2	DTXSID2020006	103-90-2	Acetaminophen	C8H9NO2	151.063328534	75
41	C8H9NO2	DTXSID6026567	134-20-3	Methyl 2-aminobenzoate	C8H9NO2	151.063328534	50

Downloadable Data



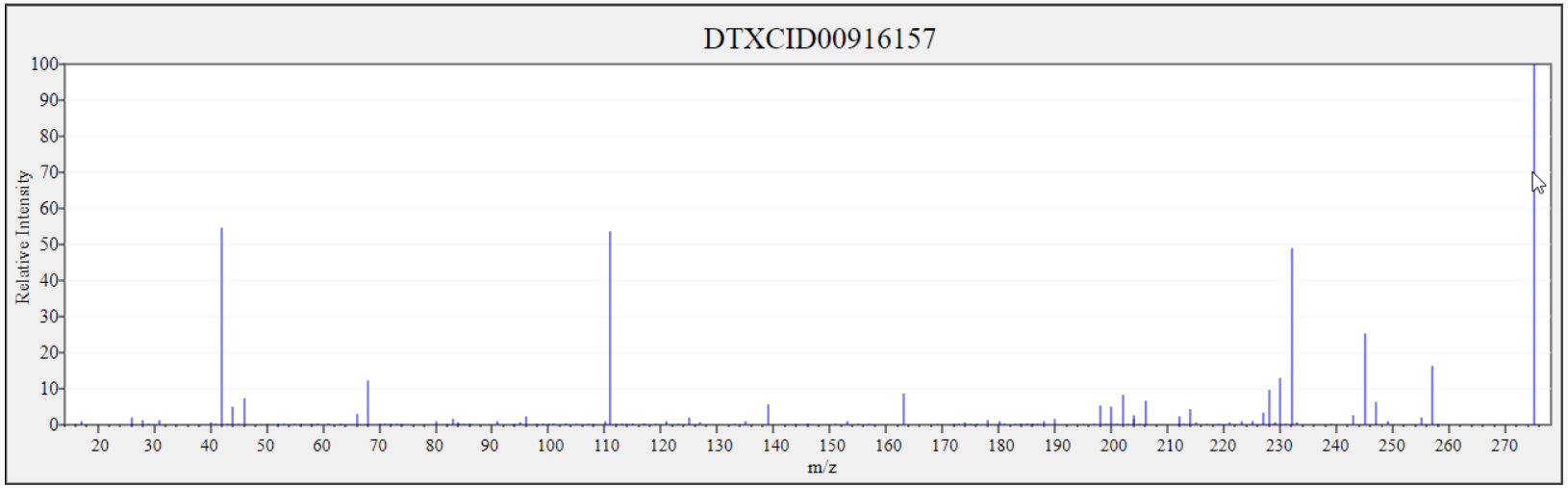
Work in Progress

- CFM-ID
  - Viewing and Downloading pre-predicted spectra
  - Search spectra against the database
- Retention Time Index Prediction
- Structure/substructure/similarity search
- Generation of MS-ready structures:
  - Upload file, download results
  - Service based generation

Predicted Mass Spectra

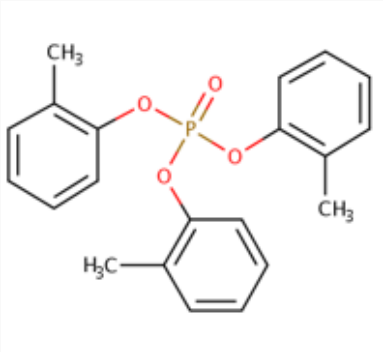
http://cfmid.wishartlab.com/

- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard

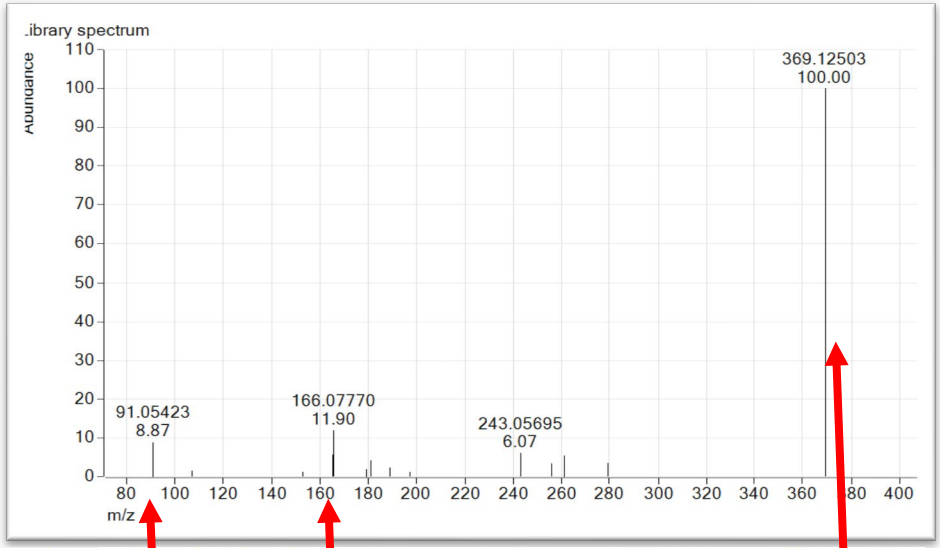


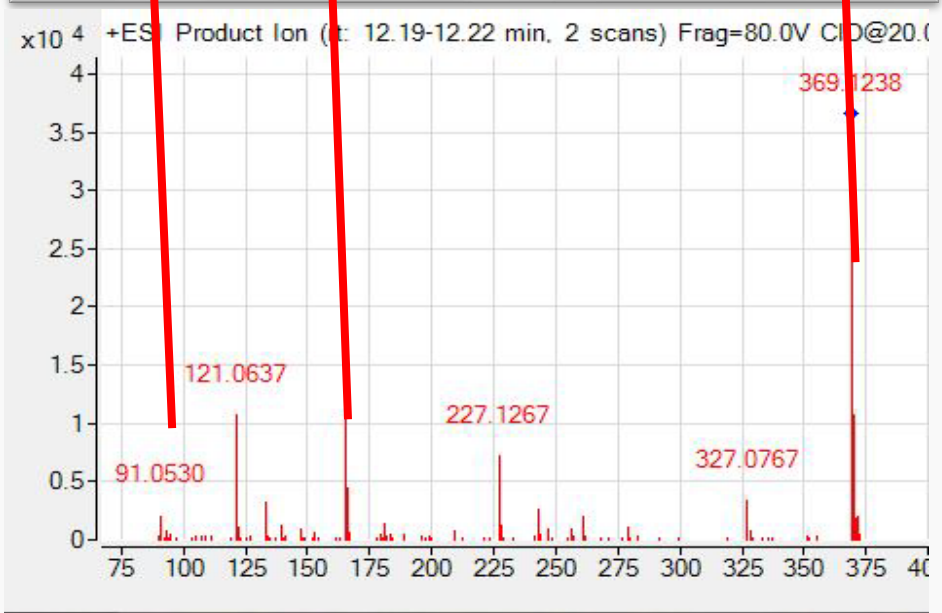
Predicted Mass Spectra

Library Fragmentation Spectra (20eV)



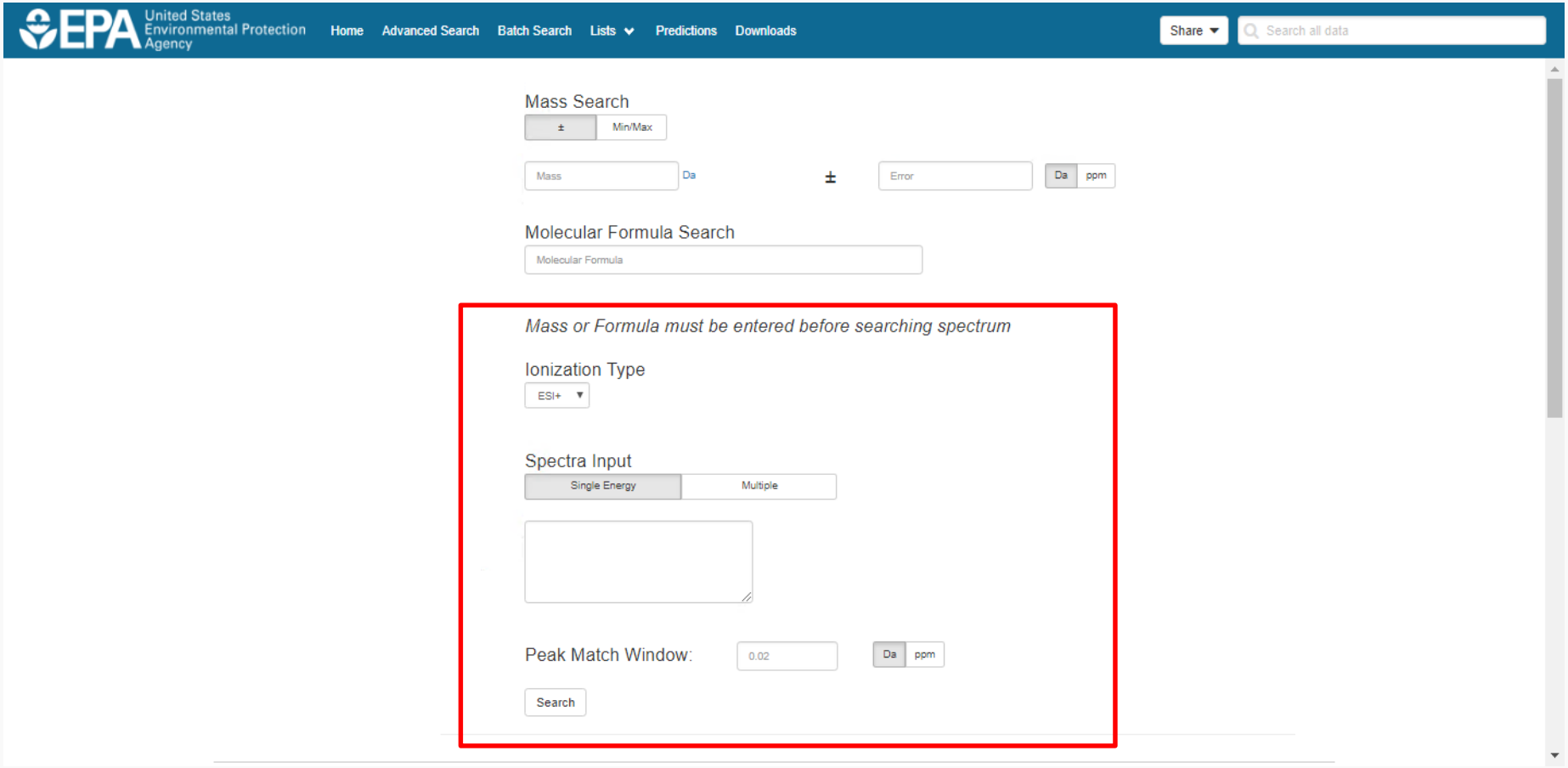
Observed Fragmentation Spectra (20eV)



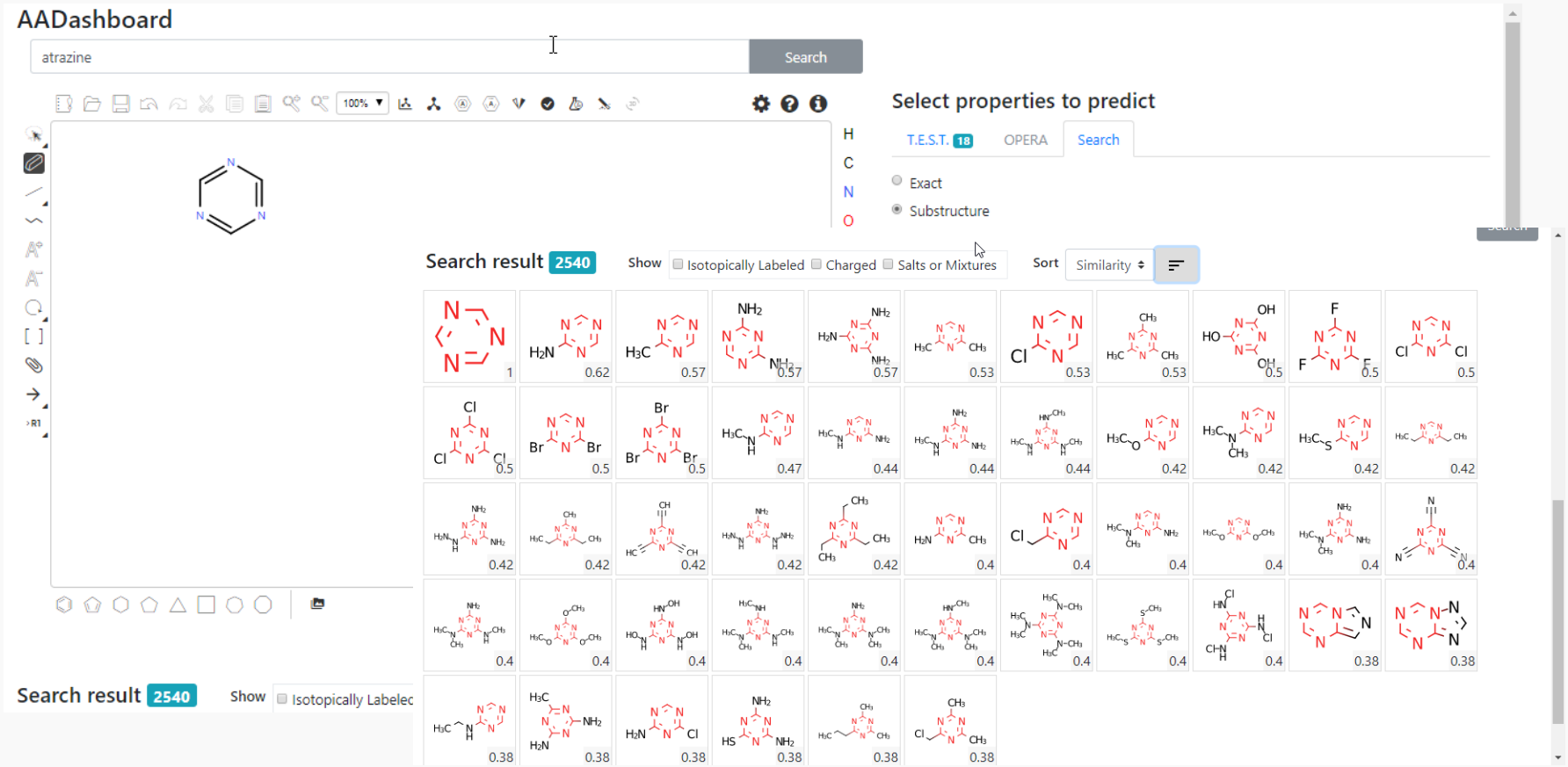


Match Score

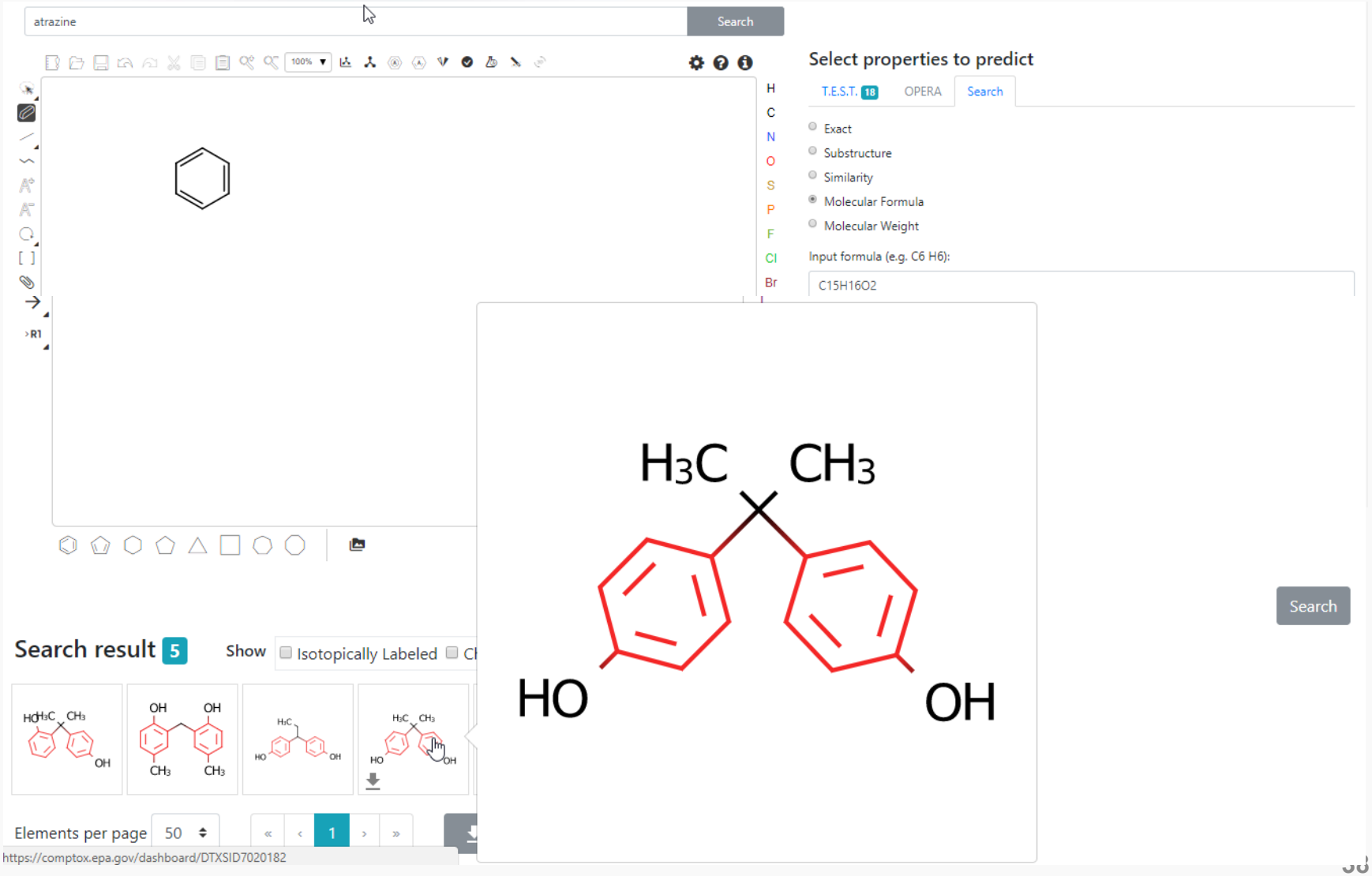
Search Expt. vs. Predicted Spectra



Prototype Development



Prototype Development



Conclusion

- The CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Multiple prediction models available for data gap filling
  - OPERA models and TEST models – PhysChem and Tox endpoints
  - Models based on *in vitro* data – classification models
  - Generalized Read-Across development in progress
- 2 years development as a CompTox Integration Hub

Acknowledgements

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