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Adapting and adopting cheminformatics tools to support mapping chemical space coverage in non-targeted analysis

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United States Environmental Protection Agency

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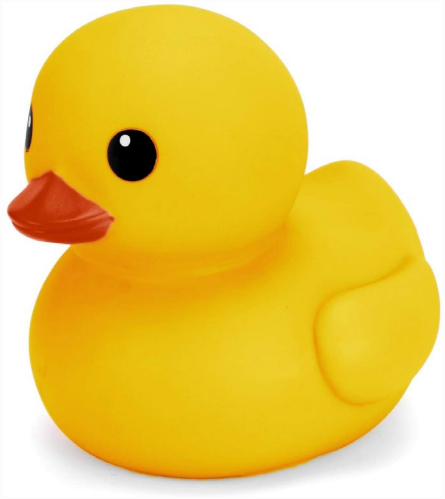
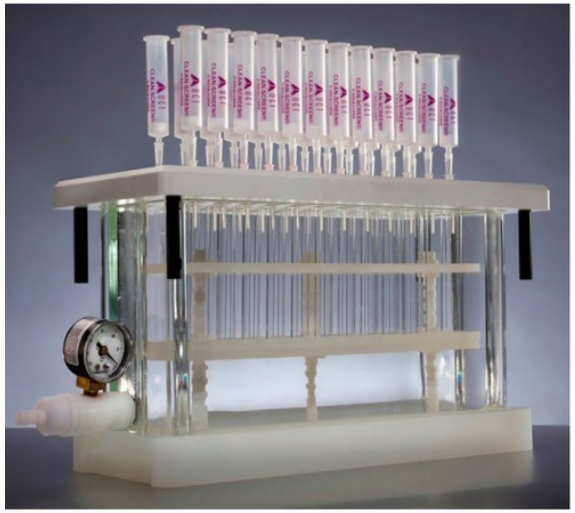
Non-targeted Analysis and Chemical Space

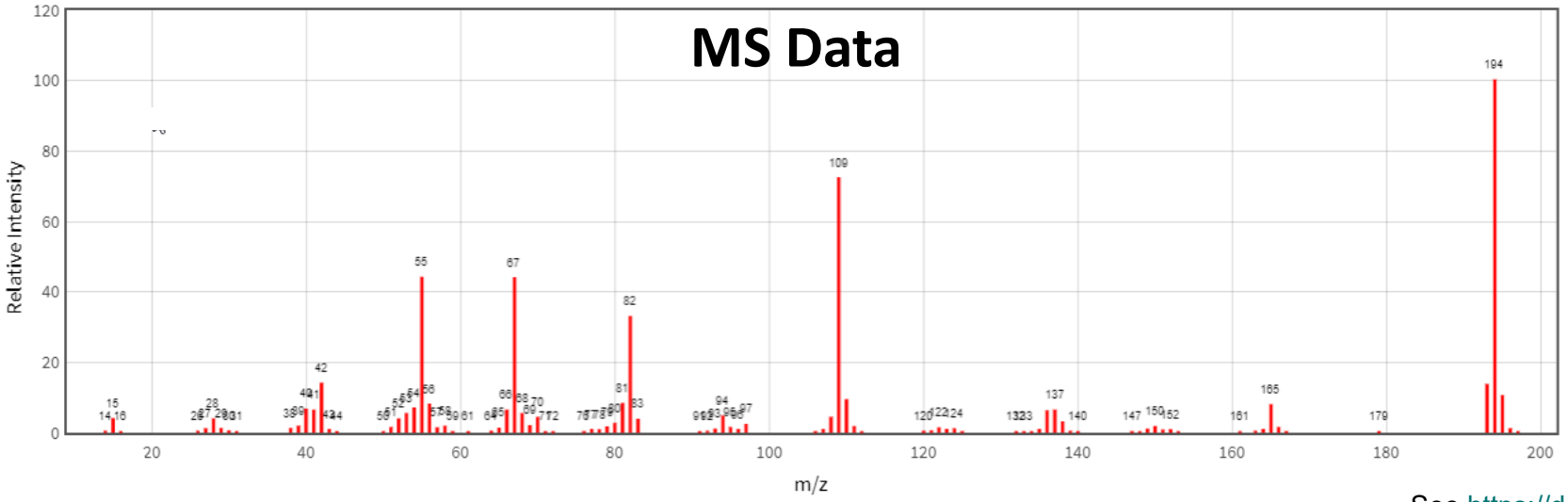


Media Sample



Extraction, Cleanup & Sample Preparation

MS Analysis



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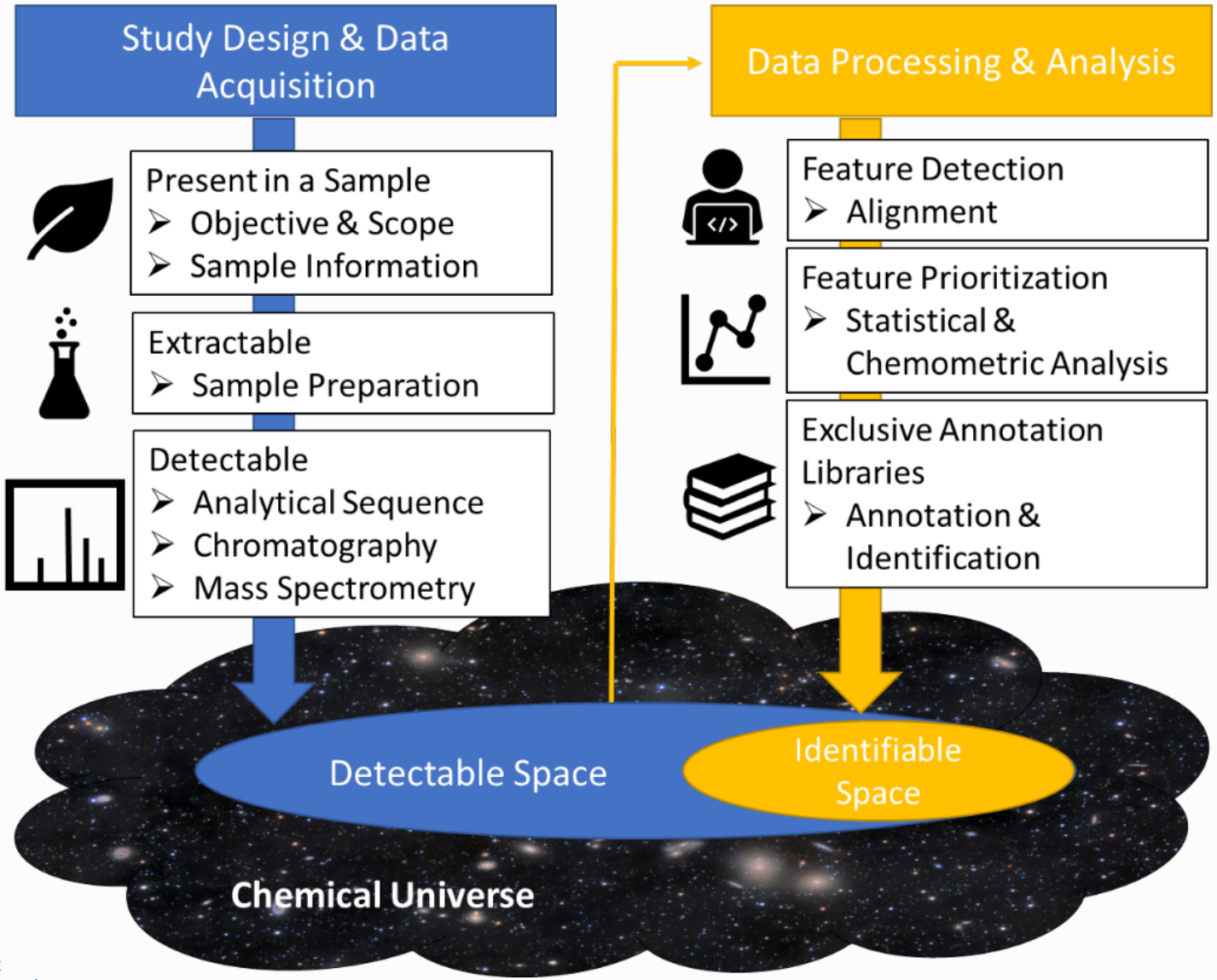
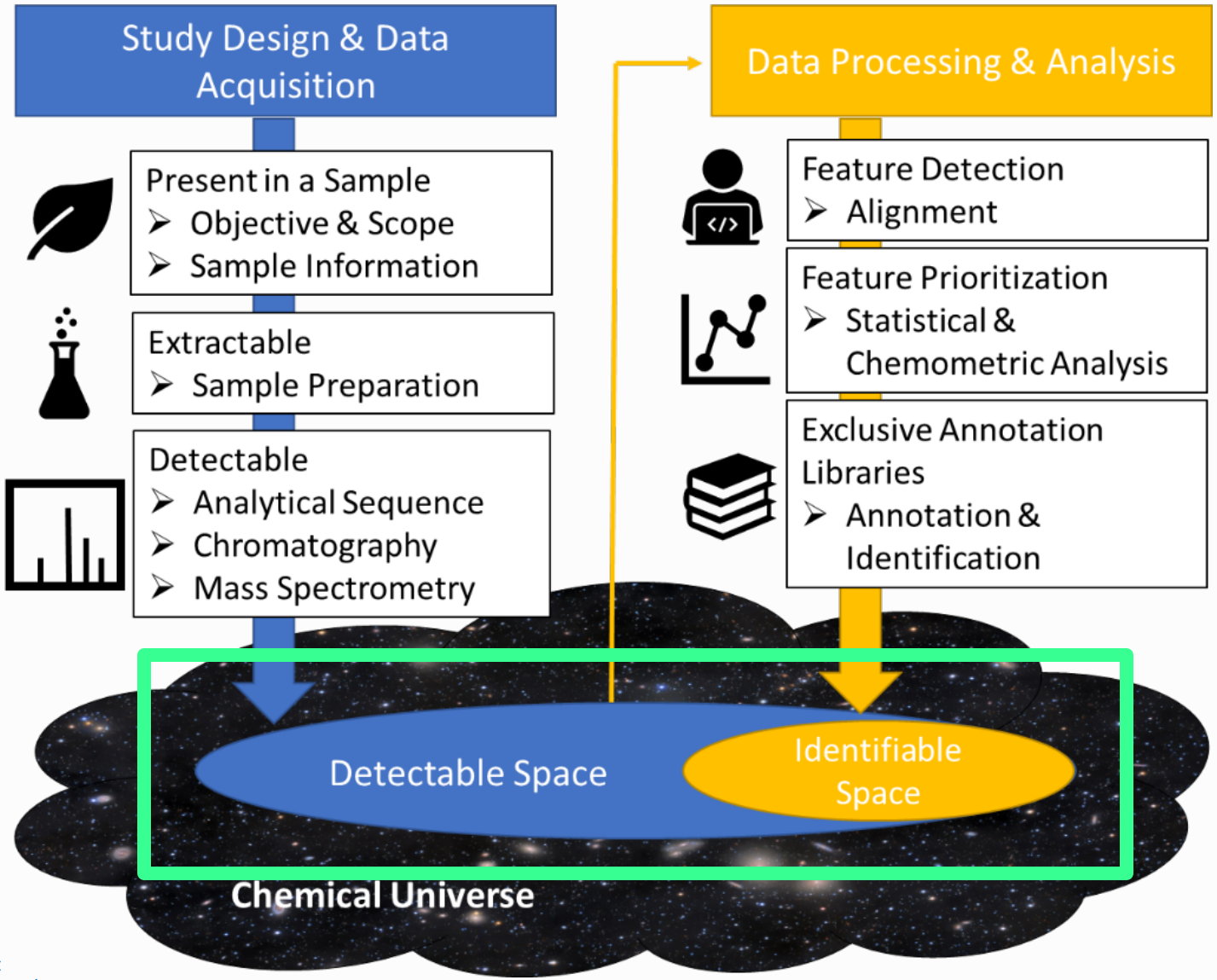
See https://doi.org/10.1021/acs.est.1c01907 for more on rubber ducky analysis.

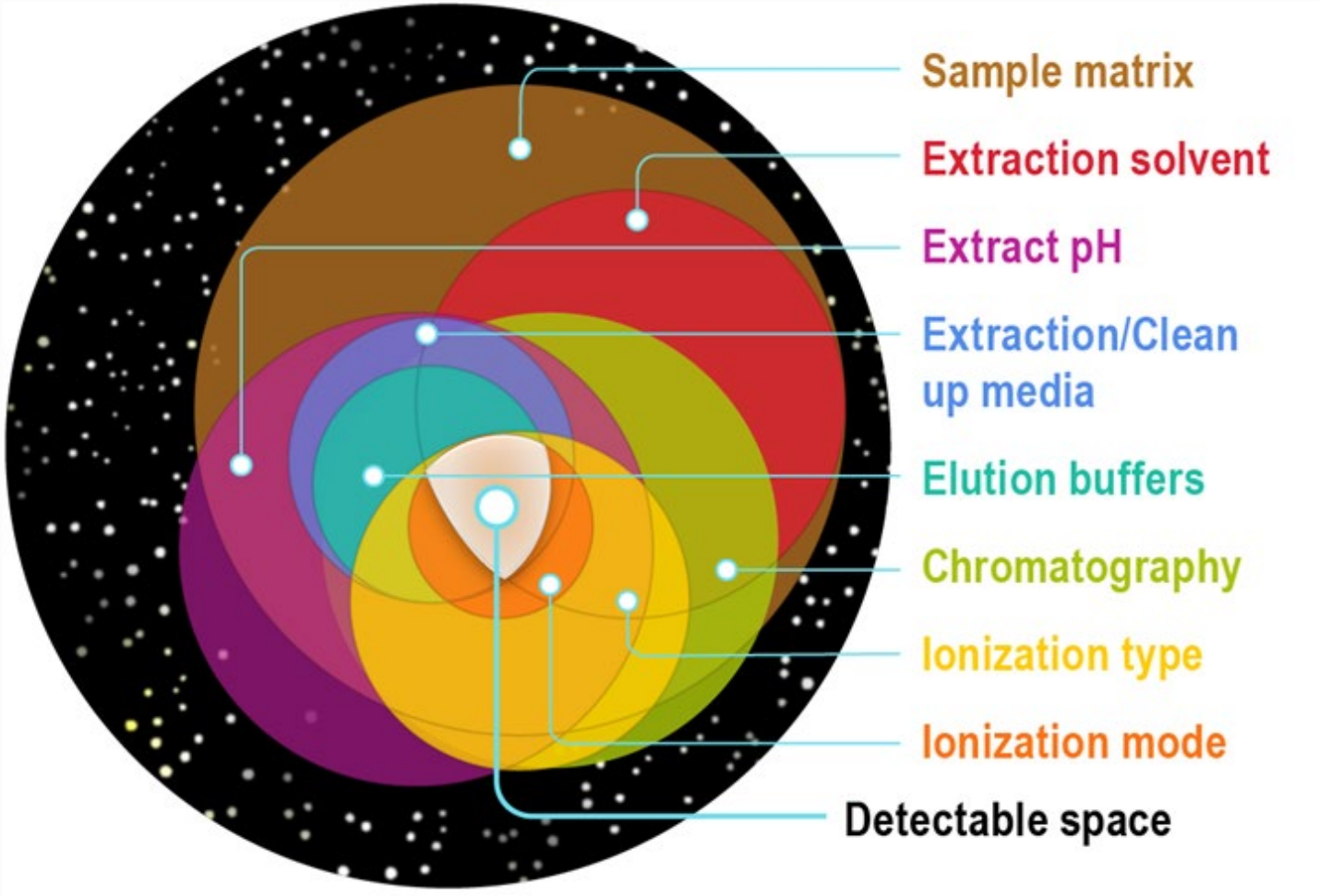
The chemical universe according to NTA



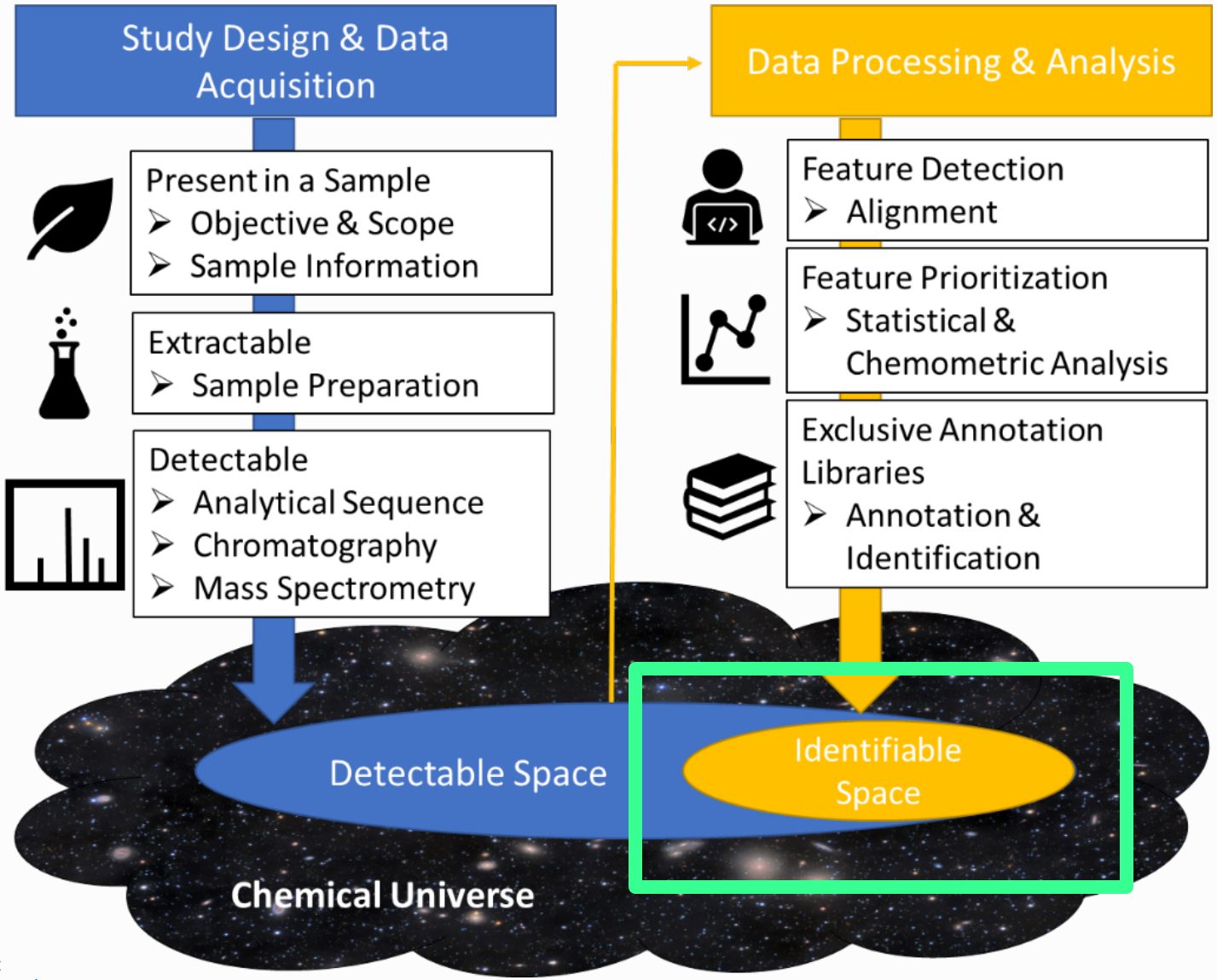
The chemical universe according to NTA



How to identify detectable space



The chemical universe according to NTA



Identifiable space

ChemSpace Tool

Categories

- Consumer Products
- Drugs
- Illicit Drugs
- Smoking&Vaping
- Pesticides
- Surfactants
- PFAS
- Food Products
- Hazardous Chemicals
- Dyes
- Plastics
- Water
- Halocarbons
- Phenols
- Exposome
- Metabolites
- Biosolids
- Biosolids QCMix

Download

Reset Checkboxes

Input Data | Average Mass | Water Solubility | Vapor Pressure | Boiling Point | LogKow | LogKoa

Show 15 entries Search:

	DTXSID	Preferred Name	CASRN	Molecular Formula	Average Mass	Water Solubility (log(mol/L))	Vapor Pressure (log(mmHg))	Boiling Point (C)	Log(Kow)	Log(Koa)
1	DTXSID7021605	Hexanedioic acid	124-04-9	C6H10O4	146.14	-0.82	-6.5	337.44	0.08	7.59
2	DTXSID2020688	Hexachlorocyclopentadiene	77-47-4	C5Cl6	272.76	-5.18	-1.22	238.99	5.04	6.91
3	DTXSID8021515	Butanoic acid	107-92-6	C4H8O2	88.11	-0.18	0.21	163.74	0.79	4.23
4	DTXSID6063199	2,4,5-T Triethanolamine salt	3813-14-7	C14H20Cl3NO6	404.67	-3.68	-4.43	314.38	0.79	9.06
5	DTXSID7020425	Dichlone	117-80-6	C10H4Cl2O2	227.04	-5.7	-5.95	346.15	2.15	7.38
6	DTXSID5020029	Acrylonitrile	107-13-1	C3H3N	53.06	0.15	2.03	77.43	0.25	2.44
7	DTXSID90866339	Butan-2-yl (2,4,5-trichlorophenoxy)acetate	61792-07-2	C12H13Cl3O3	311.58	-4.27	-4.59	342.41	4.46	8.53
8	DTXSID3020964	Nitrobenzene	98-95-3	C6H5NO2	123.11	-1.79	-0.61	210.85	1.85	3.87
9	DTXSID7021100	Parathion	56-38-2	C10H14NO5PS	291.26	-4.36	-5.17	374.96	3.83	9.33
10	DTXSID1020306	Chloroform	67-66-3	CHCl3	119.37	-1.18	2.3	61.14	1.97	2.75
11	DTXSID5024057	Dimethylamine	124-40-3	C2H7N	45.08	1.56	3.18	6.9	-0.38	2.02
12	DTXSID1027007	Propanoic anhydride	123-62-6	C6H10O3	130.14	-0.26	0.13	169.94	0.58	3.92
13	DTXSID5021881	Ethylenediamine	107-15-3	C2H8N2	60.1	1.22	1.08	117.03	-2.04	6.7
14	DTXSID1020647	Furfural	98-01-1	C5H4O2	96.08	-0.1	0.34	153.4	0.41	3.53
15	DTXSID8041329	2,4,5-T 2-Ethylhexyl	1928-47-8	C16H21Cl3O3	367.69	-4.87	-5.92	326.76	5.15	9.89

Showing 1 to 15 of 81,369 entries

Previous 1 2 3 4 5 … 5,425 Next

Each chemical substance is present in at least one category. Each chemical substance maps to a single chemical structure for the purpose of property prediction. Predicted properties were obtained from OPERA

Tweak Ranges

Average Mass: 1 to 2000

Water Solubility (log(mol/L)): -14 to 3

Vapor Pressure (log(mmHg)): -14 to 10

Boiling Point (C): -170 to 550

Octanol Water Partition Coefficient (log(Kow)): -6 to 10.5

Octanol Air Partition Coefficient (log(Koa)): -1 to 12.5

Dataset Size

81369

ChemSpace Tool

Categories

- [ ] Consumer Products
- [ ] Drugs
- [ ] Illicit Drugs
- [ ] Smoking&Vaping
- [ ] Pesticides
- [ ] Surfactants
- [ ] PFAS
- [ ] Food Products
- [ ] Hazardous Chemicals
- [ ] Dyes
- [ ] Plastics
- [ ] Water
- [ ] Halocarbons
- [ ] Phenols
- [ ] Exposome
- [ ] Metabolites
- [ ] Biosolids
- [ ] Biosolids QCMix

Download

Reset Checkboxes

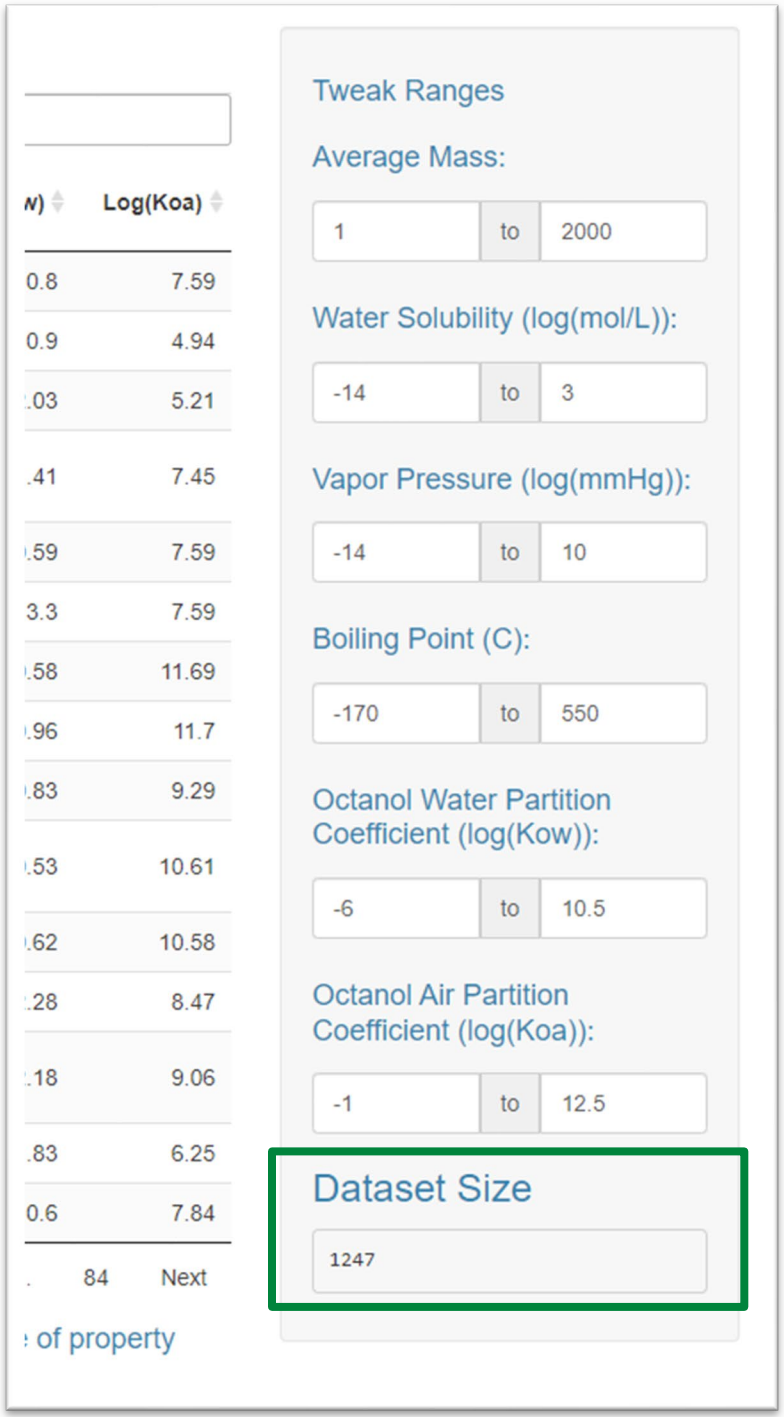
Input Data | Average Mass | Water Solubility

Show 15 entries

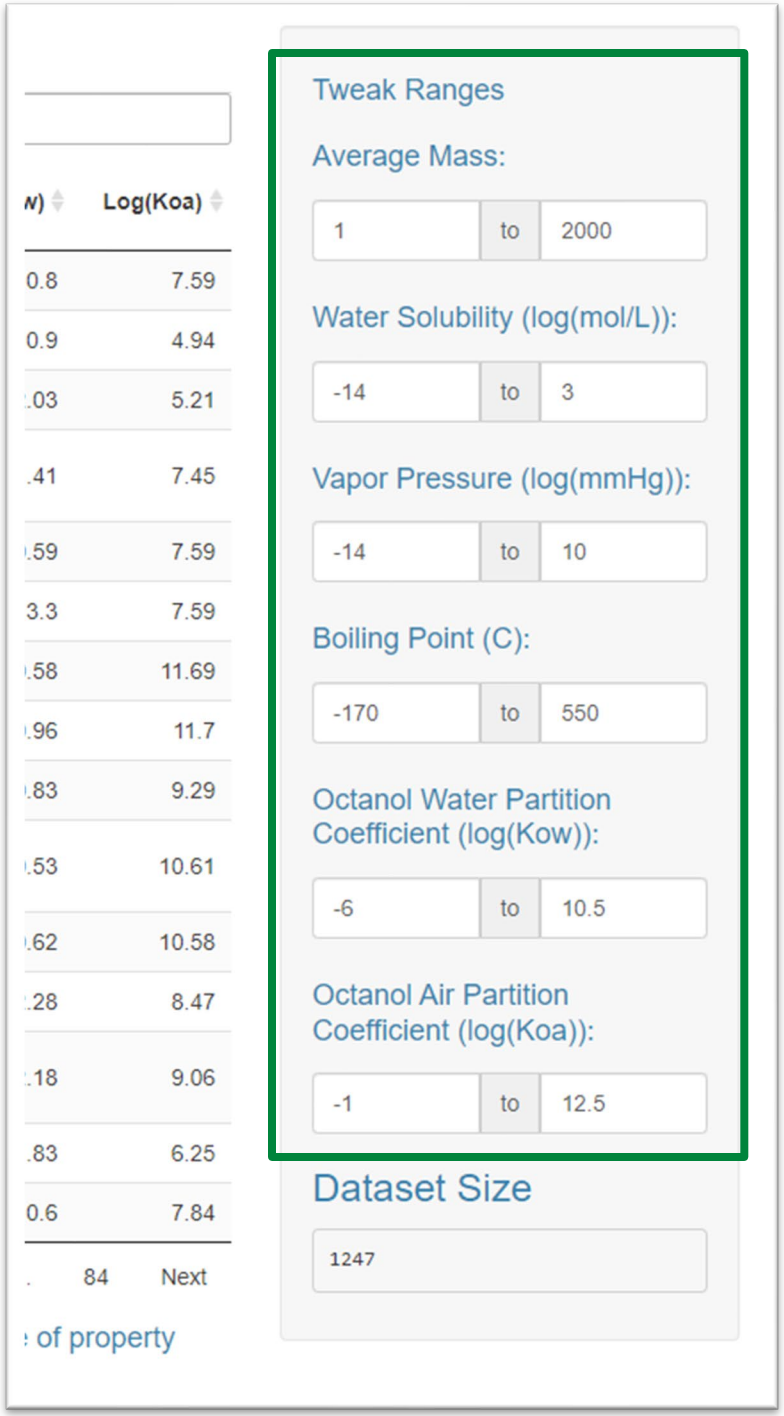
	DTXSID	Preferred Name
1	DTXSID7021605	Hexanedioic acid
2	DTXSID2020688	Hexachlorocyclopentadiene
3	DTXSID8021515	Butanoic acid
4	DTXSID6063199	2,4,5-T Triethanolamine salt
5	DTXSID7020425	Dichlone
6	DTXSID5020029	Acrylonitrile
7	DTXSID90866339	Butan-2-yl (2,4,5-trichlorophenoxy)acetate
8	DTXSID3020964	Nitrobenzene
9	DTXSID7021100	Parathion
10	DTXSID1020306	Chloroform
11	DTXSID5024057	Dimethylamine
12	DTXSID1027007	Propanoic anhydride
13	DTXSID5021881	Ethylenediamine
14	DTXSID1020647	Furfural
15	DTXSID8041329	2,4,5-T 2-Ethylhexyl

Showing 1 to 15 of 81,369 entries

Each chemical substance is present in at least
prediction. Predicted properties were obtained



N)	Log(Koa)
0.8	7.59
0.9	4.94
.03	5.21
.41	7.45
.59	7.59
3.3	7.59
.58	11.69
.96	11.7
.83	9.29
.53	10.61
.62	10.58
.28	8.47
.18	9.06
.83	6.25
0.6	7.84


Log(Koa)
0.8 7.59
0.9 4.94
.03 5.21
.41 7.45
.59 7.59
3.3 7.59
.58 11.69
.96 11.7
.83 9.29
.53 10.61
.62 10.58
.28 8.47
.18 9.06
.83 6.25
0.6 7.84
84 Next
of property
Tweak Ranges
Average Mass:
1 to 2000
Water Solubility (log(mol/L)):
-14 to 3
Vapor Pressure (log(mmHg)):
-14 to 10
Boiling Point (C):
-170 to 550
Octanol Water Partition Coefficient (log(Kow)):
-6 to 10.5
Octanol Air Partition Coefficient (log(Koa)):
-1 to 12.5
Dataset Size
1247

United States Environmental Protection Agency

ChemSpace Tool

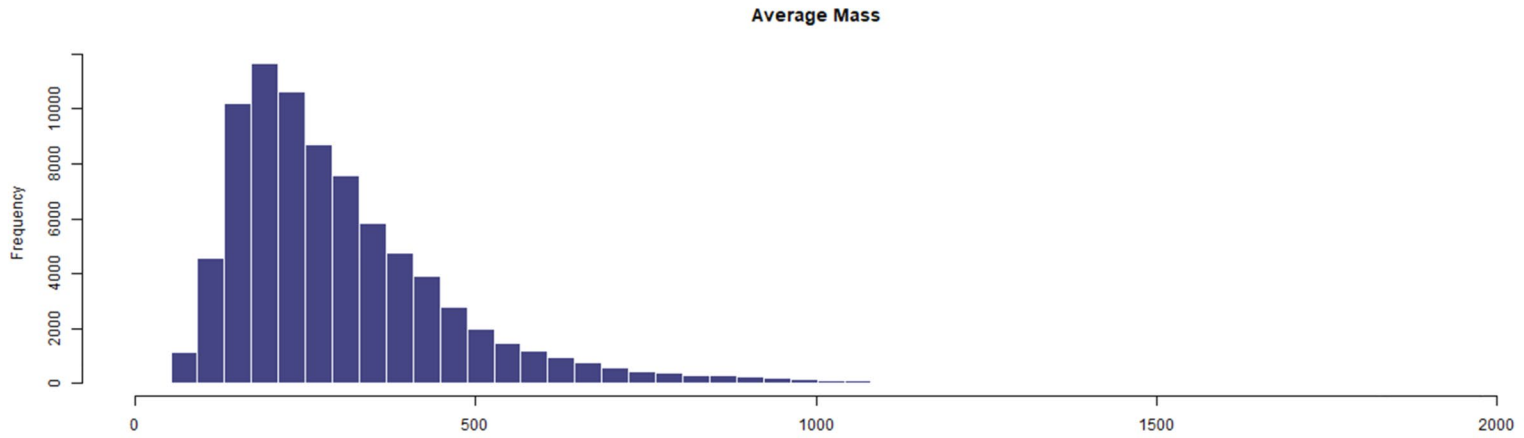
Categories

- [ ] Consumer Products
- [ ] Drugs
- [ ] Illicit Drugs
- [ ] Smoking&Vaping
- [ ] Pesticides
- [ ] Surfactants
- [ ] PFAS
- [ ] Food Products
- [ ] Hazardous Chemicals
- [ ] Dyes
- [ ] Plastics
- [ ] Water
- [ ] Halocarbons
- [ ] Phenols
- [ ] Exposome
- [ ] Metabolites
- [ ] Biosolids
- [ ] Biosolids QCMix

Download

Reset Checkboxes

Input Data | Average Mass | Water Solubility | Vapor Pressure | Boiling Point | LogKow | LogKoa



Tweak Ranges

Average Mass:

1 to 2000

Water Solubility (log(mol/L)):

-14 to 3

Vapor Pressure (log(mmHg)):

-14 to 10

Boiling Point (C):

-170 to 550

Octanol Water Partition Coefficient (log(Kow)):

-6 to 10.5

Octanol Air Partition Coefficient (log(Koa)):

-1 to 12.5

Dataset Size

81369

ChemSpace Tool

Categories

- [ ] Consumer Products
- [ ] Drugs
- [ ] Illicit Drugs
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- [ ] Surfactants
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- [ ] Food Products
- [ ] Hazardous Chemicals
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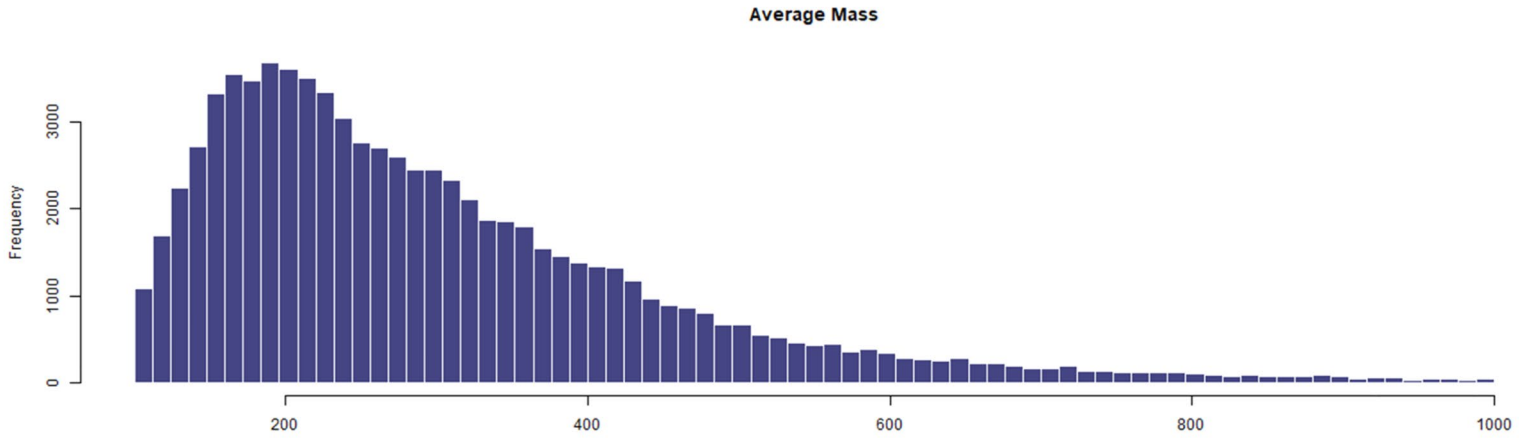
- [ ] Water
- [ ] Halocarbons
- [ ] Phenols
- [ ] Exposome
- [ ] Metabolites
- [ ] Biosolids
- [ ] Biosolids QCMix

Download

Reset Checkboxes

Input Data | Average Mass | Water Solubility | Vapor Pressure | Boiling Point | LogKow | LogKoa



Tweak Ranges

Average Mass:

100 to 1000

Water Solubility (log(mol/L)):

-14 to 3

Vapor Pressure (log(mmHg)):

-14 to 10

Boiling Point (C):

-170 to 550

Octanol Water Partition Coefficient (log(Kow)):

-6 to 10.5

Octanol Air Partition Coefficient (log(Koa)):

-1 to 12.5

Dataset Size

79021

ChemSpace Tool

Categories

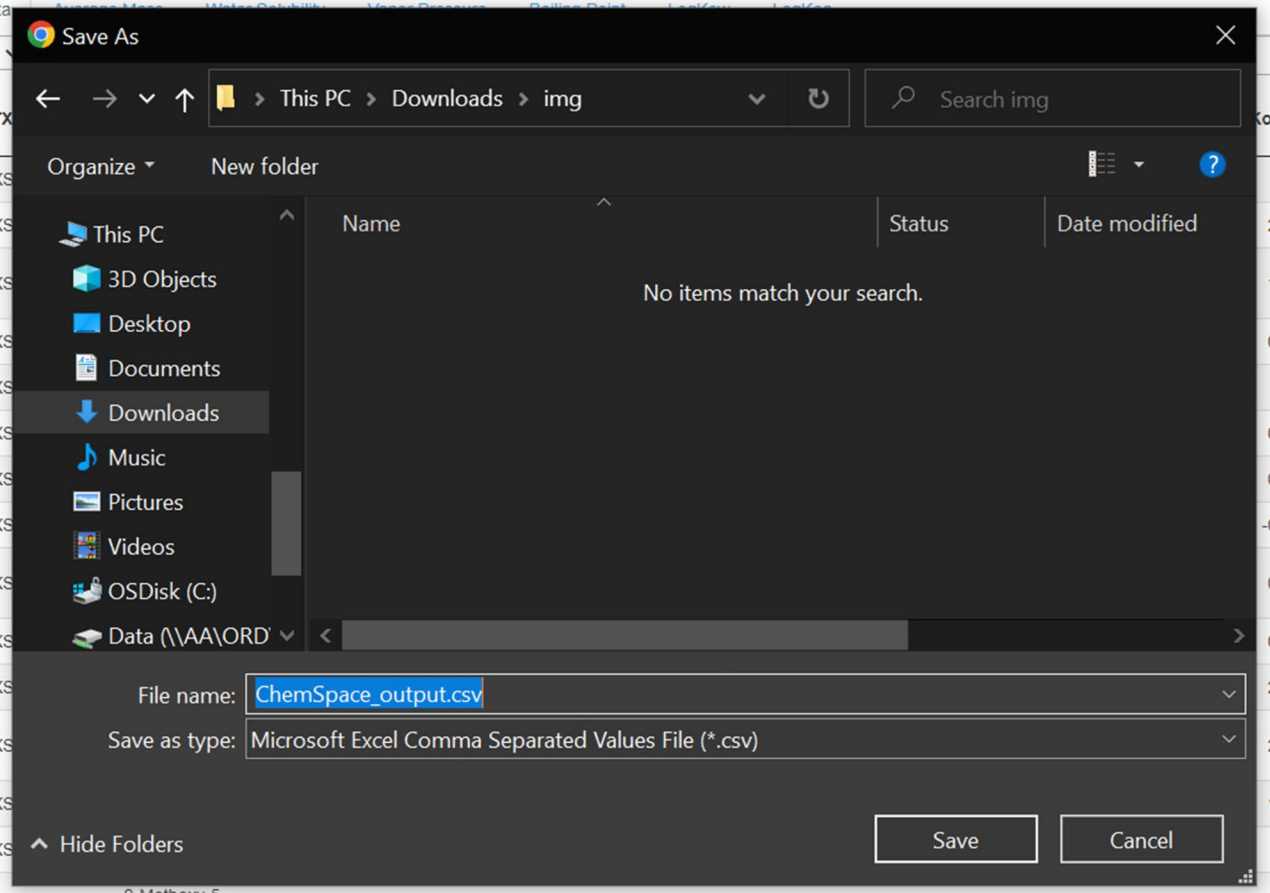
- [x] Consumer Products
- [ ] Drugs
- [ ] Illicit Drugs
- [ ] Smoking&Vaping
- [ ] Pesticides
- [ ] Surfactants
- [ ] PFAS
- [ ] Food Products
- [ ] Hazardous Chemicals
- [x] Dyes
- [ ] Plastics
- [ ] Water
- [ ] Halocarbons
- [ ] Phenols
- [ ] Exposome
- [ ] Metabolites
- [ ] Biosolids
- [ ] Biosolids QCMix

Download

Reset Checkboxes

Input Data

Show 15



	DTX								Log(Koa)
1	DTXS							0.8	7.59
2	DTXS							2.03	5.21
3	DTXS							1.41	7.45
4	DTXS							0.59	7.59
5	DTXS							3.3	7.59
6	DTXS							0.58	11.69
7	DTXS							0.96	11.7
8	DTXS							-0.83	9.29
9	DTXS							0.53	10.61
10	DTXS							0.62	10.58
11	DTXS							2.28	8.47
12	DTXS							2.18	9.06
13	DTXS							1.83	6.25
14	DTXS							0.6	7.84
15	DTXSID1020350	2-Methoxy-5-methylaniline	120-71-8	C8H11NO	137.18	-1.42	-1.49	235.44	1.74	7.28

Showing 1 to 15 of 1,210 entries

Previous 1 2 3 4 5 … 81 Next

Each chemical substance is present in at least one category. Each chemical substance maps to a single chemical structure for the purpose of property prediction. Predicted properties were obtained from OPERA.

Tweak Ranges

Average Mass: 100 to 1000

Water Solubility (log(mol/L)): -14 to 3

Vapor Pressure (log(mmHg)): -14 to 10

Boiling Point (C): -170 to 550

Octanol Water Partition Coefficient (log(Kow)): -6 to 10.5

Octanol Air Partition Coefficient (log(Koa)): -1 to 12.5

Dataset Size

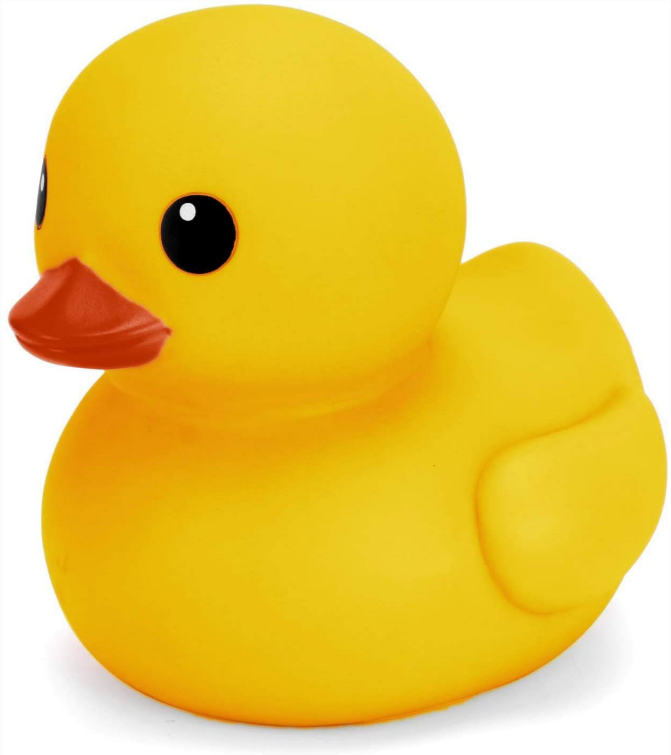
1210

Downloadable dataset matching filter criteria

	A	B	C	D	E	F	G	H	I	J	K	L
1	DTXSID	Preferred Name	CASRN	INCHIKEY	SMILES	Molecular Formula	Average M	Water Solubility (	Vapor Pressure	Boiling Point (	Log(Kow)	Log(Koa)
2	DTXSID2021238	Resorcinol	108-46-3	GHMLBKRAJCXXBS-UHFFFAOYSA-N	OC1=CC(O	C6H6O2	110.11	0.8	-3.32	279.96	0.8	7.59
3	DTXSID1021798	Quinoline	91-22-5	SMWDFEZZVXVKRB-UHFFFAOYSA-N	C1=CC2=C	C9H7N	129.16	-1.32	-1.22	237.23	2.03	5.21
4	DTXSID6025149	N,N-Dimethyl-p-phen	99-98-9	BZORFPDSXLZWJF-UHFFFAOYSA-N	CN(C)C1=C	C8H12N2	136.2	-0.99	-1.39	262.91	1.41	7.45
5	DTXSID7020716	Hydroquinone	123-31-9	QIGBRXMKCJKVMJ-UHFFFAOYSA-N	OC1=CC=C	C6H6O2	110.11	-0.18	-4.61	286.84	0.59	7.59
6	DTXSID6034972	Thymol	89-83-8	MGSRCZKZVOBKFT-UHFFFAOYSA-N	CC(C)C1=C	C10H14O	150.22	-2.26	-2.65	232.33	3.3	7.59
7	DTXSID1048700	Brilliant Green	633-03-4	NNBFNNNWANBMTI-UHFFFAOYSA-M	OS([O-])(=	C27H34N2O4S	482.64	-4.79	-7.68	365.26	0.58	11.69
8	DTXSID5020653	Gentian Violet	548-62-9	ZXJXZNDDNMQXFV-UHFFFAOYSA-M	[Cl-].CN(C	C25H30ClN3	407.99	-5.67	-7.69	353.08	0.96	11.7
9	DTXSID6021246	C.I. Basic Violet 14	632-99-5	NIKFYOSELWJIOF-SVFFXJIWSA-N	Cl.CC1=CC	C20H20ClN3	337.85	-2.17	-8.31	361.1	-0.83	9.29
10	DTXSID9020114	Auramine hydrochlor	2465-27-2	KSCQDDRPFHTIRL-UHFFFAOYSA-N	Cl.CN(C)C:	C17H22ClN3	303.83	-1.43	-6.69	330.53	0.53	10.61
11	DTXSID1025512	Malachite green	569-64-2	FDZZZRQASAIRJF-UHFFFAOYSA-M	[Cl-].CN(C	C23H25ClN2	364.92	-5.11	-6.28	354.56	0.62	10.58
12	DTXSID2020921	2-Naphthylamine	91-59-8	JBIJLHTVPXGSAM-UHFFFAOYSA-N	NC1=CC2=	C10H9N	143.19	-2.88	-3.59	300.04	2.28	8.47
13	DTXSID5020867	4,4'-Methylenebis(o-t	838-88-0	WECDUOXQLAIPQW-UHFFFAOYSA-N	CC1=C(N)C	C15H18N2	226.32	-2.86	-7.04	363.06	2.18	9.06
14	DTXSID9020295	4-Chloroaniline	106-47-8	QSNSCYSYFYORTR-UHFFFAOYSA-N	NC1=CC=C	C6H6ClN	127.57	-1.56	-1.56	231.92	1.83	6.25
15	DTXSID5041358	2,4-Diaminoanisole	615-05-4	BAHPQISAXRFLCL-UHFFFAOYSA-N	COC1=CC=	C7H10N2O	138.17	-0.39	-3.11	221.2	0.6	7.84
16	DTXSID1020350	2-Methoxy-5-methyla	120-71-8	WXWCDTXEKCVRRO-UHFFFAOYSA-N	COC1=CC=	C8H11NO	137.18	-1.42	-1.49	235.44	1.74	7.28
17	DTXSID1026164	2-Methylaniline	95-53-4	RNVCVTLRINQCPJ-UHFFFAOYSA-N	CC1=C(N)C	C7H9N	107.16	-0.83	-0.59	220.67	1.32	5.91
18	DTXSID3025091	C.I. Disperse Black 6	119-90-4	JRBJSXQPQWSCCF-UHFFFAOYSA-N	COC1=CC(	C14H16N2O2	244.29	-3.61	-8.33	356.03	1.81	9.11
19	DTXSID5023877	2-Anisidine	90-04-0	VMPITZXILSNTON-UHFFFAOYSA-N	COC1=CC=	C7H9NO	123.16	-0.99	-1.1	224.5	1.18	6.15
20	DTXSID0021094	4,4'-Oxydianiline	101-80-4	HLBLWEWZXPIGSM-UHFFFAOYSA-N	NC1=CC=C	C12H12N2O	200.24	-2.71	-6.13	350.06	1.36	8.36
21	DTXSID9021344	4,4'-Thiodianiline	139-65-1	ICNFHJVPAJKPHW-UHFFFAOYSA-N	NC1=CC=C	C12H12N2S	216.3	-2.64	-6.17	360.98	2.18	9.03
22	DTXSID6022422	4,4'-Diaminobiphenyl	101-77-9	YBRVSVVVWCFQMG-UHFFFAOYSA-N	NC1=CC=C	C13H14N2	198.27	-2.3	-5.48	397.84	1.59	8.38

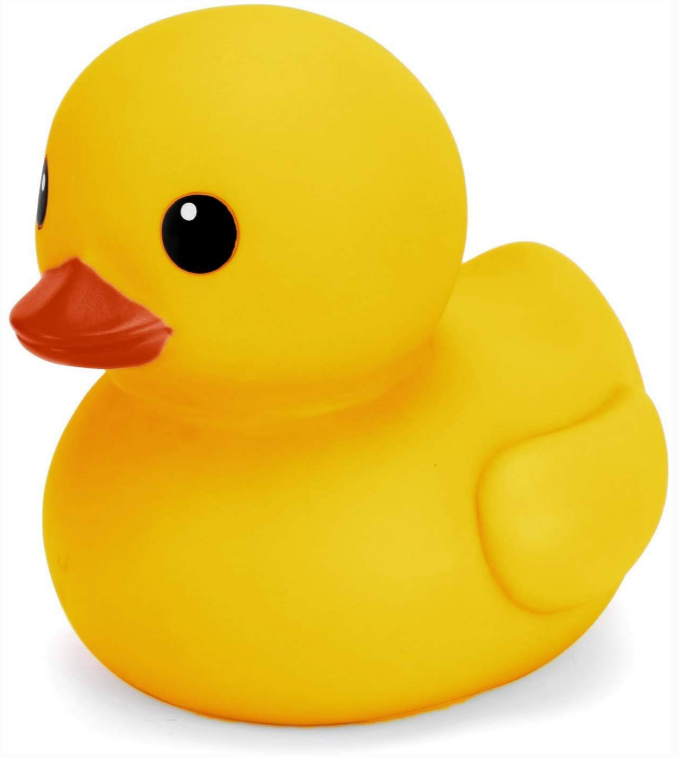
ChemSpace_output

Suspect screening example



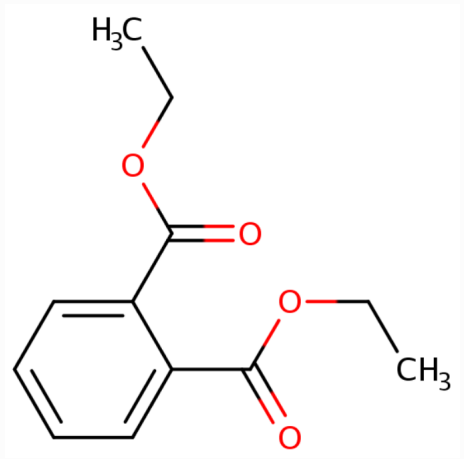
Suspect screening example

- We would like to see if plasticizers(phthalates) are in our rubber ducky.
- We own an LC-MS instrument.
- We resolve a spectrum to a formula of $C_{12}H_{14}O_4$.
- 315 potential structures based on a search of the CompTox Chemicals Dashboard.
  - This is the entirety of our ***identifiable space.***

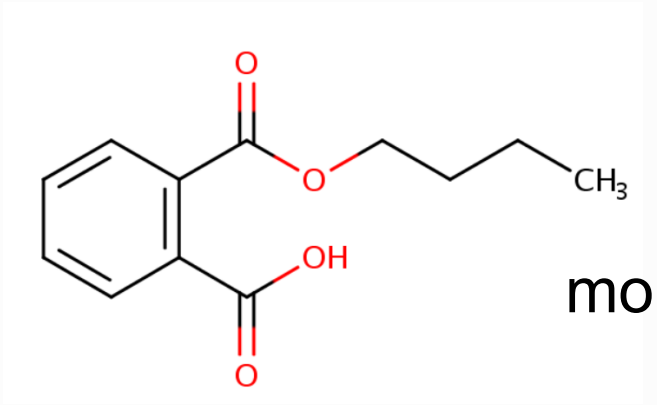


Suspect screening example

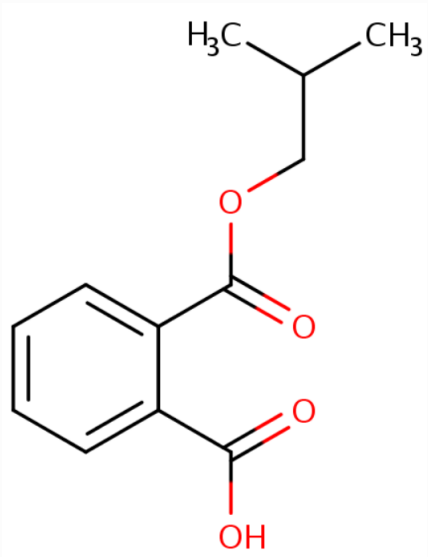
A spectrum is resolved to $C_{12}H_{14}O_4$, which could match a many of the structures, including:



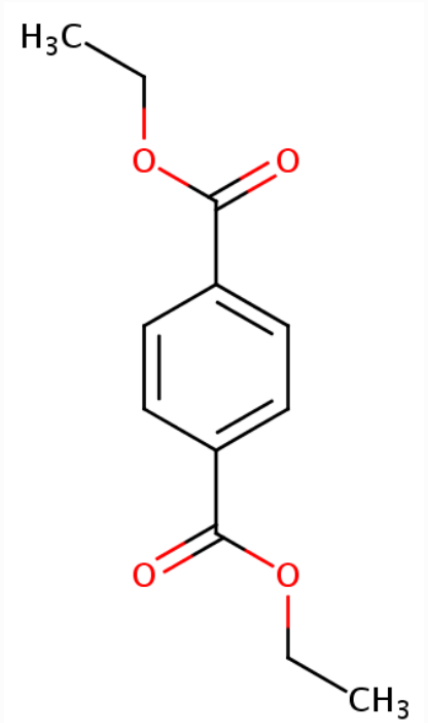
diethyl phthalate



monobutyl phthalate



monoisobutyl phthalate



diethyl terephthalate

Suspect screening example

A spectrum is resolved to $C_{12}H_{14}O_4$, which could match many structures, including:

ChemSpace Tool

Categories

- Consumer Products
- Drugs
- Illicit Drugs
- Smoking&Vaping
- Pesticides
- Surfactants
- PFAS
- Food Products
- Hazardous Chemicals
- Dyes
- Plastics
- Water
- Halocarbons
- Phenols
- Exposome
- Metabolites
- Biosolids
- Biosolids QCMix

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Reset Checkboxes

Input Data | Average Mass | Water Solubility | Vapor Pressure | Boiling Point | LogKow | LogKoa

Show 15 entries Search: C12H14O4

	DTXSID	Preferred Name	CASRN	Molecular Formula	Average Mass	Water Solubility (log(mol/L))	Vapor Pressure (log(mmHg))	Boiling Point (C)	Log(Kow)	Log(Koa)
2742	DTXSID40214422	Salicylic acid, valerate	64206-54-8	C12H14O4	222.24	-2.6	-6.21	304.79	2.34	9.04
4144	DTXSID40440007	2-Propen-1-one, 1-(3,4,5-trimethoxyphenyl)-	106331-50-4	C12H14O4	222.24	-2.28	-4.55	294.81	1.38	7.26
8503	DTXSID5052701	Monoisobutyl phthalate	30833-53-5	C12H14O4	222.24	-1.96	-6.1	304.08	2.37	9.28
14932	DTXSID4040002	Monobutyl phthalate	131-70-4	C12H14O4	222.24	-1.97	-6.21	304.76	2.37	9.04
17907	DTXSID7021780	Diethyl phthalate	84-66-2	C12H14O4	222.24	-2.33	-2.68	299.64	2.44	6.75
23298	DTXSID8060909	Diethyl terephthalate	636-09-9	C12H14O4	222.24	-2.67	-2.72	299.64	2.37	6.75
24833	DTXSID30232918	5-(Isopropyl)-4-methylphthalic acid	84029-87-8	C12H14O4	222.24	-2.59	-5.92	317.77	2.47	8.14
25831	DTXSID40992258	Methyl (4-hydroxy-3-propanoylphenyl)acetate	71662-41-4	C12H14O4	222.24	-1.73	-6.61	314.11	2.23	8.98
26323	DTXSID80221352	Ethyl 1,3-benzodioxole-5-propionate	7116-48-5	C12H14O4	222.24	-2.62	-4.26	283.39	2.14	7.55
26807	DTXSID00194019	Ethyl 3-oxo-4-phenoxybutyrate	41051-18-7	C12H14O4	222.24	-1.85	-2.9	294.86	2.06	7.42
27717	DTXSID5062683	Benzenepropanoic acid, 4-methoxy-.beta.-oxo-, ethyl ester	2881-83-6	C12H14O4	222.24	-2.39	-2.77	294.97	2.22	7.42
28190	DTXSID20987268	But-2-yne-1,4-diyl bis(2-methylprop-2-enoate)	67905-43-5	C12H14O4	222.24	-1.51	-2.56	256.74	1.87	5.72
28723	DTXSID1057826	Dimecrotic acid	7706-67-4	C12H14O4	222.24	-2.4	-4.67	306.33	2.31	9.04
30683	DTXSID50995538	2-Methylpropyl 2H-1,3-benzodioxole-5-carboxylate	74098-26-3	C12H14O4	222.24	-2.82	-4.21	287.24	2.25	7.26
30831	DTXSID1044851	2-Hydroxy-3-phenoxypropyl prop-2-enoate	16969-10-1	C12H14O4	222.24	-1.1	-5.24	314.25	2.15	9.22

Showing 1 to 15 of 35 entries (filtered from 79,021 total entries) Previous 1 2 3 Next

Suspect screening example

A spectrum is resolved to $C_{12}H_{14}O_4$, which could match many structures, including:

ChemSpace Tool

Categories

- [x] Consumer Products
- [ ] Drugs
- [ ] Illicit Drugs
- [ ] Smoking&Vaping
- [ ] Pesticides
- [ ] Surfactants
- [ ] PFAS
- [ ] Food Products
- [ ] Hazardous Chemicals
- [ ] Dyes
- [ ] Plastics
- [ ] Water
- [ ] Halocarbons
- [ ] Phenols
- [ ] Exposome
- [ ] Metabolites
- [ ] Biosolids
- [ ] Biosolids QCMix

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Reset Checkboxes

Input Data | Average Mass | Water Solubility | Vapor Pressure | Boiling Point | LogKow | LogKoa

Show 15 entries Search: C12H14O4

	DTXSID	Preferred Name	CASRN	Molecular Formula	Average Mass	Water Solubility (log(mol/L))	Vapor Pressure (log(mmHg))	Boiling Point (C)	Log(Kow)	Log(Koa)
3837	DTXSID5052701	Monoisobutyl phthalate	30833-53-5	C12H14O4	222.24	-1.96	-6.1	304.08	2.37	9.28
5914	DTXSID4040002	Monobutyl phthalate	131-70-4	C12H14O4	222.24	-1.97	-6.21	304.76	2.37	9.04
6916	DTXSID7021780	Diethyl phthalate	84-66-2	C12H14O4	222.24	-2.33	-2.68	299.64	2.44	6.75
8602	DTXSID8060909	Diethyl terephthalate	636-09-9	C12H14O4	222.24	-2.67	-2.72	299.64	2.37	6.75
10208	DTXSID1057826	Dimecrotic acid	7706-67-4	C12H14O4	222.24	-2.4	-4.67	306.33	2.31	9.04
10807	DTXSID1044851	2-Hydroxy-3-phenoxypropyl prop-2-enoate	16969-10-1	C12H14O4	222.24	-1.1	-5.24	314.25	2.15	9.22
11997	DTXSID5027277	1,3-Benzenedicarboxylic acid, diethyl ester	636-53-3	C12H14O4	222.24	-2.54	-2.72	299.64	2.33	6.75
13115	DTXSID8063917	Piperonyl isobutyrate	5461-08-5	C12H14O4	222.24	-2.62	-4.2	287.24	2.14	7.26
14844	DTXSID4041236	5-Allyl-4,7-dimethoxy-1,3-benzodioxole	523-80-8	C12H14O4	222.24	-2.77	-4.53	289.5	1.02	7.25
15064	DTXSID9047201	4-Formyl-2-methoxyphenyl isobutyrate	20665-85-4	C12H14O4	222.24	-2.65	-2.35	285.64	2.24	7.23
18205	DTXSID2020470	Diglycidyl resorcinol ether	101-90-6	C12H14O4	222.24	-2.42	-4.54	295.72	1.7	7.43
18255	DTXSID20863735	1,2-Ethanediol, 1-phenyl-, 1,2-diacetate	6270-03-7	C12H14O4	222.24	-2.61	-2.77	289.68	2.27	6.9
21764	DTXSID1047150	tert-Butyl hydrogen phthalate	33693-84-4	C12H14O4	222.24	-1.97	-6.03	303.53	1.84	9.21
26499	DTXSID80862007	Dill apiole	484-31-1	C12H14O4	222.24	-2.8	-4.53	289.5	1.03	7.25

Showing 1 to 14 of 14 entries (filtered from 27,491 total entries) Previous 1 Next

LC-MS amenability predictions can aid *detectable space*

Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis

Charles N. Lowe, Kristin K. Isaacs, Andrew McEachran, Christopher M. Grulke, Jon R. Sobus, Elin M. Ulrich, Ann Richard, Alex Chao, John Wambaugh & Antony J. Williams

Analytical and Bioanalytical Chemistry **413**, 7495–7508 (2021) | Cite this article

DTXSID	Preferred Name	SMILES	ESI+ Amenability	ESI+ Amenability Probability	ESI- Amenability	ESI- Amenability Probability
DTXSID5052701	Monoisobutyl phthalate	CC(C)COC(	Amenable	0.566	Amenable	0.617
DTXSID4040002	Monobutyl phthalate	CCCCOC(=	Amenable	0.562	Amenable	0.551
DTXSID7021780	Diethyl phthalate	CCOC(=O)	Unamenable	0.326	Unamenable	0.141
DTXSID8060909	Diethyl terephthalate	CCOC(=O)	Unamenable	0.275	Unamenable	0.121
DTXSID1057826	Dimecrotic acid	COC1=CC(	Amenable	0.759	Amenable	0.672
DTXSID1044851	2-Hydroxy-3-phenoxypropyl prop-2-enoate	OC(COC(=	Unamenable	0.256	Unamenable	0.159
DTXSID5027277	1,3-Benzenedicarboxylic acid, diethyl ester	CCOC(=O)	Unamenable	0.296	Unamenable	0.163
DTXSID8063917	Piperonyl isobutyrate	CC(C)C(=O	Unamenable	0.47	Unamenable	0.111
DTXSID4041236	5-Allyl-4,7-dimethoxy-1,3-benzodioxole	COC1=CC(	Amenable	0.625	Unamenable	0.141
DTXSID9047201	4-Formyl-2-methoxyphenyl isobutyrate	COC1=C(O	Amenable	0.527	Unamenable	0.197
DTXSID2020470	Diglycidyl resorcinol ether	C(OC1=CC	Unamenable	0.373	Unamenable	0.134
DTXSID20863735	1,2-Ethanediol, 1-phenyl-, 1,2-diacetate	CC(=O)OC	Unamenable	0.418	Unamenable	0.161
DTXSID1047150	tert-Butyl hydrogen phthalate	CC(C)(C)O	Amenable	0.557	Amenable	0.619
DTXSID80862007	Dill apiole	COC1=C(O	Amenable	0.644	Unamenable	0.153

Conclusions

- Benefits of understanding coverage of chemical space in NTA
  - Reduced method development time
  - Improved structure annotation/prioritization
  - Context for results based on chosen method
- Development of a ChemSpace Tool will continue in collaboration with analytical scientists
- A manuscript describing the vision of this tool has been submitted for peer review
  - A proof-of-concept tool is currently under development (which has been shown here)


Thank you for
Listening!