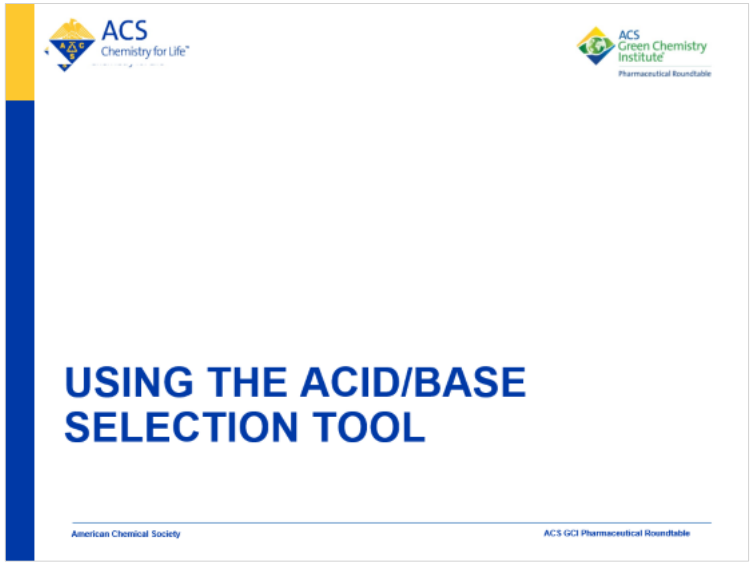
American Chemical Society

ACS GCI Pharmaceutical Roundtable

Acid/Base Selection Tool

User Guide: Charlotte Dalton, CatSci, March 2023

Update: Vittoria Valentine, ACS GCI, October 2024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USING THE ACID/BASE SELECTION TOOL
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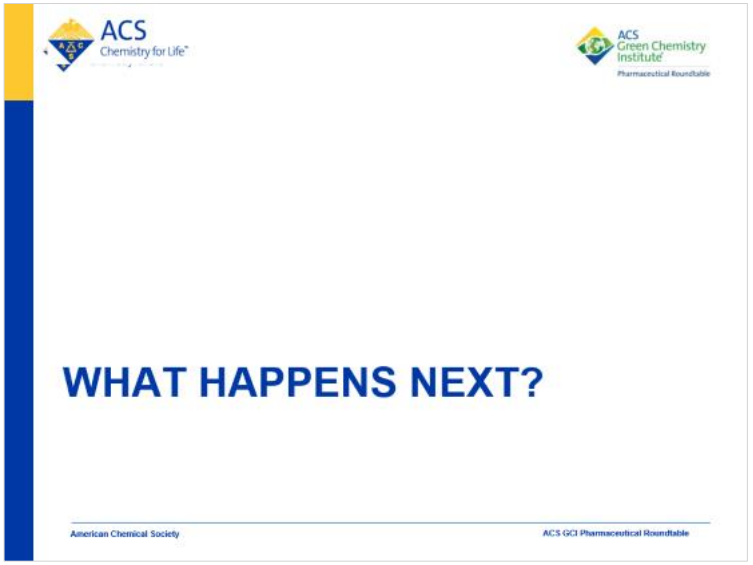
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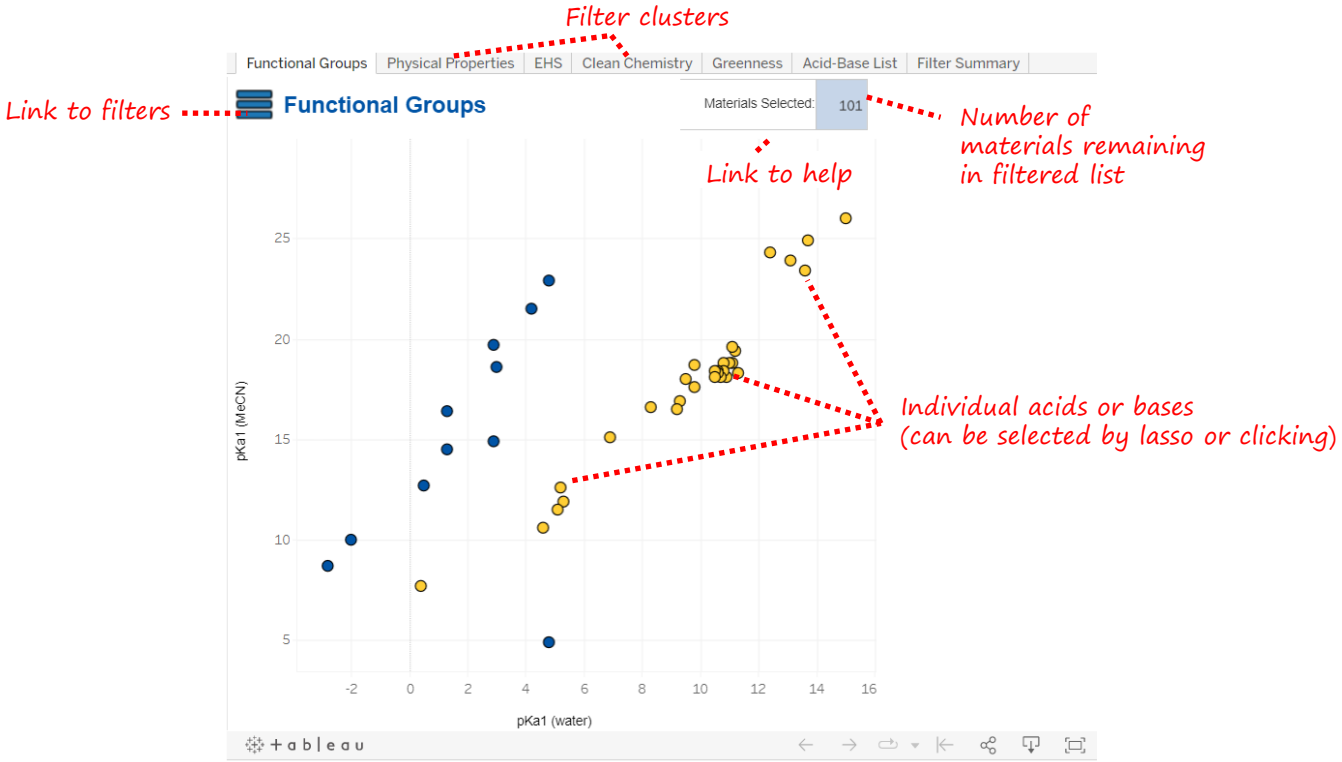
USING THE ACID/BASE SELECTION TOOL

- The Acid/Base Selection tool is similarly formatted to the ACS GCIPR Solvent Selection Tool

- This guide will outline how to use the tool and explain the different tabs of the tool
  - Functional Groups
  - Physical Properties
  - EHS
  - Clean Chemistry
  - Greenness
  - Acid/Base List
  - Filter Summary

The User Interface

- The online tool is built around Tableau™
  - Graphical distribution of acids and bases across pKa values (water and MeCN)
  - Note that materials which do not have a pKa (MeCN) listed in the data set can only be seen on the 'Acid-Base List'



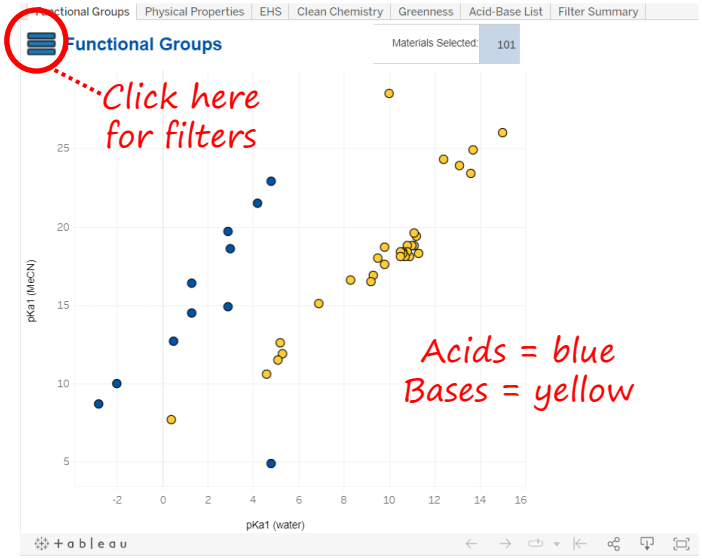
Functional Groups

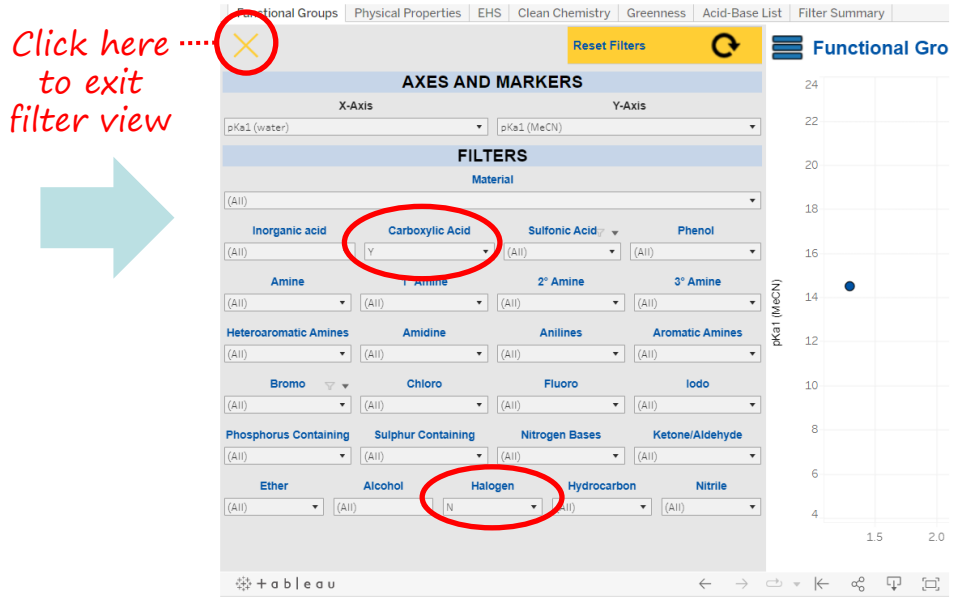
This first tab of the tool allows filtering by functional groups

E.g. the user may wish to find amine bases, or avoid halogenated materials

Change the relevant filters in the Functional Groups from ***ALL*** to ***Y*** or ***N***

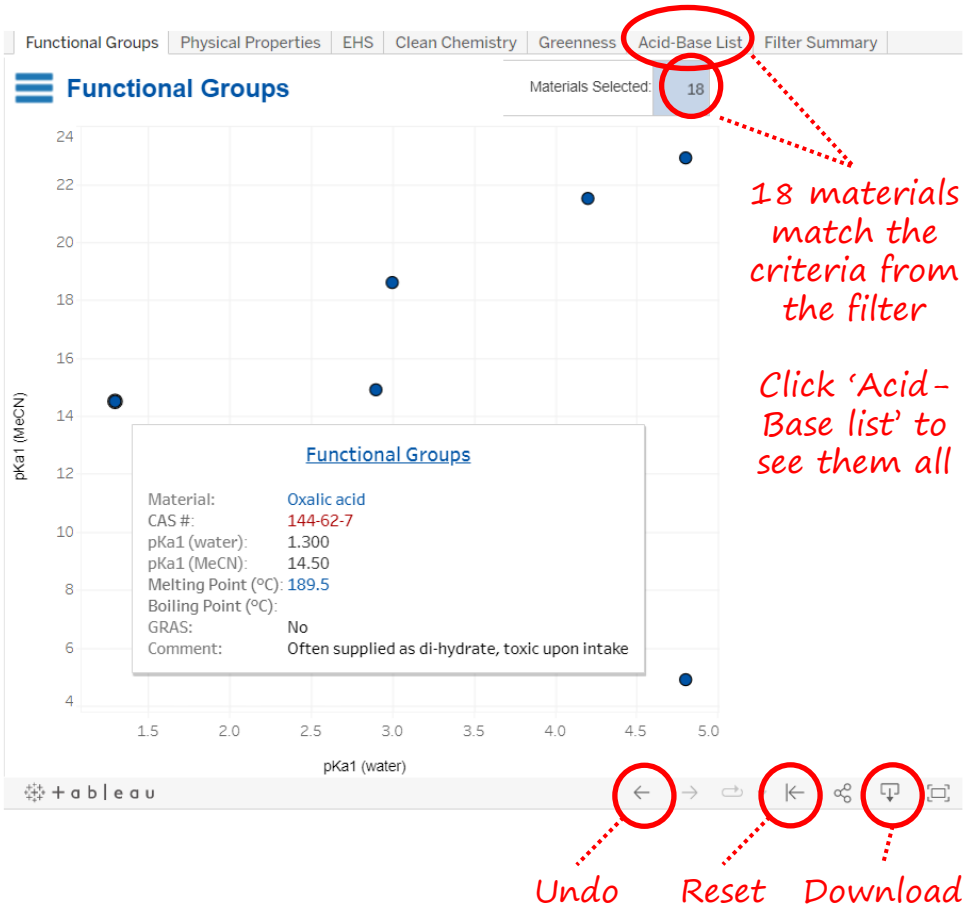
Combination of filters can be applied e.g. must be a carboxylic acid but no halogen functionality





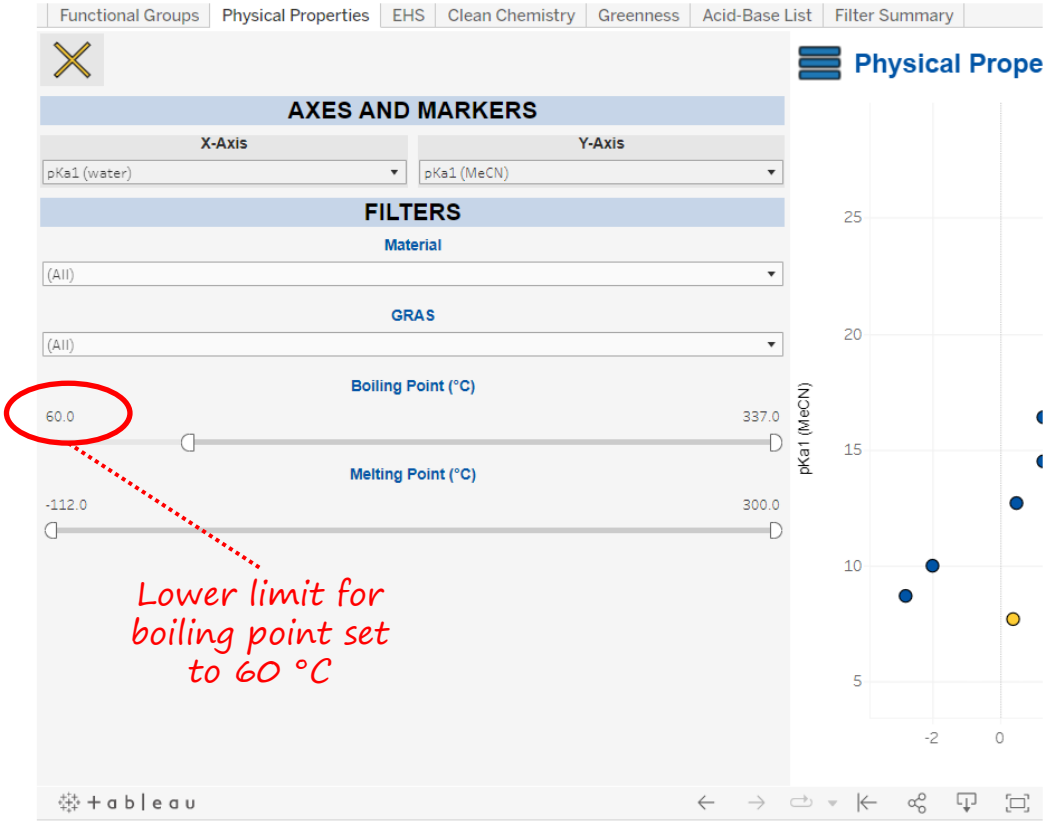
Functional Groups

- The resulting plot shows the acids/bases that meet the selected criteria
- Hover over each point to obtain the details of the material
  - Note – some materials may not be displayed if pKa data in **both** MeCN and water not available
  - Use ‘Acid-Base list’ to see all the materials meeting the selected filters
- Tableau tools allow you to undo, reset the view, download



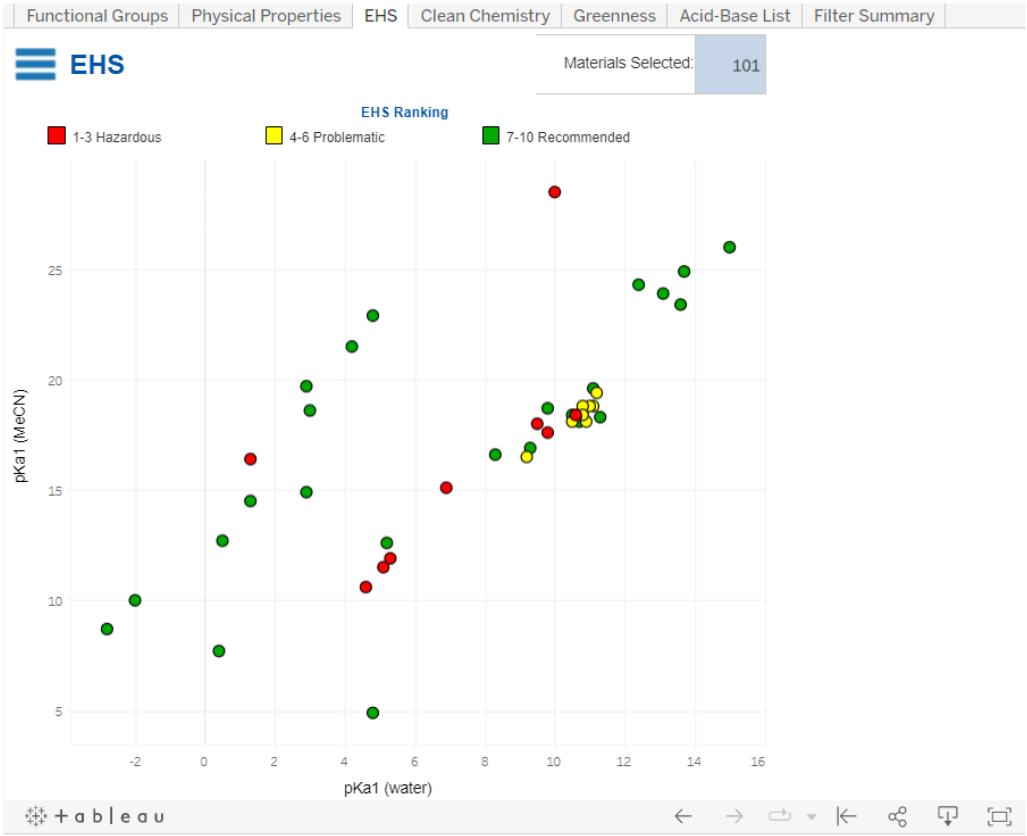
Physical Properties

- Alter numerical filters for boiling point and/or melting point by moving the sliders or typing numerical values
- Boiling point/melting point can be adjusted to identify materials that meet the processing requirements



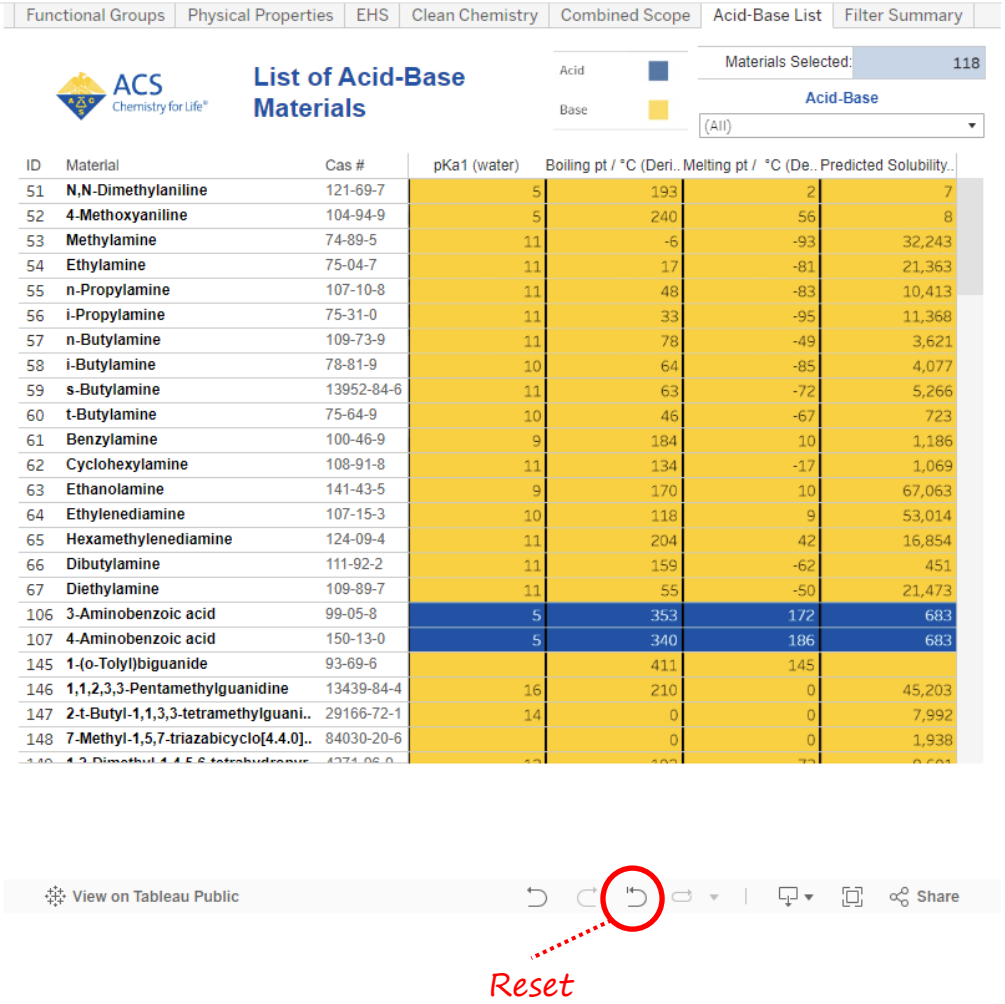
EHS, Clean Chemistry and Greenness

- These sections score the acids and bases in the tool on:
  - EHS
  - Clean Chemistry
  - Greenness
- Red colour indicates the most undesirable materials to use
- See ***Green Chem.***, 2015, **17**, 945-949 for further details



Acid-Base List

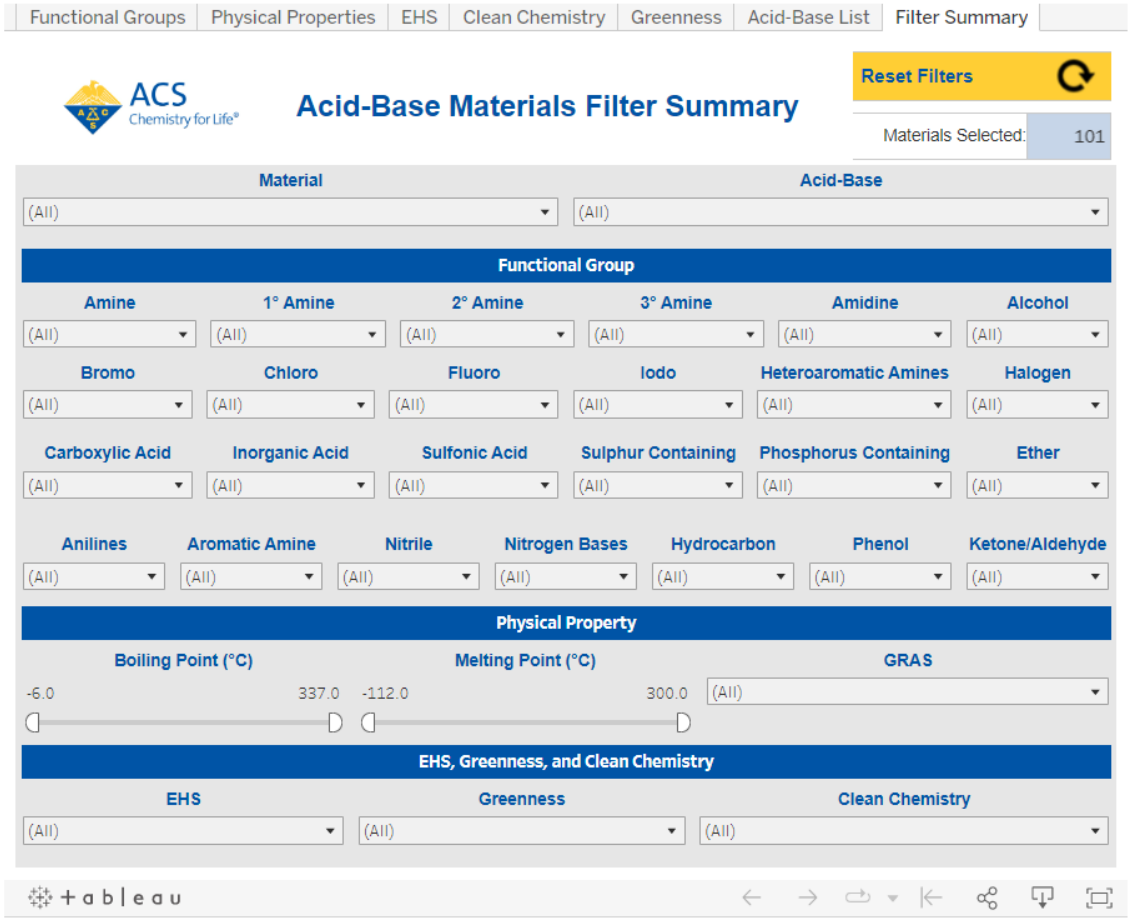
- List shows all of the acids and bases that meet all filters which have been applied
  - Acids in blue and bases in yellow
- To see the full list, use the reset button at the bottom of the screen
  - 101 materials present in the current version of the tool



ID	Material	Cas #	pKa1 (water)	Boiling pt / °C (Deri..	Melting pt / °C (De..	Predicted Solubility..
51	N,N-Dimethylaniline	121-69-7	5	193	2	7
52	4-Methoxyaniline	104-94-9	5	240	56	8
53	Methylamine	74-89-5	11	-6	-93	32,243
54	Ethylamine	75-04-7	11	17	-81	21,363
55	n-Propylamine	107-10-8	11	48	-83	10,413
56	i-Propylamine	75-31-0	11	33	-95	11,368
57	n-Butylamine	109-73-9	11	78	-49	3,621
58	i-Butylamine	78-81-9	10	64	-85	4,077
59	s-Butylamine	13952-84-6	11	63	-72	5,266
60	t-Butylamine	75-64-9	10	46	-67	723
61	Benzylamine	100-46-9	9	184	10	1,186
62	Cyclohexylamine	108-91-8	11	134	-17	1,069
63	Ethanolamine	141-43-5	9	170	10	67,063
64	Ethylenediamine	107-15-3	10	118	9	53,014
65	Hexamethylenediamine	124-09-4	11	204	42	16,854
66	Dibutylamine	111-92-2	11	159	-62	451
67	Diethylamine	109-89-7	11	55	-50	21,473
106	3-Aminobenzoic acid	99-05-8	5	353	172	683
107	4-Aminobenzoic acid	150-13-0	5	340	186	683
145	1-(o-Tolyl)biguanide	93-69-6		411	145	
146	1,1,2,3,3-Pentamethylguanidine	13439-84-4	16	210	0	45,203
147	2-t-Butyl-1,1,3,3-tetramethylguani..	29166-72-1	14	0	0	7,992
148	7-Methyl-1,5,7-triazabicyclo[4.4.0]..	84030-20-6		0	0	1,938

Filter Summary

- Contains all filter selections in the tool
- May be a useful place to start for users with multiple filters to apply
  - Can apply multiple filters without moving between tabs in the tool
  - Then once filters are applied, move to the Acid-Base list or other tabs to visualise the suitable materials



WHAT HAPPENS NEXT?

What Happens Next?

- Encourage member organisations and the wider community to use the tool to enable acid and base selection
  - Feedback to be collected from users

- Further develop the tool by including more materials and more data
  - Call for any member companies who have data sets which could be included in the next version