



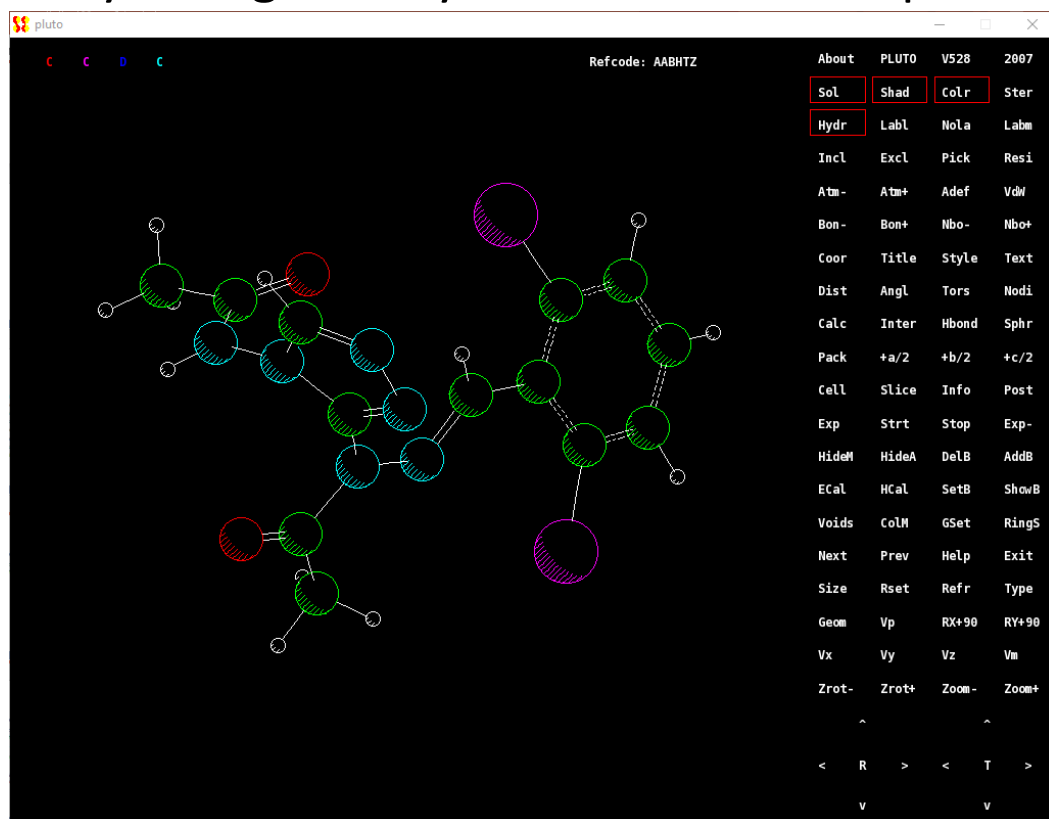
Exploring Mercury

Elna Pidcock



Mercury

- First released September 2001
- Visualisation, particularly of organic crystal structures. Replacement for Pluto...



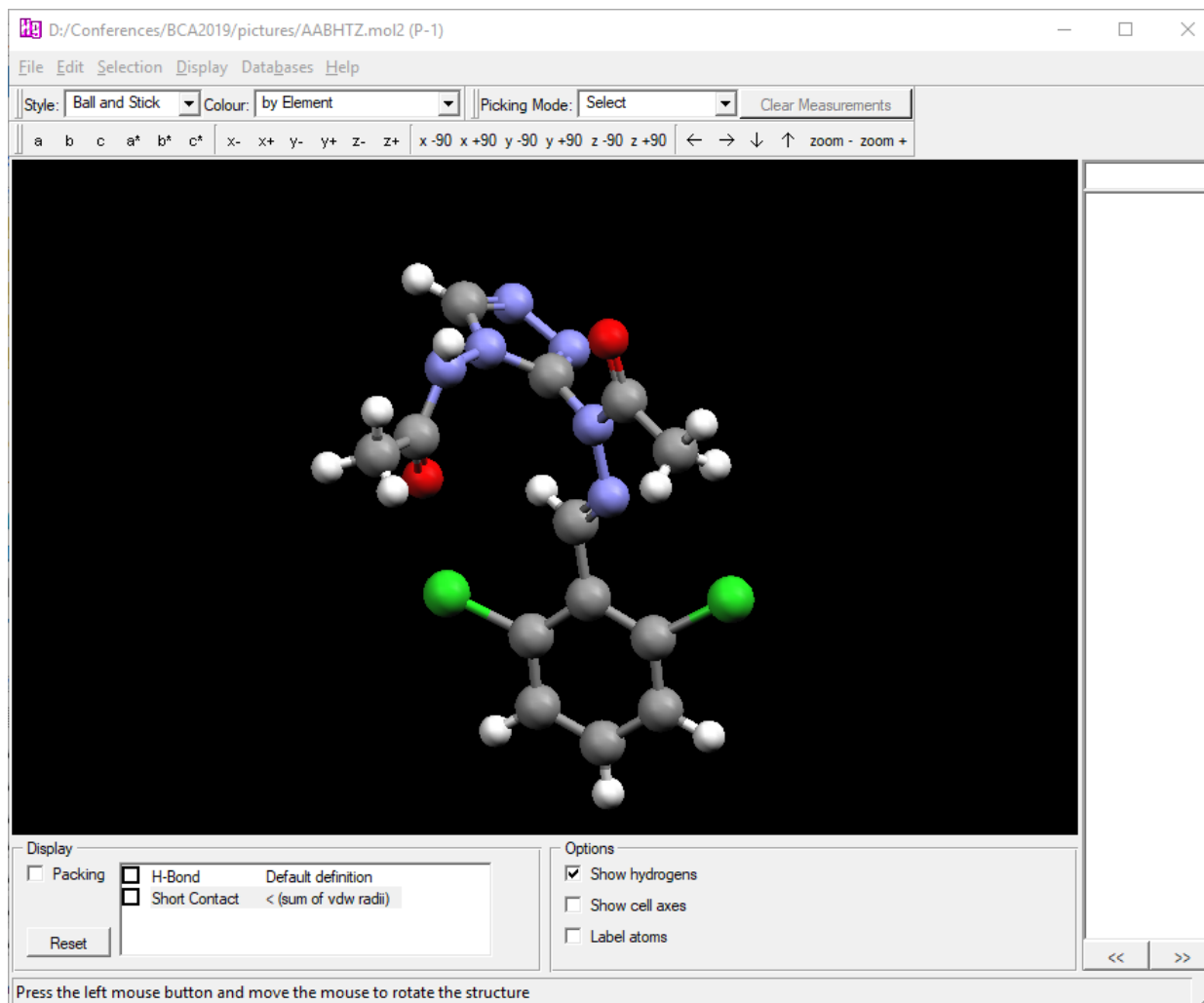


Mercury

- First released September 2001
- Visualisation, particularly of organic crystal structures. Replacement for Pluto...
- Grown significantly during that time:
 - A hub for components of the CSD System
 - Can search the CSD in a number of ways within Mercury
 - from visualisation to interrogation and exploration...



Mercury 1.0, 2001





Mercury 4.0, 2019

AABHTZ (P-1) - CSD-Enterprise

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Move Labels Clear Measurements Show Labels for Non C,H with Atom Label

Style: Ball and Stick Colour: by Element Manage Styles... Work Atom selections:

Animate... Default view: b a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: c

Structure Navigator

AABHTZ Find

Crystal Structures Spacegroup

Databases

CSD 5.40

- AABHTZ P-1
- AACANI10 P21/c
- AACANI11 P21/c
- AACFAZ Pbcn
- AACFAZ10 Pbcn
- AACMAL P21/c
- AACMHX10 Pbca
- AACRHA Pnmc
- AACRHC P-1
- AACRUB Cc
- AACRUB01 C2/c
- AADAMC P21/c
- AADMPY P-1
- AADMPY10 P-1
- AADRIB P21
- AAGAGG10 P212121
- AAGGAG10 P21
- AALCFE P21/c
- AALPRO P21/c
- AAMAND P212121
- AAMTCCO P-1
- AAMTCCO10 P-1
- AAMTXP P21/n
- AANHOX Pna21

Tree View

Multiple Structures Structures...

Display Options

Display

- Packing
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond User defined

Contacts... More Info Powder... Reset

Options

- Show hydrogens
- Depth cue
- Show cell axes
- Z-Clipping
- Label atoms
- Stereo

Press the left mouse button and move the mouse to rotate the structure



Some overlooked features? Some favourites...



It's the simple things

- Do you load .cif files into Mercury a lot?

AACANI11 (P21/c) - CSD-Enterprise

File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help

Open... Ctrl+O

Recent Files

Sketch Molecule... Ctrl+K

Auto Edit Structure on Load

Save As... Ctrl+S

POV-Ray Image...

Print in 3D...

Exit Ctrl+Q

Clear Measurements Show Labels for All atoms with Atom Label

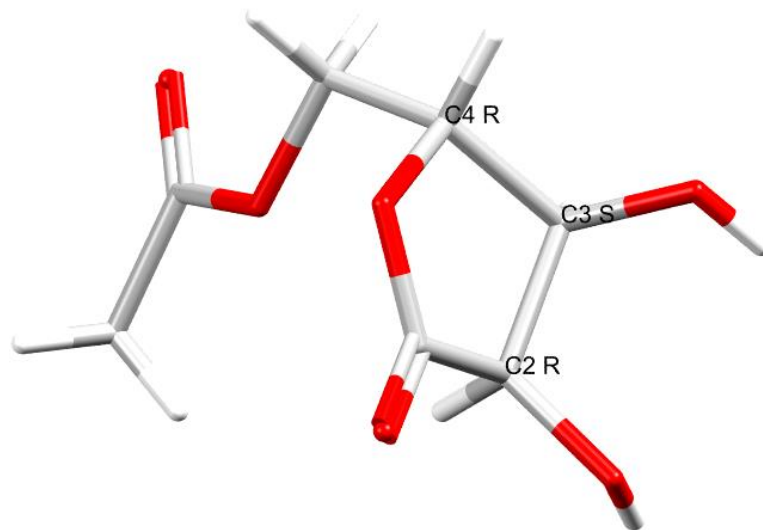
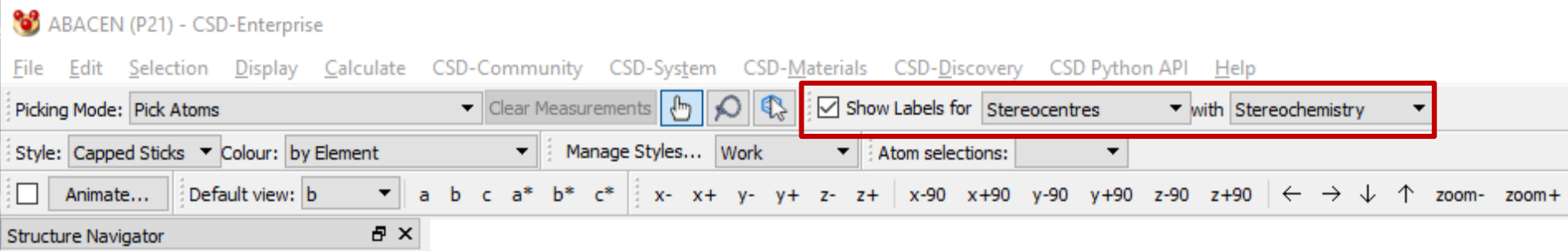
Suppression Manage Styles... Work Atom selections:

a b c a* b* c* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+



It's the simple things

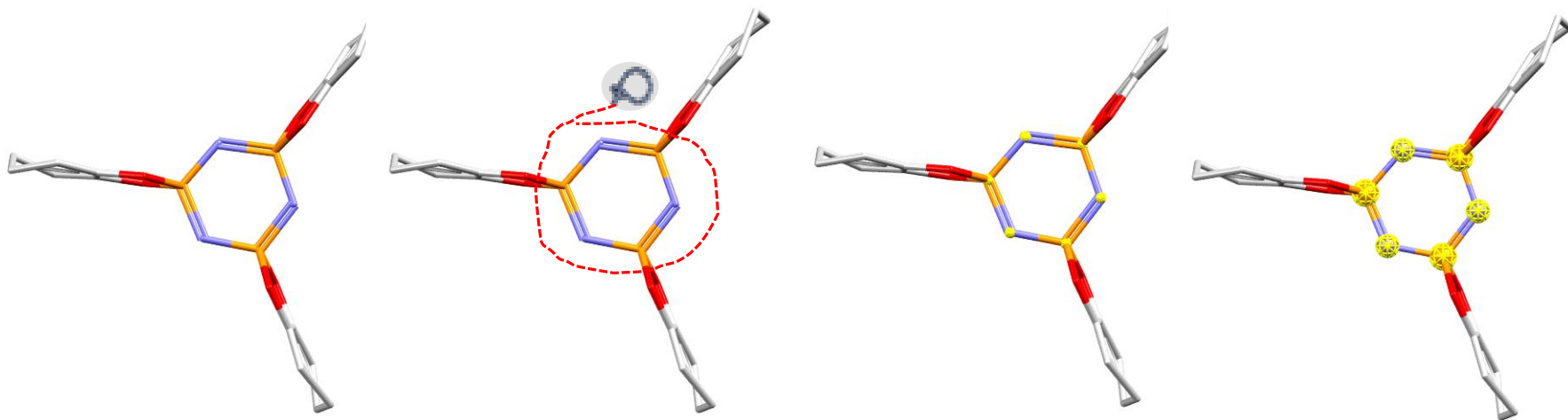
- Do you look at chiral molecules a lot?





It's the simple things

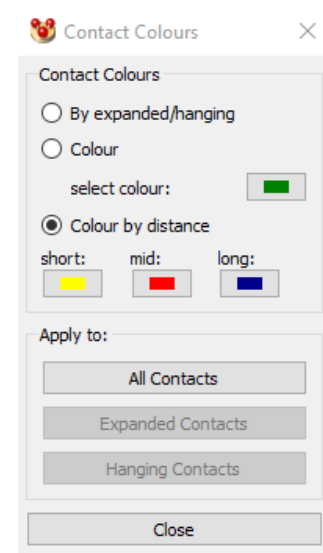
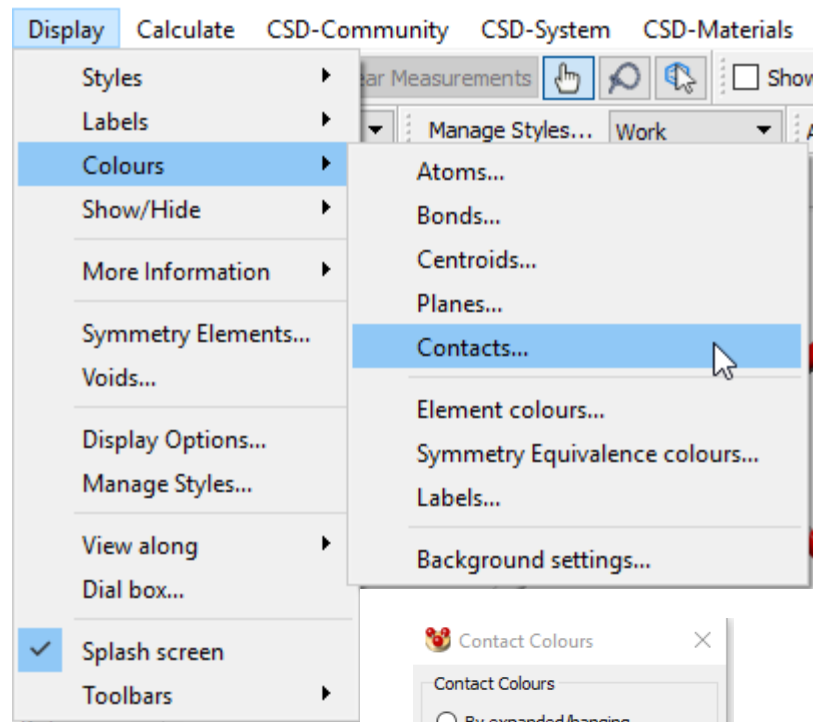
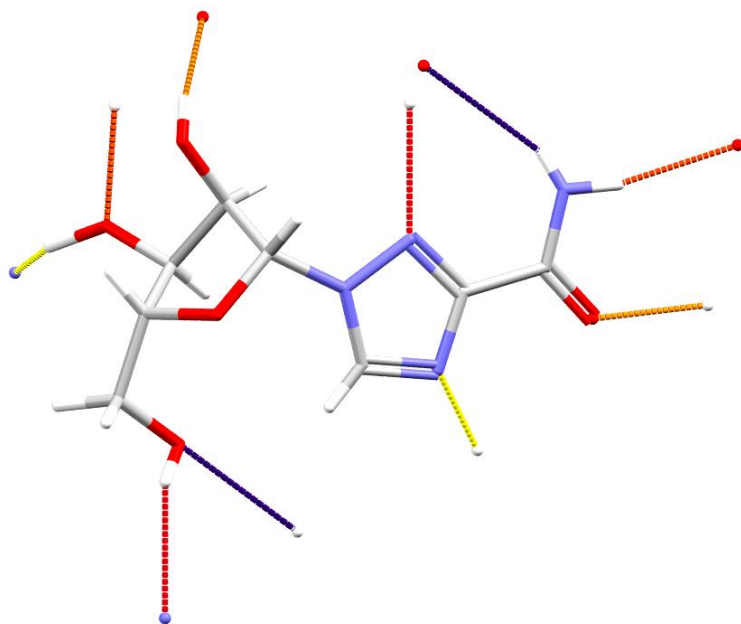
- Do you select parts of molecules often (to change display styles for example?)
- Alt-Left Mouse button invokes lasso selection





It's the simple things

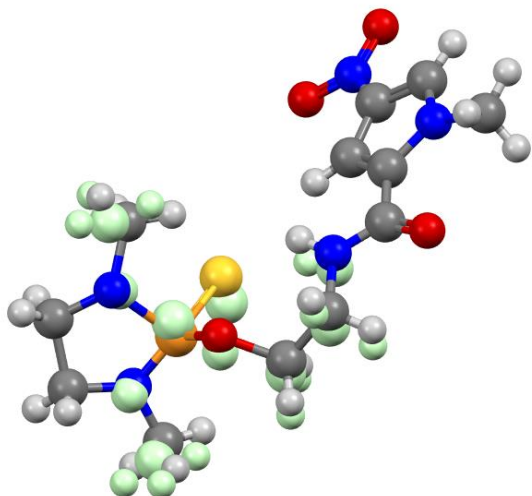
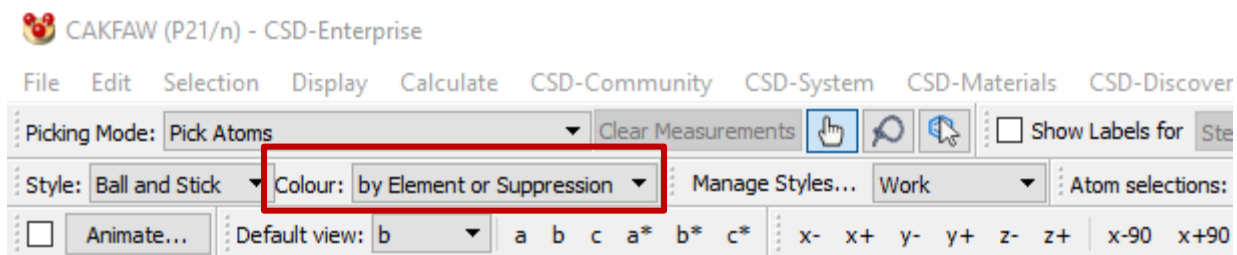
- Do you look at hydrogen bonds a lot?
- Colour by distance



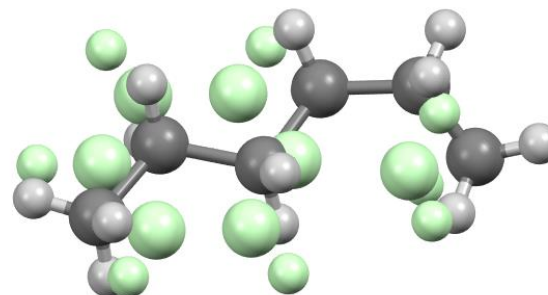


It's the simple things

- Disordered structures?



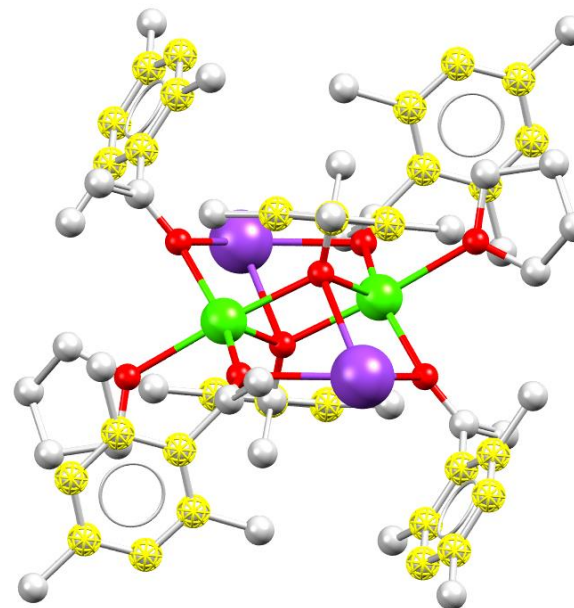
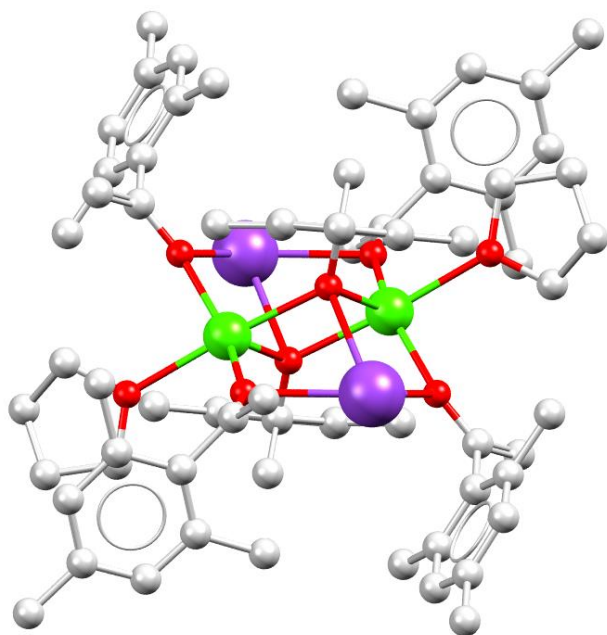
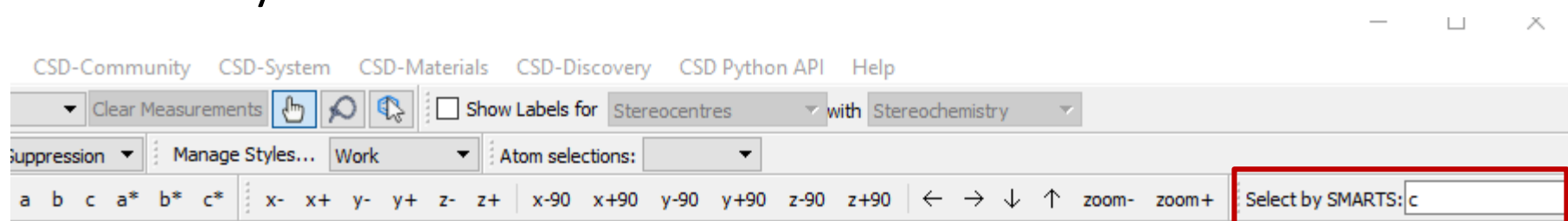
“Suppression” is our term for disordered atoms





It's the simple things

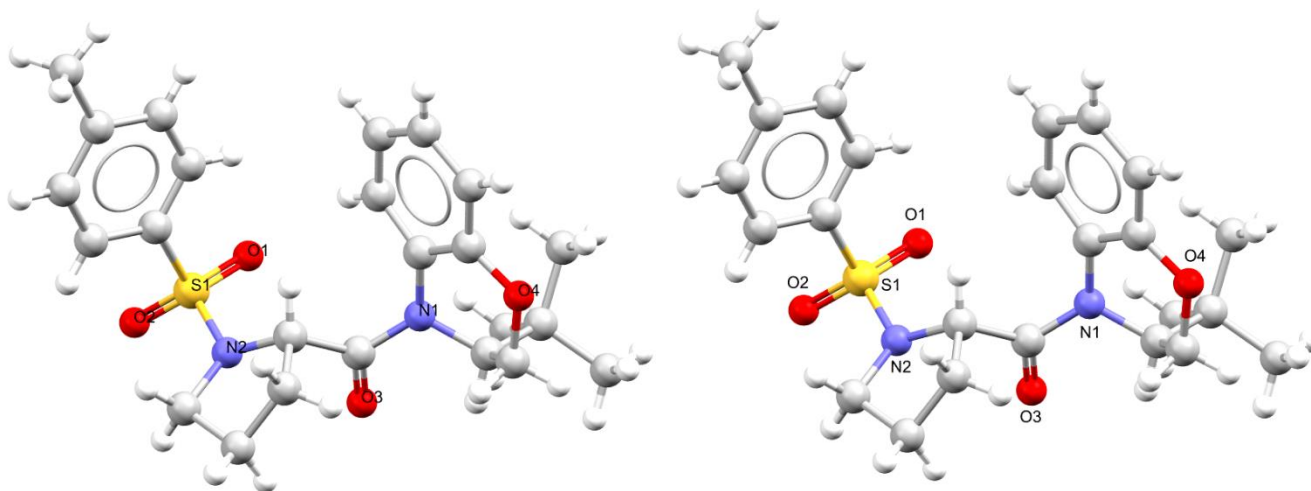
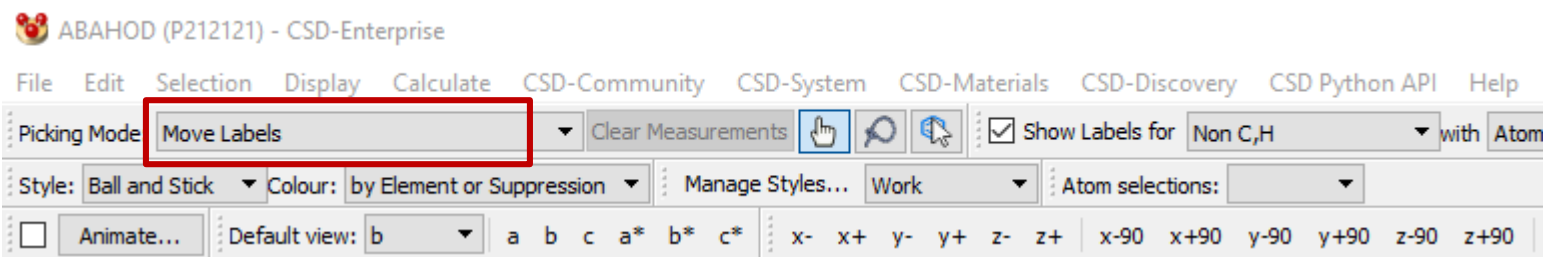
- Select by SMARTS





It's the simple things

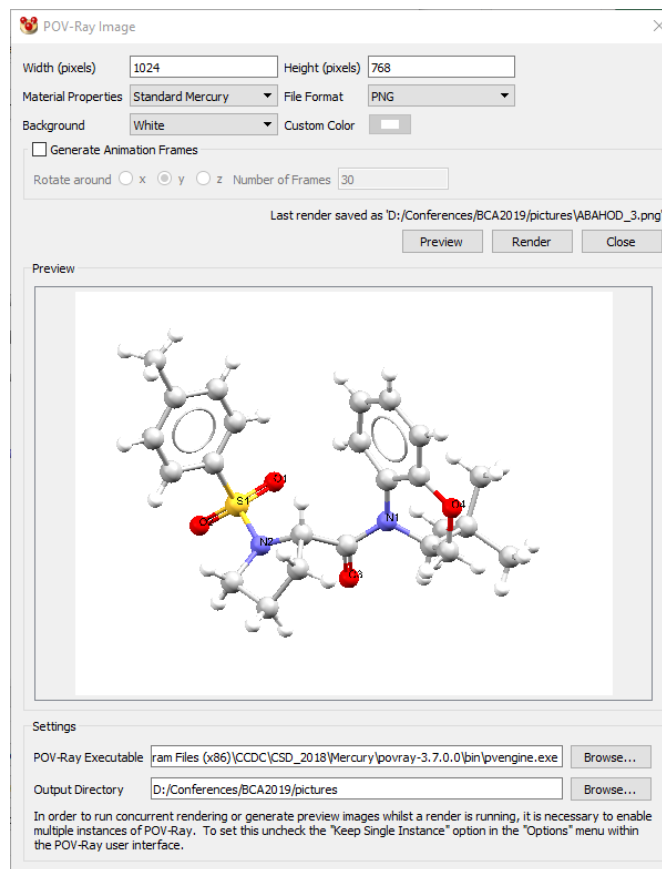
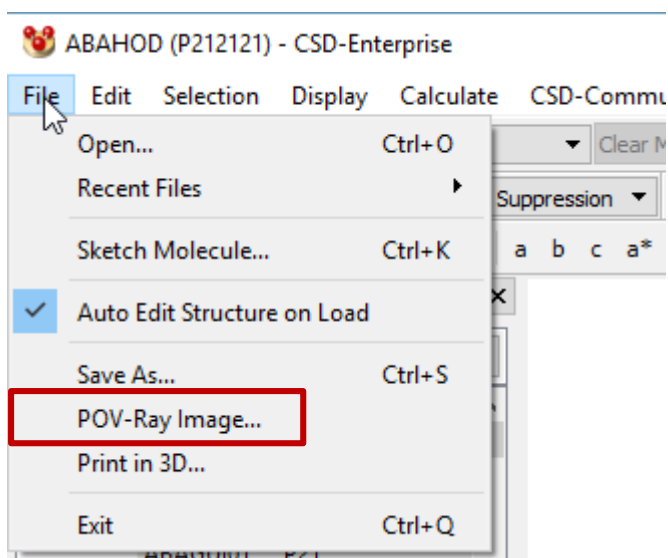
- Make pictures for publications or slides?





It's the simple things

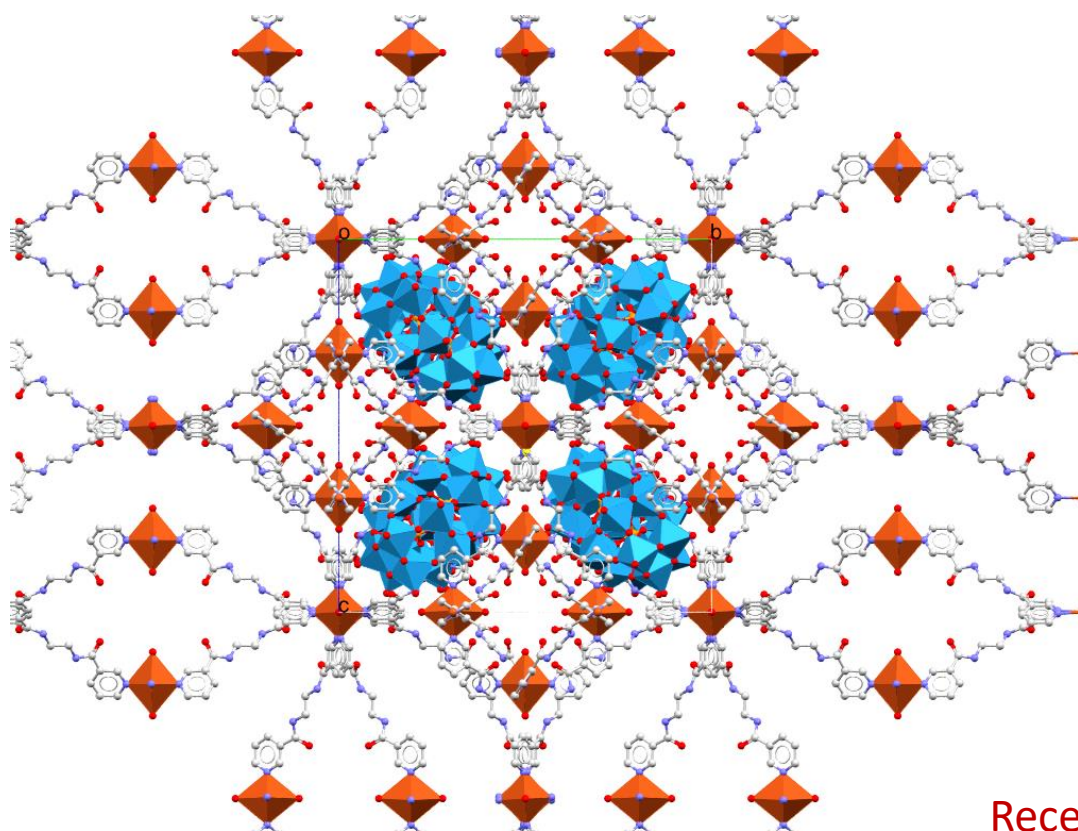
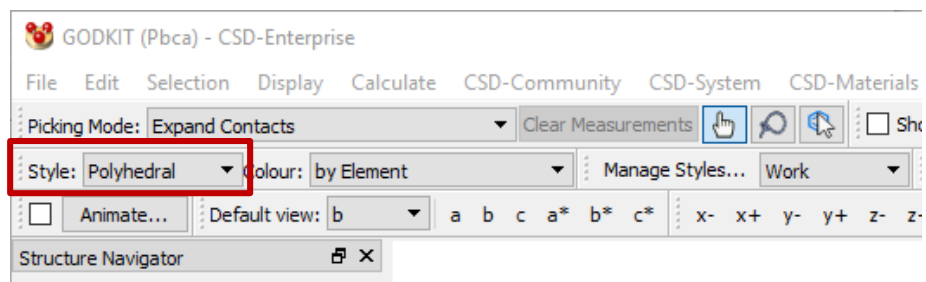
- Make pictures for publications or slides?





It's the simple things

- Work with coordination metals?

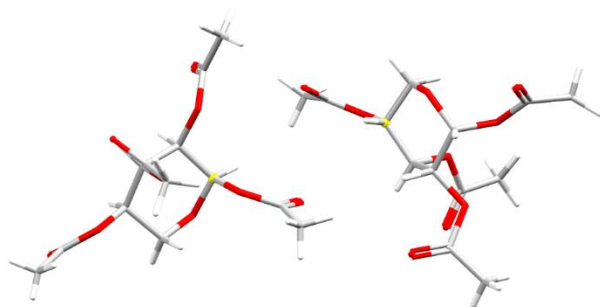


Recent update!



And a little more involved

- Molecule Overlay
- 2 molecules in the asymmetric unit and want to compare their conformations?



Automatic Molecule Overlay

Options

Select **two molecules** (by selecting at least one atom in each) then press **Overlay**. The molecules must have at least three atoms, and the same number of atoms. After overlay is complete you must select **Reset** before repeating the overlay or selecting different molecules.

Reset

Results

Flexibility	Inversion	RMSD	Max. D	Display
-	-	0.5452	1.3503	<input checked="" type="radio"/>
-	X	0.5452	1.3503	<input type="radio"/>
X	-	0.2765	0.6194	<input type="radio"/>
X	X	0.2765	0.6194	<input type="radio"/>
Original	Geometry	----	----	<input type="radio"/>

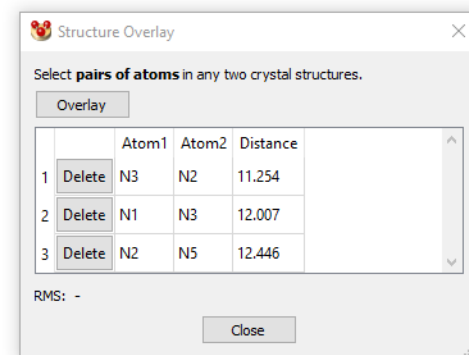
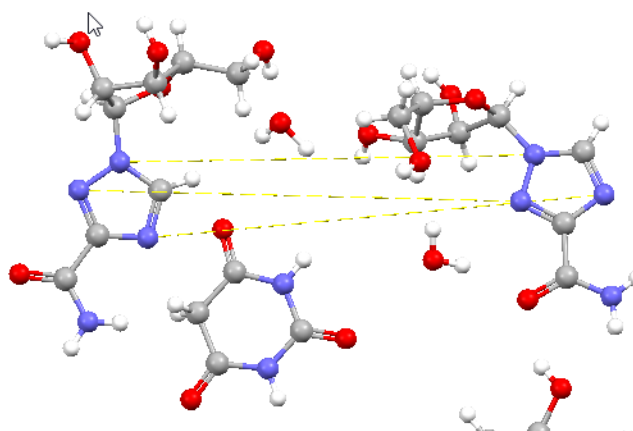
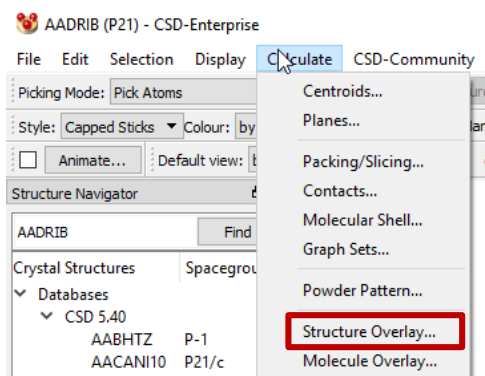
Close



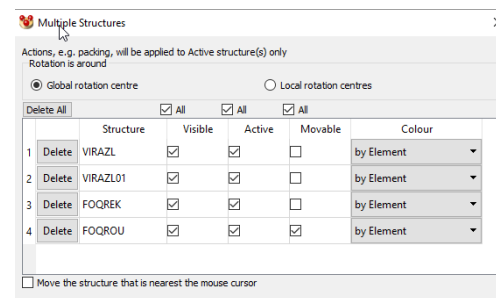


And a little more involved

- Overlaying more than 2 structures?



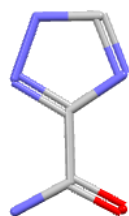
Last molecule selected is the one that moves



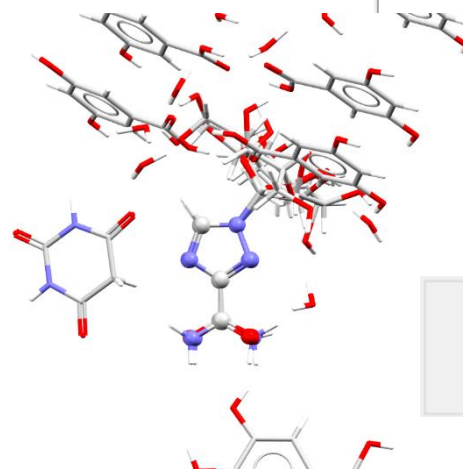
Multiple structures dialog allows you to “freeze” and hide the overlaid molecules

And a little more involved

- Want to overlay molecules from different structures? (and you don't want to use structure overlay)



Select substructure



Packing Feature_feature4_search		Options
5 hits out of 5 possible (100%)		RMS
FOQREK	1.132	
FOQRIO	1.118	
FOQROU	1.127	
VIRAZL	0	
VIRAZL01	0.097	

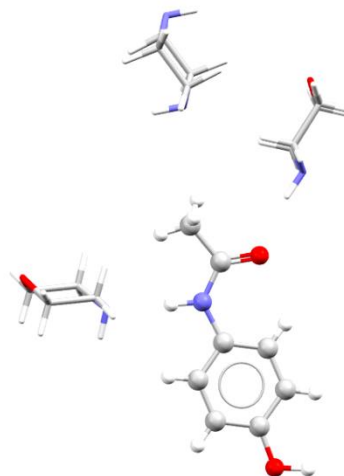
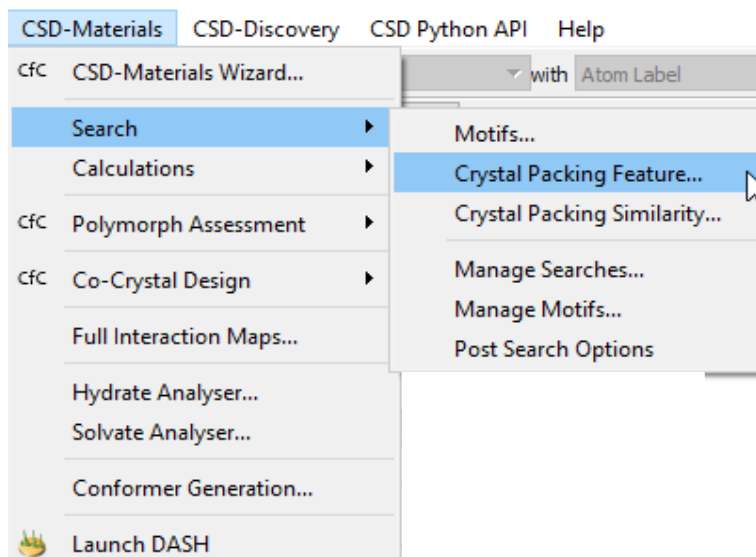
Multiple Structures

Structures...



And a little more involved

- Do you want to find all crystal structures containing a particular molecule?
 - Solid form landscape of paracetamol, ethanol solvates, anything with a common substructure, not just packing features...



Packing Feature_feature6_search	Options
85 hits	RMS
AHEPUY	0.367
AMUBAM	0.363
COKCEL	0.302
COTYOA02	0.297
COTYOA03	0.835
COTZAN02	0.193
COTZAN03	0.234
COTZAN04	0.291
COTZAN06	0.228
CUQKAC	0.545
HUMJEE	0.394
HXACAN	0
HXACAN01	0.207
HXACAN04	0.185
HXACAN06	0.211
HXACAN07	0.187
HXACAN08	0.079
HXACAN09	0.219
HXACAN10	0.195
HXACAN11	0.208
HXACAN12	0.241
HXACAN13	0.215
HXACAN14	0.215
HXACAN15	0.207
HXACAN16	0.2
HXACAN17	0.198
HXACAN18	0.196
HXACAN19	0.166
HXACAN21	0.082
HXACAN22	0.083
HXACAN23	0.092
HXACAN24	0.133
HXACAN25	0.060



And a little more involved

- Do you build subsets of structures based on a particular property? Cut and paste from Excel....

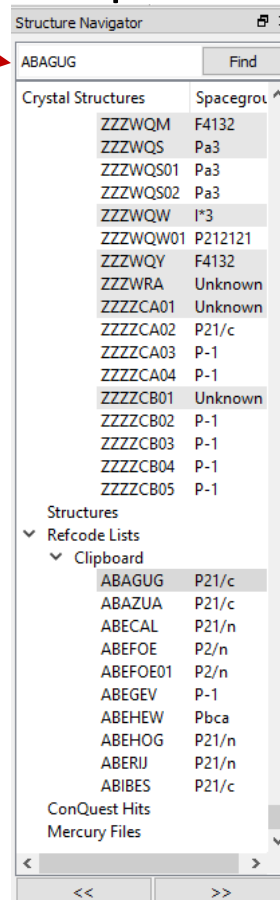
	A	B	C	G	H	I	J	K	L	M	N	O	P	R	S	T
7	Refcode	spacegr	zprime	mol_co	molecu	active.r	laxis	maxis	saxis	lm_rati	ls_ratic	ms_rati	shape_	Atoms	Aromat	Ring_A
54	ABAGUG	P21/c	0.5	1269.882	1269.882	1269.882	20.021	16.593	15.394	1.207	1.301	1.078	0.054	180	6	36
134	ABAZUA	P21/c	1	556.5447	556.5447	556.5447	19.086	12.307	11.725	1.551	1.628	1.05	0.055	80	6	36
148	ABECAL	P21/n	1	354.4418	354.4418	354.4418	20.035	9.386	3.592	2.135	5.577	2.613	0.13	46	6	35
166	ABEFOE	P2/n	0.5	618.7596	618.7596	618.7596	13.965	12.457	9.76	1.121	1.431	1.276	0.091	82	6	36
167	ABEFOE01	P2/n	0.5	618.7596	618.7596	618.7596	13.965	12.457	9.76	1.121	1.431	1.276	0.091	82	6	36
175	ABEGEV	P-1	1	620.7754	620.7754	620.7754	14.918	13.838	13.373	1.078	1.116	1.035	0.069	84	6	36
186	ABEHEW	Pbca	1	744.746	744.746	744.746	16.992	15.583	10.971	1.09	1.549	1.42	0.084	95	6	36
191	ABEHOG	P21/n	1	700.6936	700.6936	700.6936	15.065	14.07	10.708	1.071	1.407	1.314	0.087	88	6	36
283	ABERIJ	P21/n	1	694.7266	694.7266	694.7266	15.2	15.144	10.921	1.004	1.392	1.387	0.091	86	6	36
308	ABIBES	P21/c	1	492.756	492.756	492.756	14.536	12.656	9.635	1.148	1.509	1.314	0.09	64	6	36

Property in this column is the number of aromatic rings in molecule. Chosen structures with 6 aromatic rings.



And a little more involved

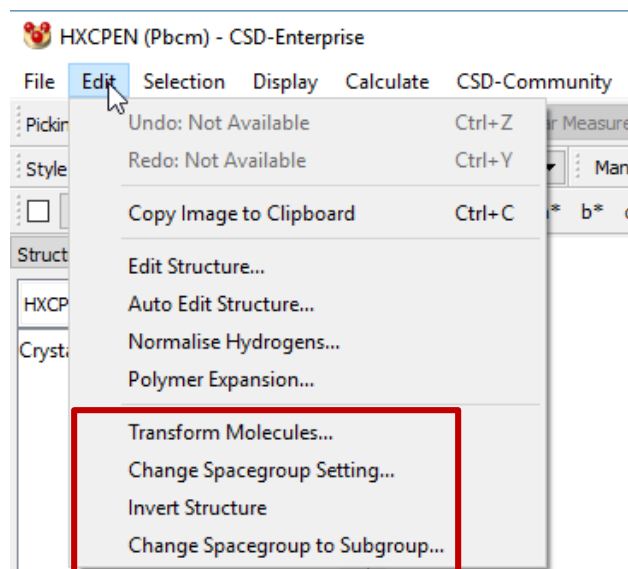
- Do you build subsets of structures based on a particular property? Cut and paste from Excel....into Mercury





And a little more involved

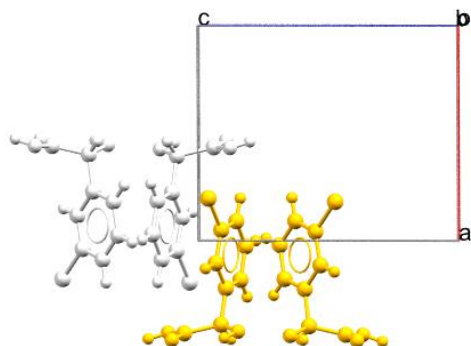
- Editing a structure
 - Invert a structure/ Invert a molecule
 - Removing symmetry by choosing a subgroup
 - Changing the space group setting: $P2_1/n$ to $P2_1/c$



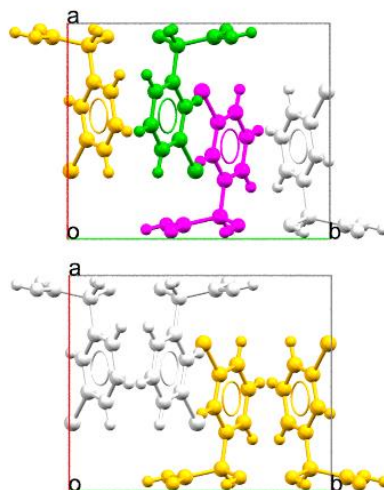


And a little more involved

- Do you explore structural changes due to phase transitions?
- FIZPEL/ FIZPEL01



P-1
Low temp



$P2_1/c$
Room Temp

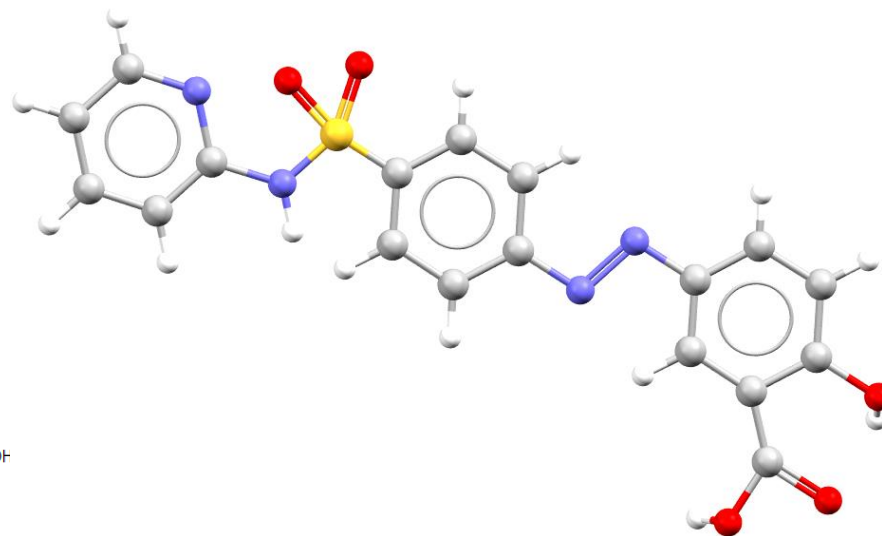
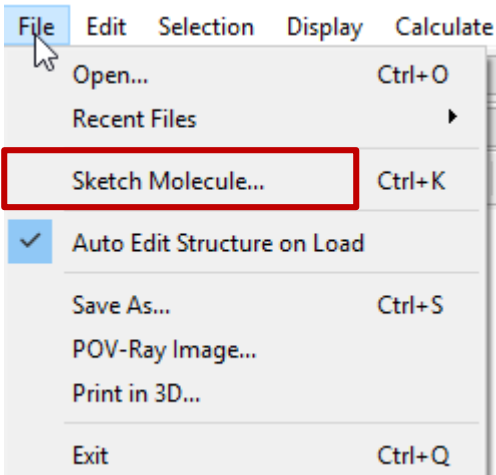
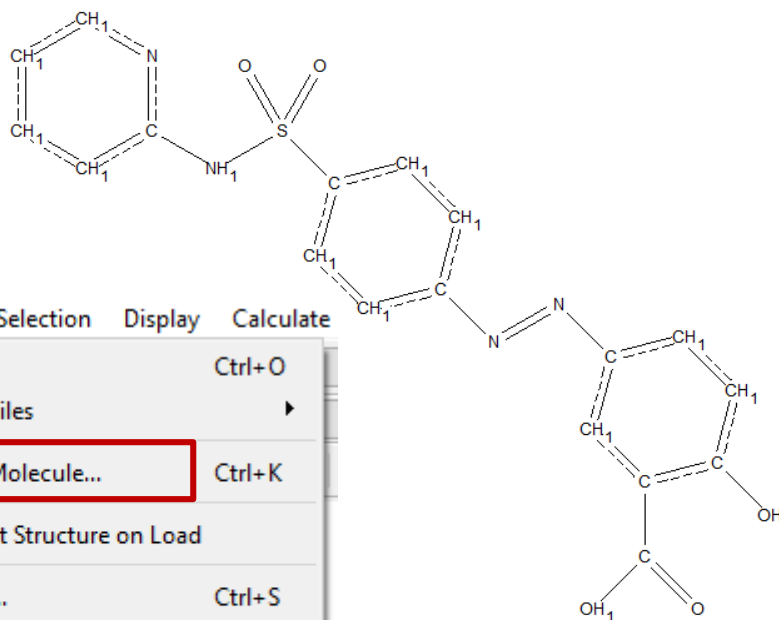
Transformed to subgroup P-1

Mirror symmetry
relationship
formalised in $P2_1/c$



And a little more involved

- Sketch a molecule and generate a conformation



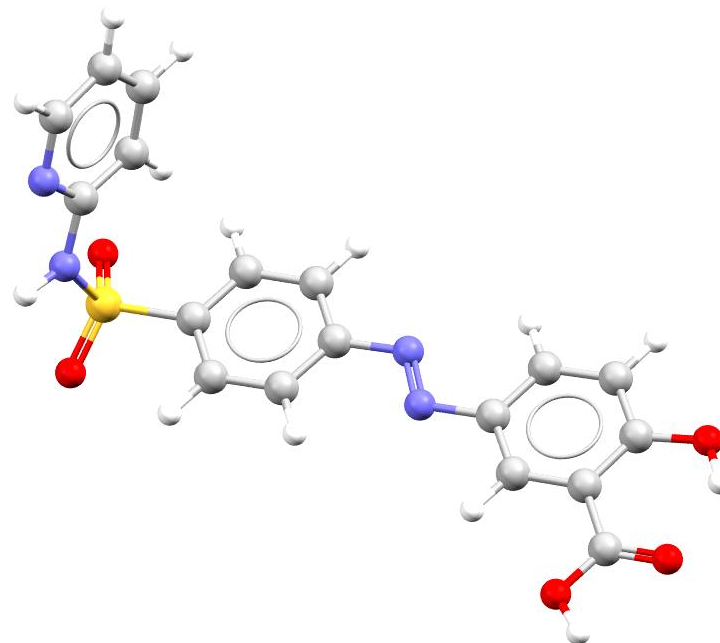
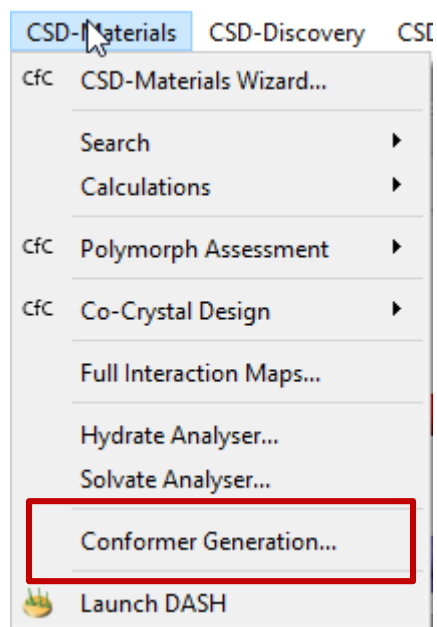
Sketcher



Mercury

And a little more involved

- Sketch a molecule and generate a conformation....





Too many to mention:

- Custom view
- Powder pattern simulation
- Links to Isostar, GOLD, Mogul etc
- Motif searching and hydrogen bond propensity calculations
- More info dialog
 - Nearest Miller Plane
 - Selecting atoms from Atoms list
- MOPAC – point group symmetry

QIZKOA

Current structure: QIZKOA

Customise... Save... Right-click on an object for options. Click on a column heading to sort rows.

Number	Label	Normal	Distance	Nearest Miller
1	mean: C3C N1C C1C O1C	0.694 0.672 -0.259	3.94423	(50 15 -25)

Structure Diagram Atoms Bonds Contacts Centroids Planes Symmetry Distances Angles Torsions All Angles All Torsions

Close



Acknowledgements – too many to mention

- Many thanks to all the developers, testers and documentation-writers at CCDC
- Many thanks to you for suggesting enhancements and new featuresand reporting bugs

Thank you!