1)1. .sdf file format – Tool tip properties

1. Properties
   -OEChem-04092001263D

2. > <protein pdb>

3. ><Data-custom field 1>
Description of entry

> <Data-custom field ...>
Description of entry

> <Data-custom field 7>
Description of entry

1)At the beginning of the sdf a ‘Properties’ section to define tooltips

2)Name of protein .pdb used eg **XX**

3)Up to 7 x selected custom data entries with description being XX characters long

1)1. .sdf file format – data entries

4. MUS-SCH-c2f-4
-OEChem-04092001263D

5. 37 39 0 0 0 0 0 0 0 0999 V2000

6. ><inspiration frags>

7. > <Data-custom field 1>
Value

> <Data-custom field ...>
Value

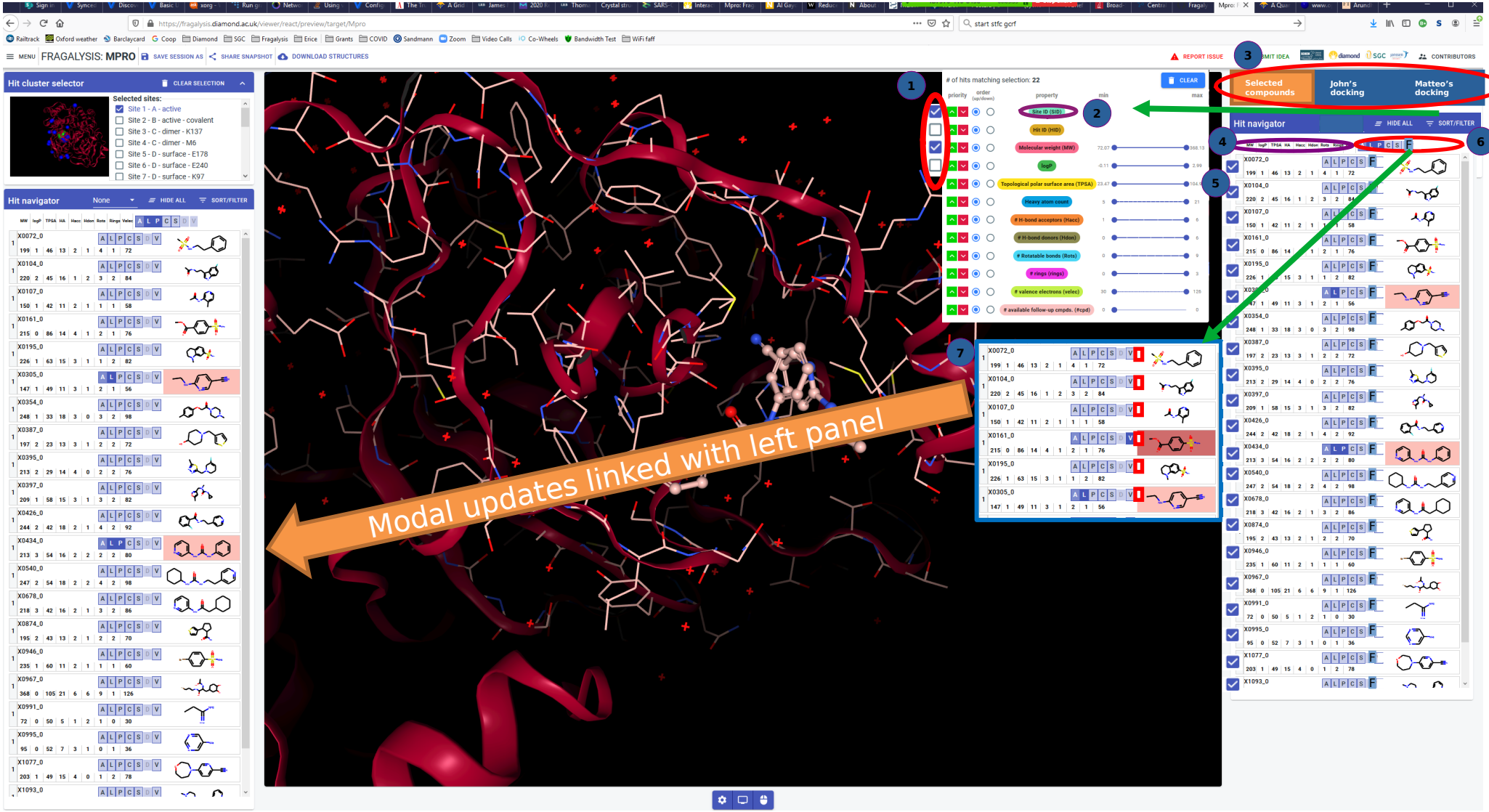
> <Data-custom field 7>
Value

4)Compound ID

5)Ligand 3D coordinates

6)Inspiration frags in format ‘x0104’

7)Up to 7 x selected data-custom field values – these will appear in Fragalysis underneath each compound


https://fragalysis.diamond.ac.uk/viewer/react/preview/target/Mpro
MENU
FRAGALYSIS: MPRO
SAVE SESSION AS
SHARE SNAPSHOT
DOWNLOAD STRUCTURES
REPORT ISSUE
SUBMIT IDEA
CONTRIBUTORS
Hit cluster selector
CLEAR SELECTION
Selected sites:
Site 1 - A - active
Site 2 - B - active - covalent
Site 3 - C - dimer - K137
Site 4 - C - dimer - M6
Site 5 - D - surface - E178
Site 6 - D - surface - E240
Site 7 - D - surface - K97
Hit navigator
None
HIDE ALL
SORT/FILTER
# of hits matching selection: 22
CLEAR
priority
order (up/down)
property
min
max
Site ID (SID)
Hit ID (HID)
Molecular weight (MW)
logP
Topological polar surface area (TPSA)
Heavy atom count
H-bond acceptors (Hacc)
H-bond donors (Hdon)
Rotatable bonds (Rots)
rings (rings)
valence electrons (velec)
available follow-up cmpds. (#cpd)
Selected compounds
John's docking
Matteo's docking
Modal updates linked with left panel
1
2
3
4
5
6
7