

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 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

Hit cluster selector

CLEAR SELECTION

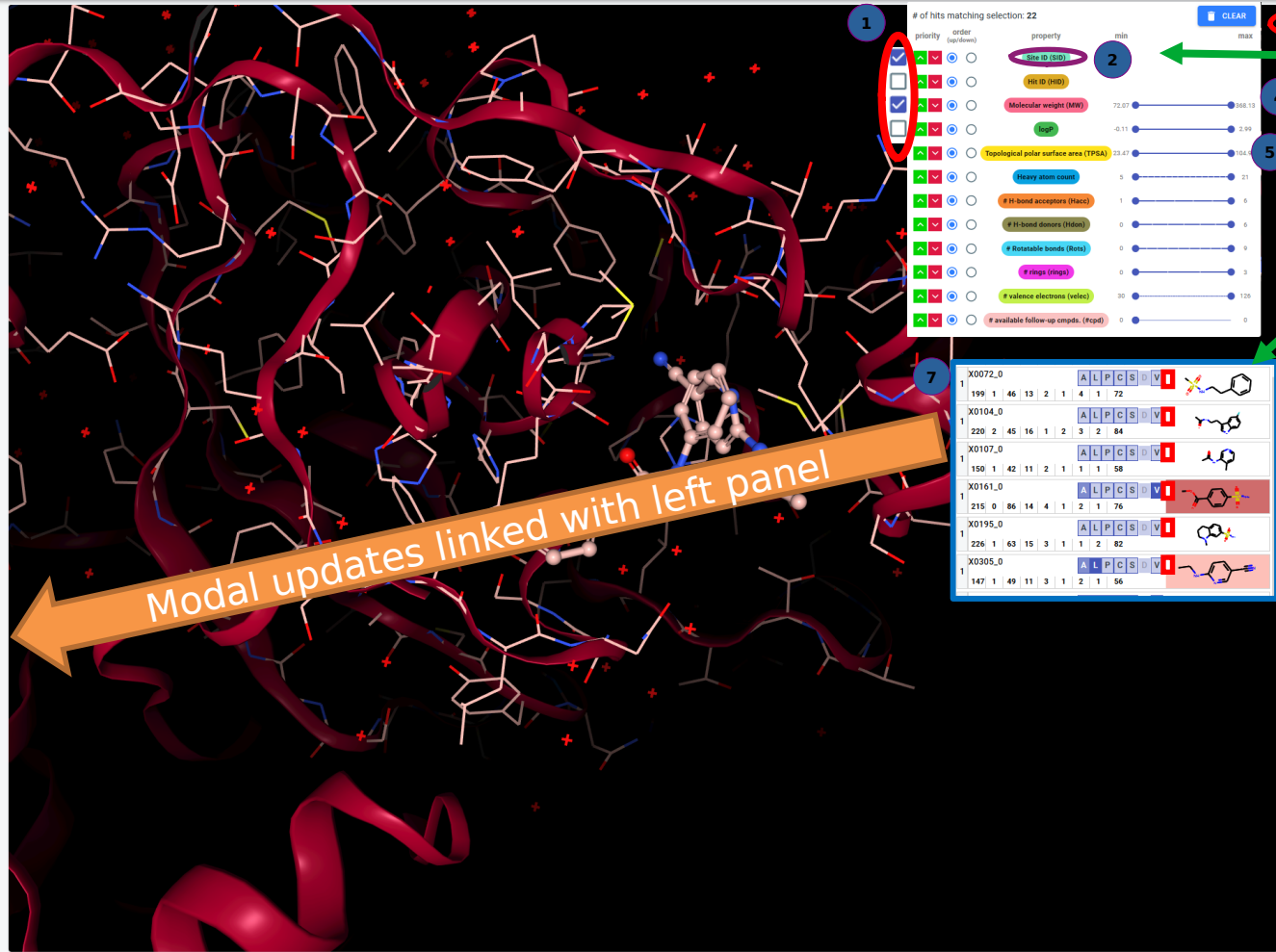
Selected sites:

- 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

MW	logP	TPSA	HA	HBD	HBA	HBD	HBA	Range	Value	A	L	P	C	S	F
X0072_0	199	1	46	13	2	1	4	1	72	A	L	P	C	S	F
X0104_0	220	2	45	16	1	2	3	2	84	A	L	P	C	S	F
X0107_0	150	1	42	11	2	1	1	1	58	A	L	P	C	S	F
X0161_0	215	0	86	14	4	1	2	1	76	A	L	P	C	S	F
X0195_0	226	1	63	15	3	1	1	2	82	A	L	P	C	S	F
X0305_0	147	1	49	11	3	1	2	1	56	A	L	P	C	S	F
X0354_0	248	1	33	18	3	0	3	2	95	A	L	P	C	S	F
X0387_0	197	2	23	13	3	1	2	2	72	A	L	P	C	S	F
X0395_0	213	2	29	14	4	0	2	2	76	A	L	P	C	S	F
X0397_0	209	1	58	15	3	1	3	2	82	A	L	P	C	S	F
X0426_0	244	2	42	18	2	1	4	2	92	A	L	P	C	S	F
X0434_0	213	3	54	16	2	2	2	2	80	A	L	P	C	S	F
X0540_0	247	2	54	18	2	2	4	2	98	A	L	P	C	S	F
X0678_0	218	3	42	16	2	1	3	2	86	A	L	P	C	S	F
X0874_0	195	2	43	13	2	1	2	2	70	A	L	P	C	S	F
X0946_0	235	1	60	11	2	1	1	1	60	A	L	P	C	S	F
X0967_0	368	0	105	21	6	6	9	1	126	A	L	P	C	S	F
X0991_0	72	0	50	5	1	2	1	0	30	A	L	P	C	S	F
X0995_0	95	0	52	7	3	1	0	1	36	A	L	P	C	S	F
X1077_0	203	1	49	15	4	0	1	2	78	A	L	P	C	S	F
X1093_0										A	L	P	C	S	F



of hits matching selection: 22

priority order (hit/lead)

property min max

- Site ID (Site)
- Hit ID (Hit)
- Molecular weight (MW)
- 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. (rcpd)

MW	logP	TPSA	HA	HBD	HBA	HBD	HBA	Range	Value	A	L	P	C	S	F
X0072_0	199	1	46	13	2	1	4	1	72	A	L	P	C	S	F
X0104_0	220	2	45	16	1	2	3	2	84	A	L	P	C	S	F
X0107_0	150	1	42	11	2	1	1	1	58	A	L	P	C	S	F
X0161_0	215	0	86	14	4	1	2	1	76	A	L	P	C	S	F
X0195_0	226	1	63	15	3	1	1	2	82	A	L	P	C	S	F
X0305_0	147	1	49	11	3	1	2	1	56	A	L	P	C	S	F

Selected compounds John's docking Matteo's docking

Hit navigator

HIDE ALL SORT/FILTER

MW	logP	TPSA	HA	HBD	HBA	HBD	HBA	Range	Value	A	L	P	C	S	F
X0072_0	199	1	46	13	2	1	4	1	72	A	L	P	C	S	F
X0104_0	220	2	45	16	1	2	3	2	84	A	L	P	C	S	F
X0107_0	150	1	42	11	2	1	1	1	58	A	L	P	C	S	F
X0161_0	215	0	86	14	4	1	2	1	76	A	L	P	C	S	F
X0195_0	226	1	63	15	3	1	1	2	82	A	L	P	C	S	F
X0305_0	147	1	49	11	3	1	2	1	56	A	L	P	C	S	F
X0354_0	248	1	33	18	3	0	3	2	95	A	L	P	C	S	F
X0387_0	197	2	23	13	3	1	2	2	72	A	L	P	C	S	F
X0395_0	213	2	29	14	4	0	2	2	76	A	L	P	C	S	F
X0397_0	209	1	58	15	3	1	3	2	82	A	L	P	C	S	F
X0426_0	244	2	42	18	2	1	4	2	92	A	L	P	C	S	F
X0434_0	213	3	54	16	2	2	2	2	80	A	L	P	C	S	F
X0540_0	247	2	54	18	2	2	4	2	98	A	L	P	C	S	F
X0678_0	218	3	42	16	2	1	3	2	86	A	L	P	C	S	F
X0874_0	195	2	43	13	2	1	2	2	70	A	L	P	C	S	F
X0946_0	235	1	60	11	2	1	1	1	60	A	L	P	C	S	F
X0967_0	368	0	105	21	6	6	9	1	126	A	L	P	C	S	F
X0991_0	72	0	50	5	1	2	1	0	30	A	L	P	C	S	F
X0995_0	95	0	52	7	3	1	0	1	36	A	L	P	C	S	F
X1077_0	203	1	49	15	4	0	1	2	78	A	L	P	C	S	F
X1093_0										A	L	P	C	S	F

Modal updates linked with left panel