
Subject: Saving 2D-structure with labels

Posted by [vijaymasand](#) on Fri, 20 May 2022 15:04:06 GMT

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Dear all

Recently, I started using Datawarrior for research work, especially for QSAR and allied areas. It is really wonderful and useful for cheminformatics. I have three requirements from developers.

(1) I want to save the 2D-structure along with the labels, please see the 'structure view' panel in the attached image. I tried 'copy view image' but it copied only the structure and not the data labels. Is there any method to copy and paste (or save) the structure along with labels?

(2) Right now, it is providing data from ChEMBL 28. Recently, ChEMBL 30 was released. Is possible to force it to download data from ChEMBL 30?

(3) In 'Look and Feel' menu could you please add 'white' as an option.

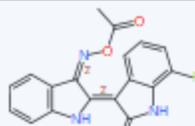
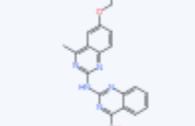
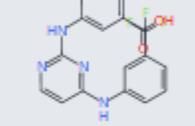
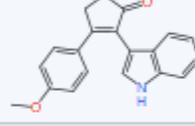
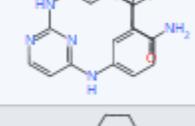
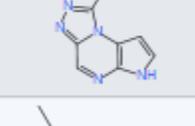
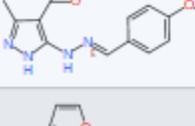
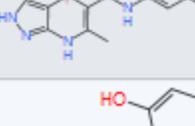
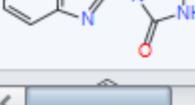
Thanks in advance.

From

Vijay

File Attachments

1) [Lables-datawarrior.png](#), downloaded 590 times

Table										
	Structure	MolRegNo	m	Value	Unit	Type	pValue	Ligand Efficiency	Binding Efficiency	
1		387278	=	20000	nM	IC50	4.7	0.26	13.93	5.8
2		1615143	=	17000	nM	IC50	4.77	0.16	8.25	4.8
3		1057688	=	16720	nM	IC50	4.78	0.25	13.75	5.5
4		2139271	=	16200	nM	IC50	4.79	0.24	12.8	5.5
5		449341	=	16000	nM	IC50	4.8	0.28	15.76	8.8
6		448944	=	16000	nM	IC50	4.8	0.24	13.16	6.6
7		2169884	=	15400	nM	IC50	4.81	0.23	11.99	5.5
8		1516286	=	15300	nM	IC50	4.82	0.37	19.96	8.5
9		456120	=	15140	nM	IC50	4.82	0.3	15.94	5.4
10		713172	=	15000	nM	IC50	4.82	0.25	12.94	5.8
11		2112246	=	15000	nM	IC50	4.82	0.33	18.12	5.5