

**Compound Tabs:** Coumarin, Benzothiazole, Pyrazole

**Search Bar:** Search:

**Filters:** HBA1, HBA2, HBD, logP, MR, MW, nF, TPSA, Name

**Compound Tabs:** All, All, All, All

**Table 1: Compound Data**

	cansmiName	ChemicalName	cansmi	formula	HBA1	HBA2	HBD	logP	MR	MW	nF	TPSA	Name
1	CCOc1c2csc(n2)N(c1=O)oc2c1ccc(c2)OC(C1=O)O)C/C CC- 10.mol	Coumarin13	CCOc1c2csc(n2)N(c1=O)oc2c1ccc(c2)OC(C1=O)O)C/C	C17H16N2O6S	7	9	2	3.3305	97.2112	376.38374	0	153.12	CC-10.mol
2	Clc1ccc(cc1)C=C1SC=C(N1n1c(C)nn(c1=O)c1cccc2oc1=O)CC- 11a.mol	Coumarin14	Clc1ccc(cc1)C=C1SC=C(N1n1c(C)nn(c1=O)c1cccc2oc1=O)	C28H19ClN4O3S	5	8	0	5.8492	151.423	526.99346	0	98.57	CC-11a.mol
3	CCOc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C CC- 11b.mol	Coumarin15	CCOc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C	C29H22N4O4S	6	9	0	5.2044	152.905	522.57438	0	107.8	CC-11b.mol
4	CCOc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C CC- 11c.mol	Coumarin16	CCOc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C	C29H21ClN4O4S	6	9	0	5.8578	157.915	557.81944	0	107.8	CC-11c.mol
5	CCOc1ccc(cc1)C=C1SC=C(N1n1c(C)nn(c1=O)c1cccc2oc1=O)CC- 11d.mol	Coumarin17	CCOc1ccc(cc1)C=C1SC=C(N1n1c(C)nn(c1=O)c1cccc2oc1=O)	C30H24N4O4S	6	9	0	5.5128	157.871	536.60096	0	107.8	CC-11d.mol
6	Cc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C CC- 11e.mol	Coumarin18	Cc1ccc(cc1)n1nc(n(c1=O)N1/C=C1c2cccc2)SC=C1c2cccc2oc1=O)C	C29H21ClN4O3S	5	8	0	6.1576	156.389	541.02004	0	98.57	CC-11e.mol
7	O=c1cc2c(cc1c1csc(n1)nc(cc1N)cc1cccc1)cc(cc2C(C)C(C)C(C)C)C/C CC- 12a.mol	Coumarin19	O=c1cc2c(cc1c1csc(n1)nc(cc1N)cc1cccc1)cc(cc2C(C)C(C)C(C)C)C/C	C29H30N4O2S	4	7	1	7.5276	149.0944	498.6391	0	115.18	CC-12a.mol
8	CCN(c1ccc(cc1)c1nn(c1)N)cc1cccc2oc1=O)CC CC- 12b.mol	Coumarin20	CCN(c1ccc(cc1)c1nn(c1)N)cc1cccc2oc1=O)CC	C25H23N5O2S	5	8	1	5.7788	134.3754	457.54742	0	118.42	CC-12b.mol
9	Clc1cccc(c1)C=NNc1ccc(n1)c1cc2cccc2oc1=O)Cl CC- 13a.mol	Coumarin21	Clc1cccc(c1)C=NNc1ccc(n1)c1cc2cccc2oc1=O)Cl	C19H11ClN3O2S	4	6	1	5.7423	111.0897	416.28054	0	95.73	CC-13a.mol
10	O=c1cc2cccc2oc1c1csc(n1)N1N=C1c1ccc(cc1C1N)N=O)O CC- 13b.mol	Coumarin22	O=c1cc2cccc2oc1c1csc(n1)N1N=C1c1ccc(cc1C1N)N=O)O	C19H13ClN4O4S	6	6	3	4.9965	114.6749	428.84892	0	156.88	CC-13b.mol

Showing 1 to 10 of 140 entries

[cum2Compounds](#) [cum2SDF](#)

**Table 2: Therapeutic Action and References**

Name	Therapeutic.Action	DOI	References
CC-10.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-11a.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-11b.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-11c.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-11d.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-11e.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-12a.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-12b.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-13a.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>
CC-13b.mol	anticancer	<a href="https://doi.org/10.1016/j.ejmc.2022.100038">https://doi.org/10.1016/j.ejmc.2022.100038</a>	<a href="https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub">https://www.sciencedirect.com/science/article/pii/S2772417422000103?via%3Dihub</a>

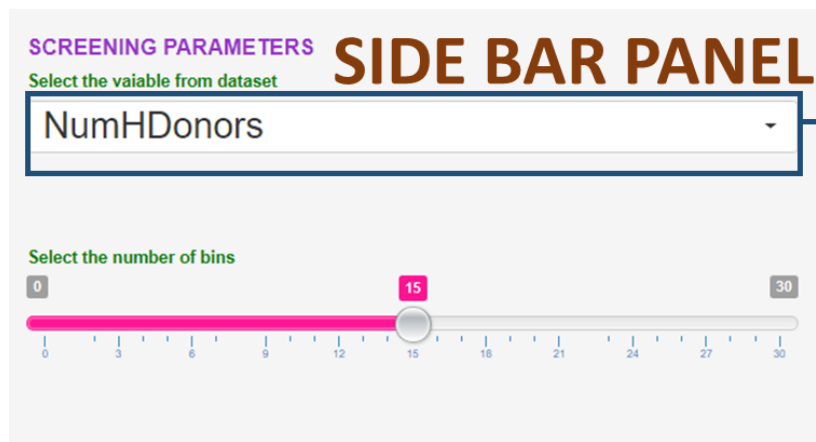
**MAIN PANEL**

**Full dataset or filtered data with all columns**

**Full dataset in .sdf format**

**Clickable references**

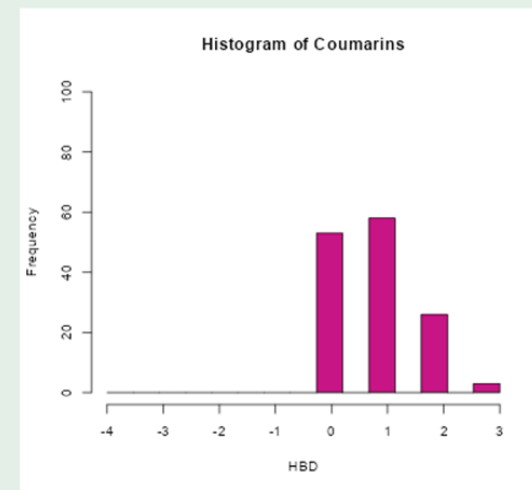
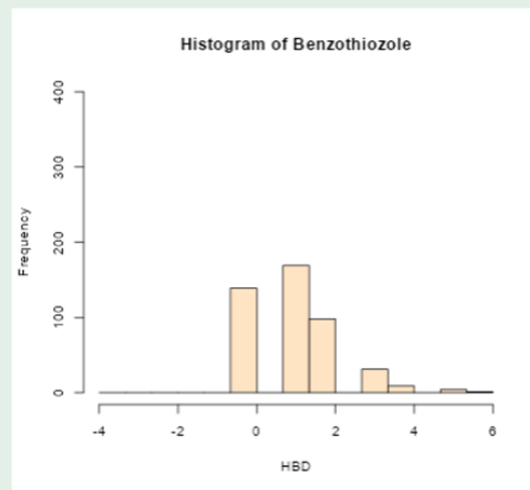
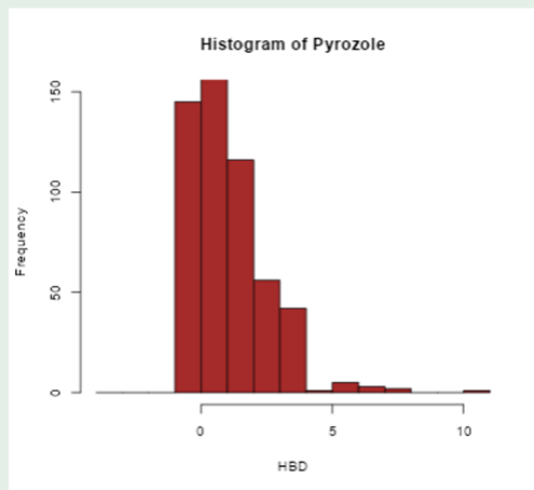
Supplementary Figure 1. The main panel with the available filters.



Select the descriptor to visualise the graph

## MAIN PANEL

### 2.Full Dataset Graphical Frequency Analysis of Descriptors



Supplementary Figure 2. Frequency of graphical visualization of the compounds corresponding to the descriptors

Coumarin
Benzothiozole
Pyrazole

Filtered applied: HBA1 > 8

Show 10 entries  
 cansmiName

Search:

formula   HBA1   HBA2   HBD   logP

	cansmiName	ChemicalName	cansmi	formula	HBA1	HBA2	HBD	logP
43	<chem>Cc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2 CC-30b.mol</chem>	Coumarin51	<chem>Cc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2</chem>	C36H32N6O3S	9	10	1	6.7873
45	<chem>Clc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2 CC-30d.mol</chem>	Coumarin53	<chem>Clc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2</chem>	C35H29ClN6O3S	9	10	1	7.1323
57	<chem>COc1c(OC)cc(cc1OC)c1cc(nn1c1ccc(cc1)S(=O)(=O)N)C(=O)OCCOc1ccc2c(c1)oc(=O)cc2 CC-36.mol</chem>	Coumarin65	<chem>COc1c(OC)cc(cc1OC)c1cc(nn1c1ccc(cc1)S(=O)(=O)N)C(=O)OCCOc1ccc2c(c1)oc(=O)cc2</chem>	C30H27N3O10S	11	13	1	5.3358
110	<chem>CCN(c1ccc2c(c1)oc(=O)c(c2)C(=O)NCCNC(=O)/C(=C/c1cc(OC)c(c(c1)OC)OC)/c1ccc(c(c1)OC)OC)CC CC-81.mol</chem>	Coumarin112	<chem>CCN(c1ccc2c(c1)oc(=O)c(c2)C(=O)NCCNC(=O)/C(=C/c1cc(OC)c(c(c1)OC)OC)/c1ccc(c(c1)OC)OC)CC</chem>	C36H41N3O9	11	12	2	5.5508

Showing 1 to 4 of 4 entries (filtered from 140 total entries)

Previous 1 Next

[cum2Compounds](#)
[cum2SDF](#)

Selected column from section 1 displayed in section 3

Download filtered data with all columns

### 3.Extracting cansmi(smiles) Column:Filtered Data

## MAIN PANEL

FilteredCoumarin

Show 10 entries  
 cansmiName

Search:

Cc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2 CC-30b.mol

Clc1ccc(cc1)/N=N/C1SC(=NC1c1cccc1)N1N=C(CC1c1ccc(cc1)/N(C)C)c1c(=O)oc2c(c1O)cccc2 CC-30d.mol

COc1c(OC)cc(cc1OC)c1cc(nn1c1ccc(cc1)S(=O)(=O)N)C(=O)OCCOc1ccc2c(c1)oc(=O)cc2 CC-36.mol

CCN(c1ccc2c(c1)oc(=O)c(c2)C(=O)NCCNC(=O)/C(=C/c1cc(OC)c(c(c1)OC)OC)/c1ccc(c(c1)OC)OC)CC CC-81.mol

Showing 1 to 4 of 4 entries

Previous 1 Next

[Filteredcum2csv](#)
[Filteredcum2sdf](#)

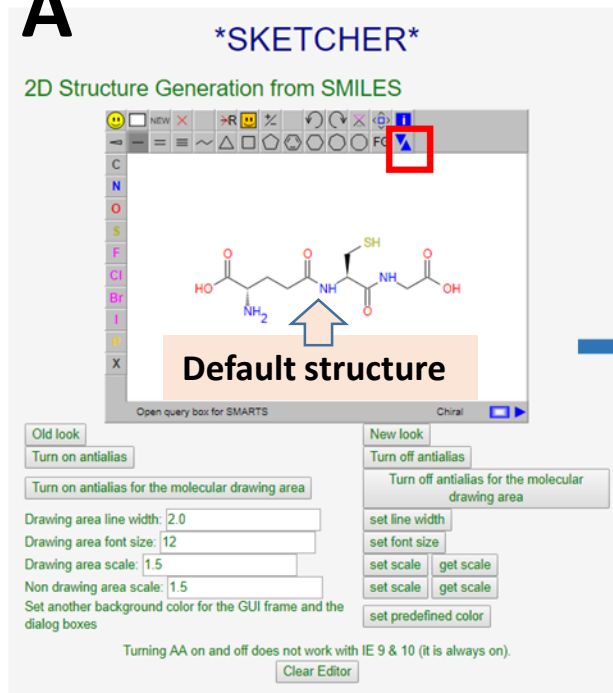
Download selected column as .sdf file

Download selected column

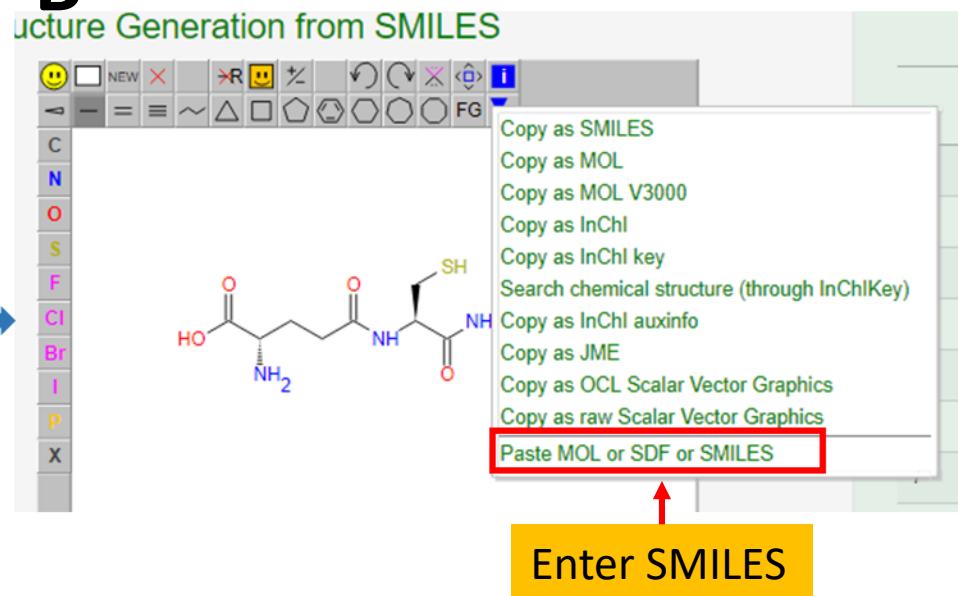
Supplementary Figure 3. Filter-based column selection and download the filtered data as .csv and .sdf files.

# SIDE BAR PANEL

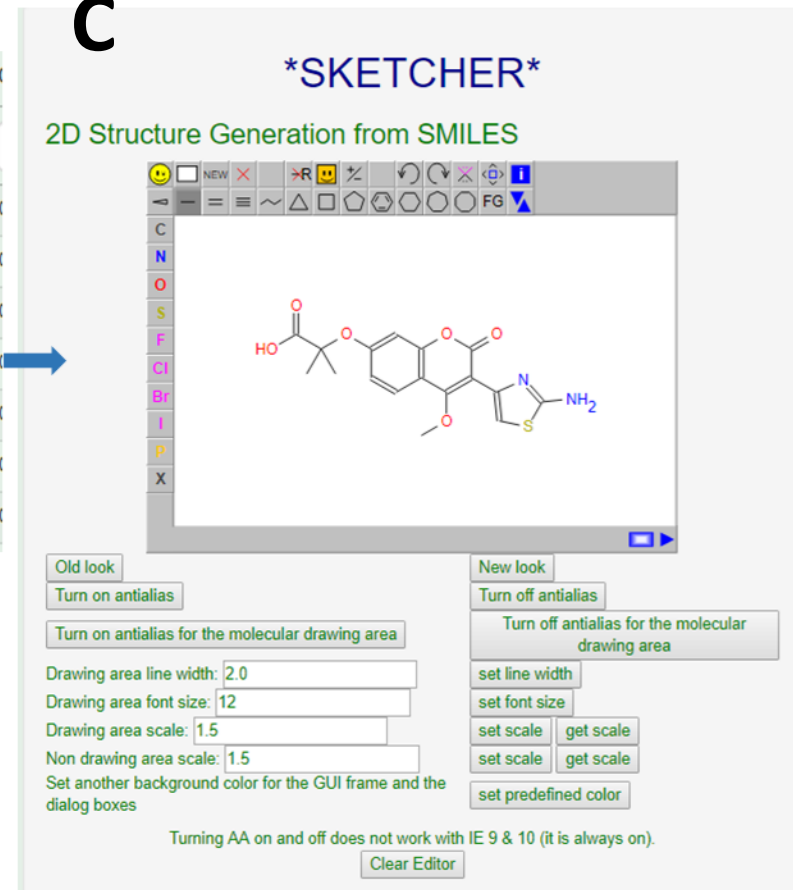
A



B

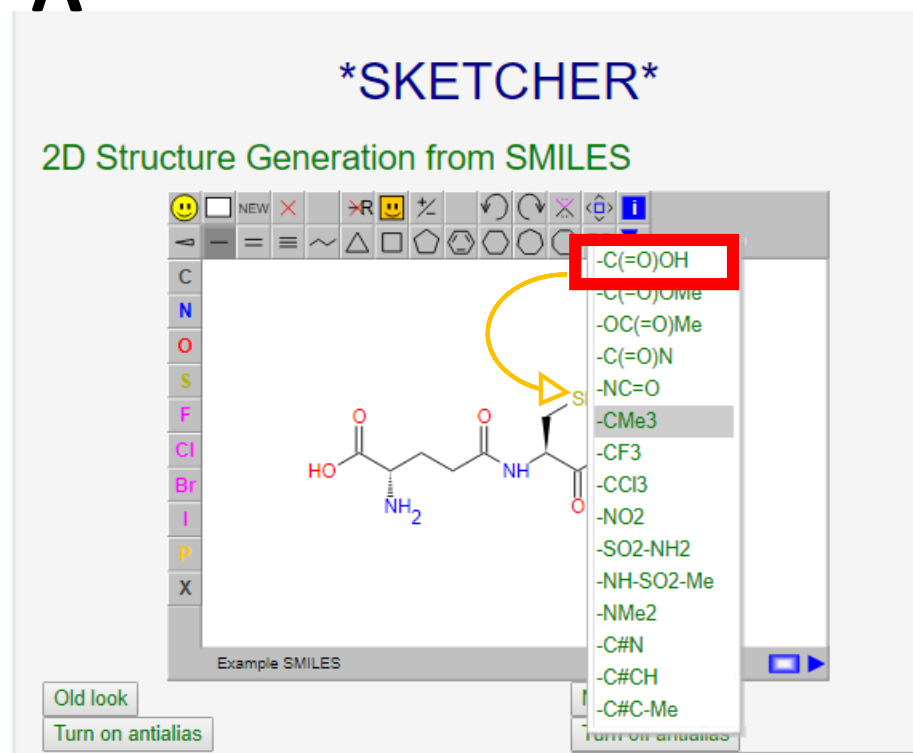
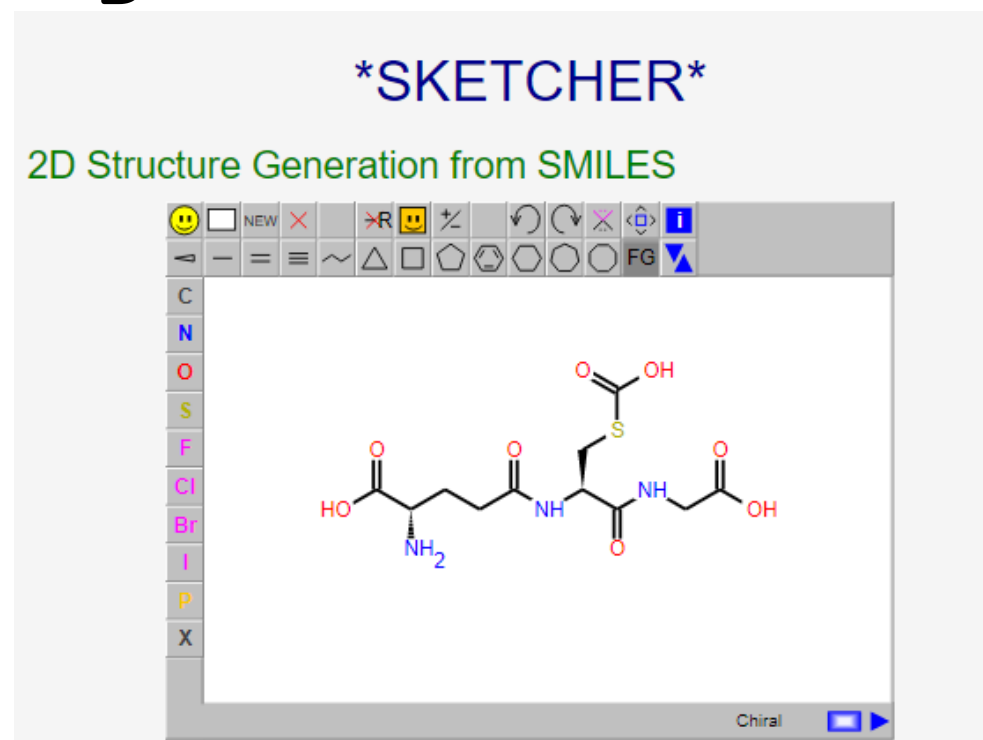


C



Structure of coumarin13

Supplementary Figure 4. The step-wise process of viewing the 2D structures of the compounds giving input as SMILES.

**A****B**

Supplementary Figure 5. Editing a given molecule.