



Drug Likeness Tool (DruLiTo)

Tutorial



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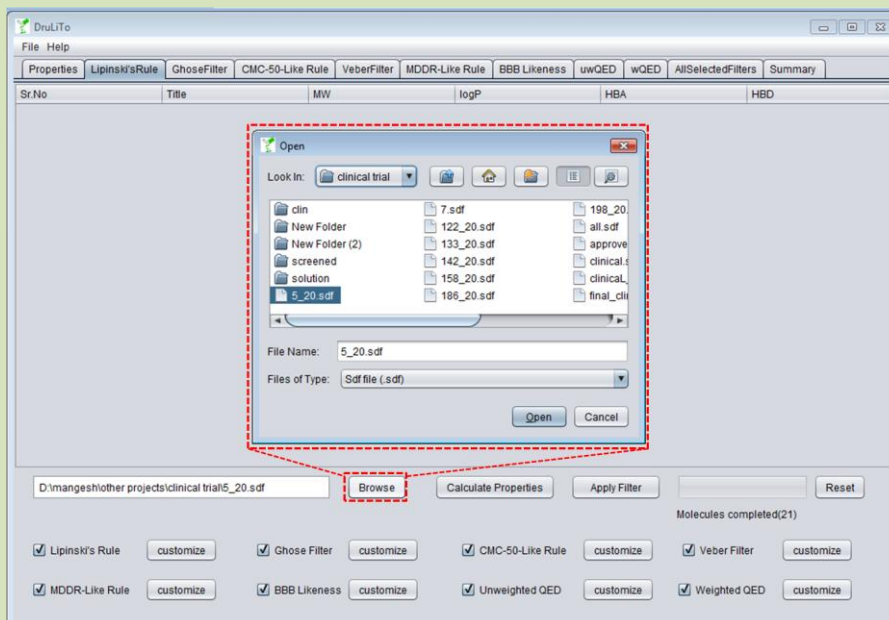
Quick Tutorial

The screenshot displays the DruLiTo software interface. At the top, there is a menu bar with 'File' and 'Help'. Below it is a toolbar with buttons for 'Properties', 'Lipinski's Rule', 'Ghose Filter', 'CMC-50-Like Rule', 'Veber Filter', 'MDDR-Like Rule', 'BBB Likeness', 'uwQED', 'wQED', 'AllSelectedFilters', and 'Summary'. The main window shows a table of molecules with columns for 'Sr. No.', 'Title', 'MW', 'logp', 'Alogp', 'HBA', 'HBD', 'TPSA', 'AMR', 'nRB', 'nAtom', 'nAcidic...', 'RC', 'nRigidB', 'nAtom...', 'nHB', and 'SAIerts'. The molecules are color-coded: green for those passing the filter and pink for those violating it. A 'Customize Lipinski's Rule of Five' dialog box is open, showing settings for Molecular Weight (500), LogP (5), H-Bond Donor (5), and H-Bond Acceptor (10). At the bottom, there is a file input field with a 'Browse' button, and buttons for 'Calculate Properties', 'Apply Filter', and 'Reset'. A status bar at the bottom indicates 'Molecules completed(21)'.

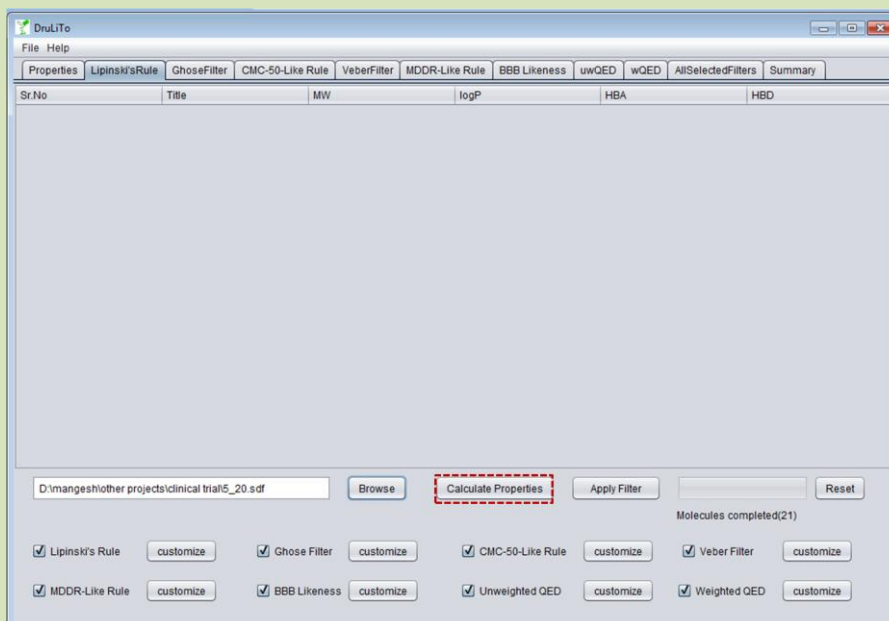
- A. Supply molecules in .mol or .sdf file format
- B. Various drug likeness filters available in DruLiTo
- C. Example window for customization of the drug likeness filter
- D. The molecules passing drug likeness filter are shown in green colour, while the molecules violating drug likeness filter are shown in pink colour
- E. Result windows for drug likeness filter
- F. The coordinates of molecules passing the drug likeness filters can be exported in .sdf file format.

HOW TO USE DRULITO

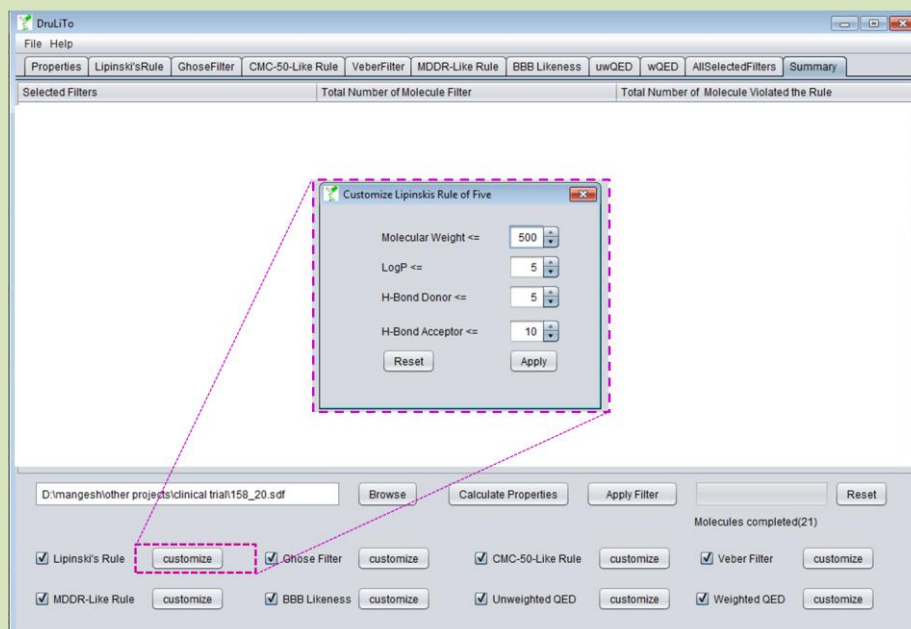
STEP1: Click on **Browse** 'Browse' button and select the molecule either in *.mol or *.sdf file format.



STEP2: Click on the **Calculate Properties** 'Calculate Properties' button which calculates all the descriptors.



STEP3: Click on the Drug likeness rule box according to the users need. The user can even customize the rules as per the need by clicking on the **Customize** 'customize' button.

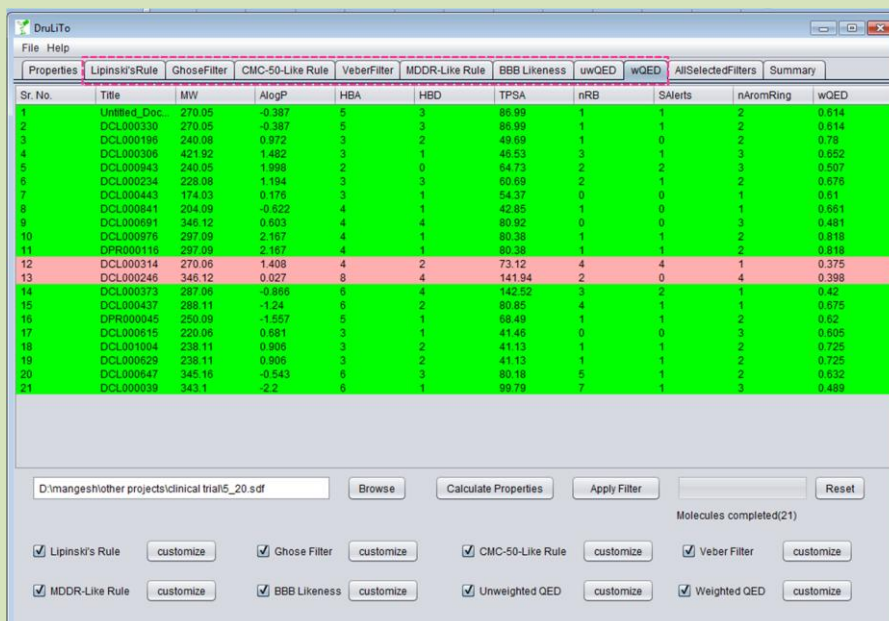


STEP4: Click on the **Apply Filter** 'Apply Filter' button to apply the selected rules.

The screenshot shows the DruLiTo application window after applying the filters. The 'Apply Filter' button is highlighted. The main window displays a table of 21 molecules with various properties.

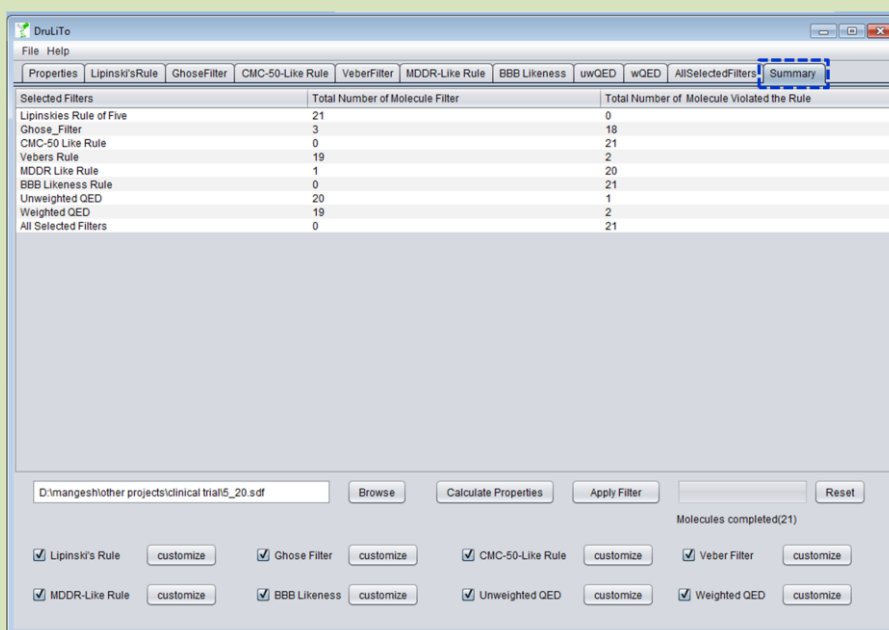
Sr. No.	Title	MW	logp	Alogp	HBA	HBD	TPSA	AMR	nRB	nAtom	nAcidic	RC	nRigidB	nAtom...	nHB	SAIerts
1	Unlitle...	270.05	1.043	-0.387	5	3	86.99	78.92	1	30	0	3	21	2	8	1
2	DCL00...	270.05	1.043	-0.387	5	3	86.99	78.92	1	30	0	3	21	2	8	1
3	DCL00...	240.08	1.379	0.972	3	2	49.69	77.44	1	30	0	3	19	2	5	0
4	DCL00...	421.92	3.411	1.482	3	1	46.53	99.67	3	34	0	3	21	3	4	1
5	DCL00...	240.05	1.533	1.998	2	0	64.73	70.11	2	26	0	3	18	3	2	2
6	DCL00...	228.08	2.048	1.194	3	3	60.69	74.61	2	29	0	2	16	2	6	1
7	DCL00...	174.03	-0.011	0.176	3	1	54.37	50.98	0	19	0	2	14	1	4	0
8	DCL00...	204.09	0.621	-0.622	4	1	42.85	58.82	1	27	0	3	16	1	5	0
9	DCL00...	346.12	1.152	0.603	4	4	80.92	106.96	0	44	0	5	30	3	8	0
10	DCL00...	297.09	2.445	2.167	4	1	80.38	92.48	1	36	0	3	22	2	5	1
11	DPR00...	297.09	2.445	2.167	4	1	80.38	92.48	1	36	0	3	22	2	5	1
12	DCL00...	270.06	1.536	1.408	4	2	73.12	65.57	4	28	0	1	15	1	6	4
13	DCL00...	346.12	-1.192	0.027	8	4	141.94	100.77	2	40	0	4	27	4	12	0
14	DCL00...	287.06	-0.217	-0.866	6	4	142.52	63.55	3	33	0	2	18	1	10	2
15	DCL00...	288.11	-0.256	-1.24	6	2	80.85	82.9	4	37	0	3	19	1	8	1
16	DPR00...	250.09	0.197	-1.557	5	1	68.49	73.01	1	29	0	3	20	2	6	1
17	DCL00...	220.06	1.545	0.681	3	1	41.46	71.53	0	25	0	4	20	3	4	0
18	DCL00...	238.11	1.576	0.906	3	2	41.13	78.21	1	32	0	3	19	2	5	1
19	DCL00...	238.11	1.576	0.906	3	2	41.13	78.21	1	32	0	3	19	2	5	1
20	DCL00...	345.16	1.791	-0.543	6	3	80.18	102.12	5	48	0	3	22	2	9	1
21	DCL00...	343.1	0.96	-2.2	6	1	99.79	99.65	7	41	0	3	19	3	7	1

STEP5: Check the respective tab of Drug likeness rules to see the conceded candidate among the molecules provided by the user.



Sr. No.	Title	MW	AlogP	HBA	HBD	TPSA	nRB	SAAlerts	nAromRing	wOED
1	Unfiltered_Dec	270.05	-0.387	5	3	86.99	1	1	2	0.614
2	DCL000330	270.05	-0.387	5	3	86.99	1	1	2	0.614
3	DCL000196	240.08	0.972	3	2	49.69	1	0	2	0.78
4	DCL000306	421.92	1.482	3	1	46.53	3	1	3	0.652
5	DCL000943	240.05	1.998	2	0	64.73	2	2	3	0.507
6	DCL000234	228.08	1.194	3	3	60.69	2	1	2	0.676
7	DCL000443	174.03	0.176	3	1	54.37	0	0	1	0.61
8	DCL000841	204.09	-0.622	4	1	42.85	1	0	1	0.661
9	DCL000991	346.12	0.603	4	4	80.92	0	0	3	0.481
10	DCL000976	297.09	2.157	4	1	80.38	1	1	2	0.818
11	DPR000115	297.09	2.157	4	1	80.38	1	1	2	0.818
12	DCL000314	270.05	1.408	4	2	73.12	4	4	1	0.375
13	DCL000245	346.12	0.027	6	4	141.94	2	0	4	0.398
14	DCL000373	287.06	-0.896	6	4	142.52	3	2	1	0.42
15	DCL000437	288.11	-1.24	6	2	80.85	4	1	1	0.675
16	DPR000045	250.09	-1.557	5	1	68.49	1	1	2	0.62
17	DCL000615	220.06	0.681	3	1	41.46	0	0	3	0.605
18	DCL001004	238.11	0.906	3	2	41.13	1	1	2	0.725
19	DCL000629	238.11	0.906	3	2	41.13	1	1	2	0.725
20	DCL000647	345.16	-0.543	6	3	80.18	5	1	2	0.632
21	DCL000939	343.1	-2.2	6	1	99.79	7	1	3	0.489

STEP6: Check the 'Summery' tab of Drug likeness rules to see the total number of candidate among the molecules passing and violating all the rules.



Selected Filters	Total Number of Molecule Filter	Total Number of Molecule Violated the Rule
Lipinski's Rule of Five	21	0
Ghose_Filter	3	18
CMC-50 Like Rule	0	21
Vebers Rule	19	2
MDDR Like Rule	1	20
BBB Likeness Rule	0	21
Unweighted QED	20	1
Weighted QED	19	2
All Selected Filters	0	21



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