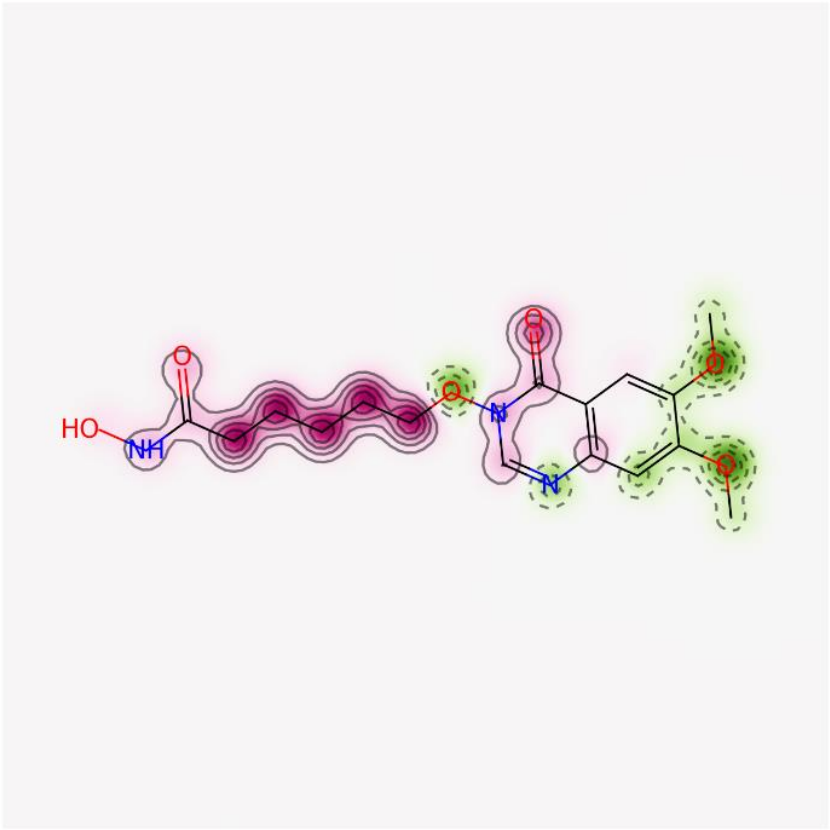
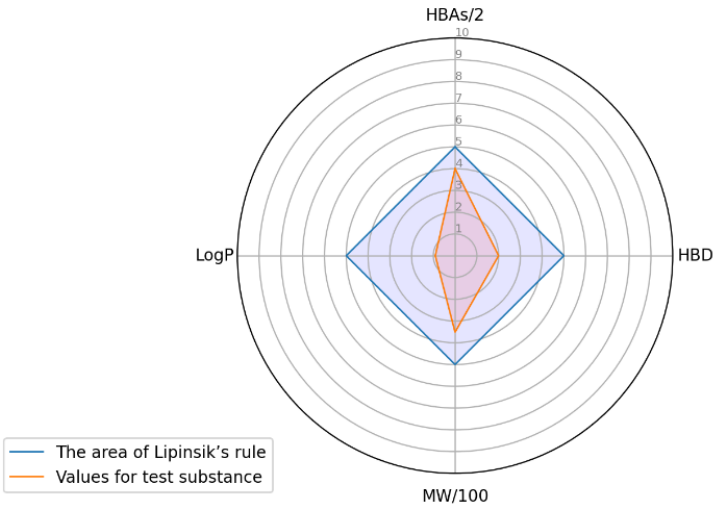
Compound V-1

The chemical fragments are colored in green (predicted to reduce inhibitory activity) or magenta (predicted to increase activity HDAC6 inhibitors). The gray isolines separate positive and negative contributions.

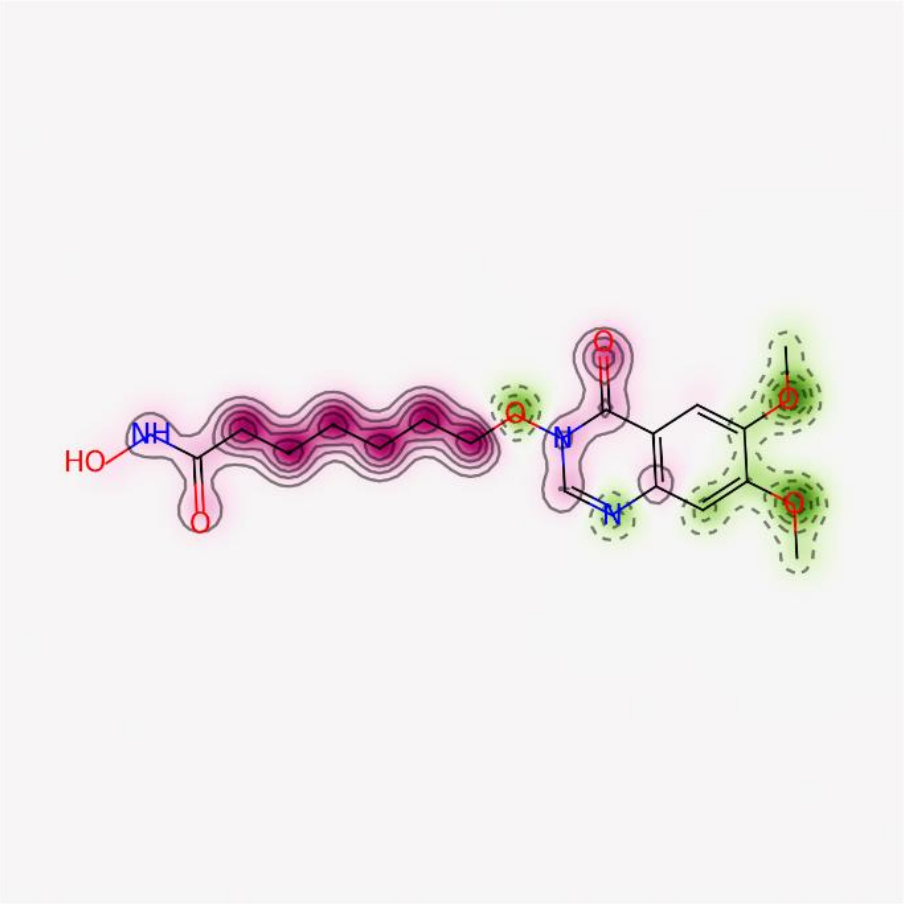
Predicted fragments contribution for compound number 1:

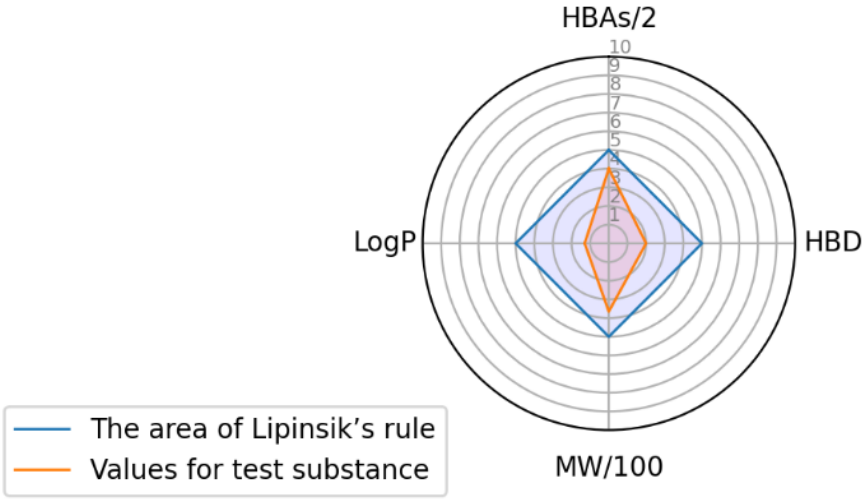




	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	351.3590	500.0000
Octanol-water coefficient(LogP)	0.9081	5.0000
Number of hydrogen bond donors (HBD)	2.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	8.0000	10.0000

Predicted fragments contribution for compound number 2:

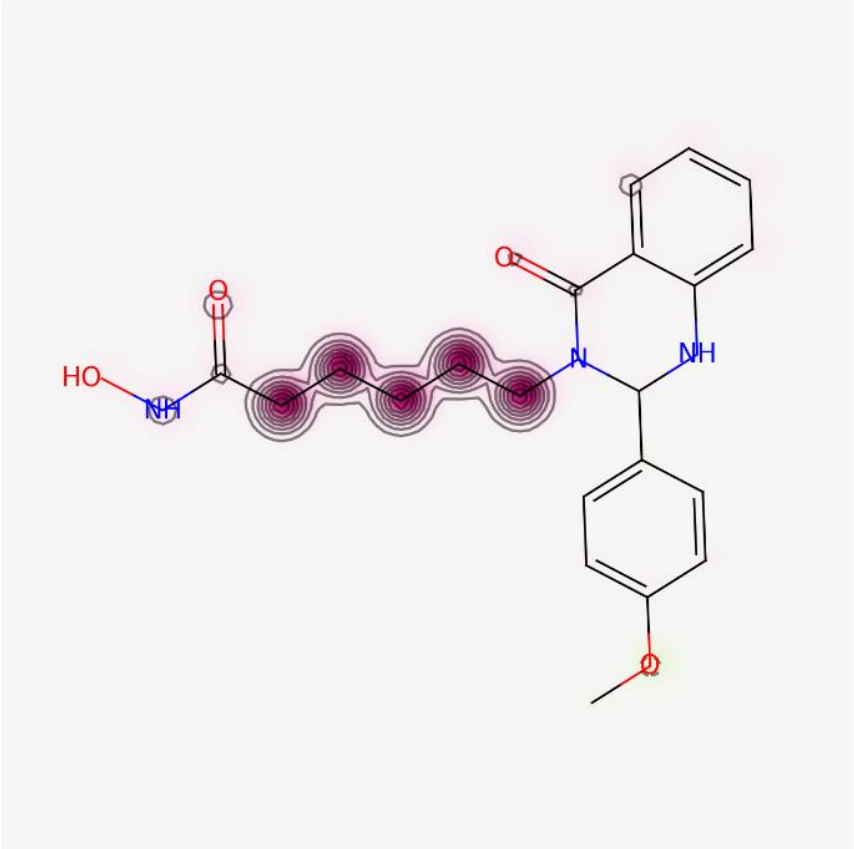


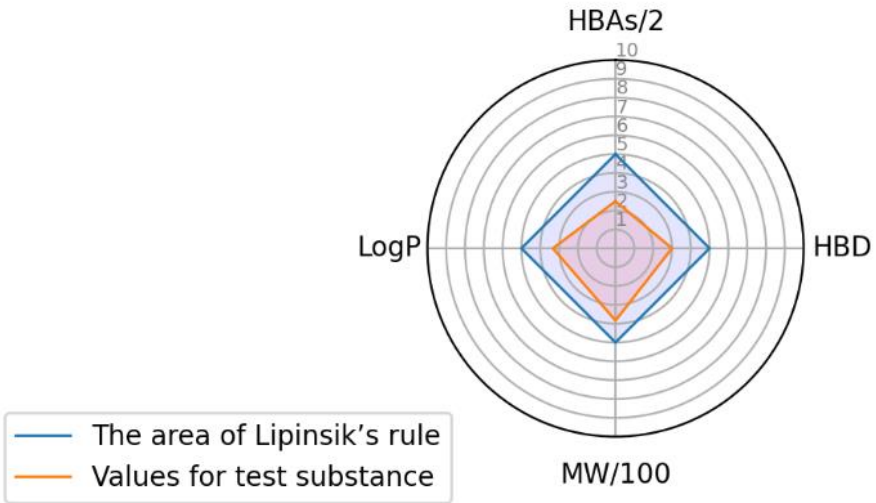


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	365.3860	500.0000
Octanol-water coefficient(LogP)	1.2982	5.0000
Number of hydrogen bond donors (HBD)	2.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	8.0000	10.0000

Compound V-5

Predicted fragments contribution for compound number 5:

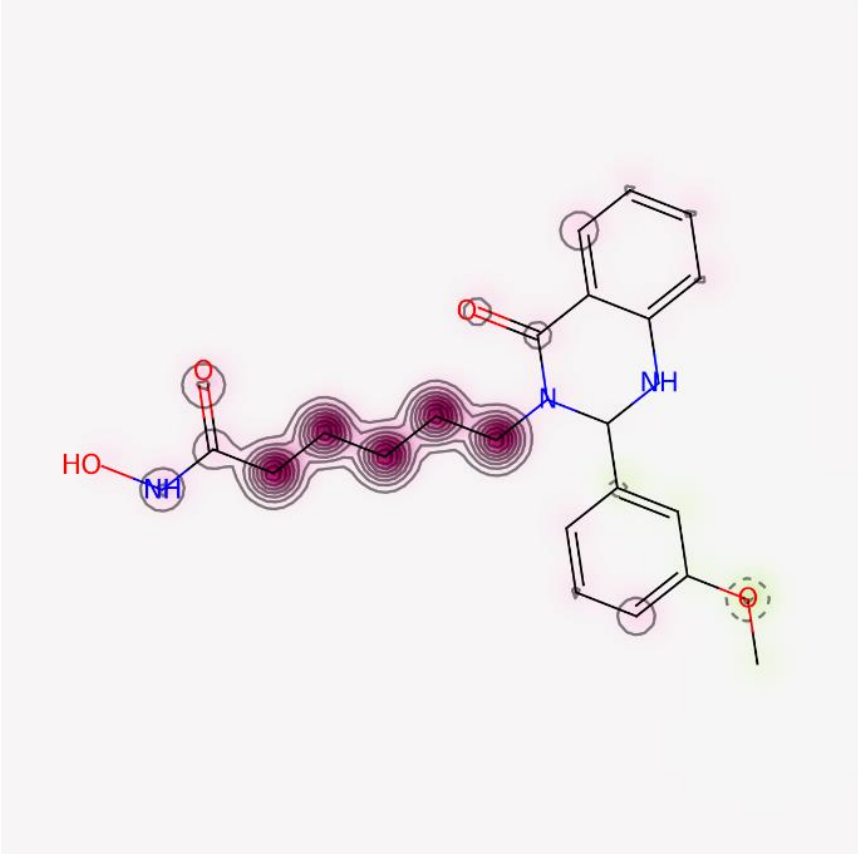


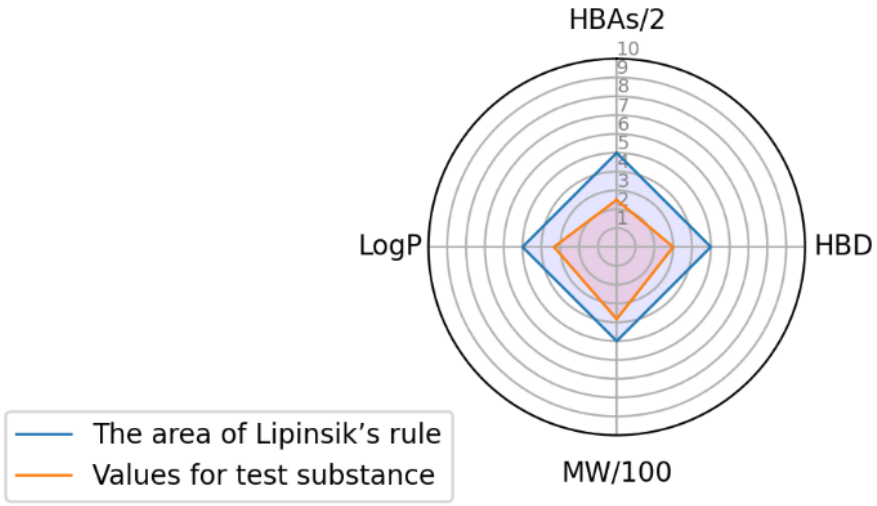


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	383.4480	500.0000
Octanol-water coefficient(LogP)	3.3275	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	5.0000	10.0000

Compound V-6

Predicted fragments contribution for compound number 6:

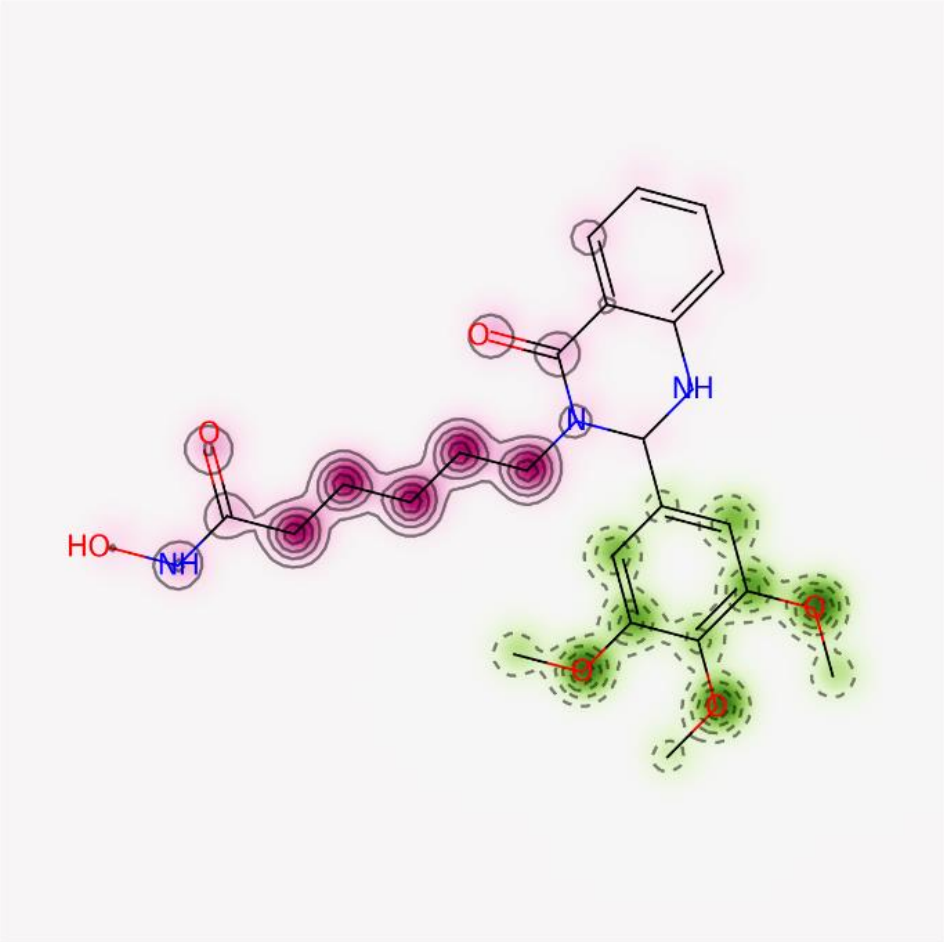


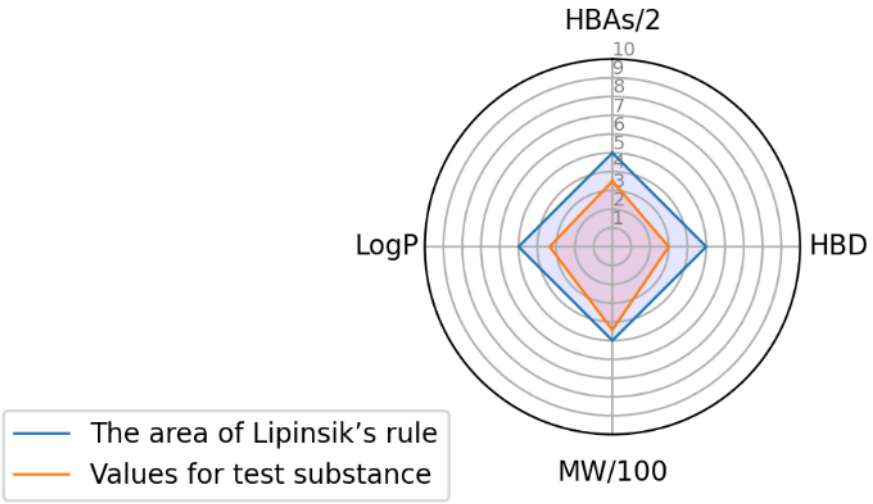


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	383.4480	500.0000
Octanol-water coefficient(LogP)	3.3275	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	5.0000	10.0000

Compound V-7

Predicted fragments contribution for compound number 7:

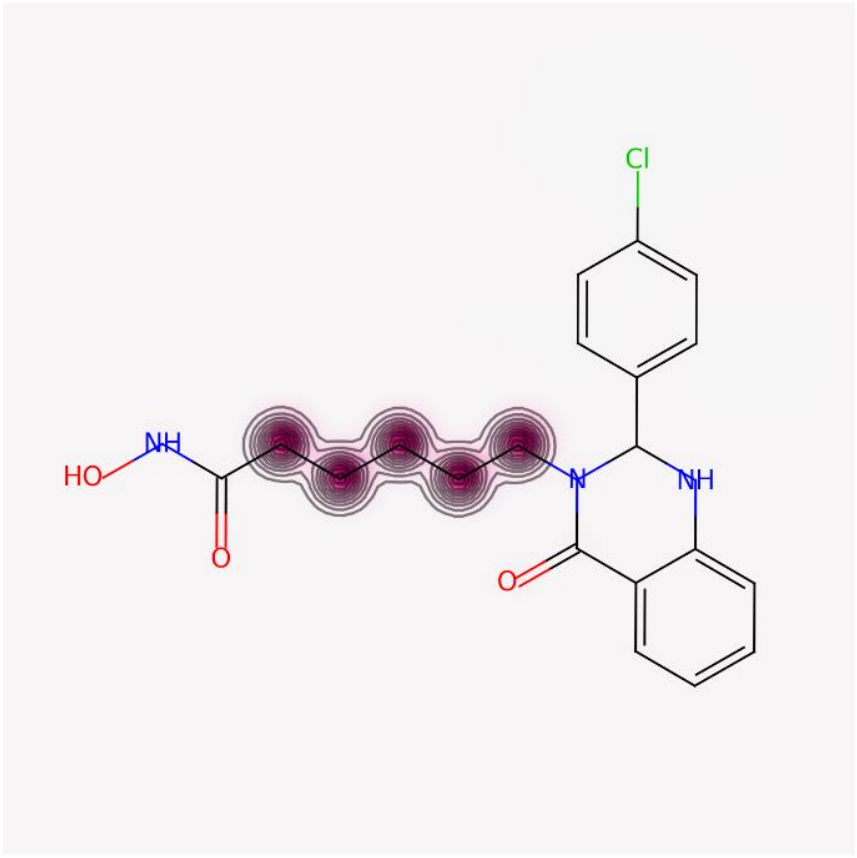


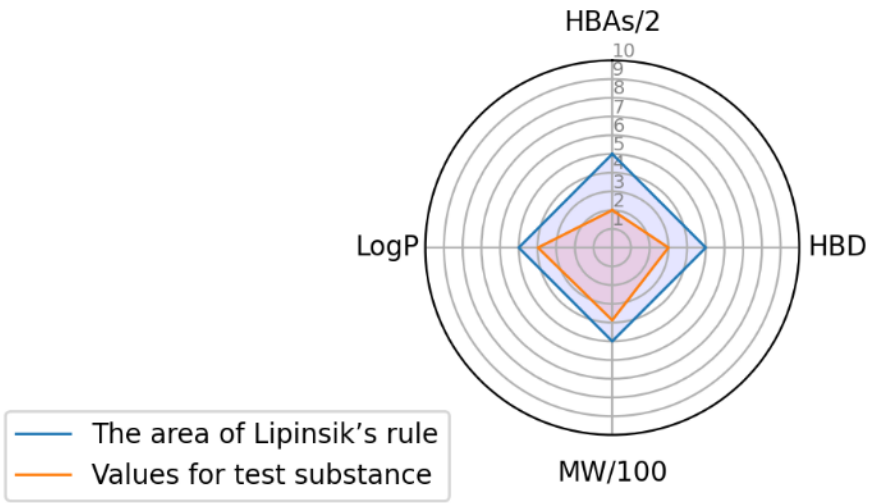


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	443.5000	500.0000
Octanol-water coefficient(LogP)	3.3447	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	7.0000	10.0000

Compound V-8

Predicted fragments contribution for compound number 8:

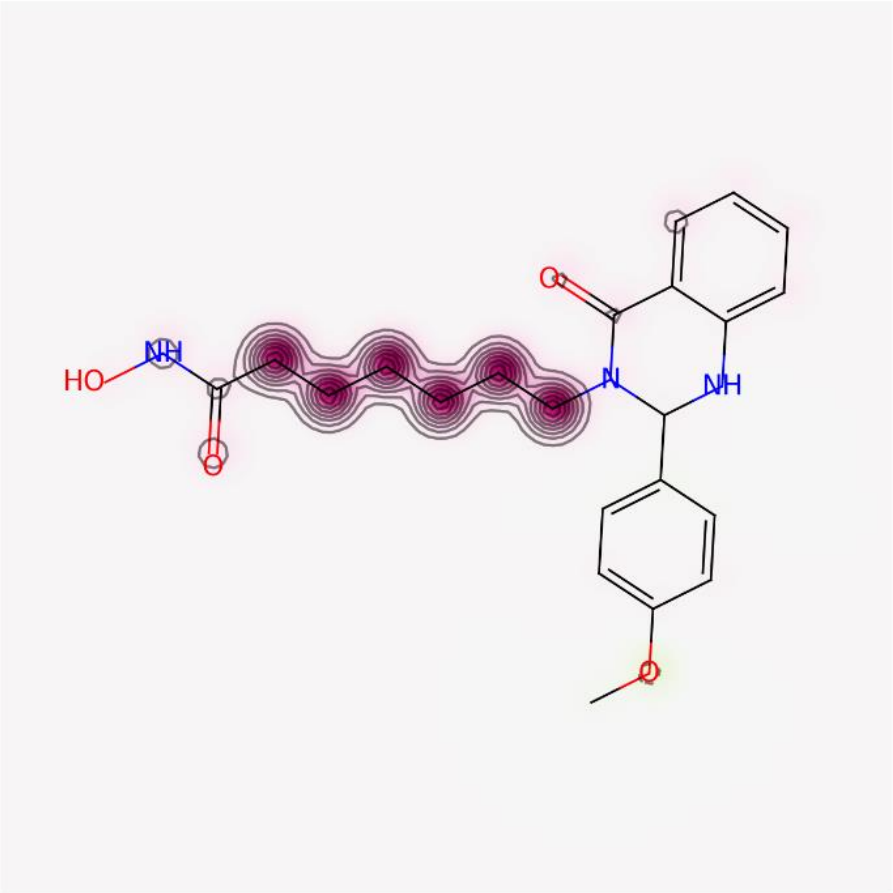


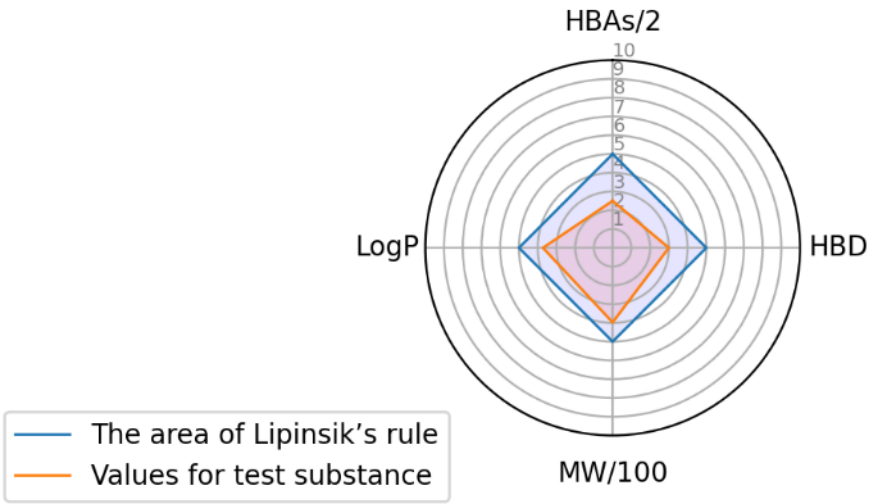


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	387.8670	500.0000
Octanol-water coefficient(LogP)	3.9723	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	4.0000	10.0000

Compound V-10

Predicted fragments contribution for compound number 10:

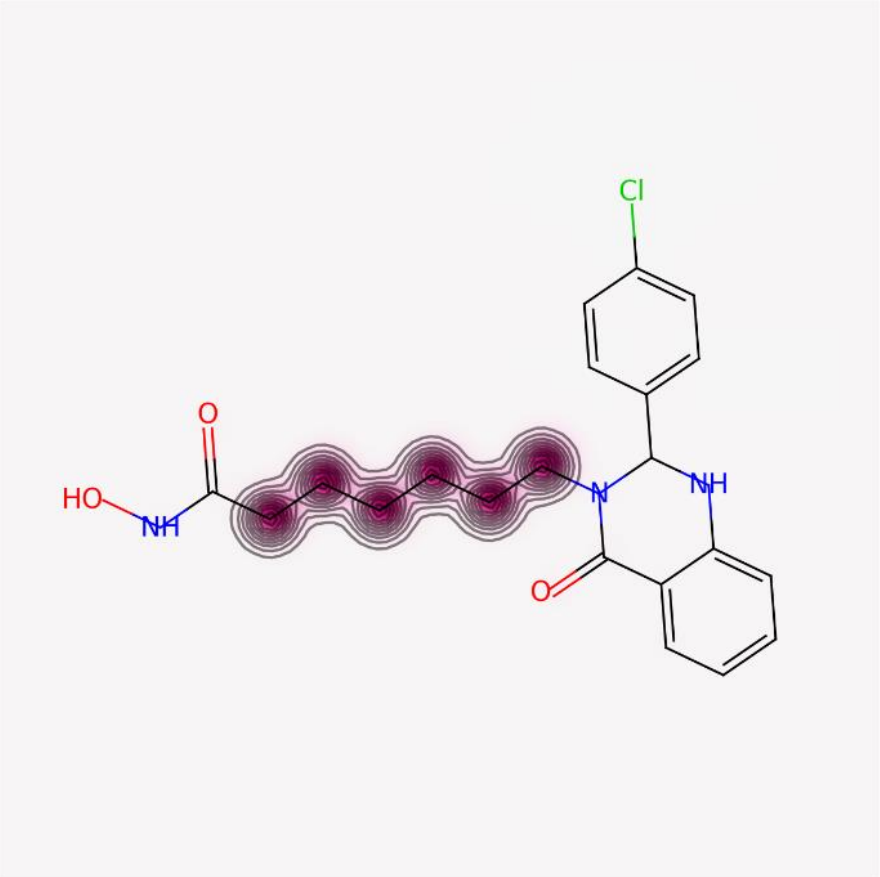


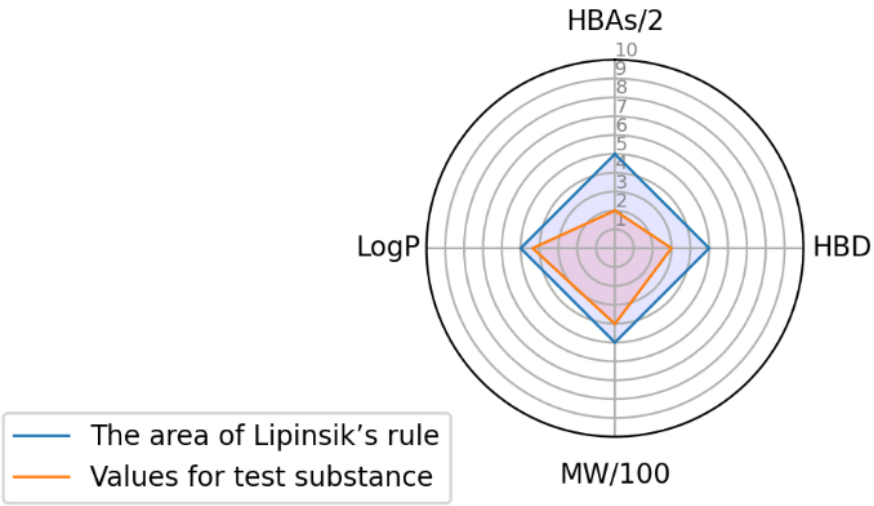


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	397.4750	500.0000
Octanol-water coefficient(LogP)	3.7176	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	5.0000	10.0000

Compound V-11

Predicted fragments contribution for compound number 11:

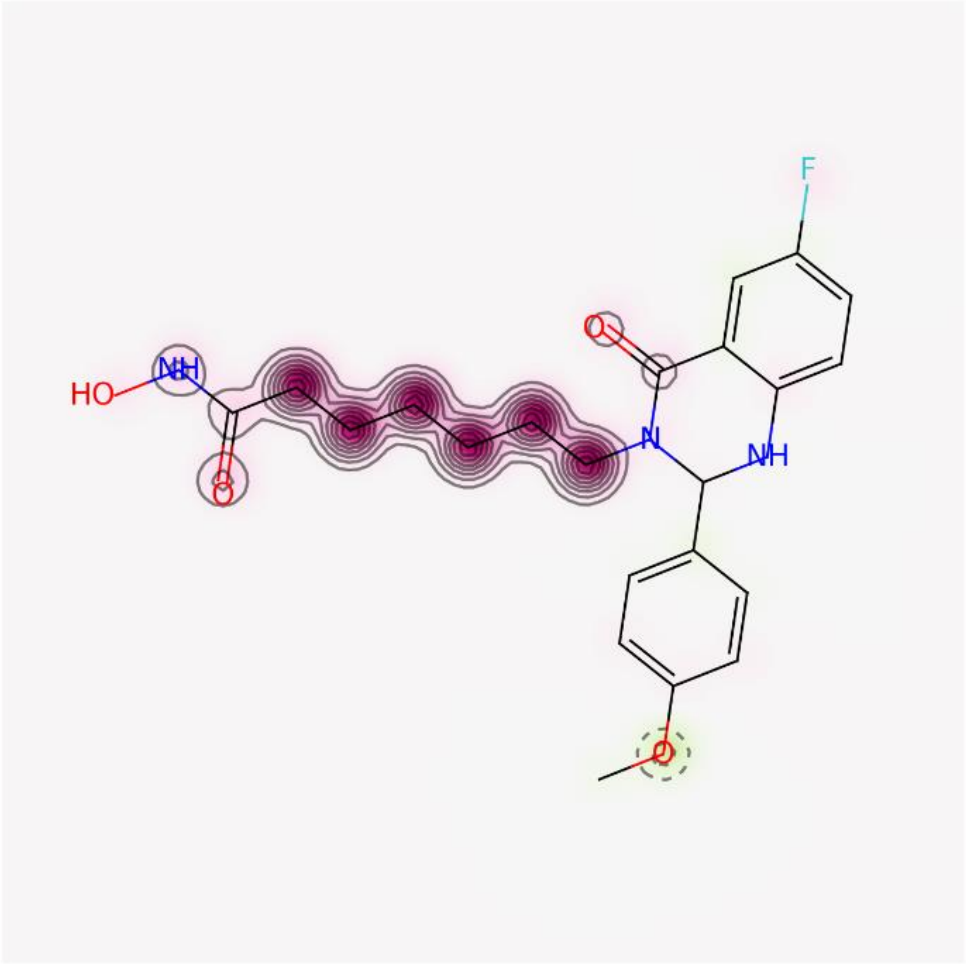


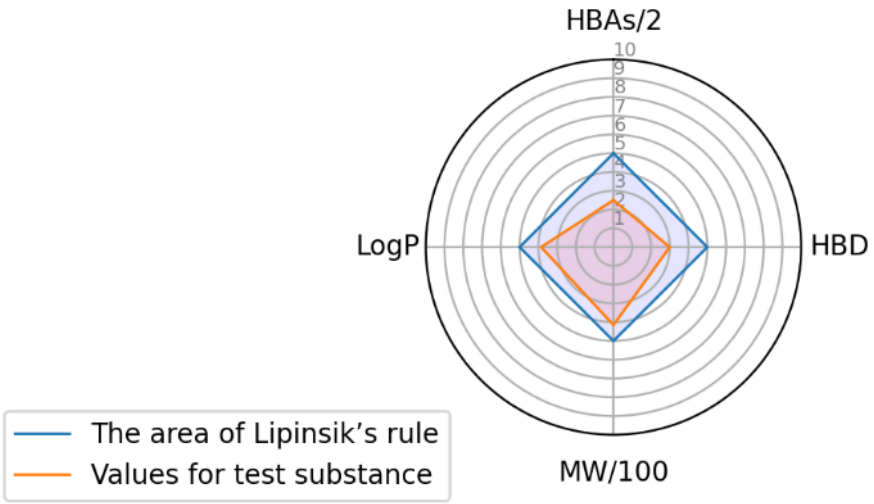


	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	401.8940	500.0000
Octanol-water coefficient(LogP)	4.3624	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	4.0000	10.0000

Compound V-12

Predicted fragments contribution for compound number 12:





	Values for the test substance	Reference value of Lipinsik's rule
Molecular weight(MW), Da	415.4650	500.0000
Octanol-water coefficient(LogP)	3.8567	5.0000
Number of hydrogen bond donors (HBD)	3.0000	5.0000
Number of hydrogen bond acceptors(HBAs)	5.0000	10.0000