Modeling of NETROPSIN and PROFLAVIN molecules and their components in the programm HyperChem

PERFORMED BY
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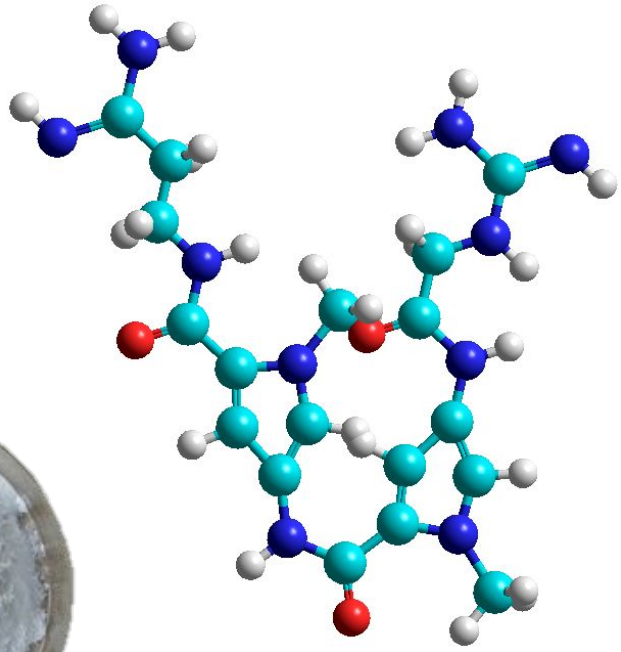
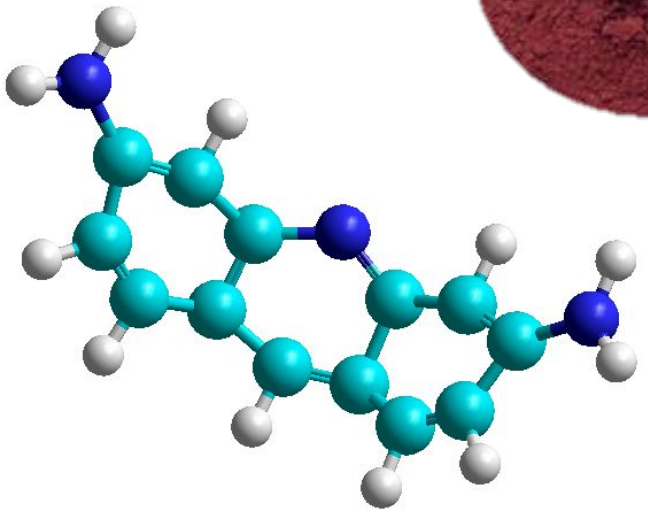
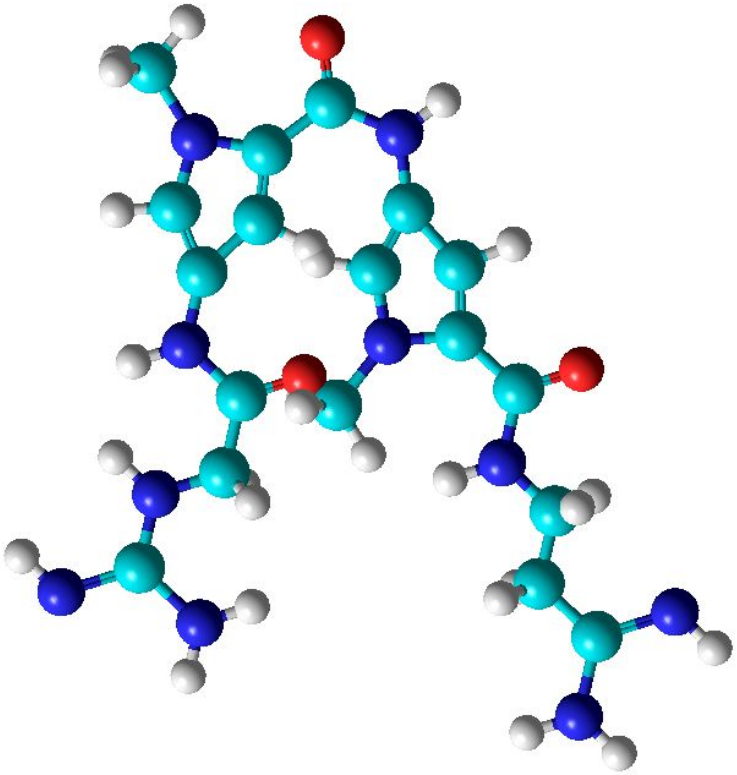
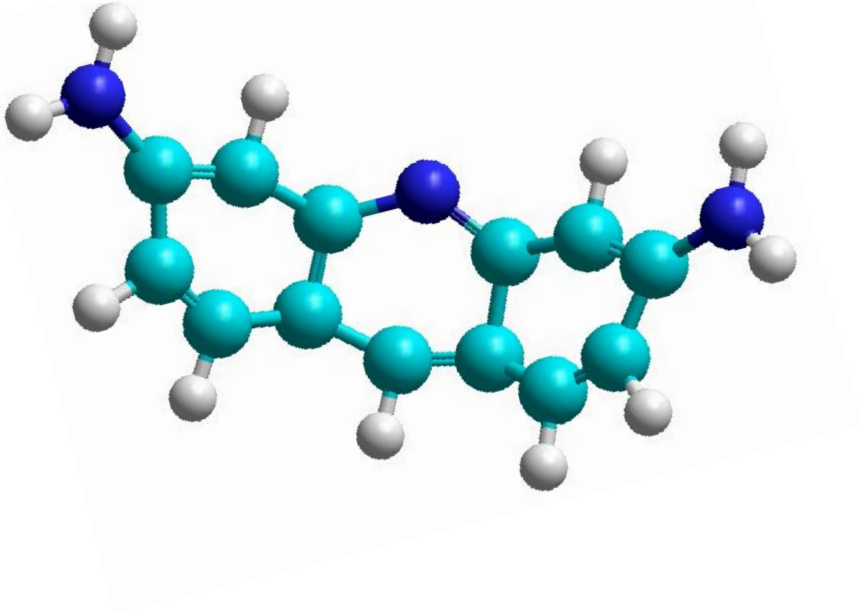
Physical-chemical and medical-biological properties of Netropsin (NT) and Proflavine (PF)



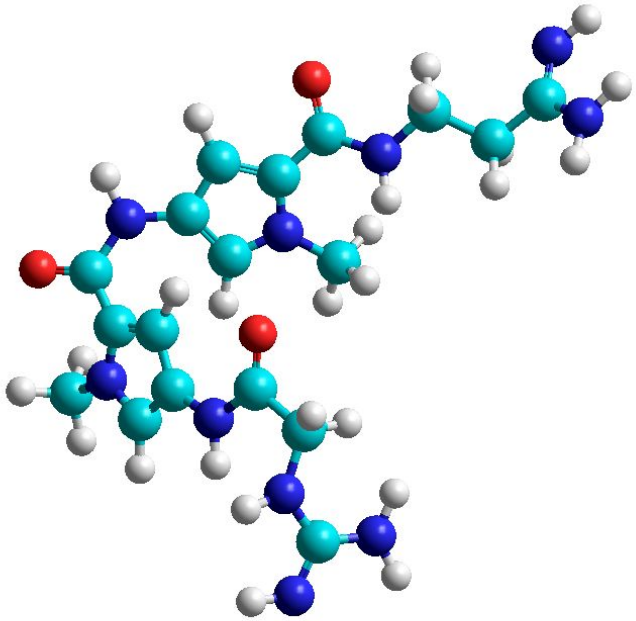


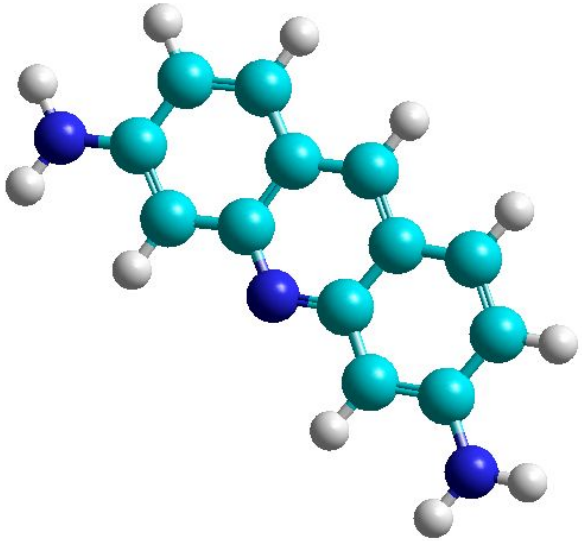
Building molecules of Netropsin (NT) and Proflavine (PF).





Optimization of molecules



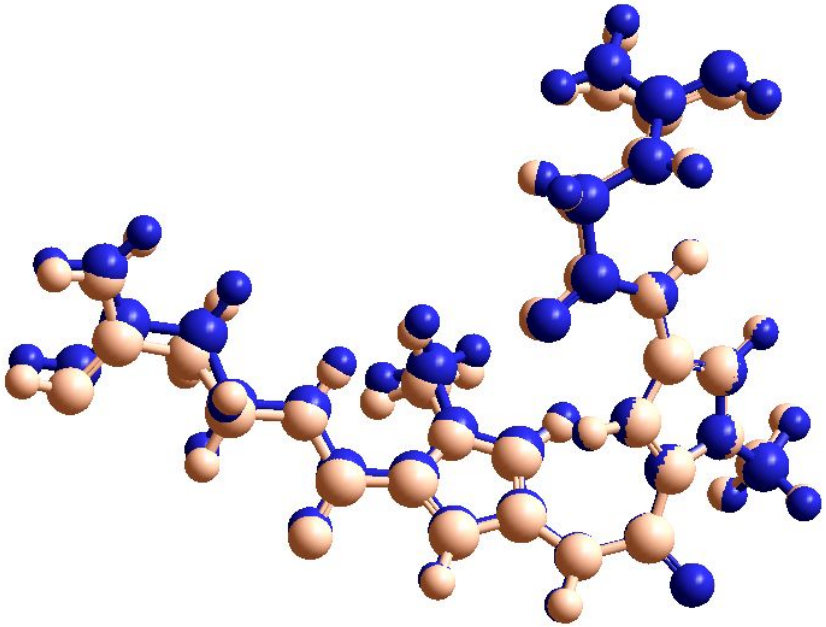


Netropsin: E = 31,509668; RMS = 0,075803;
Proflavine: E = 7,655725; RMS = 0,089366.

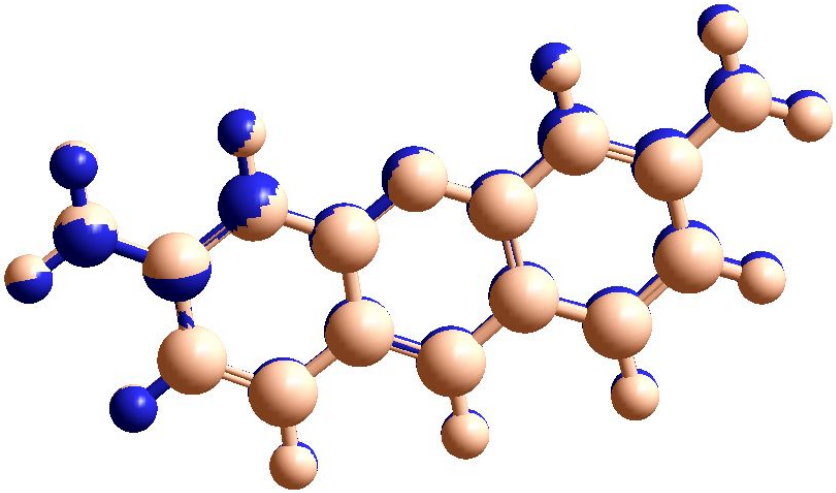
Table 1. – Value optimization energy for molecules of NETROPSIN (NT) and PROFLAVINE (PF).

File name (code_note)	E,kcal/mole	RMS
Netropsin _MM+	31,509668	0,075608
Netropsin _Amber	44,633885	0,098903
Netropsin _Opls	38,566350	0,098913
Proflavine _MM+	7,655725	0,089508
Proflavine _Amber	5,499304	0,084114
Proflavine _Opls	0,102601	0,097114
Netropsin _wat	-2027,357365	2,258891
Proflavine _wat	-883,859240	0,275568
Netropsin _bank	202,682824	78,483063
Proflavine _bank	116,466244	85,524866

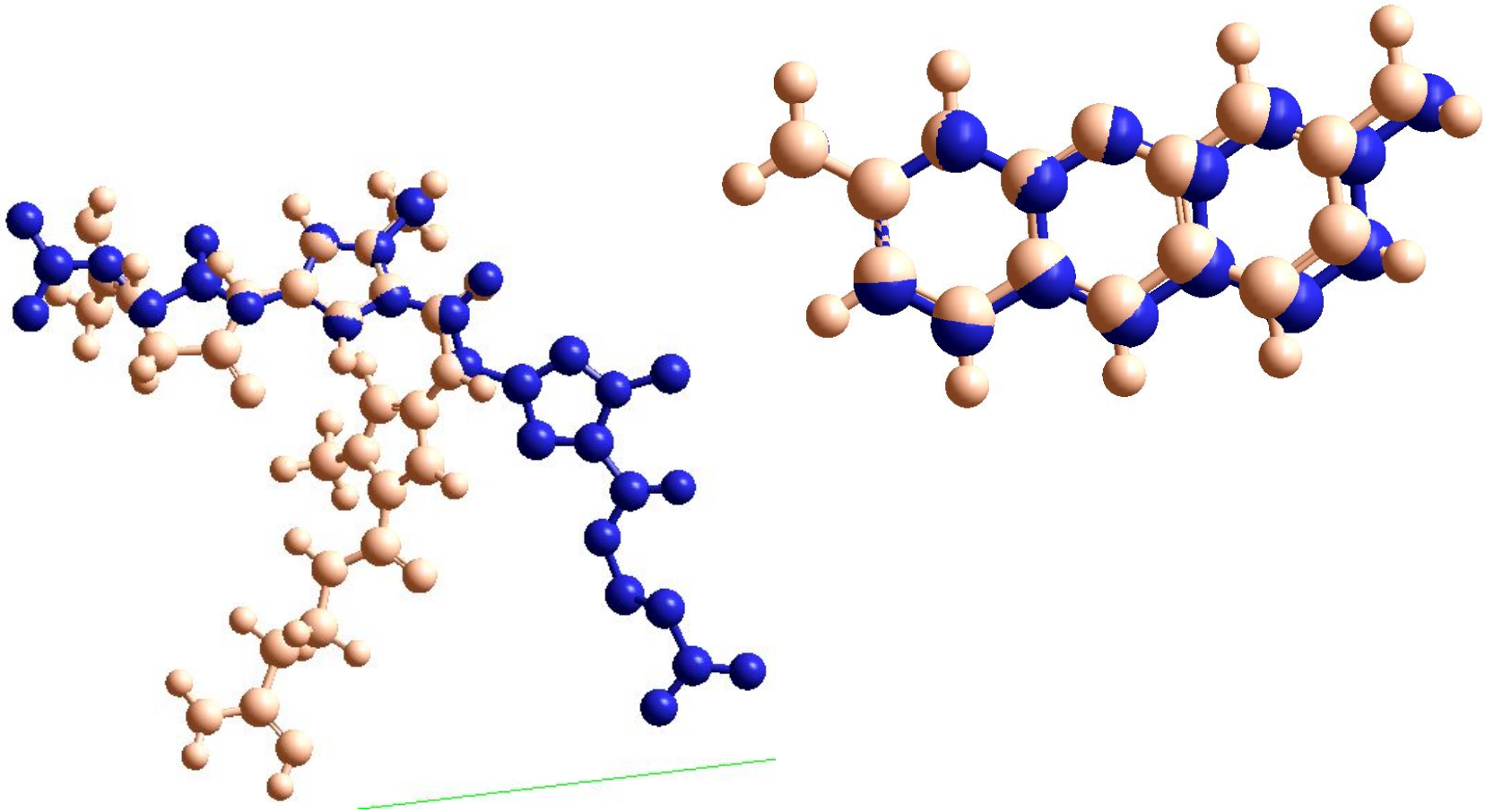
Comparison spatial forms of molecule in a vacuum, in a solution, in a complex



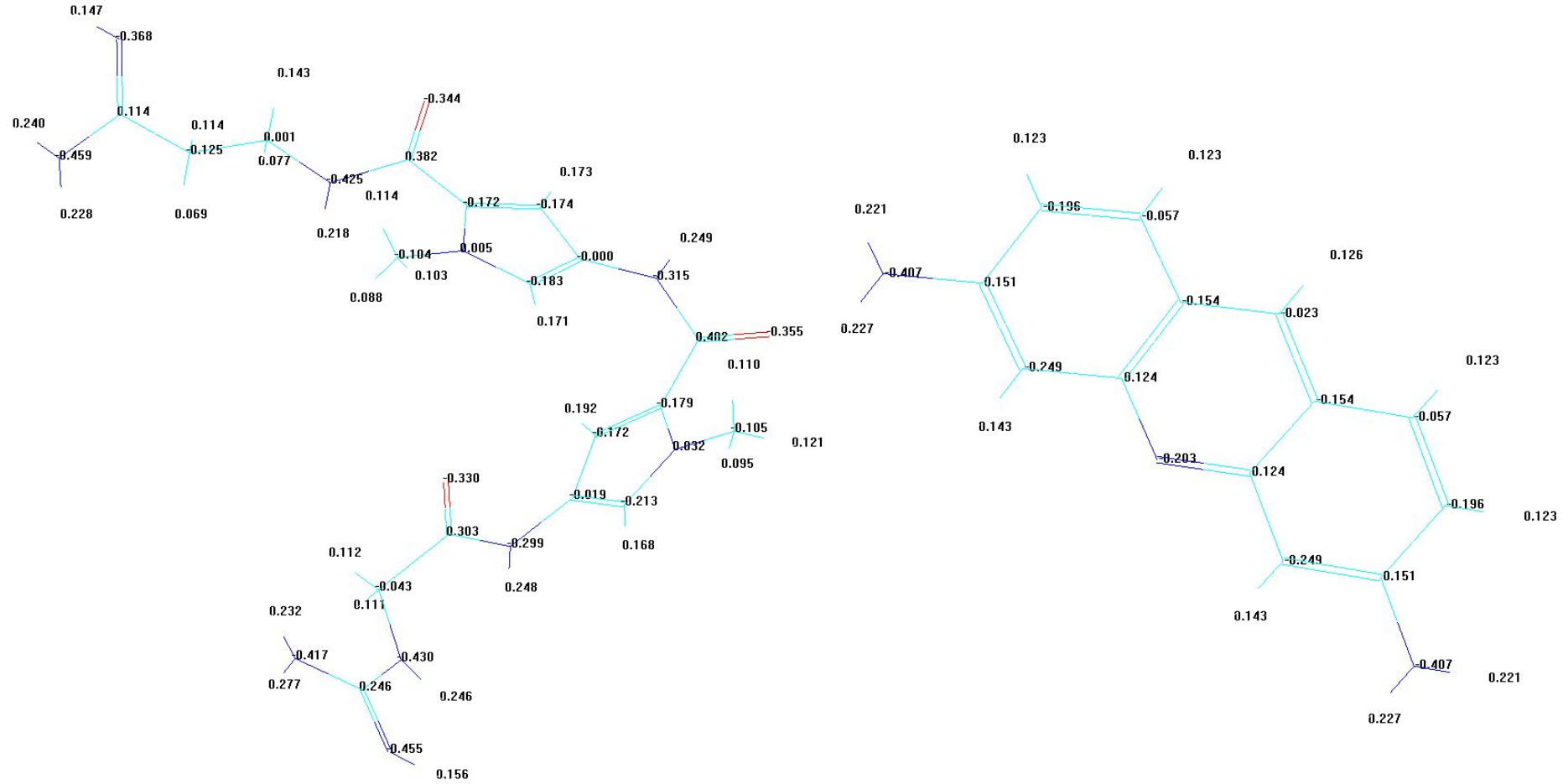
Solv and optim



Solv and bank

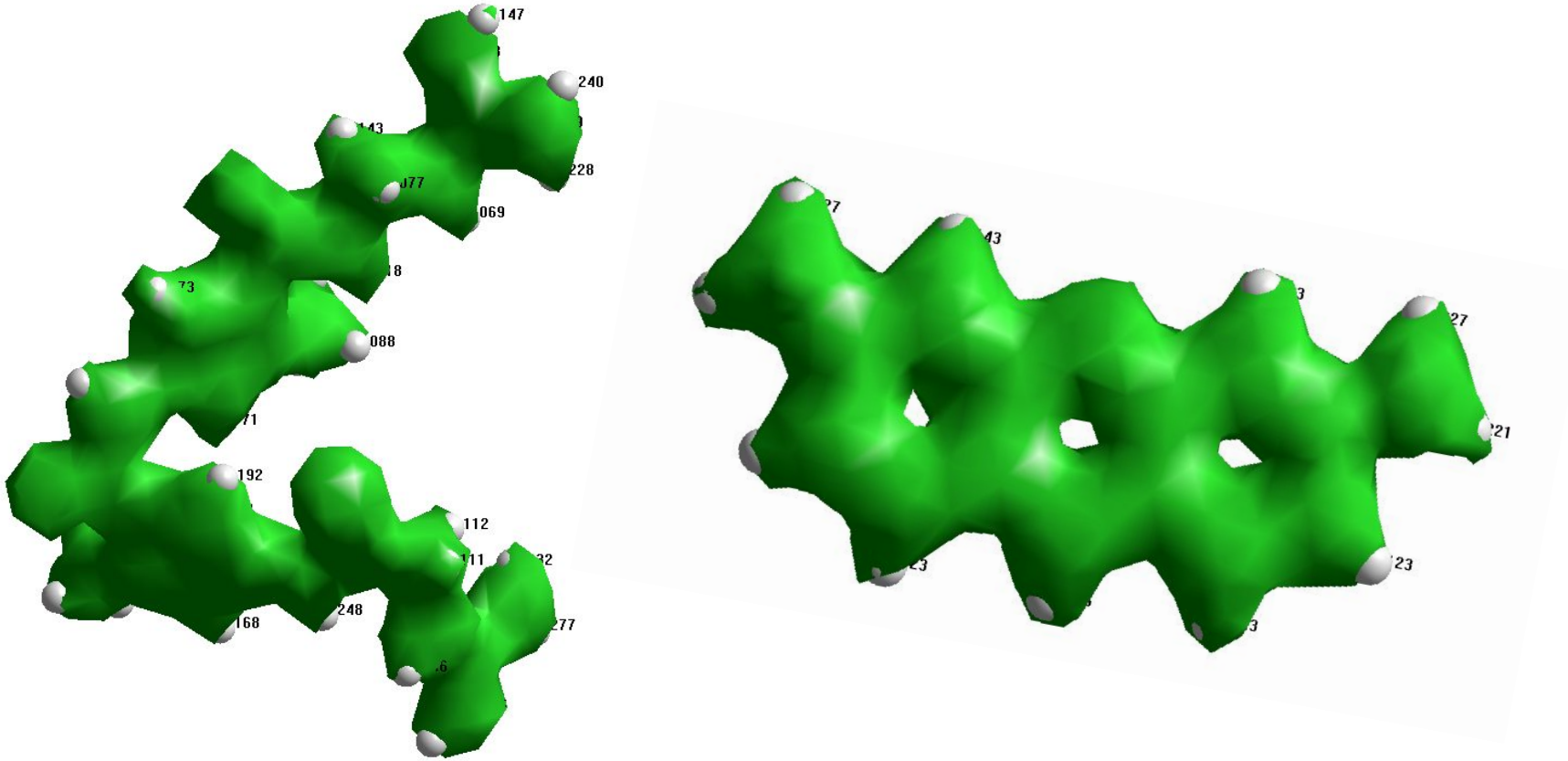


STUDYING THE PROPERTIES OF MOLECULES. THE CHARGES OF MOLECULES

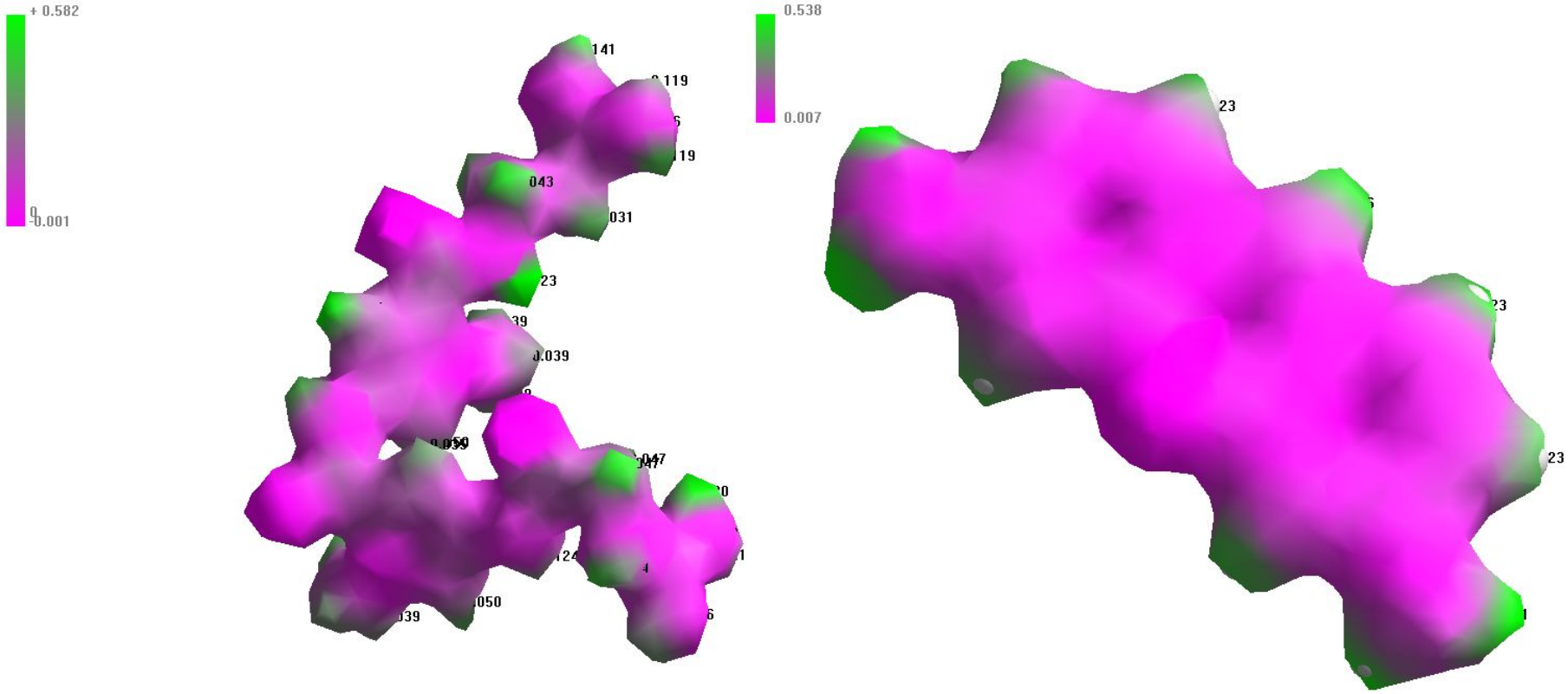


Plotting different properties of a molecule

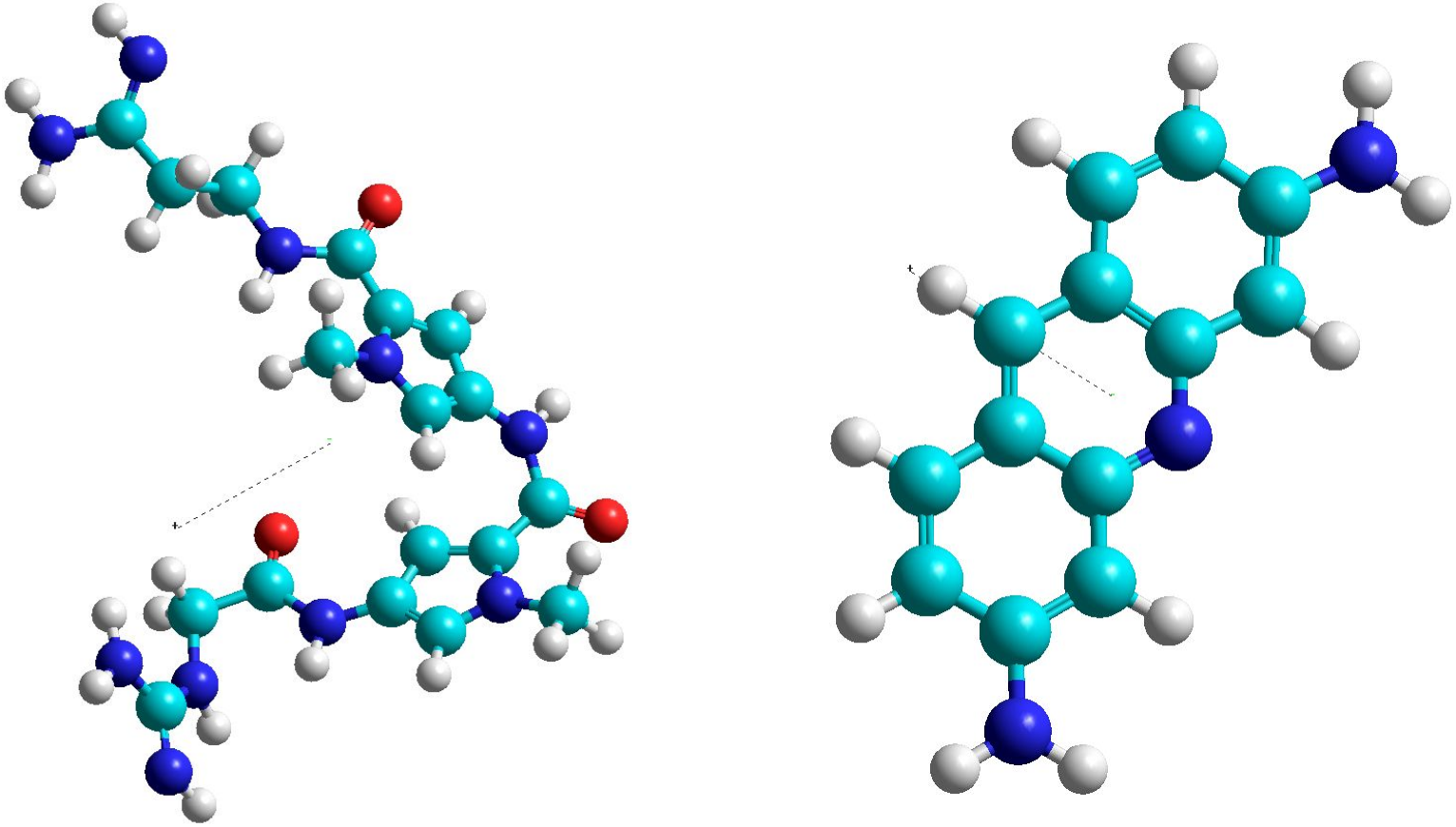
Graph of the charge density of molecules



Graph electrostatic potential of molecules Netrospin (NT) and Proflavine (PV)



Dipole moment of molecules Netrospin (NT) and Proflavine (NT)

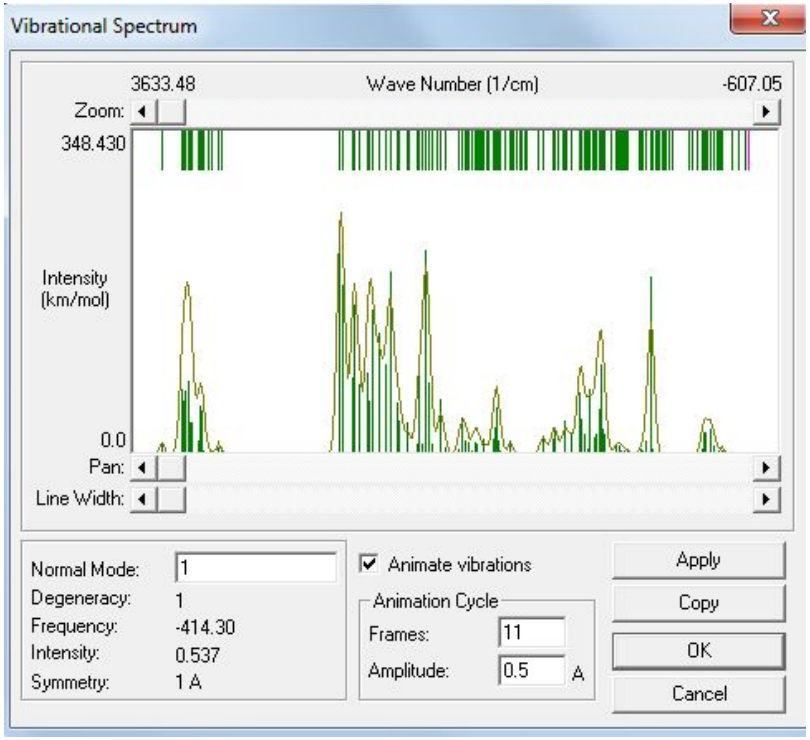


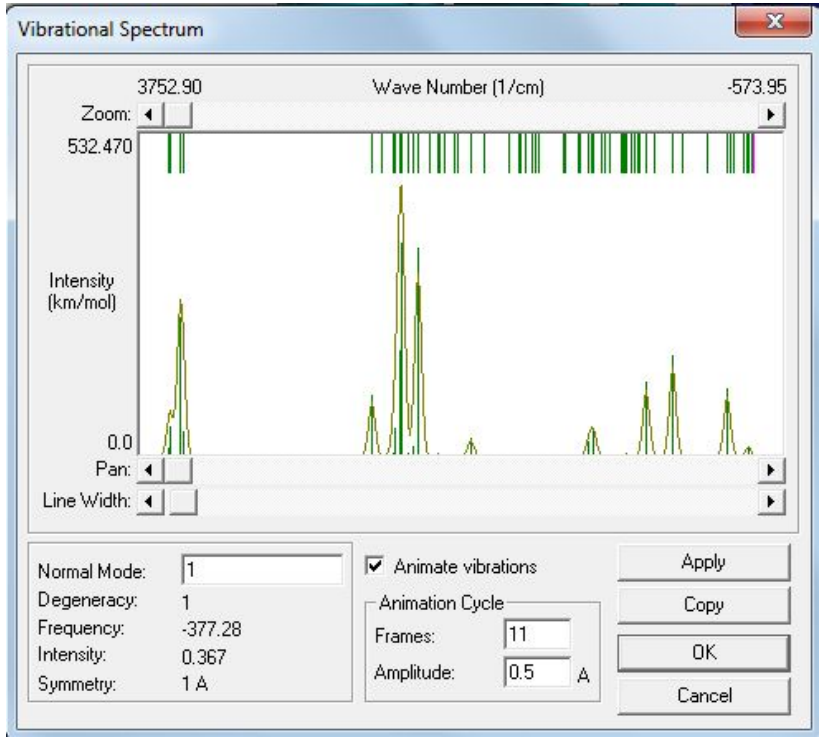
Netrospin (NT): 6,2702 (3,72431; -4,86833; 1,32067)
Proflavine (PF): 1,95123 (1,88099; -0,00991577; 0,518722).

Table 2. – Properties of molecules Netropsin (NT) and Proflavine (PF).

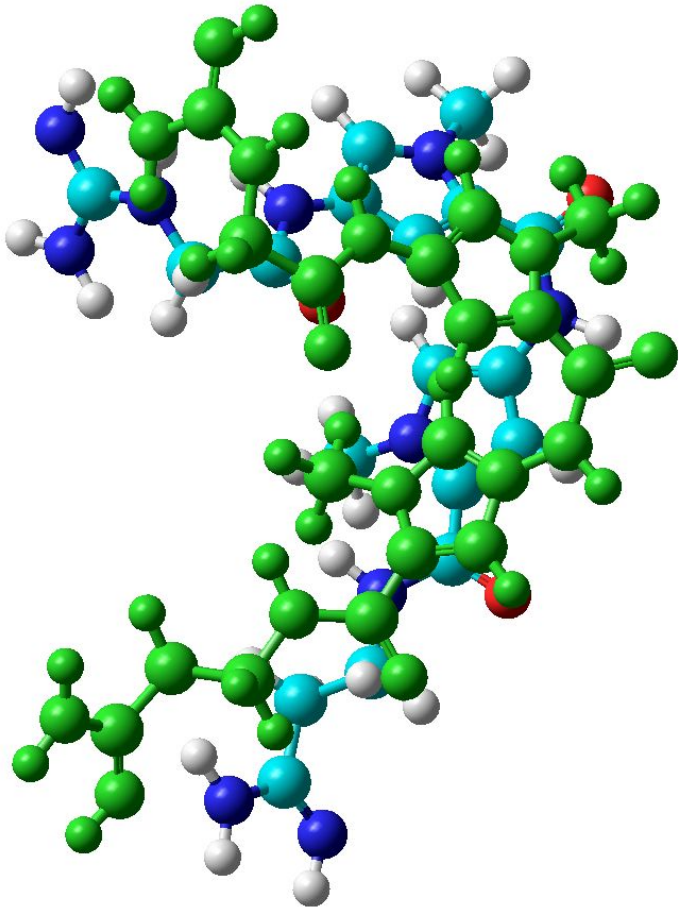
Molecule	Weight a.m.u.	Volume, A°	Surface area, A°	Energy hydration, kcal/mole	Polarizability, A°
NT	430,47	1198,30	700,84	-28,82	44,42
PF	209,25	614,63	395,29	-12,80	24,79

Analysis of molecular vibration, vibrational spectrum

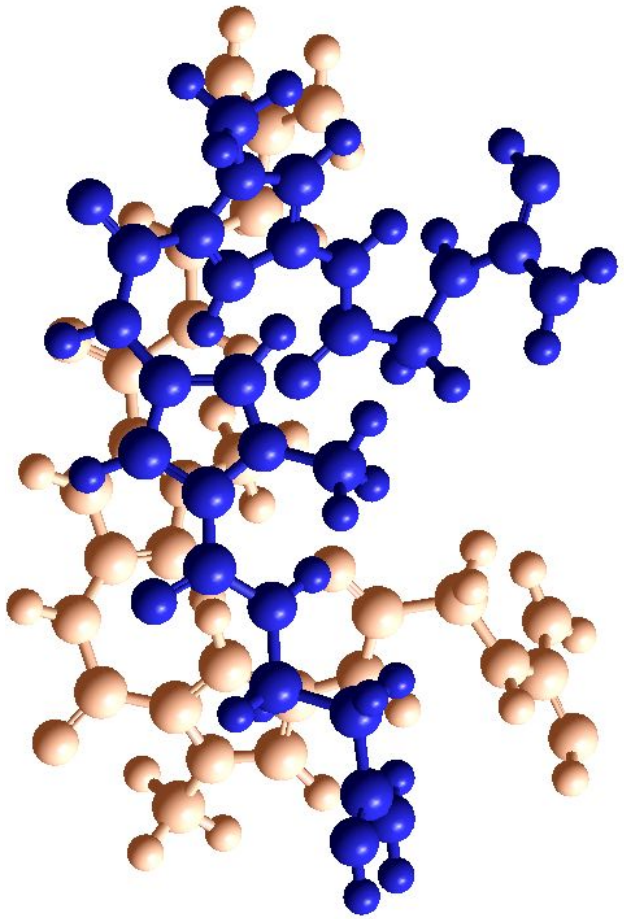


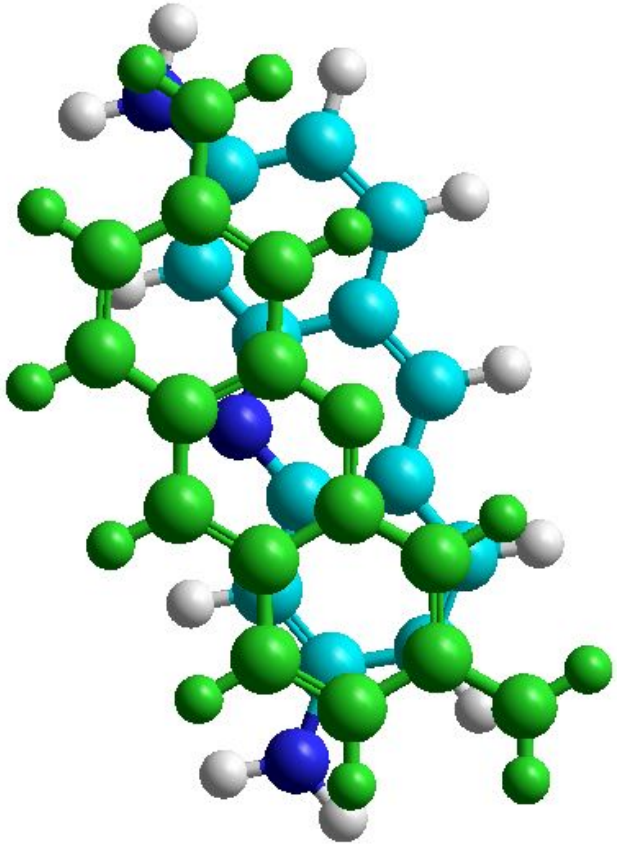


Construction of complexes self- and heteroassociative molecules

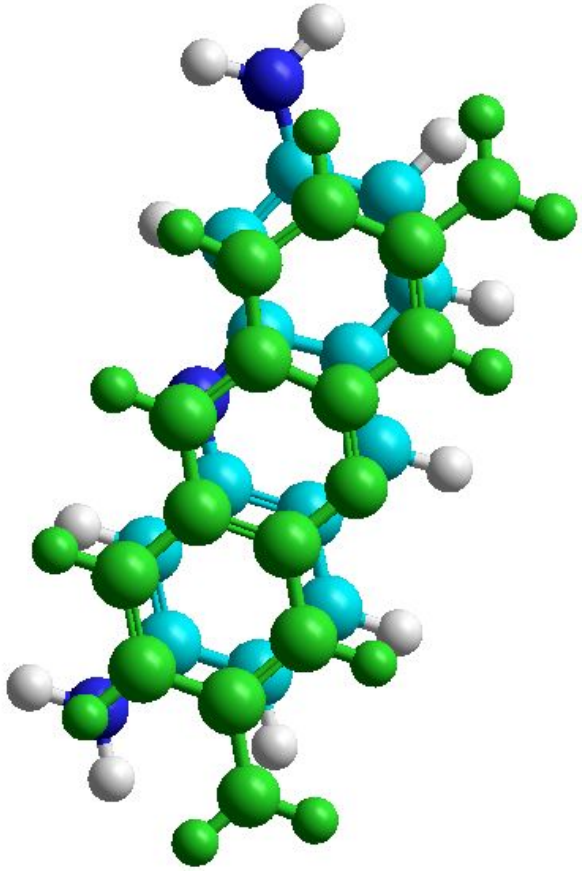


NT+NT mirror view E, kcal/mole	NT+NT inverted view E, kcal/mole
49,578064	47,822402
50,165792	50,452112
53,082138	52,394744
52,909504	55,156603
53,219878	56,046870
52,887072	55,480298
55,347948	55,852464
55,418850	55,438045
48,574037	57,272633
46,714748	50,916940

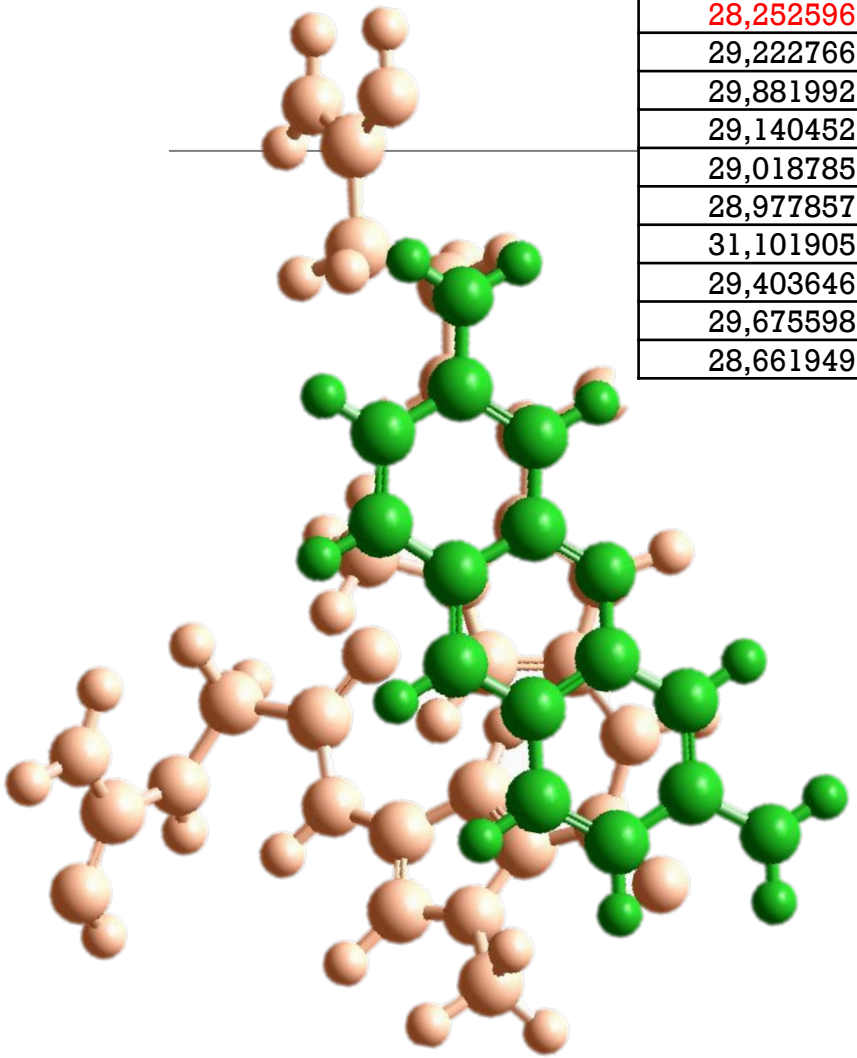


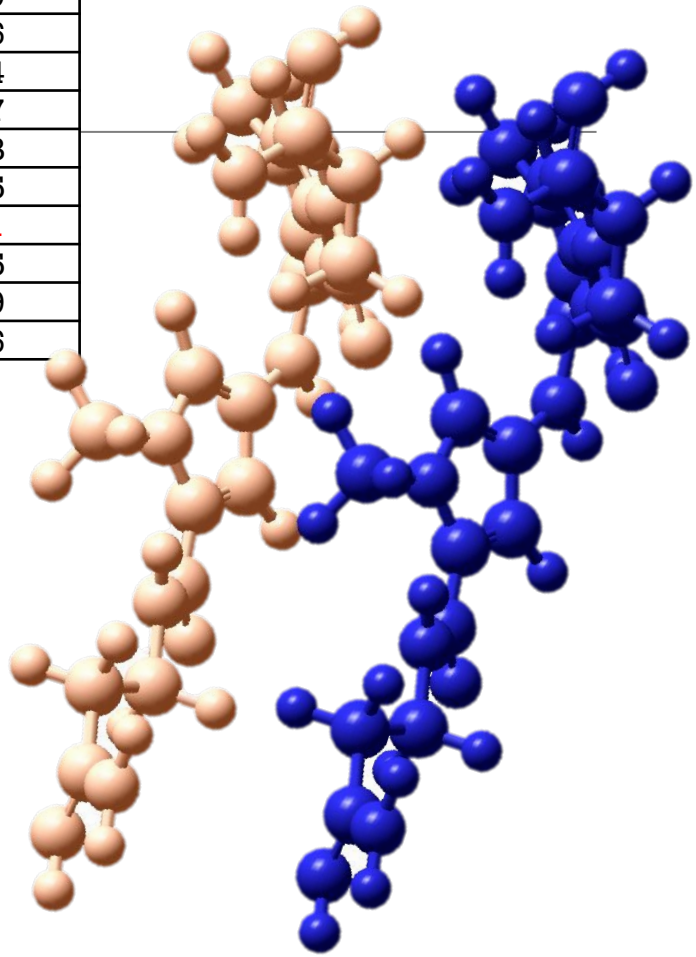


PF+PF mirror view E, kcal/mole	PF+PF inverted view E, kcal/mole
6,840576	6,313925
6,931889	6,906868
7,061646	7,460723
7,370815	7,219102
6,481654	6,803258
6,501249	6,858817
7,175762	7,073690
7,442332	7,382245
7,482286	6,924973
6,786648	6,313924



NT+PF mirror view E, kcal/mole	NT+PF inverted view E, kcal/mole
28,252596	27,516909
29,222766	27,761096
29,881992	28,963064
29,140452	29,278117
29,018785	28,956403
28,977857	28,852435
31,101905	27,430621
29,403646	28,403225
29,675598	28,764909
28,661949	28,807976





Calculating the energy of hydrophobic interactions and studying the behavior dynamic of a molecular complex

$$G_1 = 31{,}509668$$

$$G_2 = 7{,}655725$$

$$G_3 = 28{,}54897$$

$$\Delta G_{мм} = G_3 - (G_1 + G_2)$$

$$\Delta G_{мм} = 28{,}542897 - (31{,}509668 + 7{,}655725) = -10{,}622496$$

$$A_{AB} = 269{,}77\ A°$$

$$A_{A} = 679{,}63\ A°$$

$$A_{B} = 393{,}35\ A°$$

$$\Delta A = A_{AB} - A_{A} - A_{B}$$

$$\Delta A = 269{,}77 - 679{,}63 - 393{,}35 = -803{,}21\ (A°)$$

$$\Delta G_{ВДВ} = \gamma_{ВДВ} * \Delta A$$

$$\Delta G_{ВДВ} = (-38.8) * (-803,21) = 31164,548 \text{ (кал/моль*А°)},$$

$$\Delta G_{гф} = \gamma_{гф} * \Delta A$$

$$\Delta G_{гф} = 46 * (-803,21) = -36947,66 \text{ (кал/моль*А°)}$$

$$\Delta G_{сольв} = \Delta G_{ВДВ} + \Delta G_{гф}$$

$$\Delta G_{сольв} = (\gamma_{ВДВ} + \gamma_{гф}) * \Delta A = \gamma * \Delta A = 7,2 * (-803,21) = -5783,112$$

During the research:

- The molecules of NETROPSIN (NT) and PROFLAVINE(PF) were constructed ;

- Energies were calculated and structures of molecules were optimized;

- Properties of molecules were investigated ;

- Complexes of self- and heteroassociative molecules were constructed.