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The prediction on the acute toxicity of Nigella damascena fatty and essential oils

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Topicality: *in silico* methods are the pre-experimental analysis of substances. Due to the GUSAR Acute Rat Toxicity program, it is possible to predict acute toxic effects of substances in rats under *in silico* conditions, which will enable to predict the result of the experiment *in vitro*.

Purpose: to determine the acute toxic effect of *Nigella damascena* fatty and essential oils by *in silico* methods.

Materials and methods of the research: *In silico* prediction of LD50 values for rats by four types of administration (oral, intravenous, intraabdominal, subcutaneous, inhalation) using GUSAR Acute Rat Toxicity computer program. The following fatty acids (myristic acid, palmitoleic acid, arachidonic acid, oleic acid, palmitic acid, stearic acid, linoleic acid) and essential oils (thymoquinone, carvone, limonene, p-cymene, trans-anethole) oil have been selected for computer screening.

Results: This computer program is based on the SYMYX MDL toxicity database, which includes information on 1000 chemical structures with acute toxicity data in rats represented by LD50 values.

The following results have been obtained: essential oil (1. Thymoquinone: intraperitoneal injection in rats (IP) LD50 = 292,9 mg/kg; intravenous injection in rats (IV) LD50 = 41,03 mg/kg; oral administration in rats (Oral) LD50 = 1979 mg/kg; subcutaneous injection in rats (SC) LD50 = 689,8 mg/kg. 2. Carvone: Rat IP LD_{50} = 121,8 mg/kg; Rat IV LD_{50} = 34,7 mg/kg; Rat Oral LD_{50} = 1432 mg/kg; Rat SC LD_{50} = 162,9 mg/kg. 3. Limonene: Rat IP LD50 = 139,4 mg/kg; Rat IV LD50 = 35,58 mg/kg; Rat Oral LD50 = 2167 mg/kg; Rat SC LD50 = 162,1 mg/kg. 4. p-cymene: Rat IP LD50 = 722,5 mg/kg; Rat IV LD50 = 37,49 mg/kg; Rat Oral LD_{50} = 2786 mg/kg; Rat SC LD50 = 511,7 mg/kg. 5. trans-anethole: Rat IP LD50 = 559,6 mg/kg; Rat IV LD50 = 58,77 mg/kg; Rat Oral LD50 = 3243 mg/kg; Rat SC LD50 = 1085 mg/kg) and fatty oil (1. Stearic acid: Rat IP LD50 = 2269 mg/kg; Rat IV LD50 = 1425 mg/kg; Rat Oral LD50 = 4010 mg/kg; Rat SC LD50 = 4306 mg/kg. 2. Linoleic acid: Rat IP LD50 = 7208 mg/kg; Rat IV LD50 = 588,7 mg/kg; Rat Oral LD50 = 6838 mg/kg; Rat SC LD50 =

5257 mg/kg. 3. Palmitic acid: Rat IP LD50 = 2269 mg/kg; Rat IV LD50 = 1425 mg/kg; Rat Oral LD50 = 4010 mg/kg; Rat SC LD50 = 4306 mg/kg. 4. Arachidonic acid: Rat IP LD_{50} = 6788 mg/kg; Rat IV LD_{50} = 1136 mg/kg; Rat Oral LD_{50} = 7240 mg/kg; Rat SC LD_{50} = 6820 mg/kg. 5. Oleic acid: Rat IP LD50 = 7354 mg/kg; Rat IV LD50 = 744,1 mg/kg; Rat Oral LD50 = 4904 mg/kg; Rat SC LD50 = 3153 mg/kg. 6. Myristic acid: Rat IP LD_{50} = 2034,2 mg/kg; Rat IV LD_{50} = 1330 mg/kg; Rat Oral LD_{50} = 3033 mg/kg; Rat SC LD_{50} = 3716 mg/kg. 7. Palmitoleic acid: Rat IP LD50 = 6939 mg/kg; Rat IV LD50 = 698,6 mg/kg; Rat Oral LD50 = 4742 mg/kg; Rat SC LD50 = 2358 mg/kg).

Conclusion: the acute toxicity data in rats using *in silico* method, which is a more humane and more environmentally friendly method of research than the classic method of using animals, has been obtained. The obtained data will be used in the future to create new medicines.