In this work, the standard gas-phase formation enthalpies of five-membered nitrogen-containing aromatic heterocycles have been calculated using isodesmic or atomization reactions. The first method requires knowledge of the experimental gas-phase formation enthalpies of all substances participating in the corresponding reaction, while determination of the formation enthalpies via atomization reactions does not have these shortcomings. The values of the gas-phase formation enthalpies of azoles, calculated using both methods, are in good agreement with the experimental ones. The only exception is 2-methyltetrazole. The experimental value of the gas-phase formation enthalpy of 2-methyltetrazole [1] is higher than that of 1-methyltetrazole, which also contradicts the results of our calculations. This indicates that further experimental studies of the formation enthalpy of 2-methyltetrazole are necessary.

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Design and synthesis of pyrazole amide derivatives assuccinate dehydrogenase inhibitors

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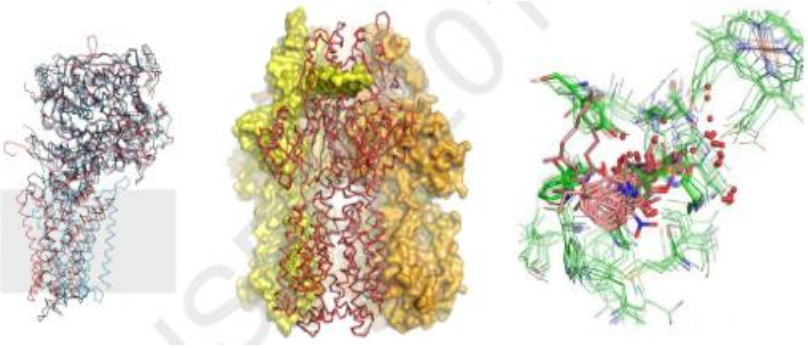
Succinate dehydrogenase inhibitors affect the respiratory chain electron transport system of pathogens by acting on the protein complex II (succinate dehydrogenase), hinder its energy metabolism, thereby inhibiting the growth of pathogenic bacteria, leading to its death. It is a method for prevention and treatment of diseases. Due to this unique mechanism of succinate dehydrogenase inhibitors and the characteristics such as low toxicity, high activity, variable structures of these inhibitors, it has gradually attracted the attention of pesticide companies and scientists in recent years [1]. As pathogens have gradually produced different degrees of resistance to existing inhibitor products [2, 3] including pyridine-ethyl-benzamides, furan amides, pyrazole-amides and others [4, 5, 6], the development of novel succinate dehydrogenase inhibitors is increasingly showing its necessity and urgency. Hereby we report the design, synthesis, fungicidal activity and SAR study of novel fluorinated pyrazole amide derivatives as succinate dehydrogenase inhibitors, which can be divided into the following parts.

1. Virtual screening model establishment (Fig. 1) of those organic molecules that can be used as candidate inhibitors via computer softwares for the likes of

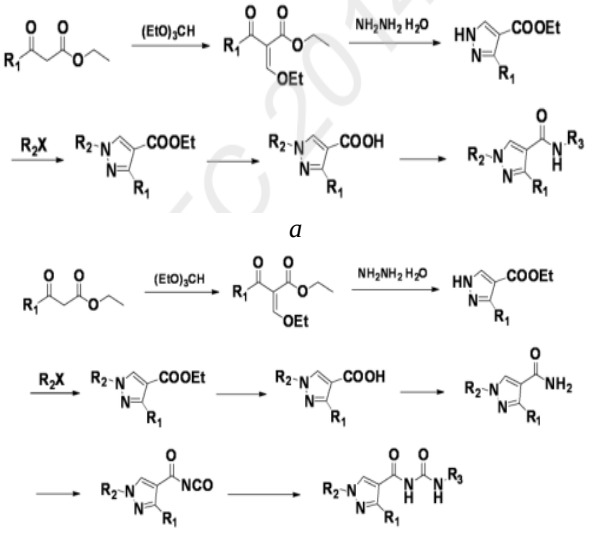
SYBYL, DOCK, eHiTS and data libraries such as ACD3D, NCI3D and DRUG LIKE, etc.



a *b* *c*

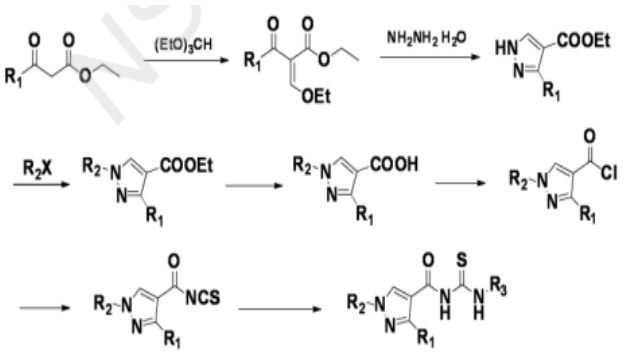
Fig. 1. Crystal structure (*a*, *b*) of SDH and docking conformation of SDH with inhibitors (*c*)

2. Rational design and green synthesis of fluorinated pyrazole amide derivatives based on the screening results (Fig. 2).



a

b



c

Fig. 2. Synthesis of fluorinated pyrazole amide derivatives (*a*, *b*, *c*)

3. The establishment of the biological activity model of the compound and the SAR (structure and activity relationship) study by taking into account the factors of hydrophobicity, electricity, and three-dimensional structure of the inhibitor compound, and followed by the synthetic optimization of the inhibitor structure as well as activity verification.

The aim of our study is to provide useful information for further discovery of novel precursor compounds with bactericidal activities, but also a theoretical and practical basis for the preparation of new, green and environmentally friendly pesticides on a global perspective.

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Tetrazole derivatives as capping ligands and precursors for nanostructured materials

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Tetrazole derivatives have received much attention in the recent years in the field of nanostructured materials [1]. This interest is due to the unique combination of properties of these multi-nitrogen heterocyclic compounds. First, it is the donor character peculiar to the tetrazole ring that determines the