

Afisarea articolelor 1-2(2) pentru cuvântul-cheie "SiRMS"

Structural, physicochemical and stereochemical interpretation of QSAR models based on simplex representation of molecular structure

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// ISSN -

Disponibil online 1 March, 2023. Descarcări-0. Vizualizări-190

Computational assessment of environmental hazards of nitroaromatic compounds: Influence of the type and position of aromatic ring substituents on toxicity

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Structural Chemistry

1(27) / 2016 / ISSN 1040-0400 /ISSNe 1572-9001

Disponibil online 23 January, 2023. Descarcări-0. Vizualizări-213



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Institutul de Dezvoltare a Societății Informaționale.

Actualizat: 19.05.2024, accesat: 19.05.2024

Disponibil: <https://ibn.idsi.md>

