

Selection of semiempirical calculation methods for insecticide development

Title	Selection of semiempirical calculation methods for insecticide development
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Abstract	Background: Insecticides are substances used to control, repel, or eradicate troublesome organisms, particularly insect-based plant pests. The discovery of new insecticide compounds fuels the ongoing development of insecticides. The integration of computational chemistry into the development of insecticidal chemicals was beneficial. Objective: This study aims to identify the most suitable method among 12 available semiempirical calculation methods in the Hyperchem application. Methods: The selection process involved comparing experimental data of the infra-red spectrum of chlorpyrifos with corresponding calculation data. Results: The largest Predicted Residual of Sum Squares (PRESS) value was observed in the INDO method of 55466.3856. Conversely, the smallest PRESS value was observed in the AM1, measuring 3242.6549. The AM1 semiempirical method yields the smallest value. Conclusion: The results indicated that the calculation chosen was the AM1 semiempirical method.
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