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*Research article*

## **QSAR study and theoretical investigation on the lethality of halogenated aliphatic hydrocarbons toward *Aspergillus (A.) Nidulans***

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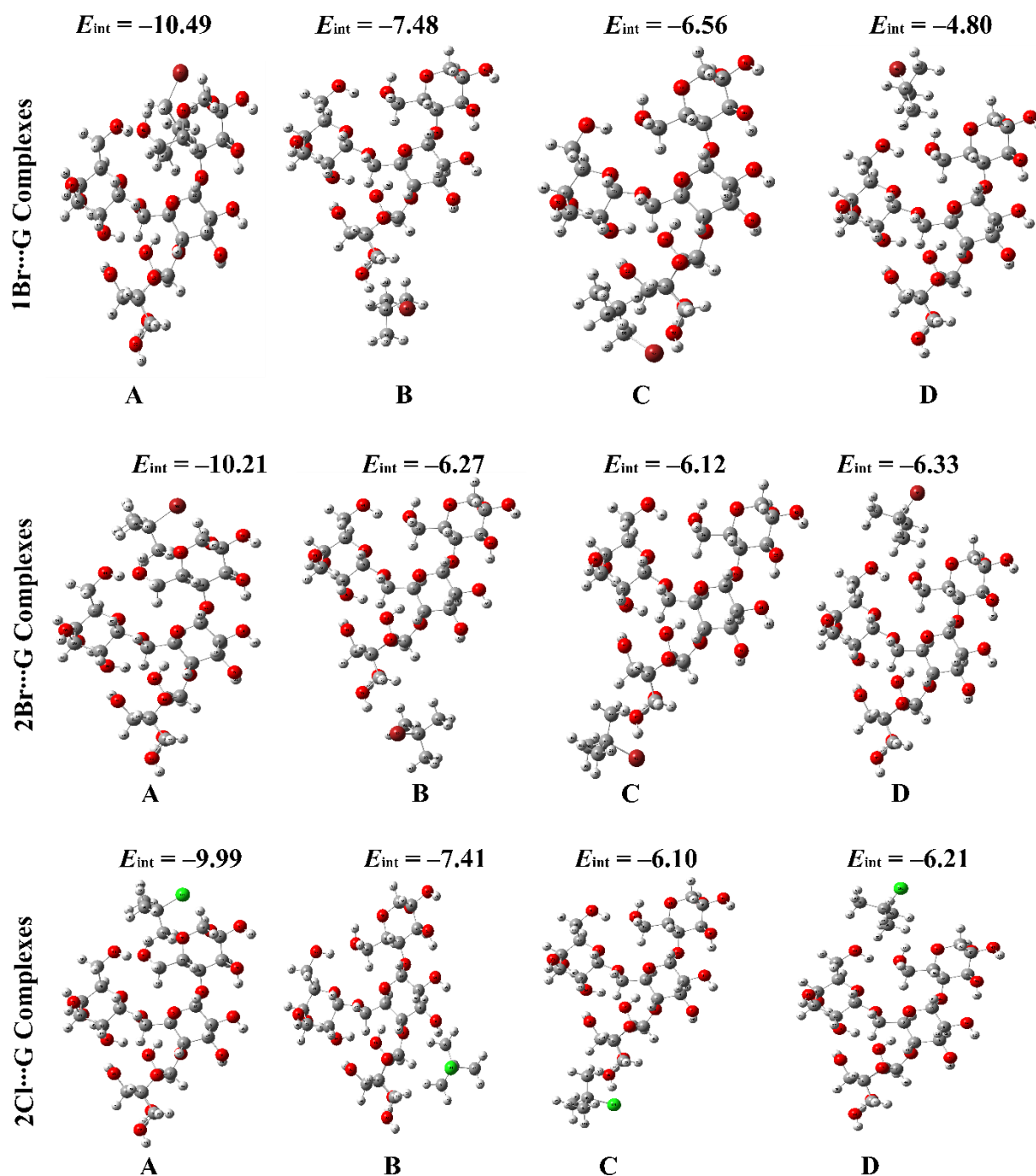
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**Figure S1.** Optimized complexes within all studied configurations of the 1-bromo-2-methylpropane (**1Br**)..., 2-bromo-2-methylpropane (**2Br**)..., and 2-chloro-2-methylpropane (**2Cl**)... $\alpha$ -glucan (**G**). Interaction energy ( $E_{\text{int}}$ ) values are in kcal/mol.

**Table S1:** A comparison between our model and those reported by Cronin et al.

	No. of HAHs	$R^2$	$s$	$F$
Our Model	55	0.897	0.219	148.766
Cronin's Model	55	0.615	0.413	44.2



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