

Supporting information

2-Methyl-6-(4-aminophenyl)-4,5-dihydro-3(2*H*)-pyridazinone synthon for some new annelated 1,2,3-selena/thiadiazoles and 2*H*-diazaphospholes with anticipated biological activity and quantum chemical calculations

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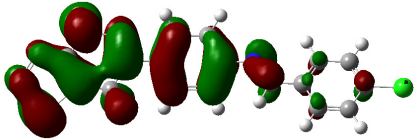
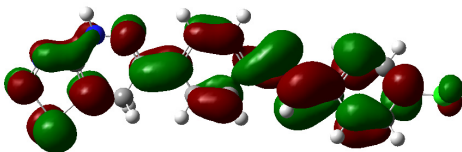
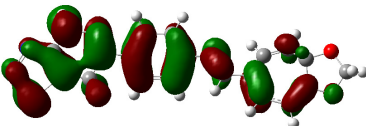
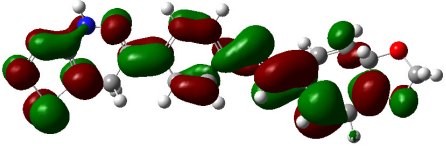
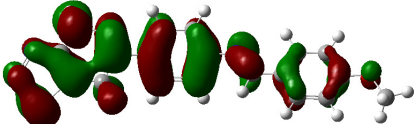
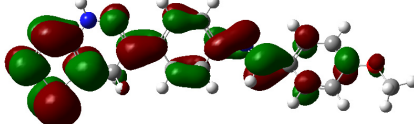
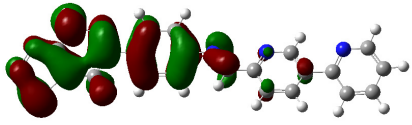
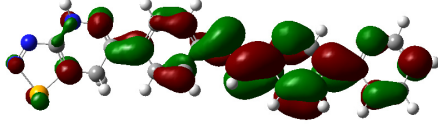
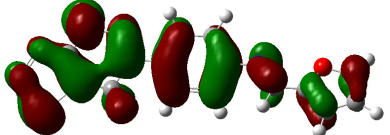
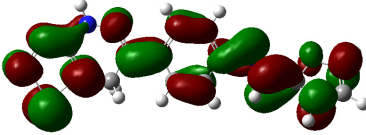
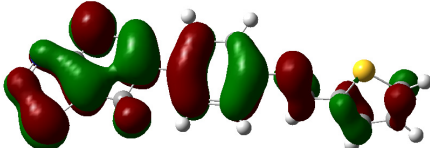
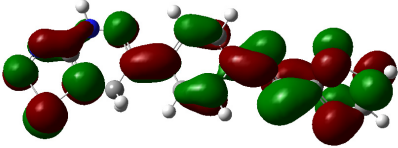
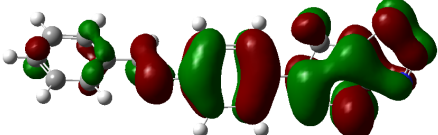
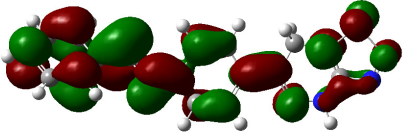
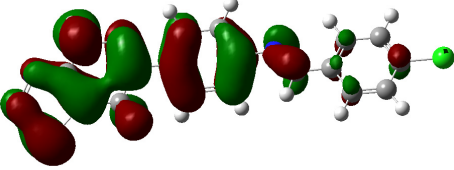
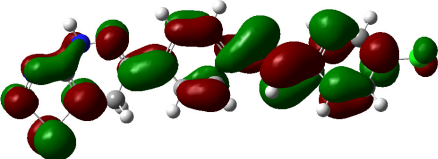
²Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, Praha, 162 06, Czechia

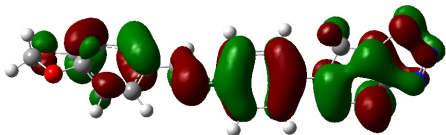
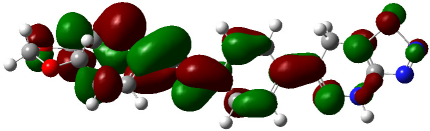
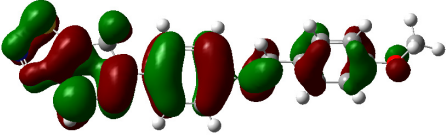
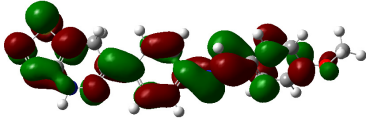
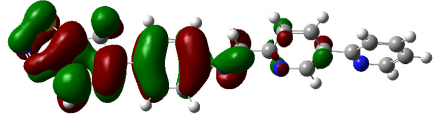
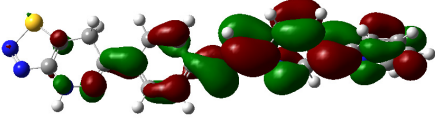
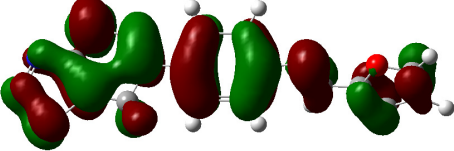
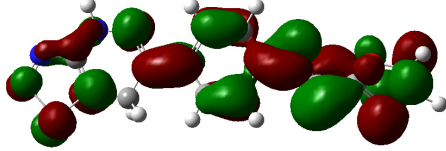
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Table S1: 3D plots of HOMO and LUMO molecular orbitals of compounds calculated using DFT(B3LYP)/6-31G+(d) method.

	HOMO	LUMO
8b		
8e		
8f		
8g		
8h		
8i		
9a		
9b		

9e		
9f		
9g		
9h		
9i	