

On the relationship between hydrogen bond strength and the formation energy in resonance-assisted hydrogen bonds

Electronic Supplementary Information

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June 30, 2021

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Table S1: IQA interaction energies (E_{int}) as well as its classical (V_{cl}) and exchange-correlation (V_{xc}) parts, for the investigated O...H RAHB contacts. The values are reported in kcal·mol⁻¹.

System	Position 1			Position 2			Position 3		
	E_{int}	V_{cl}	V_{xc}	E_{int}	V_{cl}	V_{xc}	E_{int}	V_{cl}	V_{xc}
-CF ₃	-151.00	-133.97	-17.02	-161.21	-141.09	-20.12	-162.84	-142.44	-20.39
-F	-145.79	-132.08	-13.71	-150.01	-133.22	-16.79	-193.49	-161.28	-32.21
-Cl	-142.54	-128.83	-13.71	-155.87	-137.51	-18.35	-183.98	-155.38	-28.61
-Br	-140.43	-127.26	-13.18	-156.25	-137.74	-18.51	-185.33	-155.89	-29.44
-N(CH ₃) ₂	-170.54	-149.21	-21.33	-156.33	-137.84	-18.49	-195.55	-164.03	-31.51
-OCH ₃	-163.77	-144.41	-19.36	-155.01	-136.86	-18.15	-182.75	-155.82	-26.93
-NCOCH ₃	-160.49	-141.92	-18.56	-157.31	-138.38	-18.92	-182.79	-155.76	-27.02
-NO ₂	-141.59	-128.08	-13.51	-164.28	-143.03	-21.25	-167.54	-145.27	-22.26
Malondialdehyde	-159.78	-140.19	-19.59						

Table S2: IQA interaction energies (E_{int}), formation energies (E_{form}) computed by means of the OCM (expression (3)), and H-bond interaction energies (E_{HB}) estimated via equation (4) for the investigated O...H RAHB contacts. The values are reported in kcal·mol⁻¹.

System	Position 1			Position 2			Position 3		
	E_{int}	E_{form}	E_{HB}	E_{int}	E_{form}	E_{HB}	E_{int}	E_{form}	E_{HB}
-CF ₃	-151.00	-12.23	-14.63	-161.21	-14.40	-18.20	-162.84	-11.96	-18.48
-F	-145.79	-10.24	-10.80	-150.01	-10.81	-13.87	-193.49	-13.67	-32.18
-Cl	-142.54	-9.70	-10.98	-155.87	-11.76	-16.05	-183.98	-13.01	-27.75
-Br	-140.43	-9.87	-10.49	-156.25	-12.36	-16.30	-185.33	-11.98	-28.71
-N(CH ₃) ₂	-170.54	-11.79	-19.61	-156.33	-12.20	-16.28	-195.55	-13.68	-31.78
-OCH ₃	-163.77	-13.81	-17.29	-155.01	-11.76	-15.50	-182.75	-13.58	-25.85
-NCOCH ₃	-160.49	-12.64	-16.41	-157.31	-10.85	-17.07	-182.79	-8.07	-26.01
-NO ₂	-141.59	-8.19	-10.76	-164.28	-12.78	-19.42	-167.54	-6.30	-20.49
Malondialdehyde	-159.78	-13.31	-19.59						

1 Structures of the studied systems

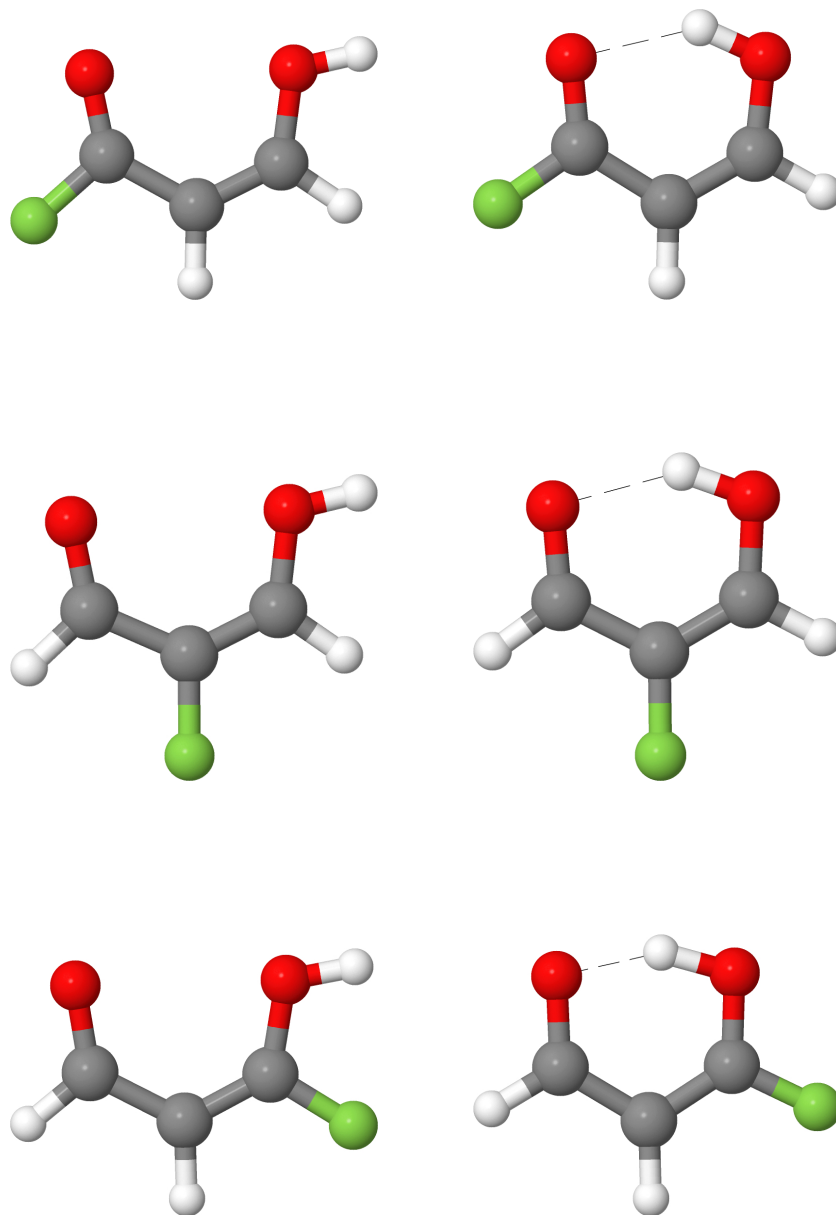


Figure S1: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by -F on the positions 1 (top), 2 (middle) or 3 (bottom).

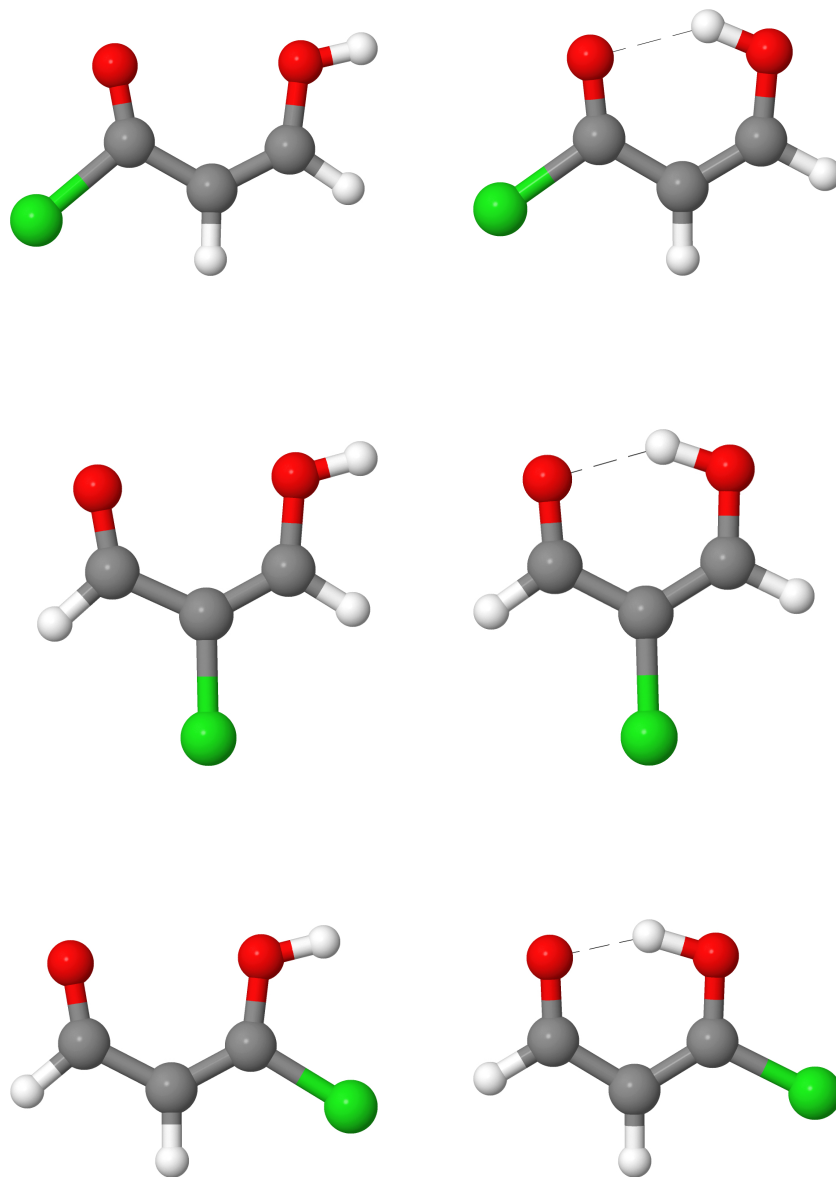


Figure S2: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by -Cl on the positions 1 (top), 2 (middle) or 3 (bottom).

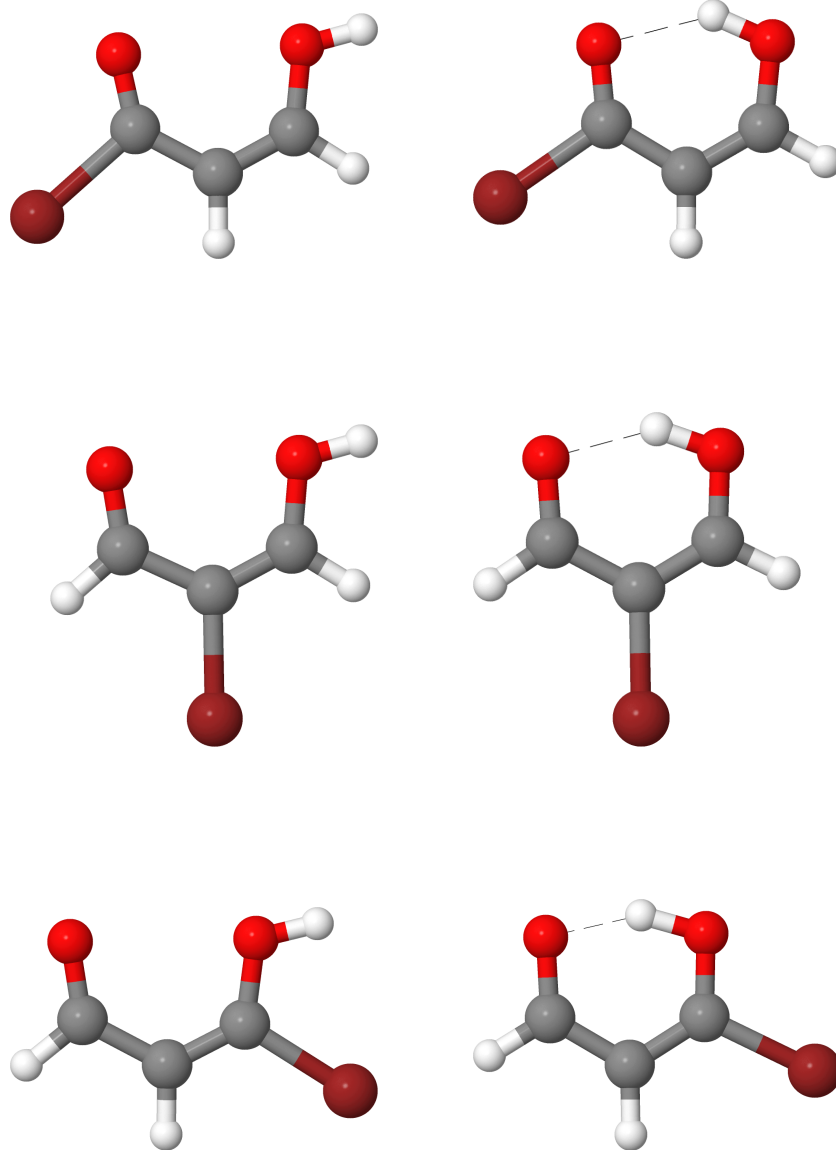


Figure S3: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by -Br on the positions 1 (top), 2 (middle) or 3 (bottom).

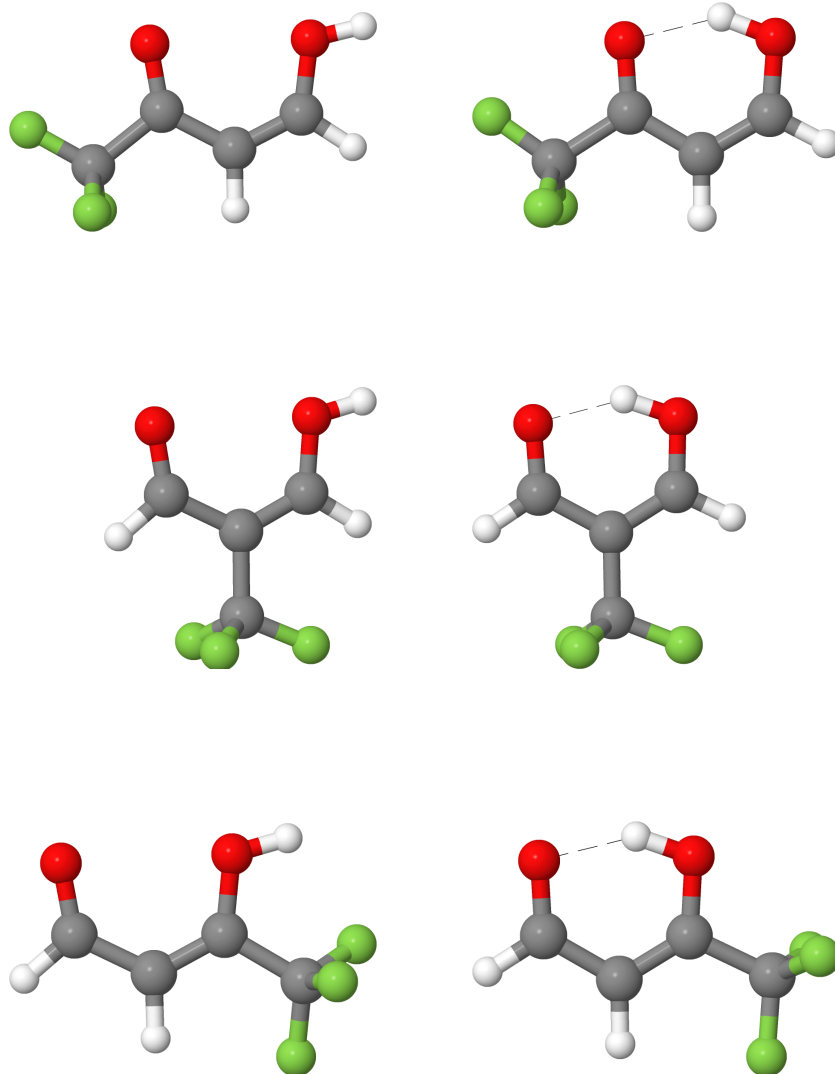


Figure S4: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by -CF_3 on the positions 1 (top), 2 (middle) or 3 (bottom).

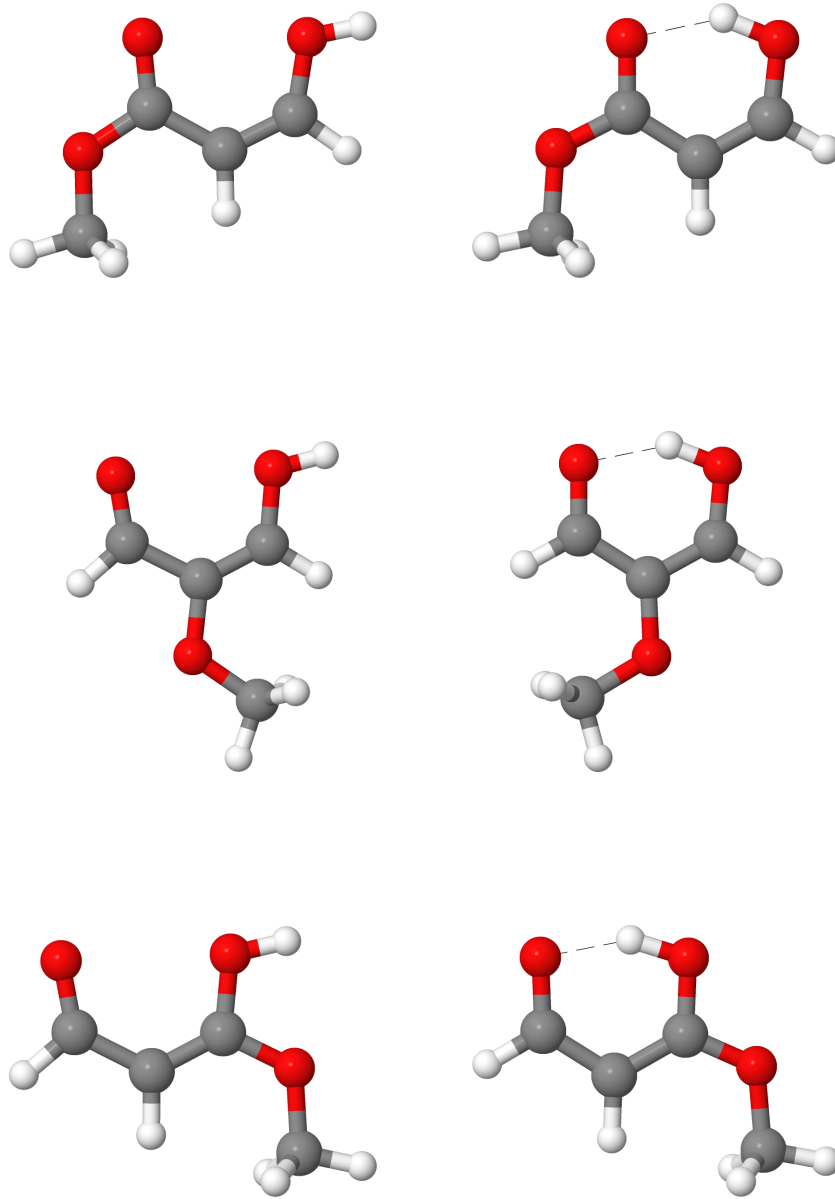


Figure S5: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by the methoxy group on the positions 1 (top), 2 (middle) or 3 (bottom).

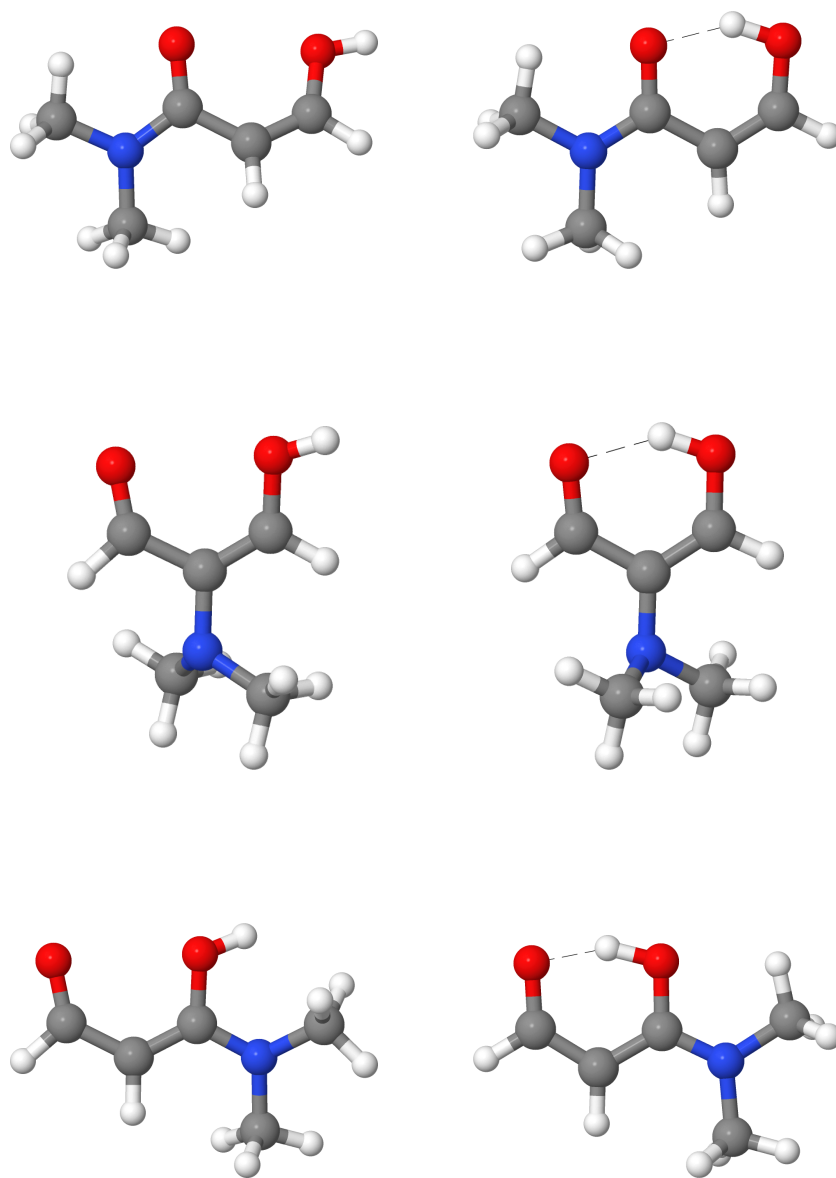


Figure S6: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by the dimetilamine group on the positions 1 (top), 2 (middle) or 3 (bottom).

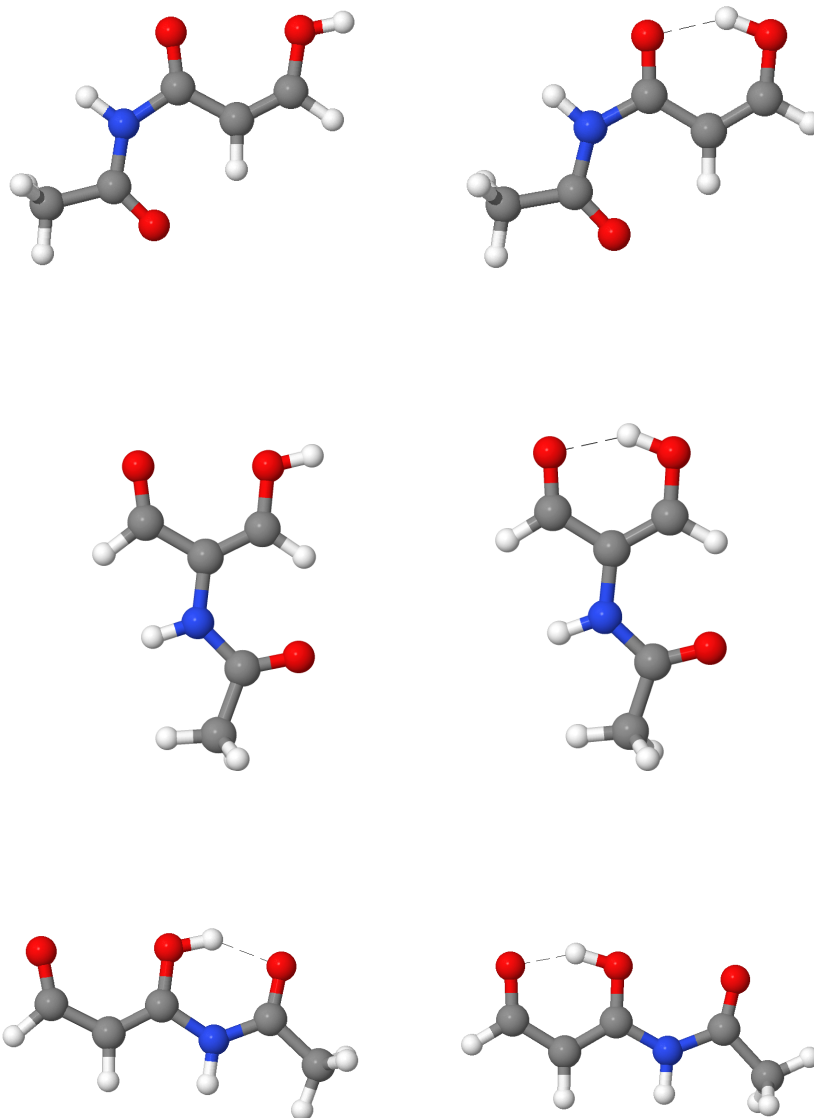


Figure S7: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by the ethanamide group on the positions 1 (top), 2 (middle) or 3 (bottom).

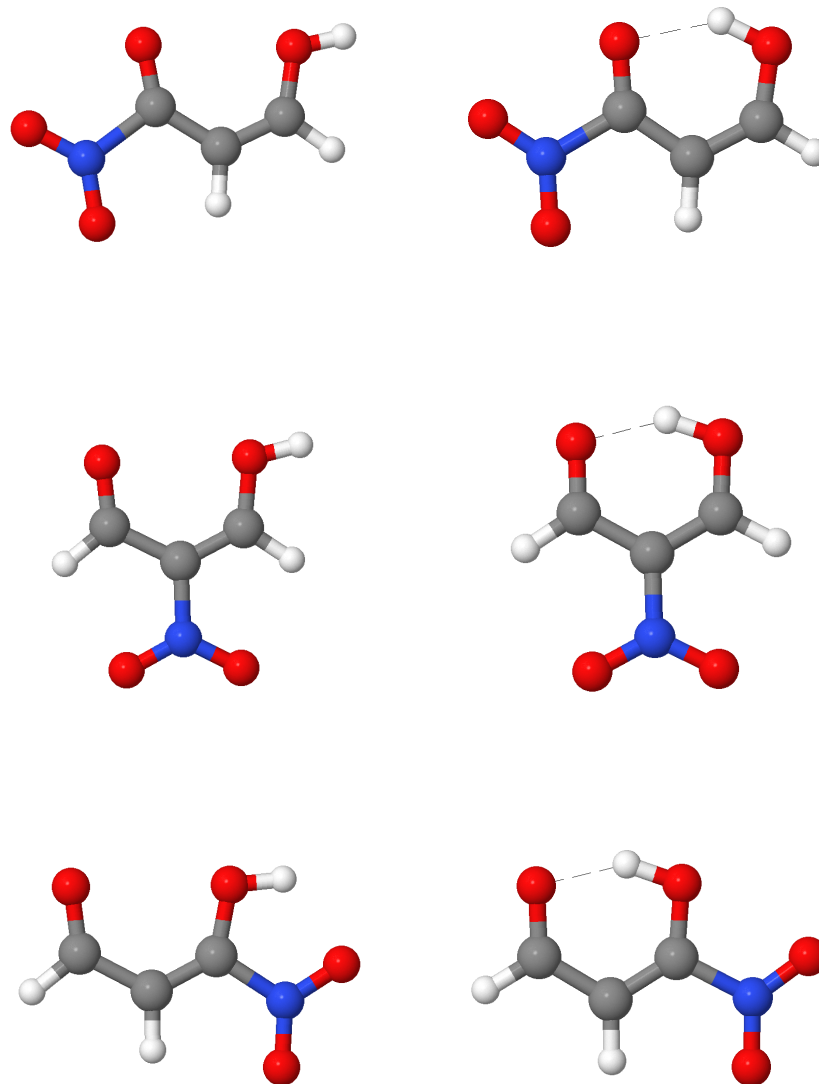


Figure S8: Structures of the open (left) and closed (right) configurations of malondialdehyde substituted by the nitro group on the positions 1 (top), 2 (middle) or 3 (bottom).