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SUPPLEMENTARY MATERIAL TO

Chemical reactivity of alliin and its molecular interactions with the protease M^{pro} of SARS-CoV-2

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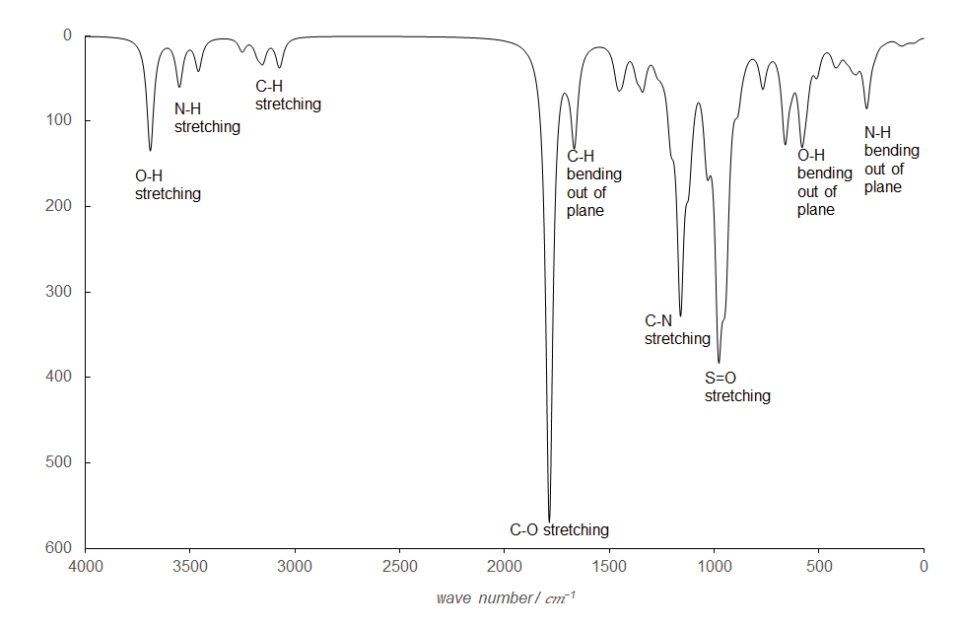

Figure S-1: Theoretical IR spectra of alliin in the aqueous phase obtained at the B3LYP/DGDZVP level of theory.

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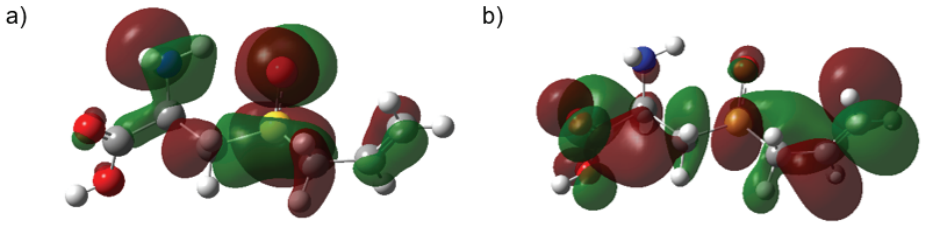

Figure S-2. HOMO and LUMO distributions on alliin obtained at the B3LYP/DGDZVP level of theory in the gas phase. In all cases the isosurfaces were obtained at 0.08 e/u.a.[3] .

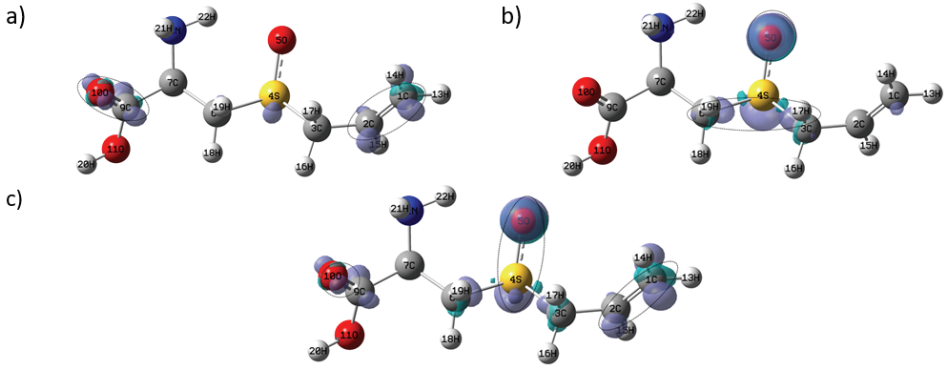

Figure S-3. Isosurfaces of Fukui Functions for alliin according to equations (9), (10) and (11) at the B3LYP/DGDZVP level of theory in the gas phase. In the case of (a) nucleophilic, (b) electrophilic and (c) free radical attacks. In all cases the isosurfaces were obtained at 0.008 e/u.a. [3]The dotted circles show the most reactive zones in each molecule.

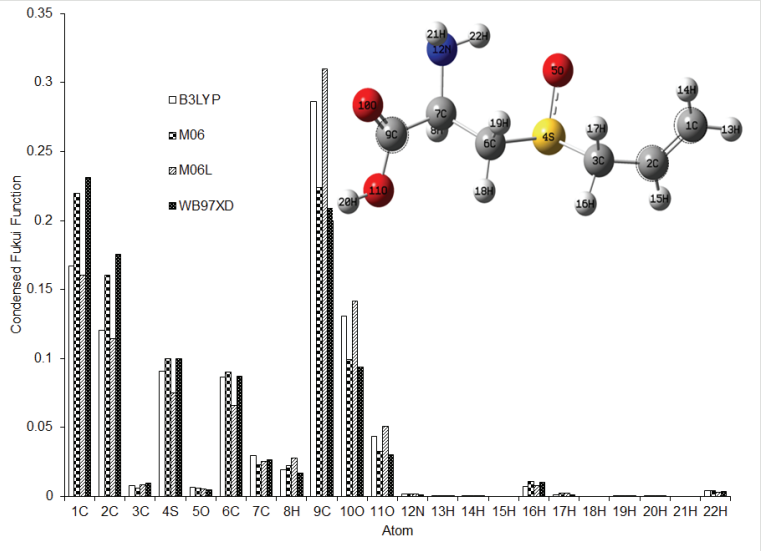

Figure S-4. Condensed Fukui function values for electrophilic attacks on alliin at the X/DGDZVP level of theory (where X=B3LYP, M06, M06L and ωB97XD), in the aqueous phase employing the Hirshfeld population and equations (12)-(14), the dashed circles show the most reactive zones in each molecule.

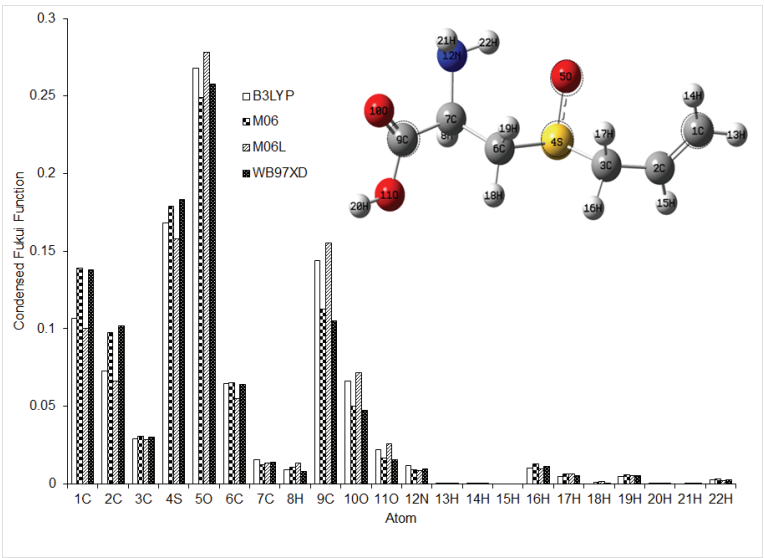

Figure S-5. Condensed Fukui function values for free radical attacks on alliin at the X/DGDZVP level of theory (where X=B3LYP, M06, M06L and ωB97XD), in the aqueous phase employing the Hirshfeld population and equations (12)-(14), the dashed circles show the most reactive zones in each molecule.

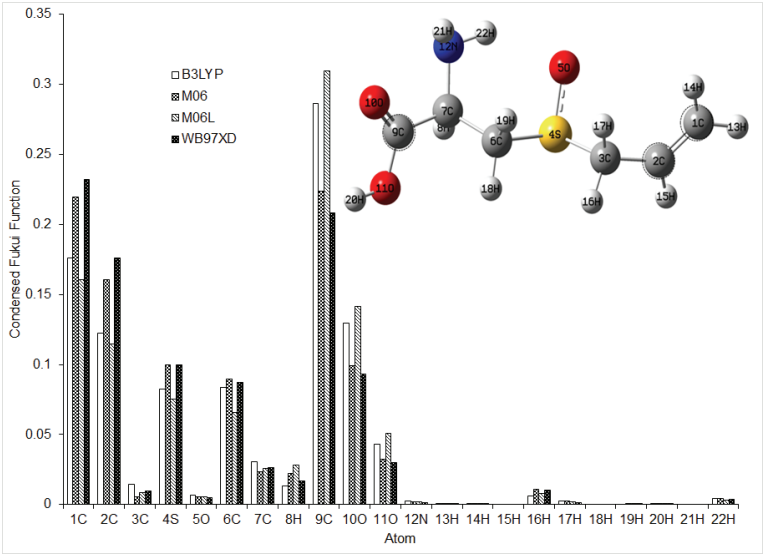

Figure S-6. Condensed Fukui function values for nucleophilic attacks on alliin at the X/DGDZVP level of theory (where X=B3LYP, M06, M06L and ωB97XD), in the gas phase employing the Hirshfeld population and equations (12)-(14), the dashed circles show the most reactive zones in each molecule.

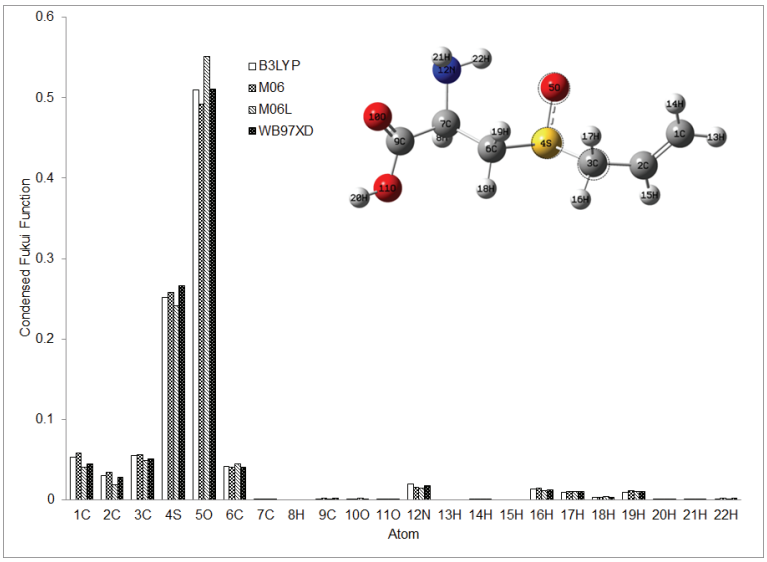

Figure S-7. Condensed Fukui function values for electrophilic attacks on alliin at the X/DGDZVP level of theory (where X=B3LYP, M06, M06L and ωB97XD), in the gas phase employing the Hirshfeld population and equations (12)-(14), the dashed circles show the most reactive zones in each molecule.

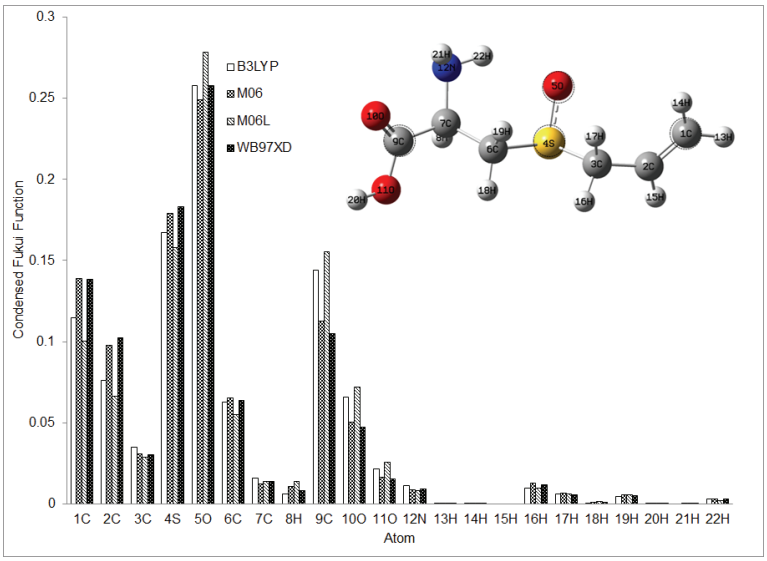

Figure S-8. Condensed Fukui function values for free radical attacks on alliin at the X/DGDZVP level of theory (where X=B3LYP, M06, M06L and ωB97XD), in the gas phase employing the Hirshfeld population and equations (12)-(14), the dashed circles show the most reactive zones in each molecule.

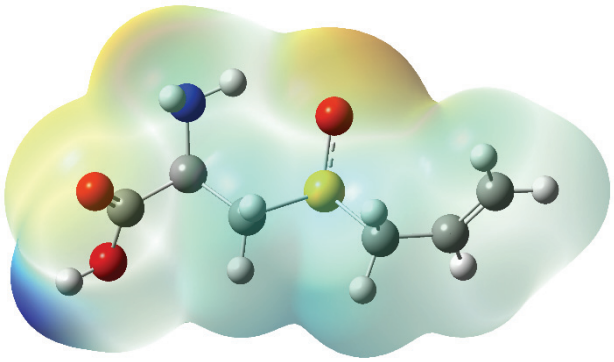

Figure S-9. Mapping of electrostatic potentials evaluated at the B3LYP/DGDZVP level of theory in the gas phase, over a density isosurface (value =0.002 e/a.u.^{3}) for alliin.

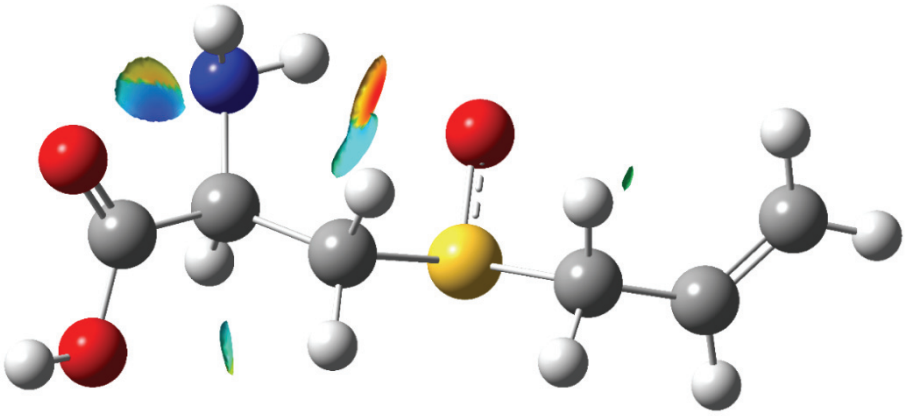

Figure S-10. Isosurface area of NCI = 0.2 for alliin in aqueous phase.

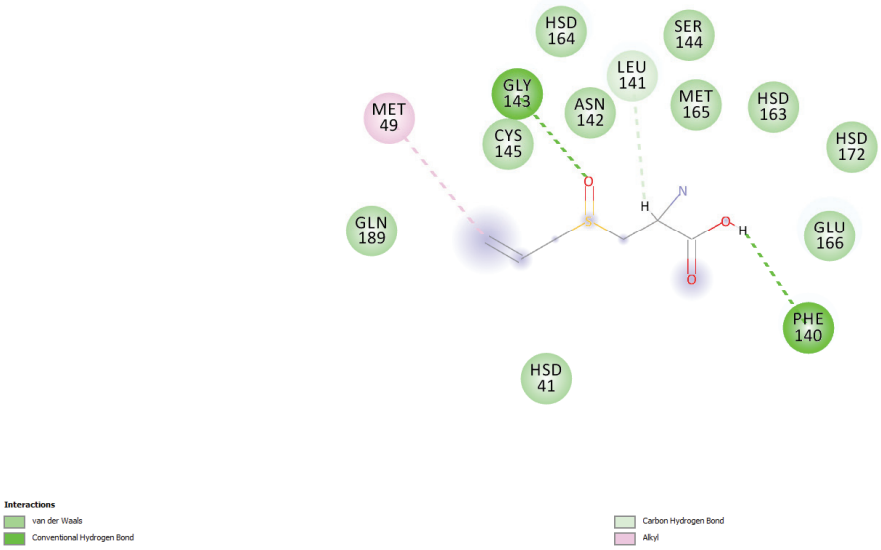

Figure S-11. 2D mapping of ligand/protein interactions for alliin.