Supplementary Material for Characterizing Molecular Interactions in Chemical Systems

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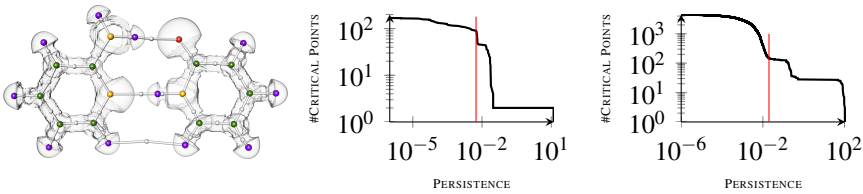
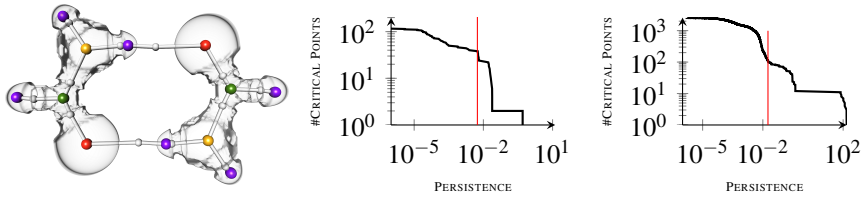
This appendix shows the persistence curves used for the extraction of the interaction sites and the Bonding graph. The left column of Figures 1–12 shows the Bonding graph of the corresponding molecules while the central and right column show the persistence curves used for the threshold selection for the simplification of the join trees (JT) and the Morse-Smale complex (MSC), respectively. Both curves exhibit characteristic slopes which are used to choose an appropriate threshold (see paper). The red vertical line highlights the chosen thresholds, respectively. Note that the strength of the slopes varies depending on the molecular structure. However, all molecules show the same characteristic behavior.



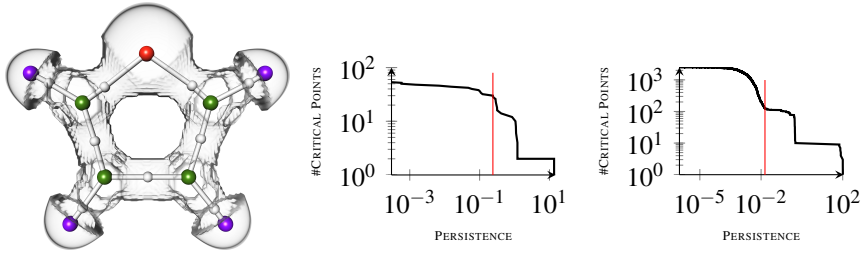
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 1: Pyridoxine-Aminopyridine



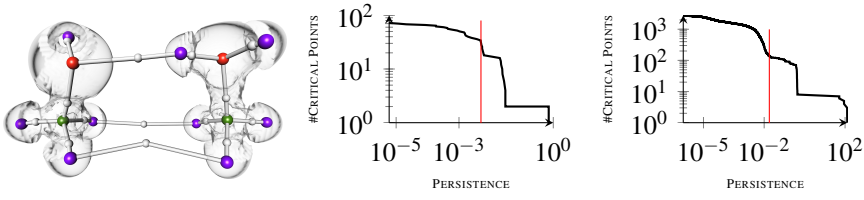
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 2: Formamide Dimer



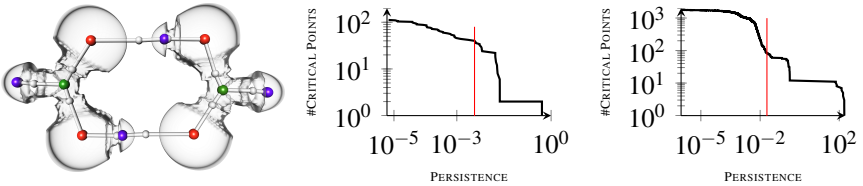
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 3: Furan



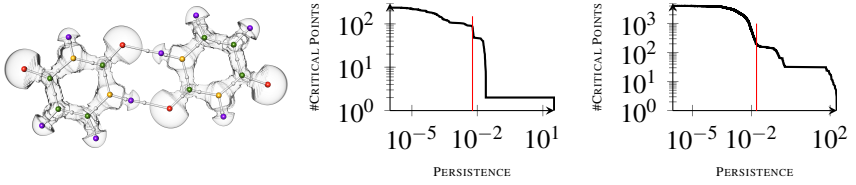
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 4: Methanol-Metanamina



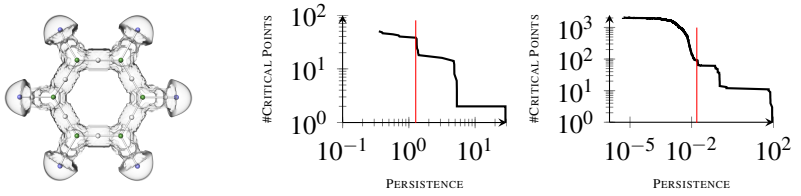
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 5: Formic-Acid Dimer



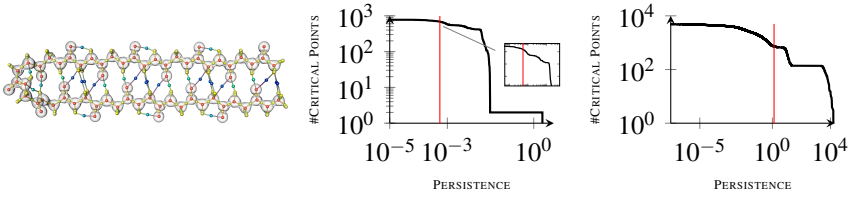
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 6: Uracil Dimer



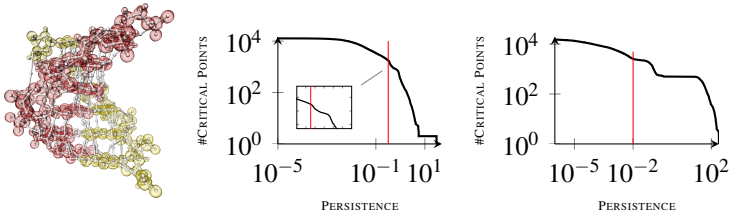
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 7: Benzene



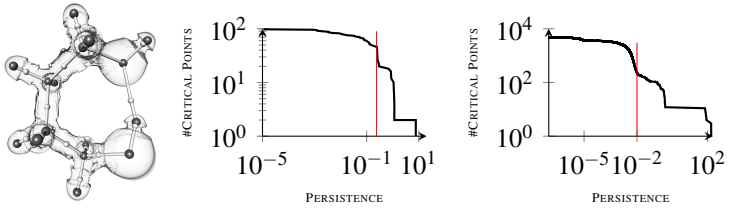
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 8: β-sheet polipeptide



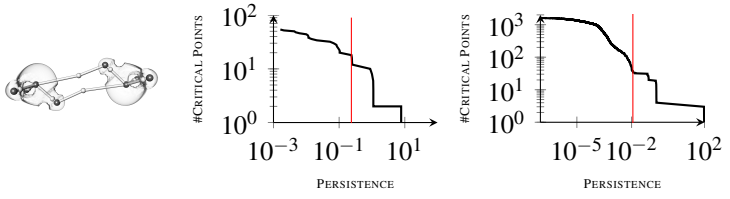
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 9: DNA



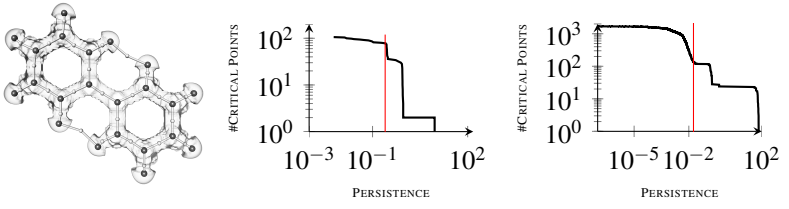
(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 10: Butane-Diol



(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 11: NH3-Dimer



(a) Bonding graph (b) Persistence JT (c) Persistence MSC

Figure 12: Biphenyl