

Supporting Information:

Multiscale End-point Screening with Extended Tight-binding Hamiltonians

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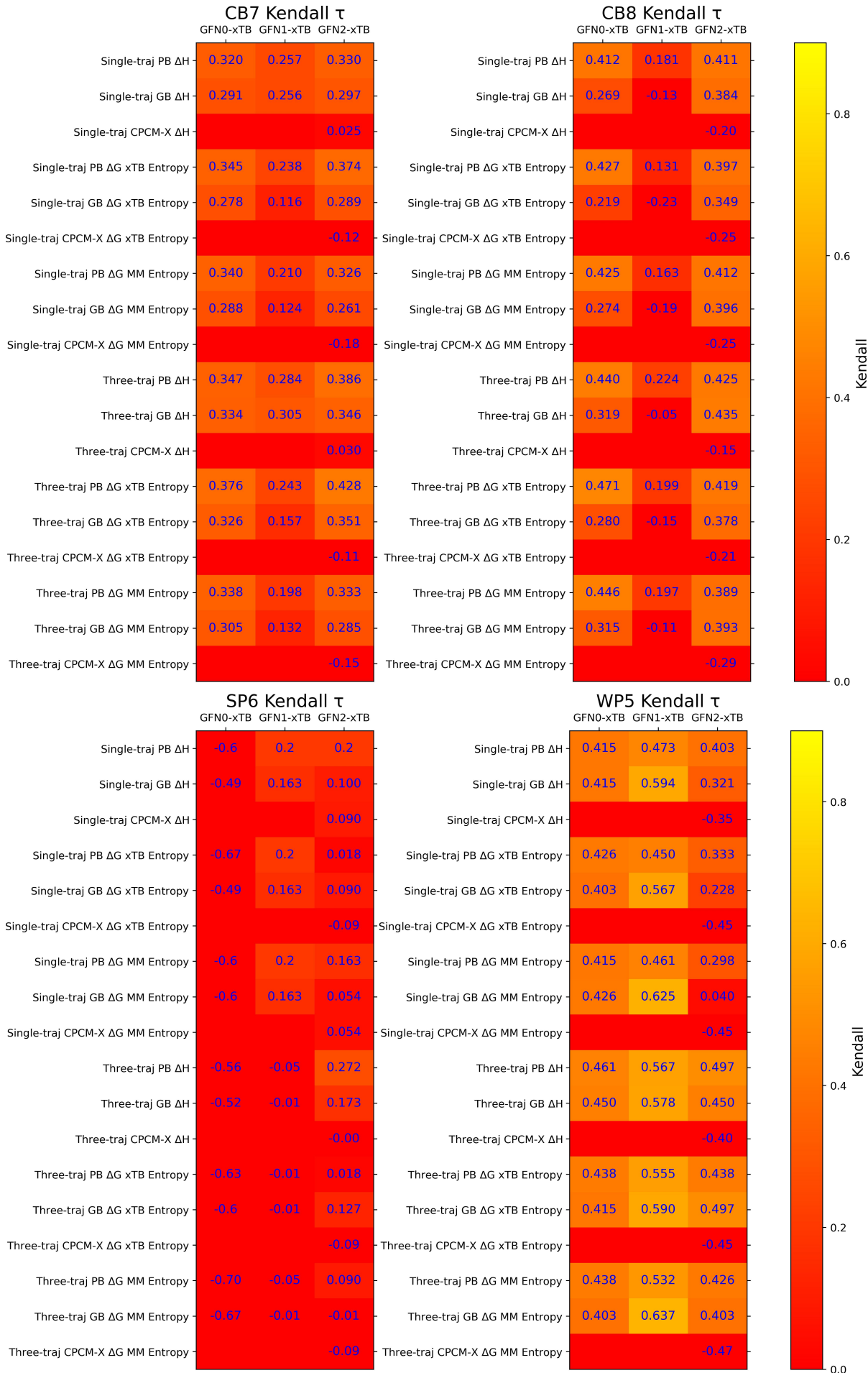
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Fig. S1. Host-specific Kendall rank coefficients.



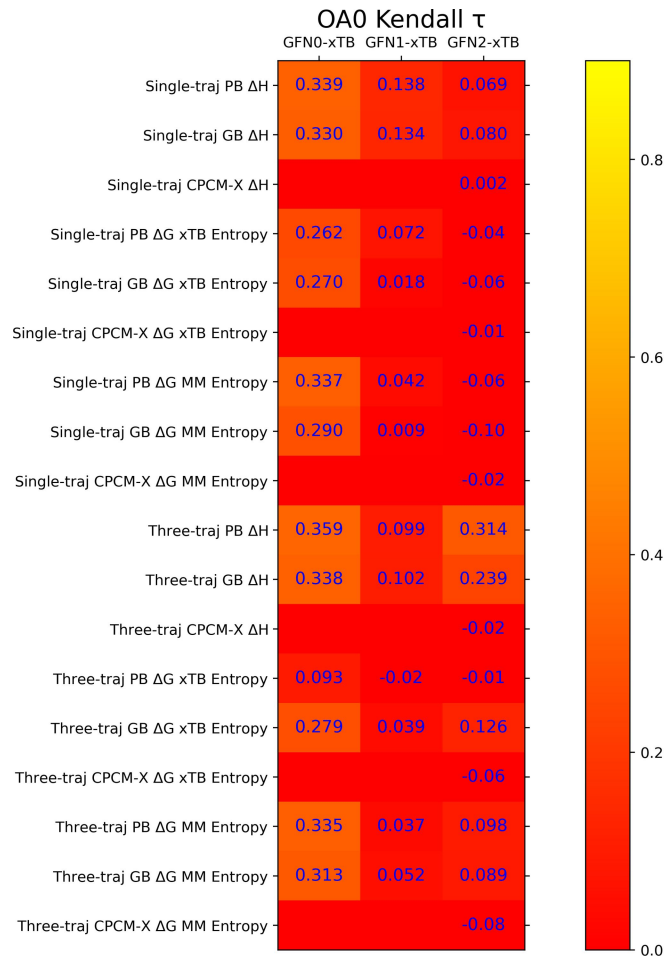
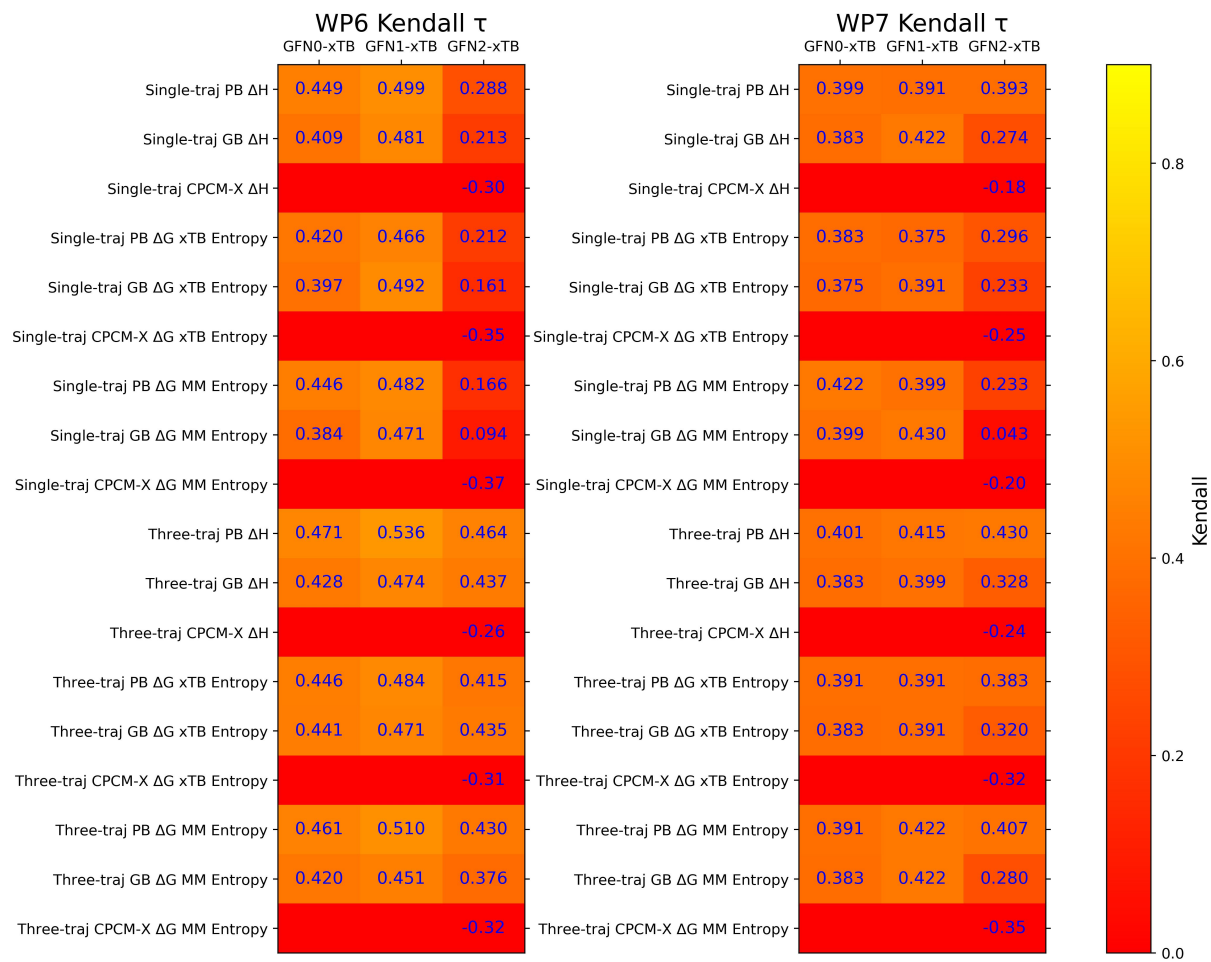
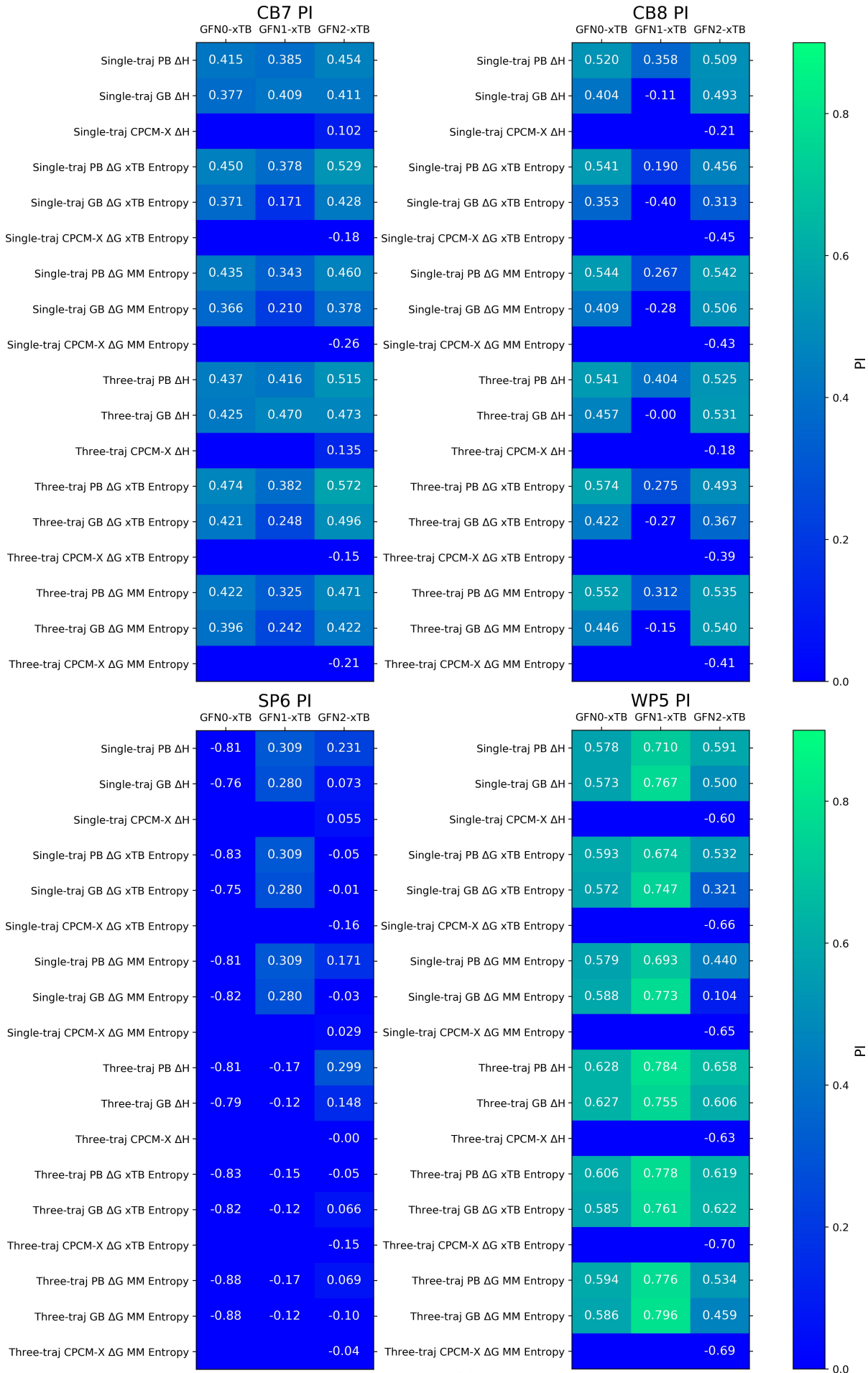


Fig. S2. Host-specific predictive index.



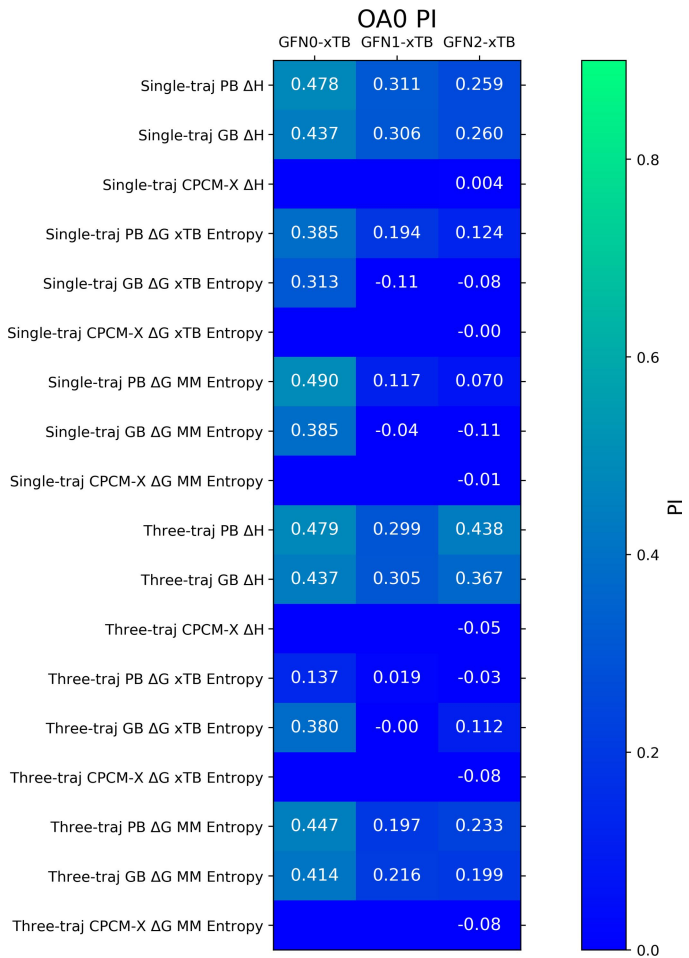
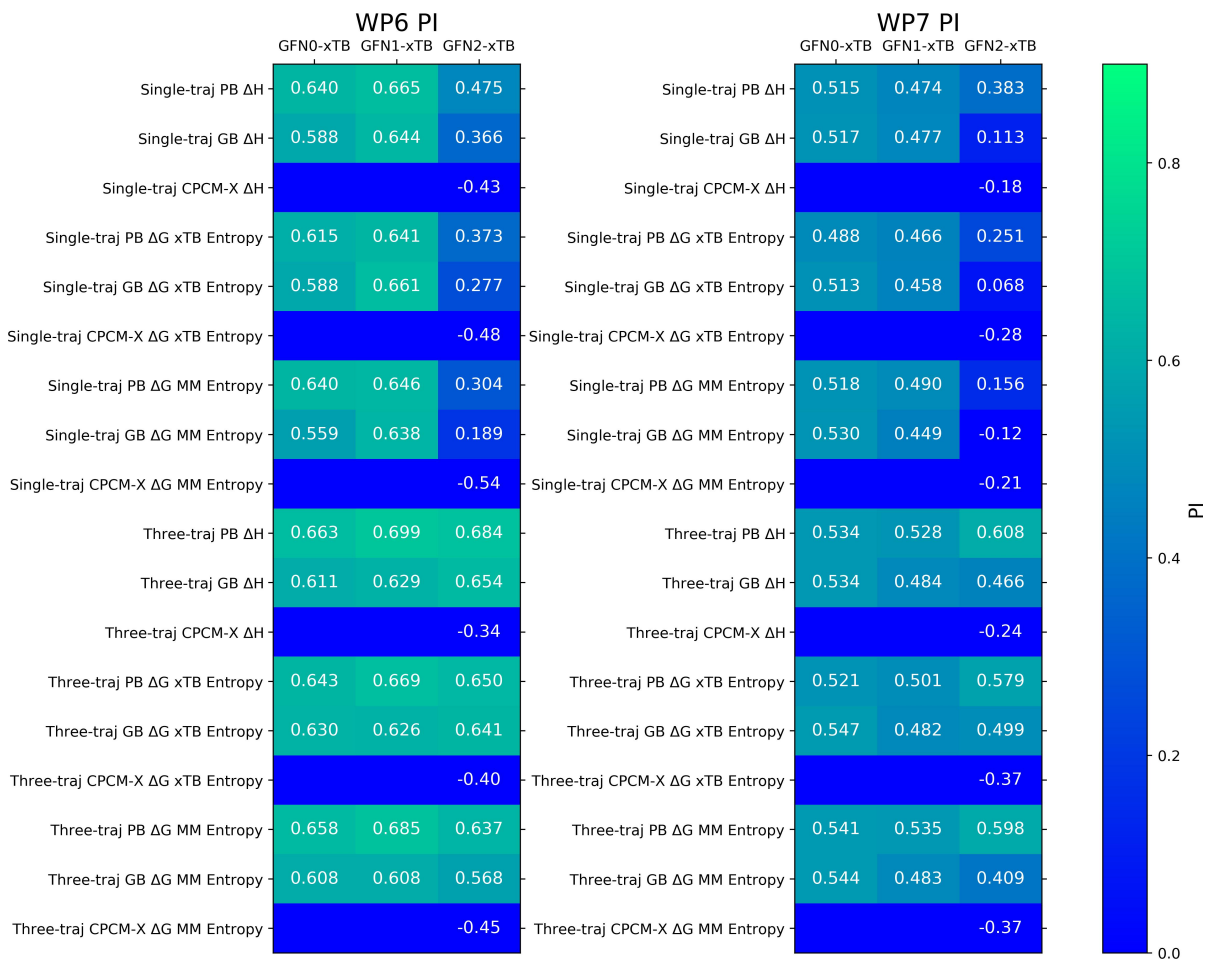
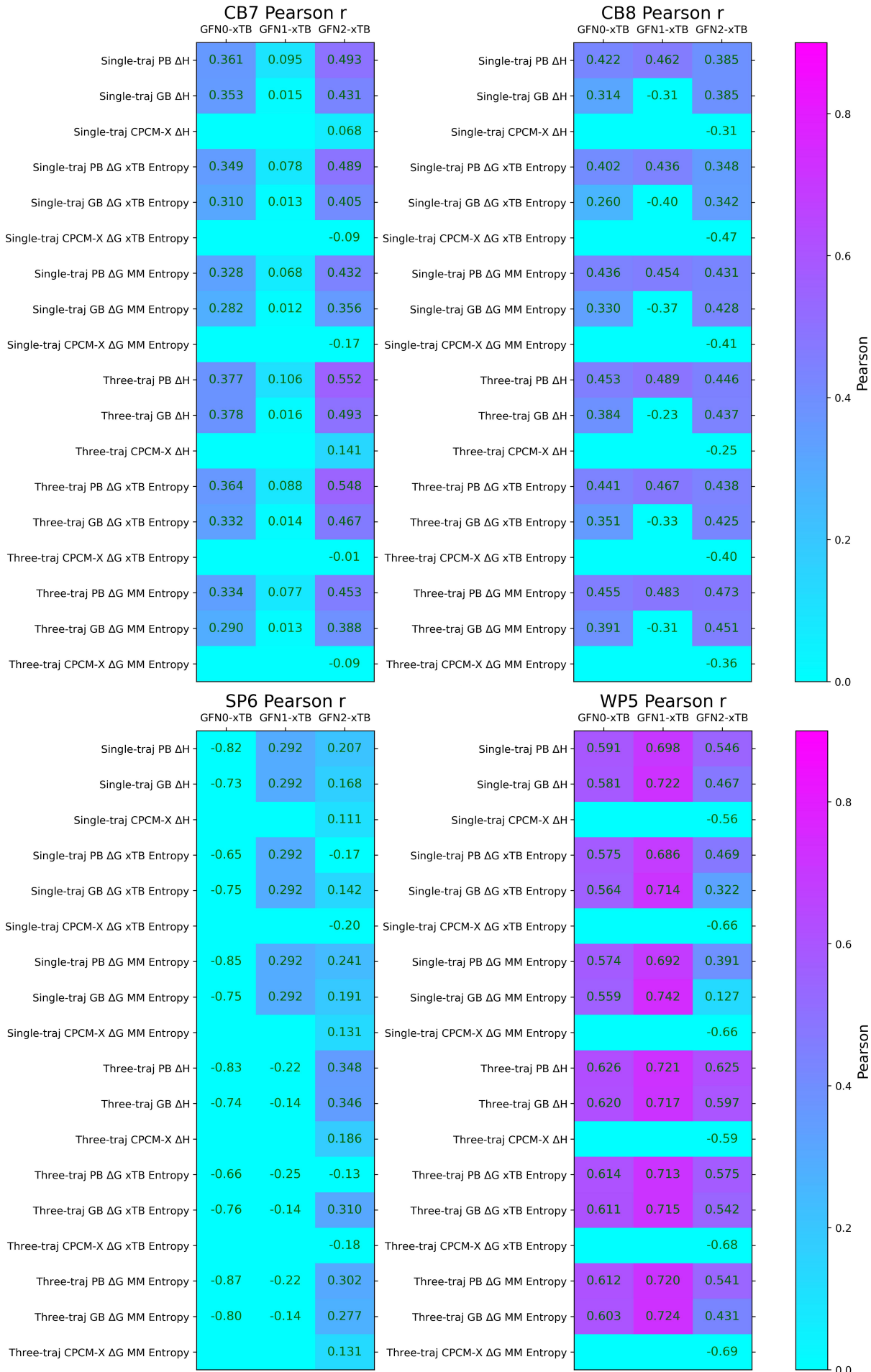
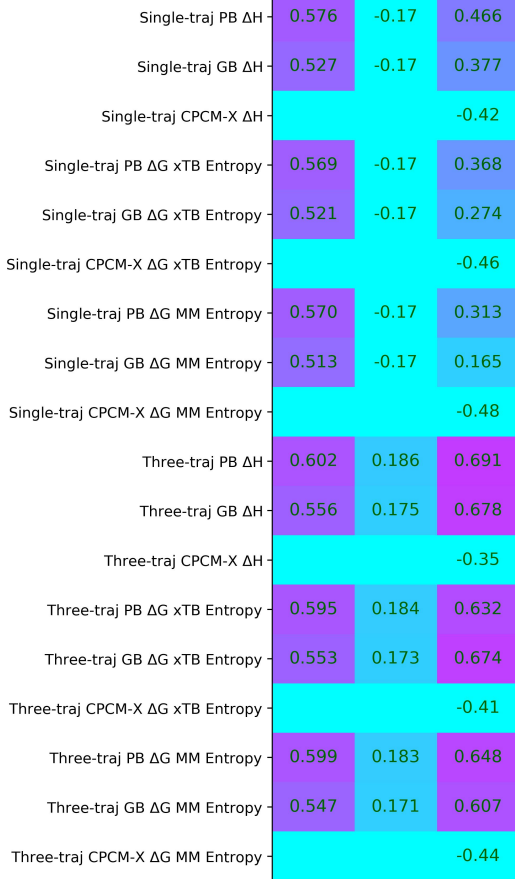


Fig. S3. Host-specific Pearson r .



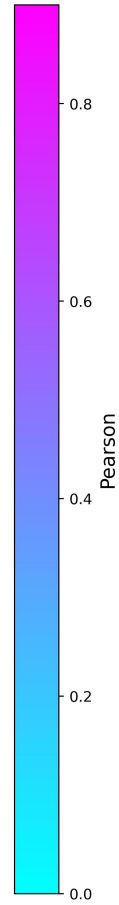
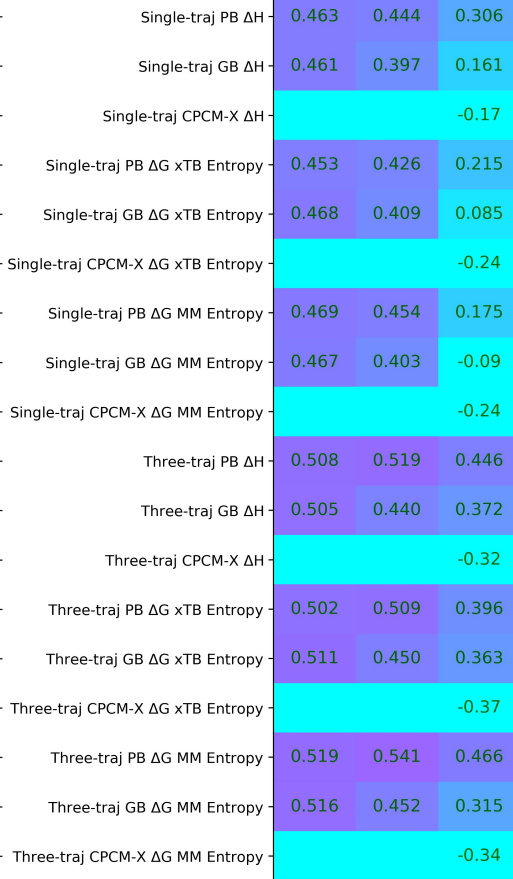
WP6 Pearson r

GFN0-xTB GFN1-xTB GFN2-xTB



WP7 Pearson r

GFN0-xTB GFN1-xTB GFN2-xTB



OA0 Pearson r

GFN0-xTB GFN1-xTB GFN2-xTB

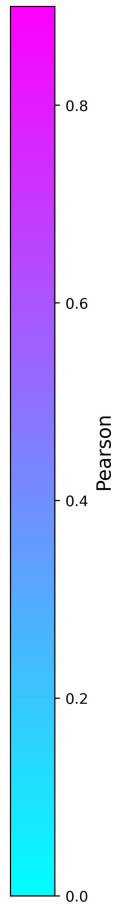
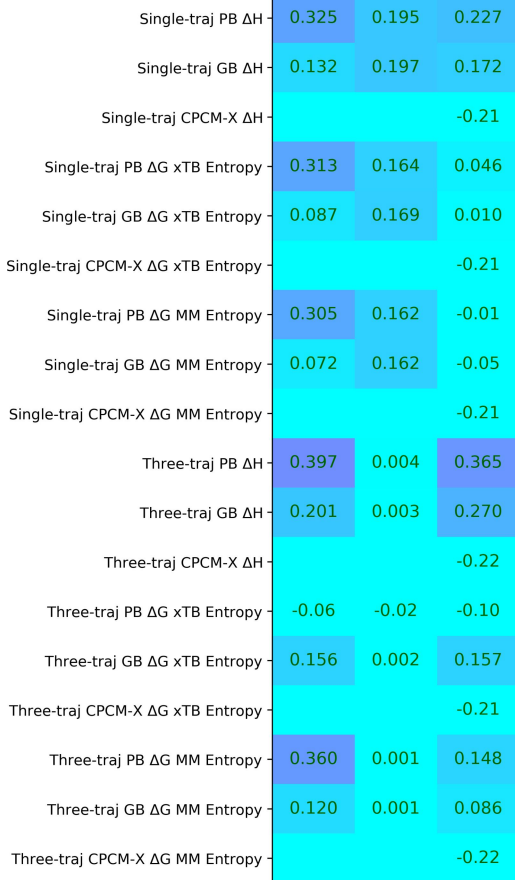


Fig. S4. Top-5 frequency maps. The N top-performing methods in each host-guest dataset are extracted and a frequency analysis is performed. The most robust technique has the largest number of occurrences in the heatmap.

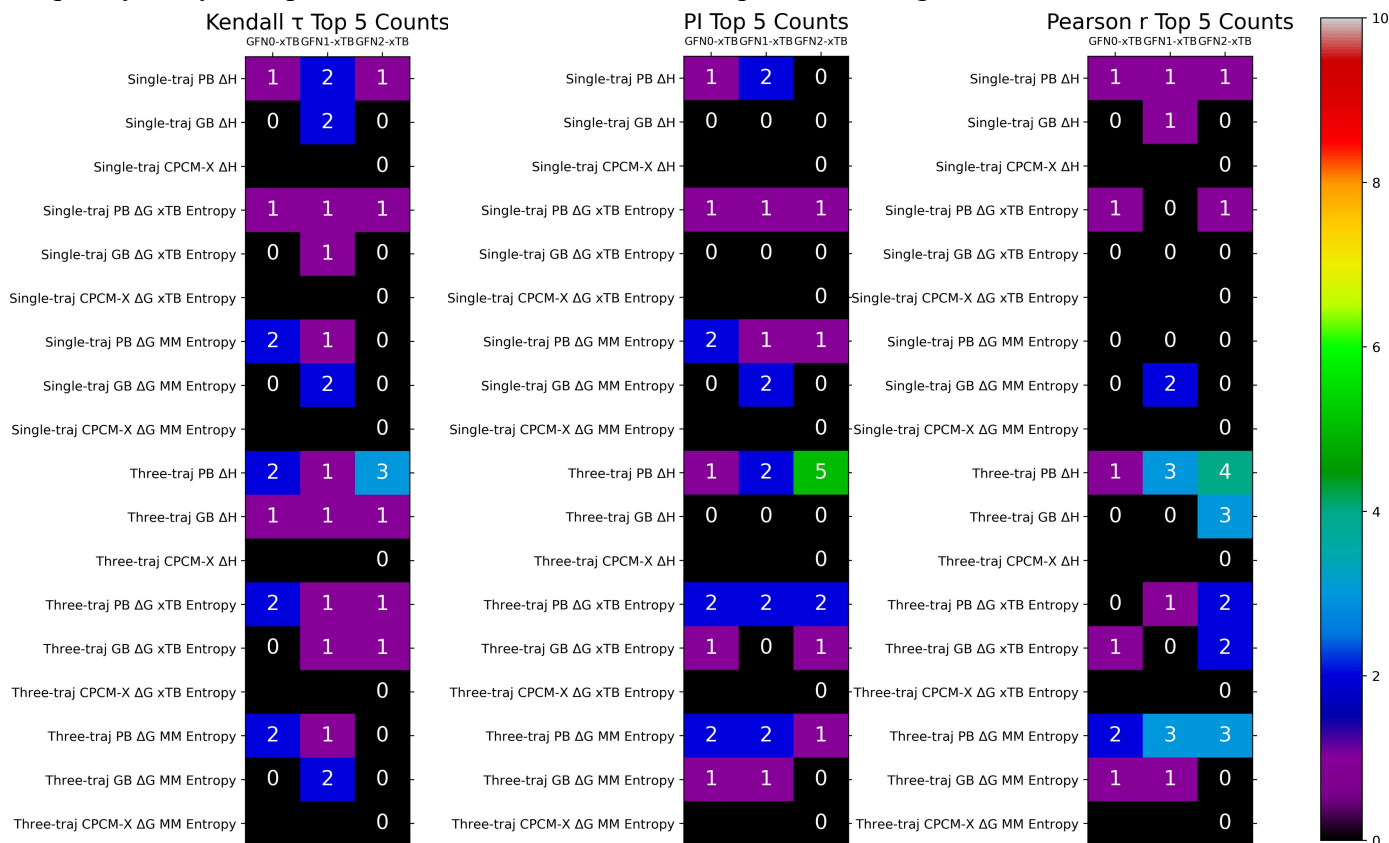


Fig. S5. Top-7 frequency maps. The N top-performing methods in each host-guest dataset are extracted and a frequency analysis is performed. The most robust technique has the largest number of occurrences in the heatmap.

