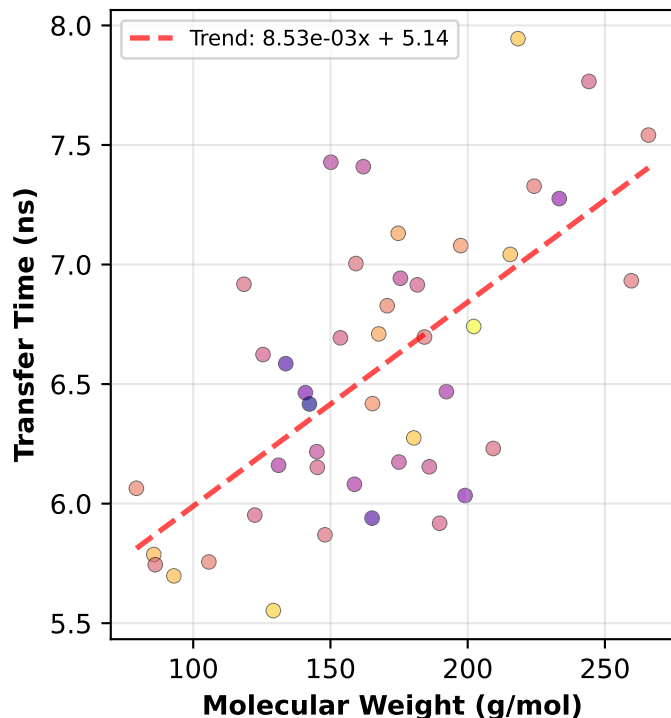
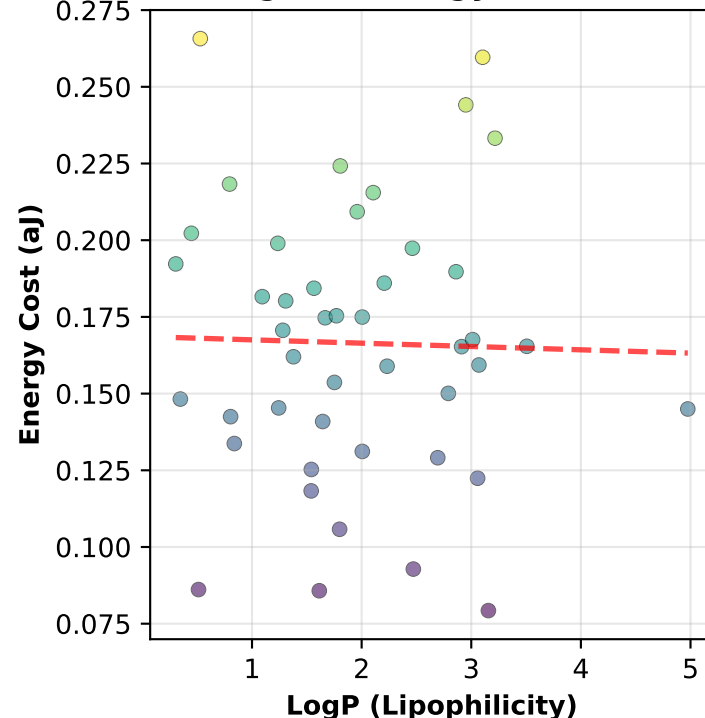


Figure 11: Molecular Property Correlations - Structure-Transfer Relationships

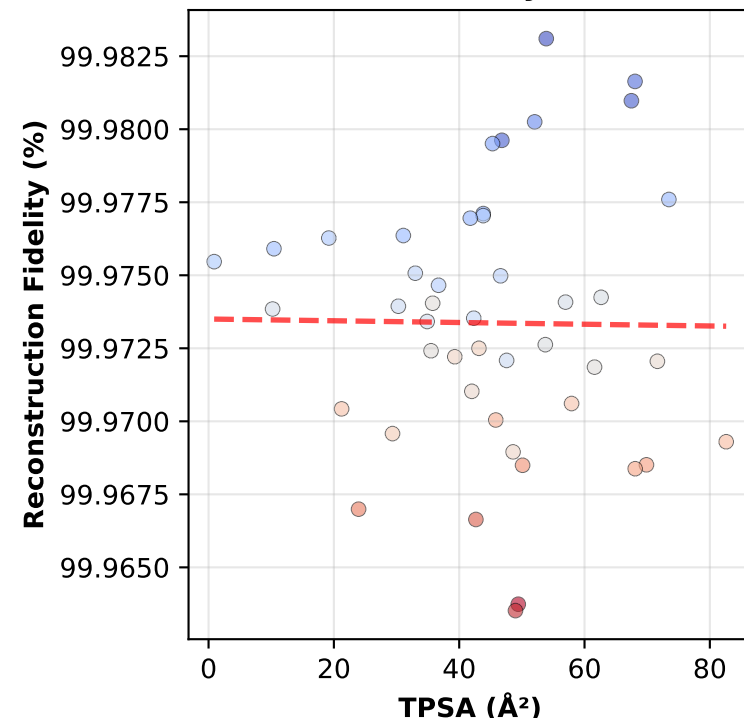
(A) MW vs Transfer Time



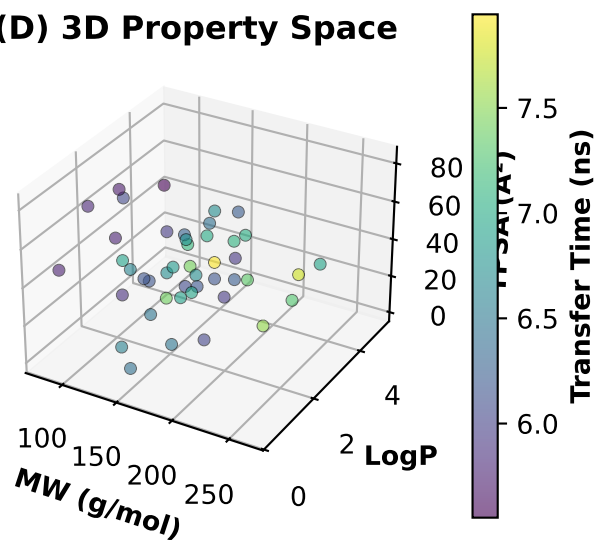
(B) LogP vs Energy



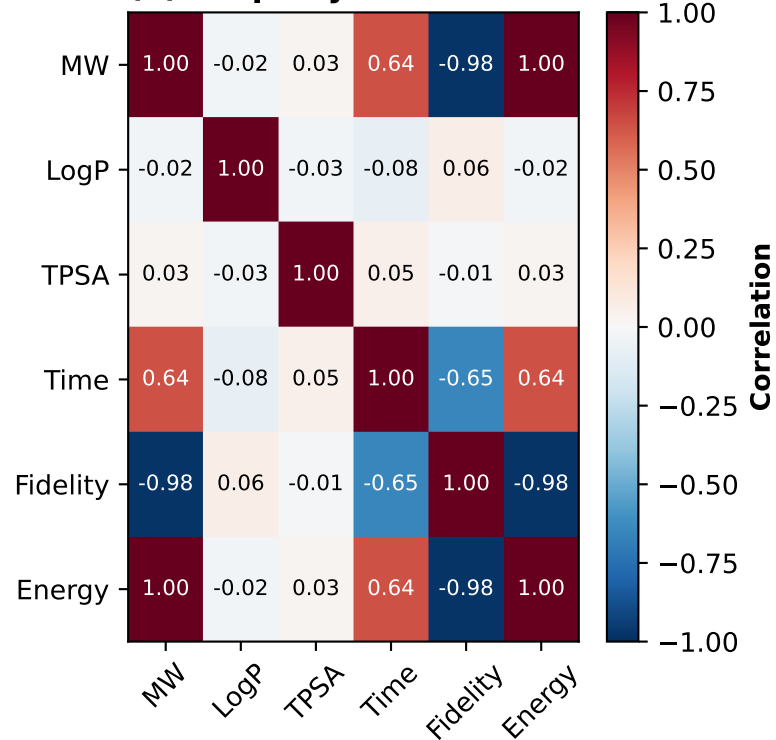
(C) TPSA vs Fidelity



(D) 3D Property Space



(E) Property Correlation Matrix



MOLECULAR PROPERTY STATISTICS

Molecular Weight:

- Mean: 166.5 g/mol
- Std: 44.1
- Range: 79.3 - 265.9

Lipophilicity (LogP):

- Mean: 1.95
- Std: 0.98
- Range: 0.30 - 4.98

TPSA:

- Mean: 44.9 Å²
- Std: 17.4
- Range: 0.9 - 82.6

Transfer Properties:

- Time: 6.56 ± 0.59 ns
- Fidelity: $99.973 \pm 0.004\%$
- Energy: 0.17 ± 0.04 aJ

Correlations:

- MW-Time: 0.637
- LogP-Energy: -0.024
- TPSA-Fidelity: -0.012