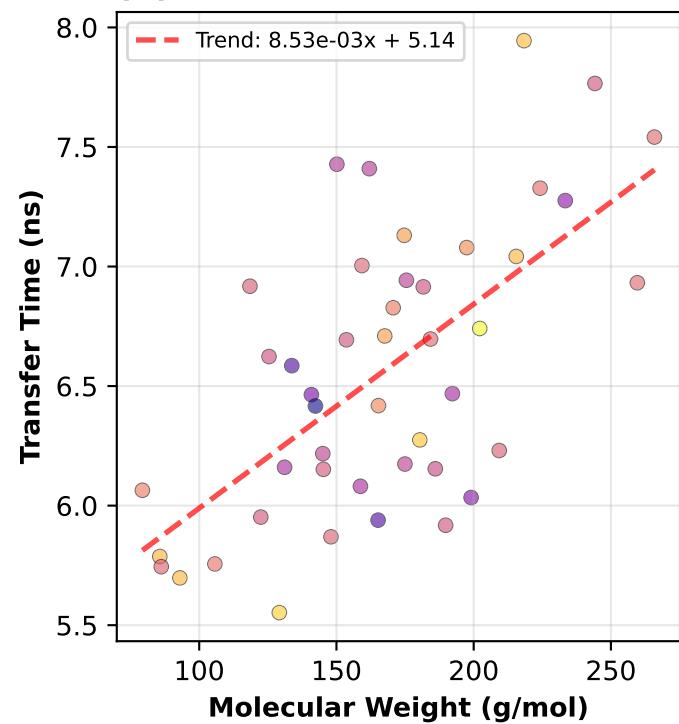
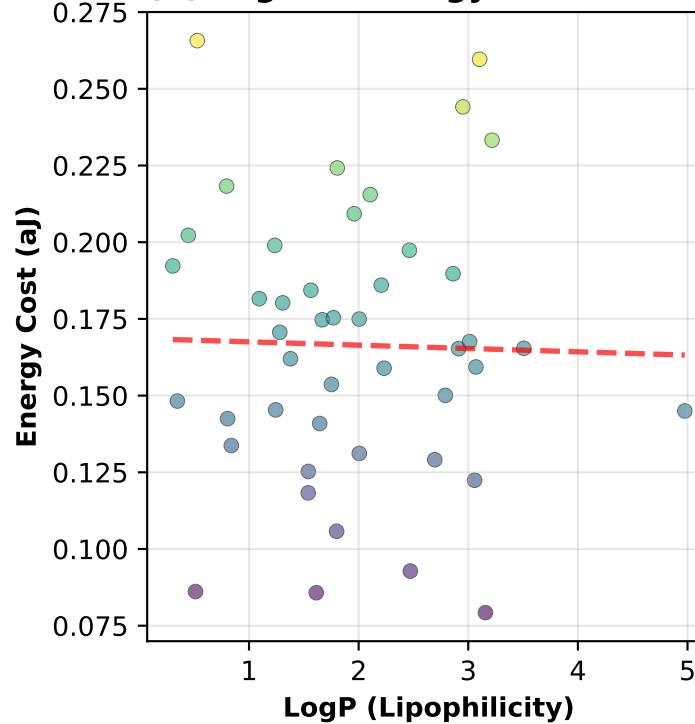


**Figure 11: Molecular Property Correlations - Structure-Transfer Relationships**

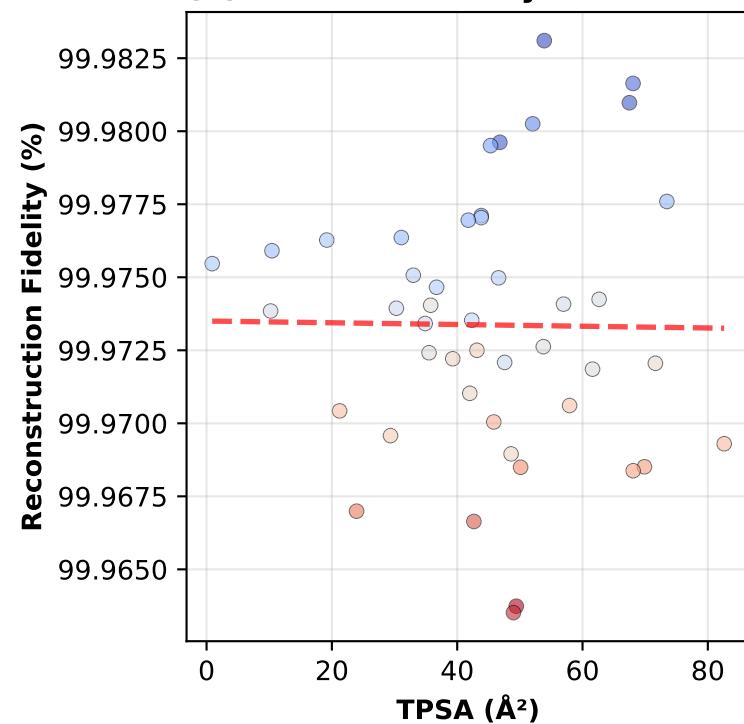
**(A) MW vs Transfer Time**



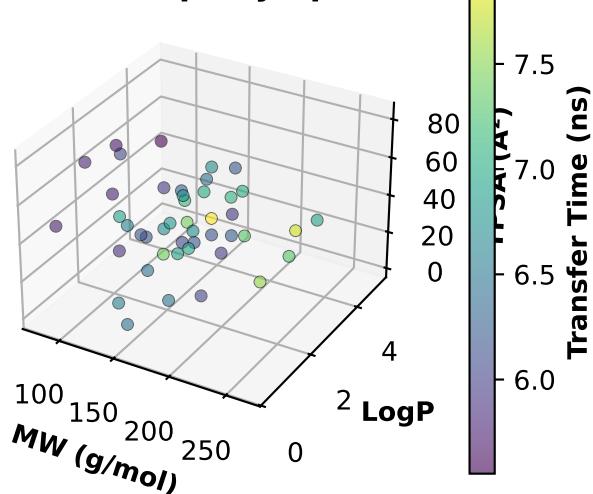
**(B) LogP vs Energy**



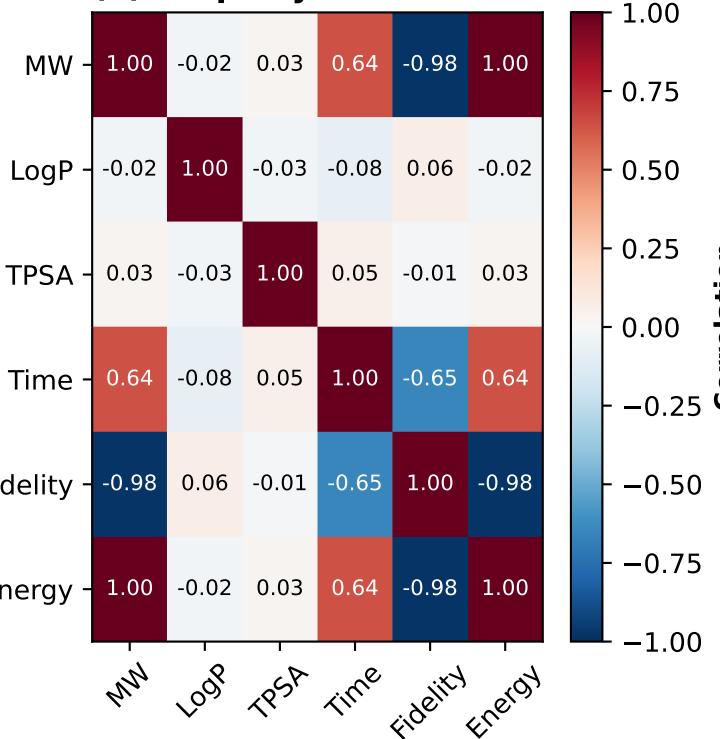
**(C) TPSA vs Fidelity**



**(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  $\text{\AA}^2$
- Std: 17.4
- Range: 0.9 - 82.6

##### Transfer Properties:

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

##### Correlations:

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