

SUPPORTING INFORMATION

Predictions of High-Order Electric Properties of Molecules: Can We Benefit From Machine Learning?

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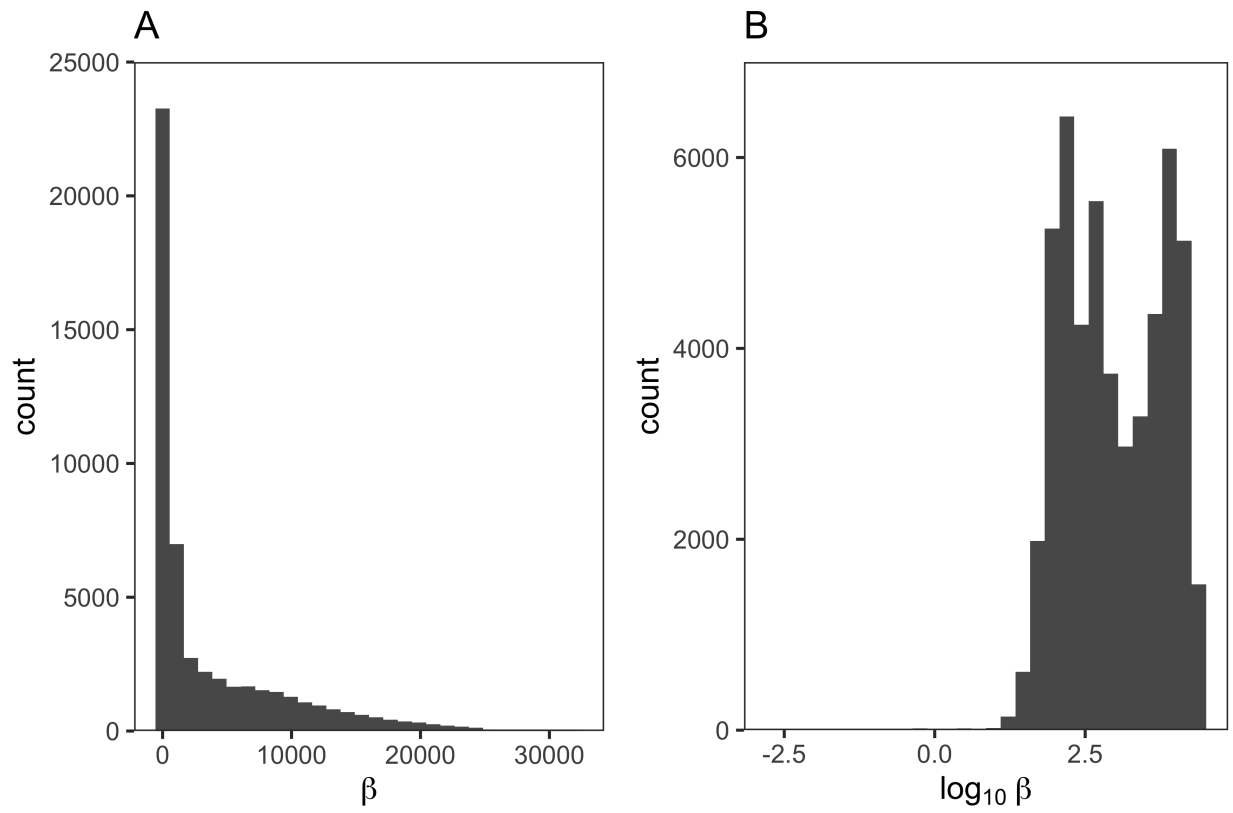


Figure S1: Histogram of (A) hyperpolarizability and (B) logarithmic transformation of hyperpolarizability.

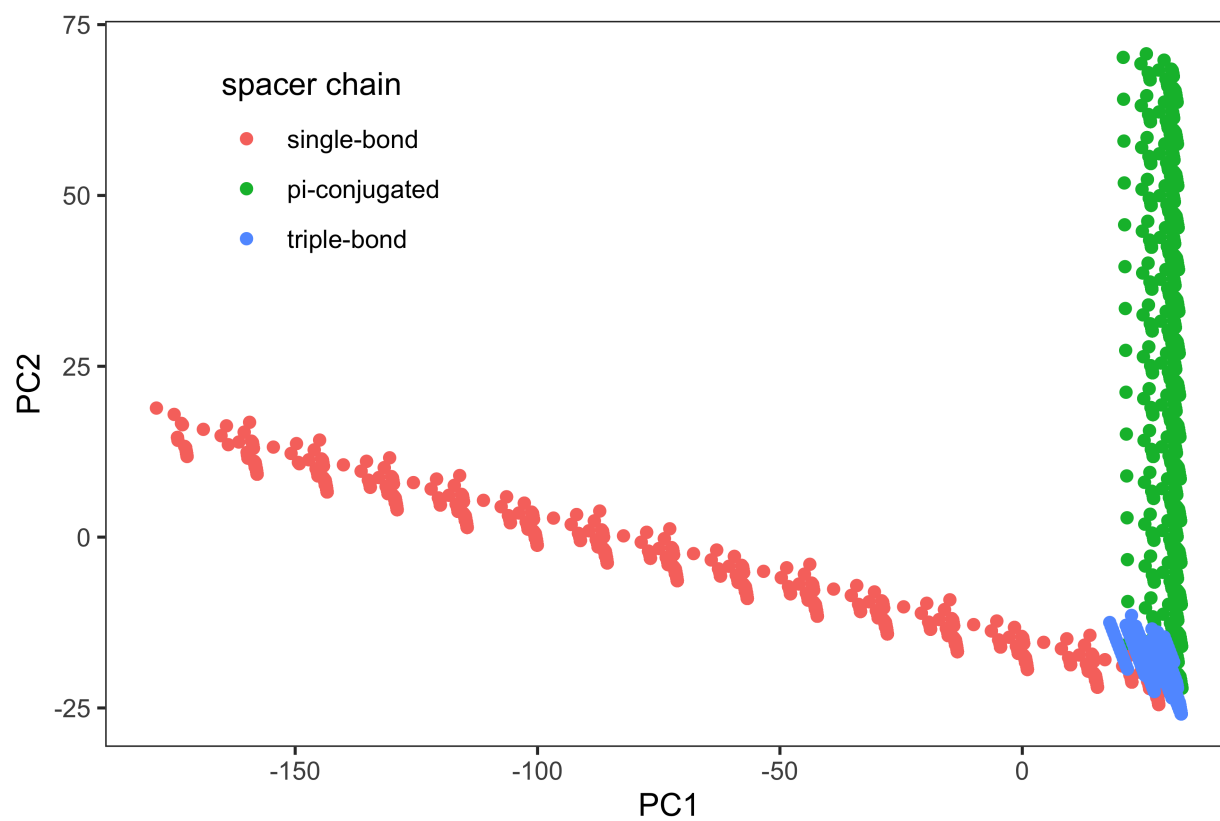


Figure S2: PCA plot based on the Klekota fingerprints for compounds containing single (red dots), alternating single/double (green dots), and single/triple (blue dots) carbon-carbon bonds