

[L2] Computational Method for Estimating Progression Saturation of Analog Series

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In chemical optimization, it is difficult to estimate when an analog series might be saturated and synthesis of additional compounds would unlikely yield further progress. Only few approaches are currently available to monitor analog series progression and aid in decision making. A new computational method is introduced to assess progression saturation of analog series by comparing existing compounds to virtual candidates. Neighborhoods of analogs in chemical space and distance relationships between existing and candidate compounds are explored. A dual scoring scheme is applied to quantify analog series saturation and estimate the progression state.