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Electronic Similarity of Molecules for Evaluation, Classification, and Discovery

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Numerical expression of molecules is important for their quantitative description. By quantification, we can apply a variety of statistical methods to observe quantitative characteristics of molecules, which are expected to facilitate evaluating their values, classifying them, and discovering their derivatives. Intrinsic structures and properties of molecules are due to their electronic structures, it is natural to quantify molecules on the basis of electronic-structure calculations.

In this presentation, we suggest a method of defining molecular similarity by applying ab initio electronic-structure calculations. It will be shown that reasonable classification of molecules is possible for the trial set shown in Scheme 1. When a reference molecule is taken as lutein A, the carotenoid molecules are top-ranked as shown in Table 1. The present computational method is also applied to investigate bioisosterism of functional groups.

Scheme 1.

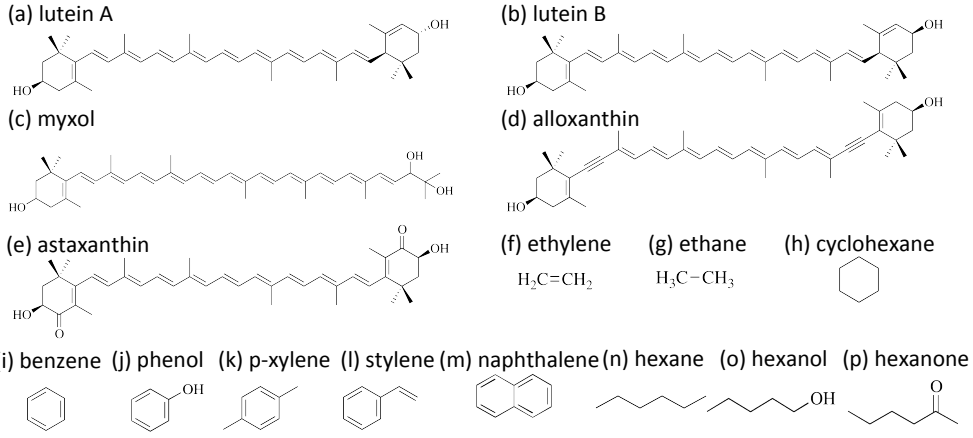

Table 1. Ranking of electronic similarity of molecules in Fig. 1.

Rank	Compd.	Similarity (%)	Rank	Compod.	Similarity (%)
1	lutein A	100.0	9	2-hexanone	31.5
2	lutein B	98.0	10	phenol	30.5
3	myxol	91.9	11	1-hexanol	29.7
4	alloxanthin	91.8	12	benzene	25.5
5	astaxanthin	77.9	13	hexane	24.9
6	p-xylene	37.7	14	ethane	20.4
7	naphthalene	37.3	15	ethylene	20.1
8	stylene	37.2	16	cyclohexane	19.2