

On evaluating the possibility of synthesizing virtually designed polymers

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Table S1 Minimum and maximum SAscore values for various polymers and their market prices.

SMILES	Polymer	SAScore	Price (\$ per g)
CC	Polyethylene	0.411798567	0.001
c1ccc(cc1)	Poly(<i>p</i> -phenylene)	0.752703786	0.18
Cc1ccc(cc1)C	Poly(<i>p</i> -xylylene)	1.065946817	0.002
Oc1ccc(cc1)	Poly[oxy(<i>p</i> -phenylene)]	1.134054422	0.66
NC(=O)c1ccc(cc1)C(=O)Nc1ccc(cc1)	Poly(<i>p</i> -phenylene terephthalamide)	1.196080089	0.1
O[SiH](C)	Poly[oxy(methylhydrosilylene)]	4.648731232	1.4
N[Si](C)(C)	Poly(1,1-dimethylsilazane)	4.907017231	38.6
Oc1ccc(c(c1)NC(=O)C1C(C(=O)O)C2C=CC1C1C2C(C1C(=O)O)C(=O)Nc1cc()ccc1N)N	Polyheteroarylene_XII	5.236793041	N/F
SC(F)(F)	Poly(thiocarbonylfluoride)	5.248370171	N/F
CC(Br)(Br)	Poly(vinylidenebromide)	5.314866543	N/F

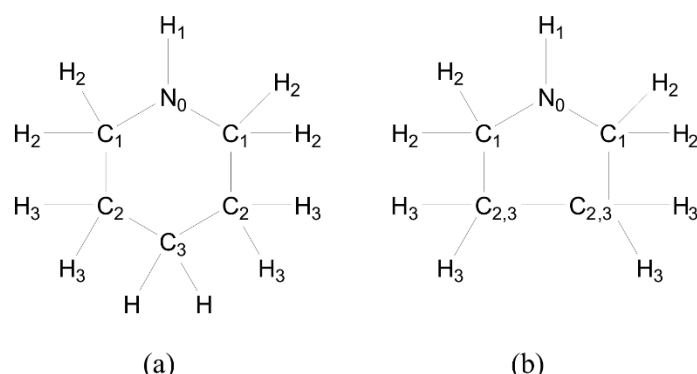


Figure S1 Example of fragmentation of (a) piperidine and (b) pyrrolidine into fragments with a topological radius of 3. The central atom in both cases is nitrogen, and the labels on the other atoms correspond to the topological radius enclosing them. For pyrrolidine with a five-membered ring, there are ambiguities regarding distant carbon atoms, for which the topological radius can be both 2 and 3. To eliminate these ambiguities, at least a six-membered ring is used for the repeating units of a cyclic polymer.