
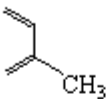








Supplementary Information:

In a classic study Houk and Munchausen^{35(a)} have demonstrated that changes in IP and EA values of dienophiles (induced by different substitutions) can be used to predict their reactivity trends in Diels-Alder (DA) reactions. The IP and EA values of the chosen dienes and dienophiles in the present study are reported in Tables S1 and S2, respectively.

Table S1: *IP* values (in eV) of the chosen Diels-Alder pairs are generated at MP2(FC)/6-31G(D,P) level.

Dienes	IP (eV)
	8.86
	8.64
	8.42
	8.47
	8.41
	7.83
	7.37
	10.08






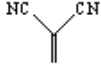
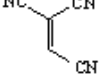
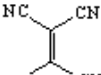



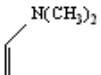


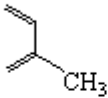





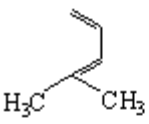


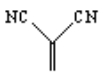
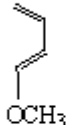
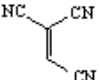
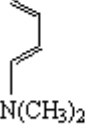
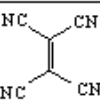





Dienophiles	IP (eV)
	12.73
	10.50
	10.20
	11.27
	11.24
	12.40
	13.34
	14.30
	9.64
	11.10
	8.65
	7.82

Table S2: *EA* values (in eV) of the chosen Diels-Alder pairs are generated at MP2(FC)/6-31G(D,P) level.

Dienes	EA (eV)	Dienophiles	EA (eV)
	-2.17		-3.85
	-2.24		-1.77
	-2.16		-1.47
	-2.25		-1.72
	-2.29		-1.07
	-2.70		-0.24
	-2.46		0.70
	-2.63		1.26
	-0.82		-3.91
			-5.69
			-4.12
			-4.23