Supporting Information for "The MC-DFT Approach Including the SCS-MP2 Energies to the New Minnesota-type Functionals "

Po-Chun Liu and Wei-Ping Hu*

Department of Chemistry and Biochemistry, National Chung Cheng University
Chia-Yi, Taiwan 621

E-mail: chewph@ccu.edu.tw

Submitted to *J. Comput. Chem.*, 2014

5 Tables, 10 Figure, 17 pages.

Table S1. Mean Unsigned Errors (kcal/mol) of MP2, SCS-MP2, MC-MP2 and MC-SCS-MP2 methods

Basis set combination	MP2	SCS-MP2
pdz	22.8	8.40
apdz	16.3	5.78
ptz	7.14	5.26
pdz/ptz	6.22	4.36
pdz/apdz/ptz	5.66	4.15
aptz	5.48	4.04
pdz/ptz/aptz	5.38	3.93
MG3S	7.14	4.83
pdz/MG3S	6.85	4.82
Pop-dp	16.31	6.53
Pop-2d2p	11.31	5.25
Pop-dp/Pop-2d2p	7.17	5.07
Pop-2df2pd	5.85	4.37
Pop-dp/Pop-2df2pd	5.66	3.86
Pop-2d2p/Pop-2df2pd	5.70	4.03
Pop-dp/Pop-2d2p/Pop-2df2pd	5.65	3.81
Pop-3df2pd	6.08	4.52
Pop-dp/Pop-3df2pd	6.04	4.26
Pop-2df2pd/Pop-3df2pd	5.81	4.35
Pop-dp/Pop-2d2p/Pop-3df2pd	5.95	4.24

Table S2. Relative Computational Cost[a] and P/C Ratios of MP2, SCS-MP2, MC-MP2 and MC-SCS-MP2 methods.

Basis set combination	MP2	SCS-MP2
pdz	4% (0.05)[b]	(0.40)
apdz	9% (0.04)	(0.33)
ptz	24% (0.08)	(0.15)
pdz/ptz	27% (0.10)	(0.19)
pdz/apdz/ptz	36% (0.09)	(0.16)
aptz	168% (0.02)	(0.04)
pdz/ptz/aptz	196% (0.02)	(0.03)
MG3S	28% (0.07)	(0.15)
pdz/MG3S	31% (0.07)	(0.14)
Pop-dp	7% (0.06)	(0.36)
Pop-2d2p	12% (0.06)	(0.30)
Pop-dp/Pop-2d2p	19% (0.10)	(0.21)
Pop-2df2pd	25% (0.12)	(0.21)
Pop-dp/Pop-2df2pd	31% (0.10)	(0.21)
Pop-2d2p/Pop-2df2pd	37% (0.08)	(0.17)
Pop-dp/Pop-2d2p/Pop-2df2pd	44% (0.07)	(0.16)
Pop-3df2pd	40% (0.07)	(0.12)
Pop-dp/Pop-3df2pd	47% (0.06)	(0.12)
Pop-2df2pd/Pop-3df2pd	53% (0.06)	(0.10)
Pop-dp/Pop-2d2p/Pop-3df2pd	59% (0.05)	(0.09)

[a]Relative to the M06-2X/aptz calculation, the cost of MP2 and SCS-MP2 is the same.

[b]Numbers in parentheses refer to the performance/cost (P/C) ratios which were defined as 1 / (relative cost × MUE^2).

Table S3. Relative Computational Cost[a] and P/C Ratios of the M08-HX functional[b].

Basis set combination	MC-M08-HX	MP2 | MC-M08-HX	MC-MP2 | MC-M08-HX
ptz	17% (0.60)[c]	25% (0.79)	51% (0.68)
pdz/apdz/ptz	31% (0.98)	40% (0.94)	65% (0.61)
aptz	68% (0.22)	76% (0.45)	102% (0.48)
pdz/ptz/aptz	88% (0.39)	97% (0.46)	123% (0.46)
MG3S	21% (1.77)	29% (1.45)	55% (1.00)
pdz/MG3S	25% (1.59)	33% (1.28)	59% (1.05)
Pop-2d2p	11% (1.53)	19% (1.47)	45% (1.43)
Pop-dp/Pop-2d2p	17% (2.08)	26% (1.85)	52% (1.26)
Pop-2df2pd	19% (1.72)	28% (1.32)	53% (1.00)
Pop-dp/Pop-2df2pd	26 % (1.59)	34% (1.27)	60% (0.91)
Pop-dp/Pop-2d2p/Pop-2df2pd	37 % (1.17)	45% (1.13)	71% (0.94)
Pop-3df2pd	26 % (1.39)	34% (1.10)	60% (0.75)
Pop-dp/Pop-3df2pd	32 % (1.09)	41% (0.97)	67% (0.75)
Pop-dp/Pop-2d2p/Pop-3df2pd	43 % (0.98)	52% (0.99)	77% (0.90)

[a]Relative to the M06-2X/aptz calculation.

[b]All the calculations in Table S3 were carried out using the Molpro 2012.1 program.

[c]Numbers in parentheses refer to the performance/cost (P/C) ratios which were defined as 1 / (relative cost × MUE^2).

Table S4. Relative Computational Cost[a] and P/C Ratios of the MN12-SX functional.

Basis set combination	MC-MN12-SX	MP2 | MC-MN12-SX	MC-MP2 | MC-MN12-SX
ptz	25% (0.29)	34 % (0.40)	59 % (0.43)
pdz/apdz/ptz	38 % (0.32)	47 % (0.49)	72 % (0.39)
aptz	173 % (0.06)	182 % (0.14)	207 % (0.15)
pdz/ptz/aptz	202% (0.07)	211% (0.12)	236% (0.14)
MG3S	35 % (0.75)	43 % (0.71)	69 % (0.49)
pdz/MG3S	39 % (0.68)	47 % (0.67)	73 % (0.47)
Pop-2d2p	11 % (1.54)	20 % (1.14)	46 % (0.63)
Pop-dp/Pop-2d2p	18 % (1.09)	27 % (0.87)	53 % (0.56)
Pop-2df2pd	32 % (0.69)	41 % (0.65)	66 % (0.45)
Pop-dp/Pop-2df2pd	39 % (0.57)	48 % (0.56)	73 % (0.41)
Pop-dp/Pop-2d2p/Pop-2df2pd	51 % (0.44)	59 % (0.46)	85 % (0.36)
Pop-3df2pd	64 % (0.32)	73 % (0.34)	98 % (0.28)
Pop-dp/Pop-3df2pd	71 % (0.30)	80 % (0.31)	105 % (0.28)
Pop-dp/Pop-2d2p/Pop-3df2pd	83 % (0.26)	91 % (0.27)	117 % (0.25)

[a]Relative to the M06-2X/aptz calculation.

[b]Numbers in parentheses refer to the performance/cost (P/C) ratios which were defined as 1 / (relative cost × MUE^2).

Table S5. Mean Unsigned Errors (kcal/mol) of Several MC-MP2 | M06-2X and MC-SCS-MP2/MC-M06-2X Methods with Various Basis Set Combinations for the MP2 and M06-2X Parts.

Basis sets combination for M06-2X	MC-M06-2X	MP2/apdz | MC-M06-2X	SCS-MP2/apdz | MC-M06-2X	SCS-MP2/aptz | MC-M06-2X	SCS-MP2/MG3S | MC-M06-2X	SCS-MP2/Pop-2df2pd | MC-M06-2X
pdz	8.37	5.34	4.48	3.64	4.01	3.91
ptz	2.92	2.72	2.51	2.4	2.46	2.46
pdz/ptz	2.22	1.76	1.71	1.75	1.78	1.79
pdz/apdz/ptz	1.54	1.52	1.51	1.50	1.51	1.50
aptz	1.99	1.78	1.68	1.66	1.67	1.67
pdz/ptz/aptz	1.55	1.47	1.43	1.44	1.45	1.44
MG3S	1.76	1.69	1.56	1.56	1.57	1.57
pdz/MG3S	1.53	1.52	1.41	1.42	1.42	1.42
Pop-dp	4.84	2.81	2.69	2.48	2.55	2.57
Pop-dp/Pop-2d2p	1.58	1.46	1.32	1.31	1.32	1.33
Pop-2df2pd	1.85	1.82	1.70	1.68	1.69	1.70
Pop-dp/Pop-2df2pd	1.75	1.73	1.51	1.53	1.54	1.54
Pop-dp/Pop-2d2p/Pop-2df2pd	1.58	1.43	1.32	1.30	1.32	1.33

	MC-MP2/[pdz/apdz/ptz] | MC-M06-2X	MC-SCS-MP2/[pdz/apdz/ptz] | MC-M06-2X	MC-SCS-MP2/[Pop-dp/Pop-2d2p/Pop-2df2pd] | MC-M06-2X
pdz	2.24	2.06	2.95
ptz	1.73	1.69	2.19
pdz/ptz	1.52	1.59	1.75
pdz/apdz/ptz	1.43	1.41	1.43
aptz	1.57	1.51	1.42
pdz/ptz/aptz	1.41	1.37	1.35
MG3S	1.55	1.39	1.36
pdz/MG3S	1.44	1.26	1.23
Pop-dp	1.84	1.75	1.61
Pop-dp/Pop-2d2p	1.32	1.22	1.27
Pop-2df2pd	1.60	1.42	1.39
Pop-dp/Pop-2df2pd	1.60	1.41	1.31
Pop-dp/Pop-2d2p/Pop-2df2pd	1.28	1.21	1.26

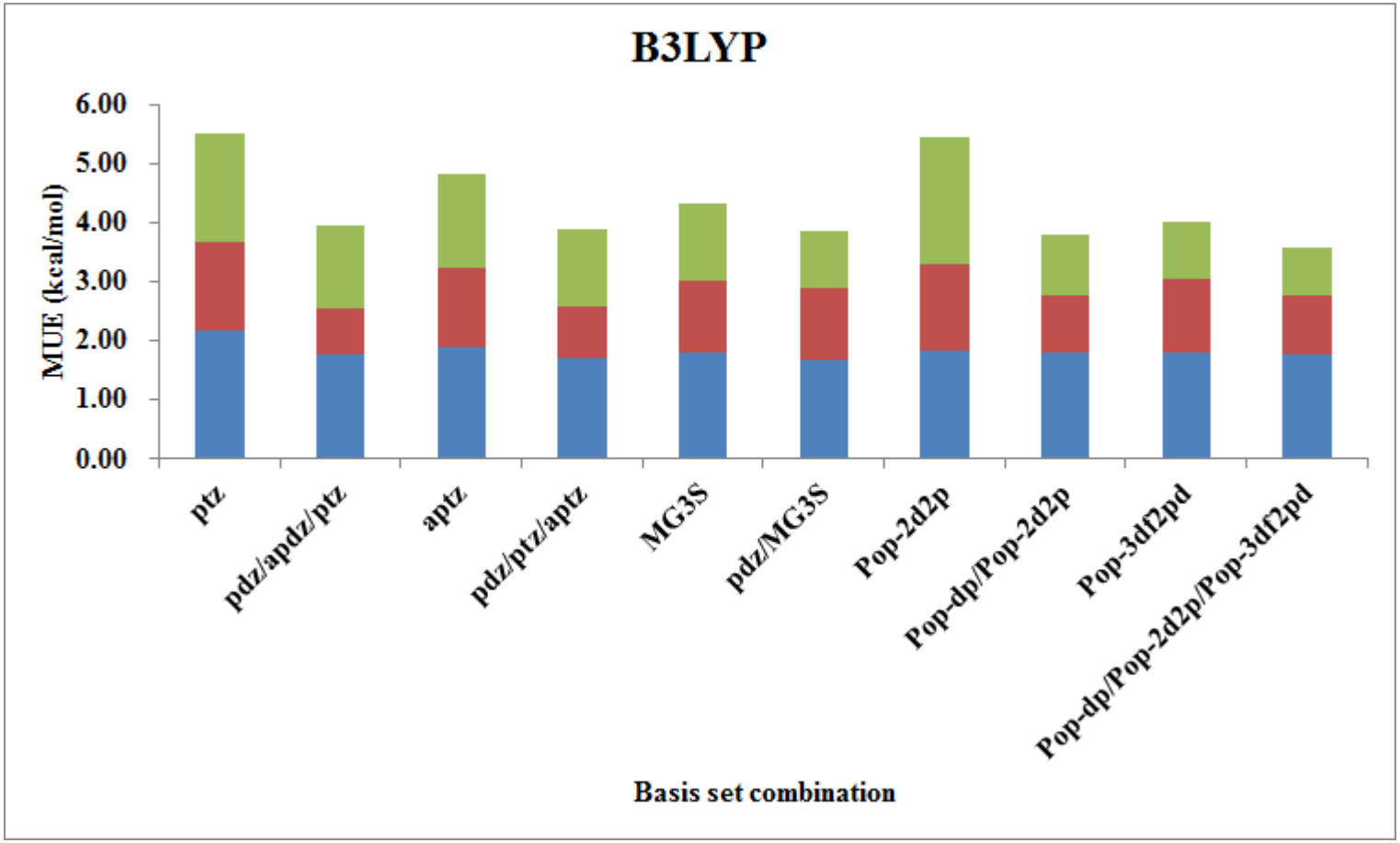

Figure S1. MUEs (kcal/mol) of the B3LYP functional using various basis sets and basis set combinations. The tops of the green, red, and blue bars were the results by the MC-DFT, SCS-MP2 | MC-DFT, and MC-SCS-MP2 | MC-DFT approaches, respectively.

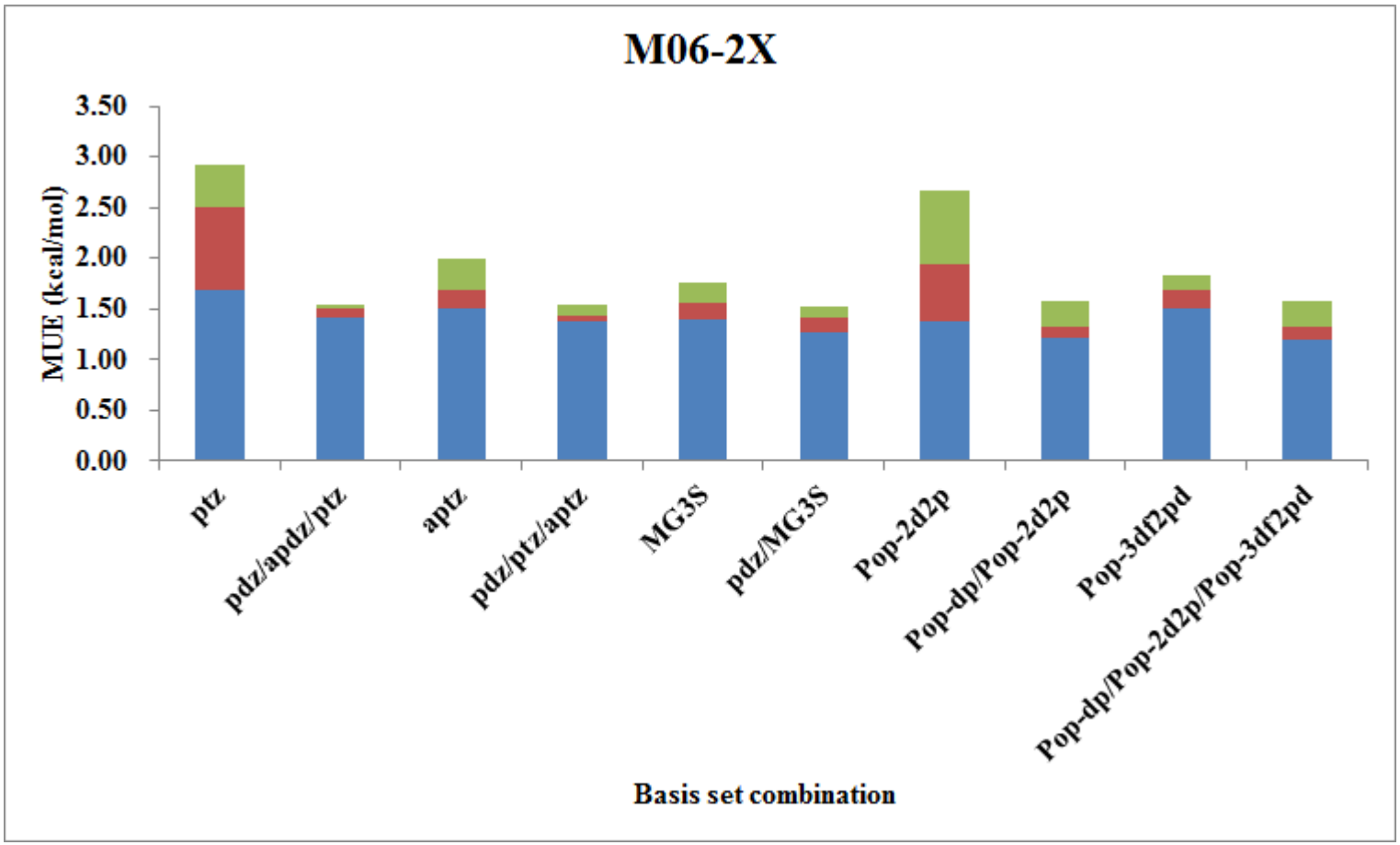

Figure S2. MUEs (kcal/mol) of the M06-2X functional using various basis sets and basis set combinations. The tops of the green, red, and blue bars were the results by the MC-DFT, SCS-MP2 | MC-DFT, and MC-SCS-MP2 | MC-DFT approaches, respectively.

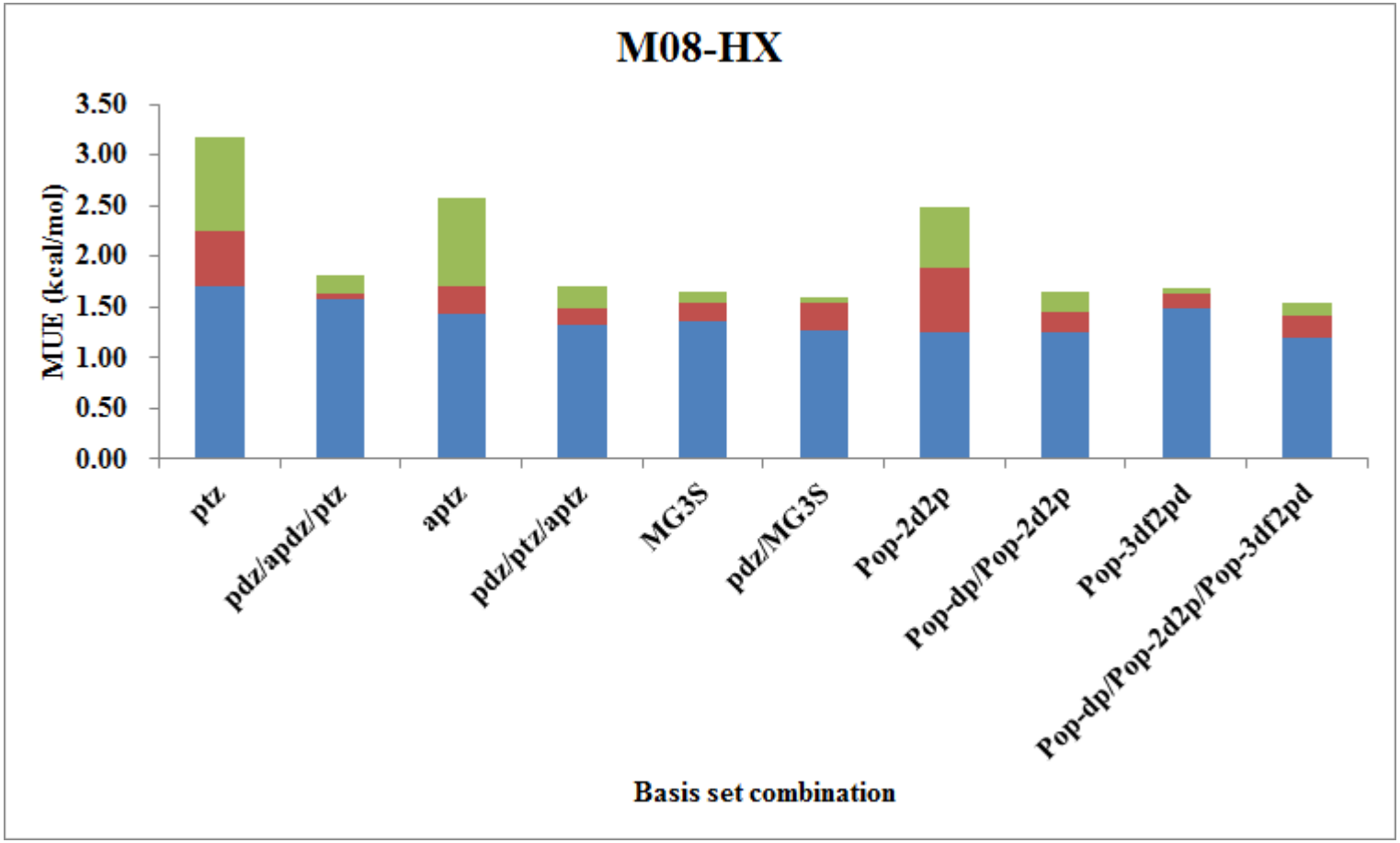

Figure S3. MUEs (kcal/mol) of the M08-HX functional using various basis sets and basis set combinations. The tops of the green, red, and blue bars were the results by the MC-DFT, SCS-MP2 | MC-DFT, and MC-SCS-MP2 | MC-DFT approaches, respectively.

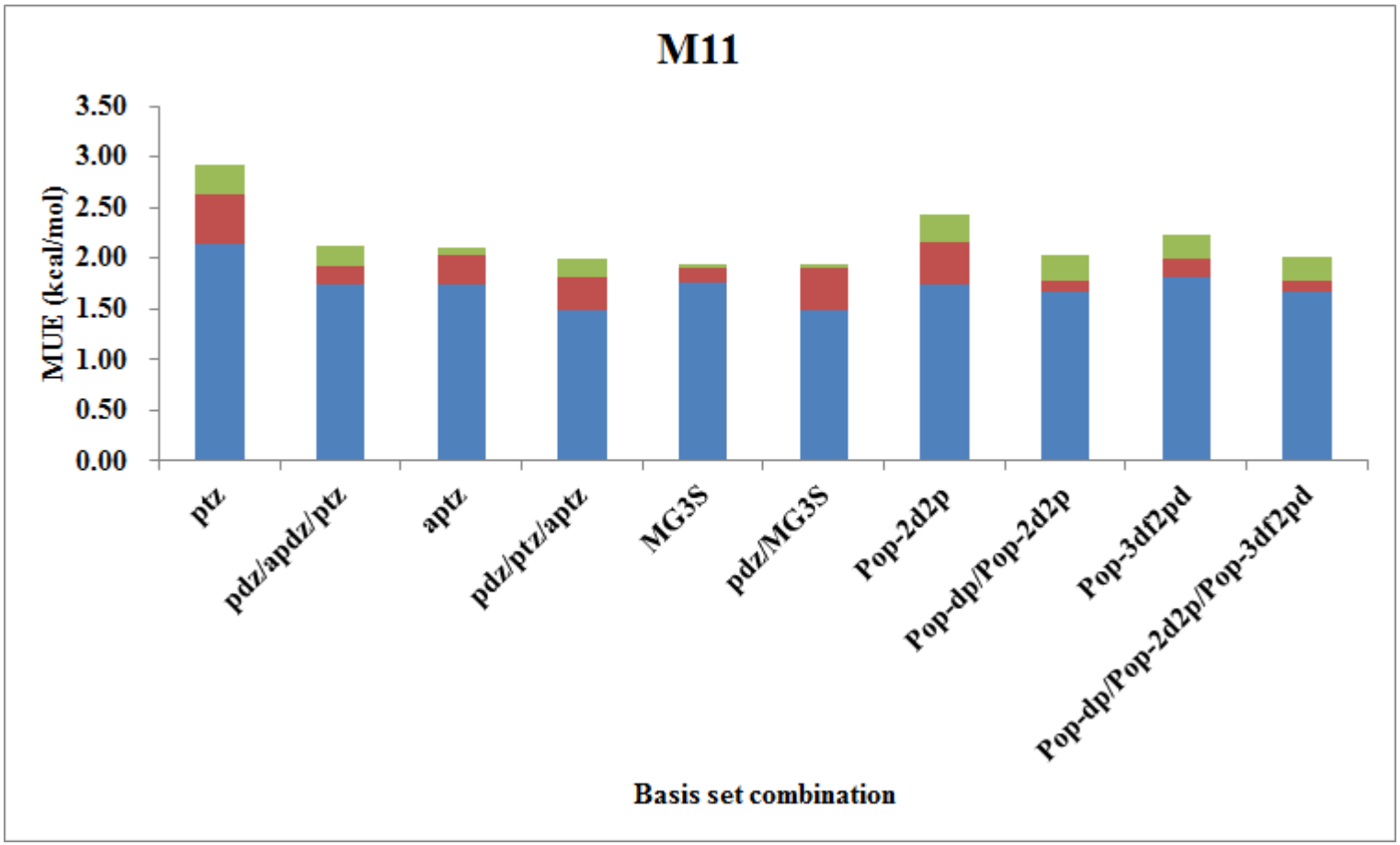

Figure S4. MUEs (kcal/mol) of the M11 functional using various basis sets and basis set combinations. The tops of the green, red, and blue bars were the results by the MC-DFT, SCS-MP2 | MC-DFT, and MC-SCS-MP2 | MC-DFT approaches, respectively.

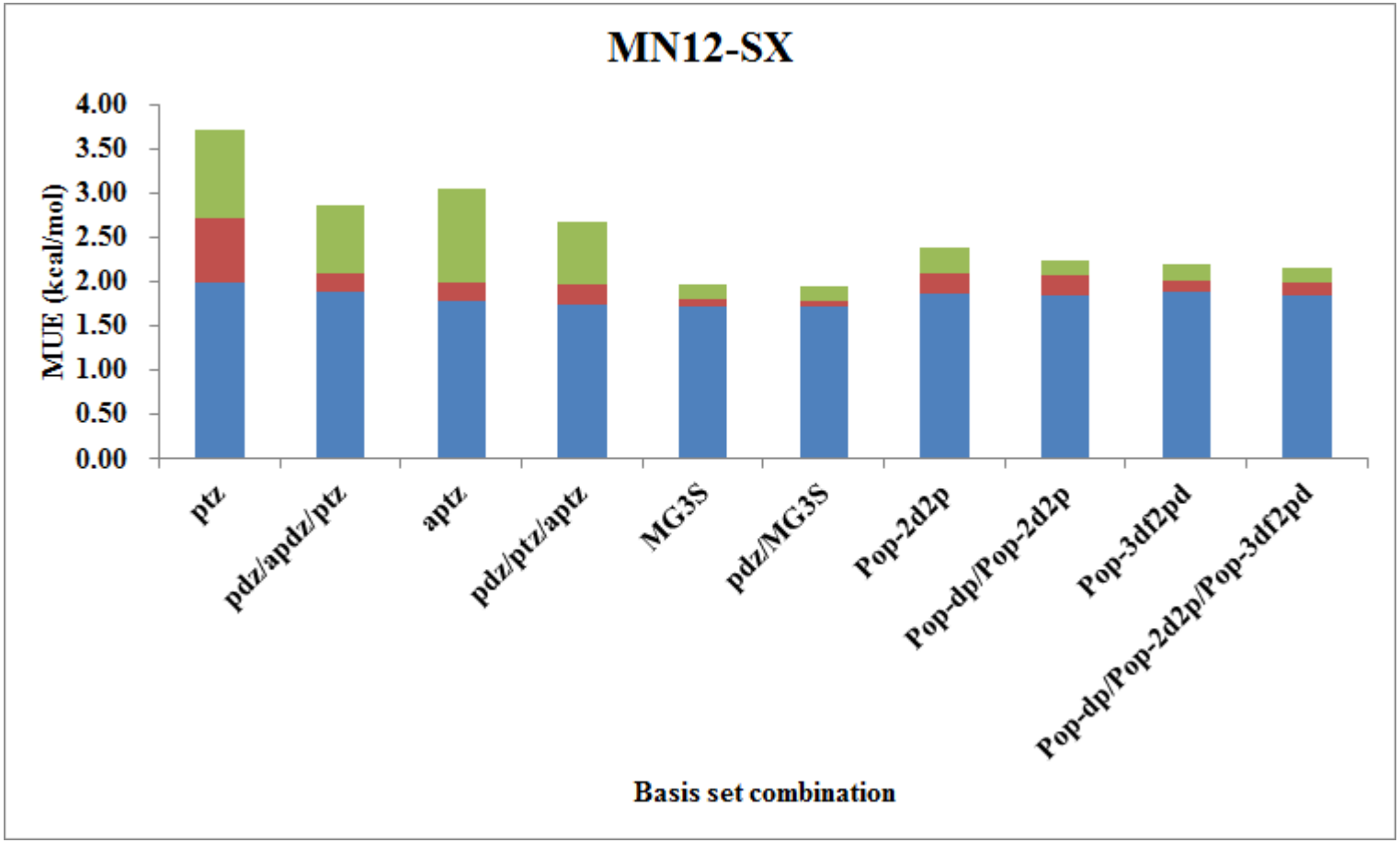

Figure S5. MUEs (kcal/mol) of the MN12-SX functional using various basis sets and basis set combinations. The tops of the green, red, and blue bars were the results by the MC-DFT, SCS-MP2 | MC-DFT, and MC-SCS-MP2 | MC-DFT approaches, respectively.

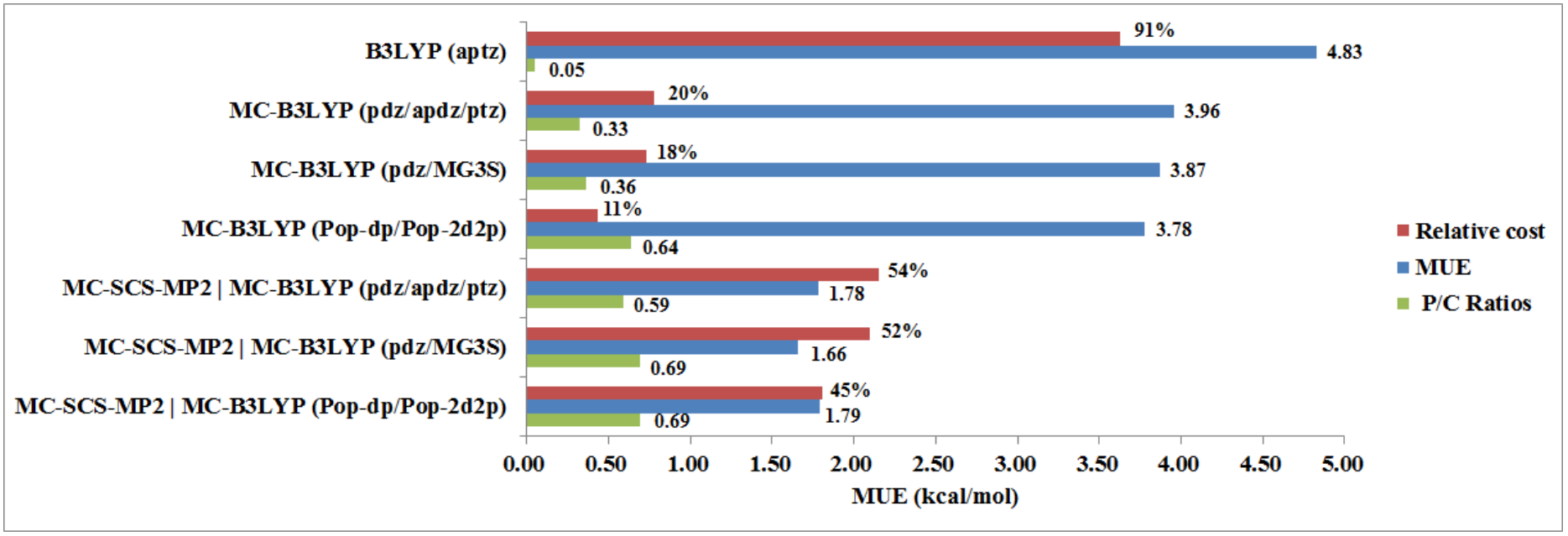

Figure S6. MUE (kcal/mol), Relative Cost (%) and P/C Ratios of Several Efficient Methods using the B3LYP functional.

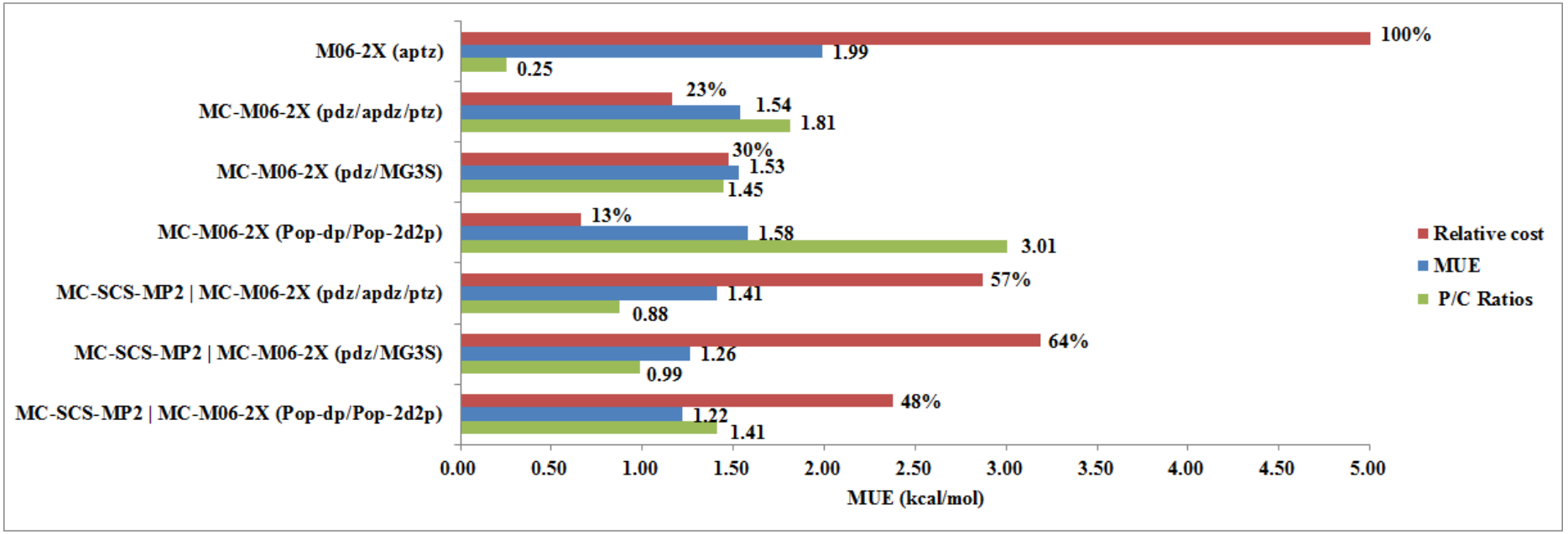

Figure S7. MUE (kcal/mol), Relative Cost (%) and P/C Ratios of Several Efficient Methods using the M06-2X functional.

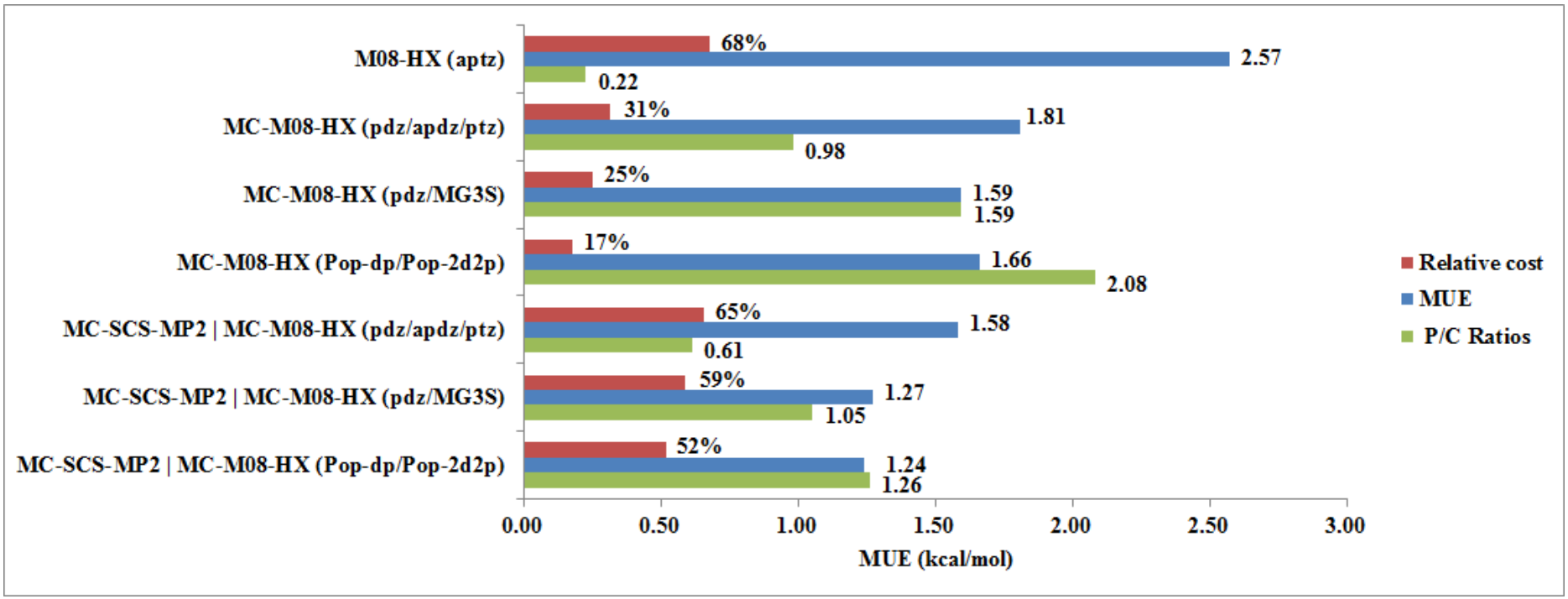

Figure S8. MUE (kcal/mol), Relative Cost (%) and P/C Ratios of the Several Efficient Methods using the M08-HX functional.

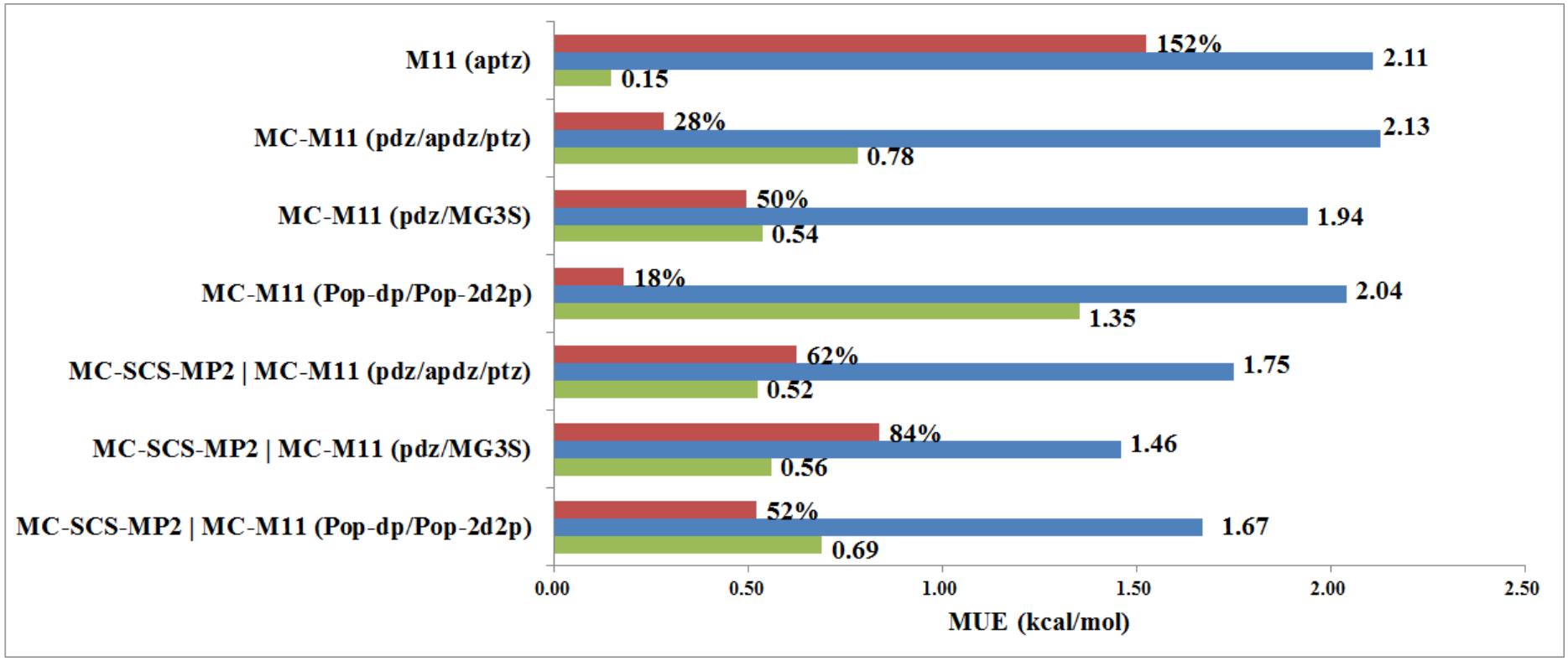

Figure S9. MUE (kcal/mol), Relative Cost (%) and P/C Ratios of the Several Efficient Methods using the M11 functional.

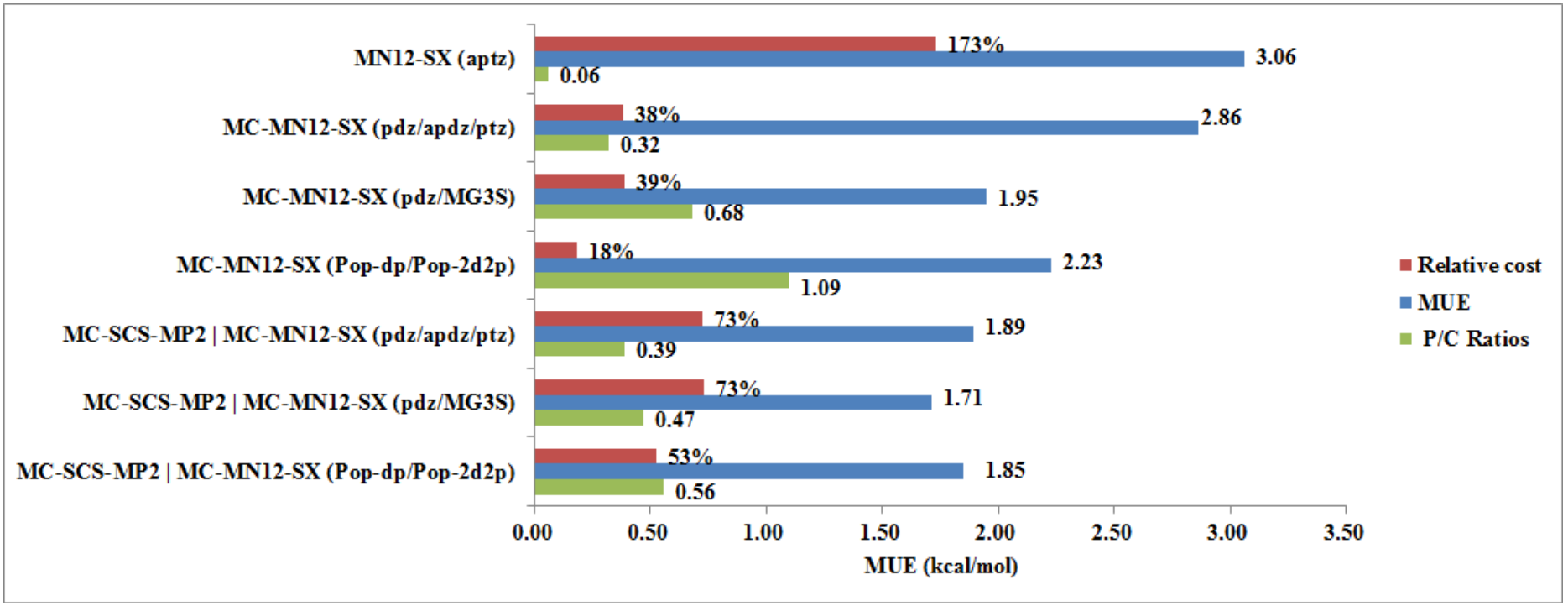

Figure S10. MUE (kcal/mol), Relative Cost (%) and P/C Ratios of the Several Efficient Methods using the MN12-SX functional.