

Mean absolute errors (ppm) in corrected  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  B3LYP/pc-2 nuclear shieldings, according to (1) our two-point correction scheme, and (2) using shifting and scaling parameters obtained via linear regression analysis.

	$^1\text{H}$	$^{13}\text{C}$	$^{19}\text{F}$
(1) excl. outliers	0.238	2.75	7.5
(1) incl. outliers	0.465	5.61	12.8
(2) excl. outliers	0.159	3.87	10.0
(2) incl. outliers	0.450	6.14	12.8