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Mean absolute errors (ppm) in corrected <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>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.

	<sup>1</sup> H	<sup>13</sup> C	<sup>19</sup> 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