Supplemental Material: A Gauge Invariant Multiscale Approach to Magnetic Spectroscopies in Condensed Phase: General Three-Layer Model, Computational Implementation and Pilot Applications

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TABLE I. Absolute chemical shifts (ppm) of pyrimidine in vacuo and solvent shifts (ppm) as obtained with different solvent representations. For the cluster approaches, two explicit water molecules are included at the QM, classical MM and FQ levels of theory, respectively, possibly including the PCM embedding (/PCM). The RMS and Max errors are reported with respect to QM/PCM.

Atom	Vacuum	QM	QEq	FQ	PCM	QM/PCM	QEq/PCM	FQ/PCM
C2	14.35	3.20	1.20	1.34	0.71	3.11	1.31	1.52
N1	-78.09	15.47	12.45	14.35	11.55	21.55	18.76	21.26
C4	18.82	-0.87	-0.98	-1.07	-1.49	-1.43	-1.77	-1.92
C5	57.56	-1.34	-0.89	-1.01	-2.20	-3.00	-2.62	-2.77
H-C4	22.62	-0.12	-0.12	-0.12	-0.12	-0.10	-0.13	-0.13
H-C2	22.01	0.23	0.17	0.17	0.09	0.19	0.15	0.17
H-C5	24.30	-0.26	-0.16	-0.18	-0.40	-0.56	-0.47	-0.50
RMS	-	5.73	13.02	8.45	15.19	-	1.61	0.42
Max	-	6.08	9.09	7.20	9.99	-	2.79	1.60