Supporting Information:

Toward the Quantum Chemical Calculation of NMR Chemical Shifts of Proteins 3: Conformational Sampling and Explicit Solvents Model

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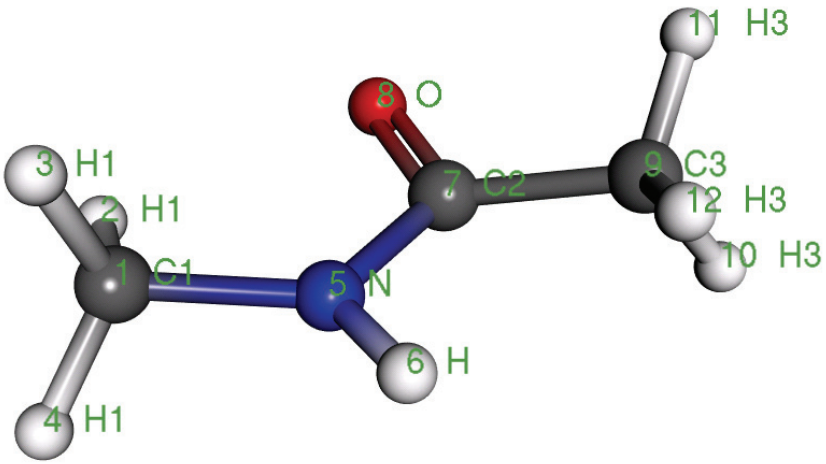

Figure S1: Numbering scheme of N-methyl acetamide used for Tables S1 to S3.

Table S1: ^{13}C chemical shifts in N-methyl acetamide (NMA) calculated with different levels of theory and basis sets: If no level of theory is given, density functional theory with the B3LYP functional was used. Atom numbering is according to Figure S1.

		A	B	C	D	E	F	G	H	I	K	L	M	N	O
		experimental	6-31G(d,p)	6-31G(d)	6-311G(d,p)	6-311G(2d,p)	ccpVDZ	ccpVTZ	ccpVQZ	MP2/6-31G(d,p)	MP2/6-311G(d,p)	MP2/6-311G(2d,p)	MP2/ccpVDZ	MP2/ccpVTZ	MP2/ccpVQZ
monomer trans	C1	28.65	24.843	24.709	25.954	25.028	24.627	25.370	26.368	26.753	28.476	25.828	25.968	27.585	30.238
	C2	177.24	156.963	154.794	168.147	168.784	159.620	170.452	174.989	154.405	162.646	164.303	153.846	167.419	171.354
	C3	24.32	22.727	22.578	24.164	23.495	23.033	23.696	24.571	24.142	24.537	24.502	23.581	24.231	24.426
monomer cis	C1		29.585	29.560	31.170	30.772	29.794	30.885	31.944	31.695	32.420	31.812	31.439	31.894	32.533
	C2		159.745	157.618	171.322	172.068	162.416	173.750	178.519	157.678	165.032	168.036	157.361	169.902	173.561
	C3		20.011	19.807	21.752	21.196	20.241	21.256	22.096	21.769	22.823	22.382	21.331	22.412	23.101
dimer trans	C1		24.565	24.593	25.121	24.262	24.012	24.651	29.046	28.806	28.959	28.393	28.031	28.587	--
	C2		158.681	156.543	170.122	170.733	161.693	171.894	177.483	156.597	164.680	167.887	156.168	169.269	--
	C3		21.799	21.649	23.373	22.681	21.967	23.027	23.298	23.337	24.079	23.534	22.747	23.886	--
dimer cis	C1		29.023	28.904	30.486	29.805	29.002	30.092	31.161	31.112	31.597	30.777	30.558	31.076	--
	C2		164.153	161.815	177.640	178.296	167.724	179.511	183.856	161.726	170.327	173.992	161.736	175.916	--
	C3		20.983	20.733	22.713	22.068	21.364	21.985	22.801	22.489	23.566	23.070	22.129	23.006	--

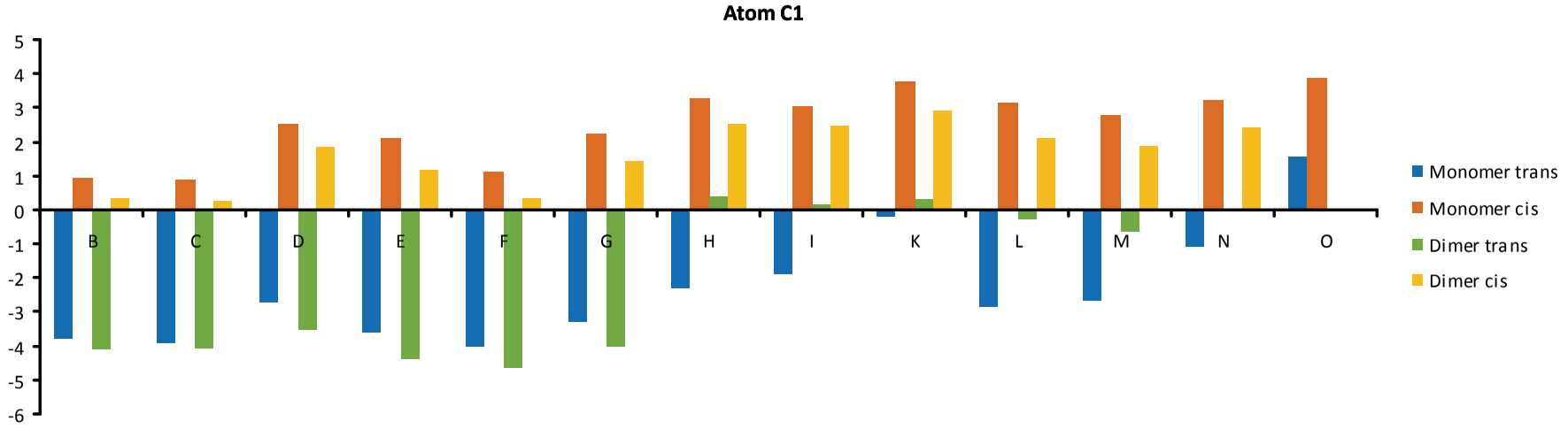

Figure S2: Errors in the ^{13}C chemical shifts of atom C1 in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S1.

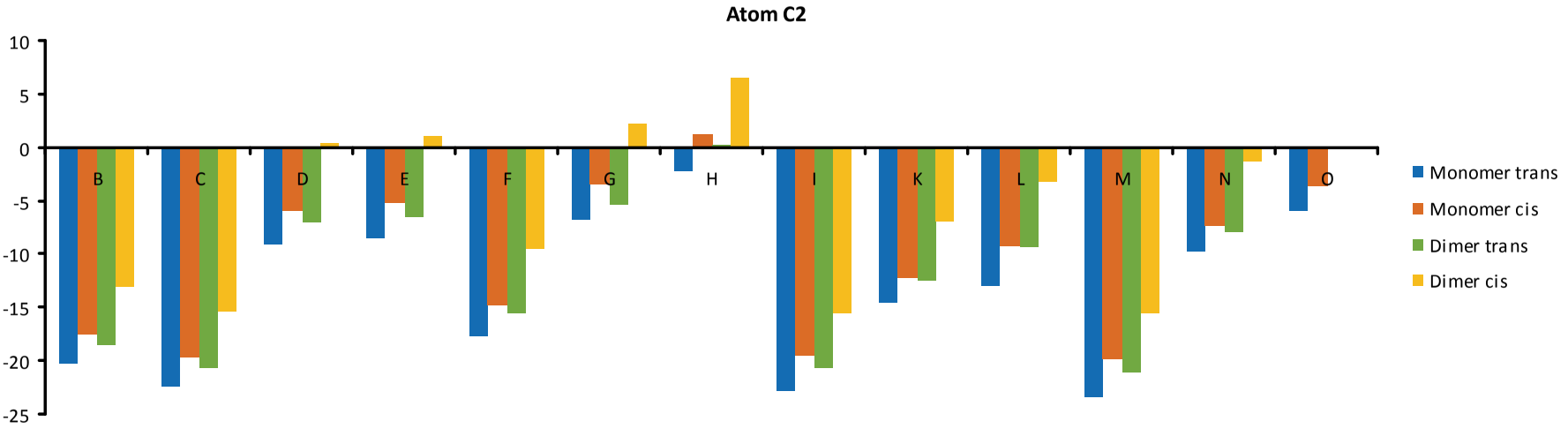

Figure S3: Errors in the ^{13}C chemical shifts of atom C2 in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S1.

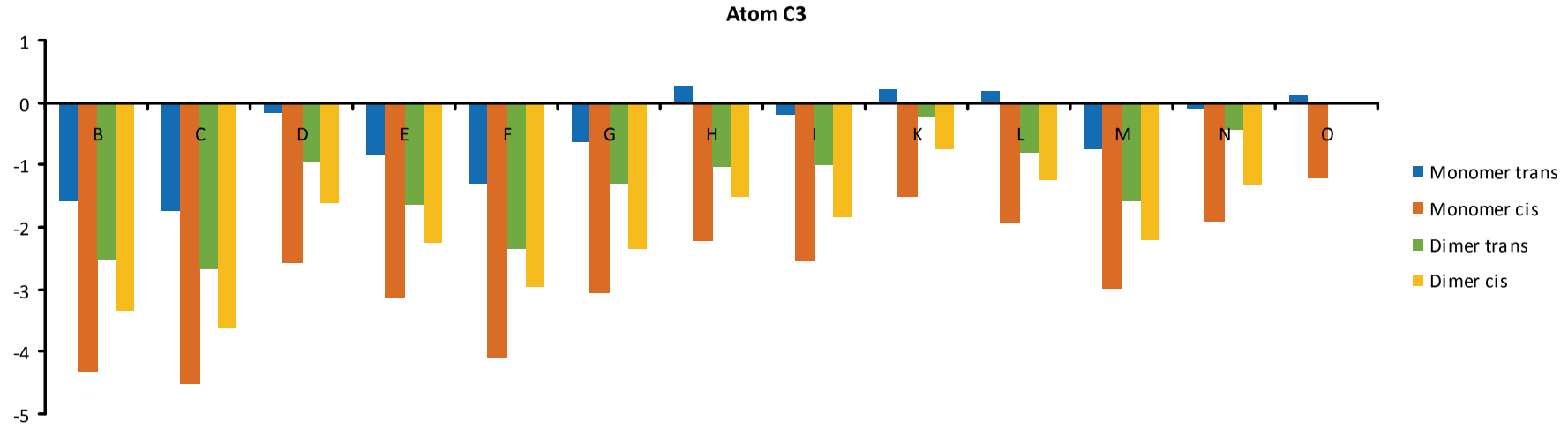

Figure S4: Errors in the ^{13}C chemical shifts of atom C3 in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S1.

Table S2: ^{1}H chemical shifts in N-methyl acetamide (NMA) calculated with different levels of theory and basis sets: If no level of theory is given, density functional theory with the B3LYP functional was used. Atom numbering is according to Figure S1.

		A	B	c	D	E	F	G	H	I	K	L	M	N	O
		experimental	6-31G(d,p)	6-31G(d)	6-311G(d,p)	6-311G(2d,p)	ccpVDZ	ccpVTZ	ccpVQZ	MP2/6-31G(d,p)	MP2/6-311G(d,p)	MP2/6-311G(2d,p)	MP2/ccpVDZ	MP2/ccpVTZ	MP2/ccpVQZ
monomer trans	H1	2.63	2.79	2.713	2.878	2.852	2.730	2.910	2.946	2.807	2.732	2.823	2.681	2.785	2.671
	H	7.73	4.28	3.906	4.265	4.321	3.953	4.596	4.774	4.215	4.050	4.278	3.579	4.590	5.059
	H2	1.90	1.59	1.547	1.664	1.618	1.465	1.694	1.741	1.600	1.618	1.574	1.430	1.636	1.697
monomer cis	H1		2.723	2.698	2.758	2.780	2.628	2.818	2.846	2.698	2.692	2.718	2.538	2.753	2.785
	H		4.005	3.570	3.988	4.005	3.582	4.339	4.573	3.977	3.755	3.977	3.330	4.270	4.587
	H2		1.761	1.717	1.768	1.763	1.611	1.839	1.878	1.769	1.729	1.742	1.562	1.794	1.846
dimer cis	H1		2.723	2.647	2.834	2.816	2.672	2.869	2.661	2.573	2.610	2.609	2.504	2.614	--
	H		7.548	6.726	7.508	7.381	7.390	7.808	8.159	7.447	7.248	7.595	7.062	8.253	--
	H2		1.573	1.524	1.676	1.642	1.478	1.719	1.728	1.656	1.713	1.663	1.449	1.725	--
dimer cis	H1		2.601	2.573	2.644	2.649	2.512	2.721	2.763	2.608	2.639	2.619	2.459	2.672	--
	H		9.333	8.041	9.194	9.294	9.211	9.800	10.026	9.038	8.897	9.454	8.779	10.265	--
	H2		1.780	1.730	1.796	1.768	1.646	1.836	1.859	1.796	1.771	1.760	1.597	1.804	--

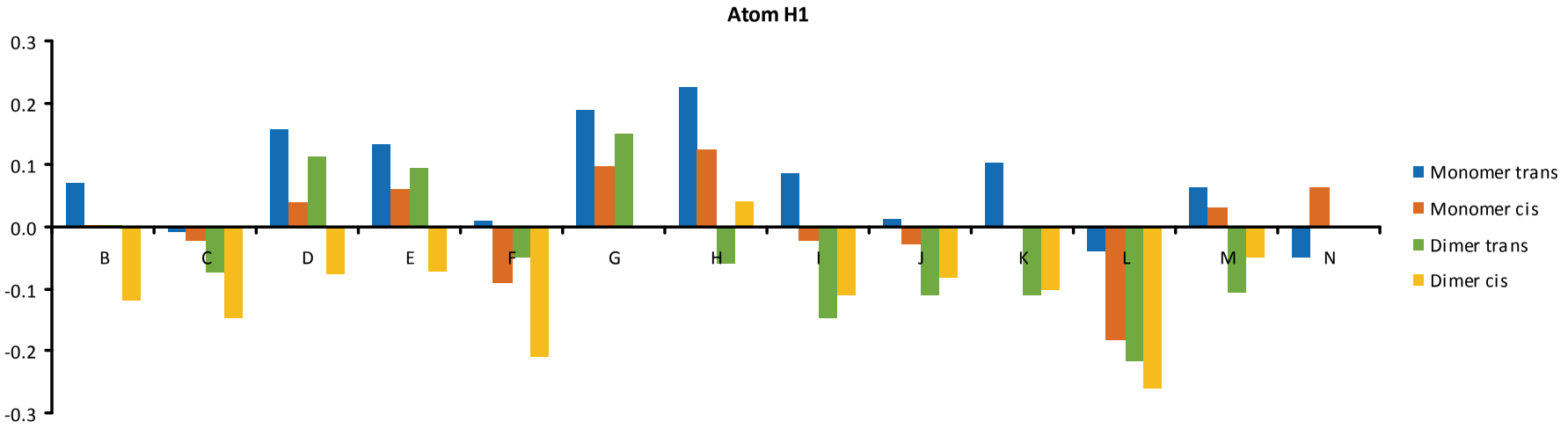

Figure S5: Errors in the ^{1}H chemical shifts of atom H1 in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S2.

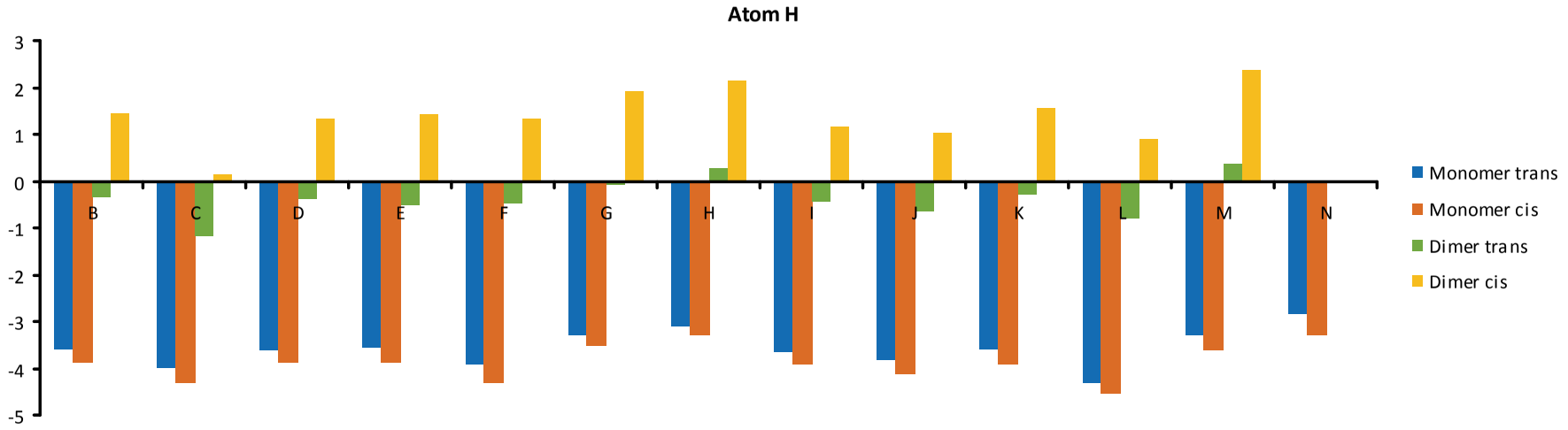

Figure S6: Errors in the ^{1}H chemical shifts of atom H in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S2.

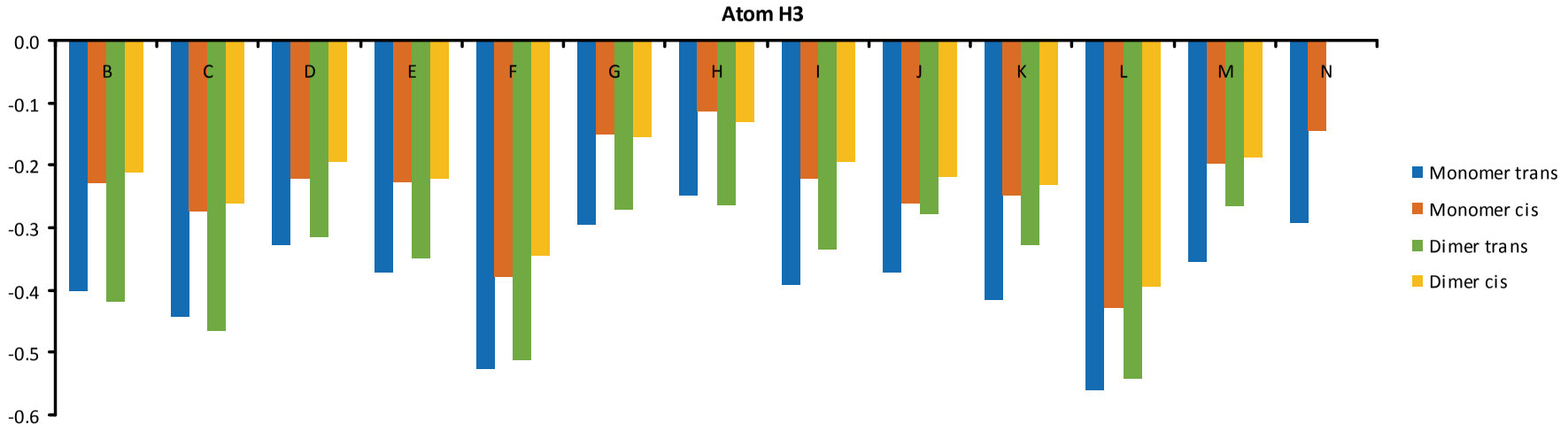

Figure S7: Errors in the ^{1}H chemical shifts of atom H3 in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S2.

Table S3: ^{15}N chemical shifts in N-methyl acetamide (NMA) calculated with different levels of theory and basis sets: If no level of theory is given, density functional theory with the B3LYP functional was used.

			A	B	C	D	E	F	G	H	I	K	L	M	N	O
			experimental	6-31G(d,p)	6-31G(d)	6-311G(d,p)	6-311G(2d,p)	ccpVDZ	ccpVTZ	ccpVQZ	MP2/6-31G(d,p)	MP2/6-311G(d,p)	MP2/6-311G(2d,p)	MP2/ccpVDZ	MP2/ccpVTZ	MP2/ccpVQZ
monomer trans	N	chemical shift	114.24	109.90	117.197	130.926	131.635	132.354	126.422	126.421	97.486	117.329	120.402	103.152	115.689	114.972
	N	error		-4.34	2.957	16.686	17.395	18.114	12.182	12.181	-16.754	3.089	6.162	-11.088	1.449	0.732
monomer cis	N	chemical shift		101.643	108.852	124.027	125.943	125.756	118.819	118.581	90.888	112.250	113.667	100.242	108.542	108.510
	N	error		101.64	108.852	124.027	125.943	125.756	118.819	118.581	90.888	112.250	113.667	100.242	108.542	108.510
dimer trans	N	chemical shift		111.525	118.023	134.242	134.804	134.615	128.714	128.415	101.220	123.527	125.577	110.201	121.405	--
	N	error		111.53	118.023	134.242	134.804	134.615	128.714	128.415	101.220	123.527	125.577	110.201	121.405	--
dimer cis	N	chemical shift		112.292	118.344	135.000	135.769	136.813	131.429	131.553	101.385	122.585	125.301	110.949	122.666	--
	N	error		112.29	118.344	135.000	135.769	136.813	131.429	131.553	101.385	122.585	125.301	110.949	122.666	--

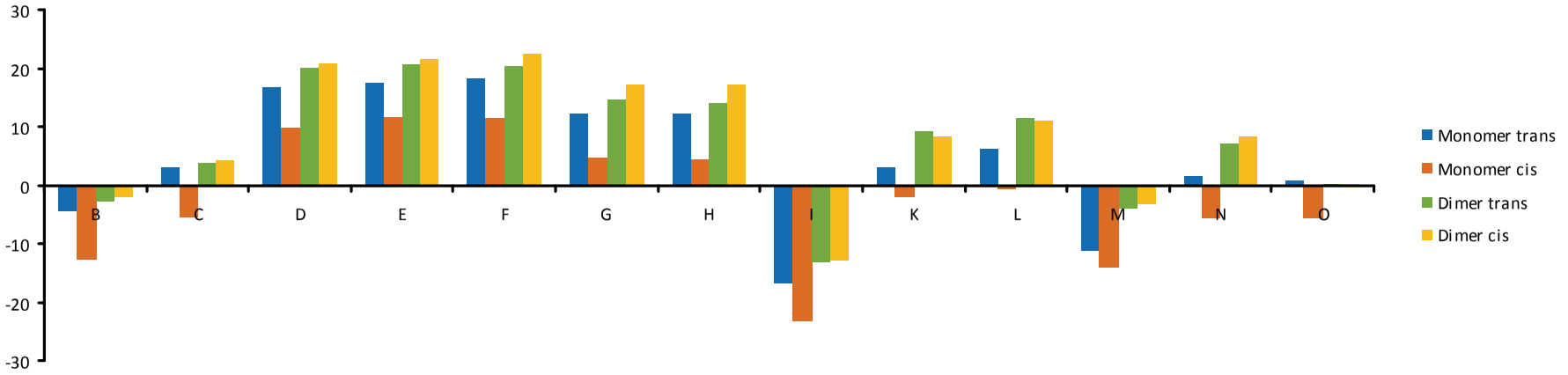

Figure S8: Errors in the ^{15}N chemical shifts in N-methyl acetamide (NMA): Naming scheme of levels of theory and basis set combinations is according to Table S3.

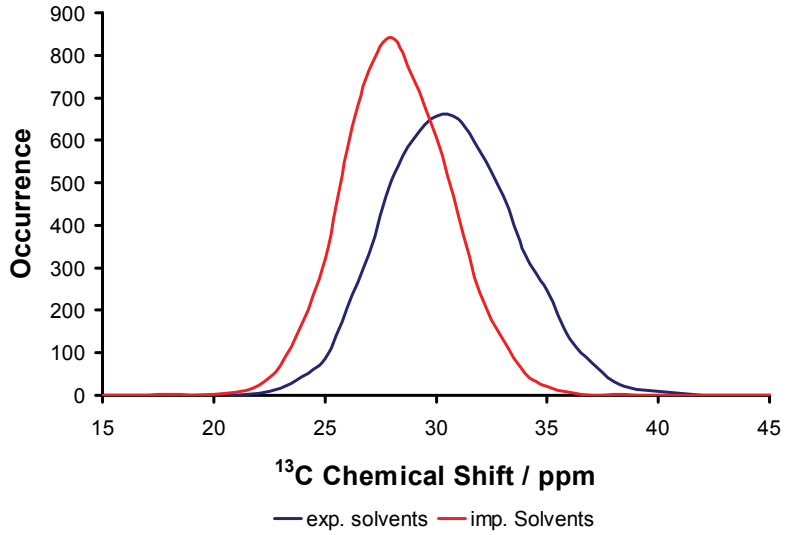

Figure S9: Probability distribution of the ^{13}C chemical shifts of the N-methyl group in N-methyl acetamide (NMA) calculated from 5000 snapshots along a 10 ns long MD simulation

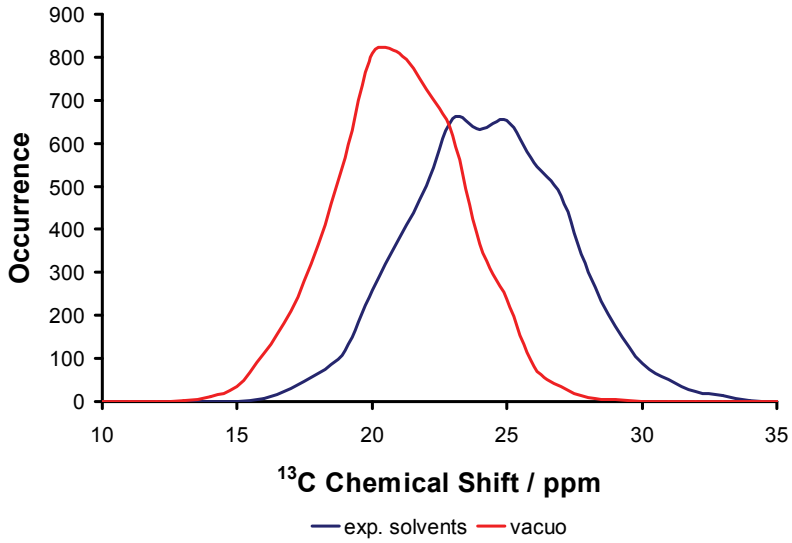

Figure S10: Probability distribution of the ^{13}C chemical shifts of the acetyl methyl group in N-methyl acetamide (NMA) calculated from 5000 snapshots along a 10 ns long MD simulation

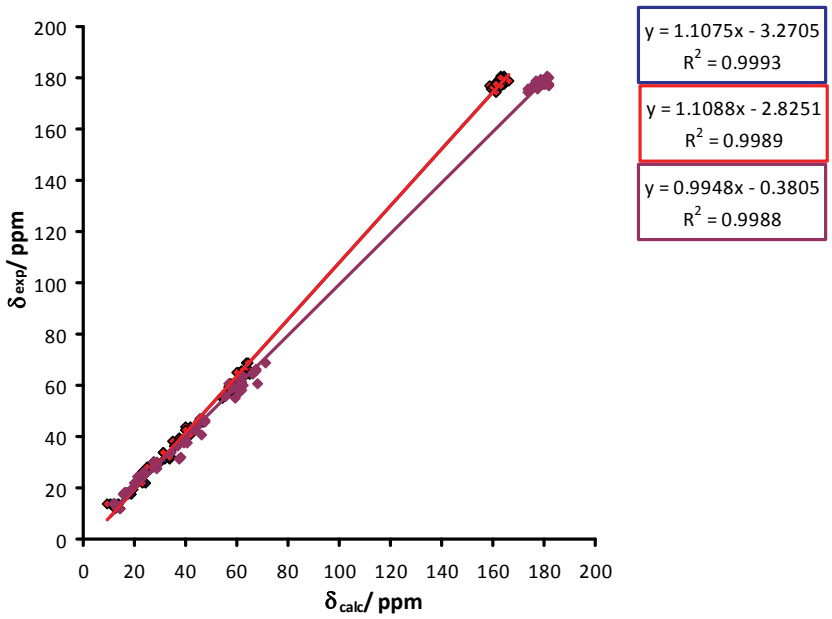

Figure S11: Correlation of ^{13}C NMR chemical shifts of all carbon atoms of the HA2 domain:
blue: B3LYP/6-31g(d), MD, explicit solvents
red: B3LYP/6-31g(d), MD, implicit solvents
magenta: B3LYP/6-311g(d), single point, implicit solvents
green: B3LYP/6-31g(d), single point, implicit solvents

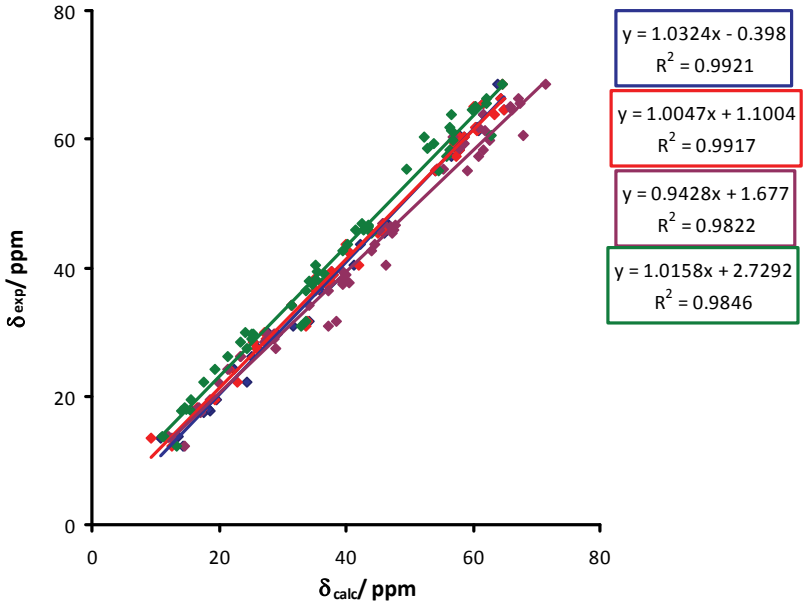

Figure S12: Correlation of ^{13}C NMR chemical shifts of aliphatic carbon atoms of the HA2 domain:
blue: B3LYP/6-31g(d), MD, explicit solvents
red: B3LYP/6-31g(d), MD, implicit solvents
magenta: B3LYP/6-311g(d), single point, implicit solvents
green: B3LYP/6-31g(d), single point, implicit solvents

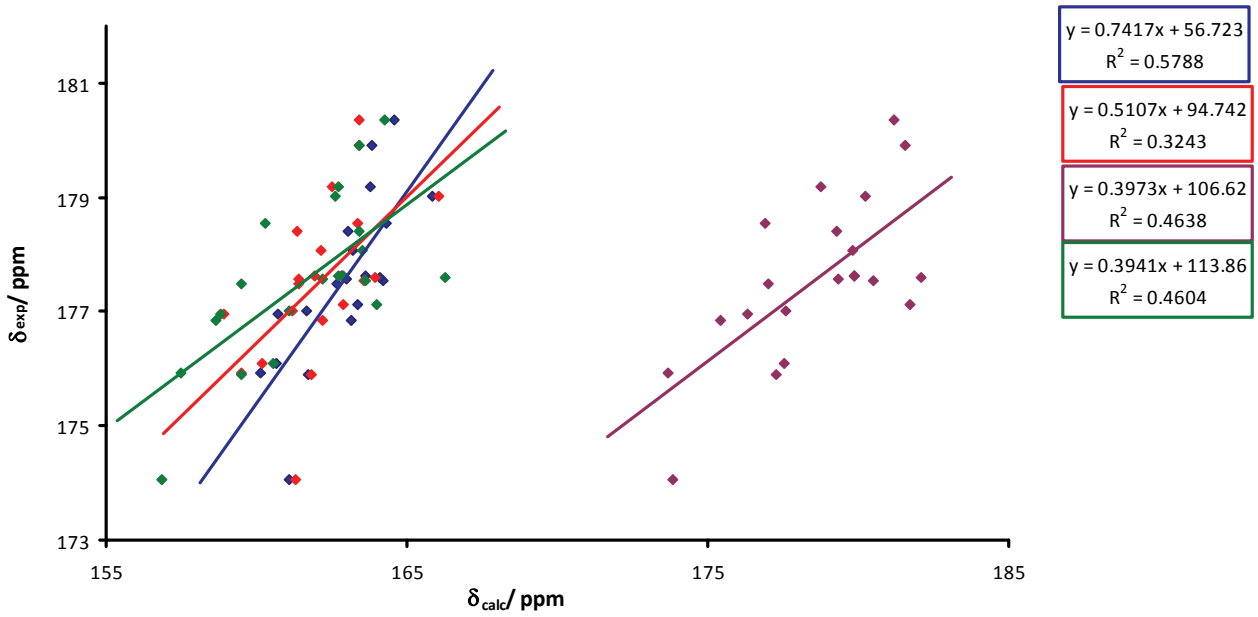

Figure S13: Correlation of ^{13}C NMR chemical shifts of the carbonyl groups of the HA2 domain:
blue: B3LYP/6-31g(d), MD, explicit solvents
red: B3LYP/6-31g(d), MD, implicit solvents
magenta: B3LYP/6-311g(d), single point, implicit solvents
green: B3LYP/6-31g(d), single point, implicit solvents