Supplementary Material

Prediction of ^{15}N NMR chemical shifts for nitrogenated aromatic compounds

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Chart S1. Compounds in the dataset with numbering on nitrogen atoms.

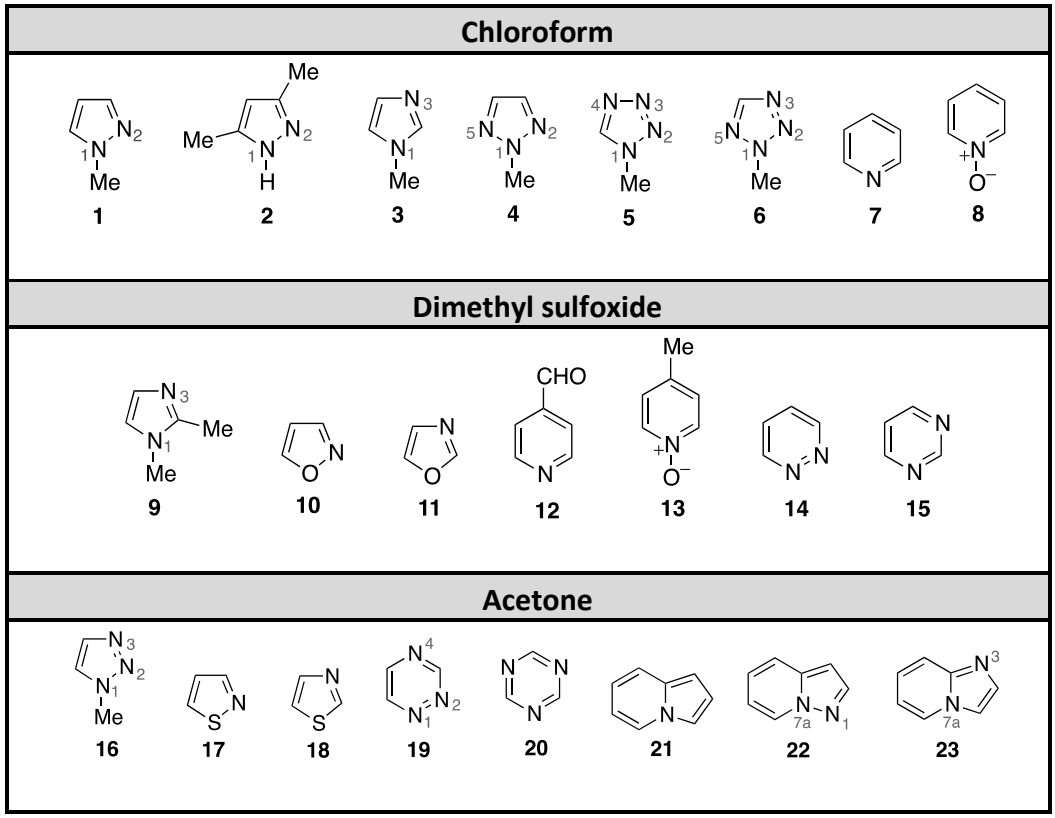

Table S1. Calculated isotropic values for nitromethane (CH_3NO_2) in various solvents using both methods described in the manuscript, SMD-MPW1PW91/6-311+G(2d,p) and CPCM-OLYP/pcSseg-2

Method	Solvent	Isotropic
1 SMD-MPW1PW91/6-311+G(2d,p)	Chloroform	-166.2851
	Dimethyl sulfoxide	-168.8624
	Acetone	-168.6584
2 CPCM-OLYP/pcSseg-2	Chloroform	-139.9247
	Dimethyl sulfoxide	-142.3360
	Acetone	-141.9767

Table S2. Calculated isotropic values, chemical shifts and deviations. GIAO NMR calculations were computed using the SMD-MPW1PW91/6-311+G(2d,p) method (M1). Effective isotropic refers to values after averaging for magnetically equivalente nitrogens. Mean absolute deviation (MAD) is provided at the end of the table

Compound	Atom	Experimental	Effective Isotropic	Chemical Shift	Deviation
1	N-1	-180.8	26.7895	-193.0746	12.3
	N-2	-76.5	-73.4330	-92.8521	16.4
2	N-1	-111.0	-37.1769	-129.1082	18.1
	N-2	-187.0	47.3964	-213.6815	26.7
3	N-1	-221.3	70.8640	-237.1491	15.8
	N-3	-125.5	-29.7875	-136.4976	11.0
4	N-1	-132.8	-23.9025	-142.3826	9.6
	N-2,N-5	-51.0	-100.0477	-66.2374	15.2
5	N-1	-154.6	1.9138	-168.1989	13.6
	N-2	-9.9	-150.9656	-15.3195	5.4
	N-3	14.6	-182.6797	16.3946	1.8
	N-4	-49.7	-102.4967	-63.7884	14.1
6	N-1	-98.4	-54.5464	-111.7387	13.3
	N-2	4.4	-159.5355	-6.7496	11.1
	N-3	-42.9	-108.4469	-57.8382	14.9
	N-4	-68.7	-77.1241	-89.1610	20.5
7	N-1	-68.7	-82.5342	-83.7509	15.1
8	N-1	-84.0	-76.5970	-89.6881	5.7
9	N-1	-221.8	70.7265	-239.5889	17.8
	N-3	-120.6	-18.0458	-150.8166	30.2
10	N-1	4.3	-144.3808	-24.4816	28.8
11	N-1	-123.7	-17.3379	-151.5245	27.8
12	N-1	-47.8	-99.3832	-69.4792	21.7
13	N-1	-94.3	-62.7552	-106.1072	11.8
14	N-1,N-2	20.4	-176.9196	8.0572	12.3
15	N-1,N-3	-84.8	-55.0859	-113.7765	29.0
16	N-1	-144.5	-12.5804	-156.0780	11.6
	N-2	-27.9	-138.7065	-29.9519	2.1
	N-3	-14.7	-126.2738	-42.3846	27.7
17	N-1	-81.5	-64.4457	-104.2127	22.7
18	N-1	-55.0	-84.2188	-84.4396	29.4
19	N-1	42.0	-204.5109	35.8525	6.1
	N-2	-2.0	-154.6913	-13.9671	12.0
	N-4	-82.0	*-61.7765*	-106.8819	24.9
20	N-1,N-3,N-5	-97.0	-40.8655	-127.7929	30.8
21	N-1	-189.8	37.2948	-205.9532	16.2
22	N-1	-93.9	-41.6269	-127.0315	33.1

23	N-7a	-144.9	-6.4909	-162.1675	17.3
	N-1	-140.0	2.7202	-171.3786	31.4
	N-7a	-179.5	27.3207	-195.9791	16.5
				MAD =	**17.5**

Table S3. Calculated isotropic values, chemical shifts and deviations. GIAO NMR calculations were computed using the SMD-MPW1PW91/6-311+G(2d,p) method (M1). Chemical shifs were scaled according to the equation y=-1.0303x – 152.85. Effective isotropic refers to values after averaging for magnetically equivalente nitrogens. Mean absolute deviation (MAD) is provided at the end of the table

Compound	Atom	Experimental	Effective Isotropic	Chemical Shift	Deviation
1	N-1	-180.8	26.7895	-180.4512	0.3
	N-2	-76.5	-73.4330	-77.1920	0.7
2	N-1	-111.0	-37.1769	-114.5466	3.5
	N-2	-187.0	47.3964	-201.6825	14.7
3	N-1	-221.3	70.8640	-225.8612	4.6
	N-3	-125.5	-29.7875	-122.1599	3.3
4	N-1	-132.8	-23.9025	-128.2233	4.6
	N-2,N-5	-51.0	-100.0477	-49.7709	1.2
5	N-1	-154.6	1.9138	-154.8218	0.2
	N-2	-9.9	-150.9656	2.6899	12.6
	N-3	14.6	-182.6797	35.3649	20.8
	N-4	-49.7	-102.4967	-47.2476	2.5
6	N-1	-98.4	-54.5464	-96.6508	1.7
	N-2	4.4	-159.5355	11.5194	7.1
	N-3	-42.9	-108.4469	-41.1172	1.8
	N-4	-68.7	-77.1241	-73.3890	4.7
7	N-1	-68.7	-82.5342	-67.8150	0.9
8	N-1	-84.0	-76.5970	-73.9321	10.1
9	N-1	-221.8	70.7265	-225.7195	3.9
	N-3	-120.6	-18.0458	-134.2574	13.7
10	N-1	4.3	-144.3808	-4.0945	8.4
11	N-1	-123.7	-17.3379	-134.9868	11.3
12	N-1	-47.8	-99.3832	-50.4555	2.7
13	N-1	-94.3	-62.7552	-88.1933	6.1
14	N-1,N-2	20.4	-176.9196	29.4303	9.0
15	N-1,N-3	-84.8	-55.0859	-96.0950	11.3
16	N-1	-144.5	-12.5804	-139.8884	4.6
	N-2	-27.9	-138.7065	-9.9407	18.0
	N-3	-14.7	-126.2738	-22.7501	8.1
17	N-1	-81.5	-64.4457	-86.4516	5.0
18	N-1	-55.0	-84.2188	-66.0794	11.1

	N-1	42.0	-204.5109	57.8576	15.9
19	N-2	-2.0	-154.6913	6.5284	8.5
	N-4	-82.0	*-61.7765*	-89.2017	7.2
20	N-1,N-3,N-5	-97.0	-40.8655	-110.7463	13.7
21	N-1	-189.8	37.2948	-191.2748	1.5
22	N-1	-93.9	-41.6269	-109.9618	16.1
	N-7a	-144.9	-6.4909	-146.1624	1.3
23	N-1	-140.0	2.7202	-155.6526	15.7
	N-7a	-179.5	27.3207	-180.9985	1.5
				MAD =	**7.3**

Table S4. Calculated isotropic values, chemical shifts and deviations. GIAO NMR calculations were computed using the CPCM-OLYP/pcSseg-2 method. Effective isotropic refers to values after averaging for magnetically equivalente nitrogens. Mean absolute deviation (MAD) is provided at the end of the table

Compound	Atom	Experimental	Effective Isotropic	Chemical Shift	Deviation
1	N-1	-180.8	25.9630	-165.8877	14.9
	N-2	-76.5	-73.7076	-66.2171	10.3
2	N-1	-111.0	-54.6541	-85.2706	25.7
	N-1	-187.0	38.5371	-178.4618	8.5
3	N-1	-221.3	67.8999	-207.8246	13.5
	N-3	-125.5	-34.3803	-105.5444	20.0
4	N-1	-132.8	-21.1297	-118.7950	14.0
	N-2,N-5	-51.0	-95.7192	-44.2055	6.8
5	N-1	-154.6	2.2085	-142.1332	12.5
	N-2	-9.9	-143.8208	3.8961	13.8
	N-3	14.6	-173.2294	33.3047	18.7
	N-4	-49.7	-103.5494	-36.3753	13.3
6	N-1	-98.4	-49.3372	-90.5875	7.8
	N-2	4.4	-150.1470	10.2223	5.8
	N-3	-42.9	-107.7172	-32.2075	10.7
	N-4	-68.7	-76.2315	-63.6932	5.0
7	N-1	-68.7	-85.2370	-54.6877	14.0
8	N-1	-84.0	-73.9904	-65.9343	18.1
9	N-1	-221.8	69.0860	-211.4220	10.4
	N-3	-120.6	-26.0070	-116.3290	4.3
10	N-1	4.3	-147.5072	5.1712	0.9
11	N-1	-123.7	-22.5957	-119.7403	4.0
12	N-1	-47.8	-107.4138	-34.9222	12.9
13	N-1	-94.3	-58.3953	-83.9407	10.4
14	N-1,N-2	20.4	-181.4784	39.1424	18.7
15	N-1,N-3	-84.8	-62.7758	-79.5602	5.2

	N-1	-144.5	-8.2197	-133.7570	10.7
16	N-2	-27.9	-133.2071	-35.4513	7.6
	N-3	-14.7	-122.6472	-46.0112	31.3
17	N-1	-81.5	-64.4457	-104.2127	22.7
18	N-1	-55.0	-86.4582	-82.2002	27.2
	N-1	42.0	-205.1439	36.4855	5.5
19	N-2	-2.0	-162.6855	-5.9729	4.0
	N-4	-82.0	*-61.4594*	-107.1990	25.2
20	N-1,N-3,N-5	-97.0	-50.8528	-117.8056	20.8
21	N-1	-189.8	35.3114	-203.9698	14.2
22	N-1	-93.9	-47.4900	-121.1684	27.3
	N-7a	-144.9	-6.8816	-161.7768	16.9
23	N-1	-140.0	-6.3666	-162.2918	22.3
	N-7a	-179.5	25.4097	-194.0681	14.6
				MAD =	**13.8**

Table S5. Calculated isotropic values, chemical shifts and deviations. GIAO NMR calculations were computed using the CPCM-OLYP/pcSseg-2 method. Chemical shifs were scaled according to the equation y=-1.0067x – 152.18. Effective isotropic refers to values after averaging for magnetically equivalente nitrogens. Mean absolute deviation (MAD) is provided at the end of the table

Compound	Atom	Experimental	Effective Isotropic	Chemical Shift	Deviation
1	N-1	-180.8	25.9630	-179.7481	2.5
	N-2	-76.5	-73.7076	-79.2901	1.5
2	N-1	-111.0	-54.6541	-98.4941	13.8
	N-1	-187.0	38.5371	-192.4215	4.0
3	N-1	-221.3	67.8999	-222.0163	0.8
	N-3	-125.5	-34.3803	-118.9281	7.9
4	N-1	-132.8	-21.1297	-132.2834	1.9
	N-2,N-5	-51.0	-95.7192	-57.1046	4.8
5	N-1	-154.6	2.2085	-155.8059	0.2
	N-2	-9.9	-143.8208	-8.6230	2.5
	N-3	14.6	-173.2294	21.0179	7.6
	N-4	-49.7	-103.5494	-49.2126	1.8
6	N-1	-98.4	-49.3372	-103.8530	4.1
	N-2	4.4	-150.1470	-2.2468	5.4
	N-3	-42.9	-107.7172	-45.0118	0.8
	N-4	-68.7	-76.2315	-76.7463	6.7
7	N-1	-68.7	-85.2370	-67.6696	2.3
8	N-1	-84.0	-73.9904	-79.0051	6.3
9	N-1	-221.8	69.0860	-223.2118	0.1
	N-3	-120.6	-26.0070	-127.3675	5.4

10	N-1	4.3	-147.5072	-4.9075	8.0
11	N-1	-123.7	-22.5957	-130.8058	5.7
12	N-1	-47.8	-107.4138	-45.3176	3.8
13	N-1	-94.3	-58.3953	-94.7234	0.9
14	N-1,N-2	20.4	-181.4784	29.3321	10.1
15	N-1,N-3	-84.8	-62.7758	-90.3083	4.2
16	N-1	-144.5	-8.2197	-145.2954	0.6
	N-2	-27.9	-133.2071	-19.3206	9.8
	N-3	-14.7	-122.6472	-29.9639	14.0
17	N-1	-81.5	-64.4457	-88.6252	5.8
18	N-1	-55.0	-86.4582	-66.4388	10.1
19	N-1	42.0	-205.1439	53.1845	12.3
	N-2	-2.0	-162.6855	10.3907	13.6
	N-4	-82.0	*-61.4594*	-91.6351	8.3
20	N-1,N-3,N-5	-97.0	-50.8528	-102.3255	4.0
21	N-1	-189.8	35.3114	-189.1704	2.1
22	N-1	-93.9	-47.4900	-105.7148	10.5
	N-7a	-144.9	-6.8816	-146.6440	0.4
23	N-1	-140.0	-6.3666	-147.1631	5.8
	N-7a	-179.5	25.4097	-179.1904	1.7
				MAD =	**5.3**

Figure S1. Linear correlations between experimental chemical shifts and calculated isotropic shielding constants for compounds in their solvents using Method 1, SMD-mPW1PW91/6-311+G(2d,p).

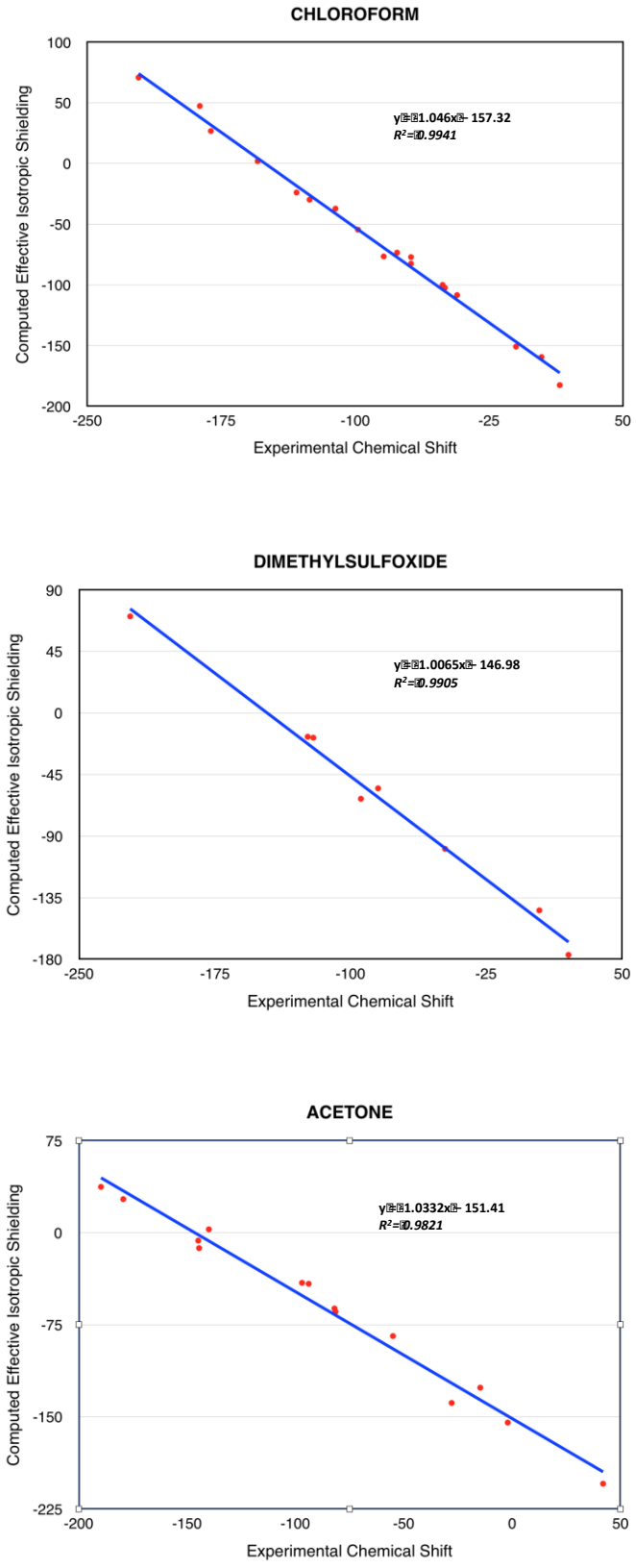

Figure S2. Linear correlations between experimental chemical shifts and calculated isotropic shielding constants for compounds in their solvents using Method 2, CPCM-OLYP/pcSseg-2.