Supplemental Material

for

Polarizable Empirical Force Field for Nitrogen-containing Heteroaromatic Compounds Based on the Classical Drude Oscillator

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Table S1) Comparison of equilibrium geometries from polarizable CHARMM and experiment.

Pyridine						
	CSD	PYRDNA01[1]	QM	Microwave[2]	Target	DRUDE
1-2	1.366±0.021	1.376	1.392	1.392	1.382	1.404
2-3	1.373±0.019	1.383	1.393	1.394	1.386	1.403
3-4	1.333±0.020	1.338	1.343	1.338	1.338	1.359
6-1-2	119.0±0.06	118.8	119.9	118.4	118.9	118.5
1-2-3	118.9±0.07	118.5	117.7	118.5	118.4	118.6
2-3-4	122.8±0.09	123.8	124.0	123.8	123.6	123.7
3-4-5	117.5±0.12	116.5	116.2	116.9	116.8	116.8
Pyrimidine						
	CSD	PRMDIN01[3]	QM	Electron Diffraction[4]	Target	DRUDE
1-2	1.374±0.01	1.387	1.393	1.393	1.387	1.398
2-3	1.337±0.01	1.339	1.344	1.340	1.340	1.341
3-4	1.324±0.01	1.337	1.342	1.340	1.336	1.342
6-1-2	116.6±0.4	116.5	116.9	116.8	116.7	116.1
1-2-3	122.6±0.6	122.6	122.3	122.3	122.5	122.6
2-3-4	117.6±0.9	115.9	115.5	115.5	116.1	115.8
3-4-5	126.8±1.0	126.7	127.5	127.6	127.2	127.0
Pyrrole						
	CSD	RUVQII[5]	QM	Microwave[6]	Target	DRUDE
5-1	1.425±0.032	1.423	1.423	1.417	1.421	1.423
1-2	1.362±0.030	1.357	1.383	1.382	1.374	1.363
2-3	1.383±0.029	1.364	1.373	1.370	1.369	1.382
5-1-2	107.6±1.2	107.0	107.5	107.4	107.3	107.5
1-2-3	108.3±1.1	108.6	107.4	107.4	107.8	108.2
2-3-4	108.0±1.4	108.8	110.1	109.8	109.6	108.6
Imidazole						
	CSD	IMAZOL13[7,8]	QM	Microwave[9]	Target	DRUDE
5-1	1.360±0.028	1.363	1.375	1. 369	1.367	1.377
1-2	1.339±0.021	1.358	1.378	1.358	1.358	1.359
2-3	1.356±0.021	1.368	1.377	1.378	1.367	1.375
3-4	1.312±0.014	1.316	1.326	1.326	1.319	1.304
4-5	1.330±0.013	1.337	1.366	1.349	1.346	1.357
5-1-2	106.30±0.74	106.08	104.9	106.3	105.9	105.41
1-2-3	110.06±0.84	109.86	111.1	109.8	110.2	109.89
2-3-4	105.20±1.52	105.05	104.9	105.4	105.2	104.55
3-4-5	111.64±1.03	112.02	111.6	111.3	111.6	113.00
4-5-1	106.75±1.14	107.00	107.6	107.2	107.1	106.60

Table S2a. Vibrational analysis of pyridine.

	Drude					MP2/6-31G*				
	Freq	PED	%	PED	%	Freq	PED	%	PED	%
1	355.6	asytor	70.0	asytor'	27.0	356.5	asytor	60.0	asytor'	26.0
2	380.3	asytor'	57.0	asytor	22.0	380.1	asytor'	60.0	asytor	25.0
3	577.0	wagCH	49.0	puck	43.0	576.3	asydef'	69.0	asydef	23.0
4	630.5	asydef'	59.0	asydef	20.0	629.6	asydef	67.0	asydef'	24.0
5	656.2	wagCH	71.0	puck	26.0	635.8	puck	83.0	wagCH	16.0
6	718.6	asydef	60.0	asydef'	20.0	691.8	wagCH	89.0		
7	750.6	wagCH	100.0			835.0	wagCH	101.0		
8	863.2	wagCH	99.0			872.8	wagCH	95.0		
9	863.6	tridef	85.0			877.8	wagCH	86.0		
10	916.4	wagCH	97.0			898.6	wagCH	86.0	asytor	16.0
11	956.5	wagCH	79.0			957.1	tridef	42.0	bondCN	32.0
12	983.4	bondCC	68.0	rockCH	23.0	996.8	bondCC	49.0	tridef	44.0
13	997.1	bondCC	70.0	rockCH	21.0	1037.6	bondCC	59.0	rockCH	33.0
14	1059.4	bondCN	46.0	bondCC	39.0	1048.7	rockCH	35.0	bondCC	31.0
15	1177.8	rockCH	73.0	bondCC	21.0	1136.9	rockCH	85.0	bondCC	15.0
16	1193.4	rockCH	64.0	bondCN	21.0	1197.1	rockCH	66.0	bondCN	22.0
17	1364.1	rockCH	56.0	bondCN	39.0	1323.1	rockCH	47.0	bondCN	40.0
18	1408.5	rockCH	86.0			1332.0	rockCH	56.0	bondCN	24.0
19	1461.4	bondCC	65.0	rockCH	27.0	1413.9	rockCH	58.0	bondCC	36.0
20	1463.1	rockCH	54.0	bondCC	36.0	1448.8	rockCH	70.0	bondCN	15.0
21	1581.1	rockCH	37.0	bondCN	35.0	1555.0	bondCC	51.0	bondCN	21.0
22	1582.2	rockCH	51.0	bondCC	25.0	1564.0	bondCC	63.0	rockCH	20.0
23	3052.0	bondCH	100.0			3035.1	bondCH	100.0		
24	3054.2	bondCH	100.0			3036.2	bondCH	100.0		
25	3056.8	bondCH	100.0			3051.6	bondCH	100.0		
26	3068.4	bondCH	100.0			3067.4	bondCH	99.0		
27	3070.3	bondCH	100.0			3073.2	bondCH	99.0		

Tabe S2b. Vibrational analysis of pyrimidine

	Drude					MP2/6-31G*				
	Freq	PED	%	PED	%	Freq	PED	%	PED	%
1	388.5	asytor'	55.0	asytor	26.0	329.2	asytor'	82.0		
2	412.8	asytor	74.0	asytor'	27.0	383.1	asytor	85.0		
3	590.7	puck	79.0			593.1	asydef	70.0	asydef'	23.0
4	650.4	asydef	62.0	asydef'	21.0	653.6	asydef'	68.0	asydef	23.0
5	728.9	asydef'	43.0	tridef	20.0	691.5	puck	59.0	wagCH3	16.0
6	755.9	wagCH1	56.0	wagCH4	15.0	764.1	wagCH1	44.0	puck	30.0
7	870.7	tridef	66.0	bondCN	17.0	887.3	wagCH1	46.0	wagCH3	17.0
8	902.6	wagCH2	52.0	wagCH4	49.0	921.4	wagCH2	47.0	wagCH4	42.0
9	928.5	wagCH3	83.0			933.7	wagCH3	58.0	asytor'	16.0
10	998.9	bondCN	48.0	rockCH	29.0	957.1	tridef	40.0	bondCN'	26.0
11	1012.8	wagCH4	30.0	wagCH2	23.0	1028.4	tridef	43.0	bondCC	41.0
12	1042.0	bondCC	63.0	bondCN'	21.0	1049.5	rockCH	45.0	bondCN	31.0
13	1105.5	bondCN	50.0	bondCN'	27.0	1108.8	bondCN'	32.0	bondCC	22.0
14	1170.3	rockCH	75.0			1192.6	rockCH	57.0	bondCN	27.0
15	1302.3	bondCN'	35.0	rockCH	28.0	1267.1	bondCN'	56.0	bondCN	28.0
16	1304.5	rockCH	73.0	bondCN	20.0	1340.9	rockCH	98.0		
17	1452.1	rockCH	61.0	bondCC	31.0	1376.1	rockCH	48.0	bondCN'	29.0
18	1528.8	bondCC	36.0	rockCH	33.0	1432.4	rockCH	74.0		
19	1574.4	bondCN'	65.0	rockCH	28.0	1542.0	bondCN	43.0	rockCH	24.0
20	1592.1	rockCH	55.0	bondCC	20.0	1549.8	bondCC	52.0	bondCN'	22.0
21	2977.3	bondCH	100.0			3040.7	bondCH	100.0		
22	3051.4	bondCH	100.0			3043.7	bondCH	100.0		
23	3053.2	bondCH	100.0			3055.3	bondCH	100.0		
24	3055.1	bondCH	100.0			3083.2	bondCH	99.0		

Table S2c. Vibrational analysis of imidazole

	Drude					MP2/6-31G*				
	Freq	PED	%	PED	%	Freq	PED	%	PED	%
1	480.0	wagNH	93.			489.2	wagNH	60.0	torsio	36.0
2	615.8	wagCH'	55.	wagCH	28.	600.2	torsio'	74.0	wagNH	18.0
3	673.2	torsio'	52.	wagCH	39.	644.0	torsio	43.0	wagCH	33.0
4	693.7	wagCH	69.	wagCH'	21.	649.3	wagCH	62.0	wagCH'	16.0
5	822.4	torsio	70.	wagCH'	21.	722.3	wagCH'	83.0		
6	883.0	rngdef	47.	rngdef'	23.	766.4	wagCH	94.0		
7	889.5	rngdef'	47.	rngdef	23.	852.5	rngdef	78.0		
8	948.8	wagCH	63.	torsio'	37.	890.2	rngdef'	76.0		
9	1012.4	bondCN	57.	bondCN'	29.	1042.6	rockCH	35.0	bondCN'	28.0
10	1033.4	rockCH'	34.	bondCN'	33.	1064.2	rockCH	26.0	rockNH	23.0
11	1077.3	rockCH	67.	bondCC	24.	1110.8	bondCN'	32.0	rockCH	25.0
12	1160.4	rockCH'	36.	rockCH	33.	1131.4	bondCN	56.0	bondCN'	31.0
13	1245.1	rockCH	28.	rockNH	24.	1226.9	rockCH'	47.0	rockCH	30.0
14	1458.5	bondCN	31.	rockCH	24.	1319.2	bondCN	49.0	rockCH	32.0
15	1502.8	bondCN	36.	rockNH	20.	1409.5	bondCN'	52.0	rockNH	27.0
16	1579.5	bondCN'	22.	bondCN	21.	1447.8	bondCN	26.0	rockCH'	24.0
17	1590.0	bondCN'	35.	bondCC	25.	1478.5	bondCC	42.0	rockCH	20.0
18	3058.1	bondCH'	99.			3120.4	bondCH	96.0		
19	3158.5	bondCH	100.			3123.8	bondCH'	95.0		
20	3164.8	bondCH	99.			3145.4	bondCH	98.0		
21	3518.3	bondNH	100.			3462.8	bondNH	100.0		

Table S2d. Vibrational analysis of pyrrole

	Drude					MP2/6-31G*				
	Freq	PED	%	PED	%	Freq	PED	%	PED	%
1	1	429.2	wagNH	94.		433.3	wagNH	68.0	torsio	21.0
2	2	552.2	torsio'	34.	wagCH	552.6	torsio'	77.0		
3	3	595.7	wagCH'	121.		596.6	wagCH	76.0		
4	4	599.9	wagCH	70.	torsio	600.4	torsio	73.0	wagNH	25.0
5	5	668.7	wagCH	82.		666.6	wagCH'	60.0	wagCH	44.0
6	6	720.9	wagCH'	59.	torsio'	727.6	wagCH	57.0	wagCH'	35.0
7	7	743.5	torsio	66.	wagCH	743.5	wagCH'	70.0	wagCH	23.0
8	8	829.4	rngdef	85.		829.1	rngdef	91.0		
9	9	850.6	rngdef'	71.		850.7	rngdef'	84.0		
10	10	997.4	bondCC	34.	rockCH'	1009.2	bondCC'	26.0	rockCH	25.0
11	11	999.7	rockCH'	33.	rockCH	1032.1	bondCC	33.0	rockCH'	25.0
12	12	1045.7	rockCH	37.	rockCH'	1069.8	rockCH'	30.0	rockCH	30.0
13	13	1051.6	bondCC	43.		1125.7	bondCC	35.0	bondCN	32.0
14	14	1130.6	rockCH	35.	rockCH'	1130.5	rockNH	35.0	bondCN	24.0
15	15	1263.6	rockNH	26.	rockCH	1260.6	rockCH	41.0	rockCH'	41.0
16	16	1386.7	bondCC'	49.		1386.7	bondCC'	41.0	bondCC	24.0
17	17	1433.1	bondCC	50.		1433.1	bondCN	60.0	rockNH	32.0
18	18	1480.0	bondCC	36.	rngdef'	1451.8	bondCC	29.0	rockCH'	23.0
19	19	1538.9	bondCN	57.	rockNH	1507.5	bondCC	59.0		
20	20	3178.9	bondCH	99.		3105.5	bondCH'	84.0		
21	21	3181.1	bondCH	99.		3115.3	bondCH'	62.0	bondCH	37.0
22	22	3215.5	bondCH'	100.		3128.5	bondCH	83.0		
23	23	3221.3	bondCH'	99.		3133.8	bondCH	62.0	bondCH'	37.0
24	24	3515.0	bondNH	100.		3476.6	bondNH	100.0		

Table S3. Rare gas-model compounds minimum interaction energy distances and energies.

	Helium				Neon			
	Drude		QM		Drude		QM	
Geom	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)
Pyridine								
1	-0.210	3.250	-0.196	3.344	-0.427	3.300	-0.693	3.380
2	-0.207	3.270	-0.172	3.440	-0.422	3.330	-0.697	3.380
3	-0.193	3.340	-0.149	3.621	-0.392	3.380	-0.646	3.460
4	-0.144	2.300	-0.109	2.914	-0.294	2.300	-0.546	2.760
5	-0.122	2.410	-0.116	2.856	-0.245	2.460	-0.576	2.740
Pyrimidine								
1	-0.220	3.250	-0.207	3.280	-0.449	3.300	-0.754	3.290
2	-0.214	3.260	-0.160	3.420	-0.435	3.310	-0.697	3.358
3	-0.202	3.300	-0.207	3.600	-0.411	3.350	-0.651	3.422
4	-0.140	2.400	-0.120	2.700	-0.293	2.400	-0.529	2.751
5	-0.140	2.400	-0.117	2.740	-0.293	2.400	-0.547	2.748
6	-0.124	2.400	-0.124	2.720	-0.250	2.450	-0.574	2.720
7	-0.224	3.220	-0.181	3.350	-0.454	3.260	-0.688	3.358
Imidazole								
1	-0.202	3.270	-0.196	3.344	-0.410	3.330	-0.693	3.380
2	-0.197	3.300	-0.172	3.440	-0.400	3.350	-0.697	3.380
3	-0.174	3.380	-0.149	3.621	-0.355	3.430	-0.646	3.460
4	-0.142	2.300	-0.109	2.914	-0.289	2.310	-0.546	2.760
5	-0.112	2.440	-0.116	2.856	-0.226	2.480	-0.576	2.740

Table S4. Water-model compounds minimum interaction energy distances and energies.

	Set LJ parameters		Final LJ parameters with NBFIX		Ab initio	
Pyridine						
Geom	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)
1	-6.42	1.85	-5.84	1.92	-6.37	1.91
2	-3.13	2.20	-2.98	2.26	-3.58	2.20
3	-1.00	2.40	-0.99	2.41	-1.47	2.32
4	-1.38	2.42	-1.38	2.42	-2.09	2.38
Pyrimidine						
Geom	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)
1	-6.06	1.83	-5.53	1.89	-5.47	2.06
2	-2.24	2.23	-2.11	2.29	-2.21	2.29
3	-1.77	2.33	-1.75	2.34	-1.91	2.30
4	-0.90	2.50	-0.87	2.54	-0.88	2.58
5	-0.92	2.39	-0.90	2.41	-1.25	2.32
6	-0.85	2.76	-0.85	2.80	-1.20	2.57
Imidazole						
Geom	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)
1	-7.06	1.84	NA	NA	-6.80	2.02
2	-0.59	2.41	NA	NA	-0.67	2.42
3	-2.18	2.26	NA	NA	-1.78	2.44
4	-1.89	2.64	NA	NA	-2.31	2.32
5	-2.95	2.33	NA	NA	-2.76	2.41
6	-1.72	2.35	NA	NA	-1.67	2.47
7	-1.72	2.35	NA	NA	-2.03	2.28
Pyrrole						
Geom	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)	Energy (kcal/mol)	Distance (Å)
1	-1.91	2.24	NA	NA	-1.57	2.37
2	-1.03	2.74	NA	NA	-1.70	2.35
3	-0.51	2.68	NA	NA	-0.87	2.44
4	-2.34	2.32	NA	NA	-2.61	2.34
5	-3.66	2.19	NA	NA	-3.41	2.33

Table S5. RMS fluctuations about the average differences and ratios between the QM and CHARMM minimum interaction energies and distances for interactions with water.*

	R_{min} (Å)		E_{min} (kcal/mol)	
Complex	Difference	Ratio	Difference	Ratio
Pyridine/Regular	0.051	0.024	0.277	0.144
Pyridine/NBFIX	0.046	0.022	0.195	0.131
Pyrimidine/ Regular	0.132	0.058	0.315	0.149
Pyrimidine/ NBFIX	0.122	0.052	0.155	0.122
Imidazole/ Regular	0.166	0.072	0.278	0.134
Pyrrole/ Regular	0.211	0.089	0.380	0.249
* RMS fluctuations were calculated as in Yin and MacKerell.[51]				

Table S6. Internal parameters for all compounds

BONDS

K_b: kcal/mol/Å^2

B_0: Å

		K_b	B_0			
!Benzene						
CD2R6A	CD2R6A	305.000	1.3750			
HDR6A	CD2R6A	340.000	1.0800			
! Pyridine						
CD2R6B	CD2R6A	361.100	1.3780			
CD2R6B	ND2R6A	407.800	1.3340			
HDR6B	CD2R6B	340.000	1.0800			
! Pyrimidine						
CD2R6B	ND2R6B	350.100	1.3120			
CD2R6C	ND2R6B	423.400	1.3220			
HDR6C	CD2R6C	320.000	1.0800			
! Imidazole						
CD2R5A	CD2R5A	410.000	1.3600			
ND2R5A	CD2R5A	400.000	1.3800			

ND2R5A	CD2R5B	400.000	1.3600			
ND2R5A	HDP1A	466.000	1.0000			
ND2R5B	CD2R5A	400.000	1.3800			
ND2R5B	CD2R5B	400.000	1.3200			
HDR5B	CD2R5B	340.000	1.0900			
HDR5A	CD2R5A	365.000	1.0830			
! Pyrrole						
HDR5C	CD2R5C	370.200	1.0800			
CD2R5A	CD2R5C	322.600	1.3970			
CD2R5C	CD2R5C	322.900	1.4300			
! Indole						
CD2R6D	CD2R5C	407.600	1.4200			
CD2R6D	CD2R6A	315.000	1.3820			
ND2R5A	CD2R6D	279.900	1.4150			
CD2R6D	CD2R6D	198.200	1.4000			
! Purine						
ND2R6B	CD2R6F	353.280	1.3100			
CD2R6F	CD2R6F	331.890	1.4690			
CD2R6F	CD2R6B	295.820	1.3980			
CD2R6F	ND2R5A	428.020	1.3810			
ND2R5B	CD2R6F	428.020	1.3810			
! 4-methyl-imidazole						
CD33A	CD2R5A	229.600	1.5000			
! Methyl-indole						
CD2R5C	CD33A	229.630	1.5000			

ANGLES

K_{theta}: kcal/mol/rad^2

$Theta_0$: degrees
K_{ub}: kcal/mol/Å^2 (Urey-Bradley)

S_0: Å

			K_{theta}	$Theta_0$	K_{ub}	S_0
!!	Aromatics					
CD2R6A	CD2R6A	CD2R6A	40.000	120.00	35.00	2.41620
HDR6A	CD2R6A	CD2R6A	30.000	120.00	22.00	2.15250
CD33A	CD2R6A	CD2R6A	45.800	122.30		
HDA3A	CD33A	CD2R6A	49.300	107.50		
!	Pyridine					
CD2R6A	CD2R6A	CD2R6B	46.100	120.00	29.80	2.44800
CD2R6A	CD2R6B	ND2R6A	27.400	119.20		
CD2R6B	ND2R6A	CD2R6B	19.600	100.00	54.20	2.28500
HDR6B	CD2R6B	CD2R6A	43.400	120.00	18.60	2.15250

HDR6B	CD2R6B	ND2R6A	25.900	112.00	32.20	2.05000
HDR6A	CD2R6A	CD2R6B	26.000	120.00	21.00	2.15250
!	Pyrimidine					
CD2R6A	CD2R6B	ND2R6B	44.300	125.0		
CD2R6B	CD2R6A	CD2R6B	60.200	128.00	33.20	2.44000
CD2R6C	ND2R6B	CD2R6B	27.500	110.00	66.70	2.20000
ND2R6B	CD2R6C	ND2R6B	17.000	135.00		
HDR6B	CD2R6B	ND2R6B	28.400	112.00	23.90	2.05000
HDR6C	CD2R6C	ND2R6B	28.400	112.00	23.90	2.05000
!	Imidazole					
CD2R5B	ND2R5A	CD2R5A	130.000	107.50		
CD2R5B	ND2R5B	CD2R5A	130.000	104.00		
HDP1A	ND2R5A	CD2R5A	30.000	125.50	20.00	2.15000
HDP1A	ND2R5A	CD2R5B	30.000	127.00	20.00	2.14000
HDP1A	ND2R5C	CD2R5A	25.000	126.00	15.00	2.13000
HDP1A	ND2R5C	CD2R5B	25.000	126.00	15.00	2.09000
HDR5B	CD2R5A	CD2R5A	22.000	130.00	15.00	2.21500
HDR5A	CD2R5A	CD2R5A	25.000	130.00	20.00	2.20000
ND2R5A	CD2R5A	CD2R5A	130.000	106.00		
ND2R5A	CD2R5A	HDR5A	25.000	124.00	20.00	2.14000
ND2R5A	CD2R5B	HDR5B	25.000	122.50	20.00	2.14000
ND2R5B	CD2R5A	CD2R5A	130.000	110.00		
ND2R5B	CD2R5A	HDR5A	25.000	120.00	20.00	2.14000
ND2R5B	CD2R5B	HDR5B	25.000	125.00	20.00	2.12000
ND2R5B	CD2R5B	ND2R5A	130.000	112.50		
!	Pyrrole					
HDR5A	CD2R5A	CD2R5C	18.63	125.00	28.00	2.17300
HDR5C	CD2R5C	CD2R5A	12.72	126.40	28.00	2.21500
HDR5C	CD2R5C	CD2R5C	23.80	126.40	28.00	2.21500
CD2R5A	CD2R5C	CD2R5C	80.00	106.40	27.90	2.26100
CD2R5A	ND2R5A	CD2R5A	119.08	106.00		
ND2R5A	CD2R5A	CD2R5C	100.02	106.00	28.00	2.24000
!	Indole					
HDR5C	CD2R5C	CD2R6D	1.7	124.7	8.3	2.3781
HDP1A	ND2R5A	CD2R6D	12.8	130.1		
CD2R6D	CD2R6A	HDR6A	43.5	122.6	19.9	2.0833

CD2R6D	CD2R5C	CD2R5A	81.9	106.1	22.5	2.2163
CD2R5C	CD2R6D	CD2R6D	81.9	106.1	22.5	2.2163
CD2R5C	CD2R6D	CD2R6A	144.3	130.9		
CD2R5A	ND2R5A	CD2R6D	81.4	108.6		
CD2R6D	CD2R6D	ND2R5A	31.4	105.5		
ND2R5A	CD2R6D	CD2R6A	132.1	130.9		
CD2R6D	CD2R6A	CD2R6A	143.5	123.8		
CD2R6D	CD2R6D	CD2R6A	50.1	126.5		
!Purine						
CD2R6C	ND2R6B	CD2R6F	26.300	121.10	75.0	2.3797
ND2R6B	CD2R6F	CD2R6F	29.820	100.50		
CD2R6F	CD2R6F	CD2R5B	58.070	117.30	9.2	2.3476
CD2R6F	ND2R5B	CD2R5B	127.910	103.00		
CD2R6F	ND2R5A	CD2R5B	137.460	109.60		
CD2R6F	ND2R5A	HDP1A	37.590	113.10	28.7	2.2021
CD2R6F	CD2R6F	CD2R6B	79.820	109.20	4.5	2.2904
ND2R6B	CD2R6B	CD2R6F	23.160	123.30		
CD2R6F	CD2R6B	HDR6B	13.060	105.10	27.6	2.1019
CD2R6F	CD2R6F	ND2R5A	111.400	96.00		
CD2R6F	CD2R6F	ND2R5B	99.820	101.50		
!tautomer	A					
CD2R6B	CD2R6F	ND2R5A	130.000	110.00		
ND2R6B	CD2R6F	ND2R5B	130.000	110.00		
!tautomer	B					
CD2R6B	CD2R6F	ND2R5B	130.000	110.00		
ND2R6B	CD2R6F	ND2R5A	130.000	110.00		
! 4-methyl-imidazole						
CD33A	CD2R5A	ND2R5A	45.800	124.0000		
CD33A	CD2R5A	CD2R5A	45.800	130.0000		
CD2R5A	CD33A	HDA3A	33.430	109.5000		
! Methyl-indole						
CD33A	CD2R5C	CD2R6D	45.800	122.3000		
CD33A	CD2R5C	CD2R5A	45.800	122.3000		
CD2R5C	CD33A	HDA3A	49.300	107.50		

DIHEDRALS

K_{chi}: kcal/mol

n: multiplicity
delta: degrees

! Benzene						
CD2R6A	CD2R6A	CD2R6A	CD2R6A	2.8000	2	180.00
HDR6A	CD2R6A	CD2R6A	CD2R6A	4.2000	2	180.00
HDR6A	CD2R6A	CD2R6A	HDR6A	2.4000	2	180.00
! Pyridine						
CD2R6A	CD2R6A	CD2R6B	ND2R6A	0.860	2	180.00
CD2R6A	CD2R6B	ND2R6A	CD2R6B	2.200	2	180.00
HDR6A	CD2R6A	CD2R6B	ND2R6A	1.200	2	180.00
HDR6B	CD2R6B	ND2R6A	CD2R6B	4.300	2	180.00
CD2R6B	CD2R6A	CD2R6A	CD2R6A	5.350	2	180.00
CD2R6A	CD2R6B	CD2R6A	CD2R6A	4.400	2	180.00
HDR6A	CD2R6A	CD2R6A	CD2R6B	3.600	2	180.00
HDR6B	CD2R6B	CD2R6A	CD2R6A	5.400	2	180.00
HDR6B	CD2R6B	CD2R6A	HDR6A	2.400	2	180.00
! Pyrimidine						
CD2R6A	CD2R6B	ND2R6B	CD2R6C	2.000	2	180.0
CD2R6B	CD2R6A	CD2R6B	ND2R6B	0.810	2	180.0
CD2R6B	ND2R6B	CD2R6C	ND2R6B	4.520	2	180.0
HDR6A	CD2R6A	CD2R6B	ND2R6B	3.420	2	180.00
HDR6B	CD2R6B	CD2R6A	CD2R6B	1.380	2	180.00
HDR6B	CD2R6B	ND2R6B	CD2R6C	10.740	2	180.00
HDR6C	CD2R6C	ND2R6B	CD2R6B	8.150	2	180.00
! Imidazole						
CD2R5B	ND2R5A	CD2R5A	CD2R5A	14.0000	2	180.00
CD2R5B	ND2R5B	CD2R5A	CD2R5A	14.0000	2	180.00
HDR5B	CD2R5B	ND2R5A	CD2R5A	3.0000	2	180.00
HDR5B	CD2R5B	ND2R5B	CD2R5A	3.0000	2	180.00
ND2R5A	CD2R5A	CD2R5A	HDR5A	3.0000	2	180.00
ND2R5A	CD2R5B	ND2R5B	CD2R5A	14.0000	2	180.00
ND2R5B	CD2R5A	CD2R5A	HDR5A	3.0000	2	180.00
ND2R5B	CD2R5A	CD2R5A	ND2R5A	14.0000	2	180.00
ND2R5B	CD2R5B	ND2R5A	CD2R5A	14.0000	2	180.00
HDR5A	CD2R5A	CD2R5A	HDR5A	2.0000	2	180.00
HDR5A	CD2R5A	ND2R5A	HDP1A	0.0000	2	180.00
HDR5A	CD2R5A	ND2R5A	CD2R5B	3.0000	2	180.00
HDR5A	CD2R5A	ND2R5B	CD2R5B	3.0000	2	180.00
HDP1A	ND2R5A	CD2R5A	CD2R5A	1.1000	2	180.00
HDR5B	CD2R5B	ND2R5A	HDP1A	0.9000	2	180.00
ND2R5B	CD2R5B	ND2R5A	HDP1A	1.1000	2	180.00
! Pyrrole						
HDR5C	CD2R5C	CD2R5A	HDR5A	0.2800	2	180.00
HDR5C	CD2R5C	CD2R5C	HDR5C	0.7000	2	180.00

HDP1A	ND2R5A	CD2R5A	CD2R5C	1.3000	2	180.00
CD2R5A	ND2R5A	CD2R5A	HDR5A	2.6000	2	180.00
CD2R5A	CD2R5C	CD2R5C	HDR5C	3.9000	2	180.00
CD2R5A	CD2R5C	CD2R5C	CD2R5A	10.9000	2	180.00
CD2R5C	CD2R5A	ND2R5A	CD2R5A	14.4000	2	180.00
CD2R5C	CD2R5C	CD2R5A	HDR5A	3.4000	2	180.00
CD2R5C	CD2R5C	CD2R5A	ND2R5A	7.8000	2	180.00
ND2R5A	CD2R5A	CD2R5C	HDR5C	1.1000	2	180.00
! Indole						
! PYRTOR+PYRTOR' pyrrole ring						
CD2R5C	CD2R6D	CD2R6D	ND2R5A	8.50	2	180.00
CD2R5C	CD2R5A	ND2R5A	CD2R6D	9.52	2	180.00
CD2R6D	CD2R5C	CD2R5A	ND2R5A	8.19	2	180.00
CD2R6D	CD2R6D	ND2R5A	CD2R5A	8.26	2	180.00
CD2R5A	CD2R5C	CD2R6D	CD2R6D	6.34	2	180.00
!BUTTERFLY motion						
CD2R5C	CD2R6D	CD2R6D	CD2R6A	1.76	2	180.00
CD2R5C	CD2R6D	CD2R6A	CD2R6A	1.68	2	180.00
ND2R5A	CD2R6D	CD2R6D	CD2R6A	1.61	2	180.00
ND2R5A	CD2R6D	CD2R6A	CD2R6A	1.93	2	180.00
CD2R5A	ND2R5A	CD2R6D	CD2R6A	2.04	2	180.00
CD2R5A	CD2R5C	CD2R6D	CD2R6A	6.61	2	180.00
! PUCK-ASYDEF+ASYDEF' phenyl ring						
CD2R6D	CD2R6D	CD2R6A	CD2R6A	1.34	2	180.00
CD2R6D	CD2R6A	CD2R6A	CD2R6A	1.38	2	180.00
CD2R6D	CD2R6A	CD2R6A	CD2R6A	0.21	2	180.00
CD2R6A	CD2R6D	CD2R6D	CD2R6A	3.46	2	180.00
! wbzCH1 wagging						
CD2R5C	CD2R6D	CD2R6A	HDR6A	0.44	2	180.00
CD2R6D	CD2R6D	CD2R6A	HDR6A	0.85	2	180.00
CD2R6D	CD2R6D	CD2R6A	HDR6A	0.07	2	180.00
ND2R5A	CD2R6D	CD2R6A	HDR6A	0.92	2	180.00
! wbzCH2 wagging						
CD2R6D	CD2R6A	CD2R6A	HDR6A	0.60	2	180.00
CD2R6D	CD2R6A	CD2R6A	HDR6A	0.60	2	180.00
! wpCH3						
HDR5C	CD2R5C	CD2R6D	CD2R6D	0.15	2	180.00
HDR5C	CD2R5C	CD2R6D	CD2R6A	0.15	2	180.00
! wpCH4						
CD2R6D	CD2R5C	CD2R5A	HDR5A	0.81	2	180.00
HDR5A	CD2R5A	ND2R5A	CD2R6D	0.81	2	180.00
! wNH						
HDP1A	ND2R5A	CD2R6D	CD2R6A	0.25	2	180.00
CD2R6D	CD2R6D	ND2R5A	HDP1A	0.25	2	180.00

! Purine						
ND2R6B	CD2R6C	ND2R6B	CD2R6F	0.10	2	180.00
ND2R6B	CD2R6B	CD2R6F	CD2R6F	0.10	2	180.00
CD2R6C	ND2R6B	CD2R6B	CD2R6F	7.80	2	180.00
CD2R6C	ND2R6B	CD2R6F	CD2R6F	7.80	2	180.00
ND2R6B	CD2R6F	CD2R6F	CD2R6B	0.10	2	180.00
HDR6C	CD2R6C	ND2R6B	CD2R6F	6.50	2	180.00
CD2R6F	CD2R6F	ND2R5A	CD2R5B	6.20	2	180.00
CD2R6F	ND2R5B	CD2R5B	ND2R5A	11.50	2	180.00
ND2R5B	CD2R6F	CD2R6F	ND2R5A	5.10	2	180.00
CD2R6F	ND2R5A	CD2R5B	ND2R5B	12.00	2	180.00
CD2R6F	CD2R6F	CD2R6B	HDR6B	0.10	2	180.0
CD2R6F	ND2R5A	CD2R5B	HDR5B	4.70	2	180.00
CD2R6F	ND2R5B	CD2R5B	HDR5B	4.70	2	180.00
CD2R6F	CD2R6F	ND2R5A	HDP1A	2.70	2	180.00
CD2R6B	CD2R6F	ND2R5A	CD2R5B	2.00	2	180.0
CD2R6B	CD2R6F	ND2R5A	HDP1A	1.00	2	180.00
HDR6B	CD2R6B	CD2R6F	ND2R5A	2.00	2	180.0
ND2R6B	CD2R6F	CD2R6F	ND2R5B	14.00	2	180.0
CD2R6B	CD2R6F	CD2R6F	ND2R5A	14.00	2	180.0
ND2R6B	CD2R6B	CD2R6F	ND2R5B	5.70	2	180.00
CD2R6C	ND2R6B	CD2R6F	ND2R5A	5.70	2	180.00
ND2R6B	CD2R6F	ND2R5A	CD2R5B	5.70	2	180.00
CD2R6F	CD2R6F	ND2R5B	CD2R5B	5.70	2	180.0
!tautomer	0					
CD2R6B	CD2R6F	ND2R5B	CD2R5B	2.0	2	180.0
ND2R6B	CD2R6F	ND2R5A	HDP1A	1.0	2	180.00
HDR6B	CD2R6B	CD2R6F	ND2R5B	2.0	2	180.0
ND2R6B	CD2R6F	CD2R6F	ND2R5A	14.0	2	180.0
CD2R6B	CD2R6F	CD2R6F	ND2R5B	14.0	2	180.0
ND2R6B	CD2R6B	CD2R6F	ND2R5A	5.7	2	180.00
CD2R6C	ND2R6B	CD2R6F	ND2R5B	5.7	2	180.00
ND2R6B	CD2R6F	ND2R5B	CD2R5B	5.7	2	180.00
! 4-methyl-imidazole						
CD33A	CD2R5A	ND2R5A	HDP1A	1.0000	2	180.00
CD33A	CD2R5A	ND2R5A	CD2R5B	3.0000	2	180.00
CD33A	CD2R5A	CD2R5A	HDR5A	2.0000	2	180.00
CD33A	CD2R5A	CD2R5A	ND2R5B	3.0000	2	180.00
HDA3A	CD33A	CD2R5A	ND2R5A	0.1900	3	0.00
HDA3A	CD33A	CD2R5A	CD2R5A	0.0000	3	0.00
! Methyl-indole						
CD33A	CD2R5C	CD2R6D	CD2R6D	3.1000	2	180.00
CD33A	CD2R5C	CD2R6D	CD2R6A	3.1000	2	180.00
CD33A	CD2R5C	CD2R5A	HDR5A	4.2000	2	180.00
CD33A	CD2R5C	CD2R5A	ND2R5A	3.0000	2	180.00
HDA3A	CD33A	CD2R5C	CD2R6D	0.0000	3	0.00
HDA3A	CD33A	CD2R5C	CD2R5A	0.0000	3	0.00

Table S7. Final nonbond parameters: Lennard-Jones parameters, charges, polarizabilities and Thole factors and LJ parameters for all compounds.

```
Lennard-Jones parameters

Atom type   epsilon    Rmin/2
CD2R6A      -0.0690    2.090  ! BENZ, benzene
CD2R6B      -0.0940    2.000  ! PYR, pyridine (adjacent to N)
CD2R6C      -0.1120    2.000  ! PYRM, pyrimidine (between 2 Ns)
CD2R6D      -0.0380    1.900  ! INDO, indole: 5,6 membered ring bisector C

HDR6A       -0.0300    1.0500 ! BENZ, benzene
HDR6B       -0.0700    0.8000 ! PYR, pyridine (on carbon adjacent to N)
HDR6C       -0.0700    0.8000 ! PYRM, pyrimidine (on carbon between 2 Ns)

ND2R6A      -0.070     1.9800 ! PYR, pyridine (N acceptor)
ND2R6B      -0.100     1.9000 ! PYRM, pyrimidine (N acceptor)


CD2R5A      -0.095     2.070  ! IMID, imidazole, CG,CD2
CD2R5B      -0.093     1.980  ! IMID, imidazole, CE1
CD2R5C      -0.050     2.090  ! PYRR, pyrrole

HDP1A       -0.0100    0.4000 ! polar hydrogen

HDR5A       -0.0550    1.2500 ! IMID, imidazole, PYRR on C adjacent to N
HDR5B       -0.0870    1.1000 ! IMID, imidazole
HDR5C       -0.0360    1.1800 ! PYRR, pyrrole

ND2R5A      -0.087     1.8610 ! IMID, imidazole (N-H donor)
ND2R5B      -0.069     1.9560 ! IMID, imidazole (N acceptor)

LJ Off diagonal terms to be used in combination with the SWM4-NDP water model
oxygen LJ parameters

CD2R6A      -0.0500    2.150  ! BENZ, benzene
CD2R6B      -0.0940    2.020  ! PYR, pyridine (adjacent to N)
CD2R6C      -0.1080    2.050  ! PYRM, pyrimidine (between 2 Ns)

ND2R6A      -0.070     2.0000 ! PYR, pyridine (N acceptor)
ND2R6B      -0.100     1.9500 ! PYRM, pyrimidine (N acceptor)
```

```
RESI PYR         0.00   ! pyridine
!
!      HD1  HE1
!       |    |
!      CD1--CE1
!      /      \
! HG--CG       NZ:
!      \      /
!      CD2--CE2
!       |    |
!      HD2  HE2
!
GROUP
ATOM CG   CD2R6A  -0.1334   ALPHA   -1.5954   THOLE 1.312
ATOM HG   HDR6A    0.2070
ATOM CD1  CD2R6A  -0.1746   ALPHA   -1.6184   THOLE 1.312
ATOM HD1  HDR6A    0.0737
ATOM CD2  CD2R6A  -0.1746   ALPHA   -1.6184   THOLE 1.312
ATOM HD2  HDR6A    0.0737
ATOM CE1  CD2R6B   0.1944   ALPHA   -1.6286   THOLE 0.988
ATOM HE1  HDR6B    0.0522
ATOM CE2  CD2R6B   0.1944   ALPHA   -1.6286   THOLE 0.988
ATOM HE2  HDR6B    0.0522
ATOM NZ   ND2R6A   0.0000   ALPHA   -1.0183   THOLE 1.057  ! fitchg ALPHA -
0.8674
ATOM LP1  LP      -0.3650

ANISOTROPY        NZ  LP1 CE1 CE2  A11 1.16107          A22 0.67785


RESI PYRM         0.00  ! pyrimidine, NA based numbering
!
!      H6
!       |   ..
!      C6---N1
!      /      \
! H5--C5       C2--H2
!      \      /
!      C4---N3
!       |   ..
!      HD2
!
GROUP
ATOM C5   CD2R6A  -0.46838  ALPHA -1.64135   THOLE 1.057
ATOM H5   HDR6A    0.15270
ATOM C6   CD2R6B   0.263165 ALPHA -1.6184    THOLE 1.169
ATOM H6   HDR6B    0.11538
ATOM C4   CD2R6B   0.263165 ALPHA -1.6184    THOLE 1.169
ATOM H4   HDR6B    0.11538
ATOM N1   ND2R6B   0.00000  ALPHA -1.02425   THOLE 1.089  ! fitchg -0.8724
ATOM LP1  LP      -0.46509
ATOM N3   ND2R6B   0.00000  ALPHA -1.02425   THOLE 1.089  ! fitchg -0.8724
ATOM LP3  LP      -0.46509
ATOM C2   CD2R6C   0.43181  ALPHA -1.6286    THOLE 0.761
ATOM H2   HDR6C    0.05696

ANISOTROPY        N1  LP1 C6  C2   A11 1.2376  A22 0.6648
ANISOTROPY        N3  LP3 C4  C2   A11 1.2376  A22 0.6648


RESI IMID        0.00 ! Imidazole, adm jr.
!
!       HD1    HE1
```

```
!        |     /
!       ND1--CE1
!      /     ||
! HG-CG       ||
!     \\      ||
!      CD2--NE2
!       |      :
!      HD2
!
GROUP

ATOM CG   CD2R5A   -0.34331     ALPHA   -1.63200  THOLE 0.949
ATOM HG   HDR5A     0.21553
ATOM CD2  CD2R5A    0.03675     ALPHA   -1.62605  THOLE 0.949
ATOM HD2  HDR5A     0.09108
ATOM ND1  ND2R5A   -0.05266     ALPHA   -1.39315  THOLE 0.670
ATOM HD1  HDP1A     0.24366
ATOM CE1  CD2R5B    0.04023     ALPHA   -1.63200  THOLE 1.568
ATOM HE1  HDR5B     0.10719
ATOM NE2  ND2R5B    0.000       ALPHA   -1.04380  THOLE 0.788
ATOM LP1  LP       -0.33847

ANISOTROPY        NE2 LP1 CE1 CD2  A11 0.808   A22 1.384


RESI PYRR          0.000 ! pyrrole
!  H2        H1
!    \ ____ /
!    C2----C1
!     |     \
!     |      N5--H5
!     |____ /
!    C3----C4
!    /      \
!  H3        H4
!
GROUP
ATOM C1   CD2R5A  -0.00431     ALPHA  -1.61755  THOLE 0.190
ATOM HP1  HDR5A    0.08384
ATOM C2   CD2R5C  -0.20244     ALPHA  -1.62095  THOLE 1.018
ATOM HP2  HDR5C    0.11235
ATOM C3   CD2R5C  -0.20244     ALPHA  -1.62095  THOLE 1.018
ATOM HP3  HDR5C    0.11235
ATOM C4   CD2R5A  -0.00431     ALPHA  -1.61755  THOLE 0.190
ATOM HP4  HDR5A    0.08384
ATOM N5   ND2R5A  -0.27227     ALPHA  -1.37785  THOLE 1.648
ATOM HP5  HDP1A    0.29339


RESI INDO        0.00 ! indole
!                  HE3
!                   |
!       HG         CE3
!       \         /  \\
!        CG-----CD2   CZ3-HZ3
!        ||     ||     |
!        CD1    CE2   CH2-HH2
!       /   \   / \  //
!     HD1    NE1   CZ2
!              |     |
!            HE1   HZ2
GROUP
```

```
ATOM CD2  CD2R6D   -0.17668     ALPHA    -1.12115    THOLE 1.344
ATOM CE2  CD2R6D    0.03338     ALPHA    -1.2529     THOLE 1.009
ATOM CZ2  CD2R6A   -0.06941     ALPHA    -1.61585    THOLE 1.300
ATOM CH2  CD2R6A   -0.08614     ALPHA    -1.61925    THOLE 1.300
ATOM CZ3  CD2R6A   -0.16212     ALPHA    -1.6184     THOLE 1.300
ATOM CE3  CD2R6A   -0.02859     ALPHA    -1.61755    THOLE 1.300
ATOM CG   CD2R5C   -0.14068     ALPHA    -1.6201     THOLE 1.346
ATOM CD1  CD2R5A    0.05490     ALPHA    -1.61755    THOLE 1.265
ATOM NE1  ND2R5A   -0.20671     ALPHA    -1.3838     THOLE 1.146
ATOM HZ2  HDR6A     0.03549
ATOM HH2  HDR6A     0.12228
ATOM HZ3  HDR6A     0.07584
ATOM HE3  HDR6A     0.07629
ATOM HG   HDR5C     0.10251
ATOM HD1  HDR5A     0.04689
ATOM HE1  HDP1A     0.32275
```

```
RESI PUR1         0.00 ! purine 7H
!
!            H6
!            |
!            C6     H9
!          //  \    |
!          N1   C5--N7\
!          |    ||     C8-H8
!          C2   C4--N9//
!         / \\ /
!       H2   N3
!
GROUP
ATOM N1   ND2R6B     0.000000     ALPHA   -0.99875    THOLE      0.916
ATOM LP1  LP        -0.337561
ATOM C2   CD2R6C     0.122627     ALPHA   -1.50025    THOLE      1.309
ATOM H2   HDR6C      0.068786
ATOM N3   ND2R6B     0.000000     ALPHA   -1.0268     THOLE      0.916
ATOM LP2  LP        -0.352369
ATOM C4   CD2R6F     0.36017      ALPHA   -1.03445    THOLE      1.170
ATOM C5   CD2R6F    -0.0662578    ALPHA   -1.26905    THOLE      1.271
ATOM C6   CD2R6B     0.18766      ALPHA   -1.62945    THOLE      1.244
ATOM H6   HDR6B      0.13229
ATOM N7   ND2R5B     0.000000     ALPHA   -0.9928     THOLE      1.065
ATOM LP3  LP        -0.264776
ATOM C8   CD2R5B    -0.13375      ALPHA   -1.52405    THOLE      1.122
ATOM H8   HDR5B      0.145501
ATOM N9   ND2R5A    -0.208358     ALPHA   -1.13985    THOLE      1.176
ATOM H9   HDP1A      0.346038

ANISOTROPY        N1  LP1 C6  C2   A11 1.2376  A22 0.6648
ANISOTROPY        N3  LP3 C4  C2   A11 1.2376  A22 0.6648
ANISOTROPY        N7  LP3 C4  C8   A11 0.808   A22 1.384
```

Figure S1. Sodium cation-model compound interaction orientations.

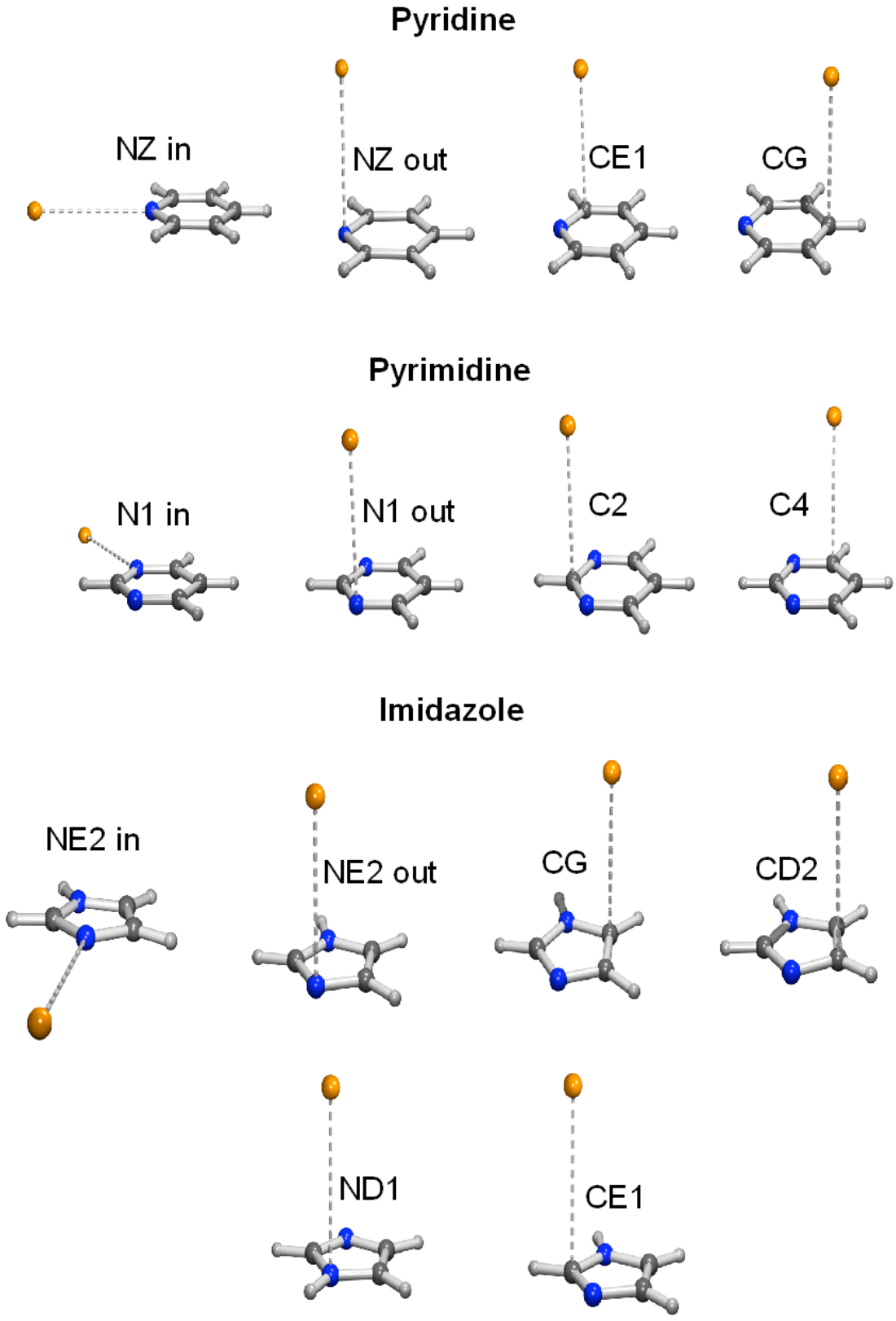


Figure S2. Rare gas-model compound interaction orientations

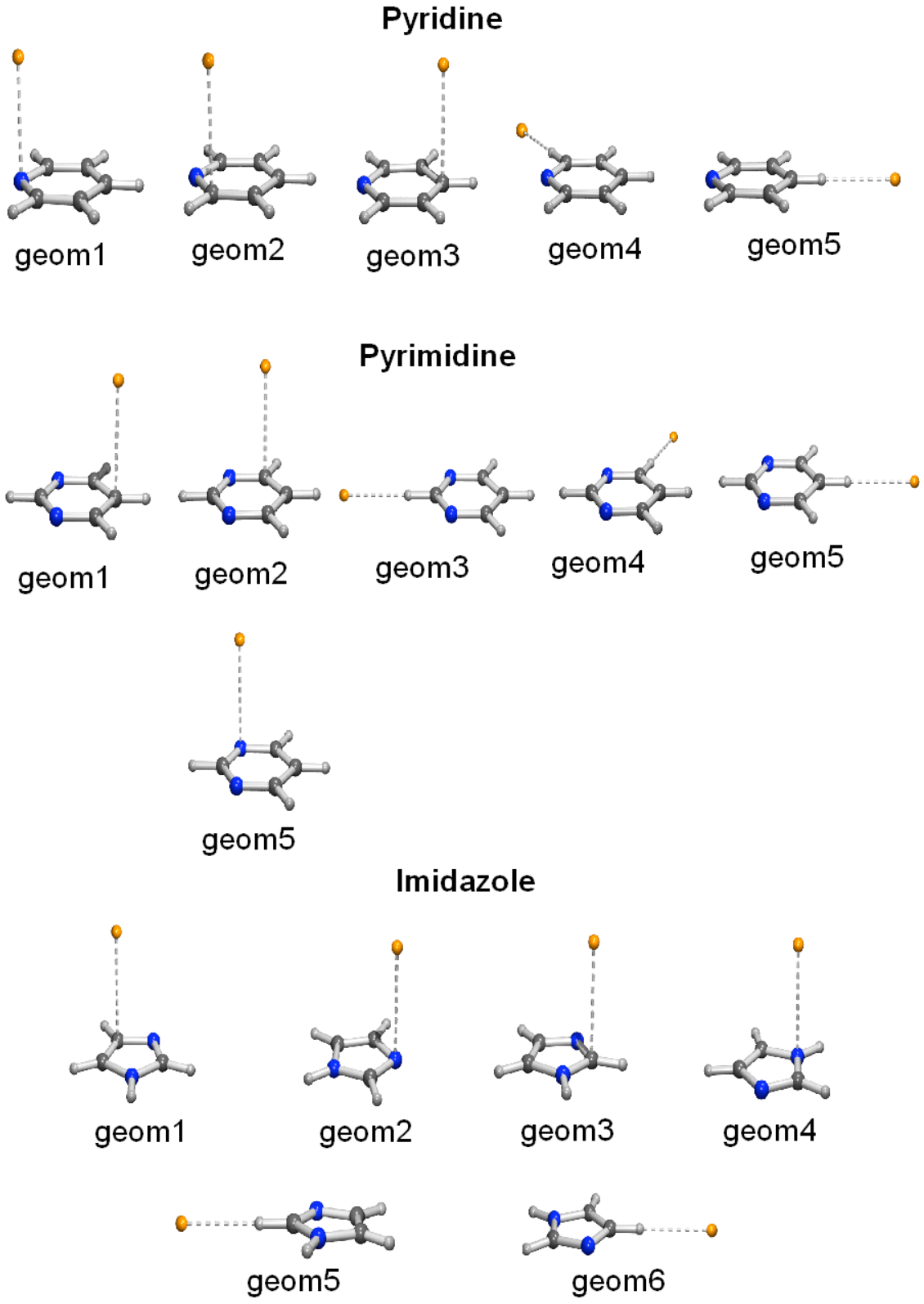


Figure S3. Model compound homodimer interaction orientations. Only in-plane orientations are considered.

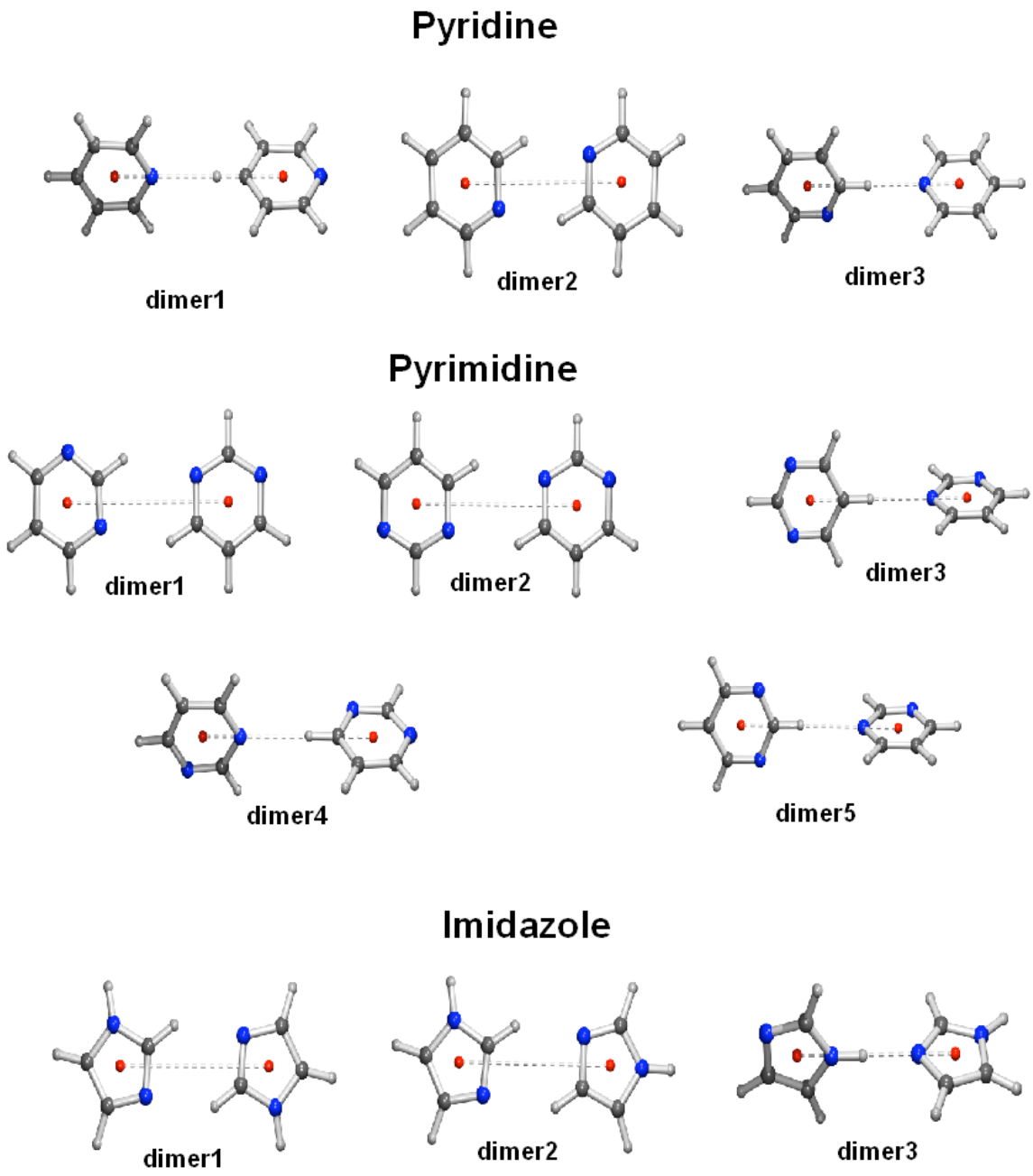


Figure S4. Interaction orientations of pyridine, pyrimidine and pyrrole with the water molecule.

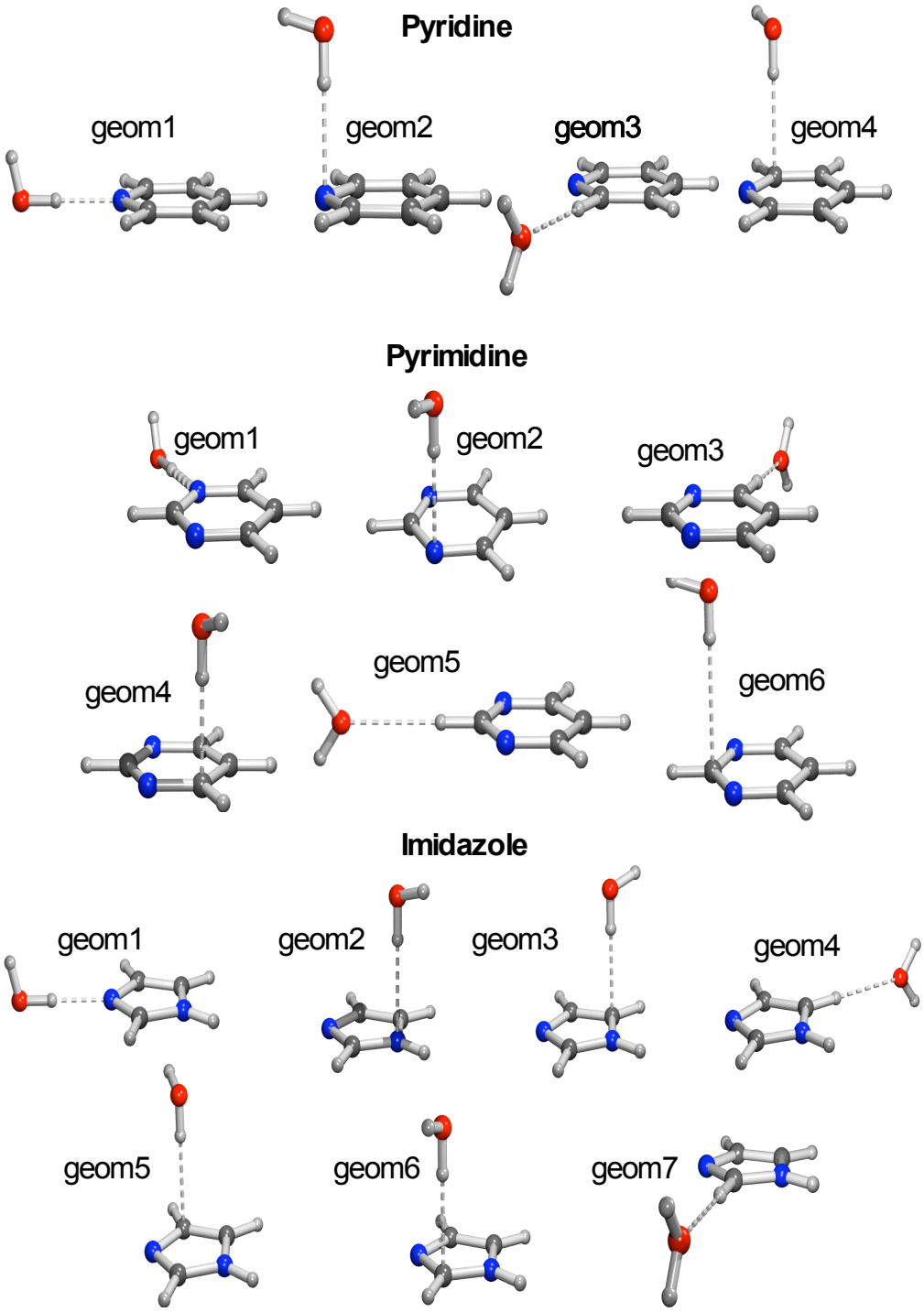
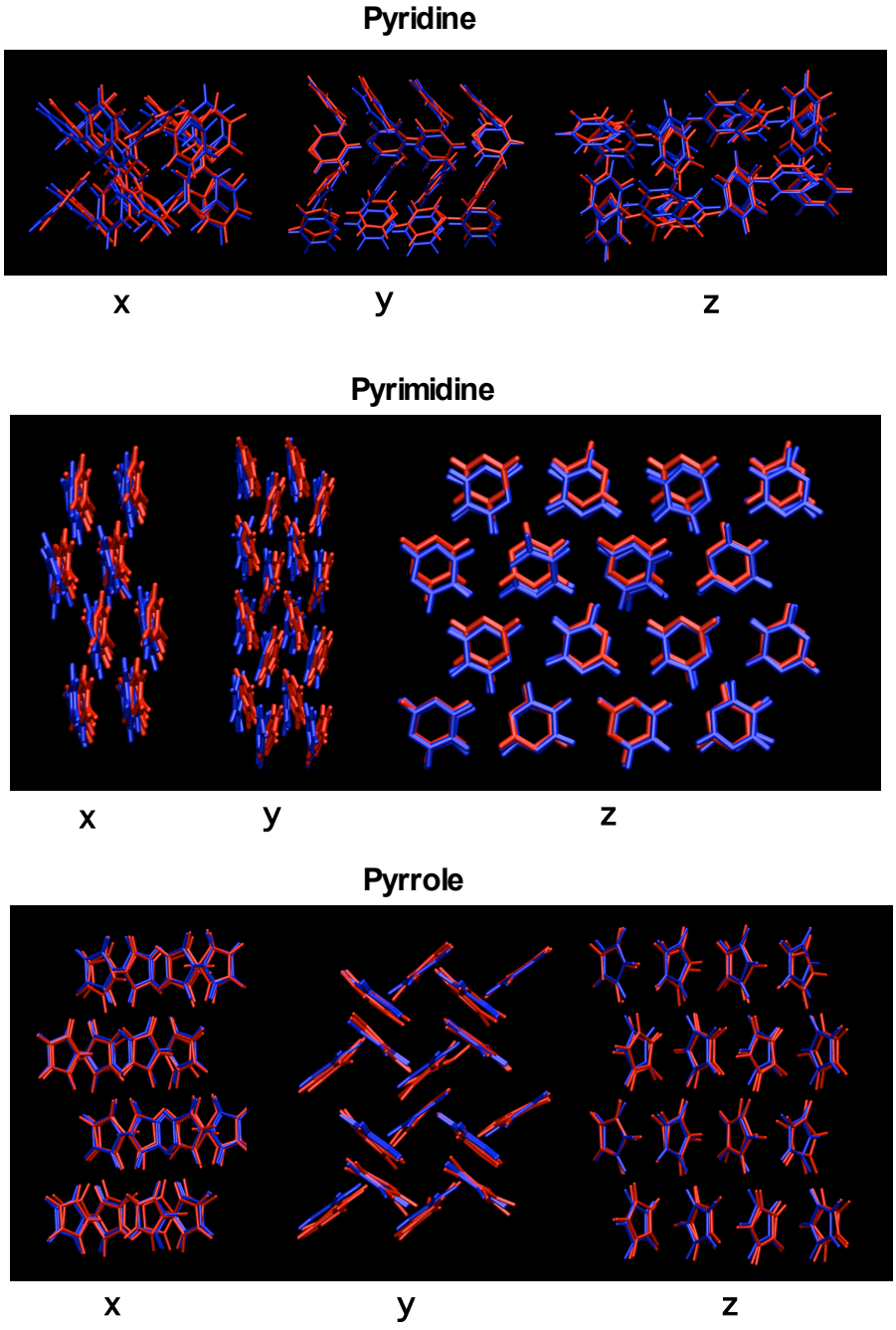


Figure S5. View of the final spashot of the MD simulation (red) superimposed on the x-ray structure (blue).



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