Supplementary Material for "Vibronic fine structure in the nitrogen 1s photoelectron spectra from Franck-Condon simulations. III. Rules for amine/imine N atoms in small N-heterocycles"

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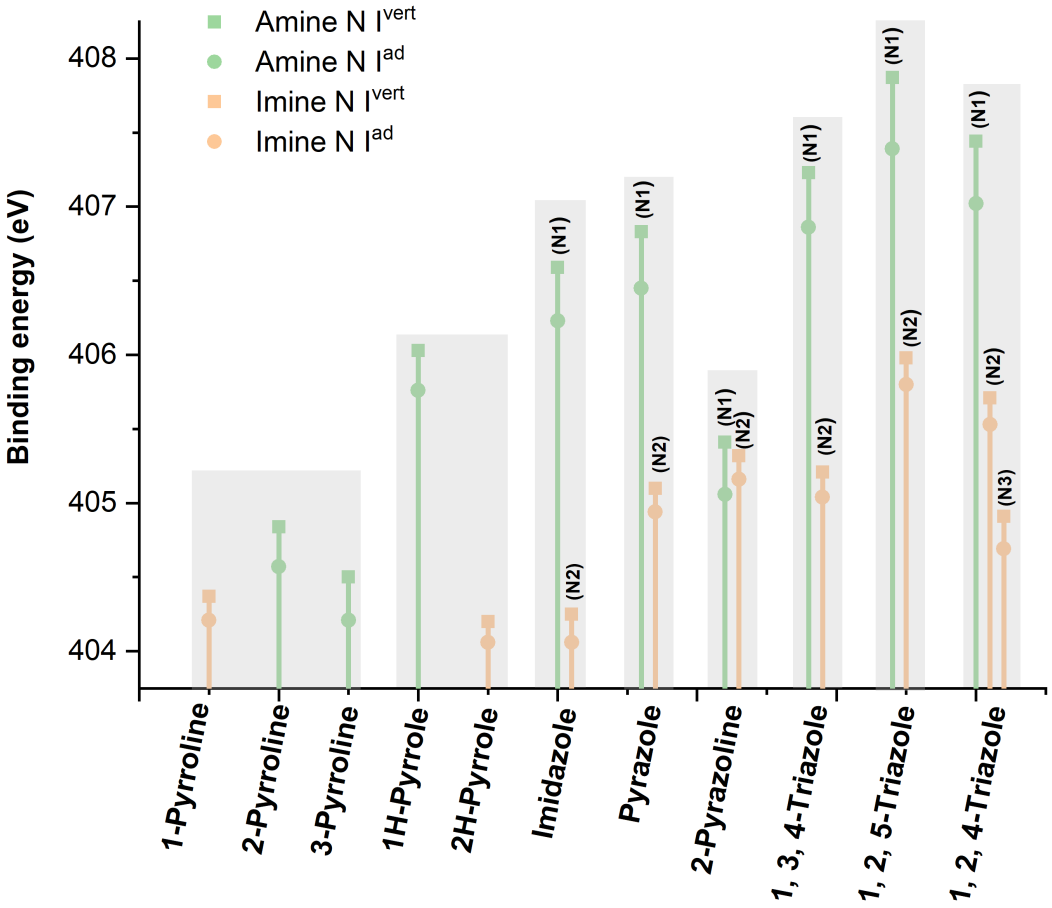

FIG. S1: Simulated vertical (I^{vert}) and adiabatic (I^{ad}) ionization potentials of 11 five-membered rings (this work) molecules. Rod tip shape differentiates between I^{vert} (square) and I^{ad} (circle) ionization potentials and the color differentiates between amine (orange) and imine (green) N atoms. Each gray area represents a group with the same molecular structure (or the same molecule).

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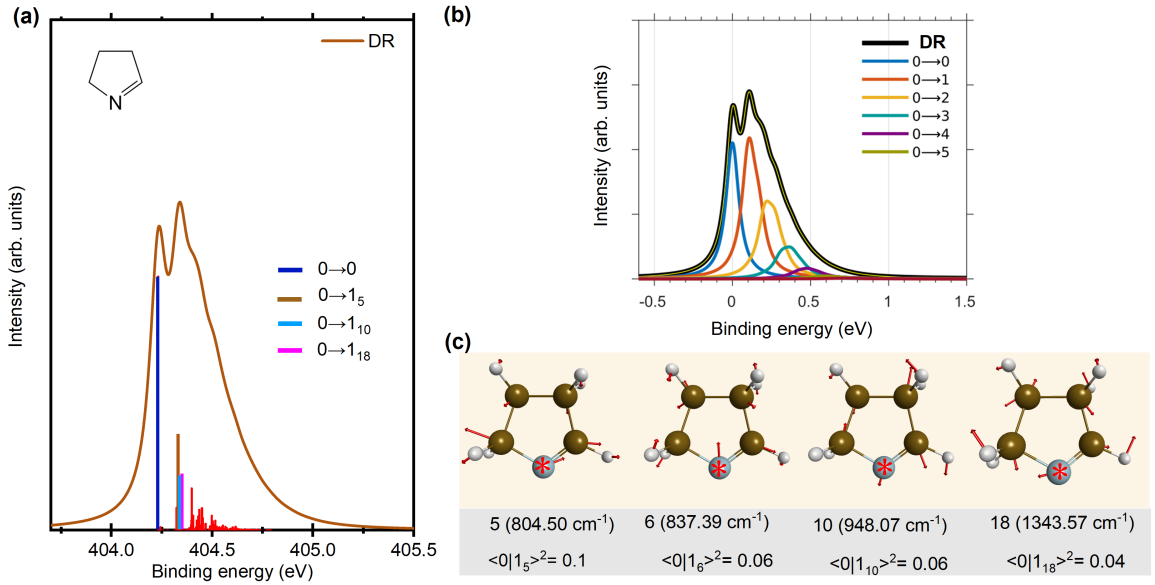


FIG. S2: (a) Simulated vibrationally-resolved N1s XPS spectrum of 1-pyrroline. (b)Analyses of contributions of different 0-n transitions until convergence. 0-0 transition energy is taken as zero. (c) Active vibrational modes are identified in the final (FCH) state. For each mode, the mode index, frequency (in parentheses), and the FC factor are shown. Asterisk denotes the core ionization center.

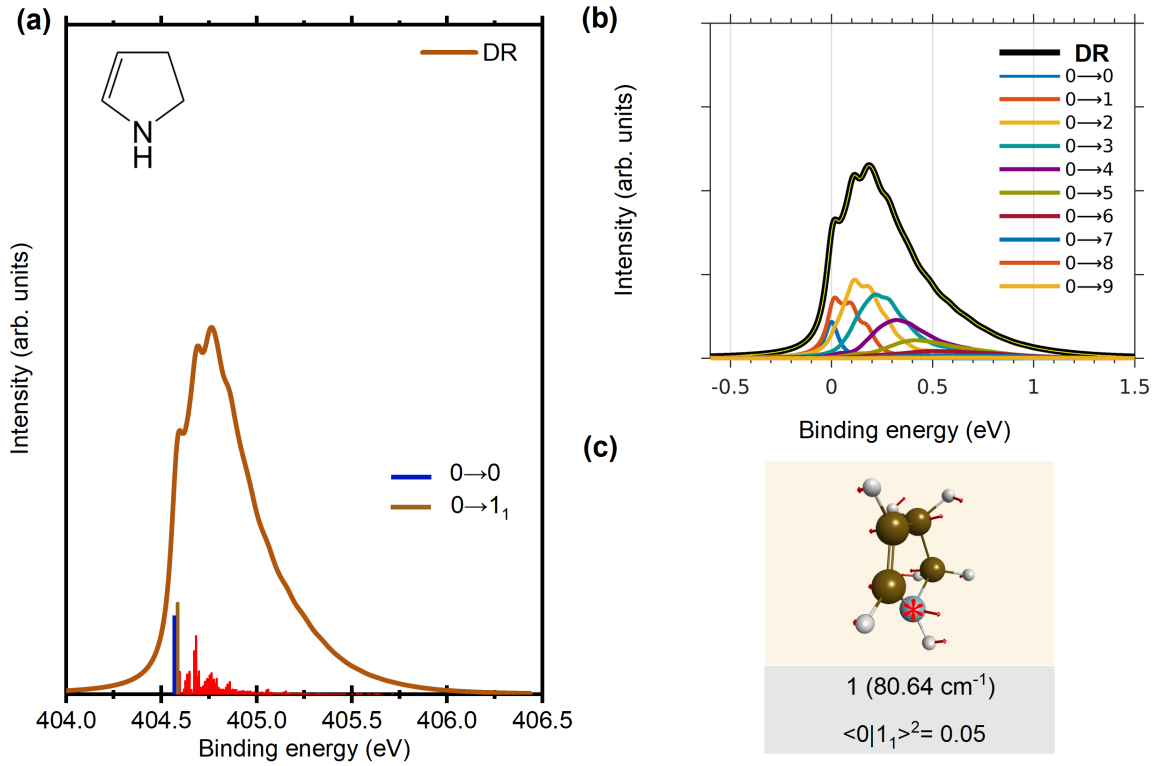


FIG. S3: The same as Fig. S2 for 2-pyrroline.

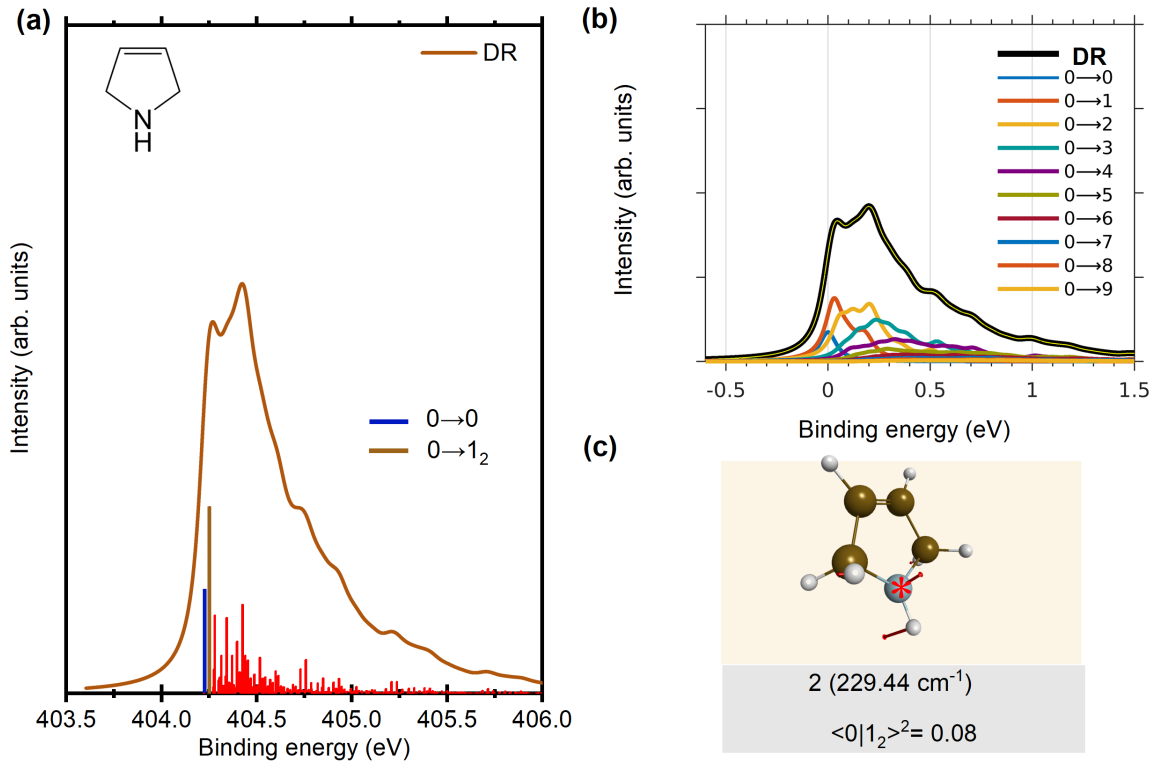


FIG. S4: The same as Fig. S2 for 3-pyrroline.

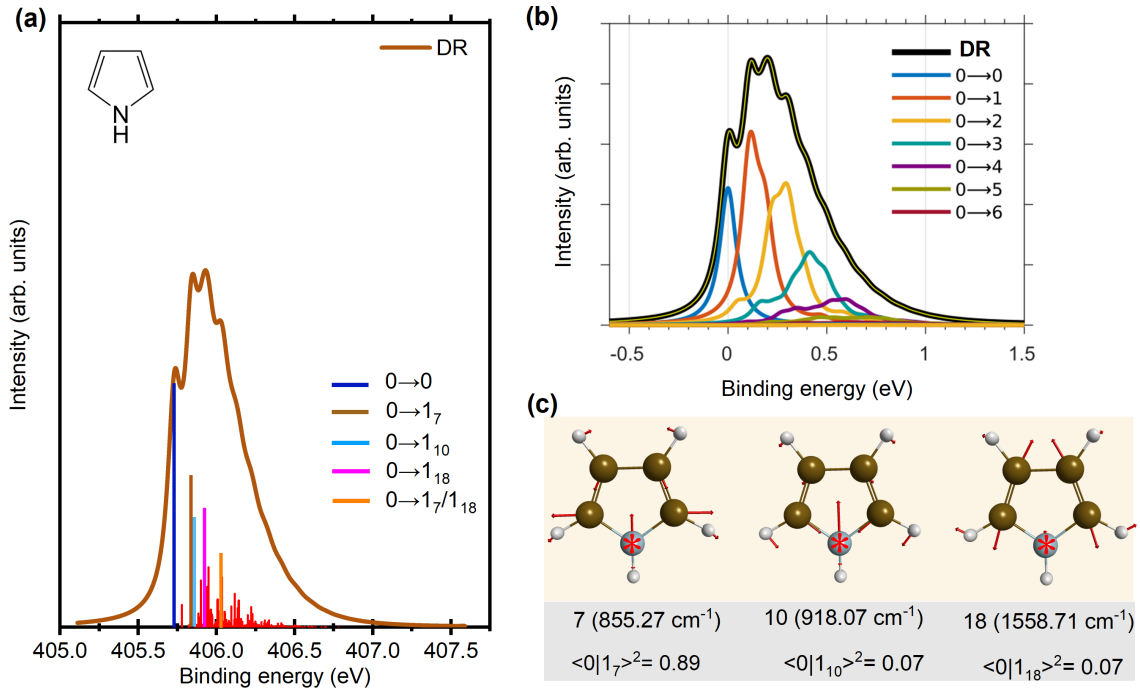


FIG. S5: The same as Fig. S2 for 1H-pyrrole.

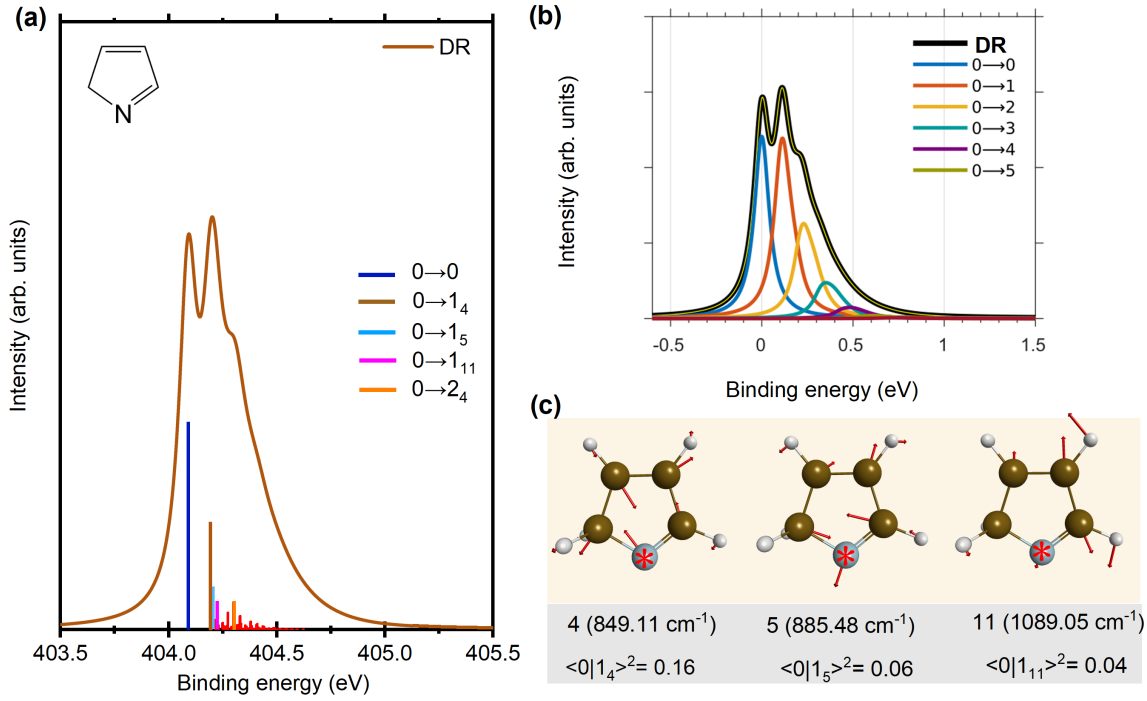


FIG. S6: The same as Fig. S2 for 2H-pyrrole.

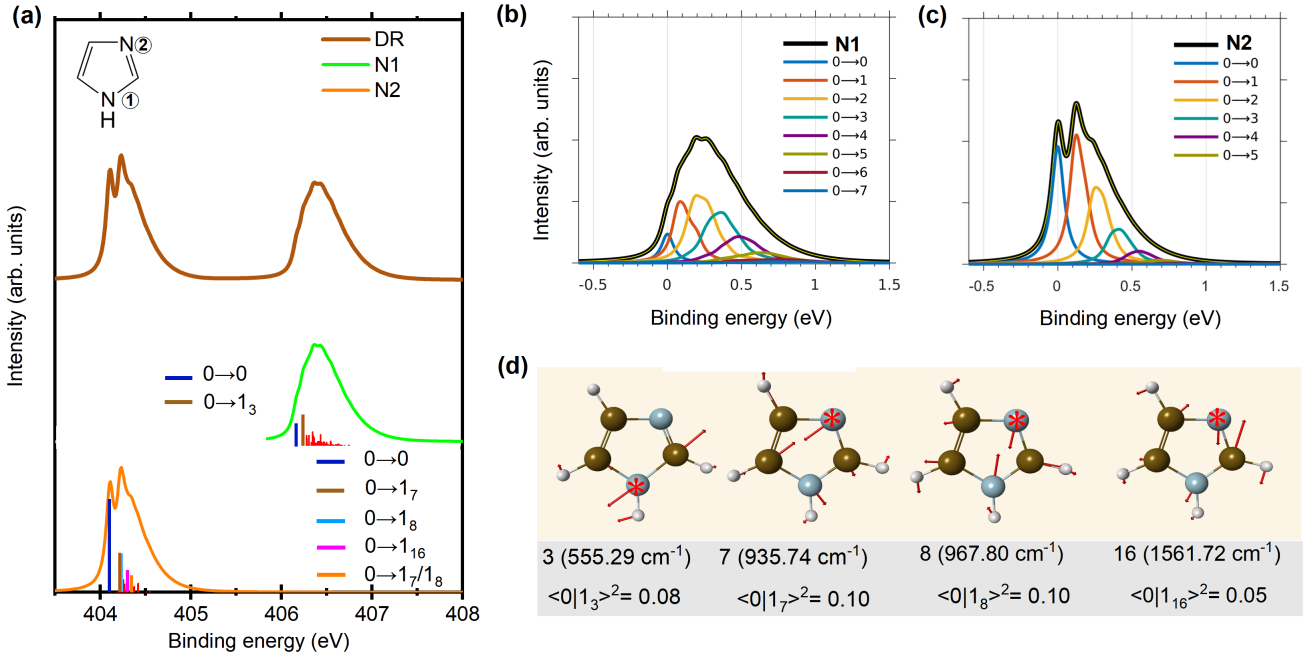


FIG. S7: (a) Simulated vibrationally-resolved N1s XPS spectrum of imidazole. (b-c)The contribution of the different 0-n transitions (until convergence) of N1 and N2. 0-0 transition energy is taken as zero. (d) Active vibrational modes are identified in the final (FCH) state. For each mode, the mode index, frequency (in parentheses), and the FC factor are shown. Asterisk denotes the core ionization center.

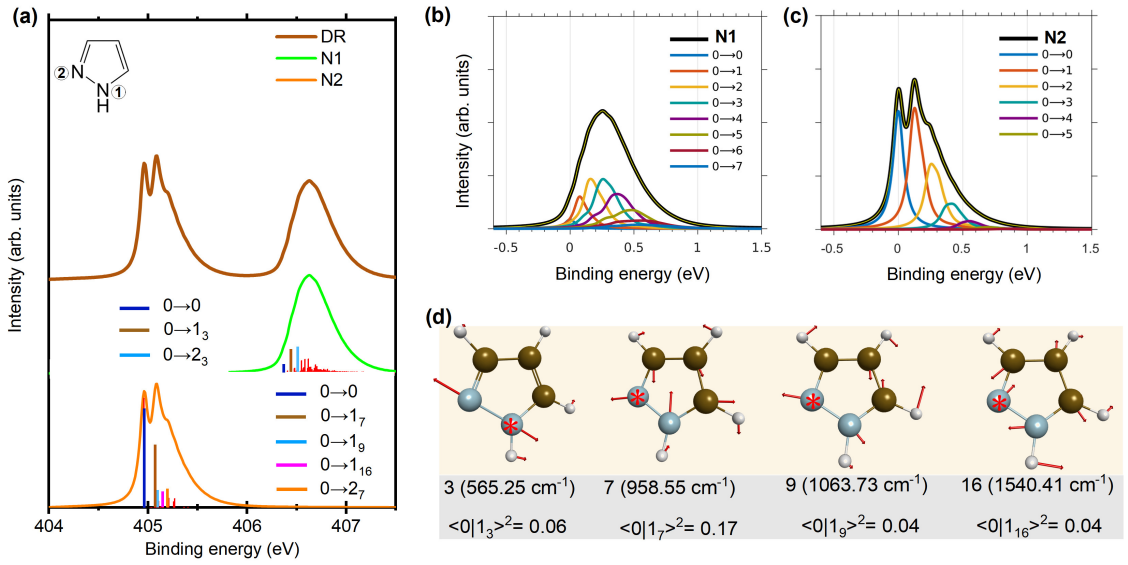


FIG. S8: The same as Fig. S7 for pyrazole.

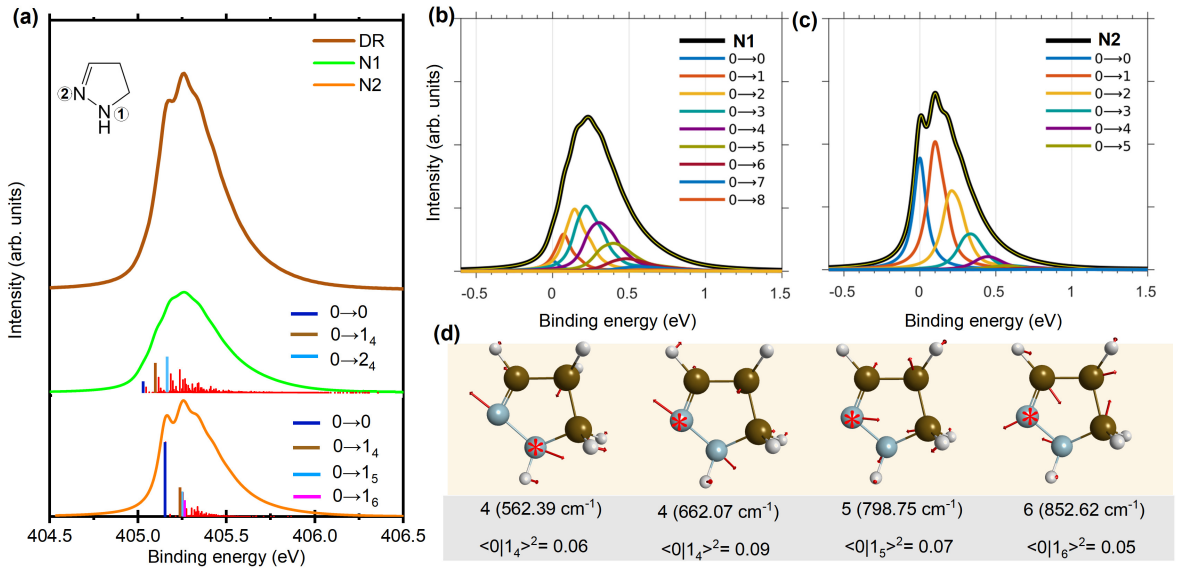


FIG. S9: The same as Fig. S7 for 2-pyrazoline.

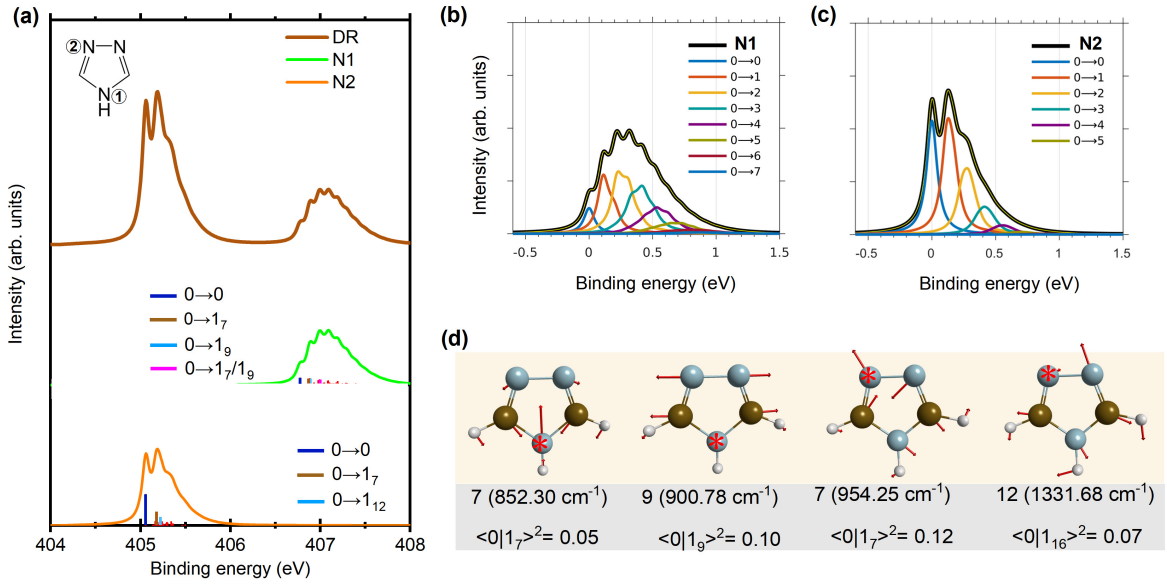


FIG. S10: The same as Fig. S7 for 1,3,4-triazole.

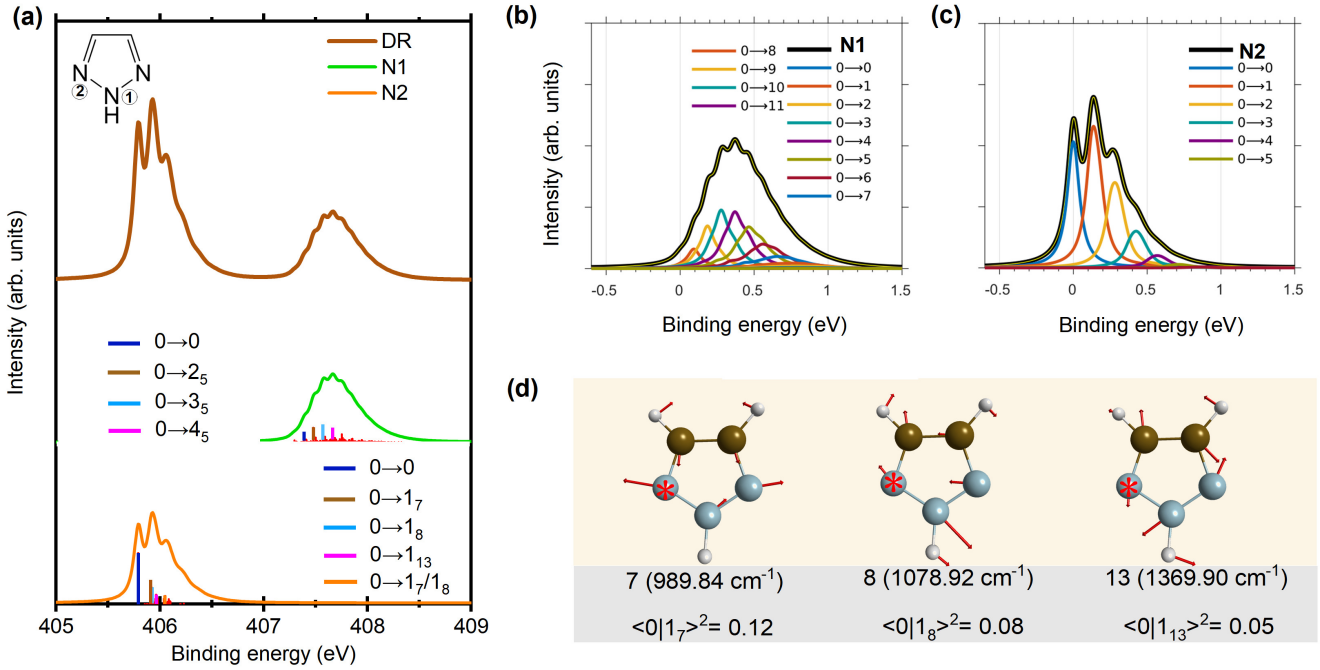


FIG. S11: The same as Fig. S7 for 1,2,5-triazole.

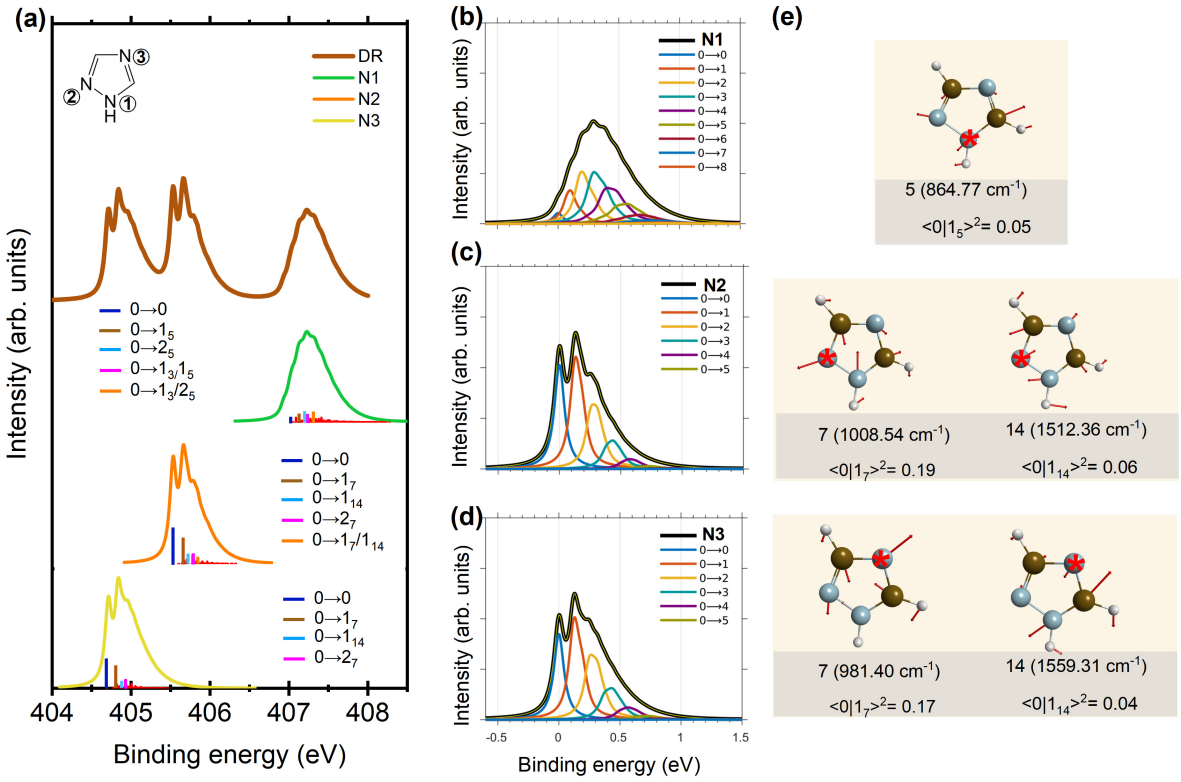


FIG. S12: (a) Simulated vibrationally-resolved N1s XPS spectrum of 1,2,4-triazole. (b-d)The contribution of the different 0-n transitions (until convergence) of N1, N2, and N3. 0-0 transition energy is taken as zero. (e) Active vibrational modes are identified in the final (FCH) state. For each mode, the mode index, frequency (in parentheses), and the FC factor are shown. Asterisk denotes the core ionization center.

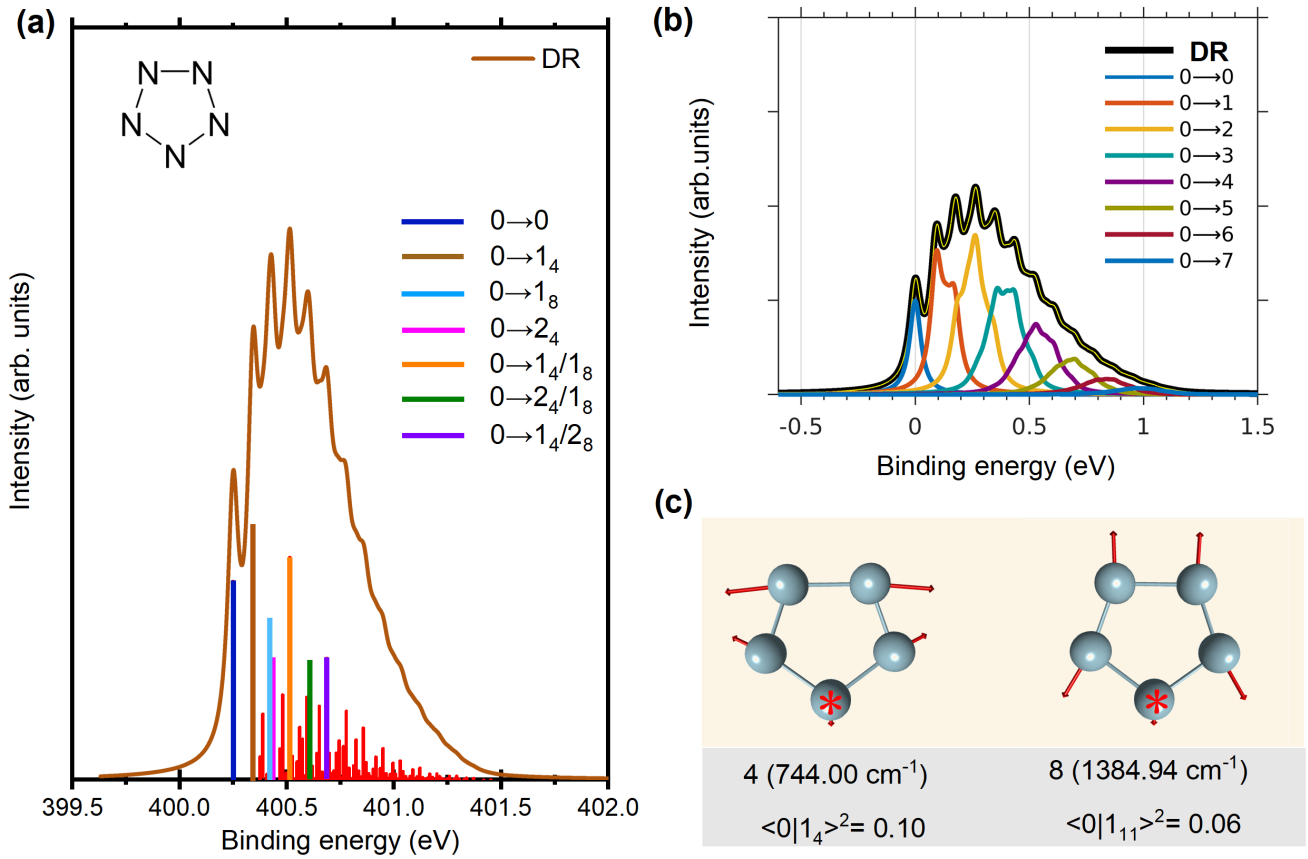


FIG. S13: The same as Fig. S2 for *cyclo*-N_5^-.

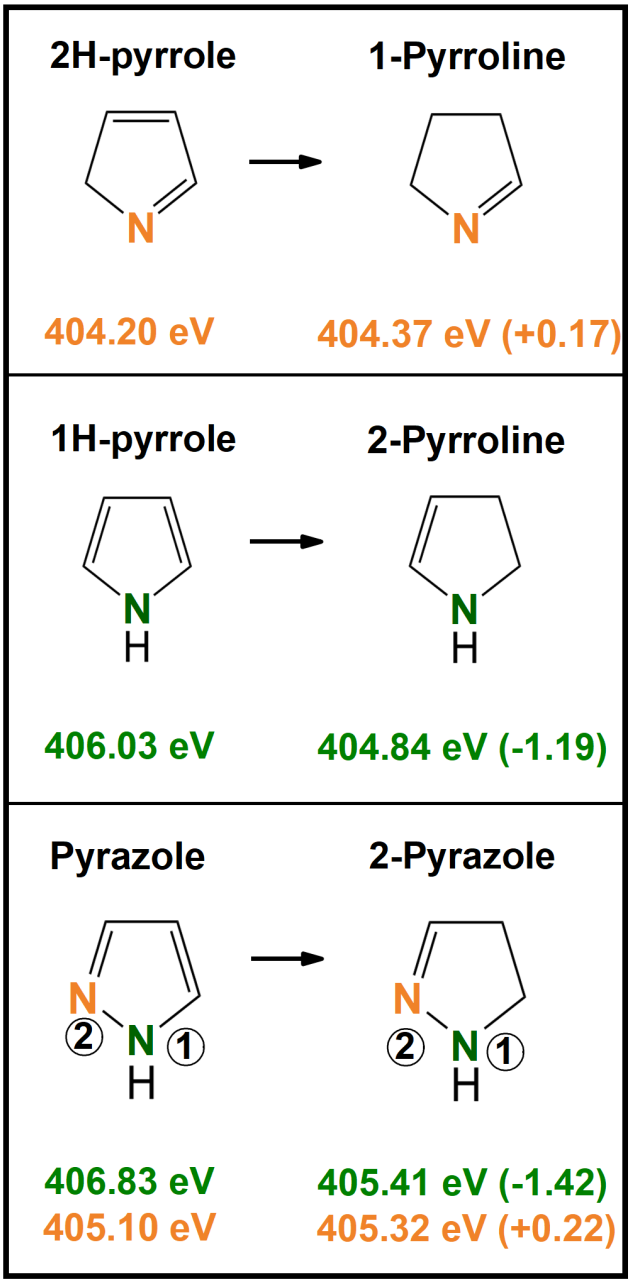


FIG. S14: Effects of hydrogenation. Comparison of computed vertical ionization potentials (I^{vert}) for selected three pairs of molecules (two molecules in each pair differ by two hydrogen atoms).

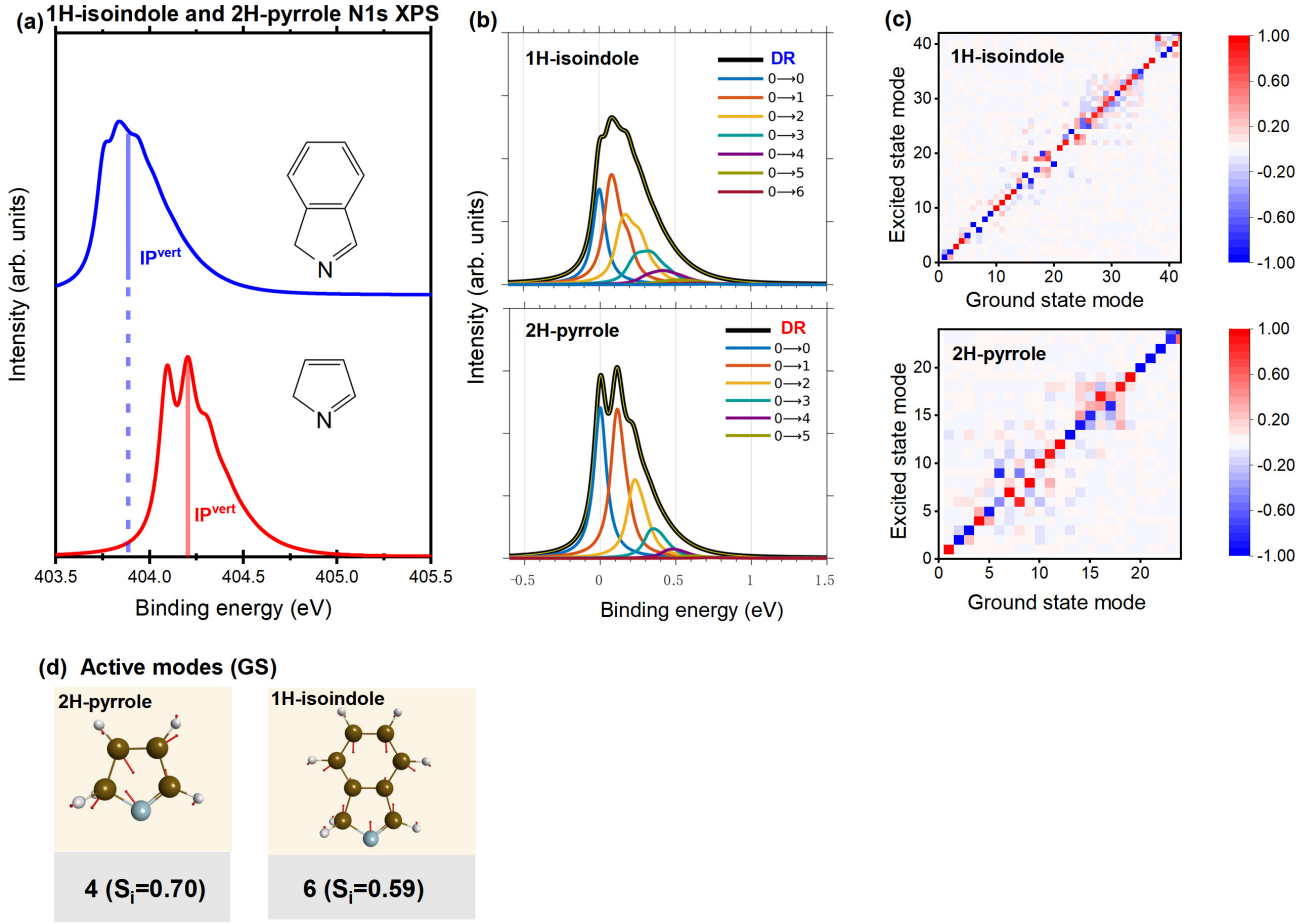


FIG. S15: A comparison of 1H-isoindole and 2H-pyrrole to see the influence of the benzene ring. (a) Computed vibrationally-resolved N1s XPS. Vertical ionization energies are indicated by vertical lines. (b) Contributions of different 0-n transitions until convergence. (c) The Duschinsky matrix. (d) Active vibrational modes are identified in the ground state. For each mode, the mode index and the Huang-Rhys factor (in parentheses) are shown.

TABLE S1: Analysis of selected vibrational modes with large Huang-Rhys factors (a threshold of $S_\mathrm{i} \geq 0.3$ was used) for the 7 azine molecules. Vibrational frequencies ω_i and the total vibrational reorganization energy (E_r) of the excited (FCH) state are given.

Molecule	N*	i	ω_i (cm^{-1})	S_i	E_r (eV)
Pyridine	N	3	602.6	0.92	0.14
Pyrimidine	N	3	620.2	0.50	0.16
		4	674.3	0.30	
Pyrazine	N	3	592.9	1.08	0.14
Pyridazine	N	3	615.6	0.72	0.18
		11	1063.6	0.40	
1,3,5-Triazine	N	4	683.3	0.67	0.18
		7	1008.2	0.35	
1,2,4-Triazine	N1	3	605.8	0.91	0.18
	N2	3	623.1	0.39	0.20
		4	704.0	0.50	
	N4	3	615.5	0.86	0.14
		10	1052.9	0.31	
1,2,4,5-Tetrazine	N	3	630.0	0.72	0.21
		7	963.8	0.48	
		10	1084.5	0.35	

TABLE S2: Analysis of selected vibrational modes with large Huang-Rhys factors (a threshold of $S_\mathrm{i} \geq 0.3$ was used) for the 17 bicyclic indole molecules. Vibrational frequencies ω_i and the total vibrational reorganization energy (E_r) of the excited (FCH) state are given. Amine (bold) and imine (lightface) N atoms are highlighted by different fonts.

Molecule	N*	i	ω_i (cm^{-1})	S_i	E_r (eV)
Indole	**N**	3	288.6	0.40	0.46
		27	1279.9	0.32	
		31	1484.0	0.56	
3-Methylindole	**N**	6	380.2	0.58	0.71
		31	1293.8	0.73	
		37	1483.7	0.38	
		51	3799.7	0.69	
3-Formylindole	**N**	2	156.1	0.36	0.49
		8	419.7	0.31	
		31	1283.6	0.45	
		36	1477.6	0.48	
		38	1604.1	0.33	
Purine	N1	6	585.3	0.73	0.22
		13	932.7	0.34	
	N2	10	788.9	0.44	0.23
		20	1215.9	0.34	
	N3	8	671.3	0.34	0.23
		13	936.2	0.44	
		14	954.5	0.42	
	N4	17	1017.8	1.60	0.91
		23	1280.8	0.34	
		24	1339.8	0.45	
		25	1405.0	0.84	
		27	1574.7	0.90	
		29	1701.2	0.66	
Adenine	N1	11	650.8	0.57	0.29
		17	906.3	0.31	
		30	1519.3	0.34	
	N2	8	568.3	0.40	0.28
	N3	18	965.4	0.73	0.25
		21	1109.5	0.30	
	N4	21	1000.3	0.97	0.80

		29	1418.0	0.37	
		31	1593.0	0.78	
		33	1678.3	0.54	
	N5	27	1359.1	0.33	0.62
		30	1472.2	0.71	
		34	1720.2	1.04	
Benzimidazole	**N1**	20	1036.0	1.54	0.86
		24	1193.4	0.33	
		27	1331.5	0.86	
		29	1486.9	0.80	
		31	1618.3	0.47	
	N2	16	974.2	0.56	0.20
4-Azaindole	**N1**	3	275.5	0.34	0.49
		26	1300.8	0.31	
		29	1449.6	0.30	
	N2	11	778.3	0.51	0.18
5-Azaindole	**N1**	30	1487.6	0.44	0.42
	N2	6	574.2	0.81	0.19
6-Azaindole	**N1**	4	389.7	0.40	0.47
		29	1451.1	0.51	
	N2	6	571.6	0.70	0.19
7-Azaindole	**N1**	26	1278.7	0.40	0.42
		29	1434.5	0.64	
		33	1688.5	0.34	
	N2	11	775.9	0.44	0.18
1*H*-isoindole	N	6	528.1	0.59	0.16
2*H*-indole	N	13	873.2	0.84	0.18
3*H*-indole	N	14	885.6	0.55	0.16
2*H*-isoindole	**N**	21	1006.3	0.47	0.32
		30	1426.9	0.78	
Indolizine	**N**	12	715.8	0.41	0.30
		26	1222.5	0.37	
7-Azaindazole	**N1**	15	920.8	0.56	0.76
		19	1059.8	1.82	
		21	1160.7	0.50	
		23	1206.8	1.03	
	N2	6	540.4	0.41	0.15
		15	945.3	0.34	
	N3	6	554.3	0.30	0.20
		10	774.0	0.42	
Pyrazolo[1,5-a]- pyrimidine	**N1**	10	681.0	0.76	0.55
		13	827.4	0.52	
		20	1054.1	0.30	
		22	1135.5	0.49	
	N2	10	787.9	0.37	0.22
	N3	7	592.3	0.35	0.19
		13	915.1	0.53	

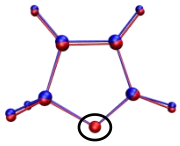
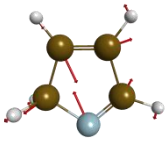
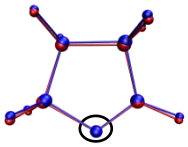
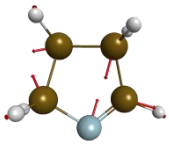
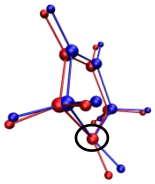
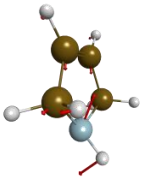
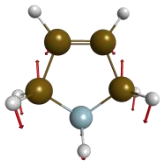
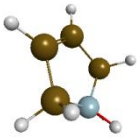
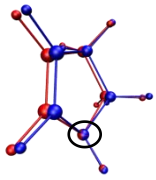
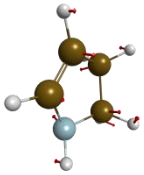
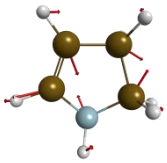
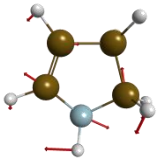
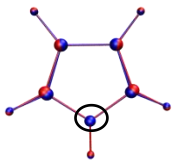
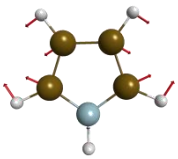
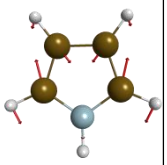
TABLE S3. Simulated vertical (I^{vert}) and adiabatic (I^{ad}) ionization potentials and their difference ($\Delta I = I^{vert} - I^{ad}$), difference in zero-point vibrational energy ($\Delta\varepsilon_0$), and the total reorganization energy (E_r) for all 35 N-heterocycle molecules studied in the three papers.

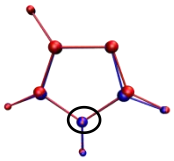
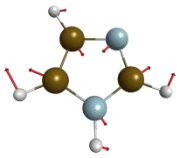
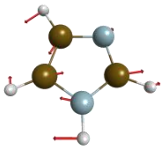
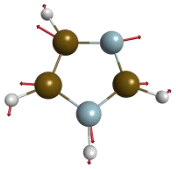
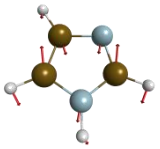
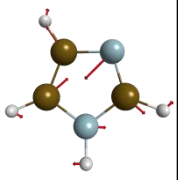
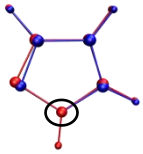
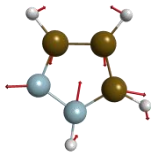
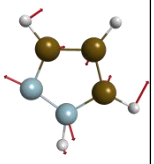
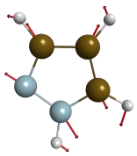
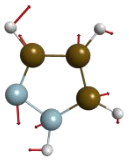
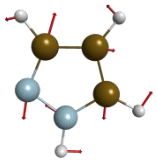
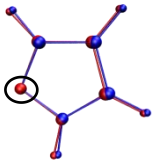
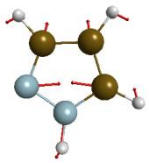
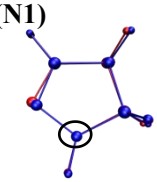
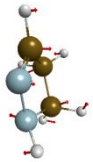
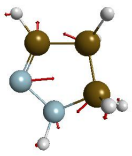
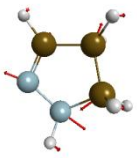
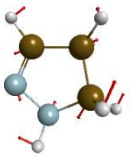
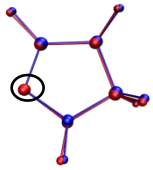
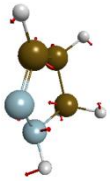
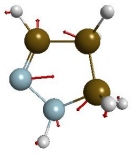
No.	Molecule	Core	I^{vert}	I^{ad}	ΔI	$\Delta\varepsilon_0$	E_r
1	2H-pyrrole		404.20	404.06	0.14	0.04	0.14
2	1-Pyrroline		404.37	404.21	0.16	0.02	0.15
3	3-Pyrroline		404.50	404.21	0.29	0.02	0.59
4	2-Pyrroline		404.84	404.57	0.27	0.00	0.32
5	1H-Pyrrole		406.03	405.76	0.27	-0.03	0.34
6	Imidazole	N1	406.59	406.23	0.36	-0.07	0.58
		N2	404.25	404.06	0.19	0.04	0.18
7	Pyrazole	N1	406.83	406.45	0.38	-0.07	0.61
		N2	405.10	404.94	0.16	0.02	0.16
8	2-Pyrazoline	N1	405.41	405.06	0.35	-0.03	0.51
		N2	405.32	405.16	0.16	0.00	0.16
9	1,3,4-triazole	N1	407.23	406.86	0.37	-0.08	0.52
		N2	405.21	405.04	0.17	0.02	0.17
10	1,2,5-triazole	N1	407.87	407.39	0.48	-0.09	0.63
		N2	405.98	405.80	0.18	-0.01	0.18
11	1,2,4-triazole	N1	407.44	407.02	0.42	0.00	0.53
		N2	405.71	405.53	0.18	0.02	0.18
		N3	407.91	404.69	0.22	-0.03	0.10
12	Pyridine		404.50	404.26	0.24	0.03	0.14
13	Pyrimidine		404.97	404.80	0.17	0.01	0.16
14	Pyrazine		405.24	405.11	0.13	0.01	0.14
15	Pyridazine		405.52	405.34	0.18	0.01	0.18
16	1,3,5-Triazine		405.49	405.30	0.19	-0.01	0.18
17	1,2,4-Triazine	N1	406.33	405.66	0.17	-0.01	0.18
		N2	406.01	405.83	0.18	-0.01	0.20
		N4	405.80	406.16	0.14	-0.01	0.14
18	1,2,4,5-Tetrazine		406.98	406.79	0.19	-0.04	0.21
19	Indole		405.68	405.29	0.39	-0.02	0.46
20	3-Methylindole		405.46	405.11	0.35	-0.01	0.71
21	3-Formylindole		406.24	405.90	0.34	-0.05	0.49
22	Adenine	N1	403.91	403.62	0.29	0.04	0.29
		N2	404.04	403.74	0.30	0.04	0.28
		N3	404.45	404.19	0.26	0.03	0.25
		N4	406.37	405.87	0.50	-0.08	0.80
		N5	405.47	405.10	0.37	-0.04	0.62
23	Purine	N1	404.48	404.27	0.21	0.01	0.22
		N2	404.83	404.60	0.23	0.00	0.23
		N3	404.73	404.49	0.24	0.02	0.23

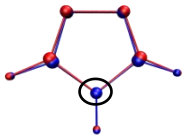
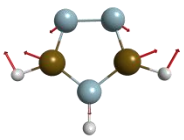
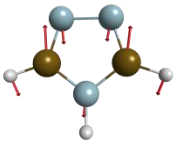
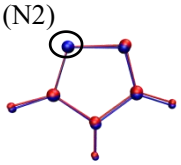
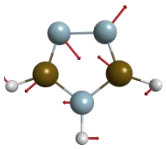
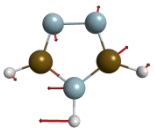
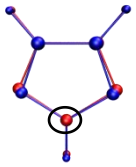
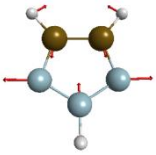
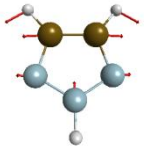
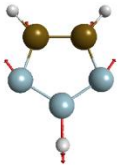
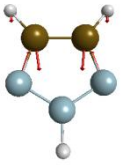
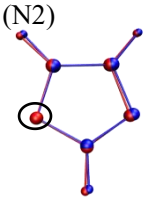
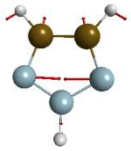
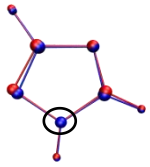
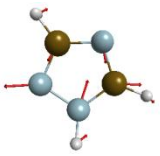
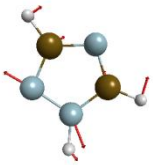
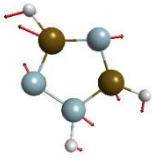
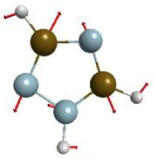
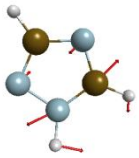
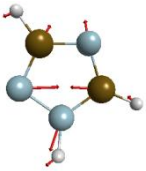
		N4	406.75	406.28	0.47	-0.10	0.91
24	Benzimidazole	N1	406.17	405.76	0.41	-0.08	0.86
		N2	404.00	403.78	0.22	0.04	0.20
25	4-Azaindole	N1	405.98	405.68	0.30	-0.03	0.49
		N2	403.81	403.63	0.18	0.04	0.18
26	5-Azaindole	N1	406.07	405.77	0.30	-0.04	0.42
		N2	403.76	403.57	0.19	0.05	0.19
27	6-Azaindole	N1	406.07	405.77	0.30	-0.04	0.47
		N2	403.77	403.60	0.17	0.04	0.19
28	7-Azaindole	N1	405.82	405.48	0.34	-0.04	0.42
		N2	404.10	403.92	0.18	0.03	0.18
29	1H-isoindole		403.88	403.71	0.17	0.04	0.16
30	2H-indole		403.31	403.13	0.18	0.05	0.18
31	3H-indole		404.52	404.36	0.16	0.00	0.16
32	2H-isoindole		406.07	405.80	0.27	-0.04	0.32
33	Indoline		406.18	405.92	0.26	-0.03	0.30
34	7-Azaindazole	N1	406.43	405.97	0.46	-0.07	0.76
		N2	405.19	405.03	0.16	0.00	0.15
		N3	404.51	404.31	0.20	0.02	0.20
35	Pyrazolo[1,5-a]pyrimidine	N1	407.15	406.75	0.40	-0.07	0.55
		N2	404.66	404.45	0.21	0.01	0.22
		N3	404.80	404.60	0.20	0.02	0.19

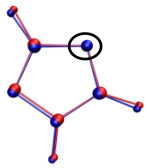
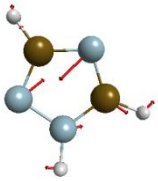
TABLE S4. Superposition of the optimized ground state and the N1s ionized state geometries (*leftmost*) and the ground-state active vibrational modes (*right*) for all 35 molecules studied in three papers of this series. The core ionization center is illustrated with a black circle. Active modes were filtered according to a threshold of HRFs ($S_i \geq 0.3$). Amine (bold) and imine (lightface) N atoms are distinguished in different fonts. For each mode, the mode index and the HRF (in parentheses) are specified. 35 molecules include 11 monocyclic compounds with five-membered rings, 7 monocyclic compounds with six-membered rings, and 17 bicyclic compounds consisting of fused five- and six-membered rings.

Part 1: 11 Monocyclic Compounds with Five-Membered Rings

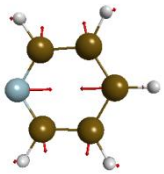
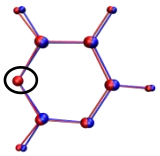
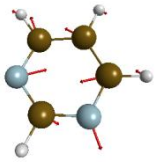
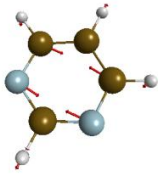
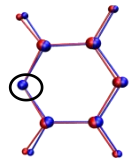
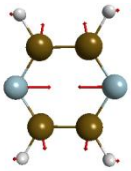
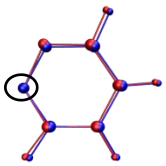
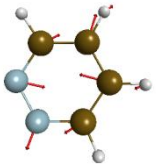
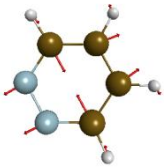
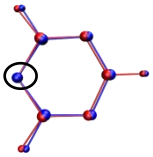
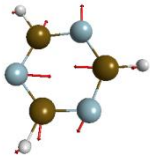
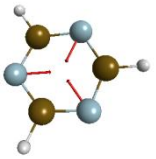
2H-pyrrole (N) 	 4 (S_i=0.70)				
1-Pyrroline (N) 	 5 (S_i=0.41)				
3-Pyrroline **(N)** 	 3 (S_i=1.39)	 19 (S_i=0.85)	 30 (S_i=0.50)		
2-Pyrroline **(N)** 	 1 (S_i=0.65)	 19 (Si=0.33)	 30 (Si=0.36)		
1H-pyrrole **(N)** 	 12 (S_i=0.40)	 18 (S_i=1.03)			

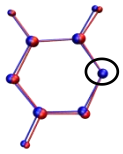
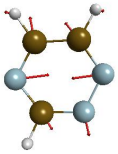
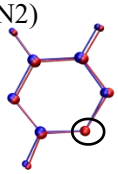
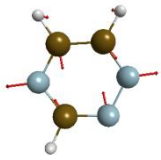
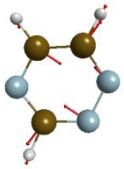
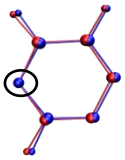
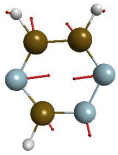
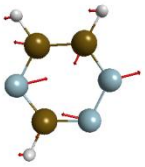
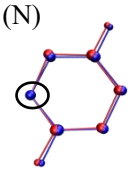
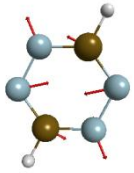
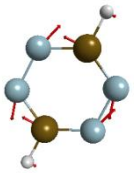
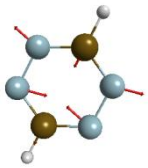
Imidazole **(N1)** 	 9 (S_i=0.36)	 10 (S_i=0.31)	 12 (S_i=0.58)	 16 (S_i=1.73)	
Imidazole (N2) 	 7 (S_i=0.72)				
Pyrazole **(N1)** 	 8 (S_i=0.59)	 9 (S_i=1.32)	 12 (S_i=0.96)	 13 (S_i=0.36)	 14 (S_i=0.59)
Pyrazole (N2) 	 8 (S_i=0.59)				
2-Pyrazoline **(N1)** 	 1 (S_i=0.37)	 6 (S_i=0.70)	 10 (S_i=1.04)	 17 (S_i=0.50)	
2-Pyrazoline (N2) 	 4 (S_i=0.33)	 6 (S_i=0.46)			

1,3,4-Triazole **(N1)** 	 10 (S_i=0.82)	 15 (S_i=1.76)			
1,3,4-Triazole (N2) 	 6 (S_i=0.56)	 15 (S_i=0.30)			
1,2,5-Triazole **(N1)** 	 7 (S_i=1.95)	 8 (S_i=0.45)	 10 (S_i=1.90)	 12 (S_i=0.42)	
1,2,5-Triazole (N2) 	 7 (S_i=0.70)				
1,2,4-Triazole **(N1)** 	 7 (S_i=0.72)	 8 (S_i=1.27)	 10 (S_i=0.50)	 12 (S_i=0.39)	 12 (S_i=0.32)
1,2,4-Triazole (N2) 	 7 (S_i=0.59)				

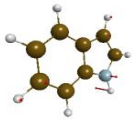
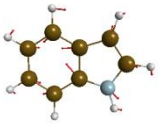
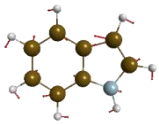
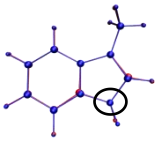
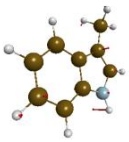
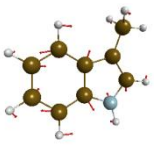
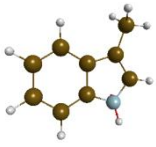
1,2,4-Triazole (N3) 	 6 (S_i=0.84)				

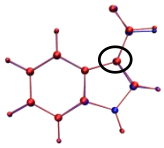
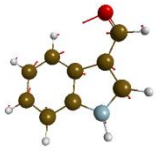
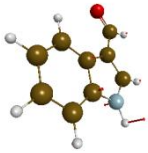
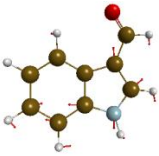
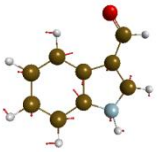
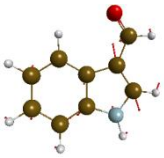
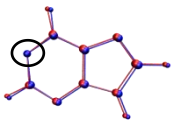
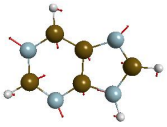
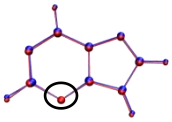
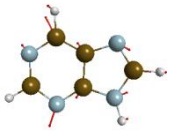
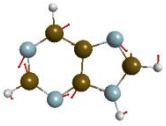
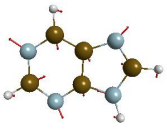
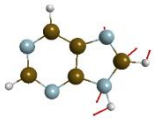
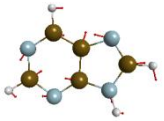
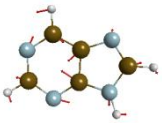
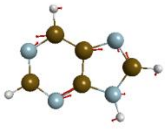
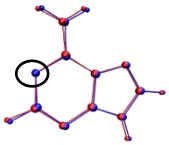
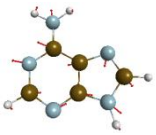
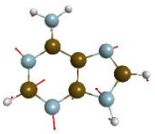
Part 2: 7 Monocyclic Compounds with Six-Membered Rings

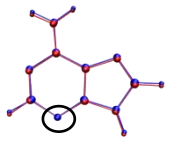
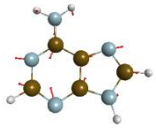
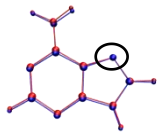
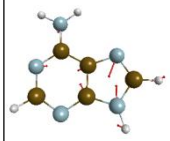
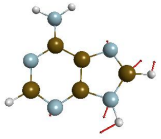
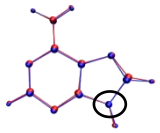
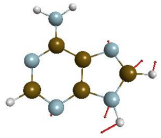
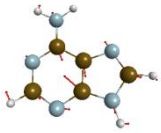
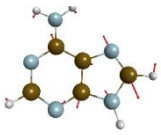
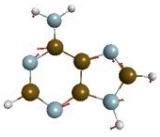
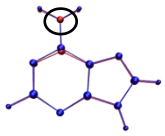
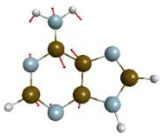
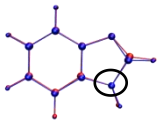
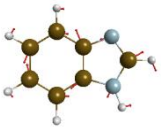
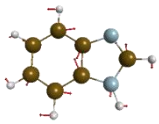
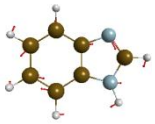
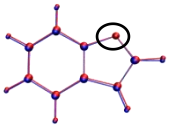
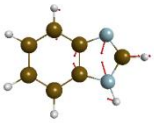
Pyridine (N) 	 3 (S_i=0.92)				
Pyrimidine (N) 	 3 (S_i=0.50)	 4 (S_i=0.30)			
Pyrazine (N) 	 3 (S_i=1.08)				
Pyridazine (N) 	 3 (S_i=0.72)	 11 (S_i=0.40)			
1,3,5-Triazine (N) 	 4 (S_i=0.67)	 11 (S_i=0.35)			

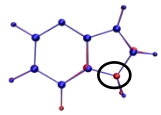
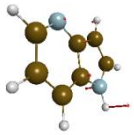
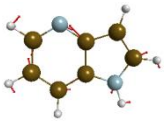
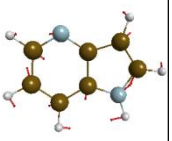
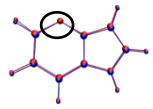
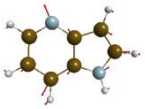
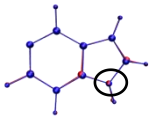
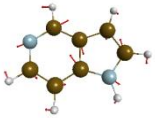
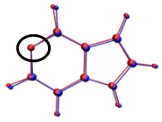
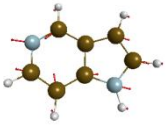
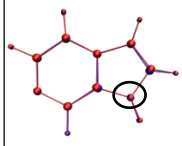
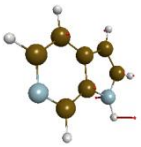
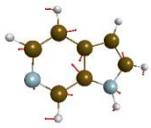
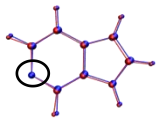
1,2,4-Triazine (N1) 	 3 (S_i=0.91)				
1,2,4-Triazine (N2) 	 3 (S_i=0.39)	 4 (S_i=0.91)			
1,2,4-Triazine (N4) 	 3 (S_i=0.39)	 10 (S_i=0.31)			
1,2,4,5-Tetrazine (N) 	 3 (S_i=0.72)	 7 (S_i=0.48)	 10 (S_i=0.35)		

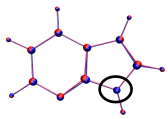
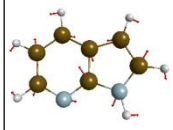
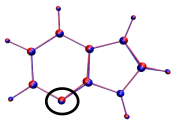
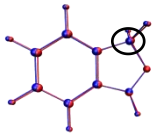
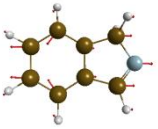
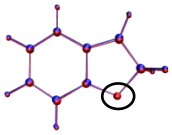
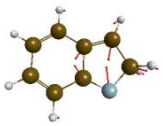
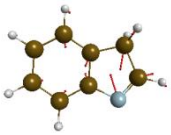
Part 3: 17 Bicyclic Compounds Consisting of Fused Five- and Six-Membered rings

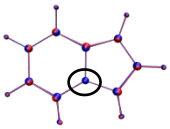
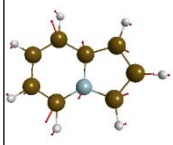
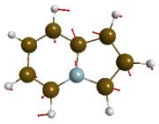
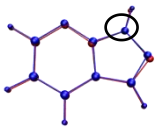
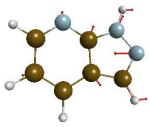
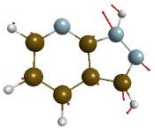
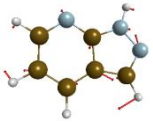
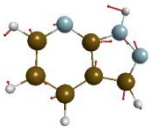
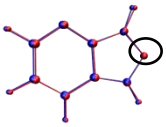
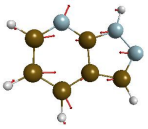
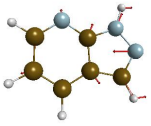
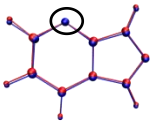
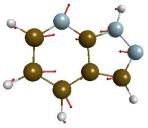
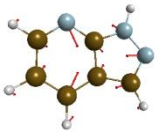
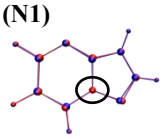
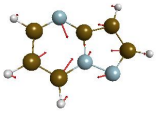
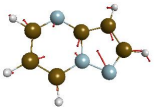
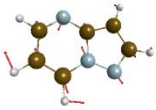
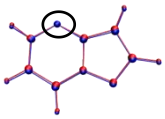
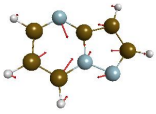
Indole **(N)** 	 3 (S_i=0.40)	 27 (S_i=0.32)	 31 (S_i=0.56)			
3-Methylindole **(N)** 	 6 (S_i=0.58)	 31 (S_i=0.73)	 37 (S_i=0.38)	 51 (S_i=0.69)		

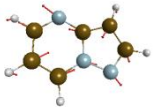
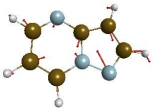
3-Formylindole **(N)** 	 2 (S_i=0.36)	 8 (S_i=0.31)	 31 (S_i=0.45)	 36 (S_i=0.48)	 38 (S_i=0.33)	
Purine (N1) 	 6 (S_i=0.73)	 13 (S_i=0.34)				
Purine (N2) 	 10 (S_i=0.44)	 20 (S_i=0.34)				
Purine (N3) 	 8 (S_i=0.34)	 13 (S_i=0.44)	 14 (S_i=0.42)			
Purine **(N4)** 	 17 (S_i=1.60)	 23 (S_i=0.34)	 24 (S_i=0.45)	 25 (S_i=0.84)	 27 (S_i=0.90)	 29 (S_i=0.66)
Adenine (N1) 	 11 (S_i=0.57)	 17 (S_i=0.31)	 30 (S_i=0.34)			

Adenine (N2) 	 8 (S_i=0.40)					
Adenine (N3) 	 18 (S_i=0.73)	 21 (S_i=0.30)				
Adenine **(N4)** 	 21 (S_i=0.97)	 29 (S_i=0.37)	 31 (S_i=0.78)	 33 (S_i=0.54)		
Adenine **(N5)** 	 27 (S_i=0.33)	 30 (S_i=0.71)	 34 (S_i=1.04)			
Benzimidazole **(N1)** 	 20 (S_i=1.54)	 24 (S_i=0.33)	 27 (S_i=0.86)	 29 (S_i=0.80)	 31 (S_i=0.47)	
Benzimidazole (N2) 	 16 (S_i=0.56)					

4-Azaindole **(N1)** 	 3 (S_i=0.34)	 26 (S_i=0.31)	 29 (S_i=0.30)			
4-Azaindole (N2) 	 11 (S_i=0.51)					
5-Azaindole **(N1)** 	 30 (S_i=0.44)					
5-Azaindole (N2) 	 6 (S_i=0.81)					
6-Azaindole **(N1)** 	 4 (S_i=0.40)	 29 (S_i=0.51)				
6-Azaindole (N2) 	 6 (S_i=0.70)					

7-Azaindole **(N1)** 	 26 (S_i=0.40)	 29 (S_i=0.64)	 33 (S_i=0.34)			
7-Azaindole (N2) 	 11 (S_i=0.44)					
1H-isoindole (N) 	 6 (S_i=0.59)					
2H-indole (N) 	 13 (S_i=0.84)					
3H-indole (N) 	 14 (S_i=0.55)					
2H-isoindole **(N)** 	 21 (S_i=0.47)	 30 (S_i=0.78)				

Indolizine **(N)** 	 12 (S_i=0.41)	 26 (S_i=0.37)				
7-Azaindazole **(N1)** 	 15 (S_i=0.56)	 19 (S_i=1.82)	 21 (S_i=0.50)	 23 (S_i=1.03)		
7-Azaindazole (N2) 	 6 (S_i=0.41)	 15 (S_i=0.34)				
7-Azaindazole (N3) 	 6 (S_i=0.30)	 10 (S_i=0.42)				
Pyrazolo[1,5-a] -pyrimidine **(N1)** 	 10 (S_i=0.76)	 13 (S_i=0.52)	 20 (S_i=0.30)	 22 (S_i=0.49)		
Pyrazolo[1,5-a] -pyrimidine (N2) 	 10 (S_i=0.37)					

Pyrazolo[1,5-a]-pyrimidine (N3) 	 7 (S_i=0.35)	 13 (S_i=0.53)				