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Supplementary Information

Substituent effects and electron delocalization in five-membered N-heterocycles

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Computational details

Geometry optimizations and all electronic structure calculations were performed using DFT with double-hybrid functional at revDSD-PBEP86-G3BJ/def2-TZVPP level of theory[1,2] (tight convergence criteria, UltraFine grid) in Gaussian 16 C.01 program.[3] This functional is one of the most accurate DFT methods as tested in several benchmarks.[1] Vibrational frequencies calculations were performed to confirm that each optimized geometry correspond to the minimum on the potential energy surface. Natural orbital calculations were performed using NBO 7 software.[4]

EDDB is a method which allows a very detailed analysis of electron delocalization directly from the information encoded in the wavefunction. In EDDB the total electron density is decomposed into the densities of electrons localized at atoms (core electrons, lone pairs), localized at chemical bonds, and delocalized between several bonds. The last density is called electron density of delocalized bonds (EDDB), from which the method takes its name. Full theory on how decomposition is performed we refer the readers to the cited articles.[5–8]

The EDDB can be further decomposed into contributions from different delocalization types. $EDDB_G$ (G - global) contains all delocalized electrons, $EDDB_H$ excludes the contribution from bonds with H atoms, while $EDDB_P$ contains only electrons delocalized in cyclic Kekulean pathway (excluding cross-ring delocalization associated in benzene with Dewar forms). Each of the delocalization types can be quantitatively analyzed in terms of contributions from electrons of σ, π and other orbital symmetries. Hence, in this paper, $EDDB_p(\pi)$ are the cyclically delocalized π electrons. The delocalized electron density grids can be visualized in the form of isosurfaces and subtracted from each other. For example, $EDDB_{G\text{-}P} = EDDB_G - EDDB_P$ function is the global electron density minus the cyclically delocalized electron density, in other words, it is a density of non-cyclically delocalized electrons. All EDDB calculations were performed using the density matrices in the NBO basis. EDDB grids were generated in cubegen subprogram available within Gaussian 16 C.01.

HOMA[9,10] and HOMED[11,12] geometric aromaticity indices were calculated from Equation 1:

$$\mathrm{HOMA, HOMED} = 1 - \frac{1}{n}\sum_{j}^{n} \alpha_j \left(d_{\mathrm{o,j}} - d_{\mathrm{j}}\right)^2 \qquad (1)$$

where *n* is the number of bonds in considered fragment, α_j is the normalization constant for *j* bond, for HOMA tabularized (but can also be calculated for specific computational level, Equation 2).

$$\alpha_j = 2\{(d_{\mathrm{o}} - d_{\mathrm{s}})^2 + (d_{\mathrm{o}} - d_{\mathrm{d}})^2\}^{-1} \qquad (2)$$

For HOMED, if the number of bonds considered is even, Equation 1 is also used. However, if the fragment has odd number of bonds, α_j in HOMED is calculated from Equations 3 or 4:

for a system with *i* double bonds and *i*+1 single bonds:

$$\alpha_j = (2i+1) \cdot \{(i+1)(d_{\mathrm{o}} - d_{\mathrm{s}})^2 + i(d_{\mathrm{o}} - d_{\mathrm{d}})^2\}^{-1} \qquad (3)$$

for a system with *i*+1 double bonds and *i* single bonds:

$$\alpha_j = (2i+1) \cdot \{i(d_{\mathrm{o}} - d_{\mathrm{s}})^2 + (i+1)(d_{\mathrm{o}} - d_{\mathrm{d}})^2\}^{-1} \qquad (4)$$

In this paper HOMA was calculated using standard parameters,[10] while HOMED was parametrized at revDSD-PBEP86-G3BJ/def2-TZVPP level of theory, using reference systems proposed by Raczynska.[11] The reference

bond lengths are provided in the Table S9. Calculation of HOMA and HOMED values, as well as EDDB grid subtraction was performed in Multiwfn program.[13]

Anisotropy of the induced current density (AICD)[14] maps were generated using Gaussian and AICD 3.03 program at B3LYP/6-311+G(d,p), NMR=CSGT, with contribution of all orbitals.

Electron donating and withdrawing properties were assessed using the cSAR method. cSAR of substituent X is calculated from Equation 5:

$$\mathrm{cSAR(X)} = q(\mathrm{X}) + q(ipso) \qquad (5)$$

where q(X) is the sum of charges at all atoms of X, and q(*ipso*) is the charge at the *ipso* atom of the substituted system, the atom to which X is attached. In this paper, Hirshfeld atomic charges were used.[15]

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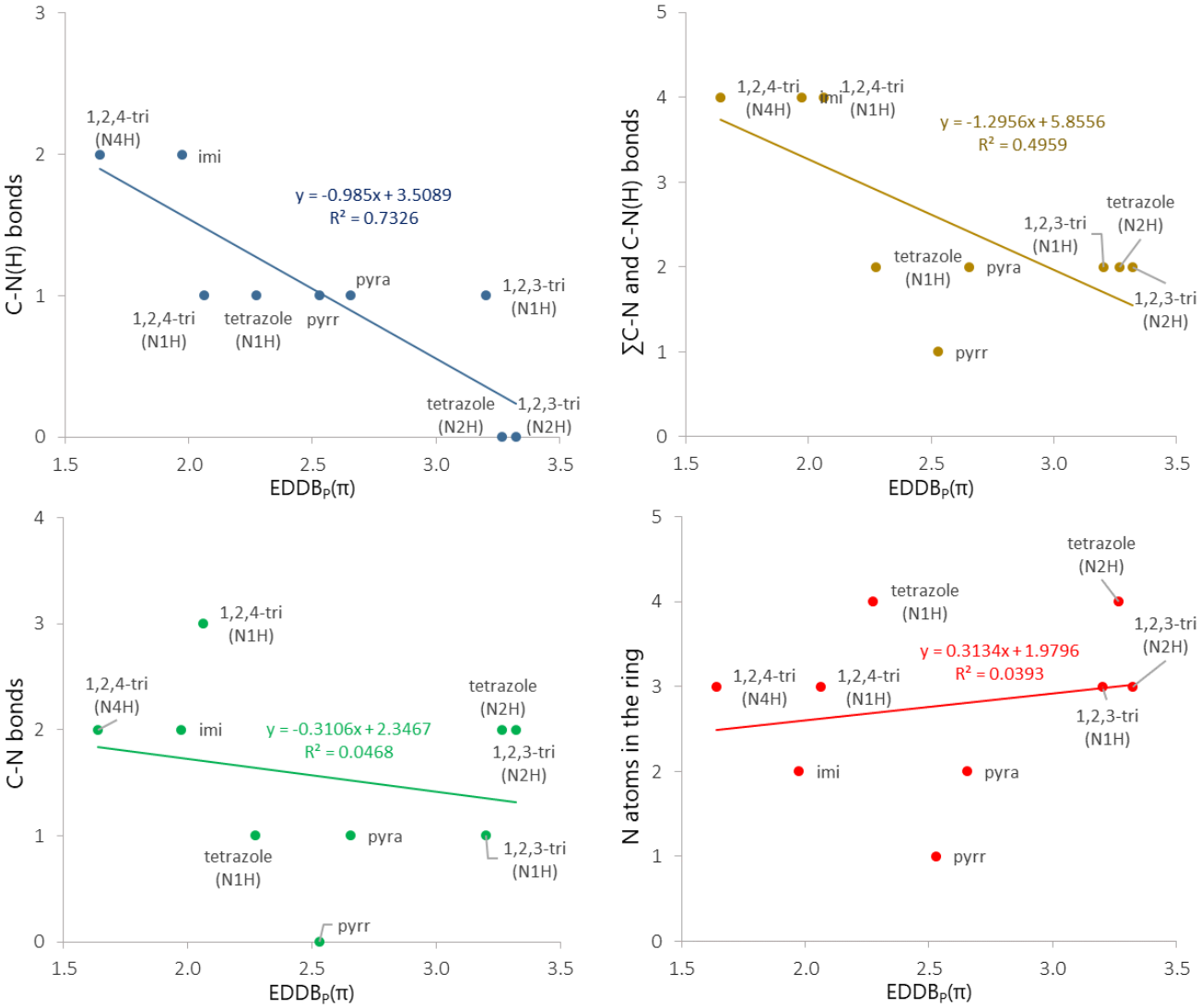
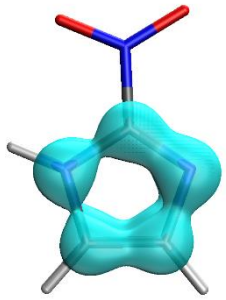
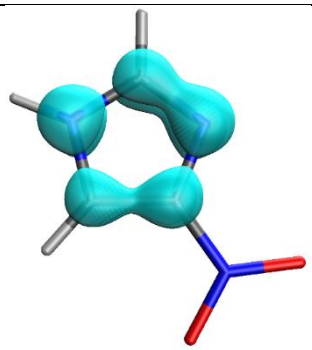
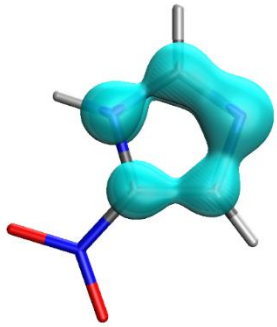
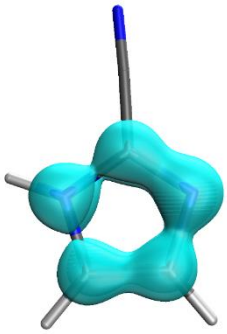
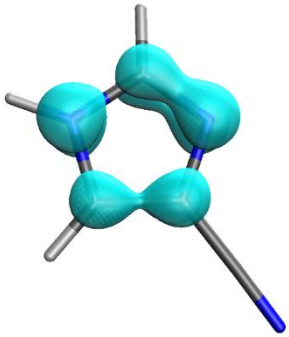
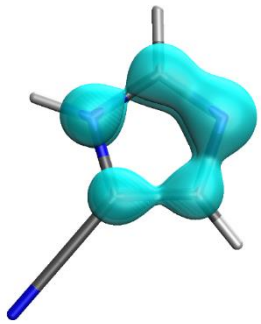
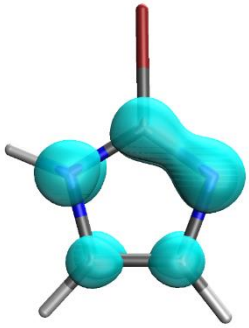
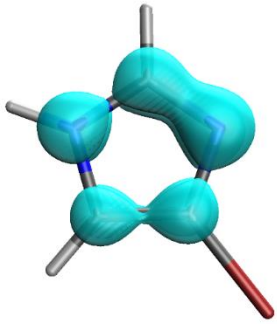
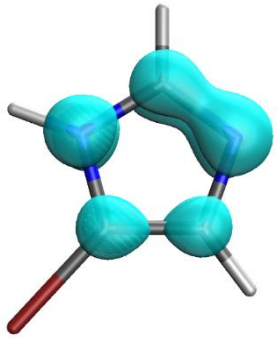
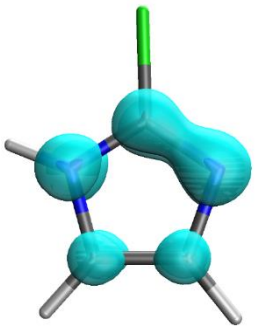
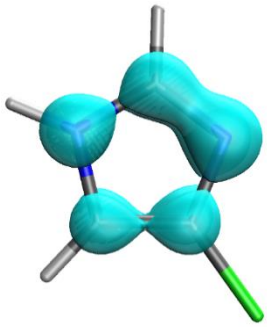
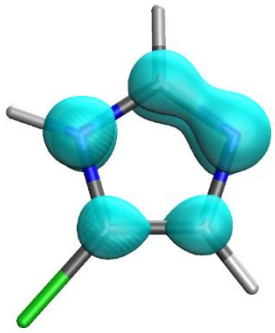


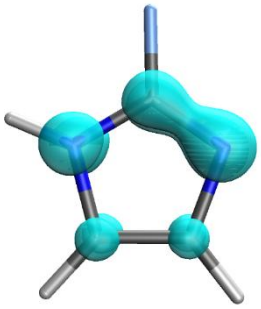
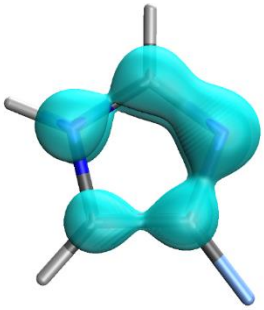
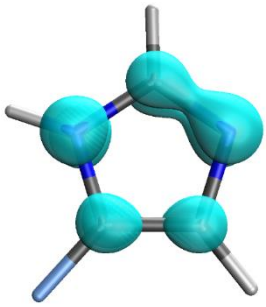
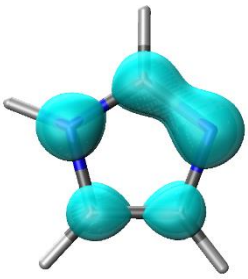
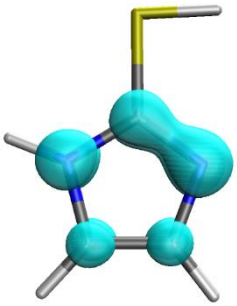
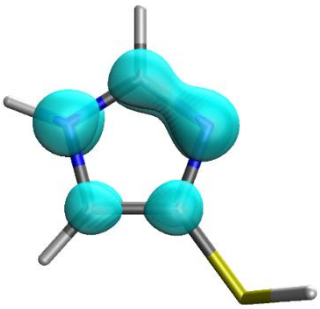
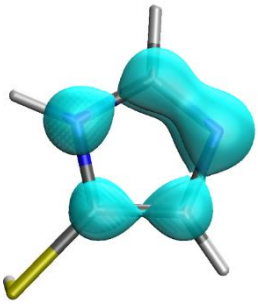
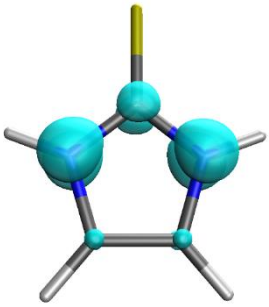
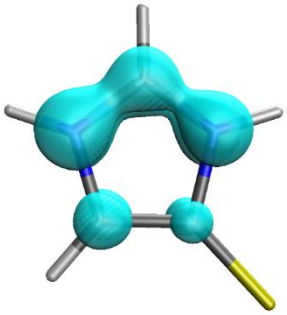
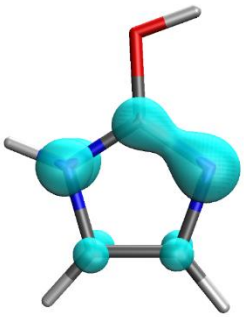
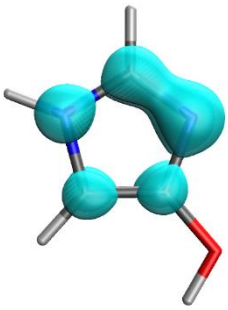
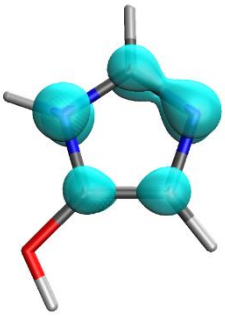
Figure S1. Relations between characteristics of five-membered N-heterocyclic rings and number of cyclically delocalized electrons, $EDDB_P(\pi)$.

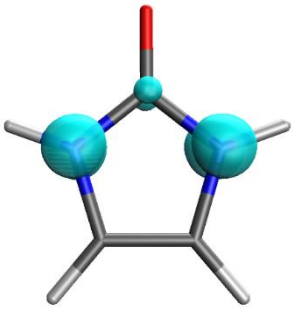
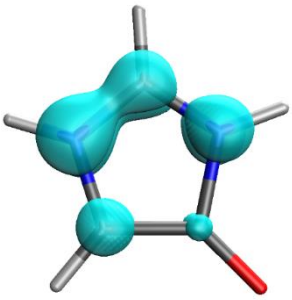
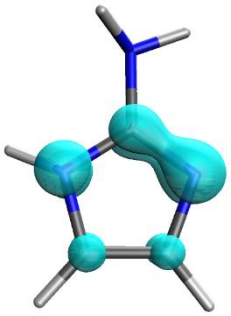
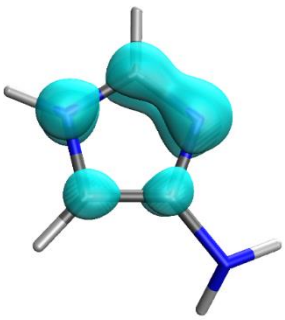
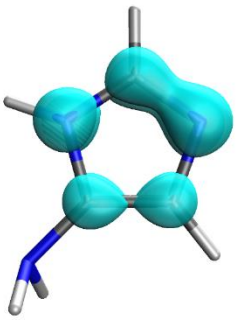
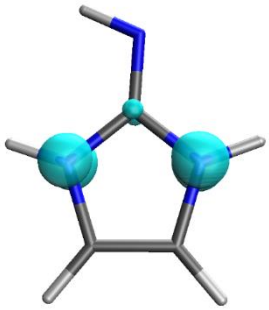
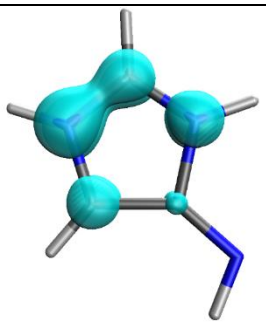
Table S1. Coefficients *a* (slope) and R^2 of linear correlations $EDDB_P(\pi)$ vs cSAR(X) presented in Figure 2.

	a	R^2
imiC2	-6.865	0.919
1,2,4-triC3 (N1H)	-5.014	0.872
pyraC3	-4.962	0.902
pyraC5	-4.252	0.785
1,2,4-triC5	-3.844	0.882
1,2,4-triC3 (N4H)	-3.703	0.926
pyrrC2	-2.621	0.448
1,2,3-triC5	-2.421	0.768
1,2,3-triC4 (N2H)	-2.383	0.290
imiC5	-2.070	0.724
imiC4	-2.018	0.781
pyrrC3	0.065	0.001
1,2,3-triC4 (N1H)	0.523	0.081
pyraC4	3.751	0.842

Table S2. Isosurfaces of $EDDB_P(\pi)$ function (0.02), representing the density of cyclically delocalized π-electrons.

X	imiC2	imiC4	imiC5
NO_2	 2.701	 2.147	 2.257
CN	 2.625	 2.054	 2.145
Br	 1.762	 2.056	 1.886
Cl	 1.708	 2.048	 1.868

F	 1.264	 1.950	 1.708
H	 **1.974**		
SH	 1.596	 1.823	 2.020
=S	 0.831	 1.310	
OH	 1.150	 1.687	 1.636

=O	 0.605	 0.896	
NH_2	 1.256	 1.624	 1.947
=NH	 0.583	 0.889	
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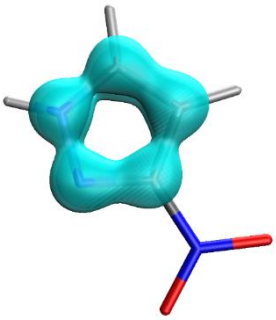
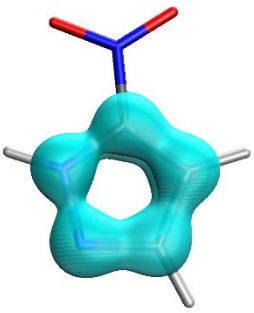
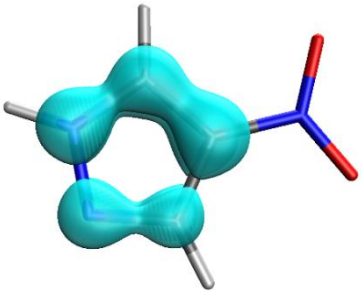
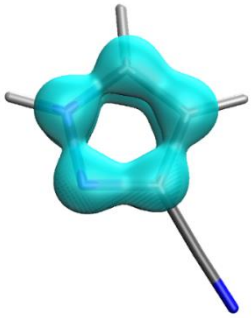
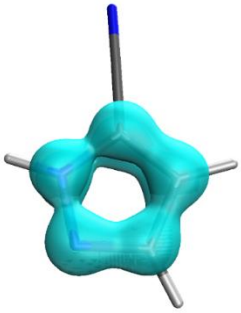
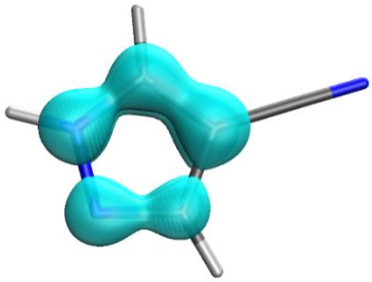
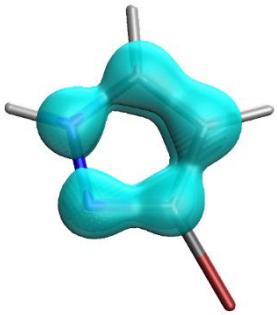
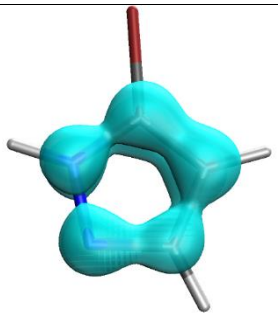
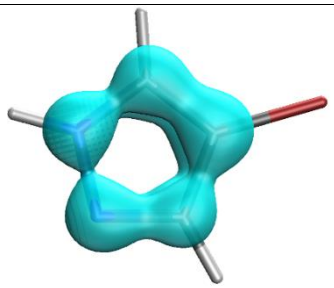
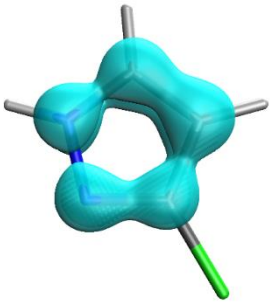
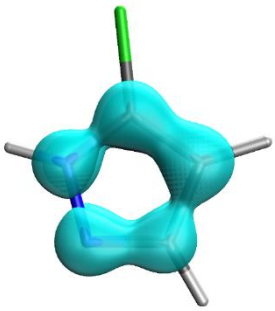
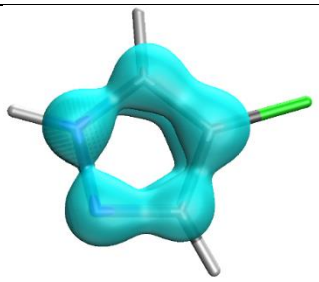
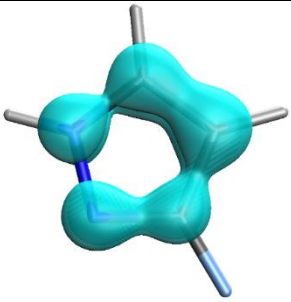
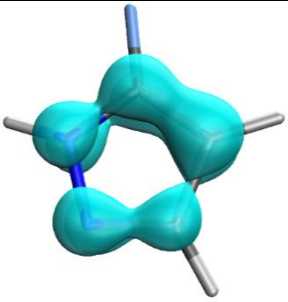
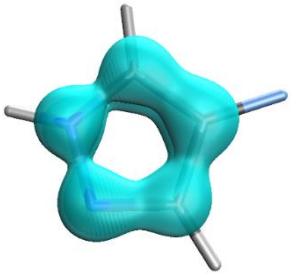
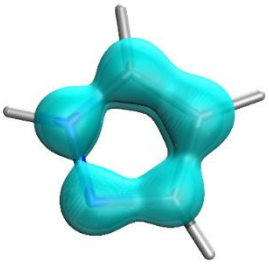
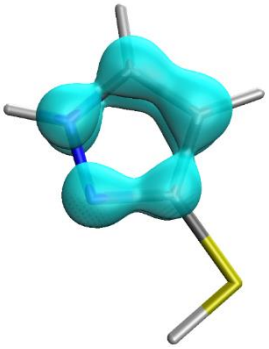
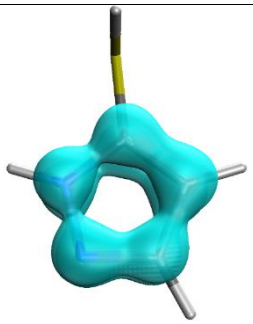
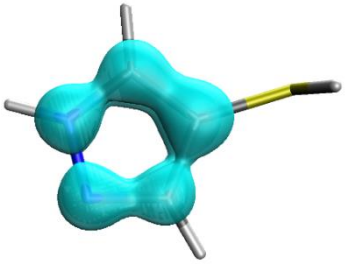
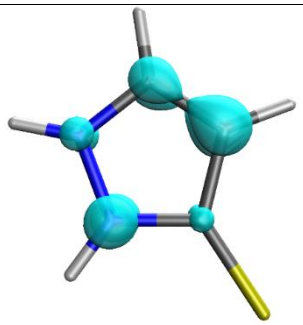
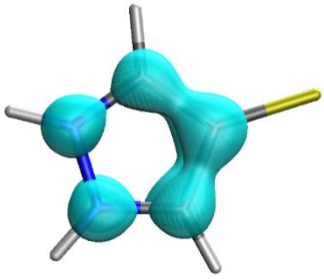
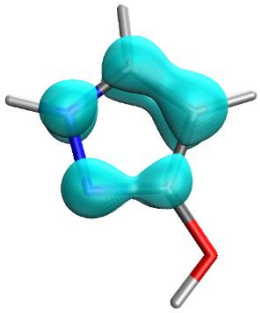
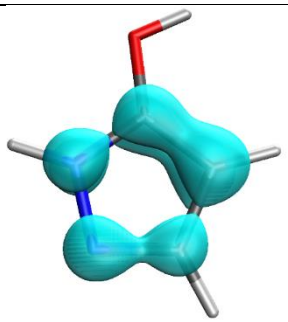
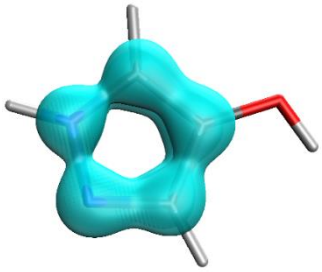
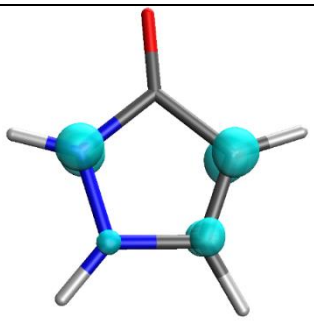
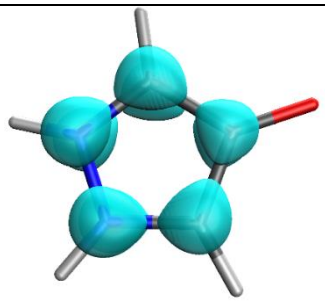
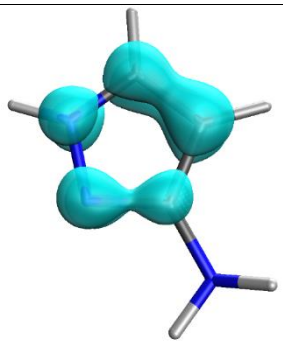
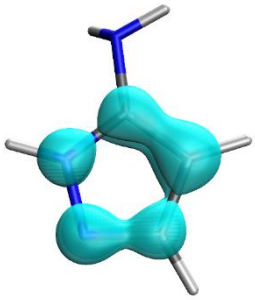
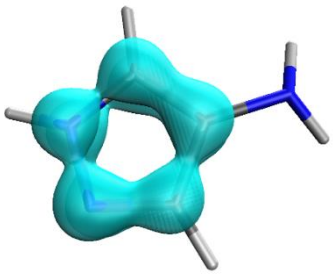
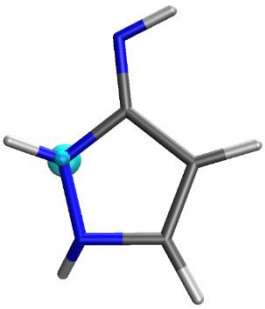
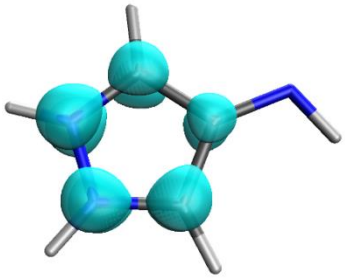
NO_2	 2.884	 3.094	 1.995
CN	 2.847	 2.944	 2.079

Br	 2.604	 2.528	 2.541
Cl	 2.521	 2.487	 2.568
F	 2.150	 2.128	 2.846
H	 2.656		
SH	 2.314	 2.861	 2.339

=S	 0.762		 2.225
OH	 1.824	 2.037	 2.905
=O	 0.491		 2.050
NH_2	 1.811	 2.159	 2.786
=NH	 0.011		 1.775
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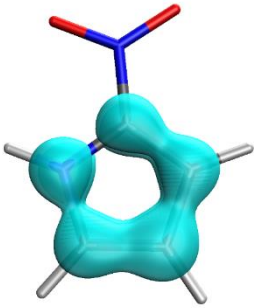
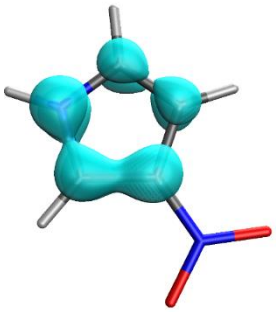
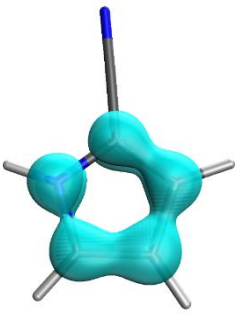
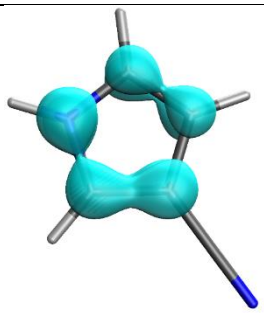
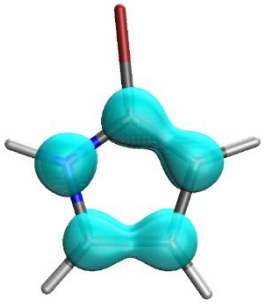
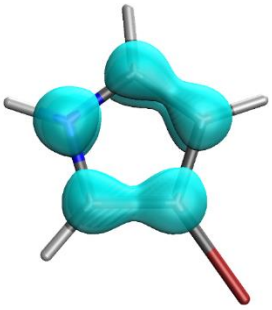
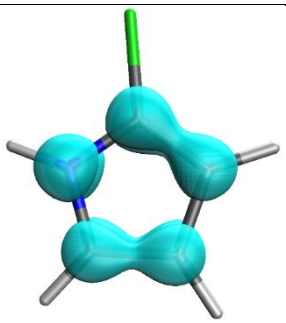
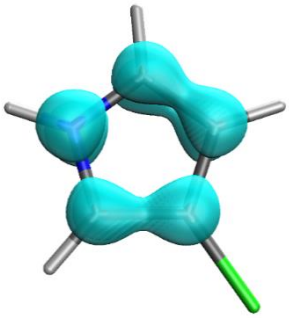
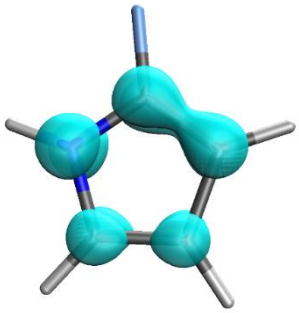
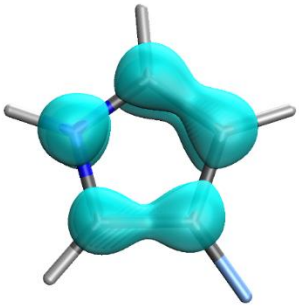
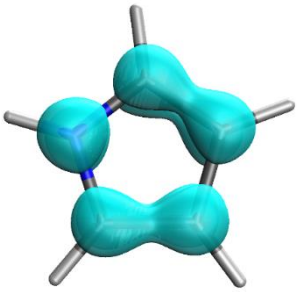
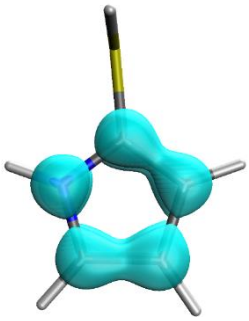
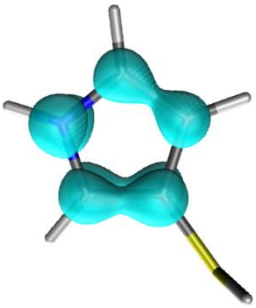
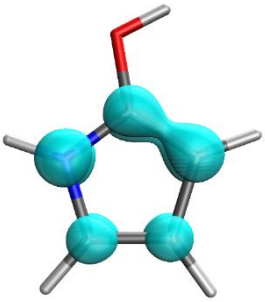
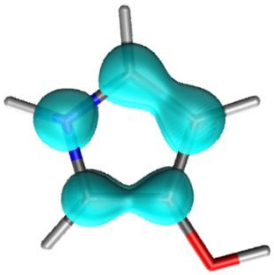
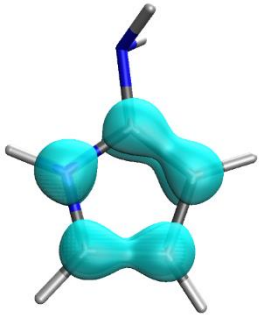
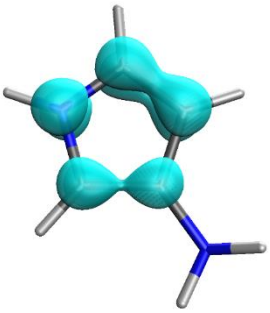
NO_2	 2.647	 2.031
CN	 2.609	 2.115
Br	 2.394	 2.462
Cl	 2.338	 2.444
F	 1.868	 2.321

H	 2.529		
SH	 2.602	 2.322	
OH	 1.728	 2.160	
NH_2	 2.459	 1.986	
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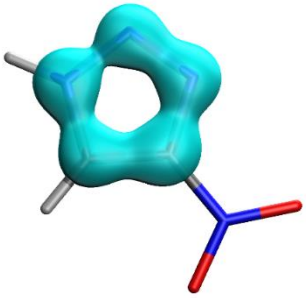
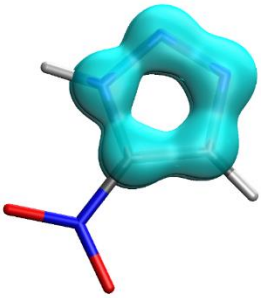
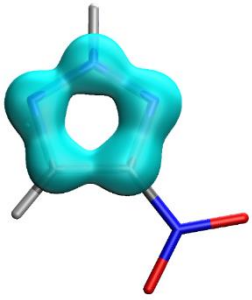
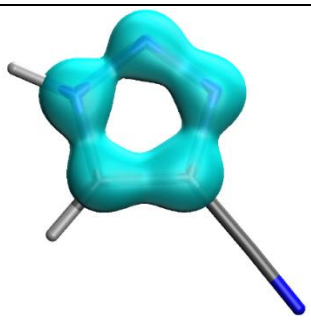
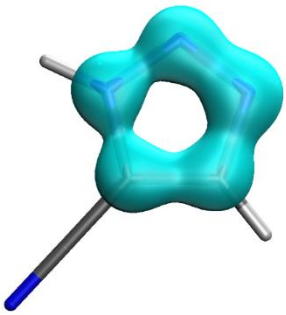
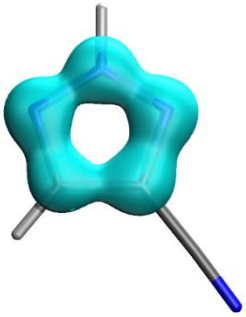
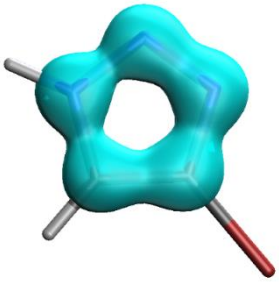
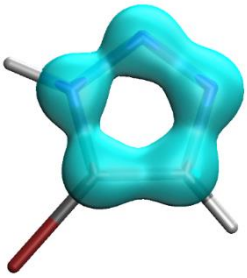
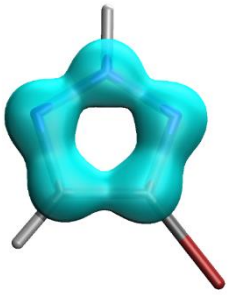
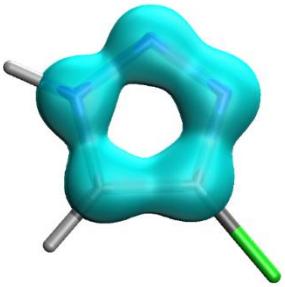
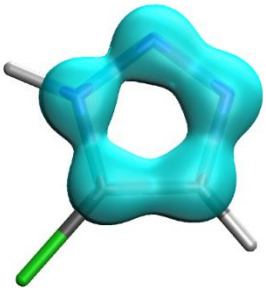
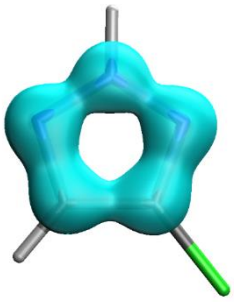
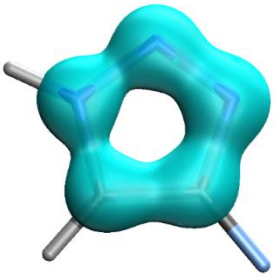
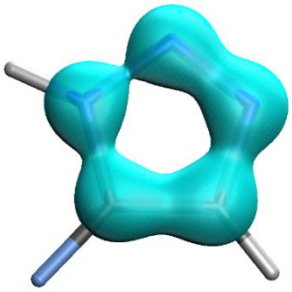
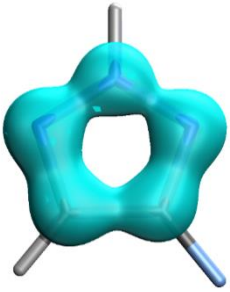
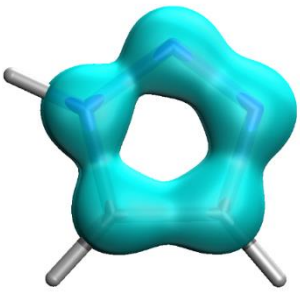
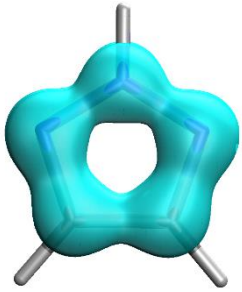
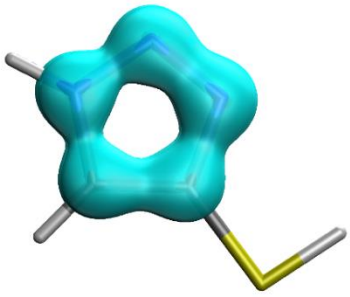
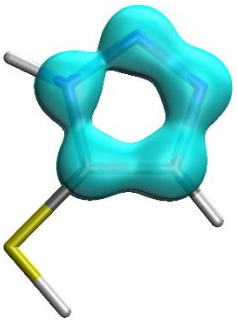
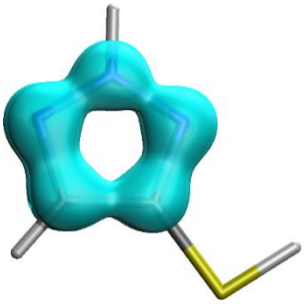
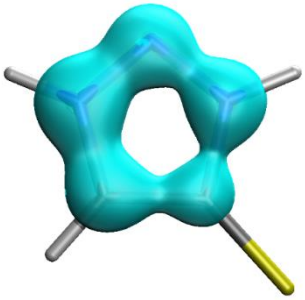
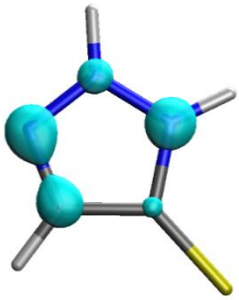
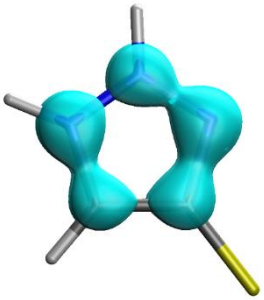
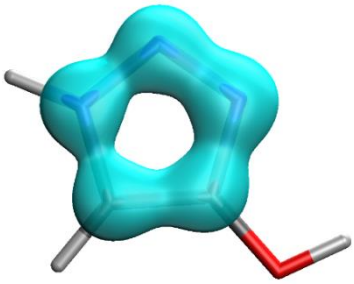
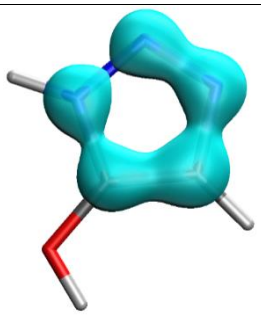
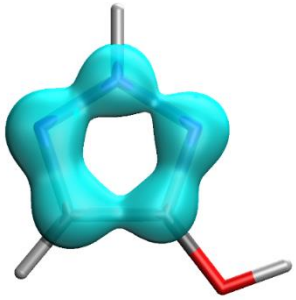
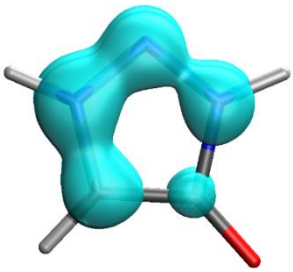
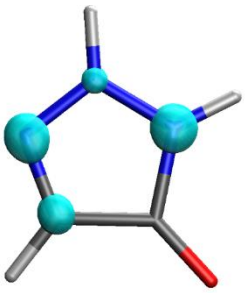
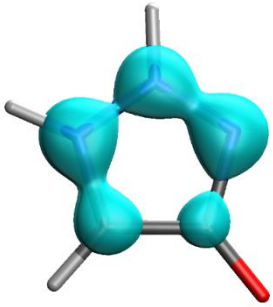
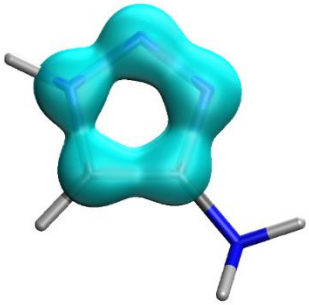
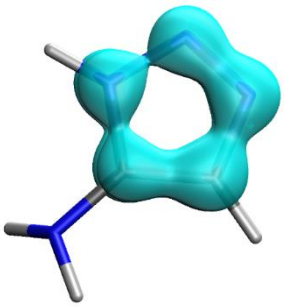
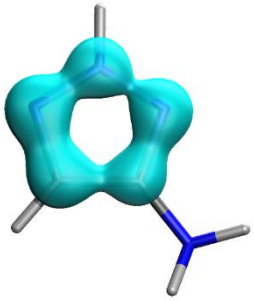
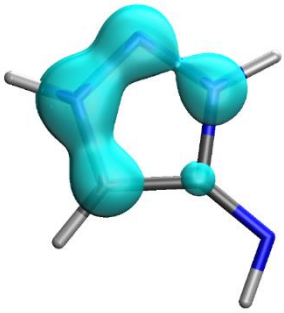
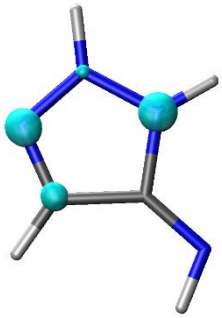
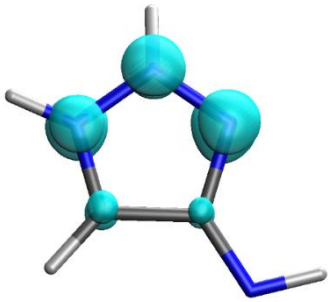
NO_2	 2.992	 3.190	 3.028

CN	 2.911	 3.124	 3.110
Br	 3.176	 3.100	 3.268
Cl	 3.192	 3.047	 3.230
F	 3.358	 2.780	 2.922
H	 3.202		 3.322

SH	 3.151	 2.886	 3.071
=S	 2.222	 0.803	 2.203
OH	 3.108	 2.602	 2.453
=O	 1.365	 0.471	 1.581
NH_2	 2.950	 2.604	 2.459

=NH	 1.113	 0.406	 0.982
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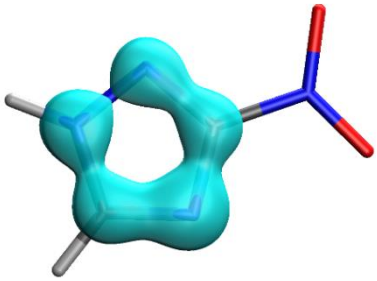
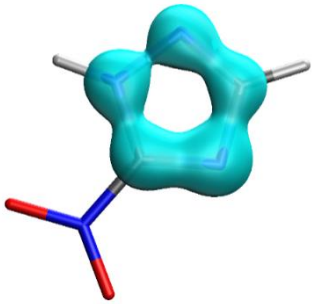
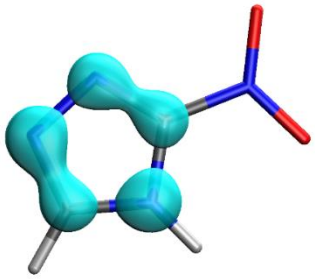
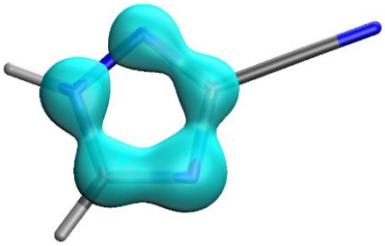
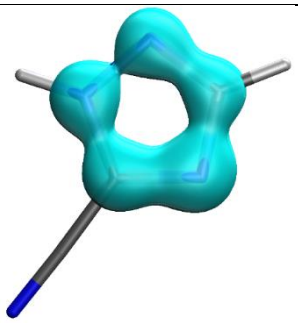
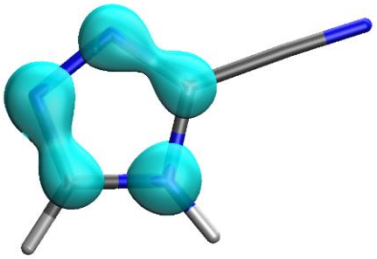
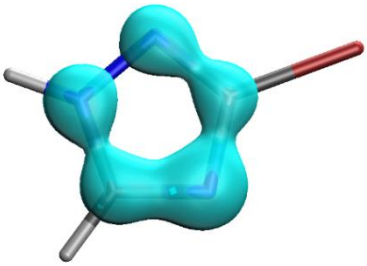
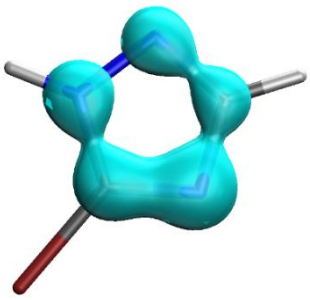
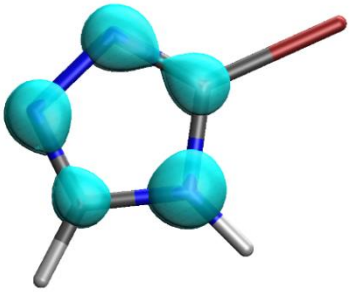
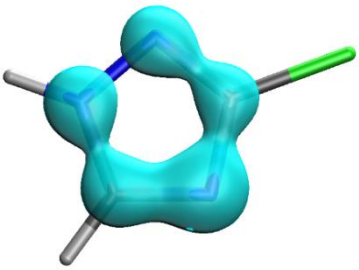
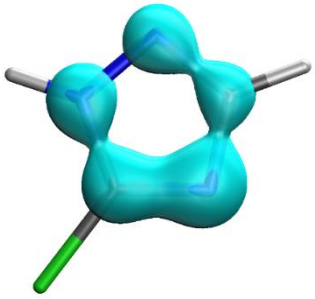
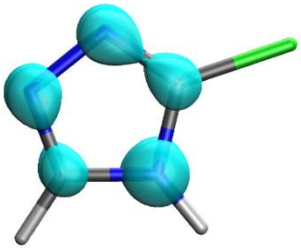
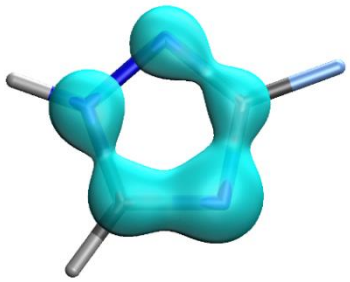
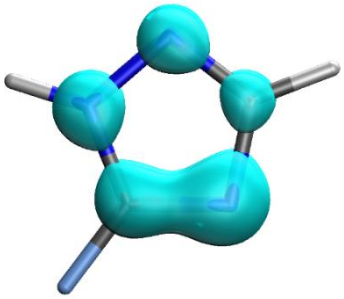
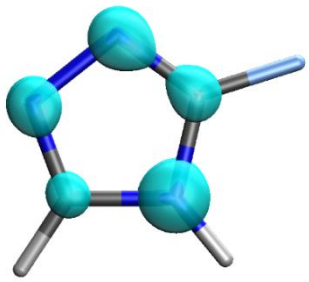
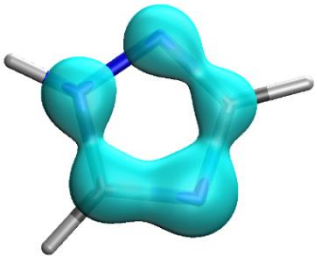
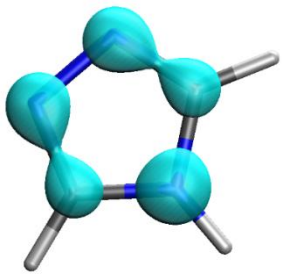
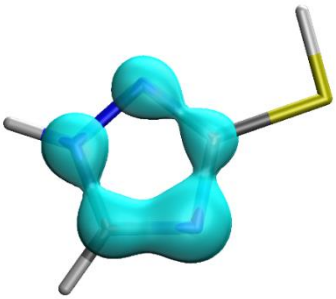
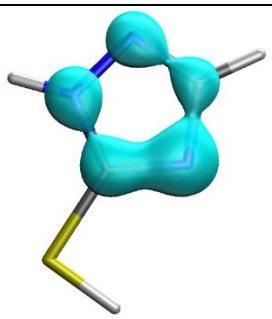
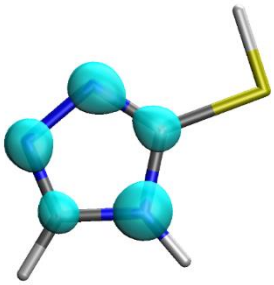
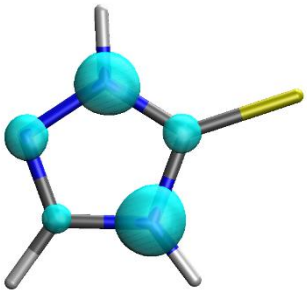
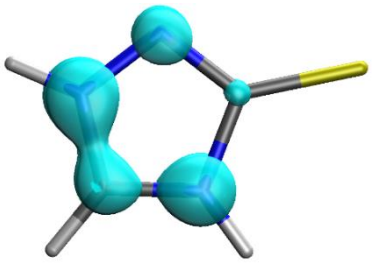
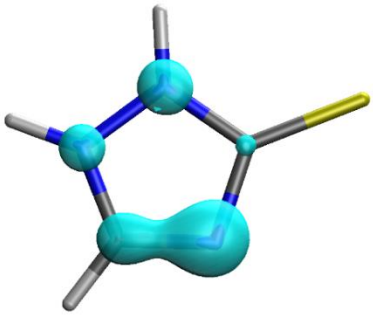
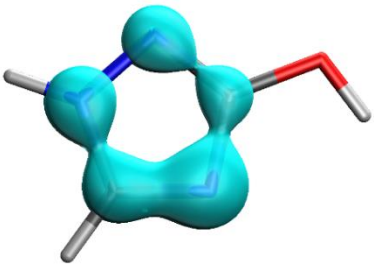
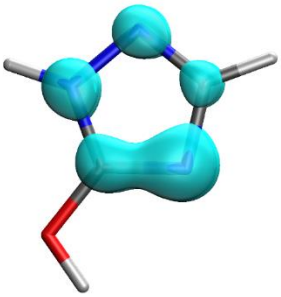
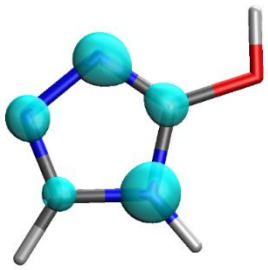
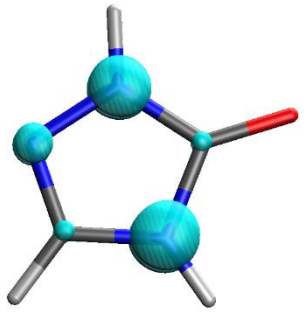
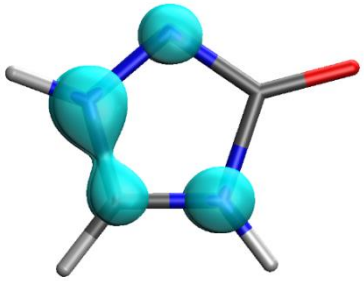
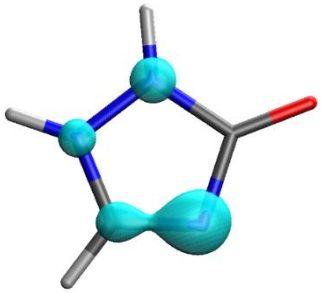
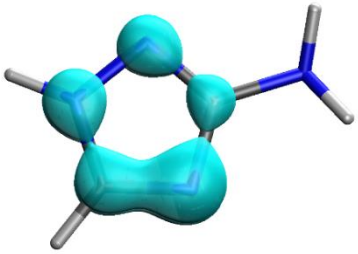
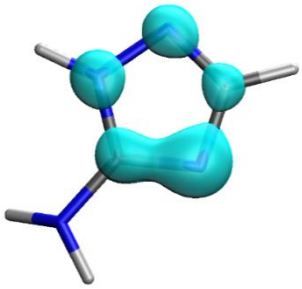
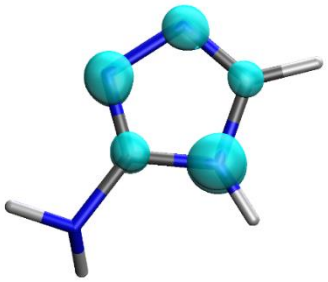
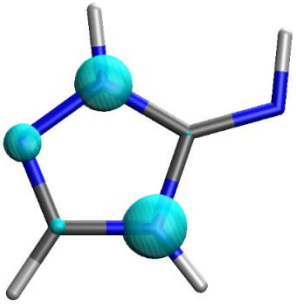
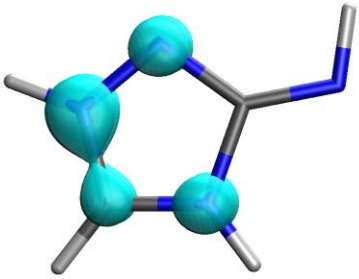
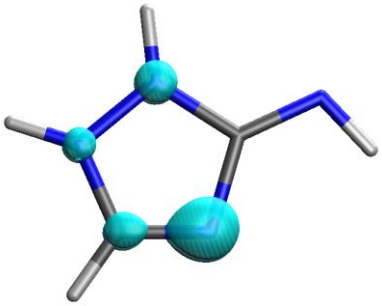
NO_2	 2.346	 2.511	 1.920
CN	 2.212	 2.498	 1.886
Br	 2.100	 1.884	 1.504
Cl	 2.046	 1.847	 1.469

F	 1.842	 1.507	 1.174
H	 2.063		 1.639
SH	 1.857	 1.772	 1.370
=S	 0.930	 0.853	 0.825
OH	 1.587	 1.443	 1.066

=O	 0.713	 0.564	 0.474
NH_2	 1.487	 1.506	 1.145
=NH	 0.619	 0.562	 0.403

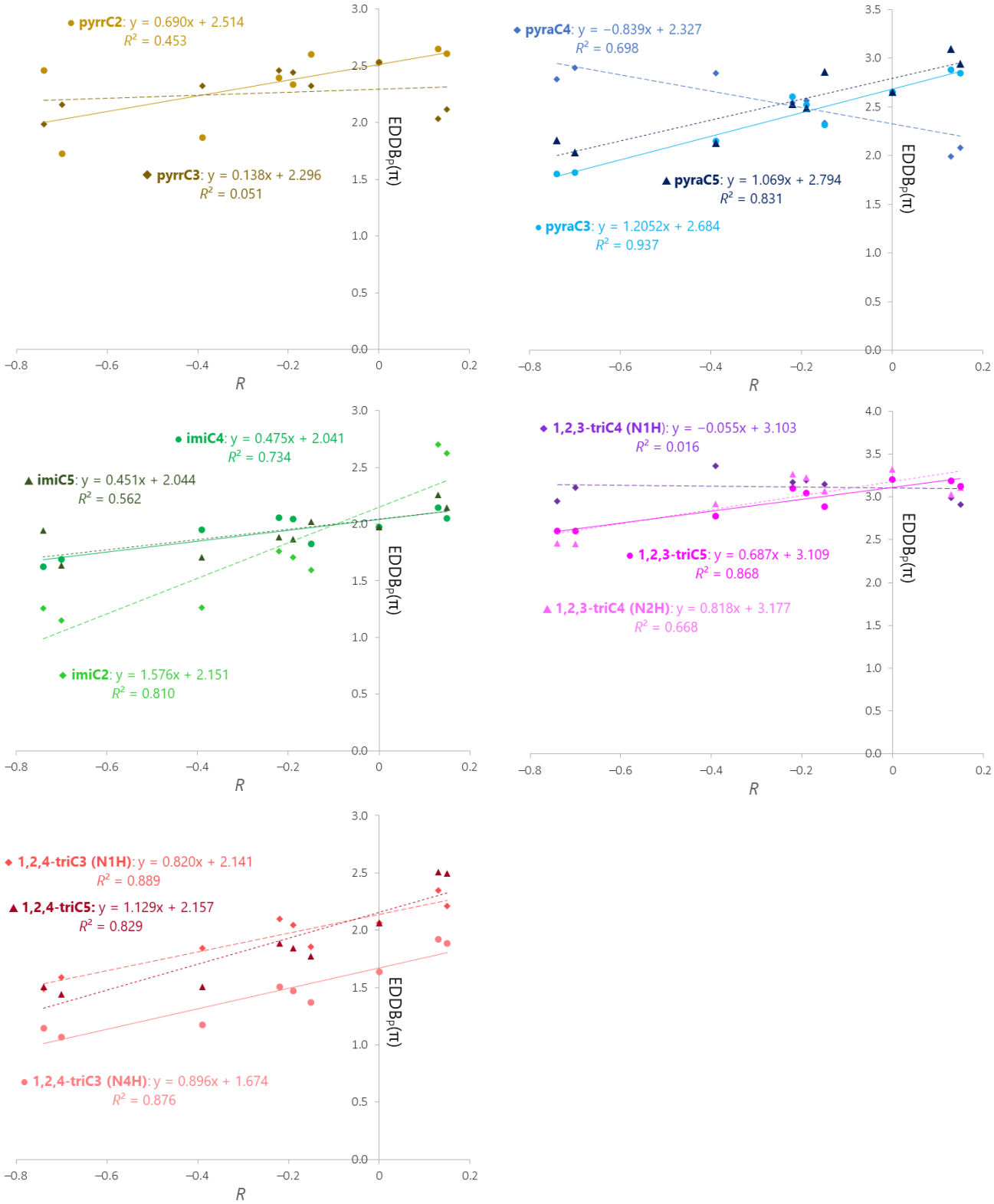
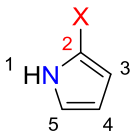
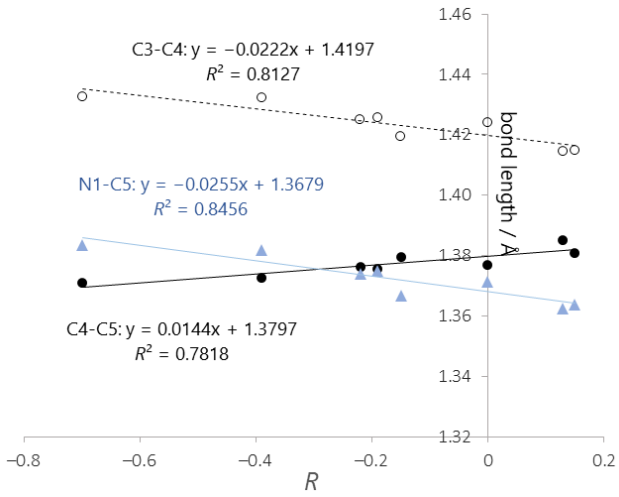
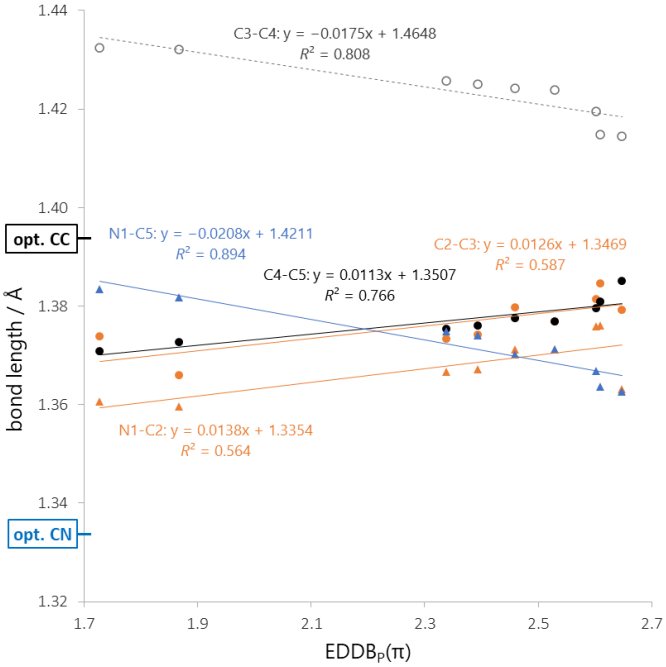


Figure S2. Relationships between $EDDB_P(\pi)$ and resonance substituent constant *R*.

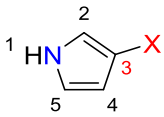
pyrrC2

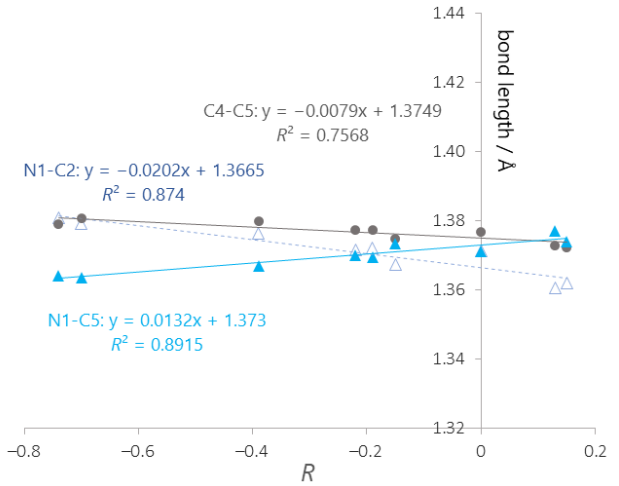


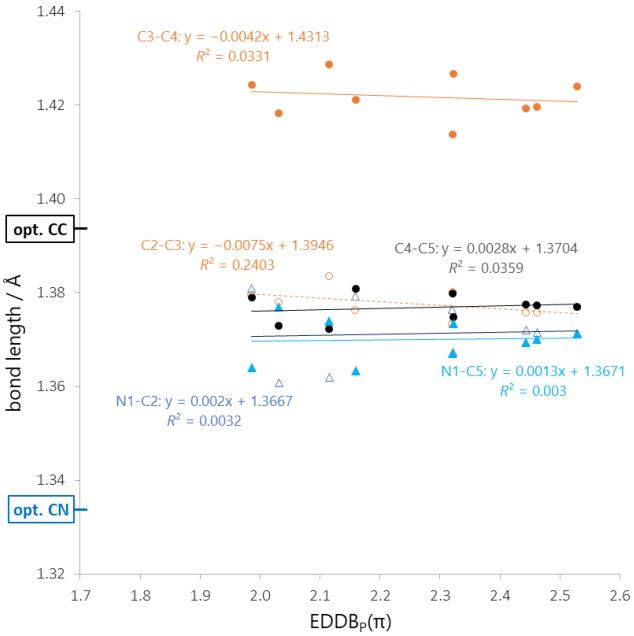




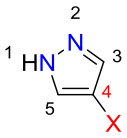
pyrrC3

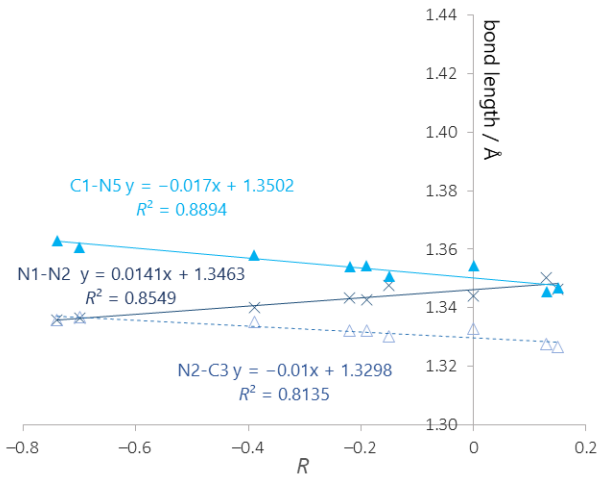


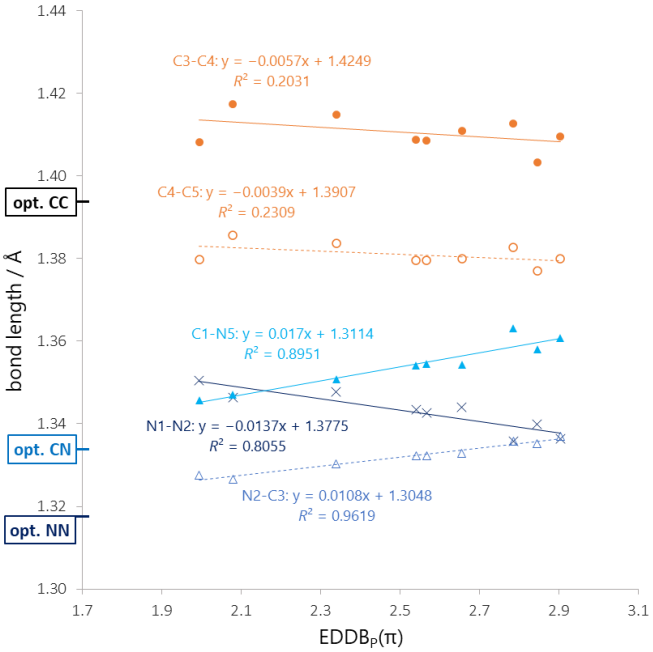




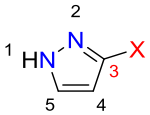
pyraC4

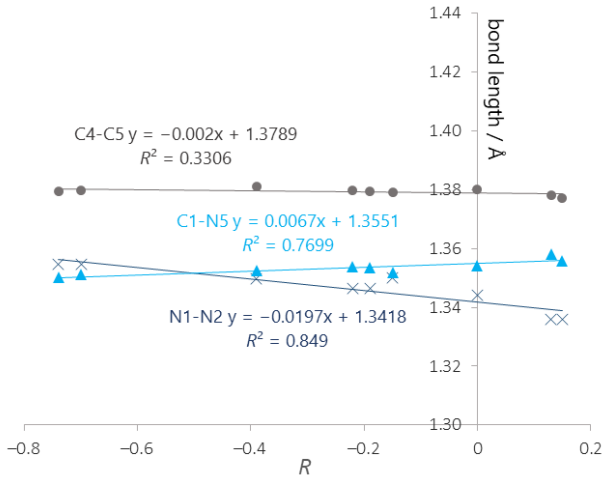


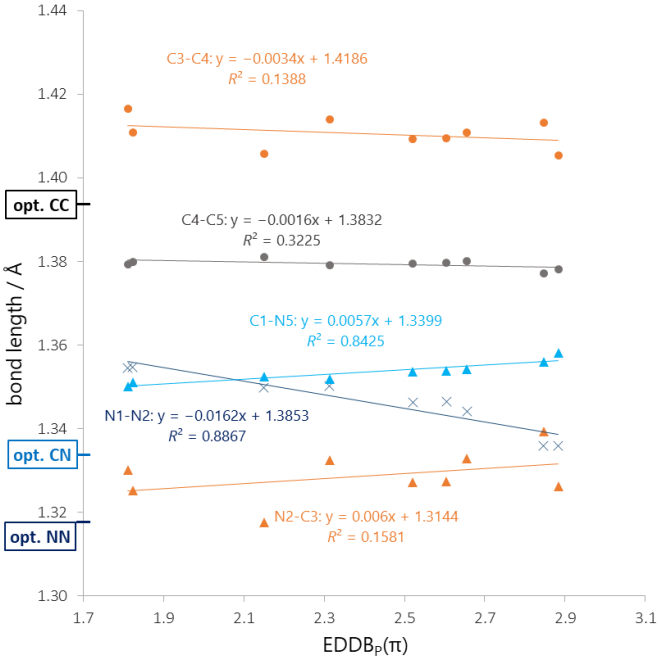




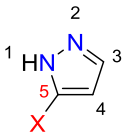
pyraC3

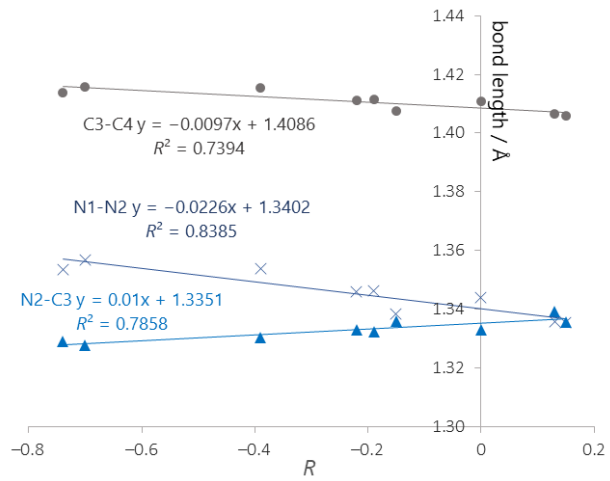


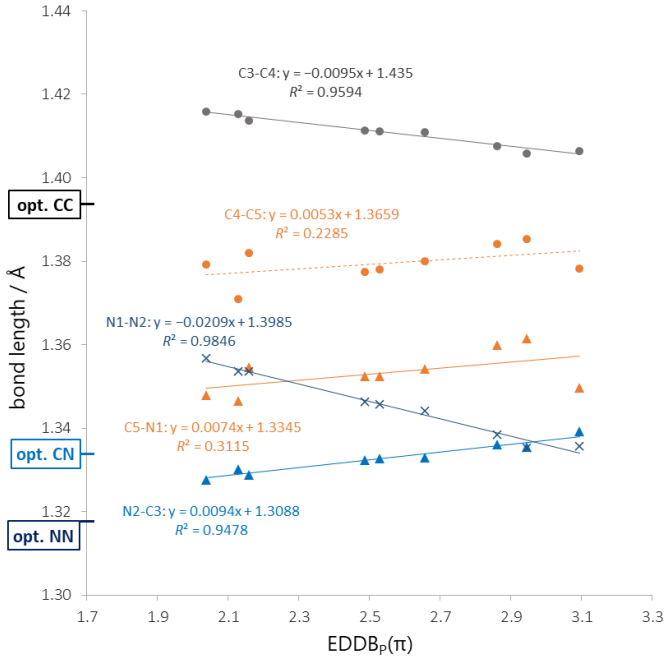




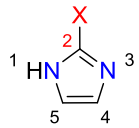
pyraC5

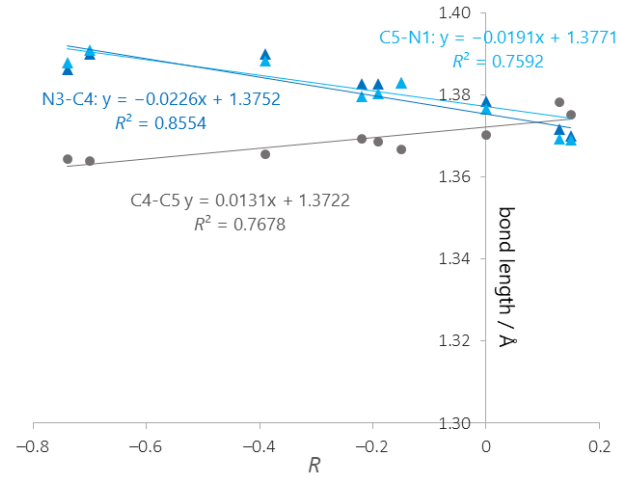


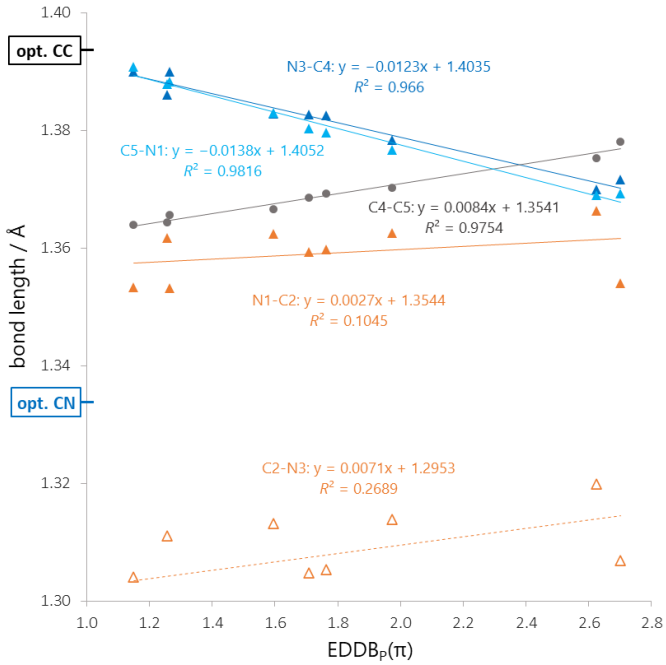




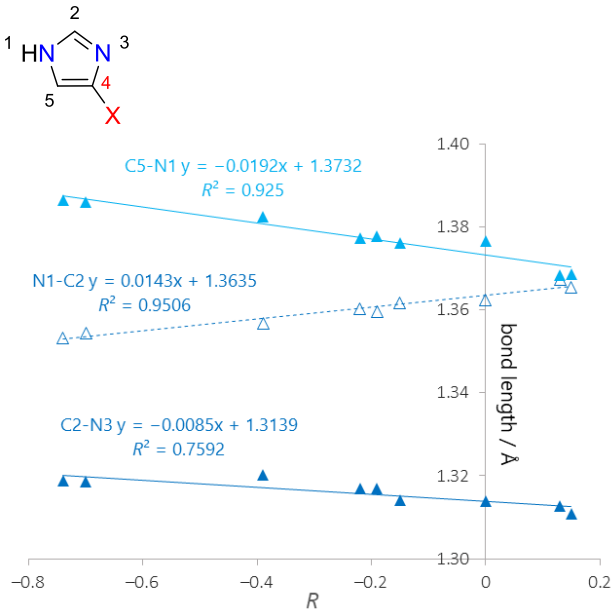
imiC2

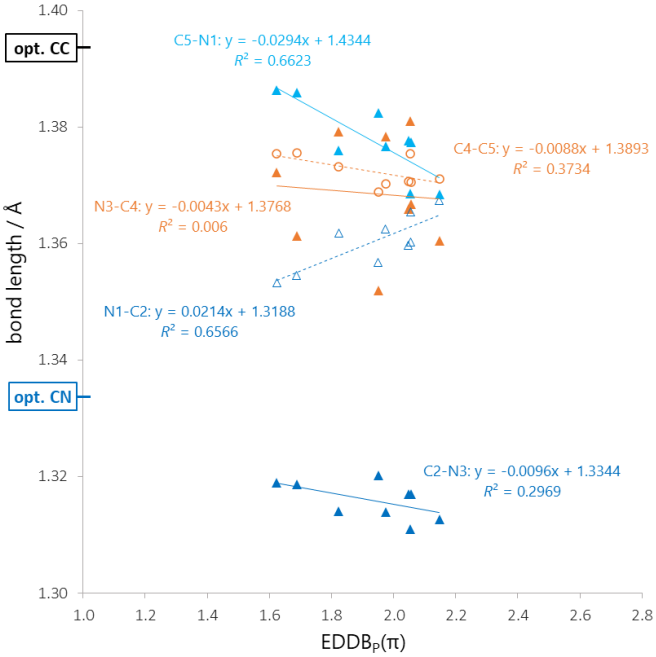




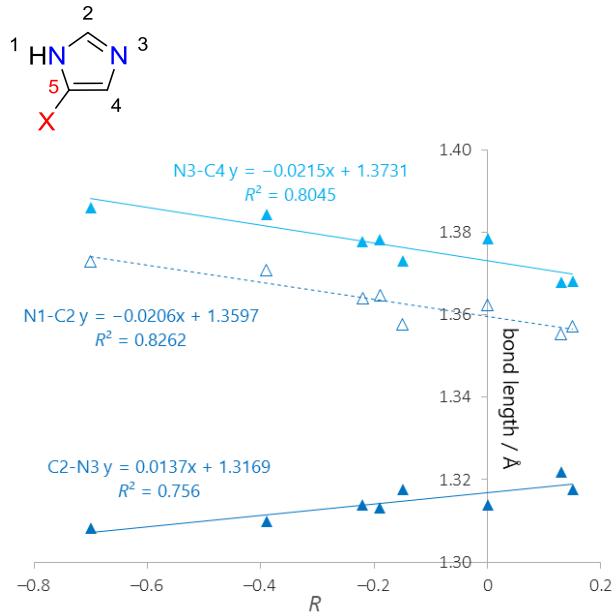


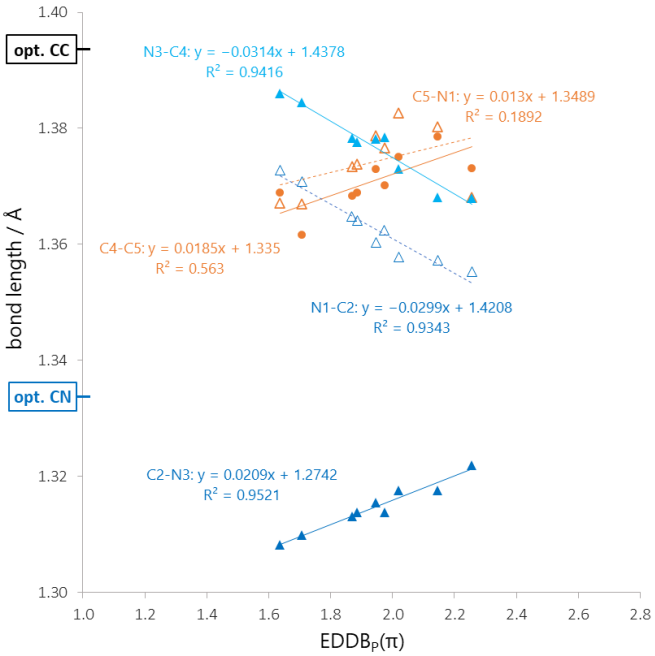
imiC4


C5-N1 y = −0.0192x + 1.3732
R² = 0.925
N1-C2 y = 0.0143x + 1.3635
R² = 0.9506
C2-N3 y = −0.0085x + 1.3139
R² = 0.7592
bond length / Å
R

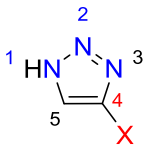

opt. CC
opt. CN
C5-N1: y = -0.0294x + 1.4344
R² = 0.6623
C4-C5: y = -0.0088x + 1.3893
R² = 0.3734
N3-C4: y = -0.0043x + 1.3768
R² = 0.006
N1-C2: y = 0.0214x + 1.3188
R² = 0.6566
C2-N3: y = -0.0096x + 1.3344
R² = 0.2969
bond length / Å
EDDBP(π)

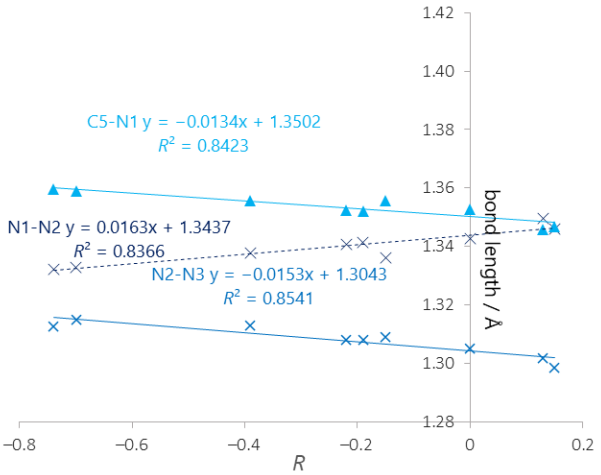
imiC5

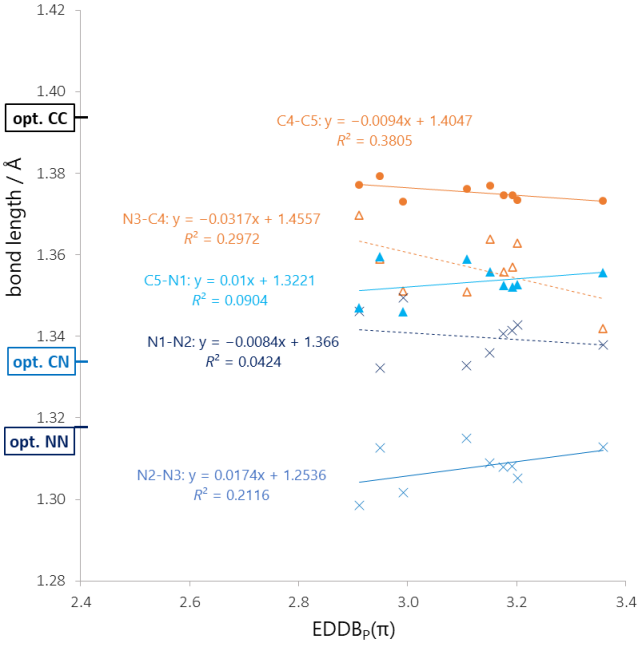

N3-C4 y = −0.0215x + 1.3731
R² = 0.8045
N1-C2 y = −0.0206x + 1.3597
R² = 0.8262
C2-N3 y = 0.0137x + 1.3169
R² = 0.756
bond length / Å
R


opt. CC
opt. CN
N3-C4: y = −0.0314x + 1.4378
R² = 0.9416
C5-N1: y = 0.013x + 1.3489
R² = 0.1892
C4-C5: y = 0.0185x + 1.335
R² = 0.563
N1-C2: y = −0.0299x + 1.4208
R² = 0.9343
C2-N3: y = 0.0209x + 1.2742
R² = 0.9521
bond length / Å
EDDBP(π)

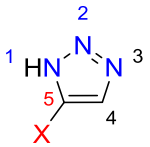
1,2,3-triC4 (N1H)

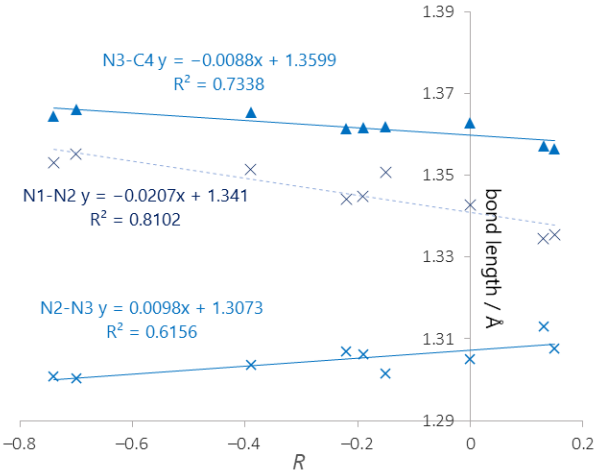


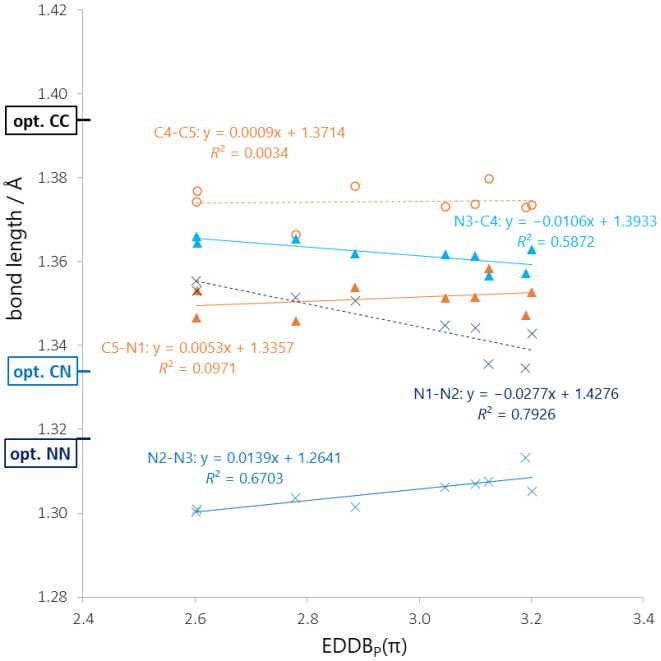




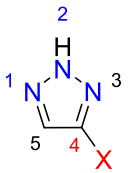
1,2,3-triC5 (N1H)

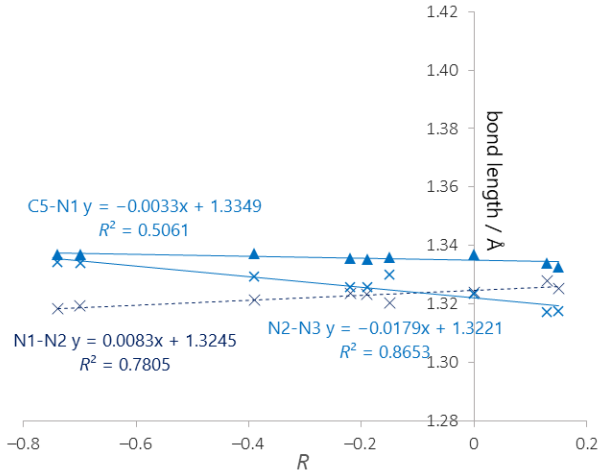


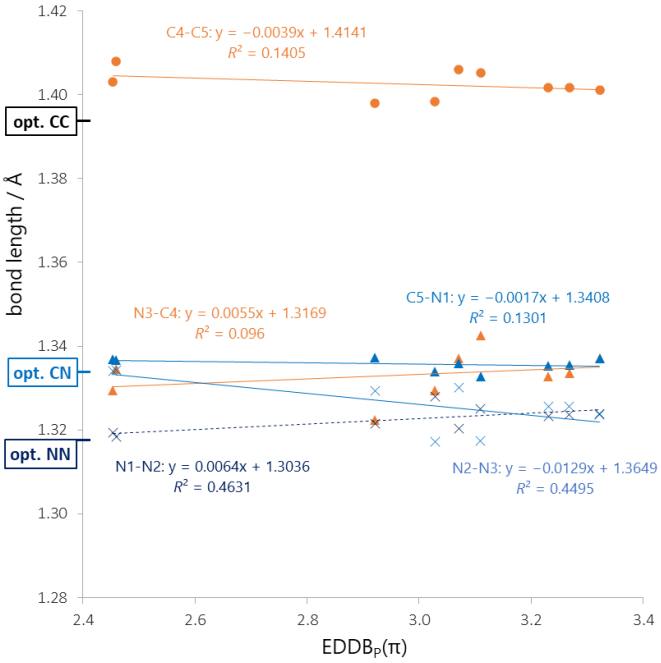




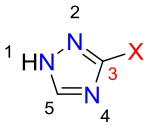
1,2,3-triC4 (N2H)

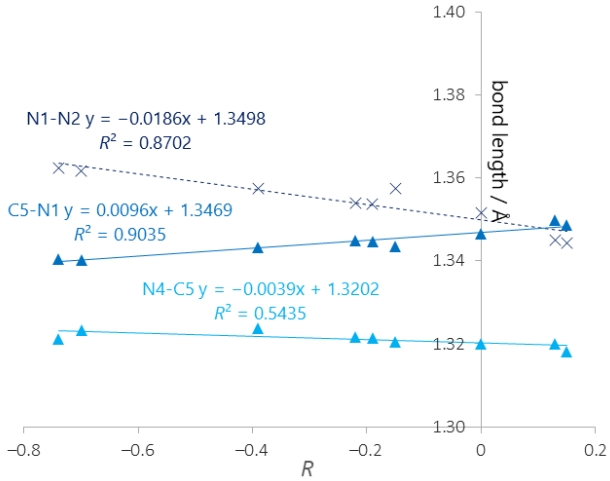


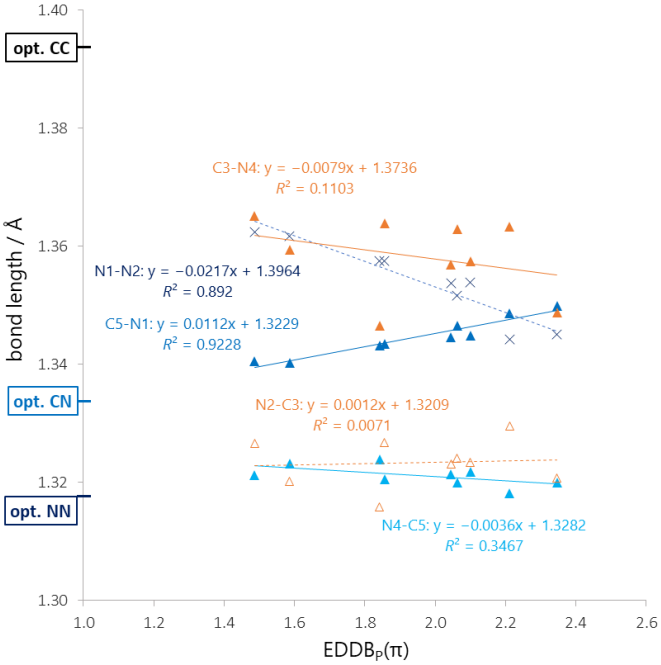




1,2,4-triC3 (N1H)







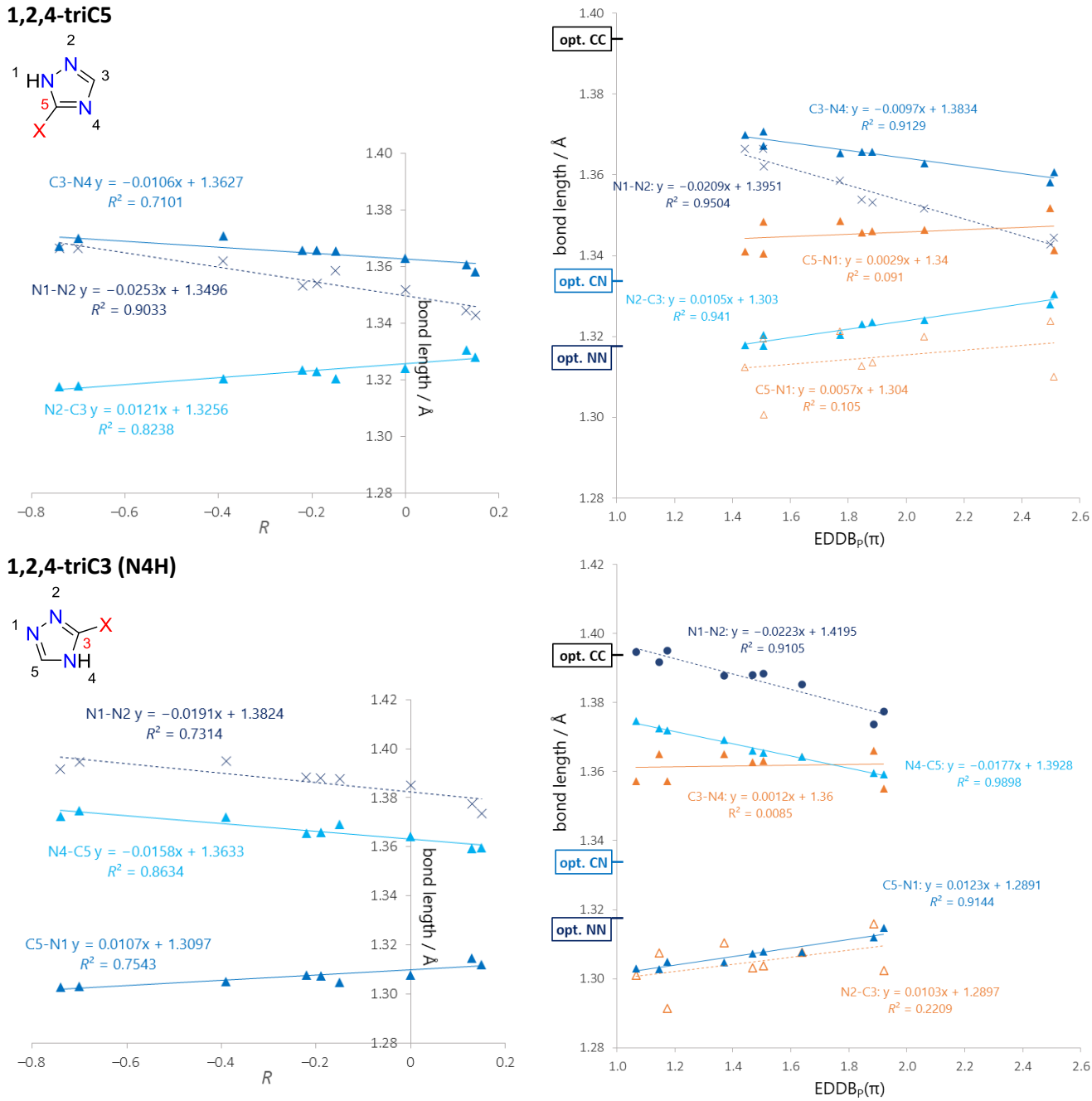


Figure S3. Relations between lengths of bonds In the ring and resonance R constants (left column) or the number of cyclically delocalized π-electrons, $EDDB_P(\pi)$ (right column).

n in sp^n hybrids (NBO analysis)

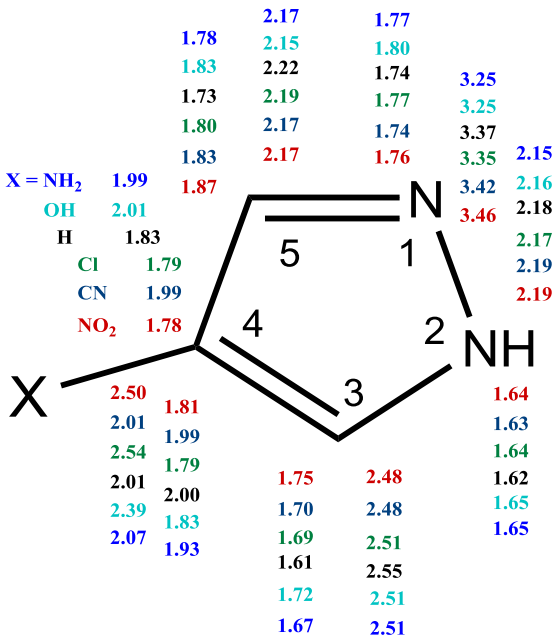


Figure S4. NBO analysis – natural hybrid orbital character of hybrids at ring atoms**.** Example – C4 substituted pyrazole derivatives (pyraC4).

Table S3. Crystallographic data found for monosubstituted compounds in CCSD.

		R constant						ref
imic4			N1-C2	C2-N3	N3-C4	C4-C5	C5-N1	
	NO2	0.13	1.3673	1.3126	1.3605	1.3711	1.3685	
	exp		1.3479	1.3187	1.3630	1.3614	1.3500	KOMHAV [1]
	Br	-0.22	1.3602	1.3170	1.3668	1.3705	1.3773	
	exp		1.3399	1.3242	1.3453	1.3606	1.3529	LUDJAX [2]
imic2			N1-C2	C2-N3	N3-C4	C4-C5	C5-N1	
	NO2	0.15	1.3673	1.3126	1.3605	1.3711	1.3685	
	exp		1.3426	1.3178	1.3703	1.3756	1.3689	CELBAW [3]
	Cl	-0.19	1.3593	1.3047	1.3827	1.3686	1.3803	
	exp		1.3243	1.3169	1.3833	1.3658	1.3796	EJEGOS [4]
	NH2	-0.74	1.3617	1.3110	1.3861	1.3644	1.3879	
	exp-nh-co-nh-ph		1.3448	1.3235	1.3910	1.3475	1.3836	CIVRUV [5]
pyrac4			N1-N2	N2-C3	C3-C4	C4-C5	C1-N5	
	NO2	0.13	1.3504	1.3275	1.4082	1.3797	1.3456	
	exp		1.3588	1.3283	1.3905	1.3796	1.3259	WIKZUL [6]
	NH2	-0.74	1.3357	1.3358	1.4127	1.3828	1.3631	
	exp		1.3457	1.3299	1.3879	1.3859	1.3540	HIWJIG [7]
1,2,3-triC4 (N1H)			N1-N2	N2-N3	N3-C4	C4-C5	C5-N1	
	NO2	0.13						
	exp		1.3451	1.3025	1.3410	1.3631	1.3226	RAMVUW [8]
	SF5	0.12	1.3427	1.3136	1.3550	1.3683	1.3324	LIPTOU [9]
1,2,4-triC3 (N1H)								
	NO2	0.13	1.3450	1.3207	1.3487	1.3199	1.3499	
	exp 1		1.3502	1.3131	1.3428	1.3290	1.3325	CIFROY [10]
	Br	-0.22	1.3539	1.3234	1.3574	1.3217	1.3449	
	exp		1.3549	1.3073	1.3458	1.3232	1.3193	BIJLEL01 [11]
	Cl	-0.19	1.3537	1.3231	1.3569	1.3214	1.3446	
	exp		1.3671	1.3133	1.3500	1.3291	1.3157	CLTRZL [12]
1,2,4-triC3 (N4H)								
			N1-N2	N2-C3	C3-N4	N4-C5	C5-N1	
	NH2	-0.74	1.3917	1.3074	1.3650	1.3724	1.3028	
	exp		1.3875	1.3375	1.3465	1.3643	1.2943	CEBPEH [13]

[1] 10.1107/S0108270191008065, [2] 10.5517/cc1j0ndl, [3] 10.1107/S010827018400384X, [4] 10.5517/ccdc.csd.cc25wqd6, [5] 10.5517/ccq5bfm, [6] 10.1107/S0108768194004180, [7] 10.5517/cc3tyys, [8] 10.5517/cc52rnm, [9] 10.1021/ol701602a, [10] G.Evrard, F.Durant, A.Michel, J.G.Fripiat, J.L.Closset, A.Copin, *Bull. Soc. Chim. Belg*. **1984**, *93*, 233, [11] 10.5517/cc5dn4b, [12] M.S.Idrissi, M.Senechal, H.Sauvaitre, M.Cotrait, C.Garrigou-Lagrange, *J.Chim.Phys.*, **1980**, *77*, 195, [13] 10.5517/ccdc.csd.cczcy5f

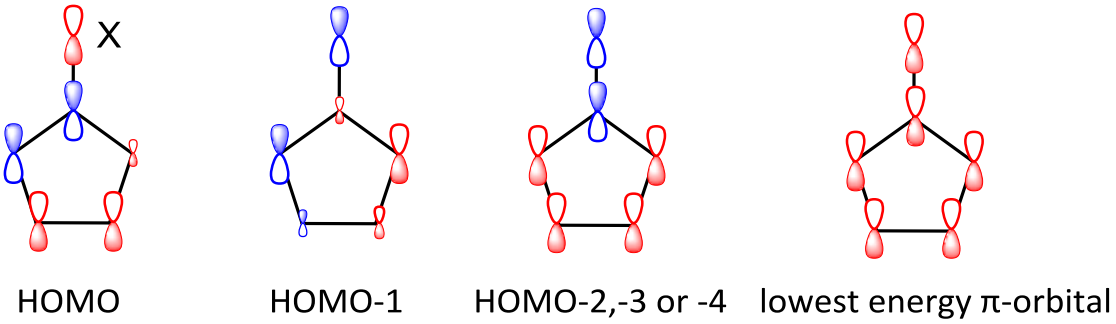
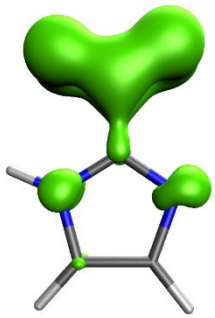
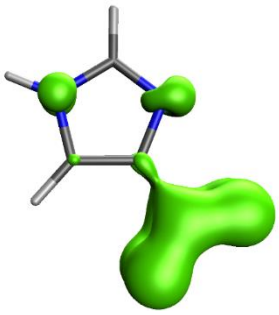
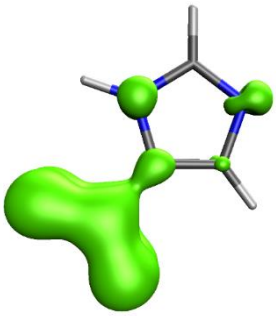
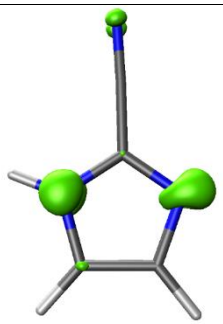
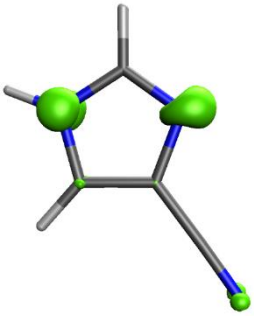
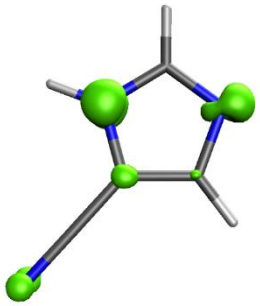
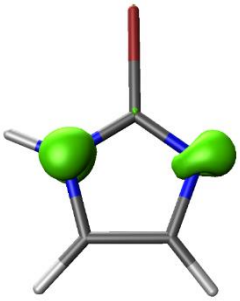
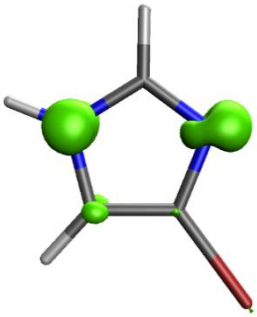
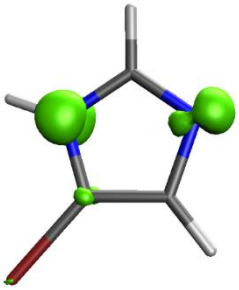
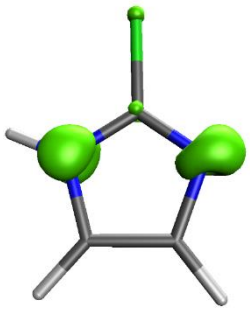
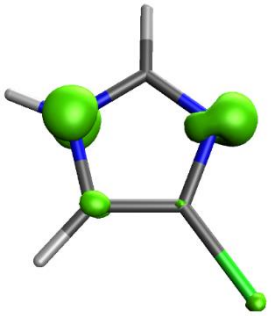
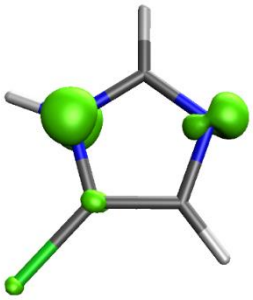
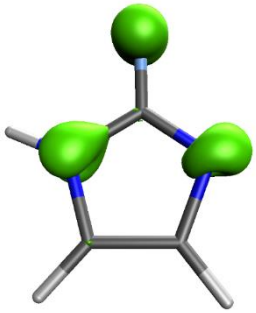
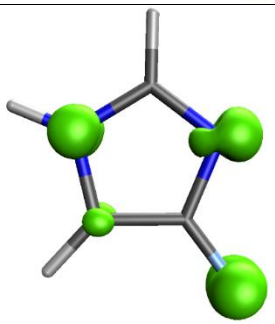
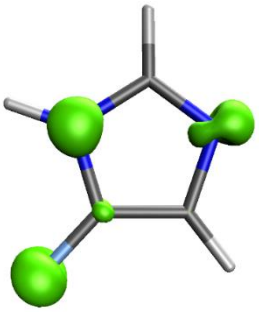
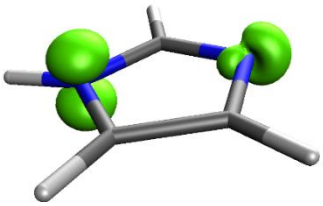
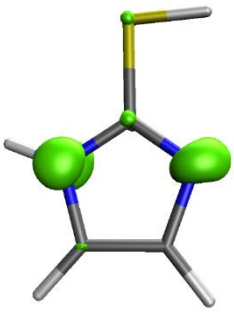
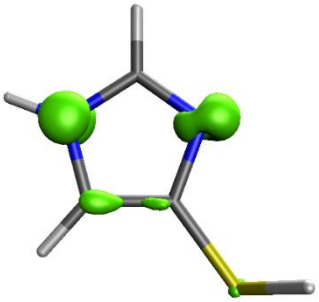
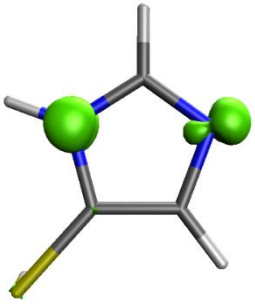
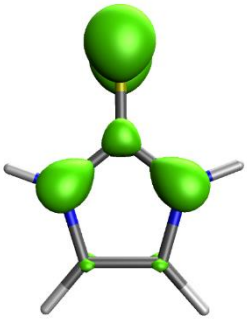
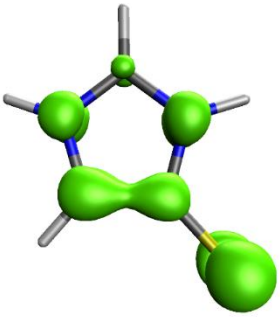
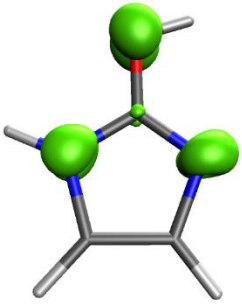
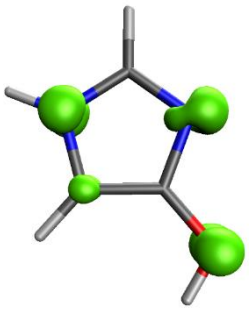
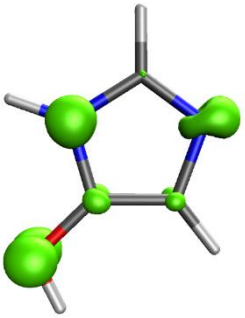
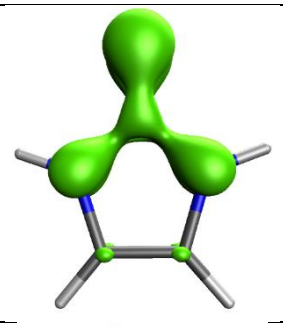
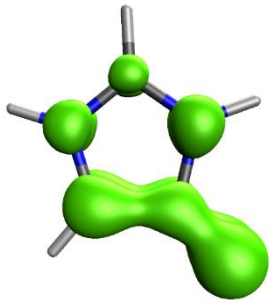
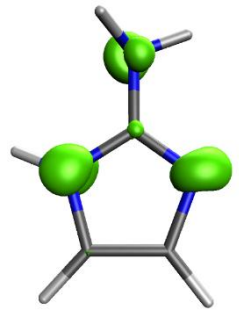
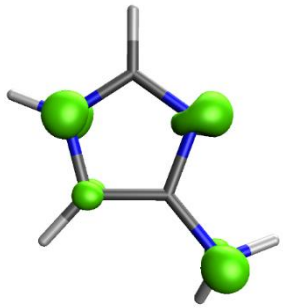
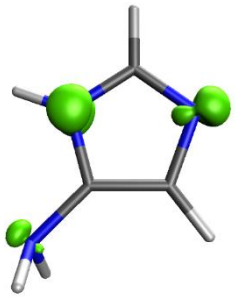
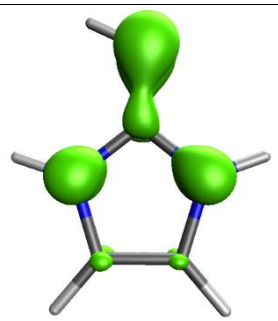
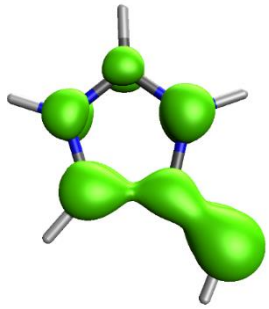


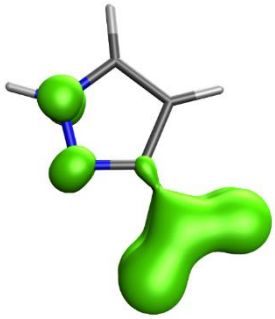
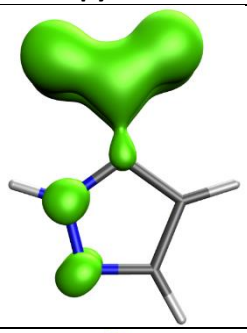
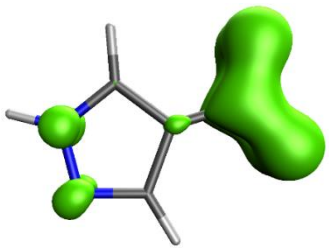
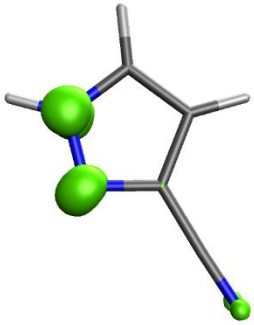
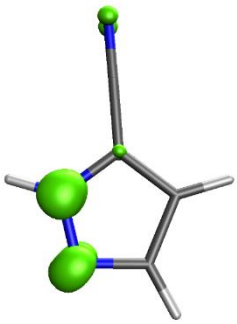
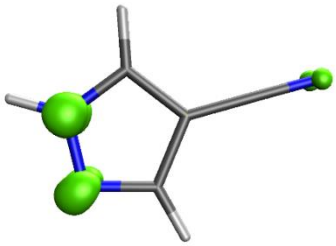
Figure S5. π-Orbital shapes independent of X substituent type.

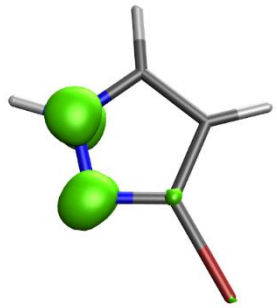
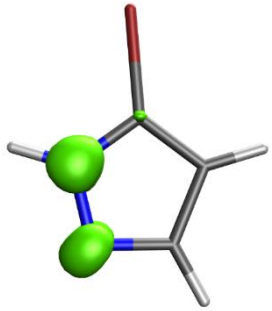
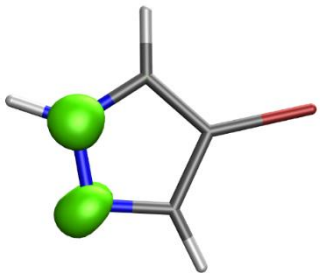
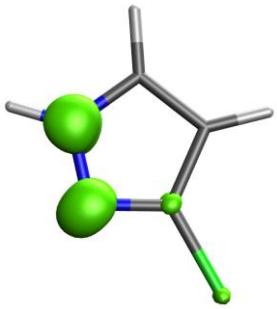
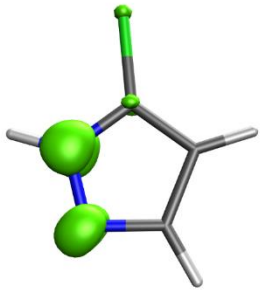
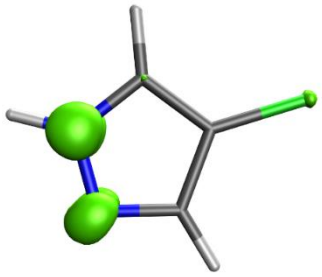
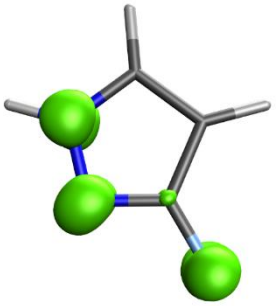
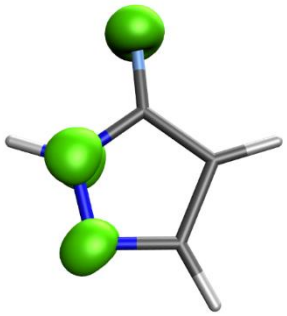
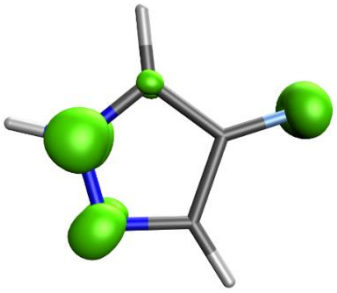
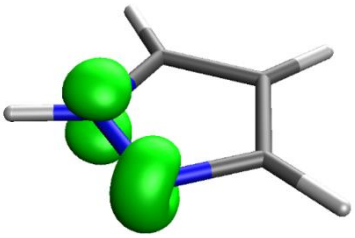
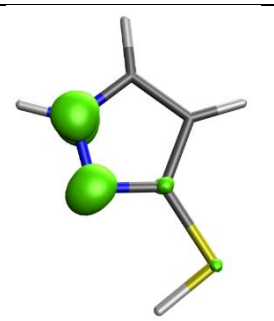
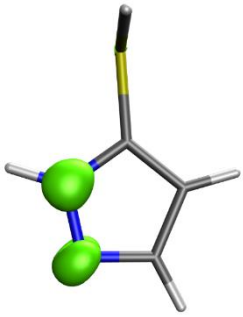
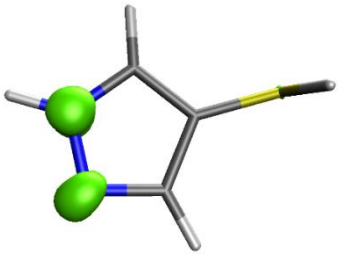
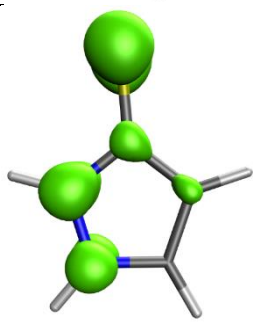
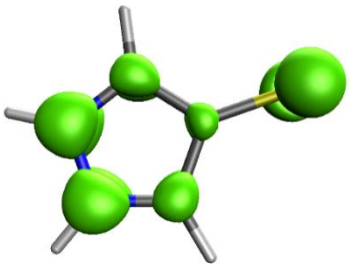
Table S4. Isosurfaces of $EDDB_{G-P}$ function (0.02 electrons) – a visual representation of non-cyclic electron delocalization.

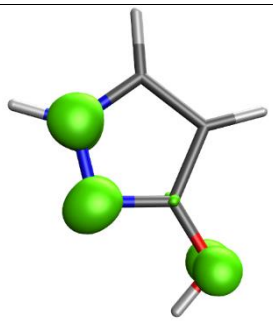
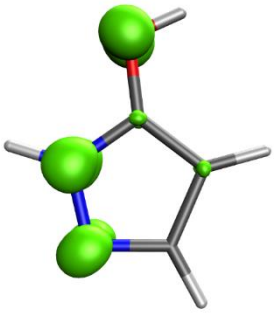
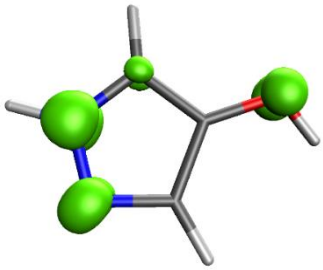
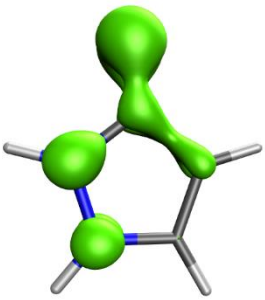
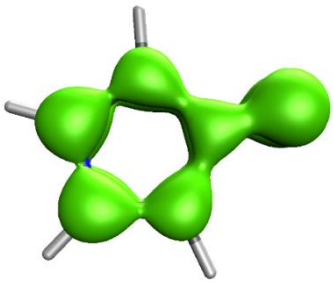
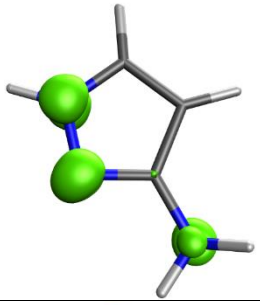
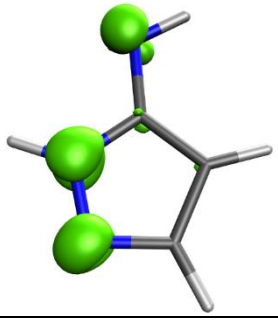
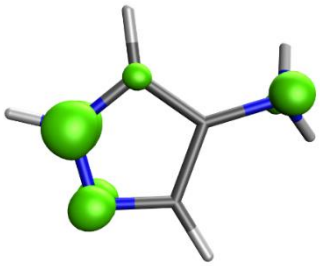
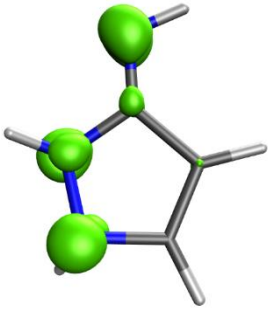
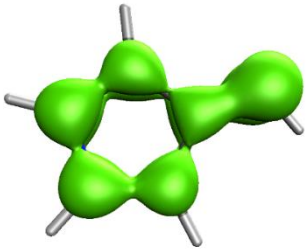
X	**imiC2**	**imiC4**	**imiC5**
NO_2			
CN			
Br			

Cl			
F			
H			
SH			
=S			
OH			

=O			
NH_2			
=NH			

	pyraC3	**pyraC5**	**pyraC4**
NO_2			
CN			

Br			
Cl			
F			
H			
SH			
=S			

OH			
=O			
NH_2			
=NH			

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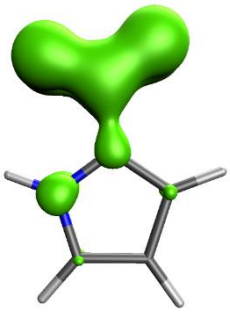
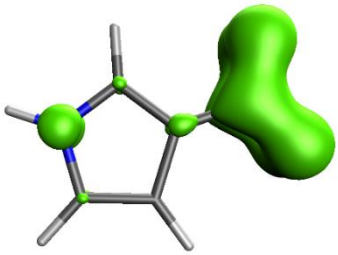
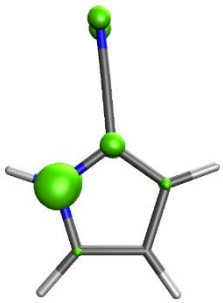
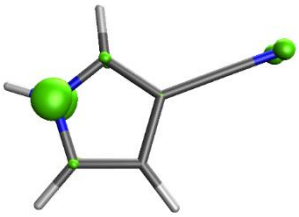
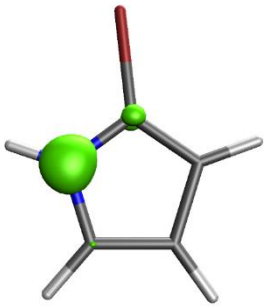
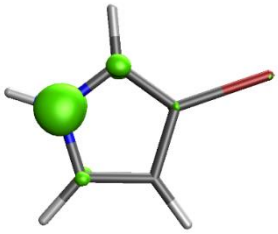
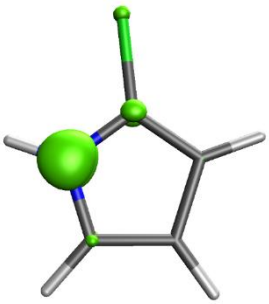
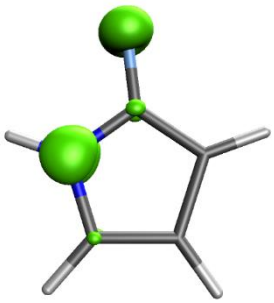
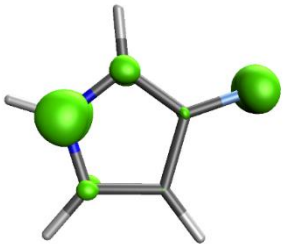
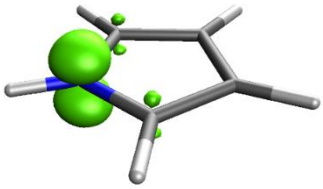
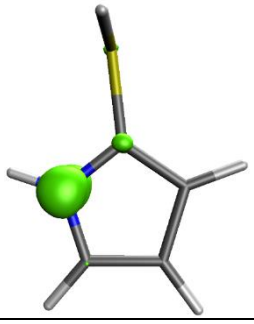
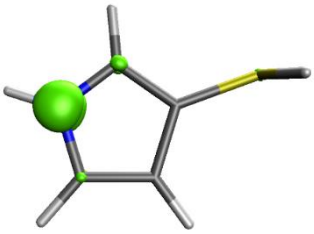
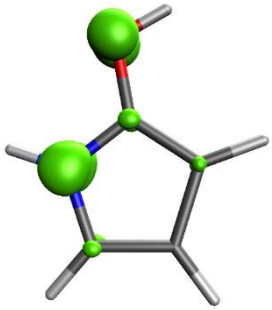
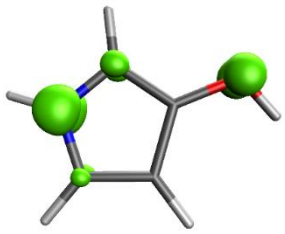
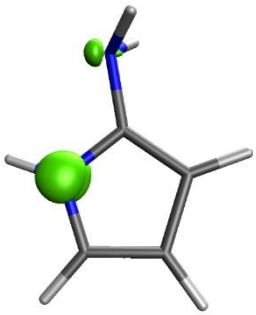
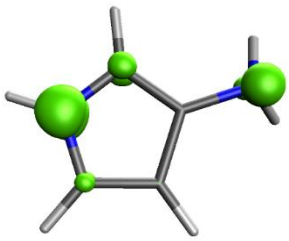
NO_2		

CN		
Br		
Cl		
F		
H		
SH		

OH		
NH_2		

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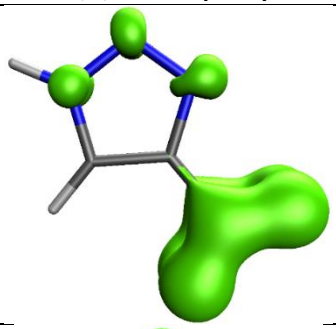
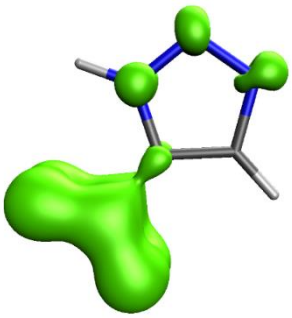
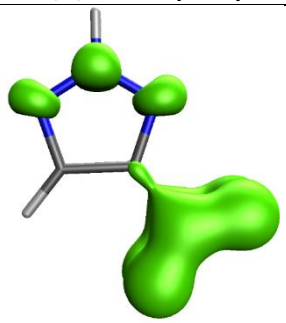
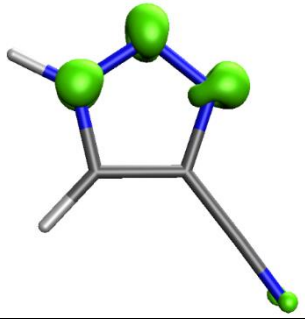
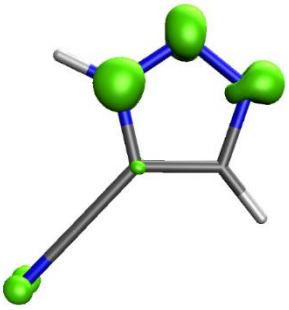
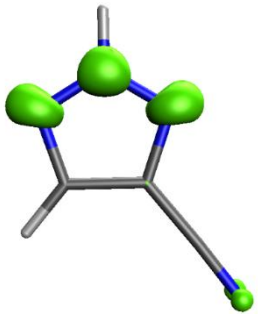
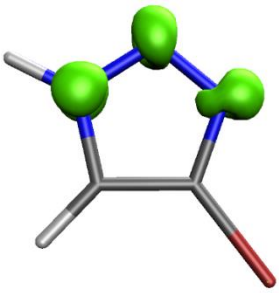
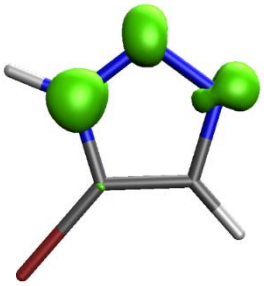
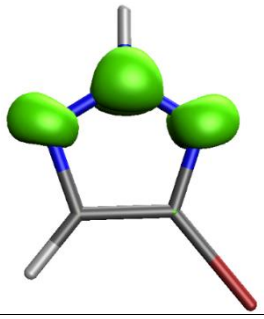
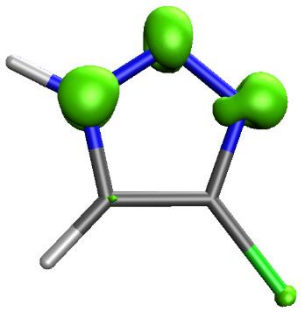
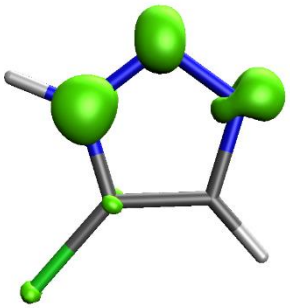
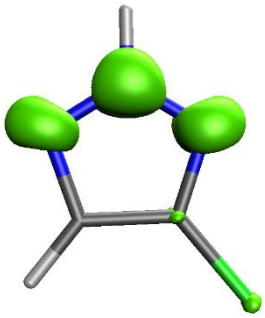
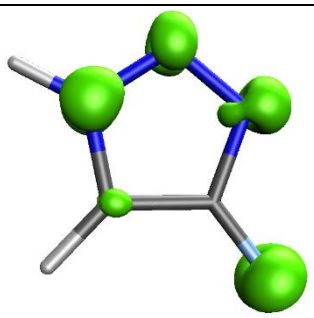
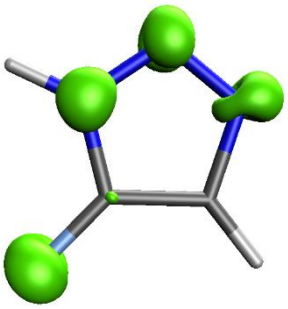
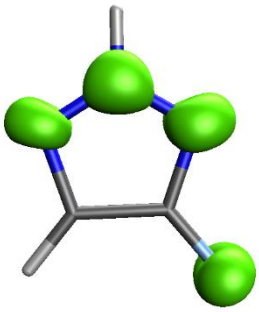
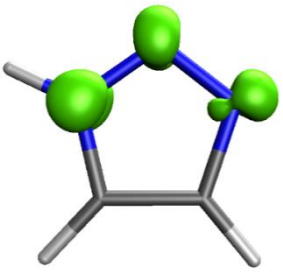
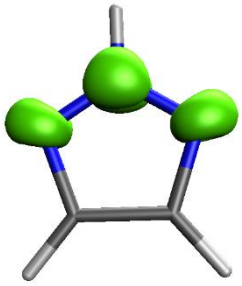
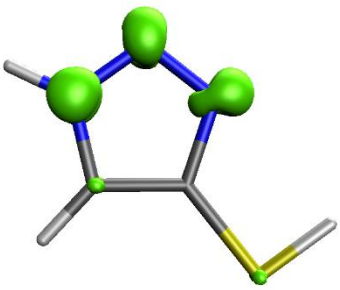
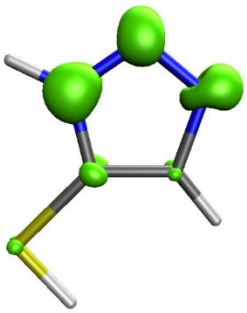
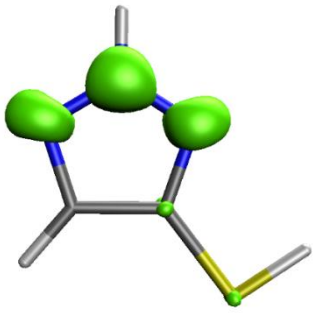
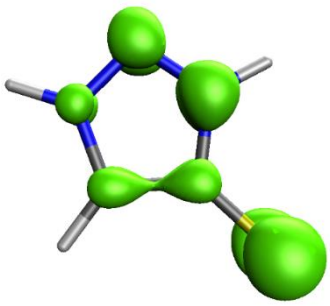
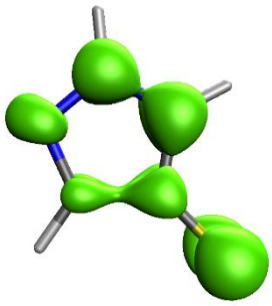
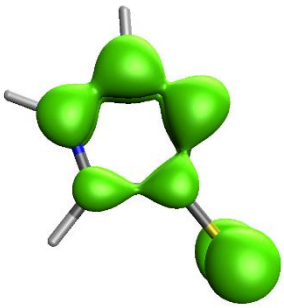
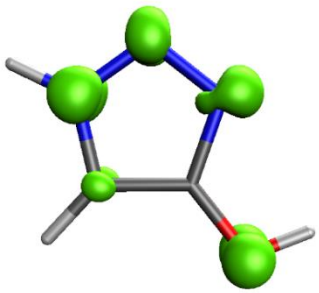
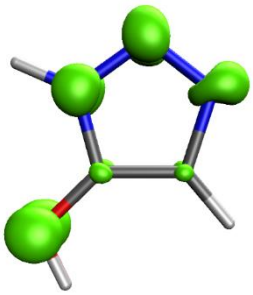
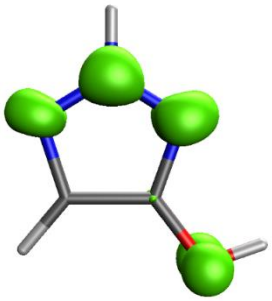
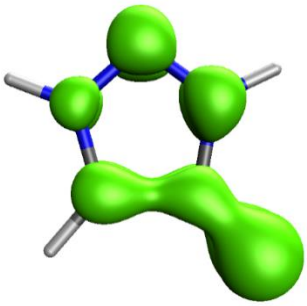
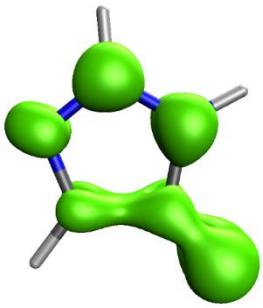
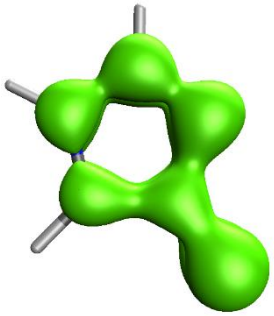
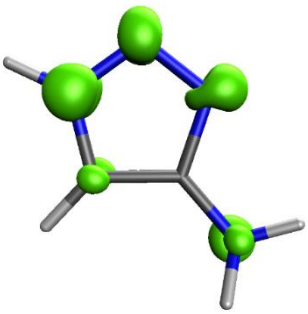
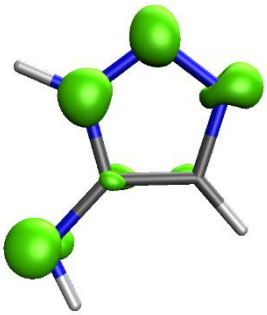
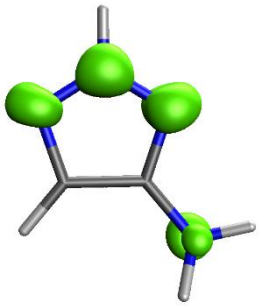
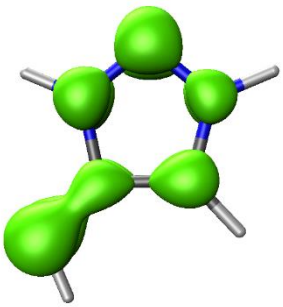
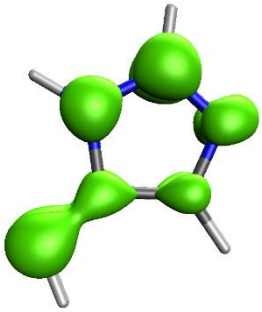
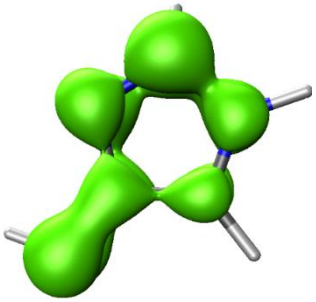
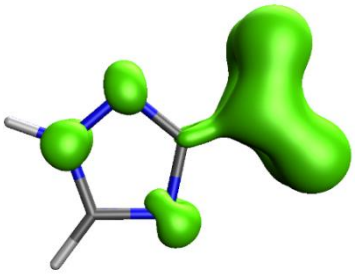
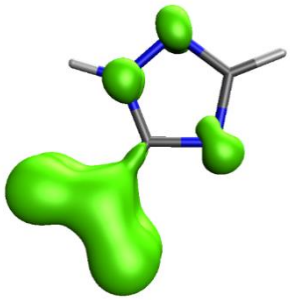
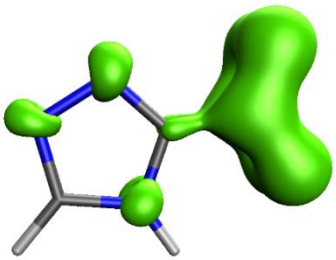
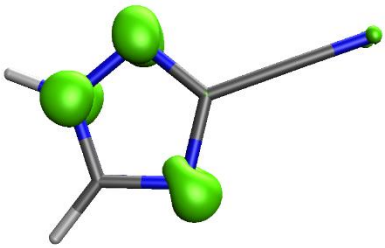
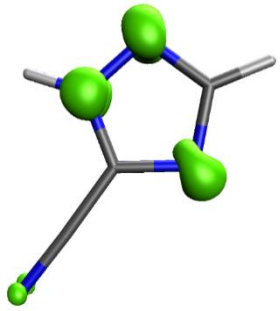
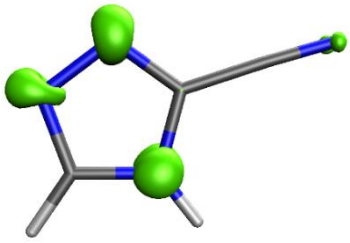
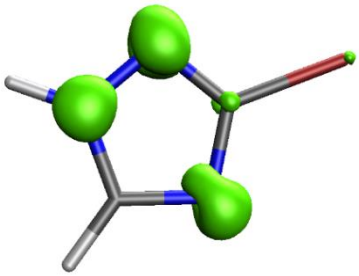
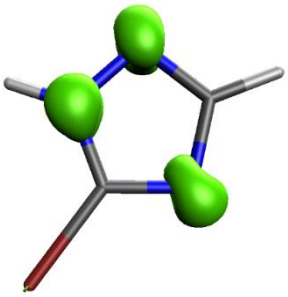
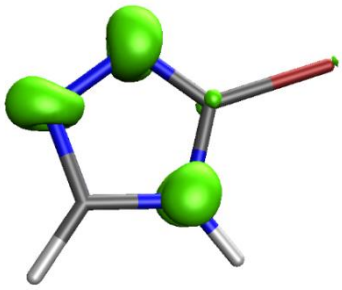
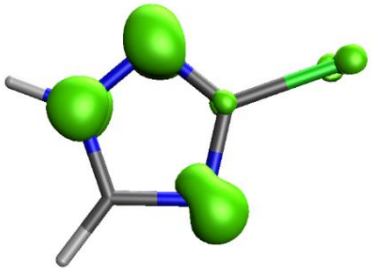
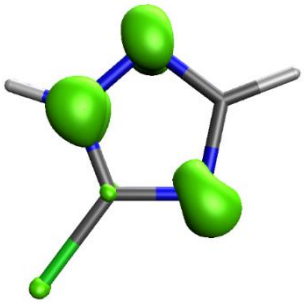
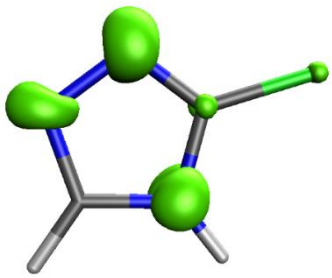
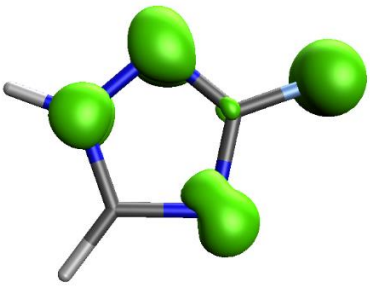
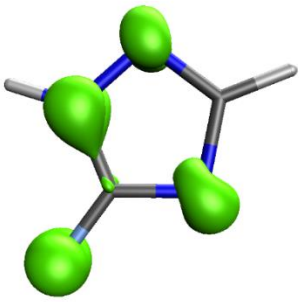
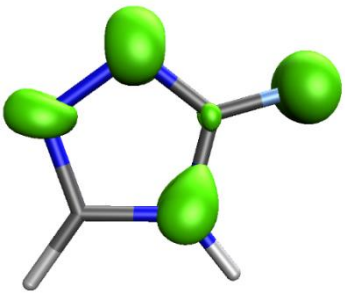
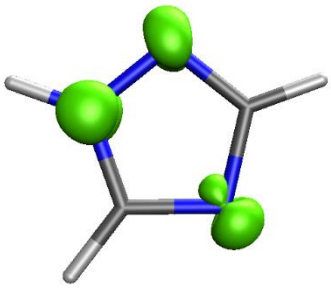
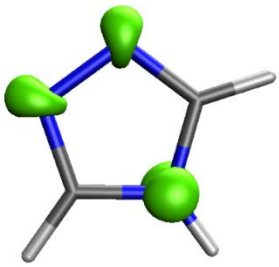
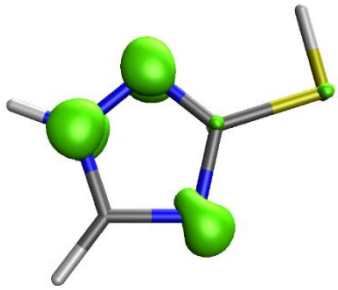
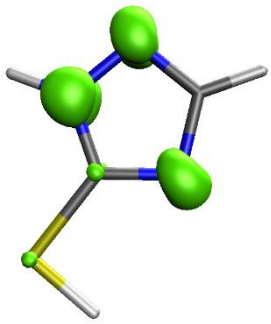
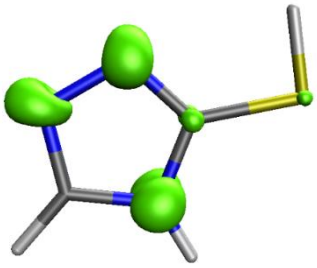
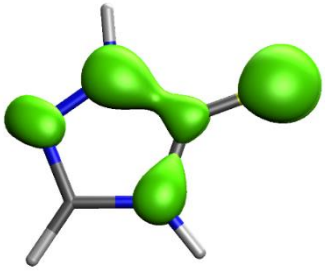
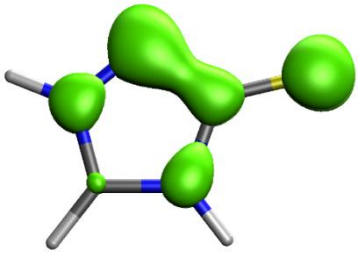
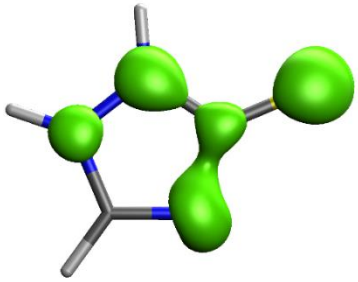
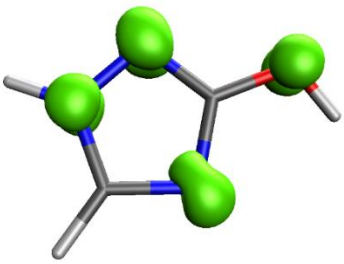
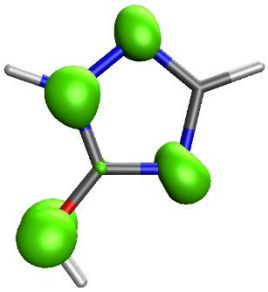
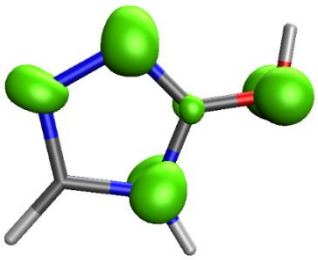
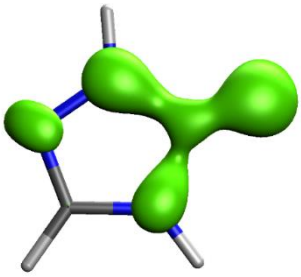
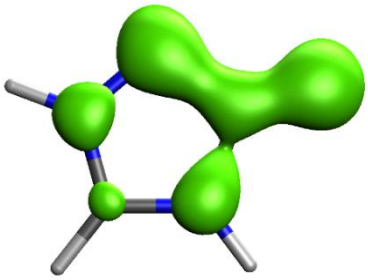
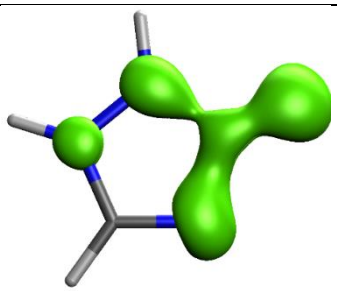
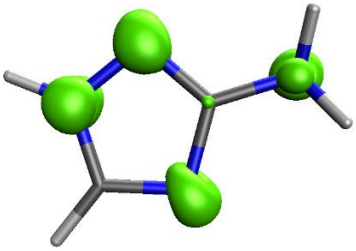
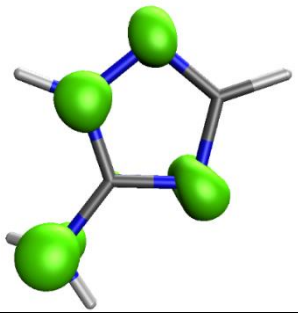
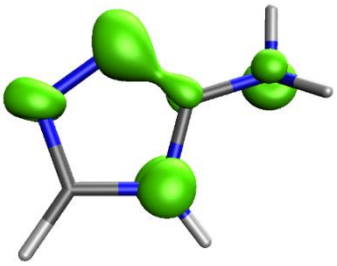
NO_2			
CN			
Br			

Cl			
F			
H			
SH			
=S			

OH			
=O			
NH_2			
=NH			

	1,2,4-triC3 (N1H)	**1,2,4-triC5 (N1H)**	**1,2,4-triC3 (N4H)**
NO_2			

CN			
Br			
Cl			
F			
H			

SH			
=S			
OH			
=O			
NH_2			

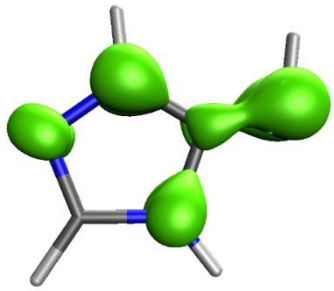
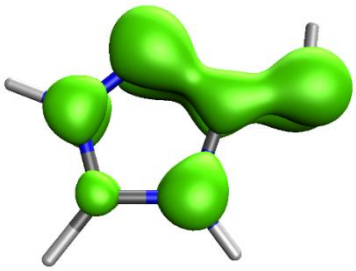
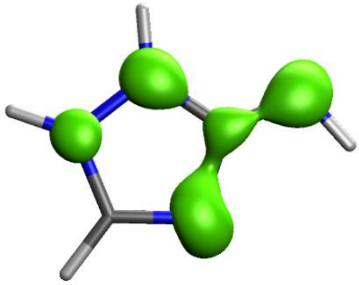
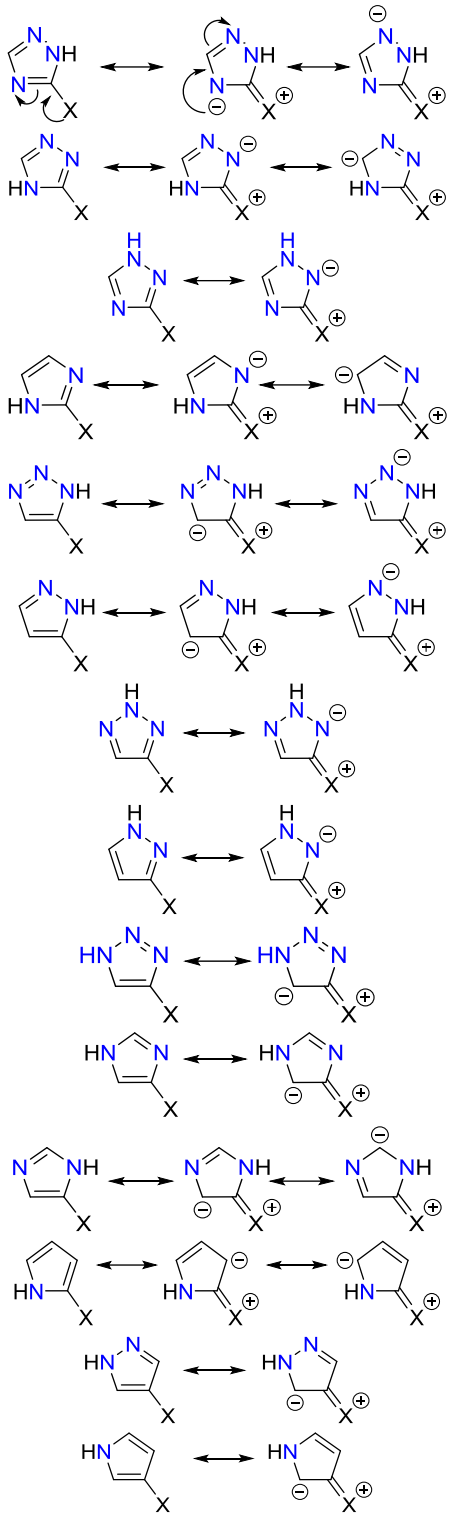
=NH			

Table S5. Values of cSAR(X) for NO_2, Cl and NH_2 substituents, the number of inductive and resonance interactions between substituent and endocyclic N atoms in each heterocycle and resonance structures associated with resonance effect of substituents.

	indN[a]	resN[b]	indN_2[c]	NO_2	Cl	NH_2
1,2,4-triC5 (N1H)	2*o*	1*o* 1*p*	1	0.000	0.119	0.230
1,2,4-triC3 (N4H)	2*o*	1*o*	1	−0.043	0.097	0.195
1,2,4-triC3 (N1H)	2*o*	1*o*	1	−0.045	0.072	0.186
imiC2	2*o*	1*o*	0	−0.056	0.079	0.182
1,2,3-triC5 (N1H)	1*o*	1*p*	2	−0.101	0.033	0.135
pyraC5	1*o*	1*p*	1	−0.112	0.024	0.126
1,2,3-triC4 (N2H)	1*o*	1*o*	2	−0.118	0.003	0.115
pyraC3	1*o*	1*o*	1	−0.128	−0.007	0.104
1,2,3-triC4 (N1H)	1*o*	0	2	−0.140	−0.016	0.092
imiC4	1*o*	0	1	−0.164	−0.034	0.079
imiC5	1*o*	0	1	−0.164	−0.014	0.062
pyrrC2	1*o*	0	0	−0.177	−0.018	0.058
pyraC4	0	0	2	−0.224	−0.095	0.020
pyrrC3	0	0	1	−0.216	−0.103	0.012

resonance (singly excited structures)[d]



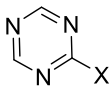
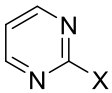
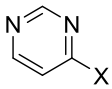
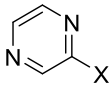
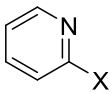
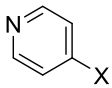
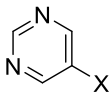
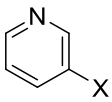
[a] indN – the number of endocyclic N atoms in *ortho* positions relative to substituent, 2o – grey shading of compound name, 1o – light grey shading, 0 – no shading.

[b] resN – the number of endocyclic N atoms interacting via resonance (singly excited structures) with substituent and their position relative to substituent: *o* – *ortho*, *p* – *para*.

[c] indN_2 – the number of non-*ortho* endocyclic N atoms interacting via induction with substituent.

[d] electron-donating substituent delocalizes negative charge, electron-withdrawing positive; the structures look similar.

Table S6. Values of cSAR(X) of NO_2, Cl and NH_2 substituents in derivatives of selected six-membered heterocycles. Data taken from *Molecules* **2021**, *26* (21), 6543.

		NO_2	Cl	NH_2
triazine		0.043	0.124	0.292
pyrimidineC2		0.000	0.083	0.244
pyrimidineC4		−0.038	0.054	0.213
pyrazine		−0.065	0.031	0.181
pyridineC2		−0.078	0.016	0.163
pyridineC4		−0.097	−0.004	0.140
pyrimidineC5		−0.118	−0.020	0.113
pyridineC3		−0.128	−0.030	0.103

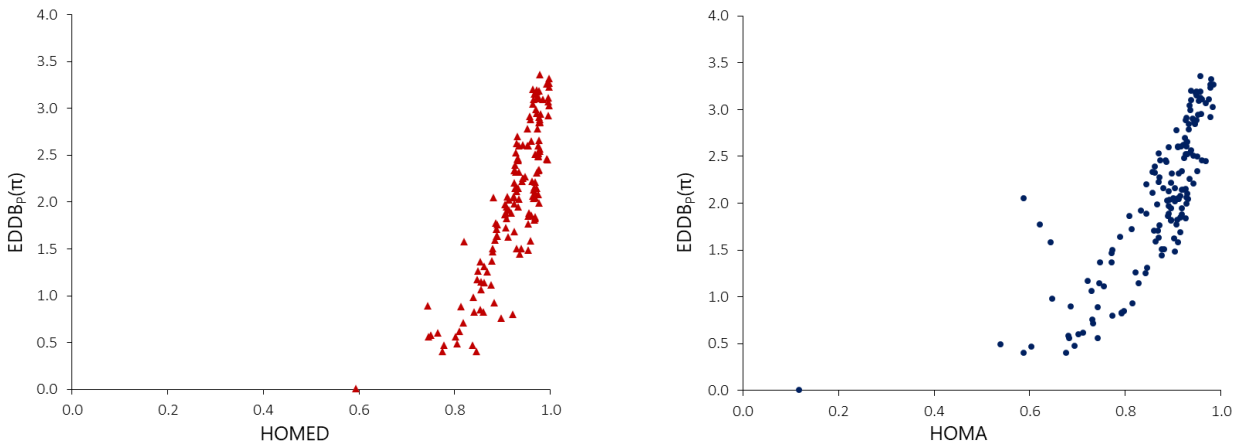
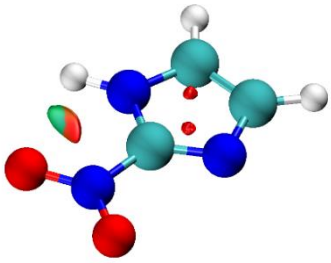
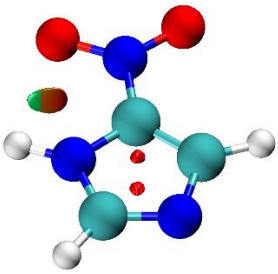


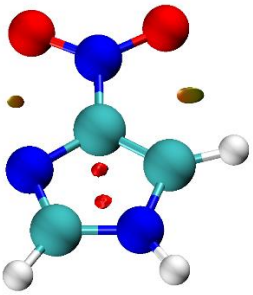
Figure S6. Relations between geometric aromaticity indices and the number of cyclically delocalized electrons from the $EDDB_P(\pi)$ function.



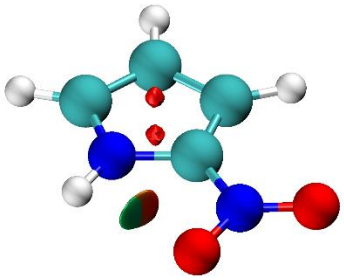
imiC2-NO2
2.410 Å, 91.9 deg



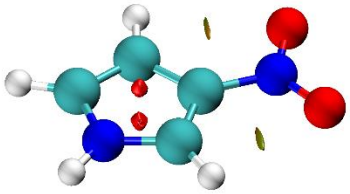
imiC5-NO2
2.461 Å, 91.01 deg



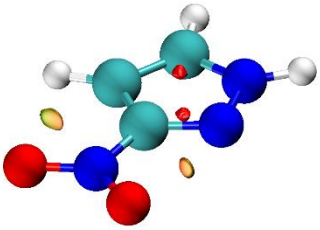
imiC4-NO2



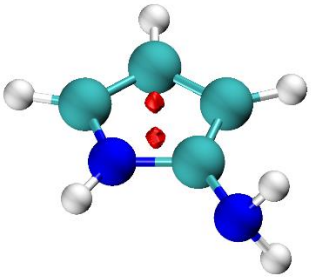
pyrrC2-NO2
2.404 Å, 93.08 deg



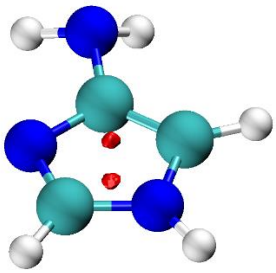
pyrrC3-NO2



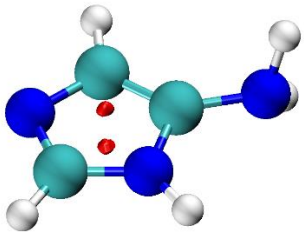
pyraC3-NO2



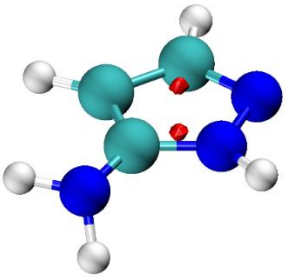
pyrrC2-NH2
2.623 Å, 65.93 deg



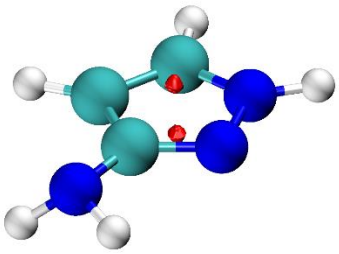
imiC4-NH2
2.474 Å, 73.95 deg



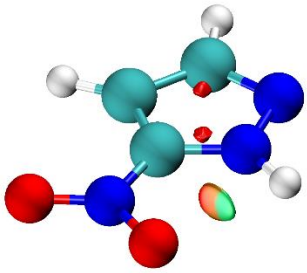
imiC5-NH2
2.674 Å, 64.21 deg



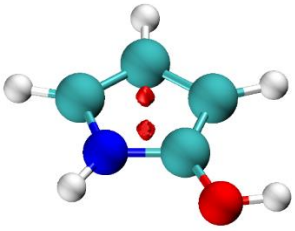
pyraC5-NH2
2.700 Å, 61.72 deg



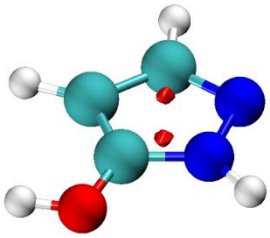
pyraC3-NH2
2.467 Å, 72.56 deg



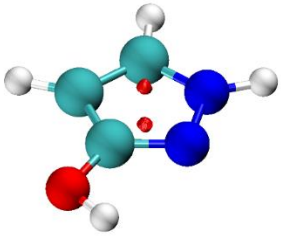
pyraC5-NO2
2.481 Å, 89.44 deg



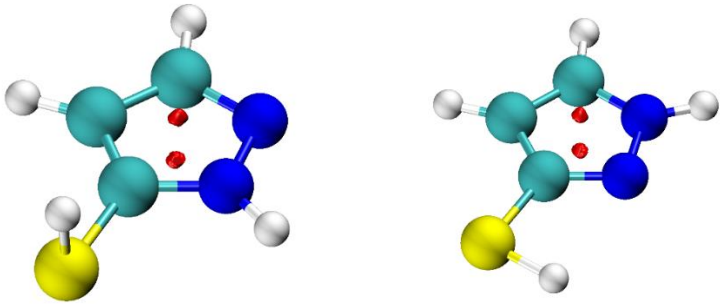
pyrrC2-OH
2.575 Å, 64.33 deg



pyraC5-OH
2.625 Å, 61.49 deg



pyraC3-OH
2.338 Å, 78.02 deg



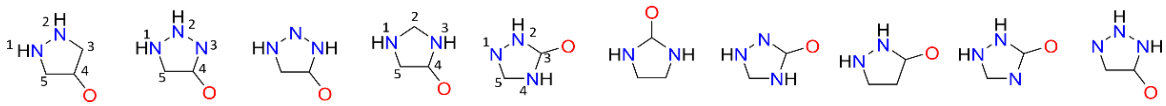
pyraC5-SH
2.966 Å, 66.75 deg

pyraC3-SH
2.574 Å, 80.99 deg

Figure S7. Non covalent interaction analysis (NCI method). Reduced density gradient isosurfaces (RDG = 0.5), colored according to the value of sgn(λ_2(r))·ρ(r). Distances and angles of DH···A *ortho* contacts (D = N,O,S; A = N,O).

Table S7. Keto, thioketo and imino forms of studied 5-membered heterocycles with their EDDB$_P$(π), cSAR(X), HOMED, CX bond lengths (d_{CX}) and ΔE values (in kcal/mol).

cyclic π-electron delocalization



EDDB$_P$(π)	2.050	1.581	1.365	0.896	0.713	0.605	0.564	0.491	0.474	0.471
HOMED	0.881	0.820	0.853	0.744	0.818	0.764	0.745	0.805	0.778	0.838
cSAR(X)	−0.416	−0.322	−0.272	−0.306	−0.165	−0.183	−0.221	−0.237	−0.167	−0.223
d_{CX}/Å	1.241	1.223	1.223	1.228	1.214	1.218	1.215	1.223	1.210	1.220
ΔE^a	33.8	45.6	15.9	7.7	−6.8	−9.0	15.6	12.5	13.5	15.9
thioketo forms (=S)										
EDDB$_P$(π)	2.225	2.203	2.222	1.310	0.930	0.831	0.853	0.762	0.825	0.803
HOMED	0.961	0.924	0.940	0.862	0.882	0.840	0.854	0.897	0.860	0.921
cSAR(X)	−0.564	−0.450	−0.389	−0.444	−0.253	−0.283	−0.333	−0.340	−0.256	−0.316
d_{CX}/Å	1.698	1.673	1.668	1.679	1.653	1.662	1.662	1.666	1.650	1.660
ΔE^b	35.3	38.8	9.7	11.1	−6.6	−8.3	14.7	14.0	16.2	17.1
imino forms (=NH)										
EDDB$_P$(π)	1.775	0.982	1.113	0.889	0.619	0.583	0.562	0.011	0.403	0.406
HOMED	0.886	0.838	0.877	0.813	0.810	0.749	0.802	0.593	0.773	0.845
cSAR(X)	−0.391	−0.279	−0.241	−0.281	−0.130	−0.150	−0.197	−0.135	−0.137	−0.188
d_{CX}/Å	1.309	1.293	1.291	1.298	1.281	1.285	1.285	1.281	1.277	1.288
ΔE^c	55.7	65.0	36.6	30.9	13.4	11.0	34.7	22.9	30.4	34.0

a – the energy of keto form relative to the enol form; b – the energy of thioketo form relative to the thiol form; c – the energy of imino form relative to the amino form.

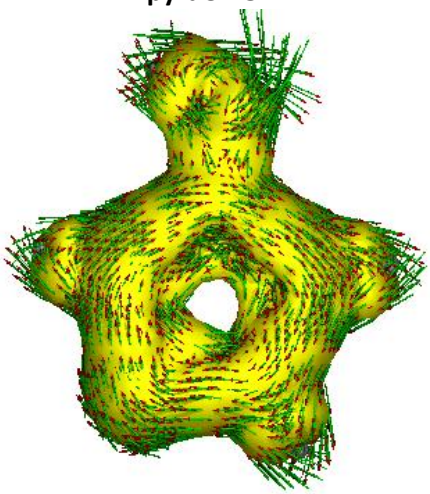
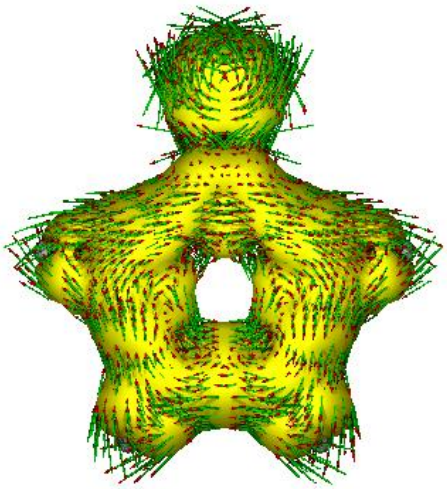
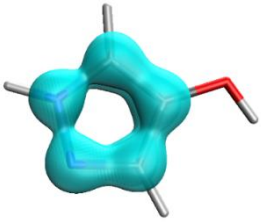
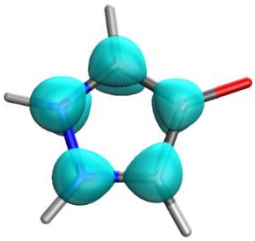
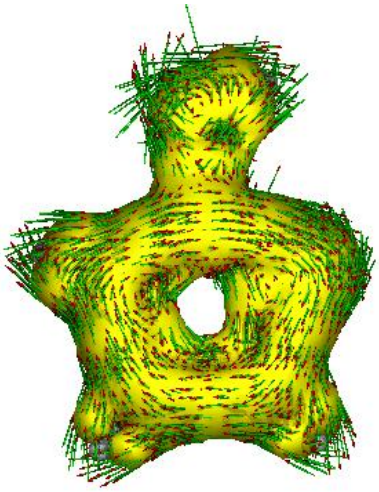
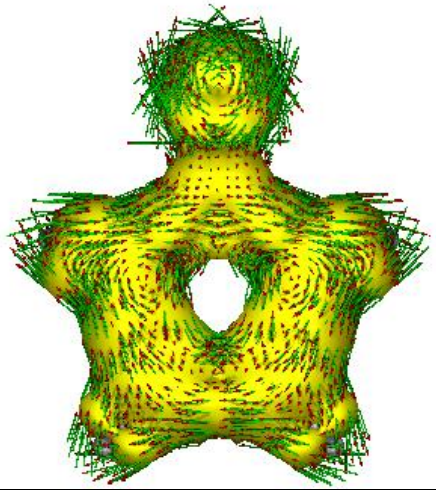
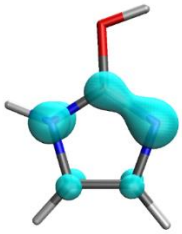
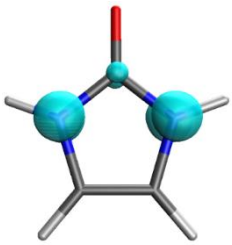
AICD	**pyraC4-OH** 	**pyraC4=O** 
$EDDB_P$	 2.905	 2.050
AICD	**imiC2-OH** 	**imiC2=O** 
$EDDB_P$	 1.150	 0.605

Figure S8. Anisotropy of the induced current density (AICD) plots (isosurface=0.03) and $EDDB_P$ isosurfaces (0.02) with corresponding populations of cyclically delocalized electrons for enol and keto forms of substituted imidazole and pyrazole.

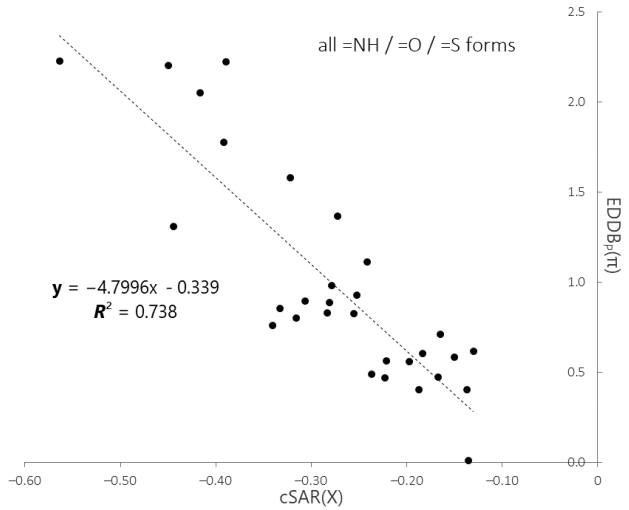
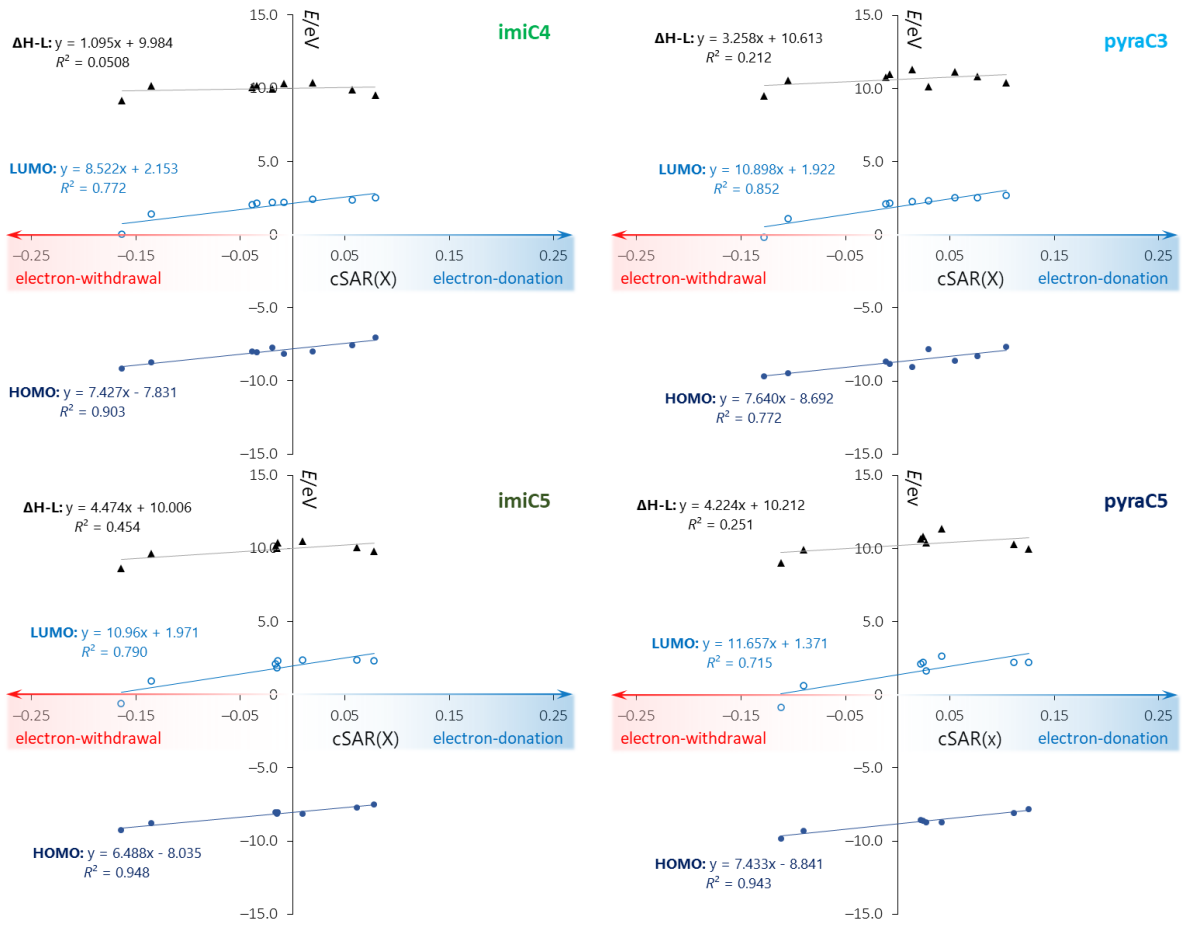
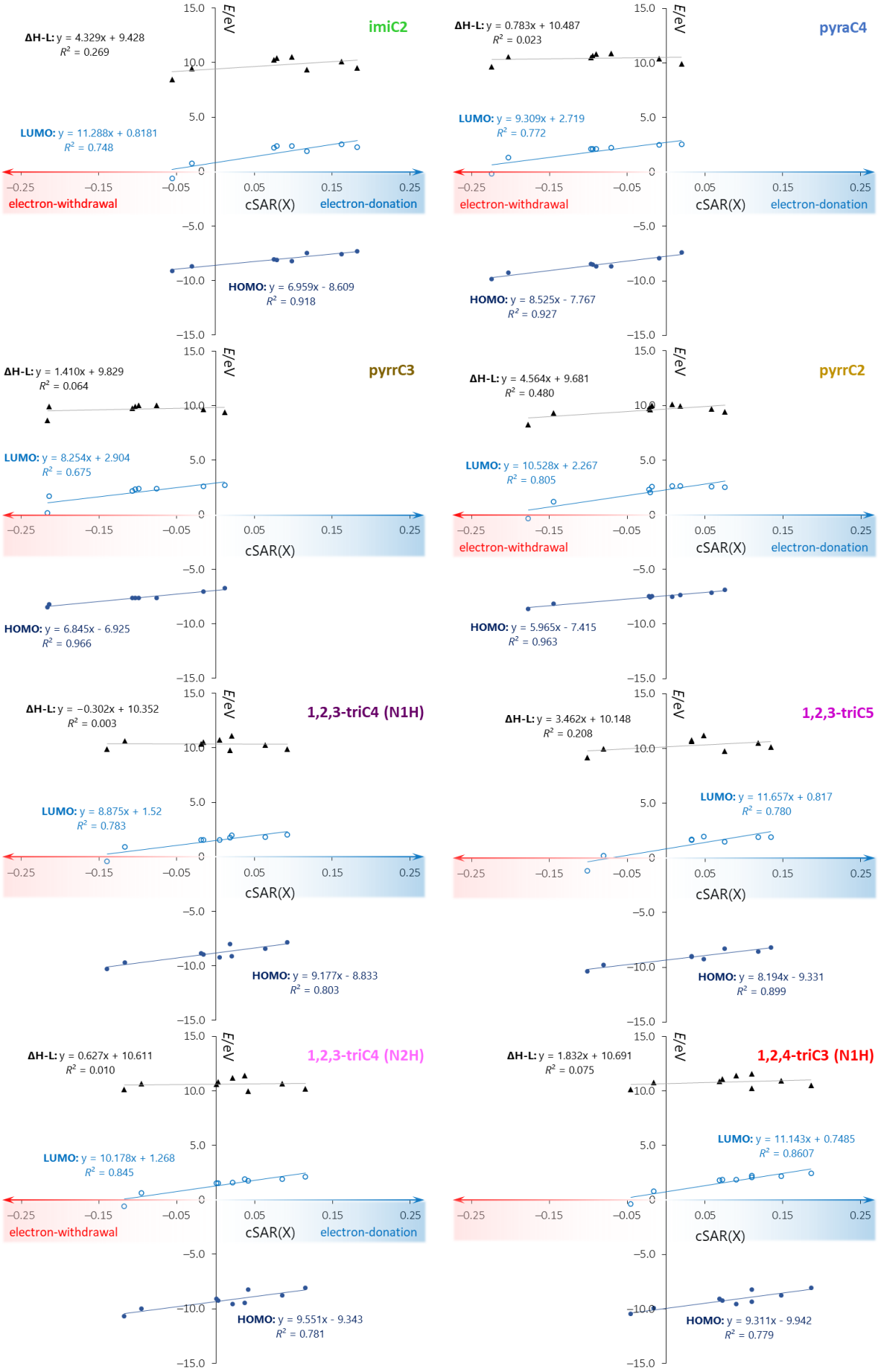


Figure S9. Correlation between the number of cyclically delocalized electrons and electron withdrawing properties of =NH/=O/=S groups for all studied heterocycles.




imiC2
ΔH-L: y = 4.329x + 9.428
R² = 0.269
LUMO: y = 11.288x + 0.8181
R² = 0.748
HOMO: y = 6.959x - 8.609
R² = 0.918
pyraC4
ΔH-L: y = 0.783x + 10.487
R² = 0.023
LUMO: y = 9.309x + 2.719
R² = 0.772
HOMO: y = 8.525x - 7.767
R² = 0.927
pyrrC3
ΔH-L: y = 1.410x + 9.829
R² = 0.064
LUMO: y = 8.254x + 2.904
R² = 0.675
HOMO: y = 6.845x - 6.925
R² = 0.966
pyrrC2
ΔH-L: y = 4.564x + 9.681
R² = 0.480
LUMO: y = 10.528x + 2.267
R² = 0.805
HOMO: y = 5.965x - 7.415
R² = 0.963
1,2,3-triC4 (N1H)
ΔH-L: y = −0.302x + 10.352
R² = 0.003
LUMO: y = 8.875x + 1.52
R² = 0.783
HOMO: y = 9.177x - 8.833
R² = 0.803
1,2,3-triC5
ΔH-L: y = 3.462x + 10.148
R² = 0.208
LUMO: y = 11.657x + 0.817
R² = 0.780
HOMO: y = 8.194x - 9.331
R² = 0.899
1,2,3-triC4 (N2H)
ΔH-L: y = 0.627x + 10.611
R² = 0.010
LUMO: y = 10.178x + 1.268
R² = 0.845
HOMO: y = 9.551x - 9.343
R² = 0.781
1,2,4-triC3 (N1H)
ΔH-L: y = 1.832x + 10.691
R² = 0.075
LUMO: y = 11.143x + 0.7485
R² = 0.8607
HOMO: y = 9.311x - 9.942
R² = 0.779
E/eV
cSAR(X)
electron-withdrawal
electron-donation

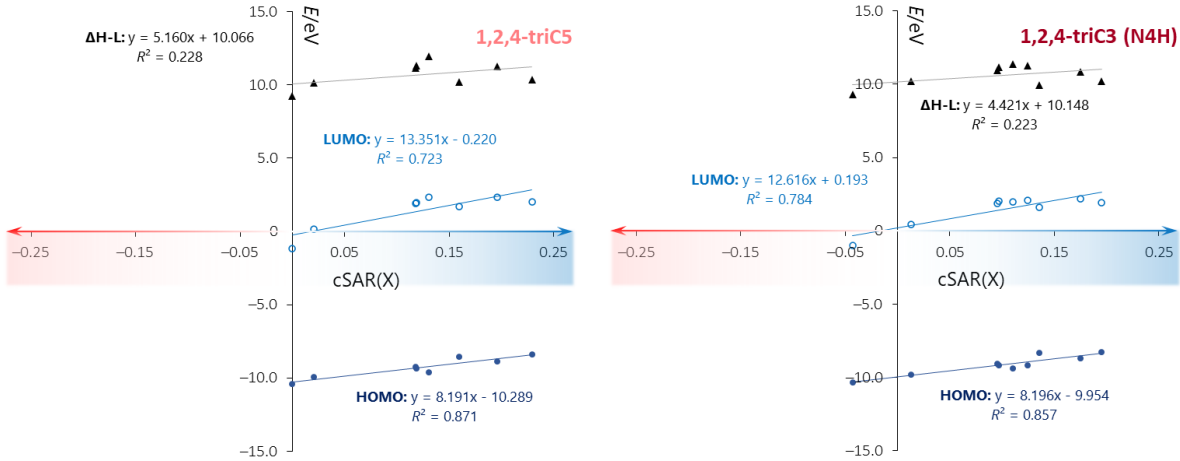


Figure S10. Energies of HOMO, LUMO and the HOMO−LUMO gap (ΔH−L) as a function of cSAR(X).

Table S8. Summary of slopes from Figure S9.

	HOMO	LUMO
1,2,4−triC3(N1H)	9.311	11.143
1,2,3−triC4(N1H)	9.177	8.875
pyraC4	8.525	9.309
1,2,3−triC4(N2H)	8.466	6.861
1,2,3−triC5(N1H)	8.194	11.657
1,2,4−triC5(N1H)	8.191	13.351
1,2,4−triC3(N4H)	8.034	7.678
pyraC3	7.640	10.898
imiC4	7.427	8.522
pyrrC3	6.844	8.254
imiC5	6.488	10.962
pyrrC2	5.965	10.528
pyraC5	5.951	4.627
imiC2	5.495	11.288

Table S9. Reference bonds lengths (Å) calculated at revDSD−PBEP86−G3BJ/def2−TZVPP level of theory and values of HOMED normalization constants α.

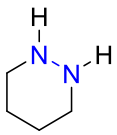
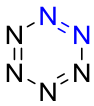
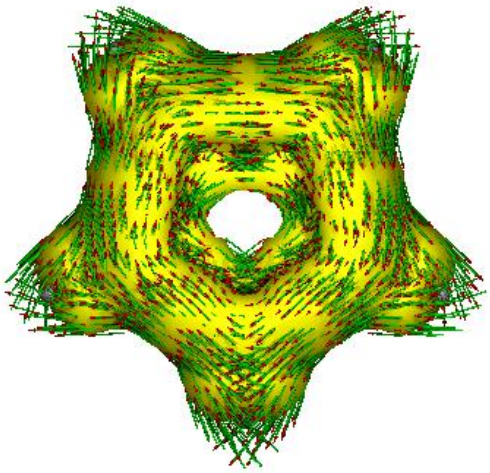
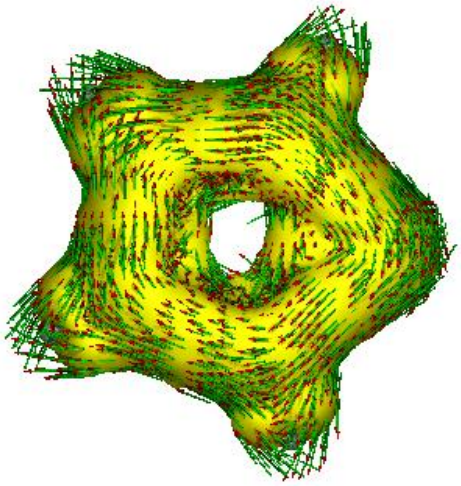
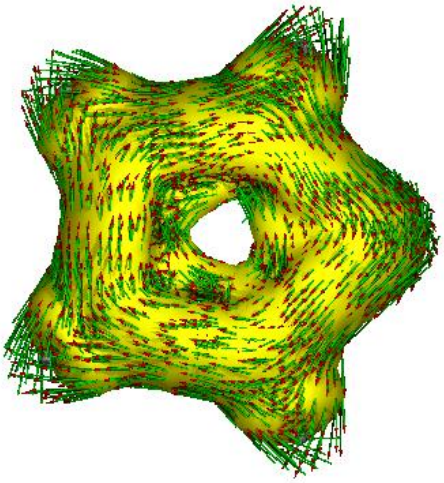
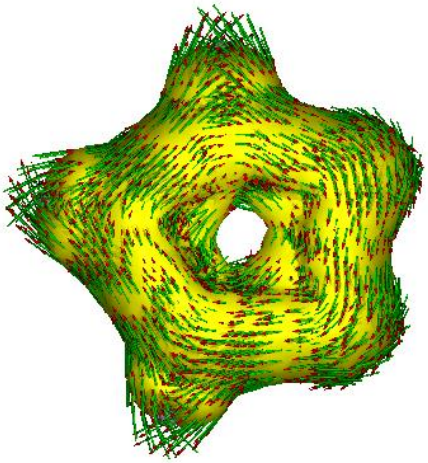
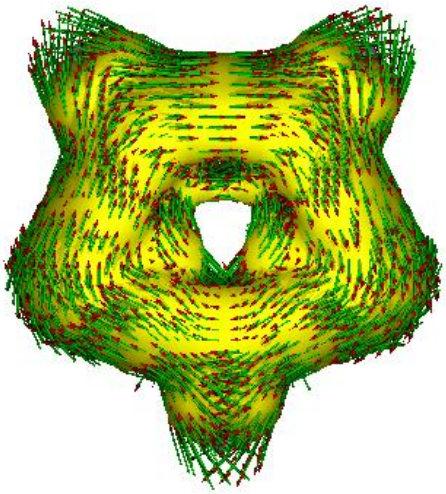
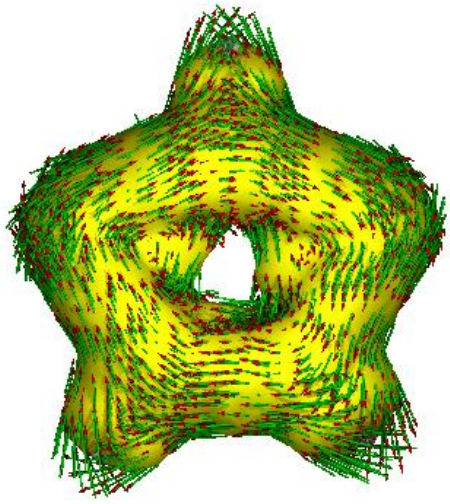
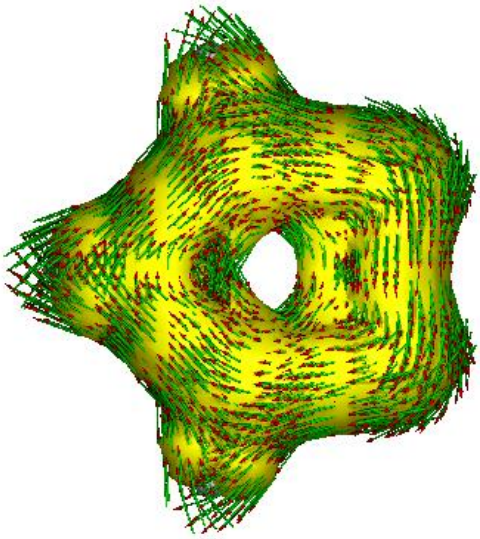
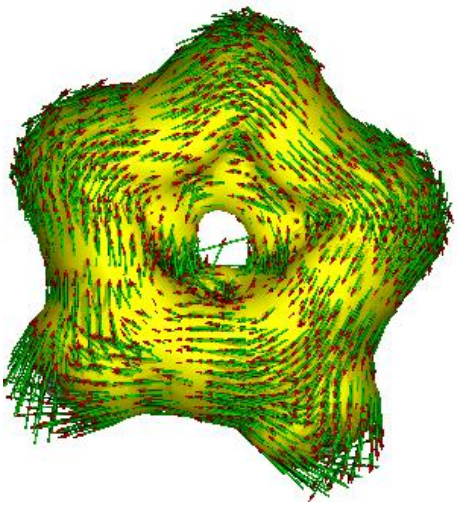
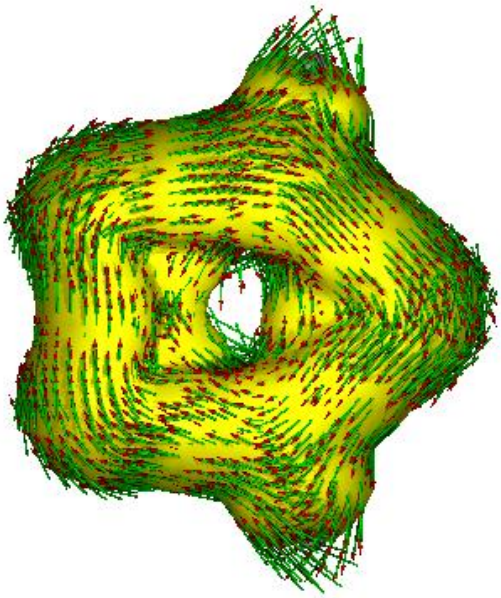
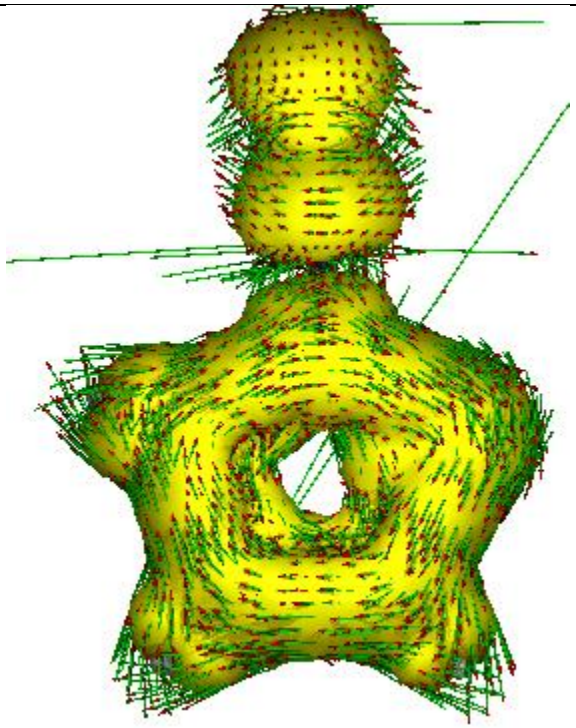
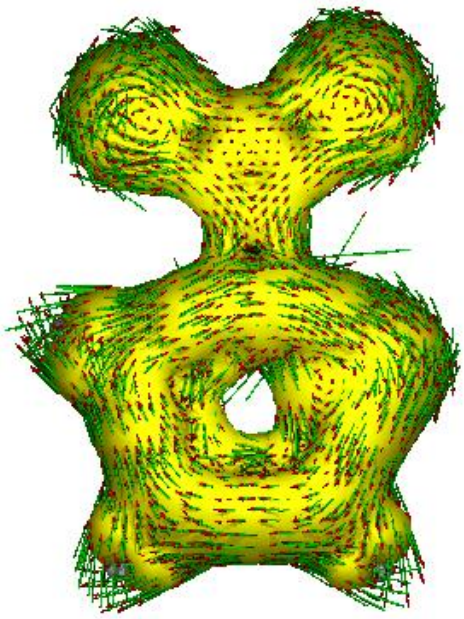
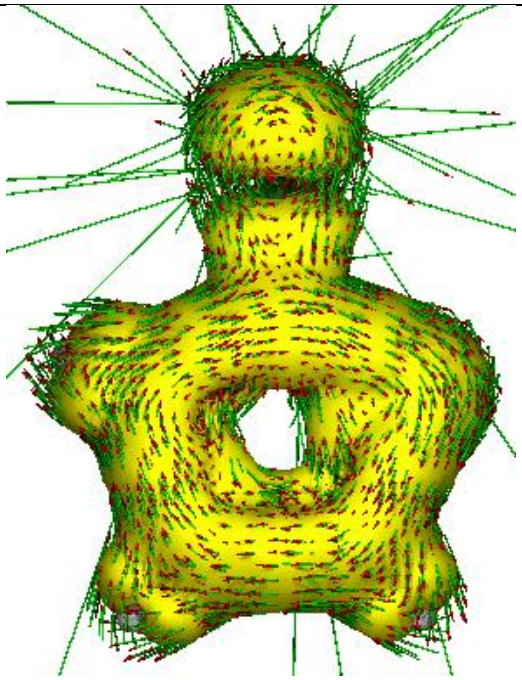
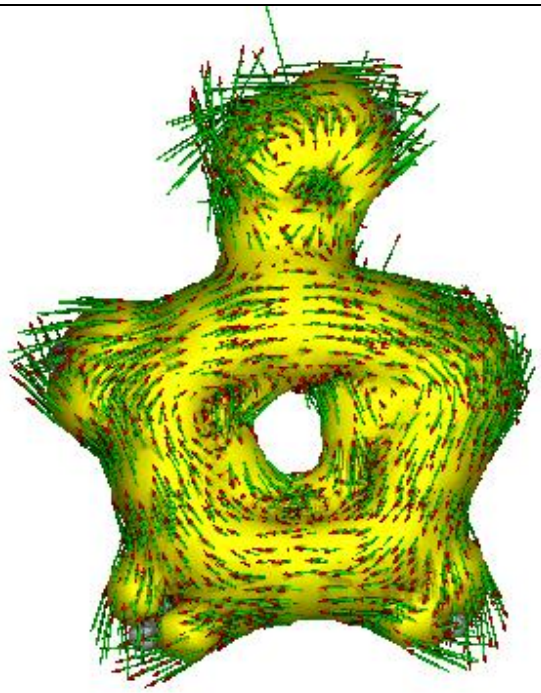
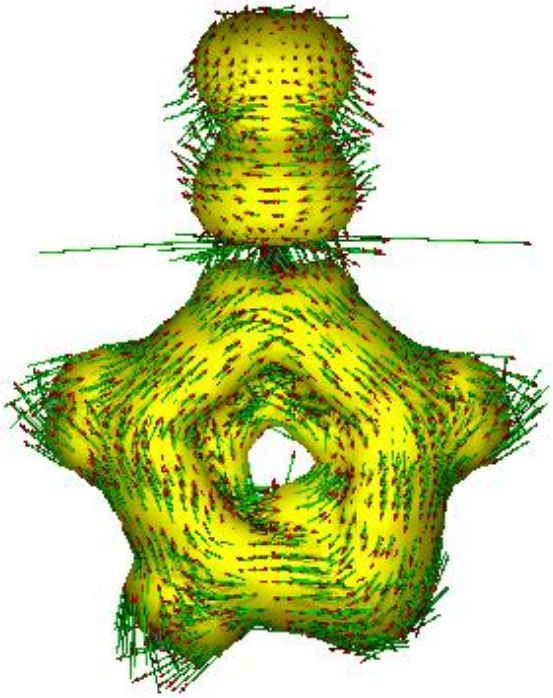
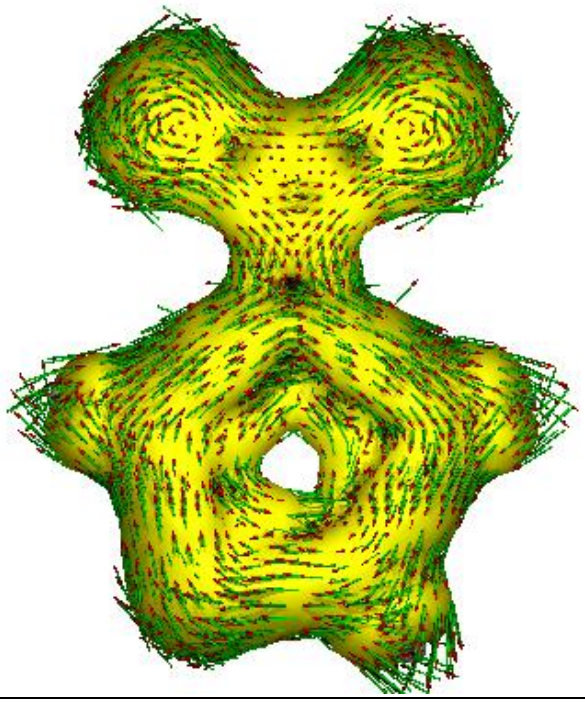
HOMED	d_s	d_d	d_o	α
CC	1.5266 ethane	1.3312 ethene	1.3936 benzene	82.226
CN	1.4643 methylamine	1.2709 methylimine	1.3337 triazine	84.611
NN	1.4687 	1.2399 	1.3175  $D6_h$	62.022

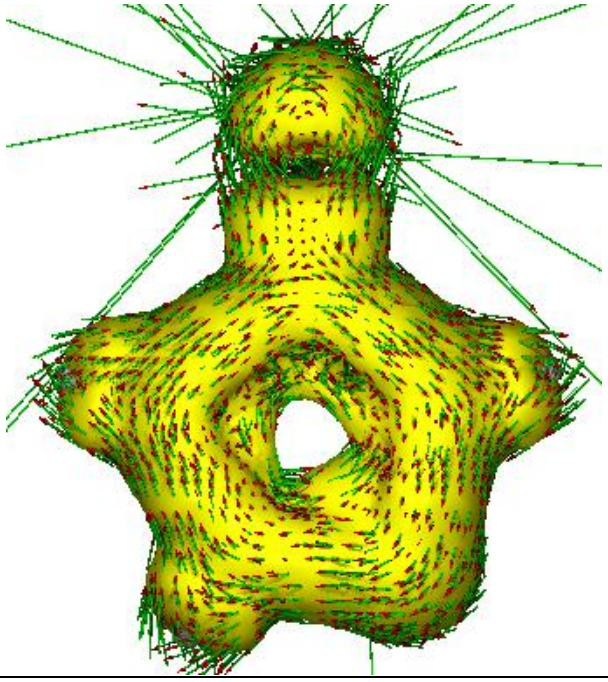
Table S10. AICD plots (isosurface = 0.03) of selected substituted and unsubstituted systems.

pyrrole	imidazole
	
pyrazole	123-triazole N1H
	
123-triazole N2H	124-triazole N1H
	

124-triazole N4H	tetrazole-N1H
	
tetrazole-N2H	imiC2-CN
	
imiC2-NO_2	imiC2-Cl

	
imiC2-OH	pyraC4-CN
	
pyraC4-NO_2	pyraC4-Cl





pyraC4-OH