

Supporting Information

for the paper:

Cooperation/Competition Between Halogen Bonds and Hydrogen Bonds in Complexes of 2,6-diaminopyridine and X-CY₃ (X = Cl, Br; Y = H, F)

Barbara Bankiewicz^{1,2,*} and Marcin Palusiak^{2,*}

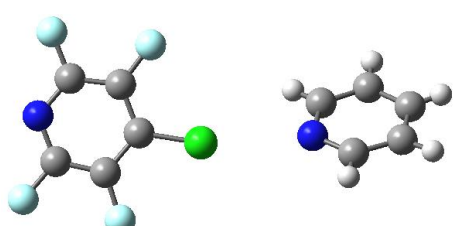
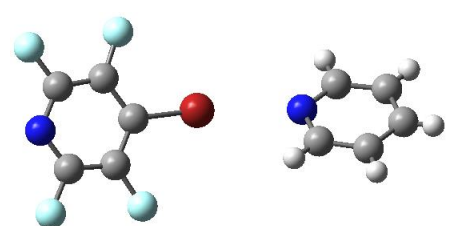
¹ *Department of Structural Chemistry, Faculty of Chemistry, University of Białystok, Ciołkowskiego 1K, 15-245 Białystok, Poland* *E-mail: b.bankiewicz@uwb.edu.pl*

² *Department of Physical Chemistry, Faculty of Chemistry, University of Łódź, Pomorska 163/165, 91-236 Łódź, Poland* *E-mail: marcin.palusiak@chemia.uni.lodz.pl*

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Table S1. Cartesian coordinates of calculated geometries of the halogen bonded complexes of pyridine with 4-chloro-2,3,5,6-tetrafluoropyridine (CSD refcode: FOFZUY) and 4-bromo-2,3,5,6-tetrafluoropyridine (CSD refcode: FOFZOS). Geometries optimized at ω B97X-D/6-311++G level of theory.

FOFZUY		Cartesian coordinates:			
E= -1352.71750066 a.u.		Cl	-0.33426200	-0.51691800	-0.25302400
 <p>Graphical representation.</p>		F	3.61569400	2.58385900	-0.18703500
		F	0.96179600	2.13321800	-0.39627300
		F	1.88488500	-2.47066800	0.18889700
		F	4.49141900	-1.80910200	0.42113500
		N	4.04077400	0.38457100	0.12735600
		C	3.15471800	1.33393800	-0.07281100
		C	1.79642600	1.11707200	-0.19559800
		C	1.32531600	-0.18621200	-0.10964500
		C	2.25701400	-1.19646200	0.09847100
		C	3.59118000	-0.84494200	0.21335300
		N	-3.33415400	-0.41786800	-0.34165900
		C	-4.45693500	-0.99021000	-0.79782400
		H	-4.37486900	-1.71376100	-1.35531200
		C	-5.72821700	-0.59956100	-0.41039600
		H	-6.58060000	-0.98360000	-0.78184000
		C	-5.86401900	0.42993000	0.50938100
		H	-6.67367800	0.76598400	0.74918400
		C	-4.71185500	1.04345500	0.98974900
		H	-4.76742600	1.82754200	1.58565900
		C	-3.48610800	0.59089000	0.52880900
		H	-2.71658200	1.00136800	0.84240200
FOFZOS		Cartesian coordinates:			
E=-3466.62211751 a.u.		Br	-0.42017700	-0.30121800	-0.42672900
 <p>Graphical representation.</p>		F	3.95295600	2.47255400	-0.00828800
		F	1.28670900	2.26887100	-0.45529000
		F	1.75082100	-2.41233400	0.16654500
		F	4.36841800	-1.97445600	0.65530700
		N	4.14627500	0.24914200	0.32269900
		C	3.36696900	1.26969600	0.04229900
		C	2.01495200	1.16357200	-0.19729900
		C	1.42303400	-0.08406300	-0.15944800
		C	2.24044600	-1.16489500	0.11825900
		C	3.57734400	-0.93233500	0.35803300
		N	-3.30592600	-0.21538200	-0.31731500
		C	-4.38196200	-0.93812100	-0.63482200
		H	-4.25671100	-1.70973800	-1.22555900
		C	-5.65728700	-0.66858500	-0.15350800
		H	-6.36286800	-1.21920600	-0.37554300
		C	-5.82553200	0.40735000	0.70900600
		H	-6.57645000	0.59456400	1.02550200
		C	-4.72255000	1.16034500	1.04496400
		H	-4.76739300	1.91439000	1.59517200
		C	-3.49140600	0.82391700	0.51589000
		H	-2.70700600	1.31328700	0.79354400

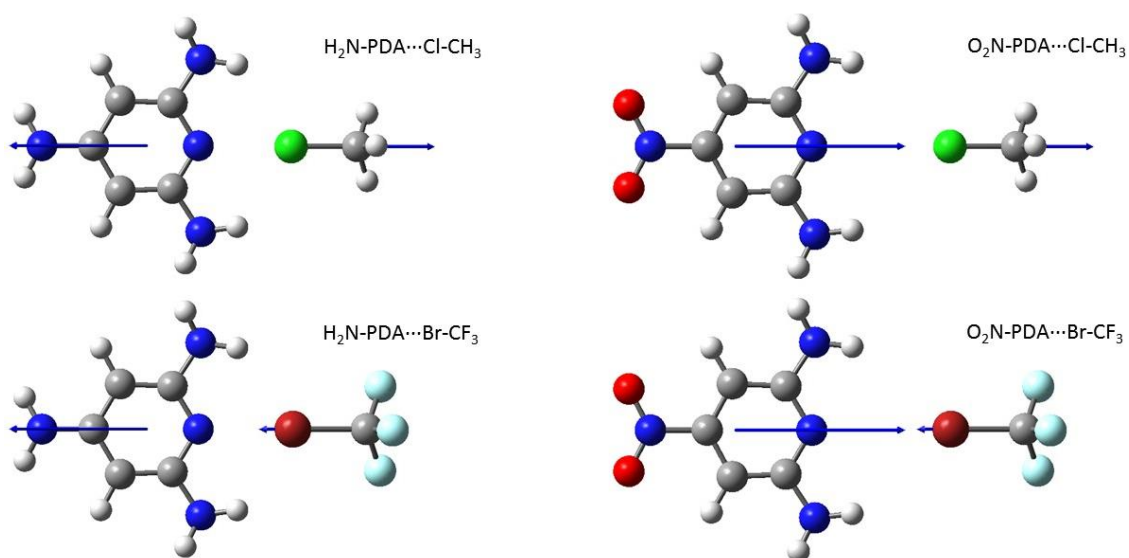


Figure S1. The orientation of dipole moment vectors of the fragments of selected complexes.

Table S2. Dipole moments of the fragments of [R-PDA][X-CY₃] and [R-Pyr][X-CY₃] complexes (ω B97X-D/6-311++G(d,p) level of theory). The dipole moments are given in Debye.

Molecule	μ
H ₂ N-PDA	2.0224
HO-PDA	2.1531
H-PDA	1.762
ON-PDA	3.5606
O ₂ N-PDA	4.6831
H ₂ N-Pyr	4.042
HO-Pyr	2.7791
H-Pyr	2.3834
ON-Pyr	0.8736
O ₂ N-Pyr	2.0883
Cl-CH ₃	2.1135
Br-CH ₃	2.0086
Cl-CF ₃	0.4602
Br-CF ₃	0.6704

Table S3. Bond lengths and selected topological parameters of distribution of electron density [a.u.] in bonds critical points for [PDA][X–CY₃] and [Pyr][X–CY₃] complexes. Electron density – ρ_{BCP} , the Laplacian of the electron density – $\nabla^2\rho_{\text{BCP}}$, potential energy density – V_{BCP} , kinetic energy density – G_{BCP} , and total energy density – H_{BCP} .

DIMER	BCP	d [Å]	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	V_{BCP}	G_{BCP}	H_{BCP}
PDA-ClCF ₃	<i>N···Cl</i>	3.057	1.19E-02	4.02E-02	-7.36E-03	8.71E-03	1.35E-03
	<i>H···Cl</i>	2.967*	-	-	-	-	-
	<i>H···Cl</i>	2.964*	-	-	-	-	-
PDA-ClCH ₃	<i>N···Cl</i>	3.218	8.67E-03	2.99E-02	-5.15E-03	6.31E-03	1.16E-03
	<i>H···Cl</i>	3.065*	3.74E-03	1.36E-02	-1.86E-03	2.63E-03	7.69E-04
	<i>H···Cl</i>	3.065*	3.74E-03	1.36E-02	-1.86E-03	2.63E-03	7.69E-04
PDA-BrCF ₃	<i>N···Br</i>	2.989	1.59E-02	4.79E-02	-9.51E-03	1.07E-02	1.24E-03
	<i>H···Br</i>	2.936	5.92E-03	2.03E-02	-2.98E-03	4.03E-03	1.05E-03
	<i>H···Br</i>	2.937	5.91E-03	2.03E-02	-2.98E-03	4.03E-03	1.05E-03
PDA-BrCH ₃	<i>N···Br</i>	3.171	1.12E-02	3.49E-02	-6.47E-03	7.60E-03	1.13E-03
	<i>H···Br</i>	3.038	4.94E-03	1.63E-02	-2.38E-03	3.23E-03	8.53E-04
	<i>H···Br</i>	3.038	4.94E-03	1.63E-02	-2.38E-03	3.23E-03	8.53E-04
Pyr-ClCF ₃	<i>N···Cl</i>	2.985	1.32E-02	4.65E-02	-8.46E-03	1.00E-02	1.58E-03
Pyr-ClCH ₃	<i>N···Cl</i>	3.402*	5.43E-03	2.02E-02	-3.10E-03	4.07E-03	9.68E-04
	<i>H···Cl</i>	3.034*	4.86E-03	1.76E-02	-2.51E-03	3.45E-03	9.43E-04
Pyr-BrCF ₃	<i>N···Br</i>	2.915	1.77E-02	5.57E-02	-1.10E-02	1.25E-02	1.44E-03
Pyr-BrCH ₃	<i>N···Br</i>	3.148	1.12E-02	3.64E-02	-6.62E-03	7.86E-03	1.24E-03

* the length of interatomic contacts larger than the sum of van der Waals radii of interacting atoms

Table S4. Bond lengths and selected topological parameters of distribution of electron density [a.u.] in bonds critical points for [ON-PDA][X-CY₃] and [ON-Pyr][X-CY₃] complexes.

DIMER	BCP	d [Å]	ρ_{BCP}	$\nabla^2\rho_{BCP}$	V_{BCP}	G_{BCP}	H_{BCP}
ON-PDA-ClCF ₃	<i>N...Cl</i>	3.078	1.14E-02	3.86E-02	-6.99E-03	8.33E-03	1.33E-03
	<i>H...Cl</i>	2.971*	4.32E-03	1.64E-02	-2.24E-03	3.17E-03	9.28E-04
	<i>H...Cl</i>	2.987*	-	-	-	-	-
ON-PDA-ClCH ₃	<i>N...Cl</i>	3.220	8.63E-03	2.99E-02	-5.14E-03	6.30E-03	1.17E-03
	<i>H...Cl</i>	2.978*	4.39E-03	1.55E-02	-2.14E-03	3.00E-03	8.64E-04
	<i>H...Cl</i>	3.134*	-	-	-	-	-
ON-PDA-BrCF ₃	<i>N...Br</i>	3.026	1.47E-02	4.49E-02	-8.76E-03	9.99E-03	1.24E-03
	<i>H...Br</i>	2.949	5.74E-03	1.97E-02	-2.86E-03	3.88E-03	1.03E-03
	<i>H...Br</i>	2.969	5.50E-03	1.90E-02	-2.76E-03	3.75E-03	9.92E-04
ON-PDA-BrCH ₃	<i>N...Br</i>	3.180	1.10E-02	3.45E-02	-6.36E-03	7.49E-03	1.13E-03
	<i>H...Br</i>	3.025	5.05E-03	1.66E-02	-2.40E-03	3.27E-03	8.72E-04
	<i>H...Br</i>	3.052	4.77E-03	1.58E-02	-2.28E-03	3.12E-03	8.36E-04
ON-Pyr-ClCF ₃	<i>N...Cl</i>	3.029	1.20E-02	4.25E-02	-7.59E-03	9.11E-03	1.52E-03
ON-Pyr-ClCH ₃	<i>N...Cl</i>	3.518*	4.24E-03	1.62E-02	-2.39E-03	3.22E-03	8.36E-04
	<i>H...Cl</i>	2.962*	5.50E-03	1.90E-02	-2.77E-03	3.76E-03	9.91E-04
ON-Pyr-BrCF ₃	<i>N...Br</i>	2.962	1.61E-02	5.12E-02	-9.89E-03	1.13E-02	1.45E-03
ON-Pyr-BrCH ₃	<i>N...Br</i>	3.176	1.05E-02	3.45E-02	-6.18E-03	7.40E-03	1.23E-03

* the length of interatomic contacts larger than the sum of van der Waals radii of interacting atoms

Table S5. Bond lengths and selected topological parameters of distribution of electron density [a.u.] in bonds critical points for [O₂N-PDA][X-CY₃] and [O₂N-Pyr][X-CY₃] complexes.

DIMER	BCP	d [Å]	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	V_{BCP}	G_{BCP}	H_{BCP}
O₂N-PDA-ClCF₃	<i>N...Cl</i>	3.073	1.12E-02	3.86E-02	-6.93E-03	8.30E-03	1.36E-03
	<i>H...Cl</i>	3.046*	-	-	-	-	-
	<i>H...Cl</i>	3.046*	-	-	-	-	-
O₂N-PDA-ClCH₃	<i>N...Cl</i>	3.211	8.73E-03	3.03E-02	-5.22E-03	6.40E-03	1.18E-03
	<i>H...Cl</i>	3.066*	3.71E-03	1.35E-02	-1.84E-03	2.61E-03	7.68E-04
	<i>H...Cl</i>	3.066*	3.72E-03	1.35E-02	-1.84E-03	2.61E-03	7.68E-04
O₂N-PDA-BrCF₃	<i>N...Br</i>	3.030	1.44E-02	4.45E-02	-8.60E-03	9.86E-03	1.26E-03
	<i>H...Br</i>	2.992	5.32E-03	1.85E-02	-2.69E-03	3.65E-03	9.63E-04
	<i>H...Br</i>	2.990	5.34E-03	1.85E-02	-2.69E-03	3.66E-03	9.67E-04
O₂N-PDA-BrCH₃	<i>N...Br</i>	3.179	1.09E-02	3.46E-02	-6.36E-03	7.51E-03	1.14E-03
	<i>H...Br</i>	3.051	4.81E-03	1.59E-02	-2.30E-03	3.14E-03	8.40E-04
	<i>H...Br</i>	3.052	4.80E-03	1.59E-02	-2.30E-03	3.14E-03	8.39E-04
O₂N-Pyr-ClCF₃	<i>N...Cl</i>	3.043	1.16E-02	4.14E-02	-7.33E-03	8.84E-03	1.51E-03
O₂N-Pyr-ClCH₃	<i>N...Cl</i>	3.461*	4.76E-03	1.79E-02	-2.69E-03	3.59E-03	9.00E-04
	<i>H...Cl</i>	3.018*	4.94E-03	1.75E-02	-2.50E-03	3.44E-03	9.40E-04
O₂N-Pyr-BrCF₃	<i>N...Br</i>	2.974	1.57E-02	5.01E-02	-9.61E-03	1.11E-02	1.45E-03
O₂N-Pyr-BrCH₃	<i>N...Br</i>	3.178	1.80E-02	5.67E-02	-1.13E-02	1.27E-02	1.46E-03

* the length of interatomic contacts larger than the sum of van der Waals radii of interacting atoms

Table S6. Bond lengths and selected topological parameters of distribution of electron density [a.u.] in bonds critical points for [HO-PDA][X-CY₃] and [HO-Pyr][X-CY₃] complexes.

DIMER	BCP	d [Å]	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	V_{BCP}	G_{BCP}	H_{BCP}
HO-PDA-ClCF ₃	<i>N...Cl</i>	3.028	1.21E-02	4.18E-02	-7.60E-03	9.02E-03	1.42E-03
	<i>H...Cl</i>	3.083*	-	-	-	-	-
	<i>H...Cl</i>	3.086*	-	-	-	-	-
HO-PDA-ClCH ₃	<i>N...Cl</i>	3.214	8.73E-03	3.01E-02	-5.20E-03	6.36E-03	1.17E-03
	<i>H...Cl</i>	3.057*	3.79E-03	1.38E-02	-1.89E-03	2.66E-03	7.78E-04
	<i>H...Cl</i>	3.081*	-	-	-	-	-
HO-PDA-BrCF ₃	<i>N...Br</i>	2.979	1.61E-02	4.89E-02	-9.70E-03	1.10E-02	1.26E-03
	<i>H...Br</i>	2.940	5.98E-03	2.05E-02	-3.02E-03	4.07E-03	1.05E-03
	<i>H...Br</i>	2.932	5.87E-03	2.02E-02	-2.98E-03	4.01E-03	1.04E-03
HO-PDA-BrCH ₃	<i>N...Br</i>	3.166	1.12E-02	3.52E-02	-6.53E-03	7.67E-03	1.14E-03
	<i>H...Br</i>	3.042	4.92E-03	1.63E-02	-2.37E-03	3.22E-03	8.50E-04
	<i>H...Br</i>	3.050	4.84E-03	1.61E-02	-2.34E-03	3.18E-03	8.42E-04
HO-Pyr-ClCF ₃	<i>N...Cl</i>	2.974	1.34E-02	4.74E-02	-8.66E-03	1.03E-02	1.60E-03
HO-Pyr-ClCH ₃	<i>N...Cl</i>	3.425*	5.18E-03	1.93E-02	-2.94E-03	3.87E-03	9.39E-04
	<i>H...Cl</i>	3.031*	4.88E-03	1.75E-02	-2.50E-03	3.44E-03	9.36E-04
HO-Pyr-BrCF ₃	<i>N...Br</i>	2.905	1.80E-02	5.67E-02	-1.13E-02	1.27E-02	1.46E-03
HO-Pyr-BrCH ₃	<i>N...Br</i>	3.148	1.12E-02	3.63E-02	-6.59E-03	7.84E-03	1.25E-03

* the length of interatomic contacts larger than the sum of van der Waals radii of interacting atoms

Table S7. Bond lengths and selected topological parameters of distribution of electron density [a.u.] in bonds critical points for [H₂N-PDA][X-CY₃] and [H₂N-Pyr][X-CY₃] complexes.

DIMER	BCP	d [Å]	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	V_{BCP}	G_{BCP}	H_{BCP}
H₂N-PDA-ClCF₃	<i>N...Cl</i>	3.009	1.25E-02	4.32E-02	-7.90E-03	9.34E-03	1.45E-03
	<i>H...Cl</i>	3.098*	-	-	-	-	-
	<i>H...Cl</i>	3.101*	-	-	-	-	-
H₂N-PDA-ClCH₃	<i>N...Cl</i>	3.219	8.69E-03	2.99E-02	-5.16E-03	6.31E-03	1.16E-03
	<i>H...Cl</i>	3.176*	-	-	-	-	-
	<i>H...Cl</i>	2.951	4.68E-03	1.64E-02	-2.28E-03	3.19E-03	9.03E-04
H₂N-PDA-BrCF₃	<i>N...Br</i>	2.958	1.67E-02	5.06E-02	-1.01E-02	1.14E-02	1.27E-03
	<i>H...Br</i>	2.931	6.02E-03	2.07E-02	-3.08E-03	4.13E-03	1.05E-03
	<i>H...Br</i>	2.929	6.05E-03	2.08E-02	-3.09E-03	4.15E-03	1.06E-03
H₂N-PDA-BrCH₃	<i>N...Br</i>	3.162	1.13E-02	3.55E-02	-6.59E-03	7.73E-03	1.14E-03
	<i>H...Br</i>	3.047	4.88E-03	1.62E-02	-2.37E-03	3.21E-03	8.44E-04
	<i>H...Br</i>	3.047	4.88E-03	1.62E-02	-2.37E-03	3.21E-03	8.44E-04
H₂N-Pyr-ClCF₃	<i>N...Cl</i>	2.951	1.41E-02	4.96E-02	-9.14E-03	1.08E-02	1.63E-03
H₂N-Pyr-ClCH₃	<i>N...Cl</i>	3.445*	4.97E-03	1.85E-02	-2.81E-03	3.72E-03	9.11E-04
	<i>H...Cl</i>	3.038*	4.80E-03	1.71E-02	-2.45E-03	3.37E-03	9.17E-04
H₂N-Pyr-BrCF₃	<i>N...Br</i>	2.881	1.89E-02	5.92E-02	-1.19E-02	1.34E-02	1.45E-03
H₂N-Pyr-BrCH₃	<i>N...Br</i>	3.134	1.15E-02	3.73E-02	-6.80E-03	8.06E-03	1.26E-03

* the length of interatomic contacts larger than the sum of van der Waals radii of interacting atoms

Table S8. Fluctuations of the electron density values at the critical points of halogen and hydrogen bonds in complexes of the [R-PDA][X-CY₃] in relation to [PDA][X-CY₃].

R	$\Delta\rho_{N\cdots X}$ (halogen bonds)			
	ClCF ₃	ClCH ₃	BrCF ₃	BrCH ₃
NH ₂	0.00063 (+5.3%)	0.00002 (+0.2%)	0.00087 (+5.5%)	0.00018 (+1,6%)
OH	0.00021 (+1.8%)	0.00005 (+0.6%)	0.00025 (+1.6%)	0.00008 (+0,7%)
NO	-0.00054 (-4.5%)	-0.00004 (-0.5%)	-0.00114 (-7.2%)	-0.00021 (-1,8%)
NO ₂	-0.00069 (-5.8%)	0.00006 (+0.7%)	-0.00142 (-8.9%)	-0.00023 (-2,0%)
R	$\Delta\rho_{H\cdots X}$ (hydrogen bonds)			
	ClCF ₃	ClCH ₃	BrCF ₃	BrCH ₃
NH ₂	-	-	0.00010 (+1.7%)	-0.00006 (-1.2%)
	-	0.00094 (+25.1%)	0.00014 (+2.4%)	-0.00006 (-1.2%)
OH	-	0.00005 (+1.4%)	0.00006 (+0.9%)	-0.00003 (-0.5%)
	-	-	-0.00004 (-0.8%)	-0.00010 (-2.0%)
NO	-	0.00065 (+11.0%)	-0.00018 (-3.1%)	0.00011 (+2.2%)
	-	-	-0.00042 (-7.0%)	-0.00017 (-3.5%)
NO ₂	-	-0.00003 (-0.6%)	-0.00060 (-10.2%)	-0.00013 (-2.7%)
	-	-0.00002 (-0.5%)	-0.00057 (-9.7%)	-0.00014 (-2.9%)

Table S9. Fluctuations of the electron density values at the critical points of halogen and hydrogen bonds in complexes of the [R-Pyr][X-CY₃] in relation to [Pyr][X-CY₃].

R	$\Delta\rho_{N\cdots X}$ (halogen bonds)			
	ClCF ₃	ClCH ₃	BrCF ₃	BrCH ₃
NH ₂	0.00091 (+6.9%)	-0.00046 (-8.5%)	0.00121 (+6.9%)	0.00029 (+2.6%)
OH	0.00025 (+1.9%)	-0.00025 (-4.6%)	0.00031 (+1.7%)	-0.00005 (-0.4%)
NO	-0.00121 (-9.2%)	-0.00119 (-21.9%)	-0.00165 (-9.3%)	-0.00071 (-6.3%)
NO ₂	-0.00157 (-11.9%)	-0.00067 (-12.3%)	-0.00207 (-11.7%)	0.00678 (+60.3%)
R	$\Delta\rho_{H\cdots X}$ (hydrogen bonds)			
	ClCF ₃	ClCH ₃	BrCF ₃	BrCH ₃
NH ₂	-	-0.00006 (-1.2%)	-	-
OH	-	0.00003 (+0.5%)	-	-
NO	-	0.00065 (+13.3%)	-	-
NO ₂	-	0.00009 (+1.8%)	-	-

Table S10. Fluctuations of the total interaction energy values of the [R-PDA][X-CY₃] and [R-Pyr][X-CY₃] complexes in relation to [PDA][X-CY₃] and [Pyr][X-CY₃].

R	ΔE_{tot}			
	ClCF ₃	ClCH ₃	BrCF ₃	BrCH ₃
<i>[R-PDA][X-CY₃] complexes</i>				
NH₂	-0.131 (+5.0%)	0.148 (-9.7%)	-0.215 (+4.8%)	0.188 (-6.5%)
OH	-0.106 (+4.0%)	0.005 (-0.3%)	-0.091 (+2.0%)	-0.023 (+0.8%)
NO	0.282 (-10.7%)	-0.348 (+22.8%)	0.513 (-11.4%)	-0.204 (+7.1%)
NO₂	0.327 (-12.4%)	-0.555 (+36.3%)	0.648 (-14.4%)	-0.275 (+9.5%)
<i>[R-Pyr][X-CY₃] complexes</i>				
NH₂	-0.336 (+12.7%)	0.137 (-9.0%)	-0.584 (+12.5%)	-0.022 (+1.4%)
OH	-0.083 (+3.1%)	-0.002 (+0.2%)	-0.141 (+3.0%)	-0.035 (+2.2%)
NO	0.460 (-17.3%)	-0.383 (+25.1%)	0.780 (-16.7%)	-0.095 (+6.0%)
NO₂	0.582 (-21.9%)	-0.495 (+32.4%)	1.002 (-21.4%)	-0.116 (+7.4%)

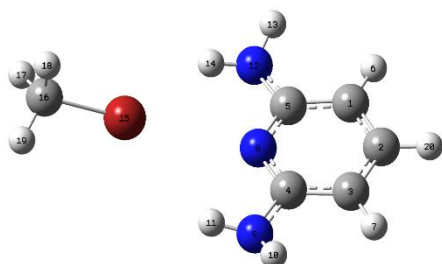
* the percentage increase or decrease of the total interaction energy was calculated relative to the [PDA][X-CY₃] and [Pyr][X-CY₃] systems

Table S11. Cartesian coordinates of calculated geometries of the studied complexes.
Geometries optimized at ω B97X-D/6-311++G(d,p) level of theory.

PDA⋯ClCF ₃		Cartesian coordinates:			
E=-1156.85391606 a.u.		C	-3.59555300	-1.20385700	0.17045500
		C	-4.26992900	-0.00198300	0.30572400
		C	-3.59776400	1.20114600	0.17085500
		C	-2.22425900	1.14826600	-0.09737600
		C	-2.22215700	-1.14839000	-0.09768200
		H	-4.10495800	-2.15525200	0.25818600
		H	-4.10888100	2.15160200	0.25882600
		N	-1.55284900	0.00056200	-0.21814600
		N	-1.49344000	2.30017100	-0.29029200
		H	-1.85491700	3.15033200	0.10702200
		H	-0.49328700	2.19318800	-0.24297800
		N	-1.48914600	-2.29894300	-0.29082500
		H	-1.84905600	-3.14964400	0.10679300
		H	-0.48923700	-2.18979700	-0.24256100
		Cl	1.50127100	0.00142300	-0.09162600
		C	3.25531400	-0.00027300	0.07518600
		F	3.80411800	-0.84738700	-0.78611200
		F	3.60581100	-0.36465400	1.30273100
		F	3.74423700	1.21164100	-0.15766800
		H	-5.33462900	-0.00300900	0.51365000
PDA⋯ClCH ₃		Cartesian coordinates:			
E=-859.11758738 a.u.		C	2.54727900	1.20339300	0.24072000
		C	3.20519700	-0.00007500	0.43605200
		C	2.54718800	-1.20349200	0.24071000
		C	1.20376200	-1.14742800	-0.15263200
		C	1.20384800	1.14743200	-0.15262200
		H	3.04763800	2.15411500	0.37655900
		H	3.04747800	-2.15425200	0.37654000
		N	0.55183500	0.00002800	-0.33839000
		N	0.47992400	-2.29367900	-0.40782800
		H	0.78340700	-3.13810400	0.04705900
		H	-0.51881900	-2.15692000	-0.43689900
		N	0.48009800	2.29374100	-0.40780600
		H	0.78365100	3.13814100	0.04707900
		H	-0.51865600	2.15706100	-0.43687600
		Cl	-2.64507200	0.00000500	0.03191500
		C	-4.41163100	0.00003900	0.33074900
		H	-4.83968700	0.89202700	-0.12093900
		H	-4.58250300	0.00031500	1.40486400
		H	-4.83964800	-0.89219800	-0.12048300
		H	4.24649900	-0.00011600	0.74085200
PDA⋯BrCF ₃		Cartesian coordinates:			
E=-3270.81908198 a.u.		C	3.83460600	1.20213000	0.13294000
		C	4.51392200	0.00009400	0.23344800
		C	3.83470200	-1.20199300	0.13291900
		C	2.44932500	-1.14981400	-0.06416200
		C	2.44923200	1.14984800	-0.06415800
		H	4.34838700	2.15312300	0.19492000
		H	4.34855100	-2.15295000	0.19488400
		N	1.77276400	-0.00001300	-0.14987000
		N	1.71469000	-2.30324500	-0.21874100
		H	2.10533400	-3.15493700	0.14583400
		H	0.71653800	-2.21086100	-0.12422800
		N	1.71452500	2.30322800	-0.21871400
		H	2.10532000	3.15502600	0.14544100
		H	0.71638300	2.21098900	-0.12406700
		Br	-1.21528400	-0.00028900	-0.06712200
		C	-3.14066200	0.00009300	0.07499600
		F	-3.64359900	1.14740000	-0.37009300
		F	-3.51981900	-0.15643200	1.33987800
		F	-3.66477700	-0.99011800	-0.64047500
		H	5.58758800	0.00013900	0.38808600

PDA \cdots BrCH₃

E=-2973.086657 a.u.



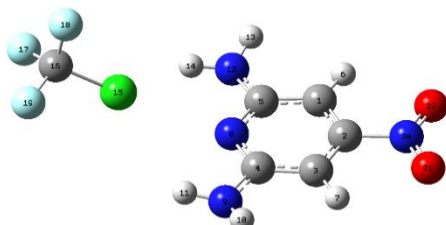
Graphical representation.

Cartesian coordinates:

C	-3.02400100	-1.20303400	0.21234600
C	-3.68809200	0.00009800	0.38547000
C	-3.02390300	1.20317400	0.21232700
C	-1.66750300	1.14835400	-0.13361000
C	-1.66759700	-1.14832700	-0.13359200
H	-3.52885800	-2.15381000	0.32947600
H	-3.52868500	2.15399100	0.32944500
N	-1.00791300	-0.00001500	-0.29347000
N	-0.94108900	2.29621900	-0.36654000
H	-1.26772000	3.14327100	0.06644800
H	0.05955400	2.17213500	-0.36998500
N	-0.94127500	-2.29625500	-0.36650600
H	-1.26796100	-3.14326900	0.06651500
H	0.05937600	-2.17224800	-0.36996400
Br	2.14862900	-0.00008800	0.01409400
C	4.07279300	0.00016700	0.28749900
H	4.48357700	-0.89306800	-0.17599900
H	4.26654400	0.00047900	1.35704400
H	4.48340200	0.89323400	-0.17648300
H	-4.73948700	0.00014300	0.65317100

O₂N-PDA \cdots ClCF₃

E=-1361.34817279 a.u.



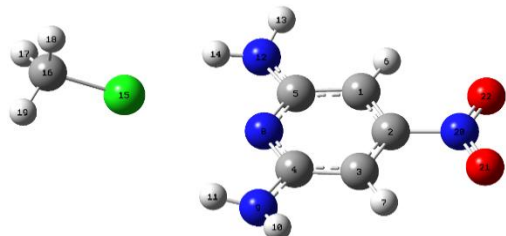
Graphical representation.

Cartesian coordinates:

C	-2.51168200	-1.21235400	-0.12305300
C	-3.13699600	0.00016200	0.07048400
C	-2.51106400	1.21229700	-0.12336100
C	-1.16962400	1.15031300	-0.52957000
C	-1.17021400	-1.15114500	-0.52926500
H	-3.03364600	-2.14611600	0.02477400
H	-3.03259700	2.14636100	0.02409200
N	-0.51959800	-0.00061100	-0.71395400
N	-0.46509400	2.29455700	-0.79091900
H	-0.79947500	3.16427000	-0.41467200
H	0.53177400	2.19796200	-0.88852800
N	-0.46621500	-2.29581800	-0.79037200
H	-0.80093200	-3.16515000	-0.41352100
H	0.53076700	-2.19953100	-0.88732900
Cl	2.49691000	-0.00144100	-0.12683100
C	4.20213600	0.00020400	0.32623700
F	4.85064500	-0.96295400	-0.31421000
F	4.33419400	-0.19737000	1.63044900
F	4.75941400	1.16326600	0.01694400
N	-4.55782300	0.00060100	0.50446000
O	-5.09337200	1.07690500	0.66802400
O	-5.09361000	-1.07537500	0.66939100

O₂N-PDA \cdots ClCH₃

E=-1063.61313144 a.u.



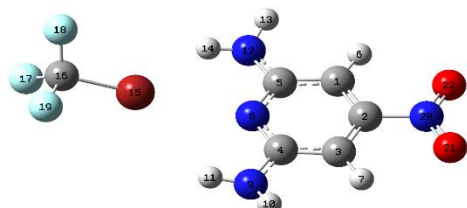
Graphical representation.

Cartesian coordinates:

C	-1.50879500	-1.21310100	-0.09235600
C	-2.15296100	-0.00006100	0.02587400
C	-1.50901300	1.21312900	-0.09201800
C	-0.12875800	1.15003000	-0.33819800
C	-0.12855700	-1.14968900	-0.33855500
H	-2.04391600	-2.14689300	-0.00328000
H	-2.04431300	2.14680300	-0.00278800
N	0.53450200	0.00024700	-0.45171500
N	0.61187800	2.29071700	-0.50838500
H	0.24776200	3.15427200	-0.14489700
H	1.61119500	2.16952800	-0.45978600
N	0.61226800	-2.29019200	-0.50911800
H	0.24825400	-3.15394600	-0.14600400
H	1.61156700	-2.16887500	-0.46047800
Cl	3.68747000	0.00018800	0.15846100
C	5.43121500	-0.00047900	0.57493400
H	5.88662100	-0.89176000	0.14982100
H	5.52976200	-0.00297100	1.65792100
H	5.88634400	0.89287500	0.15389800
N	-3.61367300	-0.00023800	0.29427200
O	-4.16615700	1.07555000	0.39593700
O	-4.16557800	-1.07616700	0.39759800

O₂N-PDA···BrCF₃

E=-3475.3128431 a.u.



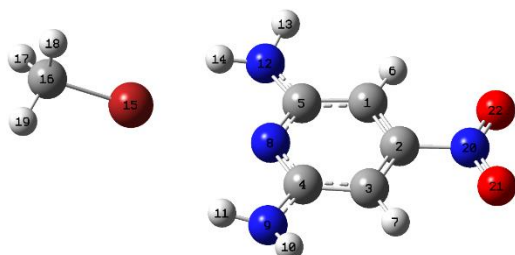
Graphical representation.

Cartesian coordinates:

C	-2.87759600	-1.21181800	-0.08190800
C	-3.51775200	0.00023000	0.05479300
C	-2.87709400	1.21197400	-0.08213700
C	-1.50404900	1.15175900	-0.36369100
C	-1.50447300	-1.15221000	-0.36318400
H	-3.41061900	-2.14570900	0.01770000
H	-3.40974700	2.14610200	0.01722700
N	-0.83839300	-0.00037400	-0.48445400
N	-0.78489200	2.29821200	-0.56096300
H	-1.16190900	3.16861000	-0.22961000
H	0.21783700	2.21597900	-0.57559200
N	-0.78561100	-2.29900700	-0.55972000
H	-1.16315900	-3.16906500	-0.22806900
H	0.21718100	-2.21695100	-0.57299900
Br	2.16506700	-0.00161400	-0.08473000
C	4.06710000	0.00051000	0.25464800
F	4.72088000	-0.57400400	-0.74775500
F	4.34273600	-0.66514500	1.37001900
F	4.51297200	1.24442800	0.38813000
N	-4.97170000	0.00058300	0.36118800
O	-5.51892400	1.07696400	0.47805400
O	-5.51968300	-1.07553000	0.47692700

O₂N-PDA···BrCH₃

E=-3177.58190197 a.u.



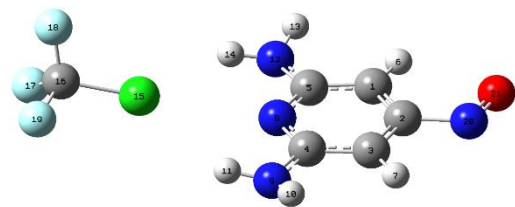
Graphical representation.

Cartesian coordinates:

C	2.05028300	1.21278900	-0.08937300
C	2.69483200	-0.00009300	0.02467300
C	2.04988800	-1.21274800	-0.08954400
C	0.66785700	-1.15040300	-0.32555900
C	0.66823000	1.15092300	-0.32539000
H	2.58627700	2.14650700	-0.00509100
H	2.58559100	-2.14664600	-0.00538700
N	0.00275800	0.00037700	-0.43136400
N	-0.06906800	-2.29265700	-0.49309400
H	0.30343200	-3.15755500	-0.14188000
H	-1.06967000	-2.18251300	-0.44679700
N	-0.06833200	2.29343600	-0.49274200
H	0.30444900	3.15818200	-0.14145800
H	-1.06896700	2.18360400	-0.44651000
Br	-3.13320500	0.00006200	0.08878300
C	-5.03221100	-0.00051900	0.50379500
H	-5.47428500	0.89279900	0.07061600
H	-5.14593800	-0.00066700	1.58462100
H	-5.47378000	-0.89396900	0.07043900
N	4.15751500	-0.00035300	0.28281600
O	4.70991900	-1.07637000	0.38141000
O	4.71029100	1.07546700	0.38148200

ON-PDA···ClCF₃

E=-1286.13415678 a.u.

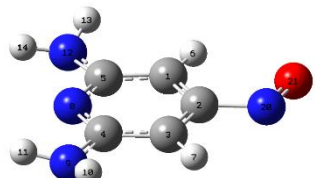


Graphical representation.

Cartesian coordinates:

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.38472402
C	1.16853050	0.00000000	2.12033719
C	2.37188792	-0.00794940	1.39545075
C	1.25266658	-0.00764726	-0.62042445
H	-0.92614319	0.01203291	-0.55880982
H	1.13925517	0.01147751	3.20241220
N	2.40446674	-0.02127514	0.06372802
N	3.58153713	0.03225721	2.03922080
H	3.61824210	-0.24239670	3.00525829
H	4.39385586	-0.17885311	1.48373148
N	1.36751415	0.03339281	-1.98710953
H	0.57504339	-0.24573086	-2.53884423
H	2.27296703	-0.19018986	-2.36552501
Cl	5.05035270	-0.66210739	-1.37326896
C	6.55601810	-1.11007677	-2.17575867
F	6.75167338	-0.35490204	-3.24776700
F	6.51802175	-2.38027853	-2.55609884
F	7.58281700	-0.94778150	-1.35160909
N	-1.21894184	0.00366535	2.18218851
O	-2.23480727	0.00210544	1.54516681

E=-988.39885635 a.u.

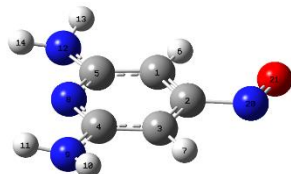
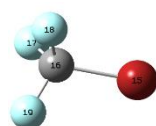


Graphical representation.

Cartesian coordinates:

Cartesian coordinates		
C	-1.93990600	-1.04795400
C	-2.50549800	0.20927200
C	-1.76036000	1.36823300
C	-0.38596700	1.21415500
C	-0.56407700	-1.08317800
H	-2.54262900	-1.94304000
H	-2.23200000	2.33718700
N	0.18535700	0.02018400
N	0.43754600	2.30079300
H	0.14006900	3.17916600
H	1.42518000	2.10435300
N	0.10138100	-2.26938600
H	-0.31573800	-3.10800300
H	1.10586000	-2.21212300
Cl	3.36421100	-0.10534100
C	5.12089500	-0.13151700
H	5.54430800	-1.04092800
H	5.25729800	-0.11168100
H	5.57868000	0.74286300
N	-3.92041900	0.42230700
O	-4.57127400	-0.58104300

E=-3400.09896949 a.u.

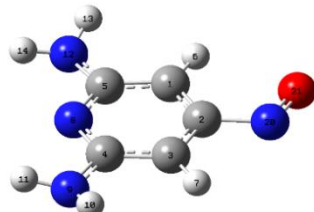


Graphical representation.

Cartesian coordinates:

C	-3.26302200	-1.06297000	-0.01807900
C	-3.88101900	0.17165100	0.08172200
C	-3.17400900	1.35536900	0.01594600
C	-1.78271500	1.25404600	-0.14978300
C	-1.87484100	-1.05226800	-0.18195700
H	-3.83581500	-1.97964600	0.02374600
H	-3.68422400	2.30755600	0.08540200
N	-1.15682700	0.07937500	-0.23499400
N	-1.00824000	2.37759700	-0.26513700
H	-1.38203100	3.25221600	0.05895700
H	-0.01219100	2.25880900	-0.18319700
N	-1.17383500	-2.22046600	-0.33279000
N	-1.60468900	-3.07644700	-0.03001600
H	-0.17350700	-2.16763500	-0.23643700
Br	1.86310900	-0.01417700	-0.06710800
C	3.78408100	-0.06536600	0.13026400
F	4.24427500	-1.28761600	-0.11212900
F	4.13618000	0.27641600	1.36483100
F	4.36383600	0.77649400	-0.71742400
N	-5.31852600	0.33175400	0.25964200
O	-5.93297700	-0.69585900	0.31963900

E=-3102.36768128 a.u.



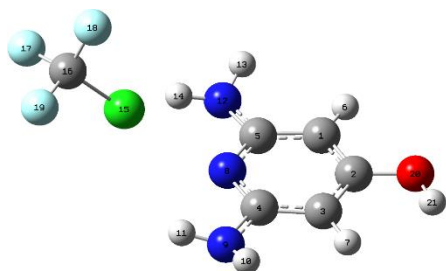
Graphical representation.

Cartesian coordinates:

C	-2.43649500	-1.05463200	-0.04333400
C	-3.03655300	0.18640100	0.09251400
C	-2.32098800	1.36454500	0.00242600
C	-0.93953800	1.24847700	-0.22736100
C	-1.05672200	-1.05416300	-0.27044800
H	-3.01634500	-1.96565700	0.01933100
H	-2.81860500	2.32080100	0.10189800
N	-0.33390800	0.06964200	-0.35074100
N	-0.14808500	2.35917100	-0.36994200
H	-0.47993800	3.23003700	0.00656700
H	0.84597000	2.20063700	-0.31940800
N	-0.36319300	-2.22319800	-0.45947400
H	-0.76998200	-3.07489700	-0.11357100
H	0.64002100	-2.15183800	-0.39566600
Br	2.81675900	-0.06223300	0.06290700
C	4.73055000	-0.13079500	0.39562300
H	5.12892900	-1.01609900	-0.09297700
H	4.88920400	-0.18107100	1.46960100
H	5.17948900	0.76831600	-0.01811300
N	-4.46069400	0.36098500	0.33646100
O	-5.08571000	-0.65965700	0.41874200

HO-PDA \cdots ClCF₃

E=-1232.08298123 a.u.



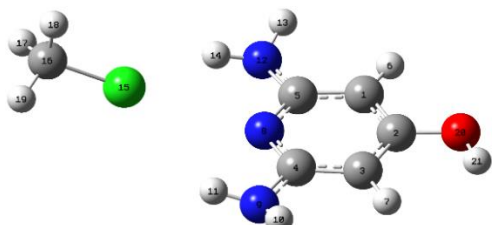
Graphical representation.

Cartesian coordinates:

C	-3.02920400	-1.21445100	0.18491000
C	-3.64141600	-0.01016200	0.49762200
C	-3.03241900	1.19651400	0.17055300
C	-1.79161800	1.13590600	-0.47021700
C	-1.79157200	-1.15464800	-0.45752600
H	-3.51120100	-2.15385000	0.41996300
H	-3.50544400	2.14859900	0.38398100
N	-1.17438600	-0.00887700	-0.76800100
N	-1.14744900	2.28724000	-0.86711300
H	-1.36230800	3.13608000	-0.37238100
H	-0.17944900	2.16894100	-1.11898300
N	-1.14309200	-2.30491200	-0.84383300
H	-1.37235600	-3.15639700	-0.36067600
H	-0.17464100	-2.19229300	-1.09515600
Cl	1.79448500	-0.00211400	-0.17227500
C	3.49507200	0.00544700	0.28476800
F	4.15246800	-0.95653000	-0.35135900
F	3.62768100	-0.18968400	1.59076500
F	4.05374200	1.16995300	-0.02352400
O	-4.84198500	-0.06478700	1.11874700
H	-5.16855000	0.82372200	1.27097700

HO-PDA \cdots ClCH₃

E=-934.34648808 a.u.



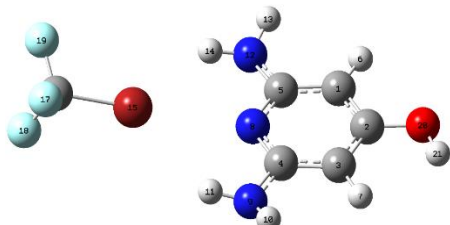
Graphical representation.

Cartesian coordinates:

C	2.15314900	1.21550900	0.07734500
C	2.82158800	0.01113700	0.23772200
C	2.15223400	-1.19623800	0.06890700
C	0.79433700	-1.13471300	-0.26125700
C	0.79763100	1.15347000	-0.25421300
H	2.67544600	2.15541200	0.19591300
H	2.66057700	-2.14839900	0.17448900
N	0.12945100	0.00868500	-0.41518600
N	0.06456300	-2.28378500	-0.48445200
H	0.38303100	-3.12552000	-0.03478400
H	-0.93429700	-2.14434300	-0.47211700
N	0.06649900	2.30048500	-0.47110300
H	0.39677800	3.14752000	-0.04093200
H	-0.93274800	2.16723100	-0.45695000
Cl	-3.04380800	-0.00687000	0.09721600
C	-4.79999700	-0.01124300	0.45206400
H	-5.24333200	0.88159300	0.01709600
H	-4.93761000	-0.01506300	1.53096300
H	-5.24062500	-0.90249700	0.01110800
O	4.13663800	0.06502300	0.55830300
H	4.48716900	-0.82455000	0.62790400

HO-PDA \cdots BrCF₃

E=-3346.04812636 a.u.



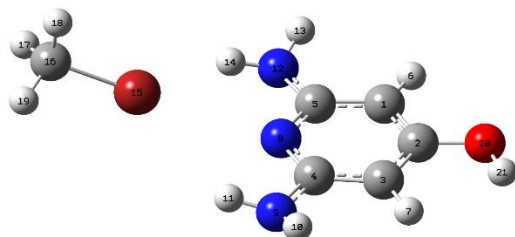
Graphical representation.

Cartesian coordinates:

C	-3.46917400	1.21371900	-0.06470700
C	-4.15059200	0.01116700	-0.17111200
C	-3.46964100	-1.19574100	-0.05948100
C	-2.08952100	-1.13920500	0.15465300
C	-2.09150200	1.15417100	0.15062900
H	-3.99868600	2.15429400	-0.13431200
H	-3.98521800	-2.14766400	-0.11937800
N	-1.40802000	0.00610100	0.24678000
N	-1.36219500	-2.29557200	0.32135300
H	-1.74209400	-3.14478500	-0.05996800
H	-0.36250500	-2.20019400	0.24746400
N	-1.36150900	2.30734100	0.31335600
H	-1.74929600	3.16142600	-0.04818200
H	-0.36188400	2.21622500	0.23816700
Br	1.56520500	0.00187000	0.06763700
C	3.48656500	-0.00530700	-0.12078200
F	3.87489900	-0.98429100	-0.93310700
F	4.07618600	-0.18469800	1.05657600
F	3.91233100	1.14817900	-0.62747800
O	-5.48536600	0.06803300	-0.37949500
H	-5.84503600	-0.81963600	-0.42467100

HO-PDA \cdots BrCH₃

E=-3048.31560167 a.u.



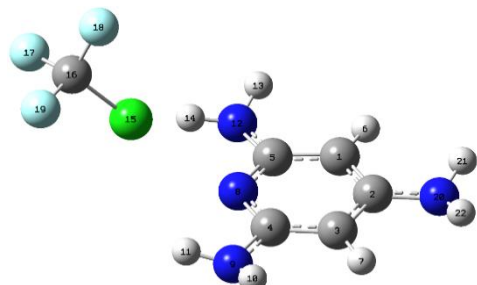
Graphical representation.

Cartesian coordinates:

C	2.64760600	1.21667000	0.07380300
C	3.31968300	0.01402700	0.23031900
C	2.65143300	-1.19447600	0.06701800
C	1.29076700	-1.13707500	-0.25159600
C	1.28956200	1.15298100	-0.24612800
H	3.16919000	2.15771300	0.18590800
H	3.16265700	-2.14560300	0.16724400
N	0.62084000	0.00582000	-0.39789200
N	0.56702800	-2.28932400	-0.47087400
H	0.89809400	-3.13252600	-0.03365700
H	-0.43353800	-2.16428600	-0.45801600
N	0.55987400	2.30005200	-0.46073600
H	0.89875100	3.14987000	-0.04331100
H	-0.44050700	2.17685500	-0.44605800
Br	-2.51283000	-0.00387100	0.05368600
C	-4.42319900	-0.00921000	0.41094200
H	-4.85550300	0.88410200	-0.03242200
H	-4.57105200	-0.01228500	1.48780000
H	-4.85177400	-0.90203300	-0.03702300
O	4.63669200	0.07099400	0.54019400
H	4.98987800	-0.81759300	0.60931800

H₂N-PDA \cdots ClCF₃

E=-1212.2185633 a.u.



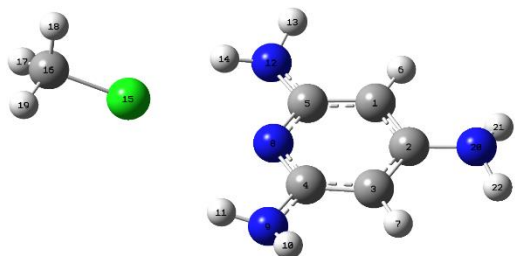
Graphical representation.

Cartesian coordinates:

C	-2.98711700	-1.20092900	0.17510200
C	-3.60134600	0.00295400	0.52437600
C	-2.98319500	1.20390900	0.17203200
C	-1.76998600	1.14182300	-0.51179400
C	-1.77376400	-1.14450900	-0.50894500
H	-3.45260200	-2.15304600	0.40191600
H	-3.44565600	2.15809800	0.39631200
N	-1.16084700	-0.00275800	-0.83683400
N	-1.13565500	2.29339600	-0.92921800
H	-1.33186100	3.13971600	-0.42246200
H	-0.17491700	2.17187600	-1.20618700
N	-1.14316400	-2.29916600	-0.92367500
H	-1.34197000	-3.14351000	-0.41462600
H	-0.18193100	-2.18122000	-1.20055500
Cl	1.77583000	-0.00418200	-0.17912300
C	3.46574900	0.00061900	0.31195500
F	4.13856600	-0.95448000	-0.31952600
F	3.57340300	-0.20731600	1.61897900
F	4.03047300	1.16860300	0.02708300
N	-4.82702600	0.00580900	1.15992700
H	-5.09010000	-0.83677100	1.64313900
H	-5.08726800	0.85050800	1.64097300

H₂N-PDA \cdots ClCH₃

E=-914.48178911 a.u.



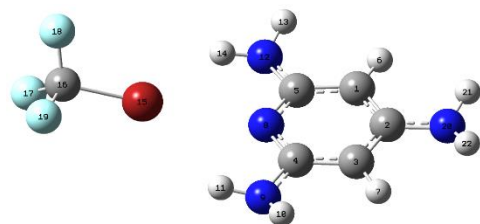
Graphical representation.

Cartesian coordinates:

C	-2.09404000	-1.23524900	0.04982600
C	-2.83972900	-0.06718800	0.21475800
C	-2.20383600	1.16718500	0.07610300
C	-0.84057600	1.17175200	-0.22111300
C	-0.73663700	-1.10968400	-0.24704200
H	-2.55574500	-2.21154900	0.14324900
H	-2.75095700	2.09602000	0.19025200
N	-0.11498700	0.06353500	-0.37704800
N	-0.15792100	2.35773500	-0.41095700
H	-0.52291200	3.17251400	0.05322000
H	0.84513000	2.26055300	-0.37154200
N	0.04993400	-2.22409700	-0.46450100
H	-0.24110900	-3.07912100	-0.02090600
H	1.04055400	-2.03864900	-0.41956000
Cl	3.06908800	0.04162300	0.09640200
C	4.83156800	-0.06182900	0.40035100
H	5.26437200	-0.76434600	-0.30837000
H	4.98989400	-0.40606500	1.41990000
H	5.26654000	0.92567100	0.26359800
N	-4.18104300	-0.13214400	0.55227700
H	-4.65245400	-0.99377400	0.33038200
H	-4.73019600	0.68603400	0.34525100

H₂N-PDA···BrCF₃

E=-3326.18389461 a.u.



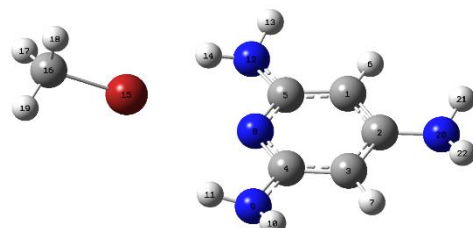
Graphical representation.

Cartesian coordinates:

C	-3.43750700	-1.20164200	0.07019200
C	-4.13245300	0.00014800	0.21360000
C	-3.43741700	1.20187400	0.07042000
C	-2.07215500	1.14474800	-0.20512700
C	-2.07222600	-1.14462500	-0.20513000
H	-3.94683300	-2.15526900	0.14528400
H	-3.94666200	2.15554800	0.14544800
N	-1.38961100	0.00006100	-0.32791700
N	-1.35110400	2.30178600	-0.40565700
H	-1.71555300	3.14943400	-0.00600300
H	-0.34957100	2.20567200	-0.36655400
N	-1.35100600	-2.30161800	-0.40535900
H	-1.71596300	-3.14935400	-0.00636200
H	-0.34951800	-2.20527000	-0.36480500
Br	1.55851100	-0.00114600	-0.08083300
C	3.47364400	0.00015900	0.15955800
F	4.08171200	-0.56743400	-0.87776900
F	3.81221400	-0.67274200	1.25628700
F	3.93125900	1.24376800	0.27921300
N	-5.49325400	0.00016800	0.44082500
H	-5.89350100	-0.84418600	0.81398200
H	-5.89343100	0.84444200	0.81424400

H₂N-PDA···BrCH₃

E=-3028.45081047 a.u.



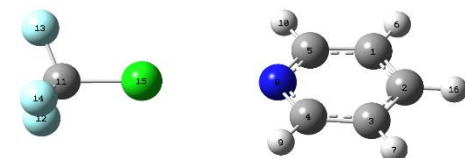
Graphical representation.

Cartesian coordinates:

C	2.63374600	1.20243300	0.06112300
C	3.32137900	-0.00004800	0.23124900
C	2.63368500	-1.20249100	0.06110000
C	1.27983800	-1.14287000	-0.27012700
C	1.27989500	1.14288500	-0.27010200
H	3.13995000	2.15587800	0.15905900
H	3.13984000	-2.15596300	0.15902600
N	0.60717200	0.00002700	-0.42499700
N	0.55472400	-2.29528600	-0.49506900
H	0.88273800	-3.13650500	-0.05158100
H	-0.44546900	-2.16787800	-0.48111500
N	0.55483900	2.29534300	-0.49501800
H	0.88287900	3.13652900	-0.05148500
H	-0.44535900	2.16798000	-0.48108700
Br	-2.51632400	0.00007400	0.06374700
C	-4.42361300	-0.00019200	0.43703900
H	-4.85829700	0.89277600	-0.00481500
H	-4.56333500	-0.00038300	1.51505900
H	-4.85810300	-0.89312300	-0.00510700
N	4.67518400	-0.00008500	0.51255500
H	5.05176900	0.84273700	0.91347600
H	5.05172800	-0.84293500	0.91345700

Pyr···ClCF₃

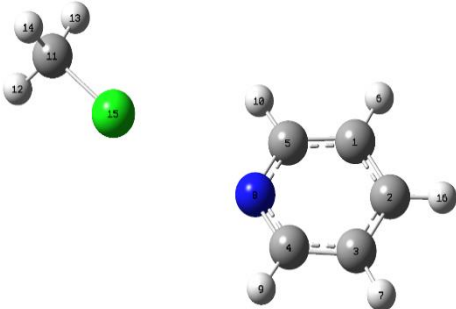
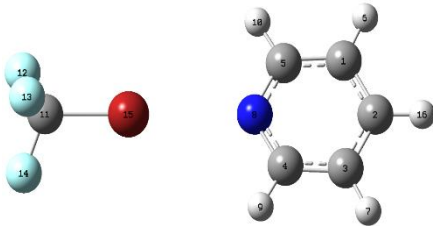
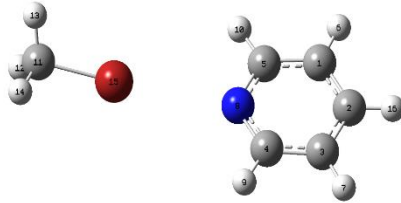
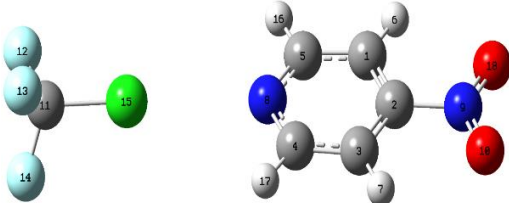
E=-1046.11281164 a.u.

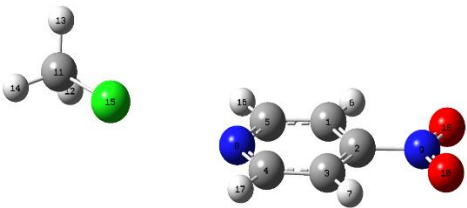
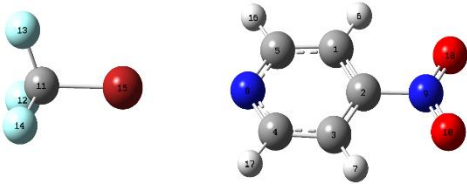
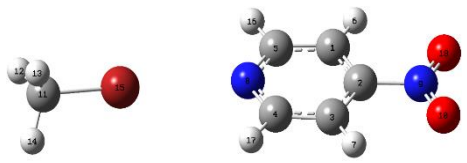


Graphical representation.

Cartesian coordinates:

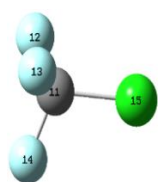
C	3.82297800	-1.19484800	0.02035300
C	4.53245700	-0.00182100	0.04669000
C	3.82591700	1.19293800	0.02052400
C	2.43808700	1.14011400	-0.03032700
C	2.43529600	-1.13861100	-0.03045200
H	4.32920900	-2.15235600	0.03963500
H	4.33445700	2.14922200	0.03994400
N	1.74658200	0.00159700	-0.05558700
H	1.85260400	2.05503900	-0.05128800
H	1.84754700	-2.05208400	-0.05151400
C	-2.99330200	-0.00017700	0.01255700
F	-3.43112500	-0.14249200	1.25964100
F	-3.48288400	-0.99940600	-0.71501600
F	-3.47803600	1.14003600	-0.46939200
Cl	-1.23800500	0.00137500	-0.03464000
H	5.61600500	-0.00317700	0.08802700

Pyr···ClCH ₃		Cartesian coordinates:			
<div>E=-748.37461895 a.u.</div> <div></div>	Graphical representation.	C	2.10218000	1.39650600	0.00424700
		C	3.26024000	0.63106200	-0.01375100
		C	3.14074000	-0.75200300	-0.01665300
		C	1.86574100	-1.30633900	-0.00114600
		C	0.87525900	0.74296000	0.01828100
		H	2.14361100	2.47929600	0.00732400
		H	4.01416200	-1.39317600	-0.03039100
		N	0.74732900	-0.58317500	0.01602100
		H	1.73553800	-2.38501000	-0.00276400
		H	-0.05318900	1.30728200	0.03224000
		C	-4.32158600	0.33749700	-0.02887300
		H	-4.85203500	-0.16195600	-0.83650100
		H	-4.29638200	1.41112200	-0.20248600
		H	-4.79633900	0.12150800	0.92559300
		Cl	-2.64108300	-0.27636900	0.01457600
		H	4.23630400	1.10333800	-0.02559100
Pyr···BrCF ₃		Cartesian coordinates:			
<div>E= -3160.07829476 a.u.</div> <div></div>	Graphical representation.	C	4.03580300	1.19405000	0.00209600
		C	4.74321300	-0.00053600	0.00402200
		C	4.03498300	-1.19464000	0.00208300
		C	2.64674800	-1.14074500	-0.00156200
		C	2.64752700	1.14110000	-0.00156100
		H	4.54421500	2.15047800	0.00353200
		H	4.54275400	-2.15140700	0.00351300
		N	1.95881700	0.00041200	-0.00348900
		H	2.05785700	-2.05354100	-0.00312900
		H	2.05926700	2.05430200	-0.00312400
		C	-2.88138500	-0.00006300	0.00217700
		F	-3.35855700	1.13680300	-0.50070600
		F	-3.35445300	-0.13211800	1.23979100
		F	-3.35893600	-1.00525900	-0.72916000
		Br	-0.95591800	0.00023900	-0.00332100
		H	5.82749300	-0.00091400	0.00702200
Pyr···BrCH ₃		Cartesian coordinates:			
<div>E=-2862.34358661 a.u.</div> <div></div>	Graphical representation.	C	3.08837400	1.26527200	0.02433000
		C	3.90848900	0.14629600	0.08037500
		C	3.32110700	-1.11102900	0.04458800
		C	1.93632300	-1.19254500	-0.04557500
		C	1.71445900	1.07488900	-0.06432700
		H	3.50073200	2.26684300	0.04952700
		H	3.91871200	-2.01382200	0.08620200
		N	1.14014200	-0.12637700	-0.09933700
		H	1.44091200	-2.15880300	-0.07519200
		H	1.03890900	1.92474000	-0.10807700
		C	-3.93886500	0.11049200	0.08373700
		H	-4.30073400	0.51365500	-0.85896500
		H	-4.19079600	0.77879900	0.90351400
		H	-4.35581100	-0.87834100	0.25822300
		Br	-2.00564000	-0.04462300	-0.01289100
		H	4.98515700	0.25311200	0.15252900
O ₂ N-Pyr···ClCF ₃		Cartesian coordinates:			
<div>E=-1250.60356002 a.u.</div> <div></div>	Graphical representation.	C	-2.66047400	1.23032900	-0.00068100
		C	-3.28805800	-0.00065200	0.00037800
		C	-2.56296600	-1.17698500	-0.00157100
		C	-1.17825000	-1.05770900	-0.00453900
		C	-1.27046400	1.22382400	-0.00378600
		H	-3.23033600	2.14903800	0.00083200
		H	-3.05753400	-2.13835800	-0.00074100
		N	-0.54012800	0.11073500	-0.00619800
		N	-4.76959200	-0.06091200	0.00317700
		O	-5.28093600	-1.16025700	0.00359400
		C	4.25932000	-0.02786000	0.00275900
		F	4.78613900	1.18268700	-0.13865600
		F	4.69620500	-0.79300400	-0.99085400
		F	4.69369400	-0.54157900	1.14749100
		Cl	2.50277800	0.05777400	-0.00870700
		H	-0.72187700	2.16017100	-0.00473300
		H	-0.55492900	-1.94624800	-0.00607600
		O	-5.36825100	0.99349100	0.00424300

O₂N-Pyr···ClCH₃		Cartesian coordinates:		
E= -952.86709191 a.u.		C	-1.00841700	-0.90753400
		C	-2.04589200	0.00516400
		C	-1.80406000	1.36577600
		C	-0.47186400	1.76365100
		C	0.28192800	-0.38899400
		H	-1.20006800	-1.97151900
		H	-2.61693300	2.07848800
		N	0.55273800	0.91429000
		N	-3.44464100	-0.48405300
		O	-4.32616500	0.34906300
		C	5.48980600	-0.74557800
		H	5.47442900	-1.49701600
		H	5.62870600	-1.21453200
		H	6.27793300	-0.01975100
		Cl	3.92012600	0.11648500
		H	1.13899300	-1.05488600
		H	-0.22156900	2.81973600
		O	-3.61500000	-1.68498000
 <p>Graphical representation.</p>				
O₂N-Pyr···BrCF₃		Cartesian coordinates:		
E=-3364.56836328 a.u.		C	2.95383000	-1.20190700
		C	3.63692600	-0.00077600
		C	2.96749900	1.20799400
		C	1.57890200	1.15380600
		C	1.56600200	-1.13194100
		H	3.48177700	-2.14533200
		H	3.50608800	2.14539800
		N	0.88941000	0.01479100
		N	5.12004400	-0.00919500
		O	5.68097100	1.06551000
		C	-4.01109000	-0.00650800
		F	-4.47745200	-0.51953500
		F	-4.47805000	-0.73742000
		F	-4.49125800	1.22720500
		Br	-2.08439100	0.00780100
		H	0.97322100	-2.04098800
		H	0.99659000	2.06956200
		O	5.66881100	-1.09014900
 <p>Graphical representation.</p>				
O₂N-Pyr···BrCH₃		Cartesian coordinates:		
E=-3066.83541418 a.u.		C	2.15443500	1.26493200
		C	2.71030100	-0.00030500
		C	1.91858600	-1.13255100
		C	0.54360100	-0.93275800
		C	0.76699700	1.33894400
		H	2.77610100	2.14891800
		H	2.35605100	-2.12109300
		N	-0.02526100	0.27042200
		N	4.18467200	-0.14563800
		O	4.63338600	-1.27233600
		C	-5.11156000	-0.25558800
		H	-5.60465800	0.70647900
		H	-5.34290200	-0.69278500
		H	-5.40101000	-0.92945200
		Br	-3.19282100	0.02846400
		H	0.27207800	2.30461600
		H	-0.13278500	-1.78119300
		O	4.84359300	0.87217700
 <p>Graphical representation.</p>				

ON-Pyr...ClCF₃

E=-1175.39065544 a.u.



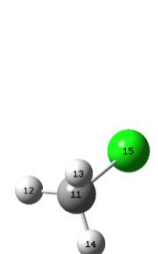
Graphical representation.

Cartesian coordinates:

C	-3.06056300	-1.05119200	-0.05032200
C	-3.68694300	0.18707300	0.01724200
C	-2.93691700	1.35104000	-0.01255500
C	-1.55468000	1.22608100	-0.10969400
C	-1.67756100	-1.05869100	-0.14605600
H	-3.63833200	-1.96676300	-0.02768800
H	-3.42361400	2.31755900	0.04096100
N	-0.93445500	0.05109600	-0.17505500
N	-5.12842200	0.36147100	0.12255100
O	-5.75312000	-0.66103600	0.15079200
C	3.84604500	-0.04291100	0.04882800
F	4.29718500	-1.28838400	0.14581200
F	4.24869000	0.63110200	1.11999300
F	4.39239300	0.51615700	-1.02525500
Cl	2.09181100	-0.02695300	-0.06856300
H	-1.13458400	-1.99705100	-0.20128600
H	-0.91985500	2.10650200	-0.13482800

ON-Pyr...ClCH₃

E=-877.65377532 a.u.



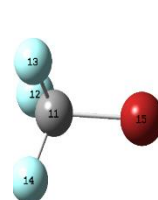
Graphical representation.

Cartesian coordinates:

C	2.27139500	1.08381700	-0.00126400
C	2.39657800	-0.30026100	0.00007000
C	1.26648500	-1.10097100	0.00180000
C	0.02592400	-0.47005500	0.00202300
C	0.98641900	1.60450600	-0.00076300
H	3.14801200	1.71946100	-0.00258600
H	1.36200400	-2.18036100	0.00291700
N	-0.11729900	0.85222300	0.00085100
N	3.67040700	-0.99975200	-0.00018300
O	4.63364500	-0.28506700	-0.00184800
C	-5.15106800	-0.64429500	-0.00496900
H	-5.93407700	0.08638200	-0.19347100
H	-5.29699200	-1.11347600	0.96525400
H	-5.13702900	-1.39506700	-0.79163300
Cl	-3.57607700	0.20761200	0.00273100
H	0.82903200	2.67867800	-0.00168900
H	-0.89295100	-1.04823800	0.00350600

ON-Pyr...BrCF₃

E=-3289.35561628 a.u.



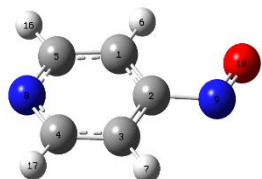
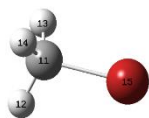
Graphical representation.

Cartesian coordinates:

C	-3.32364500	-1.04455200	-0.00543200
C	-4.00675800	0.16522400	0.00317700
C	-3.30951500	1.36165700	0.00178600
C	-1.91992300	1.29919800	-0.00841500
C	-1.93882900	-0.99126900	-0.01503300
H	-3.86041700	-1.98484200	-0.00432500
H	-3.84073400	2.30587200	0.00869200
N	-1.24722500	0.15165600	-0.01670500
N	-5.45924100	0.27572900	0.01429900
O	-6.03754300	-0.77347900	0.01508400
C	3.63514200	-0.07931800	0.00831500
F	4.05206200	-1.12646400	-0.69824900
F	4.08965500	-0.21201100	1.25130100
F	4.17787000	1.01611800	-0.51577400
Br	1.71218000	0.03451000	-0.00909700
H	-1.35063800	-1.90366400	-0.02177600
H	-1.32402200	2.20650400	-0.00990000

ON-Pyr...BrCH₃

E=-2991.6222977 a.u.



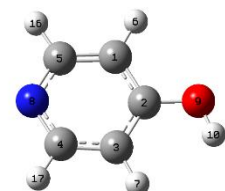
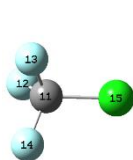
Graphical representation.

Cartesian coordinates:

C	-2.29227200	-0.99860800	0.00018200
C	-3.09993100	0.13245400	-0.00006200
C	-2.53137500	1.39531700	-0.00011600
C	-1.14224500	1.47866500	0.00013000
C	-0.92068400	-0.79848600	0.00032400
H	-2.72778600	-1.98984200	0.00022200
H	-3.15975900	2.27810300	-0.00030900
N	-0.35164500	0.40982500	0.00032800
N	-4.55359100	0.09014800	-0.00028600
O	-5.02128900	-1.01385300	-0.00018900
C	4.69240800	-0.42255900	-0.00043000
H	5.14049800	0.00604300	-0.89325600
H	4.79952900	-1.50433300	-0.00185000
H	5.14046500	0.00375200	0.89350700
Br	2.79888300	0.00842400	0.00006000
H	-0.23692400	-1.64192400	0.00049100
H	-0.64537500	2.44368000	0.00013300

HO-Pyr...ClCF₃

E=-1121.34124639 a.u.



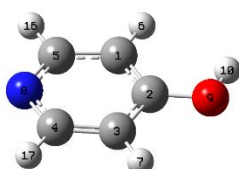
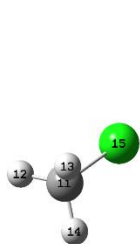
Graphical representation.

Cartesian coordinates:

C	-3.34308200	-1.20718500	0.00000600
C	-4.05508900	-0.01144100	0.01096700
C	-3.34579400	1.18640500	-0.00059300
C	-1.95927800	1.12735000	-0.02249700
C	-1.96014900	-1.14290100	-0.02173800
H	-3.86583500	-2.15492200	0.00879800
H	-3.85393200	2.14508900	0.00745800
N	-1.26130600	-0.00560500	-0.03317300
O	-5.40323800	-0.07442700	0.03261100
H	-5.77582200	0.80951700	0.03808400
C	3.46814400	0.00309300	0.00889700
F	3.95592300	-0.74099600	-0.97913200
F	3.92330800	-0.48511700	1.15871600
F	3.93921000	1.23859300	-0.13187400
Cl	1.71271900	0.00019400	-0.01768000
H	-1.37831200	-2.06013300	-0.03035700
H	-1.38176300	2.04755100	-0.03174300

HO-Pyr...ClCH₃

E=-823.6029173 a.u.



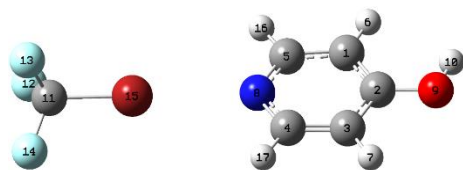
Graphical representation.

Cartesian coordinates:

C	2.61421400	1.04458500	0.00623100
C	2.80377700	-0.33393600	0.00238400
C	1.68366500	-1.15882100	-0.00626300
C	0.43295000	-0.56252600	-0.01074300
C	1.31181100	1.52756000	0.00098100
H	3.45423300	1.73189000	0.01296000
H	1.79878900	-2.23527500	-0.00946300
N	0.22815300	0.75631900	-0.00736000
O	4.02466100	-0.91474700	0.00679100
H	4.70785900	-0.24164200	0.01294700
C	-4.77230200	-0.54944400	0.01508900
H	-5.52078500	0.22141300	-0.15420200
H	-4.92482300	-1.01578100	0.98589800
H	-4.81625200	-1.29687900	-0.77396000
Cl	-3.15377600	0.21380100	-0.00645800
H	1.13758900	2.60003500	0.00385100
H	-0.46145500	-1.17914600	-0.01712800

HO-Pyr...BrCF₃

E=-3235.30682124 a.u.



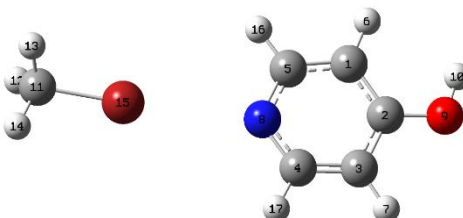
Graphical representation.

Cartesian coordinates:

C	-3.61258700	-1.18759600	0.00017700
C	-4.32337100	0.00980000	0.00004200
C	-3.61324000	1.20709100	0.00037500
C	-2.23068700	1.14581500	0.00068700
C	-2.22665900	-1.12765000	0.00097000
H	-4.11972700	-2.14670400	-0.00012300
H	-4.13772100	2.15382200	0.00028000
N	-1.53227100	0.00785900	0.00093100
O	-5.67072600	0.07137400	-0.00057000
H	-6.04379600	-0.81244900	-0.00094600
C	3.29777500	-0.00428600	0.00046800
F	3.77091100	-1.08507900	-0.61758900
F	3.77412300	-0.00173500	1.24420900
F	3.77783600	1.06899300	-0.62486900
Br	1.37241400	0.00182300	-0.00100500
H	-1.64619800	-2.04582100	0.00117800
H	-1.64853700	2.06266900	0.00076300

HO-Pyr...BrCH₃

E=-2937.57191311 a.u.



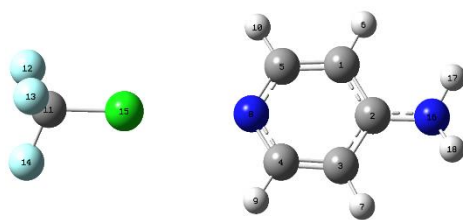
Graphical representation.

Cartesian coordinates:

C	2.62422100	-1.19496200	-0.00538000
C	3.45870900	-0.08091200	0.00881200
C	2.88050900	1.18454600	0.00505900
C	1.49804400	1.27042100	-0.01288100
C	1.25190400	-0.98586000	-0.02241600
H	3.02711600	-2.20266000	-0.00297900
H	3.50335000	2.06992000	0.01589300
N	0.68105600	0.21574900	-0.02663200
O	4.80713700	-0.16528100	0.02639100
H	5.07967200	-1.08490000	0.02641700
C	-4.38948100	-0.19680300	0.03055100
H	-4.66631300	-0.63001000	0.98854100
H	-4.67123700	-0.86163500	-0.78231600
H	-4.85714000	0.77653200	-0.09569000
Br	-2.46215500	0.03878200	-0.00421900
H	0.57468100	-1.83551500	-0.03316000
H	1.01736600	2.24431400	-0.01621200

H₂N-Pyr...ClCF₃

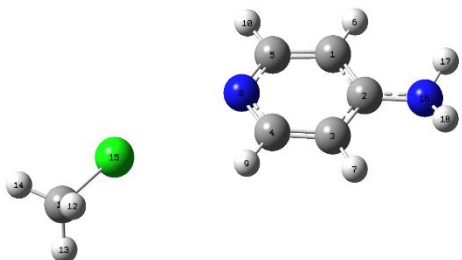
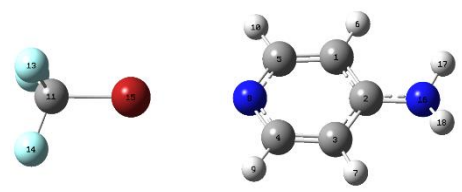
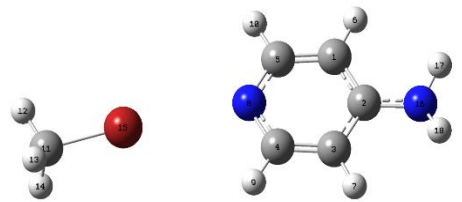
E=-1101.47801621 a.u.



Graphical representation.

Cartesian coordinates:

C	3.32474500	1.19366100	-0.00602100
C	4.05417900	-0.00088300	0.00711300
C	3.32225400	-1.19391700	-0.00618700
C	1.93995300	-1.13162500	-0.02742600
C	1.94230600	1.13423200	-0.02730000
H	3.82938400	2.15352900	-0.00241700
H	3.82492600	-2.15481100	-0.00271100
N	1.23723600	0.00203100	-0.03769800
H	1.36145500	-2.05157800	-0.03612100
H	1.36573900	2.05538900	-0.03588800
C	-3.46824000	-0.00041200	0.01194000
F	-3.95153100	1.13969400	-0.47387900
F	-3.91768700	-0.14253500	1.25583000
F	-3.95420100	-0.99992100	-0.71909800
Cl	-1.71382700	0.00139900	-0.02182000
N	5.43032600	-0.00232800	-0.01281600
H	5.90100800	0.84341200	0.26172400
H	5.89920300	-0.84911100	0.26157500

H₂N-Pyr···ClCH₃		Cartesian coordinates:		
E=-803.73904594 a.u.		C	-2.60646400	1.06550800
		C	-2.81675400	-0.31708900
		C	-1.68067200	-1.13229000
		C	-0.42942200	-0.53913900
		C	-1.30740400	1.54589500
		H	-3.44257000	1.75586100
		H	-1.77307500	-2.21313300
		N	-0.21858800	0.77760400
		H	0.46176100	-1.16056700
		H	-1.13363600	2.61875500
		C	4.79448200	-0.56509800
		H	4.85003200	-1.31269000
		H	4.93291200	-1.03174400
		H	5.54636900	0.20490300
		Cl	3.17741000	0.19934600
		N	-4.08613000	-0.85367900
		H	-4.85156900	-0.25458600
		H	-4.19576200	-1.80988500
Graphical representation.				
H₂N-Pyr···BrCF₃		Cartesian coordinates:		
E=-3215.44388743 a.u.		C	3.59164200	1.19446700
		C	4.32232000	0.00000900
		C	3.59159200	-1.19444900
		C	2.20988700	-1.13463200
		C	2.20991000	1.13467800
		H	4.09541600	2.15464000
		H	4.09536800	-2.15462100
		N	1.50807400	0.00004800
		H	1.63062800	-2.05390900
		H	1.63070700	2.05399500
		C	-3.29765600	0.00002000
		F	-3.78001600	1.08282200
		F	-3.76804900	-0.01142400
		F	-3.78023300	-1.07132500
		Br	-1.37257400	-0.00003500
		N	5.69635100	-0.00004400
		H	6.17278000	0.84728900
		H	6.17271200	-0.84740100
Graphical representation.				
H₂N-Pyr···BrCH₃		Cartesian coordinates:		
E=-2917.70826178 a.u.		C	-2.85701600	1.17524100
		C	-3.45851400	-0.08770800
		C	-2.60925000	-1.19852500
		C	-1.24193800	-0.99369200
		C	-1.47674700	1.25916400
		H	-3.45675700	2.07791600
		H	-3.01110600	-2.20581000
		N	-0.66094500	0.20621300
		H	-0.56928100	-1.84641100
		H	-0.99703100	2.23396700
		C	4.39278700	-0.18922000
		H	4.86278000	0.78422500
		H	4.70591500	-0.85968000
		H	4.63657000	-0.61433700
		Br	2.46700700	0.03937700
		N	-4.82491300	-0.23229000
		H	-5.39343300	0.56146200
		H	-5.21784500	-1.11854100
Graphical representation.				