Supplementary data

Research of the influence of anions in complexes [CuPhen(Hpz)$_2$X$_2$] (X= CF_3COO^-, Otf^-, Cl^-) on the structure and bioactivity

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Table S1. Crystal data and structure refinement parameters for **1-3**

	1	**2**	**3**
Empirical formula	$C_{22}H_{16}N_6O_4F_6Cu$	$C_{20}H_{16}N_6O_6F_6S_2Cu$	$C_{18}H_{16}Cl_2CuN_6$
CCDC	2289146	2289147	2289148
Formula weight (g mol^{-1})	605.95	678.05	450.81
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P*-1	C*2*/c	P2_1/c
a (Å)	10.1267(17)	16.084(3)	13.2386(1)
b (Å)	10.9088(18)	11.6918(17)	8.9177(13)
c (Å)	12.076(2)	16.023(3)	15.758(2)
α,	78.050(3)		
β,	72.589(3)	119.823(3)	95.674(8)
γ,	76.521(3)		
V, Å^3	1224.2(4)	2614.0(7)	1851.3(4)
Z	2	4	4
D_{calc} (g cm^3)	1.644	1.723	1.617
μ(Mo-Kα) (mm^{-1})	0.980	1.087	1.485
F(000)	610	1364	916
$2\theta_{max}$, deg.	60	60	61
Reflections collected	8632	11068	11821
Independent reflections	6507	3786	5471
R_{int}	0.0300	0.0514	0.0512
Parameters	364	186	244
GooF	1.014	1.016	1.030
R_1[a], wR_2[b] ($I > 2\sigma(I)$)	0.0629, 0.1473	0.0356, 0.0894	0.0493, 0.0856
R_1[a], wR_2[b] (all data)	0.1140, 0.1708	0.0499, 0.0972	0.0979, 0.0982
$\Delta\rho_{max}$, ρ_{min} (e/Å^3)	0.77/-0.66	0.84/-0.38	0.59/-0.88

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$. GooF = $[\Sigma w(F_o^2 - F_c^2)/\text{n-p}]^{1/2}$

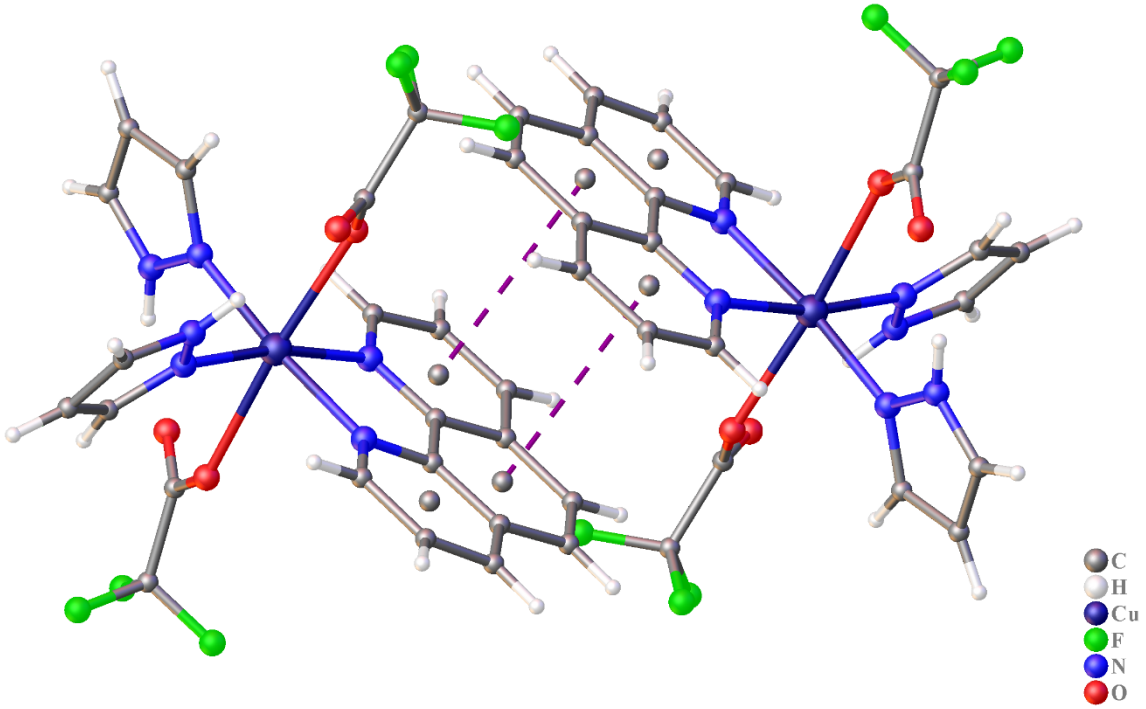

Fig. S1. π...π interactions in crystal packing of complex **1**.