molecules

MDPI

SUPPLEMENTARY MATERIAL

Probing the structural determinants of amino acid recognition: X-ray studies of crystalline ditopic host-guest complexes of the positively charged amino acids, Arg, Lys and His with a cavitand molecule.

Giovanna Brancatelli[1], Enrico Dalcanale[2], Roberta Pinalli[2,*] and Silvano Geremia[1,*]

Table S1. Experimental details for the co-crystallization experiments of the host-guest complexes of cavitand Tiiii[H, CH_3, CH_3] with the selected amino acids.

Amino acid	Amino acid Concentration in HCl 1 M(mM)	Molar Ratio cavitand:amino acid	Composition of Reservoir (v/v)
Arg	300	1:5	PEG 300 25-50%
Lys	30	2:1	PEG 300 5-15%
His	300	1:5	PEG 300 25-50%

Table S2. Crystal data and structure refinement details for the host-guest complexes

	Arg 2HCl	Lys 2HCl	His 2HCl
Empirical formula	$2(C_{36}H_{36}O_{12}P_4)$, $C_6H_{16}N_4O_2$, 2Cl, $4.4(C_2H_3F_3O)$, $3.7H_2O$	$2(C_{36}H_{36}O_{12}P_4)$, $C_6H_{16}N_2O_2$, 2Cl, $6.1(C_2H_3F_3O)$, $2.8H_2O$	$4(C_{36}H_{36}O_{12}P_4)$, $2(C_6H_{11}N_3O_2)$, 4Cl $10(C_2H_3F_3O)$, $4\ H_2O$
Formula weight	2253.06	2158.80	4546.81
T (K)	100(2)	100(2)	100(2)
λ (Å)	0.700	0.700	0.700
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	$P\ 2_1$	$P\ 2_12_12$	$P\ 2_1$
Unit cell dimensions (Å, °)	a = 12.443(1) b = 26.937(2) c = 17.394(2) β = 108.96(3)	a = 21.654(4) b = 32.439(7) c = 15.809(3)	a = 17.644(2) b = 23.627(2) c = 25.567(3) β = 93.909(4)
V (Å3)	5513.8(13)	11105(4)	10633(2)
Z	2	4	2
ϱ(calc) (g/mm^3)	1.399	1.464	1.469
μ (mm^{-1})	0.212	0.207	0.263
F(000)	2406	5060	4816
Reflections collected	18443	44450	28901
Independent reflections	18443	17357	28901
Data / restraints / parameters	18443/3/1288	17357/18/1128	28901/1753/2674
GooF	1.066	1.008	1.006
R_1, wR_2 [I>2σ(I)]	0.0749, 0.2095	0.0684, 0.1882	0.0682, 0.1548
R_1, wR_2 (all data)	0.0763, 0.2113	0.1014, 0.2112	0.1219, 0.1868
Absolute structure parameter	0.10(2)	0.09(6)	-0.03(8)
CCDC code number	1869187	1876524	1869186