J. Braz. Chem. Soc., Vol. 00, No. 00, S1-S3, 2010.
Printed in Brazil - ©2010 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

2-Chlorovinyl Tellurium Dihalides, (*p*-tol)Te[C(H)=C(C*l*)Ph]X_2 for X = C*l*, Br and I: Variable Coordination Environments, Supramolecular Structures and Docking Studies in Cathepsin B

Ignez Caracelli,*,[a] Julio Zukerman-Schpector,*,[b] Stella H. Maganhi,[b] Hélio A. Stefani,[c] Rafael Guadagnin[d] and Edward R. T. Tiekink*,[e]

[a]*Departamento de Física, Universidade Federal de São Carlos, CP 676, 13565-905 São Carlos-SP, Brazil*

[b]*Laboratório de Cristalografia, Estereodinâmica e Modelagem Molecular, Departamento de Química, Universidade Federal de São Carlos, CP 676, 13565-905 São Carlos-SP, Brazil*

[c]*Departamento de Farmácia, Faculdade de Ciências Farmacêuticas, Universidade de São Paulo, São Paulo-SP, Brazil*

[d]*Departamento de Química, Universidade Federal de São Paulo, São Paulo-SP, Brazil*

[e]*Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia*

Table S1. Complete set of data interactions

subsite	S1	S1'	S2	S2'

TeI interactions				
TeI GOLDScore: 44.97 kcal mol^{-1} $\Delta G_{binding}$: –7.10 kcal mol^{-1}				
Subsite	TeI···cathepsin interaction	distance (Å)	TeI ligand atom	1gmy atom
S2'	I2 - GLU122:OE2	3.32	I2	OE2
	C*l*3 - GLN23:HE21	2.86	**Cl3**	HE21
S1'	Te1 - GLY27:O	2.91	Te1	O
	C*l*3 - GLY27:HA1	3.24	**Cl3**	HA1
	C*l*3 - GLY27:HA2	2.44	**Cl3**	HA2
	H5 - MET196:O	3.10	H5	O
	H5 - GLY197:O	2.32	H5	O
S1	I2 - ASN72:O	3.18	I2	O
	I2 - GLY73:HA1	3.13	I2	HA1
	I2 - GLY73:HA2	3.43	I2	HA2
	Te1 - CYS29:SG	**2.971**	**Te1**	**SG**
	Te1 - GLY73:HA2	2.93	Te1	HA2
	H13 - GLY74:O	2.34	H13	O
	H15B - GLY74:O	3.14	H15B	O
S2	H1 - GLY198:O	2.48	H1	O
	H4 - GLY198:O	2.52	H4	O

*e-mail: ignez@ufscar.br, julio@power.ufscar.br, edward.tiekink@gmail.com

TeC*l* interactions

TeC*l* GOLDScore: 45.55 kcal mol^{-1}
$\Delta G_{binding}$: −7.16 kcal mol^{-1}

Subsite	TeC*l*···cathepsin interaction	distance (Å)	TeCl ligand atom	1gmy atom
S2'	C*l*3 - GLN23:HE21	2.66	**Cl3**	HE21
S1'	Te1 - GLY27:O	3.43	Te1	O
	C*l*3 - GLY27:HA2	2.91	**Cl3**	HA2
	H7 - MET196:O	2.56	H7	O
	H7 - GLY197:O	2.74	H7	O
	H8 - MET196:O	3.37	H8	O
	H8 - GLY197:O	3.26	H8	O
S1	Te1 - CYS29:SG	3.21	Te1	SG
	C*l*2 - ASN72:O	3.22	Cl2	O
	C*l*2 - GLY73:HA1	2.40	Cl2	HA1
	C*l*2 - GLY73:HA2	3.03	Cl2	HA2
	H11 - GLY74:O	3.35	H11	O
S2	C*l*3 - HIS199:HD1	2.87	Cl3	HD1
	H1 - GLY198:O	2.16	H1	O
	H4 - HIS199:ND1	3.04	H4	ND1
	H8 - GLY198:O	2.95	H8	O
	H13 - GLY198:O	3.20	H13	O
	H14 - GLY198:O	2.44	H14	O

TeBr interactions

TeBr GOLDScore: 43.09 kcal mol^{-1}
$\Delta G_{binding}$: −6.90 kcal mol^{-1}

Subsite	TeBr···cathepsin interaction	distance (Å)	TeBr ligand atom	1gmy atom
S2'	C*l*3 - GLN23:HE21	3.39	**Cl3**	HE21
	C*l*3 - GLU122:OE2	3.45	**Cl3**	OE2
S1'	Te - GLY27:O	3.21	Te	O
	C*l*3 - GLY27:HA1	2.86	**Cl3**	HA1
	C*l*3 - GLY27:HA2	2.48	**Cl3**	HA2
	H4 - GLY197:O	3.43	H4	O
	H5 - MET196:O	3.01	H5	O
	H5 - GLY197:O	2.58	H5	O
S1	Te - CYS29:SG	2.90	Te	SG
	Br2 - ASN72:O	3.43	Br2	O
	Br2 - GLY73:HA1	2.69	Br2	HA1
	Br2 - GLY73:HA2	3.15	Br2	HA2
	H13 - GLY74:O	3.32	H13	O
S2	H1 - GLY198:O	2.22	H1	O
	H4 - GLY198:O	2.66	H4	O
	H10 - GLY198:O	2.35	H10	O
	H11 - GLY198:O	3.19	H11	O

YOWMEC interactions				
YOWMEC GOLDScore: 42.79 kcal mol^{-1} $\Delta G_{binding}$: –6.87 kcal mol^{-1}				
Subsite	YOWMEC–cathepsin interaction	distance (Å)	YOWMEC ligand atom	1gmy Atom
S2'	C*l*3 - GLN23:HE21	2.93	**Cl3**	HE21
S1'	Te1 - GLY27:O	3.21	Te1	O
	C*l*3 - GLY27:HA1	3.33	**Cl3**	HA1
	C*l*3 - GLY27:HA2	2.56	**Cl3**	HA2
	H5 - MET196:O	2.98	H5	O
	H5 - GLY197:N	2.79	H5	N
	H5 - GLY197:O	2.58	H5	O
	H6 - GLY197:O	3.41	H6	O
S1	Te1 - CYS29:SG	2.90	Te1	SG
	H1 - CYS29:SG	2.98	H1	SG
	H9 - GLY74:O	2.79	H9	O
	H10 - CYS29:SG	2.59	H10	SG
	H12 - GLY74:O	2.90	H12	O
S2	H1 - GLY198:O	2.41	H1	O
	H6 - GLY198:O	2.70	H6	O
	H7 - GLY198:O	2.33	H7	O
	H8 - GLY198:N	3.42	H8	N
	H8 - GLY198:O	2.87	H8	O