

surface	fcc	ua_sca	charmm_sca	availability	SMILES
SiO2_Amorphous	000	ALA	ALA	True	C
SiO2_Amorphous	000	ARG	ARG	True	CCCNC(N)=[NH2+]
SiO2_Amorphous	000	ASN	ASN	True	CC(N)=O
SiO2_Amorphous	000	ASP	ASP	True	CC(=O)[O-]
SiO2_Amorphous	000	AAN	ASPP	False	CC(=O)O
SiO2_Amorphous	000	CYM	CYM	True	C[S-]
SiO2_Amorphous	000	CYS	CYS	True	CS
SiO2_Amorphous	000	GLN	GLN	True	CCC(N)=O
SiO2_Amorphous	000	GLU	GLU	True	CC(=O)[O-]
SiO2_Amorphous	000	GAN	GLUP	True	CCC(=O)O
SiO2_Amorphous	000	GLY	GLY	True	C
SiO2_Amorphous	000	HIS	HIS	True	CC1CNCN1
SiO2_Amorphous	000	HID	HSD	True	CC1CNCN1
SiO2_Amorphous	000	HIE	HSE	True	CC1CNCN1
SiO2_Amorphous	000	HIP	HSP	True	CC1CNCN1
SiO2_Amorphous	000	ILE	ILE	True	CCCC
SiO2_Amorphous	000	LEU	LEU	True	CC(C)C
SiO2_Amorphous	000	LYS	LYS	True	CCCC[NH3+]
SiO2_Amorphous	000	MET	MET	True	CC5C
SiO2_Amorphous	000	PHE	PHE	True	CC1CCCC1
SiO2_Amorphous	000	PRO	PRO	True	CCC
SiO2_Amorphous	000	SER	SER	True	CO
SiO2_Amorphous	000	THR	THR	True	CCO
SiO2_Amorphous	000	TRP	TRP	True	CC1C[NH]C2CCCCC12
SiO2_Amorphous	000	TYR	TYR	True	CC1CCC(O)CC1
SiO2_Amorphous	000	VAL	VAL	True	CCC