

surface	fcc	ua_sca	charmm_sca	availability	SMILES
Ag	100	ALA	ALA	True	C
Ag	100	ARG	ARG	True	CCNC(N)=[NH2+]
Ag	100	ASN	ASN	True	CC(N)=O
Ag	100	ASP	ASP	True	CC(=O)[O-]
Ag	100	AAN	ASPP	True	CC(=O)O
Ag	100	CYM	CYM	True	C[S-]
Ag	100	CYS	CYS	True	CS
Ag	100	GLN	GLN	True	CCC(N)=O
Ag	100	GLU	GLU	True	CC(=O)[O-]
Ag	100	GAN	GLUP	True	CCC(=O)O
Ag	100	GLY	GLY	True	C
Ag	100	HIS	HIS	True	CC1CNCN1
Ag	100	HID	HSD	True	CC1CNCN1
Ag	100	HIE	HSE	True	CC1CNCN1
Ag	100	HIP	HSP	True	CC1CNCN1
Ag	100	ILE	ILE	True	CCCC
Ag	100	LEU	LEU	True	CC(C)C
Ag	100	LYS	LYS	True	CCCC[NH3+]
Ag	100	MET	MET	True	CC5C
Ag	100	PHE	PHE	True	CC1CCCCC1
Ag	100	PRO	PRO	True	CCC
Ag	100	SER	SER	True	CO
Ag	100	THR	THR	True	CCO
Ag	100	TRP	TRP	True	CC1C[NH]C2CCCCC12
Ag	100	TYR	TYR	True	CC1CCC(O)CC1
Ag	100	VAL	VAL	True	CCC
Ag	110	ALA	ALA	True	C
Ag	110	ARG	ARG	True	CCNC(N)=[NH2+]
Ag	110	ASN	ASN	True	CC(N)=O
Ag	110	ASP	ASP	True	CC(=O)[O-]
Ag	110	AAN	ASPP	True	CC(=O)O
Ag	110	CYM	CYM	True	C[S-]
Ag	110	CYS	CYS	True	CS
Ag	110	GLN	GLN	True	CCC(N)=O
Ag	110	GLU	GLU	True	CC(=O)[O-]
Ag	110	GAN	GLUP	True	CCC(=O)O
Ag	110	GLY	GLY	True	C
Ag	110	HIS	HIS	True	CC1CNCN1
Ag	110	HID	HSD	True	CC1CNCN1
Ag	110	HIE	HSE	True	CC1CNCN1
Ag	110	HIP	HSP	True	CC1CNCN1
Ag	110	ILE	ILE	True	CCCC
Ag	110	LEU	LEU	True	CC(C)C
Ag	110	LYS	LYS	True	CCCC[NH3+]
Ag	110	MET	MET	True	CC5C
Ag	110	PHE	PHE	True	CC1CCCCC1
Ag	110	PRO	PRO	True	CCC
Ag	110	SER	SER	True	CO
Ag	110	THR	THR	True	CCO
Ag	110	TRP	TRP	True	CC1C[NH]C2CCCCC12
Ag	110	TYR	TYR	True	CC1CCC(O)CC1
Ag	110	VAL	VAL	True	CCC
Ag	111	ALA	ALA	True	C
Ag	111	ARG	ARG	True	CCNC(N)=[NH2+]
Ag	111	ASN	ASN	True	CC(N)=O
Ag	111	ASP	ASP	True	CC(=O)[O-]
Ag	111	AAN	ASPP	True	CC(=O)O
Ag	111	CYM	CYM	True	C[S-]
Ag	111	CYS	CYS	True	CS
Ag	111	GLN	GLN	True	CCC(N)=O
Ag	111	GLU	GLU	True	CC(=O)[O-]
Ag	111	GAN	GLUP	True	CCC(=O)O
Ag	111	GLY	GLY	True	C
Ag	111	HIS	HIS	True	CC1CNCN1
Ag	111	HID	HSD	True	CC1CNCN1
Ag	111	HIE	HSE	True	CC1CNCN1
Ag	111	HIP	HSP	True	CC1CNCN1
Ag	111	ILE	ILE	True	CCCC
Ag	111	LEU	LEU	True	CC(C)C
Ag	111	LYS	LYS	True	CCCC[NH3+]
Ag	111	MET	MET	True	CC5C
Ag	111	PHE	PHE	True	CC1CCCCC1
Ag	111	PRO	PRO	True	CCC
Ag	111	SER	SER	True	CO
Ag	111	THR	THR	True	CCO
Ag	111	TRP	TRP	True	CC1C[NH]C2CCCCC12
Ag	111	TYR	TYR	True	CC1CCC(O)CC1
Ag	111	VAL	VAL	True	CCC