

surface	fcc	ua_sca	charmm_sca	availability	SMILES
CarbonBlack	000	ALA	ALA	True	C
CarbonBlack	000	ARG	ARG	True	CCCNC(N)=[NH2+]
CarbonBlack	000	ASN	ASN	True	CC(N)=O
CarbonBlack	000	ASP	ASP	True	CC(=O)[O-]
CarbonBlack	000	AAN	ASPP	False	CC(=O)O
CarbonBlack	000	CYM	CYM	True	C[S-]
CarbonBlack	000	CYS	CYS	True	CS
CarbonBlack	000	GLN	GLN	True	CCC(N)=O
CarbonBlack	000	GUJ	GLU	True	CC(=O)[O-]
CarbonBlack	000	GAN	GLUP	True	CCC(=O)O
CarbonBlack	000	GLY	GLY	True	C
CarbonBlack	000	HIS	HIS	True	CC1CNCN1
CarbonBlack	000	HID	HSD	True	CC1CNCN1
CarbonBlack	000	HIE	HSE	True	CC1CNCN1
CarbonBlack	000	HIP	HSP	True	CC1CNCN1
CarbonBlack	000	ILE	ILE	True	CCCC
CarbonBlack	000	LEU	LEU	True	CC(C)C
CarbonBlack	000	LYS	LYS	True	CCCC[NH3+]
CarbonBlack	000	MET	MET	True	CC5C
CarbonBlack	000	PHE	PHE	True	CC1CCCCC1
CarbonBlack	000	PRO	PRO	True	CCC
CarbonBlack	000	SER	SER	True	CO
CarbonBlack	000	THR	THR	True	CCO
CarbonBlack	000	TRP	TRP	True	CC1C[NH]C2CCCCC12
CarbonBlack	000	TYR	TYR	True	CC1CCC(O)CC1
CarbonBlack	000	VAL	VAL	True	CCC