

## Supplementary Materials

Table S1. C-O distances in amino acid's carboxyl and carboxylate groups observed in different cysteine-containing crystal structures, Å.

Cysteine residue in zwitterionic state (COO <sup>-</sup> group)			
Compound	d <sub>min</sub> (C-O)	d <sub>max</sub> (C-O)	Ref.
L-cysteine L-mandelic acid	1.249(3)	1.250(3)	Fujii <i>et al.</i> , 2005
L-cysteine D-mandelic acid	1.243(3)	1.251(3)	
Orthorhombic L-cysteine	1.2357(19)	1.2588(18)	Kolesov <i>et al.</i> , 2008
Monoclinic L-cysteine	1.2435(15) 1.2539(14)	1.2650(14) 1.2551(15)	Görbitz & Dalhus, 1996
DL-cysteine-I	1.237(3)	1.254(3)	
DL-cysteine-II	1.243(5)	1.263(5)	Minkov <i>et al.</i> , 2009
Mean	<b>1.244(6)</b>	<b>1.257(6)</b>	

Cysteine residue in cationic or neutral state (COOH group)			
Compound	d(C=O)	d(C-OH)	Ref.
L-cysteine hydrochloride monohydrate	1.204(2)	1.315(2)	Chapman & Bryce, 2007
L-cysteinium L-tartrate monohydrate	1.202(4)	1.278(6)	Shan & Huang, 1999
L-cysteinium semioxalate (P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> )	1.199(2)	1.305(2)	Minkov & Boldyreva, 2008
L-cysteinium semioxalate (C2)	1.197(3)	1.312(3)	Minkov & Boldyreva, 2011
Bis(DL-cysteinium) oxalate	1.2147(15)	1.2981(15)	Drebushchak <i>et al.</i> , 2008
DL-cysteinium semioxalate	1.2082(15)	1.3050(15)	Minkov & Boldyreva, 2009

Triclinic N-acetyl-L-cysteine	1.2063(9)	1.3066(9)	Minkov <i>et al.</i> , 2012
Orthorhombic N-acetyl-L-cysteine	1.192(4)	1.314(4)	Kumar & Nangia, 2013
N-2-naphthoylcysteine	1.208(2)	1.311(2)	Katritzky <i>et al.</i> , 2009
Mean	<b>1.204(7)</b>	<b>1.305(11)</b>	