

SUPPLEMENTARY FILES

Effects of alkyl side chains on properties of aliphatic amino acids probed using quantum chemical calculations

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Table S1: Comparison of core vertical ionization energies (eV) in the aliphatic amino acids with the available experimental and other theoretical data in parentheses.

Site	Orbital	Glycine (Plekan et al.,2007)	Orbital	Alanine (Feyer et al., 2008)	Valine	Leucine	Isoleucine
OH(-C)	1a'	536.6 (540.2)	1a	536.6 (540.0)	536.5	536.5	536.5
O(=C)	2a'	535.03 (538.4)	2a	534.9 (538.2)	534.9	534.9	534.9
N	3a'	402.99 (405.4)	3a	402.9 (405.2)	402.8	402.8	402.8
C ₍₁₎	4a'		4a	293.4 (295.0)	293.4	293.3	293.4
C ₍₂₎	5a'	291.1 (292.3)	5a	291.2 (292.2)	291.0	291.0	291.0
C ₍₃₎			6a	289.8 (291.0)	290.1	289.8	290.0
C ₍₄₎			7a		289.2	289.7	289.5
C ₍₅₎			8a		289.3	289.2	289.3
C ₍₆₎			9a			289.2	289.2