Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 86 (4) S89 (2021)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Prediction of retardation factor of protein amino acids in reversed phase TLC with ethanol–sodium azide solution as the mobile phase using QSRR

SUSAN TORABI[1], FATEMEH HONARASA[2] and SAEED YOUSEFINEJAD[3]*

[1]*Deputy of Food and Drug Control, Shiraz University of Medical Sciences, Shiraz, Iran,* [2]*Department of Chemistry, Shiraz Branch, Islamic Azad University, Shiraz, Iran and* [3]*Research Center for Health Sciences, Institute of Health, Department of Occupational Health Engineering, School of Health, Shiraz University of Medical Sciences, Shiraz, Iran*

J. Serb. Chem. Soc. 86 (4) (2021) 381–391

TABLE S-I. Numerical values of the original descriptor used in Eq. (1) (before auto scaling)

Code	Name	$G_{(N\cdot\cdot O)}$	Mor24u	PW2	Mor28u	SEige
AA 1	Glycine-III	6.5	–0.105	0.517	0.092	0.637
AA 2	Alanine-III	6.52	0.06	0.578	–0.115	0.637
AA 3	Aspartic acid-III	15.5	0.095	0.572	0.03	1.134
AA 4	Arginine-III	48.96	–0.125	0.557	0.142	1.058
AA 5	Proline-III	6.43	0.034	0.563	–0.18	0.637
AA 6	Hydroxyproline-III	10.15	–0.172	0.581	–0.181	0.886
AA 7	Lysine-III	20.33	0.09	0.533	–0.183	0.778
AA 8	Glutamic acid-III	17.94	–0.135	0.568	0.124	1.134
AA 9	Serine-III	10.26	–0.135	0.557	–0.017	0.886
AA 10	Tryptophan-III	16.85	–0.024	0.582	0.09	0.778
AA 11	Valine-III	6.47	–0.032	0.588	–0.219	0.637
AA 12	Phenyl alanine-III	6.53	–0.056	0.564	–0.086	0.637
AA 13	Isoleucine-III	6.47	–0.013	0.571	–0.126	0.637
AA 14	Leucine-III	6.56	–0.142	0.572	–0.228	0.637
AA 15	Asparagine-III	20.62	–0.111	0.572	–0.023	1.026
AA 16	Methionine-III	6.48	–0.253	0.537	–0.233	0.709
AA 17	Cysteine-III	6.57	–0.092	0.557	–0.071	0.709
AA 18	Histidine-III	25.23	0.038	0.57	0.028	0.918
AA 19	Threonine-III	14.31	–0.052	0.579	0.021	0.886
AA 20	Tyrosine-III	10.26	0.018	0.588	–0.002	0.886
AA 21	Glutamine-III	4.22	0.018	0.568	–0.282	0.637

* Corresponding author. E-mail: yousefisa@sums.ac.ir