Electronic Supplementary Material (ESI) for RSC Advances.

Combined molecular docking, homology modelling and density functional theory studies to modify dioxygenase to efficiently degrade aromatic hydrocarbons

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Table A.1 Hydrophilic/hydrophobic characteristics of 20 amino acids[1]

Amino acids	Abbrevia-tion	Hydrophilic/ hydrophobic	Hydrophobic value	Amino acids	Abbrevia-tion	Hydrophilic/ hydrophobic	Hydrophobic value
Alanine	Ala	Hydrophobic	0.62	Methionine	Met	Hydrophobic	0.64
Cysteine	Cys	Hydrophilic	0.29	Asparagine	Asn	Hydrophilic	-0.85
Aspartic acid	Asp	Hydrophilic	-1.05	Proline	Pro	Hydrophobic	0.12
Glutamic acid	Glu	Hydrophilic	-0.87	Glutamine	Gln	Hydrophilic	-0.78
Phenylalanine	Phe	Hydrophobic	1.19	Arginine	Arg	Hydrophilic	-1.73
Glycine	Gly	Undetermined	0.48	Serine	Ser	Hydrophilic	-0.18
Histidine	His	Hydrophilic	-0.40	Threonine	Thr	Hydrophilic	-0.05
Isoleucine	Ile	Hydrophobic	1.38	Valine	Val	Hydrophobic	1.08
Lysine	Lys	Hydrophilic	-1.35	Tryptophan	Trp	Hydrophobic	0.81
Leucine	Leu	Hydrophobic	1.06	Tyrosine	Tyr	Hydrophobic	0.26

[1] : Cited from Reference (V. Fauchere-Pliska, *Eur. J. Med. Chem*., 1983, **18**, 369-375).