

MODELING OF DIPEPTIDES CONTAINING POTENTIAL BIOLOGICALLY ACTIVE (S)- α -PROPARGYLGYCINE, DISCLOSURE OF POSSIBLE BIOLOGICAL PROPERTIES AND TARGETED SYNTHESIS

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Considering a wide spectrum of biological properties of peptides, we found it actual to study by "Pass-online" software the range of possible biological activities of dipeptides, containing (S)- α -propargylglycine. "Pass-online" is a subsidiary tool to evaluate the general biological potential of organic drug-like molecules [1]. Table

Table

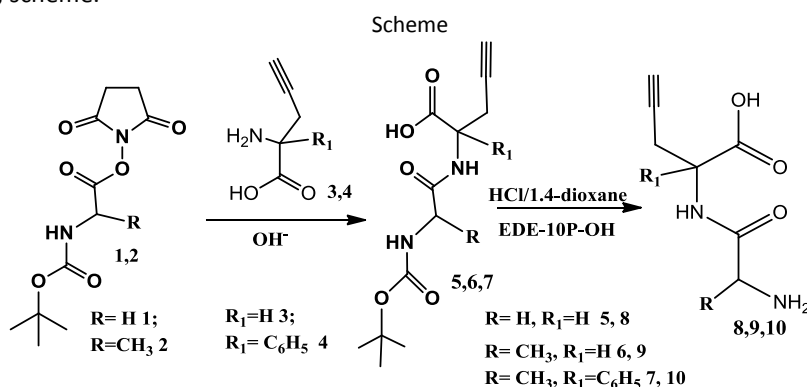
Some possible biological activities of peptides

Peptides	Anticonulsant		Protein-disulfide reductase (glutathione) inhibitor		Mucositis treatment		Cystathionine gamma-lyase inhibitor	
	Pa	Pi	Pa	Pi	Pa	Pi	Pa	Pi
Boc-glycyl-(S)-propargylglycine (5)	0,846	0,005	0,722	0,012	0,574	0,052	0,291	0,006
Glycyl-propargylglycine (12)	0,667	0,012	0,849	0,005	0,876	0,008	0,885	0,002
Boc-(S)-alanyl-(S)-propargylglycyl (6)	0,675	0,011	0,662	0,026	0,501	0,073	-	-
(S)-alanyl-(S)-propargylglycyl (13)	-	-	0,862	0,005	0,911	0,006	0,918	0,002
Boc-(S)-alanyl-(S)- α -benzylpropargylglycyl (7)	0,797	0,005	0,488	0,074	-	-	-	-
(S)-alanyl-(S)- α -benzylpropargylglycyl (14)	0,677	0,011	0,730	0,016	0,724	0,021	-	-

Pa (probability "to be active") estimates the probability of belonging of the test compound to the subclass of active compounds based on the similarity of the structure with those molecules that are most typical in this subset.

Pi (probability "to be inactive") estimates the probability of belonging of the test compound to the subclass of inactive compounds. The research results are expressed by (Pa) and (Pi) values in the range from 0 to 1.

According to the PASS predictions, the greatest probability of activity being anticipated with dipeptides (S)-alanyl-(S)-propargylglycyl (13), Glycyl-propargylglycine (12). Synthesis of the selected peptides was carried out by the method of [2], scheme.



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References

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