Proceedings International
Platinum Open Access Journal (ISSN 2668-6384)

Proceedings, Abstract
Volume 3, Issue 5, 2021, 63
https://doi.org/10.33263/Proceedings35.063

Design, Synthesis and Docking Study of Novel 4-anilinoquinazoline Derivatives for Potential EGFR Kinase Inhibitors †

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† International Conference on Advanced Materials for Next Generation Applications, 29th – 30th September, 2021 (AMNGA-2021)

Received: 10.09.2021; Revised: 20.09.2021; Accepted: 21.09.2021; Published: 29.09.2021

Abstract: According to clinical data existing since last two decades, EGFR (Epidermal Growth Factor Receptors) Inhibitors have shown significant resistance effects after six to nine-month treatment due to point mutation in NSCLC (Non-small cell lung cancer) patients. There is an imperative need for the identification of a capable scaffold that provides knowledge regarding new strategies to overcome current clinical limitations. Design and synthesis of N^4 –(2-methyl-4-nitrophenyl) quinazoline-4, 6-diamine derivatives have been prepared in four steps; in all steps, the obtained product was purified by recrystallization using suitable solvents. All synthesized compounds were characterized by Fourier-transform infrared (FT-IR), ^{1}H nuclear magnetic resonance (NMR). Results of Molecular docking analysis indicated that most of these analogs are comparable to gefitinib in their ability to inhibit against $EGFR^{T790M}$ mutant form in EGFR Kinase Domain and several also exhibited significantly enhanced anti-tumor potency in non-small cell lung cancer (NSCLC) patients. Therefore, these derivatives can be potential agents for cancer therapy, deserving further research.

Keywords: 5-nitroanthranilic acid; EGFR kinase domain; molecular docking; EGFR inhibitors; NSCLC.

Funding

This research received no external funding.

Acknowledgments

Galgotias University.

Conflicts of Interest

The authors declare no conflict of interest.