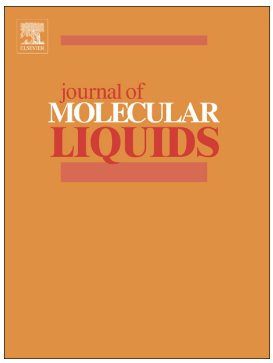


# Design, synthesis, in-silico and in-vitro evaluation of di-cationic pyridinium ionic liquids as potential anticancer scaffolds

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# Design, Synthesis, *In-silico* and *In-vitro* Evaluation of Di-Cationic Pyridinium Ionic Liquids as Potential Anticancer Scaffolds

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## ABSTRACT

An array of dicationic pyridinium ionic liquids (DILs) based hydrazone linkage were designed and synthesized via the quaternization of the appropriate bispyridine hydrazone with different phenacyl halides and led to the formation of halogenated DILs, which undergo metathesis reaction to give the specific task dicationic pyridinium liquids carrying fluorinated counter anions ($PF_6^-$, $BF_4^-$, $CF_3COO^-$). The newly synthesized DILs were well characterized using whole spectroscopic data. The Anticancer evaluation of DILs against breast and colon cancer cell lines revealed that compound **22** appears to be the most active compound in the series with $IC_{50}$ in the two-digit micromolar range. The in-vitro anticancer results were further supported by in-silico molecular docking studies revealing the highest potency of compound **22**. The docking analysis demonstrated good docking score and binding affinities of the synthesized compounds on the target protein PI3Kinase.

**Keywords**: Ionic liquids synthesis, quaternization, metathesis, dicationic ionic liquids, hydrazones, anticancer activity, molecular docking

## 1. Introduction

Cancer is one of the most compelling public health concerns worldwide. Based on the most recent statistics released by the World Health Organization (WHO) in 2015, it was estimated that about 8.8 million people passed away from cancer in that year [1]. Chemotherapy remains to be considered as the standard regime for cancer treatment [2, 3]. Despite of the improvements that have been consistently achieved in the field of chemotherapy over the last two decades, the search for new anticancer agents with significantly superior efficacy/safety ratio continues.