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## Plant Macromolecule from different species of Boraginaceae family, its synthetic monomer and their anticancer efficacy

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The 13C NMR experiments of water-soluble high-molecular preparations from different species of Boraginaceae family were carried out and simulated 13C NMR spectrum was calculated for 2-hydroxy-3-(3',4'-dihydroxyphenyl)-propionic acid residue (I) of the corresponding polyether using ACD/CNMR Version 1.1 program. Signal positions in the 13C NMR spectrum of this hypothetical structure (I) coincided satisfactory with the experimental values. According to 13C, 1H NMR, APT, 2D heteronuclear 1H/13C HSQC and 2D DOSY experiments the main structural element of these preparations was found to be a regularly substituted by 3,4-dihydroxyphenyl and carboxyl groups polyoxyethylene backbone, namely poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA) or poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene]. The synthesis of racemic monomer of PDPGA 2,3-dihydroxy-3-(3,4-dihydroxyphenyl)propionic acid (DDPPA) and its enantiomers (+)-(2R,3S)-DDPPA and (–)-(2S,3R)-DDPPA was carried out via Sharpless asymmetric dihydroxylation of trans-caffeic acid derivatives using a potassium osmate catalyst and enantiocomplementary catalysts cinchona alkaloid derivatives (DHQ)2-PHAL and (DHQD)2-PHAL as chiral auxiliaries. The opposite configuration of both enantiomers was confirmed by measurements of the optical rotation (+)/(–)-values and circular dichroism spectra. The determination of enantiomeric purity was performed by HPLC analysis. PDPGA and DDPPA exerted anti-cancer efficacy *in vitro* and in vivo against human prostate cancer (PCA) cells via targeting androgen receptor, cell cycle arrest and apoptosis without any toxicity, together with a strong decrease in prostate specific antigen level in plasma. However, our results showed that anticancer efficacy of PDPGA is more effective compared to its synthetic monomer. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

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## Synthesis and biological evaluation of BCP derivatives: A steadfast effort towards introducing a contemporary lead optimization tool.

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Potential applications of the bicyclo[1.1.1]pentane (BCP) motif, as a contemporary lead optimization tool, has generated substantial interest in medicinal chemistry.1 However, a realistic introduction of this building-block to the mainstream medicinal chemistry warrants a systematic and steadfast approach towards its development. In 2013, originating from an "out-of-the-box" notion to resolve issues pertaining to an on-going medicinal chemistry study, we recognized the need to resolve the paucity of synthetic access to BCP derivatives.2 Taking cognizance of the non-trivial chemical demeanor of the strained BCP motif, we devised contemporary strategies to secure key BCP derivatives in a scalable fashion. As an outcome, we have now secured a robust and scalable access to a variety of key intermediates such as the BCP amine (1) its 3-fluoro and 3-phenyl substituted counterparts 2 and 3, and 3-pyrazine BCP carboxylic acid (4).3-6 The newly discovered synthetic know-how was deployed to generate a library of BCP-based fragments for an 'in-house' FBDD initiative. Moreover, empowered by our synthetic studies we have also invested efforts to understand the biological behavior of BCP derivatives. In this presentation, I will narrate the background, the progress, and our future objectives related to our work on the BCP derivatives.

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