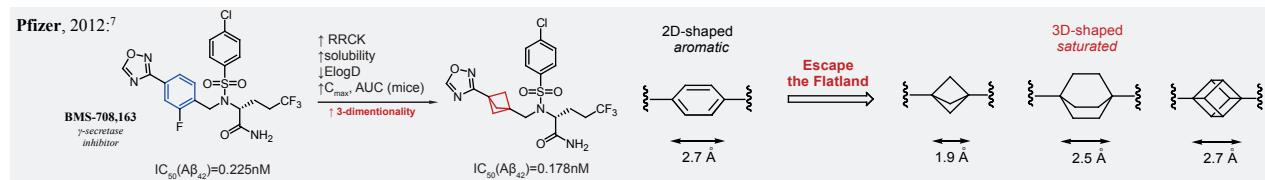


Design and synthesis of novel 3D-shaped building blocks to “Escape the Flatland”

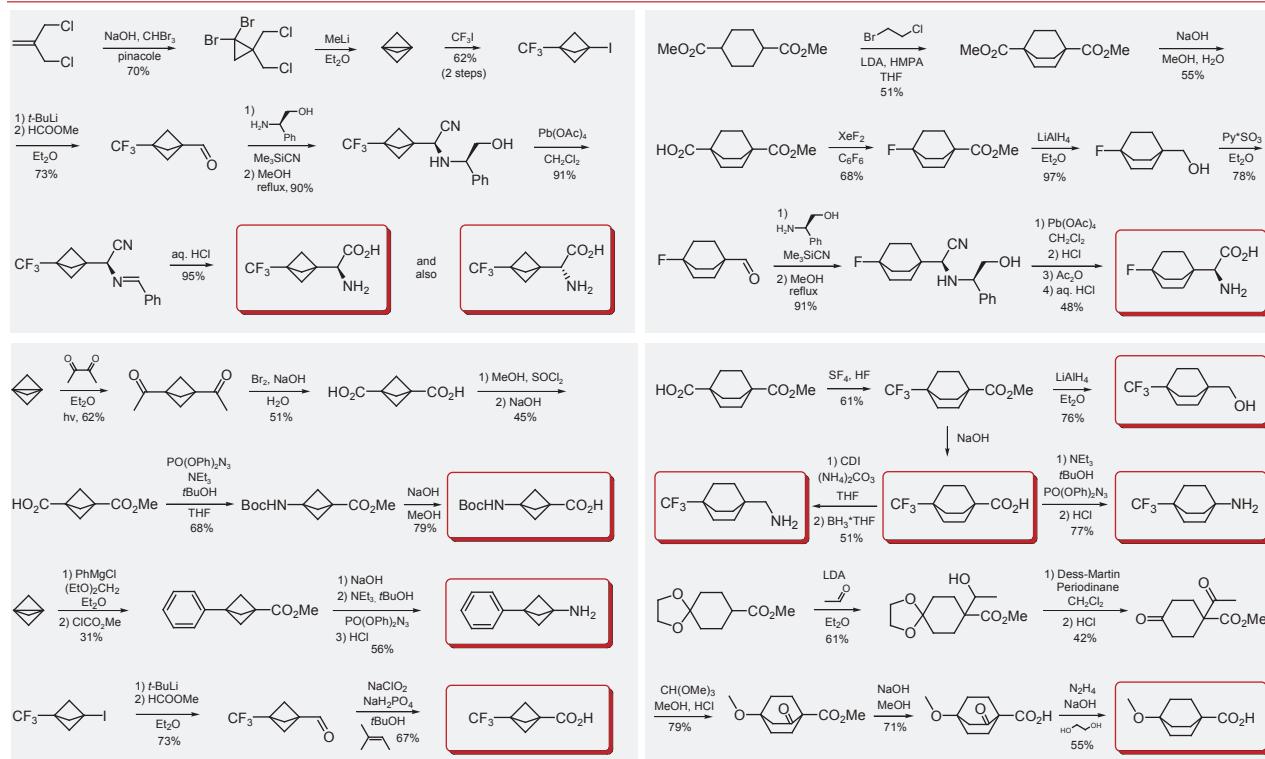
Bandak, D.; Dmytryiv Y.; Iakymenko, A.; Komarov, I.; Kokhan, S.; Korolyov, A.; Mitiuk, A.; Mykhailiuk, P.; Pavlenko, S.; Tymtsunik, A.; Tolmachev, A.

Introduction and Aim

“Escape the Flatland” concept has already gained a considerable attention in medicinal chemistry.^{1,2} Scientists are looking more and more now on 3D-shaped saturated building blocks.³⁻⁶ For example, in 2012 chemists at Pfizer showed that replacing benzene ring in BMS-108,163 by bicyclo[1.1.1]pentyl skeleton beneficially affected activity and ADMET-characteristics of the compound.⁷ In this context, herein we have carefully designed and synthesized a library novel 3D-shaped building blocks to “Escape the Flatland”.⁸⁻¹⁰



Synthesis



Results

<chem>H2N-C1CC(CO2)-C1</chem> EN300-147191	<chem>BocHN-C1CC(CO2)-C1</chem> EN300-88065	<chem>Br-C1CC(CO2)-C1</chem> EN300-90586	<chem>CF3-C1CC(CO2)-C1</chem> EN300-53511	<chem>AcO-C1CC(CO2)-C1</chem> EN300-173070	<chem>OC(=O)c1ccccc1C(=O)O</chem> EN300-152523	<chem>MeO2C-C1CC(CO2)-C1</chem> EN300-132008	<chem>OC(=O)c1ccccc1C(=O)OEt</chem> EN300-179023
<chem>CF3-C1CC(CO2)-C1</chem> EN300-97962	<chem>c1ccccc1C(=O)N</chem> EN300-171117	<chem>Br-C1CC(Otso)-C1</chem> EN300-181643	<chem>CF3-C1CC(C(=O)N)C1</chem> EN300-53088	<chem>CF3-C1CC(C(=O)NHFmoc)C1</chem> EN300-89327	<chem>OC(=O)c1ccccc1C(=O)O</chem> EN300-144843	<chem>F-C1CC(CO2)-C1</chem> EN300-106450	<chem>OC(=O)c1ccccc1C(=O)OEt</chem> EN300-203071
<chem>OC(=O)c1ccccc1C(=O)O</chem> EN300-106638	<chem>OC(=O)c1ccccc1COEt</chem> EN300-52241	<chem>OC(=O)c1ccccc1C(=O)O</chem> EN300-69426	<chem>OC(=O)c1ccccc1C=O</chem> EN300-204870	<chem>OC(=O)c1ccccc1CO</chem> EN300-211274	<chem>OC(=O)c1ccccc1CO</chem> EN300-206665	<chem>NH2c1ccccc1</chem> EN300-111973	<chem>OC(=O)c1ccccc1C(=O)NH</chem> EN300-177920

Contact

Pavel Mykhailiuk, PhD
Pavel.Mykhailiuk@mail.enamine.net
Enamine Ltd., www.enamine.net
78 Chervonotkatska St, 02660 Kyiv, Ukraine

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