

Introduction

DNA-encoded libraries combine the best from both worlds – display technologies and traditional screening approaches. Their utilization allows to cover broad chemical space within relatively short period of time and at low cost. Starting building blocks set of high quality (i.e. novelty and reactivity) comprising molecules with unique motifs with 2 or 3 orthogonal points of variation is crucial to create a high-quality DNA-encoded library. Therefore, we have selected two sets of DEL-compatible bifunctional and trifunctional building blocks from our 50 million offer of on-demand available compounds.

Compound Sets

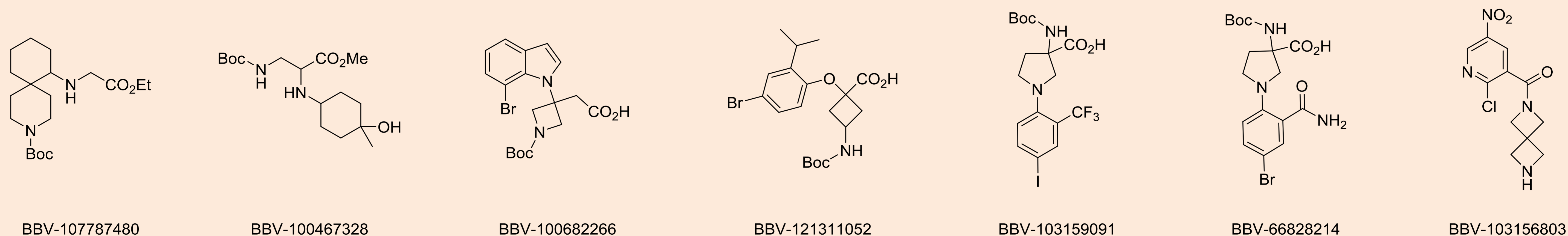
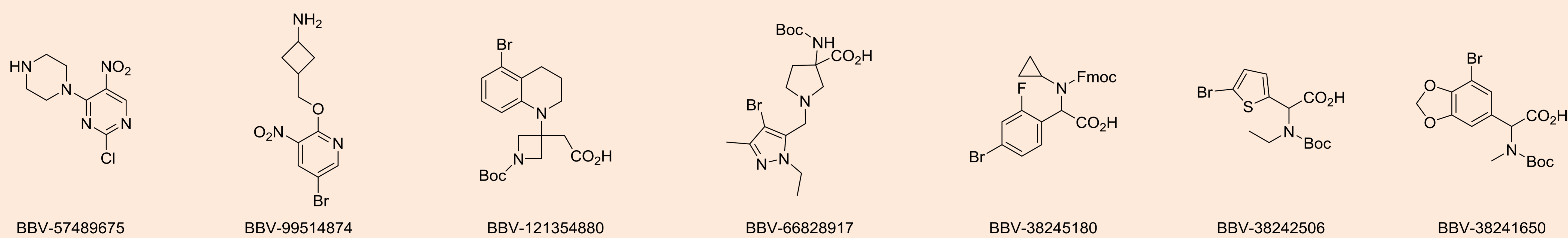
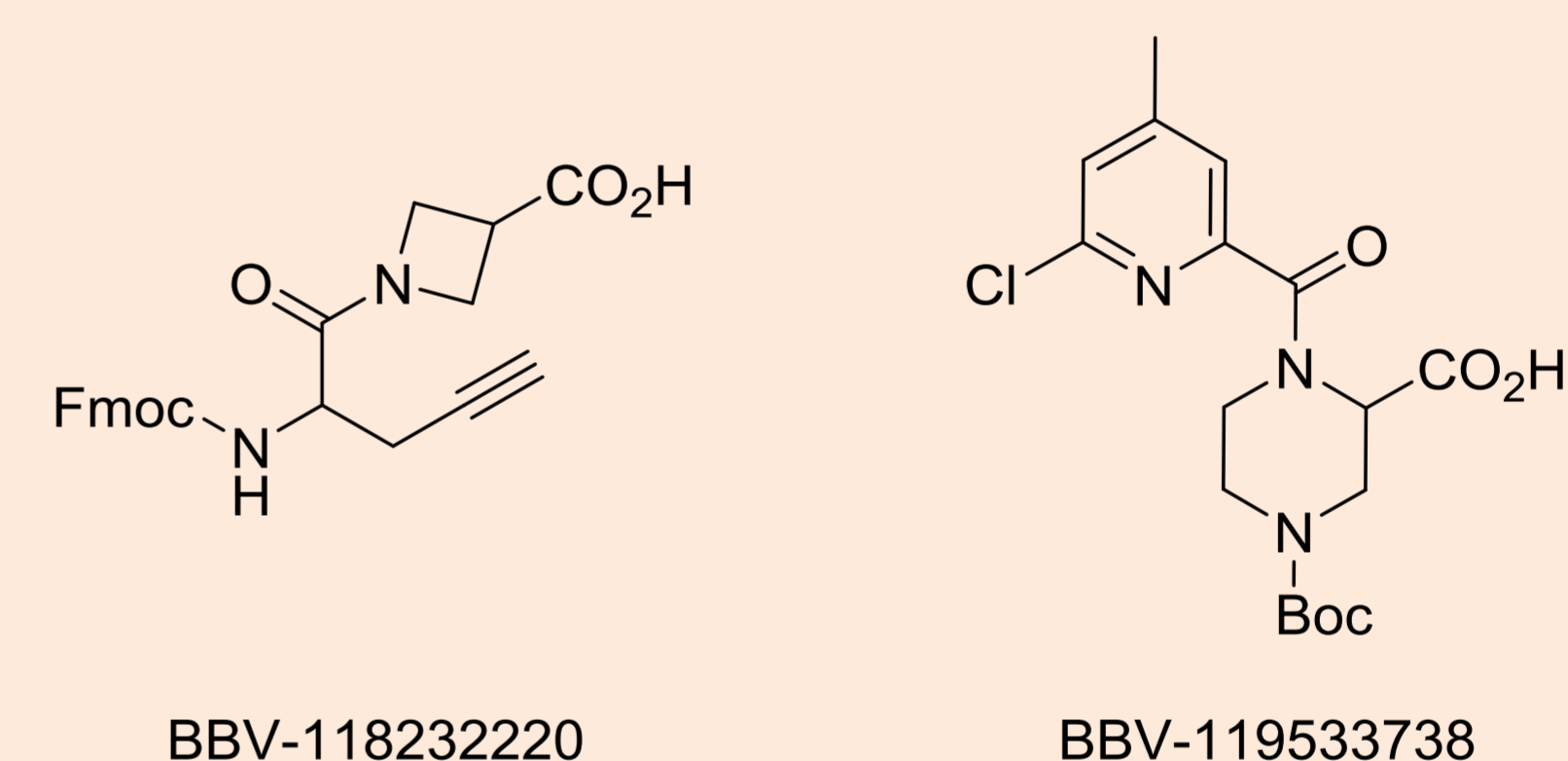
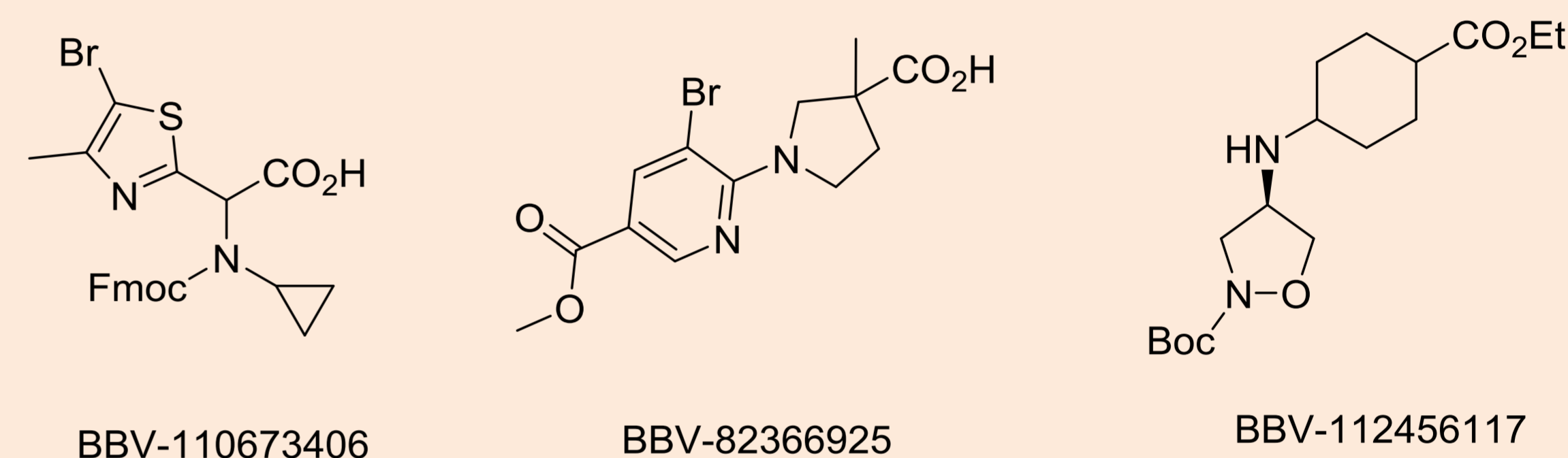
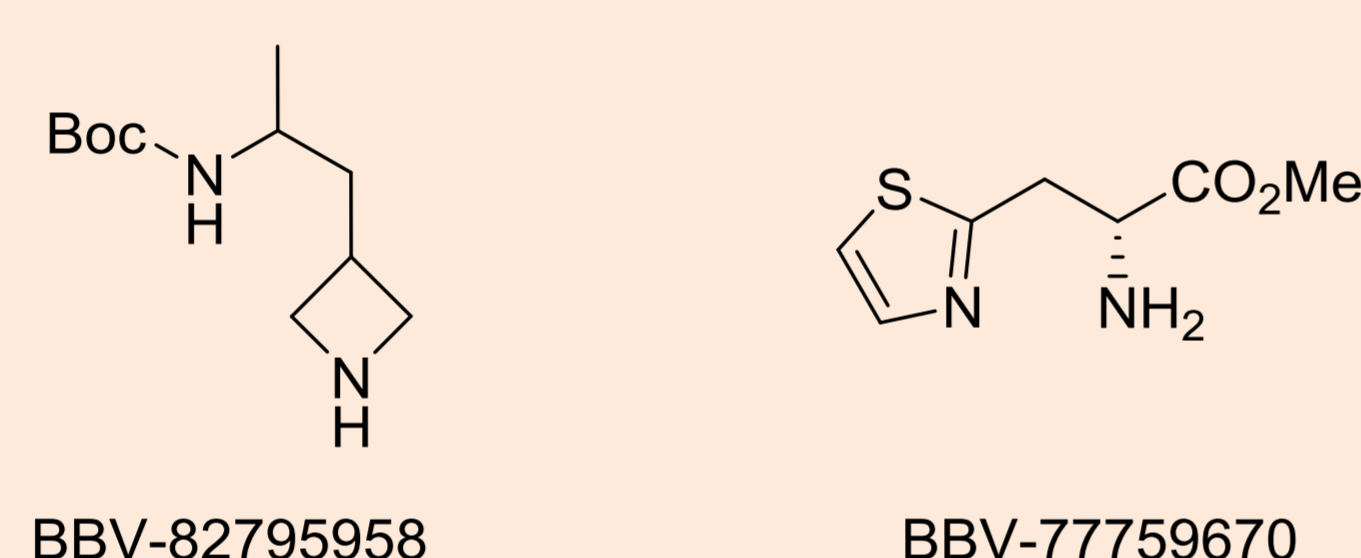
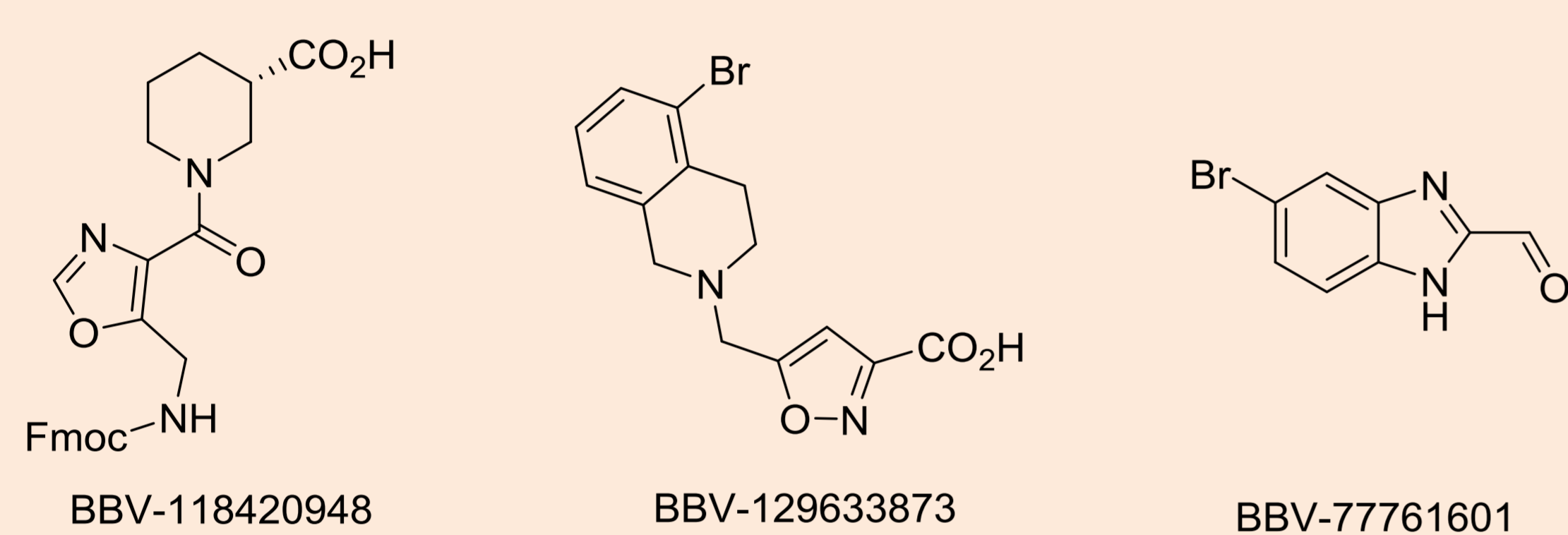
- **606,000** bifunctional and **21,000** trifunctional compounds;
- new molecules (no close analogs in the purchasable space);
- favorable physicochemical profiles (heavy atoms < 20; chiral atoms < 1; rotatable bonds < 7).

Bifunctional building blocks

Acid_Aldehyde	1,280	Aldehyde_NBoc	5,163
Acid_Alkyne	14,111	Aldehyde_Nitro	4,814
Acid_ArHal	130,921	Aldehyde_SO2X	27
Acid_Azide	13	Amine_Azide	146
Acid_Ester	7,239	Amine_Ester	82,310
Acid_Isothiocyanate	7	Amine_NBoc	270,759
Acid_NBoc	30,329	Amine_NCbz	83
Acid_NCbz	23	Amine_NFmoc	550
Acid_NFmoc	16,757	Boronates_with_Functions	37
Acid_Nitro	25,657	Ester_Isocyanates	50
Aldehyde_ArHal	14,622	Ester_SO2X	281
Aldehyde_Ester	1,215		

Trifunctional building blocks

Acid_Aldehyde_ArHal	45	Acid_NBoc_NFmoc	253
Acid_Aldehyde_Nitro	10	Acid_NBoc_Nitro	877
Acid_ArHal_Ester	874	Acid_NFmoc_Alkyne	97
Acid_ArHal_Nitro	2,953	Acid_NFmoc_ArHal	1,613
Acid_Ester_Nitro	39	Acid_NFmoc_Ester	20
Acid_NBoc_Alkyne	134	Acid_NFmoc_Nitro	67
Acid_NBoc_ArHal	3,508	Amine_ArHal_Nitro	7,847
Acid_NBoc_Ester	57	Ester_NBoc_Amine	3,131
Acid_NBoc_NCbz	24		



Availability

- Make on demand compounds, all with prices;
- 1-4 synthetic steps from in-stock reagents;
- 3-6 weeks synthesis time, 70% success rate;
- Purity 95%+ (by LCMS, NMR);
- Custom design of protecting group strategies.

Contacts

Yurii Moroz, PhD
yurii.moroz@chem-space.com
7 Deer Park Drive, Suite M-5
Monmouth Junction, NJ 08852, USA
www.chem-space.com