

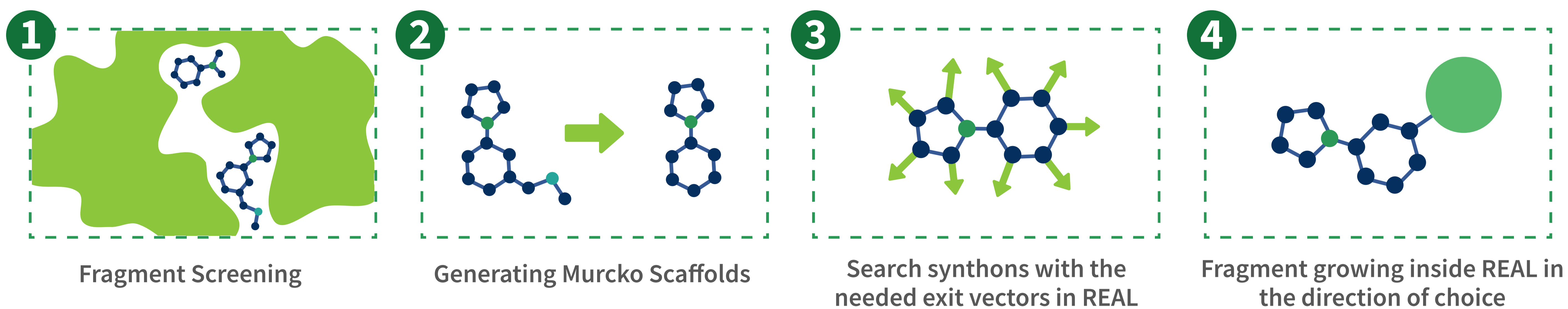
REAL Fragment Library: Efficient fragment growing inside Enamine REAL using exit vector analysis

O. Tarkhanova¹, A. Kapeliukha¹, O. Strapak¹, Y. Moroz²

¹Chemspace LLC, 85 Winston Churchill Street, Kyiv 02094, Ukraine

²Enamine Ltd, 78 Winston Churchill Street, Kyiv 02094, Ukraine

Concept - Fragment Growing Inside Enamine REAL



REAL Fragment Library

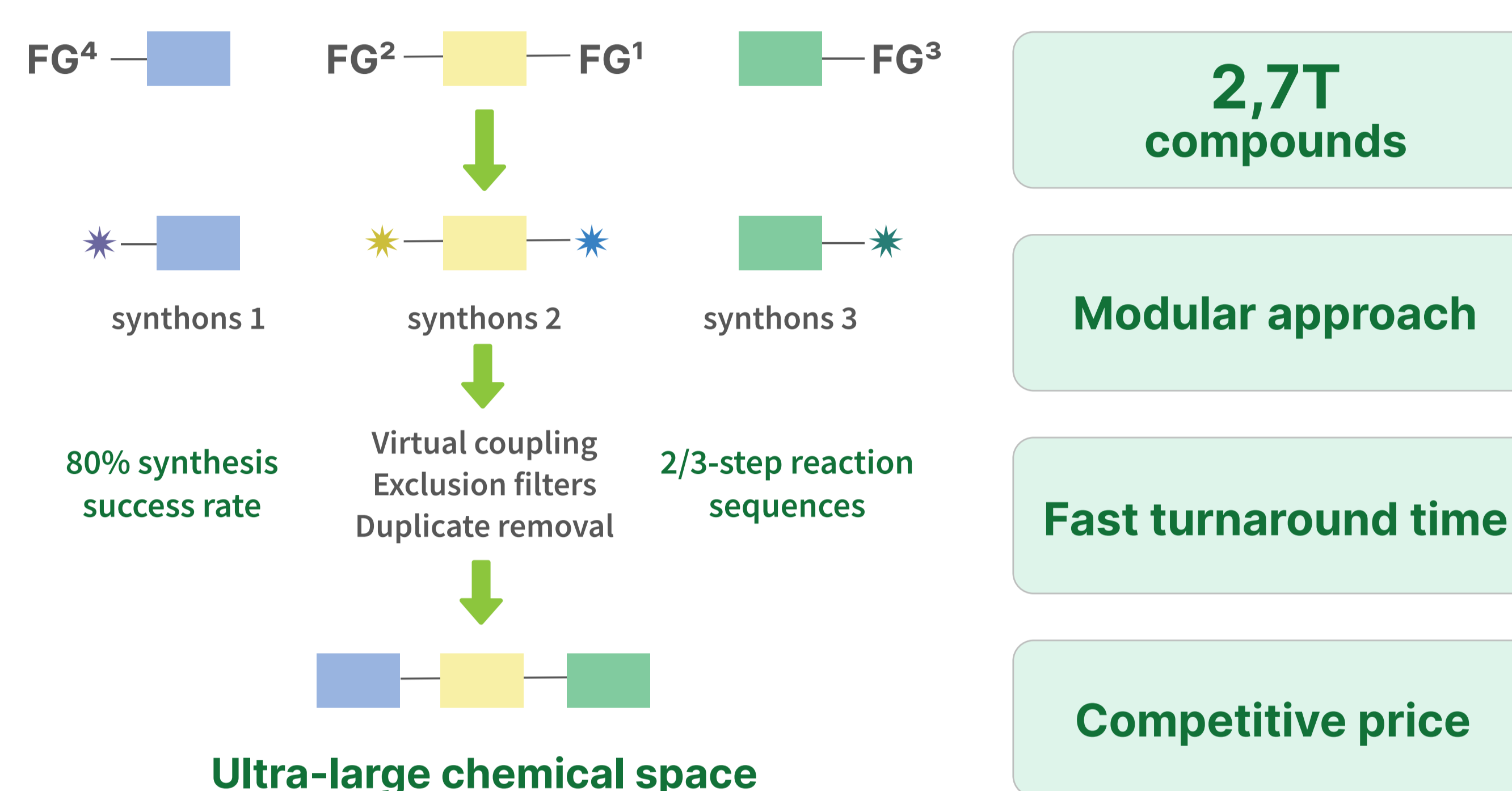
Fragment Selection Criteria:

- ✓ Coverage score ≥ 2
- ✓ N unique synthons by scaffold ≥ 5
- ✓ N unique reactions ≥ 5

Final Library

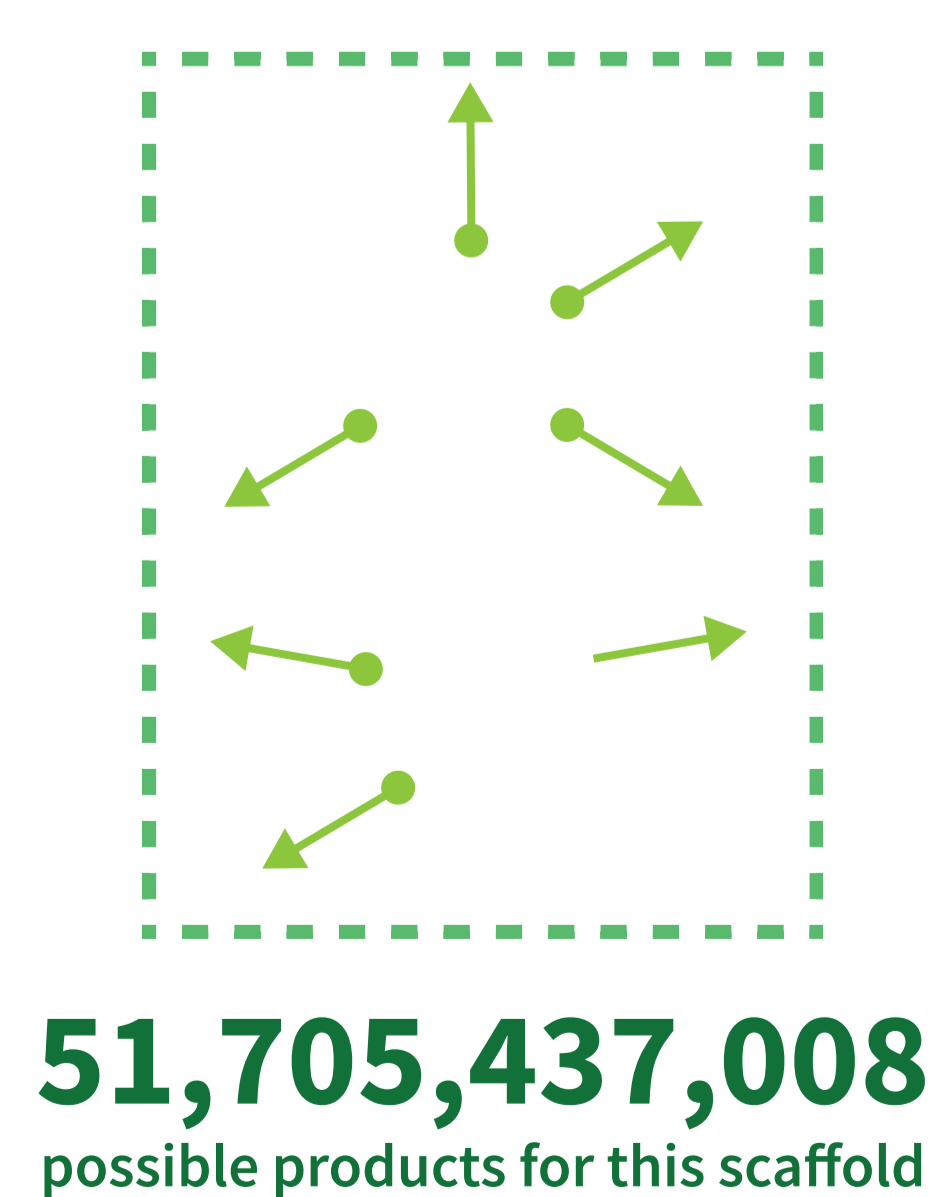
4,980 compounds

Composition of Enamine REAL



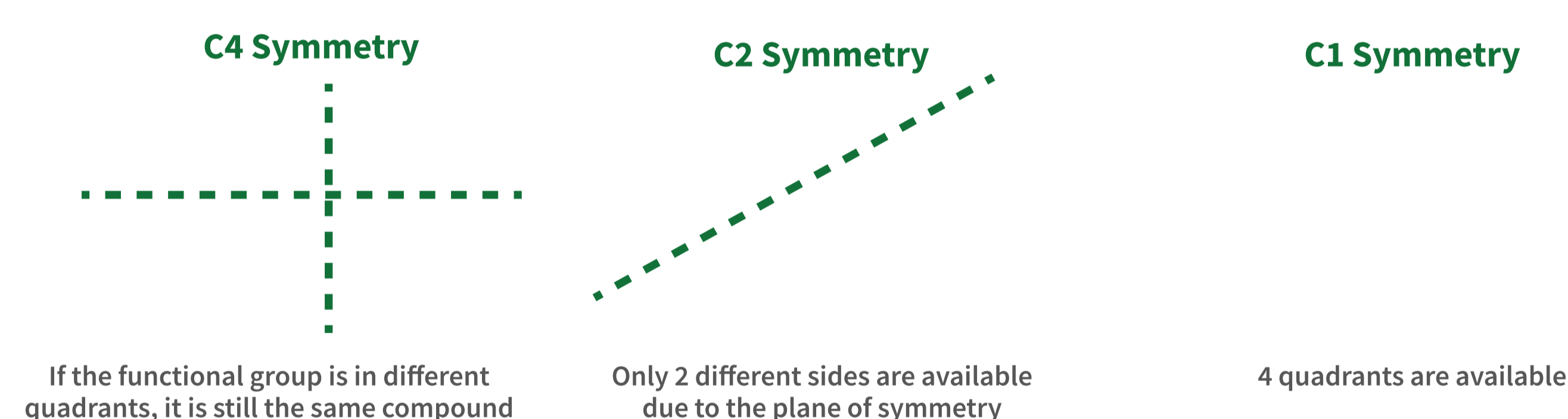
Coverage of REAL scaffolds - UMAP plot

Fragment Growing Examples

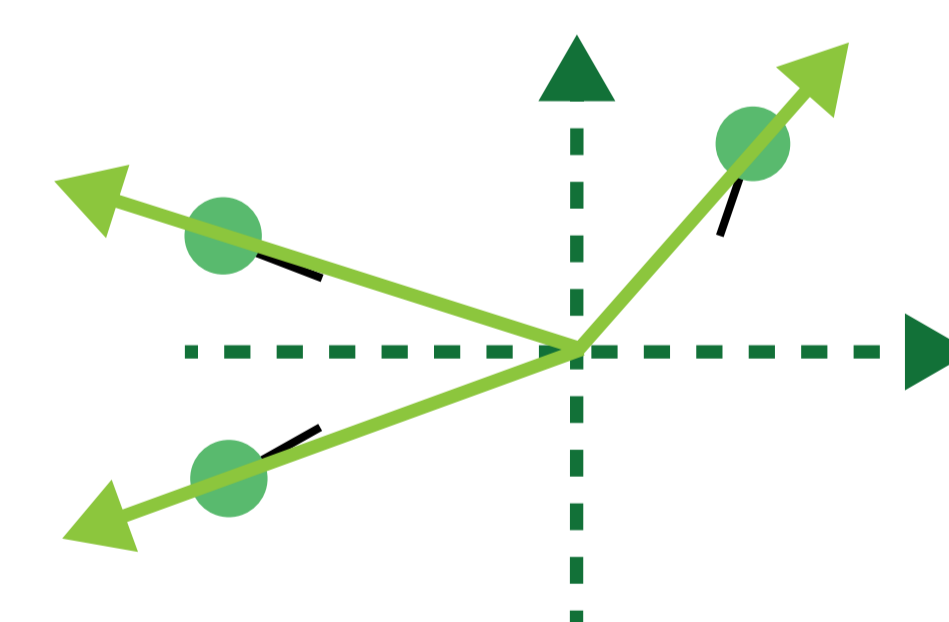


Algorithm of REAL scaffolds annotation

Custom algorithm: determining scaffold symmetry for annotation



Annotation of possible exit vectors by angle



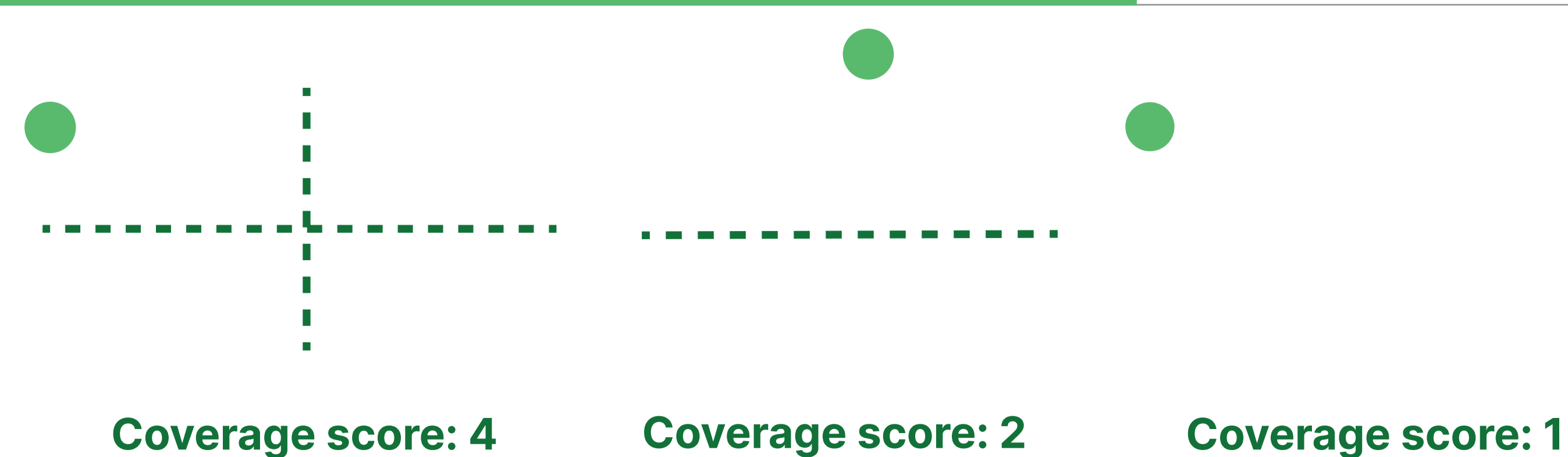
Annotation parameters:

1. Number of synthons by ID
2. Number of synthons by SMILES
3. Number of unique reactions
4. Scaffold symmetry
5. Number of reaction site angles
6. Number of quadrants
7. Coverage score

Coverage score:

1. XY symmetry -> 4
2. X or Y:
1 quadrant - 2
2 quadrants - 4
3. No symmetry -> based on N quadrants

Examples of coverage score



✉ o.tarkhanova@chem-space.com

🌐 www.chem-space.com