***Actions***

|  |  |  |
| --- | --- | --- |
| **Who** | **What**  | **By when** |
| **All** | **Review the agreed principles and email Claire stating whether you agree or would like to see changes.**  | 25th October 2018 |
| **All** | All to look through the slides on R groups and send round your thoughts.  | 25th October 2018 |
| **All** | Email Claire details of commonly used or recommended amino acid naming conventions. | 25th October 2018 |

***Attendees***

|  |  |
| --- | --- |
| **CAS** | Matthew Dunbar (CAS) |
| **Carnegie-Mellon University** | Dave Yaron |
| **EBI** | Ann Gaulton |
| **Lille University** | Maude Pupin |
| **Lilly** | Kent Holaday |
| **NextMove**  | Roger Sayle |
| **Novartis** | Yohann Potier |
| **Pfizer** | Tianhong Zhang |
|  | Sergio Rotstein |
| **Pistoia Alliance** | Claire Bellamy |
| **PubChem** | Evan Bolton |
| **Sciligence** | Tony Yuan |

**Agenda**

Peptide

* Substitutions
* R groups

Future topics

Next steps

# Peptide diversity and exploding monomer sets

The notes below capture the key questions and comments. See slides for the topic background and questions.

## Principles (tentatively) agreed

HELM should use capping monomers for C and N terminal substitutions. i.e.

 and not 

Capping monomers should be the same polymer type as the main chain of the polymer they are a part of to keep the HELM string as readable as possible.

All other types of monomer: i.e. non-terminal N substitutions and substitutions elsewhere on the amino acid, L, D and positional isomers should be defined as new monomers.

* We will not define a new branch type monomer to handle peptide substitutions.

***Action:*** Please consider the implications of these principles and email round comments if you find difficulties that we did not discuss, and you believe we should consider.

***Comments and issues***

You can have same monomer structure defined as different monomers if those monomers are different polymer types. When using - the user should select the one most appropriate to the context to help readability.

Large monomer sets are not necessarily a problem if they can be sorted in a way that makes navigation easy. For example, can you say: give me all the L forms or N substituted forms?

Naming will be critical to facilitate navigation of the monomer set.

Different R groups will be required for N and C terminal positions.

We should use statistics to identify the most common monomers, so any core set is focussed on the most frequently used. (post meeting question – should infrequent monomers be defined using in-line HELM?). Groups can then use the best practice rules for additions to this set as they need to.

# R groups

 ***Action*:** All to look through the slides on R groups and send round your thoughts.

# Next Steps

***Action:*** Let Claire know if you have a suggestion for a naming convention for peptides.