| Date/time | Fri, May 30 | Sat, May 31 | Sun, June 1 | Mon, June 2 | Tue, June 3 | Wed, June 4 | Thu, June 5 | Fri, June 6 | Sat, June 7 | Sun, June 8 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 8:30 |  | Introduction (Guerri, Spadon, Bolstad, Arnold) |  |  |  |  |  |  |  |  |
| 9:00 |  | Engineering GPCRs (M. Congreve) | Molecular modeling (J. Blaney) | Influenza virus polymerase (S. Cusack) | Protein-ligand interactions 1(G. Klebe) | Enzyme activation (J. Wells) | Targeted drug design <br> (R. Zarivach) | Antibody diversity (J. Wells) | $\begin{array}{\|l} \hline \text { Targeting PPI: } \\ \text { examples (T. } \\ \text { Blundell) } \\ \hline \end{array}$ |  |
| 9:45 |  | GPCR structures (A. Kruse) | Structural bioinformatics (A. Tramontano) | AIDS drugs + overcoming resistance (E. Arnold) | Small molecules (C. Groom) | Enzymology and drug discovery-1 (H. Danielson) | Molecular Obesity (M. Hann) | J. Blaney (2) | Podjarny (2) |  |
| 10:30 |  | Coffee | Coffee | Coffee | Coffee | Coffee | Coffee | Coffee | Coffee |  |
| 11:00 |  | Membrane protein structures (R. Stroud) | Docking (J.J. Irwin) | Talks from posters: <br> H. Kyle, J. Darby, N. Levy | Protein aggregation and DD (S. <br> Ventura) | $\begin{aligned} & \text { Buster etc. (O. } \\ & \text { Smart) } \end{aligned}$ | Talks from posters; P. Plevka, N. Radeka - Ends at 12) | Bromodomains (C.-w. Chung) | Enzymology and drug discovery -2 <br> (H. Danielson) |  |
| 11:45 |  | Epigenetics (C.-w. Chung) | Hits to drugs (G. Scapin -2) |  | Protein-ligand interactions (A. Podjarny) | Talks from posters: S. <br> Stella, J, <br> Carlsson - <br> Ends at 12:45) | Excursion 2 | Fragment screening experiences (J. Bauman) | SBDD of Diabetes drugs (G. Scapin) |  |
| 12:30 |  | Lunch | Lunch |  | Lunch | Lunch |  | Lunch | Lunch |  |
| 14:30 |  | Drug design tales (Pauptit) | Short (2-3 mins) Presentation of posters (odd numbers |  | PPI: general aspects of druggability (T. Blundell) | Short (2-3 mins) Presentation of posters (even numbers) |  | HOT TOPICS (from poster abstracts) L. De Colibus, L.Preiss, I. Prokhorova | Protein-ligand interactions 2 (G. Klebe) |  |
| 15:15 |  | WS intro | PI3K inhibitors (Bussiere) |  | CCDC | PDB (Berman) |  |  | Cusack (2) |  |
| 16:00 |  | coffee | coffee |  | coffee | coffee |  | coffee | coffee |  |
| 16:30 |  | WS: Groom, | WS: : Groom, |  | Intl Year of | WS: Prlic, |  | WS: Prlic, | Round table |  |
| 17:15 |  | Irwin, Tramontano | Irwin, Tramontano |  | crystallography talks: (Blundell, | Smart |  | Smart | Closing remarks |  |
| 18:00 |  | Introduction to Erice (M. Schmidt) | Poster Session Odd Numbers |  | Howard, Berman, Arnold) games, | Poster Session Even Numbers |  | Free | Free |  |
| 20:00 |  | Welcome buffet | Pasta party |  |  | Pizza party (Sponsored by EmeraldBio) |  |  | Good bye buffet |  |

