**mPPase meeting Wednesday, October 12, 2016 at 13-15 o´clock**

* Keni, Alexi, Niklas, Jari, Henri, Ainoleena and Gustav were present.
* We discussed about the aggregation tests performed by Niklas and Alexi (results can be found in E-Duuni):
  + on a DLS with the help of Tatu Lajunen (Zetasizer APS: <http://www.malvern.com/en/products/product-range/zetasizer-range/zet>). These were hard to analyse but maybe Päivi Tamminen (or Leena Hanski?) can help. **Gusse will check.**
  + on a nephelometer (<https://en.wikipedia.org/wiki/Nephelometer>). These were performed with Timo Oksanen. The results were showing that IAT-39-II, TL4-58 and TL2-73 might form aggregations at the highest concentrations tested; 20 and 50 µM (the files can be found in E-Duuni). However, at lower concentrations they seem to be on the save side. We still have to test them using detergent; **Niklas will prepare the samples tomorrow with Keni.**
* Parasite tests (*P. falciparum*) are performed by Ayman, results on Friday? **Gusse in contact**.
* Parasite tests (*L. donovani*) will be performed by Jaffe; in the end of the month? **Gusse in contact**.
* Keni has still the purchased cmpds (by Ainoleena) as stock solutions in DMSO (100 mM conc., around 200-500 µL); we should have them tested for purity on LC-MS by Nina Sipari (to be able to publish the results). In total around 40 cmpds (a´~30€ → 1200€). The conc. of the samples to LC-MS should be around 0.01 mg/ mL. **How will the costs be distributed (Jari, Henri, Adrian)?**
* **Tomorrow Keni and Niklas** will test 16 new cmpds on mPPase; 6 cmpds from Leeds and 10 cmpds from Alexi and Rali.
* **Alexi and Niklas will synthesize new cmpds**.
* Keni has a new crystal structure of TL2-73!!! Is it an artefact (binding randomly) or not? **We need to know it before we continue with the synthesis of the derivatives** of that cmpd (4 starting materials containing bromide has already been ordered by Alexi).
* **Gusse will apply for ERC StG**, DL is on next Tuesday.
* Keni told us that 25 mM is the lowest concentration for the stock solutions of the cmpds (DMSO limit).
* Henri told us that they will perform virtual screening with cmpds containing Br and I
* **Alexi will ask Paula** for derivatives of TL2-73 to be tested.
* **Gusse asks Adrian** about the situation of the substitution of E-Duuni to Onedrive.
* Ainoleena showed “Leeds cmpds” docked to mPPase.
* All the inhibition test results can be found in E-Duuni.
* We should update the [mPPase Compound Register-file](https://tt.eduuni.fi/sites/hy-mppase/Shared%20Documents/mPPase%20Compound%20Register.xlsx?web=1) in E-Duuni with all the results! **Who will do it?**
* This document was **written by Gusse** and a copy has been put on E-Duuni.