Following the general rules for data fusion:

- Fuse S_1, S_2 and S_3 according to SUM rule for each M_i
- Fuse M_1, M_2 and M_3 according to MAX rule

result: 1 list of fused scores for possible auxiliaries

- 3D similarity?
- Molecular modelling: crystal structure prediction?
    - CONGLOMERATE?