

Additional file 2 – Comparison of Reaction Molecular Signature and Enzyme Commission reaction partition

- a is the number of reaction pairs that are in the same set in EC and in the same set in RMS = **73408**
- b is the number of reaction pairs that are in different sets in EC and in different sets in RMS = **10142098**
- c is the number of reaction pairs that are in the same set in EC and in different sets in RMS = **9946**
- d is the number of reaction pairs that are in different sets in EC and in the same set in RMS = **232984**

$$\text{Rand Index} = \frac{a + b}{a + b + c + d} = \frac{73408 + 10142098}{73408 + 10142098 + 9946 + 232984} = 0.976$$