**The Metabolic Framework – sample queries**

1. **Identify which are the chains of metabolic reactions linking two key metabolites, (such as Leukotriene D4 and arachidonate). The query returns a chain of the shortest length only (shortest path):**

**MATCH** path = shortestPath((m1:Metabolite { MetaboliteName:"arachidonate" })-[\*..]-(m2:Metabolite{MetaboliteName:"Leukotriene D4"}))

**RETURN** path

1. **Count occurrences in metabolic reactions for each metabolite:**

**MATCH** (m:Metabolite)-[:Consumption]->(react1:Reaction), (react2:Reaction)-[:Production]->(m)

**WITH** m.MetaboliteName **as** Metabolite, count(**distinct** react1) **as** ReactConsumption, count(**distinct** react2) **AS** ReactProduction

**RETURN** Metabolite, ReactConsumption, ReactProduction, ReactConsumption + ReactProduction **as** TotalReactions

**ORDER** **BY** TotalReactions **DESC**

1. **Identify all chains of maximum 2 metabolic reactions starting from the arachidonate that do not include metabolites involved in a large number of metabolic reactions (such as proton, H2), Sodium etc..).**

**MATCH** path=((m1:Metabolite{MetaboliteName:'arachidonate'})-[r\*..4]->(m:Metabolite)) **WHERE** not((m)-->()) and none (n **IN** nodes(path) **where** "Metabolite" **in** labels(n) and n.MetaboliteName **in** ["proton", "H2O", "Sodium", "Coenzyme A", "Nicotinamide adenine dinucleotide phosphate", "Nicotinamide adenine dinucleotide phosphate - reduced", "ATP(4-)", "O2", "Bicarbonate", "Nicotinamide adenine dinucleotide", "hydrogenphosphate", "Nicotinamide adenine dinucleotide - reduced", "ADP", "water"]) **OPTIONAL** **MATCH** (catalyzer)-[r1:Catalysis]->(react:Reaction) **where** react **in** nodes(path) and ("Complex" **in** labels(catalyzer)) **RETURN** **distinct** path,r1

1. **Identify the metabolic reactions starting from the arachidonate metabolite:**

**MATCH** ({MetaboliteName:"arachidonate"})-[r1:Consumption]->(react1:Reaction)-[r3:Production]->(m2:Metabolite), ()-[r2:Catalysis]->(react1) **RETURN** r1, r2,r3