# Integrating Graph and Large Language Model with AOP-Wiki for Contextual and Semantic Parsing of Adverse Outcome Pathway Information

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# Supplementary

S-Table 1 Description of AOP nodes and their relations

|  |  |  |
| --- | --- | --- |
| S.NO | NODES | PROPERTIES |
| 1. | AOP | id  authors  name  short\_name  abstract  potential\_applications  essentiality-support  authors  references |
| 2. | KEY\_EVENT | Id  name  short\_name  description  measurement methodology  url  references |
| 3. | KEY\_EVENT\_RELATIONSHIP | name  quantitative understanding  evidence supporting taxonomic applicability  references |
| 4. | BIO\_ACTION | name  source  source id |
| 5. | BIO\_OBJECT | name  source  source id |
| 6. | BIO\_PROCESS | name  source  source id |
| 7. | STRESSORS | id  name  url |
| 8. | CHEMICAL | name  type  identifier |
| 9. | ORGAN | name  source  source-id |
| 10. | ORGANIZATION\_LEVEL | name |

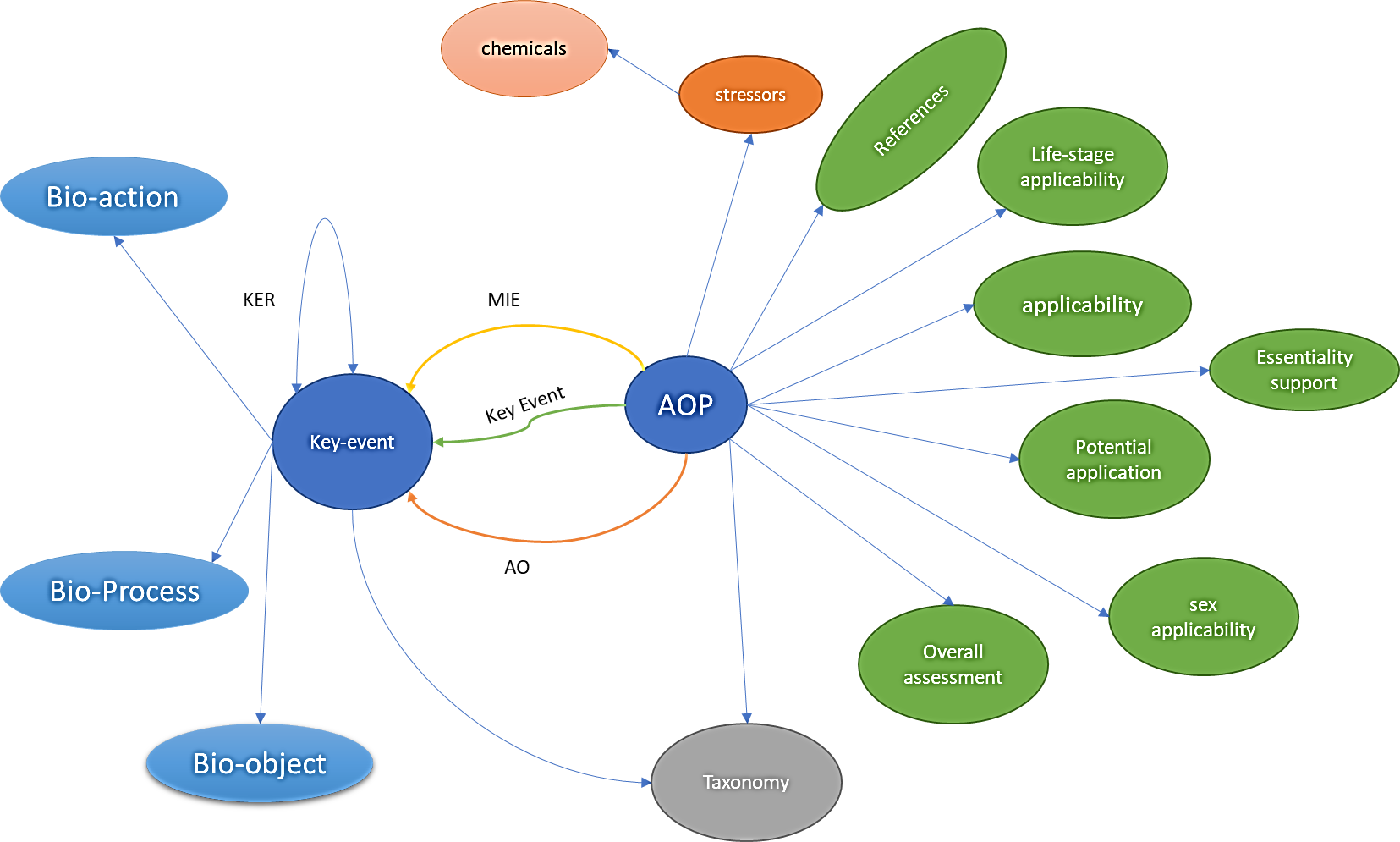
S-Table 2 Natural language and their corresponding cypher query to retrieve information from database

|  |  |
| --- | --- |
| **Natural Language Query** | **Cypher Query** |
| **Simple:** Stressors related to AOP on learning and memory impairment. | MATCH (a:AOP)-[rel1:HAS\_STRESSOR]-(b:STRESSOR)  WHERE toLower(a.name) =~ '.\*learning.\*' OR toLower(a.name) =~ '.\*memory.\*'  RETURN \* |
| **Moderate:** Provide me with a network of AOPs related to neurotoxicity and connected to key events mentioning calcium influx. | MATCH (a: AOP)-[rel1:HAS\_KEY\_EVENT]-(b:KEY\_EVENT)  WHERE toLower(a.name) =~ '.\*neuro.\*'  WITH a  MATCH (a)-[rel2:HAS\_KEY\_EVENT]-(c:KEY\_EVENT)  WHERE toLower(c.name) =~ '.\*calcium.\*'  RETURN \* |
| **Complex:** key events which lie in the shortest path connecting AOPs related to neurotoxicity. | MATCH (a:AOP)-[:HAS\_ADVERSE\_OUTCOME]-(c:KEY\_EVENT)  WHERE toLower(a.name) =~ '.\*neuro.\*'  WITH collect(a.id) as nodes  MATCH (aop1:AOP) WHERE aop1.id IN nodes  MATCH (aop2:AOP) WHERE aop2.id IN nodes AND aop1<>aop2  MATCH path = shortestPath((aop1)-[:HAS\_KEY\_EVENT\*..2]-(aop2))  RETURN path |

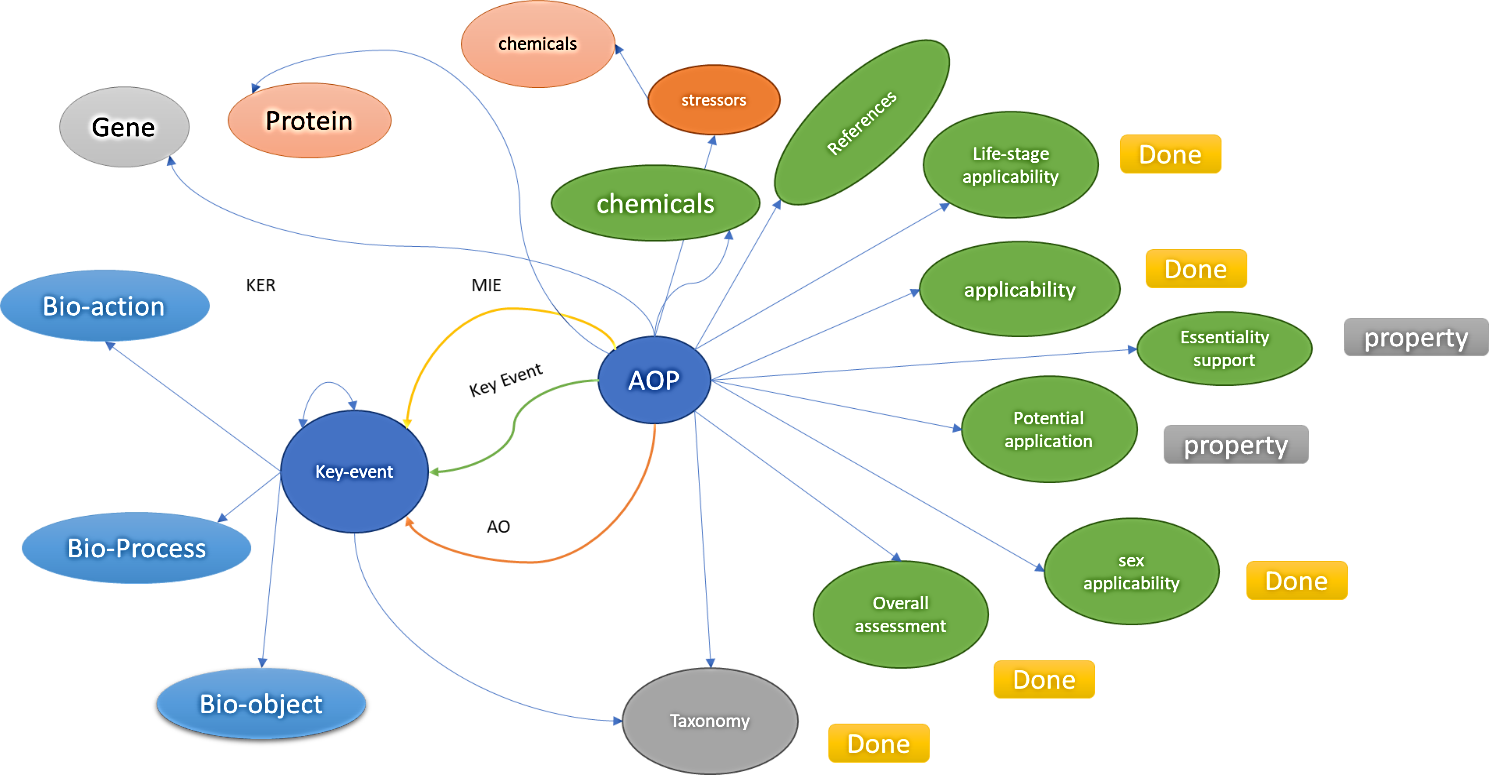
A computer screen shot of text

Description automatically generated

Figure 1 Stepwise query cyphers



S-Figure 2 Graph Schema adapted for AOP in which Key Event Relationship are edge.



S-Figure 3 Graph Schema adapted for AOP in which Key Event Relationship are edge.