DAL roadmap to reach XML server feature parity

Phase 1: DAL MVP

Scope: Demonstrate basic OData functionality and reduced complexity by enabling most common cross-context queries and removal of session handling

Target Date: End of March

Feature	OData	Comment
Unspecific browsing	`rxapiRoot/Substances`	Development: In-progress (dependency on multiple searches for single context) QE: Tests are not yet present
Unspecific pagination	`rxapiRoot/Substances$top=10` &$skip=10	Development: In-progress (dependency: completion of non selective queries) QE: Tests are not yet present
Expand properties for substances • 2nd level of Expand • Filtering within Expand (outer join with filter)	`rxapiRoot/Substances` $expand=MeltingPoints `/Substances?$filter=ReaxysRegistryNumber eq 779271&$expand=MeltingPoin`	Development: In-progress QE: Not yet approved To be discussed further with QE & PO

	`ts($expand=MeltingPointCrystallization)`
	
	`/Substances?$filter=ReaxysRegistryNumber eq 779271&$expand=NmrSpectroscopies($filter=NmrSpectroscopyLocation eq 'Paragraph 0074')`	

[Context] Substance		Development: Complete QE: Not yet approved QA: Not yet approved
[Context] Citation		Development: Complete QE: Not yet approved QA: Not yet approved
[Context] Reaction		Development: Complete QE: Not yet approved QA: Not yet approved
[Context] DPItems		Development: Complete QE: Not yet approved QA: Not yet approved

[Single Hop] Expand Citations to Substances, Reactions	`rxapiRoot/Citations?` `&$expand=` Substances	Development: In-progress QE: Not yet approved
[Single Hop] Expand Substances to Citations, Reactions		Development: In-progress QE: Not yet approved
[Single Hop] Expand Reactions to Substances, citations		Development: In-progress QE: Not yet approved
[Single Hop] Expand DPITEMS to Substances and Citations		Development: In-progress QE: • DPITEMS Context Test - Not available • Cross context Test - Not available To be done • Need consolidated definition of foreign keys (Helge)
[Multi Hop] Expand Targets to X - Approach/technical design to be completed		Not yet started (dependency on the implementation of single hop)
Structure Search		Development: Complete QE: Not yet approved QA: In progress
Order, Limit, Select, Top, Skip, Like, And, Filter		Development: Complete QE: Not yet approved

| Search by property | `/Substances?$filter=ChemicalNames/any(p:p eq 'Aspirin')`

`/Substances?$filter=ReaxysRegistryNumber eq 3587190&$expand=NmrSpectroscopies($filter=NmrSpectroscopySources/any(p:p eq 'Gmelin'))`

`/Citations?$filter=DocumentType eq 'Article'&$select=DocumentType&$expand=CitationJournal($filter=Coden eq 'AJCHAS')` | 1. Search by multipleFields
  a. Development: Complete
  b. QE: Not yet approved
2. Search by value from the subset
  a. Development: Bug-fix in-progress
  b. QE: Not yet approved |

	/Substances?$filter=ReaxysRegistryNumber eq 779271&$expand=MeltingPoints($expand=MeltingPointCrystallization($filter=CrystallizesWith))	
Reaxys API Service (deployment on Kong nonprod)		On target for end of March

Data Schema Consolidation

- virtual fields like BLL are introduced by summus and need to be documented in ds Excel and be tagged as "non-fabrication field"
- Clear definition of foreign keys between context need to be consistent. For classic Reaxys contexts columns Rolle and Verweis are used, where Rolle is of value C and Verweis defines context, such as MERKMALE, ZITATE, etc. This is not true for dpitems where DAT.MRN is referencing substances. Same for DAT links to citations.

Phase 2: existing API feature parity

Scope: Complete feature parity with existing Reaxys Data API to start migration of existing API customers

Target Date: end of 2024

Feature		Comments
[Context] MSItems		

[Context] Measurements		
[Multi Hops] Expand Targets to X (implementation)		
Reaxys API Service (integration with NeoID)		
Grouping		
Aggregation Count		
Similarity Sorting		
SMILES retrieval		
Nested expand pagination	Substances?$expand=Citations($skip=20&$top=10)	
Produce additional controllers for Patents and Articles		
SMILES search		
Support for long running queries such as complex substructure search		
Gracefully handle DAL errors • Human readable, error specific error messages		

Phase 3: XML server feature parity

XML Server Feature		
Expand Command		
Group By (filtering)		
Similarity Sorting		
XML Server Q Operator (if fulgor exposes special features for the Q operator)		
Highlighting		
Hit Only		
Any other Fulgor Capability		