Objective: Identify and define critical parameters for ligand selection and establish a set of selection criteria.

Description: The focus of this effort is to identify a selection criterion for down selection of a broad class of complexants. The selection criterion encompasses a broad facet of physiochemical properties to better suit application of chelates to the nuclear fuel cycle. Key focus points for ligand selection will include **thermodynamics**, **radiolysis resistance**, **chemical stability** (acid/based hydrolysis, reactive chemicals, etc.), **solubility**, **loading capacity, kinetics** (forward and reverse), **operational conditional range**, **dispersion numbers** (for applied systems with conditional values), **phase disengagement** (for applied systems with conditional values). Parameters will be grouped into 2 or 3 classification rankings based on their importance, and further broken down into three primary groups: physical, chemical, and process parameters.

Classification Rankings:

*High Importance*

1. **Chemical Stability** (including acid/base hydrolysis, reactive chemicals, etc.): Essential for ensuring that the ligands remain functional over the required duration of the separation process and under the chemical conditions present in nuclear fuel reprocessing.
2. **Radiolysis Resistance**: Crucial due to the radioactive nature of the materials being processed. Ligands must resist degradation under radiation to maintain their separation efficiency.
3. **Thermodynamics**: Determines the feasibility of separation processes at a fundamental level. It influences the selectivity and binding strength of ligands towards specific metal ions.

*Medium Importance*

1. **Kinetics** (forwards and reverse): Affects the speed of the separation process and the equilibrium position. Efficient kinetics ensure that separation can occur within practical time frames and is reversible if necessary.
2. **Loading Capacity**: Important for the efficiency of the separation process, determining how much material can be processed before the ligand becomes saturated,
3. **Operational Condition Range**: The ability of ligands to operate under a broad range of conditions increases the flexibility and applicability of the separation process.

*Low Importance*

1. **Solubility**: While important, solubility can often be modified or managed through the selection of solvents or conditions, making it less critical than the other parameters.
2. **Dispersion Numbers** (for applied systems with conditional values): Influences the efficiency of mass transfer between phases but is often specific to the particular system setup and thus ranked lower.
3. **Phase Disengagement** (for applied systems with conditional values): Critical for the practical separation of phases after the extraction process, but like dispersion numbers, it is highly dependent on the system design and operation parameters.

Primary Categories

*Chemical (High Importance)*

Chemical parameters are concerned with the chemical interactions and stability of the ligands in the reprocessing environment.

1. **Chemical Stability**: Critical for ensuring ligands do not degrade under the chemical conditions present in nuclear reprocessing, including resistance to acid/base hydrolysis and reactive chemicals.
2. **Radiolysis Resistance**: Essential due to the high radiation environment in nuclear fuel reprocessing, ensuring ligands maintain functionality without degrading.
3. **Thermodynamics**: Determines the fundamental feasibility and efficiency of the ligand in binding with specific metal ions, guiding the selectivity and strength of interactions.

*Process (Medium Importance)*

Process parameters involve the operational aspects and dynamics of using the ligands in the separation process.

1. **Kinetics** (forward and reverse): Influences the speed and reversibility of the separation process, affecting the practical implementation of the ligand in real-world scenarios.
2. **Loading Capacity**: Determines the amount of metal ions a ligand can bind before becoming saturated, directly impacting the throughput of the separation process.
3. **Operation Condition Range**: The ability of ligands to function effectively across a variety of operation conditions (e.g. temperature, pressure) enhances the versatility and applicability of the separation process.

*Physical (Low Importance)*

Physical parameters primarily relate to the inherent physical properties of the ligands and the physical context in which they operate.

1. **Solubility**: Pertains to the ability of the ligand to dissolve in the solvent systems used in nuclear fuel reprocessing, impacting the overall efficiency of the separation process.
2. **Phases Disengagement**: Involves the separation efficiency of the ligand-metal complex from the aqueous phases, crucial for the recovery and reuse of the ligand and/or metal.
3. **Dispersion Numbers**: Related to the distribution of the ligands and metal ions between phases, affecting mass transfer rates and separation efficiency.

This breakdown into primary groups helps in understanding the multifaceted nature of ligand selection criteria for nuclear fuel cycle chemistry aqueous separations. By focusing on physical, chemical, and process parameters, researchers can systematically evaluate and select ligands that best meet the requirements of advanced reprocessing technologies, thereby supporting the project's objectives to innovate and improve upon current methodologies.