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| Version | New Feature |
| V1 |  |
| V2 |  |
| V3 |  |
| V4 |  |
| V5 | * Check list to confirm Gunther is setup correctly. * Added a standard reaction to each batch. * Metal Coordination numbers can be interpreted as both tuples and integers. * Creation of a user selection class (acts global variables; allowing access to specific variables across different modules) |
| V6 | * Changed one reaction from the chemical space for another one. * Added unique identifiers for each reaction. |
| V7 | * Creates JSON file for automated NMR sampling. * Fine-tuned zone calibrations * Added 1 min wait times between stirs |
| V8 | * Fine-tuned zone calibrations * Ensures stock masses measured do not exceed 150% of the required mass to measure. * New checklist manager created (allows user to add own checks before a batch run) * Generation of the LCMS CSV * Created a new configurable rack for chemspeed script. * Fixed the outofplace septa problem * Bump reagent concentrations by 1.5 |
| V9 | * Changed the reaction id (for the standard reaction) * Updated the Check\_manager. * Transfer volumes now also depend on the final volume of a reaction: allowing users to keep reaction concentration consistent will varying final reaction volume. * Added reagent analysis workflow. * Changed file organisation structure |
| V10 | * Change the standard reaction to a reaction that forms a complex (simple to read reference). * Gunther dispenses sample to MS first then NMR (allows for evapouration leeway). * Automated chemical ID generation and handling. * Reagent ID are added to NMR for more quick legibility (this is paired with a printed table of reagent id + reagent structure). * Saves a log WITH the measured masses. * Removed dialdehydes from space of interest. Thus, changed USER\_SELECTION. subtype\_in\_reaction\_tuple. |
| V11 | * Better localisation of user parameters. * Better code comments (a chemist with little programming knowledge should be able to follow the script regardless if they understand python or not). * Refactored code. |
| V12 | * Changed the data structure of how batch spaces are generated, updated, and tracked. This was done by introducing a new SampleSpace class. * Introduced a method to easily retake failed batches in the workflow. * Introduced a method to easily retake failed reactions in the workflow. * Created a better method to check when stock and samples spaces have been taken. * Add a manual check for reactions or batches to be added. * Fixed bug in check\_manager.py |
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