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Details of Specific Protocols # Details on the theory and behaviour of different Protocols are listed here. Apr 28, 2026 · We are pleased to announce the release of openfe version 1.11! previous The Gufe Storage System next Show Source alias of Annotated [Quantity, FieldInfo (annotation=NoneType, required=True, validate_default=True), PlainValidator (func= _plain_quantity_validator, json_schema_input_type= Any), WithJsonSchema ... Guide to Gufe API docs gufe Change Log Welcome to gufe's documentation! # Contents: Guide to Gufe Gufe Overview Chemical Components and Systems The Gufe Protocol System Serializing ... json_schema_input_type = typing.Any json_schema = {'type': 'number'} return_type = PydanticUndefined when_used = always field production_length: NanosecondQuantity [Required] # ... The image below demonstrates how, for relative free energy calculations, you plan a network of ligand transformations starting from input SDF / MOL2 / PDB files: func = functools.partial (, unit='nanometer', convert=True) json_schema_input_type = typing.Any json_schema = {'type': ... json_schema_input_type = typing.Any json_schema = {'type': 'number'} return_type = PydanticUndefined when_used = always pydantic model ... 1. ****Setup****: Defining the simulation campaign you are going to run. 2. ****Execution****: Running and performing initial analysis of your simulation campaign. 3. ****Gather results****: Assembling the results ...

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