Appendix D

Formal Description of Scenario 2

section *Framework* **parents** *standard_toolkit*

$[CHAR, DATE, DECISION]$
$LIGAND == \operatorname{seq} CHAR$
$RECEPTOR == \operatorname{seq} CHAR$
$CONFIG == \operatorname{seq} CHAR$
$RESULT == \operatorname{seq} CHAR$
$LIGANDS == \mathbb{P}\, LIGAND$
$RECEPTORS == \mathbb{P}\, RECEPTOR$
$RESULTS == \mathbb{P}\, RESULT$
$DEEP\_ALIGN\_RESULT == \operatorname{seq} CHAR$
$LIGSIFT\_RESULT == \operatorname{seq} CHAR$
$YES\_NO ::= yes \mid no$
$USER\_INPUT == \operatorname{seq} CHAR$
$PREVIOUS\_RESULT == (LIGAND \times RECEPTOR \times CONFIG \times DATE) \mapsto RESULT$
$PREVIOUS\_RESULTS == \{PREVIOUS\_RESULT\}$

$$dockingWithConfig : (LIGAND \times RECEPTOR \times CONFIG) \rightarrowtail RESULT$$

$$\forall l : LIGAND;\ r : RECEPTOR \mid l \neq \varnothing \land r \neq \varnothing \bullet \exists c : CONFIG;\ res : RESULT \mid c \neq \varnothing \bullet dockingWithConfig(l, r, c) = res$$

Docking_AutoDockVina

$ligand? : LIGAND$
$receptor? : RECEPTOR$
$config? : CONFIG$
$result! : RESULT$

$config? \neq \varnothing \land result! = dockingWithConfig(ligand?, receptor?, config?)$

MolecularDockingEnvironment_Raccoon2

$ligands? : LIGANDS$
$receptors? : RECEPTORS$
$config? : CONFIG$
$results! : RESULTS$
$date! : DATE$

$\exists ligand? : ligands?;\ receptor? : receptors?;\ result! : results! \bullet Docking\_AutoDockVina$

ViewMolecularDockingResults

$\Xi MolecularDockingEnvironment$

$results! \neq \varnothing$

MolecularDockingResultsRepository

$repository : (LIGAND \times RECEPTOR \times CONFIG \times DATE) \leftrightarrow RESULT$
$decisionRepository : \{PREVIOUS\_RESULT\} \leftrightarrow DECISION$

$repository \neq \varnothing$

InsertUpdateMolecularDockingResultsRepository1

$\Delta MolecularDockingResultsRepository$
$l? : LIGAND$
$r? : RECEPTOR$
$c? : CONFIG$
$res? : RESULT$
$d? : DATE$

$repository' = repository \oplus \{(l?, r?, c?, d?) \mapsto res?\}$

InsertUpdateMolecularDockingResultsRepositoryMany

$\Delta MolecularDockingResultsRepository$
$dockingResults? : (LIGAND \times RECEPTOR \times CONFIG \times DATE) \leftrightarrow RESULT$
$l : LIGAND$
$r : RECEPTOR$
$c : CONFIG$
$d : DATE$

$\{(l, r, c, a, d)\} = \mathrm{dom}(dockingResults?)$
$\forall res : dockingResults? \mid \{(l, r, c, a, d)\} \bullet repository' = repository \oplus \{(l, r, c, a, d) \mapsto res\}$

InsertUpdateDecisionRepository

$\Delta MolecularDockingResultsRepository$
$previousDockingResults? : \{PREVIOUS\_RESULT\}$
$decision? : DECISION$

$decisionRepository' = decisionRepository \oplus \{previousDockingResults? \mapsto decision?\}$

SelectMolecularDockingResults

$\Xi MolecularDockingResultsRepository$

$whereL? : LIGAND$

$whereR? : RECEPTOR$

$whereC? : CONFIG$

$whereD? : DATE$

$whereRes? : RESULT$

$selectResults! : (LIGAND \times RECEPTOR \times CONFIG \times DATE) \leftrightarrow RESULT$

$lig : LIGAND$

$rec : RECEPTOR$

$con : CONFIG$

$dat : DATE$

$selectResults! = \{(whereL?, whereR?, whereC?, whereD?)\} \lhd repository \lor$

$selectResults! = \{(whereL?, whereR?, whereC?, dat)\} \lhd repository \lor$

$selectResults! = \{(whereL?, whereR?, con, whereD?)\} \lhd repository \lor$

$selectResults! = \{(whereL?, whereR?, con, dat)\} \lhd repository \lor$

$selectResults! = \{(whereL?, rec, whereC?, whereD?)\} \lhd repository \lor$

$selectResults! = \{(whereL?, rec, whereC?, dat)\} \lhd repository \lor$

$selectResults! = \{(whereL?, rec, con, whereD?)\} \lhd repository \lor$

$selectResults! = \{(whereL?, rec, con, dat)\} \lhd repository \lor$

$selectResults! = \{(lig, whereR?, whereC?, whereD?)\} \lhd repository \lor$

$selectResults! = \{(lig, whereR?, whereC?, dat)\} \lhd repository \lor$

$selectResults! = \{(lig, whereR?, con, whereD?)\} \lhd repository \lor$

$selectResults! = \{(lig, whereR?, con, dat)\} \lhd repository \lor$

$selectResults! = \{(lig, rec, whereC?, whereD?)\} \lhd repository \lor$

$selectResults! = \{(lig, rec, whereC?, dat)\} \lhd repository \lor$

$selectResults! = \{(lig, rec, con, whereD?)\} \lhd repository \lor$

$selectResults! = \{(lig, rec, con, dat)\} \lhd repository \lor$

$selectResults! = repository \rhd \{whereRes?\}$

$goodDocking : (RESULT \times USER\_INPUT) \leftrightarrow YES\_NO$

$\forall r : RESULT;\ ui : USER\_INPUT \bullet \exists threshold : \mathbb{Z};\ docking\_score : \mathbb{Z} \bullet$

$docking\_score \leq threshold \land goodDocking(r, ui) = yes$

$\lor$

$docking\_score > threshold \land goodDocking(r, ui) = no$

AssessPreviousDocking

$SelectMolecularDockingResults$
$previous\_results? : PREVIOUS\_RESULTS$
$userInput? : USER\_INPUT$
$assessedPreviousResults! : PREVIOUS\_RESULTS$

$\exists\, previous\_result : previous\_results?;\ result : RESULT \bullet$
$\{result\} = \mathrm{ran}(previous\_result) \land$
$(previous\_result \in assessedPreviousResults! \land goodDocking(result, userInput?) = yes$
$\lor$
$previous\_result \notin assessedPreviousResults! \land goodDocking(result, userInput?) = no)$

$checkPubChem : (LIGAND \times USER\_INPUT) \leftrightarrow YES\_NO$

$\forall\, l : LIGAND;\ ui : USER\_INPUT \bullet \exists\, ligand\_property : ui \bullet$
$checkPubChem(l, ui) = yes$
$\lor$
$checkPubChem(l, ui) = no$

PubChem

$SelectMolecularDockingResults$
$previous\_results? : PREVIOUS\_RESULTS$
$ui? : USER\_INPUT$
$filtered\_results! : PREVIOUS\_RESULTS$
$rec : RECEPTOR$
$con : CONFIG$
$dat : DATE$
$previous\_result : PREVIOUS\_RESULT$

$\forall\, lig : LIGAND \bullet whereL? = lig;\ previous\_result \in previous\_results?;$
$\{(lig, rec, con, dat)\} = \mathrm{dom}(previous\_result);$
$selectResults! \in filtered\_results! \land checkPubChem(lig, ui?) = yes$
$\lor$
$selectResults! \notin filtered\_results! \land checkPubChem(lig, ui?) = no$

$$
\begin{array}{|l}
makeADecisionPreviousResults : (PREVIOUS\_RESULTS \times PREVIOUS\_RESULTS) \\
\quad \leftrightarrow DECISION \\
\hline
\exists\, previous\_results\_filtered\_ligands : PREVIOUS\_RESULTS; \\
\quad previous\_results\_assessed\_docking : PREVIOUS\_RESULTS; \\
\quad d : DECISION; \bullet \\
\quad\quad \forall\, previous\_result\_filtered\_ligands : previous\_results\_filtered\_ligands; \\
\quad\quad\quad previous\_result\_assessed\_docking : previous\_results\_assessed\_docking \bullet \\
\quad\quad\quad\quad previous\_result\_filtered\_ligands = previous\_result\_assessed\_docking \land \\
\quad\quad\quad\quad makeADecisionPreviousResults(\\
\quad\quad\quad\quad\quad previous\_results\_filtered\_ligands, previous\_results\_assessed\_docking) = d
\end{array}
$$

DecisionMaker_Custom

$$
\begin{array}{|l}
assessed\_previous\_results? : PREVIOUS\_RESULTS \\
filtered\_previous\_results? : PREVIOUS\_RESULTS \\
decision! : DECISION \\
\hline
decision! = \\
makeADecisionPreviousResults(assessed\_previous\_results?, filtered\_previous\_results?) \\
\hline
\end{array}
$$