# Appendix B

# Formal Description of Framework for Systems that Use Docking Results

This appendix contains the formal description of element types and interfaces of the framework in Z notation. The choice of variable names should act as an additional explanation of the specification.

$[CHAR, DATE, ADDITIONAL\_TOOL\_RESULT, DATA\_SOURCE\_INPUT, DECISION]$

$LIGAND == \text{seq}\, CHAR$

$RECEPTOR == \text{seq}\, CHAR$

$CONFIG == \text{seq}\, CHAR$

$RESULT == \text{seq}\, CHAR$

$USER\_INPUT == \text{seq}\, CHAR$

$DATA\_SOURCE\_INFO == \text{seq}\, CHAR$

$LIGANDS == \mathbb{P}\, LIGAND$

$RECEPTORS == \mathbb{P}\, RECEPTOR$

$RESULTS == \mathbb{P}\, RESULT$

$PREVIOUS\_RESULT == (LIGAND \times RECEPTOR \times CONFIG \times DATE) \mapsto RESULT$

$$dockingWithoutConfig : (LIGAND \times RECEPTOR) \rightarrowtail RESULT$$

---

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

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

---

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

*Docking*

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

---

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

*MolecularDockingEnvironment*

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

---

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

*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*

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

---

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

*InsertUpdateDecisionRepository*

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

---

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

*SelectMolecularDockingResults*

$\Xi MolecularDockingResultsRepository$
$whereL? : LIGAND$
$whereR? : RECEPTOR$
$whereC? : CONFIG$
$whereD? : DATE$
$whereRes? : RESULT$
$selectResults! : (LIGAND \times RECEPTOR \times CONFIG \times DATE) \leftrightarrow RESULT$
$lig : LIGAND$
$rec : RECEPTOR$
$con : CONFIG$
$dat : DATE$

---

$selectResults! = \{(whereL?, whereR?, whereC?, whereD?)\} \lhd repository \lor$
$selectResults! = \{(whereL?, whereR?, whereC?, dat)\} \lhd repository \lor$
$selectResults! = \{(whereL?, whereR?, con, whereD?)\} \lhd repository \lor$
$selectResults! = \{(whereL?, whereR?, con, dat)\} \lhd repository \lor$
$selectResults! = \{(whereL?, rec, whereC?, whereD?)\} \lhd repository \lor$
$selectResults! = \{(whereL?, rec, whereC?, dat)\} \lhd repository \lor$
$selectResults! = \{(whereL?, rec, con, whereD?)\} \lhd repository \lor$
$selectResults! = \{(whereL?, rec, con, dat)\} \lhd repository \lor$
$selectResults! = \{(lig, whereR?, whereC?, whereD?)\} \lhd repository \lor$
$selectResults! = \{(lig, whereR?, whereC?, dat)\} \lhd repository \lor$
$selectResults! = \{(lig, whereR?, con, whereD?)\} \lhd repository \lor$
$selectResults! = \{(lig, whereR?, con, dat)\} \lhd repository \lor$
$selectResults! = \{(lig, rec, whereC?, whereD?)\} \lhd repository \lor$
$selectResults! = \{(lig, rec, whereC?, dat)\} \lhd repository \lor$
$selectResults! = \{(lig, rec, con, whereD?)\} \lhd repository \lor$
$selectResults! = \{(lig, rec, con, dat)\} \lhd repository \lor$
$selectResults! = repository \rhd \{whereRes?\}$

---

$additionalTool\_PR : \{PREVIOUS\_RESULT\} \leftrightarrow$
$\quad ADDITIONAL\_TOOL\_RESULT$

---

$\exists\, pr : \{PREVIOUS\_RESULT\} \bullet$
$\quad \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_PR(pr) = atr$

$$additionalTool\_DSI : \{DATA\_SOURCE\_INFO\} \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, dsi : \{DATA\_SOURCE\_INFO\} \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_DSI(dsi) = atr$$

$$additionalTool\_ATR : \{ADDITIONAL\_TOOL\_RESULT\} \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_ATR(another\_atr) = atr$$

$$additionalTool\_DSI\_PR : (\{DATA\_SOURCE\_INFO\} \times \{PREVIOUS\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, dsi : \{DATA\_SOURCE\_INFO\};\ pr : \{PREVIOUS\_RESULT\} \mid dsi \neq \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_DSI\_PR(dsi, pr) = atr$$

$$additionalTool\_UI\_PR : (USER\_INPUT \times \{PREVIOUS\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, ui : USER\_INPUT;\ pr : \{PREVIOUS\_RESULT\} \mid ui \neq \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_UI\_PR(ui, pr) = atr$$

$$additionalTool\_PR\_ATR : (\{PREVIOUS\_RESULT\} \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, pr : \{PREVIOUS\_RESULT\};\ another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid pr \notin \varnothing \wedge another\_atr \notin \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_PR\_ATR(pr, another\_atr) = atr$$

$$additionalTool\_UI\_DSI : (USER\_INPUT \times \{DATA\_SOURCE\_INFO\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, ui : USER\_INPUT;\ dsi : \{DATA\_SOURCE\_INFO\} \mid ui \neq \varnothing \wedge dsi \neq \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_UI\_DSI(ui, dsi) = atr$$

$$additionalTool\_UI\_ATR : (USER\_INPUT \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, ui : USER\_INPUT;\ another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid ui \neq \varnothing \wedge another\_atr \neq \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_UI\_ATR(ui, another\_atr) = atr$$

$$additionalTool\_DSI\_ATR : (\{DATA\_SOURCE\_INFO\} \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, dsi : \{DATA\_SOURCE\_INFO\};\ another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid dsi \neq \varnothing \wedge another\_atr \notin \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_DSI\_ATR(dsi, another\_atr) = atr$$

$$additionalTool\_UI\_DSI\_PR : (USER\_INPUT \times \{DATA\_SOURCE\_INFO\} \times \{PREVIOUS\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, ui : USER\_INPUT;\ dsi : \{DATA\_SOURCE\_INFO\};\ pr : \{PREVIOUS\_RESULT\} \mid ui \neq \varnothing \wedge dsi \neq \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_UI\_DSI\_PR(ui, dsi, pr) = atr$$

$$additionalTool\_PR\_UI\_ATR : (\{PREVIOUS\_RESULT\} \times USER\_INPUT \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, pr : \{PREVIOUS\_RESULT\};\ ui : USER\_INPUT;\ another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid pr \notin \varnothing \wedge ui \neq \varnothing \wedge another\_atr \notin \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_PR\_UI\_ATR(pr, ui, another\_atr) = atr$$

$$additionalTool\_PR\_DSI\_ATR : (\{PREVIOUS\_RESULT\} \times \{DATA\_SOURCE\_INFO\} \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT$$

$$\exists\, pr : \{PREVIOUS\_RESULT\};\ dsi : \{DATA\_SOURCE\_INFO\};\ another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid pr \notin \varnothing \wedge dsi \neq \varnothing \wedge another\_atr \notin \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet additionalTool\_PR\_DSI\_ATR(pr, dsi, another\_atr) = atr$$

$$
\begin{array}{|l}
additionalTool\_UI\_DSI\_ATR : (USER\_INPUT \times \{DATA\_SOURCE\_INFO\} \times \\
\quad \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow ADDITIONAL\_TOOL\_RESULT \\
\hline
\exists\, ui : USER\_INPUT;\ dsi : \{DATA\_SOURCE\_INFO\}; \\
\quad another\_atr : \{ADDITIONAL\_TOOL\_RESULT\} \mid ui \notin \varnothing \land dsi \neq \varnothing \land \\
\quad another\_atr \notin \varnothing \bullet \exists\, atr : ADDITIONAL\_TOOL\_RESULT \bullet \\
\quad additionalTool\_UI\_DSI\_ATR(ui, dsi, another\_atr) = atr
\end{array}
$$

*AdditionalTool*

$$
\begin{array}{|l}
userInput? : USER\_INPUT \\
dataSourceInfo? : \{DATA\_SOURCE\_INFO\} \\
previousDockingResults? : \{PREVIOUS\_RESULT\} \\
otherAdditionalToolsResults? : \{ADDITIONAL\_TOOL\_RESULT\} \\
additionalToolResult! : ADDITIONAL\_TOOL\_RESULT \\
\hline
additionalToolResult! = additionalTool\_PR(previousDockingResults?) \lor \\
additionalToolResult! = additionalTool\_DSI(dataSourceInfo?) \lor \\
additionalToolResult! = additionalTool\_ATR(otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_DSI\_PR(dataSourceInfo?, \\
\quad previousDockingResults?) \lor \\
additionalToolResult! = additionalTool\_UI\_PR(userInput?, \\
\quad previousDockingResults?) \lor \\
additionalToolResult! = additionalTool\_PR\_ATR(previousDockingResults?, \\
\quad otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_UI\_DSI(userInput?, dataSourceInfo?) \lor \\
additionalToolResult! = additionalTool\_UI\_ATR(userInput?, \\
\quad otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_DSI\_ATR(dataSourceInfo?, \\
\quad otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_UI\_DSI\_PR(userInput?, dataSourceInfo?, \\
\quad previousDockingResults?) \lor \\
additionalToolResult! = additionalTool\_PR\_UI\_ATR(previousDockingResults?, \\
\quad userInput?, otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_PR\_DSI\_ATR(previousDockingResults?, \\
\quad dataSourceInfo?, otherAdditionalToolsResults?) \lor \\
additionalToolResult! = additionalTool\_UI\_DSI\_ATR(userInput?, dataSourceInfo?, \\
\quad otherAdditionalToolsResults?)
\end{array}
$$

*ReadAnotherAdditionalToolResults*

$\Delta AdditionalTool$

$oneOrMoreAdditionalToolsResults? : \{ADDITIONAL\_TOOL\_RESULT\}$

---

$otherAdditionalToolsResults?' =$
$\quad otherAdditionalToolsResults? \cup oneOrMoreAdditionalToolsResults?$

*AdditionalDataSource*

$repository : DATA\_SOURCE\_INPUT \leftrightarrow DATA\_SOURCE\_INFO$

---

$repository \neq \varnothing$

*SelectAdditionalDataInfo*

$\Xi AdditionalDataSource$

$dataSourceInput? : DATA\_SOURCE\_INPUT$

$dataSourceInfo! : \{DATA\_SOURCE\_INFO\}$

$selectedData : DATA\_SOURCE\_INPUT \leftrightarrow DATA\_SOURCE\_INFO$

---

$selectedData = \{(dataSourceInput?)\} \lhd repository$

$dataSourceInfo! = \mathrm{ran}(selectedData)$

$makeADecisionPreviousResults : \{PREVIOUS\_RESULT\} \leftrightarrow DECISION$

---

$\exists\, pr : \{PREVIOUS\_RESULT\} \bullet \exists\, d : DECISION \bullet$
$makeADecisionPreviousResults(pr) = d$

$makeADecisionUserInputPreviousResults : (USER\_INPUT \times$
$\{PREVIOUS\_RESULT\}) \leftrightarrow DECISION$

---

$\exists\, ui : USER\_INPUT;\ pr : \{PREVIOUS\_RESULT\} \mid ui \neq \varnothing \bullet \exists\, d : DECISION \bullet$
$makeADecisionUserInputPreviousResults(ui, pr) = d$

$$makeADecisionUserInputAdditionalToolPreviousResults : (USER\_INPUT \times \{ADDITIONAL\_TOOL\_RESULT\} \times \{PREVIOUS\_RESULT\}) \leftrightarrow DECISION$$

$$\exists\, ui : USER\_INPUT;\ atr : \{ADDITIONAL\_TOOL\_RESULT\};\ pr : \{PREVIOUS\_RESULT\} \mid ui \neq \varnothing \bullet \exists\, d : DECISION \bullet makeADecisionUserInputAdditionalToolPreviousResults(ui, atr, pr) = d$$

$$makeADecisionAdditionalToolPreviousResults : (ADDITIONAL\_TOOL\_RESULT \times \{PREVIOUS\_RESULT\}) \leftrightarrow DECISION$$

$$\exists\, atr : ADDITIONAL\_TOOL\_RESULT;\ pr : \{PREVIOUS\_RESULT\} \bullet \exists\, d : DECISION \bullet makeADecisionAdditionalToolPreviousResults(atr, pr) = d$$

$$makeADecisionUserInputAdditionalTool : (USER\_INPUT \times \{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow DECISION$$

$$\exists\, ui : USER\_INPUT;\ atr : \{ADDITIONAL\_TOOL\_RESULT\} \bullet \exists\, d : DECISION \bullet makeADecisionUserInputAdditionalTool(ui, atr) = d$$

$$makeADecisionAdditionalTool : (\{ADDITIONAL\_TOOL\_RESULT\}) \leftrightarrow DECISION$$

$$\exists\, atr : \{ADDITIONAL\_TOOL\_RESULT\} \bullet \exists\, d : DECISION \bullet makeADecisionAdditionalTool(atr) = d$$

*DecisionMaker*

$userInput? : USER\_INPUT$

$additionalToolResult? : \{ADDITIONAL\_TOOL\_RESULT\}$

$previousDockingResults? : \{PREVIOUS\_RESULT\}$

$decision! : DECISION$

---

$decision! = makeADecisionUserInputAdditionalToolPreviousResults(userInput?,$
$additionalToolResult?, previousDockingResults?)$

$\lor$

$additionalToolResult? \in \varnothing \land decision! =$
$makeADecisionUserInputPreviousResults(userInput?, previousDockingResults?)$

$\lor$

$previousDockingResults? \in \varnothing \land decision! =$
$makeADecisionUserInputAdditionalTool(userInput?, additionalToolResult?)$

$\lor$

$userInput? = \varnothing \land ($
  $decision! = makeADecisionAdditionalToolPreviousResults($
    $additionalToolResult?, previousDockingResults?)$
  $\lor$
  $additionalToolResult? \in \varnothing \land decision! =$
    $makeADecisionPreviousResults(previousDockingResults?)$
  $\lor$
  $previousDockingResults? \in \varnothing \land decision! =$
    $makeADecisionAdditionalTool(additionalToolResult?))$

*Framework*

$mde : MolecularDockingEnvironment$

$mdrr : MolecularDockingResultsRepository$

$ats : \{AdditionalTool\}$

$adss : \{AdditionalDataSource\}$

$dm : DecisionMaker$

---

$mde \notin \varnothing \land mdrr \notin \varnothing \land dm \notin \varnothing$

$\forall ads : adss \bullet \exists at : ats \bullet SelectAdditionalDataInfo \neq \varnothing$