Annexe

A. Drug Development Process (DDP) Context Ontologies

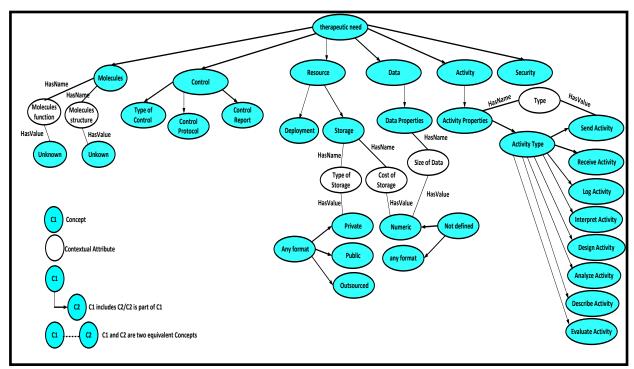


Figure A.1: Extract of the context ontology of the Process Chunk VPC1-1

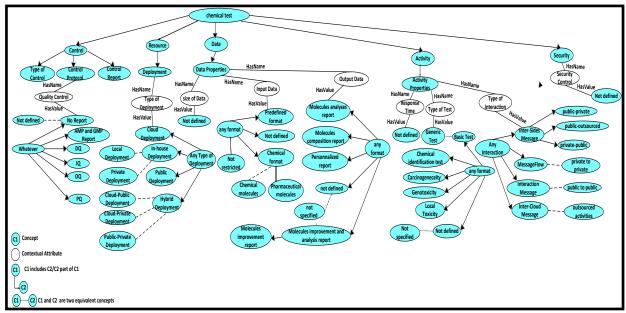


Figure A.2: Extract of the context ontology of the Process Chunk VPC3-1

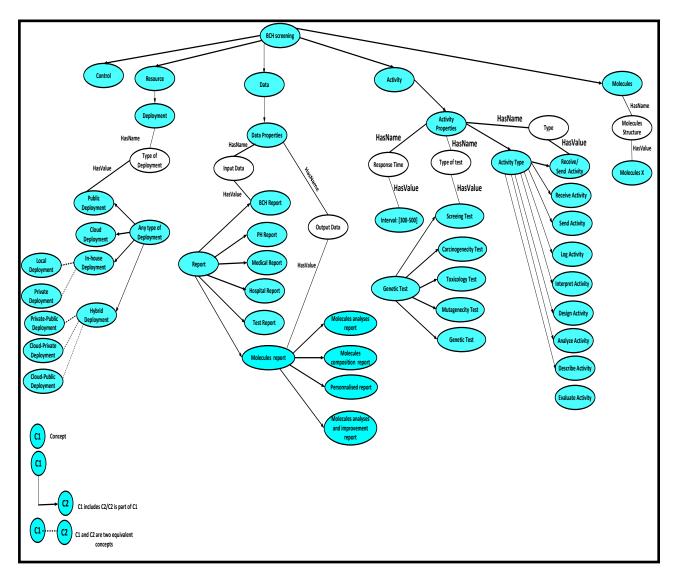


Figure A.3: Extract of the context ontology of the Process Chunk VPC4-1

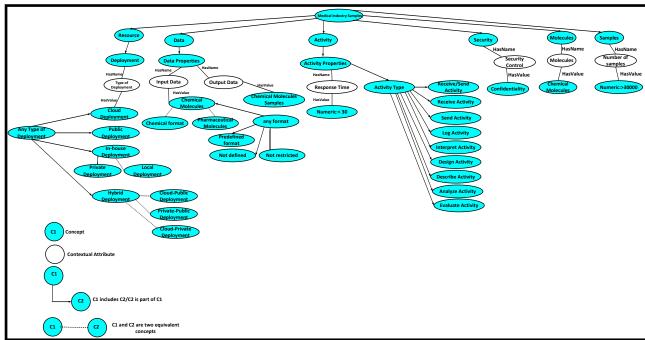


Figure A.4: Extract of the context ontology of the Process Chunk VPC6-1

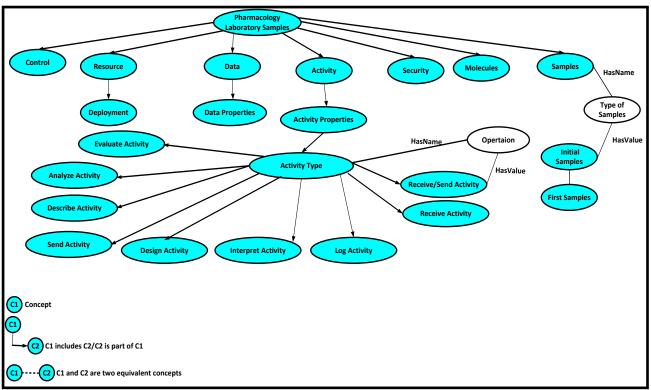


Figure A.5: Extract of the context ontology of the Process Chunk VPC7-1

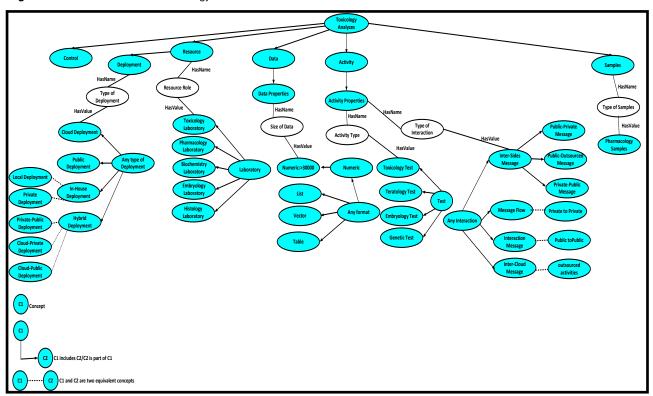
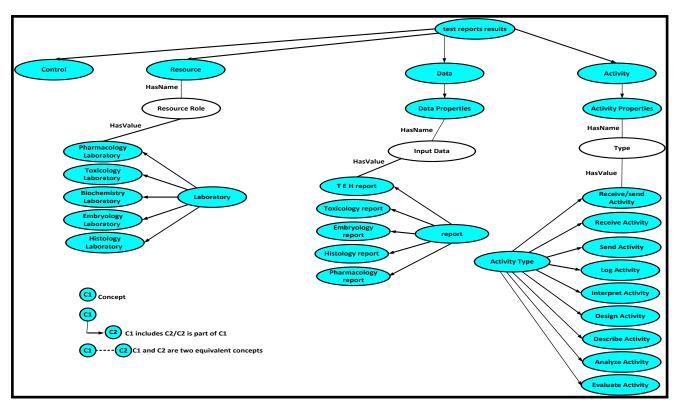
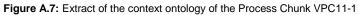


Figure A.6: Extract of the context ontology of the Process Chunk VPC8-1





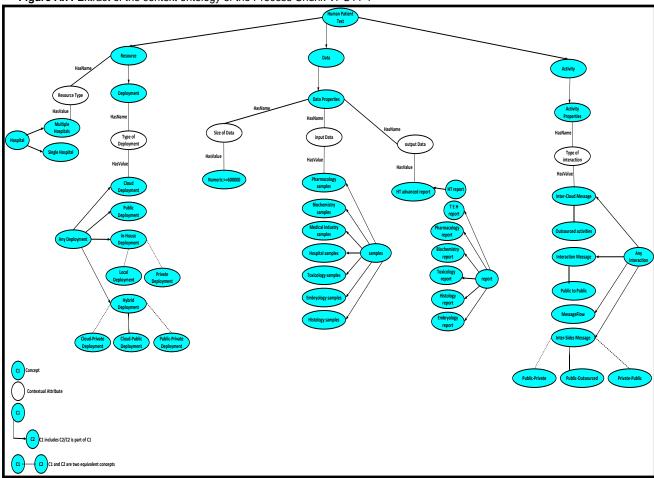


Figure A.8: Extract of the context ontology of the Process Chunk VPC12-1

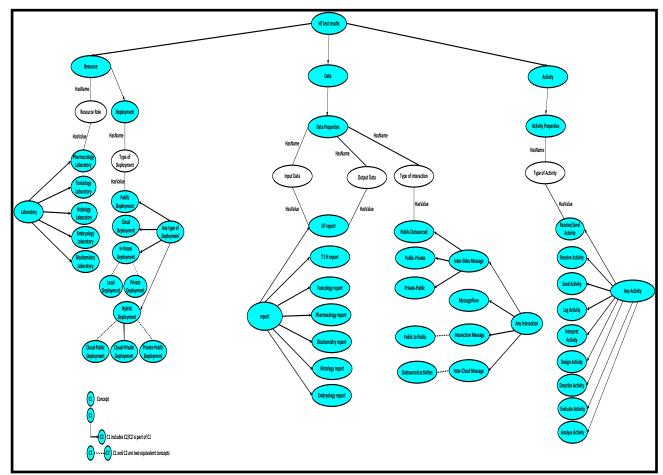


Figure A.9: Extract of the context ontology of the Process Chunk VPC13-1

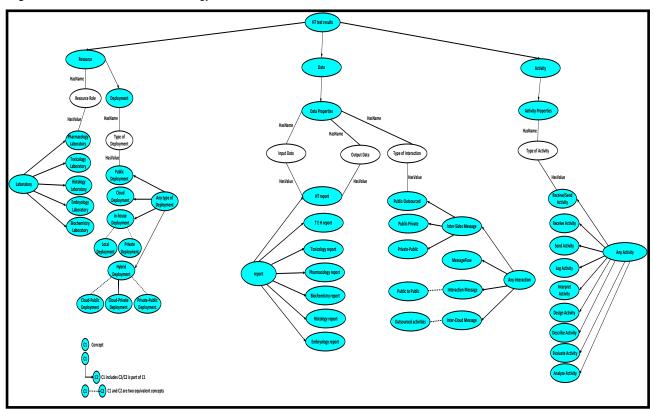


Figure A.10: Extract of the context ontology of the Process Chunk VPC14-1

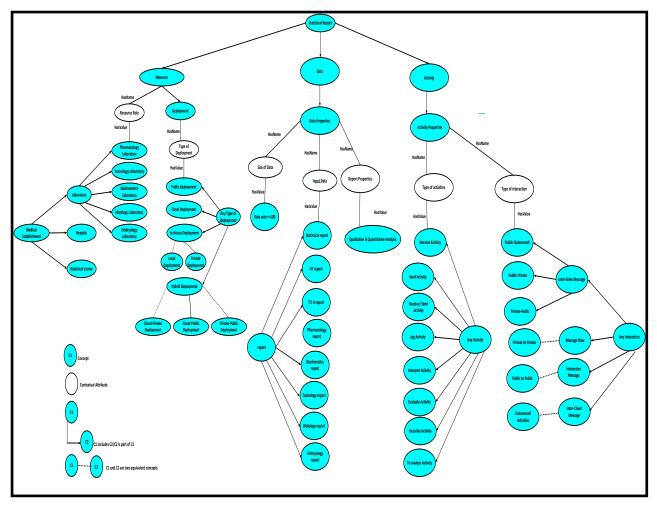


Figure A.11: Extract of the context ontology of the Process Chunk VPC15-1

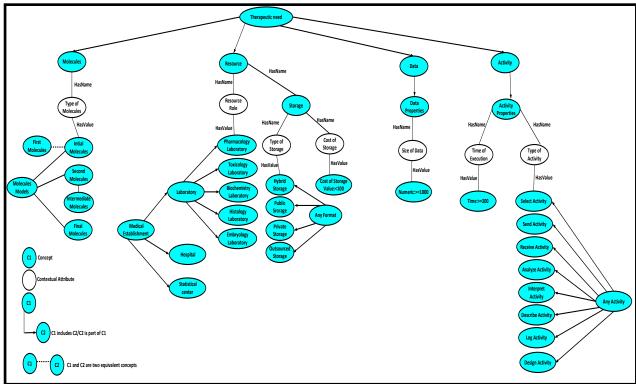


Figure A.12: Extract of the context ontology of the Process Chunk VPC1-2

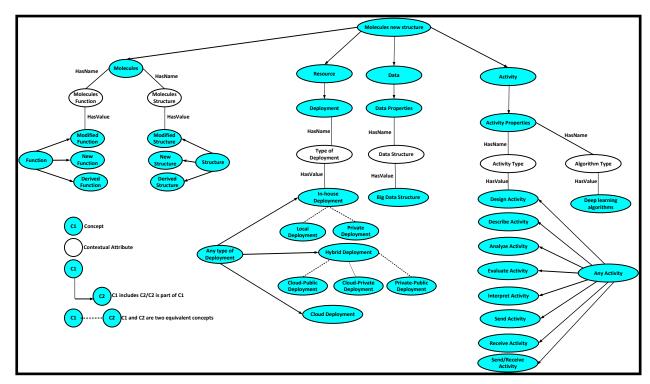


Figure A.13: Extract of the context ontology of the Process Chunk VPC2-2

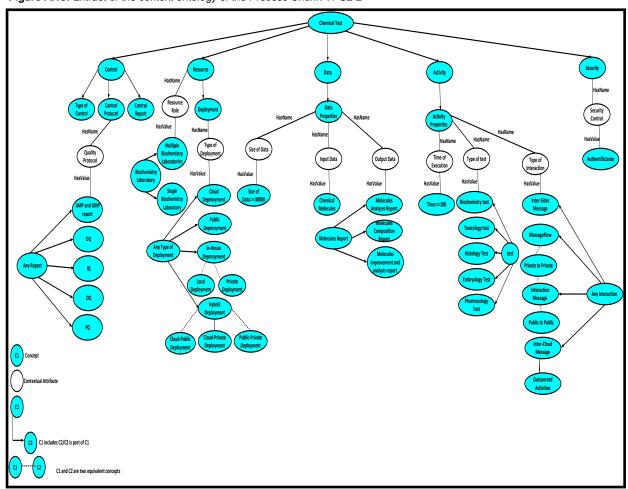


Figure A.14: Extract of the context ontology of the Process Chunk VPC2-2

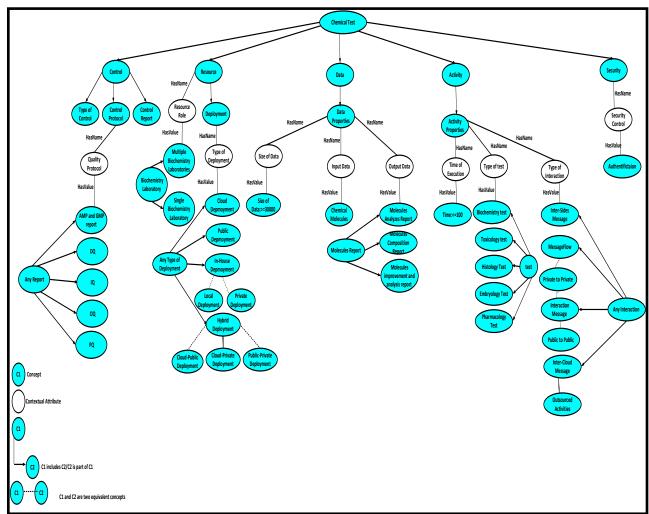


Figure A.15: Extract of the context ontology of the Process Chunk VPC3-2

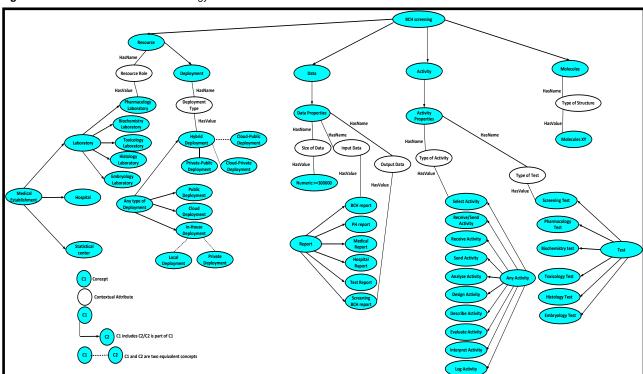


Figure A.16: Extract of the context ontology of the Process Chunk VPC4-2

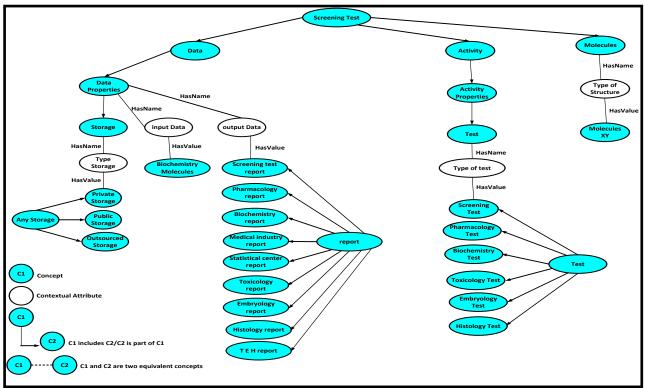


Figure A.17: Extract of the context ontology of the Process Chunk VPC5-2

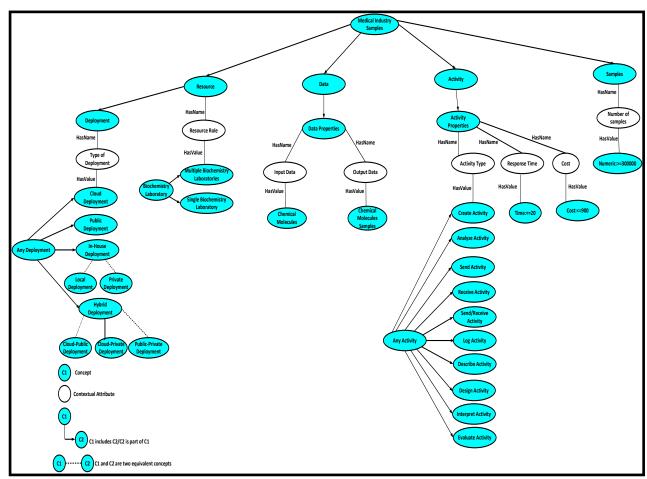


Figure A.18: Extract of the context ontology of the Process Chunk VPC6-2

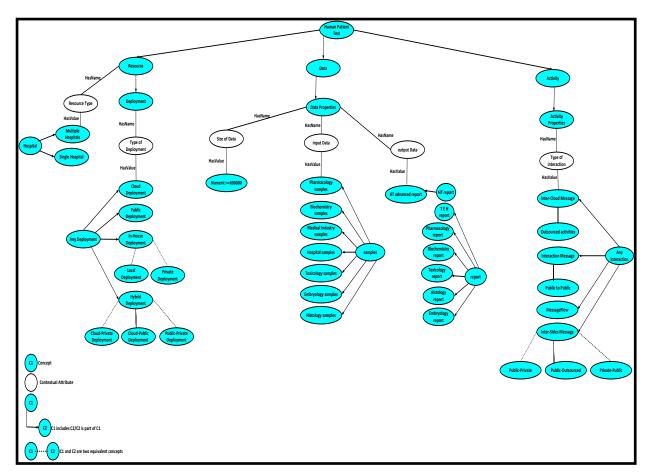


Figure A.19: Extract of the context ontology of the Process Chunk VPC12-2

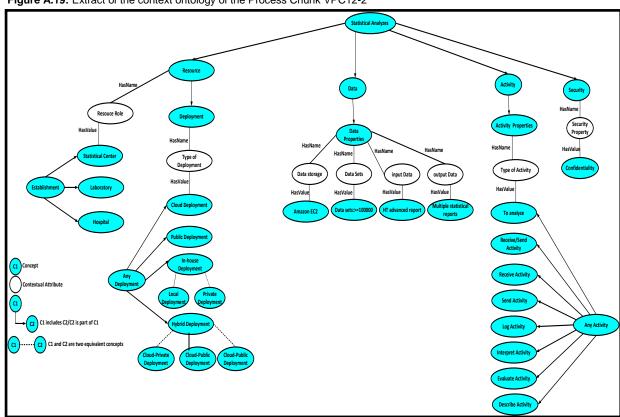


Figure A.20: Extract of the context ontology of the Process Chunk VPC14-2

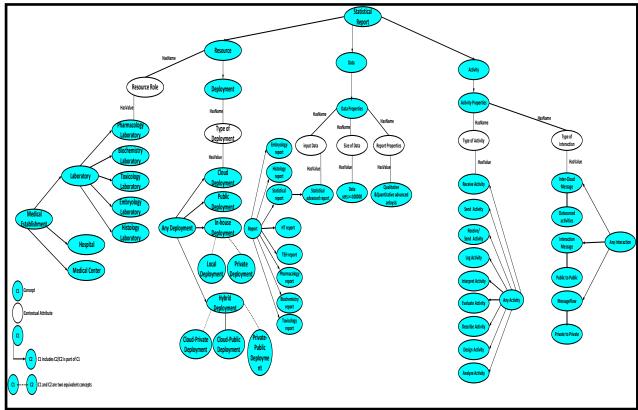
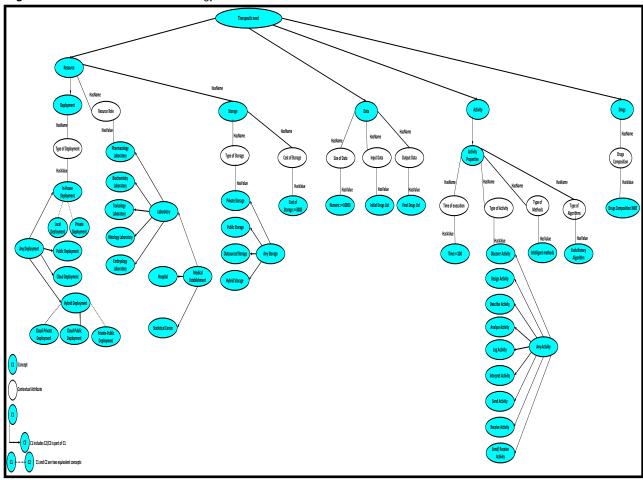


Figure A.21: Extract of the context ontology of the Process Chunk VPC15-2



 $\textbf{Figure A.22:} \ \, \textbf{Extract of the context ontology of the Process Chunk VPC1-3}$

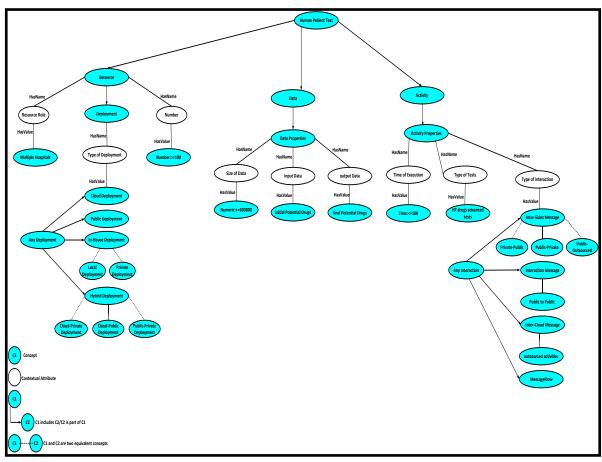


Figure A.23: Extract of the context ontology of the Process Chunk VPC12-3

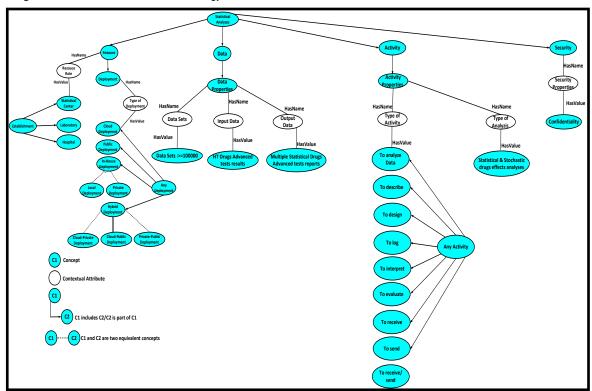


Figure A.24: Extract of the context ontology of the Process Chunk VPC14-3

B. Drug Development Process (DDP) Capacity Ontologies

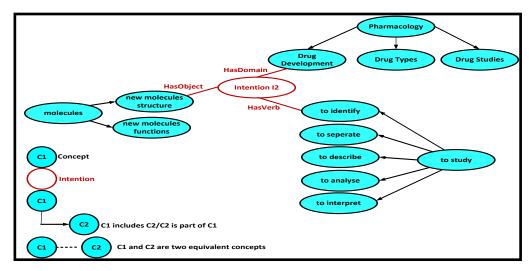


Figure B.1: Extract of the capacity ontology of the Process Chunk VPC1-1

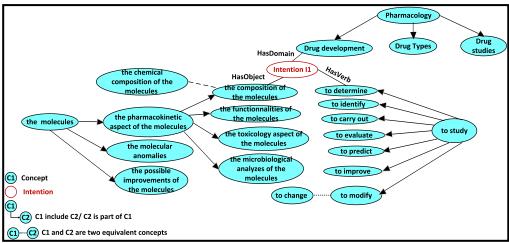


Figure B.2: Extract of the capacity ontology of the Process Chunk VPC3-1

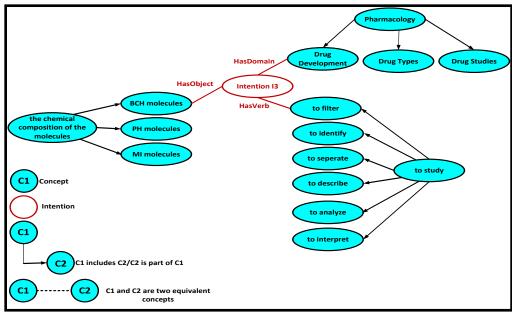


Figure B.3: Extract of the capacity ontology of the Process Chunk VPC4-1

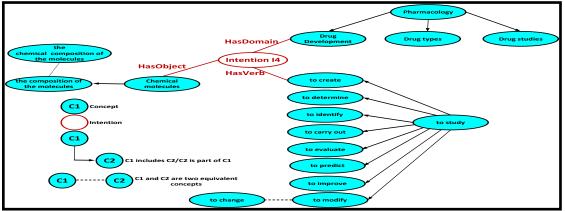


Figure B.4: Extract of the capacity ontology of the Process Chunk VPC6-1

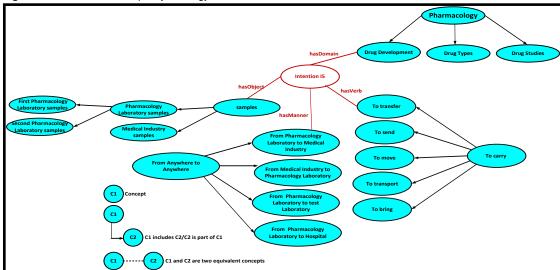


Figure B.5: Extract of the capacity ontology of the Process Chunk VPC7-1

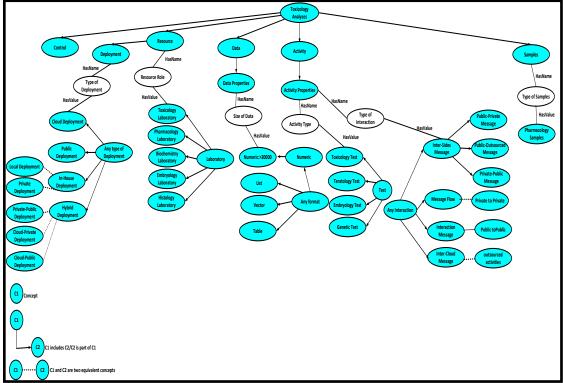


Figure B.6: Extract of the capacity ontology of the Process Chunk VPC8-1

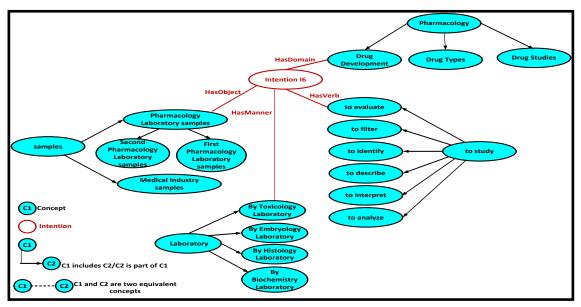


Figure B.7: Extract of the capacity ontology of the Process Chunk VPC9-1

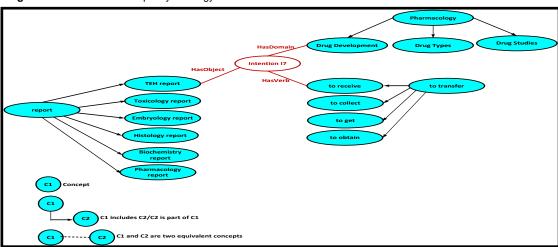


Figure B.8: Extract of the capacity ontology of the Process Chunk VPC11-1

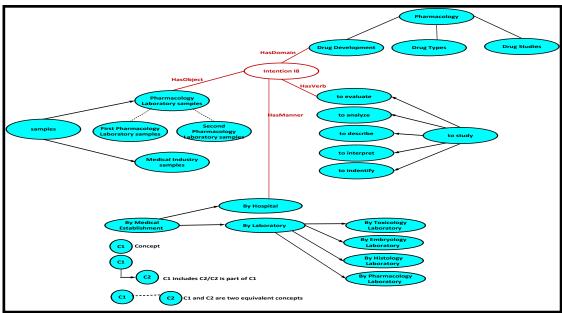


Figure B.9: Extract of the capacity ontology of the Process Chunk VPC12-1

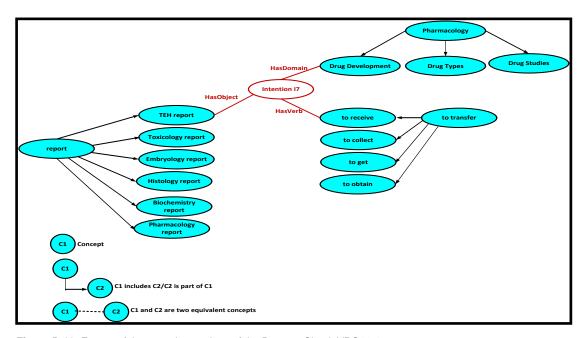


Figure B.10: Extract of the capacity ontology of the Process Chunk VPC13-1

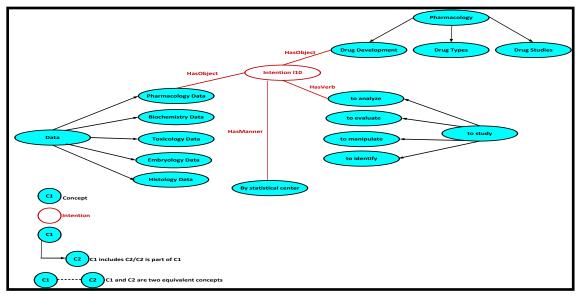


Figure B.11: Extract of the capacity ontology of the Process Chunk VPC14-1

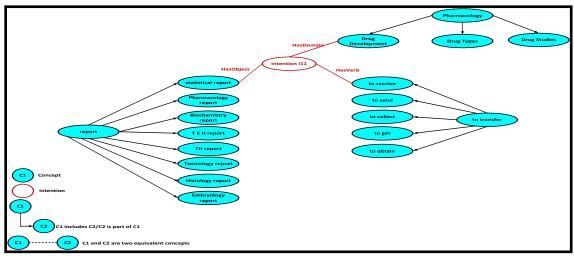


Figure B.12: Extract of the capacity ontology of the Process Chunk VPC15-1

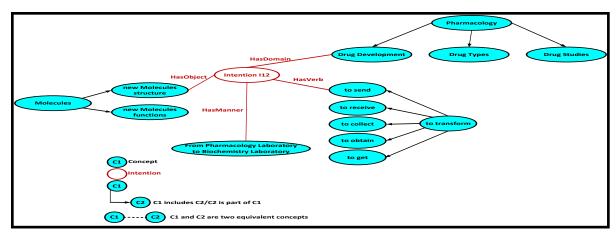


Figure B.13: Extract of the capacity ontology of the Process Chunk VPC1-2

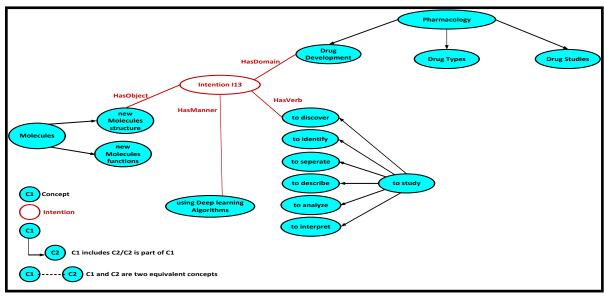


Figure B.14: Extract of the capacity ontology of the Process Chunk VPC2-2

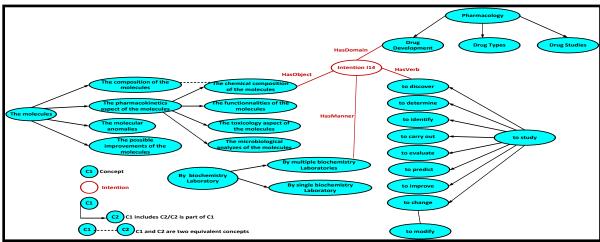


Figure B.15: Extract of the capacity ontology of the Process Chunk VPC3-2

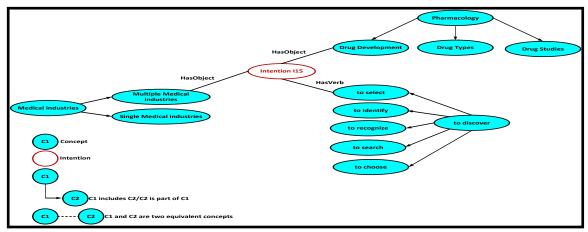


Figure B.16: Extract of the capacity ontology of the Process Chunk VPC4-2

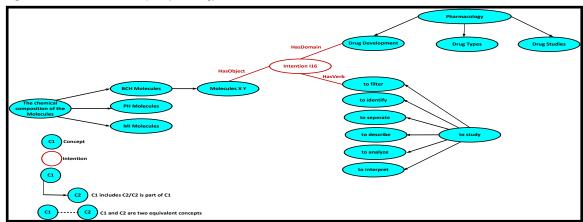


Figure B.17: Extract of the capacity ontology of the Process Chunk VPC5-2

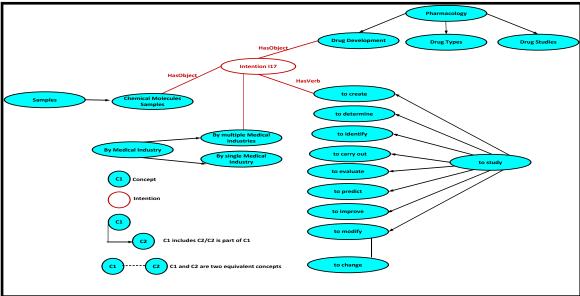


Figure B.18: Extract of the capacity ontology of the Process Chunk VPC6-2

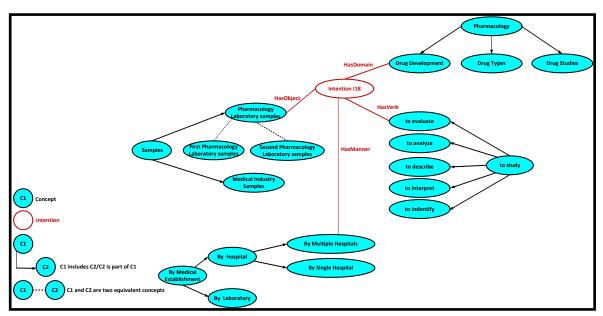


Figure B.19: Extract of the capacity ontology of the Process Chunk VPC12-2

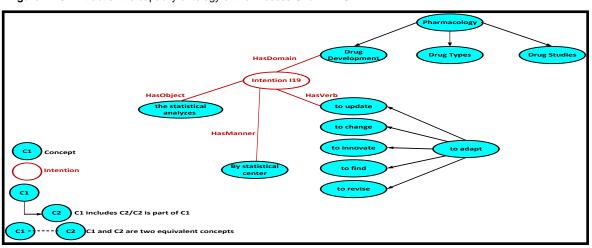


Figure B.20: Extract of the capacity ontology of the Process Chunk VPC14-2

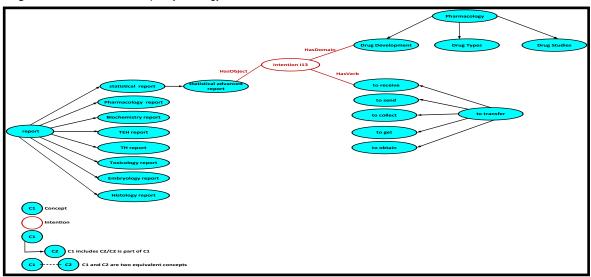


Figure B.21: Extract of the capacity ontology of the Process Chunk VPC15-2

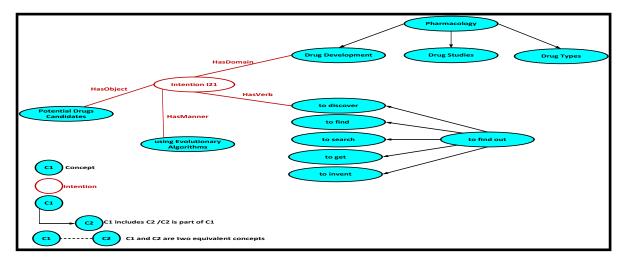


Figure B.22: Extract of the capacity ontology of the Process Chunk VPC1-3

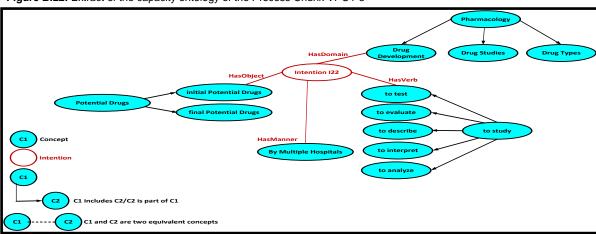


Figure B.23: Extract of the capacity ontology of the Process Chunk VPC12-3

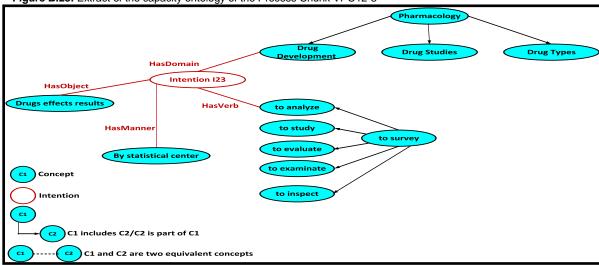


Figure B.24: Extract of the capacity ontology of the Process Chunk VPC14-3

C. Drug Development Process (DDP) SWRL Rules

 Table C.1: Sample of defined SWRL rules in our DDP domain ontology for the first CWS version

<u>'</u>	Associated CMDL rules
High-level concept	Associated SWRL rules
Therapeutic_need	Storage(?p) ^ Data_Properties(?p) ^Activity_Type(?p) ^ Molecules(?p) ^ Design_Activity(?p) -> Therapeutic_need(?p)
Molecules_structure	Molecules(?p) ^ Design_Activity(?p) ->Molecules_structure(?p)
Chemical_ test	Control_Protocol (?p)^Deployment(?p)^Data _Properties(?p) ^Activity_Properties(?p)^
	Security(?p)-> Chemical_test(?p)
BCH_screening	Deployment(?p)^Data_Properties(?p)^Activity_Properties(?p)^Receive/Send_Activity(?p)^M
_	olecules(?p) ^BCH_report(?p)^ Screening_test(?p)-> BCH_screening(?p)
Screening_test	Deployment(?p) \(^Data_Properties(?p)\^\) Activity_Properties(?p)-> Screening_test(?p)
Medical_Industry_Sa	Create_Activity(?p)^Samples(?p)^Molecules(?p)^Deployment(?p)^Data_Properties
mples	(?p)^Activity_Properties(?p)^Security(?p)-> Medical Industry Samples(?p)
Pharmacology_	Receive/Send _Activity(?p)^
Laboratory_Samples	Samples(?p)-> Pharmacology_ Laboratory _Samples(?p)
Toxicology_ Analyzes	Deployment(?p)^Cloud_Deployment(?p)^Resource
	(?p)^Toxicology_Laboratory(?p)^Data_Properties (?p)^
	Numeric:>30000(?p)^Samples(?p)^Pharmacology
	_samples(?p)^Activity_Properties(?p)^Toxicology_test(?p)^
	Inter-Sides_Message(?p)-> Toxicology_ Analyzes(?p)
Teratology_ Analyzes	Deployment(?p)^Cloud_Deployment(?p)^Resource(?p) ^Teratology_Laboratory(?p)^Data_
	Properties(?p)
	^Numeric:>30000(?p)^Samples(?p)^Pharmacology_samples(?p)^Activity_Properties(?p)^T
	eratology_test(?p)^
	Inter-Sides_Message(?p)-> Teratology_ Analyzes(?p)
Mutagenicity	Deployment(?p) ^Cloud_Deployment(?p) ^Resource(?p) ^
_ Analyzes	Mutagenicity_Laboratory(?p) ^Data_Properties (?p) ^Numeric:>30000(?p) ^Samples(?p)
	^Pharmacology_samples(?p) ^
	Activity_ Properties(?p) ^Mutagenicity_ test(?p) ^Inter-Sides_ Message(?p)
	-> Mutagenicity_ Analyzes(?p)
Test_reports_results	Activity_Properties(?p)^
	Pharmacology_test(?p)^
	Receive/Send_ Activity(?p)^
	Data_Properties(?p)^
	Toxicology _report(?p)^ Embryology _report(?p)^
	Histology _report(?p)^
	Resource(?p)^
	Pharmacology_ Laboratory(?p)-> Test_reports_results(?p)
Human _patient _Test	HP_test (?p)^Hospital(?p)^Resource(?p)^Activity _Properties(?p)^ Inter-Sides
Traman _patient _rest	_Message(?p)^Data_ Properties(?p)^Pharmacology_ samples(?p)^HT_
	report(?p)^Numeric:>300000(?p)^Deployment(?p)^Cloud_ Deployment(?p)-> Human_
	patient _Test(?p)
HT test results	Activity _Properties(?p)^
	Receive/Send _Activity(?p)^
	Data _Properties(?p)^
	HT_ report(?p)^
	Resource(?p)^
	Pharmacology_ Laboratory(?p)^
	Deployment(?p)^
	Public_ Deployment(?p)^
	Public-Outsourced(?p)-> HT_ test _results(?p)
Statistical _Analysis	Statistical _center _report(?p) ^
	Resource(?p)^
	Statistical _center(?p)^
	Data(?p) ^
	Data_ Properties(?p) ^
	Data_ sets :<=100(?p)^
	HT_ report(?p)^
	Statistical _report(?p)^
	Amazon_ EC2(?p)^
	Deployment(?p)^
	Cloud _Deployment(?p)^
	Activity _Properties(?p)^ To_ analyze_ Data(?p)
	To_ analyze_ Data(?p) -> Statistical _Analysis(?p)
Statistical _report	Resource(?p)^
Statistical _report	Pharmacology_ Laboratory(?p)^
	Data_Properties (?p)^
	data sets :<=100(?p)^
	Statistical _report(?p)^
	Qualitative &

Quantitative_ Analysis (?p)^
Report(?p)^
Deployment(?p)^
Public _Deployment(?p)^
Activity_ Properties(?p)^
Receive_ Activity(?p)^
Public-Outsourced(?p)-> Statistical _report(?p)

Table C.2: Sample of defined SWRL rules in our DDP domain ontology for the second CWS version

Table C.2: Sample of defined SWRL rules in our DDP dor	
High-level concept	Associated SWRL rules
Therapeutic_ need	Storage(?p) ^
	Date_ Properties(?p) ^
	Activity_ Properties (?p)^
	Resource (?p)^
	Pharmacology _Laboratory (?p)^
	Molecules (?p)^
	Type _of_ Storage(?p) ^
	Hybrid_ Storage(?p) ^
	Cost_ of _Storage (?p)^
	Activity_ Properties (?p)^
	Cost _Value>=1000(?p) ^
	Time _of_ execution(?p) ^
	Time>=300 (?p)^
	Select _Activity(?p)-> Therapeutic_ need (?p)
Detect_ a _new_ Molecules _structure	Molecules(?p) ^
	Activity_ Properties(?p)^
	Design _Activity(?p)^
	Data _Properties(?p)^
	Big _Data _Structure(?p)^
	Deep_ learning _Algorithms(?p)^
	Deployment(?p) ^
	In-house_ Deployment-> Detect_ a _new_ Molecules
	_structure(?p)
Chemical _test	Control _Protocol(?p) ^
_	AMP_ and _GMP_ report (?p)^
	Deployment(?p)^
	Cloud Deployment(?p)^
	Multiple _Biochemistry _Laboratories(?p) ^
	Data_ Properties(?p) ^
	Size_ of _Data:>=30000(?p)^
	Chemical_ Molecules(?p)^
	Molecules _Analyzes_ report(?p)^
	Activity_ Properties(?p)^
	Time:<=100(?p)^
	Biochemistry _test(?p) ^
	Inter-sides_ Message(?p)^
	Security(?p)^
	Authentification(?p)-> Chemical _test(?p)
PCH paragring	Deployment(?p) ^
BCH_ screening	
	Hybrid _Deployment(?p)^
	Data_ Properties(?p)^
	Activity _Properties(?p)^
	Numeric:>=30000(?p)^
	BCH _report(?p)^
	Screening _BCH _report(?p)^
	Activity_ Properties(?p)^
	select _Activity(?p)^
	Molecules(?p)^
	Molecules _XY(?p)^
	Biochemistry _Molecules(?p)^
	BCH-report(?p)^
	Screening _test(?p)^
	Resource(?p)^
	Pharmacology_ Laboratory(?p)-> BCH_ screening(?p)
Screening_test	Storage(?p)^
	Private _Storage(?p)^
	Data_Properties(?p)^
	Biochemistry_ Molecules(?p)^
	Screening_test_report(?p)^
	Activity_ Properties(?p)^
	Screeing _Test(?p)^
	Molecules(?p)^
	Molecules _XY(?p)-> Screening_test(?p)
Medical_ Industry_ Samples	Create_ Activity(?p)^

Numeric:>=300000(?p)^ Deployment(?p)^ Cloud_Deployment(?p)^ Cloud_Deployment(?p)^ Cloud_Deployment(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Activity_Properties(?p)^ Response_Time:<20(?p)^ Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Chemical_Samples(?p)-Medical_Industry_ Samples(?p) Human_patient_Test HP_advanced_test(?p)^ Multiples_Medical_Samples(?p)-Medical_Industry_ Samples(?p) HP_advanced_test(?p)^ Activity_Properties(?p)^ Multiples_Hospitals(?p)^ Resource(?p)^ Pharmacology_samples(?p)^ Pharmacology_samples(?p)^ Numeric:>=600000(?p)^ Deployment(?p)^ Cloud_Deployment(?p)> Statistical_center(?p)^ Statistical_center(?p)^ Data_(?p)^ Data_(?p)^ Data_(?p)^ Data_(?p)^ Multiple_Statistical_reports(?p)^ Amazon_EC2(?p)^ Amazon_EC2(?p)^ Pharmacology_Laboratory(?p)^ Activity_Properties(?p)^ To_analyze_Data(?p)^ Statistical_report Resource(?p)^ Pharmacology_Laboratory(?p)^ Condidentiality(?p)-Statistical_Analysis(?p) Resource(?p)^ Pharmacology_Laboratory(?p)^ Data_Properties(?p)^ Activity_Properties(?p)^ Condidentiality(?p)-Statistical_Analysis(?p) Resource(?p)^ Pharmacology_Laboratory(?p)^ Data_Properties(?p)^ Adata_sets::>=100000(?p)^ Statistical_Advanced_Report(?p)^ Outliative_Analysis(?p) Advanced_Report(?p)^ Deployment(?p)^ Cloud_Deployment(?p)^ Cloud_Deployment(?p)^ Cloud_Deployment(?p)^ Cloud_Deployment(?p)^		To 1 (0.):
Deployment(?p)^ Cloud_Deployment(?p)^ Data_Properties(?p)^ Chemical_Molecules(?p)^ Chemical_Molecules(?p)^ Activity_Properties(?p)^ Response_Time:<=20(?p)^ Molecules(?p)^ Cost:<=900(?p)^ Molecules(?p)^ Cost:<=900(?p)^ Molecules(?p)^ Cost:<=900(?p)^ Multiple_Medical_Samples(?p)>> Medical_Industry_ Samples(?p) Human_patient_Test HP_advanced_test(?p)^ Multiples_Hospitals(?p)^ Resource(?p)^ Activity_Properties(?p)^ Nativity_Properties(?p)^ Data_Properties(?p)^ Numeric:=600000(?p)^ Deployment(?p)> Deployment(?p)> Deployment(?p)> Deployment(?p)> Statistical_center_report (?p)^ Mata_sets:=100000(?p)^ Data_Properties(?p)^ Data_Properties(?p)^ Mataiscal_center_report(?p)^ Multiples_Hospitals(?p)^ Activity_Properties(?p)^ Data_Properties(?p)^ Data_Properties(?p)^ Data_Properties(?p)^ Mataiscal_center_report(?p)^ Multiple_Statistical_report(?p)^ Mataz_Center_(?p)^ Deployment(?p)^ Cloud_Deployment(?p)^ Mataz_Center_(?p)^ Deployment(?p)^ Cond_Deployment(?p)^ Activity_Properties(?p) To_analyze_Data(?p)^ Security(?p)^ Confidentiality(?p)>—Statistical_Analysis(?p) Resource(?p)^ Pharmacology_Laboratory(?p)^ Data_Properties(?p) Advanced_Report(?p)^ Qualitative & Quantitative Analysis (?p) Advanced_Report(?p)^ Deployment(?p)^ Deployment(?p)^ Cloud_Deployment(?p)^ Deployment(?p)^		Samples(?p)^
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Statistical _report Resource(?p)^ Pharmacology _Laboratory(?p)^ Data _Properties(?p) ^ data sets :>=100000(?p)^ Statistical_ Advanced_ Report(?p)^ Qualitative & Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		
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Data _Properties(?p) ^ data sets :>=100000(?p)^ Statistical_ Advanced_ Report(?p)^ Qualitative & Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^	Statistical _герогт	(1 /
data sets :>=100000(?p)^ Statistical_ Advanced_ Report(?p)^ Qualitative & Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		
Statistical_ Advanced_ Report(?p)^ Qualitative & Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		_ ' ' ' '
Qualitative & Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		
Quantitative _Analysis (?p) Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		,
Advanced_ Report(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^		
Deployment(?p)^ Cloud _Deployment(?p)^		
Cloud _Deployment(?p)^		= ' \ ' '
		1
Activity Properties(?p)^		Cloud _Deployment(?p)^
		Activity_ Properties(?p)^
Receive _Activity(?p) ^		Receive _Activity(?p) ^
Inter-Cloud_ Message(?p)-> Statistical _report(?p)		Inter-Cloud_ Message(?p)-> Statistical _report(?p)

 Table C.3: Sample of defined SWRL rules in our DDP domain ontology for the third CWS version

High-level concept	Associated SWRL rules
therapeutic _need	Storage(?p) ^
	Data_ Properties (?p) ^
	Activity _Properties(?p) ^
	Resource (?p) ^
	Pharmacology _Laboratory(?p) ^
	Deployment(?p) ^
	In-house _Deployment(?p) ^
	Drugs(?p) ^
	Drugs_ Composition_ XYW(?p) ^
	Initial_ Drugs_ List(?p) ^
	Final _Drugs_ List(?p) ^
	Private_ Storage(?p) ^
	Activity Properties(?p) ^
	Cost _Storage _Value>=3000(?p) ^
	Numeric:>=10000(?p) ^
	Time_ of _execution(?p) ^

	Time<=100(?p) ^
	discover _Activity(?p) ^
	Intelligent _methods(?p) ^
	Evolutionary_ Algorithm(?p) -> therapeutic _need(?p)
Human_ patient _Test	HP_ drugs_ advanced _tests(?p)^
	Multiple_ efficacity _tests(?p)^
	Multiples _Hospitals(?p)^
	Number:>=100(?p)^
	Resource(?p)^
	Activity Properties(?p)^
	Inter-Sides_ Message(?p)^
	Initial_ Potential_ Drugs(?p)^
	Final Potential Drugs(?p)^
	Data_ Properties(?p)^
	HT drugs advanced tests report(?p)^
	Time_ of_ execution(?p)^
	Time:<=100(?p)^
	Numeric:>=600000(?p)^
	Deployment(?p)^
	Cloud_ Deployment(?p)-> Human_ patient _Test(?p)
Statistical_ Analysis	Statistical center report (?p)
Stationical_ / that you	Resource(?p)
	Statistical _center(?p)
	Data (?p)
	Data Properties (?p)
	data sets :>=100000(?p)
	HT _ drugs_ advanced _tests_ results(?p)
	Multiple _Statistical _drugs _advanced _tests_
	reports(?p)
	Statistical & Stochastic analyzes(?p)
	Deployment(?p)
	Cloud_ Deployment(?p)
	Activity _Properties(?p)
	To _analyze_ Data(?p)
	Security(?p)
	Confidentiality(?p)-> Statistical_ Analysis(?p)

D. PC-MIC Configurator

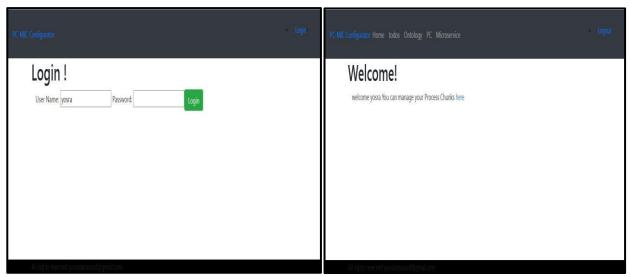


Figure C.1: PC-MIC Configurator Login Page

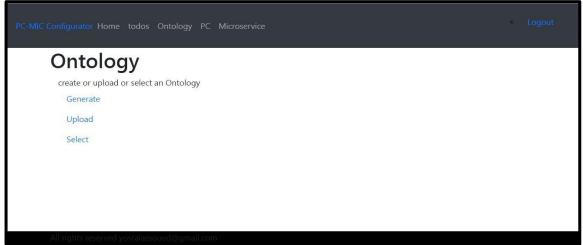


Figure C.2: Ontology Management in PC-MIC Configurator

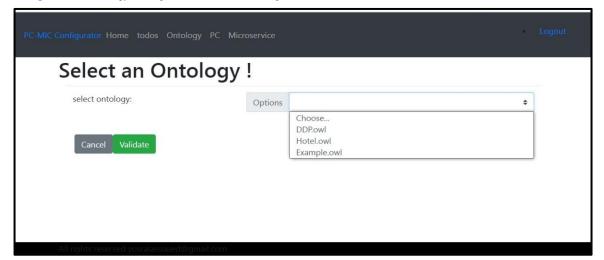


Figure C.3: Ontology Select in PC-MIC Configurator

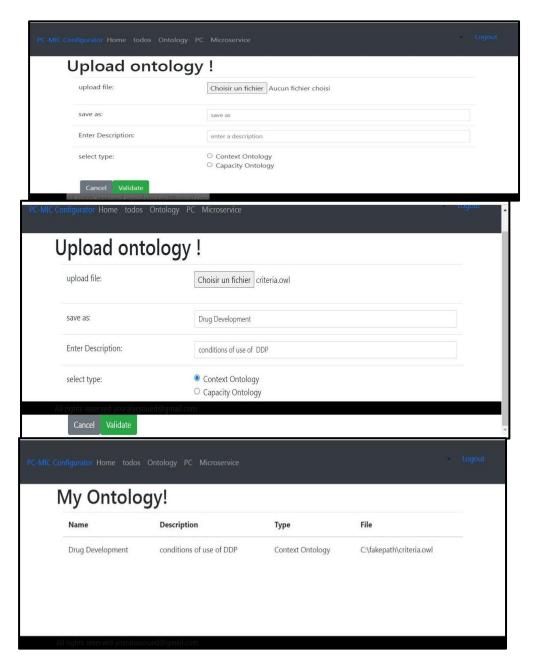


Figure C.4: Upload Ontology in PC-MIC Configurator

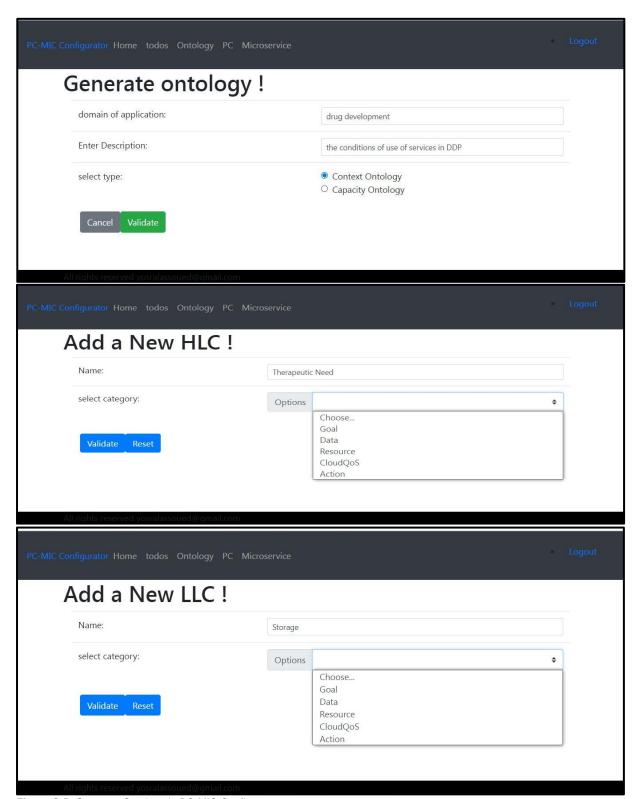


Figure C.5: Generate Ontology in PC-MIC Configurator

PC-MIC Co	nfigurator Home todos Ontology PC Micros	service	Logout			
HLC Relationships						
	Choose HLC1	Choose v				
	Choose HLC2	Choose 🗸	-			
	Choose Relationships	Choose 🔻				
Al	Validate Reset					
PC-MIC Co	nfigurator Home todos Ontology PC Micro	service	Logout			
-	HLC Relationships					
	Choose HLC1	Choose Choose				
	Choose HLC2	Therapeutic Need Molecules Structure				
	Choose Relationships	Chemical Test BCH Screening				
A	Validate Reset	Screening Test Medical Industry Samples Pharmacology Laboratory Samples Toxicology Test Teratology Test Mutagenicity Test Test Reports Results Human Patient Test				
			A second			
	nfigurator Home todos Ontology PC Micros	service	Logout			
H	HLC Relationships					
	Choose HLC1	Choose 🕶				
	Choose HLC2	Choose 🗸	_			
	Choose Relationships	Choose V				
	Validate Reset	Choose Include Exclude Equivalent				

Figure C.6: HLC Relationships in PC-MIC Configurator

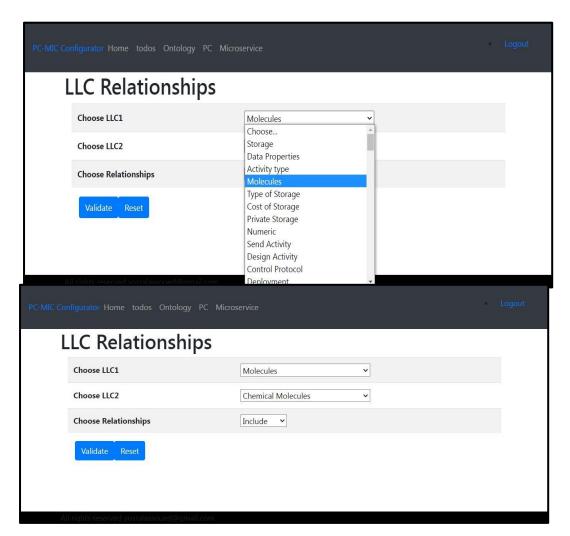


Figure C.7: LLC Relationships in PC-MIC Configurator

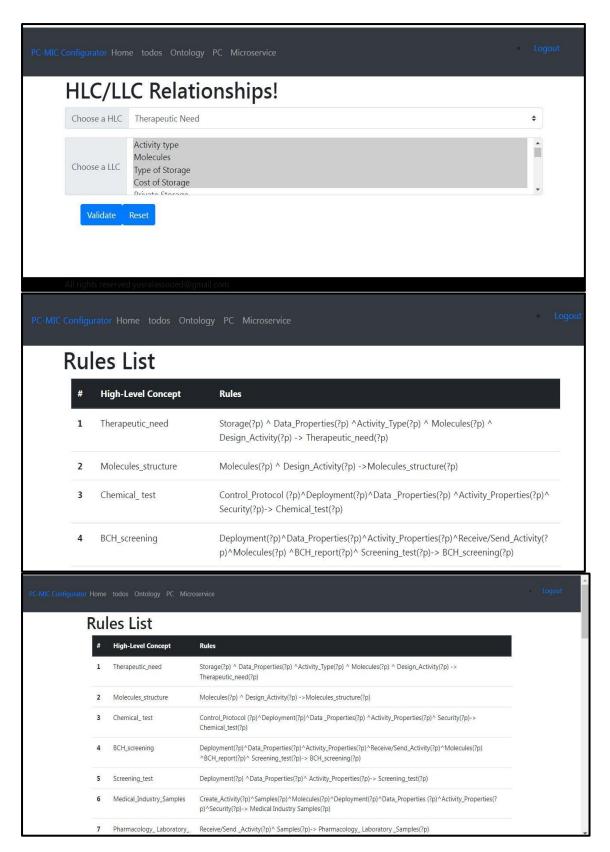


Figure C.8: SWRL Rules in PC-MIC Configurator