Annexe

A. Drug Development Process (DDP) Context Ontologies

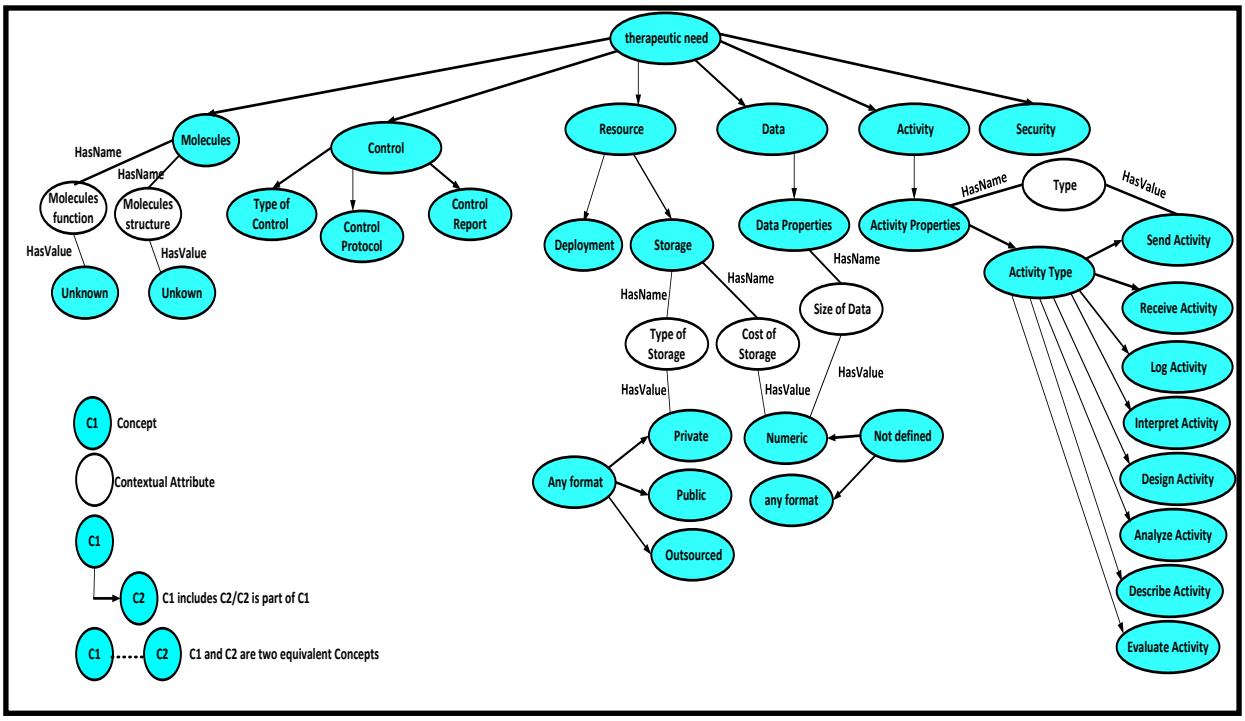

Figure A.1: Extract of the context ontology of the Process Chunk VPC1-1

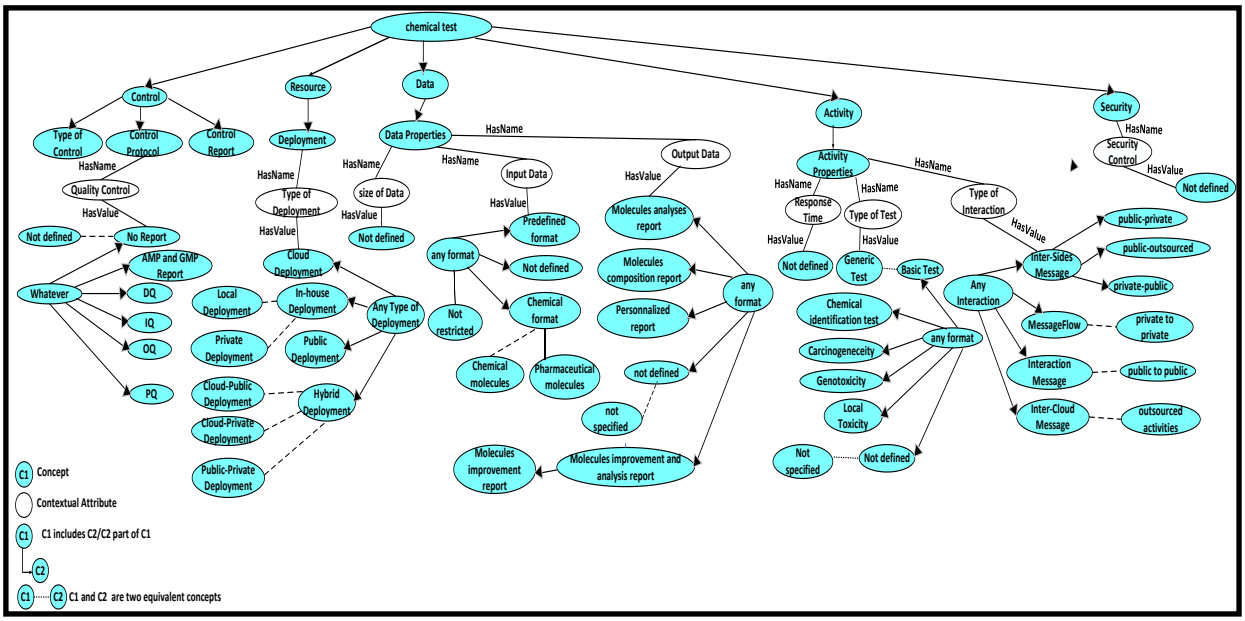

Figure A.2: Extract of the context ontology of the Process Chunk VPC3-1

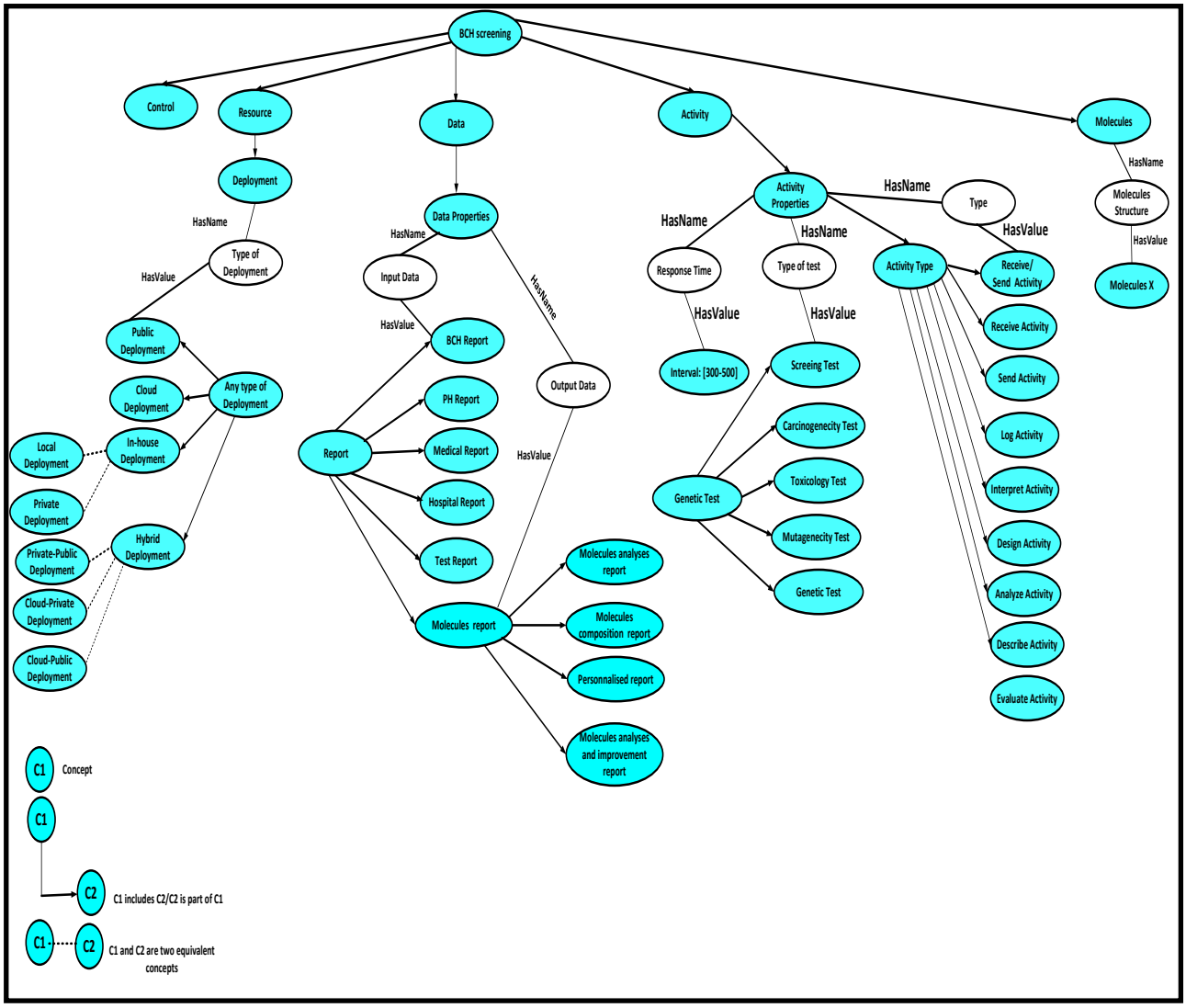

Figure A.3: Extract of the context ontology of the Process Chunk VPC4-1

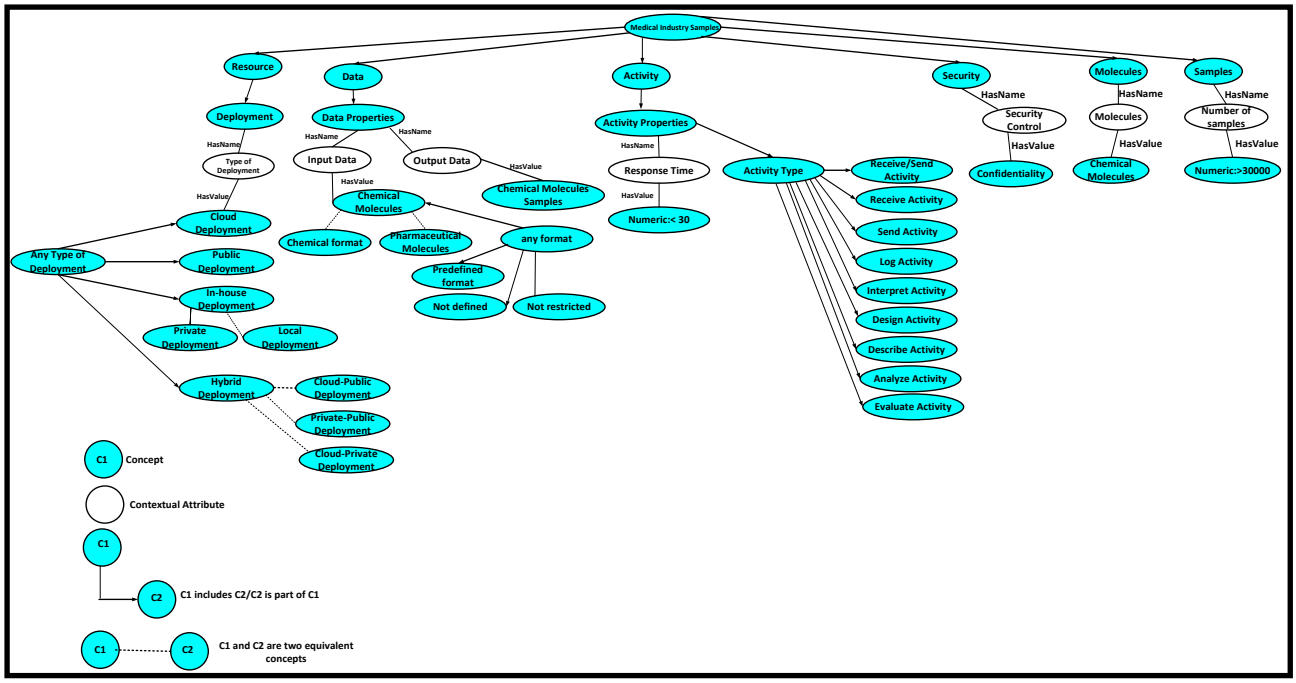

Figure A.4: Extract of the context ontology of the Process Chunk VPC6-1

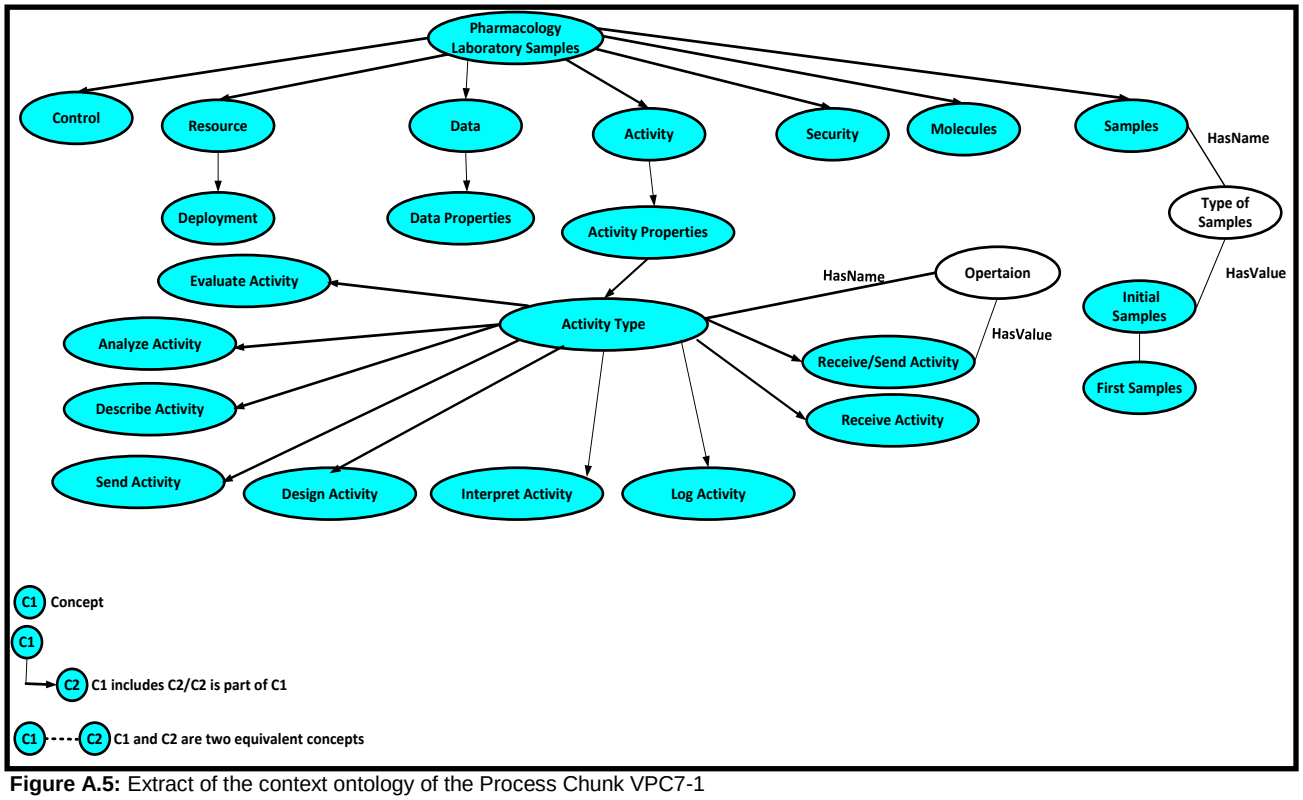

Figure A.5: Extract of the context ontology of the Process Chunk VPC7-1

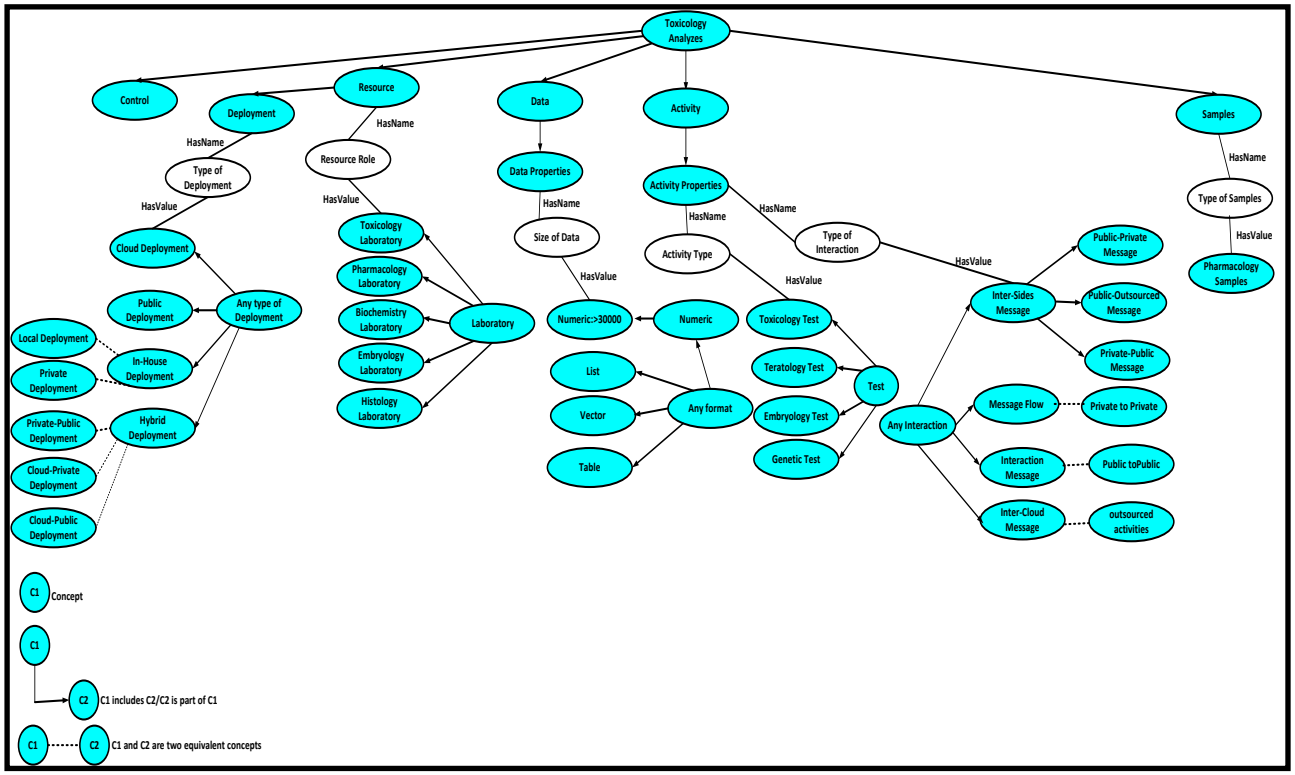

Figure A.6: Extract of the context ontology of the Process Chunk VPC8-1

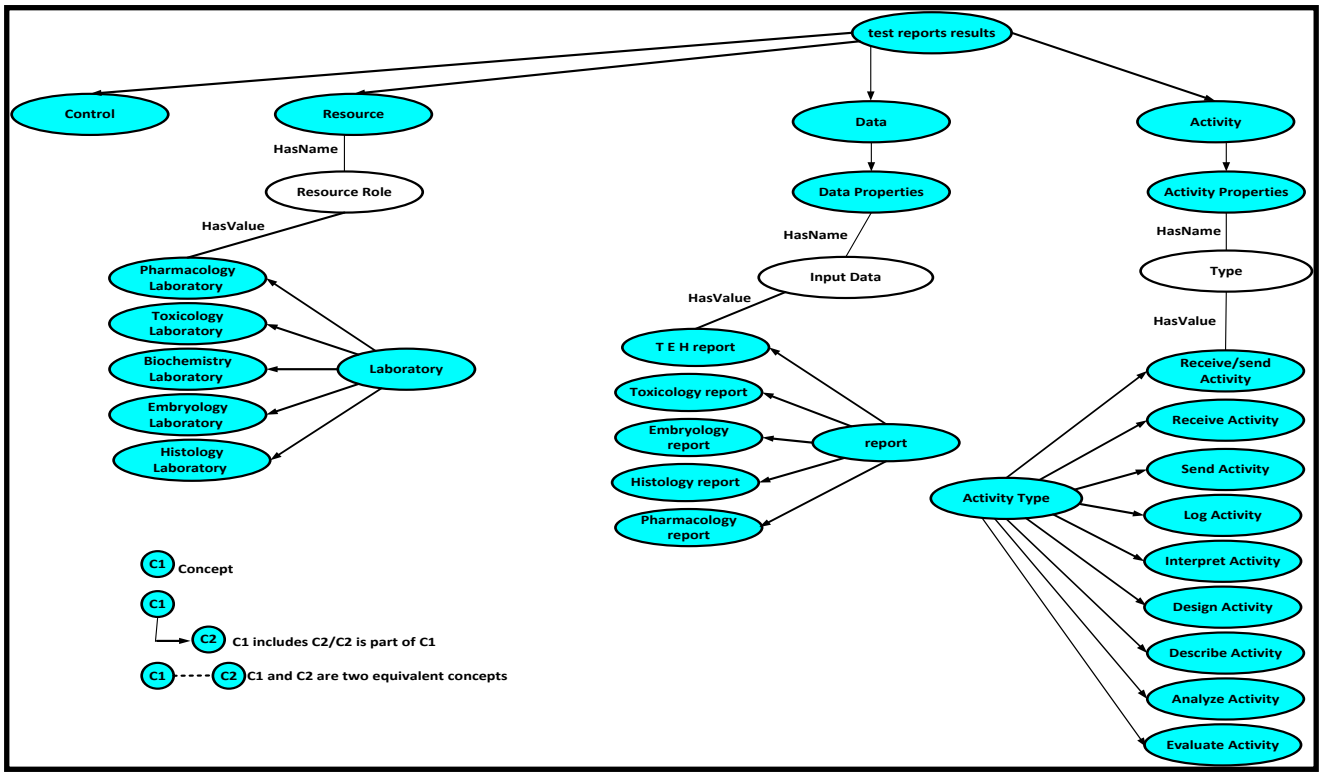

Figure A.7: Extract of the context ontology of the Process Chunk VPC11-1

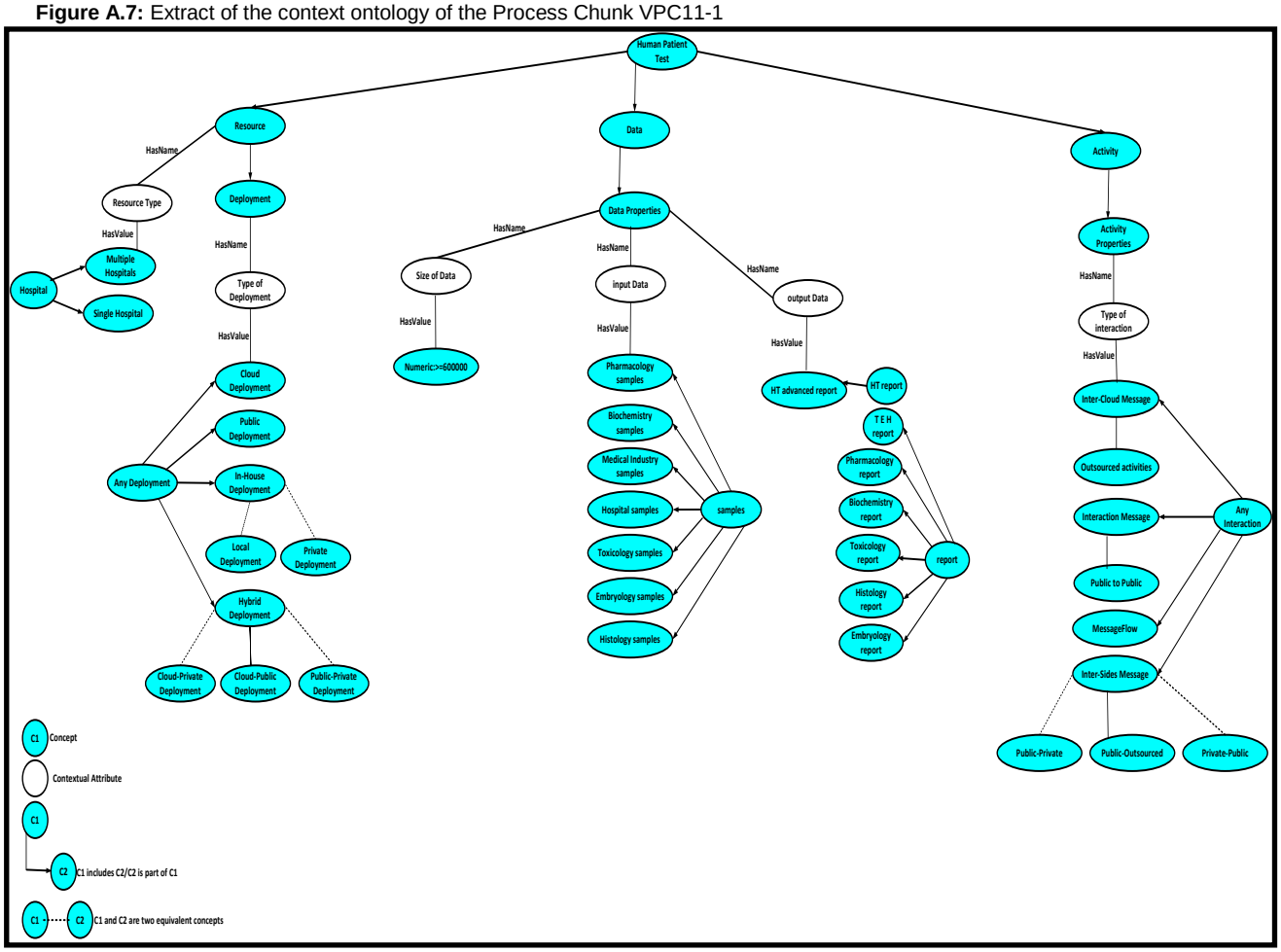

Figure A.8: Extract of the context ontology of the Process Chunk VPC12-1

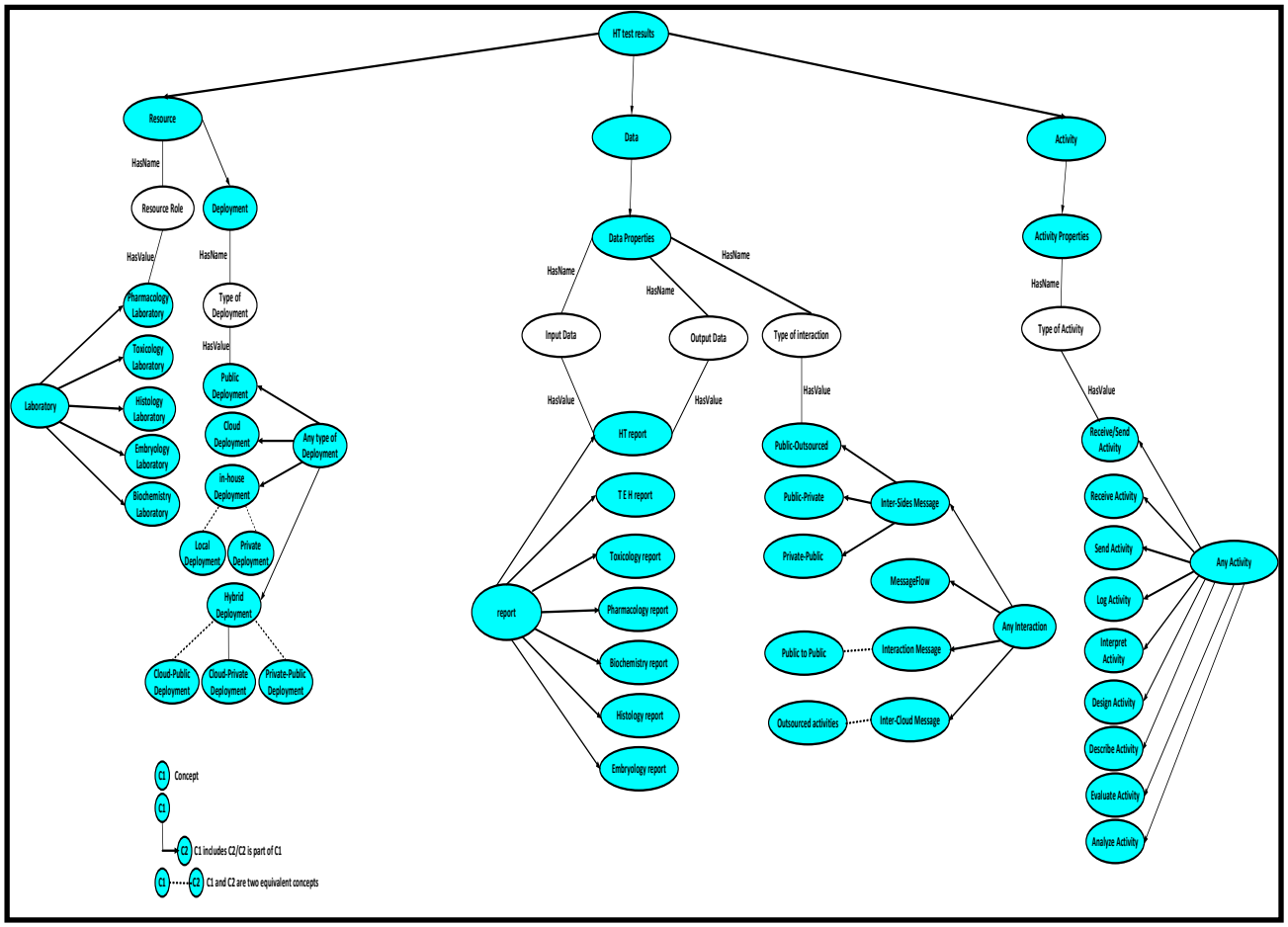

Figure A.9: Extract of the context ontology of the Process Chunk VPC13-1

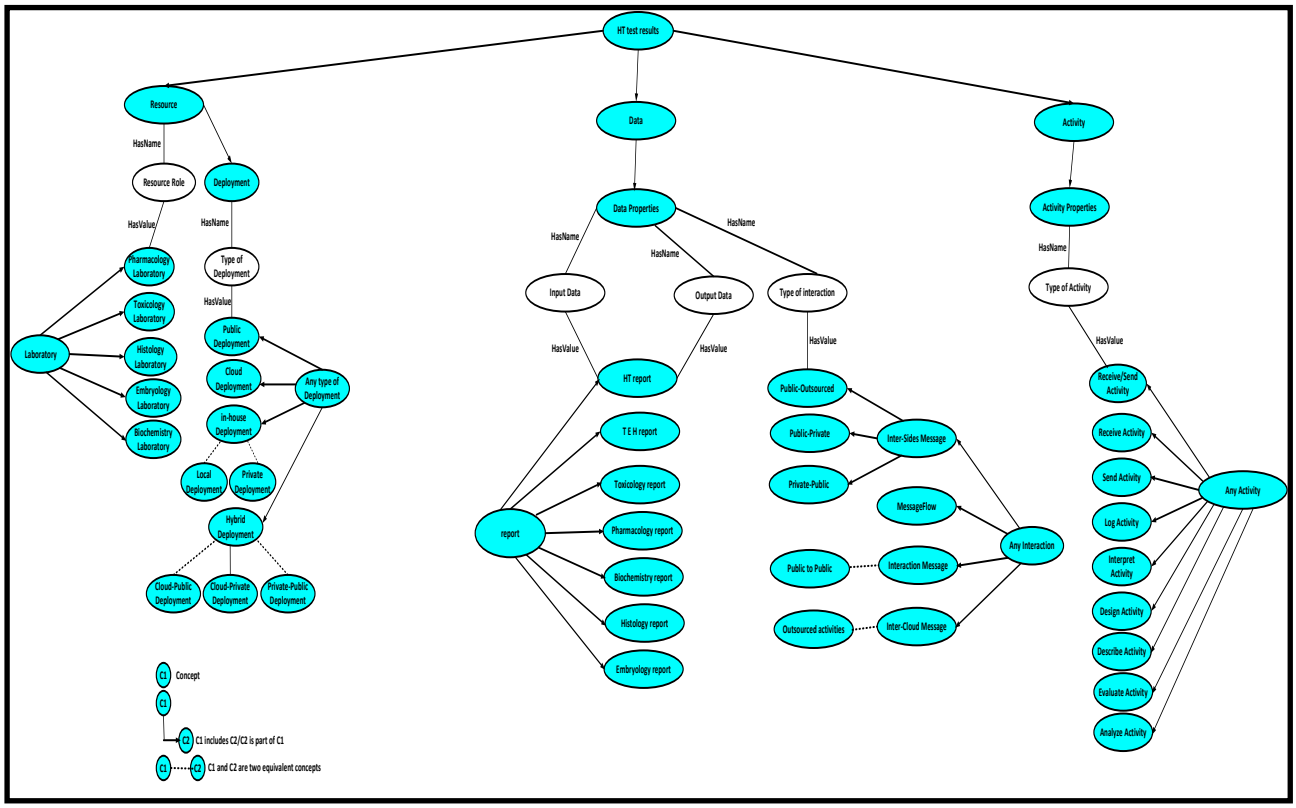

Figure A.10: Extract of the context ontology of the Process Chunk VPC14-1

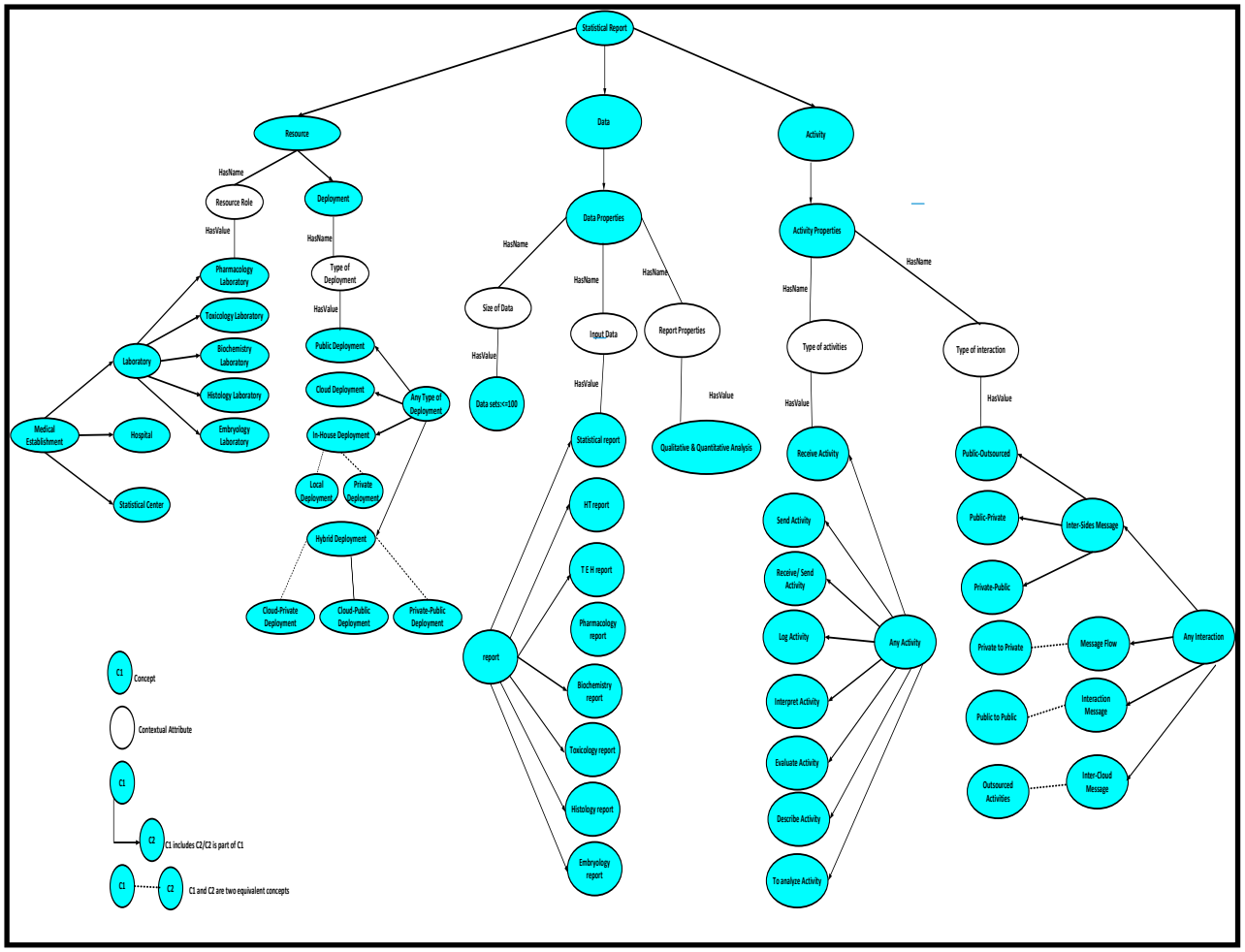

Figure A.11: Extract of the context ontology of the Process Chunk VPC15-1

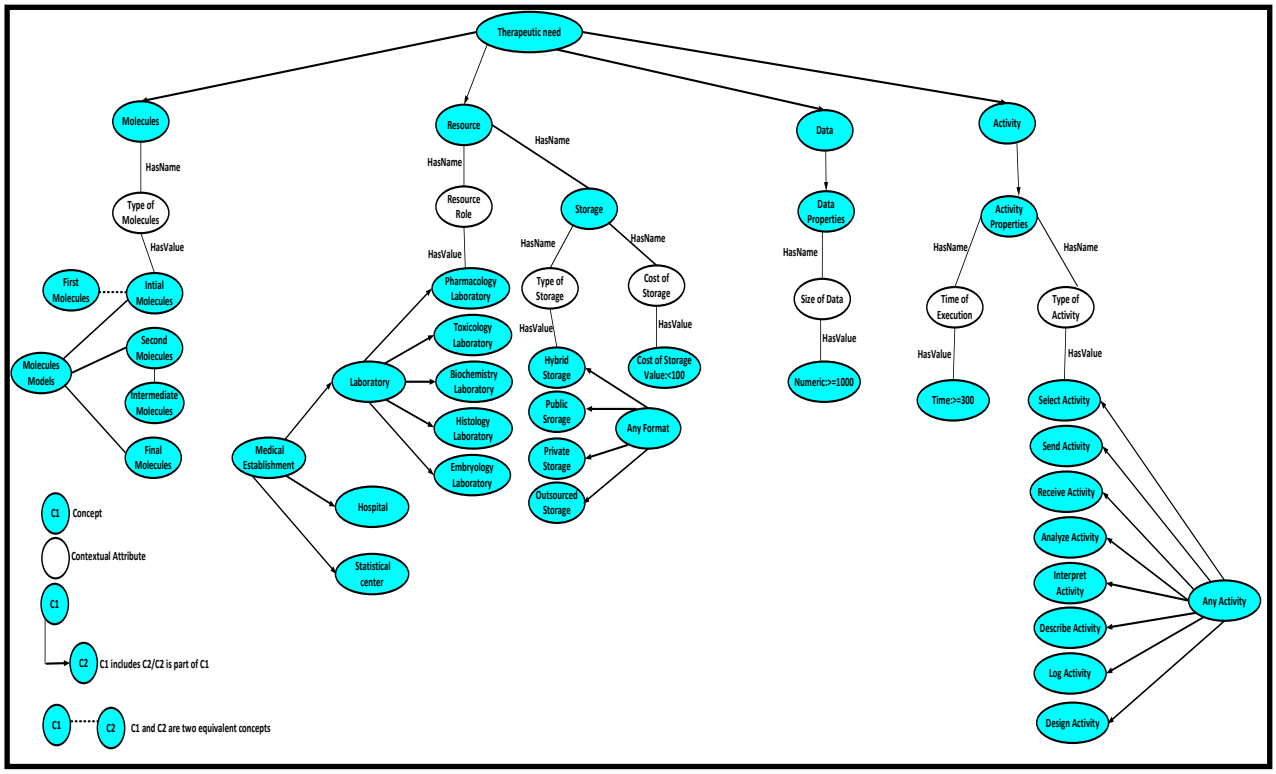

Figure A.12: Extract of the context ontology of the Process Chunk VPC1-2

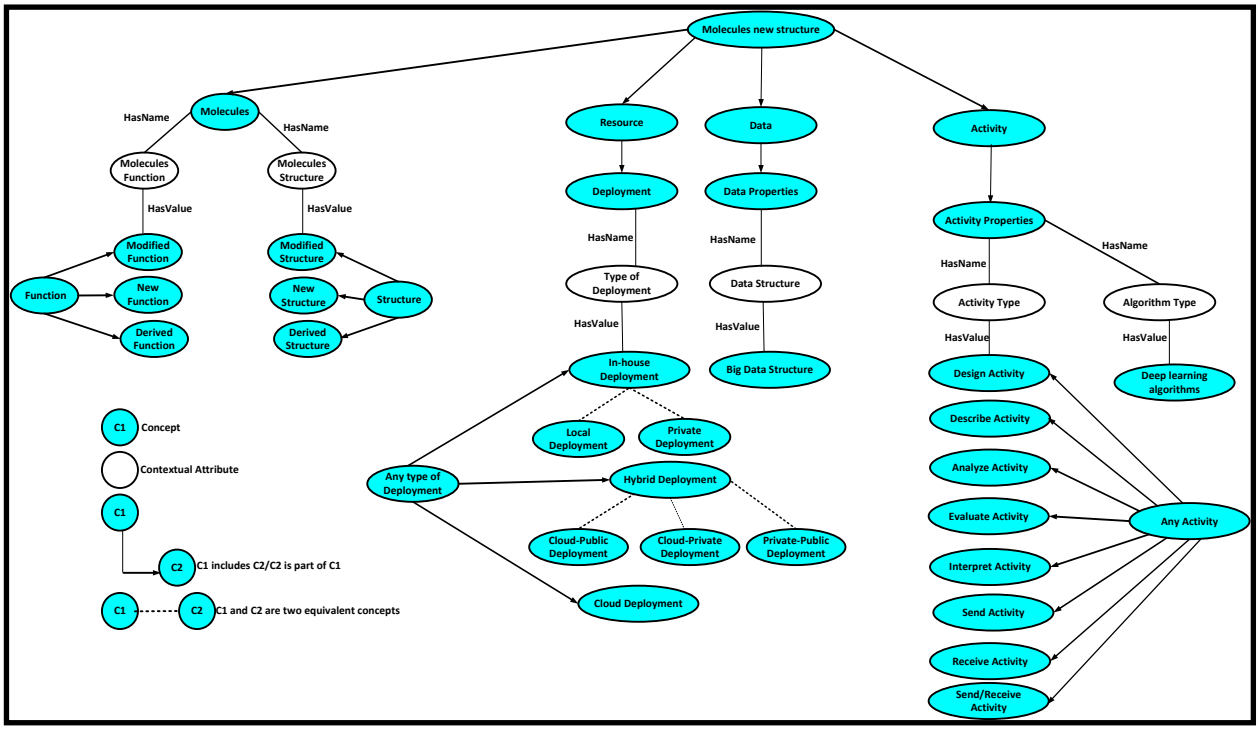

Figure A.13: Extract of the context ontology of the Process Chunk VPC2-2

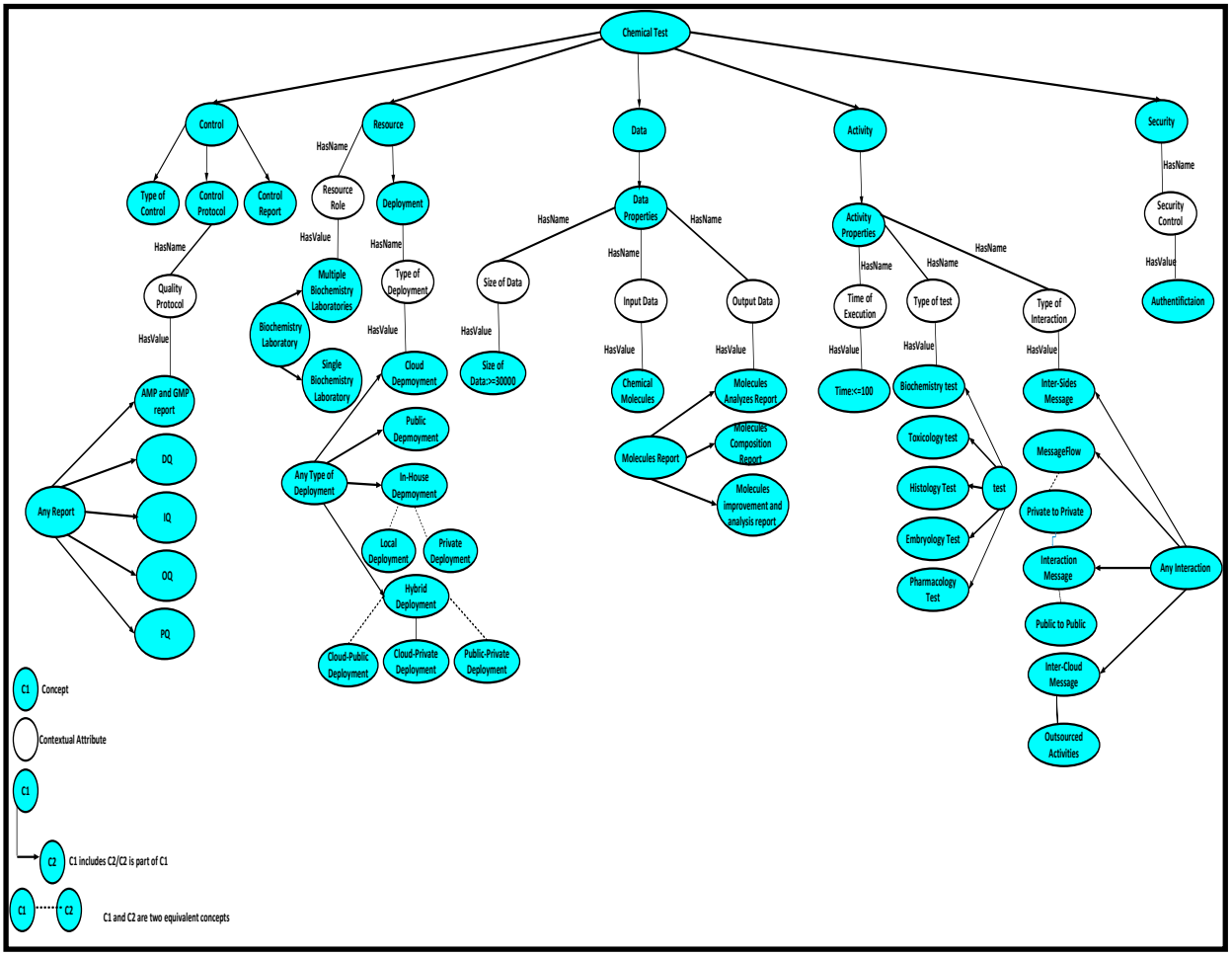

Figure A.14: Extract of the context ontology of the Process Chunk VPC2-2

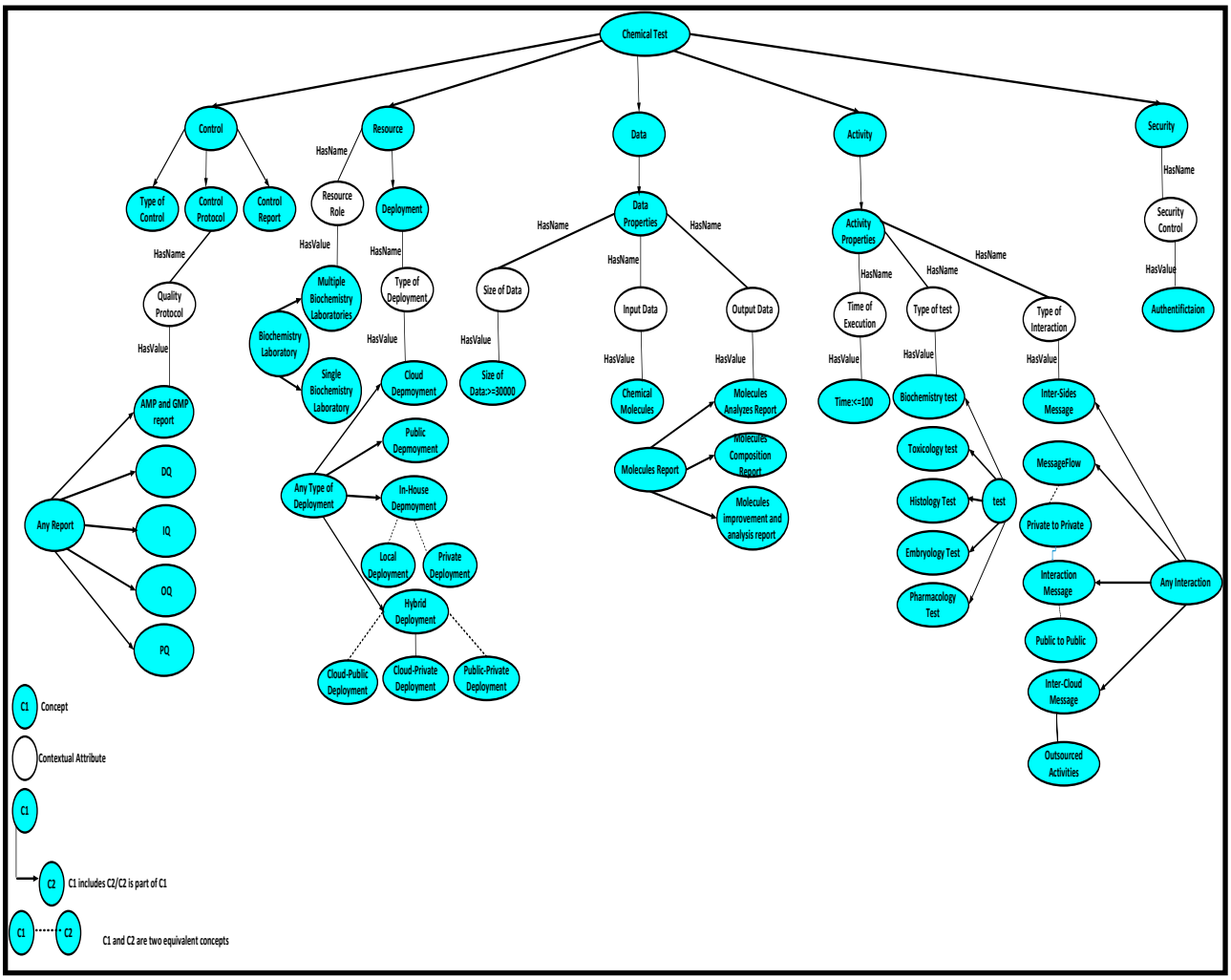

Figure A.15: Extract of the context ontology of the Process Chunk VPC3-2

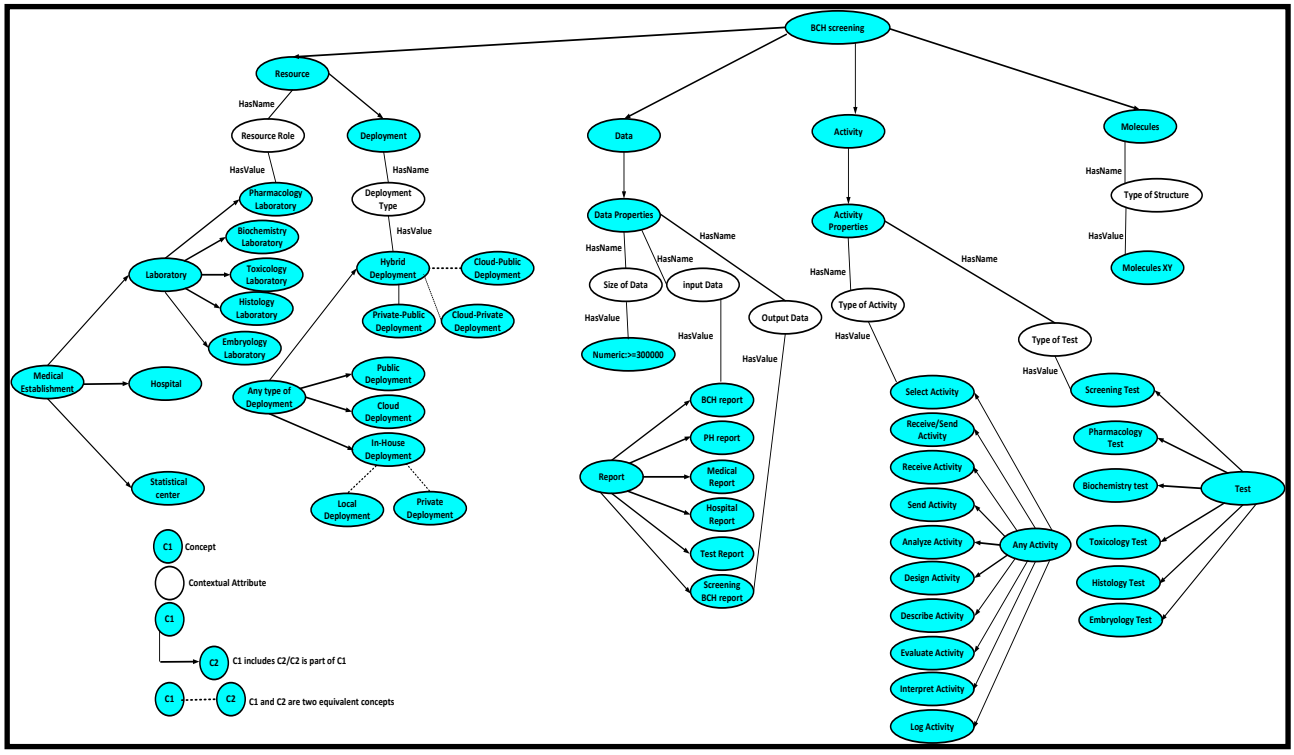

Figure A.16: Extract of the context ontology of the Process Chunk VPC4-2

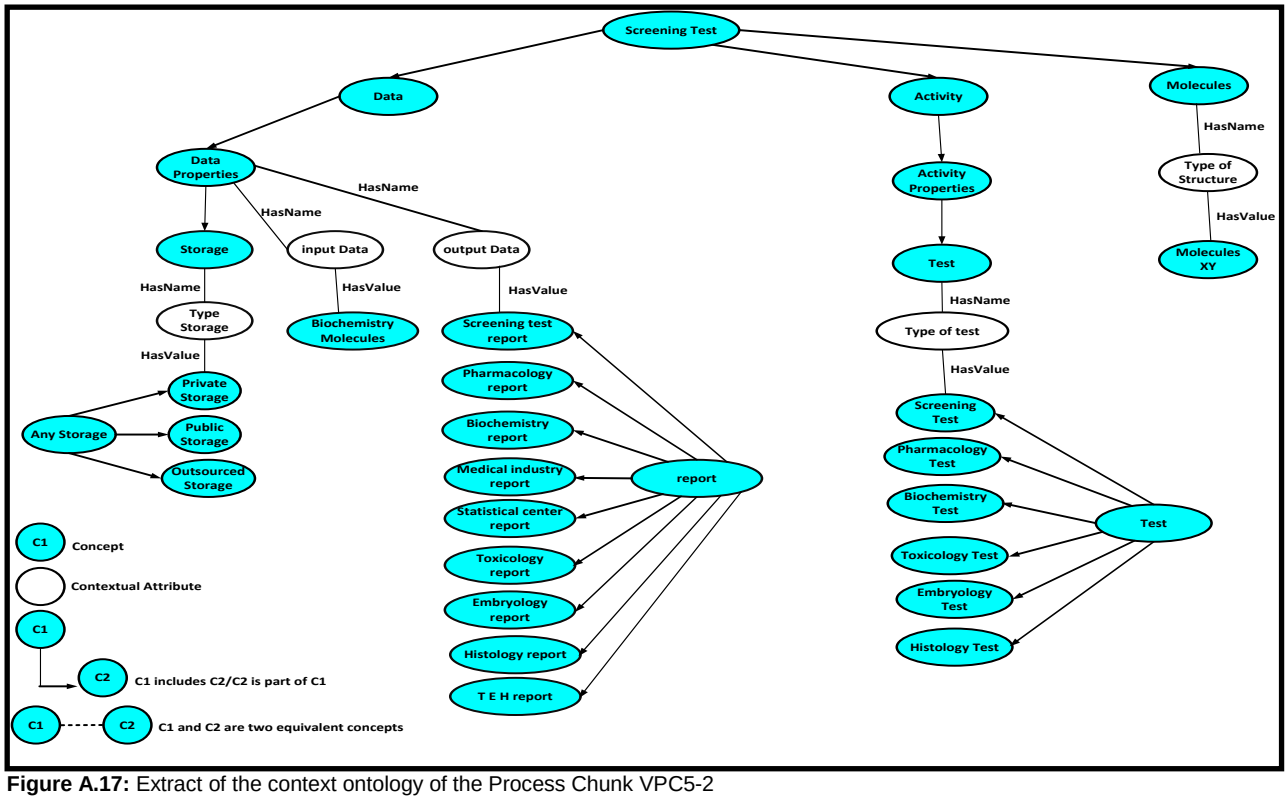

Figure A.17: Extract of the context ontology of the Process Chunk VPC5-2

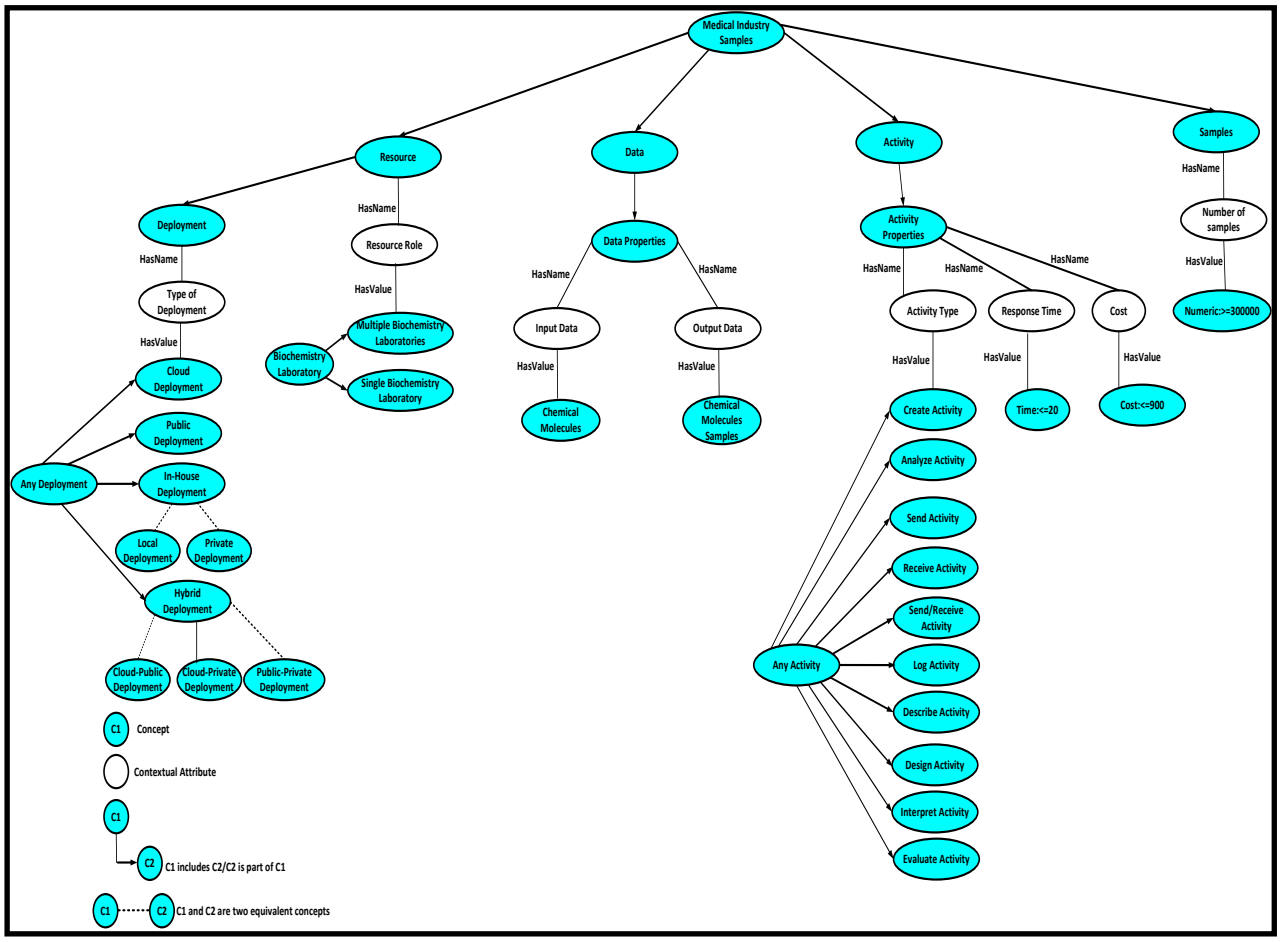

Figure A.18: Extract of the context ontology of the Process Chunk VPC6-2

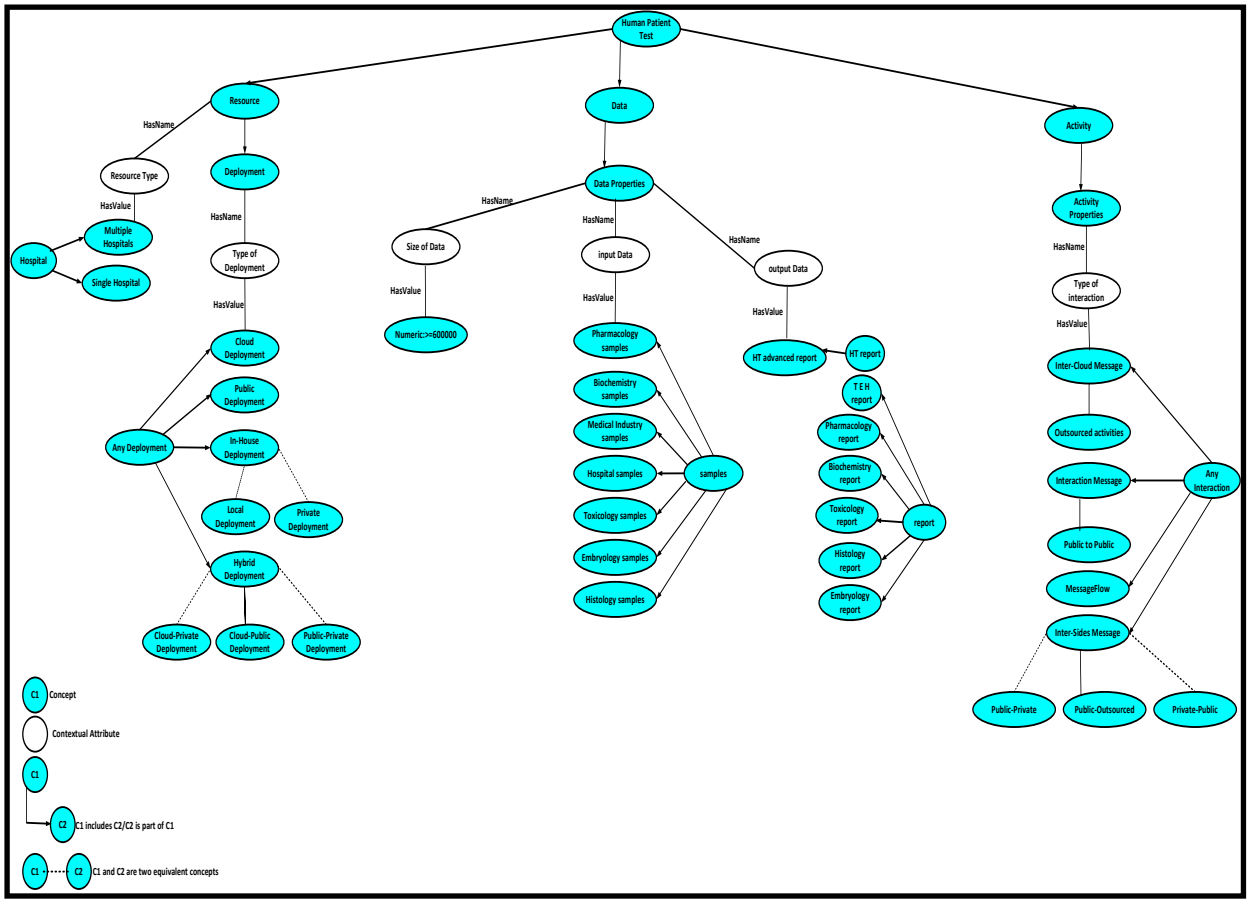

Figure A.19: Extract of the context ontology of the Process Chunk VPC12-2

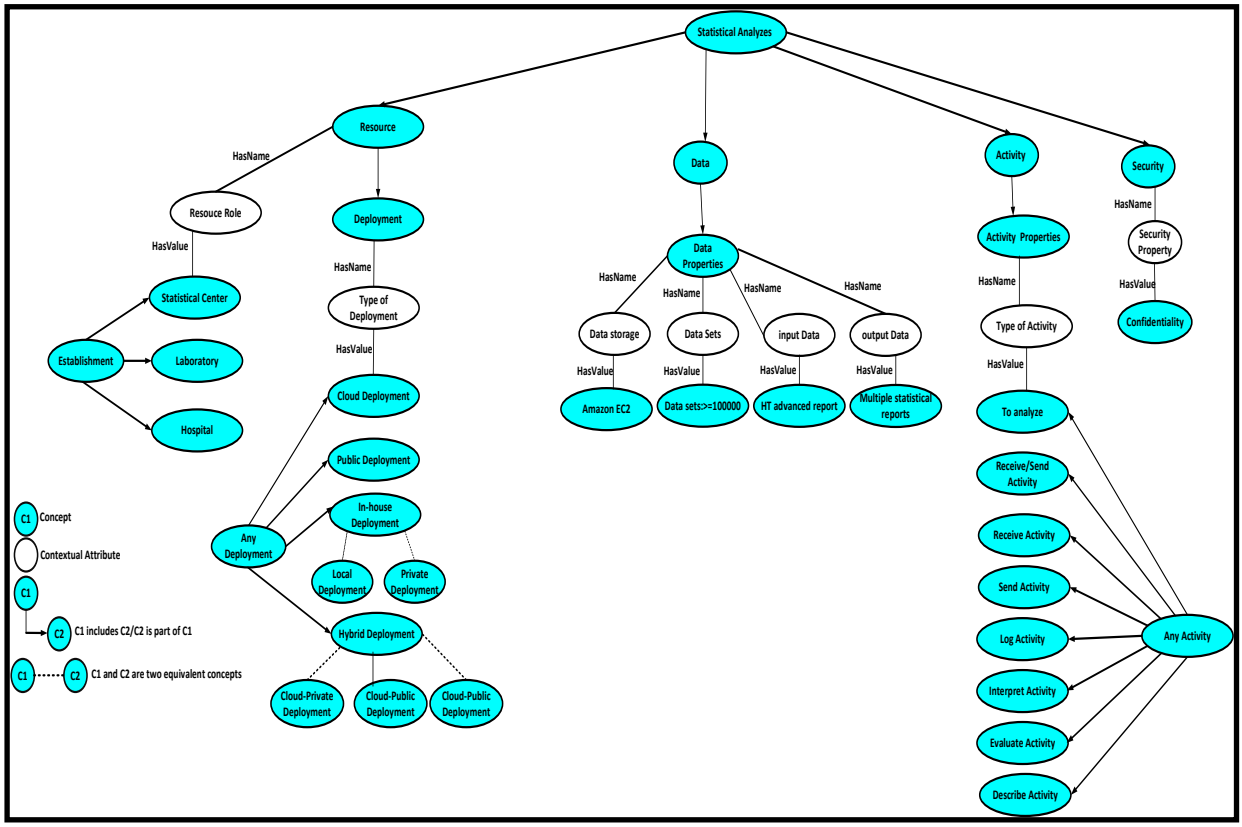

Figure A.20: Extract of the context ontology of the Process Chunk VPC14-2

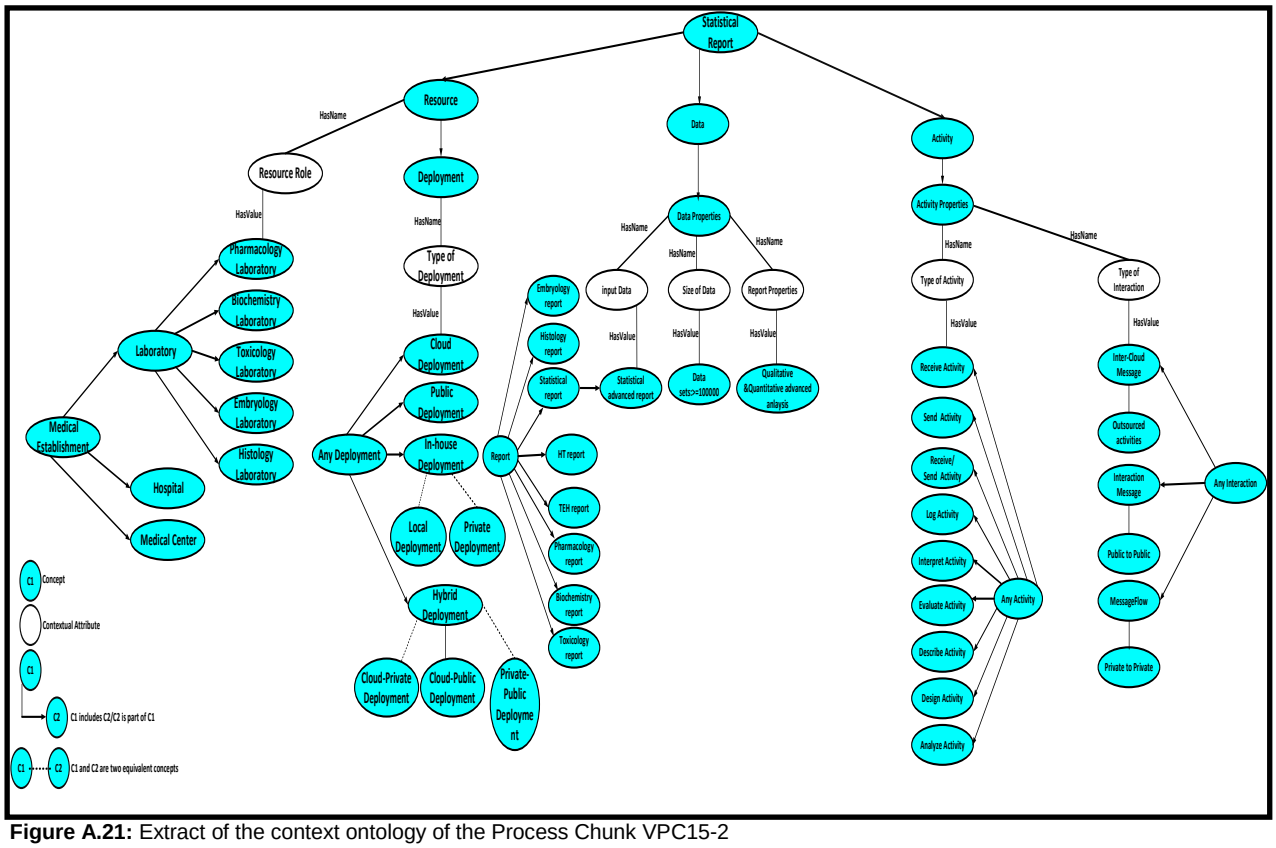

Figure A.21: Extract of the context ontology of the Process Chunk VPC15-2

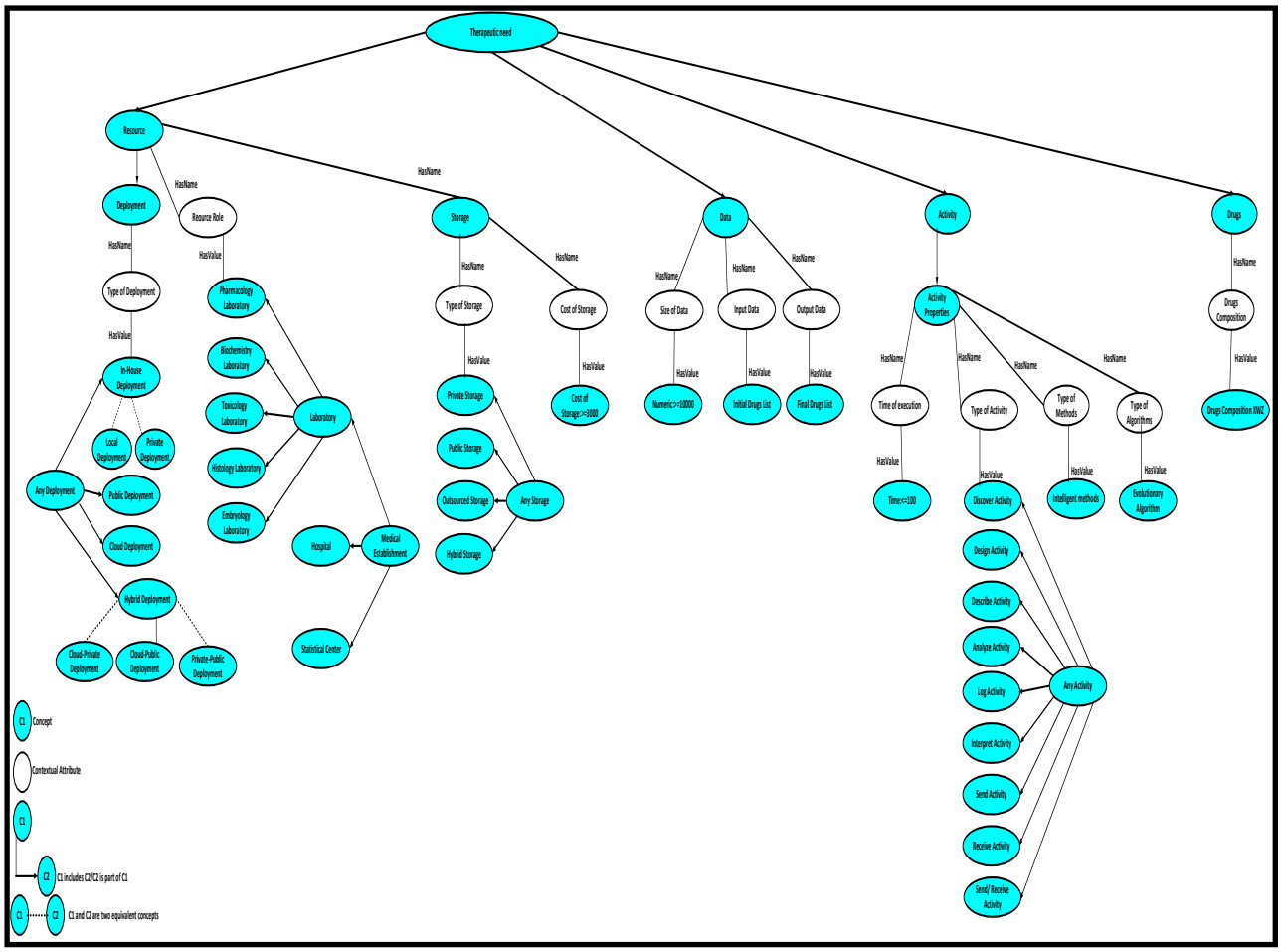

Figure A.22: Extract of the context ontology of the Process Chunk VPC1-3

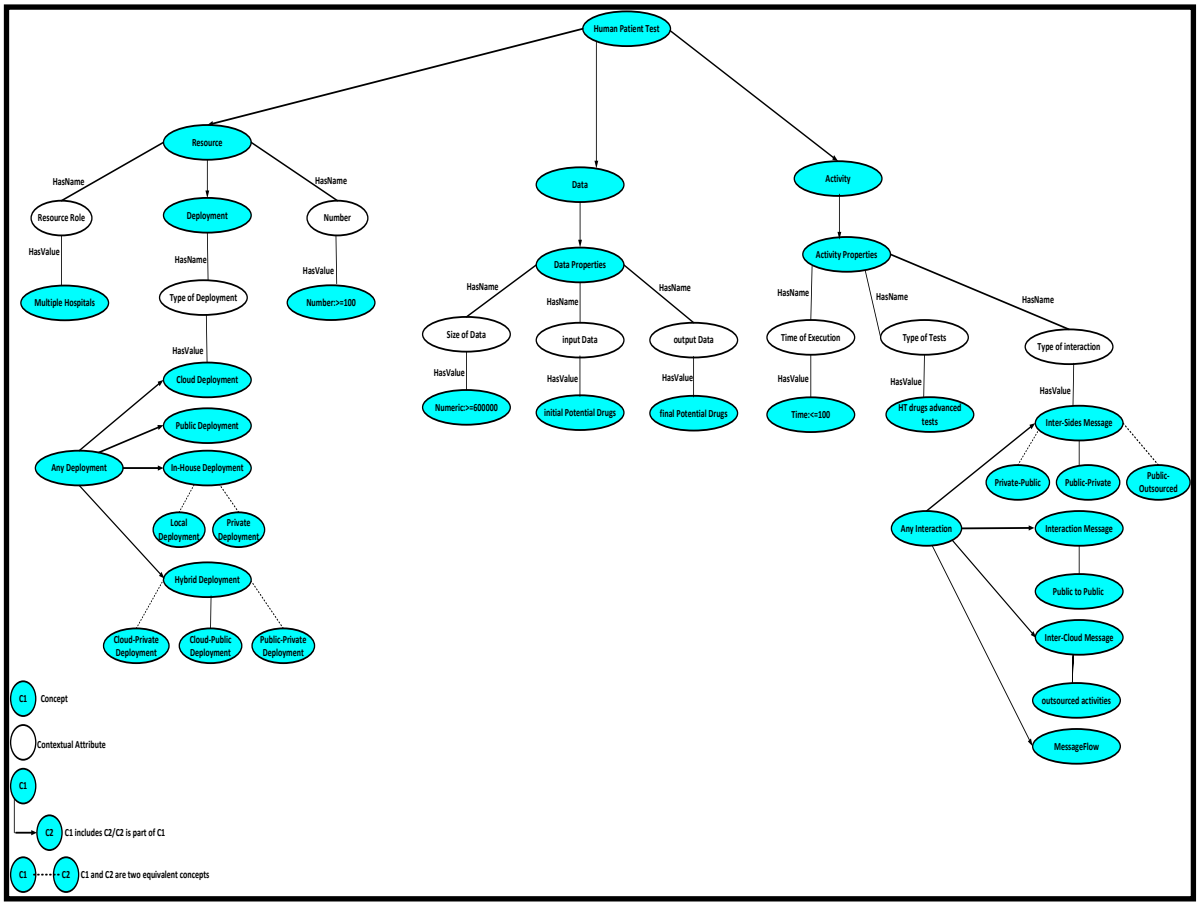

Figure A.23: Extract of the context ontology of the Process Chunk VPC12-3

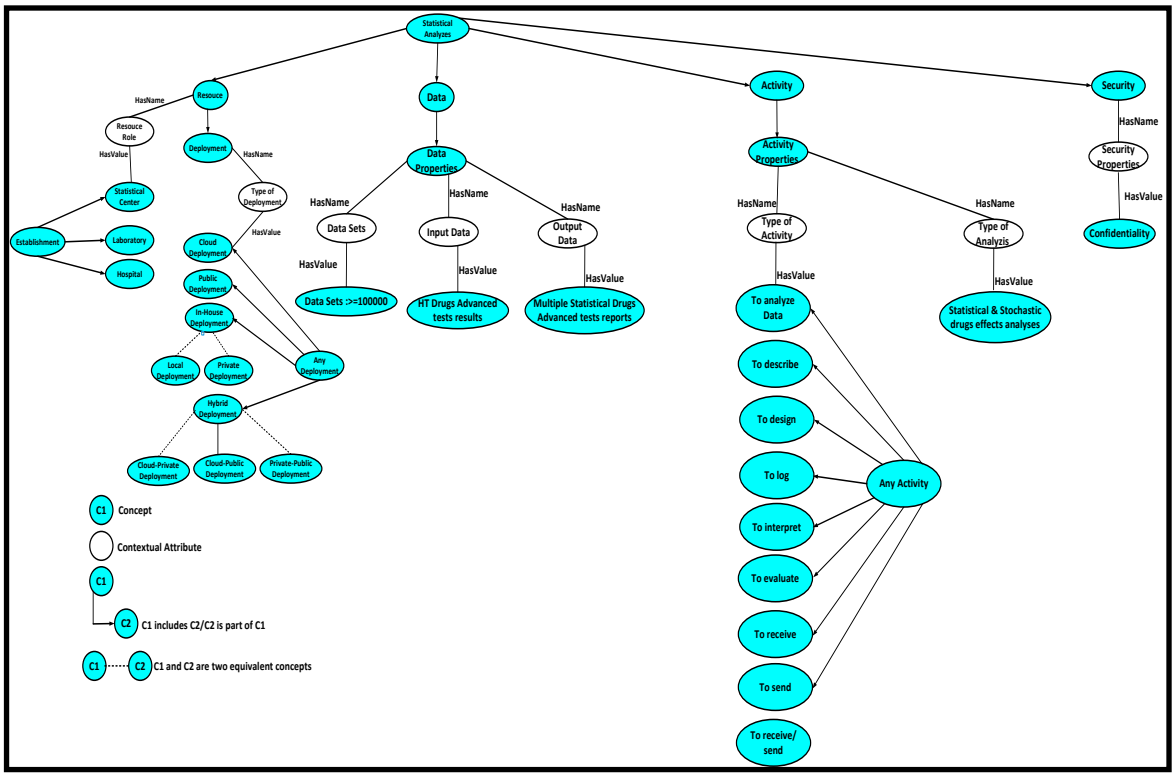

Figure A.24: Extract of the context ontology of the Process Chunk VPC14-3

B. Drug Development Process (DDP) Capacity Ontologies

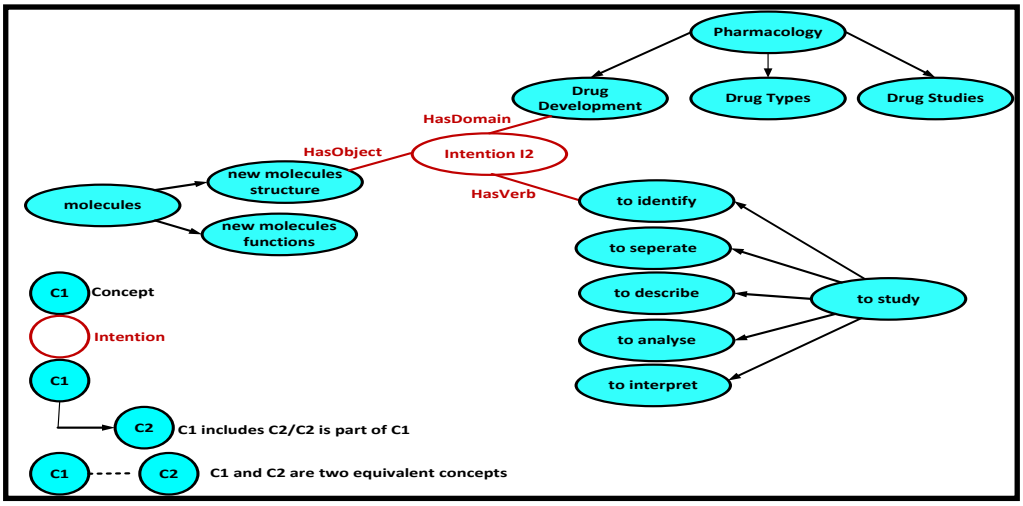

Figure B.1: Extract of the capacity ontology of the Process Chunk VPC1-1

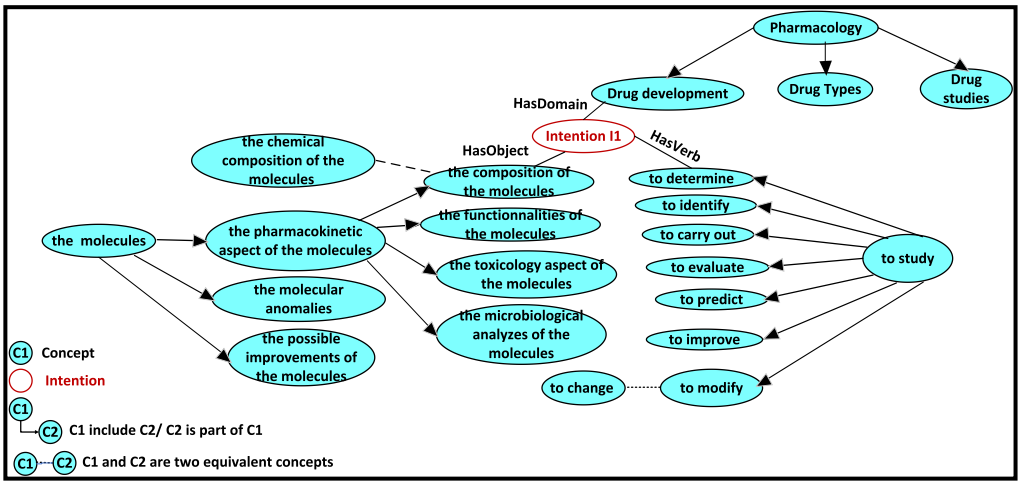

Figure B.2: Extract of the capacity ontology of the Process Chunk VPC3-1

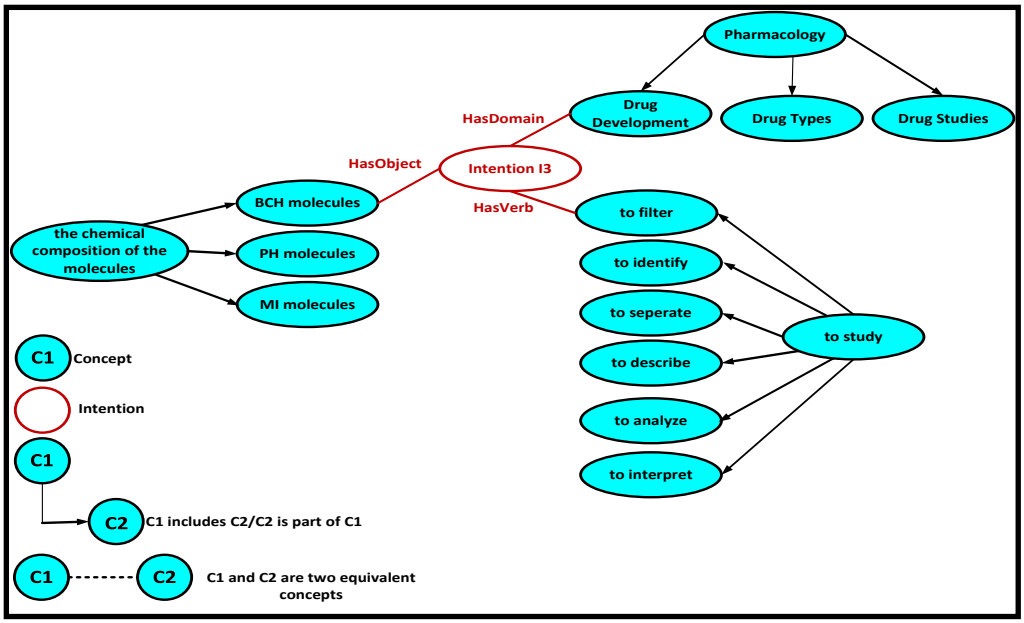

Figure B.3: Extract of the capacity ontology of the Process Chunk VPC4-1

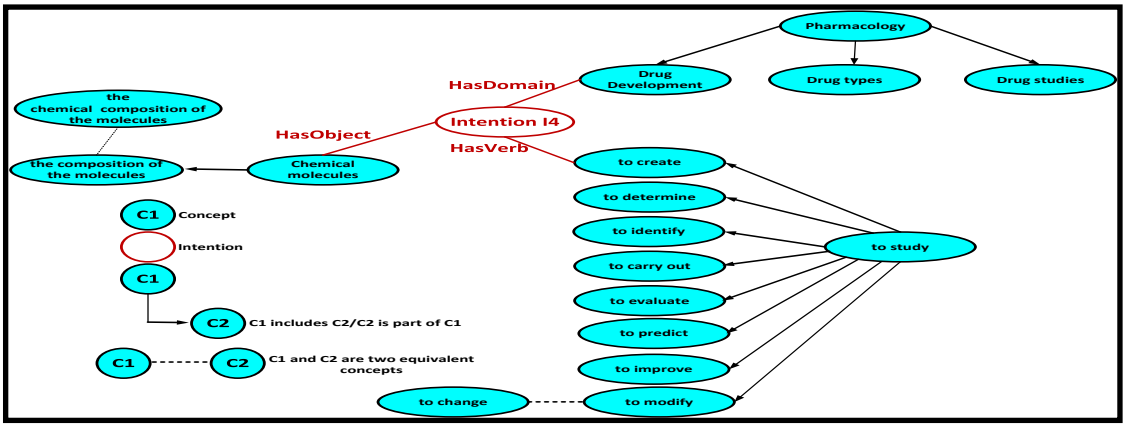

Figure B.4: Extract of the capacity ontology of the Process Chunk VPC6-1

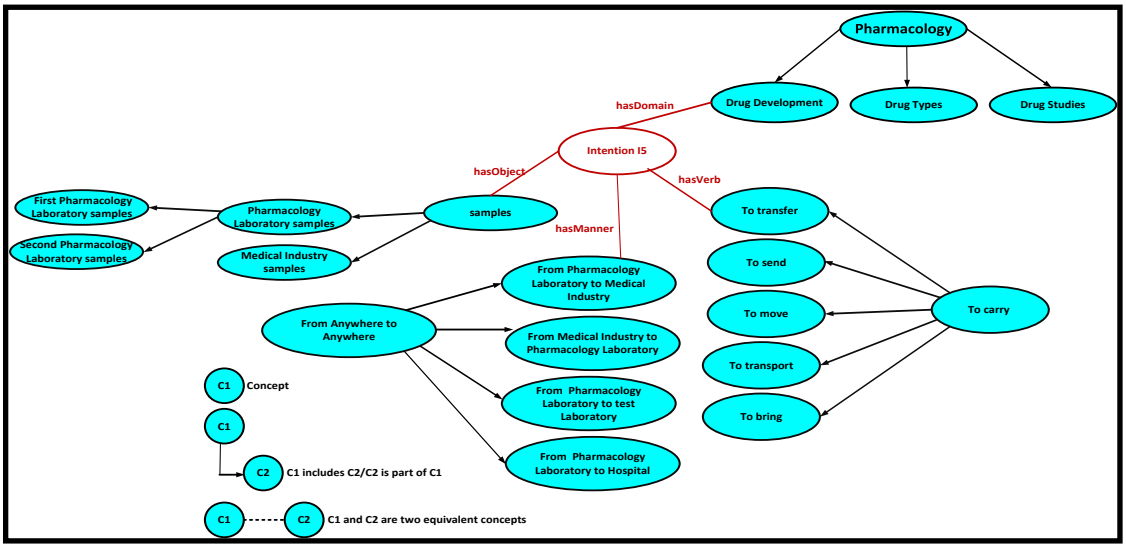

Figure B.5: Extract of the capacity ontology of the Process Chunk VPC7-1

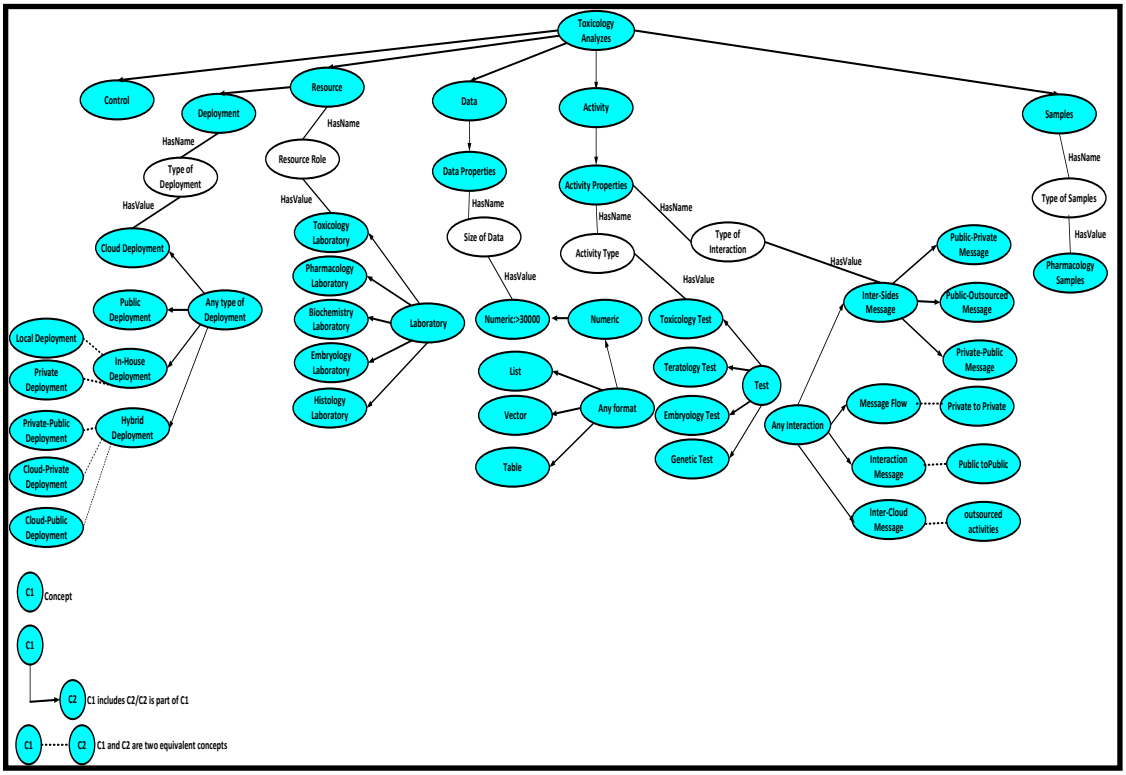

Figure B.6: Extract of the capacity ontology of the Process Chunk VPC8-1

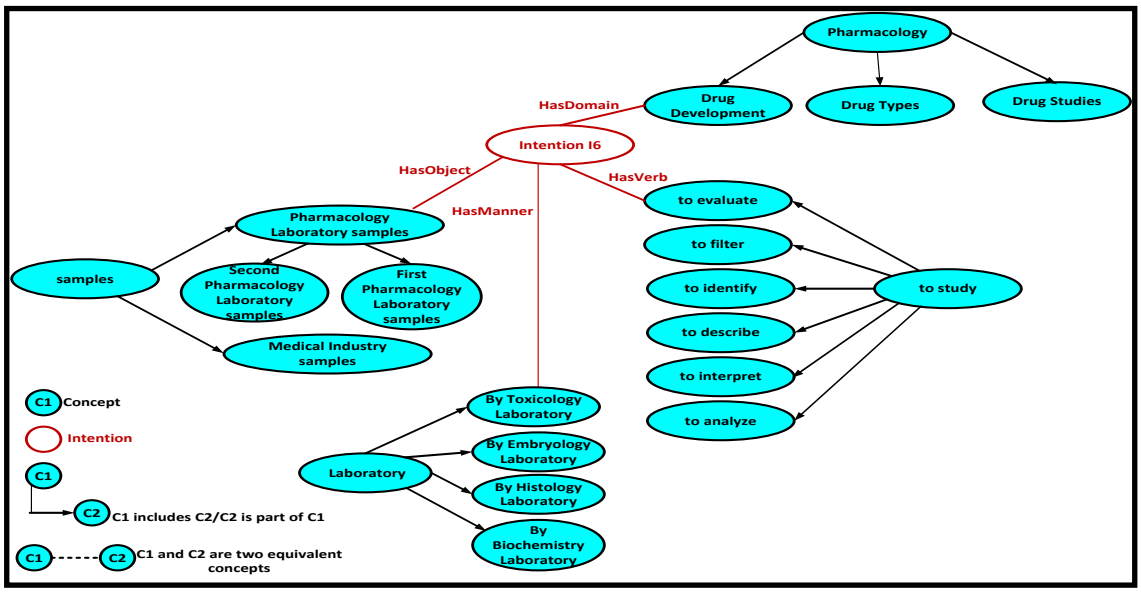

Figure B.7: Extract of the capacity ontology of the Process Chunk VPC9-1

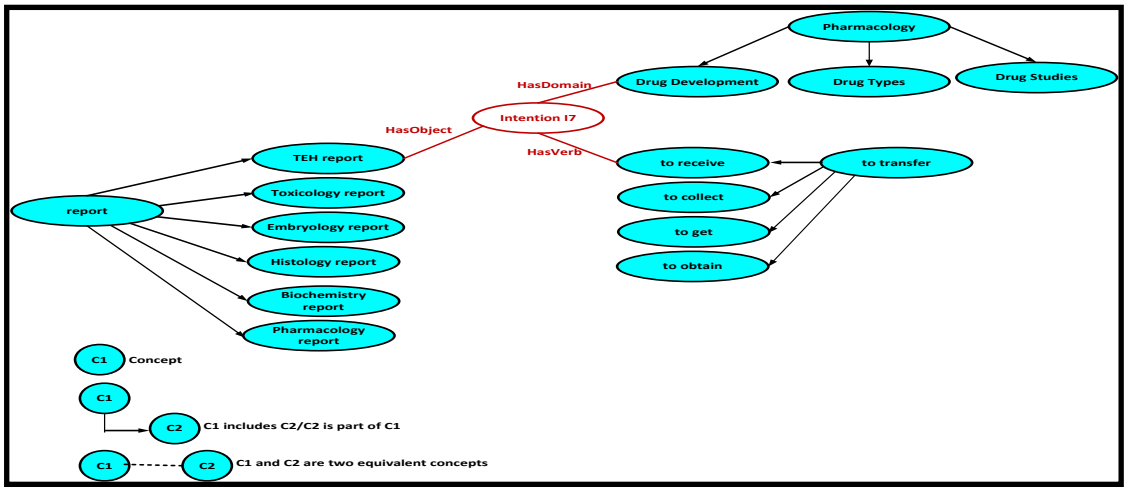

Figure B.8: Extract of the capacity ontology of the Process Chunk VPC11-1

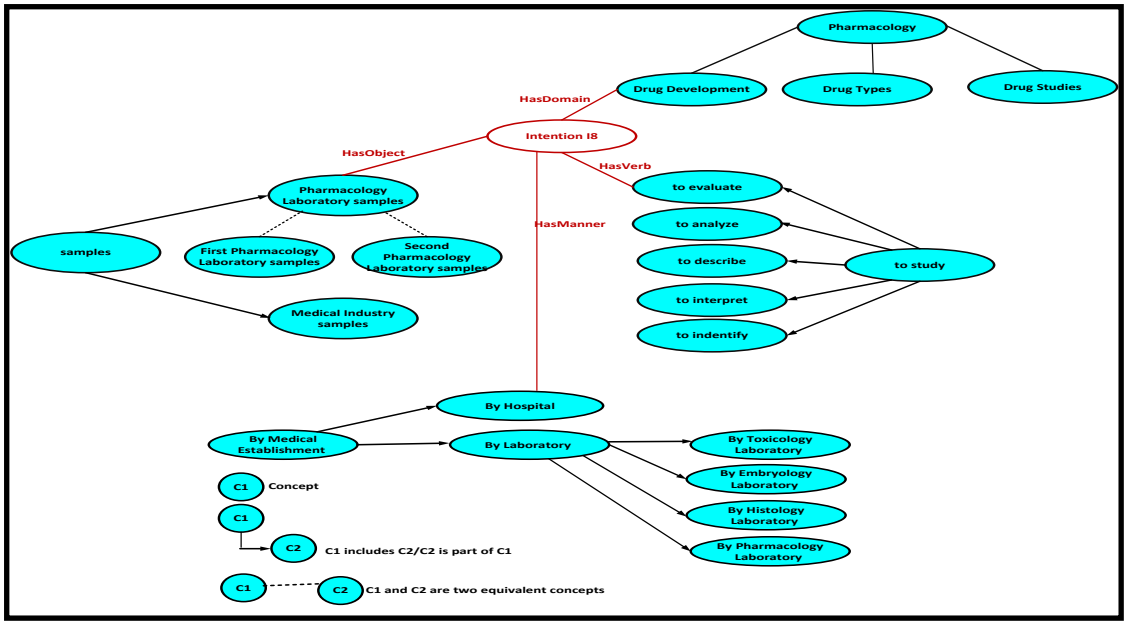

Figure B.9: Extract of the capacity ontology of the Process Chunk VPC12-1

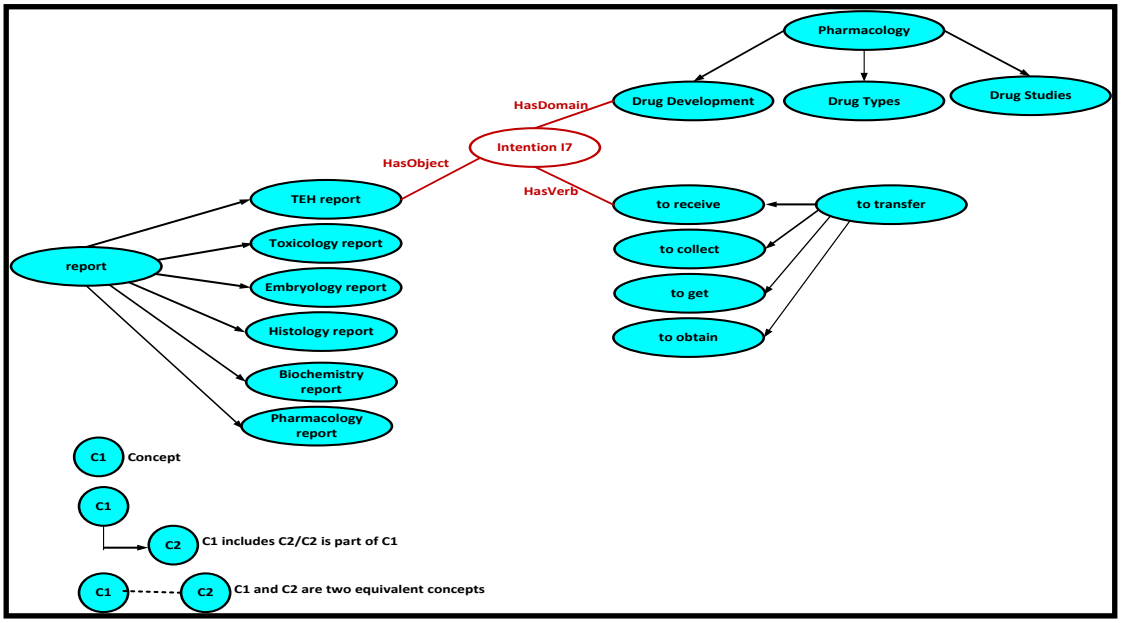

Figure B.10: Extract of the capacity ontology of the Process Chunk VPC13-1

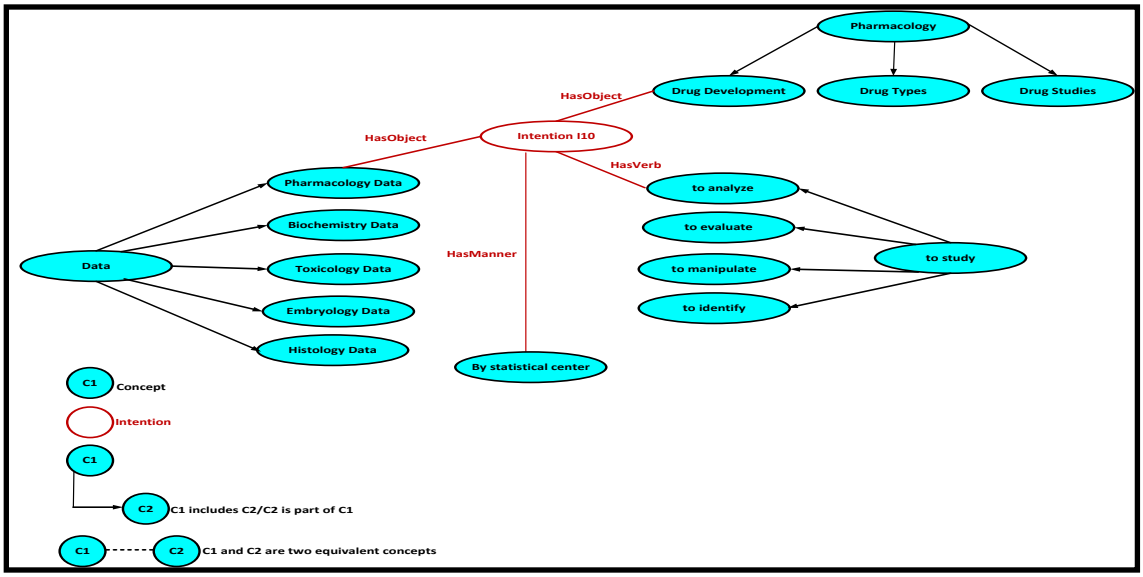

Figure B.11: Extract of the capacity ontology of the Process Chunk VPC14-1

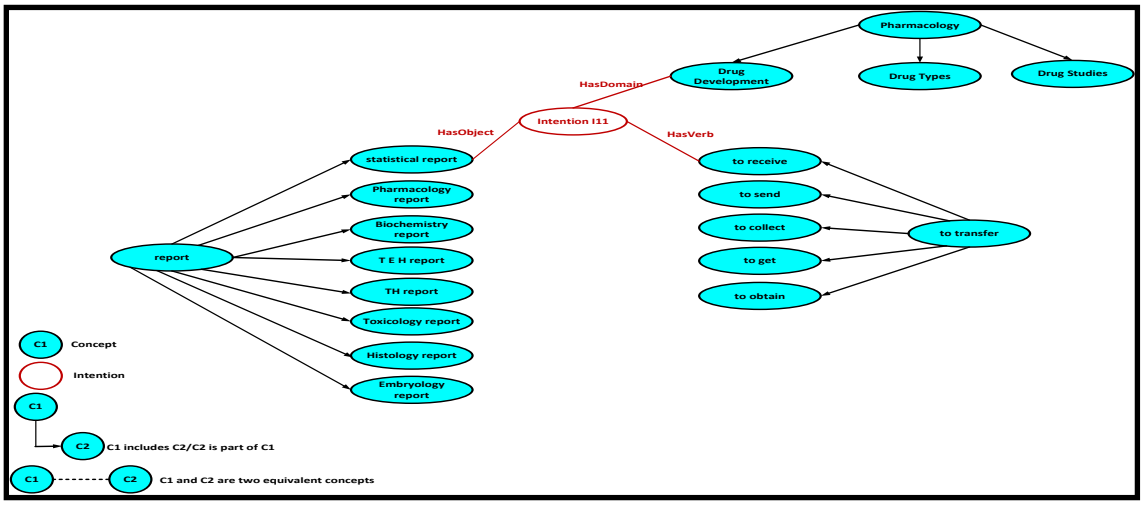

Figure B.12: Extract of the capacity ontology of the Process Chunk VPC15-1

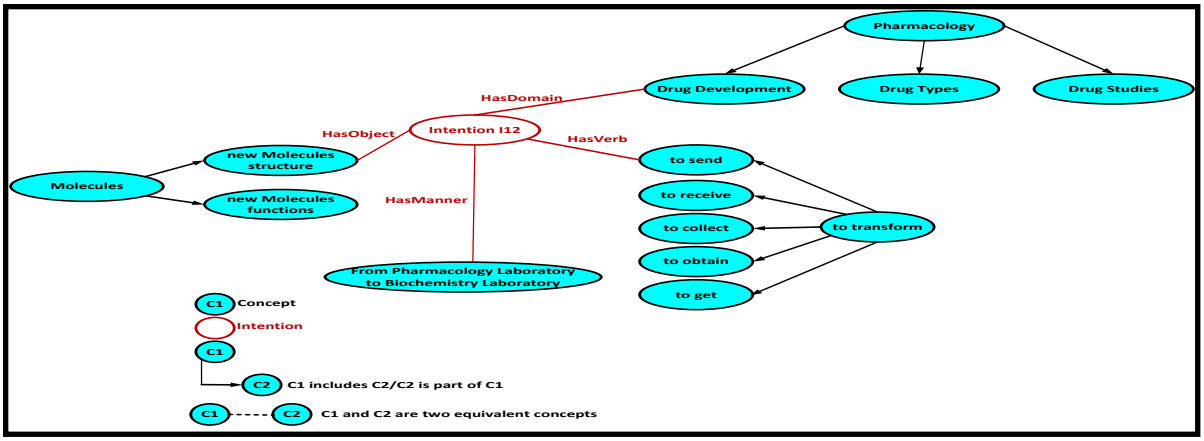

Figure B.13: Extract of the capacity ontology of the Process Chunk VPC1-2

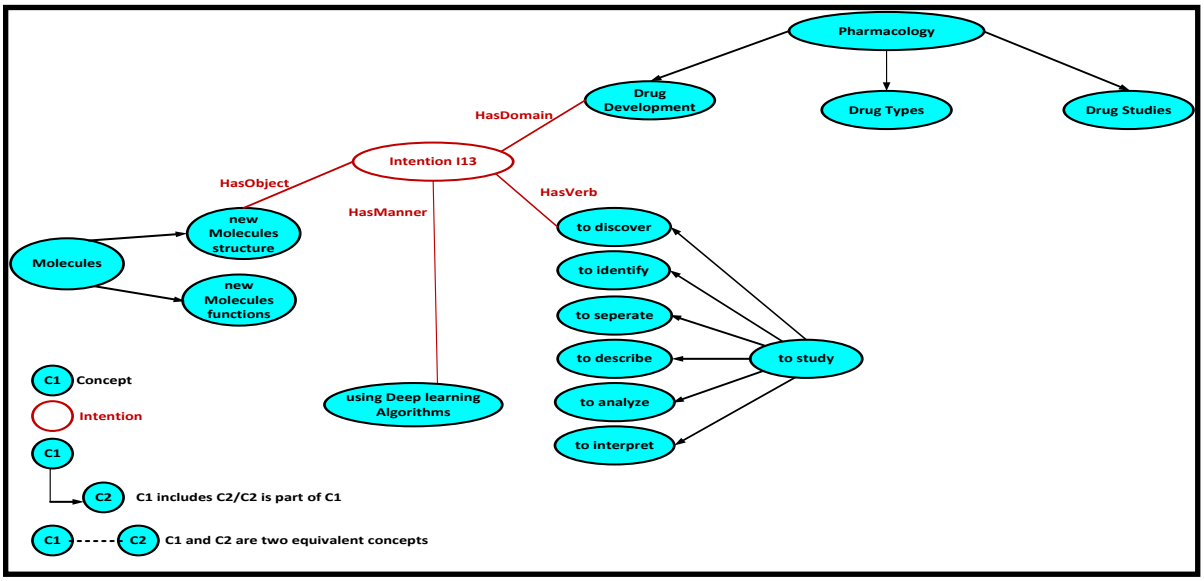

Figure B.14: Extract of the capacity ontology of the Process Chunk VPC2-2

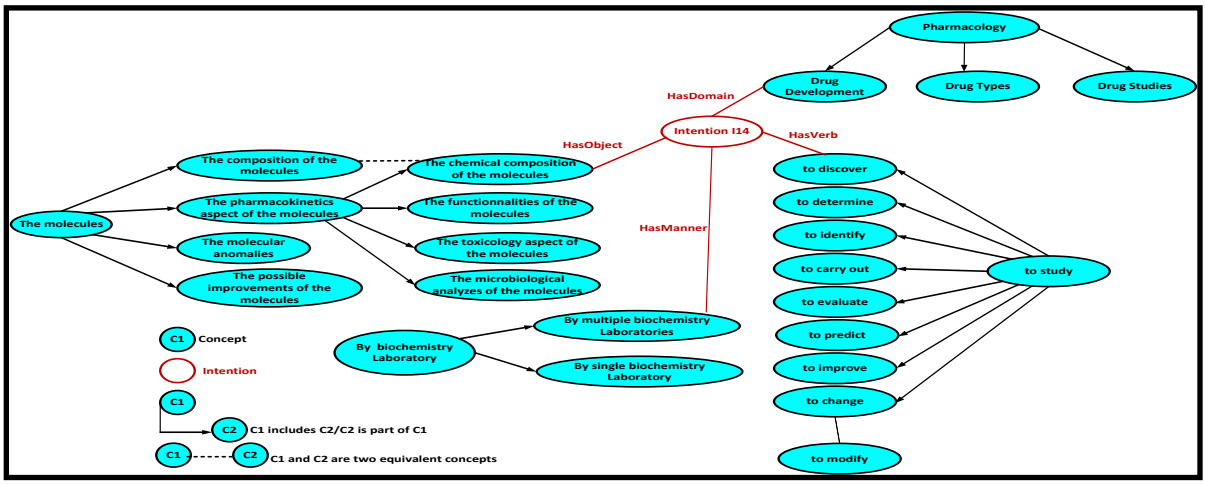

Figure B.15: Extract of the capacity ontology of the Process Chunk VPC3-2

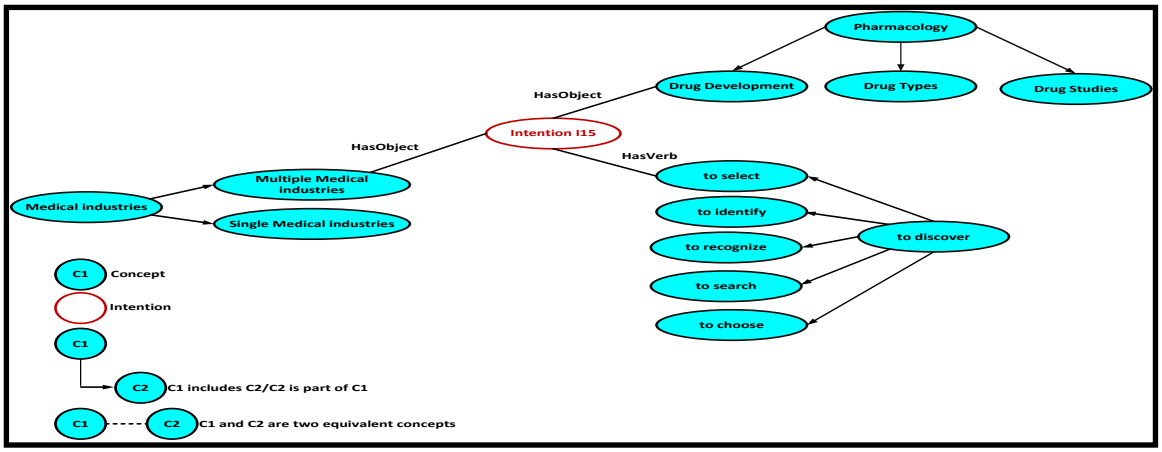

Figure B.16: Extract of the capacity ontology of the Process Chunk VPC4-2

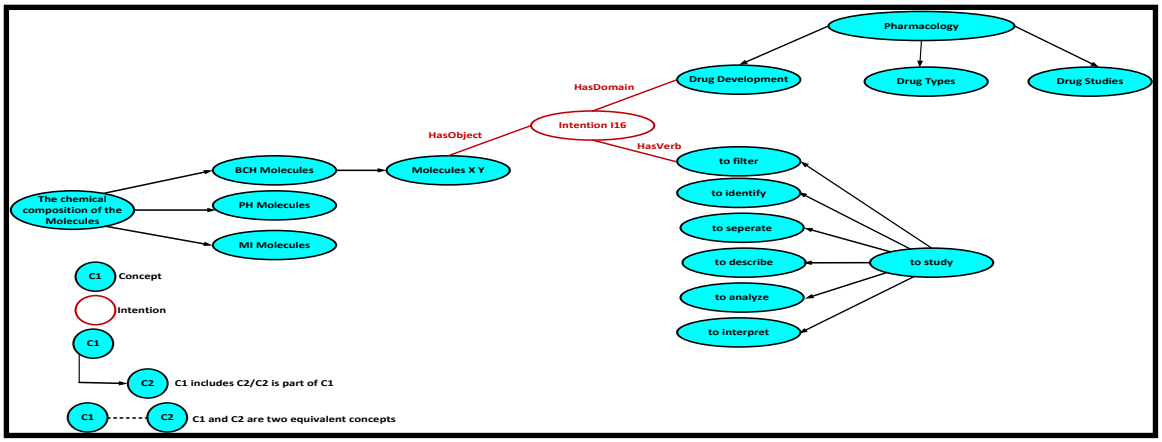

Figure B.17: Extract of the capacity ontology of the Process Chunk VPC5-2

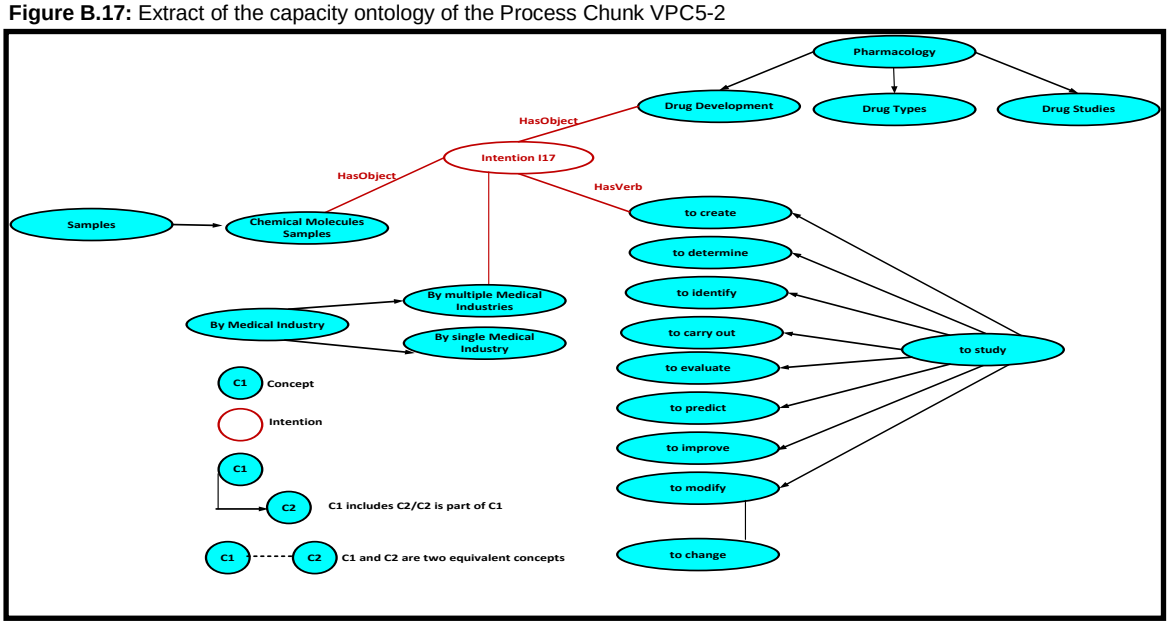

Figure B.18: Extract of the capacity ontology of the Process Chunk VPC6-2

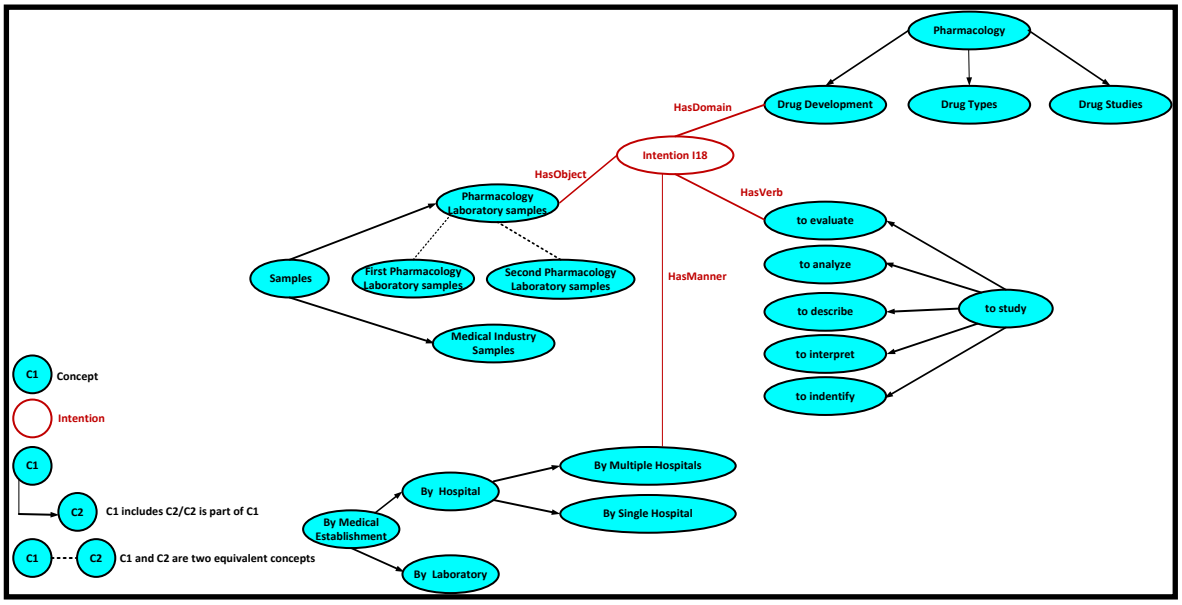

Figure B.19: Extract of the capacity ontology of the Process Chunk VPC12-2

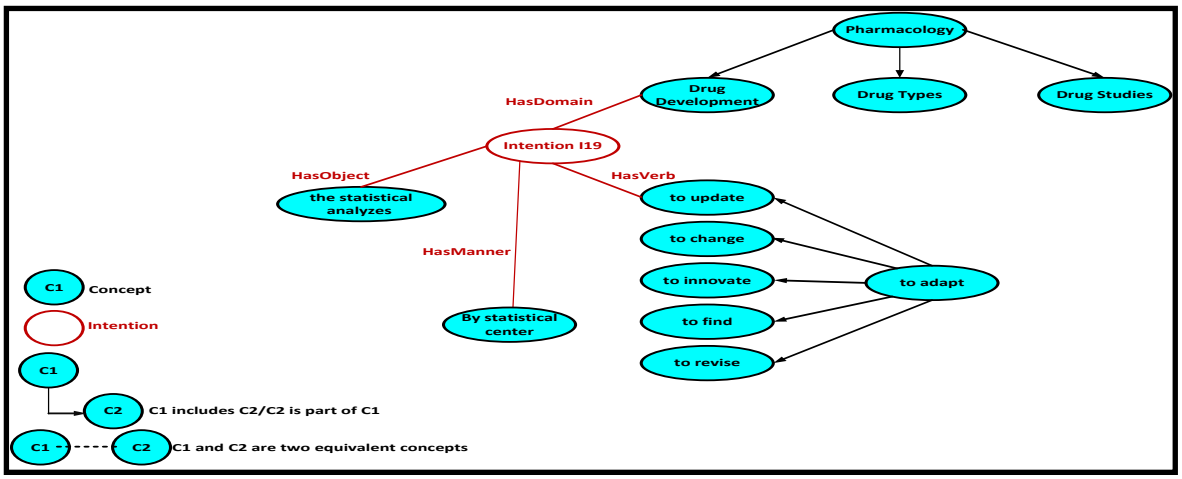

Figure B.20: Extract of the capacity ontology of the Process Chunk VPC14-2

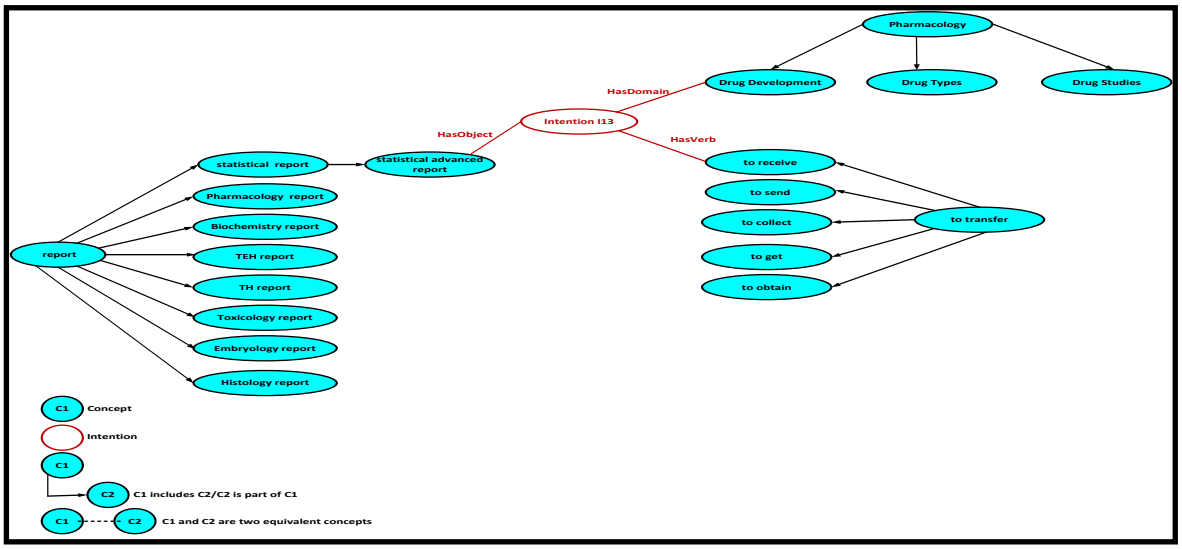

Figure B.21: Extract of the capacity ontology of the Process Chunk VPC15-2

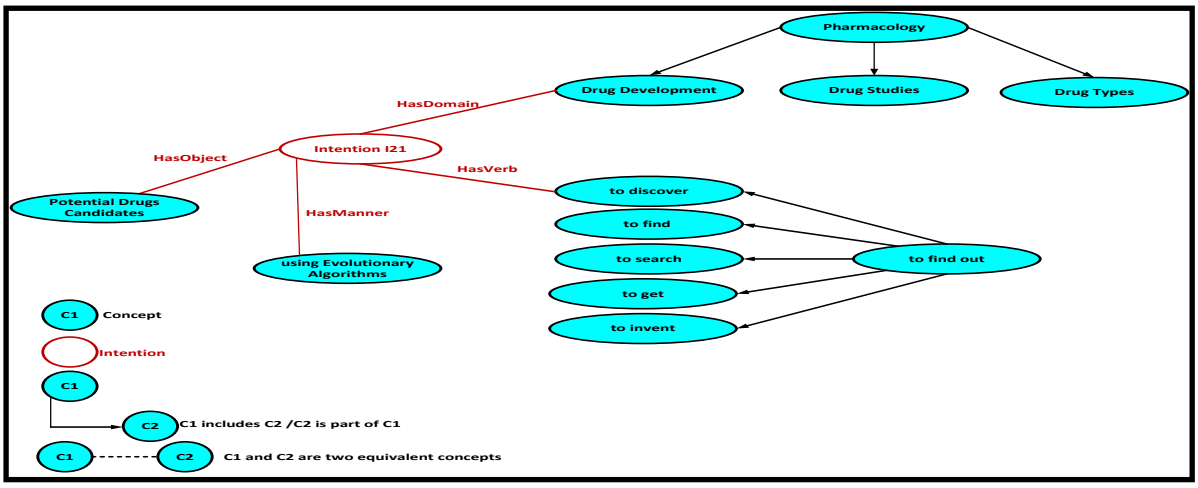

Figure B.22: Extract of the capacity ontology of the Process Chunk VPC1-3

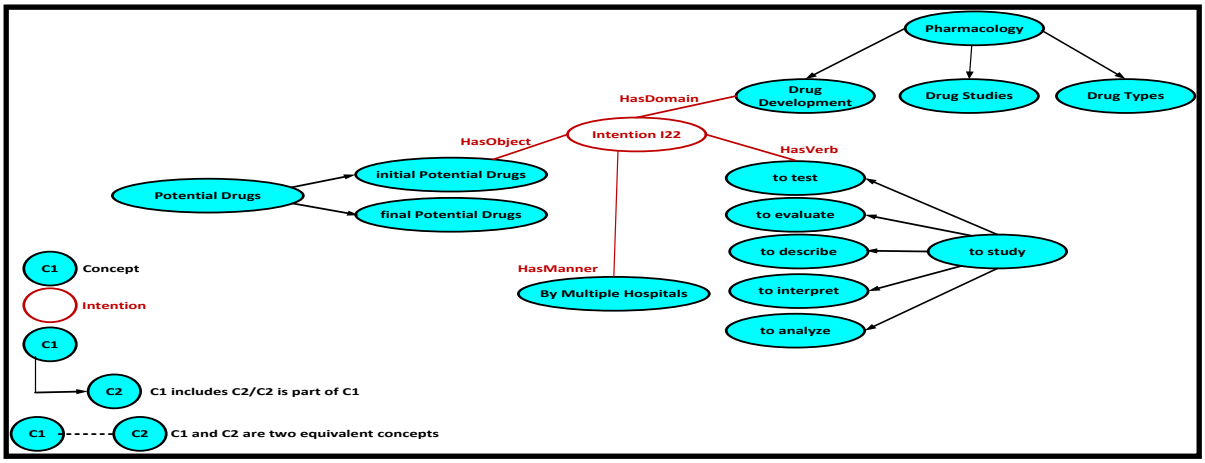

Figure B.23: Extract of the capacity ontology of the Process Chunk VPC12-3

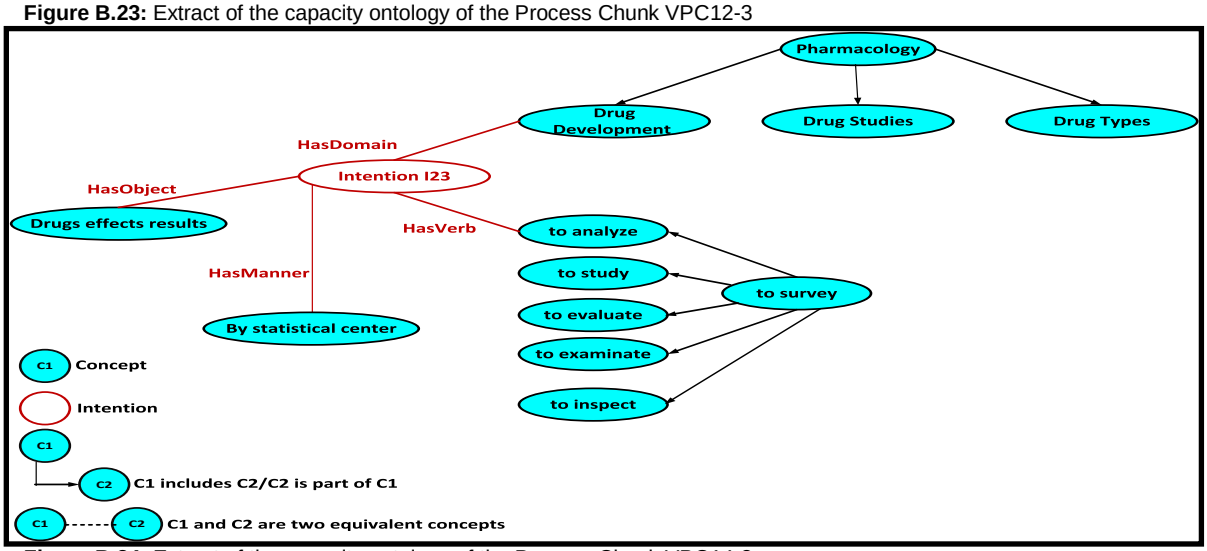

Figure B.24: Extract of the capacity ontology of the Process Chunk VPC14-3

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

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)^Molecules(?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_Samples	Create_Activity(?p)^Samples(?p)^Molecules(?p)^Deployment(?p)^Data_Properties (?p)^Activity_Properties(?p)^Security(?p)-> Medical Industry Samples(?p)
Pharmacology_ Laboratory_ Samples	Receive/Send _Activity(?p)^ 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)^Teratology_test(?p)^ Inter-Sides_Message(?p)-> Teratology_ Analyzes(?p)
Mutagenicity _ Analyzes	Deployment(?p) ^Cloud_Deployment(?p) ^Resource(?p) ^ 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 _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) -> Statistical _Analysis(?p)
Statistical _report	Resource(?p)^ 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

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)
BCH_ screening	Deployment(?p) ^ 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)^

	Samples(?p)^ Numeric:>=300000(?p)^ Deployment(?p)^ Cloud_ Deployment(?p)^ Data_ Properties(?p)^ Chemical _Molecules(?p)^ Chemical_ Molecules_Samples(?p)^ Activity_ Properties(?p)^ Response _Time:<=20(?p)^ Molecules(?p)^ Chemical _Molecules(?p)^ Cost :<=900(?p)^ Resource (?p)^ Multiple _Medical _Samples(?p)-> Medical_ Industry_ Samples (?p)
Human_patient_ Test	HP _advanced _test(?p)^ Multiples _Hospitals(?p)^ Resource(?p)^ Activity _Properties(?p)^ Inter-Cloud _Message(?p)^ Data_ Properties(?p)^ Pharmacology _samples(?p)^ HT _ advanced _report(?p)^ Numeric:>=600000(?p)^ Deployment(?p)^ Cloud _Deployment(?p)-> Human _patient _Test(?p)
Statistical_ Analysis	Statistical _center_ report (?p)^ Resource(?p)^ Statistical _center(?p)^ Data(?p) ^ Data_ Properties (?p)^ data sets :>=100000(?p)^ HT_ advanced _report(?p)^ Multiple_ Statistical_ reports(?p)^ Amazon EC2(?p)^ Deployment(?p)^ Cloud _Deployment(?p)^ Activity _Properties(?p)^ To _analyze_ Data(?p)^ Security(?p)^ Confidentiality(?p)-> Statistical _Analysis(?p)
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)^ Activity_ Properties(?p)^ Receive _Activity(?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) 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

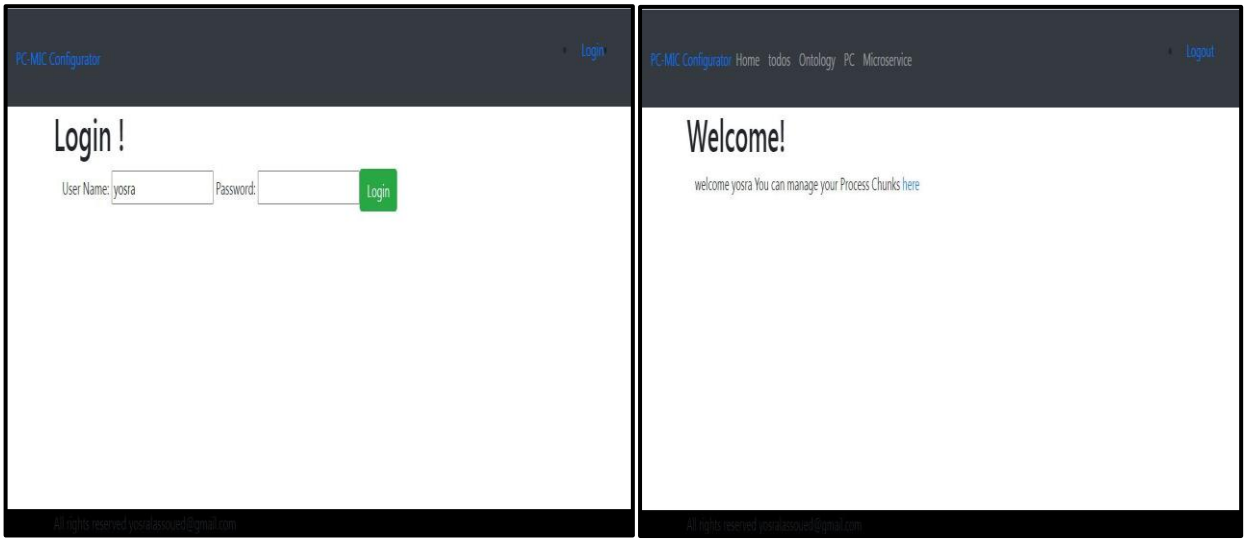

Figure C.1: PC-MIC Configurator Login Page

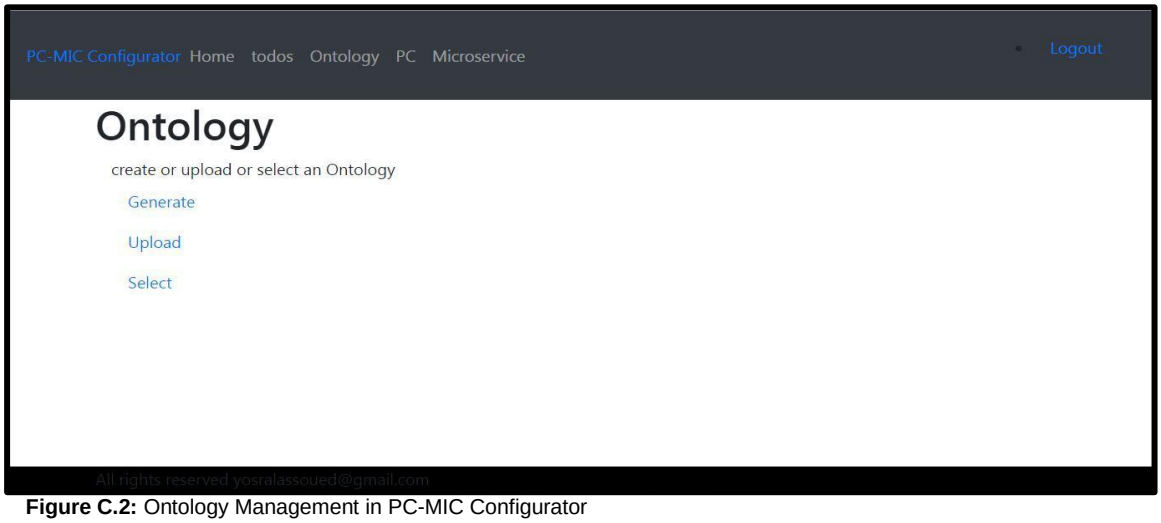

Figure C.2: Ontology Management in PC-MIC Configurator

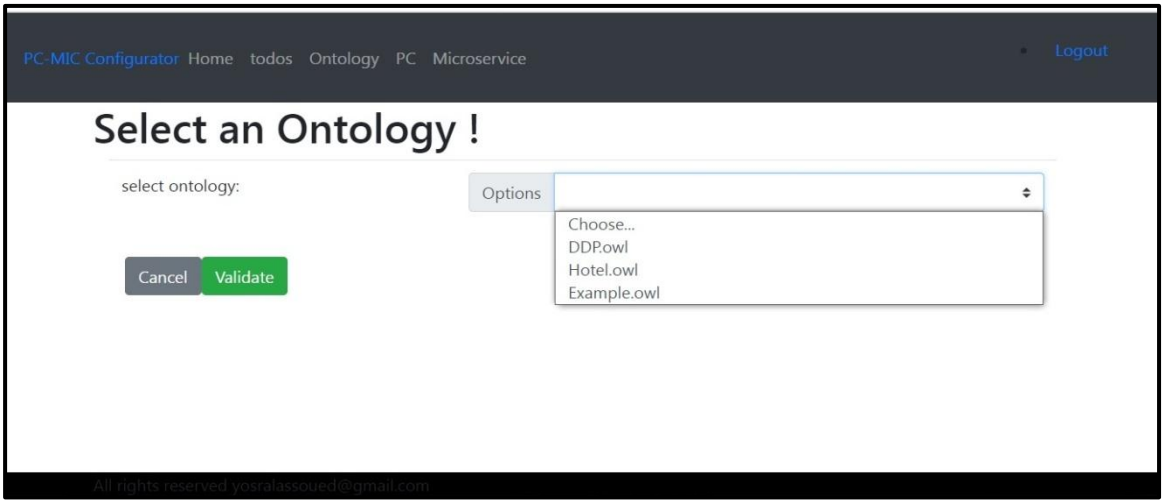

Figure C.3: Ontology Select in PC-MIC Configurator

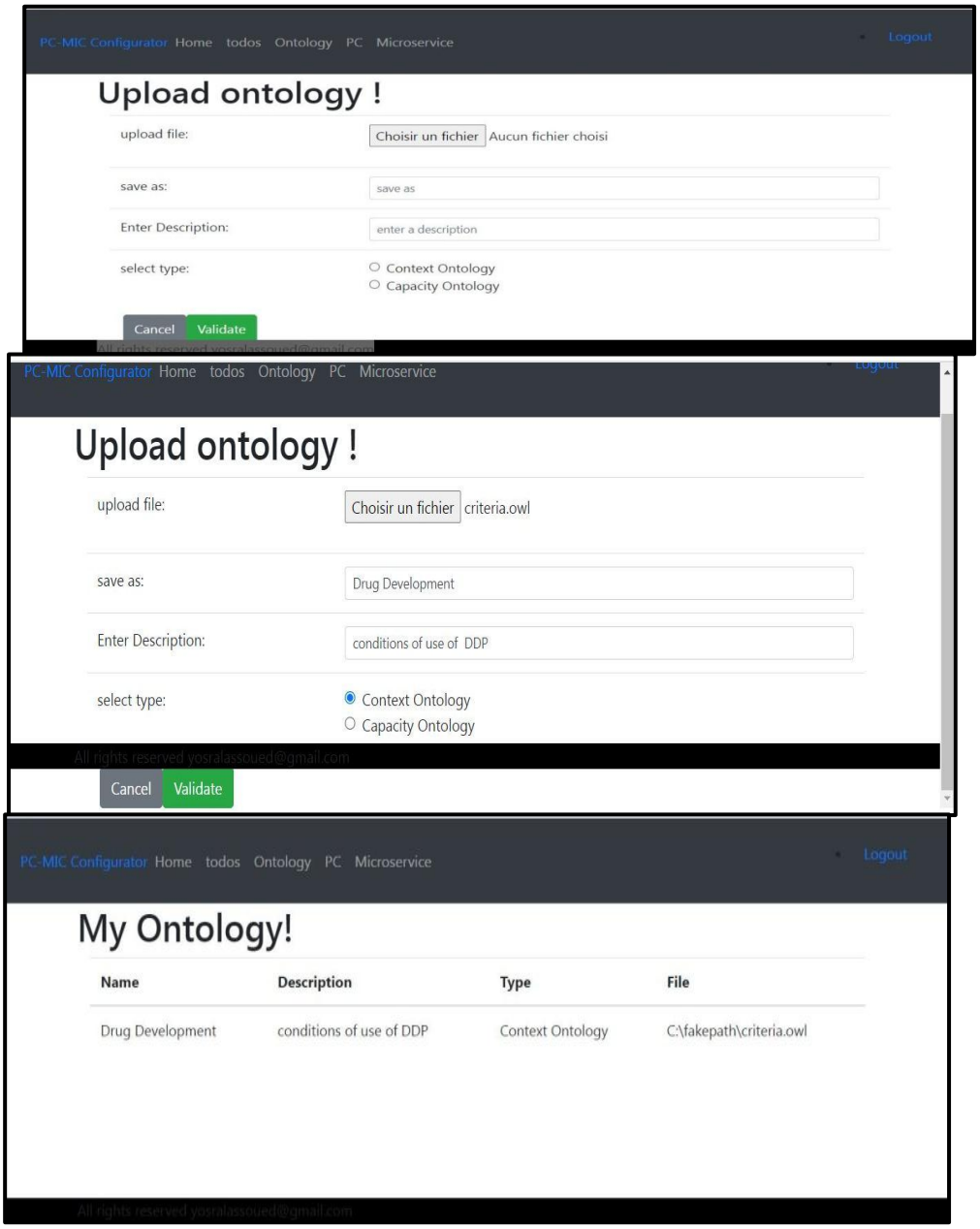

Figure C.4: Upload Ontology in PC-MIC Configurator

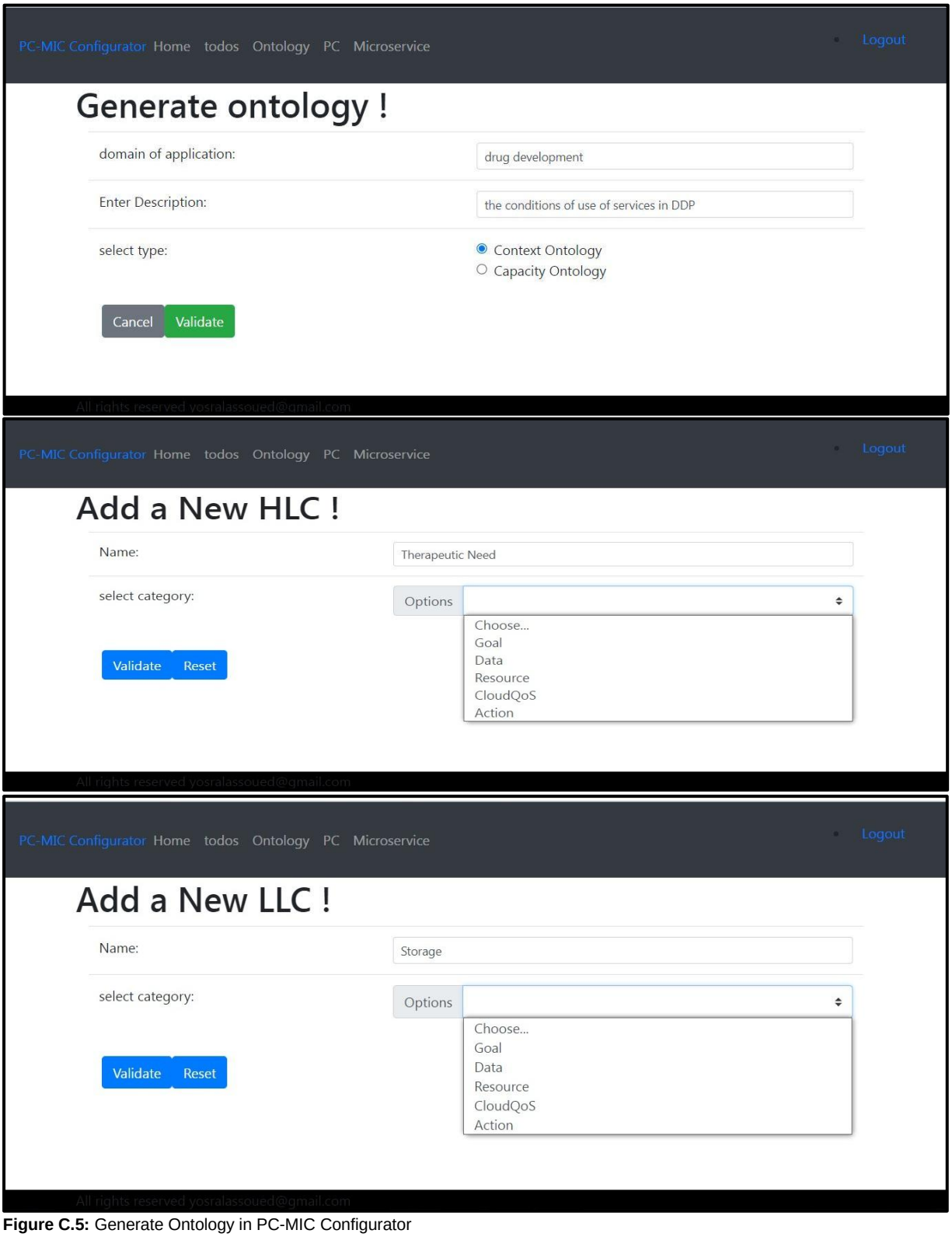

Figure C.5: Generate Ontology in PC-MIC Configurator

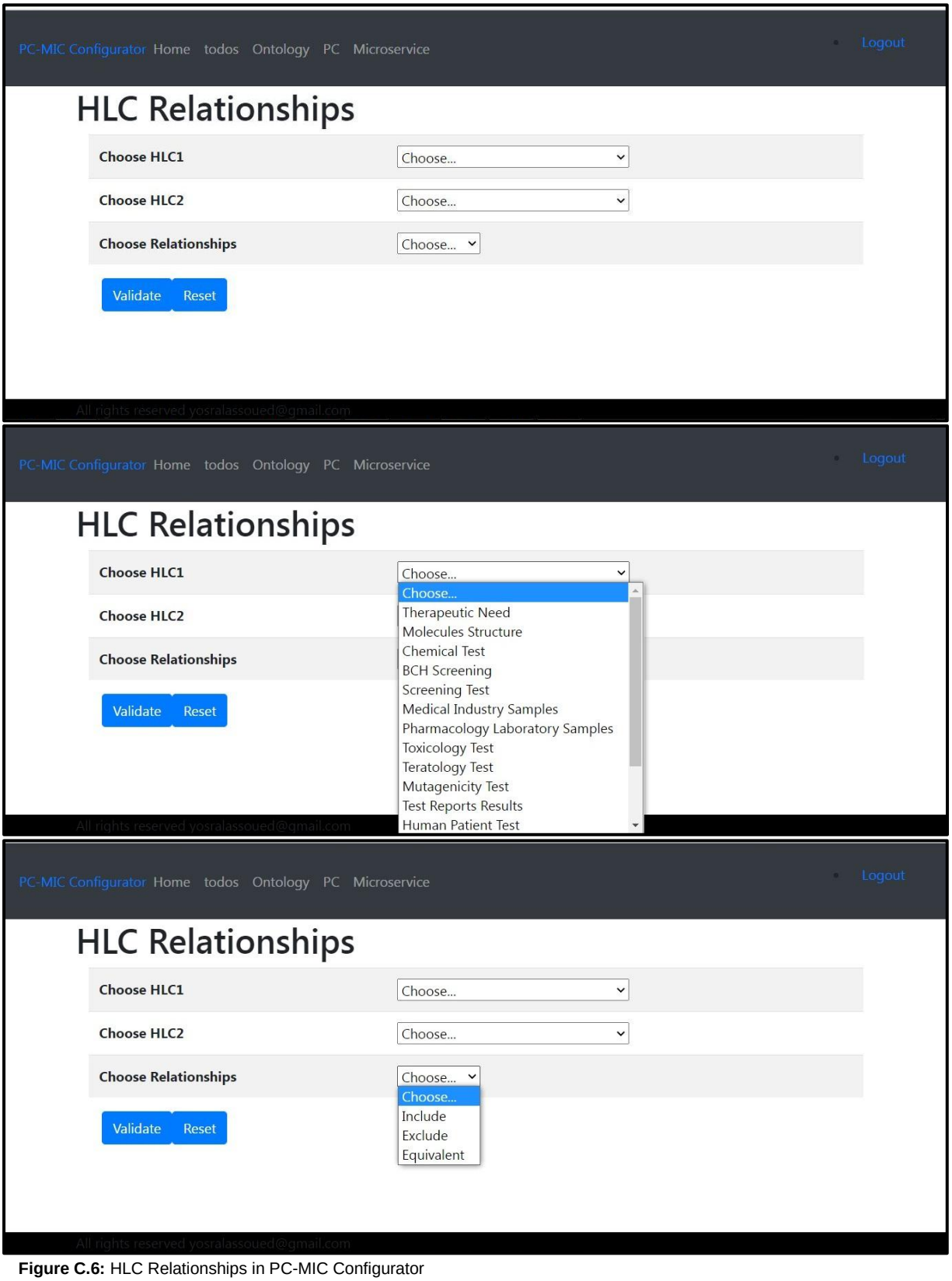

Figure C.6: HLC Relationships in PC-MIC Configurator

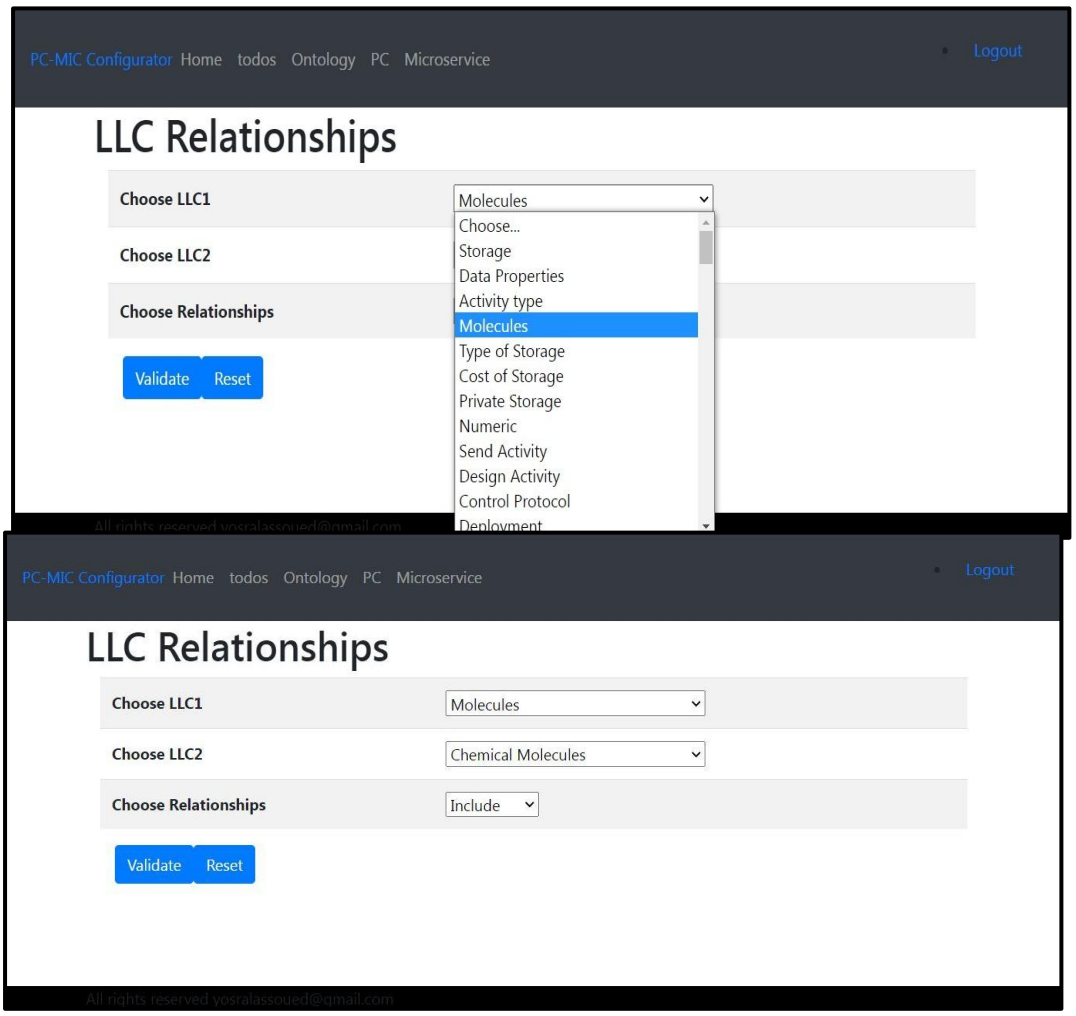

Figure C.7: LLC Relationships in PC-MIC Configurator

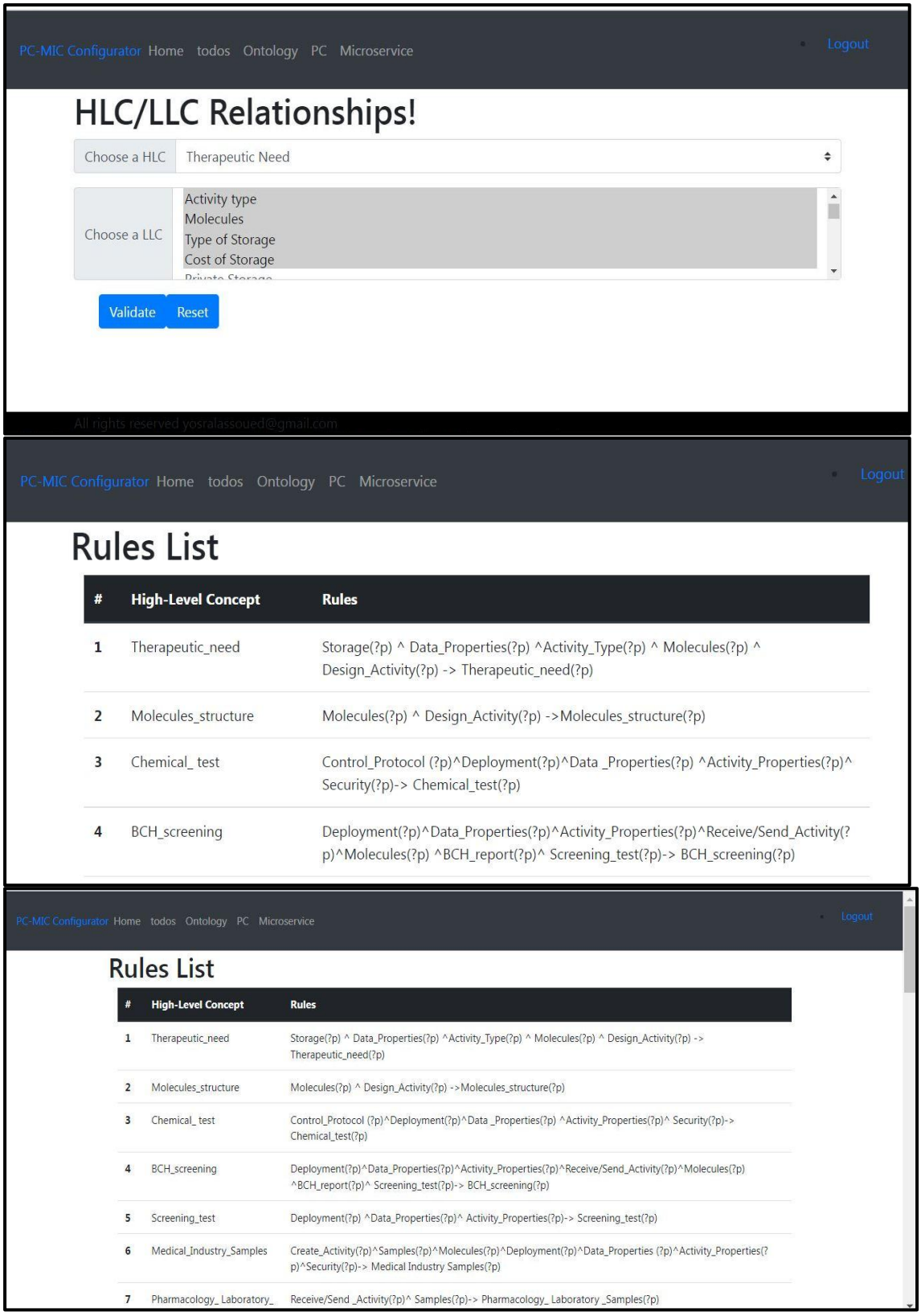

Figure C.8: SWRL Rules in PC-MIC Configurator