Moduł 10
Przypadek użycia 1
Biochemiczne badania: BRENDA

iBigWorld:
Innovations for Big Data in a Real World

UBB team

iBigWorld:2020-1-PL01-KA203-082197

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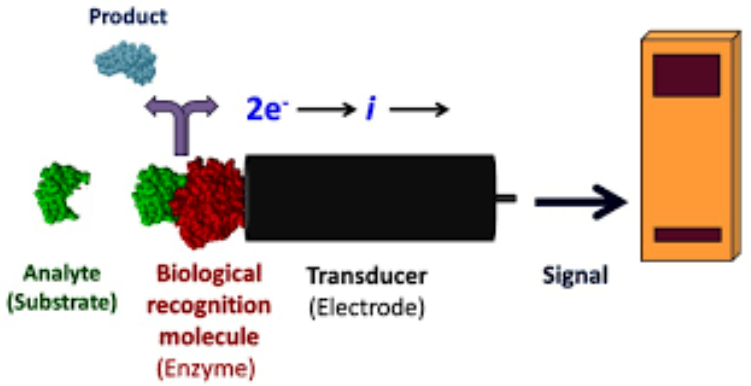
Budowa biochemicznego sensora

- Reakcje biochemiczne obejmują enzymy, substraty (aktywatory) i substancje hamujące.
- Kalibracja biosensorów wymaga przewidywania kinetyki reakcji za pomocą modeli, które należy opracować za pomocą różnych metod Big Data.
- Projekt BRENDA dostarcza nam wielu metadanych uzyskanych w wyniku wcześniejszych badań.



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Projekt biochemicznego sensora

- Analiza danych poprzez eksplorację
  - Cel: Poszukiwanie i przygotowanie danych do opracowania modelu prognozującego oddziaływanie biochemiczne enzym-substrat-inhibitor na podstawie projektu biosensora
  - Kolejne kroki:
    - Akwizycja danych biochemicznych
    - Pobranie danych
    - Agregacja
    - Wizualizacja

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Projekt biochemicznego sensora

- Konwersja bazy w .txt na format SQLite
- # cały kod znajduje się w materiałach
- brenda_file_path = "brenda_download.txt"
- database_path = "brenda.db"

- if os.path.exists(database_path):
- os.remove(database_path)
- conn = sqlite3.connect(database_path)

- brenda_iterator=parse_brenda(brenda_file_path, debug=False)

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Eksploracja danych pod kątem enzymów, substratów i inhibitorów

- Oprogramowanie KNIME może być używane do EDA za pomocą Brenda.db uzyskanego wcześniej jako baza danych SQLite.
- Dane można uzyskać za pomocą kodu EC enzymu za pomocą skonstruowanego w tym celu przepływu pracy

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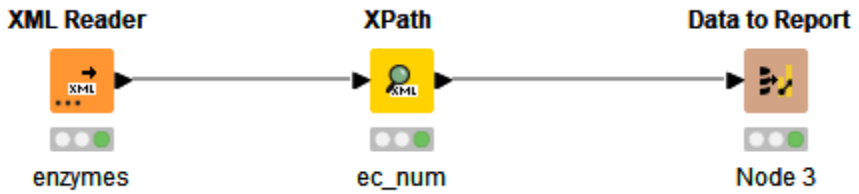
Eksploracja danych XML dla enzymów

Enzymes.xml zawiera metadane do badania enzymów (w tym referencje)

Przepływ pracy EDA dla KNIME (wzorzec)



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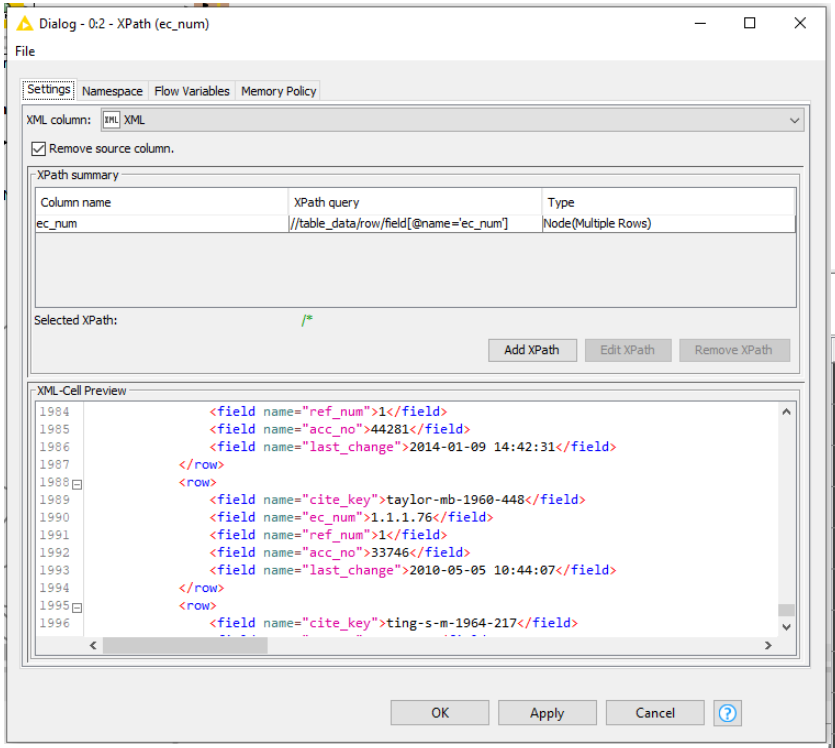
Elementy oparte na strukturze name = “ec_num”



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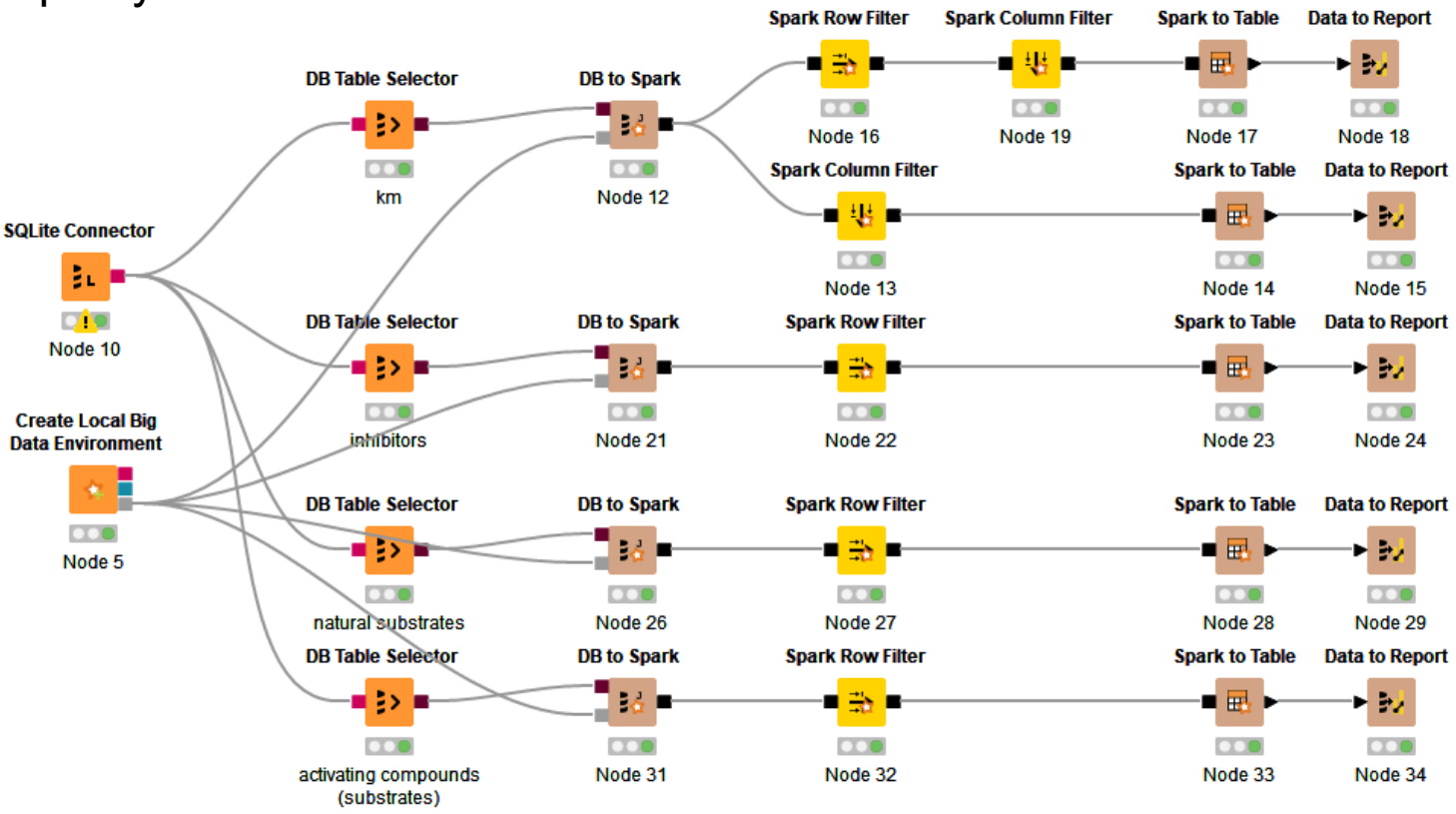
Eksploracja danych pod kątem enzymów, substratów i inhibitorów

Przepływ pracy KNIME dla EDA



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Metabolity dla enzymu z EC=3.1.1.7 (tabela ‘km’)

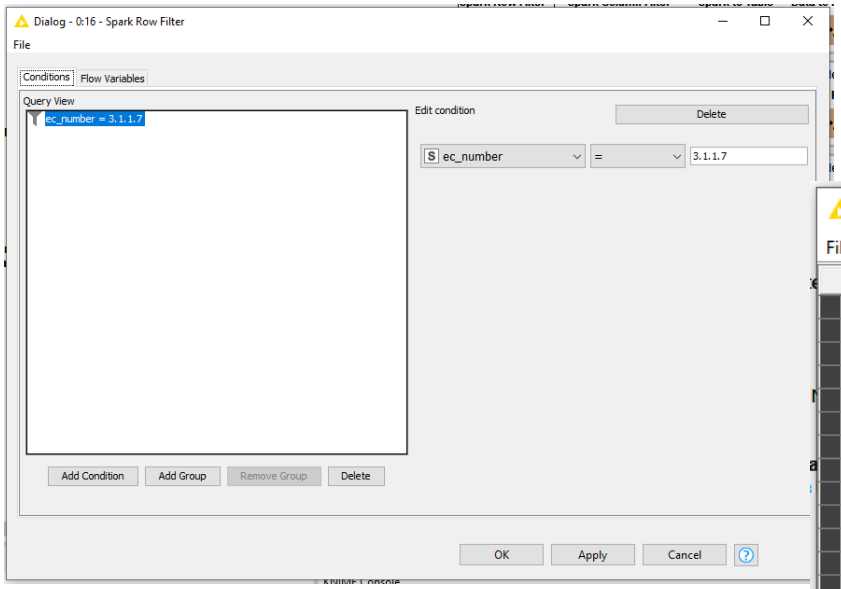

Table View - 0:18 - Data to Report

File Edit Hilite Navigation View

Row ID	ec_num...	km	temper...	ph	metabo...
Row0	3.1.1.7	-999	?	?	more
Row1	3.1.1.7	0.082	?	7.4	acetylthioch...
Row2	3.1.1.7	0.144	?	7.4	acetylthioch...
Row3	3.1.1.7	0.181	?	7.4	acetylthioch...
Row4	3.1.1.7	0.124	?	7.4	acetylthioch...
Row5	3.1.1.7	0.106	?	7.4	acetylthioch...
Row6	3.1.1.7	0.139	?	7.4	acetylthioch...
Row7	3.1.1.7	0.14	?	7.4	acetylthioch...
Row8	3.1.1.7	0.064	25	7.5	acetylthioch...
Row9	3.1.1.7	0.097	25	7.5	butyrylthioc...
Row10	3.1.1.7	0.053	37	7.4	acetylthioch...
Row11	3.1.1.7	2.24	?	8	propionylthi...
Row12	3.1.1.7	4.23	?	8	butyrylthioc...
Row13	3.1.1.7	0.67	30	7.5	butylthiocho...
Row14	3.1.1.7	0.85	30	7.5	propylthioch...
Row15	3.1.1.7	2.18	30	7.5	acetylthioch...
Row16	3.1.1.7	2.45	30	7.5	methylthioc...
Row17	3.1.1.7	0.93	30	7.5	propylthioch...
Row18	3.1.1.7	2.23	30	7.5	methylthioc...
Row19	3.1.1.7	2.28	30	7.5	acetylthioch...
Row20	3.1.1.7	1.69	30	7.5	butylthiocho...
Row21	3.1.1.7	0.769	25	7.4	Acetylcholine
Row22	3.1.1.7	4.7	?	?	butyrylthioc...
Row23	3.1.1.7	0.42	?	8	acetylthioch...
Row24	3.1.1.7	1.02	?	8	propionylthi...

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Inhibitory enzymu z EC=3.1.1.8 (tabela ‘inhibitors’)

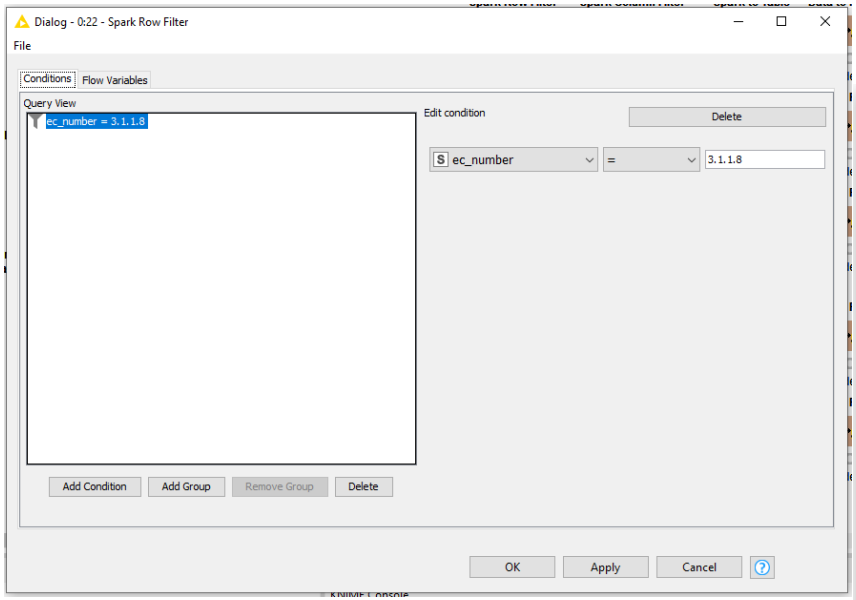

Table View - 0:24 - Data to Report

File Edit Hilite Navigation View

Row ID	entry	ec_num...	comment	inhibitor
Row0	0	3.1.1.8	?	N,N,N',N'-tetramethyl-1,6-hexane diamine
Row1	1	3.1.1.8	#1# compet...	tetrabutylammonium
Row2	2	3.1.1.8	#10# irreve...	physostigmine
Row3	3	3.1.1.8	#1# 0.1 mM...	ethopropazine hydrochloride
Row4	4	3.1.1.8	#1,36# iso ...	tetraisopropyl phosphoramide
Row5	5	3.1.1.8	?	NaCl
Row6	6	3.1.1.8	?	p-chloromercuribenzoate
Row7	7	3.1.1.8	?	iodoacetic acid
Row8	8	3.1.1.8	?	AgNO3
Row9	9	3.1.1.8	#10# comp...	atropine
Row10	10	3.1.1.8	#10# comp...	Scopolamine
Row11	11	3.1.1.8	#10# comp...	procaine
Row12	12	3.1.1.8	#10# comp...	homatropine
Row13	13	3.1.1.8	?	testosterone
Row14	14	3.1.1.8	?	methylene blue
Row15	15	3.1.1.8	?	Cycloartenol
Row16	16	3.1.1.8	#16# rever...	lovastatin
Row17	17	3.1.1.8	#16# rever...	simvastatin
Row18	18	3.1.1.8	#16# rever...	diazepam
Row19	19	3.1.1.8	?	hydralazine
Row20	20	3.1.1.8	?	p-hydroxybenzoic acid
Row21	21	3.1.1.8	#16# rever...	nifedipine
Row22	22	3.1.1.8	?	acacetin
Row23	23	3.1.1.8	?	palmatine
Row24	24	3.1.1.8	?	Jatrorrhizine

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Substraty dla enzymu z EC=3.1.1.8 (tabela ‘activating_compounds’)

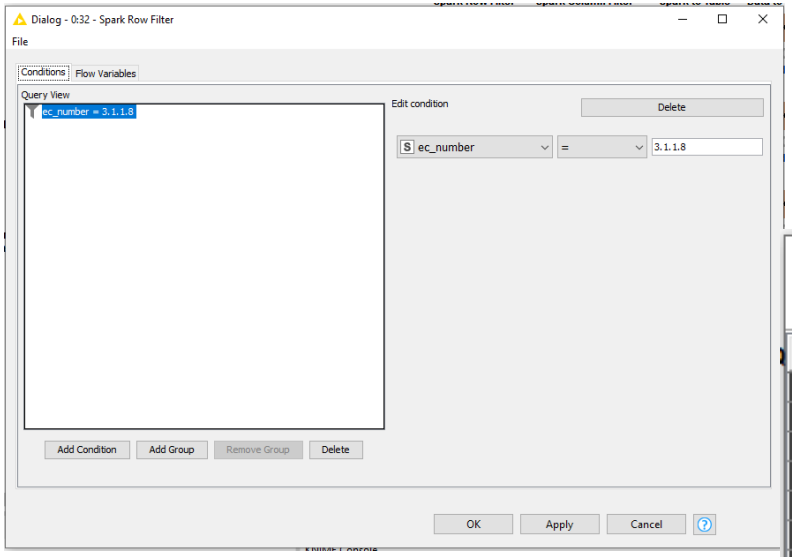

Table View - 0:34 - Data to Report

File Edit Hilite Navigation View

Row ID	entry	ec_num...	comment	activator
Row0	0	3.1.1.8	#1# 20 mM, 140% activity <14>	citrate
Row1	1	3.1.1.8	#16# nonessential activator <...	2-trimethylsi...
Row2	2	3.1.1.8	#16# substrate activation, ess...	3,3-dimethyl...
Row3	3	3.1.1.8	#16# i.e. TNT, a nonessential ...	2,4,6-trinitr...
Row4	4	3.1.1.8	#16# activating effect at acidic...	2,6-dichloro...
Row5	5	3.1.1.8	#16# activating effect at acidic...	indophenyl ...
Row6	6	3.1.1.8	#26# activating effect at acidic...	indophenyla...
Row7	7	3.1.1.8	#26# activating effect at acidic...	2,6-dichloro...
Row8	8	3.1.1.8	#5# non-substrate activation ...	homocystein...
Row9	9	3.1.1.8	#5# substrate activation, over...	Butyrylcholine
Row10	10	3.1.1.8	#5# activation kinetics and mo...	more
Row11	11	3.1.1.8	?	acetylthioch...
Row12	12	3.1.1.8	?	butyrylthioc...
Row13	13	3.1.1.8	?	propionylthi...

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Reakcja formuły dla EC=3.1.1.8 (tabela ‘natural_substrates’)

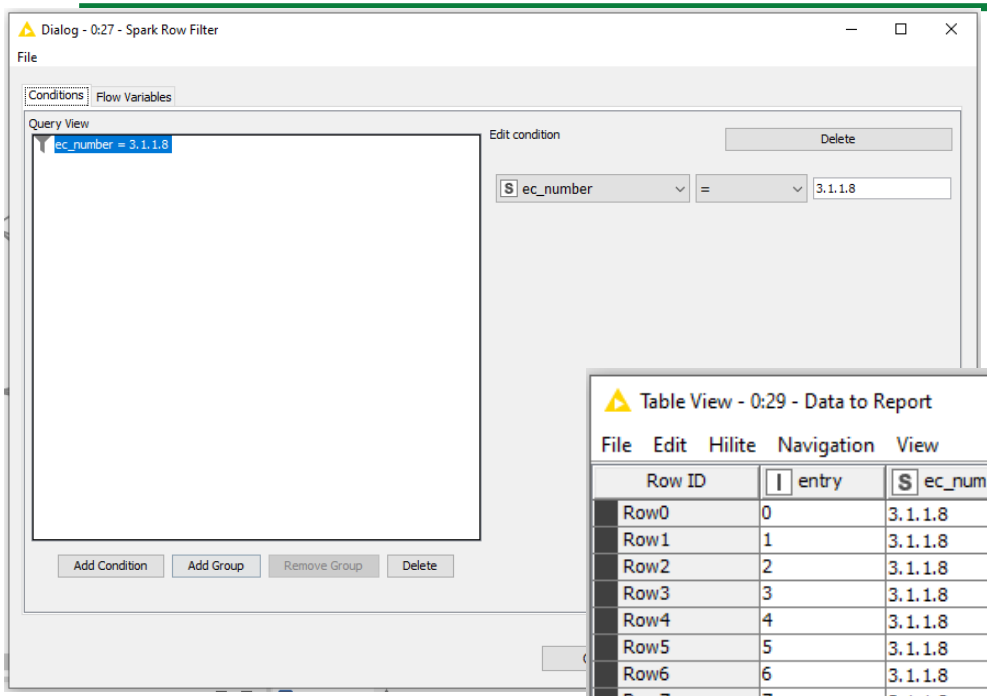

Table View - 0:29 - Data to Report

File Edit Hilite Navigation View

Row ID	entry	ec_num...	comment	reactio...	reaction_formula	reversible
Row0	0	3.1.1.8	?	?	acetylcholine + H2O = choline + acetate	?
Row1	1	3.1.1.8	?	?	acetylthiocholine + H2O = thiocholine ...	?
Row2	2	3.1.1.8	?	?	propionylthiocholine + H2O = thiocholi...	?
Row3	3	3.1.1.8	#5# BuChE ...	?	butyrylthiocholine + H2O = butyrate +...	?
Row4	4	3.1.1.8	#5# atypica...	more = ?	?	?
Row5	5	3.1.1.8	?	?	choline esters + H2O = ?	?
Row6	6	3.1.1.8	?	?	butyrylcholine + H2O = butyrate + ch...	?
Row7	7	3.1.1.8	?	?	cocaine + H2O = ecgonine methyl este...	?
Row8	8	3.1.1.8	?	?	butyrylcholine + H2O = choline + buty...	?
Row9	9	3.1.1.8	#5# BuChE ...	?	butyrylthiocholine + H2O = thiocholine...	?
Row10	10	3.1.1.8	?	?	acetylthiocholine + H2O = acetate + t...	?
Row11	11	3.1.1.8	?	?	acetylsalicylic acid + H2O = acetate + ...	?
Row12	12	3.1.1.8	?	?	benzoylcholine + H2O = benzoic acid ...	?
Row13	13	3.1.1.8	?	?	heroin + H2O = ?	?

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