

**ontochem**

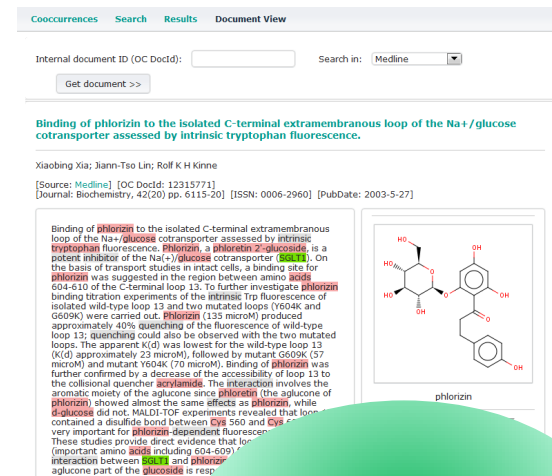
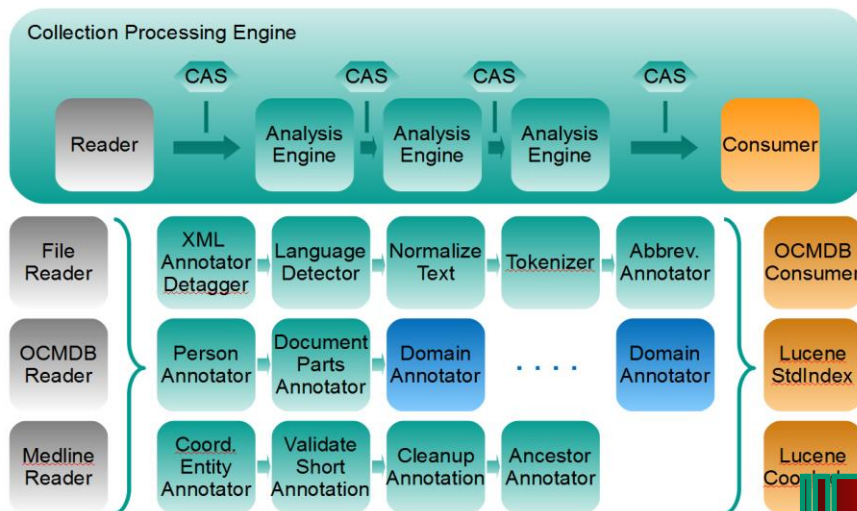
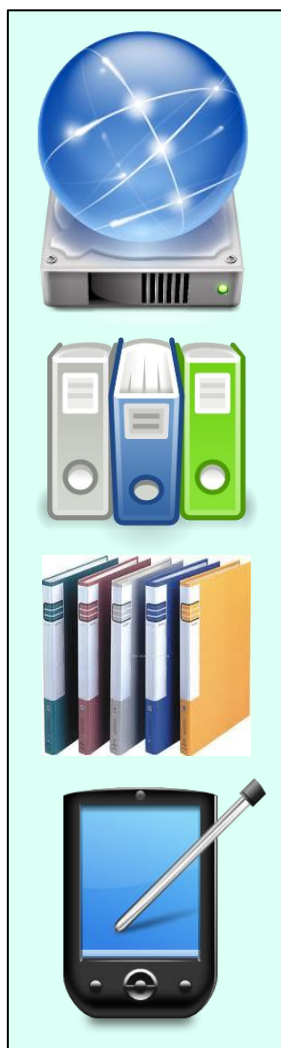
**Big Data Analytics:**

**Semantic Knowledge Discovery**

**OntoChem IT Solutions  
Company Presentation**

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## high speed document processing



**Search interfaces**

**Semantic NLP processing**

**Knowledge databases**

### IBM's Dr. Watson

To date, Watson has ingested more than 600,000 pieces of medical evidence, two million pages of text from 42 medical journals and clinical trials in the area of oncology research.

### OntoChem's OCMiner<sup>®</sup>

120 million of knowledge triples from 25 million pages of text from >2000 journals and 2.5 million full text documents within 1 week



## Input

- Pictures, Text, XML, HTML, Office documents
- PDF reader recognizes document structure (Title, Abstract, References etc.)

## High speed processing

- modular plugins for text processing and analysis
- millions of documents within days using standard hardware
- context sensitive annotations and homonym resolution
- advanced language toolbox
  - language detection, plural forms, British/American/Latin expressions, word forms, hyphens, diacritic characters, anaphora resolution, resolution of abbreviations, composite concepts, concept list expressions
- annotation confidence value

## Output

- custom formats, XML or standardized HTML for web-browser display
- document similarity based on concepts
- ontology based searching via own intranet search engine
- thematic search engines

## **Tools for creating large ontologies**

- **Ontology editors and viewers**
- **Ontology converters (obo2skos, obo2owl)**
- **Automated extraction and statistical analysis of ontology terms**
- **Chemistry ontology editor**

## **Current Ontologies** (up to 100 million terms per ontology)

- **Anatomy**
- **Authors**
- **Chemistry**
- **Companies**
- **Diseases**
- **Effects**
- **Food, flavors and fragrances**
- **Geopolitical regions**
- **Species**
- **Plants**
- **Physiology**
- **Proteins / Genes**

## Relationship extraction methods

Cooccurrences   Search   Results   Document View

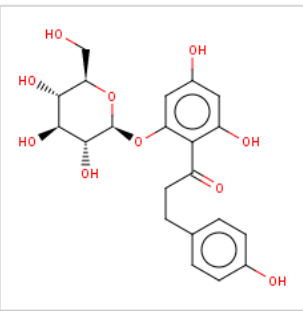
Internal document ID (OC DocId):    Search in:

**Binding of phlorizin to the isolated C-terminal extramembranous loop of the Na<sup>+</sup>/glucose cotransporter assessed by intrinsic tryptophan fluorescence.**

Xiaobing Xia; Jiann-Tso Lin; Rolf K H Kinne

[Source: [Medline](#)] [OC DocId: 12315771] [Journal: Biochemistry, 42(20) pp. 6115-20] [ISSN: 0006-2960] [PubDate: 2003-5-27]

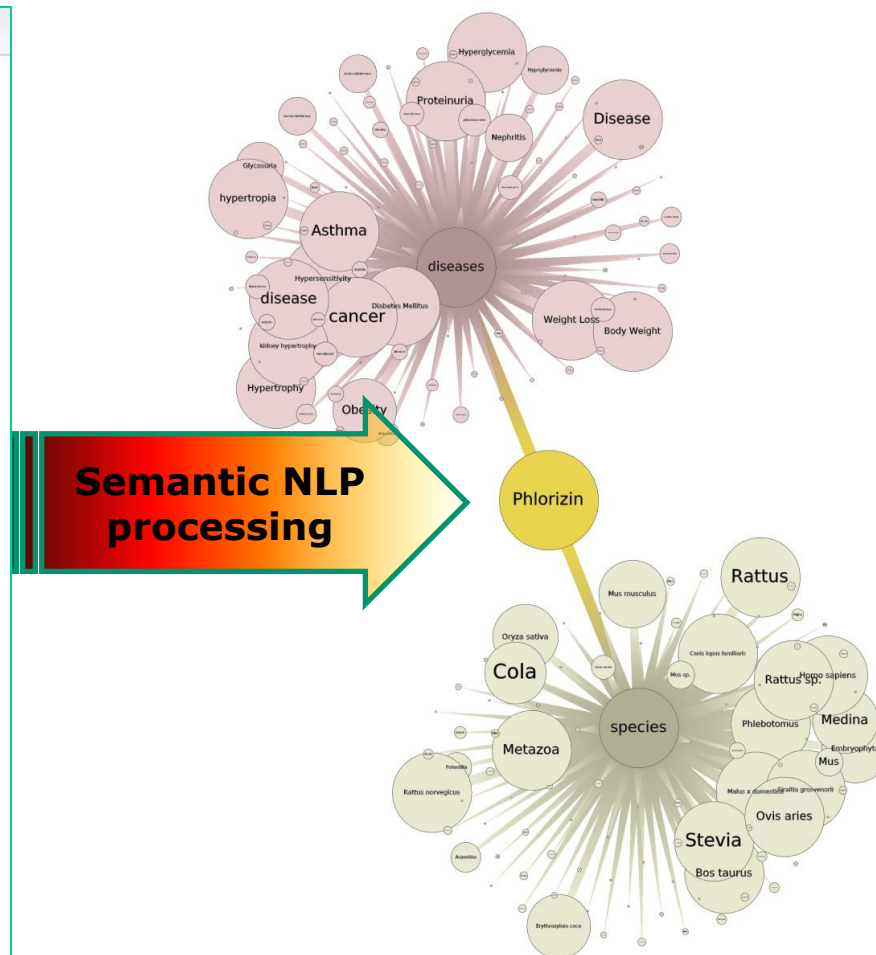
Binding of **phlorizin** to the isolated C-terminal extramembranous loop of the Na<sup>+</sup>/glucose cotransporter assessed by intrinsic **tryptophan** fluorescence. **Phlorizin**, a **phloretin 2'-glucoside**, is a potent inhibitor of the Na<sup>+</sup>/glucose cotransporter (**SGLT1**). On the basis of transport studies in intact cells, a binding site for **phlorizin** was suggested in the region between amino **acids** 604-610 of the C-terminal loop 13. To further investigate **phlorizin** binding titration experiments of the intrinsic Trp fluorescence of isolated wild-type loop 13 and two mutated loops (Y604K and G609K) were carried out. **Phlorizin** (135 microM) produced approximately 40% quenching of the fluorescence of wild-type loop 13; quenching could also be observed with the two mutated loops. The apparent K(d) was lowest for the wild-type loop 13 (K(d) approximately 23 microM), followed by mutant G609K (57 microM) and mutant Y604K (70 microM). Binding of **phlorizin** was further confirmed by a decrease of the accessibility of loop 13 to the collisional quencher **acrylamide**. The interaction involves the aromatic moiety of the aglucone since **phloretin** (the aglucone of **phlorizin**) showed almost the same effects as **phlorizin**, while **D-glucose** did not. MALDI-TOF experiments revealed that loop 13 contained a disulfide bond between **Cys** 560 and **Cys** 608 that is very important for **phlorizin**-dependent fluorescence quenching. These studies provide direct evidence that loop 13 is a site (important amino **acids** including 604-609) for the molecular interaction between **SGLT1** and **phlorizin**. They confirm that the aglucone part of the **glucoside** is responsible for this interaction.



phlorizin

Minimal confidence:

Query Term	↑
Chemistry	↑
Protein	↑
Effect	↑



apples

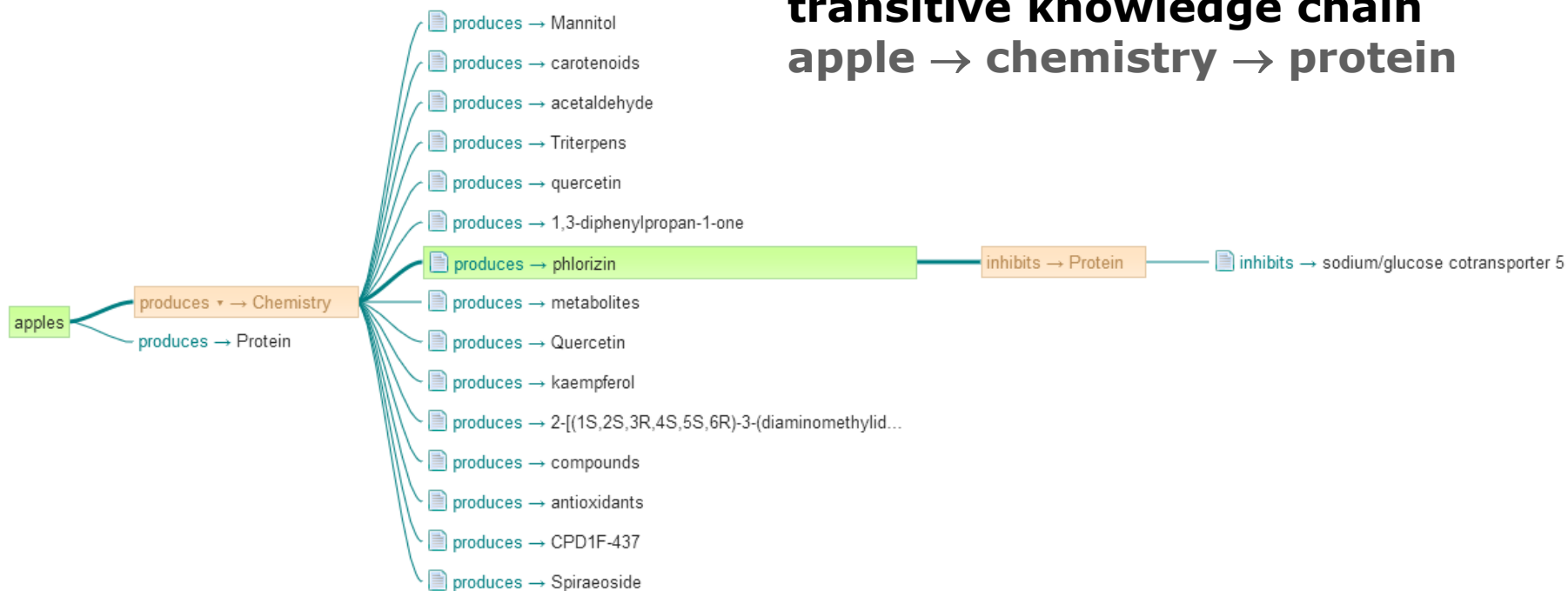
Species (plants/fungi)

Load relations

## Relations graph

done

**transitive knowledge chain**  
**apple → chemistry → protein**



## Project examples:

### General

patent analysis and freedom-to-operate

### Publishers

annotation of large document collections  
automated content analysis

### Agro, Food & Fragrances, Cosmetics

intranet Search Engine  
new anti-dandruff targets & agents  
anti-cellulite agent from natural products  
insecticides based on natural products

### Human and animal health

intranet Search Engine  
natural plant based antibiotics  
anti-cancer plant derived compounds

