

From Documents to Knowledge: Chemistry Data for Real World Evidence

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About Linguamatics



Software

Consulting

Enterprise & Cloud

- Agile, scalable, real-time NLP-based text analytics
- Rapid relationship extraction and knowledge synthesis using unique and powerful blend of methods
- Commercial out-of-the-box, deep domain expertise

Pharma/Biotech

Healthcare

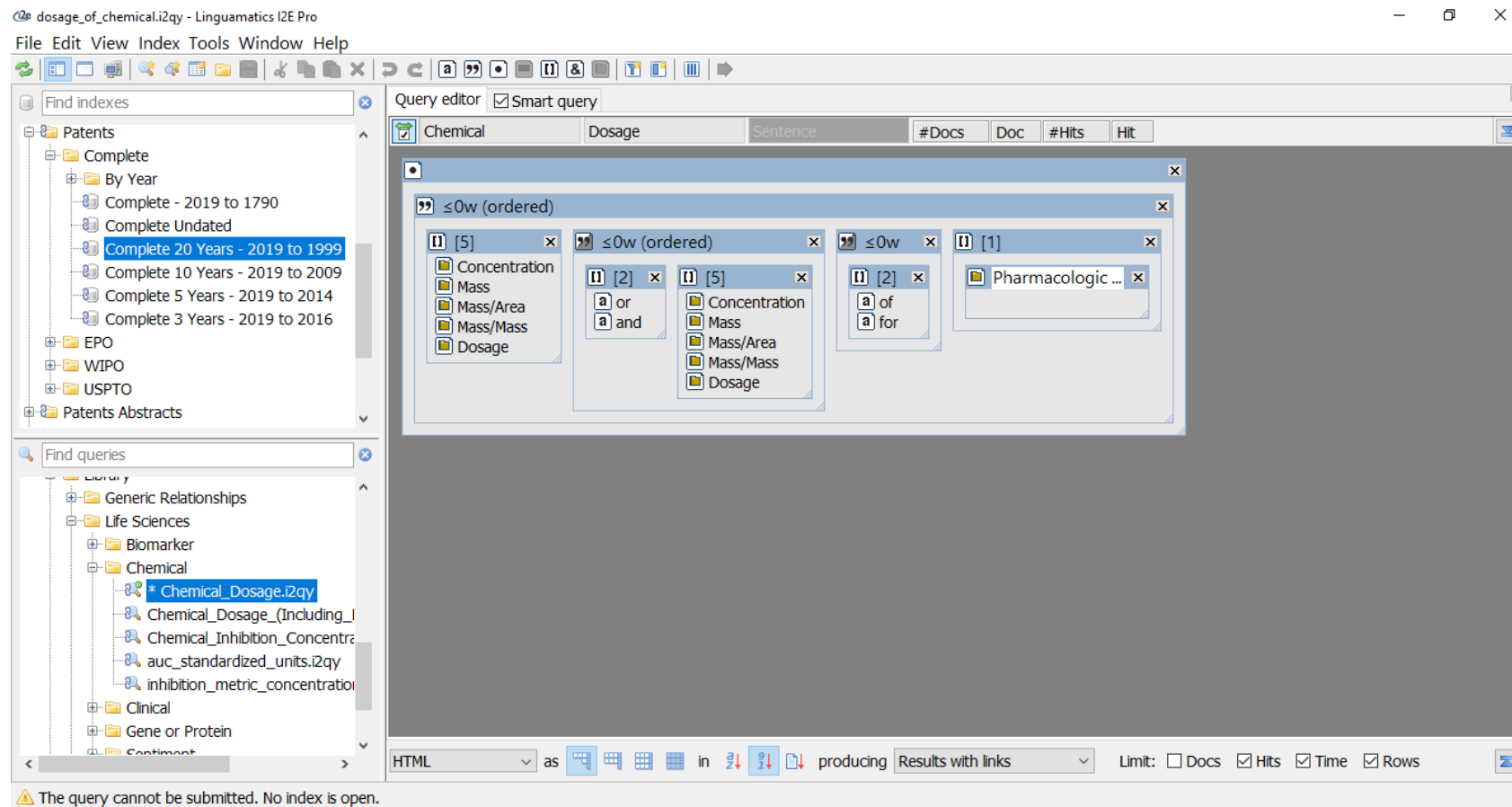
Government

Including 18 of the top 20

Including major cancer centres, health systems, academic medical centres

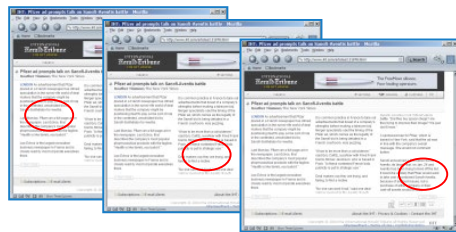
Including FDA, NIH, NCI

- ◆ Natural language processing (NLP)-based knowledge discovery platform
- ◆ Graphical view of the query
- ◆ Delivers results in real-time in structured tables
- ◆ Variety of other output formats
- ◆ Has an API
- ◆ Incorporates ChemAxon JChem



The screenshot displays the Linguamatics I2E Pro interface. On the left, a hierarchical tree view shows the 'Find indexes' and 'Find queries' sections. The 'Find indexes' section includes 'Patents' (Complete, By Year, Complete 20 Years - 2019 to 1999, etc.) and 'Patents Abstracts'. The 'Find queries' section includes 'Generic Relationships', 'Life Sciences', 'Chemical', 'Clinical', and 'Gene or Protein'. The 'Chemical' folder is expanded, showing a query named '* Chemical_Dosage.i2qy'. The main window is the 'Query editor', which shows a query graph with nodes for 'Concentration', 'Mass', 'Mass/Area', 'Mass/Mass', and 'Dosage'. The query is structured as follows: $\leq 0w$ (ordered) [5] x $\leq 0w$ (ordered) [2] x $\leq 0w$ [2] x [1]. The nodes are connected by logical operators: 'or' and 'and' between the first two nodes, 'of' and 'for' between the second and third nodes, and 'for' between the third and fourth nodes. The interface also shows a status bar at the bottom with the message: 'The query cannot be submitted. No index is open.'

From Documents to Knowledge



Web Search

LONDON An advertisement that Pfizer placed in a French newspaper has stirred speculation in the rumor-rife world of deal makers that the company might be positioning itself to play some sort of role in the contested, unsolicited bid by Sanofi-Synthelabo for Aventis.

Last Monday, Pfizer ran a full-page ad in the newspaper, as **Echo**, that described the company's most popular pharmaceutical products with the tagline, "Health is like family, you build it."

It is common practice in France to take out advertisements that boast of a company's strengths before making a takeover bid. Merger specialists said the timing of the Pfizer ad, which comes as the legality of the Sanofi bid is being debated in a French courtroom, was puzzling.

"It has to be more than a coincidence," said Eric Calhitz, a partner with Fried Frank Harris Shriver Jacobson, who is based in Paris. "In these contested French bids, publicity is put to strategic use."

A spokeswoman for Pfizer, which is based in New York, said that the ad was in line with the company's overall message. She would not comment further.

Sanofi announced a \$60 billion bid for Aventis, its larger rival, on Jan. 28 and Aventis has announced to fend off the bid.

Relationship Extraction

Assertion Clustering

Drug	Dosage	#Docs	Doc	#Hits	Hit
Cyclosporine	5 mg/kg every 1d	19	25903959	2	... control (vehicle), CSA (5 mg/kg/day) and Red + Conv ...
	25 mg/kg every 1d	15	25769608	2	... , a model group (CSA 25 mg/kg per day), and a G-Rg1 ...
	10 mg/kg every 1d	12	30018669	1	... XXMD60), IR plus cyclosporin A (10 mg/kg/day) (CSA), ...
	30 mg/kg every 1d	11	25903959	2	... and Red + Conv (CSA 30 mg/kg/day) during 3 weeks + 3 ...
	15 mg/kg every 1d	11	30574488	1	... 2.8 kg was immunosuppressed with intramuscular cyclosporine 15 mg/kg daily for 3 days prior to ...
	20 mg/kg every 1d	10	30658157	1	... renal structural damages caused by CSA (20 mg/kg/day) .
	3 mg/kg every 1d	9	29369774	1	Among them, 95 received cyclosporine (3 mg/kg/day) plus supportive care, ...
	2.5 mg/kg every 1d	7	28967549	2	... mg/wk) or cyclosporine (2.5 mg/kg/d) for 8 weeks.
	4 mg/kg every 1d	6	29727479	1	... kg-1 per week) or CyA (4 mg kg-1 per day) .
	200 mg every 1d	6	29532216	1	... , and median dosage of cyclosporine was 200 mg daily .
	2 mg/kg every 1d	5	26502369	1	... treated with either vehicle, CyA (2 mg/kg per day) , Tac (0.075 ...
	100 mg every 12h	5	30044899	1	... After 5 days' pretreatment with cyclosporine 100 mg twice daily , geometric mean Cmax of ...

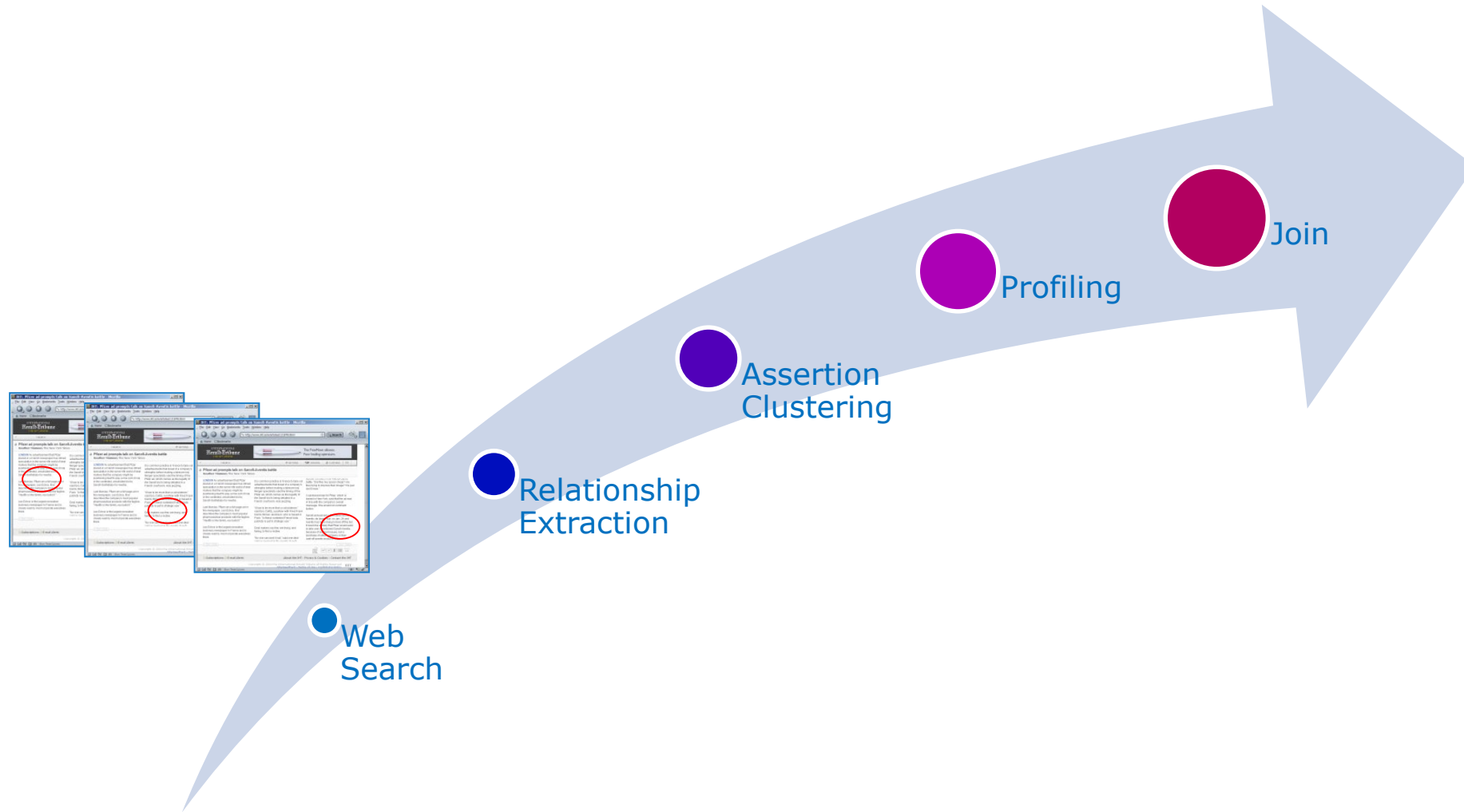
Profiling

Join

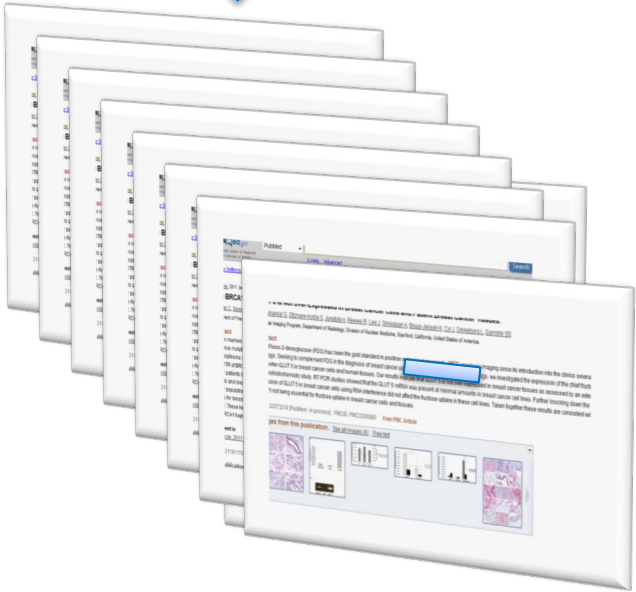
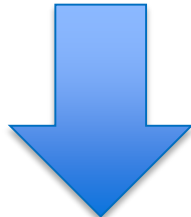
Chemical	Reln	Gene	Reln	Disease	#Docs	Doc	#Hits	Hit
Cyclosporine	inhibits	CXCL8	are upregulated in	Psoriasis	1	9588080	1	It was found out that CSA inhibits IL-8 production by stimulated THP-1 monocyte cell line in dose dependence course.
					1	8752656	1	There is ample evidence that several cytokines, including transforming growth factor-alpha (TGF-alpha), interleukin (IL)-6, and IL-8 are upregulated in psoriasis , suggesting a pathogenic role for these cytokines.

Chemical	Relation	Entity	#Docs	Doc	#Hits	Hit
Etanercept	dosage	50 mg every 7d	52	23319853	5	The aim of this study was to evaluate the proportion of patients with ankylosing spondylitis maintaining clinical remission after reduction of their subcutaneous etanercept dose to 50 mg every other week compared with that in patients receiving etanercept 50 mg weekly .
	treat	Arthritis, Rheumatoid	37	29680792	2	Pneumocystis jiroveci pneumonia in a patient taking Benepali for rheumatoid arthritis .
	cause	Sarcoidosis	2	24346918	2	Systemic sarcoidosis induced by etanercept : first Brazilian case report.
	inhibit	TNF	13	27445694	2	Combined Intrapertitoneal and Intrathecal Etanercept Reduce Increased Brain Tumor Necrosis Factor-Alpha and Asymmetric Dimethylarginine Levels and Rescues Spatial Deficits in Young Rats after Bile Duct Ligation.
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	affect	PPARA	1	28882574	1	However, neither GdCl3 nor etanercept could affect binge drinking-induced decrease of PPAR-α, ACOX, FAS, ACC and SCD protein levels, or increase of the LC3 II/LC3 I ratio and p62 protein level.

From Documents to Knowledge

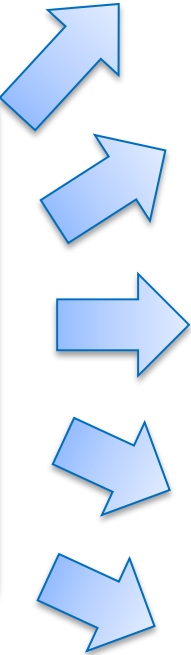


Web Search



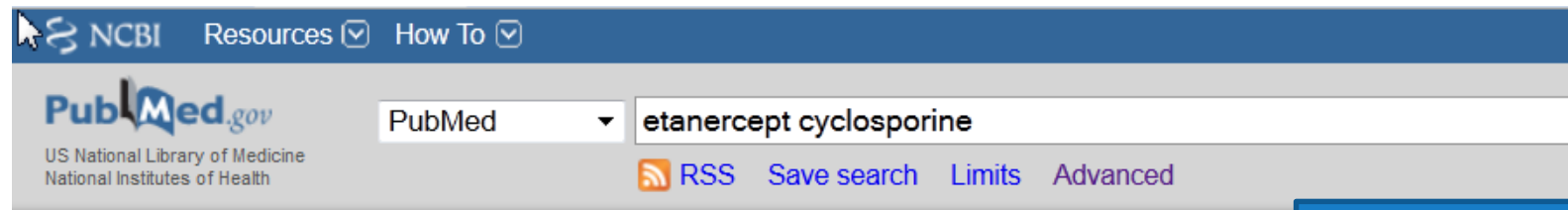
Documents, Web Pages, Folders

All these documents contain the keywords "breast cancer".
Read ALL to find the relevant ones.



Web Search of Two Terms

- ◆ Consider a search for “etanercept” and “cyclosporine”



Display Settings: Summary, 20 per page, Sorted by Recently Added

Results: 1 to 20 of 178

[Classical to Current approach for treatment of psoriasis: A Review.](#)

1. Rahman M, Alam K, Kazmi I, Ahmad MZ, Akhter S, Gupta G, Afzal M, Anwar F, Ahmad FJ. *Endocr Metab Immune Disord Drug Targets*. 2012 Mar 30. [Epub ahead of print] PMID: 22463723 [PubMed - as supplied by publisher] [Related citations](#)

[Metabolic abnormalities associated with initiation of systemic treatment for psoriasis: evidence from the Italian](#)

2. [Psocare Registry.](#)

- Gisondi P, Cazzaniga S, Chimenti S, Giannetti A, MacCarone M, Picardo M, Girolomoni G, Naldi L; Psocare S Group. *J Eur Acad Dermatol Venereol*. 2012 Feb 7. doi: 10.1111/j.1468-3083.2012.04450.x. [Epub ahead of print] PMID: 22313340 [PubMed - as supplied by publisher] [Related citations](#)

Words separated by several sentences

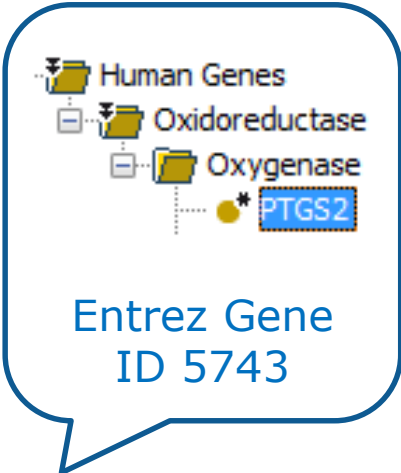
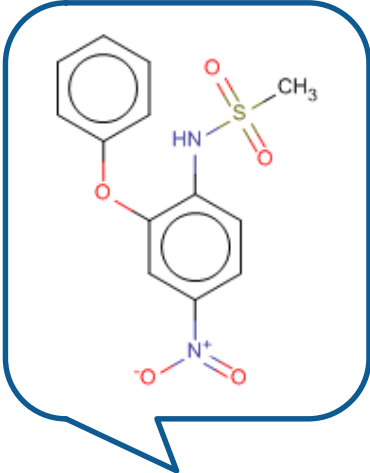
Words in adjoining sentences

Co-occurrence vs. Linguistics

- ◆ Document co-occurrence is commonly reported in search engines results.
 - Great at showing there is some association, but not what the association is.
- ◆ Would a sentence co-occurrence be any better?
 - “Etanercept and cyclosporine were the drugs most frequently prescribed at entry.”
 - “Etanercept demonstrated higher efficacy and good tolerability as replacement therapy for cyclosporine in plaque psoriasis.”
- ◆ We can use linguistics to distinguish between the specific relationships

Linguistic Processing: From Words to Meaning

Identifying entities and relations



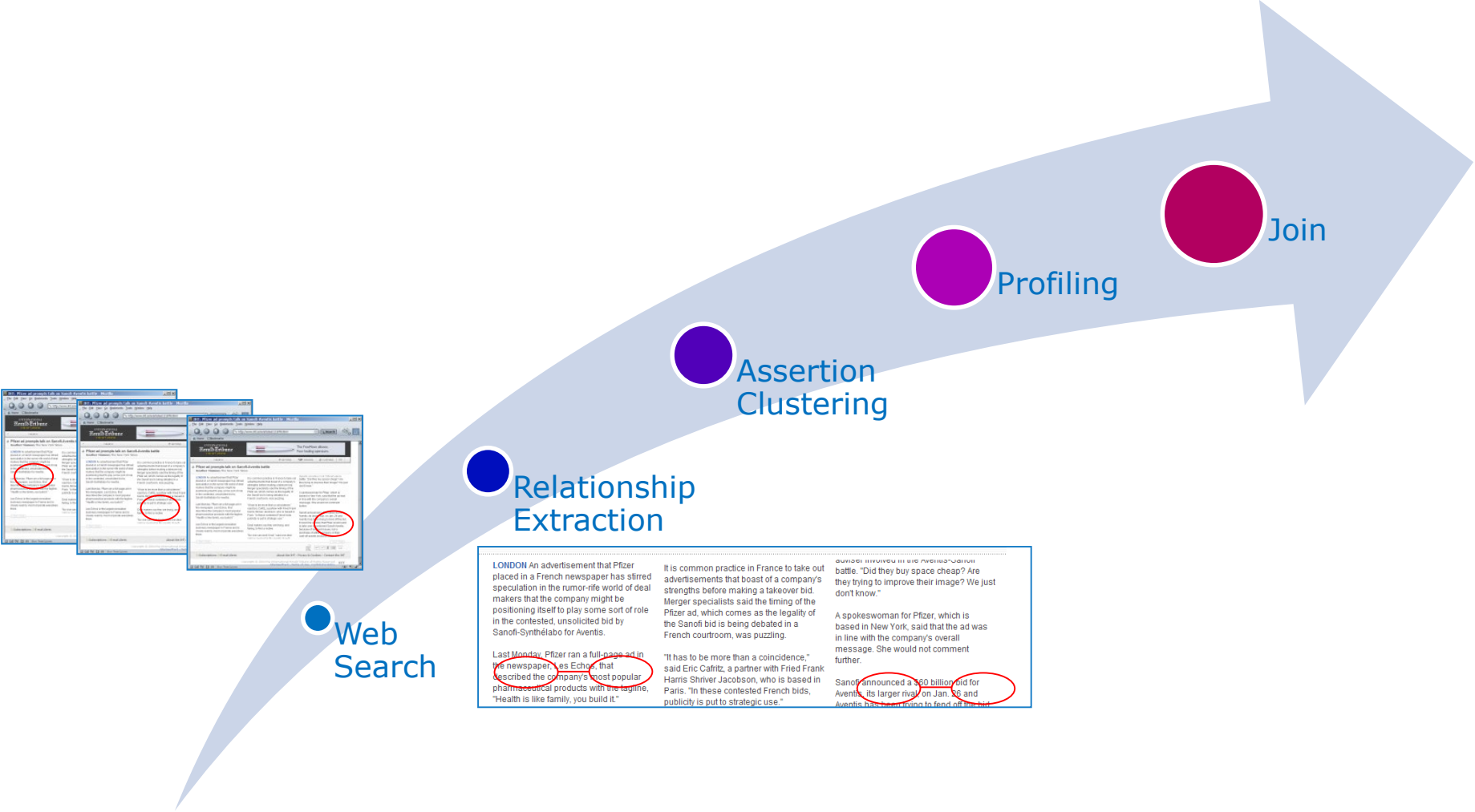
“Among them, nimesulide, a selective COX2 inhibitor, ...”

Consider linguistics to establish relationships

inhibits



From Documents to Knowledge



Linguistics and Ontologies

- ◆ Consider a search for biomarkers for a disease
 - Gene > biomarker > disease

Class1	Relation	Class2	Doc	Hit
▶ ERBB2	prognostic	Breast Neoplasms	▶ 9 19723150	1 Coordinated expression of ER, PR and HER2 define different prognostic subtypes among poorly differentiated breast carcinomas.
▶ EGFR	marker	Breast Neoplasms	▶ 3 21276138	1 Currently, CD133 is one of the best markers to characterize cancer stem cells and Her-1 is reported as an important marker for the prognosis of triple-negative breast cancer.
▶ ESR1	predictive	Breast Neoplasms	▶ 4 20437866	1 Molecular subtype approximated by quantitative estrogen receptor, progesterone receptor and Her2 can predict the prognosis of breast cancer.
▶ CD24	marker	Breast Neoplasms	▶ 4 22388757	1 It has been reported previously that: (1) normal-breast epithelial cells that are CD24-/44+ express higher levels of stem/progenitor cell-associated genes; (2) cancer cells that have undergone epithelial to mesenchymal transition display CD24-/44+ cell-surface expression, a marker for breast cancer stem cells; (3) loss of E-cadherin is a preliminary step in epithelial to mesenchymal transition; and (4) vimentin is a marker of mesenchymal phenotype.

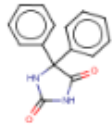
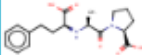
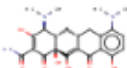
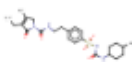
Drug Adverse Events

- ◆ What drugs containing a benzene ring and a carboxamide group have a specific adverse event?

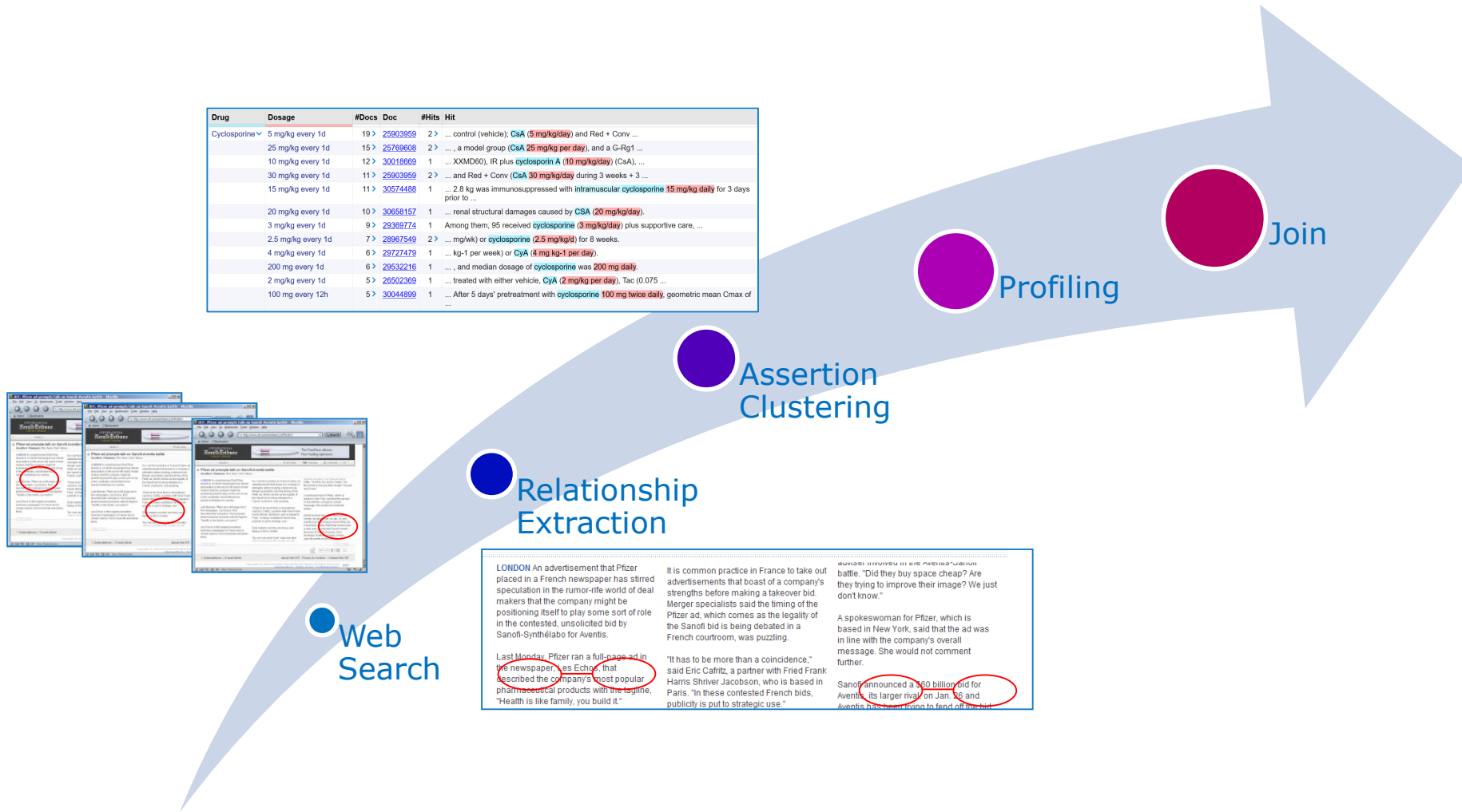
- Substructure search with Jchem in I2E



- ◆ Found 3x the number of drugs vs manual curation

Chemicals (Name to S..	Stevens-Johnson Synd..	FDA Products	Doc	Hit
silantin 	▶ Stevens-Johnson Syndrome	PHENYTOIN SODIUM	▶ 37 7317e374-847a-4b8a-851d-467a0bb9c77e	4 Phenytoin Sodium... PHENYTOIN... dermatitis, lupus erythematosus, Stevens-Johnson syndrome, and toxic epidermal necrolysis ...
enalaprilat 	▶ Stevens-Johnson Syndrome	ENALAPRIL MALEATE	▶ 66 759e0a98-9e32-4caf-936c-873ddf8b85b7	8 ENALAPRIL MALEATE... ENALAPRILAT ANHYDROUS... Skin: Exfoliative dermatitis, toxic epidermal necrolysis, Stevens-Johnson syndrome, pemphigus...
minocycline 	▶ Stevens-Johnson Syndrome	MINOCYCLINE HYDROCHLORIDE	▶ 68 13d8dea9-5f80-45e6-8a0e-9b4fd34a560f	6 MINOCYCLINE HYDROCHLORIDE... MINOCYCLINE... of nails, pruritus, toxic epidermal necrolysis, and vasculitis.
glimepiride 	▶ Stevens-Johnson Syndrome	GLIMEPIRIDE	▶ 68 4529ac93-bceb-27fe-e054-00144ff88e88	6 Glimepiride... GLIMEPIRIDE... anaphylaxis, angioedema, and Stevens-Johnson Syndrome [see

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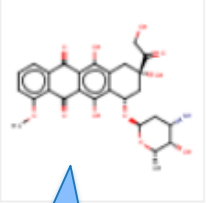
Assertion Extraction: Potential Safety Issues

Compound

In this organ

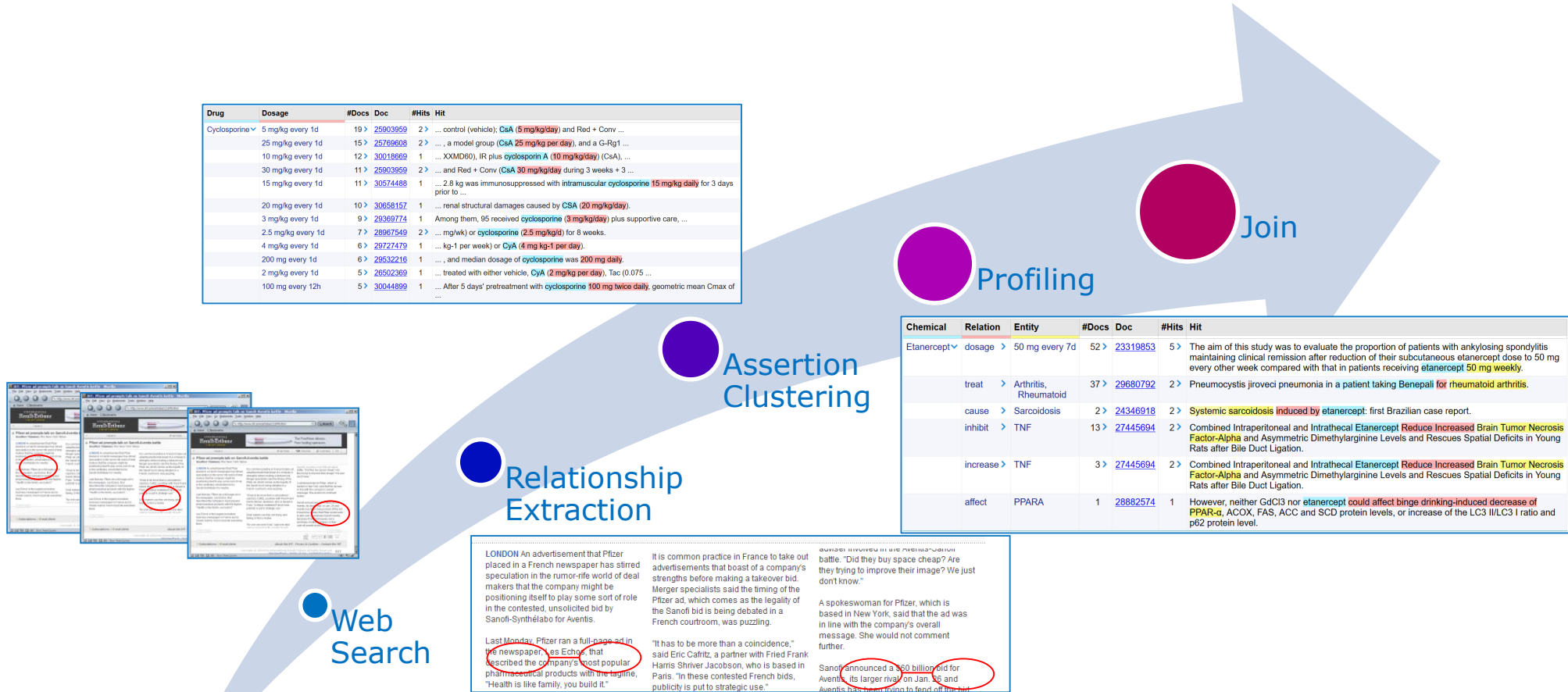
At this dosage

Searching broad range of terms

Chemical	Organ toxicity	Dosage	#Docs	Doc	#Hits	Hit
doxorubicin 	Heart	20 mg/kg	3	28344418	2	Twenty-one rats were divided into three equal groups as follows: 1) Group 1 is a control group (without any intervention), used for evaluating the basal cardiac structures and determining the normal value of cardiacs and serum oxidative markers; 2) Group 2 is the doxorubicin group (single dose i.p. 20 mg/kg doxorubicin) for detecting the cardiotoxic and systemic effects of doxorubicin; 3) Group 3 is the doxorubicin and HBO2 group (100% oxygen at 2.5 atmospheric for 90 minutes, daily), for evaluating the effect of HBO2 in doxorubicin induced cardiotoxicity.
	Liver	3 mg/kg	1	26335259	3	... limited by cardiac and hepatic toxicities. The aim of this study was to assess the hepatoprotective and cardioprotective effects of taurine zinc solid dispersions, which is a newly-synthesized taurine zinc compound, against doxorubicin-induced toxicity in Sprague-Dawley rats intraperitoneally injected with doxorubicin hydrochloride (3mg/kg) three times a week (seven injections) over 28 days. Hemodynamic parameters, levels of liver toxicity markers and oxidative stress were assessed...
	Kidney	7.19 mg/l	1	28870343	1	The toxicity level of crude extract and fractions evaluated in Vero monkey kidney cells ranged from 34 to 223 µg/mL, while doxorubicin (IC50 = 7.19 µg/mL) served as the positive control.

Chemical images provided through JChem

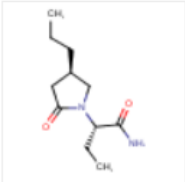
From Documents to Knowledge



Chemical Information

For a given drug

Report various properties

Chemical	Relation	Entity	#Docs	Doc	#Hits	Hit
brivaracetam 	dosage >	200 mg every 12h	3 >	27842261	1	Carbamazepine epoxide plasma concentrations were approximately doubled by brivaracetam 100 or 200mg bid.
	treat >	Seizures	8 >	29270790	1	Budget Impact Analysis of Brivaracetam Adjunctive Therapy for Partial-Onset Epileptic Seizures in Valencia Community, Spain.
		Epilepsy	3 >	26760311	1	Brivaracetam for the treatment of epilepsy.
		Epilepsies, Partial	2 >	28829199	1	The preclinical discovery and development of brivaracetam for the treatment of focal epilepsy.
		Depressive Disorder	1	19211275	1	Brivaracetam inhibits spreading depression in rat neocortical slices in vitro.
	affect	SV2A	1	26899665	1	Brivaracetam binds to synaptic vesicle glycoprotein 2a (SV2A) in the brain with greater selectivity and 15- to 30-fold higher affinity than levetiracetam, as demonstrated in preclinical models, and has demonstrated efficacy in reducing the frequency of partial onset seizures in clinical trials.
	IC50	8.2e-06 mol/l	1	25986188	1	In vitro hydrolysis of carbamazepine-epoxide in human hepatocytes was inhibited by brivaracetam, with an IC50 of 8.2µM.
	inhibit	hydrolase	1	27842261	1	Valproate and brivaracetam inhibit epoxide hydrolase and increase carbamazepine epoxide levels.

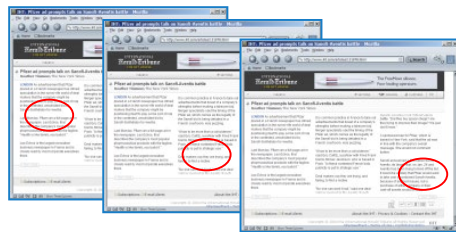
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Extracting Product Information for IDMP

IDMP (IDentification of Medicinal Products) ISO standard

Source	Section	Full Name	Invented Name Part	Strength Part	Pharmaceutical Dose ..	Intended Use Part	Flavour Part	#Hits	Hit
SmPC	1	Abacavir/Lamivudine 600 mg/300 mg film-coated tablets	Abacavir/Lamivudine	600 mg/300 mg	film-coated tablets			3	Abacavir/Lamivudine 600 mg/300 mg film- coated tablets
SmPC	1	ABILIFY 7.5 mg/ml solution for injection	ABILIFY	7.5 mg/ml	solution for injection			3	ABILIFY 7.5 mg/ml solution for injection
SmPC	1	Accupro Tablets 5 mg	Accupro	5 mg	Tablets			3	Accupro Tablets 5 mg
SmPC	1	▼ Acidex Liquid - peppermint flavour	Acidex		Liquid		peppermint flavour	3	Acidex Liquid - peppermint flavour
		Boots Heartburn Relief Peppermint Flavour	Boots			Heartburn Relief	Peppermint Flavour	3	Boots Heartburn Relief Peppermint Flavour
		Healthpoint Heartburn and Indigestion Oral Suspension	Healthpoint		Oral Suspension	Heartburn and Indigestion		3	Healthpoint Heartburn and Indigestion Oral Suspension
		LloydsPharmacy Heartburn and Indigestion Liquid Peppermint Flavoured	LloydsPharmacy		Liquid	Heartburn and Indigestion	Peppermint Flavoured	3	LloydsPharmacy Heartburn and Indigestion Liquid Peppermint Flavoured
		Peptac Peppermint Liquid	Peptac		Liquid		Peppermint	3	Peptac Peppermint Liquid
		Tesco Heartburn & Indigestion relief	Tesco			Heartburn & Indigestion relief		3	Tesco Heartburn & Indigestion relief

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overseer involved in the international battle. "Did they buy space cheap? Are they trying to improve their image? We just don't know."

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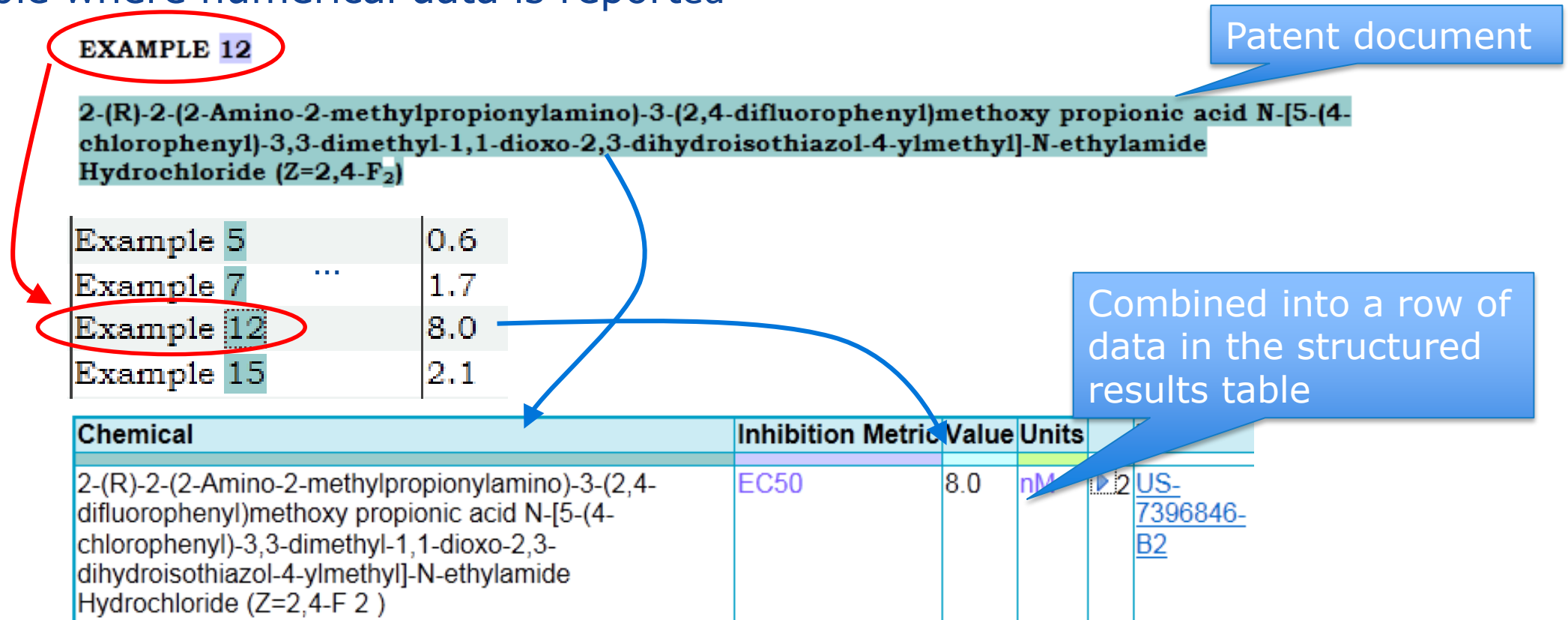
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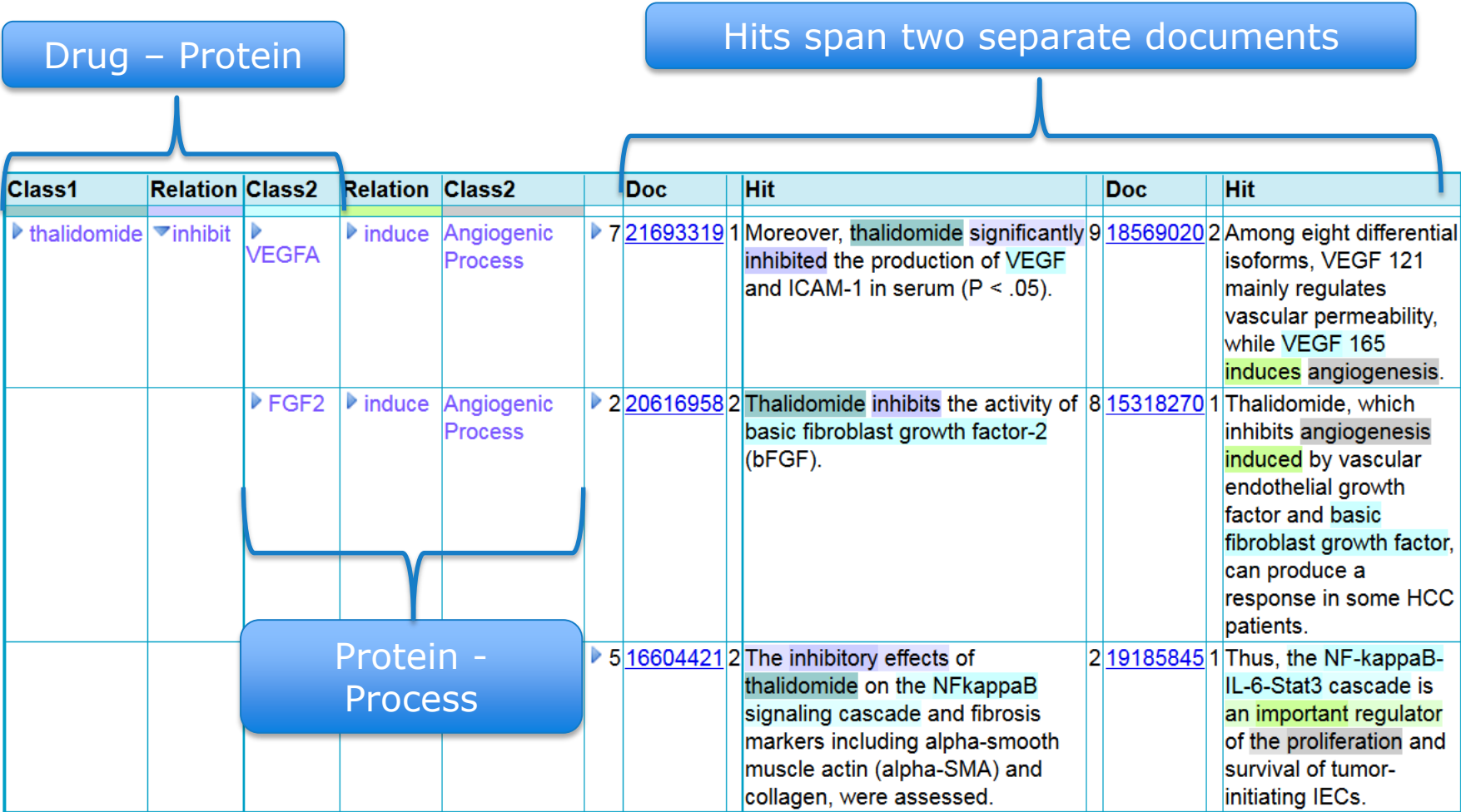
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Linking Information within Documents

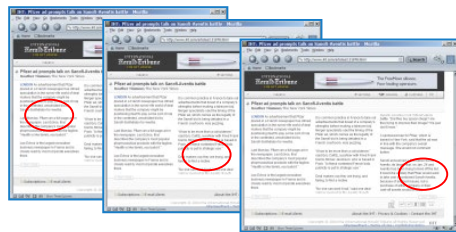
- ◆ Connecting information found in different parts of the document
- ◆ For example finding a compound as "Example 12" in a patent and linking to a table where numerical data is reported



Connecting Information Between Documents



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"It has to be more than a coincidence," said Eric Calhitz, a partner with Fried Frank Harris Shriver Jacobson, who is based in Paris. "In these contested French bids, publicity is put to strategic use."

overseer involved in the international battle. "Did they buy space cheap? Are they trying to improve their image? We just don't know."

A spokeswoman for Pfizer, which is based in New York, said that the ad was in line with the company's overall message. She would not comment further.

Sanofi announced a \$60 billion bid for Aventis, its larger rival, on Jan. 28 and Aventis has announced to fend off the bid.

Relationship Extraction

Assertion Clustering

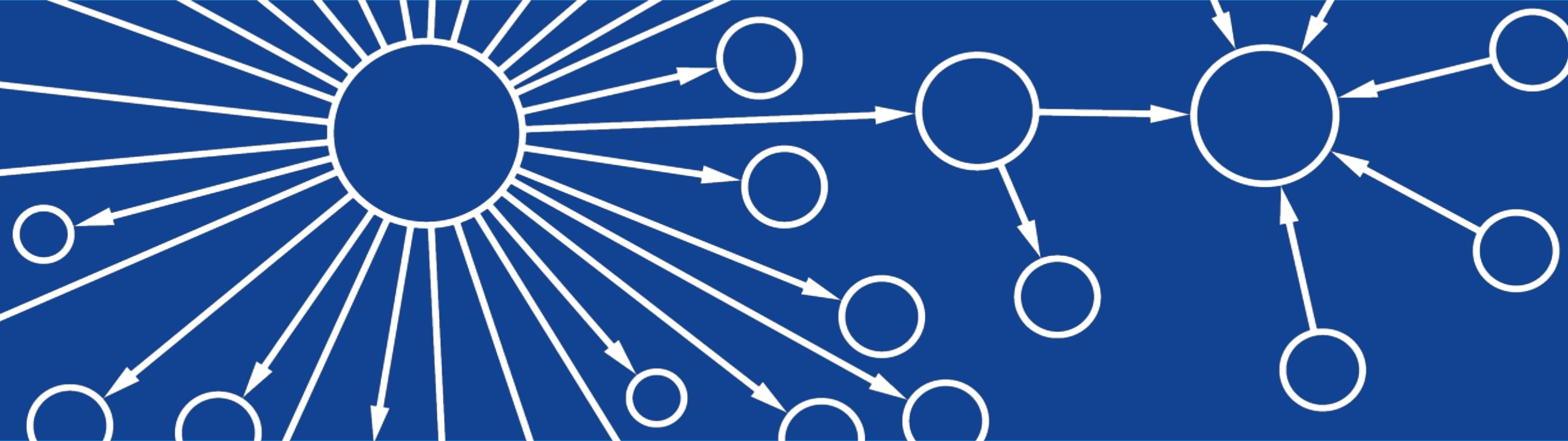
Drug	Dosage	#Docs	Doc	#Hits	Hit
Cyclosporine	5 mg/kg every 1d	19	25903959	2	... control (vehicle), CSA (5 mg/kg/day) and Red + Conv ...
	25 mg/kg every 1d	15	25769608	2	... , a model group (CSA 25 mg/kg per day), and a G-Rg1 ...
	10 mg/kg every 1d	12	30018669	1	... XXMD60), IR plus cyclosporin A (10 mg/kg/day) (CSA), ...
	30 mg/kg every 1d	11	25903959	2	... and Red + Conv (CSA 30 mg/kg/day) during 3 weeks + 3 ...
	15 mg/kg every 1d	11	30574488	1	... 2.8 kg was immunosuppressed with intramuscular cyclosporine 15 mg/kg daily for 3 days prior to ...
	20 mg/kg every 1d	10	30658157	1	... renal structural damages caused by CSA (20 mg/kg/day) .
	3 mg/kg every 1d	9	29369774	1	Among them, 95 received cyclosporine (3 mg/kg/day) plus supportive care, ...
	2.5 mg/kg every 1d	7	28967549	2	... mg/wk) or cyclosporine (2.5 mg/kg/d) for 8 weeks.
	4 mg/kg every 1d	6	29727479	1	... kg-1 per week) or CyA (4 mg kg-1 per day) .
	200 mg every 1d	6	29532216	1	... , and median dosage of cyclosporine was 200 mg daily .
	2 mg/kg every 1d	5	26502369	1	... treated with either vehicle, CyA (2 mg/kg per day) , Tac (0.075 ...
	100 mg every 12h	5	30044899	1	... After 5 days' pretreatment with cyclosporine 100 mg twice daily , geometric mean Cmax of ...

Profiling

Join

Chemical	Reln	Gene	Reln	Disease	#Docs	Doc	#Hits	Hit
Cyclosporine	inhibits	CXCL8	are upregulated in	Psoriasis	1	9588080	1	It was found out that CSA inhibits IL-8 production by stimulated THP-1 monocyte cell line in dose dependence course.
					1	8752656	1	There is ample evidence that several cytokines, including transforming growth factor-alpha (TGF-alpha), interleukin (IL)-6, and IL-8 are upregulated in psoriasis , suggesting a pathogenic role for these cytokines.

Chemical	Relation	Entity	#Docs	Doc	#Hits	Hit
Etanercept	dosage	> 50 mg every 7d	52	23319853	5	The aim of this study was to evaluate the proportion of patients with ankylosing spondylitis maintaining clinical remission after reduction of their subcutaneous etanercept dose to 50 mg every other week compared with that in patients receiving etanercept 50 mg weekly .
	treat	> Arthritis, Rheumatoid	37	29680792	2	Pneumocystis jiroveci pneumonia in a patient taking Benepali for rheumatoid arthritis .
	cause	> Sarcoidosis	2	24346918	2	Systemic sarcoidosis induced by etanercept : first Brazilian case report.
	inhibit	> TNF	13	27445694	2	Combined Intrapertitoneal and Intrathecal Etanercept Reduce Increased Brain Tumor Necrosis Factor-Alpha and Asymmetric Dimethylarginine Levels and Rescues Spatial Deficits in Young Rats after Bile Duct Ligation.
	increase	> TNF	3	27445694	2	Combined Intrapertitoneal and Intrathecal Etanercept Reduce Increased Brain Tumor Necrosis Factor-Alpha and Asymmetric Dimethylarginine Levels and Rescues Spatial Deficits in Young Rats after Bile Duct Ligation.
	affect	> PPARA	1	28882574	1	However, neither GdCl3 nor etanercept could affect binge drinking-induced decrease of PPAR-α, ACOX, FAS, ACC and SCD protein levels, or increase of the LC3 II/LC3 I ratio and p62 protein level.



Thank you!

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