

Integrating ChemAxon and Linguamatics to provide Agile, Chemistry-enabled Text Mining

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Linguamatics I2E

Flexible and scalable text mining for business-critical knowledge discovery

- ◆ NLP-based knowledge discovery platform
- ◆ Rapidly reveals structured facts and relationships by understanding meaning
- ◆ Delivers relevant, high quality results in real-time

From Documents to Knowledge

Value ↑

Join:
Creates indirect correlations and connections

Cyclosporine	Compound	Gene	Entrez	Genes	Gene-Disease	Psoriasis	Doc	Hit	Doc	Hit		
Cyclosporine	inhibit	Interferon	affect	Psoriasis	1	1789988	1	In addition, cyclosporin blocked the interferon-gamma-induced increase in epidermal L2(S)-HETE binding.	9	9856816	1	helper-1-type cytokines such as interleukin-6/gamma in psoriasis.
Cyclosporine	inhibit	IL8	affect	Psoriasis	2	9588080	8	It was found out that CSA inhibits IL-8 production by stimulated THP-1 monocyte cell.	8	11376329	2	Interleukin-6-positive neutrophils in psoriasis.
Cyclosporine	affect	CALM3	affect	Psoriasis	1	2277142	7	Cyclosporine binds to calmodulin with low affinity, and ...	7	1879887	1	Epidermal calmodulin levels in psoriasis before & after therapy.

Pharmacologic Substance	Relation	Doc	Hit			
Etanercept	causes	1	11453808	2	Clinical, histological, and immunophenotypic characteristics of injection site reactions associated with etanercept, a recombinant tumor necrosis factor alpha receptor. Fc fusion protein.	4
	Lymphoma	1	16454534	1	An increased incidence of lymphomas has been postulated to be associated with etanercept, infliximab and adalimumab; serious infections, such as tuberculosis, have also been reported with these three biologicals, all of which target TNF-alpha.	4
	inhibit	1	11961039	1	Although both infliximab and etanercept inhibited transmembrane TNF-mediated activation of human endothelial cells, infliximab was significantly more effective.	1

Drug	Dosage	Doc	Hit		
Cyclosporine	5 mg/kg/day	13	1552052	3	Patients were first treated with cyclosporine either 1.25 or 2.5 mg/kg/day (Sandimmune), in case of inadequate response the dosage was increased to a maximum of 5 mg/kg/day.
	2.5 mg/kg/day	5	1732342	2	His headache continued even after tonsillectomy and was effectively treated with cyclosporine A (3 mg/kg/day).
	3 mg/kg/day	5	10824492	3	OBJECTIVE: The objective of this study was to evaluate the efficacy and safety of the combination of 2 mg/kg/day of cyclosporin with calcipotriol ointment (50 micrograms/gm) in the treatment of severe plaque psoriasis.
	2 mg/kg/day	3	8021375	1	After the unsuccessful use of non-steroidal antiinflammatory drugs a combination therapy with cyclosporin (4 mg/kg/day) and azapropazone (300 mg 11 d.) was introduced.
	4 mg/kg/day	2	11208503	2	Male rats (10 per group) were orally administered pimecrolimus at 10 or 30 mg/kg/day, tacrolimus at 3 mg/kg/day or CSA at 20 mg/kg/day for 4 weeks.
	20 mg/kg/day	1	15093258		

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.

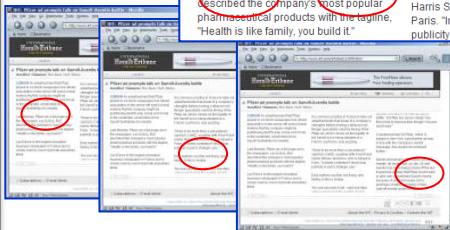
It is common for advertisements that boast of a company's strengths before making a takeover bid. Larger specialists said the timing of the Pfizer ad, which comes as the legality of the Sanofi bid is being debated in a French courtroom, was puzzling.

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.

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

Sanofi announced a \$60 billion bid for Aventis, its larger rival, on Jan. 26 and Aventis has been trying to fend off the bid.



Web Search

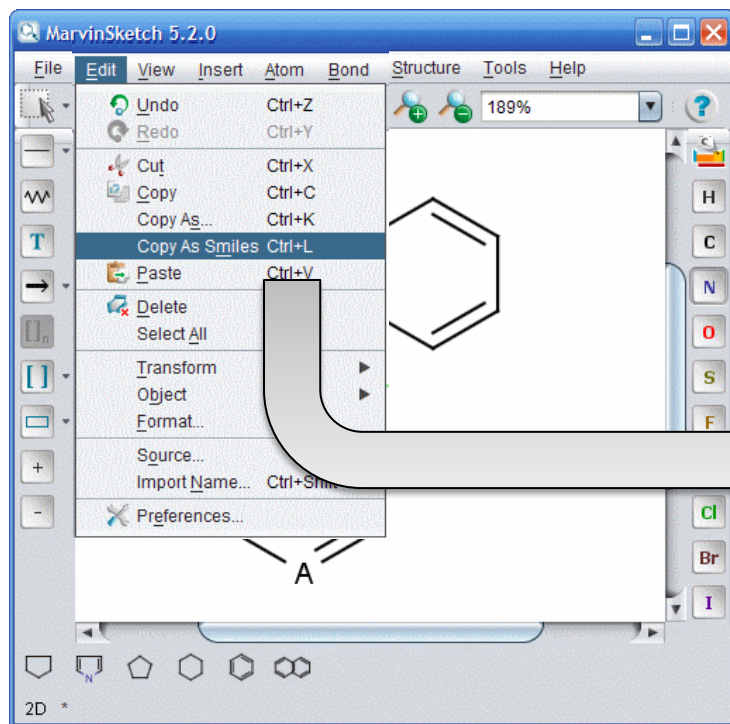
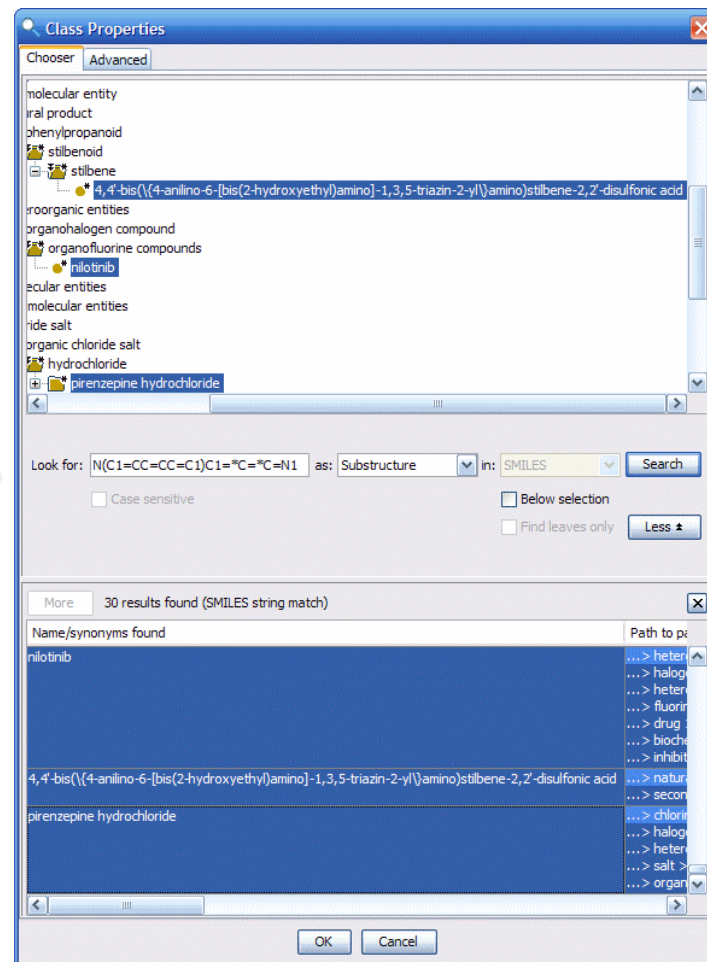
Relationship Extraction

Assertion Clustering

Profiling

Join

Structure Input: Ontology Look-up

Class Properties

Chooser Advanced

molecular entity
oral product
phenylpropanoid
stilbenoid
stilbene
4,4'-bis((4-anilino-6-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl)amino)stilbene-2,2'-disulfonic acid
inorganic entities
organohalogen compound
organofluorine compounds
nilotinib
molecular entities
molecular entities
oxide salt
organic chloride salt
hydrochloride
pirenzepine hydrochloride

Look for: N(C1=CC=CC=C1)C1=*C=*N1 as: Substructure in: SMILES Search

Case sensitive Below selection Find leaves only Less

More 30 results found (SMILES string match)

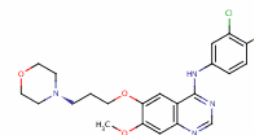
Name/synonyms found	Path to parent
nilotinib	...> heterocyclic ...> halogenated ...> heterocyclic ...> fluorinated ...> drug ...> biochemical ...> inhibitor
4,4'-bis((4-anilino-6-[bis(2-hydroxyethyl)amino]-1,3,5-triazin-2-yl)amino)stilbene-2,2'-disulfonic acid	...> natural product ...> secondary amine
pirenzepine hydrochloride	...> chlorinated ...> halogenated ...> heterocyclic ...> salt ...> organic

OK Cancel

Query Results and Visualization

Pharmacologic Substance	Targets	Entrez Genes	Doc	Hit
▼ gefitinib	▶ inhibit	AHSA1	1 17205515	Inversely, in IC1LC131, Erk and Akt pathways remained active, while Jnk and P38 pathways were inhibited by gefitinib.
	▶ treats	Dependents	1 17237287	Gefitinib inhibited DNA synthesis in a concentration-dependent fashion in 6 of 17 lines.
▼ Imatinib	▶ dosage	200 mg/day	1 17386117	Three years after treatment with different chemotherapeutic agents for progressive cutaneous Kaposi's Sarcoma with no visceral involvement, he was prescribed Imatinib (200 mg/day) for two weeks followed by 400 mg/day) after four weeks of treatment he developed anasarca, further progression of KS and agranulocytosis.
	▶ increase	DCX	1 17064569	CONCLUSION: STI571 could promote the activation/maturation of DC derived from BMMNCs of patients with CML in vitro, which might be partially responsible for the fact that the inhibitory effect of VEGF on DC NF-kappaB activation was relieved through STI571 inhibiting the overproduction of VEGF in CML.
	▶ inhibit	ABL1	▶ 1 17603257	Imatinib also inhibits the activation of VEGF receptor tyrosine kinase, resulting in a favorable response.
▼ Imatinib methanesulfonate	▶ dosage	400 mg/day	1 15161340	In patients with newly diagnosed and in the chronic phase, Imatinib mesylate resulted in higher hematologic response compared with imatinib alone, and fewer patients progressing to the accelerated phase.
	▶ increase	AIF1	1 16885745	Gleevec alone resulted in a slight increase in G2 arrest.
	▶ inhibit	ABL1	▶ 2 17436575	Gleevec inhibits the tyrosine kinase activity of ABL1.
	▶ treats	Adhesion	1 17289809	Depletion of endogenous c-Kit or inhibition of EPCs to activated EPCs both in vitro and in vivo.
▼ lapatinib	▶ inhibit	AKT1	1 17283152	In addition, lapatinib inhibited Akt phosphorylation in parental and resistant cells, and the blocking antibody alphaIR3.
	treats	Insulin-like growth factor	1 17308062	Importantly, lapatinib also inhibited insulin-like growth factor receptor signaling in parental and resistant cells, and the blocking antibody alphaIR3.
▼ nilotinib	▶ inhibit	ABL1	1 17106016	Nilotinib inhibits BCR-ABL at 20-50 times the concentration of imatinib.
	treats	International normalised ratio	1 17106016	Nilotinib inhibits BCR-ABL at 20-50 times the concentration of imatinib.
▼ vandetanib	▶ increase	ABCB1	1 17912240	In addition, ZD6474 increases the inhibition of ABCB1 by enhancing the uptake and/or decreasing the expression of ABCB1.
	inhibit	EGFR	▶ 2 17308046	In vitro, ZD6474 inhibited EGFR, VEGFR, and VEGF-induced proliferation, and

gefitinib



gefitinib

Formula	C ₂₂ H ₂₄ ClFN ₄ O ₃
Mass	446.902
Name	N-(3-chloro-4-fluorophenyl)-7-methoxy-6-[3-(morpholin-4-yl)propoxy]quinazolin-4-amine
logP	3.75
Strongest acidic pKa	16.11
Strongest basic pKa	6.85
Lipinski's rule of five	yes

Thank You!

For more information...

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