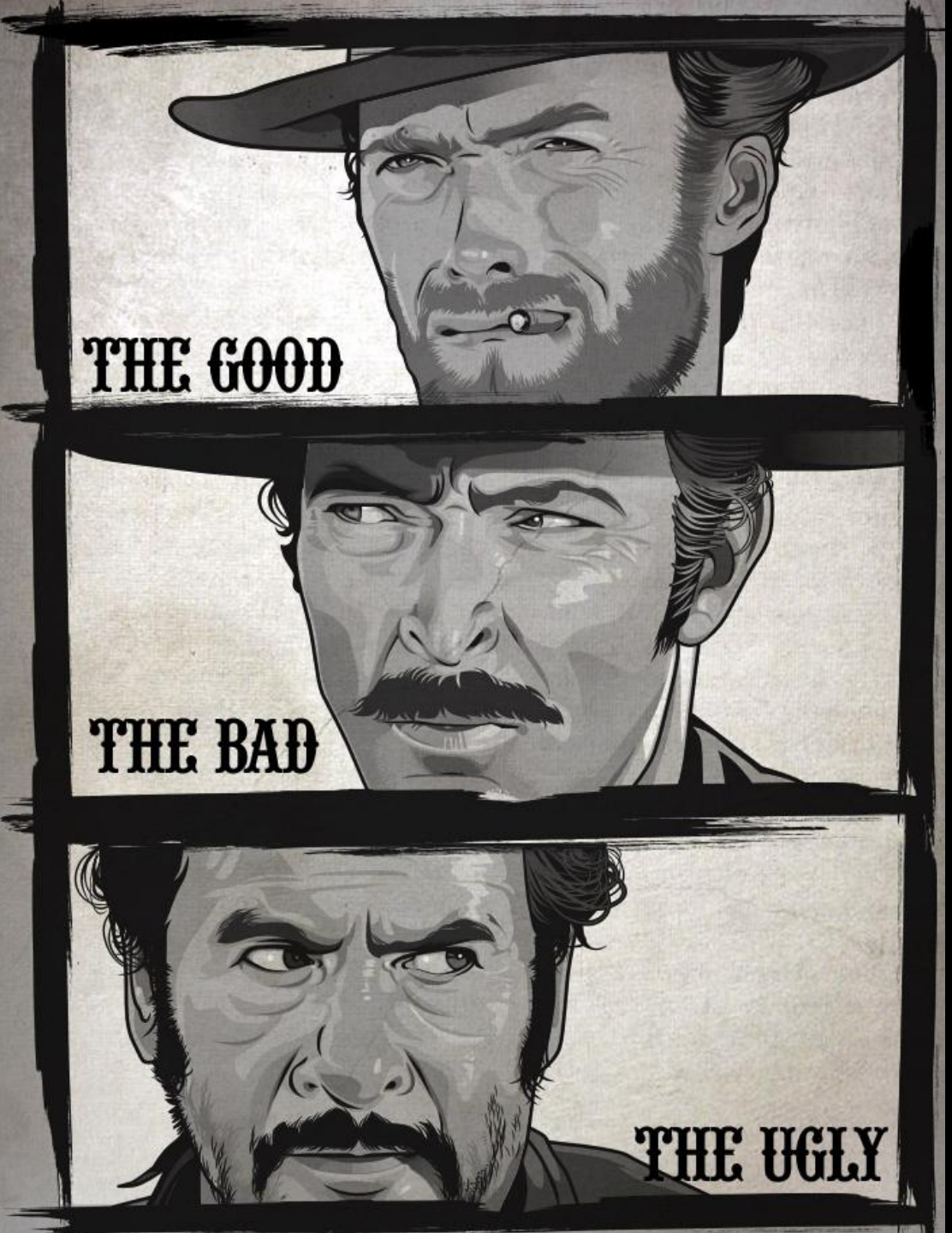
Don’t break your head, When we are just a click away!

ICIC 2012, Berlin, Germany October 14-17, 2012



Reverse Informatics

Volume of literature

Lack of Standards

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Developing a "Central Dogma"

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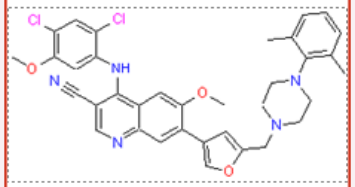
Curated Databases

RIX Database

Inhibitor | Target | Scaffold | Assignee

Compound Information

Structure



Compound ID: XX 9999	Platform Name: KINASE
Target: src kinase	Compound Type: Inhibitor
Compound Name: 4-[(2,4-dichloro-5-methoxyphenyl)-amino]-7-(5-[[4-(2,6-dimethylphenyl) piperazin-1-yl]methyl]-3-furyl)-6-methoxyquinoline-3-carbonitrile	
Use: Anticancer	Disease: Chronic myeloid leukemia

Bibliographic Information

Journal/Patent: Patent Application	Reference ID: ZZ 000	Reference: US20060035930
Publication Date: 16-Feb-2006	First Author: Diane Harris Boschelli	Assignee: Wyeth, Patent Law Group

Title: 4-(2,4-dichloro-5-methoxyphenyl)amino-6-methoxy-7-[[5-substituted -amino)methyl]-3-furyl]-3-quinolinecarbonitriles as kinase inhibitors

Activity Information

Target Class	Target Name	Family	Subfamily
non-receptor Tyrkinase	src	src	DMPK

Bioassay ID	Bioassay	Assay Type	Test System	Species	Activity parameter	Unit	Prefix	Activity Value	Remarks
B 001	Src Kinase Assay	C	Recombinant human Src enzyme	Human	IC 50	nM			
B 005	Anchorage Independent Src-Transformed Fibroblast Proliferation Assay	C	Transformed Rat2 fibroblasts	Rat	IC 50	nM			
	HT29			Mice,					

Inhibitor | Target | Scaffold | Assignee

Summary | Phylogenetic Tree | Protein Interaction | Pathway | Orthologue Data

Kinase Information

Kinase ID: K 001	Kinase Name: Src(HS)
Description: Proto-oncogene tyrosine-protein kinase Src	Synonyms:

Organism: Homo sapiens	Uniprot Code: P12931	GENA ID: GHS018950

Classification

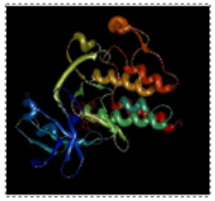
Group: TK	Family: src	Sub Family: DMPK

Family Description

The Src family, which is found in FYN (oncogene related to SRC), FGR, and YES), SRC (v-src avian sarcoma viral oncogene homologue), YES (v-yes-1 Yamaguchi sarcoma viral oncogene homologue), FGR (Gardner-Rasheed feline sarcoma viral oncogene homologue), LCK (lymphocyte-specific protein tyrosine kinase; required for antigen-activation of T-cells), HCK (hemopoietic cell kinase), and BLK (B lymphoid tyrosine kinase), has been implicated in many signal transduction pathways such as neuronal development and B-cell development. However, in C. elegans and Drosophila the Src family has only one sequence. Further, so far some reported pathways, including those for the Src family, have been different between Drosophila and mammals (Luttrell et al. 1997; Lu and Li 1999). The domain structure is conserved from worms to mammals, and the functional conservation, such as the structural plasticity of neurons, is expected.

Structure & Sequence Information

Structure



Sequence

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STGQTGYIPSNYVAPSDSIQAEEWYFGKITRRESERLLLNAENP
RGTFLVRESETTKGAYCLSVSDFDNAKGLNVKHYKIRKLDSGG
FYITSRTQFNSLQQLVAYYSKHADGLCHRLTTVCPTSKPQTQG
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LKPGTMSPEAFLQEAQVMKKLRHEKLVQLYAVVSEEPIYIVT
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KWTAPEAALYGRFTIKSDVWSFGILLTELTTKGRVPYPGMVNR
EVLDQVERGYRMPCPPECPESLHDLMCQCWRKEPEERPTFE
YLQAFLEDYFTSTEPQYQPGENL

Compounds

S. No	Name	Type	Disease	References

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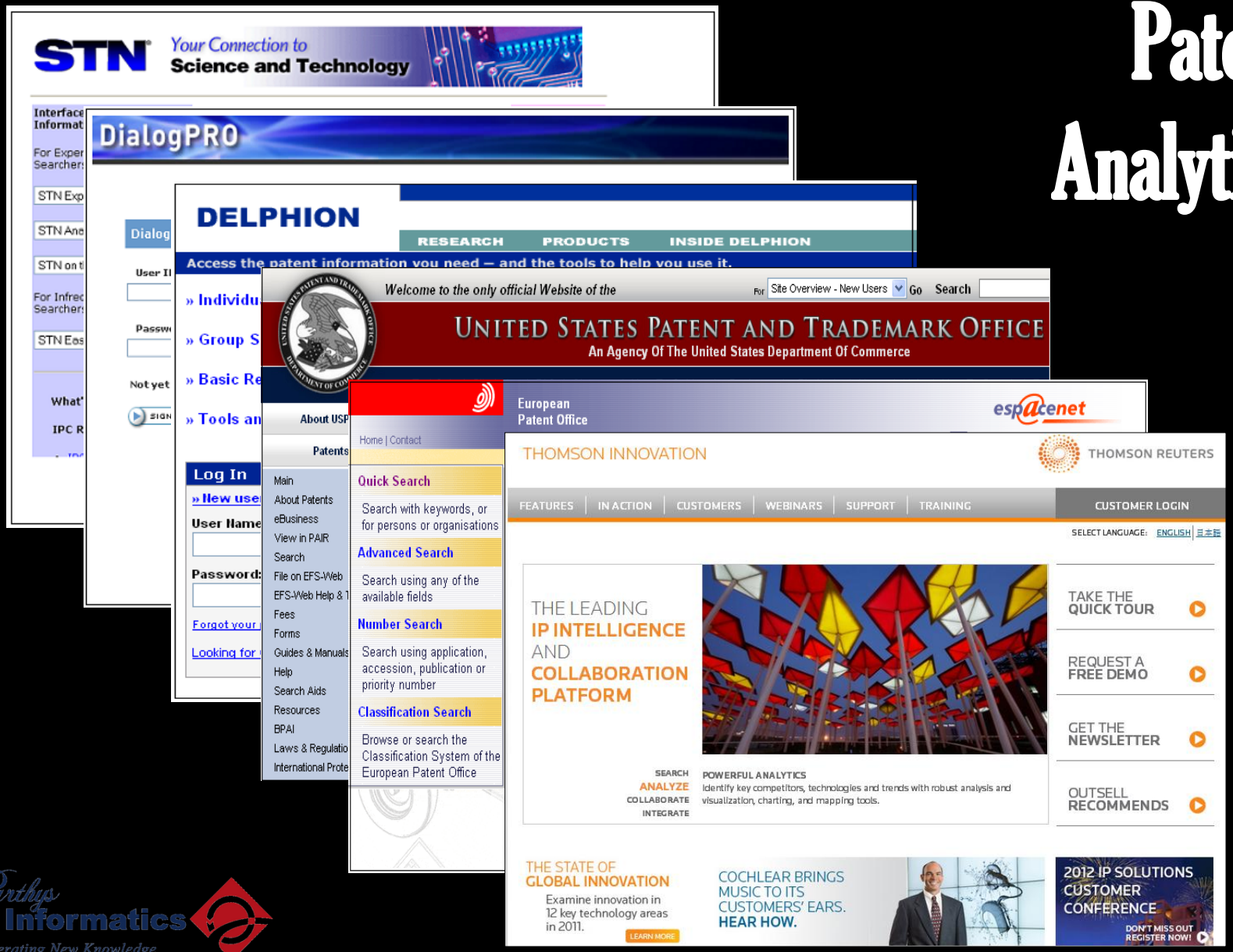
Searching is Our Business!

Patent Analytics



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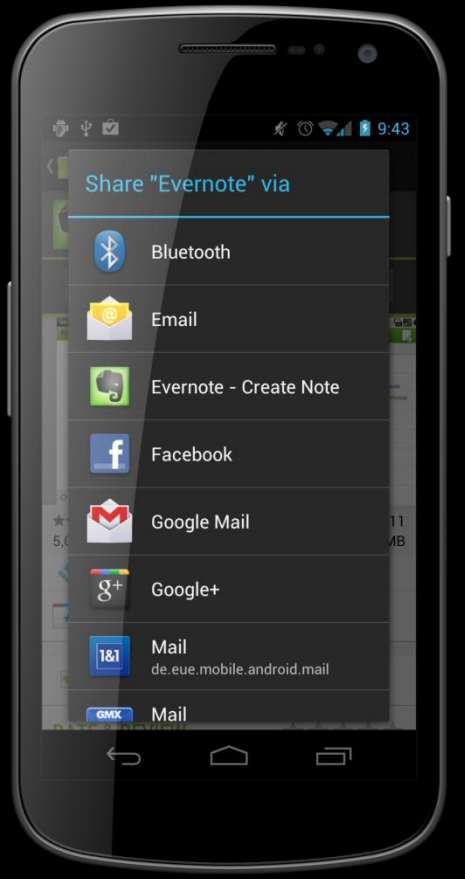
Internet for Phone Calls

Phone for Internet



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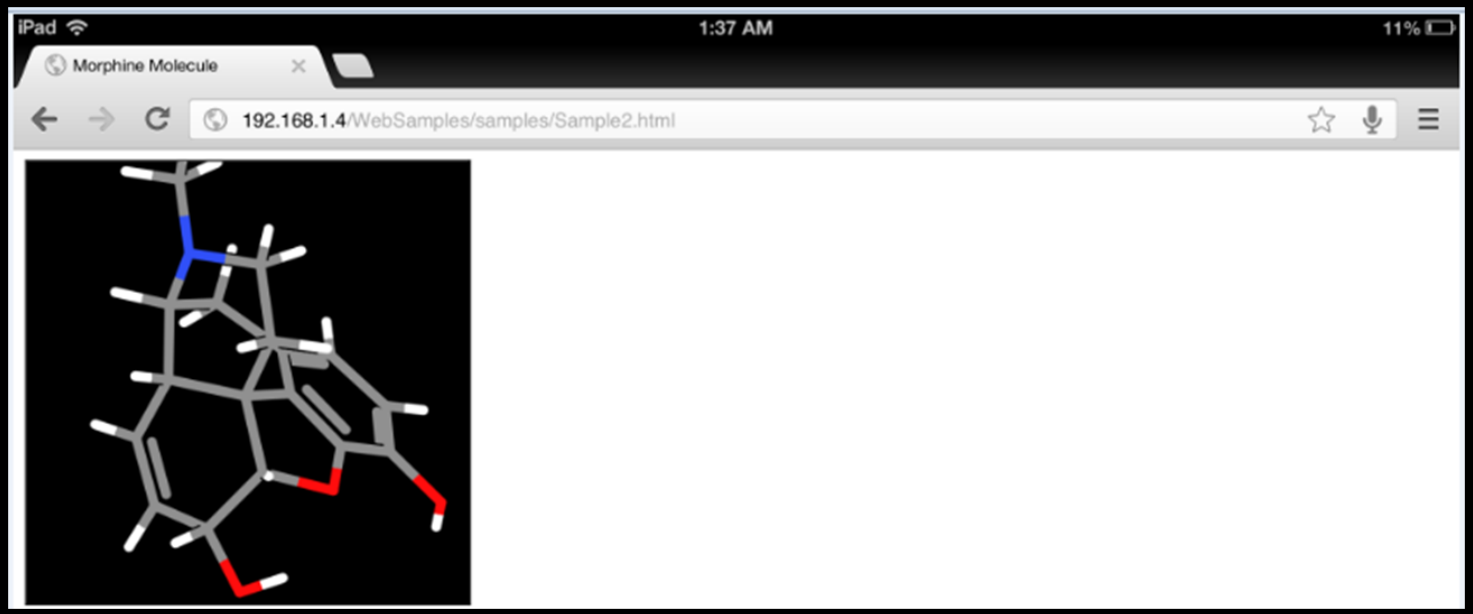
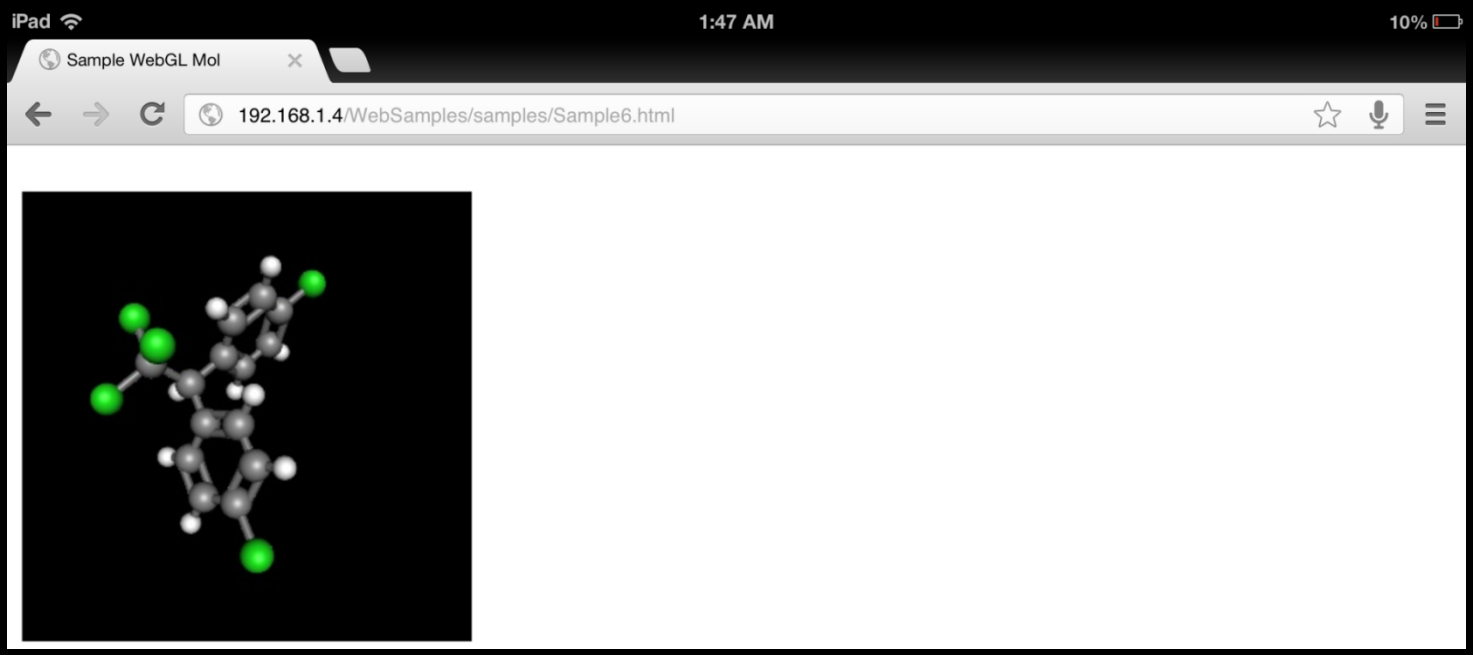


Mobile device enabled Chemistry



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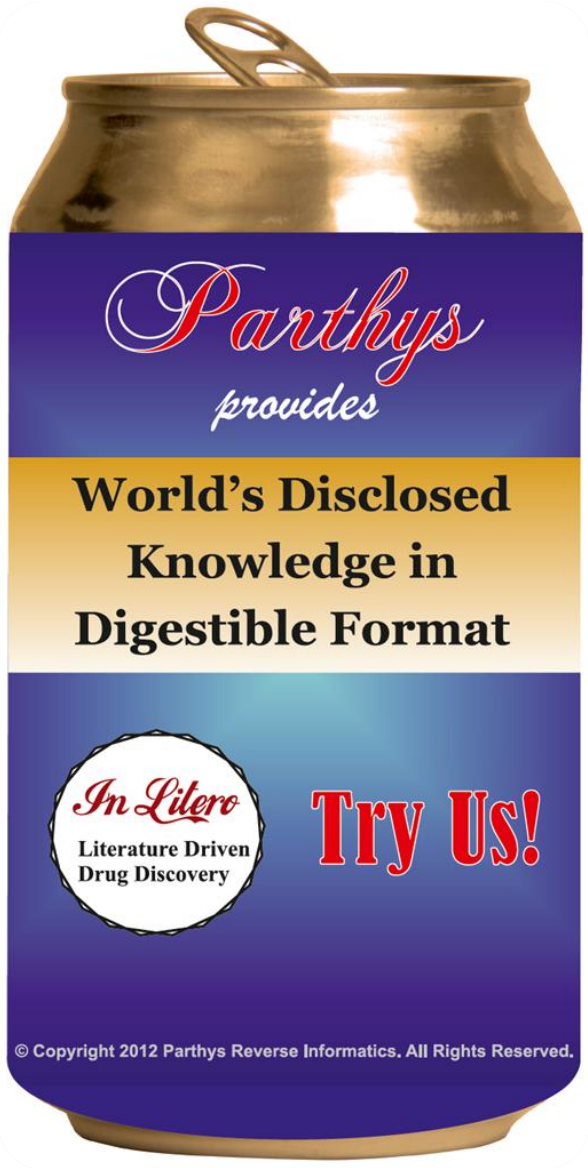

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Thank You!

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