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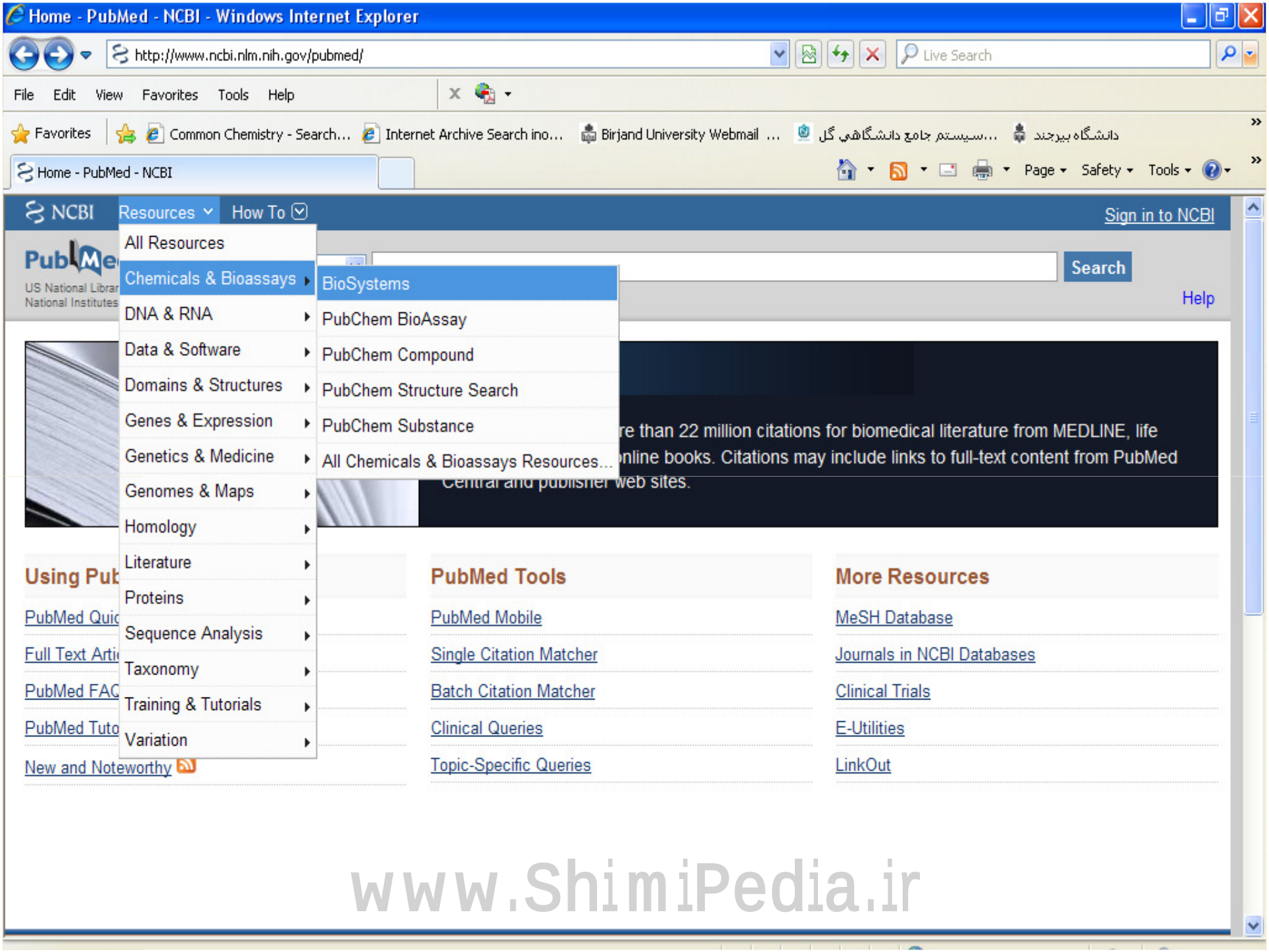

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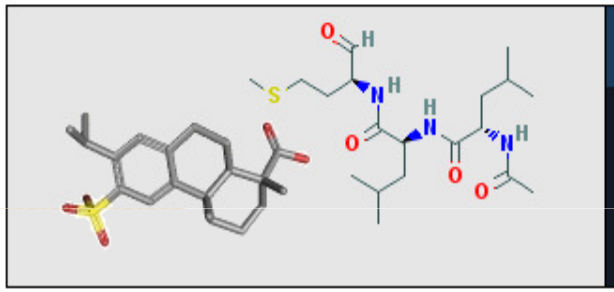

PubChem Compound

The PubChem Compound Database contains validated chemical depiction information provided to describe substances in PubChem Substance. Structures stored within PubChem Compounds are pre-clustered and cross-referenced by identity and similarity groups.

Using PubChem

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- PubChem Help
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- PubChem Publications
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PubChem Tools

- Chemical Structure Search
- BioActivity Analysis
- Deposition Gateway
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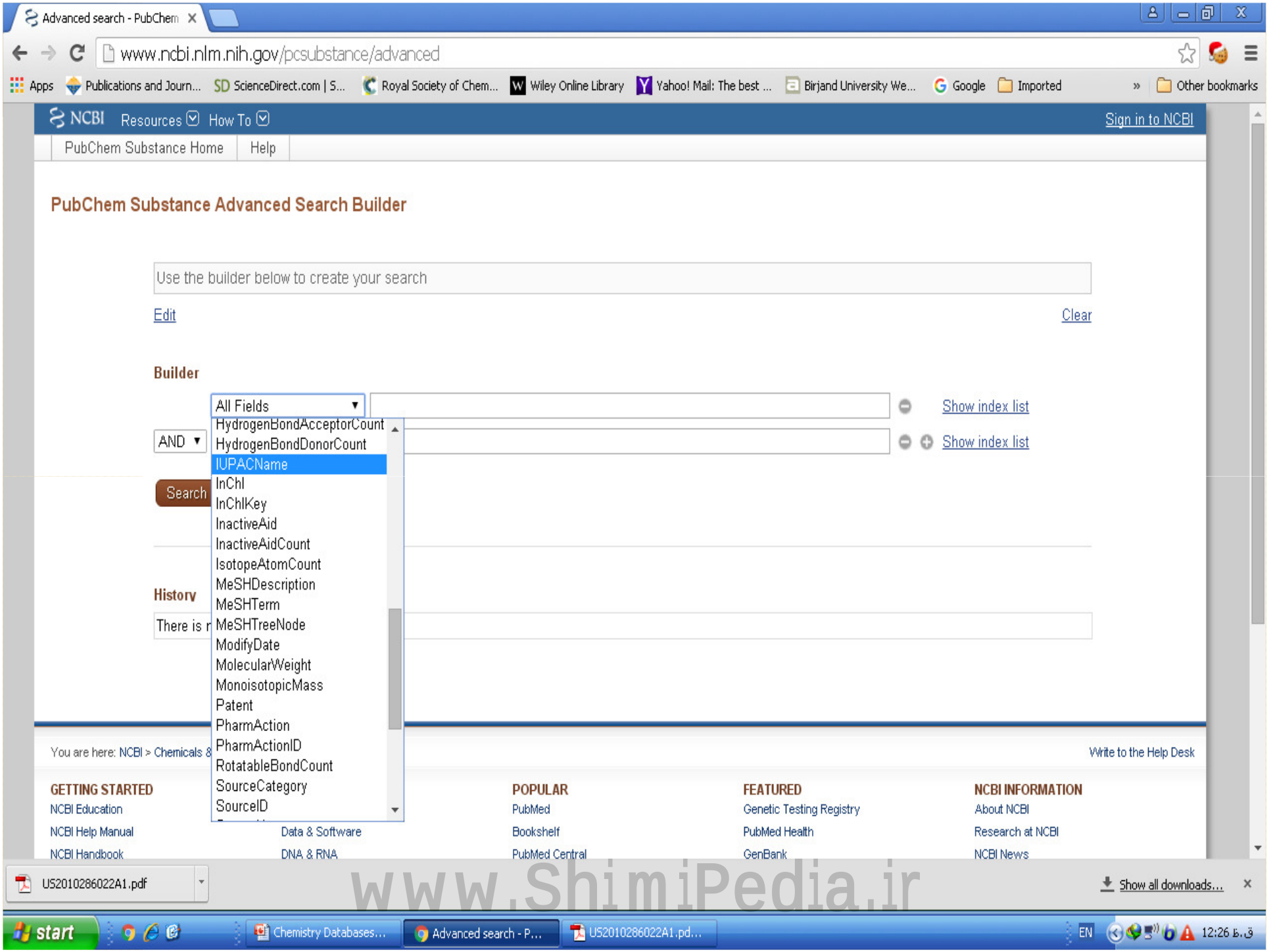
- PubChem FTP

More Resources

- PubChem Homepage
- PubChem BioAssay
- PubChem Substance
- Structure
- BioSystems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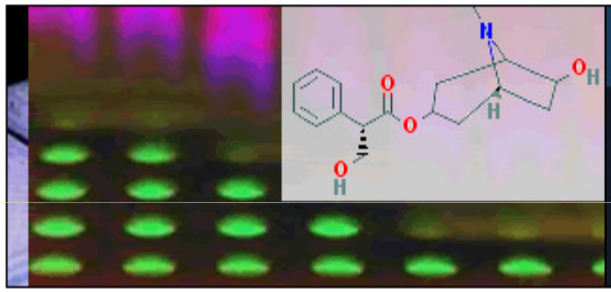

PubChem Substance

The PubChem Substance Database contains descriptions of samples, from a variety of sources, and links to biological screening results that are available in PubChem BioAssay. If the chemical contents of a sample are known, the description includes links to PubChem Compound.

Using PubChem

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- PubChem News

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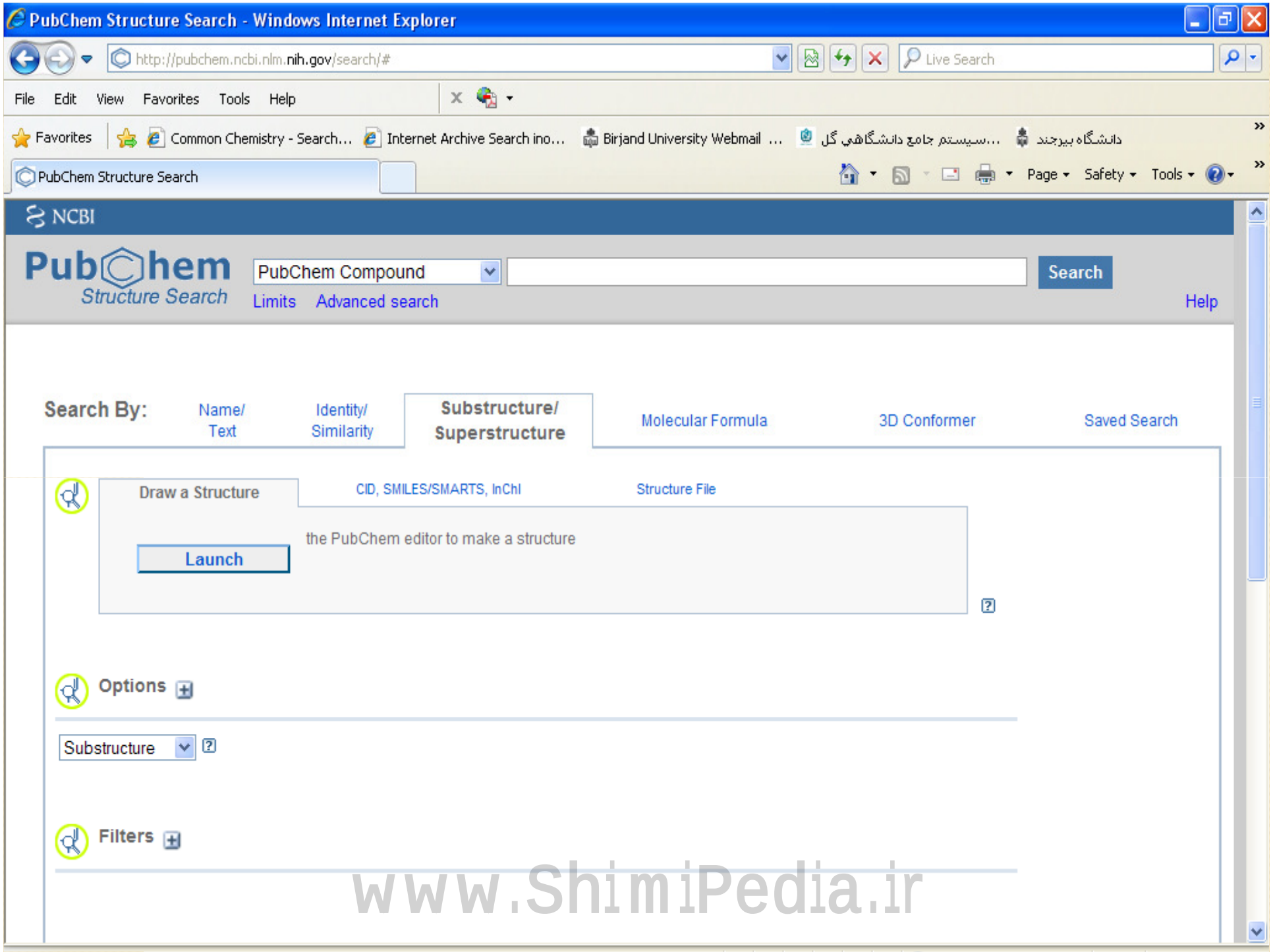
- PubChem Compound
- Structure
- BioSystems



PubChem Sketcher V2.4 - Windows Internet Explorer

http://pubchem.ncbi.nlm.nih.gov/edit2/index.html?smiles=C1(%3DCC%3DC(C%3DC1)C(C)N)C(%3DO)%

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PubChem Structure Search | PubChem Sketcher V2.4

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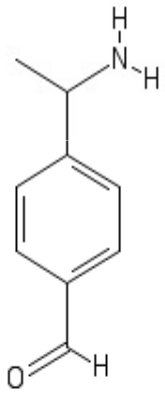

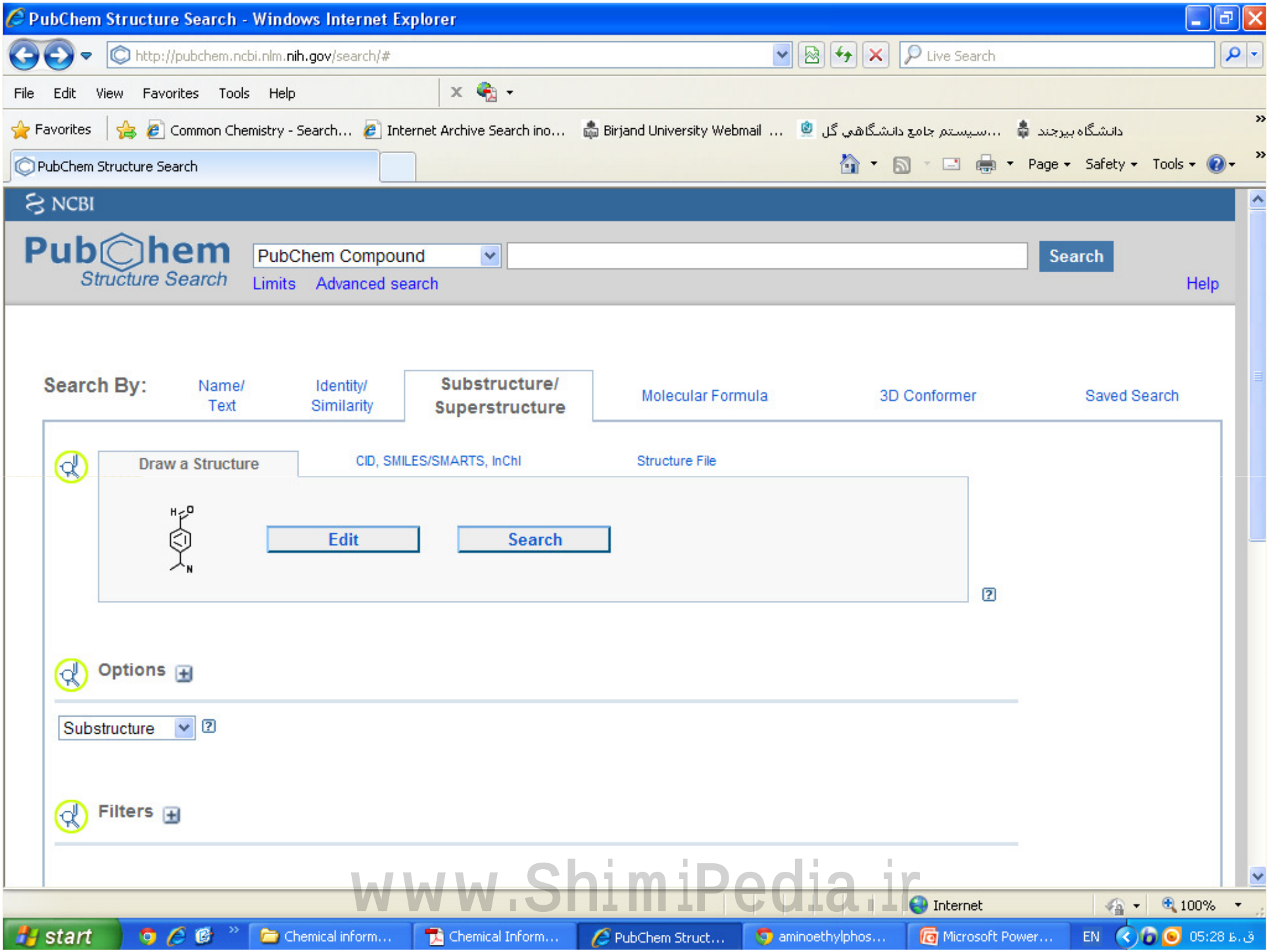
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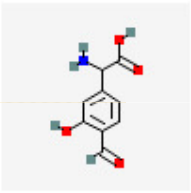
1. 

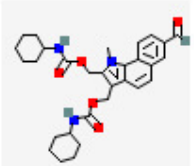
Forphenicine; 4-Formyl-3-hydroxyphenylglycine; BRN 5008292 ...

MW: 195.172060 g/mol MF: $C_9H_9NO_4$

IUPAC name: 2-amino-2-(4-formyl-3-hydroxyphenyl)acetic acid

CID: 42560

Summary Similar Compounds PubMed (MeSH Keyword)

2. 

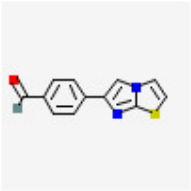
NSC683400; AC1L8VY7; NSC-683400 ...

MW: 519.631880 g/mol MF: $C_{30}H_{37}N_3O_5$

IUPAC name: [2-(cyclohexylcarbamoyloxymethyl)-7-formyl-1-methylbenzo[g]i...

CID: 388464

Summary Similar Compounds Tested in 62 BioAssays

3. 

4-imidazo[2,1-b][1,3]thiazol-6-ylbenzaldehyde; AQ-776/42801094; NSC707998 ...

MW: 228.269720 g/mol MF: $C_{12}H_8N_2OS$

IUPAC name: 4-imidazo[2,1-b][1,3]thiazol-6-ylbenzaldehyde

CID: 398284

Summary Similar Compounds

AQ-776/42801253; NSC708001; AC1L9GA9 ...

Actions on your results

BioActivity Analysis
Analyze the BioActivities of the compounds

Structure Clustering
Cluster structures based on structural similarity

Structure Download
Download the structures in various formats

Refine your results · What's this?

Chemical Properties

Rule of 5 (465)

BioActivity Experiments

BioAssays, Active (6)

BioAssays, Tested (14)

Depositor Category

Biological Properties (247)

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Journal Publishers (121)

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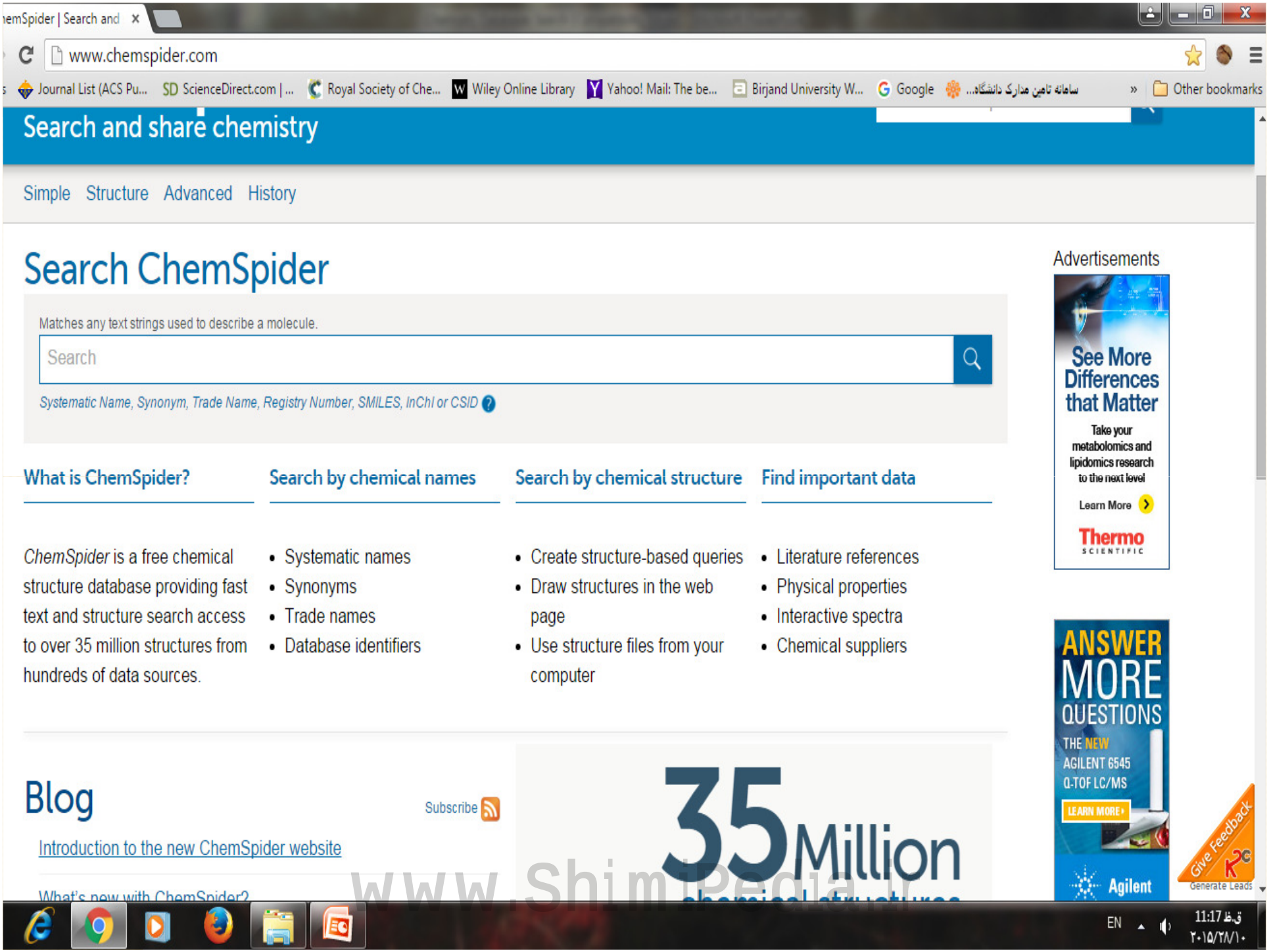

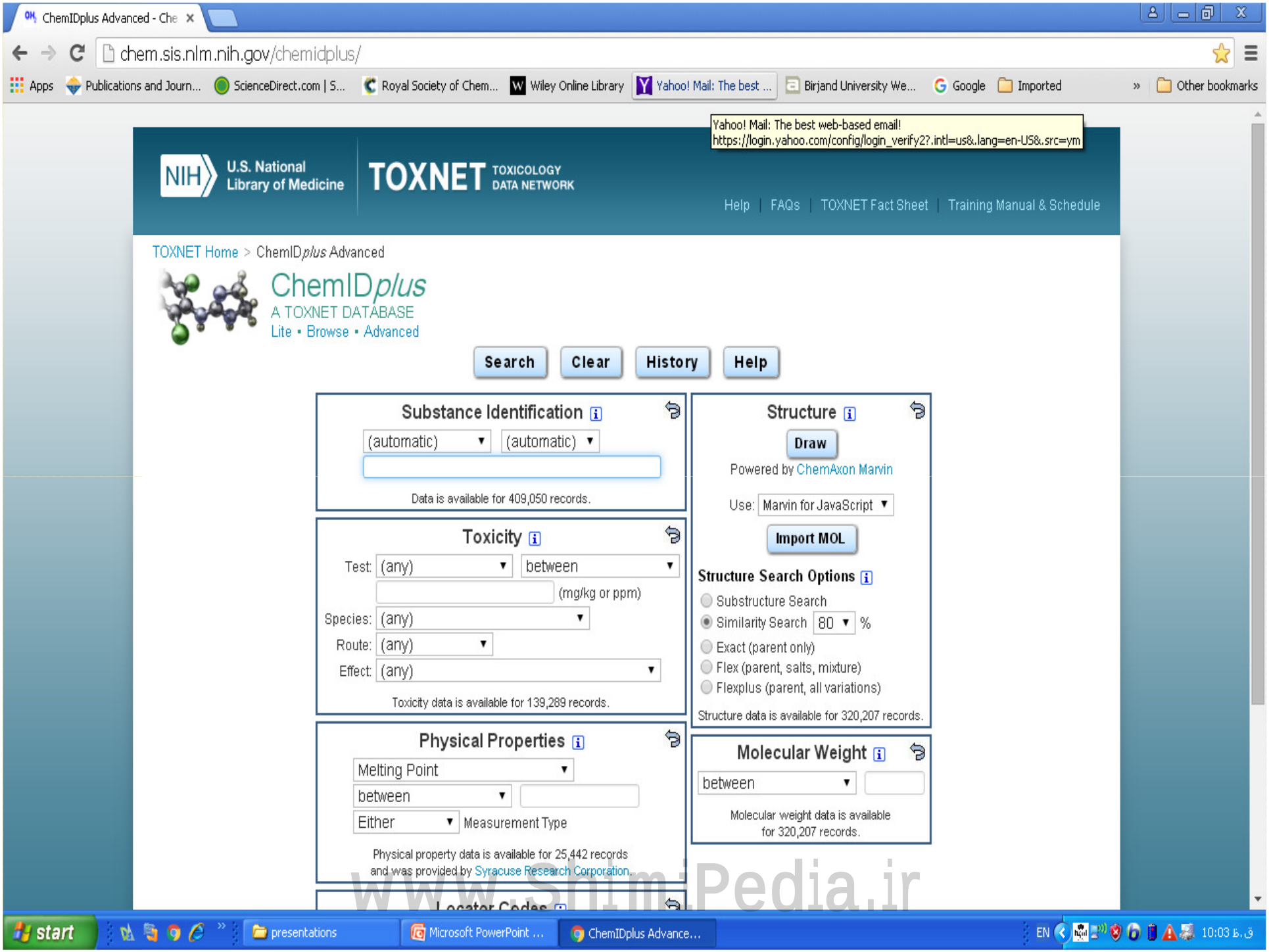
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Data is available for 409,050 records.
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Draw
Powered by ChemAxon Marvin
Use: Marvin for JavaScript
Import MOL
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Substructure Search
Similarity Search 80 %
Exact (parent only)
Flex (parent, salts, mixture)
Flexplus (parent, all variations)
Structure data is available for 320,207 records.
Toxicity
Test: (any) between
(mg/kg or ppm)
Species: (any)
Route: (any)
Effect: (any)
Toxicity data is available for 139,289 records.
Physical Properties
Melting Point
between
Either Measurement Type
Physical property data is available for 25,442 records
and was provided by Syracuse Research Corporation.
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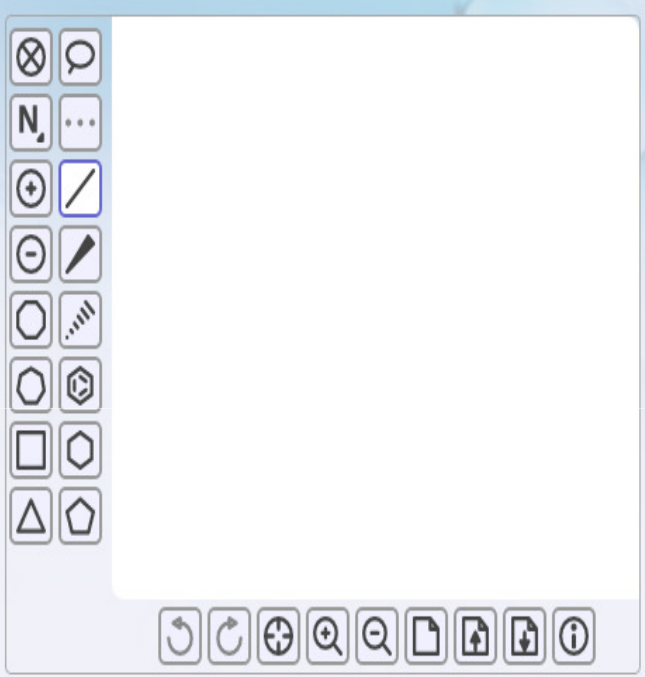

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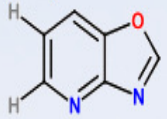
You can block substituents at a particular position by drawing explicit hydrogen atoms.



next hint...

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Name: Lipitor, Ibuprofen CAS Num: 15687-27-1 SMILES: S=C=NC

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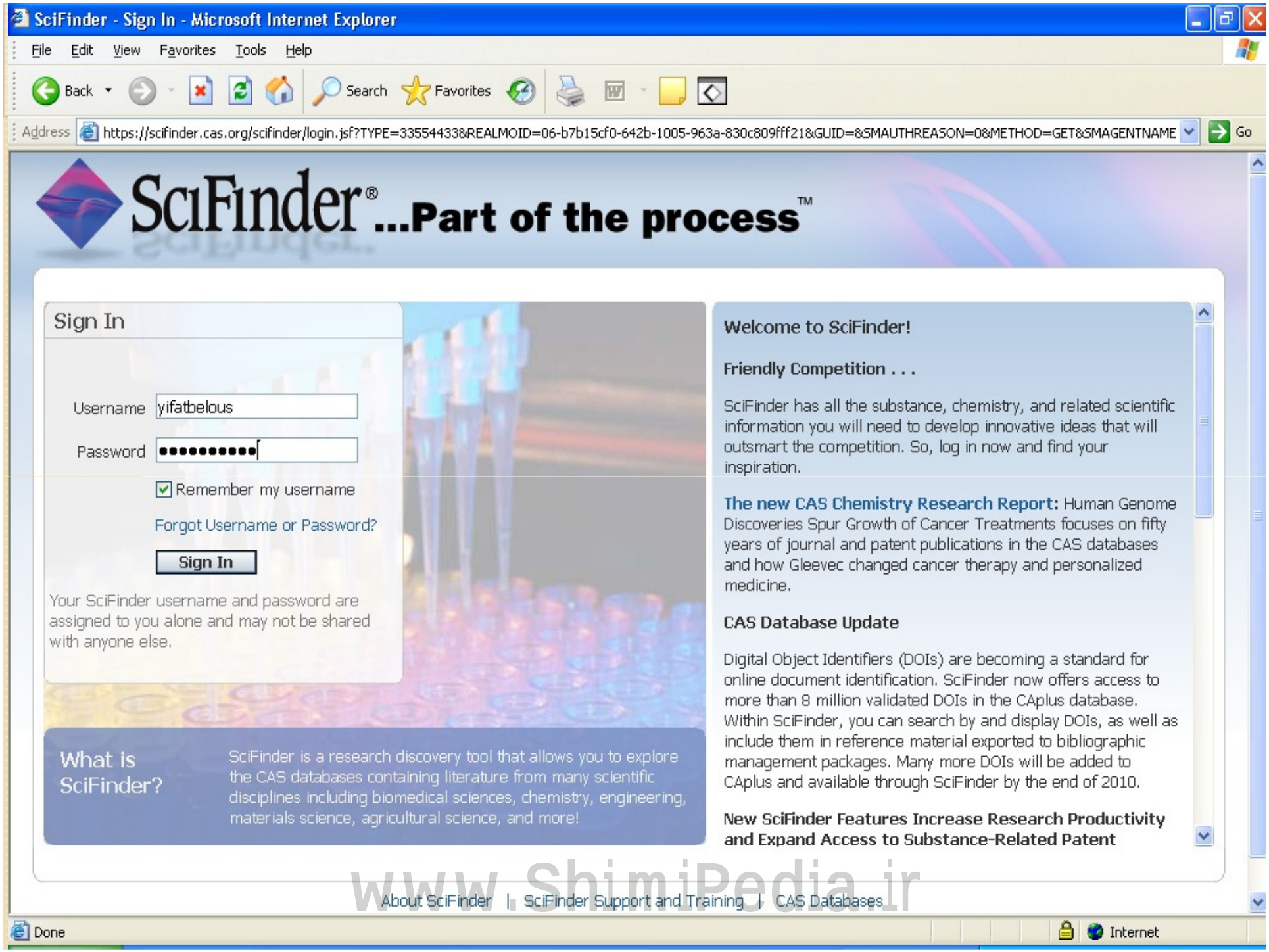

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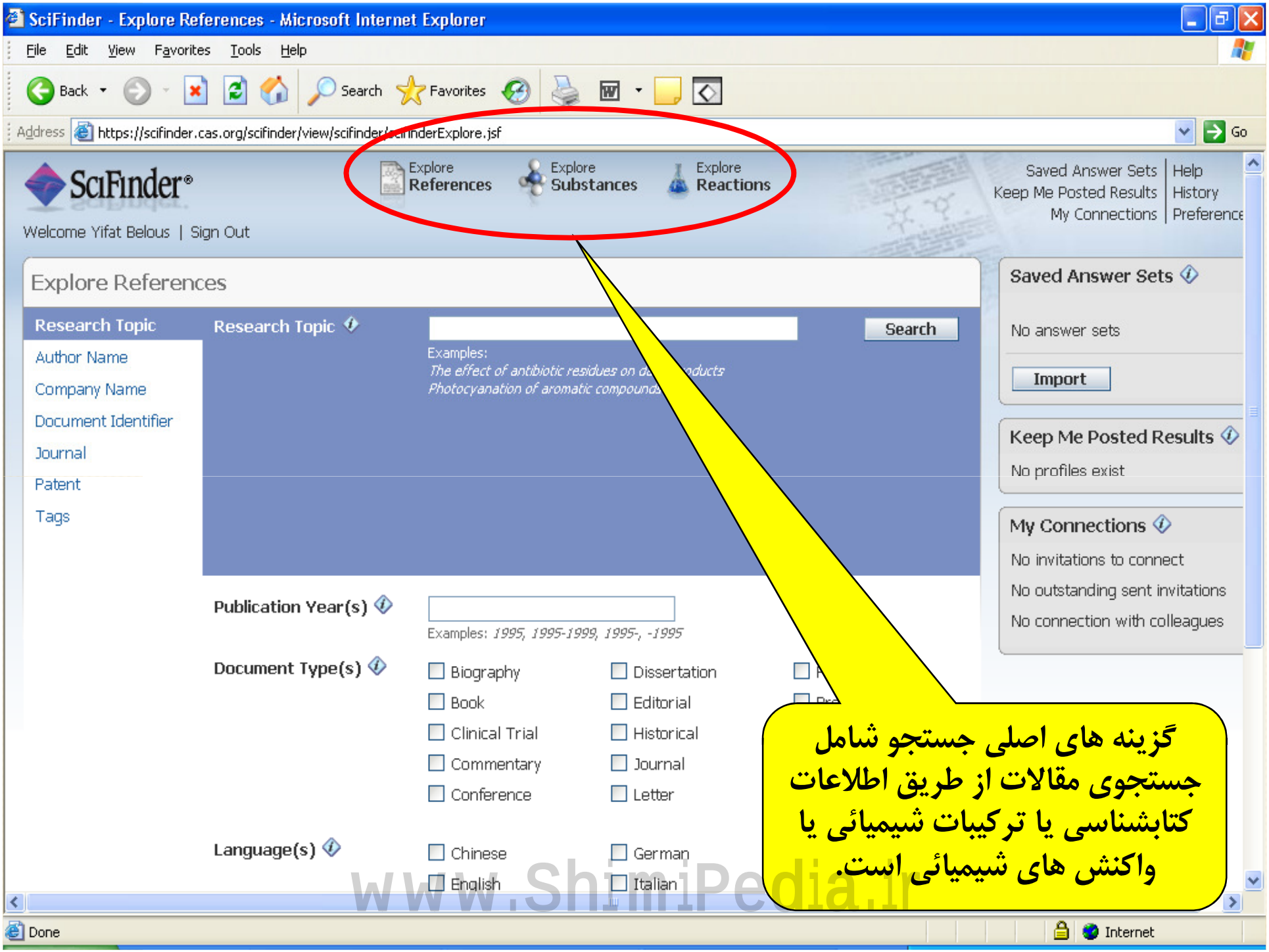
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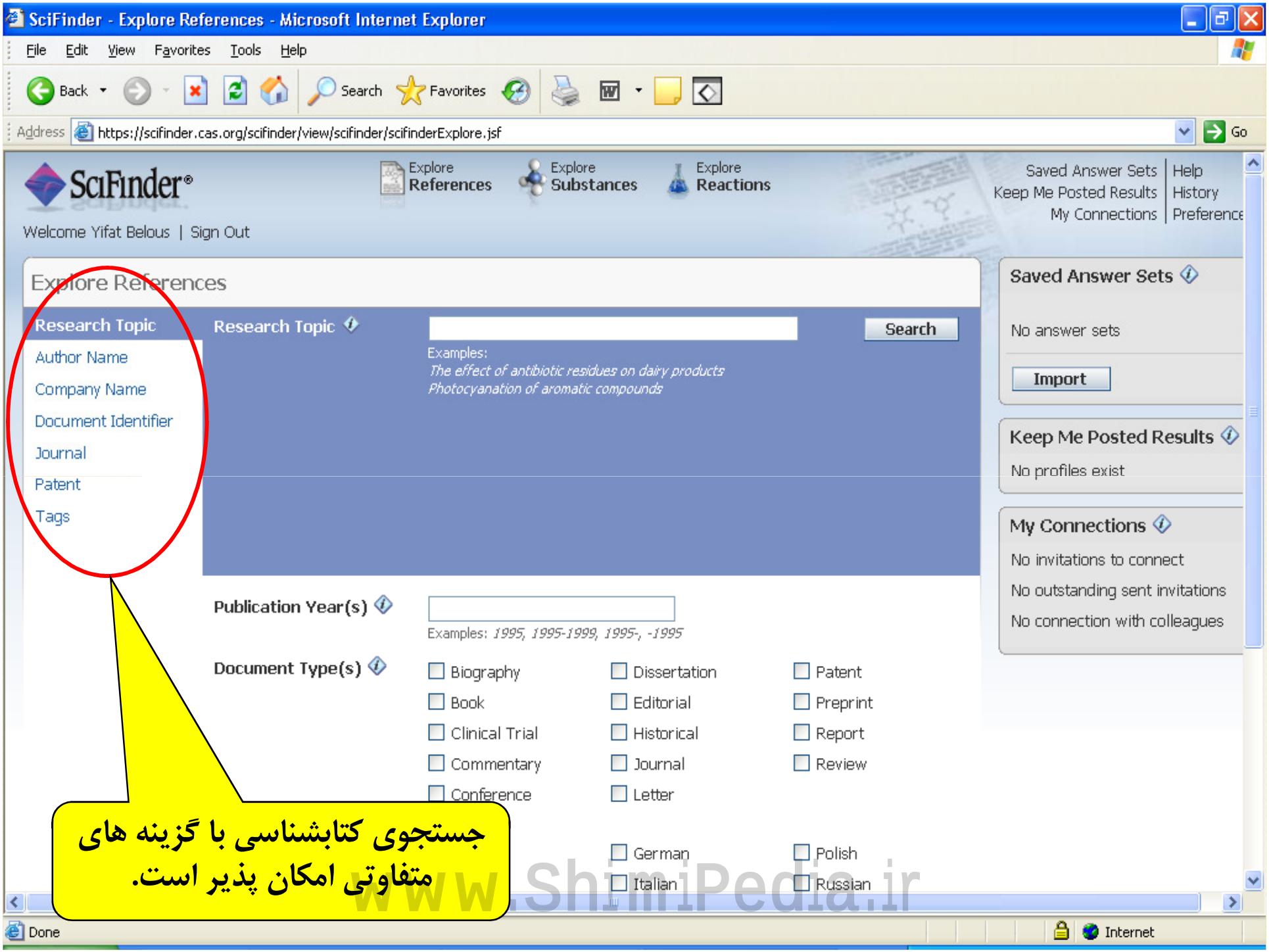
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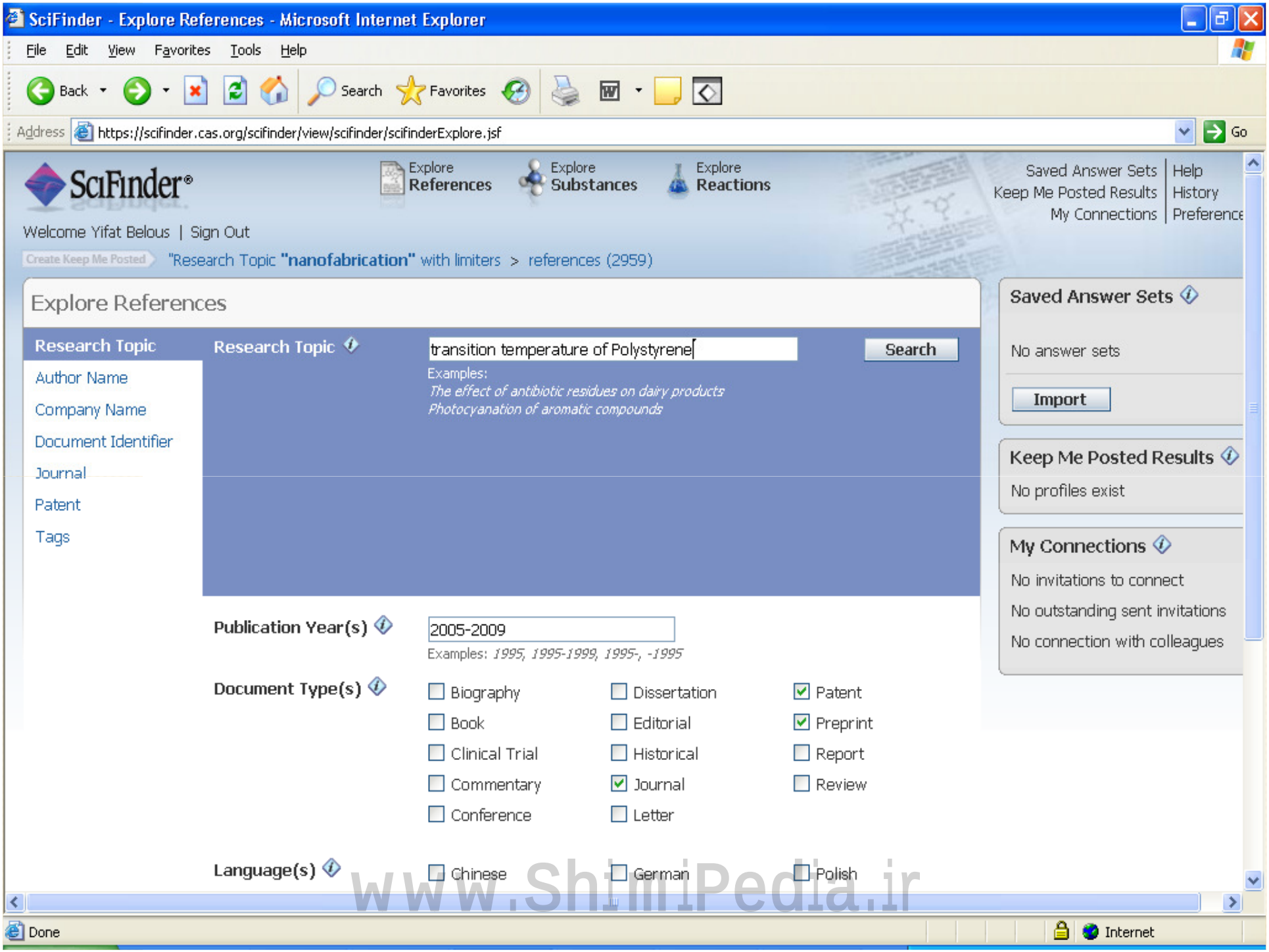

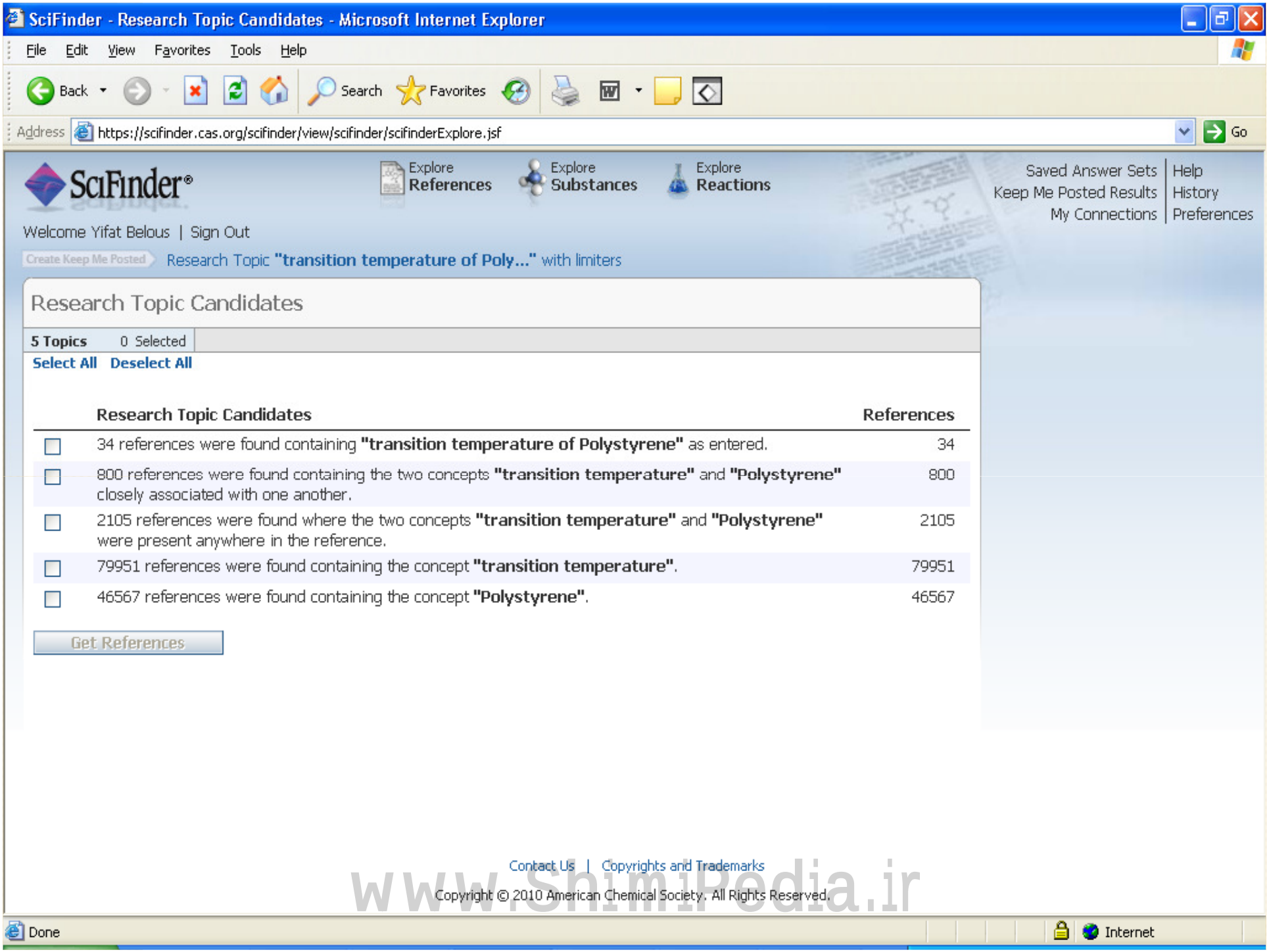

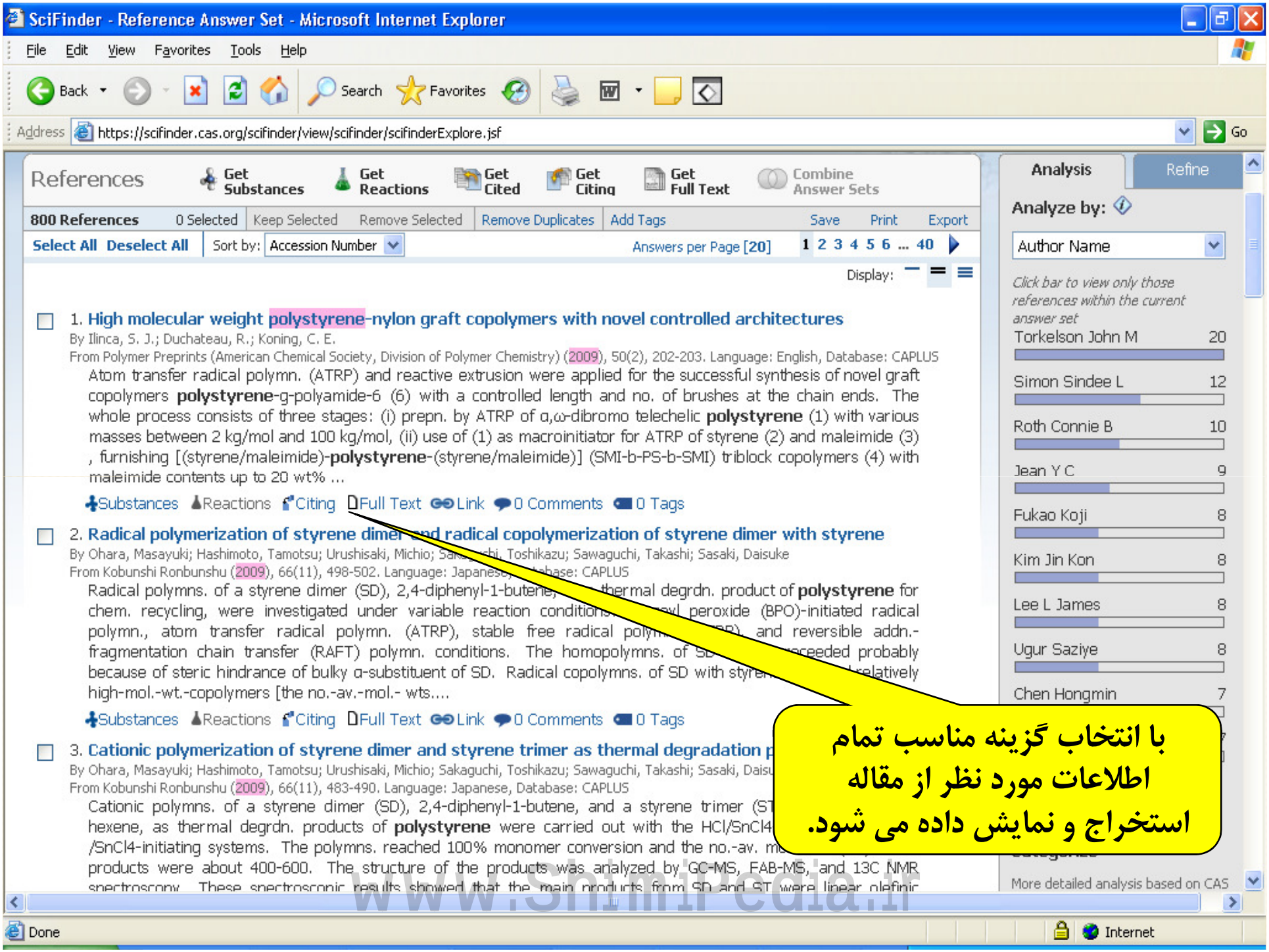

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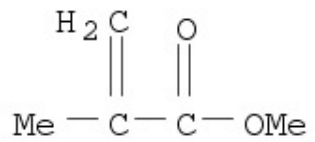
1. **Substance Detail**
9011-14-7

80-62-6
$C_5H_8O_2$



$(C_5H_8O_2)_x$

2-Propenoic acid, 2-methyl-, methyl ester, homopolymer

~85,621 References
Reactions
Commercial Sources
Regulatory Information
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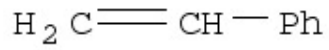
2. **Substance Detail**
9003-53-6

100-42-5
C_8H_8

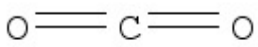


$(C_8H_8)_x$

Benzene, ethenyl-, homopolymer

~140,325 References
Reactions
Commercial Sources
Regulatory Information
Link

3. **Substance Detail**
124-38-9



CO_2

Carbon dioxide

~263,773 References
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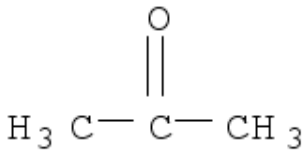
4. **Substance Detail**
67-64-1



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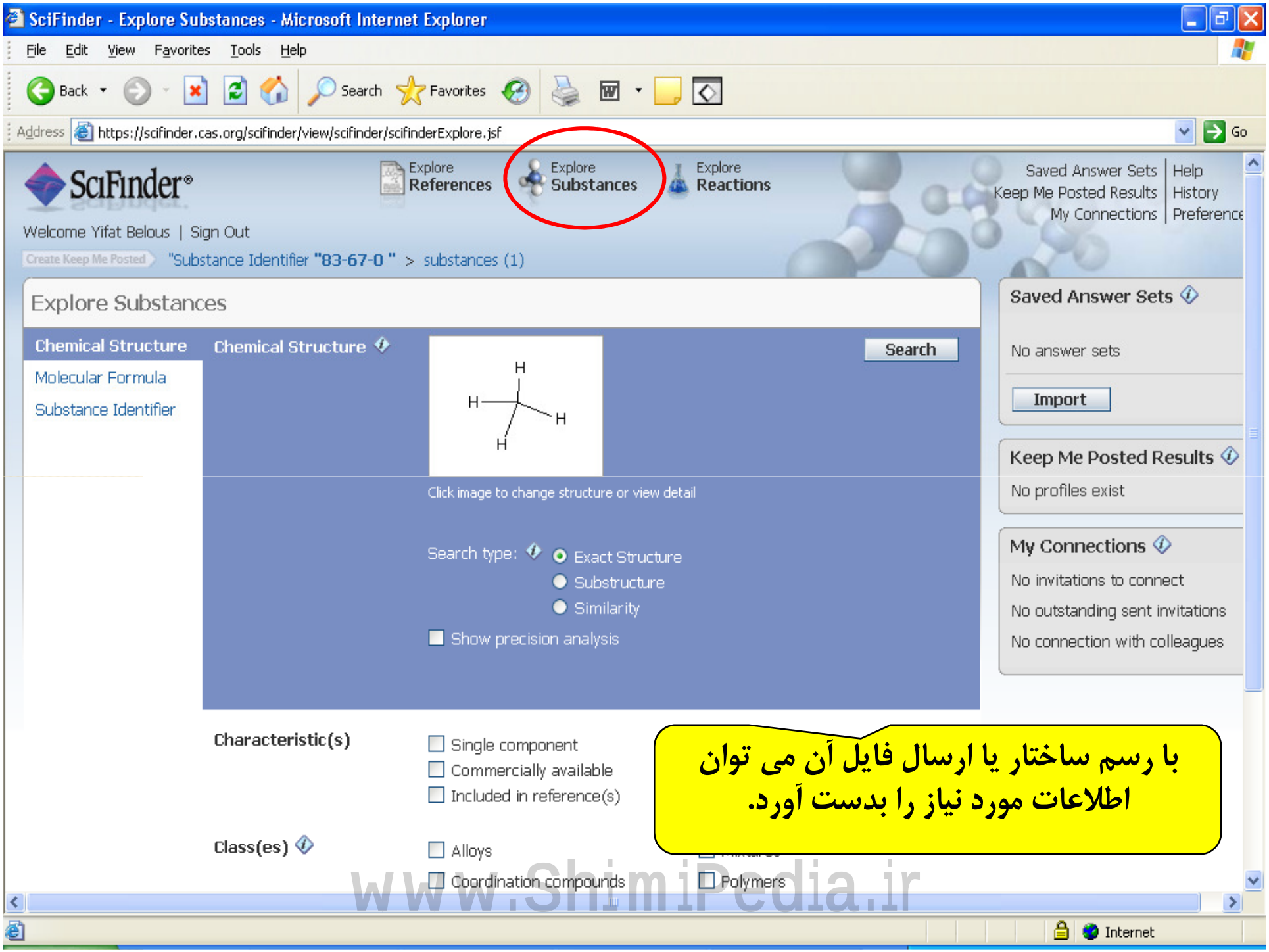
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SciFinder - Substance Answer Set - Microsoft Internet Explorer

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Create Keep Me Posted | Substance Identifier "83-67-0 " > substances (1)

Substances | Get References | Get Reactions | Get Commercial Sources | Combine Answer Sets

1 Substance 0 Selected | Keep Selected | Remove Selected | Save | Print | Export

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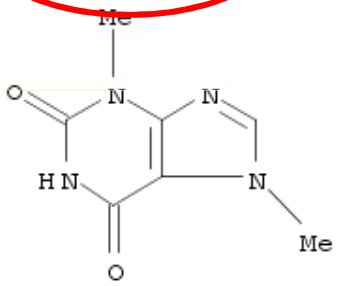
View:

1. Substance Detail
83-67-0



$C_7H_8N_4O_2$

1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-

~3,630 References
Reactions
Commercial Sources
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Analysis | Refine

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Commercially Available 1

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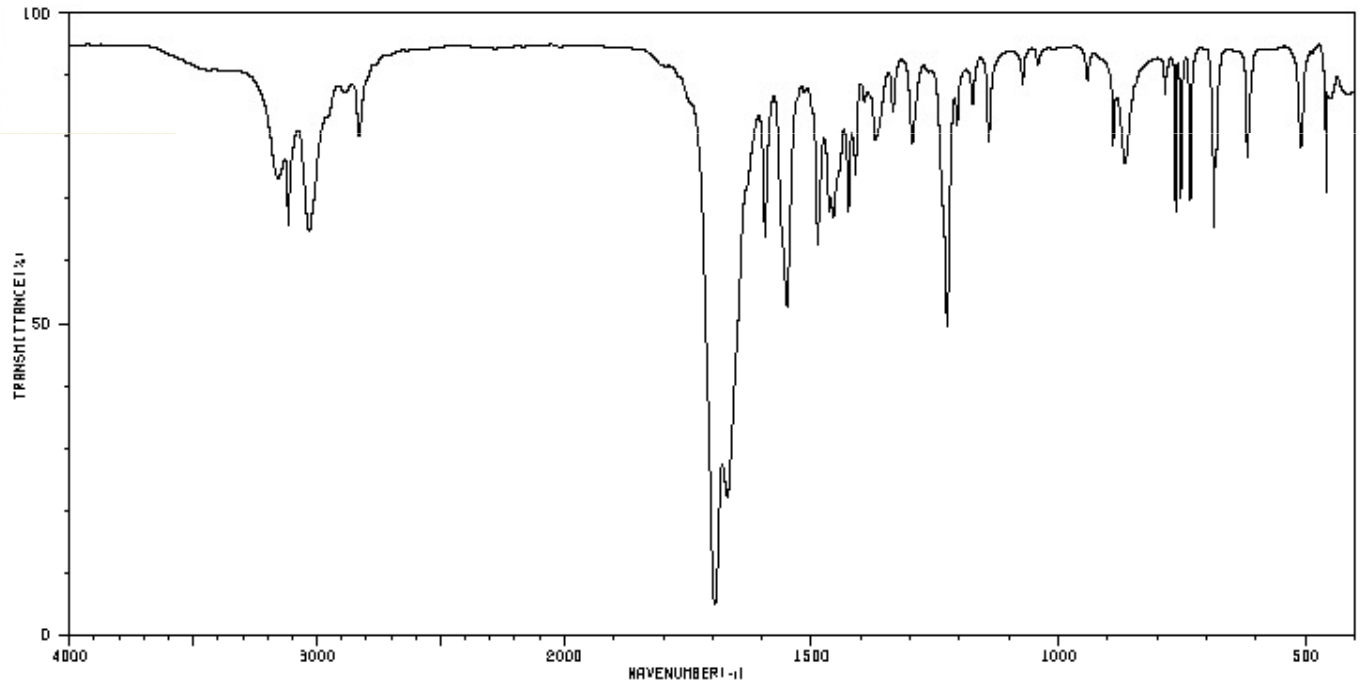
Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	1.0	pH 1 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 2 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 3 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 4 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 5 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 6 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 7 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 8 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 9 Temp: 25 °C	(55)	
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(55)	

Chemical Properties	Value	Condition	Note	Top
Koc	6.99	pH 1 Temp: 25 °C	(55)	
Koc	9.31	pH 2 Temp: 25 °C	(55)	
Koc	9.63	pH 3 Temp: 25 °C	(55)	
Koc	9.66	pH 4 Temp: 25 °C	(55)	
Koc	9.66	pH 5 Temp: 25 °C	(55)	
Koc	9.66	pH 6 Temp: 25 °C	(55)	
Koc	9.65	pH 7 Temp: 25 °C	(55)	
Koc	9.54	pH 8 Temp: 25 °C	(55)	
Koc	8.59	pH 9 Temp: 25 °C	(55)	
Koc	4.33	pH 10 Temp: 25 °C	(55)	
logD	-0.86	pH 1 Temp: 25 °C	(55)	
logD	-0.74	pH 2 Temp: 25 °C	(55)	
logD	-0.72	pH 3 Temp: 25 °C	(55)	
logD	-0.72	pH 4 Temp: 25 °C	(55)	
logD	-0.72	pH 5 Temp: 25 °C	(55)	

IR Absorption Spectrum

Print



Spectrum ID

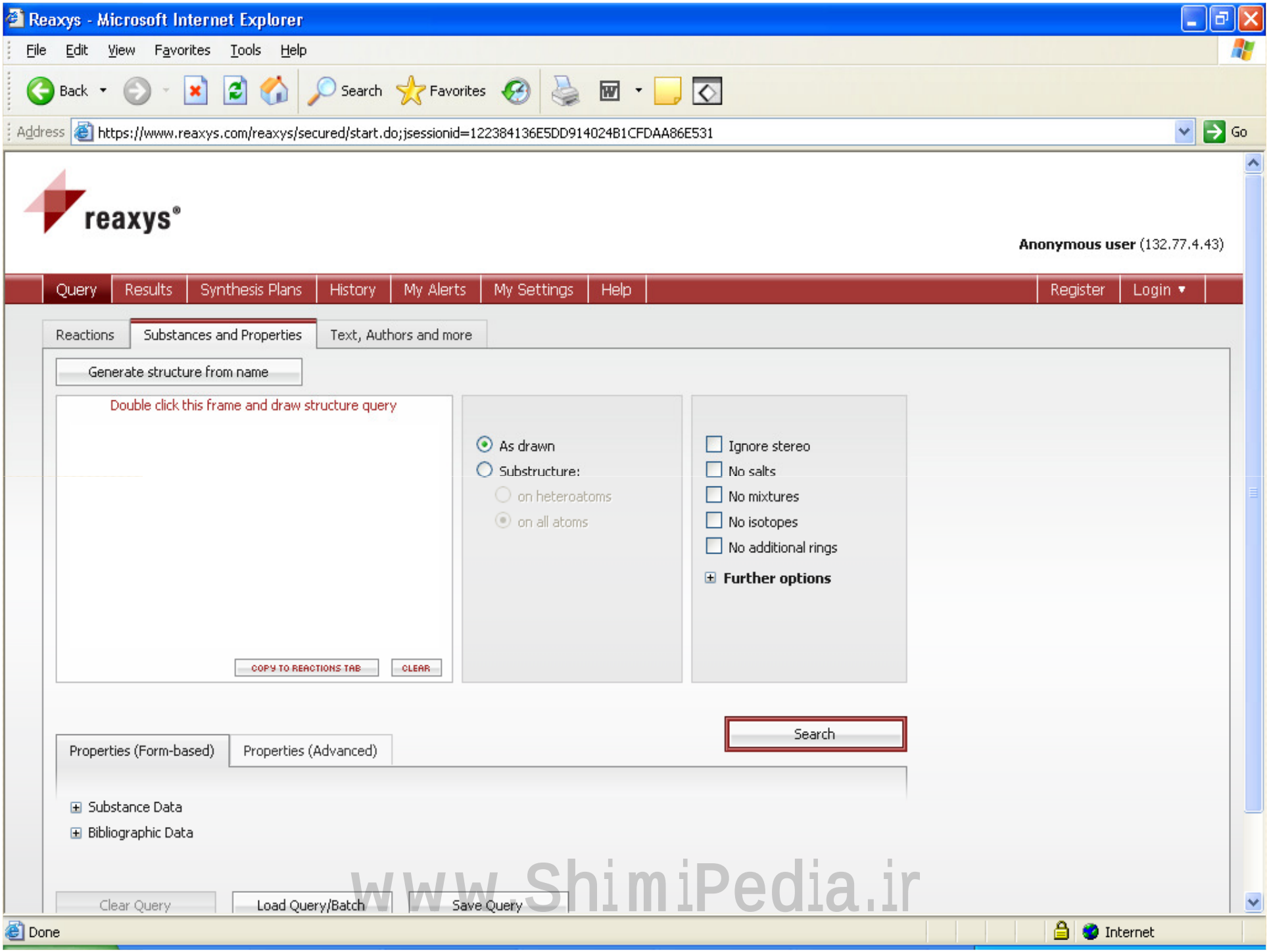
NIDA63087

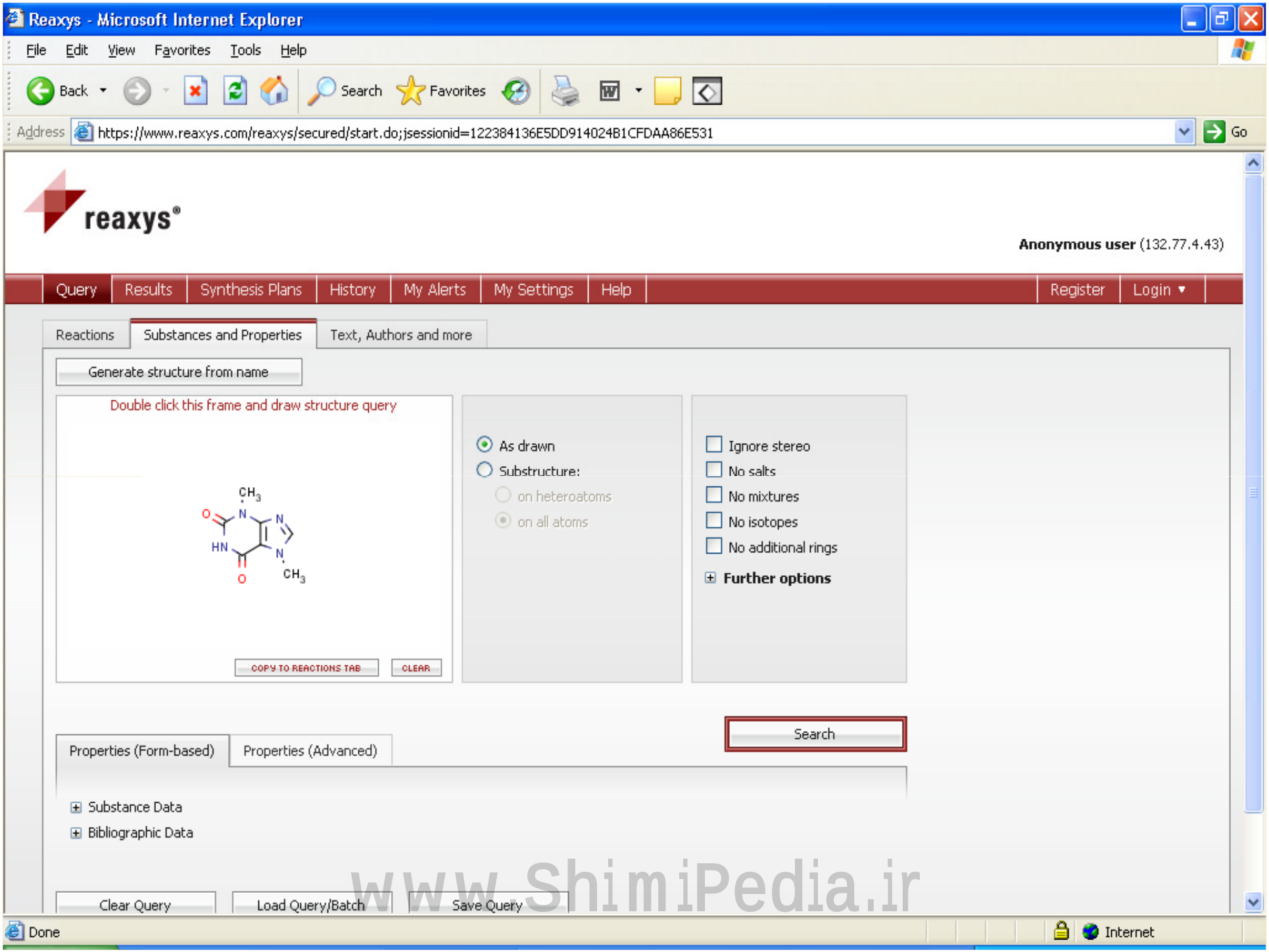
Spectrometer

Nicolet 170SX or JASCO FT/IR-410

Source

Integrated Spectral Database System of Organic Compounds. (Data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan))





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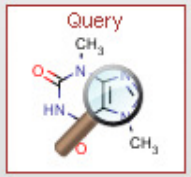

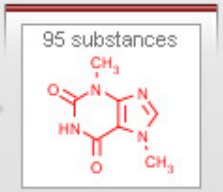

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Filter by:

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- Publication Year

Substances (Grid) | Substances (Table) | Citations

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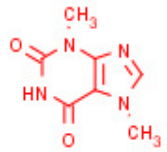
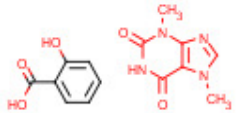
	Structure	Chemical Name	N° of preparations All Preps | All Reactions	Available Data	N° of ref.	Boiling Point
1	 Synthesize Show Details	3,7-dimethyl xanthine theobromine 3,7-dimethylxanthine 3,7-dimethylxantine paraxanthine Theobromine 3,7-dimethyl-3,7-dihydro-purine-2,6-dione	58 prep out of 368 reactions.	Identification Physical Data (167) Spectra (75) Bioactivity/Ecotox (91) Use/Application (218) Natural Product (19)	501	
2	 Show Details	3,7-dimethyl-3,7-dihydro-purine-2,6-dione, theobromine; salicylate 3,7-dimethyl-3,7-dihydro-purine-2,6-dione; salicylate (1:1) 3,7-Dimethyl-3,7-dihydro-purin-2,6-dion, Theobromin; Salicylat 3,7-Dimethyl-3,7-dihydro-purin-2,6-dion; Salicylat (1:1)	0 prep out of 1 reactions.	Physical Data (1) Spectra (1)	3	

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