

SOS 4.0 and The Ranking of Hits Using the InfoChem Algorithm for Structure Searching

Searches	Definition	Type	Relevance
XSS	Exact Structure Search	Exact Match	↓ decreasing
IXSS	Isomer Exact Structure Search		
TXSS	Tautomer Exact Structure Search		
PXSS	Parent Exact Structure Search ¹		
FlexXSS	Flexible Exact Structure Search ²		
SSS	Substructure Search	Substructure Match	

¹Finds identical main components of the query | ²Finds stereo and isotopic isomers, parent substructures and salts, tautomers or complexes containing the query structure

SOS 4.0 and The Ranking of Hits Using the InfoChem Algorithm for Reaction Searching

Searches	Definition	Type	Relevance
XRS	Exact Reaction Search	Exact Match	↓ decreasing
IXRS	Isomer Exact Reaction Search		
XRSSUB	Exact Subreaction Search		
IXRSSUB	Isomer Exact Subreaction Search		
RSS_RT Narrow ¹	Combined Reaction Substructure Search and Reaction Type Search	Reaction Substructure and Reaction Type Match	
RSS_RT Medium ²			
RSS_RT Broad ³			
RTS Narrow ¹	Overall Reaction Type Search, resulting in Similar Reactions	Overall Reaction Type Match	
RTS Medium ²			
RTS Broad ³			
RXCLUSTER Narrow ¹	Discrete Reaction Type Search, resulting in Similar individual Reaction sites	Discrete Reaction Type Match	
RXCLUSTER Medium ²			
RXCLUSTER Broad ³			

¹ Narrow – Reaction centers plus first and second atom sphere | ² Medium – Reaction centers plus first atom sphere

³ Broad – Reaction center only

