or even a crystal or spectrometrically determined 3D structure. A 3D model may also contain information about multiple low-energy conformations and atom, bond, and molecular properties such as partial atomic charge, HOMO/LUMO energy, etc.

3D Query Features. Topographical features that relate atoms, bonds, and other 3D features to each other in a pharmacophore or 3D substructure search query. Typical features include (1) objects such as atoms, centers of rings, electron lone pairs, and regions of exclusion and (2) measurements of distance, angle, dihedral angle, radius of exclusion, etc. Measurements often have a range associated with them (e.g., distance between a carbonyl oxygen and a secondary amino nitrogen is 3.4–5.0 Å).

Agent. A computer program that can run autonomously and on a schedule to perform database searches, maintenance, and reporting activities that a chemist would otherwise have to do manually. An example would be an Internet notification service that sends the chemist an e-mail notification whenever a particular database has been updated.

Application Tier. In a multi-tier architecture, the collection of programs that run on the chemist's client or workstation machine. It is the tier of programs "closest" to the chemist in the architecture. Typically this may be a Web client program or other program with a GUI that allows the chemist to interact with the architecture.

Artificial Intelligence. A branch of information science that attempts to use computer programs to perform or simulate human mental activity. Applications in chemistry include perceiving chemical structures, designing structures to fit topological or topographical criteria, designing 'novel' structures, etc. Many of the activities of AI overlap with, or contain elements of pattern recognition and data mining.

ASCII. American Standard Code for Information Interchage—a widely used system of encoding alphanumeric information into eight-bit bitsets (bytes). The expansion of information to include non-English characters requires the use of larger (16- or 32-bit) character sets such as Unicode.

Atom List. In a substructure search query, a list of allowed (or perhaps disallowed) atom types. Often represented within brackets: [Cl,Br,I].

Atom Stereochemistry. Usually refers to tetrahedral stereochemistry at a given atom, which must be a chiral or prochiral center. The stereochemistry may be local (or relative) or global (based on CIP conventions). If it is local, it usually is termed "parity" or some other nonspecific term, to distinguish it from true global stereochemistry (*R*,*S*). Local atom stereochemistry is a property of the atom and its nearest attached atoms. Global atom stereochemistry depends on the entire molecule and the stereochemistry at other chiral atoms. In some systems, the atom stereochemistry is perceived from the drawing of the structure, using "up" (wedged) and "down" (dashed) bond marks as cues. In linear notations, characters in the string can be used to specify the counterclockwise (@) or clockwise (@@) orientation of attachments at a given center.

Atom-Atom Mapping. The procedure of assigning each atom in a substructure query to a given atom in a candidate structure. The assigned structure atoms must match the query atom in all characteristics, including atom type, stereochemistry, charge, attachments, etc. In some structures, a query may map onto the structure in many ways (multiple mappings). Additionally, these mappings may overlap each other in terms of atoms and bonds, or they may be non-overlapping. Some search systems stop after the first mapping, whereas other perform exhaustive mapping, until no further mapping can be found.

Automap. A feature implemented in reaction indexing programs like REACCS, which attempts to automatically "discover" which atoms and bonds are involved in a reaction transformation (the reacting center atoms and bonds). The chemist draws the reaction or the reaction query as a set of reactants leading to a set of products, then invokes the Automap feature, which causes the reacting atoms and bonds to be marked and identified. When reacting center atoms and bonds are specified in both the query and the reactions in the database, reaction substructure searching is faster and gives fewer false hits.