This is a newly established section of MATCH, where in particular scientific software will be announced and described. We start with details on the program systems that were introduced in the preceding issue 27 of MATCH.

GENMAS and GENSTR-Systems Containing Structure Generator GEN

GENMAS is a system for generation of all possible chemical structures or substructures from any given molecular formula by the consideration of structural constraints. It distinguishes between the structural features that must be present in the output structures (MPSF-Mandatory Present Structural Fragments) and the structural features that must not be present in the output structures (MASF-Mandatory Absent Structural Fragments).

GENSTR is a system for generation of all chemical structures or substructures of organic compounds from structural fragments. The fragments can be selected from the table of standard fragments built into the system, built with a structure editor, and/or determined by the CARBON system based on ^{13}C NMR spectra. Therefore, the GENSTR system can be used with or without structures, exact or approximate molecular formula of the final structures, the number of fragments in the actual set, and/or the number and the type of free bonds can be used.

The main features of the systems:

- simple and easy to learn,
- user-friendly interface with windows and menus,
- user-friendly input of fragments and constraints,
- graphic representation of input fragments, structural constraints, and output structures,
- the generation procedure controlled by the display of intermediate results,
- the possibility to stop the generation at any time and display of already generated structures,
- the menu of standard built-in structural constraints,
- on-line, option dependent help.

Technical requirements:

- IBM XT/AT/286/386 personal computer or true compatible,
- Memory requirement: 640 K RAM or more,
- EGA/VGA/Hercules type graphic display,
- HARD DISK is recommended for GENMAS and GENSTR (each of two systems needs about 0,5 MBytes of space and for each of 1000 new generated structure it needs addional 1 MByte of space), but for CARBON it is necessary (CARBON with the collection of about 2500 ^{13}C NMR spectra and structures needs about 3 MBytes of space).

Both systems are written in Turbo Pascal programming language. For drawing chemical structures and fragments the TURBO Pascal standard graphic routines are used. GENMAS and GENSTR system (without CARBON system and the collection) are down-loaded and expanded from 1 floppy of 1.2 MBytes, CARBON with the collection comes on 3 floppies. The user manuals of about 100 pages are included.

The price:
GENMAS: 500 USD, GENSTR: 500 USD, CARBON with collection: 2000 USD

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GOLD: THE GENERATOR OF CHEMICAL STRUCTURES FOR QSAR STUDIES

The GOLD menu-driven software allows to generate the database of chemical structures with the desired structural features, which can be used for QSAR studies.
The structures obtained consist of the central fragment and of the substituents, which are generated from the sets of microfragments (of any kind) by their acyclic combining.
The sets of central fragments and microfragments are stored as WLN codes and can be modified.
The user can use the restrictions for combinations of fragments to avoid the combinatorial explosion:

- the list of forbidden neighbours for each fragment
- the maximal number of each kind of fragments in the substituent
- the maximal length of generated linear chains
- the limitations on the molecular formula.

The structures generated are saved in a text file in WLN codes, which can be automatically decoded into adjacency matrices.
The generation rate is 50 structures per second.
Hardware:

- IBM PC/AT and compatible systems
- Graphic boards: EGA,VGA
- Mouse: not required
- Minimum RAM : 640K
- Co-processor: desirable
- 300K plus 100 byte per generated structure of hard disk space are required.

Price: negotiable
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MOLGEN und MOLGEN$^+$, Strukturgeneratoren für molekulare Graphen

MOLGEN ist ein Strukturgenerator für molekulare Graphen, der als zentraler Baustein in Systemen zur molekularen Strukturerkennung gedacht ist. Er generiert, zu vorgegebenen Daten wie

- Summenformel,
- vorgeschriebenen Substrukturen (Makroatome und "goodlist"),
- verbotenen Substrukturen ("badlist"),
- Beschränkungen für Ringgrößen,
- Beschränkungen für Bindungsvielfachheiten,

alle Strukturformeln, die zu diesen Daten passen, und zwar *vollständig, effizient und redundanzfrei*. Er liefert, auf einer handelsüblichen Workstation ca. 1000 solcher Bindungsisomere pro Sekunde.

Der Generator existiert bisher in zwei Versionen, einer Version MOLGEN für *Forschung und Lehre*, sowie in einer erweiterten *Industrieversion* MOLGEN$^+$, die erheblich höheren Plattenbedarf hat. Bisher sind hierfür DOS-Versionen mit Oberfläche erhältlich. Versionen unter UNIX und VMS sind in Arbeit, ebenso Versionen, die eine Datenbank bereitstellen.

Seitens der hardware bestehen die folgenden Voraussetzungen:

- DOS-Maschine mit VGA-Graphikkarte, ein Coprozessor ist für beschleunigte Berechnung der geometrischen Darstellung der Moleküle wünschenswert, aber nicht Voraussetzung,
- 2 MB Plattenspeicher für die Version MOLGEN, ca. 120 für die Industrieversion.

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AEGIS

The structure generation program AEGIS was developed using LPA MacProlog on an Apple Macintosh computer. It requires at least an Apple Macintosh of the II series to run satisfactorily (68020 with math co-processor). Also possession of the LPA MacProlog compiler is needed. No runtime versions are currently available for distribution.
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