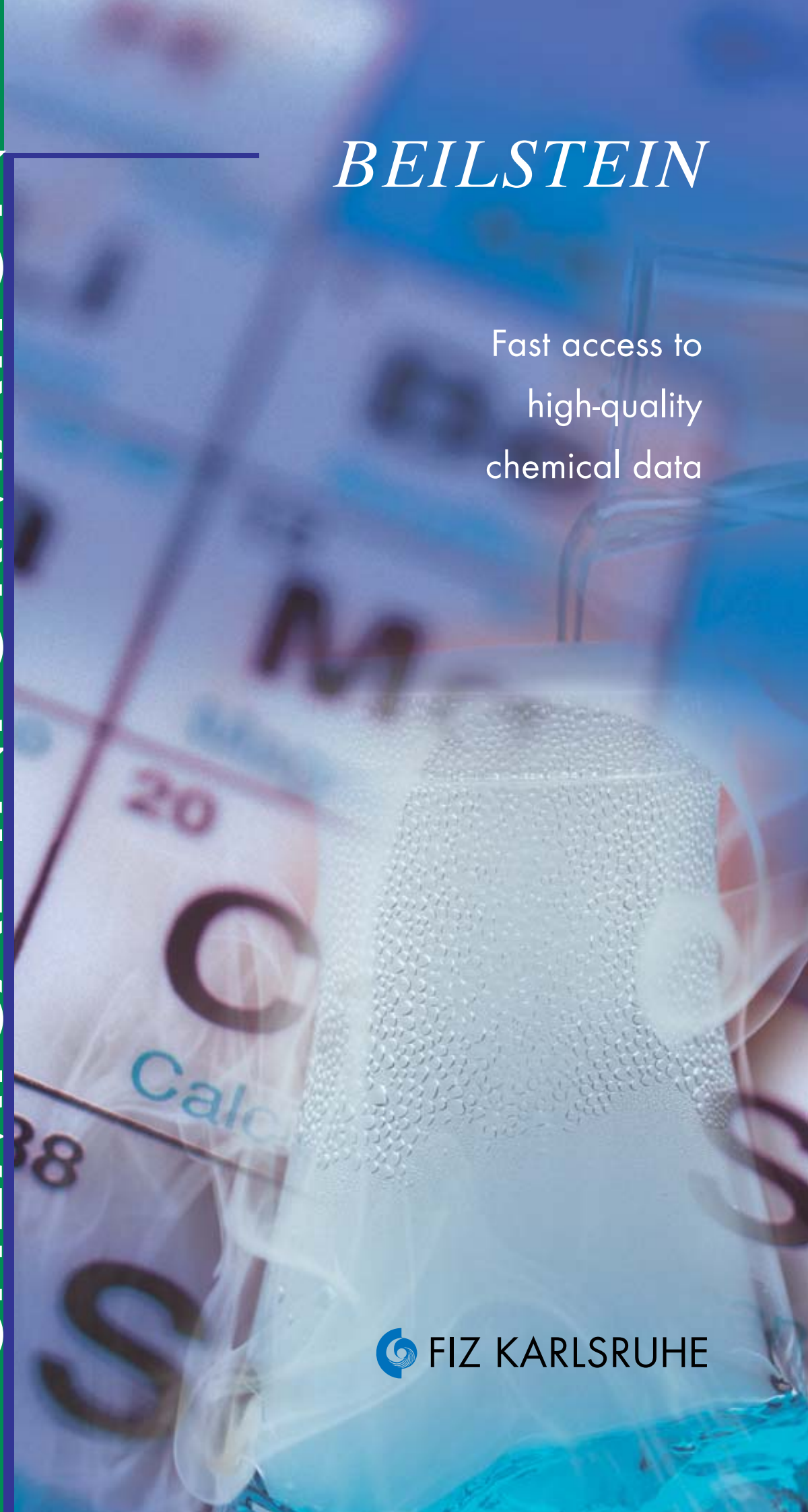
CHEMICAL INFORMATION

BEILSTEIN

Fast access to
high-quality
chemical data



FIZ KARLSRUHE

FIZ Karlsruhe provides BEILSTEIN on STN® International

For two centuries, one name has been synonymous with high-quality organic chemistry data: BEILSTEIN. In the domain of organic substances, the two factual and bibliographic databases, BEILSTEIN and BEILSTEIN Abstracts (BABS), are outstanding in providing chemical structures, facts, and reactions with nearly unlimited combinations of search possibilities.

The BEILSTEIN file draws on three different data sources:

- The Beilstein Handbook from the Basic Series to Supplement 4 covering the literature from 1779 to 1959. For more than 1.1 million compounds the complete Handbook information is available. These evaluated data are indicated as “Handbook Data” in the notes of literature references.
- Primary literature from 1960 to 1979. This data source contains appr. 3 million substances. Specific data are available for the basic properties such as melting point, boiling point, density, or refractive index. All other physical and chemical properties are available as keywords together with corresponding references to the original literature. This part of the file is being continuously updated to provide entries for more data fields.
- Primary literature data >1979. In contrast to source b) detailed information for all physical and chemical properties have been abstracted from the literature. All data fields contain references as well as data.

Topics covered include:

- Chemical data
- Electrochemical behaviour
- Electrical and magnetic properties
- Identification of substance
- Multi-component systems
- Optical properties
- Pharmacological and ecological data
- Physical and mechanical properties
- Reactions
- Spectroscopic data
- State of aggregation
- Structure and energy parameters
- Thermodynamic properties
- Transport phenomena

The BEILSTEIN database on STN offers scientists and information professionals access to the most comprehensive collection of organic chemical information.

Database Content

- Stoicheometrically defined substances (classical BEILSTEIN compounds), biomolecules, polymers, and mixtures
- More than 8.1 million organic compounds (status: October 2002)
- More than 9 million associated reactions and reaction details
- More than 35 million associated property data
- Structure images with stereochemical information
- 160,000 patents with focus on preparative methods from 1779 to 1980
- Currently, a total of 180 journals are indexed for the database.
- Access to the titles, abstracts, and bibliographic data referenced in the BEILSTEIN database is provided by the BEILSTEIN Abstracts (BABS) file for the period covering 1980 to the present.

Database Functionalities

BEILSTEIN’s rich data structure can be easily explored using sophisticated search options.

Identify your substance via

- Beilstein Registry Number
- CAS Registry Number
- Substance name
- Molecular formula
- Structure diagram

Find information on chemical data for

- Preparations
- Reactions
- Isolation from natural product
- Chemical derivatives

Determine property data such as

- Optical data
- Mechanical properties
- Multi-component system data
- Spectral properties
- Thermodynamic properties
- Pharmacological and ecological data

Use Specific Features

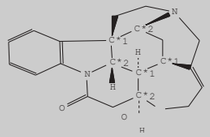
- Data Availability search
- Display of document content
- Parameter-dependent searching
- Chemical dictionary terms
- Units conversion
- Predefined and custom formats

CHEMICAL INFORMATION

Substance Identification Data and Physical Properties

```
Beilstein Records (BRN):      52979
Beilstein Pref. RN (BPR):     57-24-9
CAS Reg. Number (RN):         57-24-9
Chemical Name (CN):           strychnidin-10-one, strychnine,
                              (-)-strychnine
Molec. Formula (MF):          C21 H22 N2 O2
Molecular Weight (MW):        334.42
Lawson Number (LN):           32117
File Segment (FS):            Stereo compound
Compound Type (CTYPE):        heterocyclic
Constitution ID (CONSID):     59702
Tautomer ID (TAUTID):         56268
Beilstein Citation (BSO):     2-27-00-00723, 4-27-00-07537,
                              5-27, 6-27

Entry Date (DED):             1988/06/27
Update Date (DUPD):           2001/10/25
```



```
Atom/Bond Notes:
   1. CIP Descriptor: R
   2. CIP Descriptor: S

Field Availability:

   Code        Name                                  Occurrence
   ================================================================
   BRN         Beilstein Records                              1
   BPR         Beilstein Preferred RN                         1
   RN          CAS Registry Number                            1
   CN          Chemical Name                                  3
   MF          Molecular Formula                              1
   FW          Formular Weight                                1
   LN          Lawson Number  ...                             1
   MP          Melting Point                                 15
   MS          Mass Spectrum                                  2
   MSUS        Magnetic Susceptibility                        1
   NMR         Nuclear Magnetic Resonance                    84
   OPT         Optics                                         1
   ORP         Optical Rotatory Power                        25
   OTHE        Other Thermochemical Data                      1
   PHARM       Pharmacological Data                          39
   POT         Electrochemical Characteristics  ...          2

This substance also occurs in Reaction Documents:

   Code        Name                                  Occurrence
   ================================================================
   RX           Reaction Documents                         272
   RXREA       Substance is Reaction Reactant              253
   RXPRO       Substance is Reaction Product                19


Boiling Point:
   Value       | Press.       |Reference| Note
   (BP)        | (.P)         |     |
   (Cel)       | (Torr)       |     |
==============+==============+====+=======
   270         | 5            | 1   | 1

Reference(s):
1. Loebisch; Schoop, Monatsh.Chemical, CODEN: MOCMB7, 6,
<1885>, 851,
   Monatsh.Chemical, CODEN: MOCMB7, 7, <1886>, 83

Notes(s):
1. Handbook
```

- Identification of Beilstein compounds can be conducted via all substance identification fields (e.g. Chemical Name, Chemical Name Segment, Molecular Formula, Structure).
- For structure search, four different types are available: Exact, Family, Substructure and Closed Substructure.
- Physical data are available for
  - single components and
  - multi-component systems
- Physical data are searchable as
  - facts with
  - subfields; they contain the searchable parameter dependency of physical properties (e.g. pressure or temperature)
  - keywords
- BEILSTEIN data are experimental data (except for data gained from classical calculation methods)
- The Field Availability indicates whether or not a requested property or reaction is present for a given substance.

EcoPharm Data

```
PHARM
  Effect (.E):                  toxicity, acute
  Endpoint of Effect (.EP):     mortality
  Species or Test-System (.SP):albino mice
  Sex (.S):                     male
  Route of Application (.RA):   intravenous
  Kind of Dosing (.KD):         title comp. dissolved in
                                0.9 percent saline
  Method, Remarks (.MR):        title comp. injected into
                                the caudal vein (1 ml/kg);
                                LD50 calculated according to
                                Litchfield and Wilcoxon
                                after a 24 h observation
                                period
  Further Details (.FD):        6 mice used for each dose
  Type (.TYP):                  LD50
  Value of Type (.V):           380 mg/kg
  Results (.RE):                for comparison: LD50 of
                                quinidine 90 mg/kg and
                                propranolol 22 mg/kg
  Reference(s):
    1. Marona, H.; Pekala, E.; Filipek, B.; Maciag, D.;
    Szneler, E., Pharmazie, CODEN: PHARAT, 56(7), <2001>,
    567 - 572; BABS-6303798
```

```
ECTOX
  Effect (.E):                  toxicity to invertebrates
  Endpoint of Effect (.EP):     knockdown of insects
  Species or Test-System (.SP):Periplaneta americana (L.)
  Sex (.S):                     female
  Exposure Period (.EX):        24 hour(s)
  Method, Remarks (.MR):        insect contact in incubator
                                with vapours of title comp.
                                from filter paper impregnated
                                with title comp. solution (6
                                various concentrations);
                                incubation for 24 h at 30
                                deg C and 75 percent RH;
                                recording of insect knockdown
  Type (.TYP):                  knockdown concentration 95
  Value of Type (.V):           > 0.700 mg/cm-2
  Reference(s):
  1.Ngoh, Shay P.; Choo, Lionel E. W.; Pang, Fung Y.;
    Huang, Yan; Kini, Manjunatha R.; Ho, Shuit H.,
    Pestic.Sci., CODEN: PSSCBG, 54(3), <1998>, 261 - 268;
    BABS-6181578
```

Detailed information on the influence of chemical substances on the environment and their respective behaviour is of vital importance for drug research as well as for environmental protection. For example, it helps to plan the synthesis and evaluation of new therapeutic agents more effeciently with regard to health and environmental effects.
The influence of chemical substances on living species can have desired therapeutic effects as well as toxic adverse effects. This property is described in Pharmacological Data and Ecotoxicology. The behaviour of chemical substances in non-living ecosystems such as air, soil, and water is rather more complex and is described in several properties of Ecological Data.

Pharmacological and Toxicological Data

- Effect
- Species or test system
- Route of application
- Type
- Value
- Result
- Metabolite
- Method

Ecological Data

- Biological behaviour
- Biodegradation
- Concentration in environment
- Stability in soil
- Ecotoxicology and Exposure assessment

Reaction Data

BEILSTEIN contains the largest collection of chemical factual data and – with its 9 million reactions and reaction details – is one of the most important reaction databases. One of its main applications is the planning of synthetic routes.

Reaction Data are clearly separated in two parts:

Reaction Identification Data

- Educt
- Product

Reaction Details

- Reaction classification, e.g. preparation
- Reaction type, e.g. cyclization
- Reagent
- Catalyst
- Solvent
- Time
- Temperature
- Pressure
- pH Value
- Yield

```
Reaction:
RX
   Reaction ID (.ID):              5347186
   Reactant BRN (.RBRN):           8496283
   Reactant (.RCT):                2-iodo-benzoic acid 4-methoxy-
                                   naphthalen-1-yl ester
   Product BRN (.PBRN):            8493514
   Product (.PRO):                 12-methoxy-dibenzo<c,h>
                                   chromen-6-one
   No. of React. Details (.NVAR): 2

Reaction Details:
RX
   Reaction RID (.RID):            5347186.1
   Reaction Classification (.CL): Preparation
   Yield (.YDT):                   58 percent (BRN=8493514)
   Reagent (.RGT):                 NaOAc
   Catalyst (.CAT):                PdCl2(PPH3)2
   Solvent (.SOL):                 N,N-dimethyl-acetamide
   Time (.TIM):                    24 hour(s)
   Temperature (.T):               130 Cel
   Reaction Type (.TYP):           Cyclization
   Reference(s):
   1. Qabaja, Ghassan; Jones, Graham B., J.Org.Chem.,
      CODEN: JOCEAH, 65(21), <2000>, 7187 - 7194; BABS-6264897
RX
   Reaction RID (.RID):            5347186.2
   Reaction Classification (.CL): Preparation
   Yield (.YDT):                   65 percent (BRN=8493514)
   Reagent (.RGT):                 NaOAc
   Catalyst (.CAT):                PdCl2(PPh3)2
   Solvent (.SOL):                 N,N-dimethyl-acetamide
   Reaction Type (.TYP):           Cyclization
   Reference(s):
   1. Qabaja, Ghassan; Perchellet, Elisabeth M.; Perchellet,
      Jean-Pierre; Jones, Graham B., Tetrahedron Lett., CODEN:
      TELEAY, 41(17), <2000>, 3007 - 3010; BABS-6220208
```


Link to Beilstein Abstracts (BABS) in STN® on the Web

A platform-independent application, STN on the Web combines the widely respected and powerful STN command language functionalities with advanced web technology. Along with the full set of STN commands as well as chemical structure searching, STN on the Web offers features such as hyperlinks, images integrated in text, and context-sensitive help.

Easy access to abstracts of BEILSTEIN references is provided through:

BEILSTEIN Abstracts (**BABS**) database: Titles and abstracts of BEILSTEIN references from 1980 to the present

- **STN on the Web**: Active link from BEILSTEIN references to corresponding abstracts in BABS
- **STN Express® with** *Discover!*, the fully integrated software package: At the end of a reference, the BABS accession number is given for convenient navigation.

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FIZ Karlsruhe operates STN International in Europe.
STN (The Scientific & Technical Information Network) is the world's premier online service offering access to bibliographic, factual and full-text databases in science and technology. STN's product palette encompasses more than 210 databases with approx. 350 million documents from all fields of science and technology, among them the world's largest and most important patent files as well as subject-related business files.

STN International is jointly operated by FIZ Karlsruhe, Germany; Chemical Abstracts Service (CAS), Columbus OH, USA; and The Japan Science and Technology Corporation (JST), Tokyo.

For questions and details please contact us

FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe, Germany

Tel.: +49 (0) 7247/808-555
Fax: +49 (0) 7247/808-259
E-mail: helpdesk@fiz-karlsruhe.de
www.fiz-karlsruhe.com

or contact your local STN representative:

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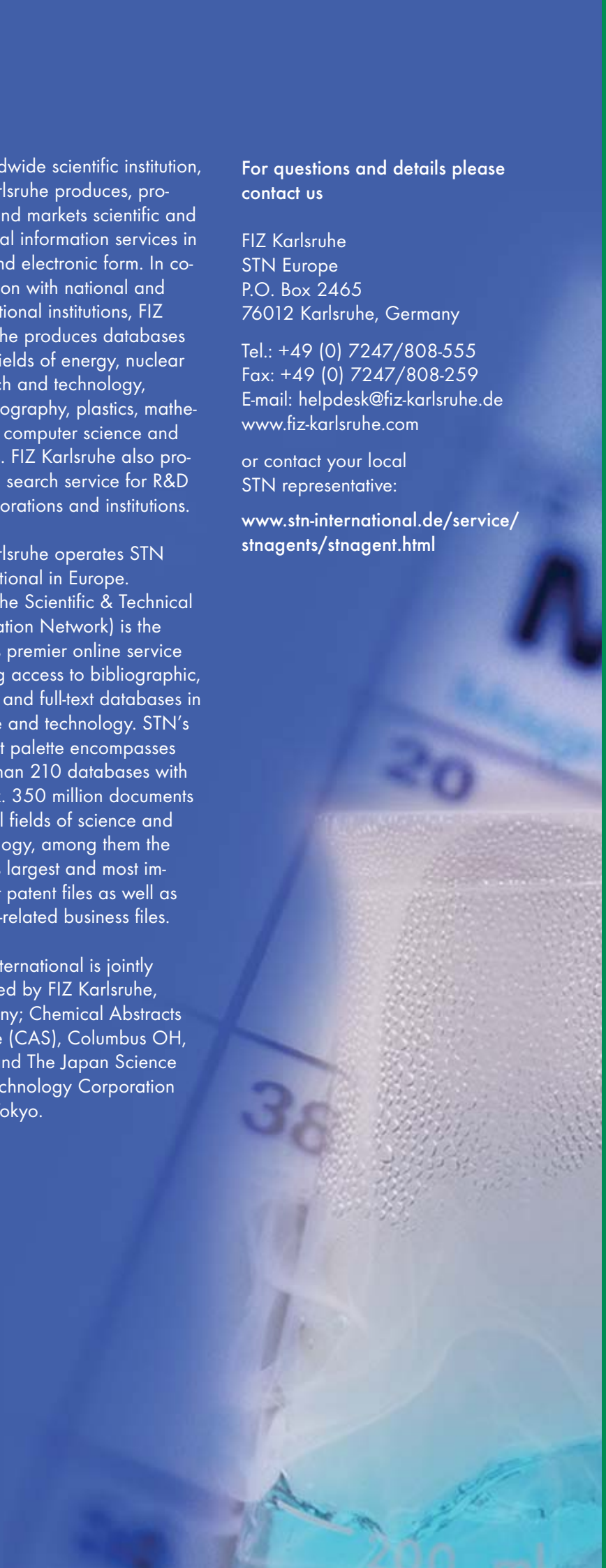

STN Service Centers

FIZ Karlsruhe
STN Europe
P.O. Box 2465
D-76012 Karlsruhe
Germany

E-mail: helpdesk@fiz-karlsruhe.de
www.fiz-karlsruhe.com
Tel.: +49 7247 808-555
Fax: +49 7247 808-259

Chemical Abstracts Service
STN North America
2540 Olentangy River Road
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U.S.A

E-mail: help@cas.org
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Toll-free for
U.S.A: 1 800 848 6533
Tel.: 1 614 447 3700
Fax: 1 614 447 3767

The Japan Science and Technology Corporation (JST)
STN Japan
5-3 Yonbancho Chiyoda-ku
Tokyo 102-0081
Japan

E-mail: helpdesk@mr.jst.go.jp
www.jst.go.jp
Tel.: +81 3 5214 8414
Fax: +81 3 5214 8410

November 2002

FIZ KARLSRUHE