

# STN<sup>®</sup>

## Exploring the Derwent Drug File on STN<sup>®</sup>

Robert Austin – FIZ Karlsruhe

# Agenda

- Introduction to the Derwent Drug File (DDF)
- Searching text, classification and indexing
- Searching for drugs and diseases
- Searching in the Derwent Drug Registry (DDR)
- Transferring results from the Derwent Drug Registry (DDR) into DDF
- Structure search example

# What is the Derwent Drug File (DDF)?

- DDF is a high quality biomedical database
- It covers all aspects of drugs from drug design to post marketing studies
- It was designed by some of the leading pharmaceutical companies
  - Using principles used for in-house systems at Roche, Sandoz, Pfizer etc.
- It started out as a printed product in 1964
- It has evolved through liaison with customers

# Main features of DDF

- Updated weekly
- All records contain English language abstracts written by Thomson Reuters
- Covers 1,150 journals from around the world
- Controlled keyword indexing including roles
- Indexing for each drug is in a separate paragraph to help eliminate false hits
- Generic searching is possible using higher terms

# DDF Subject coverage

- Analysis
- Chemistry
- Immunology
- Microbiology
- Pharmacology
- Therapy
- Biochemistry
- Endocrinology
- Metabolism
- Pharmaceuticals
- Physiology
- Toxicology

# DDF Selection rules

- All articles giving significant information on novel and established drugs
  - Isolation, Synthesis, Formulation, Pharmacology, Toxicology, Metabolism, Clinical Trials etc.
- The following are excluded
  - Routine references, Editorials, Product Reviews, Discussion
  - Unless the paper reports significant results (such as adverse effects)

## DDF selection rules (cont.)

- The following papers are not selected
  - Trivial references to drugs (e.g. reagents)
  - Incidental drug therapy (i.e. incidental to the subject of study)
  - Routine use of anaesthetics and diagnostic agents
  - Generic drug groups that are not the main topic
  - Letters containing no original data
  - Drug abuse, alcoholism, tobacco smoking
  - Environmental pollutants, poisons, non-drug carcinogens
  - Veterinary drugs, pesticides biotechnology

# DDF on STN

- 1983 – Present
  - Subscriber file DRUGU
  - Open access file DDFU
  - Comprises a literature segment (DDF) and a chemical structure registry segment (DDR)
- 1964 – 1982 (Back File)
  - Subscriber File DRUGB
  - Open File DDFB

# Example: DDF sample record

L1 ANSWER 1 OF 1 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN  
AN 2011-07419 DRUGU T  
TI Effects of rosuvastatin and allopurinol on circul **MAX display format.**  
progenitor cells in patients with congestive heart failure: The  
impact of inflammatory process and oxidative stress.  
AU Tousoulis D; Andreou I; Tsiatas M; Miliou A; Tentolouris C; Siasos  
G; Papageorgiou N; Papadimitriou C A; Dimopoulos M A; Stefanadis C  
CS Univ.Athens  
LO Athens, Greece  
SO Atherosclerosis (214, No. 1, 151-7, 2011) 2 Fig. 2 Tab. 39 Ref.  
CODEN: ATHSBL ISSN: 0021-9150  
AV Univ Athens, Sch Med, Vasilissis Sofias 114, Athens, Greece, 11528.  
(Tousoulis D, e-mail: drtousoulis@hotmail.com).  
LA English  
DT Journal  
AB This 3-group, randomized, double-blind, placebo-controlled trial  
evaluated the effects of rosuvastatin and allopurinol on the number  
of endothelial progenitor cells (EPC) in 60 patients with CHF.  
Circulating EPC was significantly increased after rosuvastatin  
treatment. The increase in EPC levels was not associated with the  
changes in the levels of the measured inflammatory and oxidative  
markers. The results show that short-term treatment with  
rosuvastatin, but not allopurinol, significantly increases the  
number of circulating EPC in patients with CHF.  
ABEX Methods 60 Patients with CHF were randomized to receive  
rosuvastatin (10 mg/day, n = 21, 19 male, mean age 65 yr),  
allopurinol (300 mg/day, n = 21, 20 male, mean age 65 yr), or  
placebo (n = 18, 16 male, mean age 66 yr) for 1 mth. Results  
Rosuvastatin significantly reduced the serum levels of total  
cholesterol, LDL and triglycerides. Rosuvastatin significantly

# Example: DDF sample record (cont.)

increased circulating EPC, as defined by the number of double-(CD34+/KDR+) and triple-(CD34+/CD133+/KDR+) EPCs, which remained unchanged in allopurinol- and placebo-treated patients. The increase in levels of CD341/KDR1 EPC induced by rosuvastatin was significantly greater vs. allopurinol and placebo. Subgroup analysis in patients receiving rosuvastatin showed that the increase in EPC numbers was similar in subjects with ischemic and non-ischemic disease (46 and 36%, respectively). A significant improvement in flow-mediated, endothelium dependent dilation was found after both rosuvastatin and allopurinol treatments. Both rosuvastatin and allopurinol showed a substantial increase in serum VEGF levels. Amino-terminal pro-brain natriuretic peptide was significantly decreased in both the rosuvastatin- and allopurinol-treated groups. Rosuvastatin significantly reduced myeloperoxidase, MMP-9 and oxidized LDL levels and caused a borderline reduction in high-sensitivity C-reactive protein and total lipid peroxides levels. A significant correlation was observed between the baseline levels of CD34+/KDR+ cells and myeloperoxidase, high-sensitivity C-reactive protein and soluble CD40 ligand. (D78)

MAX display format (cont.).

SH T Therapeutics  
CC 58 Vasoactive  
64 Clinical Trials  
CT CONGESTIVE \*TR; HEART-FAILURE \*TR; CARDIOPATHY \*TR; IN-VIVO \*FT;  
CASES \*FT; RANDOM \*FT; CLIN.TRIAL \*FT; BLIND-TEST \*FT; DOUBLE  
\*FT; PLACEBO \*FT; PROGENITOR \*FT; CELL \*FT; ENDOTHELIUM \*FT  
[01] ROSUVASTATIN \*TR; DR0030178 \*RN; ANTIARTERIOSCLEROTICS \*FT;  
HMG-COA-REDUCTASE-INHIBITORS \*FT; ANTIARTERIOSCLEROTIC \*FT; TR  
\*FT  
[02] ALLOPURINOL \*TR; ALLOPURIN \*RN; ANTIGOUTS \*FT; ANTIRHEUMATICS  
\*FT; XANTHINE-OXIDASE-INHIBITORS \*FT; TR \*FT  
FA AB; LA; CT  
FS Literature

# Text and indexing search fields on STN

- Basic Index (default text search)
  - Title
  - Abstract(s)
  - Controlled term indexing
- DDF classification and indexing fields
  - Subject Headings (“Thematic groups”) /SH
  - Classification codes (“Profile numbers”) /CC
  - Controlled term indexing (“Descriptors”) /CT
- Enzyme Number /EC

# Subject headings (Thematic groups)

- These are single letter codes to indicate the general themes of a paper
  - A – Analysis
  - C – Chemistry
  - G – Galenicals
  - S – Adverse effects
  - V – Vitamins
  - B – Biochemistry
  - E – Endocrinology
  - M – Microbiology
  - P – Pharmacology
  - T – Therapeutics

# Searching for subject headings (/SH)

- Can be searched using the single letter code (e.g. S for adverse effects) or the full definitions
  - => S S/SH
  - => S ADVERSE EFFECTS/SH
    - Either option searches for records in the adverse effects thematic group
- Example: find papers from Novartis about adverse effects
  - => S NOVARTIS/CS AND S/SH

# Classification codes (Profile numbers)

- Finer subject divisions than Subject headings (/SH)
- Many relate to drugs with particular activities
  - For example Antiallergics - 3
- Others can be used to find particular types of paper
  - Medicinal chemistry – 10
  - Adverse reactions – 35
  - Animal toxicology – 34
  - Clinical trials - 64
  - Drug delivery systems – 65
  - Drug interactions – 66
  - Drug reviews - 69
  - Drug analysis and methodology – 70
  - New drugs – 72

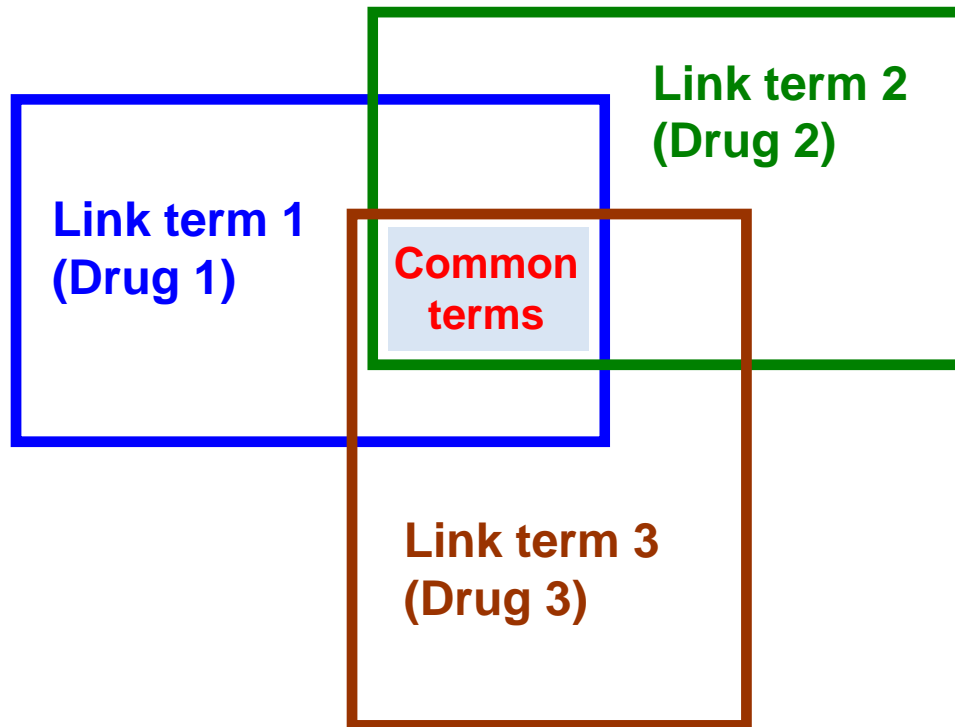
# Searching classification codes (/CC)

- Can be searched using the two digit code (e.g. 73 for Trial Preparations) or the full definition
  - => S 73/CC
  - => S TRIAL PREPARATIONS/CC
- Example: search for records concerning clinical trials carried out in Japan
  - => S JAPAN/LO AND 64/CC

# Controlled term indexing (Descriptors)

- The drug name is used as the basis for construction of a paragraph of indexing
- Keywords and roles are linked to each drug
- *Common terms* apply to the whole document, i.e. all of the indexed drugs
- *Link terms* apply to individual drugs
- Each drug has its own paragraph of indexing
- Precision searching of common and link terms is possible using the (L)-proximity operator

# Controlled term indexing (/CT)



# Example: DDF classification and indexing

SH T Therapeutics  
CC 58 Vasoactive  
64 Clinical Trials  
CT CONGESTIVE \*TR; HEART-FAILURE \*TR; CARDIOPATHY \*TR; IN-VIVO \*FT;  
CASES \*FT; RANDOM \*FT; CLIN.TRIAL \*FT; BLIND-TEST \*FT;  
\*FT; PLACEBO \*FT; PROGENITOR \*FT; CELL \*FT; ENDOTHELIUM \*FT  
[01] ROSUVASTATIN \*TR; DR0030178 \*RN; ANTIARTERIOSCLEROTICS \*FT;  
HMG-COA-REDUCTASE-INHIBITORS \*FT; ANTIARTERIOSCLEROTIC \*FT; TR  
\*FT  
[02] ALLOPURINOL \*TR; ALLOPURIN \*RN; ANTIGOUTS \*FT; ANTIRHEUMATICS  
\*FT; XANTHINE-OXIDASE-INHIBITORS \*FT; TR \*FT  
FA AB; LA; CT  
FS Literature

Subject headings (Thematic groups).

Classification codes (Profile numbers).

Common terms.

Two paragraphs contain the *link terms* relating to the two specific drugs.

# Controlled term roles

- Three different types of roles are used
  - Drug Roles
  - Disease Roles
  - Further terms (FT)
    - Indexing terms that do not apply to a particular drug or disease

# Drug Roles

- PH** – Pharmacology in humans, animals and in vitro
- TR** – Treatment of diseases in humans
- AE** – Side effects in humans and in animals
- DM** – Drug metabolism, e.g. pharmacokinetics, bioavailability
- DI** – Drug interaction
- OC** – other context, e.g. chemistry, analysis
- RC** – Reference compounds, e.g. standards, reagents

# Disease roles

- TR** – Diseases being treated in humans
- AE** – Adverse (side) effects; diseases in humans and animals caused by drugs
- OC** – Diseases in humans not being treated and not a side effect; animal models of disease

# Searching controlled terms and roles

- Use the (L)-proximity to search for controlled terms relating to a single drug (common terms are effectively present in each drug paragraph)  
E.g. => S (AMPICILLIN (L) BIOAVAILABILITY)/CT
- Use the asterisk (\*) to link a controlled term with a controlled term role of interest, e.g.  
=> S AMPICILLIN \*DM/CT  
=> S (ALLOPURINOL \*TR (L) ANTIULCER \*FT)/CT
- Alternatively (w)-Proximity may be used to link controlled terms with roles, e.g.  
=> S (AMPICILLIN (W) (TR OR DI))/CT

# Generic controlled term searching

- The generic searching capabilities are provided by the use of 'higher terms'
- The following types of higher term can be searched
  - Types of Drugs
  - Groups of Diseases
  - Types of Organisms
- Whenever a specific concept is indexed the appropriate Higher Term(s) are automatically generated

# Higher Term indexing example

- In the hierarchy below we see that E.COLI has two higher terms, namely BACT. and GRAM-NEG. so when E-COLI is indexed BACT. and GRAM-NEG. are auto-posted
- BACT.
  - GRAM-NEG.
    - E.COLI

```
CT      IN-VITRO *FT; BACT. *FT; GRAM-POS. *FT; STREPT. *FT; PNEUMONIAE
        *FT; STAPH. *FT; AUREUS *FT; GRAM-NEG. *FT; NEISSERIA *FT;
        KLEBS. *FT; SALM. *FT; PARATYPHI *FT; TYPHI *FT; E.COLI *FT;
        HAEMOPHILUS *FT; INFLUENZAE *FT; RESISTANCE *FT; SENSITIVITY *FT;
        ANTIBIOTIC *FT; MIA-GENE-INHIBITOR *FT
```

# Higher terms for drugs

- Assigned to all drugs or new compounds showing pharmacological activity
  - Drug activity – activity investigated or established the indexed paper (e.g. **ANALGESIC**)
  - Pharmacological classification – standard activity for the drug (e.g. **ANTIINFLAMMATORIES**)
  - Chemical substructure terms – chemical functions in the drug structure (e.g. **PIPERIDINE**)

# Generic searching of drugs

- To find all references where the activity has actually being referred to, use the singular form  
=> S (ANALGESIC (L) MOUSE)/CT
- To find all references to a generic class of drugs search the plural form  
=> S (ANALGESICS (L) MOUSE)/CT
- Remember to SET PLURALS OFF otherwise the generic searching will be happening by default

# Generic searching of diseases

- Higher terms allow generic searching for all diseases of a particular organ or etiology
- To search for papers relating to the treatment of lung tumours

=> S (PNEUMOPATHY \*TR (L) NEOPLASM \*TR)/CT

```
CT      MILIARY *TR; LUNG *TR; MESOTHELIOMA *TR; PNEUMOPATHY *TR;  
        NEOPLASM *TR; CASE-HISTORY *FT; IN-VIVO *FT; COMB. *FT;  
        PNEUMONECTOMY *FT; RADIOTHERAPY *FT; CYTOSTATIC *FT; GERIATRICS  
        *FT; CASES *FT; SURGERY *FT
```

# Searching for analytical techniques

- For analytical techniques search the keyword ANALYSIS
  - => S (NAPROXEN (L) ANALYSIS)/CT
    - This retrieves documents relating to some form of analytical process involving Naproxen
- You can further restrict the search by using additional controlled terms, for example
  - BLOOD-PLASMA
  - TABLET
  - CHROMATOGRAPHY

# Limiting to humans or animals

- Searching for humans
  - **HUMAN**: Studies in healthy humans, experimental studies on patients with diseases unrelated to the subject of study
  - **CASES**: Clinical studies in diseased patients
  - More specific keywords:
    - **NEONATE** 0 to 4 weeks
    - **INFANT** 0 to 2 years
    - **PEDIATRICS** 0 to 19 years
    - **ADOLESCENT** 11 to 19 years
    - **GERIATRICS** over 65 years
- Searching for animals
  - Common names are indexed (**RAT**, **MOUSE**, **DOG** etc.)
  - Latin names are only indexed if there is no common name
  - **LAB ANIMAL**: Higher term

# Searching for clinical trials

- There are two keywords that are applied to documents relating to clinical trials
  - CLIN.TRIAL
  - CASES
  - For full retrieval always OR these together
- The classification code (Profile) for clinical trials is also available (64/CC or CLINICAL TRIALS/CC)
- May also be combined with age group controlled terms (previous slide) or to age dependent studies
  - => S (NAPROXEN (L) (CASES OR CLIN.TRIAL) (L) AGE-DEPENDENCE)/CT
- For drug comparison studies search using
  - DRUG-COMPARISON

# Controlled term abbreviations

- Some general concept terms are abbreviated.  
e.g.
  - Metabolism: **METAB**
  - Toxicology: **TOX**

**Tip:** always check the thesaurus

# Searching for drug information

- Drug interactions using the DI role, e.g.
  - => S (RIFABUTIN \*DI AND RITONOVIR \*DI)/CT
  - => S (ANTIBIOTICS \*DI AND FUNGICIDES \*DI)/CT
  - => S WARFARIN \*DI/CT
- Drug metabolism using the DM role
  - => S WARFARIN \*DM/CT

## Searching for drug information (cont.)

- To search for records containing information about all drugs classified as local anesthetics  
=> S LOCAL ANESTHETICS/CT
- To search for records where local anesthetic activity is explicitly reported  
=> S LOCAL ANESTHETIC/CT
- To search for records where a specific activity of a specific drug is reported  
=> S ((LIDOCAINE \*PH OR LIDOCAINE \*TR) (L) LOCAL ANESTHETIC)/CT

# Pharmaceutics

- All pharmaceutics concepts are indexed with **PHARMACEUTICS**, plus specific descriptors
- Higher term **PHARM PREP**
  - Any type of formulation of a drug
  - Specific descriptors also assigned
    - **TABLET, CAPSULE, AEROSOL**, etc.
- When searching pharmaceutics of a specific drug, make use of the OC role
  - => **S (PARACETAMOL \* OC (L) FORMULATION (L) TABLET)/CT**
  - => **S (CHLORAMPHENICOL \*OC (L) OINTMENT)/CT**

# Searching for diseases

- Diseases are indexed as specifically as possible
- If a multi-word disease name isn't indexed, combine individual terms
- Use the Thesaurus to establish the correct search strategy
- Search in combination with AE, OC, TR roles, e.g.  
=> S HYPERTENSION \*TR
- Higher terms associated with disease
  - Anatomical: EYE-DISEASE, VASCULAR-DISEASE...
  - Etiological: INFECTION, VIRUS...
  - More than one higher term may be used in record

# The DDF Thesaurus

- Consists of 3 volumes
  - Part 1: Thesaurus A-K
  - Part 2: Thesaurus L-Z
  - Part 3: Appendices
- The keywords used in indexing are controlled by the Thesaurus
  - Lists searchable keywords
  - Higher terms associated with these keywords
  - Non-searchable synonyms and equivalent search terms

# DDF Thesaurus Appendices

- Appendix A – Definitions of Biological concept keywords
- Appendix B – Definitions of chemical substructure keywords
- Appendix C – Higher terms
- Appendix D – Keywords Out of Context
  - Grouped according to Higher Terms

Download the Derwent Drug File (DDF) Thesaurus:

[http://science.thomsonreuters.com/m/pdfs/mgr/ddf\\_thesaurus1.pdf](http://science.thomsonreuters.com/m/pdfs/mgr/ddf_thesaurus1.pdf)

# The DDF thesaurus on STN

```
=> E E.COLI/CT 5
E#   FREQUENCY   AT      TERM
--   -
E1           2           E.C.4.2.1.1/CT
E2           2           E.C.4.2.1.1 *FT/CT
E3       27820       5 --> E.COLI/CT
E4       27819           E.COLI *FT/CT
E5           2           E.COLI *RC/CT
```

```
=> E E3+ALL
E1           0       BT3  MICROORGANISMS/CT
E2       86579       BT2  BACT./CT
E3       56814       BT1  GRAM-NEG./CT
E4       27820           --> E.COLI/CT
***** END *****
```

```
=> S E3+NT
L1       58244  GRAM-NEG.+NT/CT  (87 TERMS)
```

Browse the Thesaurus using the expand command and an appropriate relationship code.

To learn more about available Thesaurus relationship codes, type **HELP RCODE** at the STN prompt (=>).

Search with relationship codes, e.g. **+NT** (all narrower terms).

# Bibliographic Search fields on STN

- Accession Number /AN
- Author /AU
- CODEN /ISN
- ISSN /ISN
- Corporate source /CS
- Journal Name /JT
- Language /LA
- Location /LO
- Publication year /PY

## Limiting a search by date

- This can be achieved using the RANGE command after the search term, e.g.  
=> **S CANCER RANGE=1996-2000**
  - Will search for records mentioning the word cancer in the basic index between 1996 and 2000
- Or the SET RANGE command can be used, e.g.  
=> **SET RANGE 1996-**
  - Subsequent searches will only include records from 1996 to date
- See **HELP SET RANGE** for more details

# Searching for conference papers

- There is no separate field for conference or congress names
- Conference name appears in abstract
- To search for conference info use the following
  - => S CONFERENCE PAPER
  - => S (CONFERENCE ABSTRACT) OR (CONGRESS ABSTRACT)
  - => S POSTER AND (CONFERENCE OR CONGRESS)
- To find a specific conference
  - => S INTERNATIONAL SYMPOSIUM ON THYROID CANCER

# DDF Back File (DDFB/DRUGB)

- Covers the period 1964 to 1982
- The file is not updated
- The same selection rules apply as to DDF
- Bibliographic data and indexing present
- Indexing format different to DDF
  - Keywords
  - Enhanced by addition of modern synonyms of old keywords
  - Ring Code – Chemical and Biological punch code

# Example: DDF Back File sample record

L1 ANSWER 1 OF 1 DRUGB COPYRIGHT 2011 THOMSON REUTERS on STN  
AN 1982-50949 DRUGB P  
TI PLASMA LEVELS AND CARDIAC ELECTROPHYSIOLOGICAL EFFECTS OF MELPERONE  
IN THE ABSENCE AND PRESENCE OF BETA-ADRENOCEPTOR BLOCKADE.  
AU PLATOU E S; REFSUM H; AMLIE J P; LANDMARK K  
LO TROMSO AND OSLO,NOR.  
SO BRIT.J.CLIN.PHARMACOL. (14, NO.4, 591P, 1982)  
LA English  
DT Journal  
FS R-X 1976-1982  
SH P Pharmacology  
CC 8 Pharmacokinetics  
9 Cardiovascular  
26 Neurology  
32 Psychotropic  
IT PSYCHOSEDATIVE BUTYROPHENONE NEUROLEPTIC MELPERONE SINGLY CF. COMB.  
& SYMPATHOLYTIC PHENOL-ETHER ATENOLOL DRUG-METAB.NEUTROPIC PLASMA  
CONC. CF. HEMODYNAMICS,EXP. BLOOD-PRESSURE HEART-RATE A.V.NODE  
REFRACTORINESS ANESTHETIZED DOG CONGRESS PSYCHOSEDATIVES  
SYMPATHOLYTICS  
MPC [01] 02& \*G; 02- \*G; 03& \*G; 032 \*G; 06& \*G; 060 \*G; 071 \*G; 096 \*G;  
10- \*G; 100 \*G; 102 \*G; 105 \*G; 111 \*G; 117 \*G; 12- \*G; 123 \*G;  
17- \*G; 170 \*G; 23- \*G; 231 \*G; 237 \*G; 306 \*G; 309 \*B; 31- \*B;  
318 \*B; 35& \*B; 364 \*B; 375 \*B; 40- \*B; 410 \*B; 45- \*B; 484 \*B;  
517 \*B; 538 \*B; 54- \*B; 544 \*B; 560 \*B; 57& \*B; 571 \*B; 577 \*B;  
58& \*B; 584 \*B; 59- \*B; 60& \*B; 607 \*B; 608 \*B; 73& \*B; 731 \*B;  
739 \*B;  
[02] 02& \*G; 03& \*G; 032 \*G; 096 \*G; 11& \*G; 11- \*G; 110 \*G; 115 \*G;  
12& \*G; 123 \*G; 124 \*G; 126 \*G; 130 \*G; 131 \*G; 18- \*G; 180 \*G;  
184 \*G; 192 \*G; 235 \*G; 237 \*G; 26& \*G; 35& \*B; 375 \*B; 45& \*B;  
458 \*B; 484 \*B; 532 \*B; 54- \*B; 560 \*B; 57& \*B; 571 \*B; 607 \*B;  
608 \*B; 73& \*B; 731 \*B; 739 \*B;

MAX display format.

# DDF Back File index terms (Descriptors)

- A series of index terms (“Descriptors”) /IT
- In a single keyword field
- Terms are arranged to provide a brief summary of the document
- Connecting non-searchable words included to make the summary more readable
- Drug and disease roles are not applied
- Derwent registry Names are not present
  - Drug name must be used as cross-filing tool
- Searchable keywords given in the thesaurus

# Agenda

- Introduction to the Derwent Drug File (DDF)
- Searching text, classification and indexing
- Searching for drugs and diseases
- **Searching in the Derwent Drug Registry (DDR)**
- Transferring results from the Derwent Drug Registry (DDR) into DDF
- Structure search example

# Derwent Drug Registry (DDR)

- Chemical substance registry for DDF, including pharmacological classification of named drugs
- CAS registry numbers available (since 1992)
- A drug substance is added to DDR when encountered for the second time in DDF
- Linked to DDF record by the DDR name
- Merged with DDF in one file on STN
  - It is the registry segment of DDFU/DRUGU

# Example: DDR sample record

=> D ALL STR

L1 ANSWER 1 OF 1 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN

AN 122449 DRUGU

FS Registry

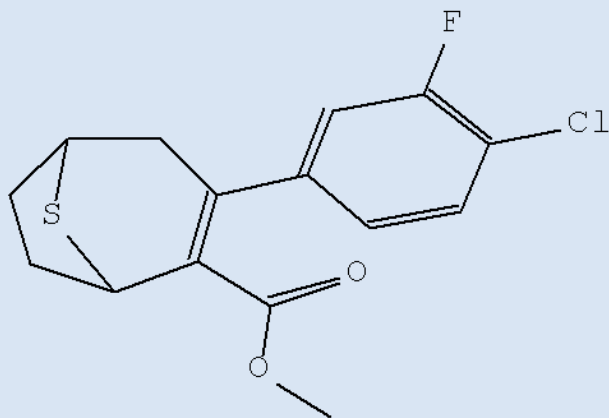
DDRN DR0186713

DDN O-3244

CT ANTISEROTONINS; DOPAMINE-ANTAGONISTS;  
SEROTONIN-TRANSPORTER-INHIBITORS; TRIAL-PREP.;  
DOPAMINE-TRANSPORTER-INHIBITORS

SS ARYLCHLORIDE; THIOPHENE; THIAPYRAN; ARYLFLUORIDE; BA-LINKED;  
CYCLOHEPTANE; BH-LINKED-CC; BRIDGE-STRUCT.; C-ESTER

**Note:** the ALL format does not already include the structure (STR) display.



# Why use DDR?

- Find drugs with a common chemical structure
  - Graphical (structure) search
  - Controlled term descriptors
- Find substances with common drug activities
  - Using controlled term descriptors
- Crossover DDR search results to DDF
  - Using the Derwent Drug Registry Name (DDRN)

# Derwent Drug Registry File

- All terms are searchable
- Thesaurus should be used to determine the correct terms
  - Activity terms
  - Substructure keywords
    - Not applied from 2007 onwards
  - Use AND to combine terms

# DDR search fields

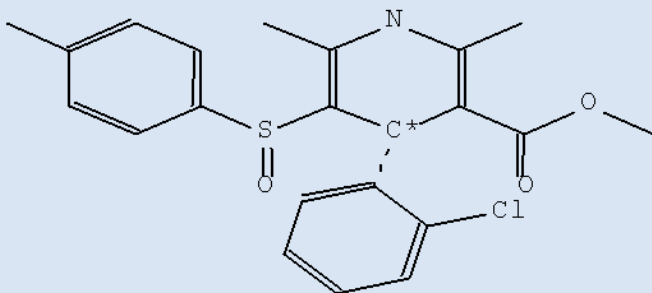
- Accession number /AN
- Derwent Drug Registry Name /DDRN
- Derwent Drug Name /DDN
- CAS Registry Number /RN
- Enzyme Commission Number /EC
- Activities /CT
- Substructure terms\* /SS

\* These keywords have not been applied to new structures since 2007.

# DDR Drug activities

- Standard drug activities are always given in the PLURAL, and are searched in the /CT field
- Limit to the DDR segment with **REGISTRY/FS**  
=> **S VASODILATORS/CT AND REGISTRY/FS**

```
L1 ANSWER 1000 OF 1422 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN
AN 33880 DRUGU
FS Registry
DDRN DR9506138
CT CALCIUM-ANTAGONISTS; VASODILATORS
SS PYRIDINE; C-ESTER; ARYLCHLORIDE; SULFOXIDE; BH-LINKED-CC; AMINOACID
```



ALL STR display format.

# DDR Chemical structures

- Chemical substructures are searchable as keywords\* (appendix B of the Thesaurus)
- If searching for two or more terms in the same structure, combine with the (L) or AND operator
- Search with the /SS field qualifier, e.g.
  - => S THIOSEMICARBAZIDE/SS
  - => S (NUCLEOSIDES (L) AZIDE)/SS

\* These keywords have not been applied to new structures since 2007.

# DDR substance identifiers

- Accession number (AN) (main record identifier)
- The Derwent Drug Name (DDN) is typically the approved name (INN), or for newer drugs the trial prep code
- The Derwent Drug Registry Name (DDRN) is used to link the record to the literature segment
- CAS Registry Number (from 1992)
- Enzyme Commission Number (EC)

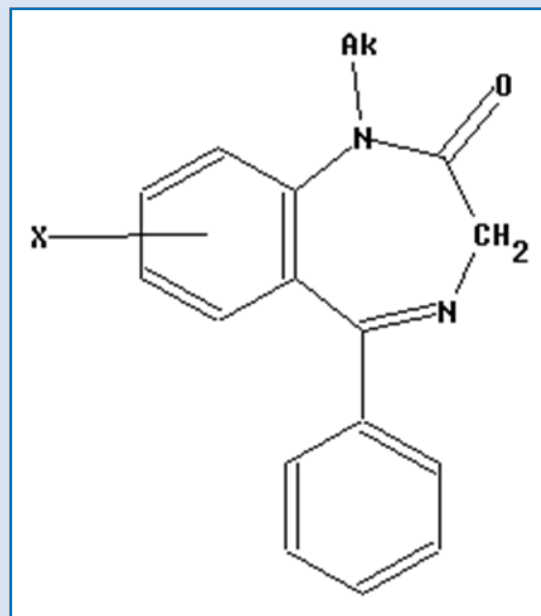
## Transferring results from Registry (DDR) to Literature (DDF) file segments

- Search the Derwent Drug Registry Name (DDRN) in the controlled term field (/CT)
- After a structure search this can be carried out using the STN TRANSFER command, e.g.
  - => **TRANSFER Lx 1- DDRN /CT**
  - Where Lx is a DDR structure search results set

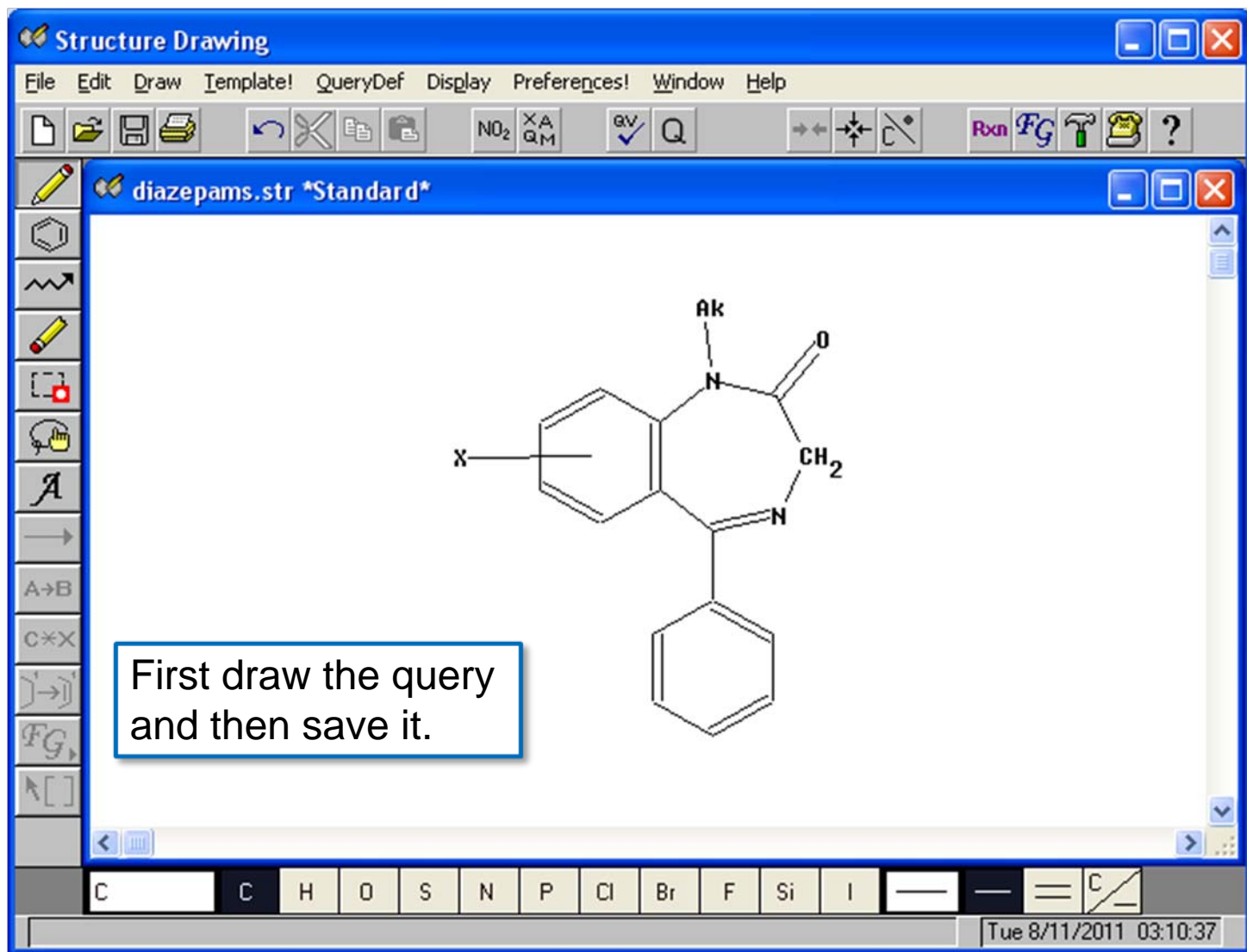
# DDF structure search example

## Search Question:

Find recent references to the adverse effects of substances represented by this structure



# Prepare the structure query



# Upload the structure query

=> **FILE DRUGU**

FILE 'DRUGU' ENTERED AT 04:40:24 ON 08 NOV 2011

COPYRIGHT (C) 2011 THOMSON REUTERS

FILE LAST UPDATED: 4 NOV 2011 <20111104/UP>

=>

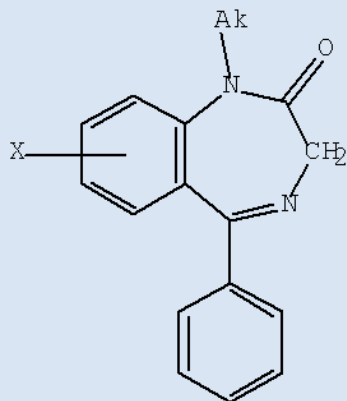
Uploading C:\....\My Documents\STN Express 8.5\Queries\diazepam.str

L1 STRUCTURE UPLOADED

=> **D**

L1 HAS NO ANSWERS

L1 STR



Upload the structure query  
(L1) via STN Express.

Structure attributes must be viewed using STN Express query preparation.

# Run the structure search

=> S L1 SSS FUL

FULL SEARCH INITIATED 04:40:57 FILE 'DRUGU'

FULL SCREEN SEARCH COMPLETED - 386 TO ITERATE

100.0% PROCESSED 386 ITERATIONS

40 ANSWERS

SEARCH TIME: 00.00.01

L2 40 SEA SSS FUL L1

Review the DDR substances  
retrieved (L2) in free-of-charge  
TRIAL display format.

=> D TRIAL 1-3

L2 ANSWER 1 OF 40 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN

AN 96914 DRUGU

SS ARYL-C-AMIDE; ARYLCHLORIDE; BH-LINKED-CC; INDOLE; SULFONIC-ACID;  
LACTAM; XANTHENE; COND.RING; ARYLFLUORIDE; BENZODIAZEPINE

L2 ANSWER 2 OF 40 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN

AN 95262 DRUGU

SS ALDIMINE; AMINOACID; ARALKYLAMINE; C-AMIDE; HYDRAZINE; PHENOL-  
ETHER; POLYPHENOL; LACTAM; BH-LINKED-CC; ARYLBROMIDE;  
ARYLCHLORIDE; BENZODIAZEPINE

L2 ANSWER 3 OF 40 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN

AN 95261 DRUGU

SS AMINOACID; ARYLBROMIDE; C-ESTER; LACTAM; BH-LINKED-CC;  
ARYLCHLORIDE; BENZODIAZEPINE

# Retrieve the DDF bibliographic results

```
=> TRANSFER L2 1- DDRN /CT
L3          TRANSFER L2 1- DDRN :          40 TERMS
L4          20512 L3/CT
```

DDF bibliographic results (L4).

```
=> S L4 (W) AE/CT AND 2010-2011/PY
L5          35 L4 (W) AE/CT AND 2010-2011/PY
```

Limit to recently published  
adverse effects results (L5).

```
=> D TI 1-4
```

```
L5 ANSWER 1 OF 35 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN
TI Effects of Multiple Doses of Lu AA21004 on the Single-Dose
Pharmacokinetics and Pharmacodynamics of Diazepam.
```

```
L5 ANSWER 2 OF 35 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN
TI Pharmacokinetics of Diazepam Administered Intramuscularly by
Autoinjector versus Rectal Gel in Healthy Subjects A Phase I,
Randomized, Open-Label, Single-Dose, Crossover, Single-Centre Study.
```

```
L5 ANSWER 3 OF 35 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN
TI 3,4-Methylenedioxymethamphetamine (MDMA) interacts with therapeutic
drugs on CYP3A by inhibition of pregnane X receptor (PXR) activation
and catalytic enzyme inhibition.
```

```
L5 ANSWER 4 OF 35 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN
TI Buccal midazolam or rectal diazepam for treatment of residential
adult patients with serial seizures or status epilepticus.
```

# Example: DDF record retrieved

=> D L5 BIB CT 4

L5 ANSWER 4 OF 35 DRUGU COPYRIGHT 2011 THOMSON REUTERS on STN  
AN 2011-26717 DRUGU T S  
TI Buccal midazolam or rectal diazepam for treatment of residential  
adult patients with serial seizures or status epilepticus.  
AU Nakken K O; Lossius M I  
CS Univ.Oslo  
LO Baerum Postterminal, Norway  
SO Acta Neurol.Scand. (124, No. 2, 99-103, 2011) 4 Tab. 21 Ref.  
CODEN: ANRSAS ISSN: 0001-6314  
AV Oslo Univ Hosp, Natl Ctr Epilepsy, POB 53, Baerum Postterminal,  
Norway, N-1306. (Nakken K O, e-mail: karl.otto.nakken@epilepsy.no).  
LA English  
DT Journal  
FA AB; LA; CT  
FS Literature  
CT EPILEPSY \*TR; ASTHENIA \*AE; ATAXIA \*AE; ENCEPHALOPATHY \*AE;  
DYSGEUSIA \*AE; NUMBNESS \*AE; ENCEPHALOPATHY \*TR; PERIPHERAL-NERVE-  
DISEASE \*AE; IN-VIVO \*FT; CASES \*FT; DRUG-COMPARISON \*FT;  
ANTICONVULSANT-AGENT \*FT  
[01] MIDAZOLAM \*TR; MIDAZOLAM \*AE; EPISTATUS \*TR; MIDAZOLAM \*RN;  
EPISTATUS \*TR; EPISTATUS \*AE; EPISTATUS \*AE; DALES \*FT;  
PSYCHOSEDATIVES \*FT; TRANQUILIZERS \*FT; GEN.ANESTHETICS \*FT;  
BENZODIAZEPINE-RECEPTOR-AGONISTS \*FT; BENZODIAZEPINE-AGONISTS \*FT;  
BUCCAL \*FT; TR \*FT; AE \*FT  
[02] DIAZEPAM \*TR; DIAZEPAM \*AE; DIAZEPAM \*RN; STESOLID \*TR; STESOLID  
\*TR; STESOLID \*AE; STESOLID \*AE; ACTAVIS \*FT; SEDATIVES \*FT;  
RELAXANTS \*FT; PSYCHOSEDATIVES \*FT; TRANQUILIZERS \*FT;  
BENZODIAZEPINE-RECEPTOR-AGONISTS \*FT; GABA-A-AGONISTS \*FT;  
GABAMINERGICS \*FT; BENZODIAZEPINE-AGONISTS \*FT;  
GABA-A-RECEPTOR-AGONISTS \*FT; TR \*FT; AE \*FT

# Summary

- Introduction to the Derwent Drug File (DDF)
- Searching text, classification and indexing
- Searching for drugs and diseases
- Searching in the Derwent Drug Registry (DDR)
- Transferring results from the Derwent Drug Registry (DDR) into DDF
- Structure search example

# Resources

DDFU/DRUGU database summary sheet:

<http://www.stn-international.com/ddfu.html>

DDF Thesaurus Part 1 A-L

[http://science.thomsonreuters.com/m/pdfs/mgr/ddf\\_thesaurus1.pdf](http://science.thomsonreuters.com/m/pdfs/mgr/ddf_thesaurus1.pdf)

DDF Thesaurus Part 2 M-Z

[http://science.thomsonreuters.com/m/pdfs/mgr/ddf\\_thesaurus2.pdf](http://science.thomsonreuters.com/m/pdfs/mgr/ddf_thesaurus2.pdf)

DDF Thesaurus Part 3 Appendices A-D

[http://science.thomsonreuters.com/m/pdfs/mgr/ddf\\_thesaurus3.pdf](http://science.thomsonreuters.com/m/pdfs/mgr/ddf_thesaurus3.pdf)

# Acknowledgement

Brian Larner, Thomson Reuters

[Brian.Larner@thomsonreuters.com](mailto:Brian.Larner@thomsonreuters.com)

# STN<sup>®</sup>

For more information ...

CAS

E-mail: [help@cas.org](mailto:help@cas.org)

Support and Training:

[www.cas.org](http://www.cas.org)

FIZ Karlsruhe

[helpdesk@fiz-karlsruhe.de](mailto:helpdesk@fiz-karlsruhe.de)

Support and Training:

[www.stn-international.de](http://www.stn-international.de)