



# How much Glyphosate Contains my Beer? –

Case Studies from the Analytical Abstracts Database on STNext

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# Agenda

- Introduction to ANABSTR
  - Value-add features
- Case studies
  - Searching for a specific analyte
  - Searching for generic substances or substance classes in ANABSTR
  - Refining searches according to the analysed media (Matrix) and the applied analytical method
- Summary



# What is ANABSTR?

- The Analytical Abstracts database (aka ANABSTR) collects worldwide literature on analytical chemistry since 1980 onwards, focusing on
  - Applied and industrial analysis
  - Chromatography and electrophoresis
  - Clinical and biochemical analysis
  - Environmental, agricultural, and food analysis
  - Pharmaceutical analysis
  - Spectroscopy and radiochemical methods
- Produced by The Royal Society of Chemistry
- ANABSTR is updated weekly
  - 505k records (December 2020)
  - approx. 200 records/week

# Sources for ANABSTR records

- Non-patent literature from about 100 core journals and other sources, including
  - books
  - conference proceedings
  - technical reports
  - standards
- Main sources<sup>1</sup>: Sens. Actuators, Talanta, Anal. Methods, Anal. Chim. Acta, Anal. Chem., Analyst, J. Chromatogr., ...
- Main selection criteria: practical measurement of a chemical species utilizing novel protocols
- approx. 20 % of the information originate from non-English language sources

<sup>1</sup>Visit <http://pubs.rsc.org/lus/analytical-abstracts/about> to see the complete list of journals indexed

# Sample ANABSTR record

<b>Bibliographic Information</b>	<b>Title</b>	TI	Determination of phthalates in toys and childcare articles made of PVC with HPLC and HPTLC.
	<b>Author</b>	AU	Hauri, U.; Schlegel, U.; Wagmann, M.; Hohl, C.* (christopher.hohl@kl.bs.ch, Kantonales Lab. Basel-Stadt, 4012 Basle, Switzerland)
	<b>Source</b>	S0	Mitt. Lebensmittelunters. Hyg. (2002) 93(3), 179-185 CODEN: MLHYFH ISSN: 1424-1307
	<b>Document Type</b>	DT	Journal
	<b>Language</b>	LA	German
<b>Value-added field</b>	<b>Abstract</b>	AB	Samples were dissolved in THF, methanol was added and any precipitate was removed. The extract was evaporated in vacuo, the residue was dissolved in acetonitrile and portions of the resulting solution were analysed on a 3 µm Nucleosil C18 column (25 cm × 4 mm i.d.), operated at 40°C, with detection at 225 nm (eluent not given). ...
	<b>Classification codes</b>	CC	*E Applied and Industrial Analysis (50000)
	<b>Controlled terms</b>	IT	Analyte(s): 85-68-7, phthalic acid benzyl butyl ester 117-81-7, phthalic acid bis-(2-ethylhexyl) ester (detmn. of, in PVC-based toys, by HPLC and HPTLC) Matrix: toys (detmn. of phthalic acid esters in PVC-based, by HPLC and HPTLC) Concepts: chromatography, liquid, high-performance (HPLC) chromatography, thin-layer, high-performance (HPTLC)

# Chemical names in ANABSTR

=> E BISPHENOL A/CN 25

E1	113	BISOPROLOL/CN
E2	13	BISOPROLOL FUMARATE/CN
E3	1170 -->	BISPHENOL A/CN
E4	1	BISPHENOL A BIS(2, 3-DIHYDROXYPROPYL) ETHER/CN
E5	1	BISPHENOL A BIS-(2, 3-DIHYDROXYPROPYL) ETHER/CN
E6	16	BISPHENOL A DERIVATIVES/CN
E7	3	BISPHENOL A DERIVATIVES, CHLORO-/CN
E8	1	BISPHENOL A DICYANATE/CN
E9	1	BISPHENOL A DIGLUCURONIDE/CN
E10	25	BISPHENOL A DIGLYCIDYL ETHER/CN
E11	1	BISPHENOL A DIGLYCIDYLETHER DIETHACRYLATE/CN
E12	1	BISPHENOL A DIGLYCIDYLETHER METHACRYLATE/CN
E13	3	BISPHENOL A DIGLYCIDYLMETHACRYLATE/CN
E14	4	BISPHENOL A DIMETHACRYLATE/CN
E15	1	BISPHENOL A DISULFATE/CN
E16	1	BISPHENOL A MONOGLUCURONIDE/CN
E17	1	BISPHENOL A MONOSULFATE/CN
...		
E23	15	BISPHENOL A, 3, 3', 5, 5' - TETRACHLORO-/CN
E24	2	BISPHENOL A, 3, 3', 5- TRIBROMO-/CN
E25	1	BISPHENOL A, 3, 3', 5- TRICHLORO-/CN



ANABSTR offers the possibility to search for a specific compound either by its chemical name or by its unique CAS Registry Number. However, delivery of CAS Registry Numbers has been discontinued by the database producer in 2016. Therefore, only searching by chemical names can be considered comprehensive.



Always use the EXPAND to verify the presence of the chemical substance of interest in the database. This will also help you to identify further specifics (e.g. *bisphenol A disulfate*) as well as unspecific derivatives (*bisphenol A derivatives*) you might want to include in the search.

# Chemical names in ANABSTR

=> **S E3** (=> **S BISPENOL A/CN**)

L1            1170 "BISPENOL A"/CN

=> **S E15** (=> **S BISPENOL A DISULFATE/CN**)

L2            1 "BISPENOL A DISULFATE"/CN

=> **S E3 AND E15**

              1170 "BISPENOL A"/CN

              1 "BISPENOL A DISULFATE"/CN

L3            0 "BISPENOL A"/CN AND "BISPENOL A DISULFATE"/CN

=> **S BISPENOL A?/CN**

L4            1317 BISPENOL A?/CN

=> **S L4 AND E15**

              1 "BISPENOL A DISULFATE"/CN

L5            1 L4 AND "BISPENOL A DISULFATE"/CN



The CN field is phrase parsed only, so searching bisphenol A in the CN field will not capture any term that includes bisphenol A but has additional words in the chemical name. Think of CN as the 'complete name.'



Either select the substances of interest from the Expand list or use appropriate truncations to include all specific and unspecific derivatives.

# ANABSTR Case Study – Searching for a specific Analyte

=> E EPOETIN/CN

E1	85	EPN/CN
E2	1	EPN OXON/CN
E3	13 -->	EPOETIN/CN
E4	8	EPOETIN ALPHA/CN
E5	4	EPOETIN BETA/CN
E6	2	EPOMEDI OL/CN

=> E ERYTHROPOI ETI N/CN

E13	3	ERYTHROMCYLAMI NE/CN
E14	1	ERYTHROPENTONI C ACID, 2- DEOXY- /CN
E15	102 -->	ERYTHROPOI ETI N/CN
E16	2	ERYTHROPTERIN/CN
E17	10	ERYTHROSE/CN
E18	3	ERYTHROSE 4- PHOSPHATE/CN

=> S E3- E5/CNA OR E15/CNA

L1 113 (EPOETIN/CNA OR "EPOETIN ALPHA"/CNA OR "EPOETIN BETA"/CNA) OR ERYTHROPOI ETI N/CNA



Search for information regarding the analysis of Erythropoietin (EPO), a essential hormone for red blood cell production. Due to its performance-enhancing effect, recombinant EPO has been widely used illicitly by athletes since the early 1990s (e.g. by cyclists).



To search for a substance specifically as the Analyte, append /CNA (Chemical Name, Analyte) to the chemical name. Please note that no EXPAND is available in this field.



# ANABSTR Case Study – Searching for a specific Analyte

(cont.)

=> S L1 AND (DOPING? OR PERFORMANCE?(3A) ENHANC? OR SPORT?)

L2 32 L1 AND (DOPING OR PERFORMANCE?(3A) ENHANCE? OR SPORT?)

=> D BIB ABS IT

L2 ANSWER X OF 32 ANABSTR COPYRIGHT 2020 RSC on STN

AN 781612 ANABSTR Full-text

TI Rapid and selective detection of recombinant human erythropoietin in human blood plasma by a sensitive optical sensor

AU Gholami, Mahnaz D.; Theiss, Frederick; Sonar, Prashant; Ayoko, Godwin A.; Izake, Emad L.

S0 Analyst (2020) 145(16), 5508–5515

AB Recombinant human erythropoietin (rHuEPO) is an important hormone drug that is used to treat several medical conditions. It is also frequently abused by athletes as a **performance enhancing** agent at **sporting** events. The time window of the rHuEPO in blood is short. Therefore, the rapid detection of rHuEPO use/abuse at points of care and in **sports** requires a selective analytical method and a sensitive sensor. Herein, we present a highly selective method for the rapid detection of rHuEPO in human blood plasma by a sensitive optical sensor. ...

IT Analyte(s):

**erythropoietin**

Matrix:

blood plasma

# Generic substances or substance classes in ANABSTR

## => E PLASTICISERS/CN 5

E1	3	PLASTIC PACKAGING/CN
E2	2	PLASTIC RAW MATERIALS/CN
E3	49 -->	PLASTICISERS/CN
E4	132	PLASTICIZERS/CN
E5	339	PLASTICS/CN



Depending how it is mentioned in the publication, a specific substance might not be indexed but rather a generic substance description or class though. Those generic substances are also indexed in the CN field.

## => E PHTHALATE/CN

E7	1	PHTHALAMIDE, SULFO- /CN
E8	57 -->	PHTHALATE/CN
E9	8	PHTHALATE DERIVATIVES/CN
E10	24	PHTHALATE ESTERS/CN
...		
E18	13	PHTHALIC ACID ALKYL ESTERS/CN
E19	207	PHTHALIC ACID BENZYL BUTYL ESTER/CN
...		
E26	331	PHTHALIC ACID BIS- (2-ETHYLHEXYL) ESTER/CN
...		
E48	22	PHTHALIC ACID DIALKYL ESTERS/CN
...		
E52	452	PHTHALIC ACID DIBUTYL ESTER/CN
...		
E77	24	PHTHALIC ACID MONOBUTYL ESTER/CN

# ANABSTR Case Study – Searching for Plasticizers

specificity

=> S PLASTICI !ERS/CNA

L1 171 PLASTICI !ERS/CNA

=> S PHTHALATE?/CNA OR E18/CNA OR E38/CNA OR

L2 790 PHTHALATE?/CNA OR "PHTHALIC ACID DI-ESTERS" /CNA OR "PHTHALIC ACID DI-ESTERS" /CNA OR "PHTHALIC ACID DI-ESTERS" /CNA OR "PHTHALIC ACID DI-ESTERS" /CNA OR "PHTHALIC ACID DI-ESTERS" /CNA

=> S E16-E17/CNA OR E19-E32/CNA OR E36-E37/CNA OR E39-E47/CNA OR E49-E67 OR E69/CNA

L3 857 ("PHTHALIC ACID 2-ETHYLHEXYL ESTER" /CNA OR "PHTHALIC ACID 2-ETHYLHEXYL HEXYL ESTER" /CNA) OR ...

=> S L1 OR L2 OR L3

L4 1426 L1 OR L2 OR L3



Plasticizers are used to increase the flexibility, transparency, durability, and longevity of plastics, such as polyvinyl chloride (PVC). Especially phthalates are used in this respect. However, they are easily released into the environment and then taken up by humans. Therefore, search for analytical studies on plasticizers in general and more specifically on phthalates.

# ANABSTR Case Study – Searching for Plasticizers (cont.)

=> D TI IND

L4 ANSWER X OF 1426 ANABSTR COPYRIGHT 2020 RSC on STN

TI Suspect screening of 200 hazardous substances in plastic toys using ultra-high-performance liquid chromatography-hybrid quadrupole time-of-flight mass spectrometry

IT Analyte(s):

colorants; plasticizers; allergens; nitrosamines; primary aromatic amines; flame-retardants; organophosphorus compounds; endocrine disruptors

... the generic substance class ...

Matrix:

toys

Concepts:

ultra-performance liquid chromatography (UPLC)

time-of-flight mass spectrometry (TOF MS)

quadrupole mass spectrometry (quadrupole MS)

precipitation

tandem mass spectrometry (tandem MS)

Depending how it is mentioned in the publication (mostly title or abstract), records will be retrieved mentioning either ...

# ANABSTR Case Study – Searching for Plasticizers (cont.)

=> D TI IND

L4 ANSWER X OF 1426 ANABSTR COPYRIGHT 2020 RSC on STN

TI Determination of phthalate esters in drinking water and edible vegetable oil samples by headspace solid phase microextraction using graphene/polyvinyl chloride nanocomposite coated fiber coupled to gas chromatography-flame ionization detector

IT Analyte(s):

phthalate esters

... a generic substance description ...

Matrix:

water

Concepts:

headspace analysis

extraction, micro-, solid-phase (SPME)

gas chromatography (GC)

flame-ionization detection (FID)

# ANABSTR Case Study – Searching for Plasticizers (cont.)

=> D TI IND

L4 ANSWER X OF 1426 ANABSTR COPYRIGHT 2020 RSC on STN

TI Development and validation of an analytical method for quantitation of monobutylphthalate, a metabolite of di-n-butylphthalate, in rat plasma, amniotic fluid, fetuses and pups by UPLC-MS/MS

IT Analyte(s):

phthalic acid monobutyl ester; **phthalic acid dibutyl ester**; biomarkers

Matrix:

blood plasma

... or the specific compound.

Concepts:

ultra-performance liquid chromatography (UPLC)

tandem mass spectrometry (tandem MS)

precipitation

extraction, liquid

# Refining searches according to the analysed media (Matrix)

## => E BLOOD/CN 5

E1	1	BLI CCA BJOERKNA/CN
E2	3	BLONANSERIN/CN
E3	9245	--> BLOOD/CN
E4	2	BLOOD CELLS/CN
E5	25738	BLOOD PLASMA/CN

## => E SOIL/CN 5

E6	41	SOFOSBUVIR/CN
E7	41	SOFT DRINKS/CN
E8	8336	--> SOIL/CN
E9	1	SOIL ACIDIFIERS/CN
E10	1	SOIL CONDITIONERS/CN

## => E BEVERAGES/CN 5

E11	6	BEVANTOLOL/CN
E12	1	BEVANTOLOL HYDROCHLORIDE/CN
E13	1143	--> BEVERAGES/CN
E14	515	BEVERAGES, ALCOHOLIC/CN
E15	626	BEVERAGES, NON-ALCOHOLIC/CN

## => E BEER/CN 5

E16	14	BEEF PRODUCTS/CN
E17	2	BEEFSTEAK FUNGUS/CN
E18	1147	--> BEER/CN
E19	53	BEESWAX/CN
E20	31	BEET/CN



Use the /CN field to explore the type of matrix available for searching in the database.

# ANABSTR Case Study – Refining searches according to the analysed media (Matrix)

=> **S (GLYPHOSAT? OR ORGANOPHOSPH? OR PESTICIDE?) /CNA**

**L1 7646 (GLYPHOSAT? OR ORGANOPHOSPH? OR PESTICIDE?) /CAN**

=> **S (BEER OR MALT OR HOPS OR BREWING MATERIALS OR BEVERAGES?) /CNM**

**L2 3501 (BEER OR MALT OR HOPS OR BREWING MATERIALS OR BEVERAGES?) /CNM**

=> **S L1 AND L2**

**L3 41 L1 AND L2**



Search for information regarding the determination of glyphosate or pesticides in general in alcoholic beverages such as beer.



To specify the analysed media (Matrix), use /CNM (Chemical Name, Matrix). Please note that no EXPAND is available in this field.



# ANABSTR Case Study – Refining searches according to the analysed media (cont.)

=> S L3 AND (HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY? OR CHROMATOGRAPHY, LIQUID, HIGH-PERFORMANCE?) /CT

L4 10 L3 AND (HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY? OR CHROMATOGRAPHY, LIQUID, HIGH-PERFORMANCE?) /CT



Use ANABSTR Controlled Terms (Concepts) to refine a search to the applied analytical method.

=> D TI IND

L4 ANSWER X OF 10 ANABSTR COPYRIGHT 2020 RSC on STN

TI Evaluation of selected buffers for simultaneous determination of ionic and acidic pesticides including glyphosate using anion exchange chromatography with mass spectrometric detection

IT Analyte(s):

glyphosate; pesticides

Matrix:

beer

Concepts:

high-performance liquid chromatography (HPLC)

tandem mass spectrometry (tandem MS)

ion-exchange chromatography

# SELECT CIT to extract reference data

=> **SEL CIT L3 1-**

**E1 THROUGH E37 ASSIGNED**

=> **D SEL**



**SELECT CIT allows you to extract the reference data from the source documents in ANABSTR and have them automatically converted to a citation format for searching in SCISEARCH or HCAPLUS. SEL CIT selects first author, publication year, volume, first page, and a truncation symbol with /RE appended.**

E1	1	AHMED F E, 2001, V20, P649, ?/RE
E2	1	BRITO N M, 2002, V957, P201, ?/RE
E3	1	BU Y L, 1997, V15, P499, ?/RE
E4	1	CHARLTON A J, 2008, V618, P196, ?/RE
E5	1	CHEN H D, 2008, V133, P1182, ?/RE
E6	1	DASGUPTA S, 2011, V1218, P6780, ?/RE
E7	1	GOURSAUD J, 1978, V32, P975, ?/RE
E8	1	HARTL A, 1990, V130, P984, ?/RE
...		
E36	1	XU M L, 2014, V49, P97, ?/RE
E37	1	ZHAO Q, 2013, V405, P4765, ?/RE

# Enhance your search with citation data

=> **FIL SCISEARCH** (=> **FIL HCAPLUS**)

=> **S E1-E37**

L5 947 ("AHMED F E, 2001, V20, P649, ?"/RE OR "BRITO N M, 2002, V957, P201, ?"/RE OR "BU Y L, 1997, V15, P499, ?"/RE OR "CHARLTON A J, 2008, V618, P196, ?"/RE OR "CHEN H D, 2008, V133, P1182, ?"/RE ...

=> **D TI**

L5 ANSWER x OF 947 SCISEARCH COPYRIGHT (c) 2020 Clarivate Analytics on STN  
TI A review of the analytical methods used for beer ingredient and finished product analysis and quality control

L5 ANSWER x OF 947 SCISEARCH COPYRIGHT (c) 2020 Clarivate Analytics on STN  
TI Tracking, Behavior and Fate of 58 Pesticides Originated from Hops during Beer Brewing

L5 ANSWER x OF 947 SCISEARCH COPYRIGHT (c) 2020 Clarivate Analytics on STN  
TI Development and Validation of a Method for the Determination of Pesticide Residues in Beer by Liquid Chromatography-Mass Spectrometry

# Summary

- ANABSTR is an important database when looking for analytical studies on a specific chemical substance
- Value-added indexing is performed on the basis of three main aspects: the analyte, matrix and technique used
- ANABSTR is a very timely, up-to-date database
- The narrow scientific focus and unique search capabilities make ANABSTR a good starting point for further exploring the content on STN

# Contact Us



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