ReaxysFile™ on STN: Property Information from Patents

Introduction

ReaxysFile contains property information from journals as well as from patents. The main areas excerpted from patents are reactions/preparations, uses of compound, spectral data (e.g. NMR data), bioactivity (e.g. metabolism, toxicological data) and basic physical data (e.g. melting point).

The information is derived from selected patents:

- IPC Classes C07 (Organic Chemistry); A61K and secondary IPC C07 (Medicinal, Dental, Cosmetic Preparations) and C09B (Dyes)
- English-language patents from these IPC classes are excerpted from the PCT (WIPO), European (EPO) and USPTO Patent Offices

Only one family member is indexed, most often the first published patent document or an English language equivalent ("yes" in table indicates the relevant patent, see DIS ALLPAT in example 3).

Patent Specific Data (PSD)

PSD is treated like a property field. It is directly related to the substance and therefore listed in the Field Availability. It includes the following information:

- Prophetic compounds

Compounds similar producible according to the preparation claimed in the patent

- Related Markush structures

A defined compound A references a "related Markush structure" B. The related Markush structure B may reference other defined compounds including A.

- Location in patent (substance-related)

Points to a specific "Claim", "page", "line" or "column" of the indexed patent

Example 1:
Search and display of related Markush structures and corresponding properties

```
ANSWER 8 OF 9 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

Accession Number (AN):          11323042
Chemical Name (CN):             palladium bis(2,4-pentanedionate),
                                platinum(II) bis(acetylacetonate),
                                platinum(II) bis(acetylacetonato),
                                bis(acetylacetonato)platinum(II),
                                bis(acetylacetonete)platinum(II),
                                platinum(II) bis-acetylacetonate,
                                bis-acetyl acetonate platinum
Lin. Struct. Formula (LSF):     <Pt(CH3COCHCH3CO)2>
Molec. Formula (MF):            C10 H14 O4 Pt
Formula Weight (FW):            393.299
Compound Type (CTYPE):          Coordination compound
InChi Key: (INCHI):             KLFRPGNCEJNEKU-FDGPNNRMSA-L
Alternate InChi Key:(AINCHI): KLFRPGNCEJNEKU-OZCANJGIDM
Markush Ref. Count (MARKREF): 1
Entry Date (DED):               2008/06/16
Update Date (DUPD):             2011/03/17
```

```
 Field Availability:
      Code      Name                              Occurrence
      ================================================
      AN        Accession Number                         1
      CN        Chemical Name                            7
      LSF       Linearized Structure Formula             1
      …
      PSD       Patent Specific Data                     4
      QCC       Quantum Chemical Calculations            3
      RAS       Raman Spectrum                           1
      SLB       Solubility (MCS)                         1
      USC       Use of Compound                          1
      UVS       UV and Visible Spectrum                  7
   …
Patent Specific Data:
PSD
      Prophetic compound:              prophetic catalyst
      Location in Patent:              Page/page column 5
      Reference(s):
      1. Patent: LIQUID POLYMER; …
PSD
      Related Markush Structure:       11337539
      Reference(s):
      1. Patent: Selective hydrogenation of nitro groups of halonitro aromatic
         compounds; …
      Prophetic compound:              prophetic catalyst
      Reference(s):
      1. Patent: Process for the Preparation of enantiomerically enriched
         compounds; …
PSD
      Location in Patent:              Claim
      Reference(s):
      1. Patent: Preparation of acetals; …

=> s 11337539/an
L10           1 11337539/AN

=> d

L10  ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

      Accession Number (AN):          11337539
      Compound Type (CTYPE):          markush structure
      Markush Ref. Count (MARKREF):   0
      Entry Date (DED):               2008/06/16
      Update Date (DUPD):             2010/02/17

      No structure diagram available for this Document

   Field Availability:
      Code      Name                            Occurrence
      ================================================
      AN        Accession Number                         1
      CTYPE     Compound Type                            1
      MARKREF   Markush Reference Count                  1
      DED       Entry Date                               1
      DUPD      Update Date                              1
      LB        Substance Label                          1
      PSD       Patent Specific Data                     1
      USC       Use of Compound                          1

=> d psd usc

L10  ANSWER 1 OF 1 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

Patent Specific Data:
PSD
      Location in Patent:              Claim 1
      Reference(s):
      1. Patent: Selective hydrogenation of nitro groups of halonitro aromatic
         compounds;…

Use of Compound:
USC
      Use Pattern (.PT):               Complex for preparation of supported
                                       catalyst for hydrogenation of nitro groups
                                       of halonitro compounds
      Reference(s):
      1. Patent: Selective hydrogenation of nitro groups of halonitro aromatic
         compounds; …
```

Searching Bibliographic Patent Information

The focus of ReaxysFile is on physical, chemical and bioactivity properties, not on searching patent specific data like classifications or Application Numbers. However, a couple of fields are searchable:

- Patent Assignee /PA
- Inventor /IN
- Patent Number /PN
- Patent Kind Code /PK
- Title /TI
- Language /LA

To restrict a search to bibliographic information in substance documents, append (.SUB)to the search field code, e.g. /PA.SUB. To restrict a search to reaction information, append (.RX) to the search field code, e.g. /PA.RX.

Example 2:
Search for product selectivity studies of reactions (patents) published by the BASF company

```
=> e product/rx.subj
E1          1074       NOT/RX.SUBJ
E2          4371       OF/RX.SUBJ
E3        176517  -->  PRODUCT/RX.SUBJ
E4        134863       PRODUCT DISTRIBUTION/RX.SUBJ
E5         42626       PRODUCT DISTRIBUTION / SELECTIVITY/RX.SUBJ
E6          8250       PURIFICATION/RX.SUBJ
E7          8250       PURIFICATION / WORK UP/RX.SUBJ
E8         15615       QUANTUM/RX.SUBJ
E9         15615       QUANTUM YIELD/RX.SUBJ
E10       146879       RATE/RX.SUBJ
E11       146879       RATE CONSTANT/RX.SUBJ
E12         1074       REACT/RX.SUBJ

=> s e5
L23       42626 "PRODUCT DISTRIBUTION / SELECTIVITY"/RX.SUBJ

=> e basf/pa
E1          3990       BASELL/PA
E2             1       BASES/PA
E3        156120  -->  BASF/PA
E4             1       BASFAKTIENGESELLSCHAFT/PA
E5             2       BASFAKTIENGLESELLSCHAFT/PA
E6             3       BASFORD/PA
E7          3639       BASHA/PA
E8             5       BASHAI/PA
E9            20       BASHAR/PA
E10            6       BASHAROVA/PA
E11            4       BASHFORD/PA
               30       BASHIARDES/PA

=> s e3 and l23
          156120 BASF/PA
L24          748 BASF/PA AND L23

=> d

L24  ANSWER 1 OF 748 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

Reaction:
RX
      Reaction ID:                    30080298
      Reactant AN (.RAN):             5802393
      Reactant (.RCT):                (R)-sec-butylidene(1-phenylethyl)amine
      Product AN (.PAN):              5802508, 8615068
      Product (.PRO):                 RR-(R)-sec-butylidene(1-phenylethyl)amine,
                                      RS-(R)-sec-butylidene(1-phenylethyl)amine
      React. Struct. Keywords (.SKW): mapped reaction
      Record type (.RTYP):            full reaction
      Number of Bond Changes (.NBC):  4
      No. of React. Details (.NVAR):  1, 5802393, 5802508, 8615068
      Det. React. reactants (.BLC):   5802393, 5802508, 8615068
      No. of References (.NUMREF):    1

Reaction Details:
```

```
RX
      Reaction RID (.RID):              30080298.1
      Reaction Classification (.CL):    Chemical behaviour
      Reagent (.RGT):                   hydrogen
      Catalyst (.CAT):                  passivated Cu/Ni/Mo (13/40/1)/ZrO2
      Solvent (.SOL):                   methanol
      Time (.TIM):                      12
      Temperature (.T):                 100 Cel
      Pressure (.P):                    52505.3 Torr
      Other Conditions (.COND):         Inert atmosphere
      Subject Studied (.SUBJ):          Product distribution / selectivity
      Location (.LCN):                  Page/Page column 13
      Fulltext of reaction (.TXT):      II. General Method BDiaselective
                                        Hydrogenation of
                                        (R)-Sec-Butylidene(1-Phenyl-Ethyl)Amine
                                        (Schiff Base of (R)-(1-Phenylethyl)Amine
                                        with 2-Butanone)A mixture of
                                        (R)-sec-butylidene(1-phenylethyl)amine
                                        (imine); solvent and passivated catalyst,
                                        as specified in table 3, was initially
                                        charged in each case in a 300 ml
                                        autoclave. Subsequently, the mixture was
                                        inertized with nitrogen and heated to
                                        100.deg. C. Subsequently, at this
                                        temperature, hydrogen was injected up to
                                        the desired pressure, as likewise
                                        specified in each case in table 3, and,
                                        when the internal pressure declined,
                                        brought back to the desired pressure.
                                        After the run times specified in table 3
                                        in each case, measured from injection of
                                        hydrogen, a sample was taken and was
                                        analyzed by gas chromatography. The
                                        results are reported in table 3 below.
      Example label (.LB):              II.3.5
      Reactant AN (.RCAN):              3587189
      Solvent AN (.SOLAN):              1098229
      Number of R. steps (.STP):        1
      Yield optical (.YDO):             82 percent de
      Reference(s):
      1. Patent: PROCESS FOR DIASTEREOSELECTIVE CONVERSION OF CHIRAL IMINES;…
      For details see ALLPAT (Example 3)
```

All Patents (ALLPAT)

List of all bibliographic patent information available for a specific substance or reaction.
Note: It is recommended to SET LINE 100

Example 3:
ALLPAT for record of Example 2

```
=> set line 100
SET COMMAND COMPLETED

=> d allpat

L3   ANSWER 1 OF 748 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

     All Patents:
     ALLPAT

   Reference:          Patent
   Title:              PROCESS FOR DIASTEREOSELECTIVE CONVERSION OF CHIRAL IMINES
   Patent Number:      US2010/274053
   Inventor:           Siegel, Wolfgang; Hahn, Thilo; Staeb, Tobias
   Patent Assignee:    BASF SE
   Abstract:           Diastereoselective conversion of chiral imines of the formula I
                       to amines of the formula II where the R1 to R4 radicals are
                       each as defined in the description and R1 and R2 are different
                       than one another, by converting the imine of the formula I in
                       the presence of hydrogen and a heterogeneous copper-containing
                       catalyst.
```

```
Main IPC:          C07C 211/45
                   Priority Number      Priority Date
                   EP2007-150290        2007/12/21
PATENT INFORMATION

Patent Title:      PROCESS FOR DIASTEREOSELECTIVE CONVERSION OF CHIRAL IMINES

Patent Number  Kind Code  Publ. Date  Application No  Filing Date   Indexed Patent
WO2009/80511   A1         2009/07/02  WO2008-EP67191  2008/12/10    ---
EP2234958      A1         2010/10/06  EP2008-864515   2008/12/10    ---
US2010/274053  A1         2010/10/28  US2010-746868   2010/06/08    yes
---            ---         ---        EP2007-150290   2007/12/21    ---
```

All References (ALLREF)

List of all references available for a specific substance.

Note: the amount of information available for a specific reference reflects modified indexing philosophy. Citations might have only basic bibliographic information.

Example 4:

ALLREF for Accession Number 16701594

```
ANSWER 678 OF 6974 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on
STN

Accession Number (AN):          16701594
…

All References:
ALLREF

Reference:     Chen, Hai-ling; Li, Qian-shu; Xie, Yaoming; King, R. Bruce;
               Schaefer III, Henry F., Polyhedron, CODEN: PLYHDE, 29,
               <2010>, 2177 - 2184

Reference:     Bruce, Michael I.; Zaitseva, Natasha N.; Skelton, Brian W.;
               White, Allan H.; Fox, Mark A.; Low, Paul J., Dalton
               Transactions, CODEN: DTARAF, 39, <2010>, 1222 - 1234
Title:         Syntheses and molecular structures of some tricobalt
               carbonyl clusters containing
               2,4,6-trimethyl-1,3,5-trithiane
Abstract:      Reactions of CCo3 carbonyl clusters Co3(.my. 3-CR)(CO)9
               with 2,4,6-trimethyl-1,3,5-trithiane (S Me3) have given
               Co3(.my.3-CR)(.my.3- SMe3)(CO)6 <R = H (1), CCSiMe3 (2)>. A
               small amount of the coupled-alkyne product Me3SiC2<Co
               2(CO)6>C2<Co2(.my.-S Me3)(CO)4>CCSiMe3 (3) was isolated
               from the latter reaction. The reaction of Co3(.my.3-CCCSiMe
               3)(.my.3-SMe3)(CO)6 (2) with AuCl(PPh3) in the presence of
               NaOMe gave Co3<.my. 3-CCCAu(PPh3)>(.my.3-SMe3)(CO) 6 (4),
               which in turn reacts with Co3(.my.3-CBr) (CO)9 in the
               presence of catalytic amounts of Pd(PPh 3)4 and CuI to give
               <(OC)9Co 3>(.my.-CCCC)<Co3(.my.3-SMe3)(CO) 6> (5). Further
               substitution of 5 with SMe3 gave symmetrical
               <Co3(.my.3-SMe3)(CO) 6>2(.my.-CCCC) (6), also obtained from
               a reaction between <Co3(CO)9>2(.my.-CCCC) and two
               equivalents of SMe3. Similar substitution of
               Co3<.my.3-C(CC) 2<Ru(dppe)Cp*>>(CO)9 with SMe3 gave
               Co3<.my.3-C(CC)2<Ru(dppe)Cp*>> (.my.3-SMe3)(CO)6 (7). In
               all of these compounds, the SMe3 ligand caps the basal face
               of the CCo3 cluster on the opposite side to the .my.3-CR
               group. The three S donors occupy axial sites, with all CO
               groups being in equatorial sites. Reactions of
               Co3(.my.3-CBr)(CO)9 with S Me3 gave only
               Co3(.my.3-CX)(.my.3- SMe3)(CO)6 <X = C(O)NMe2 (8), CO2H
               (9)>. The redox properties and electronic structure of the
               C4-bridged bis-cluster 6 have been investigated through a
               combination of cyclic voltammetry, IR
               spectroelectrochemistry and DFT calculations, with
               comparisons made with suitablemodel systems. Single-crystal
               X-ray diffraction structure determination s of 1, 2, 3, 4
               and 8 are reported.
```

Reference: Aime, S.; Milone, L.; Valle, M., Inorganica Chimica Acta, CODEN: ICHAA3, 18, <1976>, 9 - 12

Reference: Slivinskii, E. V.; Rozovskii, A. Ya.; Korneeva, G. A.; Kurkin, V. I., Kinetics and Catalysis, CODEN: KICAA8, 39, <1998>, 764 - 774, Kinetika i Kataliz, CODEN: KNKTA4, 39, <1998>, 832 - 843

Reference: Sugihara, Takumichi; Wakabayashi, Akihito; Takao, Hiroko; Imagawa, Hiroshi; Nishizawa, Mugio, Chemical Communications (Cambridge, United Kingdom), CODEN: CHCOFS, <2001>, 2456 - 2457
Title: Synthesis of cyclopentadienones catalyzed by methylidynetricobalt nonacarbonyl
Abstract: Easily prepared and air-stable methylidynetricobalt nonacarbonyl could be used as a catalyst for the intramolecular <2+2+1>-cocyclization of diynes and carbon monoxide producing cyclopentadienones.

Reference: Sugihara, Takumichi; Wakabayashi, Akihito; Nagai, Yasuko; Takao, Hiroko; Imagawa, Hiroshi; Nishizawa, Mugio, Chemical Communications (Cambridge, United Kingdom), CODEN: CHCOFS, <2002>, 576 - 577
Title: Methylidynetricobalt nonacarbonyl catalyzed cyclotrimerization of alkynes
Abstract: A cobalt carbonyl cluster, methylidynetricobalt nonacarbonyl, catalyzed inter- and intramolecular cyclotrimerization of alkynes producing substituted benzene derivatives in good to excellent yields.

Reference: Sugihara, Takumichi; Yamaguchi, Masahiko, Journal of the American Chemical Society, CODEN: JACSAT, 120, <1998>, 10782 - 10783
Title: The Pauson-Khand reaction catalyzed by the methylidynetricobalt nonacarbonyl cluster <12>

Reference: Xiang, Si Fen; Bakke, Albert A.; Chen, Hsiang-Wen; Eyermann, C. J.; Hoskins, James L.; et al., Organometallics, CODEN: ORGND7, 1, <1982>, 698 - 703

Reference: Vollmer, David L.; Gross, Michael L.; Waugh, Russell J.; Bruce, Michael I.; Bowie, John H., Organometallics, CODEN: ORGND7, 13, <1994>, 3564 - 3571

Reference: Tsoy, A. A.; Korneeva, G. A.; Kayumov, F. F.; Grudtsyn, Yu. D.; Slivinskii, E. V.; et al., Russian Chemical Bulletin, CODEN: RCBUEY, 42, <1993>, 1320 - 1326, Izvestiya Akademi Nauk, Seriya Khimicheskaya, CODEN: IASKEA, 42, <1993>, 1388 - 1393

Reference: Howard, Martin W.; Kettle, Sidney F.; Oxton, Ian A.; Powell, Donald B.; Sheppard, Norman; Skinner, Phillip, Journal of the Chemical Society, Faraday Transactions 2: Molecular and Chemical Physics, CODEN: JCFTBS, 77, <1981>, 397 - 404

Reference: Granozzi, Gaetano; Tondello, Eugenio; Ajo, David; Casarin, Maurizio; Aime, Silvio; Osella, Domenico, Inorganic Chemistry, CODEN: INOCAJ, 21, <1982>, 1081 - 1084

Reference: Evans, John, Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999), CODEN: JCDTBI, <1980>, 1005 - 1011

Reference: Deshmukh, Prabodh; Dutta, T. K.; Hwang, J. L.-S.; Housecroft, C. E.; Fehlner, T. P., Journal of the American Chemical Society, CODEN: JACSAT, 104, <1982>, 1740 - 1742

Reference: DeKock, Roger L.; Fehlner, Thomas P., Surface Science, CODEN: SUSCAS, 119, <1982>, 391 - 398

Reference: Costa, Newton C. V.; Lloyd, D. Robert; Brint, Paul; Pelin, William K.; Spalding, Trevor R., Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999), CODEN: JCDTBI, <1982>, 201 - 206

Reference: Chesky, Peter T.; Hall, Michael B., Inorganic Chemistry, CODEN: INOCAJ, 20, <1981>, 4419 - 4425

Reference: Leung, P.; Coppens, P.; McMullan, R. K.; Koetzle, T. F., Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry, CODEN: ACBCAR, 37, <1981>, 1347 - 1352

Reference: Hitchcock, Adam P.; McGlinchey, Michael J.; Johnson, Allen L.; Walter, Wendy K.; Jigato, Manolo Perez; et al., Journal of the Chemical Society, Faraday Transactions 1, CODEN: JCFTEV, 89, <1993>, 3331 - 3346

Reference: Diana, E.; Gambino, O.; Rossetti, R.; Stanghellini, P. L.; Albiez, T.; et al., Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy, CODEN: SAMCAS, 49, <1993>, 1247 - 1260

Reference: DeKock, Roger L.; Deshmukh, Prabodh; Dutta, T. K.; Fehlner, T. P.; Housecroft, C. E.; Hwang, Jane L.-S., Organometallics, CODEN: ORGND7, 2, <1983>, 1108 - 1116

Reference: Binsted, Norman; Cook, Stephen L.; Evans, John; Greaves, G. Neville; Price, Richard J., Journal of the American Chemical Society, CODEN: JACSAT, 109, <1987>, 3669 - 3676

Reference: Aitchison, Alison A.; Farrugia, Louis J., Organometallics, CODEN: ORGND7, 6, <1987>, 819 - 829

Reference: Onaka, Satoru; Takagi, Sigeru; Furuta, Hiroyuki; Kato, Yoshio; Mizuno, Atushi, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 63, <1990>, 42 - 46

Title: 17O NMR study of metal carbonyl cluster compounds. IV. The substituent effect on the 17O NMR chemical shifts for a series of tri-nuclear metal carbonyl cluster compounds

Abstract: 17O NMR spectra have been measured for series of cobalt carbonyl cluster derivatives, RCCo3(CO)(9-x)- (PPh3)(x), (RC2R')Co(3-x-y)Fe(x)Mo(y)(CO)(9-y)Cp(y), and R(3-x)Sn<Co(CO)4>(x+1). The small 17O-chemical shift differences due to the change of R and/or introduction of PPh3 have been interpreted in terms of the electron buffer action of the Co3 core for RCCo3(CO)(9-x)(PPh3)(x). Good linear correlations between 17O-chemical shifts and CO stretching frequencies have been observed for these derivatives. Some effect of the magnetic anisotropy resulted from the ring current along the metal-triangle on 17O-chemical shifts has been suggested for metal-triangle clusters.

Reference: Worth, Gillian H.; Robinson, Brian H.; Simpson, Jim, Journal of Organometallic Chemistry, CODEN: JORCAI, 387, <1990>, 337 - 356

Reference: Bor, G., Proc. Symp. Coord.Chem., Tihany, Ung., 1964 (1965) S. 361/71, C.A., CODEN: PTRMAD, 65, <1966>, 1593

Reference: Patent
For details see display format ALLPAT

Reference: Co: Org.Verb.2, 3.1.3.5, page 152 - 167

Reference: Robinson, B. H., J. N. Z. Inst. Chem., CODEN: JNZCAH, 33, <1969>, 45 - 50, C.A., CODEN: JNZCAH, 71, <1969>, 54762

Reference: Robinson, B. H.; Tham, W. S., Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical, CODEN: JCSIAP, <1968>, 1784 - 1787

Reference: Mays, M. J.; Simpson, R. N. F., Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical, CODEN: JCSIAP, <1968>, 1444 - 1447

Reference: Ercoli, R.; Santambrogio, E.; Tettamanti Casagrande, G., Chimica e l'Industria (Milan, Italy), CODEN: CINMAB, 44, <1962>, 1344 - 1349

Reference: Bor, G.; Marko, L.; Marko, B., Chemische Berichte, CODEN: CHBEAM, 95, <1962>, 333 - 340

Reference: Alami, Mohamed Kalam; Dahan, Francoise; Bonnet, Jean-Jacques; Mathieu, Rene, Organometallics, CODEN: ORGND7, 7, <1988>, 1391 - 1394

Example 5:
Display for older patents (most of them have no TI/AB or further patent information)

```
=> d 30 rx allpat

L16  ANSWER 30 OF 52005 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

Reaction:
RX
      Reaction ID (.ID):              26815644
      Reactant AN (.RAN):             1919922, 3587189
      Reactant (.RCT):                N,N-dimethyl-cyclohexylamine, hydrogen
      Product AN (.PAN):              2689488
      Product (.PRO):                 (CH3)2(cyclo-C6H11)N*BH3
      React. Struct. Keywords (.SKW): failed mapping
      Record type (.RTYP):            no reaction scheme, has preparation
      No. of React. Details (.NVAR):  2
      Preparation reactants (.BLB):   1919922, 3587189, 2689488
      Det. React. reactants (.BLC):   1919922, 3587189, 2689488
      No. of References (.NUMREF):    5

      All Patents:
      ALLPAT

    Reference:          Patent
    Patent Number:      FR1186995
    Patent Assignee:    Studiengesellschaft Kohle m.b.H.

    Reference:          Patent
    Patent Number:      GB855881
    Patent Assignee:    Studiengesellschaft Kohle m.b.H.

    Reference:          Patent
    Patent Number:      DE1056137
    Patent Assignee:    Studiengesellschaft Kohle m.b.H.

    Reference:          Patent
    Patent Number:      DE1048586
    Patent Assignee:    Studiengesellschaft Kohle m.b.H.
```

Appendix

Examples for properties derived from patents:

```
Reaction:
RX
      Reaction ID (.ID):              29875874
      Product AN (.PAN):              20838133
      Product (.PRO):                 6-methoxy-7-n-butoxy-4-(3-trifluoromethyl-
                                      4-fluoroanilino)-benzo<d><1,2,3>triazine
      React. Struct. Keywords (.SKW): half reaction
      Record type (.RTYP):            half reaction, has preparation
      No. of React. Details (.NVAR):  1
      Preparation reactants (.BLB):   20838133
      No. of References (.NUMREF):    1

Reaction Details:
RX
      Reaction RID (.RID):            29875874.1
      Reaction Classification (.CL):  Preparation (half reaction)
      Location (.LCN):                Page 19 column 10
      Example label (.LB):            23
      Number of R. steps (.STP):      1
      Reference(s):
      1. Patent: THE AROMATIC RING TRIAZINE DERIVATIVES AND THE USES THEREOF;…
```

```
Use of Compound:
USC
      Use Pattern (.PT):              modulation of activity of liver X
                                      receptors (LXR) and Farnesoid X receptors
                                      (FXR)
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
USC
      Use Pattern (.PT):              hypocholesterolemia
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
USC
      Use Pattern (.PT):              atherosclerosis
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
USC
      Use Pattern (.PT):              myocardial infarction
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
USC
      Use Pattern (.PT):              ischemic stroke
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
USC
      Use Pattern (.PT):              obesity
      Reference(s):
      1. Patent: LXR AND FXR MODULATORS; …
```

```
Nuclear Magnetic Resonance:
NMR
      Nucleus (.NUC):                 1H
      Solvents (.SOL):                methanol-d4
      Original Text (.TXT):           NMR (400 MHz, CD3OD) : 7.27 (d, J= 3.2 Hz,
                                      IH), 7.20-7.14 (m, 2H), 6.93 (t, J = 6.8
                                      Hz, IH), 6.85 (s, IH), 6.79 (s, IH), 3.60
                                      (q, J = 2.8 Hz, IH), 3.49 (br s, 2H), 3.19
                                      (dd, J= 18.8, 6.0 Hz, IH), 3.07 (dd, J=
                                      13.2, 3.2 Hz, IH), 2.84-2.78 (m, 2H), 2.37
                                      (d, J= 12.4 Hz, IH), 1.86 (d, J = 12.4 Hz,
                                      IH), 1.79-1.69 (m, 2H), 1.56-1.10 (m, HH),
                                      0.84 (t, J= 7.6 Hz, 3H).
      Frequency (.F):                 400 MHz
      Note(s) (.COM):                 Signals given
      Reference(s):
      1. Patent: (+)-3-HYDROXYMORPHINAN DERIVATIVES AS NEUROPROTECTANTS;…
```

Mass Spectrum:

MS

Description (.KW): ESI (Electrospray ionisation), LCMS (Liquid chromatography mass spectrometry)

Reference(s):

1. Patent: (+)-3-HYDROXYMORPHINAN DERIVATIVES AS NEUROPROTECTANTS; …

UV and Visible Spectrum:

Description (.KW)	Solvent (.SOL)	Absorption Maxima (.AM) (nm)	Ref.
UV/VIS reflection maximum(a)	chloroform	282	1

Reference(s):

1. Patent: ANTIMICROBIAL POLYMERS AND COATINGS; …

Infrared Spectrum:

Description (.KW)	Orig. Text (.TXT)	Ref.
in KBr	IR (KBr): 3300, 3277, 1577, 1501 , 1367, 1280, 1184.	1

Reference(s):

1. Patent: ANTITUMOR 1,2-DIPHENYLPYRROLE COMPOUNDS AND THEIR PREPARATION…

Refractive Index:

Value (RI) (--)	Temp. (.T) (Cel)	Wavelen. (.W) (nm)	Ref.
1.5692	22.2	589	1

Reference(s):

1. Patent: NITROGENOUS HETEROCYCLIC COMPOUNDS AND FUNGICIDES FOR AGRICULTURAL AND HORTICULTURAL USE; …

Pharmacological Data:

PHARM

Effect (.E):	neuroprotective
Species or Test-System (.SP):	HT22 hippocampal neuron cells of mouse
Kind of Dosing (.KD):	as trifluoroacetate salt
Method, Remarks (.MR):	Experimental Example 1: Cell cytotoxicity testHT22 cells (mouse hippocampal neuron, SaIk Institute and KRIBB) were plated in a 96-well plate at a density of 3 x 103 cells/well for 16 hrs before treatment. The cells were treated with five millimolar glutamate and various concentrations of the inventive compounds and incubated for 24 hrs in a growth media (DMEM with 10percent FBS and 1percent penicillin streptomycin). Then, the cells were treated with3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT, Sigma.(R).) for 4 hrs and absorbance of each well was measured with a plate reader at a wavelength of 450 nm. <Da-Qing, et. al, Anti-oxidant and anti-inflammatory activities of macelignan in murine hippocampal cell line and primary culture of rat microglia cells, BBRC, 2005, 331, 1264-1269>.Table 1 shows the results of cell cytotoxicity test of the compounds of Examples 1 to 134 and a comparative compound, 3-HM.eta.Br. hi Table 1, EC50 is neuroprotective effect against glutamate toxicity and CC50 is cytotoxicity of the compounds. The EC50 values were statistically analyzed using Prizm.(R). (GraphPad Software Inc., San Diego, CA., USA).
Type (.TYP):	EC50
Value of Type (.V):	0.459 .my.mol/l

Reference(s):

1. Patent: (+)-3-HYDROXYMORPHINAN DERIVATIVES AS NEUROPROTECTANTS;…

Melting Point:

Value (MP) (Cel)	Ref.
237 - 239	1

Reference(s):

1. Patent: BICYCLIC DERIVATIVES OF AZABICYCLIC CARBOXAMIDES, PREPARATION THEREOF AND THERAPEUTIC USE THEREOF; …

Boiling Point:

Value (BP) (Cel)	Press. (.P) (Torr)	Ref.
55 - 60	0.080258 - 0.09976	1

Reference(s):

1. Patent: METHOD FOR PRODUCING ACRYLATE DERIVATIVE, ACRYLATE DERIVATIVE, AND INTERMEDIATE THEREOF; …

Crystal Property Description:

CPD

(CPD):	blue

Reference(s):

1. Patent: (+)-3-HYDROXYMORPHINAN DERIVATIVES AS NEUROPROTECTANTS; …

Kinematic Viscosity:

Value (KV) (cm**2/s)	Temp. (.T) (Cel)	Ref.
342.4	25	1

Reference(s):
1. Patent: Photopolymerizable functional radical-containing organosilicon

Dynamic Viscosity:

Value (DV) (g/cm*s)	Temp. (.T) (Cel)	Ref.
75.52	24.9	1

Reference(s):
1. Patent: EPOXY COMPOUND AND PROCESS FOR PRODUCING THE EPOXY COMPOUND; …

Patent Specific Data:

PSD
Prophetic compound: prophetic catalyst
Location in Patent: Page 13 column 6;
Reference(s):
1. Patent: Use of a mixture of an ordered intermetallic compound and an inert material as a catalyst and corresponding hydrogenation processes;…