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## 8. FIGURES

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Figure 1: Cumulative excretion of radioactivity after single oral administration of  $^{14}\text{C}$ -4,4'-sulphonyldiphenol at a target dose level of 300 mg/kg bw to male and female rats, respectively

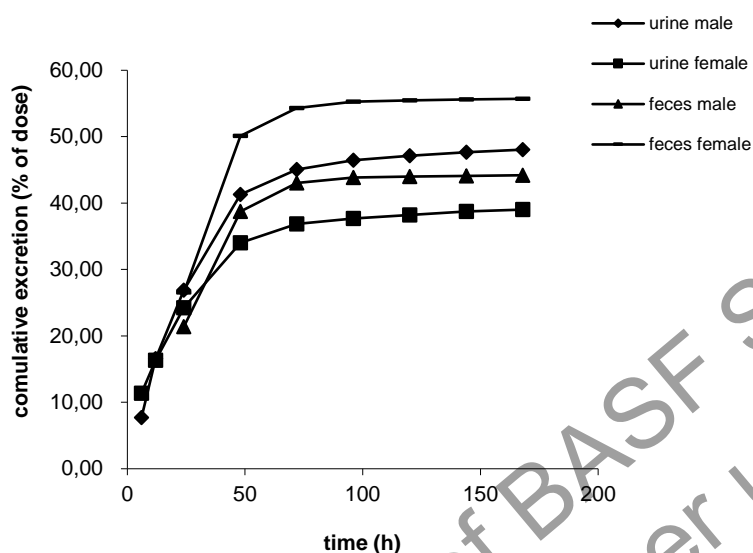


Figure 2: Cumulative excretion of radioactivity after single oral administration of  $^{14}\text{C}$ -4,4'-sulphonyldiphenol at a target dose level of 30 mg/kg bw to male and female rats, respectively

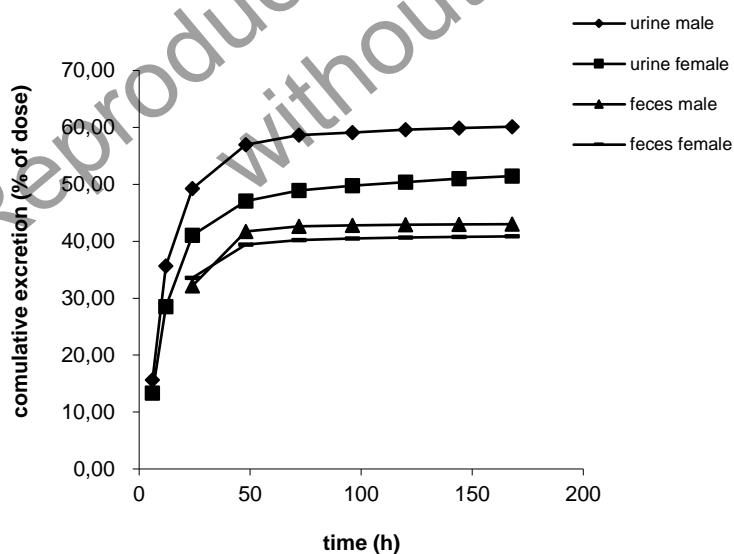


Figure 3: Cumulative excretion of radioactivity after 14 daily oral administrations of DHDPS and one oral administration of  $^{14}\text{C}$ -4,4'-sulphonyldiphenol on day 15 (30 mg/kg bw) to male and female rats, respectively

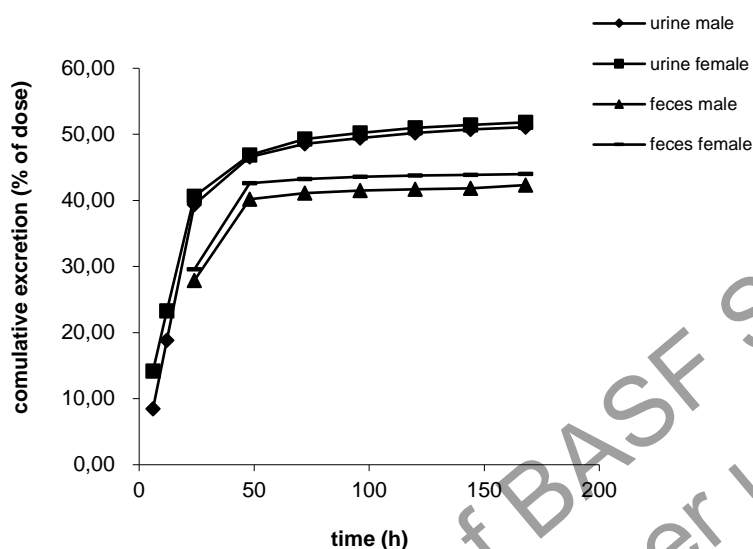


Figure 4: Mean plasma concentrations of radioactivity after single oral administration of  $^{14}\text{C}$ -4,4'-sulphonyldiphenol at a target dose level of 300 mg/kg bw to male and female rats

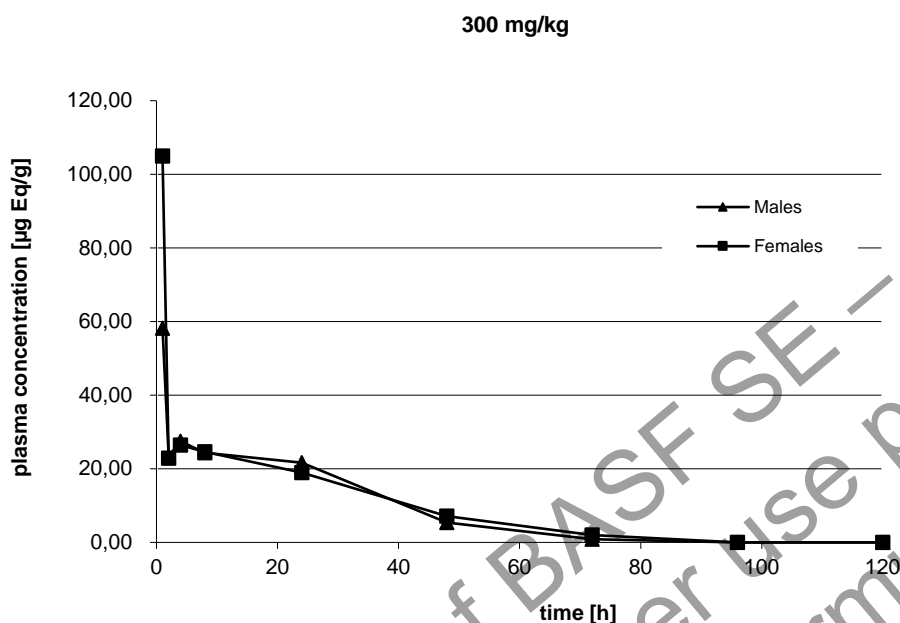
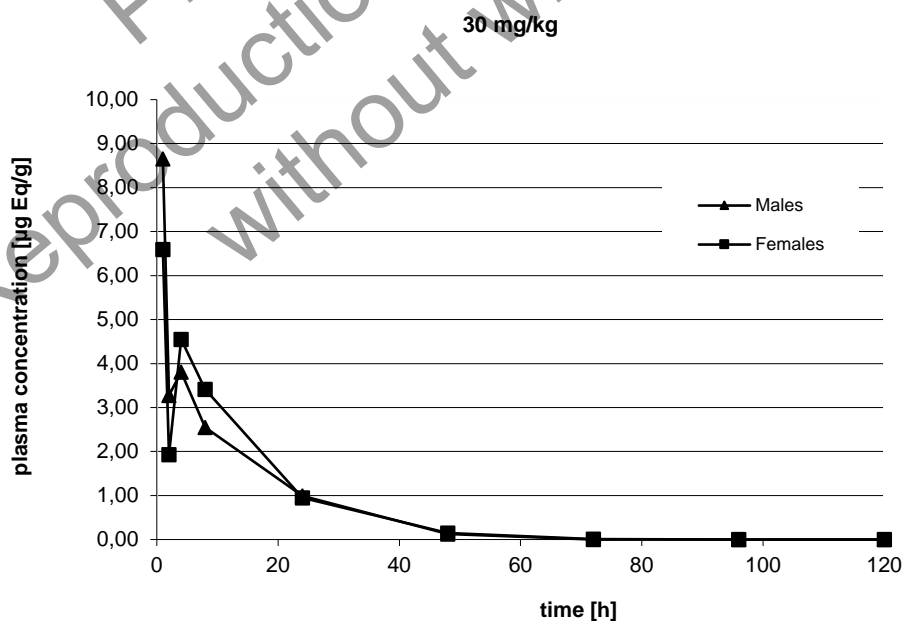


Figure 5: Mean plasma concentrations of radioactivity after single oral administration of  $^{14}\text{C}$ -4,4'-sulphonyldiphenol at a target dose level of 30 mg/kg bw to male and female rats



## 9. APPENDICES

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Appendix 1: Certificate of Analysis of the radio-labeled test substance

$^{14}\text{C}$ -4,4'-sulphonyldiphenol

**17/0423-1**  
added 04.09.18

  
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**Certificate of Analysis**

Reg.No. : 63265      Batch No. : 1248-1101  
Label : phenyl-U-C14  
Study Code : IL1248\_1017

|  |  |
|--|--|
|  | CL-No.   |
|  | CAS No. 80-09-1  |
|  | Core Project   |
|  | Internal (Metabolite) Code                                       |
|  | Molecular Formula $\text{C}_{12}\text{H}_{10}\text{O}_4\text{S}$ |
|  | Molecular Weight (unlabelled) 250.27                             |

IUPAC-Name: 4,4'-dihydroxydiphenylsulfone  
Solvent: Acetonitrile  
Homogeneity: given

|                                      |                       |                    |
|--------------------------------------|-----------------------|--------------------|
| Specific Activity: 59.6 MBq/g        | Determination by: LSC | Date: Dec 18, 2017 |
| Concentration of AI: 4.45 mg/g       | HPLC                  | Dec 18, 2017       |
| Specific Activity of AI: 13.2 MBq/mg | calculated            | Dec 18, 2017       |
| Radiochemical Purity: 98.8 %         | RHPLC                 | Dec 18, 2017       |
| Chemical Purity: 90.3 %              | calculated            | Dec 18, 2017       |

**Additional Information**  
Storage Advice: keep in freezer (approx. -18°C)


Recipients should ensure that the label information on the corresponding substance container(s) correspond(s) with that on this Certificate of Analysis

Study Director:       Study Completion Date: August 06, 2018

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Released August 06, 2018 by 

Appendix 2: Certificate of Analysis of the  $^{13}\text{C}$ -labeled test substance  
 $^{13}\text{C}$ -4,4'-Dihydroxydiphenylsulfon

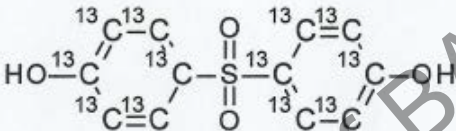
**17/0532-1**  
added 04.09.18

  
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### Certificate of Analysis

|              |                                     |             |           |
|--------------|-------------------------------------|-------------|-----------|
| Reg.No. :    | 63265                               | Batch No. : | 1248-2101 |
| Label :      | phenyl-1,2,3,4,5,6- $^{13}\text{C}$ |             |           |
| Study Code : | IL1248_2001                         |             |           |



|                               |  |
|-------------------------------|--|
| CL-No.                        |  |
| CAS No.                       | 80-09-1  |
| Core Project                  |  |
| Internal (Metabolite) Code    |  |
| Molecular Formula             | $\text{C}_{12}\text{H}_{10}\text{O}_2\text{S}$ |
| Molecular Weight (unlabelled) | 250.27   |

**IUPAC-Name:** 4,4'-dihydroxydiphenylsulfone  
**Homogeneity:** given  
**Chemical Purity:** 94,0 %  
**Determination by:** HPLC / calculated  
**Date:** Dec 08, 2017  
**Additional Information**  
**Storage Advice:** keep in freezer (approx. -18°C)

*Recipients should ensure that the label information on the corresponding substance container(s) correspond(s) with that on this Certificate of Analysis*

**Study Director:** [Redacted]      **Study Completion Date:** April 23, 2018  
**Issued on :** August 31, 2018      **Issued by :** [Redacted]

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Released April 23, 2018 by [Redacted]



## Appendix 3: Characterization of "4,4'-dihydroxydiphenylsulfone"

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## Final Report

Characterization of "4,4'-dihydroxydiphenylsulfone"  
Study No. 16L00571 (confidential)



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|                                |   |
|--------------------------------|---|
| Test item                      | "4,4'-dihydroxydiphenylsulfone"                                 |
| Chemical identity              | 4,4'-dihydroxydiphenylsulfone (DHDPS)                           |
| Batch identification           | 03508136W0  |
| Date of production (test item) | Nov 23, 2016  |
| Origin of test item            | [REDACTED]  |
| PSN                            | 05/0066-8   |
| CAS no.                        | 80-09-1   |
| Sponsor                        | [REDACTED]  |
| Date of receipt of order       | Nov 29, 2016  |
| Date of receipt of test item   | Dec 01, 2016  |
| Testing facility               | Competence Center Analytics, BASF SE, D-67056 Ludwigs-<br>hafen |
| Study director                 | [REDACTED]  |
| Storage cond. test item        | ambient temperature   |
| Test period                    | Dec 13 – Jan 10, 2017   |
| Storage of records             | GLP archives, Competence Center Analytics                       |
| Storage of sample of test item | Archives, Competence Center Analytics                           |

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**Summary of results**

|  |   |
|--|---|
| Appearance and homogeneity                           | The test item are white powderlike crystals. It is obviously homogeneous.   |
| Identity via $^1\text{H}$ -NMR spectroscopy          | The $^1\text{H}$ -NMR spectrum shows the expected signals for the given structure.  |
| Identity via $^{13}\text{C}$ -NMR spectroscopy       | The $^{13}\text{C}$ -NMR spectrum shows the expected signals for the given structure.   |
| Content of identified main component and by-products | $w(\text{C}_{12}\text{H}_{10}\text{O}_4\text{S}) = 99.9 \text{ g/100 g}$ via $^1\text{H}$ -NMR spectroscopy<br>By-products were not observed. |

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**1 Appearance and homogeneity**

|                    |   |
|--------------------|---|
| Method             | Visual inspection at room temperature.                                    |
| Result             | The test item are white powderlike crystals. It is obviously homogeneous. |
| Date of test       | Dec 13, 2016  |
| Head of laboratory |   |

**2 Identity by  $^1\text{H}$ -NMR spectroscopy**

|                    |   |
|--------------------|---|
| Method             | $^1\text{H}$ -NMR spectroscopy  |
| Apparatus          | Bruker AV3-500p   |
| Reagents           | solvent: [D6]-DMSO (Euriso-top)<br>reference: Tetramethylsilane (TMS) (Cambridge Isotope Lab)   |
| Sample preparation | In a suitable vial, the test item was dissolved in [D6]-DMSO containing TMS. The resulting solution was transferred into a 5 mm NMR tube for measurement. |
| Test parameters    | Measuring frequency = 500 MHz, measuring temperature = 298 K; further parameters see at $^1\text{H}$ -NMR spectrum displayed in figure on page 7.         |
| Result             | The $^1\text{H}$ -NMR spectrum shows the expected signals for the given test item. For assignments see spectrum on page 7.                                |
| Date of test       | Jan 10, 2015  |
| Head of laboratory |   |

**3 Identity of by  $^{13}\text{C}$ -NMR spectroscopy**

|                    |   |
|--------------------|---|
| Method             | $^{13}\text{C}$ -NMR spectroscopy   |
| Apparatus          | Bruker AV3-500p (PG/01992)  |
| Reagents           | solvent: [D6]-DMSO (Euriso-top, ord. no. D010-H)<br>reference: Tetramethylsilane (TMS) (Cambridge Isotope Lab))   |
| Sample preparation | In a suitable vial, the test item was dissolved in [D6]-DMSO containing TMS. The resulting solution was transferred into a 5 mm NMR tube for measurement. |
| Test parameters    | Measuring frequency = 126 MHz, measuring temperature = 298 K; further parameters see at $^{13}\text{C}$ -NMR spectrum displayed in figure on page 8.      |

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|                    |   |
|--------------------|---|
| Result             | The $^{13}\text{C}$ -NMR spectrum shows the expected signals for the given test item.<br>For assignments see spectrum |
| Date of test       | Jan 10, 2017  |
| Head of laboratory |   |

#### 4 Content of identified main and by-products

|                    |   |
|--------------------|---|
| Method             | Quantitative $^1\text{H}$ -NMR spectroscopy   |
| Apparatus          | Bruker AV3-500p   |
| Reagents           | solvent [D6]-DMSO (Euriso-top)<br>reference: Tetramethylsilane (TMS) (Cambridge Isotope Lab))   |
| Internal Standard  | 1,3,5-Trimethoxy benzene (Sigma Aldrich)<br><br>Molecular Weight: 168.19 g/mol<br>Purity: 99.9 g/100 g (for calc.)  |
| Sample preparation | Test item and internal standard were weighed into a suitable vial and dissolved in [D6]-DMSO containing TMS. The resulting solution was transferred into a 5 mm NMR tube. |
| Test parameters    | Measuring frequency = 500 MHz, measuring temperature 298 K; further parameters see at $^1\text{H}$ -NMR spectrum displayed in figure on page 9.                           |
| Evaluation         | The content of test item was calculated by using the following equation:  |

$$w = \frac{E_{St} \cdot I_K \cdot M_K \cdot A_{St} \cdot R_{St}}{E_P \cdot I_{St} \cdot M_{St} \cdot A_K}$$

$w$  = mass fraction [g/100 g]  
 $I_K$  = peak intensity test item  
 $I_{St}$  = peak intensity standard  
 $E_P$  = weighed test item  
 $E_{St}$  = weighed standard

$A_K$  = protones/molecule of test item  
 $A_{St}$  = protones/molecule of standard  
 $M_K$  = molecular weight test item  
 $M_{St}$  = molecular weight standard  
 $R_{St}$  = purity standard



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**Result**

For quantitation triplicate determinations were carried out. Evaluation was performed by using 3 protons/molecule of the internal standard (at ~ 6.1 ppm) and 8 selected protons/molecule of the analyte (at ~ 6.9 and 7.7 ppm). An exemplary spectrum is displayed in figure on page 9):

| Det. | test item      |                                | internal standard |                                | resulting mass fraction<br>w(C <sub>12</sub> H <sub>10</sub> O <sub>4</sub> S)<br>[g/100 g] |
|------|----------------|--------------------------------|-------------------|--------------------------------|---|
|      | weight<br>[mg] | peak intensity<br>[area units] | weight<br>[mg]    | peak intensity<br>[area units] |   |
| 1    | 41.69          | 3581.78                        | 20.84             | 1000.00                        | 99.8  |
| 2    | 38.87          | 2547.93                        | 27.40             | 1000.00                        | 100.1   |
| 3    | 27.73          | 1919.10                        | 25.90             | 1000.00                        | 99.9  |
| mean |                |                                |                   |                                | 99.9 ± 0.2  |

Date of test Jan 10, 2017

Head of laboratory

Feb 07, 2017  
Date

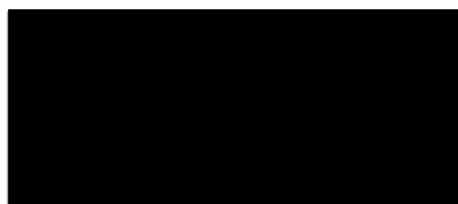
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GLP Compliance Statement

This study was conducted in accordance with the OECD Principles of Good Laboratory Practice and the GLP Principles of the German "Chemikaliengesetz" (Chemicals Act).



Feb 07, 2017

Date

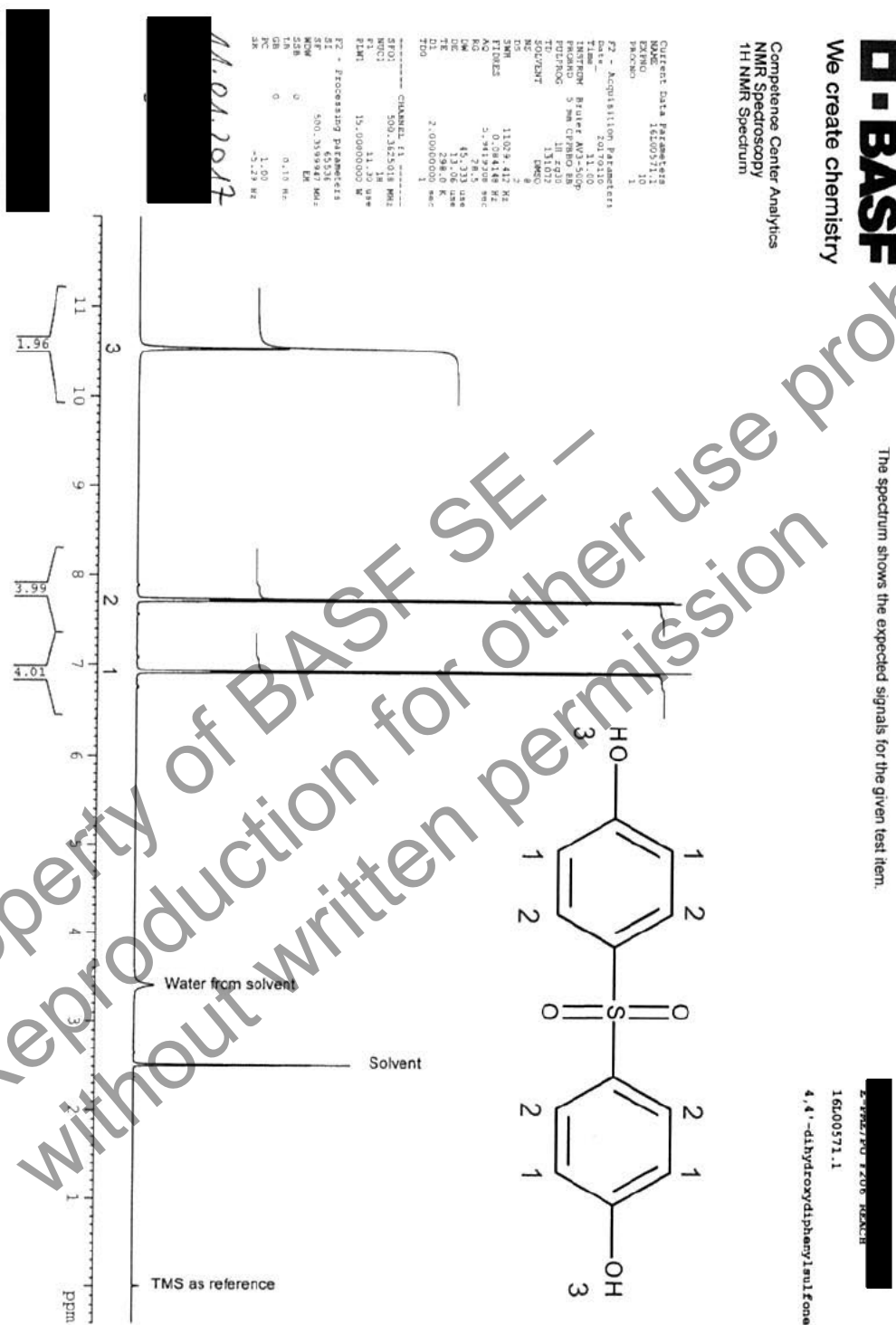
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## Final Report

## Characterization of "4,4'-dihydroxydiphenylsulfone"

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<sup>1</sup>H-NMR-spectrum

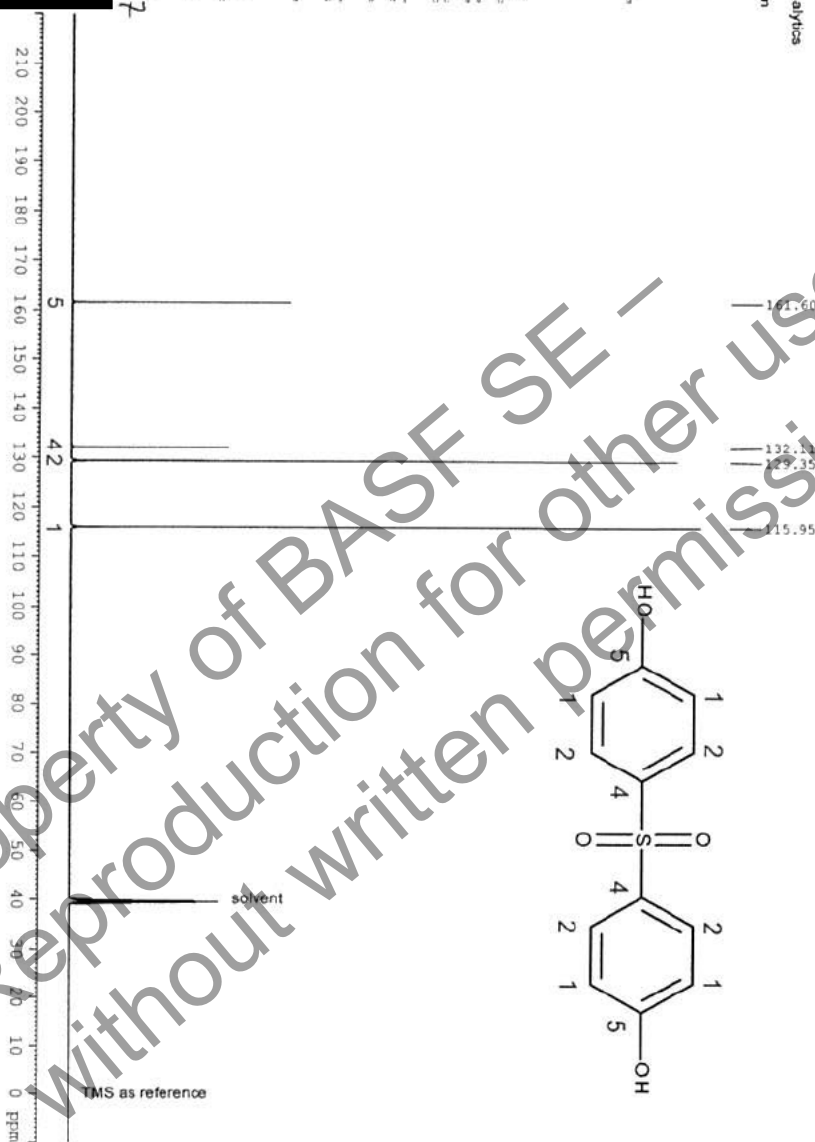


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11.01.2017

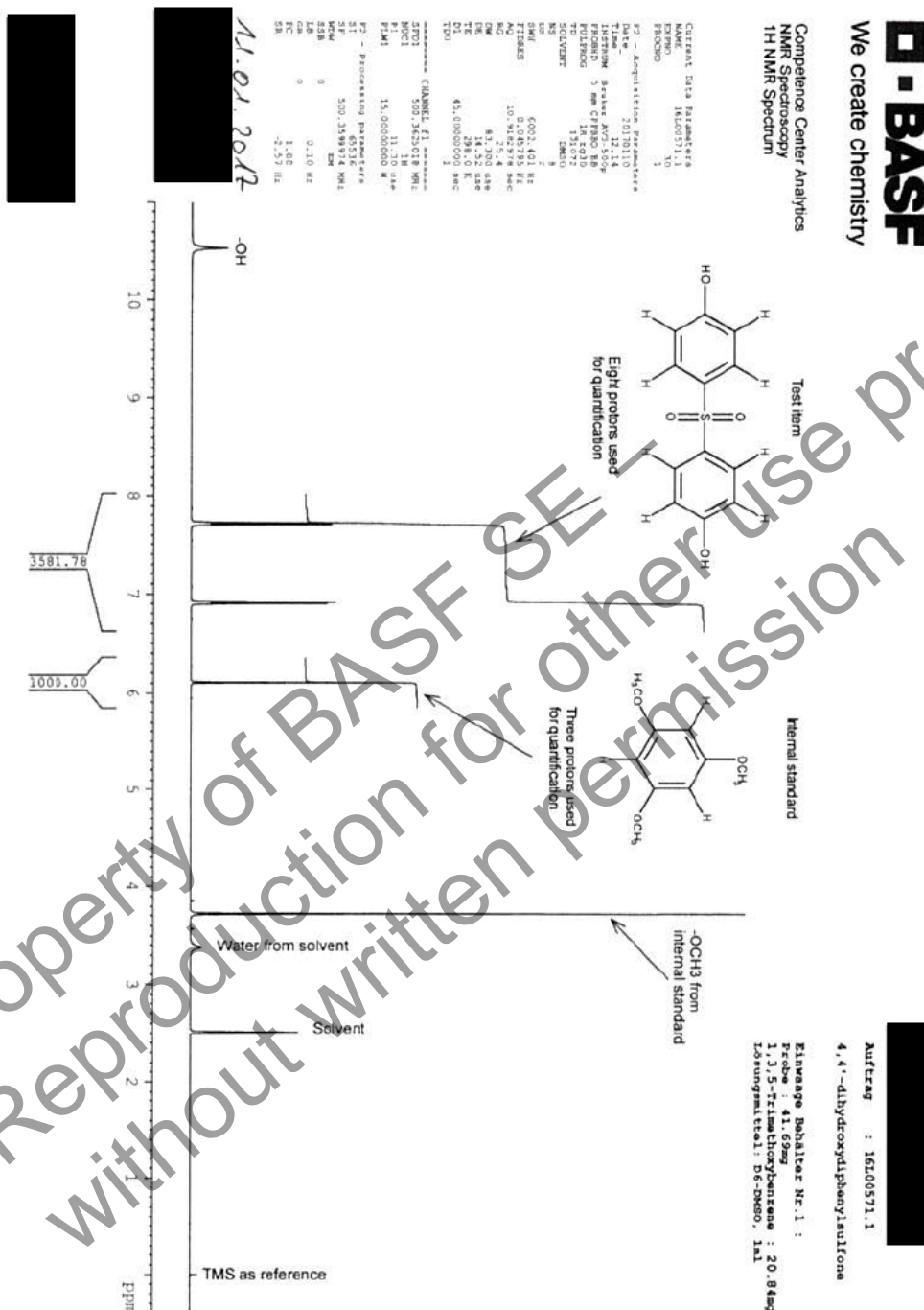
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The spectrum shows the expected signals for the given test item

4,4'-dihydroxydiphenylsulfone  
16L00571.1

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**Characterization of "4,4'-dihydroxydiphenylsulfone"**  
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Quant. <sup>1</sup>H NMR spectrum

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**Statement of the Quality Assurance Unit**

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The Quality Assurance Unit inspects all studies in accordance with the OECD Principles of Good Laboratory Practice and the GLP Principles of the German "Chemikaliengesetz" (Chemicals Act). The particular items inspected in this study are listed below.

The study-based inspections in terms of the Competence Center Analytics include "study-based inspections" and "process-based inspections" as defined in the Consensus Document "Quality Assurance and GLP" of the OECD.

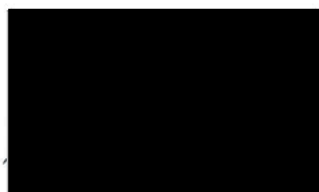
Additionally the Quality Assurance Unit inspects the laboratories of the department Competence Center Analytics in regular intervals (equates to "facility-based inspections"). Findings are reported to study director and to management.

Verification of study plan: Dec 12, 2016

| Inspection of | Date of inspection | Reported to study director and management |
|---------------|--------------------|---|
| Raw data      | Jan 23, 2017       | Feb 07, 2017                              |
|               | Feb 07, 2017       |   |
| Final report: | Jan 23, 2017       | Feb 07, 2017                              |
|               | Feb 07, 2017       |   |

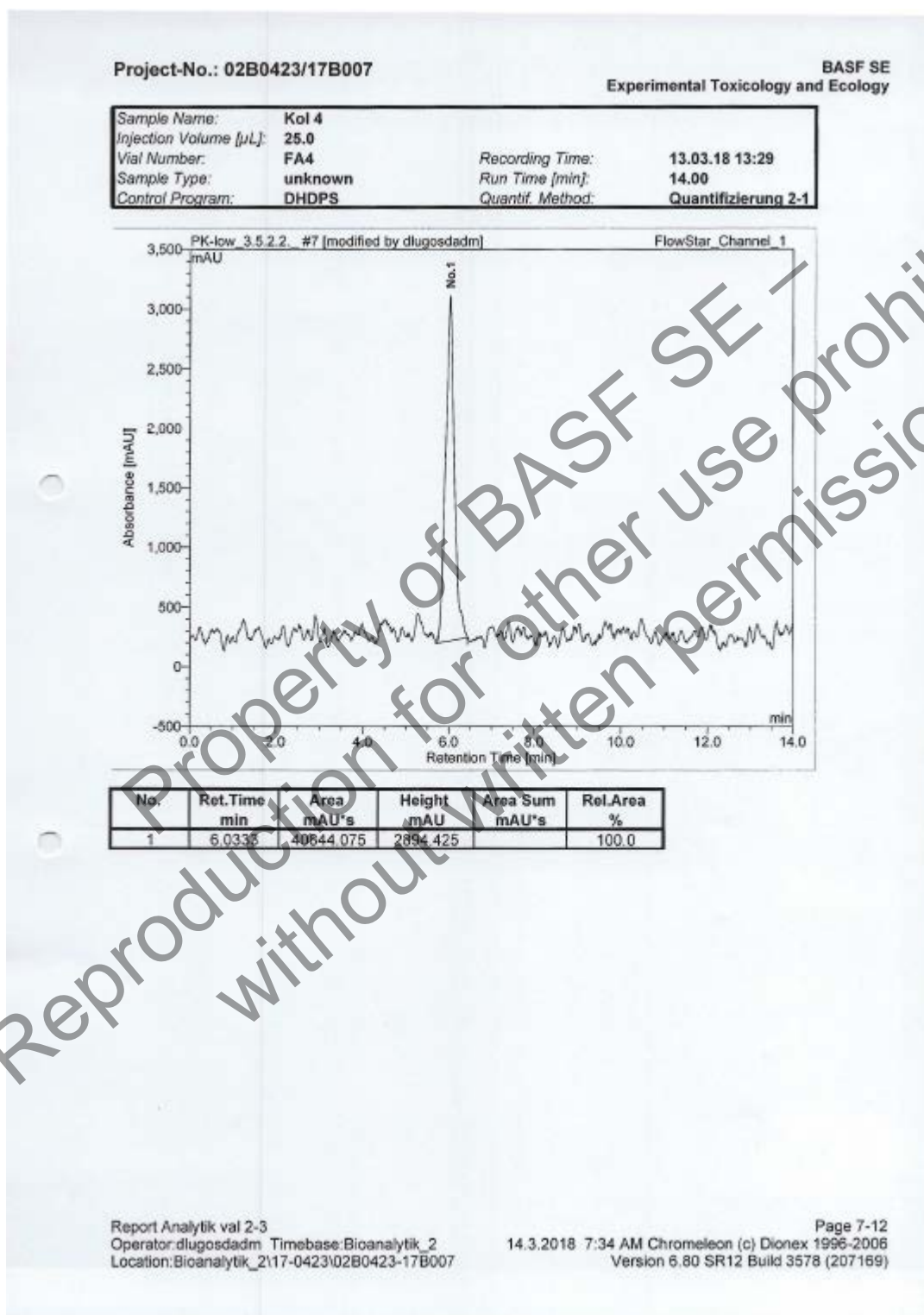
The final report reflects the raw data.

Ludwigshafen



*Feb 07, 2017*  
Date

Appendix 4: Sample HPLC-Radio-Chromatogram of test-substance preparation  
(concentration control before administration, experiment 2)



Appendix 5: Sample HPLC-Radio-Chromatogram of test-substance preparation  
(concentration control after administration, experiment 2)

