

# Chemotion-ELN: digitization systems for chemists

Patrick Hodapp (Stefan Bräse group)

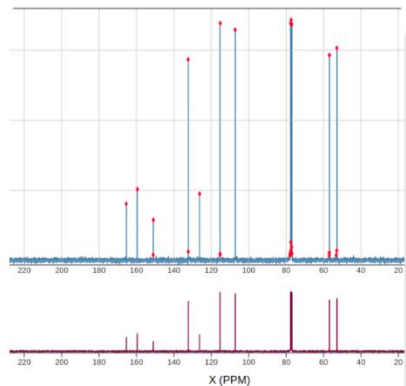
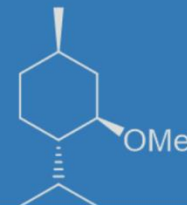
INSTITUTE OF ORGANIC CHEMISTRY - Stefan Bräse Group Karlsruhe



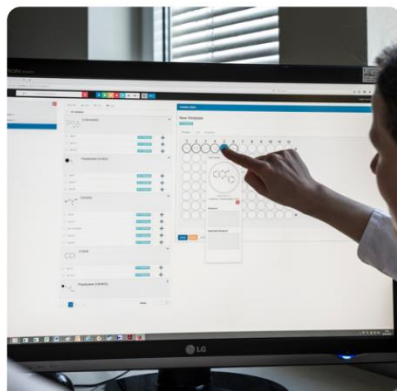
**Chemotion**  
*funded by*  
**DFG**



## Electronic Laboratory Notebook & Repository for Research Data



Spectra Viewer

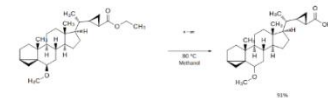


Electronic Lab Notebook

dated on 4-2-2019

Biosynthesis  
use of Technology

Reaction: A-FUHFF-LHFFFAFDFSC-GUZYJTHAS-LHFFFAFDFSC-NLHFF-NBMM-NLHFF-ZZZ



91%

1 liter (200 mg, 230 µmol, 1.06 equiv) and potassium hydroxide (200 mg, 3.57 mmol, 15.9 equiv) in methanol (15 mL) was refluxed for 1 h to raise temperature the solution was acidified with 1M HCl and extracted with EtOAc (3 x 15 mL). The combined organic extracts were dried on sodium sulfate under reduced pressure. The residue was purified by flash chromatography (Phenomenex/ODS, 4.1 to 2.1) to yield 0.5 g, 234 µmol, 91% yield.

formation for publication and purification details:  
was purified by flash chromatography (Phenomenex/ODS, 4.1 to 2.1) to yield the acid as a white solid (0.5 g, 232 µmol, 91% yield).

1.90 18(C)H40(O)5 1469.11 1.7116727272919 4.40 1.58 12 2209 426 13 15267 10 2526 321(888 4 2418 2526)4 252 1 403 4 27 20158 15 16 17 18 19 20 21 22 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

Chemotion Repository

SMILES

```
OP1=C(COC1C2C3C4C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40C41C42C43C44C45C46C47C48C49C50C51C52C53C54C55C56C57C58C59C60C61C62C63C64C65C66C67C68C69C70C71C72C73C74C75C76C77C78C79C80C81C82C83C84C85C86C87C88C89C90C91C92C93C94C95C96C97C98C99C100C101C102C103C104C105C106C107C108C109C110C111C112C113C114C115C116C117C118C119C120C121C122C123C124C125C126C127C128C129C130C131C132C133C134C135C136C137C138C139C140C141C142C143C144C145C146C147C148C149C150C151C152C153C154C155C156C157C158C159C160C161C162C163C164C165C166C167C168C169C170C171C172C173C174C175C176C177C178C179C180C181C182C183C184C185C186C187C188C189C190C191C192C193C194C195C196C197C198C199C200C201C202C203C204C205C206C207C208C209C210C211C212C213C214C215C216C217C218C219C220C221C222C223C224C225C226C227C228C229C230C231C232C233C234C235C236C237C238C239C240C241C242C243C244C245C246C247C248C249C250C251C252C253C254C255C256C257C258C259C260C261C262C263C264C265C266C267C268C269C270C271C272C273C274C275C276C277C278C279C280C281C282C283C284C285C286C287C288C289C290C291C292C293C294C295C296C297C298C299C300C301C302C303C304C305C306C307C308C309C310C311C312C313C314C315C316C317C318C319C320C321C322C323C324C325C326C327C328C329C330C331C332C333C334C335C336C337C338C339C340C341C342C343C344C345C346C347C348C349C350C351C352C353C354C355C356C357C358C359C360C361C362C363C364C365C366C367C368C369C370C371C372C373C374C375C376C377C378C379C380C381C382C383C384C385C386C387C388C389C390C391C392C393C394C395C396C397C398C399C400C401C402C403C404C405C406C407C408C409C410C411C412C413C414C415C416C417C418C419C420C421C422C423C424C425C426C427C428C429C430C431C432C433C434C435C436C437C438C439C440C441C442C443C444C445C446C447C448C449C450C451C452C453C454C455C456C457C458C459C460C461C462C463C464C465C466C467C468C469C470C471C472C473C474C475C476C477C478C479C480C481C482C483C484C485C486C487C488C489C490C491C492C493C494C495C496C497C498C499C500
```

ChemScanner

Visit us on Youtube

# Access to research data: Key challenges

AIMS: Infrastructure: Access to research data  
Improve reproducibility of scientific work  
Accelerate and facilitate scientific work

## Device Integration



- Remote work
- Data transfer



## Electronic Lab Notebook

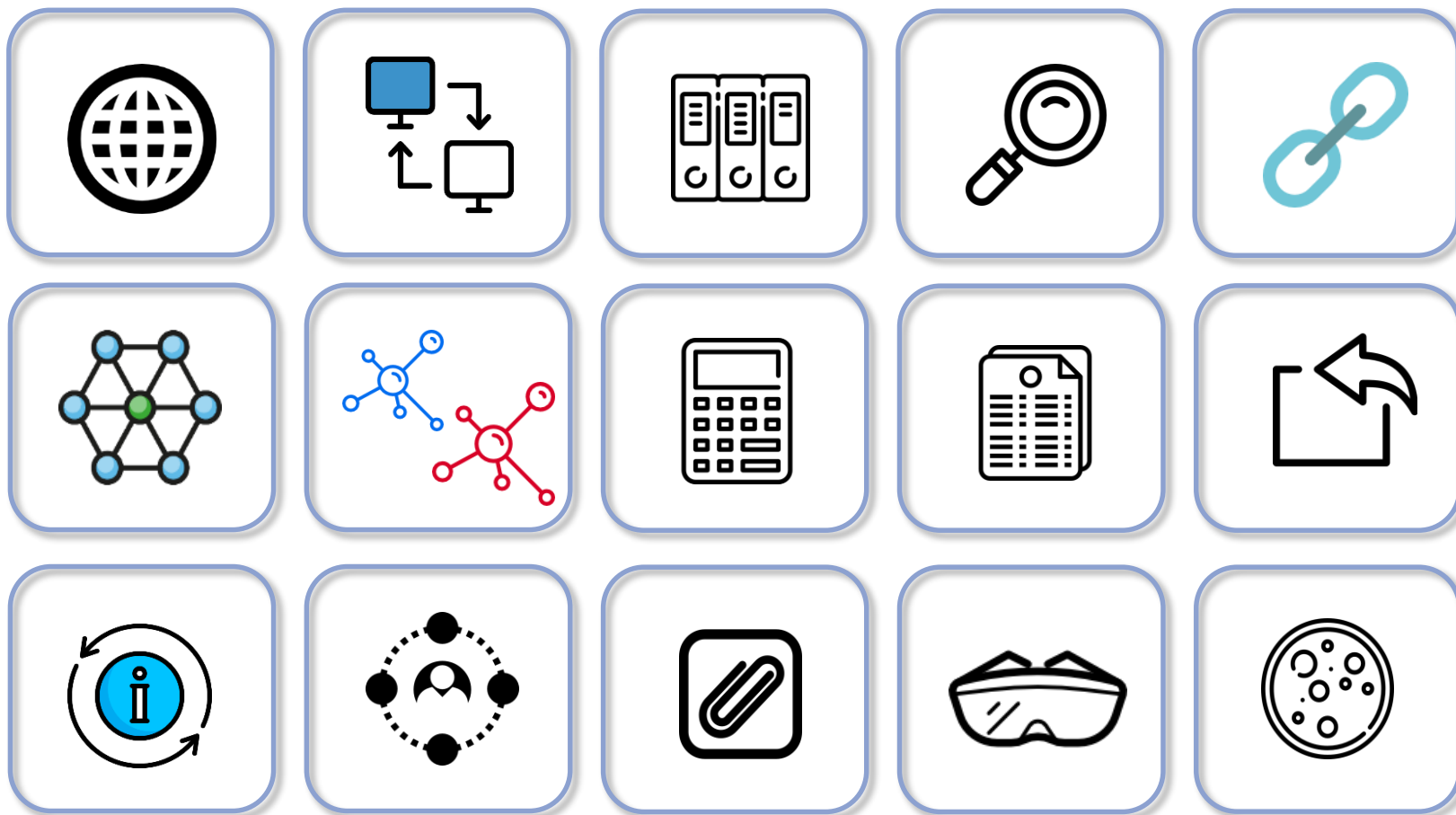
- Digital storage
- Processing of data



## Repository

- Open Access
- No limitation (file types)
- Interoperability





**OPEN SOURCE**

Source: Our findings &  
S. Kanza, C. Willoughby, N. Gibbins, R. Whitby, J.G. Frey, J. Erjavac, K. Zupanic, M. Hren, K. Kovac, *J Cheminfo*. **2017**, 9:31.

# Electronic Lab Notebook - Management

← → ↻ <https://complat-eln.ioc.kit.edu/#/collection/7/> 🔍 ⭐ 📄 🔄 🏠

Chemotion ▾ All ▾ IUPAC, InChI, SMILES, ... 📄 ✖ 🏠 📄 📄 🔄 + ▾ 🔍 ▾ 0

Nicole Jung ▾ 🏠

📄 Collections 🔧

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- chemotion.net +
- Labjournal Nicole 1 +
- Chemical Database +
- Biological Database
- Collaborations
- Data for Supervisor
- Calculation ETL properties
- Imported data +
- Beilstein Extraction
- Extraction KP
- Molecules with calculated data +






🔍 My shared collections

🔍 Shared with me

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- by JPK +
- by HK +
- by STM +
- by SUK +
- by SVS +
- by JEW +
- by FA +
- by RB +
- ... +

🔍 1021(0) ⬆️ 158(0) ⚙️ 3(0) 📄 1(0)

From To Sample P ▾

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 <chem>C16F4N4O2</chem>	<span>🏠</span> <span>▾</span>
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 <chem>C18F9N3O2</chem>	<span>🏠</span> <span>▾</span>
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 <chem>C15HF10NO2</chem>	<span>🏠</span> <span>▾</span>

« 1 2 3 4 5 ... »

Show 15

# Electronic Lab Notebook - Management

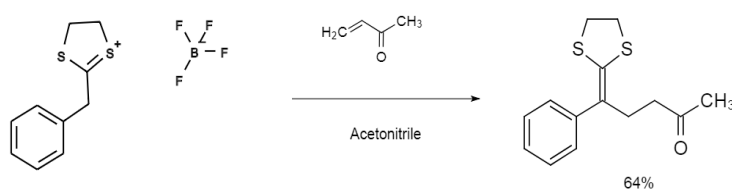
Secure | <https://eln.chemotion.net/#/collection/192/reaction/336>

Chemotion | All | IUPAC, InChI, SMILES, ... | Logged in as Nicole Jung

Collections: 219(0), 62(0), 1(0), 1(0)

Selected: NJu-145 NJu-R24-A, NJu-R243 According to General Procedure 2a

Reaction: NJu-R243 According to General Procedure 2a



Scheme Properties References Analyses Green Chemistry Zotero

Starting materials	Ref	T/R	Amount	Conc	Equiv
<b>A</b> NJu-772 2-benzyl-4,5-dihydro-1,3-dithiol-1-...	t	1000	mg 0.00 ml	3.544 mmol	708.9 mmol/l 1.000

Reactants	Reagents	T/R	Amount	Conc	Yield
<b>B</b> but-3-en-2-one	t	298.1	mg 0.00 ml	4.253 mmol	850.6 mmol/l 1.200

Products	T/R	Amount	Conc	Yield	
<b>P1</b> NJu-773 NJu-R243-A 5-(1,3-dithiolan-2-ylidene)-5-phen...	r	599.8	mg 0.00 ml	2.268 mmol	453.7 mmol/l 64%

Solvents

Name: According to General Procedure 2a | Status: Select... | Temperature: Temperature... °C

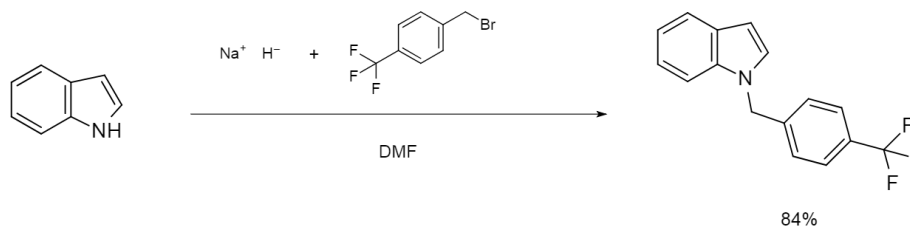
Role: Parts of GP | According to: [Home]

« 1 2 3 4 5 » Show 15

# Electronic Lab Notebook - Reactions

JEW-176 JEW-R51-A JEW-R99

JEW-R99



Scheme Properties References Analyses Green Chemistry SciFINDER

Starting materials		Ref	T/R	Amount		Conc		Equiv					
+ JEW-246-2 1H-indole			t	300.0	mg	0.00	ml	2.561	mmol	853.6	mmol/l	1.000	
Reactants		Reagents											
+ sodium;hydride			t	153.6	mg	0.00	ml	3.841	mmol	1280	mmol/l	1.500	
+ 1-(bromomethyl)-4-(trifluoromethyl)benzene			t	734.6	mg	0.00	ml	3.073	mmol	1024	mmol/l	1.200	
Products		T/R	Amount		Conc		Yield						
+ P1 JEW-293 JEW-R99-A 1-[[4-(trifluoromethyl)phenyl]methyl]indole		r	591.1	mg	0.00	ml	2.147	mmol	715.8	mmol/l	84%		

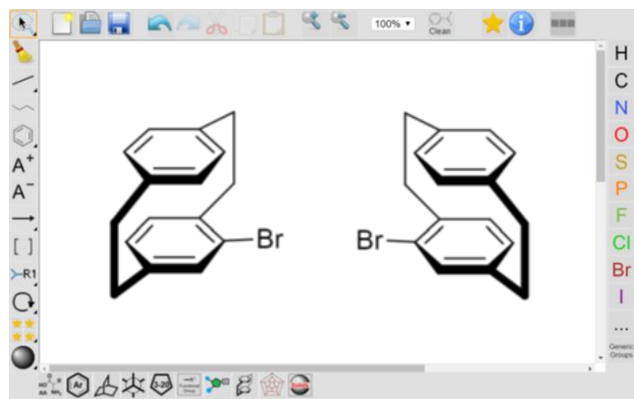
Name  
Name...

Status  
Successful

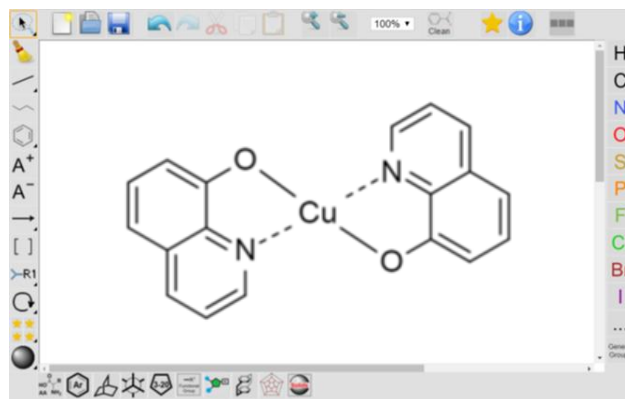
Temperature  
Temperature... °C

Role

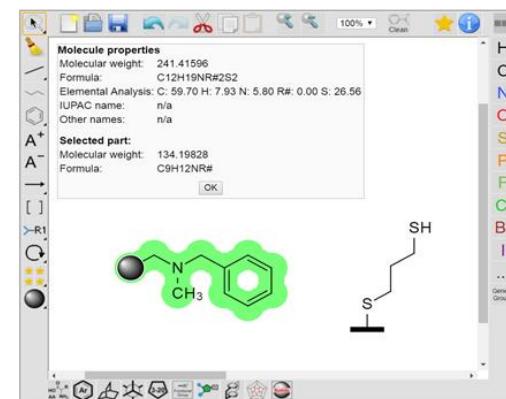
Differentiation of planar  
chiral compounds



Coordination  
chemistry enabled



Supported Material  
and Surfaces







## Reporting Functions



# ELN – Reporting: Document Types

## Supporting Information: Standard

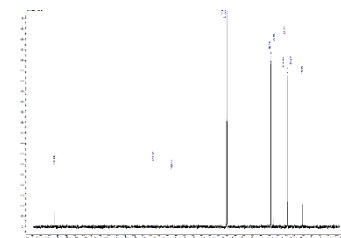
4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)



Name: 4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one; Formula: C<sub>18</sub>H<sub>24</sub>O<sub>2</sub>S<sub>2</sub>; CAS: -;  
SMILES: CCCC(C)C(=O)CC(C1=CC=C(C=C1)C2=CC3=C(C=C2)S4=CC=CC=C3S4)C5=CC=CC=C5;  
UNII: 407534; Molecular Mass: 334.500; Exact Mass: 334.142; EA, C: 68.21; H: 7.81;  
O: 4.78; S: 19.17.

According to General Procedure 2a: [A2a] 2-benzyl-1,3-dithiane-4H-1,3-dithian-1-ium  
tetrafluoroborate (0.154 g, 0.55 mmol, 1.0 equiv), (BnO)<sub>2</sub>Sn-O-3-one (0.50 g, 0.60  
mmol, 1.20 equiv), (C) acetonitrile (3.00 mL), Yield (D&S) = 64% (0.113 g, 0.37 mmol).  
The obtained crude product was purified via flash-chromatography on silica gel using  
cyclohexane/ethyl acetate 10:1, R<sub>f</sub> = 0.73 (cyclohexane/ethyl acetate 2:1 = 19, N<sub>2</sub>O).  
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, ppm) δ = 0.96-0.96 (m, 3H), 1.26-1.45 (m, 6H), 2.05-2.15 (m,  
2H), 2.12-2.15 (m, 2H), 2.75-4.2 (m, 2H), 2.75-3.84 (m, 2H), 3.79-2.58 (m, 1H), 3.99-3.66  
(m, 1H), 3.89-3.88 (m, 1H), 6.99-7.04 (m, 2H), 7.28-7.39 (m, 3H); <sup>13</sup>C NMR (125 MHz,  
CDCl<sub>3</sub>, ppm) δ = 14.0, 24.4, 24.4, 29.5, 29.6, 30.8, 31.9, 31.9, 47.7, 127.6, 127.6, 128.0  
(C), 129.2 (C), 138.8, 142.8, 207.6; EI (m/z, 70 eV, 69 °C): 334 (3), [M]<sup>+</sup>: 277 (6), 235  
(22), 208 (70), 195 (20), 169 (22), 152 (100), 134 (80), 119 (50), 109 (33), 101 (57), 95 (28),  
91 (21), 81 (29), 69 (33), 55 (28); HRMS-MS (m/z): [M]<sup>+</sup> calcd for C<sub>18</sub>H<sub>24</sub>O<sub>2</sub>S<sub>2</sub>: 334.1420; found:  
334.1421; IR (ATR, ν): 2921, 2825, 1763, 1596, 1466, 1441, 1419, 1354, 1301, 1279, 1160,  
1121, 1072, 1051, 874, 878, 783, 751, 727, 707, 645, 609, 541, 464 cm<sup>-1</sup>.

## Supporting Information: Collection of Spectra



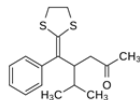
## Supporting Information: Excel-Lists Identifier

Index	Reference	File Name	File Path	File Size	File Type	File Date	File Description
1	1	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
2	2	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
3	3	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
4	4	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
5	5	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
6	6	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
7	7	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
8	8	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
9	9	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier
10	10	4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	C:\Users\johannes\Desktop\4-((1,3-dithian-2-ylidene)phenyl)methyl)octan-2-one (50)	1.2 MB	Excel 2007-2019 Workbook	2023-10-27	Supporting Information: Excel-Lists Identifier

## Project Reports



#### 4.9 4-((1,3-Dithiolan-2-ylidene)(phenyl)methyl)-5-methylhexan-2-one (4e)



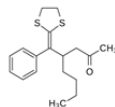
Name: 4-((1,3-Dithiolan-2-ylidene)(phenyl)methyl)-5-methylhexan-2-one; Formula:  $C_{17}H_{22}OS_2$ ; CAS: -; Smiles: CC(C(C(=C1SCCS1)c1ccccc1)CC(=O)C)C; InChI: AJUPULBPXRSZPK-UHFFFAOYSA-N; Molecular Mass: 306.4860; Exact Mass: 306.1112; EA: C, 66.62; H, 7.24; O, 5.22; S, 20.92.

According to General Procedure 2b: {A1a} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.551 mmol, 1.00 equiv); {B3e} (E)-5-methylhex-3-en-2-one (0.074 g, 0.660 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D4e} = 85% (0.144 g, 0.471 mmol).

The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1.  $R_f$  = 0.63 (cyclohexane/ethyl acetate 2:1).

$^1H$  NMR (500 MHz,  $CDCl_3$ , ppm)  $\delta$  = 0.90 (d,  $J$  = 6.6 Hz, 3H), 1.12 (d,  $J$  = 6.6 Hz, 3H), 1.60–1.69 (m, 1H), 2.16 (s, 3H), 2.37 (dd,  $J$  = 16.6 Hz,  $J$  = 8.9 Hz, 1H), 2.53 (dd,  $J$  = 16.6 Hz,  $J$  = 4.8 Hz, 1H), 3.04 (td,  $J$  = 9.3 Hz,  $J$  = 4.7 Hz, 1H), 3.20–3.24 (m, 2H), 3.36–3.40 (m, 2H), 7.13–7.16 (m, 2H), 7.27–7.31 (m, 1H), 7.33–7.37 (m, 2H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ , ppm)  $\delta$  = 20.6, 21.2, 29.8, 31.1, 37.1, 37.7, 45.8, 50.3, 127.1, 128.1 (2C), 129.1, 129.3 (2C), 136.8, 141.2, 207.9; EI ( $m/z$ , 70 eV, 60 °C): 306 (38) [M]<sup>+</sup>, 263 (100), 221 (52), 191 (11), 113 (13), 69 (19); HRMS–EI ( $m/z$ ): [M]<sup>+</sup> calcd for  $C_{17}H_{22}OS_2$ : 306.1107; found, 306.1108; IR (ATR,  $\bar{\nu}$ ): 2964, 2924, 1710, 1586, 1472, 1440, 1404, 1369, 1301, 1278, 1169, 1110, 1071, 1026, 917, 889, 843, 816, 793, 749, 702, 652, 590, 563, 501, 425, 400  $cm^{-1}$ .

#### 4.10 4-((1,3-dithiolan-2-ylidene)(phenyl)methyl)octan-2-one (4f)



Name: 4-((1,3-dithiolan-2-ylidene)(phenyl)methyl)octan-2-one; Formula:  $C_{18}H_{24}OS_2$ ; CAS: -; Smiles: CCCCC(C(=C1SCCS1)c1ccccc1)CC(=O)C; InChI: XLPWXCGXHOGTNX-UHFFFAOYSA-N; Molecular Mass: 320.5126; Exact Mass: 320.1269; EA: C, 67.45; H, 7.55; O, 4.99; S, 20.01.

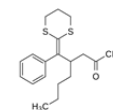
According to General Procedure 2a: {A1a} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.553 mmol, 1.00 equiv); {B3f} (E)-oct-3-en-2-one (0.084 g, 0.666 mmol, 1.21 equiv); {C} acetonitrile (5.00 mL); Yield {D4f} = 90% (0.160 g, 0.498 mmol).

The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1 +  $NEt_3$  (1%).  $R_f$  = 0.45 (cyclohexane/ethyl acetate 2:1).

$^1H$  NMR (500 MHz,  $CDCl_3$ , ppm)  $\delta$  = 1.04–1.09 (t,  $J$  = 7.2 Hz, 3H), 1.44–1.63 (m, 6H), 2.29 (s, 3H), 2.49 (dd,  $J$  = 16.6 Hz,  $J$  = 7.0 Hz, 1H), 2.63 (dd,  $J$  = 16.4 Hz,  $J$  = 7.0 Hz, 1H), 3.37–

3.41 (m, 2H), 3.41–3.48 (m, 1H), 3.54–3.57 (m, 2H), 7.24–7.28 (m, 2H), 7.43–7.48 (m, 1H), 7.49–7.54 (m, 2H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ , ppm)  $\delta$  = 13.9, 22.6, 29.6, 30.0, 33.2, 37.1, 37.8, 43.2, 47.9, 127.1, 128.2 (2C), 129.3 (2C), 129.4, 135.9, 140.7, 207.6; EI ( $m/z$ , 70 eV, 120 °C): 320 (58) [M]<sup>+</sup>, 263 (100), 221 (22), 195 (20), 152 (49); HRMS–EI ( $m/z$ ): [M]<sup>+</sup> calcd for  $C_{18}H_{24}OS_2$ : 320.1263; found, 320.1265; IR (ATR,  $\bar{\nu}$ ): 2953, 2923, 2855, 1711, 1597, 1580, 1489, 1438, 1420, 1356, 1278, 1159, 1105, 1072, 1031, 978, 847, 750, 702, 645, 541  $cm^{-1}$ .

#### 4.11 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one (5f)



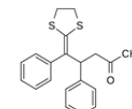
Name: 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one; Formula:  $C_{19}H_{26}OS_2$ ; CAS: -; Smiles: CCCCC(C(=C1SCCS1)c1ccccc1)CC(=O)C; InChI: UOHJUSHNULFLRZ-UHFFFAOYSA-N; Molecular Mass: 334.5391; Exact Mass: 334.1425; EA: C, 68.21; H, 7.83; O, 4.78; S, 19.17.

According to General Procedure 2a: {A2a} 2-benzyl-5,6-dihydro-4H-1,3-dithiin-1-ium tetrafluoroborate (0.156 g, 0.525 mmol, 1.00 equiv); {B3f} (E)-oct-3-en-2-one (0.080 g, 0.630 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D5f} = 64% (0.113 g, 0.337 mmol).

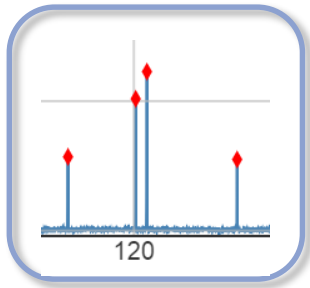
The obtained crude product was purified via flash-chromatography on silica gel using cyclohexane/ethyl acetate 10:1.  $R_f$  = 0.73 (cyclohexane/ethyl acetate 2:1 + 1%  $NEt_3$ ).

$^1H$  NMR (500 MHz,  $CDCl_3$ , ppm)  $\delta$  = 0.90–0.96 (m, 3H), 1.26–1.45 (m, 6H), 2.05–2.15 (m, 2H), 2.12–2.15 (m, 3H), 2.27–2.42 (m, 2H), 2.75–2.86 (m, 2H), 2.91–2.98 (m, 1H), 2.99–3.06 (m, 1H), 3.80–3.88 (m, 1H), 6.99–7.04 (m, 2H), 7.28–7.39 (m, 3H);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ , ppm)  $\delta$  = 14.0, 22.6, 24.4, 29.5, 29.5, 29.6, 30.0, 33.0, 38.7, 47.7, 127.6, 128.0 (2C), 129.2 (2C), 138.8, 142.6, 207.6; EI ( $m/z$ , 70 eV, 60 °C): 334 (33) [M]<sup>+</sup>, 277 (61), 235 (22), 208 (70), 195 (26), 169 (22), 152 (100), 134 (80), 119 (29), 109 (33), 105 (37), 95 (28), 91 (21), 81 (26), 69 (55), 55 (28); HRMS–EI ( $m/z$ ): [M]<sup>+</sup> calcd for  $C_{19}H_{26}OS_2$ : 334.1420; found, 334.1421; IR (ATR,  $\bar{\nu}$ ): 2921, 2852, 1703, 1596, 1560, 1487, 1419, 1354, 1301, 1279, 1160, 1121, 1072, 1031, 914, 878, 783, 751, 727, 707, 645, 609, 541, 444  $cm^{-1}$ .

#### 4.12 (E)-5-(1,3-dithiolan-2-yl)-4,5-diphenylpent-4-en-2-one (4g)



Name: (E)-5-(1,3-dithiolan-2-yl)-4,5-diphenylpent-4-en-2-one; Formula:  $C_{20}H_{20}OS_2$ ; CAS: -; Smiles: CC(=O)CC(C(=C1SCCS1)c1ccccc1)c1ccccc1; InChI: LRVYWKBWUOILMV-UHFFFAOYSA-N; Molecular Mass: 340.5022; Exact Mass: 340.0956; EA: C, 70.55; H, 5.92; O, 4.7; S, 18.83.



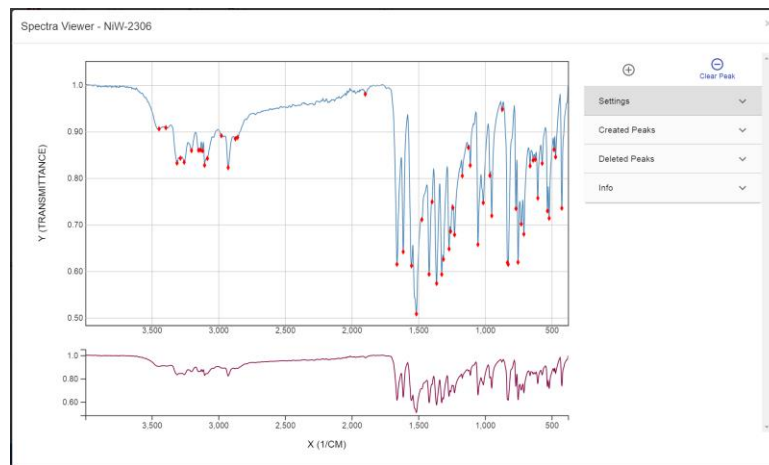
## Analysis (13C NMR and IR)

# Electronic Lab Notebook - Analysis

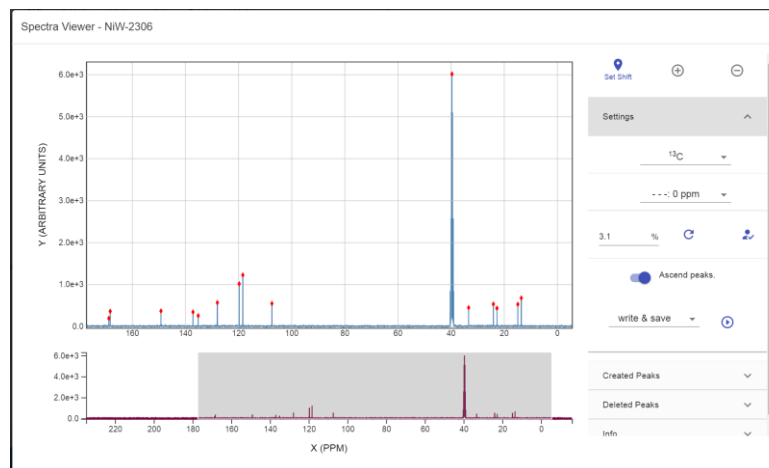
Inbox 10

Unsorted

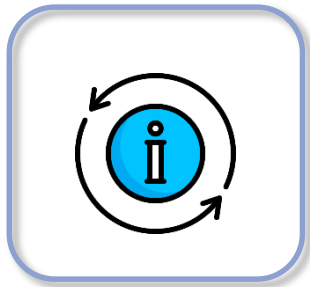
- PH-711 1H ...
- HK-004.dx
- PH681 13C...
- HK004.jpg
- HK004HR...
- sgr-100.pea...
- PH681 13C...
- PH-711 1H.dx
- PH681 19F...
- HK004C.pe...



IR (ATR,  $\tilde{\nu}$ ) = 3445, 3394, 3310, 3285, 3257, 3201, 3149, 3135, 3119, 3104, 3082, 2978, 2927, 2873, 2856, 1898, 1660, 1613, 1551, 1514, 1473, 1419, 1397, 1363, 1324, 1312, 1269, 1258, 1241, 1228, 1170, 1125, 1111, 1052, 1013, 963, 949, 870, 832, 826  $\text{cm}^{-1}$ .

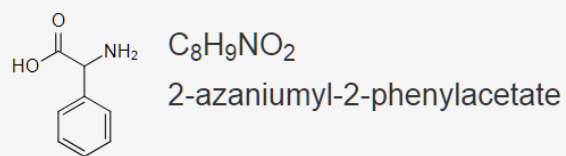


$^{13}\text{C}$  NMR (100 MHz, ppm)  $\delta$  = 168.2, 149.1, 137.0, 135.1, 127.9, 119.6, 118.3, 107.3, 23.9, 13.4.



**Connection to external information**

# Electronic Lab Notebook - External Information



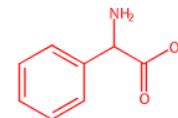
NJ-1302



PubChem

2. **2835-06-5** 🔍

~1652 📄 🧪 ~130 🧪



$C_8H_9NO_2$   
Benzeneacetic acid,  $\alpha$ -amino-

▶ **Key Physical Properties**

[Regulatory Information](#)  
[Spectra](#)  
[Experimental Properties](#)

ZGUNAGUHMKGQNY-UHFFFAOYSA-N



STRUCTURE



PHARMACOLOGY



LITERATURE



PATENTS

**PubChem CID:** 25200329

**Molecular Formula:**  $C_8H_9NO_2$

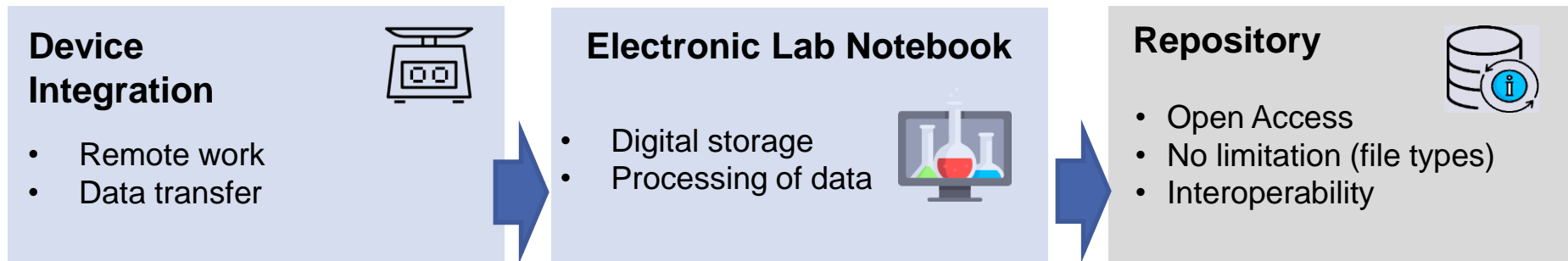
**Molecular Weight:** 151.165 g/mol

**InChI Key:** ZGUNAGUHMKGQNY-UHFFFAOYSA-N

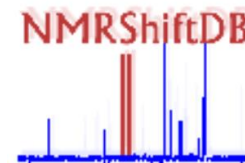
[2-Phenylglycine](#) is a metabolite described in normal human urine (PMID: [14473597](#)) and plasma (PMID: [5888801](#)).

# Access to research data: Key challenges

AIMS: Infrastructure: Access to research data  
 Improve reproducibility of scientific work  
 Accelerate and facilitate scientific work



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## Science Data Center SDC - MoMaF



Presseinformation 021/2019


### Molekül- und Materialforschung: Daten leicht teilen

„Science Data Center für Molekulare Materialforschung“ entwickelt Digitalisierungsbausteine für wissenschaftliche Daten – von Erfassung über Prozessierung bis zur öffentlichen Archivierung.



Daten aus vielen Laboren nachhaltig und gemeinschaftlich nutzen, ist das Ziel des neuen Science Data Centers MoMaF (Foto: Laila Tkotz, KIT)

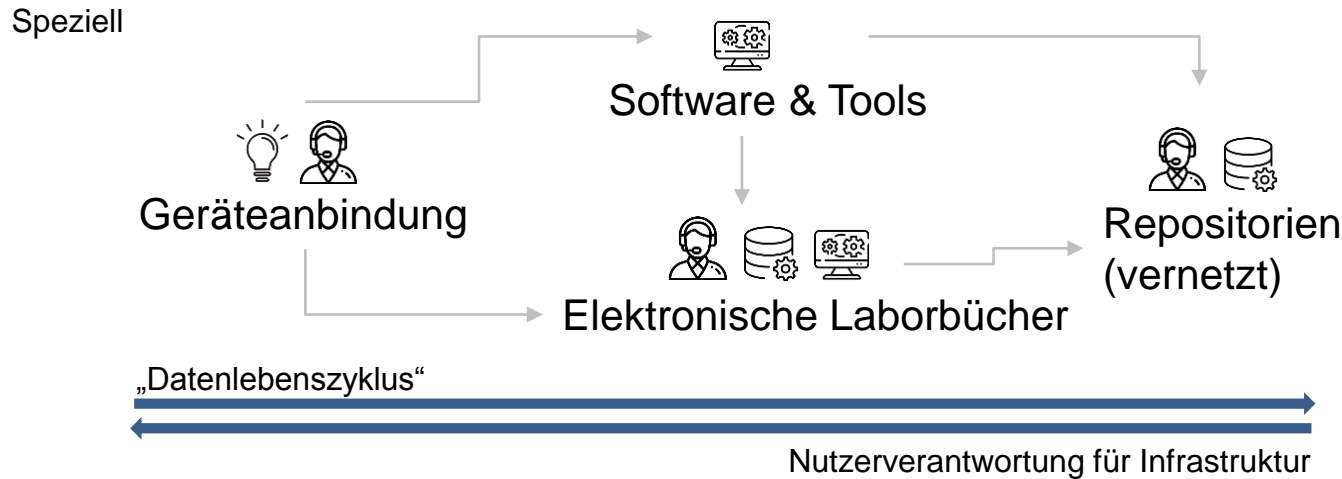
Dezember 2018



Rat für  
Informations  
Infrastrukturen

In der Breite und forschungsnah: Handlungsfähige Konsortien

Dritter Diskussionsimpuls zur Ausgestaltung einer Nationalen Forschungsdateninfrastruktur (NFDI) für die Wissenschaft in Deutschland



Übergreifend

Datenstandards  
& Formate

Communities

Juristische Aspekte

**Konzepte**

- Modell-Entwicklung
- Software-Entwicklung
- Beratung/  
techn Support
- Betrieb

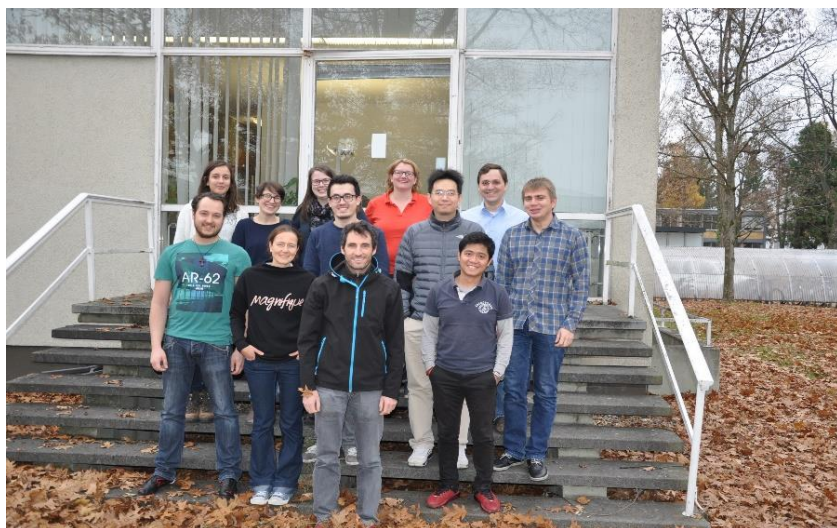
# Thank you for your attention



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KIT-SCC  
KIT-ITG



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# Further information about the Electronic Laboratory Notebook

- <https://www.chemotion.net>
- Recommended Internet-Browser:  
Google Chrome
- <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0240-0>
- <https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0292-9>

