Chemotion-ELN: digitization systems for chemists

Patrick Hodapp (Stefan Bräse group)

INSTITUTE OF ORGANIC CHEMISTRY - Stefan Bräse Group Karlsruhe

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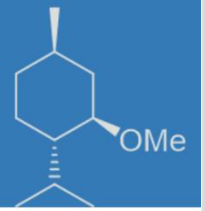
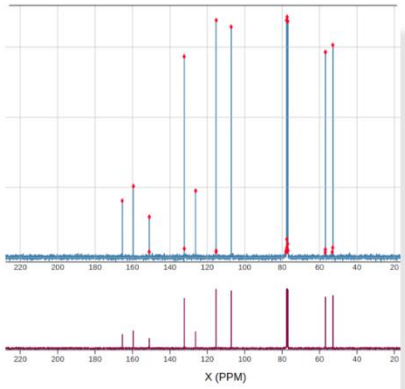
Projects funded by DFG Deutsche Forschungsgemeinschaft

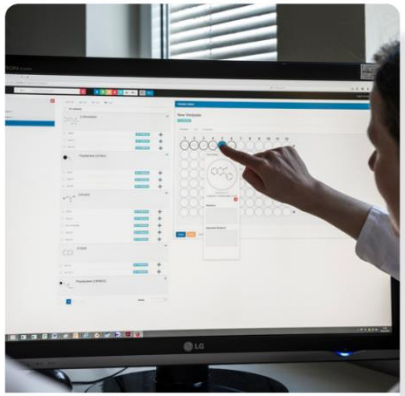
CHEMOTION

Electronic Laboratory Notebook & Repository for Research Data

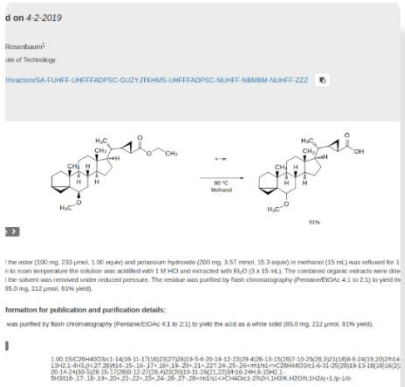




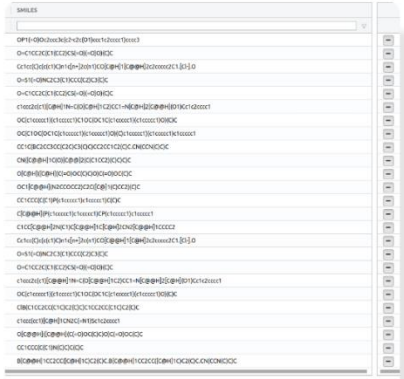
Spectra Viewer



Electronic Lab Notebook



Chemotion Repository



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

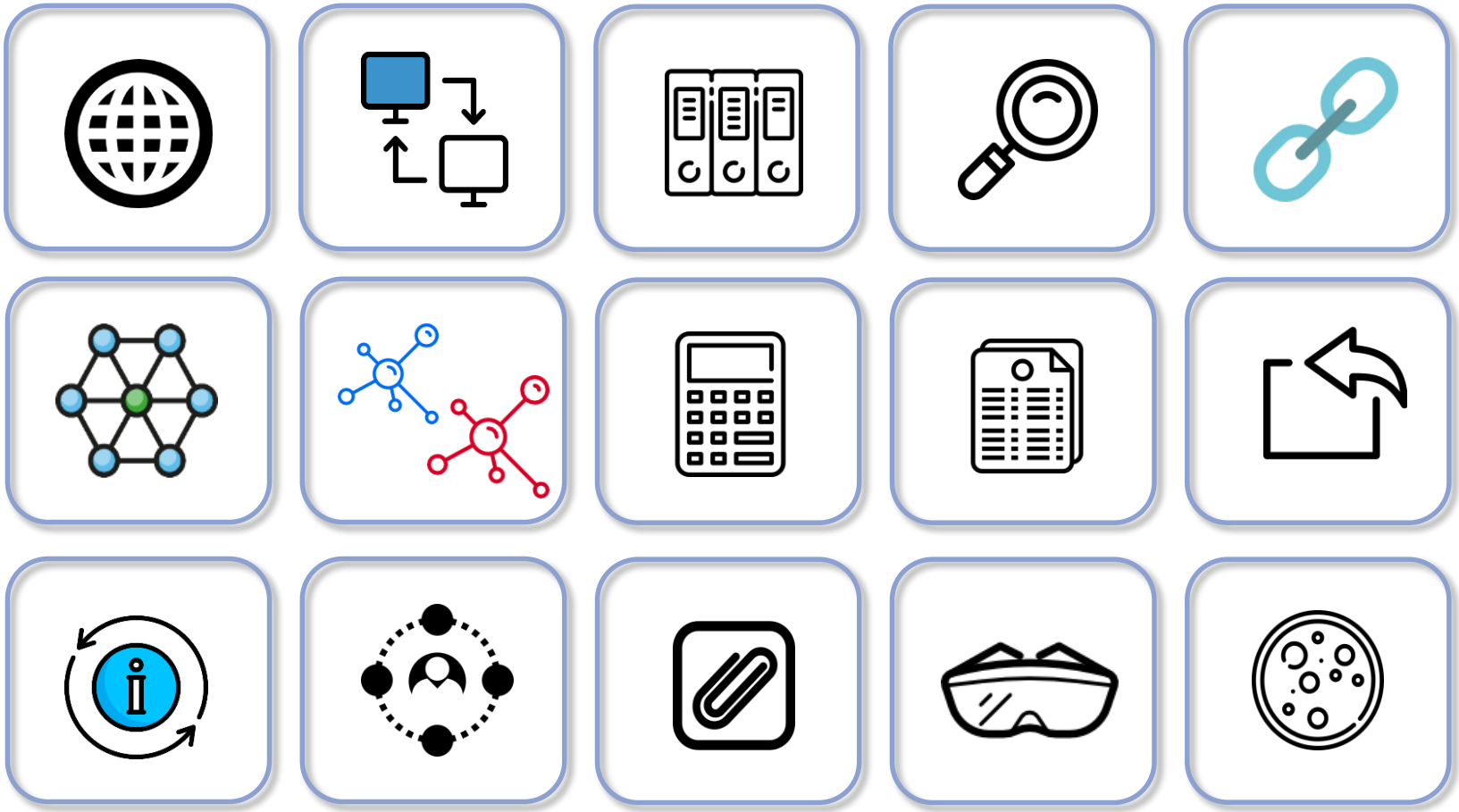
Electronic Lab Notebook

- Digital storage
- Processing of data

Repository

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

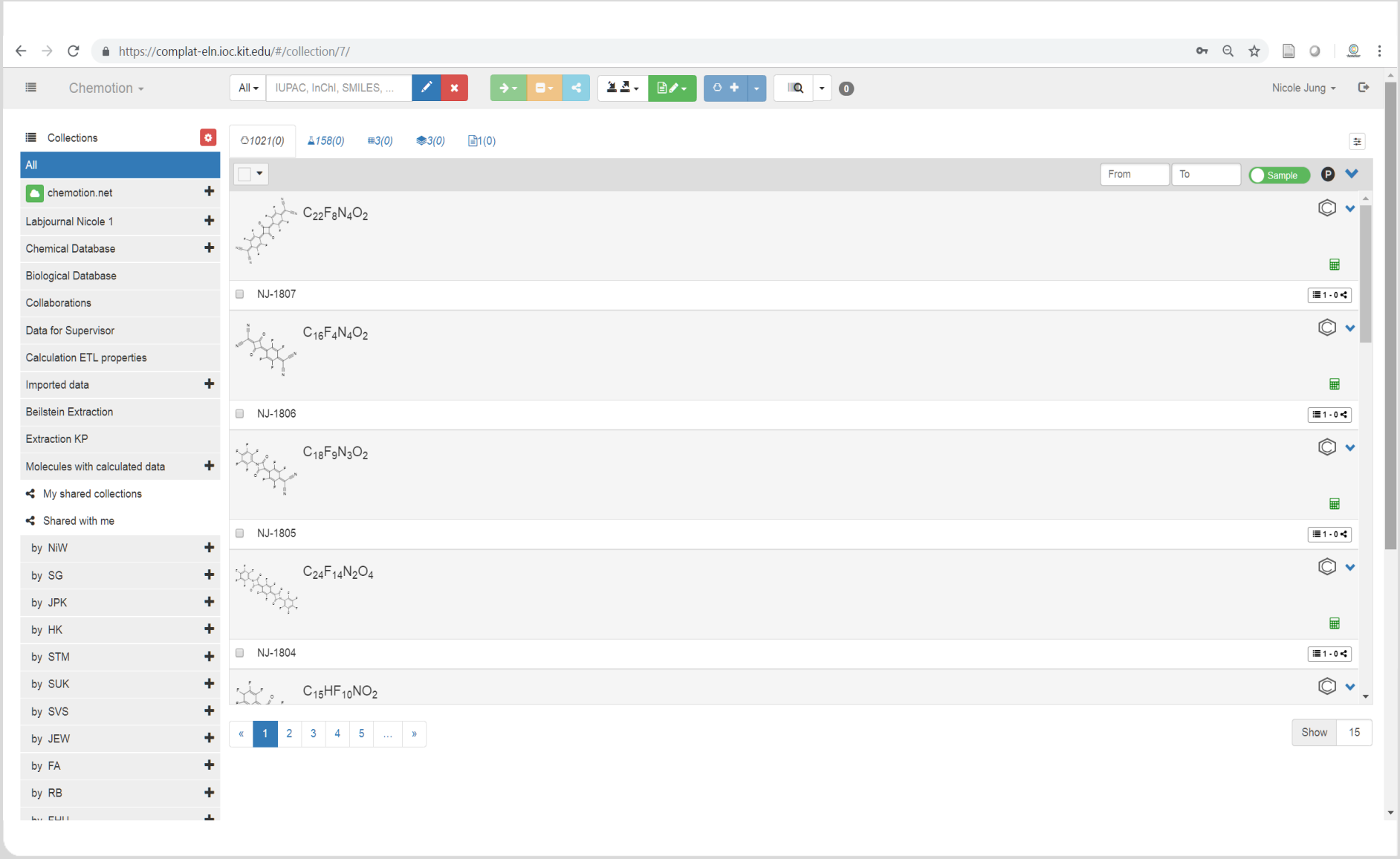
Chemotion Electronic Lab Notebook



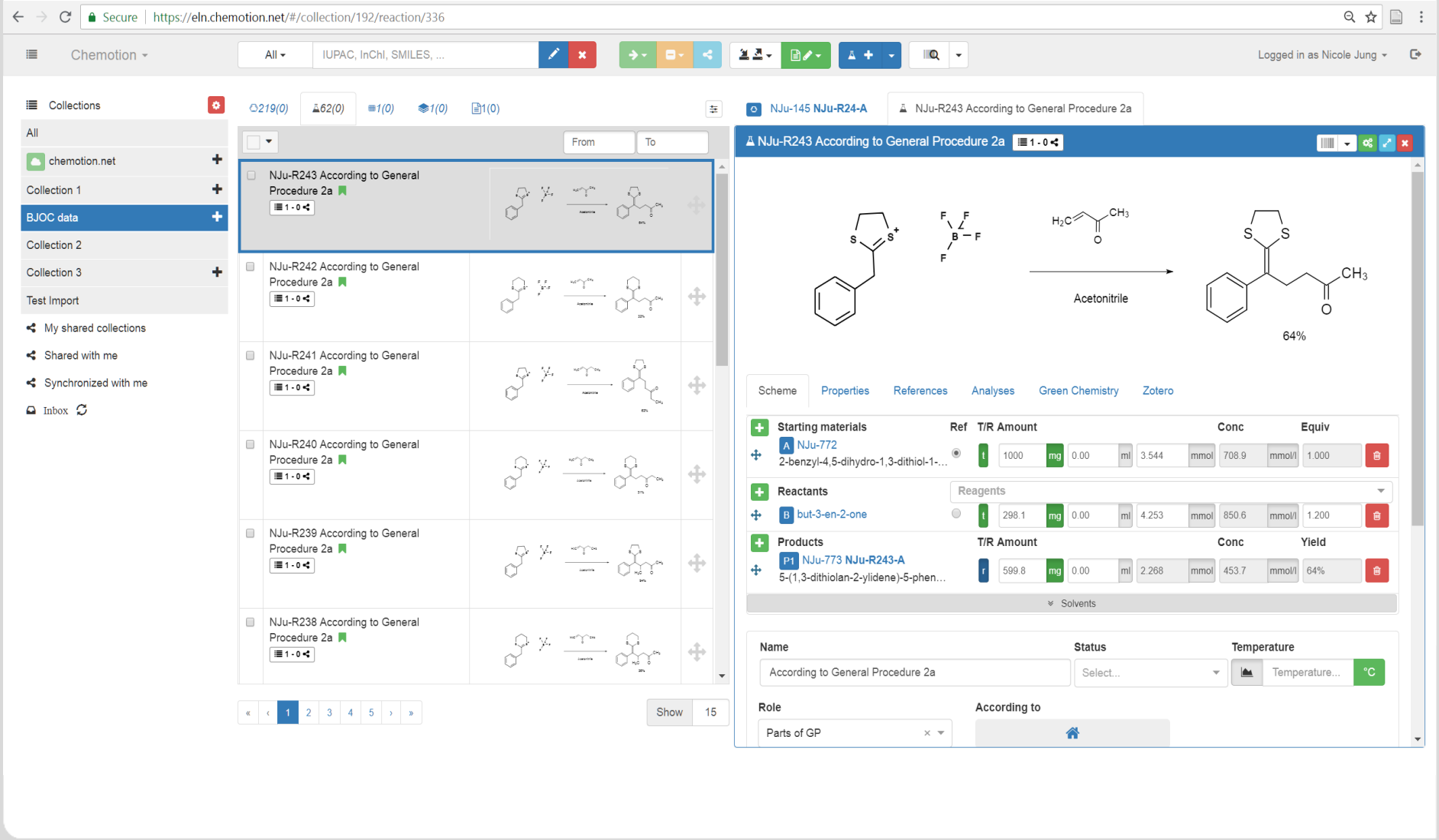
OPEN SOURCE

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.

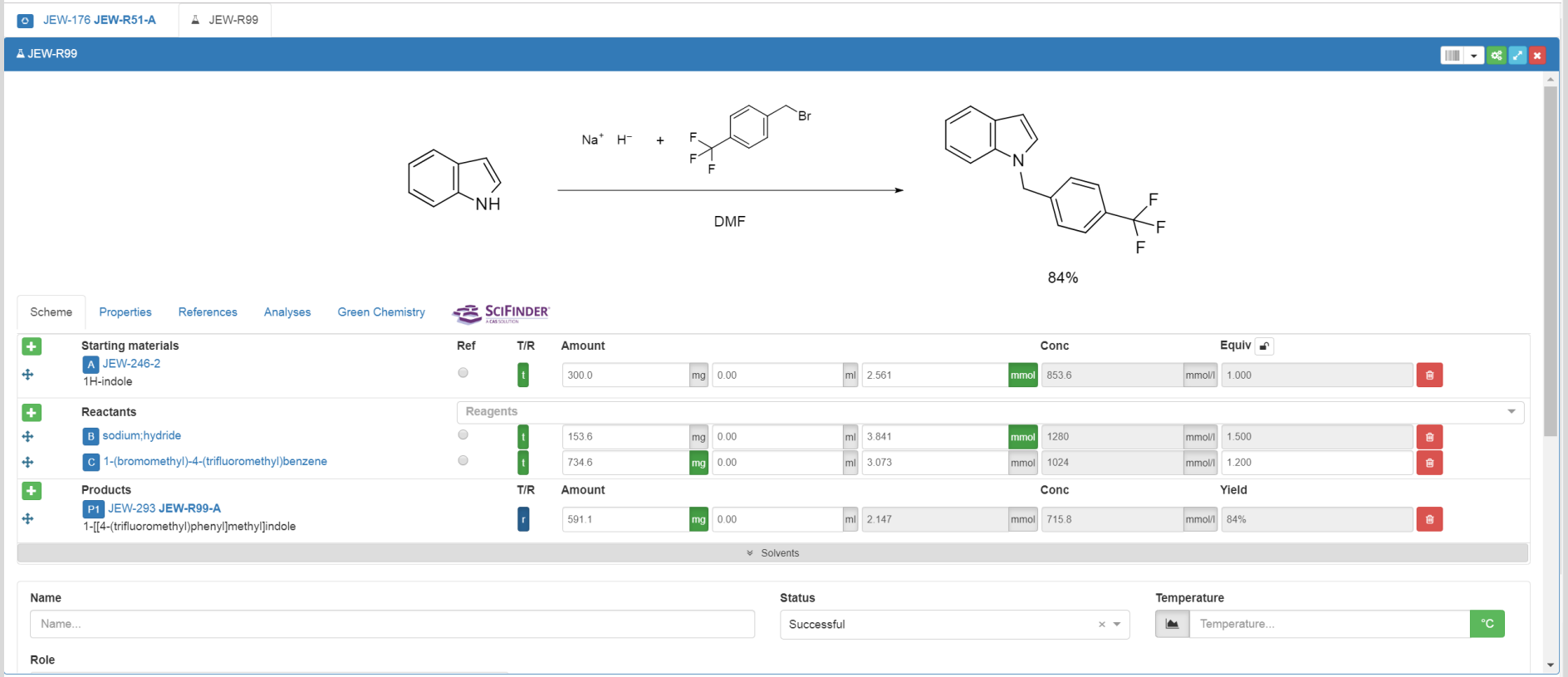
Electronic Lab Notebook - Management



Electronic Lab Notebook - Management

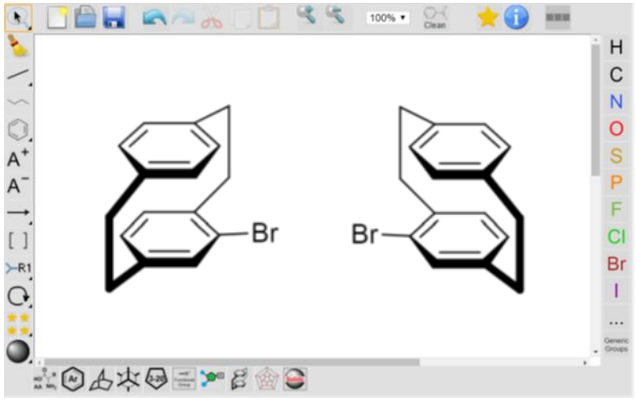


Electronic Lab Notebook - Reactions

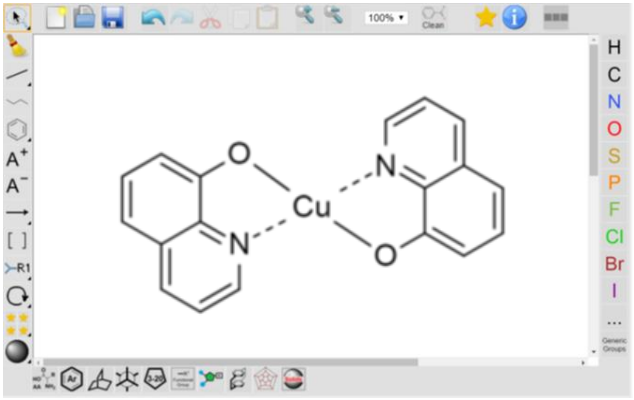


Electronic Lab Notebook - Structure Editor

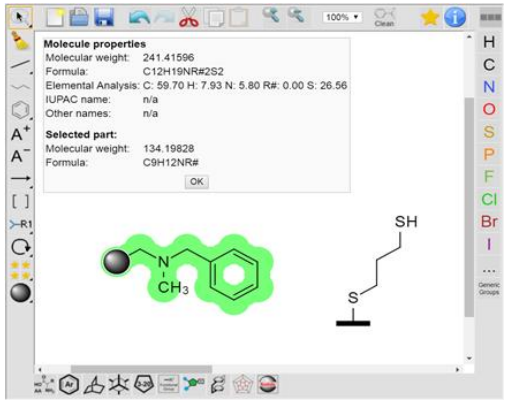
Differentiation of planar chiral compounds



Coordination chemistry enabled



Supported Material and Surfaces

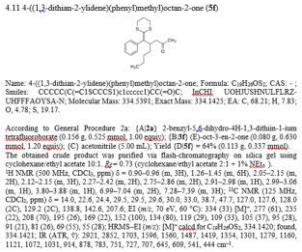


Electronic Lab Notebook - Management

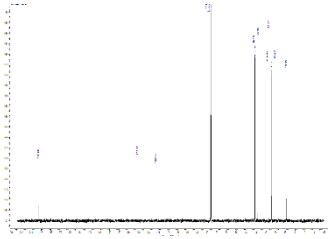
Reporting Functions

ELN – Reporting: Document Types

Supporting Information: Standard

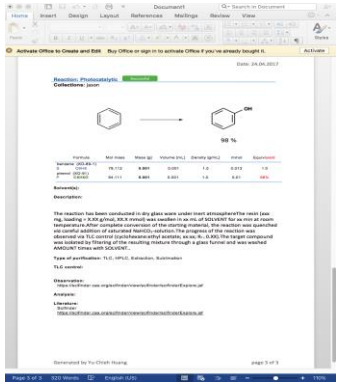


Supporting Information: Collection of Spectra



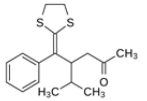
Supporting Information: Excel-Lists Identifier

Project Reports



ELN – reporting and Supporting Information

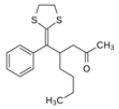
4.9 4-((1,3-Dithiolan-2-ylidene)(phenyl)methyl)-5-methylhexan-2-one (**4e**)



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: {A|**1a**} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.551 mmol, 1.00 equiv); {B|**3e**} (E)-5-methylhex-3-en-2-one (0.074 g, 0.660 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D|**4e**} = 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).
^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ = 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) δ = 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]$^+$, 263 (100), 221 (52), 191 (11), 113 (13), 69 (19); HRMS–EI (*m/z*): [M]$^+$ calcd for $C_{17}H_{22}OS_2$, 306.1107; found, 306.1108; IR (ATR, ṽ): 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}.

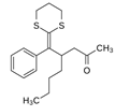
4.10 4-((1,3-dithiolan-2-ylidene)(phenyl)methyl)octan-2-one (**4f**)



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: {A|**1a**} 2-benzyl-4,5-dihydro-1,3-dithiol-1-ium tetrafluoroborate (0.156 g, 0.553 mmol, 1.00 equiv); {B|**3f**} (E)-oct-3-en-2-one (0.084 g, 0.666 mmol, 1.21 equiv); {C} acetonitrile (5.00 mL); Yield {D|**4f**} = 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).
^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ = 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) δ = 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]$^+$, 263 (100), 221 (22), 195 (20), 152 (49); HRMS–EI (*m/z*): [M]$^+$ calcd for $C_{18}H_{24}OS_2$, 320.1263; found, 320.1265; IR (ATR, ṽ): 2953, 2923, 2855, 1711, 1597, 1580, 1489, 1438, 1420, 1356, 1278, 1159, 1105, 1072, 1031, 978, 847, 750, 702, 645, 541 cm^{-1}.

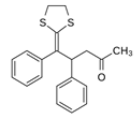
4.11 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one (**5f**)



Name: 4-((1,3-dithian-2-ylidene)(phenyl)methyl)octan-2-one; Formula: $C_{19}H_{26}OS_2$; CAS: - ; Smiles: CCCCC(C(=C1SCCCS1)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: {A|**2a**} 2-benzyl-5,6-dihydro-4H-1,3-dithiin-1-ium tetrafluoroborate (0.156 g, 0.525 mmol, 1.00 equiv); {B|**3f**} (E)-oct-3-en-2-one (0.080 g, 0.630 mmol, 1.20 equiv); {C} acetonitrile (5.00 mL); Yield {D|**5f**} = 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).
^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ = 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) δ = 14.0, 22.6, 24.4, 29.5, 29.5, 29.6, 30.0, 33.0, 38.7, 47.7, 127.0, 127.6, 128.0 (2C), 129.2 (2C), 138.8, 142.6, 207.6; EI (*m/z*, 70 eV, 60 °C): 334 (33) [M]$^+$, 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]$^+$ calcd for $C_{19}H_{26}OS_2$, 334.1420; found, 334.1421; IR (ATR, ṽ): 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}.

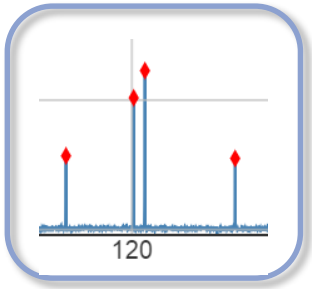
4.12 (E)-5-(1,3-dithiolan-2-yl)-4,5-diphenylpent-4-en-2-one (**4g**)



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: LRVYWKBWOILOMV-UHFFFAOYSA-N; Molecular Mass: 340.5022; Exact Mass: 340.0956; EA: C, 70.55; H, 5.92; O, 4.7; S, 18.83.

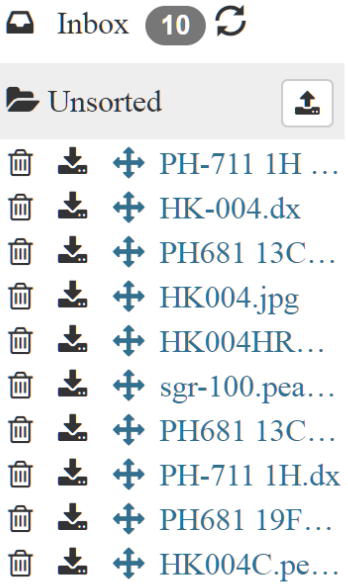
Addition of dithi(ol)anylium tetrafluoroborates to α, β-unsaturated ketones, Huang, Y.-C.; Nguyen, A.; Gräßle, S.; Vanderheiden, S.; Jung, N.; Bräse, S**. 2018**. *Beilstein Journal of Organic Chemistry*, 14, 515–522.

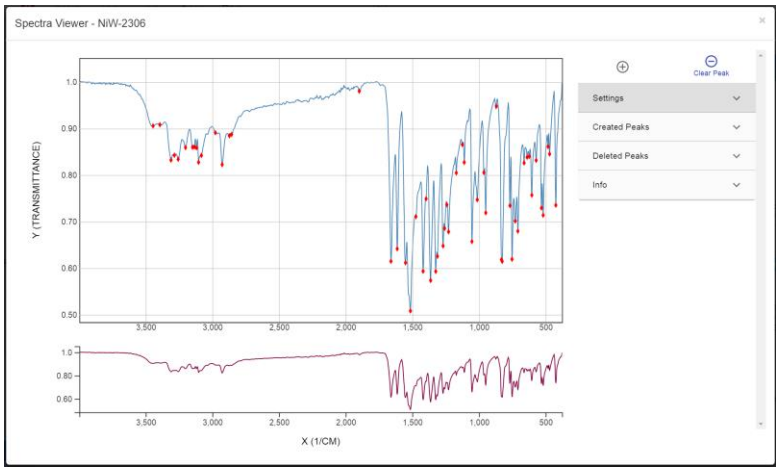
Electronic Lab Notebook - Management

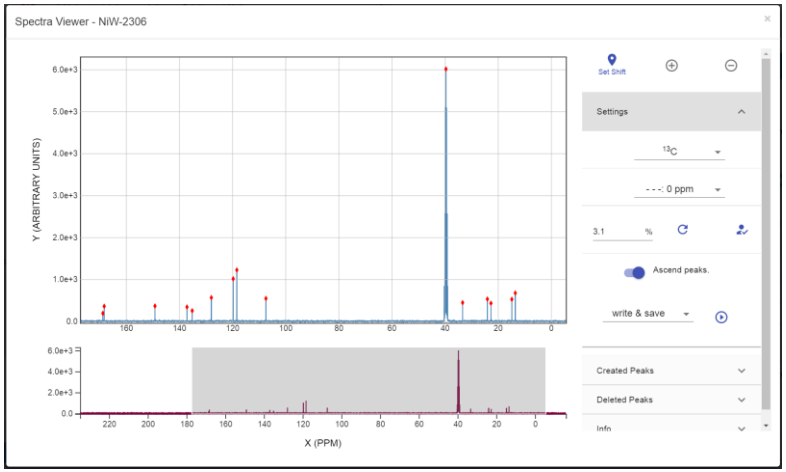


Analysis (13C NMR and IR)

Electronic Lab Notebook - Analysis



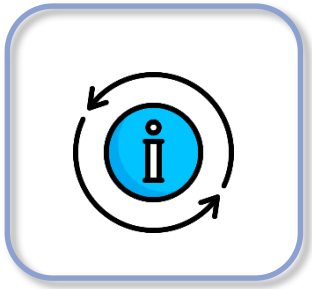




IR (ATR, ṽ) = 3445, 3394, 3310, 3285, 3257, 3201, 3149, 3135, 3119, 3104, 3082, 2978, 2927, 2873, 2856, 1898, 1660, 1613, 1551, 1514, 1473, 1419, 1397, 1363, 1324, 1312, 1269, 1258, 1241, 1228, 1170, 1125, 1111, 1052, 1013, 963, 949, 870, 832, 826 cm^{-1}.

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

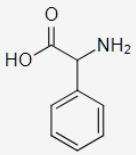
Electronic Lab Notebook - Management



Connection to external information

Electronic Lab Notebook - External Information

SciFinder A CAS SOLUTION

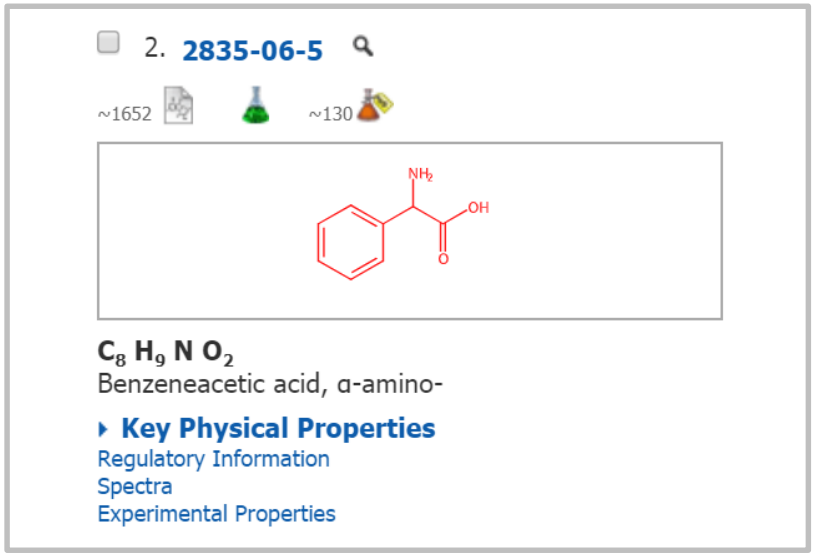


$C_8H_9NO_2$

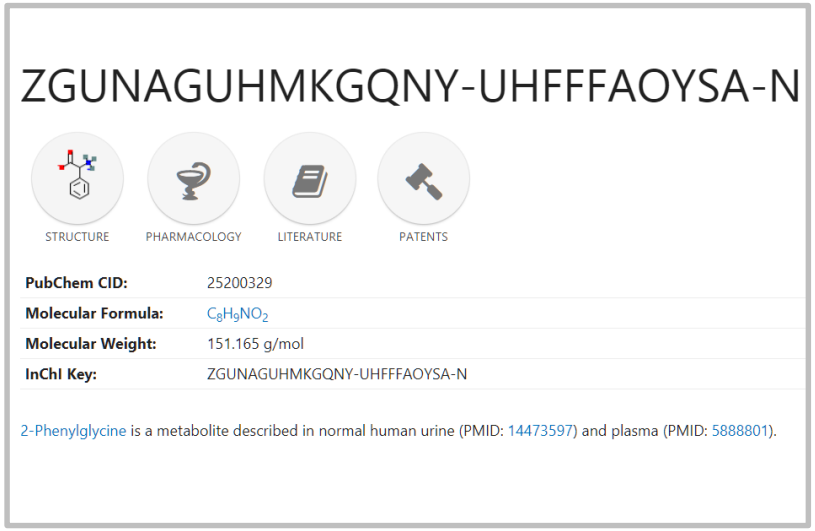
2-azaniumyl-2-phenylacetate

NJ-1302

4 - 0



PubChem



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

Chemotion

figshare

NMRShiftDB

RADAR

www.chemotion-repository.net

Science Data Center MoMaF und NFDI4Chem

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.

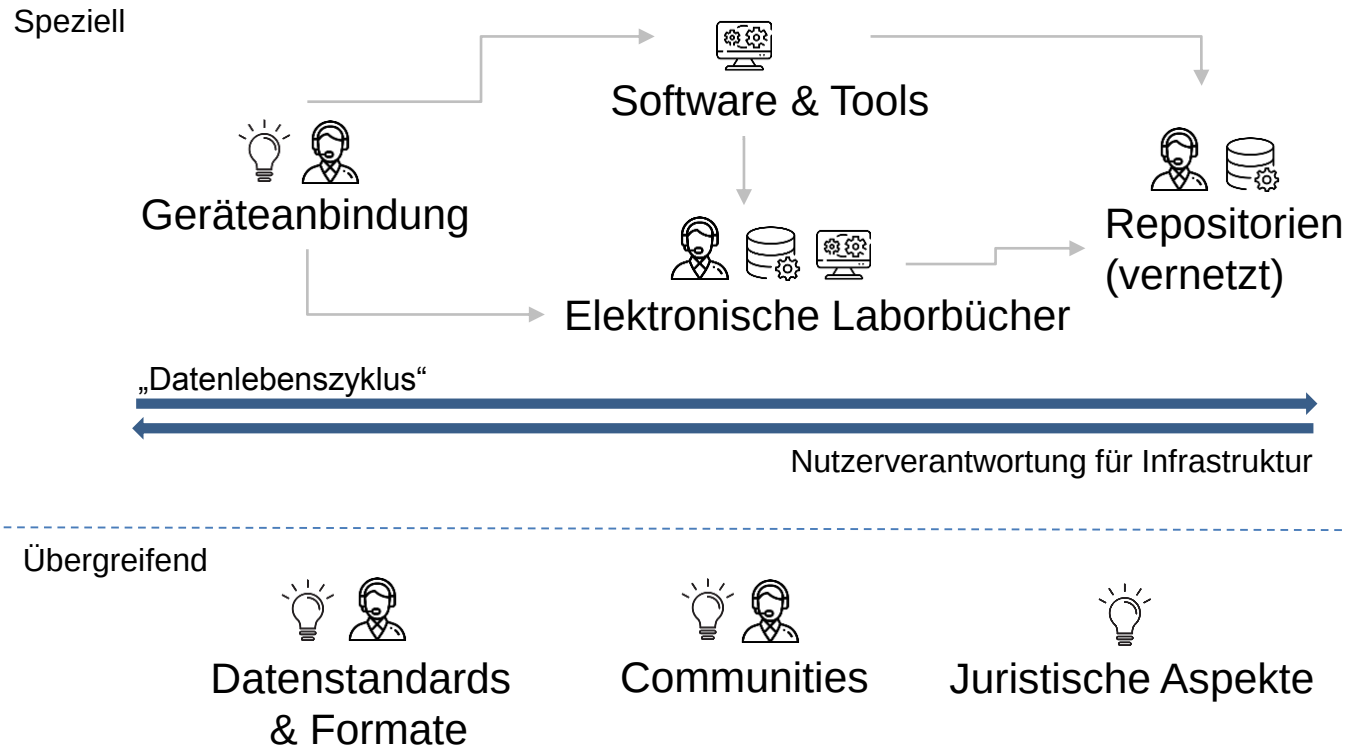
Daten aus vielen Laboren nachhaltig und gemeinschaftlich nutzen, ist das Ziel des neuen Science Data Centers MoMaF (Foto: Laila Tkotz, KIT)

Dezember 2018

In der Breite und forschungsnah: Handlungsfähige Konsortien

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

Chemotion-ELN NFDI4Chem



Konzepte

Modell-Entwicklung

Software-Entwicklung

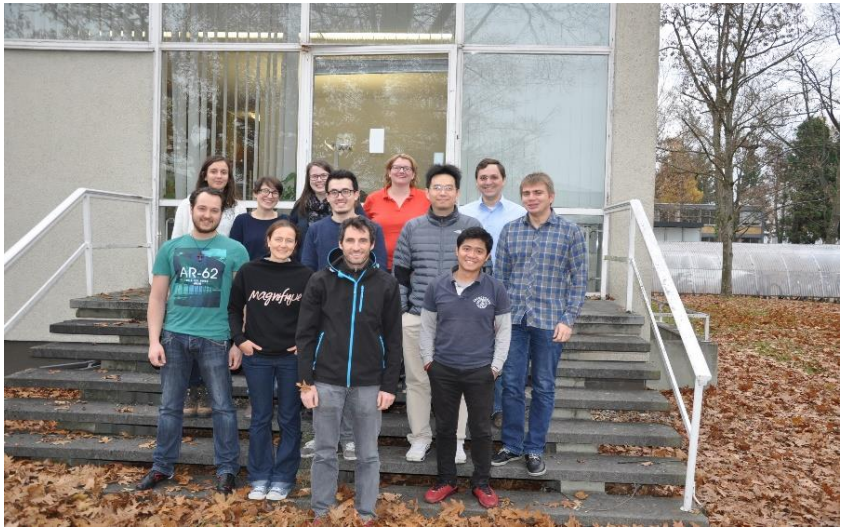
Beratung/
techn Support

Betrieb

Thank you for your attention

KIT-Bibliothek
KIT-SCC
KIT-ITG

Icons made by *Freepik*, *Madebyoliver*, *Anatoli*, *Dinosoft*, *Vectors market*, *Zlatko Najdenovski,* and *Gregor Cresnar* from www.flaticon.com



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