
IOCB SERVICE DAYS

Presentation of services by:
Research-Service Groups / Service Groups / Core Facilities

20
23

Drug Discovery Group

Pavel Majer



ÚOCHB AV
CR
IOCB PRAGUE



Automated peptide synthesis (M. Blechová, A. Prichodko)

Fmoc strategy using two instruments, Liberty Blue synthesizers

Group	Number of peptides
Bouřa	6
Cígler	10
Cvačka	10
Hocek	11
Jungwirth	4
Konvalinka	10
Majer	7
Maletínská	18
Marek	2
Mareš	13
Rulíšek	5
Řezáčová	22
Stříšovský	20
Vondrášek	7
Vrábel	1
Zoll	4
Total:	150

2022 overview



- 53 Peptides (roughly 1/3) were further modified by manual synthesis which included binding of special amino acids (45) or formation of disulfide bridges (8).
- Approx. 70% peptides contained up to 20 AA, the remainder were longer peptides up to 45 AA.
- Collaboration with mass spectrometry department frequently used for service MS measurement.

Manual peptide and small molecule synthesis

(M. Hradilek)



Users and number of synthesized compounds:

Year 2022, Group:

Hocek	12
Marek	2
Konvalinka	5
Mareš	9
Vondrášek	1
Jungwirth	6
Cígler	7

Year 2021, Group:

Hocek	19
Birkuš	1
Konvalinka	10
Zoll	1
Vondrášek	7
Jungwirth	12
Cígler	7
Polášek	2

Synthesis of peptides containing unusual modification on C-, N-terminus or on side chains of peptide:

- Acetylation,
- Biotinylation,
- Methylation,
- Phosphorylation,
- Small molecule modification, Azidation, Alkynylation,
- PEGylation,
- Fluorescent and FRET peptides, Cyclic and Bicyclic peptides (C-N, C-S, S-S cyclization),
- Peptidomimetics,
- Small Library synthesis,
- Fluorescent dye synthesis.

Amino Acid Analysis (AAA) - LC-MS FACILITY (R. Souček)

Department	NHD-AAA	OPA-HPLC	LC/MS	Stability studies	Total (2022)
Drug Discovery (Majer)	11	18	336		365
Prot. of Human Pathogens (Konvalinka)	36	29	263		328
Synthetic Nanochemistry (Cígler)	0	0	285		285
HBV Cure (Birkuš)	47	85	0		132
Intermembrane Proteolysis (Strišovský)	58	44	0		102
Neurosteroids (Kudová)	0	0	68	4	68
Cathepsin Proteases in Pathol. (Mareš)	12	13	8		33
Chemistry and Biol. of Insulin (Jiráček)	4	11	8		23
Bioinformatics (Vondrášek)	10	8	0		18
Structural Biology (Řezáčová)	14	4	0		18
Analytical Laboratory (Matějková)	8	6	0		14
Functional Potential of NA (Curtis)	0	1	0		1
Total 2022	200	219	968	4	



- Two instruments, classic ninhydrine derivatization and newer OPA-HPLC analyzer
- The LC/MS unit 6230 LC/MS TOF (Agilent Technologies) This instrument combines a rapid resolution HPLC with very short run times, superior sensitivity and selectivity, an electrospray (ESI) source, and a time-of-flight (TOF) mass analyzer

Protein sequencing (Z. Vobůrka)

Users and number of samples analyzed in 2022:

Stříšovský	6
Jiráček	72
Maloy Řezáčová	11
Lébl	6
Majer	19
Mareš	73
Konvalinka	11
Zoll	2
Pichová	7
Kečkéšová	6

- N-terminal amino acid sequencing by Edman degradation using the Procise Protein Sequencing System (Applied Biosystems, 491 HT or 494 cLC Protein Sequencer).

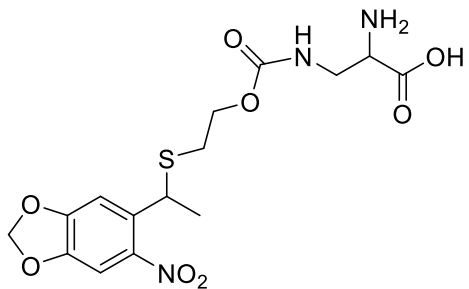


How to reach us.....

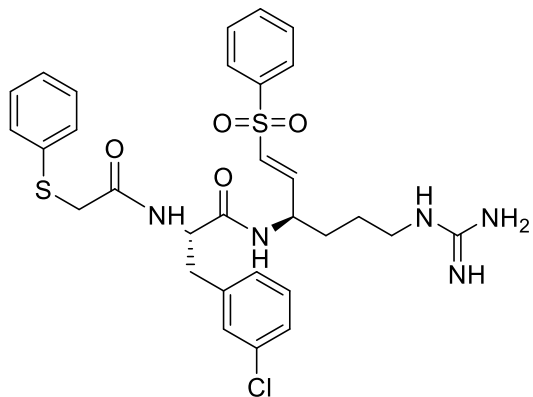
- In person...talk to anyone from our group
- Phone, email...etc.
- For peptides, there is a simple form, Mirka or Martin can help
- Material cost of peptide synthesis is paid by customers (likely to be changed)

Compounds made by Ivan Šnajdr

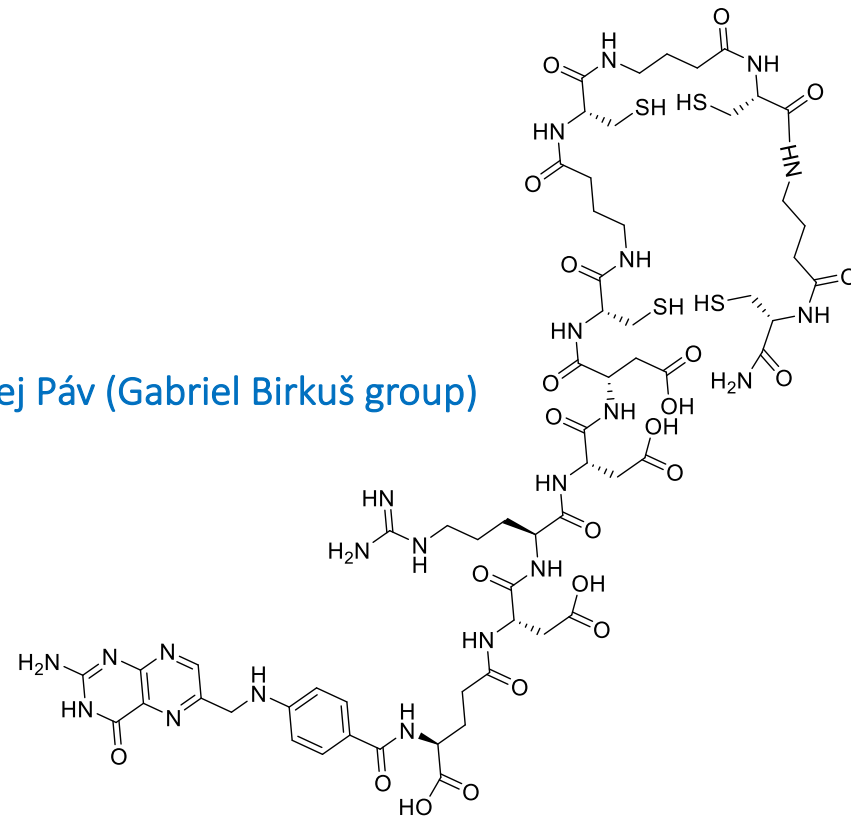
IS-103-064



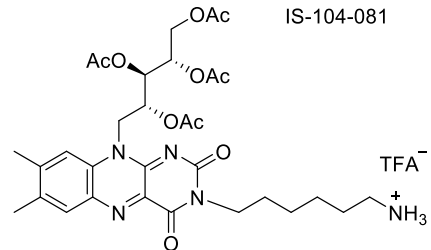
for **Tat'ána Majerová** (Jan Konvalinka group)



for Petra Rubešová (10 derivatives, Michael Mareš group)

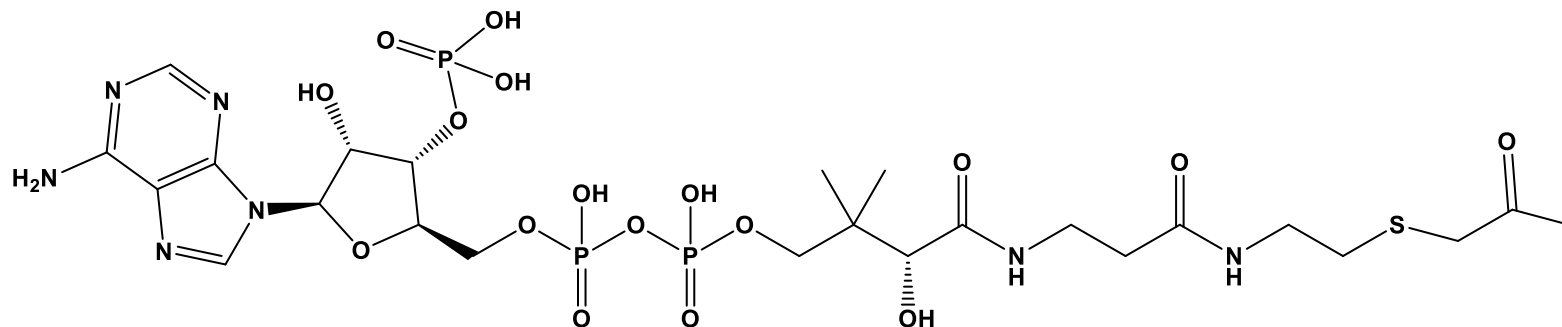


IS-104-081

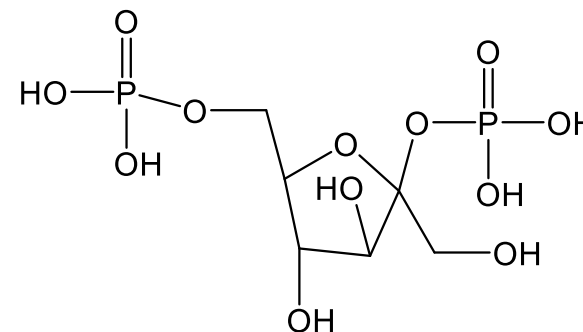


for Pavel Šácha (Jan Konvalinka group)

Compounds made by Marcela Krečmerová



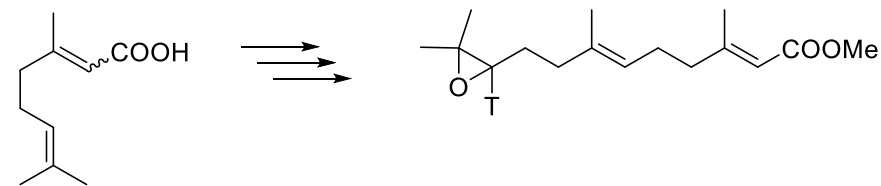
for Václav Veverka (Pavlína Řezáčová group)



for Iva Pichová

Int. J. Mol. Sci. **2021**, 22, Article No. 1483.

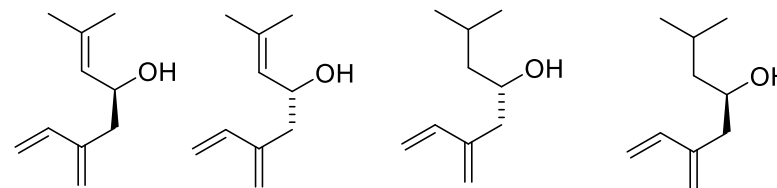
Compounds made by Aleš Machara



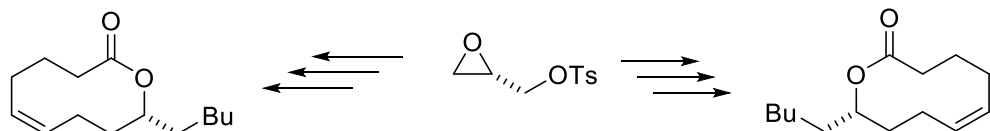
geranic acid

radiolabeled juvenile hormone JHIII
in collaboration with [Aleš Marek](#)

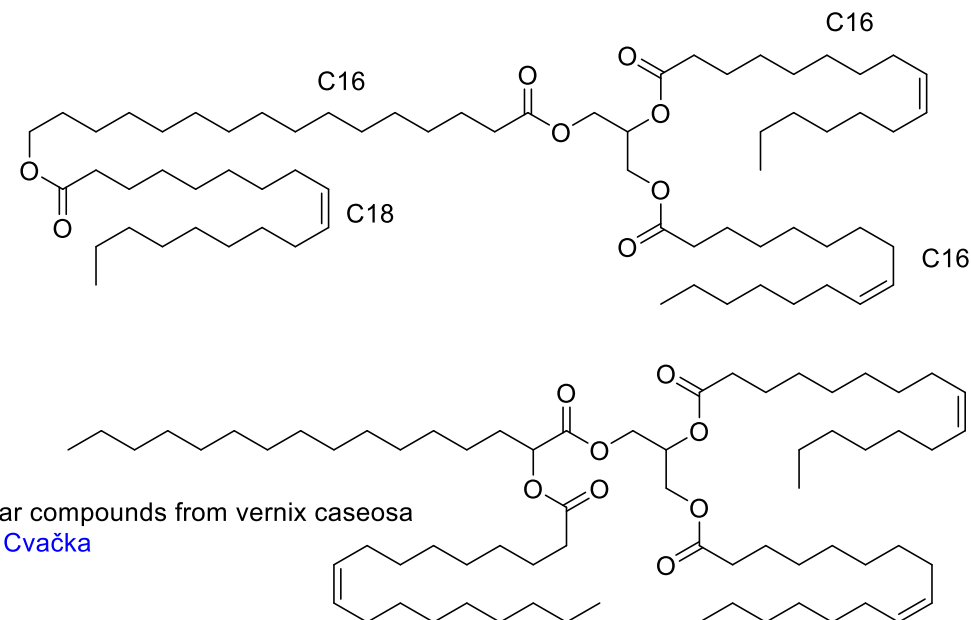
Insect Biochemistry and Molecular Biology 139: 103671 (2021)



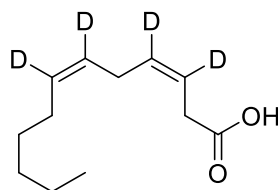
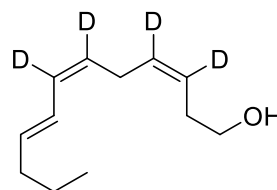
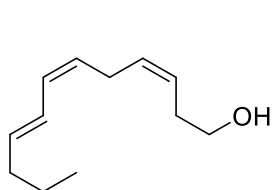
enantiopure bark beetle pheromones
BMC Biology 19: 16 (2021)



enantiodivergent synthesis of queen termite pheromone for [Robert Hanus](#)
Journal of Natural Products 81 (10): 2266-2274 (2018)

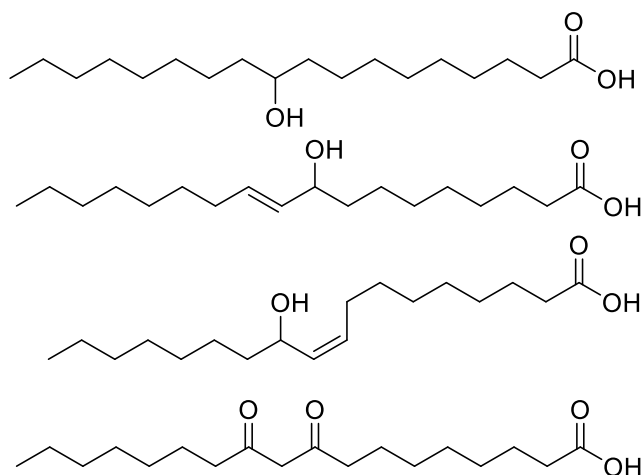


and similar compounds from vernix caseosa
for [Josef Cvačka](#)



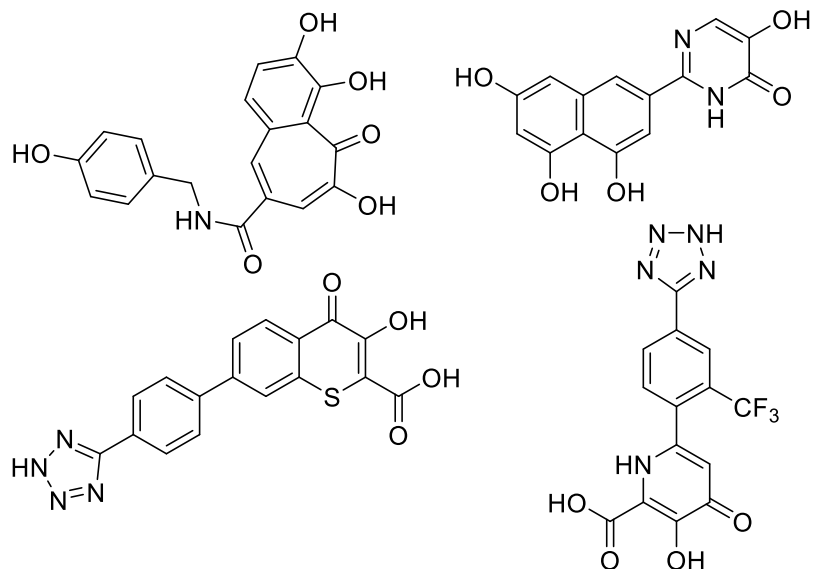
(3Z,6Z,8E)-dodeca-3,6,8-trien-1-ol
trail pheromone of termites; made for [Robert Hanus](#)

More compounds made by Aleš Machara



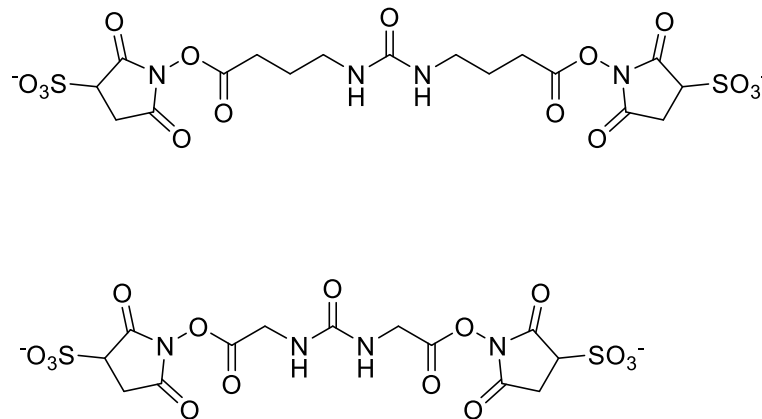
small library of oxidized fatty acids
for [Iva Pichová](#) and [Luboš Rulišek](#)

Computational and Structural Biotechnology Journal 20:1378–1388 (2022)

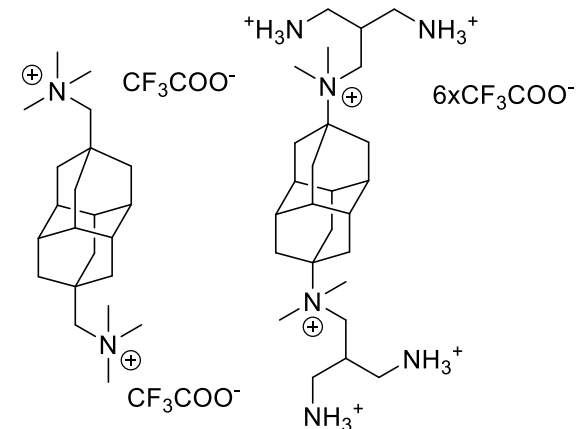


large library of compounds that can chelate two metal ions
for [Milan Kožíšek](#)

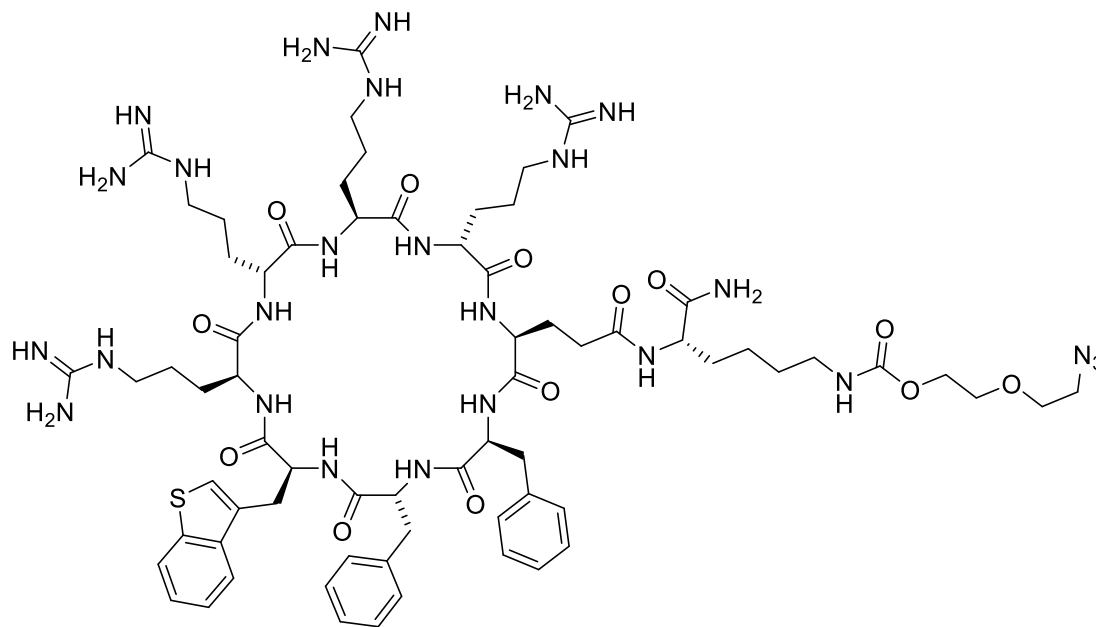
European Journal of Medicinal Chemistry 208: 112754 (2020)



crazy (cross-linking) stuff for [Josef Cvačka](#)



more crazy stuff for [Pavel Hobza](#)



cell-penetrating peptide sequence with bioorthogonal functional group
originally for [Milan Kožíšek](#)

Compounds made by Martin Hradilek

Cyclic peptide for [Milan Kožíšek](#) ([Jan Konvalinka](#) group)

Cyclic azidopeptide for [Milan Kožíšek](#) ([Jan Konvalinka](#) group)

Compounds made by Martin Hradilek

Cyclic peptide for [Milan Kožíšek](#) ([Jan Konvalinka](#) group)

Alkyne peptide for [Milan Kožíšek](#) ([Jan Konvalinka](#) group)

Compounds made by Martin Hradilek

DOTA-aminosulfonamides for Jiří Brynda (Pavlína Řezáčová group)