

Porada vedoucích

Meeting with Team Leaders



IOCB Compound Archive

Petr Jansa



IOCB

IOCB

- 10 groups of organic chemistry
- up to 140 organic chemists

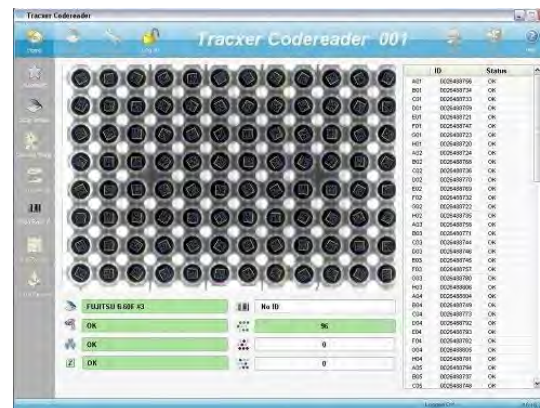
- NMR 2500 compounds/year
- elemental analysis 2000 compounds/year
- MS 4600 compounds/year

Up to 2500 compounds are produced at UOCHB every year.

After publishing „waste“

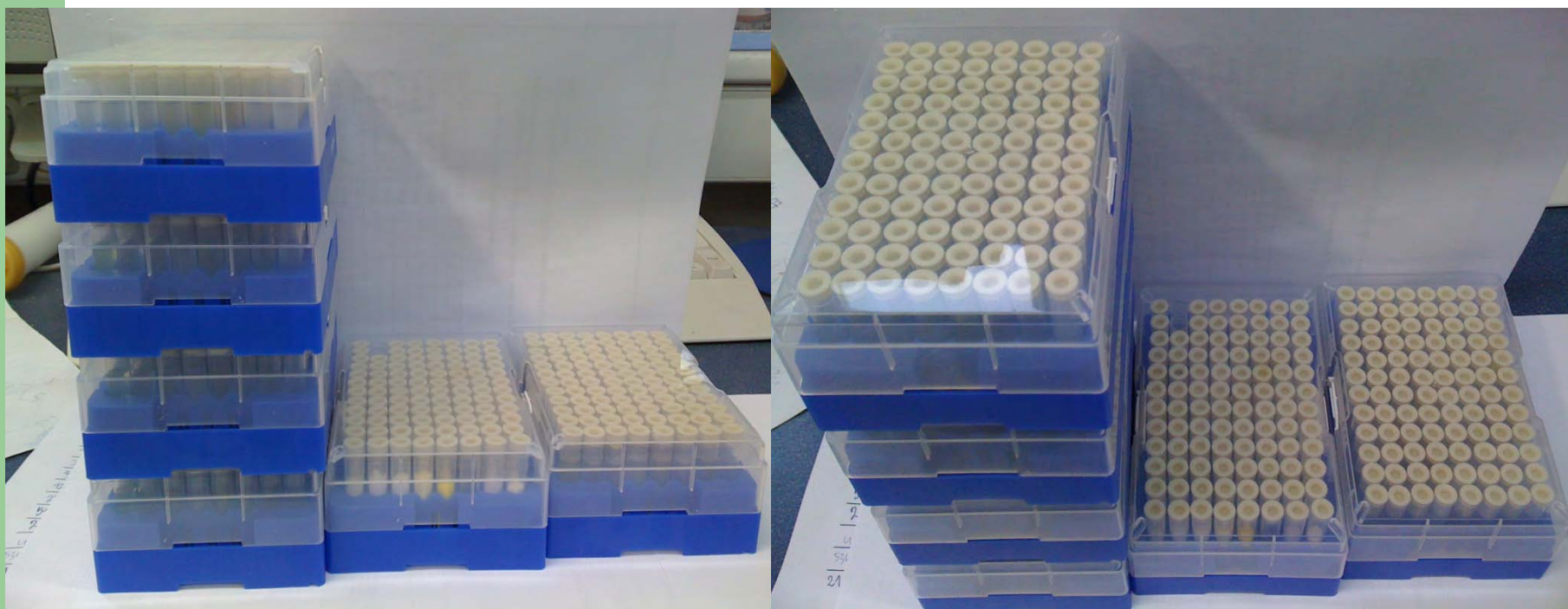
Project: Antonín Holý Library (AHL) of chemical compounds

Phase 1 – supported by Prof. Holý – equipment, racks and tubes



Project: Antonín Holý Library (AHL) reality

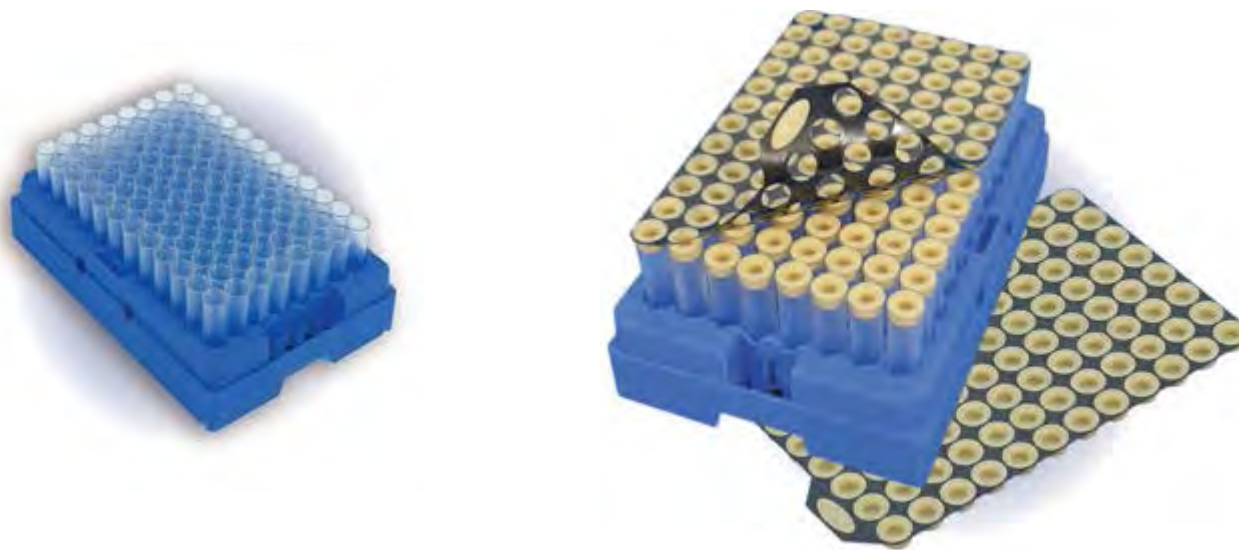
Phase 2 – collecting compounds (now 576 compounds)



Current capacity is 96 compounds per week (more than **4000** per year)

Project: Antonín Holý Library (AHL) of chemical compounds

Phase 3 – new racks and tubes (supported by Dr. Janeba)
– storing of all compounds of Prof. Holy



Material for storing of 10 000 compounds

Project: Antonín Holý Library (AHL) of chemical compounds

- long time storing of **ALL** compounds (-20°C, in dry pure DMSO, argon)
- effective management (storing, distribution, recovery, saving quantities)
- biological screening – antiproliferative (group of Dr. Kaiserová-Mertlíková)
 - antimicrobial (Army of the Czech Republic)
 - (virology, immunology, BIOMEDREG)

= publications and patents

10.div - DIVA - C:\Users\Petr Jansa\Desktop\data z lab\Publikace\AHL\10.div

File Edit Insert Format Data Analysis Window Help

G15

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	
	Rack	Position	Allies code	Allies name	Allies institution	Sample added	Structure	Library code	Concentration (mM in DMSO)	additive/ comment	Solid sample (mg)	Vial code (A)	Vial code (B)	Vial code (C)	Vial code (D)	Vial code (E) solid	XTT (%) CCRF-CEM	XTT IC50 (uM) CCRF-CEM	XTT (%) HeLa S3	XTT IC50 (uM) HeLa S3	XTT (%) CCRF-HL60	XTT IC50 (uM) HL60	XTT (%) CCRF-HepG2	
112	2	B4	PJ-677 B	Jansa Petr	IOCB	13.5.2011		112	50,1518		214	21713023	21713119	21712543	21712639	21712735	12			106		121		100
115	2	B7	PJ-695	Jansa Petr	IOCB	13.5.2011		115	50										122		111		111	
31	1	C7	PJ-489	Jansa Petr	IOCB	21.4.2011		31	2,49997	H									97		111		102	
36	1	C12	PJ-K-R	Jansa Petr	IOCB	21.4.2011		36	50										102		114		100	
76	1	G4	PJ-503	Jansa Petr	IOCB	21.4.2011		76	2,50307	N									63		83		48	
55	1	E7	PJ-N-3	Jansa Petr	IOCB	21.4.2011		55	50										130		112		100	
93	1	H9	PJ-426 O	Jansa Petr	IOCB	21.4.2011		93	50,0998										83		117		108	
66	1	F6	PJ-K-I	Jansa Petr	IOCB	21.4.2011		66	50	N									110		116		105	
81	1	G9	PJ-433	Jansa Petr	IOCB	21.4.2011		81	2,49809	NH3	227	21713376	21713280	21713472	21712896	21712992	68		99		108		90	
185	2	H5	H-2007	Holý Antonín	IOCB	13.5.2011		185	50,1054		245	21713096	21713192	21712616	21712712	21712808	73							
119	2	B11	PJ-464	Jansa Petr	IOCB	13.5.2011		119	25		383	21713030	21713126	21712550	21712646	21712742	74							
138	2	D6	PJ-KR1-17	Jansa Petr	IOCB	13.5.2011		138	49,9158		368	21713049	21713145	21712569	21712665	21712761	75							
139	2	D7	PJ-KR1-18	Jansa Petr	IOCB	13.5.2011		139	50		167	21713050	21713146	21712570	21712666	21712762	76							
53	1	E5	PJ-N-1	Jansa Petr	IOCB	21.4.2011		53	50		561	21713348	21713252	21713444	21712868	21712964	79							
127	2	C7	PJ-KR1-6	Jansa Petr	IOCB	13.5.2011		127	50		238	21713038	21713134	21712558	21712654	21712750	79							
164	2	F8	PJ-KR2-16	Jansa Petr	IOCB	13.5.2011		164	50		399	21713075	21713171	21712595	21712691	21712787	79							
165	2	F9	PJ-KR2-17	Jansa Petr	IOCB	13.5.2011		165	50		177	21713076	21713172	21712596	21712692	21712788	79							
155	2	E11	PJ-KR2-7	Jansa Petr	IOCB	13.5.2011		155	50		418	21713066	21713162	21712586	21712682	21712778	81							
63	1	F3	PJ-N-10	Jansa Petr	IOCB	21.4.2011		63	40		8	21713358	21713262	21713454	21712878	21712974	82							
106	2	A10	PJ-198	Jansa Petr	IOCB	13.5.2011		106	12,5		156	21713017	21713113	21712537	21712633	21712729	82							

Set 1: Table Set 1: Report

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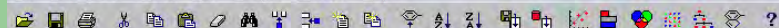
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Multiple Selection Viewer



Structure 1 of 1

Clone Deselect

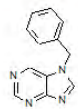


J3 16,66666

	A Rack	B Position	C Allies code	D Allies name	E Allies institution	F Sample added	G Structure	H Search Hits	I Library code	J Concentration (mM in DMSO)	K additive/ comment	L Solid sample (mg)	M Vial code (A)	N Vial code (B)	O Vial code (C)	P Vial code (D)	Q Vial code (E) solid	R XTT (%) CCRF-CEM	S XTT IC50 (uM) CCRF-CEM	T XTT (%) HeLa S3	U XTT IC50 (uM) HeLa S3	V XTT (%) CCRF-HL60	W XTT IC50 (uM) HL60	X CCF
112	2	B4	PJ-677 B	Jansa Petr	IOCB	13.5.2011		1	112	50,1518		214	21713023	21713119	21712543	21712639	21712735	12		106		121		100
37	1	D1	PJ-164	Jansa Petr	IOCB	21.4.2011		1	37	25		559	21713332	21713236	21713428	21712852	21712948	105						
99	2	A3	PJ-164	Jansa Petr	IOCB	13.5.2011		1	99	16,6667		51	21713010	21713106	21712530	21712626	21712722	105						
80	1	G8	PJ-556	Jansa Petr	IOCB	21.4.2011		0	80	25		399							48±0,025	21	2,15±0,25	16	0,78±0,011	43
79	1	G7	PJ-550	Jansa Petr	IOCB	21.4.2011		0	79	12,5		32							22±0,15	27	3,94±0,37	21	3,02±0,08	41
43	1	D7	PJ-350 rac	Jansa Petr	IOCB	21.4.2011		0	43	50		245							52±0,50	90		75		104
46	1	D10	PJ-66 rac	Jansa Petr	IOCB	21.4.2011		0	46	50		316							17±0,20	81		71	8,32±0,64	95
48	1	D12	PJ-333 rac	Jansa Petr	IOCB	21.4.2011		0	48	25		372							53±0,25	59	14,2±0,1	32	>15	94
187	2	H7	PJ-416 A	Jansa Petr	IOCB	13.5.2011		0	187	50		507							55±0,16	7	4,04±0,19	9	9,10±0,45	
190	2	H10	PJ-393	Jansa Petr	IOCB	13.5.2011		0	190	50		150							59±0,29	69	10,4±0,6	70	9,57±0,53	100
45	1	D9	PJ-66	Jansa Petr	IOCB	21.4.2011		0	45	50		169							78±0,26	94		81		100
47	1	D11	PJ-333	Jansa Petr	IOCB	21.4.2011		0	47	50		145	21713342	21713246	21713438	21712862	21712958	25	5,06±0,28	80		59	14,1±0,1	100
39	1	D3	PJ-32A	Jansa Petr	IOCB	21.4.2011		0	39	50		400	21713334	21713238	21713430	21712854	21712950	10	7,25±0,11	95		27	6,51±0,68	103
186	2	H6	PJ-670 A	Jansa Petr	IOCB	13.5.2011		0	186	50		85	21713097	21713193	21712617	21712713	21712809	10	7,56±0,53	37	12,2±0,4	35	>15	120
191	2	H11	PJ-662	Jansa Petr	IOCB	13.5.2011		0	191	13,746		0	21713102	21713198	21712622	21712718	21712814	16	7,60±0,34	15	6,36±0,15	27	10,0±0,76	109
54	1	E6	PJ-N-2	Jansa Petr	IOCB	21.4.2011		0	54	50		742	21713349	21713253	21713445	21712869	21712965	8		62		96		98
114	2	B6	PJ-629	Jansa Petr	IOCB	13.5.2011		0	114	25		99	21713025	21713121	21712545	21712641	21712737	11		104		119		102
115	2	B7	PJ-695	Jansa Petr	IOCB	13.5.2011		0	115	50		625	21713026	21713122	21712546	21712642	21712738	12		122		111		111
31	1	C7	PJ-489	Jansa Petr	IOCB	21.4.2011		0	31	2,49997	HS	219	21713326	21713230	21713422	21712846	21712942	14		97		111		102
36	1	C12	PJ-K-R	Jansa Petr	IOCB	21.4.2011		0	36	50		891	21713331	21713235	21713427	21712851	21712947	16		102		114		100

Substructure Search

Structure:



Search Options:

- ☒ Reorder sheet
- ☒ New hit count column
- ☒ Highlight substructure
- ☒ Align by substructure
- ☐ New sheet for hits

Paste Read File...

Help:

Select a substructure either by using copy and paste, or by reading a structure file.

Search Cancel Help

Set 1: Table Set 1: Report

Data Size: 1176 rows, 26 columns Selected: Area 1R X 1C Extracting structures... 0 jobs pending



Project: Antonín Holý Library (AHL) of chemical compounds

Special thanks to: Prof. Antonín Holý
Dr. Zlatko Janeba
Assoc. Prof. Martin Fusek
Assoc. Prof. Jiří Krechl
Dr. Zdeněk Havlas

staff of the analytical laboratory

A few remarks:

- Divide into 1, building blocks 2, screening compounds
- Add stock on/off
- Add virtual compounds
- Price categories (1-5)
- Block licensed material

Campus Remodeling update

Jiří Špička







Budova C

Zahájeno: 7/2010

Dokončeno: 9/2011
(předpoklad)





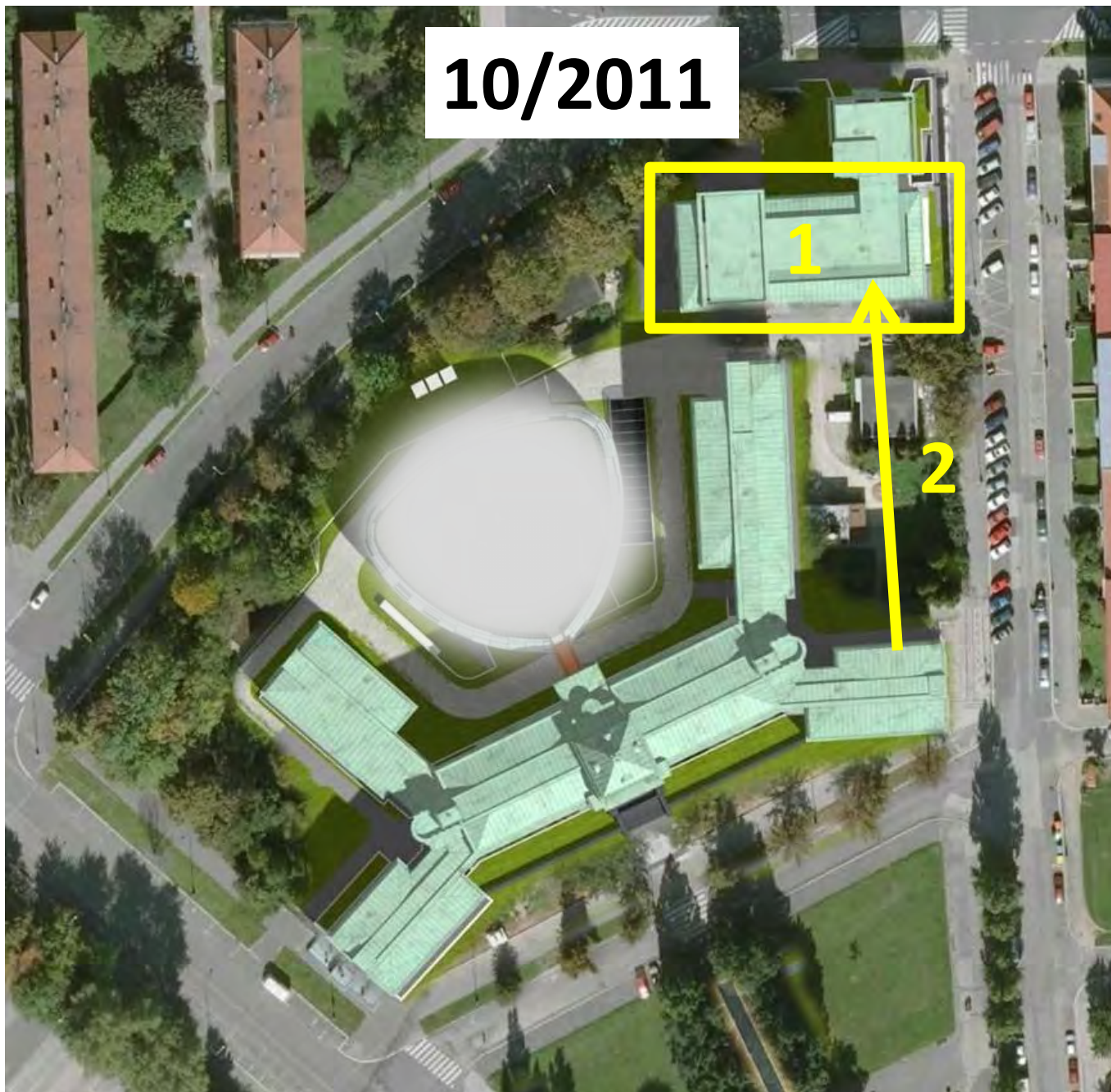
Papírenská – hala B (2. etapa)

Dokončeno: 2012 ?

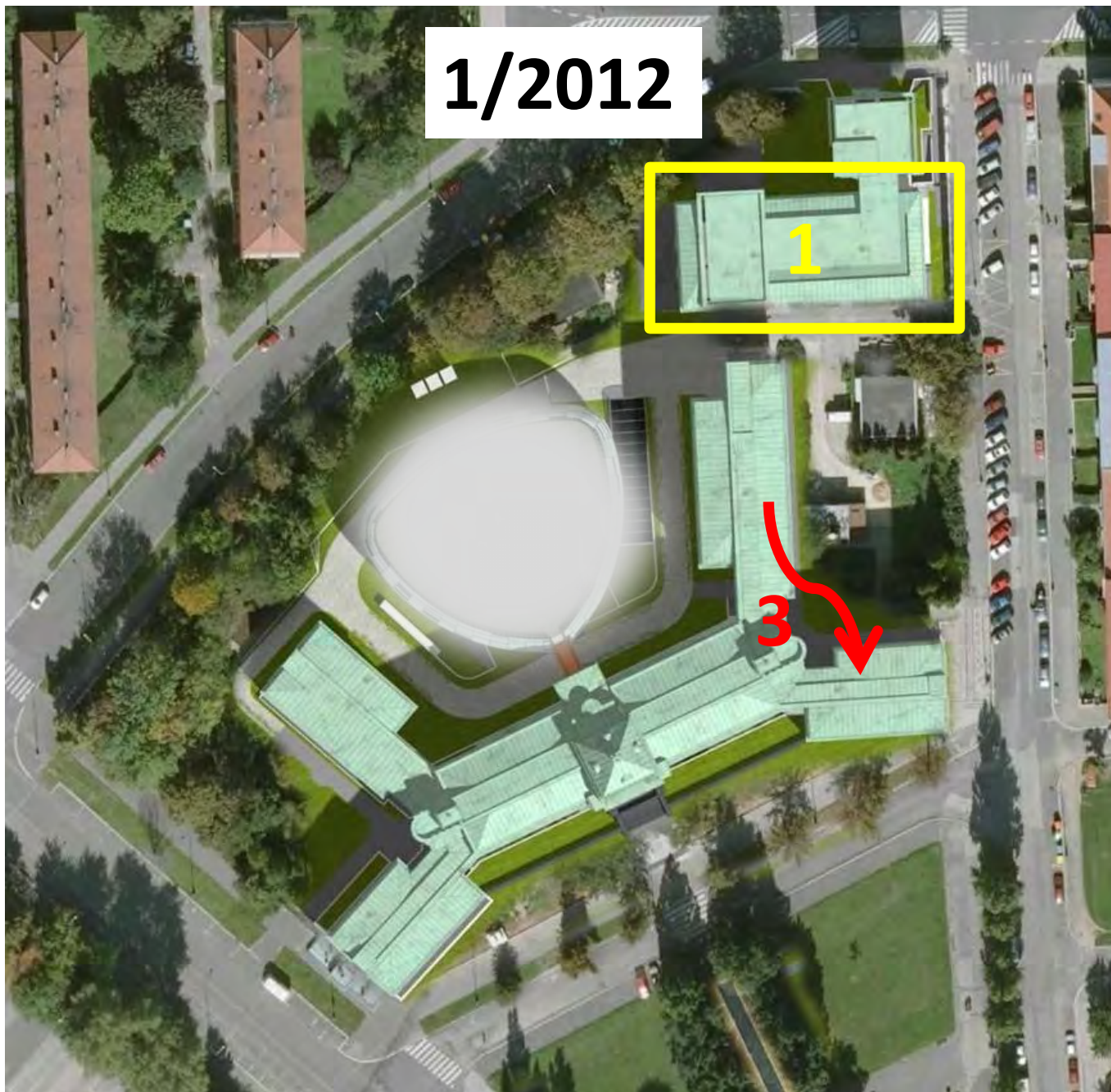


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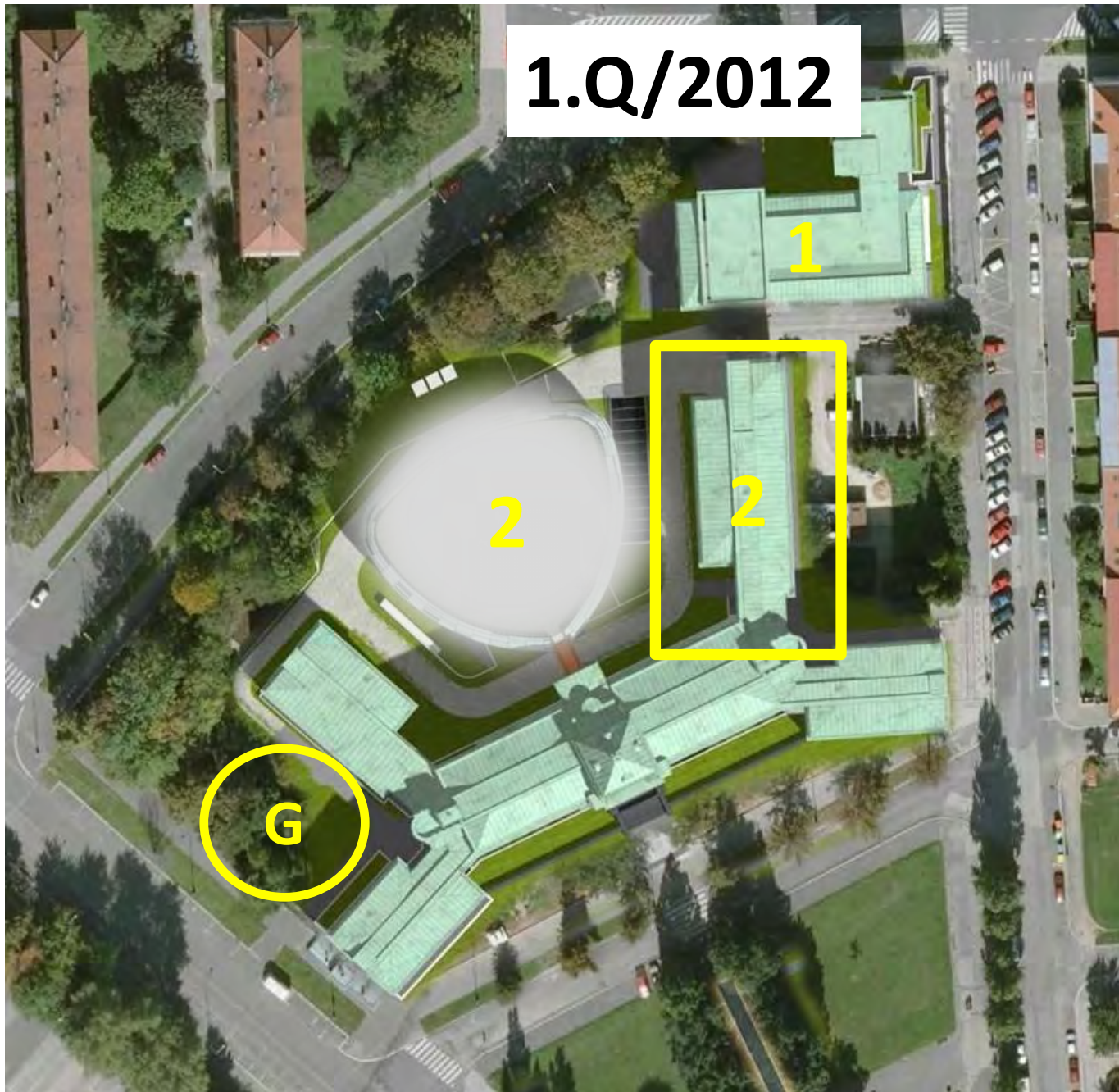
10/2011



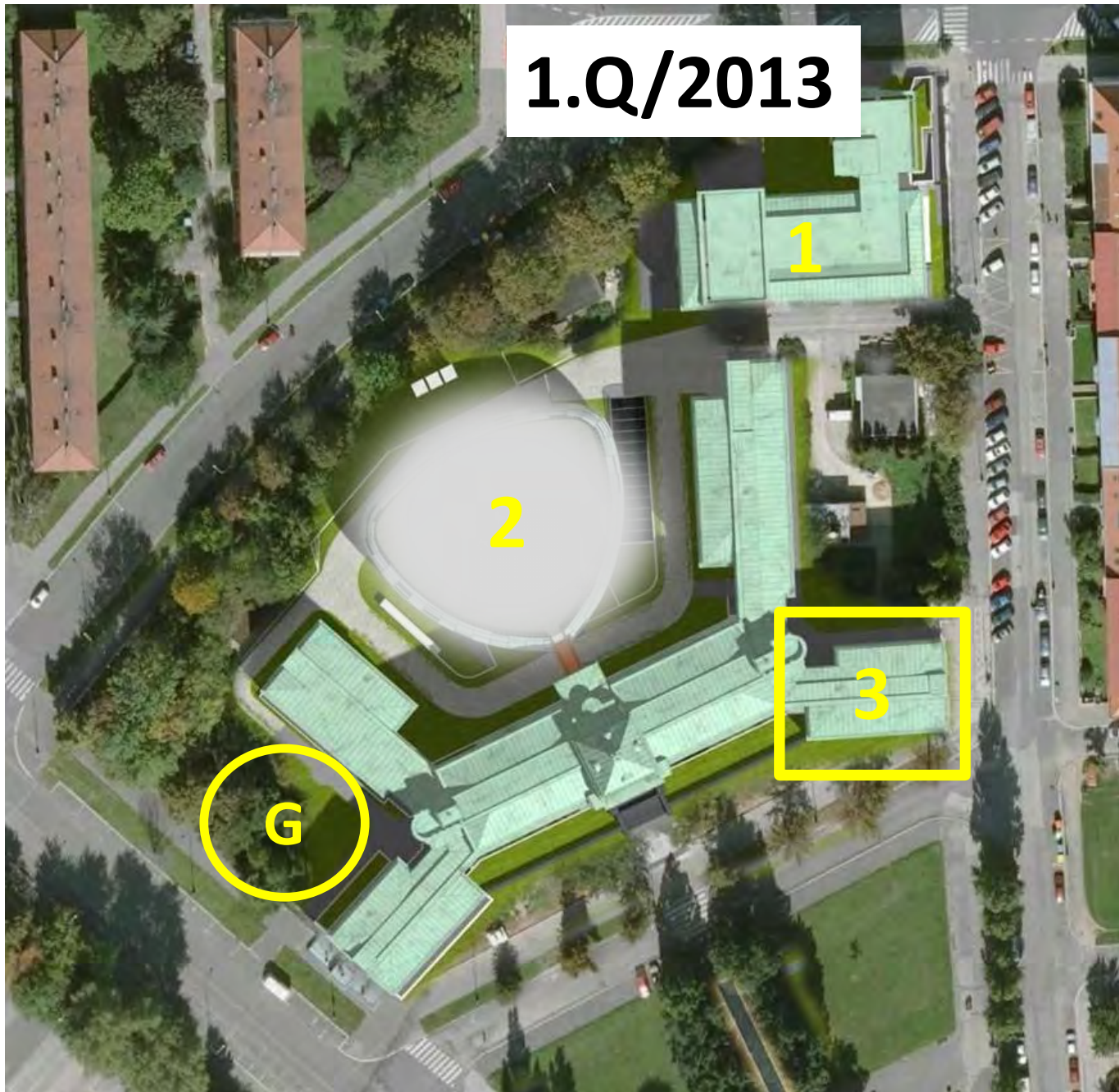
1/2012



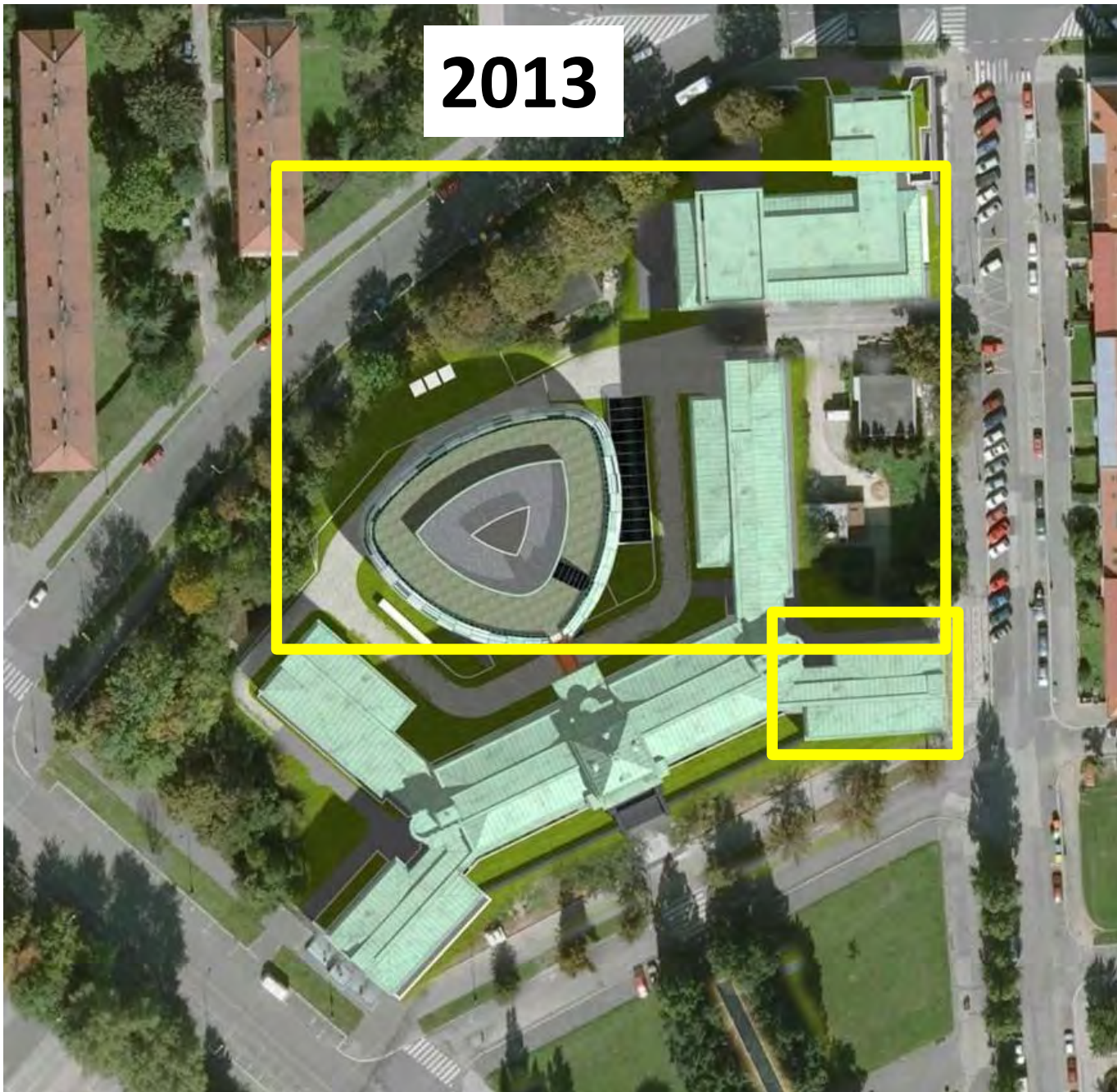
1.Q/2012



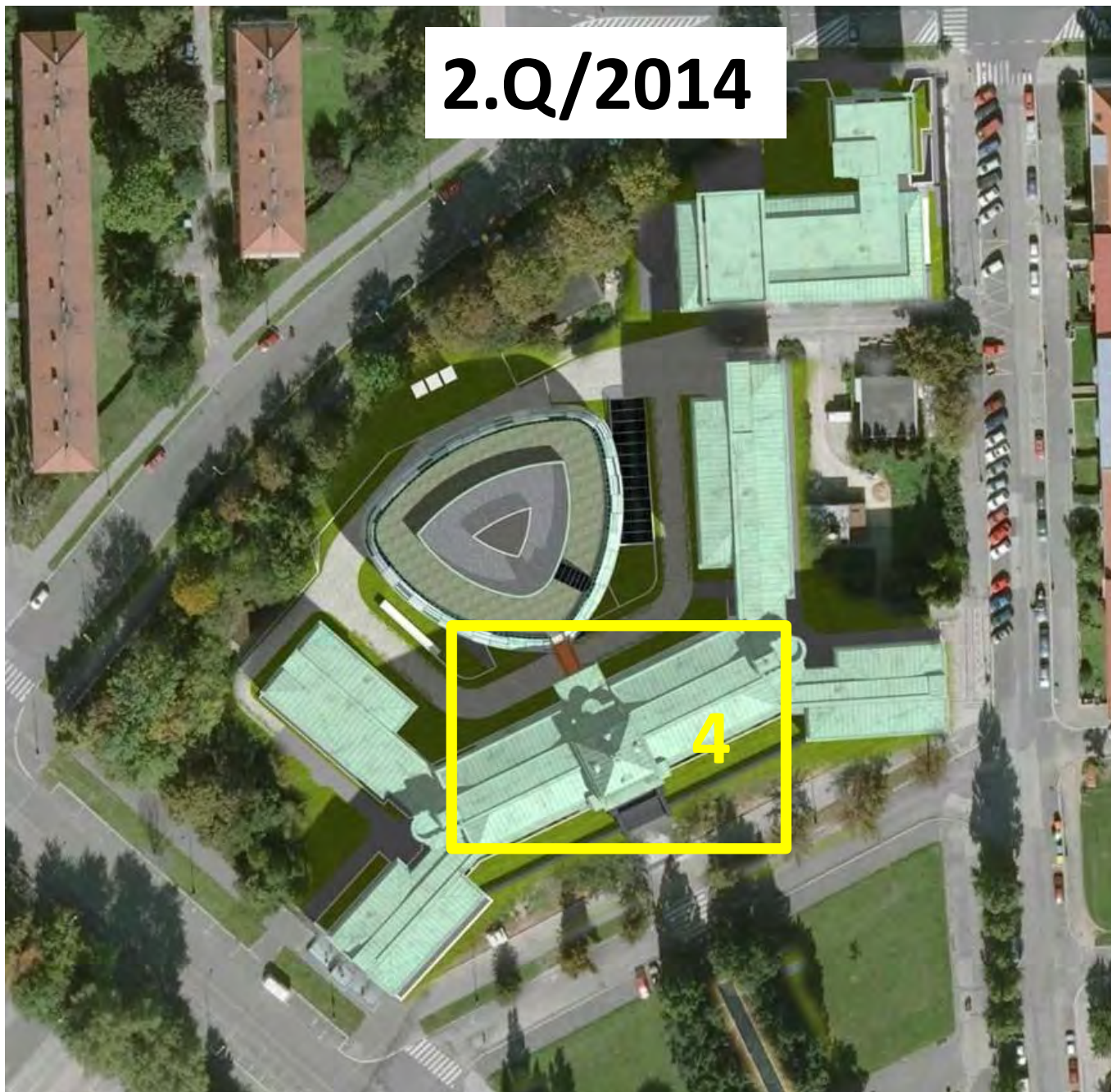
1.Q/2013



2013



2.Q/2014



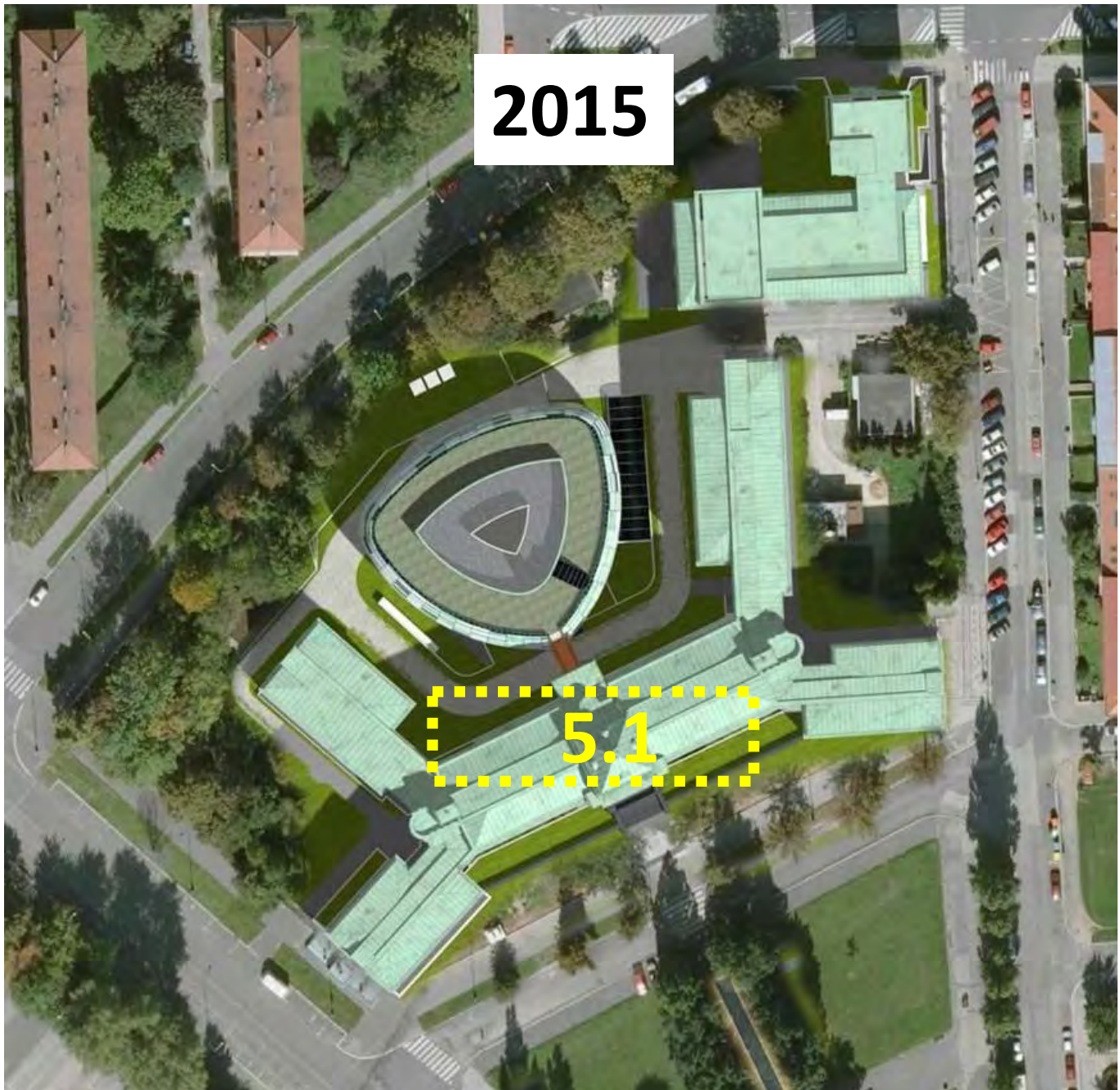
2014/15



5

2015

5.1



Rekonstrukce a dostavba areálu ÚOCHB AV ČR, v.v.i. harmonogram

BUDOVA „C“ – 9/2011

BUDOVA „B“ – polovina 2013

BUDOVA „A“ – 2014/15

Evaluation of the scientific teams

Reports: first week of December
Reviews: end of February
On-site meeting: third week of March
Results: end of March

Review reports: organized by Technipolis, UK



New International Advisory Board

Chairman:

Dr. Alexander Wlodawer, molecular crystallography

Members:

Prof. Karl-Heinz Altmann, pharmaceutical biology

Prof. Dr. Wilhelm Boland, chemical ecology

Prof. Cynthia J. Burrows, organic & biological chemistry

Prof. Dr. Burkhard König, organic chemistry

Prof. Dr. med Hans-Georg Kräusslich, virology

Prof. Ing. Dr. Marko D. Mihovilovic, organic chemistry, biocatalysis

Prof. Barry V. L. Potter, FMedSci, medicinal and biological chemistry

Prof. Dr. Walter Thiel, theoretical chemistry

Prof. Frank Turecek, physical chemistry, mass spectrometry



Postdoctoral and Sabbatical Programs

Meeting of the Selection Committee: September 29, 2011

Deadline for applications: September 21, 2011



CCCC

Collection will be converted into ChemPlusChem (Wiley)

Starting January 2012

Michal Hocek: co-chairman



Invited Lecture Series

October 19, 2011

Prof. Ada E. YONATH

Structural Biology Department, Weizmann Institute of Science, Rehovot, Israel

The Amazing Ribosome

November 24, 2011

Prof. Jeremy SANDERS

Department of Chemistry, University of Cambridge, Cambridge, UK

Adventures in Molecular Recognition: Dynamic Combinatorial Chemistry and Supramolecular Nanotubes



Chemický jarmark

Chemical Fair

Friday, September 23
Vítězné náměstí (Kulat'ák)

2011 – Year of Chemistry



Free discussion

