

Contents

Preface *xvii*

Part I Inspiration *1*

1	The Next Big Developments – The Lab of the Future	3
	<i>Richard Shute and Nick Lynch</i>	
1.1	Introduction	3
1.2	Discussion	3
1.2.1	People/Culture	4
1.2.2	Process	5
1.2.3	Lab Environment and Design	6
1.2.4	Data Management and the “Real Asset”	7
1.2.4.1	Data in the Hypothesis-driven, Research Lab	7
1.2.4.2	Data in the Protocol-driven Lab	8
1.2.4.3	New Data Management Developments	9
1.2.5	New Technology	11
1.2.5.1	Lab Automation Integration and Interoperability	12
1.2.5.2	Quantum Computing and the Lab of the Future	16
1.2.5.3	Impact of AI and ML	18
1.2.6	New Science	19
1.2.6.1	New Science in Health Care	19
1.2.6.2	New Science in the Life Sciences Domain	20
1.2.6.3	Other Important New Science Areas	21
1.3	Thoughts on LotF Implementation	22
1.4	Conclusion	22
	References	24

Part II Knowledge Base 33

2	Crucial Software-related Terms to Understand	35
	<i>Luka Murn</i>	
2.1	Digital Revolution	35
2.2	Computers	35
2.2.1	Programs, Instructions, and Programming Languages	37
2.2.2	Hardware and Software	38
2.2.3	Operating Systems	38
2.2.4	Abstraction	40
2.2.5	Virtualization	40
2.3	Internet	41
2.3.1	World Wide Web (WWW)	42
2.3.2	Web Applications	43
2.3.3	Web Applications in Comparison With Traditional Applications	44
2.4	Cloud Computing	47
2.4.1	Classification of Cloud Services	48
2.4.1.1	IaaS (infrastructure as a service)	49
2.4.1.2	PaaS (platform as a service)	49
2.4.1.3	SaaS (software as a service)	49
2.4.2	Cloud Deployment Models	50
2.4.2.1	Public Cloud	50
2.4.2.2	Private Cloud	51
2.4.2.3	Hybrid Cloud	51
2.4.3	Issues and Considerations	51
2.5	Computer Platforms	52
2.5.1	Desktop/Laptop/PC	53
2.5.1.1	Desktop Applications	53
2.5.2	Mobile	54
2.5.2.1	Mobile Applications	55
2.5.3	Server/Web	55
2.5.3.1	Web Browser	56
2.5.4	Embedded	56
2.5.5	Cross-platform	56
2.6	Applications	57
2.7	Values of Software	58
2.7.1	Features	58
2.7.2	Design	58
2.8	Software Development	58
2.9	Software Product Lifecycle	59
2.10	Software Design	61
2.10.1	Code	61
2.10.2	Data	63
2.11	Software Quality	64
2.12	Software Integration	65

2.12.1	API	66
2.12.2	Middleware	67
2.12.3	Authentication and Authorization	67
2.12.4	Internet of Things	67
2.13	Data-flow Modeling for Laboratories	67
2.14	Software Licensing	70
2.14.1	Proprietary Software Licenses	70
2.14.2	Open Source	70
	References	72
3	Introduction to Laboratory Software Solutions and Differences Between Them	75
	<i>Tilen Kranjc</i>	
3.1	Introduction	75
3.2	Types of Software Used in Laboratories	76
3.2.1	Electronic Lab Notebook (ELN)	76
3.2.2	Laboratory Information Management System (LIMS)	78
3.2.3	Laboratory Execution System (LES)	80
3.2.4	Laboratory Data Management System (LDMS)	80
3.2.5	Chromatography Data Management System (CDMS)	80
3.2.6	Process Analytical Technology (PAT) Software	81
3.2.7	Automation Scheduling Software	82
3.2.8	Laboratory Instrument Software	82
3.2.9	Middleware and Robotic Process Automation (RPA)	83
3.2.10	Data Analysis Software	83
3.2.11	Enterprise Resource Planning (ERP)	84
	References	84
4	Data Safety and Cybersecurity	85
	<i>Luka Murn</i>	
4.1	Introduction	85
4.1.1	Magnetic Storage	85
4.1.2	Solid-state Drives	86
4.2	Data Safety	86
4.2.1	Risks	86
4.2.2	Measures	87
4.2.2.1	Backups	87
4.2.2.2	Data Replication	88
4.3	Cybersecurity	88
4.3.1	Threat Model	89
4.3.1.1	Untargeted/Oppportunistic Attacks	89
4.3.1.2	Targeted Attacks	90
4.3.2	Risks	90
4.3.2.1	Physical Access	91
4.3.2.2	Software Access	91

- 4.3.2.3 Privileged Users 93
- 4.3.2.4 Data in Transit 93
- 4.3.2.5 Social Engineering 94
- 4.3.3 Measures 96
 - 4.3.3.1 Physical Protection 96
 - 4.3.3.2 Software and Infrastructural Measures 96
 - 4.3.3.3 Encryption 97
 - 4.3.3.4 Policies and Processes 99
 - 4.3.3.5 Education 99
 - 4.3.3.6 Third-party Security Review 100
- References 100

5 FAIR Principles and Why They Matter 101

Keith Russell

- 5.1 Introduction 101
- 5.2 What Is the Value of Making Data FAIR? 101
- 5.3 Considerations in Creating Lab-based Data to Prepare for It to Be FAIR 102
- 5.4 The FAIR Guiding Principles Overview 104
 - References 104

6 The Art of Writing and Sharing Methods in the Digital Environment 107

Lenny Teytelman and Emma Ganley

- 6.1 Introduction 107
- 6.2 Tools and Resources for Tracking, Developing, Sharing, and Disseminating Protocols 109
 - 6.2.1 Tools for Organizing and Tracking Your Protocols 109
- 6.3 Making Your Protocols Public 110
- 6.4 The Art of Writing Methods 111
 - References 113

Part III Practical 115

7 How to Approach the Digital Transformation 117

Jana Erjavec, Matjaž Hren, and Tilen Kranjc

- 7.1 Introduction 117
- 7.2 Defining the Requirements for Your Lab 118
 - 7.2.1 Digitization Versus Digitalization Versus Digital Transformation 118
 - 7.2.2 Defining the Approach and Scope for Your Lab – Digitization, Digitalization, or Digital Transformation? 119
 - 7.2.2.1 Which Challenges Do I Have Now? 120
 - 7.2.2.2 Which Challenges Need My Immediate Attention? 121
 - 7.2.2.3 Which Challenges Do I See in the Future? 121

7.2.2.4	What is My Long-term Business Strategy?	122
7.2.2.5	How Will Changes Affect My Current Business?	122
7.2.2.6	How Will I Manage Legacy Data?	123
7.2.2.7	How Will I Get People to Cooperate?	124
7.3	Evaluating the Current State in the Lab	124
7.3.1	Defining the Overall Goals of the Digitalized Laboratory	124
7.3.1.1	Example	124
7.3.2	Defining the Data Flows	125
7.3.3	Describing the Processes	127
7.3.4	Identifying the Bottlenecks	128
7.3.4.1	Bottlenecks in Data Flow Optimization	128
7.3.4.2	Efficiency and Integrity of Data Flows	128
7.3.4.3	Example: Make Data Machine Readable	129
7.3.5	Opportunities in Process Optimization	130
7.3.5.1	Time-consuming Processes	130
7.3.5.2	General Laboratory Processes	131
7.3.6	Gap Analysis	131
7.3.6.1	Example	132
	References	133
8	Understanding Standards, Regulations, and Guidelines	135
	<i>Matjaž Hren</i>	
8.1	Introduction	135
8.2	The Need for Standards and Guidelines	136
8.3	How Does Digitalization Relate to Standards and Guidelines	137
8.3.1	Standards Should Affect the Selection of the Tools for Digitalization	137
8.3.2	Digital Tools Promote Good Practices	138
8.4	Challenges Related to Digitalization in Certified Laboratories	140
8.5	Can Digital Strategy be Implemented without Certification?	141
	References	142
9	Interoperability Standards	143
	<i>Sören Hohmann</i>	
9.1	SiLA	144
9.2	AnIML	145
9.3	Allotrope	146
9.4	Conclusion	147
10	Addressing the User Adoption Challenge	149
	<i>Jana Erjavec</i>	
10.1	Introduction	149
10.2	Identify Key Stakeholders and Explain the Reasons for Change	151
10.3	Establish a Steering Committee	152
10.4	Define the Project Objectives, Expected Behaviour, and Timeline	153
10.5	Check for Understanding and Encourage Debate	154

10.6	Acknowledge Ideas and Communicate Progress	155
10.7	Provide a Feedback Mechanism	155
10.8	Set Up Key Experience Indicators and Monitor Progress	156
10.8.1	Happiness	156
10.8.2	Engagement	157
10.8.3	Adoption	157
10.9	Gradually Expand to a Larger Scale	158
10.10	Conclusions	159
	References	160

11 Testing the Electronic Lab Notebook and Setting Up a Product Trial 161

Blazka Orel

11.1	Introduction	161
11.2	The Product Trial	161
11.3	The Importance of a Product Trial	162
11.4	Setting Up a Product Trial	163
11.4.1	Phase I: Planning	163
11.4.2	Phase II: Conceptualization	164
11.4.3	Phase III: Testing	166
11.4.4	Phase IV: Reporting	170
11.5	Good Practices of Testing a Product	171
11.5.1	Taking the Time for Planning	172
11.5.2	Having a Bigger Picture in Mind	172
11.5.3	Keeping Your Testers Motivated	173
11.5.4	Systematic Evaluation of Products	173
11.5.5	Cooperating with Vendors	174
11.6	Conclusions	174
	References	175

Part IV Case Studies 177

12 Understanding and Defining the Academic Chemical Laboratory's Requirements: Approach and Scope of Digitalization Needed 179

Samantha Kanza

12.1	Types of Chemistry Laboratory	179
12.2	Different Stages of Digitalization	179
12.3	Preparatory Stage	180
12.3.1	Digitalization Requirements	181
12.3.2	Issues and Barriers to Adoption	181
12.3.3	Suggested Solutions	181
12.4	Laboratory Stage	182
12.4.1	Digitalization Requirements	182

- 12.4.2 Issues and Barriers to Adoption 183
- 12.4.3 Suggested Solutions 184
- 12.5 Transferal Stage 185
 - 12.5.1 Digitalization Requirements 185
 - 12.5.2 Issues and Barriers to Adoption 185
 - 12.5.3 Suggested Solutions 186
- 12.6 Write-up Stage 186
 - 12.6.1 Digitalization Requirements 186
 - 12.6.2 Issues and Barriers to Adoption 187
 - 12.6.3 Suggested Solutions 187
- 12.7 Conclusions and Final Considerations 188
- References 189

- 13 Guidelines for Chemistry Labs Looking to Go Digital 191**
Samantha Kanza
 - 13.1 Understanding the Current Setup 191
 - 13.2 Understanding Your Scientists and Their Needs 192
 - 13.3 Understanding User-based Technology Adoption 193
 - 13.4 Breaking Down the Barriers Between Science and Technology 195
 - 13.5 Making Your Laboratory Team Understand Why This Is Necessary 195
 - 13.6 Working with Domain Experts 195
 - 13.7 Choosing the Right Software 196
 - 13.8 Changing Attitude and Organization 196
 - References 197

- 14 Electronic Lab Notebook Implementation in a Diagnostics Company 199**
Casey Scott-Weathers
 - 14.1 Making the Decision 199
 - 14.2 Problems with Paper Notebooks 199
 - 14.3 Determining Laboratory's Needs 200
 - 14.4 Testing 201
 - 14.5 A Decision 201
 - 14.6 How to Structure the ELN 202
 - 14.7 Conclusion 203

- 15 Identifying and Overcoming Digitalization Challenges in a Fast-growing Research Laboratory 205**
Dorothea Höpfner
 - 15.1 Why Going Digital? 205
 - 15.2 Steps to Introduce ELNs in Lab Practice 207
 - 15.2.1 Step 1: Getting to Know the Market or What We Can Expect of an ELN 207
 - 15.2.2 Step 2: Defining the Needs of Our Lab and Our Requirements for an ELN 208

15.2.2.1	Data Structure	209
15.2.2.2	Compatibility with Databases	209
15.2.2.3	Flexibility of Documentation Style	209
15.2.2.4	Report Options	210
15.2.2.5	Speed	210
15.2.3	Step 3: Matching Steps 1 and 2 and Testing Our Best Options	210
15.2.4	Step 4: Getting Started in Implementing the ELN	211
15.3	Creating the Mindset of a Digital Scientist	213
15.4	The Dilemma of Digitalization in Academia	214
16	Turning Paper Habits into Digital Proficiency	217
	<i>Tessa Grabinski</i>	
16.1	Five Main Reasons for the Implementation of a Digital System to Manage the Research Data	217
16.1.1	Scale-up of the Laboratory	218
16.1.2	Protocol Management Issues	218
16.1.3	Environmental and Financial Factors	218
16.1.4	Introducing the Benefits of Technology to Younger Employees	219
16.1.5	Remote Access to Data by Authorized Supervisors	219
16.2	The Six-step Process of Going from Paper to Digital	219
16.2.1	Defining the Specific Needs of the Laboratory	219
16.2.2	Testing the Software and Defining the Standard Way to Use It	220
16.2.3	Organizing the Collaboration Between Lab Members and Supervisors	221
16.2.4	Managing Projects and Setting Up Work Processes	222
16.2.5	Versioning of Protocols and Keeping the Protocol Repository Up to Date	225
16.2.6	Choosing to Digitize Only New Projects	226
16.3	Onboarding All Team Members and Enhancing the Adoption of the New Technology in the Lab	226
16.4	Benefits of Switching from Paper to Digital	230
17	Going from Paper to Digital: Stepwise Approach by the National Institute of Chemistry (Contract Research)	231
	<i>Samo Andresek and Simona L. Hartl</i>	
17.1	Presentation of our CVTA Laboratory	231
17.2	Data Management Requirements Explained in Detail	231
17.2.1	Meaning of ALCOA	232
17.2.2	FDA and CFR 21 Part 11	233
17.2.3	MHRA and GxP Data Integrity Guidance and Definitions	233
17.2.4	Definition of Terms and Interpretation of Requirements	235
17.3	Going from Paper to Digital	240
17.4	Implementation of SciNote (ELN) to CVTA System	241
17.4.1	Some of CVTA user's Requirements (URS)	242

17.4.2	From Documentation Review and Approval to ELN Implementation	242
17.4.3	Step-by-Step Implementation of Change Control Management in SciNote	244
17.4.3.1	Creating Projects in SciNote	245
17.4.3.2	Creating a Workflow	245
17.4.3.3	Creating the Tasks and Protocol Steps	245
17.4.3.4	Filtering, Overview of Data and Inventory for Change Control Management	246
17.4.3.5	Audit Trail of Changes	246
17.4.3.6	Overview of all Activities	246
17.4.4	Organization and Signing of CVTA Documentation in ELN SciNote Due to User Roles and Permissions	250
17.4.4.1	Managing the Team Roles and Responsibilities within SciNote	250
17.4.4.2	Managing Projects for Efficient Work with Clients	250
17.5	Suggestions for Improvements and Vision for the Future	251
	References	251
18	Wet Lab Goes Virtual: In Silico Tools, ELNs, and Big Data Help Scientists Generate and Analyze Wet-lab Data	253
	<i>Jungjoon Lee and Yoonjoo Choi</i>	
18.1	CRISPR-Cas9 Explained	254
18.2	Introduction of the Digital Solutions and ELN into the Laboratory	255
18.3	The Role of the ELN and In Silico Tools in the Genome-editing Process	255
18.3.1	Designing sgRNA	255
18.3.2	Issues with Paper-based Processes and the Use of ELN	256
18.3.3	High-content Imaging for the Target Discovery	256
18.3.4	Plant Virtual Laboratory	257
18.4	The Role of the ELN and In Silico Tools in the Protein Design Process	258
18.4.1	Protein Modeling	258
18.4.2	Protein Redesign	259
18.4.3	Importance of Keeping the Electronic Records	260
18.4.4	Development of Therapeutic Antibodies	260
18.4.5	Importance of Electronic Lab Notebook for Communication Between Team Members	262
	References	263
19	Digital Lab Strategy: Enterprise Approach	265
	<i>Cesar Tavares</i>	
19.1	Motivation	265
19.1.1	Which Problem Do We Want to Solve?	265
19.1.2	New Problems Require New Answers	266
19.2	Designing a Flexible and Adaptable Architecture	267

- 19.3 There is Only One Rule: No Rules 269
- 19.4 The Lab Digitalization Program Compass 270
- 19.5 Conclusion 273
- References 273

Part V Continuous Improvement 275

- 20 Next Steps – Continuity After Going Digital 277**
Klemen Zupancic
- 20.1 Are You Ready to Upgrade Further? 277
- 20.2 Understanding the Big Picture 277
- 20.3 What to Integrate First? 279
- 20.3.1 Integrations 280
- 20.3.2 Laboratory Equipment – Concepts of IoT and Lab 4.0 281
- 20.3.2.1 Does the Equipment Support Integrations? 281
- 20.3.2.2 How Often Is the Instrument Being Used? 282
- 20.3.2.3 Is There a High Chance for Human Error? 282
- 20.3.2.4 Do You Need One- or Two-way Sync? 282
- 20.3.2.5 Is the Equipment Using Any Standards? 282
- 20.3.2.6 Is Equipment Cloud Connected? 282
- 20.3.3 Data Repositories 282
- 20.3.4 Data Analytics Tools 283
- 20.3.5 Other Types of Integrations 284
- 20.3.5.1 Scientific Search Engines and Literature Management 284
- 20.3.5.2 Data Sharing 284
- 20.3.5.3 Publishing 285
- 20.3.5.4 Upgrading Plans 285
- 20.4 Budgeting 285
- 20.5 Continuous Improvement as a Value 286
- References 286

Part VI Vision of the Future and Changing the Way We Do Science 287

- 21 Artificial Intelligence (AI) Transforming Laboratories 289**
Dunja Mladenic
- 21.1 Introduction to AI 289
- 21.1.1 Opportunities 289
- 21.1.2 Needs 290
- 21.1.3 Challenges 290
- 21.2 Artificial Intelligence in Laboratories 291
- 21.2.1 Data Preprocessing 291
- 21.2.2 Data Analytics 292

21.3	Process Monitoring	293
21.4	Discussion – Human in the Loop	294
	References	295
22	Academic’s Perspective on the Vision About the Technology Trends in the Next 5–10 Years	297
	<i>Samantha Kanza</i>	
22.1	Hybrid Solutions	297
22.2	Voice Technologies	298
22.3	Smart Assistants	298
22.4	Internet of Things	298
22.5	Robot Scientists	299
22.6	Making Science Smart – Incorporating Semantics and AI into Scientific Software	300
22.7	Conclusions	300
	References	301
23	Looking to the Future: Academic Freedom Versus Innovation in Academic Research Institutions	303
	<i>Alastair Downie</i>	
23.1	Introduction	303
23.2	Corporate Culture Versus Academic Freedom	303
23.3	Spoiled for Choice, but Still Waiting for the Perfect Solution	304
23.4	Building a Single, Shared Infrastructure for Research Data Management	305
23.5	A Journey of a Thousand Miles Begins with a Single Step	307
	Reference	308
24	Future of Scientific Findings: Communication and Collaboration in the Years to Come	309
	<i>Lenny Teytelman and Emma Ganley</i>	
24.1	Preprints: Reversing the Increased Time to Publish	309
24.2	Virtual Communities	310
24.3	Evolving Publishing Models	312
24.4	Funders Are Starting to Play a Role in Facilitating and Encouraging Rapid Sharing and Collaboration	312
24.5	Conclusion	314
	References	314
25	Entrepreneur’s Perspective on Laboratories in 10 Years	317
	<i>Tilen Kranjc</i>	
25.1	Data Recording	317
25.2	Recognition of Voice and Writing	318
25.3	Data Recording in the Future	318
25.4	Experimental Processes	318

25.5	Research Project Management	319
25.6	Experimental Planning	319
25.7	Virtual Reality	320
25.8	Smart Furniture	320
25.9	Experiment Execution	321
25.10	Laboratory Automation Trends	321
25.11	Cloud Laboratories	322
25.12	Data Analysis Trends	323
25.13	Artificial Intelligence	324
25.14	Data Visualizations and Interpretation	325
25.15	Databases	325
25.16	Conclusion	326
	References	326

Index	329
--------------	-----