

Index

A

Accuracy, 25, 58, 79, 106, 114, 118, 120, 135, 144, 147, 195, 224
Accuracy measures, 106
Amino acid, 2, 8, 211, 217, 218, 220
Artificial neural networks, 35, 36, 91, 95, 185, 188
Associative Experimental Design (AED), 34, 38, 39, 53, 223
Auto-focusing, 151, 152, 155
Auto-focusing, active, 155
Auto-focusing, passive, 155
Automated image scoring, 58, 83
AutoSherlock, 208

B

Batch method, 15
Bayesian classifier, 60, 87, 91, 95, 185, 189, 191, 192
Binding, 2, 54, 212, 213, 218
Binding analysis, 53
Binding reaction, 12
Bin – Recall, 51
Birefringent precipitate, 23
Boundary uniformity, 72
Bray–Curtis dissimilarity measure, 44
Bright spots, 23, 26

C

Categories of classification, 225
Categories of protein crystallization, 28, 58, 86, 105, 110, 126, 200, 205
Chemical cross linking, 217
Chemical distance, 43

Chemical space, 9–11, 33–35, 37, 43, 145, 200, 208, 224
Chemical space mapping, 208
Circular Dichroism (CD), 219
Classification, 29, 35, 58, 60, 75, 77, 86, 87, 94, 95, 103, 105, 126, 135, 146, 152, 175, 177, 185, 199, 224, 225
Classification accuracy, 75, 126, 189
Classification, 3-class (non-crystals, likely-leads, and crystals), 105
Classification, crystals, 69, 111
Classification, likely-leads, 110
Classification, non-crystals, 110
Clear drop, 28, 36, 58, 84, 86, 110
Cocktail distance coefficient (CD_{coeff}), 43
Convolutional neural networks, 115
Co-occurrence matrix, 97
Cryogenic Electron Microscopy (Cryo-EM), 214, 215
Crystal growth, 3, 27, 125, 127, 131, 135, 136, 140, 141, 144, 152, 178, 206, 223
Crystallization of complexes, 17, 145
Crystallization pathway, 3–6, 18, 57
Crystallization phase, 21, 84, 140, 202, 223
Crystallization screening, 2, 4, 5, 9, 11, 12, 14, 33, 46
Crystallization space, 10, 36
Crystal miss, 29, 75, 77, 79, 224
CrystalNet, 115, 116, 224
Crystal nucleation, 3, 5, 9, 26, 53, 226
Crystal size, 54, 126, 131, 132, 146, 153, 216
Crystal size growth, 139, 144, 147
Crystal symmetry, 213
Crystal X2, 46, 61, 63, 64, 68, 91, 103, 113, 117, 119, 131, 188, 193
CrystPro, 130, 144, 146

D

3D crystals, 26, 27
 3D crystals, large, 23, 28, 225
 3D crystals, small, 23, 28
 Decision tree, 60, 87, 91, 92, 118, 146, 182, 185, 188
 Deep convolutional neural network, 60, 87, 88
 Deep learning, 115, 224, 226
 Depth of field, 151, 153, 155
 Dialysis, 13
 Diffraction resolution, 18, 53, 145, 213
 Dimensionality reduction, 92, 118
 Diviner, 128
 Droplet boundary, 58
 Dye-binding assay, 128

E

Edge detection, Canny, 59, 93, 132–134, 179, 182
 Edge detection, Sobel, 59, 86, 93, 126, 169, 170, 172, 173, 175
 Emission filter, 62
 Emission spectrum, 218
 Emission wavelength, 63
 Euler angle, 215
 Euler number, 59, 86
 Excitation, 62, 68, 78
 Excitation source, 131
 Excitation wavelength, 63

F

Family of conditions, 40, 47, 49, 50, 53, 226
 Feature analysis, 88
 Feature extraction, 58, 59, 61, 64–66, 69, 70, 77, 78, 86–88, 91, 96, 103, 112–114, 119, 120, 126, 138, 152, 175, 178, 182, 185–189, 193, 195, 224
 Feature normalization, 92
 Feature reduction, 87, 91, 105, 106, 118
 Feature selection, 84, 92, 93, 107, 118, 119, 185, 194
 Features, graph, 101
 Features, histogram, 78, 83, 86, 88, 91, 96, 98, 106, 109–111, 114, 118, 119, 126, 185, 189, 194
 Features, histogram autocorrelation, 119
 Features, intensity, 69, 96, 118, 194
 Features, regions, 71, 78, 99, 106, 111, 119
 Features, shape adaptive, 101
 Features, spatiotemporal, 139

Features, texture, 59, 86, 88, 98, 112, 126, 185
 Femtosecond X-ray laser, 216
 Fluorescence microscopy, 61, 225
 Fluorescence Resonance Energy Transfer (FRET), 218
 Fluorescent probe, 12, 63, 126, 145, 218
 Focal stacking, 151, 156, 164, 165, 168
 Focal Stacking, Neighborhood Based (NBFS), 158
 Focal Stacking, Pixel Based (PBFS), 158
 Focal stacking, transformation based, 158
 FocusALL, 161, 164, 166, 172, 175, 225
 Full factorial design, 33, 34

G

Gabor wavelet, filter, 59, 86
 Genetic algorithm, 36, 59, 60, 87, 88
 Gray-level co-occurrence matrix, 59, 86, 126, 183
 Grayscale conversion, 67
 Green level co-occurrence matrix, 97
 Grid screening, 10, 11, 34, 35

H

Hampton's score, 91
 Harris Corner Response Measure (HCRM), 159, 160
 Heavy precipitate, 22, 26
 Hierarchical classification, 28, 105, 114, 116, 225
 High-throughput rate, 59, 87
 High-throughput system, 57, 58, 83, 125, 224, 226
 Histogram, 59, 96
 Hough transform, 59, 86, 88, 126
 Hydrophobic-binding dye, 218

I

Image acquisition, 62, 64, 78, 79, 113, 151, 154, 155, 204, 223
 Image down-sampling, 65
 Image processing, 16, 58, 59, 61, 64, 66, 79, 86, 88, 91, 93, 113, 126, 129, 132, 152, 202, 204, 215
 Image registration, 138
 Image segmentation, 64, 67, 177, 179, 224
 Image thresholding, 64, 68, 93, 99, 132, 147, 178, 179, 224, 226
 Incomplete factorial cocktails, 208
 Incomplete factorial design, 125

Incomplete factorial experiment, 10, 34, 36
Incomplete factorial screen, 11, 12, 35
INFAC, 11
Integral histogram, 59, 86
Integral membrane proteins, 17
Intensity histogram, 96, 97, 167, 179, 183
Intensity statistics, 59, 70, 86, 88, 100, 194
IXpressGenes, Inc., 46, 61, 64, 91, 103, 131, 188, 193, 200

L

Labile zone, 3–5, 7
Laplacian, 158, 194
Laplacian filter, 156
Laplacian pyramid filter, 59, 86, 126, 179
Light Emitting Diode (LED), 63, 131
Light precipitate, 24, 26
Light scattering, 5, 6, 212
Linear discriminant analysis, 60, 87, 120
Liquid–liquid diffusion screening, 13

M

MacroScope, 201
Max-Class ensemble method, 76
Mean Decrease in Accuracy (*MDA* – *RF*), 92, 93, 107
Measure of symmetry, 73
Metastable zone, 3, 4
Microcrystal, 28, 36, 58, 84, 86, 110, 126, 215
minimal-Redundancy-Maximal-Relevance (mRMR) criterion, 185
Misclassification, 29, 75, 76, 84, 88, 109, 119, 224
Multilayer perceptron neural network, 75, 76, 88

N

Naming inconsistency, 225
Needle crystals, 26, 27
Neural networks, 35
Neutron diffraction, 28, 54, 212
Noise removal, 66
Non-faceted crystals, 4, 23, 26, 28, 50
Nuclear Magnetic Resonance (NMR), 213, 214
Nucleation, 3, 6, 145
Nucleation event, 31
Nucleation rate, 9

O

Optimization, 18, 26, 36, 42, 47, 49, 53, 54, 57, 58, 63
Optimization crystallization conditions, 31
Optimization experiments, 16, 30
Optimization methods, 35, 40
Optimization of cocktails, 34, 35, 41
Optimization of conditions, 37, 39, 50, 126, 208
Optimization problems, constrained and unconstrained, 36
Optimization screen, 43, 45, 47, 49, 50
Optimization screening, 54
Optimization strategies, 22
Optimization tests, 9
Optimization trials, 131
Optimizing concentration values, 42, 45, 53
Optimizing conditions, 126

P

Phase diagram, 3
Phase separation, 22, 26, 29, 36, 40, 42, 84, 103, 110
Phase transition, 24, 26
Plate, 16, 21, 138, 152
Plate analysis, 145
Plate, crystallization, 24, 63, 128
Plate, crystallization screening, 12
Plate crystals, 27, 47, 111, 179
PlateDB, 208
Plate imaging system, 145
Plate, screening, 16
Plate view, 200, 207
Plate visualization, 200
Plate well, 200
Plate, 96-well, 64, 201
Plate, 1536-well, 201
Precipitate, 3–5, 23, 26, 28, 29, 36, 42, 58, 69, 77, 86, 126, 130, 154
Principle Components Analysis (PCA), 83, 91, 92, 106
Prioritization of reagents, 42
Prioritized cocktails, 43
Prohibited combinations, 41, 42
Protein crystallization, 1, 8, 18, 226
Protein molecule, 2, 8, 12, 126, 128, 213, 216

Q
Quenching, 145

R

Radon-Laplacian, 59, 86
Random forest, 60, 87, 95, 112, 116, 118, 185, 188
Random screen, 10, 11
Ranked category, 110
Ranking cocktails, 224
Ranking conditions, 50
Ranking features, 93, 118, 119
Ranking methods, 50
Ranking prioritized cocktails, 42, 43, 53
Real-time analysis, 64, 84, 88, 129
Real-time application, 113
Real-time autofocus, 156
Real-time classification, 195
Real-time classifier, 88
Real-time microscope, 223
Real-time system, 57, 126, 224
Region segmentation, 94, 129, 137
Robotic image acquisition, 57
Robotic methods, 14
Robotic microscopy, 60, 135
Robotic setup, 9, 16, 57, 61, 125
Robotic system, 57, 61, 83, 126
RoCKS, 200, 204, 205
Running time, 58, 59, 224

S

Scoring, 21, 22, 24, 26, 30, 31, 45, 51, 57, 131, 199, 200, 205
Scoring, expert, 85
Scoring, image, 78
Scoring, levels, 58
Scoring methods, 58
Scoring outcome, 39, 42, 46
Scoring procedure, 22
Scoring, real-time, 117, 119
Scoring scale, 21, 22
Scoring system, 36, 75, 91
Screen designing, 43
Screening analysis, 11, 22, 39, 47, 53, 223
Screening cocktails, 63
Screening conditions, 11
Screening experiments, 5, 8, 9, 14, 31, 34, 215, 226
Screening factors, 39
Screening, genetic algorithm, 12, 36
Screening, incomplete factorial design, 34
Screening kits, 9
Screening methods, 9, 10, 12, 34, 223, 224
Screening, neural networks, 35
Screening process, 8, 9

Screening solution, 21
Screening solution volume, 9
Screens, ranking, 50
Second virial coefficient, 5–7
Seed crystals, 50
Self-organizing neural networks, 60, 87, 88
Shape-adaptive Discrete Cosine Transform (SA-DCT), 101
Significance ratio, 43
Solubility line, 3, 7, 22
Soluble protein zone, 3
Soundness and completeness, 191, 195
Sparse matrix sampling, 10, 35
Sparse matrix screen, 10
Spatio-temporal analysis, 125, 130, 132, 135, 146, 223
Stochastic multiparameter optimization, 12
Super-thresholding, 178, 185, 188, 192, 195, 226
Super-thresholding, posteriori, 187, 189, 193
Super-thresholding, priori, 186, 189, 194
Supervised thresholding, 180
Support Vector Machines (SVM), 60, 87, 91, 95, 118
Symmetry, 8

T

Temporal analysis, 128, 129
Thresholding, global, 178
Thresholding, green percentile, 67, 68, 94, 179
Thresholding, local, 178
Thresholding, morphological, 94
Thresholding, Otsu's, 67, 76, 77, 93, 114, 132, 136, 177, 185, 189
Time analysis, 103, 106, 193
Timing analysis, 75, 112, 116
Trace fluorescent labeling, 12, 17, 26, 39, 61, 69, 91, 113, 119, 125, 131, 145, 207, 208, 226

V

Vapor diffusion, 14
Vector quantization, 60, 87
Visualization, 199
Visualization display, 225
Visualization interface, 199, 204
Visualization software, 199, 200, 203
Visualization, plate well, 203
Visualization, screening results, 16
Visualizaton, color coding, 201, 204, 207

Visualizaton, glyphs, [202](#)
Visualizaton, multiple light sources, [207](#)
Visualizaton, region-of-interest, [202](#)
Visualizaton, sequential view, [207](#)
Visualizaton, thumbnails, [200](#)
Visualizaton, time course, [206](#)
Visual-X2, [200](#), [203](#), [205](#)
Vollath-F4, [156](#), [169](#), [172](#)
Vollath-F5, [156](#)

W
Well-plate, [61](#), [125](#)

X
X-ray beam, [127](#)
X-ray crystallography, [1](#), [126](#), [213](#)
X-ray diffraction, [10](#), [57](#), [153](#), [211](#)
X-ray Free Electron Laser (XFEL), [215](#), [216](#)
XtalPIMS, [200](#), [206](#), [207](#)