

Supporting Information: Cluster Analysis

A Day in the Life: Characterization of Doctoral Bench Research in Synthetic Chemistry using Phenomenological Case Studies

Elizabeth W. Kelley*

Chemistry Department, University of Chicago, 5735 S Ellis Ave, Chicago, IL, 60637, USA

*ewkelley@uchicago.edu

CONTENTS

- CrossTabs count data for Equipment, Technique, and Purpose codes p. 2-4
 - The count data was used to conduct the cluster analysis.
- Cluster silhouette values and cluster sizes p. 5
 - Silhouette values demonstrate the fit of the cluster analysis for an 8-cluster model.
- Cluster count composition graphs p. 6-9
 - These graphs illustrate the codes which clustered into each cluster and the proportion they represent of their overall code categories.

Table S5. CrossTabs between Equipment and Purpose.

	PURPOSE	Analyze results	Avoid contamination	Enable next step only	Enable repetition via measurements	Enable repetition via records	Maintain work relationships	Maximize product yield	Optimization - analyze results	Optimization - avoid contamination	Optimization - enable repetition via measurements	Optimization - maximize product yield	Optimization - purify product	Optimization - synthesize product	Preserve amount of supply	Preserve product integrity	Protect equipment	Protect people	Purify product	Reduce personal annoyance	Synthesize product	TOTAL
EQUIPMENT	REF #	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	
Automated column	E1					4	1				4	2	13						15			35
Balance	E2				65															2		71
Calculator	E3	1			1	16															17	35
Column	E4		2									1							16			19
Computer	E5	116											1								1	118
Fridge	E6															1						1
Fume hood	E7		18	1				1		5		1	6				50	1	5	74		162
Glovebox	E8		7	18													2					27
Heat gun	E9	4	3										5									12
Human body	E10	4	64					70	6	23	1	21	37	18			2		55			301
In-house utilities	E11		5				26											2				33
Monkey bars & clamps	E12									1		1	11				3				32	48
Oven	E13		6																			6
Phone	E14					10			4					1							1	16
PPE	E15																	75		6		81
Propane torch	E16		3																			3
Records	E17	33				49	8		9		2			2		10		1		2	1	117
Rotatory evaporator	E18		8									61	119				2		8			198
Schlenk line	E19		12	5								2	9				6		9			45
Solvent system	E20		1					1							1							3
Sonicator	E21		2									10										12
Standard glassware	E22		1	1			4		1	1		66	6	19	1				64			164
Static gun	E23										8			1								9
Stir plate & bar magnet	E24													6			5					11
Sundry items	E25	1	21	1			3	2	32	2		14	11	4	12	1	5	5		4	9	127
Temperature bath	E26													4	1						6	11
TLC chamber & stain	E27	16							2													18
Transfer tools - gas	E28		13		1																	14
Transfer tools - liquid	E29	52	156	12	10		1	83	15			1	8		3		8	2	63	1	55	470
Transfer tools - solid	E30	15	34		10		2	2	3	40	15	7		11	1		11	7	14	9	33	214
UV lamp	E31	16							9													25
Waste collector	E32		9															32				41
TOTAL		258	365	38	87	79	45	159	81	72	30	187	226	66	21	12	94	125	249	98	155	2447

Table S6. CrossTabs between Equipment and Technique.

		Table of Cross-tab between Equipment and Technique																															
	TECHNIQUE	Air-free mass transfer	Airstream evaporation	Chemical drawing software usage	Cleaning & waste disposal	Column chromatography	Dissolution	Glassware drying	Glovebox operation	Inventory management	Laboratory & workspace management	Light-sensitive reaction management	Liquid-liquid extraction	Literature searching	Mass measurement - liquid	Mass measurement - solid	Mass transfer - liquid	Mass transfer - phase change	Mass transfer - solid	NMR analysis	NMR sample preparation	Notebook management	PPE management	Rotatory evaporation	Schlenk line operation	Solution drying & gravity filtration	Solvent system operation	Sonication	Temperature bath manipulation	Thin-layer chromatography	Vacuum filtration	TOTAL	
EQUIPMENT	REF #	T 1	T 2	T 3	T 4	T 5	T 6	T 7	T 8	T 9	T 10	T 11	T 12	T 13	T 14	T 15	T 16	T 17	T 18	T 19	T 20	T 21	T 22	T 23	T 24	T 25	T 26	T 27	T 28	T 29	T 30		
Automated column	E1				1	34																										35	
Balance	E2														2	69																71	
Calculator	E3																					34								1		35	
Column	E4				2	17																										19	
Computer	E5			1		1								3							113											118	
Fridge	E6									1																						1	
Fume hood	E7		7		23	5				1	123	1													1						1	162	
Glovebox	E8							1	26																							27	
Heat gun	E9				3																				5						4	12	
Human body	E10	1			23	17	35	3		3	2		83			9	1	4	33		1			10	34	1			3	31	7	301	
In-house utilities	E11				3						1												3	26								33	
Monkey bars & clamps	E12		9								39																					48	
Oven	E13							6																								6	
Phone	E14																					12								4		16	
PPE	E15										3												78									81	
Propane torch	E16							3																								3	
Records	E17								7	12						2					8	50					3			35		117	
Rotatory evaporator	E18																							198								198	
Schlenk line	E19																								45							45	
Solvent system	E20																										3					3	
Sonicator	E21																											12				12	
Standard glassware	E22					15				1	1		109				7	2	9		1			2	4	6					7	164	
Static gun	E23															8			1													9	
Stir plate & bar magnet	E24				3		5				1													2								11	
Sundry items	E25	1			6				6	14	25	2	6						9				2	18	8					30		127	
Temperature bath	E26																2												9			11	
TLC chamber & stain	E27																													18		18	
Transfer tools - gas	E28		13												1																	14	
Transfer tools - liquid	E29		15		154	14	7			14			65		26		56		9		18			33	4	1	1		1	47	5	470	
Transfer tools - solid	E30				33	15	2	2	9							4			66				16	2	3			2	57	3	214		
UV lamp	E31																													25		25	
Waste collector	E32				41																											41	
TOTAL			39	7	1	292	118	49	15	48	46	195	3	263	3	29	92	64	8	127	113	28	96	83	305	103	11	7	12	15	252	23	2447

Numbers are squished vertically to fit on the page (e.g., $\frac{1}{3}$ is 13).

Table S7. CrossTabs between Technique and Purpose.

	PURPOSE	Analyze results	Avoid contamination	Enable next step only	Enable repetition via measurements	Enable repetition via records	Maintain work relationships	Maximize product yield	Optimization - analyze results	Optimization - avoid contamination	Optimization - enable repetition via measurements	Optimization - maximize product yield	Optimization - purify product	Optimization - synthesize product	Preserve amount of supply	Preserve product integrity	Protect equipment	Protect people	Purify product	Reduce personal annoyance	Synthesize product	TOTAL
TECHNIQUE	REF #	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	
Air-free mass transfer	T1		14															1			24	39
Airstream evaporation	T2											1	1						4	1		7
Chemical drawing software usage	T3																				1	1
Cleaning & waste disposal	T4		242				3		1	6							3	36		1		292
Column chromatography	T5					4	2	6		1		10	29						66			118
Dissolution	T6							41				2		5							1	49
Glassware drying	T7		10											3				2				15
Glovebox operation	T8		12	18			5										2			11		48
Inventory management	T9		6	12			4					5			1	12		2		2	2	46
Laboratory & workspace management	T10		4	2					2	3		1	22	5	1		53	2		77	23	195
Light-sensitive reaction management	T11							2				1										3
Liquid-liquid extraction	T12	1	19				2	24				79	1				4		133			263
Literature searching	T13	3																				3
Mass measurement - liquid	T14				13			9													7	29
Mass measurement - solid	T15		9		67						14									2		92
Mass transfer - liquid	T16	4						26			1	1		6	2				3		21	64
Mass transfer - phase change	T17													8								8
Mass transfer - solid	T18		6		6			23	1		15			26	1				1		48	127
NMR analysis	T19	113																				113
NMR sample preparation	T20	17	1						9										1			28
Notebook management	T21	1				74								3							18	96
PPE management	T22		3															77		3		83
Rotatory evaporation	T23		12				26	15		2		71	129		10		22	5	13			305
Schlenk line operation	T24		21	5						1		3	44	6	2		10		10	1		103
Solution drying & gravity filtration	T25							2											9			11
Solvent system operation	T26		1				3	1							1						1	7
Sonication	T27		2									10										12
Temperature bath manipulation	T28											1		4	1						9	15
Thin-layer chromatography	T29	119	2		1	1			68	59					2							252
Vacuum filtration	T30		1	1				10				2							9			23
TOTAL		258	365	38	87	79	45	159	81	72	30	187	226	66	21	12	94	125	249	98	155	2447

Figure S2. Cluster Sizes for an 8-Cluster Model.

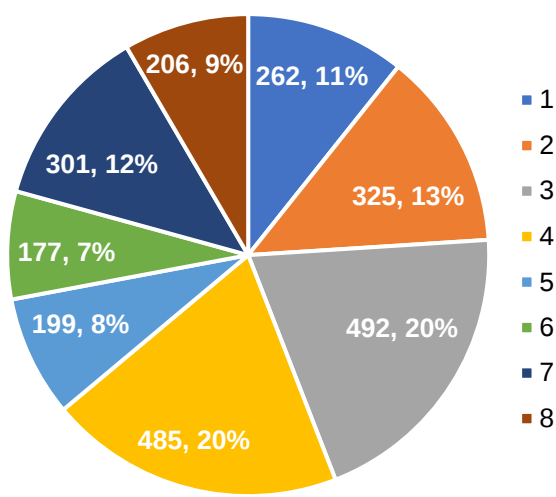
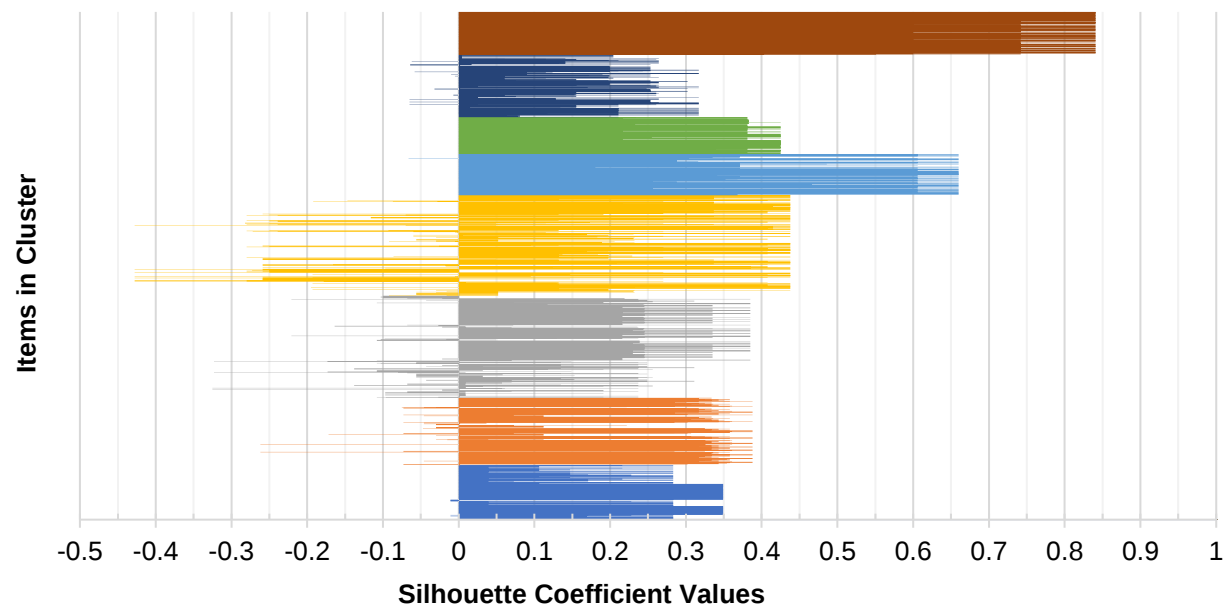


Figure S3. Silhouette Values for an 8-Cluster Model.



Average $k = .2670$ (8-cluster local maximum k after testing up to 10 clusters)

Figure S4. Summary of Cluster 1: Analyzing NMRs and Preparing Chemicals.

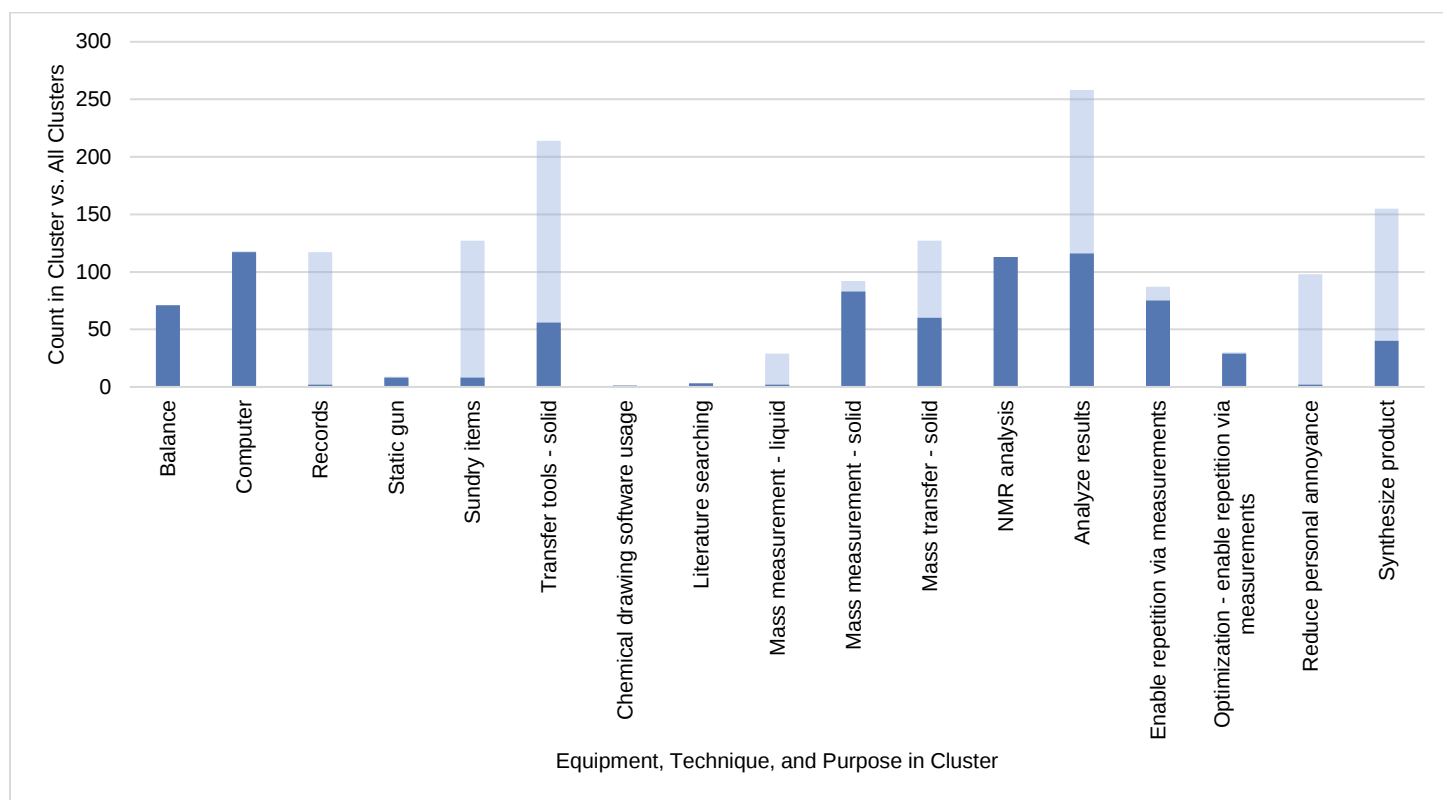


Figure S5. Summary of Cluster 2: Making NMR Samples and Running TLCs.

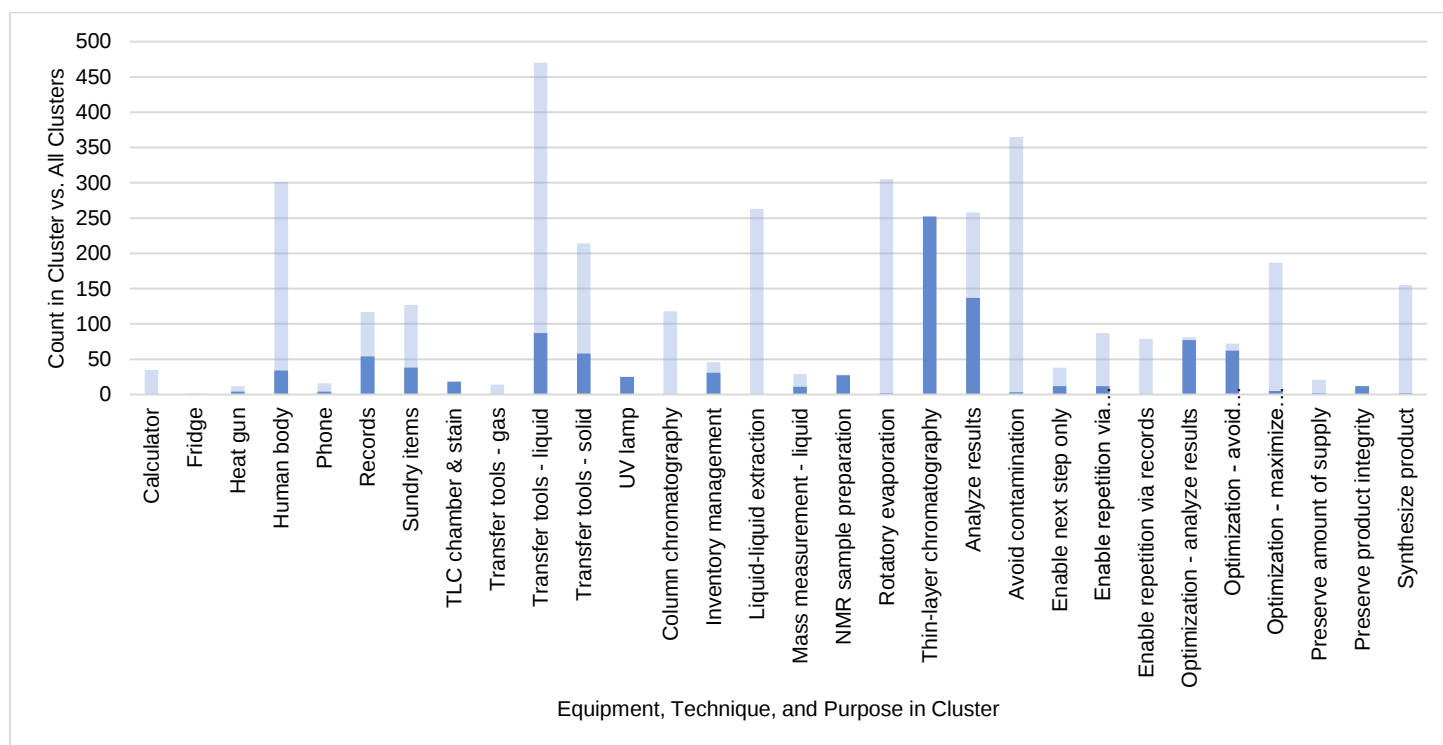


Figure S6. Summary of Cluster 3: Purifying Crude Mixtures.

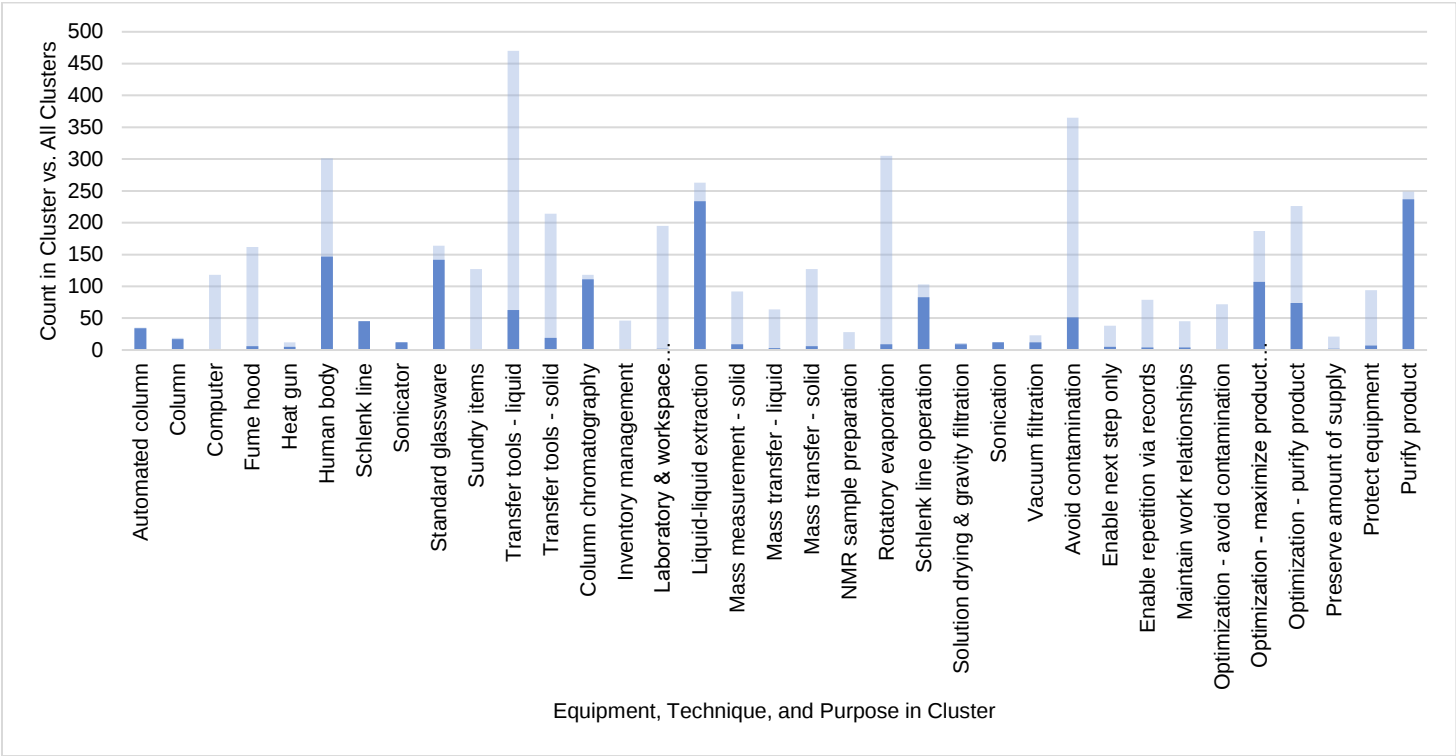


Figure S7. Summary of Cluster 4: Using Scientific Equipment and Room Infrastructure.

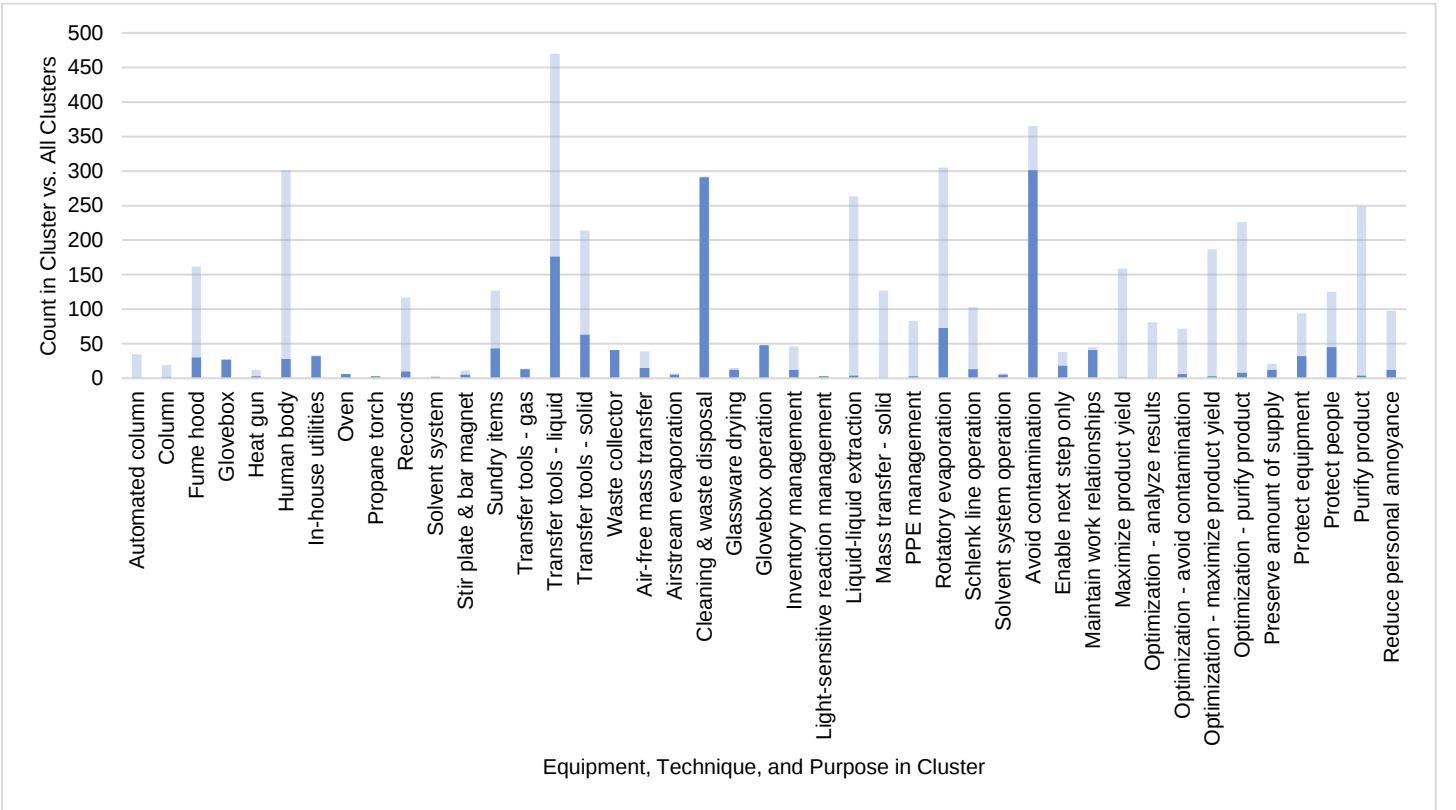


Figure S8. Summary of Cluster 5: Working in a Fume Hood.

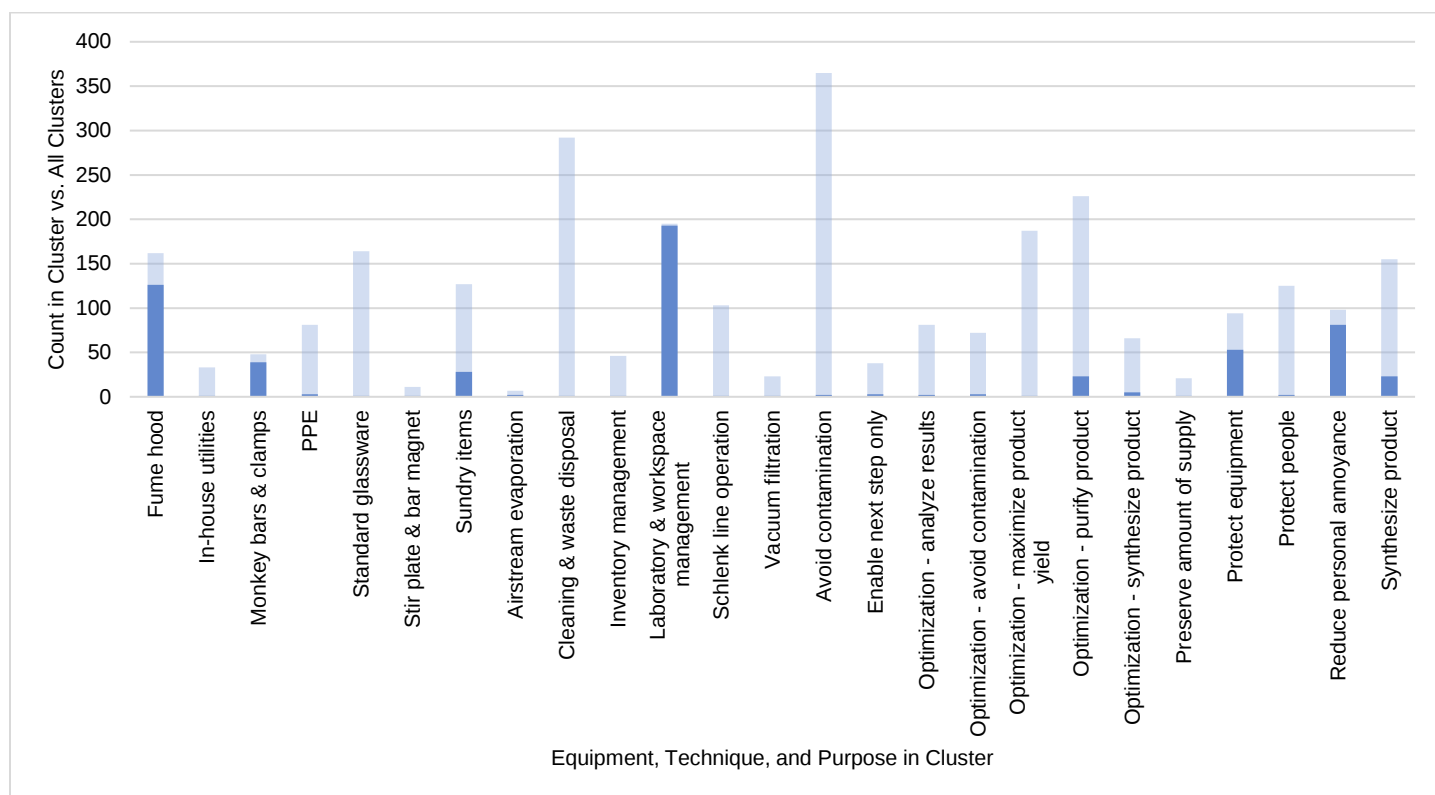


Figure S9. Summary of Cluster 6: Staying Safe and Using a Notebook.

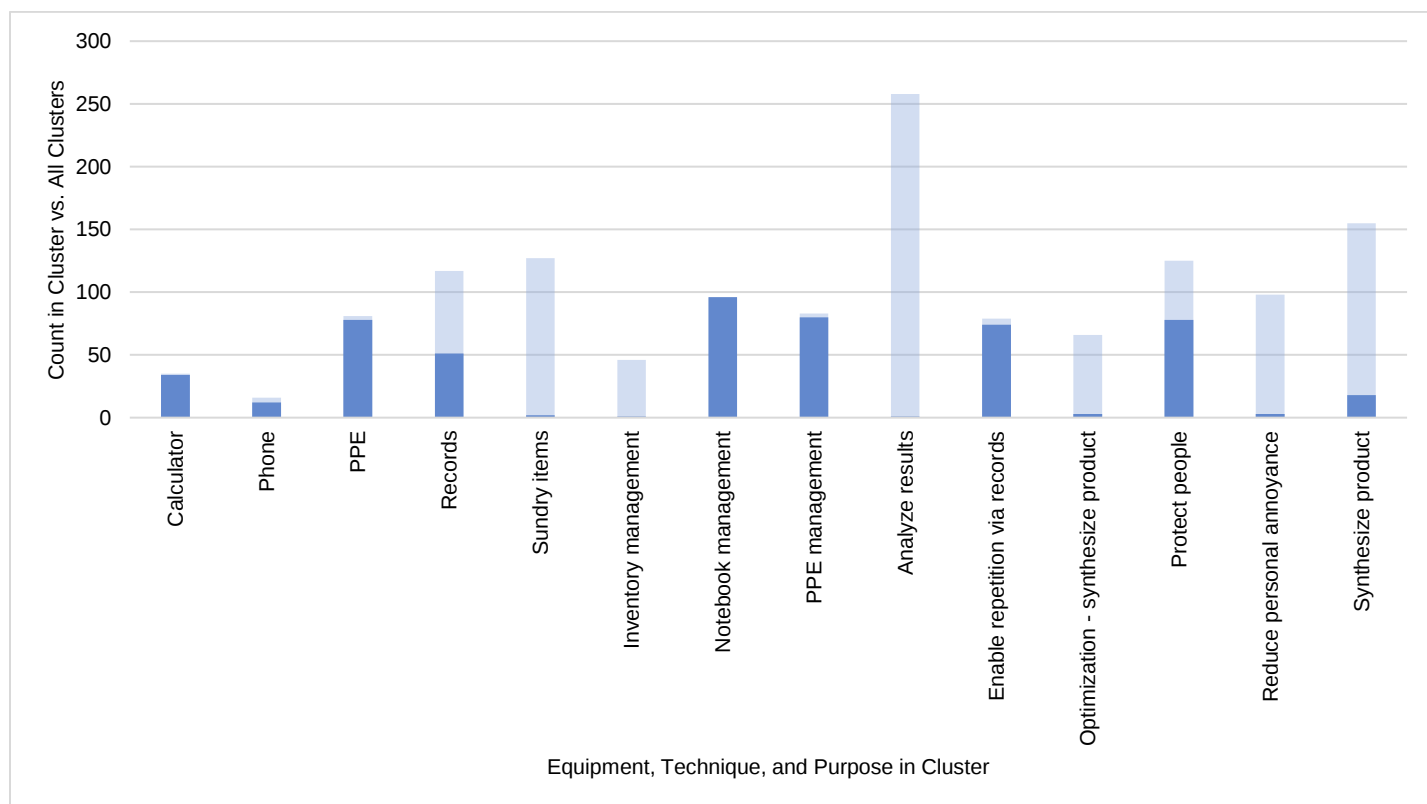


Figure S10. Summary of Cluster 7: Setting up and Monitoring Reactions.

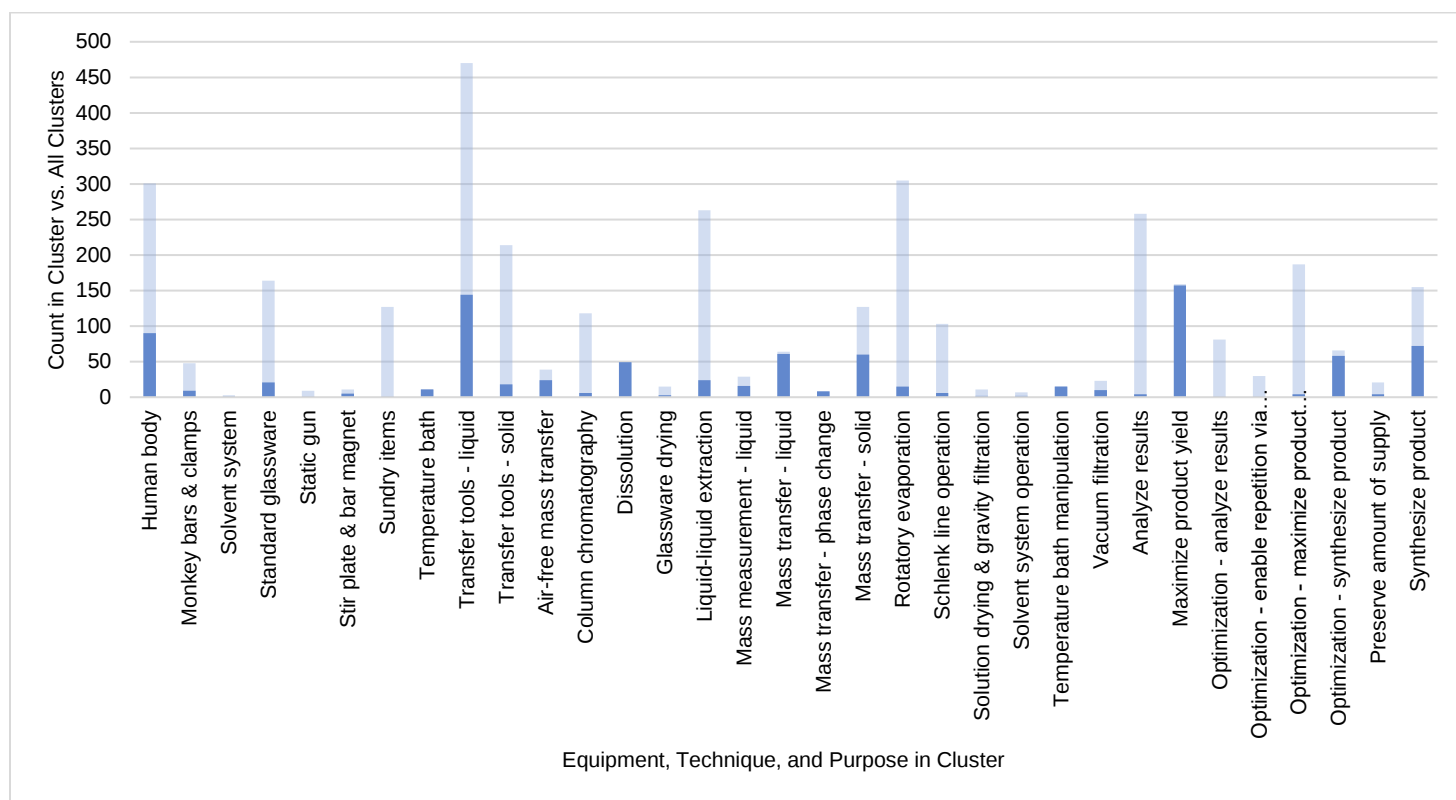


Figure S11. Summary of Cluster 8: Rotatory Evaporating.

