Investigation of the prognostic value for metabolic and Raman spectroscopic erythrocyte profiling in sepsis

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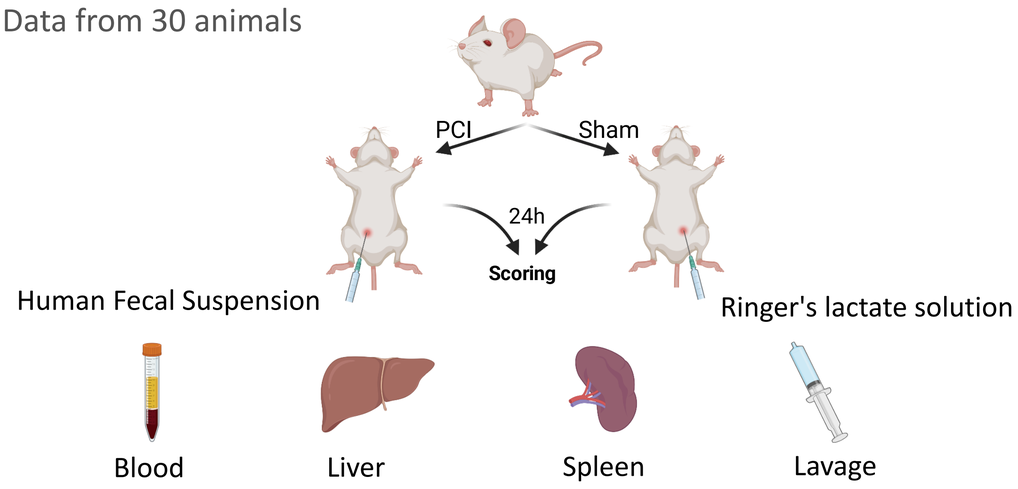
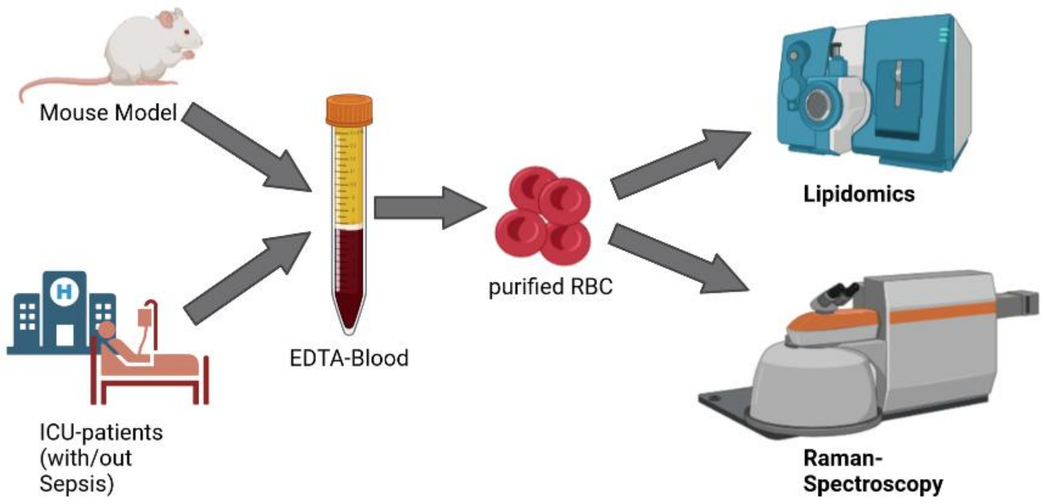
Experimental setup and data collection

- PCI mouse model for investigation of possible biomarkers in sepsis
- Focus on the spectral composition of red blood cells (RBCs)
- Data collection via lipidomics and Raman spectroscopy
- Data from 30 animals





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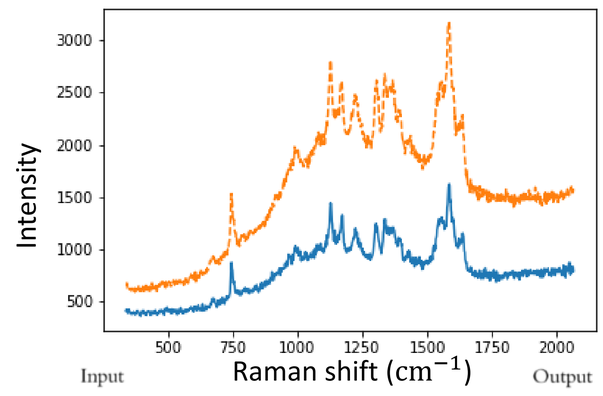
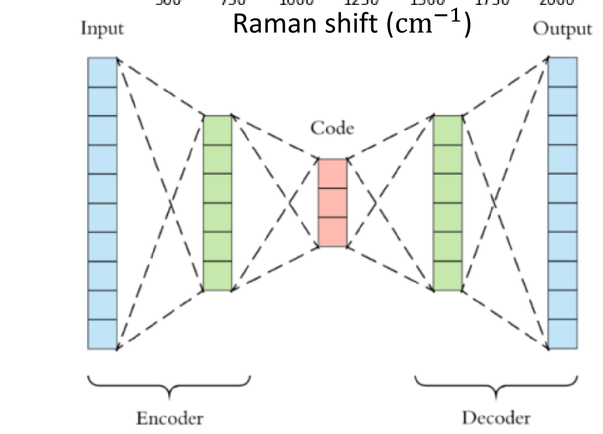
Data fusion

- Lipid data is naturally tabular
- Raman data is high-dimensional and needs to be merged with tabular data
- Preprocessing of Raman data: Whittaker baseline subtraction and area-under-the-curve normalization
- Preprocessing of lipidomic data: area-under-the-curve normalization
- Use of an autoencoder to convert Raman spectra to tabular form

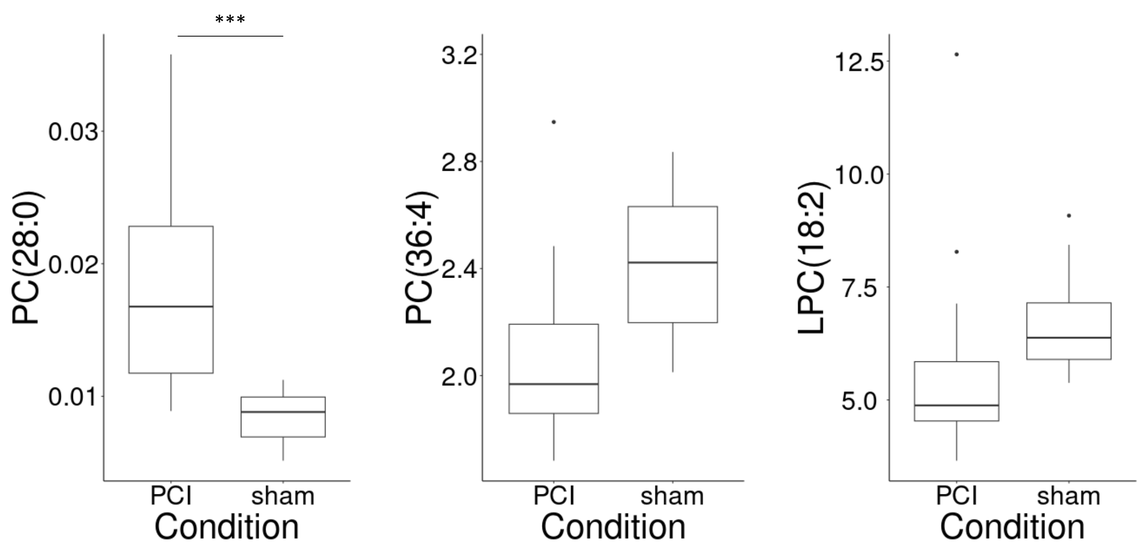
ANEST	License	d18:1 So	d18:1 So1P	C12 SM	C14 SM	C16 SM	C18:1 SM	C18:0 SM	C20 SM	C22 SM	C24:1 SM	C24 SM	C26:1 SM	Raman Dim 1	Raman Dim 2	Raman Dim 3
73925	UKJ-19-010	0,56	4,00	0,57	5,52	21,64	0,82	6,34	15,47	61,03	233,16	99,06	10,67	0,40	0,25	7,13
73927	UKJ-19-010	0,52	4,18	0,96	4,89	20,08	1,36	7,43	16,97	53,19	170,47	75,46	8,18	0,36	0,23	5,37
73928	UKJ-19-010	0,40	2,57	0,51	3,22	25,60	1,94	7,36	18,92	54,24	177,04	83,31	8,57	0,35	0,20	3,67
73929	UKJ-19-010	0,74	3,43	0,95	5,23	19,20	1,30	6,67	15,79	38,77	128,98	59,67	6,02	0,28	0,21	7,46
73984	UKJ-19-010	0,42	2,22	0,21	3,63	14,54	0,78	5,50	14,32	46,87	164,20	73,78	7,81	0,32	0,23	5,34
73985	UKJ-19-010	0,73	1,65	0,29	4,15	17,25	1,18	4,59	14,77	44,08	156,23	73,86	8,12	0,27	0,21	6,43
73876	UKJ-19-010	1,15	4,99	1,33	5,75	53,71	2,30	28,16	121,23	395,14	989,77	460,36	46,80	0,47	0,37	4,51
73877	UKJ-19-010	1,38	1,11	0,17	2,54	23,69	1,30	5,72	17,05	55,54	157,46	69,34	6,03	0,35	0,21	5,27
73878	UKJ-19-010	2,30	0,69	0,26	1,27	33,27	2,47	8,26	16,27	54,44	134,54	71,65	5,45	0,25	0,18	6,16
73965	UKJ-19-010	2,98	2,24	0,11	2,57	12,82	0,64	3,27	8,68	32,96	78,87	38,31	3,75	0,51	0,29	11,63
73966	UKJ-19-010	0,79	6,12	2,02	13,76	60,28	5,25	34,65	163,82	519,99	1679,60	796,09	82,83	0,68	0,44	7,23
73968	UKJ-19-010	0,91	5,81	1,37	4,82	35,66	4,38	26,31	77,31	229,55	716,21	329,64	41,05	0,42	0,31	5,43

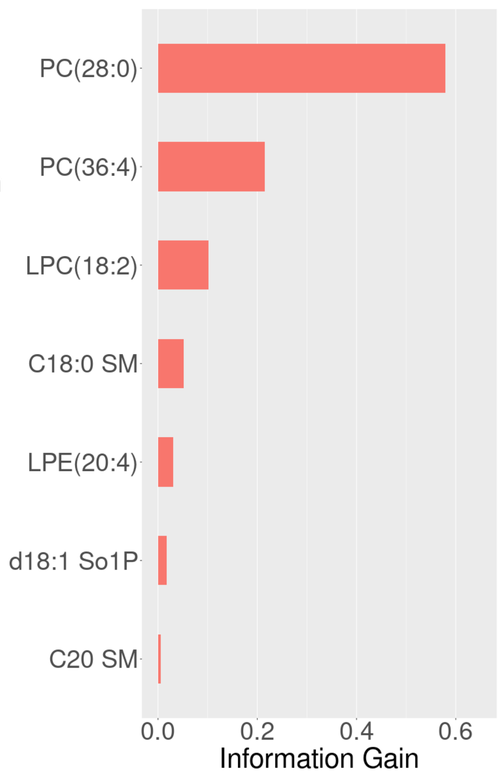


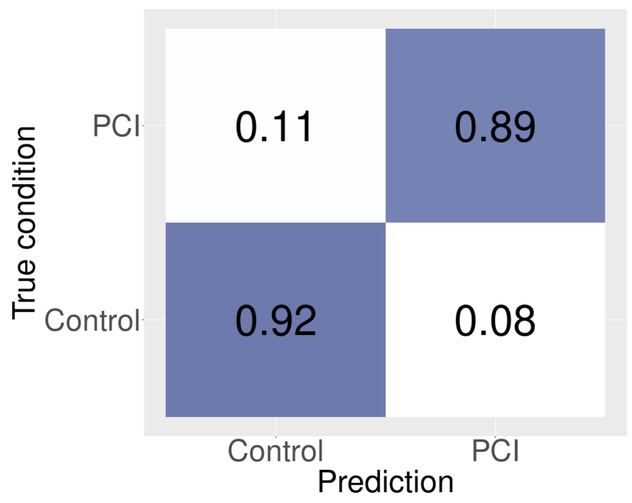


Data analysis

- Direct use of XGBoost[1] on tabular data
- Fivefold cross-validation for evaluating prediction
- Use XGBoost to identify the most informative features
- Phosphatidylcholine 28:0 (PC(28:0)) is the most informative lipid
- PC(28:0) is the only lipid that is statistically significant between PCI and sham







Summary

- Data fusion of Raman and lipidomics
- Machine learning-assisted classification and key feature identification
- Sepsis status correlates with RBC lipid composition
- Lipidomics as a potential biomarker for sepsis

Outlook

- Further investigation of the role of Raman spectra
- Translation to patient data

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References

[1] Chen, T., & Guestrin, C. (2016). XGBoost: A Scalable Tree Boosting System. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (pp. 785–794). New York, NY, USA: ACM.