

Supplementary information

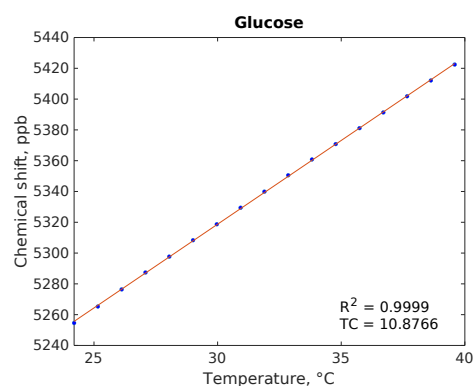
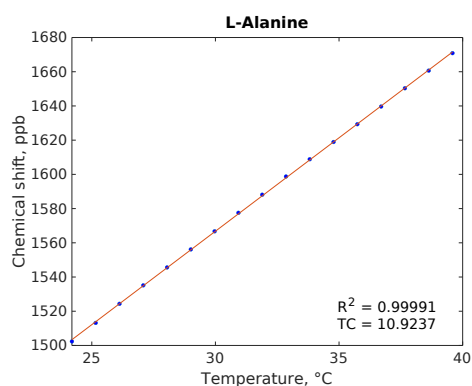
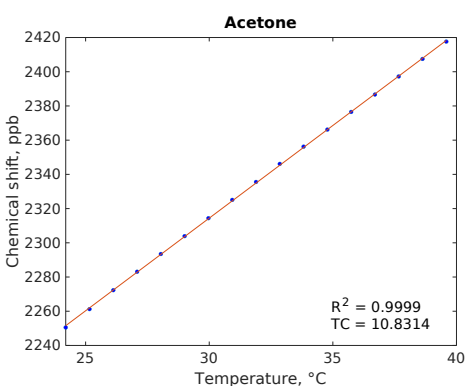
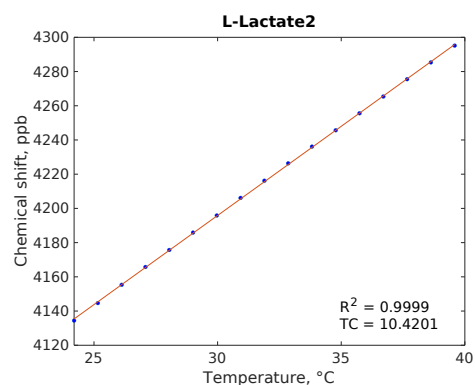
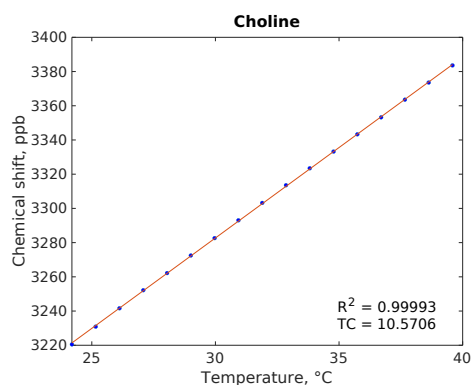
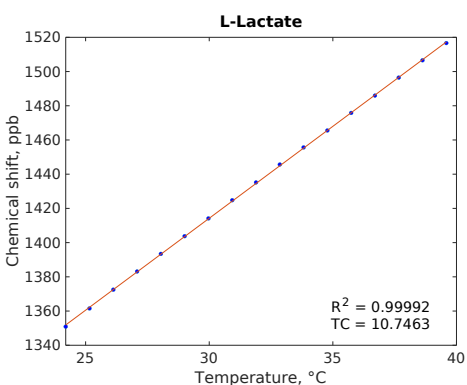
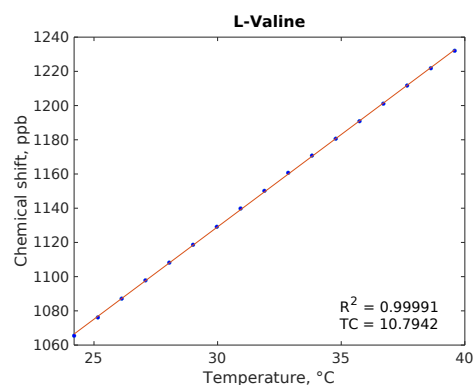
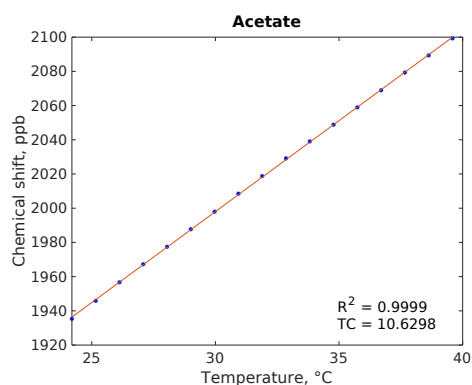
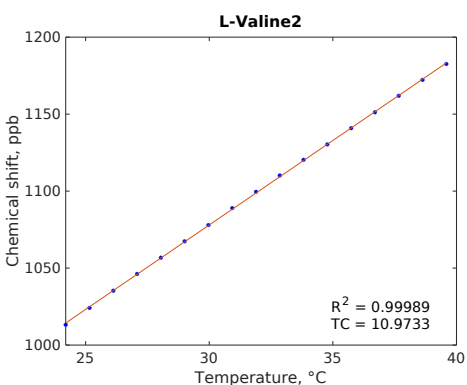
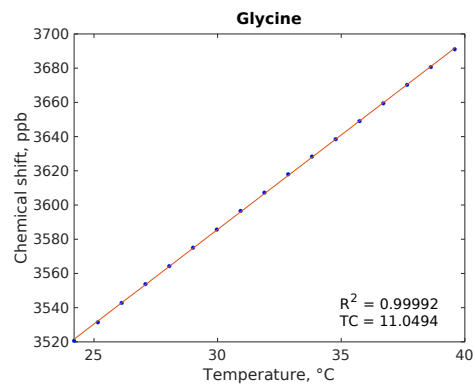
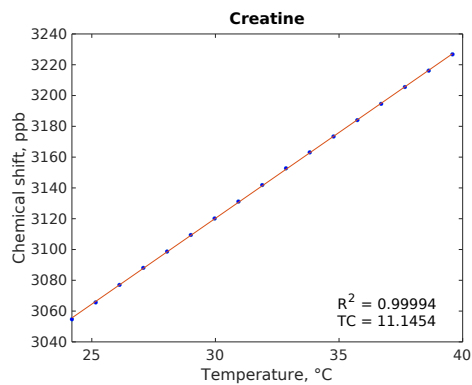
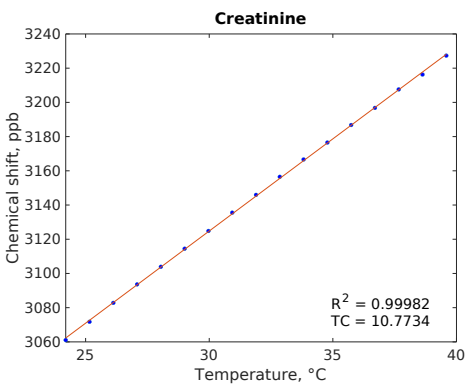
for

Variable-temperature NMR spectroscopy for metabolite identification in biological materials

Ewa K. Nawrocka^{a,b}, Mateusz Urbańczyk^{a,c}, Kamil Koziński^a, and Krzysztof Kazimierczuk^a

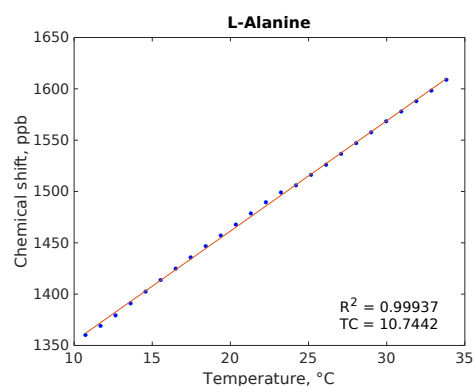
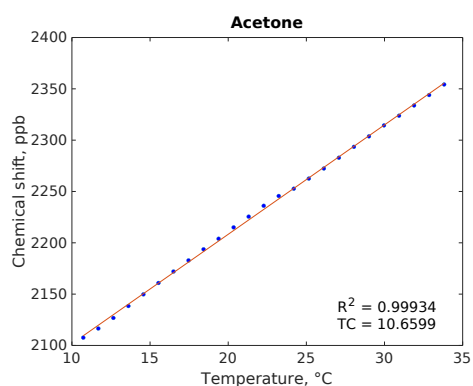
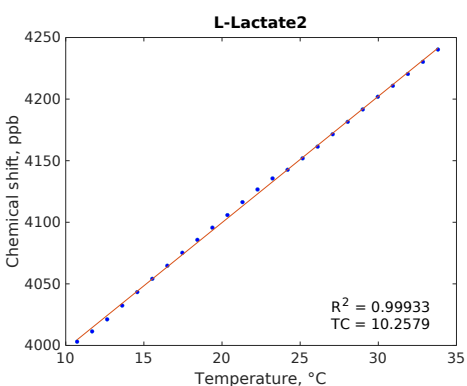
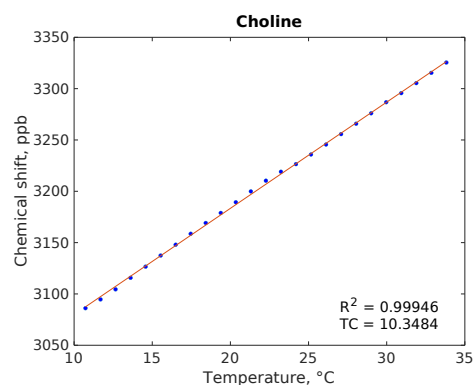
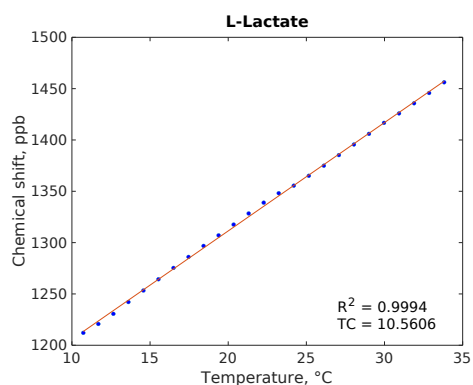
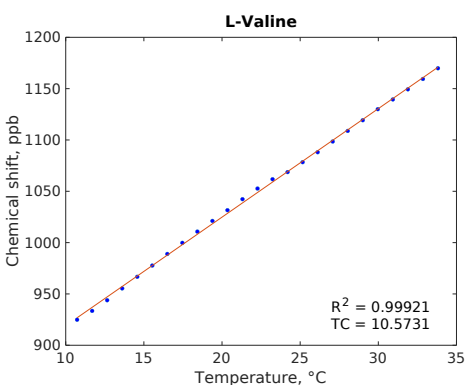
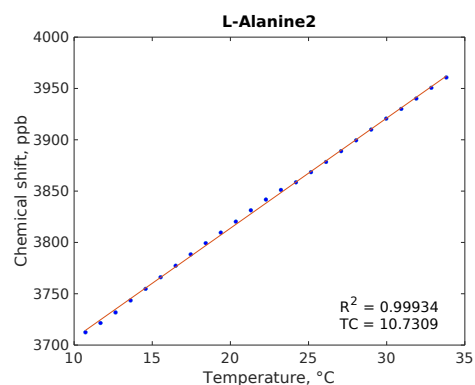
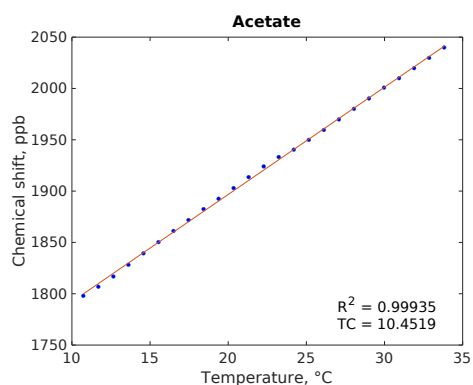
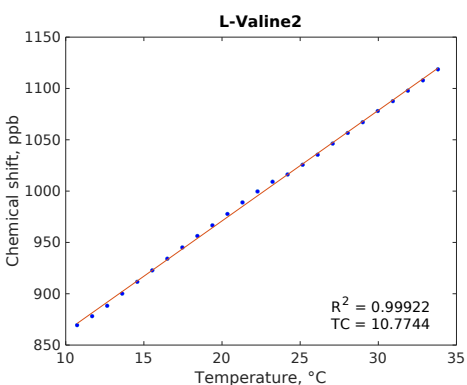
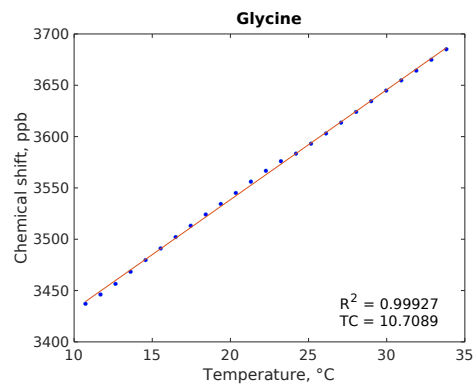
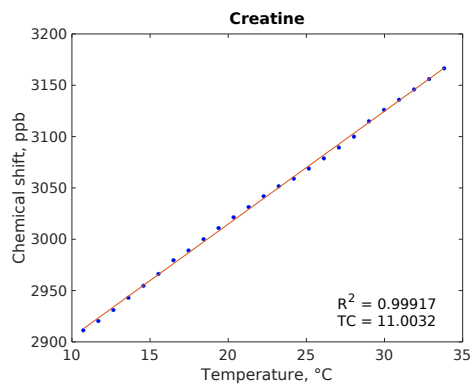
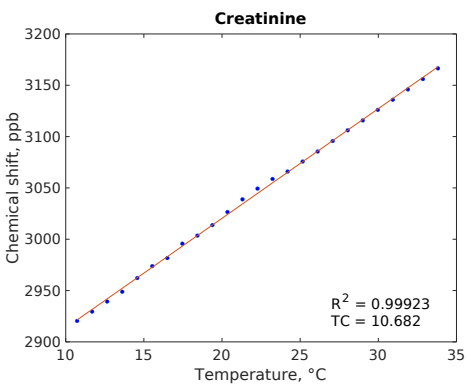
- a) Centre of New Technologies, University of Warsaw, ul. Banacha 2C, 02-097 Warsaw, Poland
- b) Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland
- c) Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

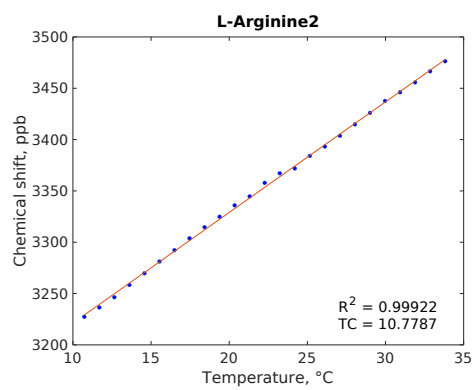
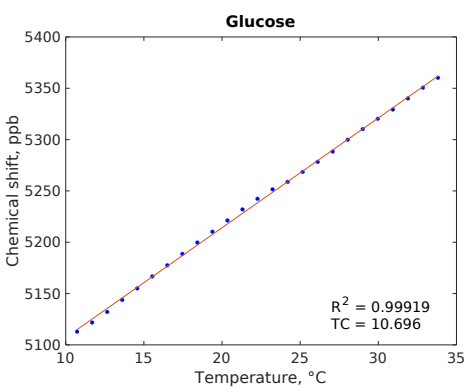
Chemical shift dependence, ppb, on temperature, °C, for metabolites from the first artificial mixture. Temperature coefficients (TCs) as a slope of the linear function. For all diagrams, the coefficient of determination R^2 is shown.



**Chemical shift dependence¹, ppb, on temperature, °C,
for NIST1950 plasma sample (experiment lasting 21 h).
Temperature coefficients (TCs) as a slope of the linear
function. For all diagrams, the coefficient of
determination R^2 is shown.**

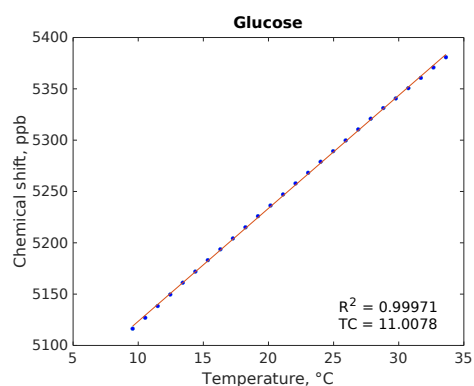
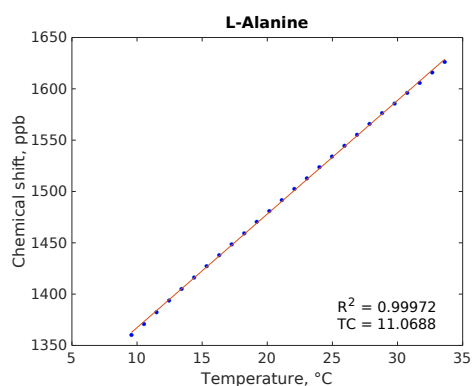
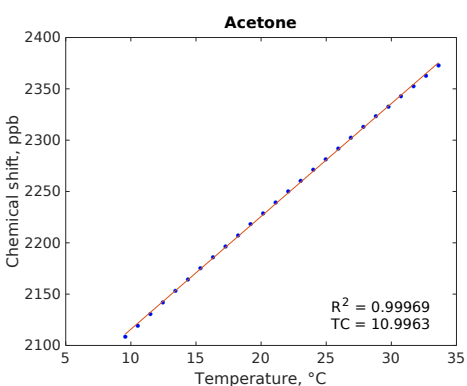
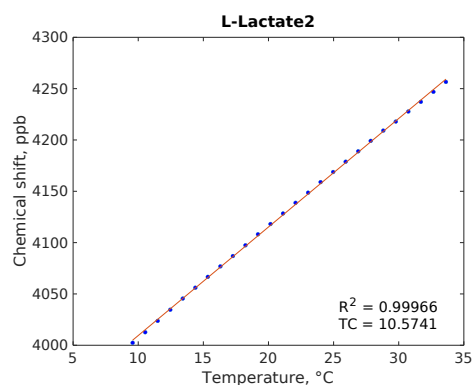
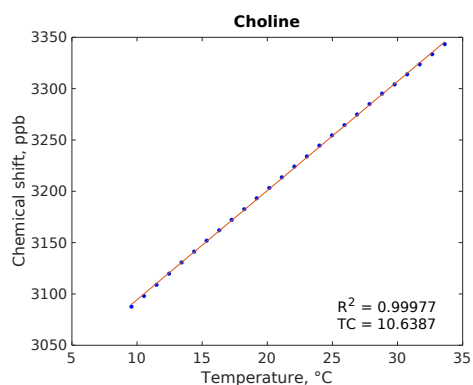
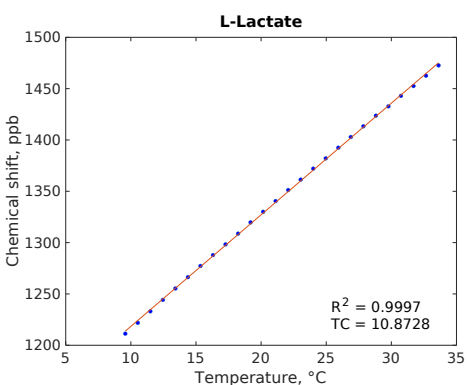
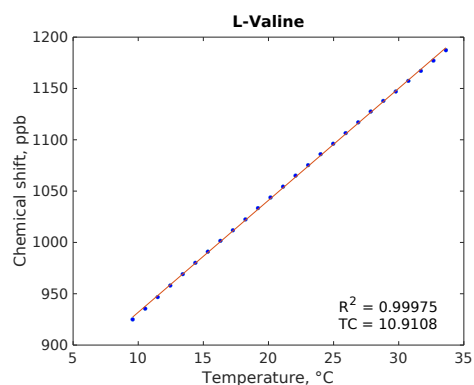
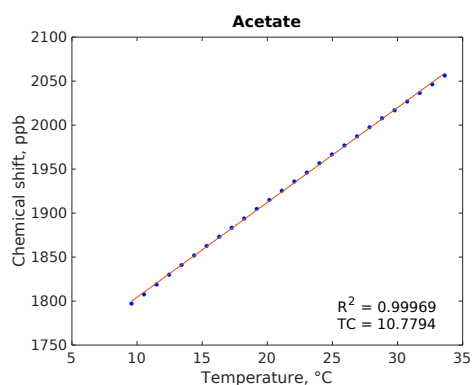
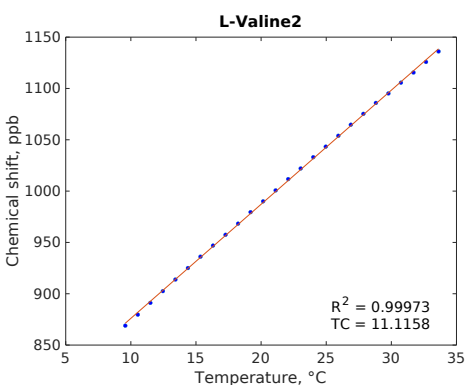
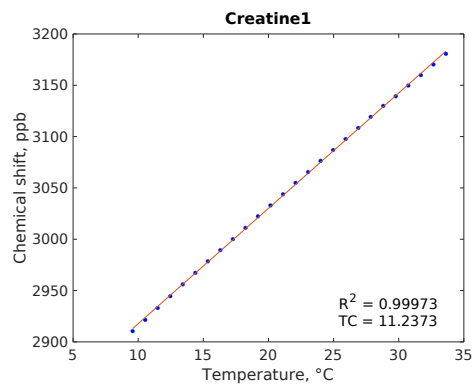
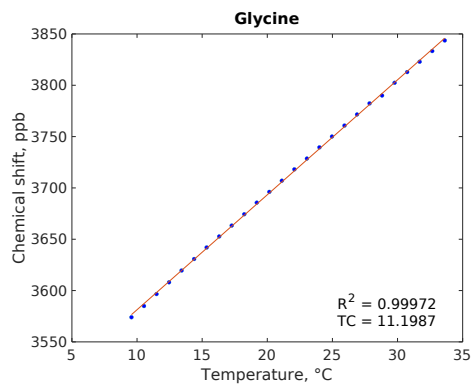
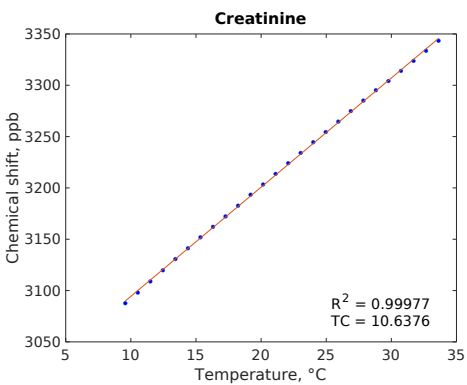
1 Raw data, before referencing to Lactate peak





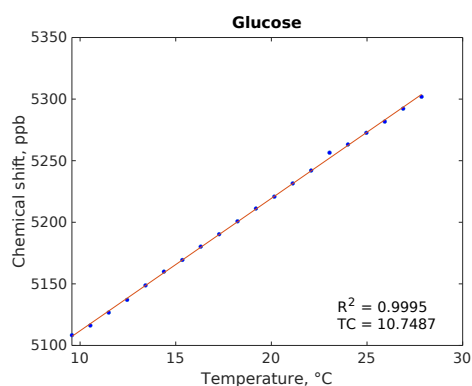
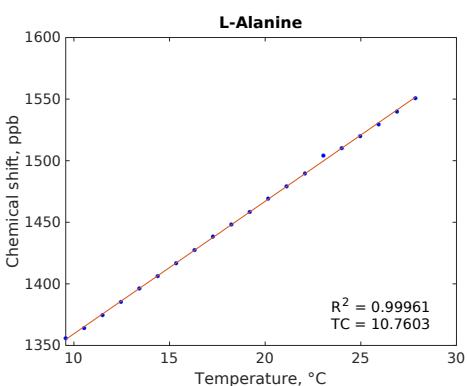
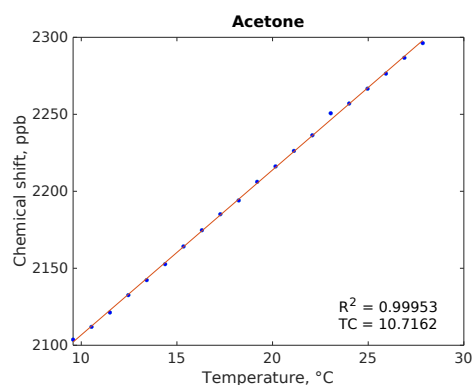
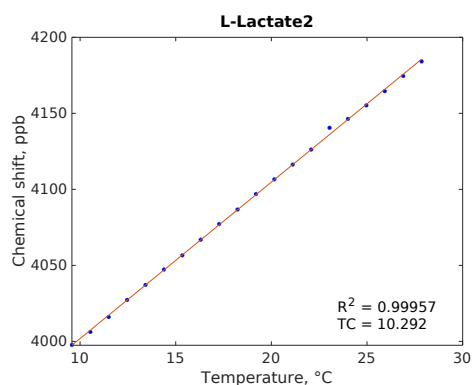
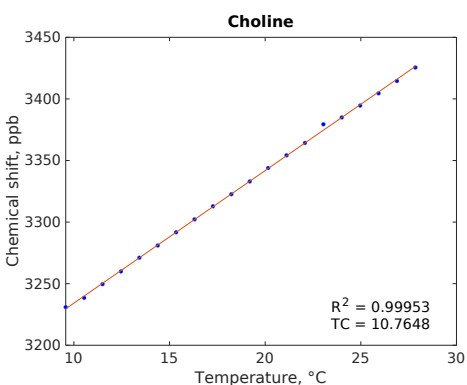
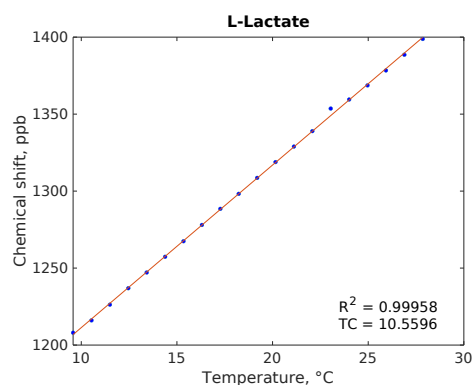
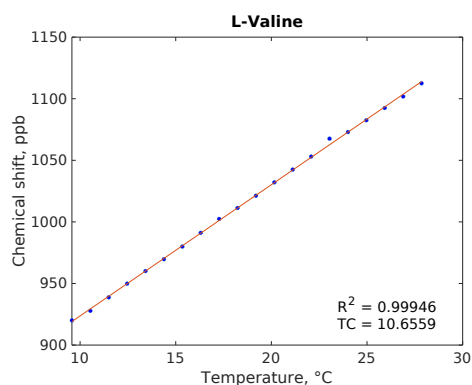
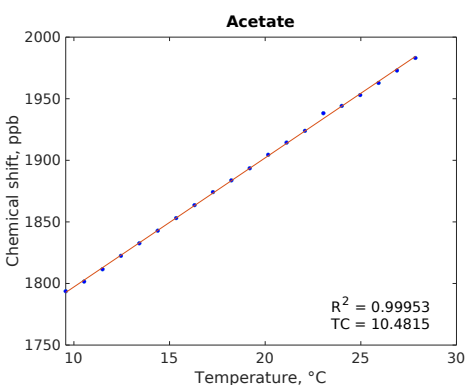
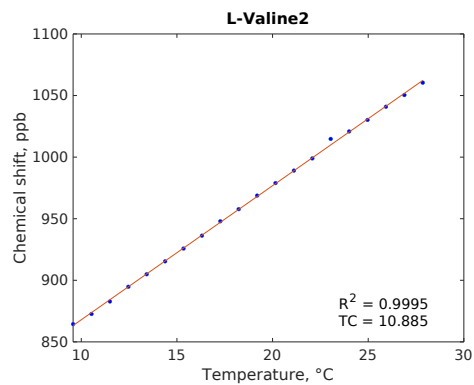
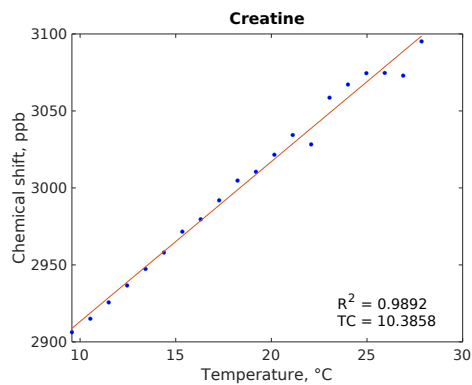
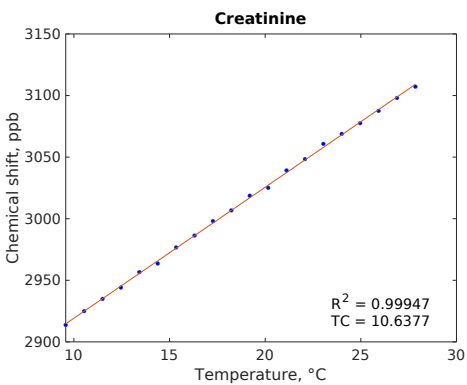
Chemical shift dependence¹, ppb, on temperature, °C, for mouse serum. Temperature coefficients (TCs) as a slope of the linear function. For all diagrams, the coefficient of determination R^2 is shown.

1 Raw data, before referencing to Lactate peak



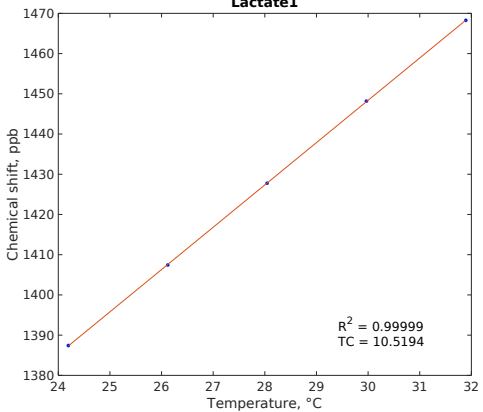
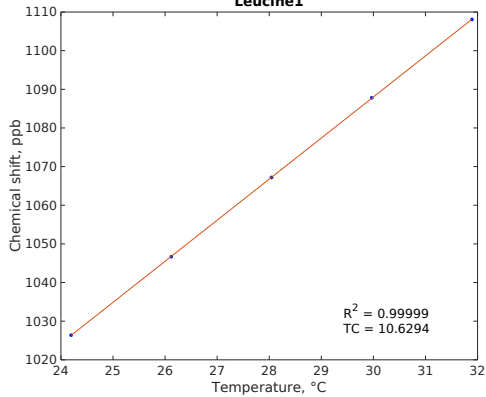
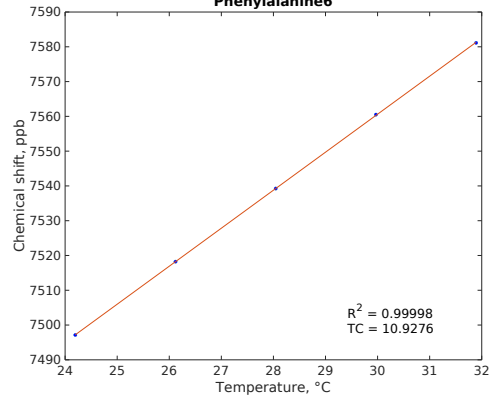
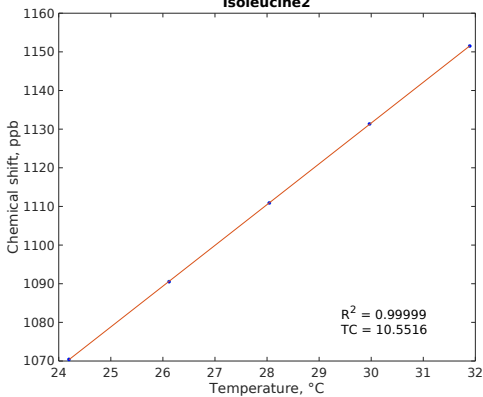
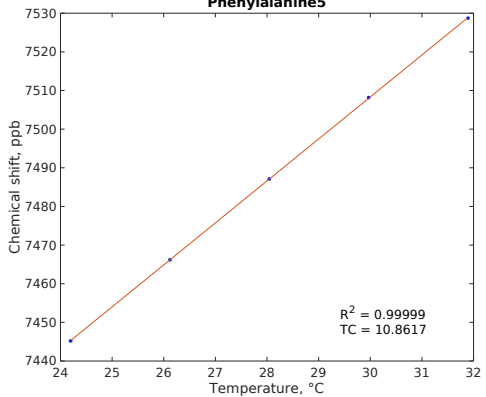
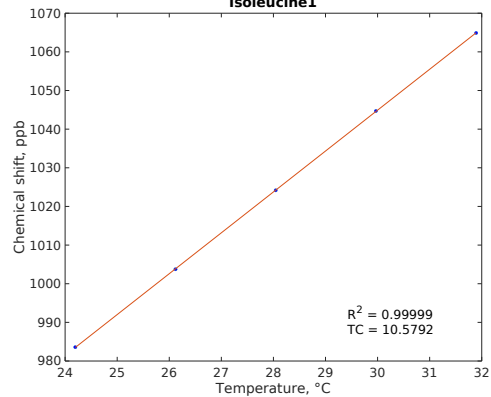
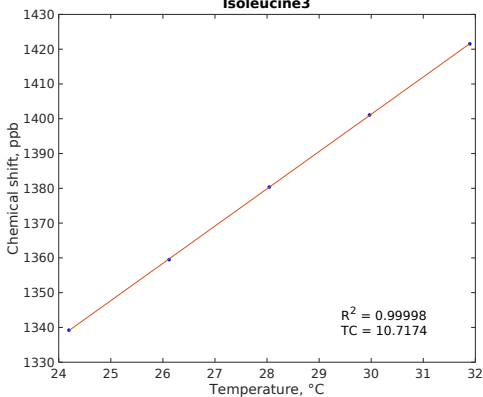
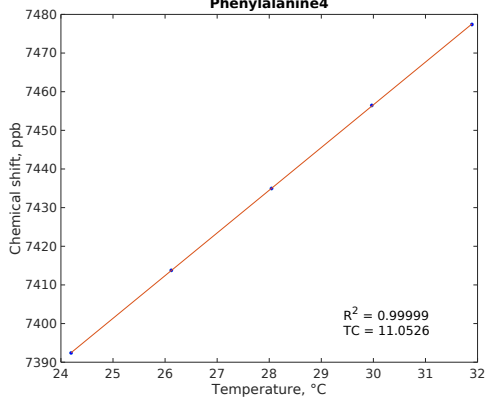
Chemical shift dependence¹, ppb, on temperature, °C, for NIST1950 plasma sample (experiment lasting 1 h). Temperature coefficients (TCs) as a slope of the linear function. For all diagrams, the coefficient of determination R^2 is shown.

1 Raw data, before referencing to Lactate peak



**Chemical shift dependence¹, ppb, on temperature, °C,
for metabolites from the artificial mixture 2.
Temperature coefficients (TCs) as a slope of the linear
function. For all diagrams, the coefficient of
determination R^2 is shown.**

1 Raw data, before referencing to Lactate peak

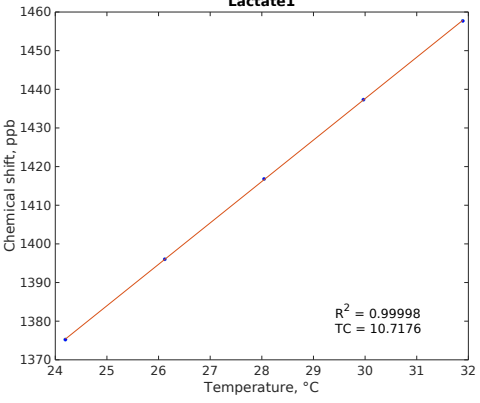
Lactate1**Leucine1****Phenylalanine6****Isoleucine2****Phenylalanine5****Isoleucine1****Isoleucine3****Phenylalanine4**

Chemical shift dependence¹, ppb, on temperature, °C, for metabolites from artificial mixture 3. Temperature coefficients (TCs) as a slope of the linear function. For all diagrams, the coefficient of determination R^2 is shown.

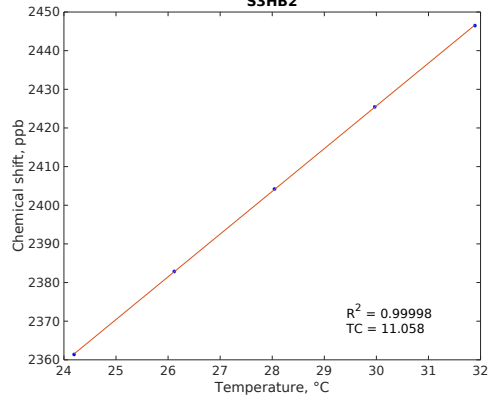
1 Raw data, before referencing to Lactate peak

S3HB - Sodium 3-hydroxybutyrate

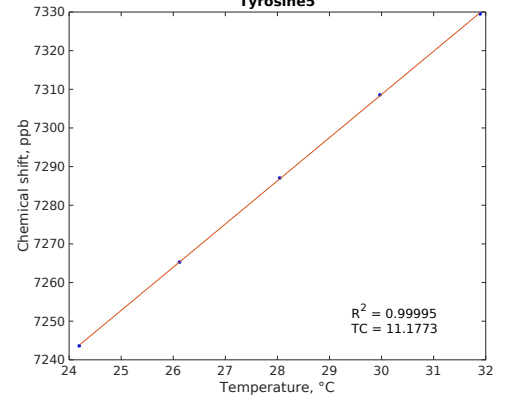
Lactate1



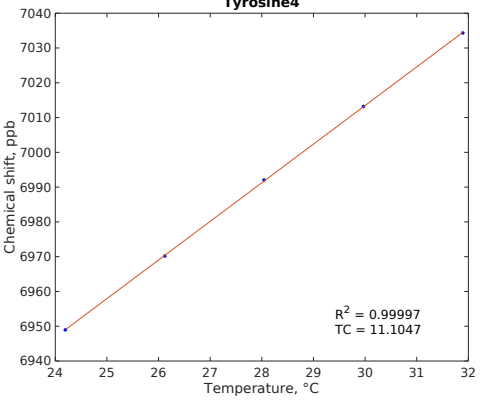
S3HB2



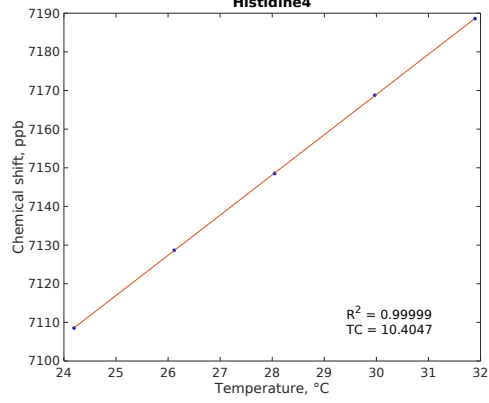
Tyrosine5



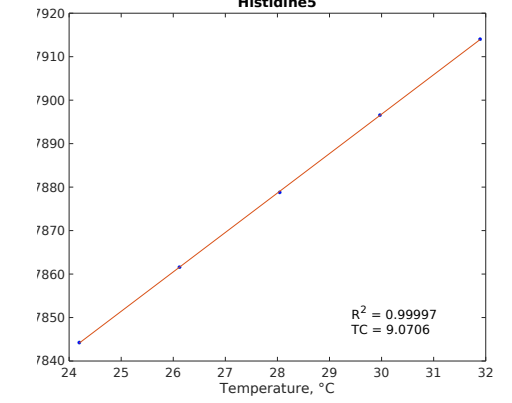
Tyrosine4



Histidine4



Histidine5



	Chem. shift, ppm	Temperature coefficients (TC), ppb/K after referencing to Lactate peak				
		Art. mixture	NIST1950 (21 h)	NIST1950 (1 h)	Mouse serum	NIST1950 (1 h) after Radon proc.
Alanine	1.51	10.93	10.93	10.95	10.94	10.90
Lactate*	1.36	10.75	10.75	10.75	10.75	10.75
Lactate	4.14	10.44	10.48	10.42	10.45	10.46
Acetate	1.95	10.64	10.67	10.63	10.65	10.66
Acetone	2.26	10.85	10.90	10.83	10.87	10.94
Choline	3.23	10.53	10.95	10.57	10.51	10.60
Glucose	5.26	10.88	10.94	10.88	10.88	10.85
Creatinine	3.07	10.87	10.82	10.77	10.51	
Creatine	3.065	11.19	10.57	11.15	11.11	11.31
Valine	1.08	10.76	10.84	10.79	10.78	10.87
Valine	1.02	10.96	11.07	10.97	10.99	11.01
Leucine	1.03	10.85	10.84		10.80	
Isoleucine	0.99	10.81	10.76		10.79	
Isoleucine	1.07	10.79	10.73		10.76	
Isoleucine	1.31	10.93	10.82		10.90	
Phenylalanine	7.39	11.27	11.30		11.47	
Phenylalanine	7.43	11.04	11.90		10.86	
Phenylalanine	7.49	11.14	11.12		11.07	
Tyrosine	6.94	11.11	11.16		11.24	
Tyrosine	7.24	11.17	11.22		11.33	
Histidine	7.11	10.45	10.58		10.61	
Histidine	7.84	9.36	9.57		9.61	
S3HB**	2.35	11.03	11.01		11.10	

* Treated as a TC reference

** Sodium 3-hydroxybutyrate