

Mittwoch 27. März 2002 9:50 - 11:10



EUROPEAN COMMISSION

JOINT RESEARCH CENTRE

Institute for Reference Materials and Measurements

Geel, Belgium



The energy of interaction between water and surfaces of biological Reference Materials



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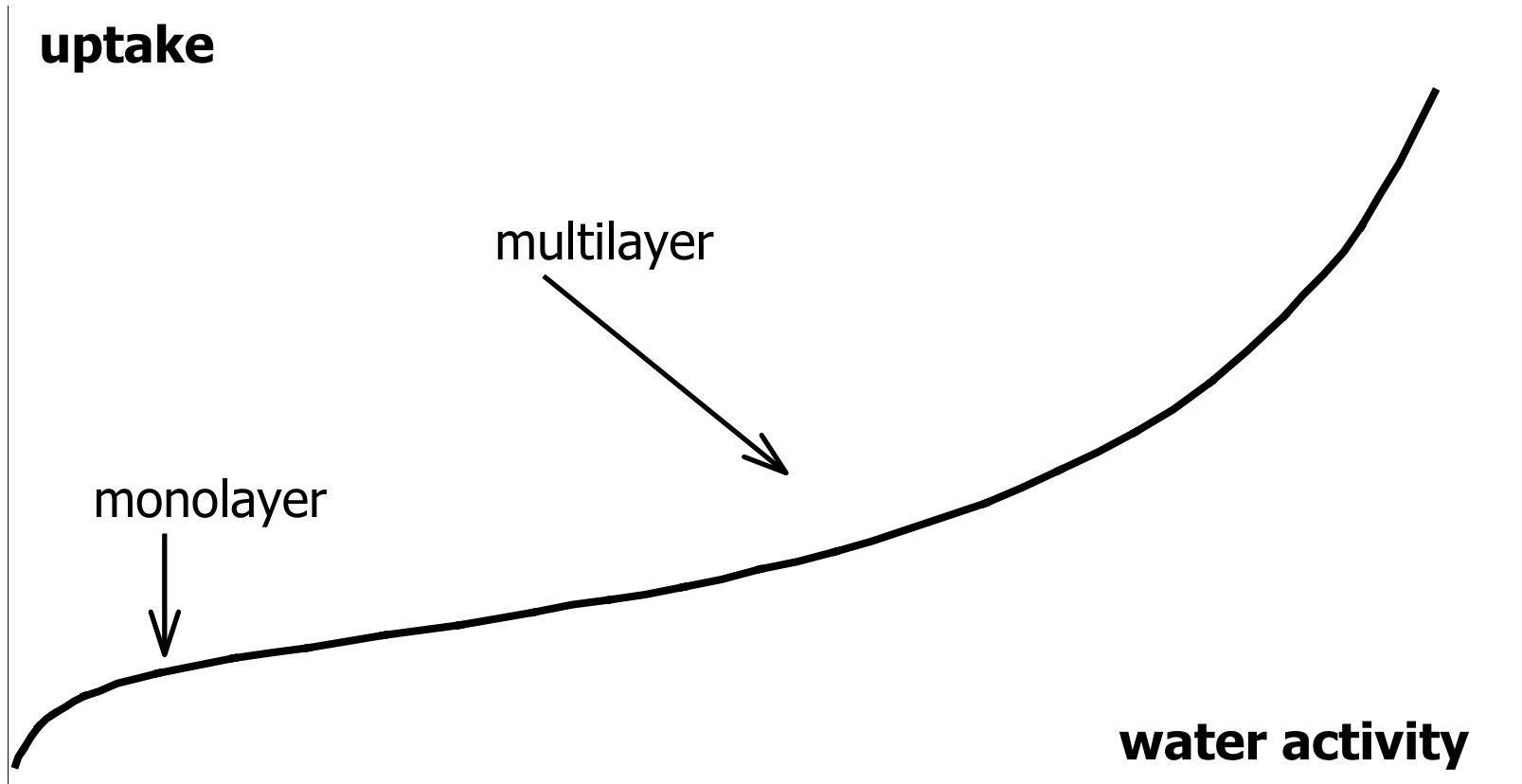
Terms in use to describe “bound water”

- bound water
- solid-like water
- imbibed water
- immobilised water
- ice-like water
- monolayer water
- sorbed water
- water of crystallisation
- water of hydration
- unfreezable water
- non-solvent water
- water available for certain processes

van den Berg (1981)



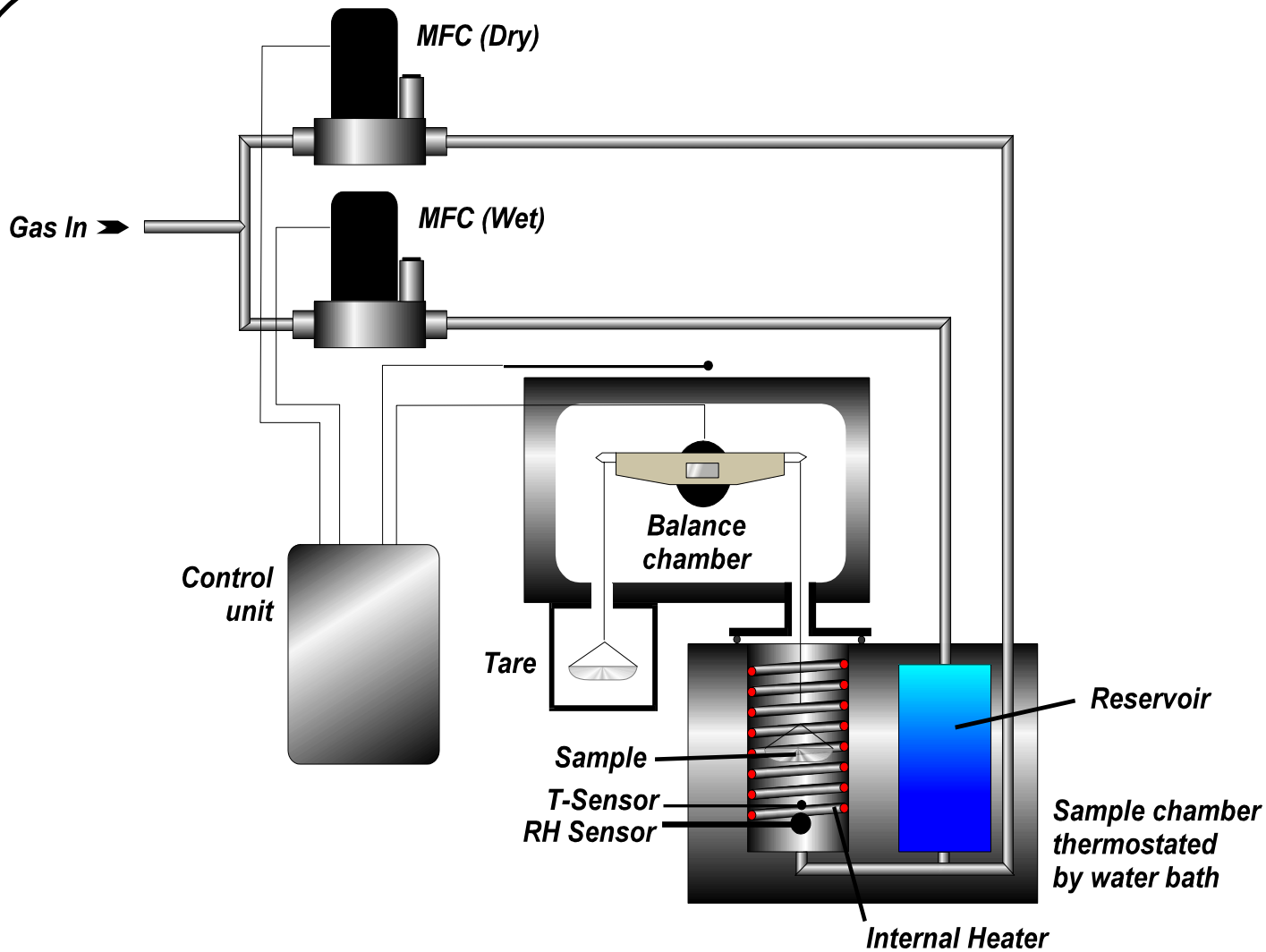
sorption isotherm

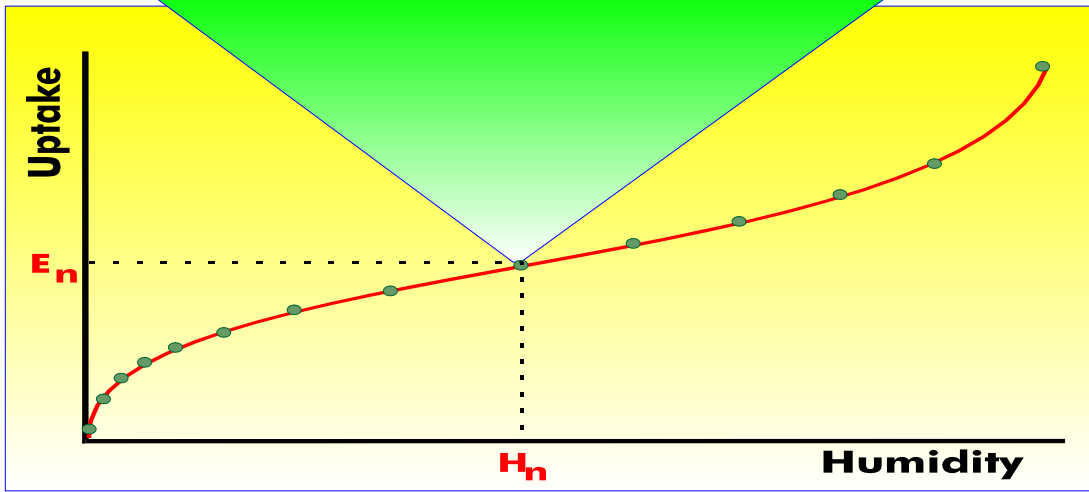
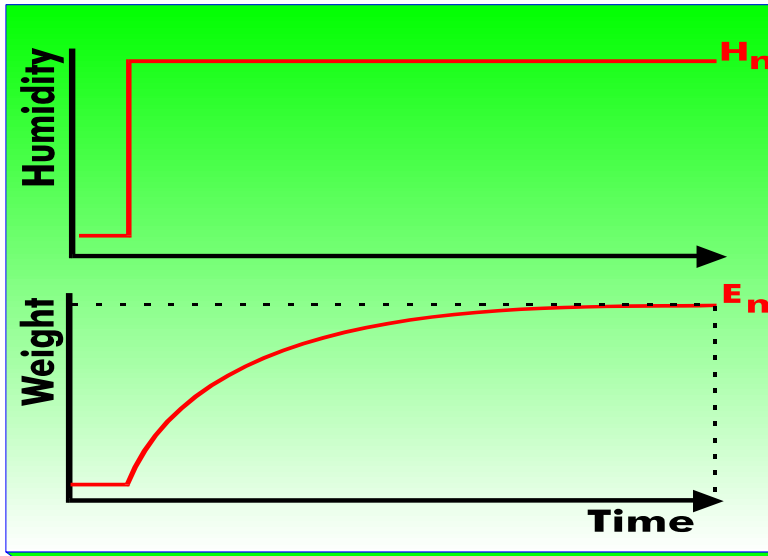




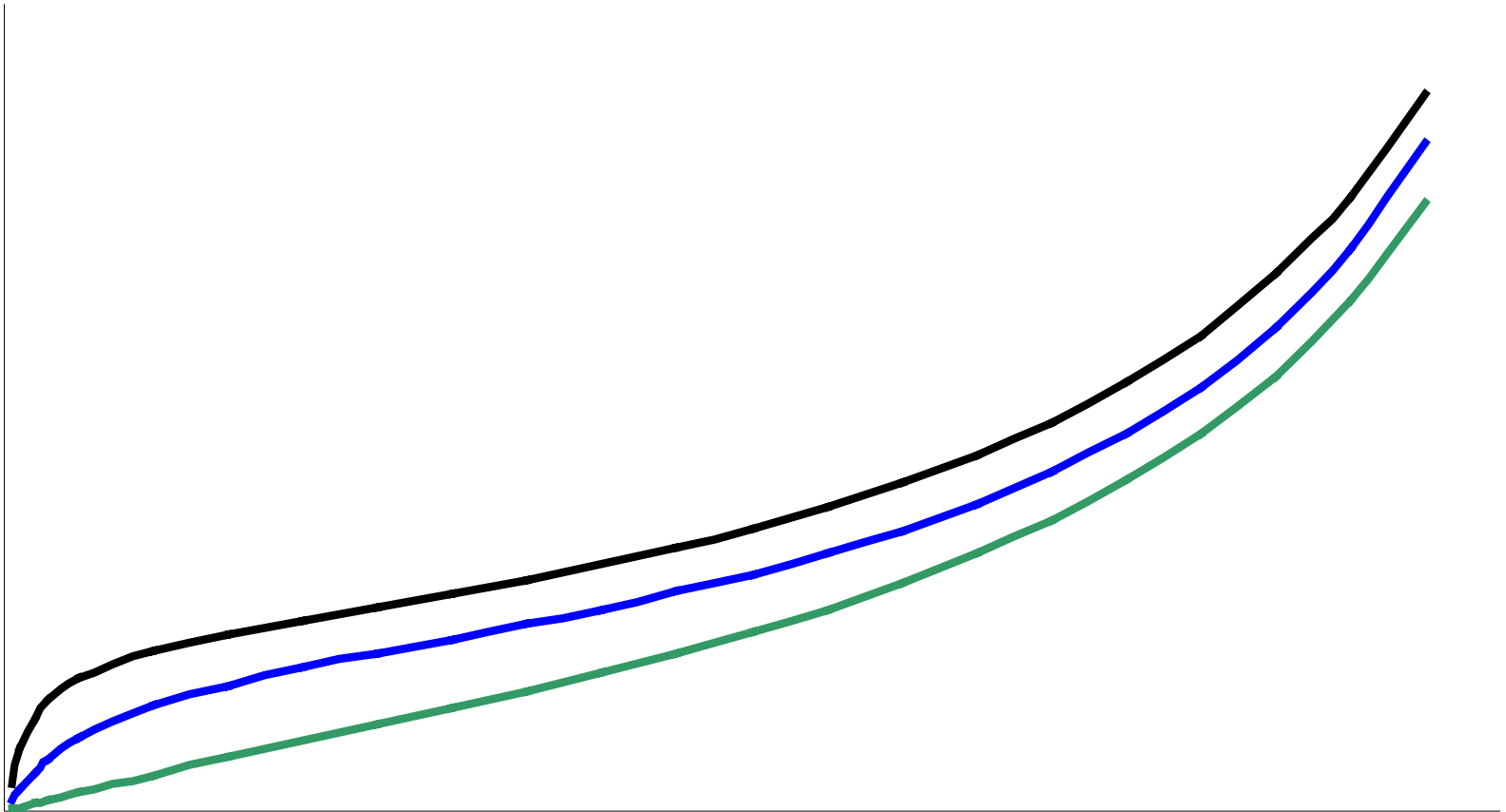
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effect of temperature



applying Clausius-Clapeyron on sorption isotherms

isosteric heat of sorption, q_{st}

$$\left[\frac{\partial \ln p}{\partial T} \right]_n = \frac{q_{st}}{RT^2}$$

latent heat of evaporation

water: $H_L \approx 44 \text{ kJ/mol}$

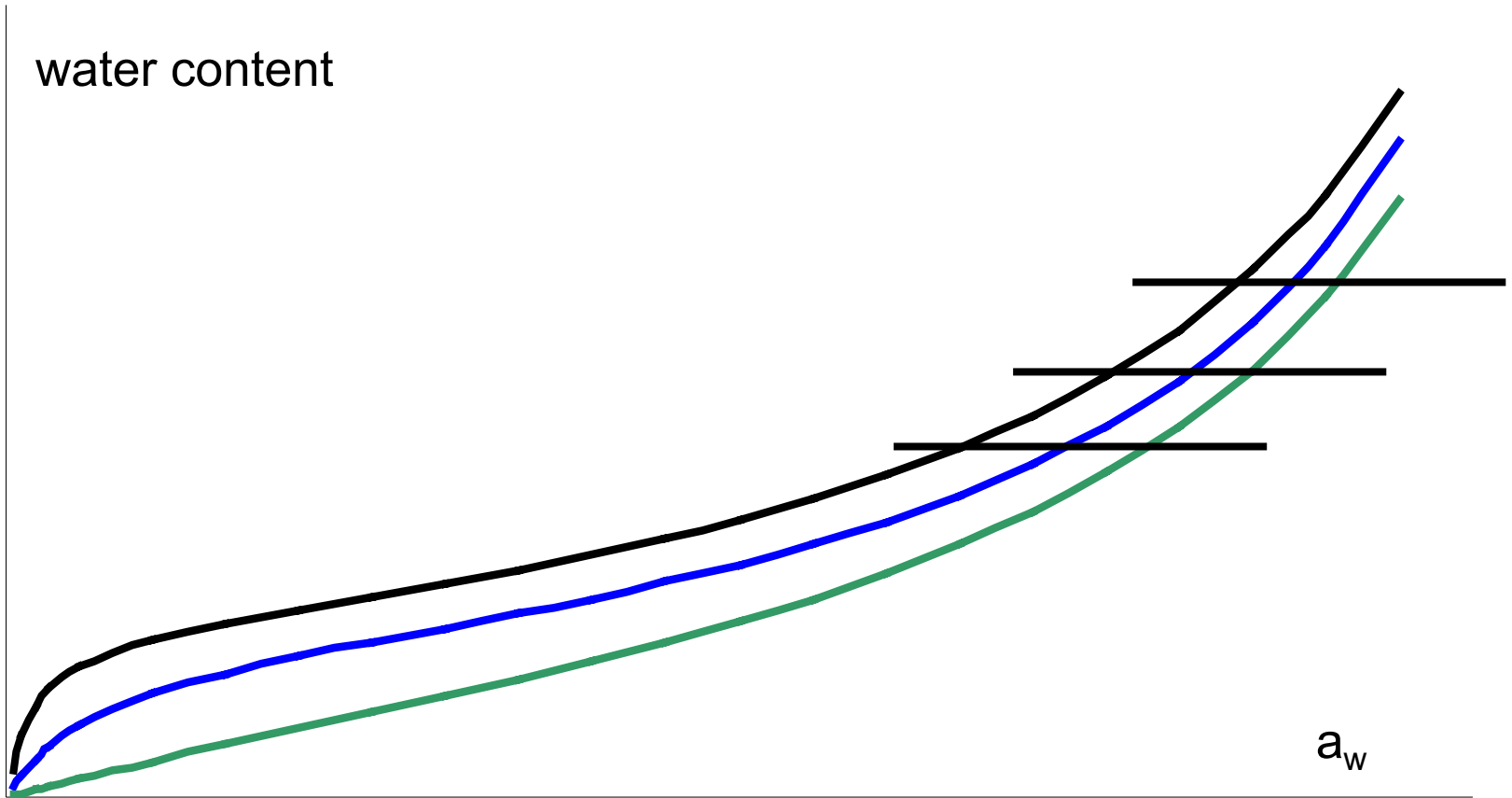
$$\left[\frac{\partial \ln p_0}{\partial T} \right]_n = \frac{H_L}{RT^2}$$

net isosteric heat of sorption, $q_{st,net}$

$$\left[\frac{\partial \ln(p/p_0)}{\partial T} \right]_n = \left[\frac{\partial \ln(a_w)}{\partial T} \right]_n = \frac{q_{st,net}}{RT^2}$$



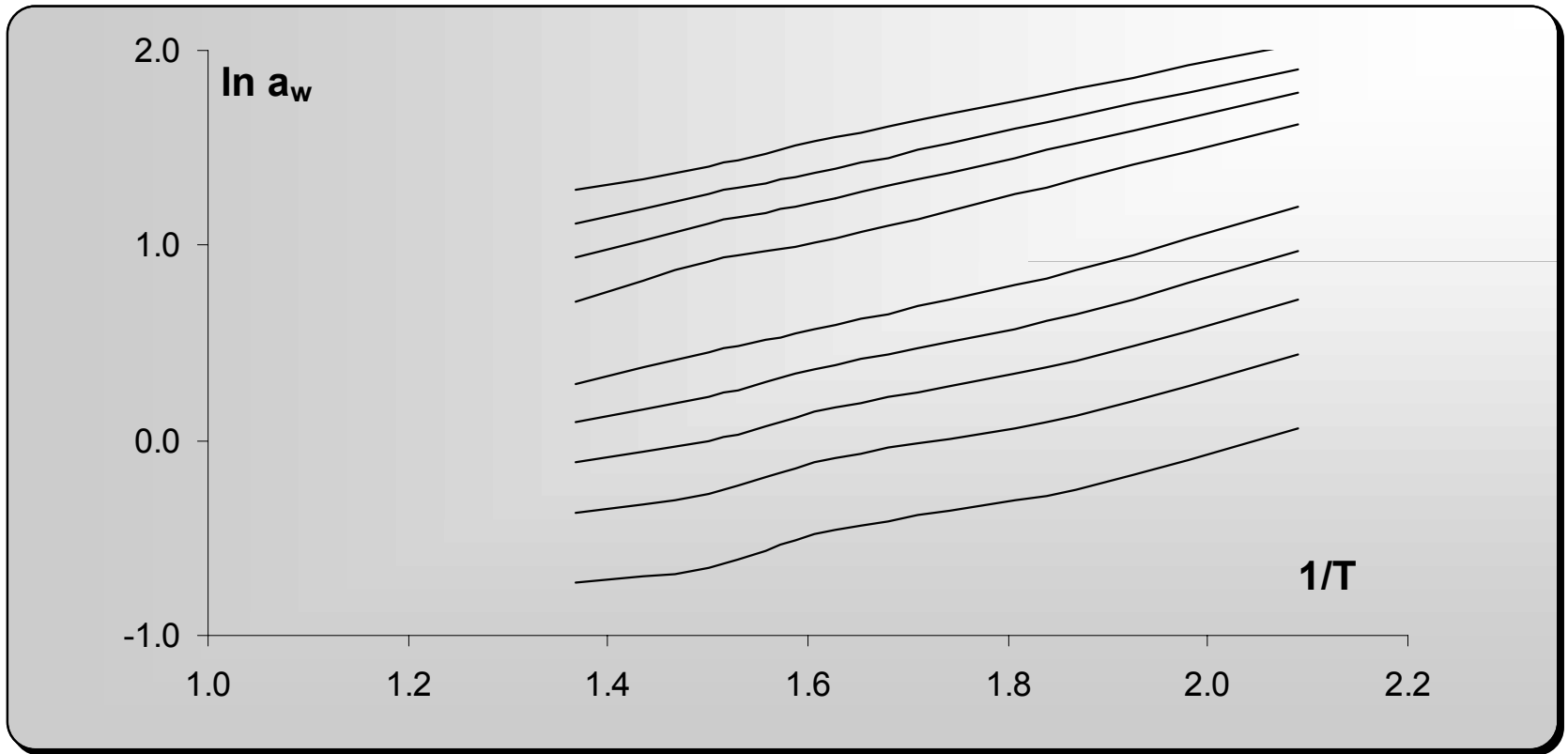
water content



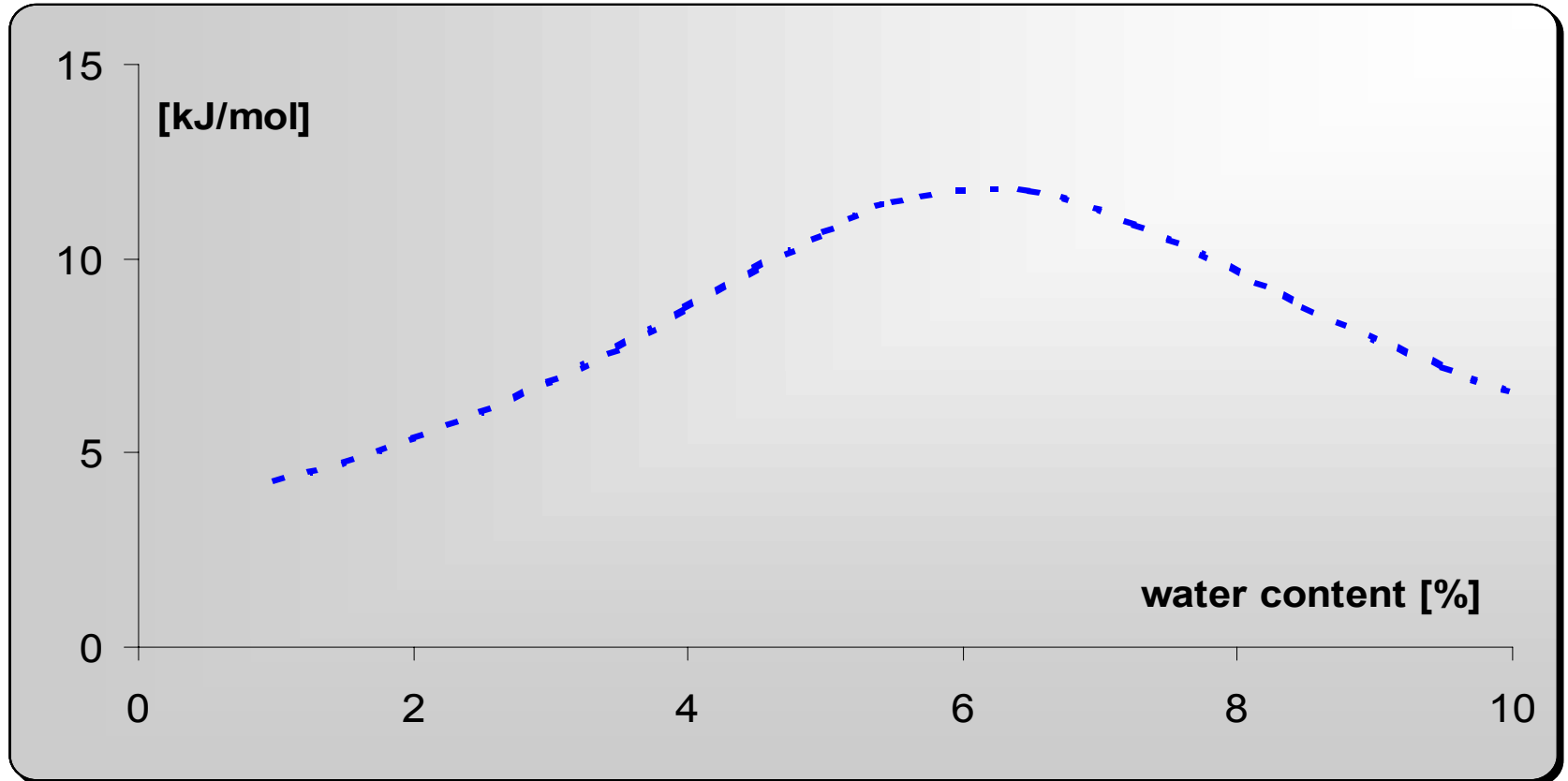
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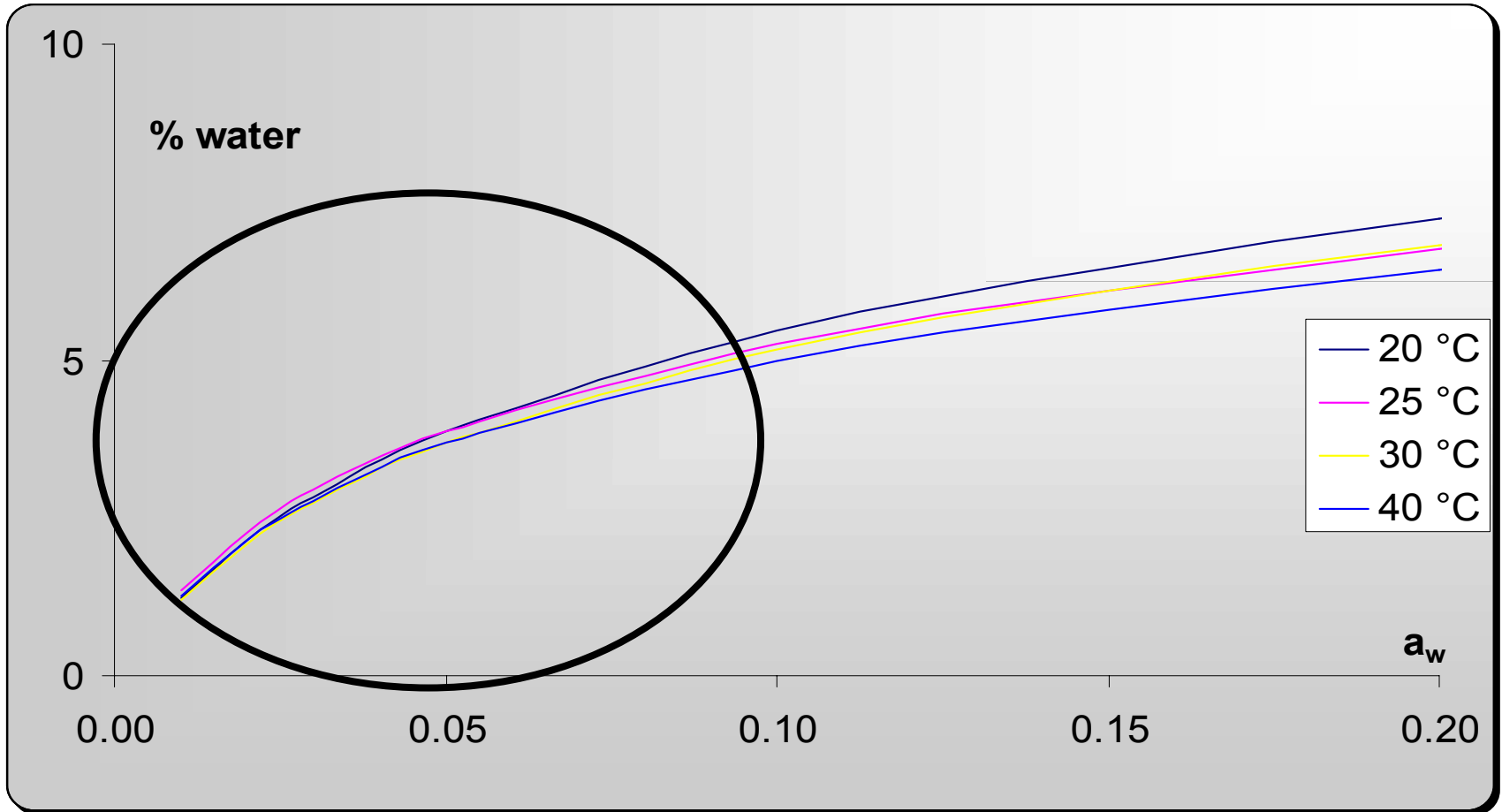
plotting $\ln a_w$ versus $1/T$ at different water contents



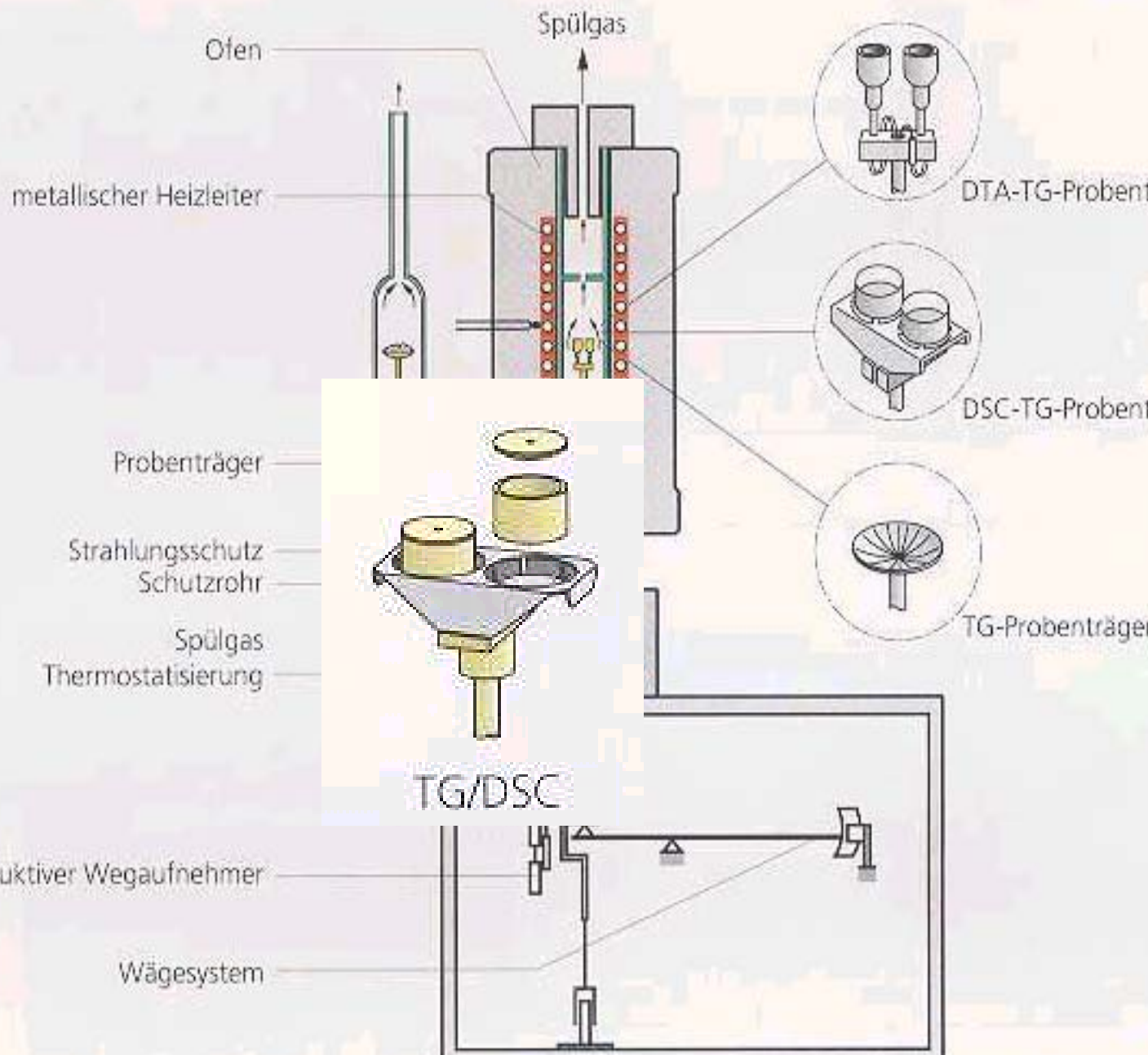
results is graph for net isosteric heat of sorption



lack of accuracy in the low- a_w -range



Schema STA 409 EP



STA as a tool to assess binding energy of water on biological surfaces directly

- equilibrating samples at different relative humidities
- evaluating temperature program
- recording mass loss and energy peaks



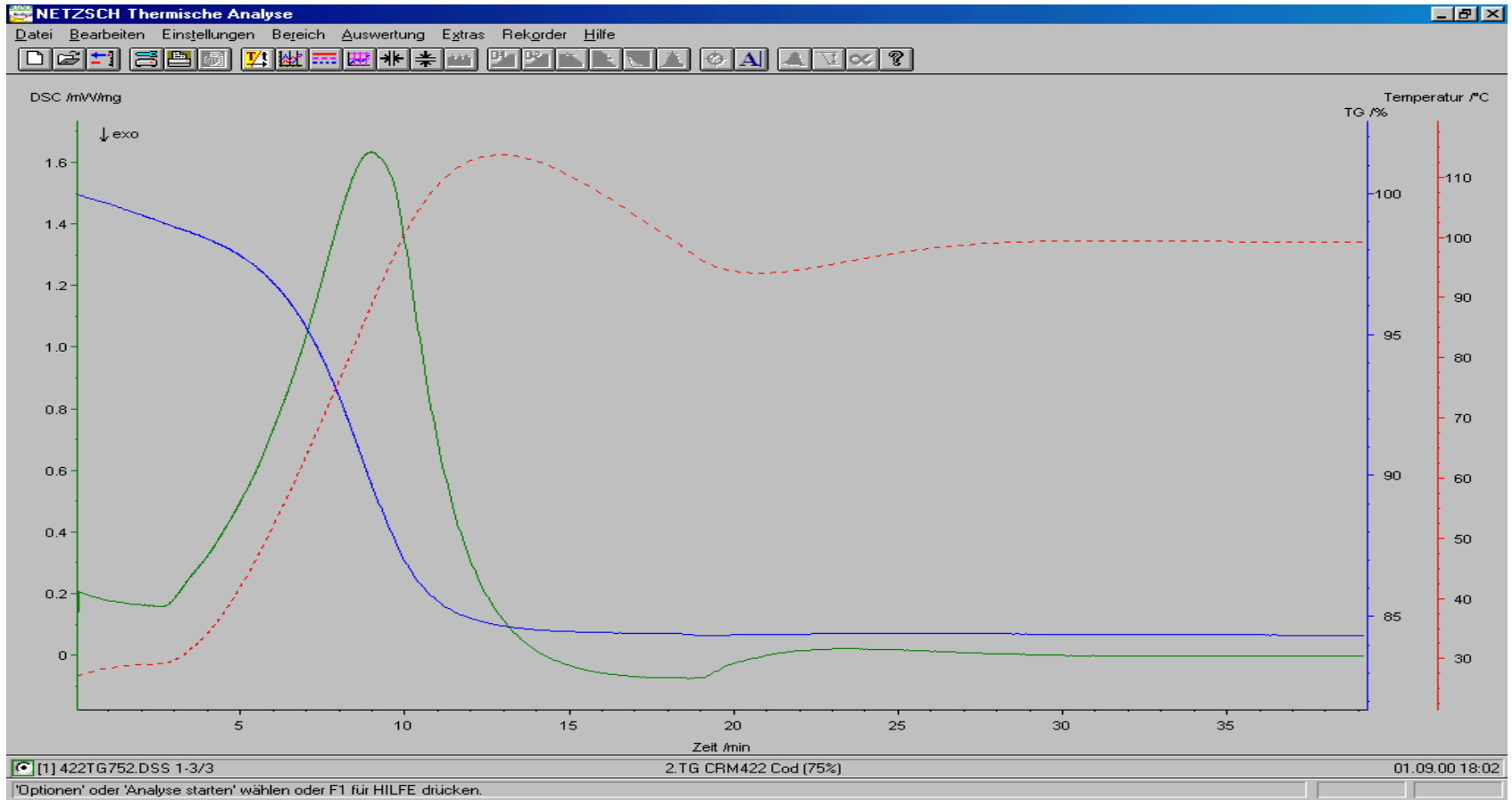
“low tech, but high efficiency” sample preparation



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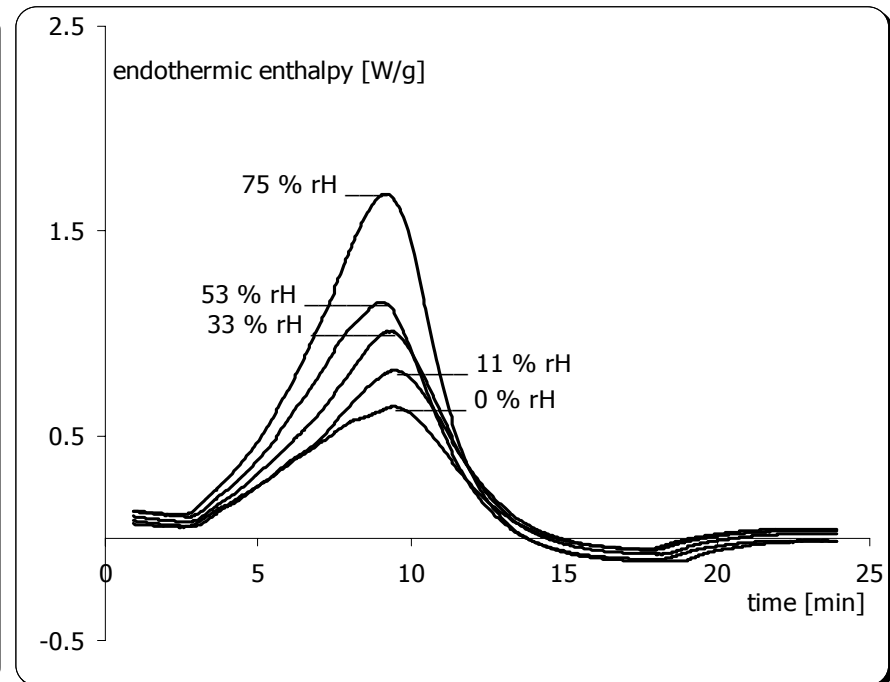
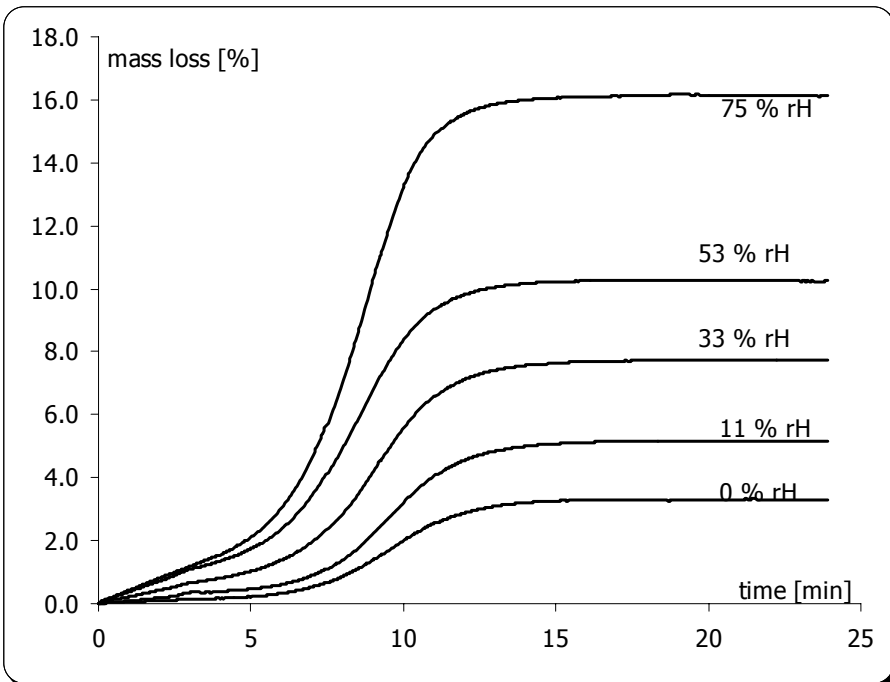
exemplary graph for STA (cod, equilibr. at 75 % rH)



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summary of graphs for STA (cod)



results for sample 1 - CRM 422 - cod muscle

water [%]	Qst,net [kJ/mol]	H _{evap} [kJ/mol]				
		75 % rH water: 20.6 % - 5.5 %	53 % rH water: 10.8 % - 1.8 %	33 % rH water: 7.4 % - 0.7 %	11 % rH water: 5.2 % - 0.4 %	0 % rH water: 3.1 % - 0.1 %
0	-					
1	-					86
2	88					
3	93					
4	90					
5	77					
6	58					
7	41					
8	29					
9	21					
10	16					
11	12					
12	9					
13	7					
14	6					
15	5					
16	4					
17	3					
18	2					
19	1					
20	1					



results for sample 2 - RM 405 - whole grain wheat flour

water [%]	Qst,net [kJ/mol]	H _{evap} [kJ/mol]				
		75 % rH water: 15.8 % - 3.4 %	53 % rH water: 12.4 % - 2.0 %	33 % rH water: 9.4 % - 1.4 %	11 % rH water: 6.1 % - 0.5 %	0 % rH water: 4.0. % - 0.1 %
0	-					
1	-					
2	-					
3	19	18	23	32	43	46
4	20					
5	21					
6	22					
7	21					
8	18					
9	15					
10	12					
11	10					
12	8					
13	7					
14	6					
15	5					
16	4					
17	4					
18	3					
19	3					
20	3					



results for sample 3 - CRM 063r - skim milk powder

water [%]	Q _{st,net} [kJ/mol]	H _{evap} [kJ/mol]				
		75 % rH water: 13.4 % - 4.6 %	53 % rH water: 7.8 % - 1.2 %	33 % rH water: 6.4 % - 0.9 %	11 % rH water: 5.3 % - 0.8 %	0 % rH water: 2.7 % - 0.2 %
0	-					
1	-					94
2	-					
3	-				51	
4	29			44		
5	43		28			
6	40					
7	25	21				
8	16					
9	11					
10	8					
11	6					
12	4					
13	3					
14	3					
15	2					
16	2					
17	1					
18	1					
19	1					
20	0					



results for sample 4 - whole milk powder

water [%]	Q _{st,net} [kJ/mol]	H _{evap} [kJ/mol]				
		75 % rH water: 9.4 % - 2.3 %	53 % rH water: 5.2 % - 2.3 %	33 % rH water: 4.5 % - 0.4 %	11 % rH water: 3.8 % - 0.3 %	0 % rH water: 1.7 % - 0.2 %
0	-					
1	-					
2	-					
3	4					
4	57					
5	25					
6	12					
7	7					
8	5					
9	3					
10	2					
11	2					
12	1					
13	1					
14	0					
15	0					
16	0					
17	0					
18	0					
19	0					
20	0					



summary

- STA is well applicable on biological and environmental matrices
- overcomes shortcomings of $q_{st,net}$ calculated from WSIs at low water activities
- is a suitable technique for cross checking $q_{st,net}$ data in the overlapping range
- increases knowledge of heat deterioration processes when combined with mass spectrometry



Thank you very much
for your patience!

Discussion is open

