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Experiment Setup

Proposal #	8038
Proposal Name	Benchmarking different approaches to predict small angle profiles from proteins
Start Date	19/7/2019
End Date	21/7/2019, some samples measured 13/12/2019
Principal Scientist	Andrew Whitten (ANSTO - ACNS)
Email Address	andrew.whitten@ansto.gov.au
Local Contact	A Whitten
Experiment Description	
Affiliation	
Contact Number(s)	
Wavelength	Å
Wavelength Resolution	0.10
Standard/High res'n NVS	High resolution (NVS43), tilted to -6 degrees on eve of first day in July Low resolution (NVS40) at 0 tilt in December
Apx Softzero	0.5
samx Softzero	-2.5
samy	845
samz	227.7
Sample Environment	20 position,no shroud
T/P/Field Set-point	15
Cells Used	helmas
Sample Alignment Date	
Sensitivity File Date	

Experiment Configuration

Configurations	**low q**	**med q**	**high q**
Name of config	L1=L2=6m_central	L1=4m_L2=1p3m	
L_1	6m	4m	
L_2	6m	1.3m	
# guides	G6	G7	
Det y	5200	510	
Det offset	-5	5	
Source ap diameter	50	50	
Guard ap diameter	12.5	12.5	
apx diameter	12.5	12.5	
Beamstop #	2	2	

bsx	38.5	37	
bsz	259	259	
Beam centre (x,z)	config.beamcenterx = 91.62 config.beamcenterz = 95.96	config.beamcenterx = 91.63 config.beamcenterz = 96.27	
Qmin	0.008	0.04	
Qmax	0.11	0.45	
H_2O or buffer S rate	6663 (NVS=-6 degrees tilt)	153 147 (NVS=0tilt) 237 703 (NVS=-6)	
D_2O or buffer S rate	1696 (NVS=- 6 degrees tilt)	34 309 (NVS =0tilt) 53 745 (NVS=-6 tilt)	
MT cell S rate	713 (NVS= - 6)	10 384 (NVS=0 tilt) 15 753 (NVS=-6 tilt)	
MT beam T rate	586 (NVS= - 6, att=9)	1,174 (att=9, NVS=0tilt) 1,900 (att=9, NVS=-6tilt)	

NVS at 0 tilt:

L1=4m_L2=1p3m			
Position	**Name**	**Thickness**	**Scattering**
1	0_Lys_Buffer	1.0	0178743
2	0_Lys_halfConc	1.0	0178744
3	0_Lys	1.0	0178745
4	100_Lys_Buffer	2.0	0178746
5	100_Lys_halfConc	2.0	0178747
6	100_Lys	2.0	0178748
7	0_UOx_Buffer	1.0	0178749
8	0_UOx_halfConc	1.0	0178750
9	0_UOx	1.0	0178751
10	100_UOx_Buffer	2.0	0178752
11	100_UOx_halfConc	2.0	0178753
12	100_UOx	2.0	0178754
18	BLOCKED_BEAM	1.0	0178755
19	EMPTY_CELL	0.0	0178756

L1=L2=6m_central				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_Lys_Buffer	1.0	0178757	
2	0_Lys_halfConc	1.0	0178758	
3	0_Lys	1.0	0178759	
4	100_Lys_Buffer	2.0	0178760	
5	100_Lys_halfConc	2.0	0178761	
6	100_Lys	2.0	0178762	
7	0_UOx_Buffer	1.0	0178763	
8	0_UOx_halfConc	1.0	0178764	
9	0_UOx	1.0	0178765	
10	100_UOx_Buffer	2.0	0178766	

11	100_UOx_halfConc	2.0	0178767	
12	100_UOx	2.0	0178768	
19	EMPTY_CELL	0.0	0178769	
20	EMPTY_BEAM	1.0	0178770	

Changed NVS to -6 degrees tilt:

L1=L2=6m_central			
Position	**Name**	**Thickness**	**Scattering**
1	0_Lys_Buffer	1.0	0178771
2	0_Lys_halfConc	1.0	0178772
3	0_Lys	1.0	0178773
4	100_Lys_Buffer	2.0	0178774
5	100_Lys_halfConc	2.0	0178775
6	100_Lys	2.0	0178776
7	0_UOx_Buffer	1.0	0178777
8	0_UOx_halfConc	1.0	0178778
9	0_UOx	1.0	0178779
10	100_UOx_Buffer	2.0	0178780
11	100_UOx_halfConc	2.0	0178781
12	100_UOx	2.0	0178782
18	BLOCKED_BEAM	1.0	0178783
19	EMPTY_CELL	0.0	0178784

L1=4m_L2=1p3m				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_Lys_Buffer	1.0		0178787
2	0_Lys_halfConc	1.0		0178788
3	0_Lys	1.0		0178789
4	100_Lys_Buffer	2.0		0178790
5	100_Lys_halfConc	2.0		0178791
6	100_Lys	2.0		0178792
7	0_UOx_Buffer	1.0		0178793
8	0_UOx_halfConc	1.0		
20	EMPTY_BEAM	1.0	0178786	

Sample			**L1=L2=6m_central**	**L1=4m_L2=1p3m**
Position	**Name**	**Thickness**	**Scattering**	**Scattering**
1	0_Lys_Buffer	1.0	0178771	0178787
2	0_Lys_halfConc	1.0	0178772	0178788
3	0_Lys	1.0	0178773	0178789
4	100_Lys_Buffer	2.0	0178774	0178790
5	100_Lys_halfConc	2.0	0178775	0178791
6	100_Lys	2.0	0178776	0178792

7	0_UOx_Buffer	1.0	0178777	0178793
8	0_UOx_halfConc	1.0	0178778	
9	0_UOx	1.0	0178779	
10	100_UOx_Buffer	2.0	0178780	
11	100_UOx_halfConc	2.0	0178781	
12	100_UOx	2.0	0178782	
18	BLOCKED_BEAM	1.0	0178783	
19	EMPTY_CELL	0.0	0178784	

L1=4m_L2=1p3m				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_GI_Buffer	1.0		0178795
2	0_GI_halfConc	1.0		0178796
3	0_GI	1.0		0178797
4	100_GI_Buffer	2.0		0178798
5	100_GI_halfConc	2.0		0178799
6	100_GI	2.0		0178800
8	0_UOx_halfConc	1.0		0178801
9	0_UOx	1.0		0178802
10	100_UOx_Buffer	2.0		0178803
11	100_UOx_halfConc	2.0		0178804
12	100_UOx	2.0		0178805
18	BLOCKED_BEAM	1.0		0178806
19	EMPTY_CELL	0.0		0178807
20	EMPTY_BEAM	1.0	0178794	

L1=L2=6m_central				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_GI_Buffer	1.0	0178808	0178820
2	0_GI_halfConc	1.0	0178809	0178821
3	0_GI	1.0	0178810	0178822
4	100_GI_Buffer	2.0	0178811	0178823
5	100_GI_halfConc	2.0	0178812	0178824
6	100_GI	2.0	0178813	0178825
13	APD1	1.0	0178814	
14	APD2	1.0	0178815	
15	APD3	1.0	0178816	
16	APD4	1.0	0178817	
17	APD5	1.0	0178818	
20	EMPTY_BEAM	1.0	0178819	

Sample			**L1=4m_L2=1p3m**	**L1=L2=6m_central**
Position	**Name**	**Thickness**	**Scattering**	**Scattering**
1	0_GI_Buffer	1.0	0178795	0178820
2	0_GI_halfConc	1.0	0178796	0178821
3	0_GI	1.0	0178797	0178822

4	100_GI_Buffer	2.0	0178798	0178823
5	100_GI_halfConc	2.0	0178799	0178824
6	100_GI	2.0	0178800	0178825
8	0_UOx_halfConc	1.0	0178801	
9	0_UOx	1.0	0178802	
10	100_UOx_Buffer	2.0	0178803	
11	100_UOx_halfConc	2.0	0178804	
12	100_UOx	2.0	0178805	
18	BLOCKED_BEAM	1.0	0178806	
19	EMPTY_CELL	0.0	0178807	

L1=4m_L2=1p3m				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_RNase_Buffer	1.0		0178827
2	0_RNase_halfConc	1.0		0178828
3	0_RNase	1.0		0178829
4	100_RNase_Buffer	2.0		0178830
5	100_RNase_halfConc	2.0		0178831
6	100_RNase	2.0		0178832
7	0_Xylanase_Buffer	1.0		0178833
8	0_Xylanase_halfConc	1.0		0178834
9	0_Xylanase	1.0		0178835
10	100_Xylanase_Buffer	2.0		0178836
11	100_Xylanase_halfConc	2.0		0178837
12	100_Xylanase	2.0		0178838
20	EMPTY_BEAM	1.0	0178826	

L1=L2=6m_central				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	0_RNase_Buffer	1.0	0178839	0178852
2	0_RNase_halfConc	1.0	0178840	0178853
3	0_RNase	1.0	0178841	0178854
4	100_RNase_Buffer	2.0	0178842	0178855
5	100_RNase_halfConc	2.0	0178843	0178856
6	100_RNase	2.0	0178844	0178857
7	0_Xylanase_Buffer	1.0	0178845	0178858
8	0_Xylanase_halfConc	1.0	0178846	0178859
9	0_Xylanase	1.0	0178847	0178860
10	100_Xylanase_Buffer	2.0	0178848	0178861
11	100_Xylanase_halfConc	2.0	0178849	0178862
12	100_Xylanase	2.0	0178850	0178863
20	EMPTY_BEAM	1.0	0178851	

Sample			**L1=4m_L2=1p3m**	**L1=L2=6m_central**
Position	**Name**	**Thickness**	**Scattering**	**Scattering**
1	0_RNase_Buffer	1.0	0178827	0178852

2	0_RNase_halfConc	1.0	0178828	0178853
3	0_RNase	1.0	0178829	0178854
4	100_RNase_Buffer	2.0	0178830	0178855
5	100_RNase_halfConc	2.0	0178831	0178856
6	100_RNase	2.0	0178832	0178857
7	0_Xylanase_Buffer	1.0	0178833	0178858
8	0_Xylanase_halfConc	1.0	0178834	0178859
9	0_Xylanase	1.0	0178835	0178860
10	100_Xylanase_Buffer	2.0	0178836	0178861
11	100_Xylanase_halfConc	2.0	0178837	0178862
12	100_Xylanase	2.0	0178838	0178863

13/12/2021 - Remeasuring the small proteins directly from SEC without further concentration. Same instrument setup as previously, however, using low resolution velocity selector at 0 tilt, 10% wavelength resolution.

L1=4m_L2=1p3m				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	EMPTY_BEAM	1.0	0220312	
2	BLOCKED_BEAM	1.0		0220322
3	0_Lys_Buffer	1.0		0220321
4	0_RNase_Buffer	1.0		0220320
5	0_Lys_3p3mg	1.0		0220319
6	0_RNase_3p3mg	1.0		0220318
7	100_Lys_Buffer	1.0		0220317
8	100_RNase_Buffer	1.0		0220316
9	100_Lys_3p3mg	1.0		0220315
10	100_RNase_3p0mg	1.0		0220314
11	EmptyCell	1.0		0220313

L1=L2=6m_central				
Position	**Name**	**Thickness**	**Transmission**	**Scattering**
1	EMPTY_BEAM	1.0	0220323	
2	BLOCKED_BEAM	1.0		0220342
3	0_Lys_Buffer	1.0	0220324	0220341
4	0_RNase_Buffer	1.0	0220325	0220340
5	0_Lys_3p3mg	1.0	0220326	0220339
6	0_RNase_3p3mg	1.0	0220327	0220338
7	100_Lys_Buffer	1.0	0220328	0220337
8	100_RNase_Buffer	1.0	0220329	0220336
9	100_Lys_3p3mg	1.0	0220330	0220335
10	100_RNase_3p0mg	1.0	0220331	0220334
11	EmptyCell	1.0	0220332	0220333

Sample			L1=4m_L2=1p3m	L1=L2=6m_central
Position	**Name**	**Thickness**	**Scattering**	**Scattering**
2	BLOCKED_BEAM	1.0	0220322	0220342
3	0_Lys_Buffer	1.0	0220321	0220341
4	0_RNase_Buffer	1.0	0220320	0220340
5	0_Lys_3p3mg	1.0	0220319	0220339
6	0_RNase_3p3mg	1.0	0220318	0220338
7	100_Lys_Buffer	1.0	0220317	0220337
8	100_RNase_Buffer	1.0	0220316	0220336
9	100_Lys_3p3mg	1.0	0220315	0220335
10	100_RNase_3p0mg	1.0	0220314	0220334
11	EmptyCell	1.0	0220313	0220333