

	Experiment title: Structural studies of Apical Merozoite Antigen 1 (AMA1) from <i>Plasmodium vivax</i>	Experiment number: 30-01-578
Beamline: BM30A	Date of experiment: from: 13.11.2002 to: 14.11.2002	Date of report:
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Report:

Crystals of Apical Merozoite Antigen 1 (AMA1) give weak diffraction, precluding the possibility to screen heavy atom derivatives on a rotating anode source. This has required that the screening be done at a synchrotron beam-line. During the experiment, crystals of AMA1 soaked in three different heavy atom salts were tested : K_2PtCl_6 , K_2PtCl_4 , $K_2Pt(CN)_4$.

Each heavy atom-soaked crystal was first screened by taking a fluorescence spectrum to detect the presence of the heavy atom. If present by this test, diffraction data were collected and analysed for the anomalous signal. The $K_2Pt(CN)_4$ and K_2PtCl_6 soakings showed no fluorescence signal and were thus discarded. The K_2PtCl_4 derivative showed an anomalous signal at the peak wavelength (1.071916 Å) and collection was therefore continued at the inflection wavelength (1.072176 Å). A more careful data treatment showed that the anomalous signal dropped rapidly with increasing Bragg angle, reaching noise level at about 5 Å resolution. We have been unable to interpret the Patterns so far.

Results of data treatment (with HKL) after merging Friedel pairs shows high values of χ^2 to about 6 Å only, suggesting that the Platinum atoms possess a degree of disorder:

(1) peak wavelength

Shell	Lower	Upper	Average	Average	Norm.	Linear	Square
limit	Angstrom	I	error	stat.	Chi**2	R-fac	R-fac
99.00	7.53	1777.9	44.5	44.5	7.008	0.030	0.056
	7.53	5.98	595.5	19.1	19.1	2.027	0.031
	5.98	5.22	490.2	19.3	19.3	1.481	0.036
	5.22	4.74	509.8	21.9	21.9	1.051	0.032
	4.74	4.40	541.1	25.8	25.8	1.026	0.034
	4.40	4.14	390.6	23.2	23.2	1.114	0.046
	4.14	3.94	292.3	23.2	23.2	1.110	0.066
	3.94	3.77	227.5	24.1	24.1	1.226	0.091
	3.77	3.62	167.3	26.7	26.7	1.019	0.120
	3.62	3.50	166.8	28.6	28.6	1.134	0.135
	3.50	3.39	115.4	31.3	31.3	1.028	0.201
	3.39	3.29	90.5	32.7	32.7	0.996	0.244
	3.29	3.20	64.8	35.0	35.0	0.947	0.331
	3.20	3.12	46.0	39.1	39.1	1.084	0.566
	3.12	3.05	42.2	44.9	44.9	1.169	0.606
All reflections		397.2	28.7	28.7	1.541	0.061	0.057

(2) edge wavelength

Shell	Lower	Upper	Average	Average	Norm.	Linear	Square
limit	Angstrom	I	error	stat.	Chi**2	R-fac	R-fac
99.00	7.53	4345.5	100.5	100.5	3.974	0.018	0.020
	7.53	5.98	1504.3	43.1	43.1	1.411	0.020
	5.98	5.22	1221.3	39.8	39.8	1.050	0.022
	5.22	4.74	1262.8	42.0	42.0	0.998	0.020
	4.74	4.40	1264.1	47.0	47.0	0.882	0.022
	4.40	4.14	967.6	41.0	41.0	0.914	0.027
	4.14	3.94	699.6	37.5	37.5	0.945	0.037
	3.94	3.76	554.9	37.1	37.1	0.929	0.045
	3.76	3.62	407.4	34.6	34.6	0.897	0.057
	3.62	3.49	392.6	37.0	37.0	1.026	0.069
	3.49	3.39	273.2	34.6	34.6	1.016	0.100
	3.39	3.29	210.9	33.0	33.0	1.033	0.121
	3.29	3.20	141.3	36.7	36.7	1.153	0.199
	3.20	3.12	98.7	42.2	42.2	0.935	0.315
	3.12	3.05	81.2	43.9	43.9	1.005	0.408
All reflections		927.6	43.7	43.7	1.182	0.036	0.025