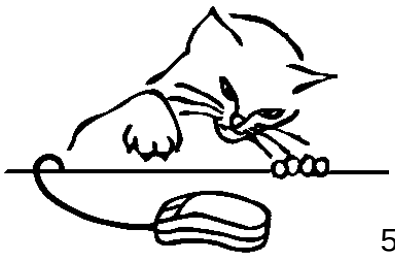
Eindhoven, 6 November 1997



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Case Study: About handling overlapping GPC peaks with DAx

- the first page shows a plot of the measurement data as they were supplied to us. The data were in a comma separated ASCII file, which DAx read without a need for user intervention (that is, the frequency and other parameters were correctly retrieved from the file without further user input).
  The peaks in the plot have been labeled with the Mw at the peak top and with the weight averaged Mw for the entire peak. To calculate Mw's based on elution volumes, a calibration is needed. We created a dummy calibration for this purpose.
- the second page has a plot and a table of this calibration.
- the third page contains an enlargement of the area between 1100 and 1500 seconds, where two peaks overlap. Peaks are again labeled with Mw at peak top and weight averaged Mw, as are the graphs on all remaining pages.
  DAx has the ability to automatically allocate shoulder peaks. That is, whenever two or more peaks are not baseline separated, DAx will consider the possibility that the peaks form a cluster of a main peak and one or more shoulder peaks. In the example, DAx considered the leftmost of the two overlapping peaks the main peak, and marked the right peak as a shoulder peak.
- the fourth page contains a plot of the same area. The leftmost peak was now made the shoulder peak. DAx conveniently lets you do this using the mouse.
- the fifth page contains a plot in which the overlapping peaks are treated equally. Note that the Mw at peak top is always the same, since the peak top has the same location. But the weight averaged Mw changes as more or less area is assigned to a peak.
- the sixth page compares the measurement data with two purely Gaussian peaks with the same peak top and peak height, and a standard deviation cooresponding to the statistical standard deviation. The standard deviations were derived from the measurement data as displayed on the fifth page, i.e. without marking either peak as a shoulder peak.
- the seventh page compares the measurement data with the sum of the two purely Gaussian peaks. Parameters for the Gaussian peaks clearly need to be further refined to get an acceptable fit.

PP van Mierlo, M.Sc.Eng. 

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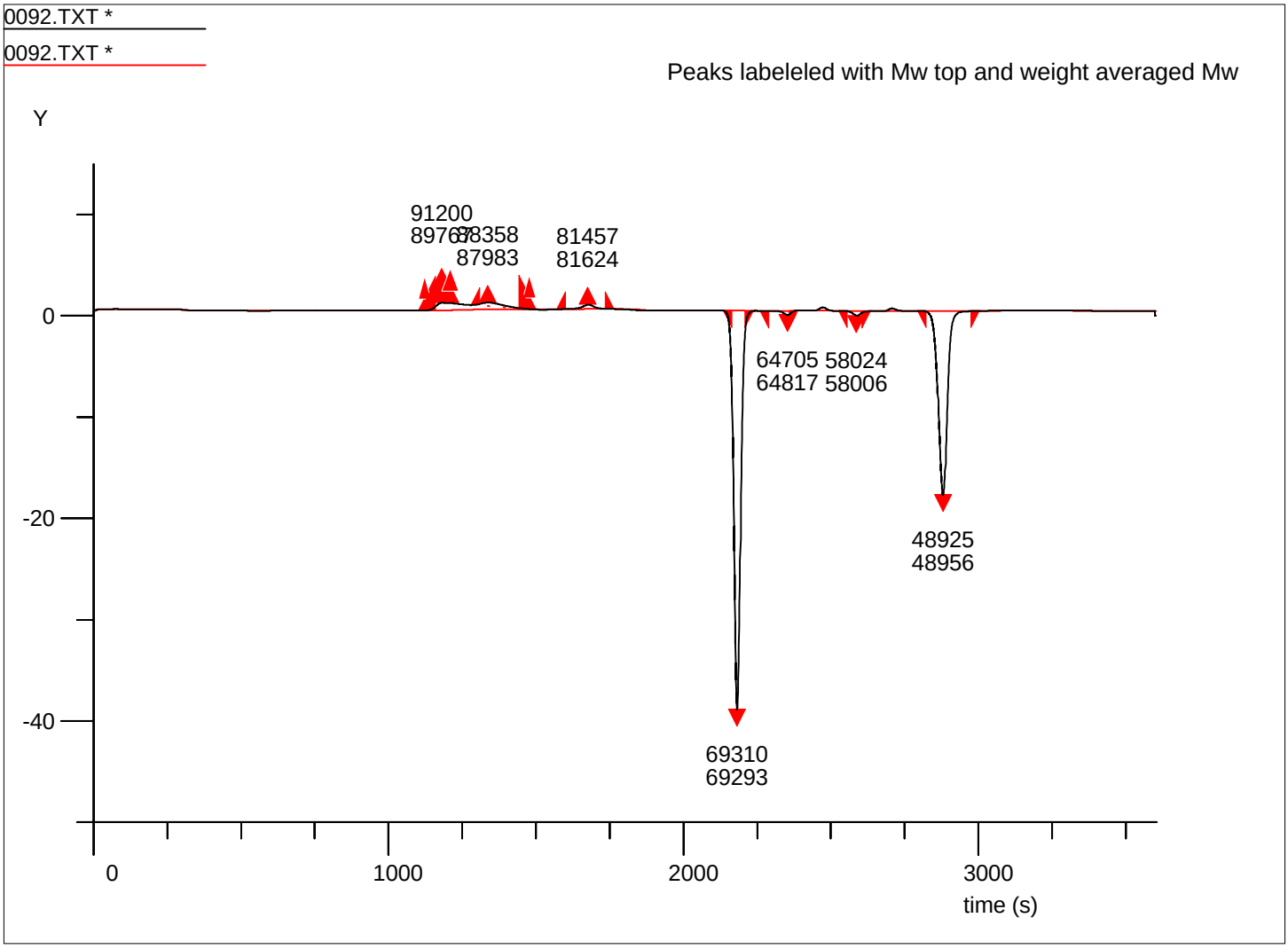
Measurement Report: Overlapping GPC peaks

G:\CSERVE\DOWNLOAD\BRILJA~1\009 31/10/97 20:28:58
0092.TXT * measured 00/00/00 00:00:00 by



Point to point noise (V): 0.0084803 (0.02%); RMS Noise (V): 0.0042401 (0.01%)

Peak	Begin (s)	Top (s)	End (s)	Top (V)	Annotation	Area (V.s)	Mp	Mn	Mw	Mz	D
1S	1102.000	1182.000	1501.000	0.7619		122.92	91200	89744	89767	89789	1.000
2s	1282.000	1338.000	1482.000	0.3605		31.475	88358	87979	87983	87988	1.000
3	1572.000	1677.000	1765.000	0.38602		20.188	81457	81620	81624	81628	1.000
4	2136.000	2183.000	2239.000	-39.38		-1028	69310	69292	69293	69294	1.000
5	2261.000	2354.000	2388.000	-0.38521		-10.364	64705	64814	64817	64820	1.000
6	2528.000	2587.000	2634.000	-0.44307		-13.911	58024	58003	58006	58009	1.000
7	2794.000	2881.000	3005.000	-18.135		-633.1	48925	48951	48956	48961	1.000
7 of 7 peaks						1859.9					

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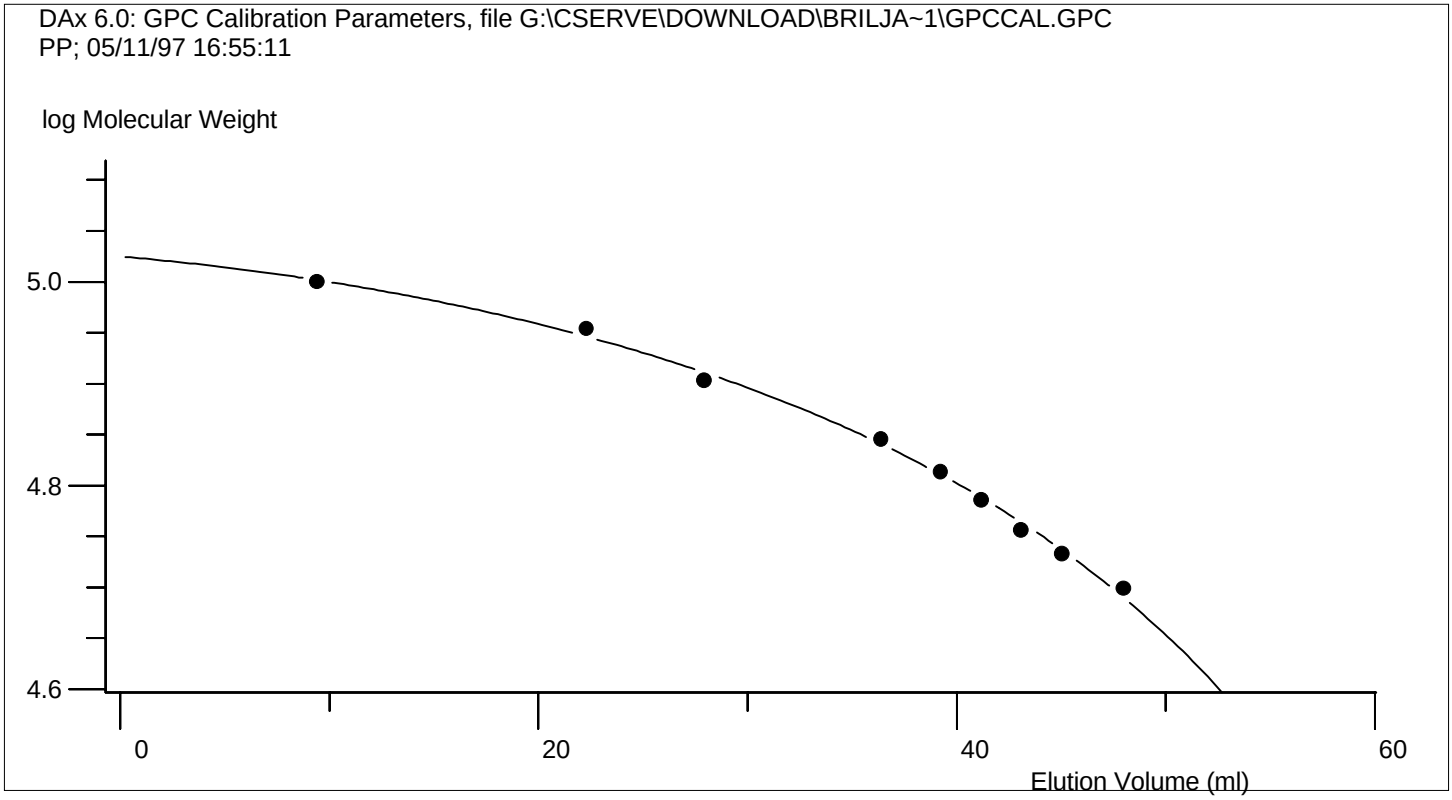
GPC Calibration Data



GPC Calibration Parameters G:\CSERVE\DOWNLOAD\BRILJA~1\GPCCAL.GPC

	Polyn.Par	Used?	EV (ml)	Mw	Check	Data
1	1.0591E+05	Yes	48.017	50000	48924.8	0092.TXT *
2	-440.34	Yes	45.067	54000	54492.2	0092.TXT *
3	-15.545	Yes	43.117	57000	58023.9	0092.TXT *
4		Yes	41.217	61000	61351.3	0092.TXT *
5		Yes	39.233	65000	64704.9	0092.TXT *
6		Yes	36.383	70000	69309.8	0092.TXT *
7		Yes	27.950	80000	81456.9	0092.TXT *
8		Yes	22.300	90000	88358.1	0092.TXT *
9		Yes	9.417	100000	100383	0092.TXT *

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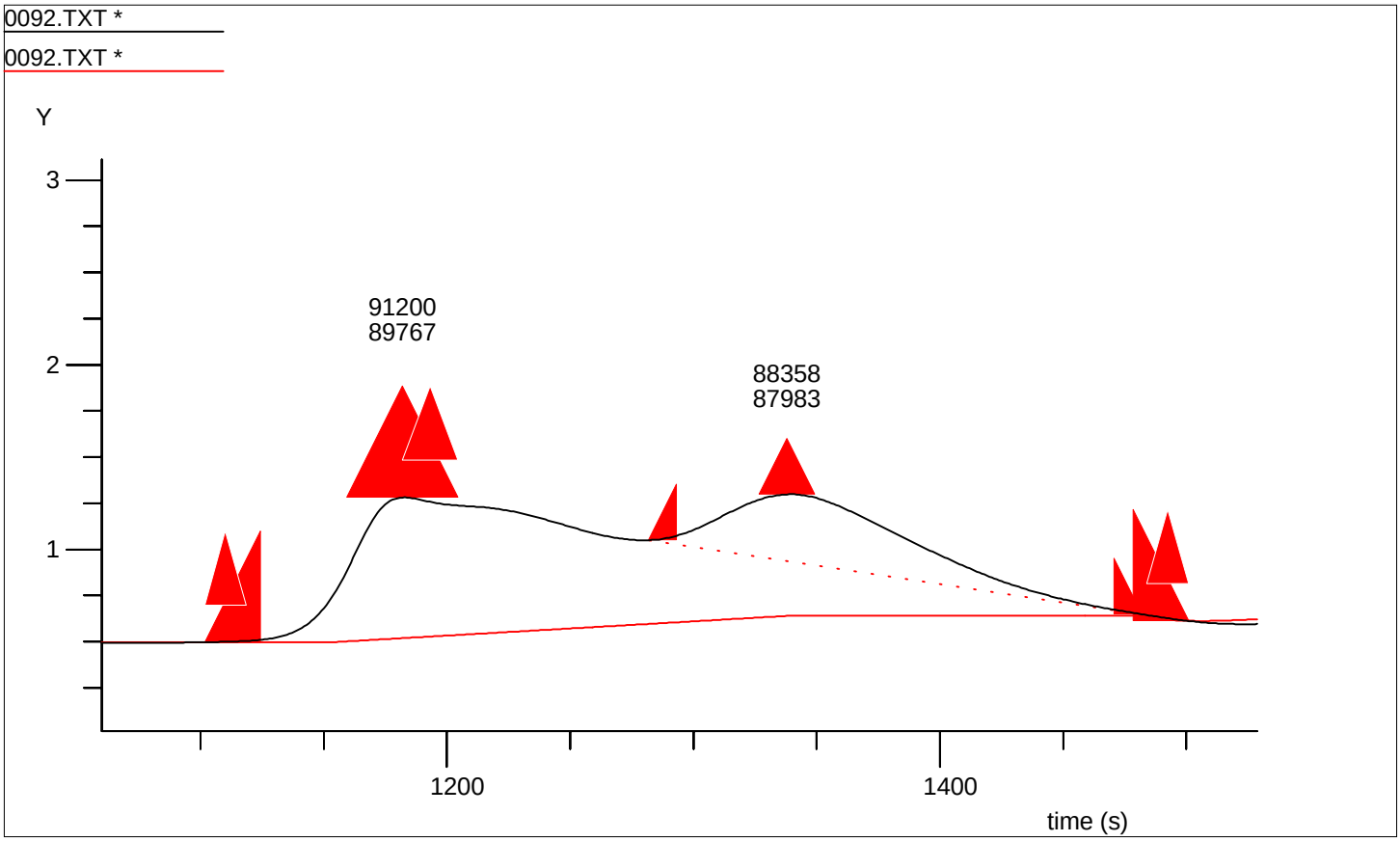
Detail; right peak was automatically designated as a shoulder



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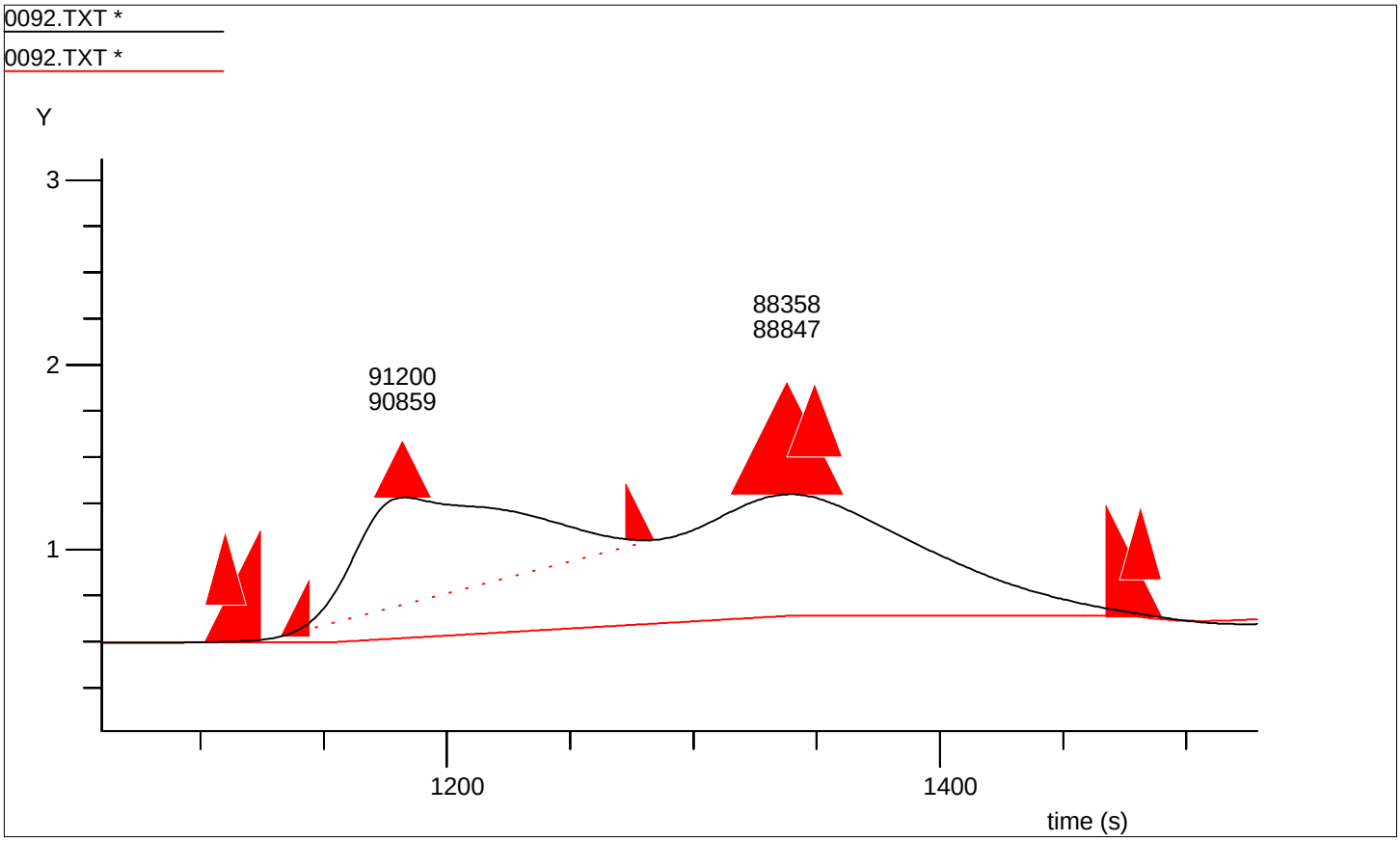
Detail; left peak has been made shoulder



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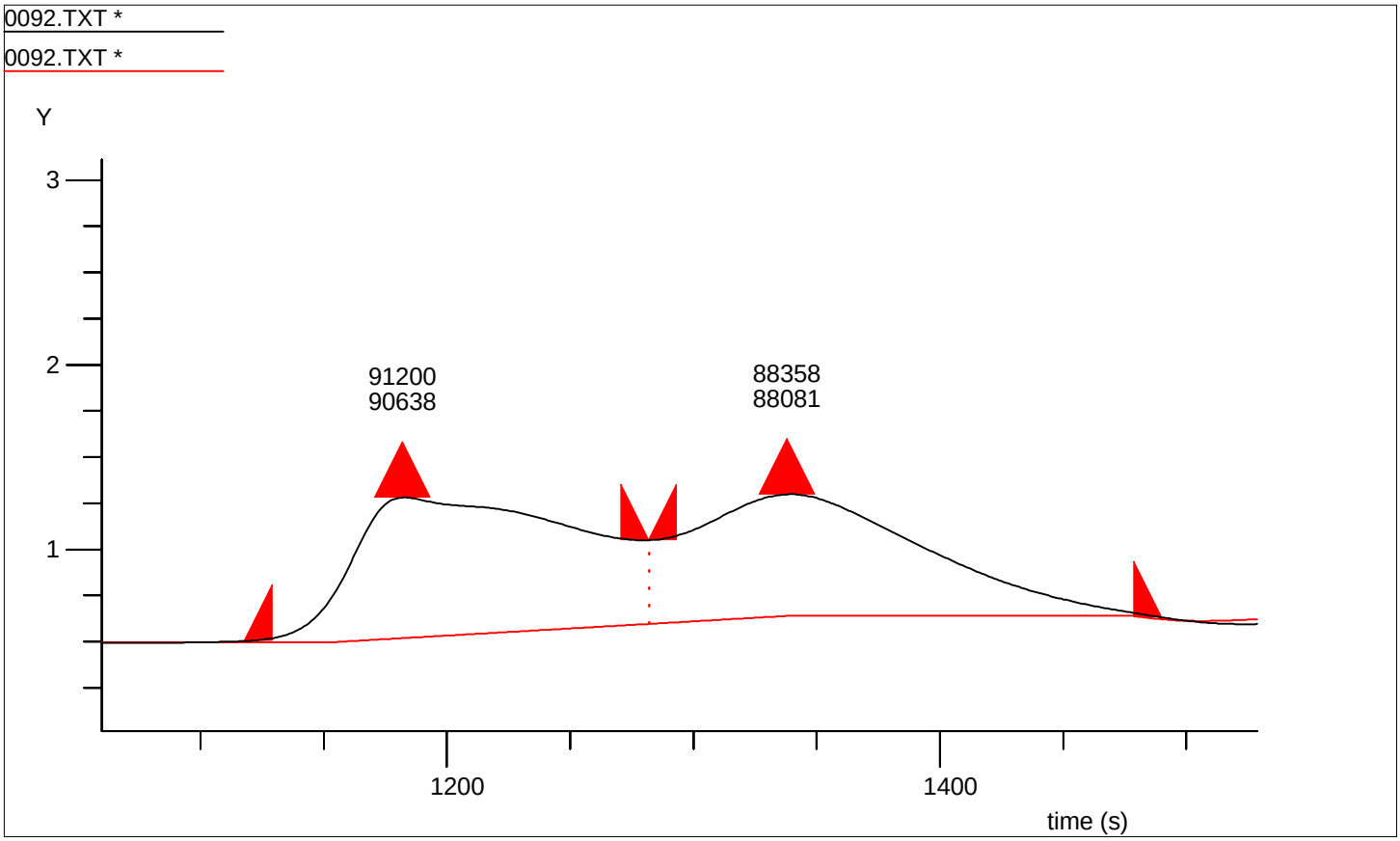
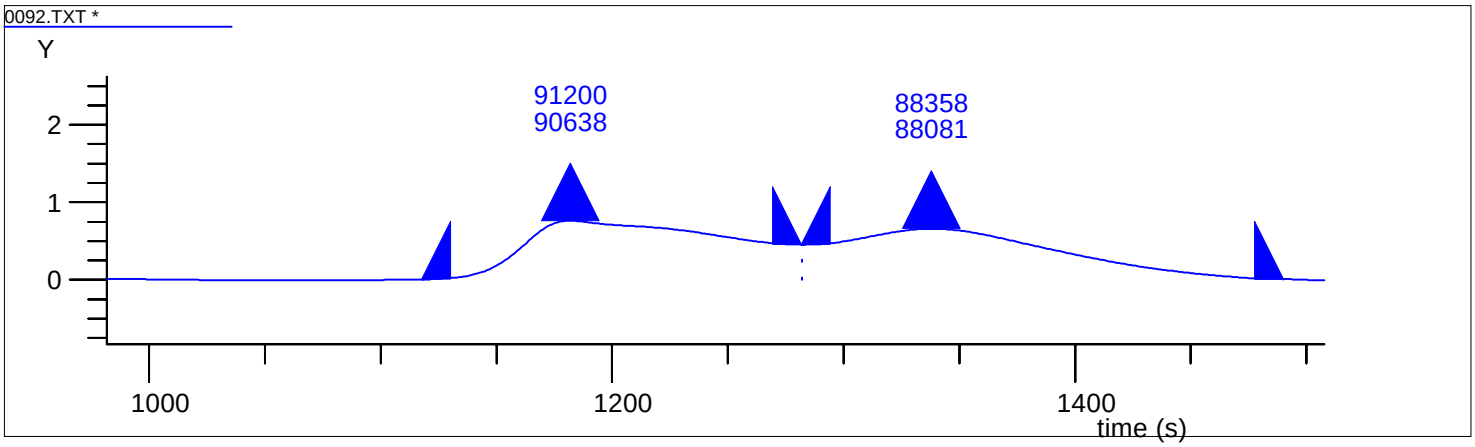
Detail; no shoulder peaks being used

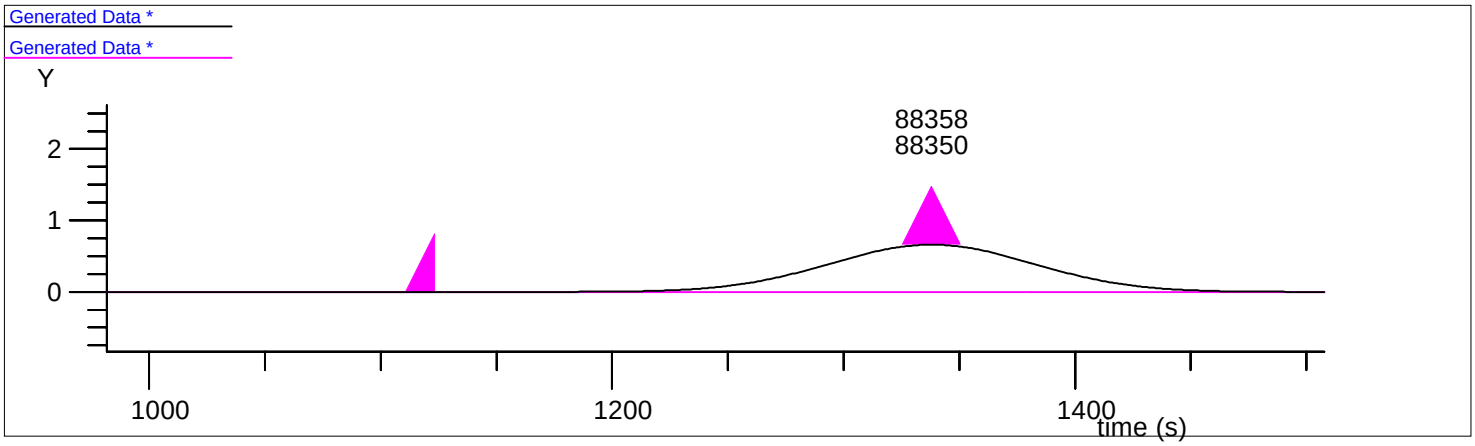


Comparison with Gaussian curves



Point to point noise (V): 0.0084803 (0.02%); RMS Noise (V): 0.0042401 (0.01%)

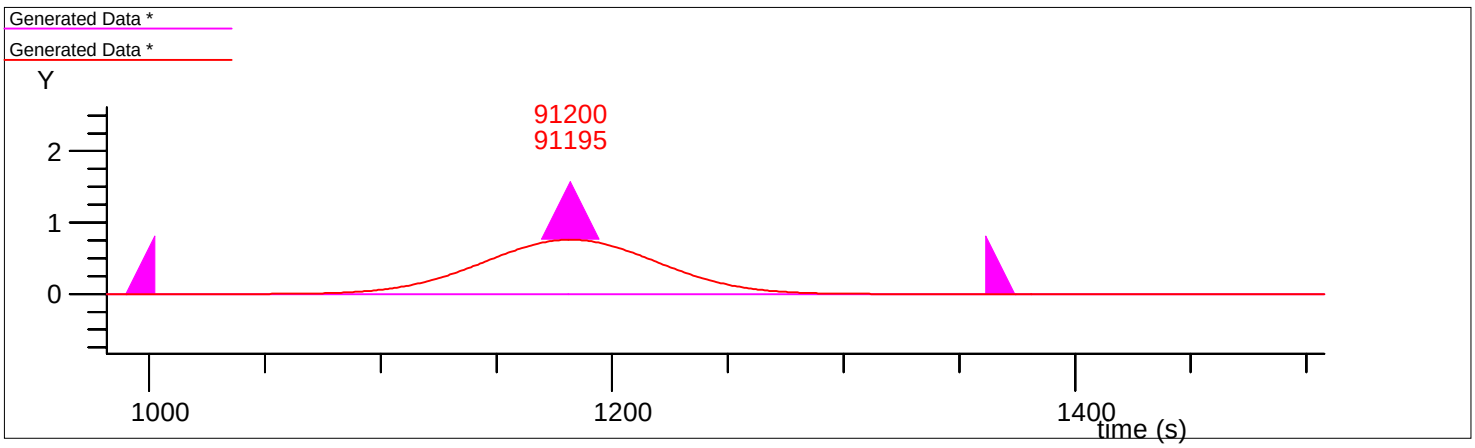
Peak	Begin (s)	Top (s)	End (s)	Top (V)	Area (V.s)	Mp	Mn	Mw	Mz	D
1	1118.000	1182.000	1282.000	0.7619	80.086	91200	90633	90638	90642	1.000
2	1282.000	1338.000	1490.000	0.6582	74.675	88358	88073	88081	88089	1.000
2 of 2 peaks					3525.4					



Point to point noise (V): 0 (0.00%); RMS Noise (V): 0 (0.00%)

Peak	Begin (s)	Top (s)	End (s)	Top (V)	Area (V.s)	Mp	Mn	Mw	Mz	D
1 of 1 peaks					71.568					
1	1111.000	1338.000	1565.000	0.66	71.568	88358	88342	88350	88358	1.000

(more)



Point to point noise (V): 0.015058 (1.98%); RMS Noise (V): 4.6674E-10 (0.00%)

Peak	Begin (s)	Top (s)	End (s)	Top (V)	Area (V.s)	Mp	Mn	Mw	Mz	D
1	990.000	1182.000	1374.000	0.76	69.038	91200	91190	91195	91199	1.000

(more)

DAx 6.0: PP 05/11/97 18:21:42

Data Set	Measured	Disk File	Description
0092.TXT *	00/00/00 00:00:00;	G:\CSERVE\DOWNLOAD\BRILJA~1\PIPO2.Dd1	
Generated Data *	00/00/00 00:00:00;	*	
Generated Data *	00/00/00 00:00:00;	G:\CSERVE\DOWNLOAD\BRILJA~1\PIPO2.Db1 *	Sum of two generated Gaussian curves