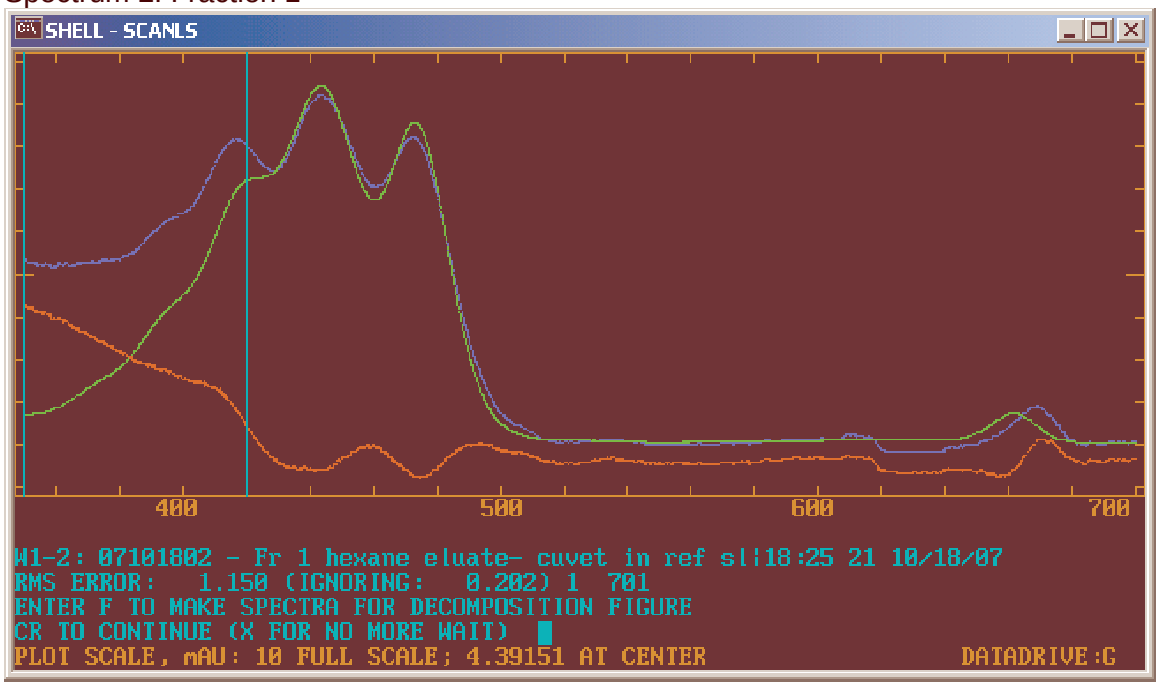
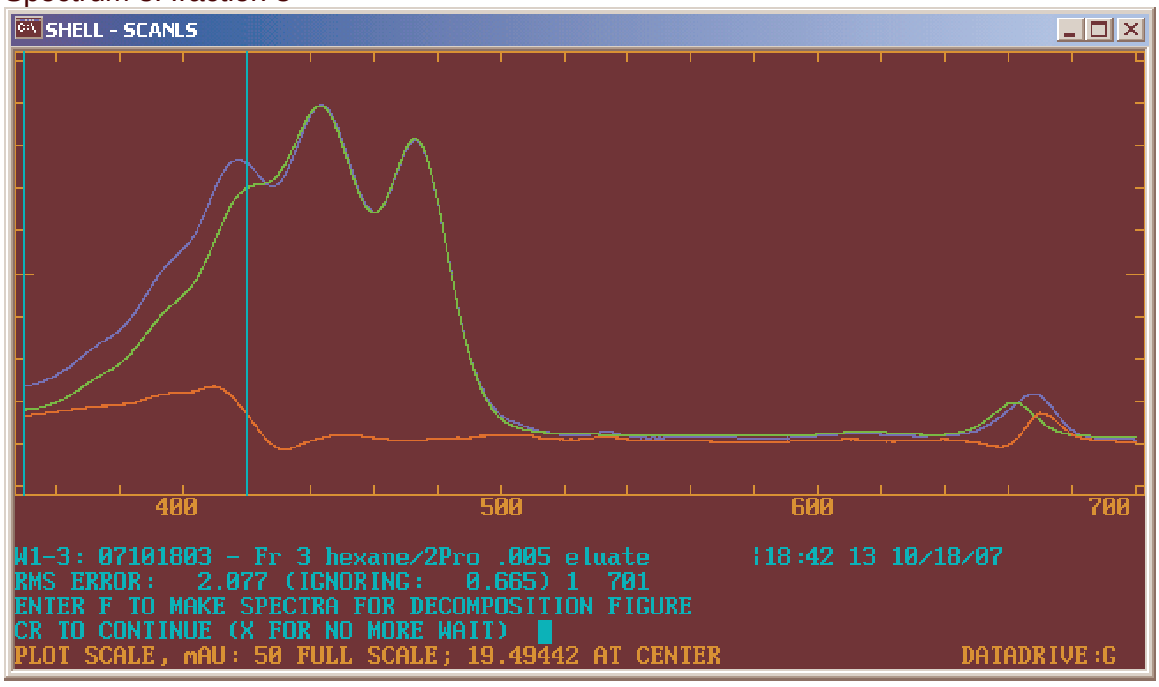
Each screen displays the fit to one of the experimental spectra (blue). The constructed fit is green, and the residual is red. In this case the wavelength-region below 420 is being ignored in the fitting procedure. The spectra are fractions from a sucrose-column separation of spinach pigments, in hexane as they are eluted. They are being fit with standard spectra of beta carotene, chlorophyl a, and chlorophyl b which were constructed from spectra #6, 10 and 12 (so those spectra fit perfectly). Spectra 2 and 3 do not fit well because of additional component(s) apparently with peaks at 668 and 410 nm. It is immediately obvious that the fit is poor and the results should not be taken seriously. Once the additional component has been identified and its spectrum included, these fractions can be analyzed also. (spectrum 2 is 0.02 AUFS, and a baseline glitch at 620 nm is apparent)

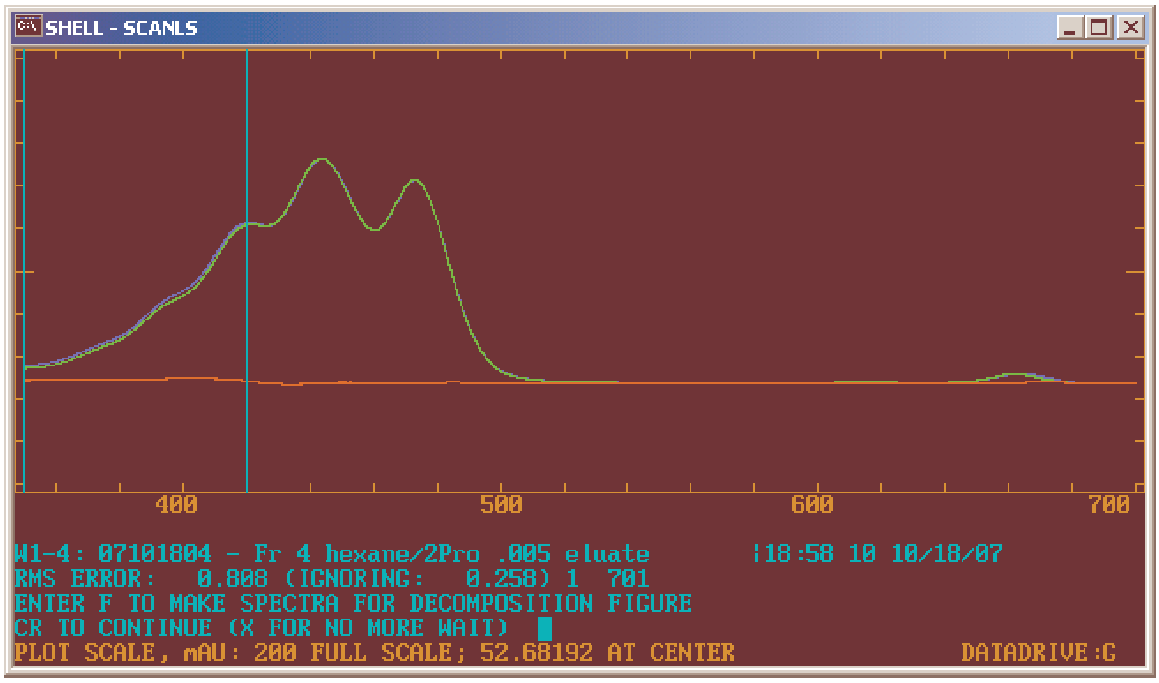
Spectrum 2: Fraction 1

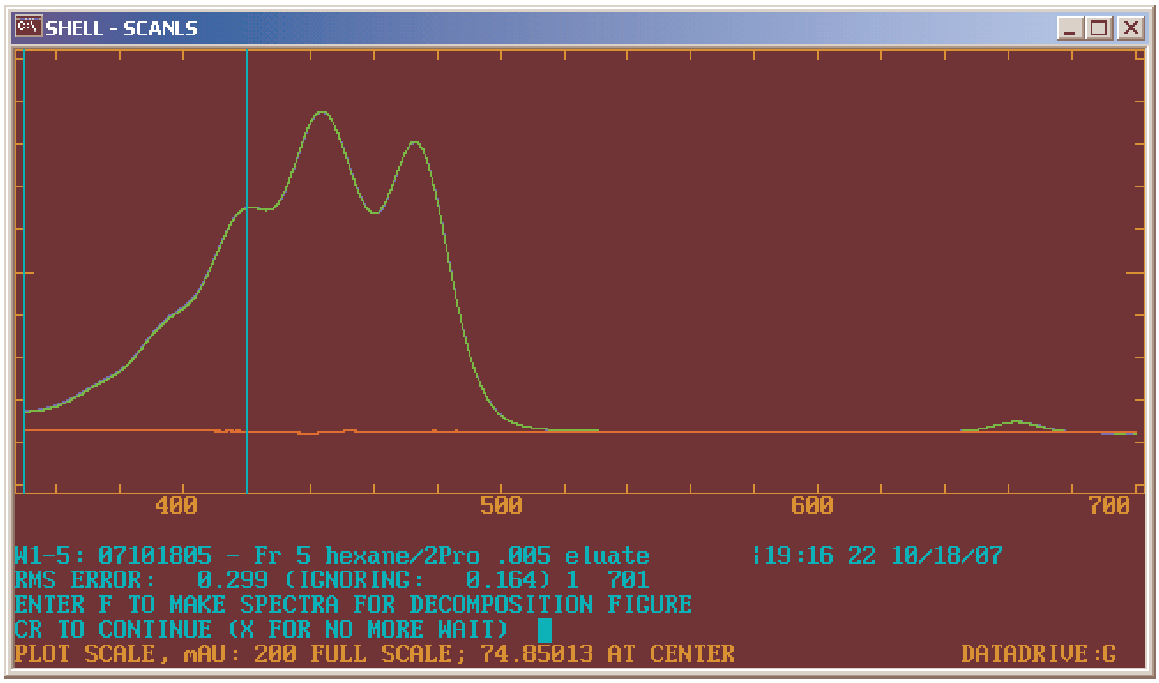


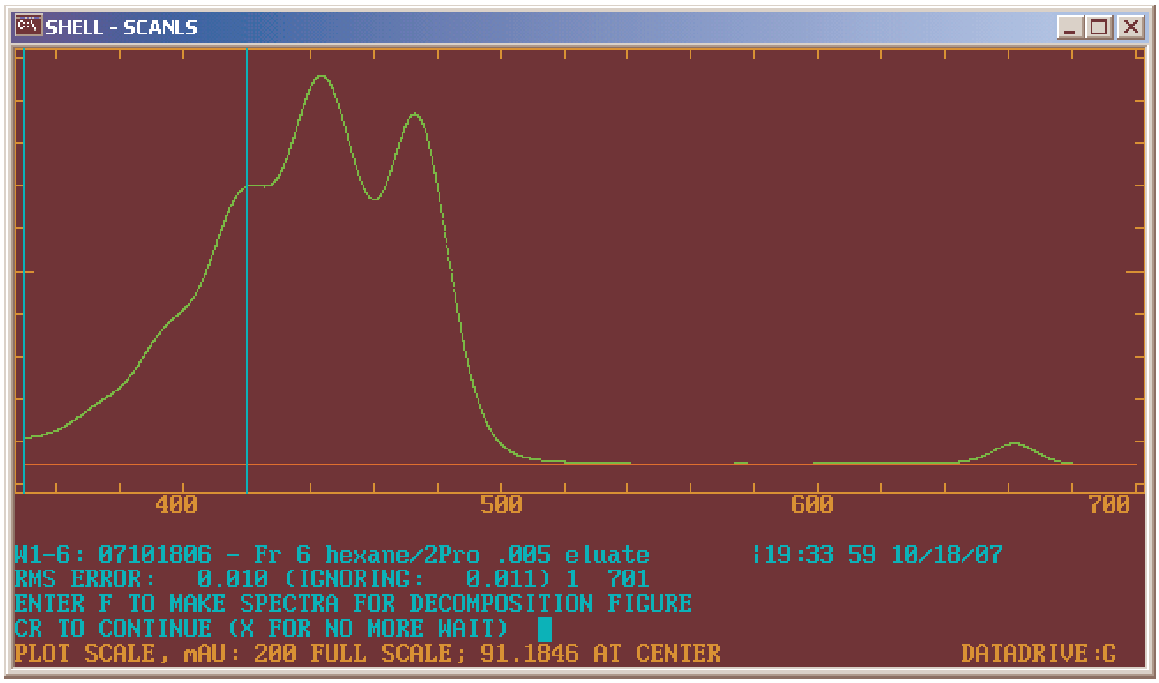
Spectrum 3: fraction 3

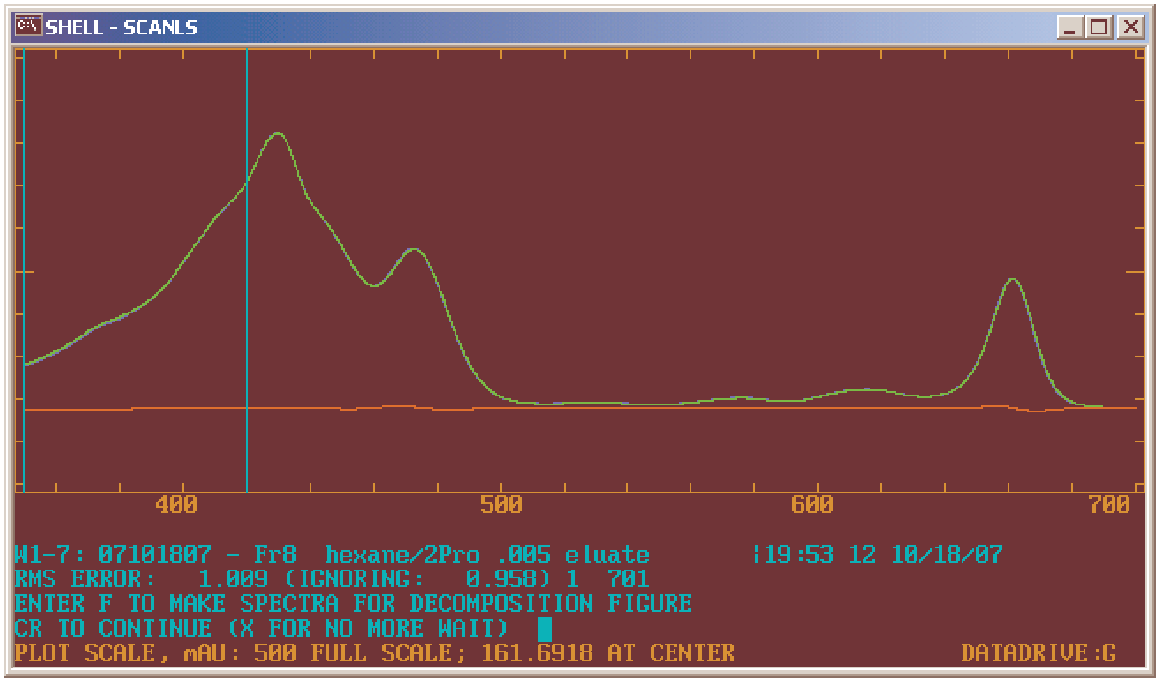


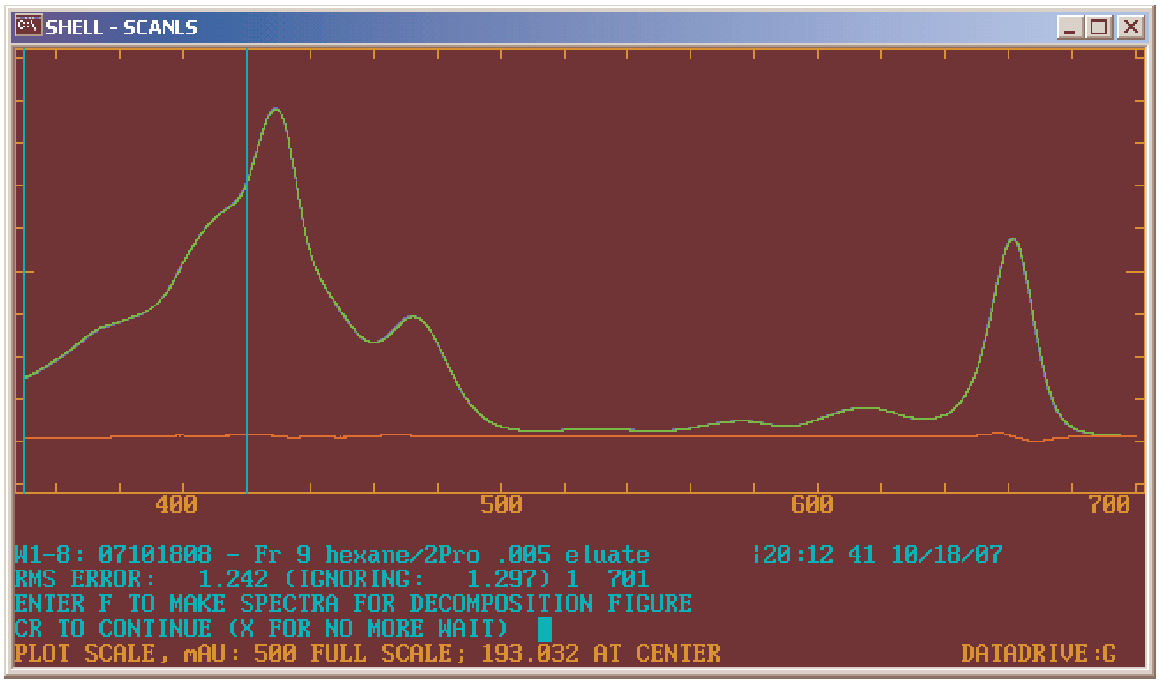
Spectra 4 to 13 fit well, apparently no other component is eluting here. Carotenoid peaks in

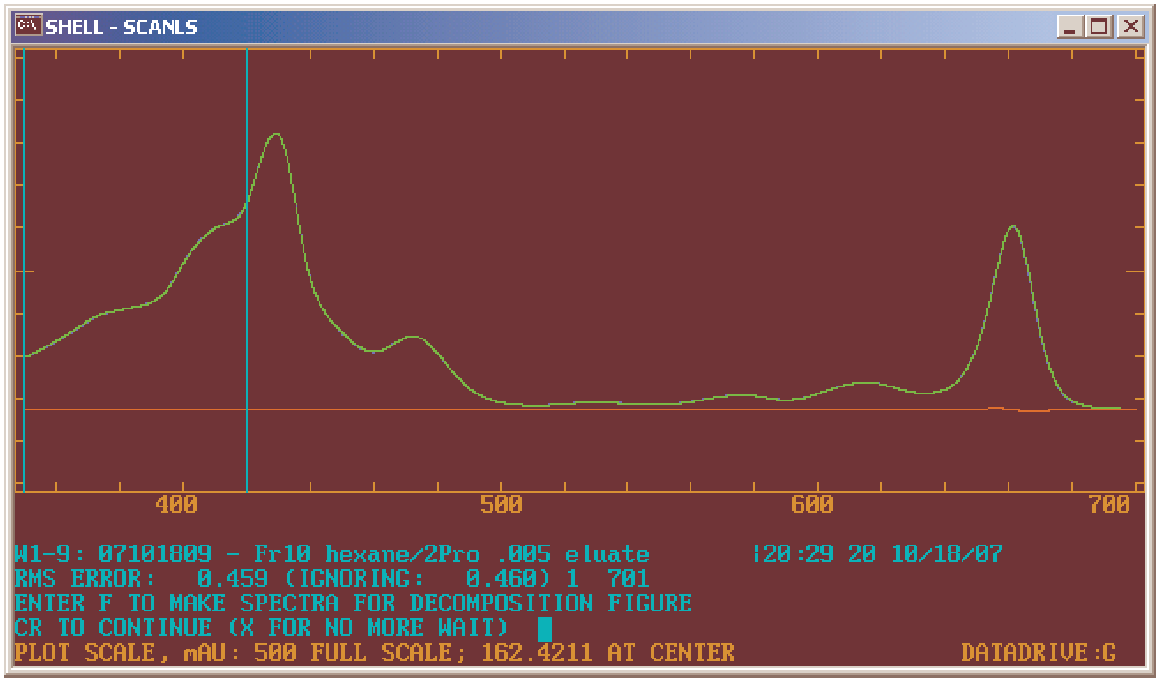


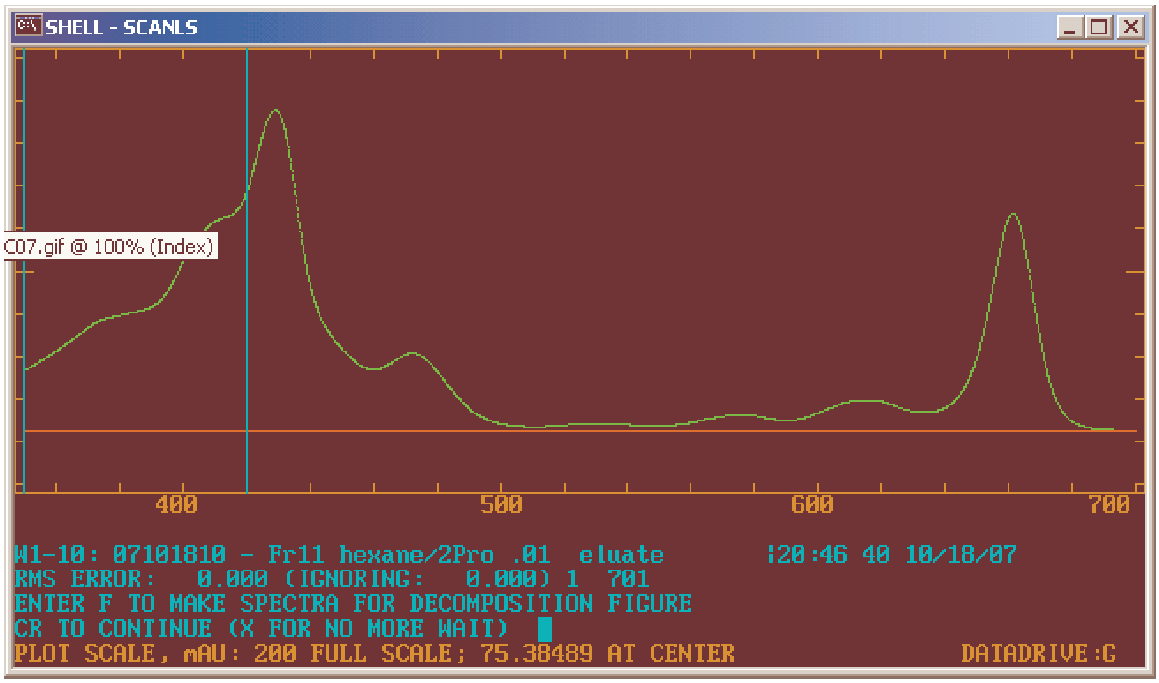


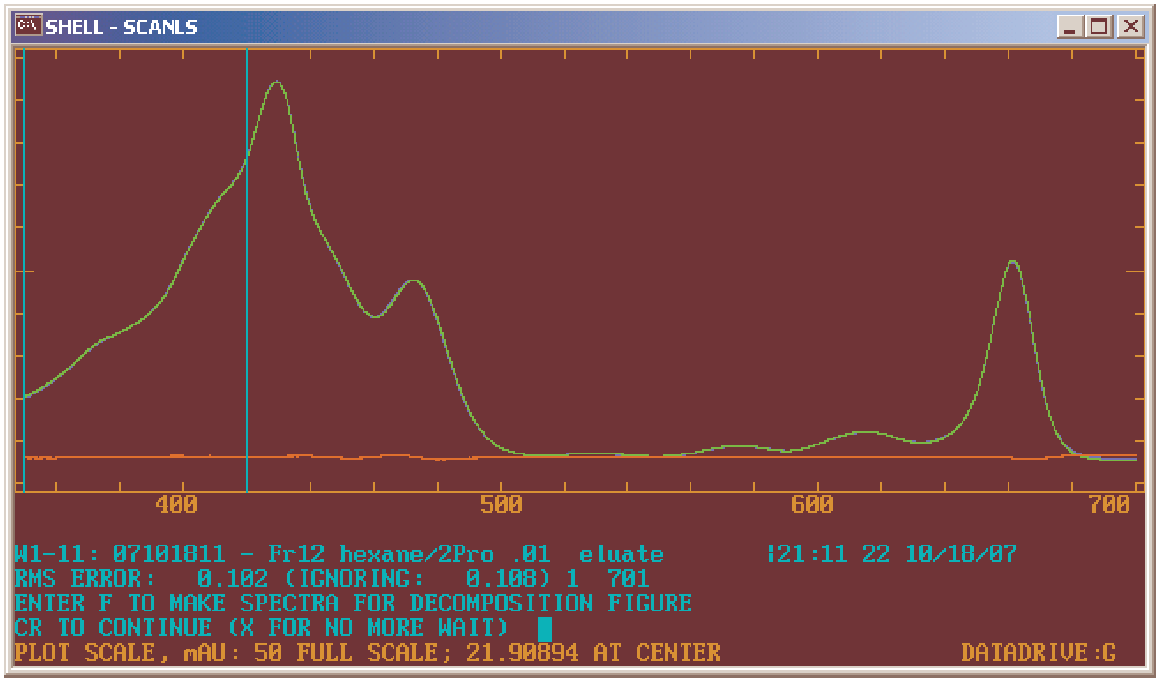

SHELL - SCANLS
400
500
600
700
W1-6: 07101806 - Fr 6 hexane/2Pro .005 eluate 19:33 59 10/18/07
RMS ERROR: 0.010 (IGNORING: 0.011) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 200 FULL SCALE; 91.1846 AT CENTER
DATADRIVE:G

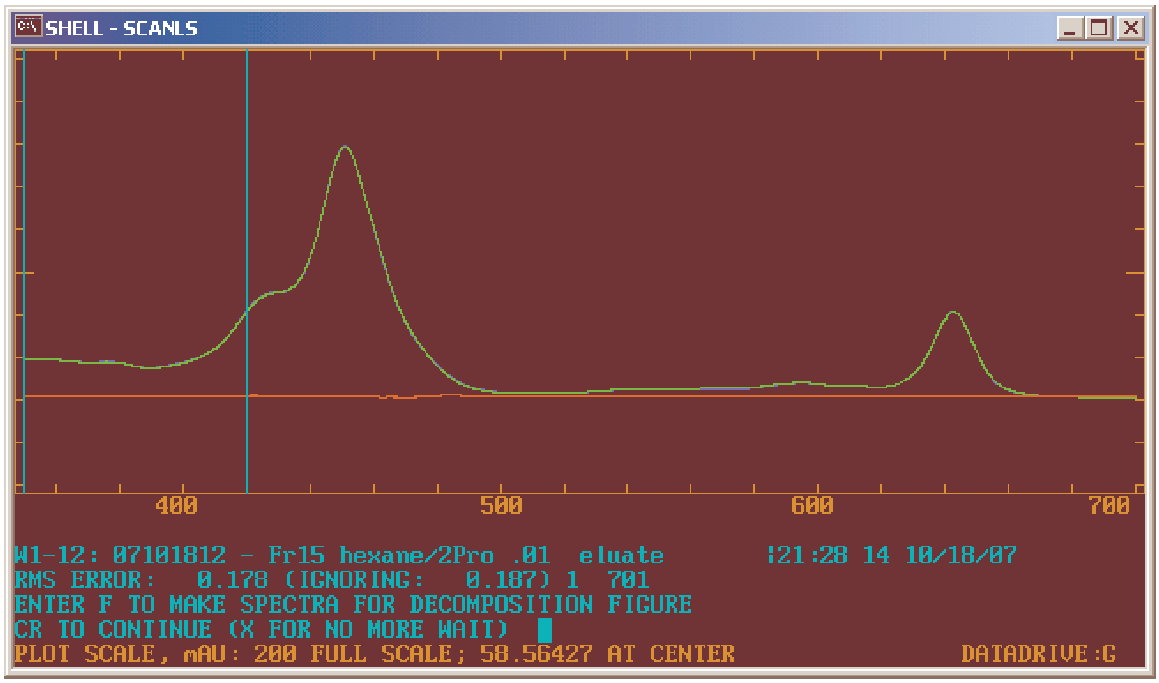

SHELL - SCANLS
400
500
600
700
W1-7: 07101807 - Fr8 hexane/2Pro .005 eluate 19:53 12 10/18/07
RMS ERROR: 1.009 (IGNORING: 0.958) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 500 FULL SCALE; 161.6918 AT CENTER
DATADRIVE:G

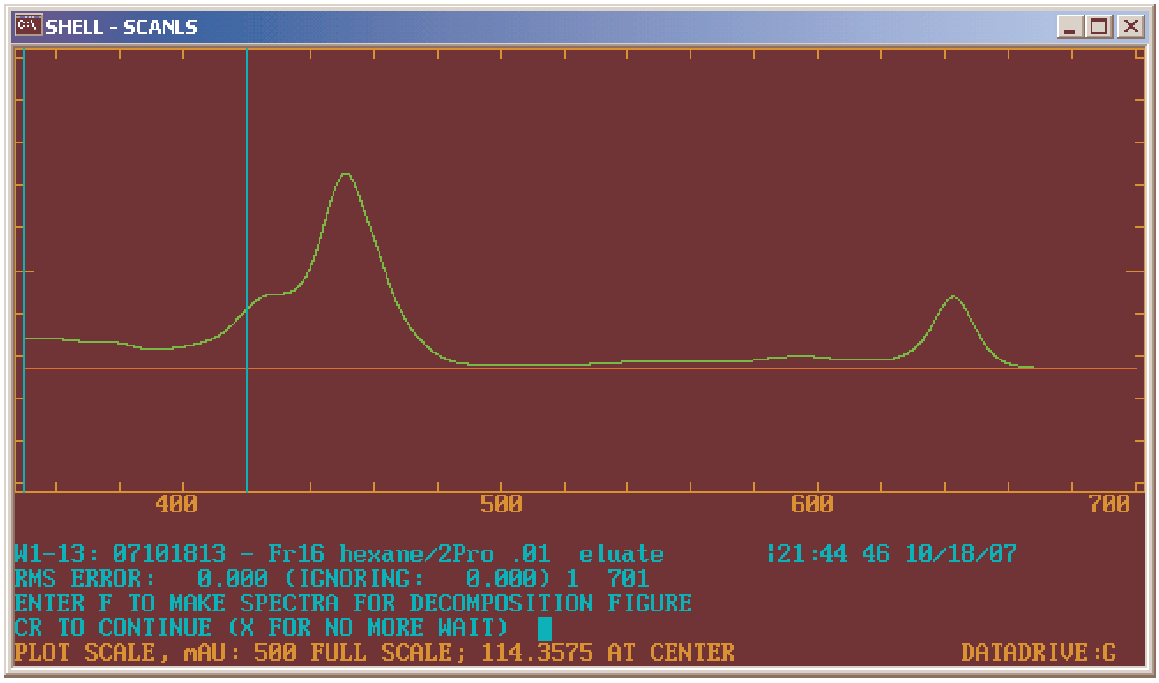

SHELL - SCANLS
400
500
600
700
W1-8: 07101808 - Fr 9 hexane/2Pro .005 eluate 20:12 41 10/18/07
RMS ERROR: 1.242 (IGNORING: 1.297) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 500 FULL SCALE; 193.032 AT CENTER
DATADRIVE:C


SHELL - SCANLS
400
500
600
700
W1-9: 07101809 - Fr10 hexane/2Pro .005 eluate 20:29 20 10/18/07
RMS ERROR: 0.459 (IGNORING: 0.460) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 500 FULL SCALE; 162.4211 AT CENTER
DATADRIVE:C

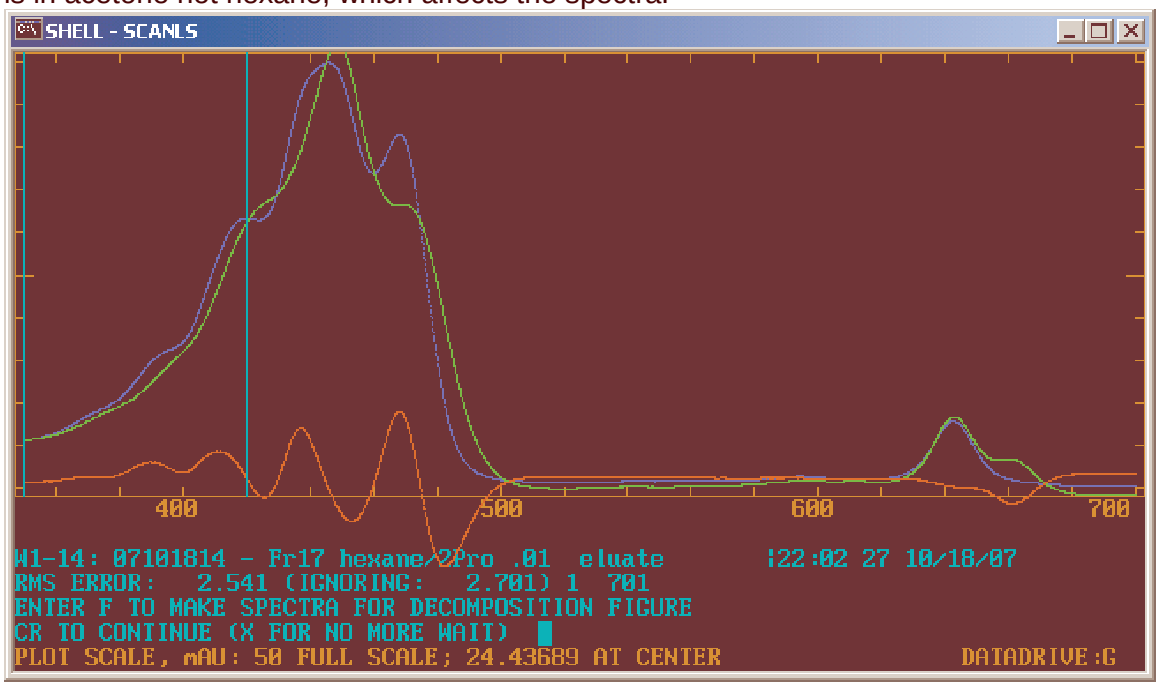

SHELL - SCANLS
C07.gif @ 100% (Index)
400
500
600
700
W1-10: 07101810 - Fr11 hexane/2Pro .01 eluate ¦20:46 40 10/18/07
RMS ERROR: 0.000 (IGNORING: 0.000) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 200 FULL SCALE; 75.38489 AT CENTER
DAIADRIVE:C


SHELL - SCANLS
400
500
600
700
W1-11: 07101811 - Fr12 hexane/2Pro .01 eluate ¦21:11 22 10/18/07
RMS ERROR: 0.102 (IGNORING: 0.108) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 50 FULL SCALE; 21.90894 AT CENTER
DAIADRIVE:C


SHELL - SCANLS
400
500
600
700
W1-12: 07101812 - Fr15 hexane/2Pro .01 eluate ¦21:28 14 10/18/07
RMS ERROR: 0.178 (IGNORING: 0.187) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 200 FULL SCALE; 58.56427 AT CENTER
DAIADRIVE:G


SHELL - SCANLS
400
500
600
700
W1-13: 07101813 - Fr16 hexane/2Pro .01 eluate ¦21:44 46 10/18/07
RMS ERROR: 0.000 (IGNORING: 0.000) 1 701
ENTER F TO MAKE SPECTRA FOR DECOMPOSITION FIGURE
CR TO CONTINUE (X FOR NO MORE WAIT)
PLOT SCALE, mAU: 500 FULL SCALE; 114.3575 AT CENTER
DAIADRIVE:G

Spectra 14 and 15 do not fit adequately. Clearly another component is present. Also 15 is in acetone not hexane, which affects the spectra.



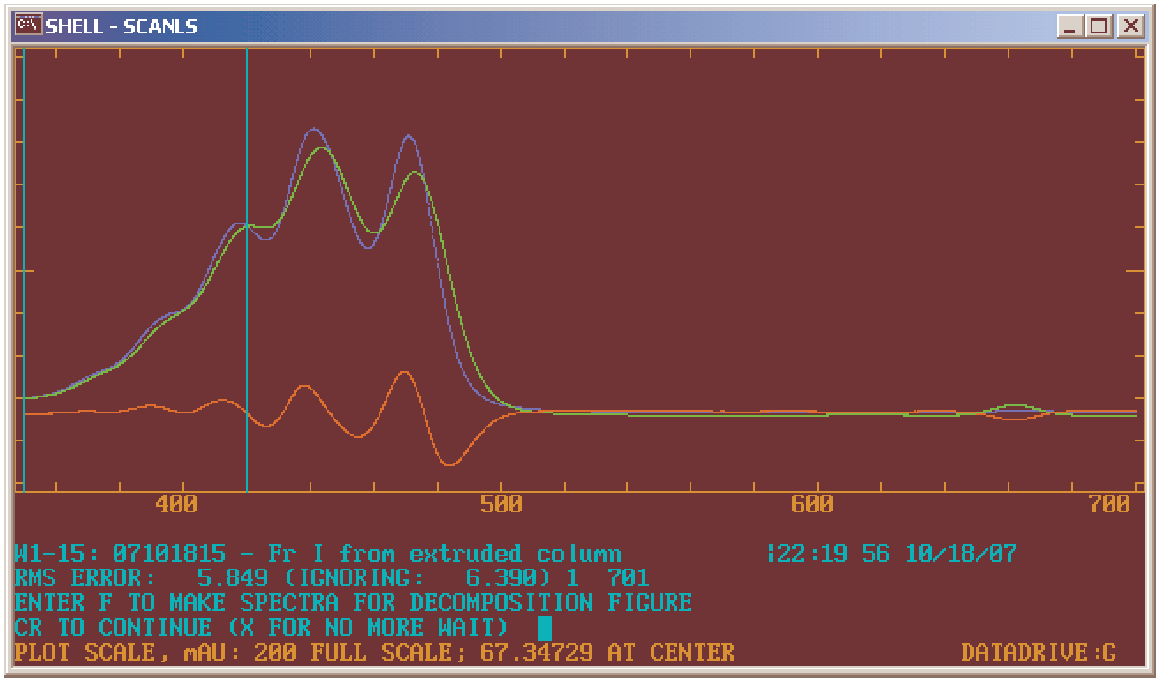


Table of results. Each row corresponds to one spectrum. Columns 2,3,4 give the concentration of the three analytes, column 5 is the baseline offset required for best fit. The next-to last column is the magnitude of the spectrum, and the last is the rms error in mAU of the fit. Note 6, 10, and 13 fit perfectly because they were used in constructing the basis. Spectrum 1 is a baseline that was subtracted from all including itself, so it gets a perfect zero.

HEXANE3C.LFT

SPECTRUM	b-Carot	Clphl-a	Clphl-b	baseline	magnit	error
1	0.000	0.000	0.000	0.000	0.000	0.000
2	0.045	0.006	0.000	0.017	4.042	1.150
3	0.208	0.037	-0.002	0.012	16.404	2.077
4	0.582	0.037	-0.001	0.005	40.883	0.808
5	0.835	0.042	-0.001	-0.006	57.728	0.299
6	1.000	0.090	-0.000	-0.000	70.642	0.010
7	0.819	1.483	0.004	0.013	119.111	1.009
8	0.354	2.264	0.003	0.025	129.861	1.242
9	0.052	2.104	-0.000	0.021	106.047	0.459
10	0.000	1.000	-0.000	0.000	48.982	0.000
11	0.079	0.230	0.004	-0.018	15.429	0.102
12	0.052	0.007	0.477	-0.016	30.811	0.178
13	-0.000	-0.000	1.000	-0.000	58.405	0.000
14	0.172	0.036	0.104	-0.058	17.864	2.541
15	0.699	0.044	-0.004	-0.025	48.918	5.849

Units are arbitrary because we have not normalized the standard spectra to a particular concentration like 1 uM.