Hyperpositive non-linear effects: enantiodivergence and modelling

Yannick Geiger, Thierry Achard, Aline Maisse-François and Stéphane Bellemin-Laponnaz.

Supplementary Information

Summary

I: Supplementary Methods

I.1 Experimental procedures

All reagents and dry solvents were purchased from commercial chemical suppliers (Acros, Alfa Aesar, Sigma-Aldrich and TCI Europe) and used without further purification, except for benzaldehyde which was dried, distilled and stored under argon over 4 Å molecular sieves prior to use. 1.2 M $ZnMe_2$ solutions in toluene were prepared from pure $ZnMe_2$ (purchased from Strem chemicals) and dry toluene in a N_2-filled glovebox in a 10-20 mL-scale and stored outside the glovebox, at 4 °C and protected from light, in a Young's tap-equipped Schlenk tube; the solutions were consumed within 3 weeks. (1*R*,2*S*)-(-)- and (1*S*,2*R*)-(+)-*N*-methylephedrine ((-)-NME and (+)-NME) were prepared from the respective ephedrine enantiomer according to a literature procedure; spectral data were identical to those reported.[1] Enantiomeric excesses were determined on a Varian 3900 gas chromatograph equipped with a CP-8400 autosampler and a Chiraldex G-TA capillary column (25 m long, 250 µm in diameter) with helium as carrier gas.

I.1.1 General procedure for (-)-NME-catalysed addition of dialkylzincs to benzaldehyde

In a N_2-filled glovebox, (1*R*,2*S*)-*N*-methylephedrine[1] (17.9 mg, 20 mol%, 100 µmol) and a magnetic stirring bar were placed in an oven-dried vial, which was then closed with a septum-containing screwcap. The vial was put out of the glovebox and dry toluene (0.4 mL) followed by a 1.2 M $ZnMe_2$ solution in toluene (0.5 mL, 1.2 equiv, 600 µmol) were added via syringe; gas evolution occurred upon $ZnMe_2$ addition. The mixture stirred for 10 min, then benzaldehyde (51 µL, 1 equiv, 500 µmol) was added via syringe. The solution stirred at room temperature for 48h, then was quenched carefully with 3 M aqueous HCl under vigorous stirring. The organic phase was then analysed by chiral stationary phase GC.

To obtain the experimental NLE curves the ligand ee was adjusted by preparing appropriate mixtures of the (1*R*,2*S*)-(-)- and (1*S*,2*R*)-(+)-enantiomers of NME. For the catalysts loading screening at 0 °C the amount of NME was reduced to the indicated catalyst loading shown in Figure 5a and the amount of dry toluene increased to keep the benzaldehyde concentration at 0.56 M; below 10 mol%, the reactions were scaled up (1.0-1.5 mL $ZnMe_2$ solution) to allow sufficiently precise weighing of NME. For temperature screenings, the reaction temperature was adapted as indicated in Figure 6a; reactions at room temperature fluctuated between 20 and 25 °C (always starting at 25 °C). The reaction time was increased to 4 days (7 days if the catalyst loading was lower than 20 mol%) for reaction conducted at 0 °C. The product ee and conversions were determined by GC. Full details of the starting material quantities, reaction conditions and results, including for the previously published NBE runs, are found in the SI_Experimental_Data.xlsx file.

Note: the reference concentration for the NME-catalysed runs (0.56 M benzaldehyde) is slightly lower than the one used previously for NBE (0.83 M). At 0.83 M, the runs with NME exhibited the formation of a white precipitate upon addition of $ZnMe_2$ at high ee_L and high catalyst loading, which most likely is a homochiral aggregate (cf. Supplementary Figure 6 for an exemplary ee_P vs $[Cat_{tot}]$-plot). Thus, the

catalytic runs were diluted to 0.56 M to allow full solubilisation of the catalyst. Previous investigations with NBE showed that comparable dilution of the reaction medium alters only slightly ee_P.[2]

I.1.2 GC analysis

Supplementary Table 1 | GC retention times of the catalysis products issued from the enantioselective addition of $ZnEt_2$ and $ZnMe_2$ to benzaldehyde.

Reagent	Product	t_{major} [min]	t_{minor} [min]
$ZnMe_2$	(R)-1-phenyl-1-ethanol	23.4	24.7

Oven temperature: 110°C; Helium pressure: 16 psi; split: 1/20. The separation conditions were determined by injecting racemic versions of the corresponding product. The product's absolute configuration was deducted from earlier reports using the same catalyst.[3] The chromatograms are listed in section III: Supplementary Chromatograms. The product/benzaldehyde response ratio, used to determine the reaction's conversions, was determined from a calibration curve which was obtained by injecting mixtures of benzaldehyde and racemic 1-phenyl-1-ethanol in toluene of known concentration. The data can be found in the Calibration Curve-sheet of the SI_Experimental_Data.xlsx file.

Note: benzyl alcohol is formed as a side-product in dialkylzinc additions, which is occasionally seen as a trace peak in the GC chromatograms (retention time slightly lower than of the R-enantiomer of the 1-phenyl-1-ethanol product).

I.1.3 Kinetic measurements

The kinetic runs were performed in the same conditions as those with NBE,[2] with the same reactant quantities and concentrations as in Supplementary Figure 6 (0.83 M benzaldehyde), at 30 °C and on a 1.5-2.0 mL $ZnMe_2$-scale. The ligand was placed in an oven-dried and argon-filled Schlenk tube, then $ZnMe_2$ was added via syringe, followed by toluene. The mixture stirred for 10 min at 30 °C, then benzaldehyde was added via syringe. A DS AgX Comp probe connected to a ReactIR 15 was mounted onto the Schlenk tube and IR recording was started precisely 30 s after benzaldehyde injection. Acquisition parameters: 2000 to 650 cm^{-1}, 4 cm^{-1} resolution; one acquisition every 5 min; 128 scans per acquisition (82 s acquisition time), 20-40 h reaction time (cf. corresponding rate profiles in the SI_Experimental_Data.xlsx file). The background was recorded each time in the empty (but argon-filled) Schlenk tube before addition of the ligand.

The kinetic profiles (Supplementary Fig. 5) were obtained by integrating the 1739 to 1675 cm^{-1} region of the IR spectra (benzaldehyde ν(C=O) at 1706 cm^{-1}) from a single point baseline at 1739 cm^{-1}; the solvent was subtracted from the spectra using a previously recorded spectrum of pure toluene at 30 °C. The first acquisition of each run was approximated to correspond to the initial benzaldehyde

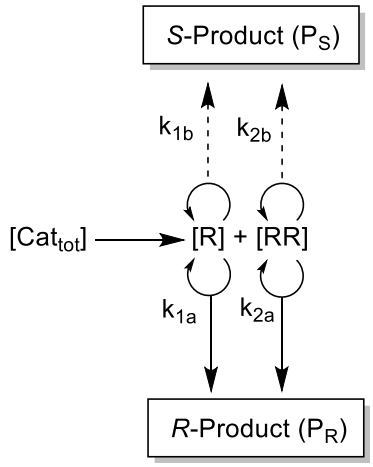
concentration and all following points of the corresponding run were normalised to that value. The complete rate profile data (including the previously published runs with NBE[2]) can be found in the Sup. Figure 5a and 5b-sheets of the SI_Experimental_Data.xlsx file.

Note: no precipitate appeared at this concentration (0.83 M benzaldehyde) at 30 °C, cf. Supplementary Figure 6.

I.2 Mathematical treatment

Note: full data of the mathematical simulations (ee_P *vs* $[Cat_{tot}]$, ee_P *vs* ee_L, $k_{obs}/[Cat_{tot}]$ vs $[Cat_{tot}]$, k_{obs} vs ee_L and *c* vs catalyst loading-plots) can be found in the

I.2.1 Model I: ee_P vs $[Cat_{tot}]$



$k_1 = k_{1a} + k_{1b}$
$k_2 = k_{2a} + k_{2b}$

$2R \rightleftharpoons RR$ (K_{Homo})

$ee_1 = (k_{1a}-k_{1b})/k_1$
$ee_2 = (k_{2a}-k_{2b})/k_2$

$ee_P = (P_R - P_S)/(P_R + P_S)$

$$[Cat_{tot}] = [R] + 2[RR] \quad \text{(I)}$$

$$K_{Homo} = \frac{[RR]}{[R]^2} \quad \text{(II)}$$

Replacement of [RR] in equation (II) through (I) gives a 2nd-order equation in [R] whose only positive root is described by equation (III):

$$[R] = \frac{\sqrt{1 + 8K_{Homo}[Cat_{tot}]} - 1}{4K_{Homo}} \quad \text{(III)}$$

The only catalytically active species are the monomeric (R) and the dimeric (RR) complexes. Their enantioselectivities for the synthesis of the R-product are described by ee_1 and ee_2, respectively.

The chiral products P_R and P_S are synthesised according to the following reaction equation:

$$Cat_i + Rea + Sub \xrightarrow{k_{i\,a,b}} Cat_i + P_{R,S}$$

With Cat_i referring to R and RR as catalysts, which give P_R and P_S from the substrate (Sub) and the reactant (Rea) with the respective kinetic constant $k_{i\,a,b}$.

If we define the catalytic reaction giving the chiral product as the rate-limiting step, with only one catalyst, reactant and substrate molecule involved, the reaction's kinetics are expressed by:

$$\frac{d[P_{R,S}]}{dt} = k_{i\,a,b}[Cat_i][Rea][Sub]$$

If the different $[Cat_i]$ are constant over time, we can insert the integrated forms of the kinetic equations into the term for ee_P, simplify and rearrange to make ee_1 and ee_2 appear:

$$ee_P = \frac{\sum_i k_{ia}[Cat_i][Rea][Sub]t - \sum_i k_{ib}[Cat_i][Rea][Sub]t}{\sum_i k_{ia}[Cat_i][Rea][Sub]t + \sum_i k_{ib}[Cat_i][Rea][Sub]t}$$

$$\Leftrightarrow ee_P = \frac{[R]k_{1a} + [RR]k_{2a} - ([R]k_{1b} + [RR]k_{2b})}{[R]k_{1a} + [RR]k_{2a} + ([R]k_{1b} + [RR]k_{2b})}$$

$$\Leftrightarrow ee_P = \frac{[R](k_{1a} - k_{1b}) + [RR](k_{2a} - k_{2b})}{[R](k_{1a} + k_{1b}) + [RR](k_{2a} + k_{2b})}$$

$$\Leftrightarrow ee_P = \frac{[R]k_1ee_1 + [RR]k_2ee_2}{[R]k_1 + [RR]k_2}$$

Elimination of [RR] using equation (II) gives:

$$\Leftrightarrow ee_P = \frac{[R]k_1ee_1 + [R]^2K_{Homo}k_2ee_2}{[R]k_1 + [R]^2K_{Homo}k_2}$$

$$\Leftrightarrow ee_P = \frac{k_1ee_1 + [R]K_{Homo}k_2ee_2}{k_1 + [R]K_{Homo}k_2}$$

Elimination of [R] with equation (III) and introduction of the factor *γ* gives:

$$\Leftrightarrow ee_P = \frac{k_1 ee_1 + \left(\frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}}\right) K_{Homo} k_2 ee_2}{k_1 + \left(\frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}}\right) K_{Homo} k_2}$$

$$\Leftrightarrow ee_P = \frac{ee_1 + \gamma \frac{k_2}{k_1} ee_2}{1 + \gamma \frac{k_2}{k_1}} \quad (1)$$

$$\gamma = \frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4} \quad (2)$$

The "Model I ee_P vs $[Cat_{tot}]$"-sheet in the SI_Simulated_NLE_xlsx-file allows the computation of ee_P *vs* $[Cat_{tot}]$-plots with free choice of the parameters K_{Homo}, k_2/k_1, ee_1 and ee_2.

I.2.2 Model I: kinetic rate law

First, the general kinetic equation is established:

$$-\frac{d[Sub]}{dt} = k_1[R][Rea][Sub] + k_2[RR][Rea][Sub]$$

$$\Leftrightarrow -\frac{d[Sub]}{dt} = (k_1[R] + k_2[R]^2 K_{Homo})[Rea][Sub]$$

[R] can be substituted using equation (III):

$$\Leftrightarrow -\frac{d[Sub]}{dt} = \left(k_1 \frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}} + k_2 \left(\frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}}\right)^2 K_{Homo}\right)[Rea][Sub]$$

$$\Leftrightarrow -\frac{d[Sub]}{dt} = \left(k_1 \frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}} + k_2 \frac{\left(\sqrt{1+8K_{Homo}[Cat_{tot}]}-1\right)^2}{16K_{Homo}}\right)[Rea][Sub]$$

If [Rea] = [Sub], the equation simplifies to:

$$\Leftrightarrow -\frac{d[Sub]}{dt} = \left(k_1 \frac{\sqrt{1+8K_{Homo}[Cat_{tot}]}-1}{4K_{Homo}} + k_2 \frac{\left(\sqrt{1+8K_{Homo}[Cat_{tot}]}-1\right)^2}{16K_{Homo}}\right)[Sub]^2$$

➔ This corresponds to a standard 2nd-order rate law of type:

$$-\frac{d[Sub]}{dt} = k_{obs}[Sub]^2 \quad (6)$$

$$with\ k_{obs} = k_1 \frac{\sqrt{1 + 8K_{Homo}[Cat_{tot}]} - 1}{4K_{Homo}} + k_2 \frac{\left(\sqrt{1 + 8K_{Homo}[Cat_{tot}]} - 1\right)^2}{16K_{Homo}} \quad (9)$$

Integration over [Sub] and t give the integrated form of the 2nd-order rate law:

$$\Leftrightarrow -\int_{[Sub]_0}^{[Sub]_t} \frac{d[Sub]}{[Sub]^2} = k_{obs}\int_0^t dt$$

$$\Leftrightarrow [Sub]_t^{-1} - [Sub]_0^{-1} = k_{obs}t$$

$$\Leftrightarrow [Sub]_t^{-1} = [Sub]_0^{-1} + k_{obs}t \text{ (linearised form of equation (7))}$$

$$[Sub]_t = \left(\frac{1}{[Sub]_0} + k_{obs}t\right)^{-1} \quad (7)$$

$$with\ k_{obs} = k_1 \frac{\sqrt{1 + 8K_{Homo}[Cat_{tot}]} - 1}{4K_{Homo}} + k_2 \frac{\left(\sqrt{1 + 8K_{Homo}[Cat_{tot}]} - 1\right)^2}{16K_{Homo}} \quad (9)$$

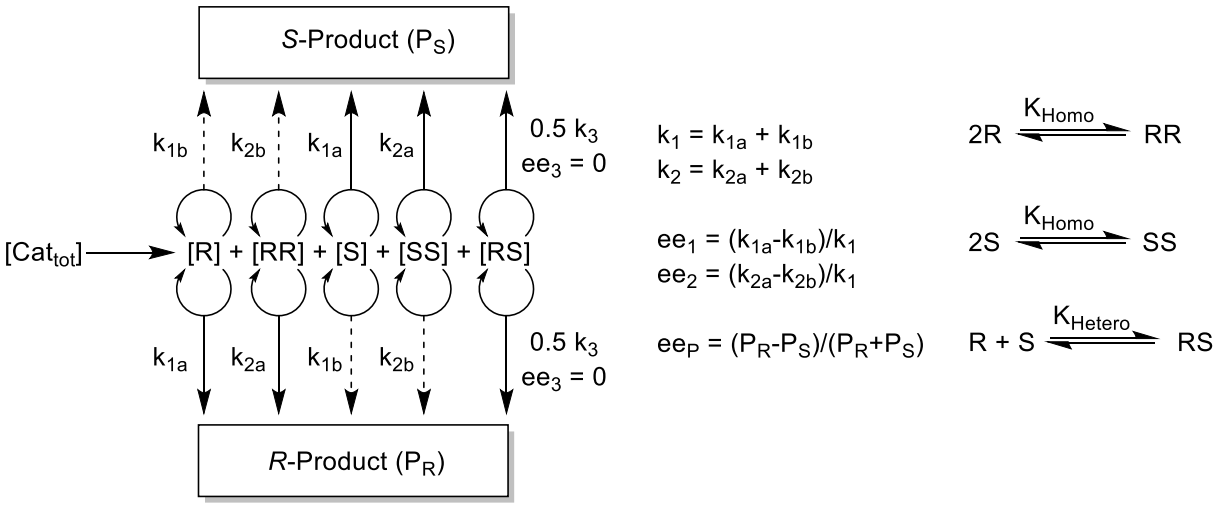
If [Rea]≠[Sub], then the general form of the integrated 2nd-order rate law applies:

$$\ln\frac{[Rea]_t[Sub]_0}{[Sub]_t[Rea]_0} = k_{obs}([Rea]_0 - [Sub]_0)t$$

I.2.2.1 Variable Time-normalised analysis (VTNA) of simulated rate profiles (Figure 9)

Rate profiles were obtained from equations (7) and (9) using different parameter sets (K_{Homo}, k_1 and k_2); for each parameter set, several rate profiles with different [Cat_{tot}] were generated. Then, the rate profiles were normalised to their respective catalyst concentration using the excel spreadsheet provided by Nielsen and Burés.[4] The catalyst order *c* of two normalised rate profiles from an identical parameter set, but different [Cat_{tot}], was determined visually. *c* was then plotted against the mean [Cat_{tot}] of the two respective rate profiles used in order to obtain *c vs* [Cat_{tot}]-plots. The "Fig. 9"-sheet in the XXX file provides the *c vs* [Cat_{tot}] datasets, simulated rate profiles and derived time-normalised rate profiles, which allow the independent verification of *c* for the given dataset.

I.2.3 Model II: ee_P vs ee_L



$$K_{Homo} = \frac{[RR]}{[R]^2} = \frac{[SS]}{[S]^2} \quad \text{(II)}$$

$$K_{Hetero} = \frac{[RS]}{[R][S]} \quad \text{(IV)}$$

$$[Cat_{tot}] = [R] + 2[RR] + [S] + 2[SS] + 2[RS] \quad \text{(V)}$$

As will be shown in the following, obtaining an equation of type $ee_P = f(ee_L)$ is difficult in this case. We will first develop an equation of type $ee_P = f(\alpha)$, then $ee_L = f(\alpha)$ and define the limits of α.

I.2.3.1 Expression for $ee_P = f(\alpha)$

The rate-limiting reaction step and its general kinetic rate law are the same as in Model I. The general expression for ee_P becomes:

$$ee_P = \frac{\sum_{i\ a,b\rightarrow \boldsymbol{P_R}} k_{i\ a,b}[Cat_i][Rea][Sub]t - \sum_{i\ a,b\rightarrow \boldsymbol{P_S}} k_{i\ a,b}[Cat_i][Rea][Sub]t}{\sum_{i\ a,b\rightarrow \boldsymbol{P_R}} k_{i\ a,b}[Cat_i][Rea][Sub]t + \sum_{i\ a,b\rightarrow \boldsymbol{P_S}} k_{i\ a,b}[Cat_i][Rea][Sub]t}$$

$$\Leftrightarrow ee_P$$
$$= \frac{[R]k_{1a} + [RR]k_{2a} + [S]k_{1b} + [SS]k_{2b} + 0.5[RS]k_3 - ([S]k_{1a} + [R]k_{1b} + [SS]k_{2a} + [RR]k_{2b} + 0.5[RS]k_3)}{([R]k_{1a} + [RR]k_{2a} + [S]k_{1b} + [SS]k_{2b} + 0.5[RS]k_3) + ([R]k_{1b} + [RR]k_{2b} + [S]k_{1a} + [SS]k_{2a} + 0.5[RS]k_3)}$$

$$\Leftrightarrow ee_P = \frac{[R](k_{1a} - k_{1b}) + [RR](k_{2a} - k_{2b}) - \big([S](k_{1a} - k_{1b}) + [SS](k_{2a} - k_{2b})\big)}{[R](k_{1a} + k_{1b}) + [RR](k_{2a} + k_{2b}) + [S](k_{1a} + k_{1b}) + [SS](k_{2a} + k_{2b}) + [RS]k_3}$$

$$\Leftrightarrow ee_P = \frac{([R] - [S])k_1 ee_1 + ([RR] - [SS])k_2 ee_2}{([R] + [S])k_1 + ([RR] + [SS])k_2 + [RS]k_3}$$

The dimeric complexes [RR], [SS] and [RS] are eliminated using equations (II) and (IV):

$$\Leftrightarrow ee_P = \frac{([R] - [S])k_1 ee_1 + ([R]^2 - [S]^2)K_{Homo}k_2 ee_2}{([R] + [S])k_1 + ([R]^2 + [S]^2)K_{Homo}k_2 + [R][S]K_{Hetero}k_3}$$

Since [R] and [S] appear simultaneously in sums and products, it is difficult to isolate one of both without ending up with complicated terms. Thus, we will apply a technique used by Noyori[5] in his model for DAIB: the introduction of parameters α and β through equations (VI) and (VII):

$$\alpha = [R] + [S] \quad \text{(VI)}$$

$$\beta = [R][S] \quad \text{(VII)}$$

The combination (VI) and (VII), while supposing [R] is the major catalyst enantiomer (i. e. ee_L is defined as (R-S)/(R+S)), gives (VIII) and (IX):

$$[R] = \frac{\alpha + \sqrt{\alpha^2 - 4\beta}}{2} \quad \text{(VIII)}$$

$$[S] = \frac{\alpha - \sqrt{\alpha^2 - 4\beta}}{2} \quad \text{(IX)}$$

Equations (VI), (VII), (VIII) and (IX) now allow us to eliminate [R] and [S] :

$$\Leftrightarrow ee_P = \frac{\left(\left(\frac{\alpha + \sqrt{\alpha^2 - 4\beta}}{2}\right) - \left(\frac{\alpha - \sqrt{\alpha^2 - 4\beta}}{2}\right)\right)k_1 ee_1 + \left(\left(\frac{\alpha + \sqrt{\alpha^2 - 4\beta}}{2}\right)^2 - \left(\frac{\alpha - \sqrt{\alpha^2 - 4\beta}}{2}\right)^2\right)K_{Homo}k_2 ee_2}{\alpha k_1 + \left(\left(\frac{\alpha + \sqrt{\alpha^2 - 4\beta}}{2}\right)^2 + \left(\frac{\alpha - \sqrt{\alpha^2 - 4\beta}}{2}\right)^2\right)K_{Homo}k_2 + \beta K_{Hetero}k_3}$$

$$\Leftrightarrow ee_P = \frac{\sqrt{\alpha^2 - 4\beta}k_1 ee_1 + \left(\frac{\alpha^2 + 2\alpha\sqrt{\alpha^2 - 4\beta} + (\alpha^2 - 4\beta)}{4} - \frac{\alpha^2 - 2\alpha\sqrt{\alpha^2 - 4\beta} + (\alpha^2 - 4\beta)}{4}\right)K_{Homo}k_2 ee_2}{\alpha k_1 + \left(\frac{\alpha^2 + 2\alpha\sqrt{\alpha^2 - 4\beta} + (\alpha^2 - 4\beta)}{4} + \frac{\alpha^2 - 2\alpha\sqrt{\alpha^2 - 4\beta} + (\alpha^2 - 4\beta)}{4}\right)K_{Homo}k_2 + \beta K_{Hetero}k_3}$$

$$\Leftrightarrow ee_P = \frac{\sqrt{\alpha^2 - 4\beta}k_1 ee_1 + \alpha\sqrt{\alpha^2 - 4\beta}K_{Homo}k_2 ee_2}{\alpha k_1 + (\alpha^2 - 2\beta)K_{Homo}k_2 + \beta K_{Hetero}k_3}$$

$$\Leftrightarrow ee_P = \frac{\sqrt{\alpha^2 - 4\beta}\left(ee_1 + \alpha K_{Homo}\frac{k_2}{k_1}ee_2\right)}{\alpha + (\alpha^2 - 2\beta)K_{Homo}\frac{k_2}{k_1} + \beta K_{Hetero}\frac{k_2'}{k_1}} \quad (3)$$

The same principle will be applied to ee_L. Both ee_P and ee_L then are described as functions of α (we will later develop the expression for β, which is itself a function of α). NLE curves can then be drawn by choosing appropriate α-values which will give paired ee_P/ee_L datapoints.

I.2.3.2 Expression for $ee_L = f(\alpha)$

$$ee_L = \frac{\sum Cat_{iR} - \sum Cat_{iS}}{[Cat_{tot}]}$$

$$\Leftrightarrow ee_L = \frac{[R] + 2[RR] + [RS] - ([S] + 2[SS] + [RS])}{[Cat_{tot}]}$$

$$\Leftrightarrow ee_L = \frac{([R] - [S]) + 2([RR] - [SS])}{[Cat_{tot}]}$$

Substitution by equations (II), (IV) and (V) gives :

$$\Leftrightarrow ee_L = \frac{([R] - [S]) + 2K_{Homo}([R]^2 - [S]^2)}{[Cat_{tot}]}$$

Replacement of [R] and [S] through equations (VIII) and (IX) gives :

$$\Leftrightarrow ee_L = \frac{\sqrt{\alpha^2 - 4\beta} + 2K_{Homo}\alpha\sqrt{\alpha^2 - 4\beta}}{[Cat_{tot}]}$$

$$\Leftrightarrow ee_L = \frac{\sqrt{\alpha^2 - 4\beta}(1 + 2\alpha K_{Homo})}{[Cat_{tot}]} \quad (4)$$

I.2.3.3 Expression for β = f(α)

To express β as a function of α, we start from equation (V) into which we integrate equations (II) and (IV):

$$[Cat_{tot}] = [R] + 2[RR] + [S] + 2[SS] + 2[RS]$$

$$\Leftrightarrow [Cat_{tot}] = [R] + 2K_{Homo}[R]^2 + [S] + 2K_{Homo}[S]^2 + 2K_{Hetero}[R][S]$$

$$\Leftrightarrow [Cat_{tot}] = [R] + [S] + 2K_{Homo}([R]^2 + [S]^2) + 2K_{Hetero}\beta$$

We then eliminate [R] and [S] using equations(VI), (VII), (VIII) and (IX) and rearrange for β:

$$\Leftrightarrow [Cat_{tot}] = \alpha + 2K_{Homo}(\alpha^2 - 2\beta) + 2K_{Hetero}\beta$$

$$\Leftrightarrow [Cat_{tot}] = \alpha + 2K_{Homo}\alpha^2 - 4K_{Homo}\beta + 2K_{Hetero}\beta$$

$$\Leftrightarrow 4K_{Homo}\beta - 2K_{Hetero}\beta = \alpha + 2K_{Homo}\alpha^2 - [Cat_{tot}]$$

$$\Leftrightarrow \beta = \frac{(\alpha + 2K_{Homo}\alpha^2 - [Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}} \quad (5)$$

The division precludes that $K_{Hetero} \neq 2K_{Homo}$. This the point which separates a (+)-NLE ($K_{Hetero} > 2K_{Homo}$) from a (-)-NLE ($K_{Hetero} < 2K_{Homo}$).

In summary:

$$\text{NLE (Model II):} \begin{cases} ee_L = \frac{\sqrt{\alpha^2-4\beta}(1+2\alpha K_{Homo})}{[Cat_{tot}]} \\ ee_P = \frac{\sqrt{\alpha^2-4\beta}\left(ee_1+\alpha K_{Homo}\frac{k_2}{k_1}ee_2\right)}{\alpha+(\alpha^2-2\beta)K_{Homo}\frac{k_2}{k_1}+\beta K_{Hetero}\frac{k_2'}{k_1}} \end{cases}$$

$$\text{with } \beta = \frac{(\alpha+2K_{Homo}\alpha^2-[Cat_{tot}])}{4K_{Homo}-2K_{Hetero}}$$

I.2.3.4 Limiting values for α

To build an NLE curve from $ee_P = f(\alpha)$ and $ee_L = f(\alpha)$, we need to define the range of α we may use. In the following we will define the minimum (α_{min}) and maximum (α_{max}) α-values. Both are defined through the minimum (0) and maximum (1) values ee_L can take.

(a) α_{min}: $0 \leq ee_L$

$$0 \leq \frac{\sqrt{\alpha^2 - 4\beta}(1 + 2\alpha K_{Homo})}{[Cat_{tot}]}$$
$$\Longrightarrow 0 \leq \sqrt{\alpha^2 - 4\beta}\ or\ 0 \leq (1 + 2\alpha K_{Homo})$$
$$\Longrightarrow 0 \leq \alpha^2 - 4\beta$$

Development of β using equation (5) gives a 2nd-order inequality:

$$\Leftrightarrow 0 \leq \alpha^2 - 4\frac{(\alpha + 2K_{Homo}\alpha^2 - [Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}}$$
$$\Leftrightarrow 0 \leq \frac{(4K_{Homo} - 2K_{Hetero})\alpha^2}{4K_{Homo} - 2K_{Hetero}} + \frac{-4\alpha - 8K_{Homo}\alpha^2 + 4[Cat_{tot}]}{4K_{Homo} - 2K_{Hetero}}$$
$$\Leftrightarrow 0 \leq \frac{-4\alpha + (-4K_{Homo} - 2K_{Hetero})\alpha^2 + 4[Cat_{tot}]}{4K_{Homo} - 2K_{Hetero}}$$
$$\Leftrightarrow 0 \leq \frac{4\alpha + (4K_{Homo} + 2K_{Hetero})\alpha^2 - 4[Cat_{tot}]}{2K_{Hetero} - 4K_{Homo}}$$
$$\Longrightarrow 0 \leq (2K_{Homo} + K_{Hetero})\alpha^2 + 2\alpha - 2[Cat_{tot}]$$

The last step is valid only if $K_{Hetero} > 2K_{Homo}$ (positive non-linear effect); if $K_{Hetero} < 2K_{Homo}$ it results in multiplication with a negative value which switches the sign of the inequality. Solution of the 2nd-order inequality gives:

$$\Leftrightarrow \alpha_{\pm} \geq \frac{-2 \pm \sqrt{4 - 4(-2[Cat_{tot}])(2K_{Homo} + K_{Hetero})}}{4K_{Homo} + 2K_{Hetero}}$$
$$\Leftrightarrow \alpha_{\pm} \geq \frac{-1 \pm \sqrt{1 + 2[Cat_{tot}](2K_{Homo} + K_{Hetero})}}{2K_{Homo} + K_{Hetero}}$$

Since α = [R]+[S] must be a positive number, α_+ is the only significant root:

$$\Longrightarrow \alpha_{min} \geq \frac{\sqrt{1 + 2[Cat_{tot}](2K_{Homo} + K_{Hetero})} - 1}{2K_{Homo} + K_{Hetero}} \quad (X)$$

α_{min} defines 0 as the lower limit of ee_L but also of ee_P (cf. the corresponding equation) in case of a (+)-NLE. For a (-)-NLE the inequality is switched, α_{min} then becomes the *maximal* value α can reach.

2nd factor = 0 :

$$0 = (1 + 2\alpha K_{Homo})$$

$$-1 = 2\alpha K_{Homo}$$

$$-\frac{1}{2K_{Homo}} = \alpha$$

➔ Without significance, since α must be positive.

(b) α_{max}: $1 \geq ee_L$

$$1 \geq \frac{\sqrt{\alpha^2 - 4\beta}(1 + 2\alpha K_{Homo})}{[Cat_{tot}]}$$

$$\Leftrightarrow [Cat_{tot}] \geq \sqrt{\alpha^2 - 4\beta}(1 + 2\alpha K_{Homo})$$

Since both sides of the inequality have to be positive values, we can quadrate the inequality to eliminate the square root, leading to a quartic equation:

$$\Leftrightarrow [Cat_{tot}]^2 \geq (\alpha^2 - 4\beta)(1 + 2\alpha K_{Homo})^2$$

$$\Leftrightarrow [Cat_{tot}]^2 \geq \left(\alpha^2 - 4\left(\frac{(\alpha + 2K_{Homo}\alpha^2 - [Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}}\right)\right)(1 + 2\alpha K_{Homo})^2$$

$$\Leftrightarrow [Cat_{tot}]^2 \geq \left(\frac{(4K_{Homo} - 2K_{Hetero})\alpha^2}{4K_{Homo} - 2K_{Hetero}} + \frac{(-4\alpha - 8K_{Homo}\alpha^2 + 4[Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}}\right)(1 + 2\alpha K_{Homo})^2$$

$$\Leftrightarrow [Cat_{tot}]^2 \geq \left(\frac{(-4\alpha - (4K_{Homo} + 2K_{Hetero})\alpha^2 + 4[Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}}\right)(1 + 4\alpha K_{Homo} + 4\alpha^2 K_{Homo}^2)$$

$$\begin{aligned}\Leftrightarrow [Cat_{tot}]^2 \geq & \left(\frac{(2\alpha + (2K_{Homo} + K_{Hetero})\alpha^2 - 2[Cat_{tot}])}{K_{Hetero} - 2K_{Homo}}\right) \\ & + \left(\frac{(8\alpha^2 K_{Homo} + 4K_{Homo}(2K_{Homo} + K_{Hetero})\alpha^3 - 8\alpha K_{Homo}[Cat_{tot}])}{K_{Hetero} - 2K_{Homo}}\right) \\ & + \left(\frac{(8\alpha^3 K_{Homo}^2 + 4K_{Homo}^2(2K_{Homo} + K_{Hetero})\alpha^4 - 8\alpha^2 K_{Homo}^2[Cat_{tot}])}{K_{Hetero} - 2K_{Homo}}\right)\end{aligned}$$

The next step is valid only if $K_{Hetero} > 2K_{Homo}$, otherwise the sign of the inequality changes:

$$\begin{aligned}\Leftrightarrow [Cat_{tot}]^2(K_{hetero} - 2K_{Homo}) & \\ \geq (2 - 8K_{Homo}[Cat_{tot}])\alpha + (2K_{Homo} + K_{Hetero} + 8K_{Homo} - 8K_{Homo}^2[Cat_{tot}])\alpha^2 & \\ + (2K_{Homo} + K_{Hetero} + 8K_{Homo}^2)\alpha^3 + 4K_{Homo}^2(2K_{Homo} + K_{Hetero})\alpha^4 - 2[Cat_{tot}] &\end{aligned}$$

$$\Leftrightarrow 0 \geq (2 - 8K_{Homo}[Cat_{tot}])\alpha + (10K_{Homo} + K_{Hetero} - 8K_{Homo}^2[Cat_{tot}])\alpha^2 + (2K_{Homo} + K_{Hetero} + 8K_{Homo}^2)\alpha^3 + 4K_{Homo}^2(2K_{Homo} + K_{Hetero})\alpha^4 - \left(2[Cat_{tot}] + [Cat_{tot}]^2(K_{hetero} - 2K_{Homo})\right)$$

$$\Leftrightarrow 0 \geq 4K_{Homo}^2(2K_{Homo} + K_{Hetero})\alpha^4 + (2K_{Homo} + K_{Hetero} + 8K_{Homo}^2)\alpha^3 + (10K_{Homo} + K_{Hetero} - 8K_{Homo}^2[Cat_{tot}])\alpha^2 + (2 - 8K_{Homo}[Cat_{tot}])\alpha - \left(2[Cat_{tot}] + [Cat_{tot}]^2(K_{Hetero} - 2K_{Homo})\right) \quad \text{(XI)}$$

Equation (XI) can then be solved numerically to obtain the upper limit of α, which is α_{max} (however, it may give spurious results depending on the software used). If $K_{Hetero} > 2K_{Homo}$ then α_{max} becomes the *lower* limit of α.

The "Model II ee_P vs ee_L"-sheet in the SI_Simulated_NLE_xlsx-file allows the computation of ee_P *vs* ee_L-plots with free choice of the parameters $[Cat_{tot}]$, K_{Homo}, K_{Hetero}, k_1, k_2, k_2', ee_1 and ee_2. For this, the user has to set up manually a range of α-values that serve as a base to obtain ee_P vs ee_L-datasets. The first α-value, α_{min}, is automatically calculated from the inserted parameters (cf. equation (X), it can be either the minimum or maximum α if K_{Hetero} > or < $2K_{Homo}$, respectively). Upon change of K_{Homo}, K_{Hetero} or $[Cat_{tot}]$ the α-values may have to be readjusted to obtain enough datapoints that span from 0 to 100% ee_L.

I.2.4 Model II: kinetic rate law

First, the general kinetic equation is established and rearranged:

$$-\frac{d[Sub]}{dt} = k_1[R][Rea][Sub] + k_1[S][Rea][Sub] + k_2[RR][Rea][Sub] + k_2[SS][Rea][Sub] + k_2'[RS][Rea][Sub]$$

$$\Leftrightarrow -\frac{d[Sub]}{dt} = (k_1([R] + [S]) + k_2([RR] + [SS]) + k_2'[RS])[Rea][Sub]$$

$$\Leftrightarrow -\frac{d[Sub]}{dt} = (k_1([R] + [S]) + k_2K_{Homo}([R]^2 + [S]^2) + k_2'K_{Hetero}[R][S])[Rea][Sub]$$

[R] and [S] are then replaced by α and β using equations (VI)-(IX) and it is assumed that [Rea]=[Sub]:

$$\Leftrightarrow -\frac{d[Sub]}{dt} = (k_1\alpha + k_2K_{Homo}(\alpha^2 - 2\beta) + k_2'K_{Hetero}\beta)[Rea][Sub]$$

$$\Leftrightarrow -\frac{d[Sub]}{dt} = (k_1\alpha + k_2 K_{Homo}(\alpha^2 - 2\beta) + k_2' K_{Hetero}\beta)[Sub]^2$$

➔ This corresponds to a standard 2nd-order rate law of type:

$$-\frac{d[Sub]}{dt} = k_{obs}[Sub]^2 \quad (6)$$

$$[Sub]_t = \left(\frac{1}{[Sub]_0} + k_{obs}t\right)^{-1} \quad (7)$$

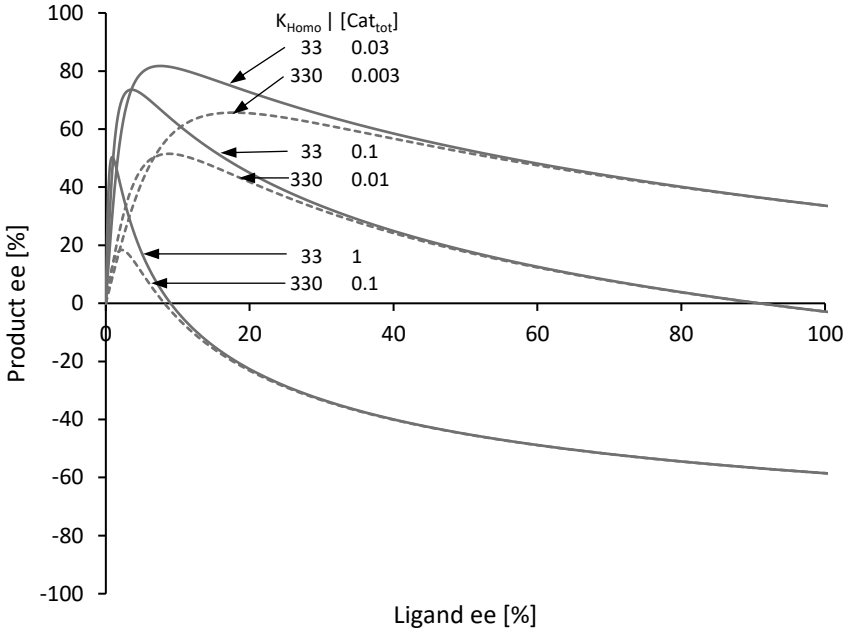
$$with\ k_{obs} = k_1\alpha + k_2 K_{Homo}(\alpha^2 - 2\beta) + k_2^{'} K_{Hetero}\beta \quad (10)$$

$$ee_L = \frac{\sqrt{\alpha^2 - 4\beta}(1 + 2\alpha K_{Homo})}{[Cat_{tot}]}\ and\ \beta = \frac{(\alpha + 2K_{Homo}\alpha^2 - [Cat_{tot}])}{4K_{Homo} - 2K_{Hetero}} \quad (4)\ \&\ (5)$$

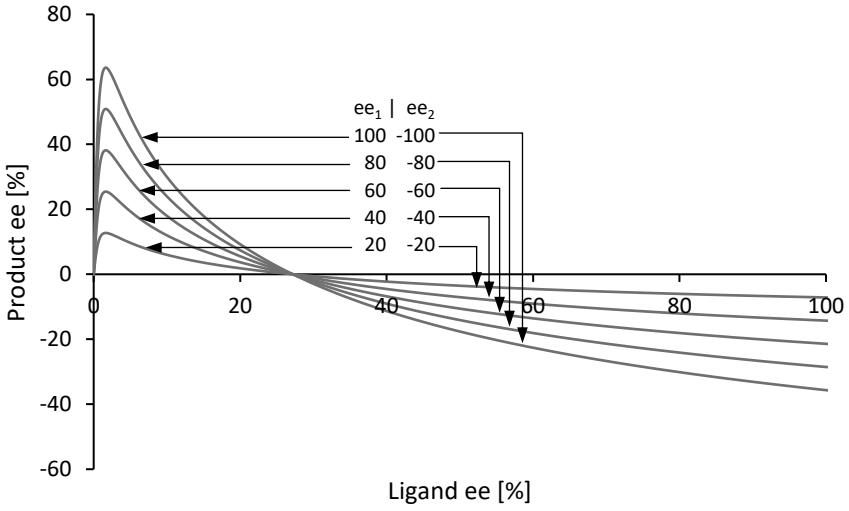
The expressions for ee_L and β (equations (4) and (5)) as well as the maximum and minimum values for α have been established in in section I.2.3. As for the ee_P *vs* ee_L-plots, k_{obs} *vs* ee_L-plots can be established by choosing appropriate values of α, which give paired k_{obs} and ee_L datapoints. The integrated form of the kinetic rate law is, as for Model I, given by equation (7) (cf. section I.2.2). If [Rea]≠[Sub], the integrated form of the 2nd-order rate law is given by:

$$\ln\frac{[Rea]_t[Sub]_0}{[Sub]_t[Rea]_0} = k_{obs}([Rea]_0 - [Sub]_0)t$$

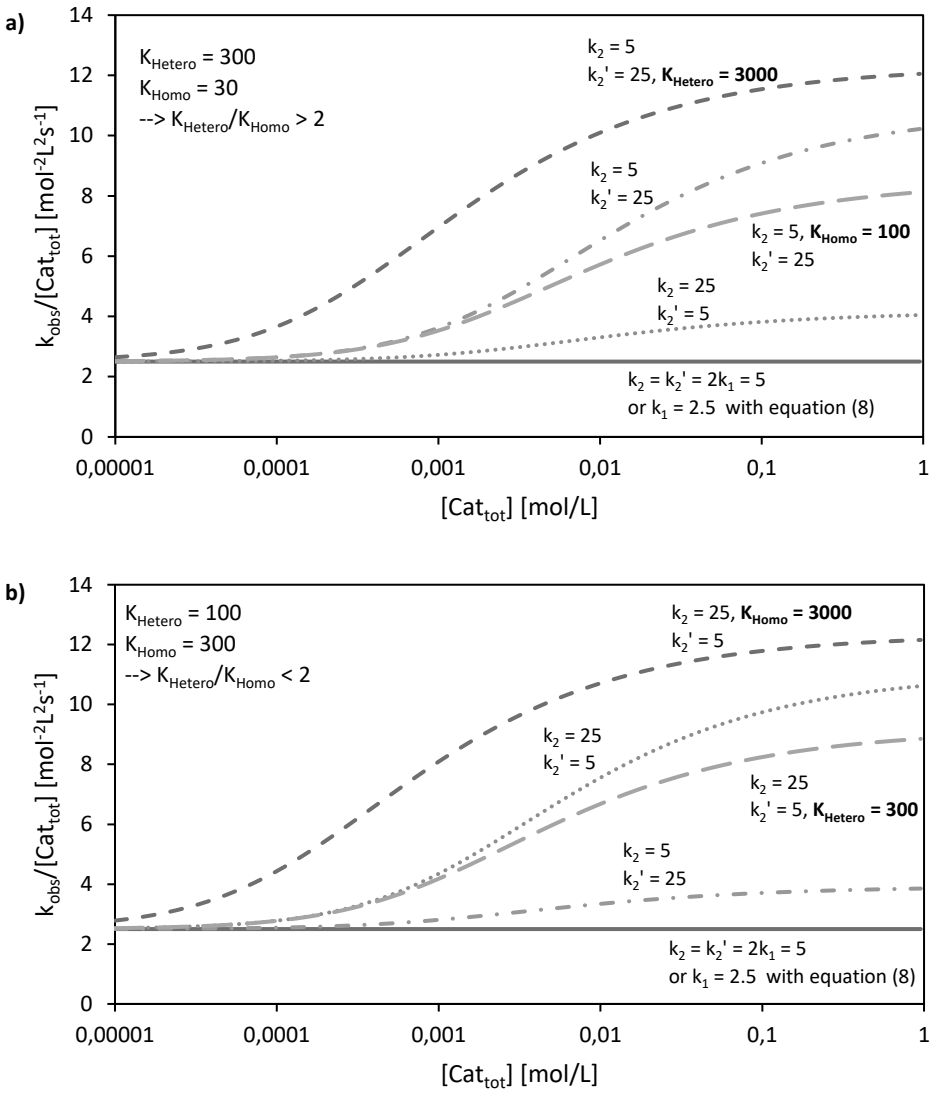
II: Supplementary Figures



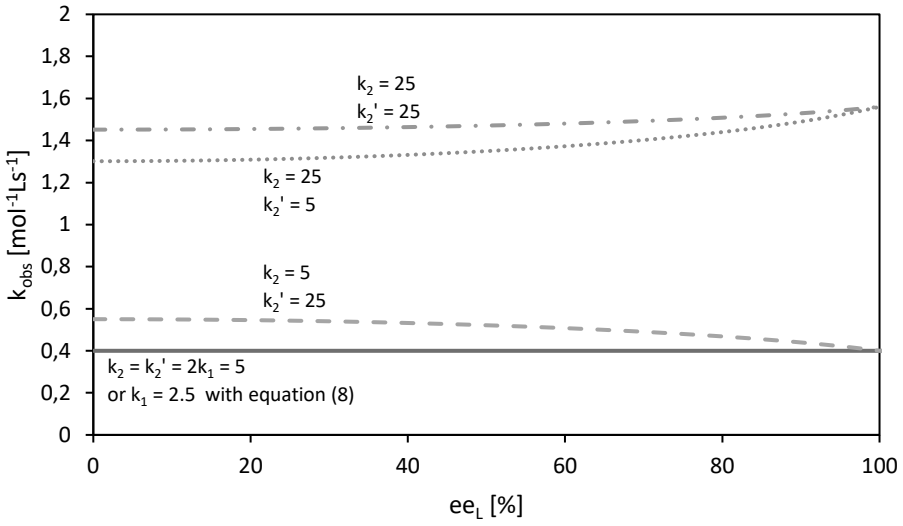
Supplementary Figure 1: Comparison of $[Cat_{tot}]$- and K_{Homo}-variations in NLE-simulations using Model II, with $k_1/k_2 = 1$, $k_3 = 0$, $K_{Hetero} = 10000$, $ee_1 = 100$ and $ee_2 = -100$. For a given curve (blue full line), simultaneous multiplication of K_{Homo} and division of $[Cat_{tot}]$ by the same number leads to a new curve (grey dashed line). Both have the same ee_P^{100}-value and are essentially identical for ee_L higher than 50; at lower ee_L, the new curve deviates to lower ee_P values.



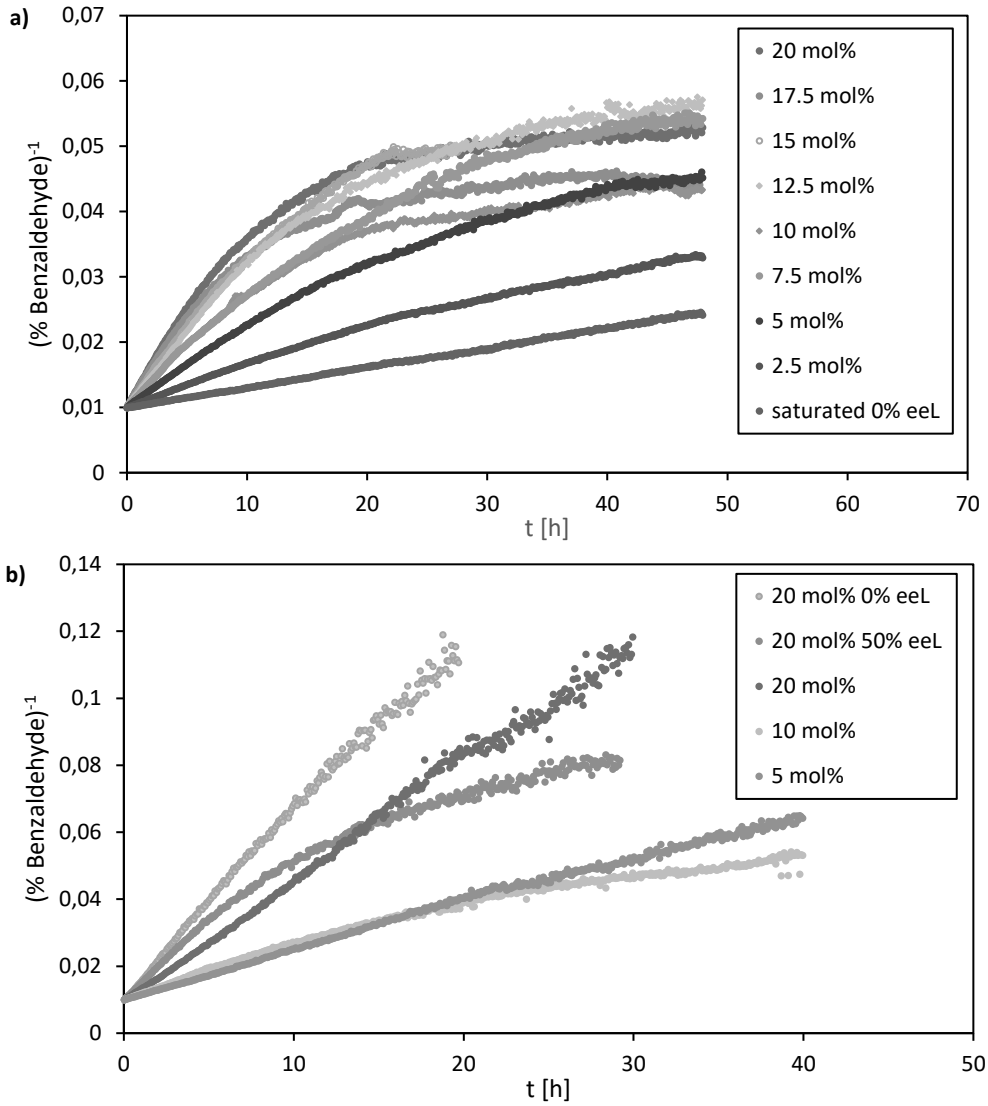
Supplementary Figure 2: Simultaneous decrease of the absolute values of ee_1 and ee_2 (with a constant ee_1/ee_2-ratio of -1) in NLE-simulations using Model II, with $k_1/k_2 = 1$, $k_3 = 0$, $K_{Homo} = 100$, $K_{Hetero} = 330000$ and $[Cat_{tot}] = 0.11$. The decrease leads to a compression of the curve: ee_P^{100} increases and ee_P^{max} decreases. On the other hand, ee_L^0 and ee_L^{max} stay constant.



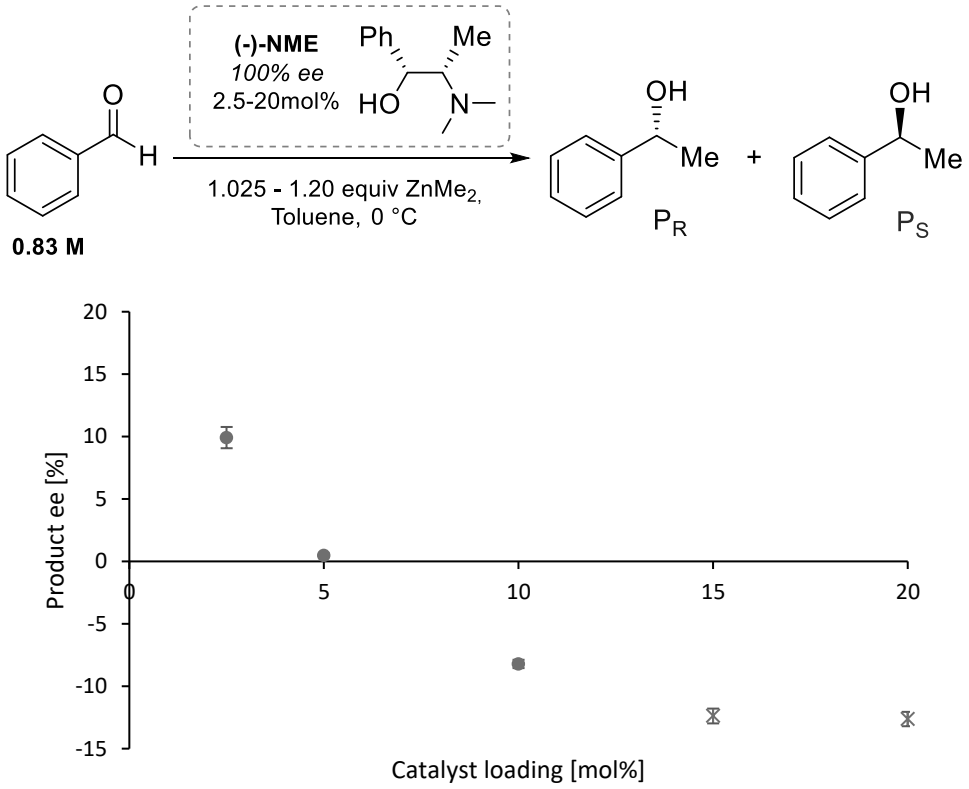
Supplementary Figure 3: Simulated $k_{obs}/[Cat_{tot}]$ vs $[Cat_{tot}]$-plots computed from equation (10) at $ee_L = 0$ (cf. section I.2.3.4(a)) with a) $K_{Hetero} = 300$, $K_{Homo} = 30$ and b) $K_{Hetero} = 100$, $K_{Homo} = 300$, unless noted otherwise. In all plots $k_1 = 2.5$, k_2 and k_2' as indicated. In contrast to the case with enantiopure ligand (Figure 7a in the main text) the shape of plots the plots is not only determined by k_2/k_1 but also by k_2'/k_1. If $k_2 = k_2' = 2k_1$ the plot is flat, regardless of K_{Homo} and K_{Hetero} (blue full line in a) and b)). Increasing k_2 (orange dotted line) and k_2' (green dashed/dotted line) both enhance $k_{obs}/[Cat_{tot}]$ with increasing $[Cat_{tot}]$, the effect being more pronounced with k_2' in a) ($K_{Hetero}/K_{Homo} > 2$) or with k_2 in b) ($K_{Hetero}/K_{Homo} < 2$). When $k_2 \neq k_2'$, increasing the dimerization constant associated to the higher rate constant amplifies the curve (blue dashed lines). On the other hand, increasing the K associated to the lower k depletes the curve (grey long-dashed lines).



Supplementary Figure 4: Simulated k_{obs} vs ee_L-plots computed from equations (10), (4) and (5) (K_{Homo} = 30, K_{Hetero} = 10, [Cat_{tot}] = 0.16, k_1 = 2.5, k_2 and k_2' as indicated). Since in this example $K_{Hetero}/K_{Homo} < 2$, the plot's slope is positive when increasing both k_2 and k_2' to 25 (green dashed/dotted line), which stands in contrast to what is seen Figure 7b in the main text. Here, the homochiral dimers are prevalent over the heterochiral ones, which leads to an overall k_{obs} increase at any ee_L (not only at high ee_L as in Figure 7b) when increasing k_2 (orange dotted line). On the other hand, an increase of k_2' has only little effect (grey dashed line). As discussed in the main text, $k_2 = k_2' = 2k_1 = 5$ results in a constant k_{obs} over varying ee_L (blue full line).



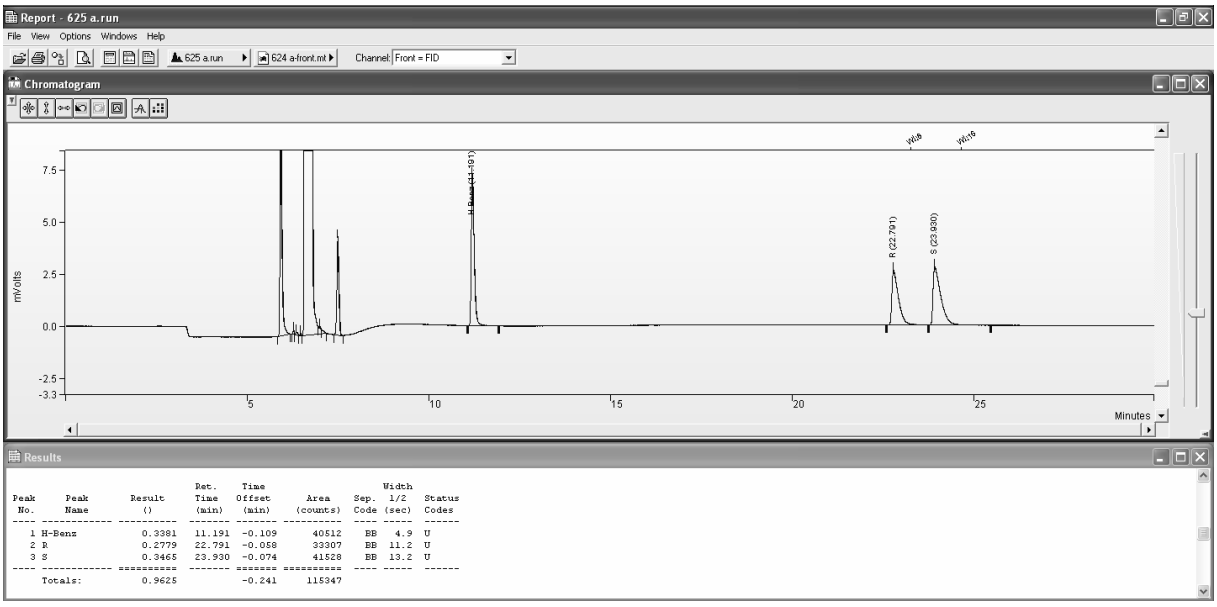
Supplementary Figure 5: Experimental (% Benzaldehyde)$^{-1}$ vs time-plots of a) NBE (original data from ref. [2]), b) NME-catalysed reactions. The ligands were used in their enantiopure form unless noted otherwise, at the indicated catalyst loading. The grey line in a) was obtained from 20 mol% racemic NBE which mostly precipitates. The mostly curved plots indicate a non-constant k_{obs} over time, which suggest a participation of the substrate/reactant and/or of the reaction product in the catalytic system.



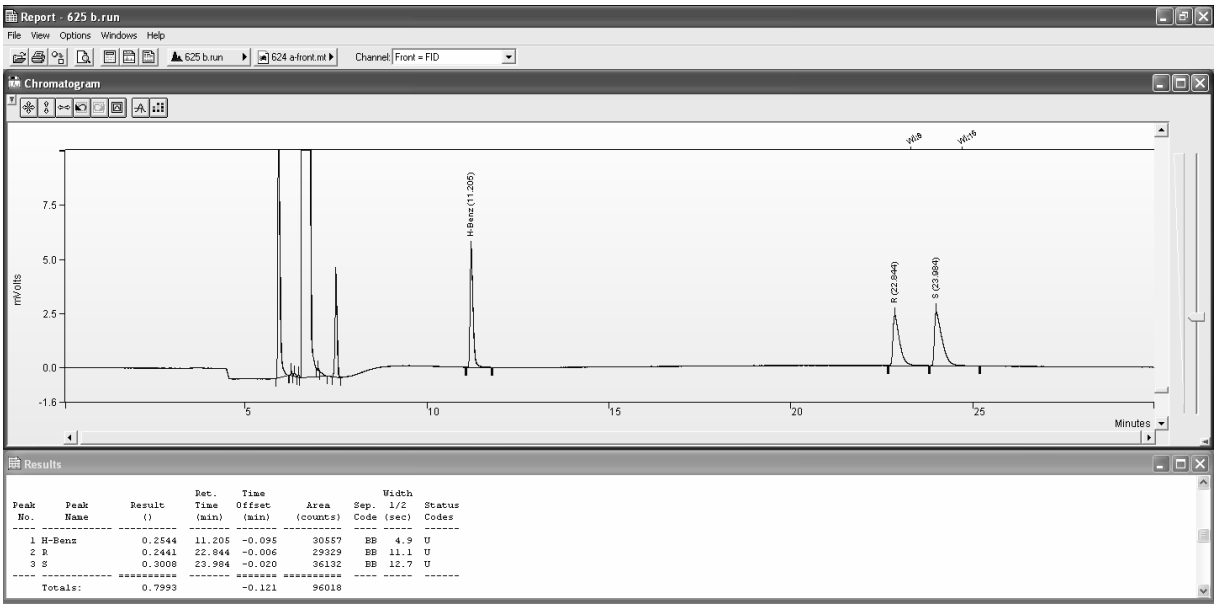
Supplementary Figure 6: Catalyst loading screening of the (-)-NME-catalysed addition of $ZnMe_2$ to 0.83 M benzaldehyde at 0 °C. Each point is the mean of three independent experiments; the vertical bars depict standard deviations. The product ee is defined as $(P_R-P_S)/(P_R+P_S)$. Upon addition of $ZnMe_2$ to 20 and 15 mol% (-)-NME (blue crosses), a white precipitate appeared which vanished over the course of the reaction; the runs with lower catalyst loading (blue dots) didn't exhibit any precipitate. This supports the hypothesis of a partly soluble homochiral aggregate which saturates the solution only when the catalyst concentration is sufficiently high. Therefore, the amount of soluble catalyst was limited by the aggregate's solubility in the runs at 15 and 20 mol%, which explains their similar ee_P-values. The vanishing of the precipitate over the course of the reaction can be explained by the continuous production of P_R and P_S, leading to catalyst-product-adducts which drive the solubilisation of the homochiral aggregate.

III: Supplementary Chromatograms

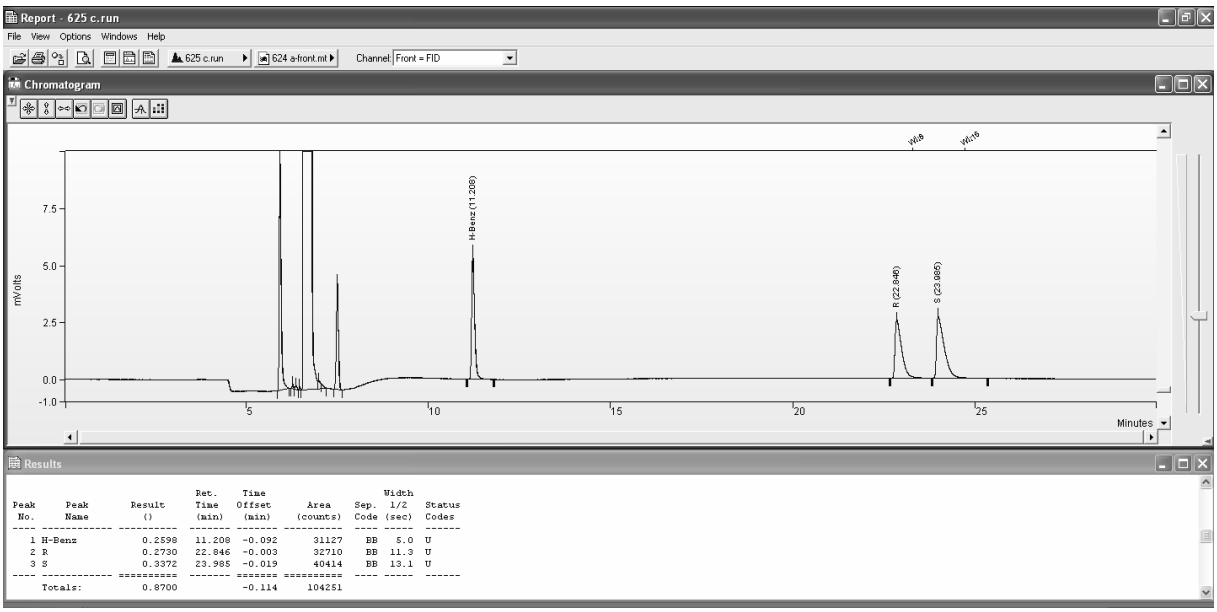
III.1 Figure 2a (NME)



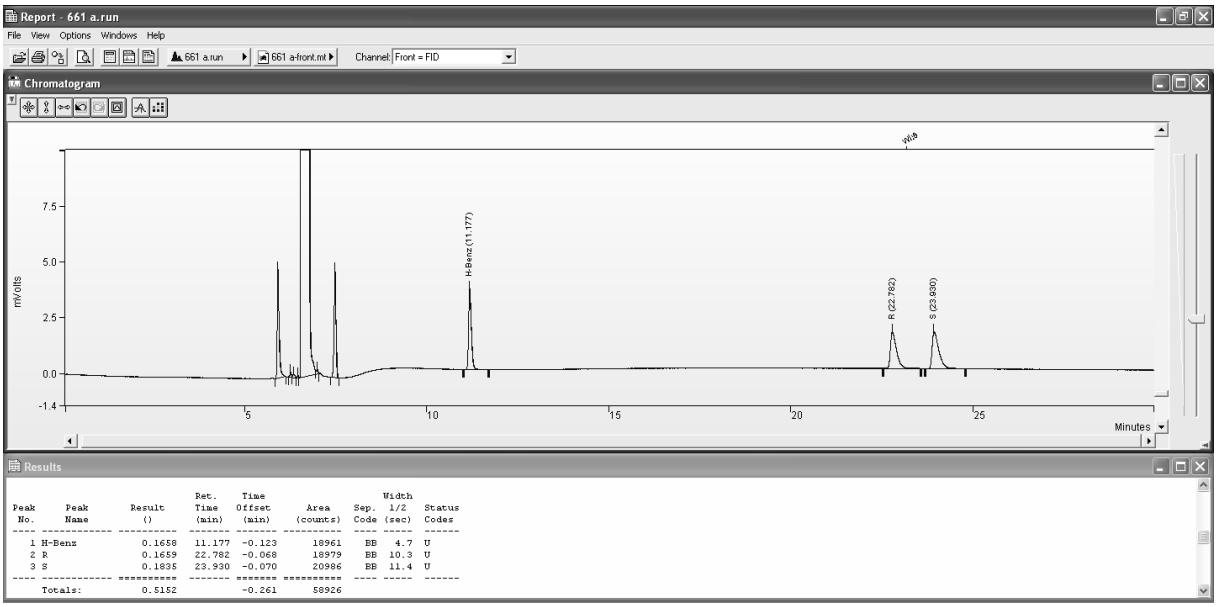
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.3381	11.191	-0.109	40512	BB	4.9	U
2	R	0.2779	22.791	-0.058	33307	BB	11.2	U
3	S	0.3465	23.930	-0.074	41528	BB	13.2	U
	Totals:	0.9625		-0.241	115347			



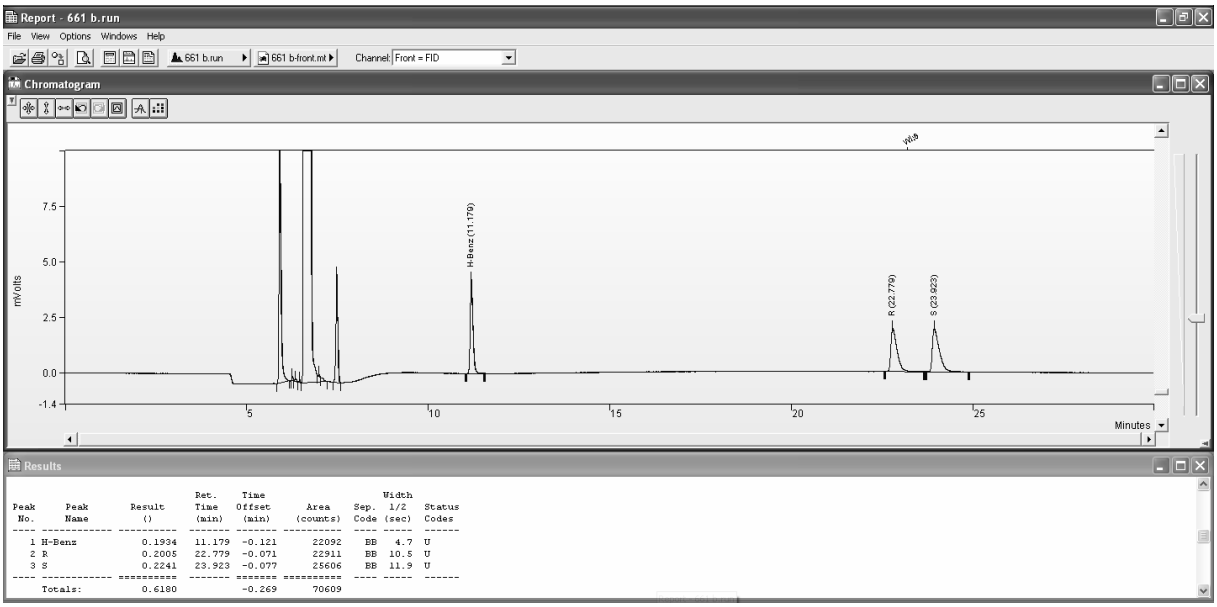
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2544	11.205	-0.095	30557	BB	4.9	U
2	R	0.2441	22.844	-0.006	29329	BB	11.1	U
3	S	0.3008	23.984	-0.020	36132	BB	12.7	U
	Totals:	0.7993		-0.121	96018			



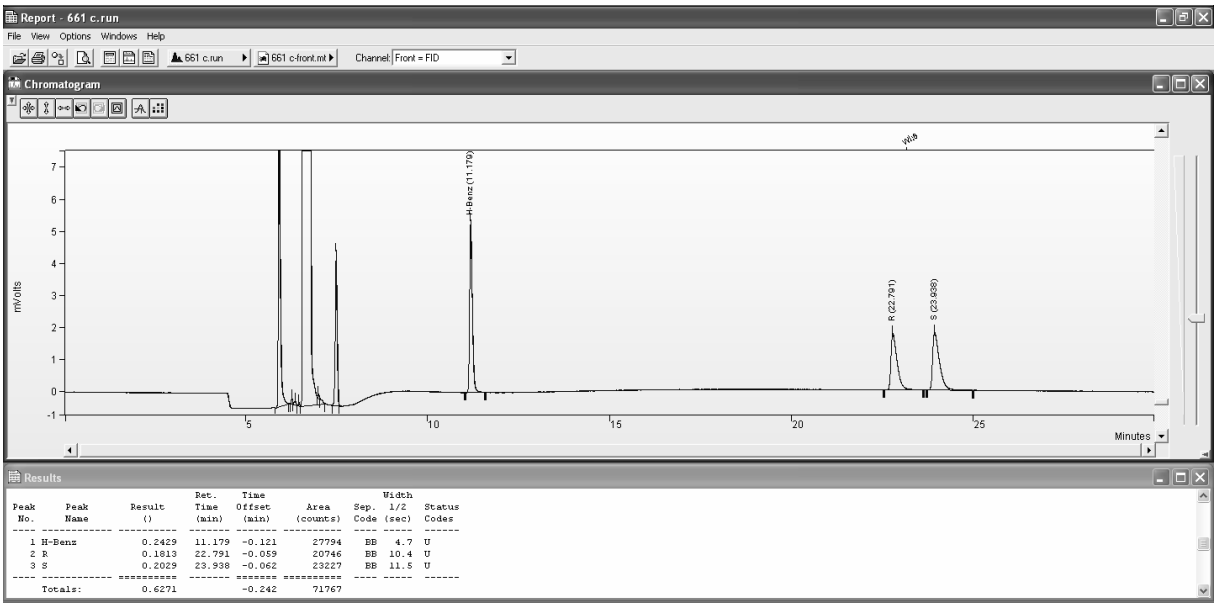
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2598	11.208	-0.092	31127	BB	5.0	U
2	R	0.2730	22.846	-0.003	32710	BB	11.3	U
3	S	0.3372	23.985	-0.019	40414	BB	13.1	U
	Totals:	0.8700		-0.114	104251			



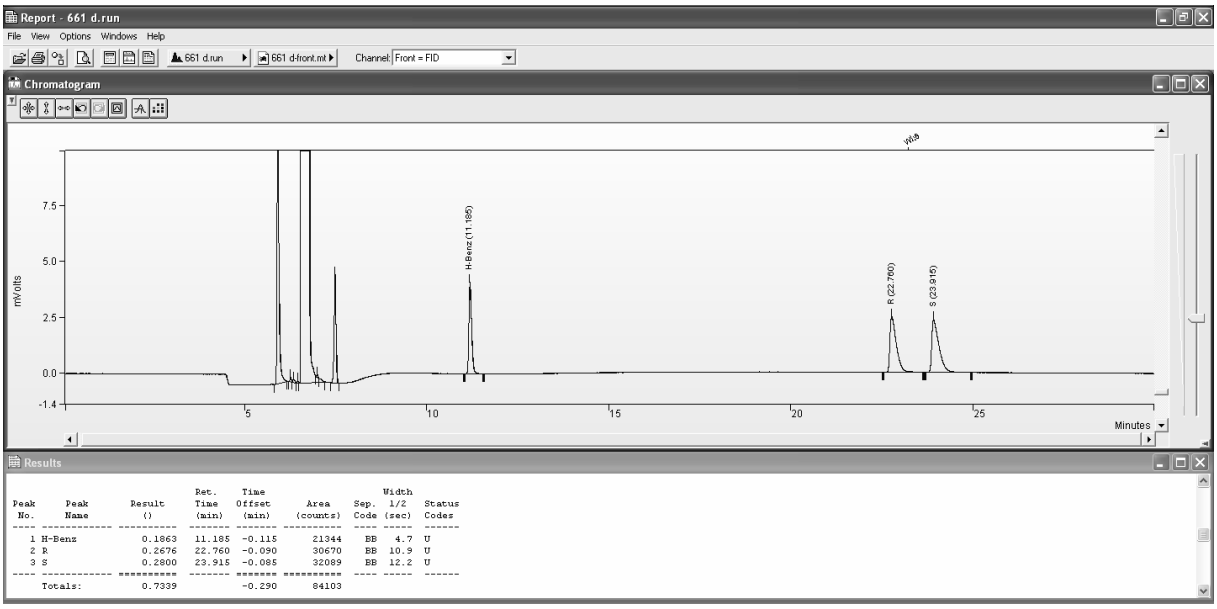
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1658	11.177	-0.123	18961	BB	4.7	U
2	R	0.1659	22.782	-0.068	18979	BB	10.3	U
3	S	0.1835	23.930	-0.070	20986	BB	11.4	U
	Totals:	0.5152		-0.261	58926			



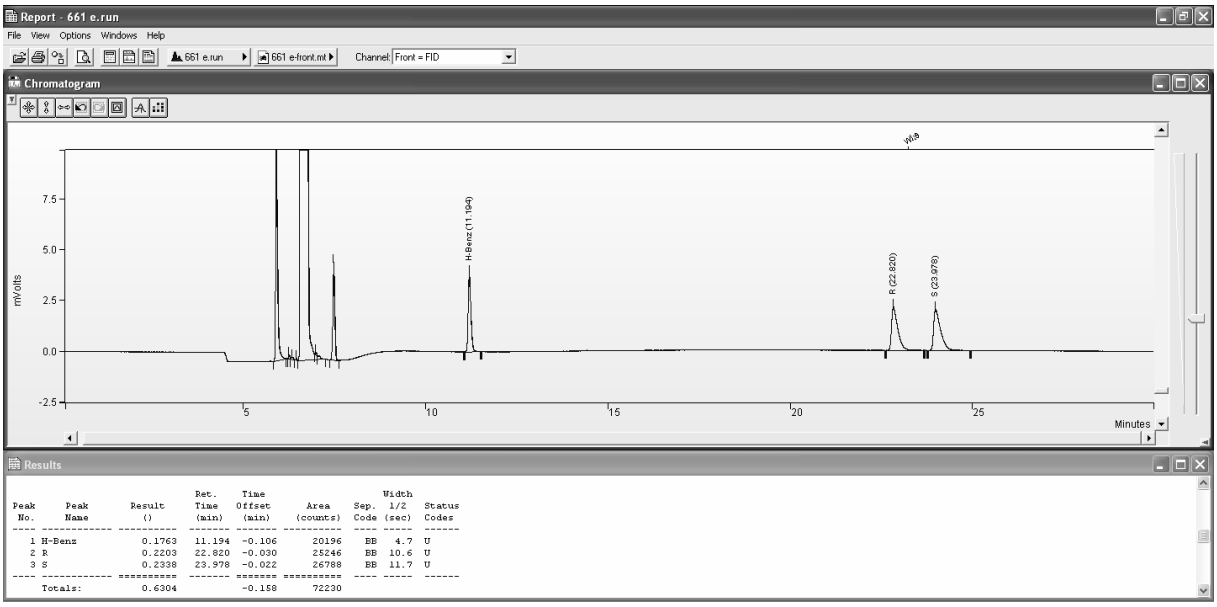
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1934	11.179	-0.121	22092	BB	4.7	U
2	R	0.2005	22.779	-0.071	22911	BB	10.5	U
3	S	0.2241	23.923	-0.077	25606	BB	11.9	U
	Totals:	0.6180		-0.269	70609			



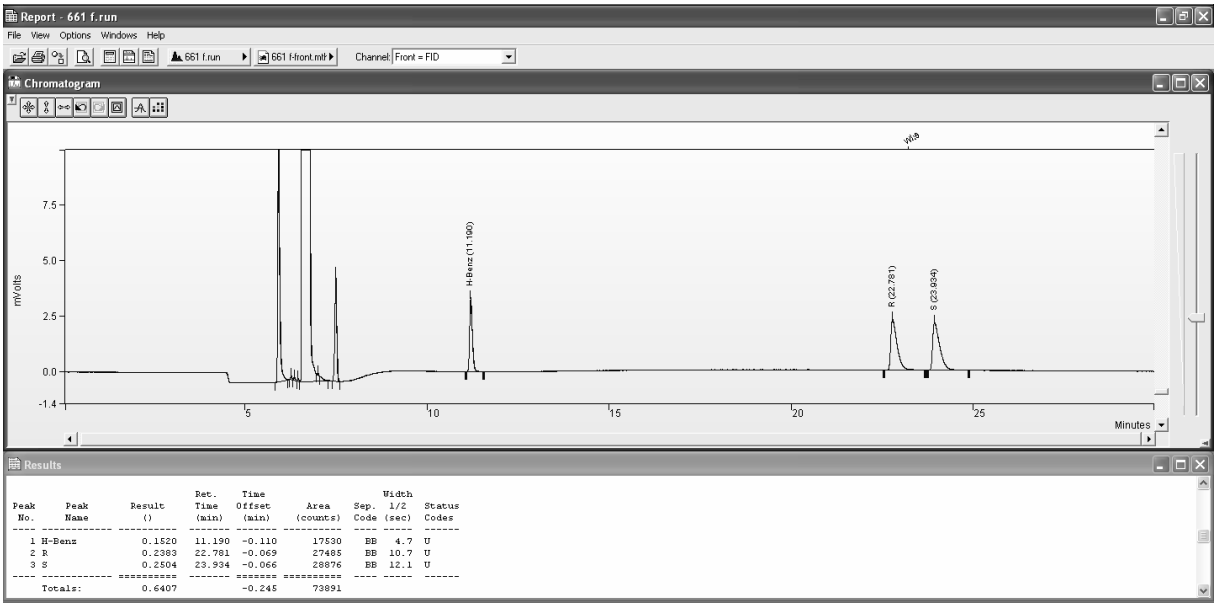
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2429	11.179	-0.121	27794	BB	4.7	U
2	R	0.1813	22.791	-0.059	20746	BB	10.4	U
3	S	0.2029	23.938	-0.062	23227	BB	11.5	U
	Totals:	0.6271		-0.242	71767			



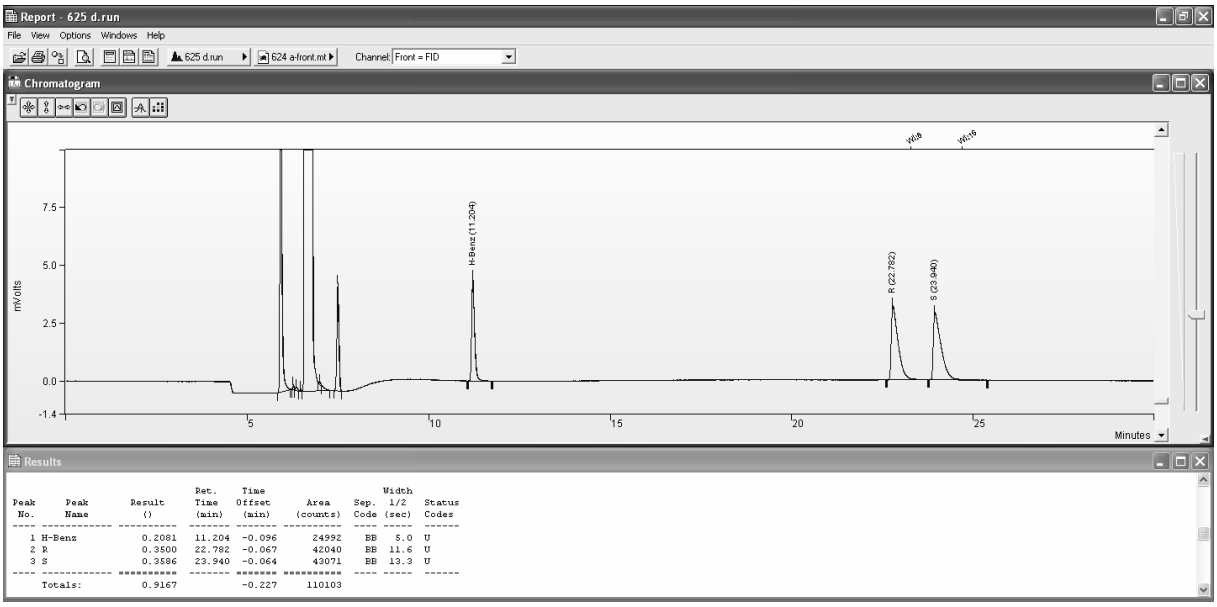
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1863	11.185	-0.115	21344	BB	4.7	U
2	R	0.2676	22.760	-0.090	30670	BB	10.9	U
3	S	0.2800	23.915	-0.085	32089	BB	12.2	U
Totals:		0.7339		-0.290	84103			



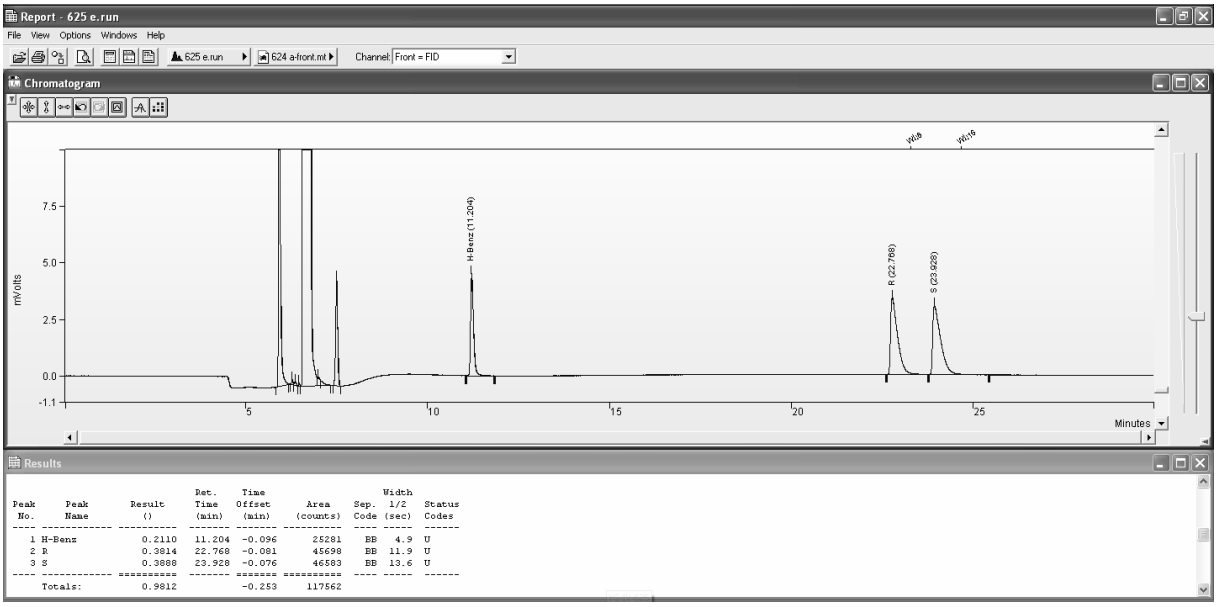
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1763	11.194	-0.106	20196	BB	4.7	U
2	R	0.2203	22.820	-0.030	25246	BB	10.6	U
3	S	0.2338	23.978	-0.022	26788	BB	11.7	U
Totals:		0.6304		-0.158	72230			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1520	11.190	-0.110	17530	BB	4.7	U
2	R	0.2383	22.781	-0.069	27485	BB	10.7	U
3	S	0.2504	23.934	-0.066	28876	BB	12.1	U
Totals:		0.6407		-0.245	73891			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2081	11.204	-0.096	24992	BB	5.0	U
2	R	0.3500	22.782	-0.067	42040	BB	11.6	U
3	S	0.3586	23.940	-0.064	43071	BB	13.3	U
Totals:		0.9167		-0.227	110103			



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2110	11.204	-0.096	25281	BB	4.9	U
2	R	0.3814	22.768	-0.081	45698	BB	11.9	U
3	S	0.3888	23.928	-0.076	46583	BB	13.6	U
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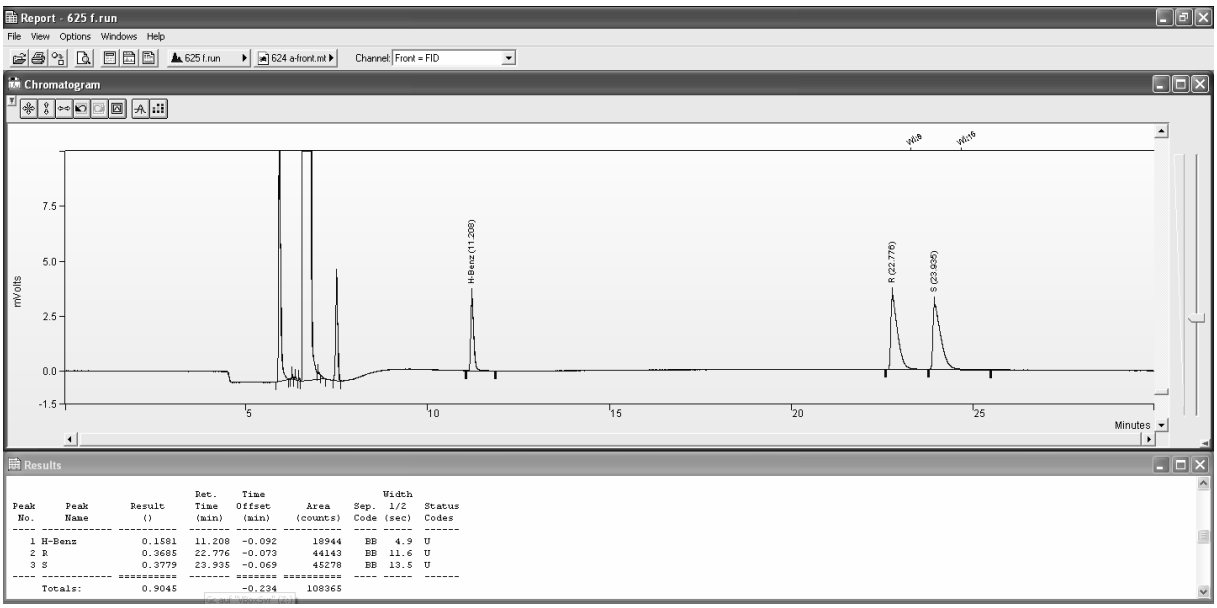
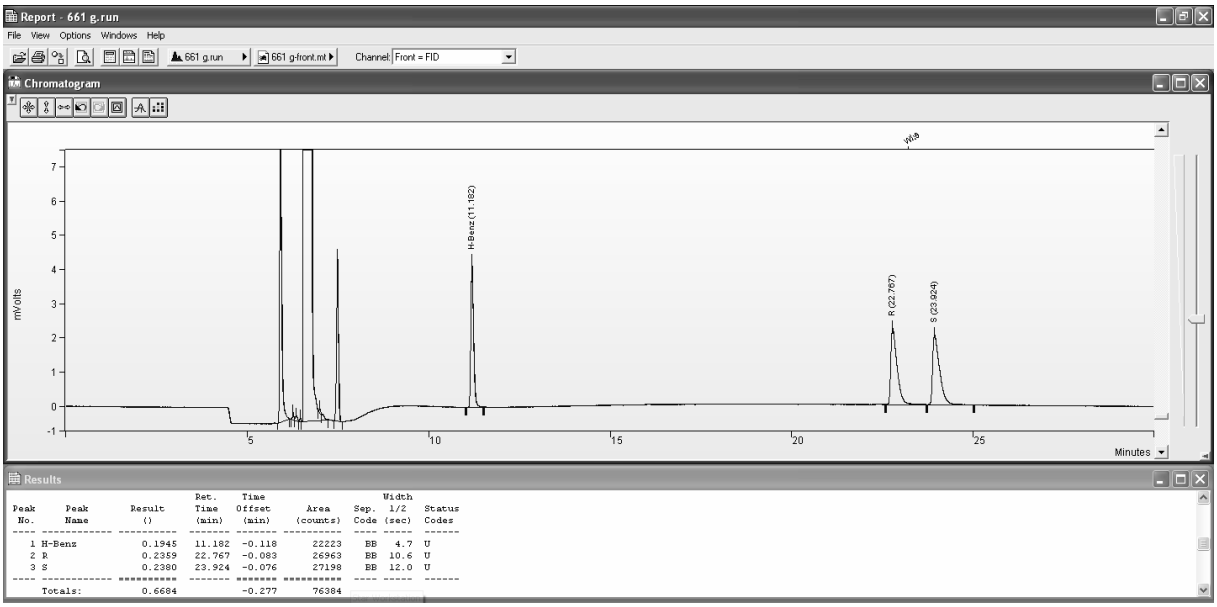


Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1581	11.208	-0.092	18944	BB	4.9	U
2	R	0.3685	22.776	-0.073	44143	BB	11.6	U
3	S	0.3779	23.935	-0.069	45278	BB	13.5	U
Totals:		0.9045		-0.234	108365			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Minutes
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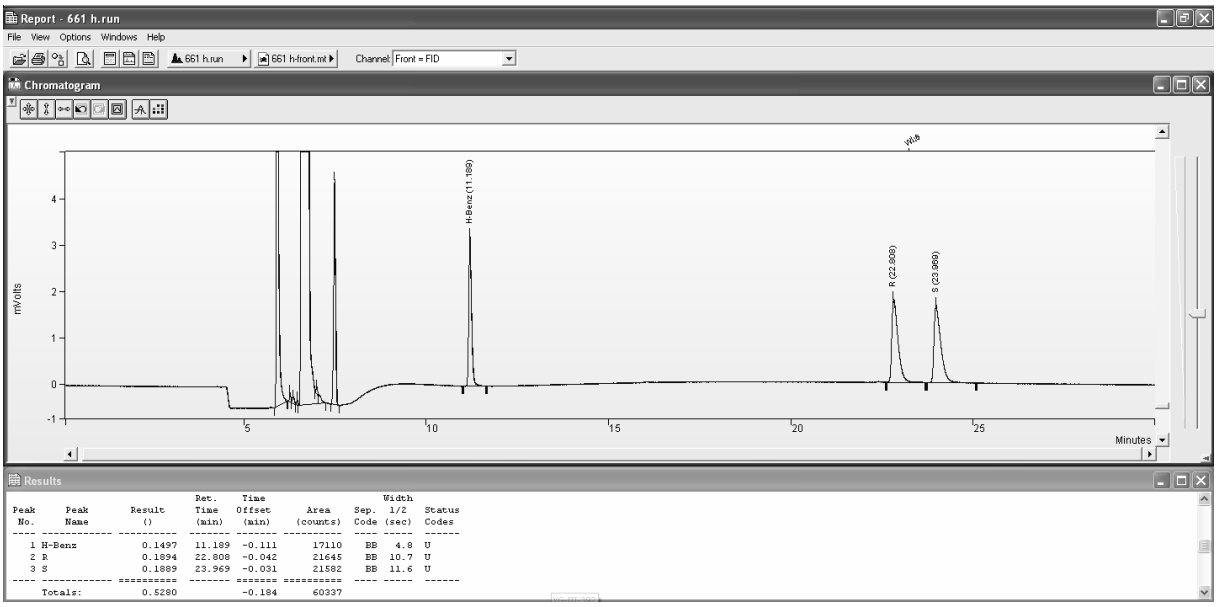
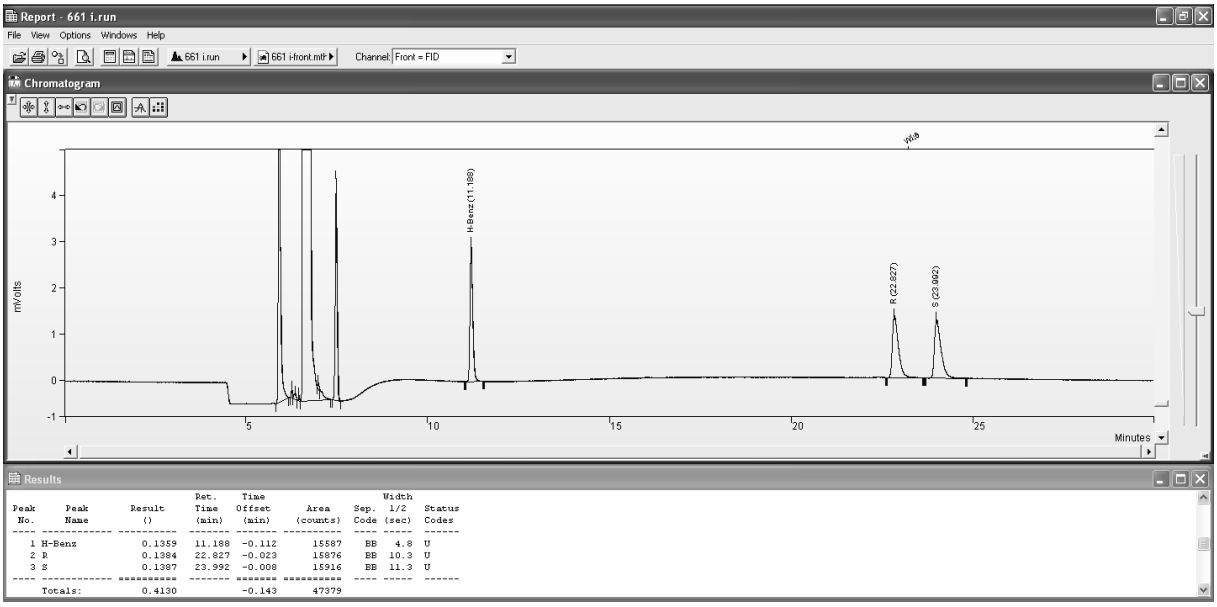
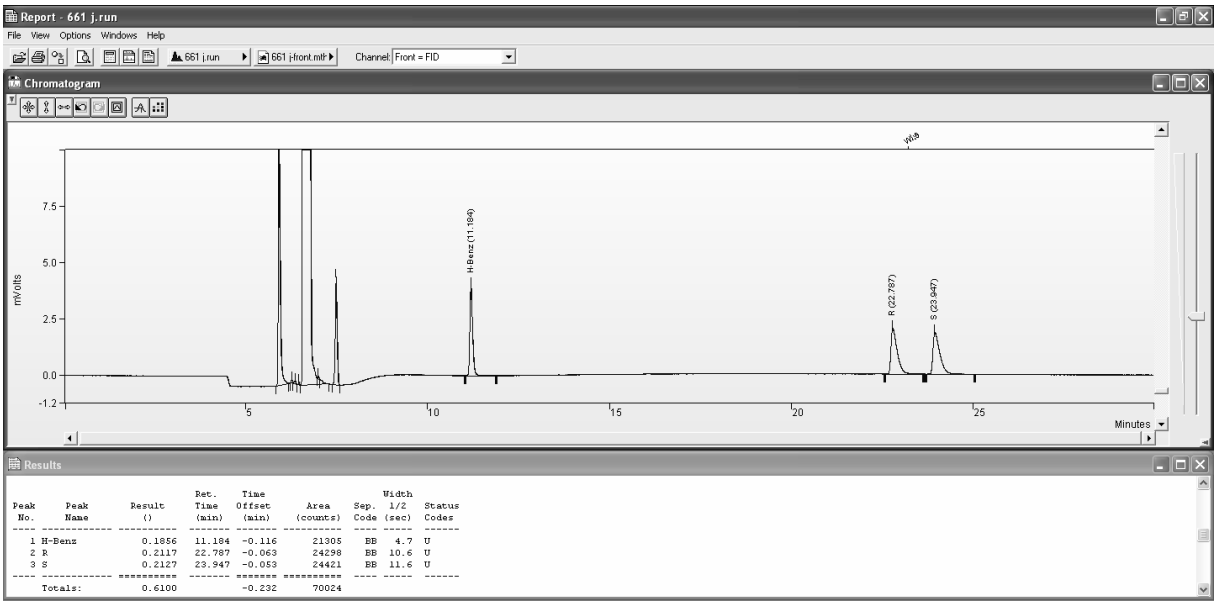
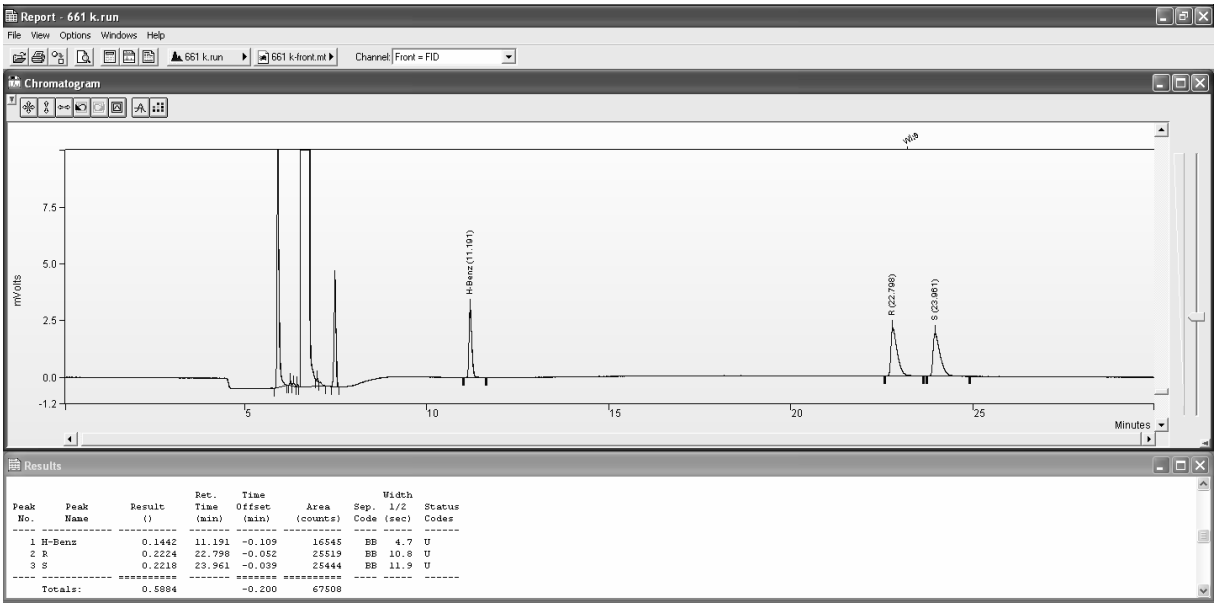
S (23.924)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1945 11.182 -0.118 22223 BB 4.7 U
2 R 0.2359 22.767 -0.083 26963 BB 10.6 U
3 S 0.2380 23.924 -0.076 27198 BB 12.0 U
Totals: 0.6684 -0.277 76384


Report - 661 h.run
File View Options Windows Help
661 h.run
661 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.189)
R (22.808)
S (23.969)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1497 11.189 -0.111 17110 BB 4.8 U
2 R 0.1894 22.808 -0.042 21645 BB 10.7 U
3 S 0.1889 23.969 -0.031 21582 BB 11.6 U
Totals: 0.5280 -0.184 60337

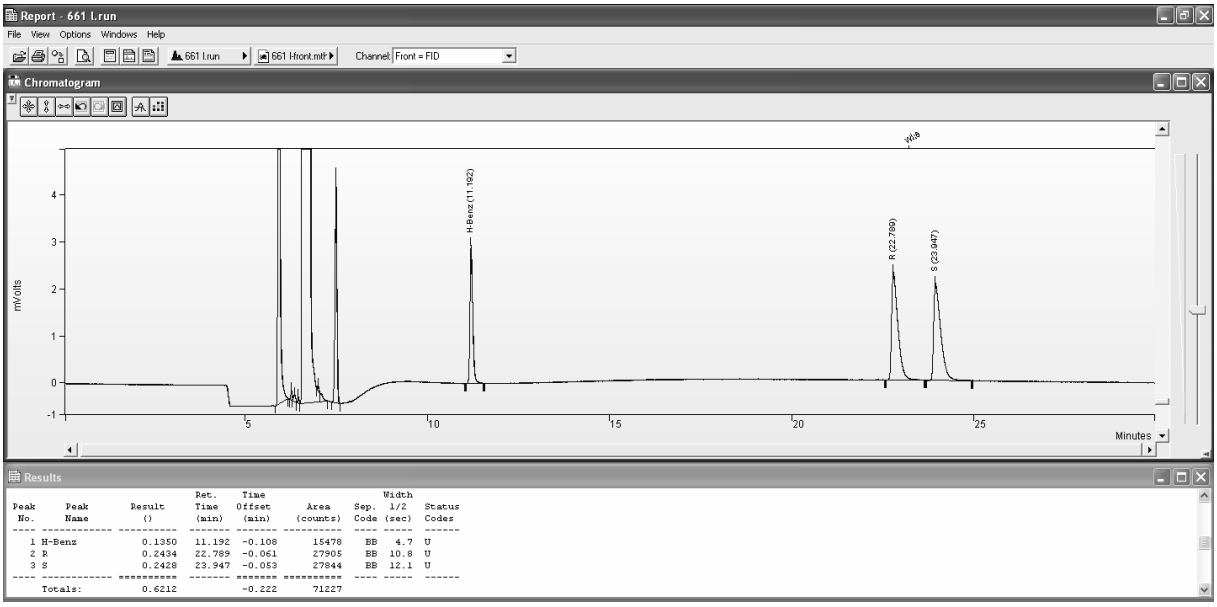

Report - 661 i.run
File View Options Windows Help
661 i.run
661 i-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.188)
R (22.827)
S (23.982)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1359 11.188 -0.112 15587 BB 4.8 U
2 R 0.1384 22.827 -0.023 15876 BB 10.3 U
3 S 0.1387 23.992 -0.008 15916 BB 11.3 U
Totals: 0.4130 -0.143 47379



Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1856	11.184	-0.116	21305	BB	4.7	U
2	R	0.2117	22.787	-0.063	24298	BB	10.6	U
3	S	0.2127	23.947	-0.053	24421	BB	11.6	U
	Totals:	0.6100		-0.232	70024			

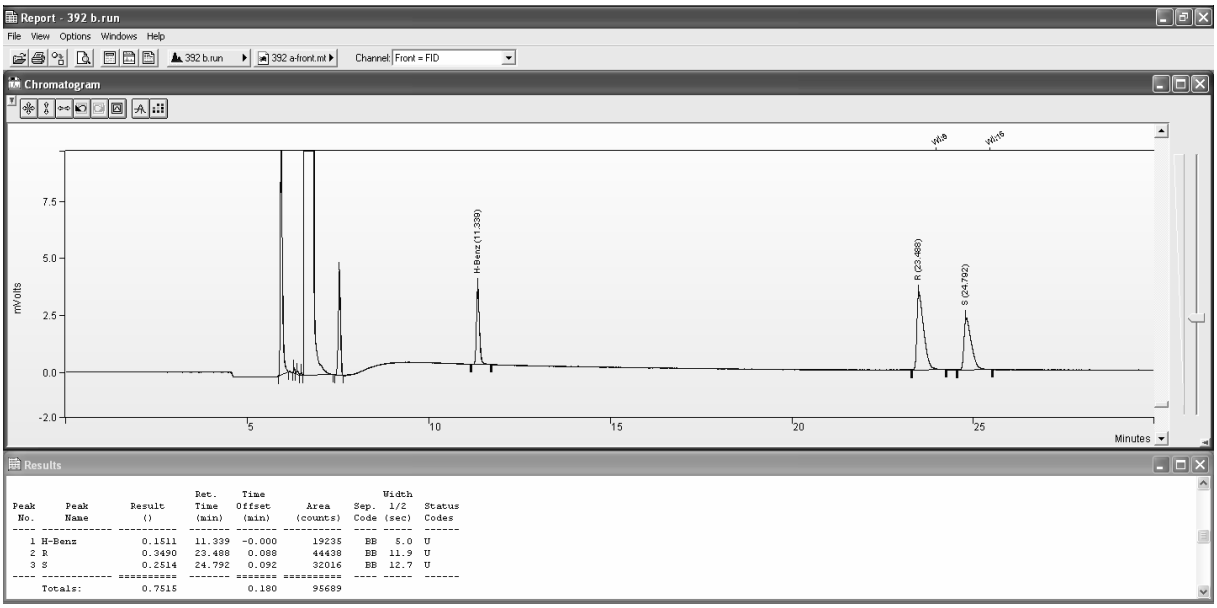


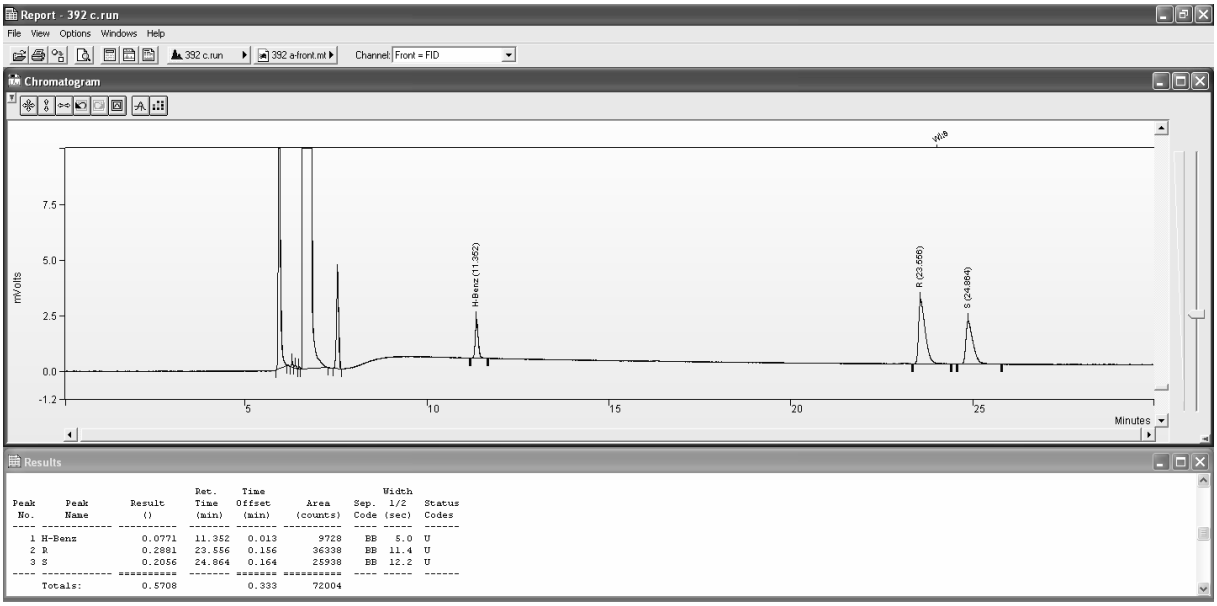
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1442	11.191	-0.109	16545	BB	4.7	U
2	R	0.2224	22.798	-0.052	25519	BB	10.8	U
3	S	0.2218	23.961	-0.039	25444	BB	11.9	U
	Totals:	0.5884		-0.200	67508			

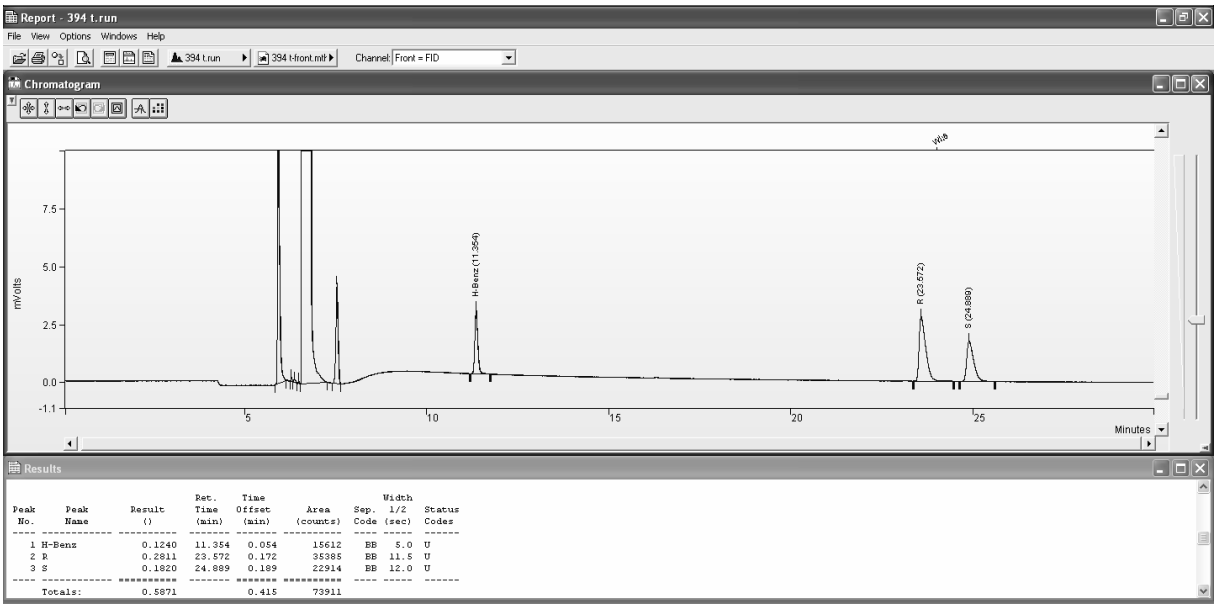


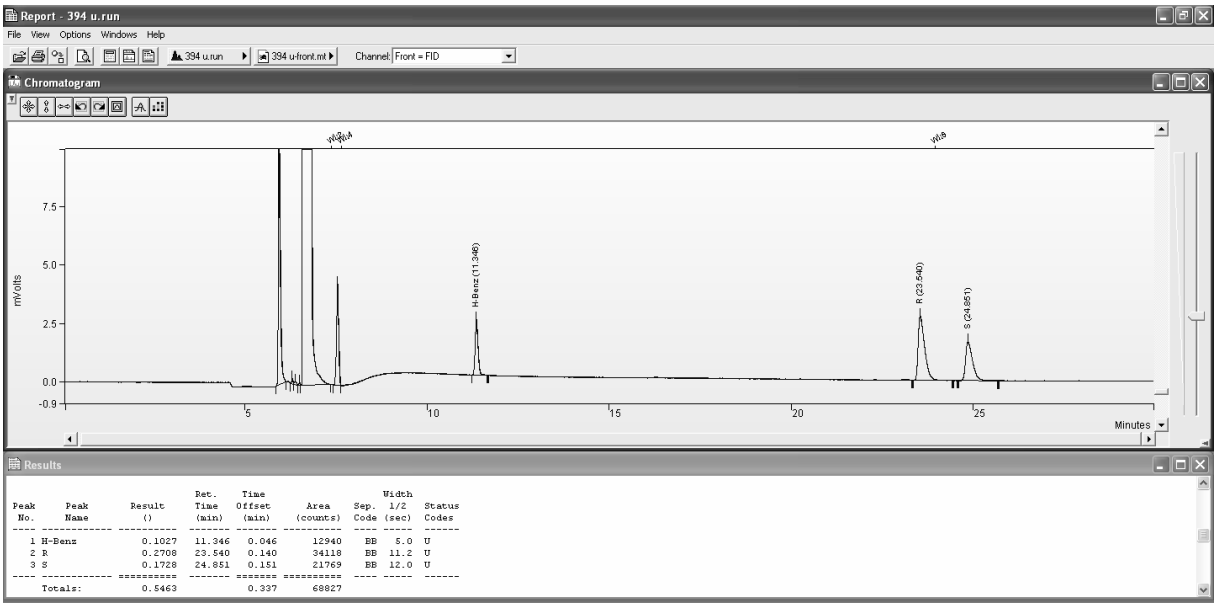
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1350	11.192	-0.108	15478	BB	4.7	U
2	R	0.2434	22.789	-0.061	27905	BB	10.8	U
3	S	0.2428	23.947	-0.053	27844	BB	12.1	U
	Totals:	0.6212		-0.222	71227			

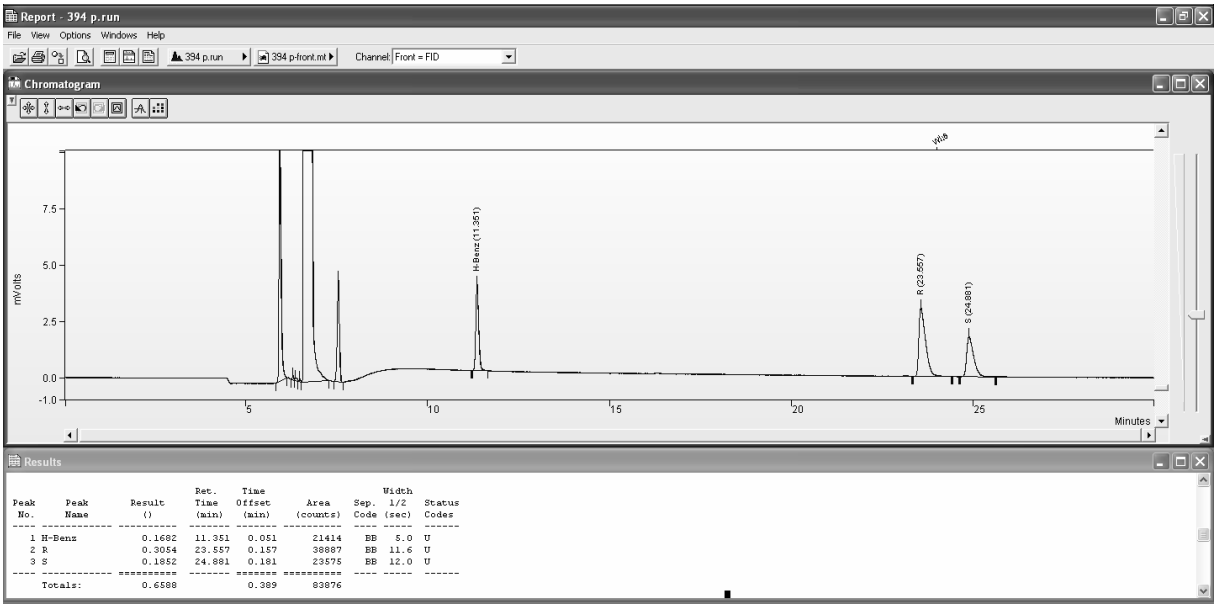
III.2 Figure 2a (NBE)

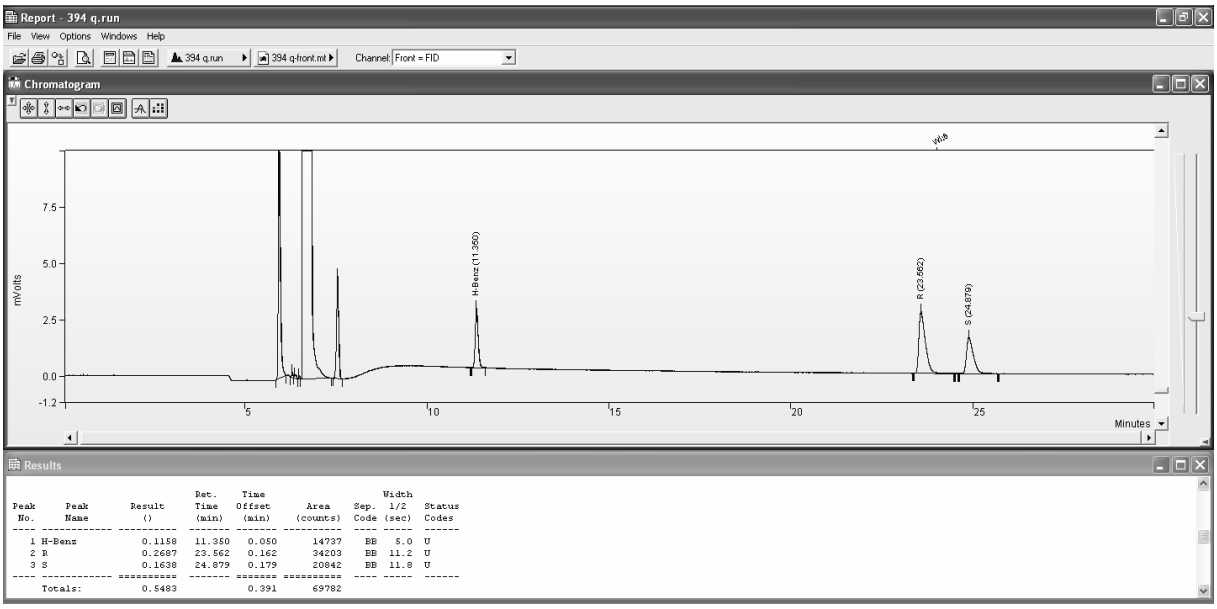




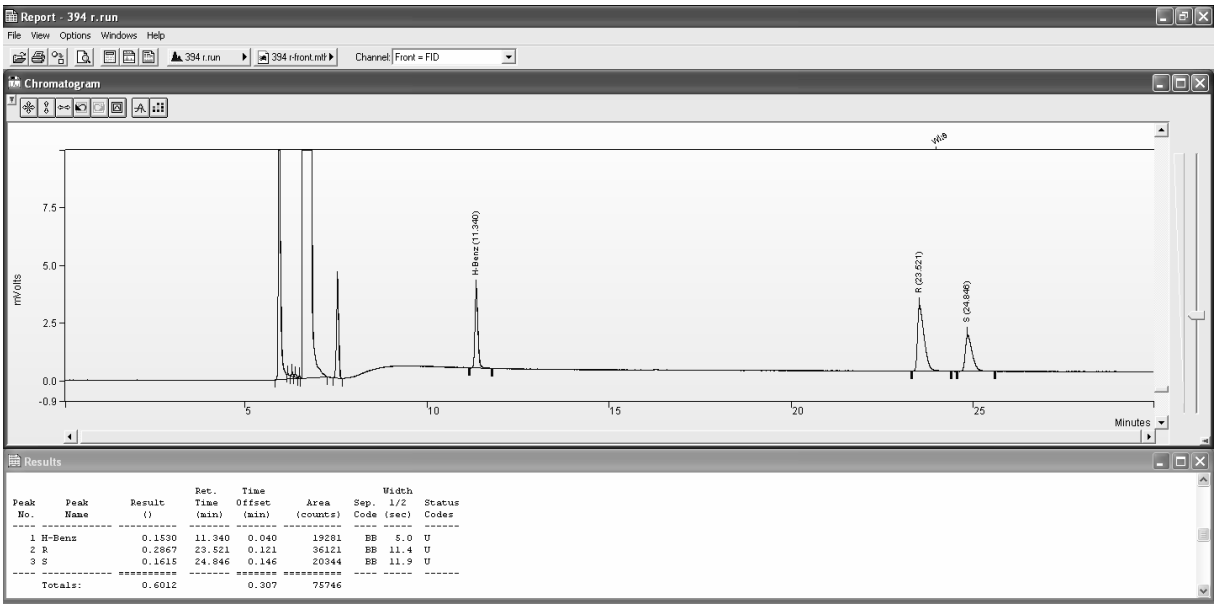

Report - 394 t.run
File View Options Windows Help
394 t.run
394 t-front.mth
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.354)
R (23.572)
S (24.889)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1240 11.354 0.054 15612 BB 5.0 U
2 R 0.2811 23.572 0.172 35385 BB 11.5 U
3 S 0.1820 24.889 0.189 22914 BB 12.0 U
Totals: 0.5871 0.415 73911


Report - 394 u.run
File View Options Windows Help
394 u.run
394 u-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.346)
R (23.540)
S (24.851)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1027 11.346 0.046 12940 BB 5.0 U
2 R 0.2708 23.540 0.140 34118 BB 11.2 U
3 S 0.1728 24.851 0.151 21769 BB 12.0 U
Totals: 0.5463 0.337 68827

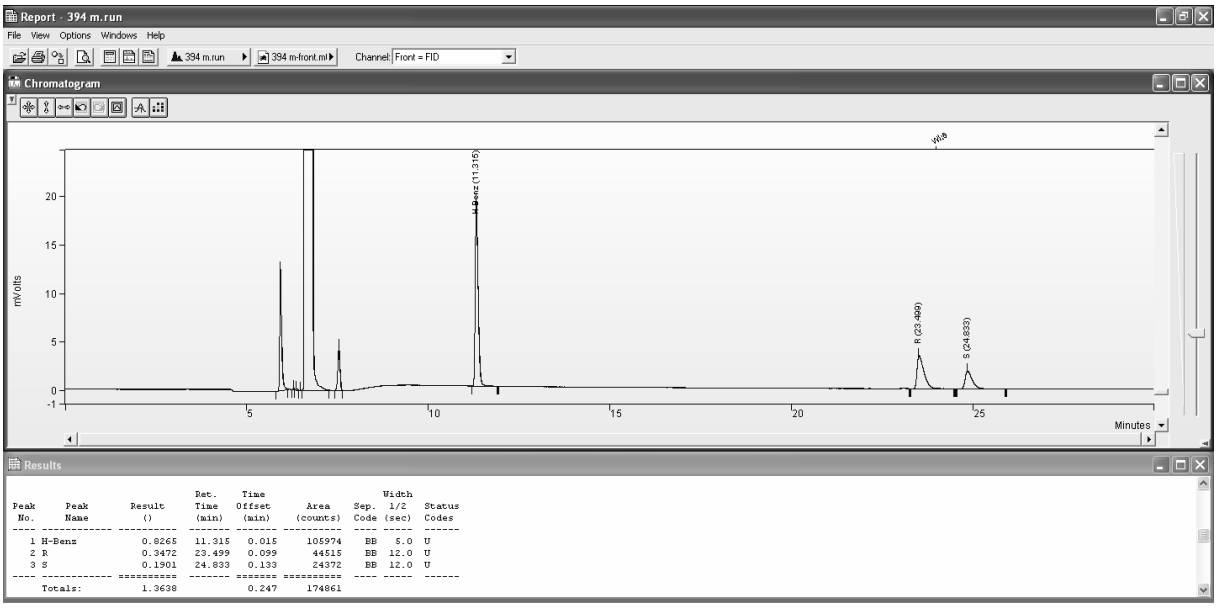

Report - 394 p.run
File View Options Windows Help
394 p.run
394 p-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.351)
R (23.557)
S (24.881)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1682 11.351 0.051 21414 BB 5.0 U
2 R 0.3054 23.557 0.157 38887 BB 11.6 U
3 S 0.1852 24.881 0.181 23575 BB 12.0 U
Totals: 0.6588 0.389 83876



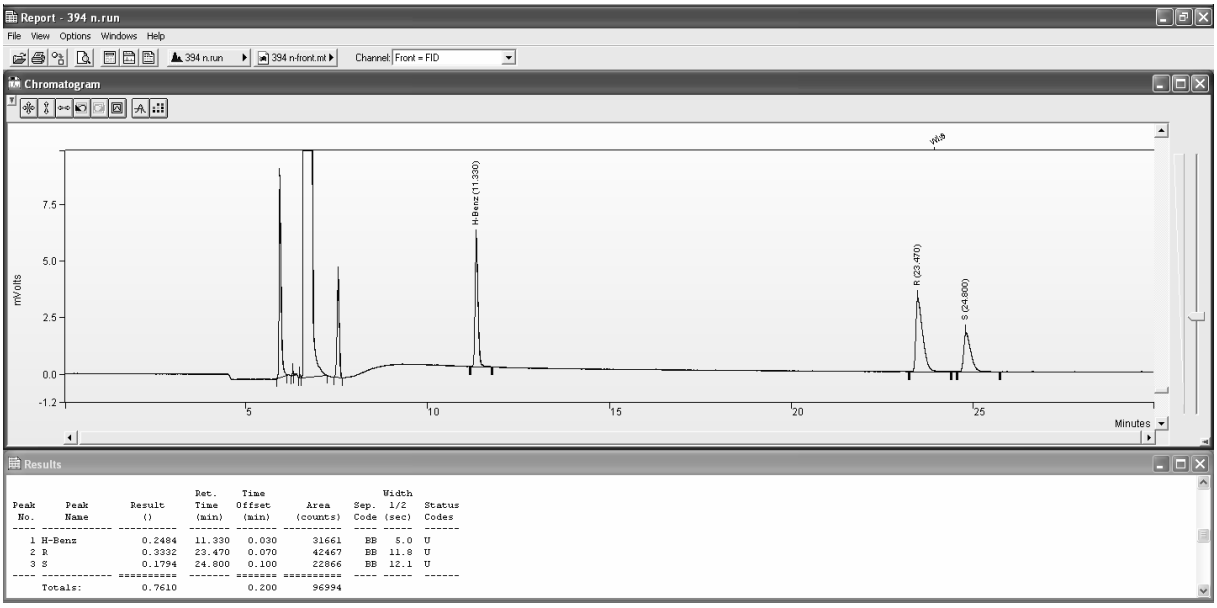
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1158	11.350	0.050	14737	BB	5.0	U
2	R	0.2687	23.562	0.162	34203	BB	11.2	U
3	S	0.1638	24.879	0.179	20842	BB	11.8	U
	Totals:	0.5483		0.391	69782			

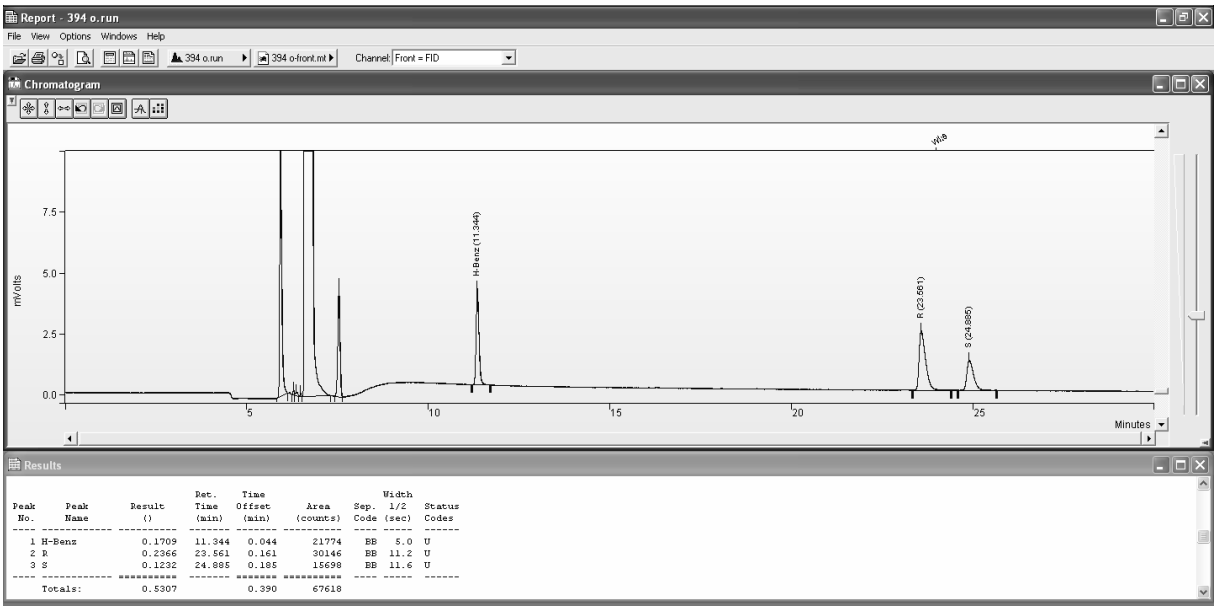


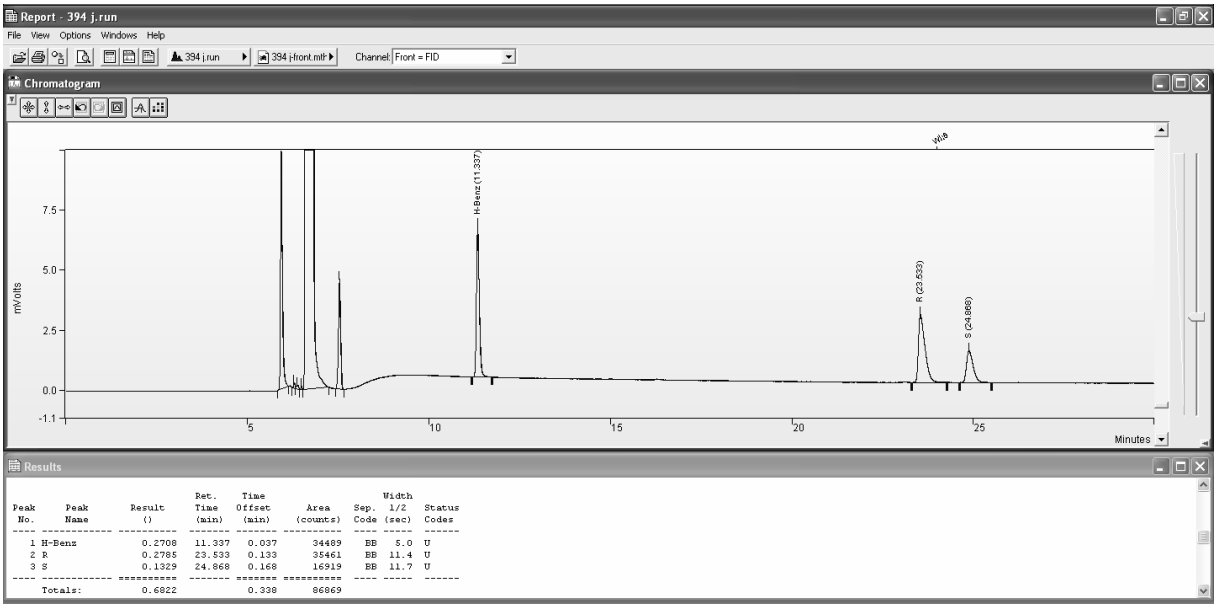
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1530	11.340	0.040	19281	BB	5.0	U
2	R	0.2867	23.521	0.121	36121	BB	11.4	U
3	S	0.1615	24.846	0.146	20344	BB	11.9	U
	Totals:	0.6012		0.307	75746			

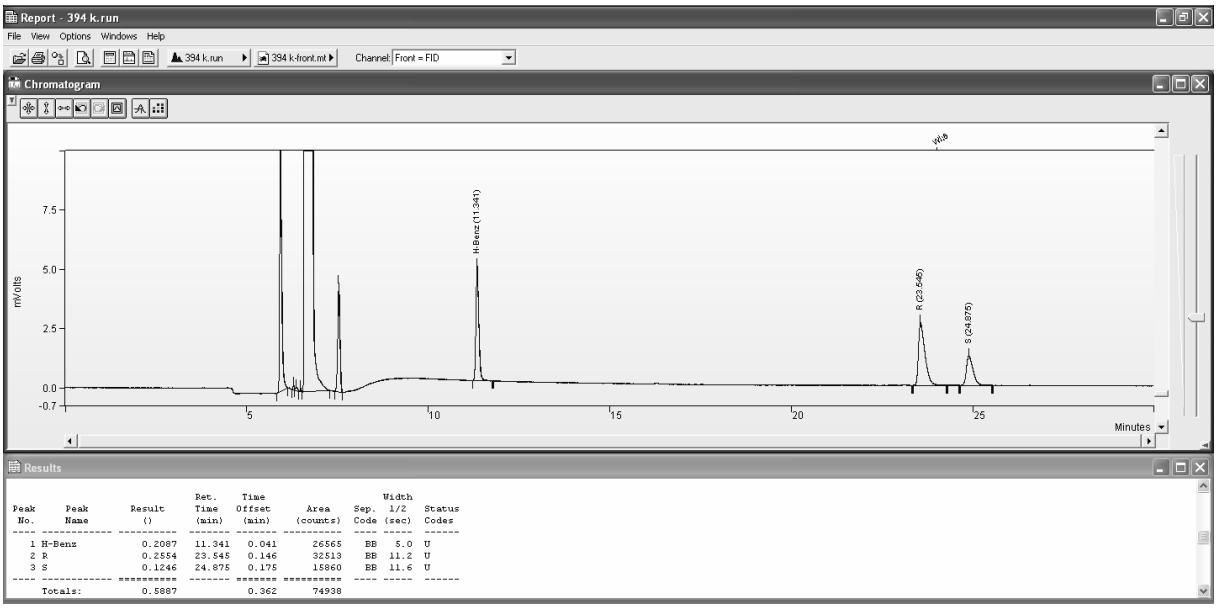


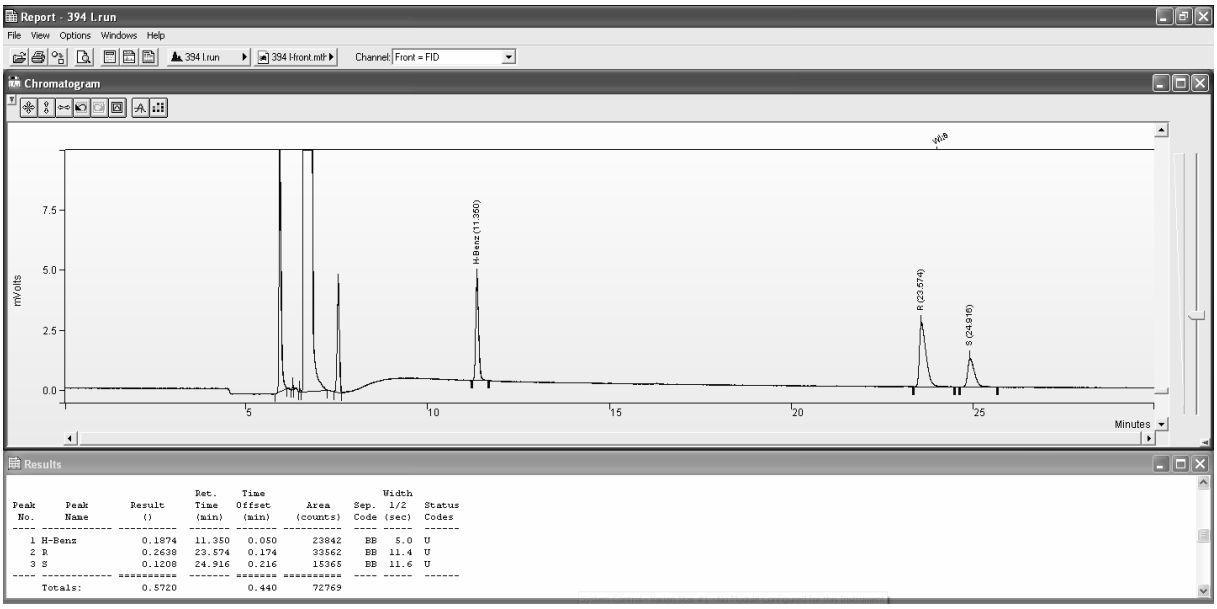
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.8265	11.315	0.015	105974	BB	5.0	U
2	R	0.3472	23.499	0.099	44515	BB	12.0	U
3	S	0.1901	24.833	0.133	24372	BB	12.0	U
	Totals:	1.3638		0.247	174861			

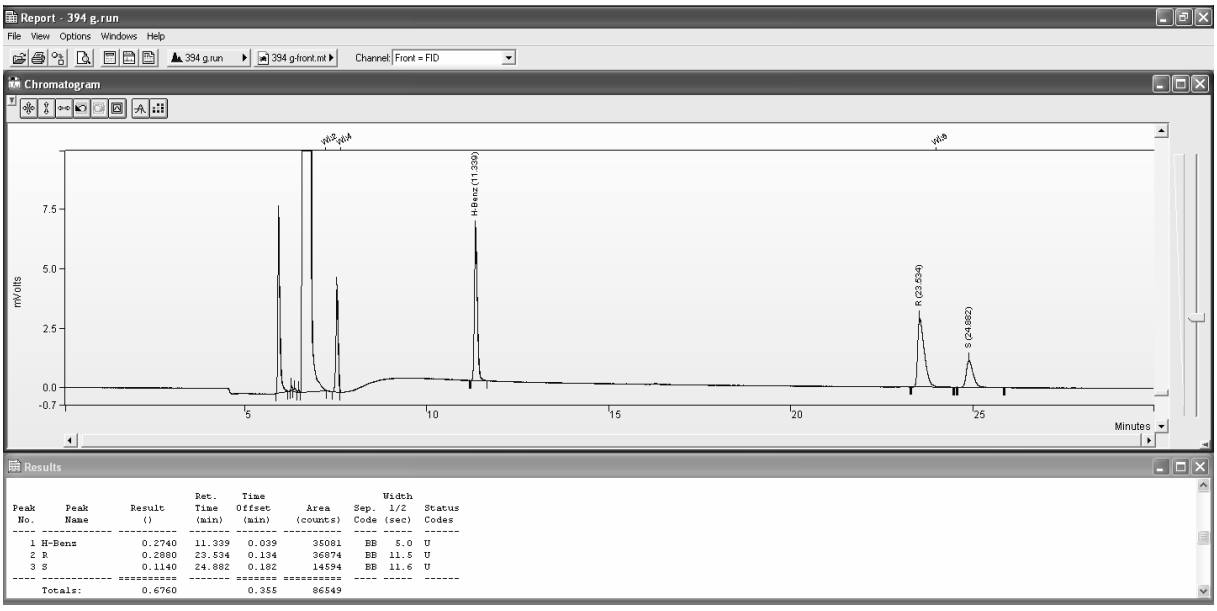

Report - 394 n.run
File View Options Windows Help
394 n.run
394 n-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.330)
R (23.470)
S (24.800)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2484 11.330 0.030 31661 BB 5.0 U
2 R 0.3332 23.470 0.070 42467 BB 11.8 U
3 S 0.1794 24.800 0.100 22866 BB 12.1 U
Totals: 0.7610 0.200 96994

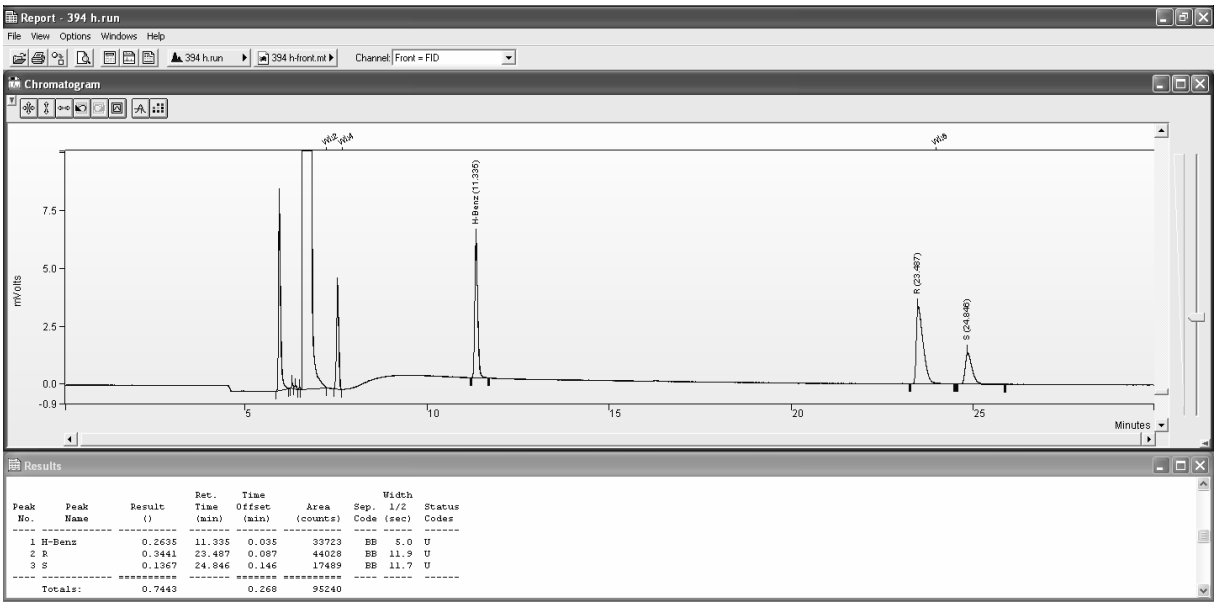

Report - 394 o.run
File View Options Windows Help
394 o.run
394 o-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.344)
R (23.561)
S (24.885)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1709 11.344 0.044 21774 BB 5.0 U
2 R 0.2366 23.561 0.161 30146 BB 11.2 U
3 S 0.1232 24.885 0.185 15698 BB 11.6 U
Totals: 0.5307 0.390 67618

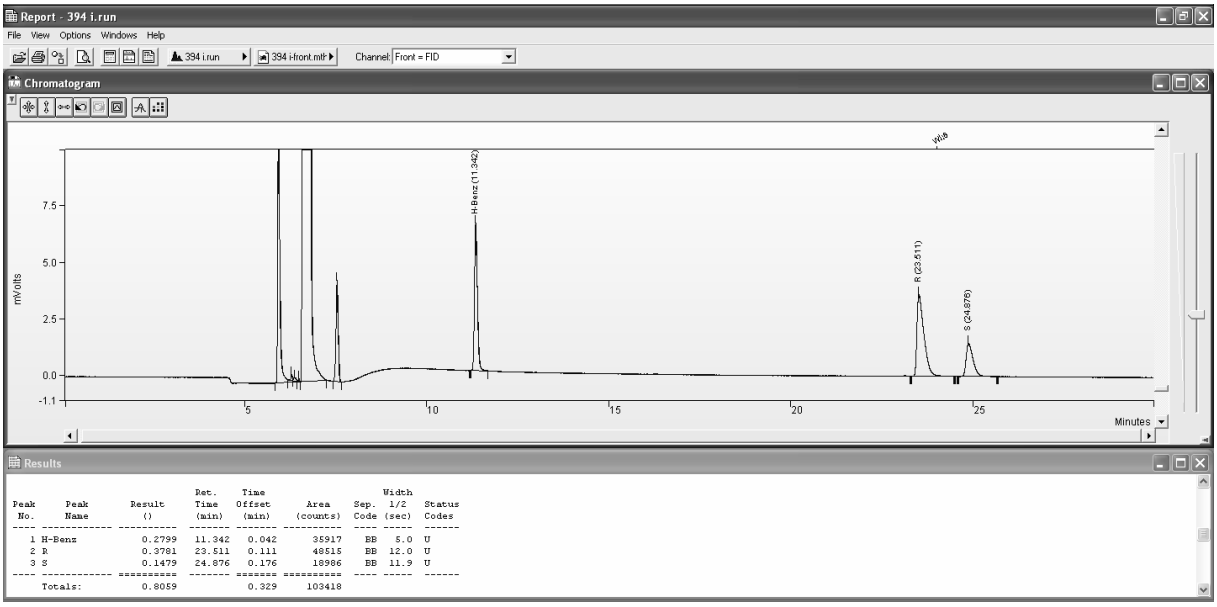

Report - 394 j.run
File View Options Windows Help
394 j.run
394 j-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.337)
R (23.533)
S (24.868)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2708 11.337 0.037 34489 BB 5.0 U
2 R 0.2785 23.533 0.133 35461 BB 11.4 U
3 S 0.1329 24.868 0.168 16919 BB 11.7 U
Totals: 0.6822 0.338 86869

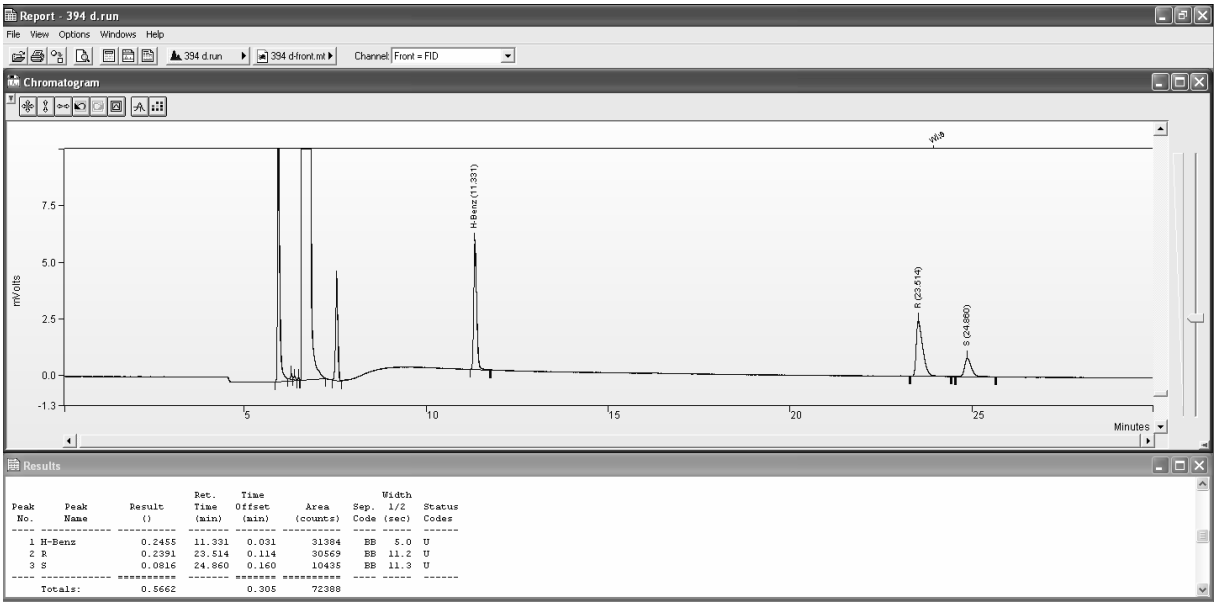

Report - 394 k.run
File View Options Windows Help
394 k.run
394 k-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.341)
R (23.545)
S (24.875)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2087 11.341 0.041 26565 BB 5.0 U
2 R 0.2554 23.545 0.146 32513 BB 11.2 U
3 S 0.1246 24.875 0.175 15860 BB 11.6 U
Totals: 0.5887 0.362 74938

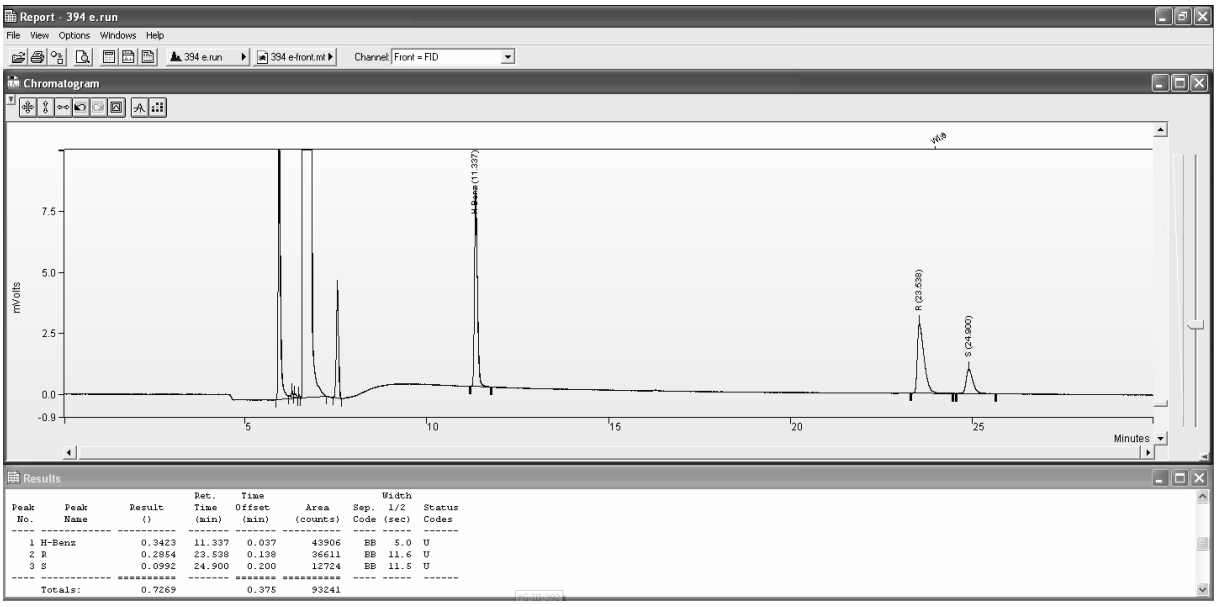

Report - 394 l.run
File View Options Windows Help
394 l.run
394 l-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.350)
R (23.574)
S (24.916)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1874 11.350 0.050 23842 BB 5.0 U
2 R 0.2638 23.574 0.174 33562 BB 11.4 U
3 S 0.1208 24.916 0.216 15365 BB 11.6 U
Totals: 0.5720 0.440 72769

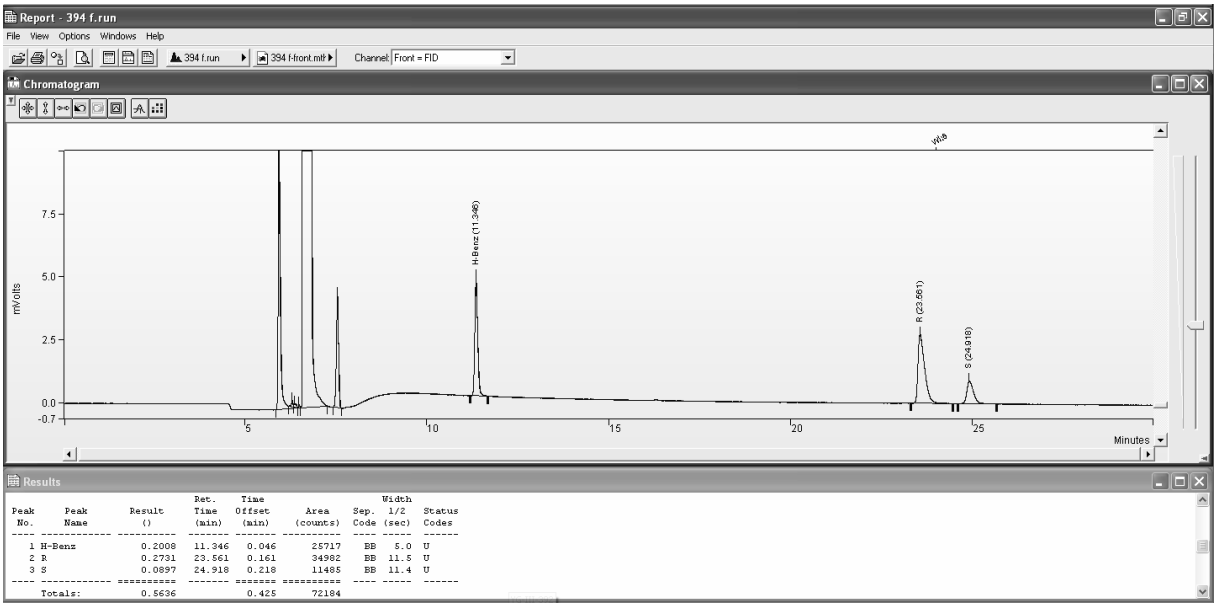

Report - 394 g.run
File View Options Windows Help
394 g.run
394 g-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.339)
R (23.534)
S (24.882)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2740 11.339 0.039 35081 BB 5.0 U
2 R 0.2880 23.534 0.134 36874 BB 11.5 U
3 S 0.1140 24.882 0.182 14594 BB 11.6 U
Totals: 0.6760 0.355 86549

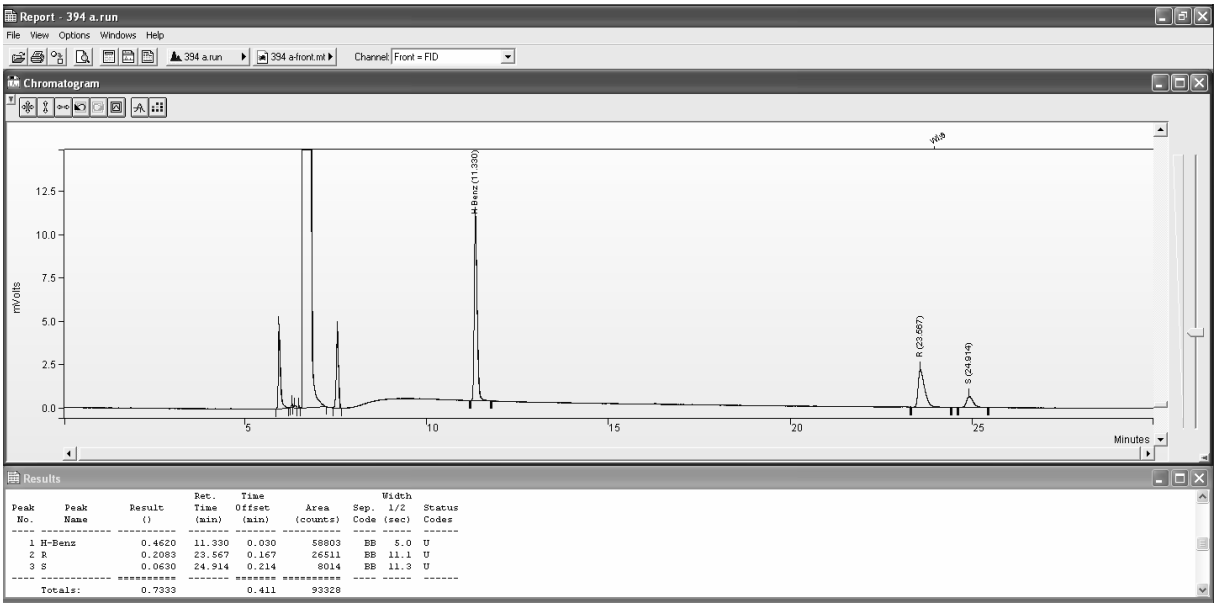

Report - 394 h.run
File View Options Windows Help
394 h.run
394 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.335)
R (23.487)
S (24.846)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2635 11.335 0.035 33723 BB 5.0 U
2 R 0.3441 23.487 0.087 44028 BB 11.9 U
3 S 0.1367 24.846 0.146 17489 BB 11.7 U
Totals: 0.7443 0.268 95240

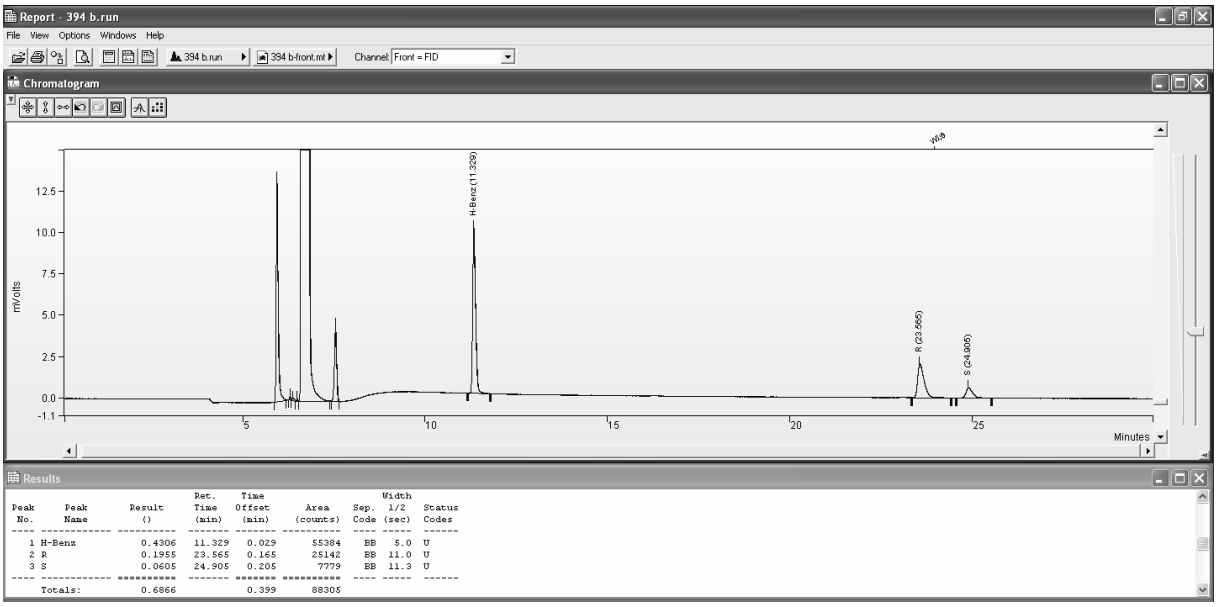

Report - 394 i.run
File View Options Windows Help
394 i.run
394 i-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.342)
R (23.511)
S (24.876)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2799 11.342 0.042 35917 BB 5.0 U
2 R 0.3781 23.511 0.111 48515 BB 12.0 U
3 S 0.1479 24.876 0.176 18986 BB 11.9 U
Totals: 0.8059 0.329 103418

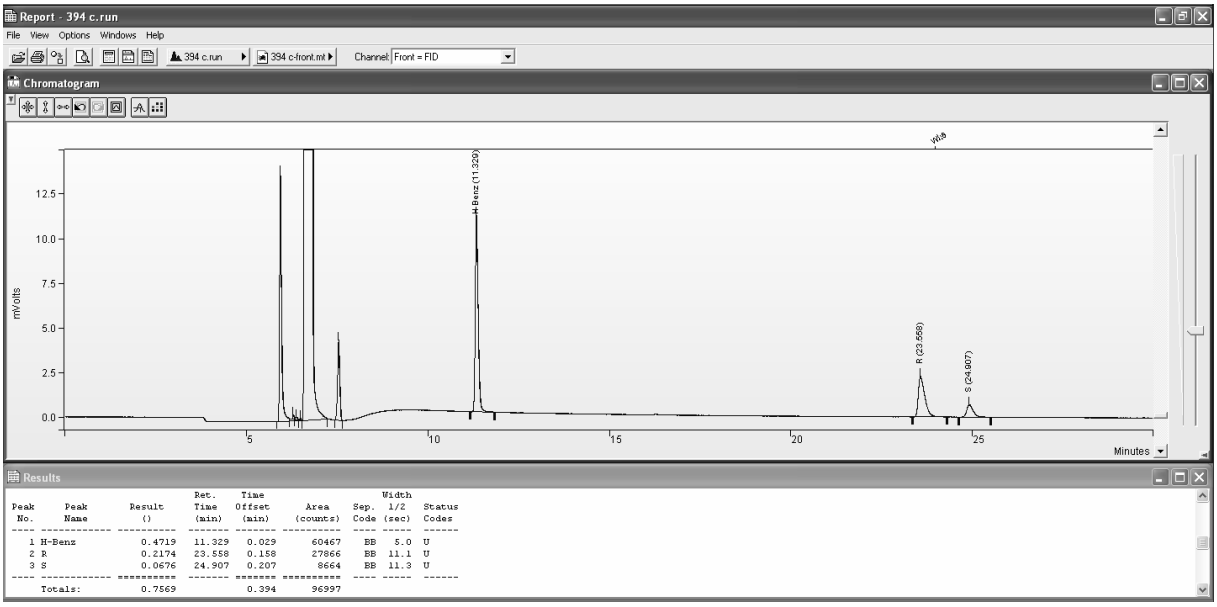

Report - 394 d.run
File View Options Windows Help
394 d.run
394 d-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.331)
R (23.514)
S (24.860)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2455 11.331 0.031 31384 BB 5.0 U
2 R 0.2391 23.514 0.114 30569 BB 11.2 U
3 S 0.0816 24.860 0.160 10435 BB 11.3 U
Totals: 0.5662 0.305 72388

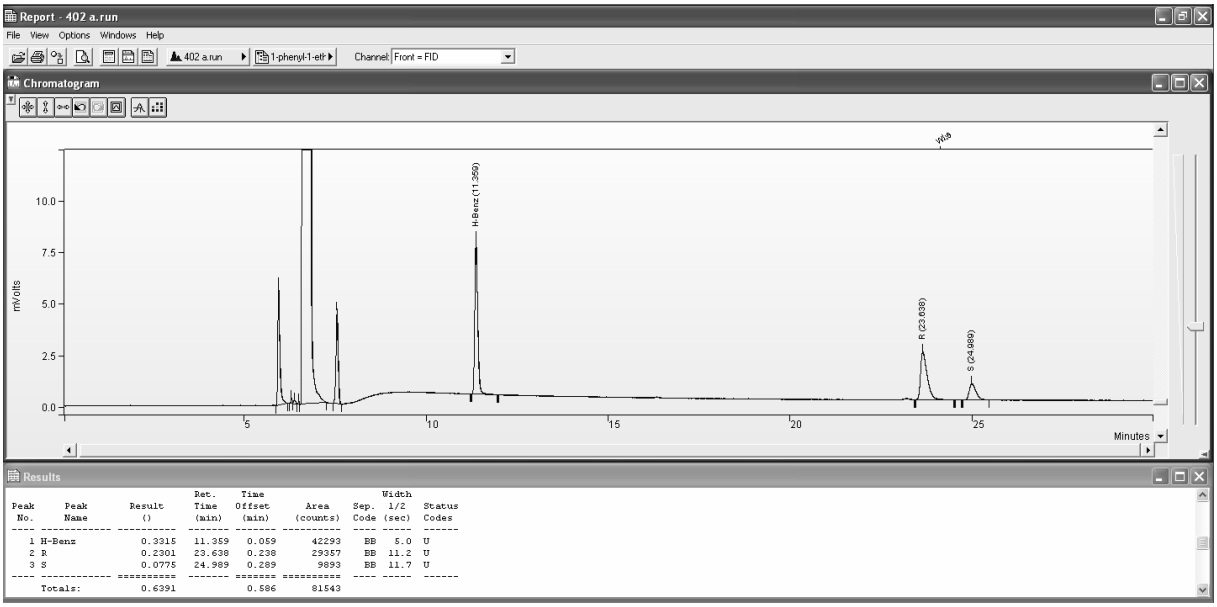

Report - 394 e.run
File View Options Windows Help
394 e.run
394 e-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.337)
R (23.538)
S (24.900)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3423 11.337 0.037 43906 BB 5.0 U
2 R 0.2854 23.538 0.138 36611 BB 11.6 U
3 S 0.0992 24.900 0.200 12724 BB 11.5 U
Totals: 0.7269 0.375 93241

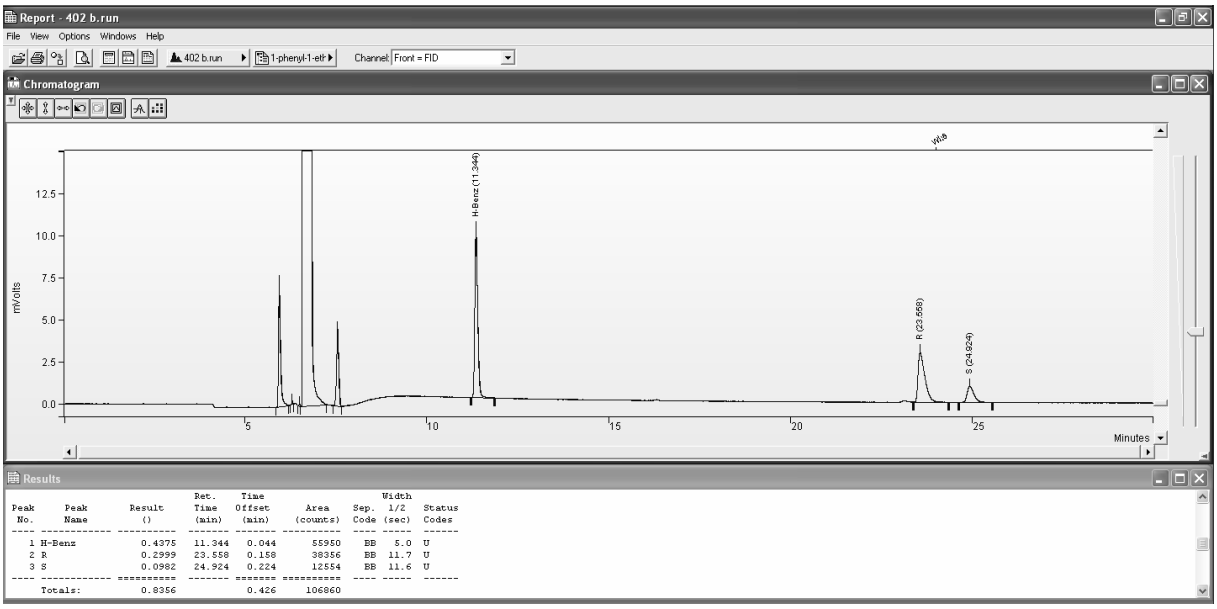

Report - 394 f.run
File View Options Windows Help
394 f.run
394 f-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.346)
R (23.561)
S (24.918)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2008 11.346 0.046 25717 BB 5.0 U
2 R 0.2731 23.561 0.161 34982 BB 11.5 U
3 S 0.0897 24.918 0.218 11485 BB 11.4 U
Totals: 0.5636 0.425 72184

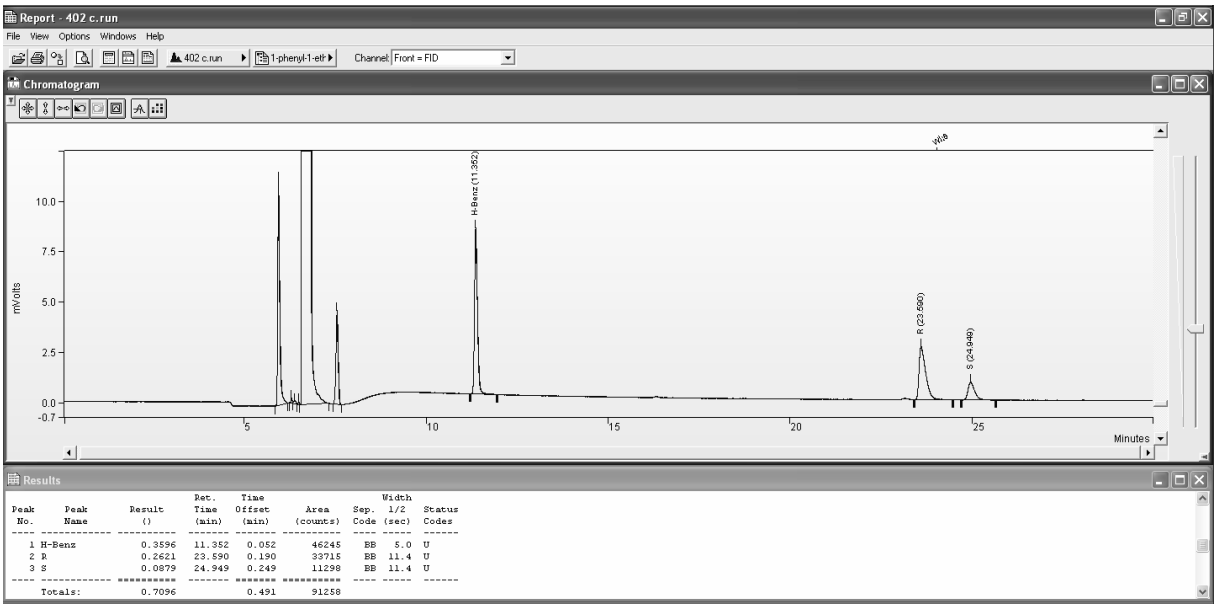

Report - 394 a.run
File View Options Windows Help
394 a.run
394 a-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.330)
R (23.567)
S (24.914)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4620 11.330 0.030 58803 BB 5.0 U
2 R 0.2083 23.567 0.167 26511 BB 11.1 U
3 S 0.0630 24.914 0.214 8014 BB 11.3 U
Totals: 0.7333 0.411 93328

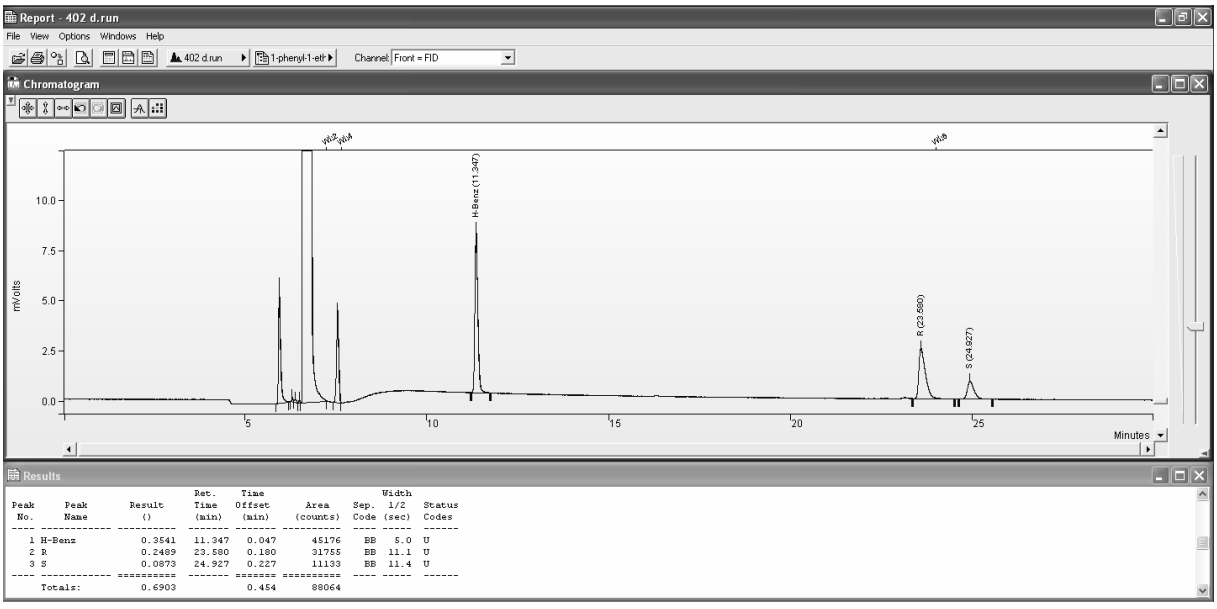

Report - 394 b.run
File View Options Windows Help
394 b.run
394 b-front.ml
Channel Front = FID
Chromatogram
mV
H-Benz (11.329)
R (23.565)
S (24.905)
mV/olts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4306 11.329 0.029 55384 BB 5.0 U
2 R 0.1955 23.565 0.165 25142 BB 11.0 U
3 S 0.0605 24.905 0.205 7779 BB 11.3 U
Totals: 0.6866 0.399 88305

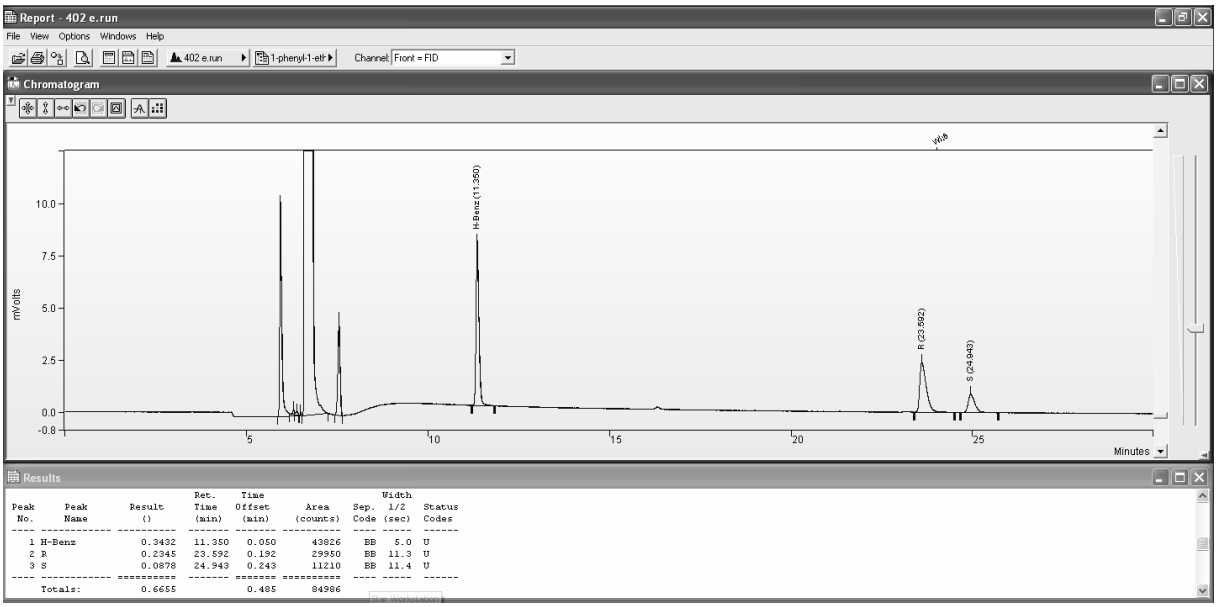

Report - 394 c.run
File View Options Windows Help
394 c.run
394 c-front.ml
Channel Front = FID
Chromatogram
mV
H-Benz (11.329)
R (23.558)
S (24.907)
mV/olts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4719 11.329 0.029 60467 BB 5.0 U
2 R 0.2174 23.558 0.158 27866 BB 11.1 U
3 S 0.0676 24.907 0.207 8664 BB 11.3 U
Totals: 0.7569 0.394 96997

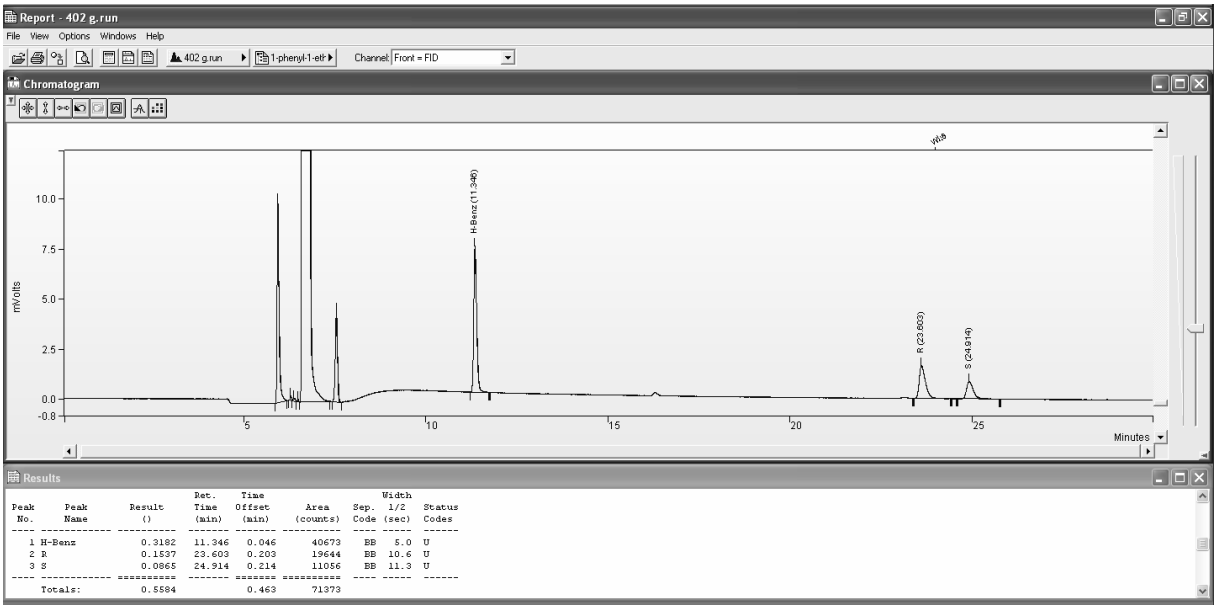

Report - 402 a.run
File View Options Windows Help
402 a.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mV
H-Benz (11.359)
R (23.638)
S (24.989)
mV/olts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3315 11.359 0.059 42293 BB 5.0 U
2 R 0.2301 23.638 0.238 29357 BB 11.2 U
3 S 0.0775 24.989 0.289 9893 BB 11.7 U
Totals: 0.6391 0.586 81543

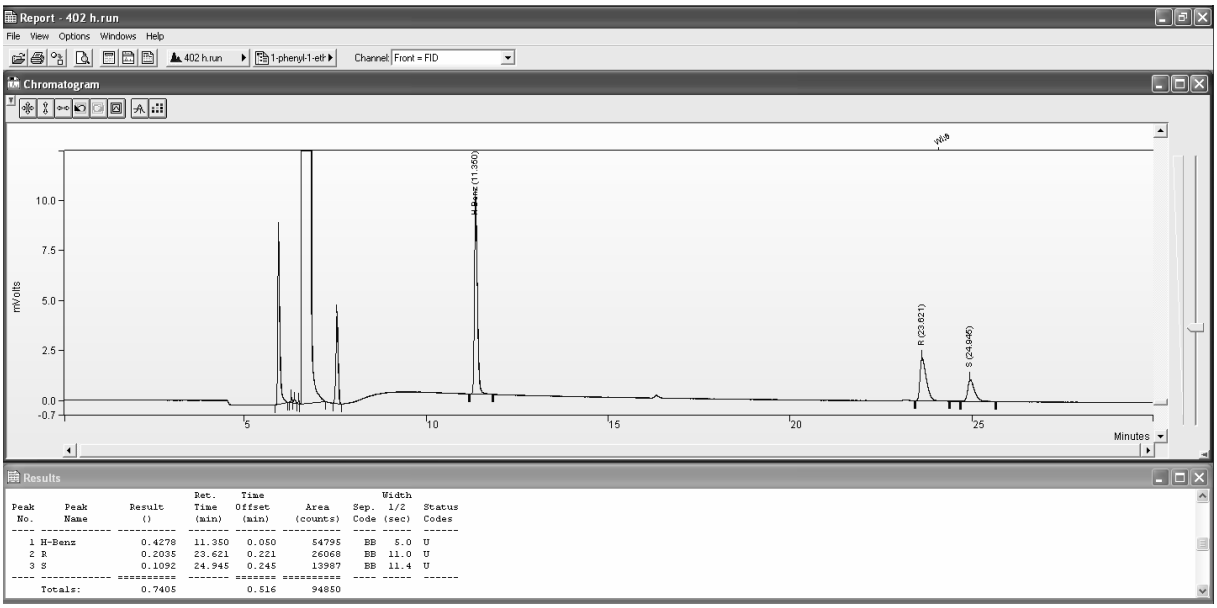

Report - 402 b.run
File View Options Windows Help
402 b.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
WvB
H-Benz (11.346)
R (23.558)
S (24.924)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4375 11.344 0.044 55950 BB 5.0 U
2 R 0.2999 23.558 0.158 38356 BB 11.7 U
3 S 0.0982 24.924 0.224 12554 BB 11.6 U
Totals: 0.8356 0.426 106860

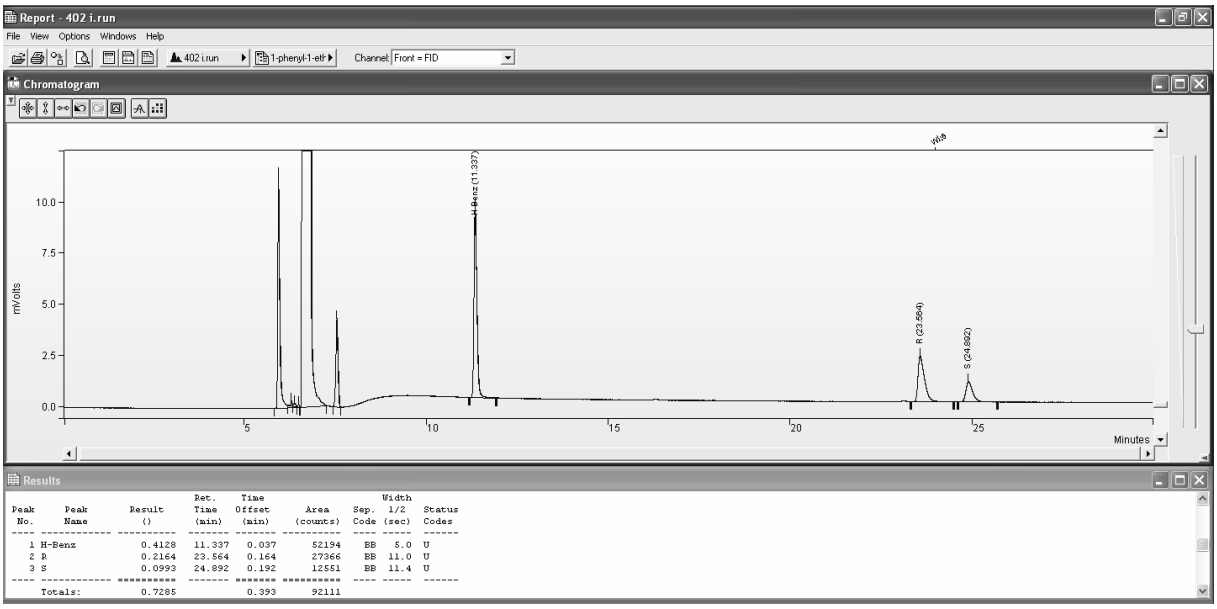

Report - 402 c.run
File View Options Windows Help
402 c.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
WvB
H-Benz (11.352)
R (23.590)
S (24.949)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3596 11.352 0.052 46245 BB 5.0 U
2 R 0.2621 23.590 0.190 33715 BB 11.4 U
3 S 0.0879 24.949 0.249 11298 BB 11.4 U
Totals: 0.7096 0.491 91258

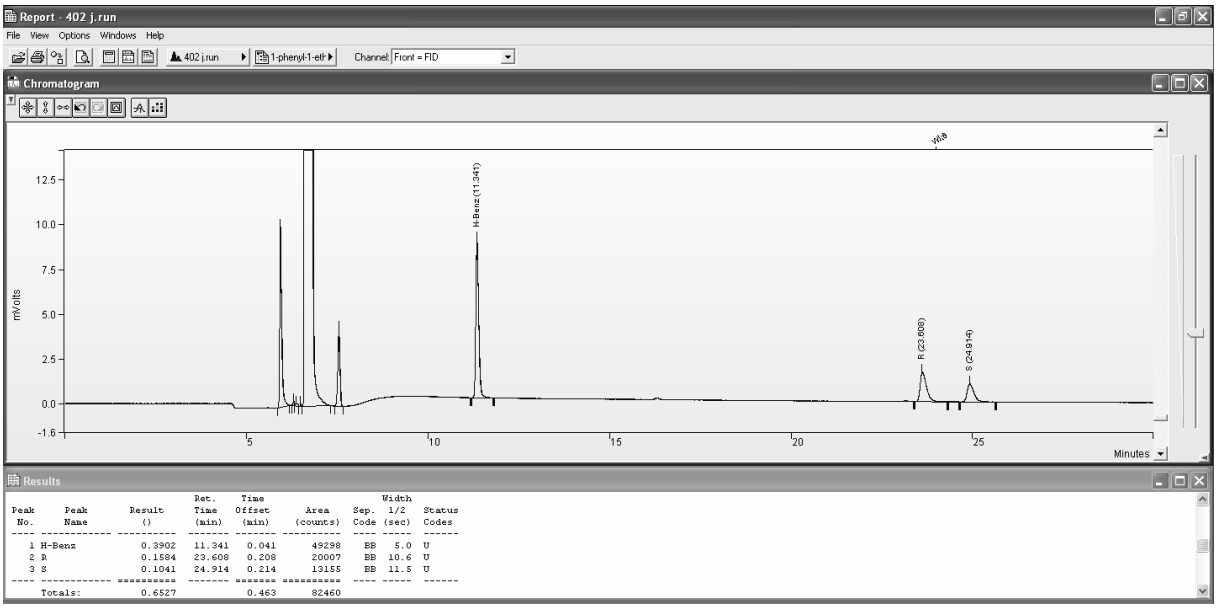

Report - 402 d.run
File View Options Windows Help
402 d.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
WvB
WvM
H-Benz (11.347)
R (23.560)
S (24.927)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3541 11.347 0.047 45176 BB 5.0 U
2 R 0.2489 23.580 0.180 31755 BB 11.1 U
3 S 0.0873 24.927 0.227 11133 BB 11.4 U
Totals: 0.6903 0.454 88064

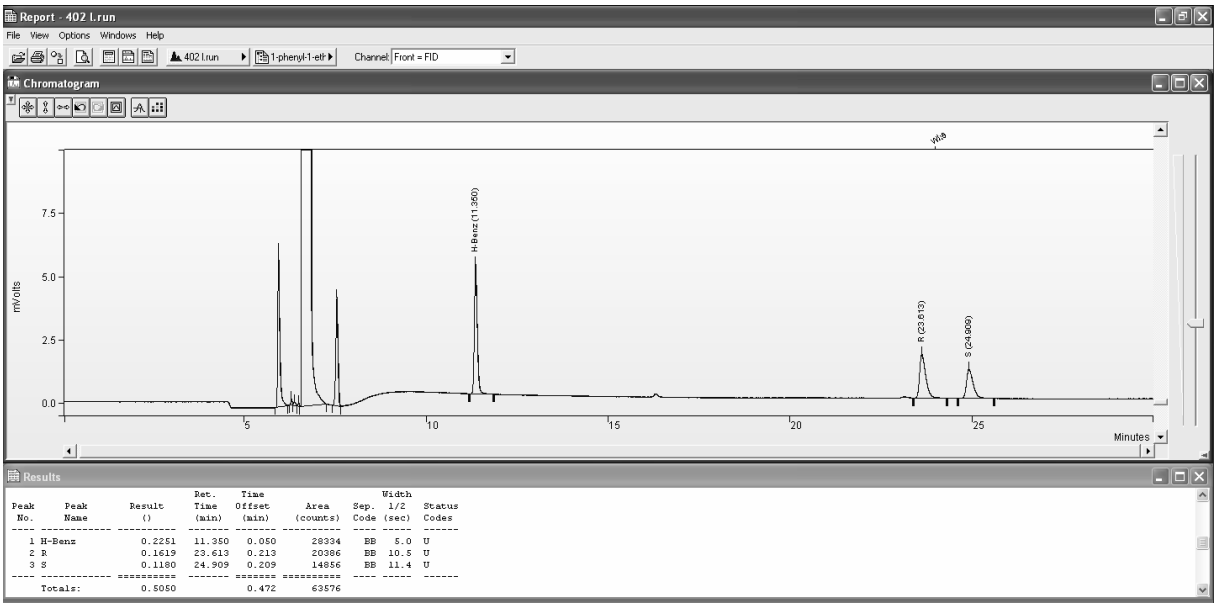

Report - 402 e.run
File View Options Windows Help
402 e.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.350)
R (23.592)
S (24.943)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3432 11.350 0.050 43826 BB 5.0 U
2 R 0.2345 23.592 0.192 29950 BB 11.3 U
3 S 0.0878 24.943 0.243 11210 BB 11.4 U
Totals: 0.6655 0.485 84986


Report - 402 g.run
File View Options Windows Help
402 g.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.346)
R (23.603)
S (24.914)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3182 11.346 0.046 40673 BB 5.0 U
2 R 0.1537 23.603 0.203 19644 BB 10.6 U
3 S 0.0865 24.914 0.214 11056 BB 11.3 U
Totals: 0.5584 0.463 71373

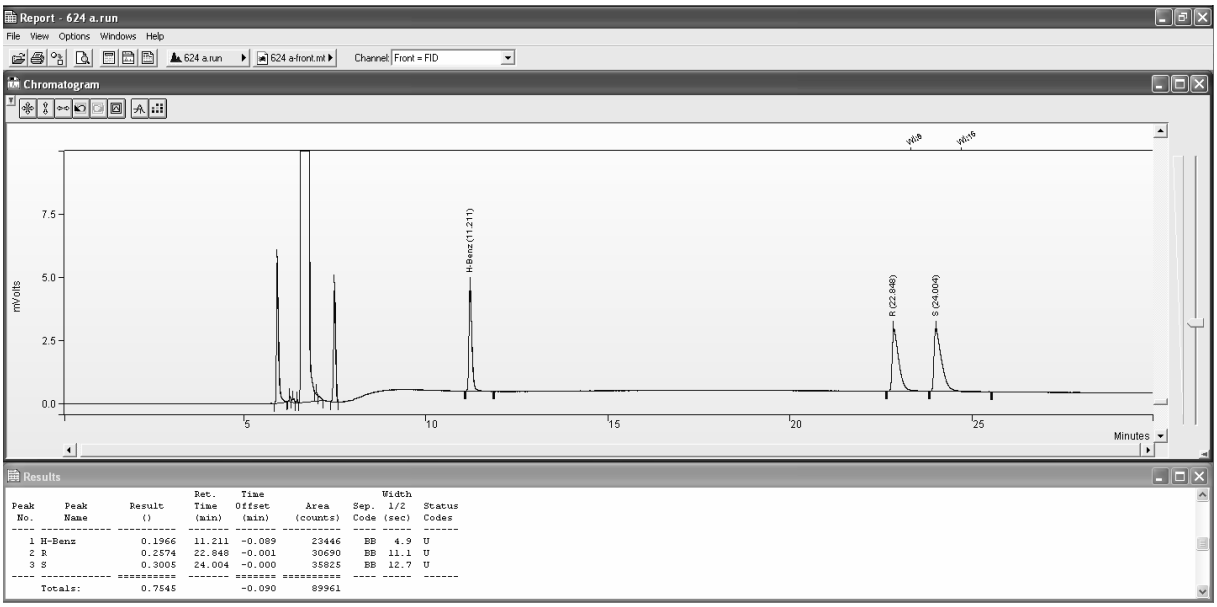

Report - 402 h.run
File View Options Windows Help
402 h.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.360)
R (23.621)
S (24.945)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4278 11.350 0.050 54795 BB 5.0 U
2 R 0.2035 23.621 0.221 26068 BB 11.0 U
3 S 0.1092 24.945 0.245 13987 BB 11.4 U
Totals: 0.7405 0.516 94850

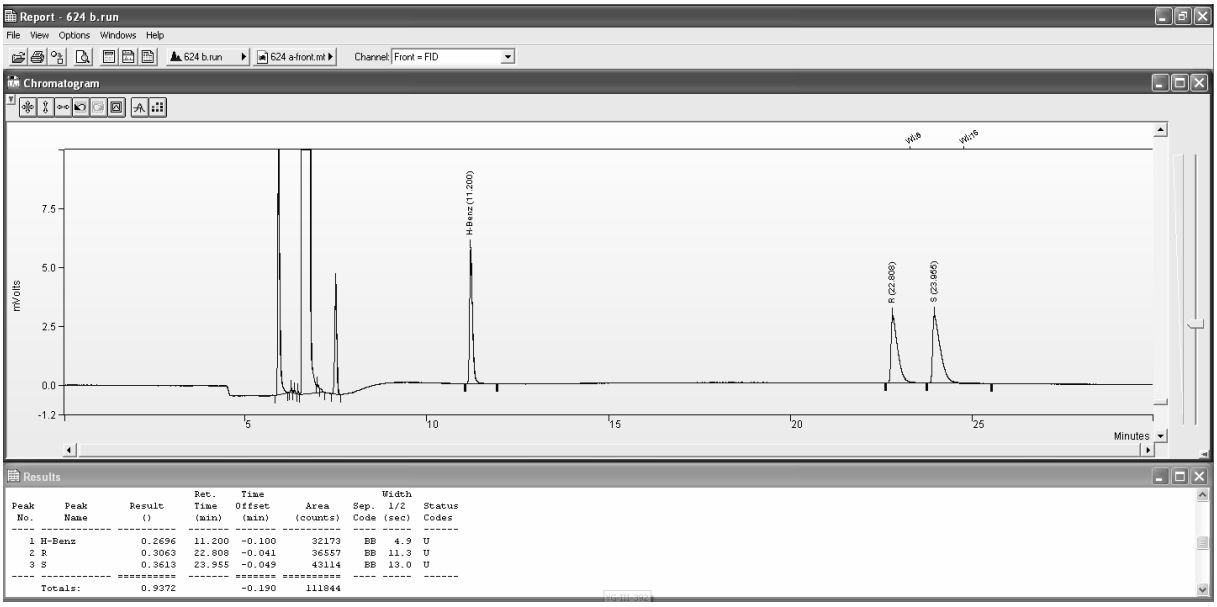

Report - 402 i.run
File View Options Windows Help
402 i.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.337)
R (23.564)
S (24.892)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4128 11.337 0.037 52194 BB 5.0 U
2 R 0.2164 23.564 0.164 27366 BB 11.0 U
3 S 0.0993 24.892 0.192 12551 BB 11.4 U
Totals: 0.7285 0.393 92111

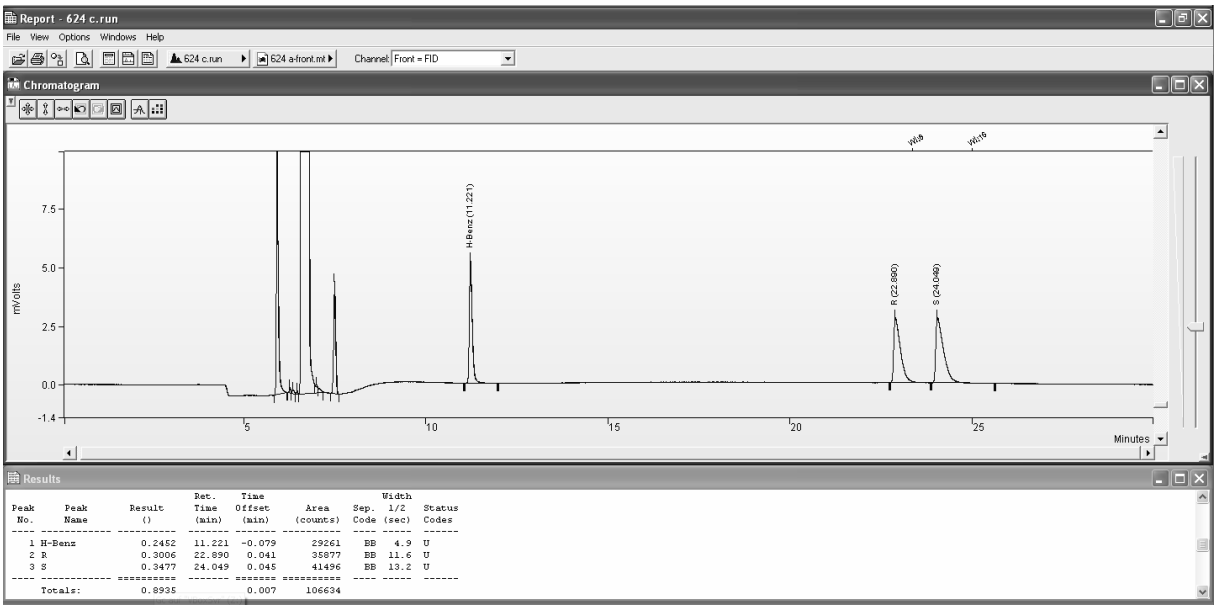

Report - 402 j.run
File View Options Windows Help
402 j.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.341)
R (23.608)
S (24.914)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3902 11.341 0.041 49298 BB 5.0 U
2 R 0.1584 23.608 0.208 20007 BB 10.6 U
3 S 0.1041 24.914 0.214 13155 BB 11.5 U
Totals: 0.6527 0.463 82460

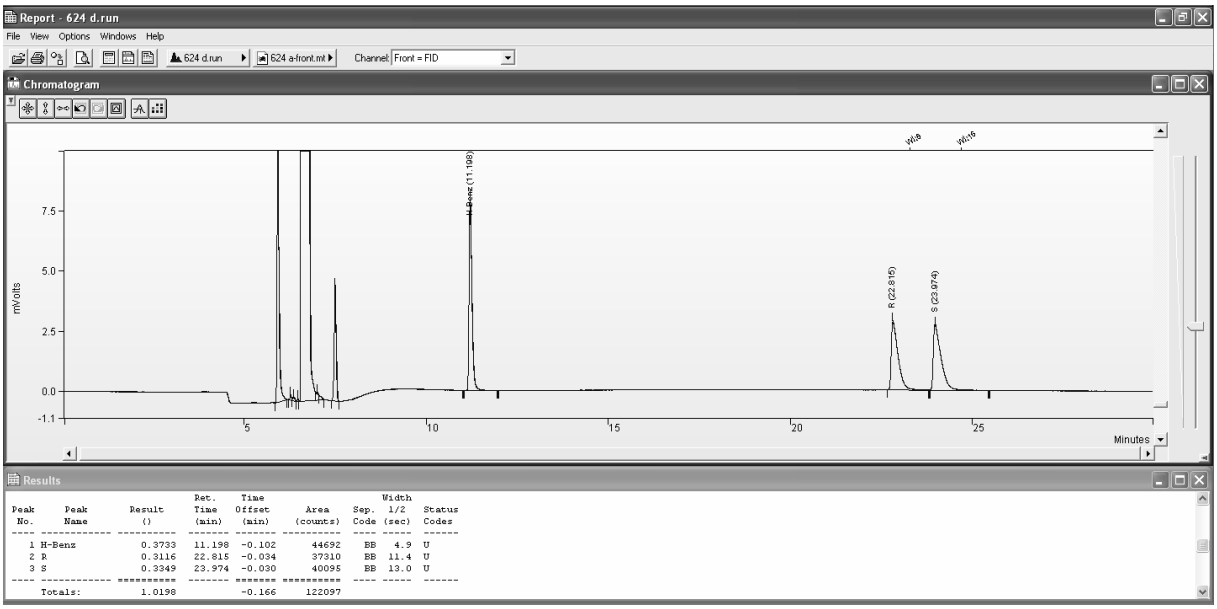

Report - 402 l.run
File View Options Windows Help
402 l.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.350)
R (23.613)
S (24.909)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2251 11.350 0.050 28334 BB 5.0 U
2 R 0.1619 23.613 0.213 20386 BB 10.5 U
3 S 0.1180 24.909 0.209 14856 BB 11.4 U
Totals: 0.5050 0.472 63576

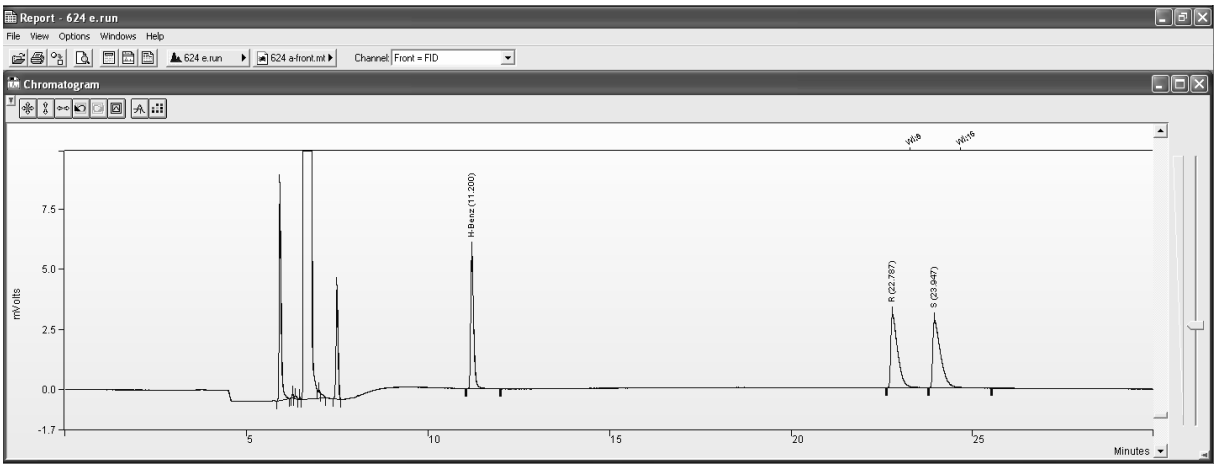
III.3 Figure 2b (NME)

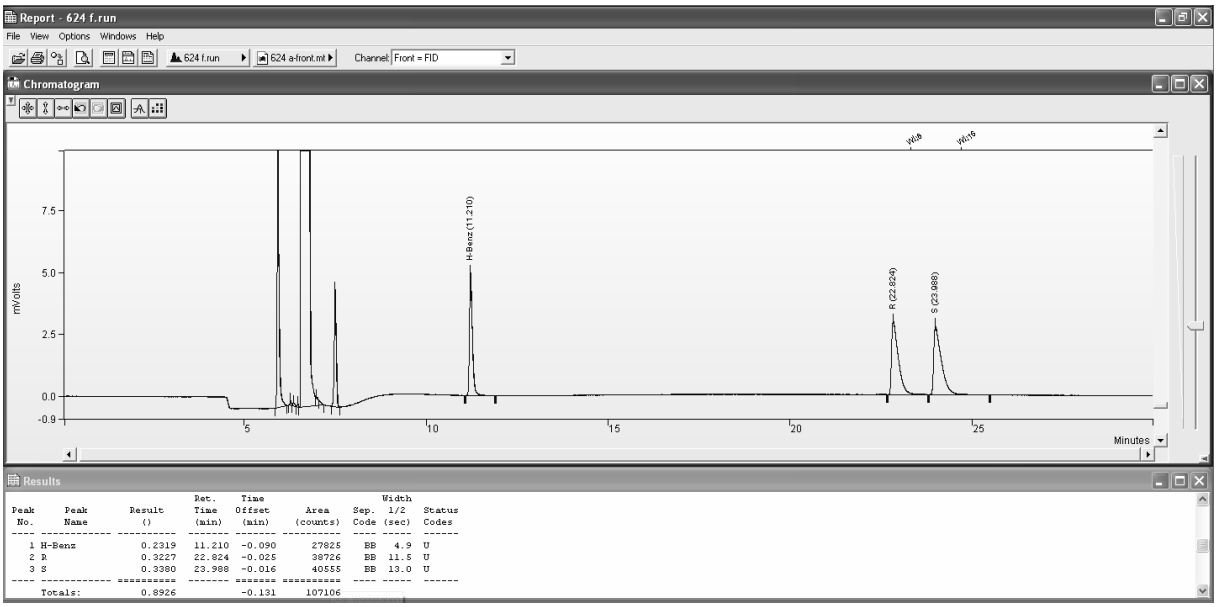


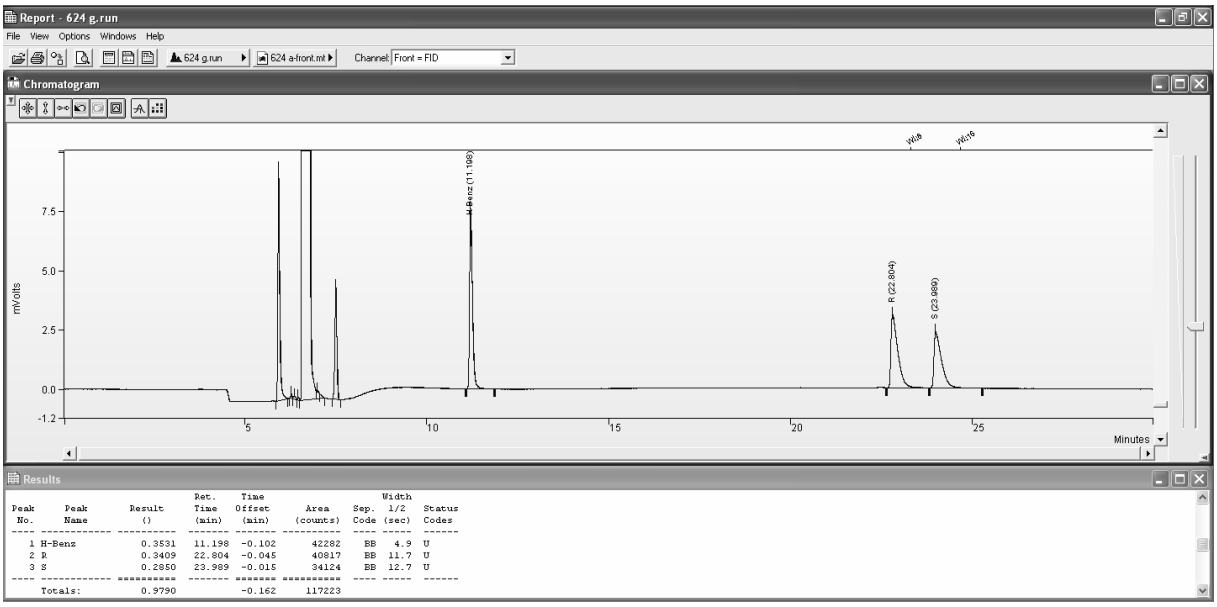


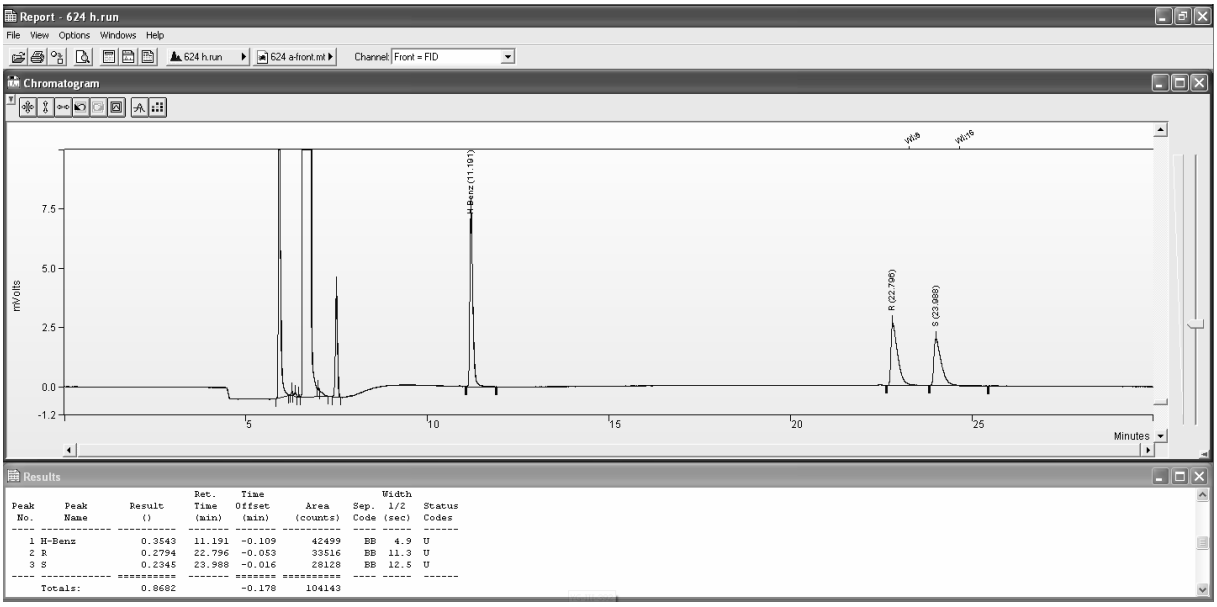

Report - 624 c.run
File View Options Windows Help
624 c.run
624 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.221)
R (22.890)
S (24.049)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2452 11.221 -0.079 29261 BB 4.9 U
2 R 0.3006 22.890 0.041 35877 BB 11.6 U
3 S 0.3477 24.049 0.045 41496 BB 13.2 U
Totals: 0.8935 0.007 106634

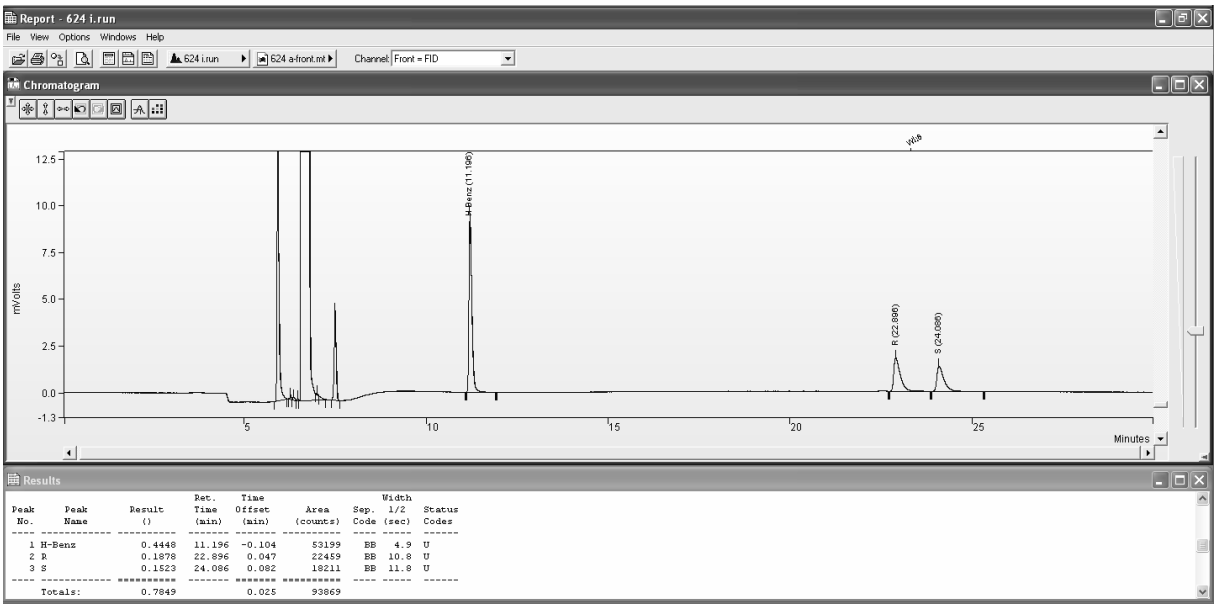

Report - 624 d.run
File View Options Windows Help
624 d.run
624 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.198)
R (22.815)
S (23.974)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3733 11.198 -0.102 44692 BB 4.9 U
2 R 0.3116 22.815 -0.034 37310 BB 11.4 U
3 S 0.3349 23.974 -0.030 40095 BB 13.0 U
Totals: 1.0198 -0.166 122097

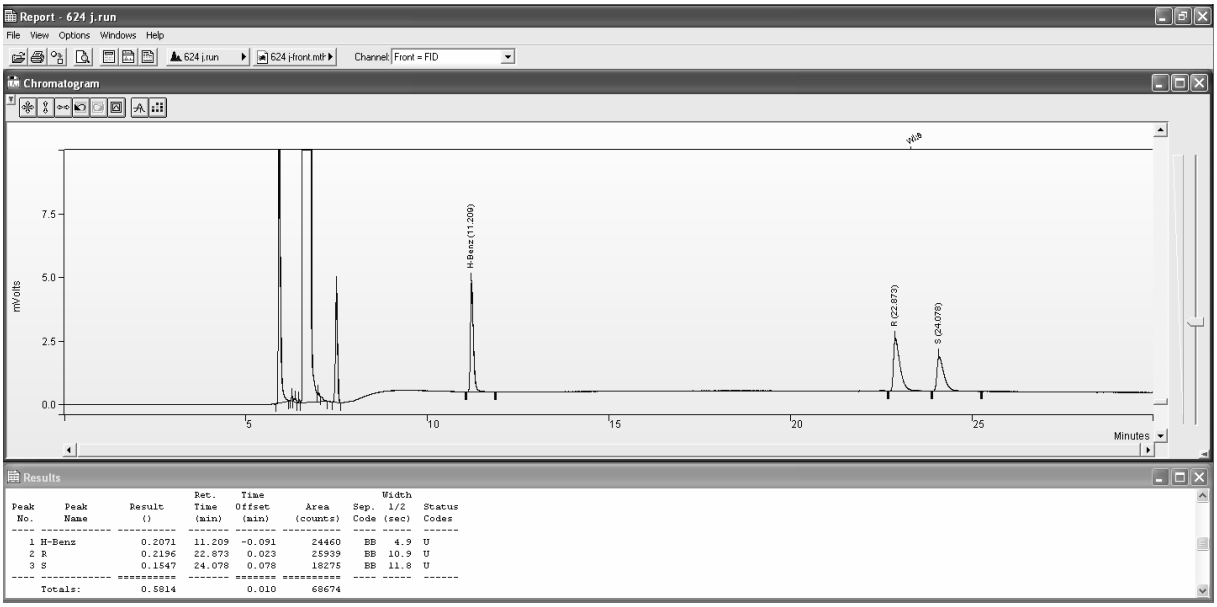

Report - 624 e.run
File View Options Windows Help
624 e.run
624 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.200)
R (22.787)
S (23.947)
mVolts
Minutes

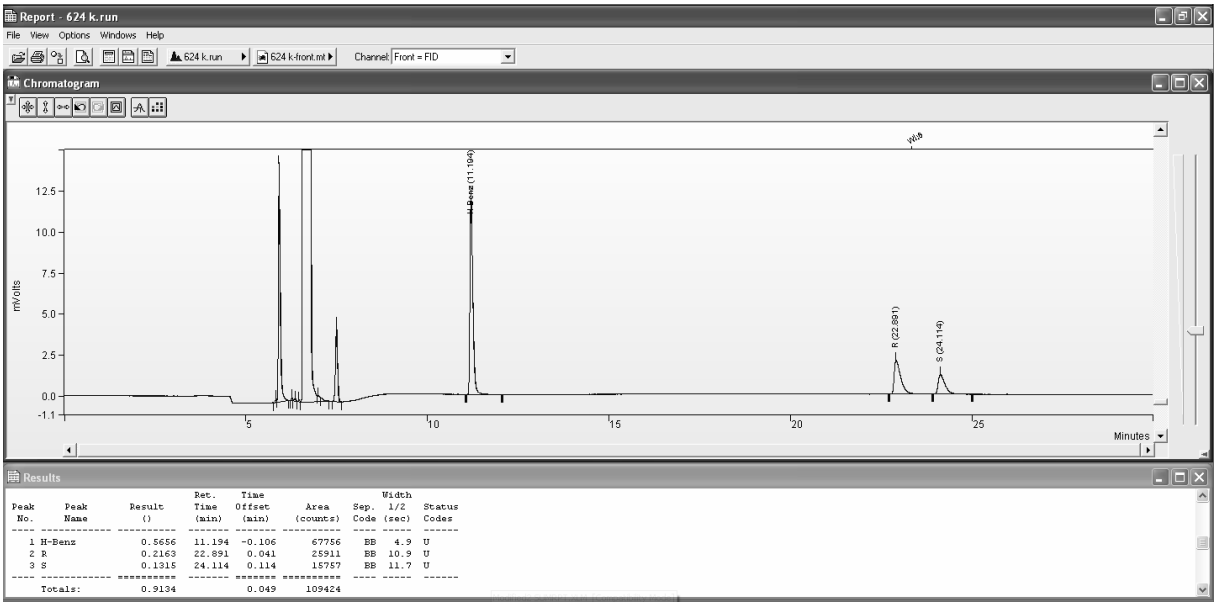

Report - 624 f.run
File View Options Windows Help
624 f.run
624 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.210)
R (22.824)
S (23.988)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2319 11.210 -0.090 27825 BB 4.9 U
2 R 0.3227 22.824 -0.025 38726 BB 11.5 U
3 S 0.3380 23.988 -0.016 40555 BB 13.0 U
Totals: 0.8926 -0.131 107106

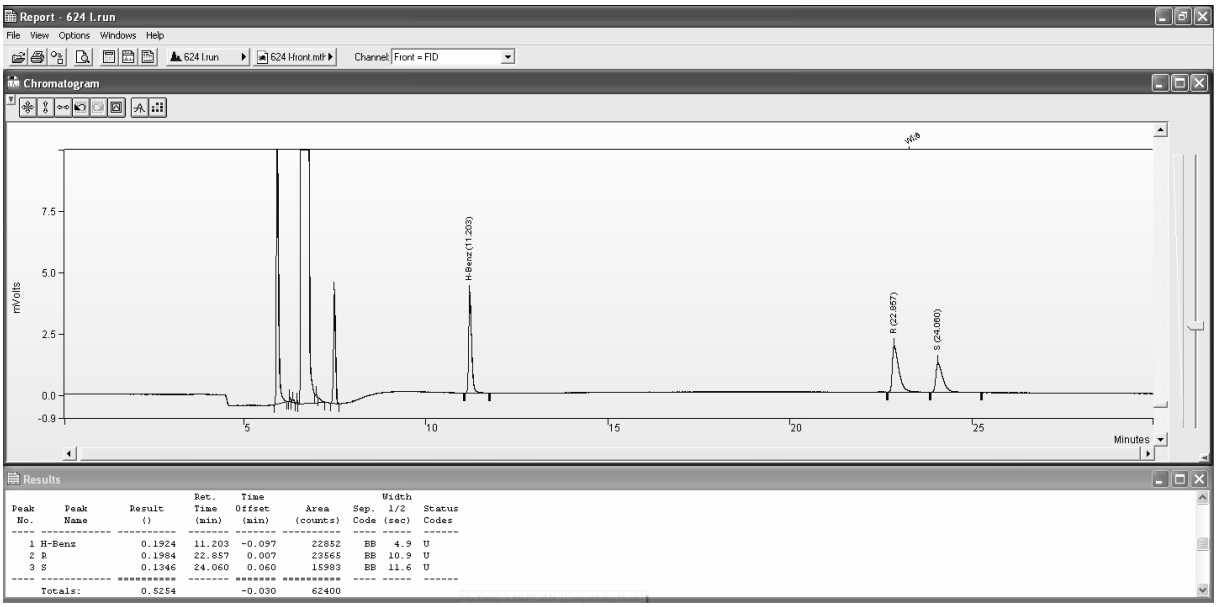

Report - 624 g.run
File View Options Windows Help
624 g.run
624 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.198)
R (22.804)
S (23.988)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3531 11.198 -0.102 42282 BB 4.9 U
2 R 0.3409 22.804 -0.045 40817 BB 11.7 U
3 S 0.2850 23.989 -0.015 34124 BB 12.7 U
Totals: 0.9790 -0.162 117223


Report - 624 h.run
File View Options Windows Help
624 h.run
624 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.191)
R (22.796)
S (23.988)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3543 11.191 -0.109 42499 BB 4.9 U
2 R 0.2794 22.796 -0.053 33516 BB 11.3 U
3 S 0.2345 23.988 -0.016 28128 BB 12.5 U
Totals: 0.8682 -0.178 104143

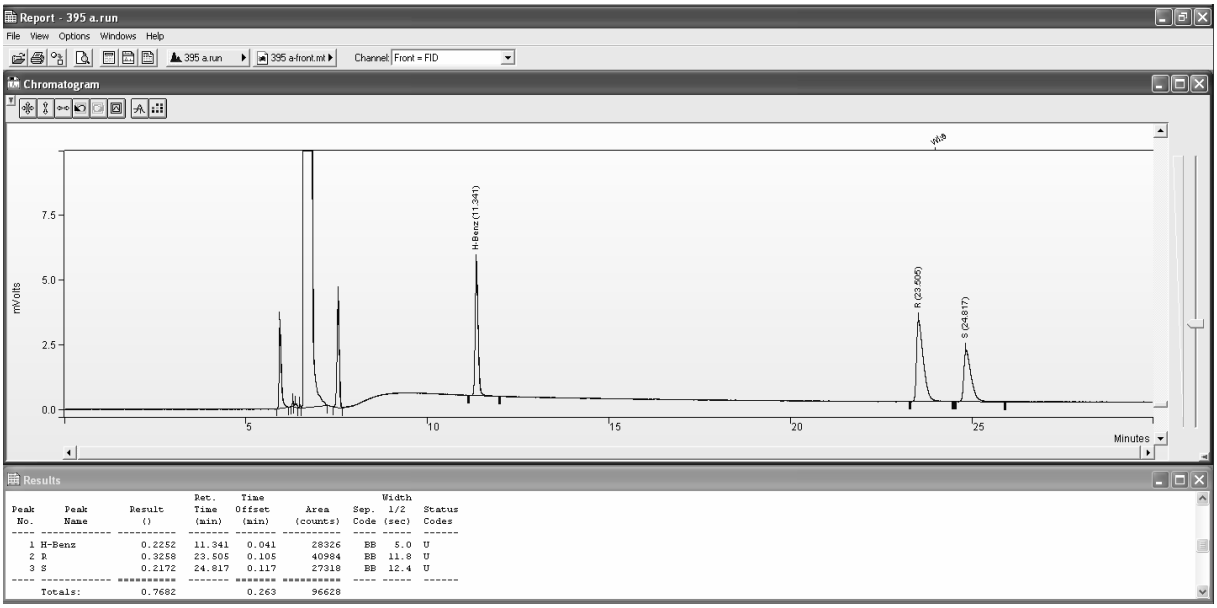

Report - 624 i.run
File View Options Windows Help
624 i.run
624 a-front.mt
Channel: Front = FID
Chromatogram
WL8
H-Benz (11.196)
R (22.896)
S (24.086)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4448 11.196 -0.104 53199 BB 4.9 U
2 R 0.1878 22.896 0.047 22459 BB 10.8 U
3 S 0.1523 24.086 0.082 18211 BB 11.8 U
Totals: 0.7849 0.025 93869

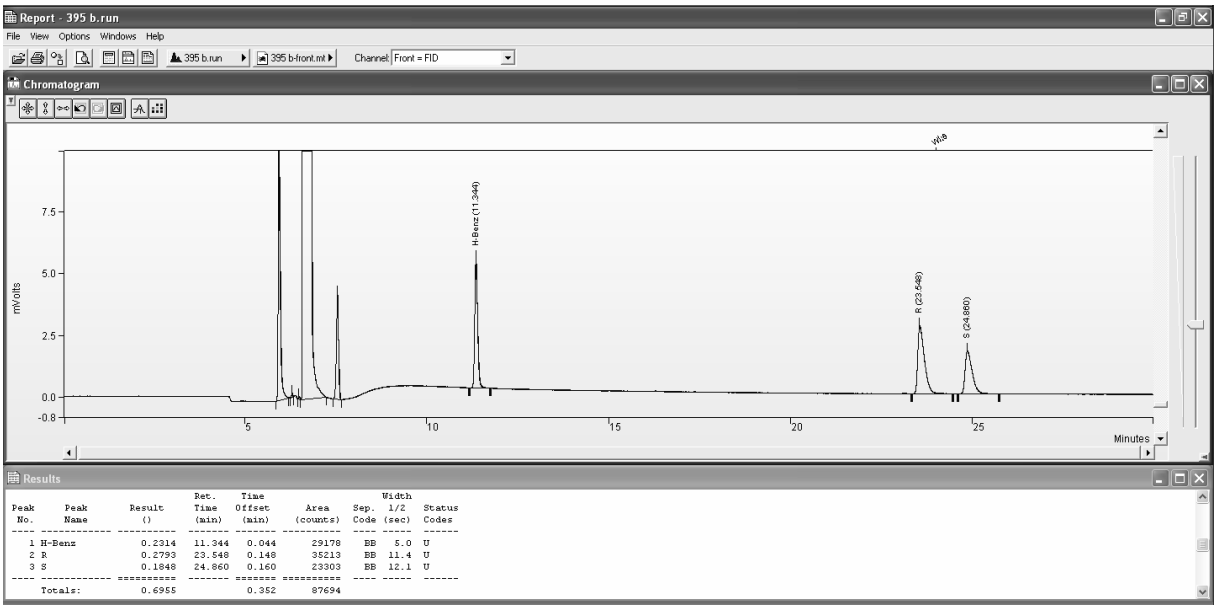

Report - 624 j.run
File View Options Windows Help
624 j.run
624 j-front.mt
Channel: Front = FID
Chromatogram
WL8
H-Benz (11.209)
R (22.873)
S (24.078)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2071 11.209 -0.091 24460 BB 4.9 U
2 R 0.2196 22.873 0.023 25939 BB 10.9 U
3 S 0.1547 24.078 0.078 18275 BB 11.8 U
Totals: 0.5814 0.010 68674

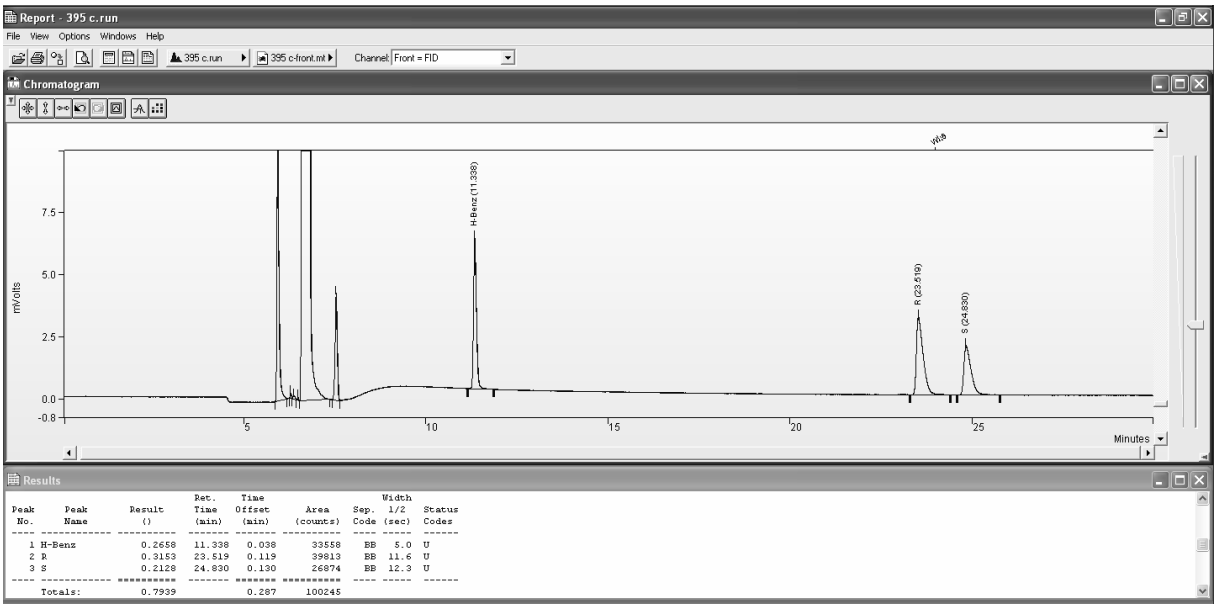

Report - 624 k.run
File View Options Windows Help
624 k.run
624 k-front.mt
Channel: Front = FID
Chromatogram
WL8
H-Benz (11.194)
R (22.891)
S (24.114)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5656 11.194 -0.106 67756 BB 4.9 U
2 R 0.2163 22.891 0.041 25911 BB 10.9 U
3 S 0.1315 24.114 0.114 15757 BB 11.7 U
Totals: 0.9134 0.049 109424

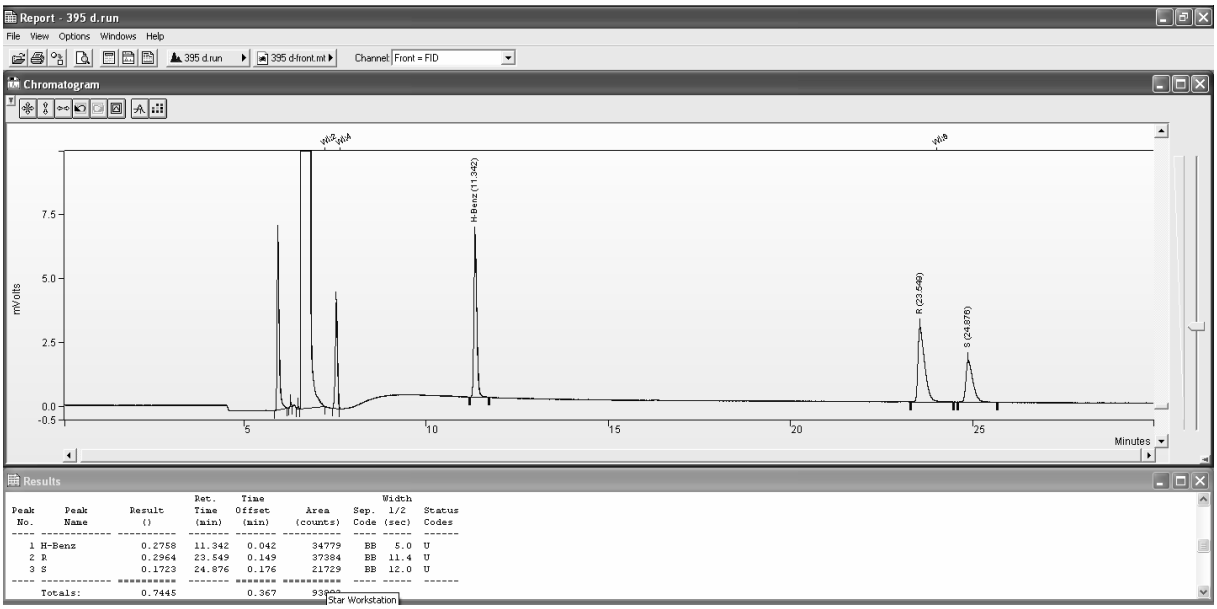

Report - 624 l.run
File View Options Windows Help
624 l.run
624 Hront.mth
Channel Front = FID
Chromatogram
mV/dIts
7.5
5.0
2.5
0.0
-0.9
5
10
15
20
25
Minutes
H-Benz (11.203)
R (22.857)
S (24.060)
Results
Peak No. Peak Name Result () Ret. Time (min) Time Offset (min) Area (counts) Sep. Code Width 1/2 (sec) Status Codes
1 H-Benz 0.1924 11.203 -0.097 22852 BB 4.9 U
2 R 0.1984 22.857 0.007 23565 BB 10.9 U
3 S 0.1346 24.060 0.060 15983 BB 11.6 U
Totals: 0.5254 -0.030 62400

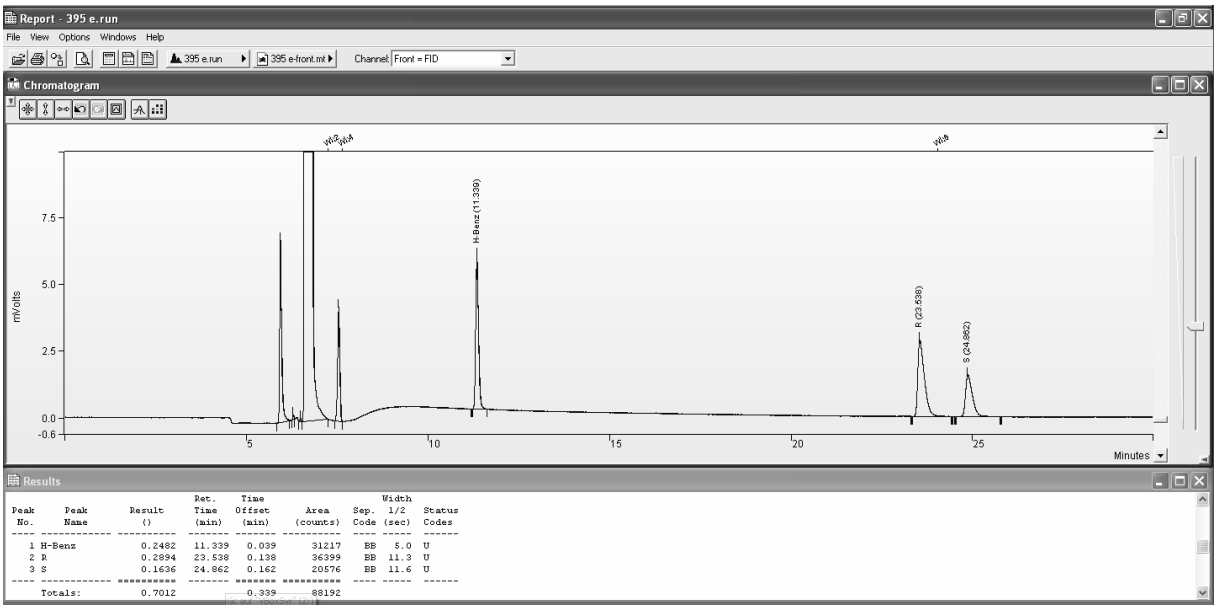
III.4 Figure 2b (NBE)

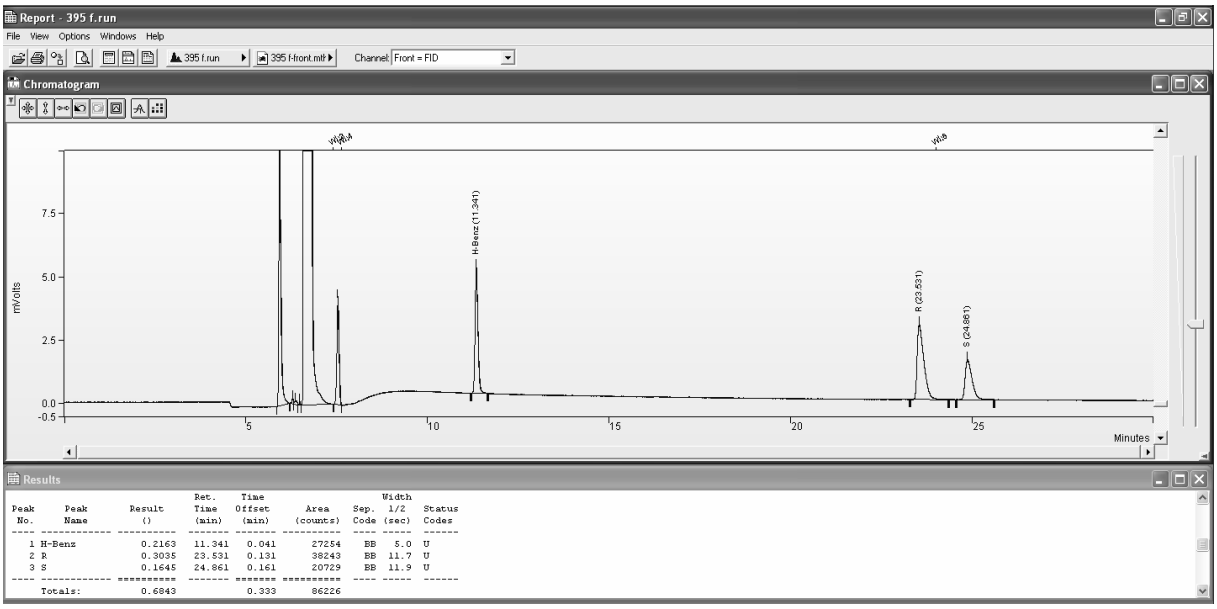


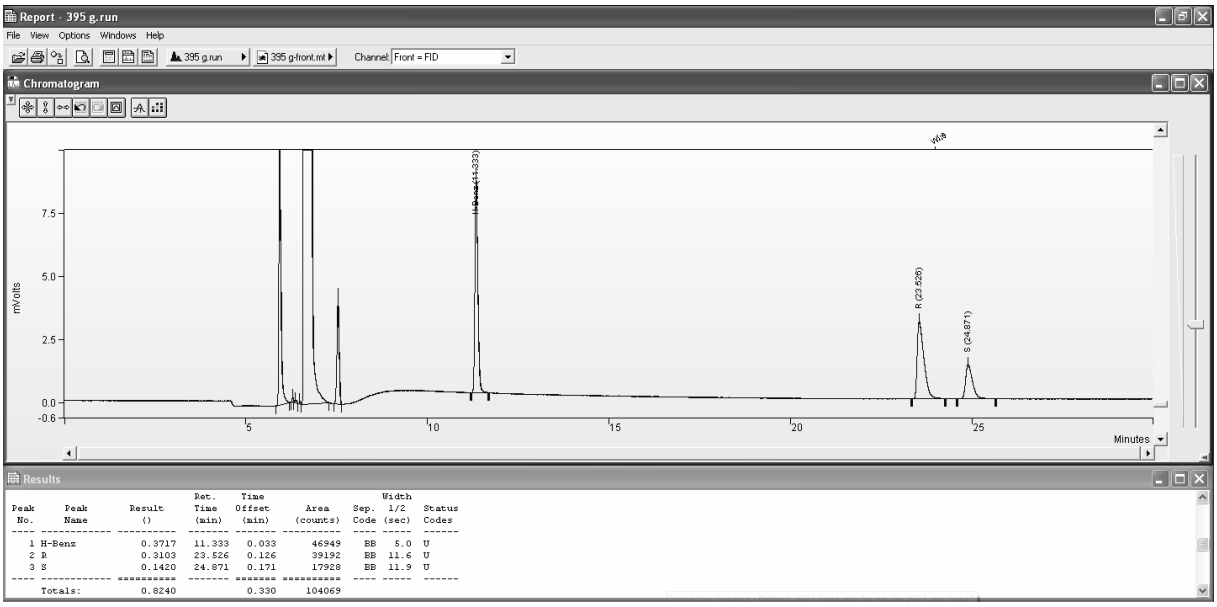


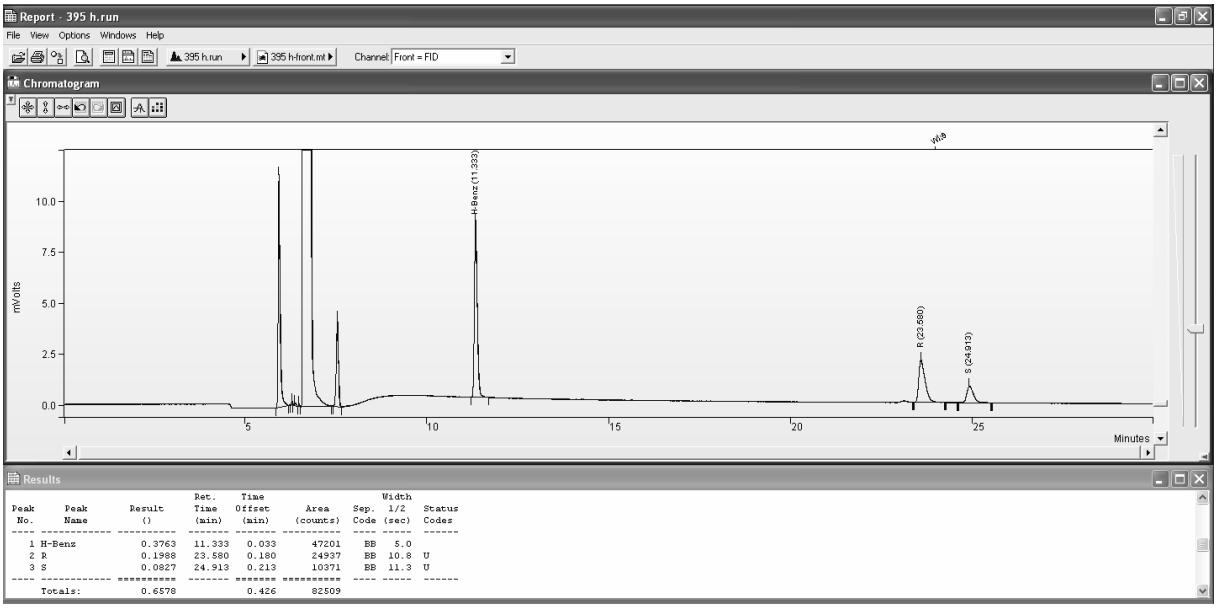

Report - 395 c.run
File View Options Windows Help
395 c.run
395 c-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.338)
R (23.419)
S (24.830)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2658 11.338 0.038 33558 BB 5.0 U
2 R 0.3153 23.519 0.119 39813 BB 11.6 U
3 S 0.2128 24.830 0.130 26974 BB 12.3 U
Totals: 0.7939 0.287 100245

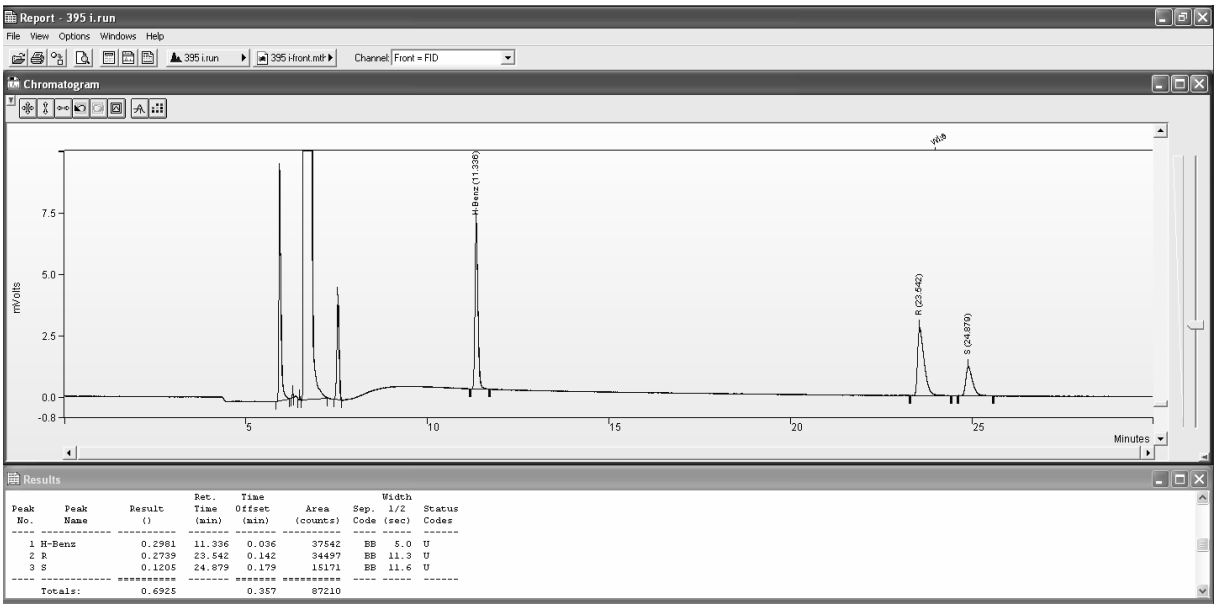

Report - 395 d.run
File View Options Windows Help
395 d.run
395 d-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.342)
R (23.549)
S (24.876)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2758 11.342 0.042 34779 BB 5.0 U
2 R 0.2964 23.549 0.149 37384 BB 11.4 U
3 S 0.1723 24.876 0.176 21729 BB 12.0 U
Totals: 0.7445 0.367
Star Workstation

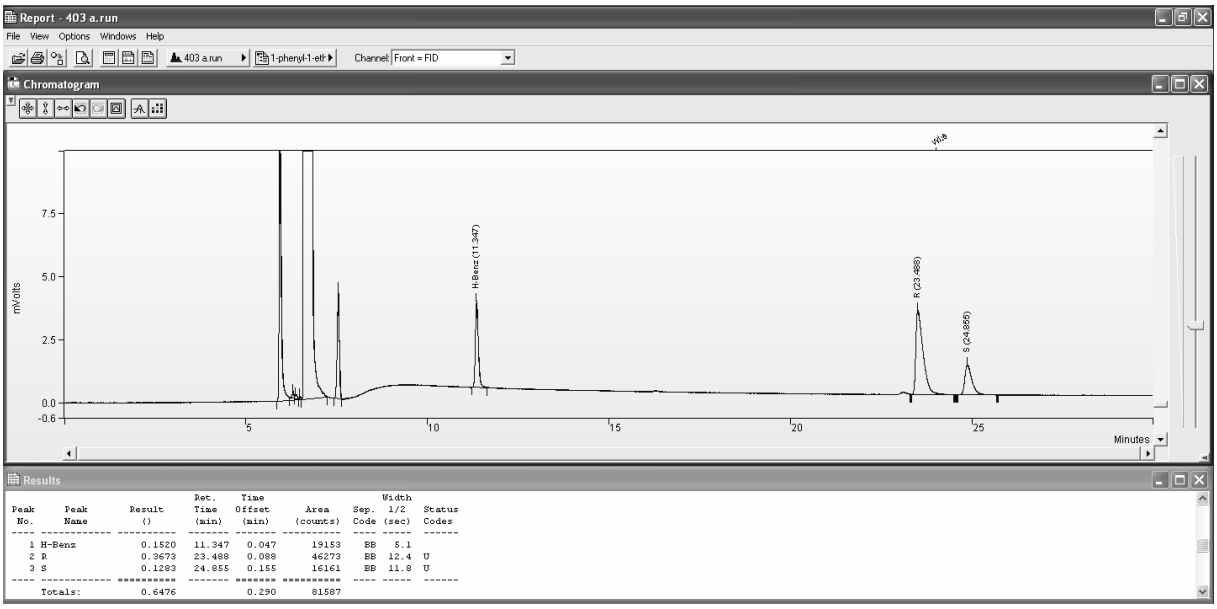

Report - 395 e.run
File View Options Windows Help
395 e.run
395 e-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.339)
R (23.538)
S (24.862)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2482 11.339 0.039 31217 BB 5.0 U
2 R 0.2894 23.538 0.138 36399 BB 11.3 U
3 S 0.1636 24.862 0.162 20576 BB 11.6 U
Totals: 0.7012 0.339 88192

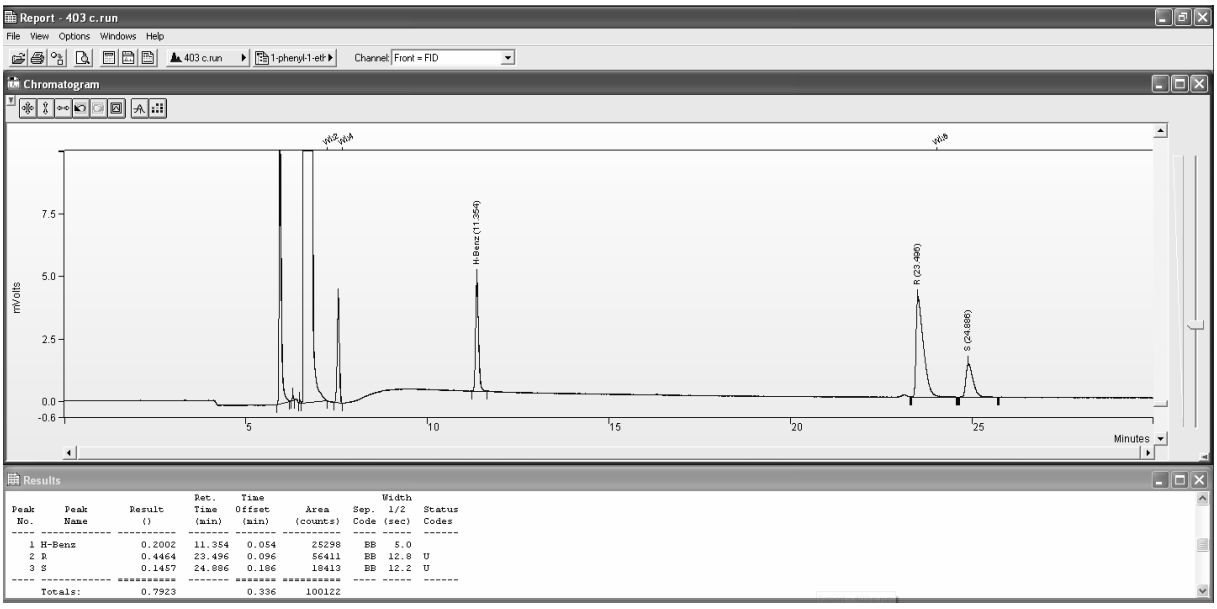

Report - 395 f.run
File View Options Windows Help
395 f.run
395 f-front.mtf
Channel Front = FID
Chromatogram
mV/olts
H-Benz (11.341)
R (23.531)
S (24.861)
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2163 11.341 0.041 27254 BB 5.0 U
2 R 0.3035 23.531 0.131 38243 BB 11.7 U
3 S 0.1645 24.861 0.161 20729 BB 11.9 U
Totals: 0.6843 0.333 86226


Report - 395 g.run
File View Options Windows Help
395 g.run
395 g-front.mtf
Channel Front = FID
Chromatogram
mV/olts
R (23.526)
S (24.871)
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3717 11.333 0.033 46949 BB 5.0 U
2 R 0.3103 23.526 0.126 39192 BB 11.6 U
3 S 0.1420 24.871 0.171 17928 BB 11.9 U
Totals: 0.8240 0.330 104069

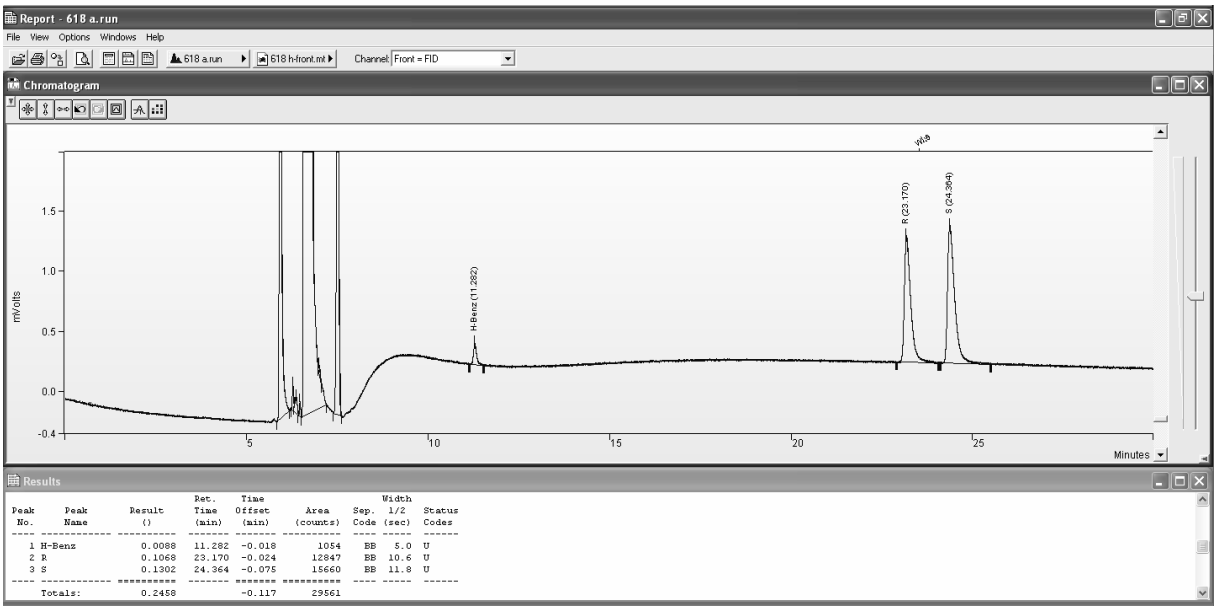

Report - 395 h.run
File View Options Windows Help
395 h.run
395 h-front.mtf
Channel Front = FID
Chromatogram
mV/olts
H-Benz (11.333)
R (23.580)
S (24.913)
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.3763 11.333 0.033 47201 BB 5.0
2 R 0.1988 23.580 0.180 24937 BB 10.8 U
3 S 0.0827 24.913 0.213 10371 BB 11.3 U
Totals: 0.6578 0.426 82509


Report - 395 i.run
File View Options Windows Help
395 i.run
395 i-front.mth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.336)
R (23.542)
S (24.879)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2981 11.336 0.036 37542 BB 5.0 U
2 R 0.2739 23.542 0.142 34497 BB 11.3 U
3 S 0.1205 24.879 0.179 15171 BB 11.6 U
Totals: 0.6925 0.357 87210

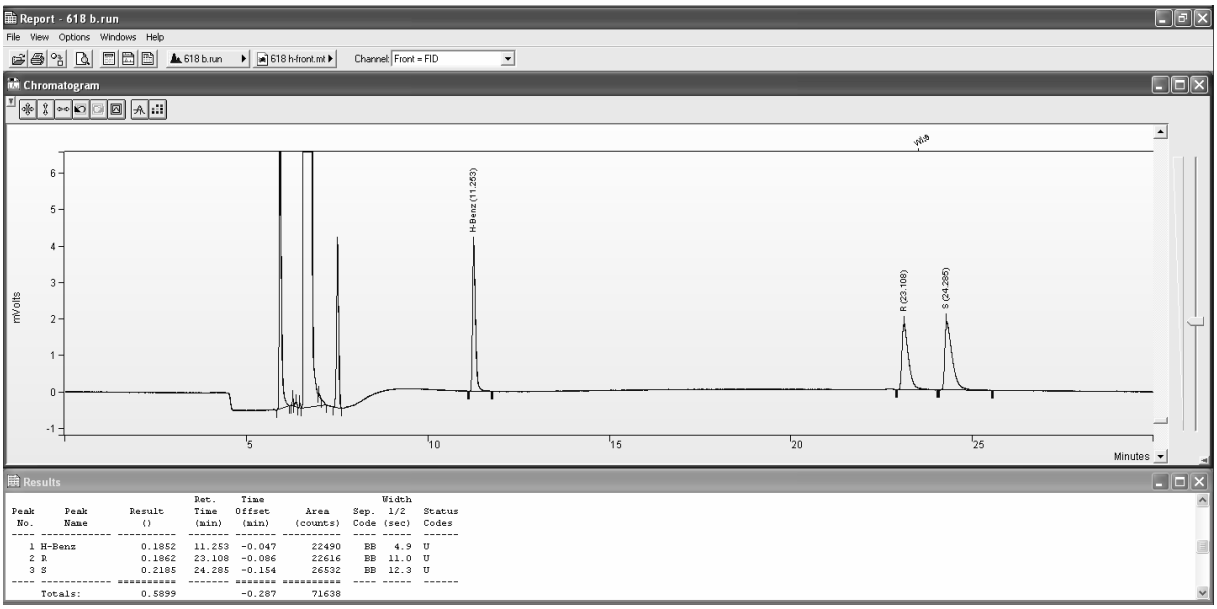

Report - 403 a.run
File View Options Windows Help
403 a.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.347)
R (23.488)
S (24.855)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1520 11.347 0.047 19153 BB 5.1
2 R 0.3673 23.488 0.088 46273 BB 12.4 U
3 S 0.1283 24.855 0.155 16161 BB 11.8 U
Totals: 0.6476 0.290 81587


Report - 403 c.run
File View Options Windows Help
403 c.run
1-phenyl-1-eth
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.354)
R (23.496)
S (24.886)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2002 11.354 0.054 25298 BB 5.0
2 R 0.4464 23.496 0.096 56411 BB 12.8 U
3 S 0.1457 24.886 0.186 18413 BB 12.2 U
Totals: 0.7923 0.336 100122

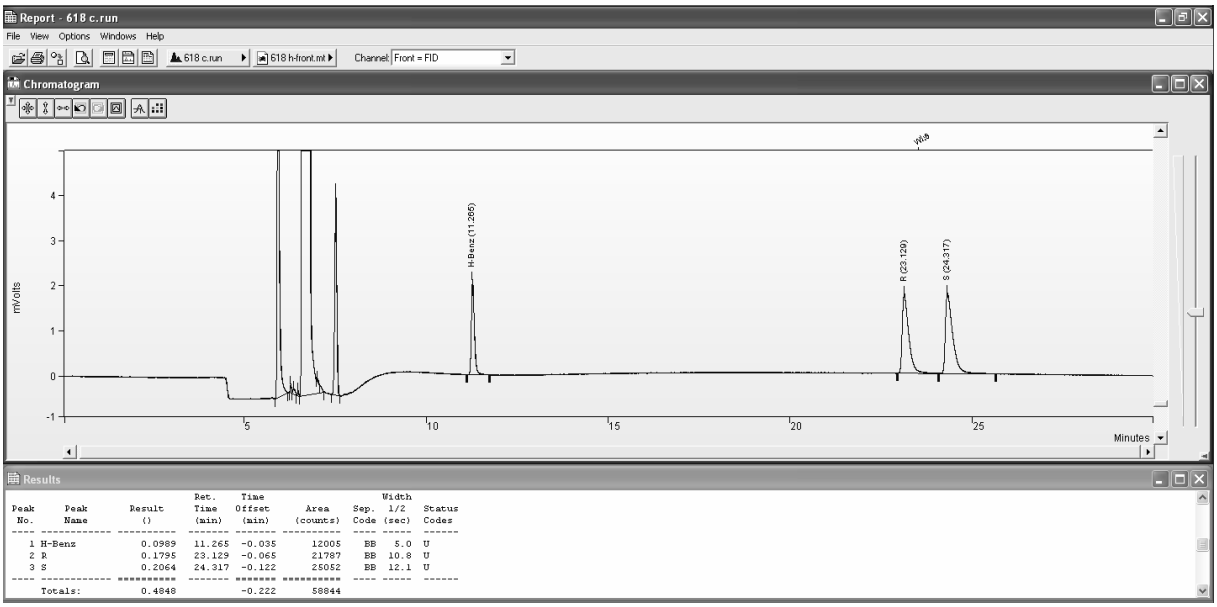
III.5 Figure 3a



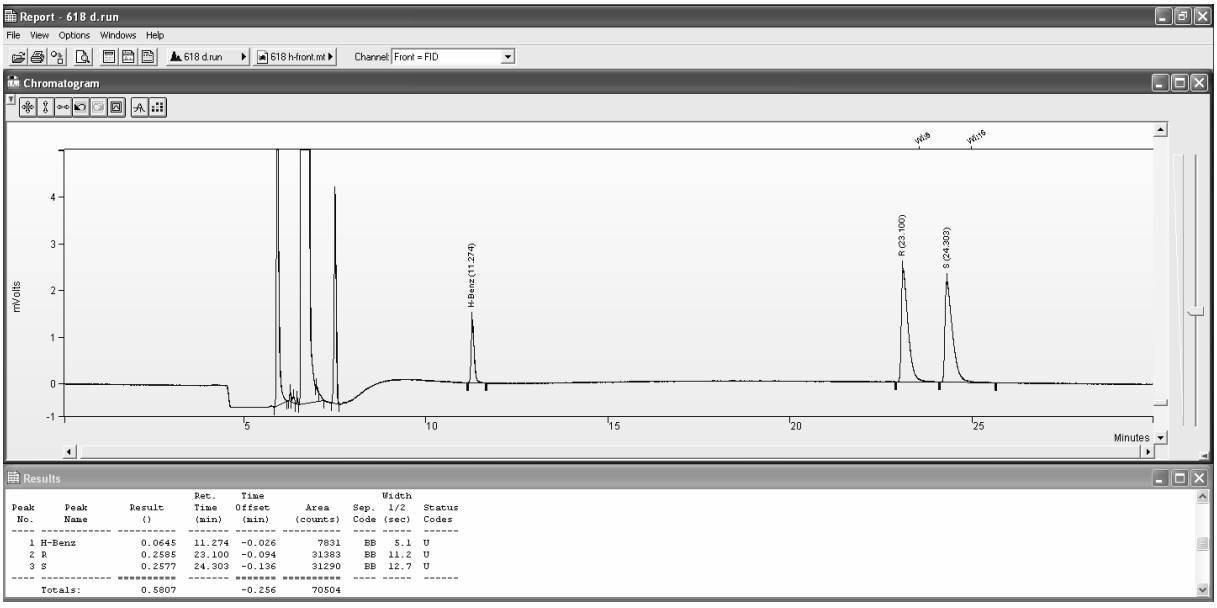
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0088	11.282	-0.018	1054	BB	5.0	U
2	R	0.1068	23.170	-0.024	12847	BB	10.6	U
3	S	0.1302	24.364	-0.075	15660	BB	11.8	U
Totals:		0.2458		-0.117	29561			



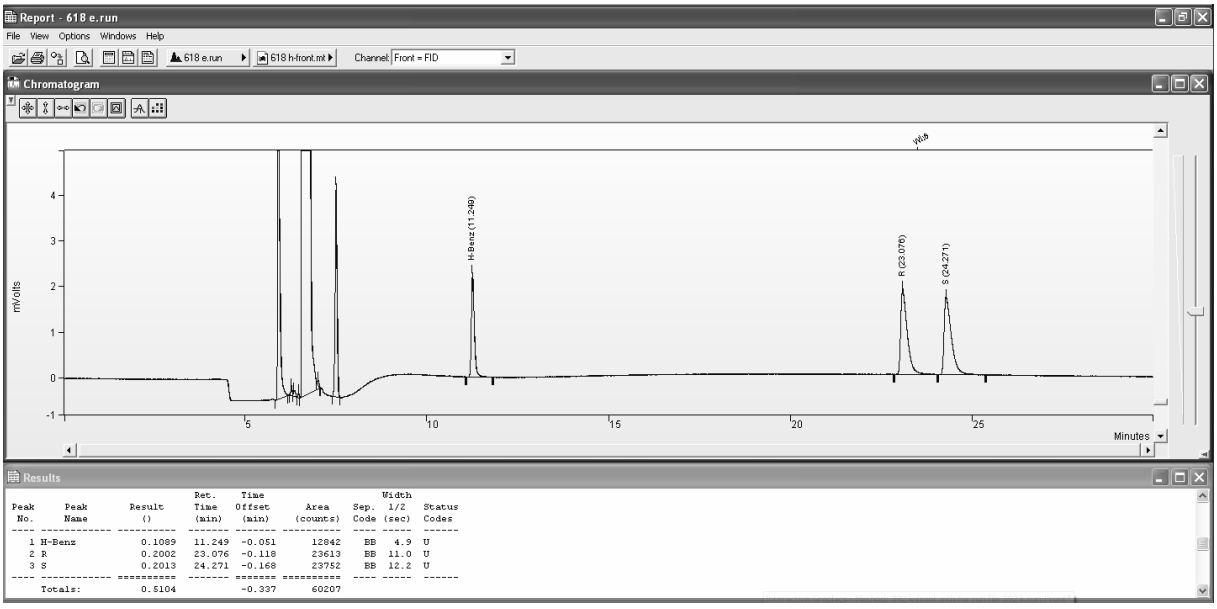
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1852	11.253	-0.047	22490	BB	4.9	U
2	R	0.1862	23.108	-0.086	22616	BB	11.0	U
3	S	0.2185	24.285	-0.154	26532	BB	12.3	U
Totals:		0.5899		-0.287	71638			



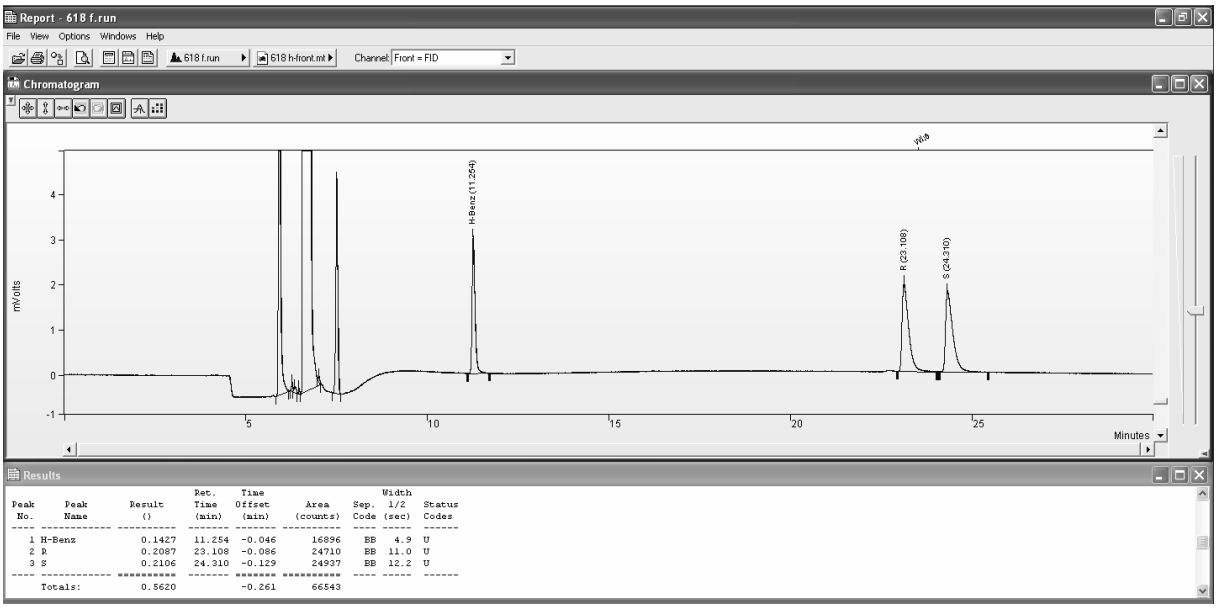
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0989	11.265	-0.035	12005	BB	5.0	U
2	R	0.1795	23.129	-0.065	21787	BB	10.8	U
3	S	0.2064	24.317	-0.122	25052	BB	12.1	U
	Totals:	0.4848		-0.222	58844			

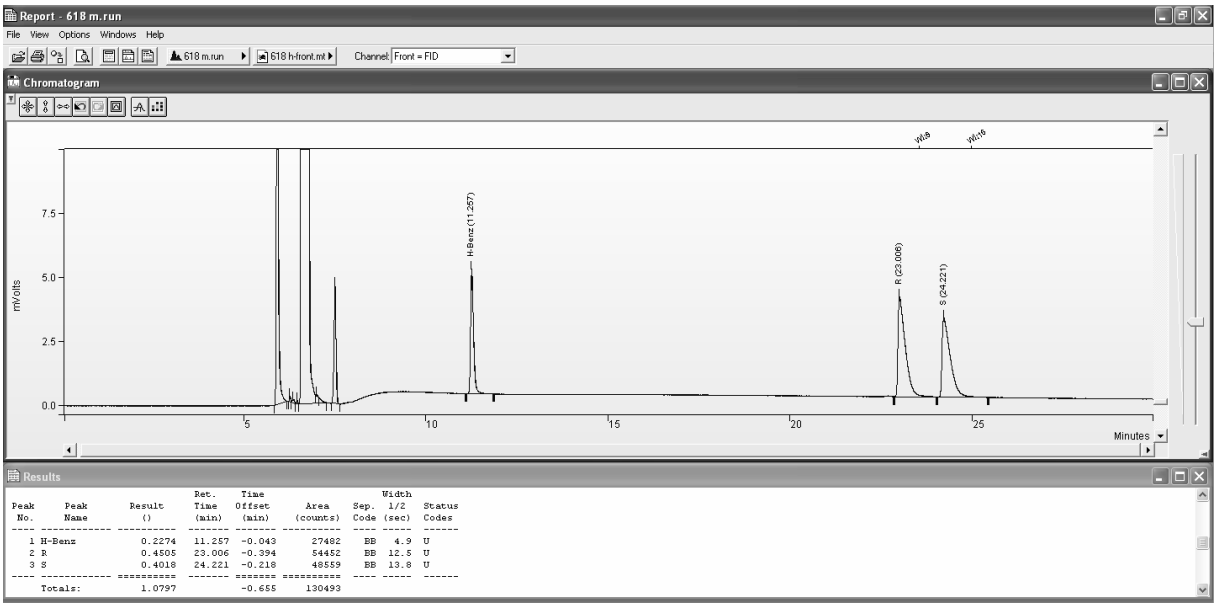


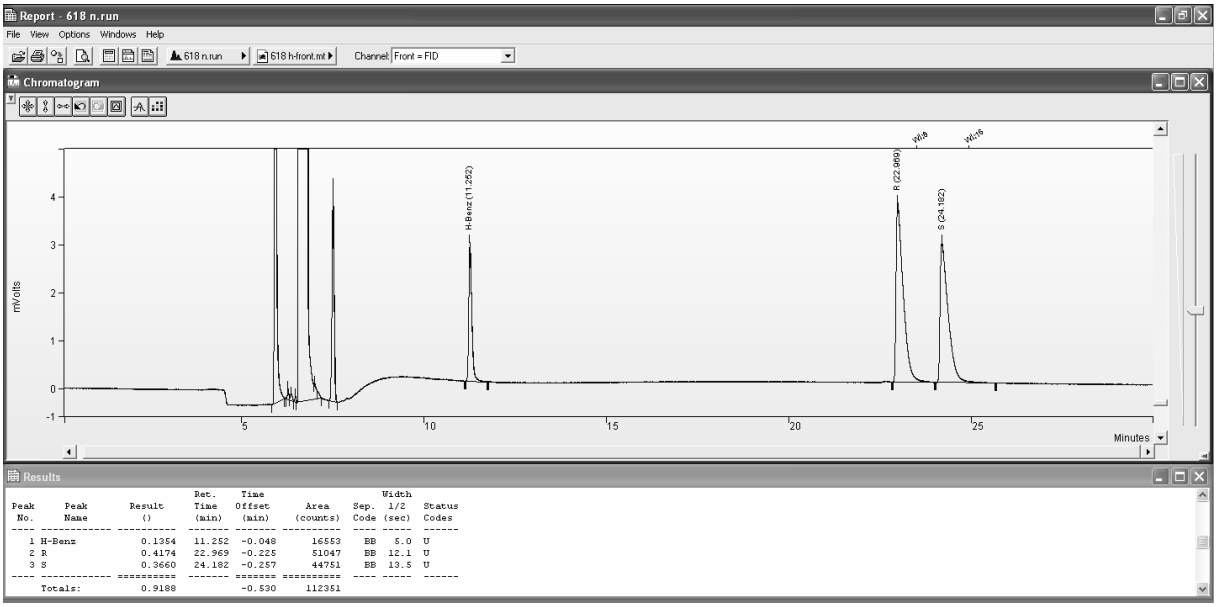
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0645	11.274	-0.026	7831	BB	5.1	U
2	R	0.2585	23.100	-0.094	31383	BB	11.2	U
3	S	0.2577	24.303	-0.136	31290	BB	12.7	U
	Totals:	0.5807		-0.256	70504			

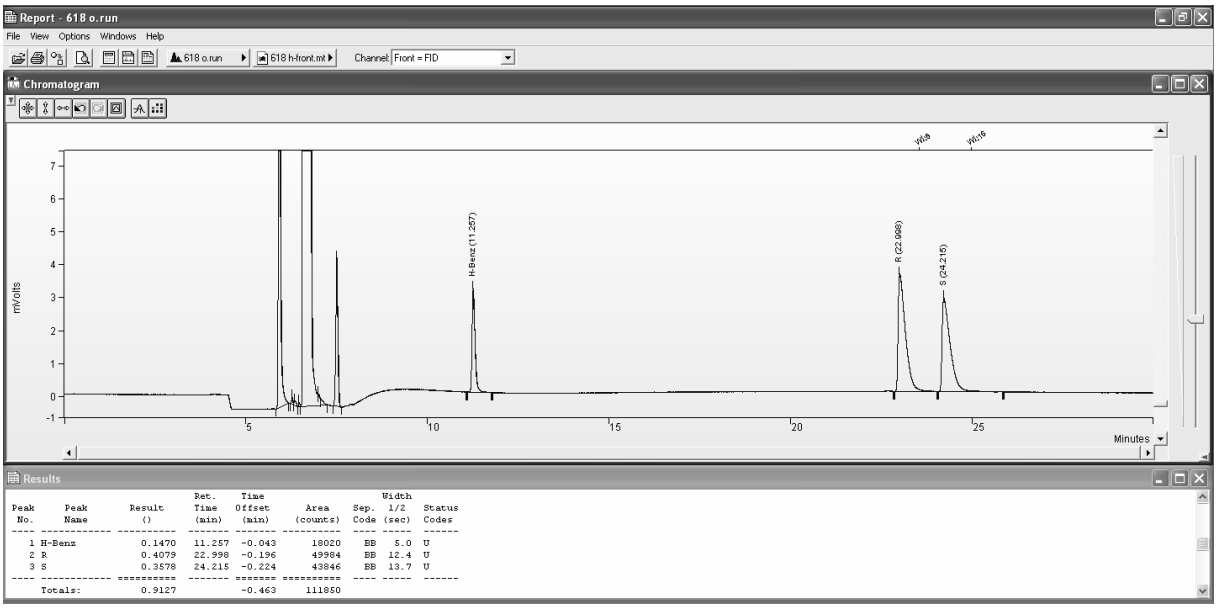


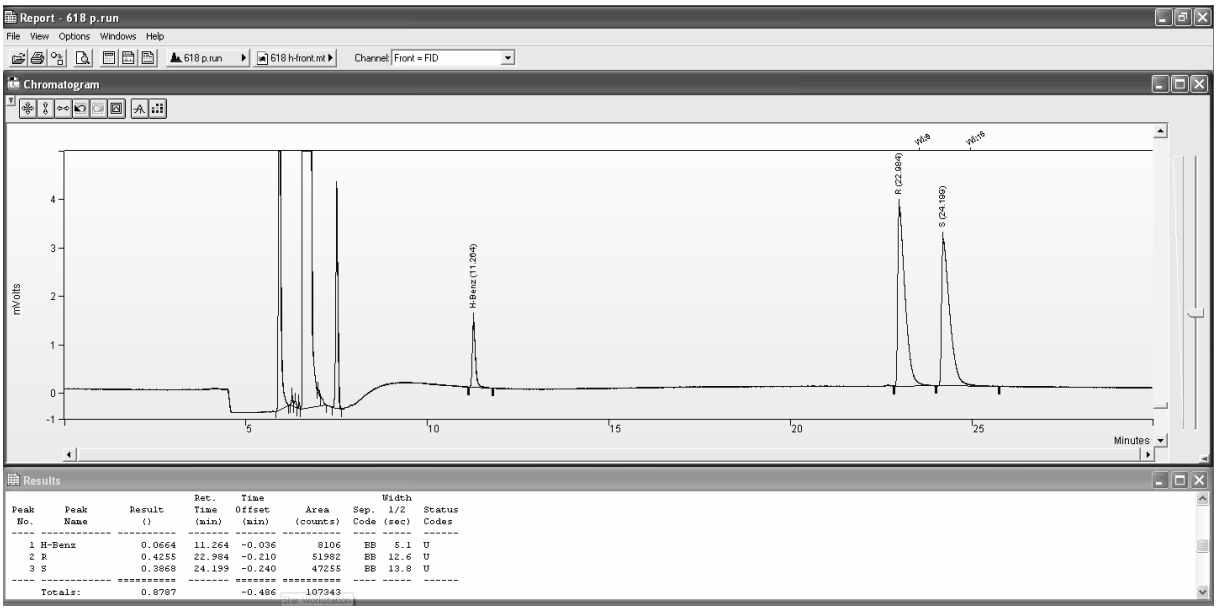
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1089	11.249	-0.051	12842	BB	4.9	U
2	R	0.2002	23.076	-0.118	23613	BB	11.0	U
3	S	0.2013	24.271	-0.168	23752	BB	12.2	U
	Totals:	0.5104		-0.337	60207			

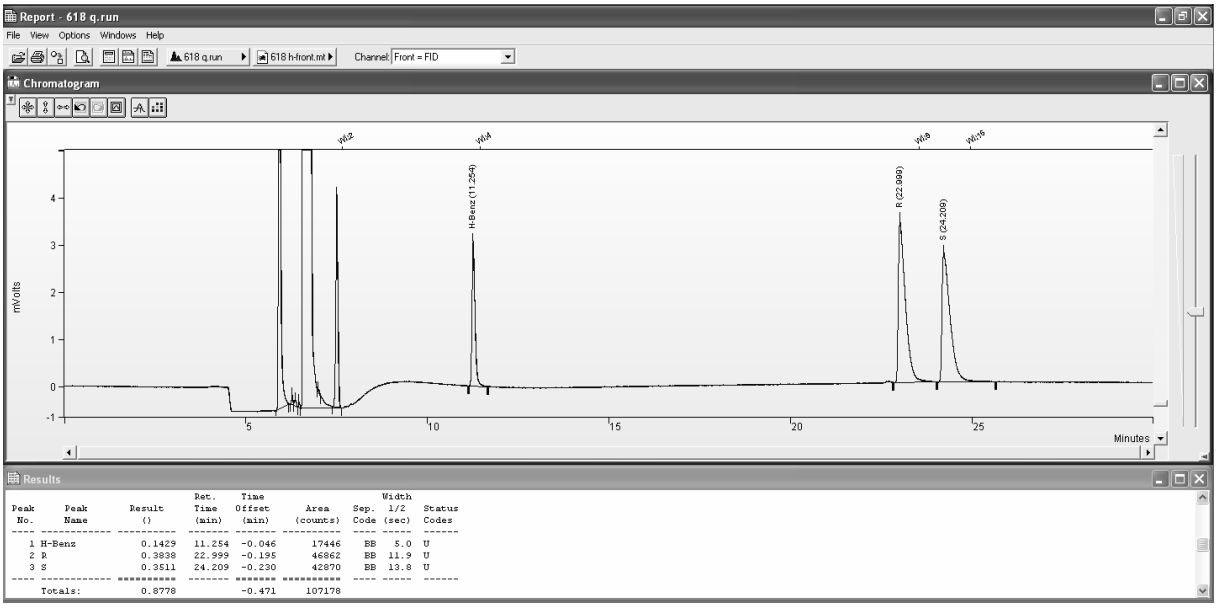

Report - 618 f.run
File View Options Windows Help
618 f.run
618 h-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.254)
R (23.108)
S (24.310)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1427 11.254 -0.046 16896 BB 4.9 U
2 R 0.2087 23.108 -0.086 24710 BB 11.0 U
3 S 0.2106 24.310 -0.129 24937 BB 12.2 U
Totals: 0.5620 -0.261 66543

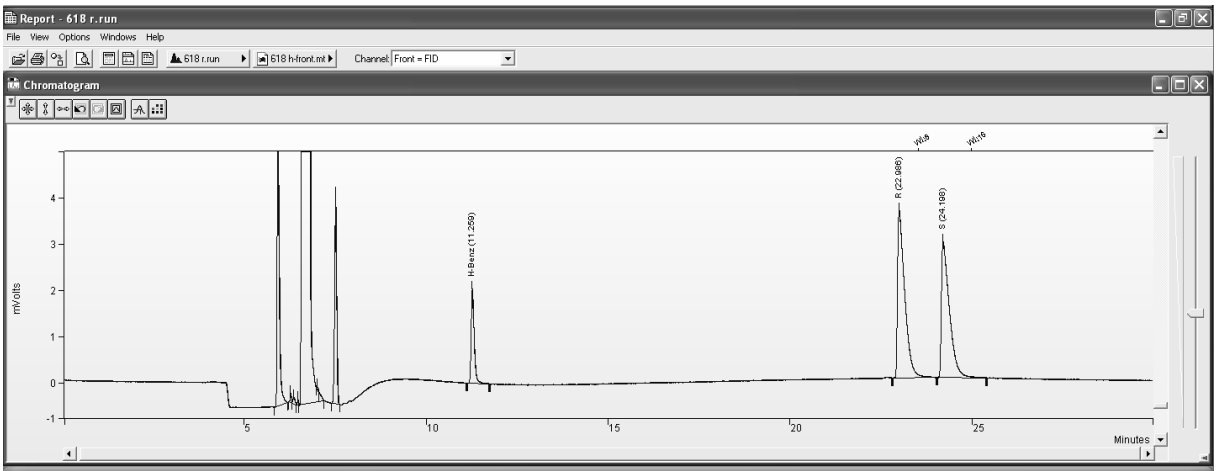

Report - 618 m.run
File View Options Windows Help
618 m.run
618 h-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.257)
R (23.006)
S (24.221)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2274 11.257 -0.043 27482 BB 4.9 U
2 R 0.4505 23.006 -0.394 54452 BB 12.5 U
3 S 0.4018 24.221 -0.218 48559 BB 13.8 U
Totals: 1.0797 -0.655 130493


Report - 618 n.run
File View Options Windows Help
618 n.run
618 h-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.252)
R (22.969)
S (24.182)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1354 11.252 -0.048 16553 BB 5.0 U
2 R 0.4174 22.969 -0.225 51047 BB 12.1 U
3 S 0.3660 24.182 -0.257 44751 BB 13.5 U
Totals: 0.9188 -0.530 112351


Report - 618 o.run
File View Options Windows Help
618 o.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.257)
R (22.998)
S (24.215)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1470 11.257 -0.043 18020 BB 5.0 U
2 R 0.4079 22.998 -0.196 49984 BB 12.4 U
3 S 0.3578 24.215 -0.224 43846 BB 13.7 U
Totals: 0.9127 -0.463 111850


Report - 618 p.run
File View Options Windows Help
618 p.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.264)
R (22.984)
S (24.199)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0664 11.264 -0.036 8106 BB 5.1 U
2 R 0.4255 22.984 -0.210 51982 BB 12.6 U
3 S 0.3868 24.199 -0.240 47255 BB 13.8 U
Totals: 0.8787 -0.486 107343

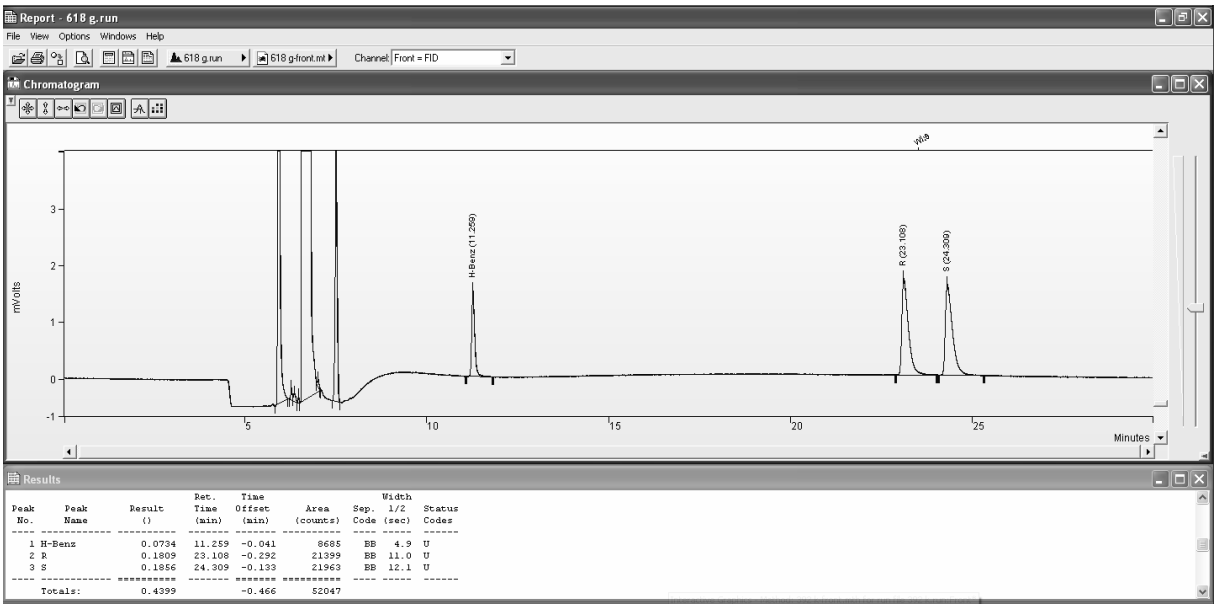

Report - 618 q.run
File View Options Windows Help
618 q.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.254)
R (22.999)
S (24.209)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1429 11.254 -0.046 17446 BB 5.0 U
2 R 0.3838 22.999 -0.195 46862 BB 11.9 U
3 S 0.3511 24.209 -0.230 42870 BB 13.8 U
Totals: 0.8778 -0.471 107178

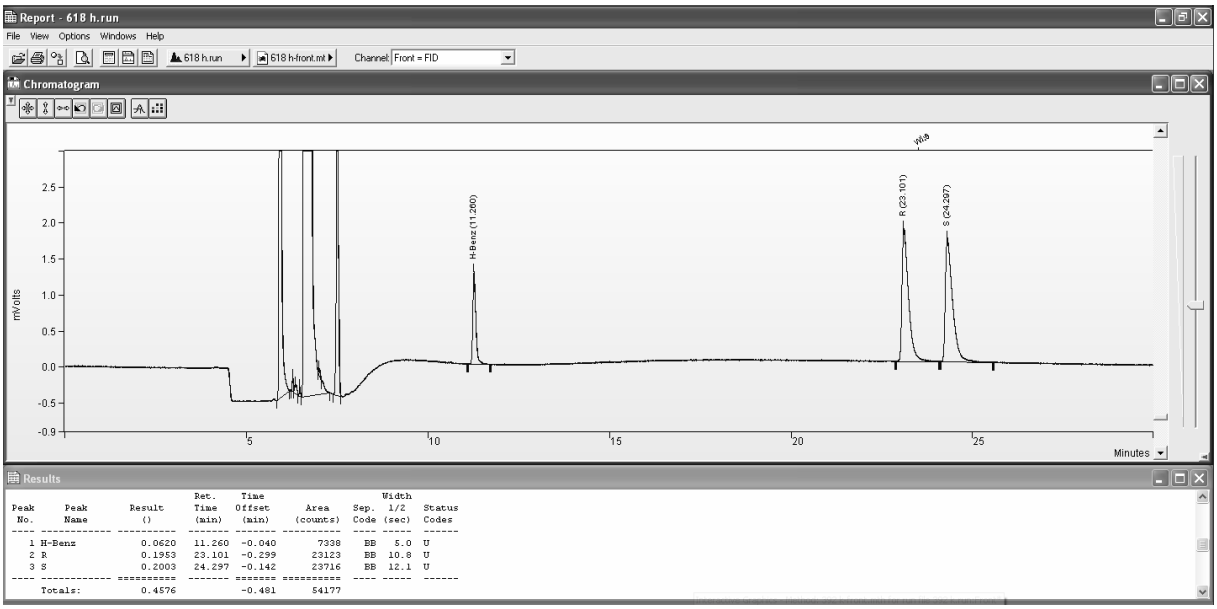


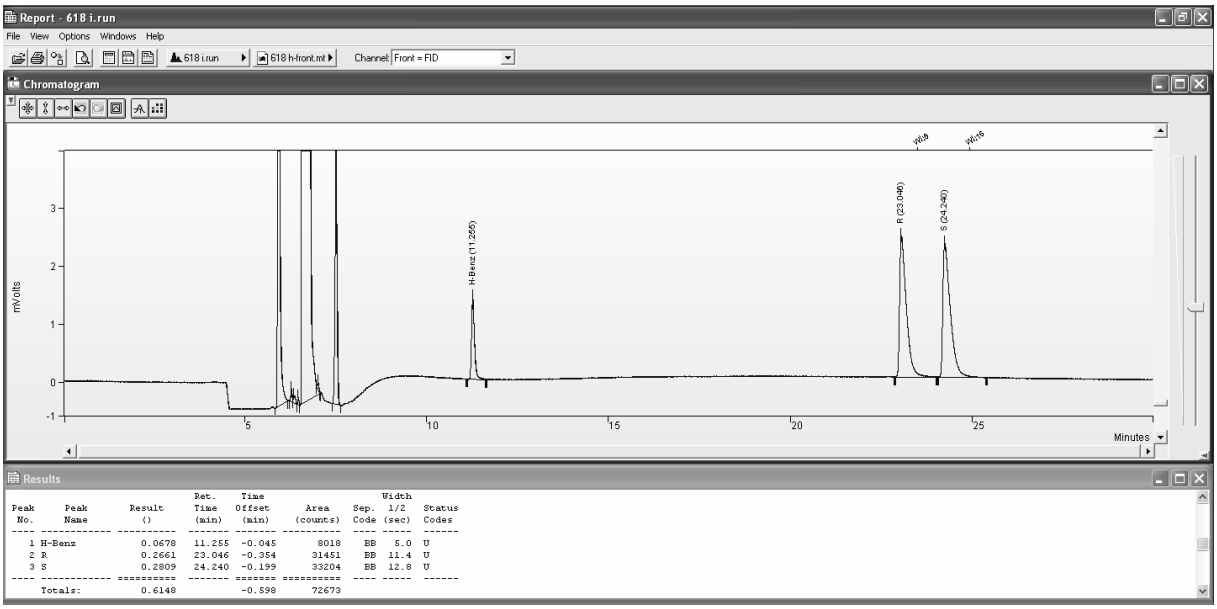
Results

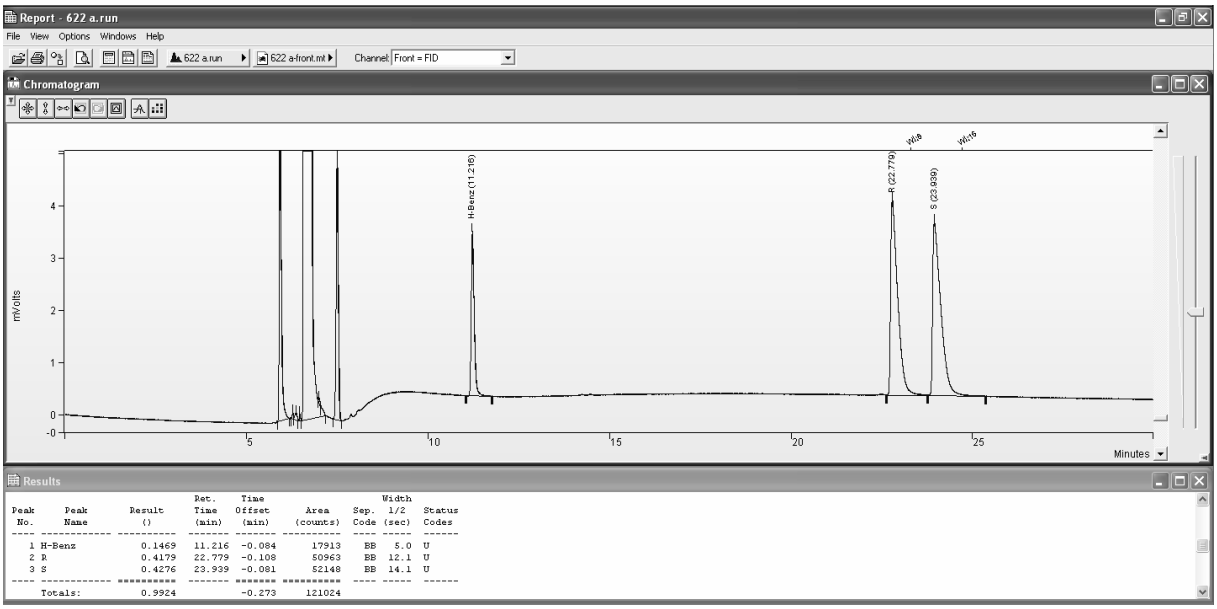
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0969	11.259	-0.041	11832	BB	5.0	U
2	R	0.4110	22.986	-0.208	50211	BB	12.3	U
3	S	0.3690	24.198	-0.241	45074	BB	13.6	U
	Totals:	0.8769		-0.490	107117			

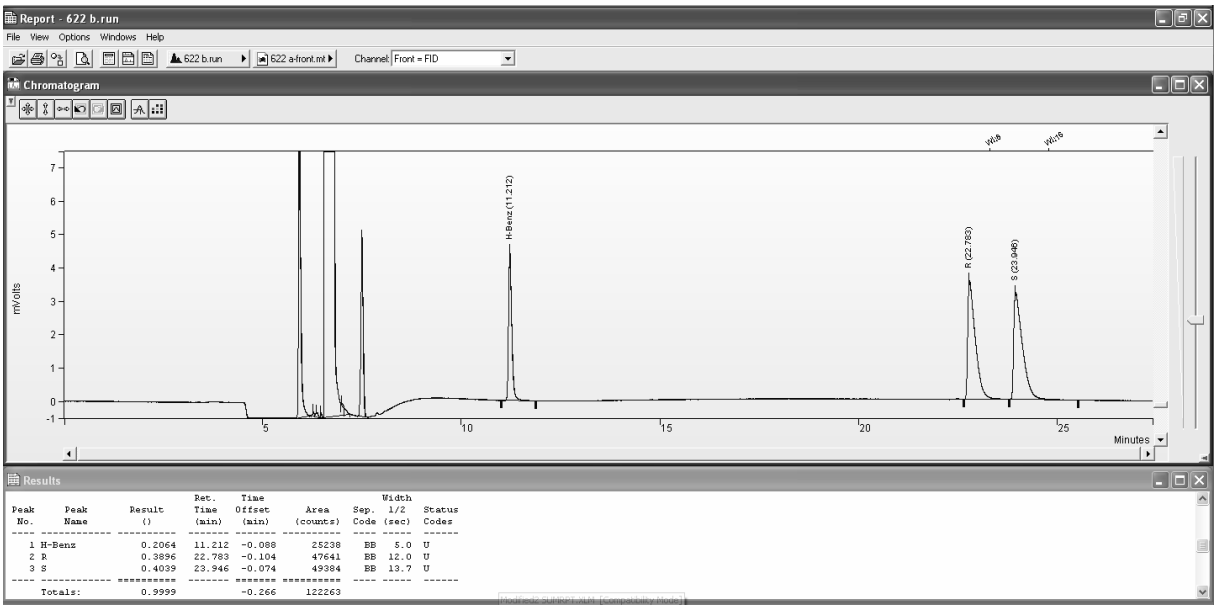
III.6 Figure 3b ((-)-NME)

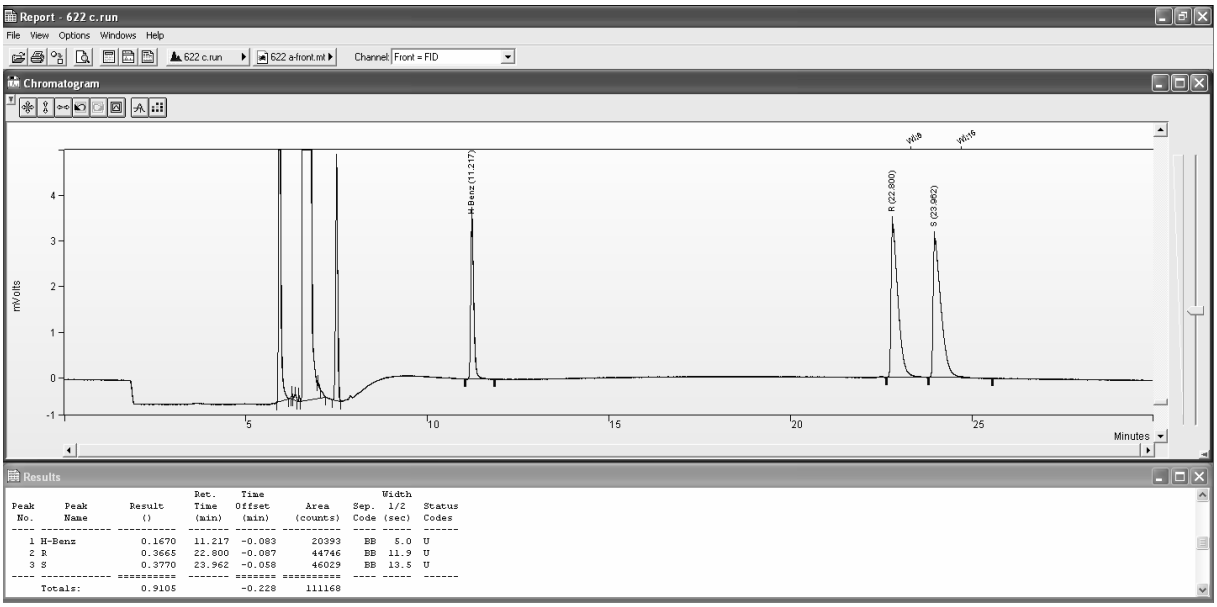




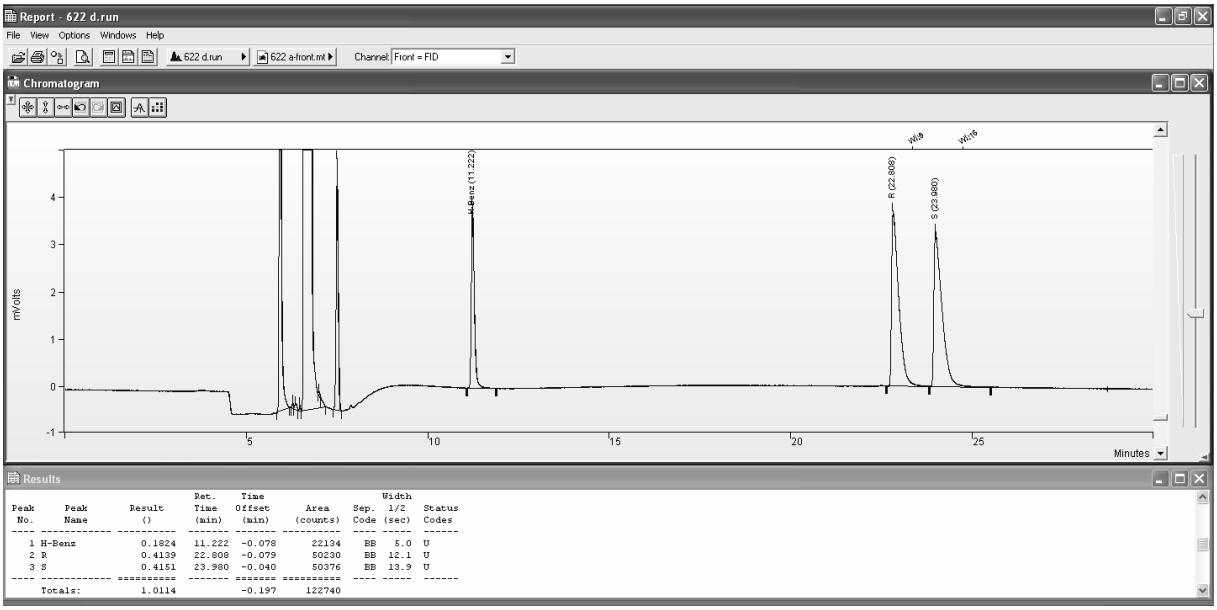

Report - 618 i.run
File View Options Windows Help
618 i.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.255)
R (23.046)
S (24.240)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0678 11.255 -0.045 8018 BB 5.0 U
2 R 0.2661 23.046 -0.354 31451 BB 11.4 U
3 S 0.2809 24.240 -0.199 33204 BB 12.8 U
Totals: 0.6148 -0.598 72673


Report - 622 a.run
File View Options Windows Help
622 a.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.216)
R (22.779)
S (23.939)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1469 11.216 -0.084 17913 BB 5.0 U
2 R 0.4179 22.779 -0.108 50963 BB 12.1 U
3 S 0.4276 23.939 -0.081 52148 BB 14.1 U
Totals: 0.9924 -0.273 121024

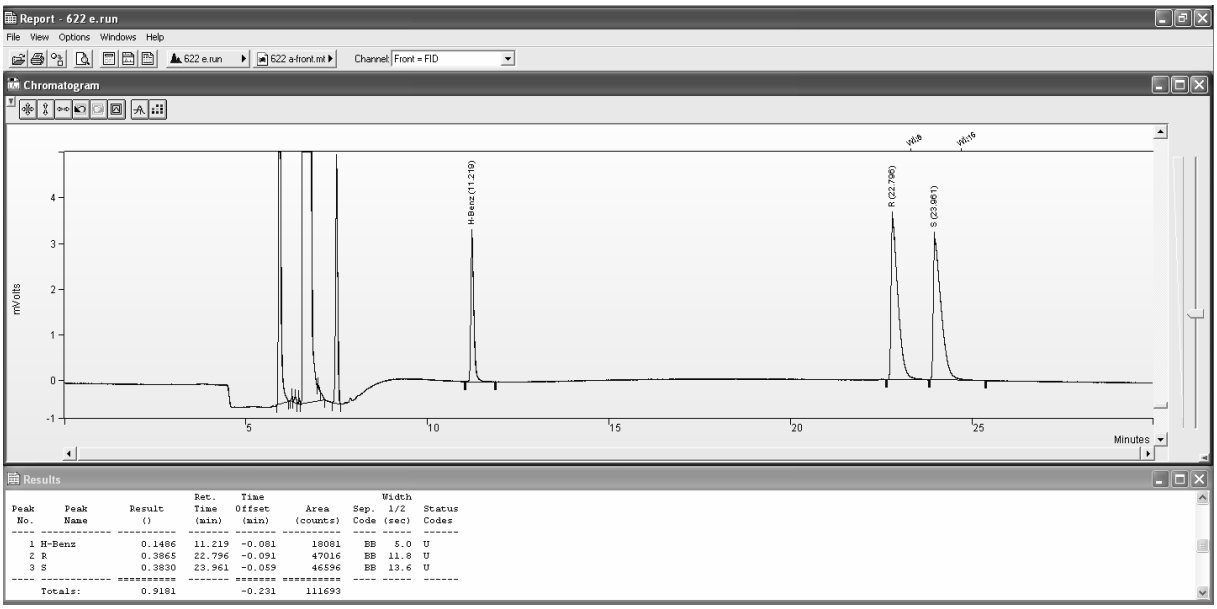

Report - 622 b.run
File View Options Windows Help
622 b.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.212)
R (22.783)
S (23.946)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2064 11.212 -0.088 25238 BB 5.0 U
2 R 0.3896 22.783 -0.104 47641 BB 12.0 U
3 S 0.4039 23.946 -0.074 49384 BB 13.7 U
Totals: 0.9999 -0.266 122263



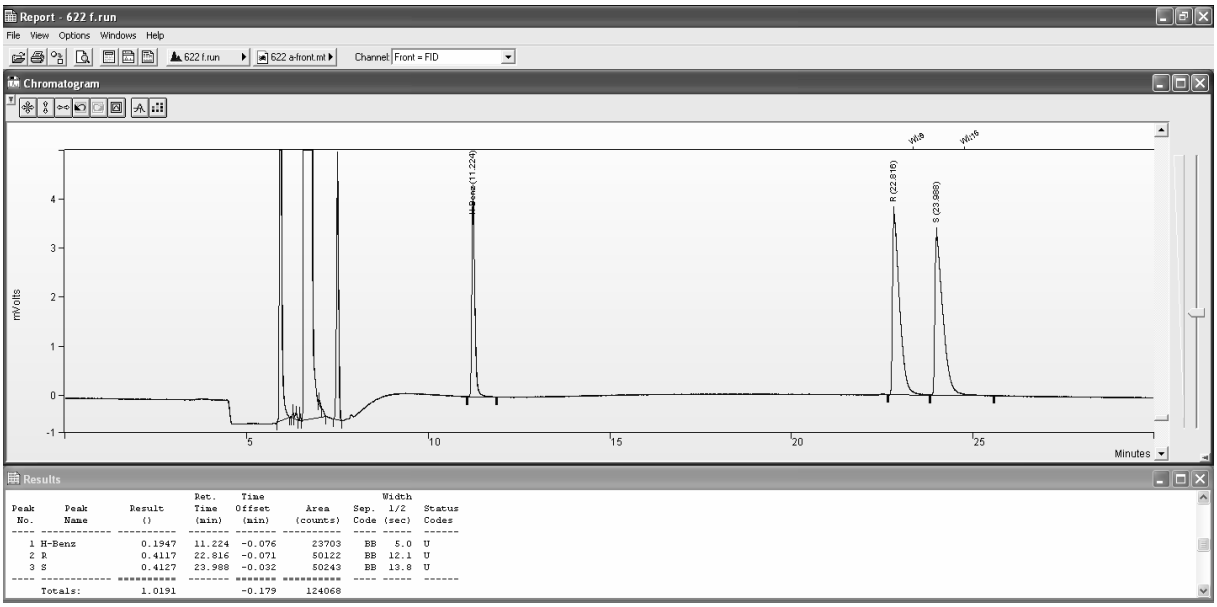
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1670	11.217	-0.083	20393	BB	5.0	U
2	R	0.3665	22.800	-0.087	44746	BB	11.9	U
3	S	0.3770	23.962	-0.058	46029	BB	13.5	U
	Totals:	0.9105		-0.228	111168			

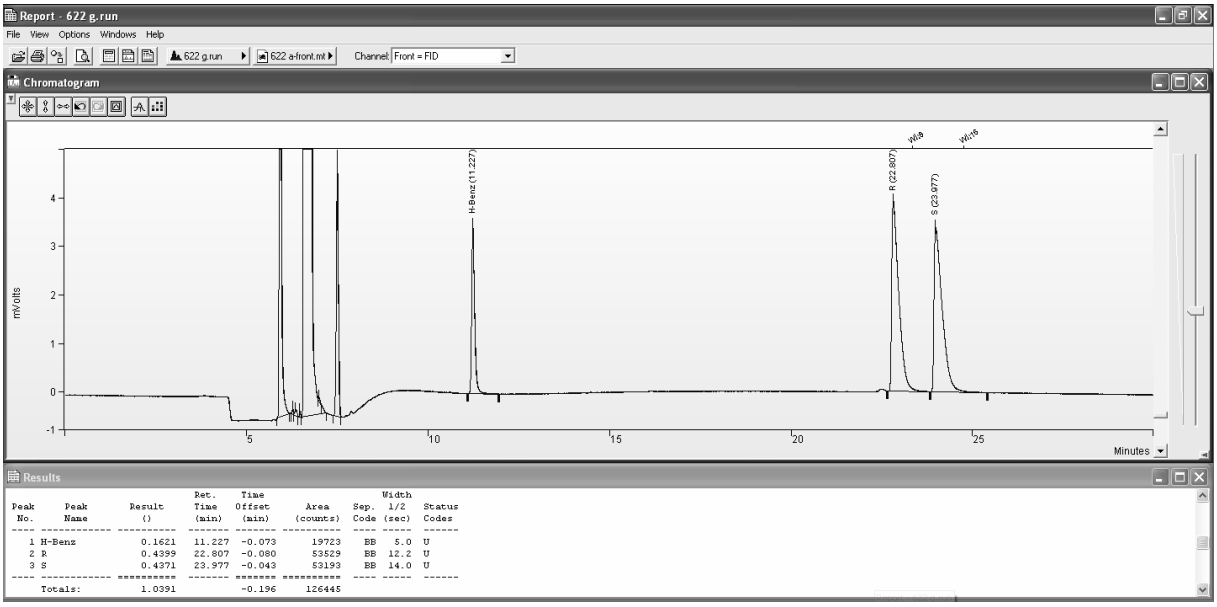


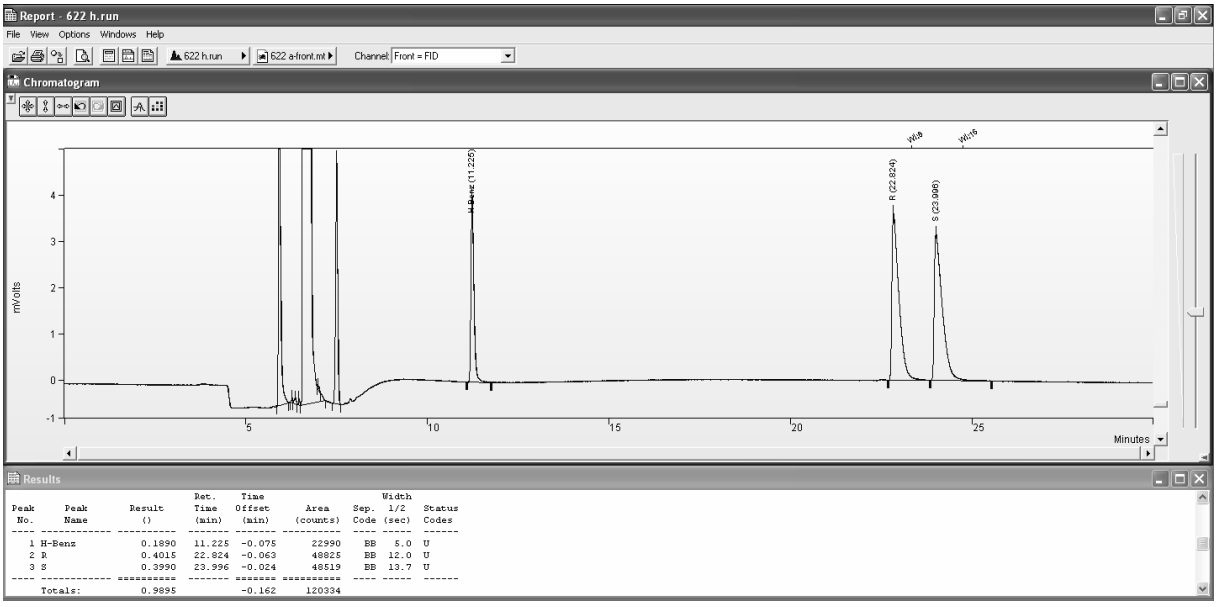
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1824	11.222	-0.078	22134	BB	5.0	U
2	R	0.4139	22.808	-0.079	50230	BB	12.1	U
3	S	0.4151	23.980	-0.040	50376	BB	13.9	U
	Totals:	1.0114		-0.197	122740			

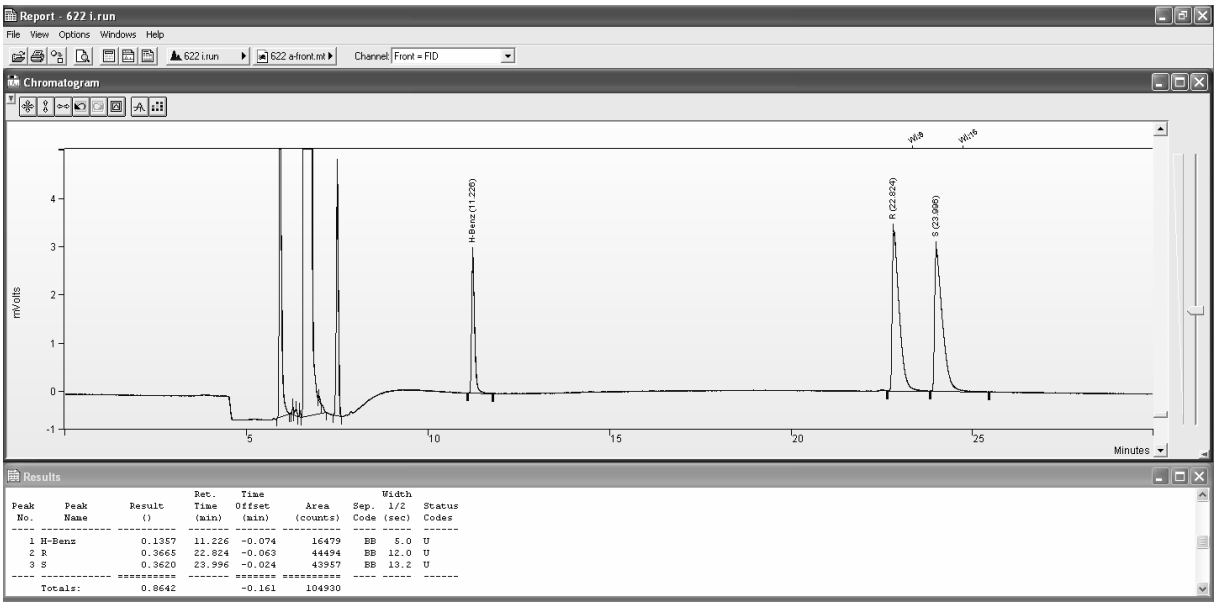


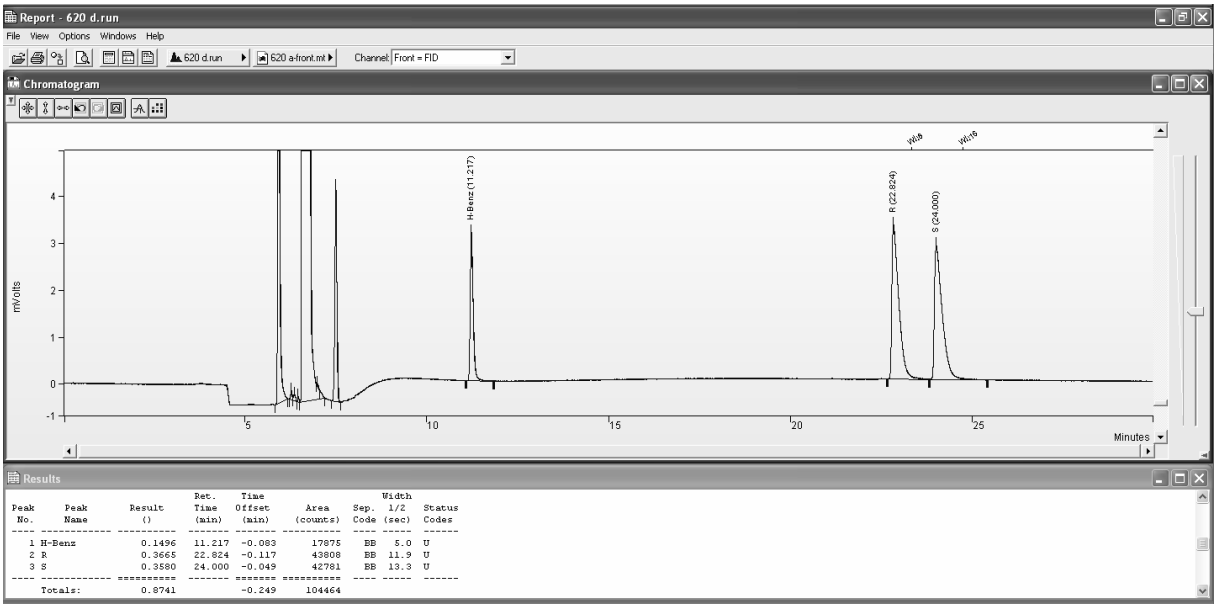
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1486	11.219	-0.081	18081	BB	5.0	U
2	R	0.3865	22.796	-0.091	47016	BB	11.8	U
3	S	0.3830	23.961	-0.059	46596	BB	13.6	U
	Totals:	0.9181		-0.231	111693			

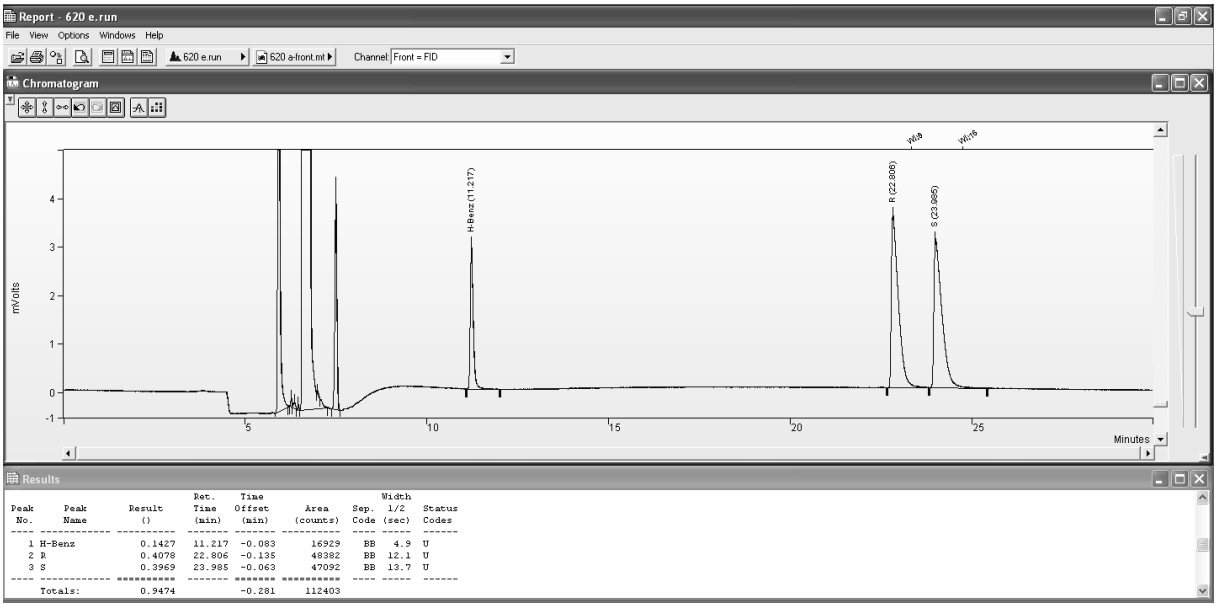

Report - 622 f.run
File View Options Windows Help
622 f.run
622 a-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.224)
R (22.816)
S (23.988)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1947 11.224 -0.076 23703 BB 5.0 U
2 R 0.4117 22.816 -0.071 50122 BB 12.1 U
3 S 0.4127 23.988 -0.032 50243 BB 13.8 U
Totals: 1.0191 -0.179 124068

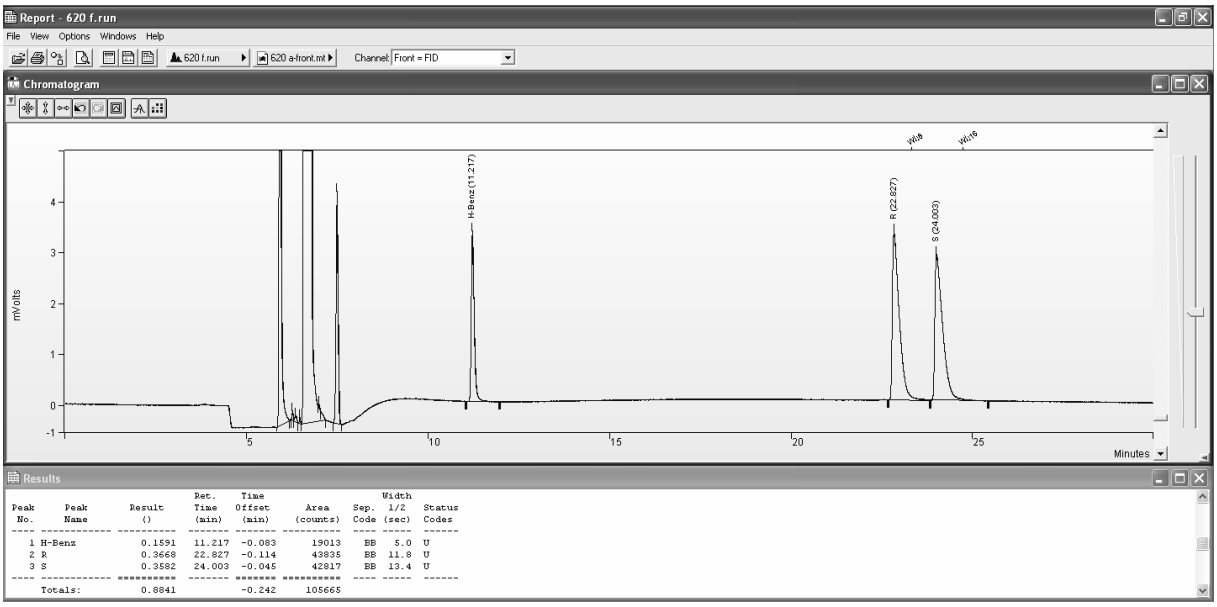

Report - 622 g.run
File View Options Windows Help
622 g.run
622 a-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.227)
R (22.807)
S (23.977)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1621 11.227 -0.073 19723 BB 5.0 U
2 R 0.4399 22.807 -0.080 53529 BB 12.2 U
3 S 0.4371 23.977 -0.043 53193 BB 14.0 U
Totals: 1.0391 -0.196 126445

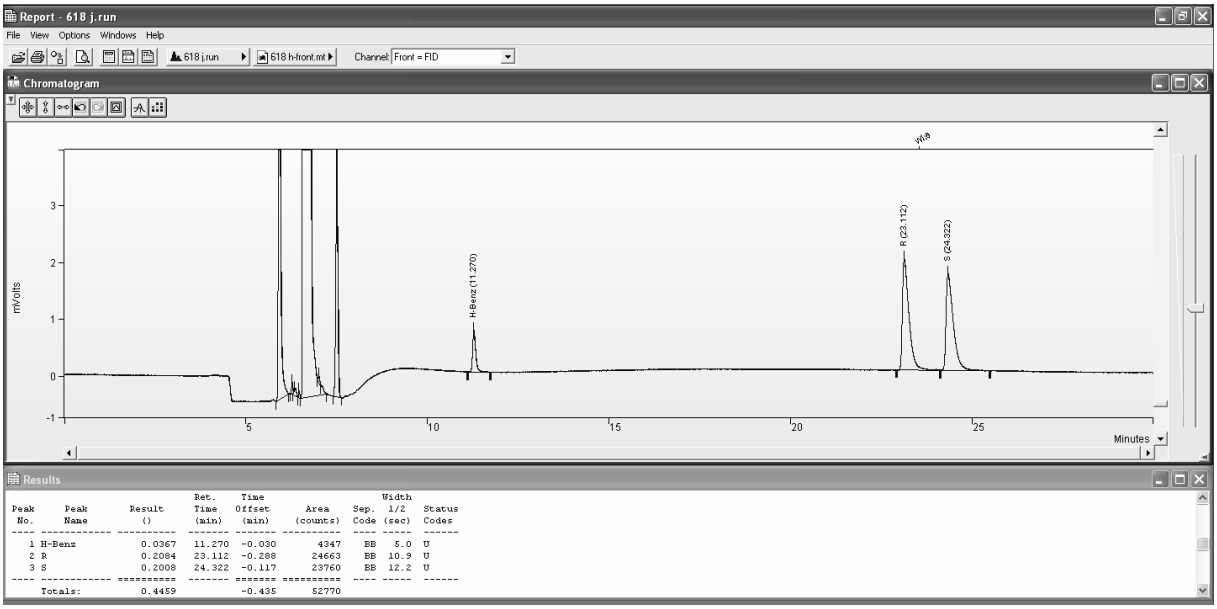

Report - 622 h.run
File View Options Windows Help
622 h.run
622 a-front.mt
Channel Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.225)
R (22.824)
S (23.986)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1890 11.225 -0.075 22990 BB 5.0 U
2 R 0.4015 22.824 -0.063 48825 BB 12.0 U
3 S 0.3990 23.996 -0.024 48519 BB 13.7 U
Totals: 0.9895 -0.162 120334

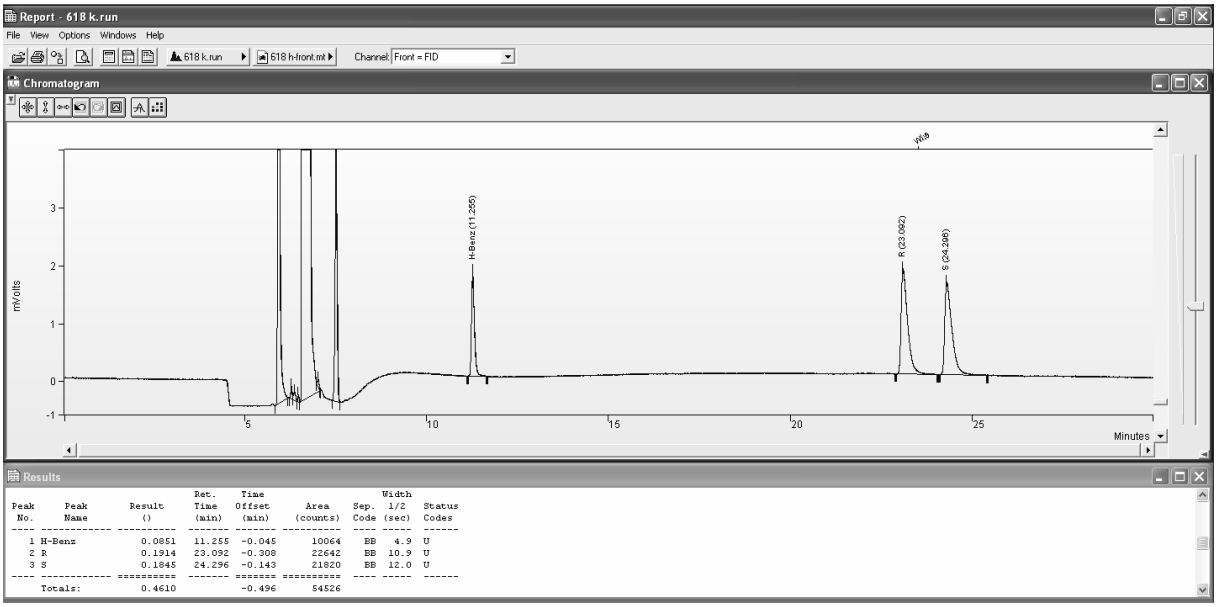

Report - 622 i.run
File View Options Windows Help
622 i.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.226)
R (22.824)
S (23.996)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1357 11.226 -0.074 16479 BB 5.0 U
2 R 0.3665 22.824 -0.063 44494 BB 12.0 U
3 S 0.3620 23.996 -0.024 43957 BB 13.2 U
Totals: 0.8642 -0.161 104930

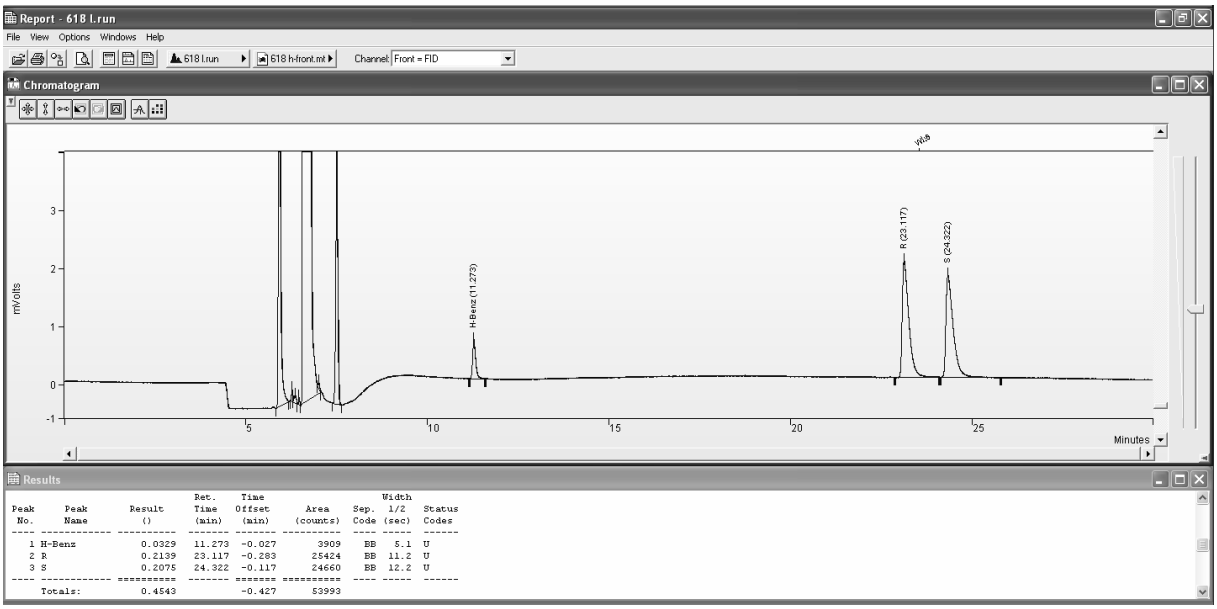

Report - 620 d.run
File View Options Windows Help
620 d.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.217)
R (22.824)
S (24.000)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1496 11.217 -0.083 17875 BB 5.0 U
2 R 0.3665 22.824 -0.117 43808 BB 11.9 U
3 S 0.3580 24.000 -0.049 42781 BB 13.3 U
Totals: 0.8741 -0.249 104464

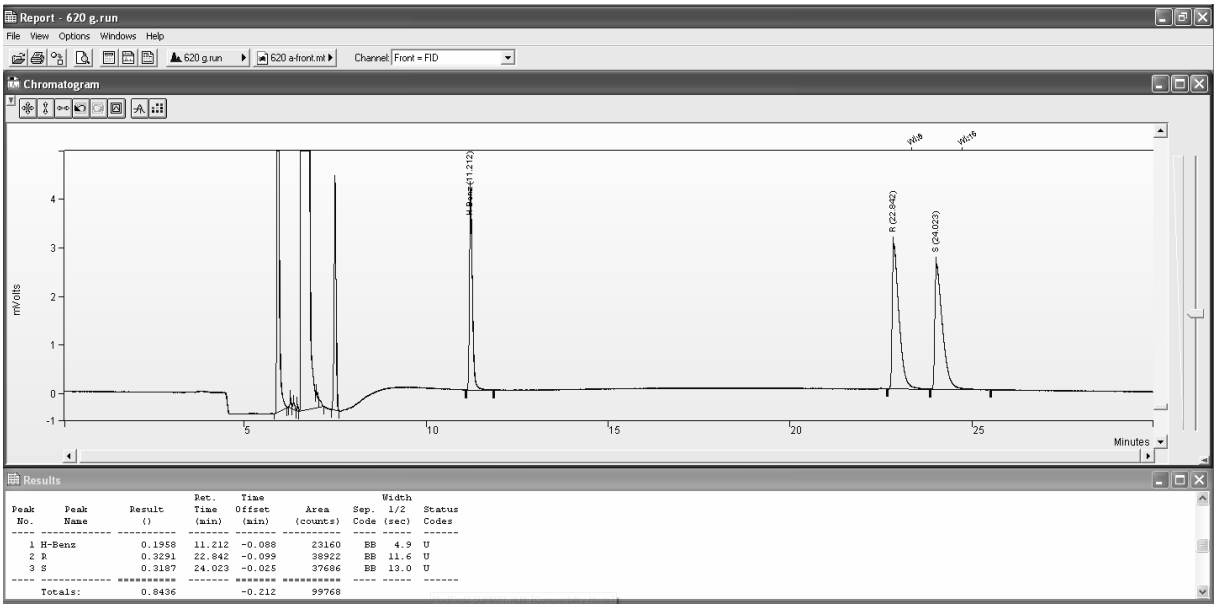

Report - 620 e.run
File View Options Windows Help
620 e.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.217)
R (22.806)
S (23.985)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1427 11.217 -0.083 16929 BB 4.9 U
2 R 0.4078 22.806 -0.135 48382 BB 12.1 U
3 S 0.3969 23.985 -0.063 47092 BB 13.7 U
Totals: 0.9474 -0.281 112403

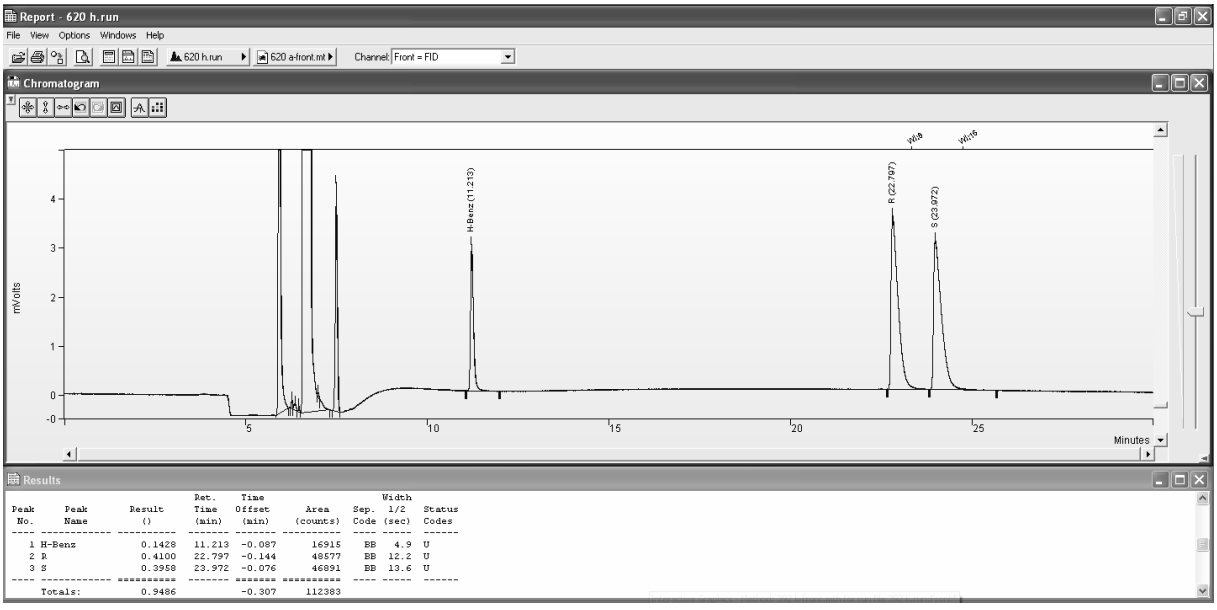

Report - 620 f.run
File View Options Windows Help
620 f.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.217)
R (22.827)
S (24.003)
Wdb
Wdb
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1591 11.217 -0.083 19013 BB 5.0 U
2 R 0.3668 22.827 -0.114 43835 BB 11.8 U
3 S 0.3582 24.003 -0.045 42817 BB 13.4 U
Totals: 0.8841 -0.242 105665

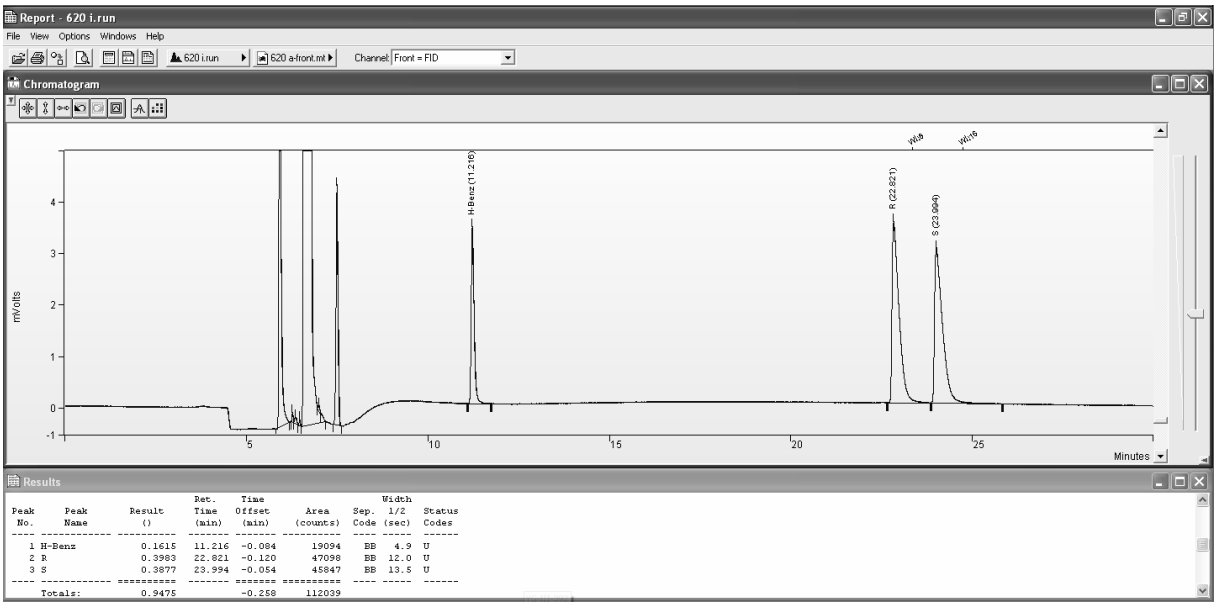

Report - 618 j.run
File View Options Windows Help
618 j.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.270)
R (23.112)
S (24.322)
Wdb
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0367 11.270 -0.030 4347 BB 5.0 U
2 R 0.2084 23.112 -0.288 24663 BB 10.9 U
3 S 0.2008 24.322 -0.117 23760 BB 12.2 U
Totals: 0.4459 -0.435 52770

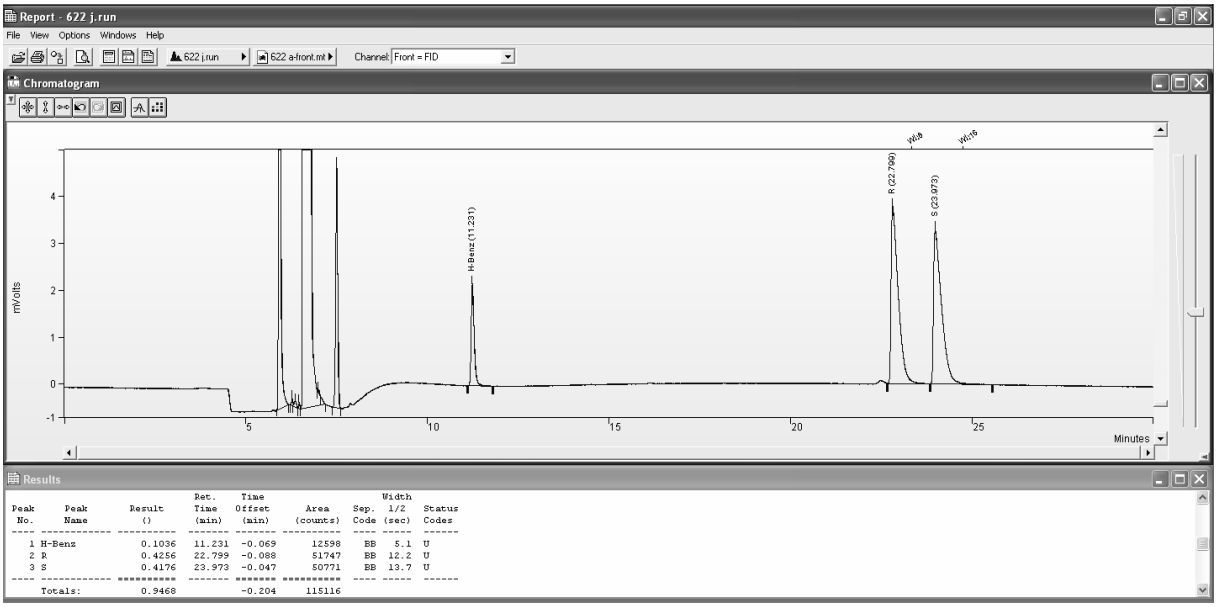

Report - 618 k.run
File View Options Windows Help
618 k.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.255)
R (23.092)
S (24.296)
Wdb
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0851 11.255 -0.045 10064 BB 4.9 U
2 R 0.1914 23.092 -0.308 22642 BB 10.9 U
3 S 0.1845 24.296 -0.143 21820 BB 12.0 U
Totals: 0.4610 -0.496 54526

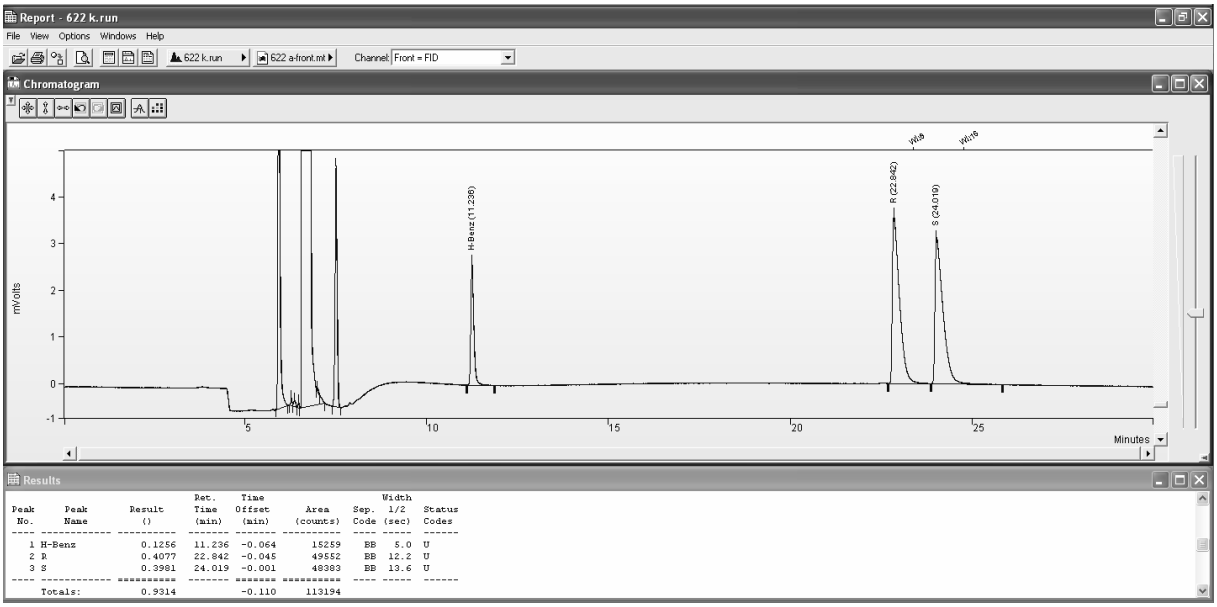

Report - 618 l.run
File View Options Windows Help
618 l.run
618 h-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.273)
R (23.117)
S (24.322)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0329 11.273 -0.027 3909 BB 5.1 U
2 R 0.2139 23.117 -0.283 25424 BB 11.2 U
3 S 0.2075 24.322 -0.117 24660 BB 12.2 U
Totals: 0.4543 -0.427 53993

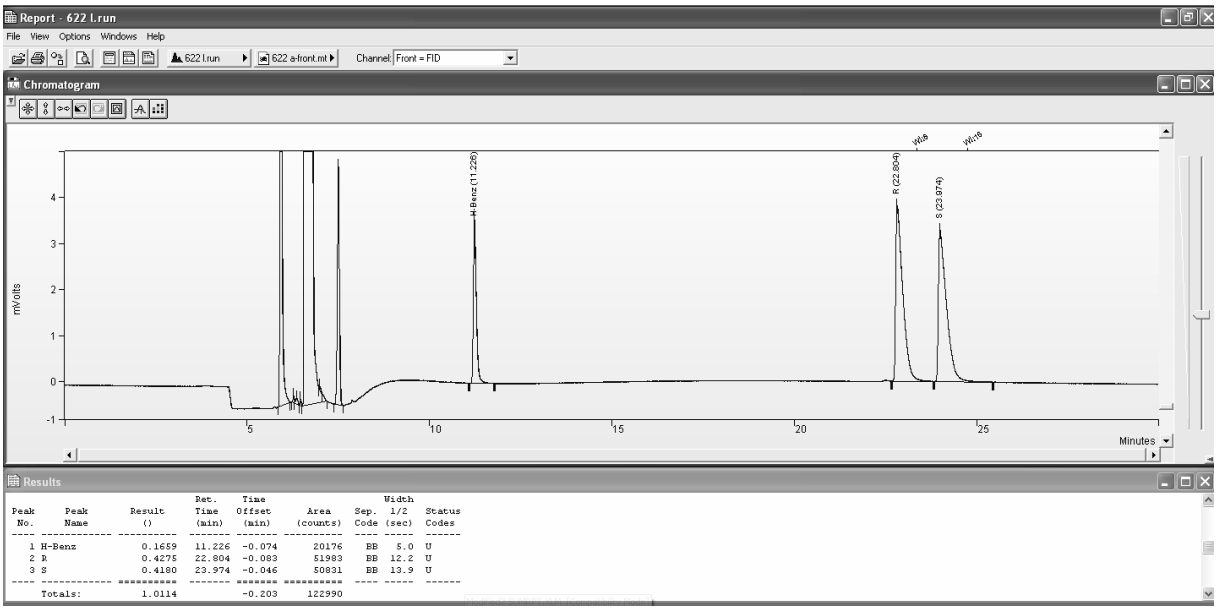

Report - 620 g.run
File View Options Windows Help
620 g.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.212)
R (22.842)
S (24.023)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1958 11.212 -0.088 23160 BB 4.9 U
2 R 0.3291 22.842 -0.099 38922 BB 11.6 U
3 S 0.3187 24.023 -0.025 37686 BB 13.0 U
Totals: 0.8436 -0.212 99768

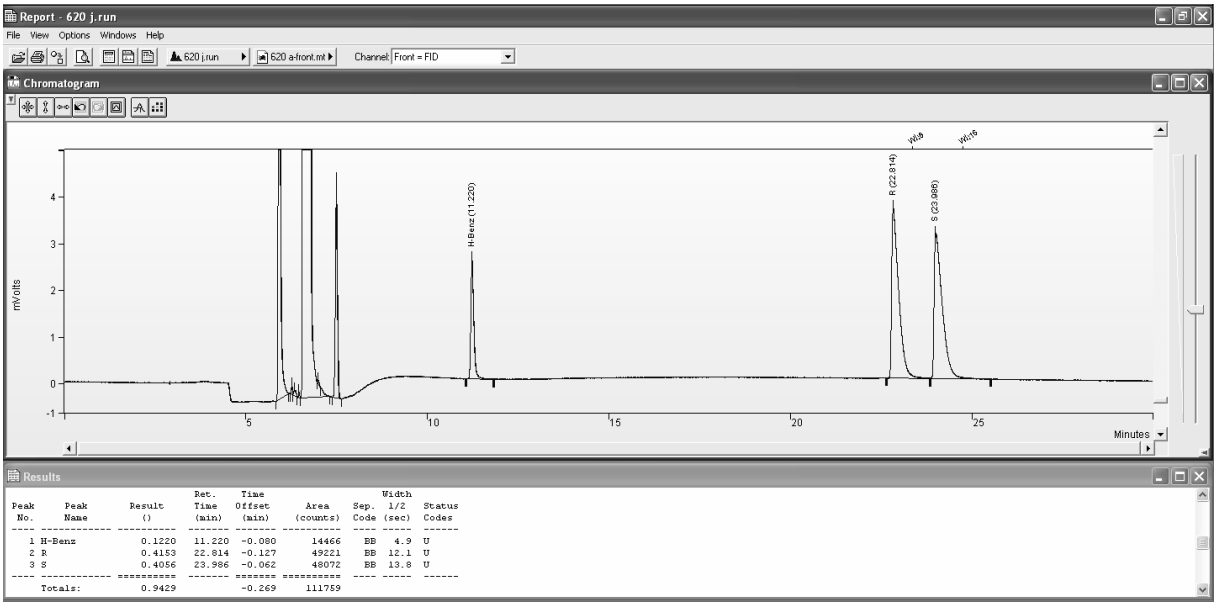

Report - 620 h.run
File View Options Windows Help
620 h.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.213)
R (22.797)
S (23.972)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1428 11.213 -0.087 16915 BB 4.9 U
2 R 0.4100 22.797 -0.144 48577 BB 12.2 U
3 S 0.3958 23.972 -0.076 46891 BB 13.6 U
Totals: 0.9486 -0.307 112383

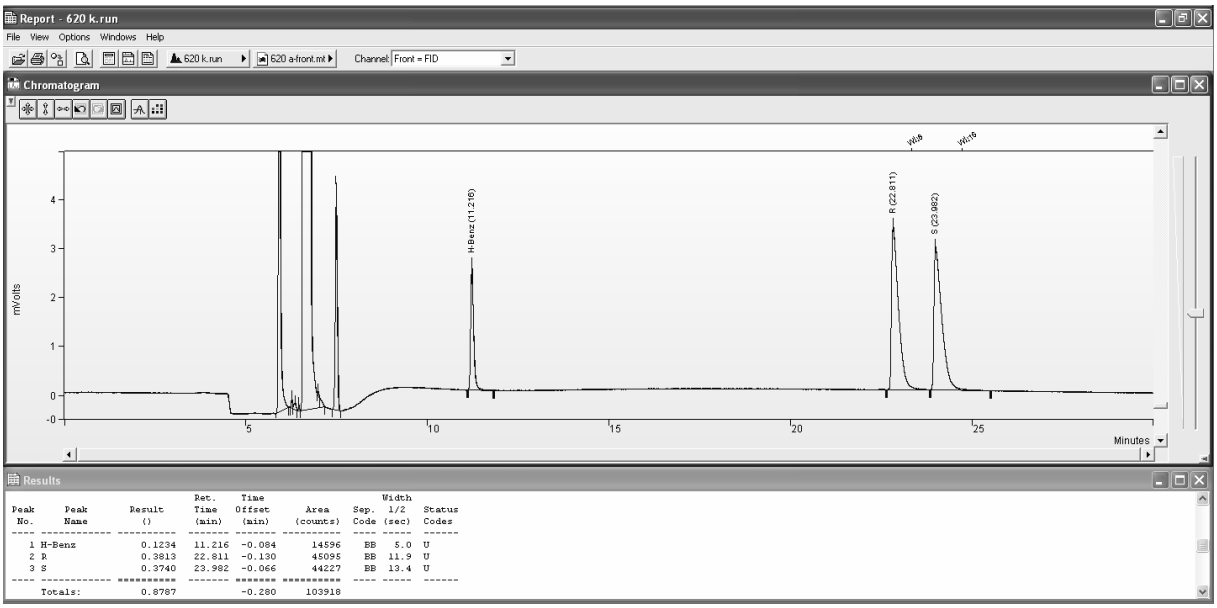

Report - 620 i.run
File View Options Windows Help
620 i.run
620 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.216)
R (22.821)
S (23.994)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1615 11.216 -0.084 19094 BB 4.9 U
2 R 0.3983 22.821 -0.120 47098 BB 12.0 U
3 S 0.3877 23.994 -0.054 45847 BB 13.5 U
Totals: 0.9475 -0.258 112039

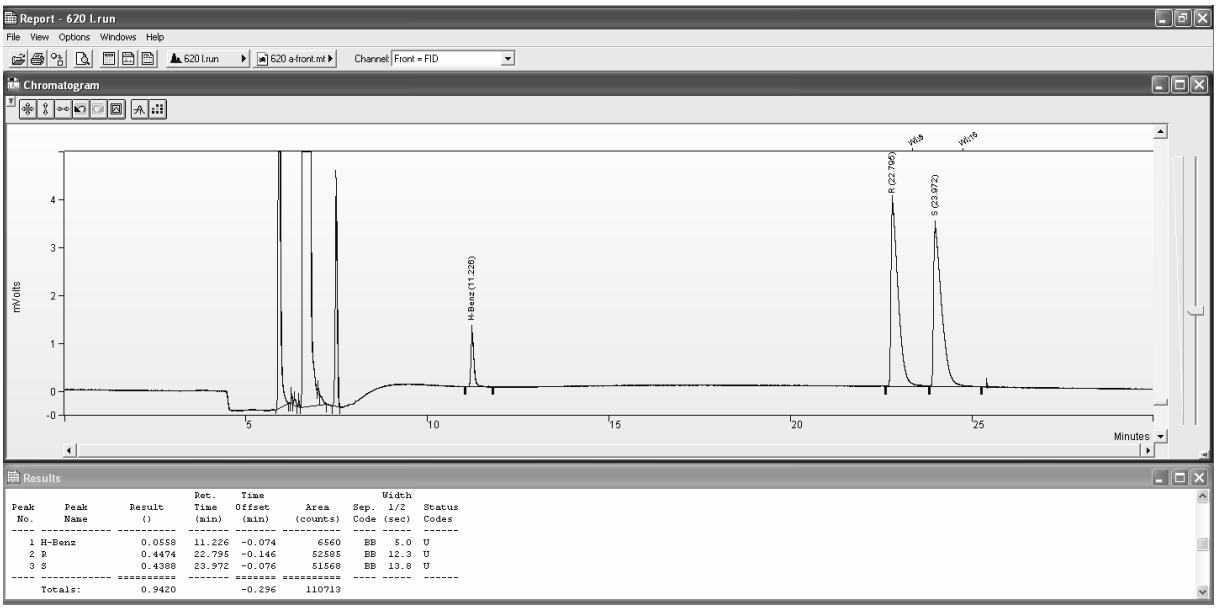

Report - 622 j.run
File View Options Windows Help
622 j.run
622 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.231)
R (22.799)
S (23.973)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1036 11.231 -0.069 12598 BB 5.1 U
2 R 0.4256 22.799 -0.088 51747 BB 12.2 U
3 S 0.4176 23.973 -0.047 50771 BB 13.7 U
Totals: 0.9468 -0.204 115116

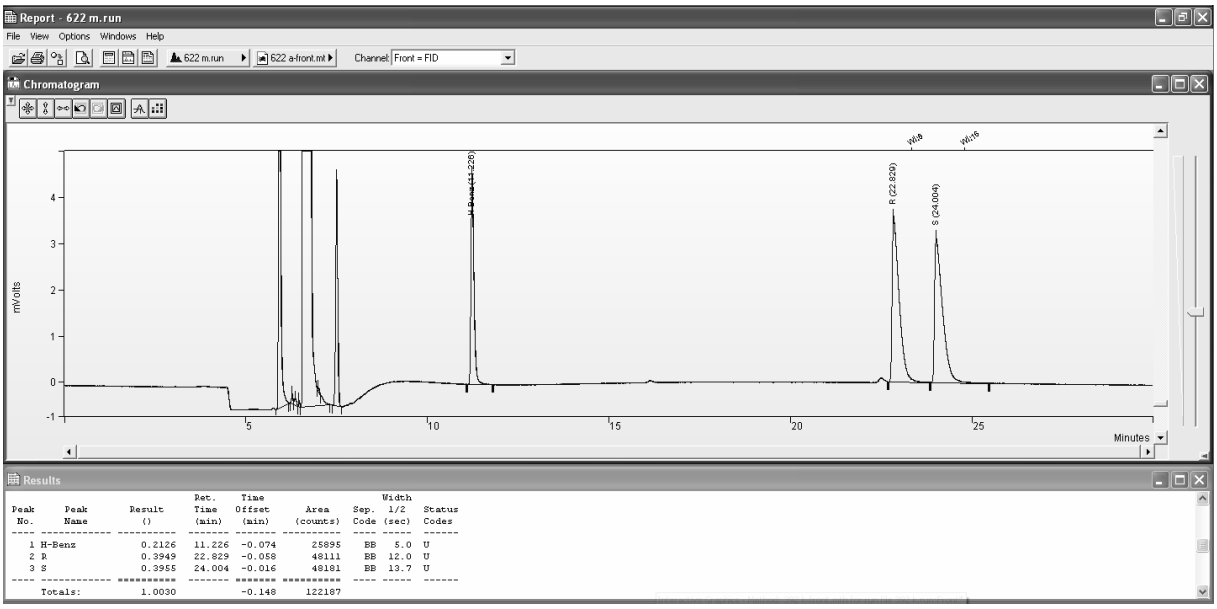

Report - 622 k.run
File View Options Windows Help
622 k.run
622 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.236)
R (22.842)
S (24.019)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1256 11.236 -0.064 15259 BB 5.0 U
2 R 0.4077 22.842 -0.045 49552 BB 12.2 U
3 S 0.3981 24.019 -0.001 48383 BB 13.6 U
Totals: 0.9314 -0.110 113194

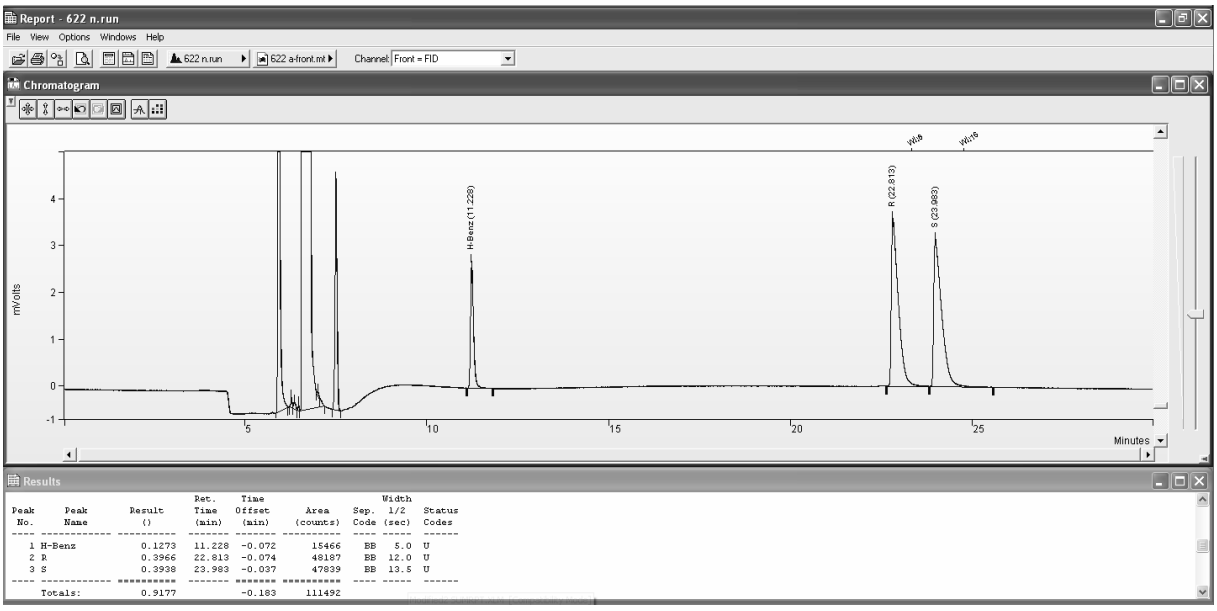

Report - 622 l.run
File View Options Windows Help
622 l.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.226)
R (22.804)
S (23.974)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1659 11.226 -0.074 20176 BB 5.0 U
2 R 0.4275 22.804 -0.083 51983 BB 12.2 U
3 S 0.4180 23.974 -0.046 50831 BB 13.9 U
Totals: 1.0114 -0.203 122990

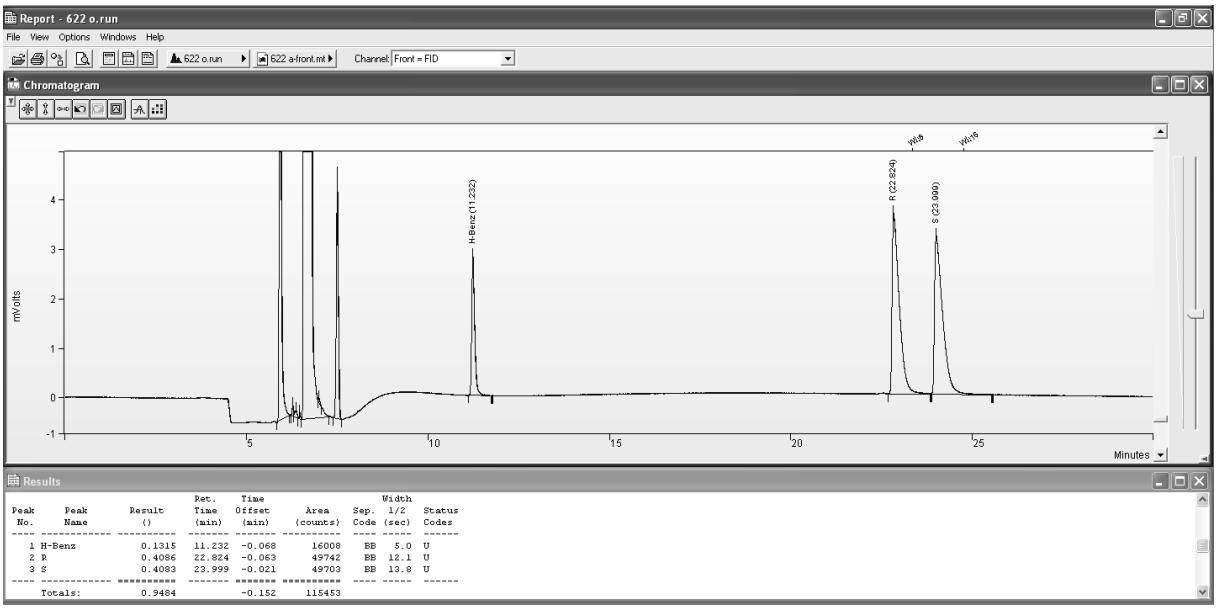

Report - 620 j.run
File View Options Windows Help
620 j.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.220)
R (22.814)
S (23.986)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1220 11.220 -0.080 14466 BB 4.9 U
2 R 0.4153 22.814 -0.127 49221 BB 12.1 U
3 S 0.4056 23.986 -0.062 48072 BB 13.8 U
Totals: 0.9429 -0.269 111759


Report - 620 k.run
File View Options Windows Help
620 k.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.216)
R (22.811)
S (23.982)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1234 11.216 -0.084 14596 BB 5.0 U
2 R 0.3813 22.811 -0.130 45095 BB 11.9 U
3 S 0.3740 23.982 -0.066 44227 BB 13.4 U
Totals: 0.8787 -0.280 103918

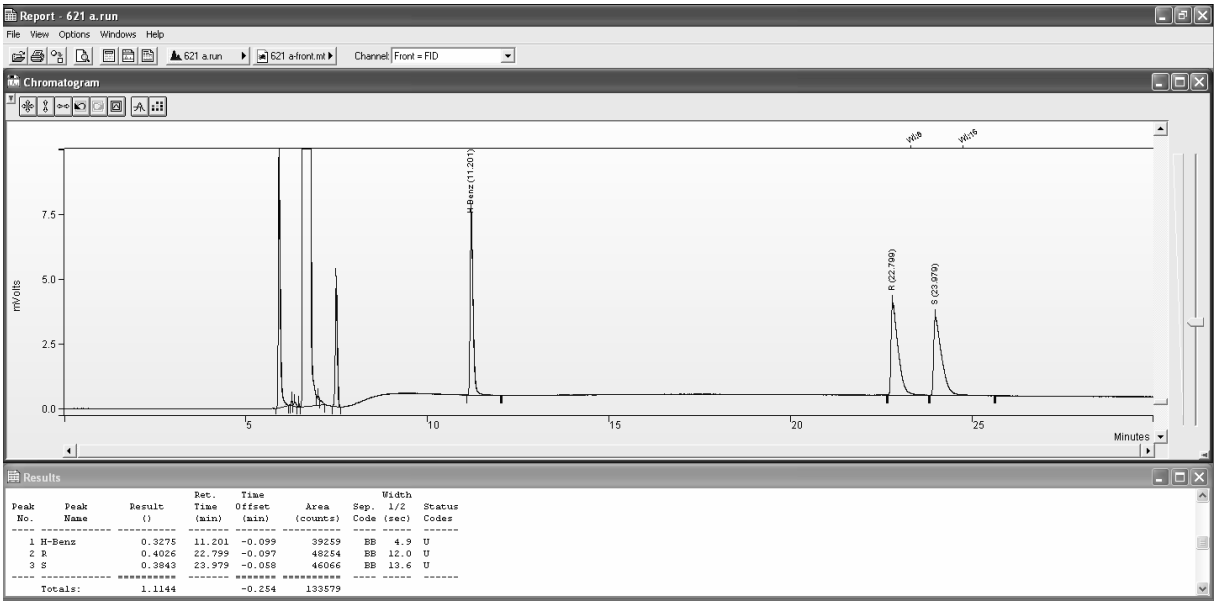

Report - 620 l.run
File View Options Windows Help
620 l.run
620 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.226)
R (22.795)
S (23.972)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.0558 11.226 -0.074 6560 BB 5.0 U
2 R 0.4474 22.795 -0.146 52585 BB 12.3 U
3 S 0.4388 23.972 -0.076 51568 BB 13.8 U
Totals: 0.9420 -0.296 110713

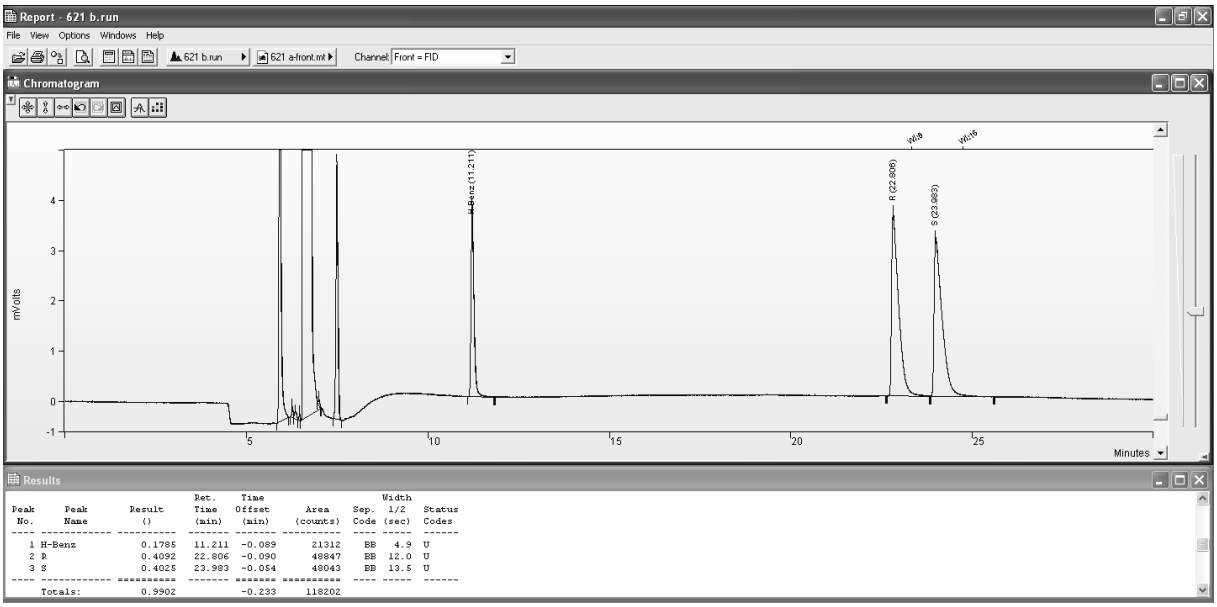

Report - 622 m.run
File View Options Windows Help
622 m.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
R (22.829)
S (24.004)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2126 11.226 -0.074 25895 BB 5.0 U
2 R 0.3949 22.829 -0.058 48111 BB 12.0 U
3 S 0.3955 24.004 -0.016 48181 BB 13.7 U
Totals: 1.0030 -0.148 122187

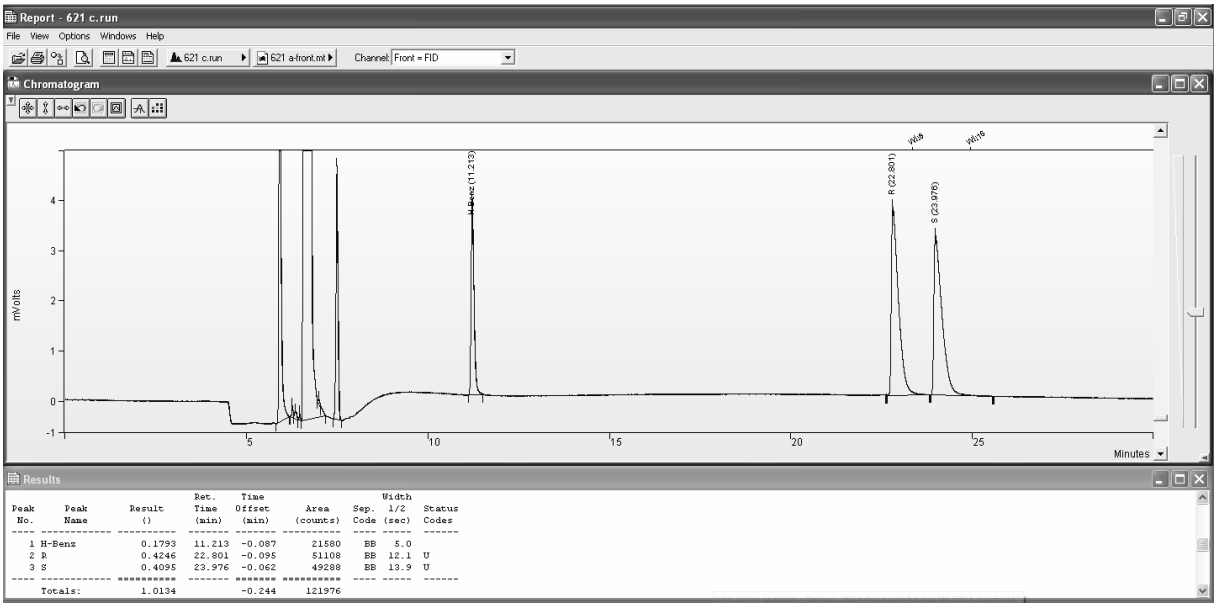

Report - 622 n.run
File View Options Windows Help
622 n.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.228)
R (22.813)
S (23.983)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1273 11.228 -0.072 15466 BB 5.0 U
2 R 0.3966 22.813 -0.074 48187 BB 12.0 U
3 S 0.3938 23.983 -0.037 47839 BB 13.5 U
Totals: 0.9177 -0.183 111492

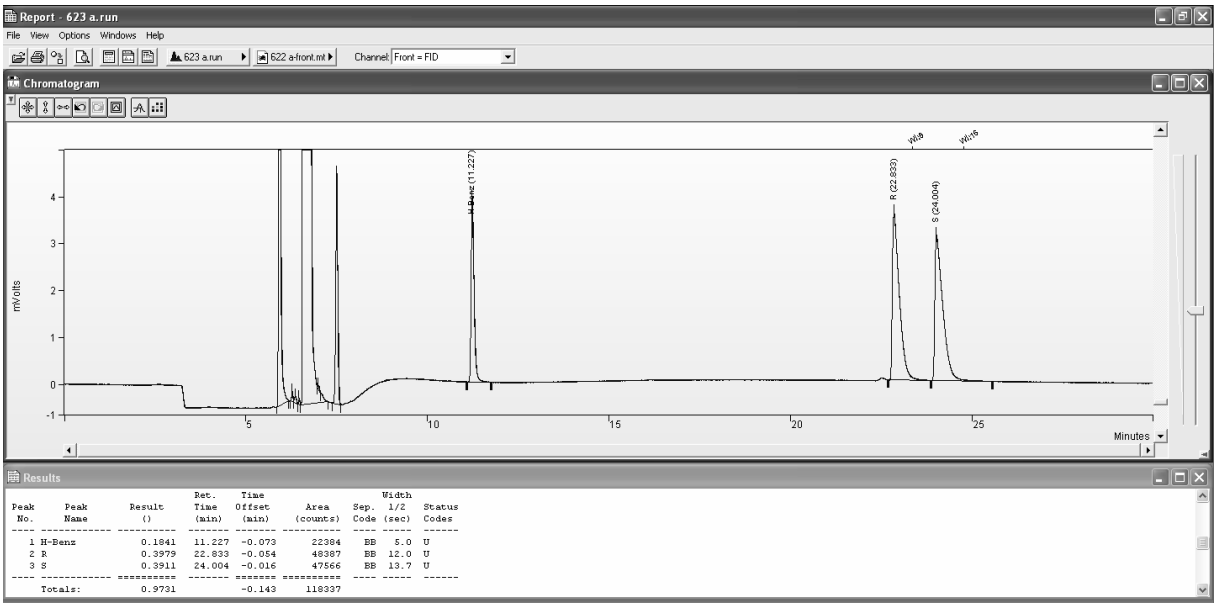


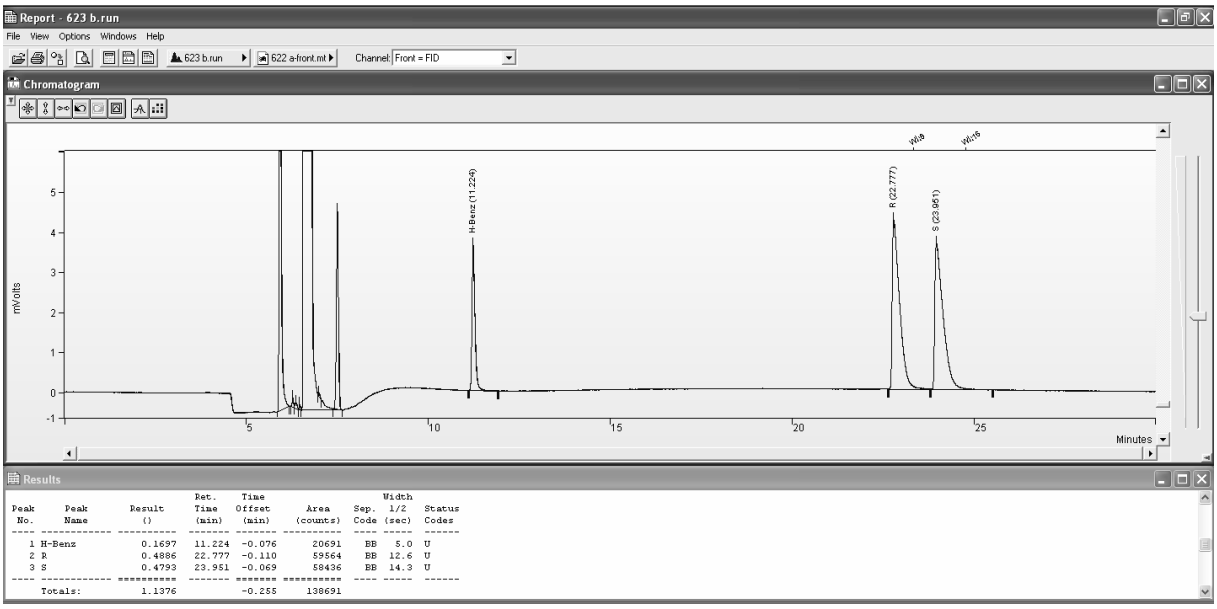
III.7 Figure 3b ((+)-NME)

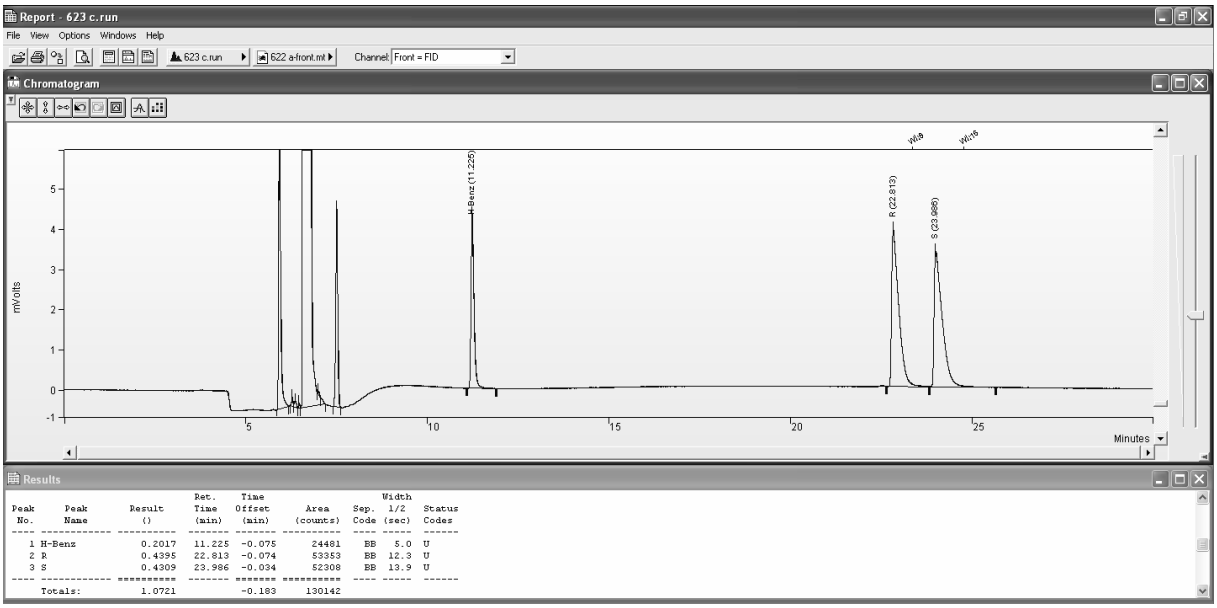


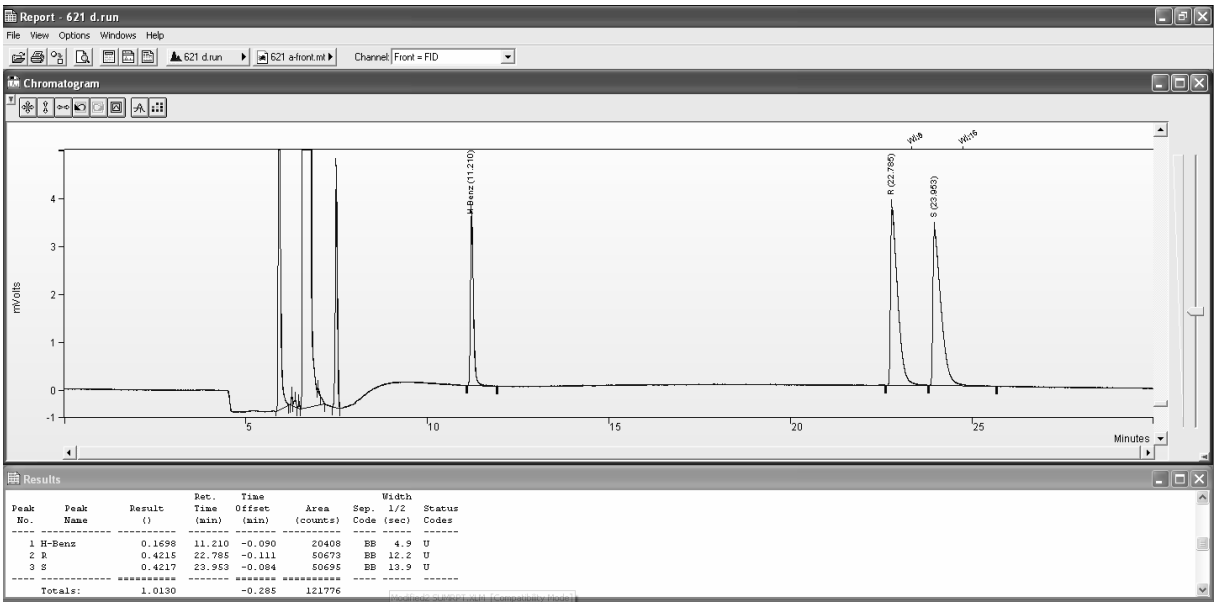

Report - 621 b.run
File View Options Windows Help
621 b.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.211)
R (22.806)
S (23.983)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1785 11.211 -0.089 21312 BB 4.9 U
2 R 0.4092 22.806 -0.090 48847 BB 12.0 U
3 S 0.4025 23.983 -0.054 48043 BB 13.5 U
Totals: 0.9902 -0.233 118202

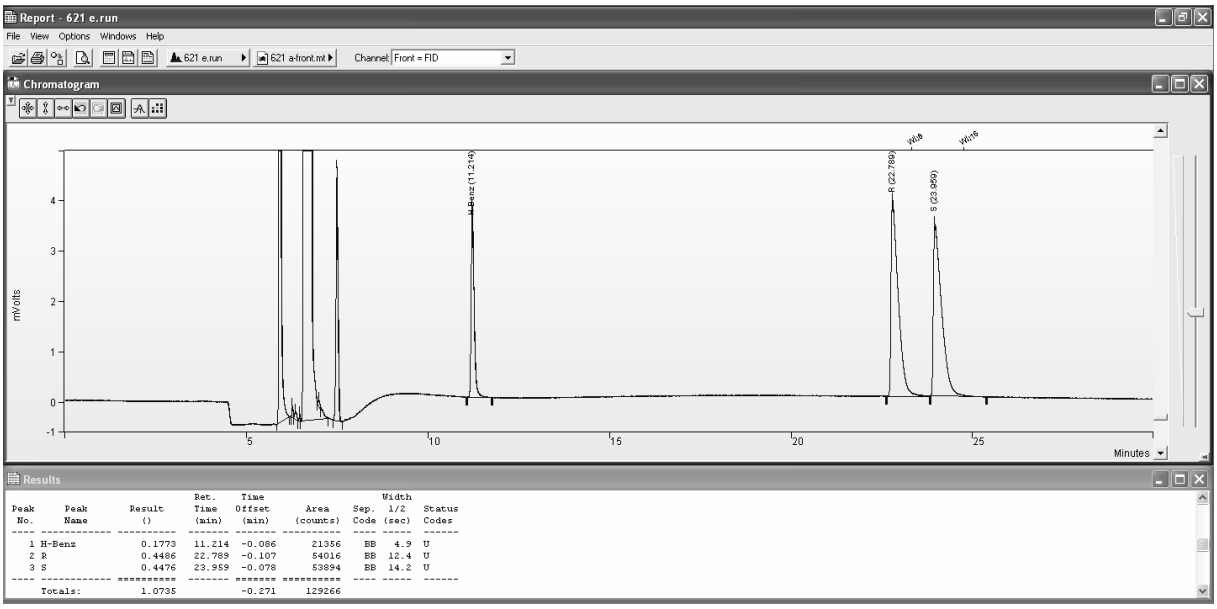

Report - 621 c.run
File View Options Windows Help
621 c.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.213)
R (22.801)
S (23.976)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1793 11.213 -0.087 21580 BB 5.0
2 R 0.4246 22.801 -0.095 51108 BB 12.1 U
3 S 0.4095 23.976 -0.062 49288 BB 13.9 U
Totals: 1.0134 -0.244 121976

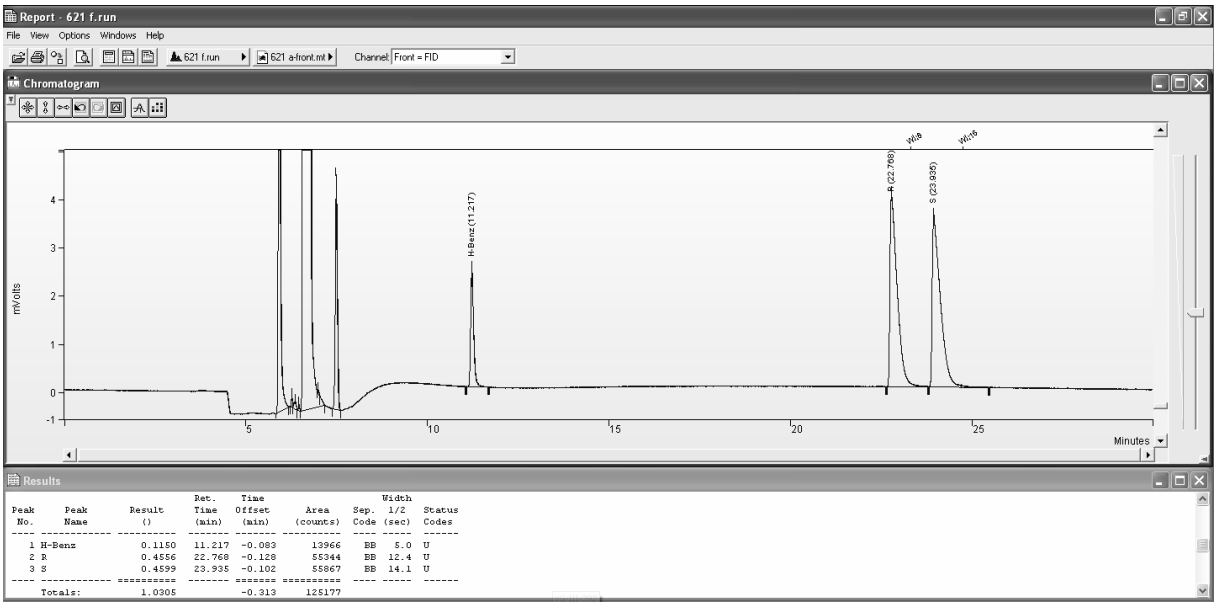

Report - 623 a.run
File View Options Windows Help
623 a.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.227)
R (22.833)
S (24.004)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1841 11.227 -0.073 22384 BB 5.0 U
2 R 0.3979 22.833 -0.054 49387 BB 12.0 U
3 S 0.3911 24.004 -0.016 47566 BB 13.7 U
Totals: 0.9731 -0.143 119337

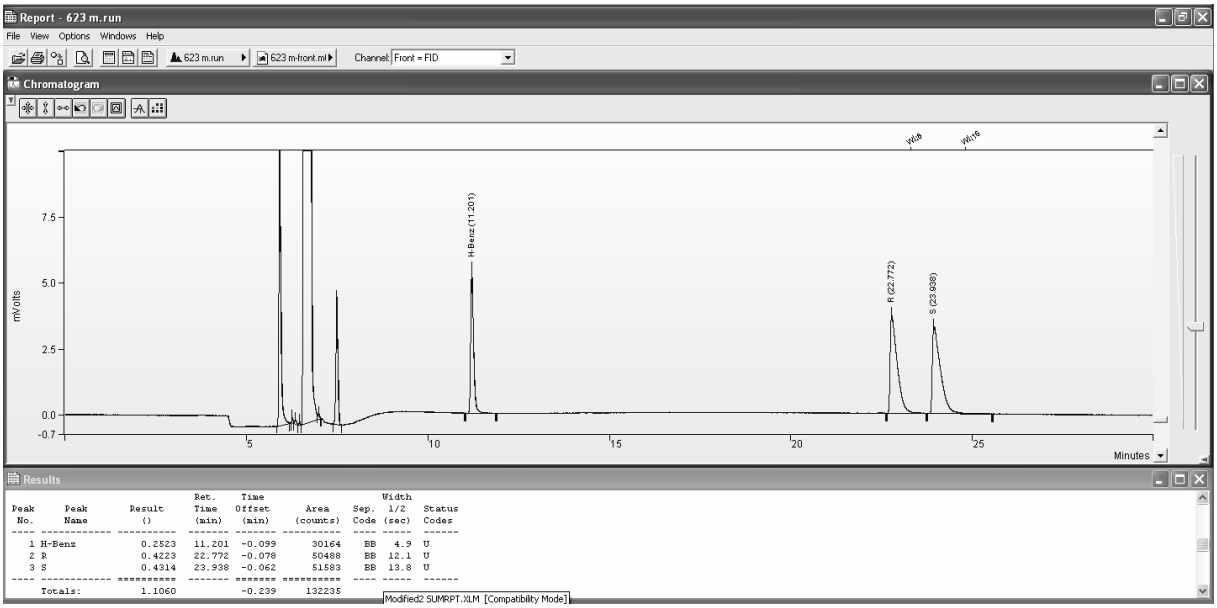

Report - 623 b.run
File View Options Windows Help
623 b.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.224)
R (22.777)
S (23.951)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1697 11.224 -0.076 20691 BB 5.0 U
2 R 0.4886 22.777 -0.110 59564 BB 12.6 U
3 S 0.4793 23.951 -0.069 58436 BB 14.3 U
Totals: 1.1376 -0.255 138691

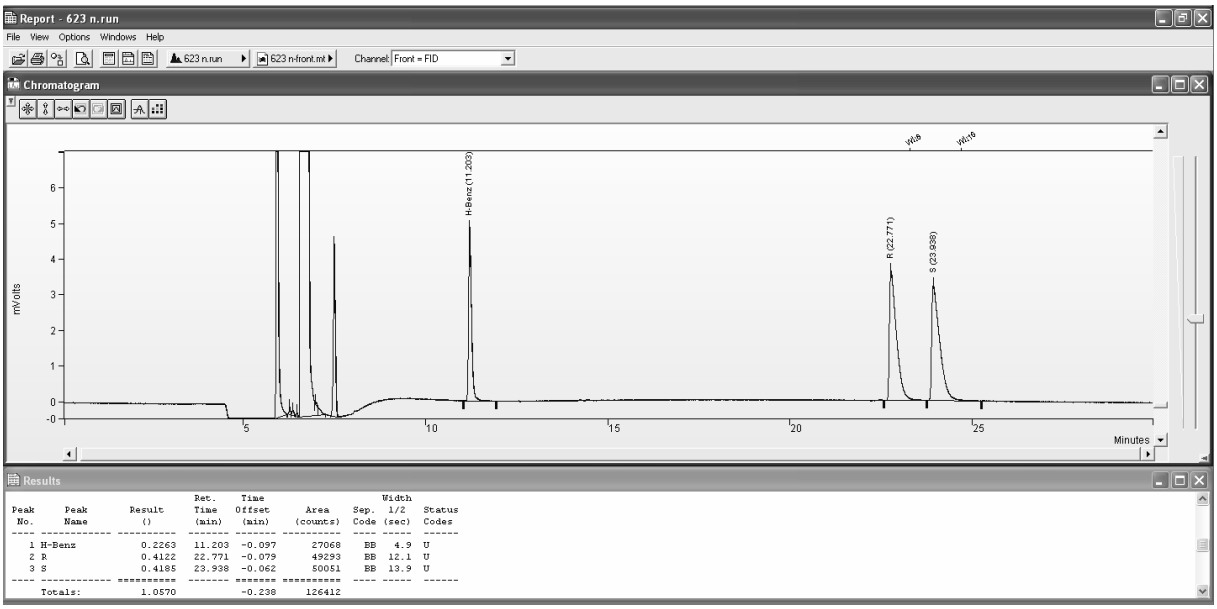

Report - 623 c.run
File View Options Windows Help
623 c.run
622 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.225)
R (22.813)
S (23.986)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2017 11.225 -0.075 24481 BB 5.0 U
2 R 0.4395 22.813 -0.074 53353 BB 12.3 U
3 S 0.4309 23.986 -0.034 52308 BB 13.9 U
Totals: 1.0721 -0.183 130142


Report - 621 d.run
File View Options Windows Help
621 d.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.210)
R (22.785)
S (23.953)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1698 11.210 -0.090 20408 BB 4.9 U
2 R 0.4215 22.785 -0.111 50673 BB 12.2 U
3 S 0.4217 23.953 -0.084 50695 BB 13.9 U
Totals: 1.0130 -0.285 121776

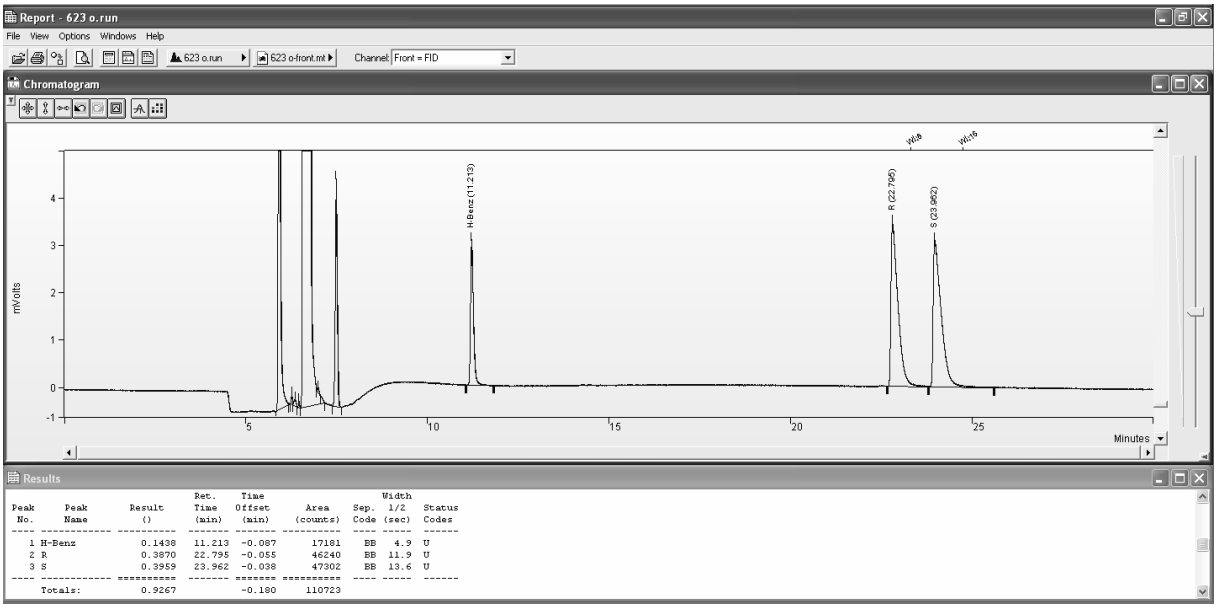

Report - 621 e.run
File View Options Windows Help
621 e.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.214)
R (22.789)
S (23.959)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1773 11.214 -0.086 21356 BB 4.9 U
2 R 0.4486 22.789 -0.107 54016 BB 12.4 U
3 S 0.4476 23.959 -0.078 53894 BB 14.2 U
Totals: 1.0735 -0.271 129266


Report - 621 f.run
File View Options Windows Help
621 f.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.217)
R (22.768)
S (23.935)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1150 11.217 -0.083 13966 BB 5.0 U
2 R 0.4556 22.768 -0.128 55344 BB 12.4 U
3 S 0.4599 23.935 -0.102 55867 BB 14.1 U
Totals: 1.0305 -0.313 125177

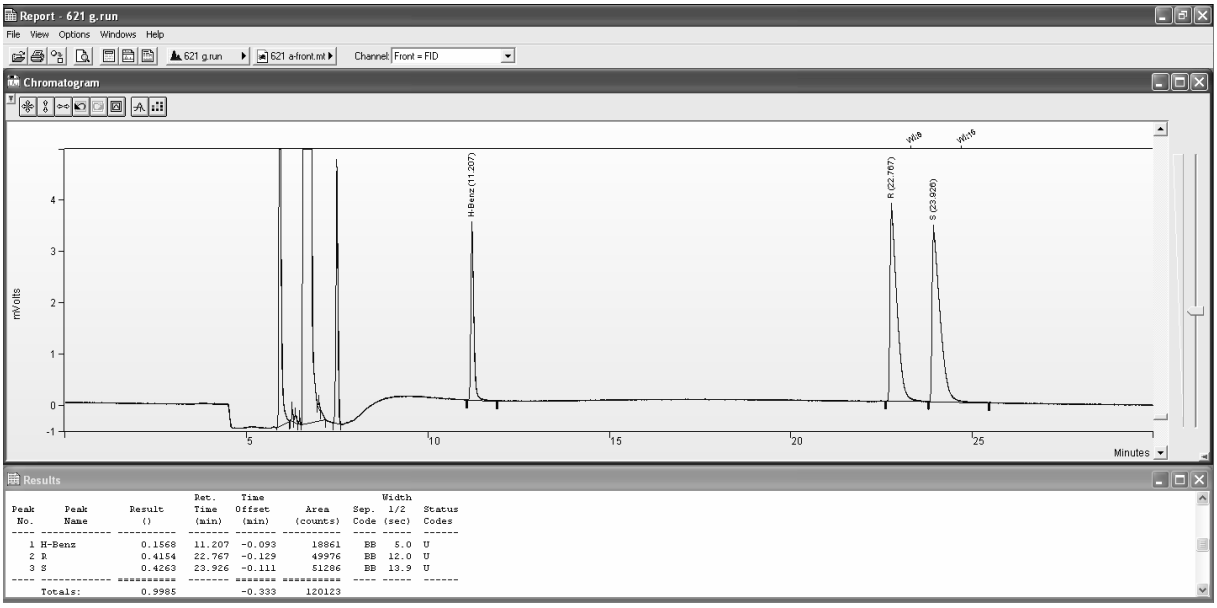

Report - 623 m.run
File View Options Windows Help
623 m.run
623 m-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.201)
R (22.772)
S (23.938)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2523 11.201 -0.099 30164 BB 4.9 U
2 R 0.4223 22.772 -0.078 50488 BB 12.1 U
3 S 0.4314 23.938 -0.062 51583 BB 13.8 U
Totals: 1.1060 -0.239 132235
Modified2 SUMRPT.XLM [Compatibility Mode]



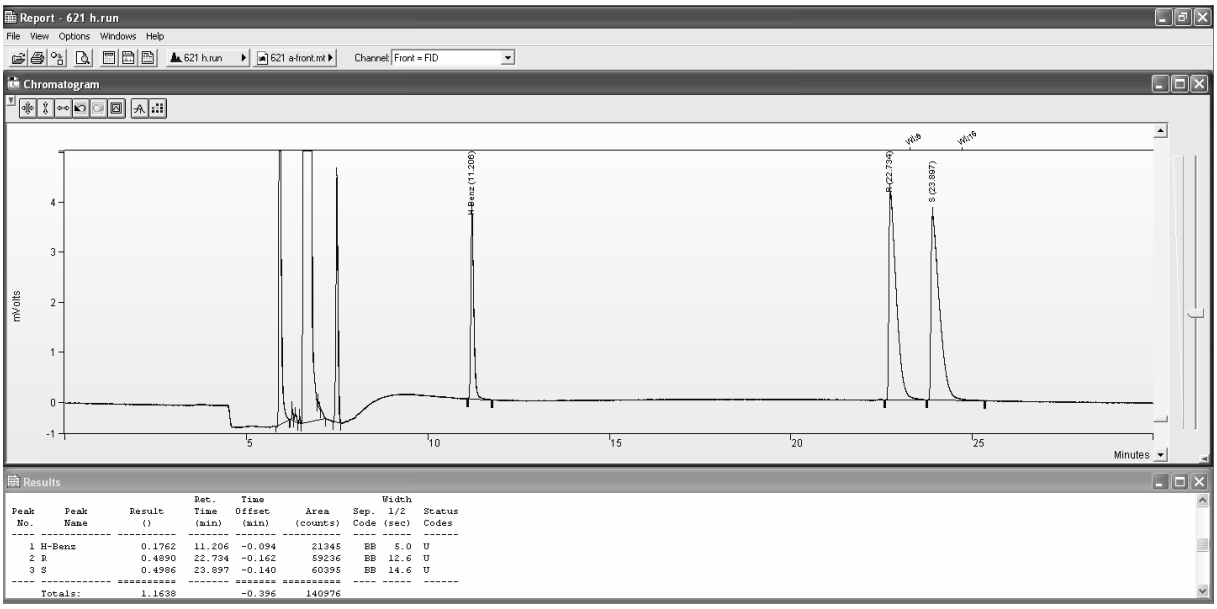
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.2263	11.203	-0.097	27068	BB	4.9	U
2	R	0.4122	22.771	-0.079	49293	BB	12.1	U
3	S	0.4185	23.938	-0.062	50051	BB	13.9	U
	Totals:	1.0570		-0.238	126412			

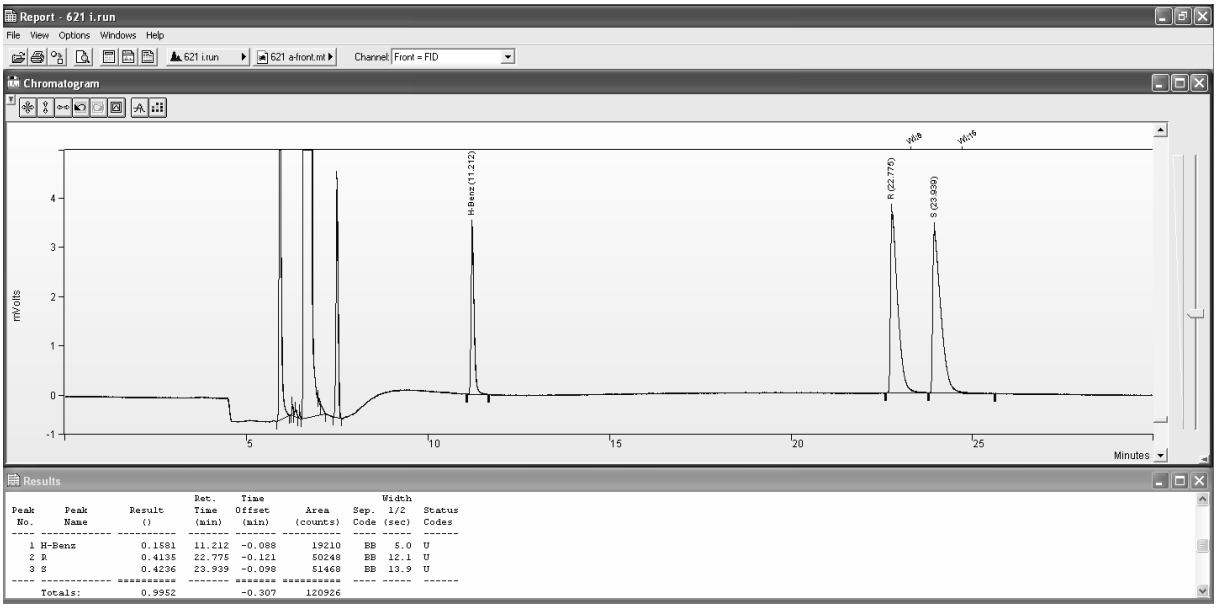


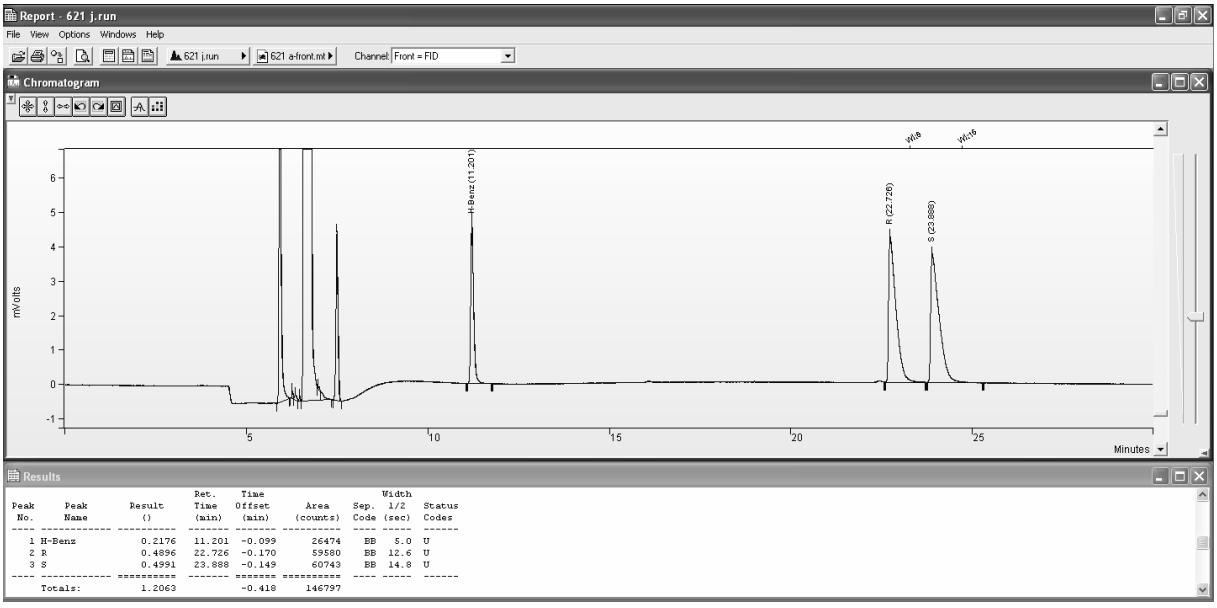
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1438	11.213	-0.087	17181	BB	4.9	U
2	R	0.3870	22.795	-0.055	46240	BB	11.9	U
3	S	0.3959	23.962	-0.038	47302	BB	13.6	U
	Totals:	0.9267		-0.180	110723			

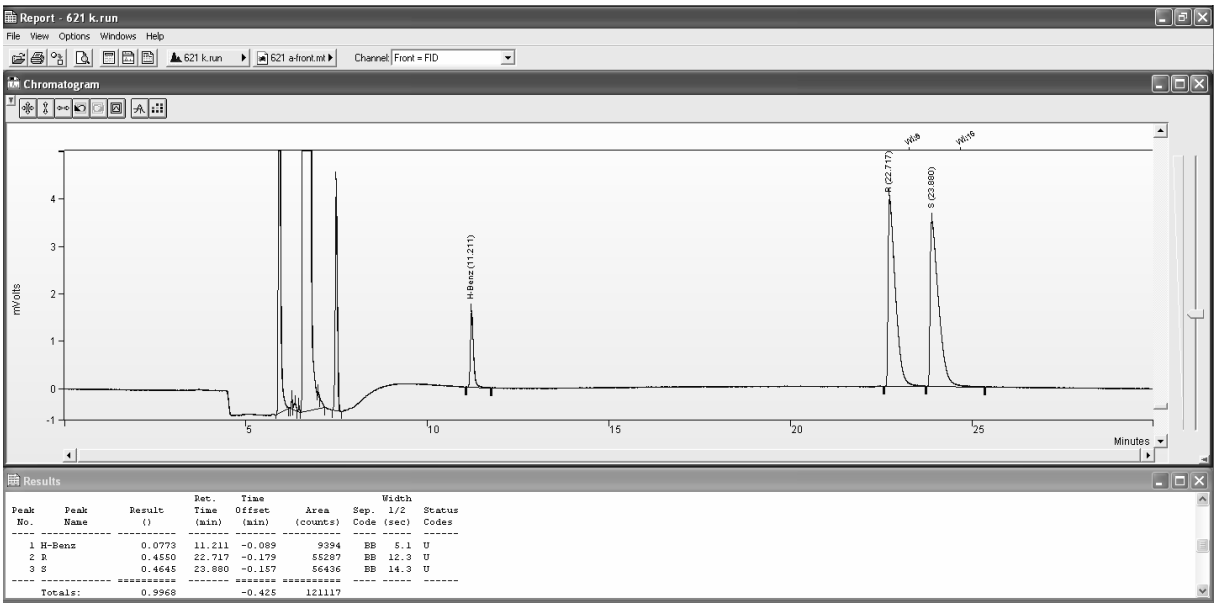


Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1568	11.207	-0.093	18861	BB	5.0	U
2	R	0.4154	22.767	-0.129	49976	BB	12.0	U
3	S	0.4263	23.926	-0.111	51286	BB	13.9	U
	Totals:	0.9985		-0.333	120123			

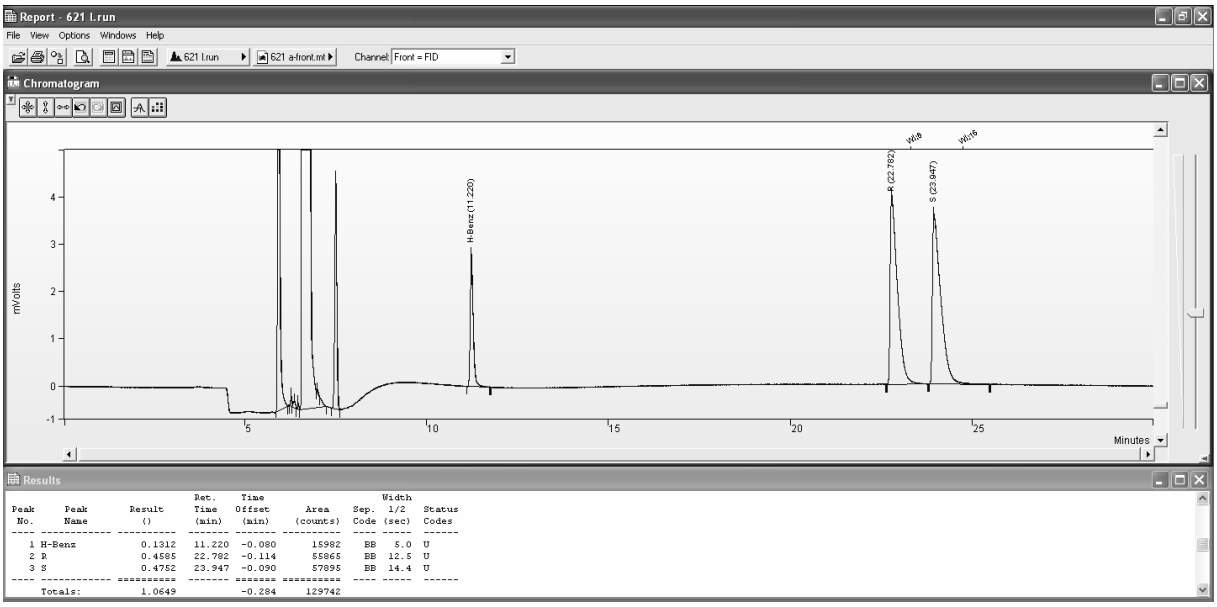

Report - 621 h.run
File View Options Windows Help
621 h.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.206)
R (22.734)
S (23.897)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1762 11.206 -0.094 21345 BB 5.0 U
2 R 0.4890 22.734 -0.162 59236 BB 12.6 U
3 S 0.4986 23.897 -0.140 60395 BB 14.6 U
Totals: 1.1638 -0.396 140976


Report - 621 i.run
File View Options Windows Help
621 i.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.212)
R (22.775)
S (23.939)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1581 11.212 -0.088 19210 BB 5.0 U
2 R 0.4135 22.775 -0.121 50248 BB 12.1 U
3 S 0.4236 23.939 -0.098 51468 BB 13.9 U
Totals: 0.9952 -0.307 120926

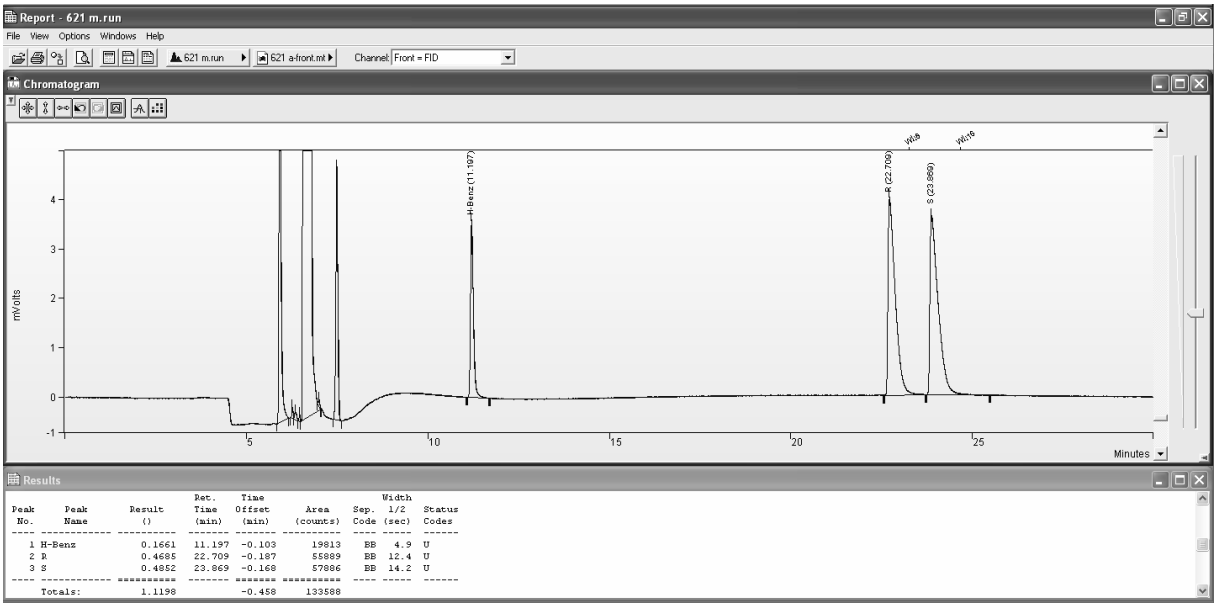

Report - 621 j.run
File View Options Windows Help
621 j.run
621 a-front.mt
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.201)
R (22.726)
S (23.888)
Wid
Wid
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2176 11.201 -0.099 26474 BB 5.0 U
2 R 0.4896 22.726 -0.170 59580 BB 12.6 U
3 S 0.4991 23.888 -0.149 60743 BB 14.8 U
Totals: 1.2063 -0.418 146797



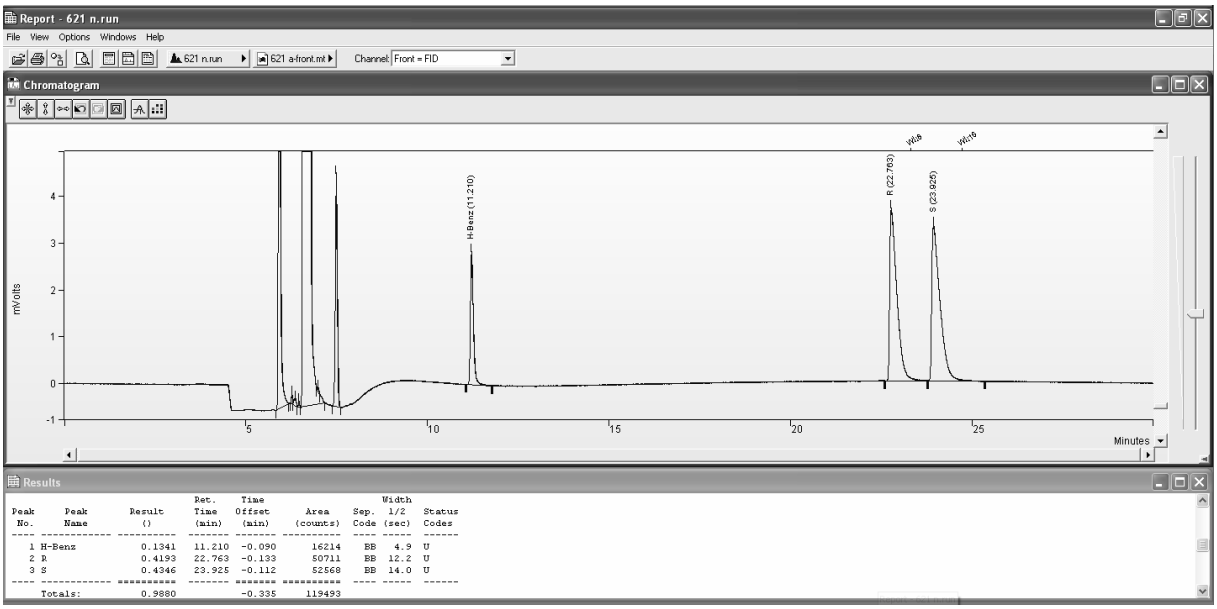
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0773	11.211	-0.089	9394	BB	5.1	U
2	R	0.4550	22.717	-0.179	55287	BB	12.3	U
3	S	0.4645	23.880	-0.157	56436	BB	14.3	U
Totals:		0.9968		-0.425	121117			

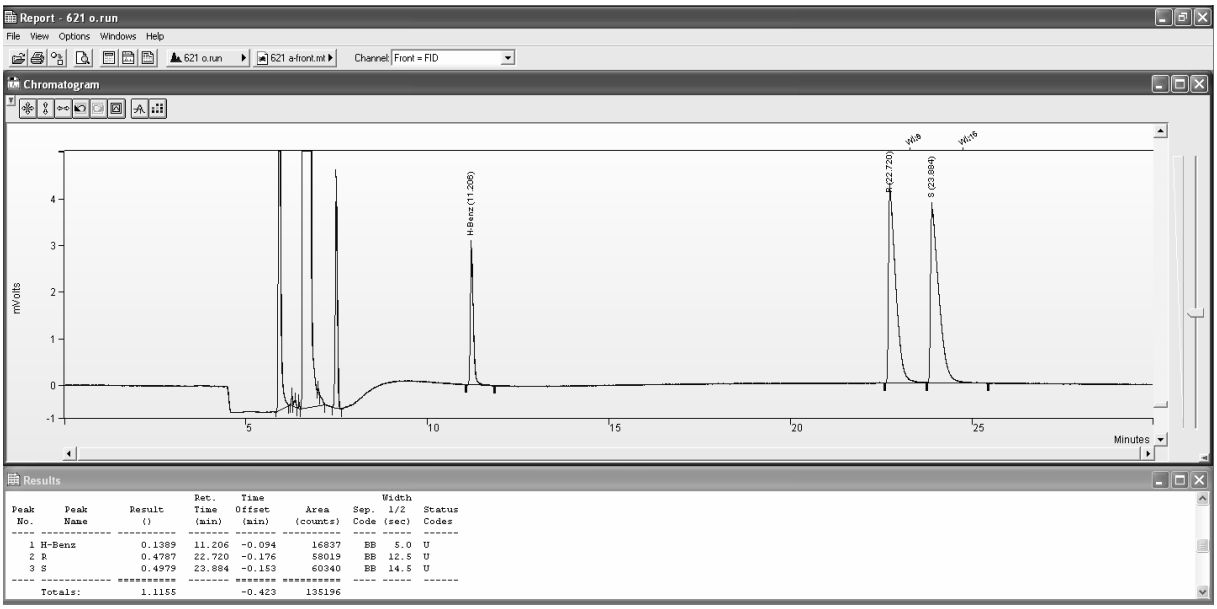


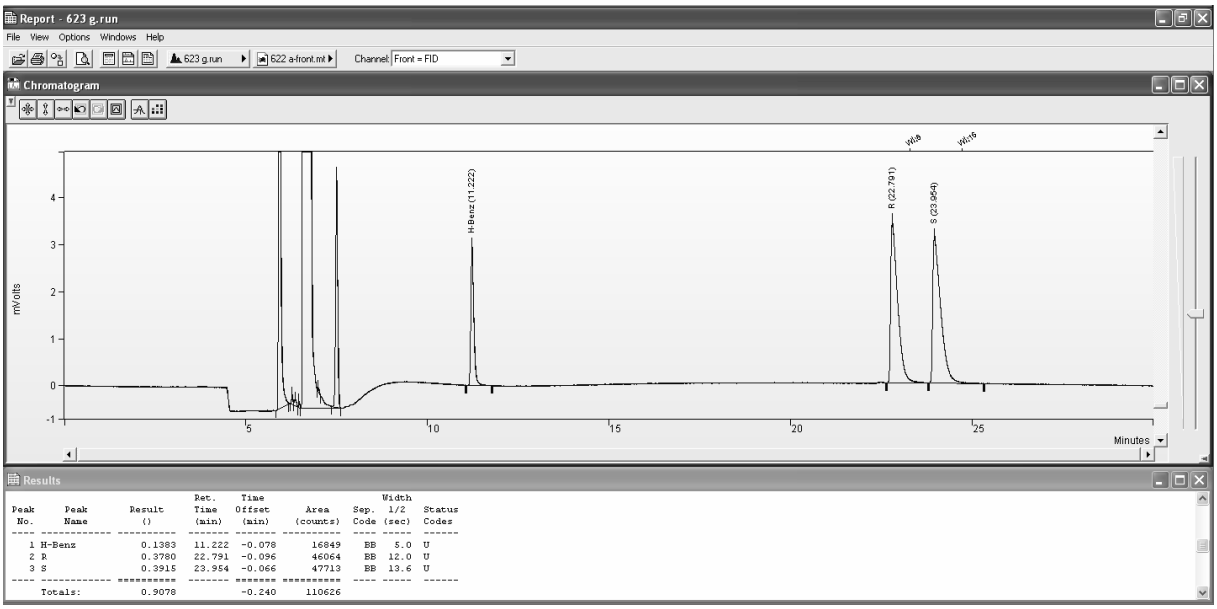
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1312	11.220	-0.080	15982	BB	5.0	U
2	R	0.4585	22.782	-0.114	55965	BB	12.5	U
3	S	0.4752	23.947	-0.090	57895	BB	14.4	U
Totals:		1.0649		-0.284	129742			

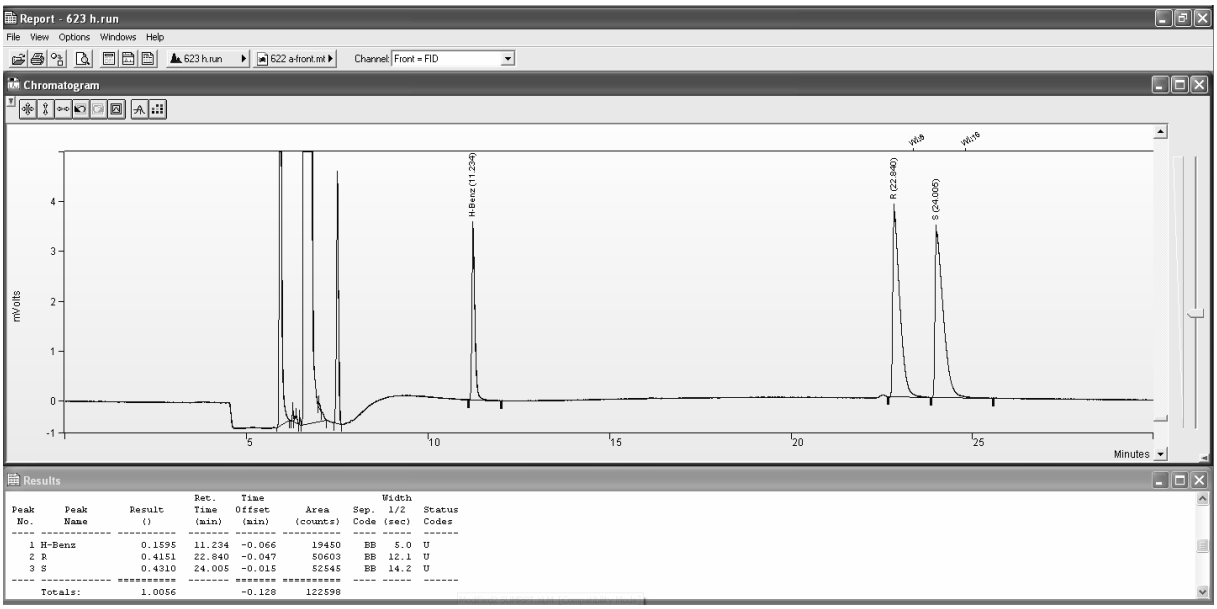


Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1661	11.197	-0.103	19813	BB	4.9	U
2	R	0.4685	22.709	-0.187	55889	BB	12.4	U
3	S	0.4852	23.869	-0.168	57886	BB	14.2	U
Totals:		1.1198		-0.458	133588			

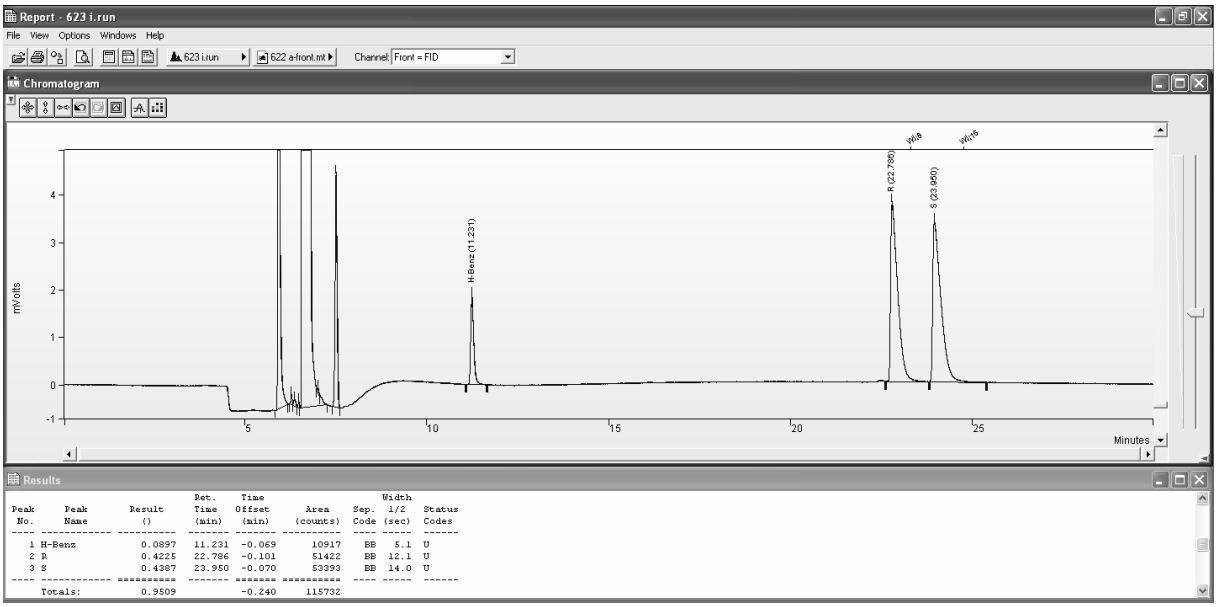

Report - 621 n.run
File View Options Windows Help
621 n.run
621 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.210)
R (22.763)
S (23.925)
Wid8
Wid16
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1341 11.210 -0.090 16214 BB 4.9 U
2 R 0.4193 22.763 -0.133 50711 BB 12.2 U
3 S 0.4346 23.925 -0.112 52568 BB 14.0 U
Totals: 0.9880 -0.335 119493


Report - 621 o.run
File View Options Windows Help
621 o.run
621 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.206)
R (22.720)
S (23.884)
Wid8
Wid16
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1389 11.206 -0.094 16837 BB 5.0 U
2 R 0.4787 22.720 -0.176 58019 BB 12.5 U
3 S 0.4979 23.884 -0.153 60340 BB 14.5 U
Totals: 1.1155 -0.423 135196

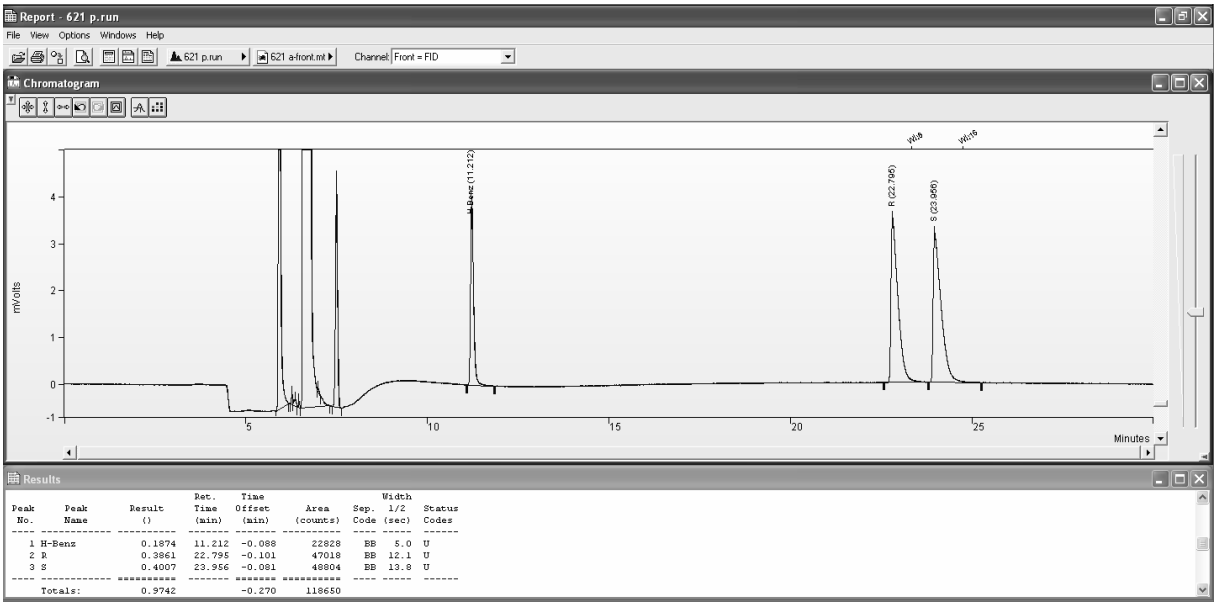

Report - 623 g.run
File View Options Windows Help
623 g.run
622 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz (11.222)
R (22.791)
S (23.954)
Wid8
Wid16
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1383 11.222 -0.078 16849 BB 5.0 U
2 R 0.3780 22.791 -0.096 46064 BB 12.0 U
3 S 0.3915 23.954 -0.066 47713 BB 13.6 U
Totals: 0.9078 -0.240 110626



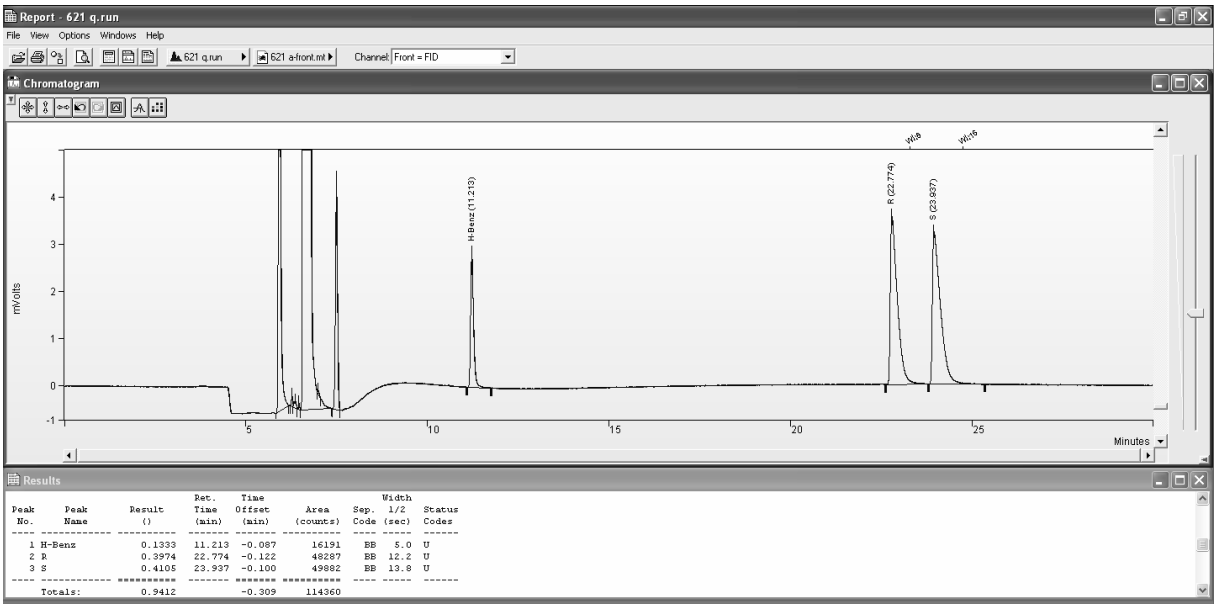
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1595	11.234	-0.066	19450	BB	5.0	U
2	R	0.4151	22.840	-0.047	50603	BB	12.1	U
3	S	0.4310	24.005	-0.015	52545	BB	14.2	U
	Totals:	1.0056		-0.128	122598			

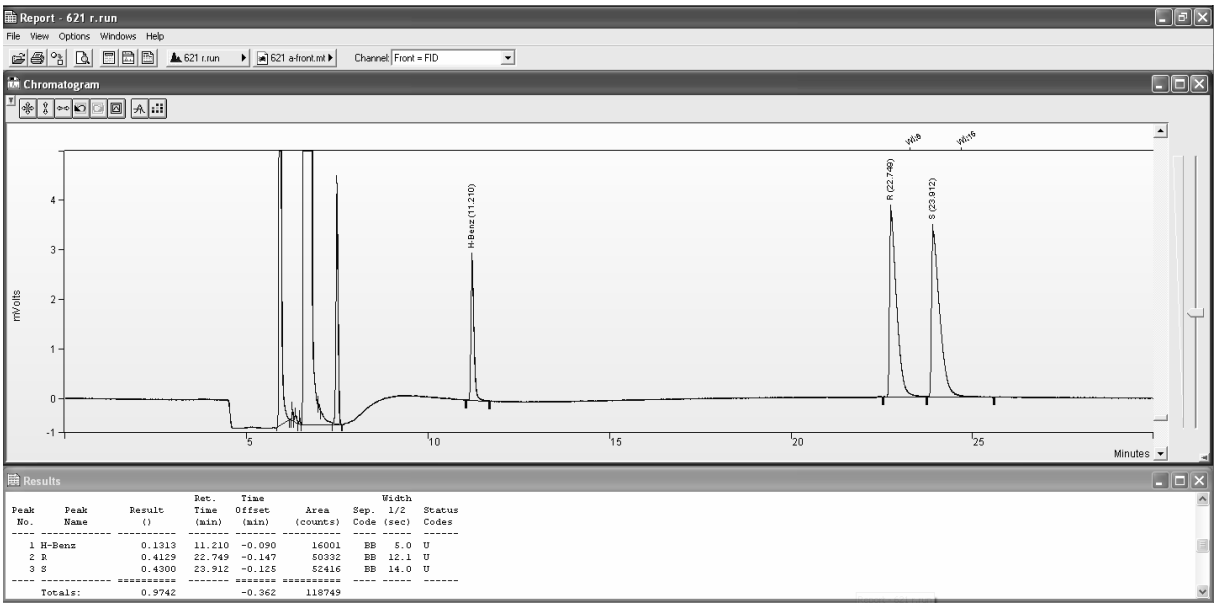


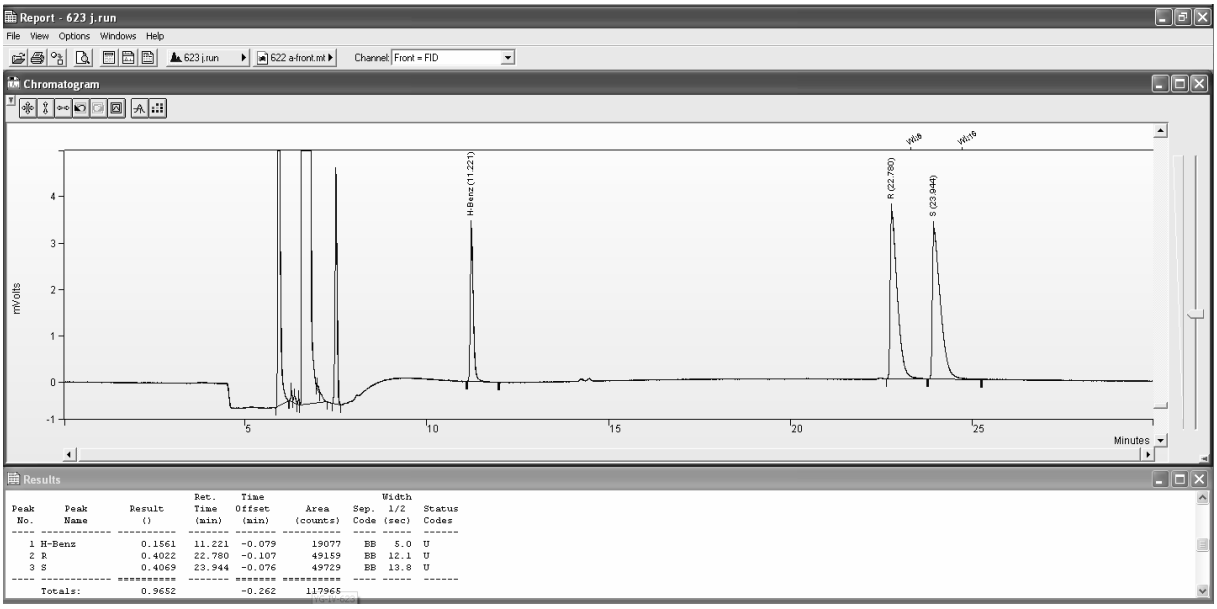
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.0897	11.231	-0.069	10917	BB	5.1	U
2	R	0.4225	22.786	-0.101	51422	BB	12.1	U
3	S	0.4387	23.950	-0.070	53393	BB	14.0	U
	Totals:	0.9509		-0.240	115732			

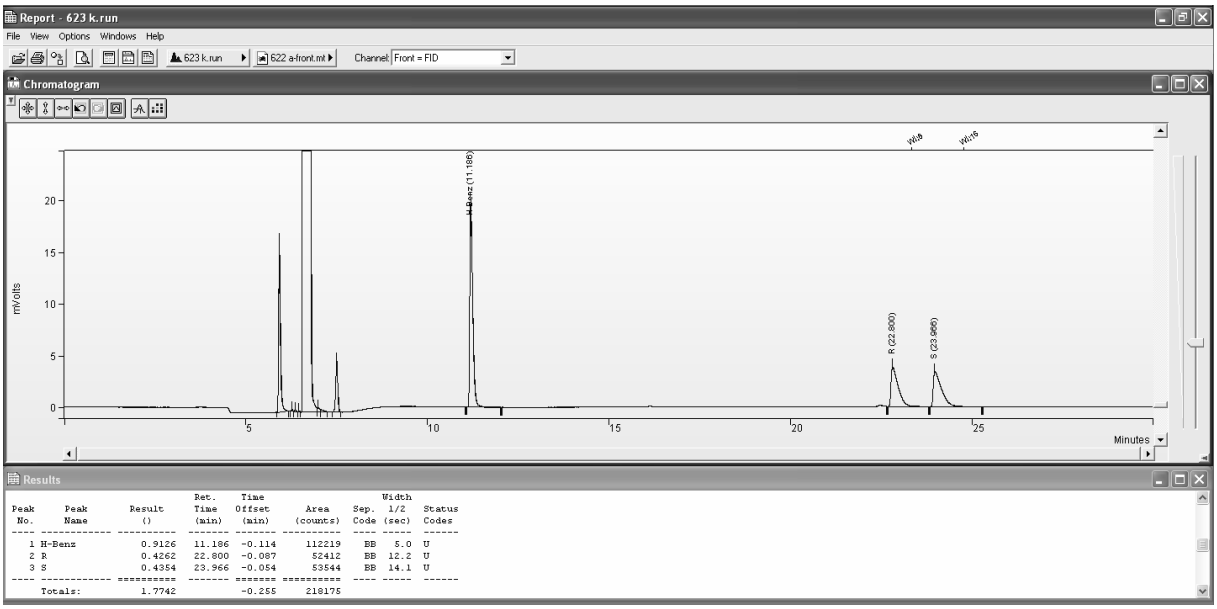


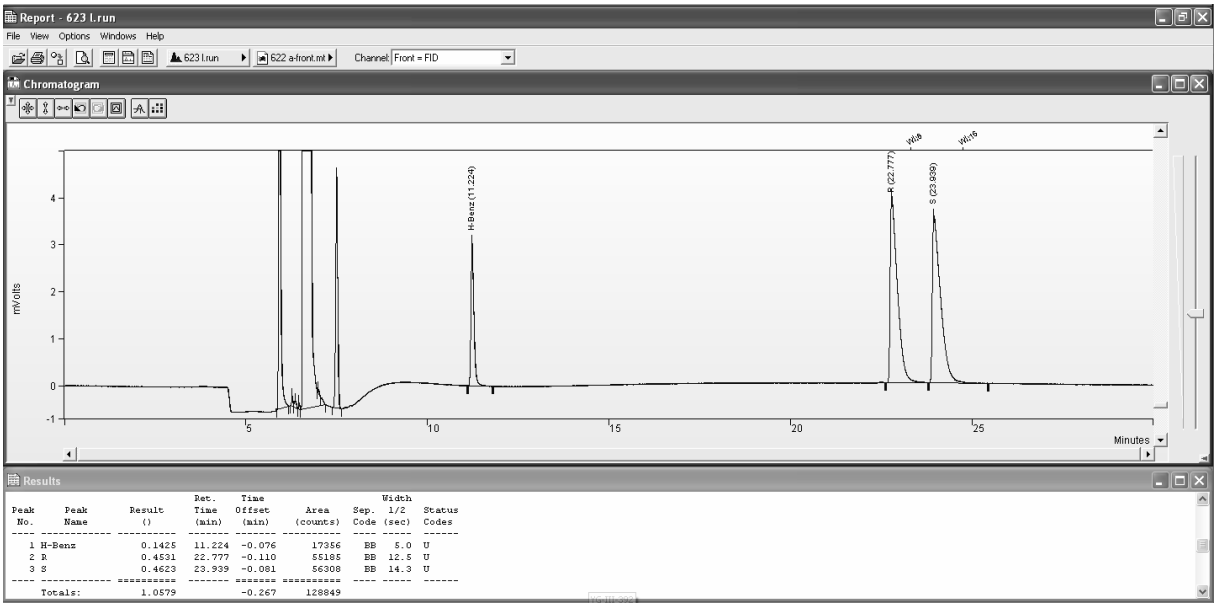
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.1874	11.212	-0.088	22828	BB	5.0	U
2	R	0.3861	22.795	-0.101	47018	BB	12.1	U
3	S	0.4007	23.956	-0.081	48804	BB	13.8	U
	Totals:	0.9742		-0.270	118650			


Report - 621 q.run
File View Options Windows Help
621 q.run
621 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz(11.213)
R (22.774)
S (23.937)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1333 11.213 -0.087 16191 BB 5.0 U
2 R 0.3974 22.774 -0.122 48287 BB 12.2 U
3 S 0.4105 23.937 -0.100 49882 BB 13.8 U
Totals: 0.9412 -0.309 114360

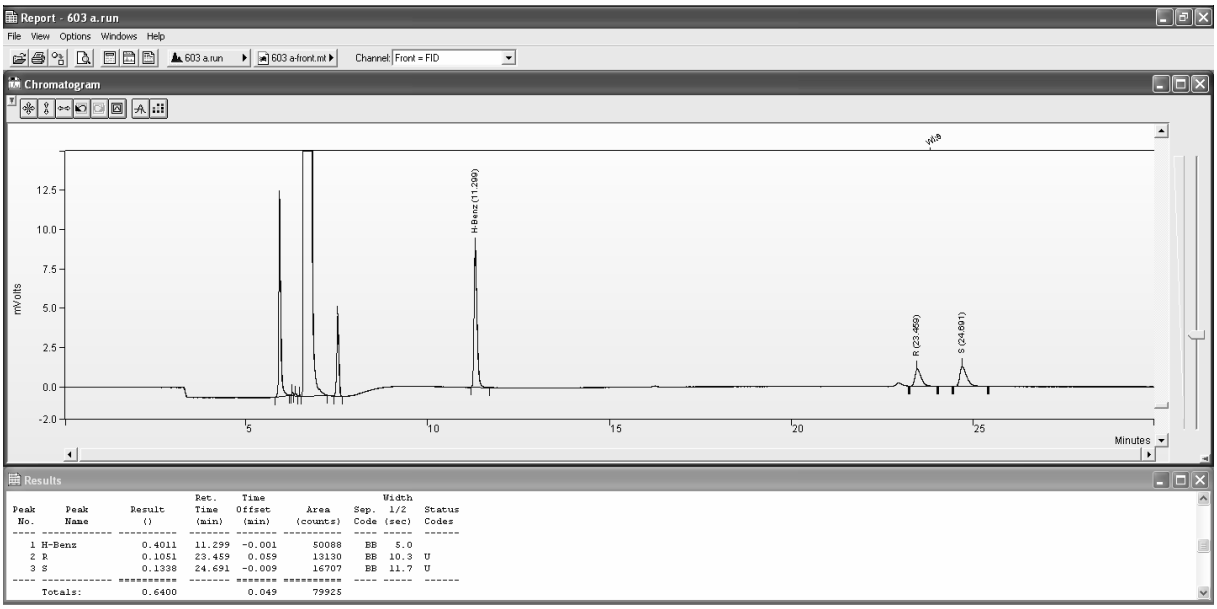

Report - 621 r.run
File View Options Windows Help
621 r.run
621 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz(11.210)
R (22.749)
S (23.912)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1313 11.210 -0.090 16001 BB 5.0 U
2 R 0.4129 22.749 -0.147 50332 BB 12.1 U
3 S 0.4300 23.912 -0.125 52416 BB 14.0 U
Totals: 0.9742 -0.362 118749

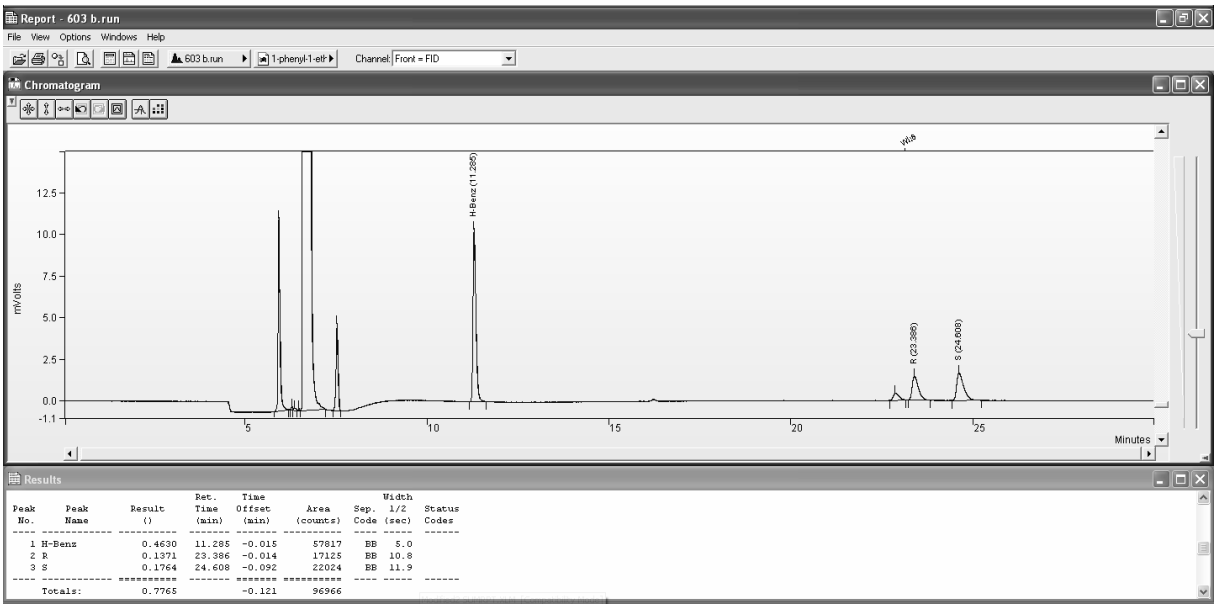

Report - 623 j.run
File View Options Windows Help
623 j.run
622 a-front.mt
Channel: Front = FID
Chromatogram
H-Benz(11.221)
R (22.780)
S (23.944)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1561 11.221 -0.079 19077 BB 5.0 U
2 R 0.4022 22.780 -0.107 49159 BB 12.1 U
3 S 0.4069 23.944 -0.076 49729 BB 13.8 U
Totals: 0.9652 -0.262 117965

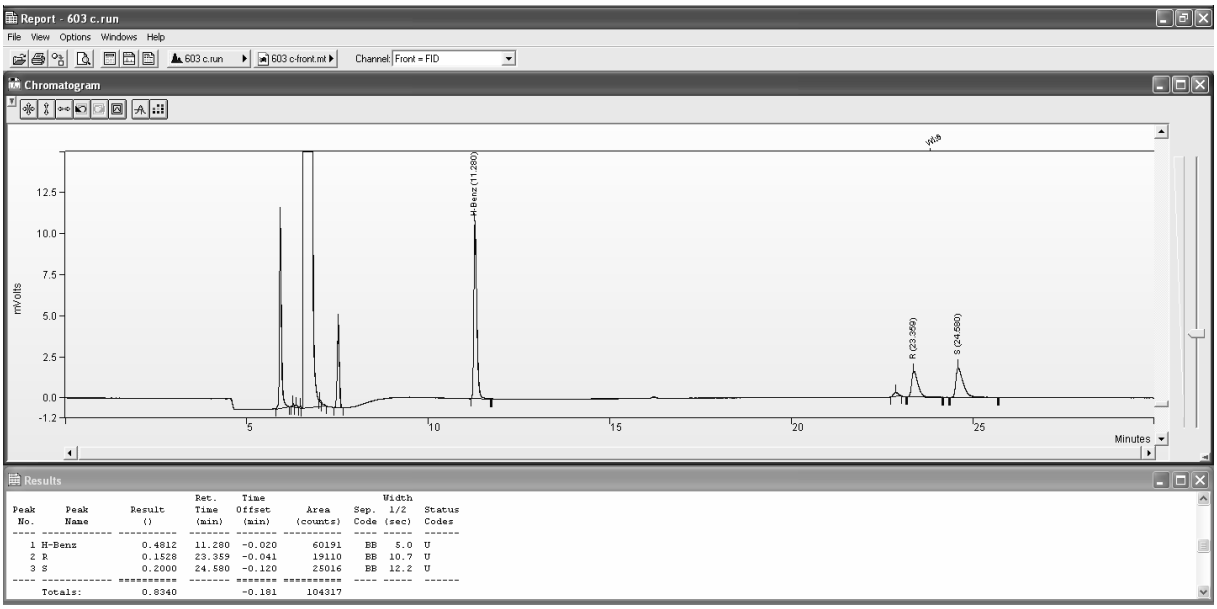

Report - 623 k.run
File View Options Windows Help
623 k.run
622 a-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.186)
R (22.800)
S (23.966)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.9126 11.186 -0.114 112219 BB 5.0 U
2 R 0.4262 22.800 -0.087 52412 BB 12.2 U
3 S 0.4354 23.966 -0.054 53544 BB 14.1 U
Totals: 1.7742 -0.255 218175

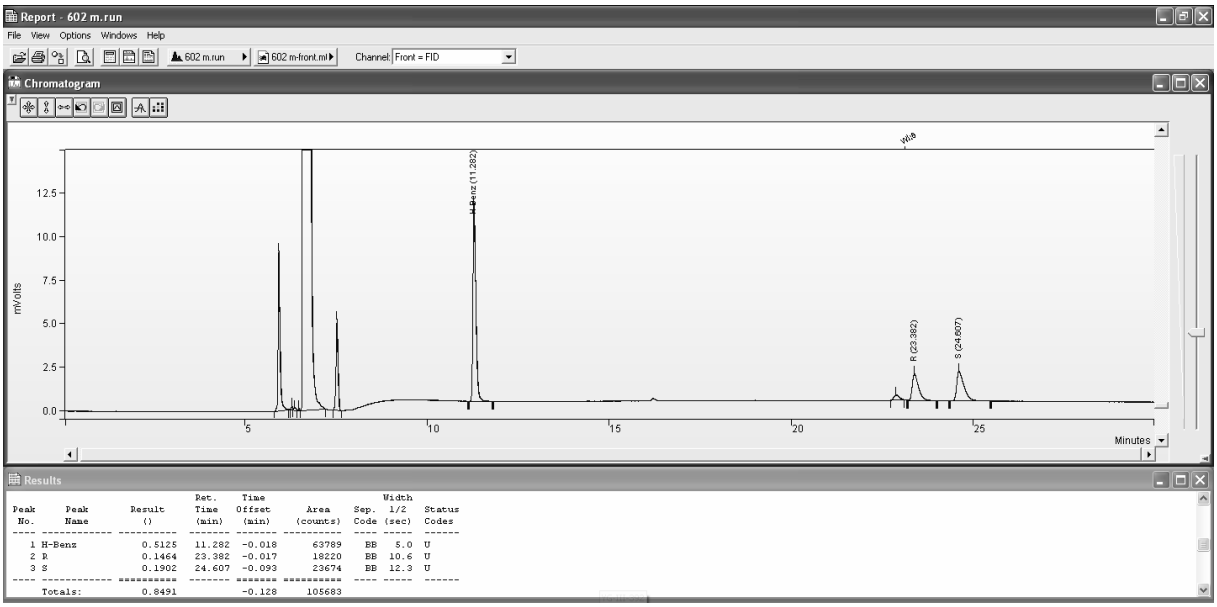

Report - 623 l.run
File View Options Windows Help
623 l.run
622 a-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.224)
R (22.777)
S (23.939)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.1425 11.224 -0.076 17356 BB 5.0 U
2 R 0.4531 22.777 -0.110 55185 BB 12.5 U
3 S 0.4623 23.939 -0.081 56308 BB 14.3 U
Totals: 1.0579 -0.267 128849

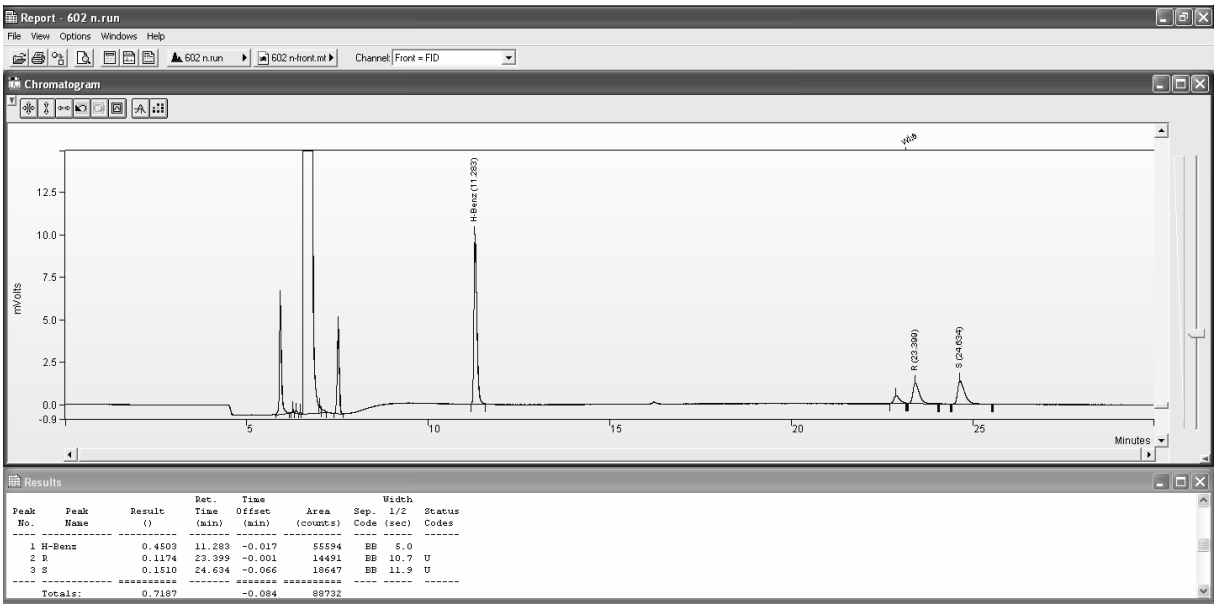
III.8 Sup. Figure 6

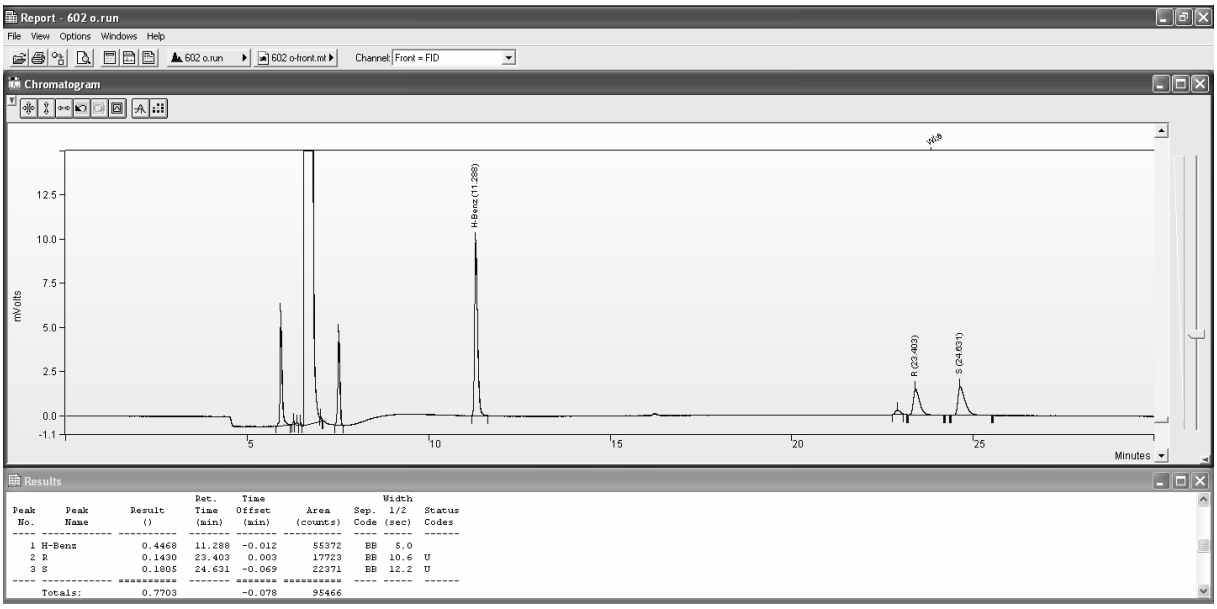




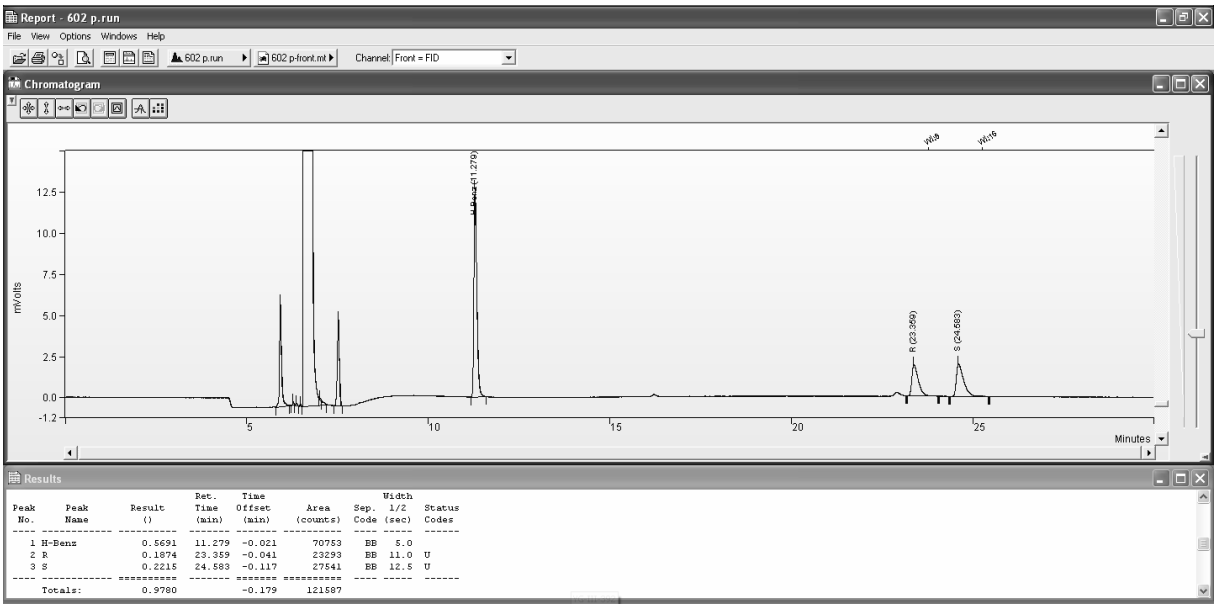

Report - 603 c.run
File View Options Windows Help
603 c.run
603 c-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.280)
R (23.399)
S (24.580)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4812 11.280 -0.020 60191 BB 5.0 U
2 R 0.1528 23.359 -0.041 19110 BB 10.7 U
3 S 0.2000 24.580 -0.120 25016 BB 12.2 U
Totals: 0.8340 -0.181 104317


Report - 602 m.run
File View Options Windows Help
602 m.run
602 m-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.282)
R (23.382)
S (24.607)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5125 11.282 -0.018 63789 BB 5.0 U
2 R 0.1464 23.382 -0.017 18220 BB 10.6 U
3 S 0.1902 24.607 -0.093 23674 BB 12.3 U
Totals: 0.8491 -0.128 105683

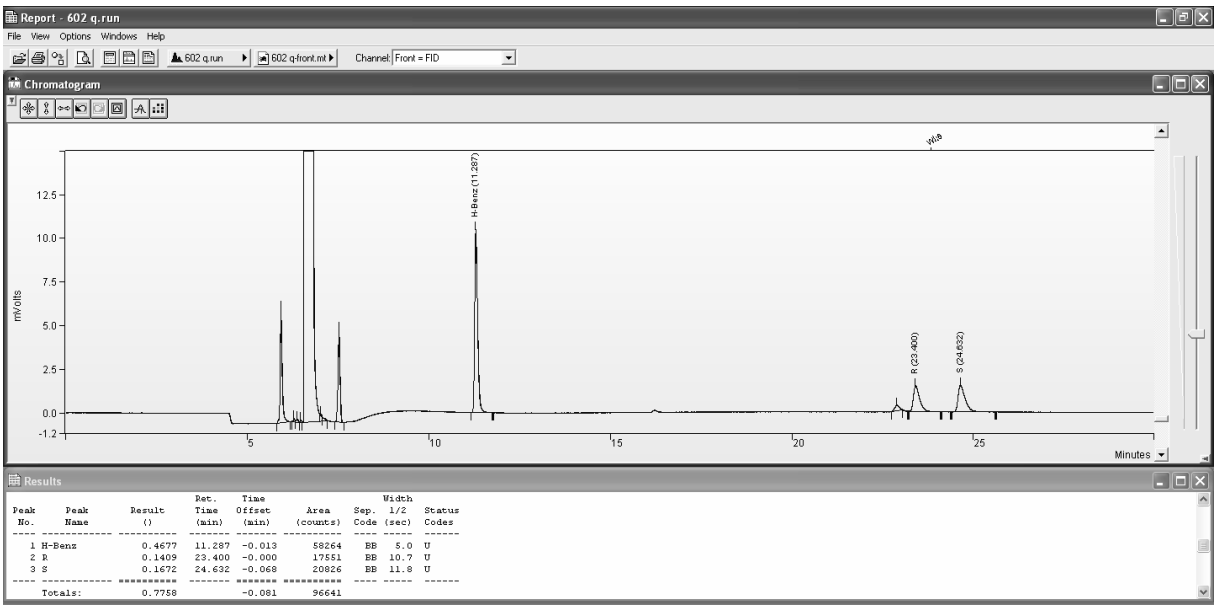

Report - 602 n.run
File View Options Windows Help
602 n.run
602 m-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.283)
R (23.399)
S (24.634)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4503 11.283 -0.017 55594 BB 5.0
2 R 0.1174 23.399 -0.001 14491 BB 10.7 U
3 S 0.1510 24.634 -0.066 18647 BB 11.9 U
Totals: 0.7187 -0.084 88732



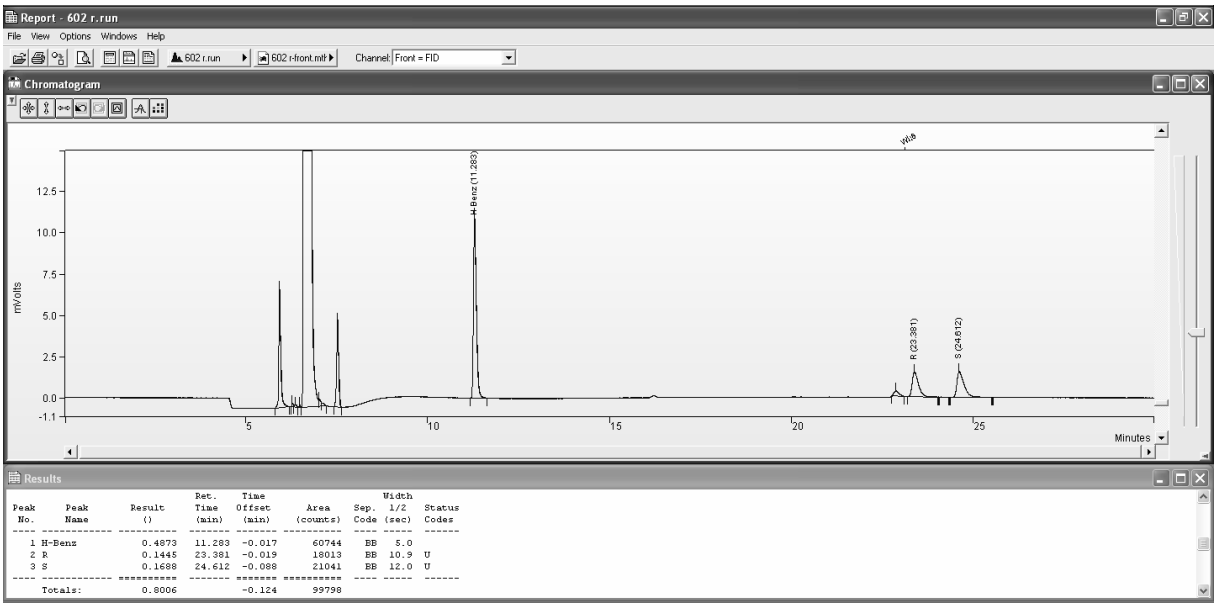
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.4468	11.288	-0.012	55372	BB	5.0	
2	R	0.1430	23.403	0.003	17723	BB	10.6	U
3	S	0.1805	24.631	-0.069	22371	BB	12.2	U
	Totals:	0.7703		-0.078	95466			

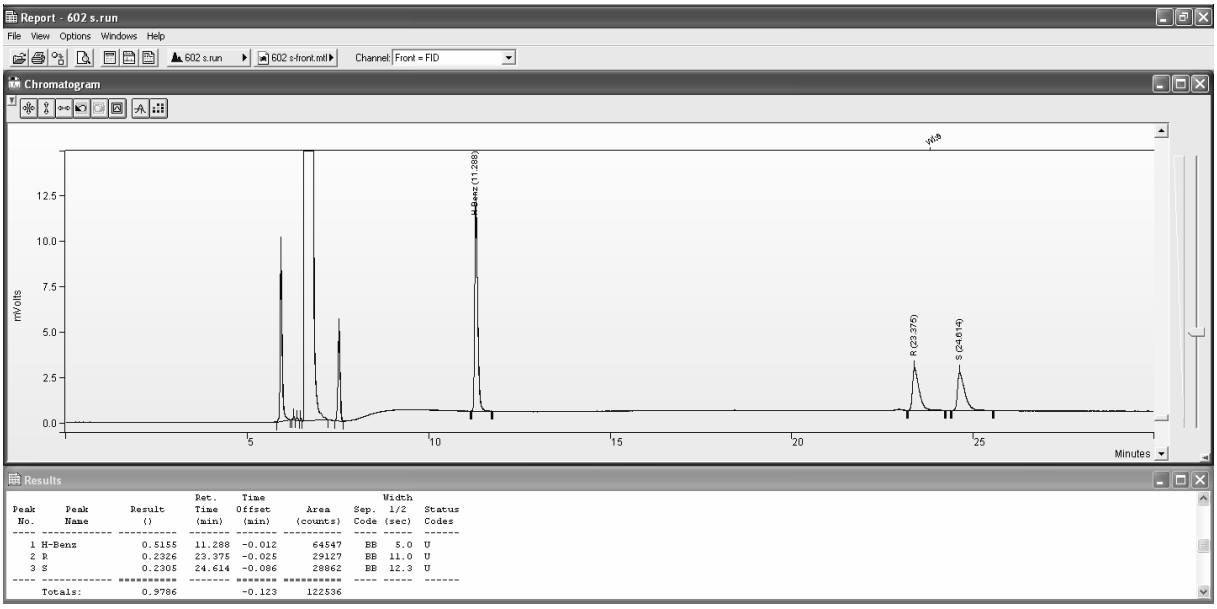


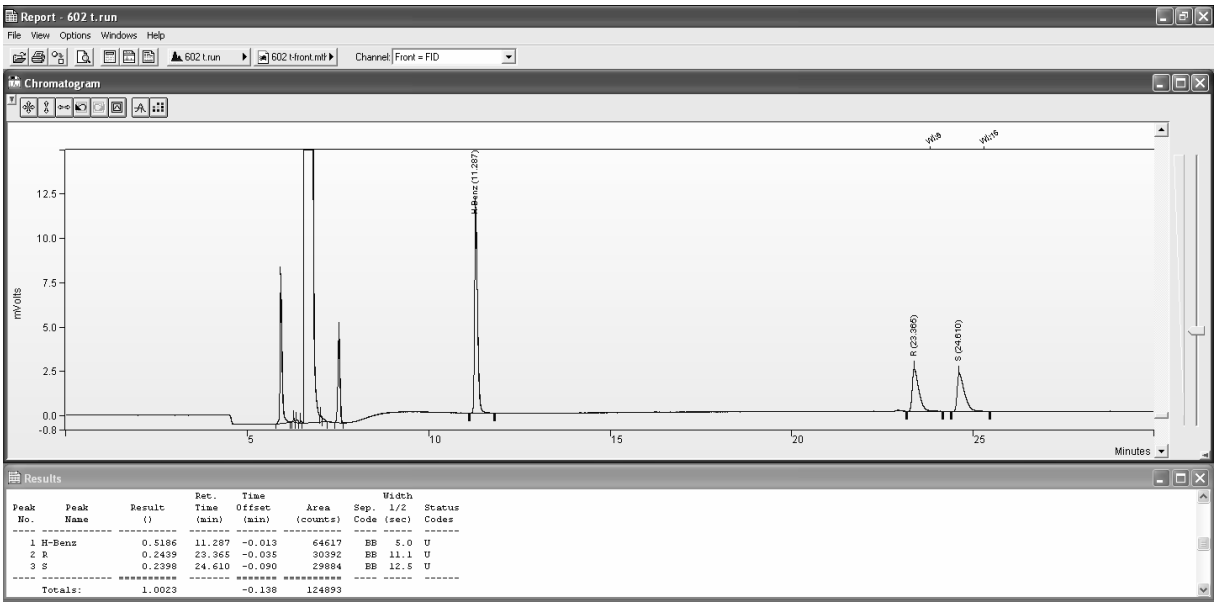
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.5691	11.279	-0.021	70753	BB	5.0	
2	R	0.1874	23.359	-0.041	23293	BB	11.0	U
3	S	0.2215	24.583	-0.117	27541	BB	12.5	U
	Totals:	0.9780		-0.179	121587			

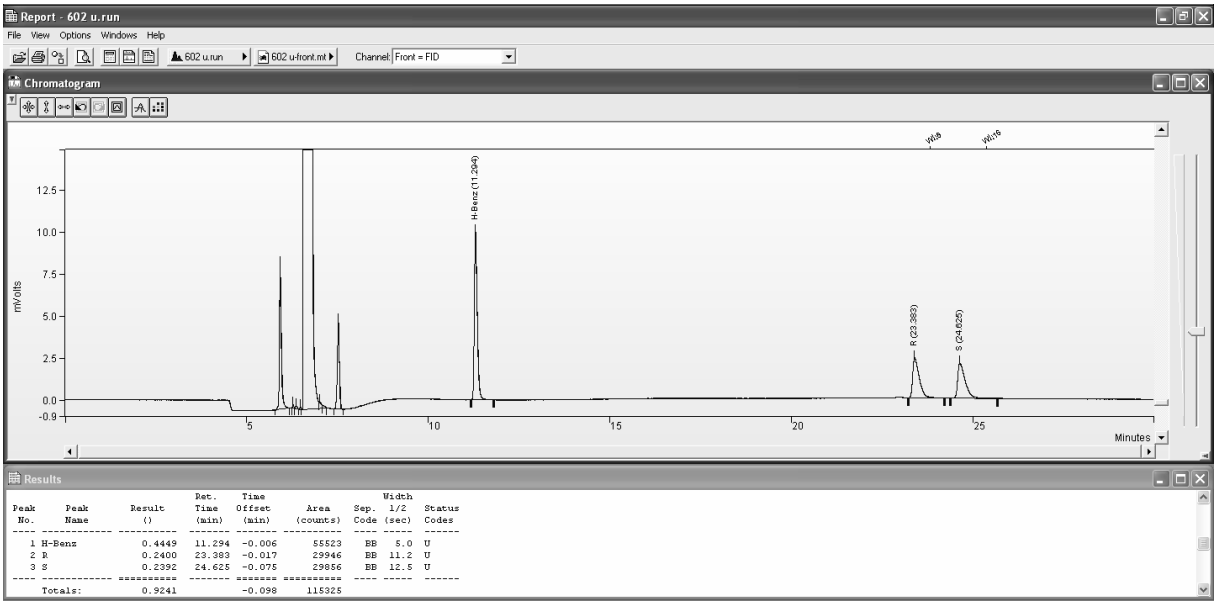


Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.4677	11.287	-0.013	58264	BB	5.0	U
2	R	0.1409	23.400	-0.000	17551	BB	10.7	U
3	S	0.1672	24.632	-0.068	20826	BB	11.8	U
	Totals:	0.7758		-0.081	96641			

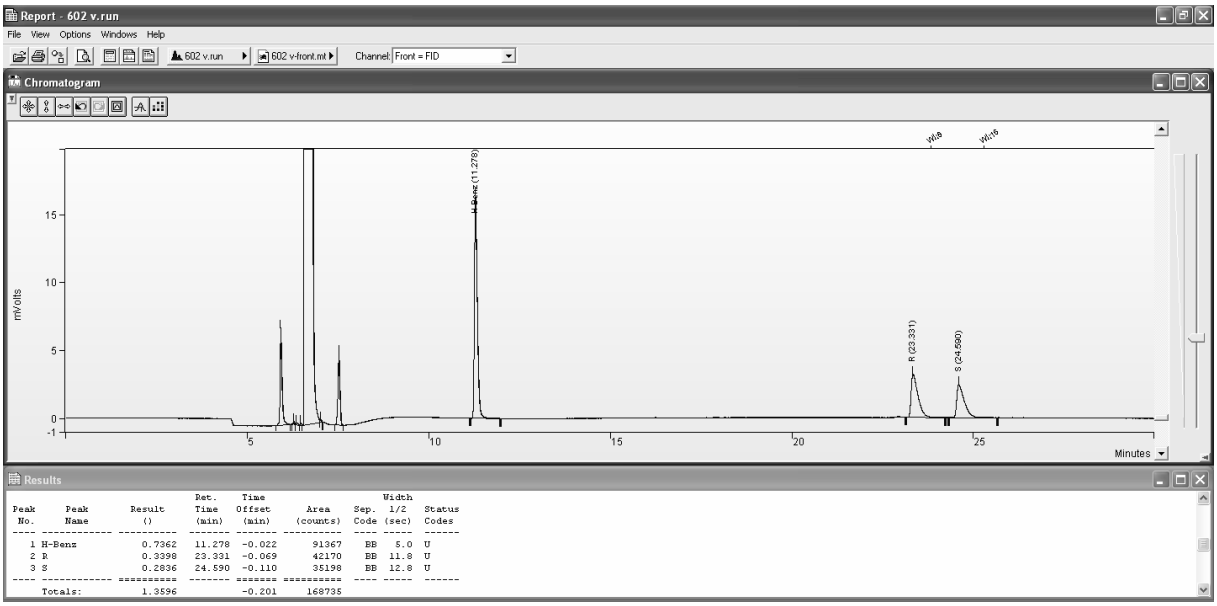

Report - 602 r.run
File View Options Windows Help
602 r.run
602 r-front.mtf
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.283)
R (23.381)
S (24.612)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4873 11.283 -0.017 60744 BB 5.0
2 R 0.1445 23.381 -0.019 18013 BB 10.9 U
3 S 0.1688 24.612 -0.088 21041 BB 12.0 U
Totals: 0.8006 -0.124 99798


Report - 602 s.run
File View Options Windows Help
602 s.run
602 s-front.mtf
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.288)
R (23.375)
S (24.614)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5155 11.288 -0.012 64547 BB 5.0 U
2 R 0.2326 23.375 -0.025 29127 BB 11.0 U
3 S 0.2305 24.614 -0.086 28862 BB 12.3 U
Totals: 0.9786 -0.123 122536

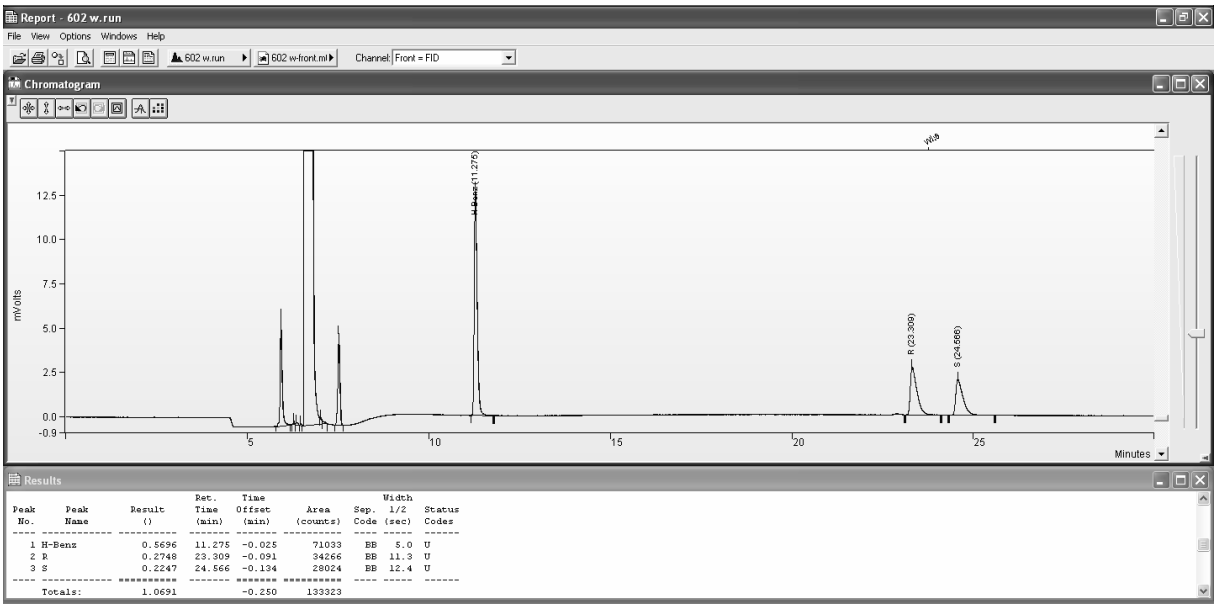

Report - 602 t.run
File View Options Windows Help
602 t.run
602 t-front.mtf
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz (11.287)
R (23.366)
S (24.610)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5186 11.287 -0.013 64617 BB 5.0 U
2 R 0.2439 23.365 -0.035 30392 BB 11.1 U
3 S 0.2398 24.610 -0.090 29884 BB 12.5 U
Totals: 1.0023 -0.138 124893

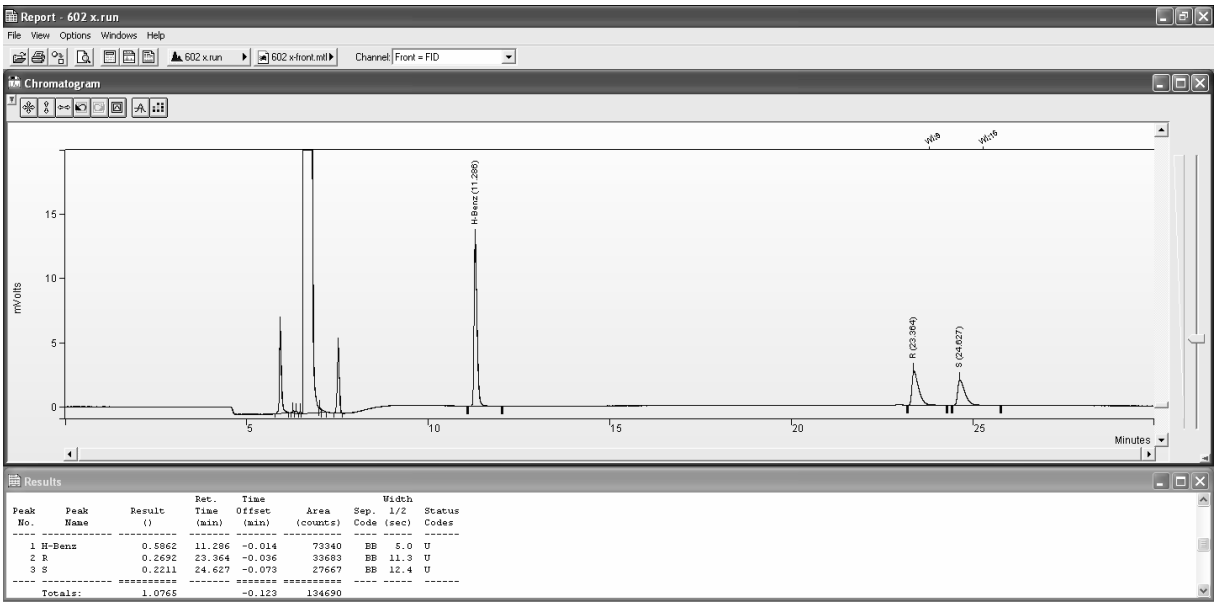


Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.4449	11.294	-0.006	55523	BB	5.0	U
2	R	0.2400	23.383	-0.017	29946	BB	11.2	U
3	S	0.2392	24.625	-0.075	29856	BB	12.5	U
	Totals:	0.9241		-0.098	115325			

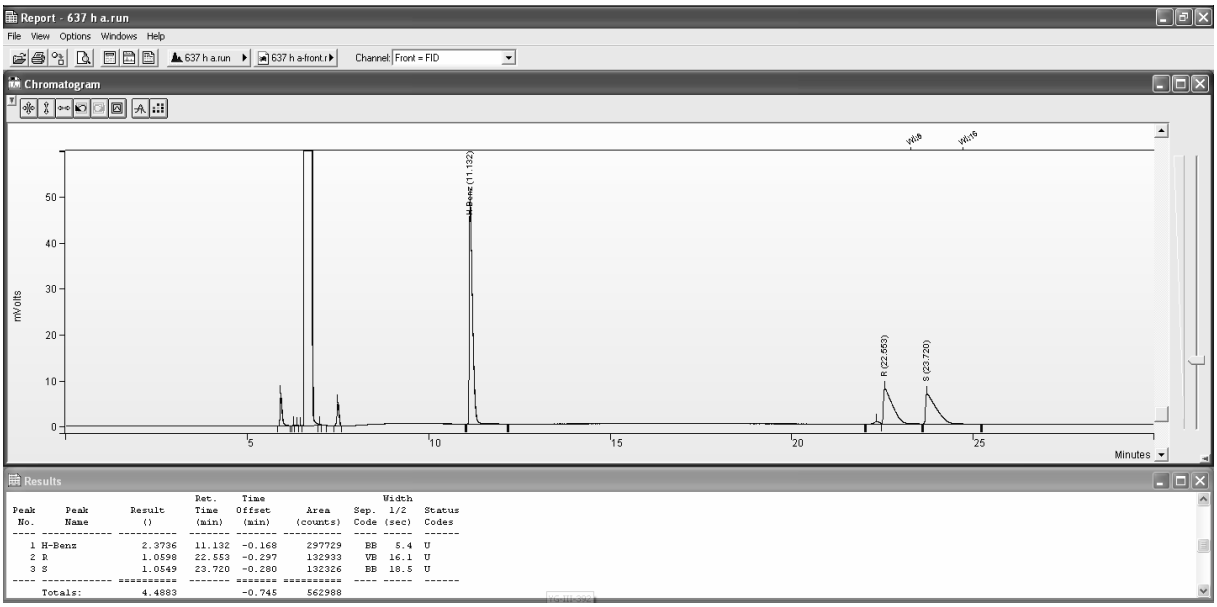


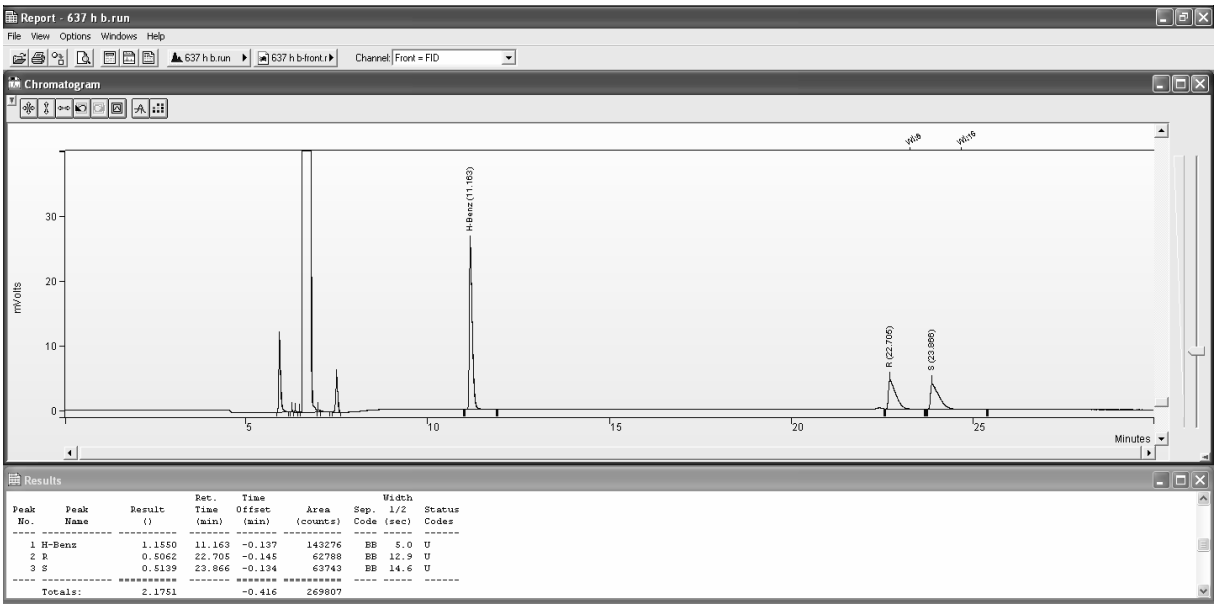
Peak No.	Peak Name	Result ()	Ret. Time (min)	Time Offset (min)	Area (counts)	Sep. Code	Width 1/2 (sec)	Status Codes
1	H-Benz	0.7362	11.278	-0.022	91367	BB	5.0	U
2	R	0.3398	23.331	-0.069	42170	BB	11.8	U
3	S	0.2836	24.590	-0.110	35198	BB	12.8	U
	Totals:	1.3596		-0.201	168735			

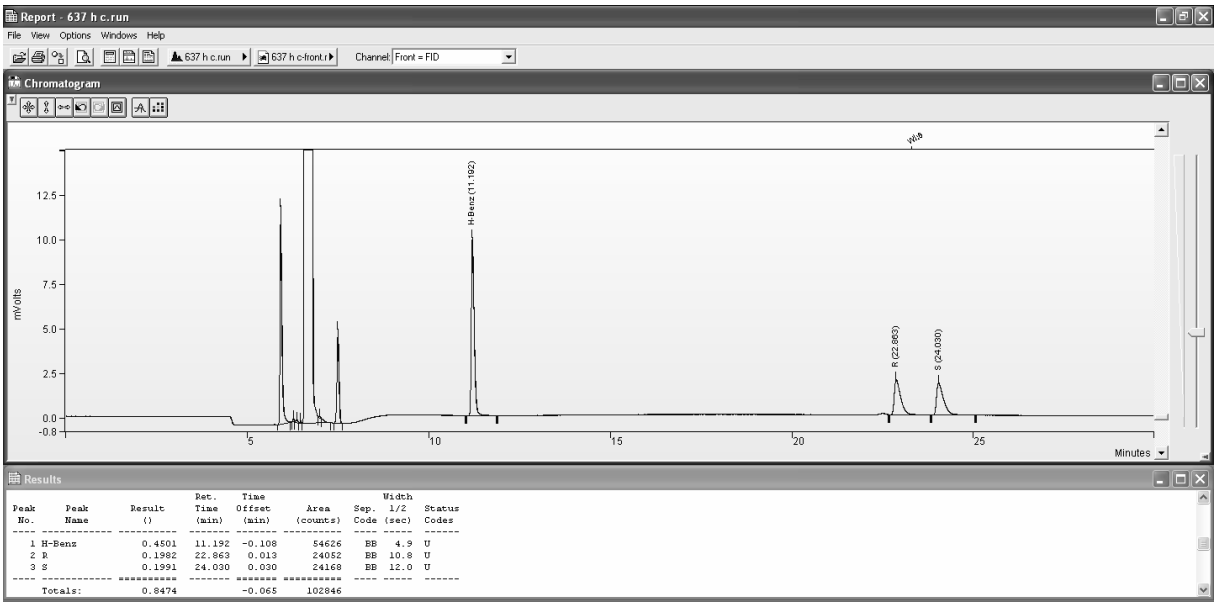

Report - 602 w.run
File View Options Windows Help
602 w.run
602 w-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.275)
R (23.309)
S (24.666)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5696 11.275 -0.025 71033 BB 5.0 U
2 R 0.2748 23.309 -0.091 34266 BB 11.3 U
3 S 0.2247 24.566 -0.134 28024 BB 12.4 U
Totals: 1.0691 -0.250 133323

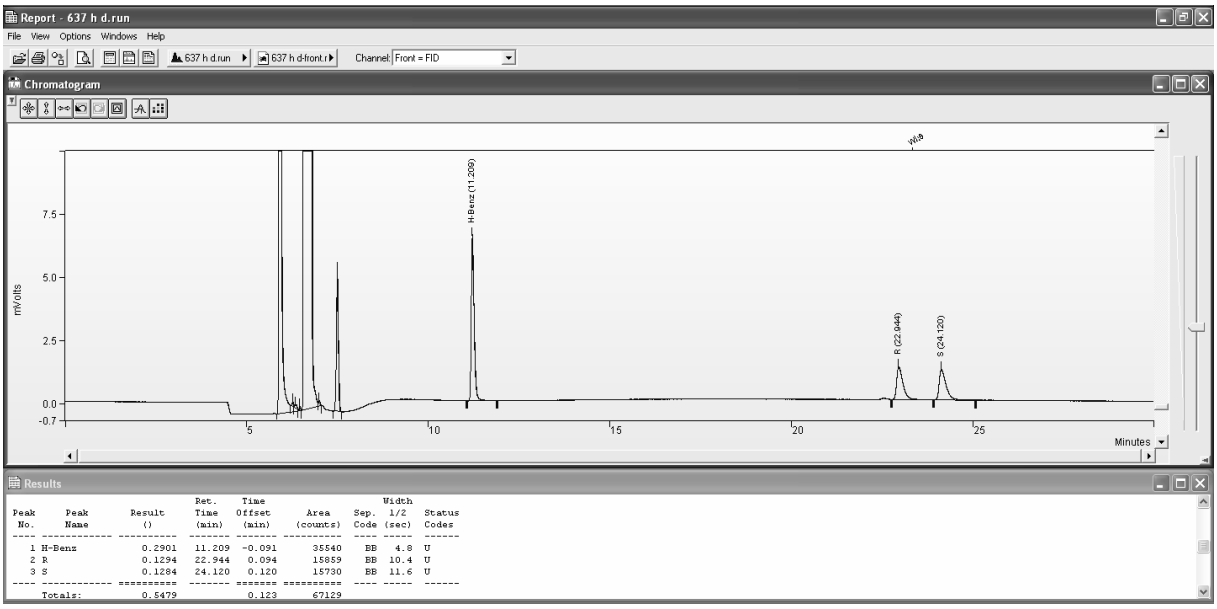

Report - 602 x.run
File View Options Windows Help
602 x.run
602 x-front.ml
Channel: Front = FID
Chromatogram
mVolts
Minutes
H-Benz(11.286)
R (23.364)
S (24.627)
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.5862 11.286 -0.014 73340 BB 5.0 U
2 R 0.2692 23.364 -0.036 33683 BB 11.3 U
3 S 0.2211 24.627 -0.073 27667 BB 12.4 U
Totals: 1.0765 -0.123 134690

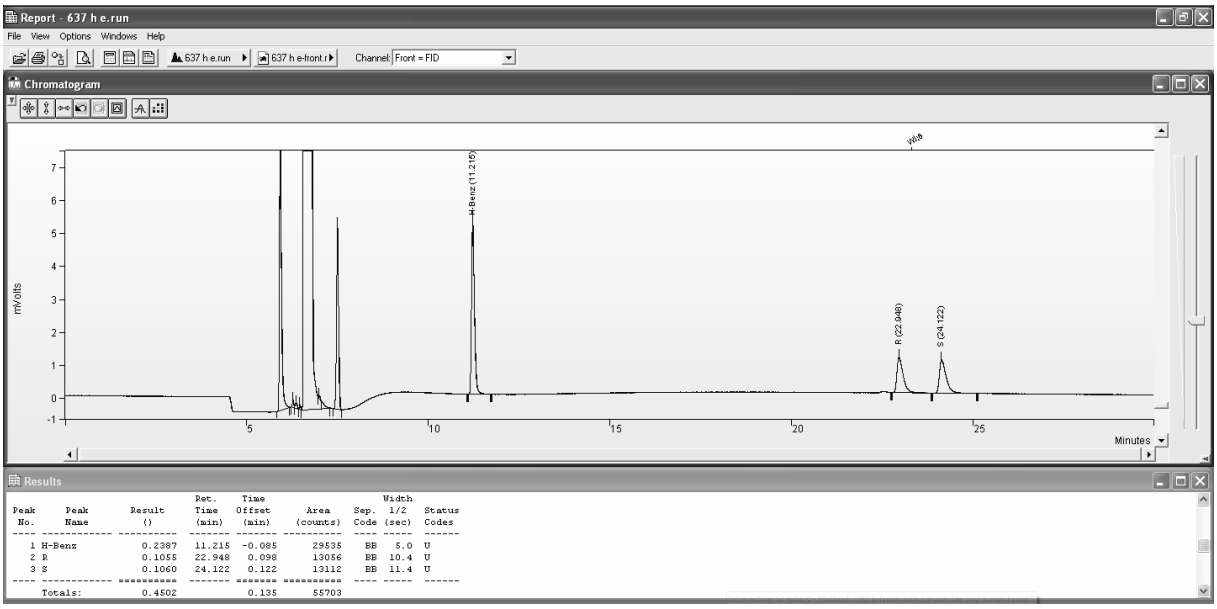
III.9 Benzaldehyde/1-phenyl-1-ethanol calibration curve






Report - 637 h c.run
File View Options Windows Help
637 h c.run
637 h c-front.r
Channel: Front = FID
Chromatogram
WB
H-Benz (11.192)
R (22.863)
S (24.030)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.4501 11.192 -0.108 54626 BB 4.9 U
2 R 0.1982 22.863 0.013 24052 BB 10.8 U
3 S 0.1991 24.030 0.030 24168 BB 12.0 U
Totals: 0.8474 -0.065 102846


Report - 637 h d.run
File View Options Windows Help
637 h d.run
637 h d-front.r
Channel: Front = FID
Chromatogram
WB
H-Benz (11.209)
R (22.944)
S (24.120)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2901 11.209 -0.091 35540 BB 4.8 U
2 R 0.1294 22.944 0.094 15859 BB 10.4 U
3 S 0.1284 24.120 0.120 15730 BB 11.6 U
Totals: 0.5479 0.123 67129


Report - 637 h e.run
File View Options Windows Help
637 h e.run
637 h e-front.r
Channel: Front = FID
Chromatogram
WB
H-Benz (11.215)
R (22.948)
S (24.122)
mVolts
Minutes
Results
Peak No. | Peak Name | Result () | Ret. Time (min) | Time Offset (min) | Area (counts) | Sep. Code | Width 1/2 (sec) | Status Codes
1 H-Benz 0.2387 11.215 -0.085 29535 BB 5.0 U
2 R 0.1055 22.948 0.098 13056 BB 10.4 U
3 S 0.1060 24.122 0.122 13112 BB 11.4 U
Totals: 0.4502 0.135 55703

IV: References

1 G. D. Potter, M. C. Baird and S. P. C. Cole, A new series of titanocene dichloride derivatives bearing chiral alkylammonium groups; assessment of their cytotoxic properties, *Inorg. Chim. Acta*, 2010, **364**, 16–22.

2 Y. Geiger, T. Achard, A. Maisse-François and S. Bellemin-Laponnaz, Hyperpositive nonlinear effects in asymmetric catalysis, *Nat. Catal.*, 2020, **3**, 422–426.

3 M. Watanabe and K. Soai, Enantioselective addition of diethylzinc to aldehydes using chiral polymer catalysts possessing a methylene spacer, *J. Chem. Soc., Perkin Trans. 1*, 1994, 837–842.

4 C. D.-T. Nielsen and J. Burés, Visual kinetic analysis, *Chem. Sci.*, 2019, **10**, 348–353.

5 M. Kitamura, S. Suga, H. Oka and R. Noyori, Quantitative Analysis of the Chiral Amplification in the Amino Alcohol-Promoted Asymmetric Alkylation of Aldehydes with Dialkylzincs, *J. Am. Chem. Soc.*, 1998, **120**, 9800–9809.