Supplementary Information for

Iron-catalyzed epoxidation of olefins using hydrogen peroxide

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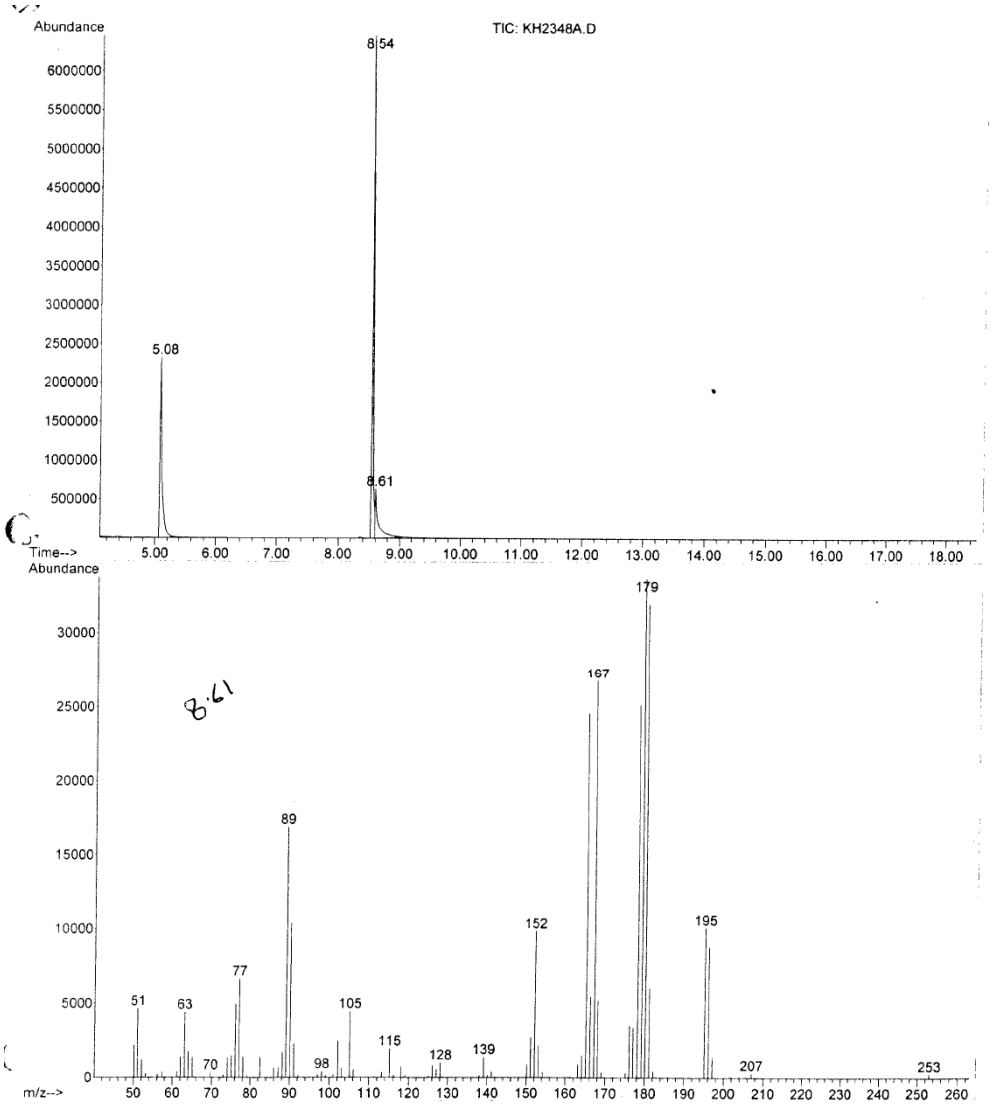
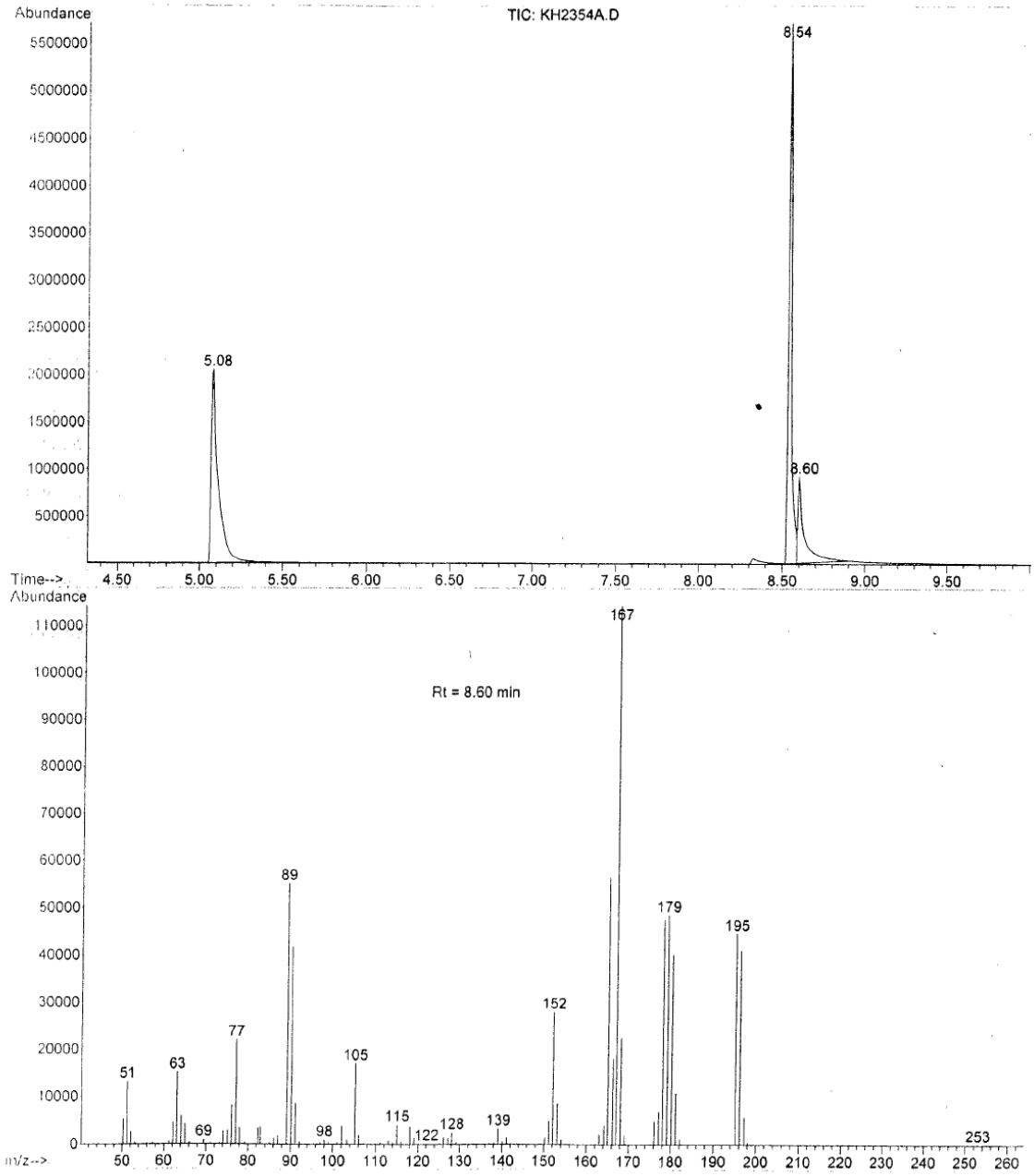
GC Traces and Mass Spectra of Selected Products Given in Table 1:

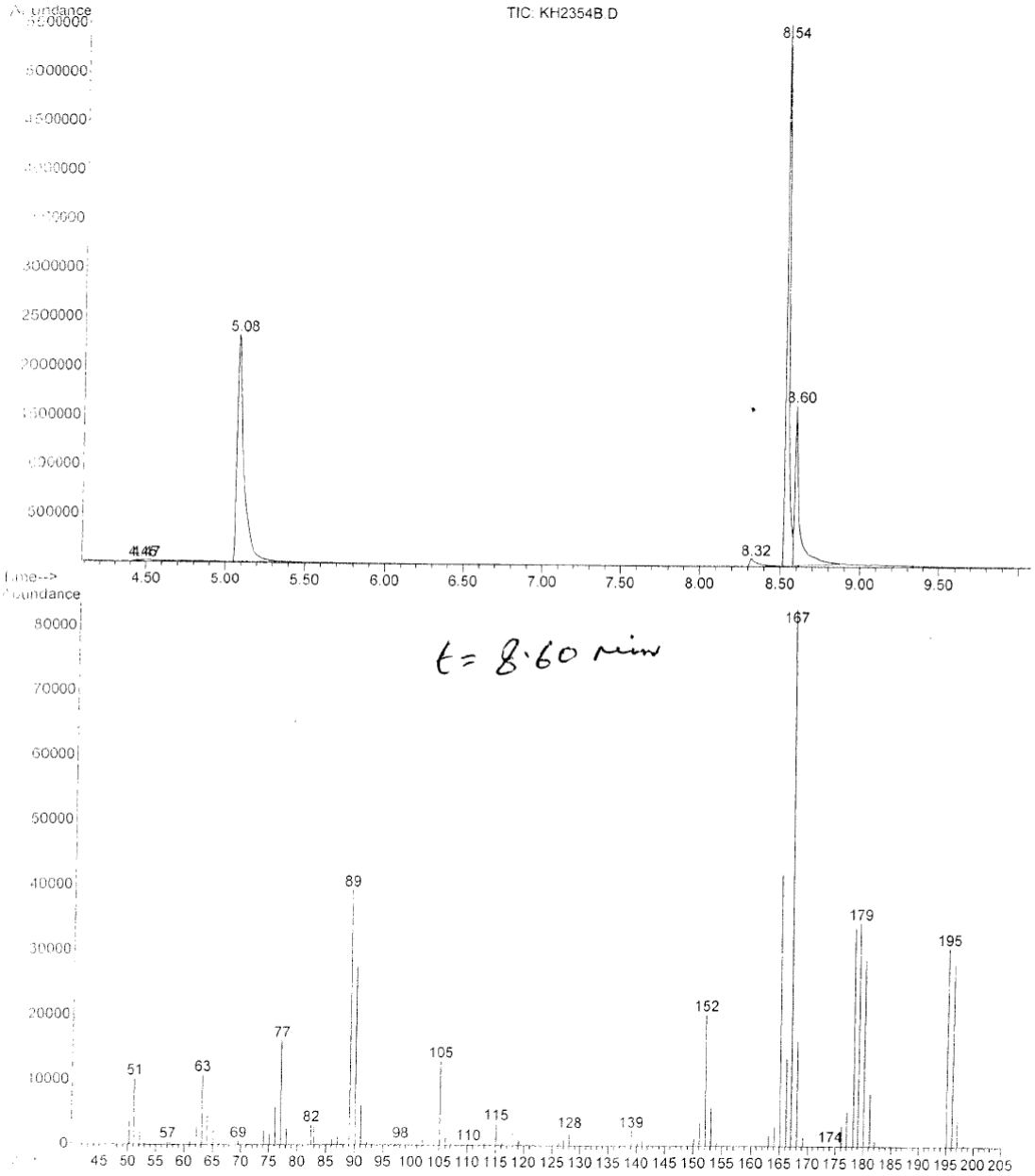
Entry 1: Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.61 min.



Entry 5: Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.60 min.

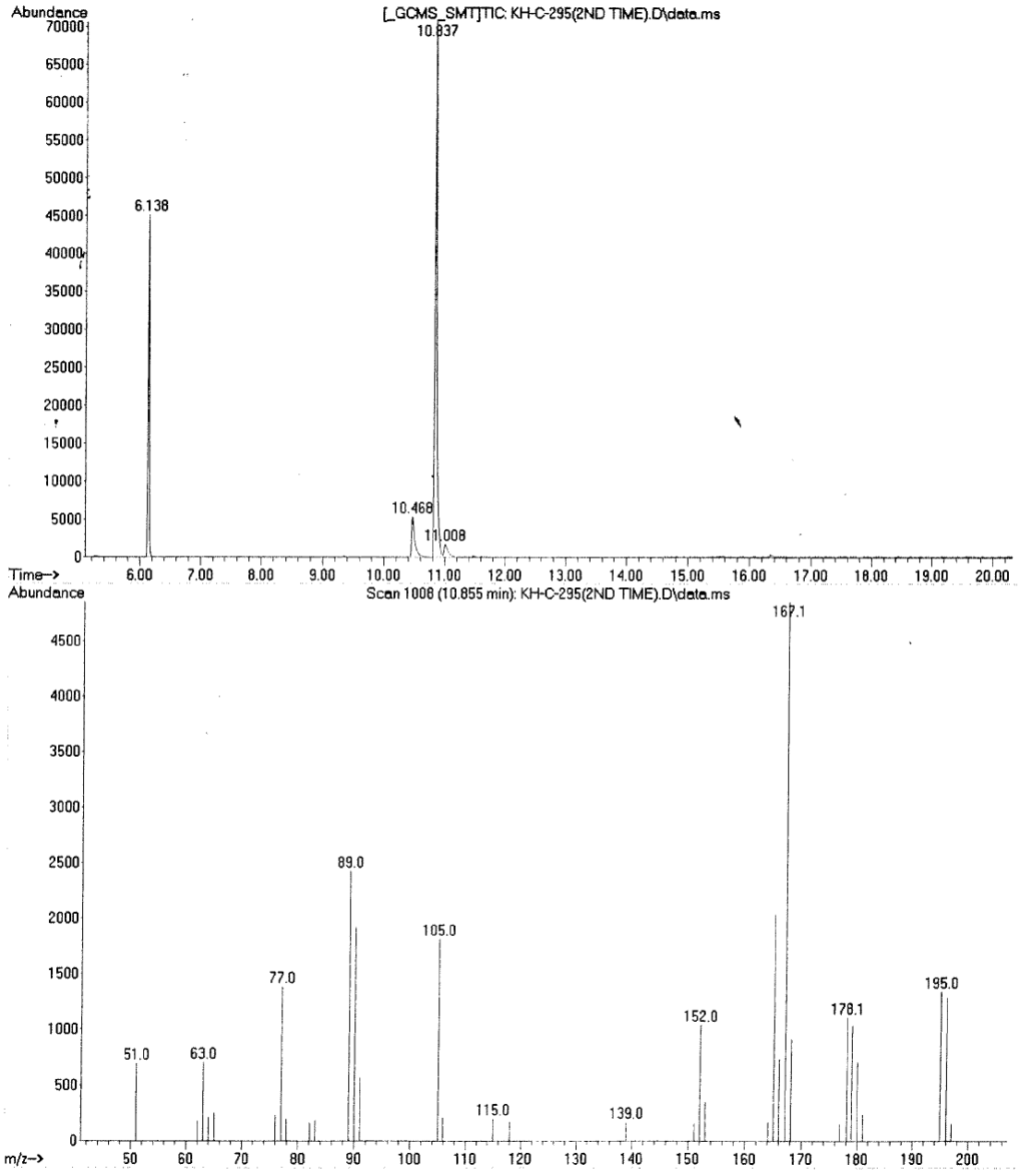


Entry 6 at room temperature (for Entry 6 at 65 °C see Table 2, Entry 1, below): Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.60 min. Isomer of *trans*-Stilbene oxide, R_t = 8.32 min.

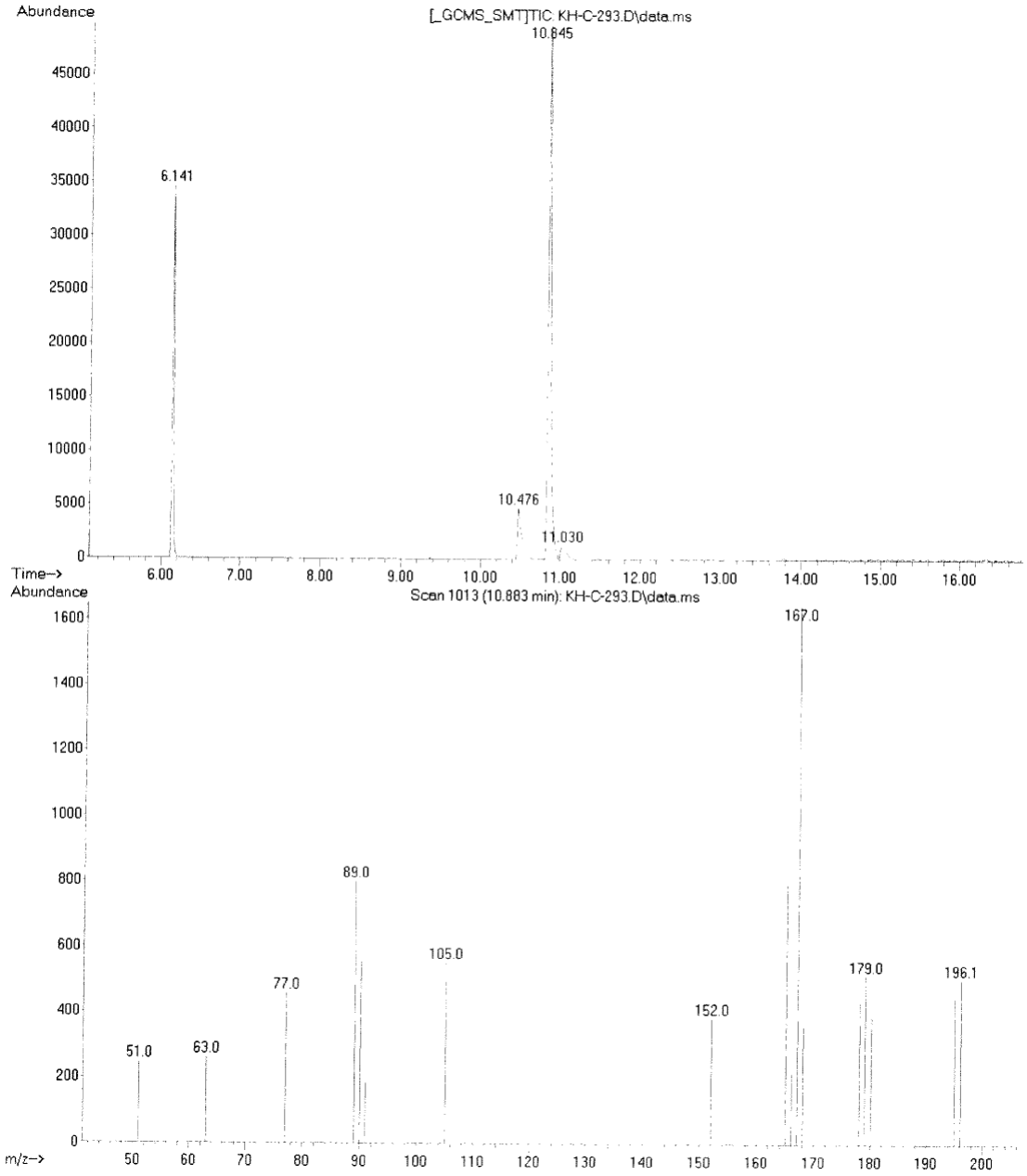


GC Traces and Mass Spectra of Selected Products Given in Table 2:

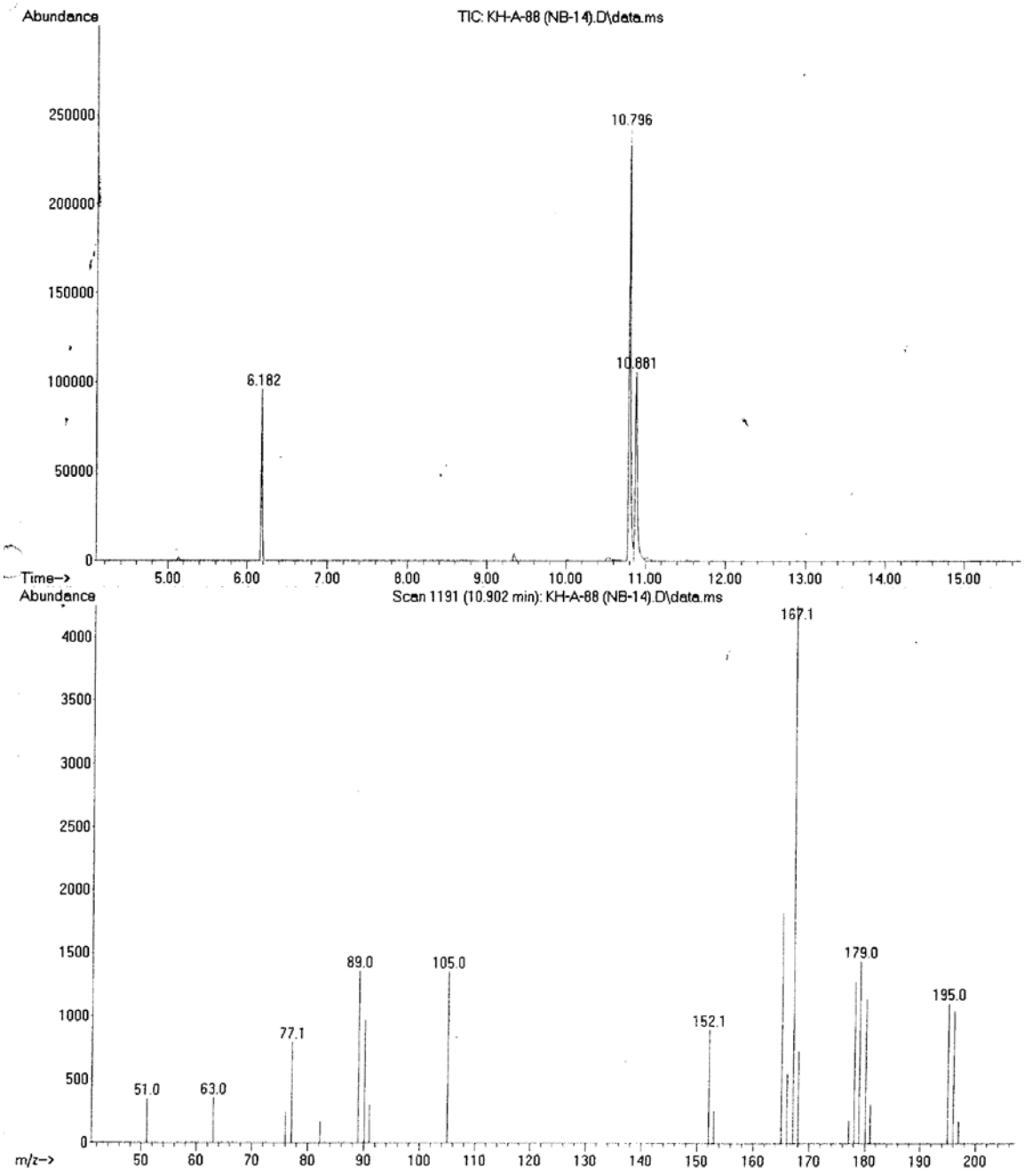
Entry 1 (Also Table 1, Entry 6 at 65 °C and Table 3, Entry 5): Dodecane internal standard, R_t = 6.138 min. *trans*-Stilbene oxide, R_t = 10.837 min. Isomer of *trans*-Stilbene oxide, R_t = 10.468 min. Unidentified by-product, R_t = 11.008 min.



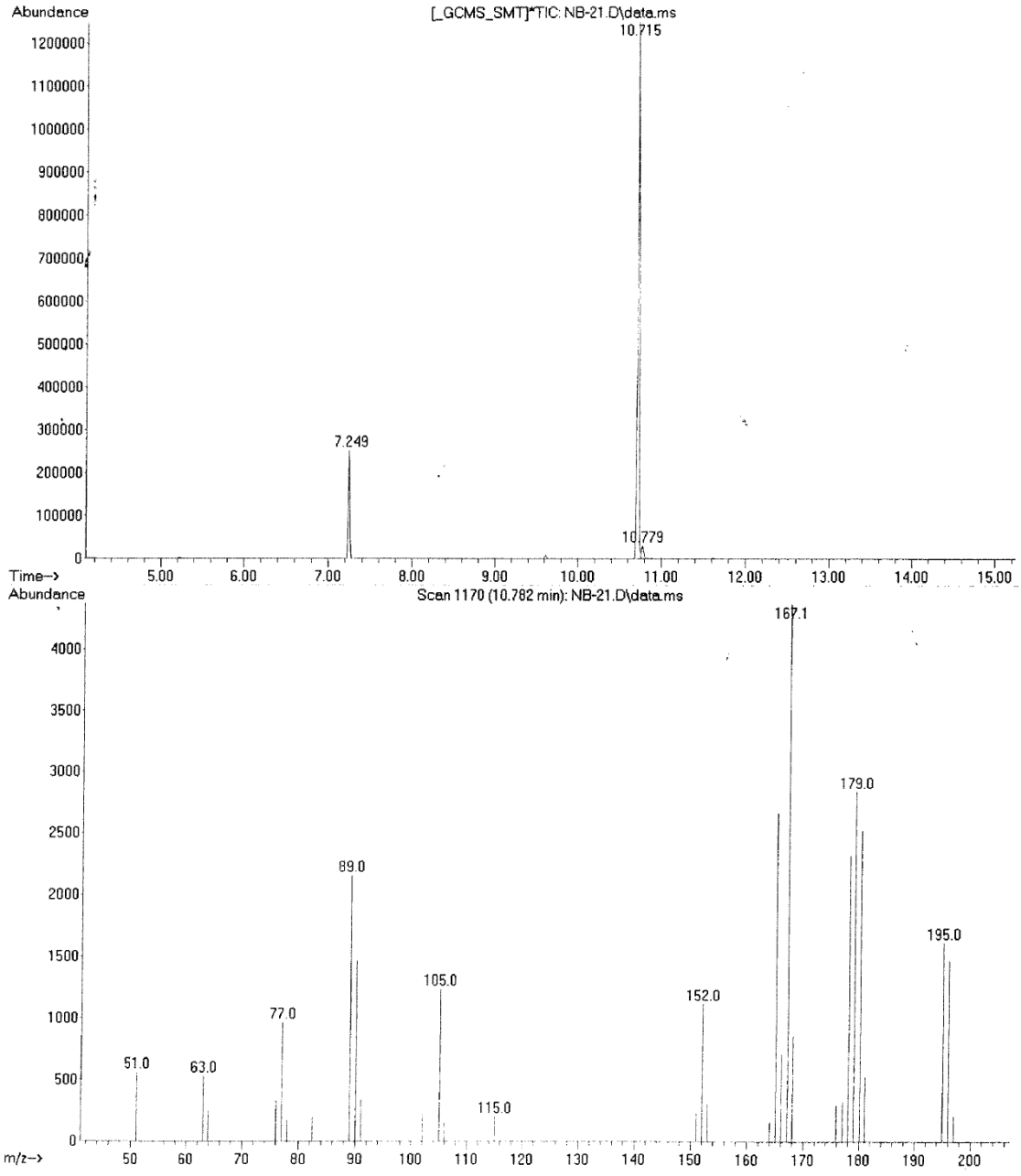
Entry 2: Dodecane internal standard, R_t = 6.141 min. *trans*-Stilbene oxide, R_t = 10.845 min. Isomer of *trans*-Stilbene oxide, R_t = 10.476 min. Unidentified by-product, R_t = 11.030 min.



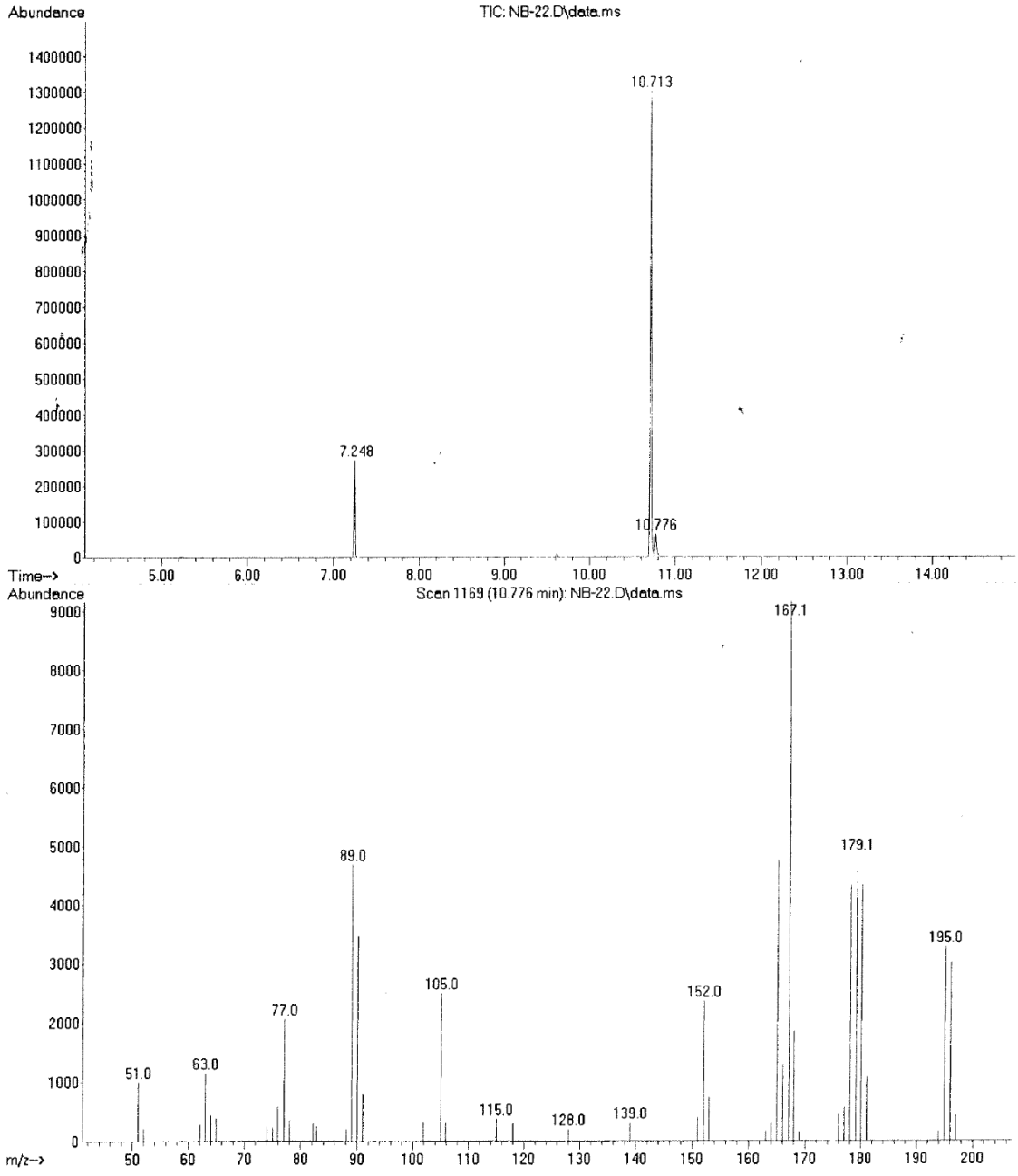
Entry 6: Dodecane internal standard, R_t = 6.182 min. *trans*-Stilbene, R_t = 10.796 min. *trans*-Stilbene oxide, R_t = 10.881 min.



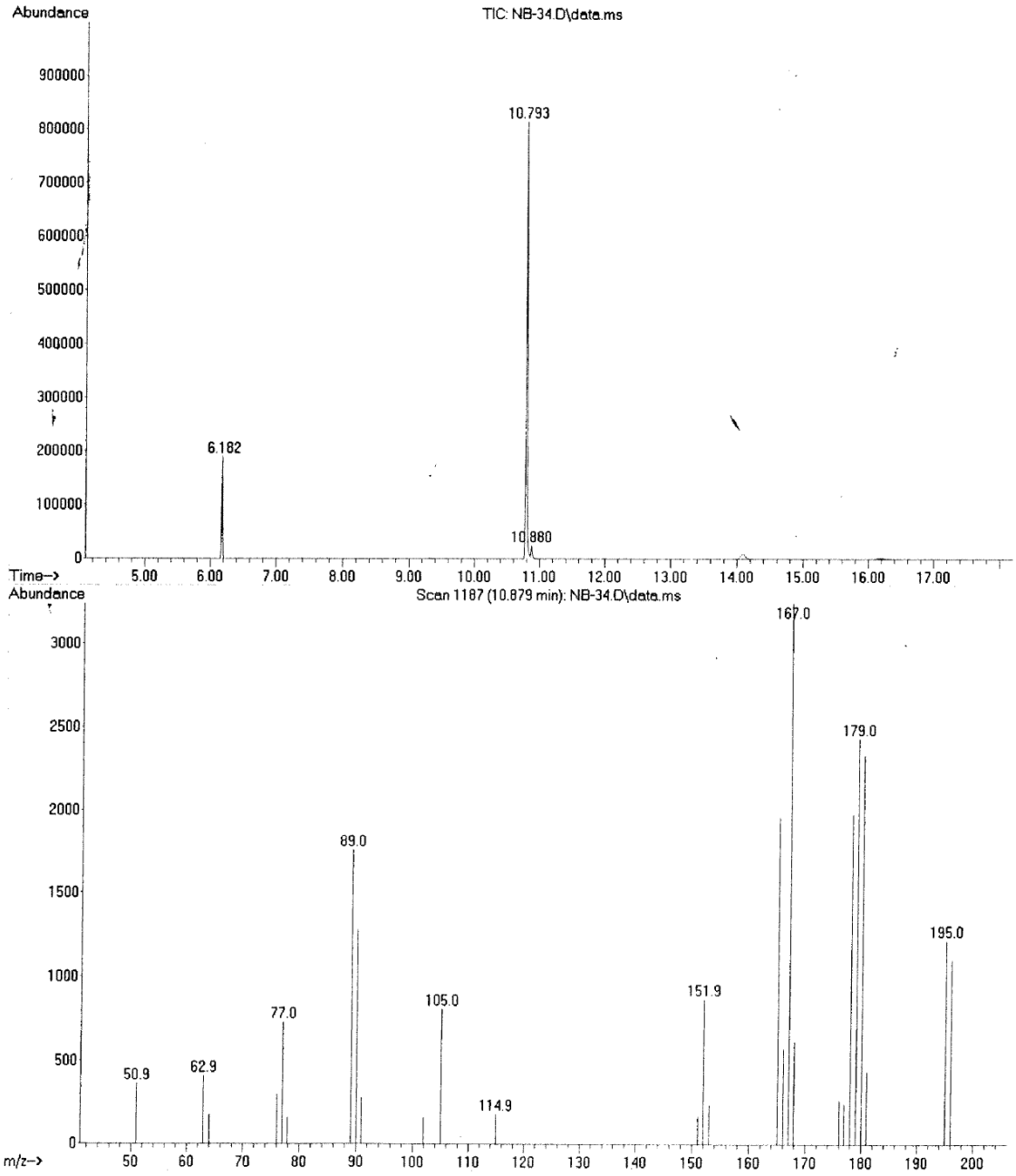
Entry 7: Dodecane internal standard, R_t = 7.249 min. *trans*-Stilbene, R_t = 10.715 min. *trans*-Stilbene oxide, R_t = 10.779 min.



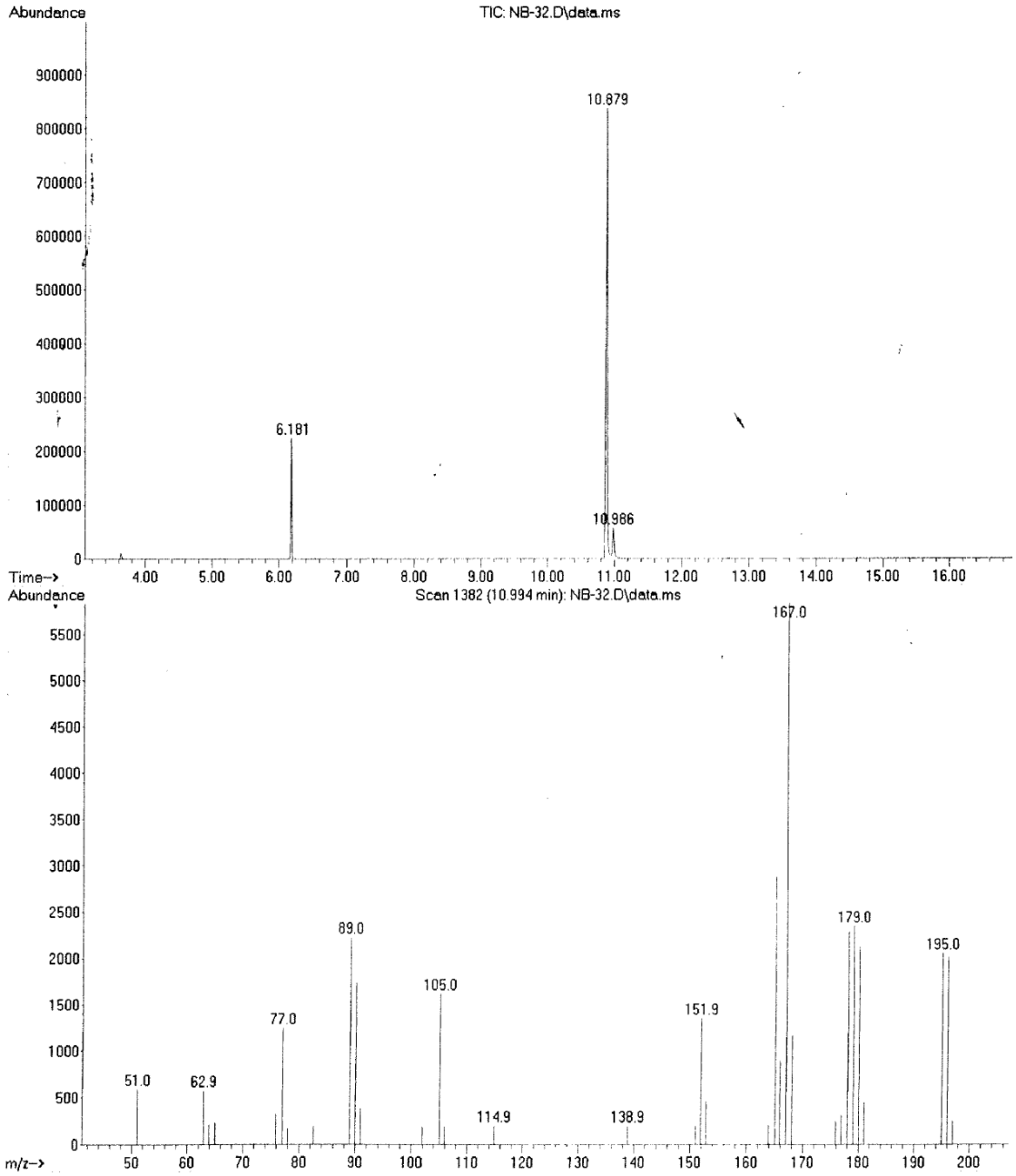
Entry 8: Dodecane internal standard, R_t = 7.248 min. *trans*-Stilbene, R_t = 10.713 min. *trans*-Stilbene oxide, R_t = 10.776 min.



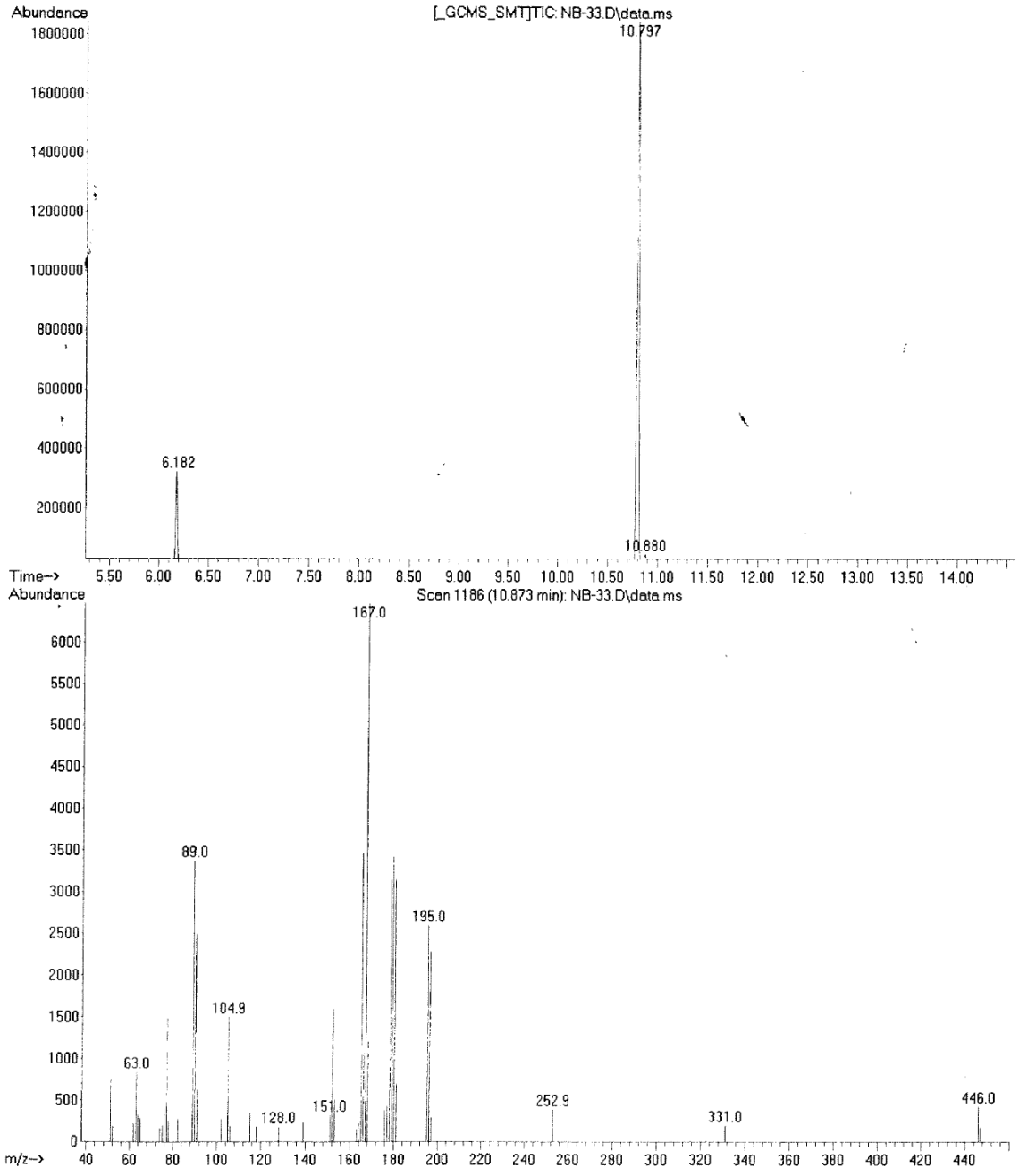
Entry 9: Dodecane internal standard, R_t = 6.182 min. *trans*-Stilbene, R_t = 10.793 min. *trans*-Stilbene oxide, R_t = 10.880 min.



Entry 10: Dodecane internal standard, R_t = 6.181 min. *trans*-Stilbene, R_t = 10.879 min. *trans*-Stilbene oxide, R_t = 10.986 min.

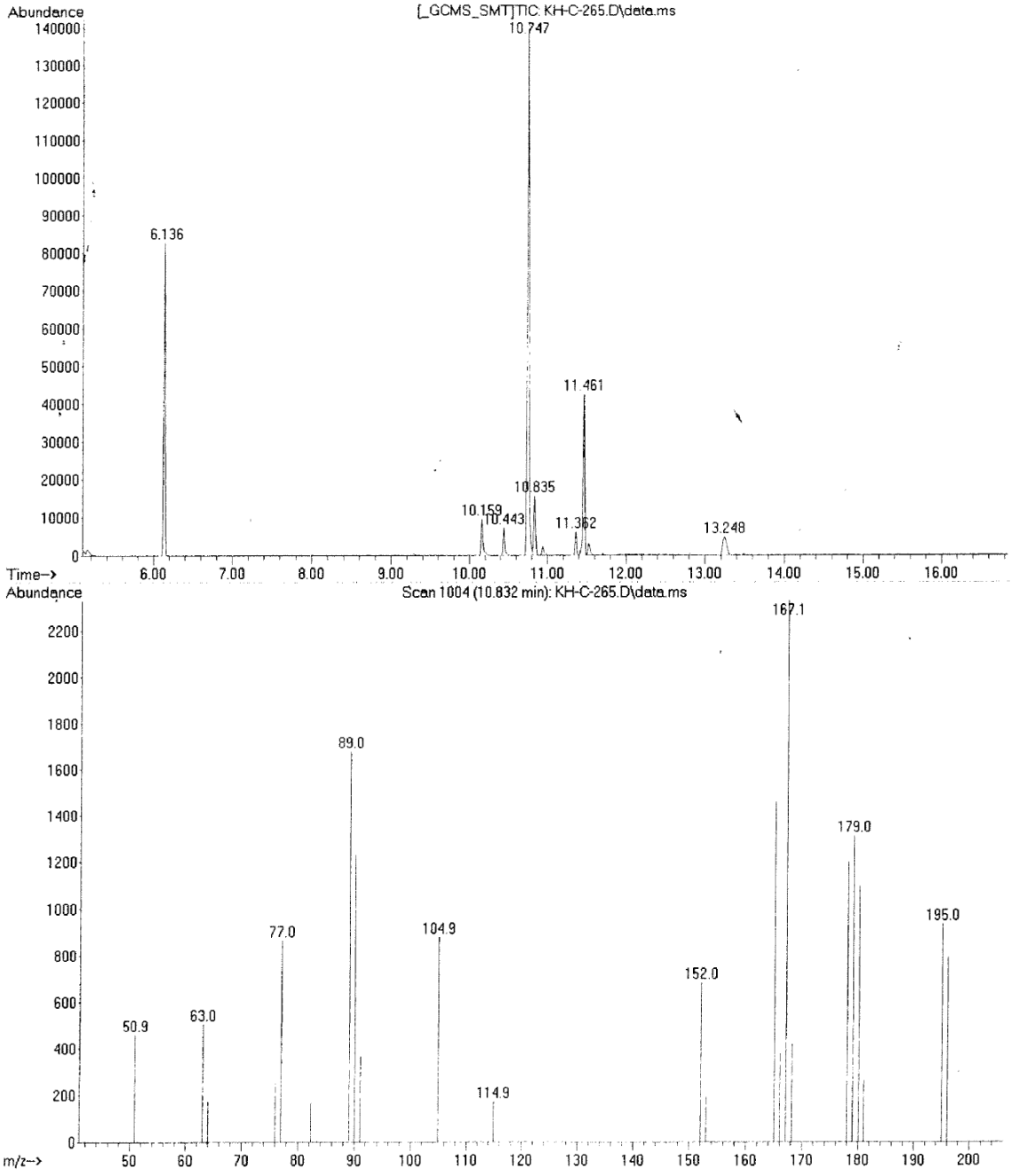


Entry 11: Dodecane internal standard, R_t = 6.182 min. *trans*-Stilbene, R_t = 10.797 min. *trans*-Stilbene oxide, R_t = 10.880 min.

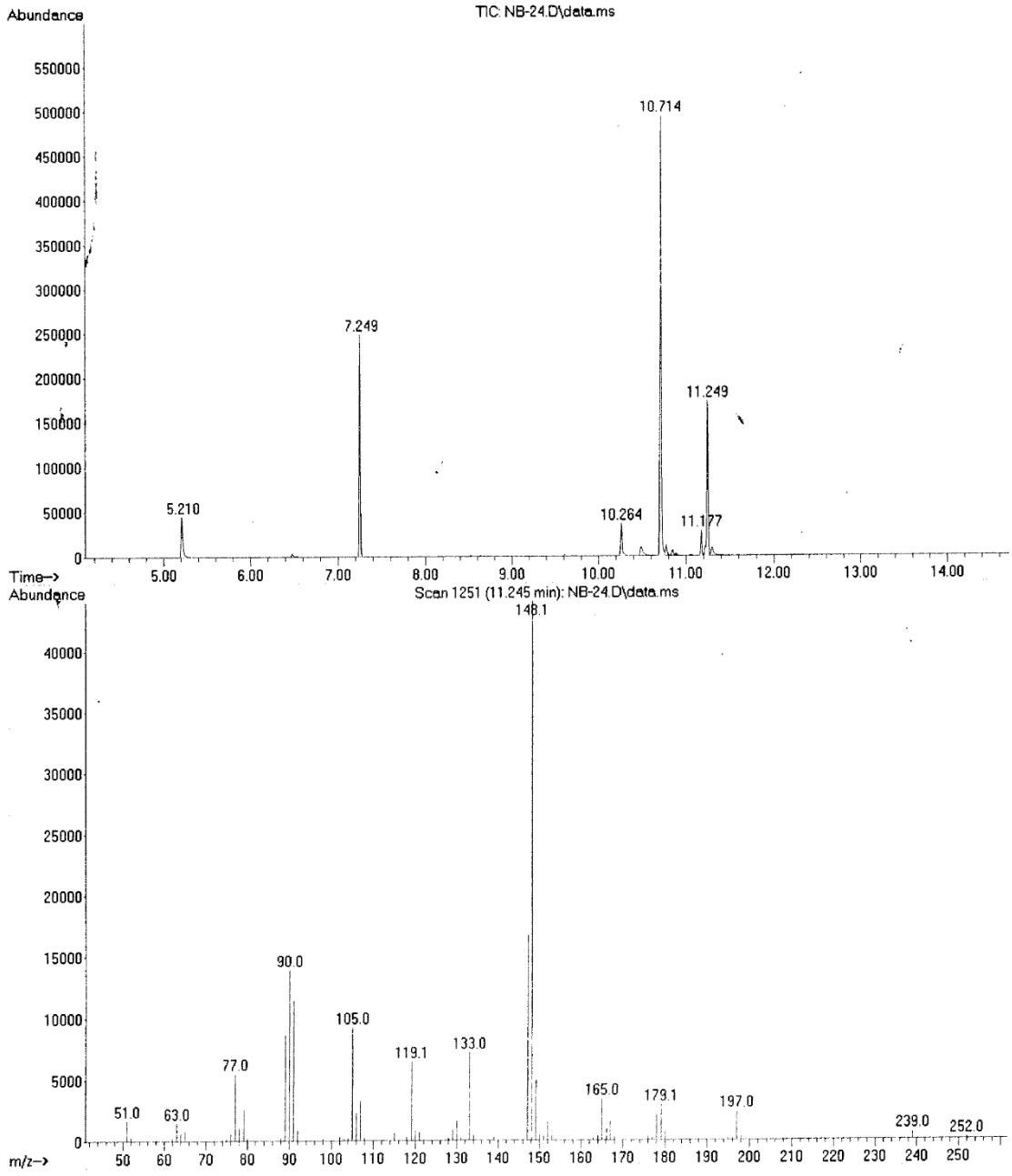


GC Traces and Mass Spectra of Selected Products Given in Table 3:

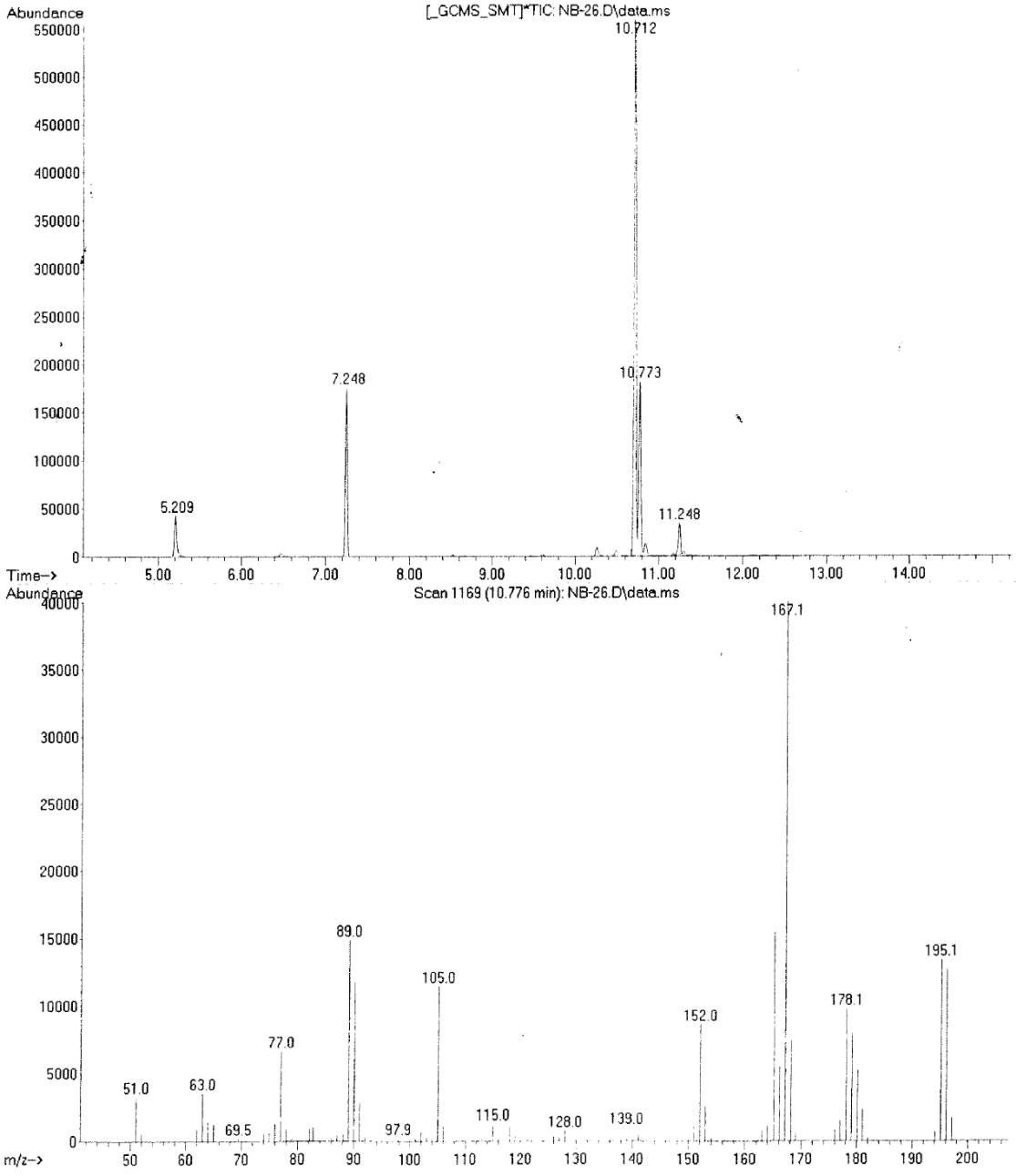
Entry 1: Dodecane internal standard, R_t = 6.136 min. *trans*-Stilbene, R_t = 10.747 min. *trans*-Stilbene oxide, R_t = 10.835 min. Isomer of *trans*-Stilbene oxide, R_t = 10.443 min. 1,2-diphenylethane-1,2-diol, R_t = 11.461 min. Other peaks in GC trace have not been identified.



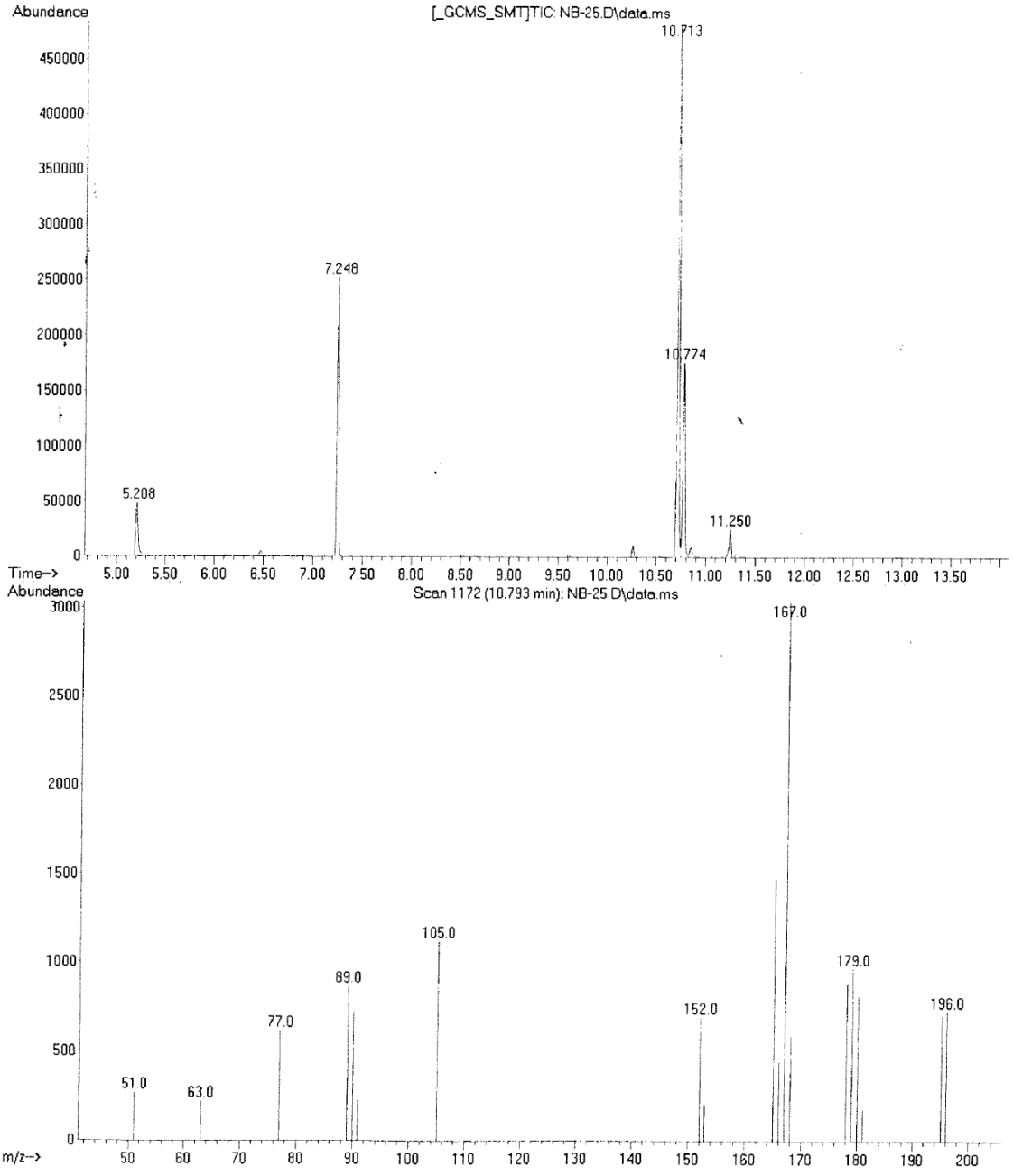
Entry 2: Dodecane internal standard, R_t = 7.249 min. *trans*-Stilbene, R_t = 10.714 min. By-products: benzaldehyde, R_t = 5.210 min. and 1,2-diphenylethane-1,2-diol, R_t = 11.249 min. Other peaks in GC trace have not been identified.



Entry 3: Dodecane internal standard, R_t = 7.248 min. *trans*-Stilbene, R_t = 10.712 min. *trans*-Stilbene oxide, R_t = 10.773 min. By-products: benzaldehyde, R_t = 5.209 min. and 1,2-diphenylethane-1,2-diol, R_t = 11.248 min.

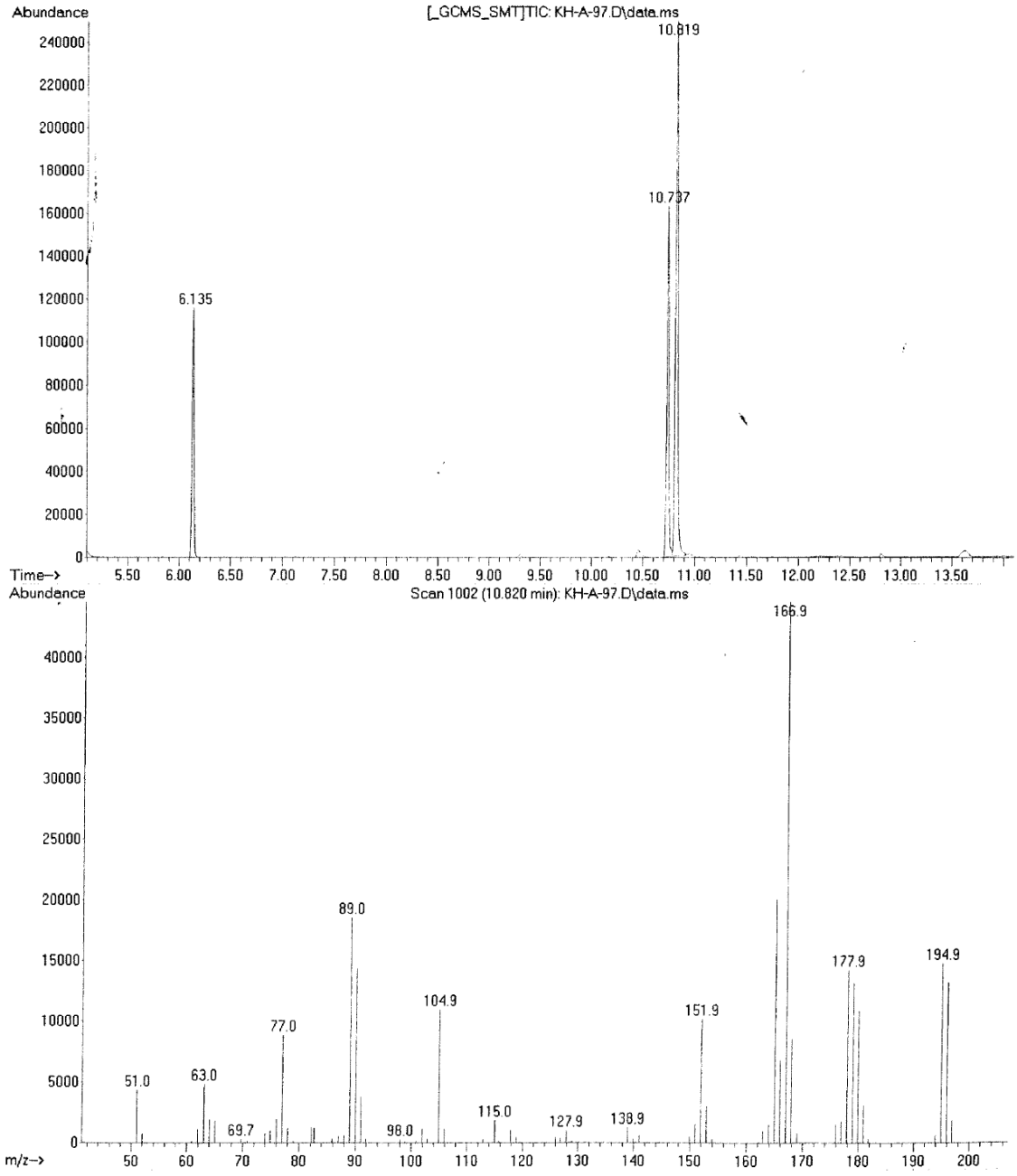


Entry 4: Dodecane internal standard, R_t = 7.248 min. *trans*-Stilbene, R_t = 10.713 min. *trans*-Stilbene oxide, R_t = 10.774 min. By-products benzaldehyde, R_t = 5.208 min. and 1,2-diphenylethane-1,2-diol, R_t = 11.250 min.

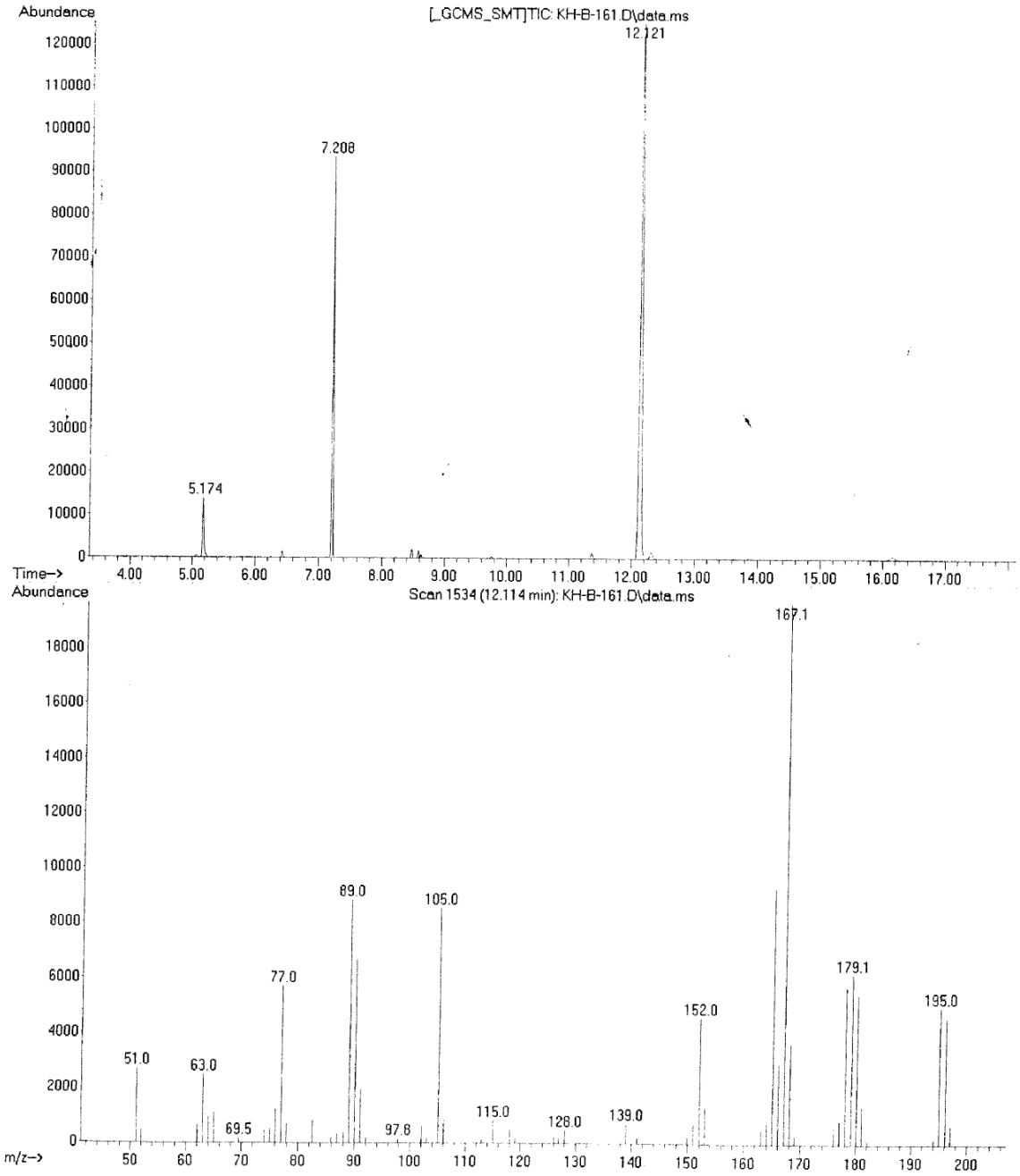


Entry 5: See Table 2, Entry 1.

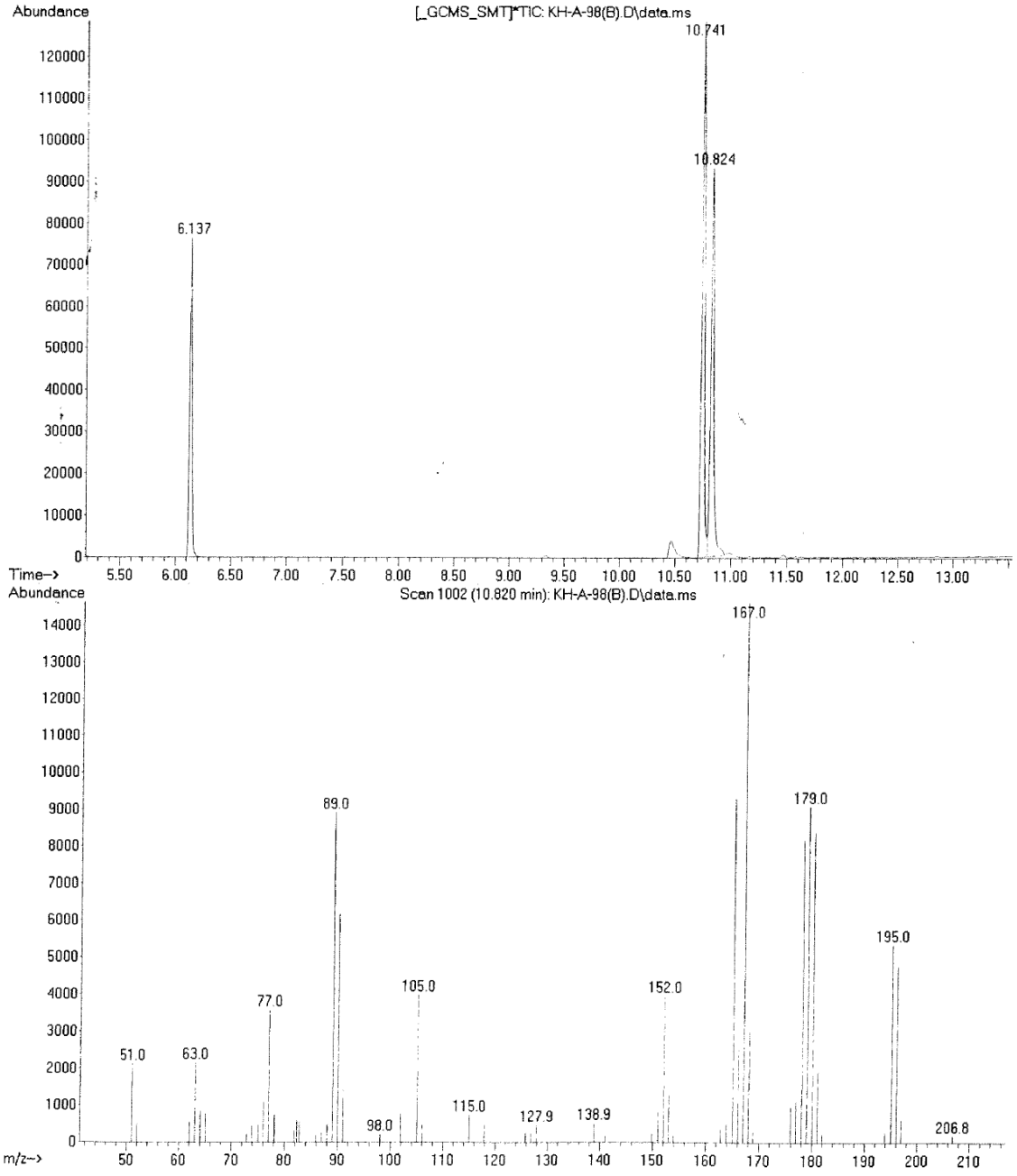
Entry 6: Dodecane internal standard, R_t = 6.135 min. *trans*-Stilbene, R_t = 10.737 min. *trans*-Stilbene oxide, R_t = 10.819 min.



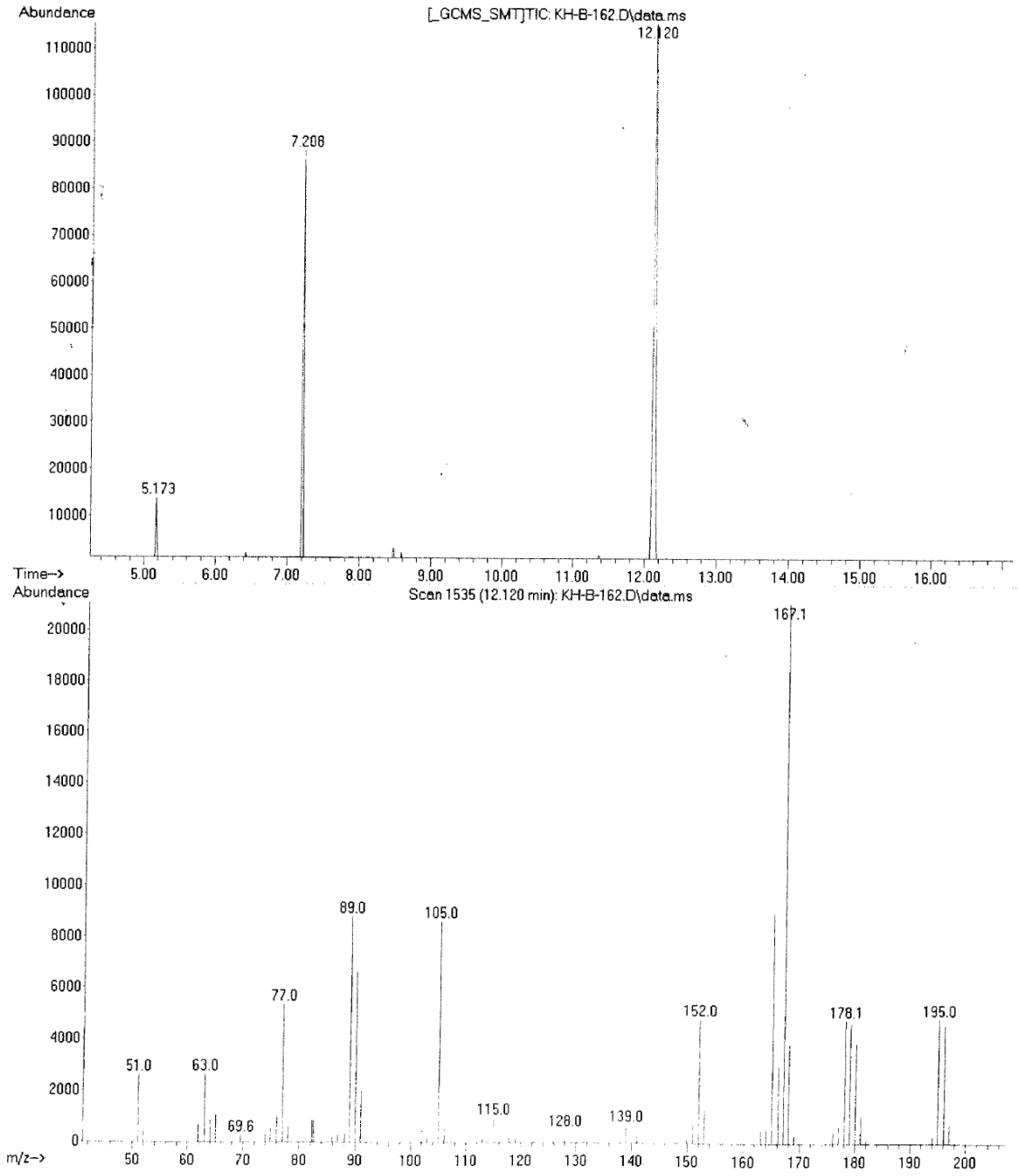
Entry 6 (using 3.0 mmol H_2O_2, condition *c* in Table 3 footnote): Dodecane internal standard, R_t = 7.208 min. *trans*-Stilbene oxide, R_t = 12.121 min. By-product benzaldehyde, R_t = 5.174 min.



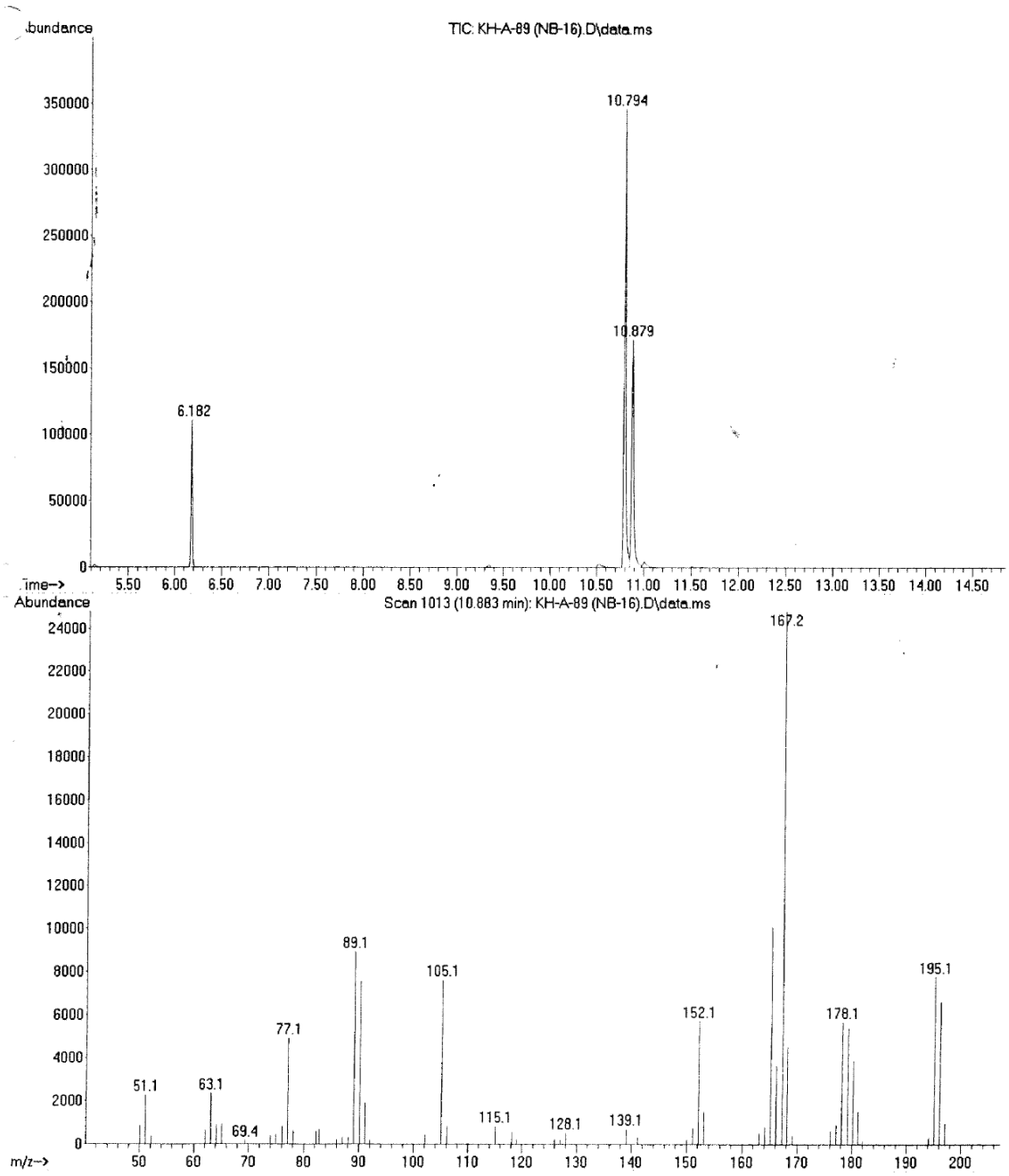
Entry 7: Dodecane internal standard, R_t = 6.137 min. *trans*-stilbene, R_t = 10.741 min. *trans*-Stilbene oxide, R_t = 10.824 min.



Entry 7 (using 3.0 mmol H_2O_2, condition *c* in Table 3 footnote): Dodecane internal standard, R_t = 7.208 min. *trans*-Stilbene oxide, R_t = 12.120 min. By-product benzaldehyde, R_t = 5.173 min.

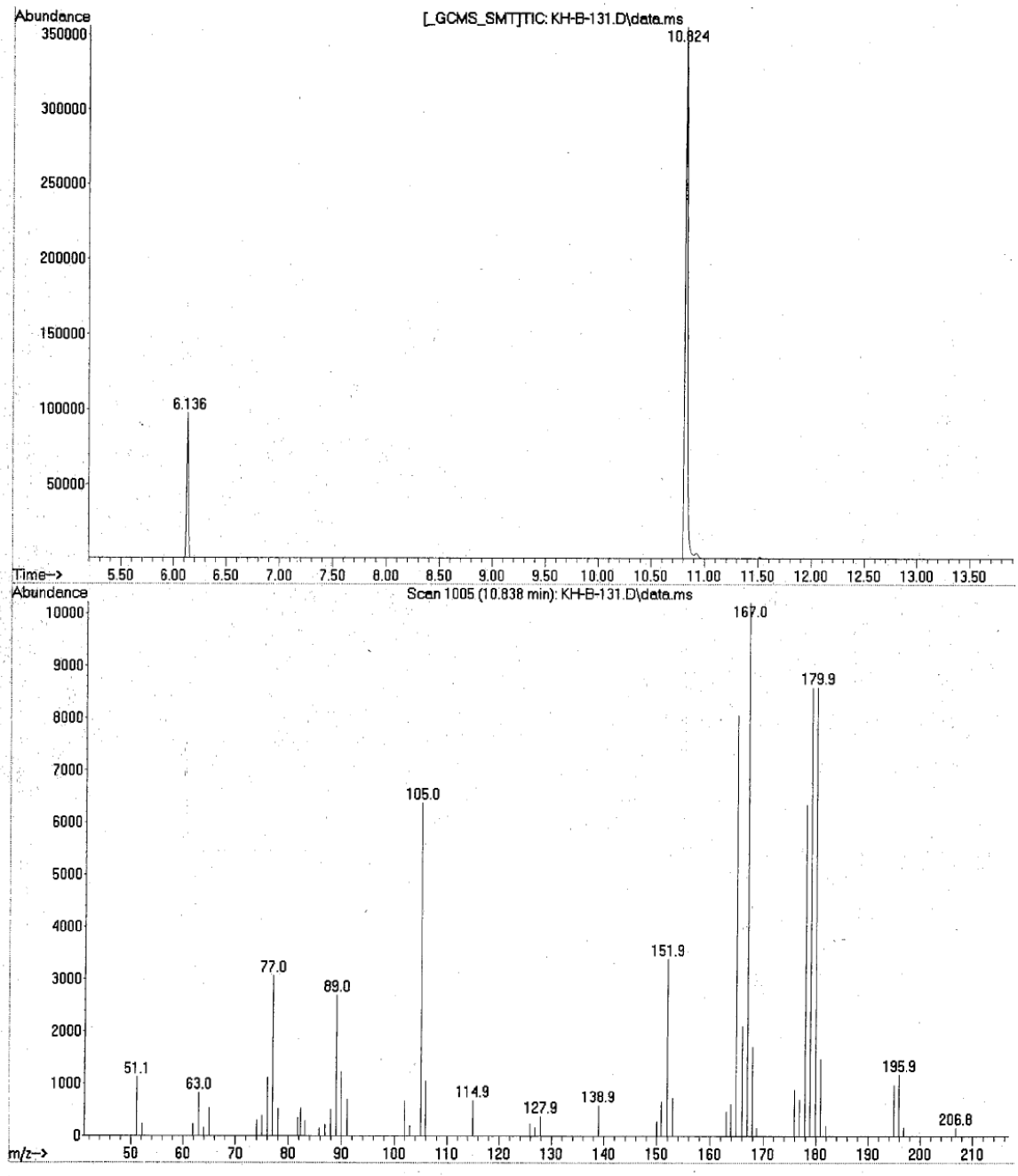


Entry 8: Dodecane internal standard, R_t = 6.182 min. *trans*-stilbene, R_t = 10.794 min. *trans*-Stilbene oxide, R_t = 10.879 min.

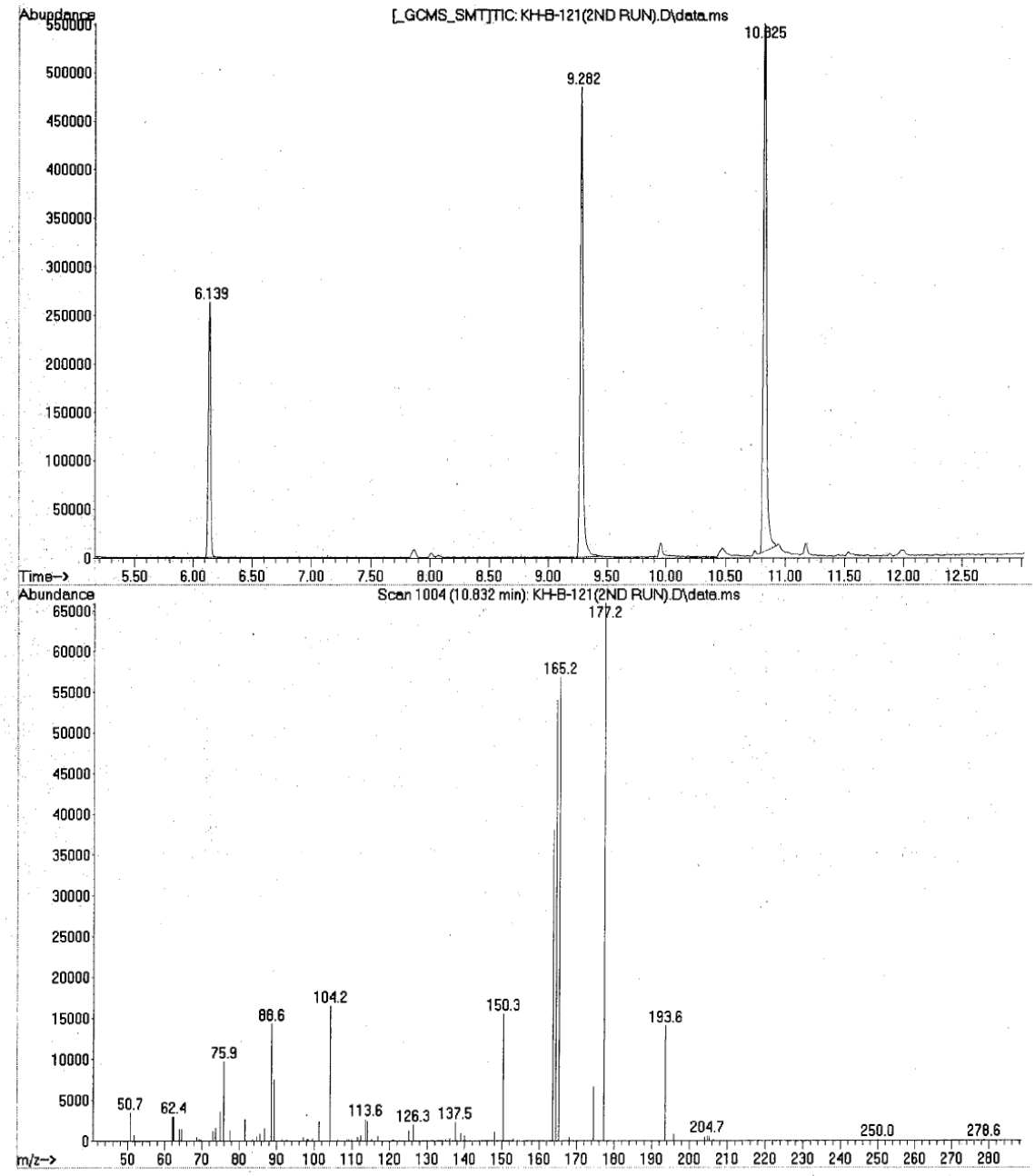


GC Traces and Mass Spectra of Selected Products Given in Table 4:

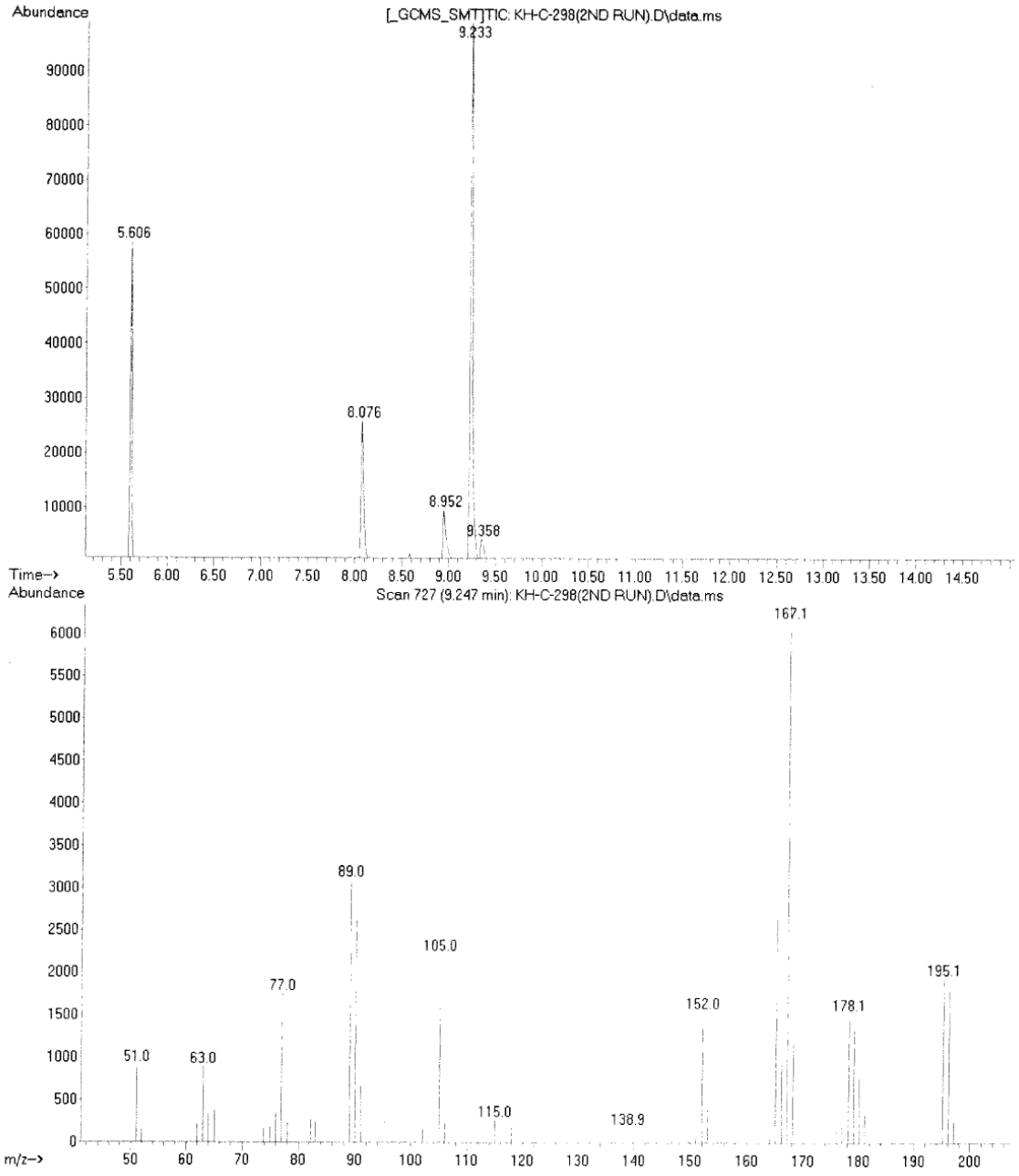
Entry 1: Dodecane internal standard, R_t = 6.136 min. *trans*-Stilbene oxide, R_t = 10.824 min.



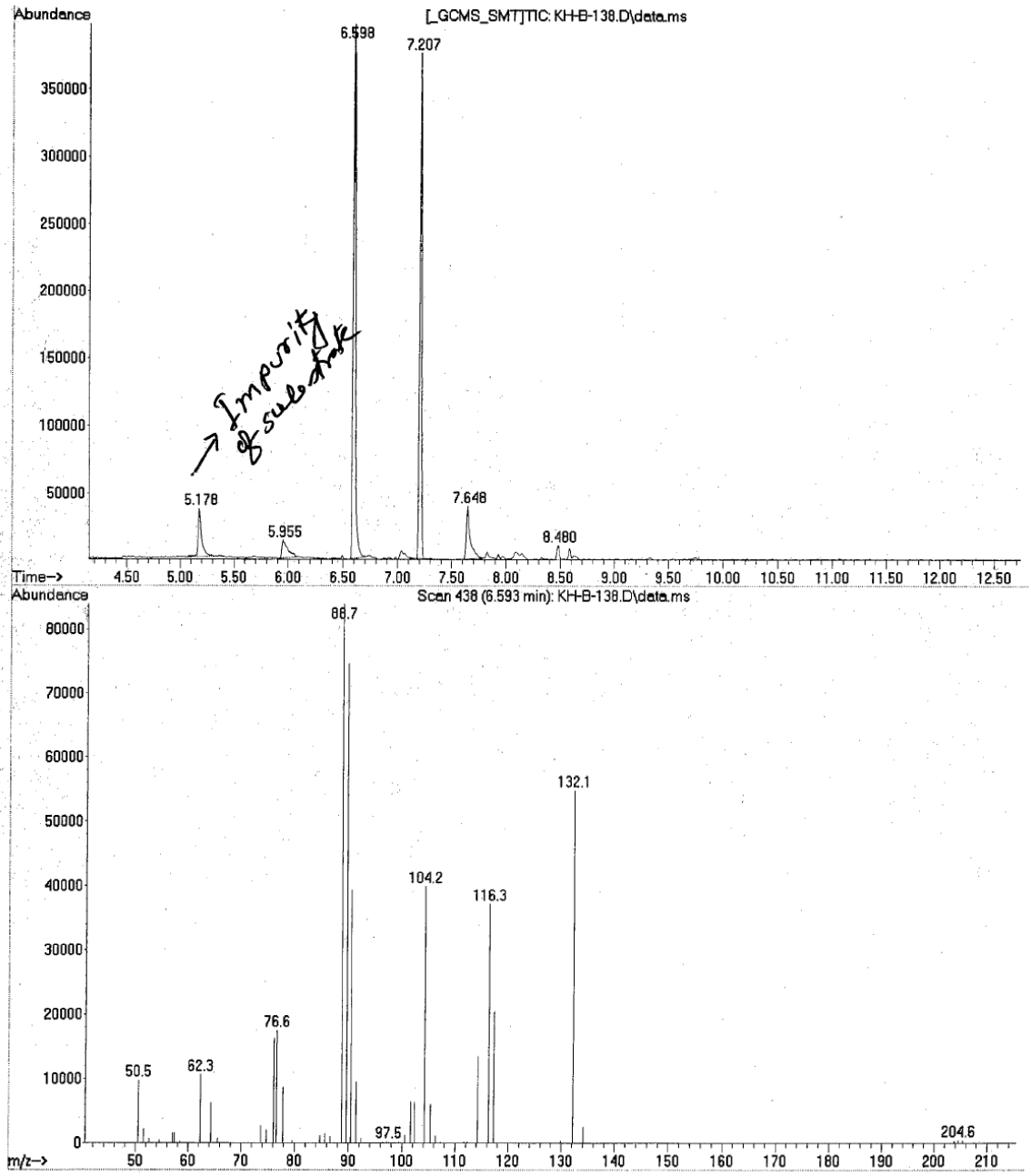
Entry 2: Dodecane internal standard , R_t = 6.139 min. *cis*-Stilbene , R_t = 9.282 min. *trans*-Stilbene oxide, R_t = 10.825 min.



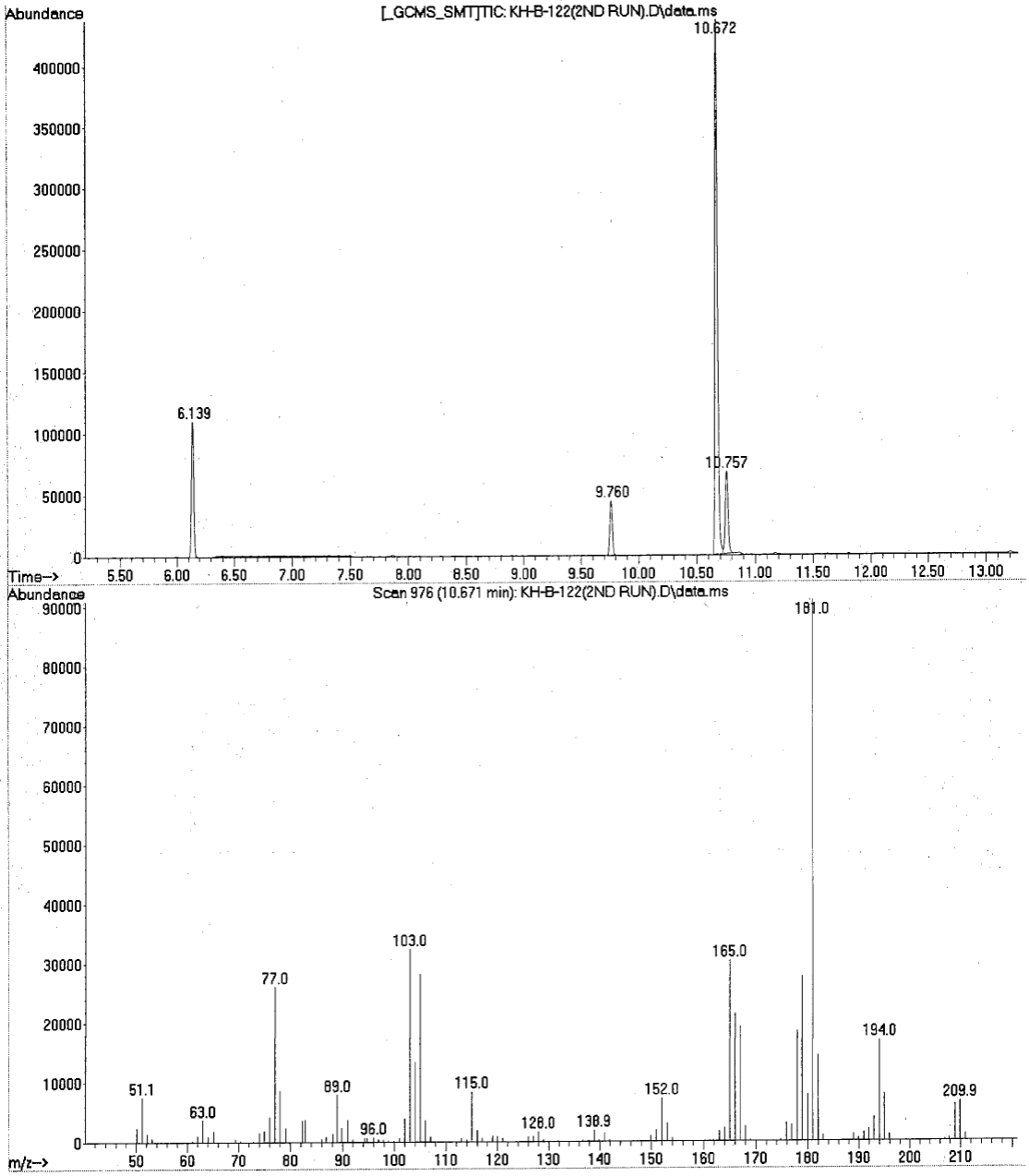
Entry 2 (after heating to 62 °C for 48 h, condition *b* in Table 4 footnote): Dodecane internal standard, R_t = 5.606 min. *cis*-Stilbene, R_t = 8.076 min. Isomer of *trans*-Stilbene oxide, R_t = 8.952 min. *trans*-Stilbene oxide (confirmed by ^{1}H NMR), R_t = 9.233 min. Unidentified by-product R_t = 9.358 min.



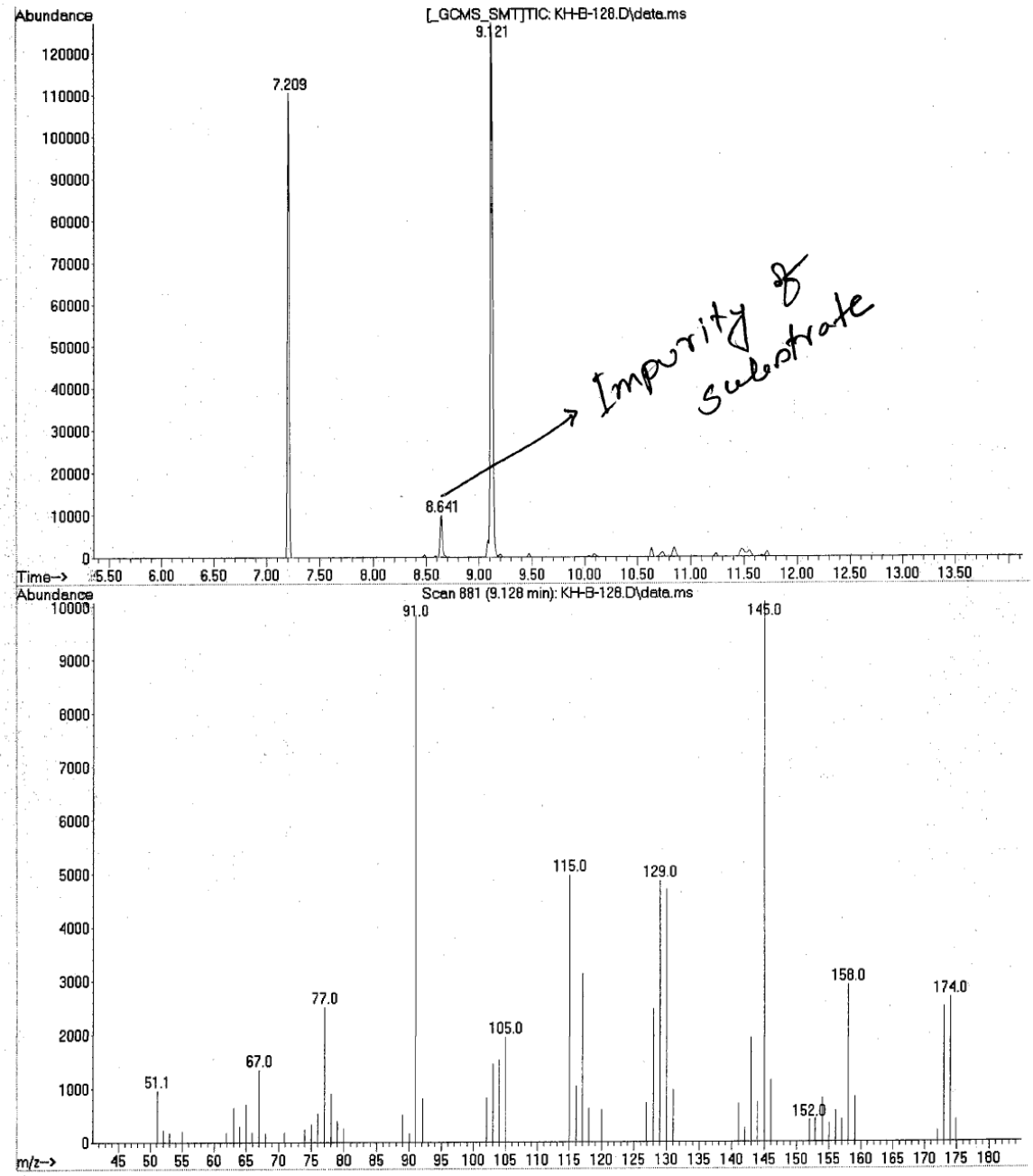
Entry 3: Impurity of substrate, R_t = 5.178 min. *trans*-β-methyl styrene oxide, R_t = 6.598 min. Dodecane internal standard, R_t = 7.207 min. Unidentified by products, R_t = 7.648 and 8.460 min.



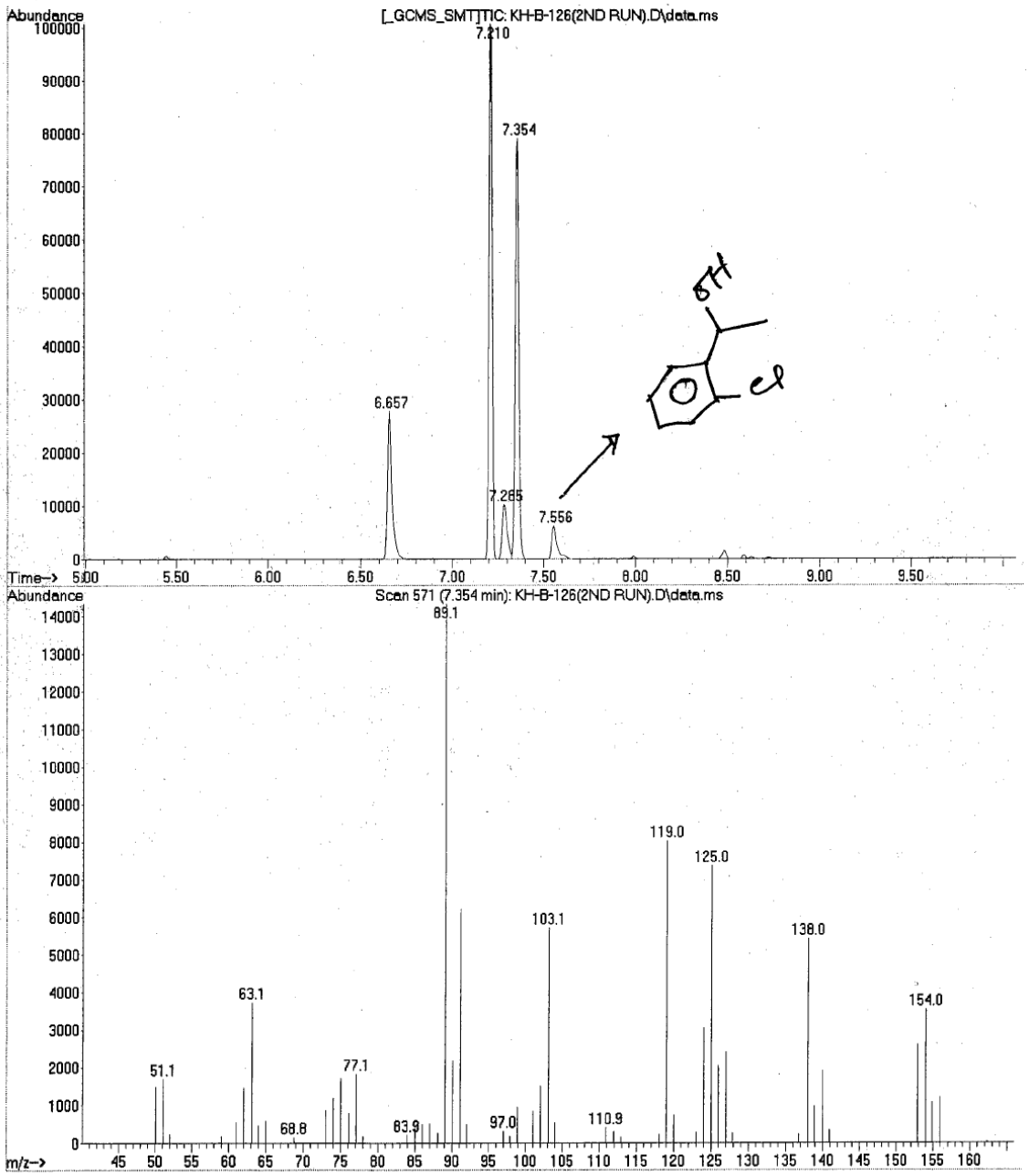
Entry 4 : Dodecane internal standard, R_t = 6.139 min. *trans-α*-Methylstilbene oxide, R_t = 10.672 min. Isomer of *trans-α*-methylstilbene oxide R_t = 9.760 min. *trans-α* Methylstilbene: R_t = 10.757 min.



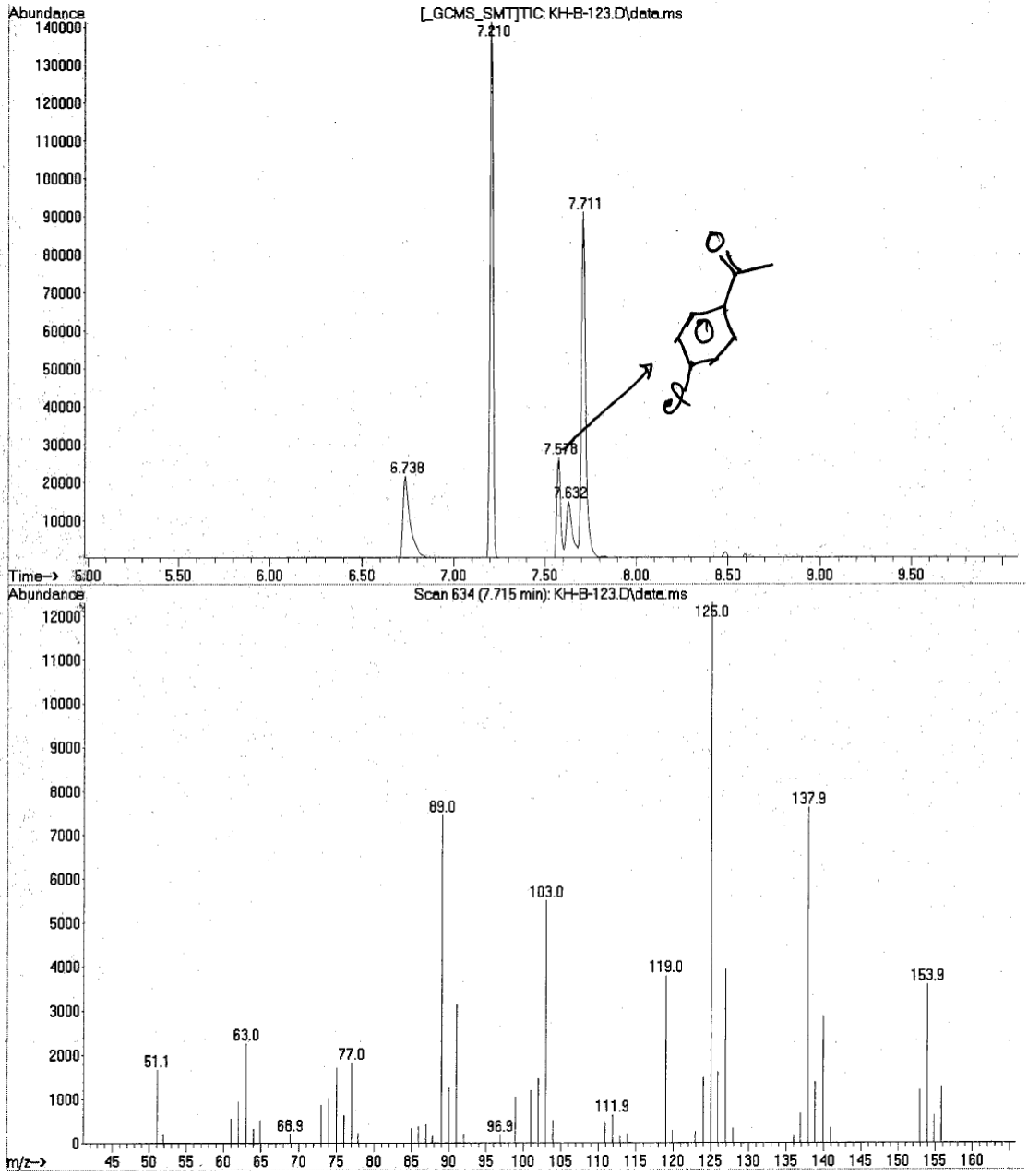
Entry 5: Dodecane internal standard, R_t = 7.209 min. 1-phenyl-1-cyclohexene oxide, R_t = 9.121 min. Impurity of substrate, R_t = 8.641 min.



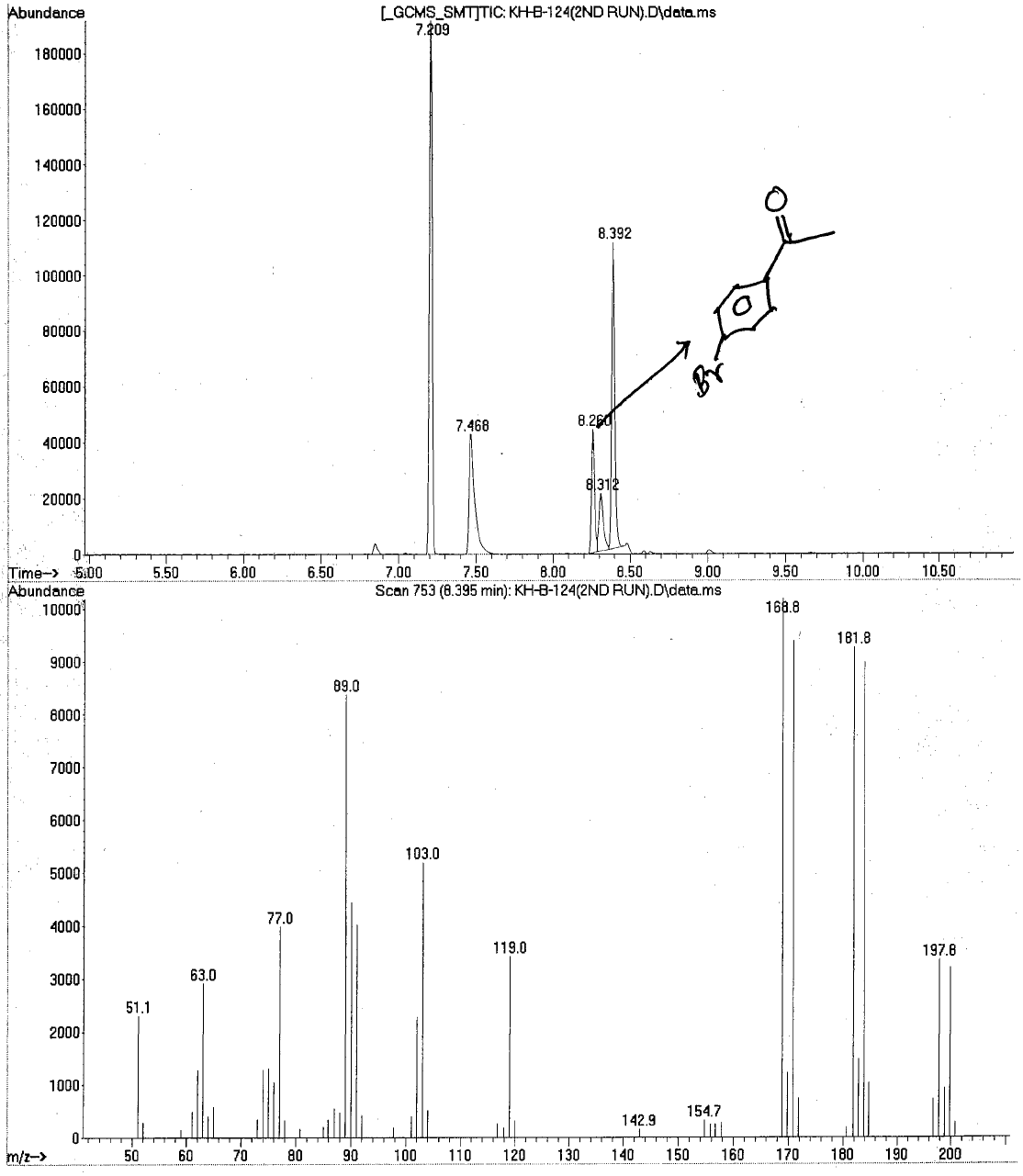
Entry 6. 2-Chlorostyrene, R_t = 6.657 min. Dodecane internal standard, R_t = 7.210 min. 1-(2-chlorophenyl) ethanone, R_t = 7.265 min. 2-chlorostyrene oxide, R_t = 7.354 min. 1-(2-chlorophenyl) ethanol, R_t = 7.556 min**.**



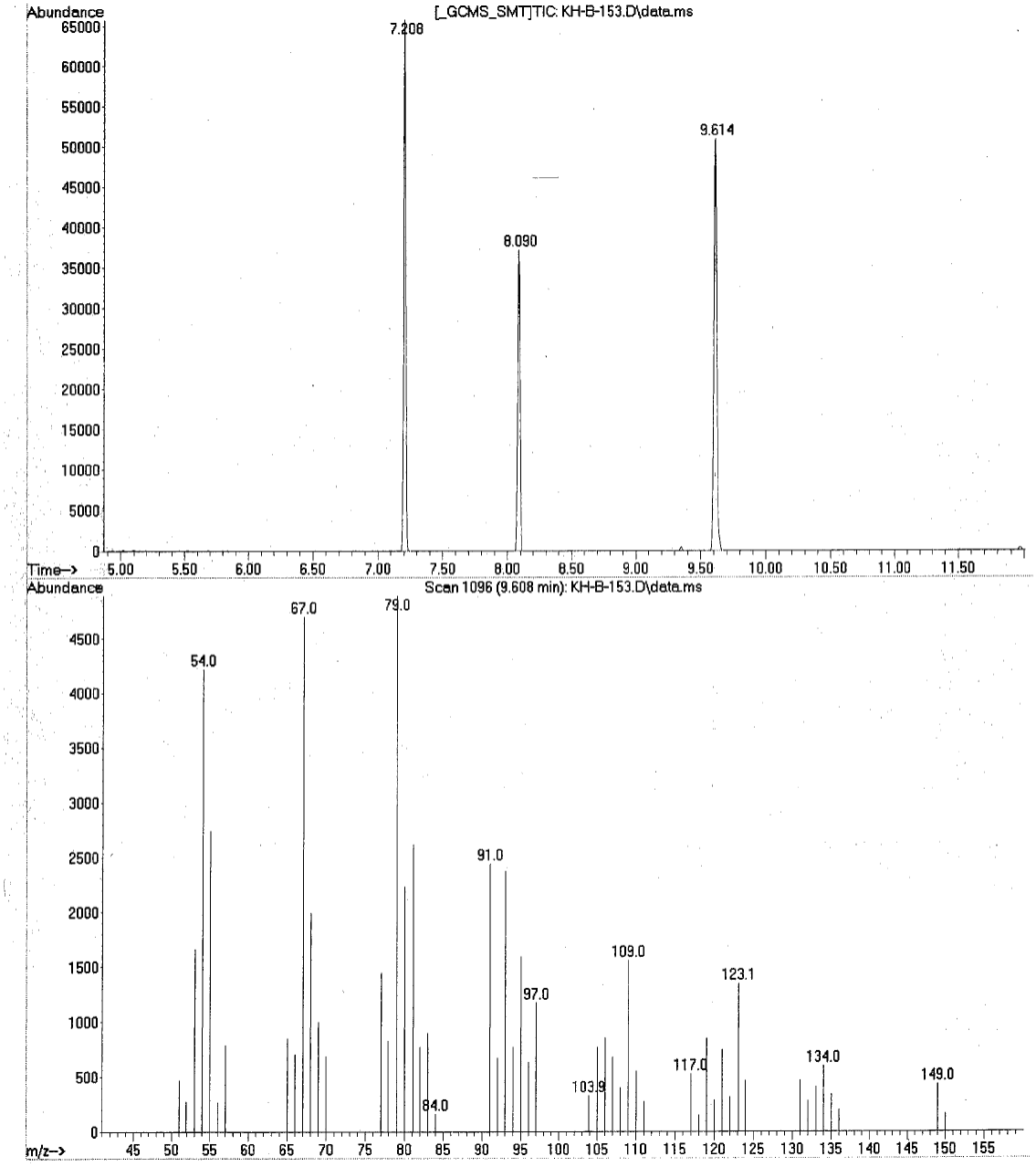
Entry 7: 4-Chlorostyrene, R_t = 6.738 min. Dodecane internal standard, R_t = 7.210 min. 1-(4-chlorophenyl) ethanone, R_t = 7.578 min. 4-chlorostyrene oxide, R_t = 7.632 and 7.711 min. Confirmed against standard 4-chlorostyrene oxide R_t = 7.632 and 7.711 min.



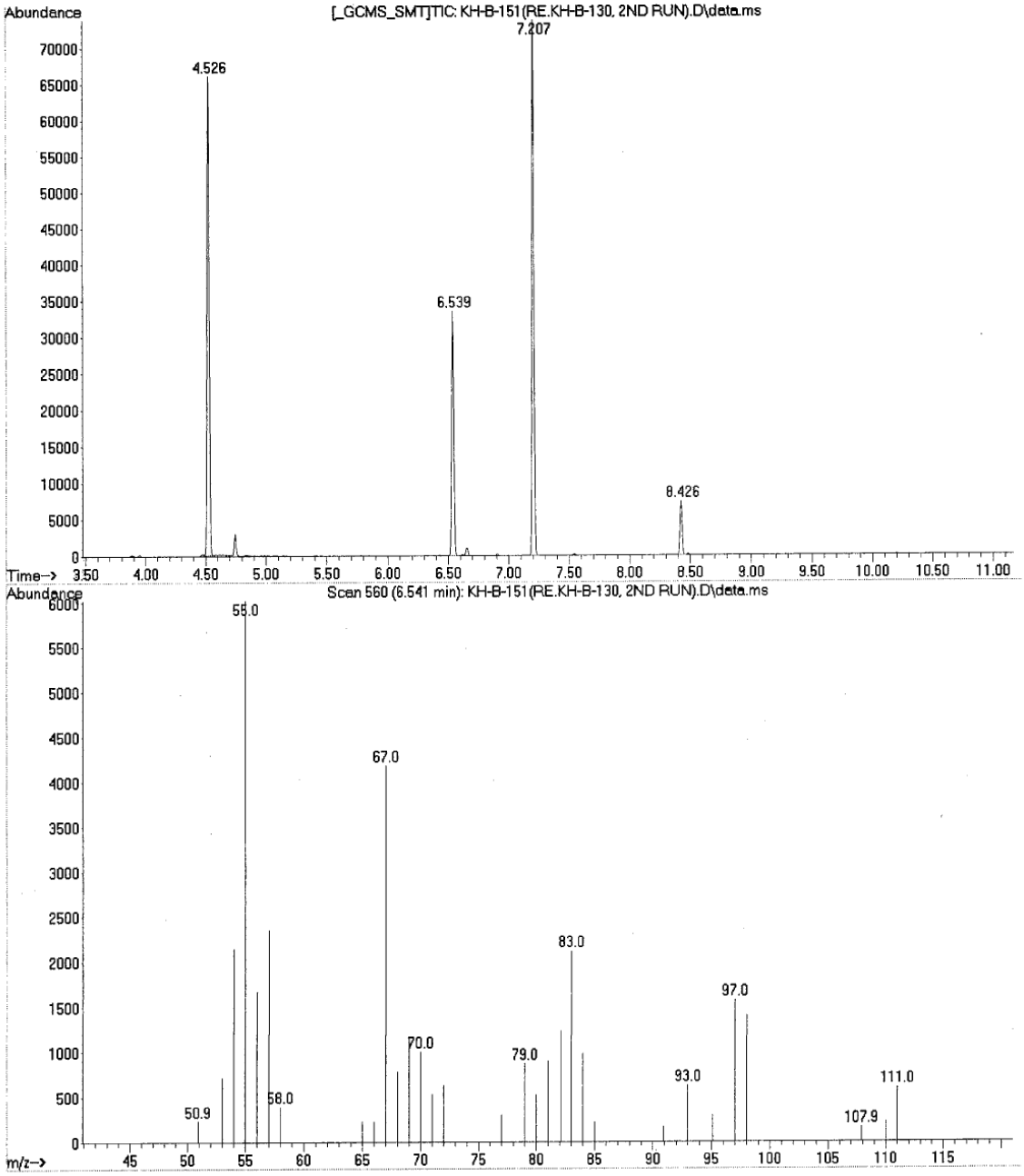
Entry 8: Dodecane internal standard, R_t = 7.209 min. 4-Bromostyrene, R_t = 7.468 min. 1-(4-bromophenyl) ethanone, R_t = 8.260 min. 4-bromorostyrene oxide, R_t = 8.312 and 8.392 min. Confirmed against standard 4-bromostyrene oxide: R_t = 8.312 and 8.392 min.



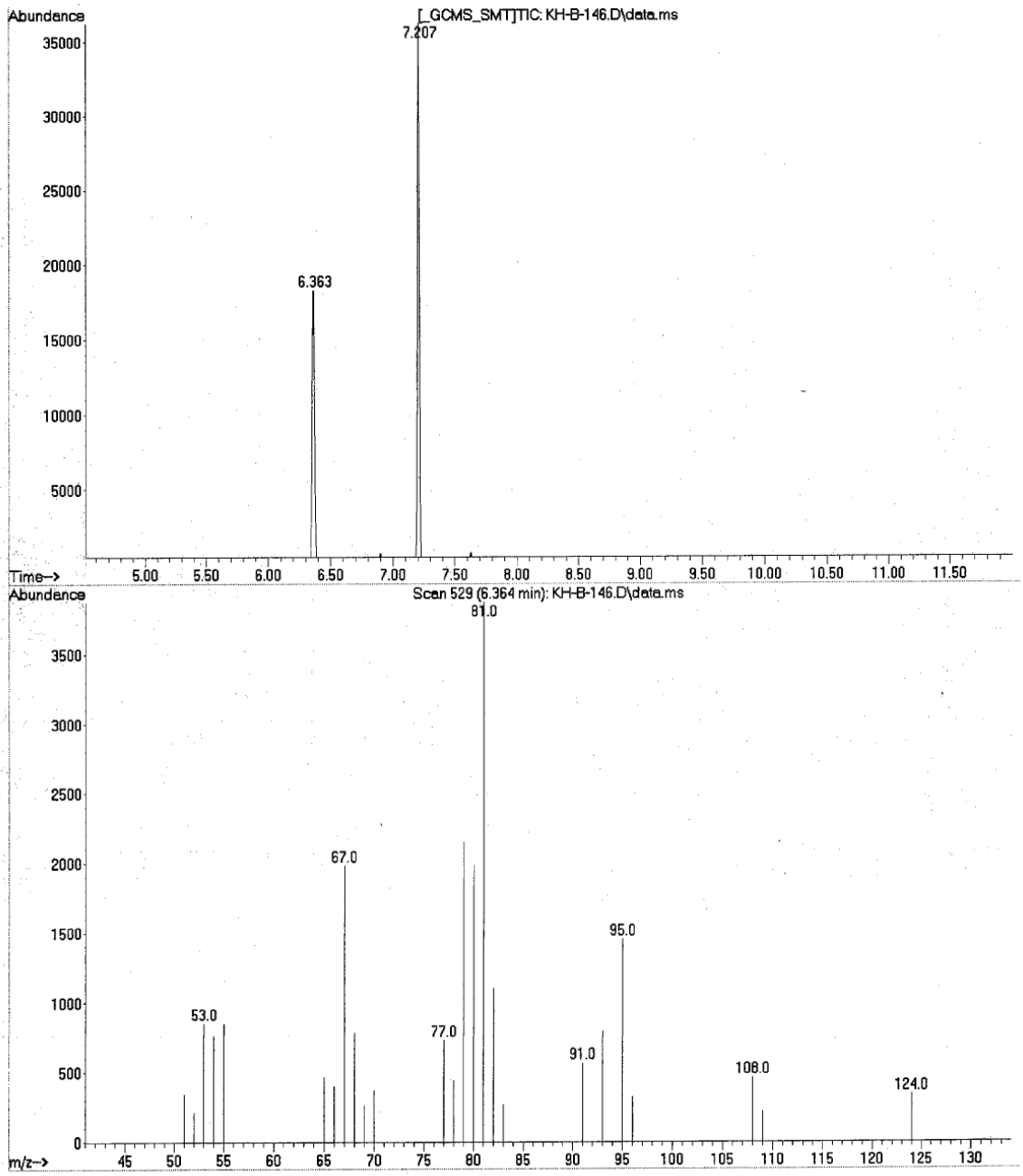
Entry 9: Dodecane internal standard, R_t = 7.208 min. *trans,trans,cis*-1,5,9-cyclododecatriene, R_t = 8.090 min. 13-oxo-bicyclo[10.1.0]trideca-4,8-diene, R_t = 9.614 min. Epoxide product also characterized by ^{1}H NMR.



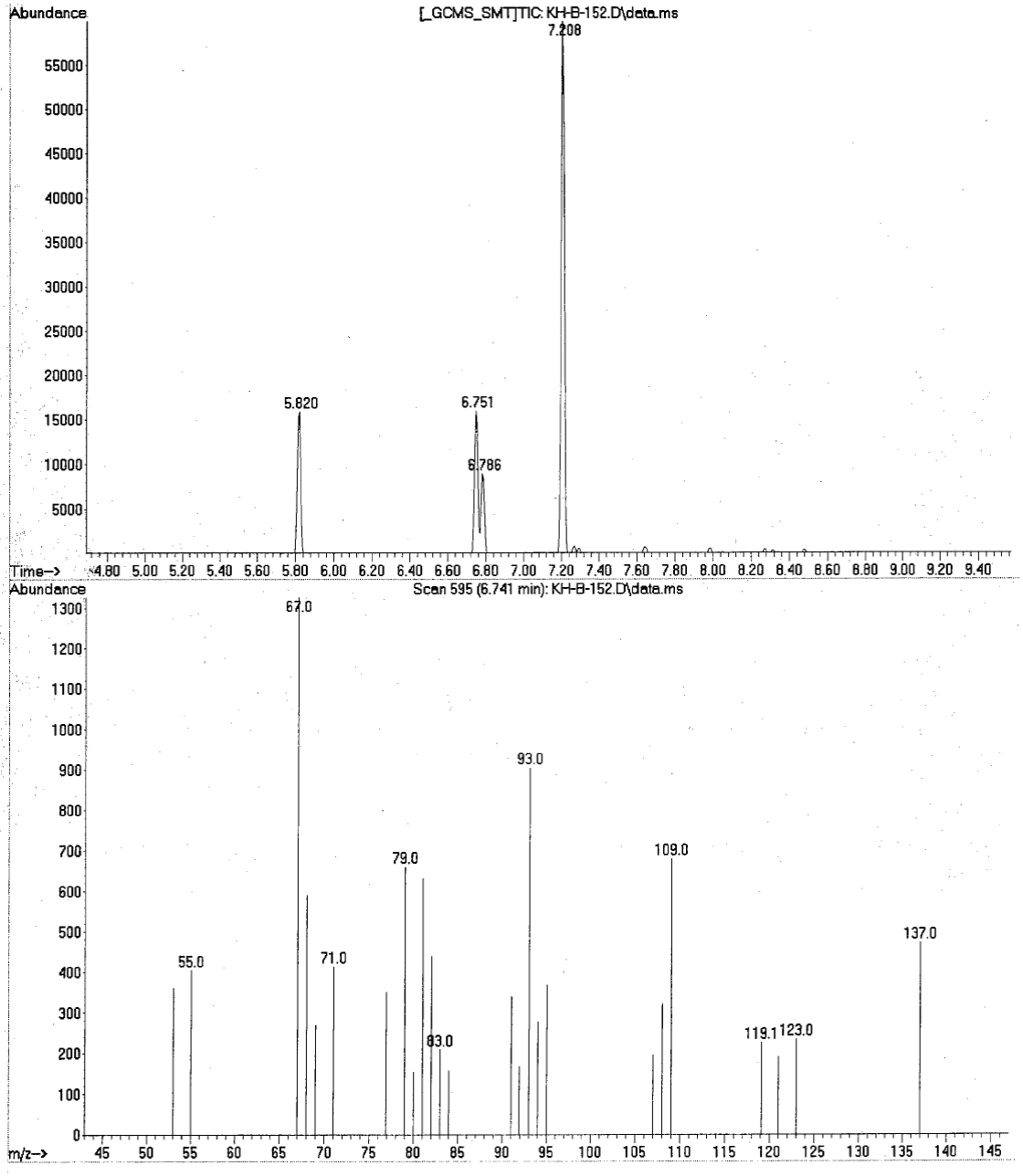
Entry 10: *cis*-Cyclooctene, R_t = 4.526min. *cis*-Cyclooctene oxide, R_t = 6.539 min. Dodecane internal standard, R_t = 7.207 min. By product 8-chlorocyclooctene, R_t = 8.426 min. Epoxide product also characterized by ^{1}H NMR.



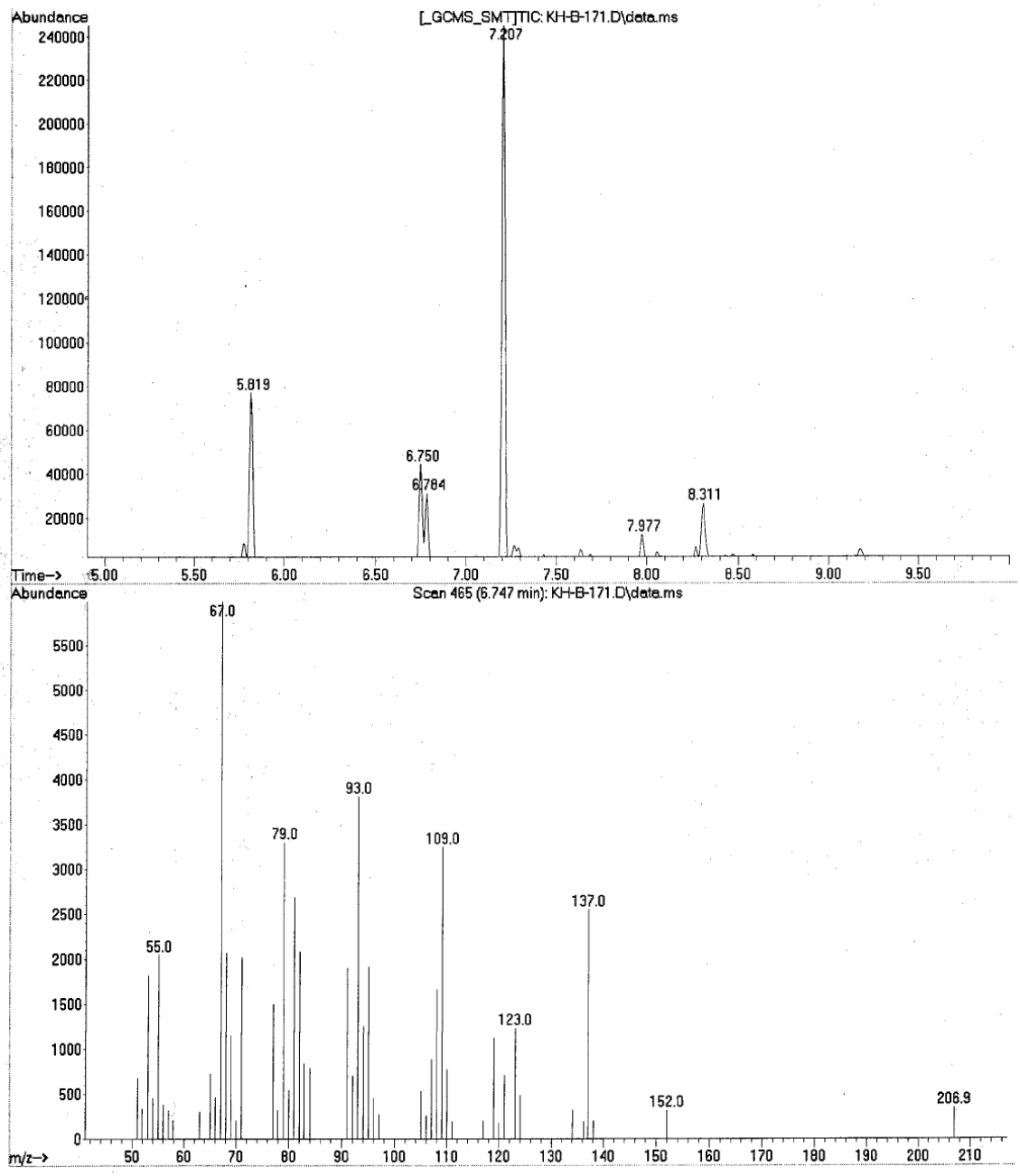
Entry 11: 1,3-cyclooctadiene oxide, R_t = 6.363 min. Dodecane internal standard, R_t = 7.207 min.



Entry 12: R (+) Limonene, R_t = 5.820 min. (+) limonene oxide, R_t = 6.751 and 6.786 min. Dodecane internal standard, R_t = 7.208 min. Confirmed against standard (+) limonene oxide, R_t = 6.751 and 6.786 min.

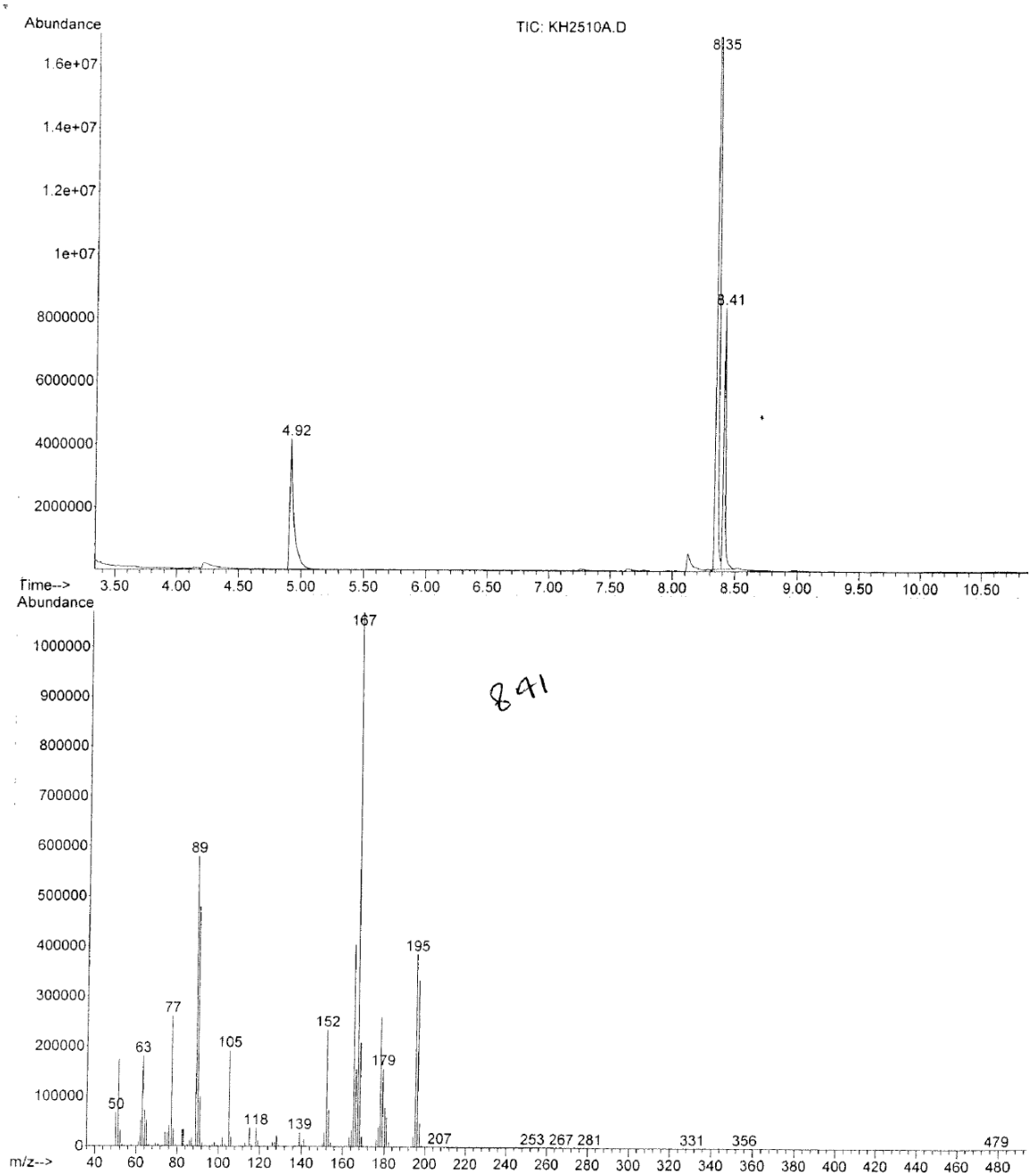


Entry 13: S (-) Limonene, R_t = 5.819 min. (-) limonene oxide, R_t = 6.750 and 6.784 min. Dodecane internal standard, R_t = 7.207 min. Unidentified oxidized products at R_t = 7.977 and 8.311 min.

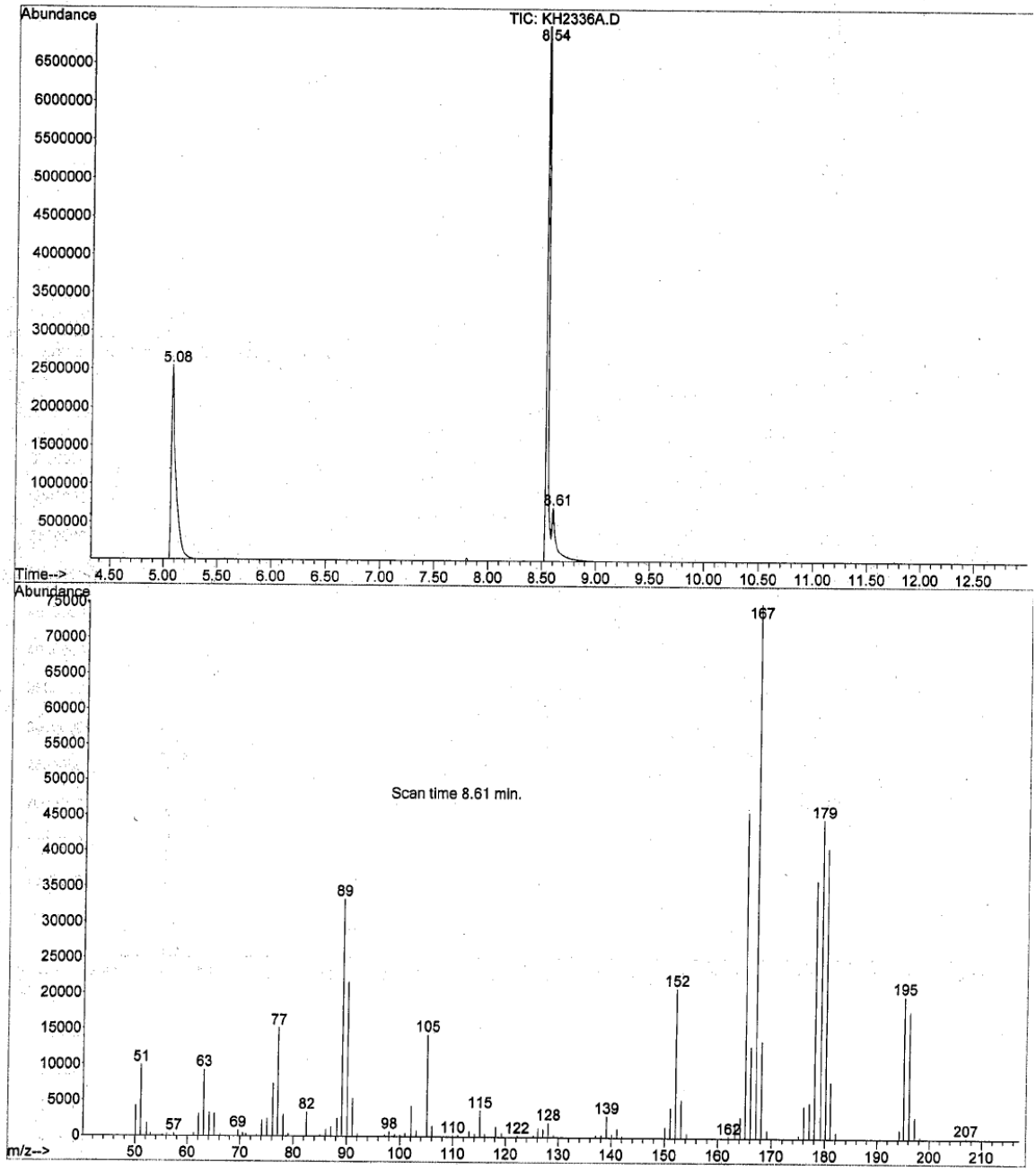


GC Traces and Mass Spectra of Selected Products Given in Table 5:

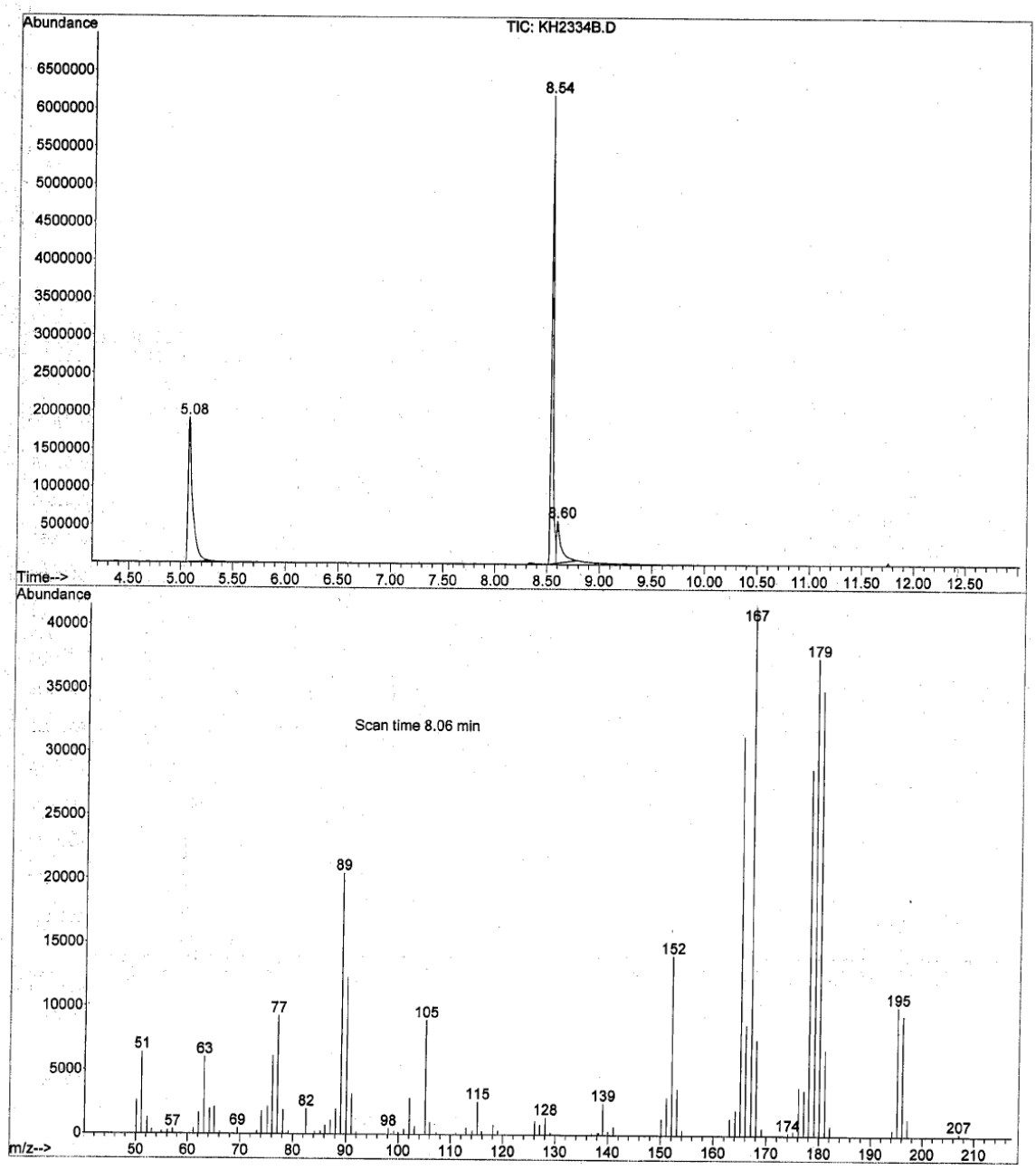
Entry 1: Dodecane internal standard, R_t = 4.92 min. *trans*-Stilbene, R_t = 8.35 min. *trans*-Stilbene oxide, R_t = 8.41 min.



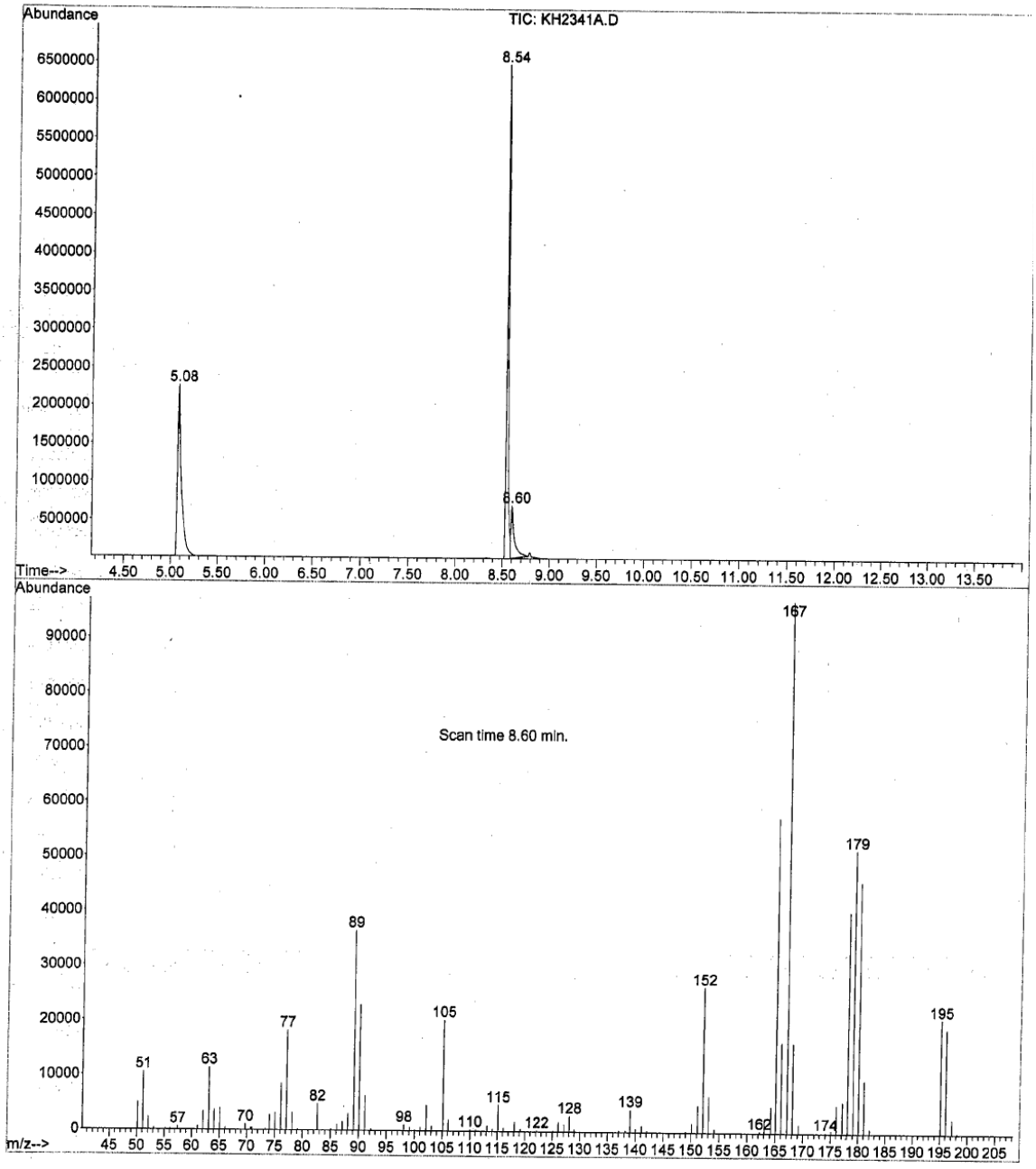
Entry 2: Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.61 min.



Entry 3: Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.60 min.

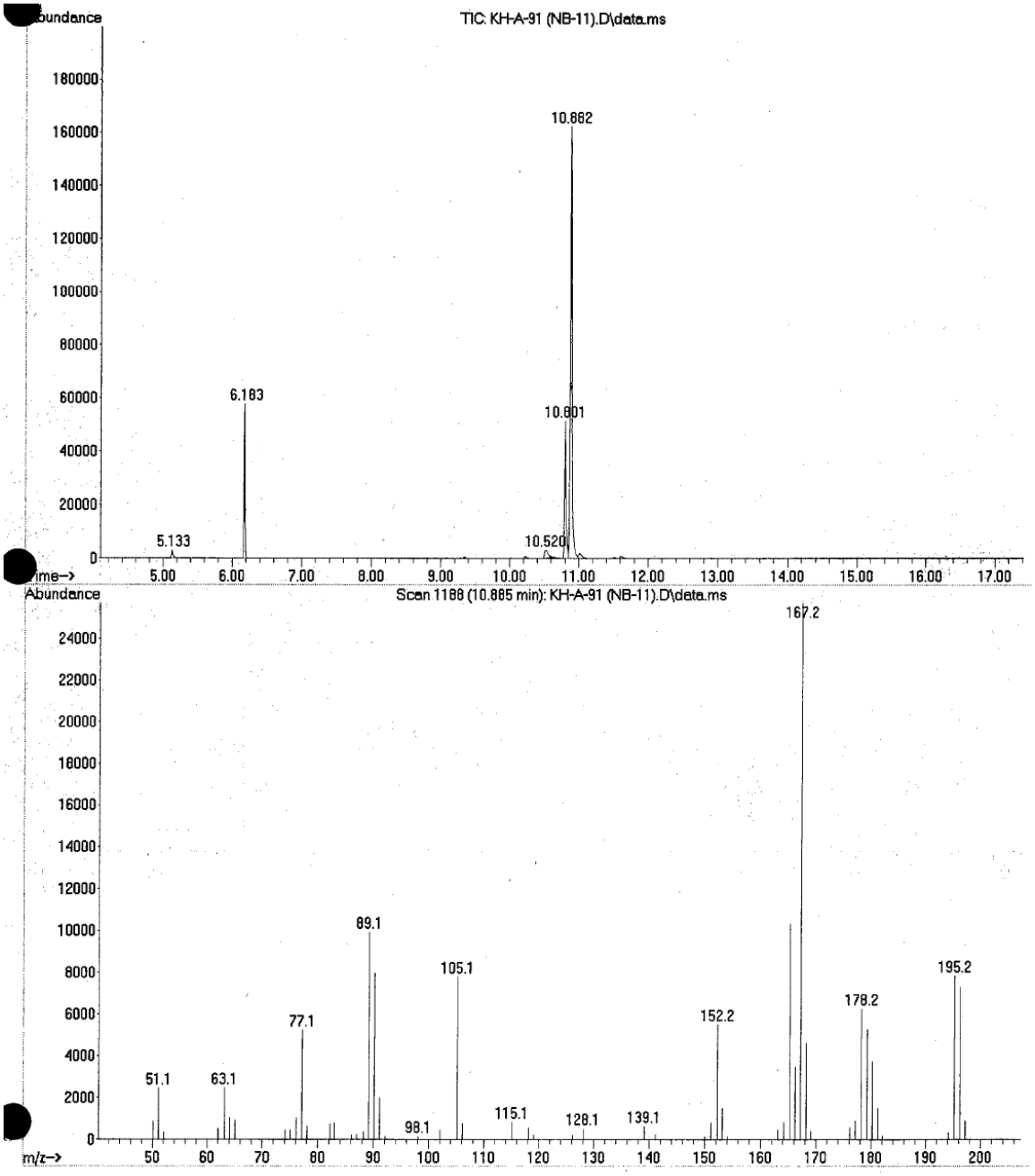


Entry 4: Dodecane internal standard, R_t = 5.08 min. *trans*-Stilbene, R_t = 8.54 min. *trans*-Stilbene oxide, R_t = 8.60 min.

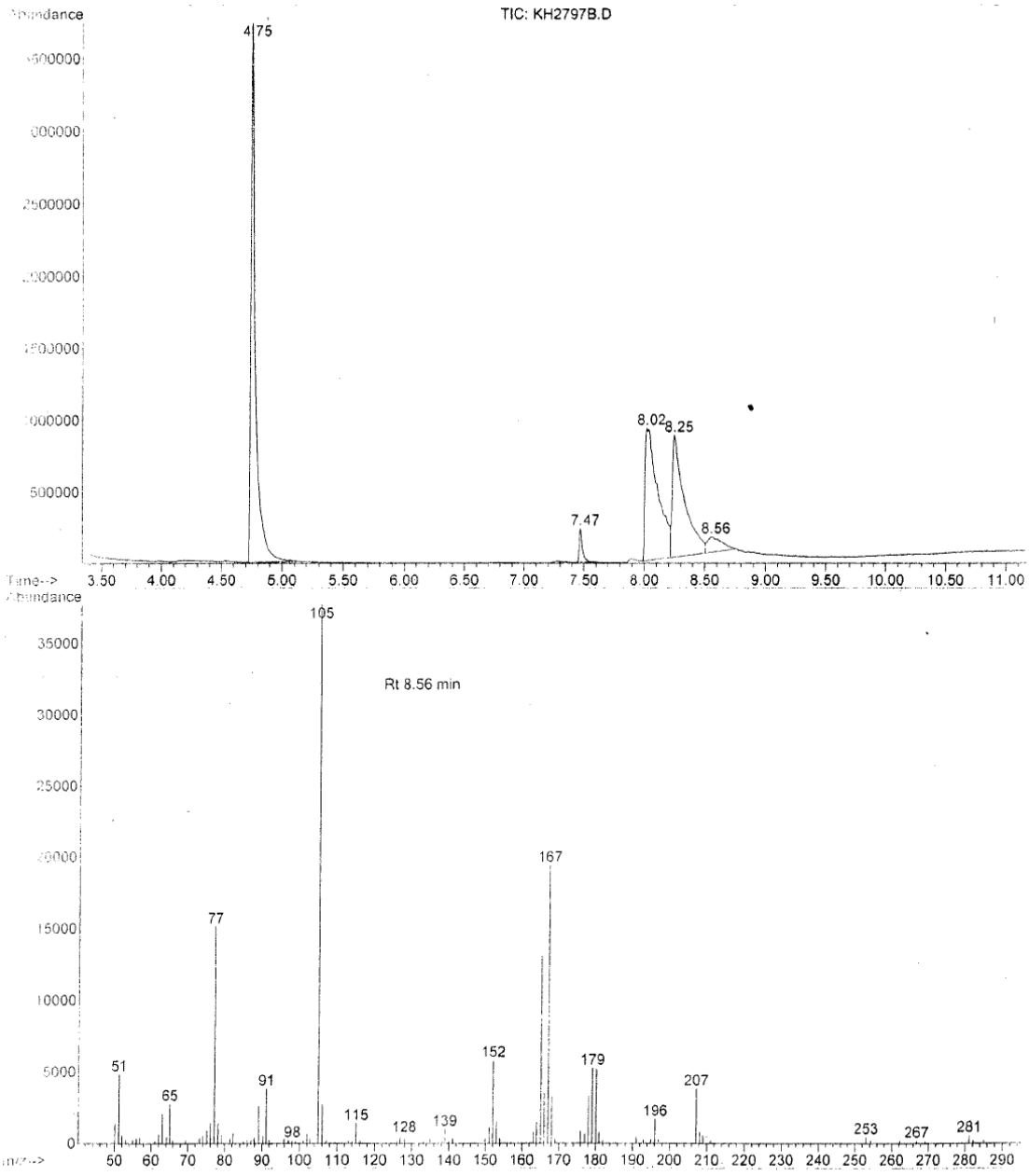


GC Traces and Mass Spectra of Selected Products Given in Table 6:

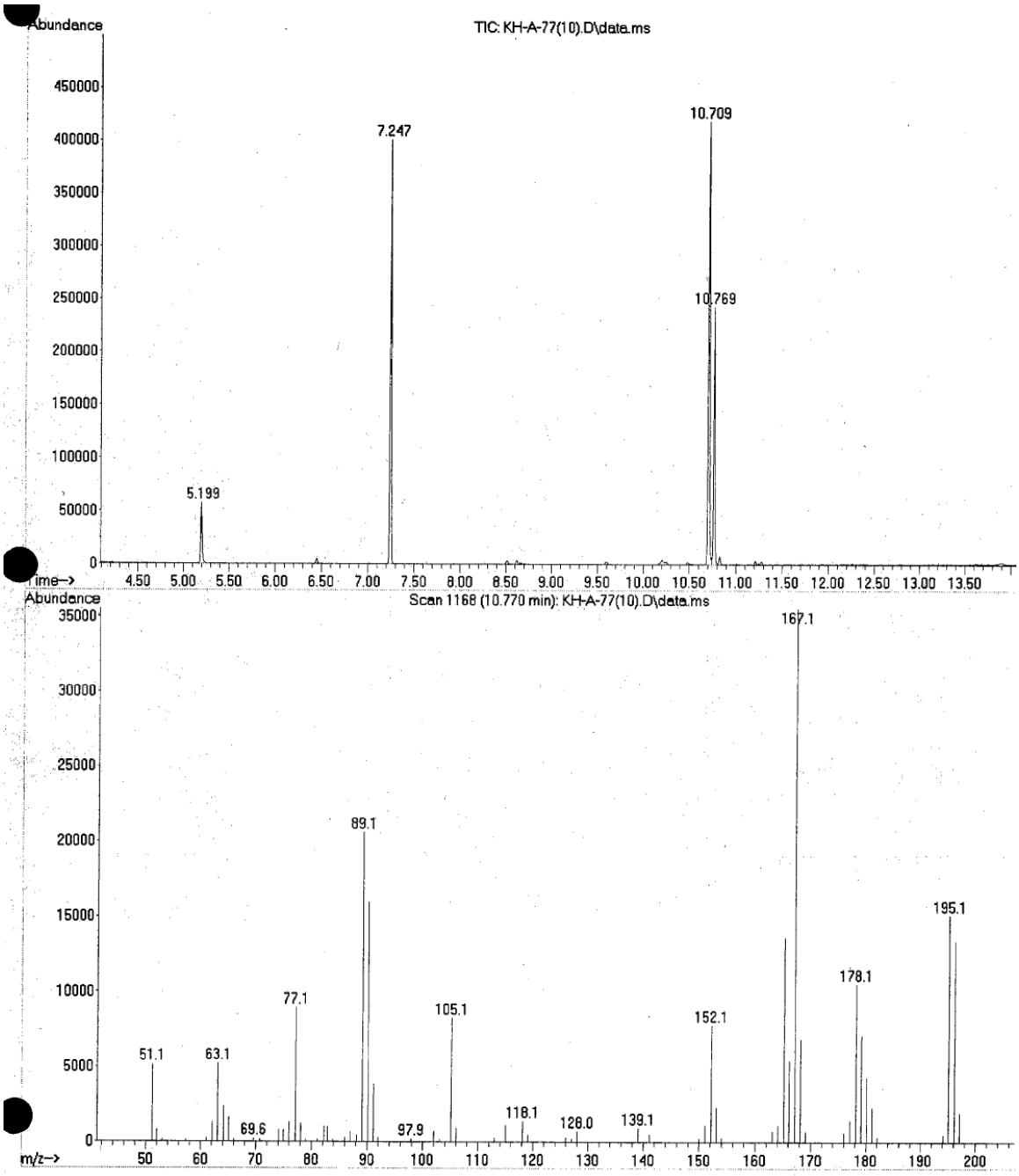
Entry 1: Dodecane internal standard, R_t = 6.183 min. *trans*-Stilbene, R_t = 10.801 min. *trans*-Stilbene oxide, R_t = 10.882 min. Isomer of trans-stilbene oxide R_t = 10.520 min. Unidentified by-product R_t = 5.133 min.



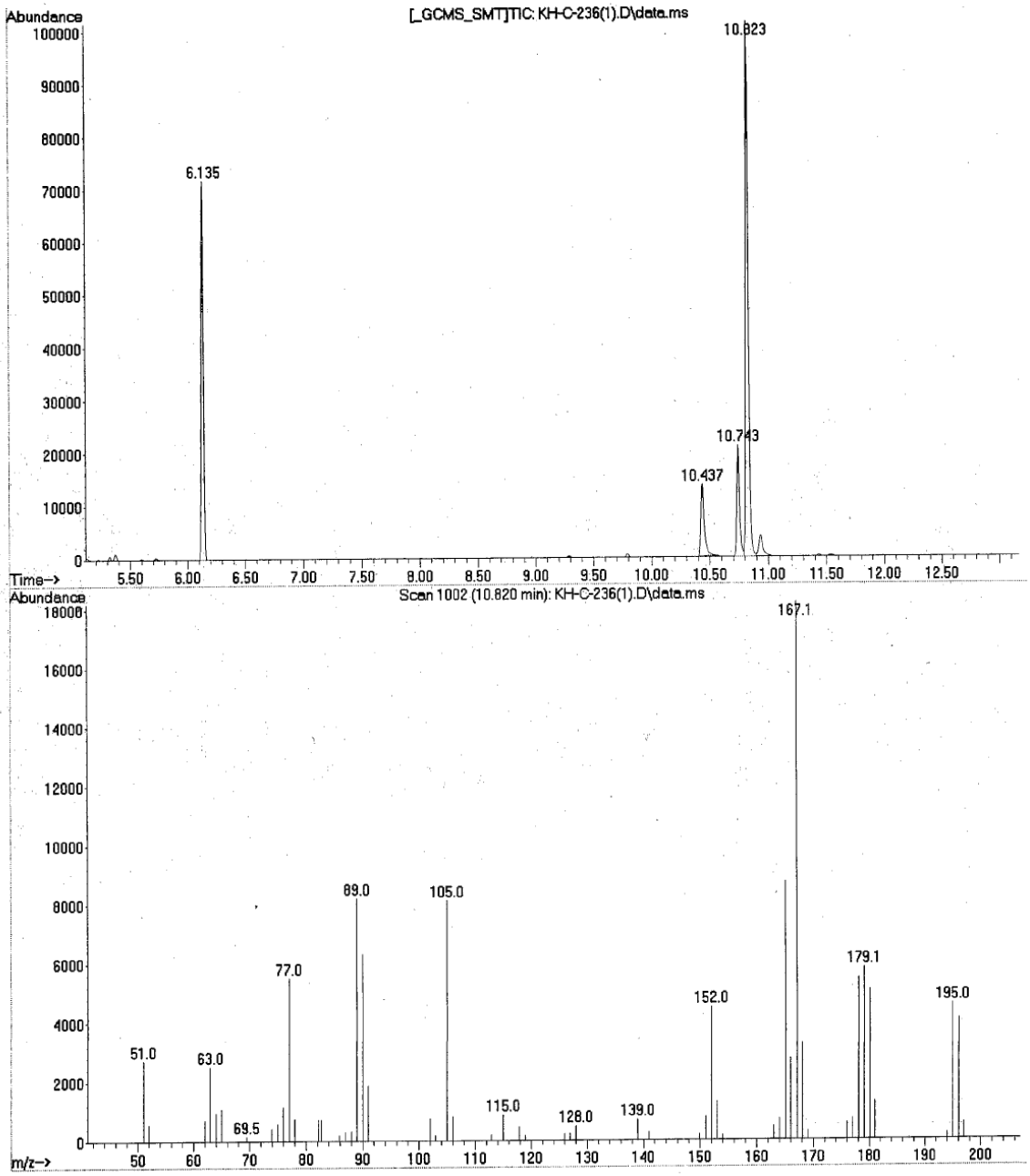
Entry 2: Dodecane internal standard, R_t = 4.75 min. *trans*-Stilbene, R_t = 8.25 min. *trans*-Stilbene oxide, R_t = 8.02 min. and R_t = 8.56 min. Unidentified by-product R_t = 7.47 min.



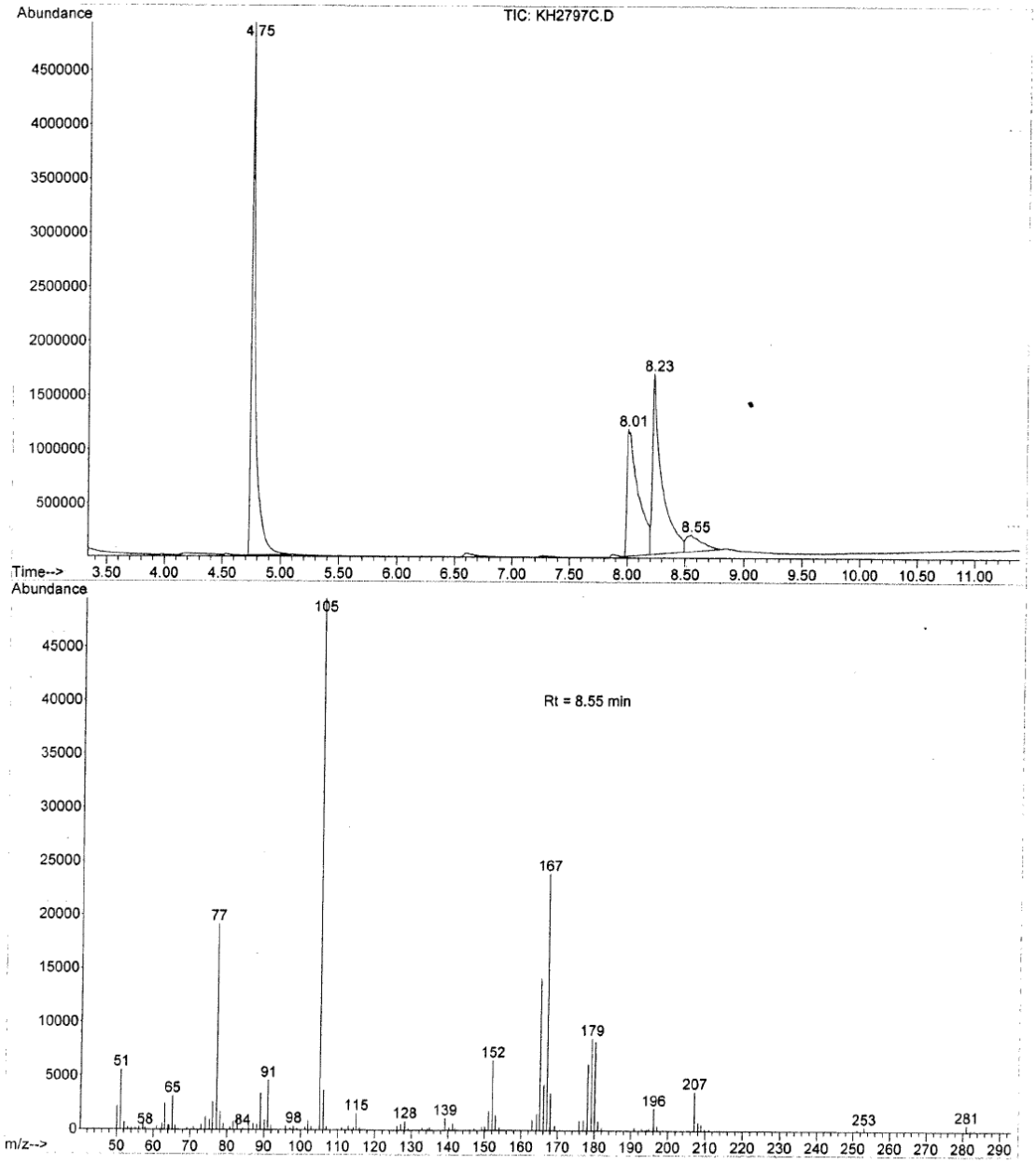
Entry 3: Dodecane internal standard, R_t = 7.247 min. *trans*-Stilbene, R_t = 10.709 min. *trans*-Stilbene oxide, R_t = 10.769 min. By-product benzaldehyde, R_t = 5.199 min.



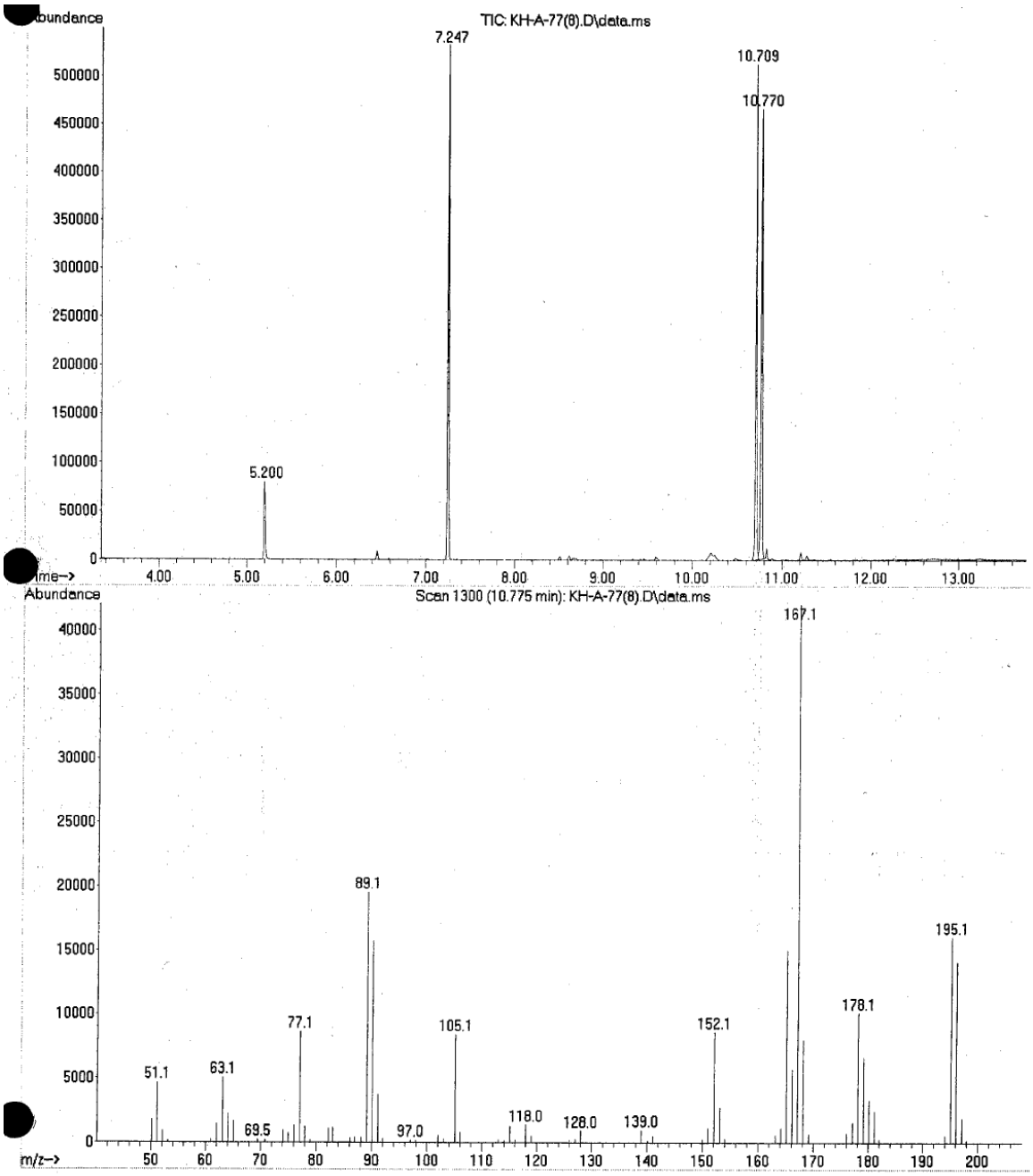
Entry 4: Dodecane internal standard, R_t = 6.135 min. *trans*-Stilbene, R_t = 10.743 min. *trans*-Stilbene oxide, R_t = 10.823 min. Isomer of *trans*-Stilbene oxide, R_t = 10.437 min.



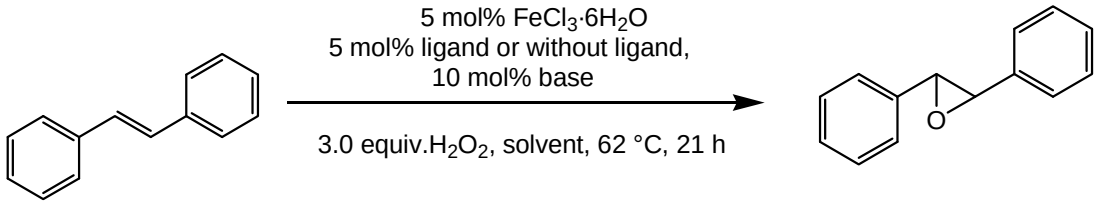
Entry 5: Dodecane internal standard, R_t = 4.75 min. *trans*-Stilbene, R_t = 8.23 min. *trans*-Stilbene oxide, R_t = 8.01 min. and R_t = 8.55 min.



Entry 6: Dodecane internal standard, R_t = 7.247 min. *trans*-Stilbene, R_t = 10.709 min. *trans*-Stilbene oxide, R_t = 10.770 min. By-product benzaldehyde, R_t = 5.200 min.

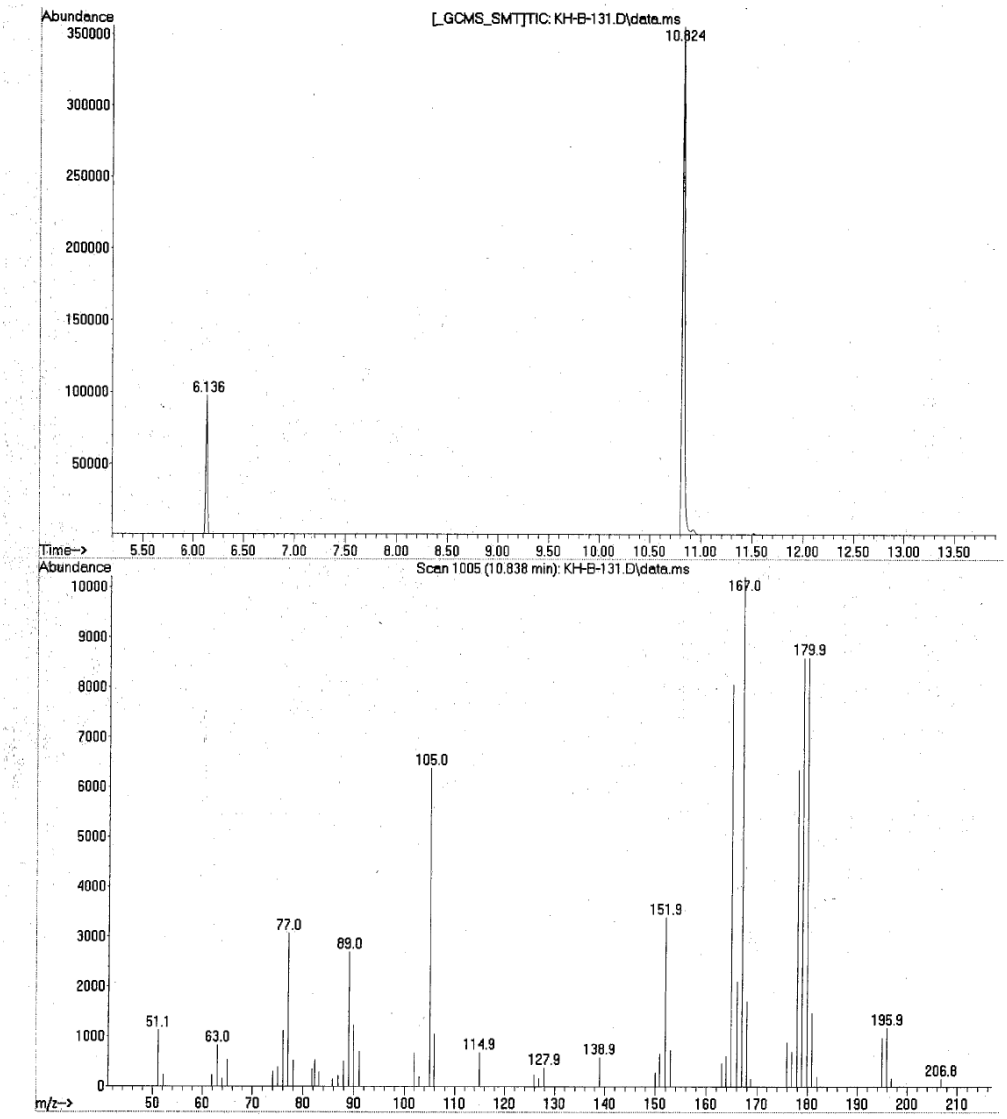


Reaction progress monitoring: Epoxidation of *trans*-stilbene (Figure 3A & B)



Catalytic systems: A) $FeCl_3 \cdot 6H_2O$ and 1-methylimidazole
B) $FeCl_3 \cdot 6H_2O$, 1-methylimidazole and proligand H_2**L7**

A) $FeCl_3 \cdot 6H_2O$ and 1-methylimidazole, GC-MS spectrum after 21 h.
Dodecane internal standard, R_t = 6.136 min. *trans*-Stilbene oxide, R_t = 10.824 min.



B) $FeCl_3 \cdot 6H_2O$, 1-methylimidazole and proligand H_2**L7**. GC-MS spectrum after 19 h.

Dodecane internal standard, R_t = 6.136 min. *trans*-Stilbene, R_t = 10.743 min. *trans*-Stilbene oxide, R_t = 10.821 min. Isomer of *trans*-stilbene, R_t = 9.290 min.