

Electronic Supplementary Information for

Catalytic Alkylation of Aryl Grignard Reagents by Iron(III)
Amine-bis(phenolate) Complexes

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Crystallographic Data for (2)

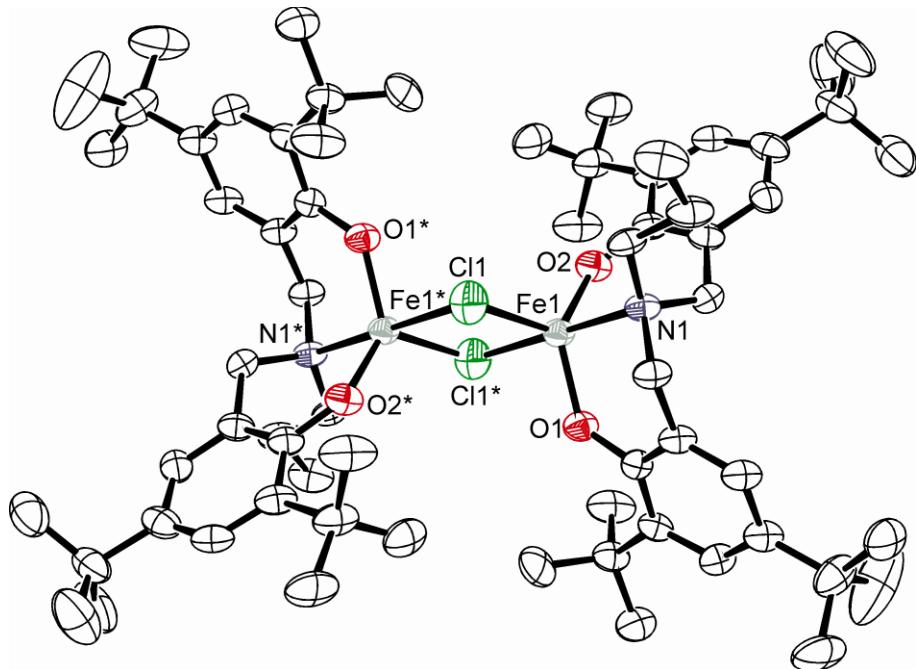


Figure S1: Molecular structure (ORTEP) and partial atom labelling of **2**. Ellipsoids shown at 50% probability. Hydrogen atoms omitted for clarity.

Table S1: Crystallographic data and refinements for **2**

Chemical formula	C ₆₆ H ₁₀₂ Cl ₂ Fe ₂ N ₂ O ₄	V/ Å ³	1663(2)
Formula Weight	1170.14	Z	1
T/K	123(2)	D/g cm ⁻³	1.168
Crystal Color, Habit	Brown, irregular	μ(Mo-Kα)/cm ⁻¹	5.60
Crystal dimensions/mm	0.22 × 0.19 × 0.15	F(000)	630
Crystal System	Triclinic	θ range for collection/°	2.77 to 25.00
Space Group	P-1 (#2)	Reflections collected	11654
a/ Å	10.248(8)	Independent reflections	5702
b/ Å	11.616(9)	R(int)	0.1134
c/ Å	14.662(12)	R, wR ² (all)	0.1381, 0.3897
α/°	99.827(14)	R, wR ² [I > 2σ(I)]	0.1327, 0.3793
β/°	104.057(12)	GOF on F ²	1.627
γ/°	92.03(2)		

Table S2: Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe(1)	Fe(1)	3.3654(11) ⁽¹⁾	Fe1	O1	1.834(4)
Fe1	O2	1.825(4)	Fe1	N1	2.184(4)
Fe1	C11	2.315(3)	Fe1	Cl1	2.495(3) ⁽¹⁾
Cl1	Fe1	2.495(3) ⁽¹⁾	O1	C1	1.351(6)
O2	C33	1.353(6)	N1	C16	1.480(6)
N1	C19	1.491(6)	N1	C15	1.506(6)
C1	C14	1.397(7)	C1	C2	1.407(7)
C2	C7	1.376(7)	C2	C3	1.532(7)
C3	C6	1.504(8)	C3	C5	1.539(7)
C3	C4	1.540(8)	C7	C8	1.402(7)
C8	C13	1.373(7)	C8	C9	1.512(8)
C9	C10	1.498(12)	C9	C12	1.512(9)
C9	C11	1.522(11)	C13	C14	1.383(7)
C14	C15	1.491(7)	C16	C17	1.509(8)
C17	C18	1.505(8)	C19	C20	1.488(6)
C20	C21	1.375(7)	C20	C33	1.387(7)
C21	C22	1.391(8)	C22	C27	1.384(9)
C22	C23	1.539(8)	C23	C25	1.507(9)
C23	C24	1.517(11)	C23	C26	1.538(10)
C27	C28	1.377(8)	C28	C33	1.415(7)
C28	C29	1.544(8)	C29	C32	1.495(10)
C29	C30	1.554(8)	C29	C31	1.558(8)

Symmetry Operators: (1) -x + 1, -y + 1, -z + 1

Table S3: Selected bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Fe(1)	Cl(1) ⁽¹⁾	91.27(7)	Cl(1)	Fe(1)	O(1)	112.12(12)
Cl(1)	Fe(1)	O(2)	118.89(12)	Cl(1)	Fe(1)	N(1)	91.86(11)
Cl(1) ⁽¹⁾	Fe(1)	O(1)	89.18(13)	Cl(1) ⁽¹⁾	Fe(1)	O(2)	89.23(13)
Cl(1) ⁽¹⁾	Fe(1)	N(1)	176.57(11)	O(1)	Fe(1)	O(2)	128.99(15)
O(1)	Fe(1)	N(1)	90.93(16)	O(2)	Fe(1)	N(1)	88.04(16)
Fe(1)	Cl(1)	Fe(1) ⁽¹⁾	88.73(6)	Fe(1)	O(1)	C(1)	134.8(3)
Fe(1)	O(2)	C(33)	137.5(3)	Fe(1)	N(1)	C(15)	105.9(3)
Fe(1)	N(1)	C(16)	113.0(3)	Fe(1)	N(1)	C(19)	105.9(2)
C(15)	N(1)	C(16)	110.2(3)	C(15)	N(1)	C(19)	109.0(3)
C(16)	N(1)	C(19)	112.5(4)	O(1)	C(1)	C(2)	121.3(4)
O(1)	C(1)	C(14)	118.2(4)				

Symmetry Operators: (1) -x + 1, -y + 1, -z + 1

Table S4: Selected torsion angles (°)

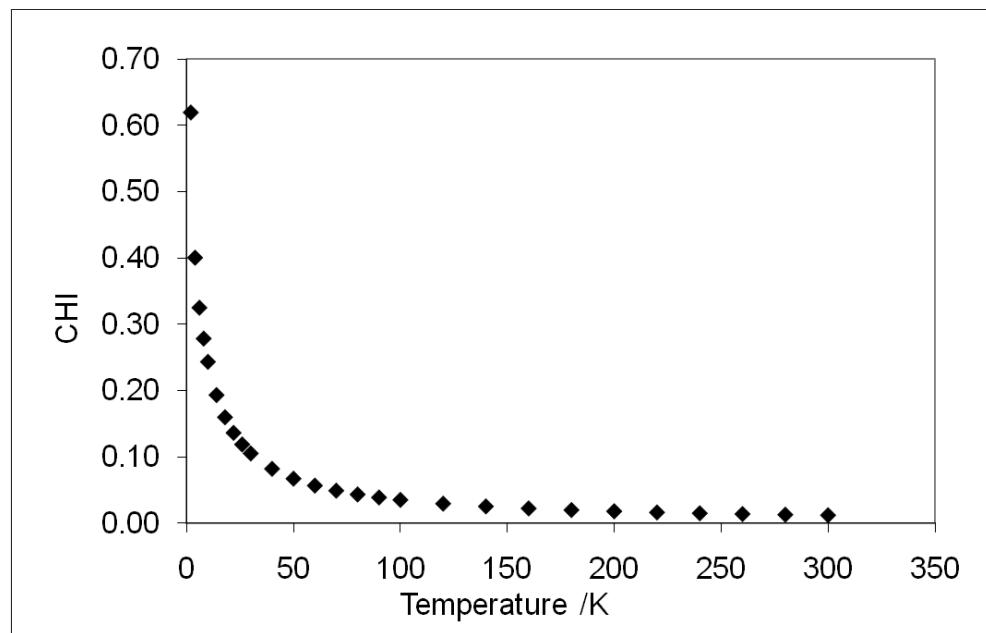
atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl(1)	Fe(1)	O(1)	C(1)	-107.8(3)	O(1)	Fe(1)	Cl(1)	Fe(1) ⁽¹⁾	-89.63(14)
Cl(1)	Fe(1)	O(2)	C(33)	100.3(4)	O(2)	Fe(1)	Cl(1)	Fe(1) ⁽¹⁾	89.82(15)
Cl(1)	Fe(1)	N(1)	C(15)	83.0(2)	Cl(1)	Fe(1)	N(1)	C(16)	-37.8(3)
Cl(1)	Fe(1)	N(1)	C(19)	-161.4(2)	N(1)	Fe(1)	Cl(1)	Fe(1) ⁽¹⁾	178.61(12)
Cl(1) ⁽¹⁾	Fe(1)	O(1)	C(1)	161.1(3)	O(1)	Fe(1)	Cl(1) ⁽¹⁾	Fe(1) ⁽¹⁾	112.11(12)
Cl(1) ⁽¹⁾	Fe(1)	O(2)	C(33)	-168.7(4)	O(2)	Fe(1)	Cl(1) ⁽¹⁾	Fe(1) ⁽¹⁾	-118.88(12)
Cl(1) ⁽¹⁾	Fe(1)	N(1)	C(15)	-121(2)	Cl(1) ⁽¹⁾	Fe(1)	N(1)	C(16)	118.3(19)
Cl(1) ⁽¹⁾	Fe(1)	N(1)	C(19)	-5(2)	N(1)	Fe(1)	Cl(1) ⁽¹⁾	Fe(1) ⁽¹⁾	-156(2)
O(1)	Fe(1)	O(2)	C(33)	-80.4(4)	O(2)	Fe(1)	O(1)	C(1)	72.8(4)
O(1)	Fe(1)	N(1)	C(15)	-29.2(2)	O(1)	Fe(1)	N(1)	C(16)	-149.9(3)
O(1)	Fe(1)	N(1)	C(19)	86.5(2)	N(1)	Fe(1)	O(1)	C(1)	-15.4(3)
O(2)	Fe(1)	N(1)	C(15)	-158.2(2)	O(2)	Fe(1)	N(1)	C(16)	81.1(3)
O(2)	Fe(1)	N(1)	C(19)	-42.5(2)	N(1)	Fe(1)	O(2)	C(33)	9.2(4)
Fe(1)	O(1)	C(1)	C(2)	-149.3(3)	Fe(1)	O(1)	C(1)	C(14)	29.9(6)
Fe(1)	O(2)	C(33)	C(20)	9.4(6)	Fe(1)	O(2)	C(33)	C(28)	-171.7(3)
Fe(1)	N(1)	C(15)	C(14)	65.0(4)	Fe(1)	N(1)	C(16)	C(17)	-171.4(3)
Fe(1)	N(1)	C(19)	C(20)	67.8(4)					

Symmetry Operators: (1) -x + 1, -y + 1, -z + 1

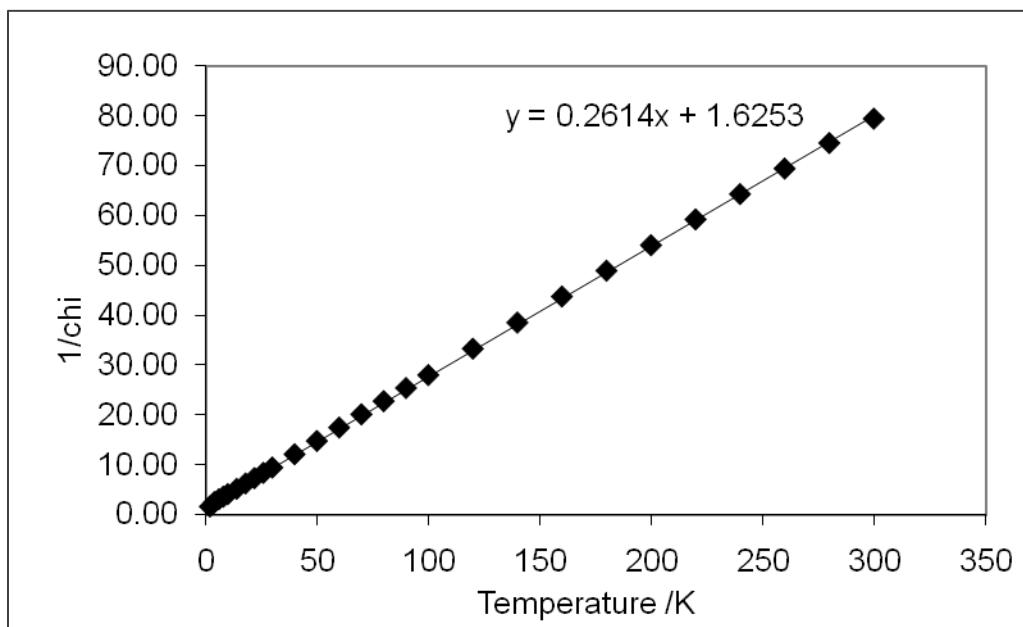
The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Variable Temperature Magnetic Data for (1)

Magnetic susceptibility, χ , (per iron) vs. temperature for (1)



Inverse of Susceptibility vs. temperature for (1)



¹H NMR data of cross-coupled products and radical clock experiments

Entry 1: 1-cyclohexylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.44 (m, 1H, ArCH); 1.36-1.80 (m, 10H, CH₂).

Entry 2: 1-cyclohexyl-3-methoxybenzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.79 (s, 3H, OCH₃); 2.47 (m, H, ArCH); 1.46-1.86 (m, 10H).

Entry 3: 1-cyclohexyl-4-fluorobenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.47 (m, 1H, ArCH); 1.39-1.84 (m, 10H, CH₂).

Entry 5: 1-cyclohexylnaphthalene. ¹H NMR (500 MHz, CDCl₃, δ): 3.32 (m, 1H, ArCH); 1.55-2.03 (m, 10H, CH₂).

Entry 6: 1-cyclohexyl-4-methylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 7.08 (m, 4H); 2.45 (m, 1H, ArCH); 2.30 (s, 3H, ArCH₃); 1.81 (m, 5H CH₂); 1.27 (m, 5H, CH₂).

Entry 7: 1-cyclohexyl-2-methylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 7.14 (m, 4H, ArH); 2.70 (m, 1H, ArCH); 2.33 (s, 3H, ArCH₃); 2.15 (m, 5H, CH₂); 1.53 (m, 2H, CH₂); 1.39 (m, 3H, CH₂).

Entry 8: 1-cyclohexyl-4-methoxybenzene. ¹H NMR (500 MHz, CDCl₃, δ): 7.13 (d, 2H); 6.84 (d, 2H); 3.79 (s, 3H, OCH₃); 2.44 (m, 1H, ArCH); 1.81 (m, 5H, CH₂); 1.30 (m, 5H, CH₂).

Entry 9: 1-benzyl-2-methylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.79 (s, 2H, CH₂); 2.33 (s, 3H, ArCH₃).

Entry 10: 2-benzyl-1,3-dimethylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 4.05 (s, 2H, ArCH₂Ar); 2.23 (s, 6H, ArCH₃).

Entry 11: 1,3-bis(2-methylbenzyl)benzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.93 (s, 4H, ArCH₂Ar); 2.23 (s, 6H, ArCH₃).

Entry 12: 1,3-bis(2,6-dimethylbenzyl)benzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.74 (s, 4H, CH₂); 2.24 (s, 6H, ArCH₃).

Entry 13: 1-(3-chloropropyl)-2-methylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.51 (t, 2H, CH₂Cl); 2.70 (t, 2H, ArCH₂); 2.33 (s, 3H, ArCH₃); 1.84 (m, 2H, ArCH₂CH₂).

Entry 14: 1-(3-chloropropyl)-4-fluorobenzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.51 (dd, 2H, CH₂Cl); 2.75 (t, 2H, ArCH₂); 2.05 (t, 2H, CH₂).

Entry 15: 1-(4-chlorobutyl)-2-methylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 3.56 (m, 2H, CH₂Cl); 2.62 (m, 2H, ArCH₂); 1.81 (m, 2H, CH₂CH₂Cl); 1.69 (m, 2H, ArCH₂CH₂).

Entry 16: 1-methyl-2-octylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 7.41 (s, br, 4H, ArH); 2.71 (t, 2H, ArCH₂); 2.45 (s, 3H, ArCH₃); 1.74 (m, 2H, CH₂CH₃); 1.44 (m, 10H, CH₂); 1.03 (t, 3H, CH₂CH₃).

Entry 17: 1,3-dimethyl-2-octylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.58 (m, 2H, ArCH₂); 2.34 (s, 6H, ArCH₃); 1.89 (m, 2H, ArCH₂CH₂); 1.28 (s, 10H, CH₂); 0.88 (dd, 3H, CH₃).

Entry 19: 1-methyl-2-propylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.58 (m, 2H, ArCH₂); 2.29 (s, 3H, ArCH₃); 1.60 (dt, 2H, ArCH₂); 0.98 (m, 2H, CH₃).

Entry 20: 1-fluoro-4-propylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.60 (t, 2H, ArCH₂); 1.66 (m, 2H, CH₂); 0.92 (t, 3H, CH₃).

Entry 21: 1,3-dimethyl-2-propylbenzene. ¹H NMR (500 MHz, CDCl₃, δ): 2.41 (t, 2H, ArCH₂); 2.32 (s, 6H, ArCH₃); 1.45(m, 2H, ArCH₂CH₂); 0.92 (t, 3H, CH₃).

Entry 23: 1-sec-butyl-4-methoxybenzene. ^1H NMR (500 MHz, CDCl_3 , δ): 3.78 (s, 3H, OCH_3); 2.27 (m, 1H, ArCH); 1.42 (dt, 2H, CHCH_2); 1.12 (t, 3H, CHCH_3); 0.87 (t, 3H, CH_2CH_3).

Entry 24: 1-sec-butyl-2-methylbenzene. ^1H NMR (500 MHz, CDCl_3 , δ): 2.33 (m, H, ArCH); 2.09 (s, 3H, ArCH_3); 1.46 (m, 2H, ArCH_2); 1.29 (m, 3H, CHCH_3); 0.92 (t, 3H, CH_2CH_3).

Entry 25: sec-butylbenzene. ^1H NMR (500 MHz, CDCl_3 , δ): 2.35 (m, H, ArCH); 1.45 (m, 2H, CHCH_2); 1.33 (m, 3H, CHCH_3); 0.95 (t, 3H, CH_2CH_3).

Entry 26: 1-sec-butyl-4-methylbenzene. ^1H NMR (500 MHz, CDCl_3 , δ): 2.38 (s, 3H, ArCH_3); 2.34 (m, H, ArCH); 1.55 (m, 2H, CHCH_2); 1.26 (m, 3H, CHCH_3); 0.88 (m, 3H, CH_2CH_3).

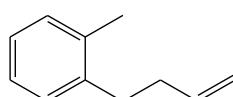
Entry 27: 2-(2-methylphenethyl)-1,3-dioxane. ^1H NMR (500 MHz, CDCl_3 , δ): 4.52 (t, H, CH); 4.12(m, 2H, OCH); 3.75(m, 2H, OCH); 2.71 (m, 2H, ArCH_2); 2.31(s, 3H, ArCH_3); 2.01 (m, 2H, $\text{CH}_2\text{CH}_2\text{CH}$); 1.87(m, 2H, $\text{CH}_2\text{CH}_2\text{CH}_2$).

Entry 29: ethyl 6-o-tolylhexanoate. ^1H NMR (500 MHz, CDCl_3 , δ): 4.12 (q, 2H, CH_2CH_3); 2.89 (t, 2H, ArCH_2); 2.59 (dd, 2H, CH_2CO); 2.30 (s, 3H, ArCH_3); 1.66 (m, 2H, ArCH_2CH_2 ; 2H, $\text{CH}_2\text{CH}_2\text{CO}$); 1.40 (dt, 3H, CH_3).

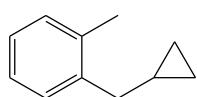
Entry 30: ethyl 6-(4-fluorophenyl)hexanoate. ^1H NMR (500 MHz, CDCl_3 , δ): 4.15 (qq, 2H, OCH_2); 2.61 (m, 2H, ArCH_2); 2.32 (m, 2H, CH_2CO); 1.65 (m, 2H, ArCH_2CH_2 ; 2H, $\text{CH}_2\text{CH}_2\text{CO}$); 1.30 (m, 2H, $\text{ArCH}_2\text{CH}_2\text{CH}_2$; m, 3H, CH_3).

Entry 32: 2-phenylbicyclo[2.2.1]heptane. ^1H NMR (500 MHz, CDCl_3 , δ): 2.73 (m, H, ArCH); 2.33 (t, 2H, CHCH_2CH); 1.42-1.78 (m, 8H).

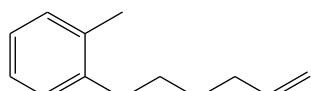
NMR Data for “Radical Clock” Experiments



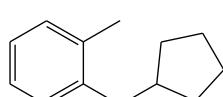
1-(but-3-enyl)-2-methylbenzene (500 MHz, CDCl_3 , δ): 5.81(ddt, $=\text{CH}$, 1H,); 4.97(m, $=\text{CH}_2$, 2H,); 2.59(m, CH_2 , 2H,); 2.29(s, CH_3 , 3H,); 2.09(m, CH_2 , 2H,).



1-(cyclopropylmethyl)-2-methylbenzene (500 MHz, CDCl_3 , δ): 2.61(m, CH_2 , 2H,); 2.30(s, CH_3 , 3H,); ~1.5(m, C_3H_5 , 5H).



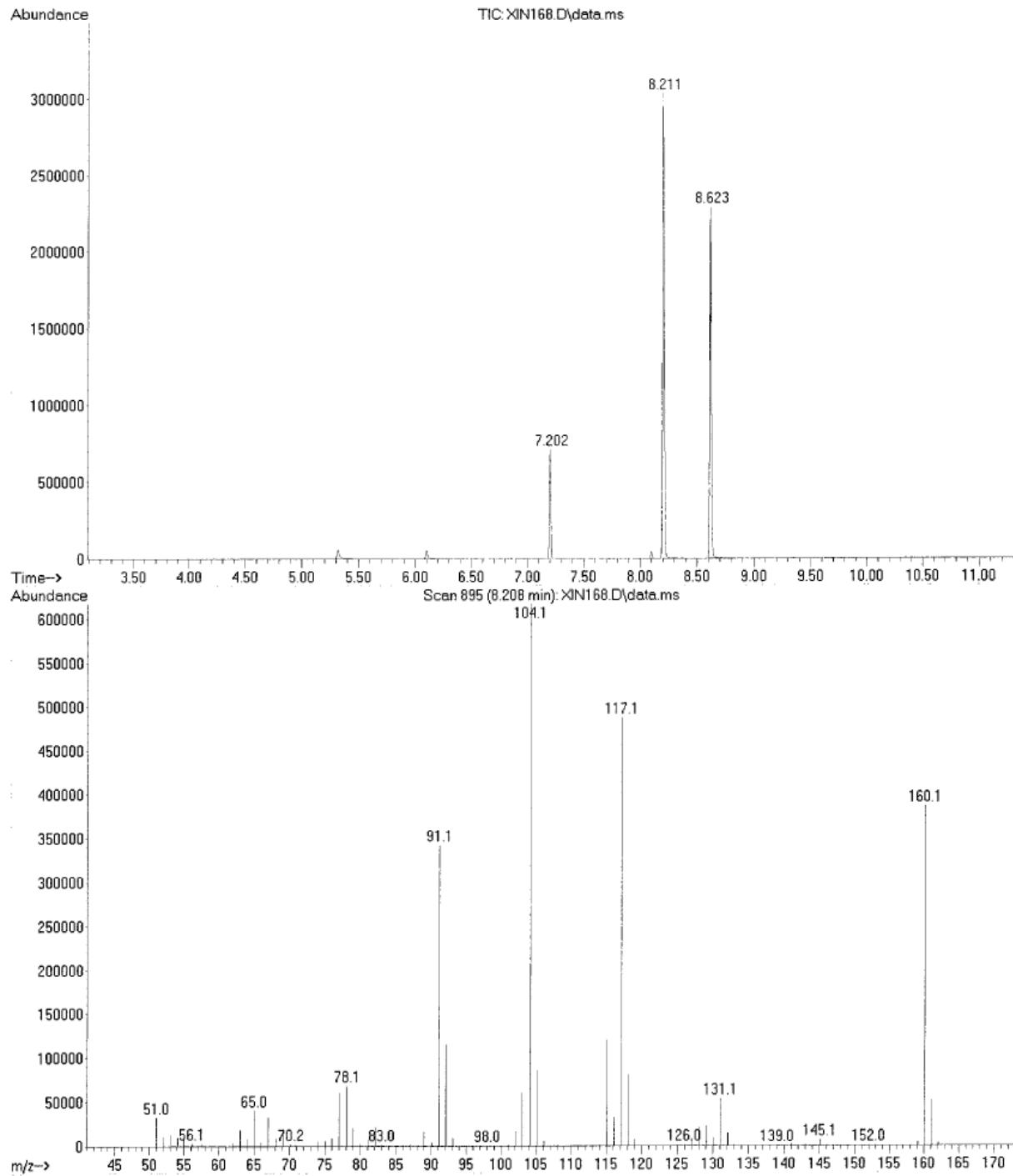
1-(hex-5-enyl)-2-methylbenzene (500 MHz, CDCl_3 , δ): 5.88(m, $=\text{CH}$, 1H,); 5.02(dd, $=\text{CH}_2$, 2H,); 2.69(m, CH_2 , 2H,); 2.30(s, CH_3 , 3H,); 2.14(m, CH_2 , 2H,).



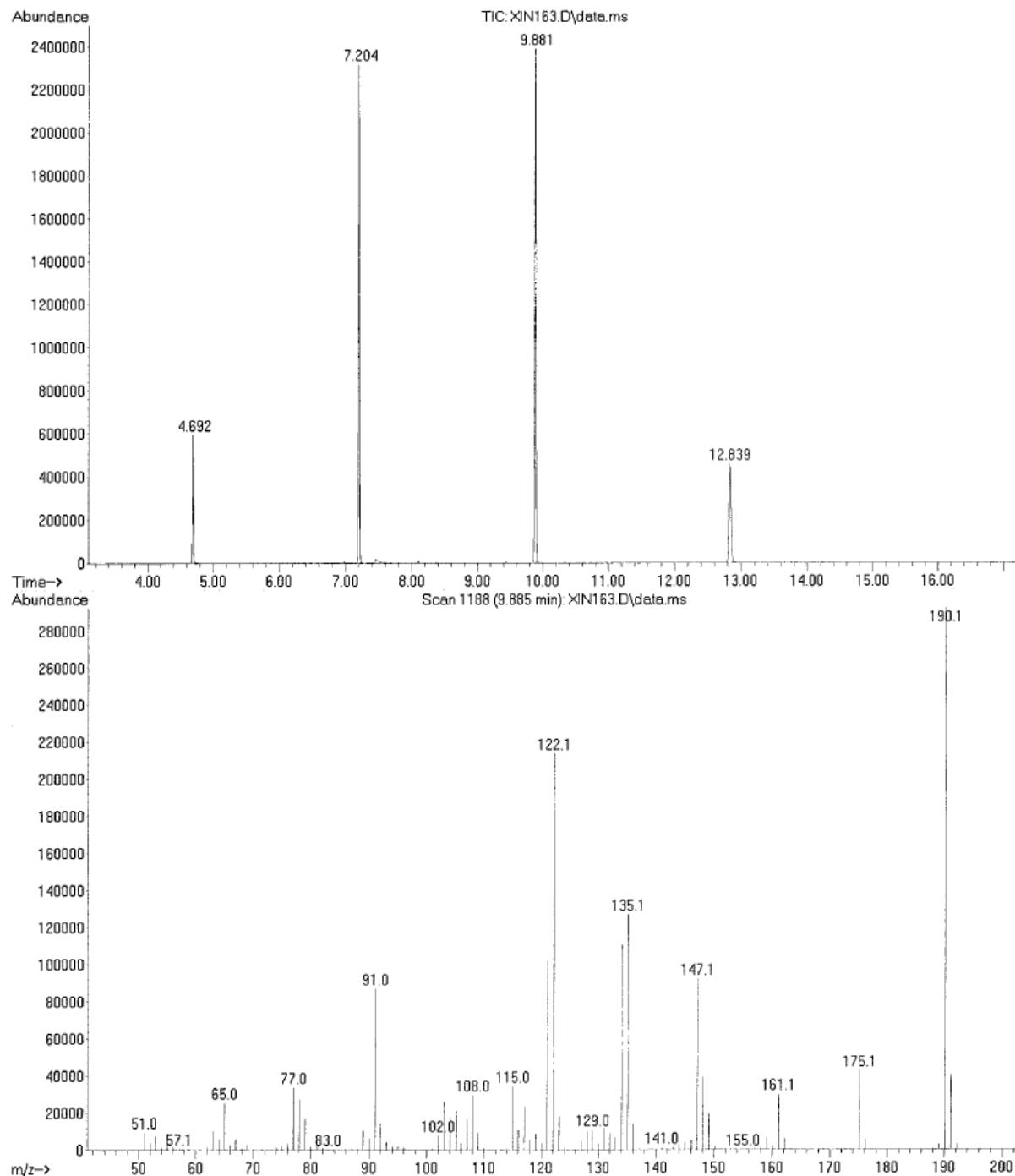
1-(cyclopentylmethyl)-2-methylbenzene (500 MHz, CDCl_3 , δ): 2.33(m, CH_2 , 2H,); 2.30(s, CH_3 , 3H,); 2.01(m, CH , 1H).

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

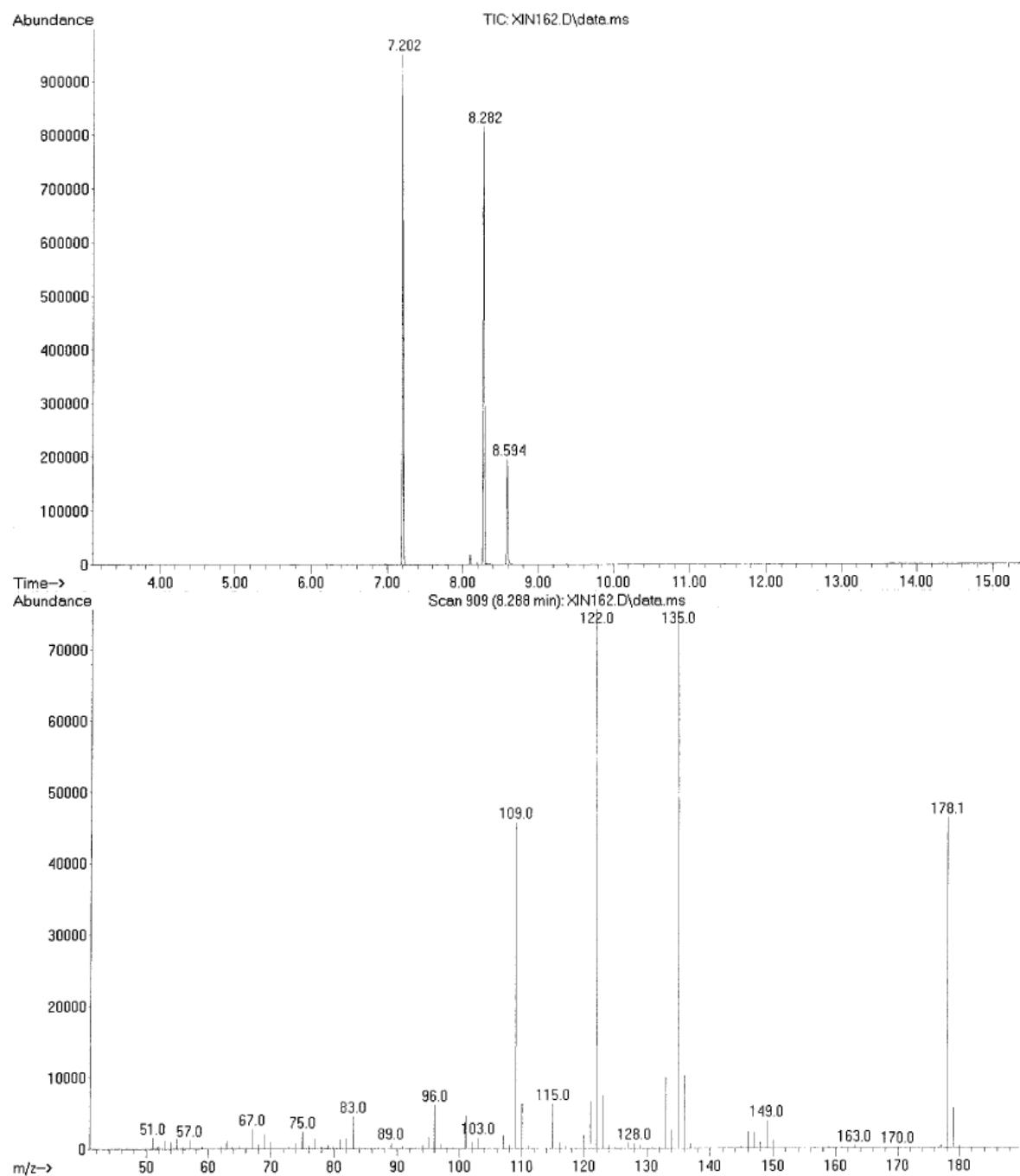
Entry 1: Dodecane internal standard: $R_t = 7.202$ min. Cyclohexylbenzene: $R_t = 8.211$ min. By-product, biphenyl: $R_t = 8.623$ min.



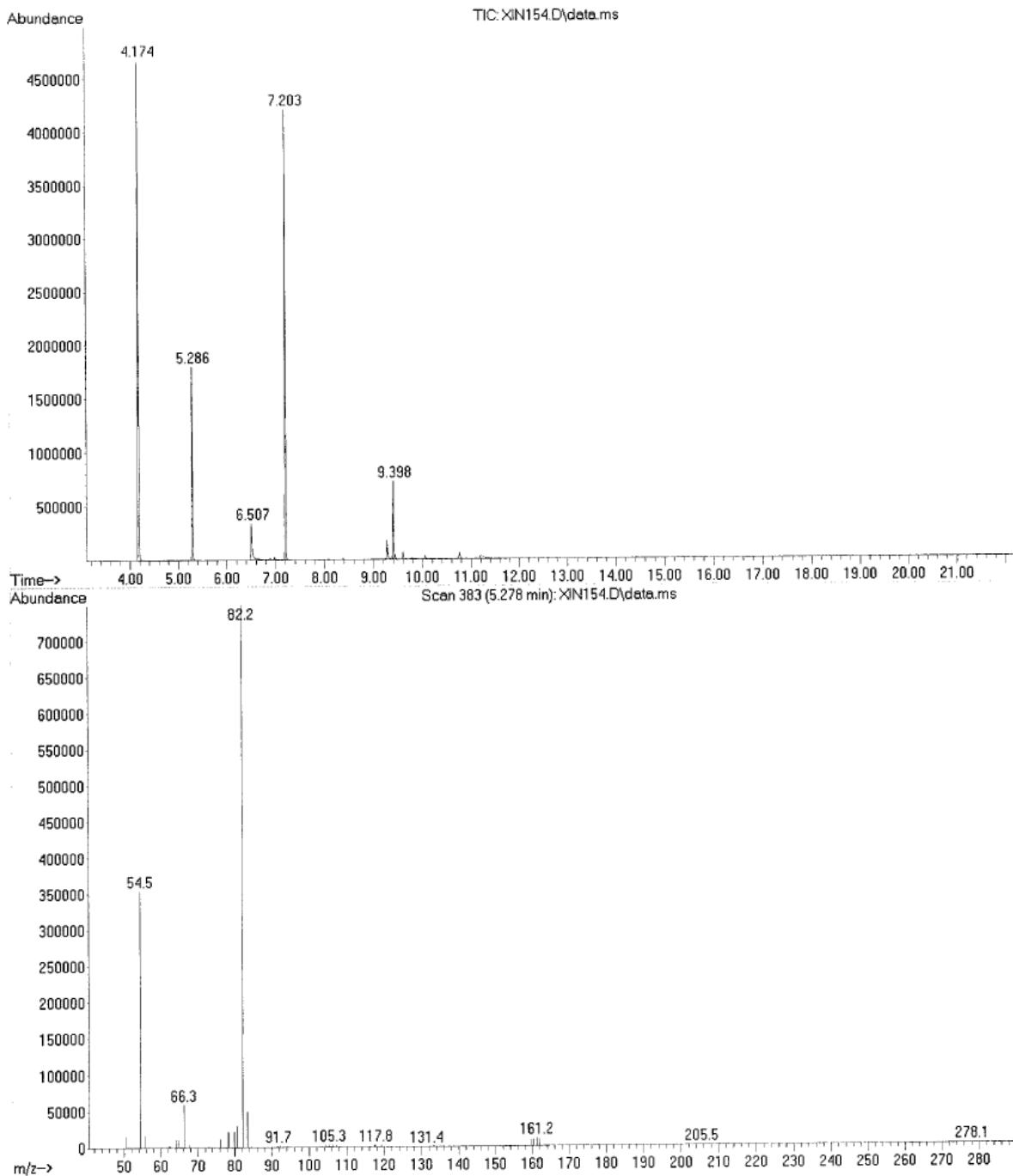
Entry 2: Dodecane internal standard: $R_t = 7.204$ min. 1-cyclohexyl-3-methoxybenzene: $R_t = 9.881$ min.
By-product, 3,3'-dimethoxybiphenyl, $R_t = 12.839$ min.



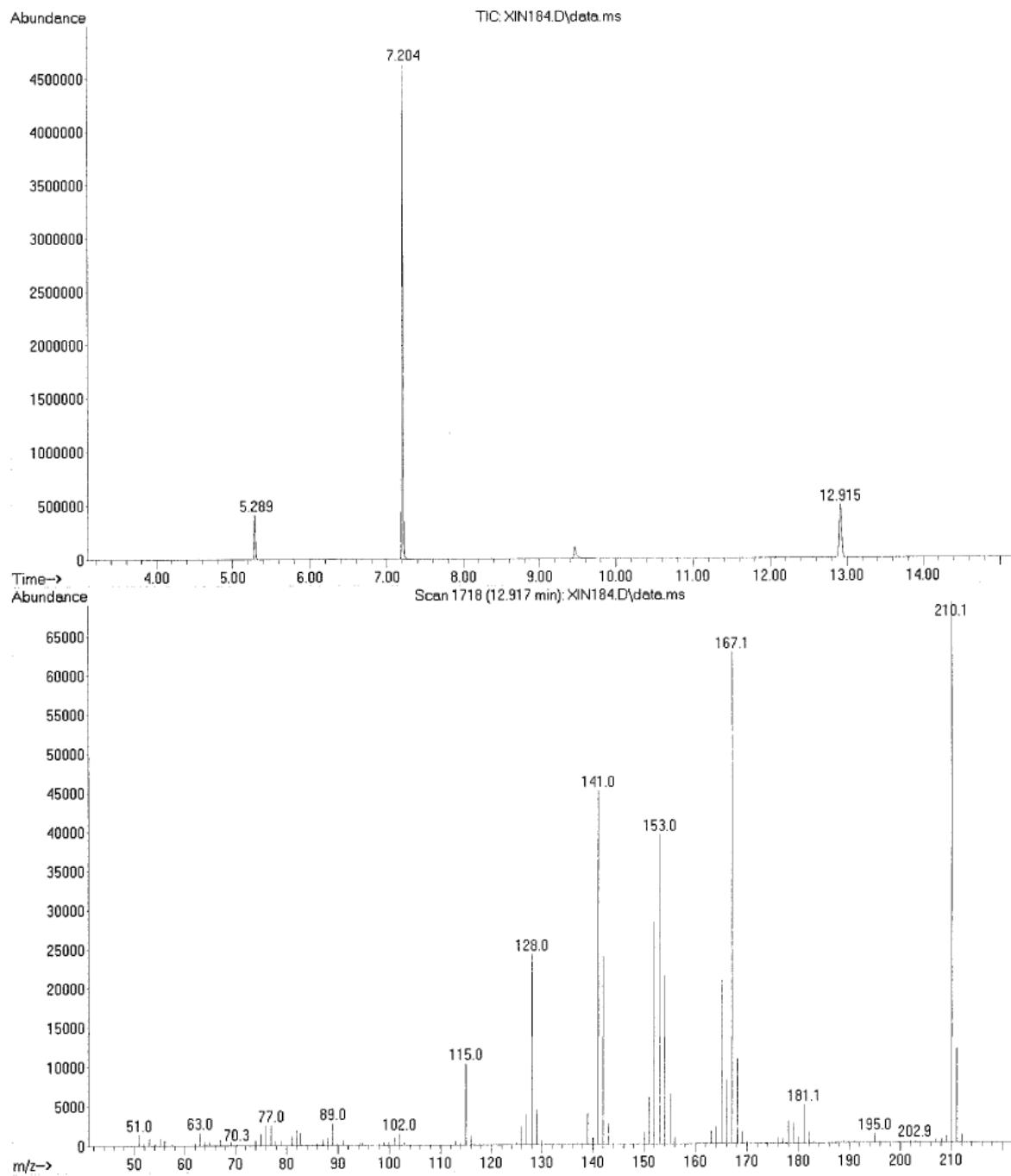
Entry 3: Dodecane internal standard: $R_t = 7.202$ min. 1-cyclohexyl-4-fluorobenzene: $R_t = 8.282$ min.
By-product, 4,4'-difluorobiphenyl: $R_t = 8.594$ min.



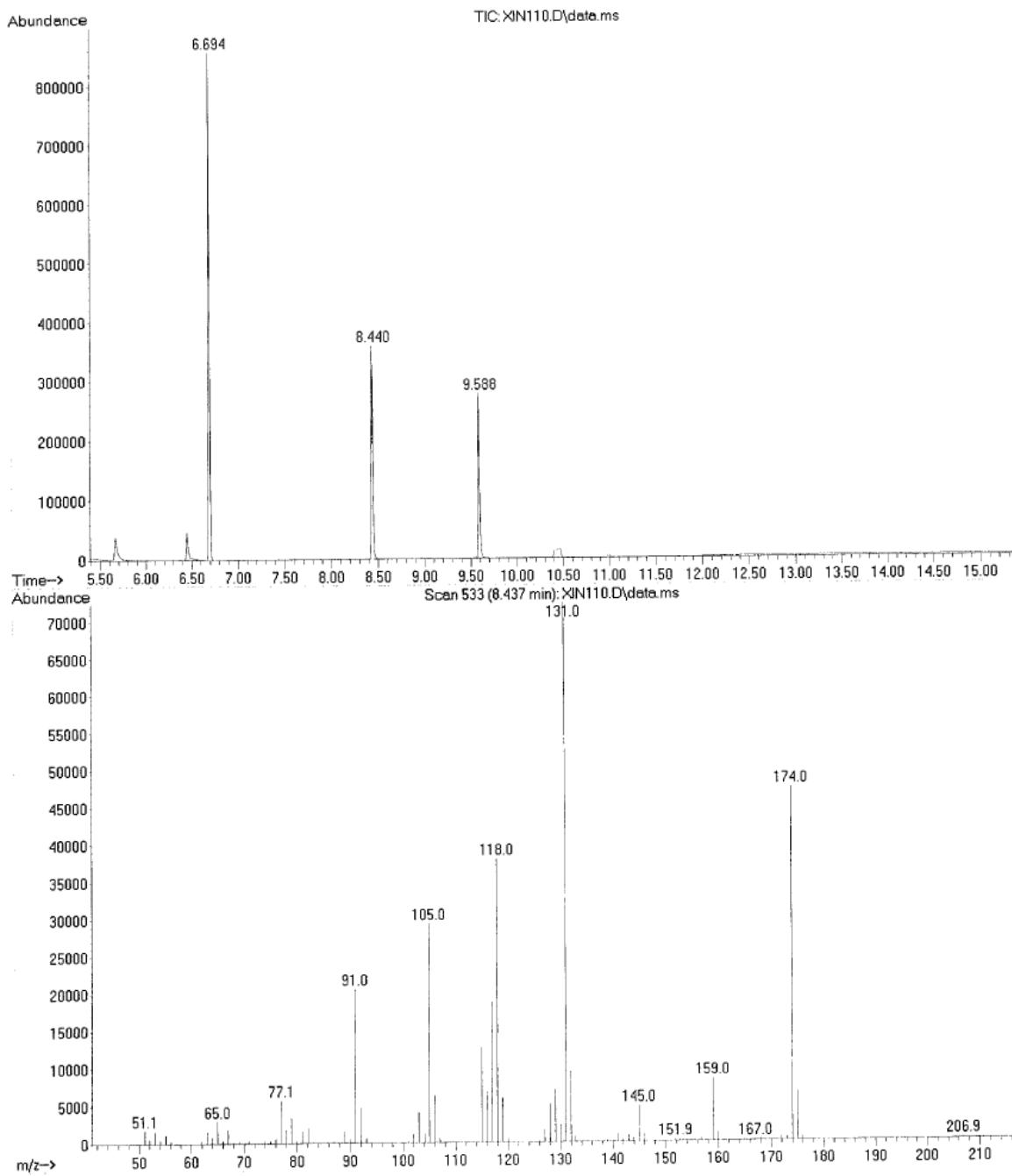
Entry 4 (MW method): Dodecane internal standard: $R_t = 7.203$ min. Cyclohexene: $R_t = 5.286$ min.
Starting material, cyclohexyl bromide: $R_t = 4.174$ min.



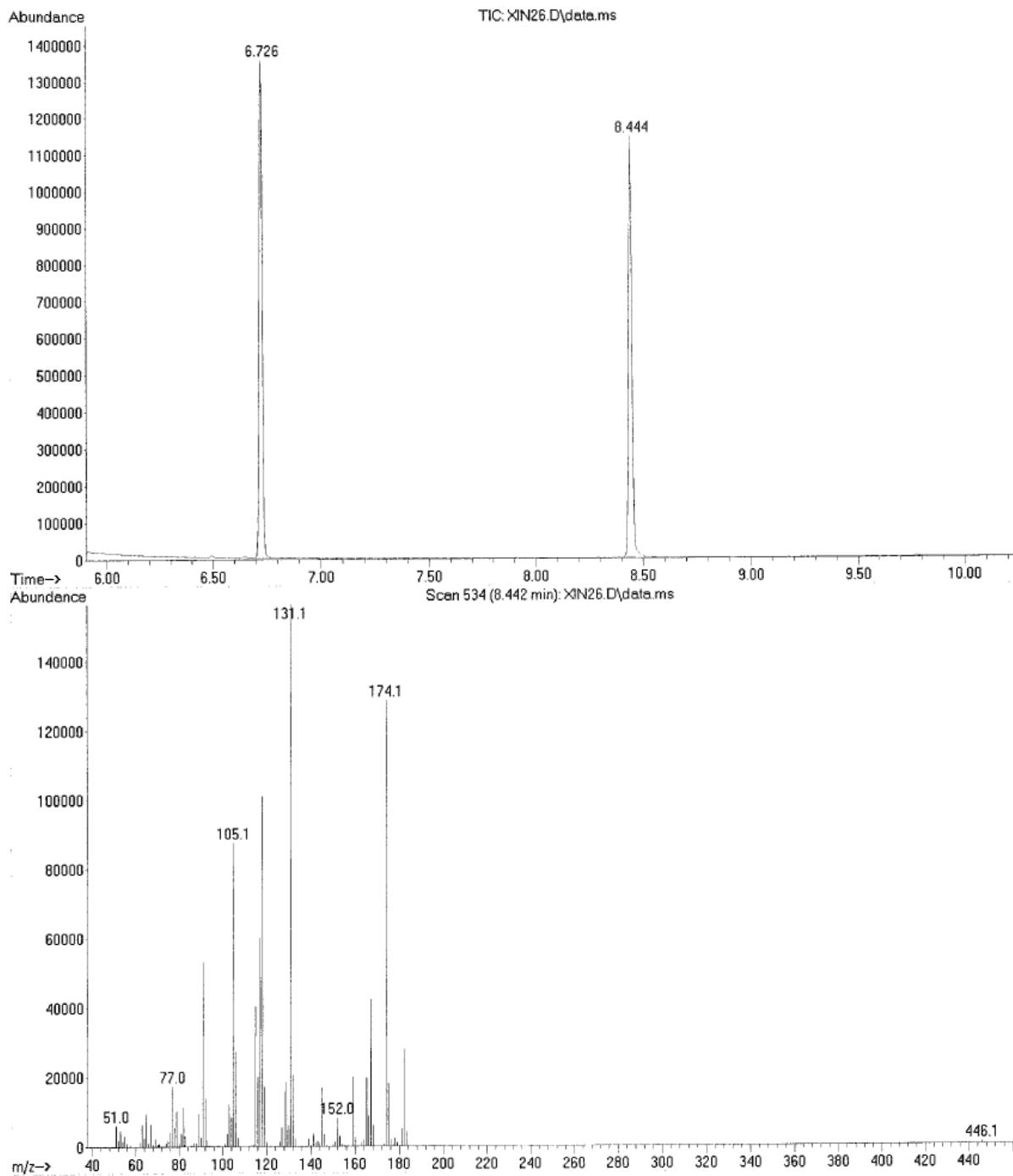
Entry 5: Dodecane internal standard: $R_t = 7.204$ min. 1-cyclohexylnaphthalene: $R_t = 12.915$ min.



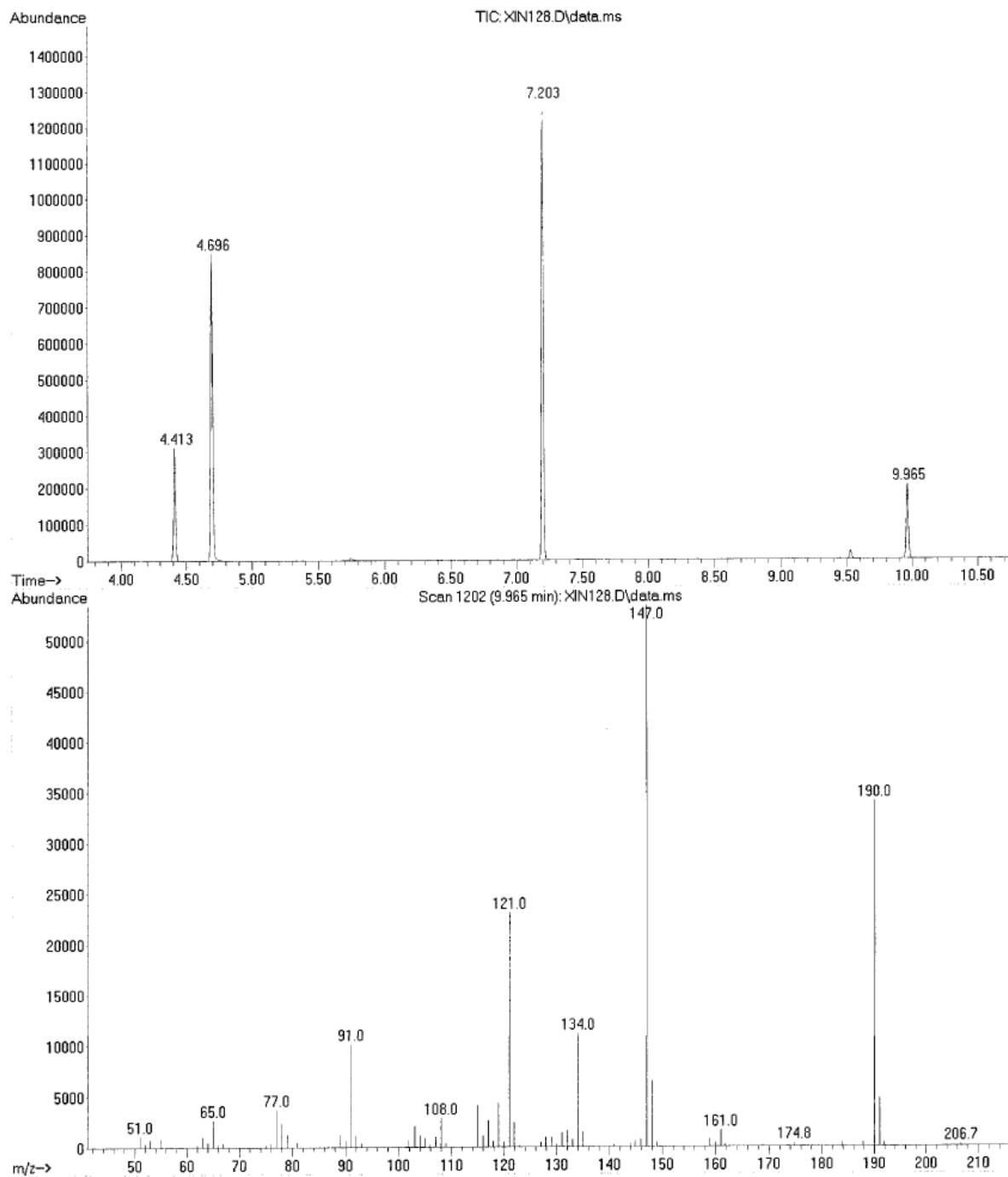
Entry 6: Dodecane internal standard: $R_t = 6.694$ min. 1-cyclohexyl-4-methylbenzene: $R_t = 8.440$ min.
By-product, 4,4'-dimethylbiphenyl: $R_t = 9.588$ min.



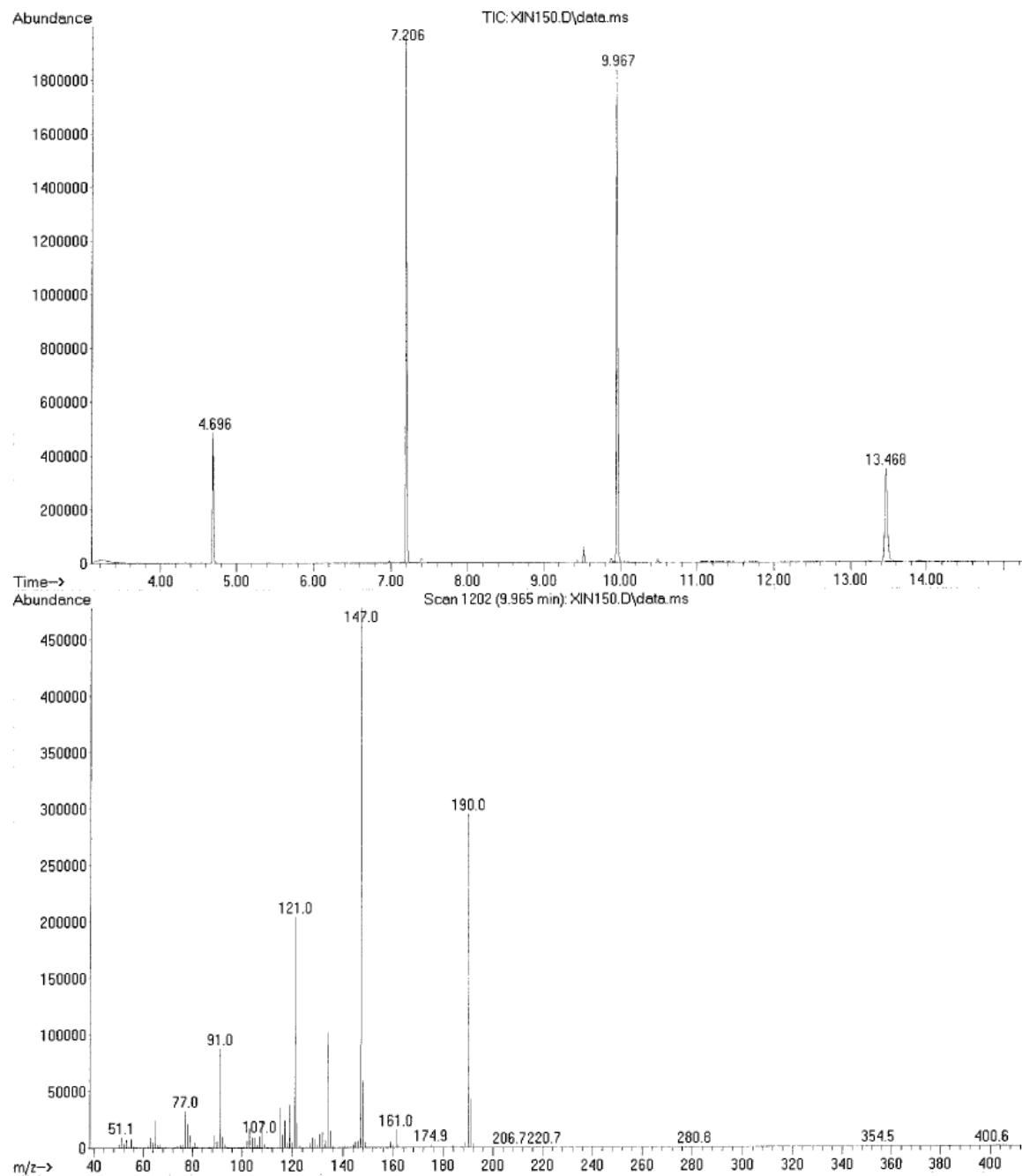
Entry 7: Dodecane internal standard: $R_t = 6.726$ min. 1-cyclohexyl-2-methylbenzene: $R_t = 8.444$ min.



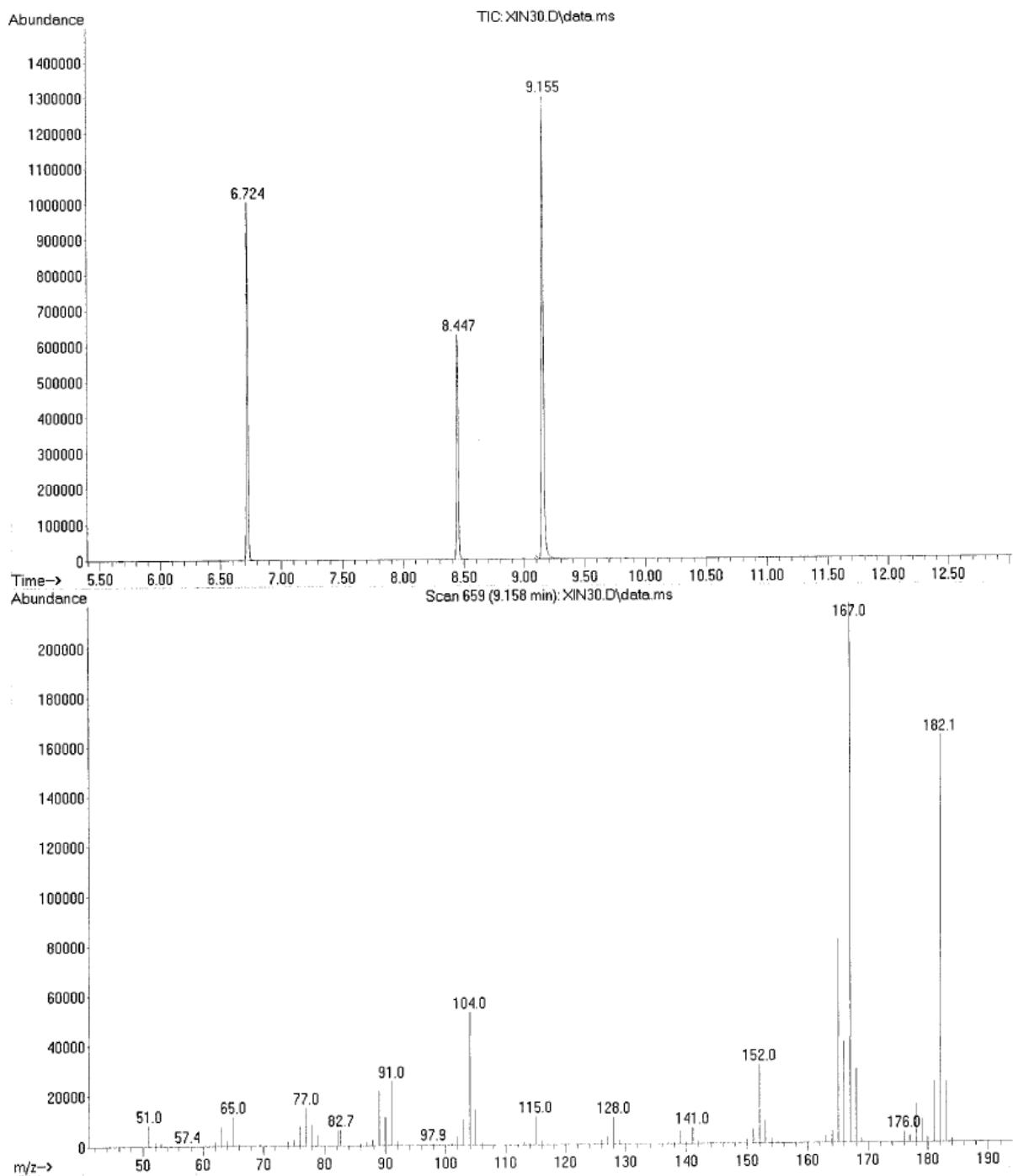
Entry 8 (Heated to 40 °C): Dodecane internal standard: $R_t = 7.203$ min. 1-cyclohexyl-4-methoxybenzene: $R_t = 9.965$ min. Starting material, cyclohexyl chloride: $R_t = 4.413$ min.



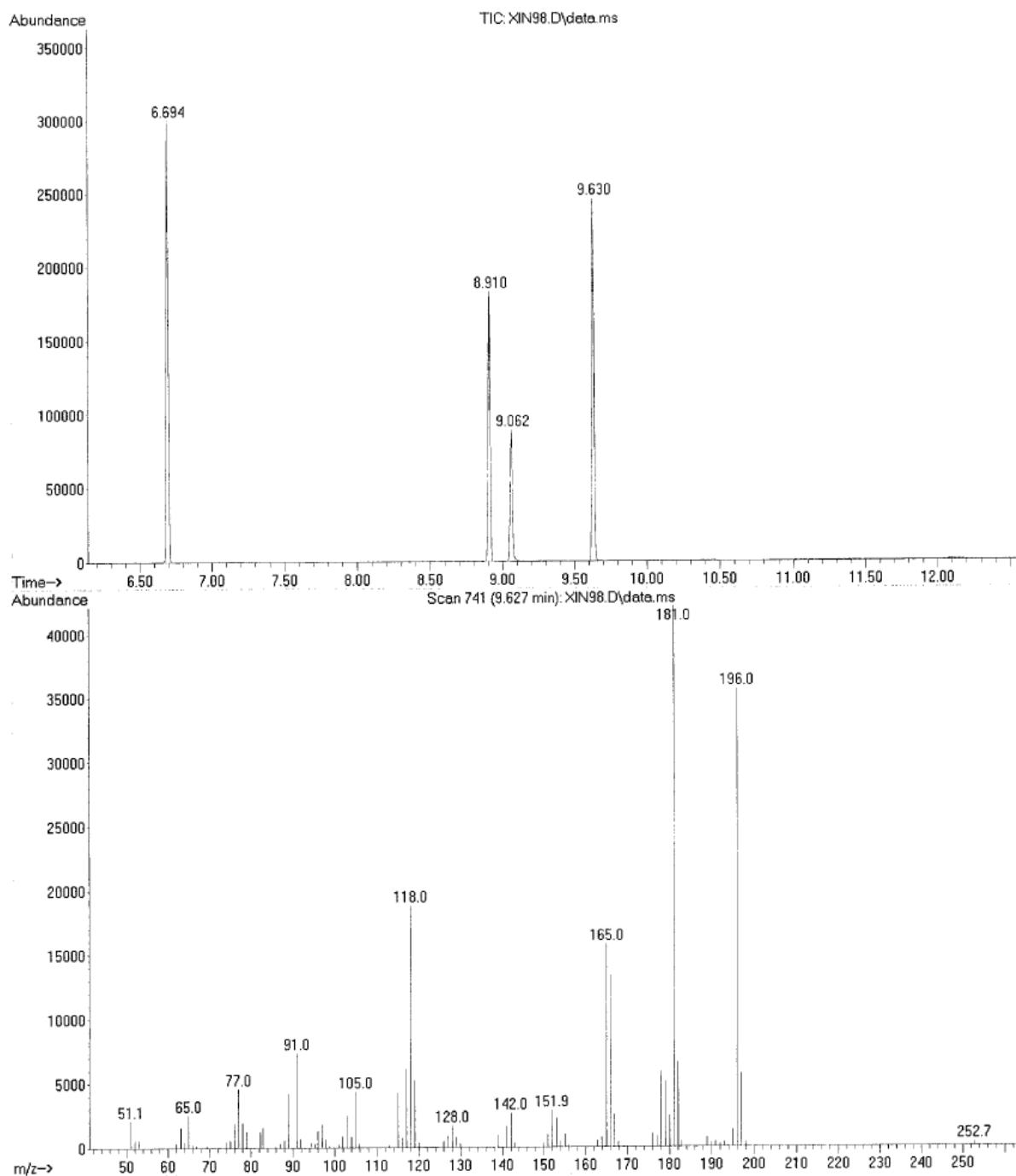
Entry 8 (MW method): Dodecane internal standard: $R_t = 7.206$ min. 1-cyclohexyl-4-methoxybenzene, $R_t = 9.967$ min. By-product: 4,4'-dimethoxybiphenyl, $R_t = 13.468$ min.



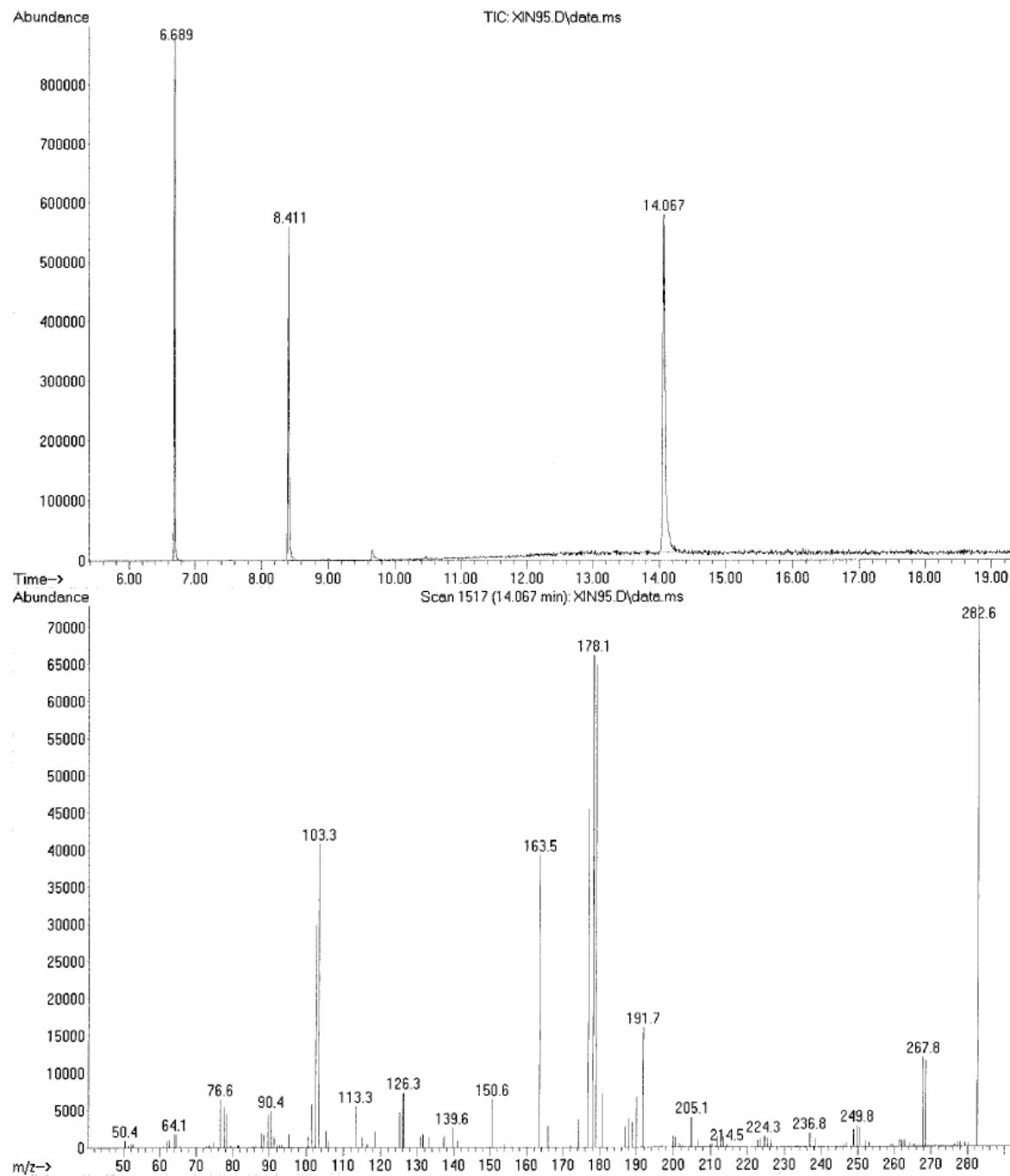
Entry 9: Dodecane internal standard $R_t = 6.724$ min. 1-benzyl-2-methylbenzene, $R_t = 9.155$ min.
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.447$ min.



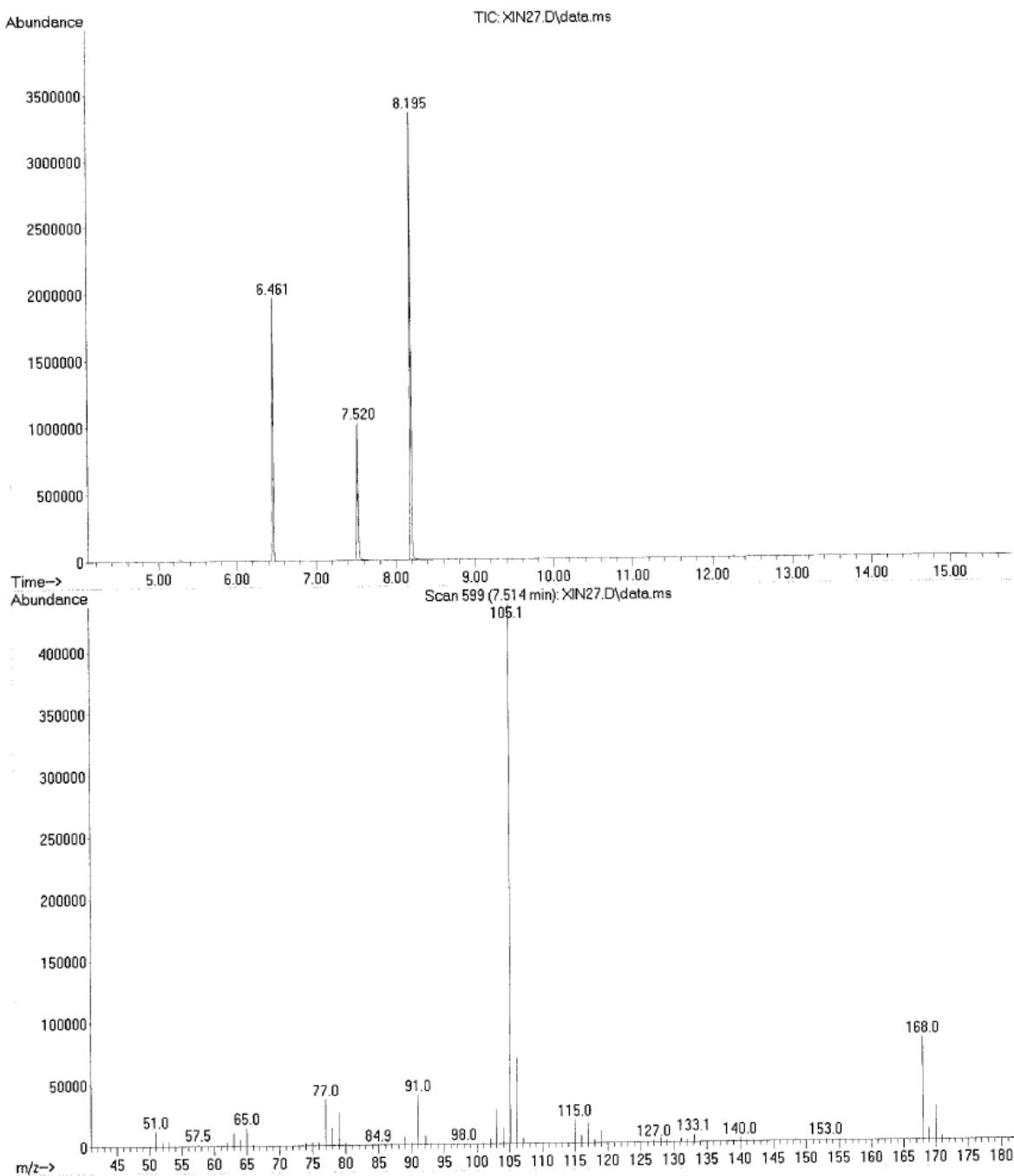
Entry 10: Dodecane internal standard $R_t = 6.694$ min. 2-benzyl-1,3-dimethylbenzene, $R_t = 9.630$ min.
By-product: 2,2',6,6'-tetramethylbiphenyl, $R_t = 8.910$ min. 1,2-diphenylethane, $R_t = 9.062$ min.



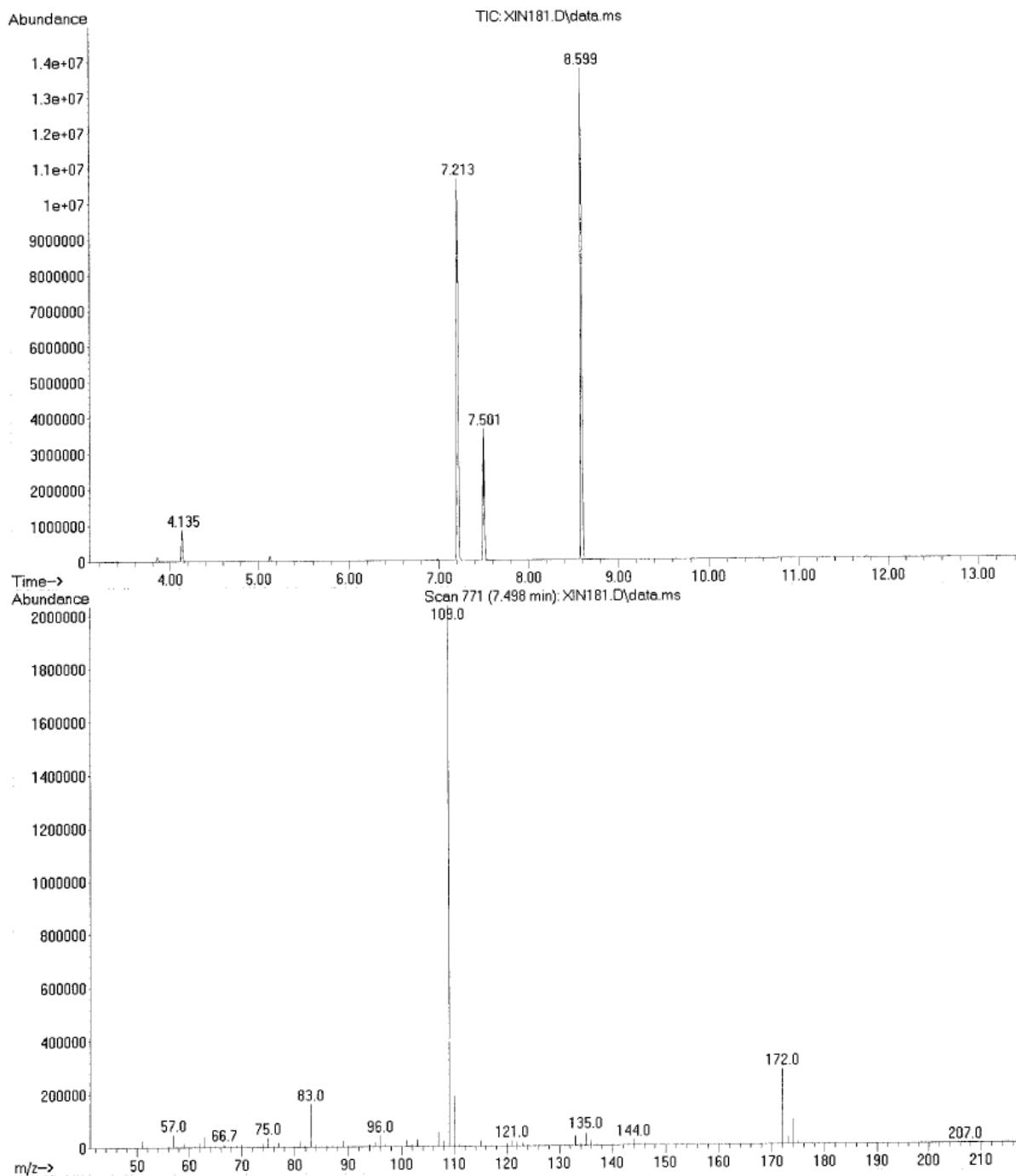
Entry 11: Dodecane internal standard $R_t = 6.689$ min. 1,3-bis(2-methylbenzyl)benzene, $R_t = 14.067$ min.
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.411$ min.



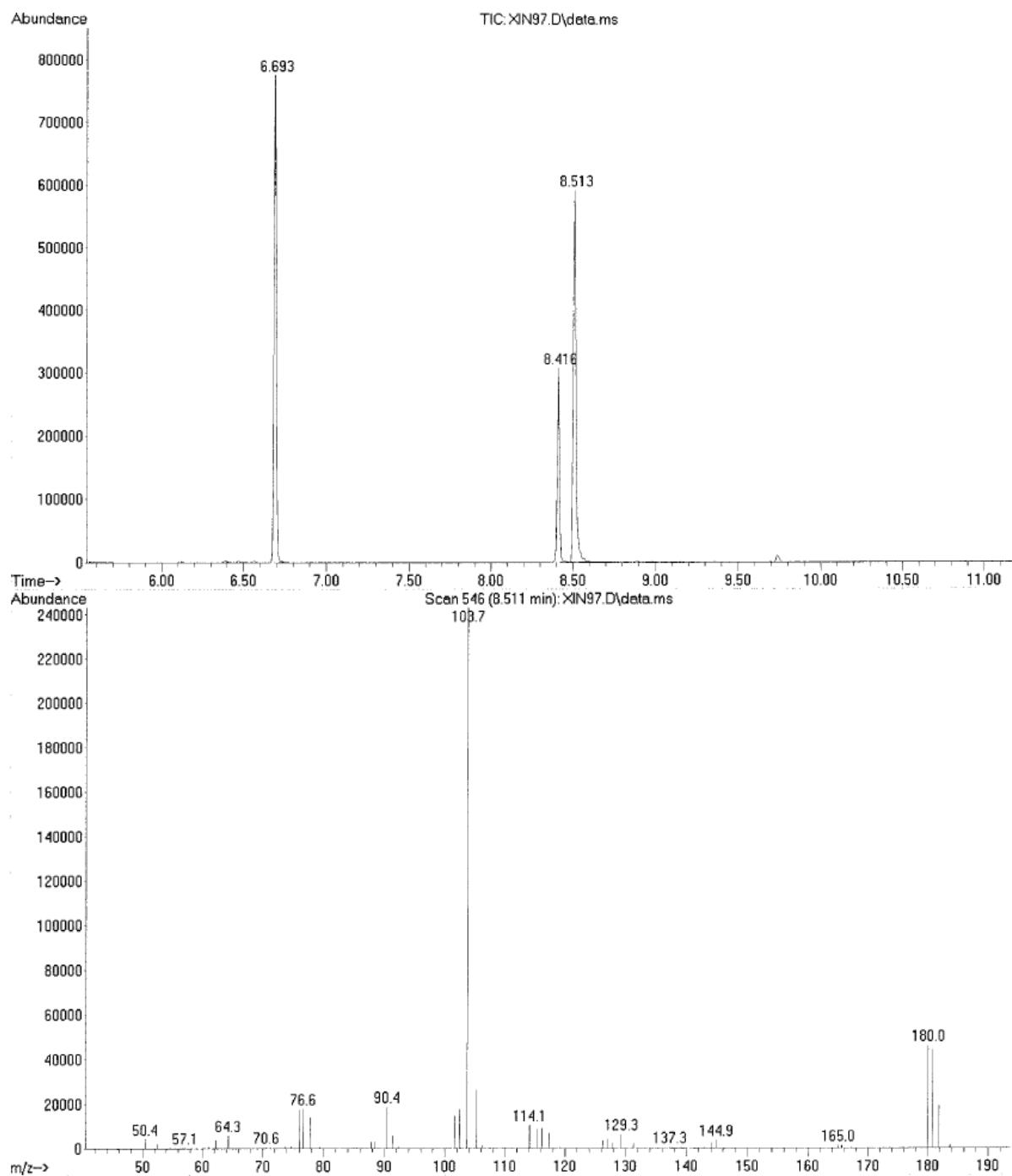
Entry 13: Dodecane internal standard $R_t = 6.461$ min. 1-(3-chloropropyl)-2-methylbenzene, $R_t = 7.520$ min. By-product: 2,2'-dimethylbiphenyl, $R_t = 8.195$ min.



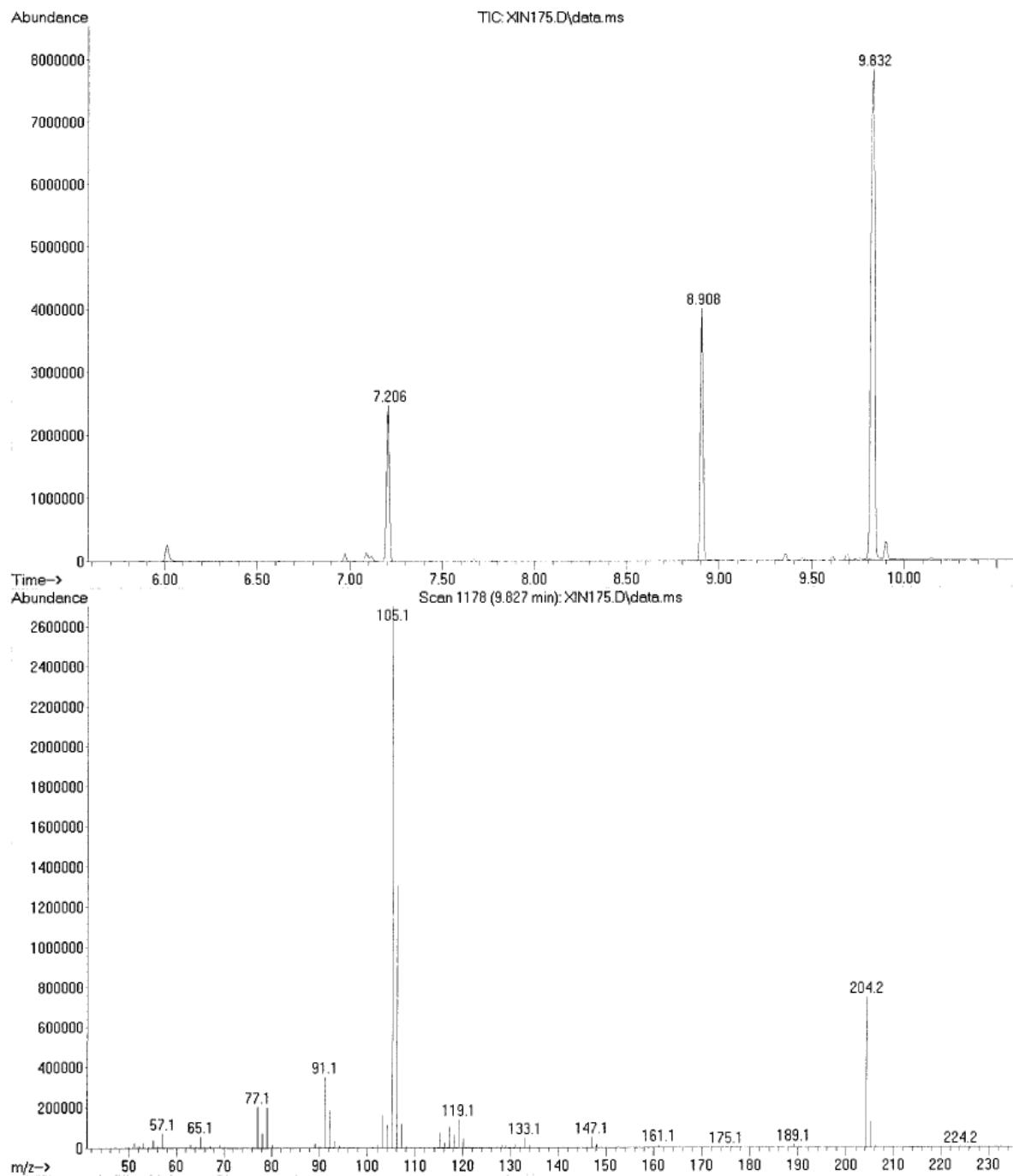
Entry 14 (MW method): Dodecane internal standard $R_t = 7.213$ min. 1-(3-chloropropyl)-4-fluorobenzene, $R_t = 7.501$ min. By-product: 4,4'-difluorobiphenyl, $R_t = 8.599$ min.



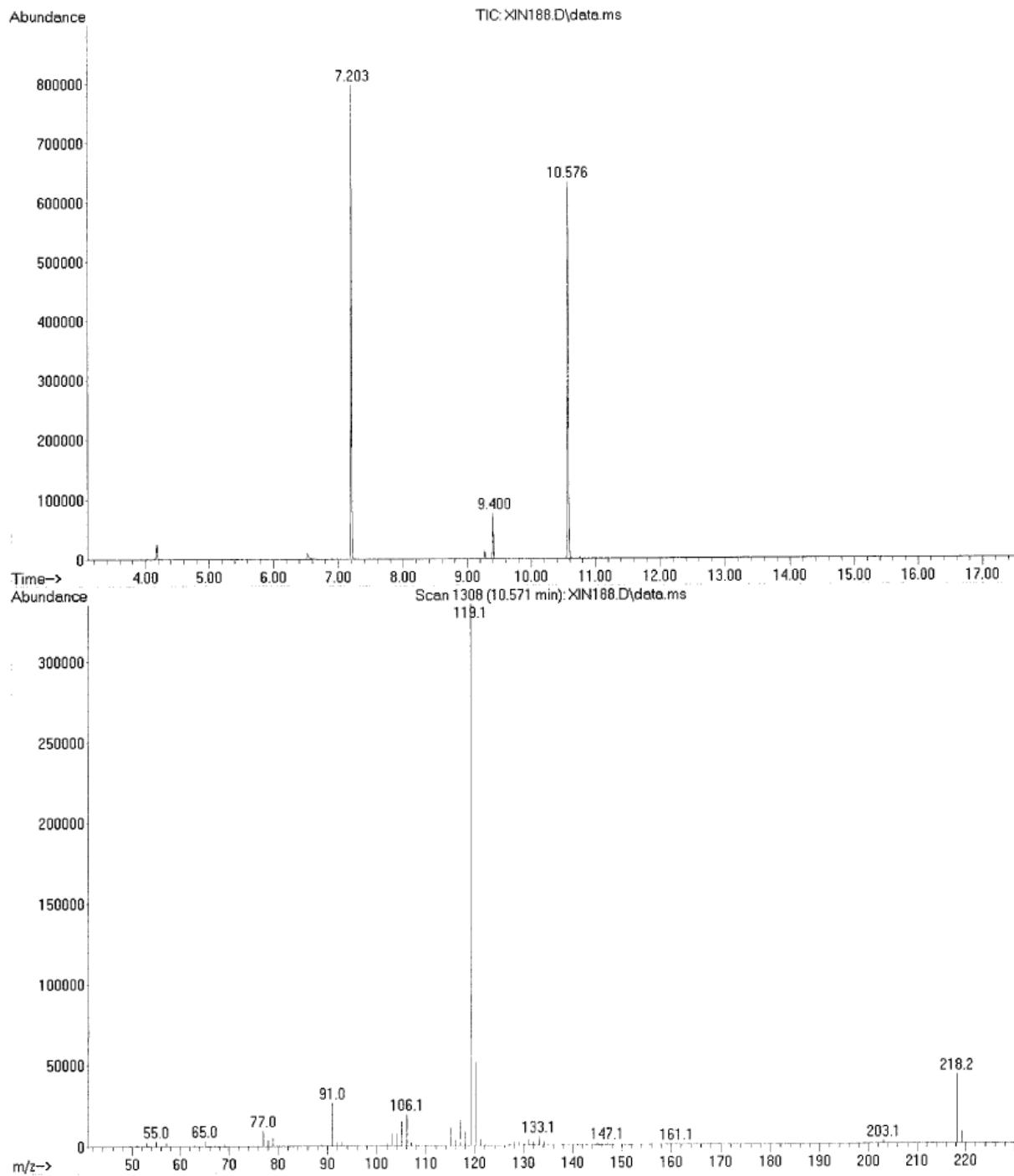
Entry 15: Dodecane internal standard $R_t = 6.693$ min. 1-(4-chlorobutyl)-2-methylbenzene, $R_t = 8.513$ min. By-product: 2,2'-dimethylbiphenyl, $R_t = 8.416$ min.



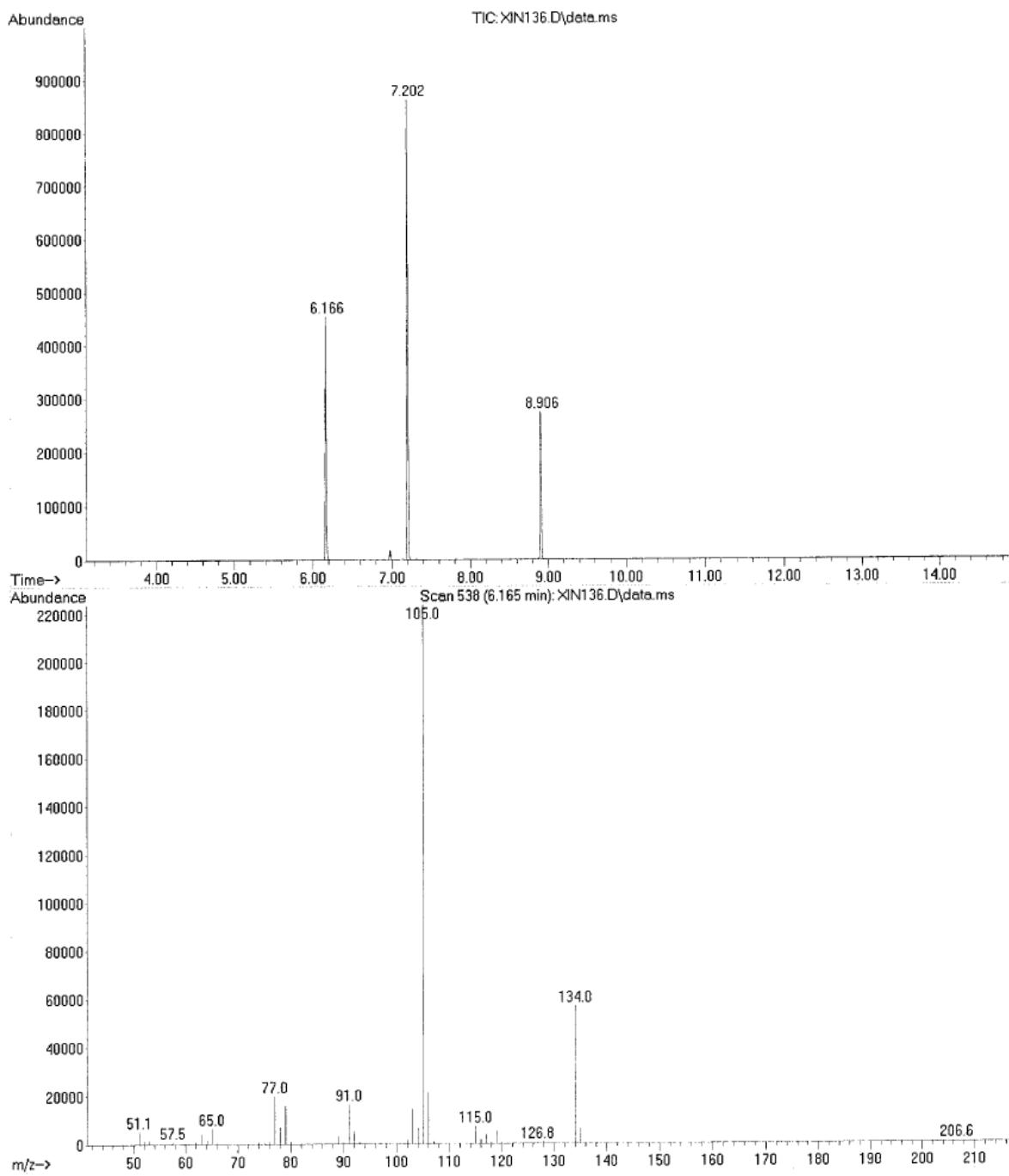
Entry 16: Dodecane internal standard $R_t = 7.206$ min. 1-methyl-2-octylbenzene, $R_t = 9.832$ min.
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.908$ min.



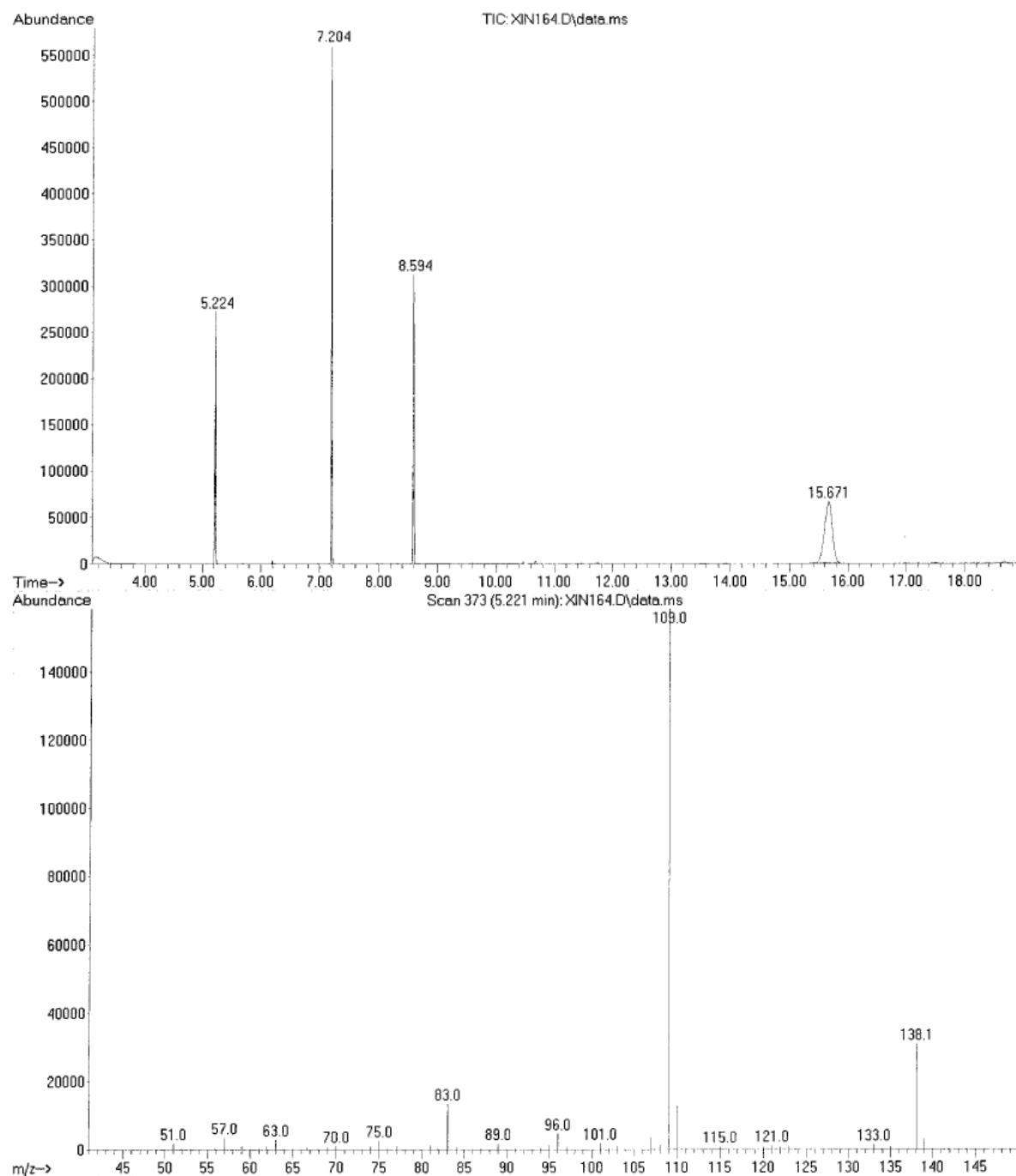
Entry 17 (MW method): Dodecane internal standard $R_t = 7.203$ min. 1,3-dimethyl-2-octylbenzene, $R_t = 10.576$ min. By-product: 2,2',6,6'-tetramethylbiphenyl, $R_t = 9.400$ min.



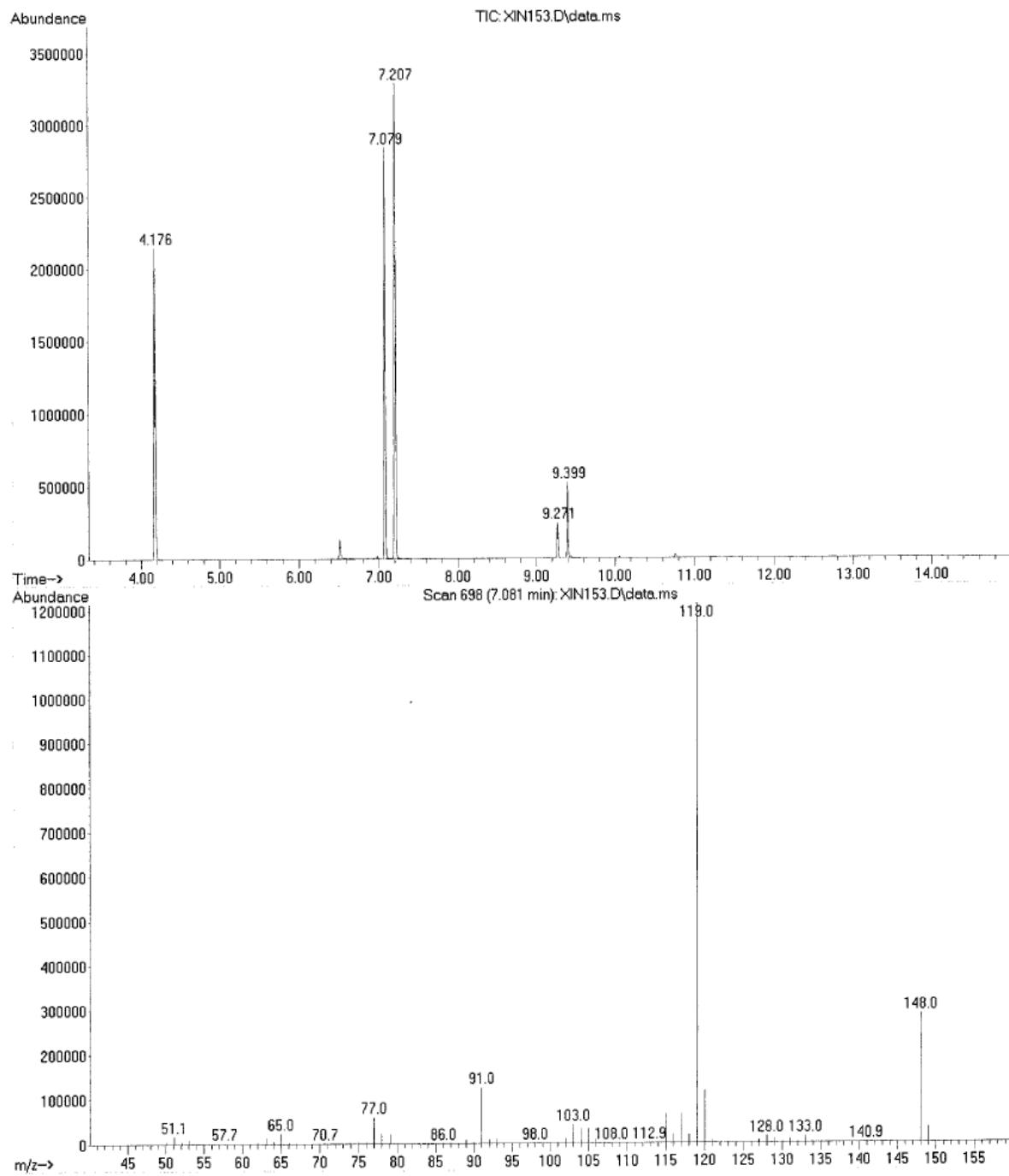
Entry 19: Dodecane internal standard $R_t = 7.202$ min. 1-methyl-2-propylbenzene, $R_t = 6.166$ min.
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.906$ min.



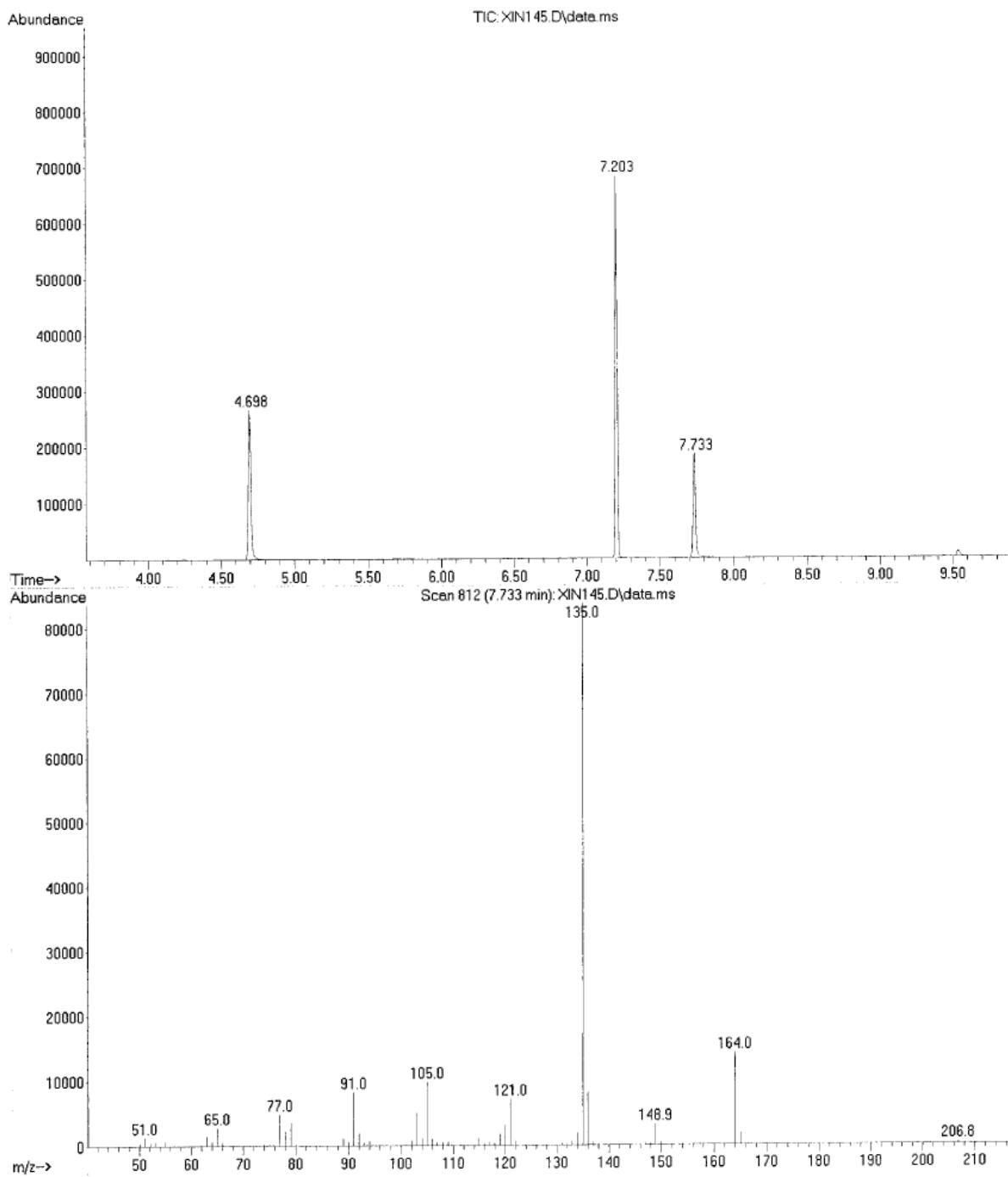
Entry 20: Dodecane internal standard $R_t = 7.204$ min. 1-fluoro-4-propylbenzene, $R_t = 5.224$ min.
By-product: 4,4'-difluorobiphenyl, $R_t = 8.594$ min.



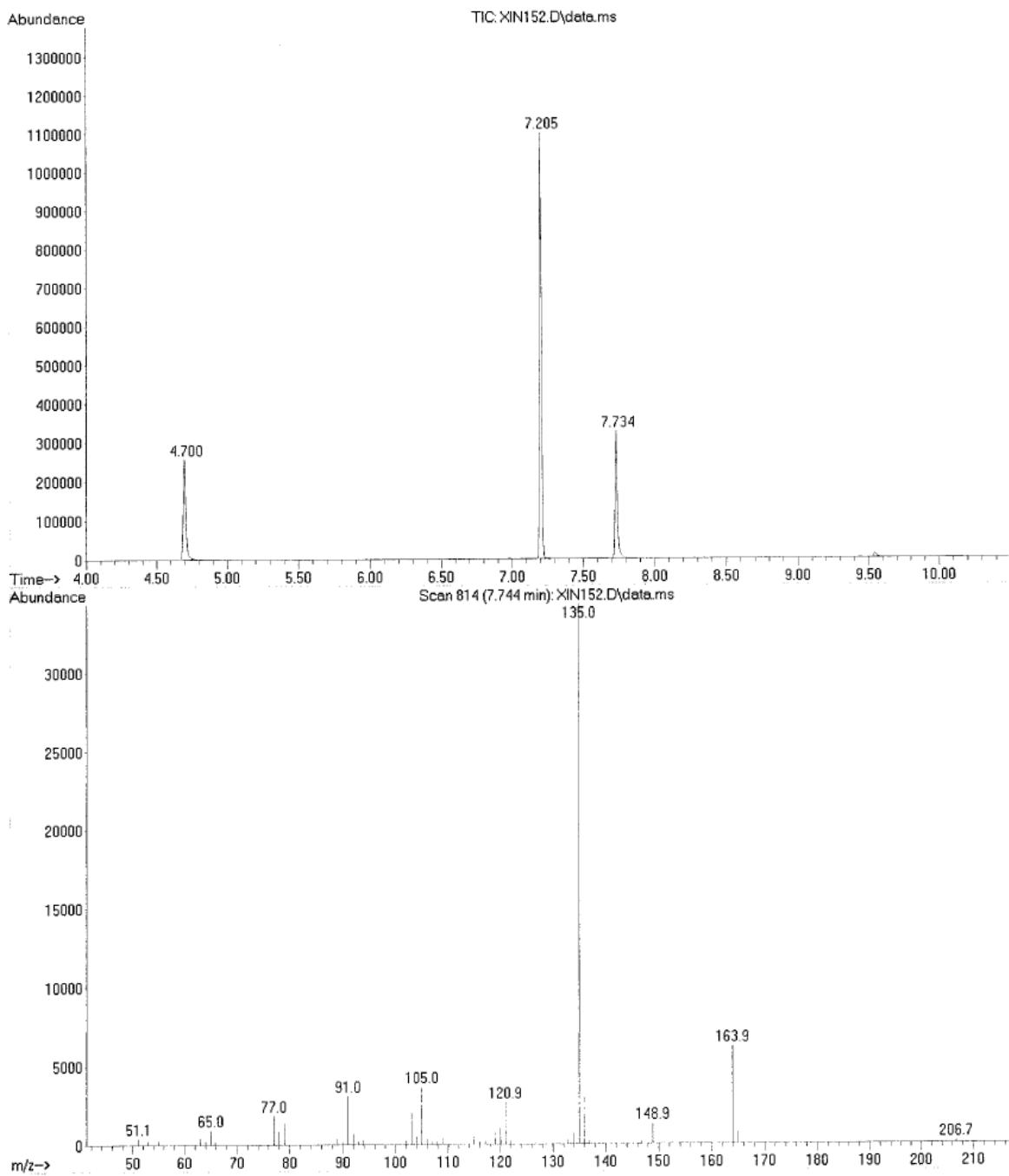
Entry 21 (MW method): Dodecane internal standard $R_t = 7.207$ min. 1,3-dimethyl-2-propylbenzene, $R_t = 7.079$ min. By-product: 2,2',6,6'-tetramethylbiphenyl, $R_t = 9.399$ min.



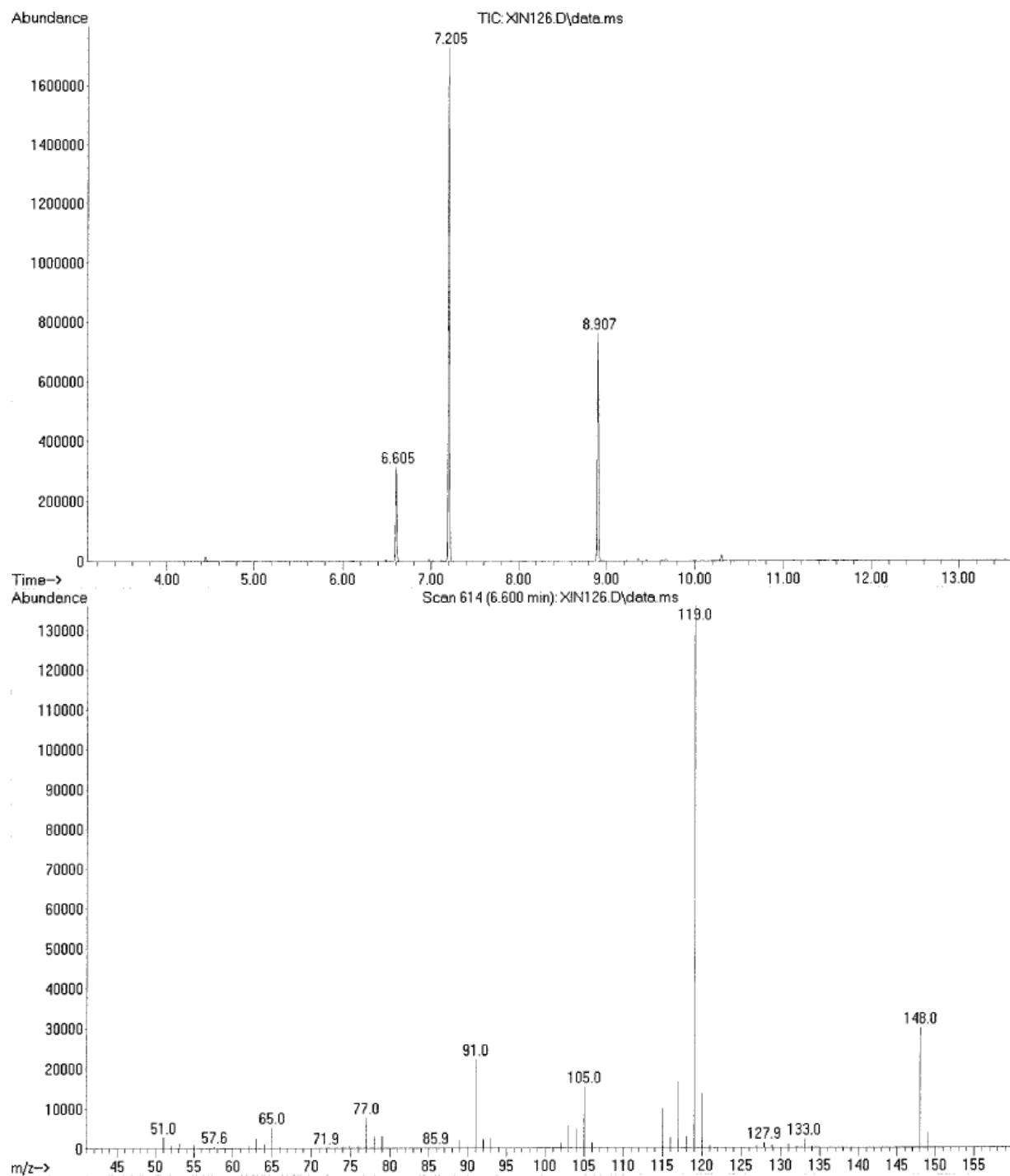
Entry 23: Dodecane internal standard $R_t = 7.203$ min. 1-*sec*-butyl-4-methoxybenzene, $R_t = 7.733$ min.



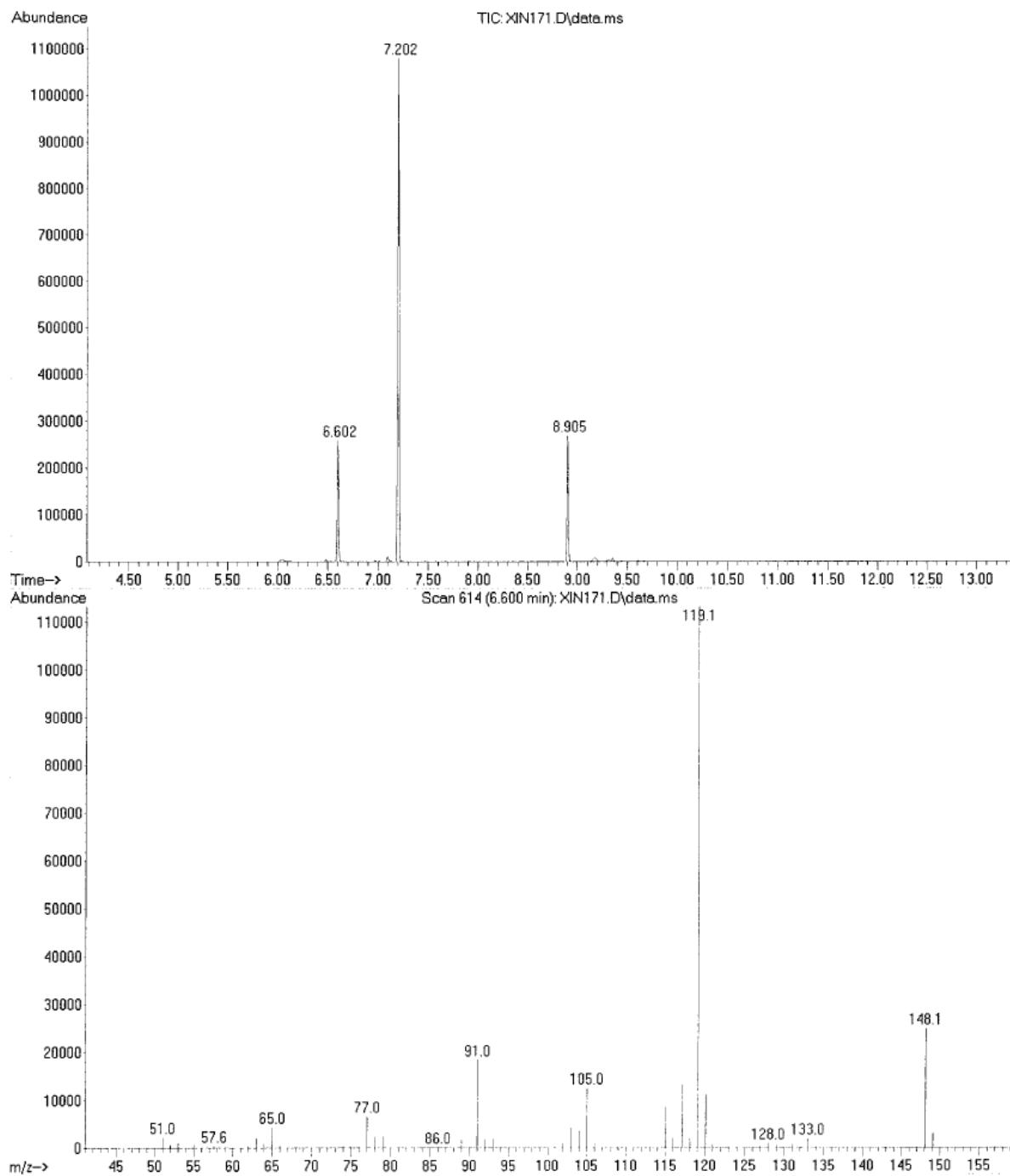
Entry 23 (MW method): Dodecane internal standard $R_t = 7.205$ min. 1-sec-butyl-4-methoxybenzene, $R_t = 7.734$ min.



Entry 24: Dodecane internal standard $R_t = 7.205$ min. 1-*sec*-butyl-2-methylbenzene, $R_t = 6.605$ min.
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.907$ min.

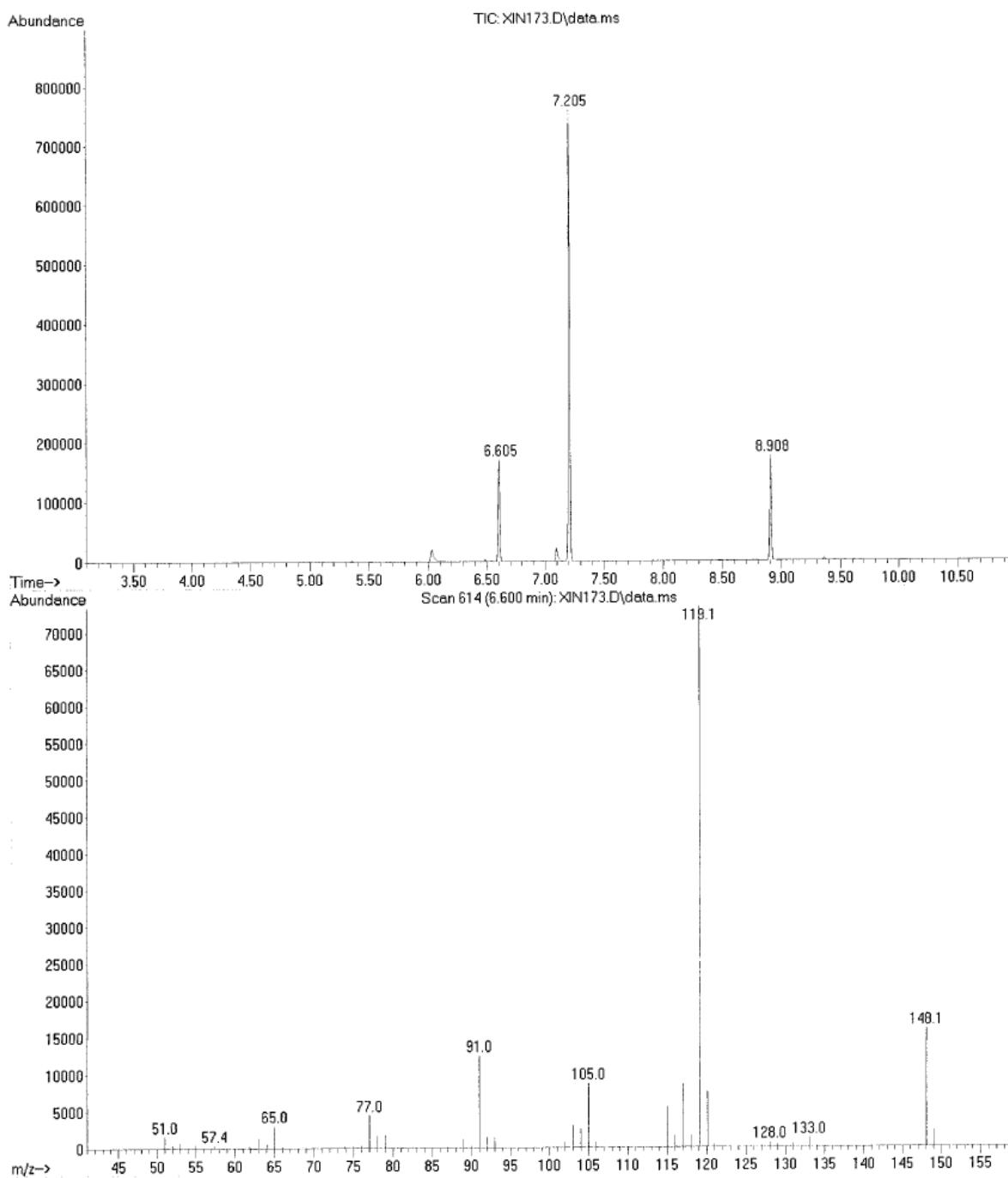


Entry 24 (MW method): Dodecane internal standard $R_t = 7.202$ min. 1-sec-butyl-2-methylbenzene, $R_t = 6.602$ min. By-product: 2,2'-dimethylbiphenyl, $R_t = 8.905$ min.

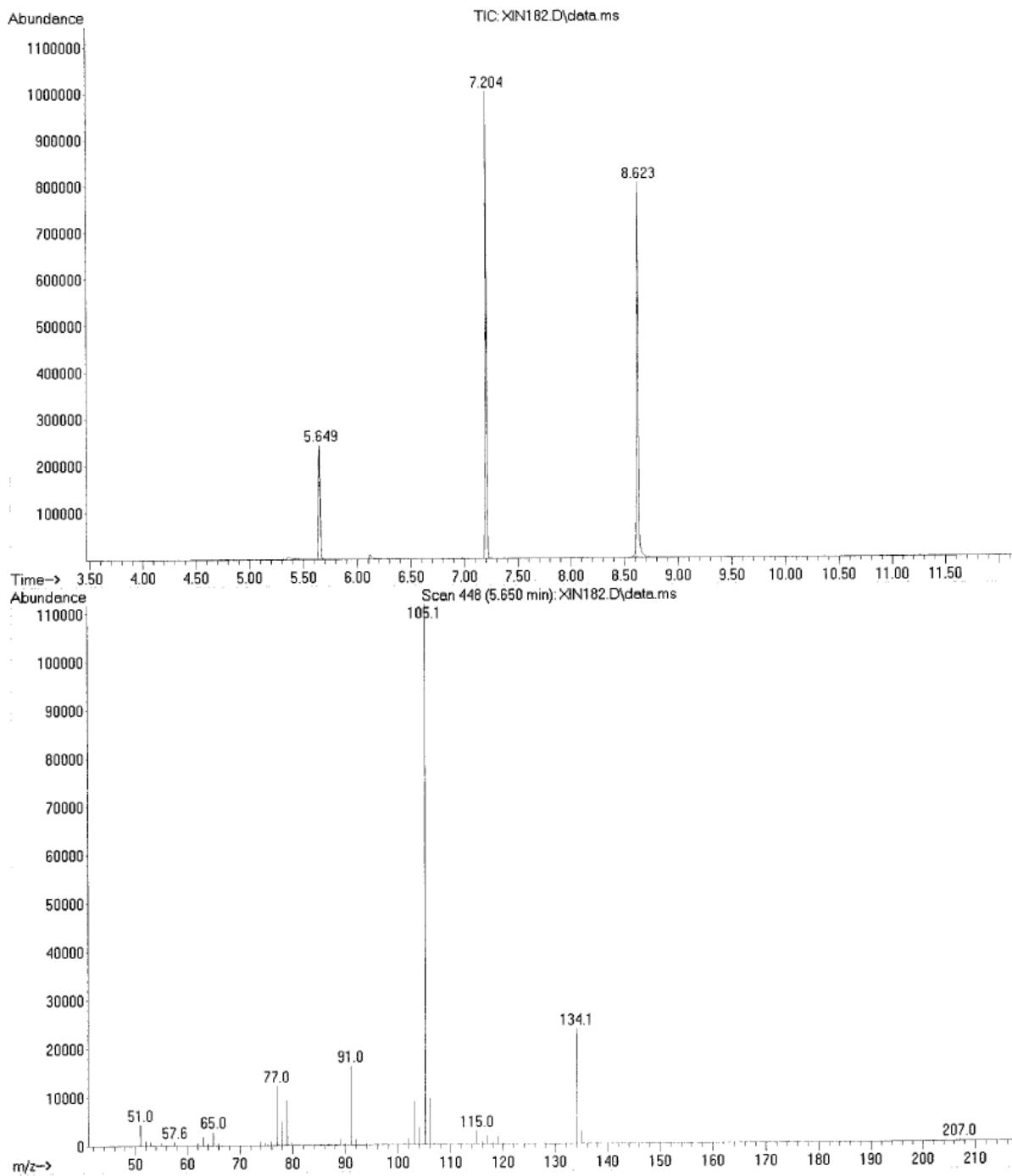


Entry 24 (MW method at 180 °C): Dodecane internal standard $R_t = 7.205$ min.

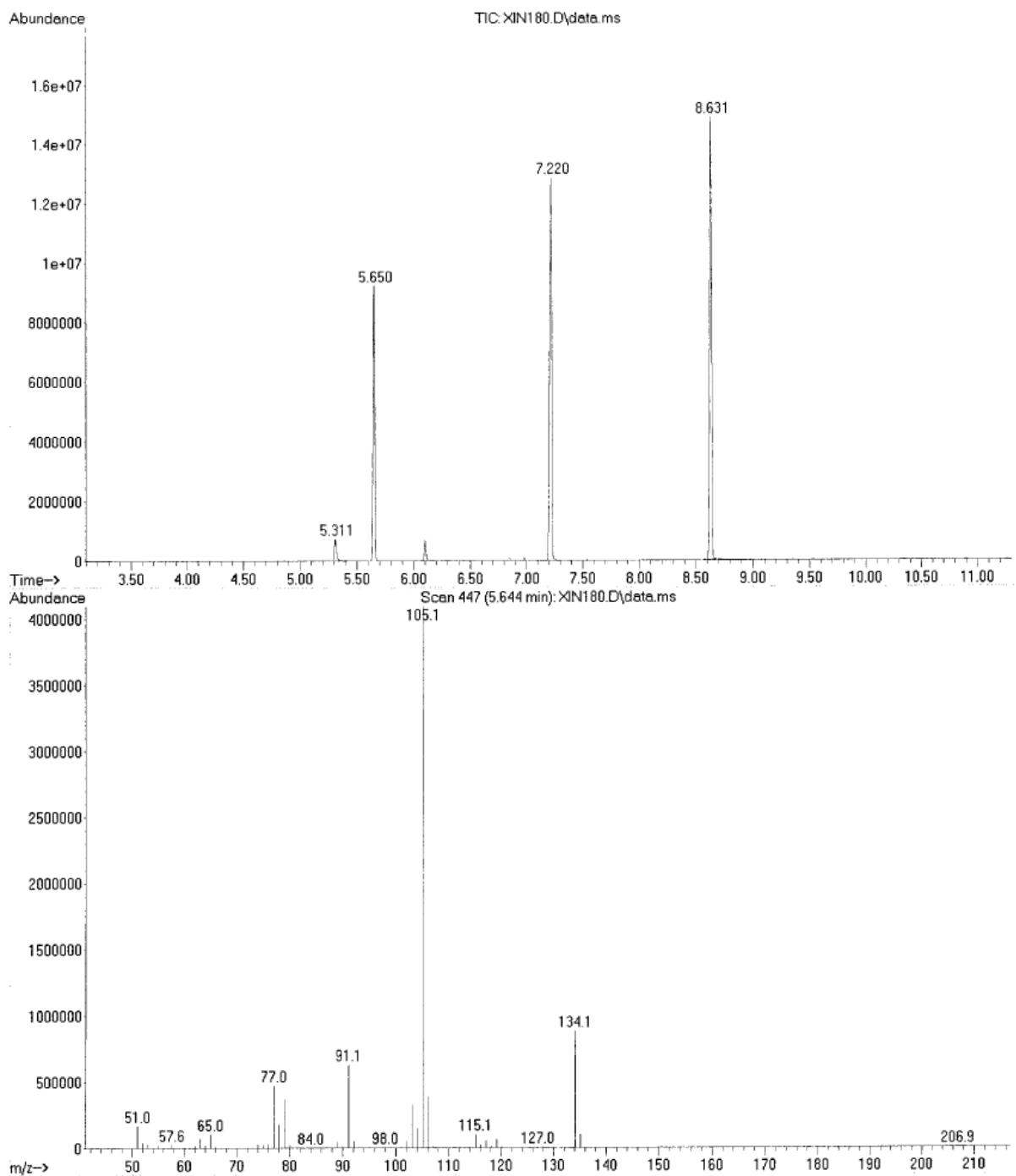
1-sec-butyl-2-methylbenzene, $R_t = 6.605$ min. By-product: 2,2'-dimethylbiphenyl, $R_t = 8.908$ min.



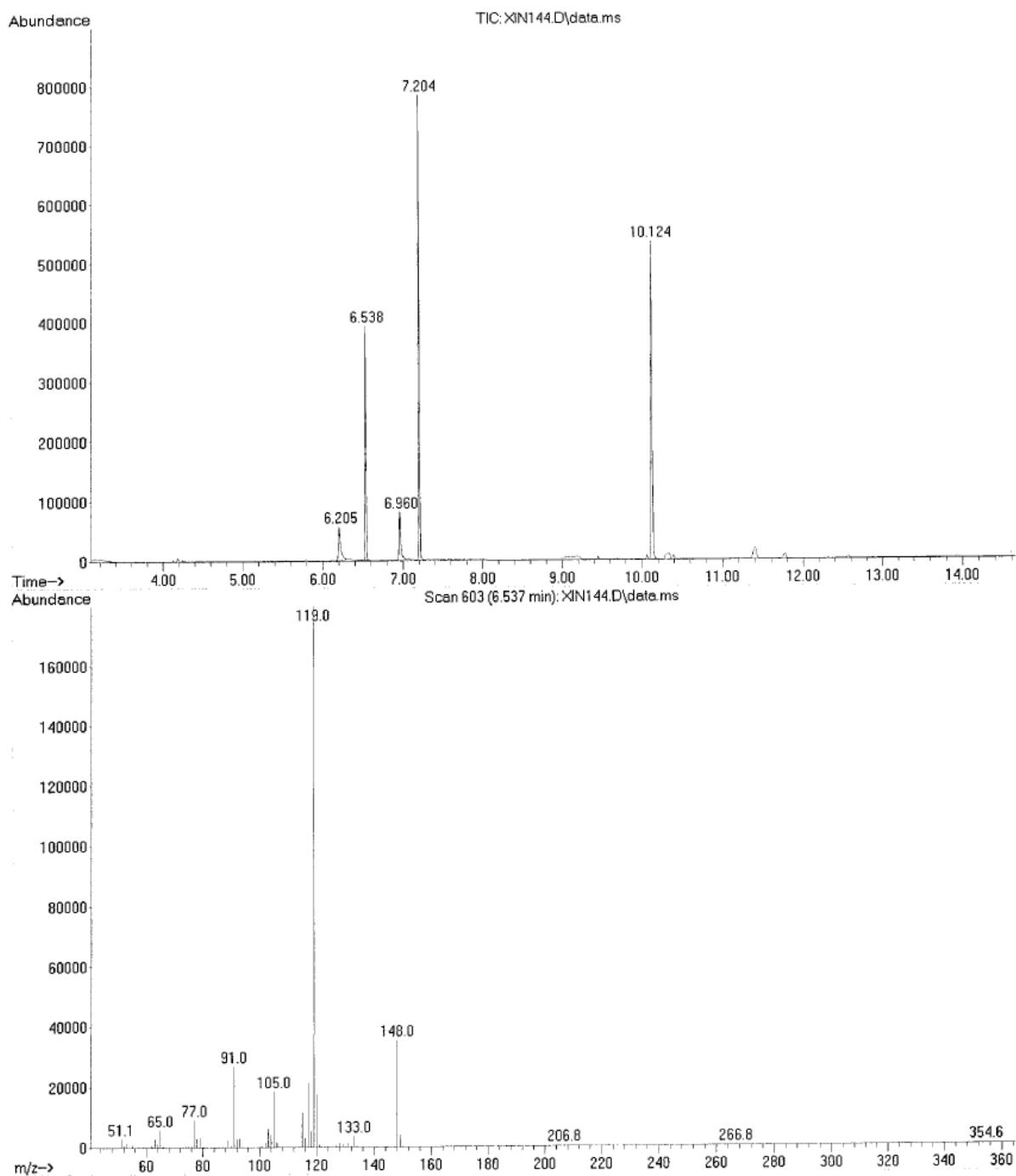
Entry 25: Dodecane internal standard $R_t = 7.204$ min. *sec*-butylbenzene, $R_t = 5.649$ min. By-product: biphenyl, $R_t = 8.623$ min.



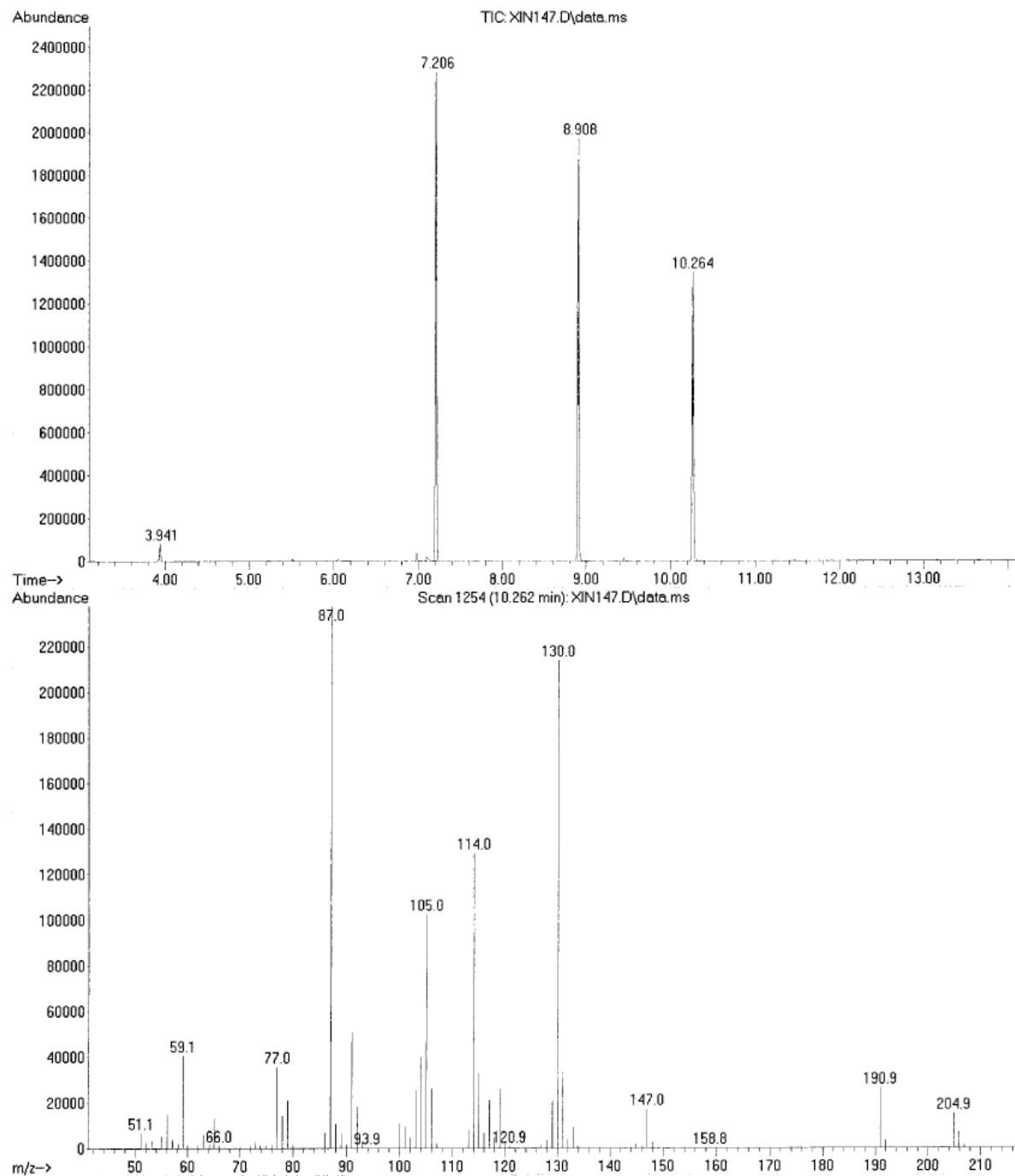
Entry 25 (MW method): Dodecane internal standard $R_t = 7.220$ min. *sec*-butylbenzene, $R_t = 5.650$ min.
By-product: biphenyl, $R_t = 8.631$ min.



Entry 26: Dodecane internal standard $R_t = 7.204$ min. *sec*-butylbenzene, $R_t = 6.538$ min. By-product: 4,4'-dimethylbiphenyl, $R_t = 10.124$ min.

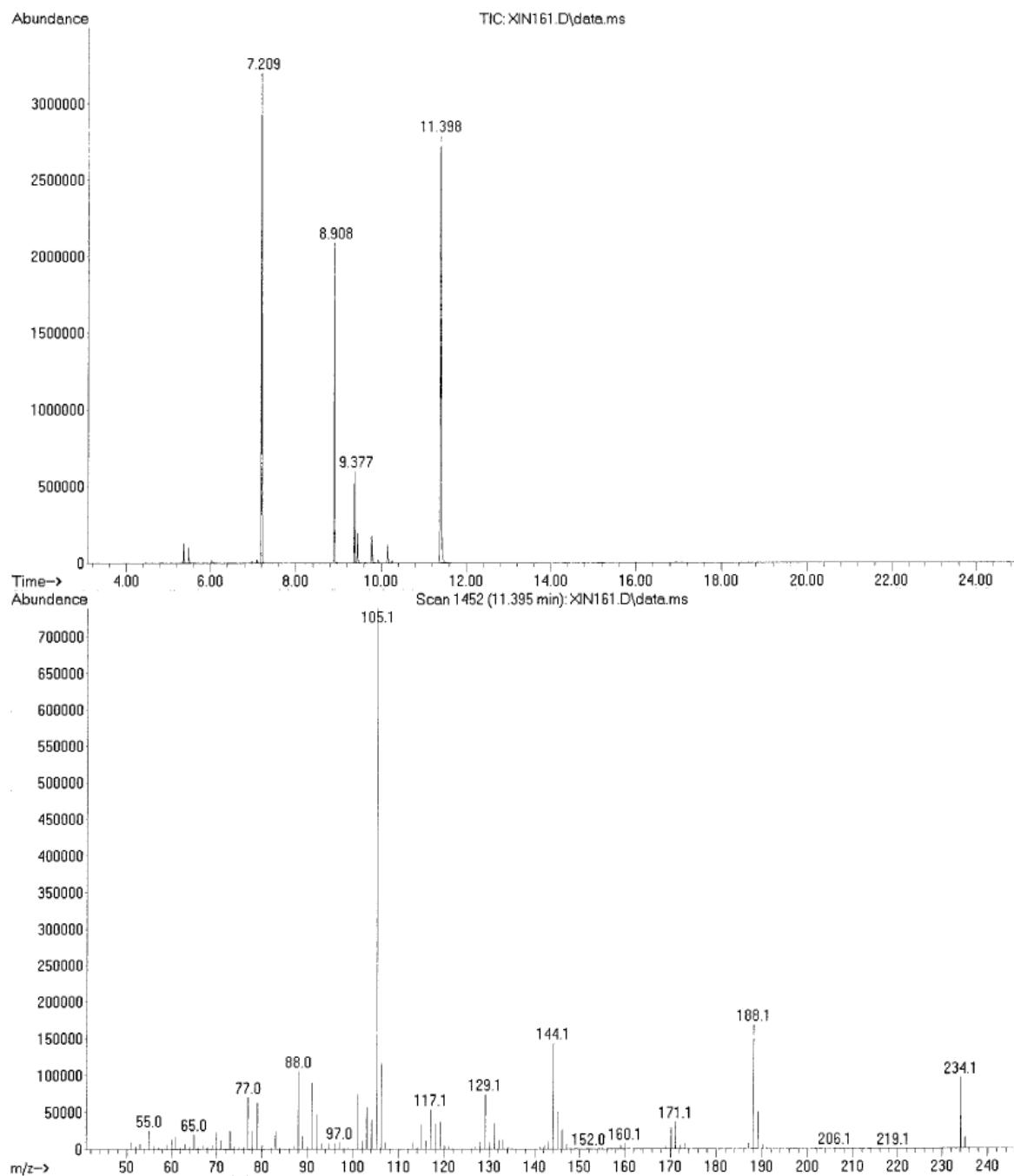


Entry 27: Dodecane internal standard $R_t = 7.206$ min. 2-(2-methylphenethyl)-1,3-dioxane, $R_t = 10.264$ min. By-product: 2,2'-dimethylbiphenyl, $R_t = 8.908$ min.

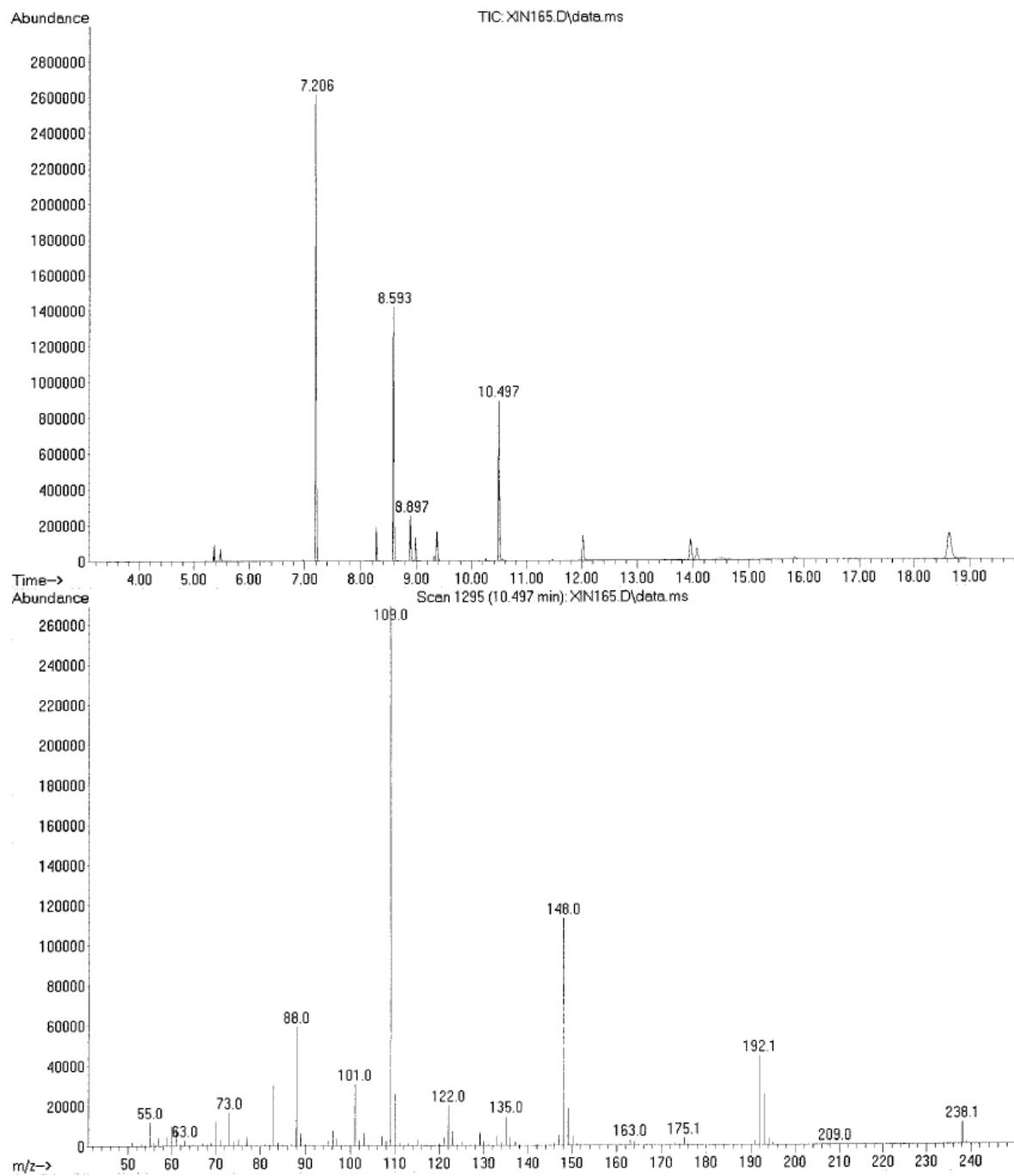


Entry 29: Dodecane internal standard $R_t = 7.209$ min. Ethyl-6-*o*-tolylhexanoate, $R_t = 11.398$ min.

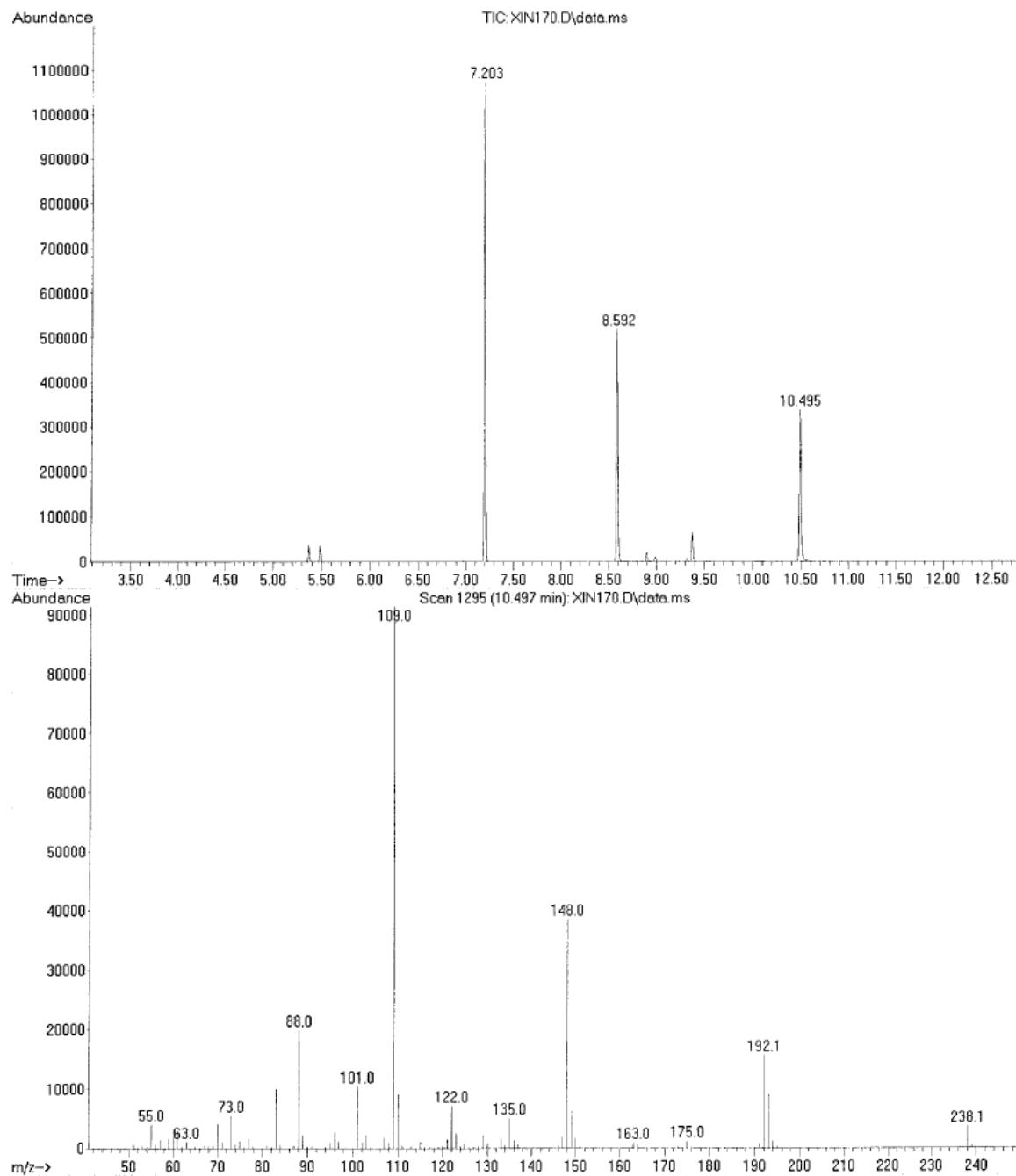
By-product: 2,2'-dimethylbiphenyl, $R_t = 8.908$ min. Other small peaks are impurities from the starting material, ethyl-6-bromohexanoate.



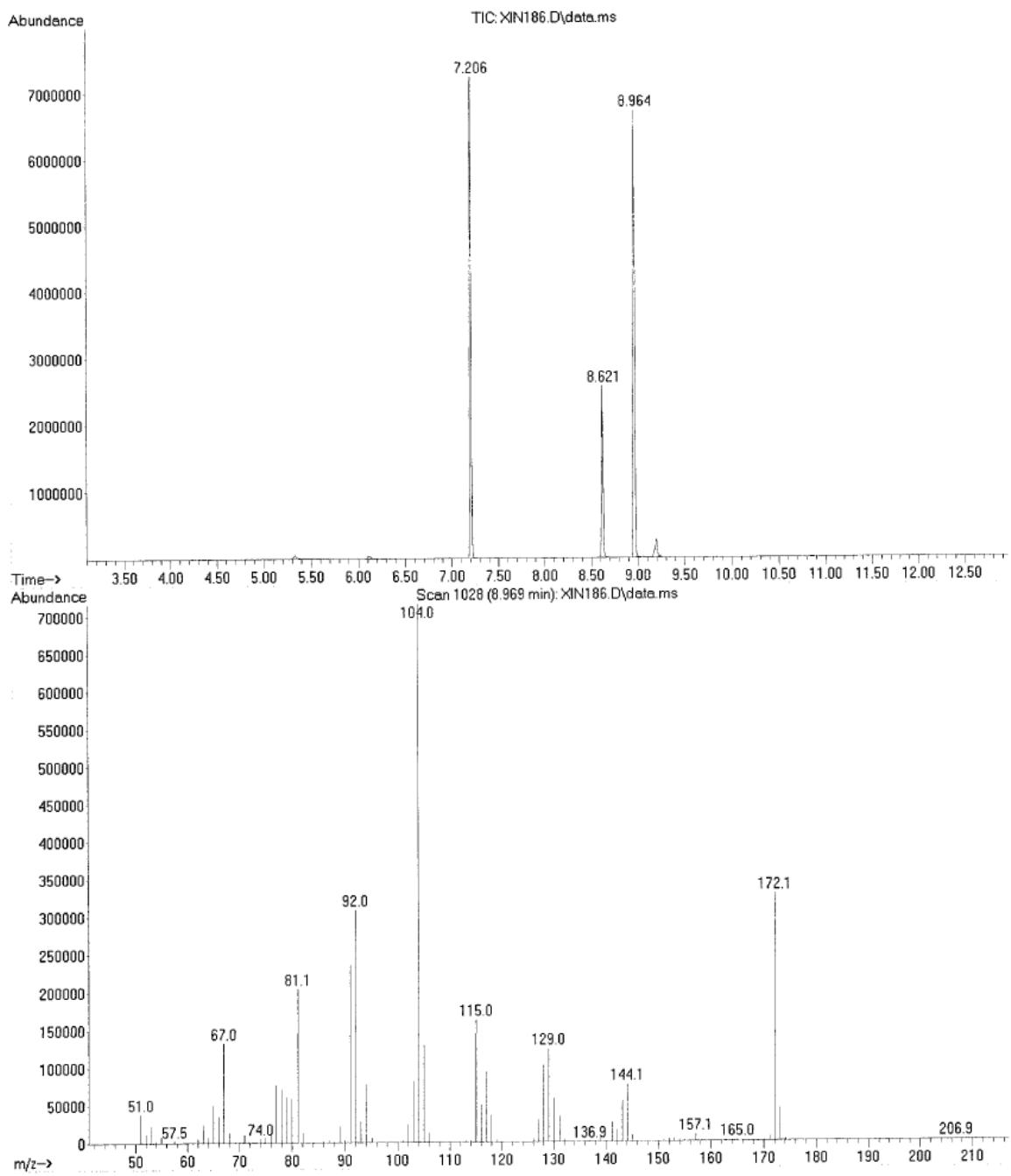
Entry 30: Dodecane internal standard $R_t = 7.206$ min. Ethyl 6-(4-fluorophenyl)hexanoate, $R_t = 10.497$ min. By-product: 4,4'-difluorobiphenyl, $R_t = 8.593$ min.



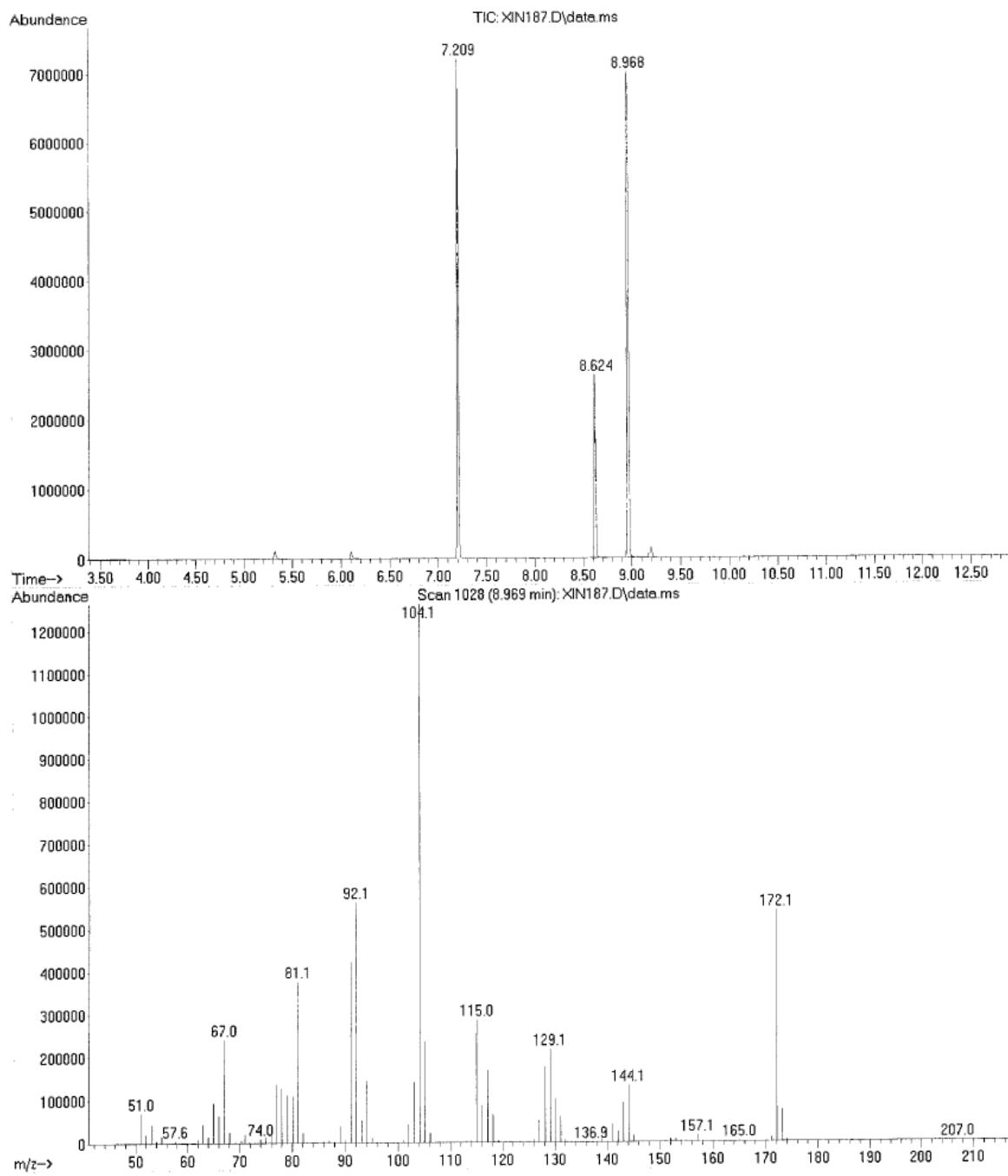
Entry 30 (MW method): Dodecane internal standard $R_t = 7.203$ min; Ethyl 6-(4-fluorophenyl)-hexanoate, $R_t = 10.495$ min. By-product: 4,4'-difluorobiphenyl, $R_t = 8.592$ min.



Entry 32: Dodecane internal standard $R_t = 7.206$ min. (1S,2S,4R)-2-phenylbicyclo[2.2.1]heptane, $R_t = 8.964$ min. By-product: biphenyl, $R_t = 8.621$ min.



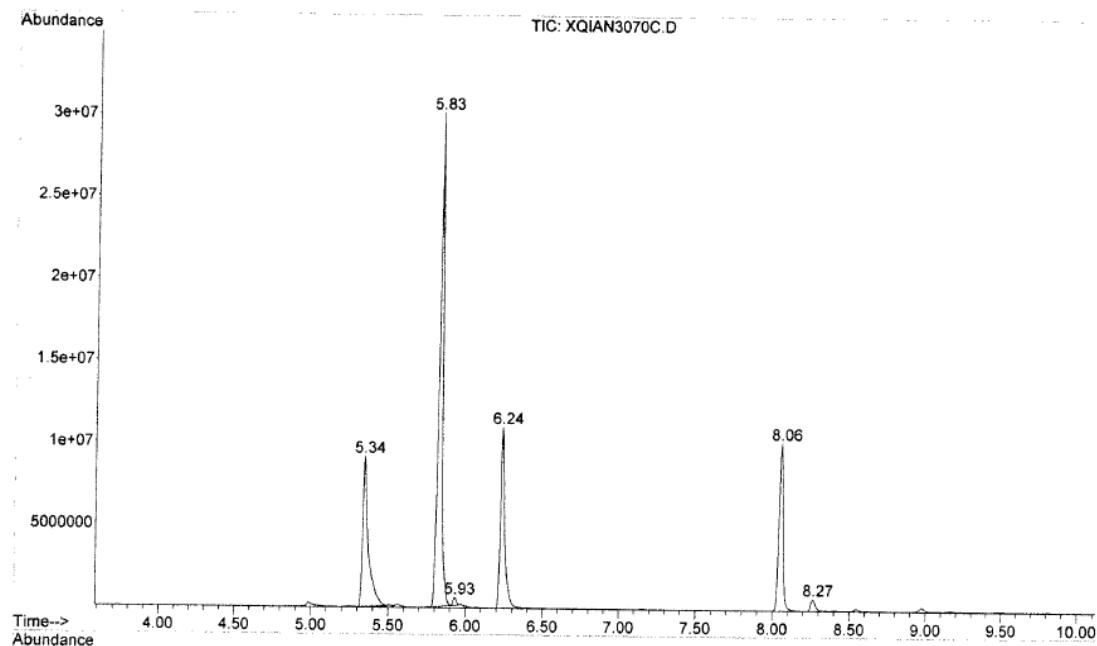
Entry 32 (MW method): Dodecane internal standard $R_t = 7.209$ min. (1S,2S,4R)-2-phenylbicyclo[2.2.1]heptane, $R_t = 8.968$ min. By-product: biphenyl, $R_t = 8.624$ min.



GC traces of radical clock experiments

Dodecane internal standard $R_t = 5.83$ min. 1-(but-3-enyl)-2-methylbenzene, $R_t = 5.34$ min.

1-(cyclopropylmethyl)-2-methylbenzene, $R_t = 6.24$ min. 2,2'-dimethylbiphenyl, $R_t = 8.06$ min.



Dodecane internal standard $R_t = 5.83$ min. 1-(hex-5-enyl)-2-methylbenzene, $R_t = 7.39$ min.

1-(cyclopentylmethyl)-2-methylbenzene, $R_t = 7.98$ min. 2,2'-dimethylbiphenyl, $R_t = 8.05$ min.

