Supporting Information

High Affinity InhA Inhibitors With Activity Against Drug Resistant Strains of *Mycobacterium Tuberculosis*

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Synthesis of the Alkyl Diphenyl Ethers.

Reaction A. The aryl halide (7.35 mmol), phenol (14.7 mmol), Cs_2CO_3 (32.3 mmol), $(CuOTf)_2$•PhH (0.735 mmol, 5.0 mol % Cu), ethyl acetate (0.125 mmol, 5.0 mol %), 1-naphthoic acid (32.3 mmol), molecular sieves 4 Å (1.8 g) and toluene (15 mL) were added to a oven-dried 50 mL two-necked round-bottomed flask sealed with a septum which was purged with nitrogen, and heated to 110 °C under nitrogen. Upon cooling to RT, dichloromethane was added and the organic phase was obtained by filtration. This solution was washed with 5% NaOH. The aqueous layer was then extracted with dichloromethane and the combined organic layers were washed with brine, dried over Mg_2SO_4 and concentrated under vacuum to give the crude product. This was then purified by flash chromatography on silica gel (5% ethyl acetate/hexane).

Reaction B. $ZnCl_2$ (0.5 M solution in tetrahydrofuran; 9.0 mL, 4.52 mmol) was added by syringe to a round bottom flask sealed with a rubber septum and purged with nitrogen. The appropriate alkyl magnesium chloride or alkyl magnesium bromide (1.0 M solution in THF; 4.0 mL, 4.26 mmol) was then added dropwise by syringe, and the resulting solution was stirred at room temperature for 20 min. *N*-methylpyrrolidinone (4.7 mL) was then added to the flask by syringe, followed by 21.7 mg (0.0426 mmol) of $Pd(P(t\text{-}Bu)_3)_2$ and 500 mg (2.13 mmol) of 4-chloro-2-methoxy-1-phenoxybenzene after 5 min. The flask was then fitted with a reflux condenser and refluxed for 48 h at 130 °C. The flask was then gradually cooled to RT, and 20 mL of a 1.0 M aqueous HCl solution was added. The resulting mixture was extracted with diethyl ether, the ether extract was washed with water, and then the organic layer was dried over anhydrous $MgSO_4$ and concentrated under vacuum to give the crude product. This was then purified by flash chromatography on silica gel (5% ethyl acetate/hexane).

Reaction C. A solution of 455 mg (1.8 mmol) boron tribromide in 1.8 mL of dichloromethane (1.0 M solution) was added to a solution of the 4-substituted-2-methoxy-1-phenoxy-benzene (1.4 mmol) in 3 mL of dry dichloromethane at - 70 °C under nitrogen. The reaction mixture was stirred at -70 °C for 1 h and then at RT for 3 h. When TLC analysis showed that the reaction had reached completion, the reaction mixture was quenched with methanol at -70 °C and concentrated to give an oil. A suspension of this oil in dichloromethane was washed with 10 % aqueous sodium bicarbonate solution and the organic layer was drawn off, washed sequentially with water then brine and dried over $MgSO_4$. The organic layer was filtered, concentrated under vacuo to give the crude product which was then purified by flash chromatography on silica gel (5% ethyl acetate/hexane).

1-(4-Ethyl-2-methoxyphenoxy)benzene. Reaction A was used to convert 4-ethyl-2-methoxyphenol and iodobenzene to the title product: yellow liquid (48%); ^{1}H NMR (200MHz) ($CDCl_3$) δ 7.50-6.81 (m,8H), 3.86 (s,3H), 2.77-2.68 (q,3H), 1.38-1.31 (t,3H).

5-Ethyl-2-phenoxyphenol (**2PP**). Reaction C was used to convert 1-(4-ethyl-2-methoxyphenoxy)benzene to the title product. Flash chromatography gave the product as a light brown oil (68%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at >97% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^{1}H NMR (300MHz) ($CDCl_3$) δ 7.39-7.34 (m, 2H), 7.17-7.11 (m, 1H), 7.07-7.03 (m,2H), 6.97-6.96 (d,1H), 6.88-6.86 (d,1H), 6.76-6.71 (d,1H), 5.67 (s,1H), 2.70-2.62 (q, 2H), 1.32-1.27 (t, 3H); HRMS (EI-MS M^+) calculated for $C_{14}H_{14}O_2$ 214.0994, found 214.0986.

4-Chloro-2-methoxy-1-phenoxy-benzene. Reaction A was used to convert 4-chloro-2-methoxy-phenol and iodobenzene to the title compound: white solid (53%); ^{1}H NMR (250 MHz) ($CDCl_3$) δ 7.35-

6.94 (m, 8H), 3.87 (s,3H); ^{13}C NMR (250 MHz, $CDCl_3$) δ 157.55, 151.88, 143.73, 129.53, 122.69, 121.66, 120.79, 118.80, 116.40, 113.33, 56.06; HRMS (EI-MS M^+) calculated for $C_{13}H_{11}ClO_2$ 234.0447, found 234.0443.

4-Butyl-2-methoxy-1-phenoxybenzene. Reaction B was used to couple butyl-magnesium chloride and 4-chloro-2-methoxy-1-phenoxy-benzene to the title compound: light brown oil (31%); ^1H NMR (300MHz) ($CDCl_3$) δ 7.41-7.29 (m,3H), 7.22-7.13 (m,1H), 7.09-6.93 (m,5H), 6.88-6.87 (d,1H), 6.83-6.79 (dd,1H), 3.88 (s, 3H), 2.67-2.66 (t,1.4H), 1.75-1.64 (m,1.5H), 1.47-1.39 (m,1.6H), 1.03-0.98 (t,2H).

5-Butyl-2-phenoxyphenol (4PP). Reaction C was used to convert 4-butyl-2-methoxy-1-phenoxybenzene to the title compound. Flash chromatography gave the product as a clear light yellow oil (82%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at 99% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^1H NMR (300MHz) ($CDCl_3$) δ 7.45-7.36 (t,2H), 7.23-7.15 (t,1H), 7.12-7.05 (d,2H), 6.95 (s,1H) 6.88-6.79 (d,1H), 6.67-6.65 (dd,1H), 5.58 (s, 1H), 2.67-2.61 (t,2H), 1.75-1.64 (m,2H), 1.43-1.30 (m,2H), 0.96-0.91 (t,3H); HRMS (EI-MS M^+) calculated for $C_{16}H_{18}O_2$ 242.1307, found 242.1311.

2-Methoxy-4-pentyl-1-phenoxybenzene. Reaction B was used to convert pentyl-magnesium chloride and 4-chloro-2-methoxy-1-phenoxy-benzene to the title compound: light brown oil (26%); ^1H NMR (300MHz) ($CDCl_3$) δ 7.38-7.32 (m,2H), 7.13-7.06 (m,1H), 7.04-6.97 (m,3H), 6.92-6.91 (d,1H), 6.84-6.80 (dd,1H), 3.91 (s, 3H), 2.71-2.68 (t,2H), 1.72-1.68 (m,2H), 1.47-1.44 (m,4H), 1.03-1.00 (t,3H).

5-Pentyl-2-phenoxyphenol (5PP). Reaction C was used to convert 2-methoxy-4-pentyl-1-phenoxybenzene to the title compound. Flash chromatography gave the product as a clear light yellow oil (77%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at 99% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^1H NMR (300MHz) ($CDCl_3$) δ 7.37-7.31 (m,2H), 7.14-7.01 (m,4H), 6.92-6.91 (s,1H), 6.85-6.82 (d,1H), 6.70-6.67 (dd,1H), 5.58 (s, 1H), 2.61-2.56 (t,2H), 1.67-1.62 (m,2H), 1.39-1.34 (m,4H), 0.96-0.92 (t,3H). HRMS (EI-MS M^+) calculated for $C_{17}H_{20}O_2$ 256.1463, found 256.1459.

1-(2-Methoxy-4-hexylphenoxy)benzene. Reaction B was used to convert hexyl-magnesium bromide and 4-chloro-2-methoxy-1-phenoxy-benzene to the title compound: clear oil (28%); ^1H NMR (300MHz) ($CDCl_3$) δ 7.36-6.80 (m,8H), 3.90 (s,3H), 2.71-2.66 (t,2H), 1.74-1.67 (m,2H), 1.42-1.33 (m,6H), 1.01-0.97 (t,3H).

5-Hexyl-2-phenoxyphenol (**6PP**). Reaction C was used to convert 1-(4-hexyl-2-methoxyphenoxy)benzene to the title product. Flash chromatography gave the product as a clear light yellow oil (86%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at 99% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^1H NMR (300MHz) ($CDCl_3$) δ 7.35-7.31 (t,2H), 7.11-7.07 (t,1H), 7.02-7.0 (t,2H), 6.88 (d,1H), 6.82-6.80 (d,1H), 6.67-6.65 (dd,1H), 5.48 (s, 1H), 2.58-2.54 (t,2H), 1.65-1.59 (m,2H), 1.35-1.27 (m,6H), 0.91-0.88 (t,3H). HRMS (EI-MS M^+) calculated for $C_{18}H_{22}O_2$ 270.1620, found 270.1615.

1-(2-Methoxy-4-octylphenoxy)benzene. Reaction B was used to convert octyl-magnesium chloride and 4-chloro-2-methoxy-1-phenoxy-benzene to the title compound: clear oil (73%);. ^1H NMR

(300MHz) ($CDCl_3$) δ 7.36-6.90 (m,8H), 3.90 (s,3H), 2.69-2.65 (t,2H), 1.72-1.68 (m,2H), 1.42-1.36 (m,10H), 1.00-0.94 (t,3H).

5-Octyl-2-phenoxyphenol (8PP) Reaction C was used to convert 1-(2-methoxy-4-octylphenoxy)benzene to the title compound. Flash chromatography gave the product as a clear light yellow oil (84%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at 99% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^1H NMR (300MHz) ($CDCl_3$) δ 7.35-7.31 (m,2H), 7.11-7.07 (t,1H), 7.02-7.0 (t,2H), 6.89-6.88 (d,1H), 6.82-6.80 (d,1H), 6.67-6.65 (dd,1H), 5.48 (s, 1H), 2.58-2.54 (t,2H), 1.63-1.59 (m,2H), 1.39-1.30 (m,10H), 0.91-0.88 (t,3H). HRMS (EI-MS M^+) calculated for $C_{20}H_{26}O_2$ 298.1933, found 298.1932.

2-Methoxy-1-phenoxy-4-tetradecylbenzene. Reaction B was used to convert tetradecylmagnesium chloride and 4-chloro-2-methoxy-1-phenoxy-benzene to the title compound: light brown oil (65 %); ^1H NMR (300MHz) ($CDCl_3$) δ 7.43-7.32 (m,2.6 H), 7.20-7.06 (m,2H), 7.03-6.97 (m,3H), 6.90-6.89 (d,1H), 6.82-6.79 (dd,1H), 3.89 (s, 3H), 2.70-2.65 (t,2H), 1.73-1.62 (m,2.3H), 1.40-1.38 (m,25H), 0.98-0.94 (t,3.6H). ESI-MS calculated for $C_{27}H_{40}O_2$ 396.61, found 269.2, 327.1, 397.3, 411.2.

5-Tetradecyl-2-phenoxyphenol (14PP) Reaction C was used to convert 2-methoxy-1-phenoxy-4-tetradecylbenzene to the title compound. Flash chromatography gave the product as a clear light yellow oil (82%). The identify of the product was verified by NMR and EI-MS methods and the purity of the product was estimated at 99% by NMR spectroscopy. Relevant NMR and EI-MS spectra are presented below. ^1H NMR (300MHz) ($CDCl_3$) δ 7.33-7.30 (m,2H), 7.12-7.07 (m,1H), 7.02-6.99 (m,2H), 6.89-6.88 (d,1H), 6.82-6.80 (d,1H),6.68-6.64 (dd,1H), 5.43 (s, 1H), 2.55 (t,2H), 1.64-1.59 (m,2H), 1.33-1.27 (m,24H), 0.91-0.87 (t,3H). HRMS (EI-MS M^+) calculated for $C_{26}H_{38}O_2$ 382.2872, found 382.2868.

Supplementary Table 1. Data collection and refinement statistics (Molecular Replacement)

	5-Octyl-2-phenoxyphenol (8PP)	5-Pentyl-2-phenoxyphenol (5PP)	Triclosan (TCN)
Data collection			
Space group	$C222_1$	C2	C2
Cell dimensions			
a, *b*, *c* (Å)	82.3, 100.3, 379.3	100.2, 82.1, 189.8	100.0, 81.8, 188.7
α, β, γ (°)	90.0, 90.0, 90.0	90.0, 95.4, 90.0	90.0, 95.7, 90.0
Resolution (Å)	40-2.6 (2.7-2.6)	40-2.8 (2.9-2.8)	50-2.3 (2.4-2.3)
R_{sym}	11.2 (45.7)	11.9 (35.0)	10.3 (18.6)
$I / \sigma I$	13.3 (3.3)	16.1 (4.3)	16.0 (7.4)
Completeness (%)	96.4 (97.3)	98.4 (93.9)	90.0 (84.1)
Redundancy	3.6 (3.6)	7.5 (6.7)	2.6 (2.5)
Refinement			
Resolution (Å)	2.6	2.8	2.3
No. reflections	44,393	37,542	60,723
R_{work} / R_{free}	22.8 / 28.8	24.2 / 29.5	26.8 / 33.3
No. atoms			
Protein	11,398	11,463	11,271
Ligand/ion	264 (NAD) 40 (8PP)	264 (NAD) 114 (5PP)	264 (NAD) 102 (TCL)
Water			
B-factors			
Protein	40.5	32.5	32.6
Ligand/ion	38.1 (NAD) 37.9 (8PP)	26.9 (NAD) 35.0 (5PP)	32.4 (NAD) 53.3 (TCL)
Water	25.0	-	-
R.m.s. deviations			
Bond lengths (Å)	0.016	0.016	0.014
Bond angles (°)	1.4	1.5	1.5

Supplementary Table 1 Legend

$R_{sym} = \Sigma_{hkl}\Sigma_i|I_i-\langle I\rangle|/\Sigma_{hkl}\Sigma_i\langle I\rangle$ where I_i is the i^{th} measurement and $\langle I\rangle$ is the weighted mean of all measurements of I. $\langle I\rangle/\langle\sigma I\rangle$ indicates the average of the intensity divided by its average standard deviation. Numbers in parentheses refer to the respective highest resolution data shell in each data set. $R_{cryst}=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ where F_o and F_c are the observed and calculated structure factor amplitudes. R_{free} same as R_{cryst} for 5% of the data randomly omitted from the refinement. Ramachandran statistics indicate the fraction of residues in the most favored, additionally allowed, generously allowed, and disallowed regions of the Ramachandran diagram, as defined by the program PROCHECK (*1*).

1. Laskowski, R. A., Macarthur, M. W., Moss, D. S., and Thornton, J. M. (1993) Procheck - a program to check the stereochemical quality of protein structures. *J. Appl. Crystallogra. 26*, 283-291.

Supplementary Table 2. Primer Sequences Used for Quantitative Real Time PCR.

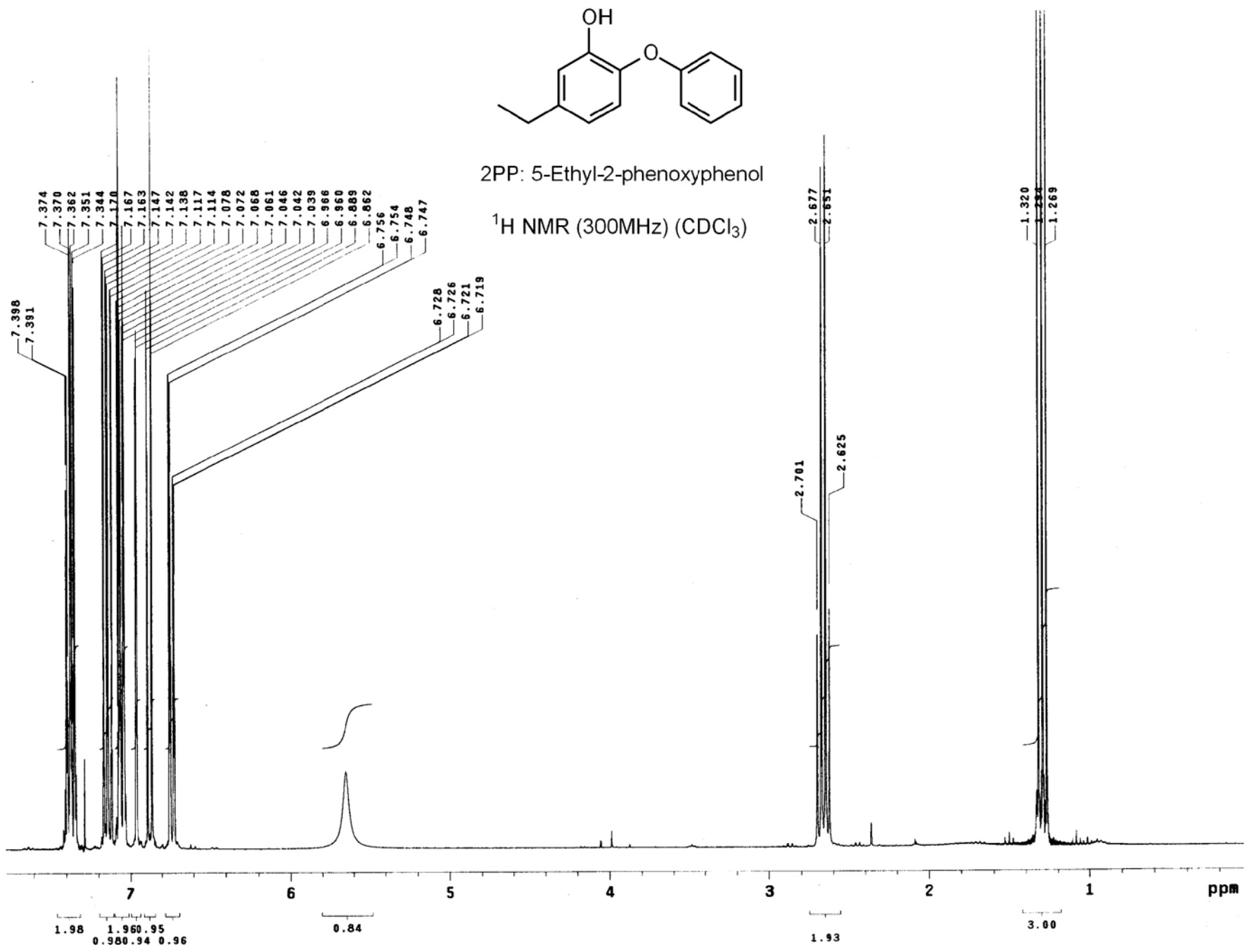
A. Gene[a]	Forward Primer	Reverse Primer
sigA	TTCGCGCCTACCTCAAACAG	GCTAGCTCGACCTCTTCCTCG
fabD	ACCCTGGTCTCCCAGCTCAC	AGTTCGCGTTTGGCGATACC
kasA	TGCTCATCGAGACGGAGGAG	CTACCGGCACGAACACCATC
rv1685c	ACTTCGGCACCAAACAGCAG	AACCGAGTTCCTCGACAGGC
rv1687c	GGTCGGGCAAGACAACACTG	AGAGTTCGGCGAAGTAGCGG
rv3160c	CTGGACTACCTGCATGCTTC	CCATCTCCGCGACTAGCTCC
rv3161c	CAGGGTTCCCTTCAGCGTTC	GCGGAATAAAGCCGAACCAC

B. Gene[b]	Forward Primer	Reverse Primer
dnaA	GCATTCAAACGCAGCTACCG	TGTTGGCATTGTGCAAGGTG
rv0077c	TGACGTGTTCTTCGCACTCG	GGGGAATCCACCATCGAGAA
rv0711	GCCCTGACCAATGTGCTGAC	CGGTGACCTGGGTGATGGTA
rv1072	GGTGAAGGCTTGGGCTTACG	ATCTGATCAGCCGCATCGAA
inhA	CGATCGGCTGGAACATGAAG	CCGTCGGCGTAGATGATGTC
rv1557	GGAACTGGCGCTGGCTAACT	CGGCGGCAGATAGAAGGAGT
rv1686c	CATTGTGGCGTTCTGGTTCC	AATAGACCGAGCCCGACACC
rv2253	GACACCGCAAGAAGGCAATG	TCACGAGGTACTGCCCGTTC
rv3486	ATTGTCTGCGGCACACTGGT	TGCAGTGCTCGGAGTTTGGT

Supplementary Table 2 Legend

[a]Primer sequences obtained from Betts et al. (*2*) and B. Primers designed using the Primer3 website (http://frodo.wi.mit.edu/cgi-bin/primer3/primer3-www.cgi)

2. Betts, J. C., McLaren, A., Lennon, M. G., Kelly, F. M., Lukey, P. T., Blakemore, S. J., and Duncan, K. (2003) Signature gene expression profiles discriminate between isoniazid-, thiolactomycin-, and triclosan-treated Mycobacterium tuberculosis. *Antimicrob. Agents Chemother. 47*, 2903-13.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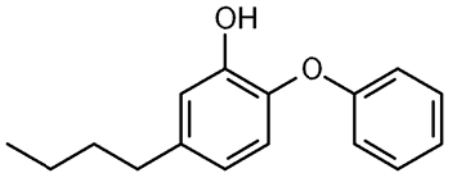
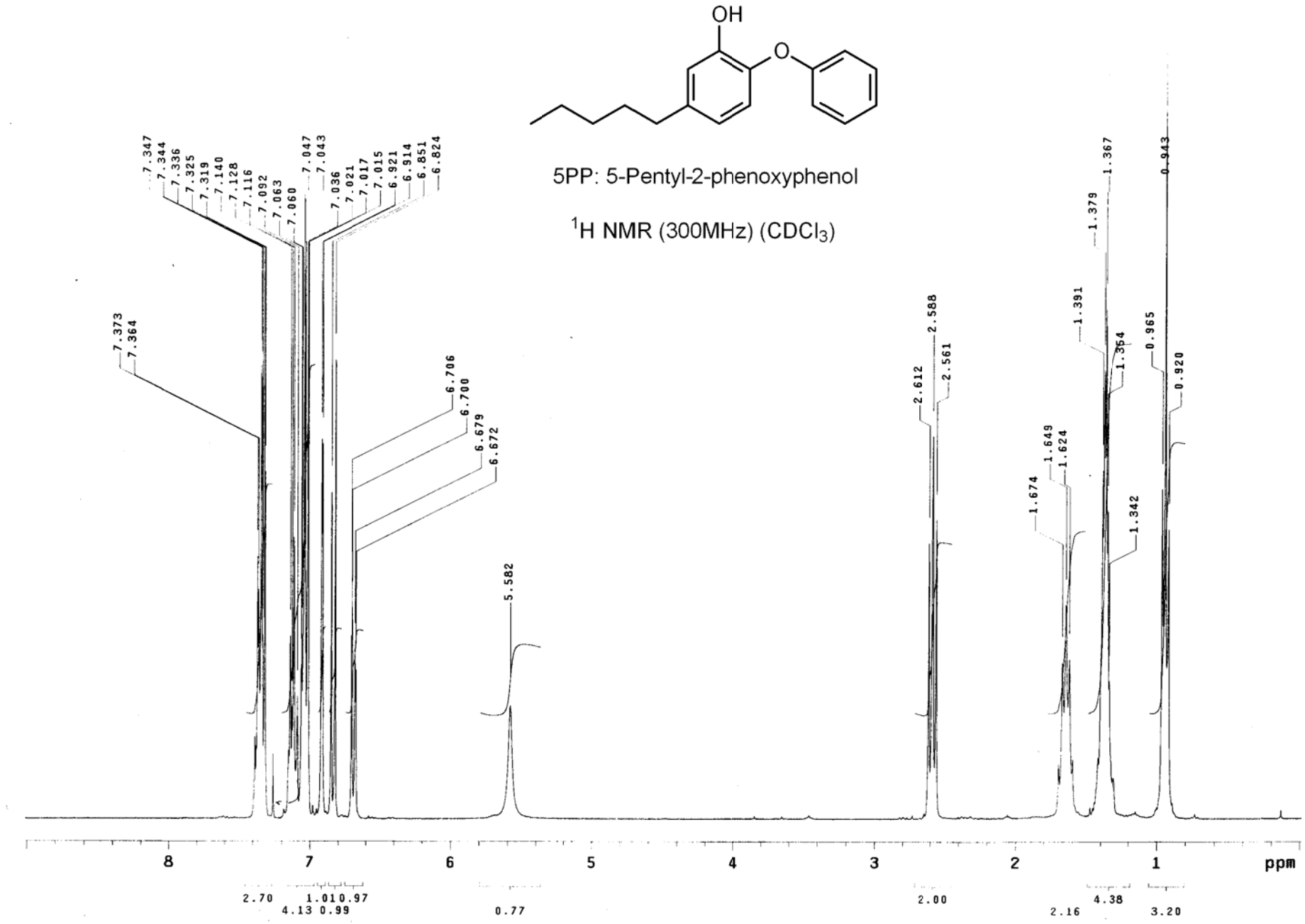


4PP: 5-Butyl-2-phenoxyphenol

^{1}H NMR (300MHz) ($CDCl_3$)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1H NMR (300MHz) (CDCl3)
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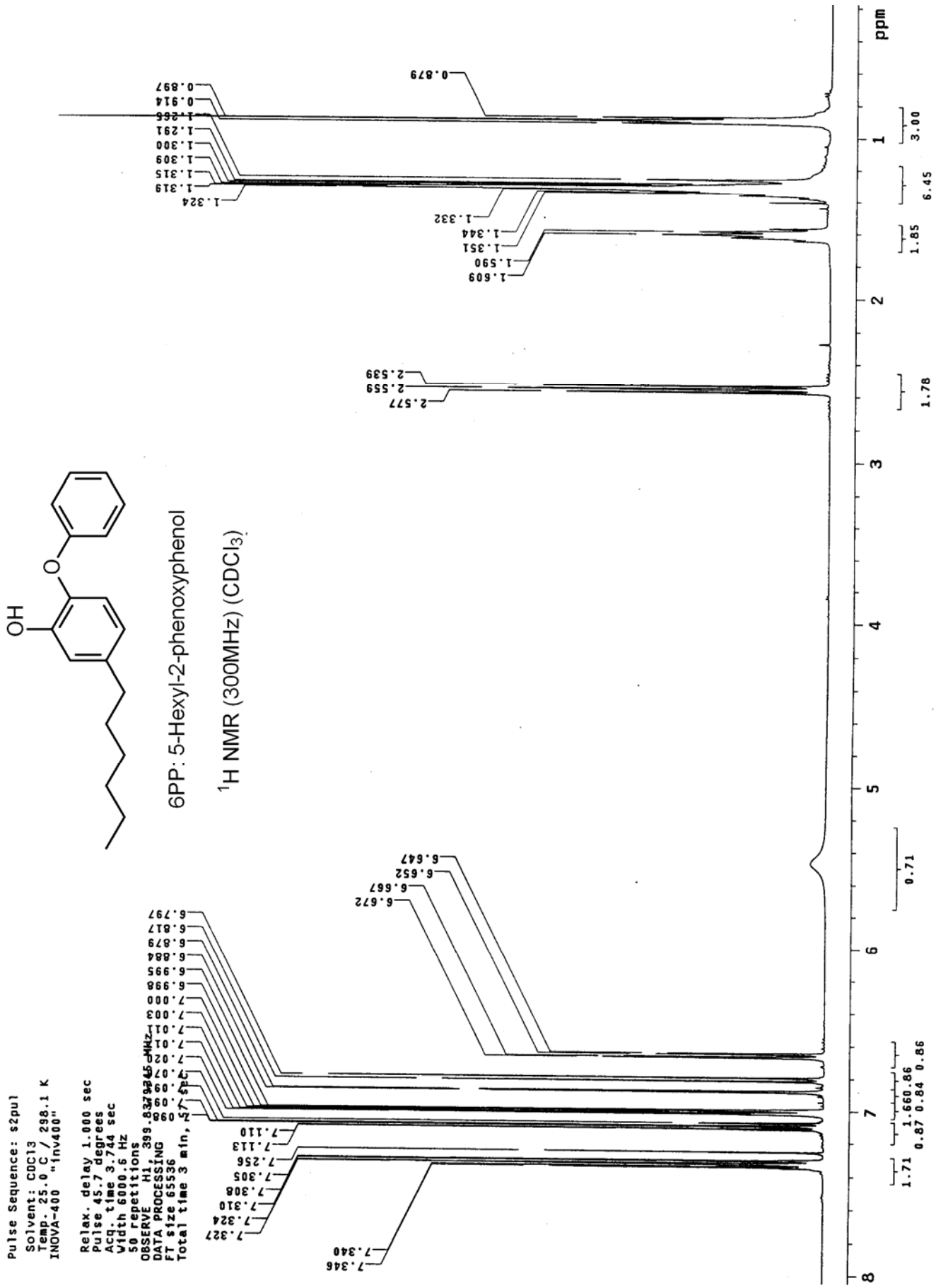
6PP: 5-Hexyl-2-phenoxyphenol
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DATA PROCESSING
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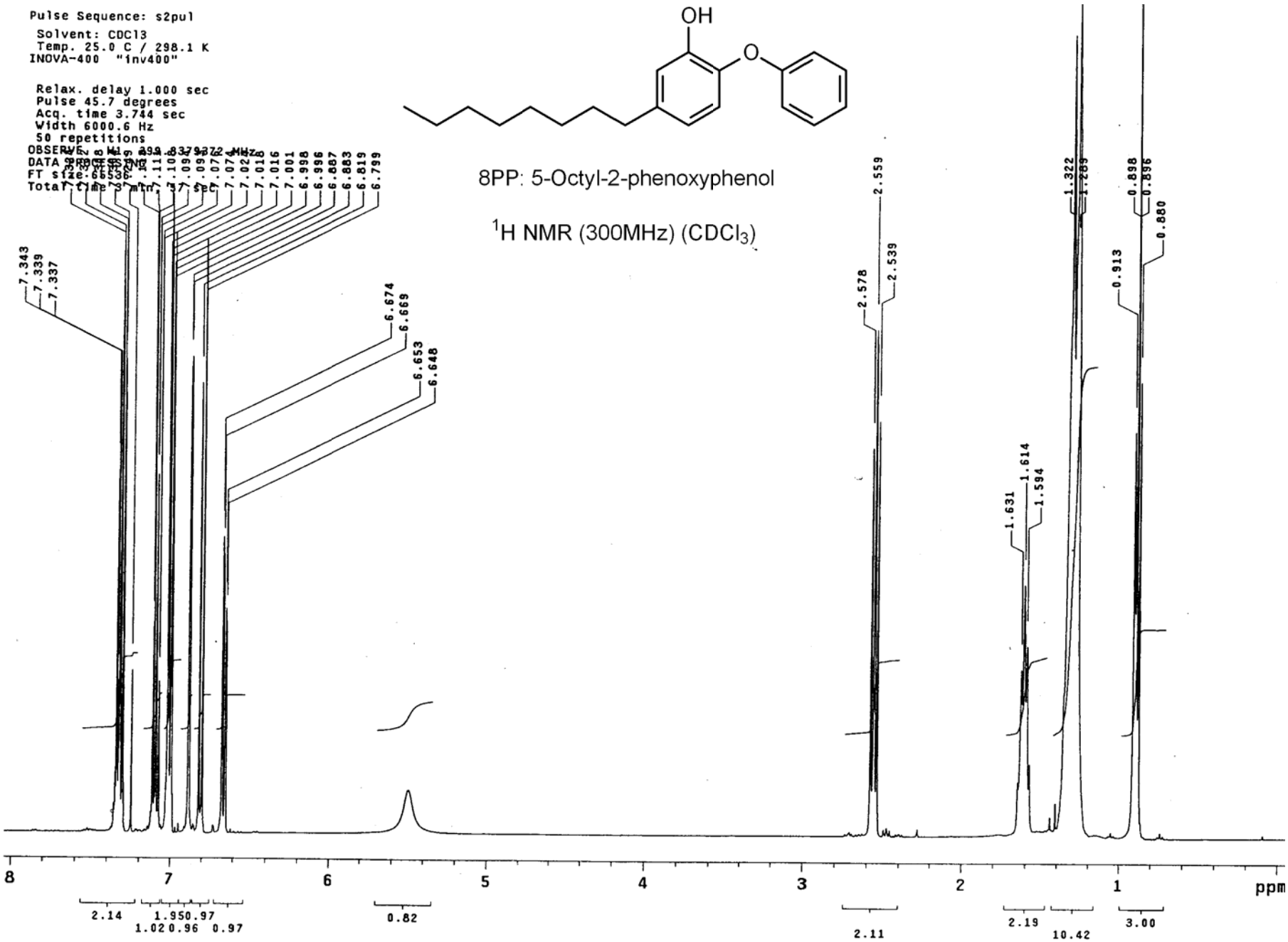
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Pulse 45.7 degrees
Acq. time 3.744 sec
Width 6000.6 Hz
50 repetitions
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8PP: 5-Octyl-2-phenoxyphenol
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7.337
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7.022
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6.648
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2.559
2.539
1.631
1.614
1.594
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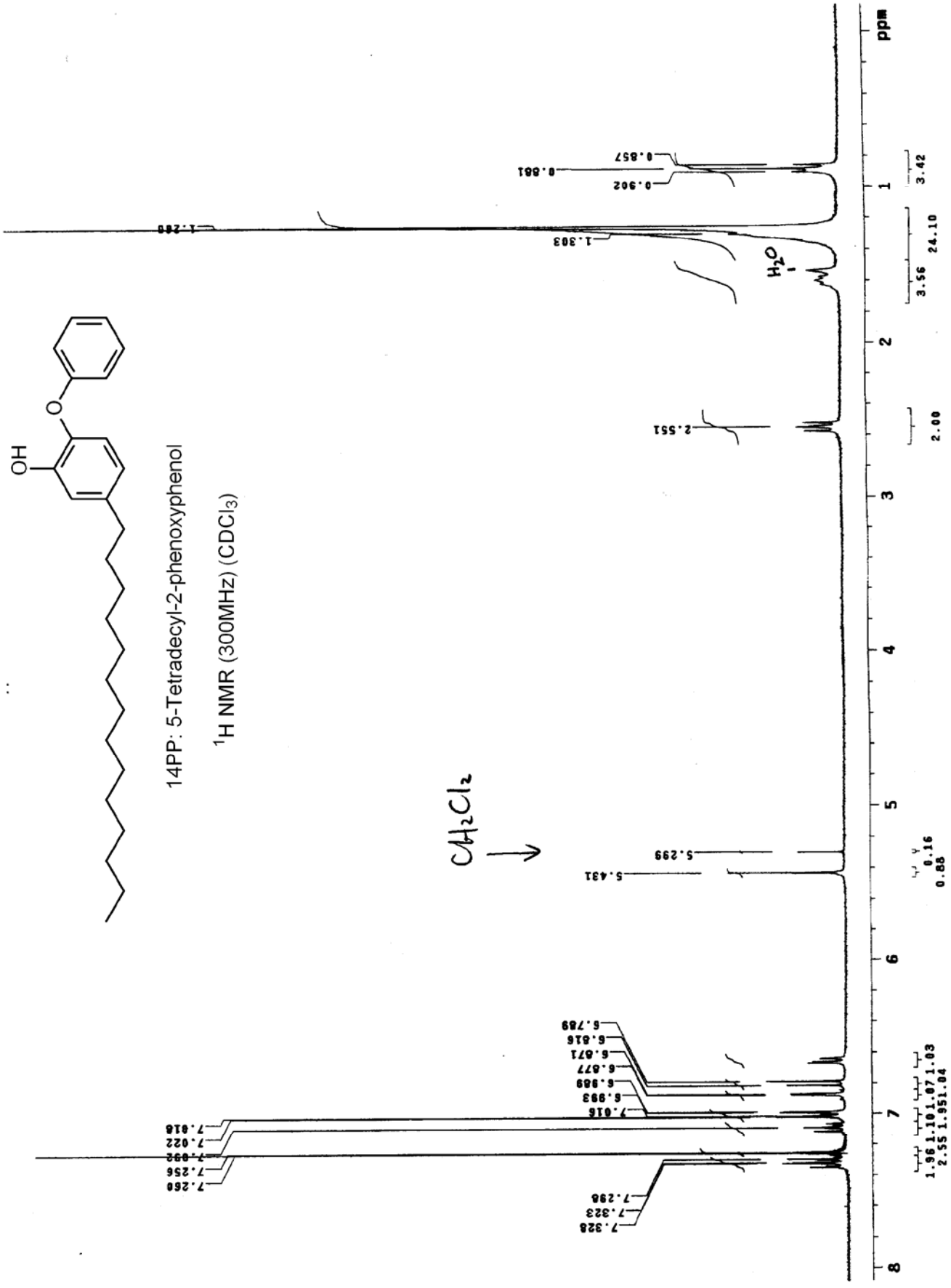
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O
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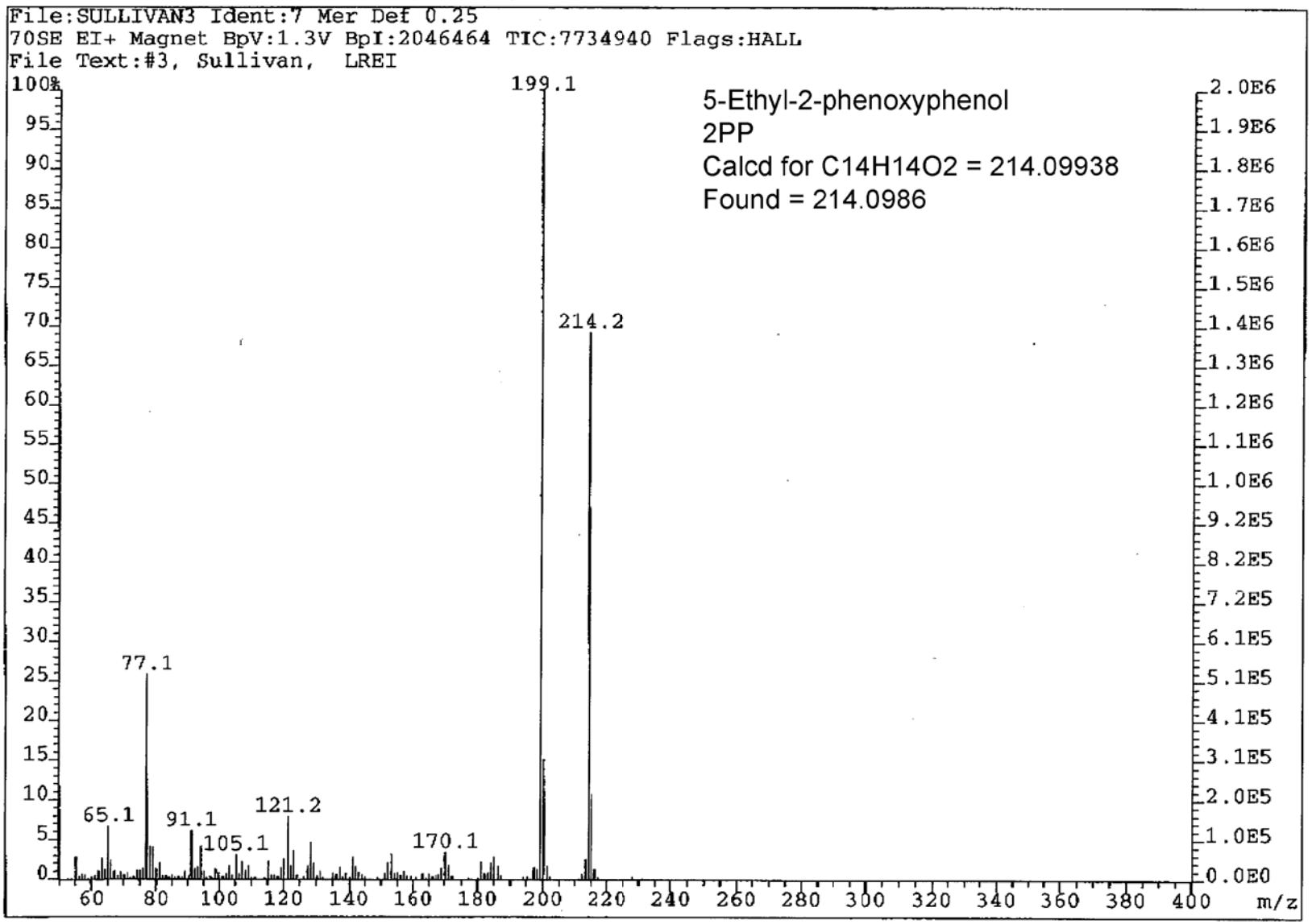
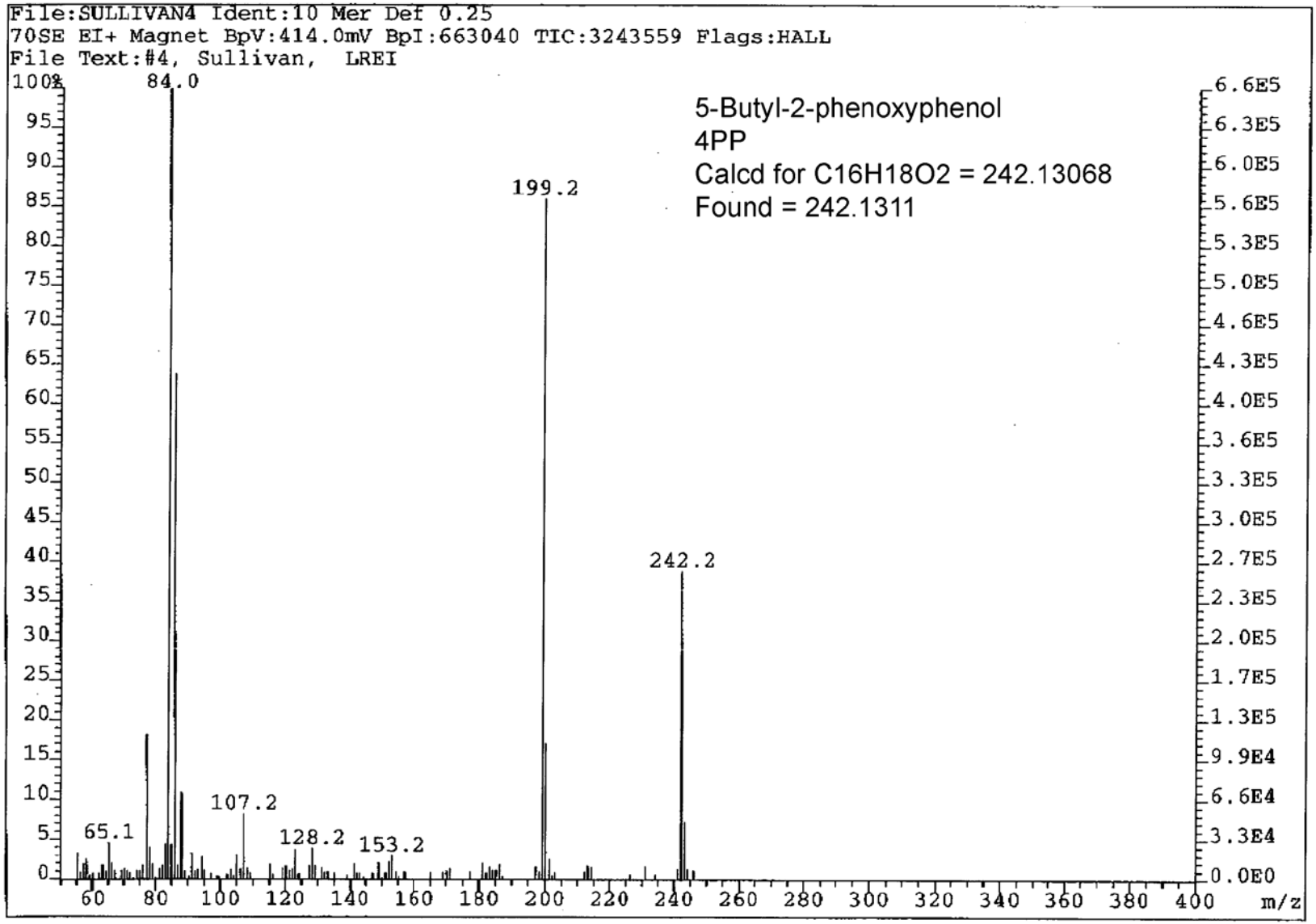
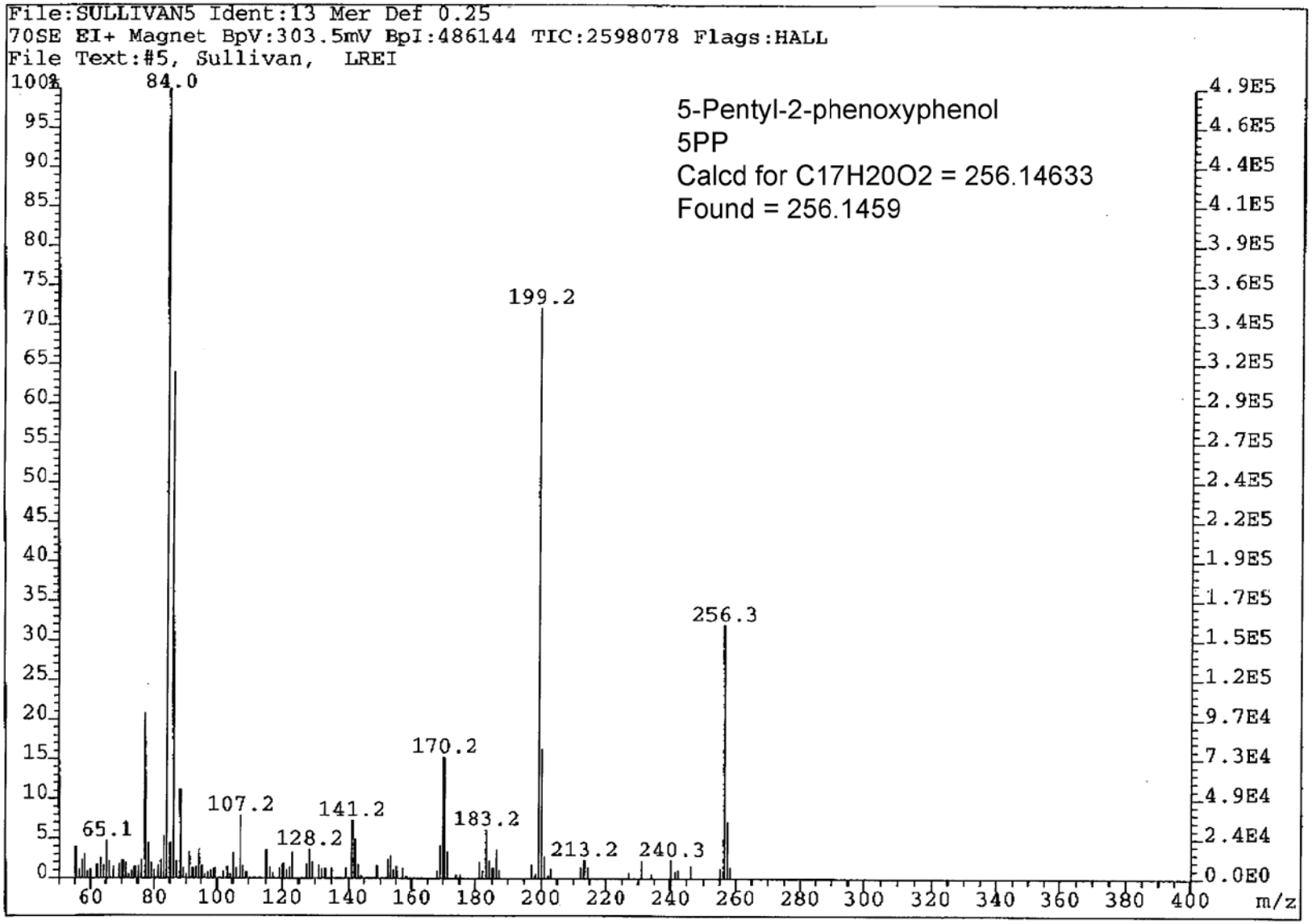
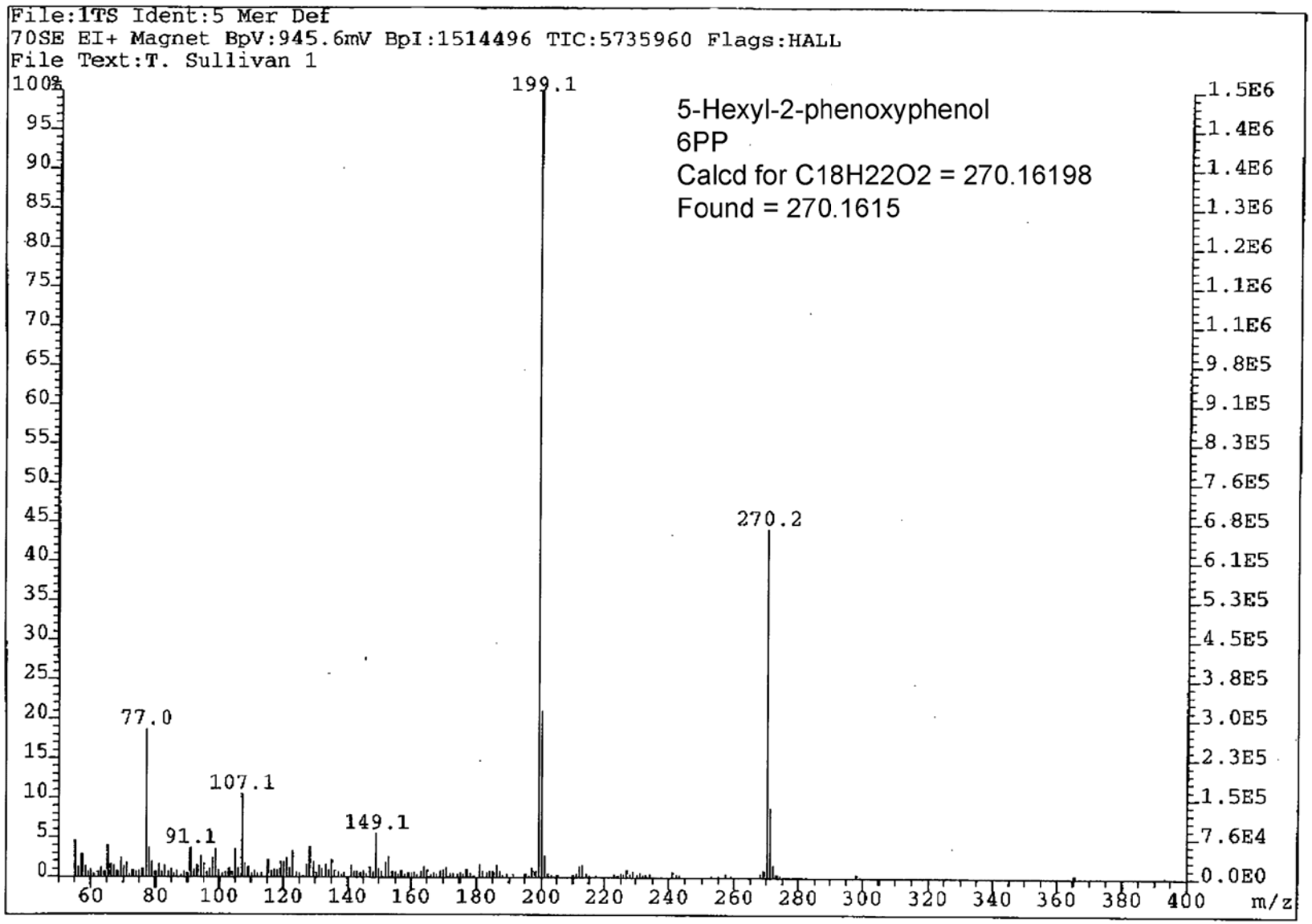
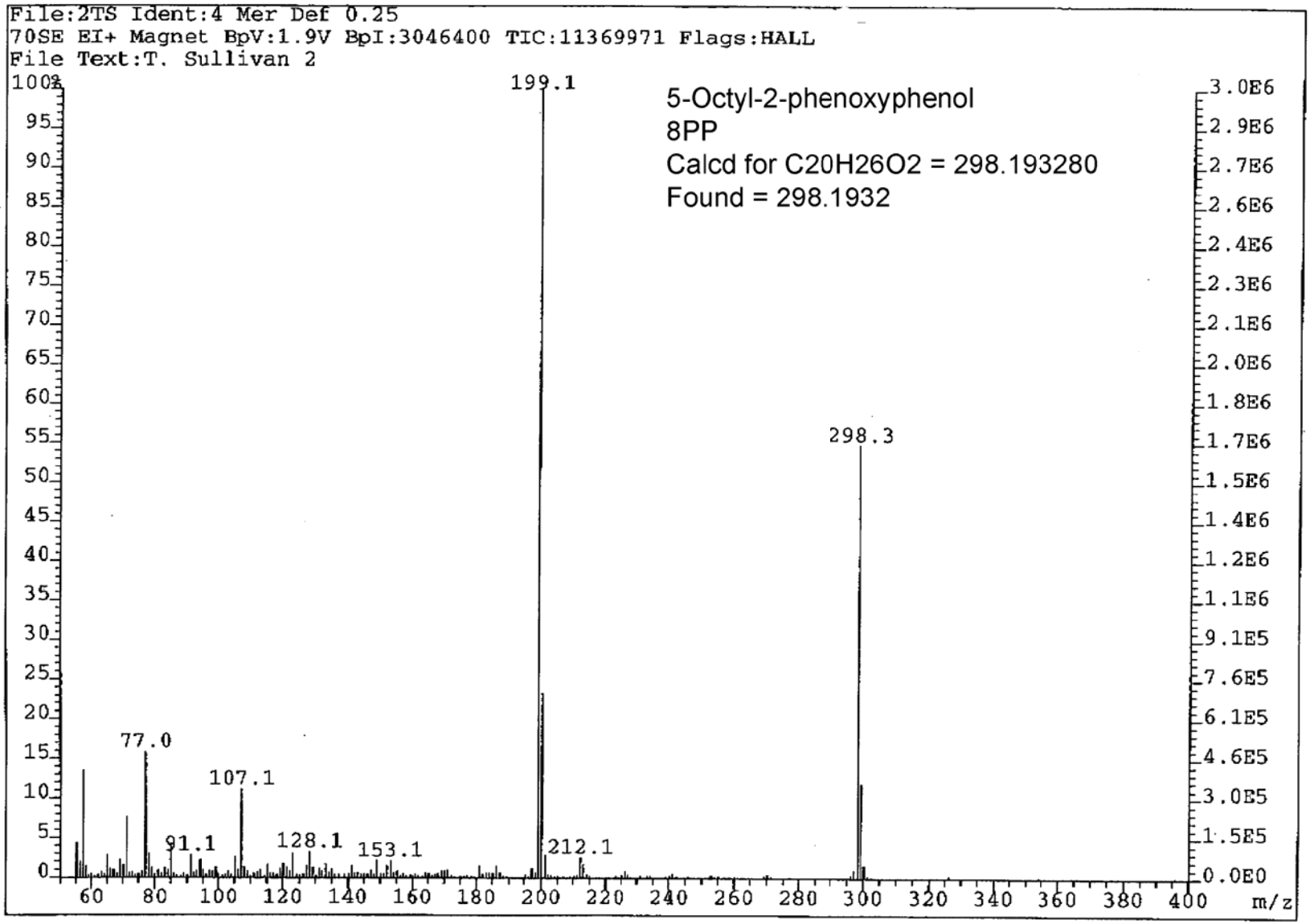
0.881
0.902
2.551
5.299
5.431
6.789
6.816
6.871
6.877
6.989
6.993
7.016
7.258
7.323
7.298
7.268
7.256
7.092
7.022
7.018
3.42
24.10
3.56
2.00
0.16
0.88
1.96 1.10 1.07 1.03
2.55 1.95 1.04

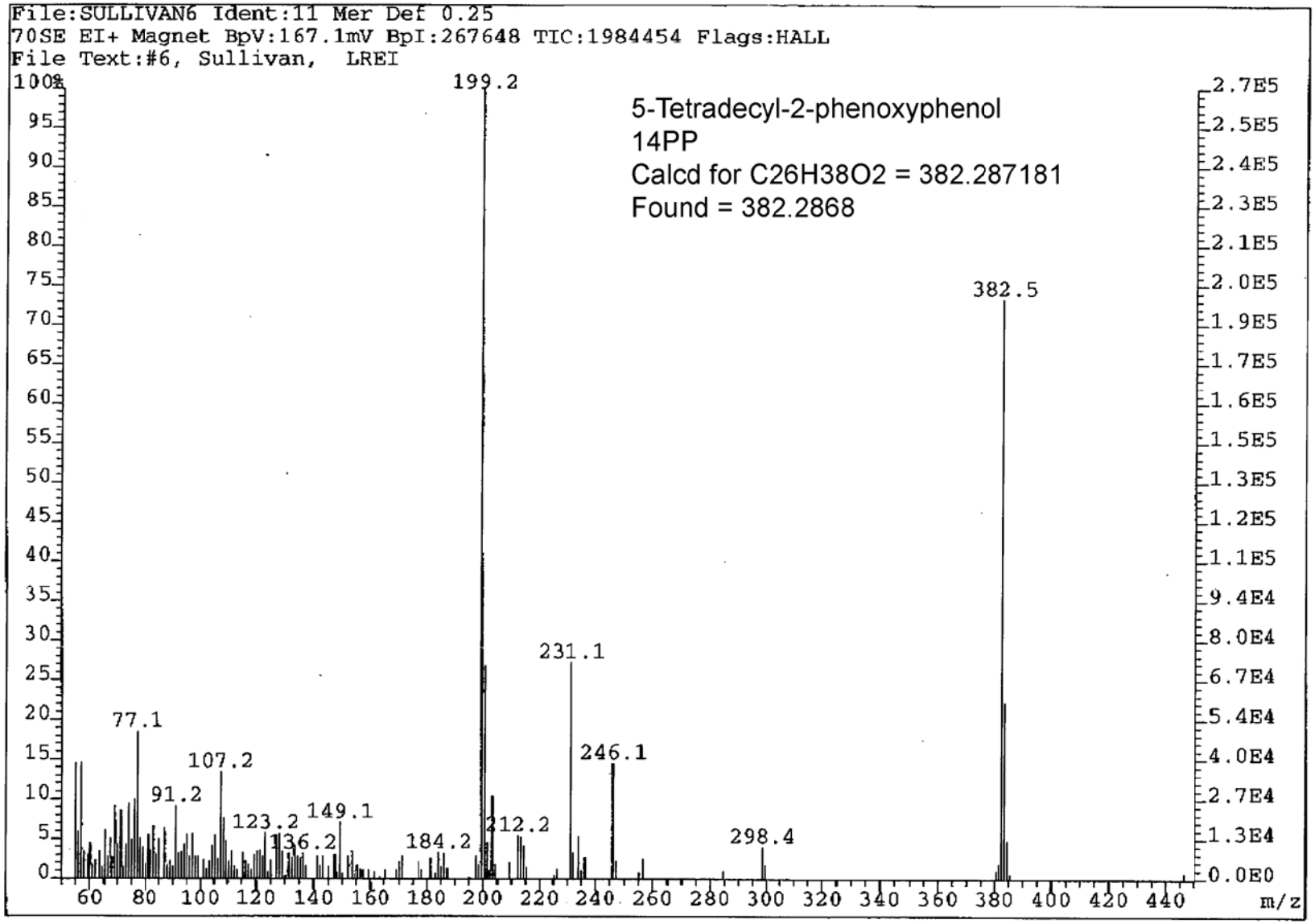

File:SULLIVAN3 Ident:7 Mer Def 0.25
70SE EI+ Magnet BpV:1.3V BpI:2046464 TIC:7734940 Flags:HALL
File Text:#3, Sullivan, LREI
5-Ethyl-2-phenoxyphenol
2PP
Calcd for C14H14O2 = 214.09938
Found = 214.0986
199.1
214.2
77.1
65.1
91.1
105.1
121.2
170.1
m/z


File:SULLIVAN4 Ident:10 Mer Def 0.25
70SE EI+ Magnet BpV:414.0mV BpI:663040 TIC:3243559 Flags:HALL
File Text:#4, Sullivan, LREI
5-Butyl-2-phenoxyphenol
4PP
Calcd for C16H18O2 = 242.13068
Found = 242.1311
84.0
199.2
242.2
107.2
65.1
128.2
153.2
m/z


File:SULLIVAN5 Ident:13 Mer Def 0.25
70SE EI+ Magnet BpV:303.5mV BpI:486144 TIC:2598078 Flags:HALL
File Text:#5, Sullivan, LREI
5-Pentyl-2-phenoxyphenol
5PP
Calcd for C17H20O2 = 256.14633
Found = 256.1459
84.0
199.2
256.3
170.2
107.2
141.2
183.2
128.2
65.1
213.2
240.3
m/z


File:1TS Ident:5 Mer Def
70SE EI+ Magnet BpV:945.6mV BpI:1514496 TIC:5735960 Flags:HALL
File Text:T. Sullivan 1
5-Hexyl-2-phenoxyphenol
6PP
Calcd for C18H22O2 = 270.16198
Found = 270.1615
199.1
270.2
77.0
107.1
91.1
149.1
m/z


File:2TS Ident:4 Mer Def 0.25
70SE EI+ Magnet BpV:1.9V BpI:3046400 TIC:11369971 Flags:HALL
File Text:T. Sullivan 2
5-Octyl-2-phenoxyphenol
8PP
Calcd for C20H26O2 = 298.193280
Found = 298.1932
199.1
298.3
77.0
107.1
91.1
128.1
153.1
212.1
m/z


File:SULLIVAN6 Ident:11 Mer Def 0.25
70SE EI+ Magnet BpV:167.1mV BpI:267648 TIC:1984454 Flags:HALL
File Text:#6, Sullivan, LREI
5-Tetradecyl-2-phenoxyphenol
14PP
Calcd for C26H38O2 = 382.287181
Found = 382.2868
199.2
382.5
231.1
246.1
77.1
107.2
91.2
123.2
149.1
136.2
184.2
212.2
298.4
m/z