

SUPPLEMENTARY MATERIAL

For

Synthesis and Characterisation of Arsenolipids: Naturally Occurring Arsenic Compounds in Fish and Algae

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¹H & ¹³C NMR spectra for:

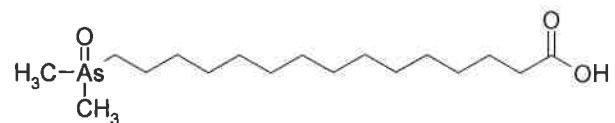
- 15-dimethylarsinyl pentadecanoic acid (**1**, As-FA 362)
- 19-Dimethylarsinyl-nonadecanoic acid (**2**, As-FA 418)
- 17-dimethylarsinyl-9-heptadecenoic acid (**3**, As-FA 388)
- 16-dimethylarsinyl-9-hexadecenoic acid (**4**, As-FA 374)
- 1-dimethylarsinyl-pentadecane (**5**, As-HC 332)
- 1-dimethylarsinyl-heptadecane (**6**, As-HC 360)

¹H NMR spectra for:

- 1-Dimethylarsinyltricosane (**7**, As-HC 444)

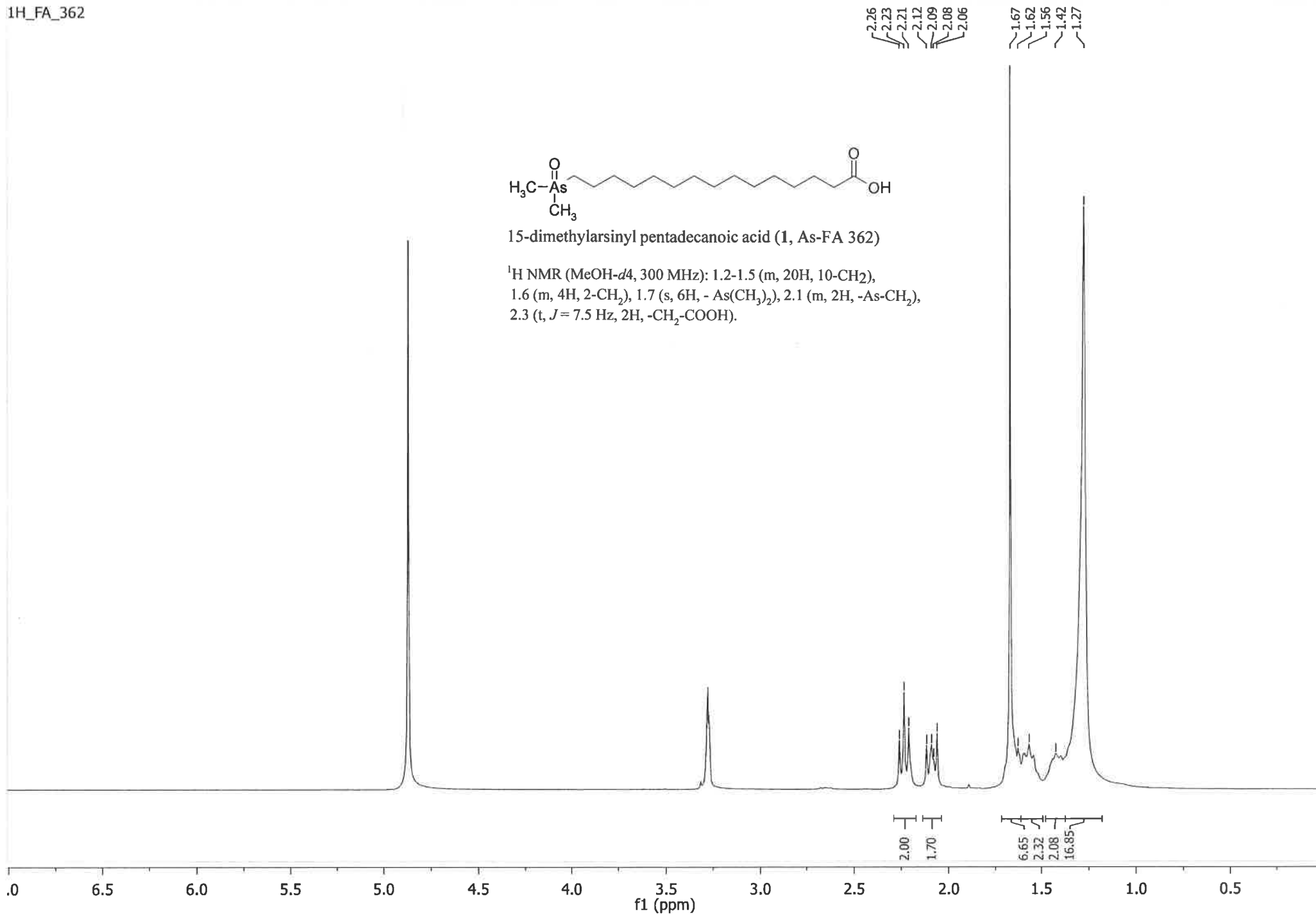
High resolution mass spectra & tandem mass spectra for:

- 15-dimethylarsinyl pentadecanoic acid (**1**, As-FA 362)
- 19-Dimethylarsinyl-nonadecanoic acid (**2**, As-FA 418)
- 17-dimethylarsinyl-9-heptadecenoic acid (**3**, As-FA 388)
- 16-dimethylarsinyl-9-hexadecenoic acid (**4**, As-FA 374)
- 1-dimethylarsinyl-pentadecane (**5**, As-HC 332)
- 1-dimethylarsinyl-heptadecane (**6**, As-HC 360)
- 1-Dimethylarsinyltricosane (**7**, As-HC 444)



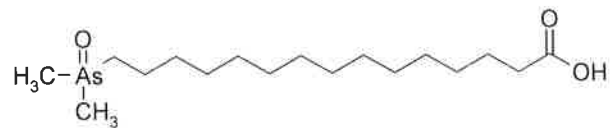
15-dimethylarsinyl pentadecanoic acid (1, As-FA 362)

^1H NMR (MeOH- d_4 , 300 MHz): 1.2-1.5 (m, 20H, 10-CH₂),
1.6 (m, 4H, 2-CH₂), 1.7 (s, 6H, -As(CH₃)₂), 2.1 (m, 2H, -As-CH₂),
2.3 (t, $J = 7.5$ Hz, 2H, -CH₂-COOH).



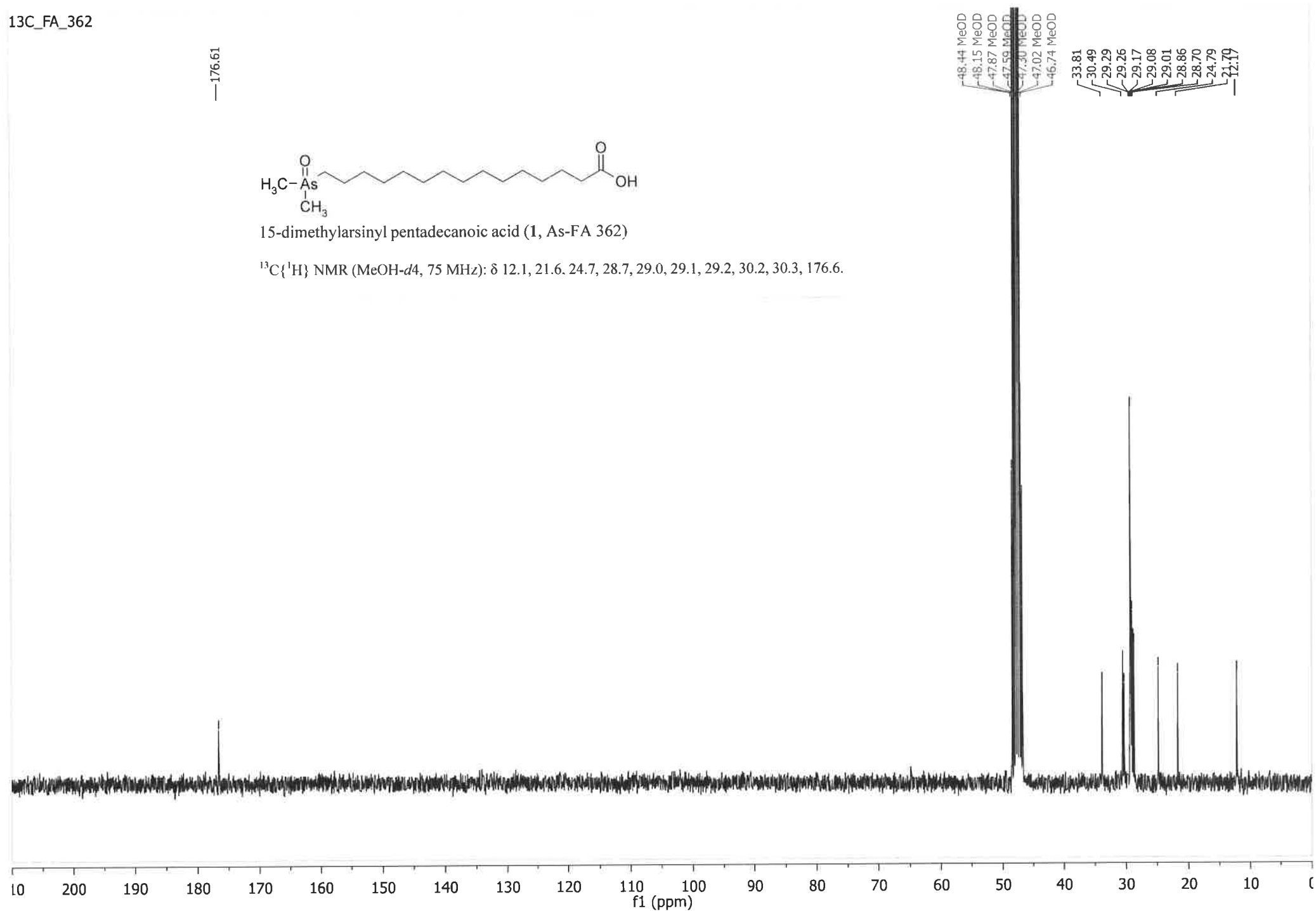
13C_FA_362

—176.61

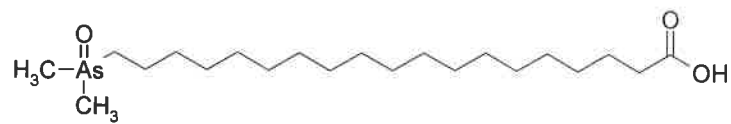


15-dimethylarsinyl pentadecanoic acid (1, As-FA 362)

$^{13}\text{C}\{^1\text{H}\}$ NMR (MeOH- d_4 , 75 MHz): δ 12.1, 21.6, 24.7, 28.7, 29.0, 29.1, 29.2, 30.2, 30.3, 176.6.

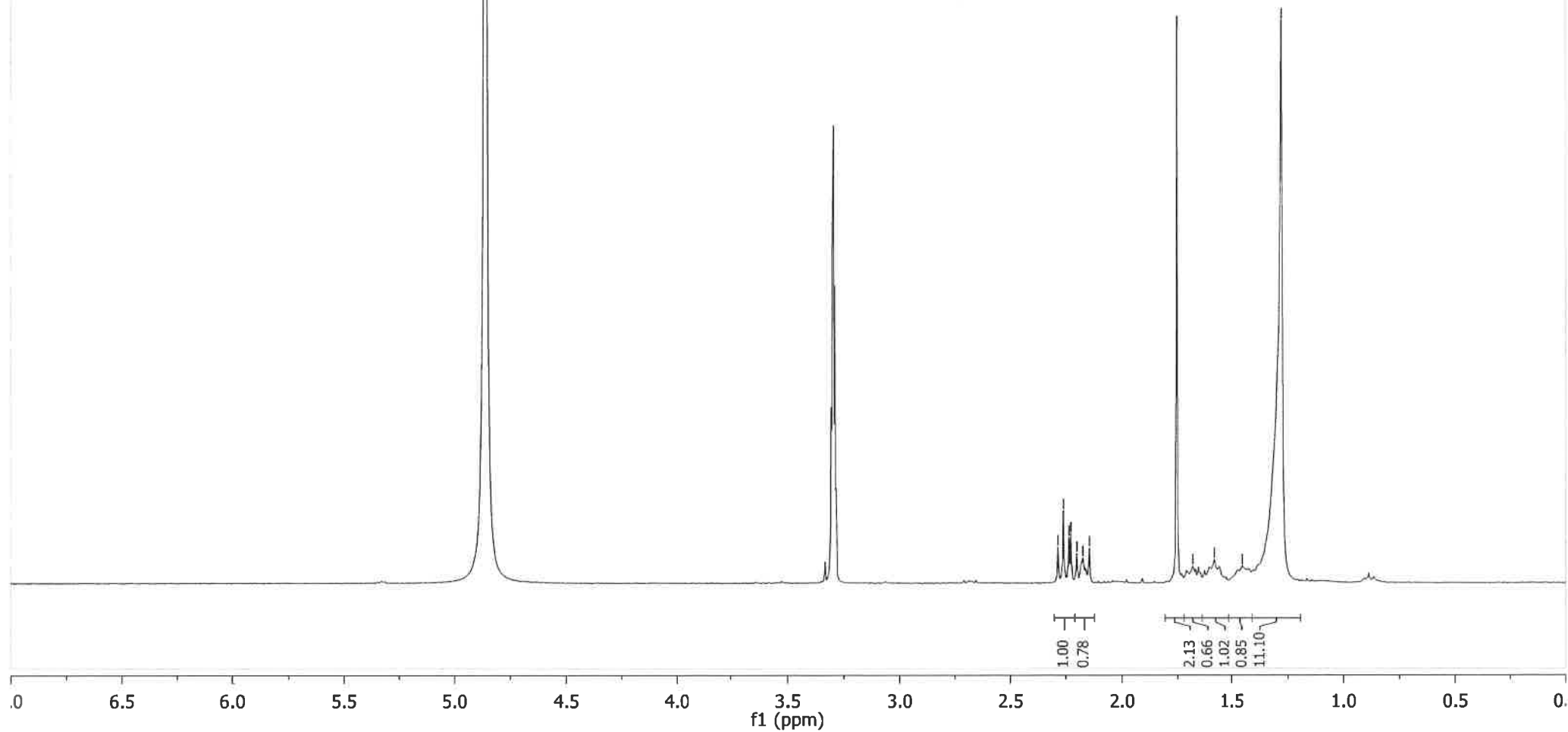


2.28
 2.26
 2.24
 2.23
 2.20
 2.18
 2.15
 1.75
 1.68
 1.58
 1.45
 1.28



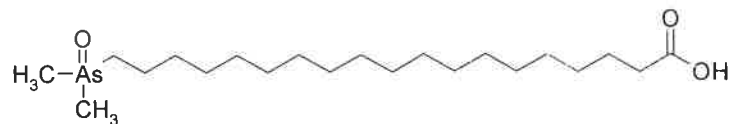
19-Dimethylarsinyl-nonadecanoic acid (2, As-FA 418)

^1H NMR (MeOH-*d*₄, 300 MHz): δ 1.3-1.5 (m, 28H, 14-CH₂), 1.6 (m, 2H, -CH₂),
 1.7 (m, 2H, -CH₂), 1.75 (s, 6H, -As(CH₃)₂), 2.20 (m, 2H, -As-CH₂),
 2.28 (t, $J = 7.5$ Hz, 2H, -CH₂-COOH).



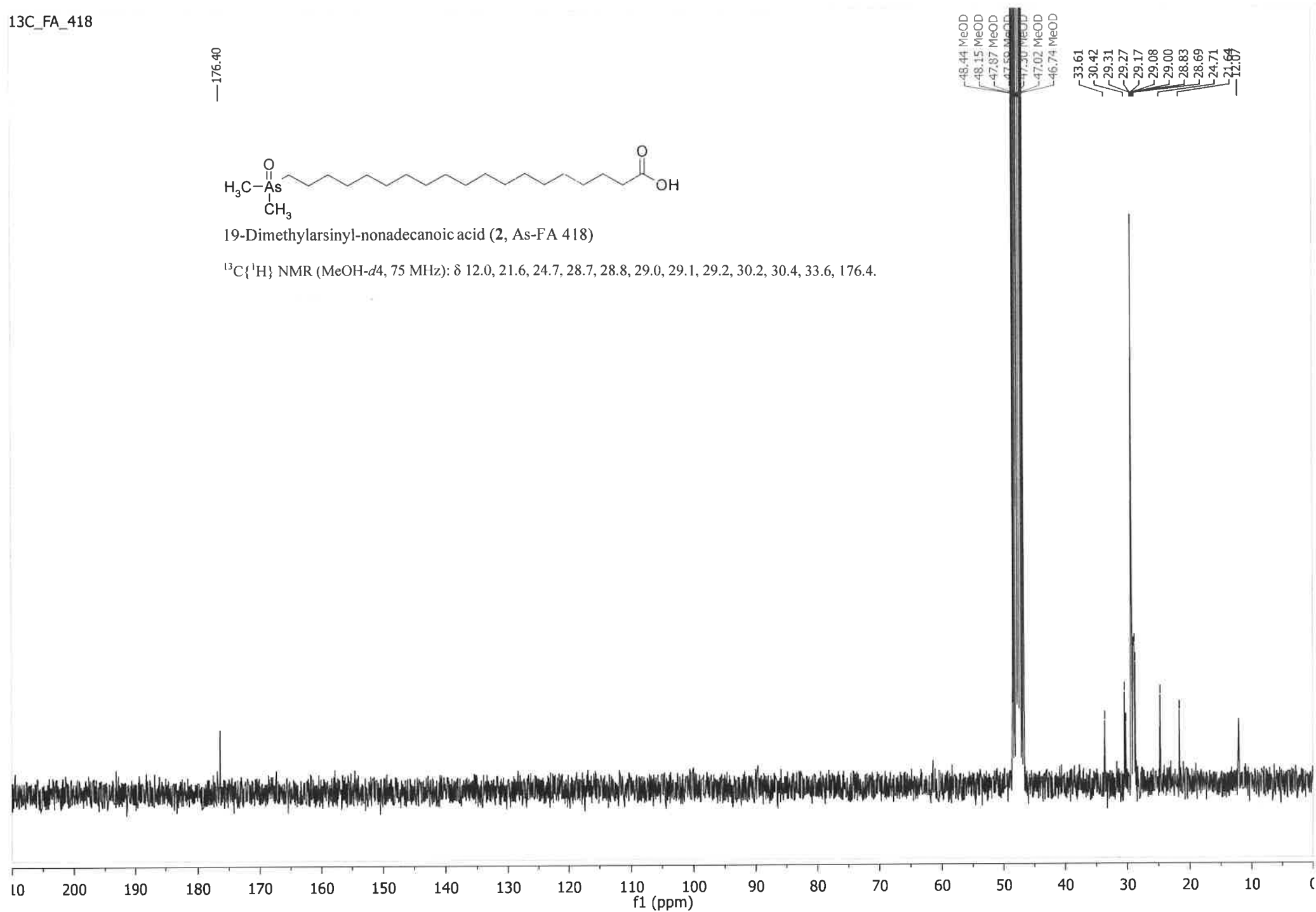
13C_FA_418

—176.40

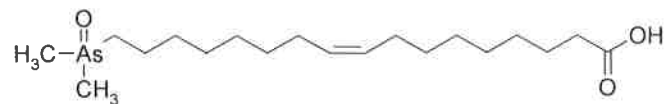


19-Dimethylarsinyl-nonadecanoic acid (**2**, As-FA 418)

$^{13}\text{C}\{^1\text{H}\}$ NMR (MeOH-*d*₄, 75 MHz): δ 12.0, 21.6, 24.7, 28.7, 28.8, 29.0, 29.1, 29.2, 30.2, 30.4, 33.6, 176.4.

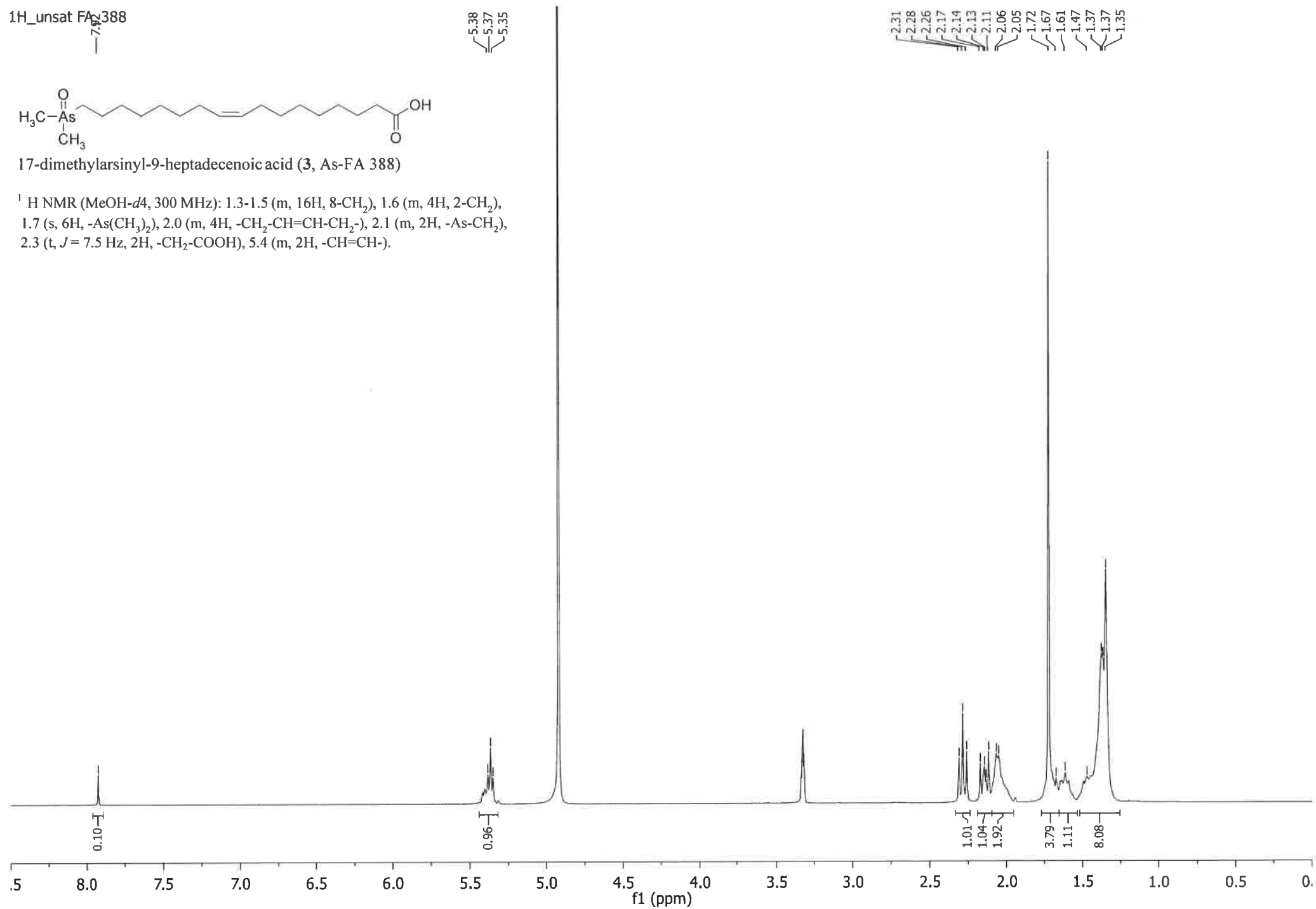


1H_unsat FA 388



17-dimethylarsinyl-9-heptadecenoic acid (**3**, As-FA 388)

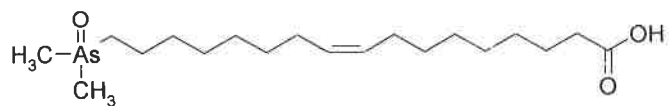
$^1\text{H NMR}$ (MeOH- d_4 , 300 MHz): 1.3-1.5 (m, 16H, 8-CH₂), 1.6 (m, 4H, 2-CH₂), 1.7 (s, 6H, -As(CH₃)₂), 2.0 (m, 4H, -CH₂-CH=CH-CH₂-), 2.1 (m, 2H, -As-CH₂), 2.3 (t, $J = 7.5$ Hz, 2H, -CH₂-COOH), 5.4 (m, 2H, -CH=CH-).



13C_unsat FA_388

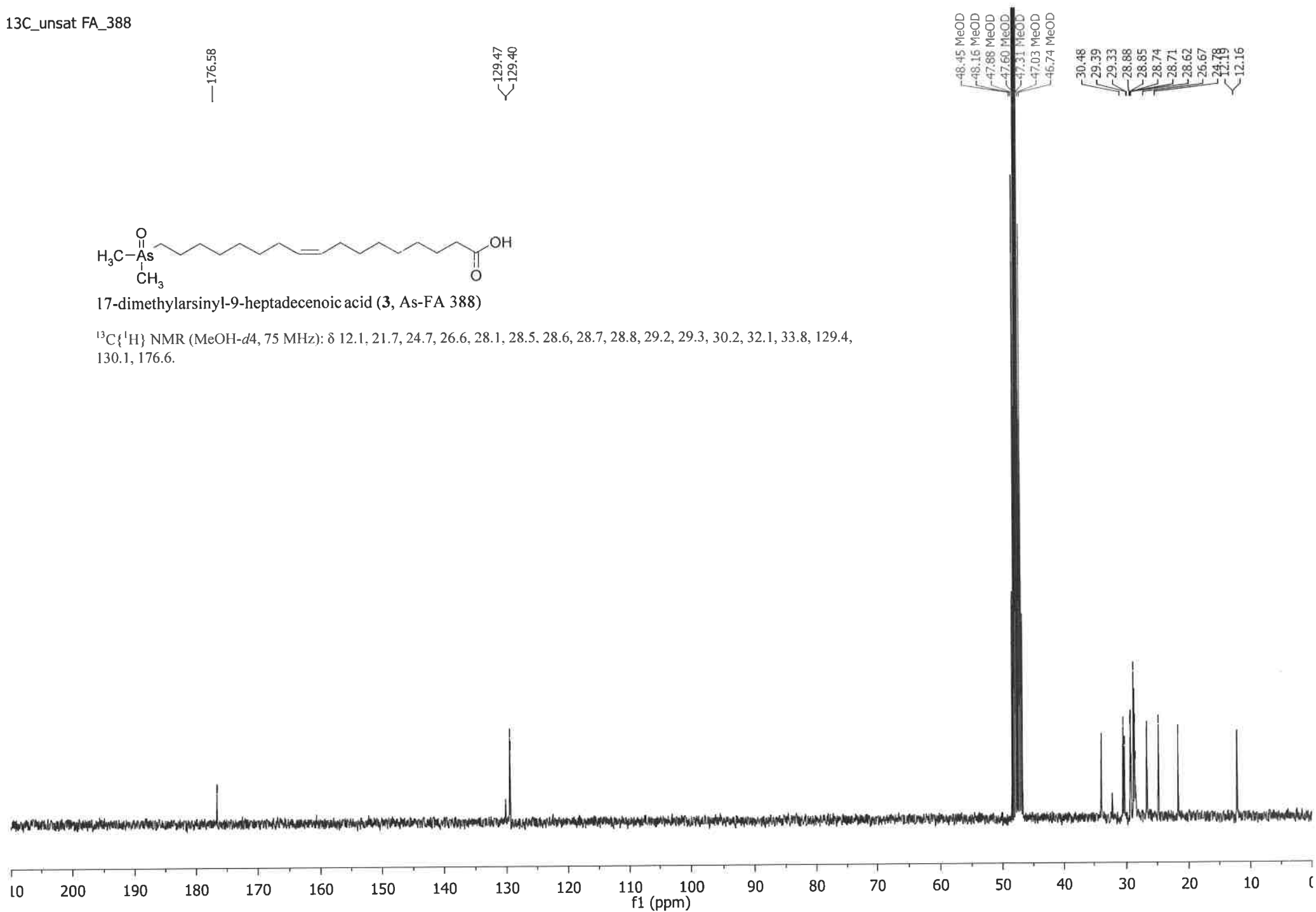
176.58

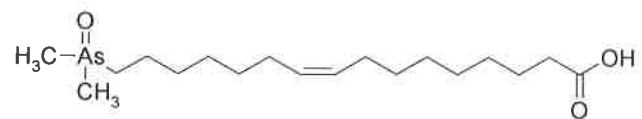
129.47
129.40



17-dimethylarsinyl-9-heptadecenoic acid (**3**, As-FA 388)

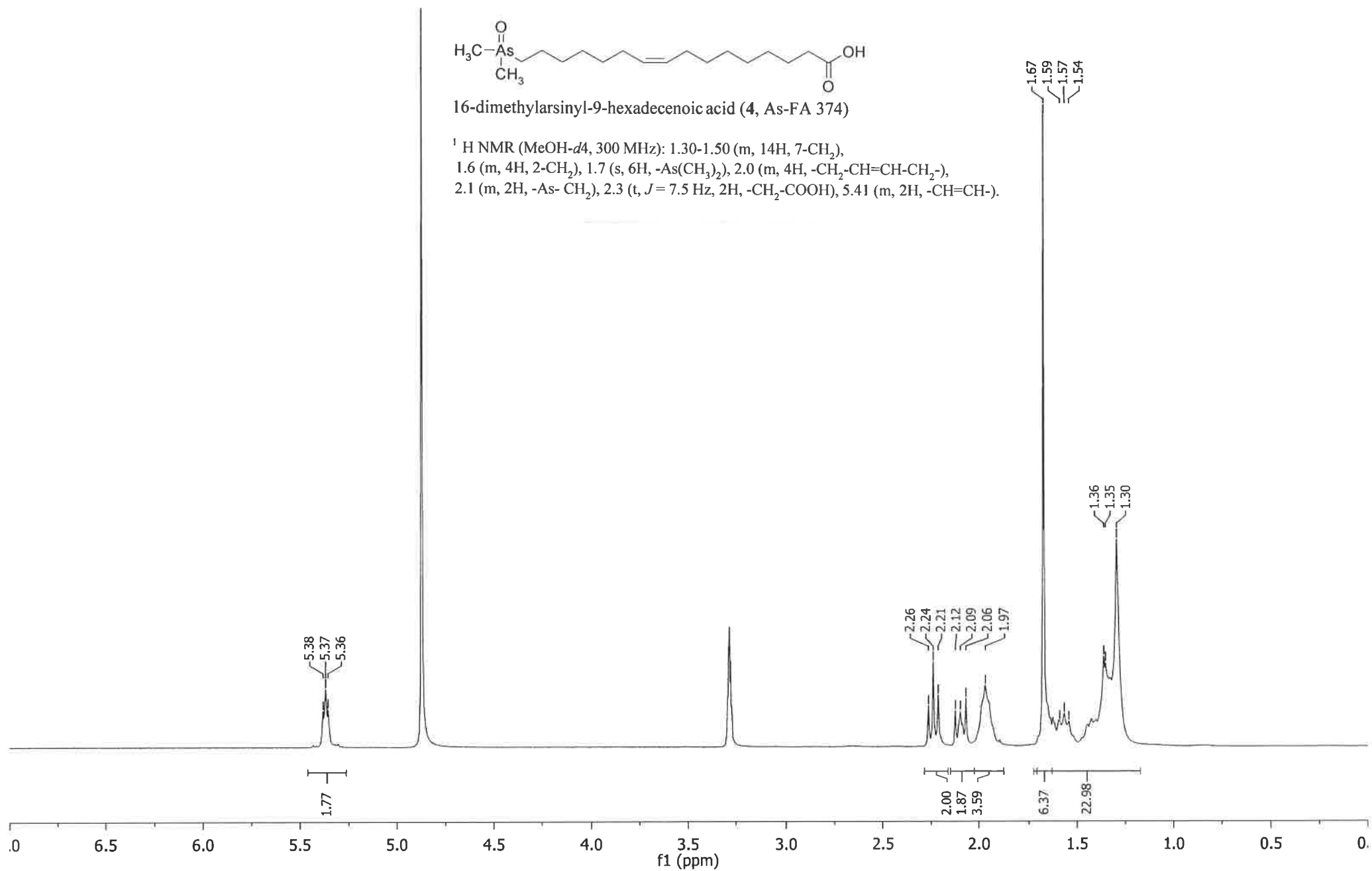
$^{13}\text{C}\{^1\text{H}\}$ NMR (MeOH-*d*₄, 75 MHz): δ 12.1, 21.7, 24.7, 26.6, 28.1, 28.5, 28.6, 28.7, 28.8, 29.2, 29.3, 30.2, 32.1, 33.8, 129.4, 130.1, 176.6.



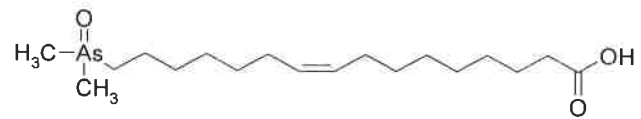


16-dimethylarsinyl-9-hexadecenoic acid (4, As-FA 374)

^1H NMR (MeOH- d_4 , 300 MHz): 1.30-1.50 (m, 14H, 7- CH_2),
 1.6 (m, 4H, 2- CH_2), 1.7 (s, 6H, -As(CH_3) $_2$), 2.0 (m, 4H, - CH_2 -CH=CH- CH_2 -),
 2.1 (m, 2H, -As- CH_2), 2.3 (t, $J = 7.5$ Hz, 2H, - CH_2 -COOH), 5.41 (m, 2H, -CH=CH-).

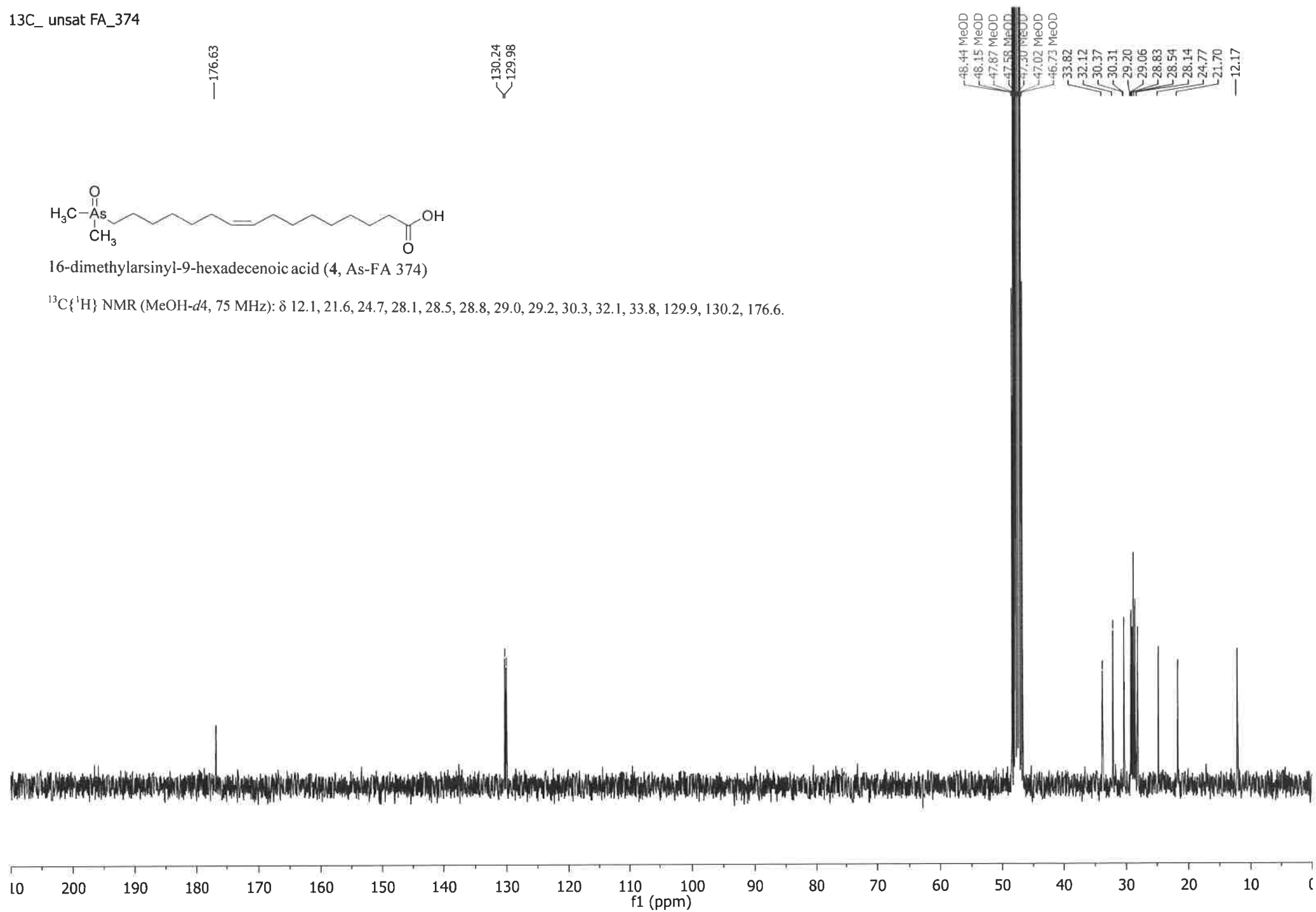


13C_ unsat FA_374

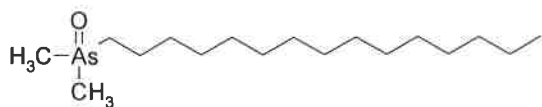


16-dimethylarsinyl-9-hexadecenoic acid (4, As-FA 374)

$^{13}\text{C}\{^1\text{H}\}$ NMR (MeOH-*d*4, 75 MHz): δ 12.1, 21.6, 24.7, 28.1, 28.5, 28.8, 29.0, 29.2, 30.3, 32.1, 33.8, 129.9, 130.2, 176.6.



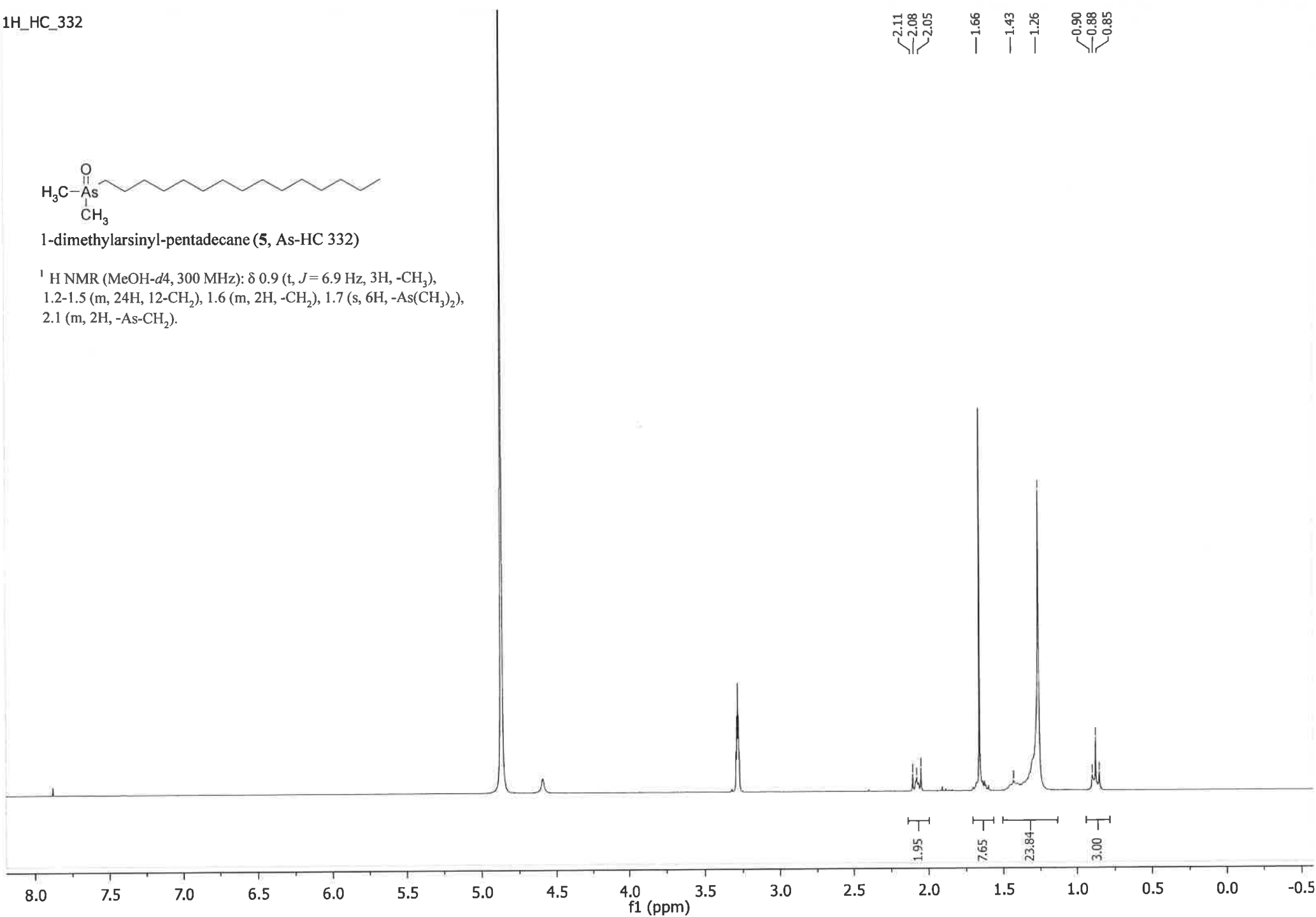
1H_HC_332



1-dimethylarsinyl-pentadecane (5, As-HC 332)

¹H NMR (MeOH-*d*₄, 300 MHz): δ 0.9 (t, *J* = 6.9 Hz, 3H, -CH₃),
1.2-1.5 (m, 24H, 12-CH₂), 1.6 (m, 2H, -CH₂), 1.7 (s, 6H, -As(CH₃)₂),
2.1 (m, 2H, -As-CH₂).

2.11
2.08
2.05
— 1.66
— 1.43
— 1.26
0.90
0.88
0.85



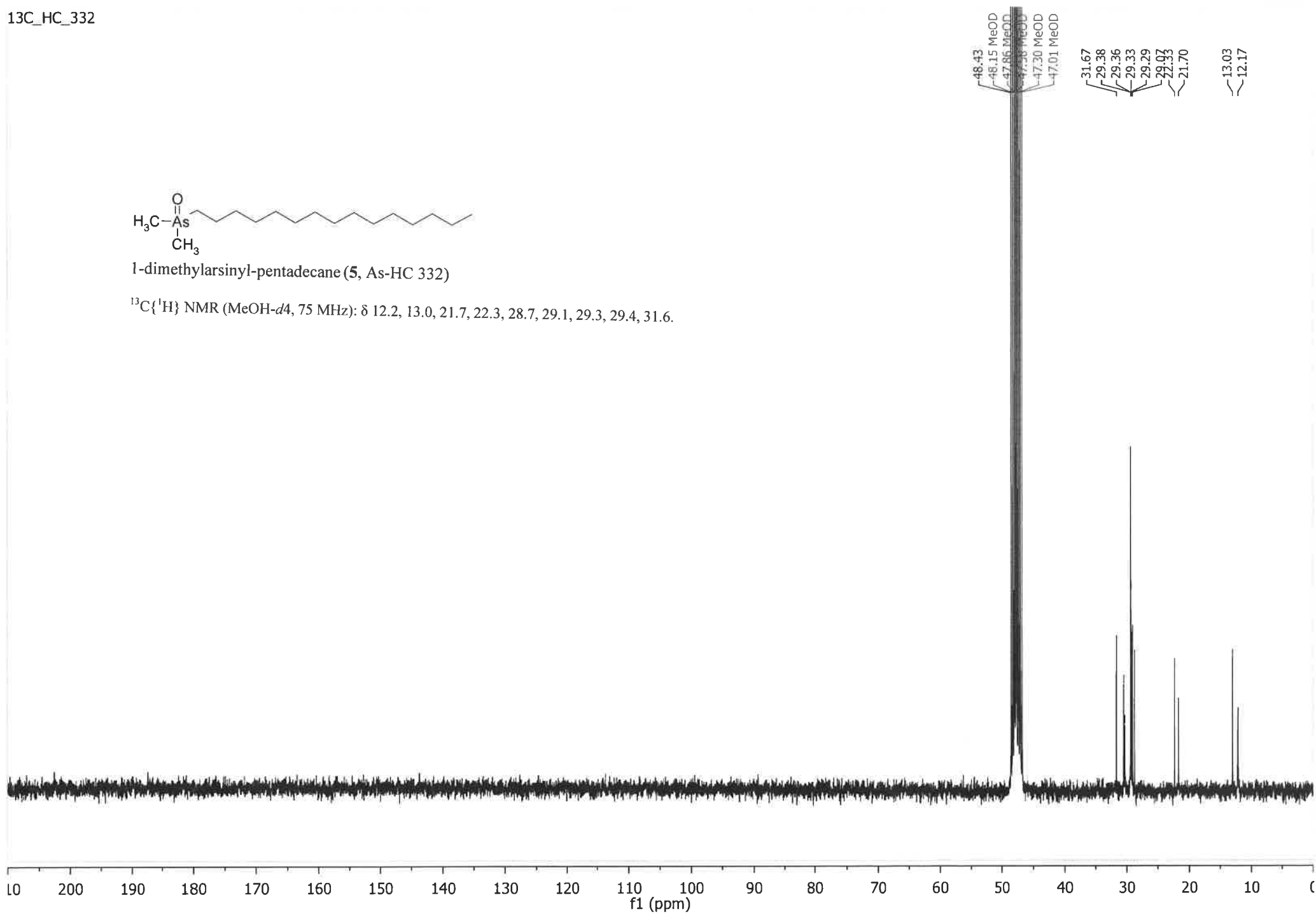
1.95
7.65
23.84
3.00

13C_HC_332

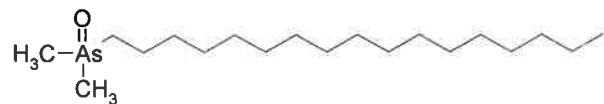


1-dimethylarsinyl-pentadecane (**5**, As-HC 332)

$^{13}\text{C}\{^1\text{H}\}$ NMR (MeOH-*d*₄, 75 MHz): δ 12.2, 13.0, 21.7, 22.3, 28.7, 29.1, 29.3, 29.4, 31.6.

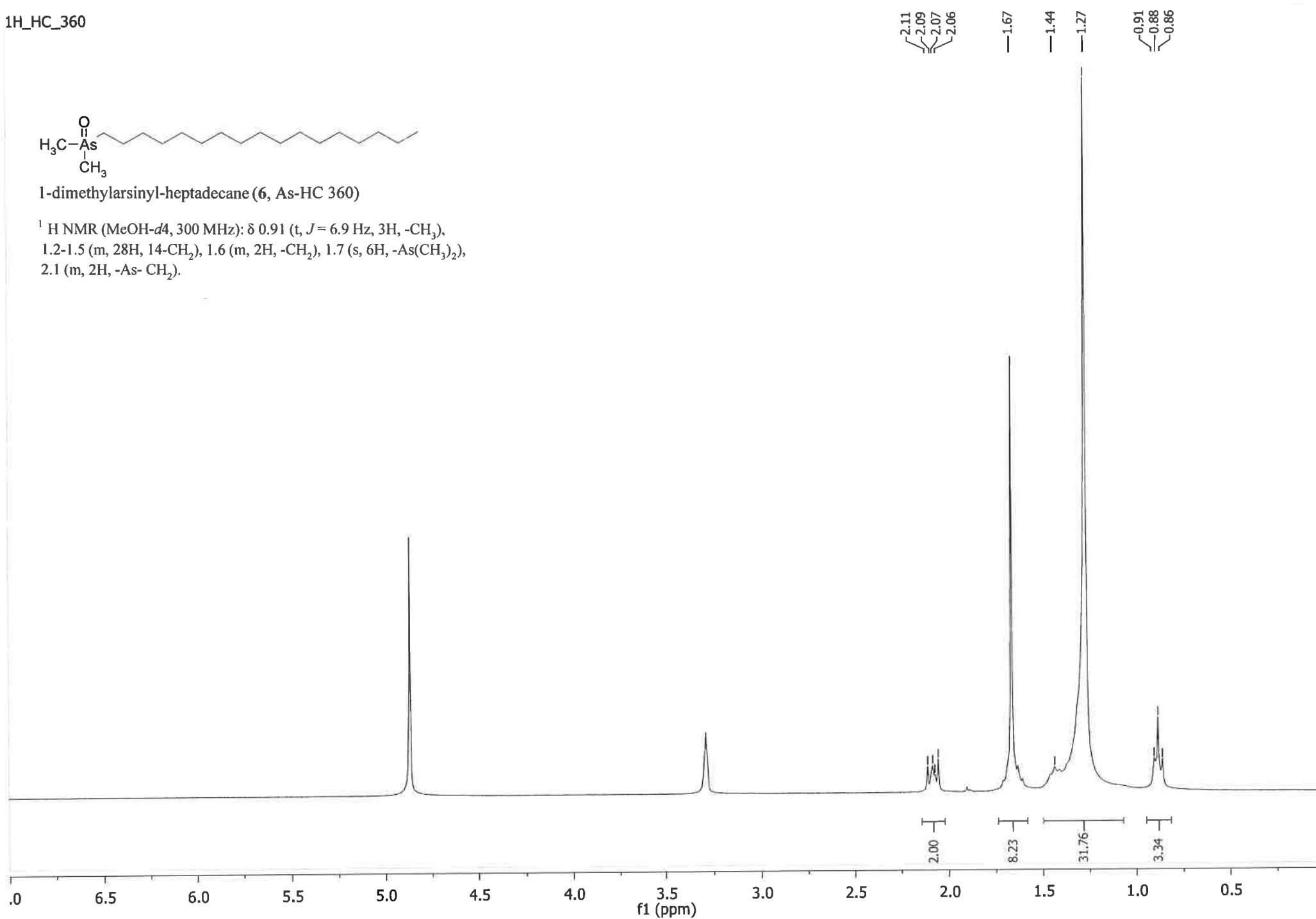


1H_HC_360

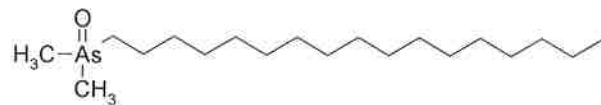


1-dimethylarsinyl-heptadecane (6, As-HC 360)

¹H NMR (MeOH-*d*₄, 300 MHz): δ 0.91 (t, *J* = 6.9 Hz, 3H, -CH₃),
1.2-1.5 (m, 28H, 14-CH₂), 1.6 (m, 2H, -CH₂), 1.7 (s, 6H, -As(CH₃)₂),
2.1 (m, 2H, -As-CH₂).

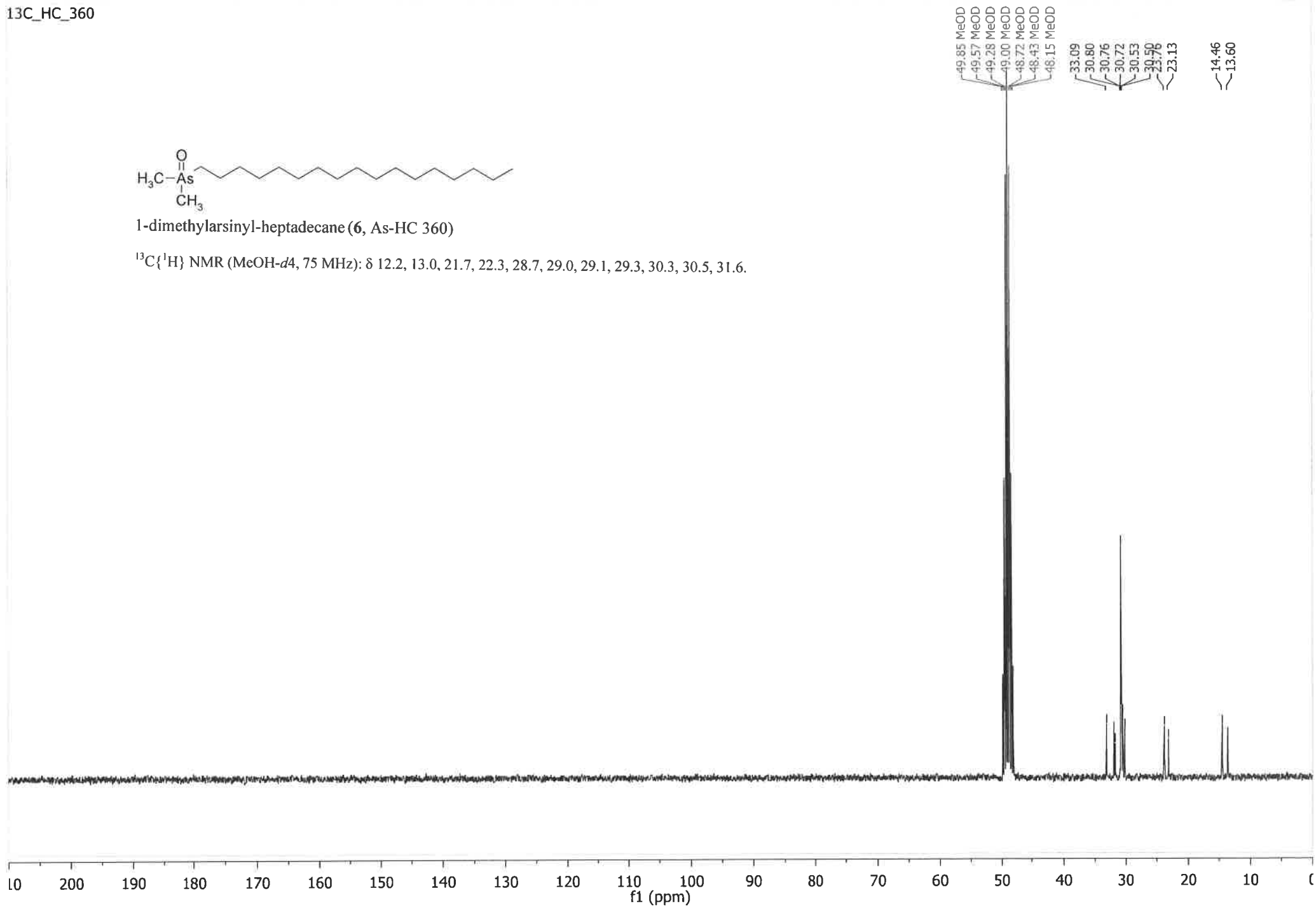


¹³C_HC_360

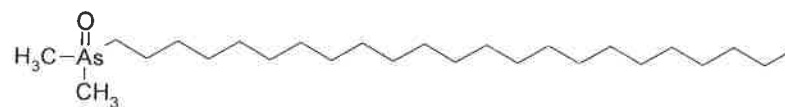


1-dimethylarsinyl-heptadecane (6, As-HC 360)

¹³C{¹H} NMR (MeOH-*d*₄, 75 MHz): δ 12.2, 13.0, 21.7, 22.3, 28.7, 29.0, 29.1, 29.3, 30.3, 30.5, 31.6.

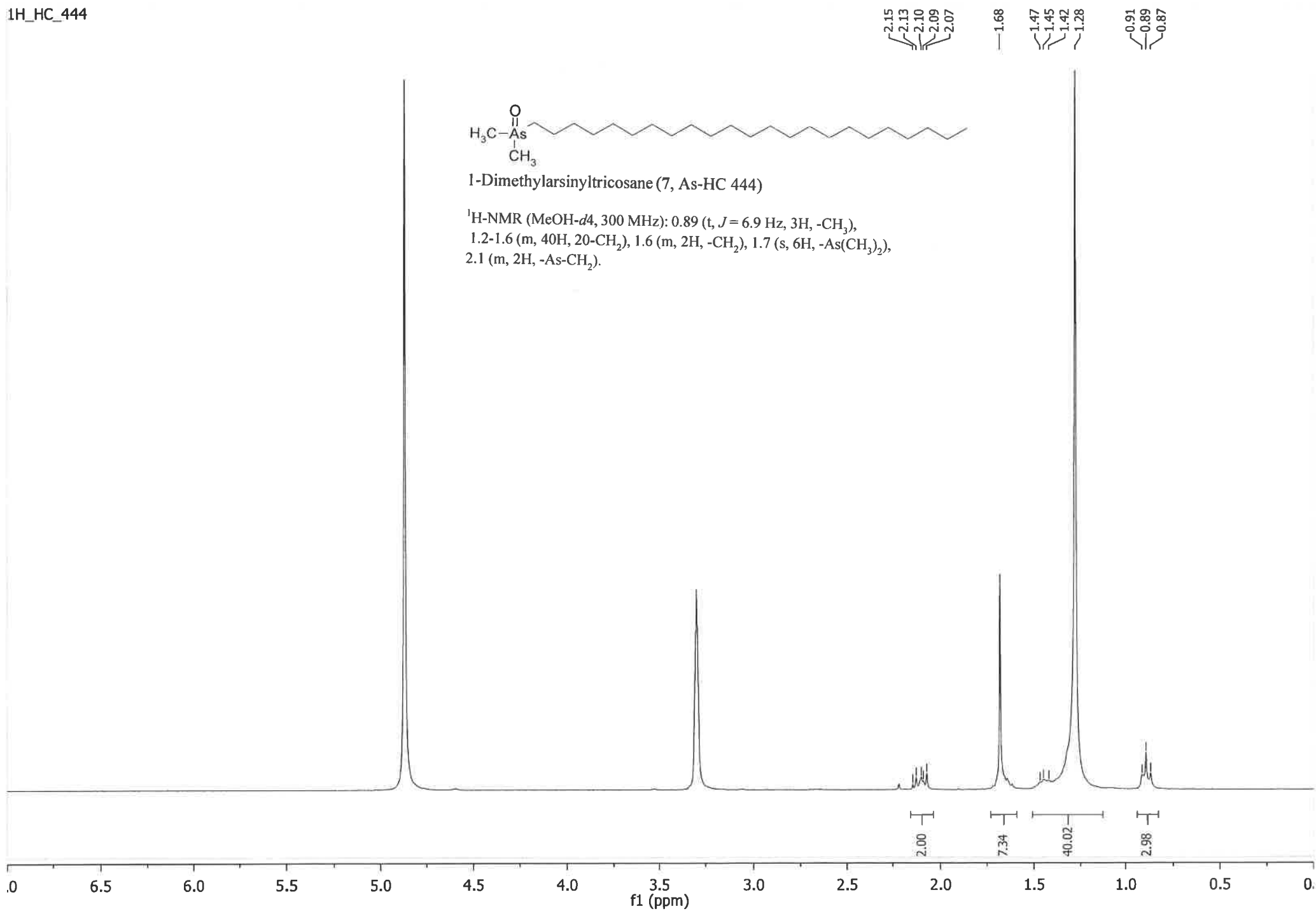


1H_HC_444



1-Dimethylarsinyltricosane (7, As-HC 444)

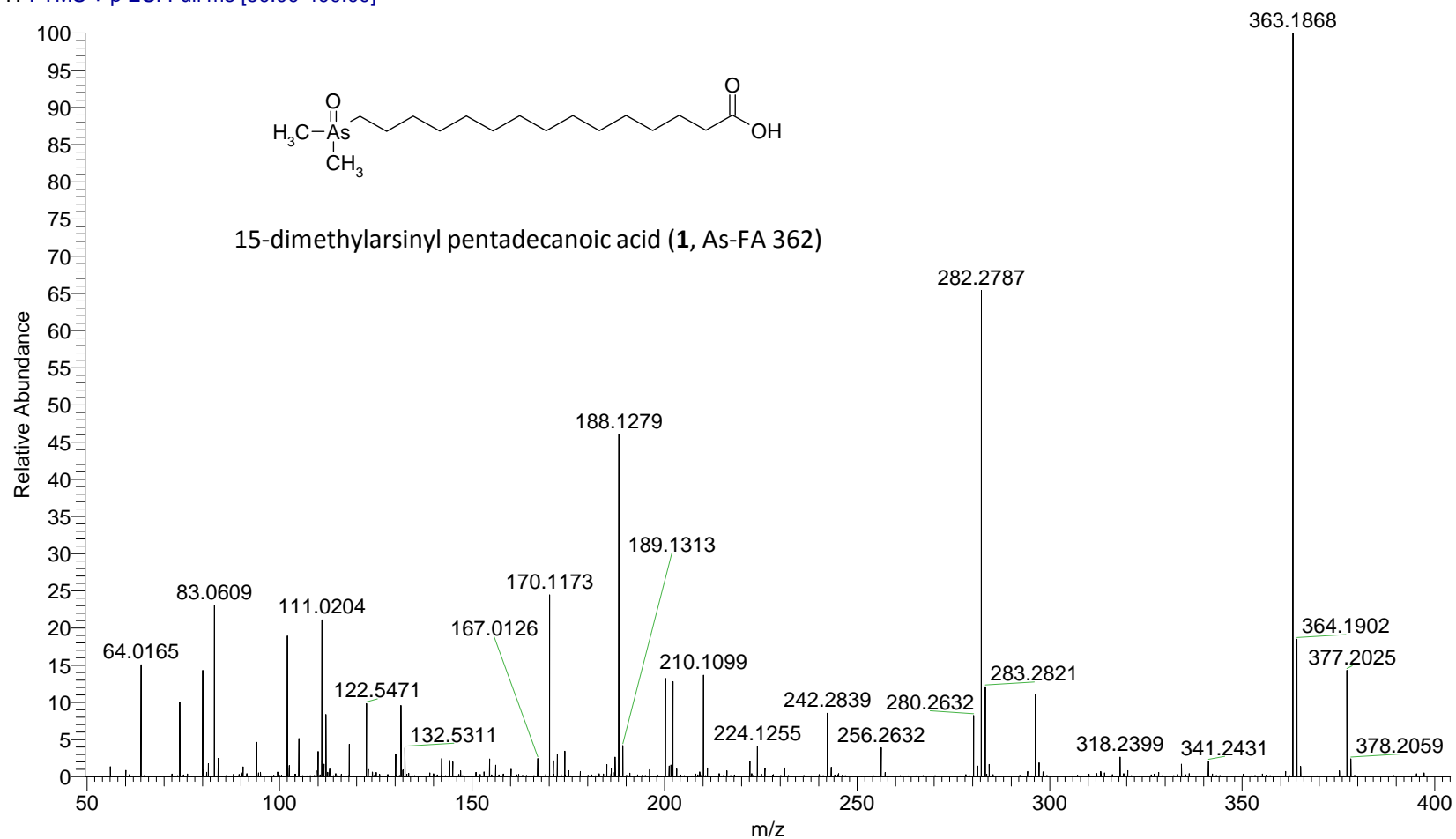
¹H-NMR (MeOH-*d*₄, 300 MHz): 0.89 (t, *J* = 6.9 Hz, 3H, -CH₃),
1.2-1.6 (m, 40H, 20-CH₂), 1.6 (m, 2H, -CH₂), 1.7 (s, 6H, -As(CH₃)₂),
2.1 (m, 2H, -As-CH₂).



FA 362 acetonitrile

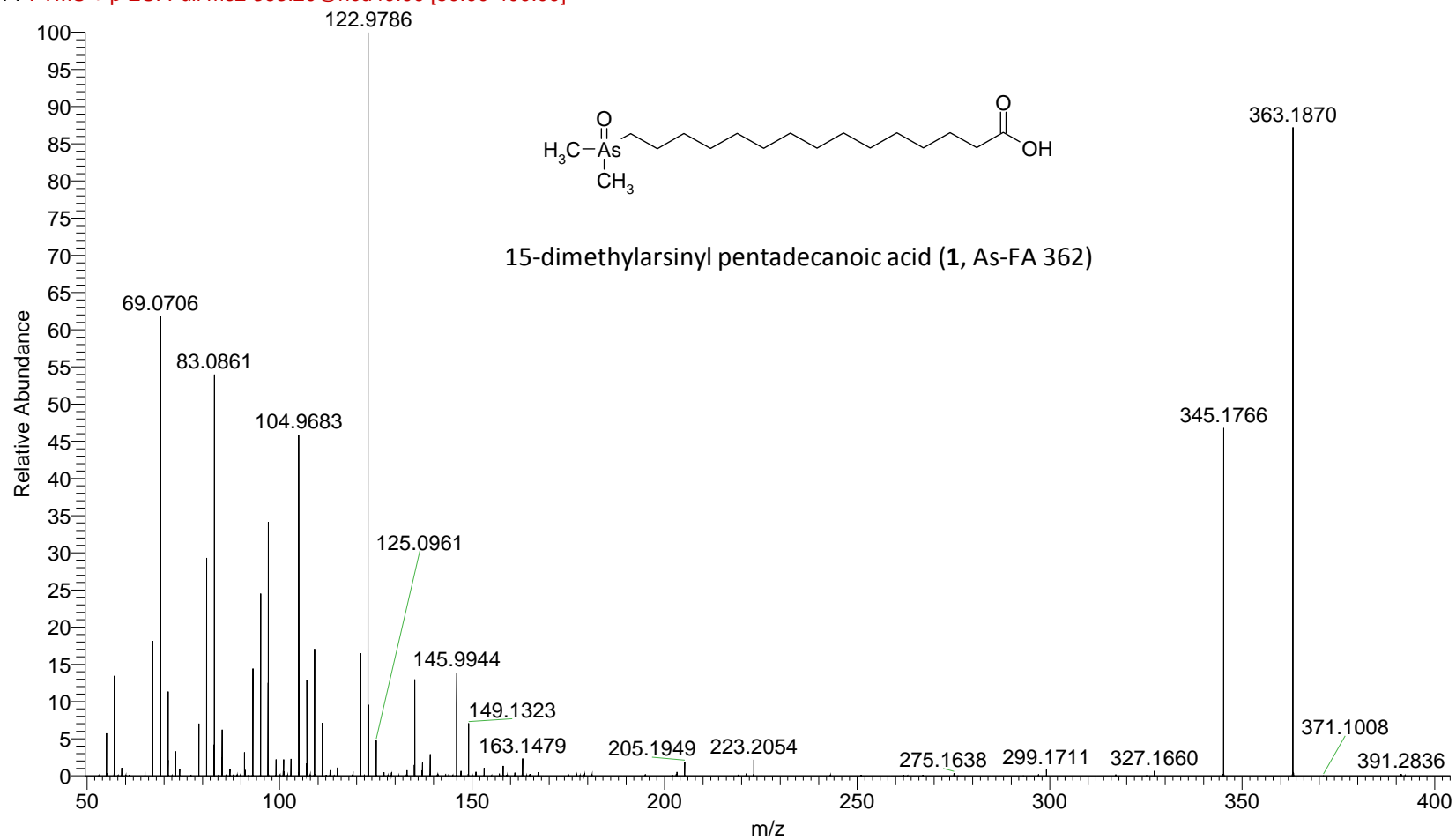
13032601 #1905-2084 RT: 29.43-31.13 AV: 180 NL: 3.08E8

T: FTMS + p ESI Full ms [50.00-400.00]



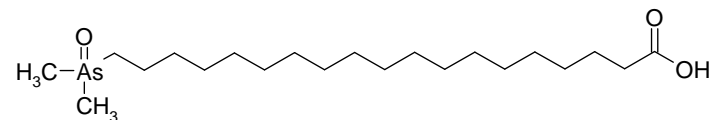
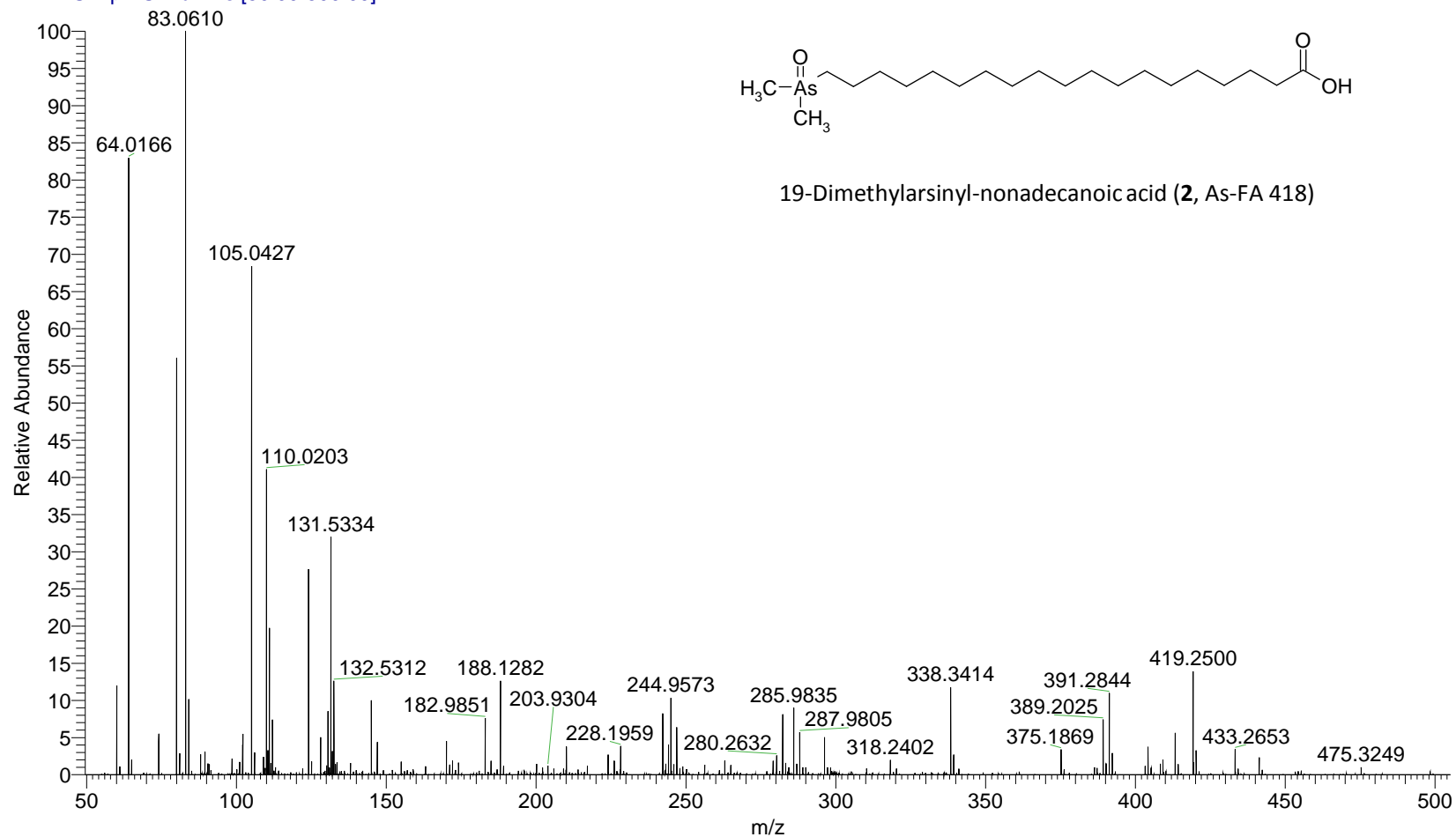
13032601 #1384-1476 RT: 20.73-22.09 AV: 55 NL: 1.03E6

F: FTMS + p ESI Full ms2 363.20@hcd40.00 [50.00-400.00]



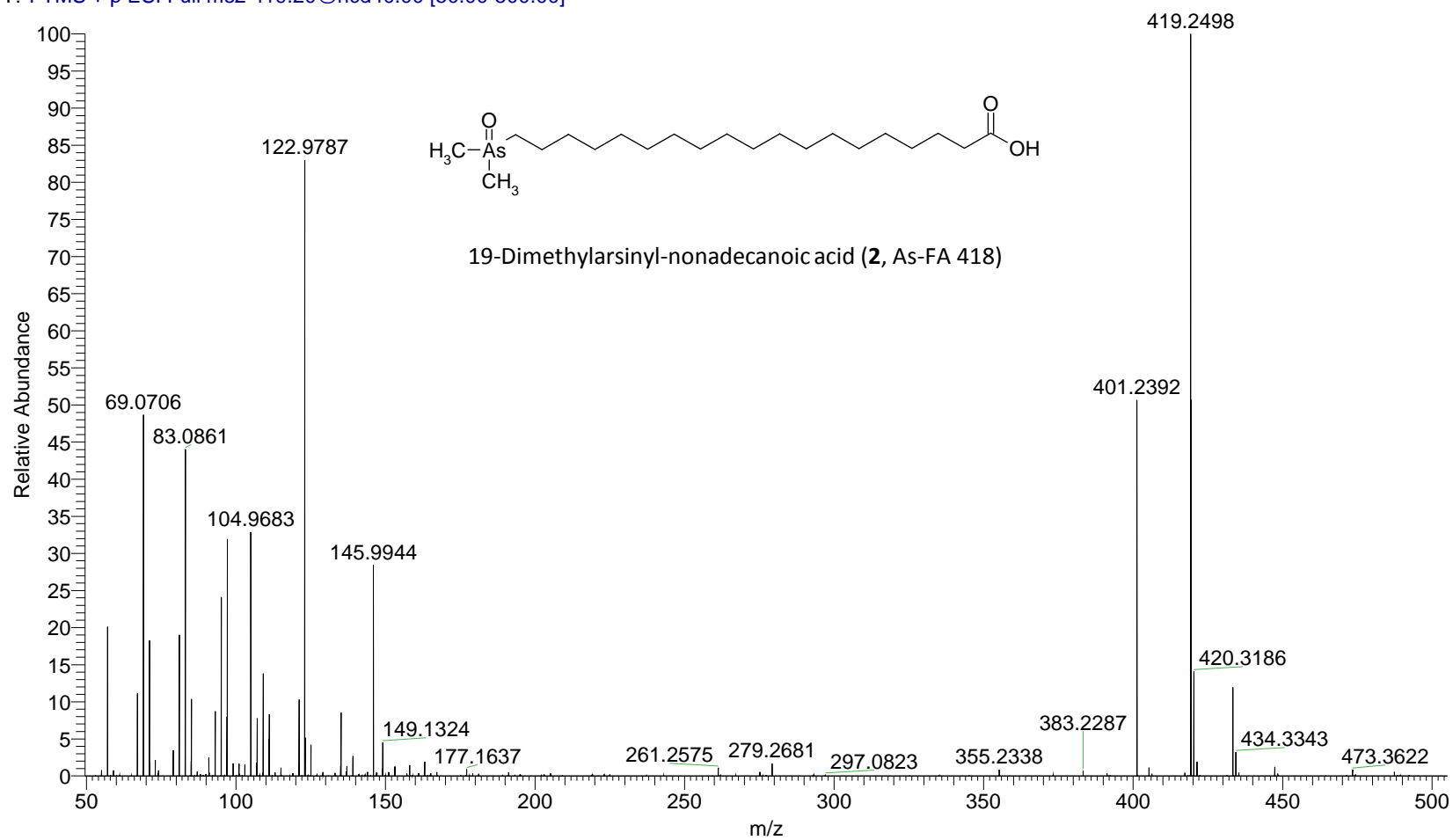
FA As 418 acetonitrile

13032606 #3598-3723 RT: 17.03-17.39 AV: 121 NL: 9.34E6
T: FTMS + p ESI Full ms [50.00-500.00]



19-Dimethylarsinyl-nonadecanoic acid (**2**, As-FA 418)

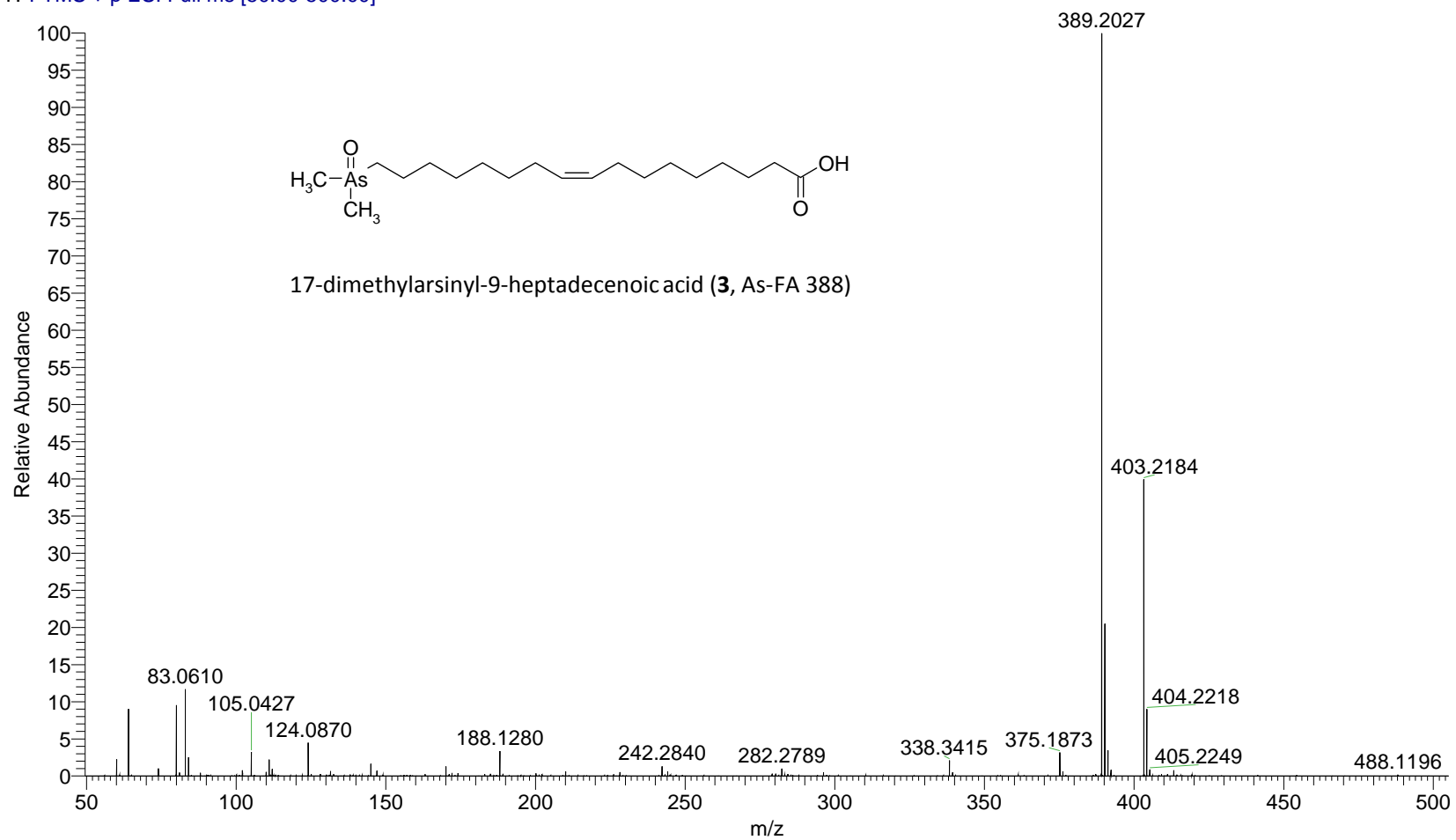
13032606 #3787-3823 RT: 18.50-19.21 AV: 37 NL: 1.89E5
T: FTMS + p ESI Full ms2 419.20@hcd40.00 [50.00-500.00]



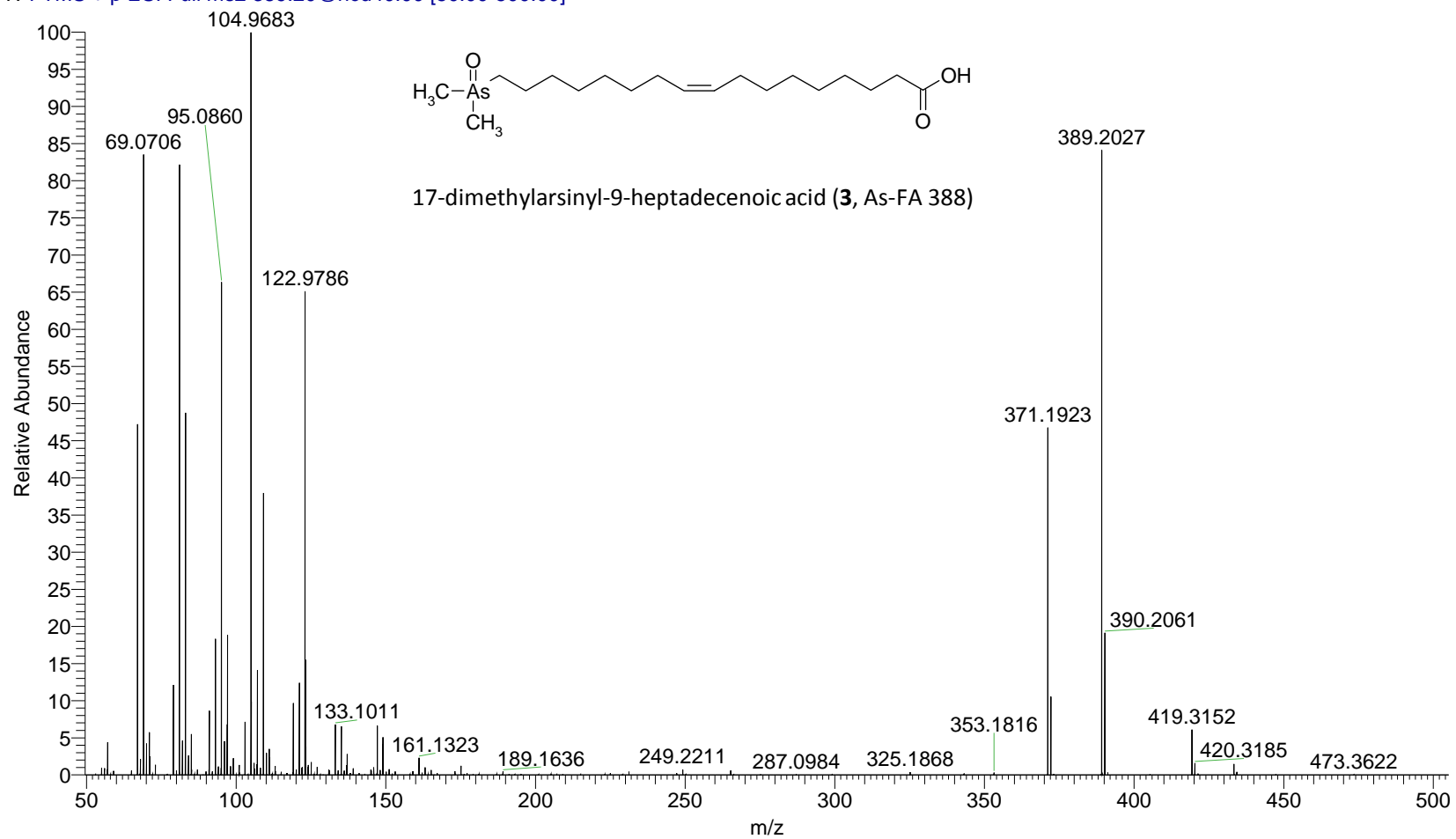
FA 388 acetonitrile

13032605 #1807-1819 RT: 17.94-18.06 AV: 13 NL: 2.50E7

T: FTMS + p ESI Full ms [50.00-500.00]



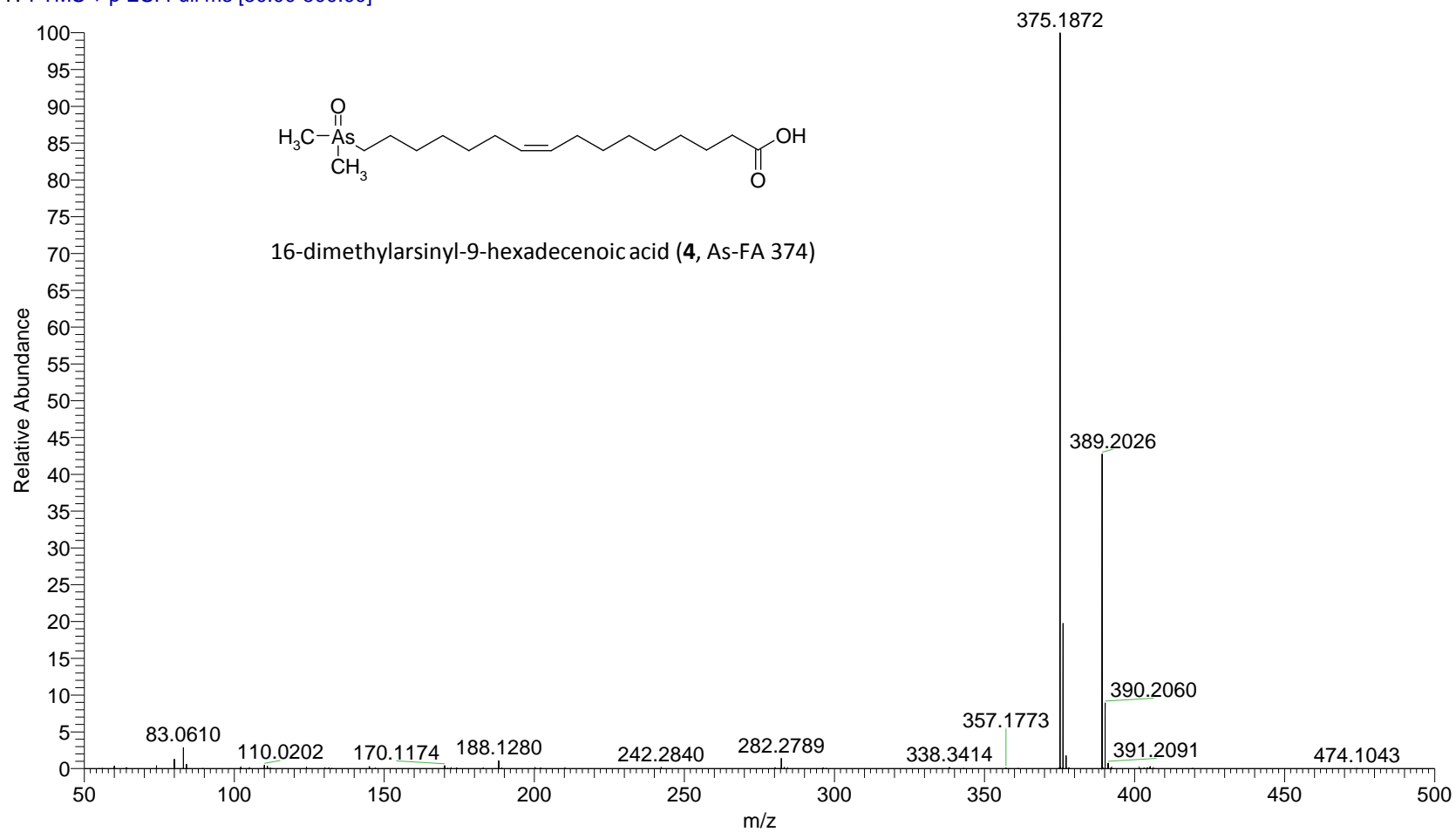
13032605 #1484-1522 RT: 14.95-15.29 AV: 39 NL: 3.27E6
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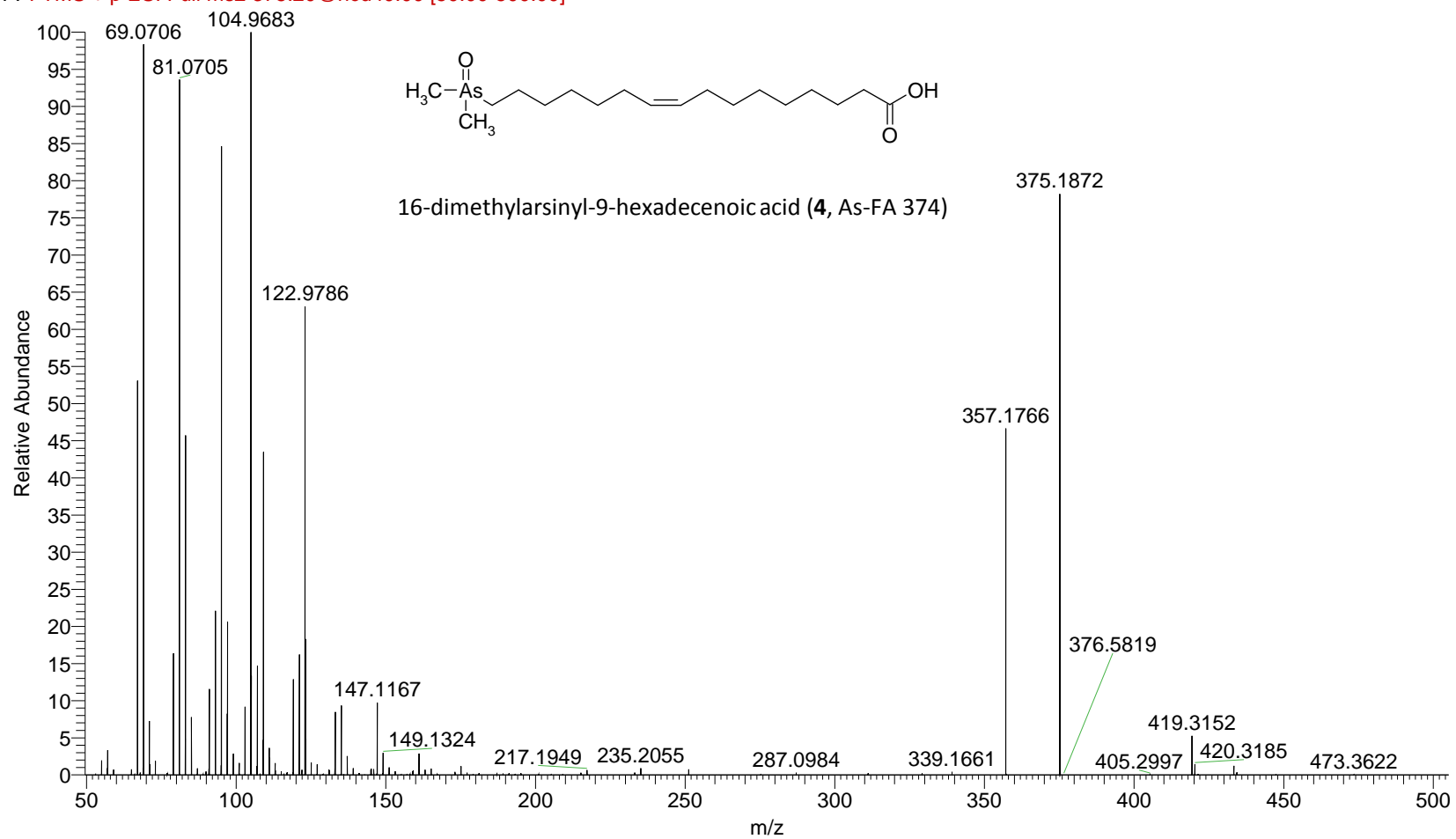
FA 374

13032604 #200 RT: 1.89 AV: 1 NL: 5.89E8

T: FTMS + p ESI Full ms [50.00-500.00]



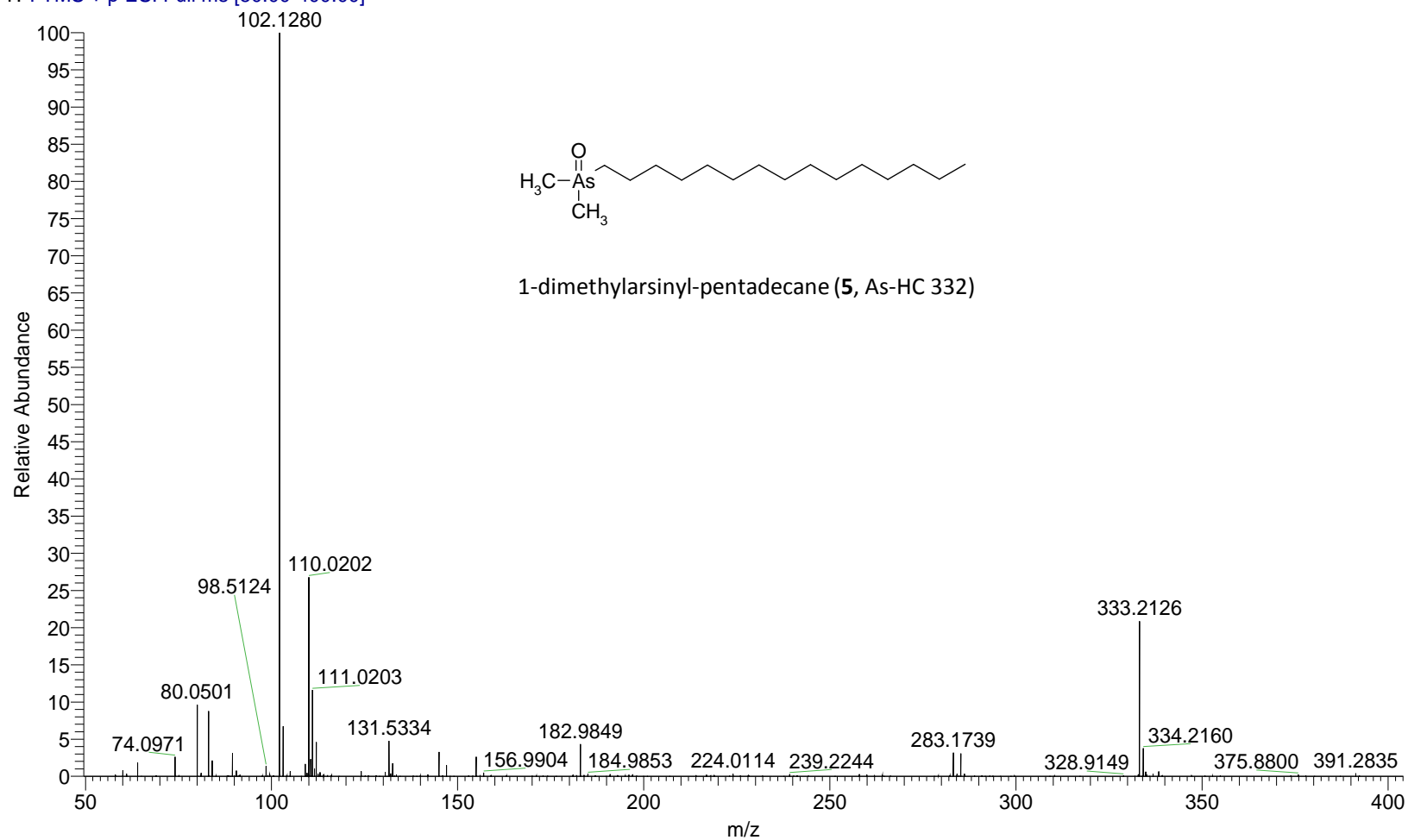
13032604 #827-880 RT: 7.81-8.29 AV: 54 NL: 2.37E7
F: FTMS + p ESI Full ms2 375.20@hcd40.00 [50.00-500.00]



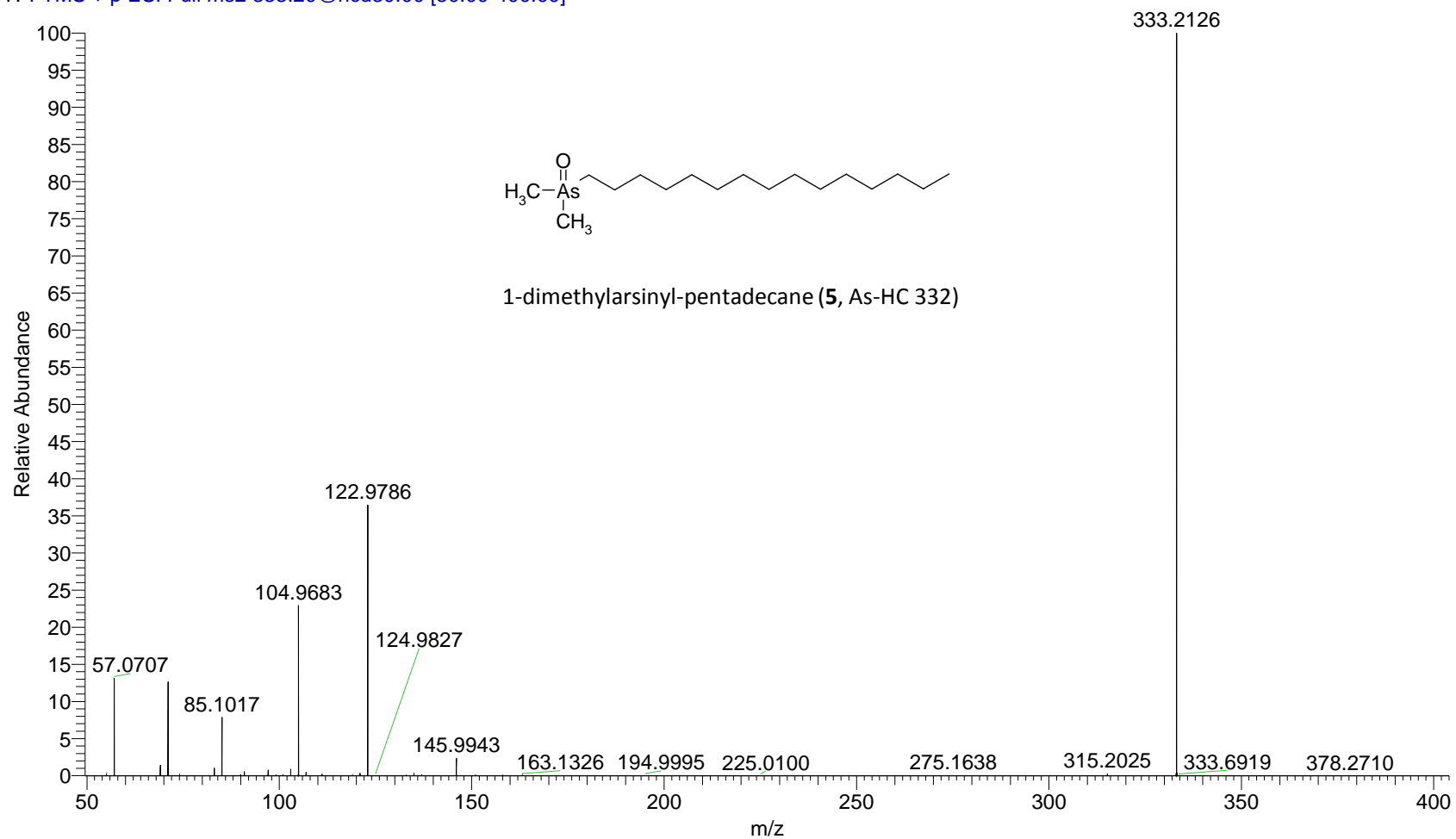
HA 332 acetonitrile

13032501 #667-671 RT: 8.44-8.48 AV: 5 NL: 5.71E8

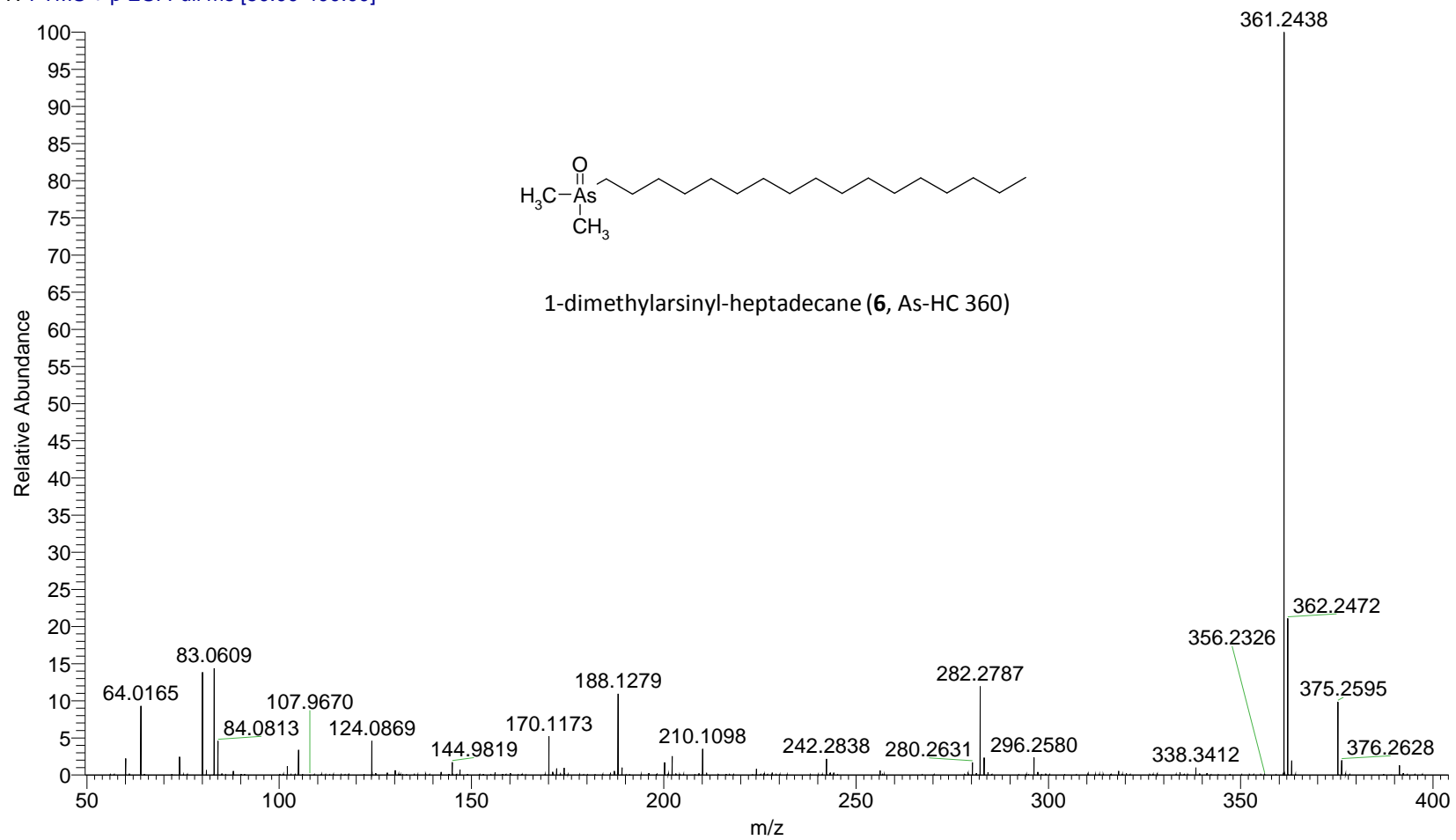
T: FTMS + p ESI Full ms [50.00-400.00]



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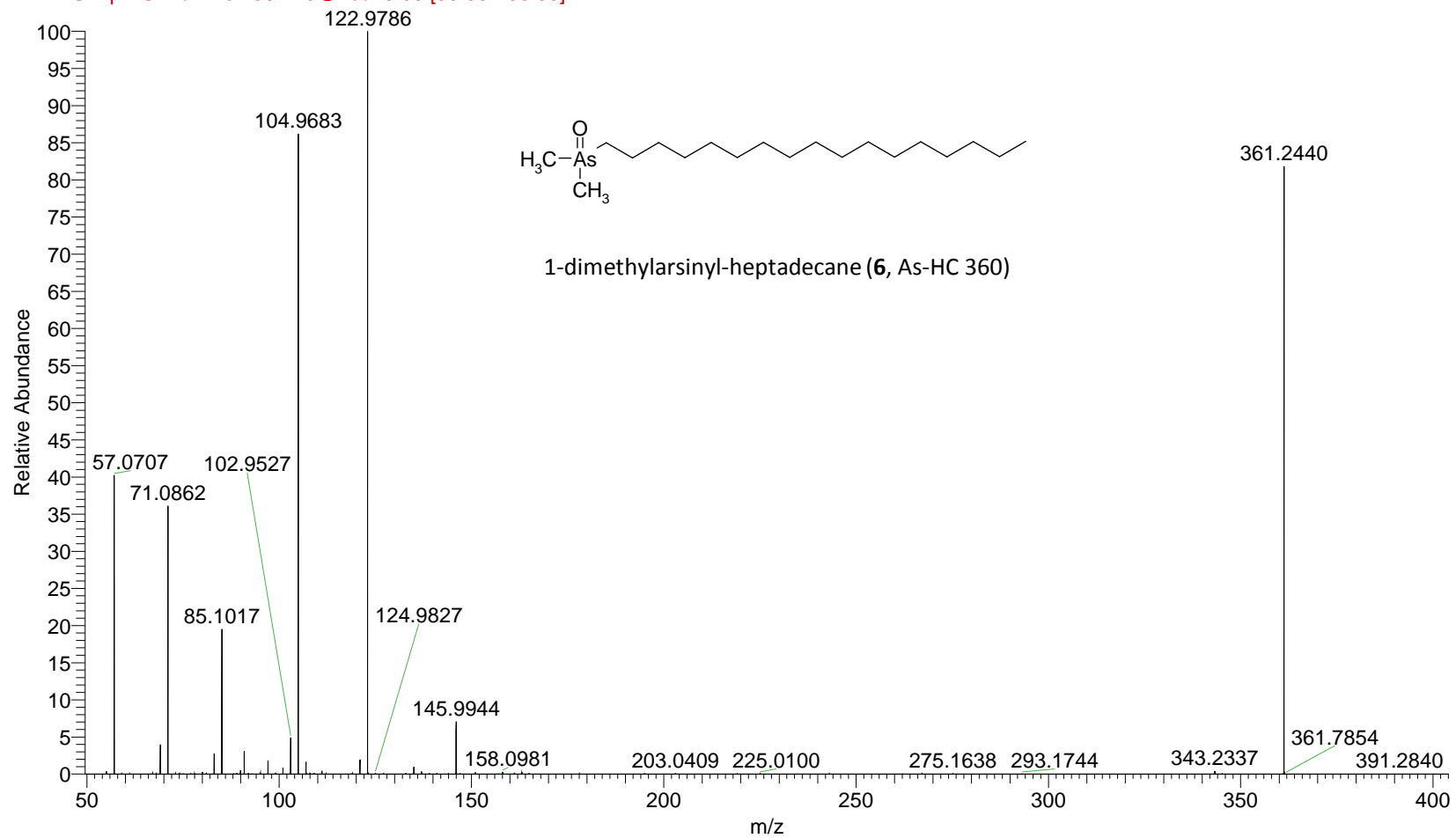
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HA 360 acetonitrile

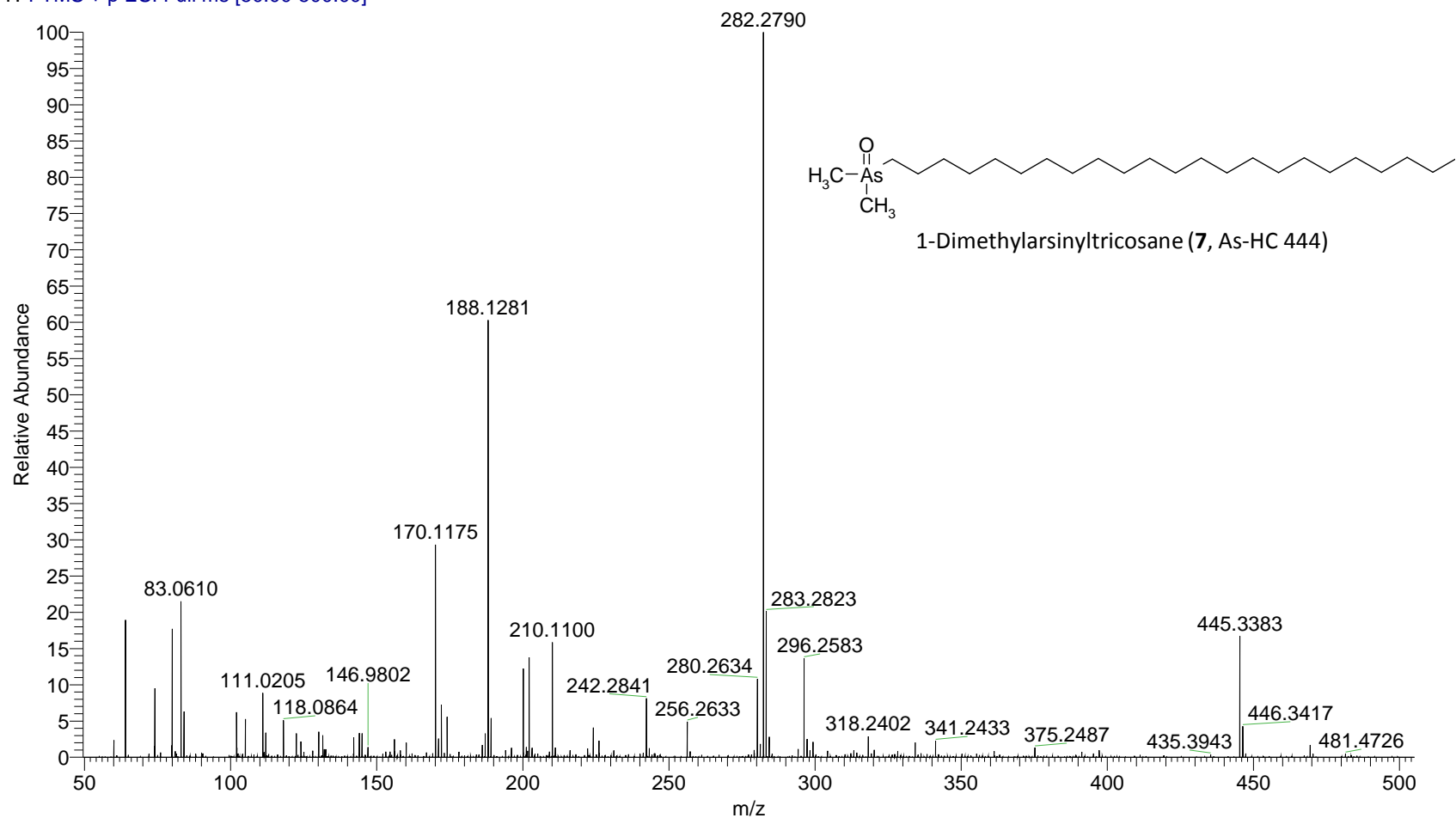
13032602 #274-329 RT: 2.87-3.48 AV: 41 NL: 5.10E6

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HA 444 acetonitrile

13032603 #645-766 RT: 7.20-8.35 AV: 122 NL: 2.43E8
T: FTMS + p ESI Full ms [50.00-500.00]



13032603 #112-658 RT: 2.30-4.88 AV: 95 NL: 4.07E6
F: FTMS + p ESI Full ms2 445.30@hcd40.00 [50.00-500.00]

