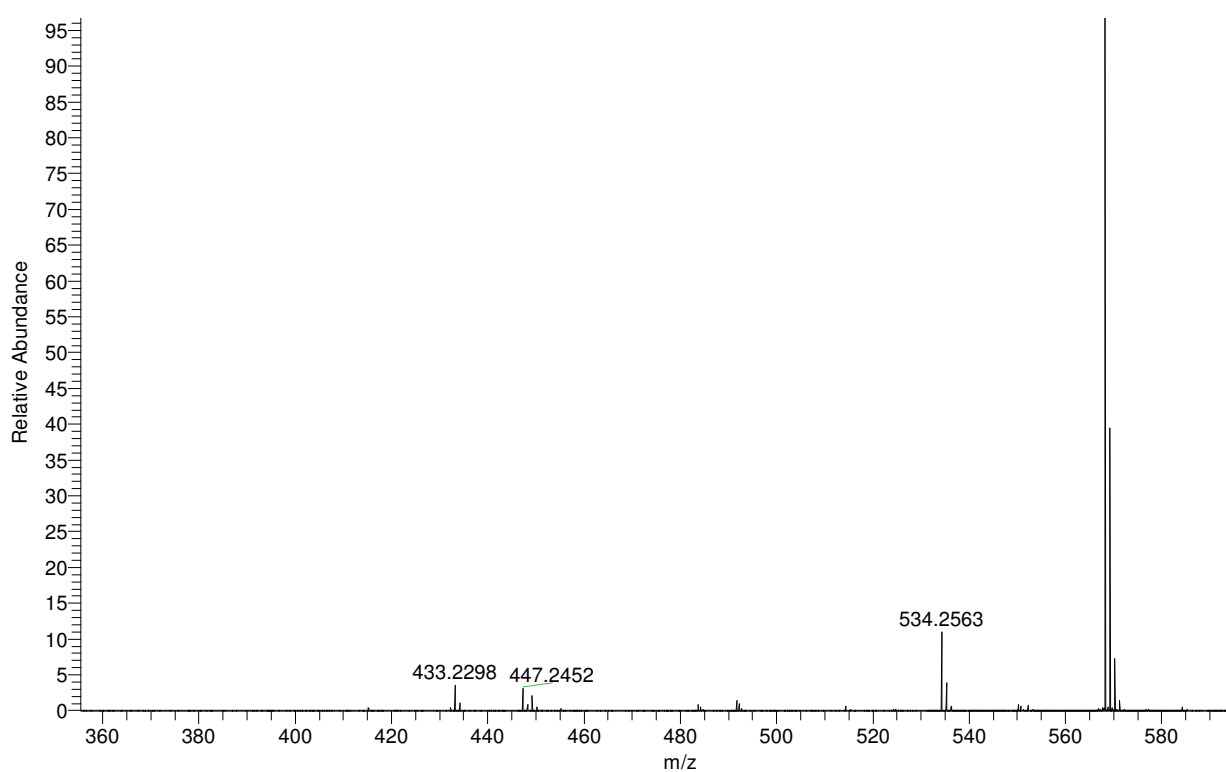


General experimental and instrumentation details and spectra for AP123

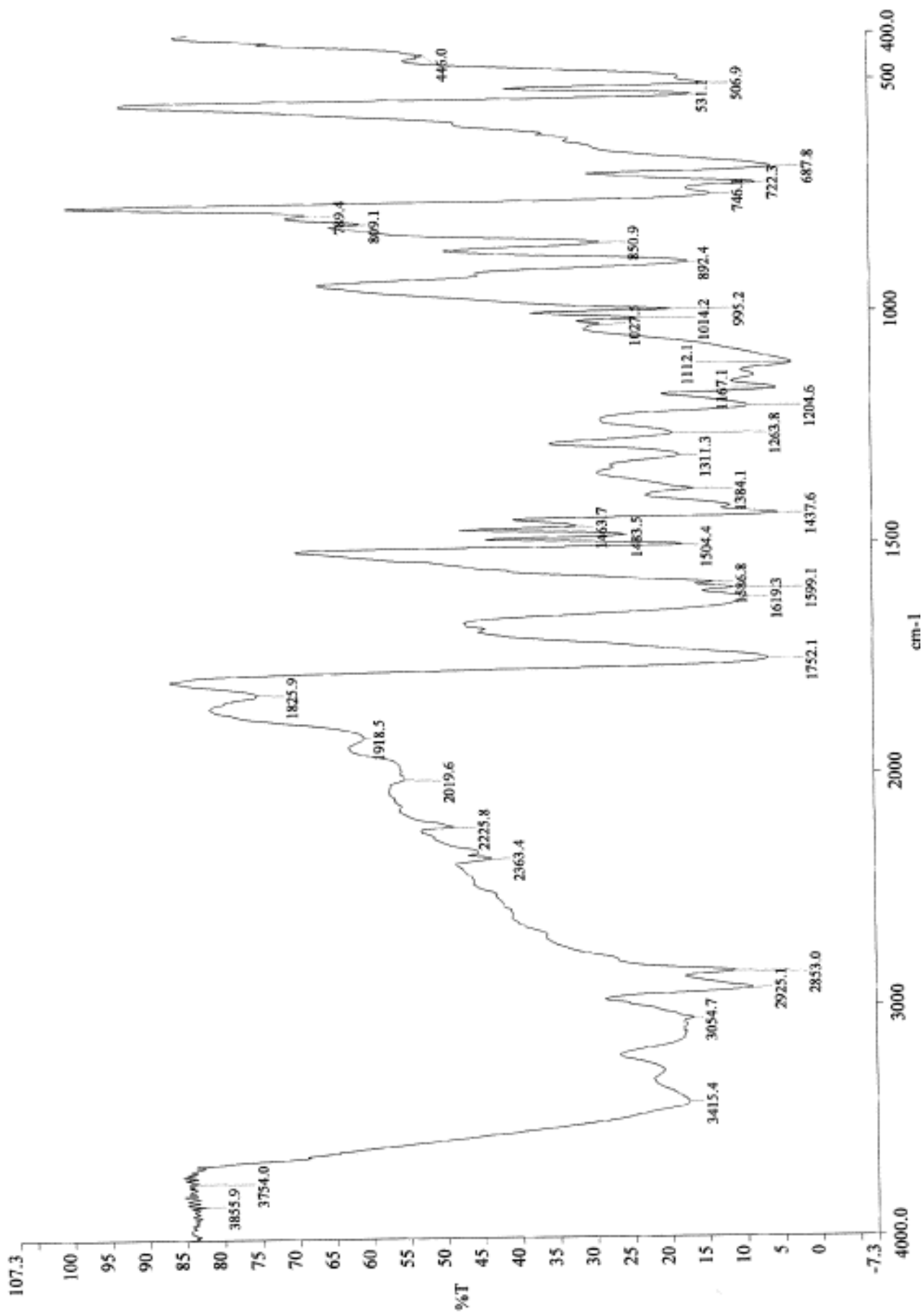
General information

For general information regarding synthetic and analytical chemistry methods, see reference **28**. (Le Trionnaire S, Perry A, Szczesny B, Szabo C, Winyard PG, Whatmore JL, et al. The synthesis and functional evaluation of a mitochondria-targeted hydrogen sulfide donor, (10-oxo-10-(4-(3-thioxo-3H-1,2-dithiol-5-yl)phenoxy)decyl)triphenylphosphonium bromide (AP39). *Med Chem Commun.* 2014; (5):728-36. doi: 10.1039/C3MD00323J.)

AP123 high-resolution mass spectrum:



AP123 infrared spectrum (KBr disc):

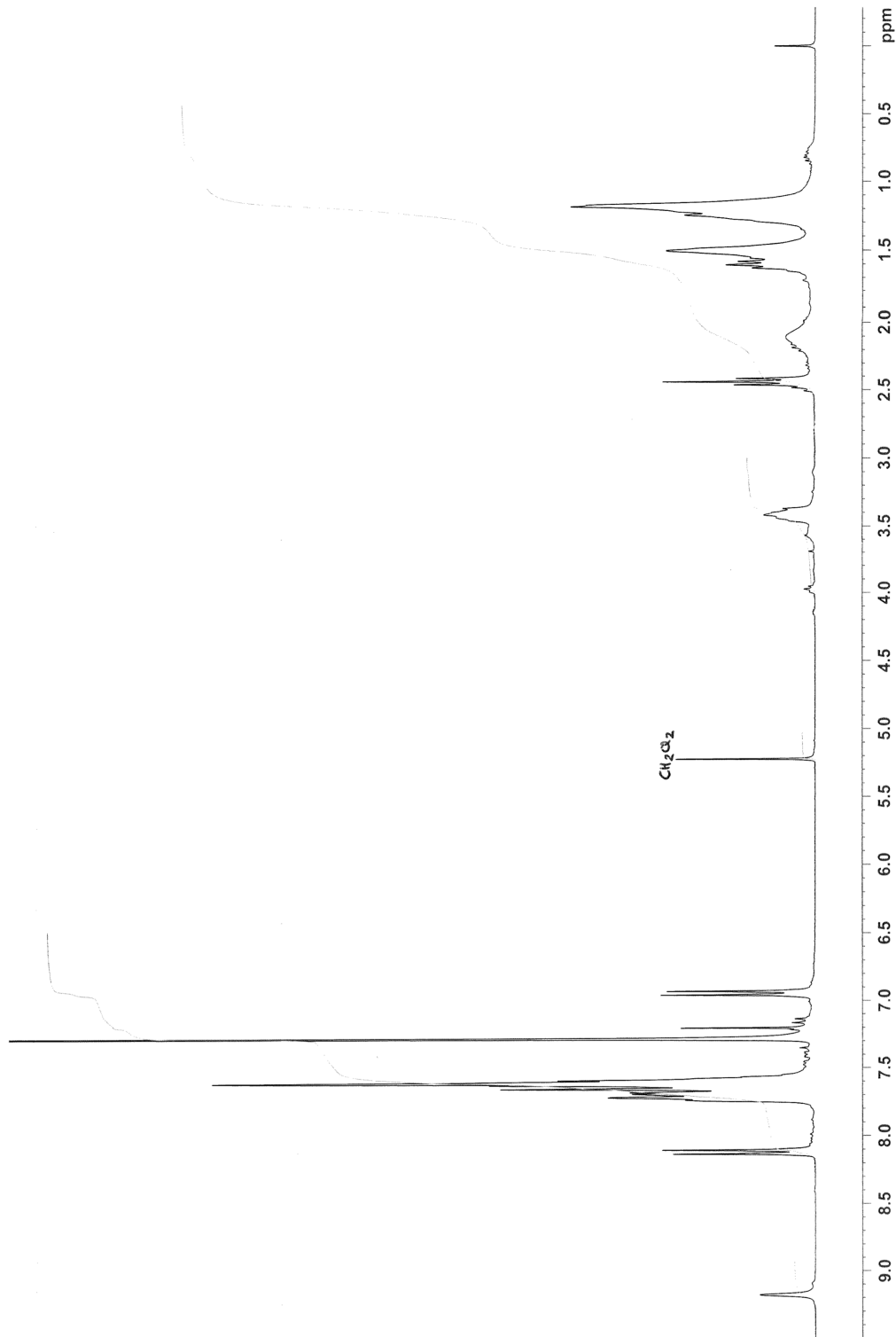


AP123 ¹H NMR spectrum (300 MHz; CDCl₃):



NAME AP123
EXPNO 20
PROCNO 1
Date_ 20130619
Time_ 14.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SF01 300.1318534 MHz
SI 32768
SF 300.1300241 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AP123

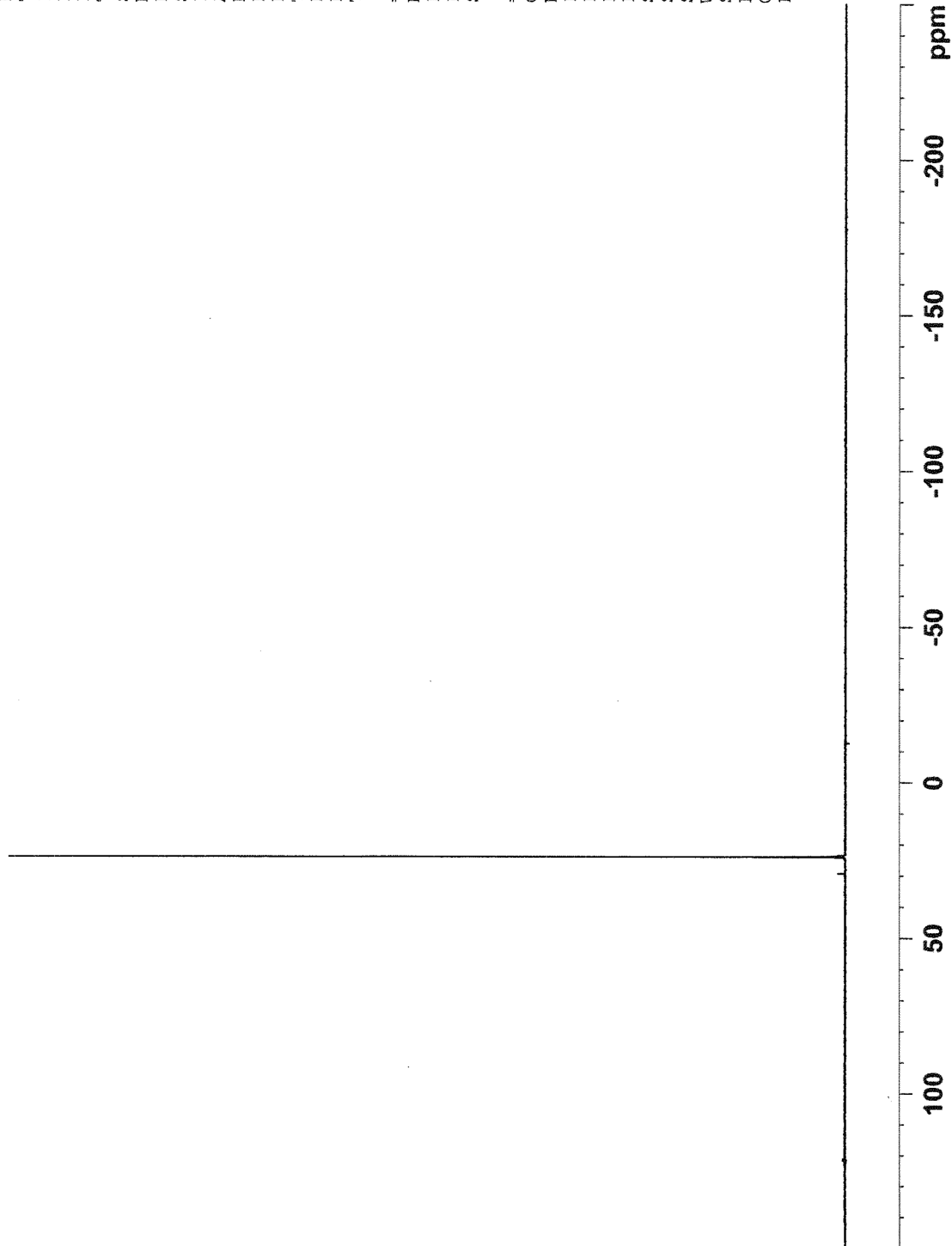
AP123 ³¹P NMR spectrum (121 MHz; CDCl₃):



NAME AP123
 EXPNO 21
 PROCNO 1
 Date_ 20130619
 Time_ 15.08
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 48661.801 Hz
 FIDRES 0.742520 Hz
 AQ 0.6734324 sec
 RG 20642.5
 DW 10.275 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 31P
 P1 6.00 usec
 PL1 5.00 dB
 SFO1 121.4887762 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 23.00 dB
 PL13 24.00 dB
 SFO2 300.1312005 MHz
 SI 32768
 SF 121.4948510 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



AP123 ¹³C NMR spectrum (75 MHz; CDCl₃):



```

NAME AP123
EXPNO 12
PROCNO 1
Date_ 20130618
Time_ 11.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.821908 sec
RG 380.3
DW 27.900 usec
DE 6.50 usec
TE 299.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL12 23.00 dB
PL13 24.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

AP123?

