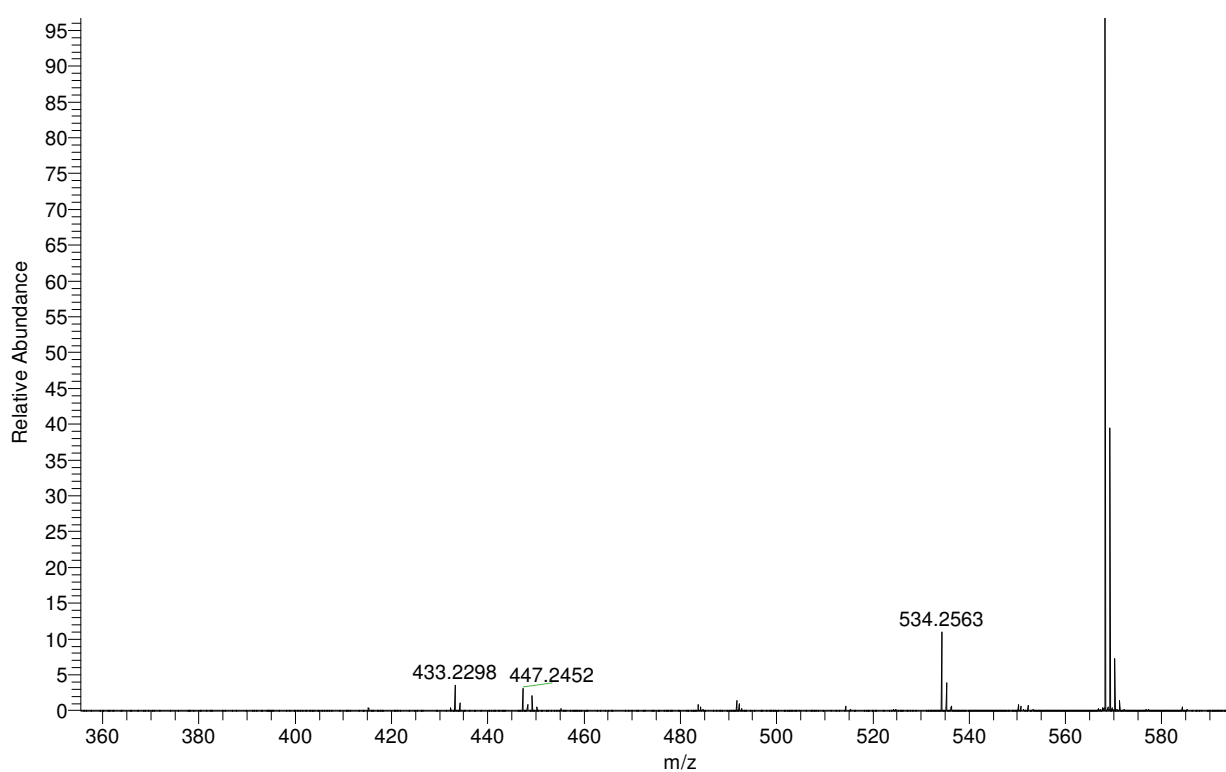


## General experimental and instrumentation details and spectra for AP123

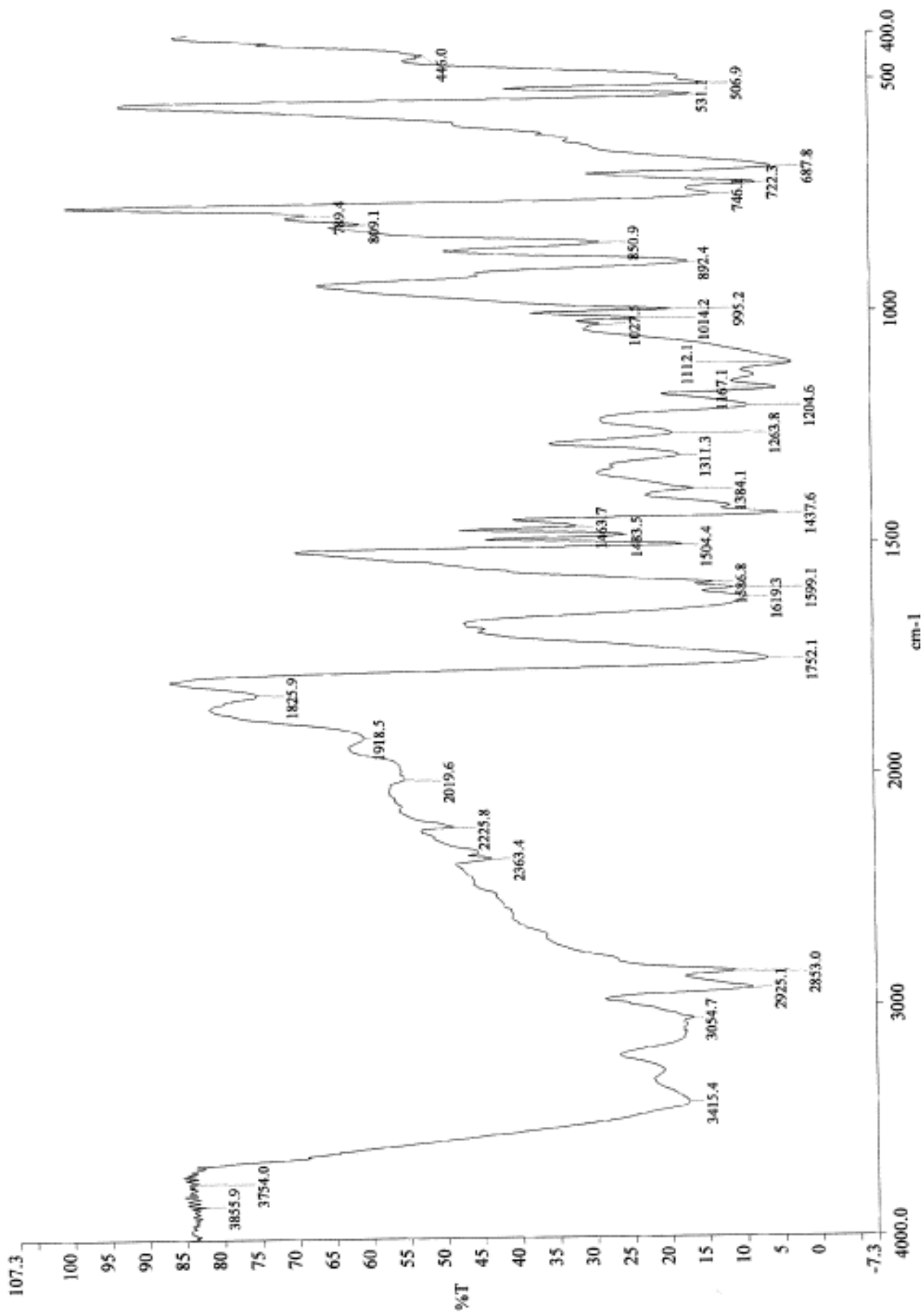
### General information

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):

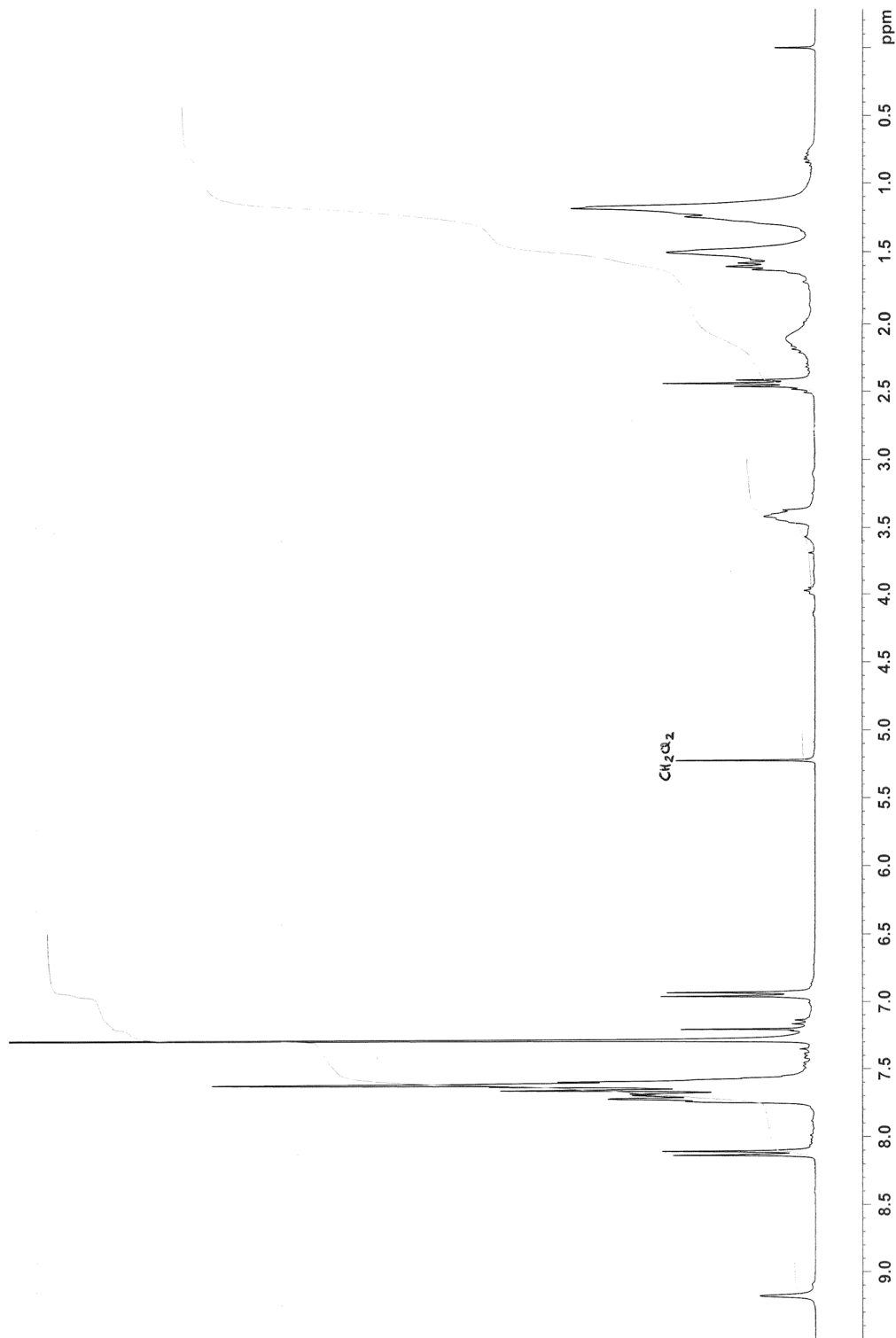


# AP123 <sup>1</sup>H NMR spectrum (300 MHz; CDCl<sub>3</sub>):



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  
TDO 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

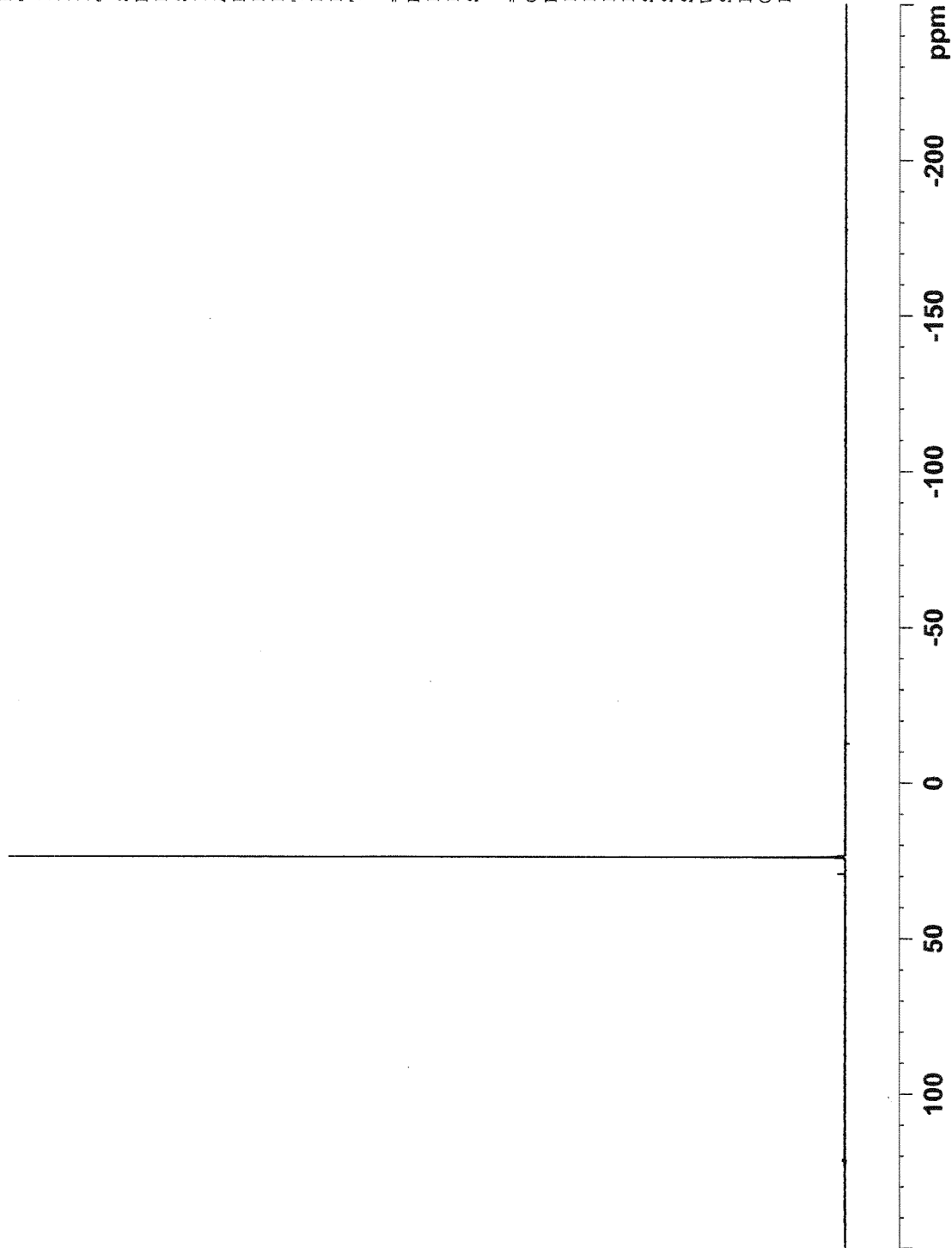
AP123 <sup>31</sup>P NMR spectrum (121 MHz; CDCl<sub>3</sub>):



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 <sup>13</sup>C NMR spectrum (75 MHz; CDCl<sub>3</sub>):



```

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?

