

Supporting Information

Synthesis of Unsymmetrical Sulfides and Their Oxidation to Sulfones to Discover Potent Antileishmanial Agents

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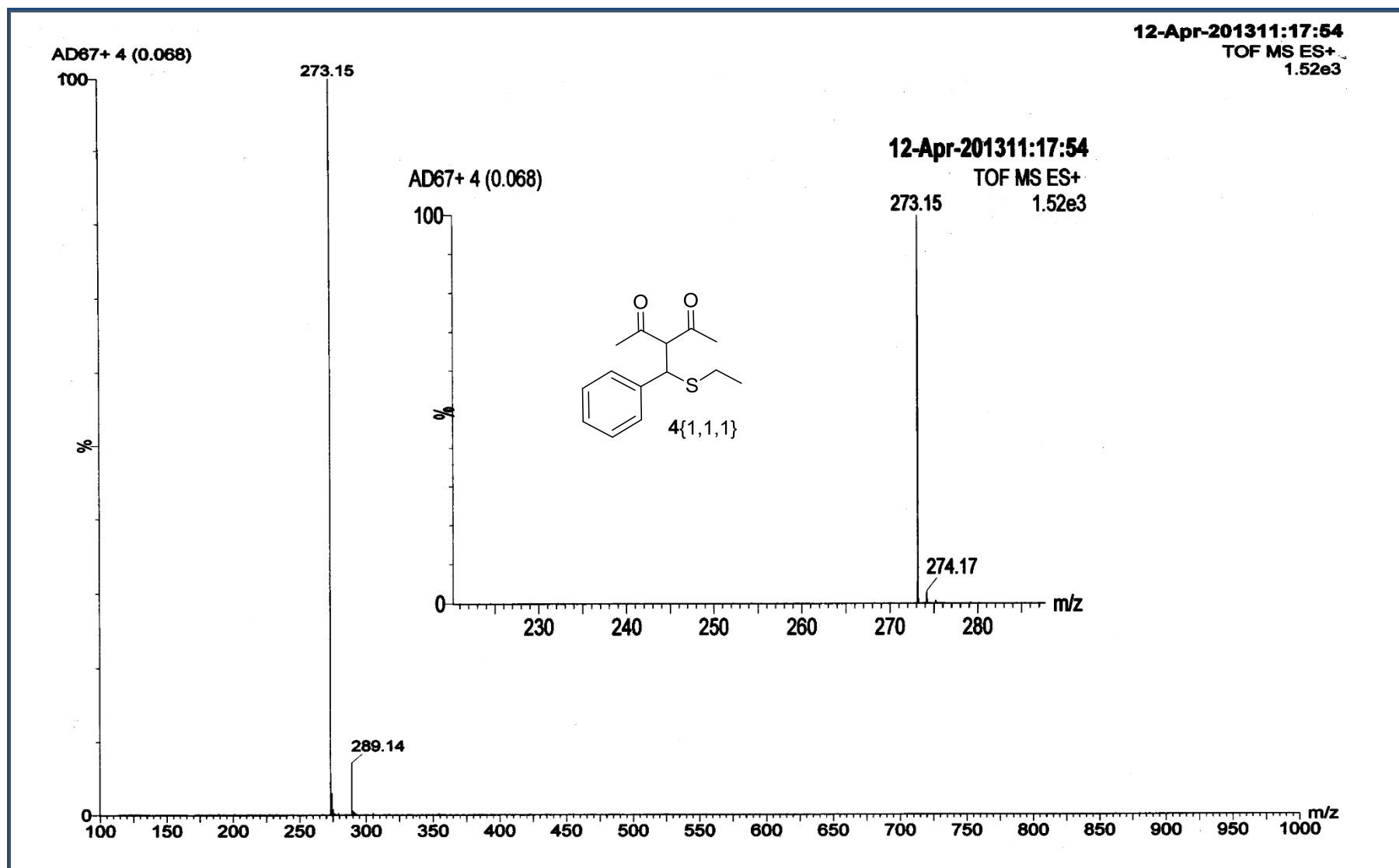
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• Copies of ESI-MS spectra of Compounds	2-69



AD68+ 22 (0.37)

100

287.18

%

273.17

0

100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 m/z

12-Apr-2013 11:40:06

TOF MS ES+

3.84e3

12-Apr-2013 11:40:06

TOF MS ES+

3.84e3

AD68+ 22 (0.376)

100

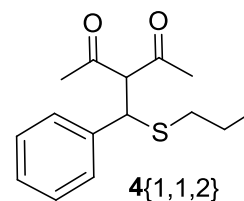
287.18

0

273.17

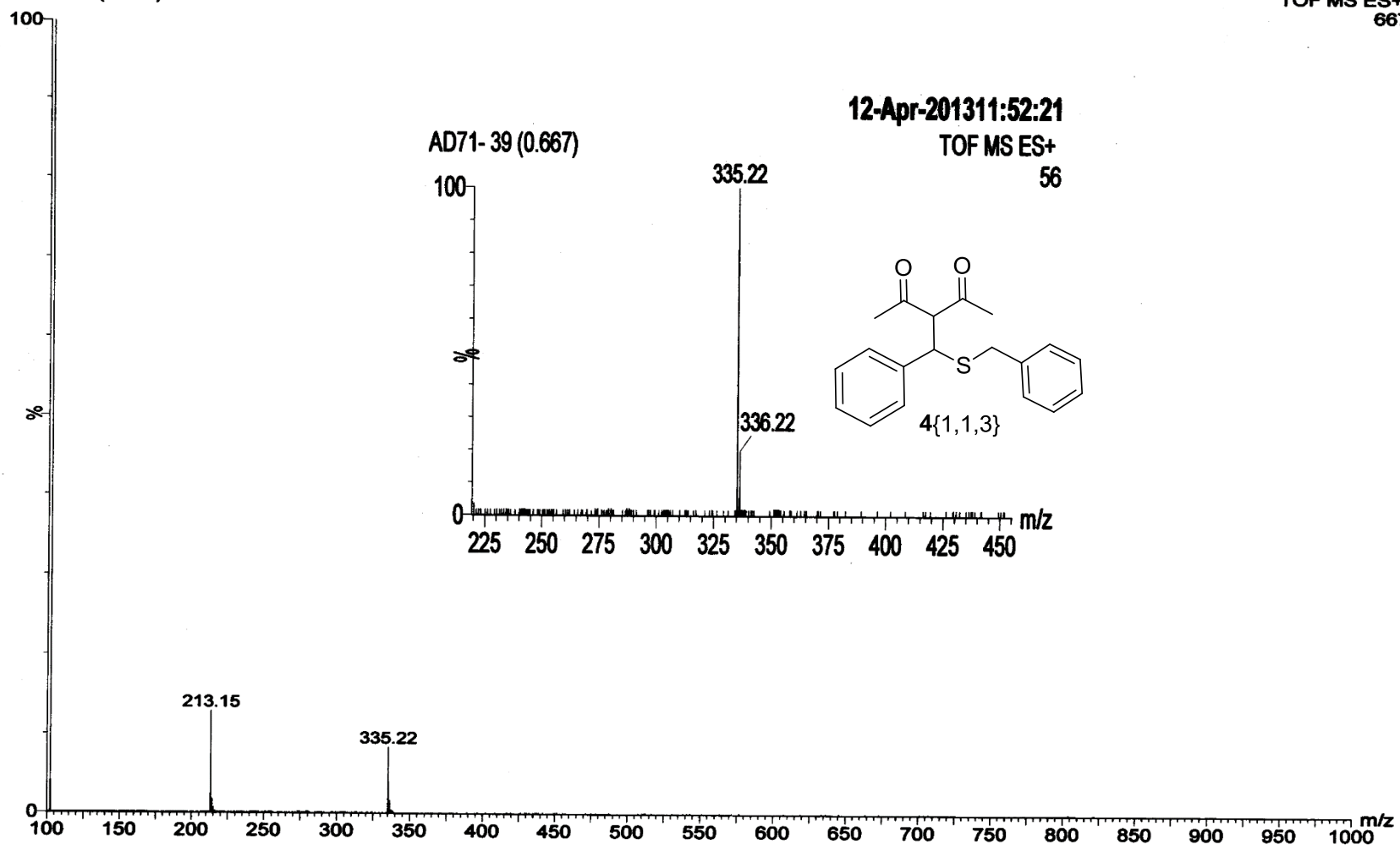
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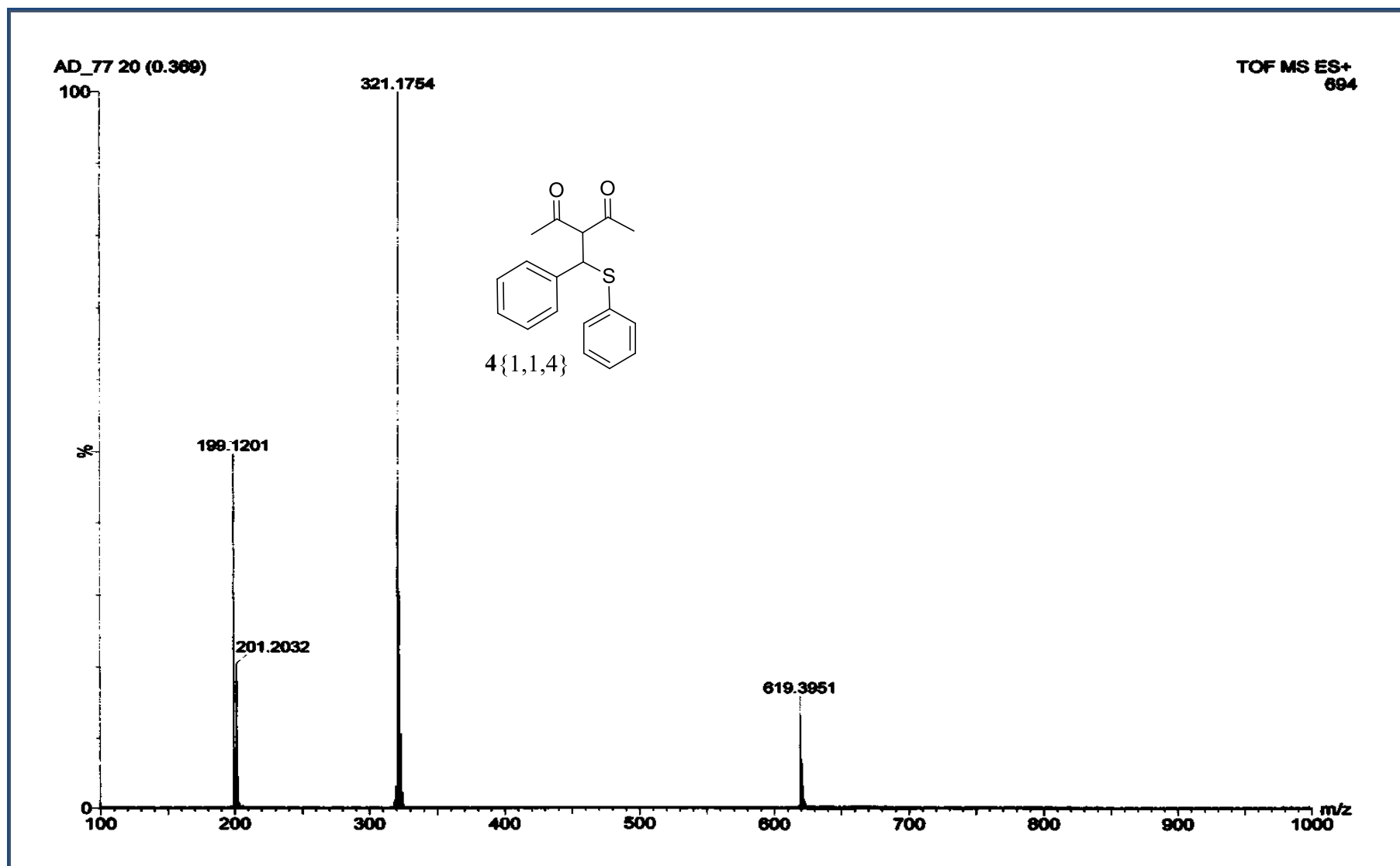
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AD71- 39 (0.667)

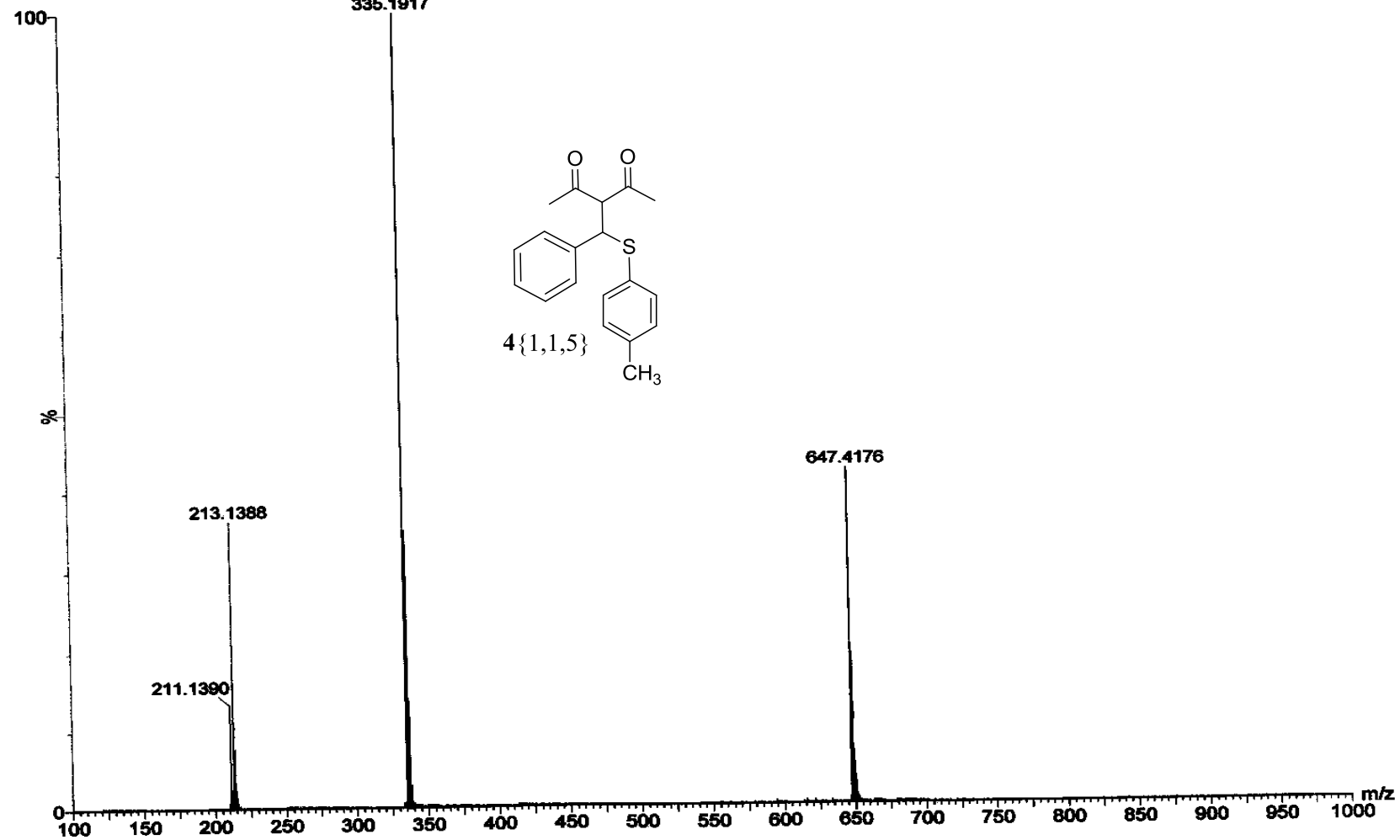
12-Apr-2013 11:52:21
TOF MS ES+
667





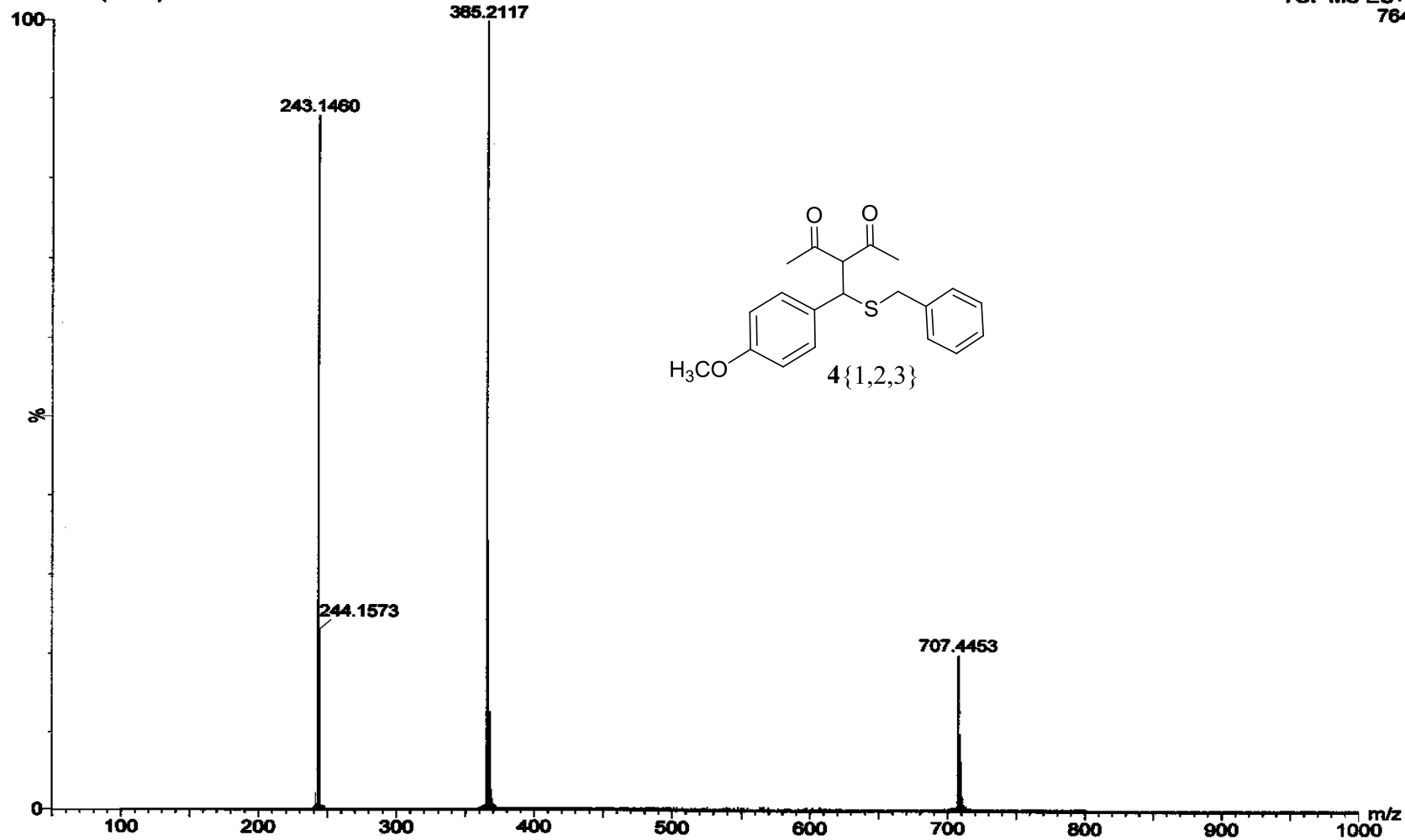
AD_78 32 (0.590)

TOF MS ES+
955



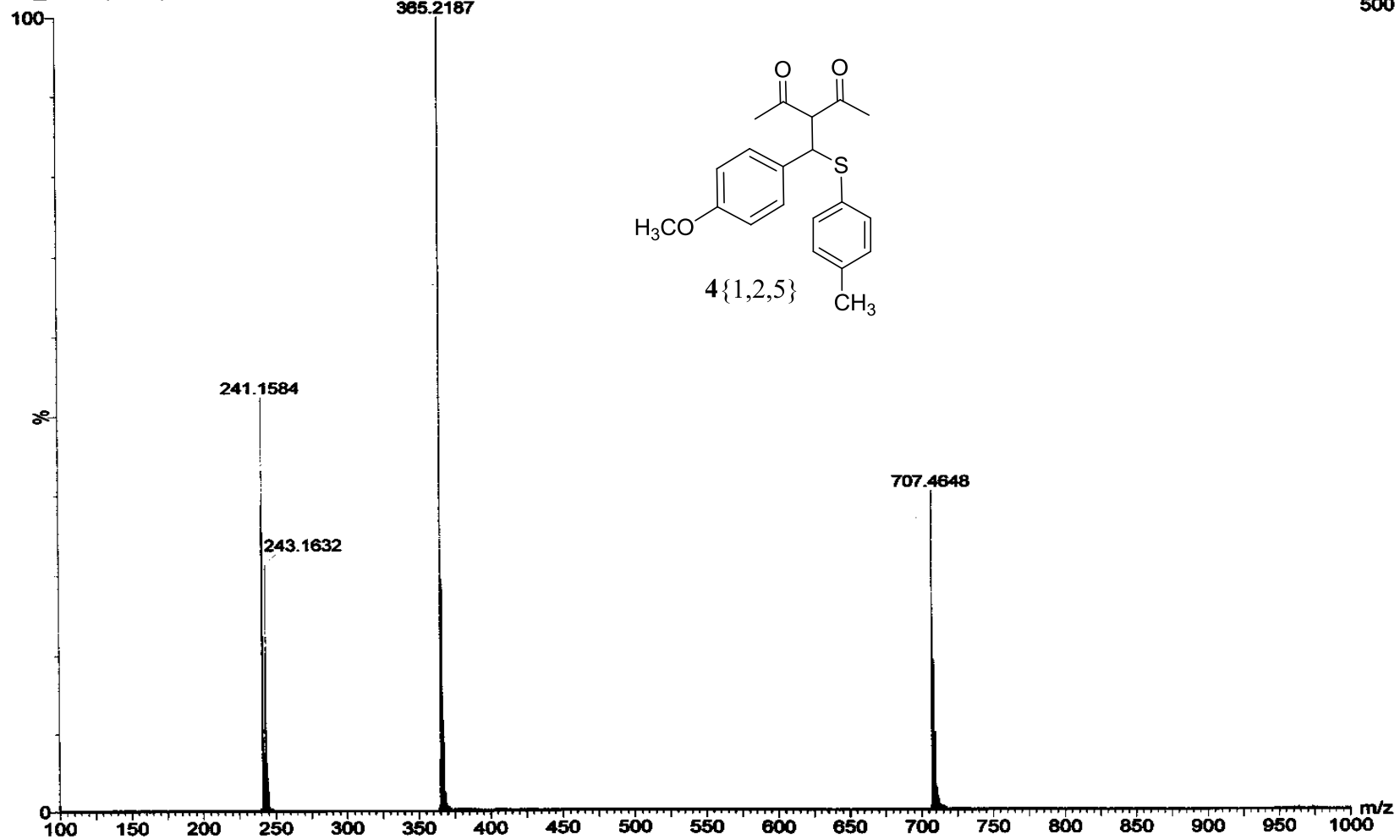
AD-86 55 (1.014)

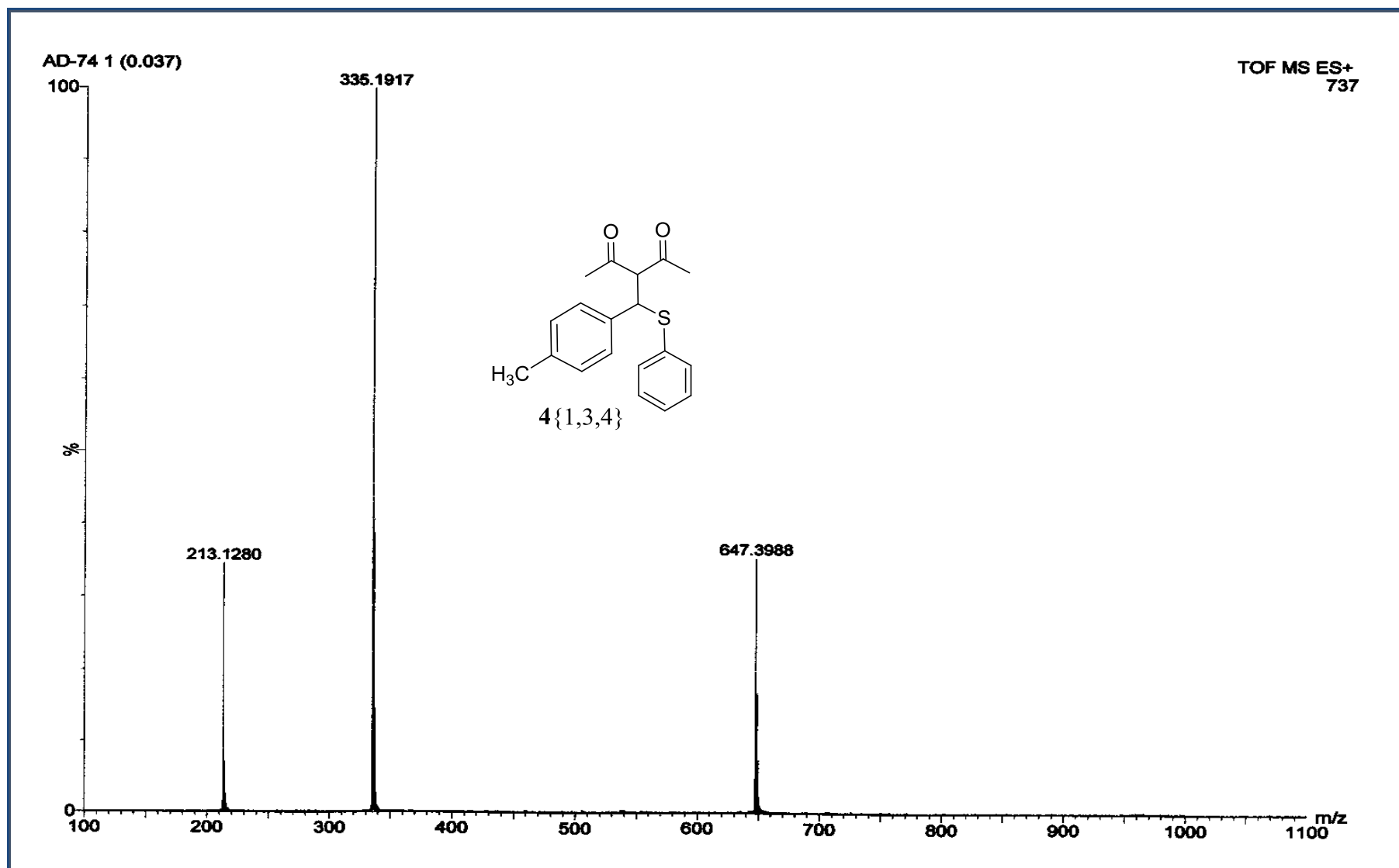
TOF MS ES+
764



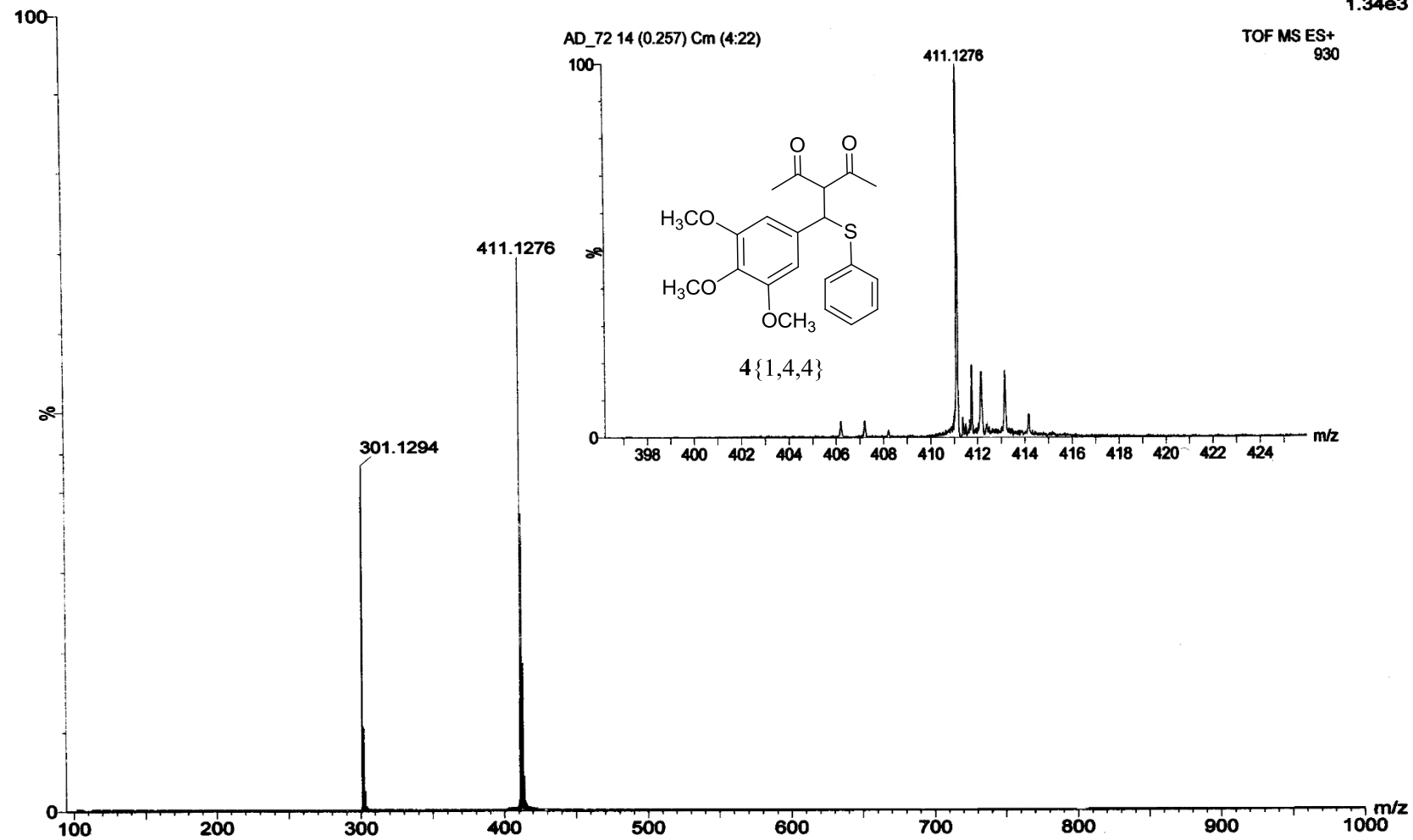
AD_75 12 (0.221)

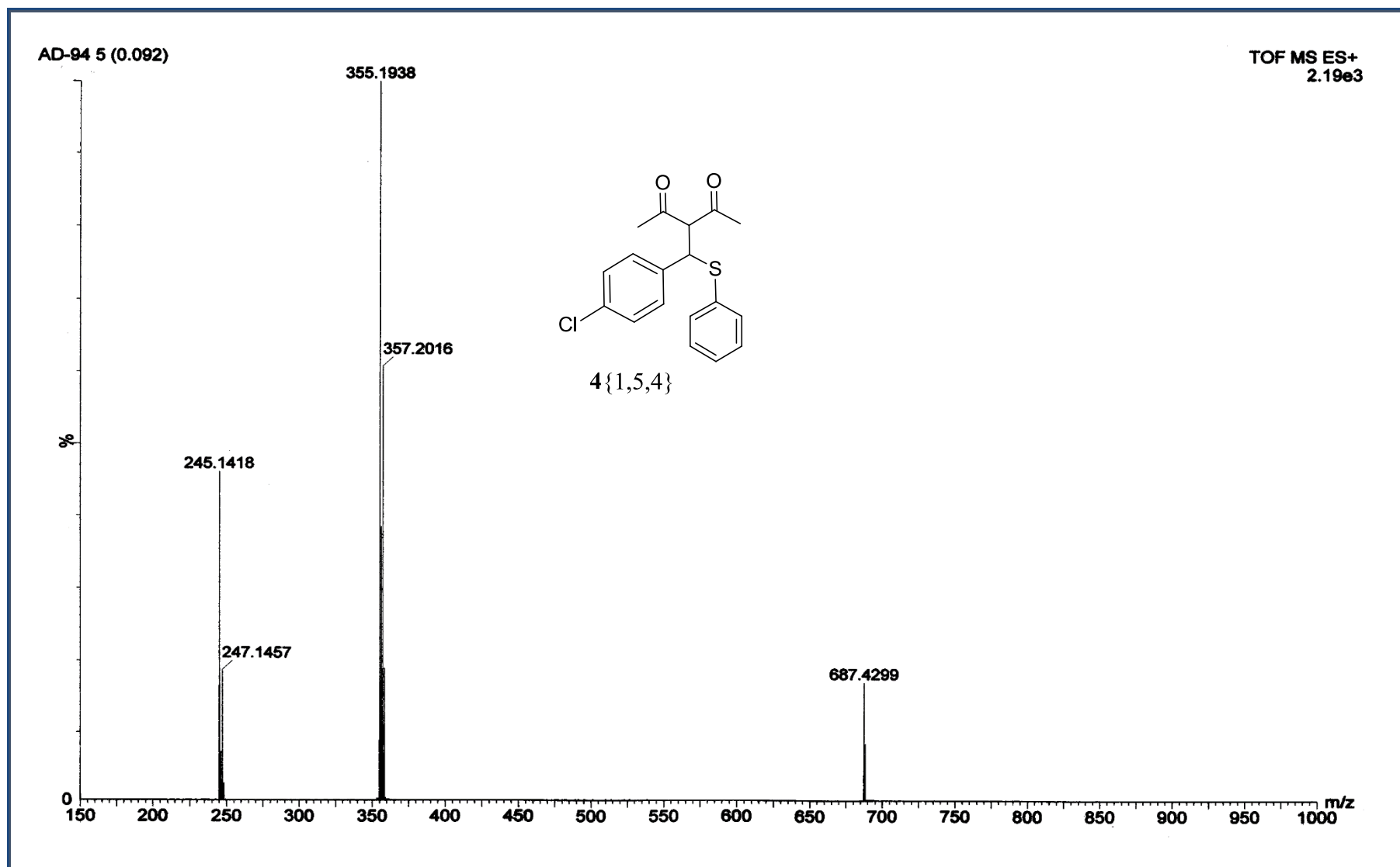
TOF MS ES+
500

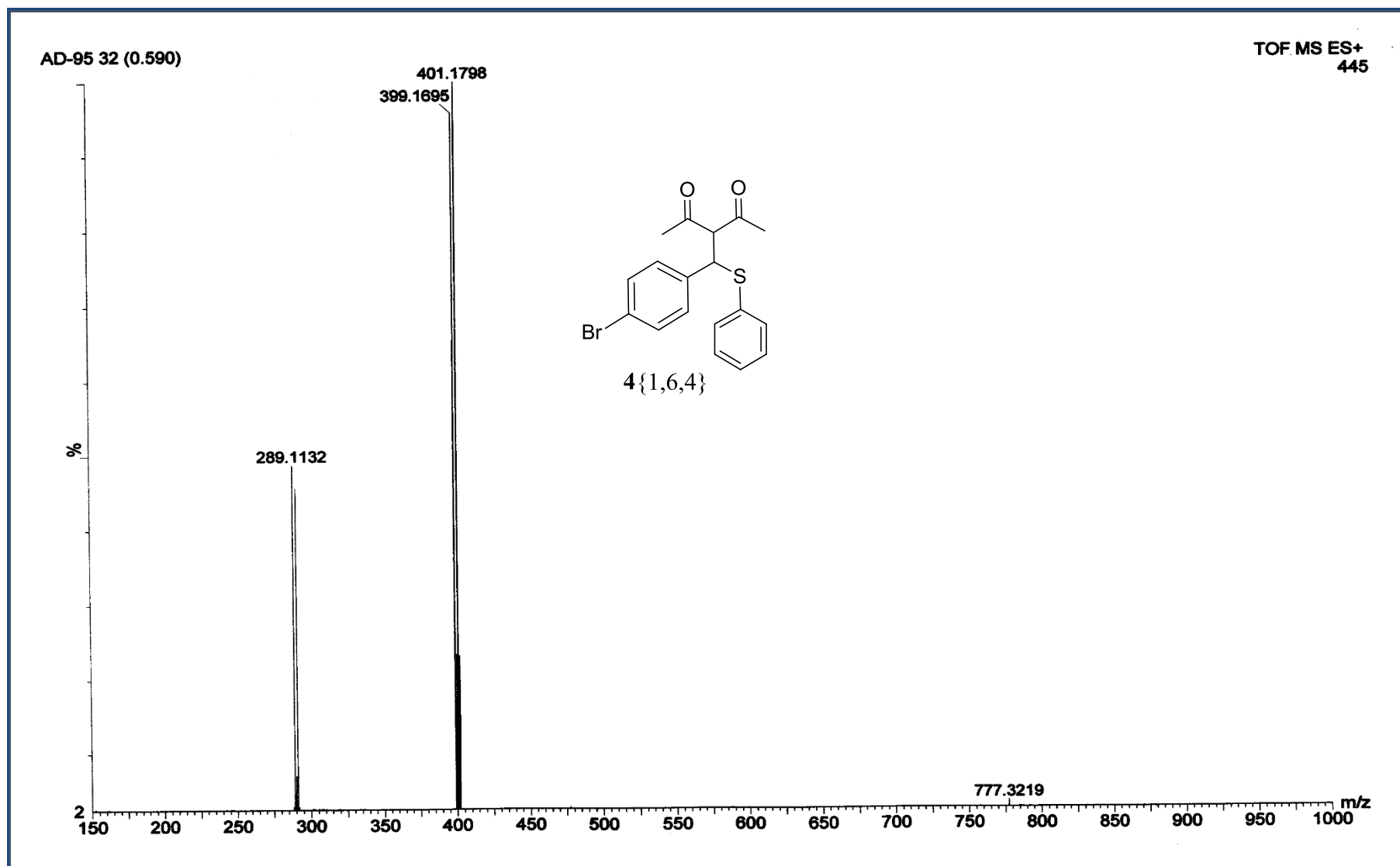




AD_72 14 (0.257) Cm (4:22)

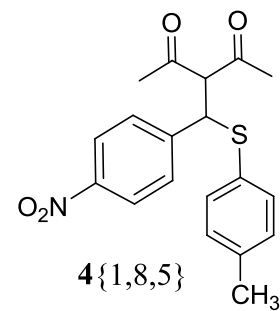
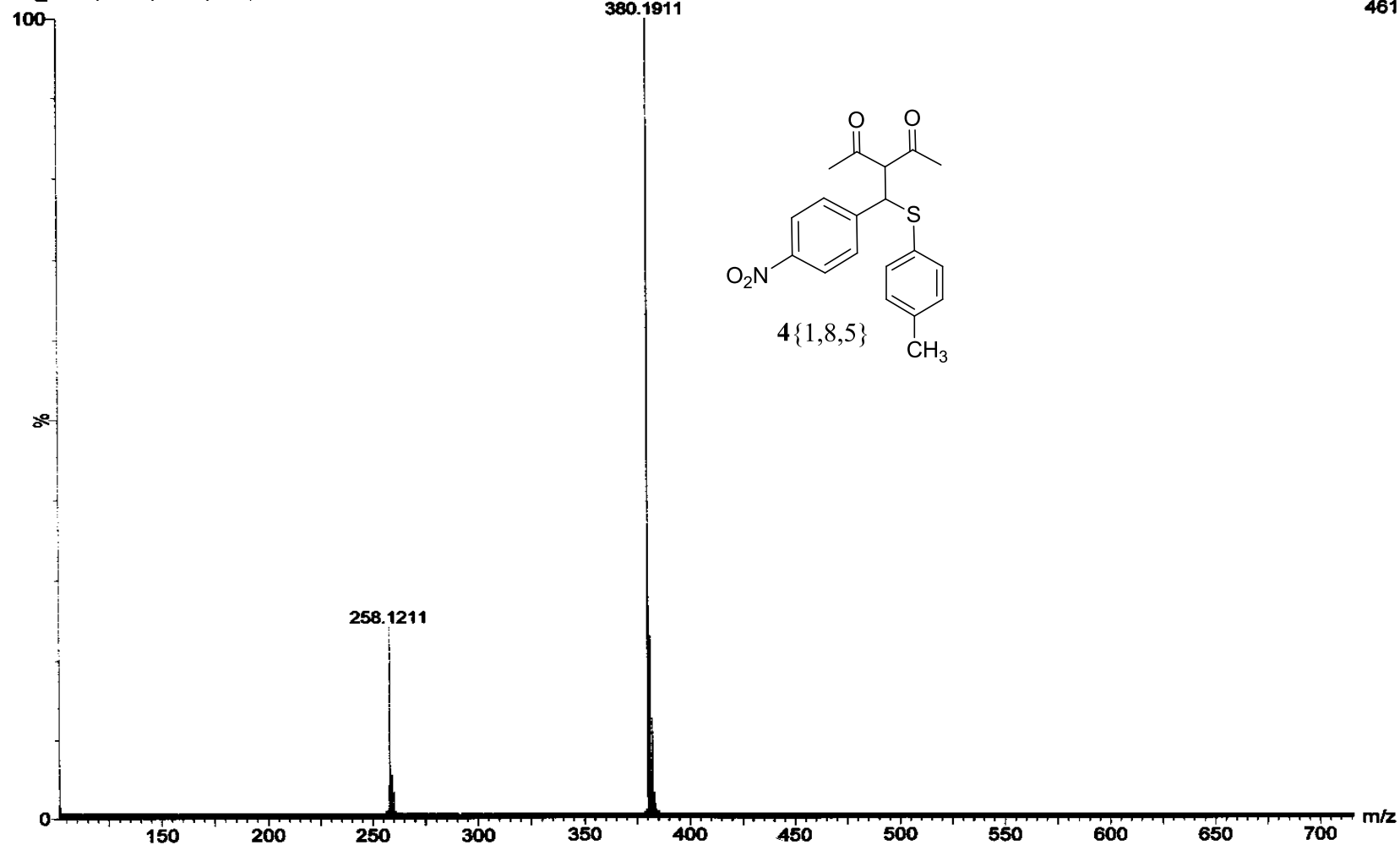






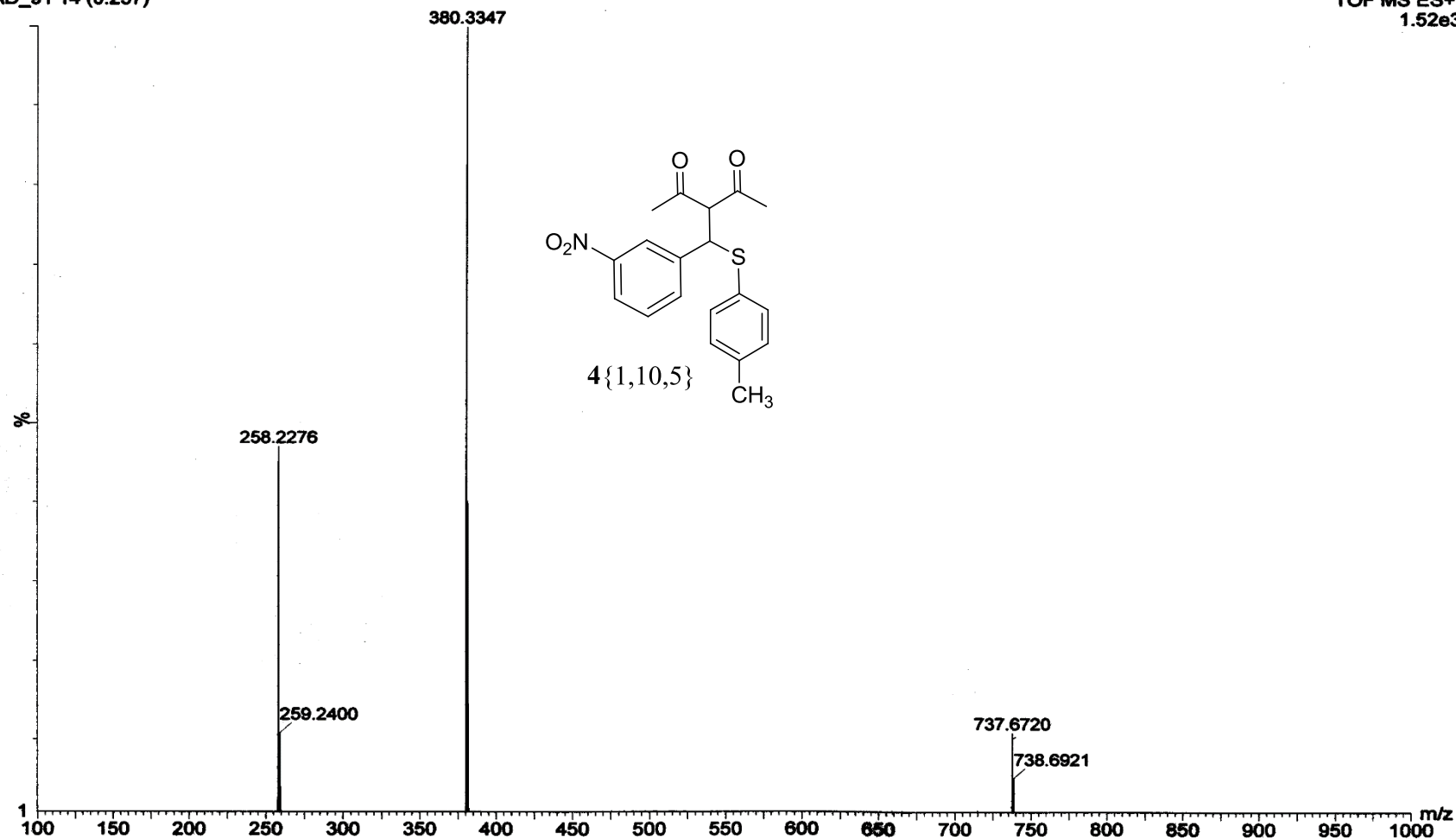
AD_73 4 (0.074) Cm (4:10)

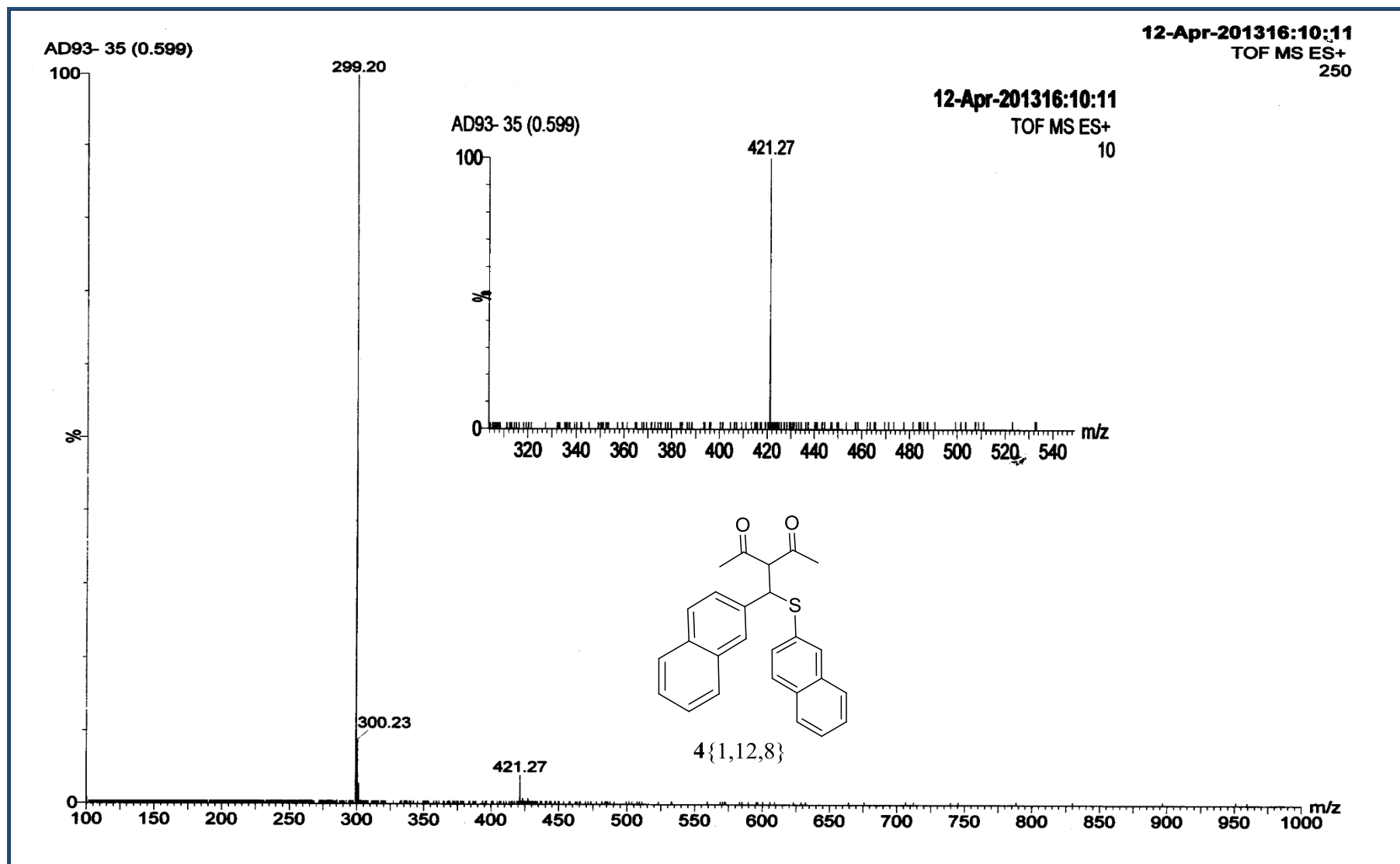
TOF MS ES+
461



AD_91 14 (0.257)

TOF MS ES+
1.52e3



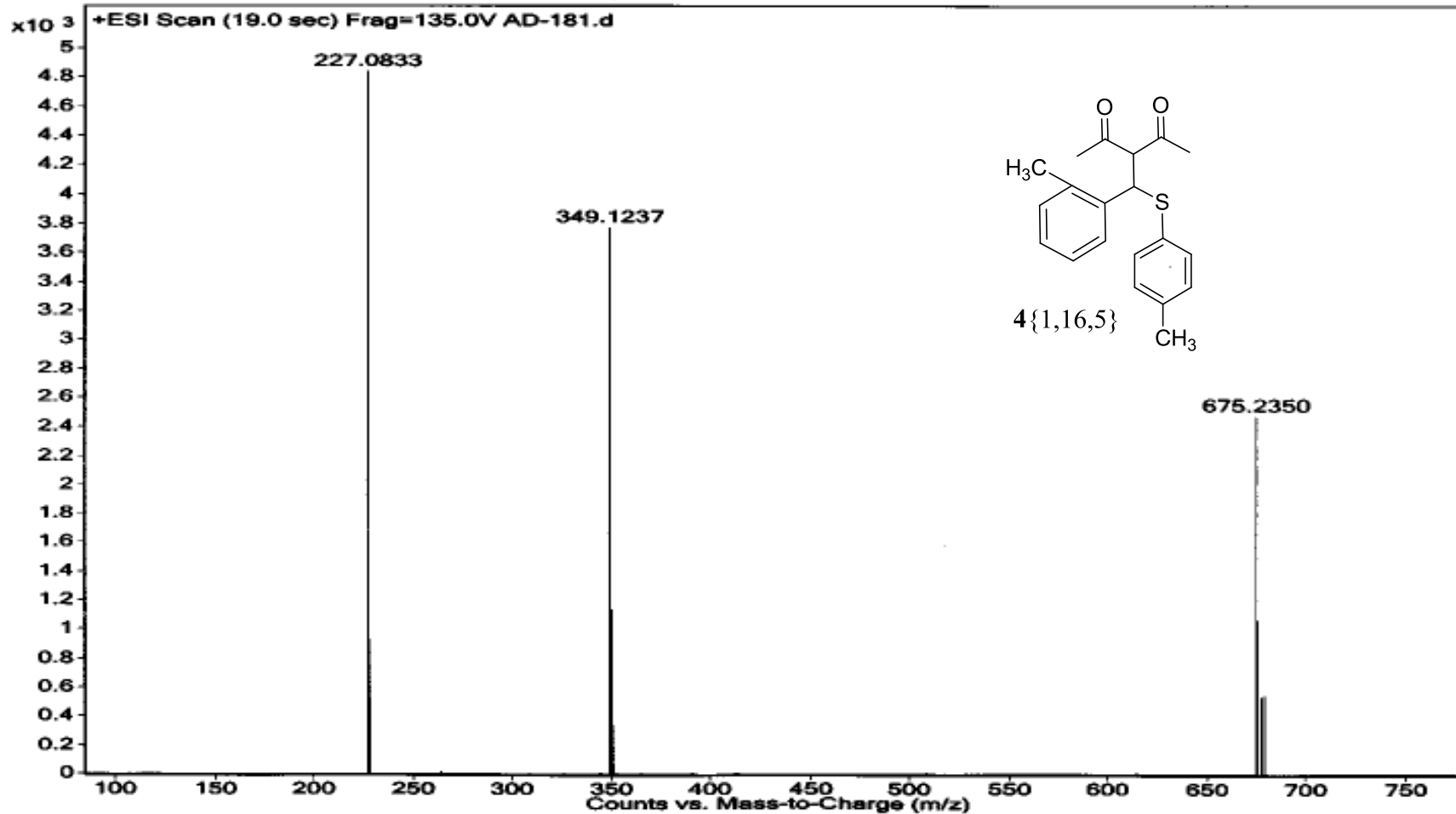


Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time

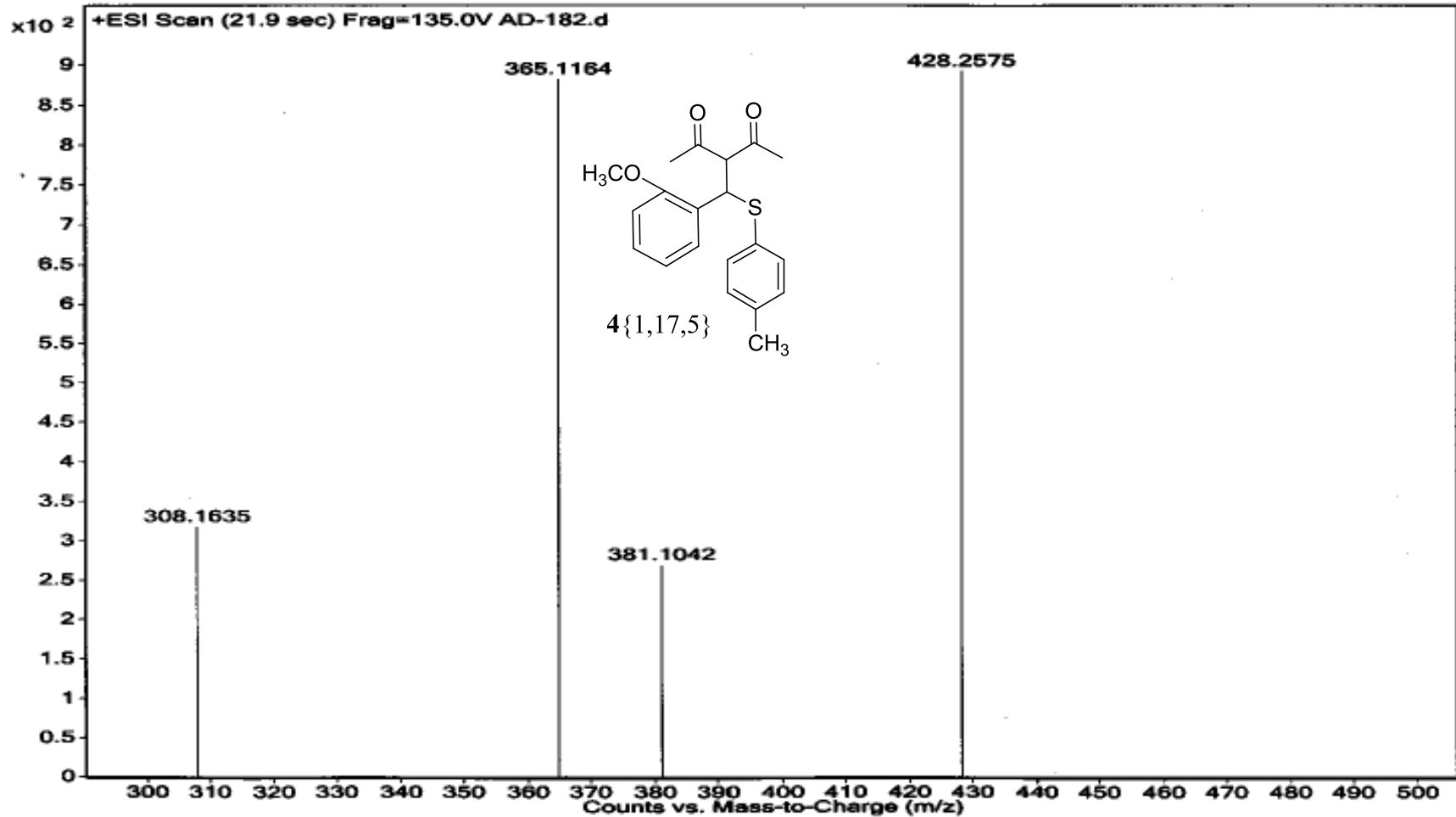


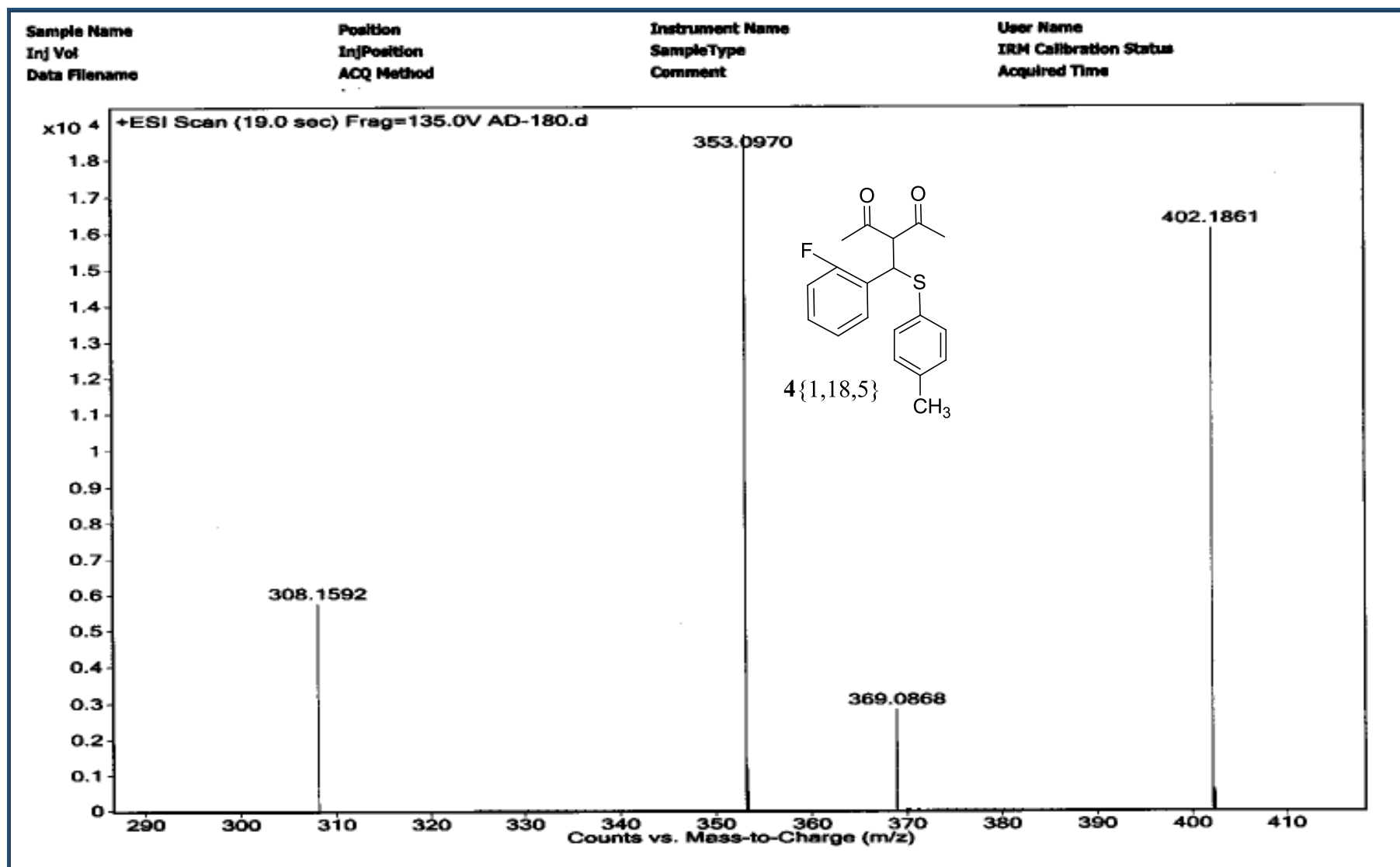
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Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



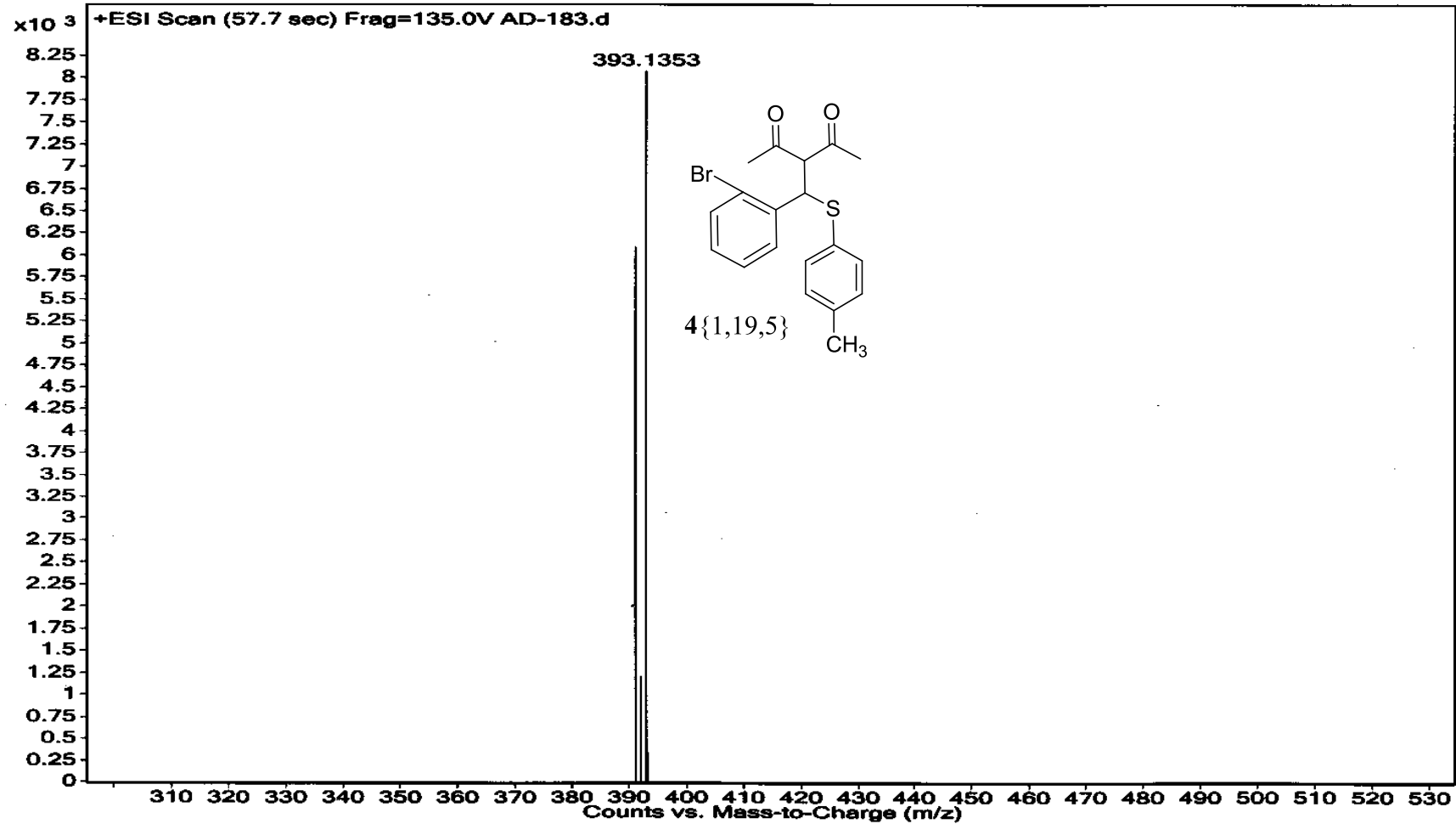


Sample Name
Inj Vol
Data Filename

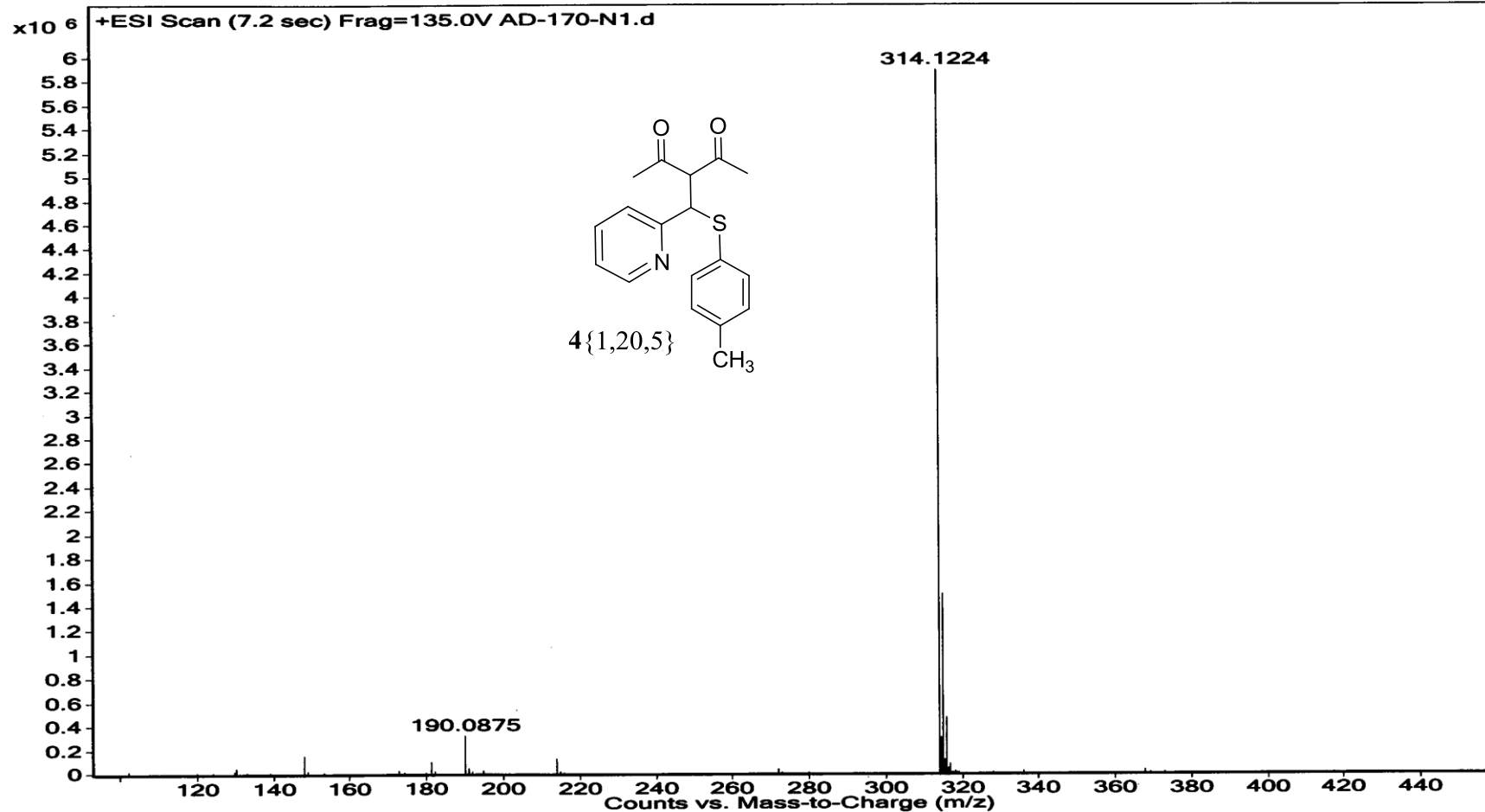
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

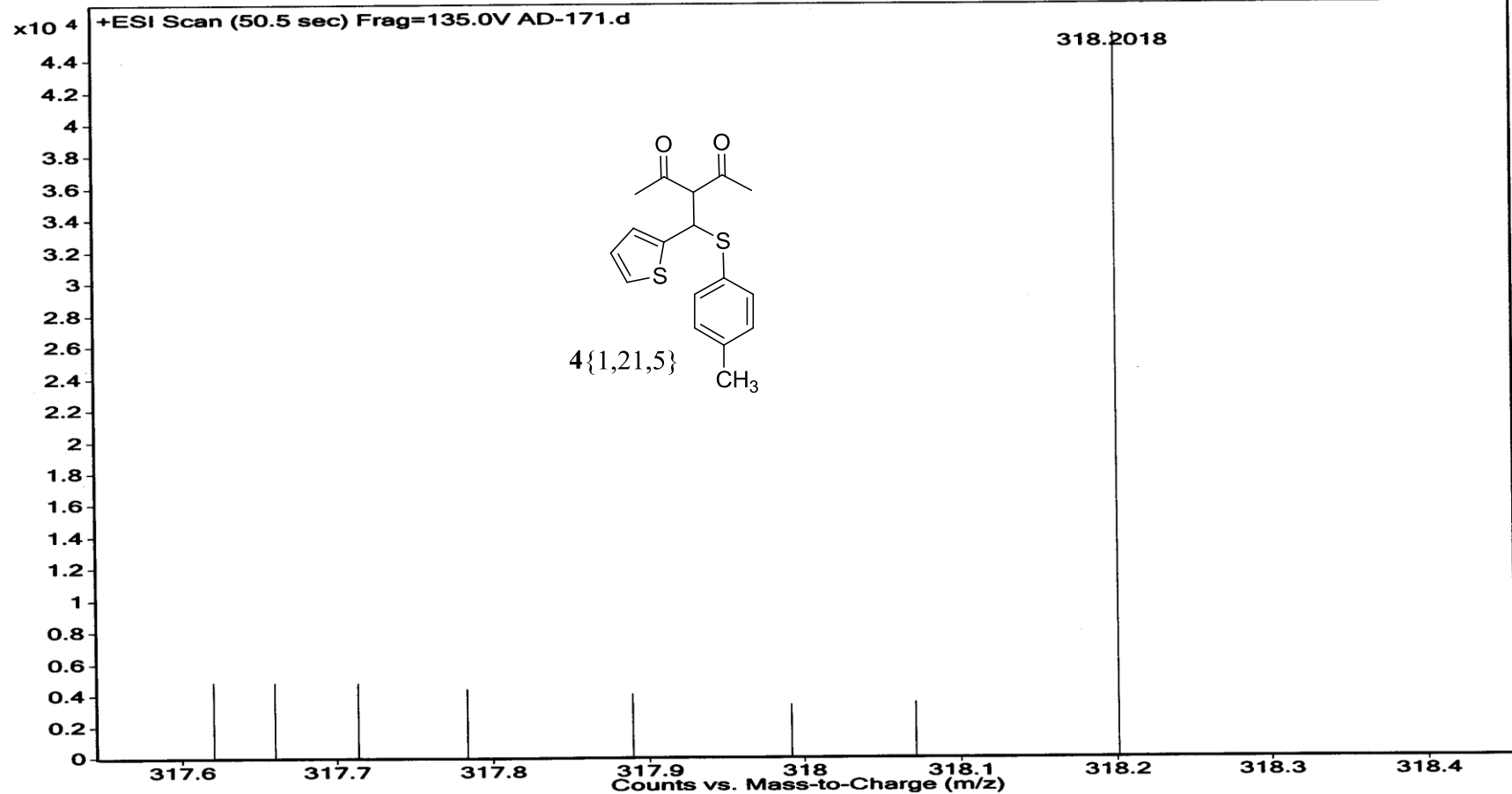
User Name
IRM Calibration Status
Acquired Time

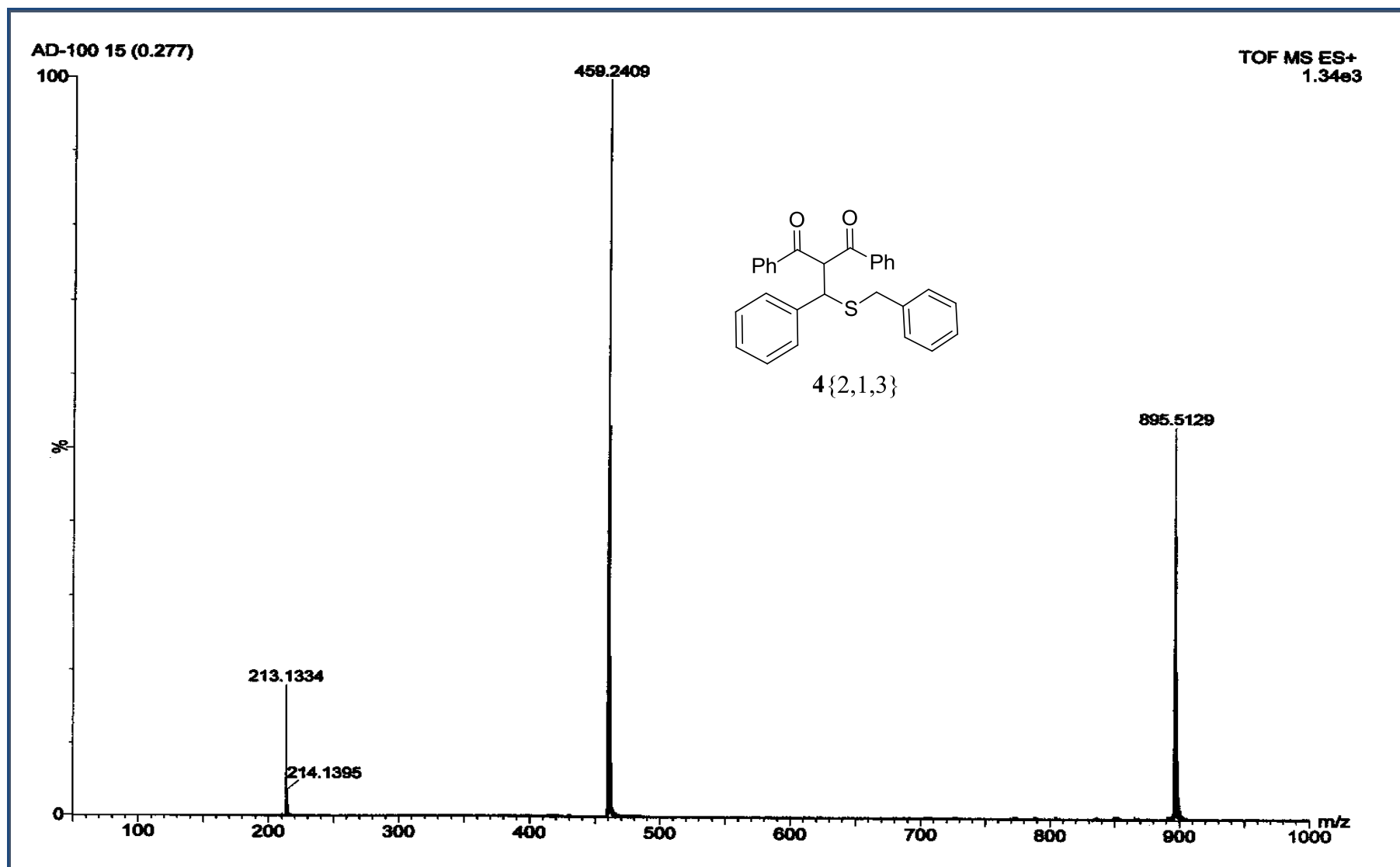


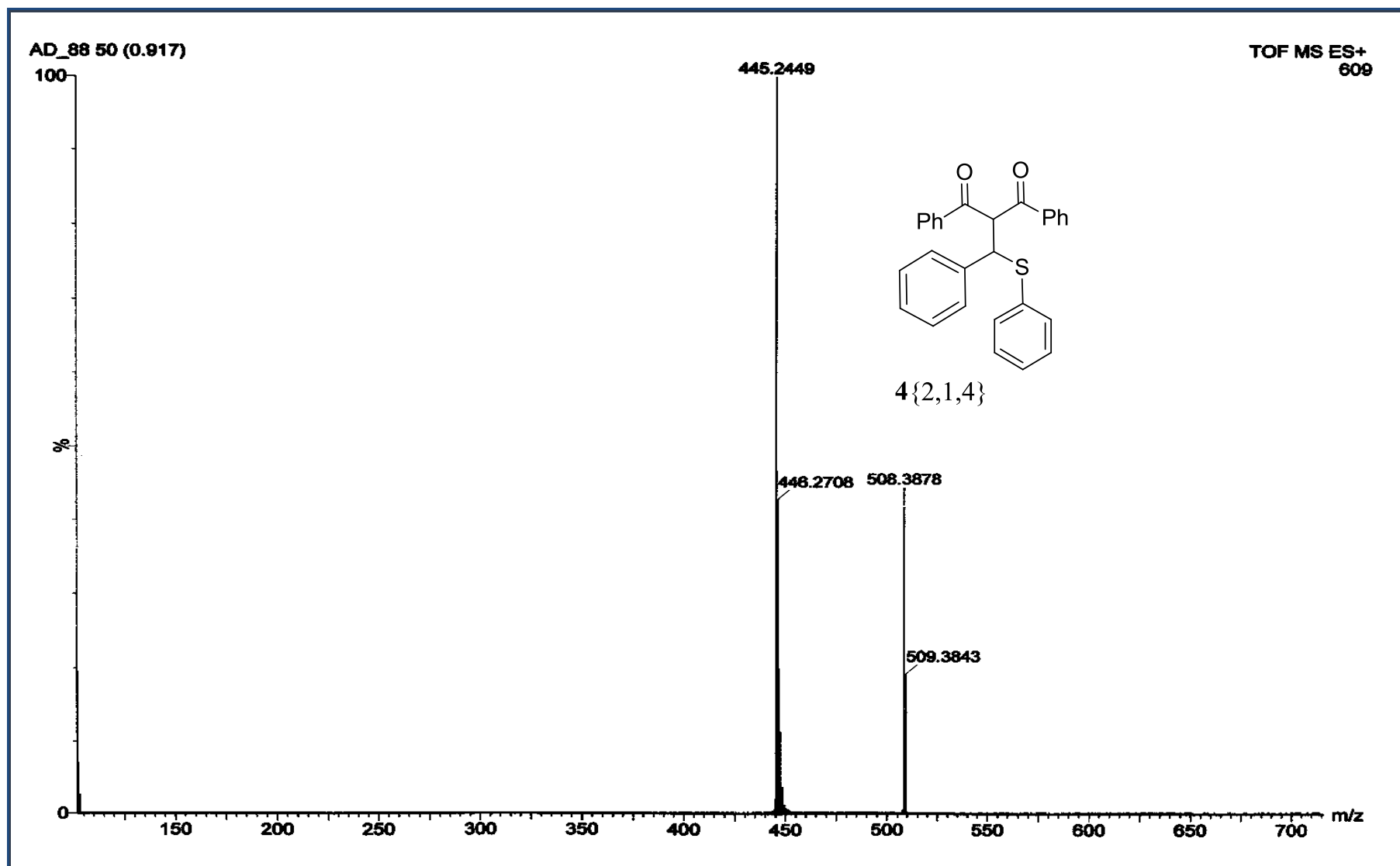
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Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	AD-170-N1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable

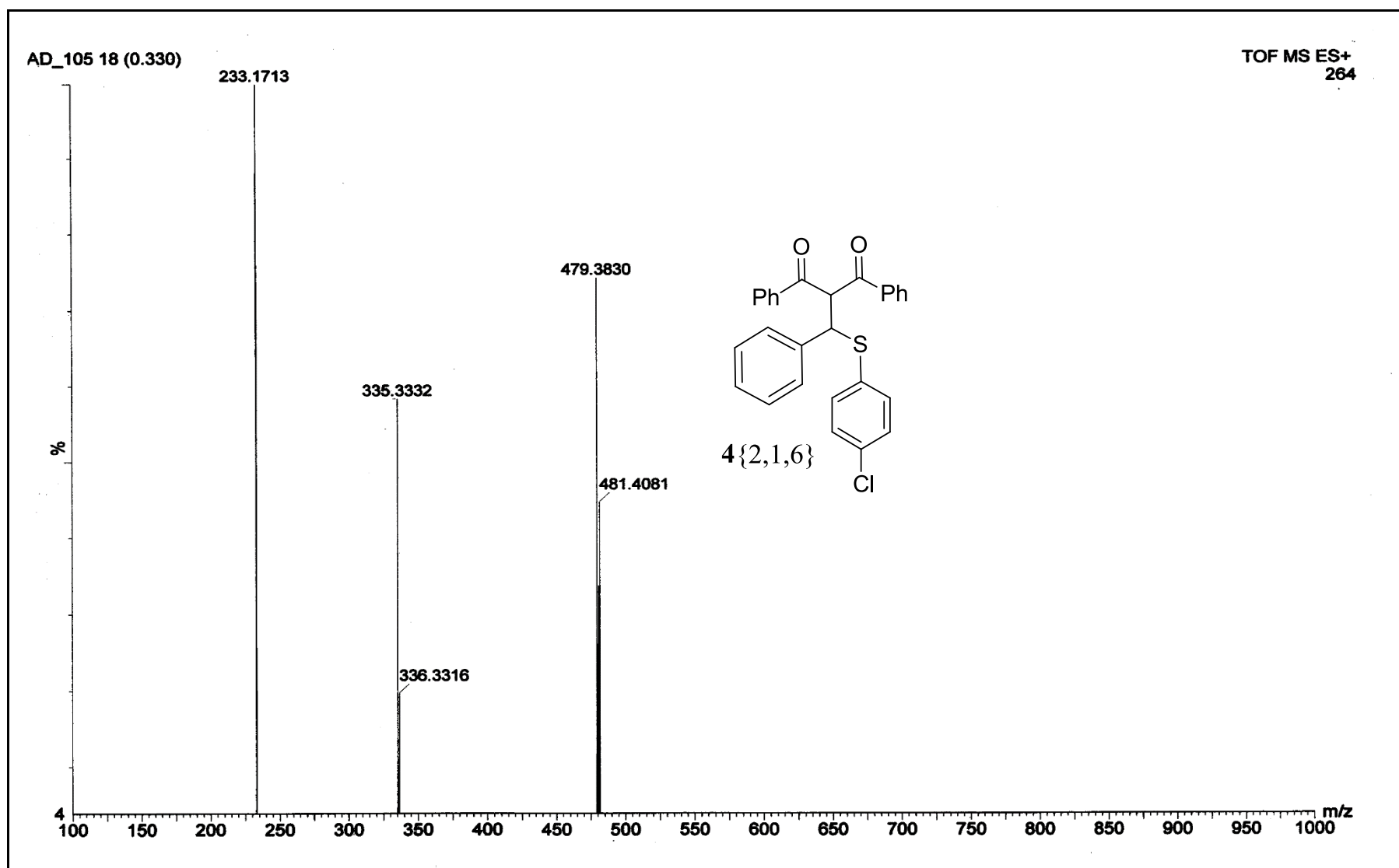


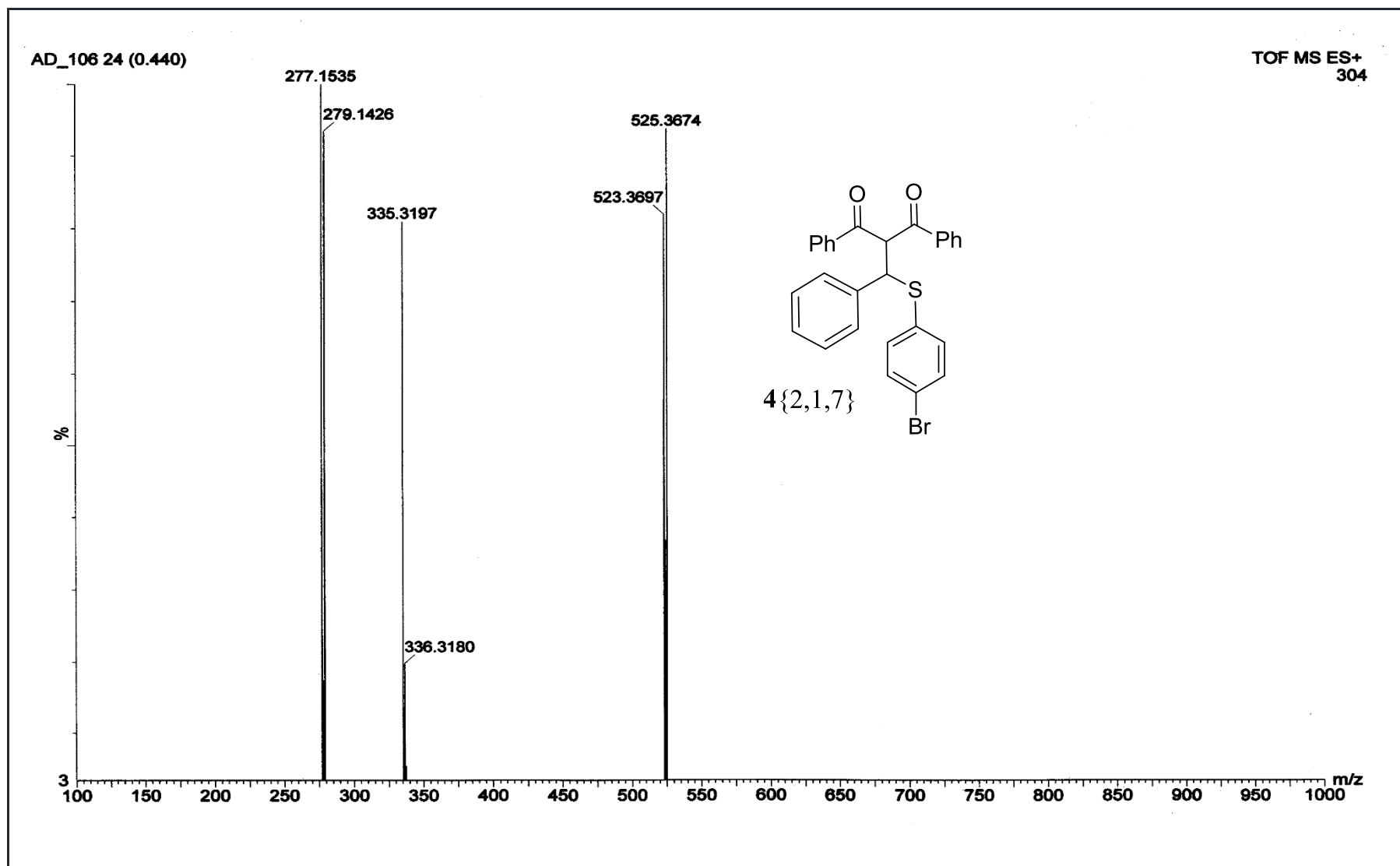
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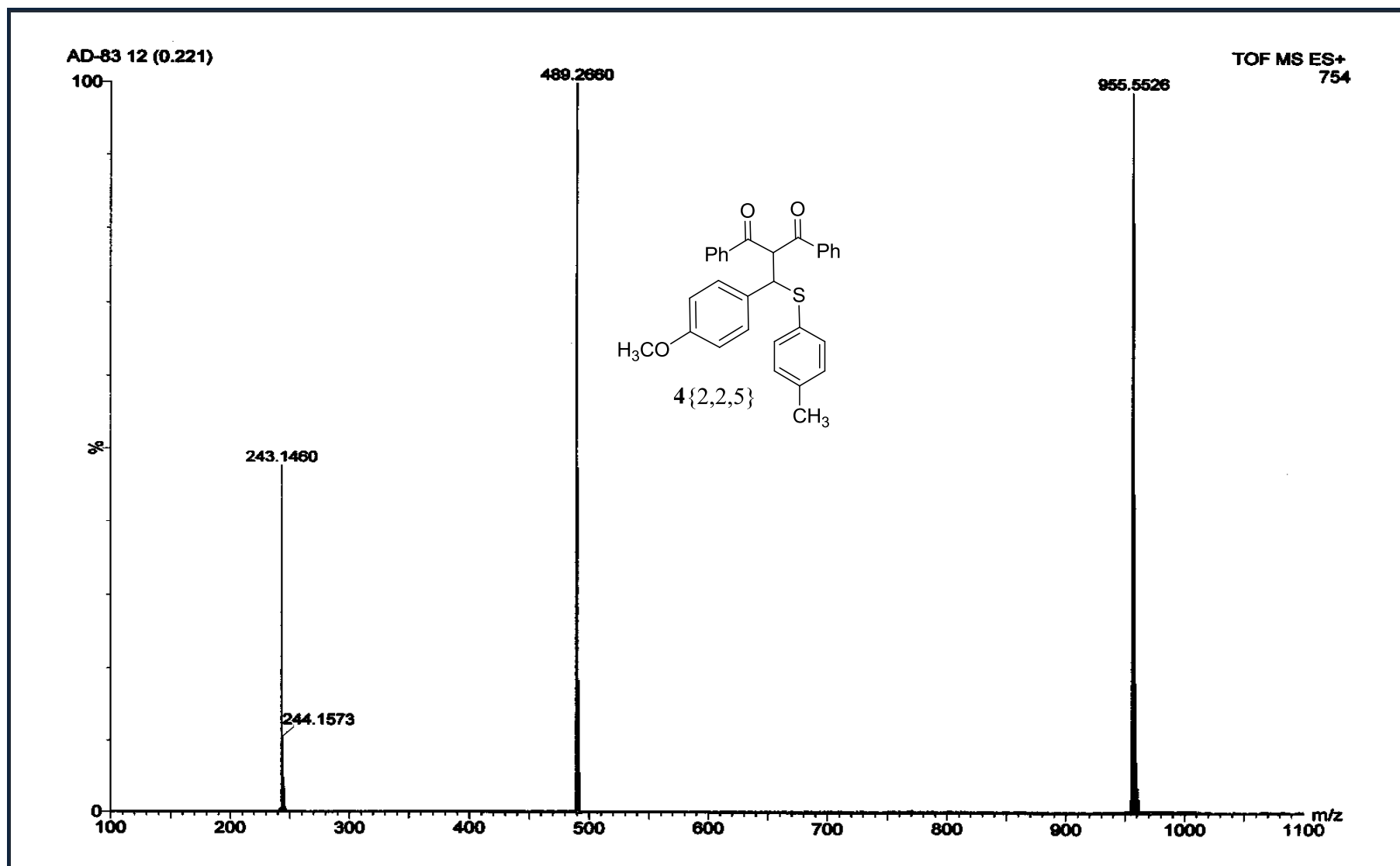


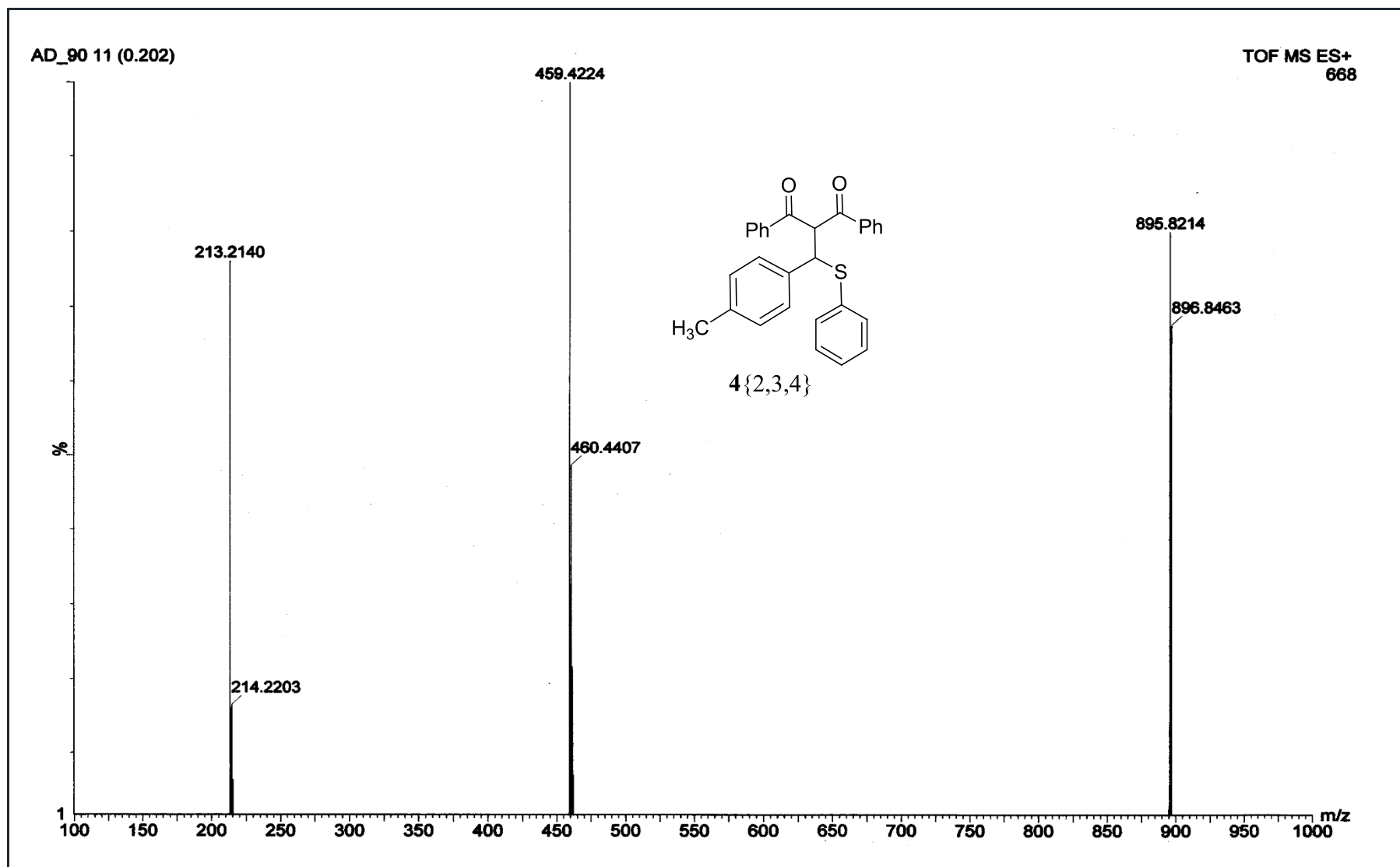






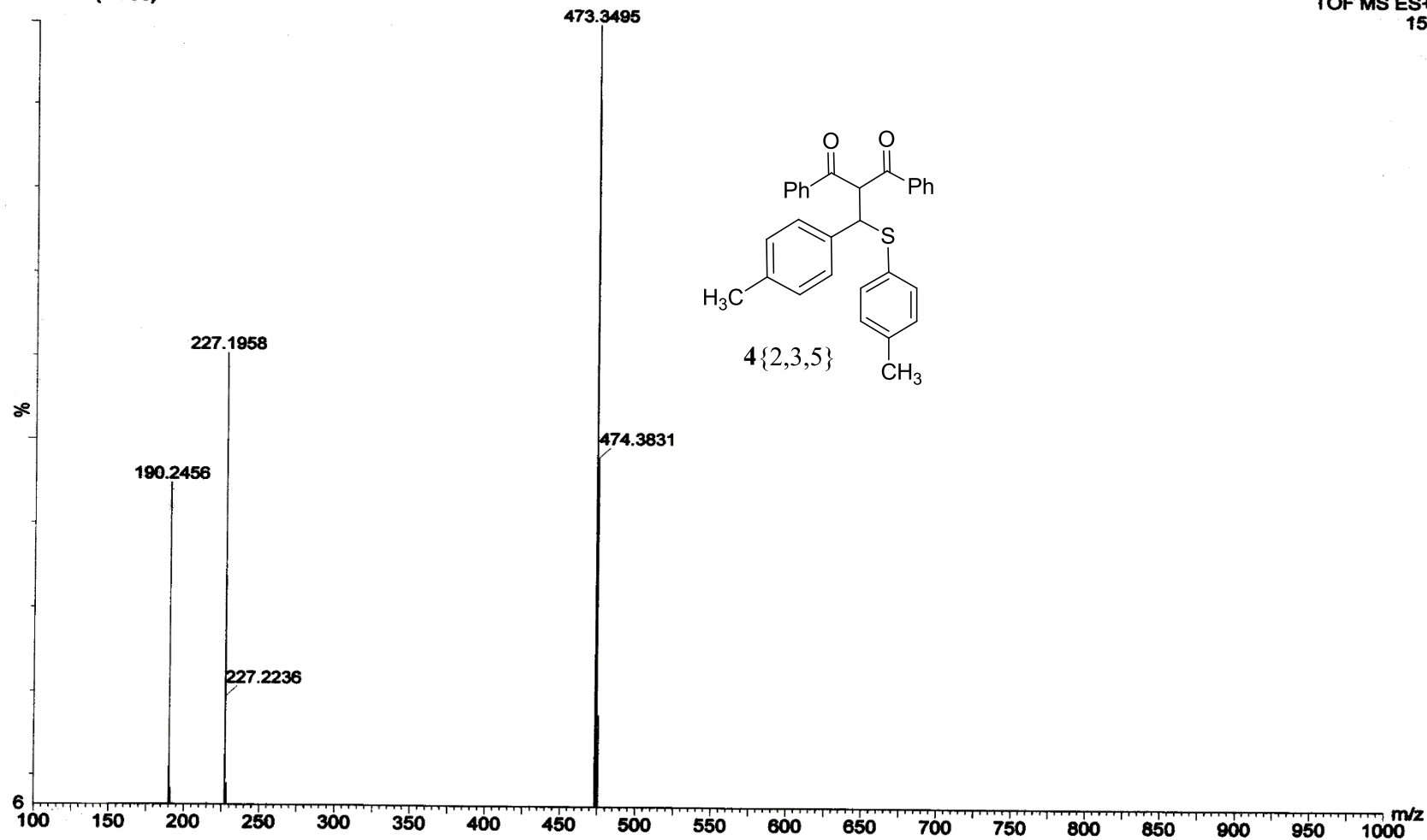






AD-122 38 (0.700)

TOF MS ES+
154



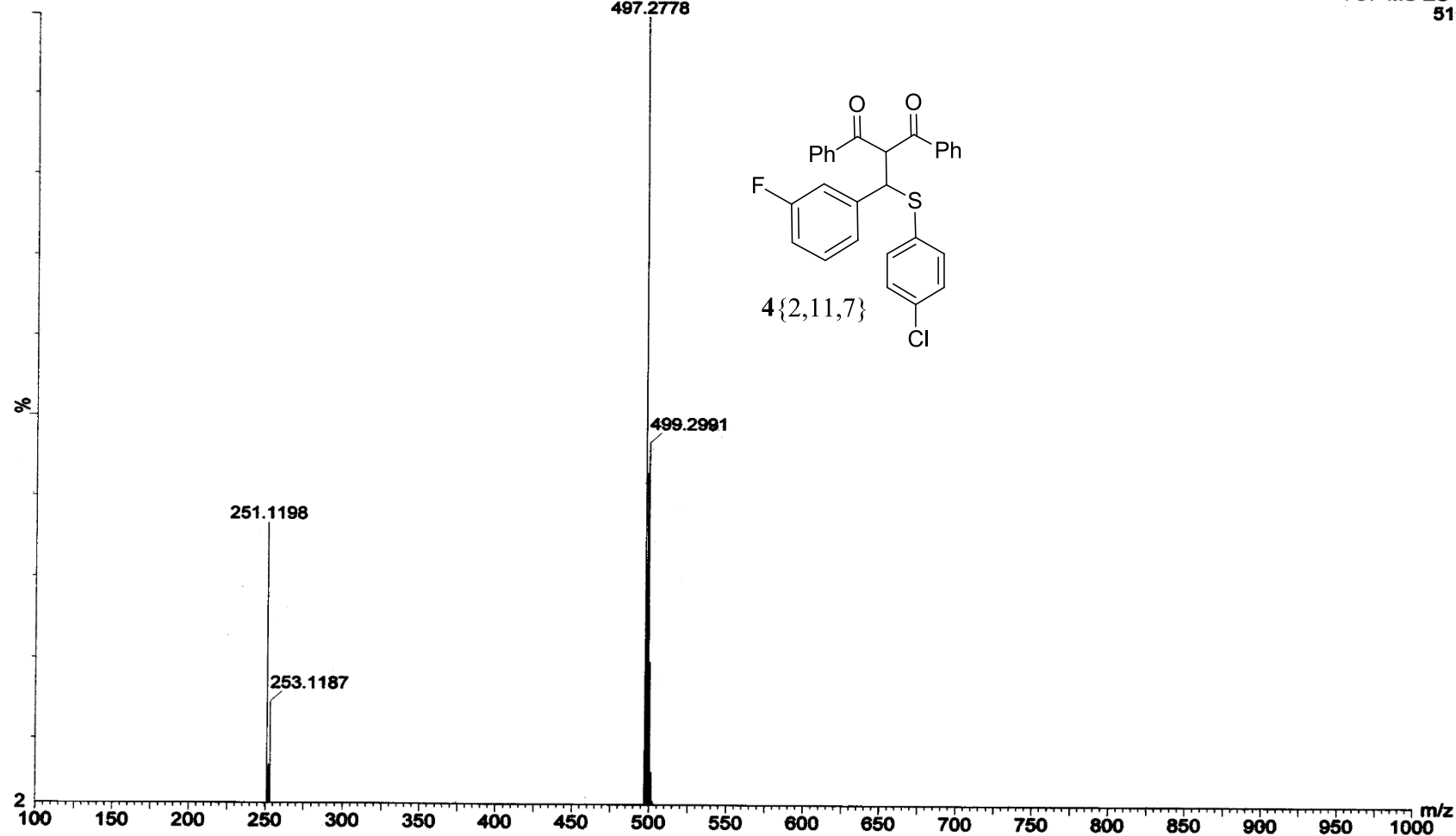
AD-118 32 (0.590)

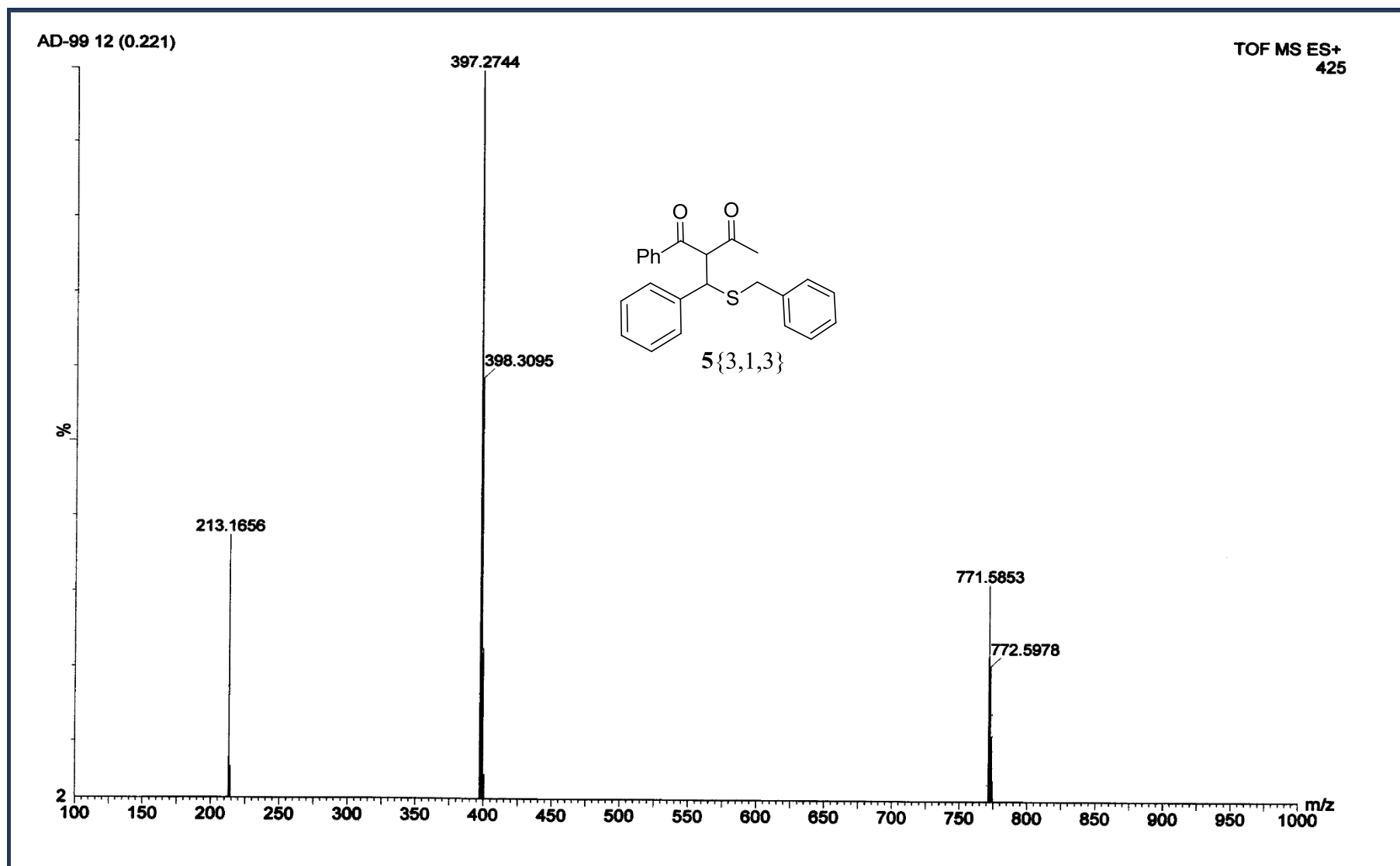
TOF MS ES+
176



AD-117 42 (0.774)

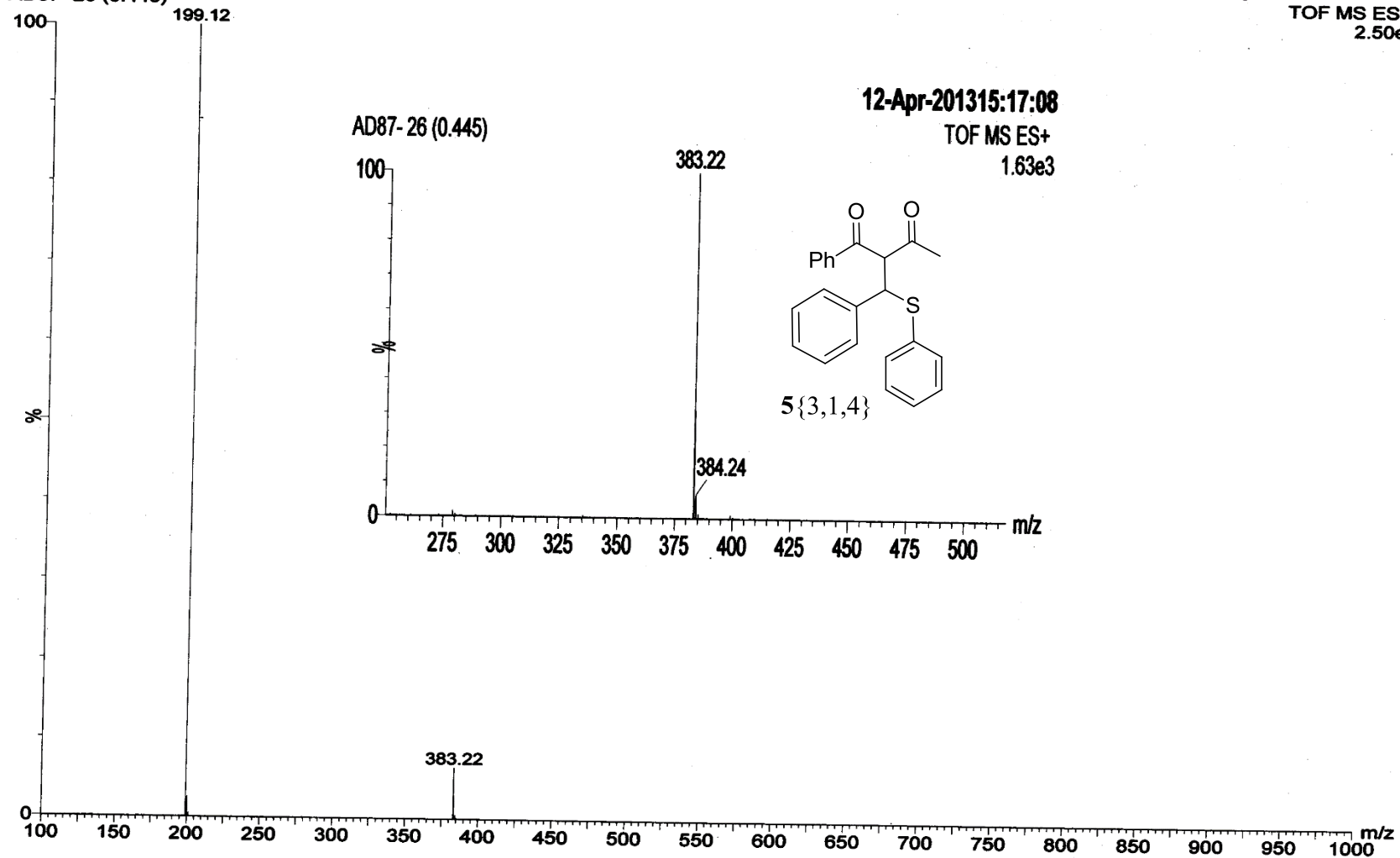
TOF MS ES+
515





AD87- 26 (0.445)

199.12



12-Apr-2013 15:17:08

TOF MS ES+
2.50e4

12-Apr-2013 15:17:08

TOF MS ES+
1.63e3

AD87- 26 (0.445)

100

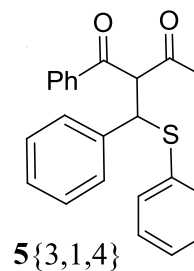
383.22

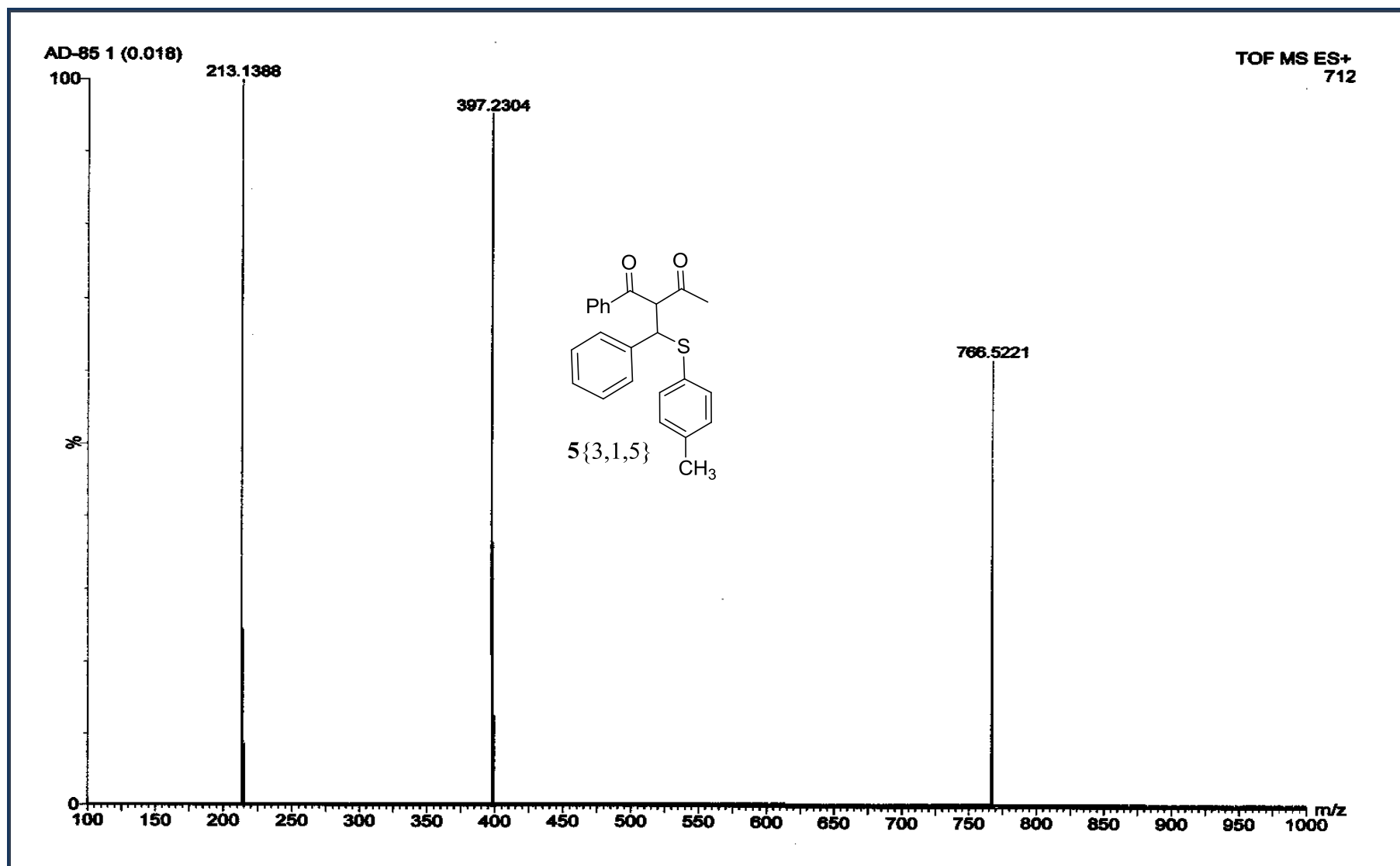
%

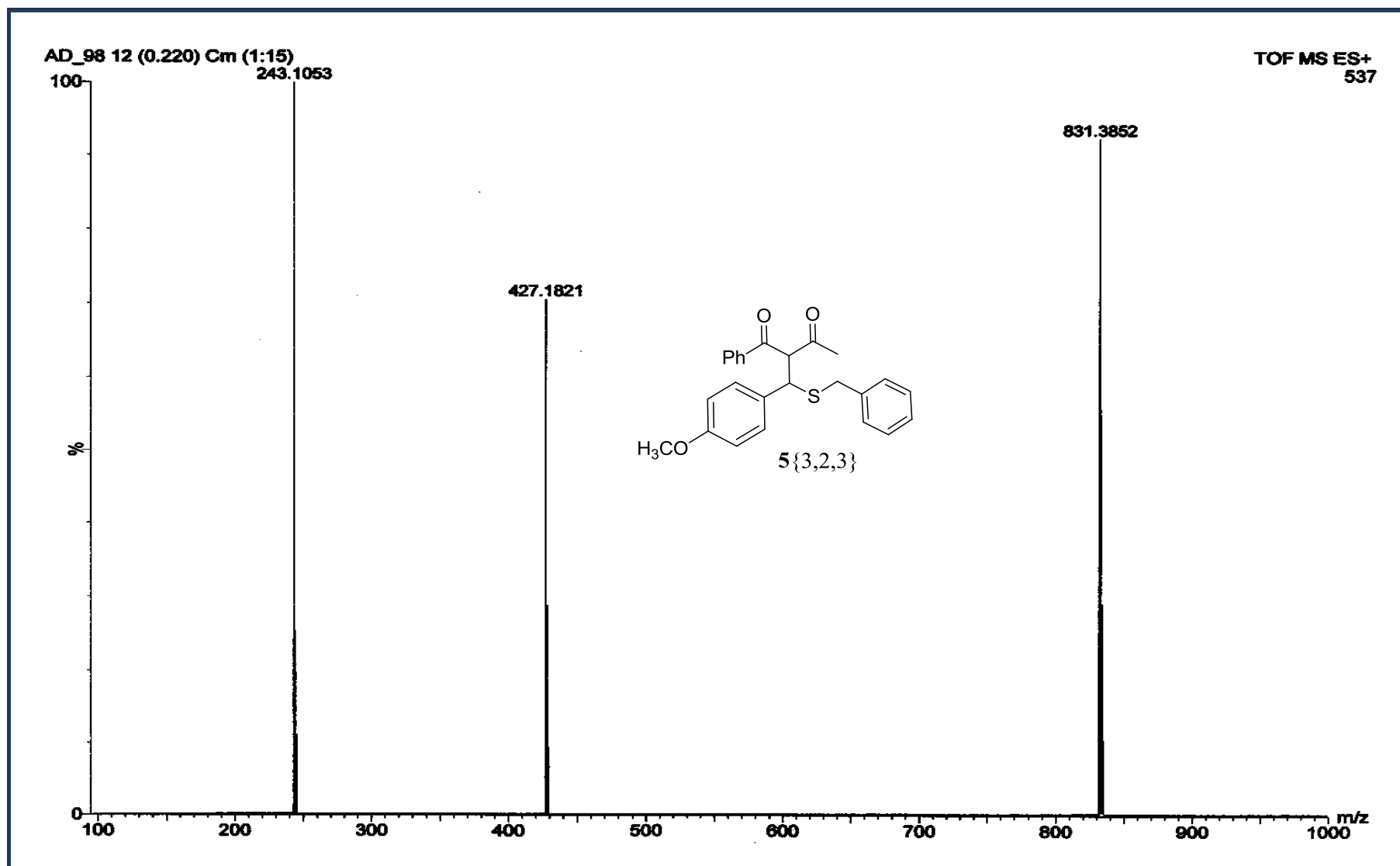
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0

275 300 325 350 375 400 425 450 475 500 m/z

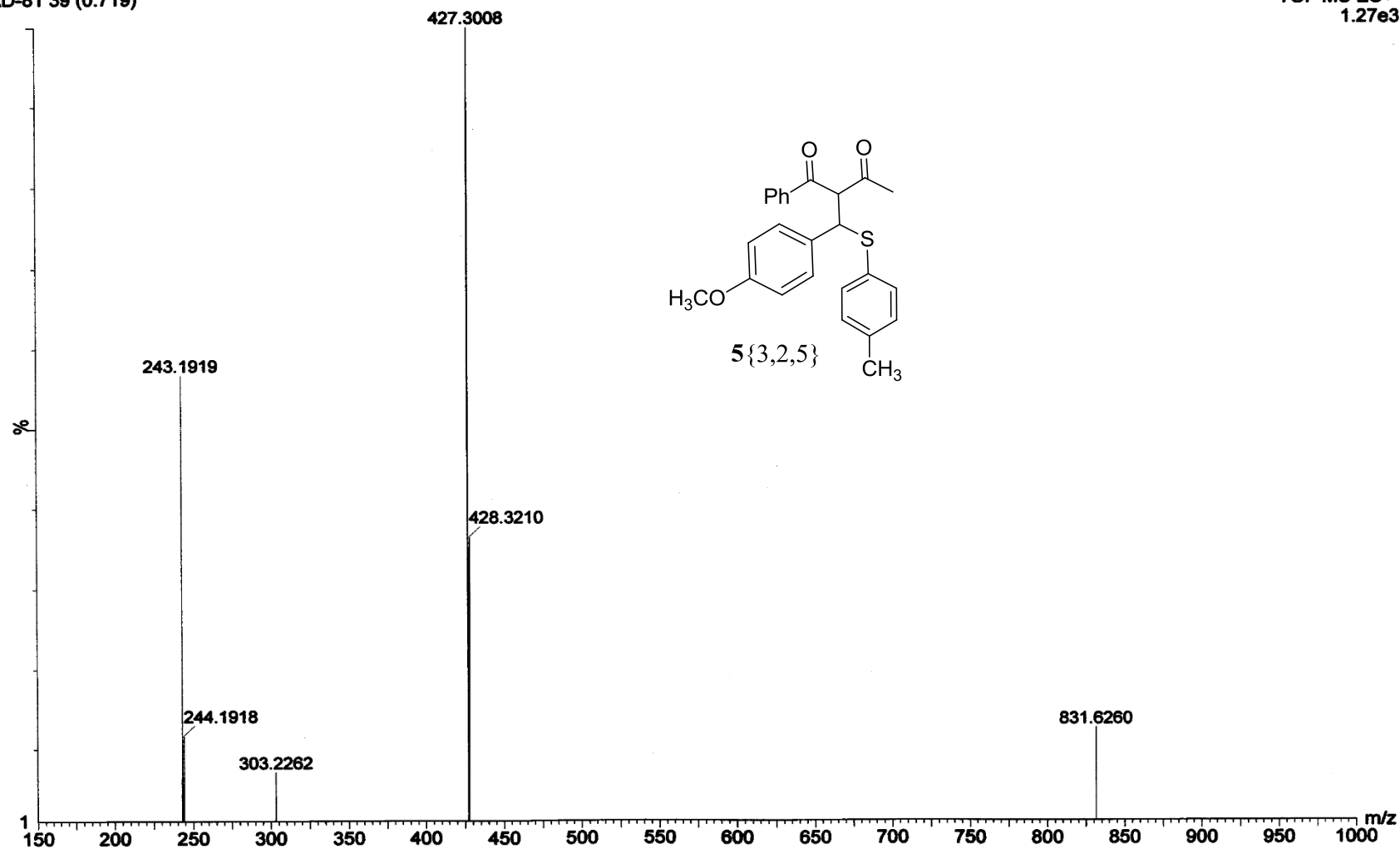






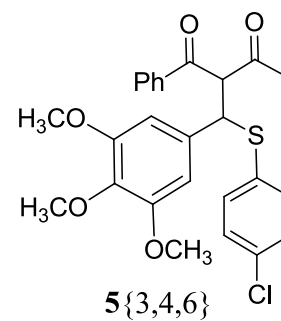
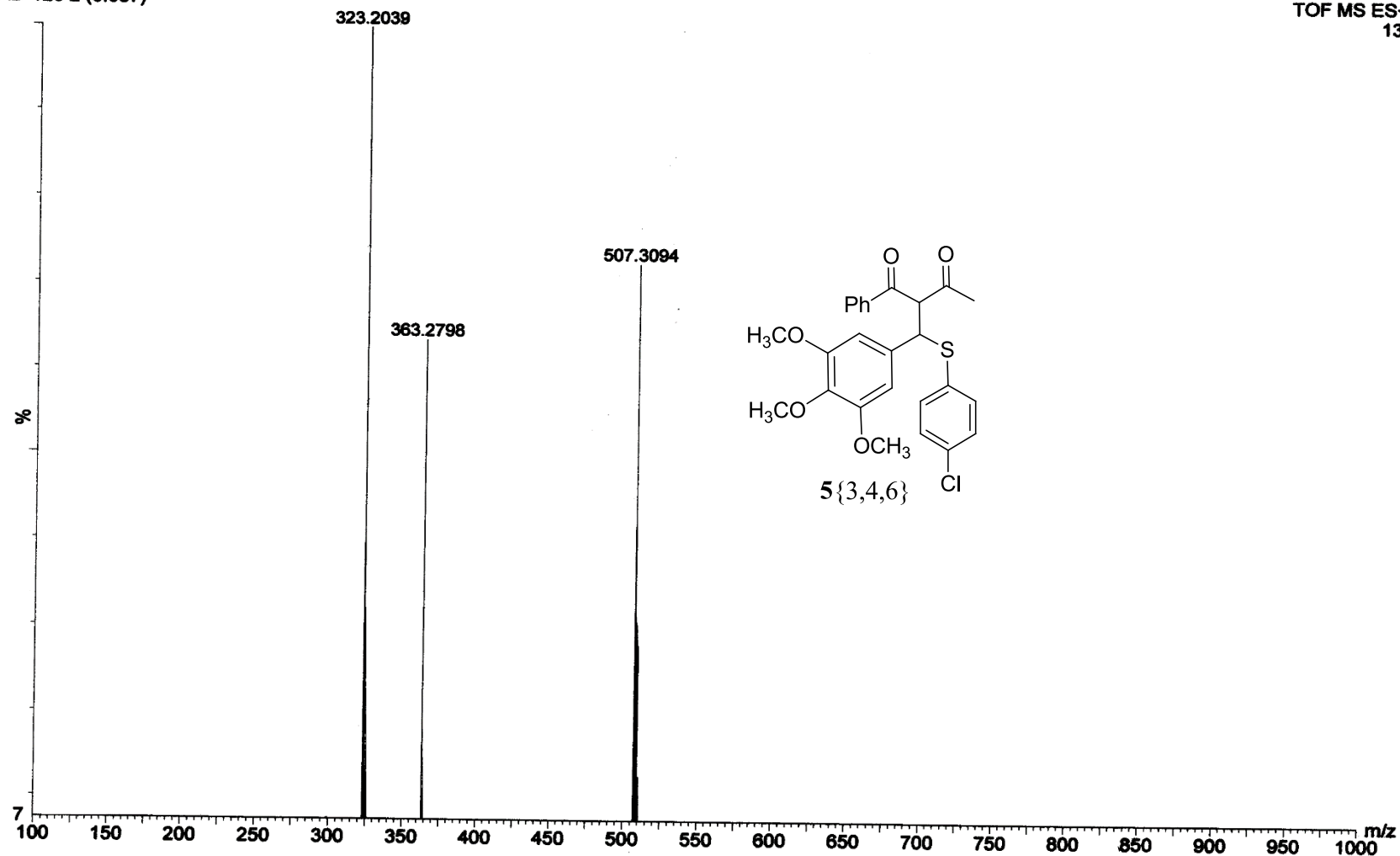
AD-81 39 (0.719)

TOF MS ES+
1.27e3



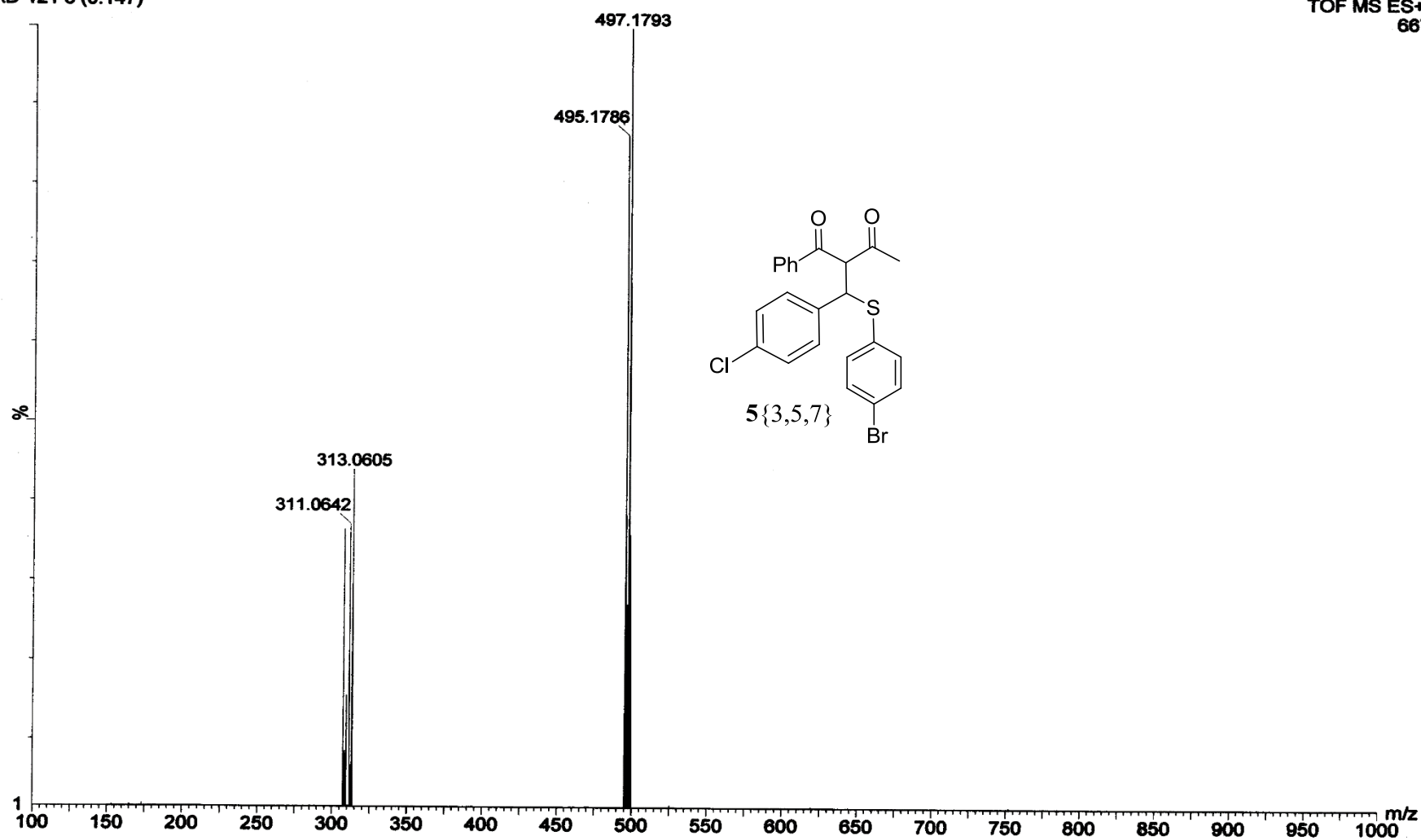
AD-120 2 (0.037)

TOF MS ES+
134



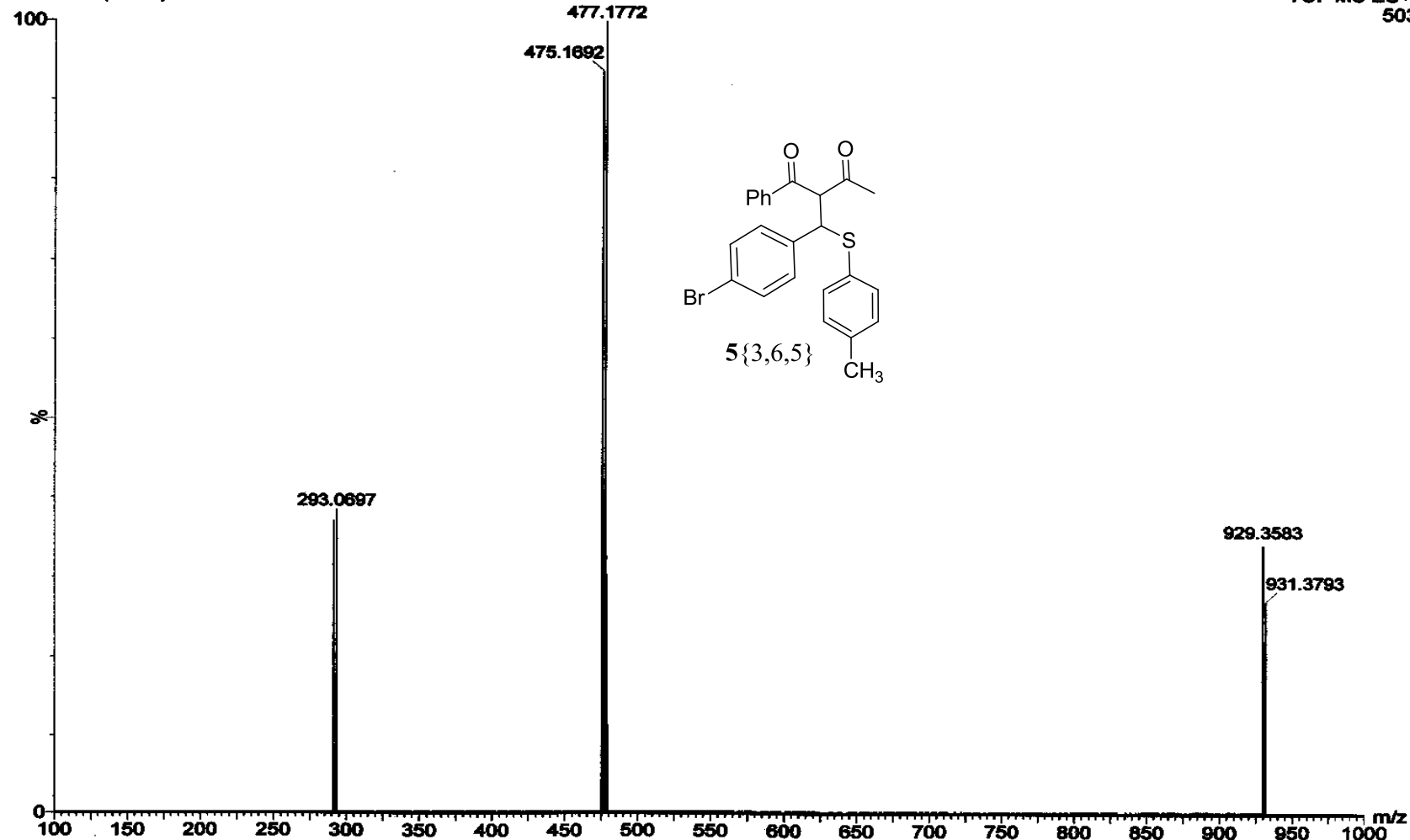
AD-121 8 (0.147)

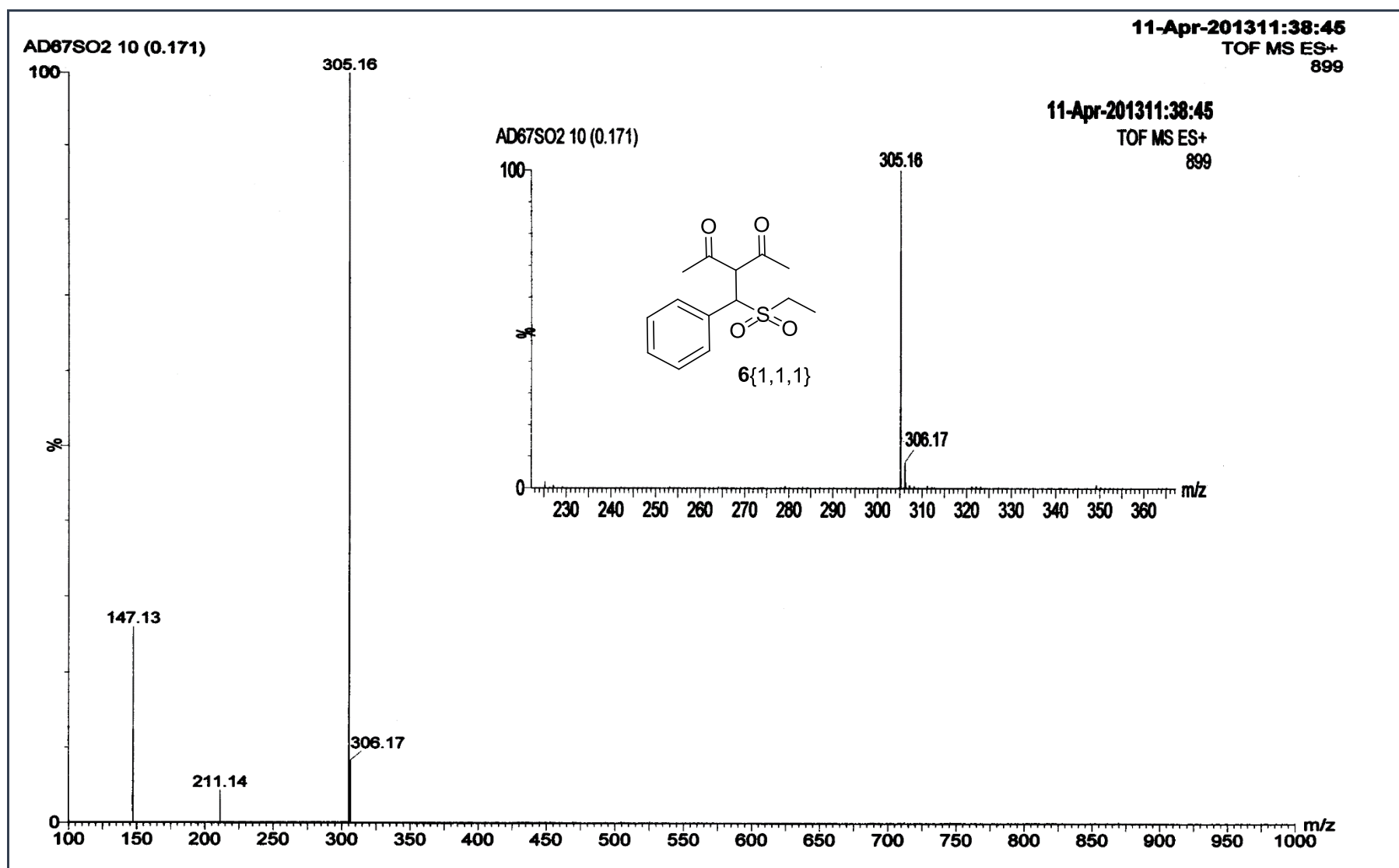
TOF MS ES+
667

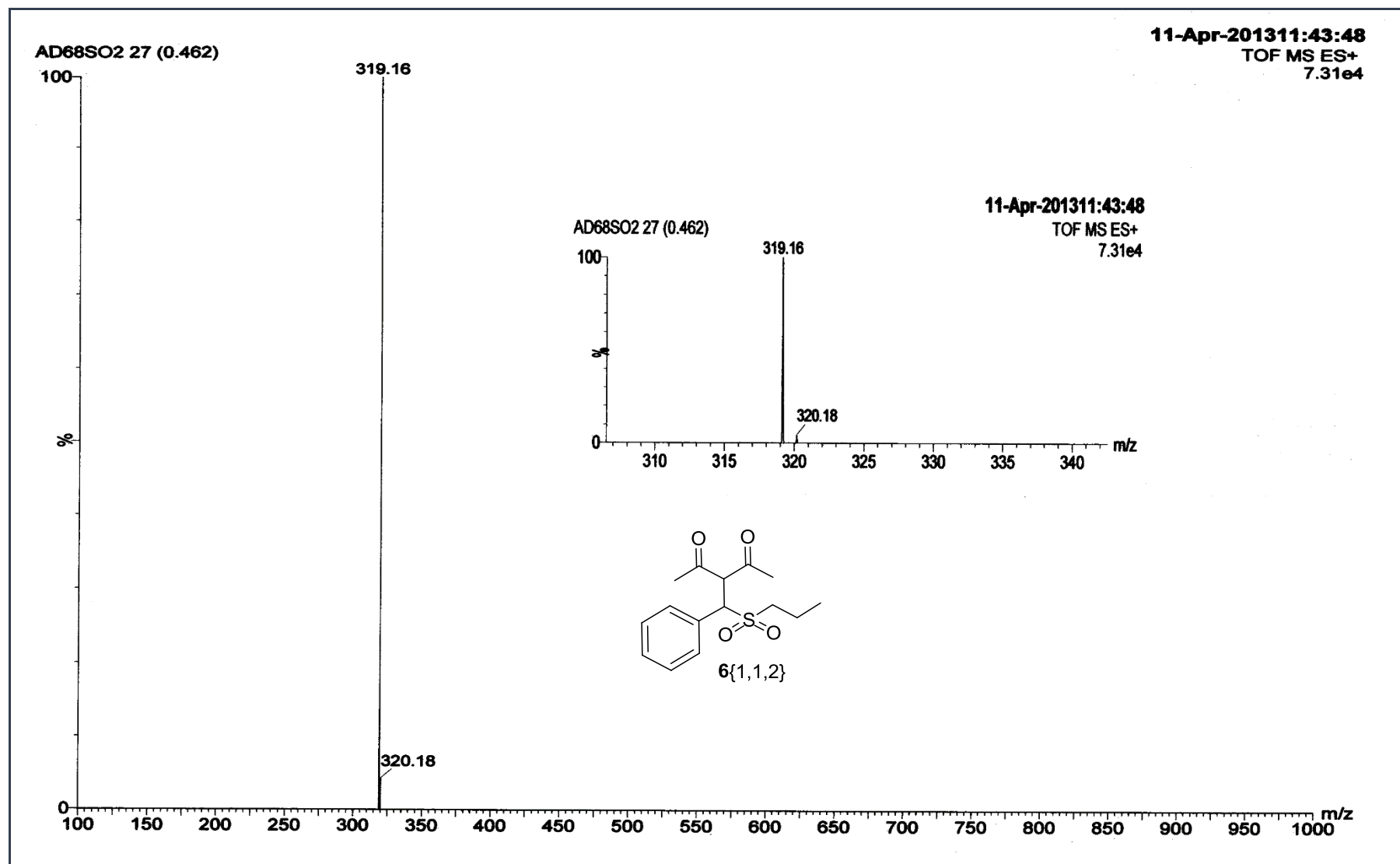


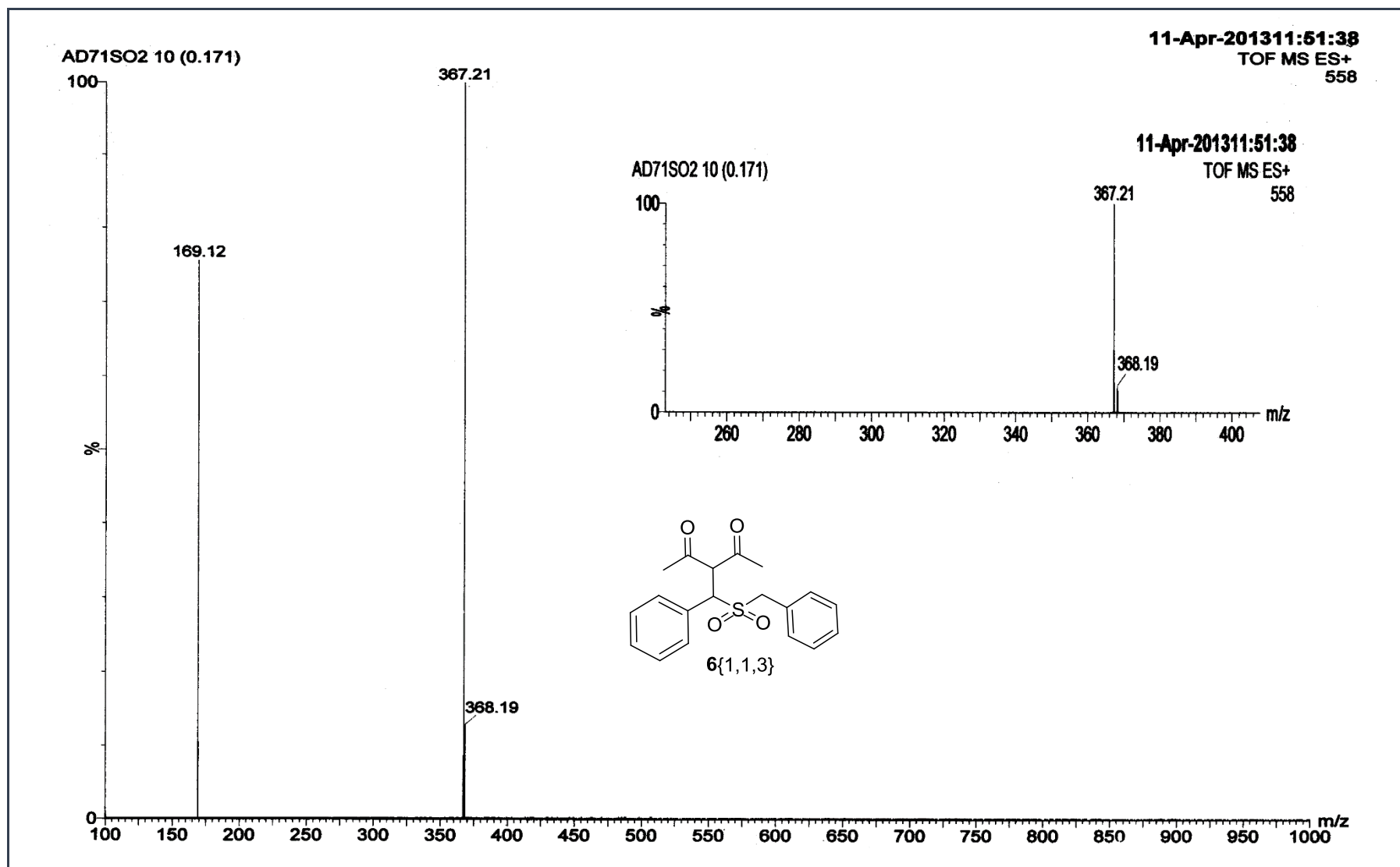
AD-96 14 (0.258)

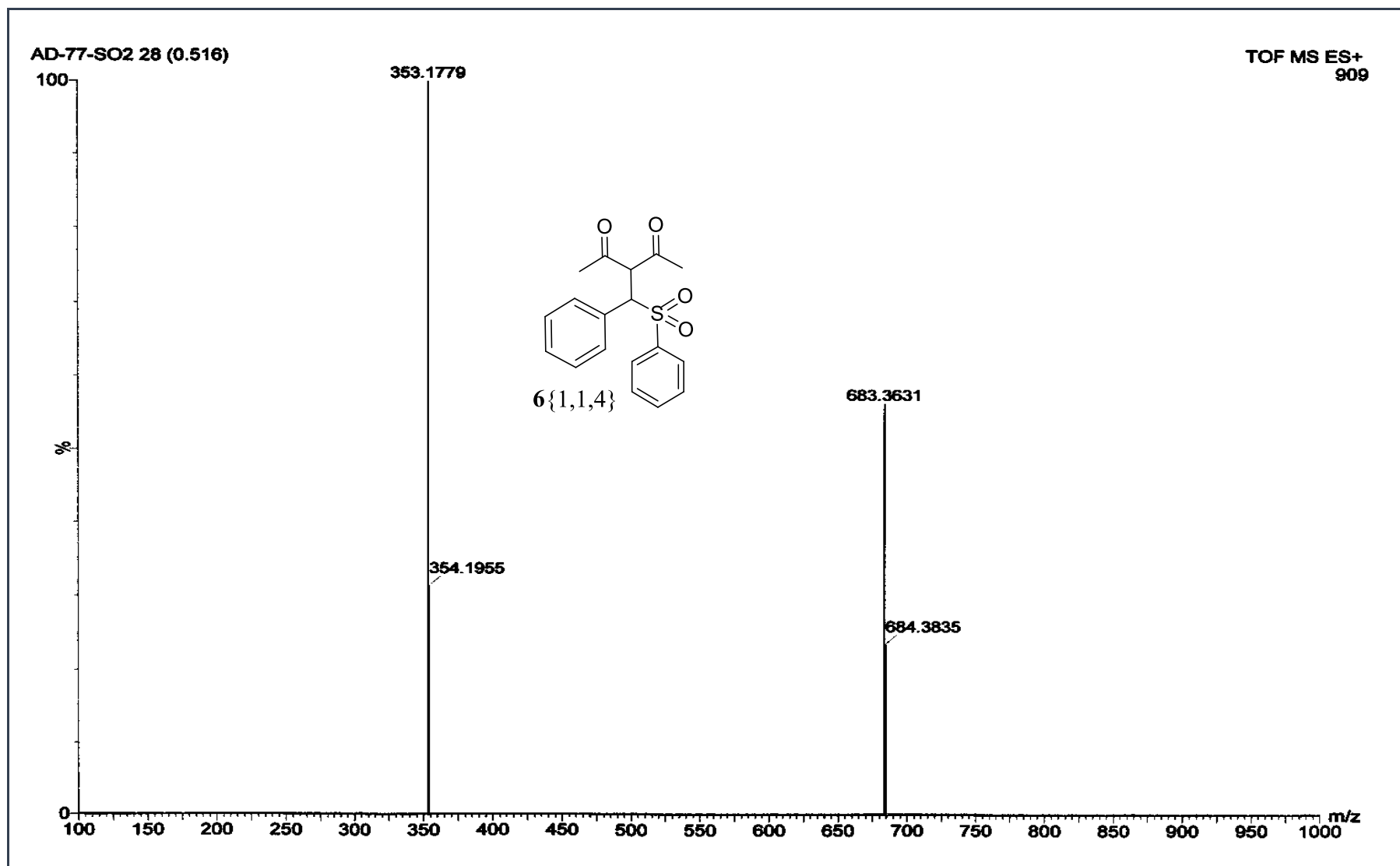
TOF MS ES+
503

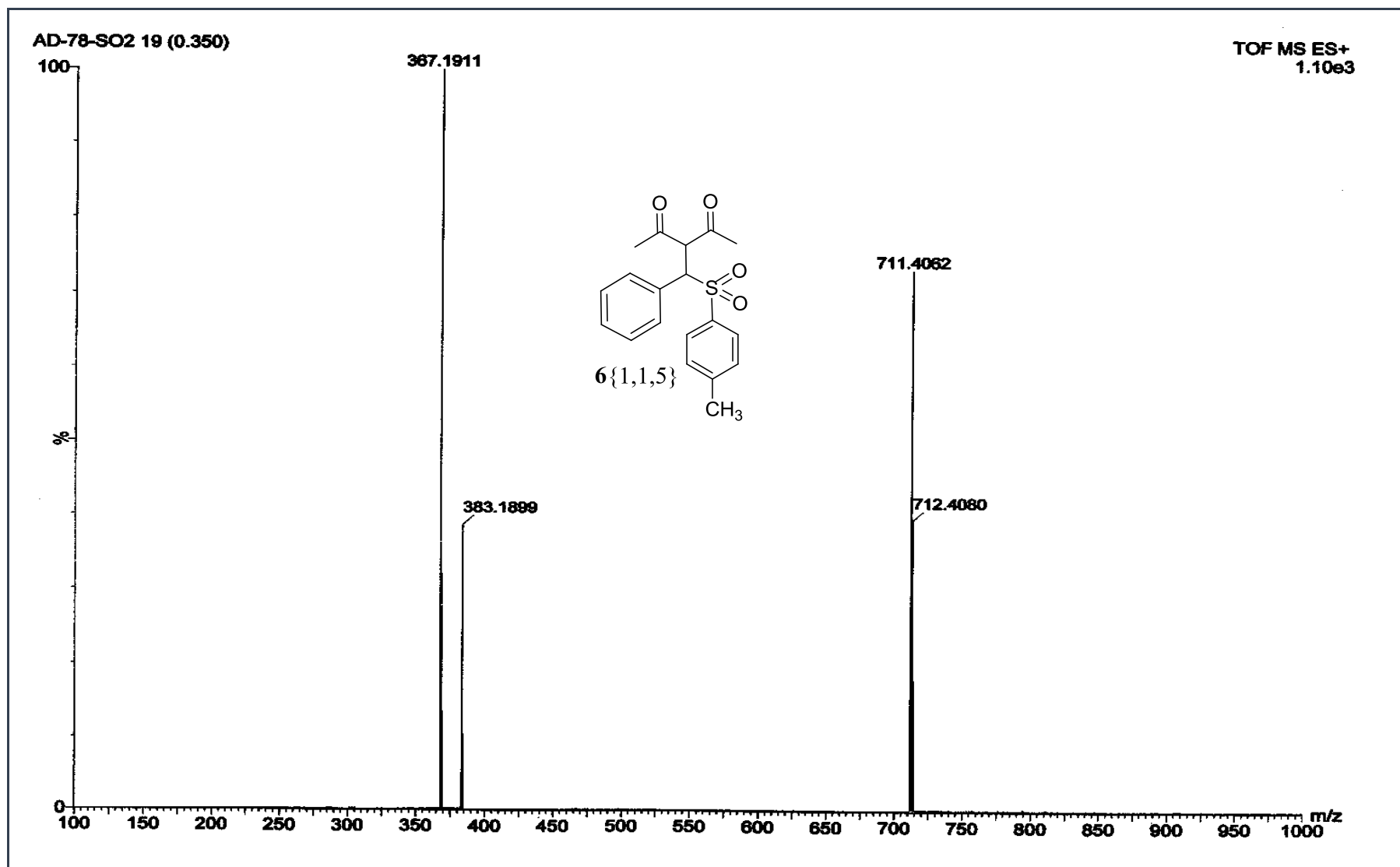


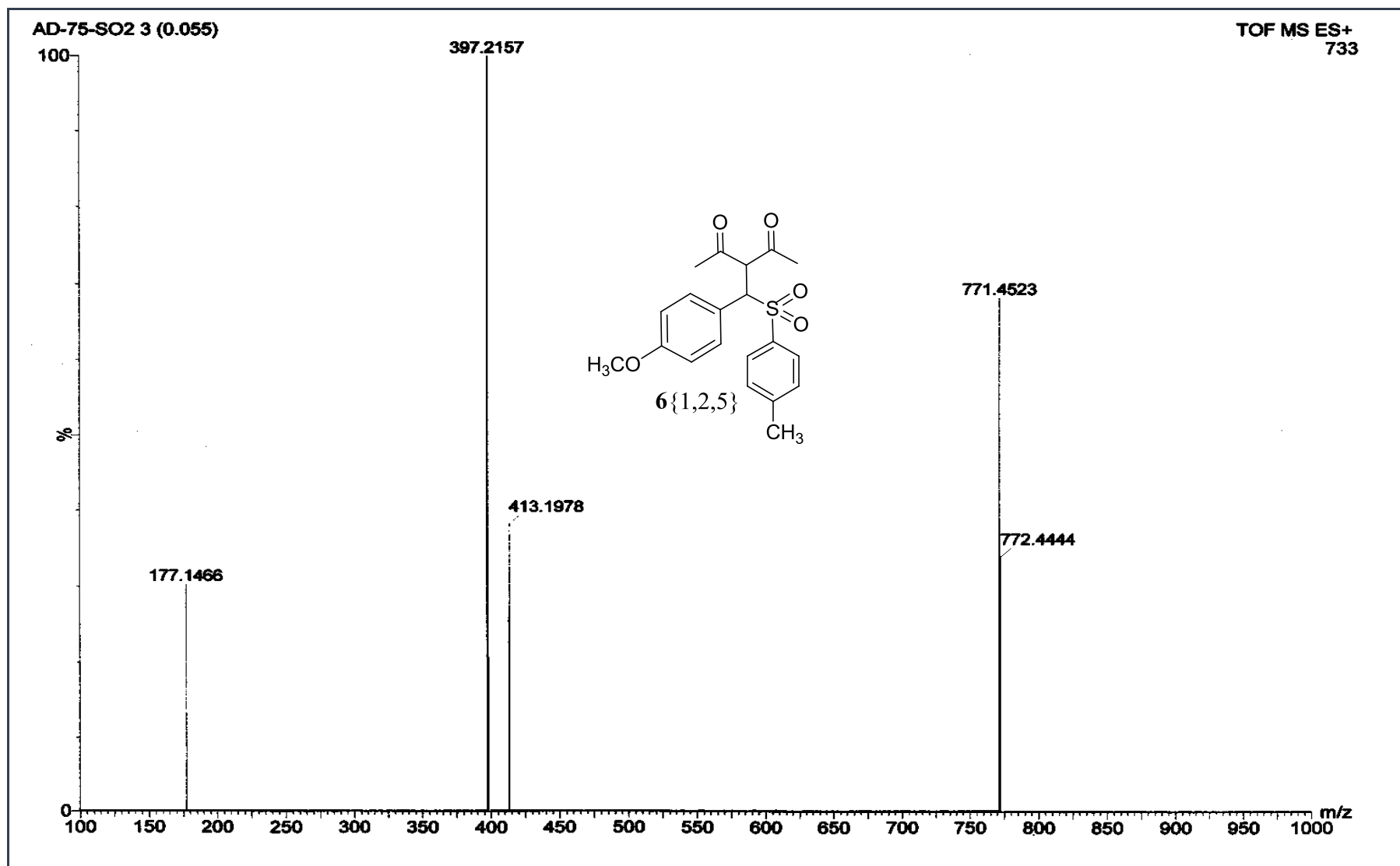


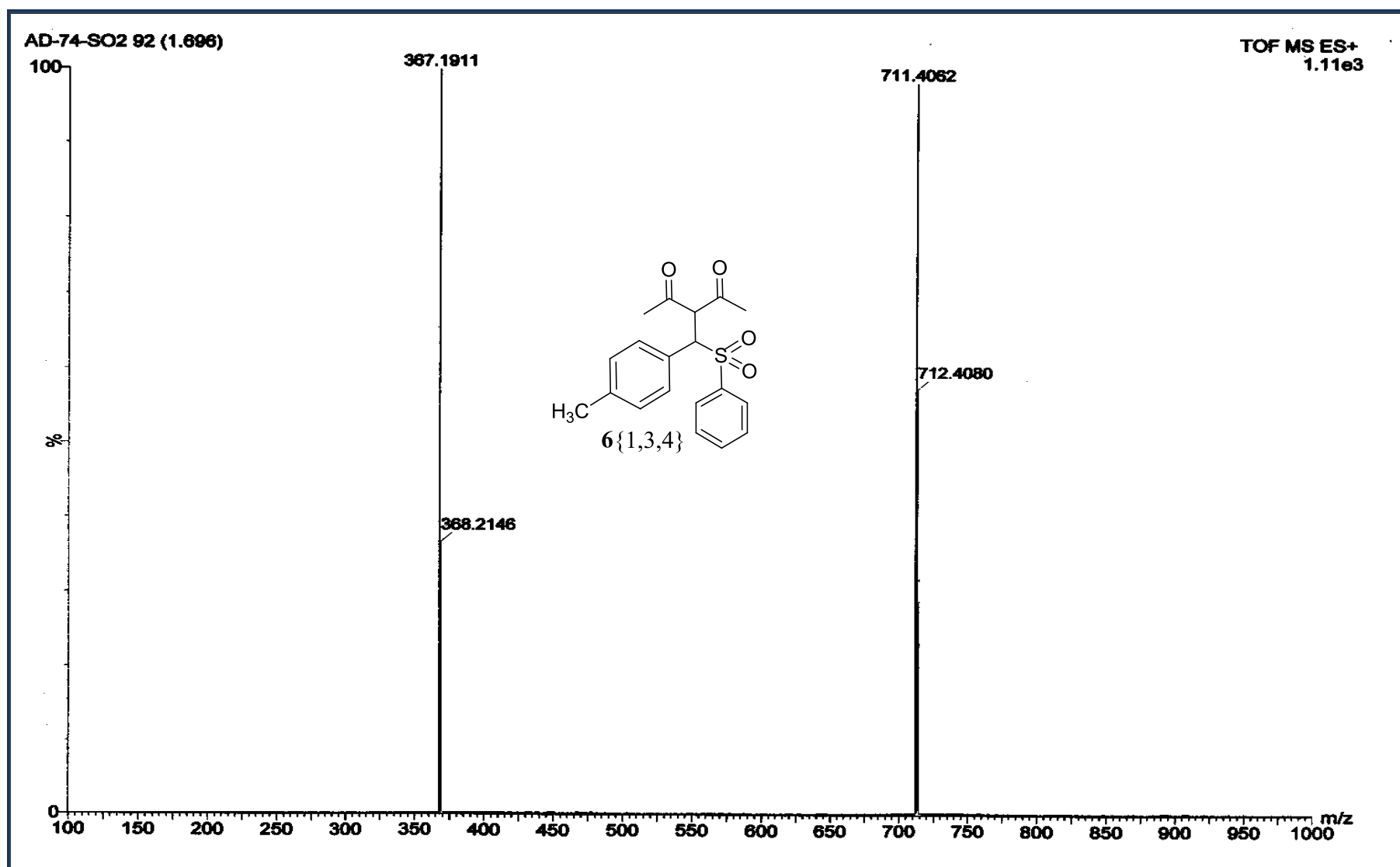


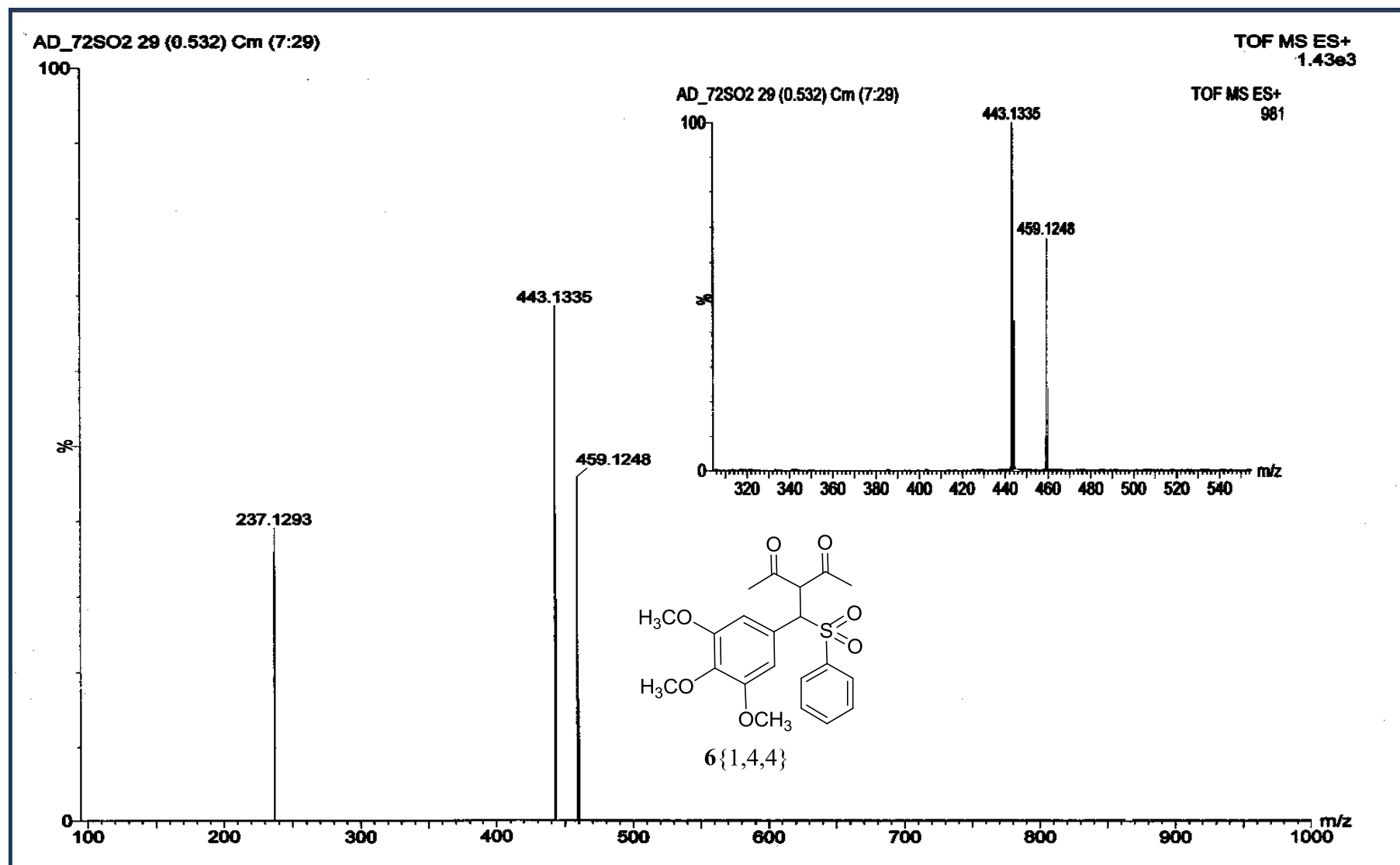


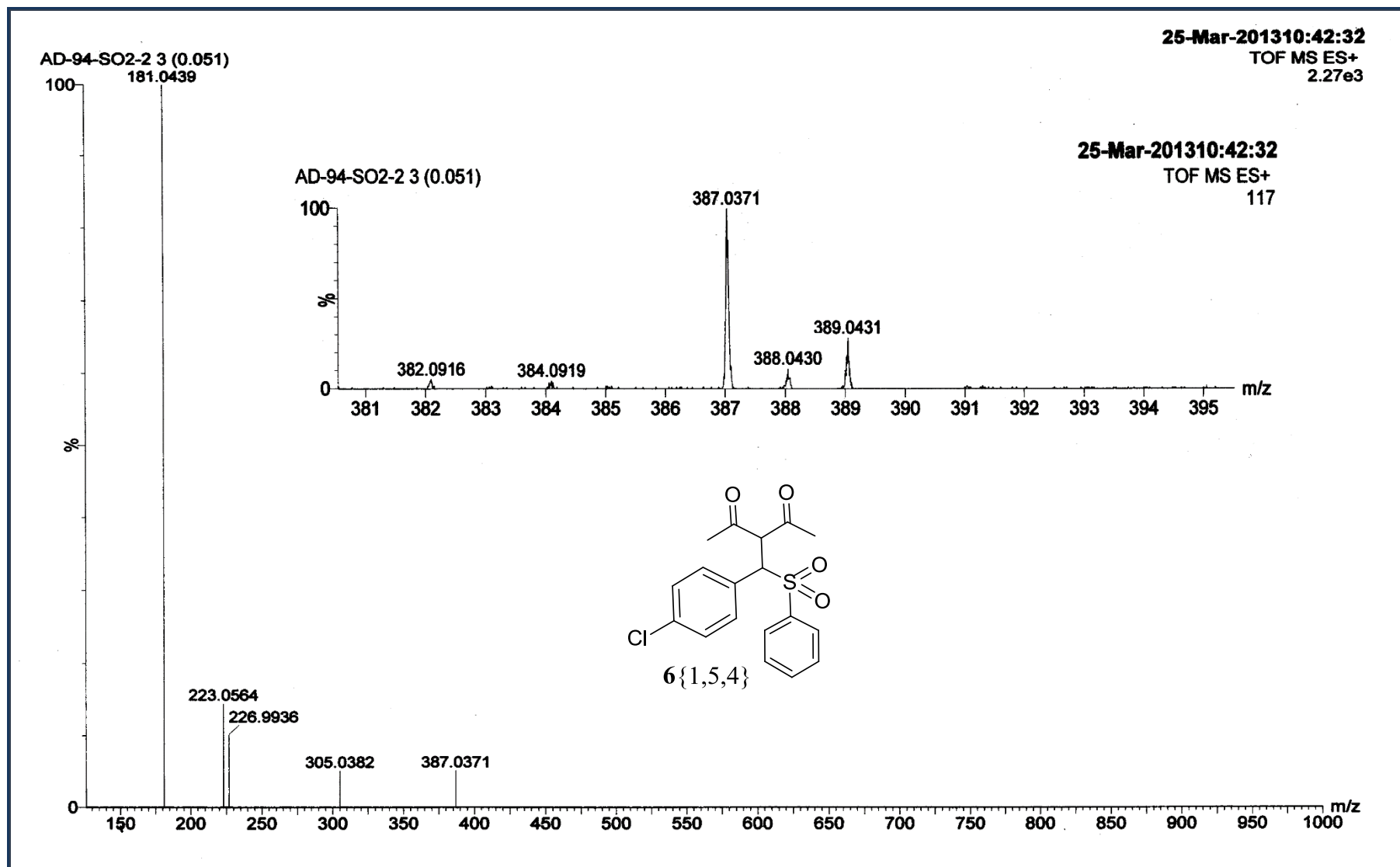


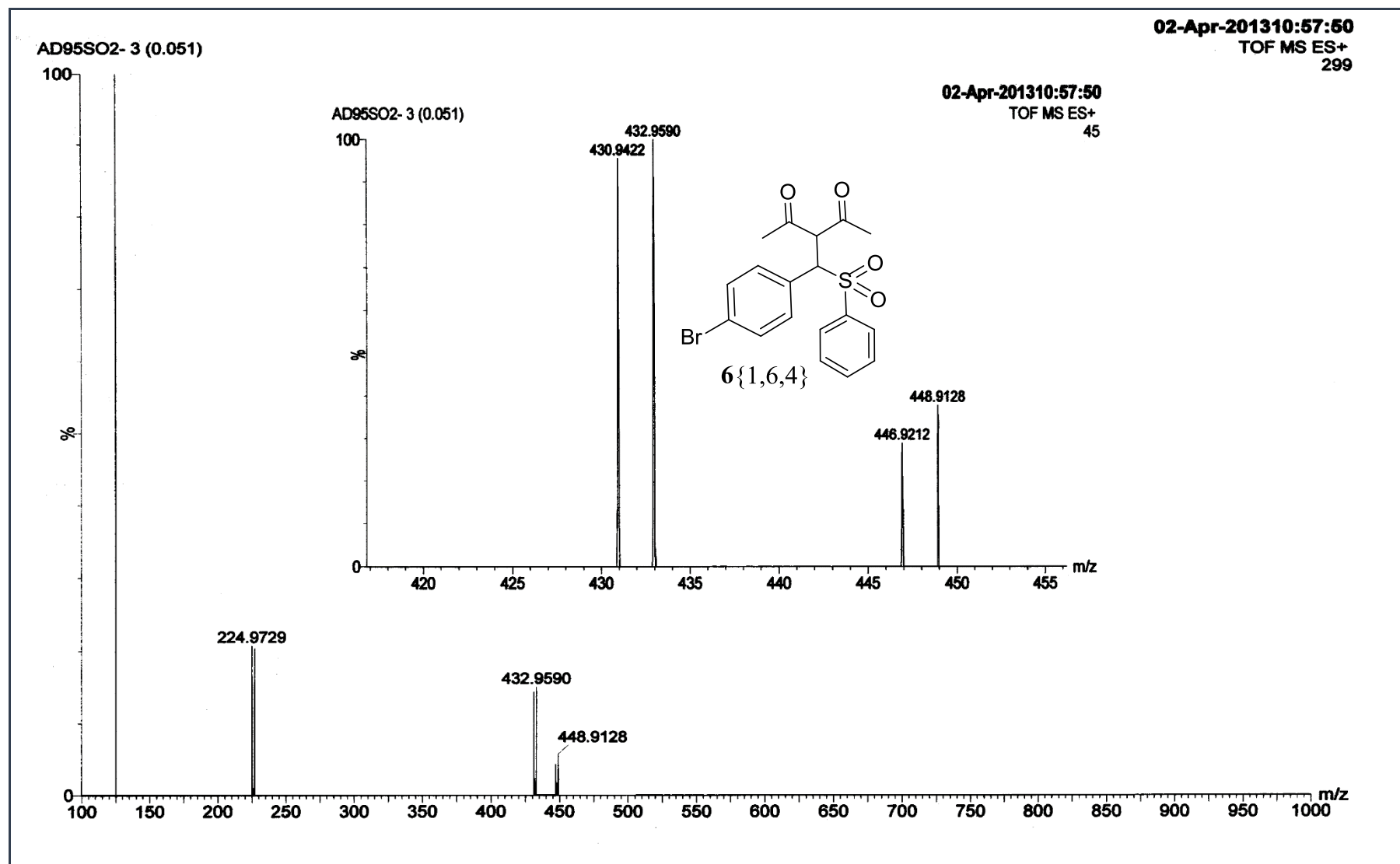












AD-73-SO2 78 (1.457)

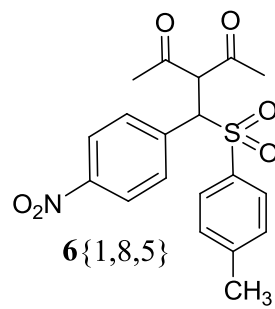
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100

407.2409

796.4552

%



797.4633

408.2666

0

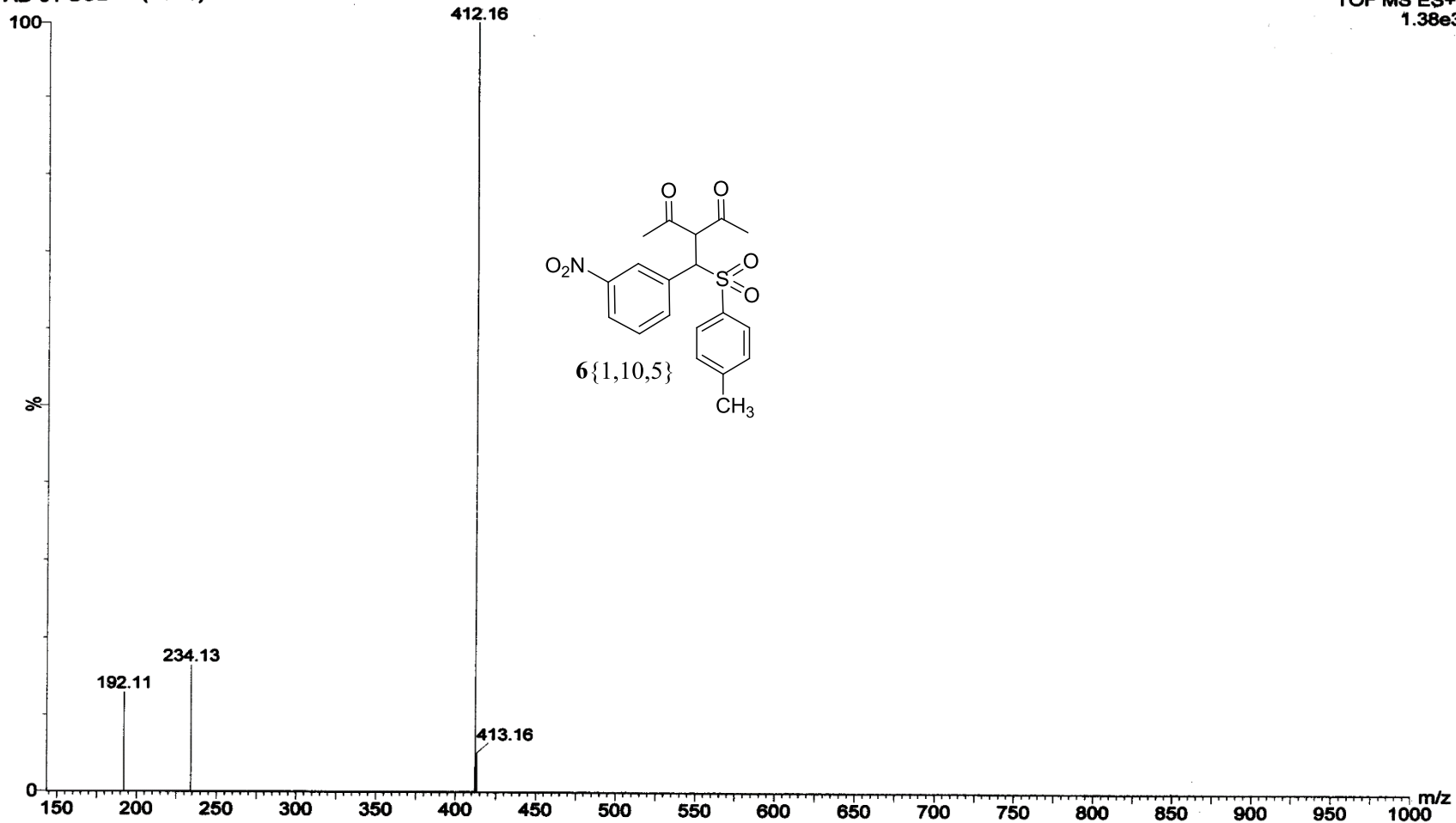
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AD-91-SO2 22 (0.376)

22-Mar-2013 17:31:32

TOF MS ES+

1.38e3



02-Apr-2013 11:53
TOF MS ES+
742

AD_80SO2 6 (0.103)

100

%

AD_80SO2 6 (0.103)

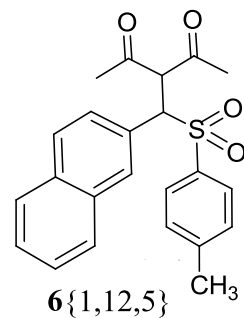
100

%

412.1364

417.1213

418.1203



m/z

144.9967

417.1213

m/z

AD-93-SO2 3 (0.051)

100
197.08

175.02

%

0

150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 m/z

AD-93-SO2 3 (0.051)

100

%

0

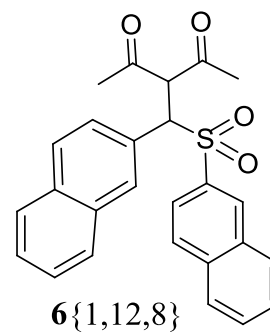
435 440 445 450 455 460 465 470 475 480 485 490 495 m/z

453.09

454.11

469.06

470.07



6{1,12,8}

453.09

25-Mar-2013 10:33:52

TOF MS ES+

2.00e4

25-Mar-2013 10:33:52

TOF MS ES+

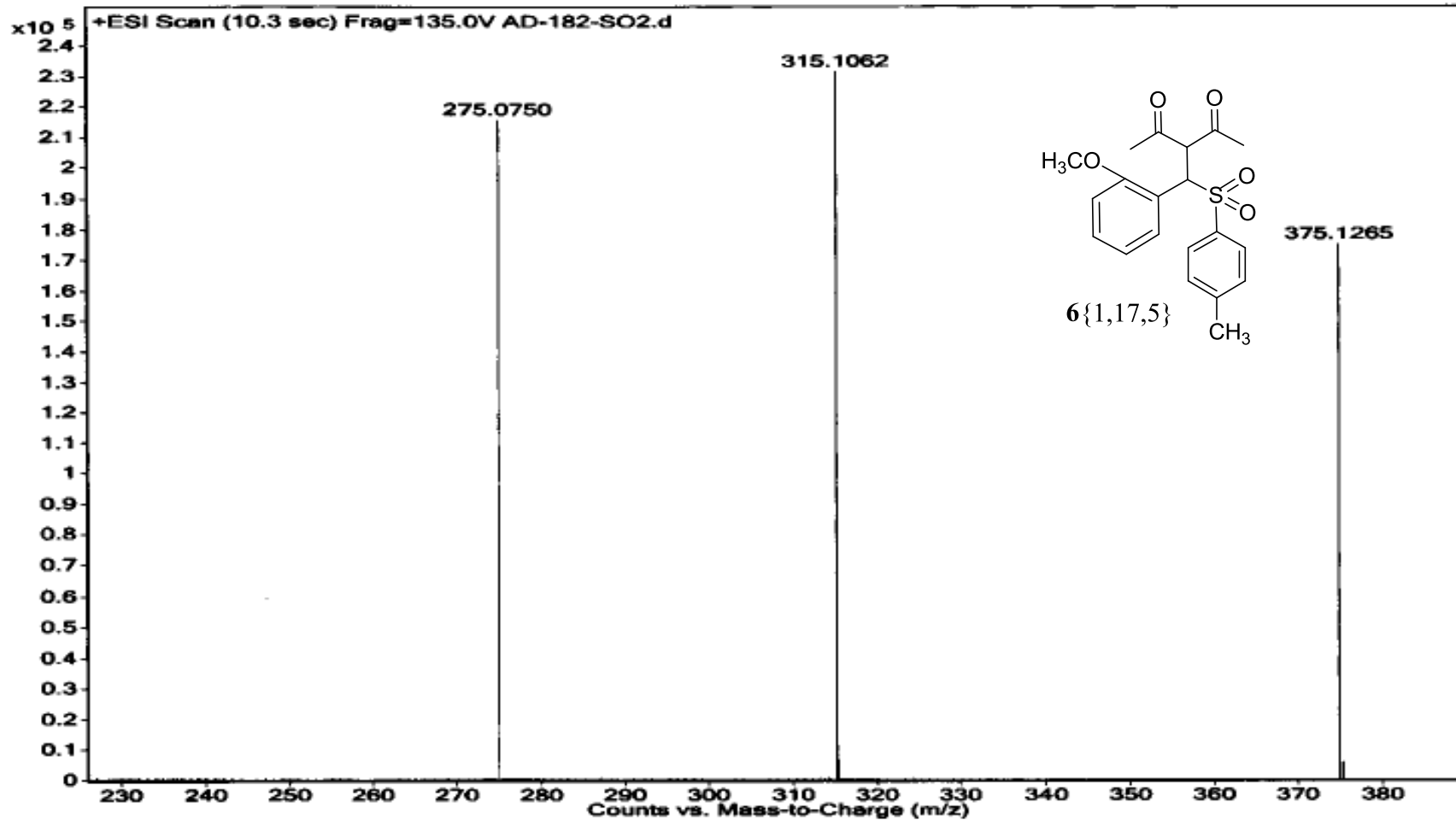
849

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time

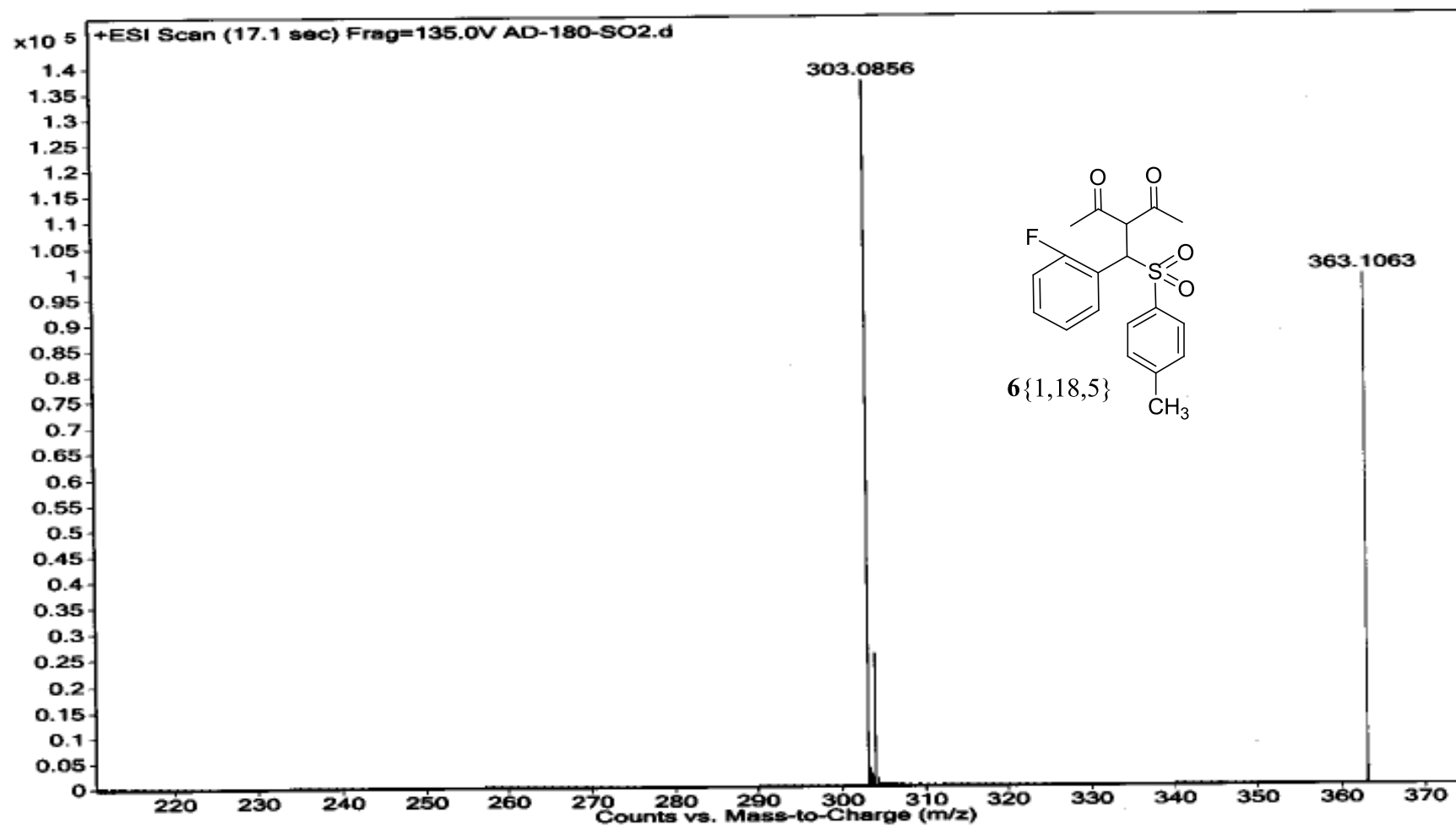


Sample Name
Inj Vol
Data Filename

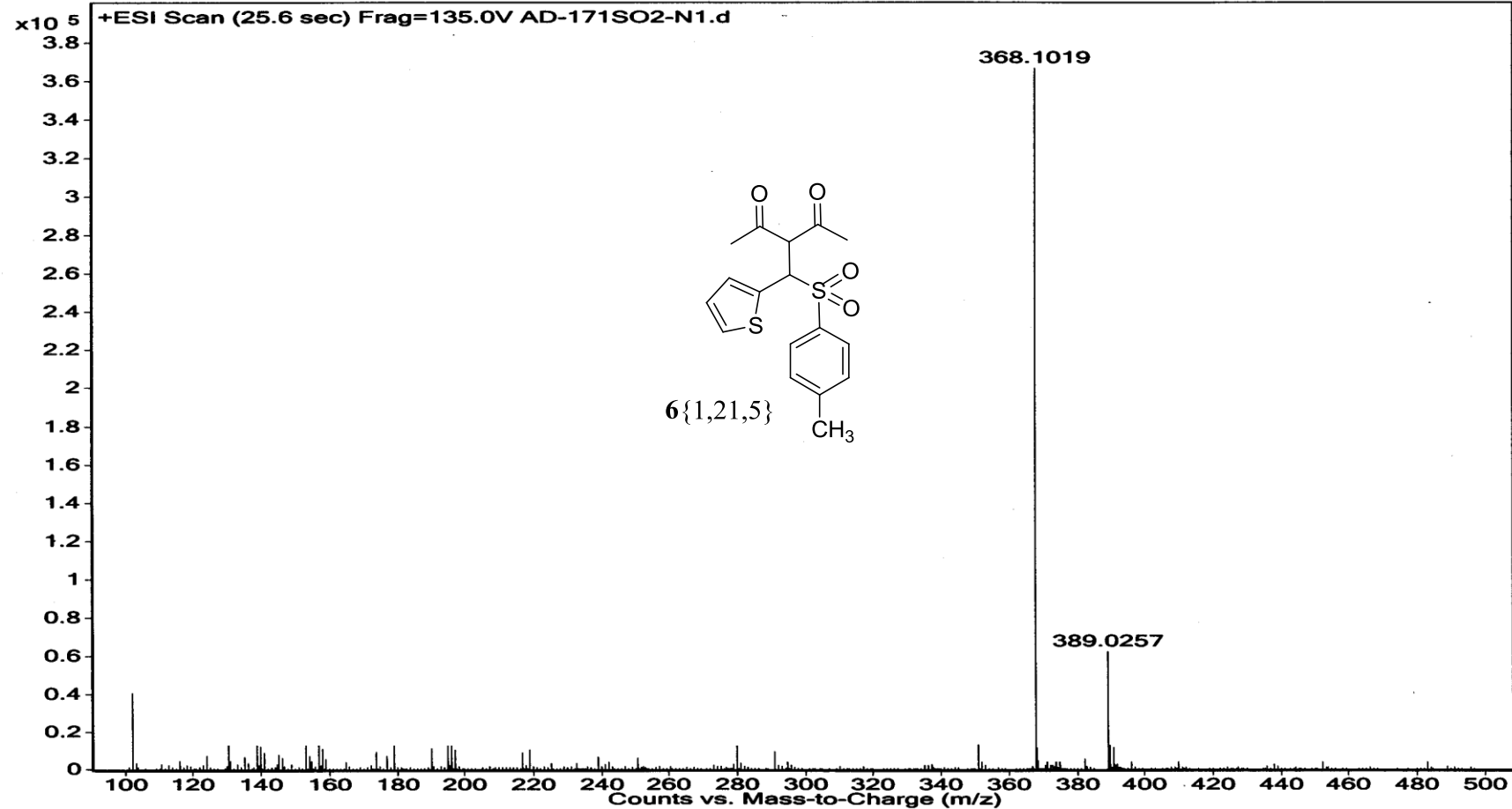
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
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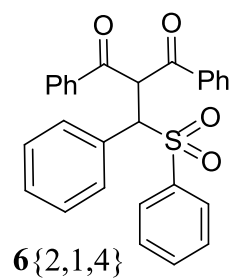
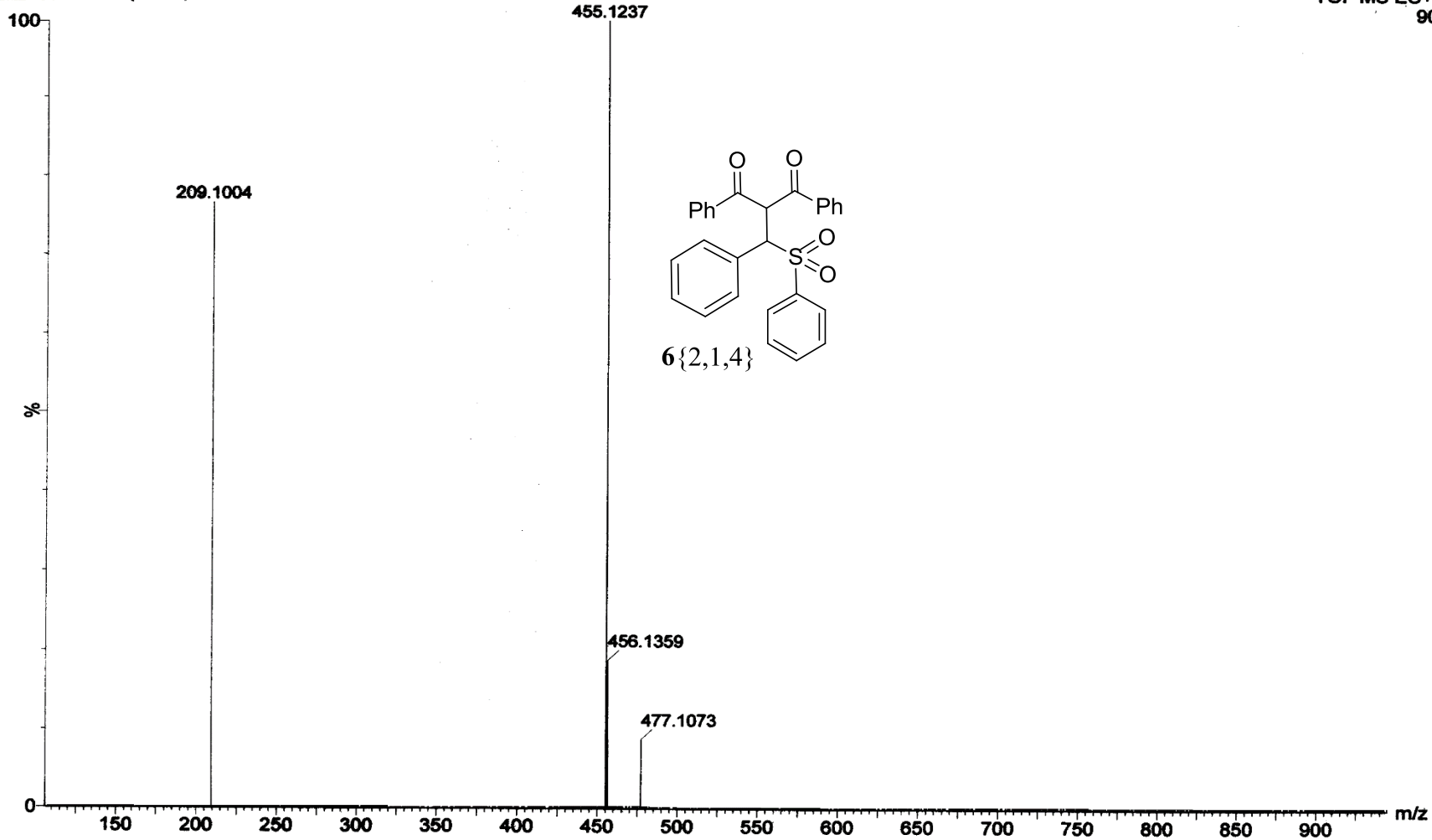


88-SO2 1 (0.017)

25-Mar-2013 10:52:06

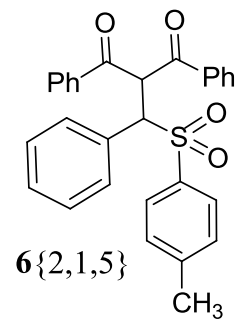
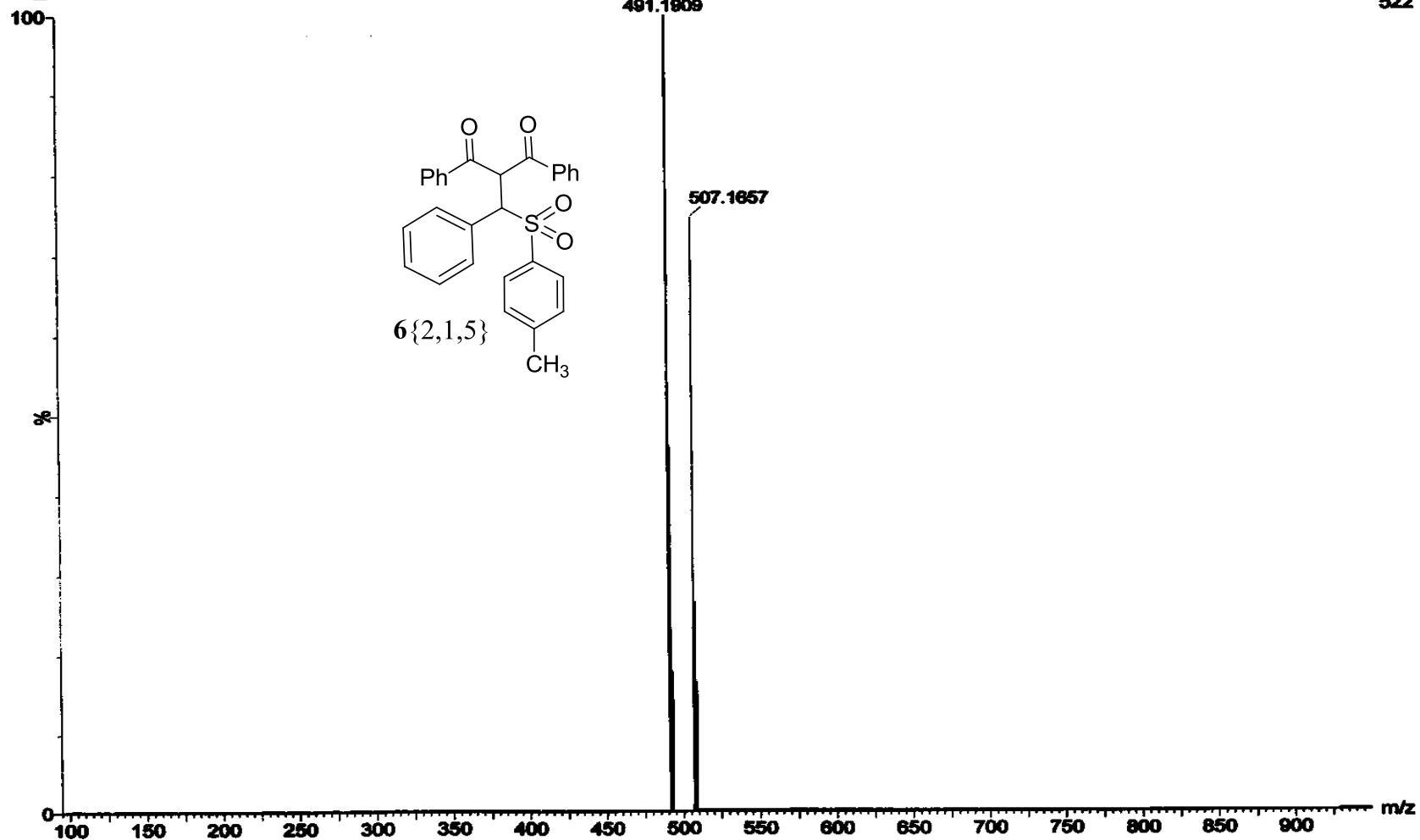
TOF MS ES+

90



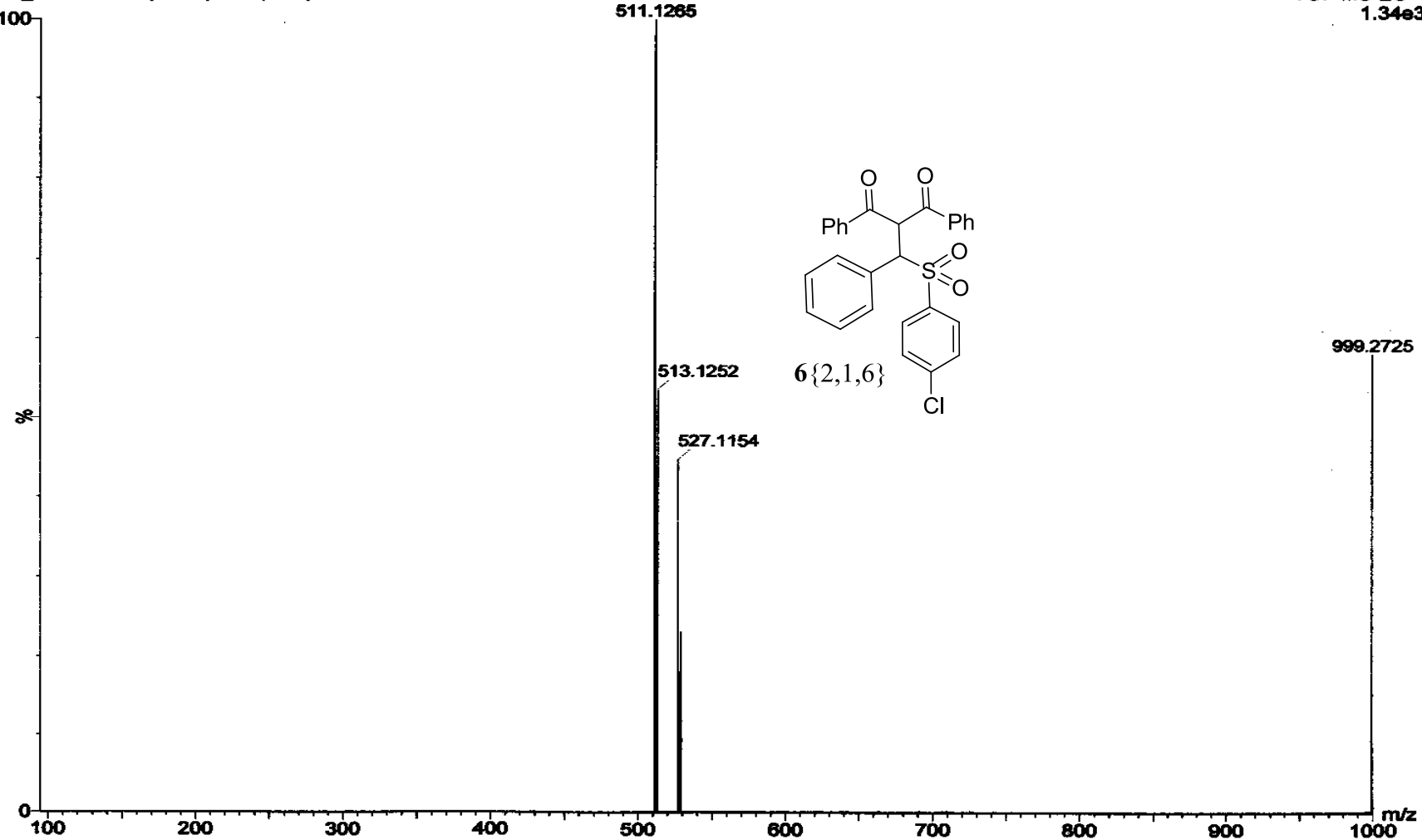
AD_97SO2 19 (0.348) Cm (4:23)

TOF MS ES+
522



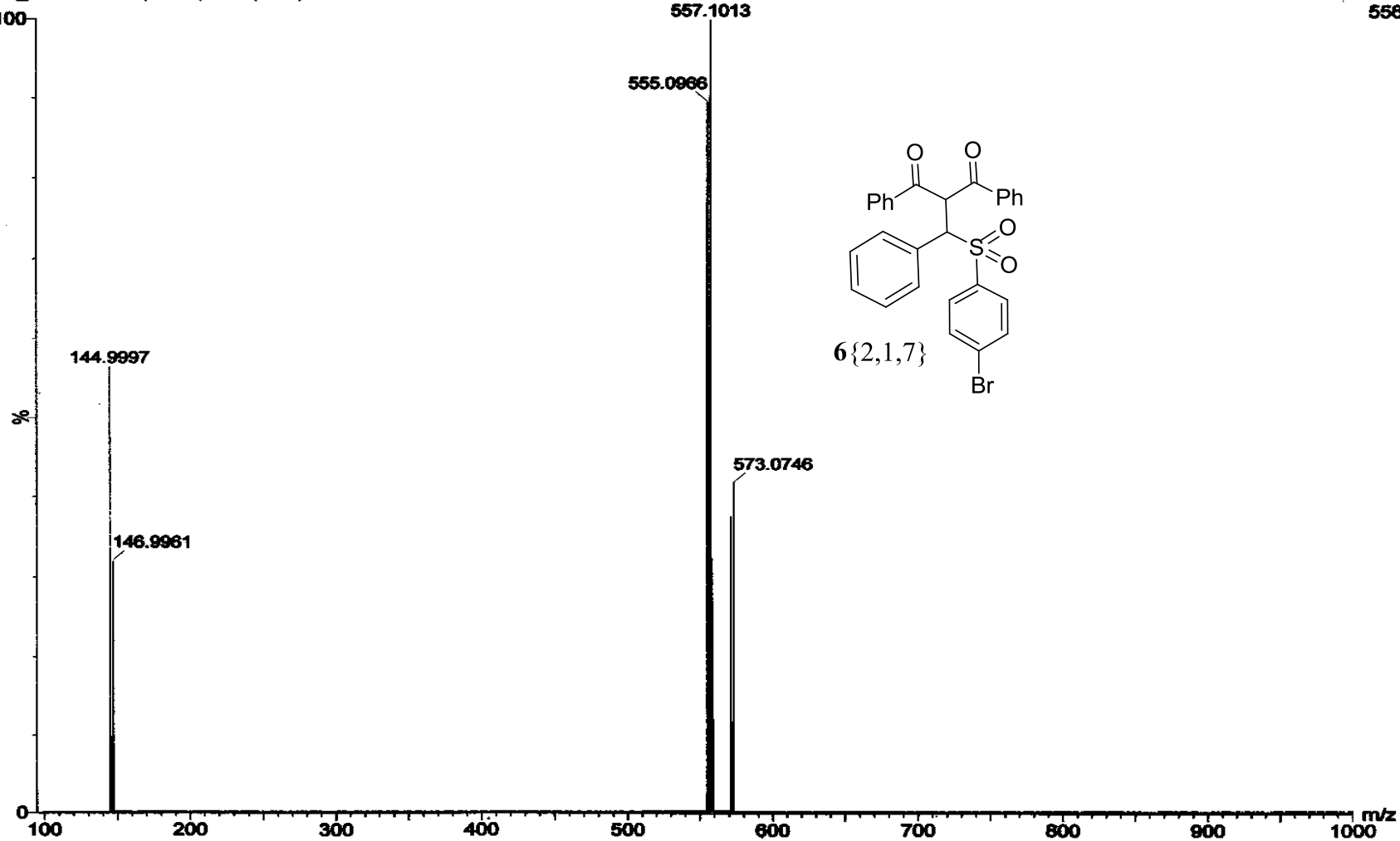
AD_105SO2 37 (0.678) Cm (3:41)

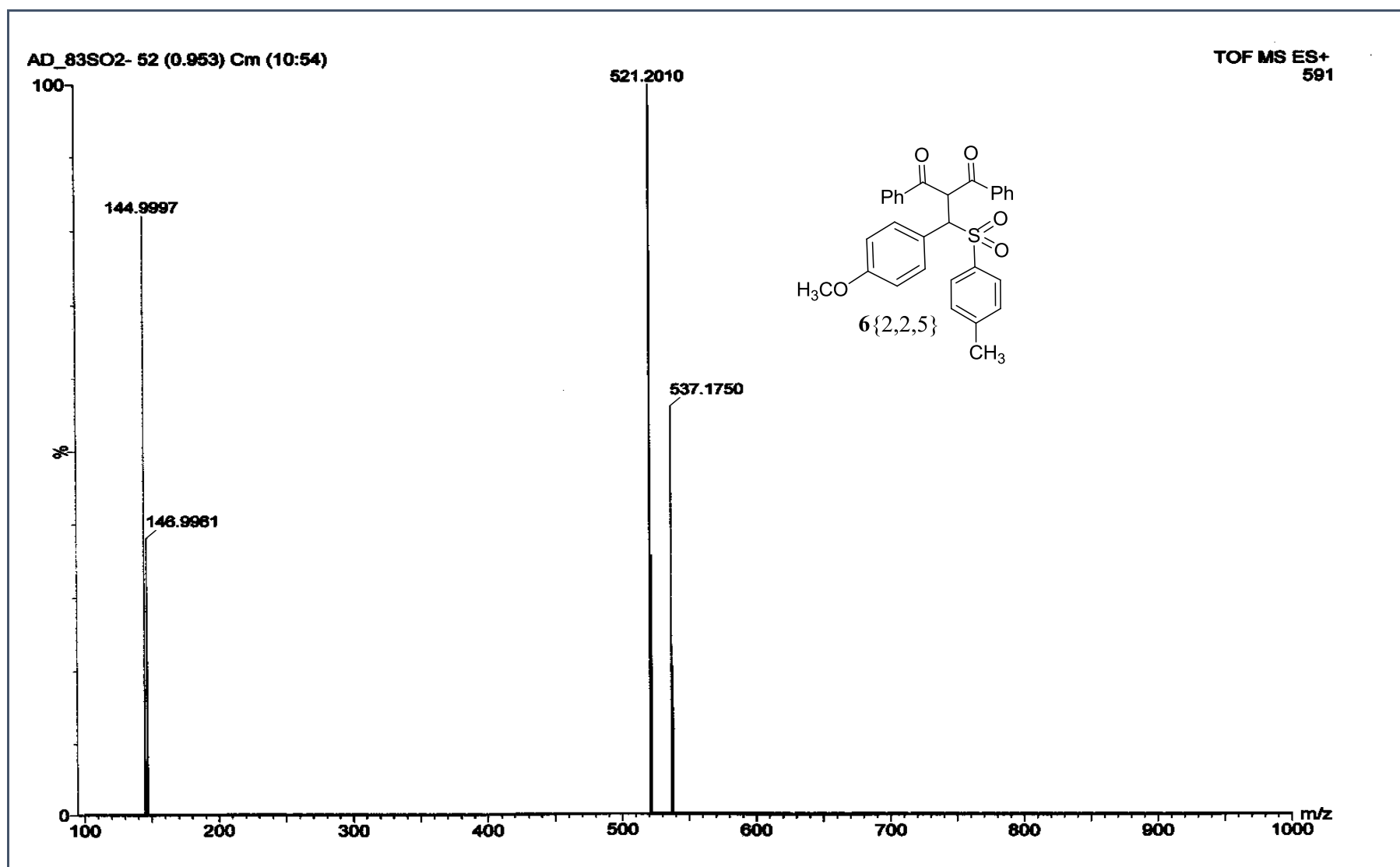
TOF MS ES+
1.34e3

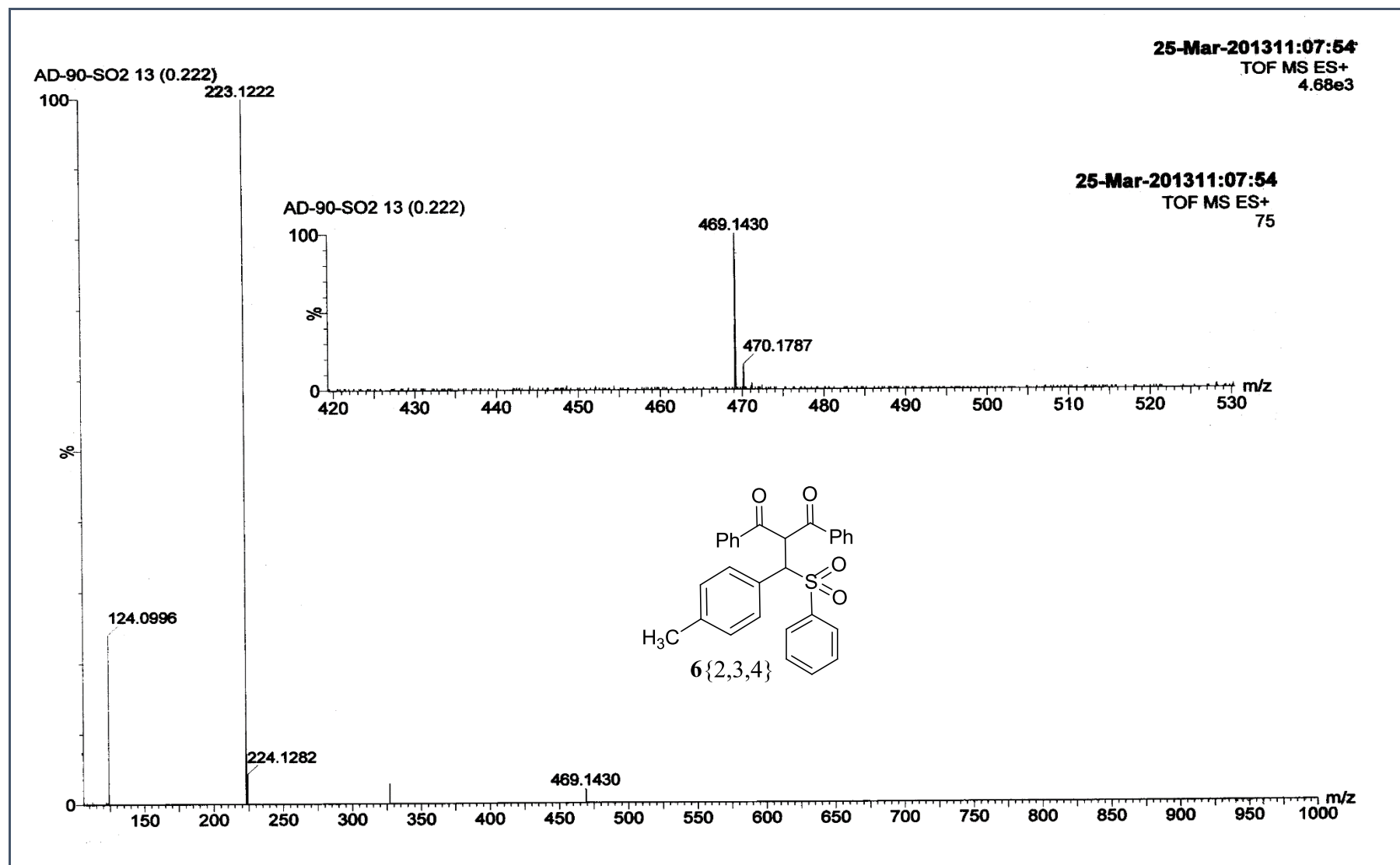


AD_106SO2 18 (0.330) Cm (6:34)

TOF MS ES+
556







AD_122SO2 37 (0.678) Cm (33:40)

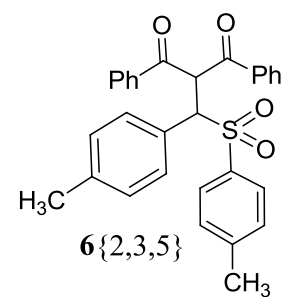
TOF MS ES+
684

100

%

505.1952

521.1758



0

100

200

300

400

500

600

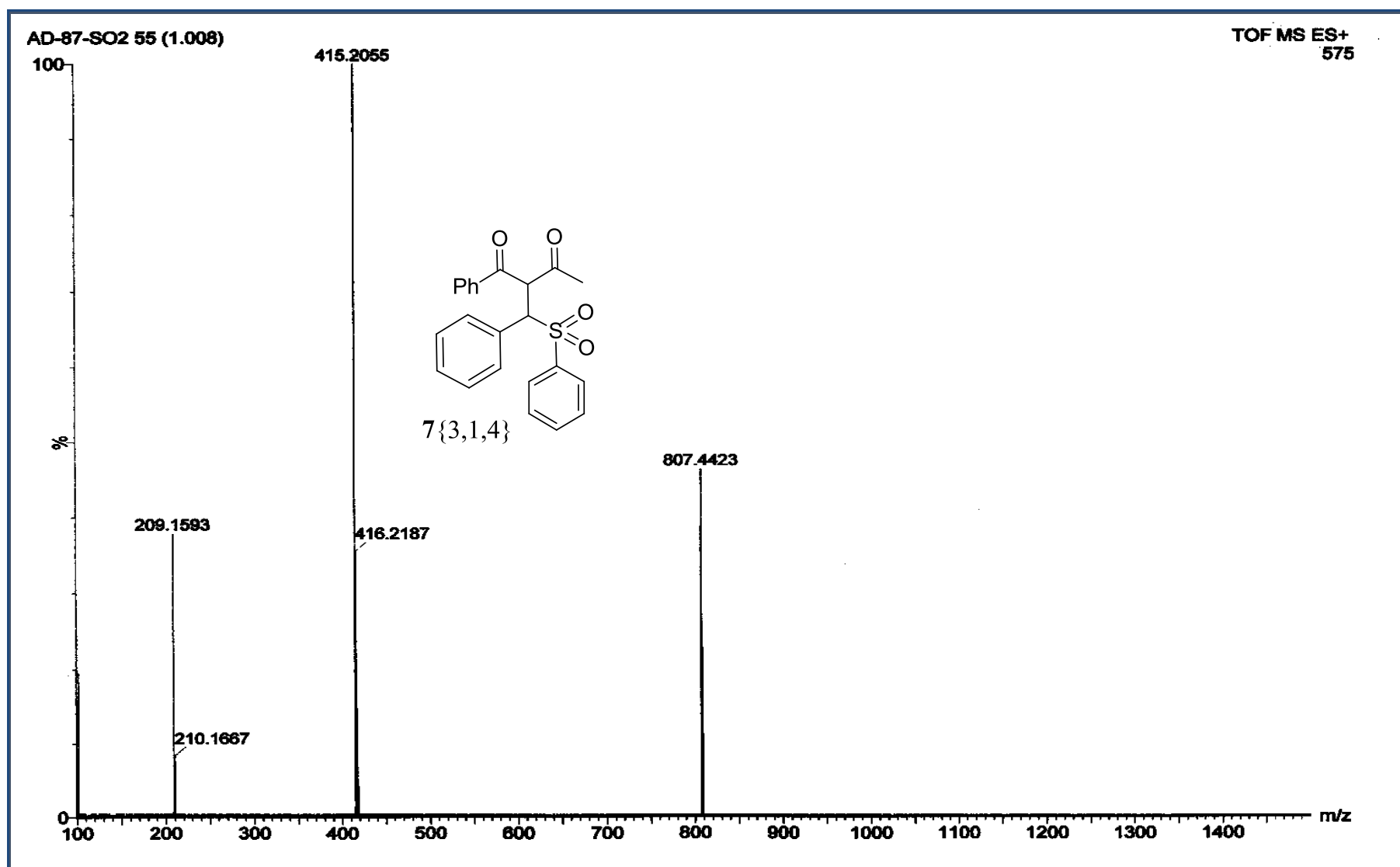
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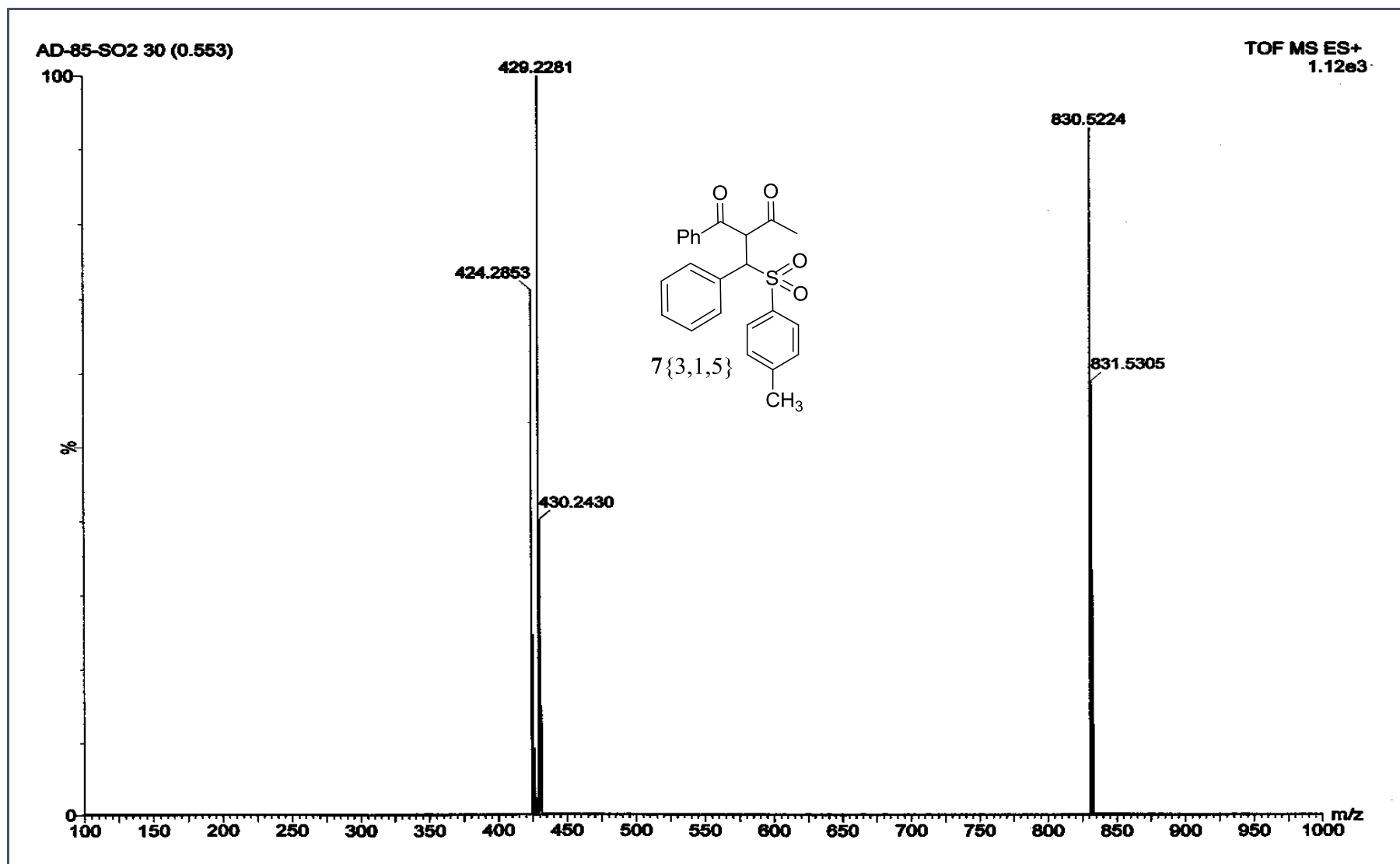
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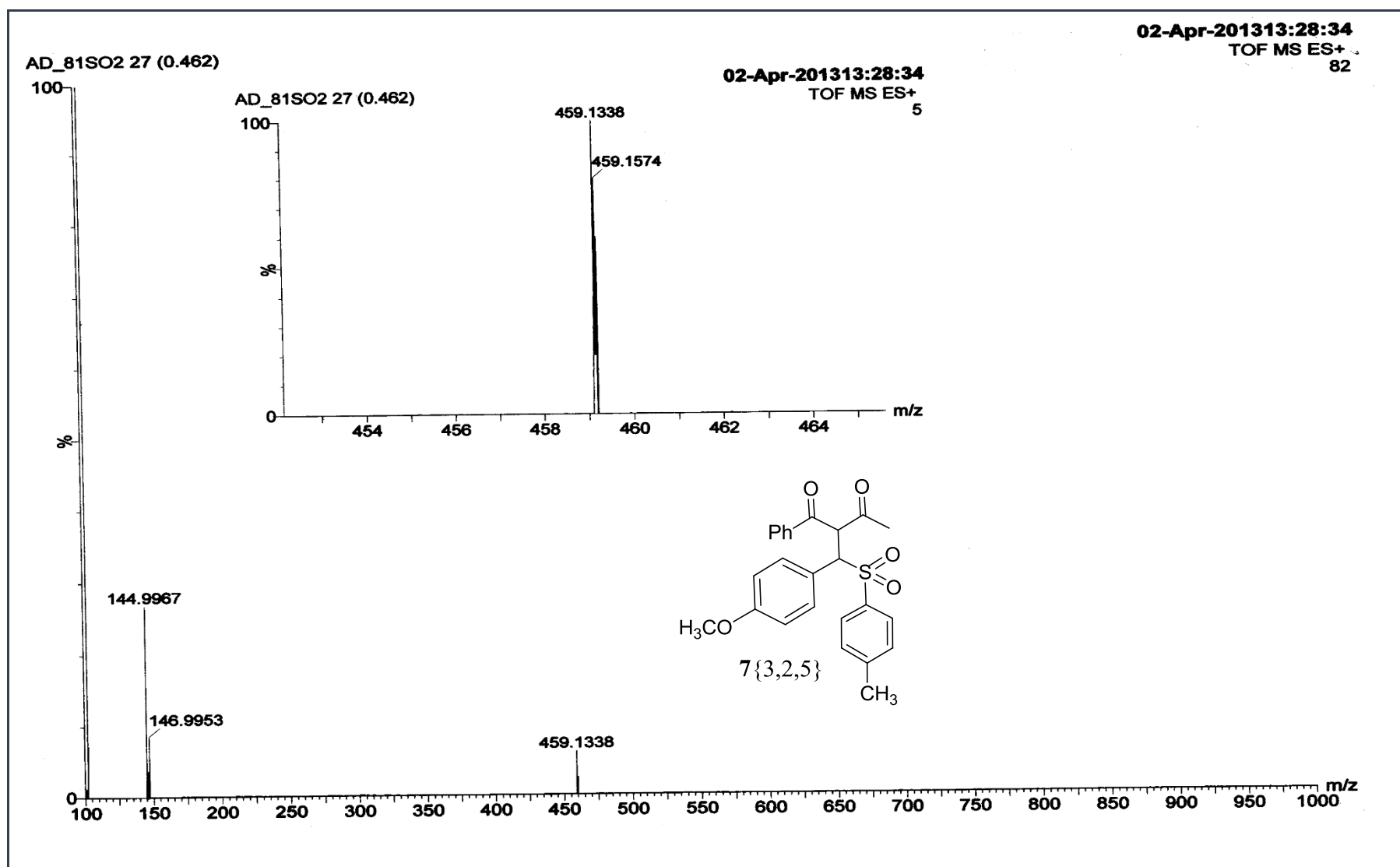
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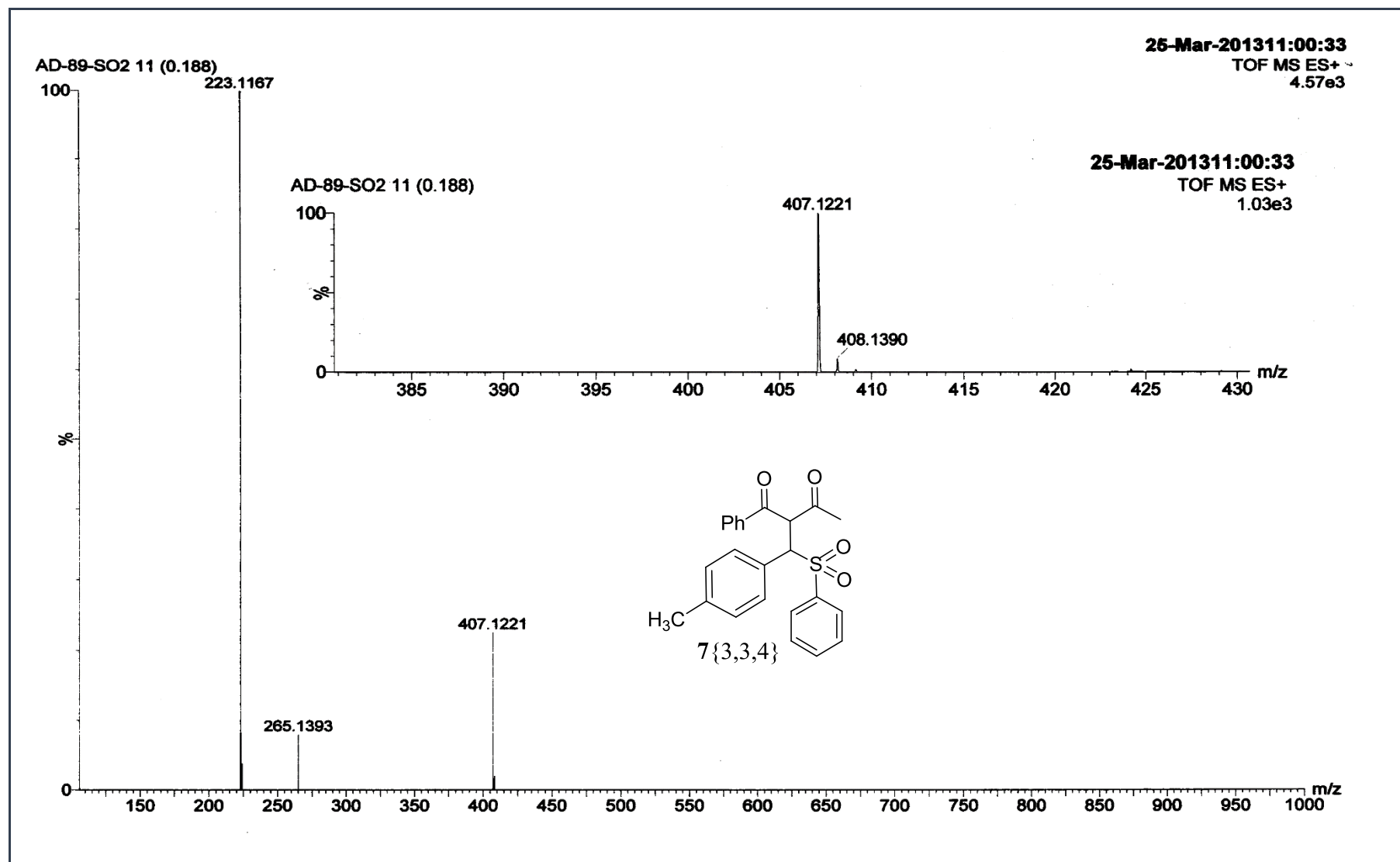
1000

m/z



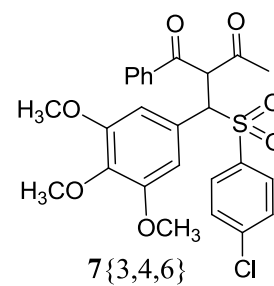
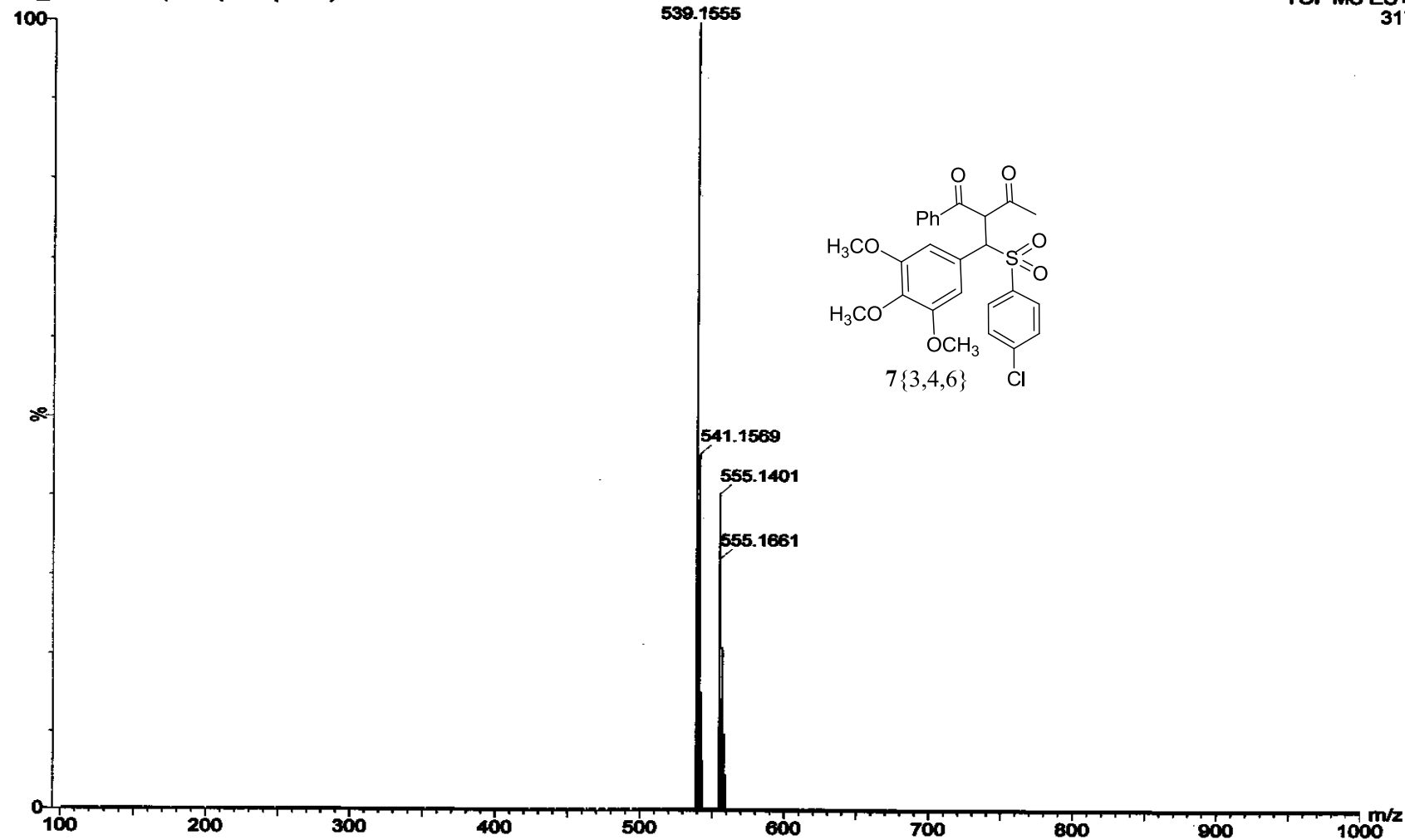






AD_120SO2 39 (0.715) Cm (34:39)

TOF MS ES+
317



AD_121SO2 11 (0.202) Cm (11:33)

TOF MS ES+
1.07e3

