

Supporting Information

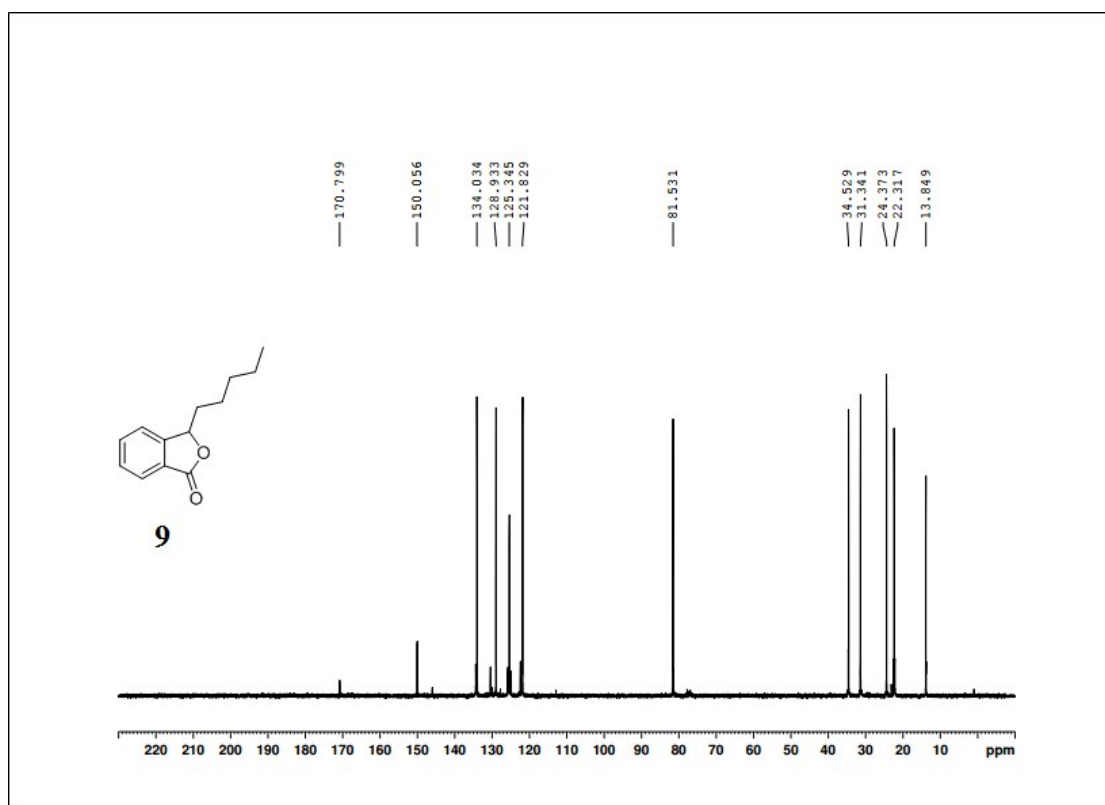
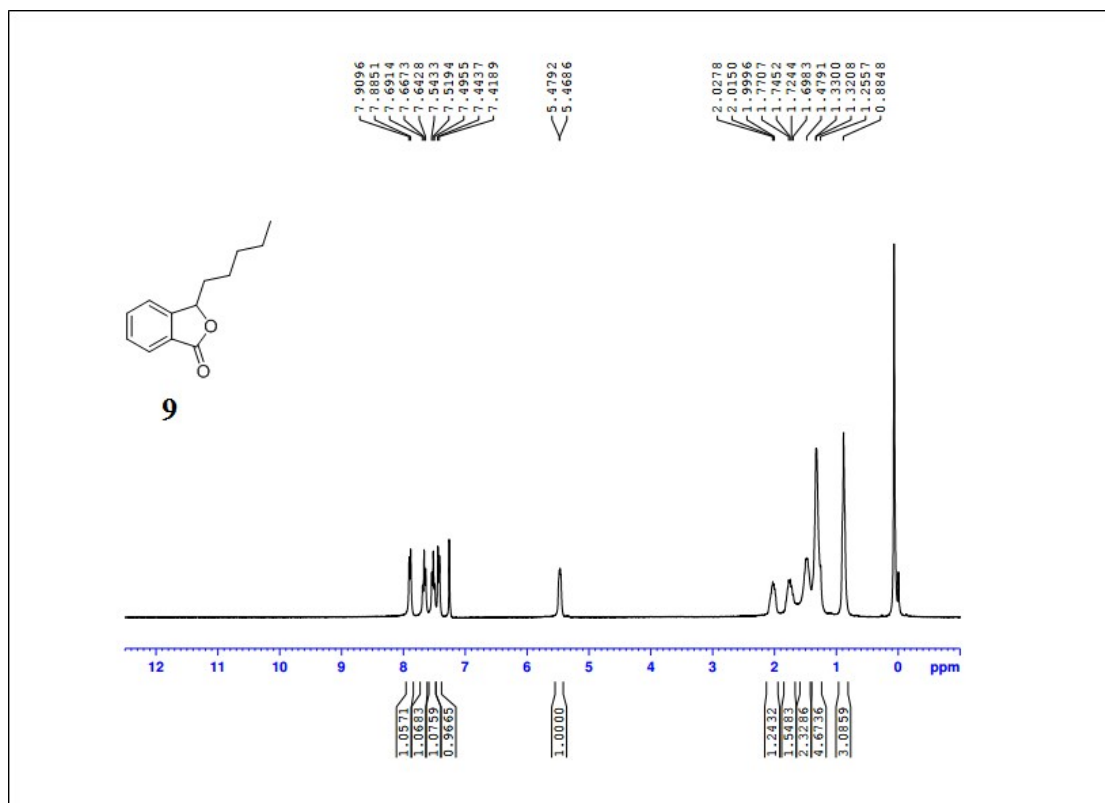
**Enantiomers of 3-Pentylbenzo[c]thiophen-1(3H)-one: Preparation and
Evaluation of Anti-Ischemic Stroke Activities**

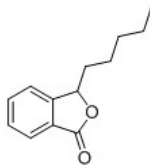
Yanlin Jian,^{‡*a*} Jing Ji,^{‡*b*} Zhangjian Huang,^{‡*a*} Yang Gao,^{*a*} Xiao Sheng,^{*a*} Wei Yin,^{*a*} Dayong Zhang,^{*a*}
Huiji,^{*b*} and YihuaZhang^{*a*}

Content: some spectra of related compounds

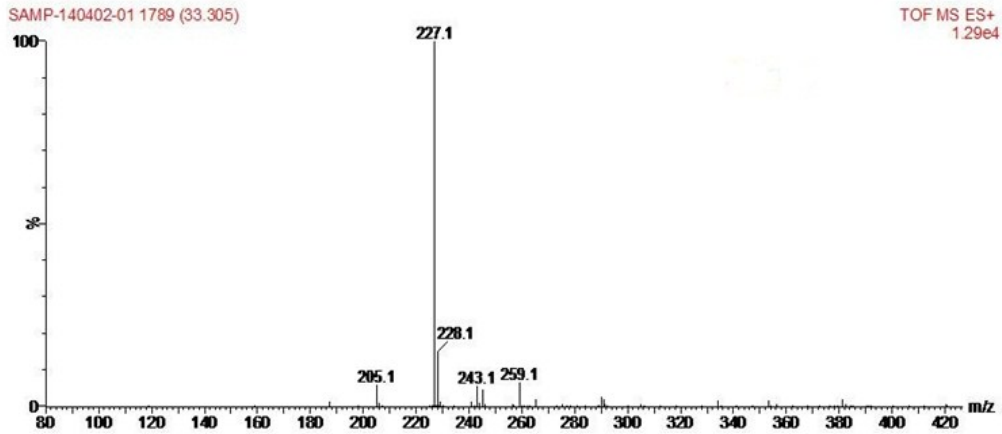
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1. ^1H , ^{13}C NMR, ESI-MS and ESI-HRMS spectra of (*S*)-**9**, (*R*)-**9**, (*S*)-**12**, (*R*)-**12**, (*S*)-**1**, (*R*)-**1**





9



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

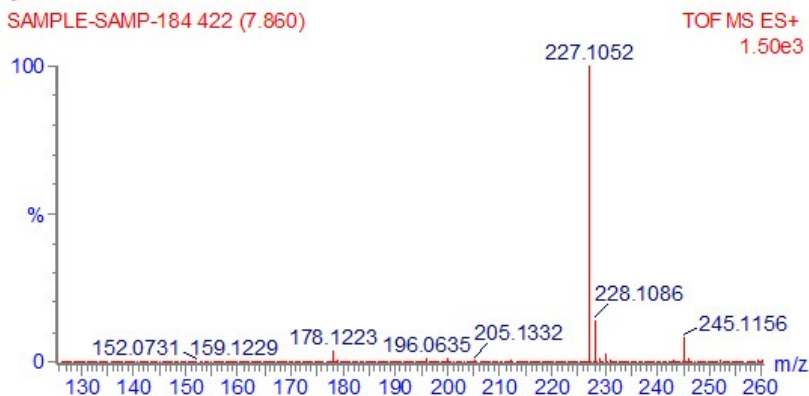
204 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 Na: 0-1

9

SAMPLE-SAMP-184 422 (7.860)



Minimum:

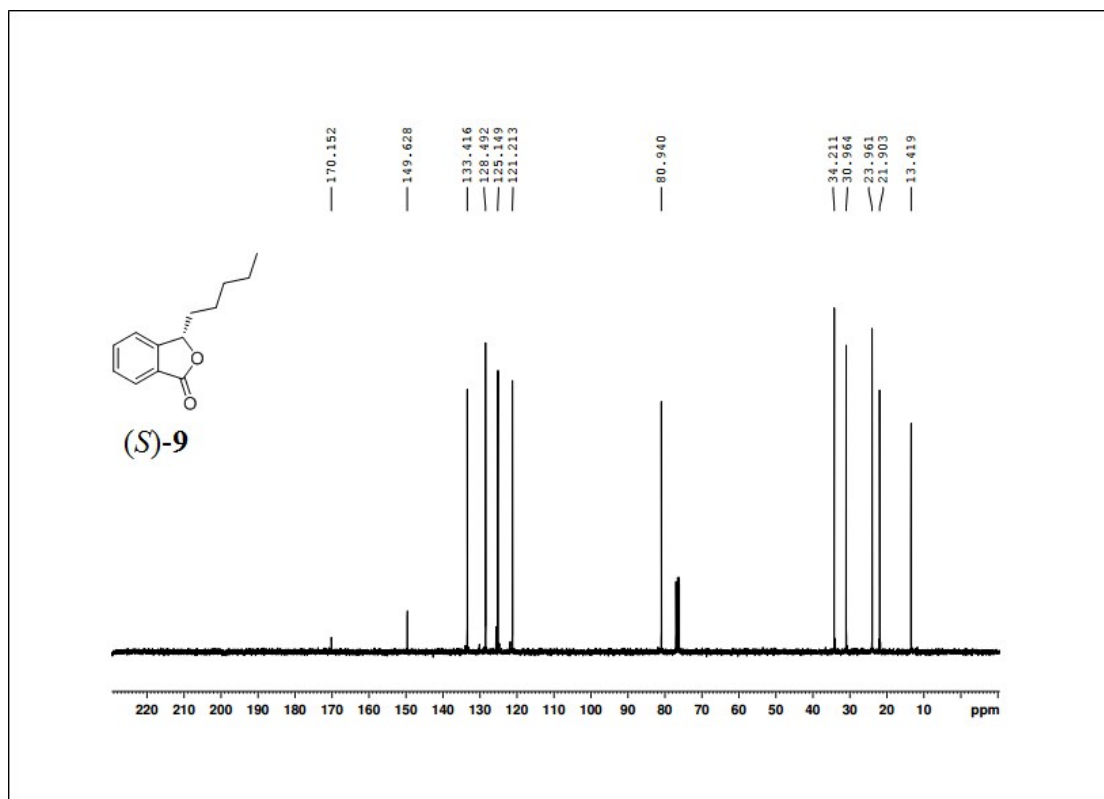
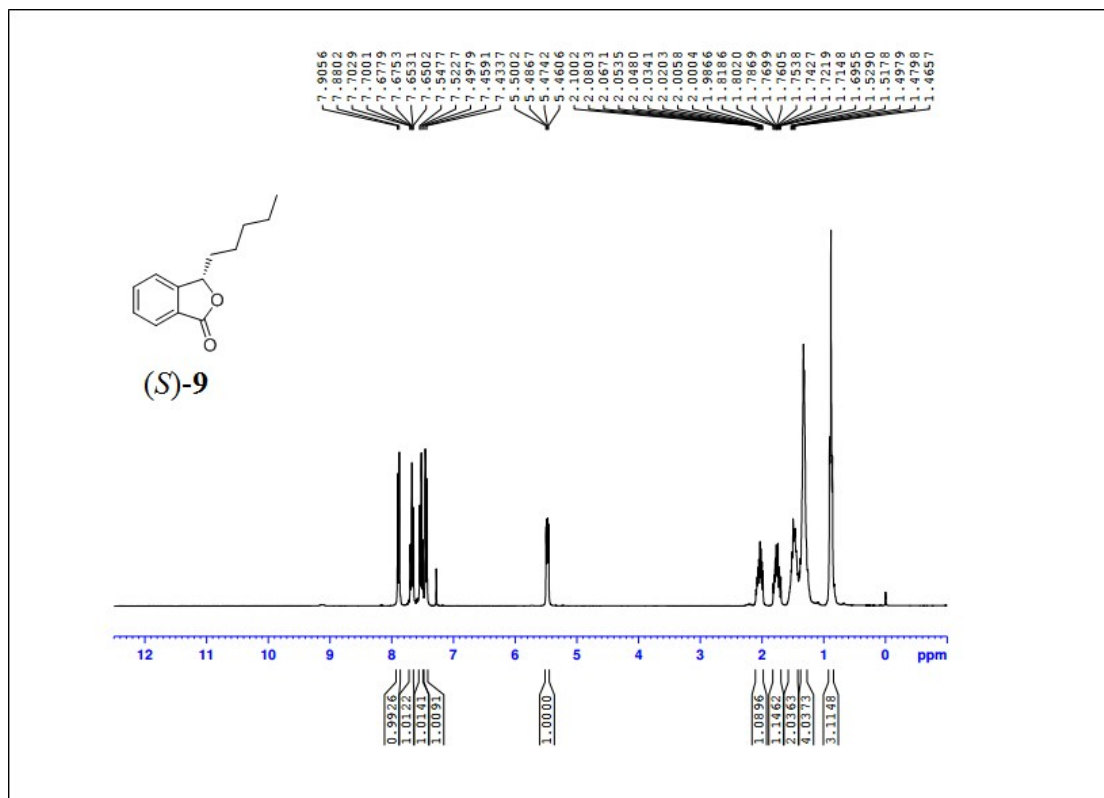
-1.5

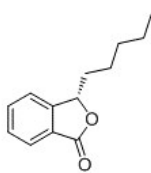
Maximum:

5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
227.1052	227.1048	0.4	1.8	5.5	1.3	C13 H16 O2 Na

Figure 1. Spectra of compound 9



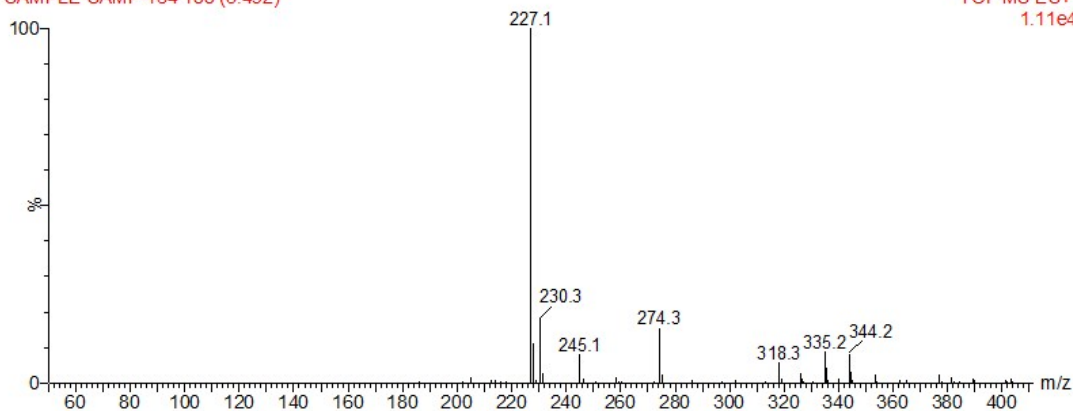


(S)-9

S-9

SAMPLE-SAMP-164 188 (3.492)

TOF MS ES+
1.11e4



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

204 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

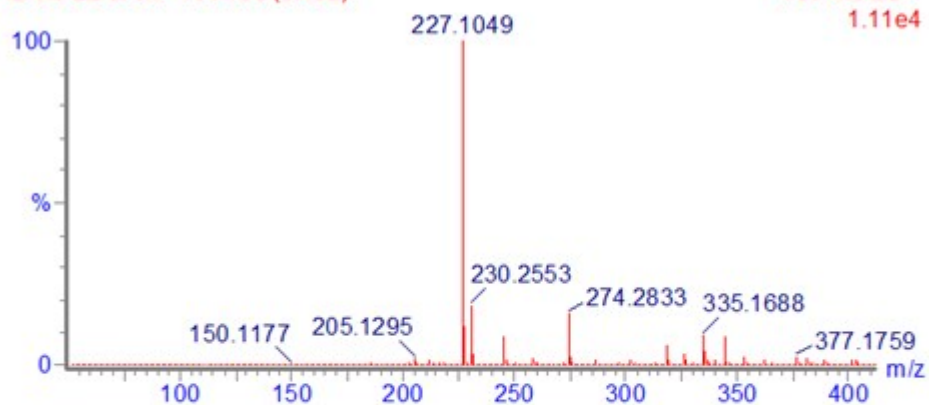
Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 Na: 0-1

S-9

SAMPLE-SAMP-164 188 (3.492)

TOF MS ES+
1.11e4



Minimum:

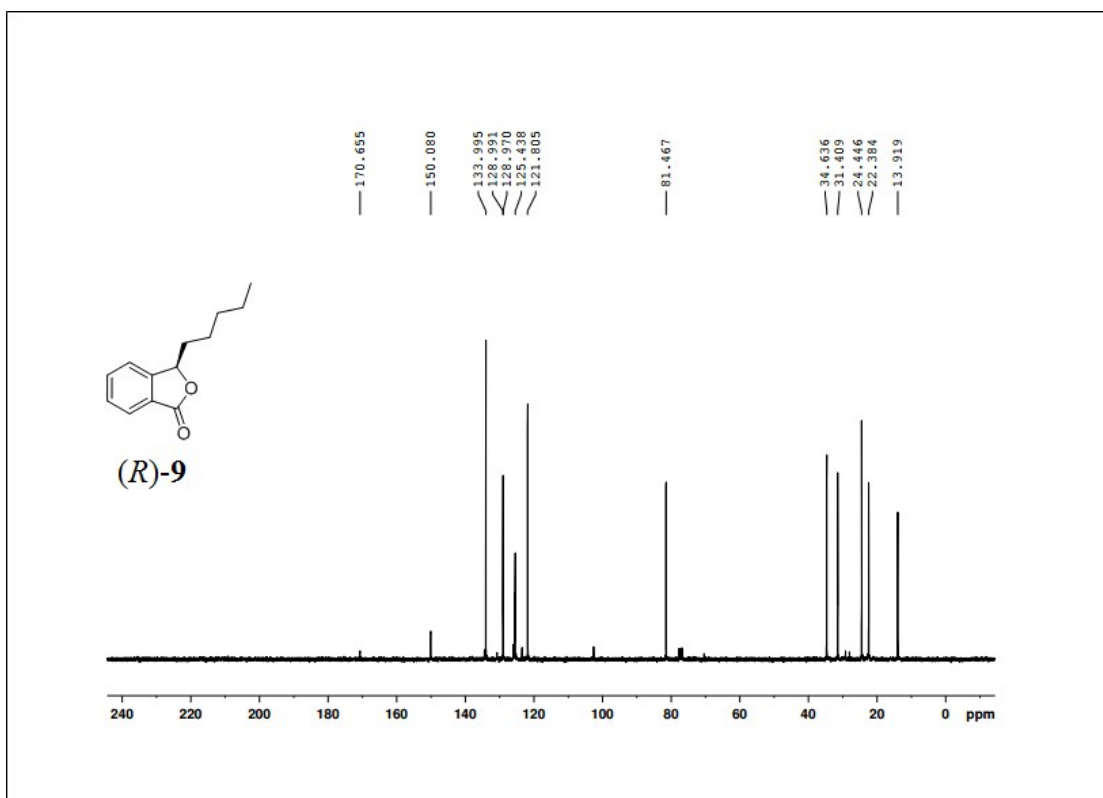
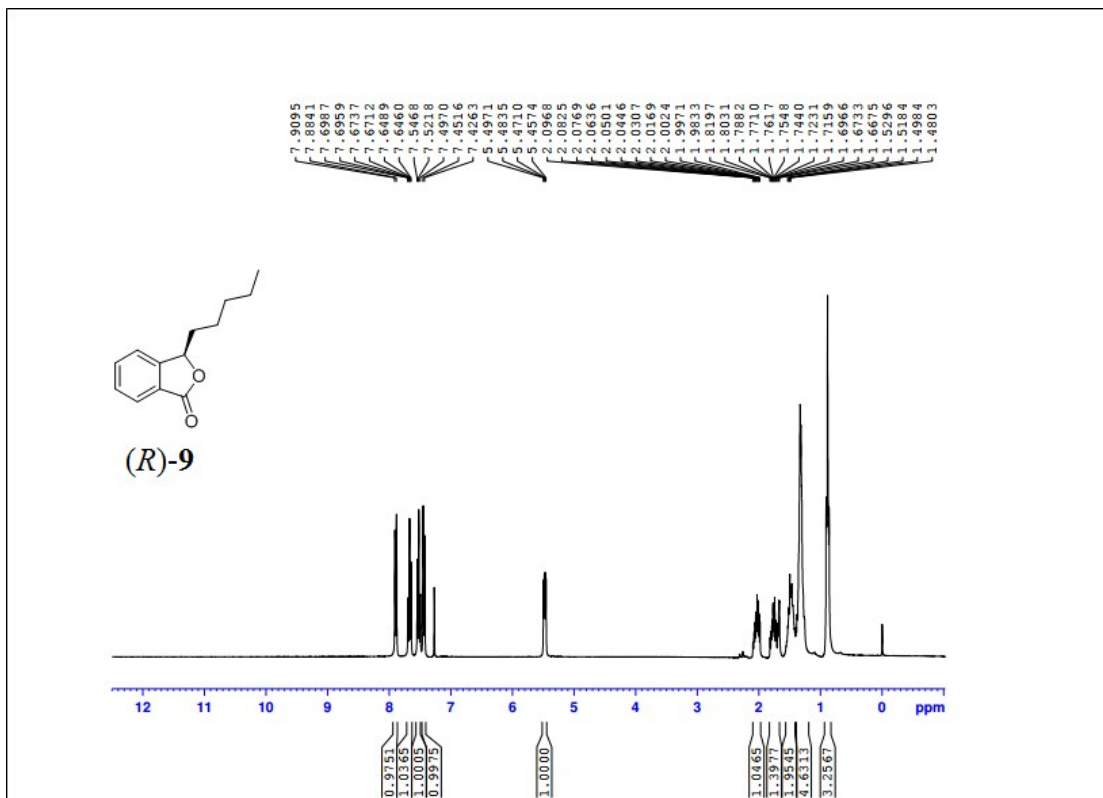
-1.5

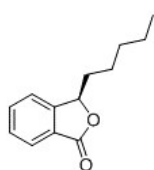
Maximum:

5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
227.1049	227.1048	0.1	0.4	5.5	72.4	C13 H16 O2 Na

Figure 2. Spectra of compound (S)-9



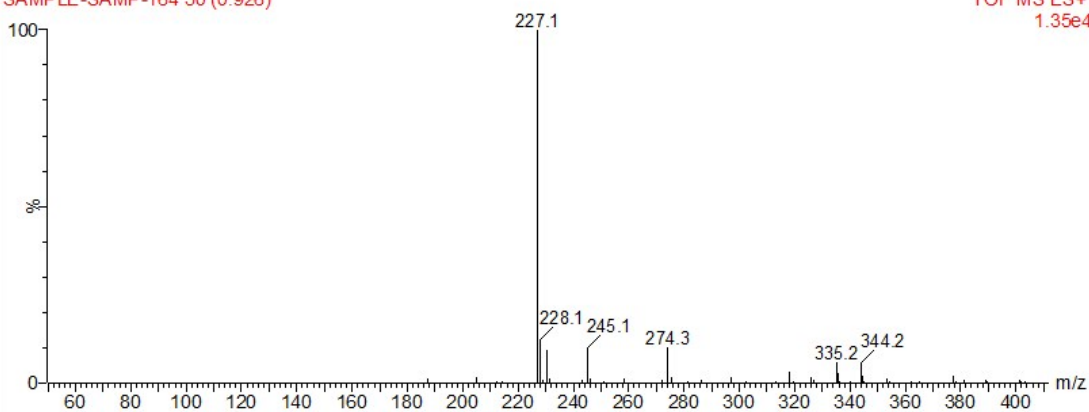


(R)-9

R-9

SAMPLE-SAMP-164 50 (0.926)

TOF MS ES+
1.35e4



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

204 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

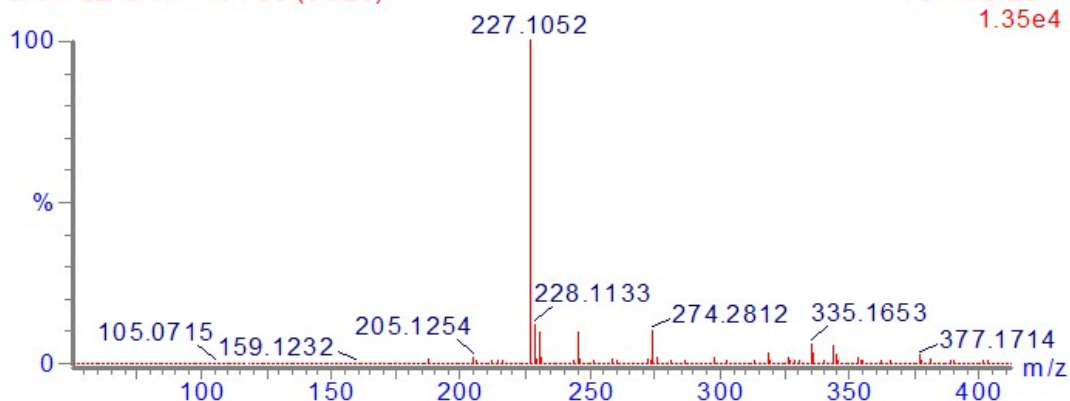
Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 Na: 0-1

R-9

SAMPLE-SAMP-164 50 (0.926)

TOF MS ES+
1.35e4



Minimum:

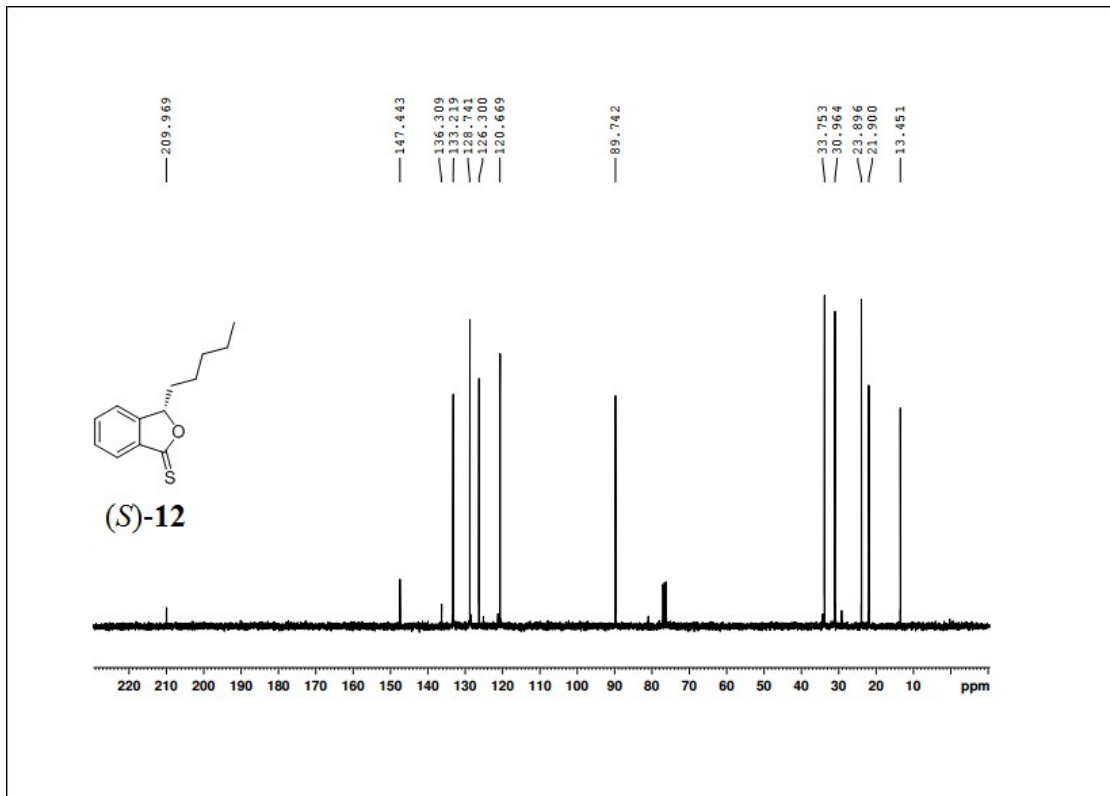
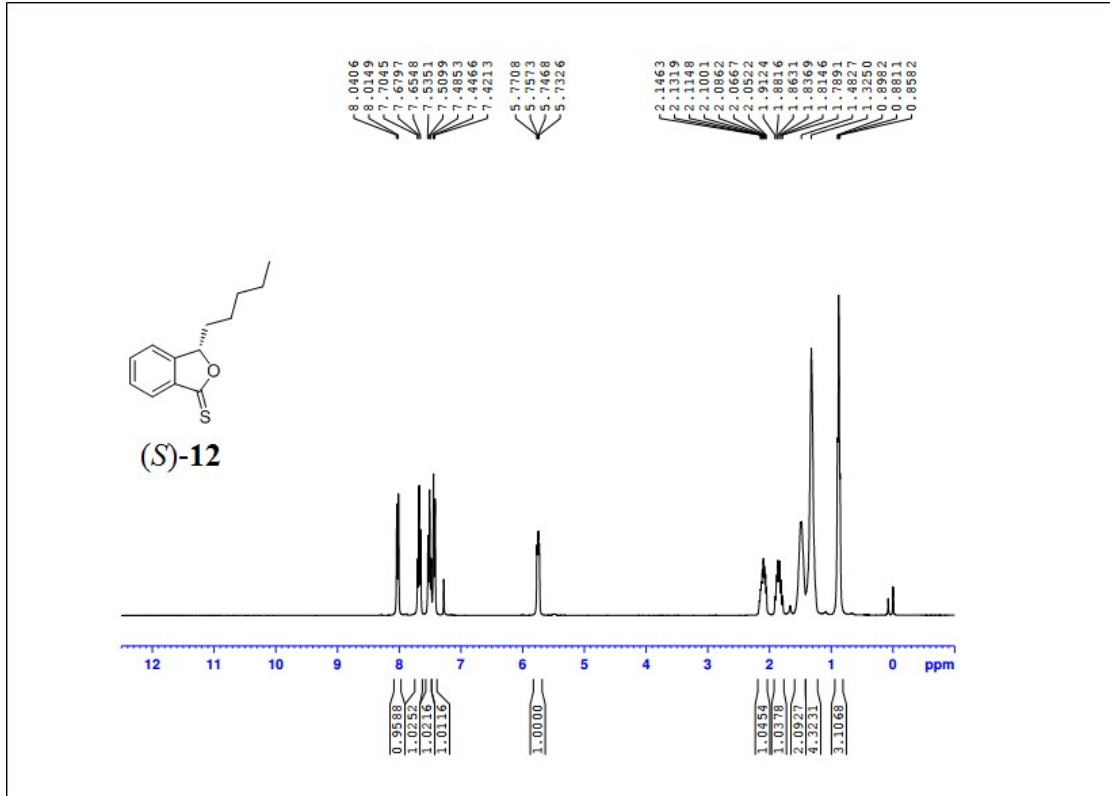
-1.5

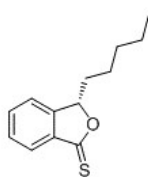
Maximum:

5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
227.1052	227.1048	0.4	1.8	5.5	39.7	C13 H16 O2 Na

Figure 3. Spectra of compound (R)-9

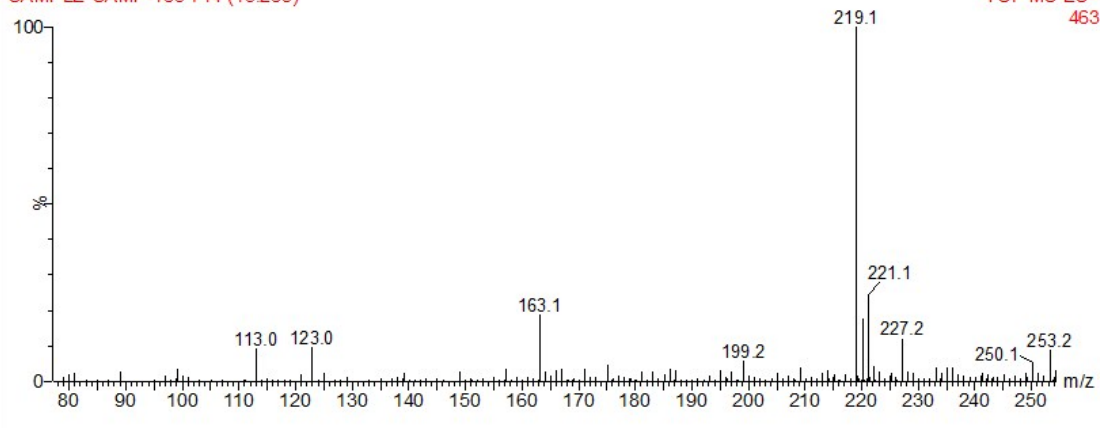




(S)-12

S-12

SAMPLE-SAMP-163 714 (13.265)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

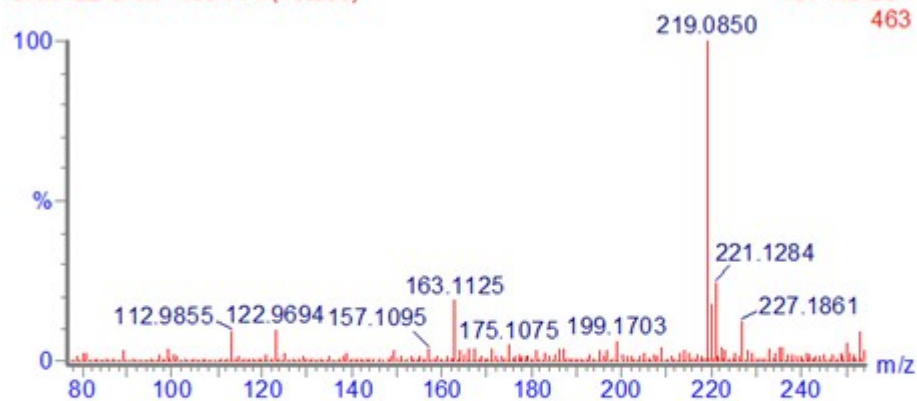
198 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 S: 0-1

S-12

SAMPLE-SAMP-163 714 (13.265)



Minimum:

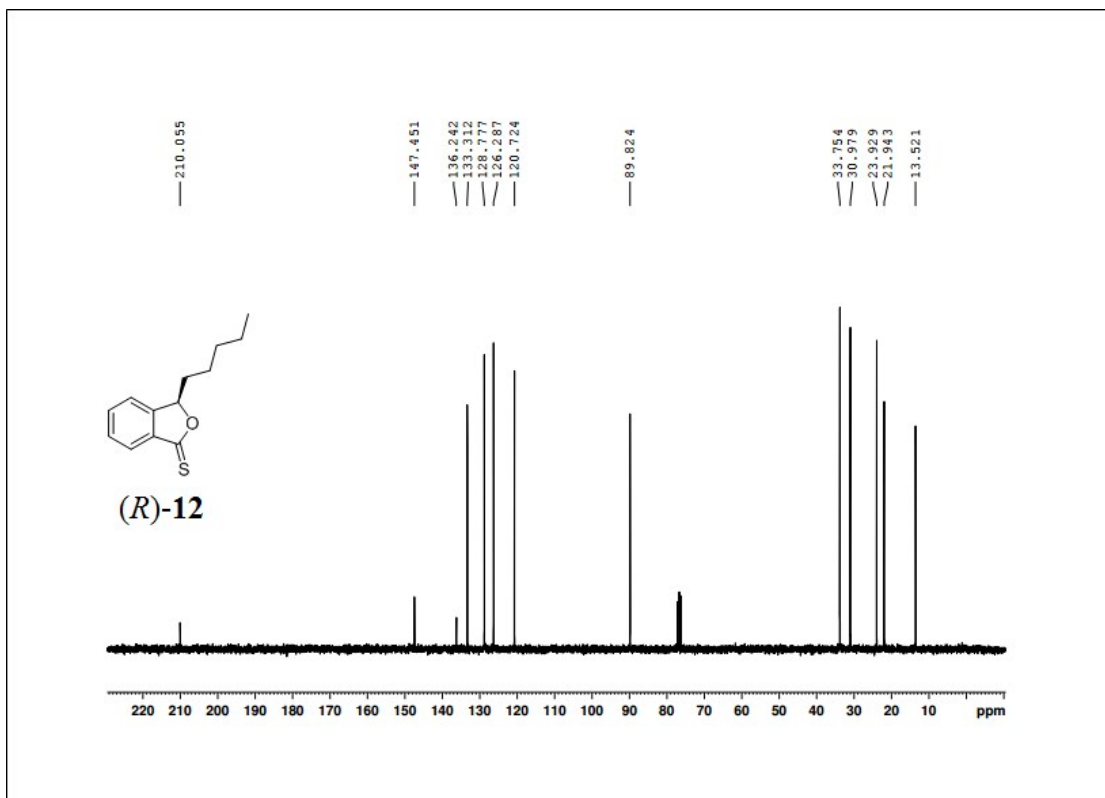
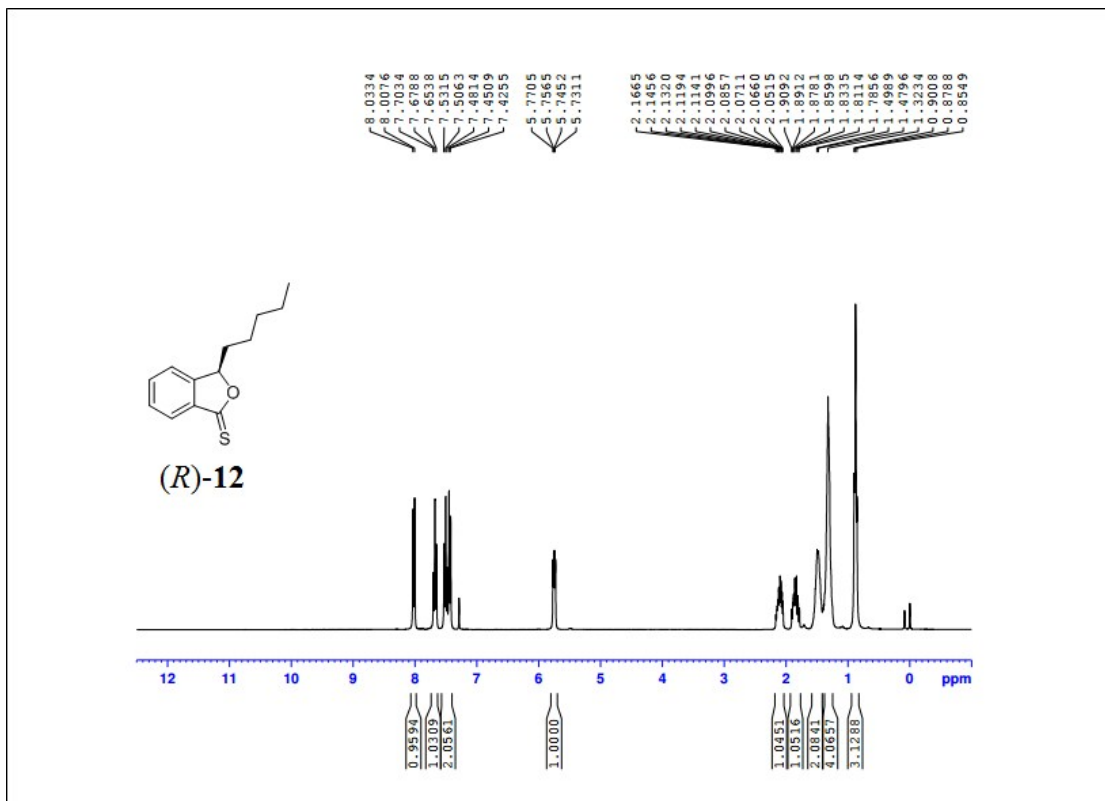
-1.5

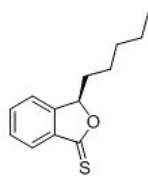
Maximum:

5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.0850	219.0844	0.6	2.7	6.5	2773158.3	C13 H15 O S

Figure 4. Spectra of compound (S)-12

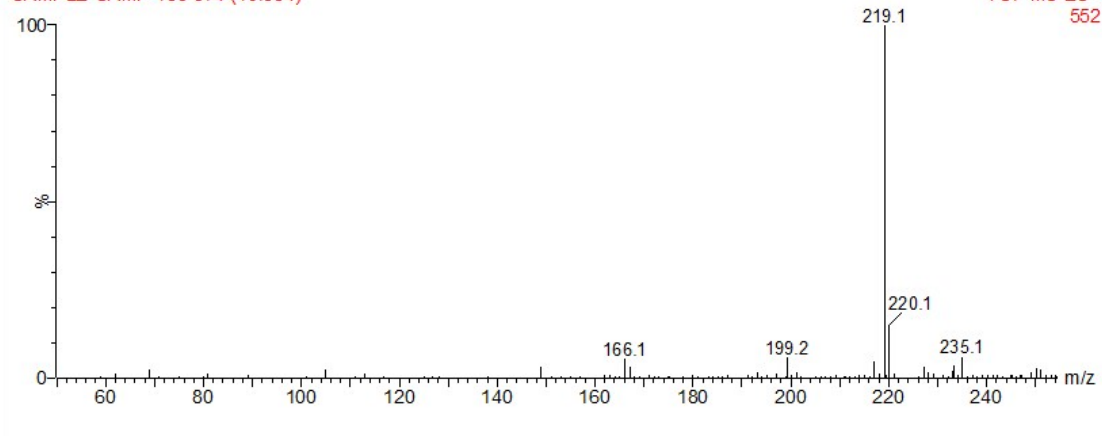




(R)-12

R-12

SAMPLE-SAMP-163 574 (10.664)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

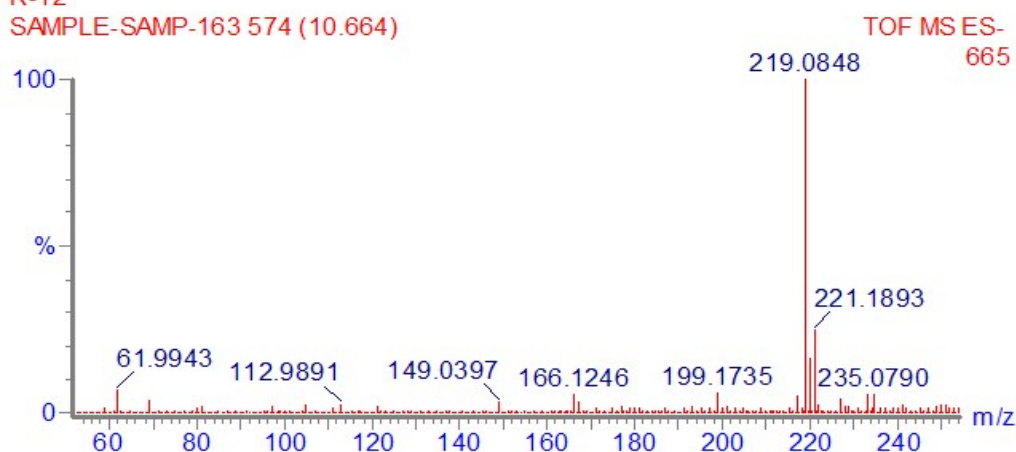
198 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 S: 0-1

R-12

SAMPLE-SAMP-163 574 (10.664)



Minimum:

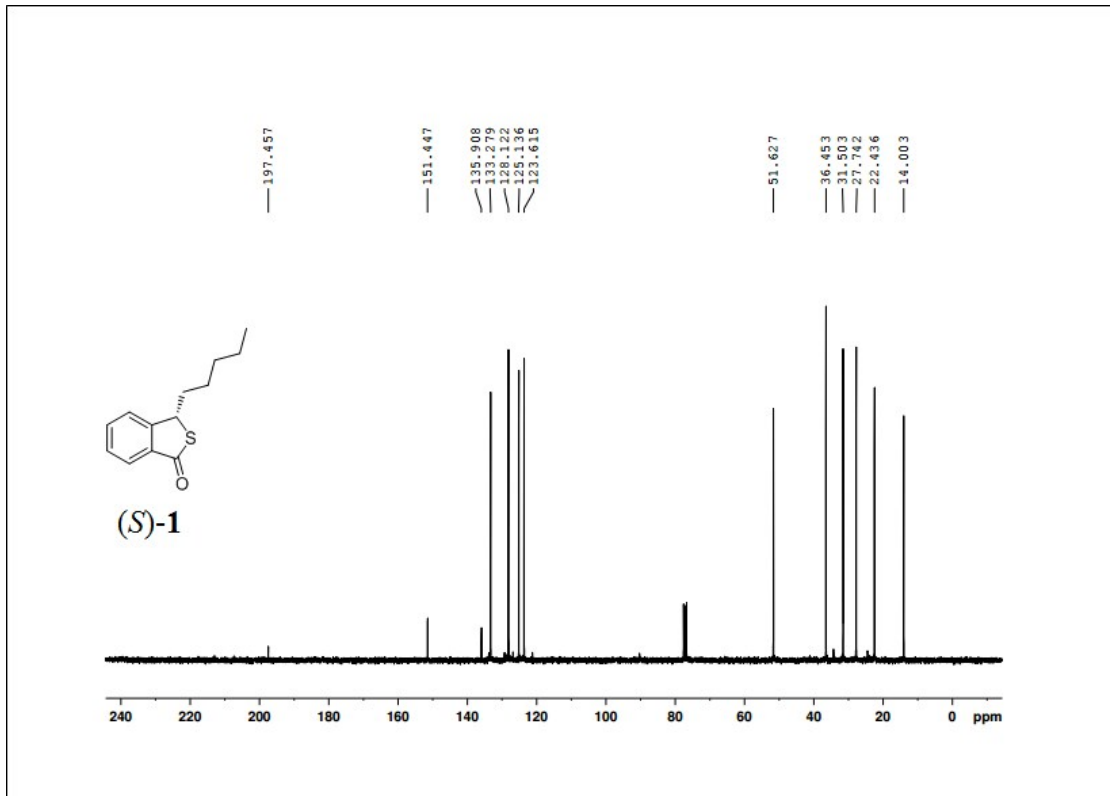
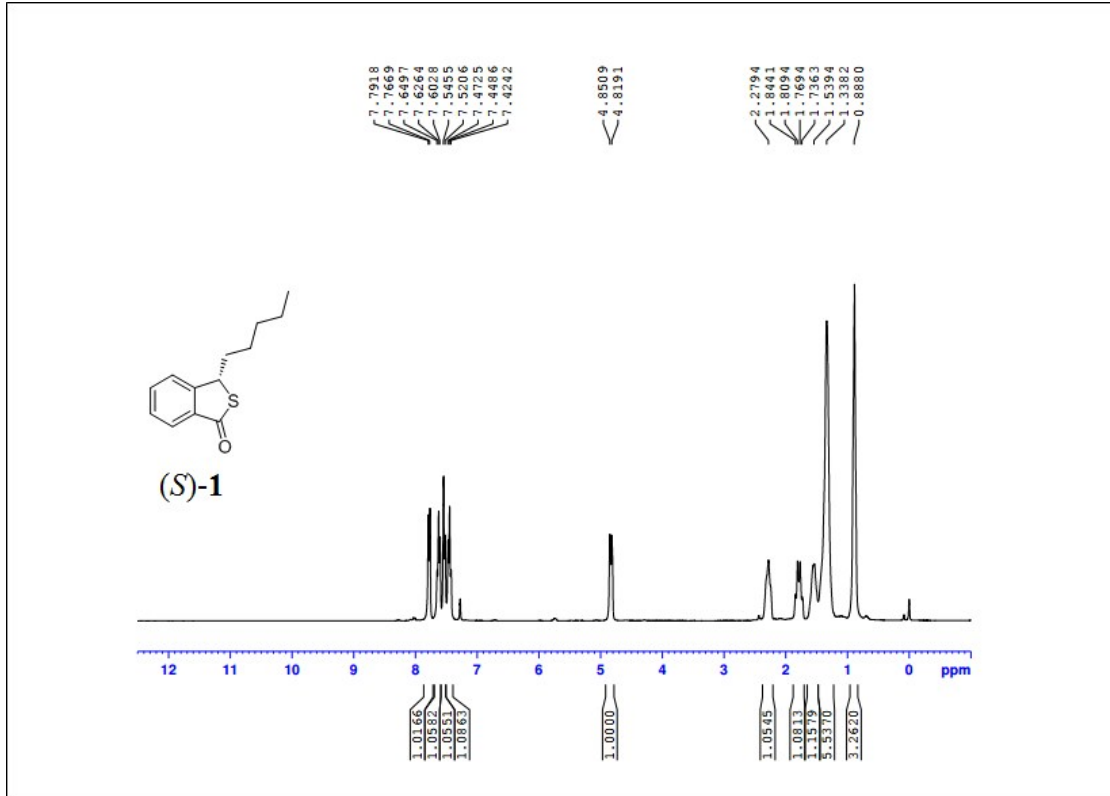
-1.5

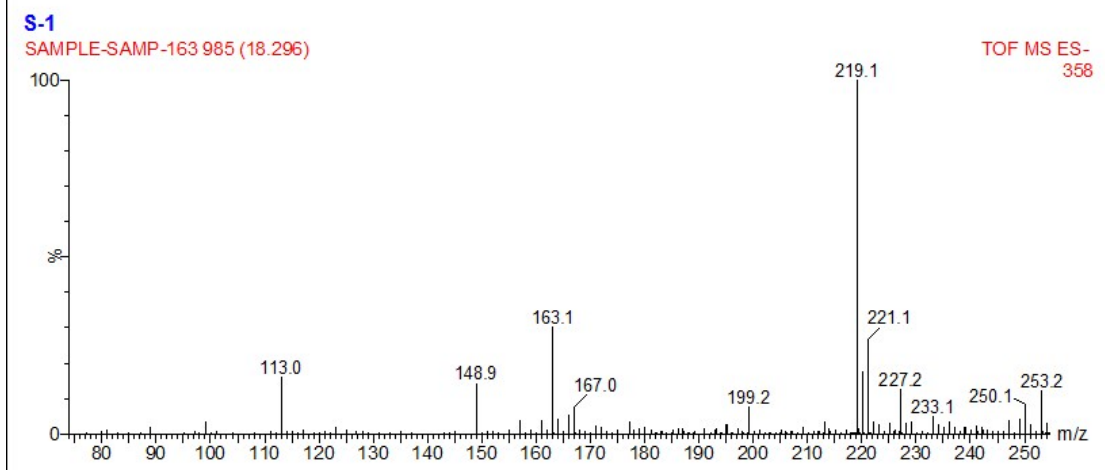
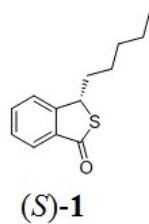
Maximum:

5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.0848	219.0844	0.4	1.8	6.5	2773253.5	C ₁₃ H ₁₅ O S

Figure 5. Spectra of compound (R)-12





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

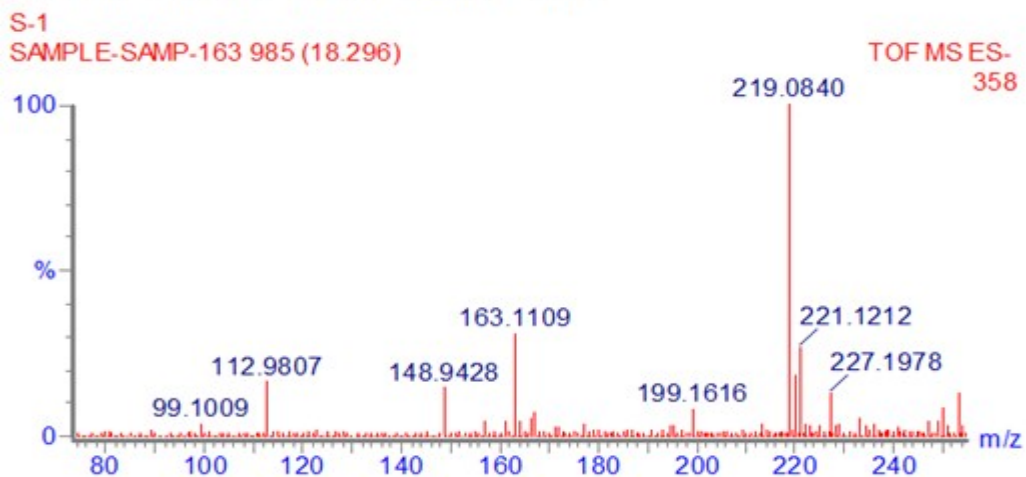
Selected filters: None

Monoisotopic Mass, Even Electron Ions

198 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 S: 0-1



Minimum:

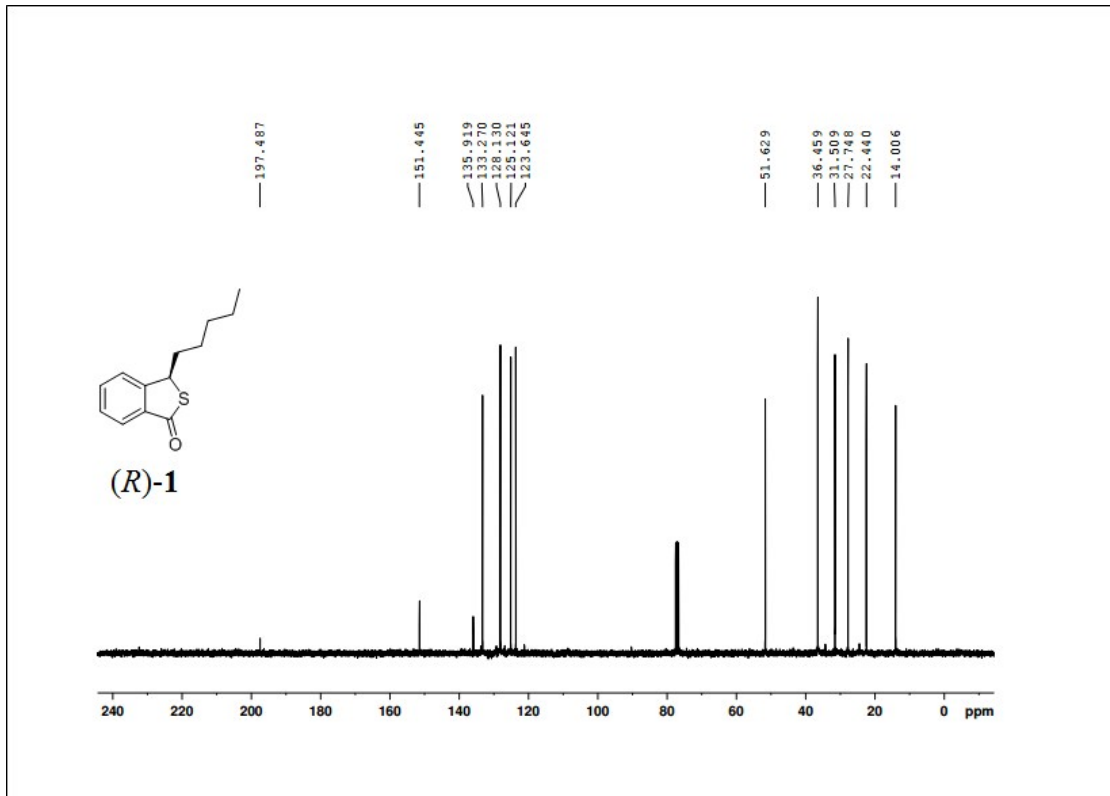
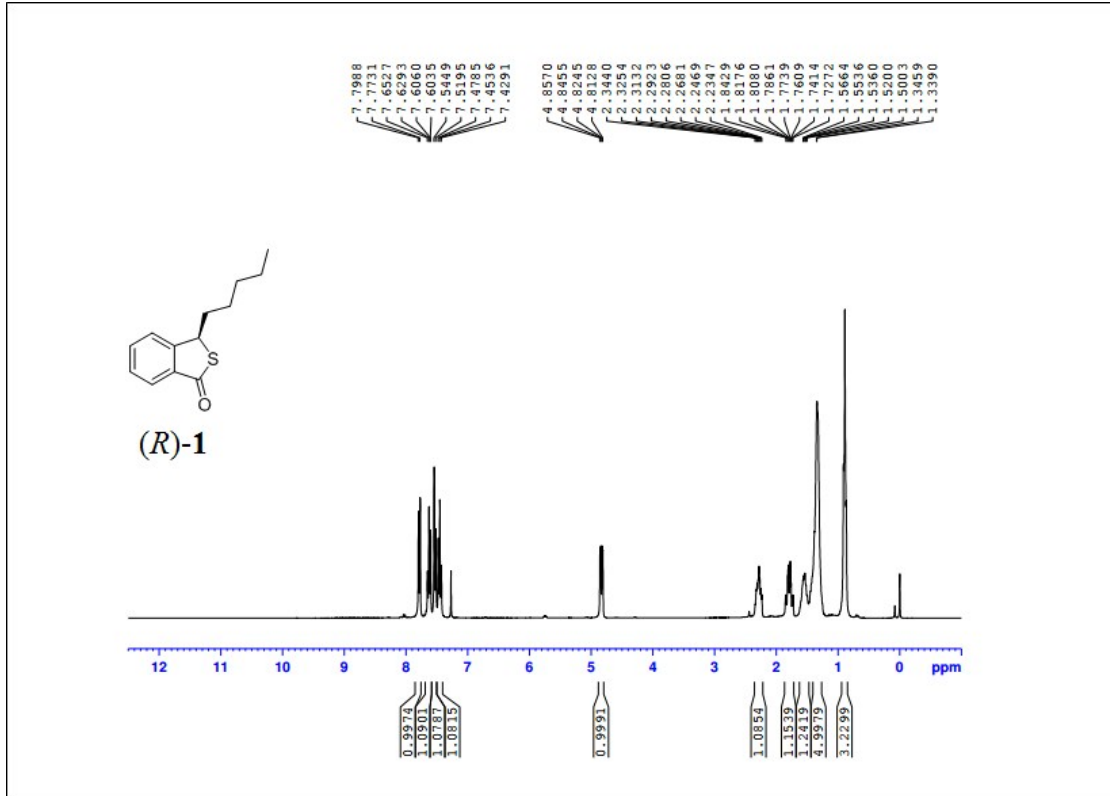
-1.5

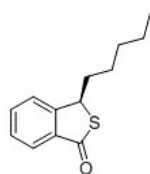
Maximum:

5.0 5.0 20.0

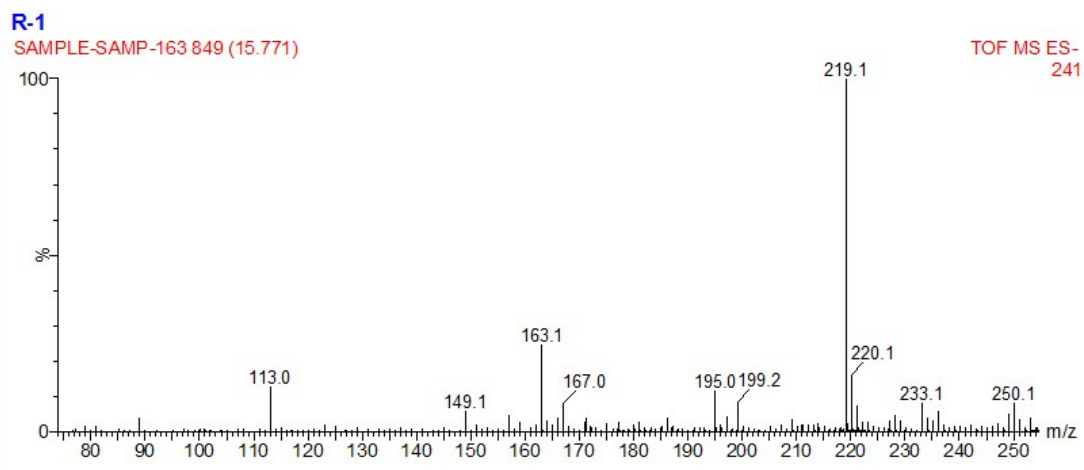
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.0840	219.0844	-0.4	-1.8	6.5	2773110.5	C ₁₃ H ₁₅ O S

Figure 6. Spectra of compound (S)-1





(R)-1



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 20.0

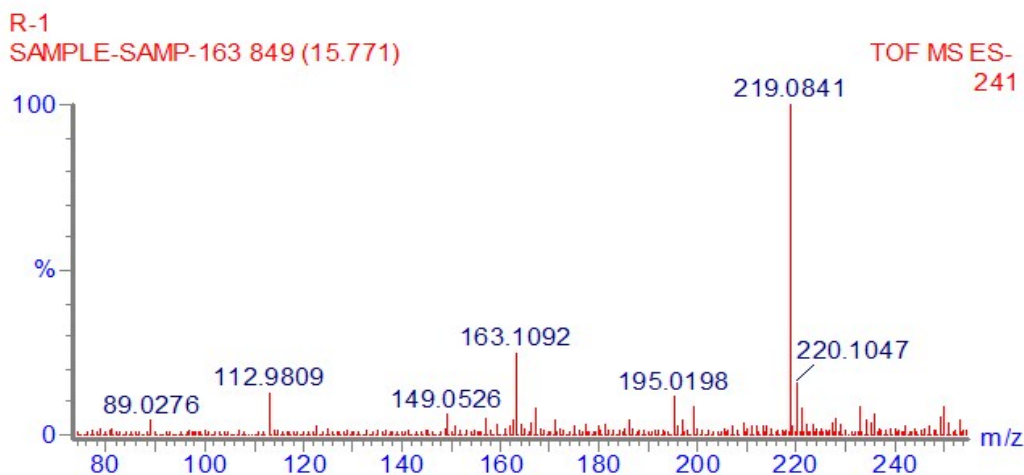
Selected filters: None

Monoisotopic Mass, Even Electron Ions

198 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-5 O: 0-5 S: 0-1



Minimum:

-1.5

Maximum:

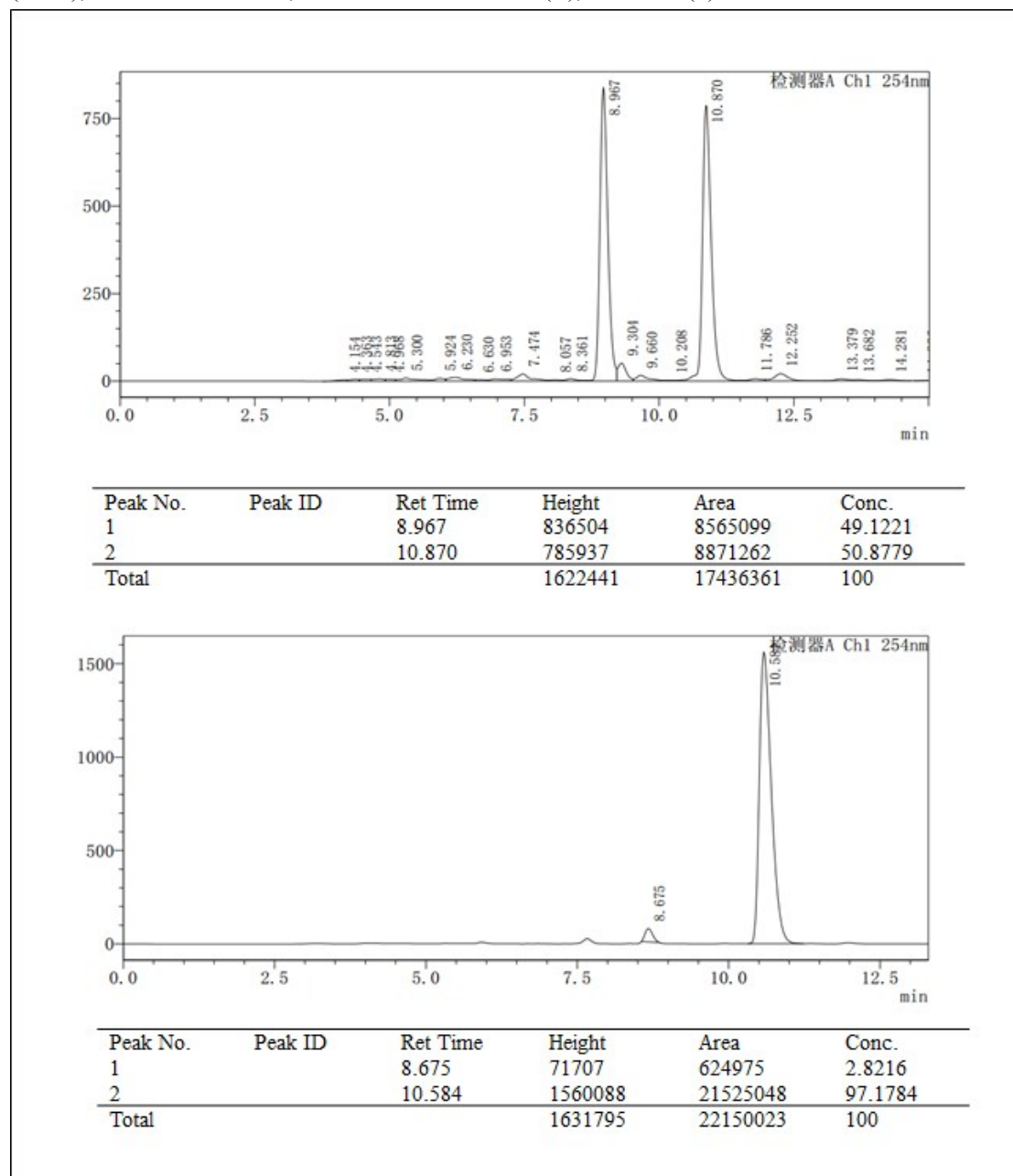
5.0 5.0 20.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.0841	219.0844	-0.3	-1.4	6.5	1.3	C ₁₃ H ₁₅ O S

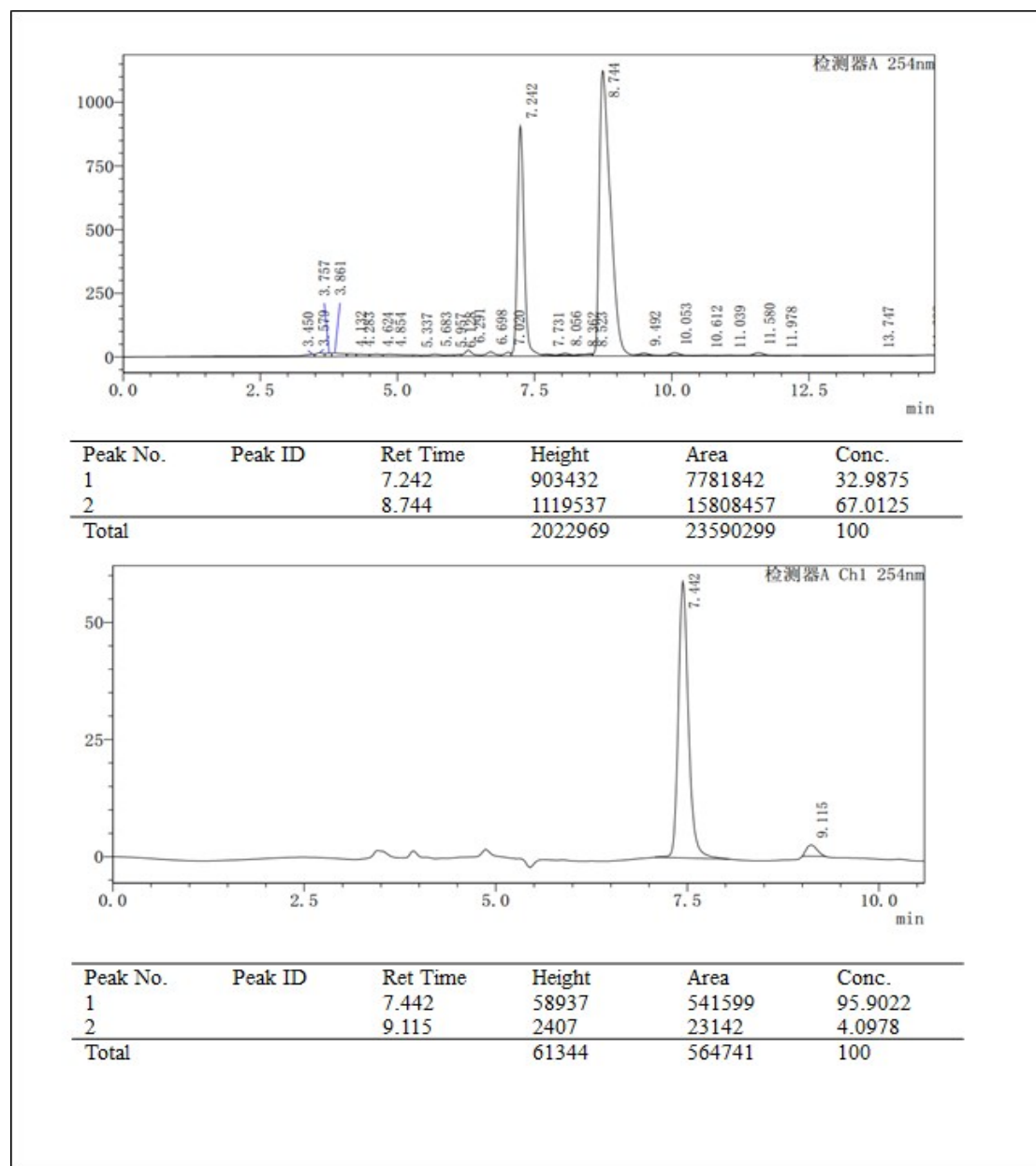
Figure 7. Spectra of compound (R)-1

2. HPLC spectra for the enantiomeric excess of (*S*)-**1** and (*R*)-**1** prepared by chemical synthesis in combination with chiral resolution

2.1. (*S*)-3-pentylbenzo[*c*]thiophen-1(3*H*)-one ((*S*)-**1**). 94.4% ee. HPLC: chiralpak AD-H column (0.46 cm I.D. × 25 cm L × 5 μm); detected at 254 nm; n-hexane/EtOH/diethylamine = 98/2/0.1 (v/v/v); flow = 1.0 mL/min; retention time: 8.6 min (*R*), 10.6 min (*S*).

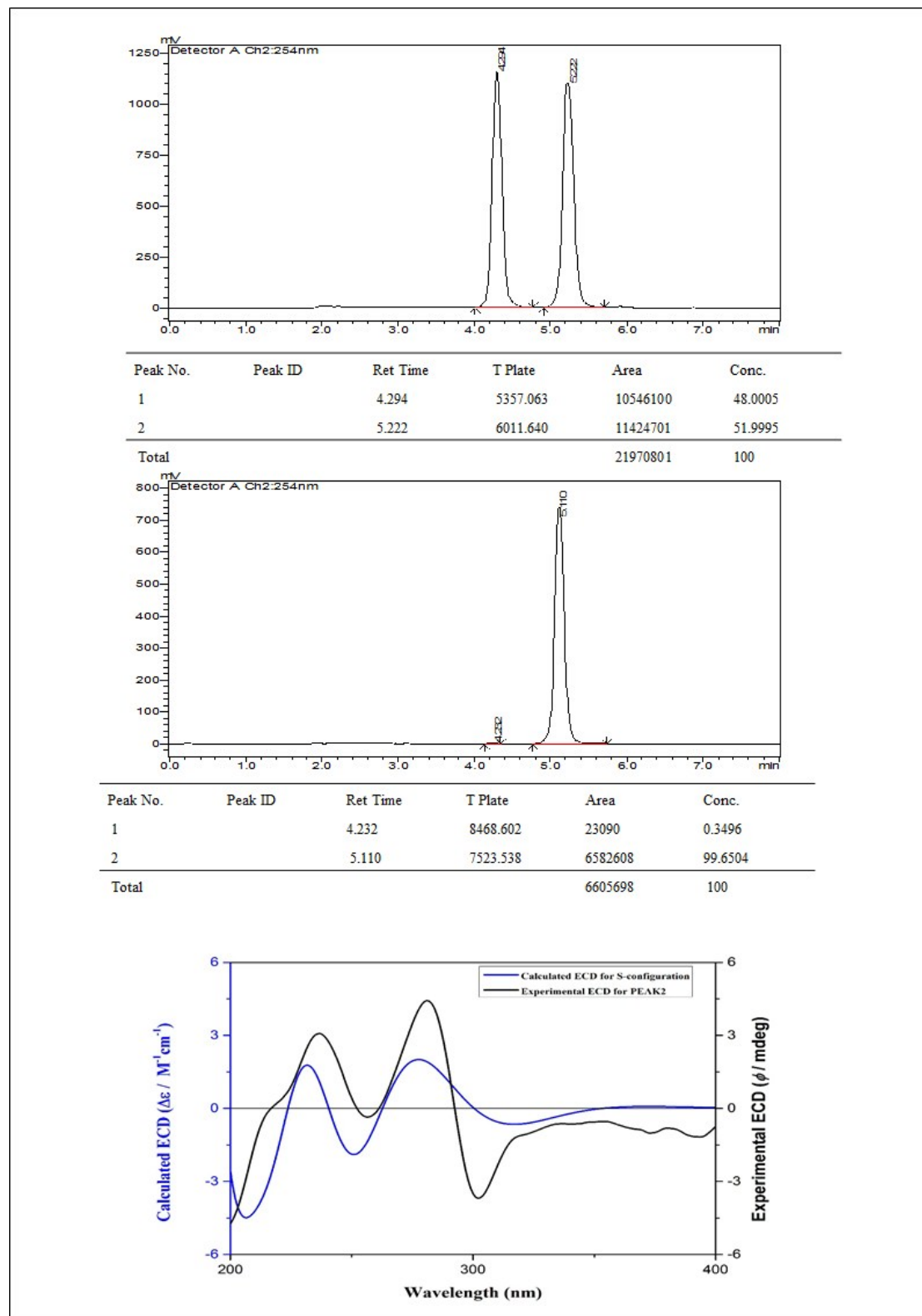


2.2. (*R*)-3-pentylbenzo[*c*]thiophen-1(3*H*)-one ((*R*)-**1**). 91.8% ee. HPLC: chiralpak AD-H column (0.46 cm I.D. × 25 cm L × 5 μm); detected at 254 nm; n-hexane/EtOH/diethylamine = 98/2/0.1 (v/v/v); flow = 1.0 mL/min; retention time: 7.4 min (*R*), 9.1 min (*S*).



3. HPLC and EDC spectra of (*S*)- and (*R*)-**1** prepared by preparative HPLC chiral columns

3.1. (*S*)-3-pentylbenzo[*c*]thiophen-1(3*H*)-one ((*S*)-**1**). 99.3% ee. HPLC: chiralpak AD-H column (0.46 cm I.D. × 25 cm L × 5 μm); detected at 254 nm; n-hexane/EtOH/diethylamine = 98/2/0.1 (v/v/v); flow = 1.0 mL/min; retention time: 4.2 min (*R*), 5.1 min (*S*).



3.2. (*R*)-3-pentylbenzo[*c*]thiophen-1(3*H*)-one ((*R*)-**1**). 99.2% ee. HPLC: chiralpak AD-H column (0.46 cm I.D. × 25 cm L × 5 μm); detected at 254 nm; n-hexane/EtOH/diethylamine = 98/2/0.1 (v/v/v); flow = 1.0 mL/min; retention time: 4.2 min (*R*), 5.2 min (*S*).

