

The novel chiral 2(5*H*)-furanone sulfones possessing terpene moiety: synthesis and biological activity

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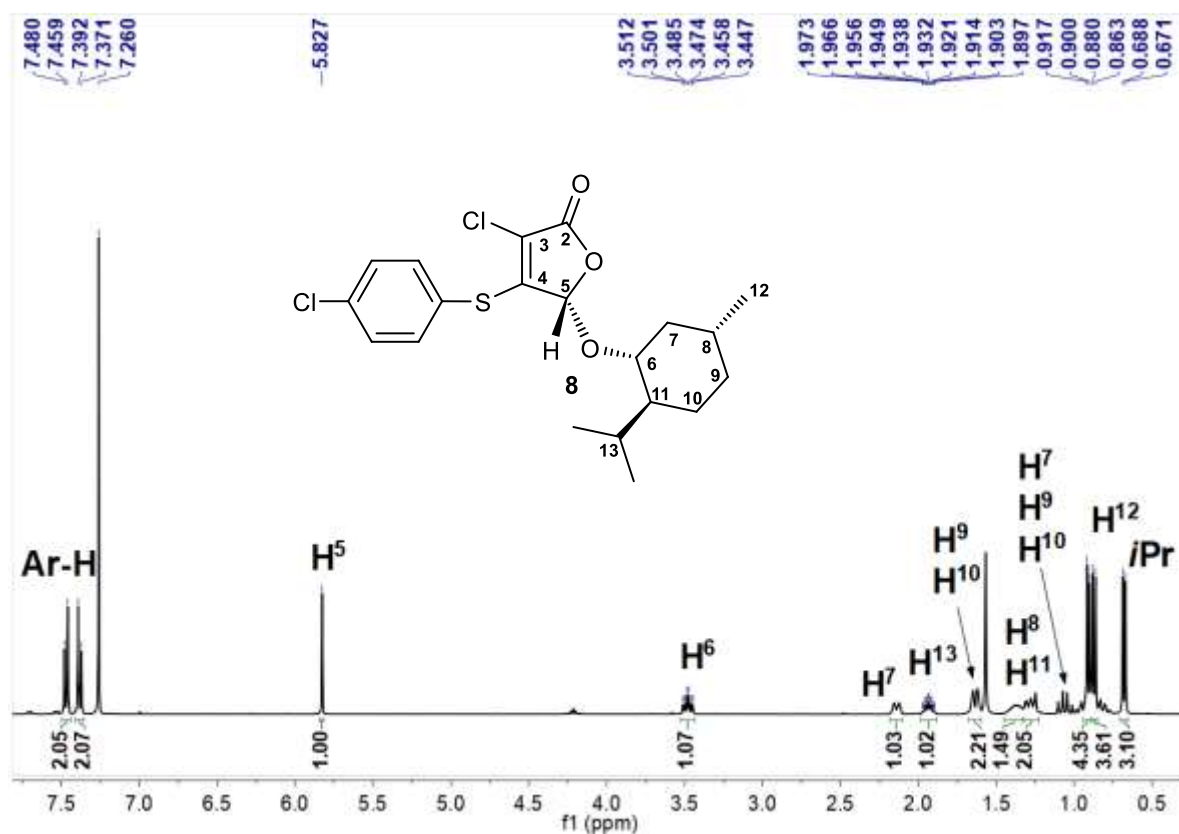
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⁶ N.I. Lobachevsky Institute of Mathematics and Mechanics, Kazan Federal University, 18 Kremlyovskaya Street, 420008 Kazan, Russia

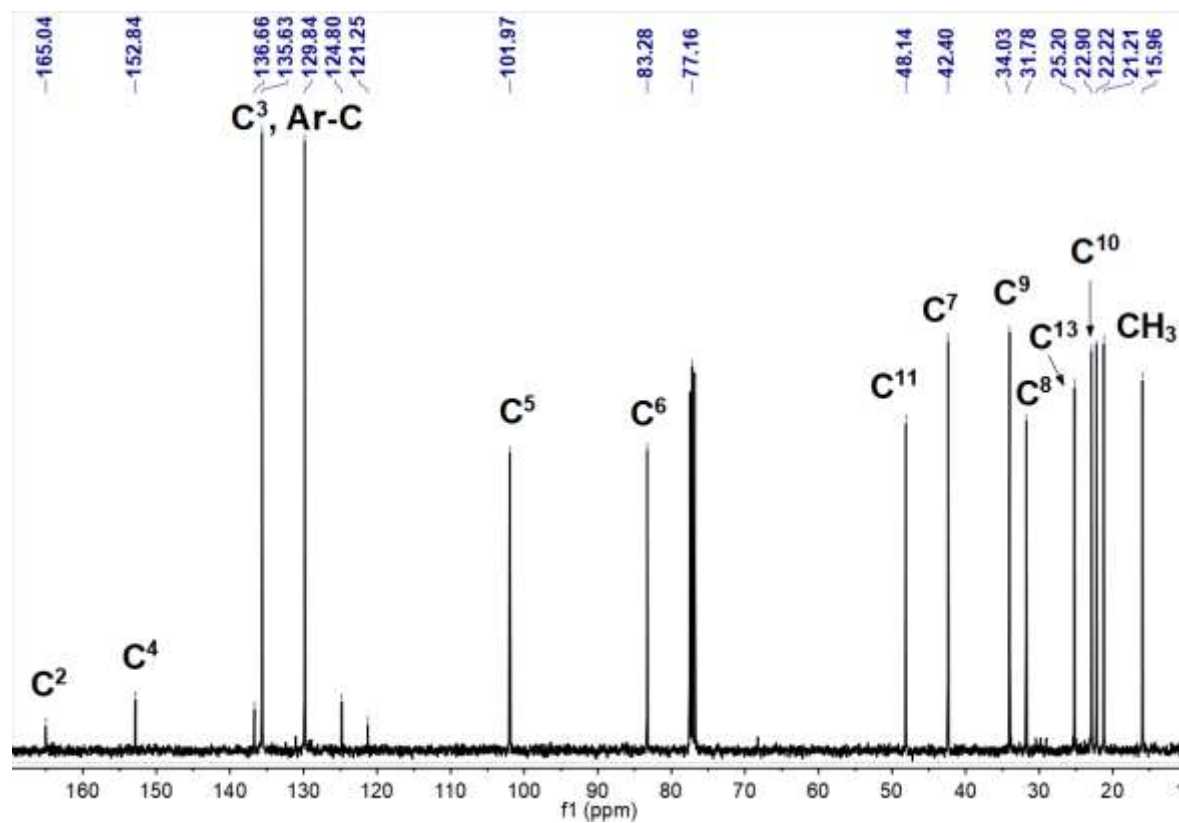
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^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of thioethers

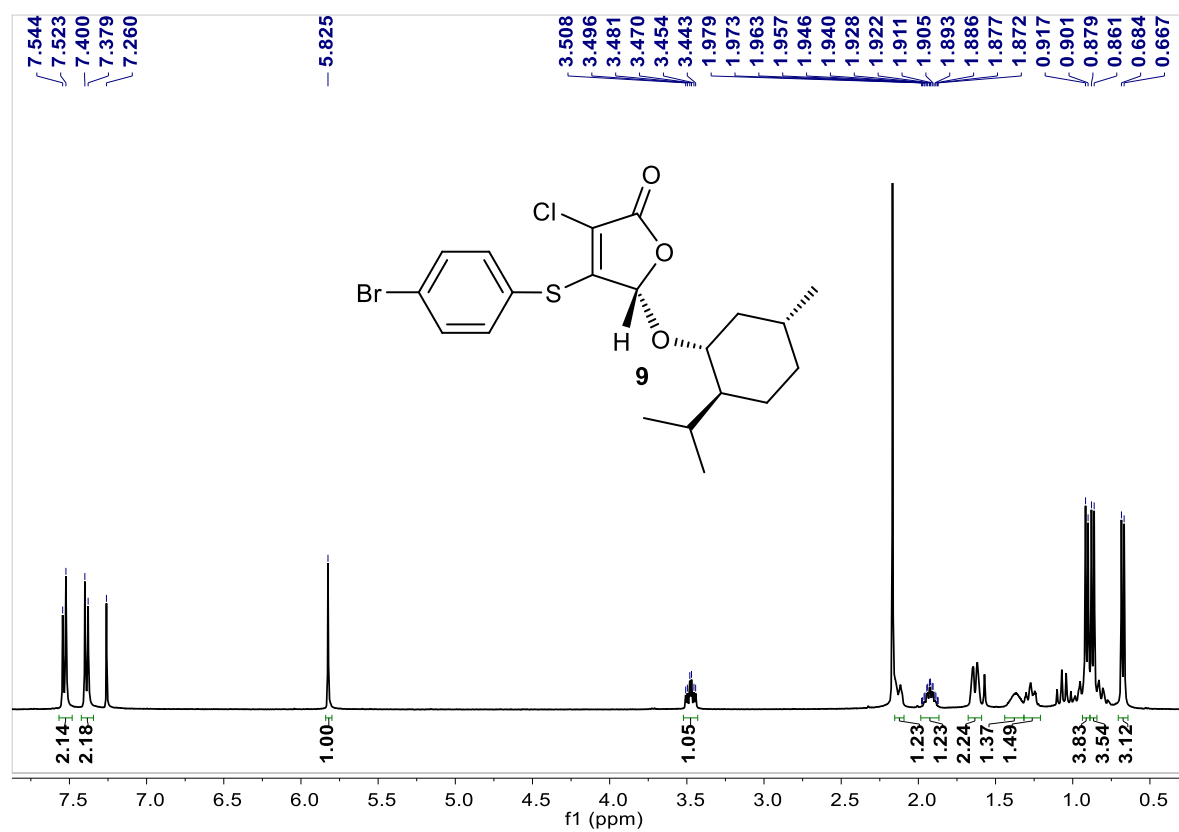
a)



b)

**Figure S1.** ^1H (a) and $^{13}\text{C}\{^1\text{H}\}$ (b) NMR spectra of compound **8** (CDCl_3).

a)



b)

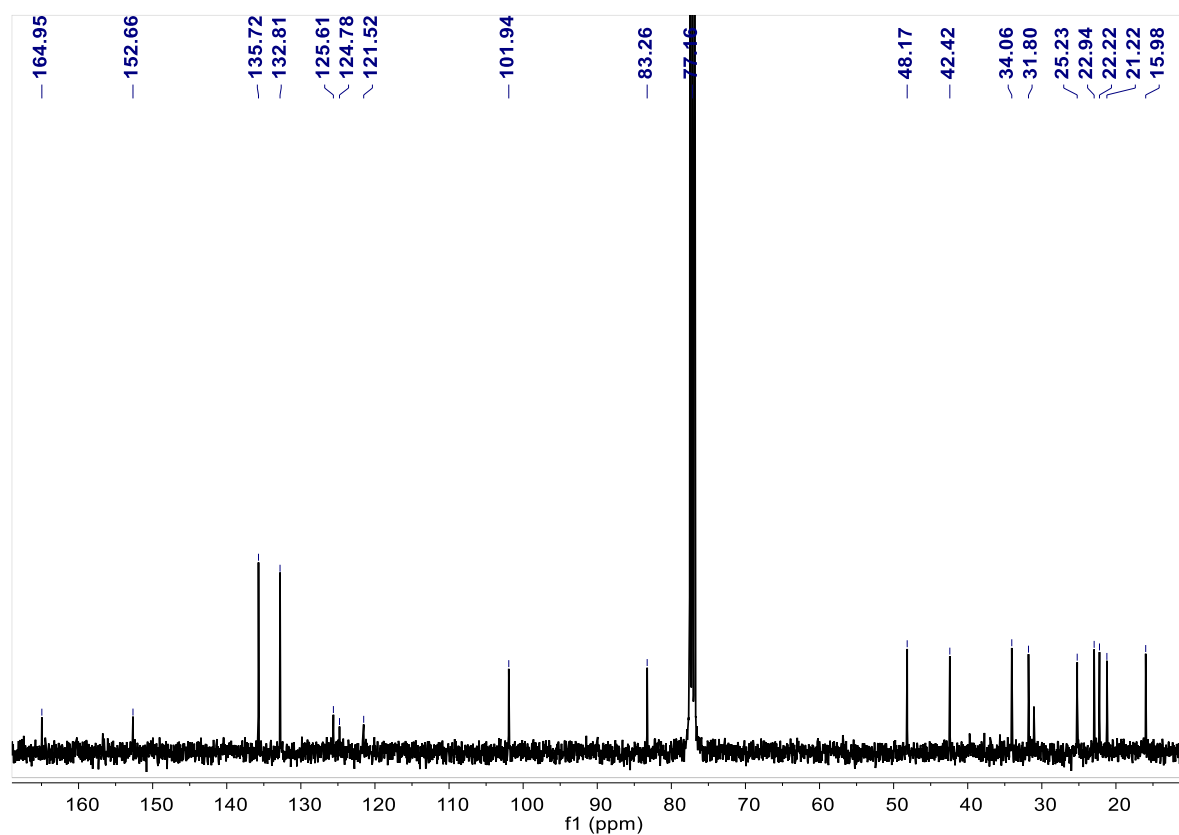
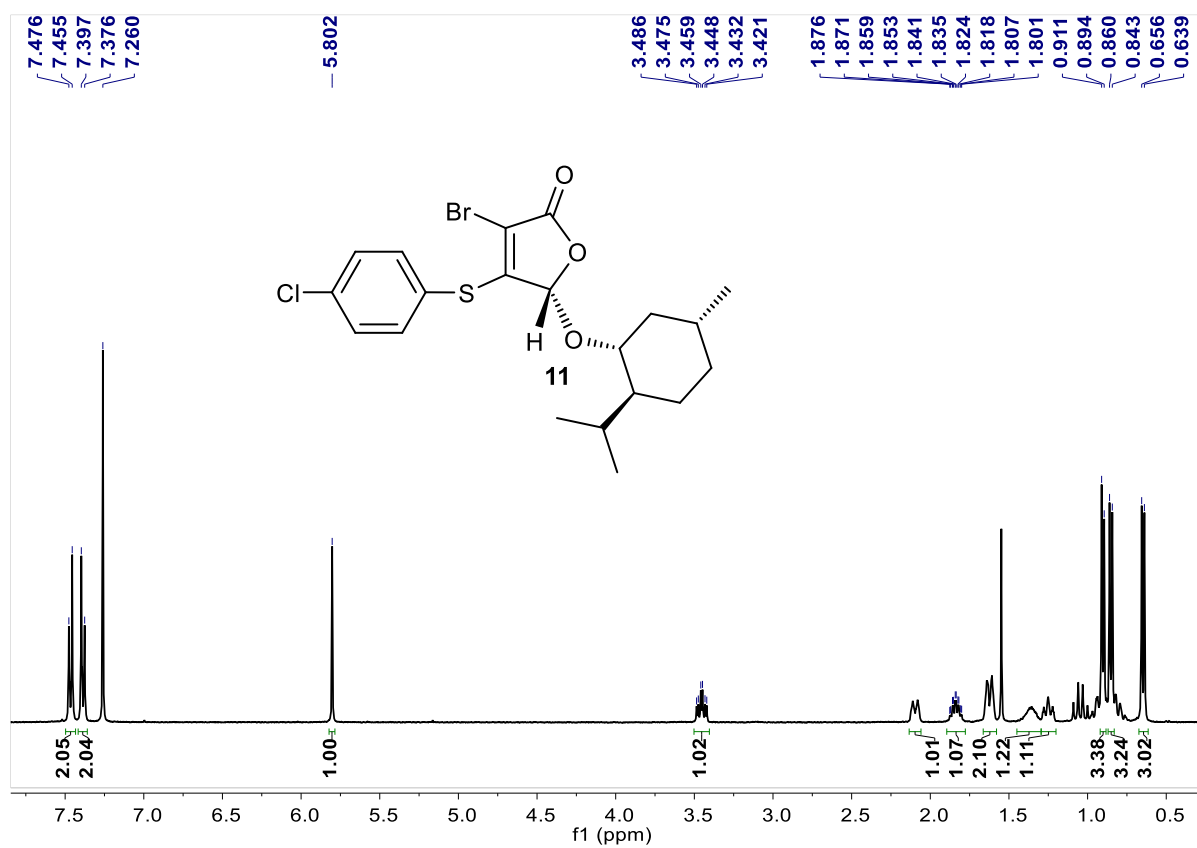


Figure S2. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **9** (CDCl₃).

a)



b)

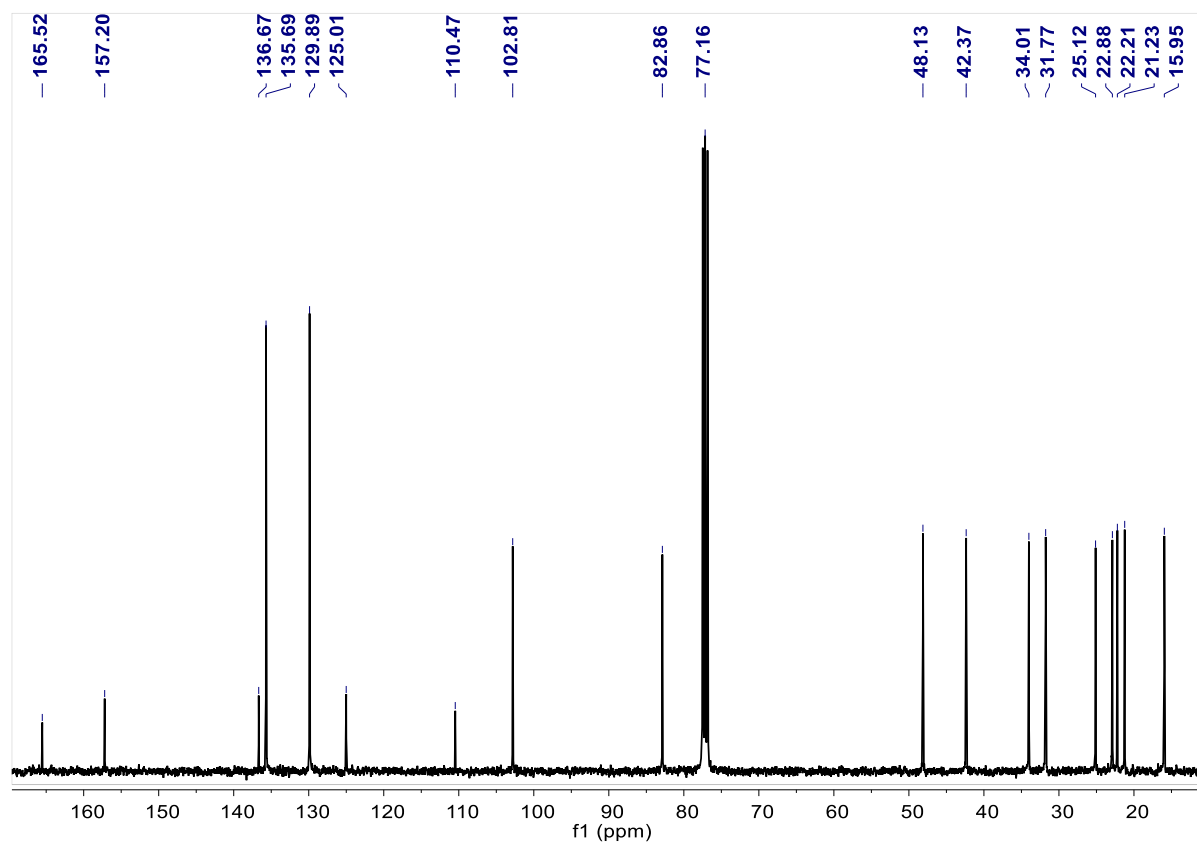
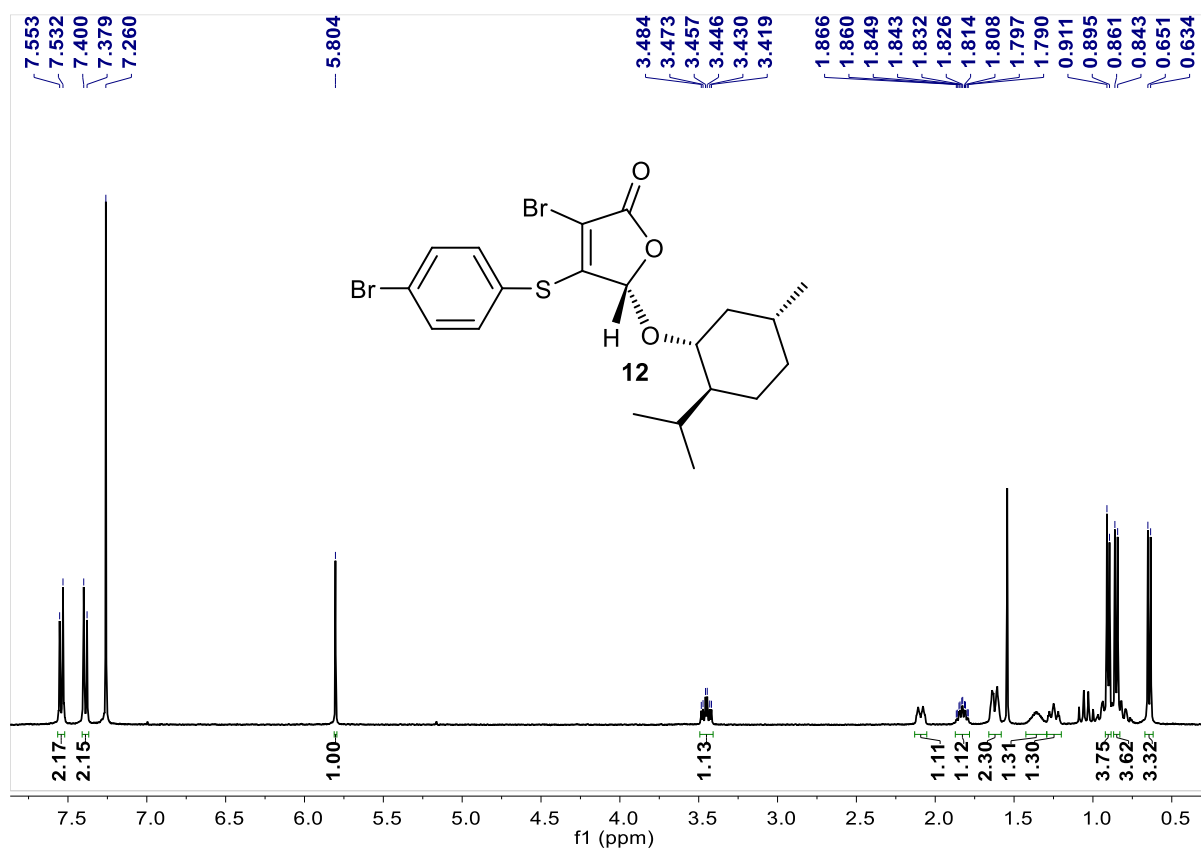


Figure S4. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound 11 (CDCl₃).

a)



b)

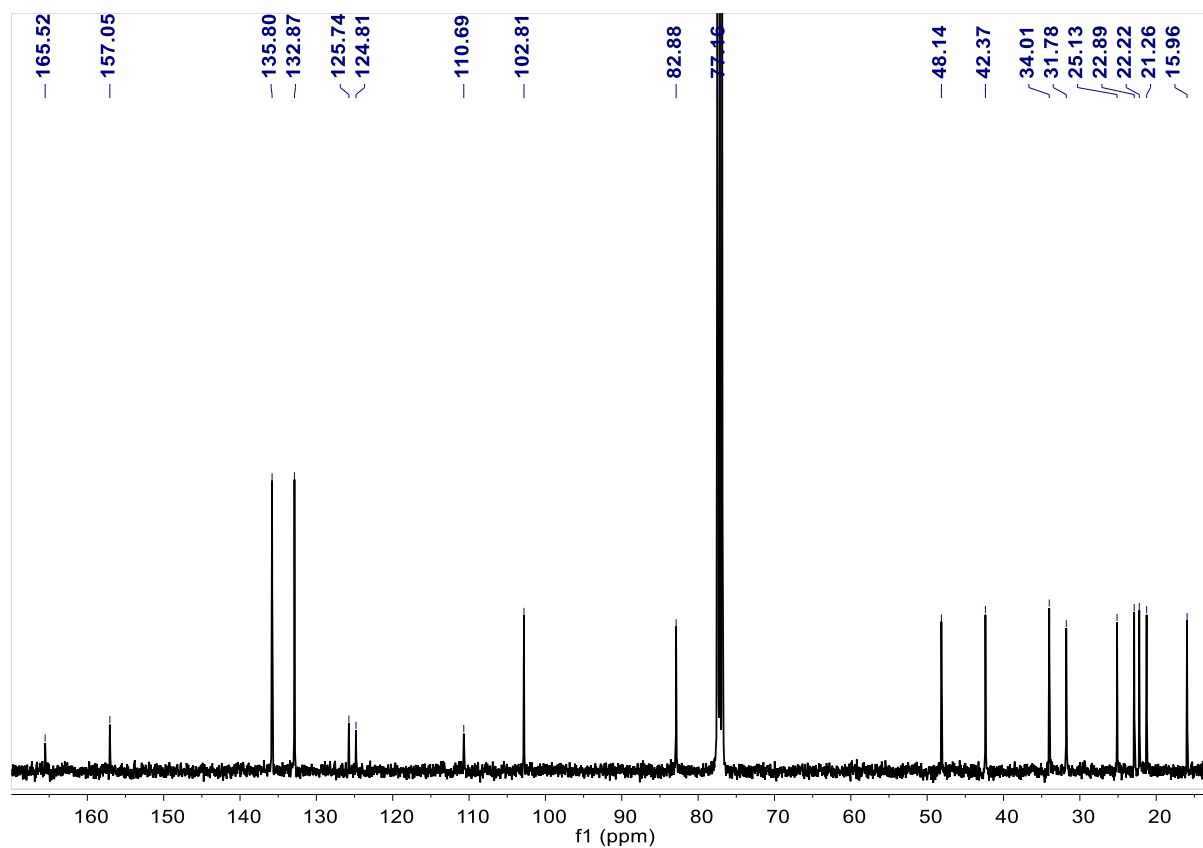
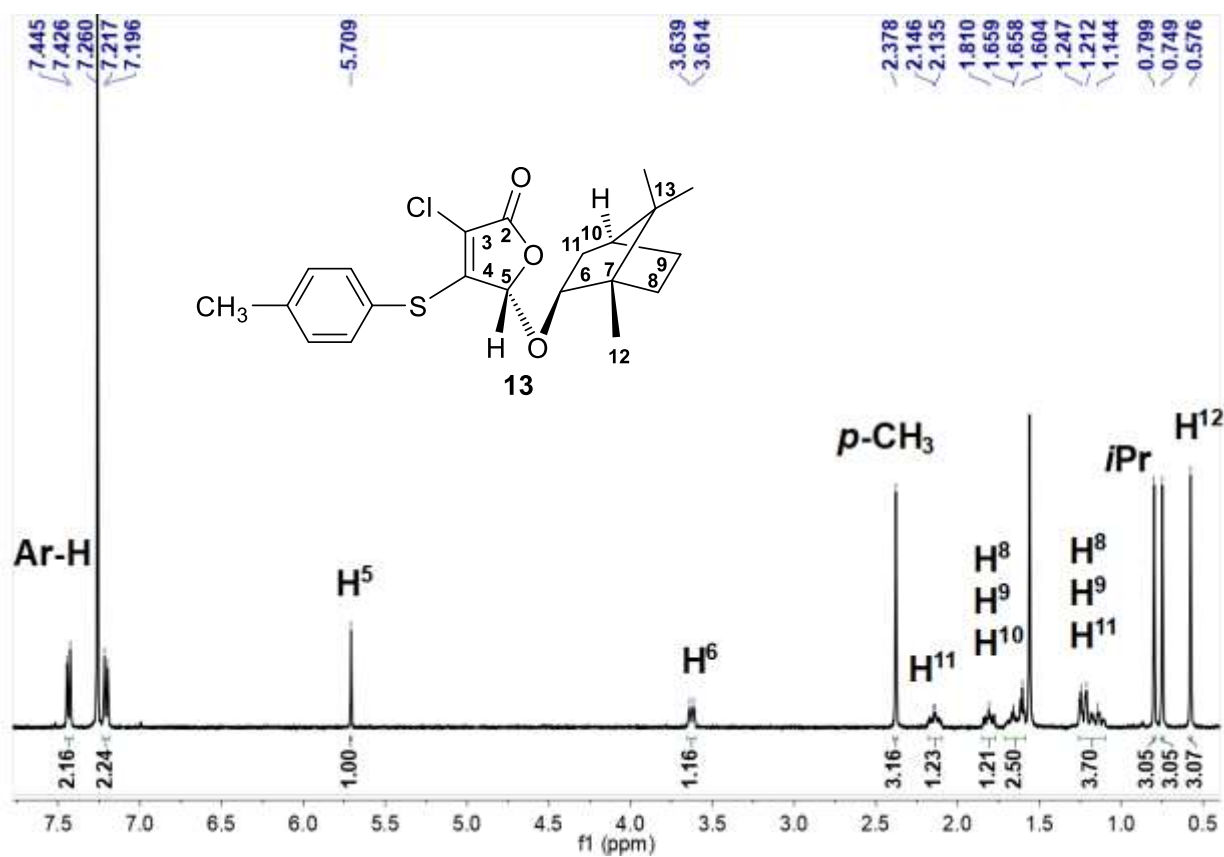


Figure S5. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **12** (CDCl₃).

a)



b)

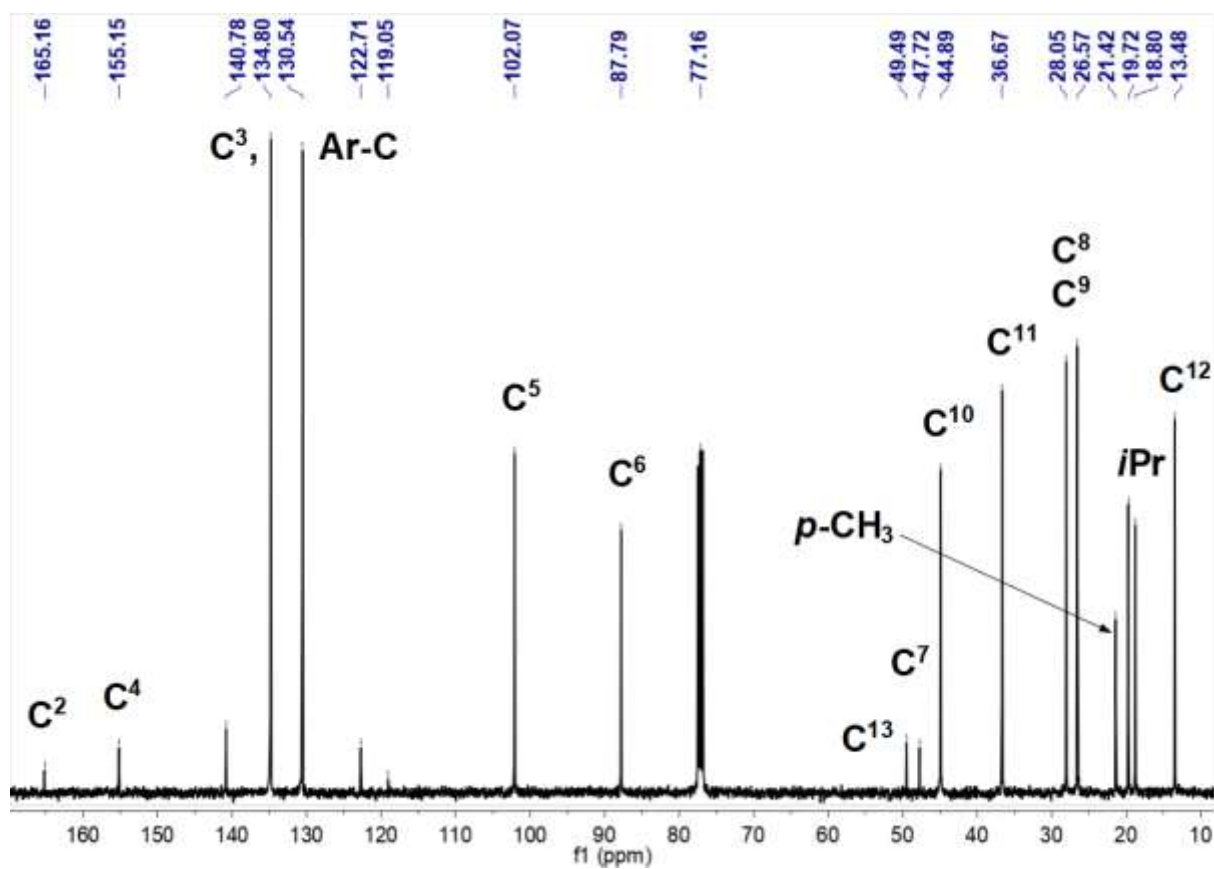
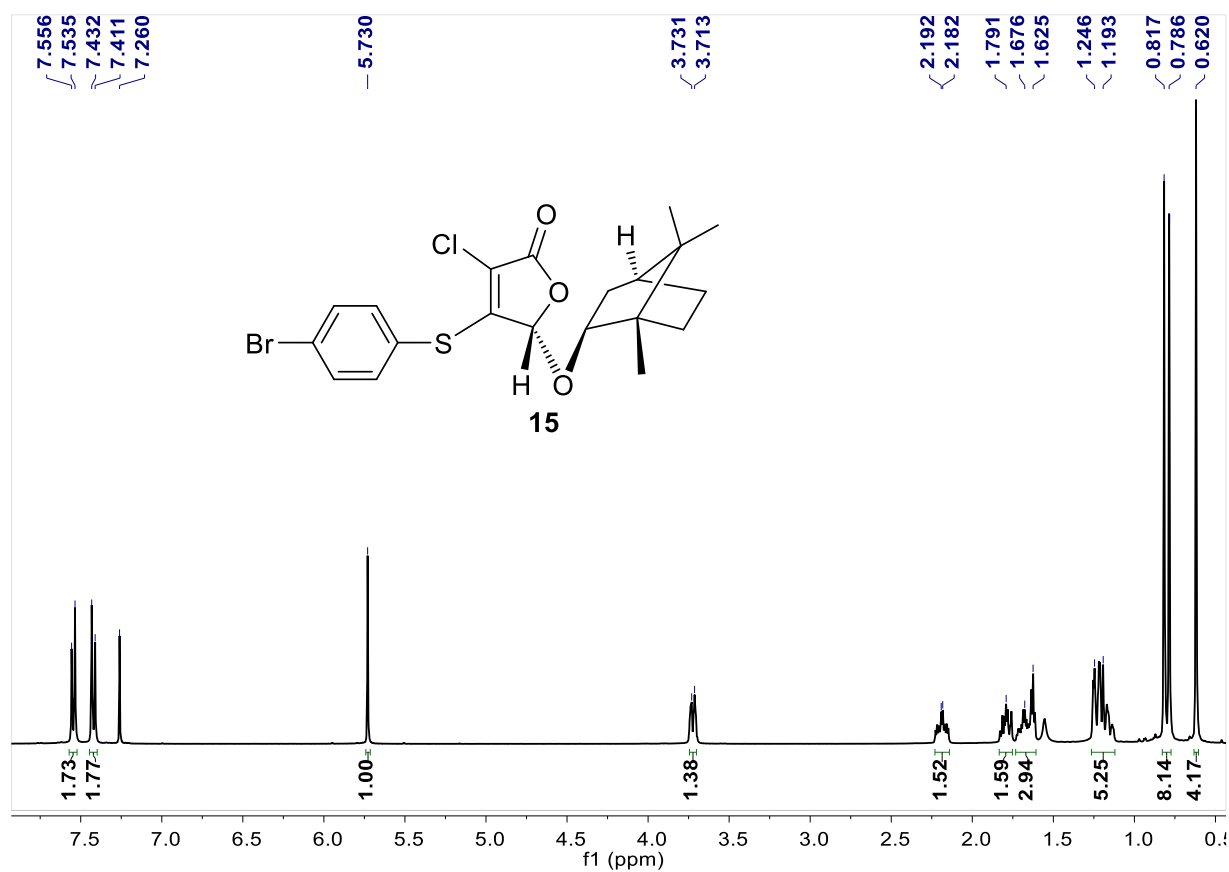


Figure S6. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **13** (CDCl₃).

a)



b)

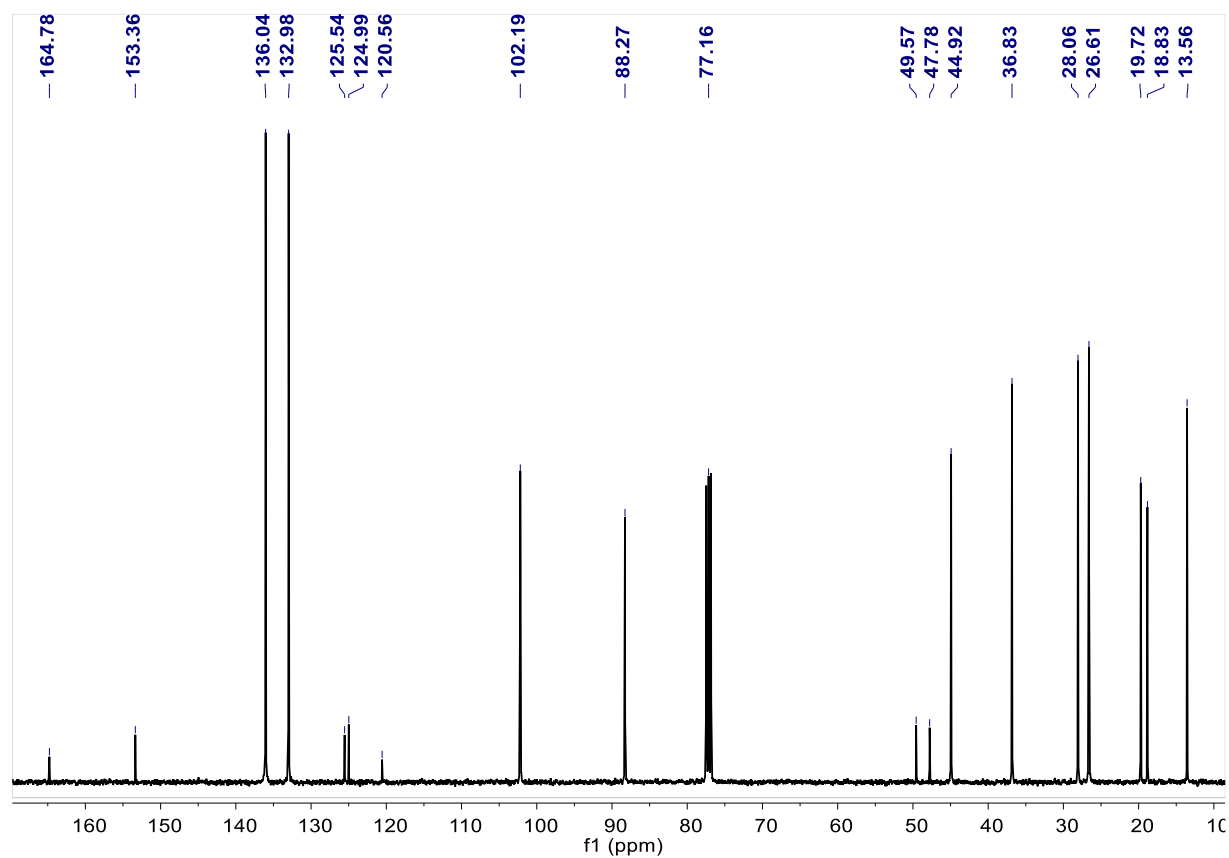
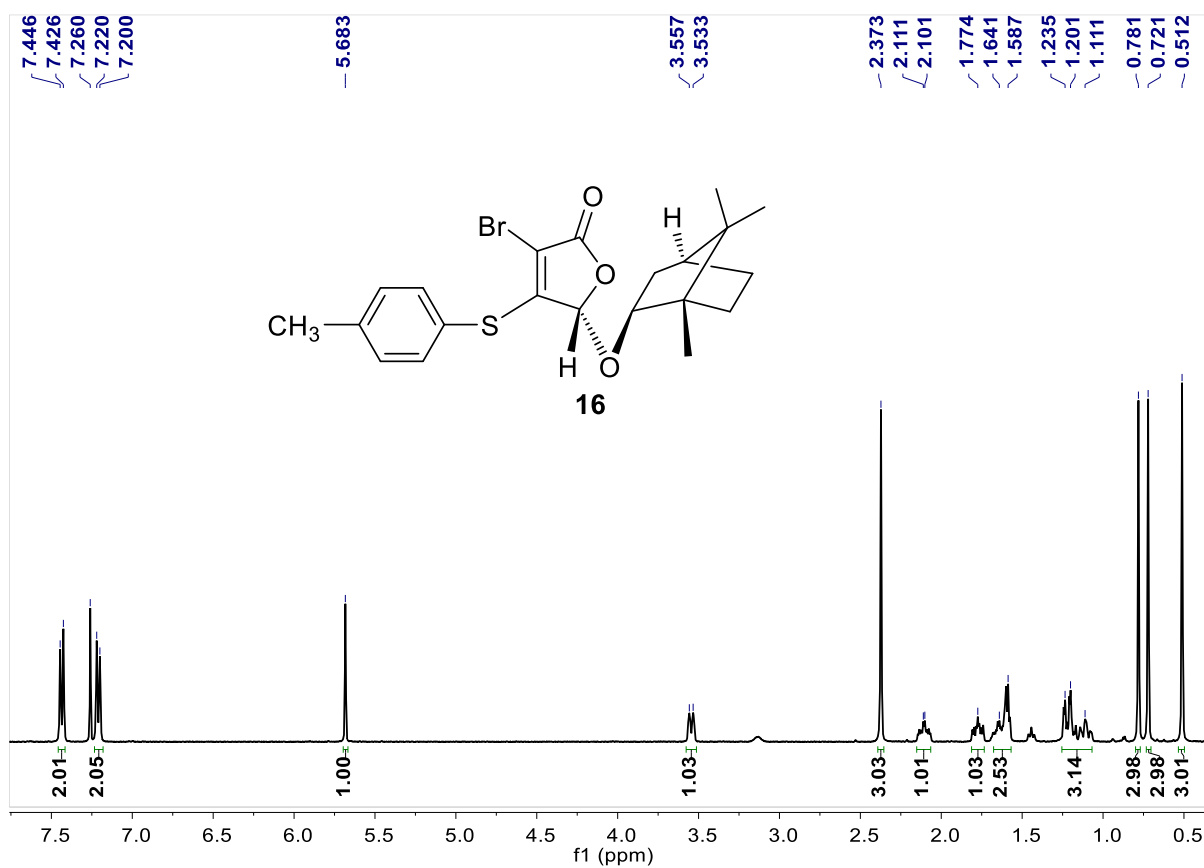


Figure S7. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **15** (CDCl₃).

a)



b)

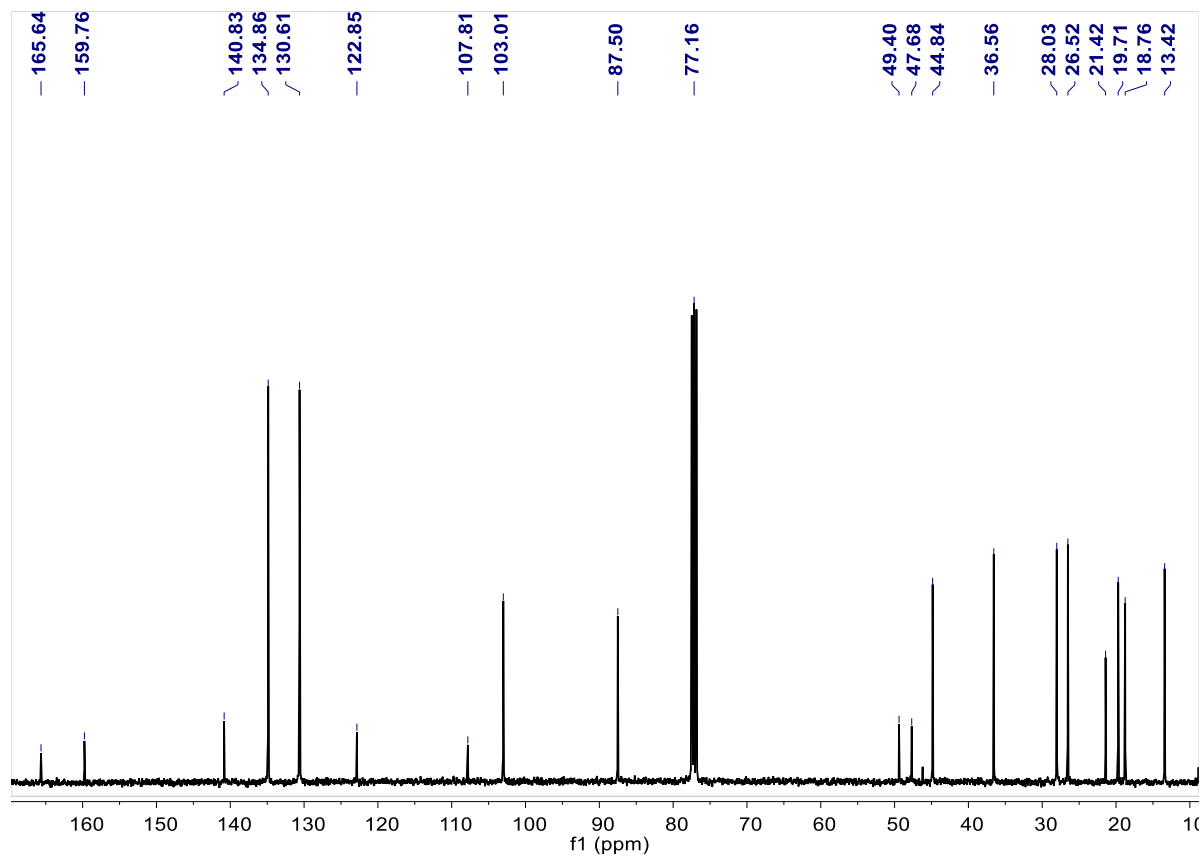
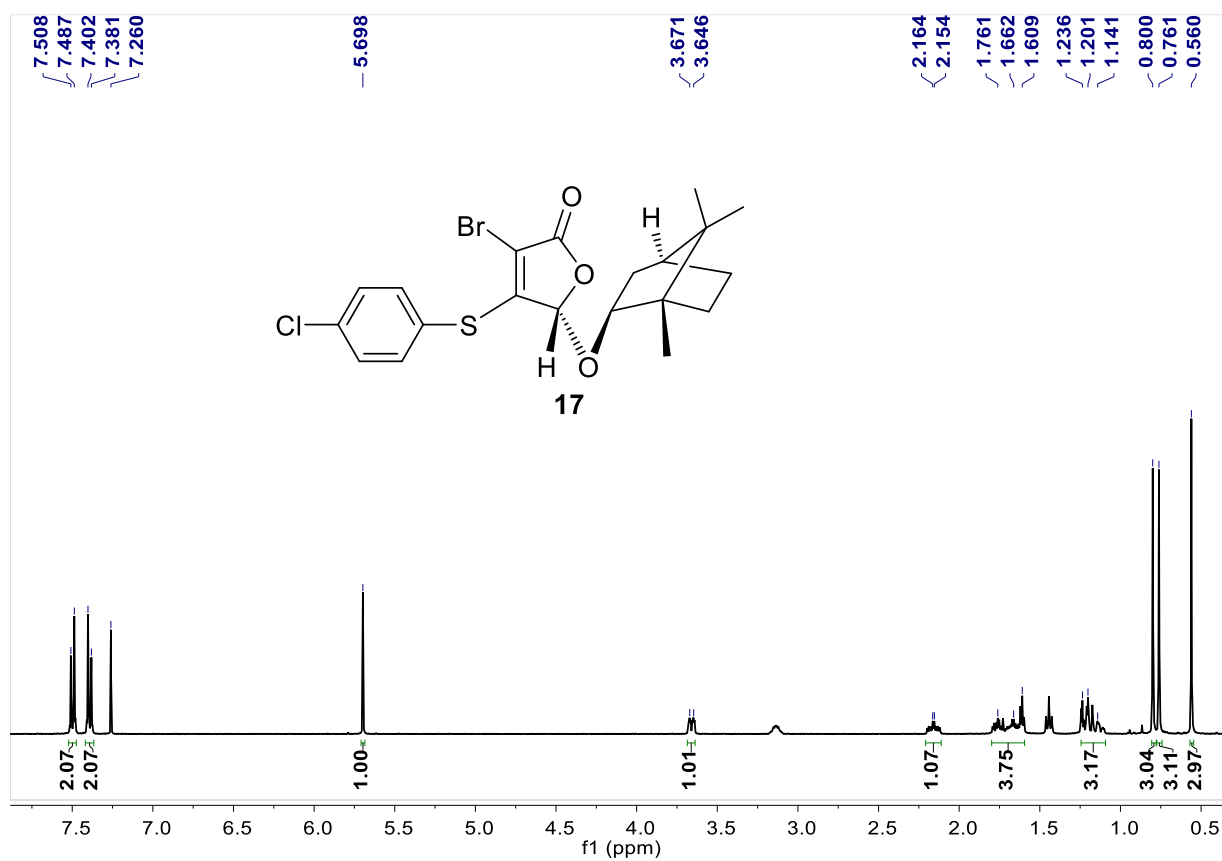


Figure S8. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **16** (CDCl₃).

a)



b)

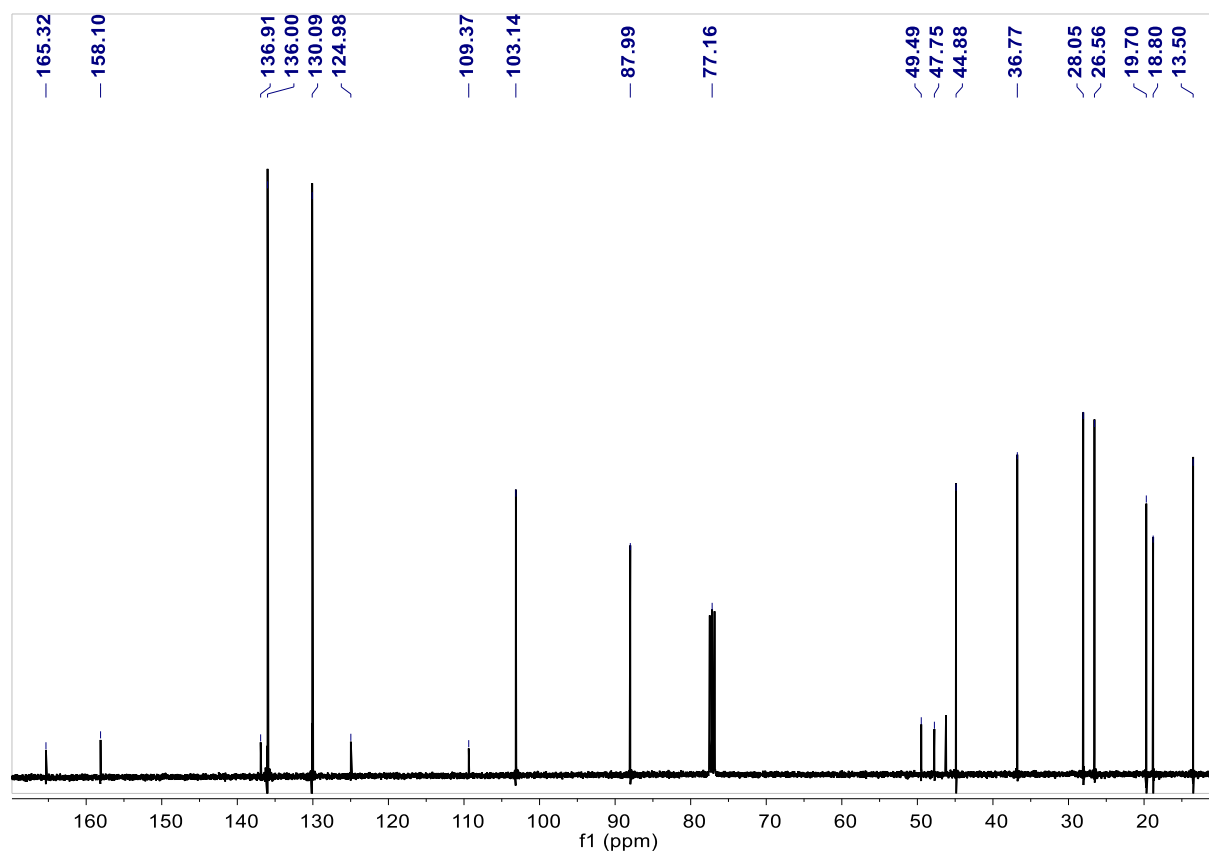
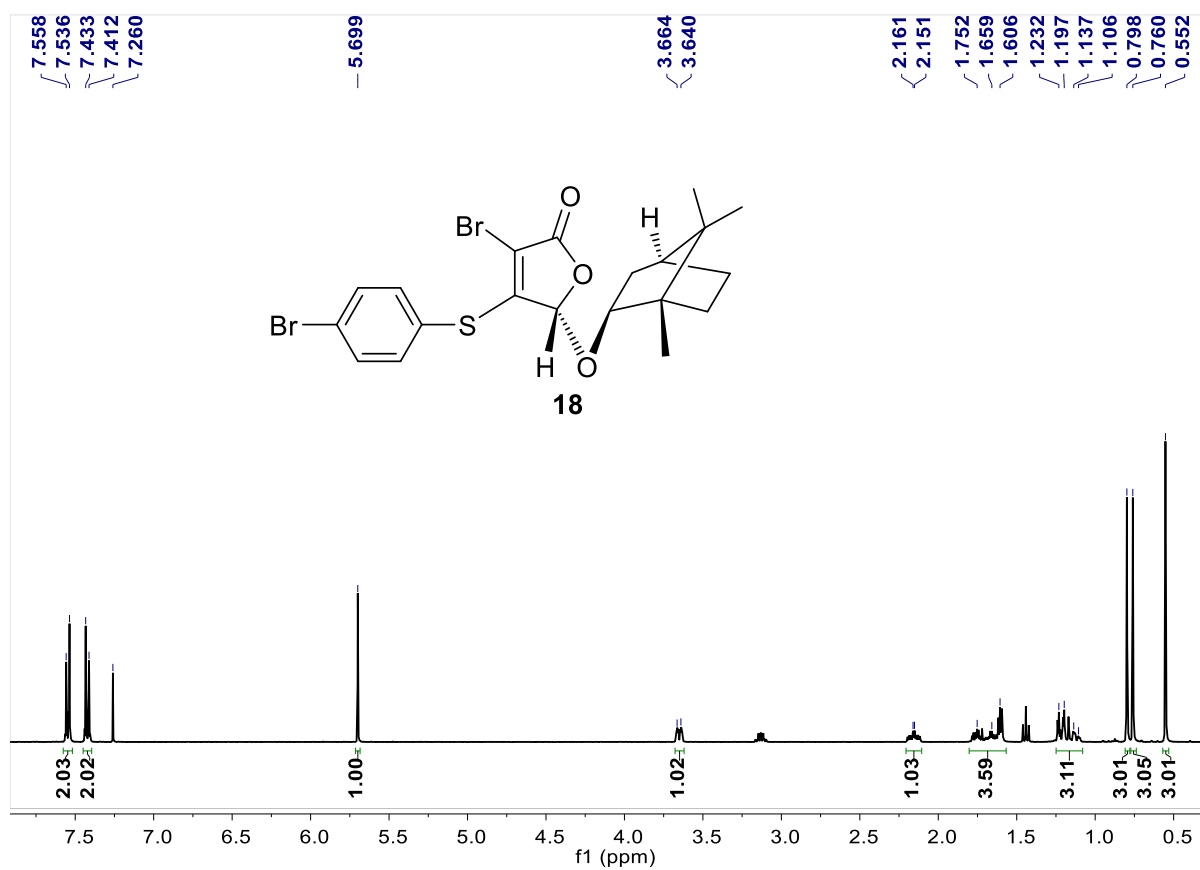


Figure S9. ^1H (a) and $^{13}\text{C}\{^1\text{H}\}$ (b) NMR spectra of compound **17** (CDCl_3).

a)



b)

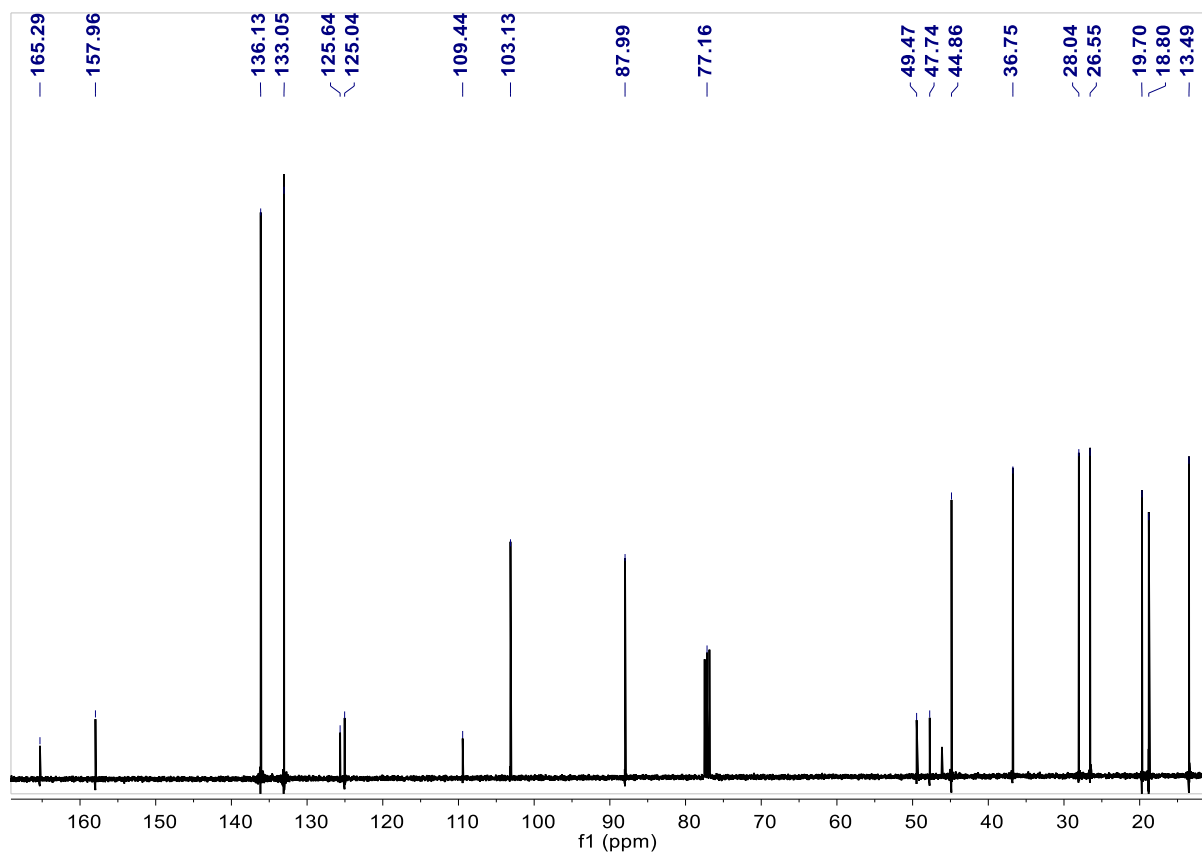
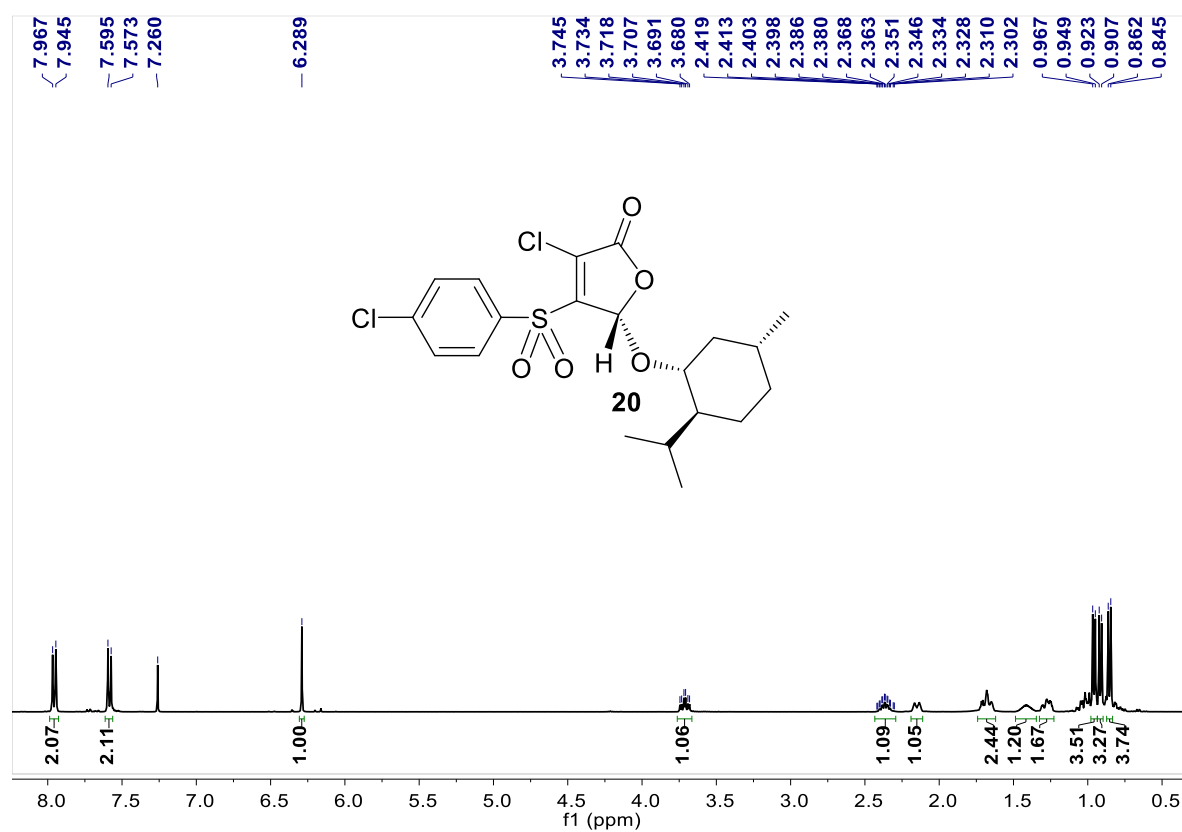


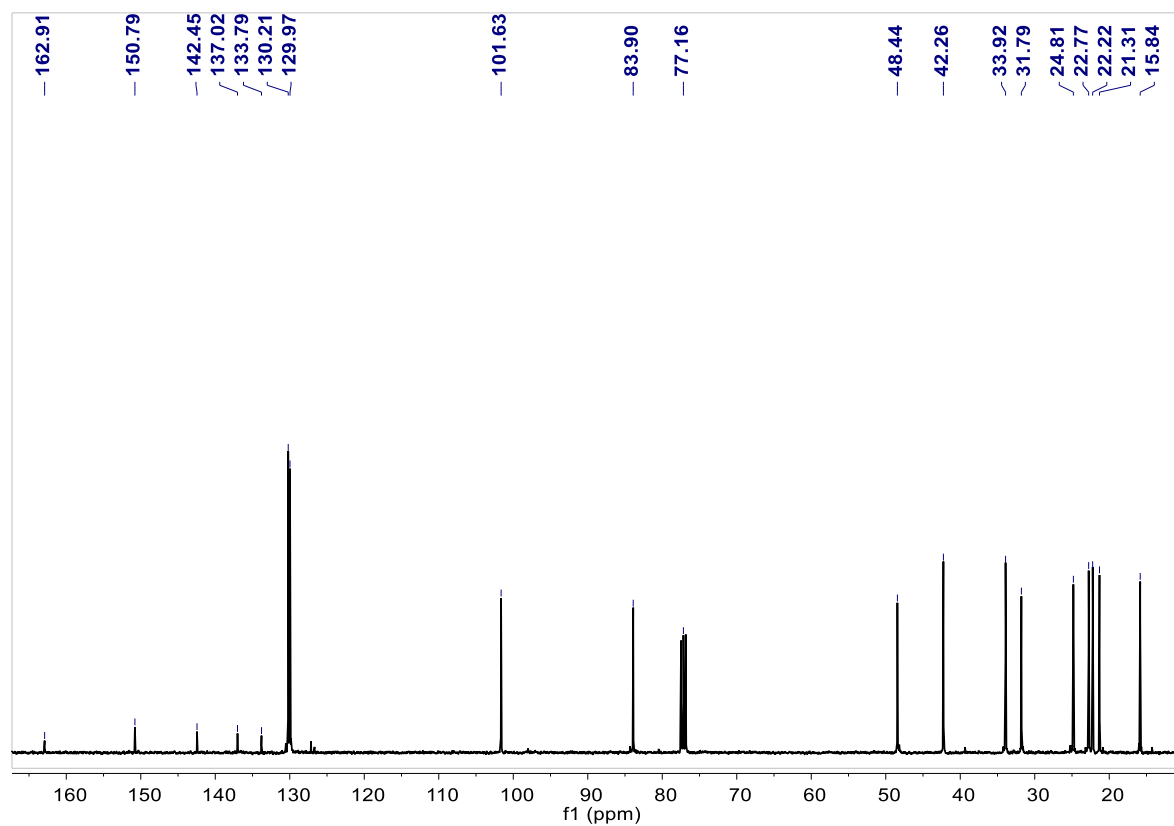
Figure S10. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **18** (CDCl₃).

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of sulfones

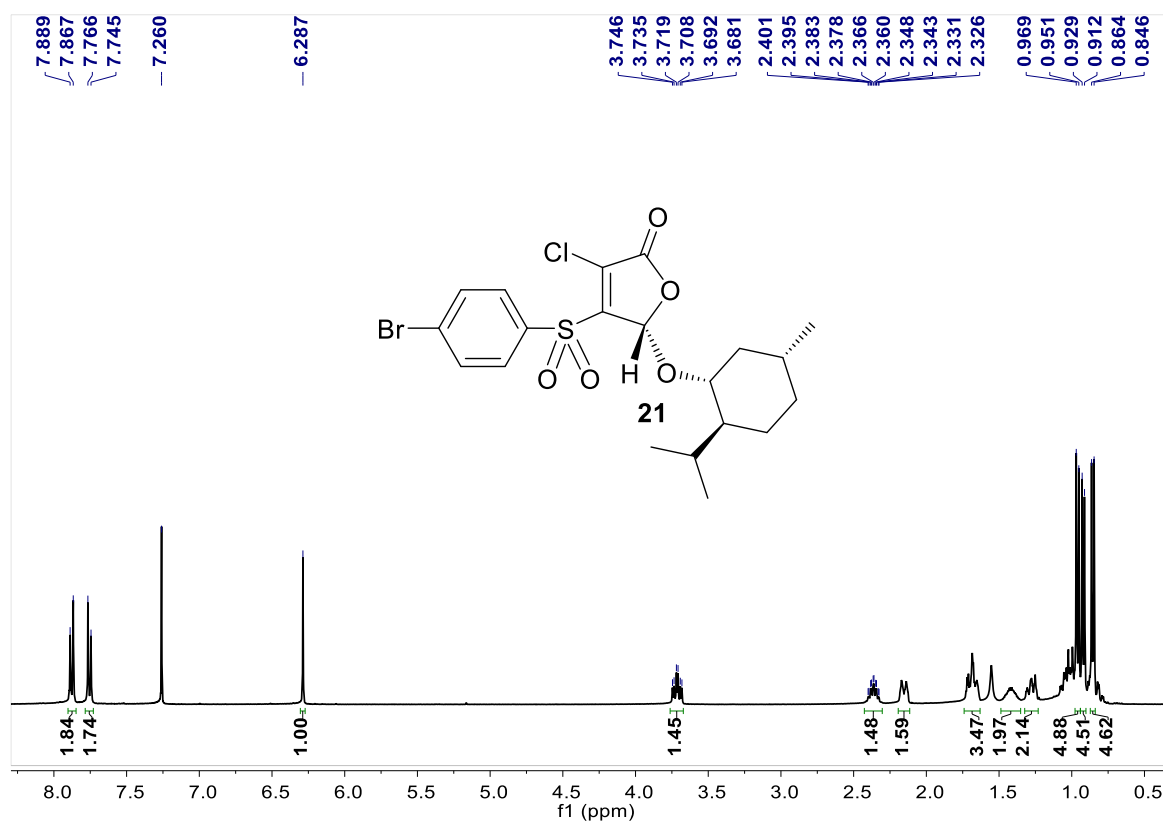
a)



b)

**Figure S11.** ^1H (a) and $^{13}\text{C}\{^1\text{H}\}$ (b) NMR spectra of compound **20** (CDCl₃).

a)



b)

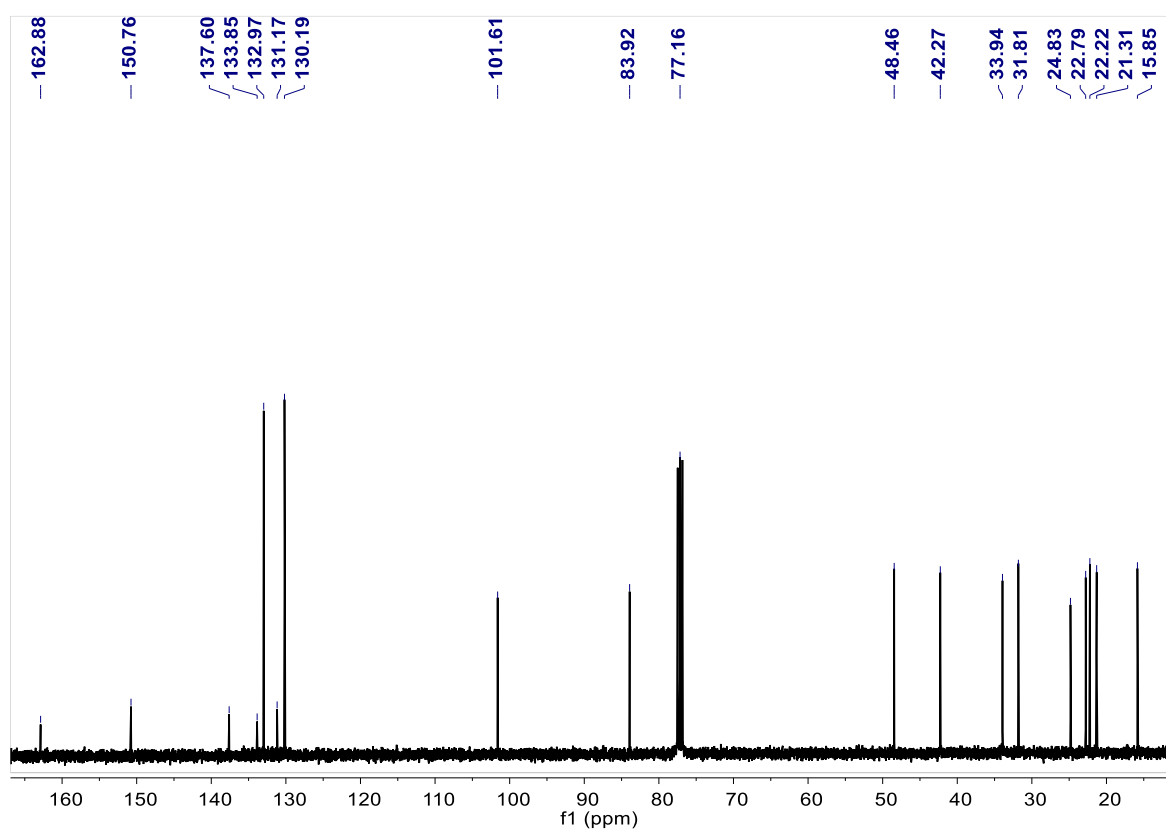
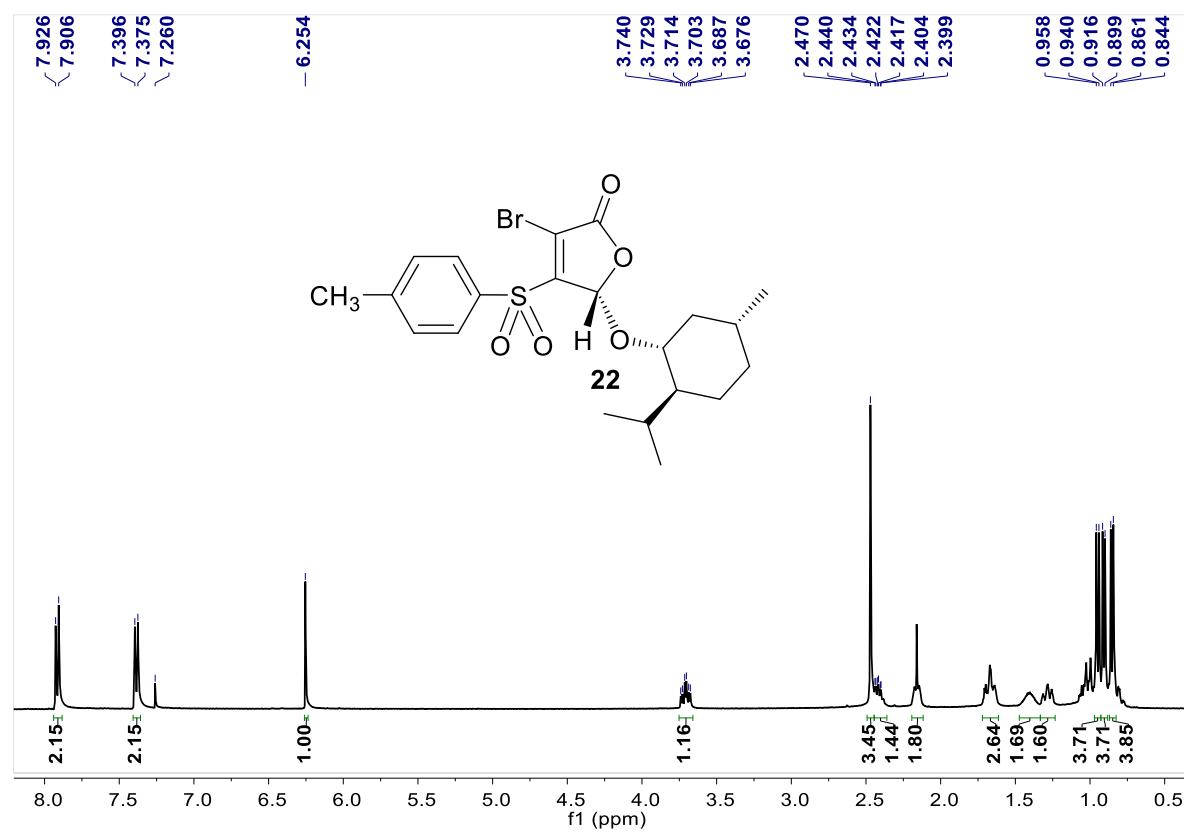


Figure S12. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **21** (CDCl₃).

a)



b)

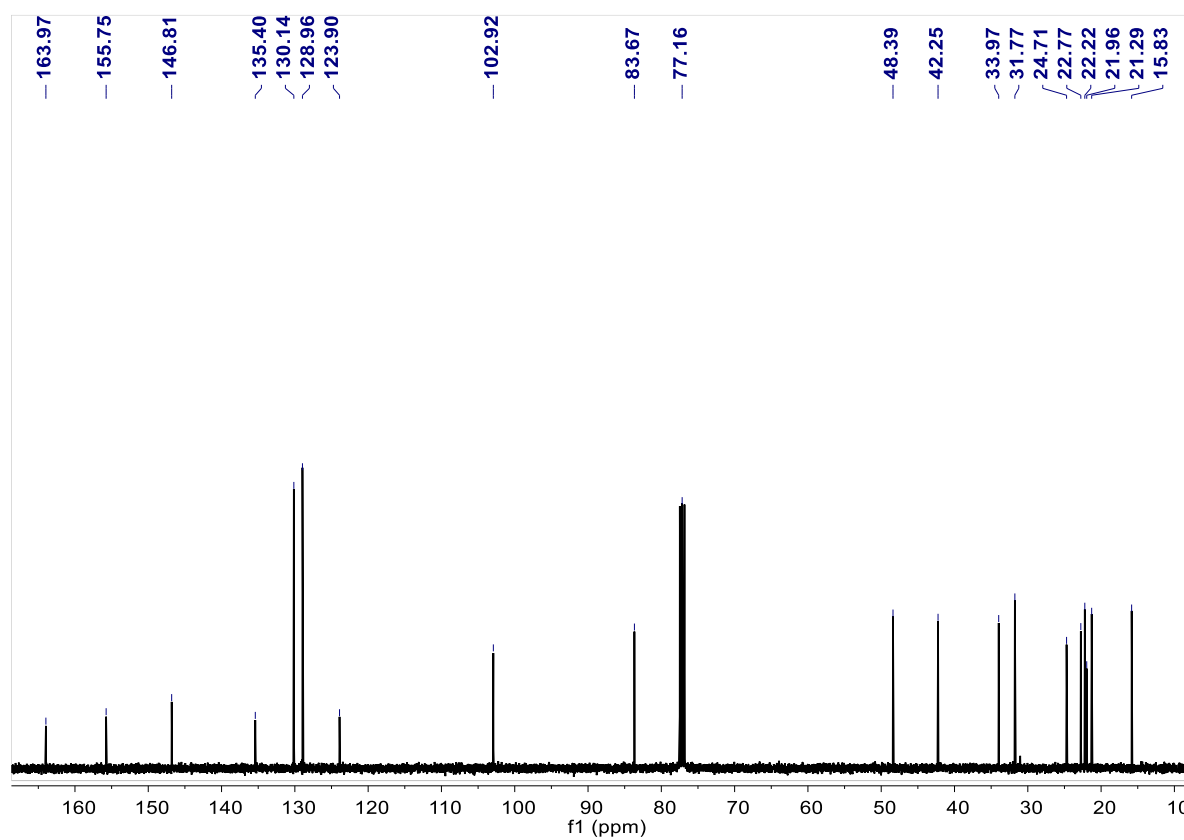
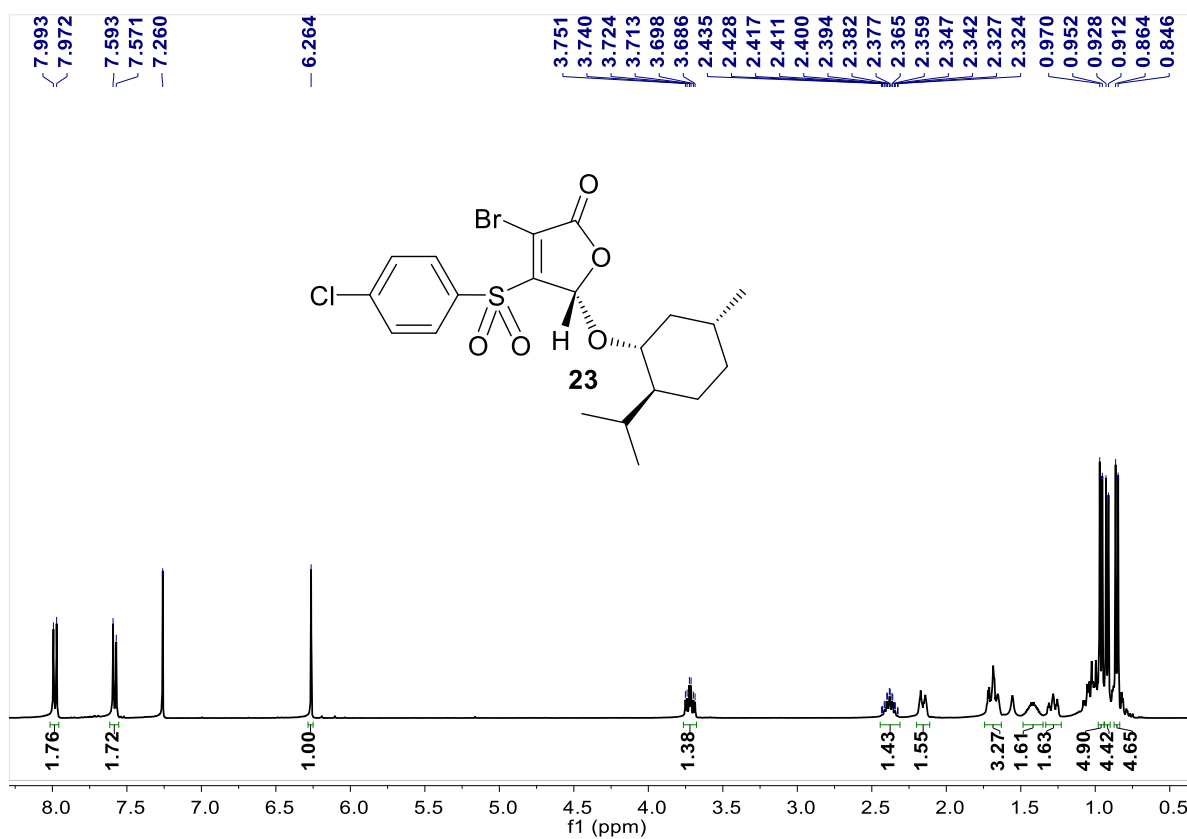


Figure S13. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **22** (CDCl₃).

a)



b)

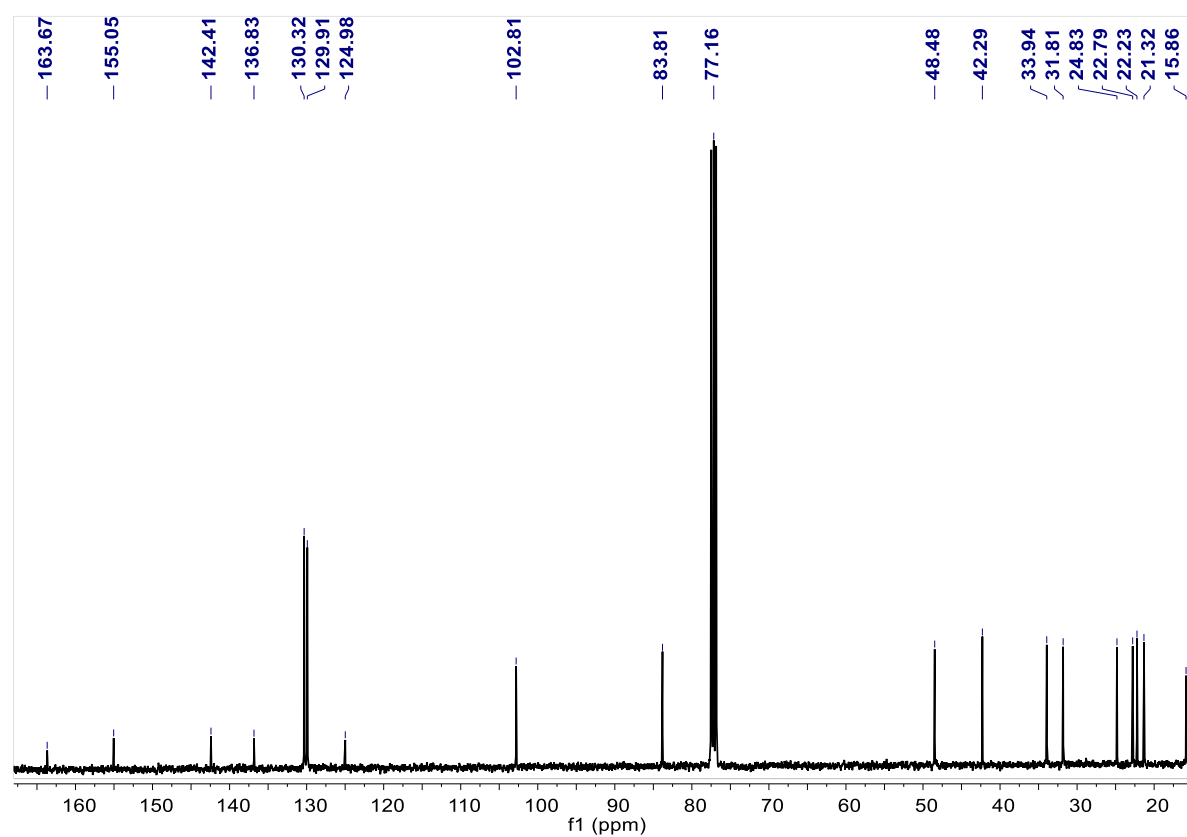
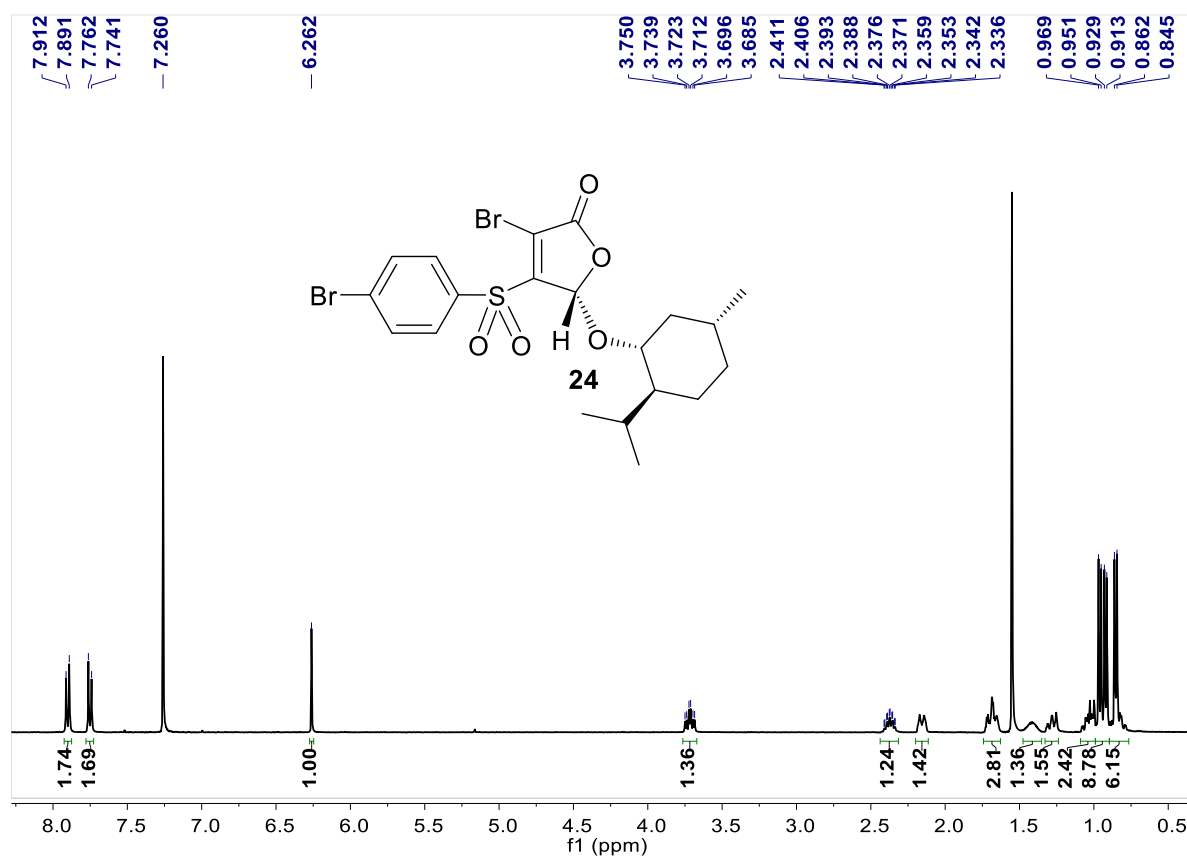


Figure S14. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **23** (CDCl₃).

a)



b)

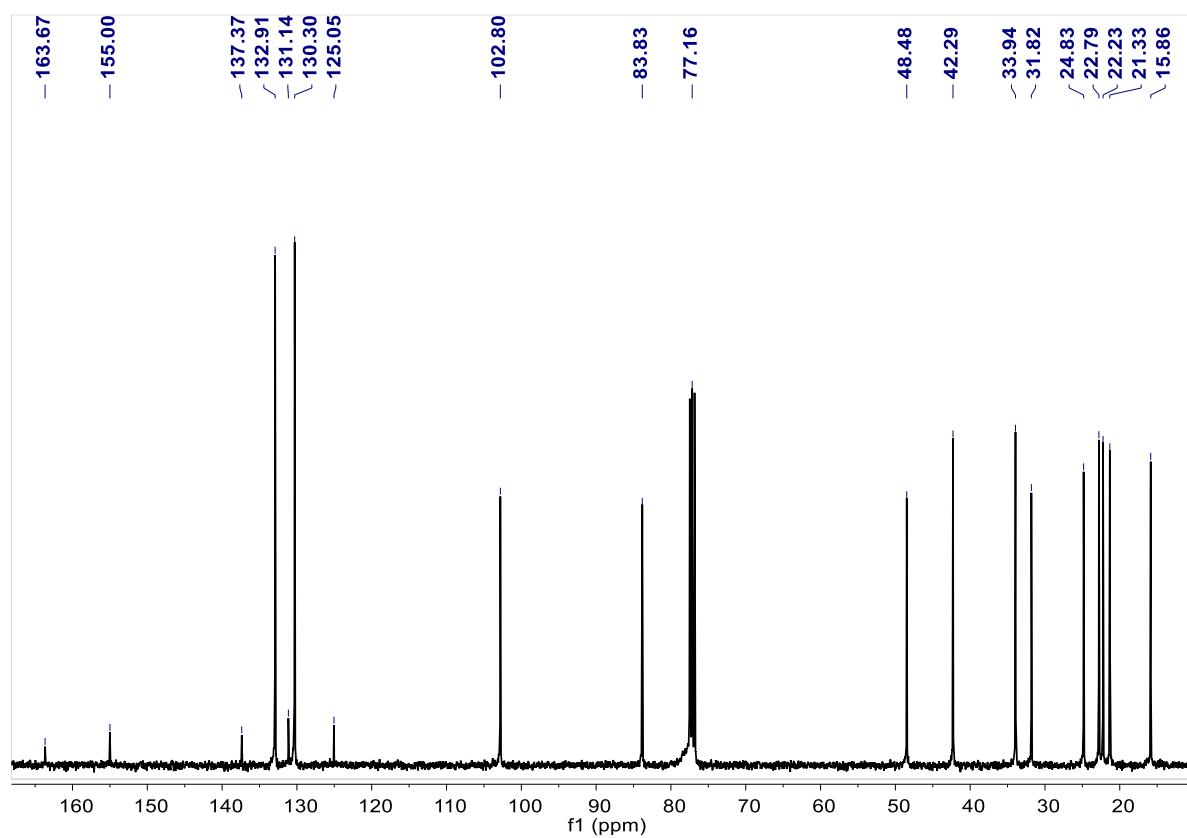
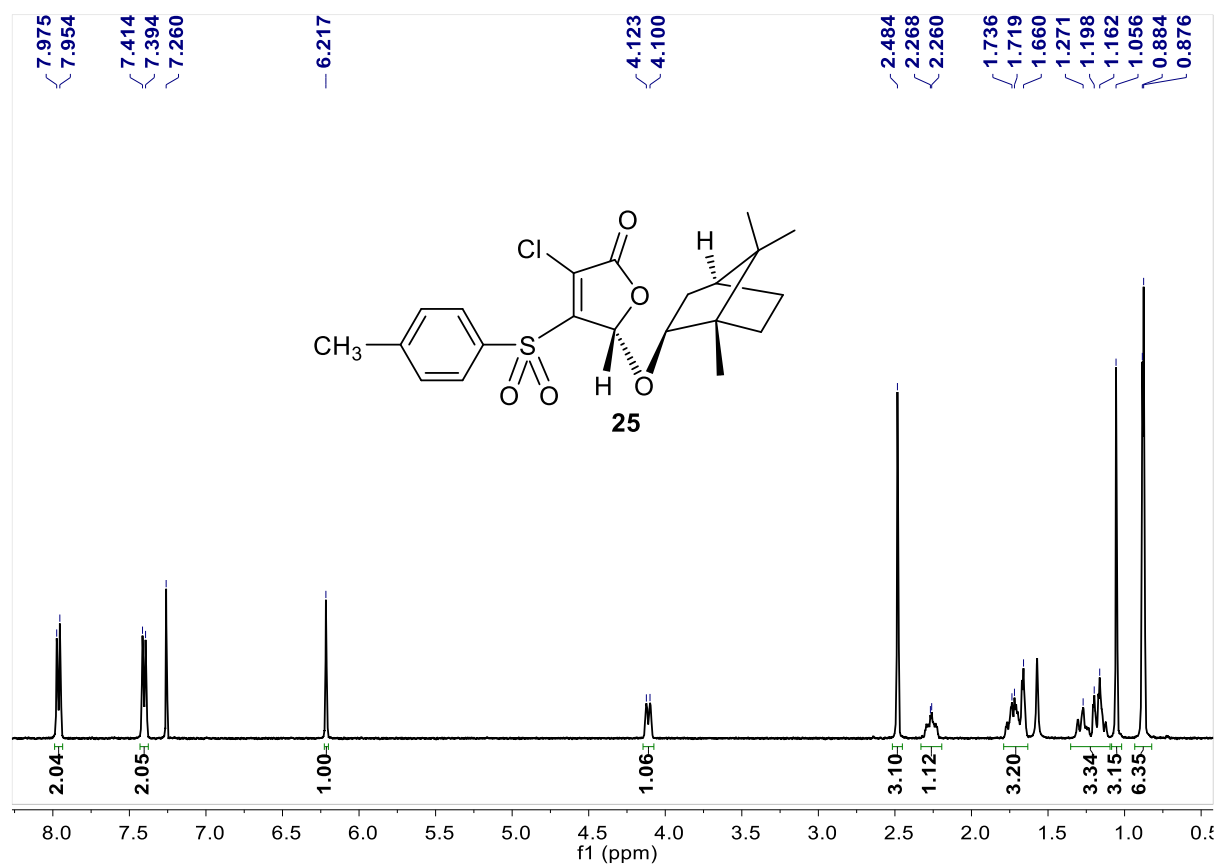


Figure S15. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **24** (CDCl₃).

a)



b)

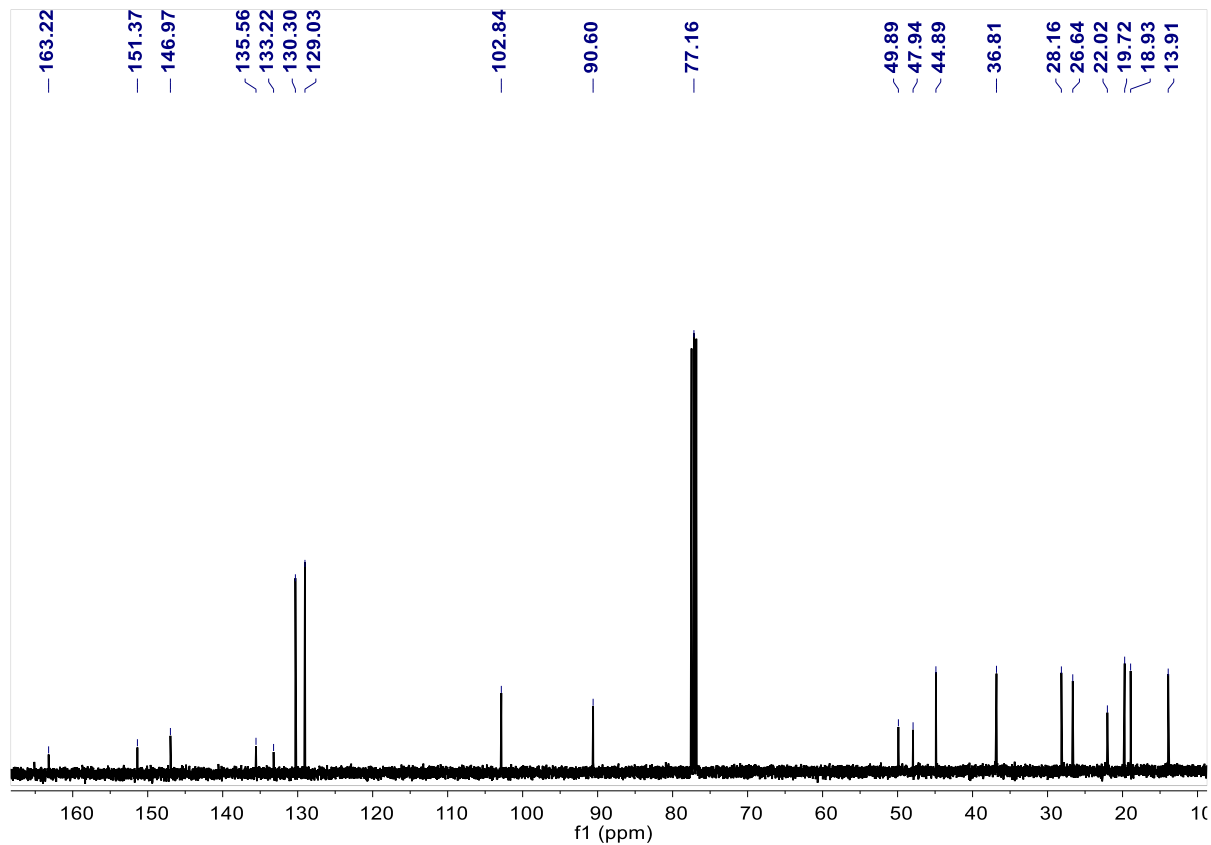
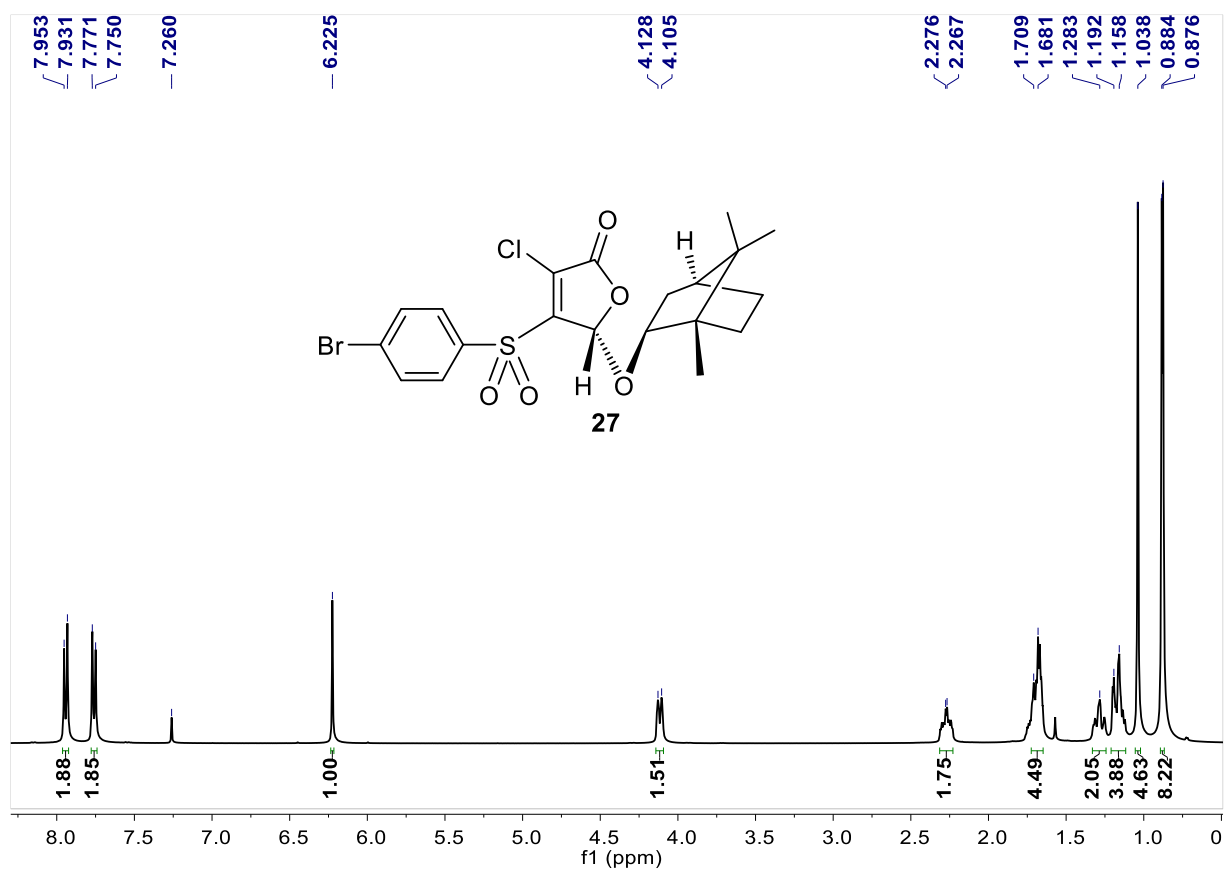


Figure S16. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **25** (CDCl₃).

a)



b)

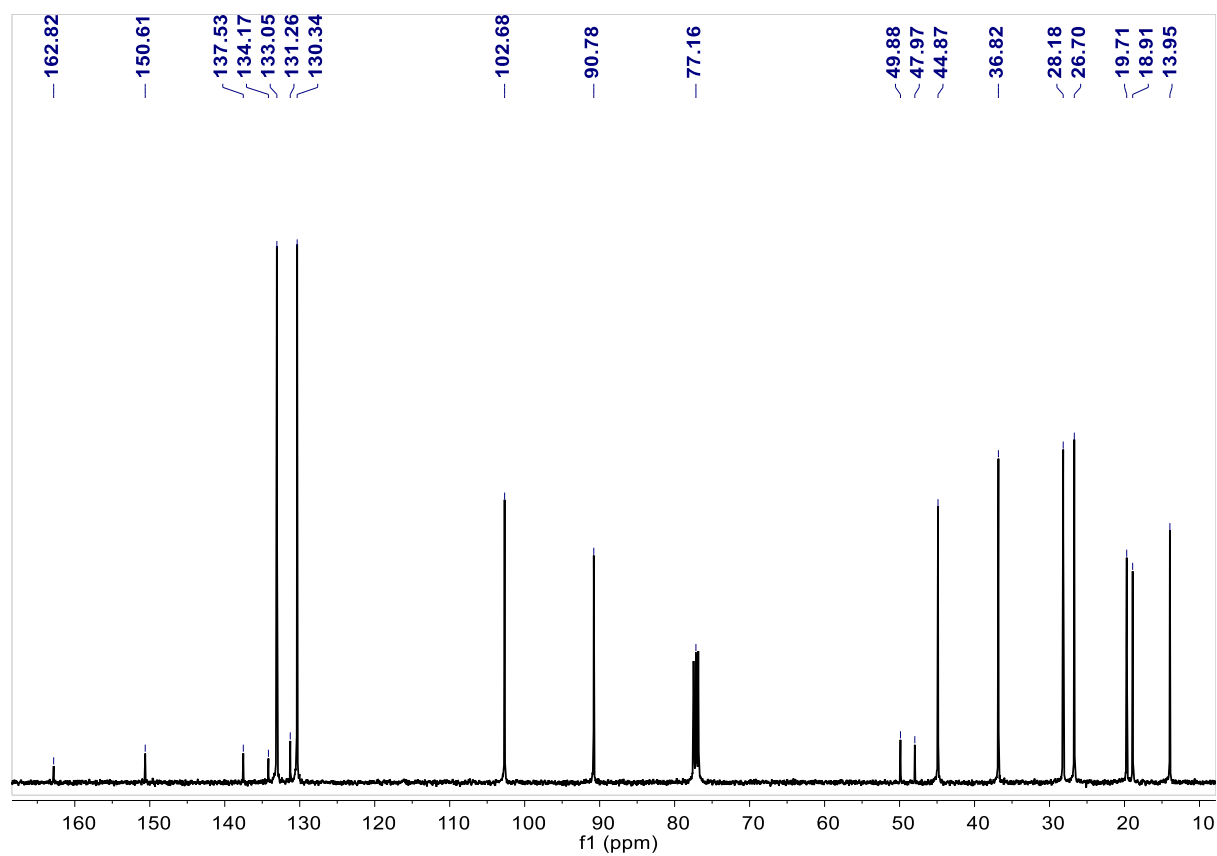
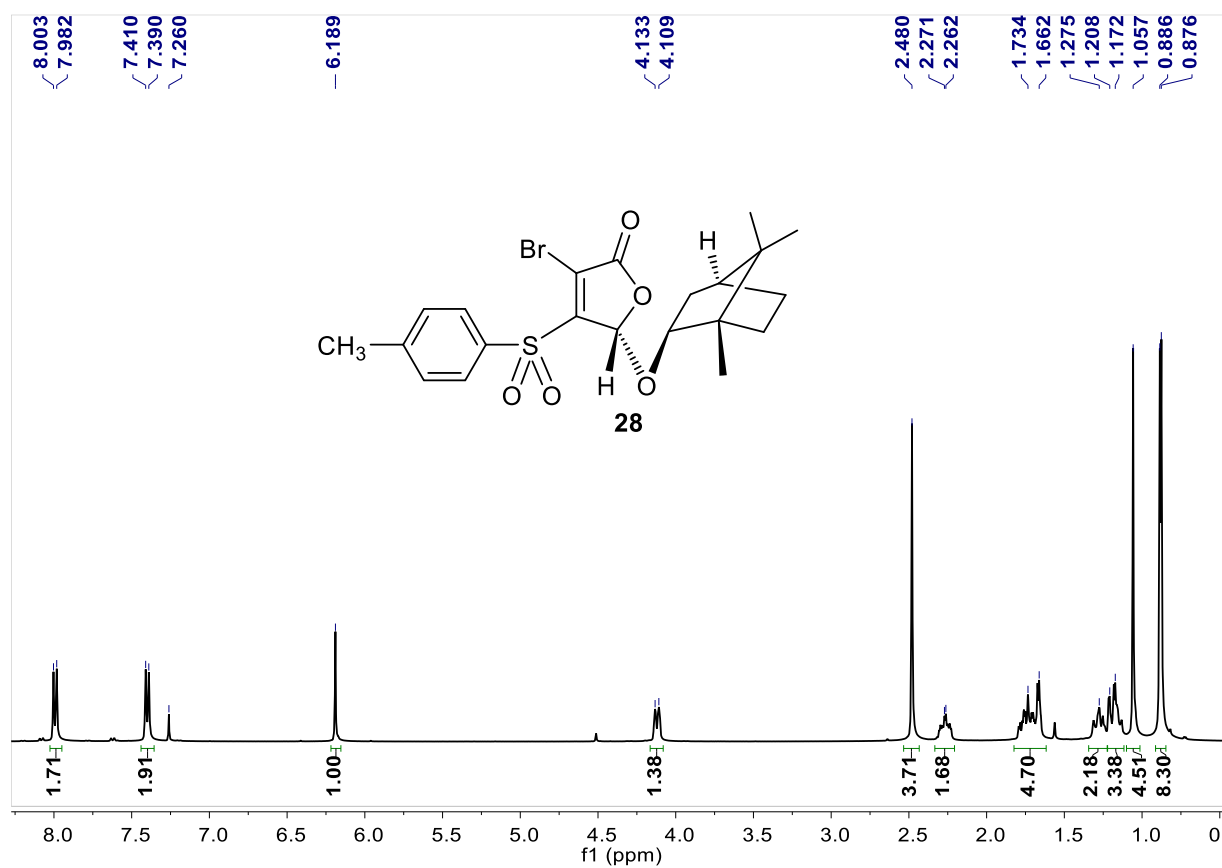


Figure S17. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **27** (CDCl₃).

a)



b)

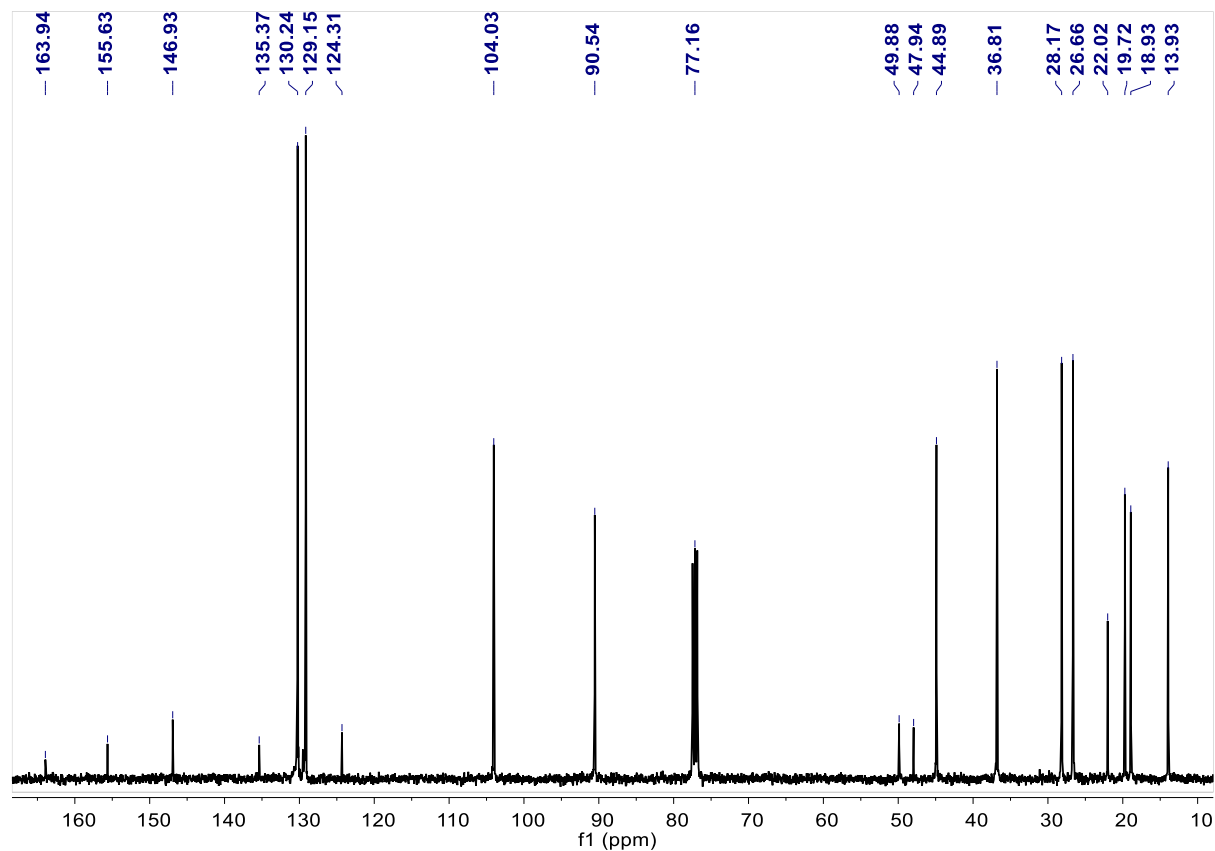
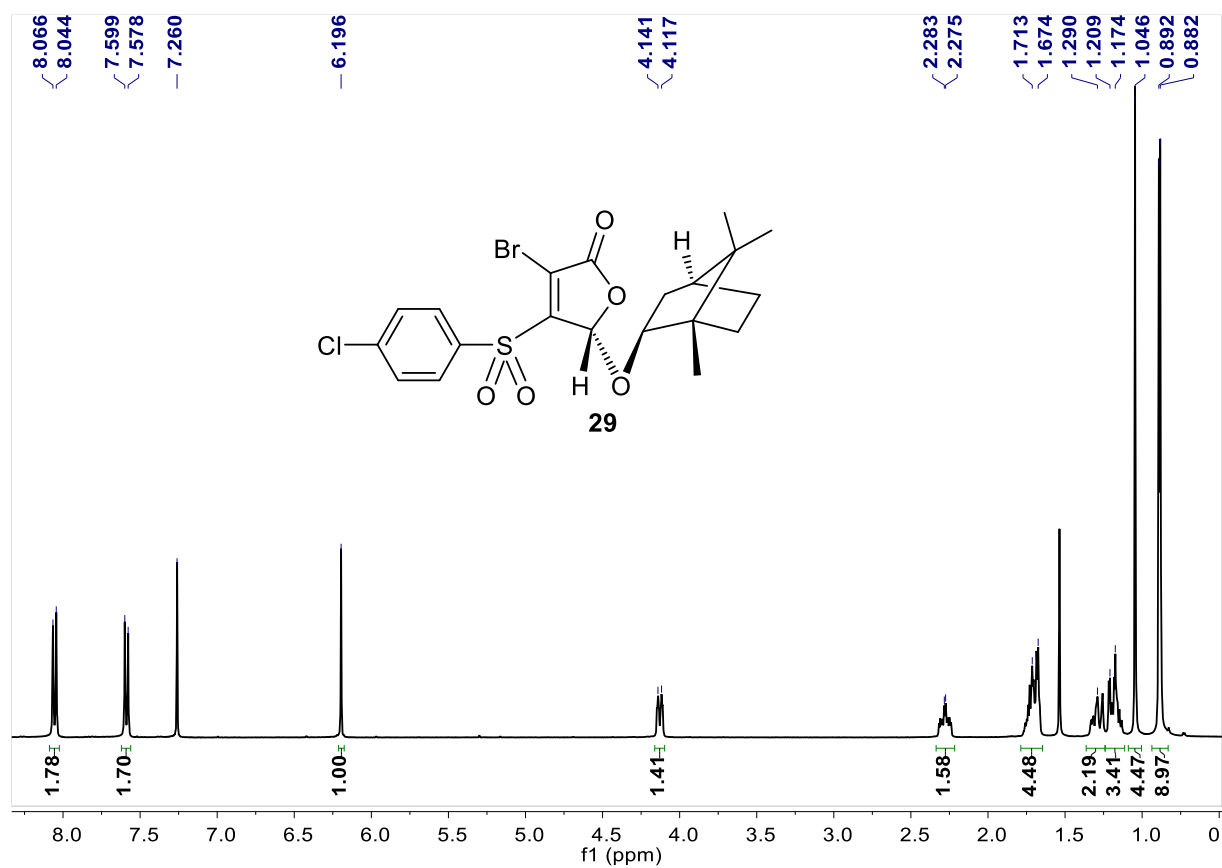


Figure S18. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **28** (CDCl₃).

a)



b)

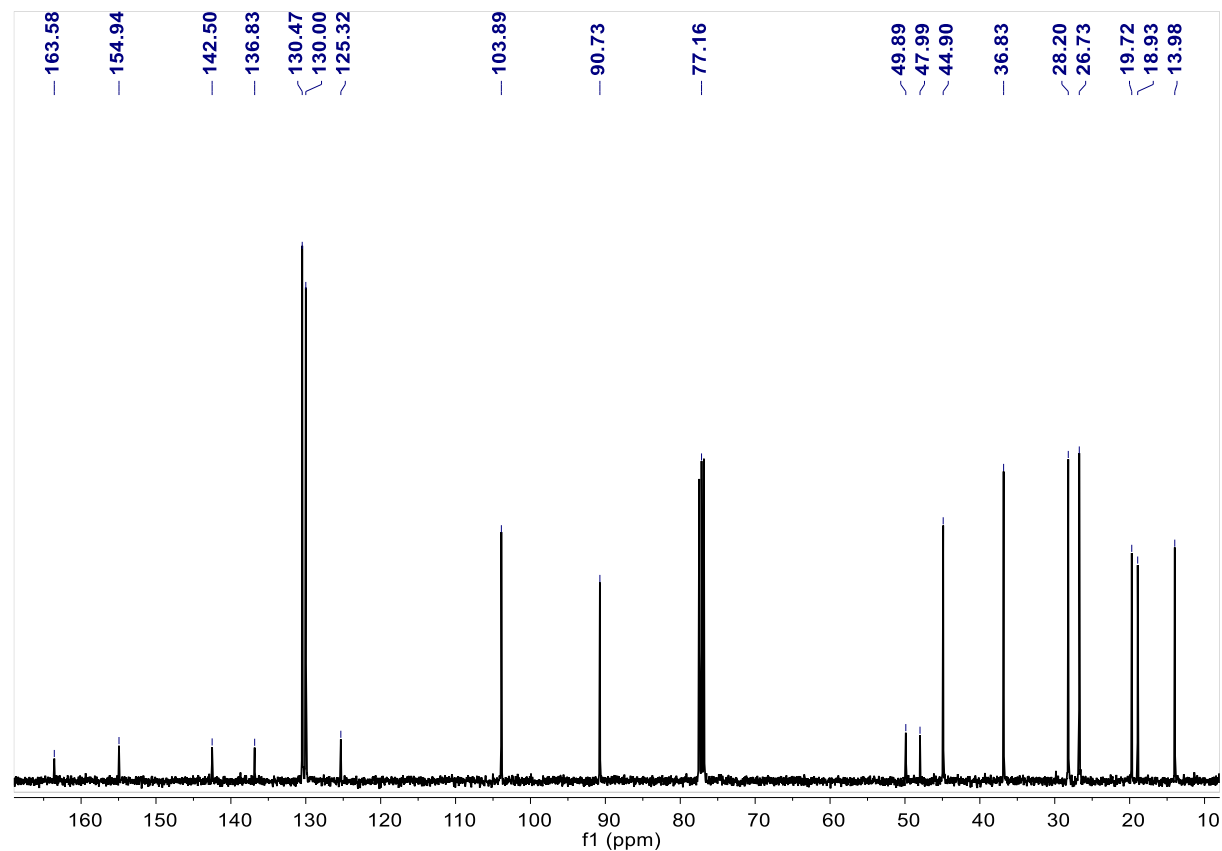
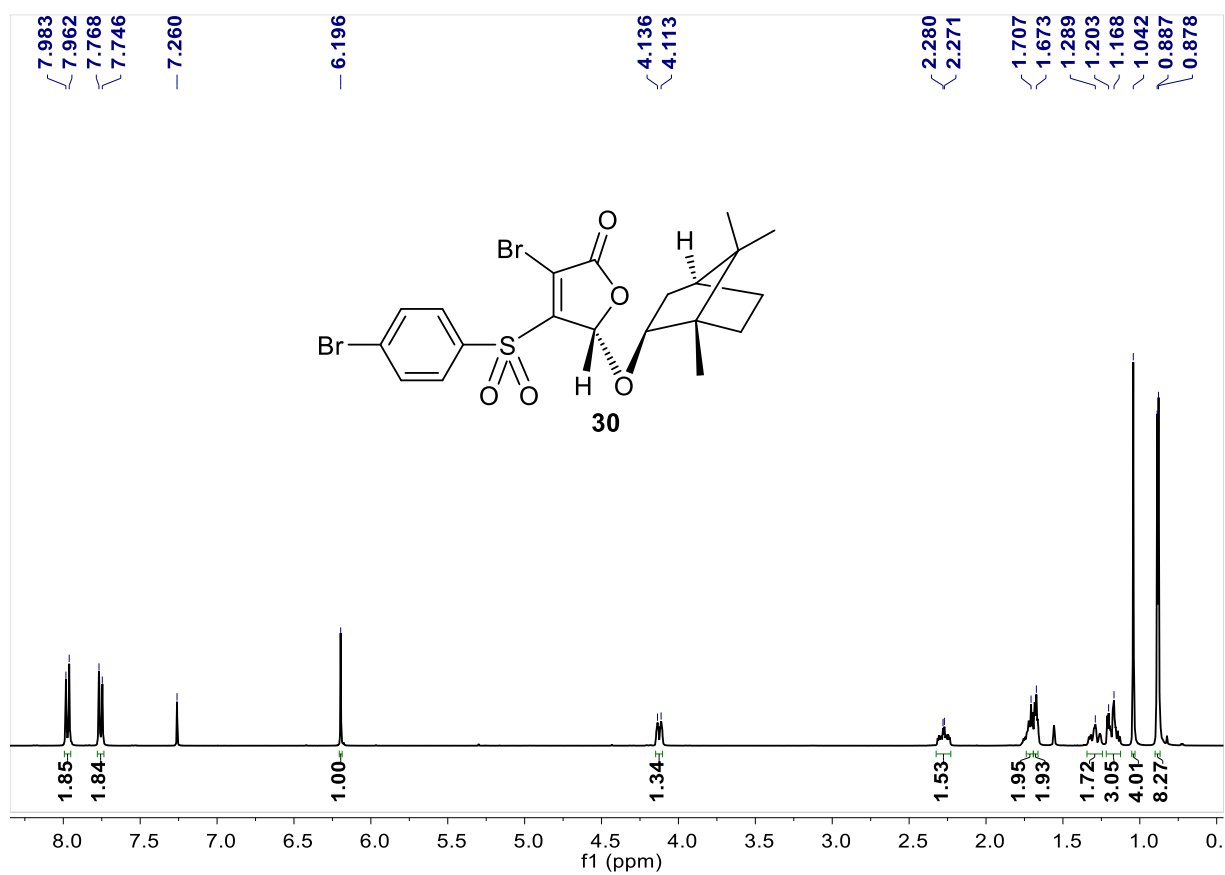


Figure S19. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **29** (CDCl₃).

a)



b)

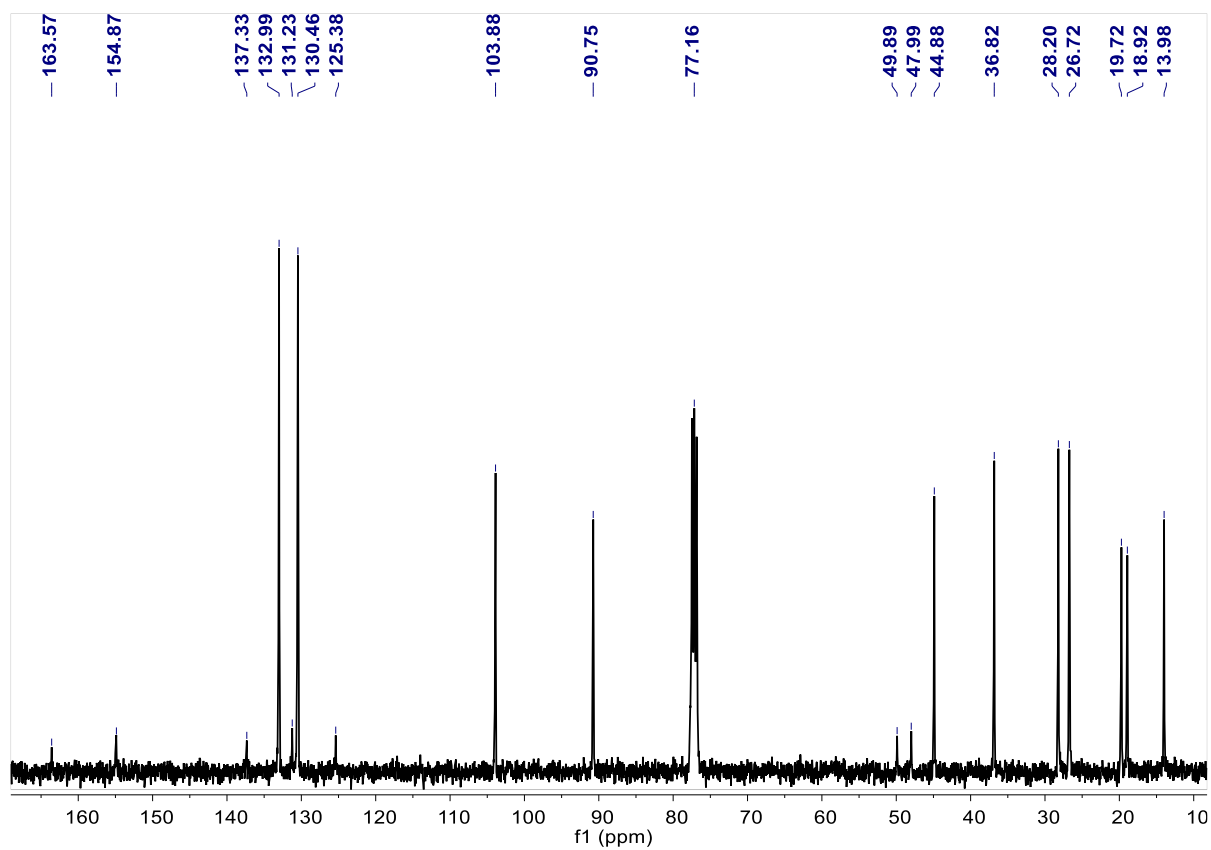
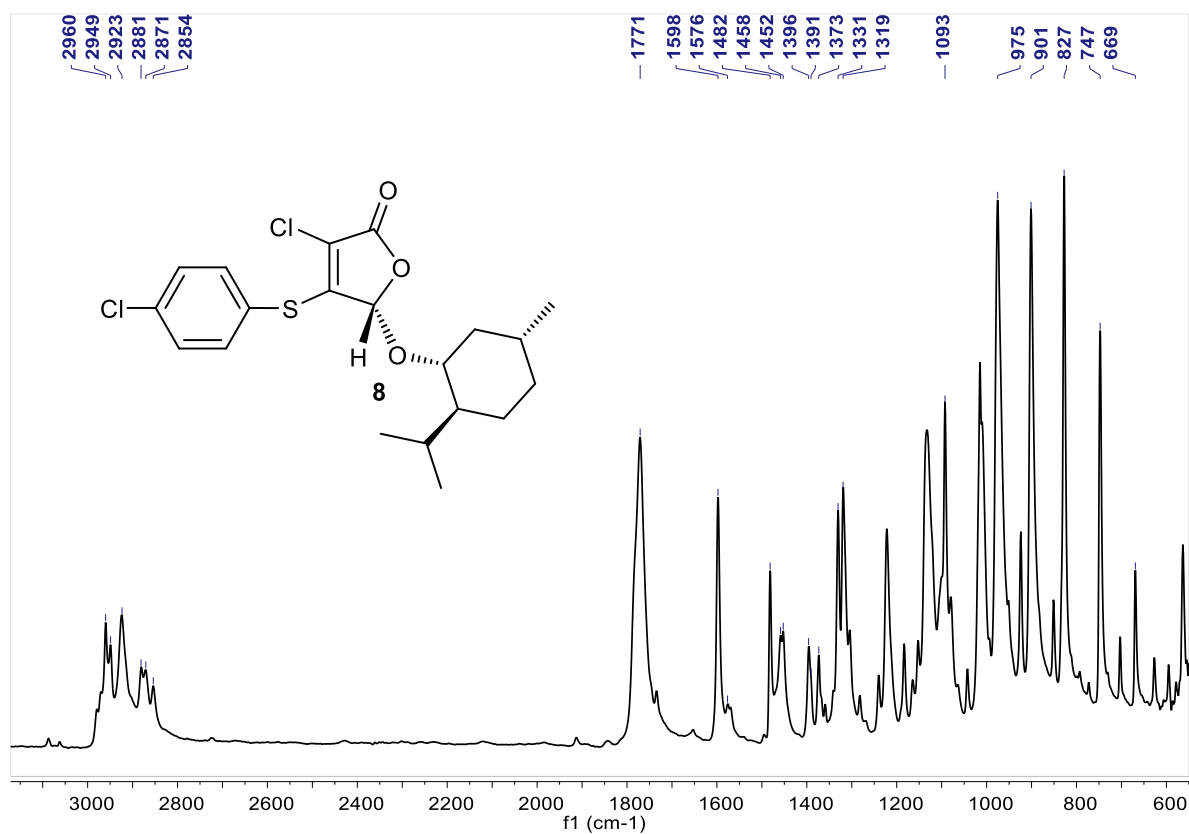


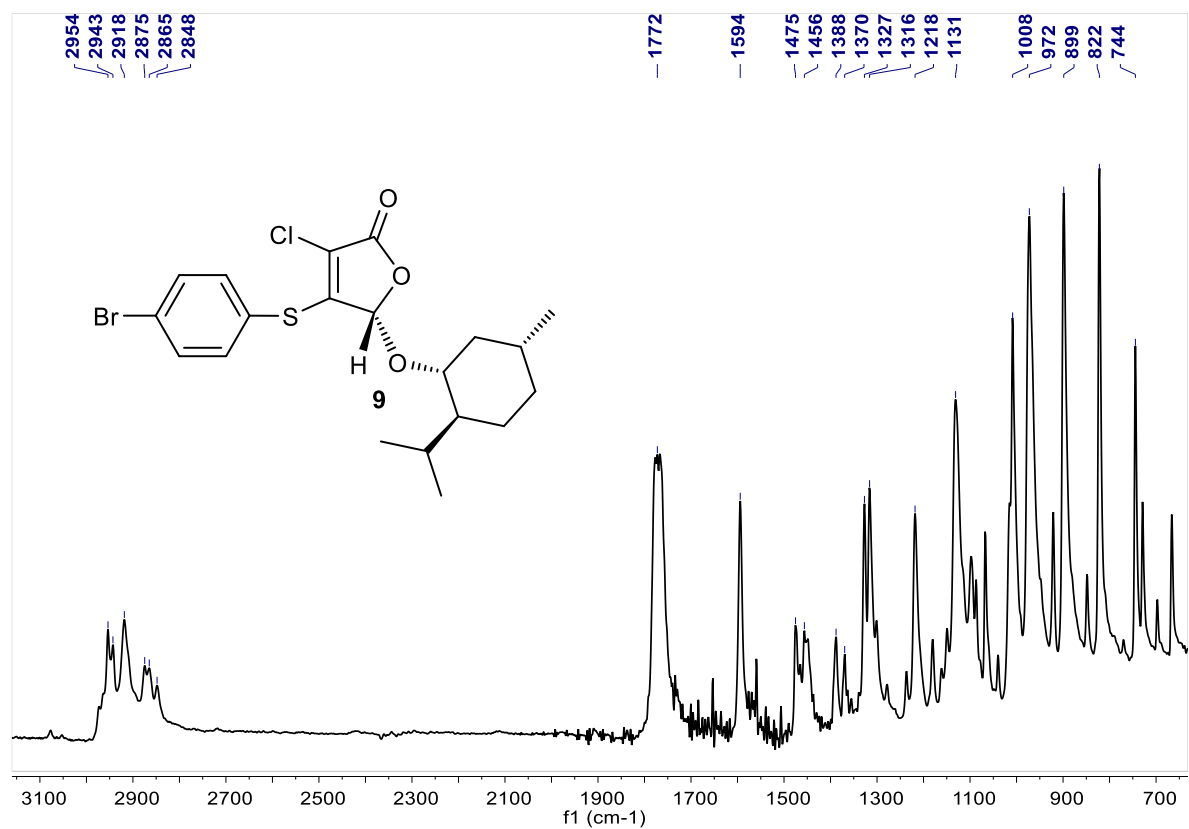
Figure S20. ¹H (a) and ¹³C{¹H} (b) NMR spectra of compound **30** (CDCl₃).

IR spectra of thioethers

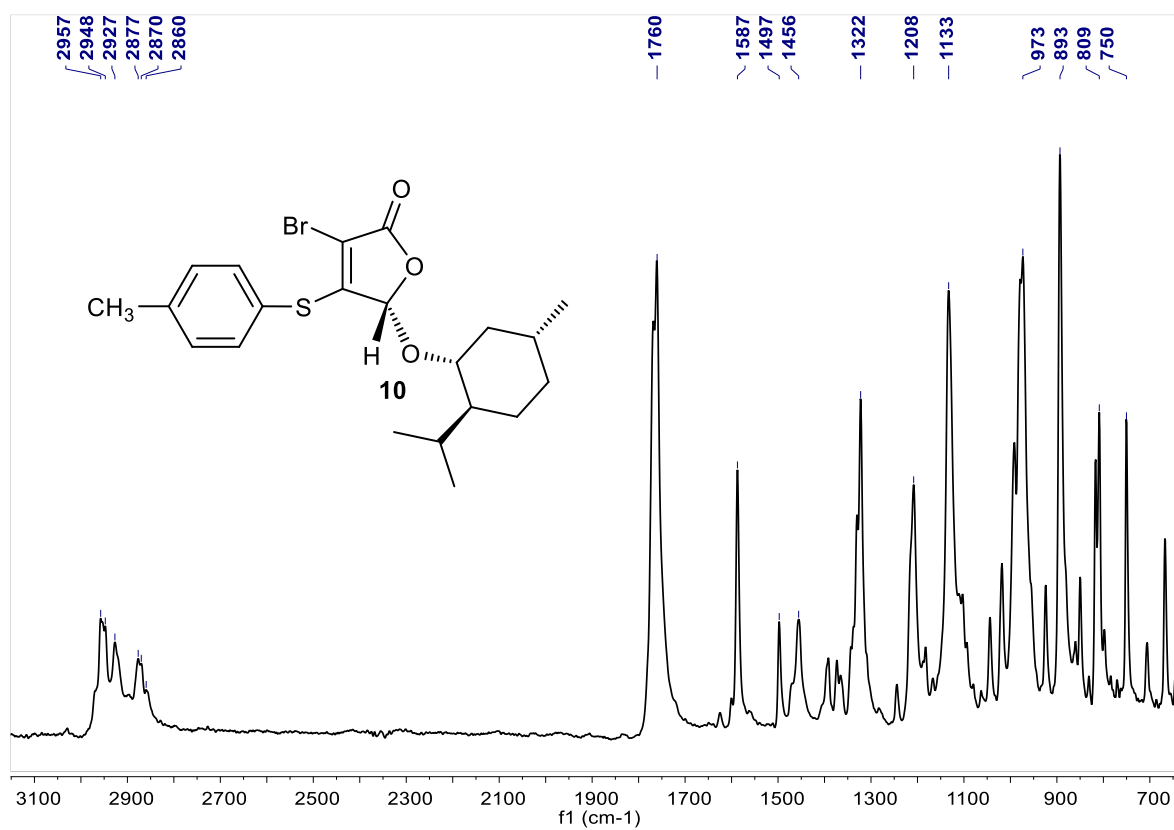
a)



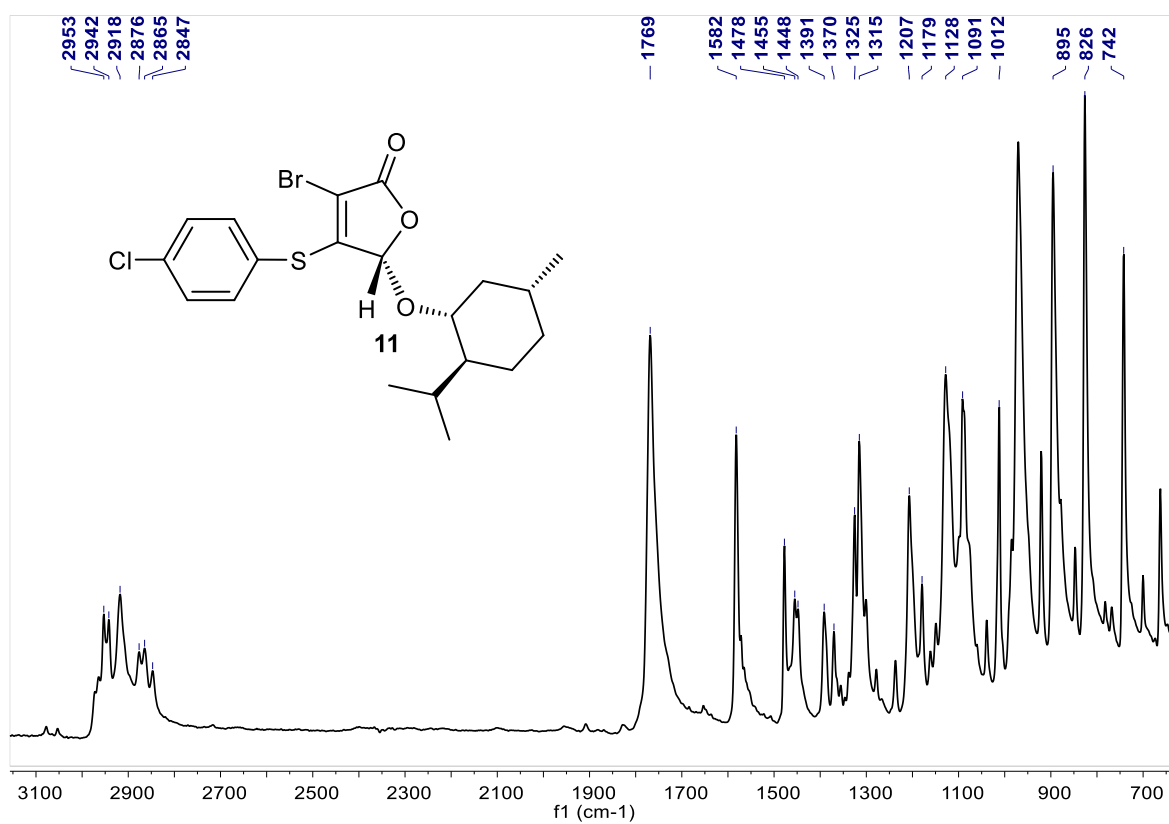
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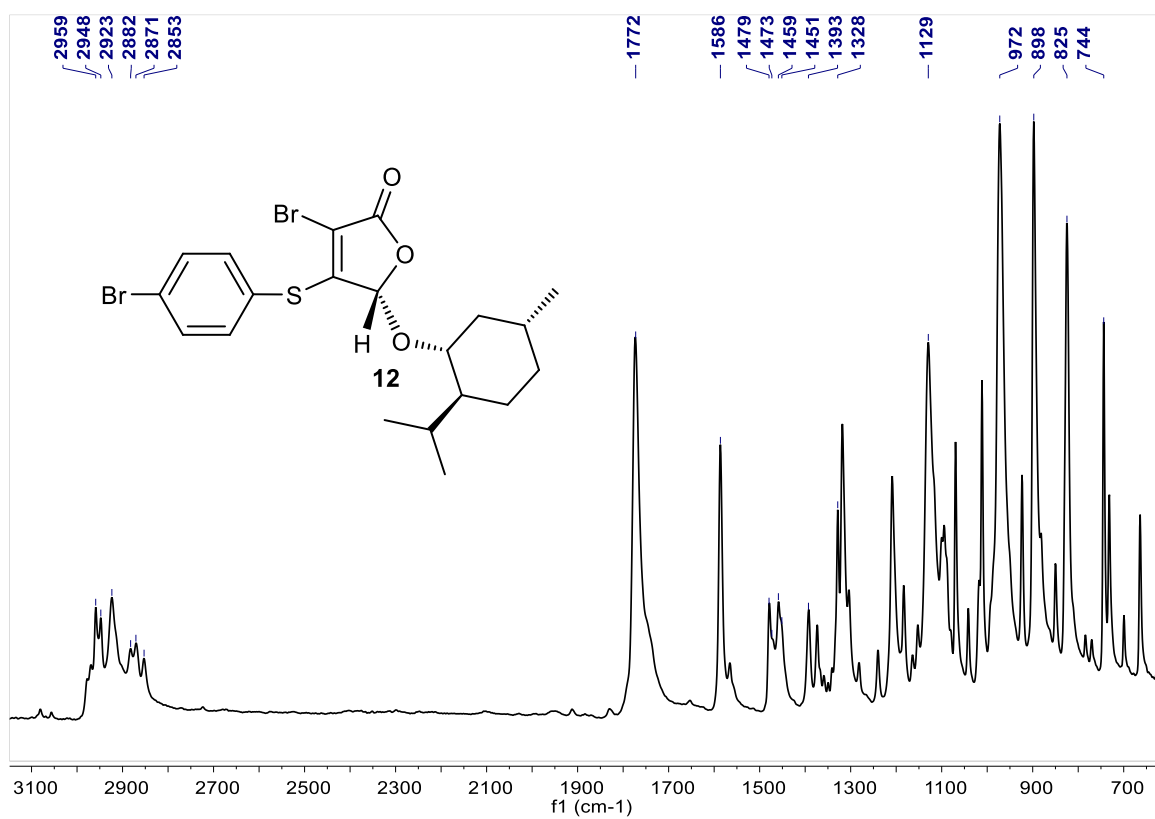
c)



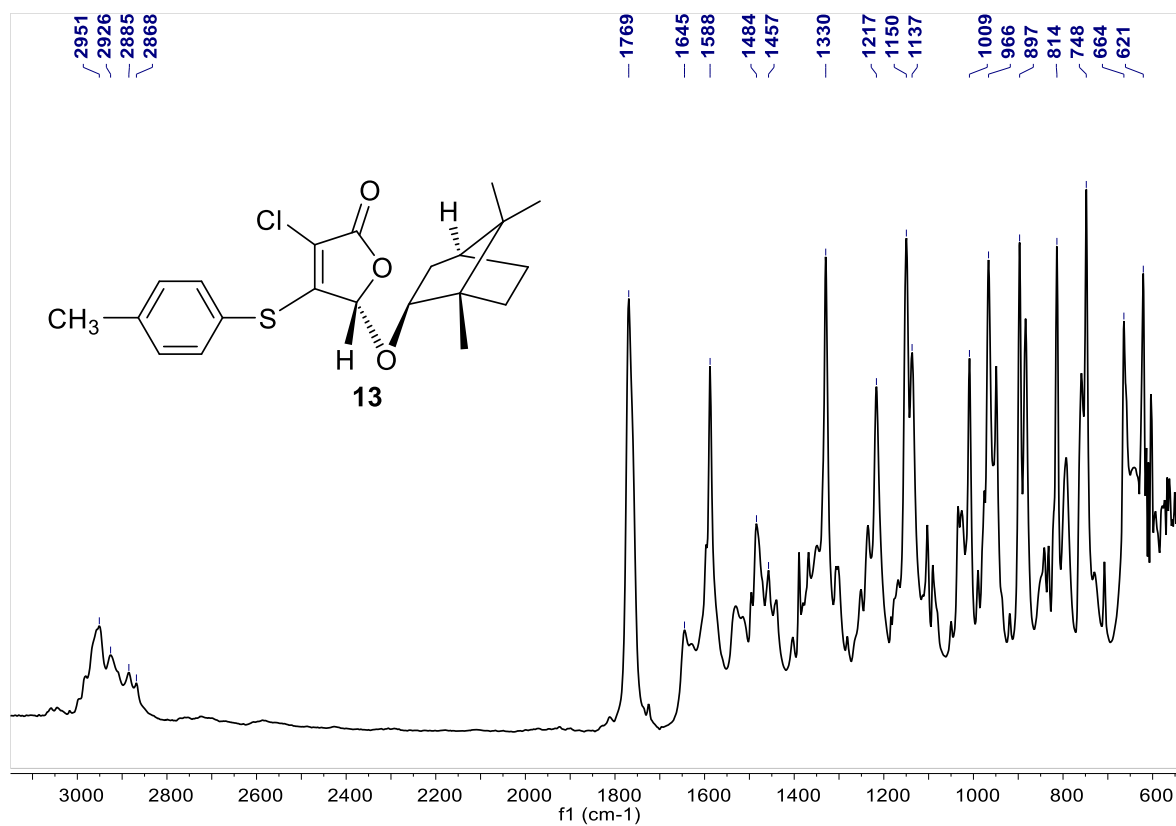
d)



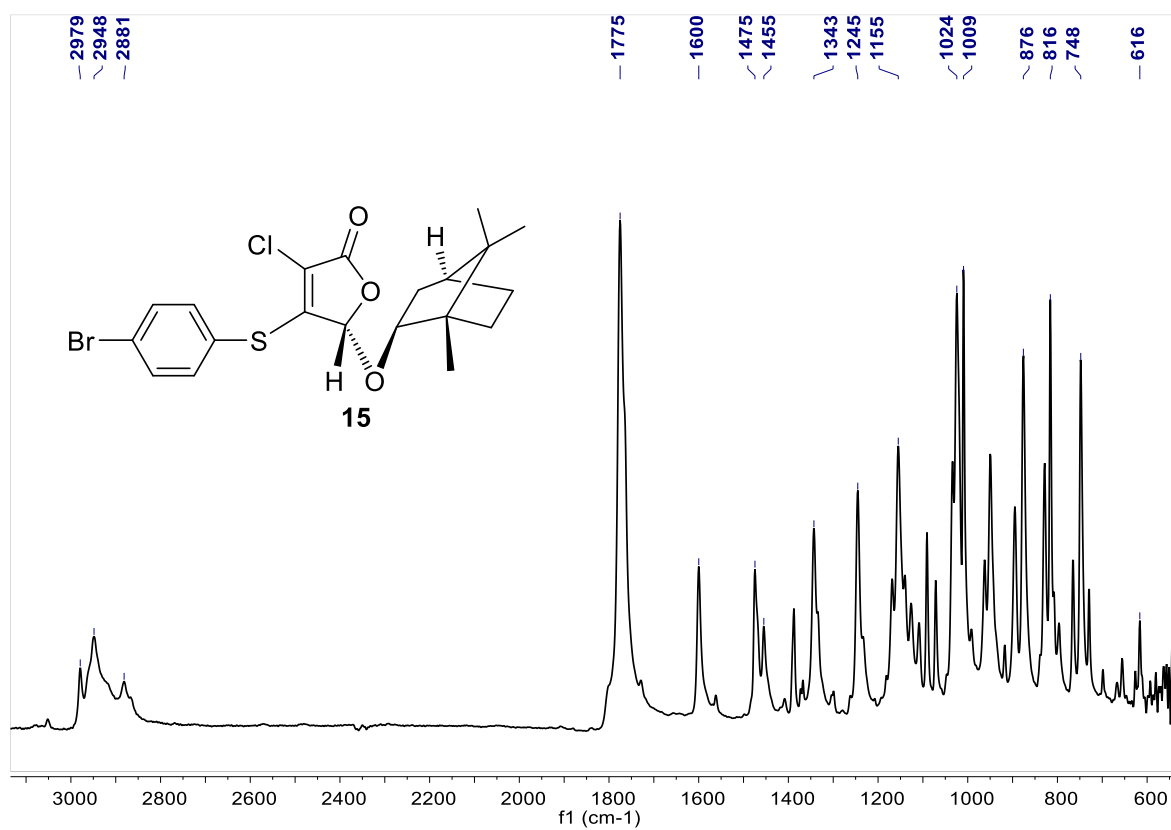
e)



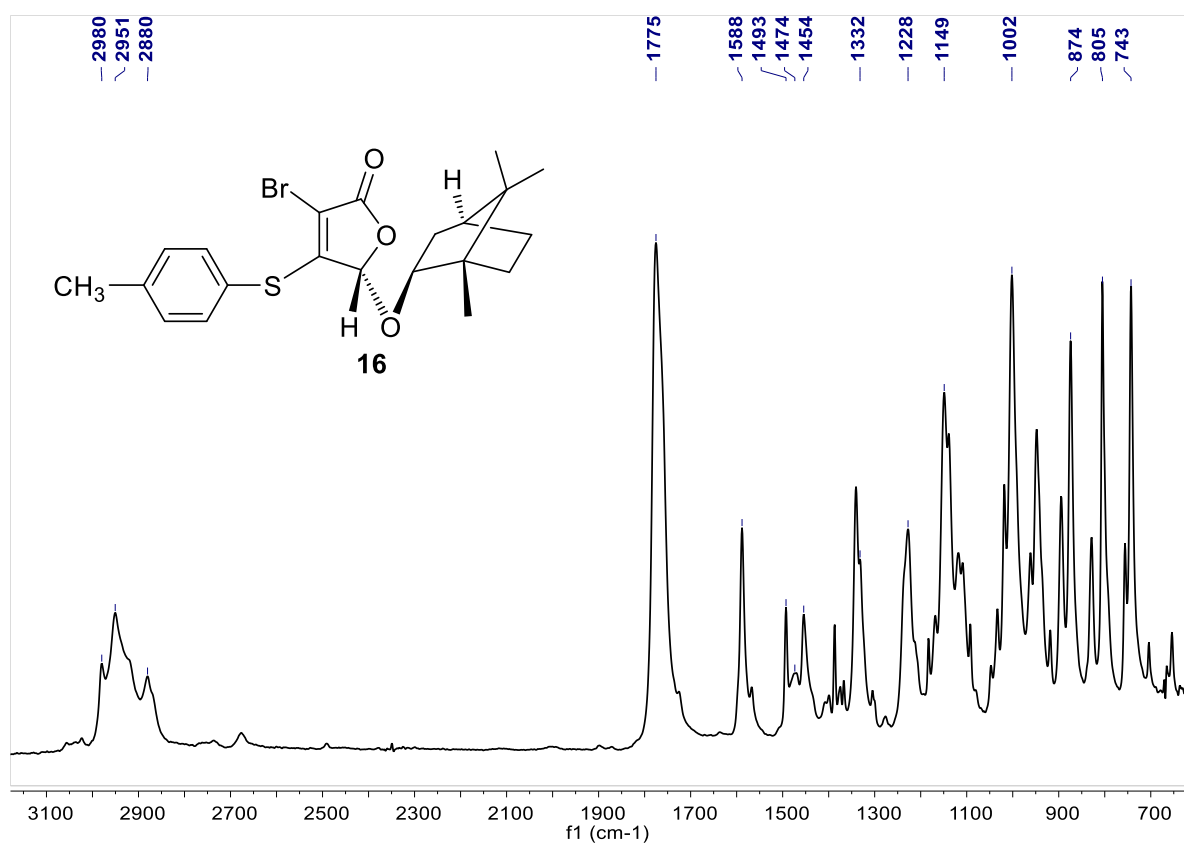
f)



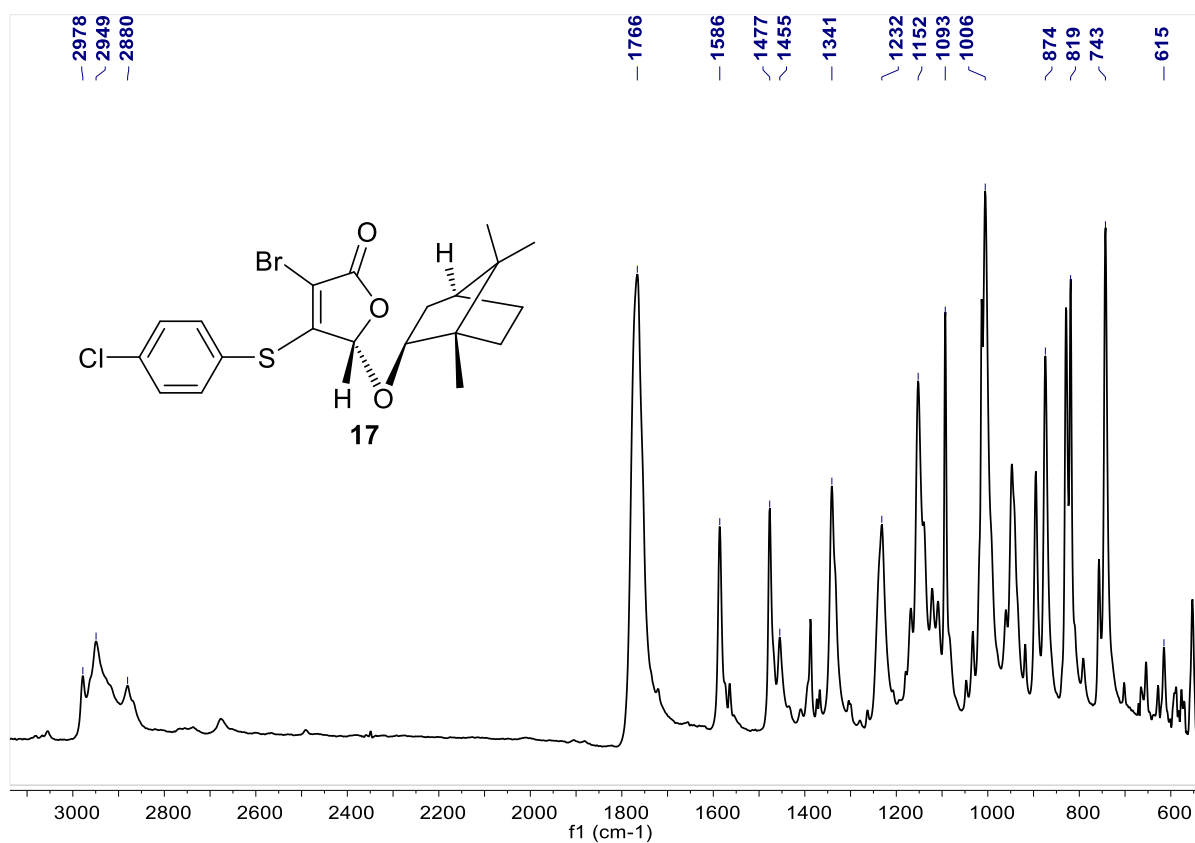
g)



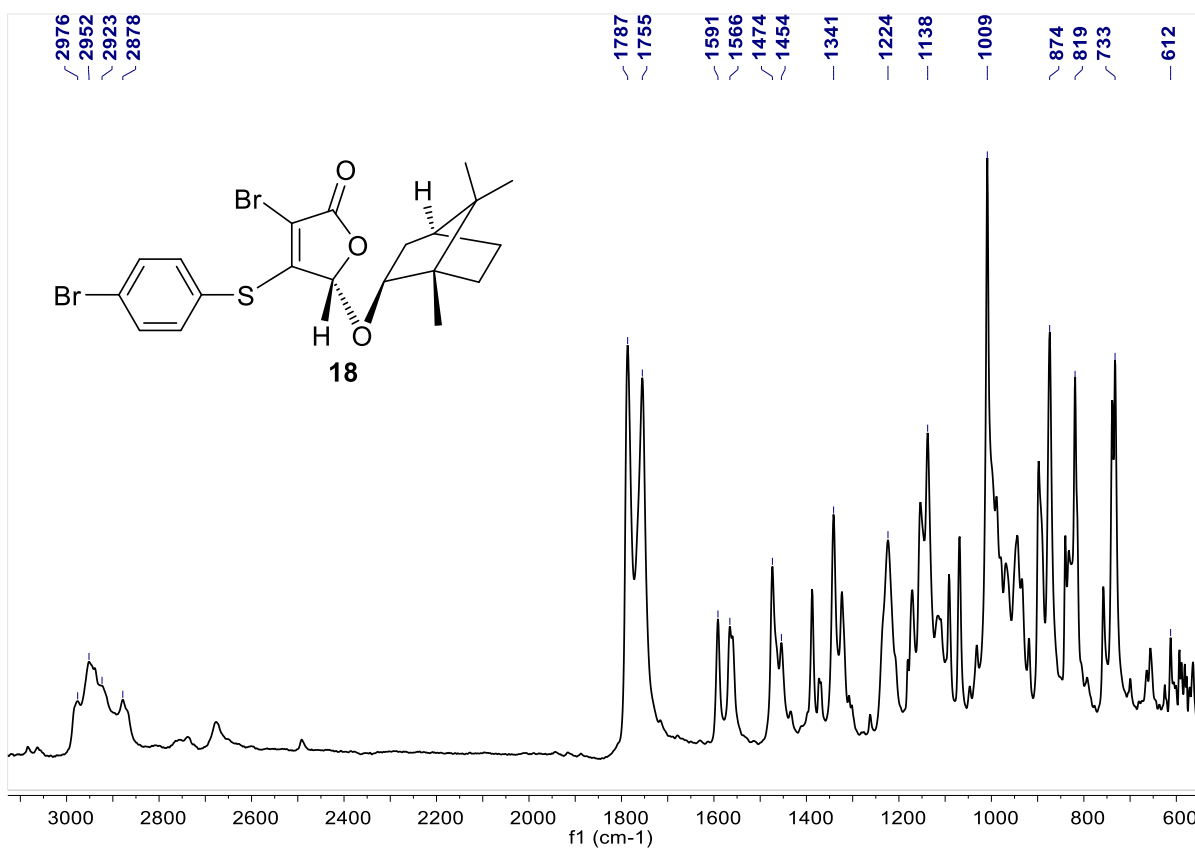
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i)

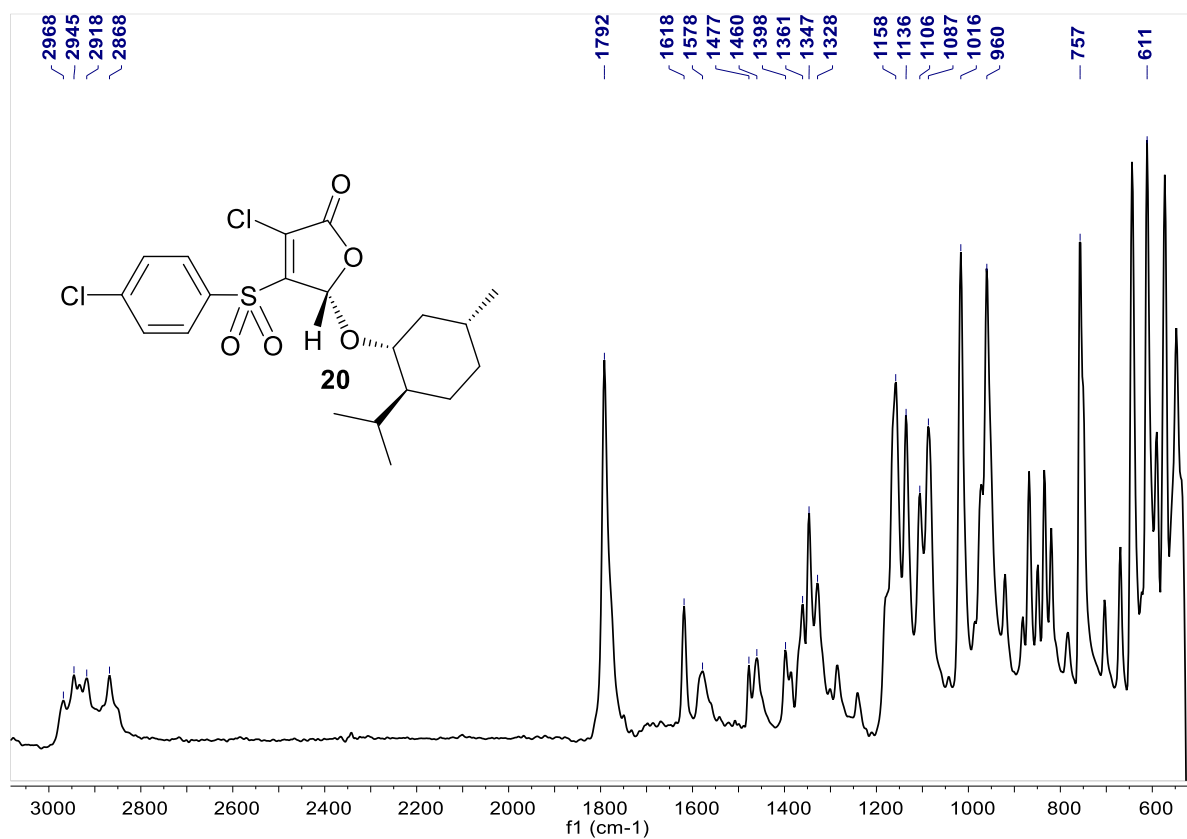


j)

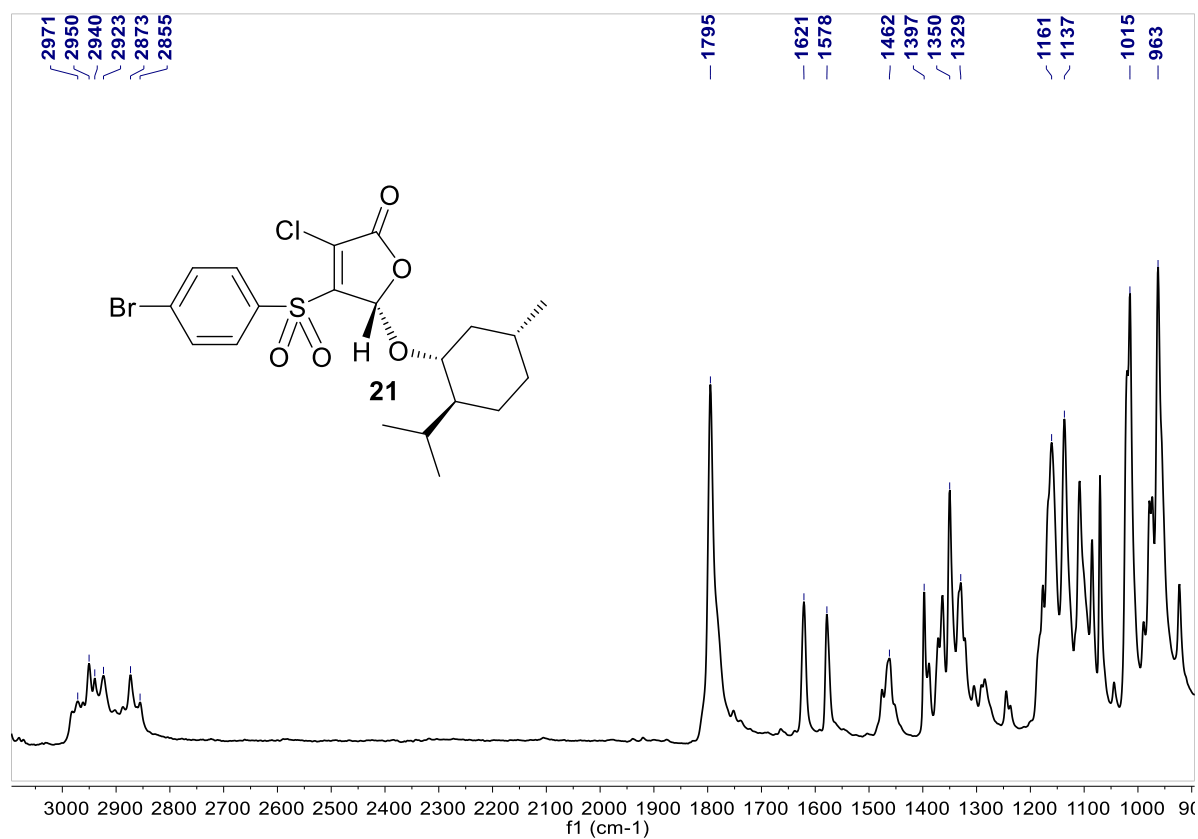
**Figure S21.** IR spectra of thioethers **8–18**.

IR spectra of sulfones

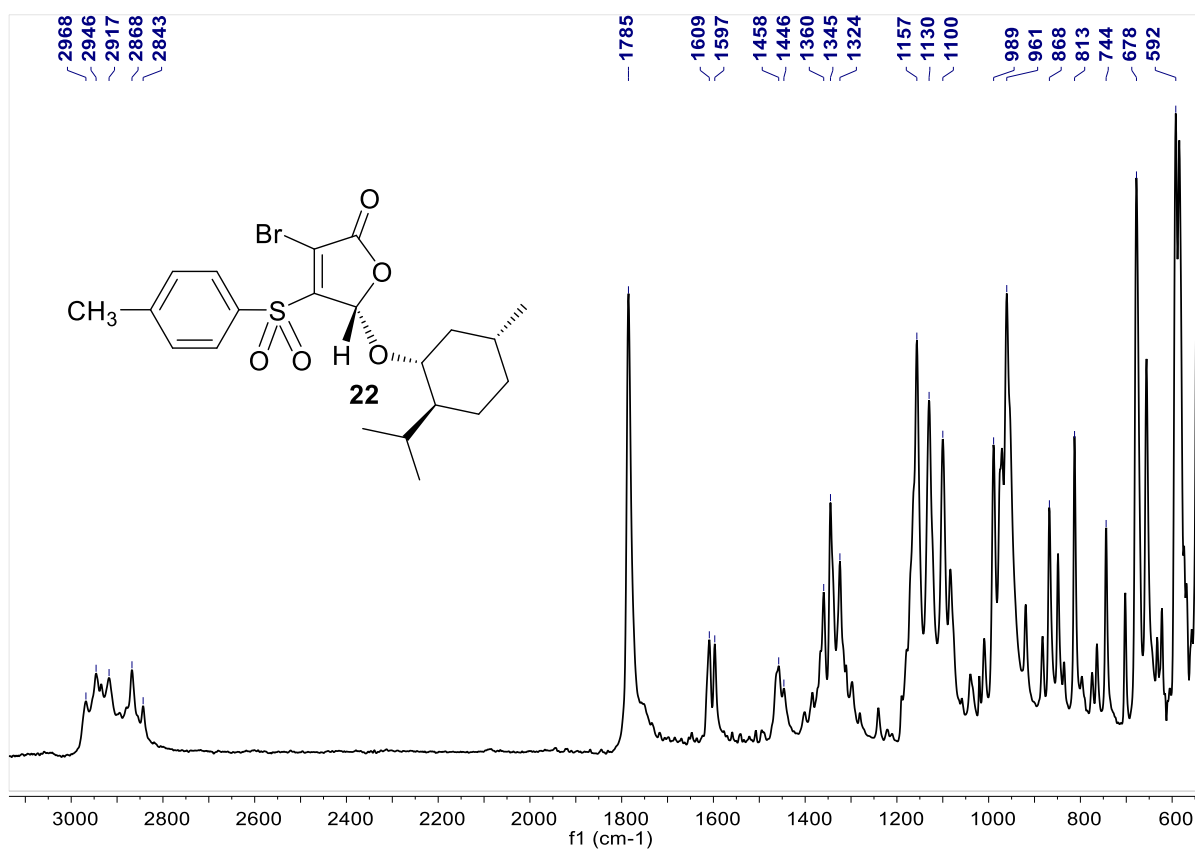
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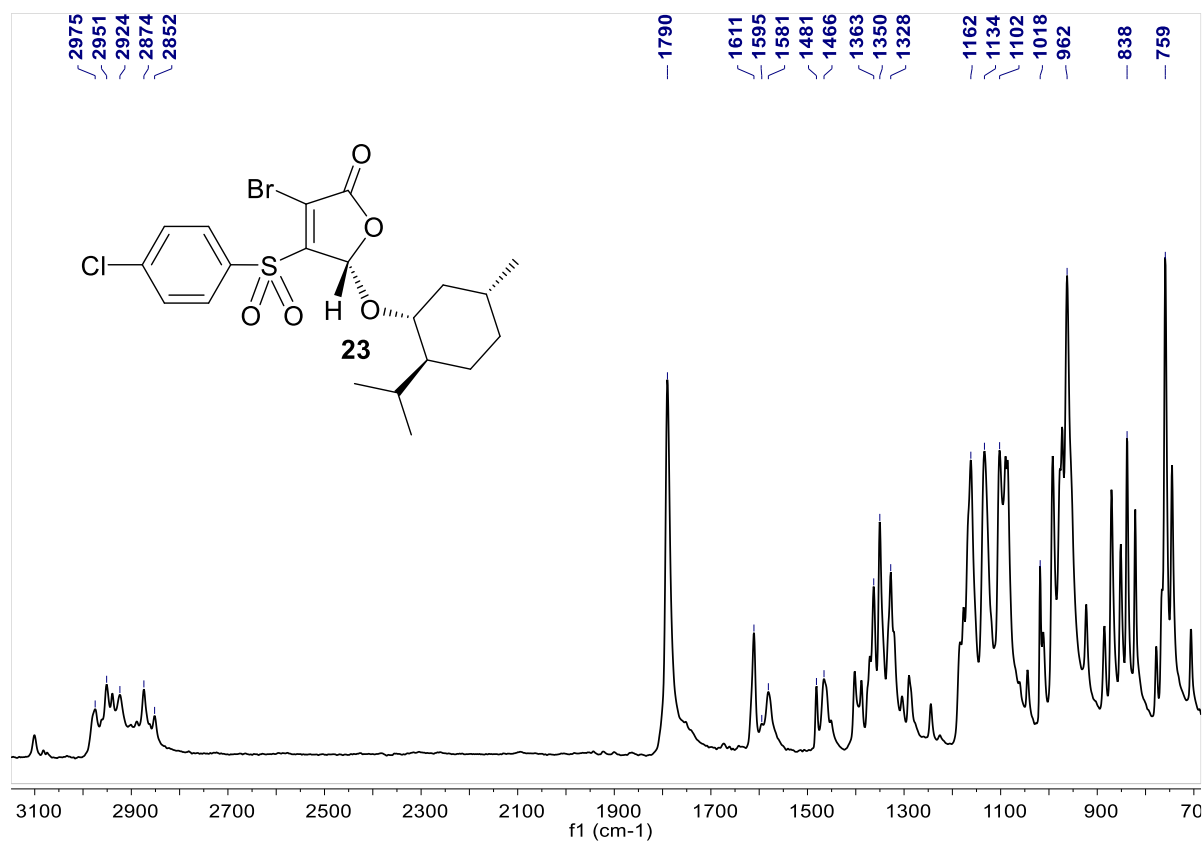
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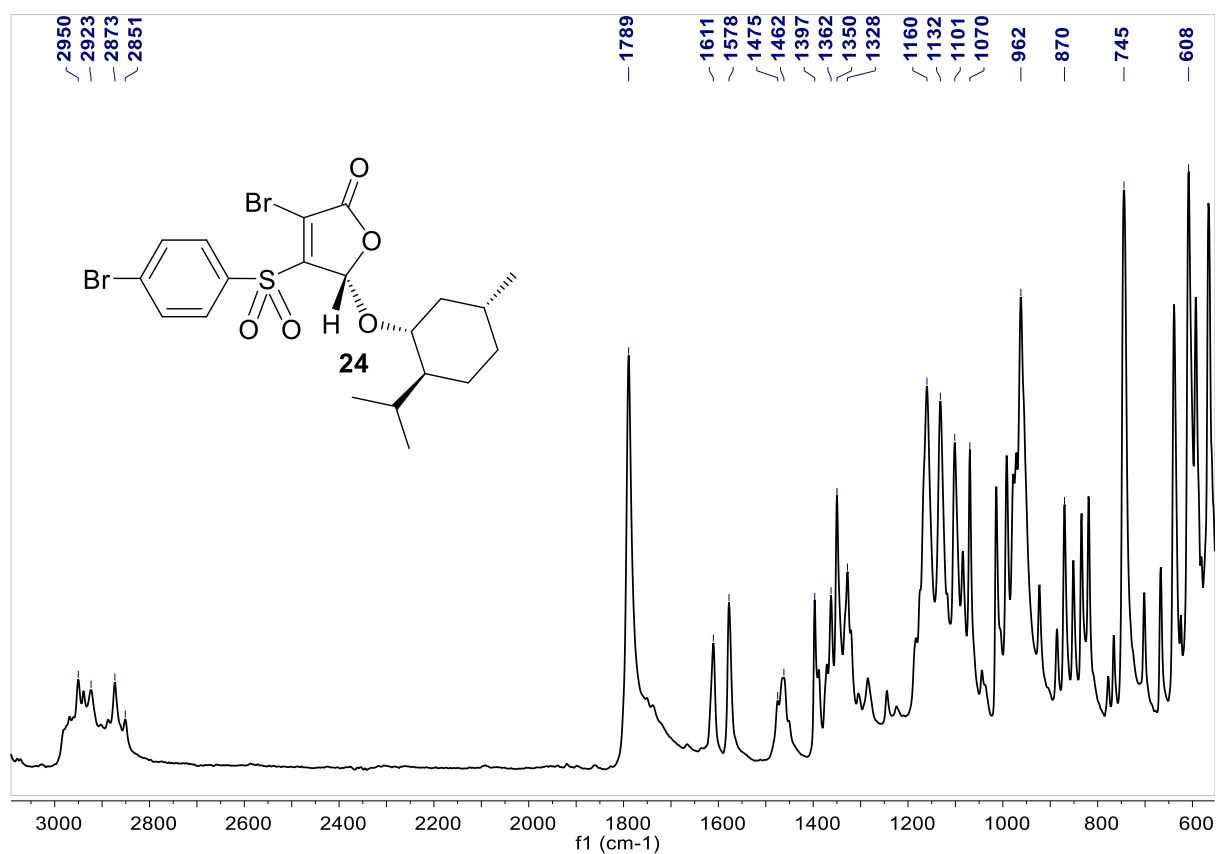
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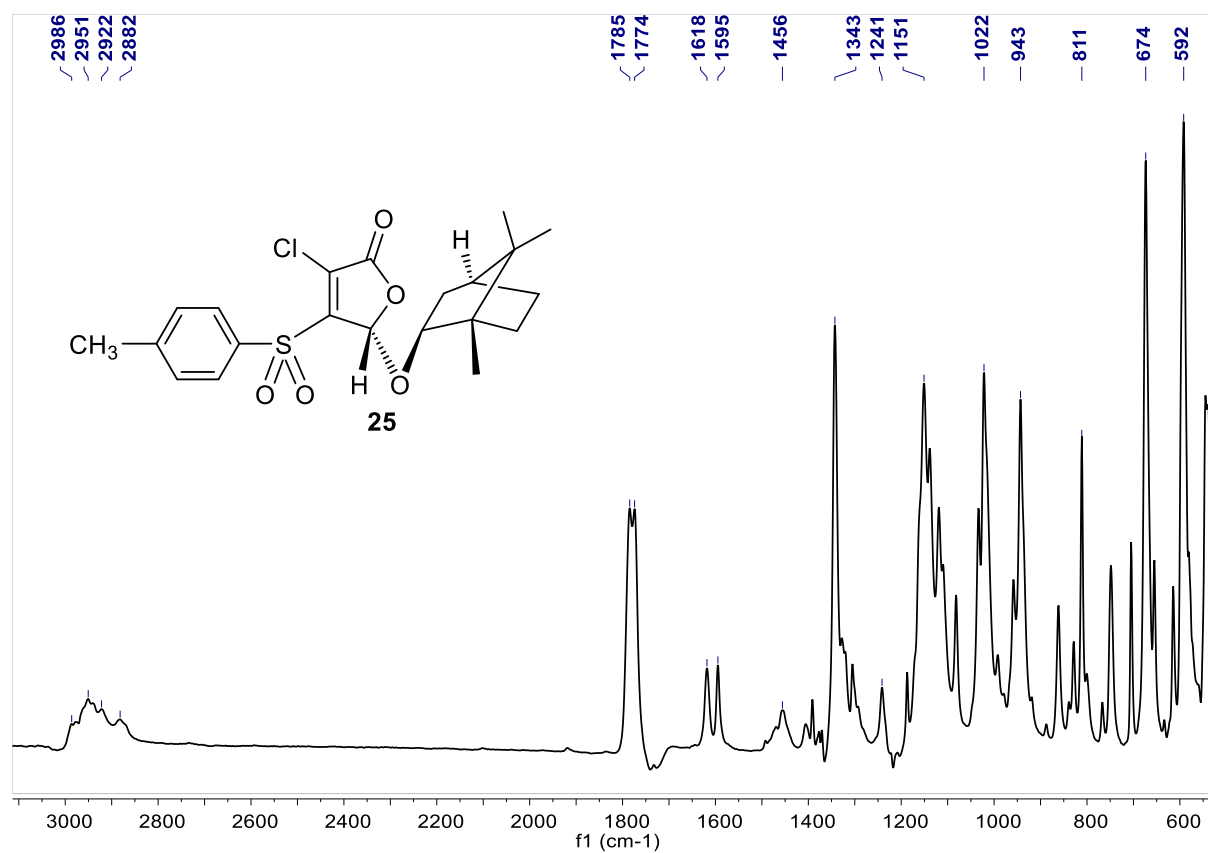
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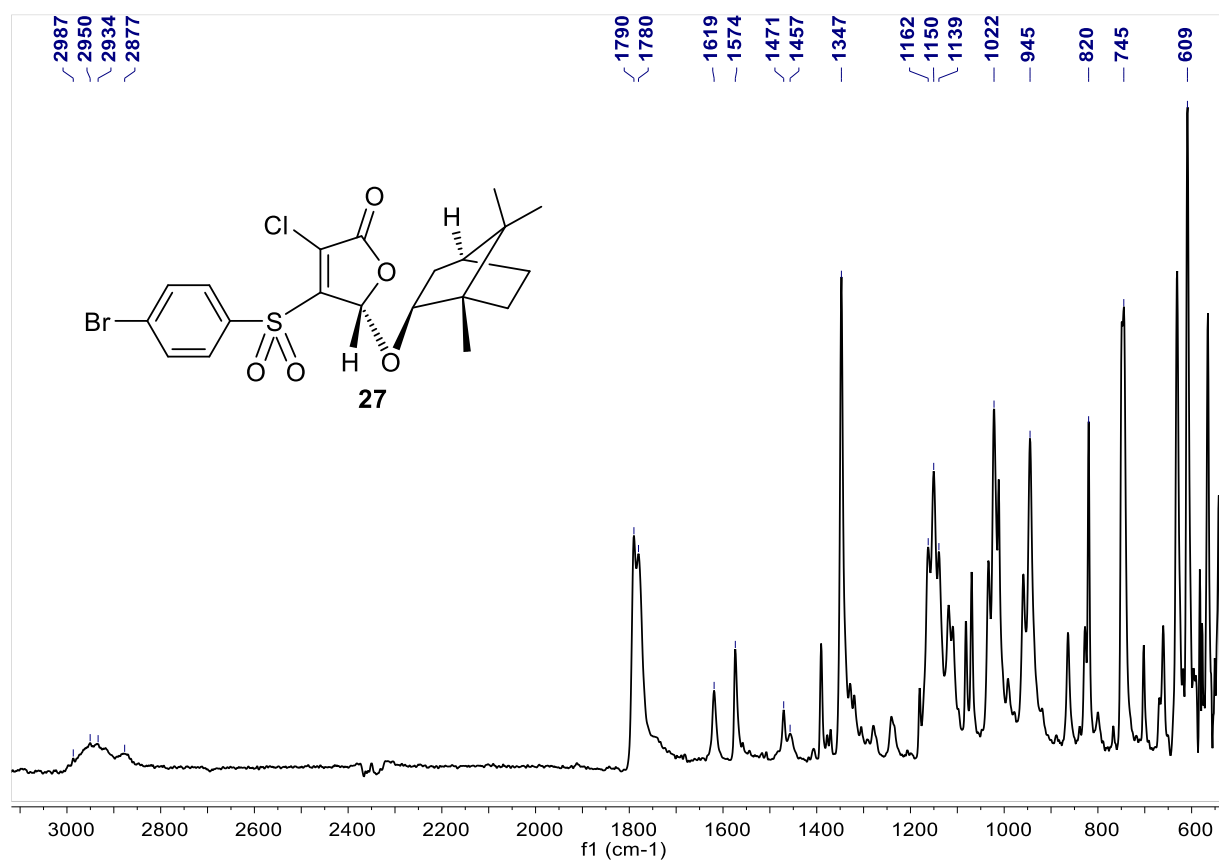
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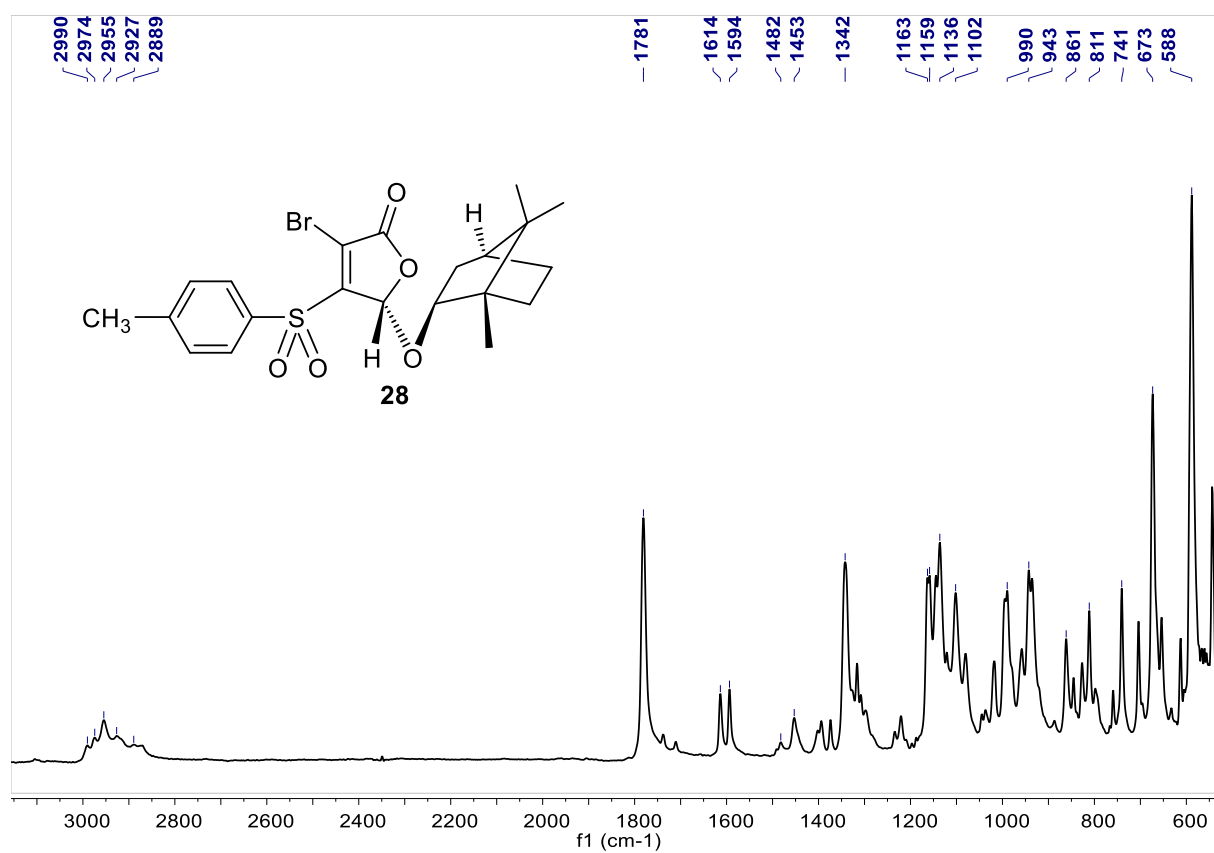
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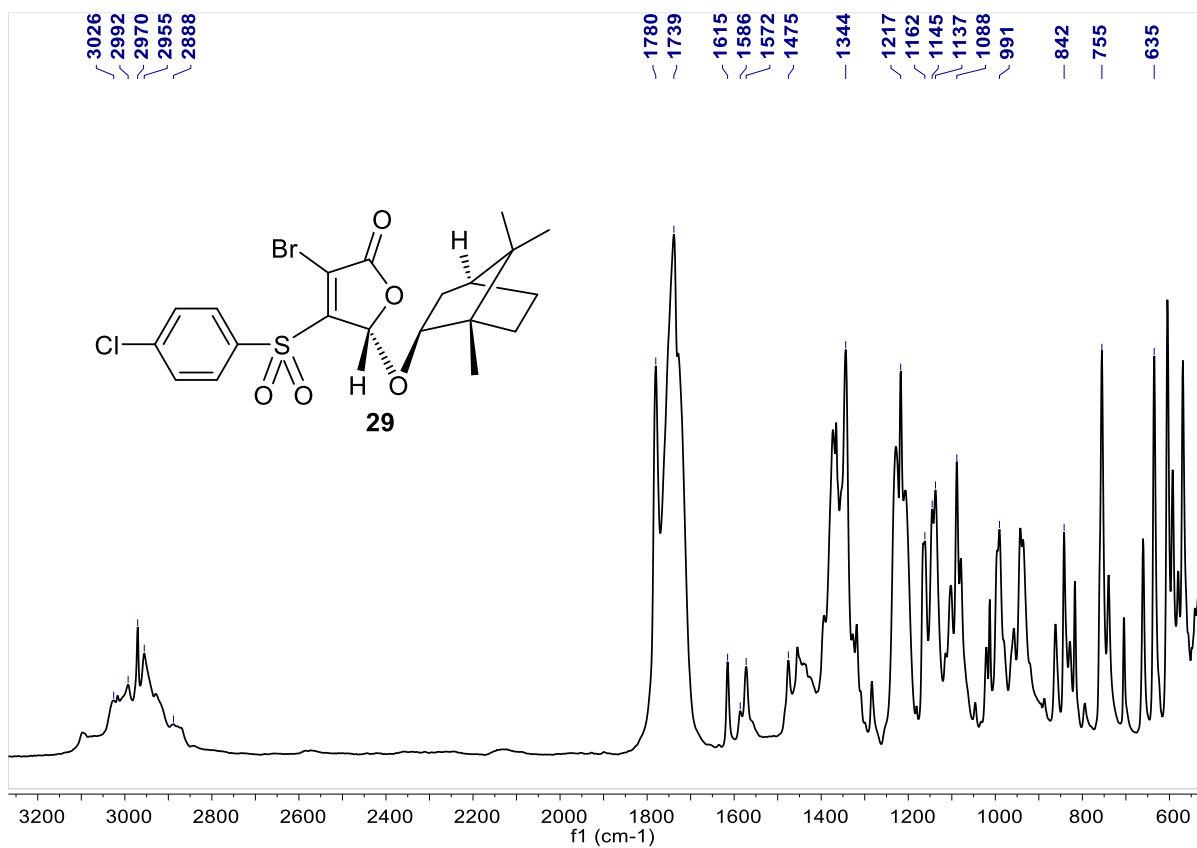
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h)



i)



j)

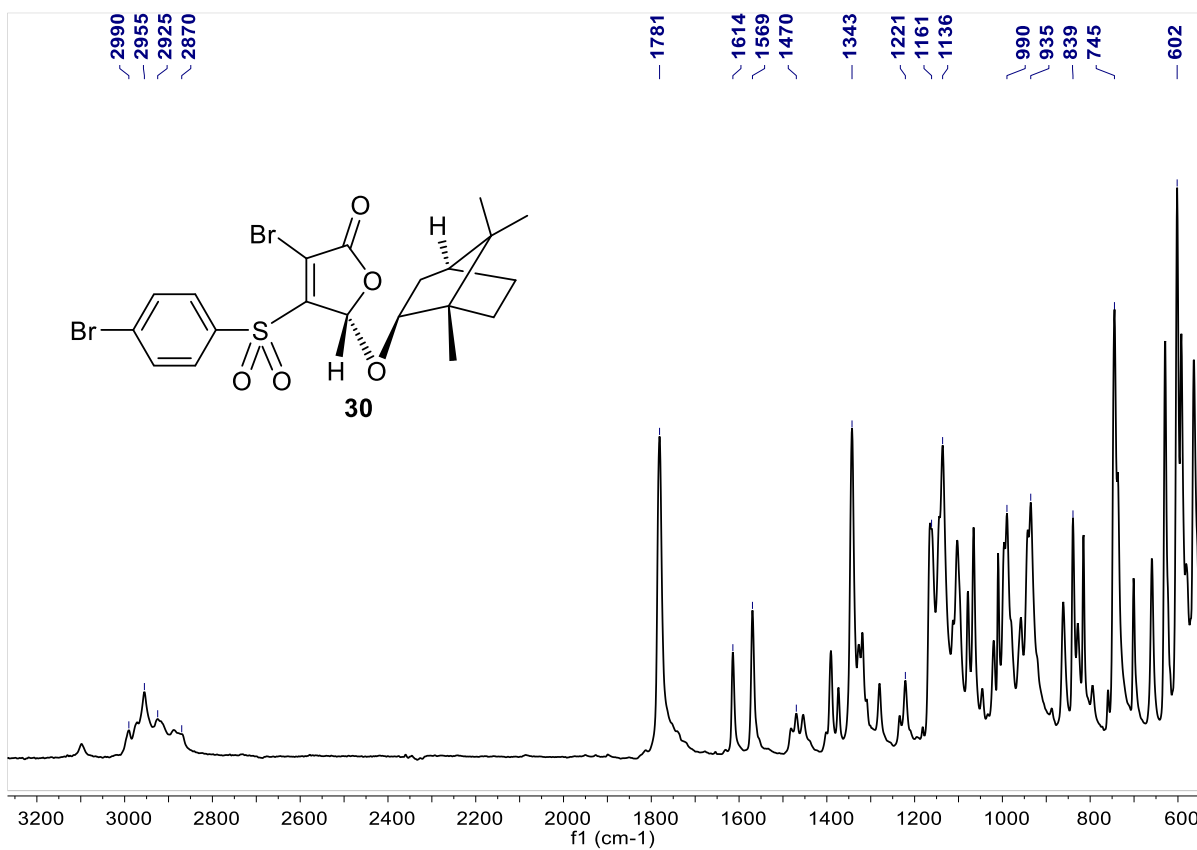


Figure S22. IR spectra of sulfones **20–30**.

a)

32

Mass Spectrum SmartFormula Report

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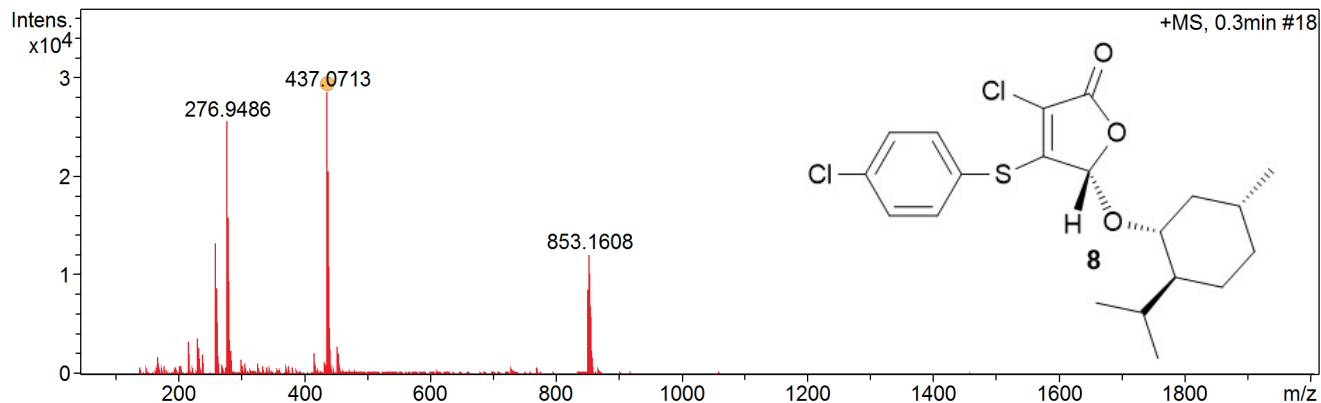
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Mass Spectrum SmartFormula Report

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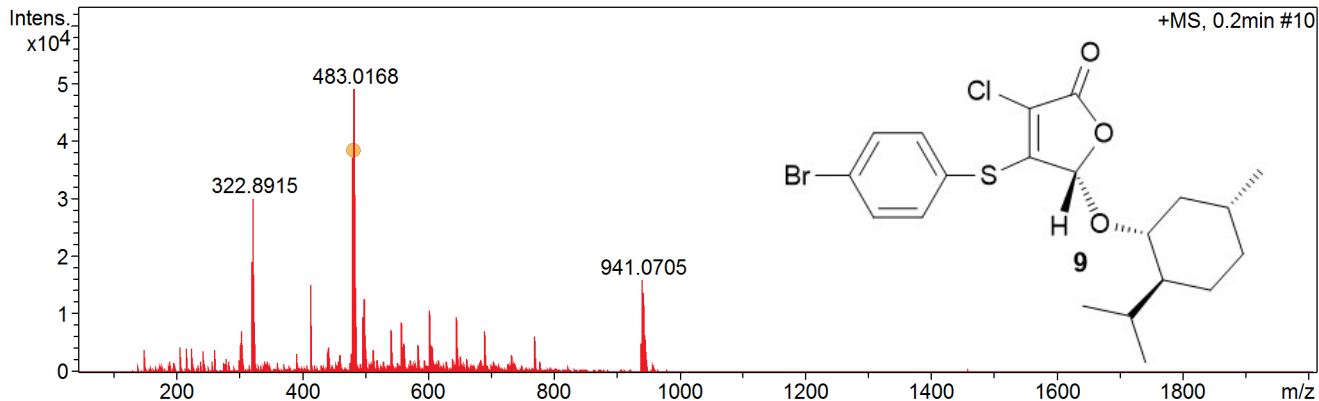
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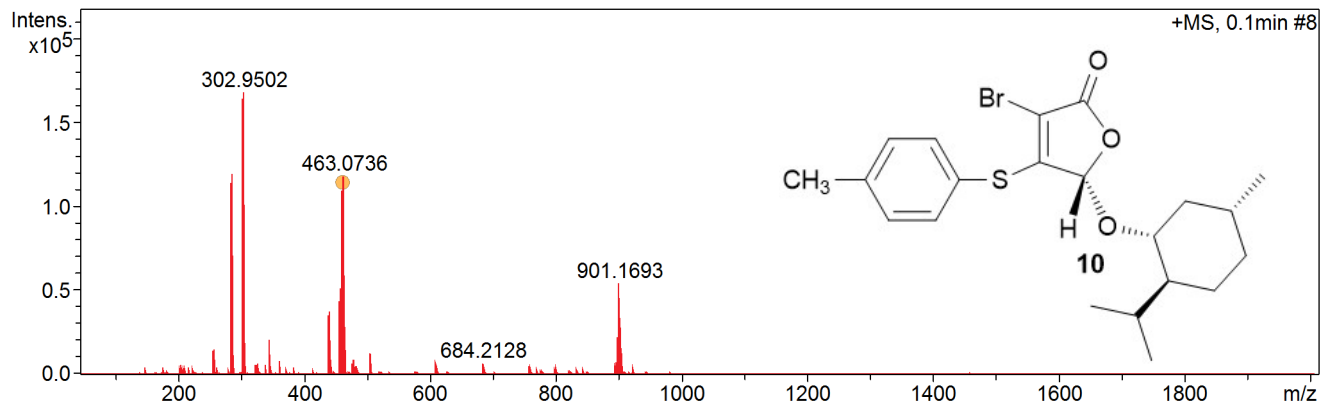
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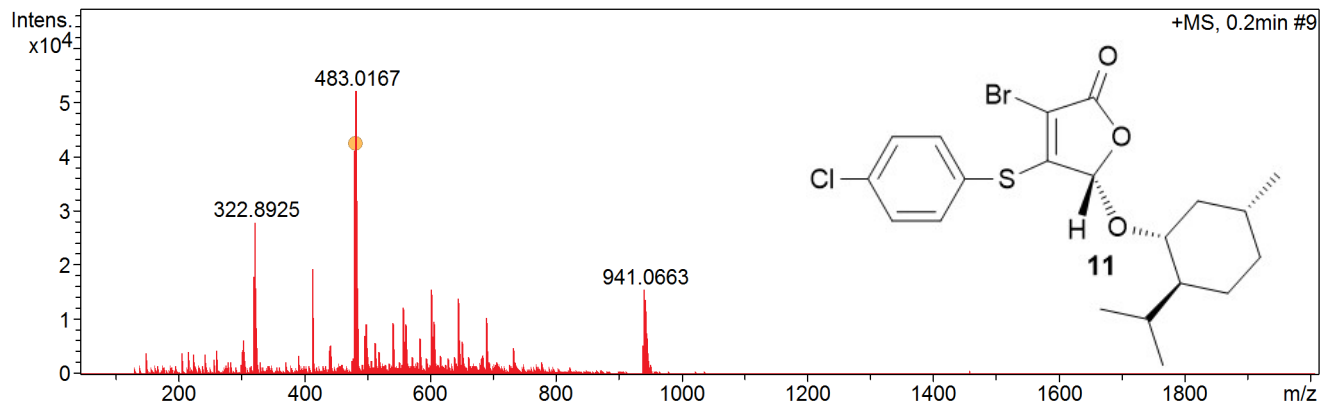
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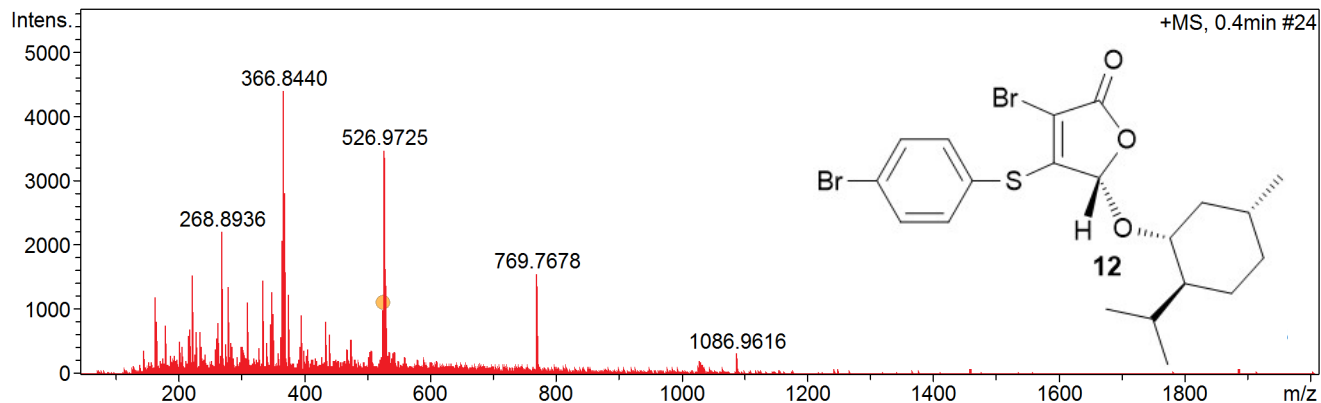
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Mass Spectrum SmartFormula Report

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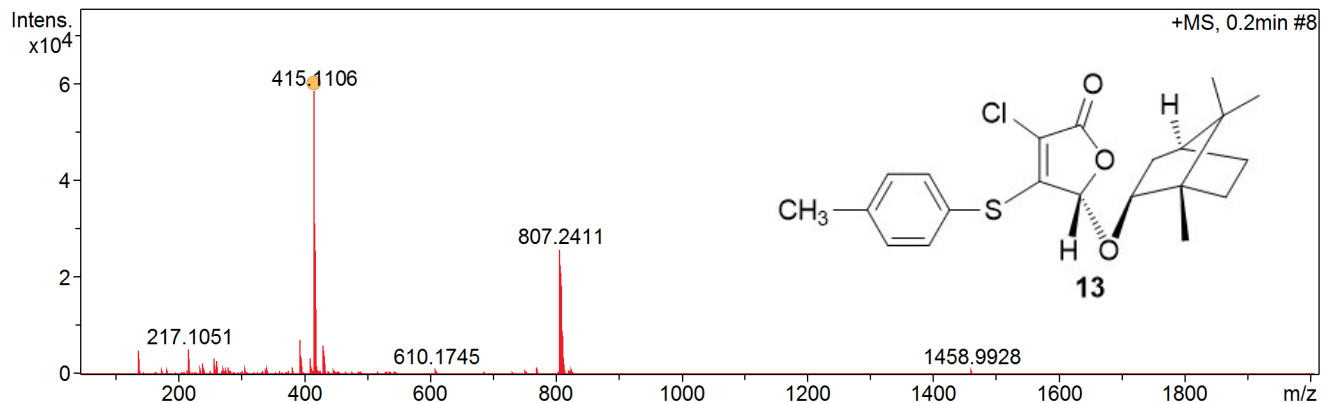
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Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
415.1106	1	C21H25ClNaO3S	415.1105	-0.1	18.8	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

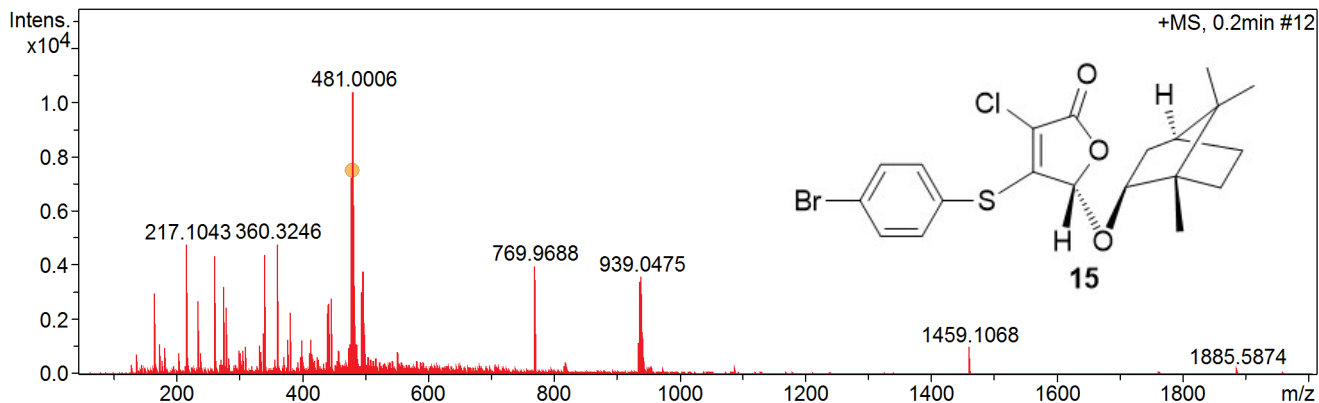
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Rg-B2
 Comment

Acquisition Date 2018/03/22 11:18:43

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
479.0062	1	C20H22BrClNaO3S	479.0054	-1.6	16.6	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

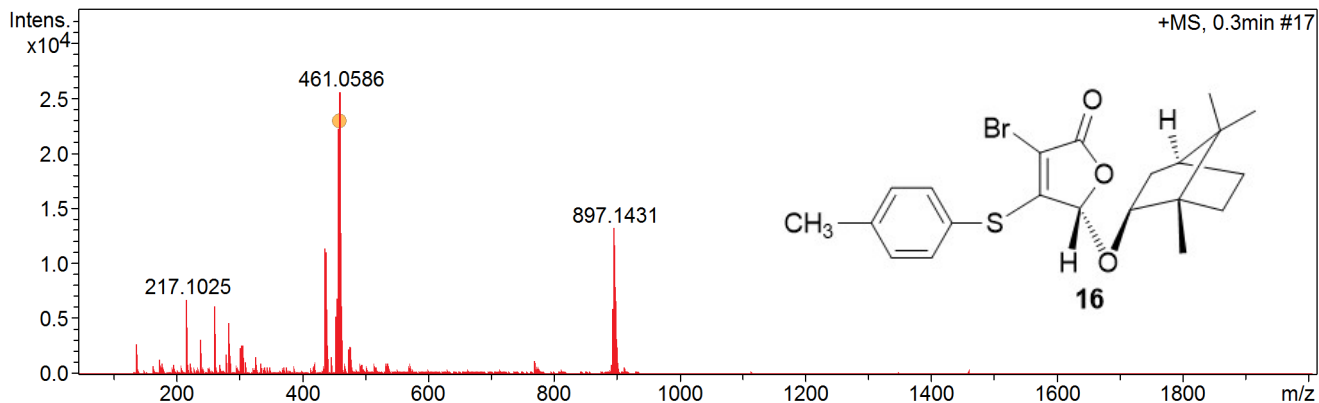
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Rg-S3
 Comment

Acquisition Date 2018/03/27 9:51:04

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
459.0599	1	C ₂₁ H ₂₅ BrNaO ₃ S	459.0600	0.2	34.8	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

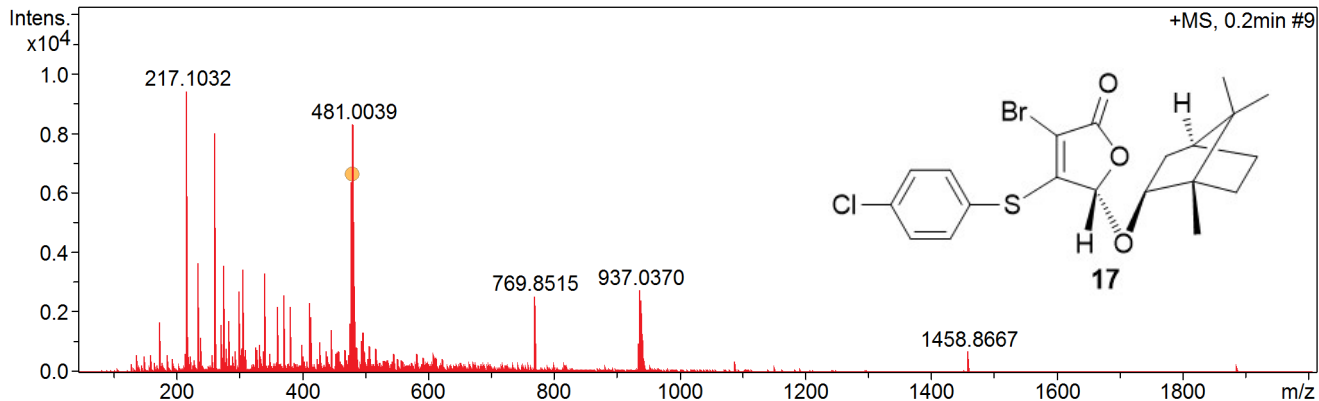
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Faz-L1
 Comment

Acquisition Date 2018/03/23 15:12:45

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
479.0056	1	C ₂₀ H ₂₂ BrClNaO ₃ S	479.0054	-0.4	35.4	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Faz-T1
 Comment

Acquisition Date 2018/03/26 11:45:19

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

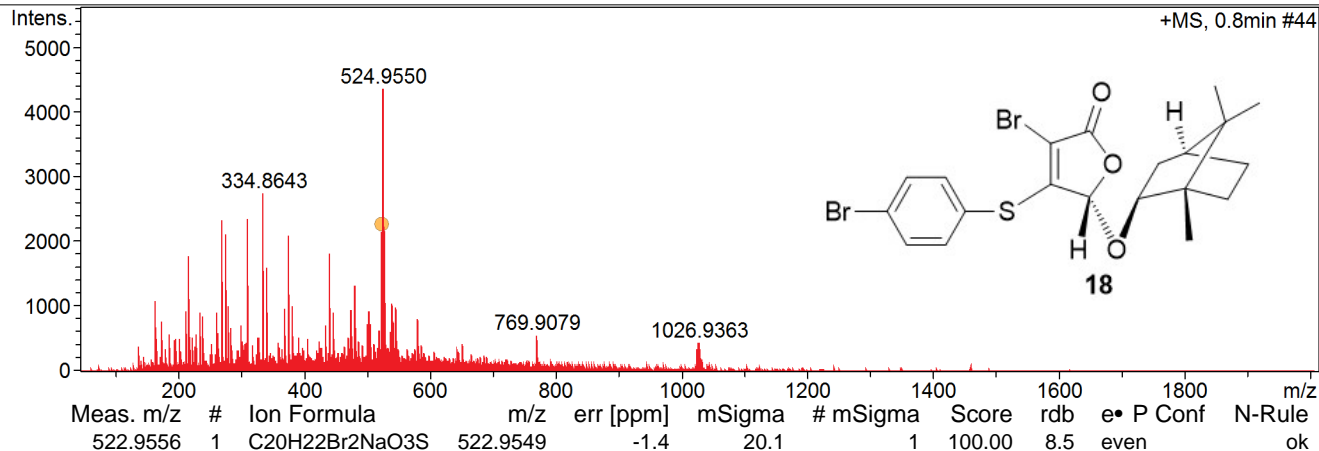


Figure S23. Mass spectra of thioethers 8–18.

a)

Mass Spectrum SmartFormula Report

Analysis Info

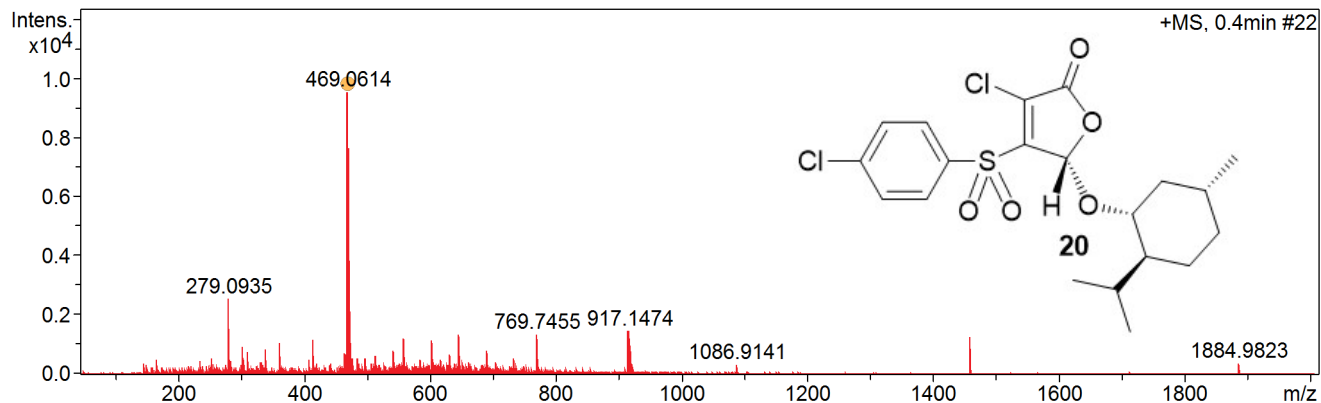
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name R10
 Comment

Acquisition Date 2018/06/16 12:05:09

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
469.0614	1	C ₂₀ H ₂₄ Cl ₂ NaO ₅ S	469.0614	0.0	51.2	1	100.00	7.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

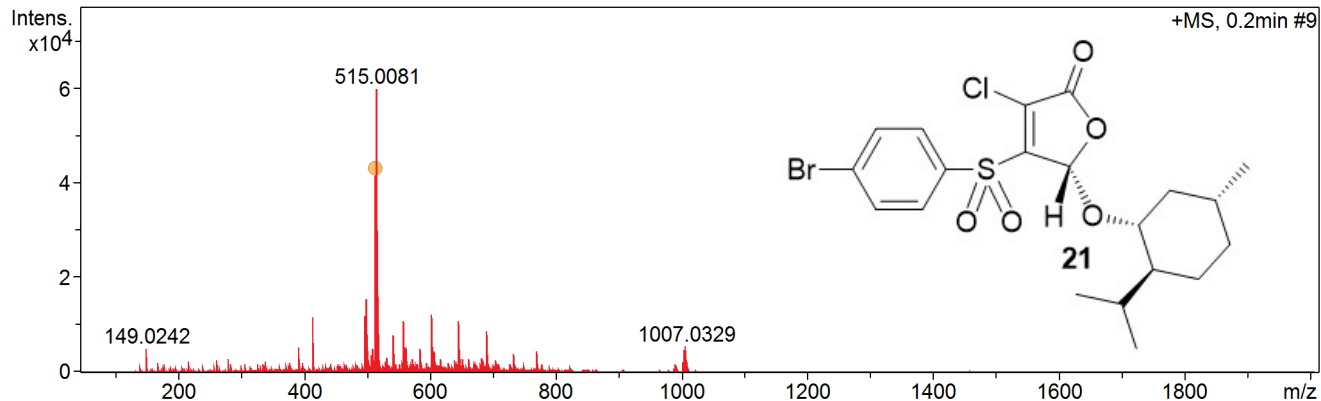
Analysis Name D:\Data\User
Method lcms_esi_pos_low.m
Sample Name ZR-E2
Comment

Acquisition Date 2018/03/05 14:13:22

Operator BDAL@DE
Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
513.0110	1	C20H24BrClNaO5S	513.0109	-0.3	21.2	1	100.00	7.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

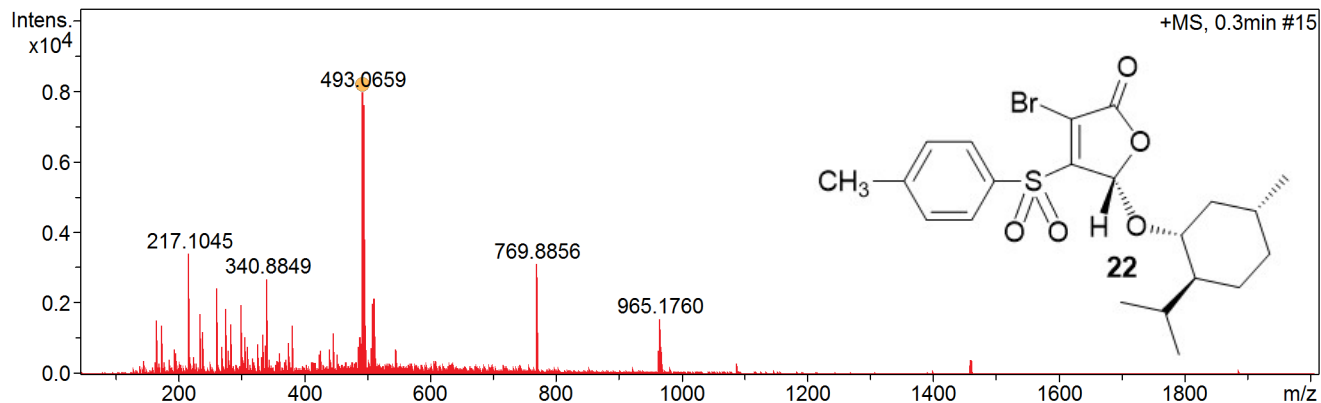
Analysis Name D:\Data\User
Method lcms_esi_pos_low.m
Sample Name ZR-I1
Comment

Acquisition Date 2018/03/13 14:51:30

Operator BDAL@DE
Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
493.0659	1	C21H27BrNaO5S	493.0655	-0.8	35.2	1	100.00	7.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

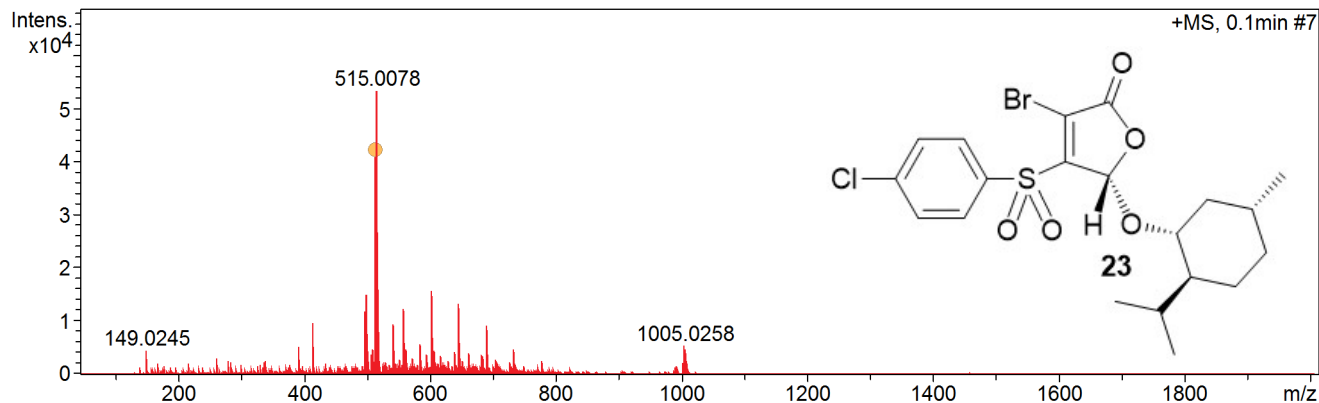
Analysis Name D:\Data\User
Method lcms_esi_pos_low.m
Sample Name ZR-F1
Comment

Acquisition Date 2018/03/05 14:13:22

Operator BDAL@DE
Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
513.0106	1	C20H24BrClNaO5S	513.0109	0.5	17.3	1	100.00	7.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

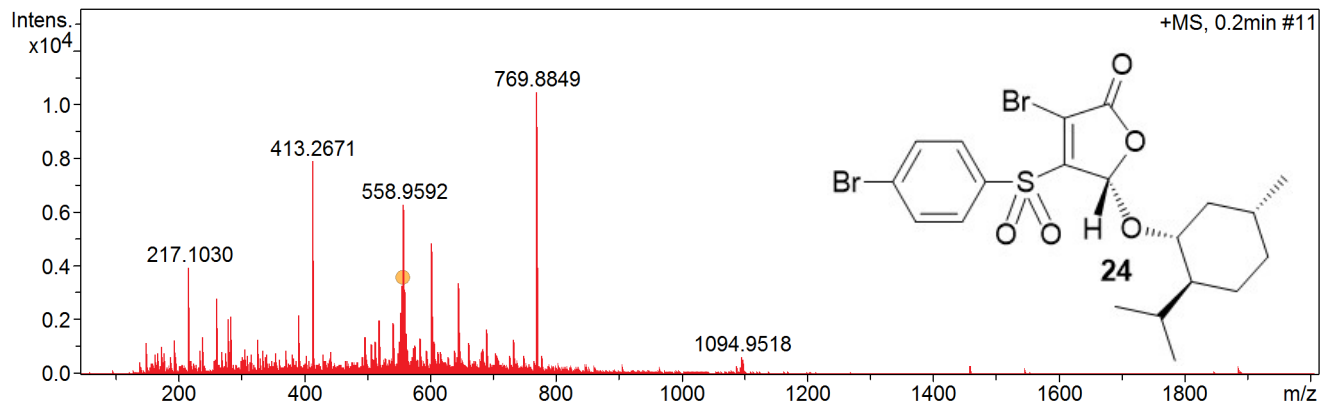
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name ZR-A1
 Comment

Acquisition Date 2018/03/13 14:47:13

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
556.9610	1	C ₂₀ H ₂₄ Br ₂ NaO ₅ S	556.9603	-1.1	31.7	1	100.00	7.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

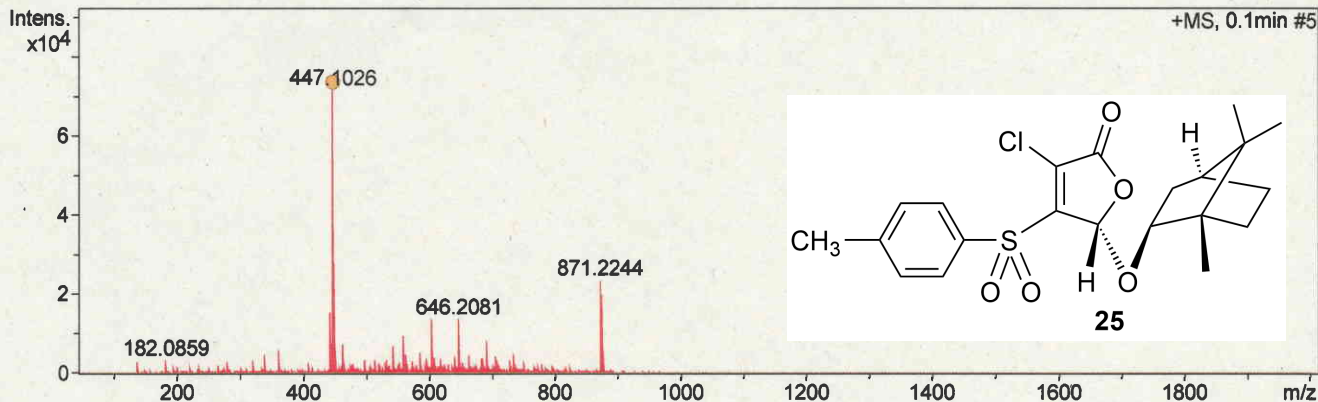
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Method lcms_esi_pos_low.m
Sample Name SR1
Comment

Acquisition Date 3/30/2017 4:18:23 PM

Operator BDAL@DE
Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
447.1026	1	C21H25ClNaO5S	447.1003	-5.1	13.0	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

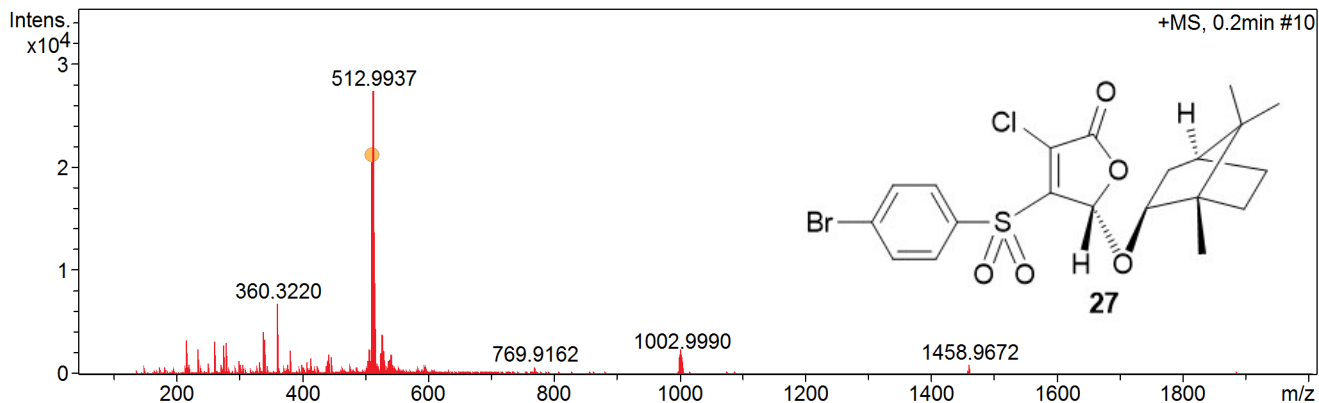
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Rg-Z1
 Comment

Acquisition Date 2018/03/22 12:31:02

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
510.9956	1	C20H22BrClNaO5S	510.9952	-0.9	10.4	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

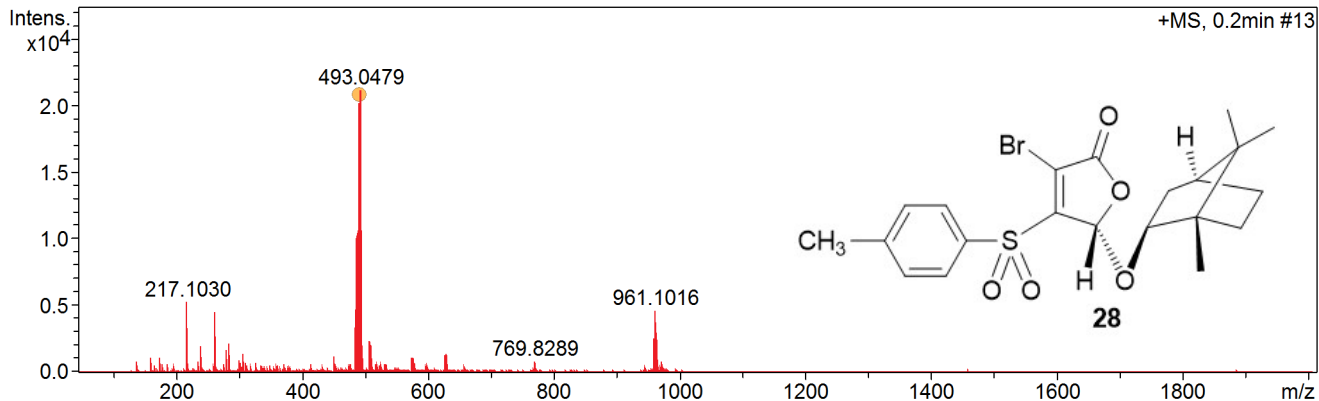
Analysis Name D:\Data\User
Method lcms_esi_pos_low.m
Sample Name Rg-G1
Comment

Acquisition Date 2018/03/23 15:08:58

Operator BDAL@DE
Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
491.0498	1	C ₂₁ H ₂₅ BrNaO ₅ S	491.0498	0.1	12.0	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

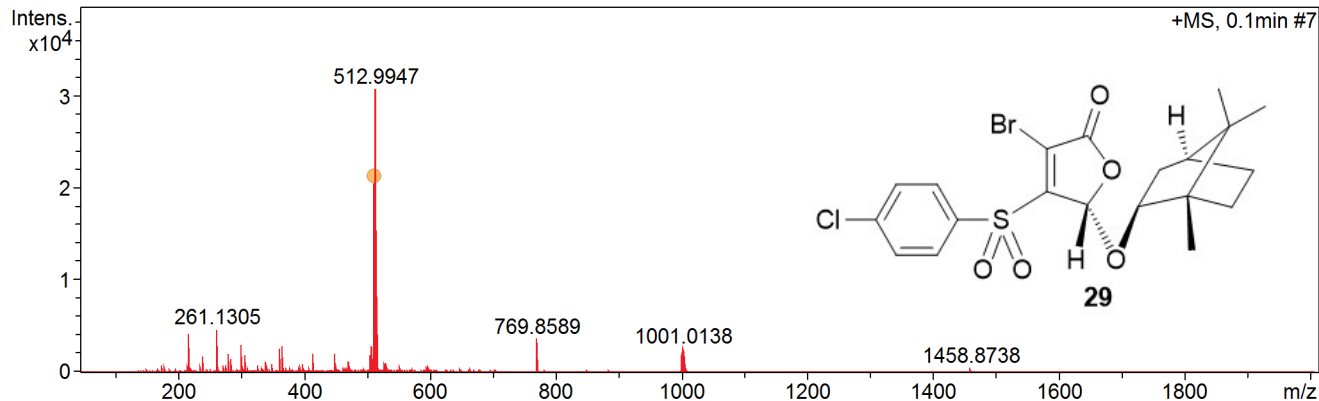
Analysis Name D:\Data\User
 Method lcms_esi_pos_low.m
 Sample Name Faz-X6
 Comment

Acquisition Date 2018/03/23 15:24:02

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e• P Conf	N-Rule
510.9950	1	C20H22BrClNaO5S	510.9952	0.4	30.8	1	100.00	8.5	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\User Data\Regina\SR6_1-6_01_706.d
 Method lcms_esi_pos_low.m
 Sample Name SR6
 Comment

Acquisition Date 3/30/2017 4:37:27 PM

Operator BDAL@DE
 Instrument micrOTOF II 8213750.10448

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	10.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

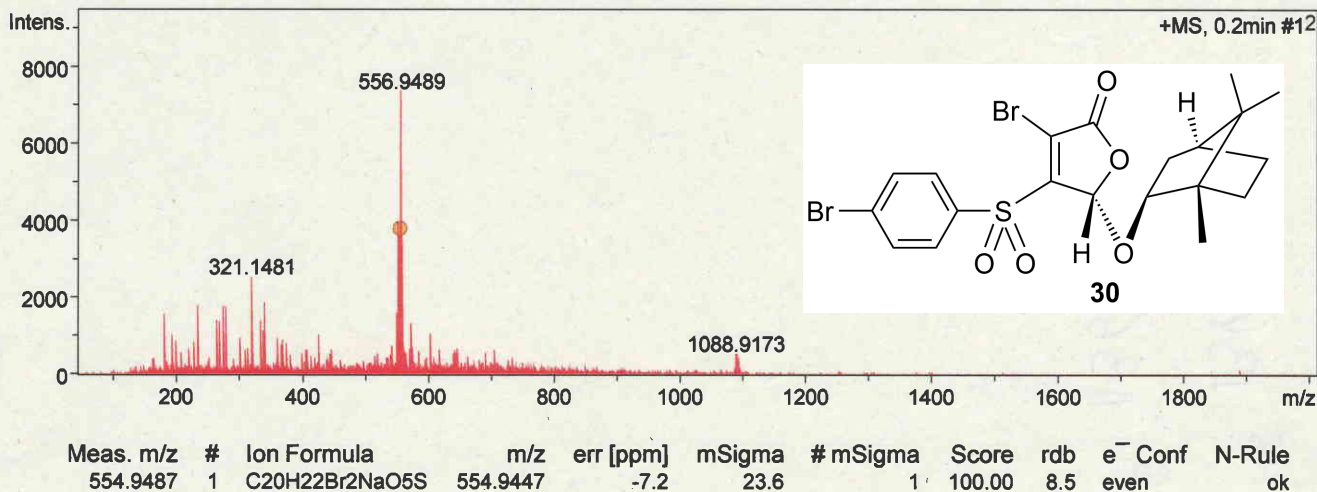
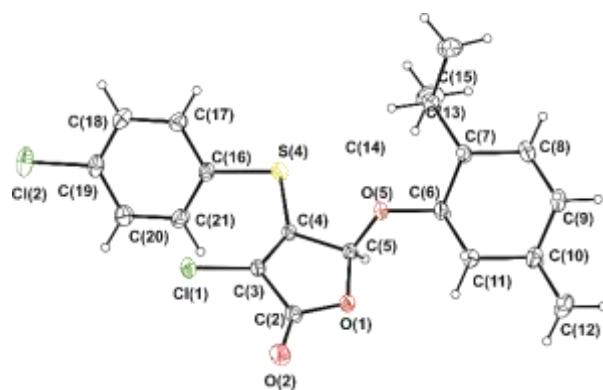


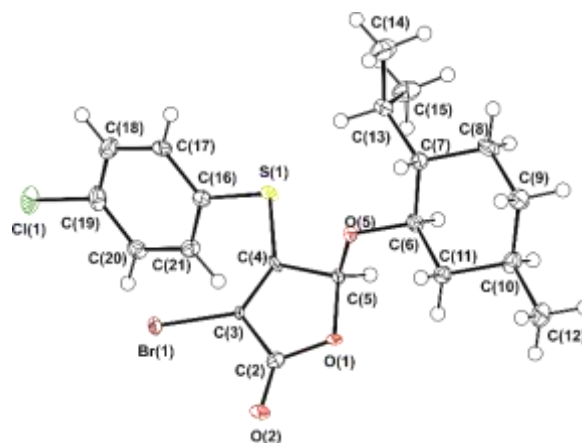
Figure S24. Mass spectra of sulfones 20–30.

Single crystal X-ray analysis

a)



b)



c)

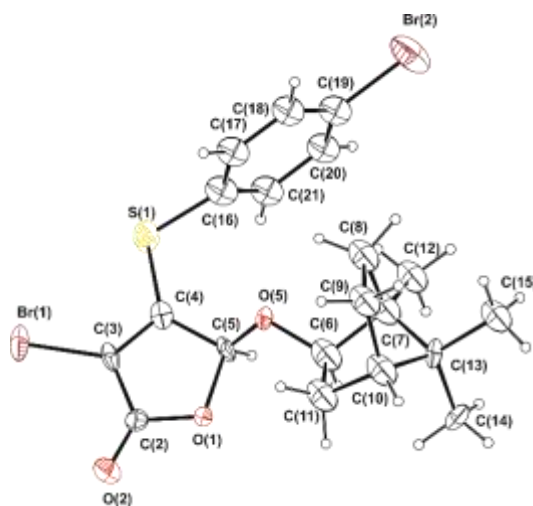
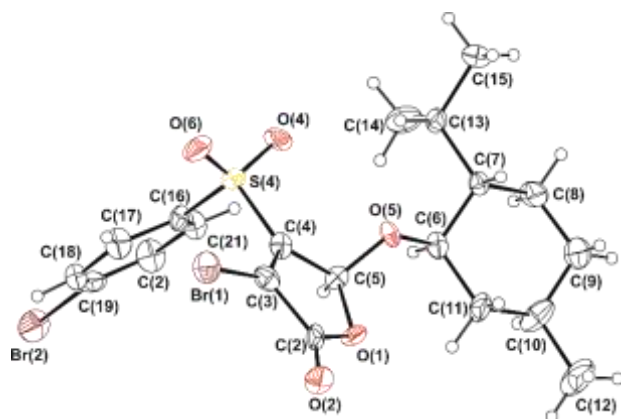
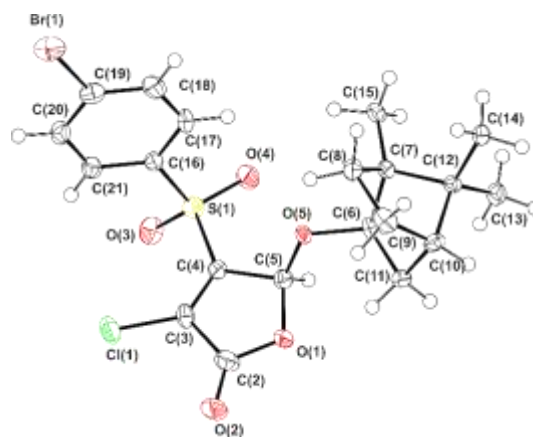


Figure S25. Molecular structure of thioethers **8** (a), **11** (b) and **18** (c) in the crystal.

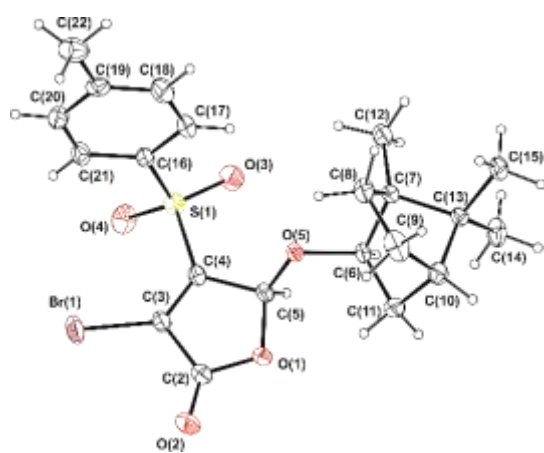
a)



b)



c)



d)

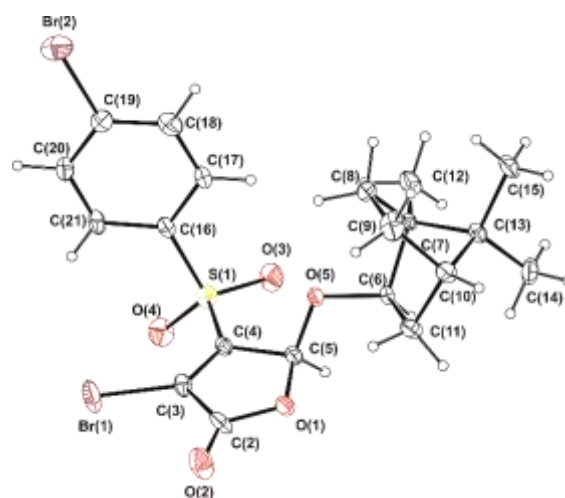


Figure S26. Molecular structure of sulfones **24** (a), **27** (b), **28** (c) and **30** (d) in the crystal.

Table S1. Crystal data, data collection and structure refinement details for crystals **5a**, **7**, **8**, **11**, **16**, **18**, **19**, **24**, **26–28** and **30**

Compound	5a	7	8	11	16	18
Empirical formula	C ₁₄ H ₁₈ Cl ₂ O ₃	C ₂₁ H ₂₇ ClO ₃ S	C ₂₀ H ₂₄ Cl ₂ O ₃ S	C ₂₀ H ₂₄ BrClO ₃ S	C ₂₁ H ₂₅ BrO ₃ S	C ₂₀ H ₂₂ Br ₂ O ₃ S
Formula weight	305.18	394.93	415.35	459.81	437.37	502.24
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	trigonal	monoclinic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁	<i>P</i> 3 ₂	<i>P</i> 2 ₁
<i>a</i> /Å	7.384(4)	10.274(5)	6.637(3)	6.7968(4)	15.742(7)	7.2279(19)
<i>b</i> /Å	7.920(4)	10.768(5)	8.087(3)	8.0082(4)	15.742(7)	29.569(8)
<i>c</i> /Å	25.943(13)	19.382(9)	19.288(8)	18.6589(11)	7.496(14)	10.475(3)
α	90	90	90	90	90	90
β	90	90	92.015(5)	91.688(4)	90	109.608(7)
γ	90	90	90	90	120	90
Volume, Å ³	1517.2(14)	2144.3(17)	1034.6(7)	1015.17(10)	1609(4)	2108.9(10)
<i>Z</i> and <i>Z'</i>	4 and 1	4 and 1	2 and 1	2 and 1	3 and 1	4 and 2
Calculated density, g cm ⁻³	1.336	1.223	1.333	1.504	1.354	1.582
Absorption coefficient, mm ⁻¹	0.429	0.292	0.431	2.276	2.030	3.959
<i>F</i> (000)	640	840	436	472	678	1008
Θ range for data collection	2.7° to 28.0°	2.1° to 28.0°	2.1° to 28.0°	3.7° to 28.0°	3.0° to 27.0°	3.6, 27.0
Index ranges	-9 ≤ <i>h</i> ≤ 9, -10 ≤ <i>k</i> ≤ 4, -34 ≤ <i>l</i> ≤ 34	-13 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -25 ≤ <i>l</i> ≤ 24	-8 ≤ <i>h</i> ≤ 8, -10 ≤ <i>k</i> ≤ 10, -25 ≤ <i>l</i> ≤ 25	-8 ≤ <i>h</i> ≤ 8, -10 ≤ <i>k</i> ≤ 10, -24 ≤ <i>l</i> ≤ 24	-20 ≤ <i>h</i> ≤ 20, -19 ≤ <i>k</i> ≤ 20, -5 ≤ <i>l</i> ≤ 9	-4 ≤ <i>h</i> ≤ 9, -37 ≤ <i>k</i> ≤ 36, -13 ≤ <i>l</i> ≤ 13
Reflections collected	13916	19674	9419	17063	13251	17907
Independent reflections [<i>R</i> (int)]	3643 [0.115]	5159 [0.079]	4844, 0.044	4796, 0.057	3245 [0.2383]	8928 [0.1070]
Observed Data [<i>I</i> > 2σ(<i>I</i>)]	2000	2606	3774	3975	1067	3638
Data / parameters	3643/212	5159/239	4844, 238	4796, 235	3245/178	8928/343
Goodness-of-fit on <i>F</i> ²	0.95	0.96	0.94	1.05	0.94	0.96
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0572, <i>wR</i> ₂ = 0.0957	<i>R</i> ₁ = 0.0512, <i>wR</i> ₂ = 0.1019	<i>R</i> ₁ = 0.0417 <i>wR</i> ₂ = 0.0833	<i>R</i> ₁ = 0.0483 <i>wR</i> ₂ = 0.1046	<i>R</i> ₁ = 0.0790 <i>wR</i> ₂ = 0.1677	<i>R</i> ₁ = 0.0840 <i>wR</i> ₂ = 0.2011
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.1263, <i>wR</i> ₂ = 0.1197	<i>R</i> ₁ = 0.1207, <i>wR</i> ₂ = 0.1265	<i>R</i> ₁ = 0.0558 <i>wR</i> ₂ = 0.0894	<i>R</i> ₁ = 0.0658 <i>wR</i> ₂ = 0.1115	<i>R</i> ₁ = 0.2570 <i>wR</i> ₂ = 0.2500	<i>R</i> ₁ = 0.2144 <i>wR</i> ₂ = 0.2646
Flack parameter	-0.06(7)	0.05(8)	-0.07(5)	-0.002(6)	0.05(4)	0.011(12)
Largest diff. peak and hole, e Å ⁻³	-0.21 and 0.21	-0.166 and 0.037	-0.227 and 0.186	-0.599 and 1.811	-0.339 and 0.327	-0.98 and 0.87

Table S1 continued. Crystal data, data collection and structure refinement details for crystals **5a**, **7**, **8**, **11**, **16**, **18**, **19**, **24**, **26–28** and **30**

Compound	19	24	26	27	28	30
Empirical formula	C ₂₁ H ₂₇ ClO ₅ S	C ₂₀ H ₂₄ Br ₂ O ₅ S	C ₂₀ H ₂₂ Cl ₂ O ₅ S	C ₂₀ H ₂₂ BrClO ₅ S	C ₂₁ H ₂₅ BrO ₅ S	C ₂₀ H ₂₂ Br ₂ O ₅ S
Formula weight	426.93	536.27	445.34	489.79	469.37	534.24
Crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	6.371(3)	9.652(7)	10.154(3)	10.0530(13)	10.2462(19)	10.094(10)
<i>b</i> /Å	17.650(7)	9.994(7)	11.250(3)	11.2524(11)	11.346(2)	11.199(10)
<i>c</i> /Å	19.166(8)	23.147(15)	18.301(6)	18.191(2)	18.312(4)	18.418(17)
α	90	90	90	90	90	90
β	90	90	90	90	90	90
γ	90	90	90	90	90	90
Volume, Å ³	2155.2(16)	2233(3)	2090.6(11)	2057.8(4)	2128.8(7)	2082(3)
<i>Z</i> and <i>Z'</i>	4 and 1	4 and 1	4 and 1	4 and 1	4 and 1	4 and 1
Calculated density, g cm ⁻³	1.316	1.595	1.415	1.581	1.464	1.704
Absorption coefficient, mm ⁻¹	0.303	3.751	0.439	2.258	2.058	4.023
<i>F</i> (000)	904	1080	928	1000	968	1072
Θ range for data collection	1.6° to 26.0°	3.9° to 27.0°	4.3, 27.0	2.7° to 27.0°	3.8, 28.0	3.8, 27.0
Index ranges	-7 ≤ <i>h</i> ≤ 12, -21 ≤ <i>k</i> ≤ 21, -23 ≤ <i>l</i> ≤ 23	-7 ≤ <i>h</i> ≤ 12, -12 ≤ <i>k</i> ≤ 11, -29 ≤ <i>l</i> ≤ 29	-12 ≤ <i>h</i> ≤ 6, -14 ≤ <i>k</i> ≤ 14, -23 ≤ <i>l</i> ≤ 23	-12 ≤ <i>h</i> ≤ 12, -14 ≤ <i>k</i> ≤ 14, -23 ≤ <i>l</i> ≤ 22	-13 ≤ <i>h</i> ≤ 7, -14 ≤ <i>k</i> ≤ 14, -24 ≤ <i>l</i> ≤ 24	-9 ≤ <i>h</i> ≤ 12, -13 ≤ <i>k</i> ≤ 14, -22 ≤ <i>l</i> ≤ 23
Reflections collected	20910	16527	17858	25768	19651	17894
Independent reflections [<i>R</i> (int)]	4089, 0.167	4851, 0.248	4542 [0.056]	4467, 0.105	5115 [0.082]	4543 [0.146]
Observed Data [<i>I</i> > 2σ(<i>I</i>)]	2062	1748	3494	3309	2844	2237
Data / parameters	4089, 257	4851, 256	4542/253	4467, 256	5115/257	4543/256
Goodness-of-fit on <i>F</i> ²	1.05	0.89	1.03	0.99	1.01	1.02
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0976 <i>wR</i> ₂ = 0.0853	<i>R</i> ₁ = 0.0723 <i>wR</i> ₂ = 0.1155	<i>R</i> ₁ = 0.0523 <i>wR</i> ₂ = 0.1054	<i>R</i> ₁ = 0.0455 <i>wR</i> ₂ = 0.0776	<i>R</i> ₁ = 0.0511 <i>wR</i> ₂ = 0.1000	<i>R</i> ₁ = 0.0582 <i>wR</i> ₂ = 0.1128
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.2105 <i>wR</i> ₂ = 0.1048	<i>R</i> ₁ = 0.2427 <i>wR</i> ₂ = 0.1666	<i>R</i> ₁ = 0.0735 <i>wR</i> ₂ = 0.1152	<i>R</i> ₁ = 0.0759 <i>wR</i> ₂ = 0.0879	<i>R</i> ₁ = 0.1225 <i>wR</i> ₂ = 0.1233	<i>R</i> ₁ = 0.1563 <i>wR</i> ₂ = 0.1462
Flack parameter	-0.04(6)	0.02(3)	-0.09(4)	-0.005(9)	-0.007(6)	-0.019(13)
Largest diff. peak and hole, e Å ⁻³	-0.273 and 0.235	-0.523 and 0.549	-0.25 and 0.30	-0.463 and 0.423	-0.31 and 0.58	-0.65 and 0.43