

Supporting Information

Design, Synthesis And Biological Evaluation of Soluble 2,5-Diketopiperazines Derivatives As Potential Antifouling Agents

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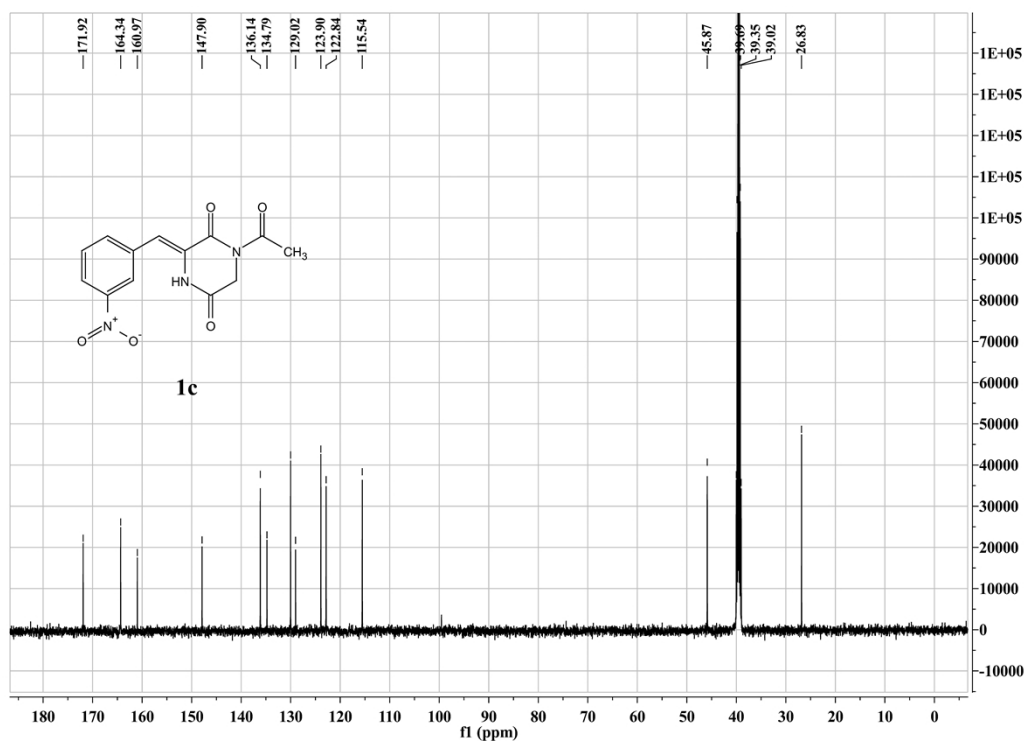
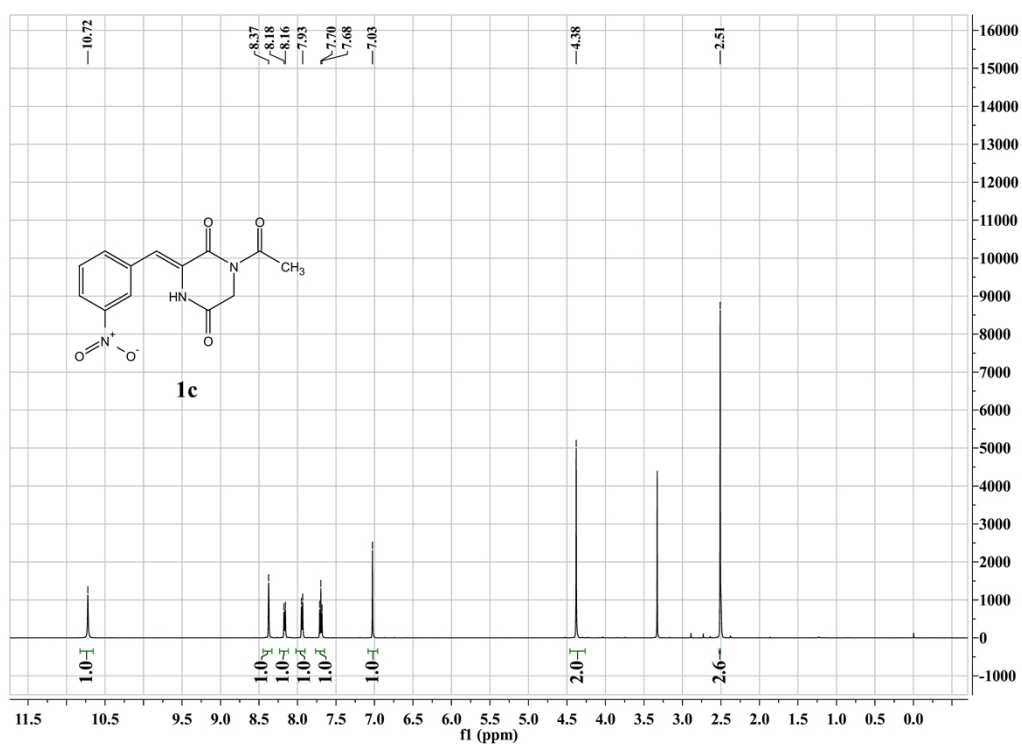
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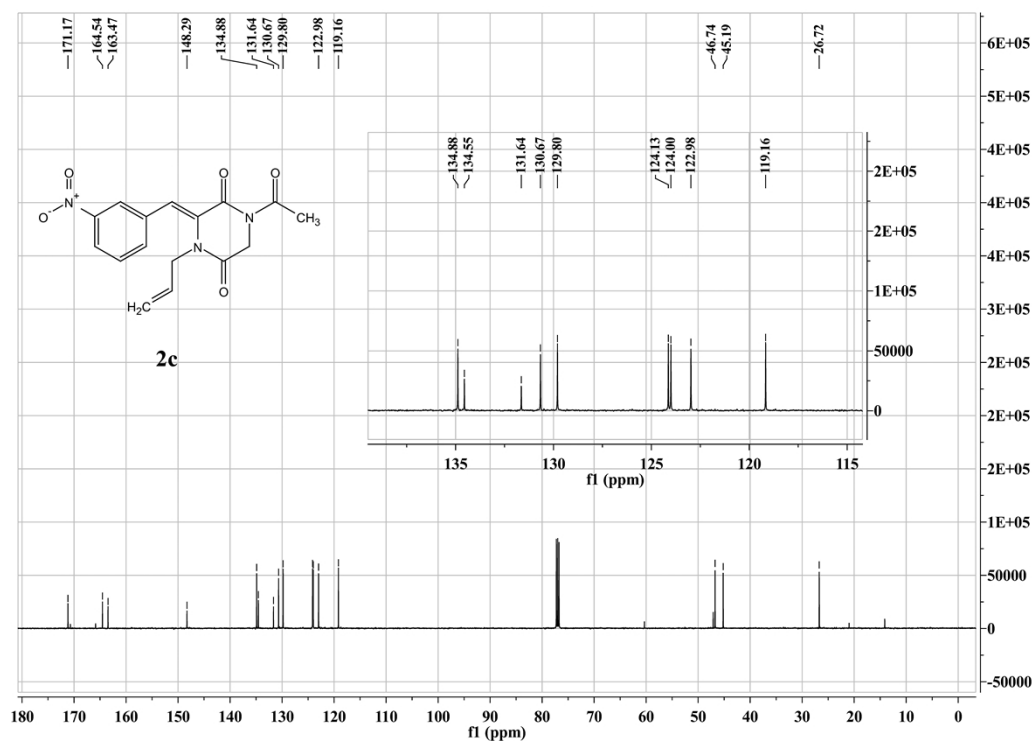
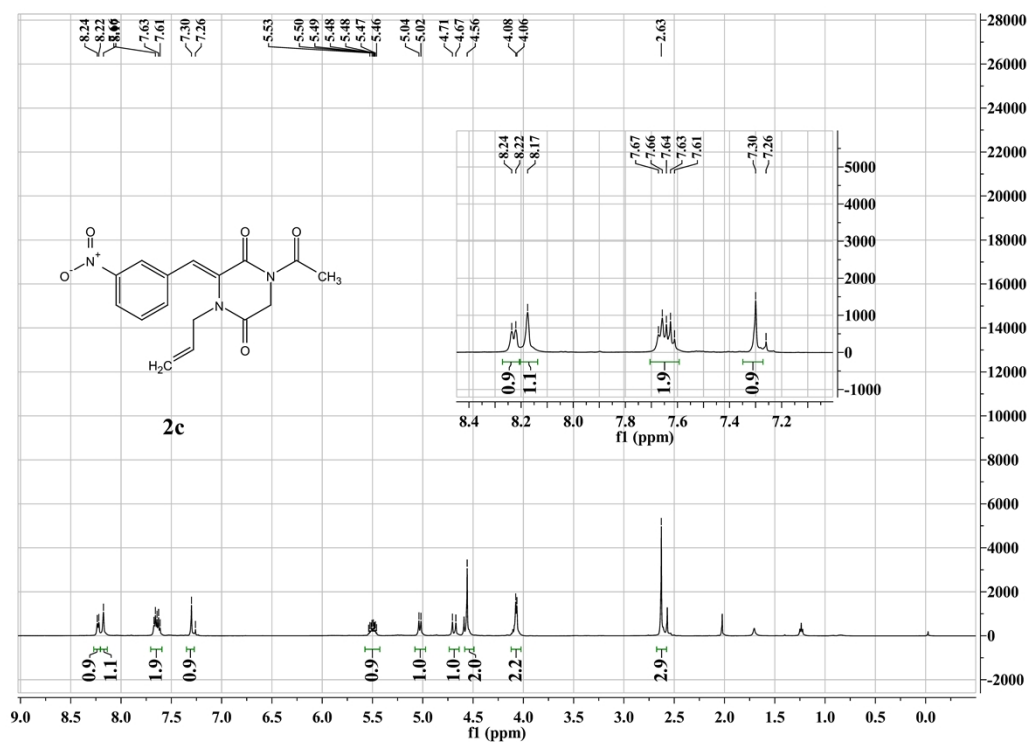
* Author to whom correspondence should be addressed; E-Mail: yonghongliu@scsio.ac.cn; Tel./Fax: +86-020-8902-3244.

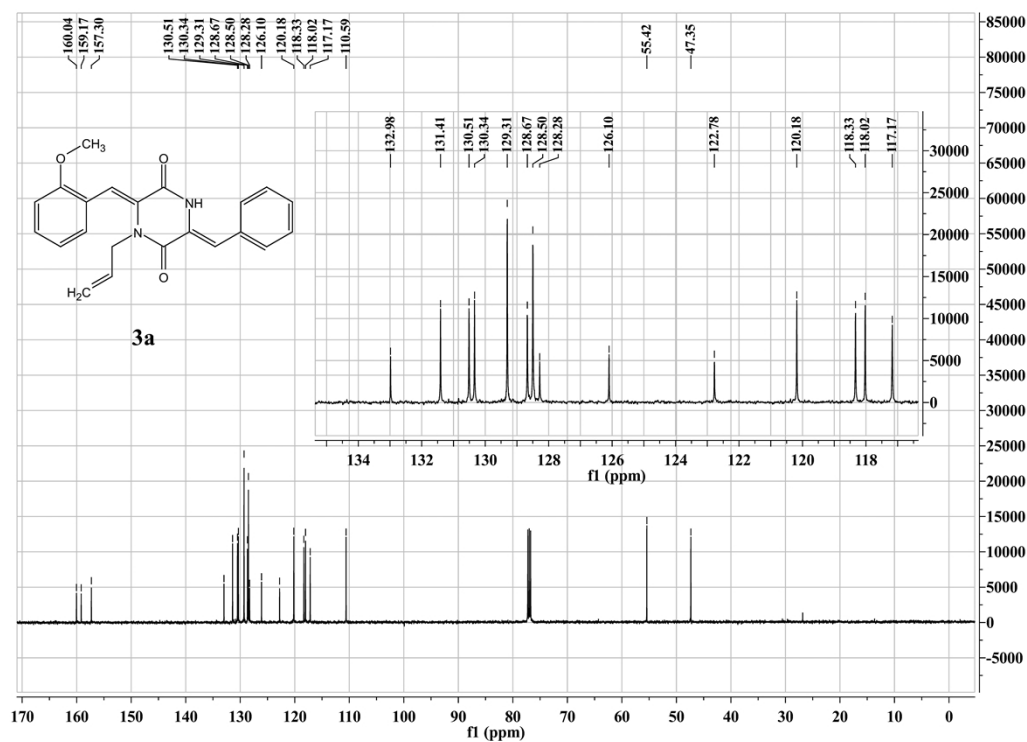
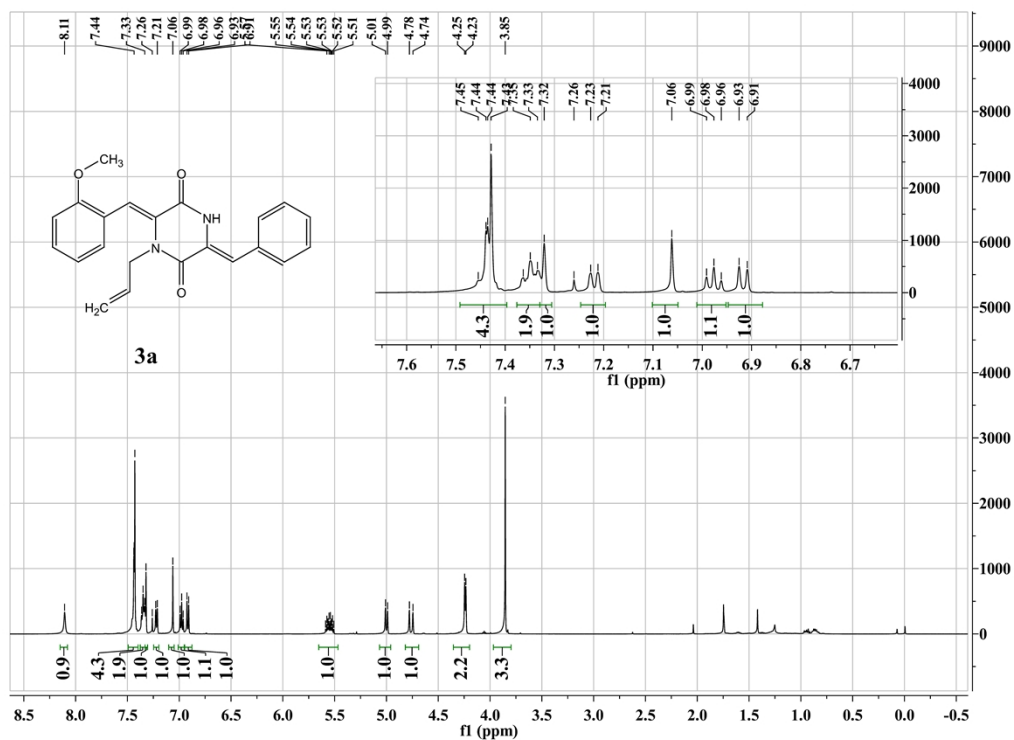
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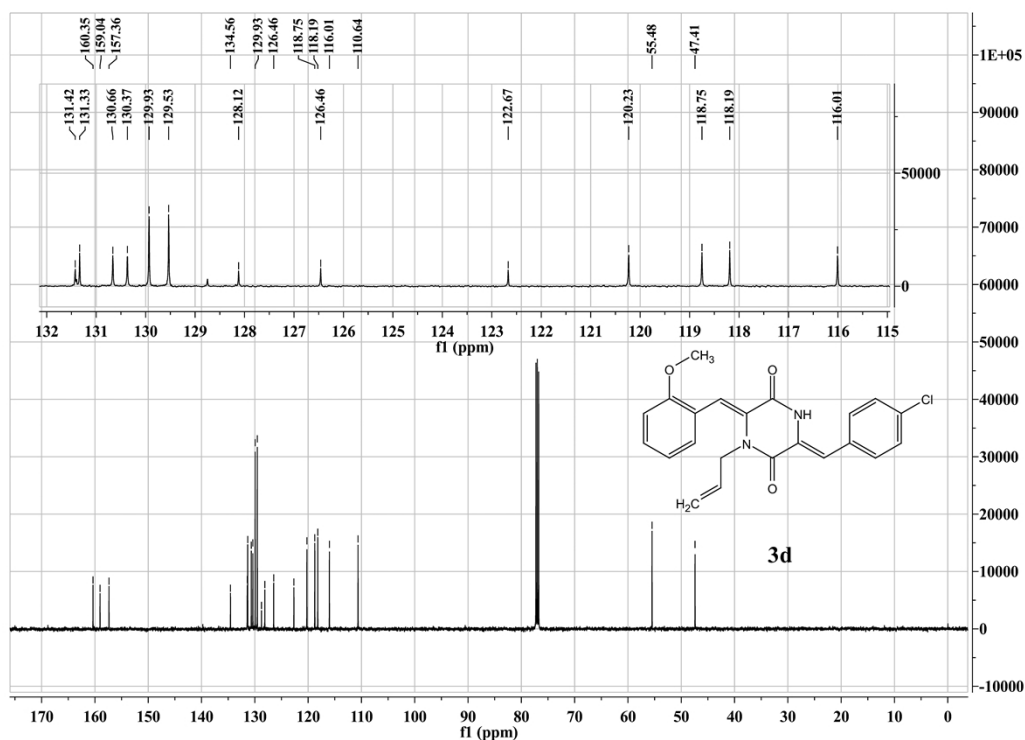
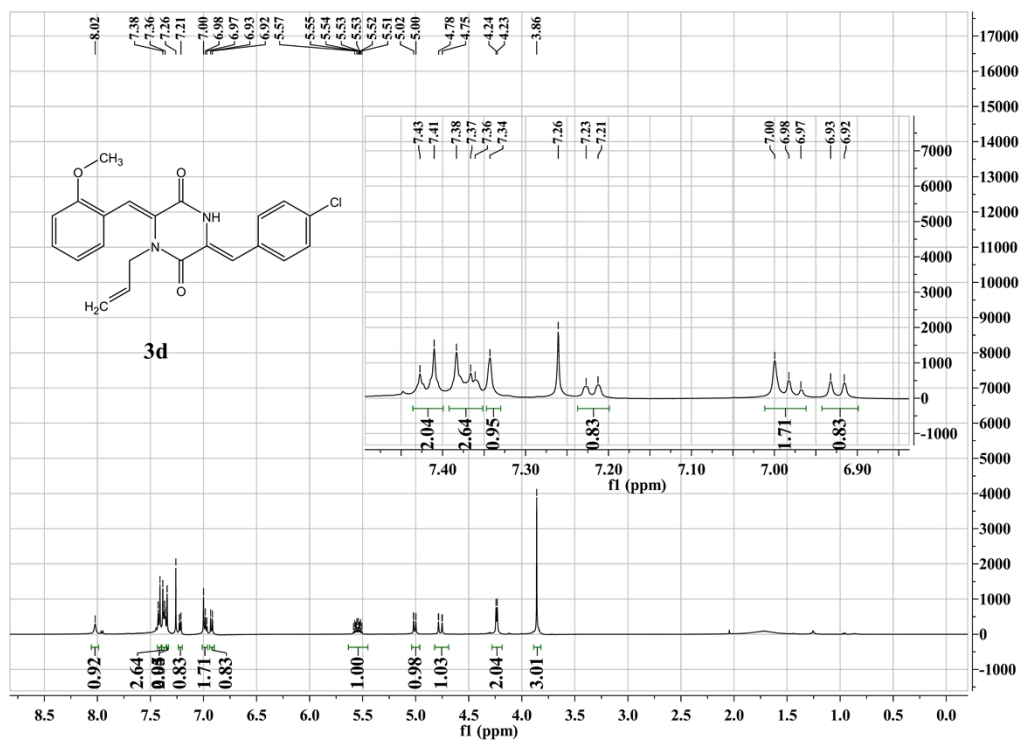
1. ¹ H and ¹³ C NMR of compounds 1c , 2c , 3a , 3d , 3f-g , 3j-m	Page S1-S10
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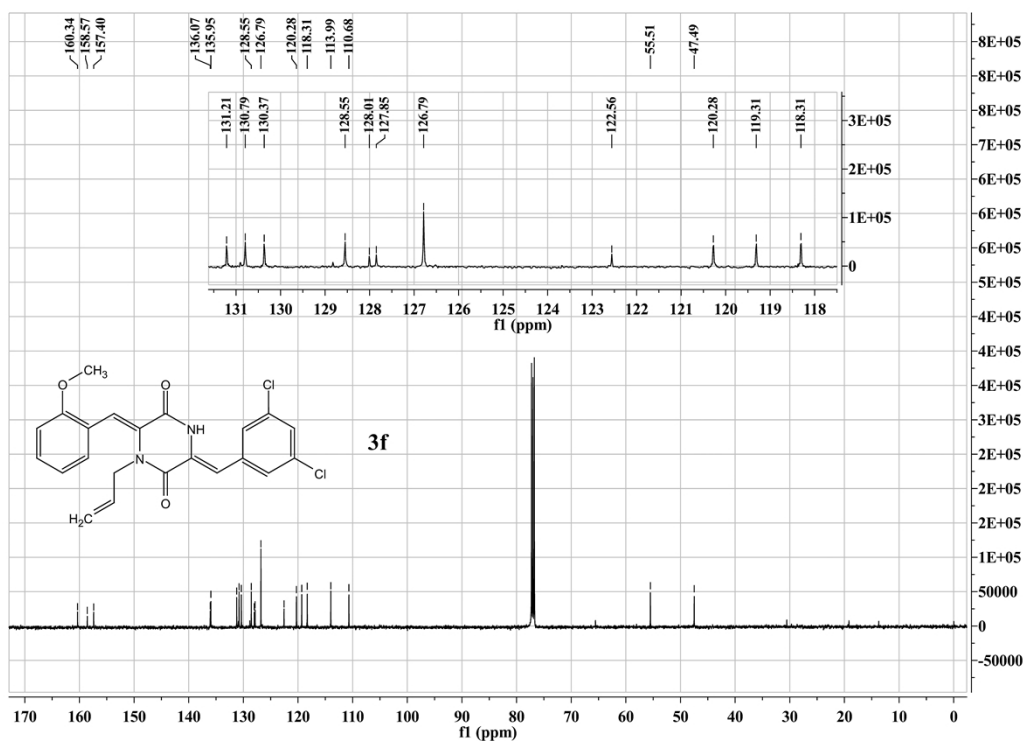
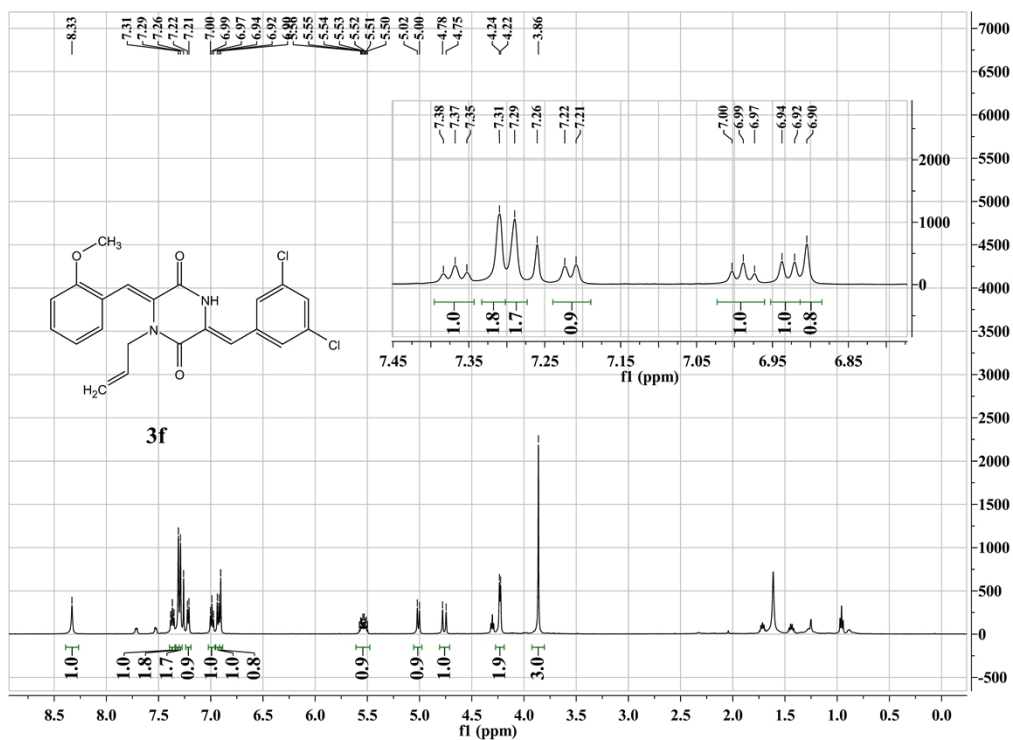
1. ^1H and ^{13}C NMR of compounds **1c**, **2c**, **3a**, **3d**, **3f-g**, **3j-m**

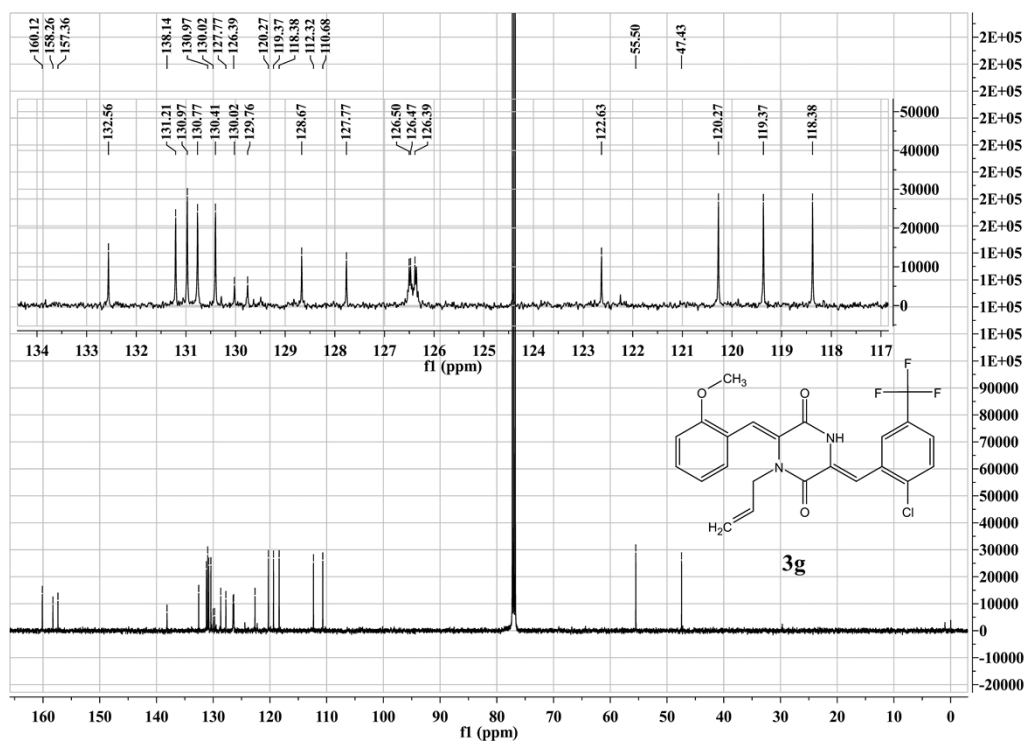
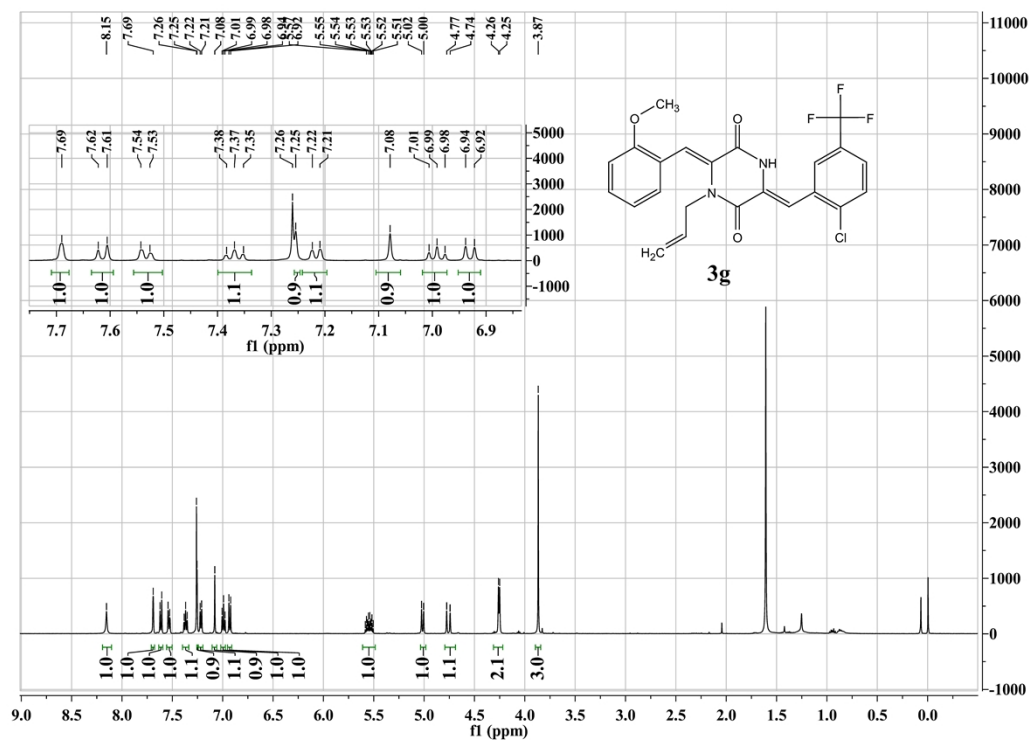


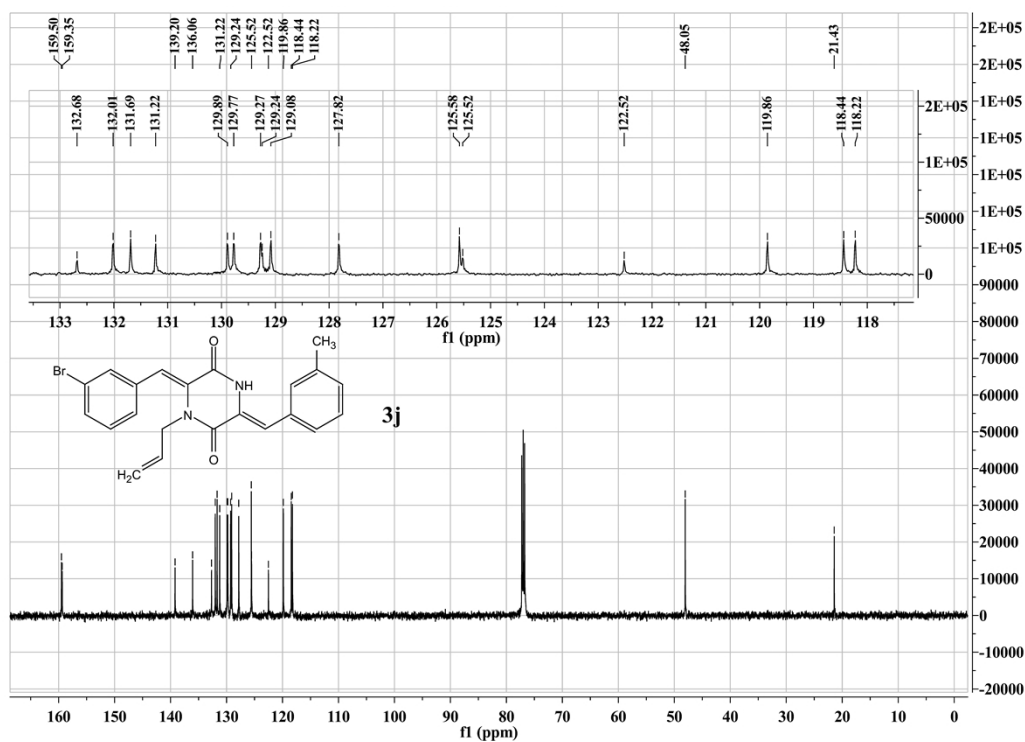
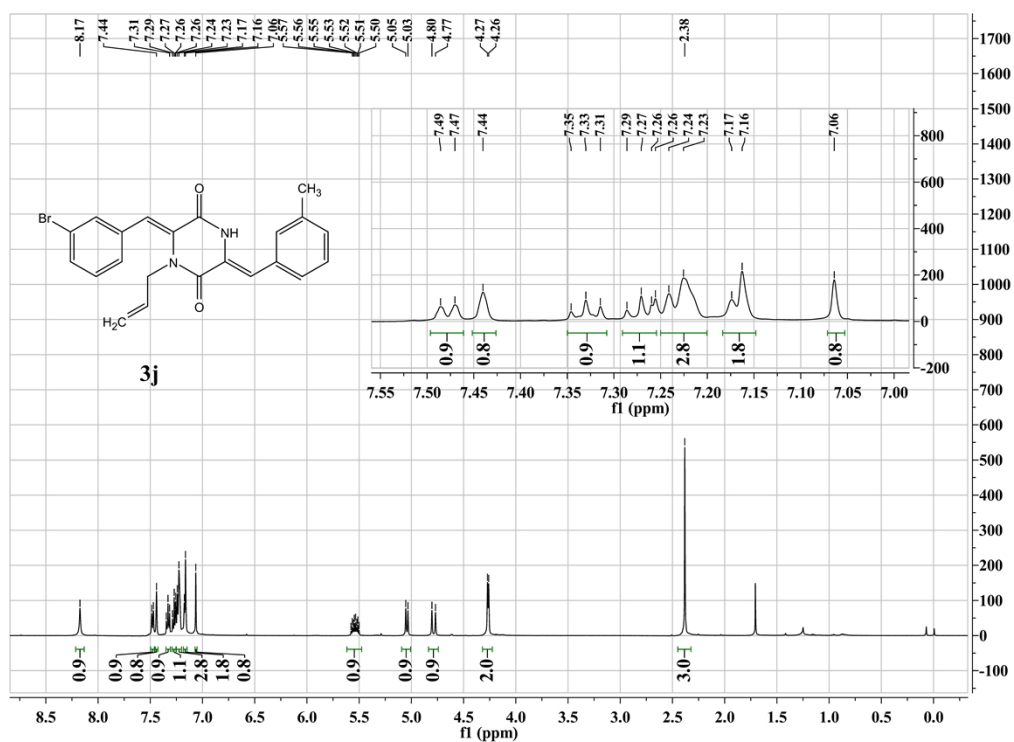


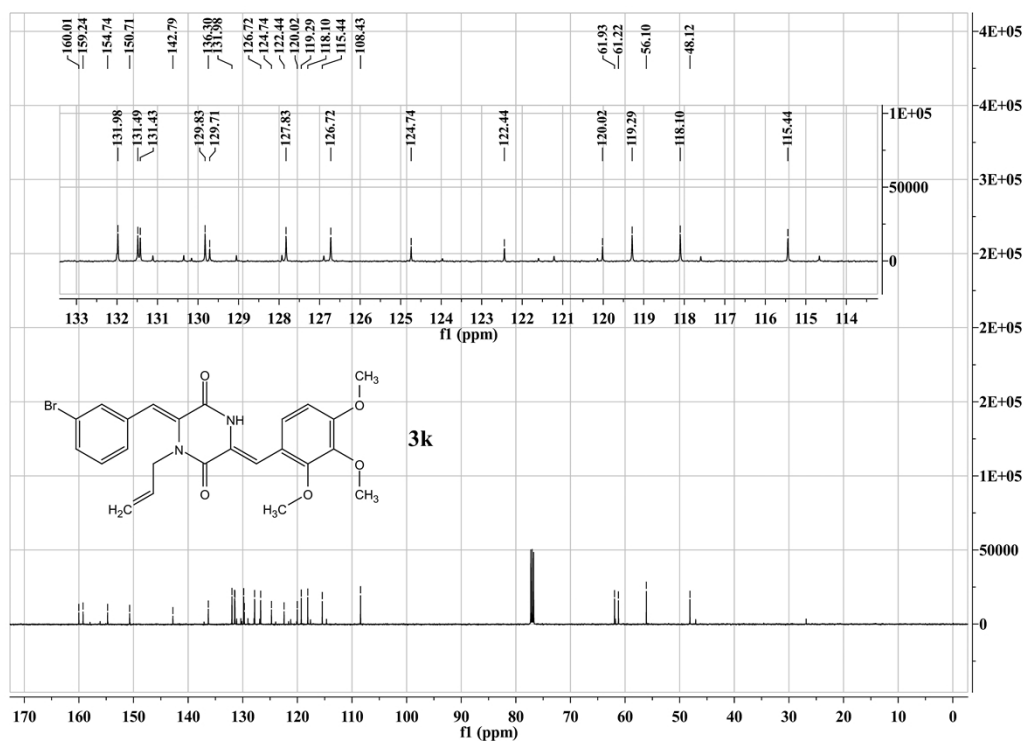
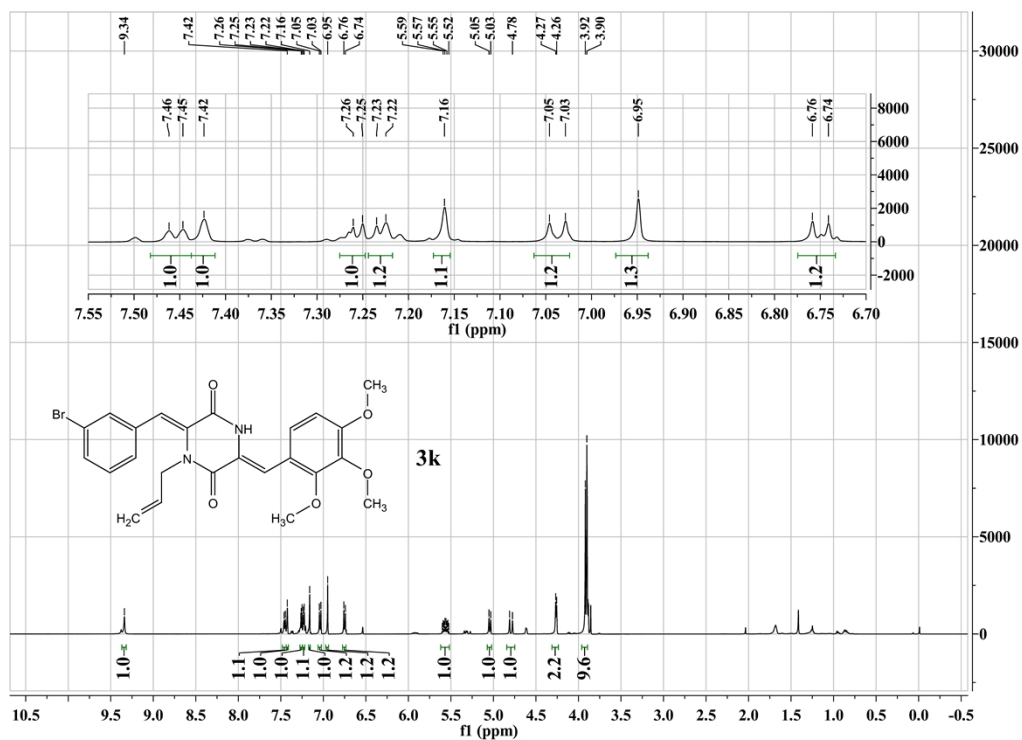


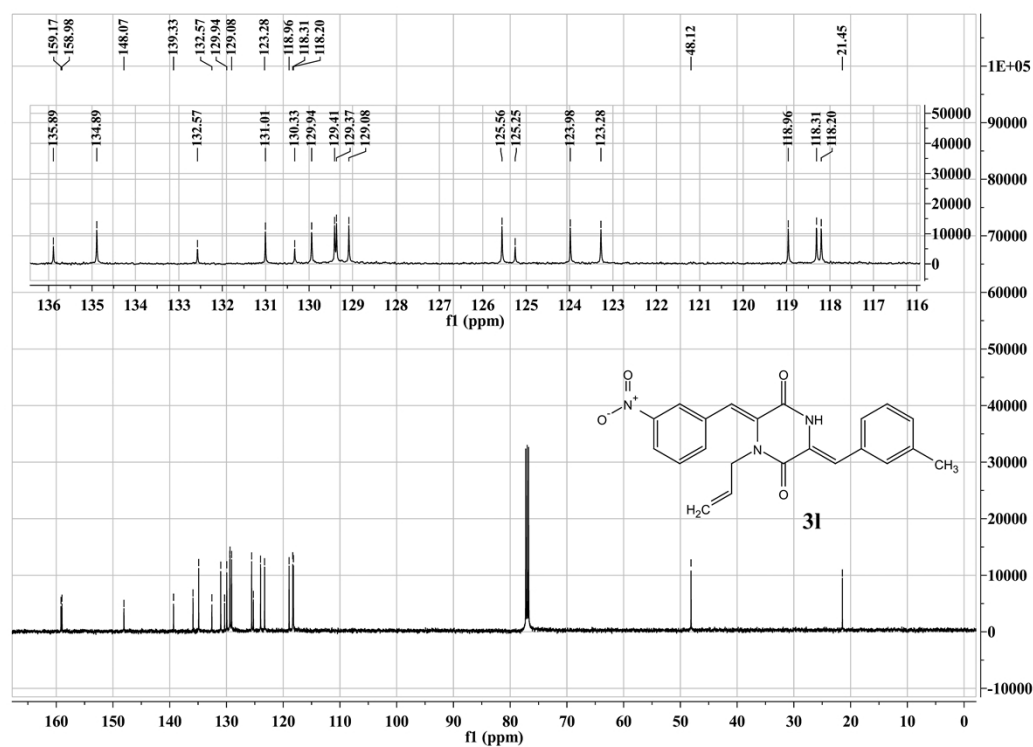
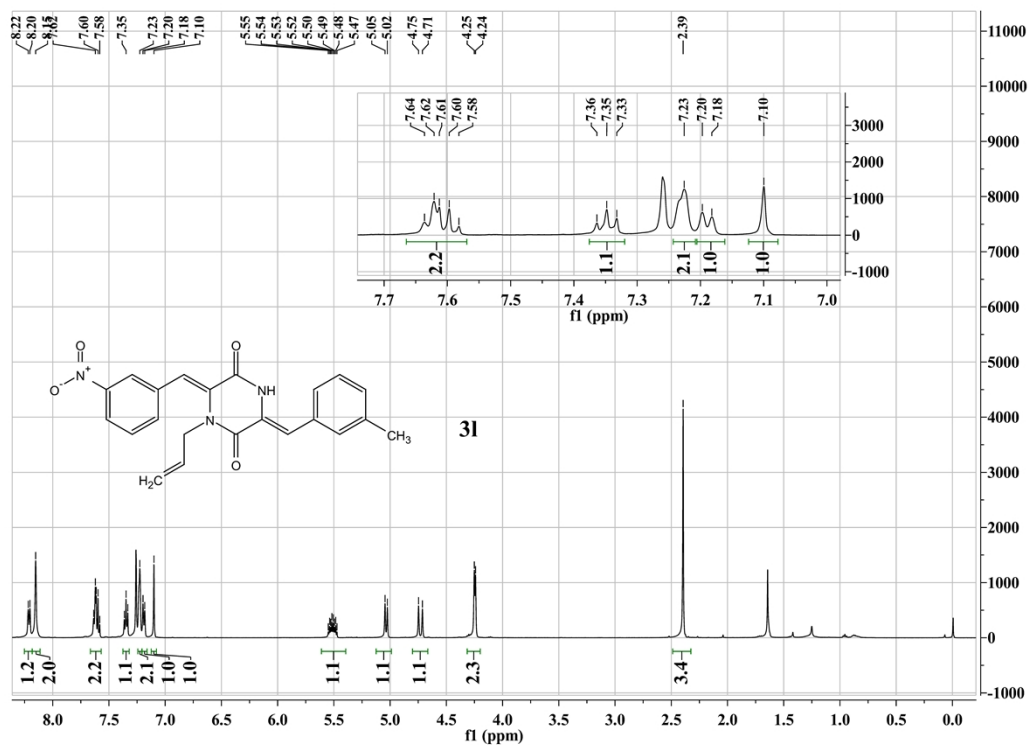


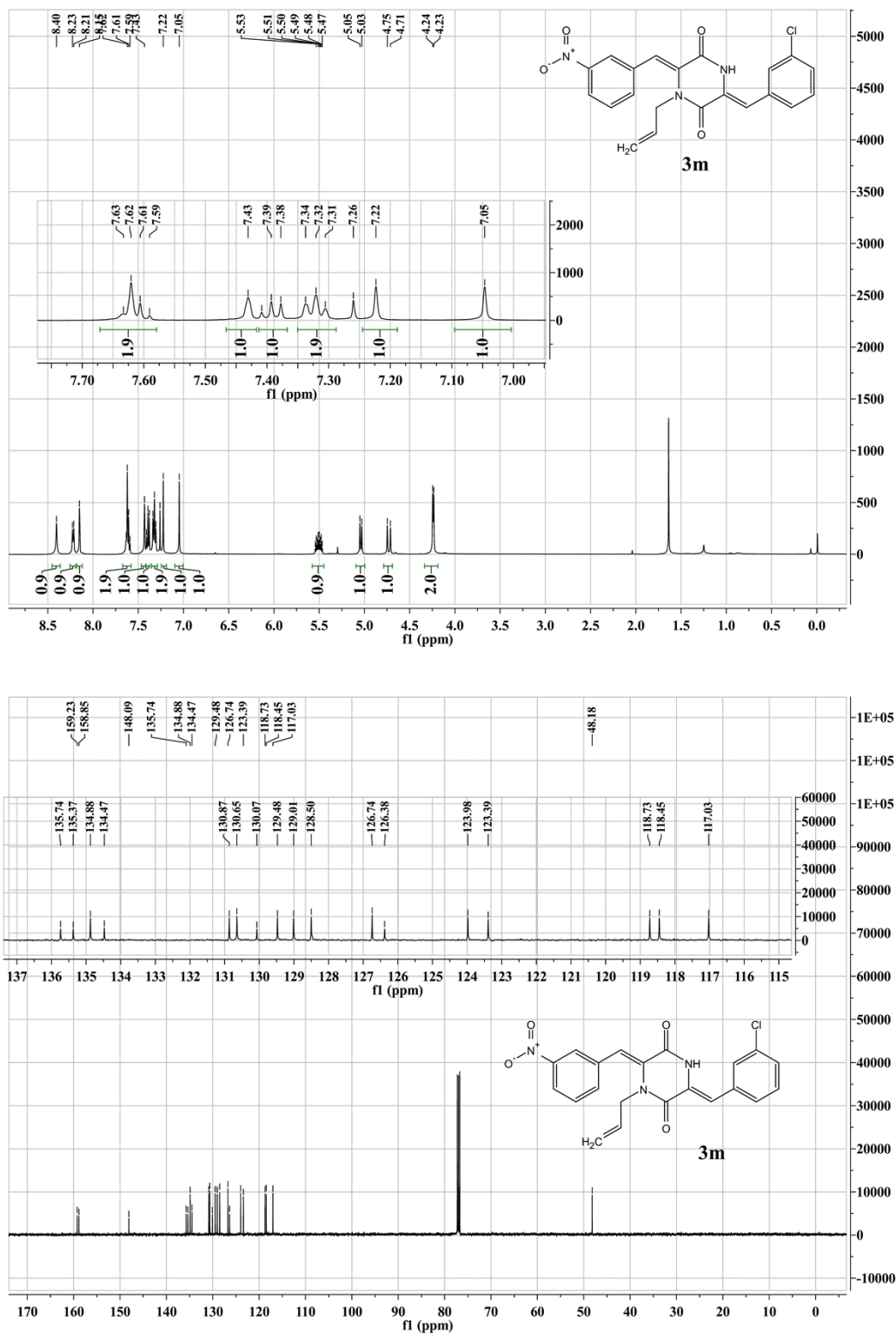




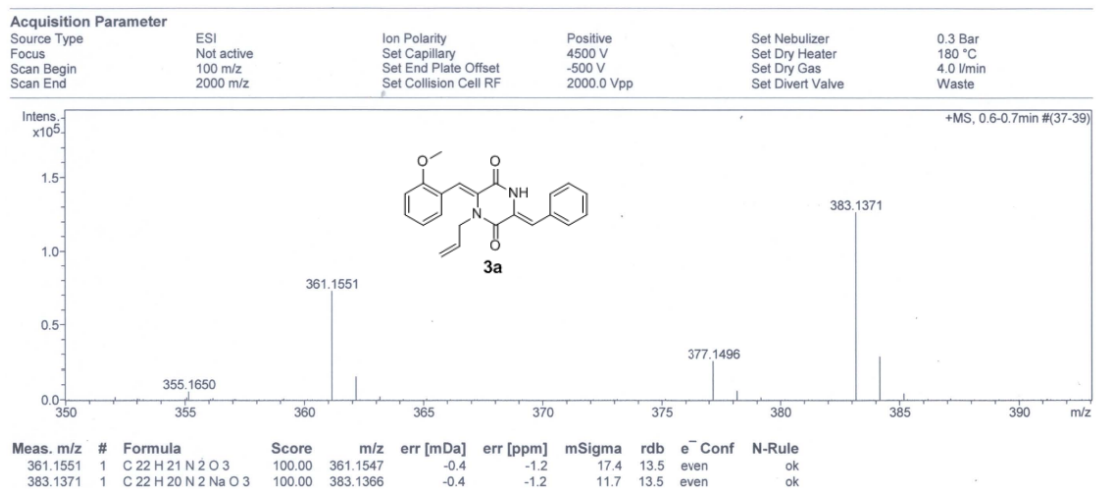
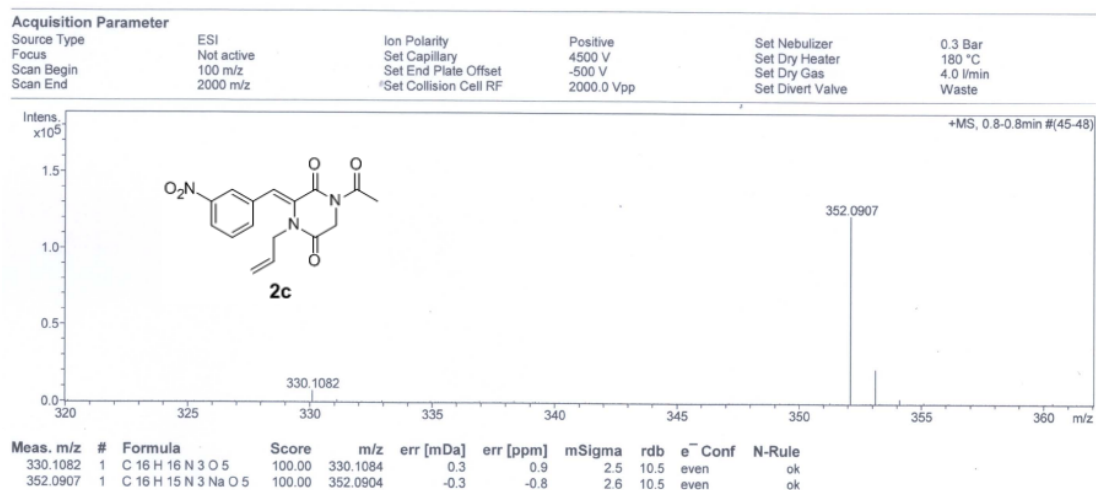
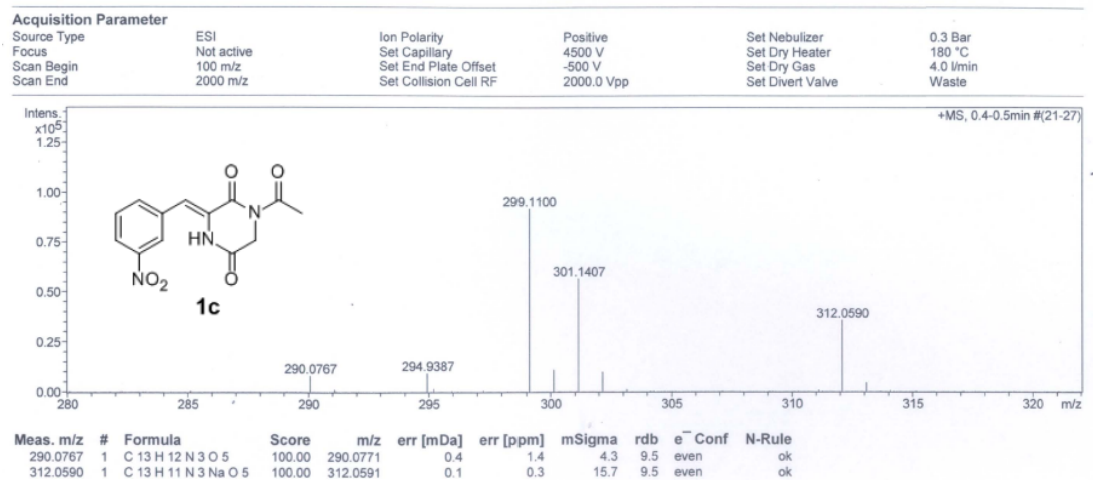






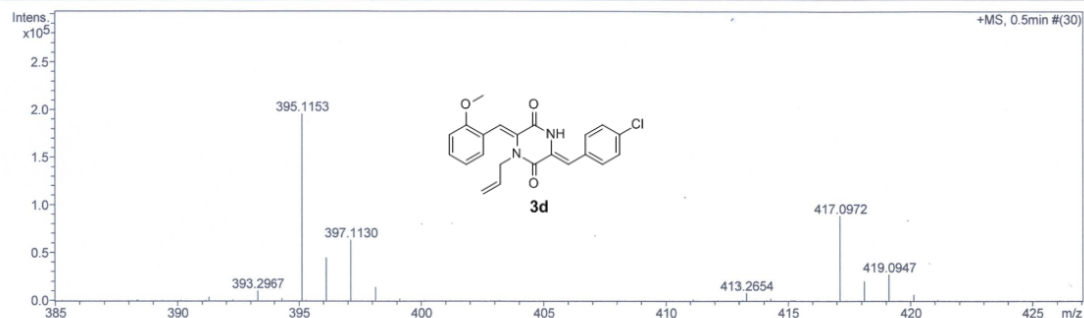


2. HRMS of compounds **1c**, **2c**, **3a**, **3d**, **3f-g**, **3j-m**



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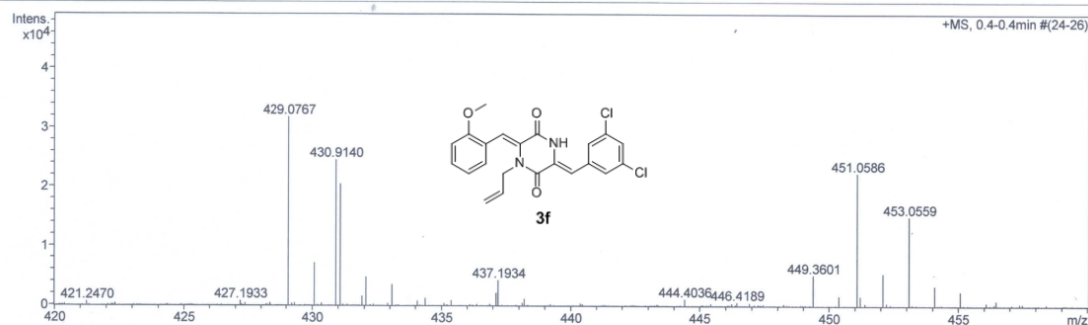
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Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
395.1153	1	C ₂₂ H ₂₀ ClN ₂ O ₃	100.00	395.1157	0.4	1.0	16.2	13.5	even	ok
417.0972	1	C ₂₂ H ₁₉ ClN ₂ NaO ₃	83.55	417.0976	0.4	1.0	23.0	13.5	even	ok

Acquisition Parameter

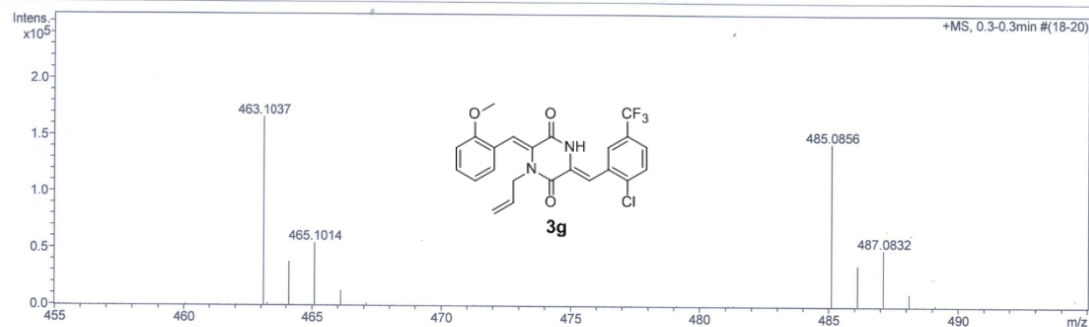
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Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
429.0767	1	C ₂₂ H ₁₉ Cl ₂ N ₂ O ₃	100.00	429.0767	-0.0	-0.0	16.6	13.5	even	ok
451.0586	1	C ₂₂ H ₁₈ Cl ₂ N ₂ NaO ₃	99.11	451.0587	0.1	0.3	10.1	13.5	even	ok

Acquisition Parameter

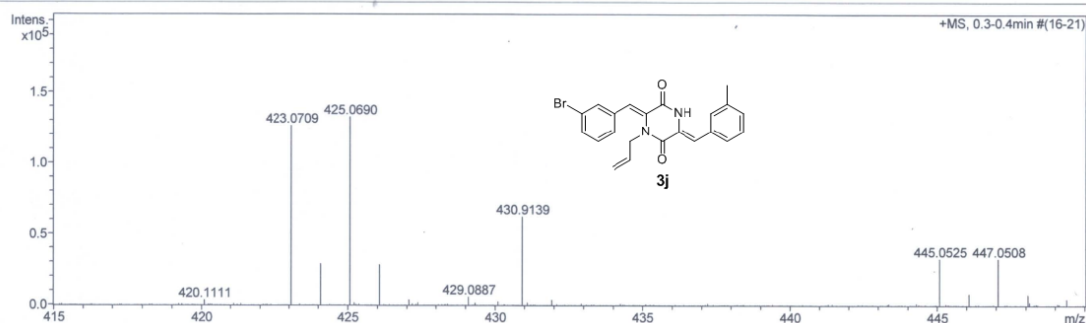
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Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
463.1037	1	C ₂₃ H ₁₉ ClF ₃ N ₂ O ₃	100.00	463.1031	-0.6	-1.3	17.4	13.5	even	ok
485.0856	1	C ₂₃ H ₁₈ ClF ₃ N ₂ NaO ₃	100.00	485.0850	-0.5	-1.1	5.5	13.5	even	ok

Acquisition Parameter

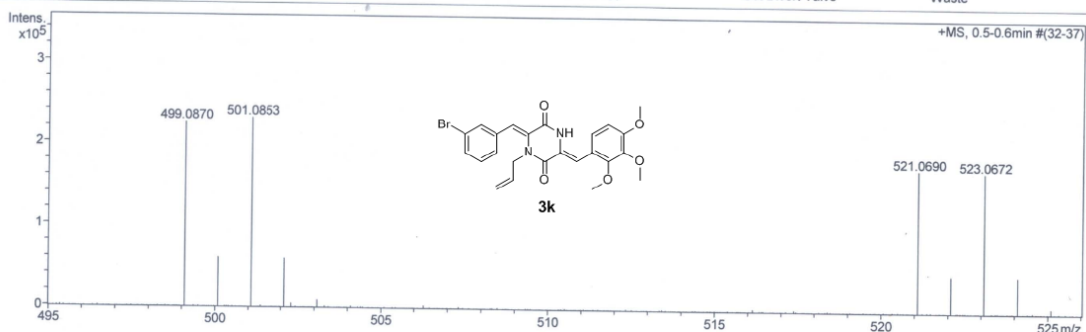
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Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
423.0709	1	C ₂₂ H ₂₀ BrN ₂ O ₂	100.00	423.0703	-0.6	-1.4	23.1	13.5	even	ok
445.0525	1	C ₂₂ H ₁₉ BrN ₂ NaO ₂	100.00	445.0522	-0.3	-0.7	8.1	13.5	even	ok

Acquisition Parameter

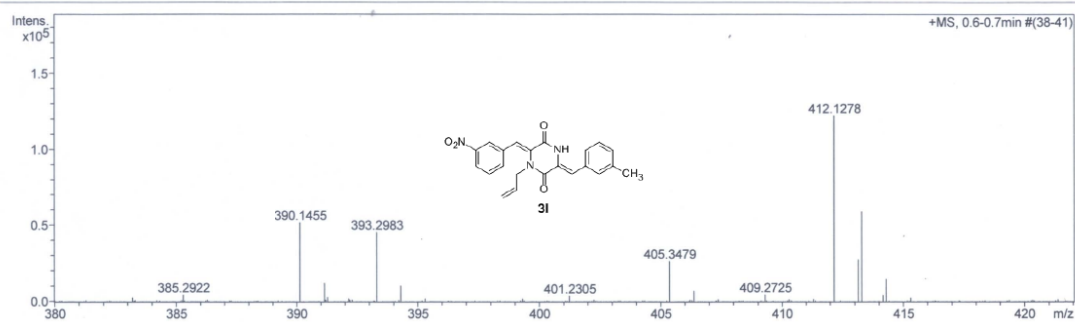
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Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
499.0870	1	C ₂₄ H ₂₄ BrN ₂ O ₅	100.00	499.0863	-0.7	-1.4	4.3	13.5	even	ok
521.0690	1	C ₂₄ H ₂₃ BrN ₂ NaO ₅	100.00	521.0683	-0.8	-1.5	10.4	13.5	even	ok

Acquisition Parameter

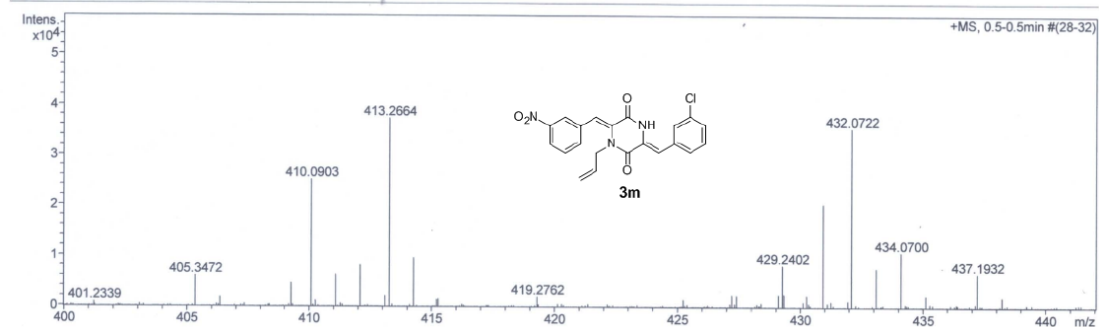
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Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
390.1455	1	C ₂₂ H ₂₀ N ₃ O ₄	100.00	390.1448	-0.6	-1.6	9.1	14.5	even	ok
412.1278	1	C ₂₂ H ₁₉ N ₃ NaO ₄	91.47	412.1268	-1.1	-2.6	13.8	14.5	even	ok

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule
410.0903	1	C ₂₁ H ₁₇ ClN ₃ O ₄	100.00	410.0902	-0.1	-0.2	13.6	14.5	even	ok	ok
432.0722	1	C ₂₁ H ₁₆ ClN ₃ NaO ₄	100.00	432.0722	-0.1	-0.1	25.7	14.5	even	ok	ok