Supplementary Information

Synthesis, cytotoxic activity and drug combination study of tertiary amine derivatives of 2',4'-dihydroxyl-6'-methoxyl-3',5'-dimethylchalcone

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HR-ESIMS, ^{1}H-NMR, and ^{13}C-NMR spectra of synthesized compounds (**1**, and **2a**–**2f**) are provided in the following pages.

HR-ESIMS of 1

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MS\data\201511\wangchen_ON3-18-2_pos_6_01_850.d	Acquisition Date	11/24/2015 10:23:25 PM
Method	LC_Direct Infusion_pos_100-1000mz.m	Operator	SCSIO
Sample Name	wangchen_ON3-18-2_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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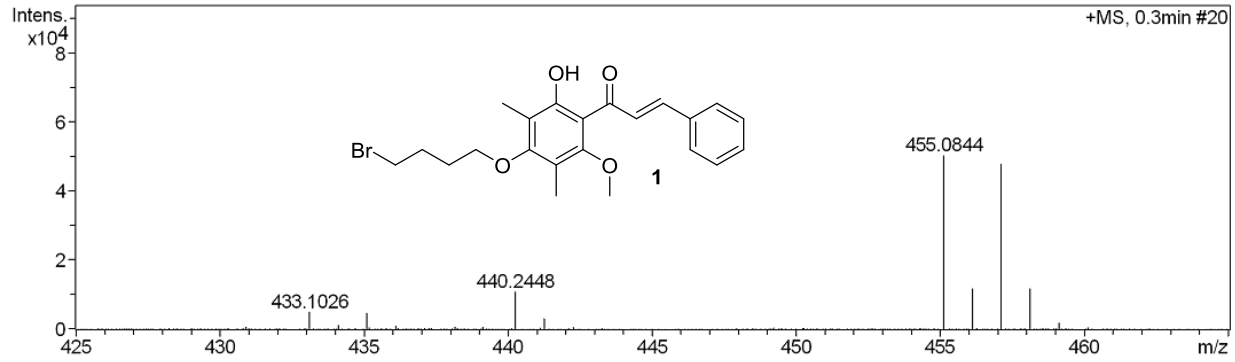
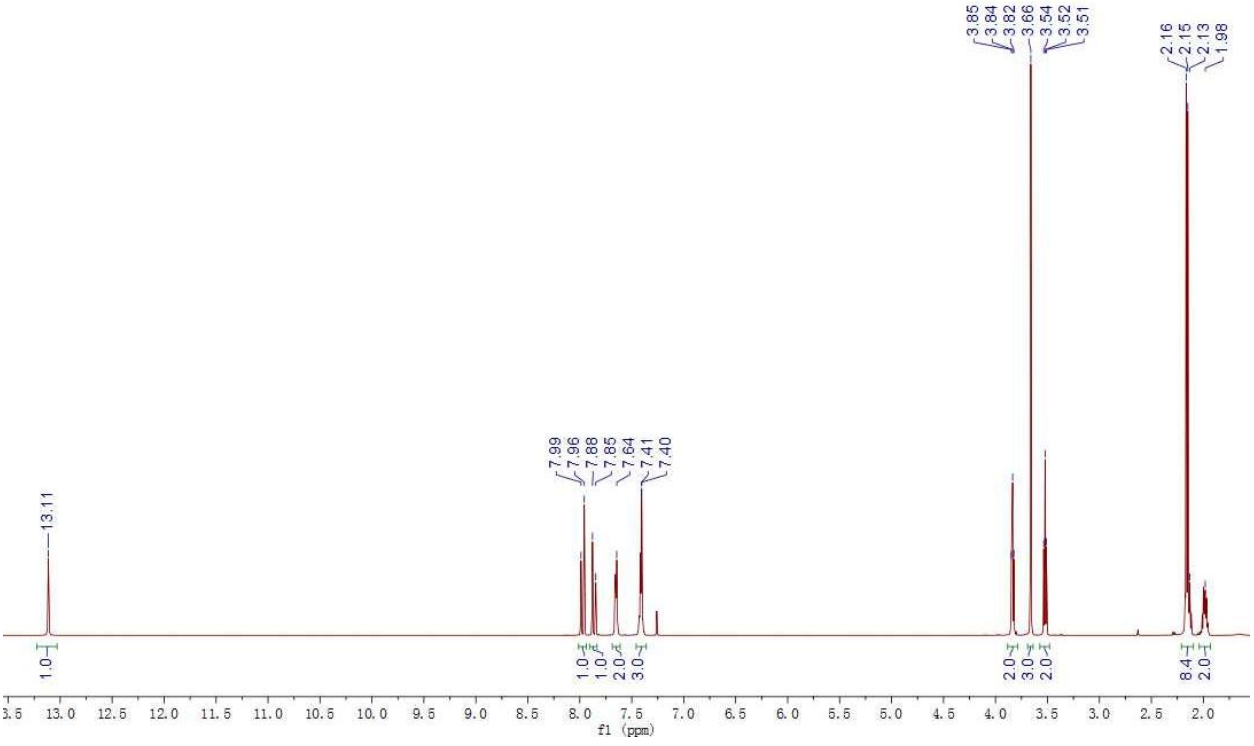
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
433.1026	1	C 22 H 26 Br O 4	100.00	433.1009	-4.0	-1.7	40.2	9.5	even	ok
455.0844	1	C 22 H 25 Br Na O 4	68.85	455.0828	-3.5	-1.6	22.4	9.5	even	ok
887.1807	1	C 44 H 50 Br 2 Na O 8	8.89	887.1765	-4.8	-4.2	15.1	18.5	even	ok

^{1}H-NMR of 1 in $CDCl_3$



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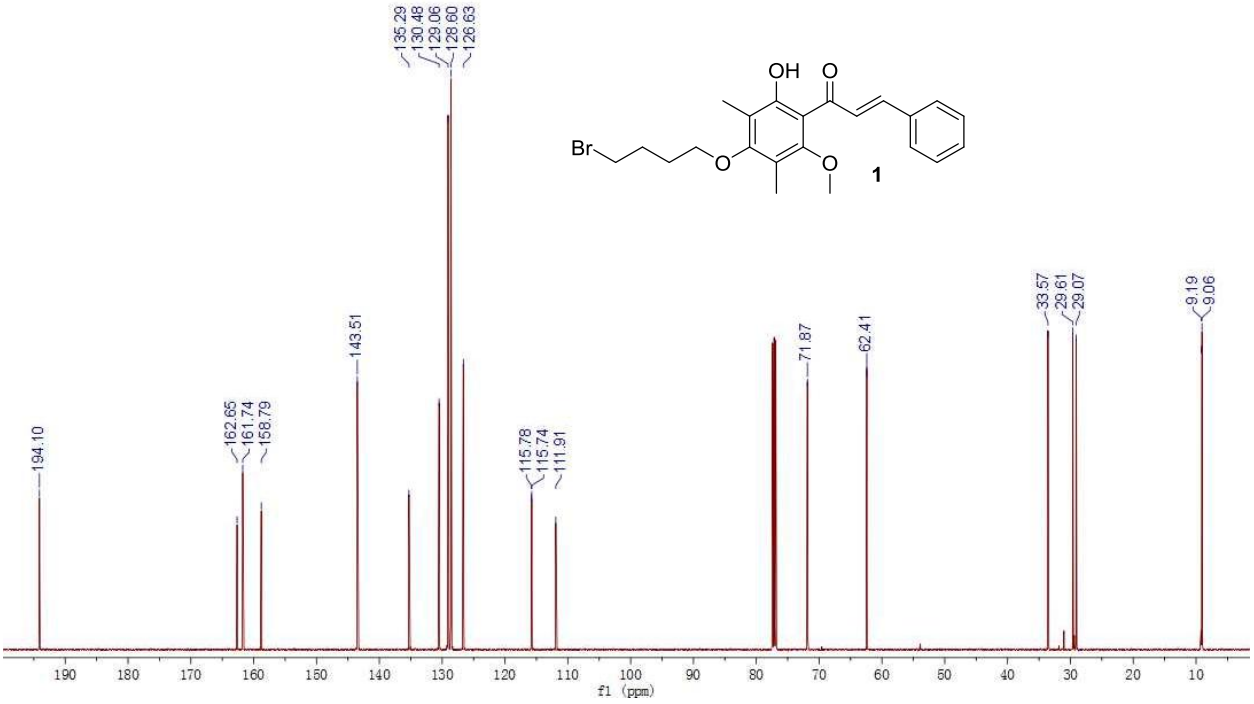

HR-ESIMS of 2a

Mass Spectrum SmartFormula Report

Analysis Info

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Method	LC_Direct Infusion_pos_100-1000mz.m	Operator	SCSIO
Sample Name	wangchen_ON3-22_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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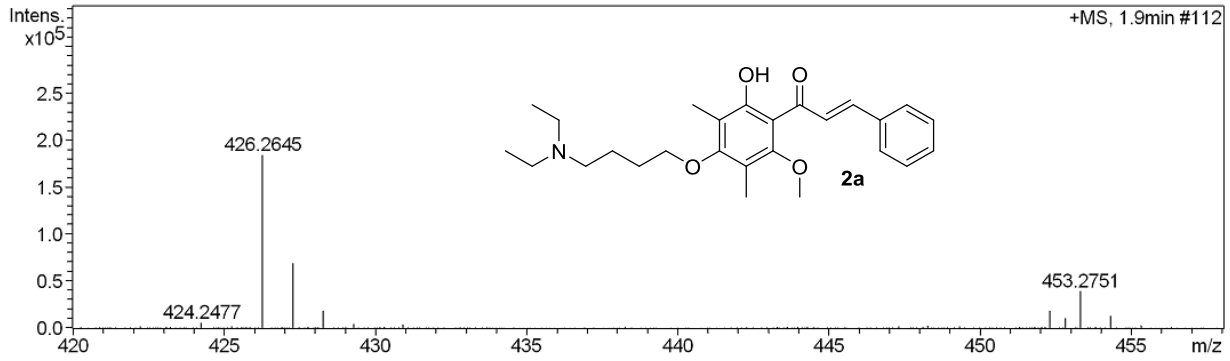
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



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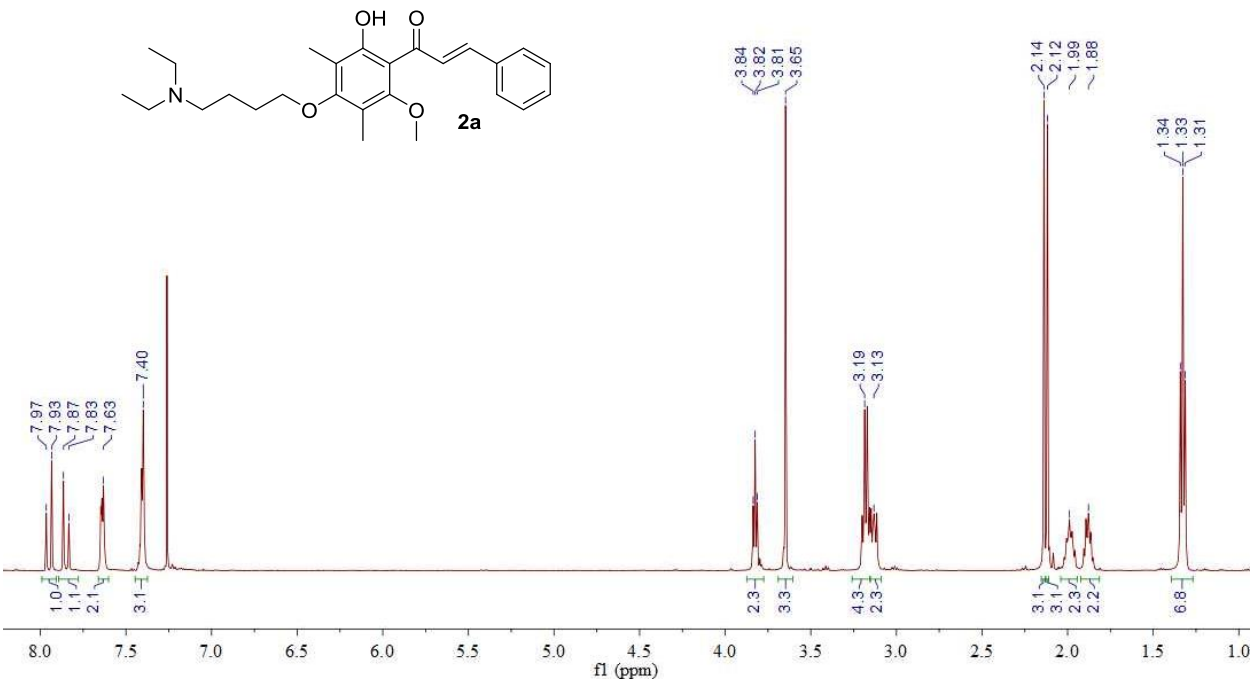
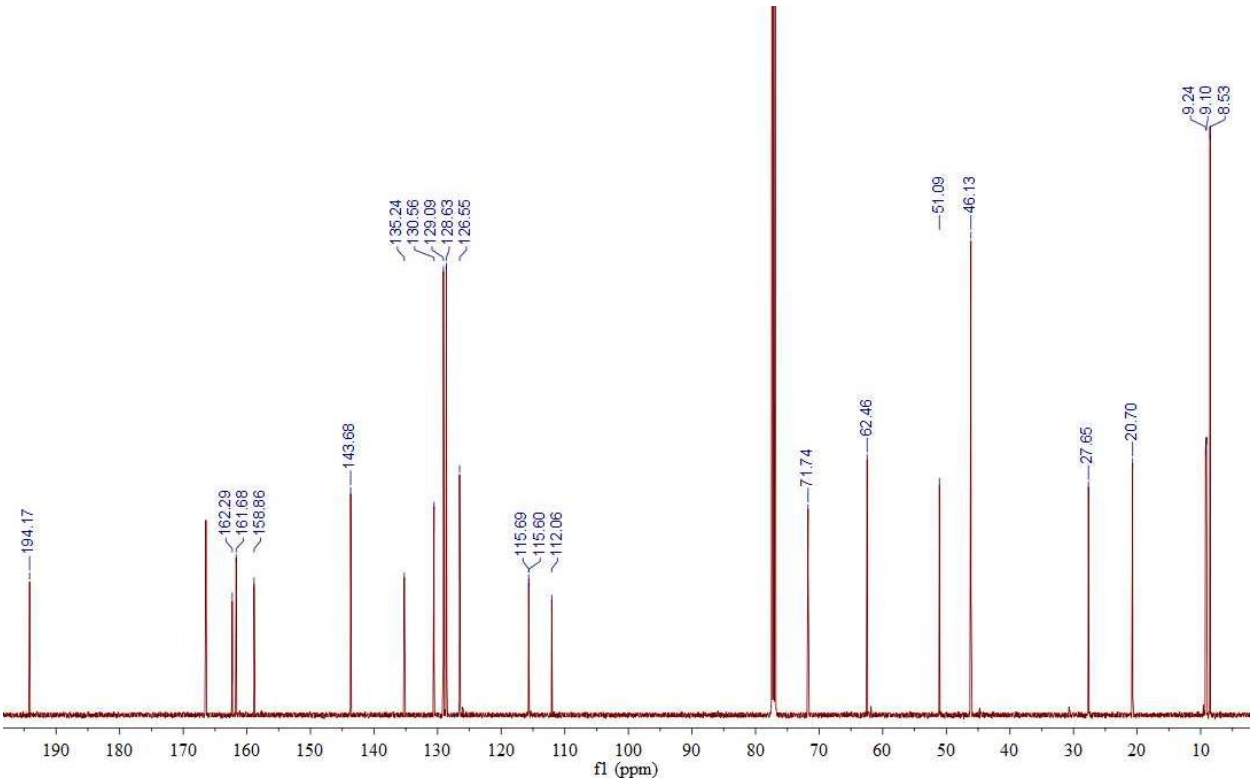
426.2645	1	C 26 H 36 N O 4	64.04	426.2639	-1.5	-0.6	55.0	9.5	even	ok
448.2451	1	C 26 H 35 N Na O 4	1.56	448.2458	1.6	0.7	169.1	9.5	even	ok

^{1}H-NMR of 2a in $CDCl_3$



^{13}C-NMR of 2a in $CDCl_3$



HR-ESIMS of 2b

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	wangchen_ON3-23_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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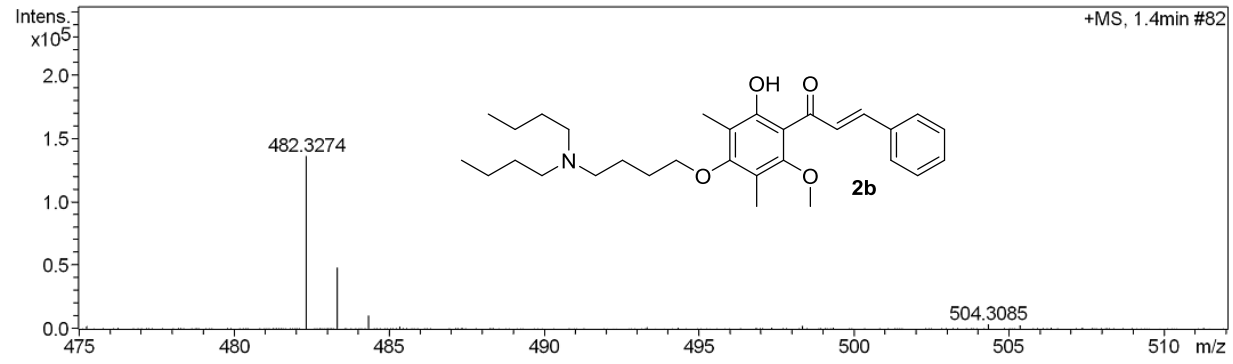
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



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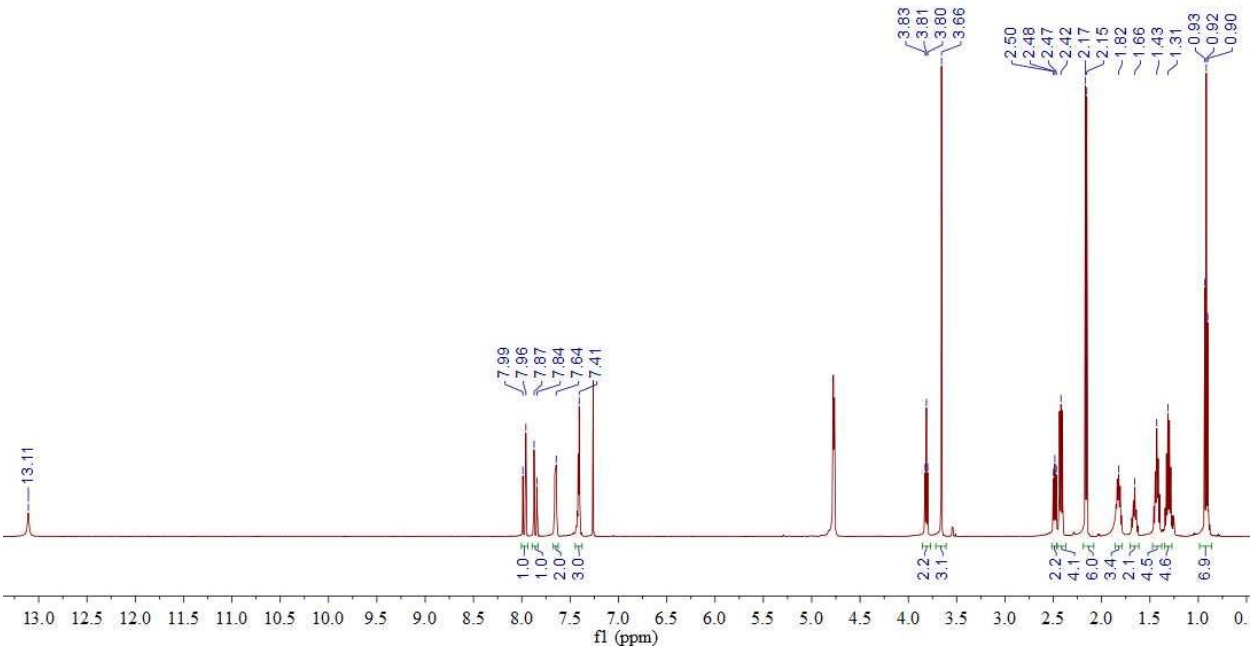
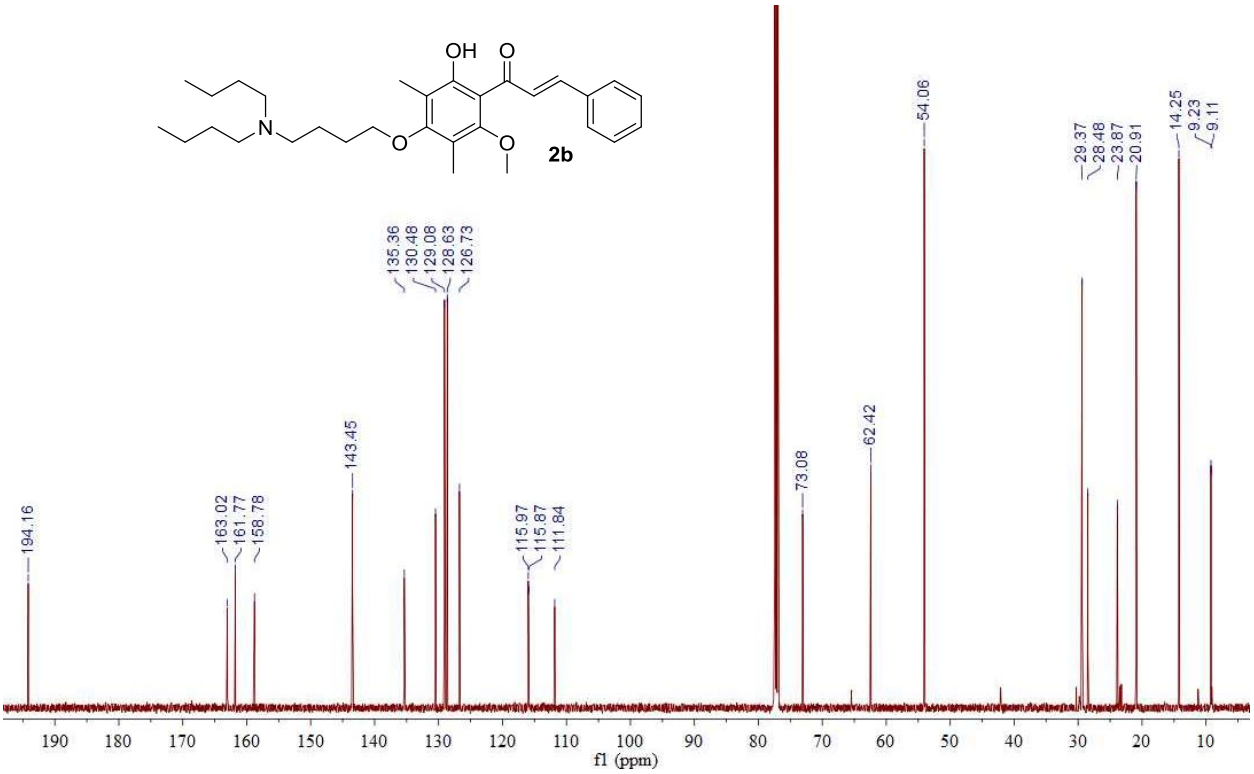
482.3274	1	C 30 H 44 N O 4	76.24	482.3265	-1.8	-0.9	10.6	9.5	even	ok
504.3085	1	C 30 H 43 N Na O 4	78.01	504.3084	-0.2	-0.1	188.4	9.5	even	ok

^{1}H-NMR of 2b in $CDCl_3$



^{13}C-NMR of 2b in $CDCl_3$



HR-ESIMS of 2c

Mass Spectrum SmartFormula Report

Analysis Info

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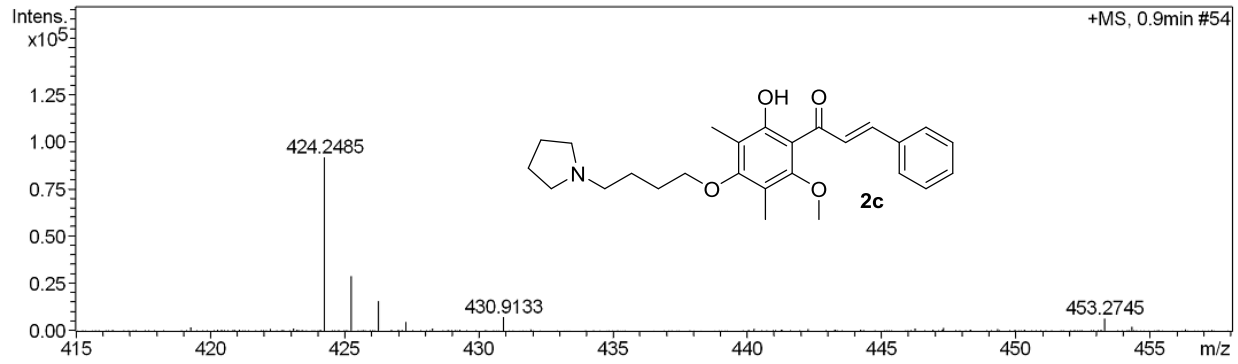
Sample Name	wangchen_ON3-19_pos	Instrument / Ser#	maXis 29
Comment			

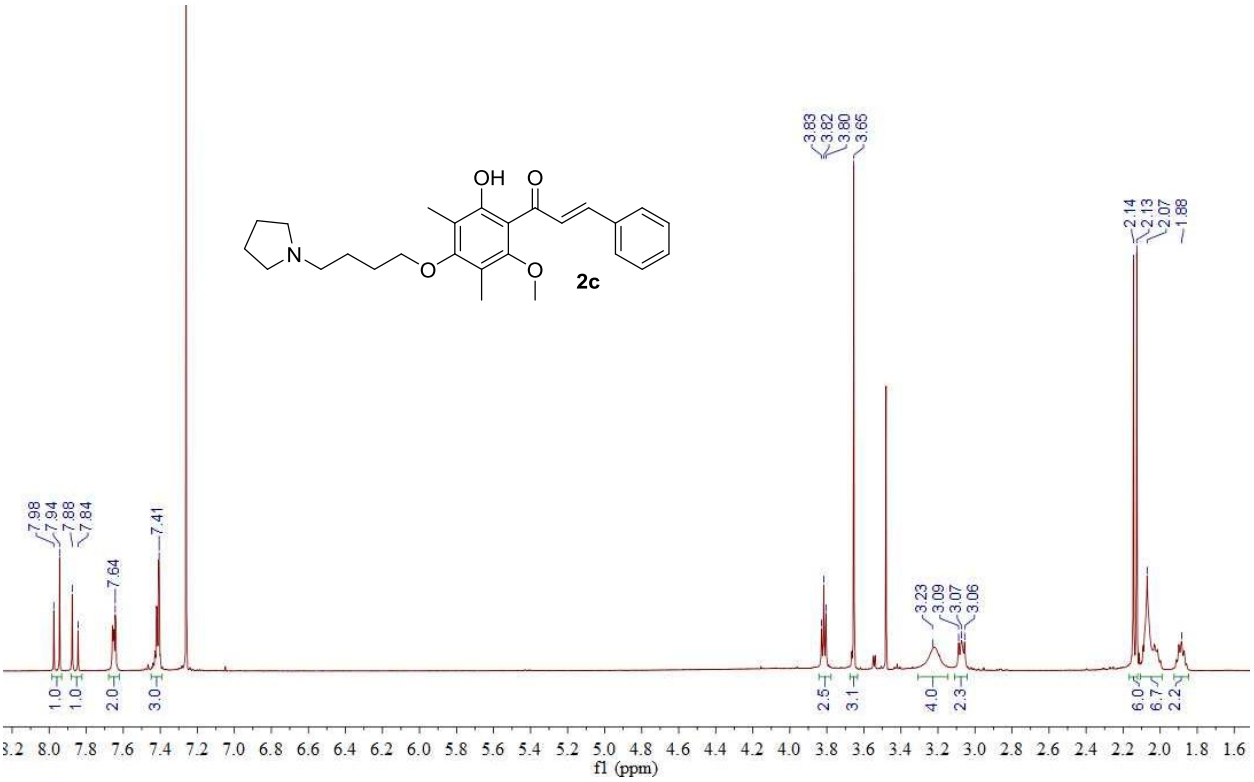
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste

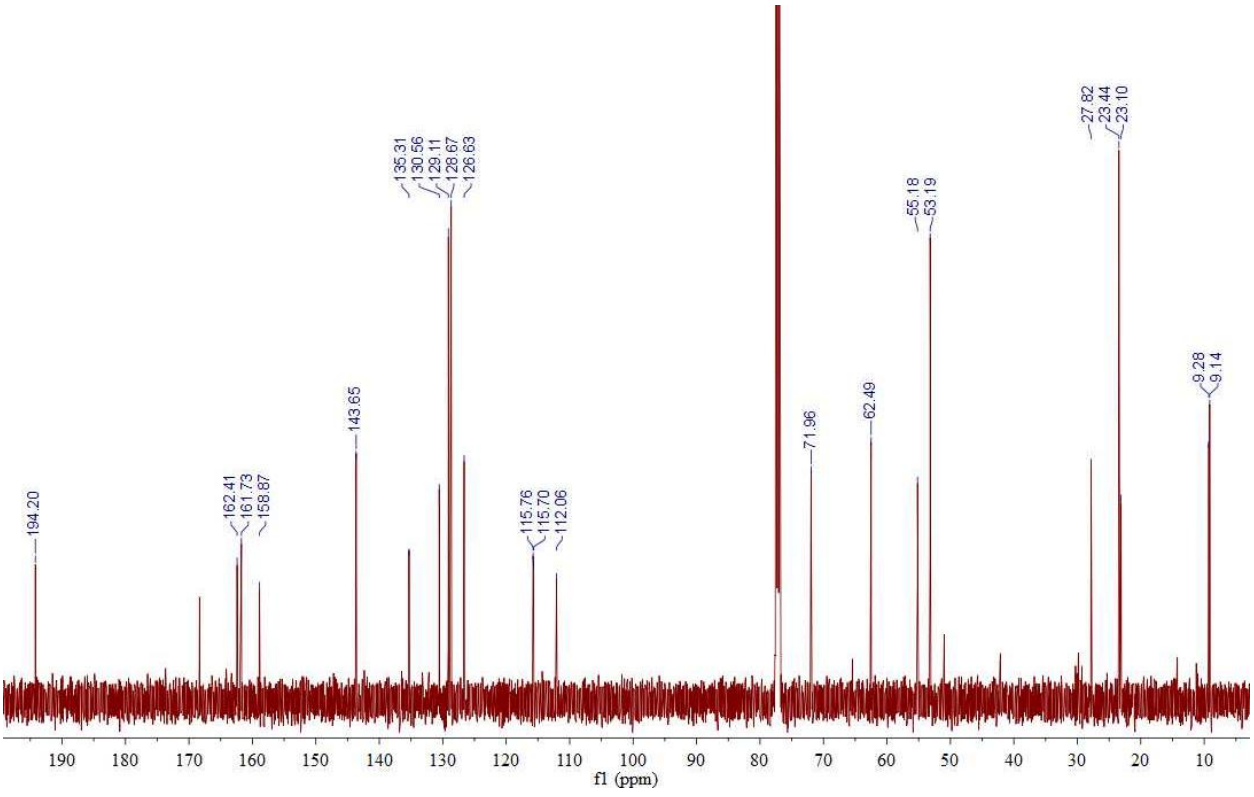


Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
424.2485	1	C 26 H 34 N O 4	100.00	424.2482	-0.7	-0.3	69.7	10.5	even	ok
446.2296	1	C 26 H 33 N Na O 4	95.72	446.2302	1.4	0.6	35.4	10.5	even	ok

^{1}H-NMR of 2c in $CDCl_3$



^{13}C-NMR of 2c in $CDCl_3$



HR-ESIMS of 2d

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	wangchen_ON3-20-1_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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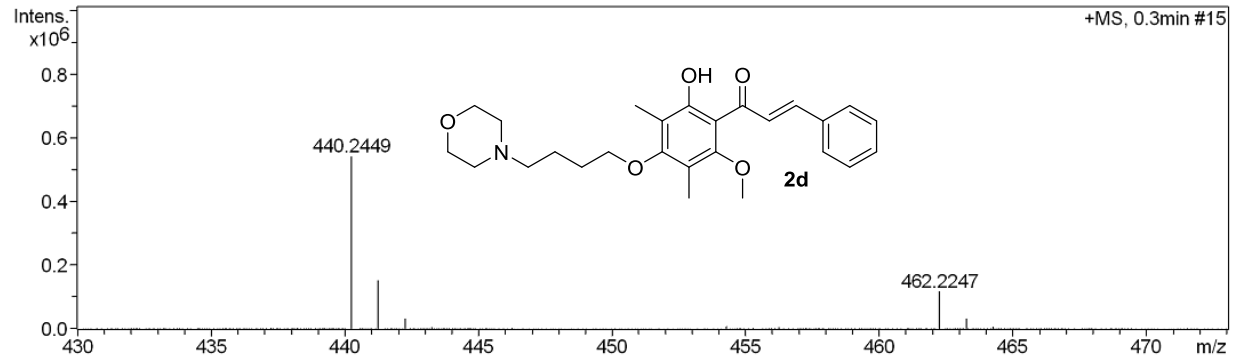
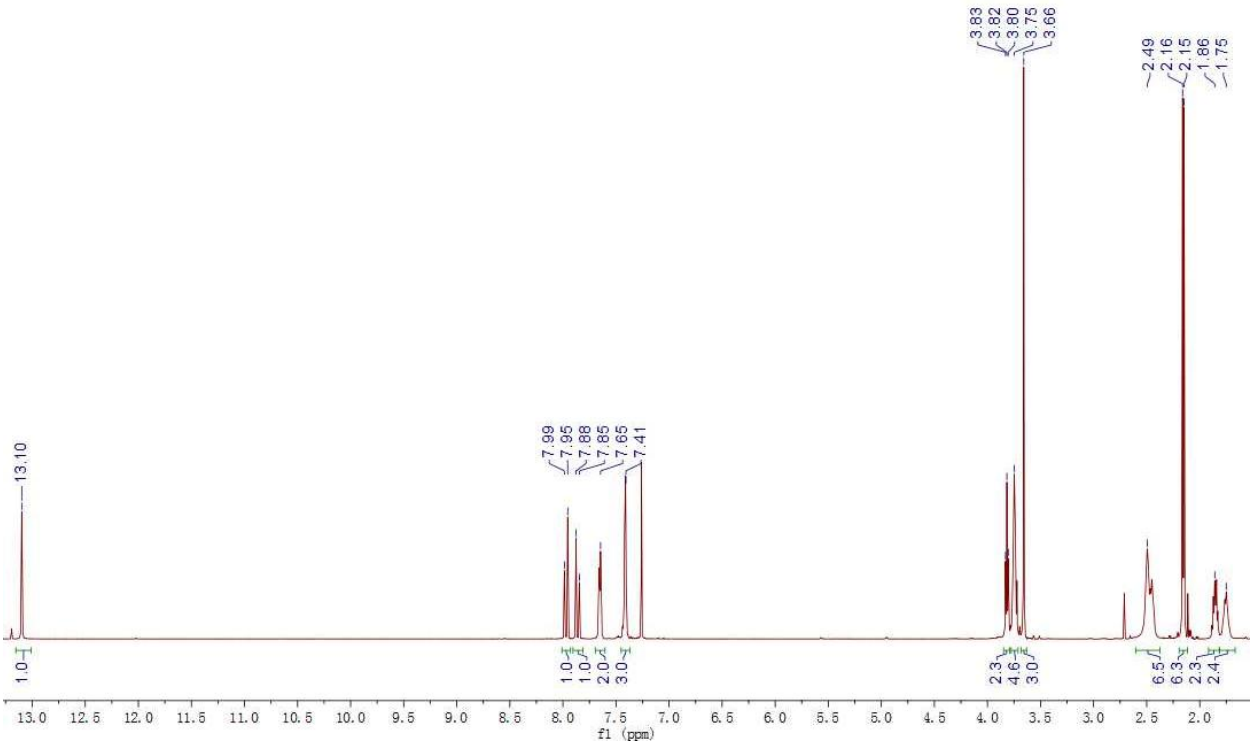
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste

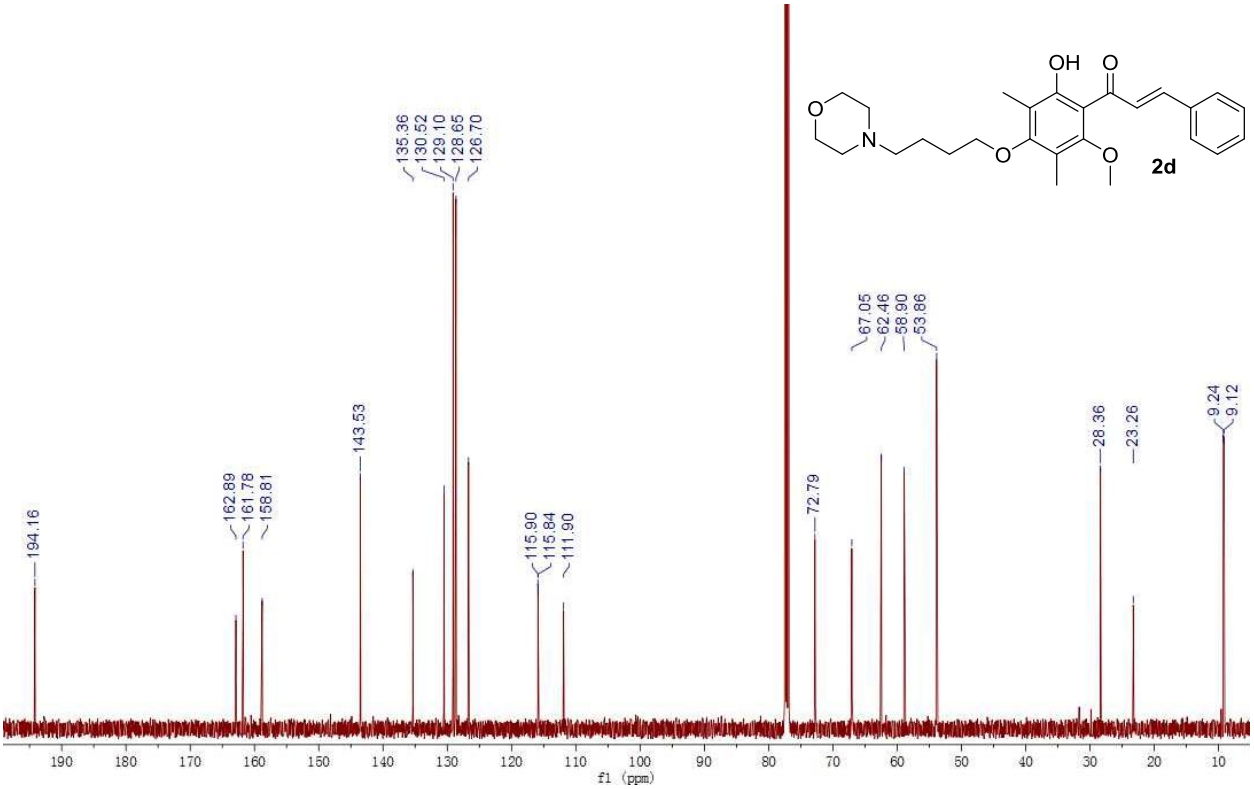


Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
440.2449	1	C 26 H 34 N O 5	55.45	440.2431	-3.9	-1.7	7.1	10.5	even	ok
462.2247	1	C 26 H 33 N Na O 5	84.25	462.2251	0.9	0.4	15.6	10.5	even	ok

^{1}H-NMR of 2d in $CDCl_3$



^{13}C-NMR of 2d in $CDCl_3$



HR-ESIMS of 2e

Mass Spectrum SmartFormula Report

Analysis Info

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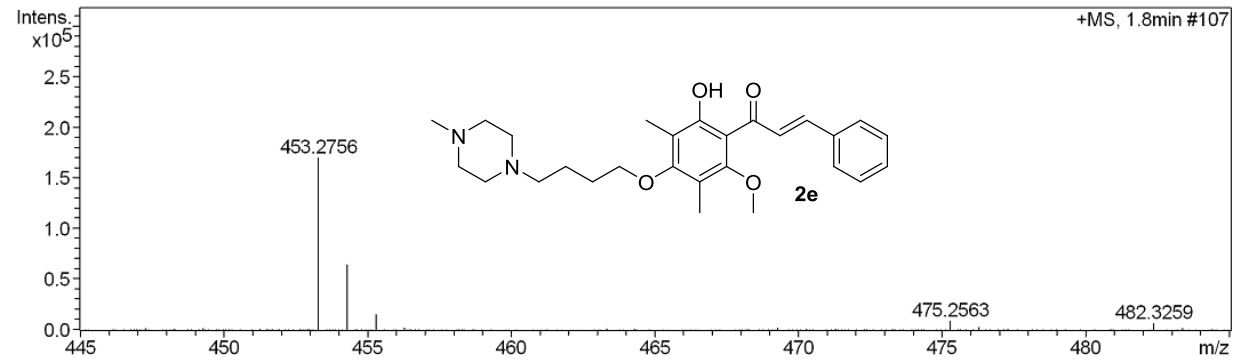
Method	LC_Direct Infusion_pos_100-1000mz.m	Operator	SCSIO
Sample Name	wangchen_ON3-21_pos	Instrument / Ser#	maXis 29
Comment			

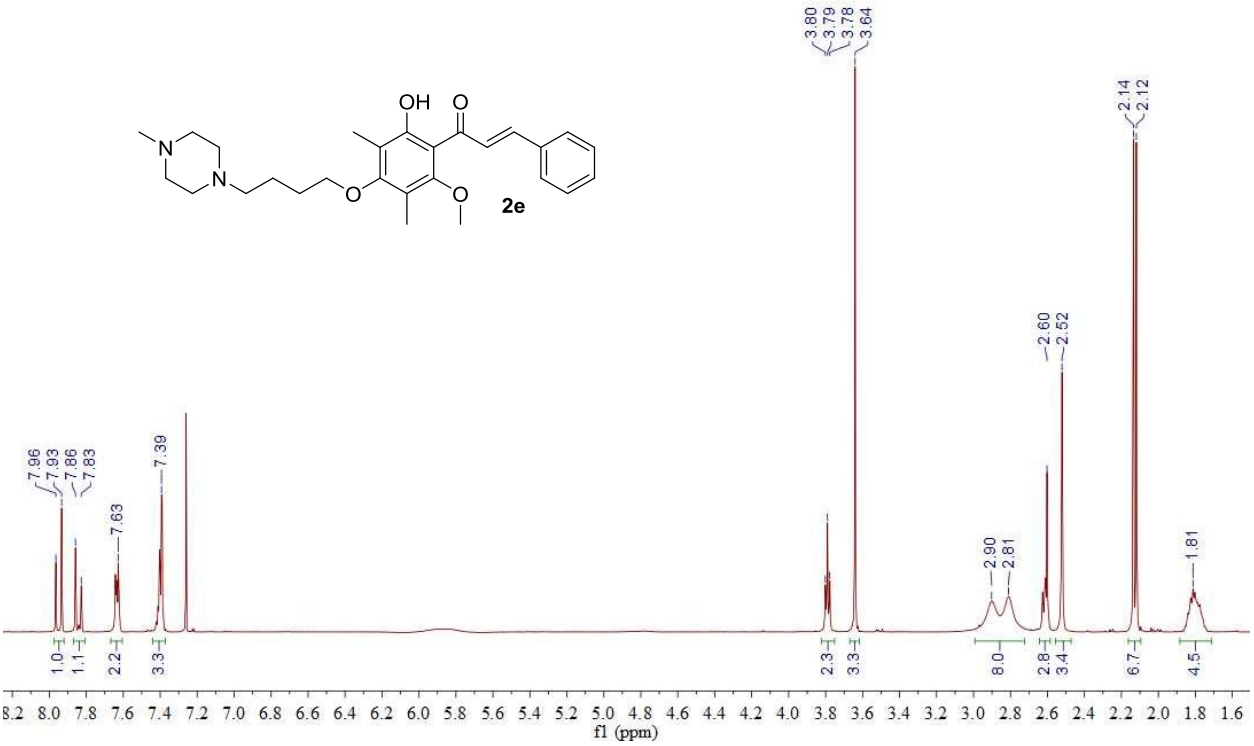
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste

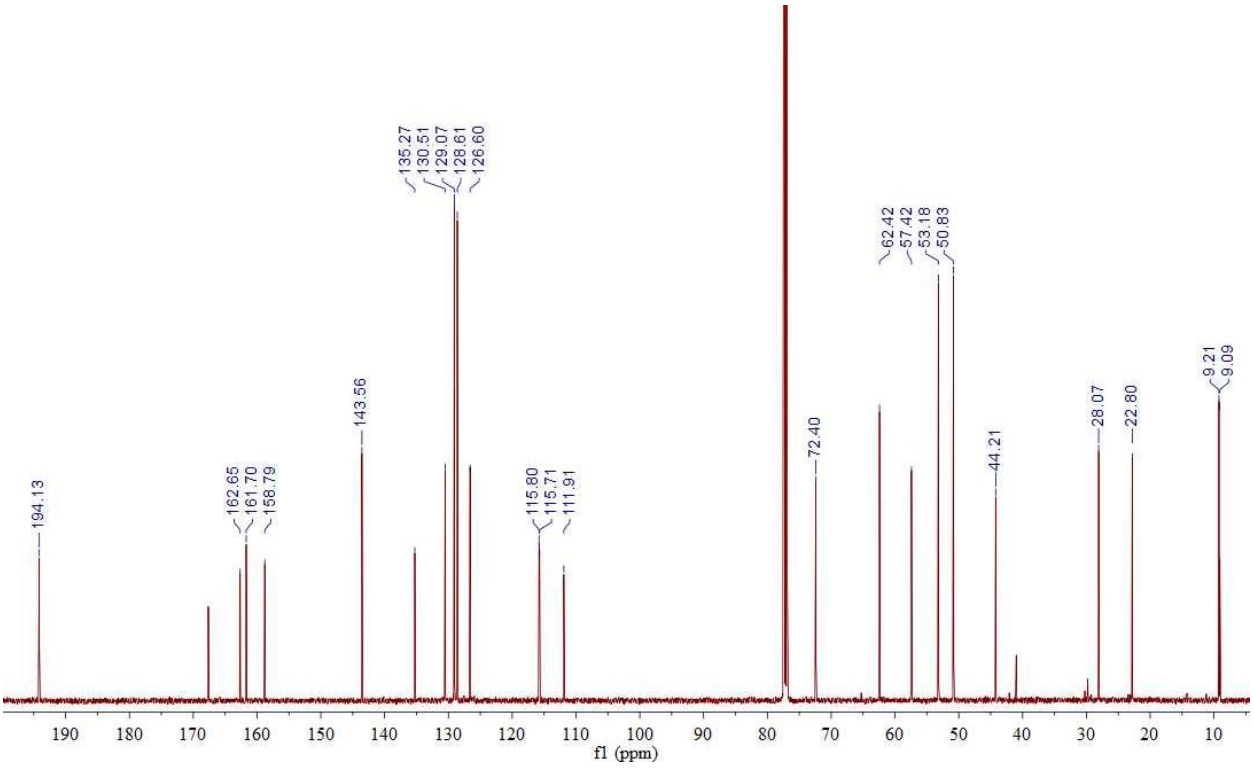


Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e¯ Conf	N-Rule
453.2756	1	C 27 H 37 N 2 O 4	67.67	453.2748	-1.7	-0.8	39.6	10.5	even	ok
475.2563	1	C 27 H 36 N 2 Na O 4	92.37	475.2567	0.8	0.4	13.9	10.5	even	ok

^{1}H-NMR of 2e in $CDCl_3$



^{13}C-NMR of 2e in $CDCl_3$



HR-ESIMS of 2f

Mass Spectrum SmartFormula Report

Analysis Info

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Sample Name	wangchen_ON3-25_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

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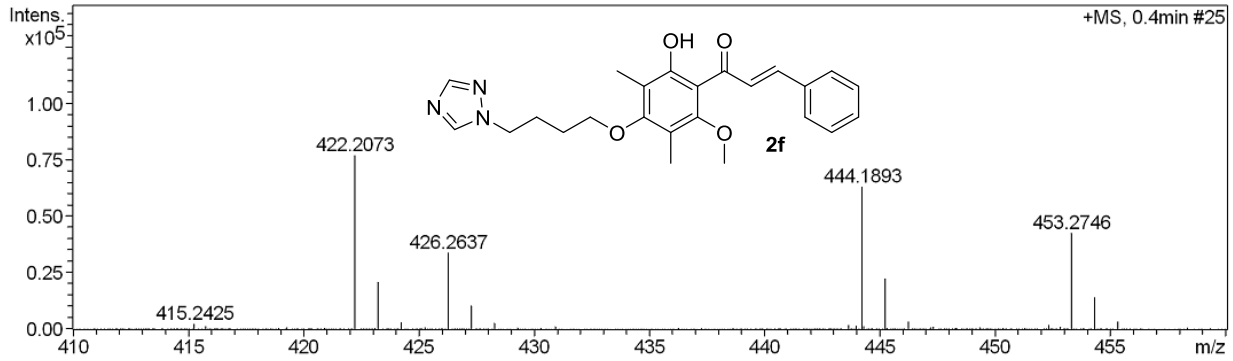
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste



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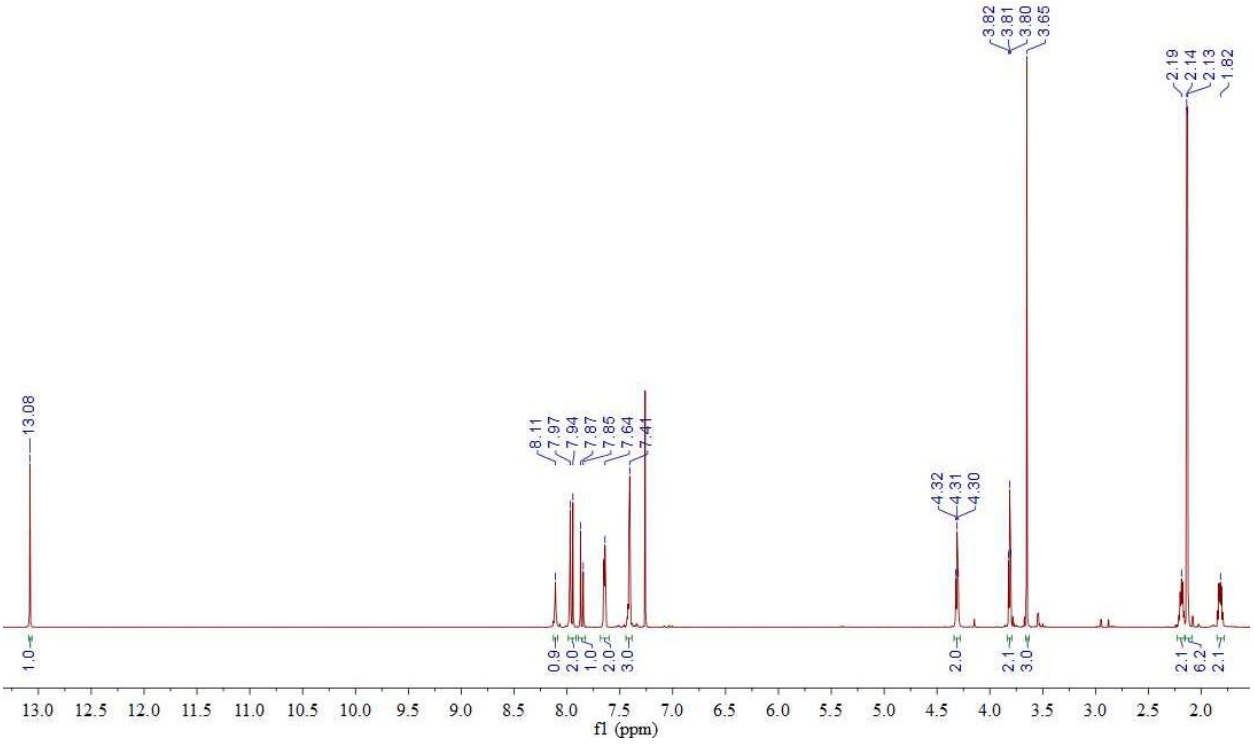
422.2073	1	C 24 H 28 N 3 O 4	100.00	422.2074	0.3	0.1	3.1	12.5	even	ok
444.1893	1	C 24 H 27 N 3 Na O 4	100.00	444.1894	0.2	0.1	47.6	12.5	even	ok

^{1}H-NMR of 2f in $CDCl_3$



^{13}C-NMR of 2f in $CDCl_3$