

Supporting Information for

Synthesis and Evaluation of New Sterol Derivatives as Potential Antitumor Agents

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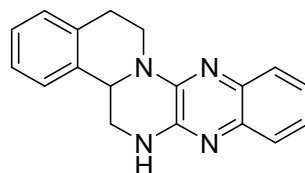
b. Experimental Teaching Center, Chongqing Medical University, Chongqing, People's Republic of China, 401331; cqjy0708@126.com

c. Department of Pharmacy, The First Affiliated Hospital of Chongqing Medical University, Chongqing, People's Republic of China, 40016 ; 36360496@qq.com

d. Correspondence: 86487165@qq.com; Tel.: +86-023-68485983. Prof. Dr.Yu Yu and Dr.Yuan Zhang are both corresponding authors of this paper.

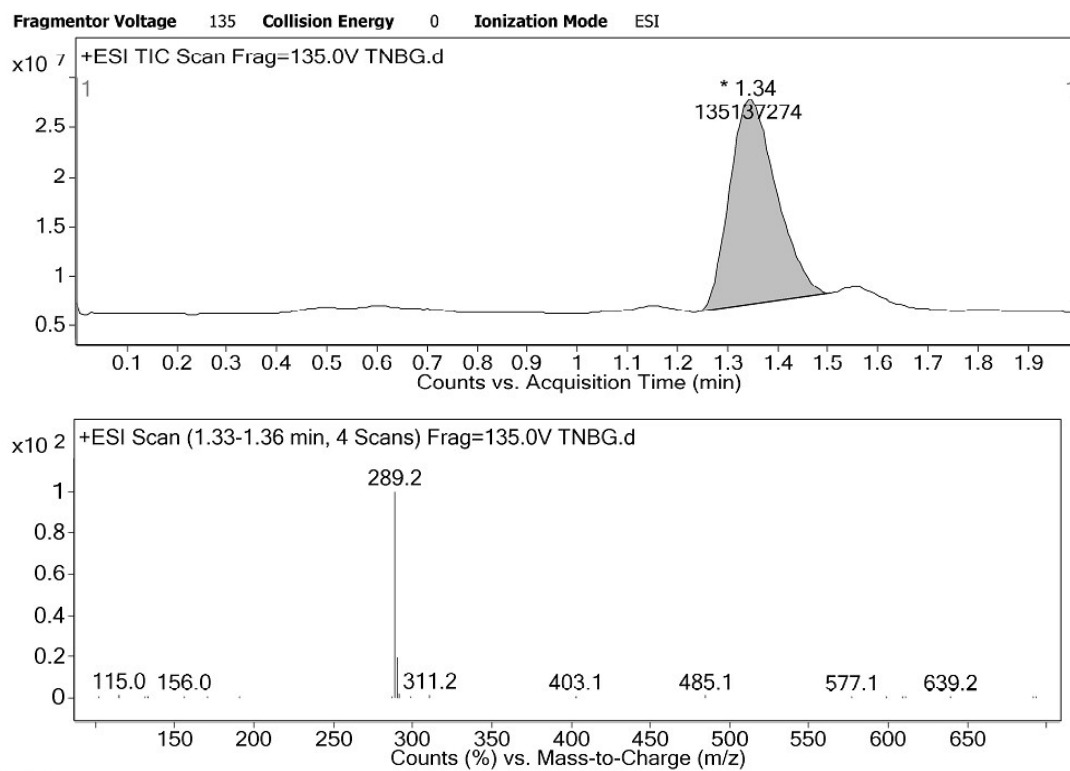
Some representative spectra:

TNBG

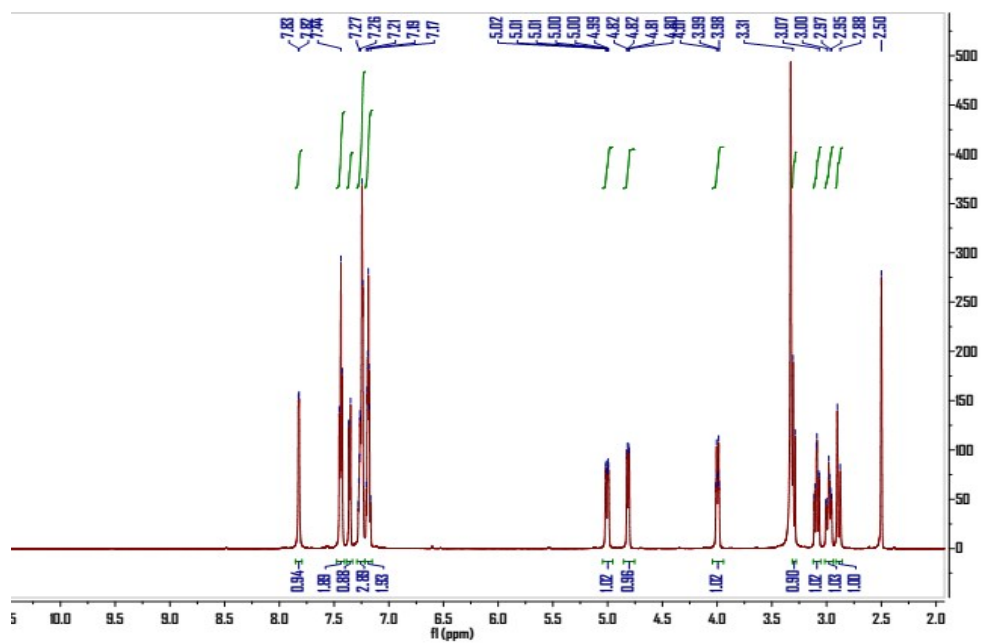


TNBG MW:288.3464

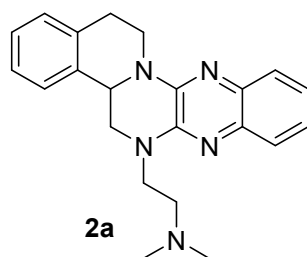
LC-MS Spectrum



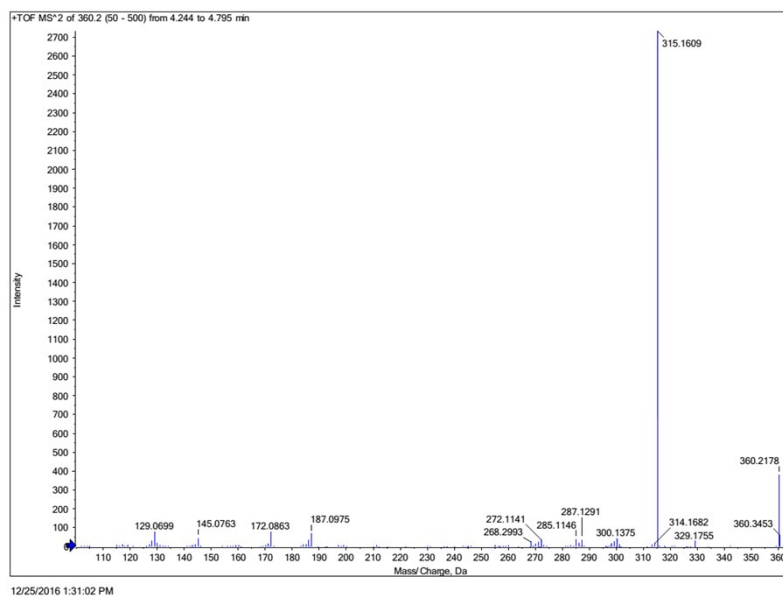
¹H NMR Spectrum



2a:



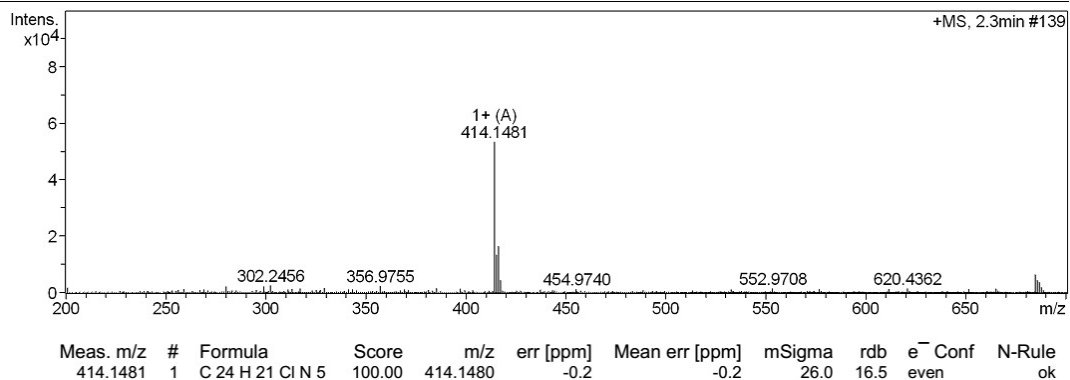
HRMS Spectrum



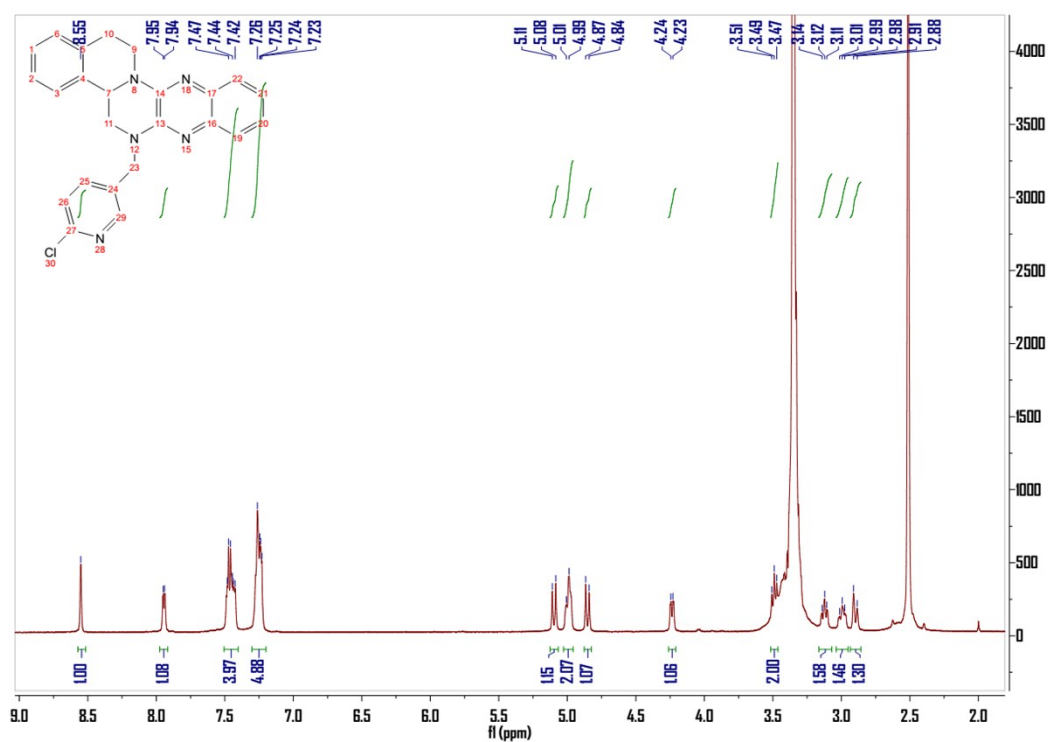
¹H NMR Spectrum

Acquisition Parameter

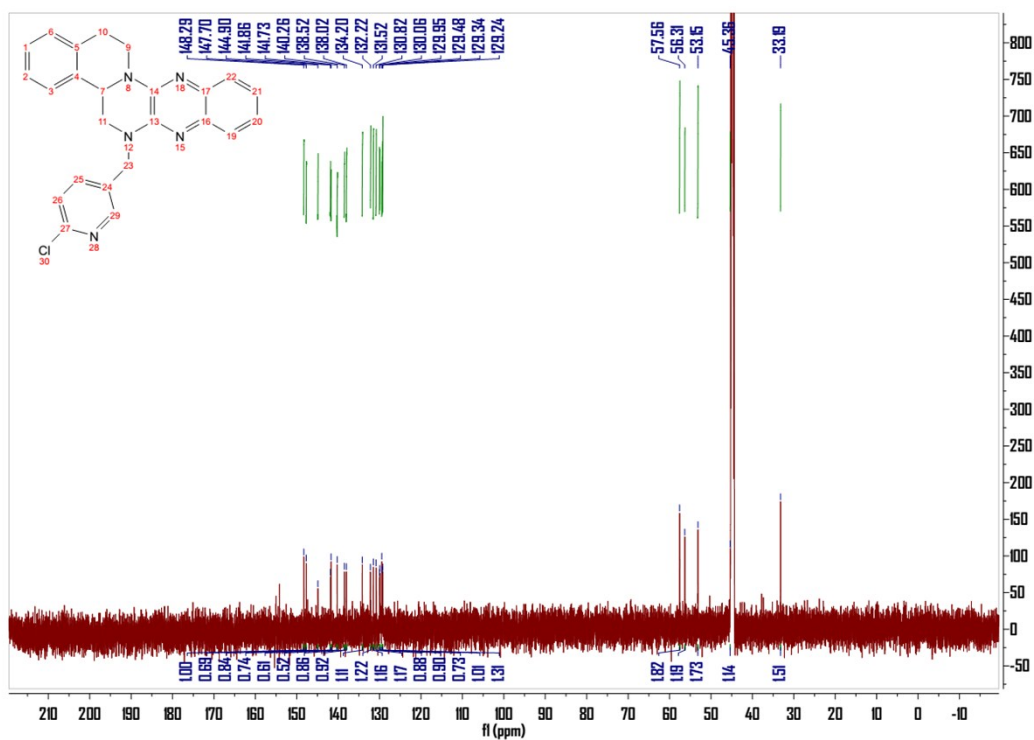
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



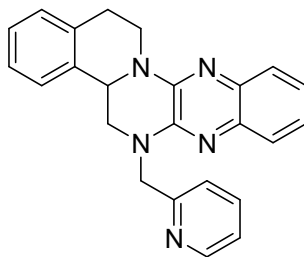
¹H NMR Spectrum



¹³C NMR Spectrum



2C:



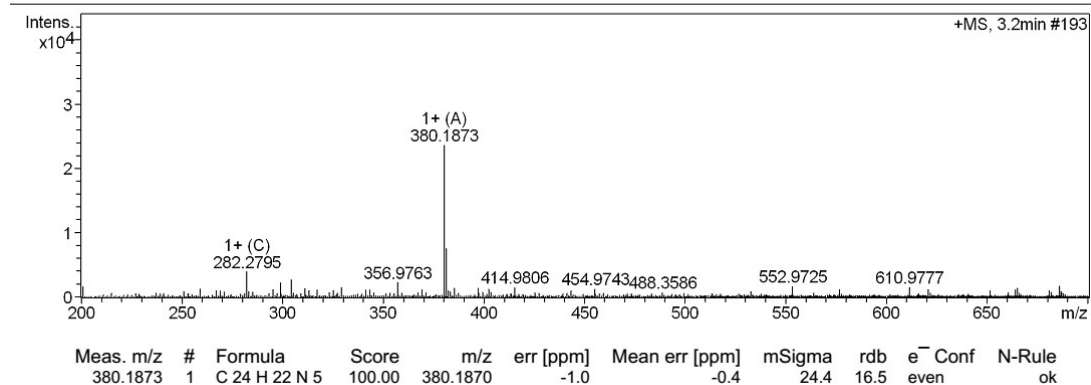
HRMS Spectrum

Acquisition Parameter

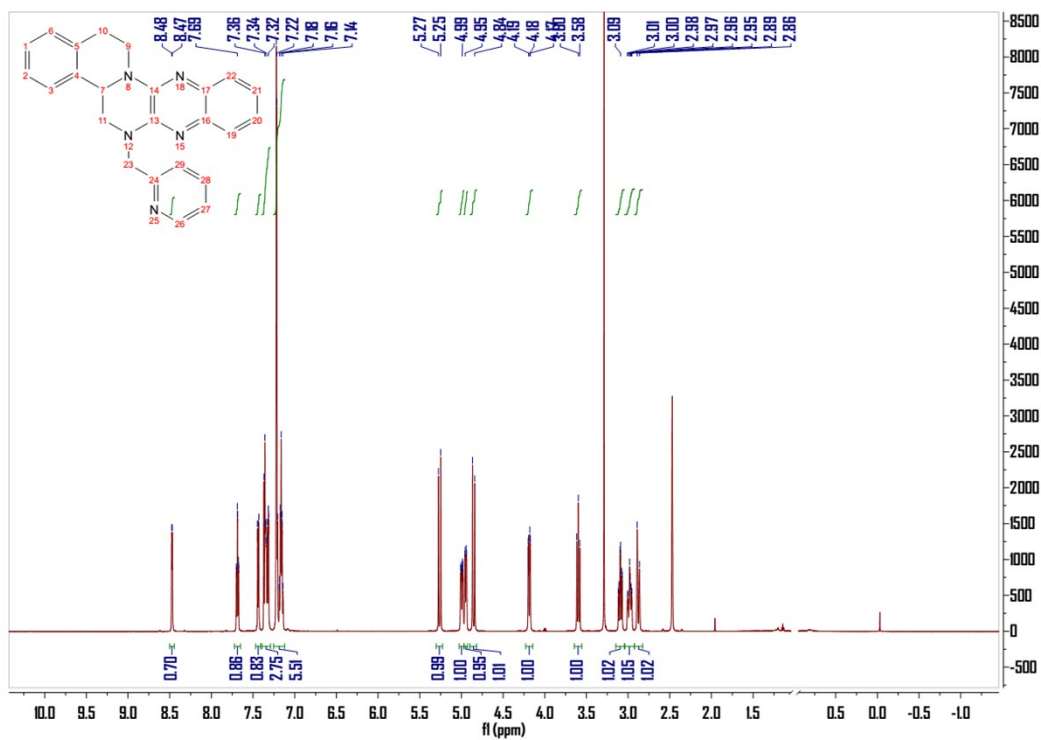
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Ion Polarity Positive
Set Capillary 4000 V
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Set Collision Cell RF 600.0 Vpp

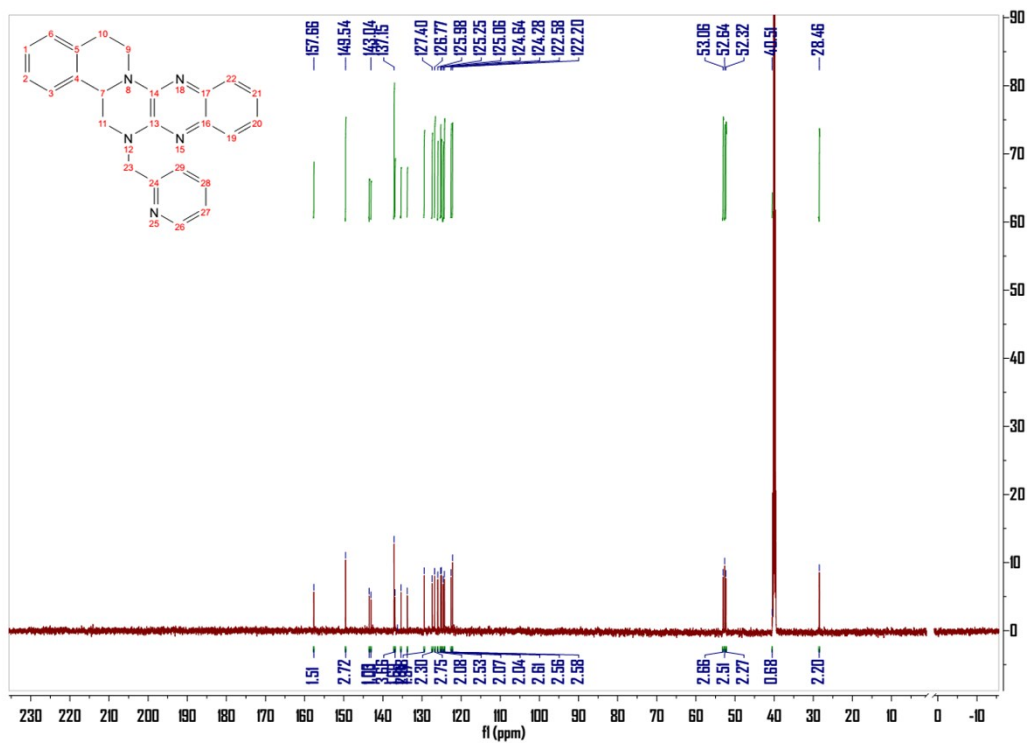
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Set Dry Heater 220 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste



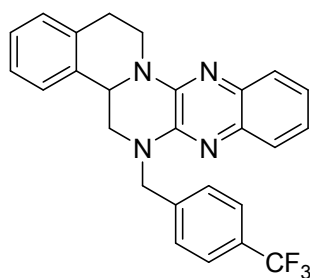
¹H NMR Spectrum



¹³C NMR Spectrum



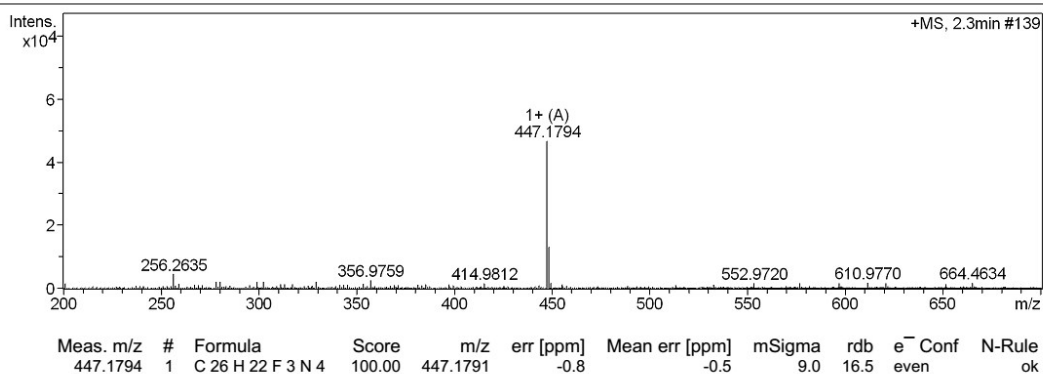
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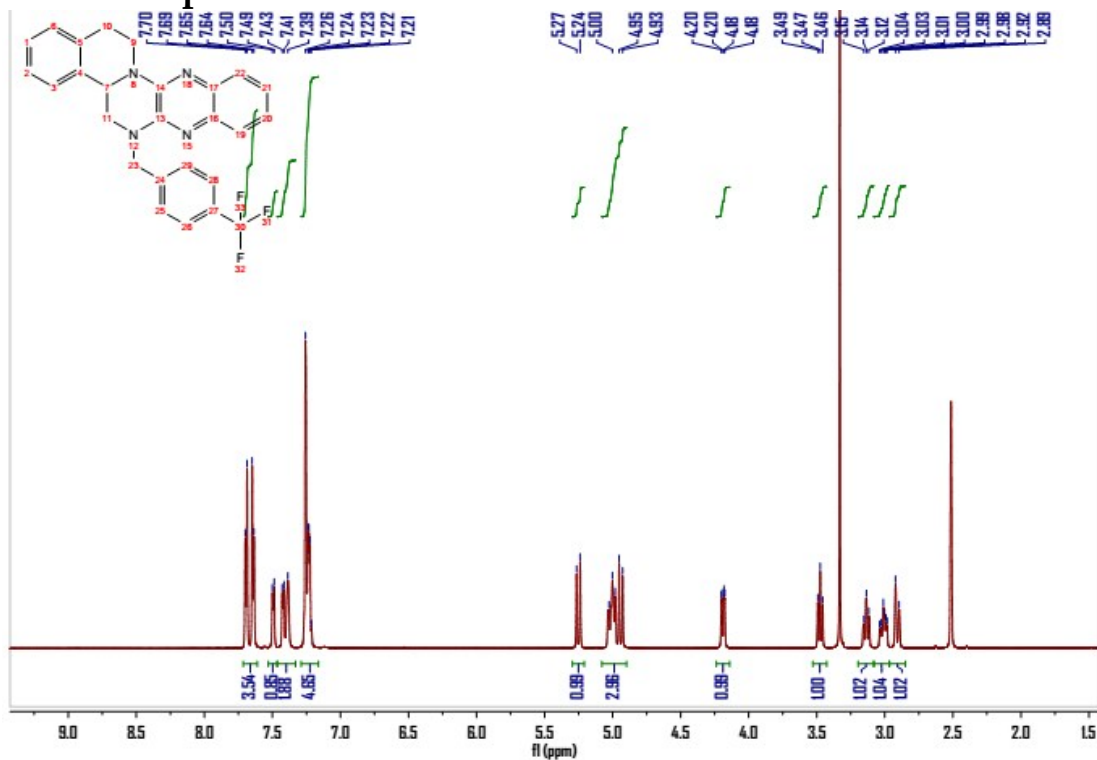
HRMS Spectrum

Acquisition Parameter

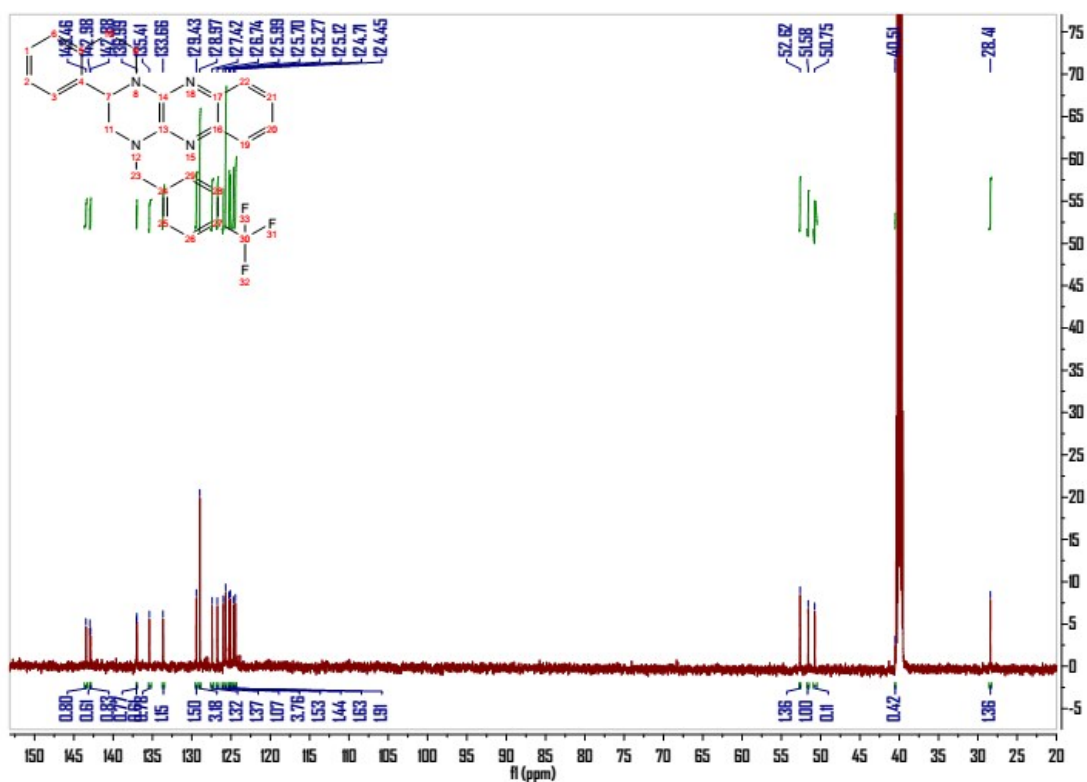
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Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



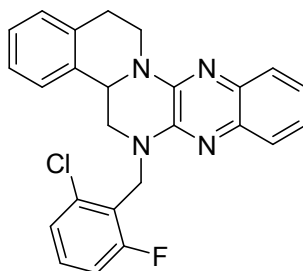
¹H NMR Spectrum



¹³C NMR Spectrum



2e:



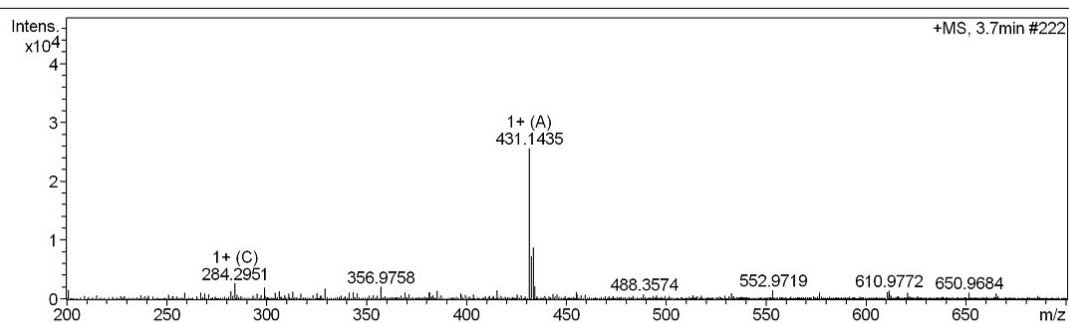
HRMS Spectrum

Acquisition Parameter

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Focus Not active
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Scan End 1500 m/z

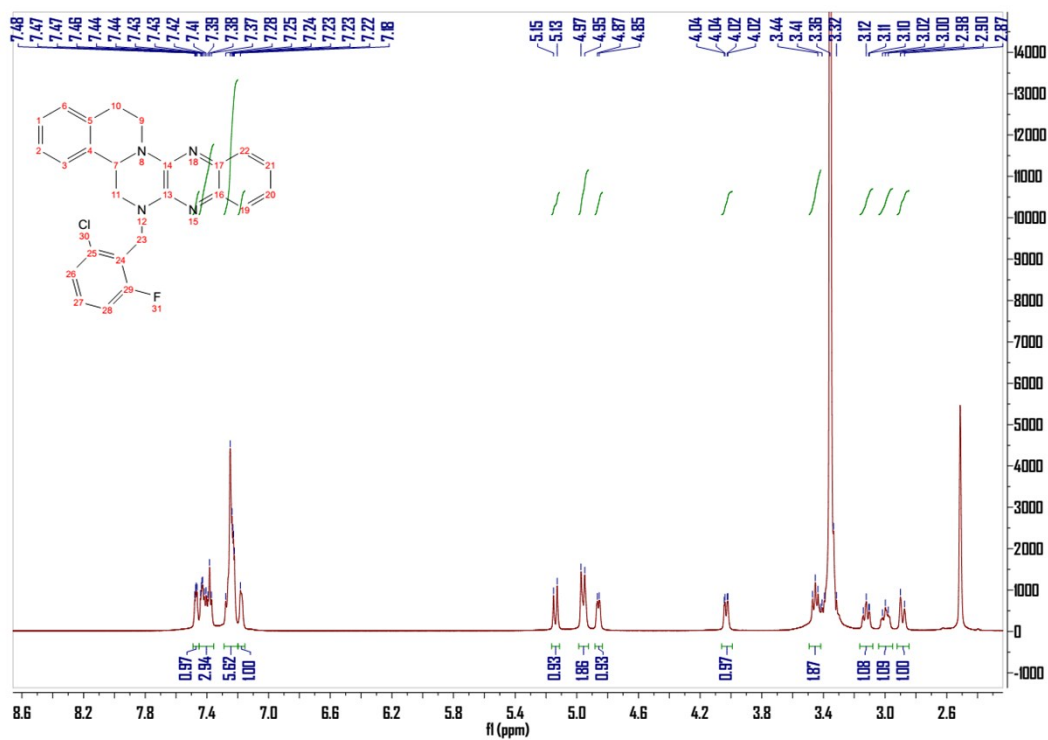
Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Collision Cell RF 600.0 Vpp

Set Nebulizer 1.0 Bar
Set Dry Heater 220 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste

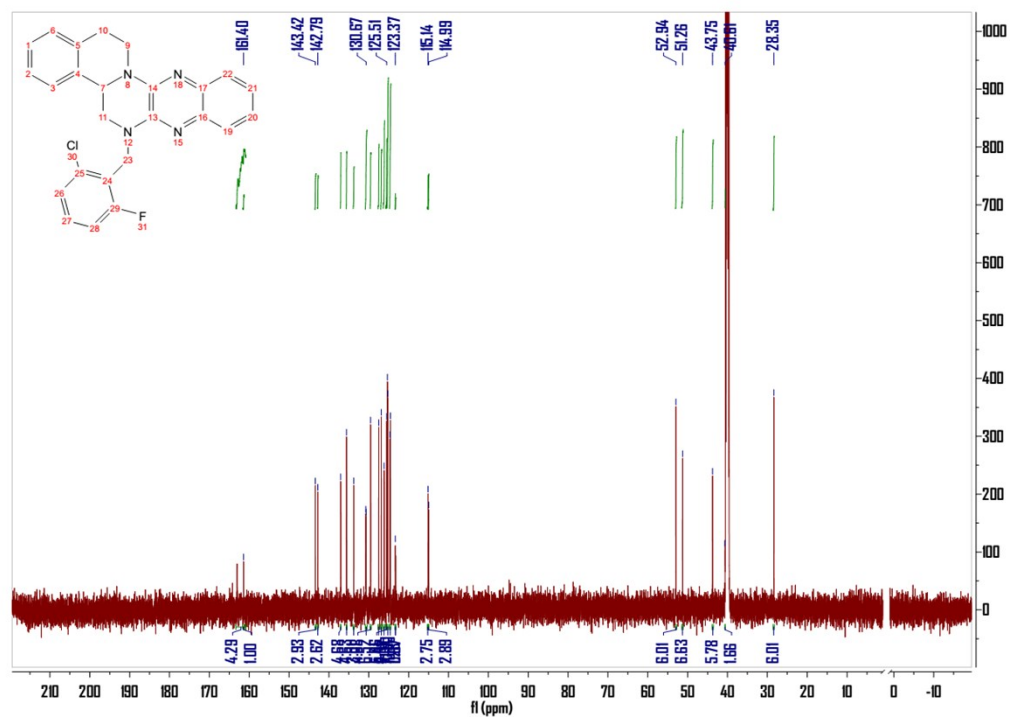


Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e ⁻ Conf	N-Ru le
431.1435	1	C ₂₅ H ₂₁ ClF ₁ N ₄	100.00	431.1433	-0.4	-0.8	8.6	16.5	even	ok

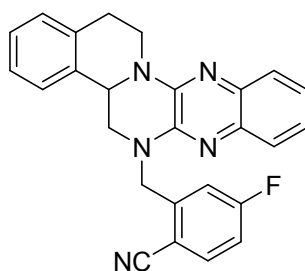
¹H NMR Spectrum



¹³C NMR Spectrum



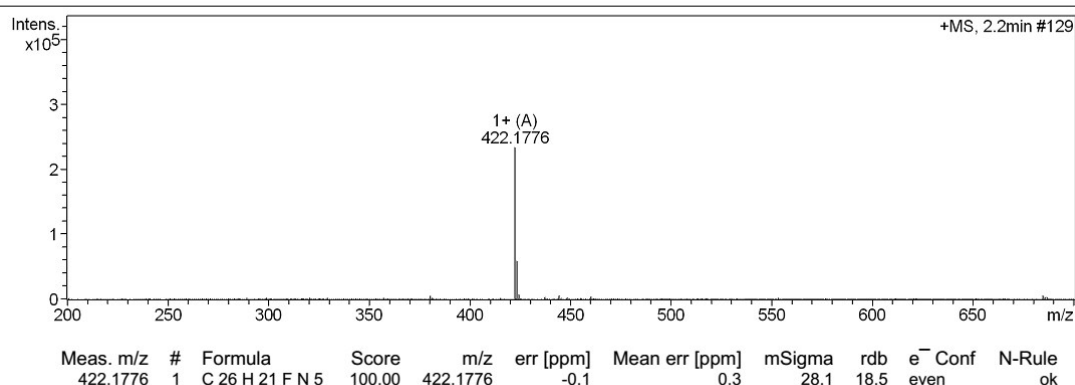
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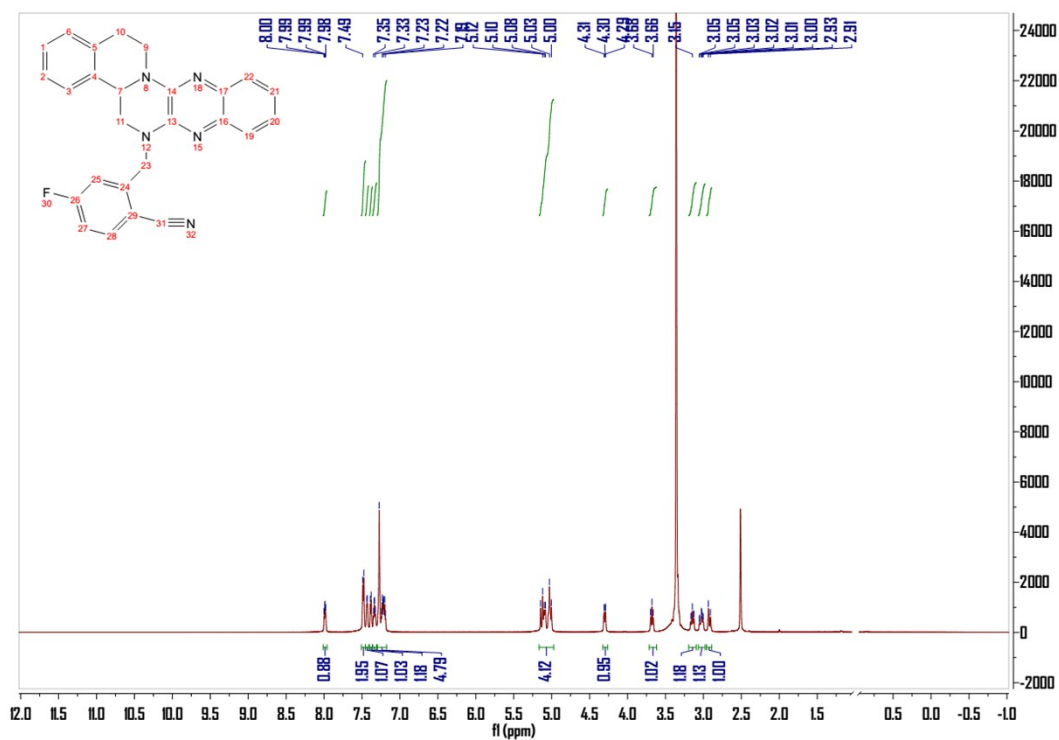
HRMS Spectrum

Acquisition Parameter

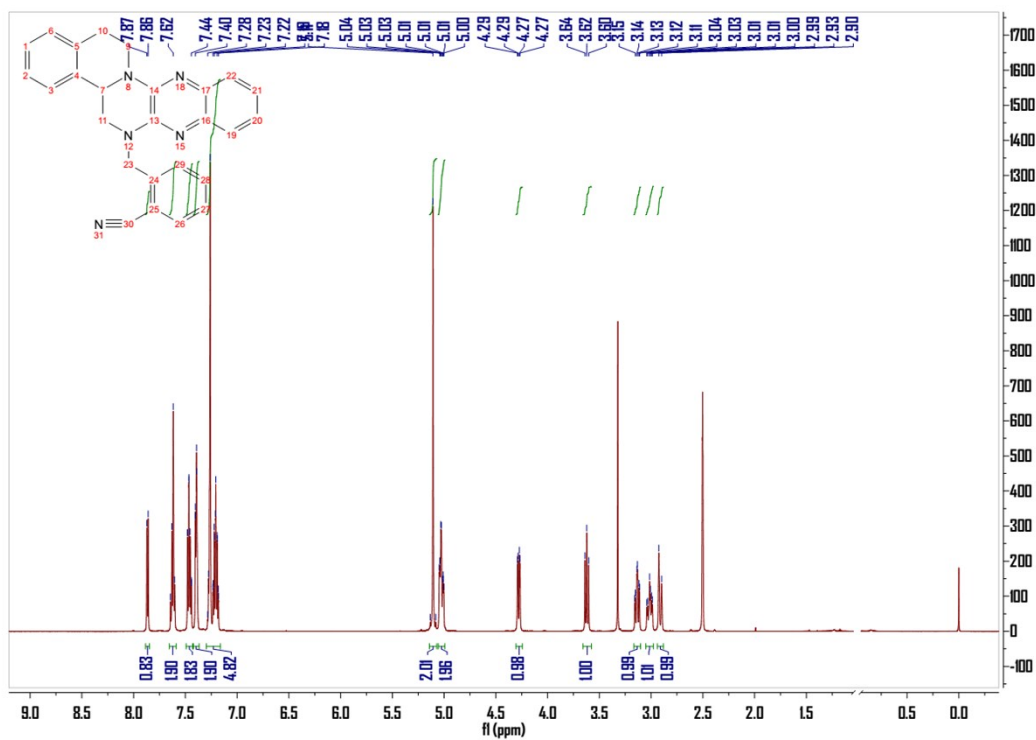
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Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



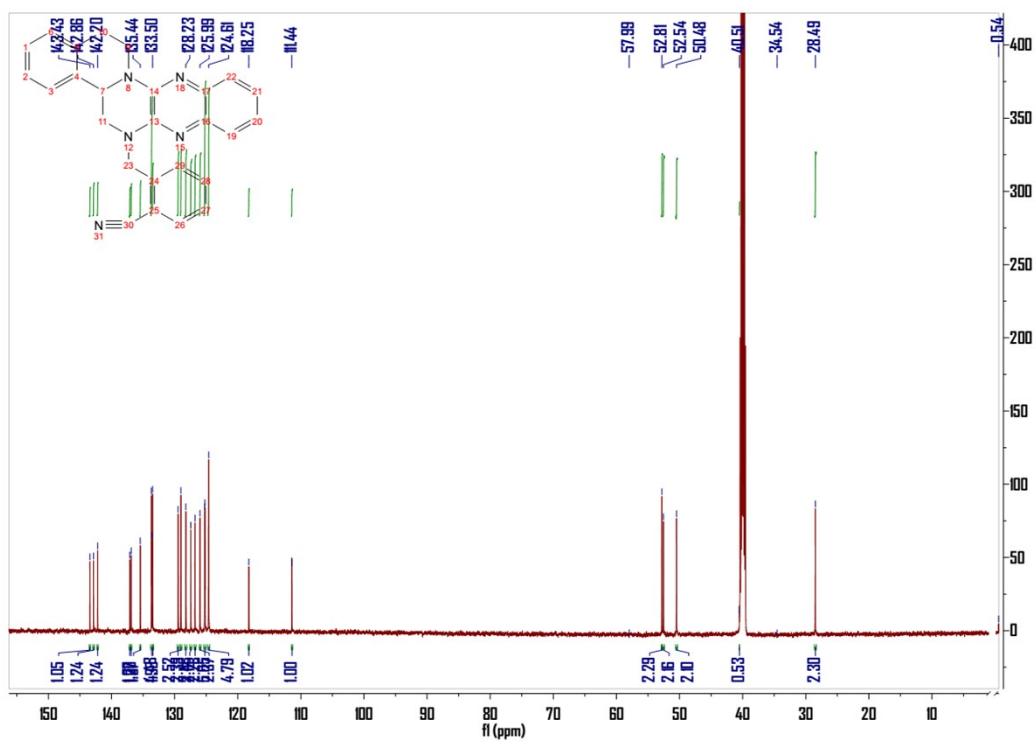
¹H NMR Spectrum



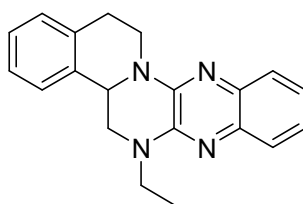
¹³C NMR Spectrum



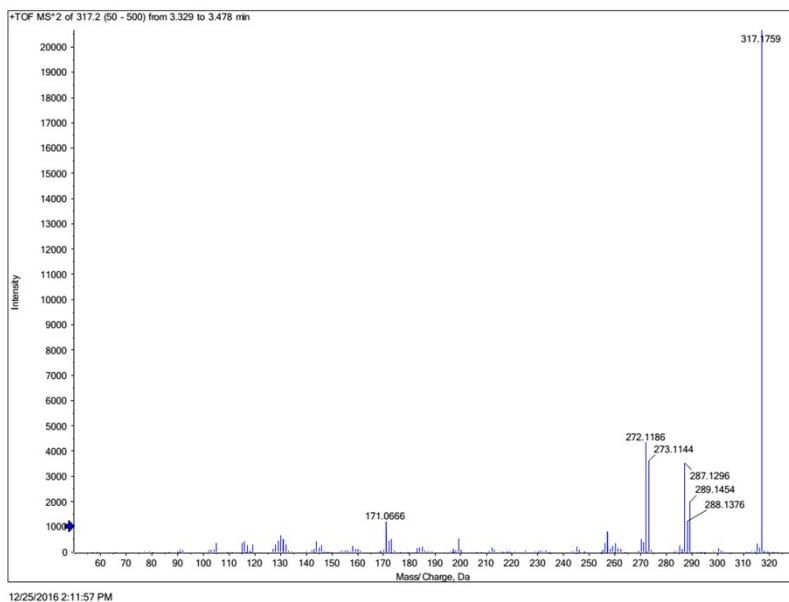
¹³C NMR Spectrum



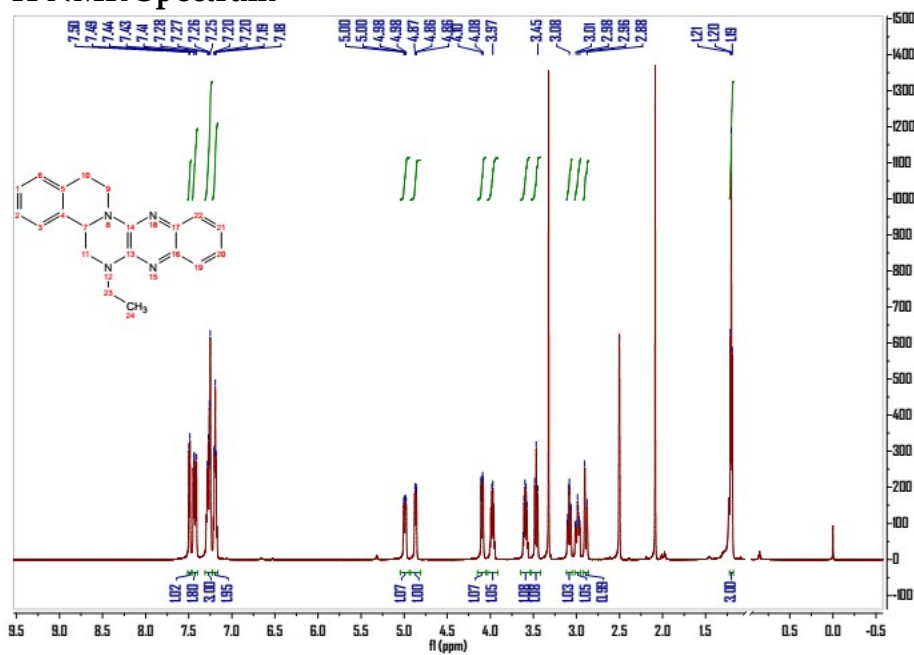
2h:



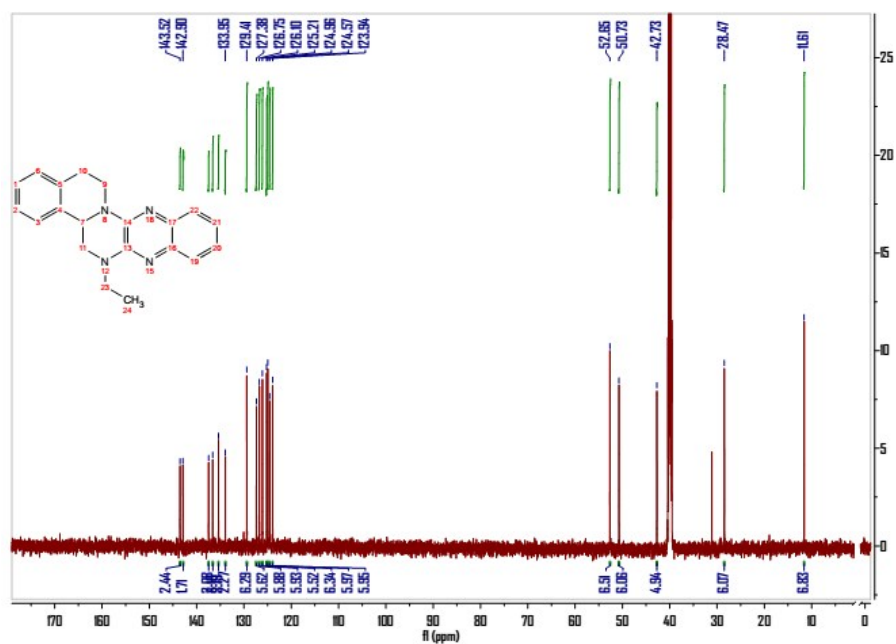
HRMS Spectrum



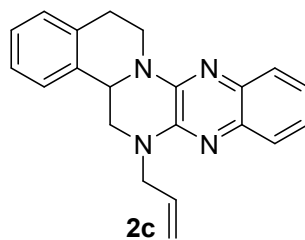
¹H NMR Spectrum



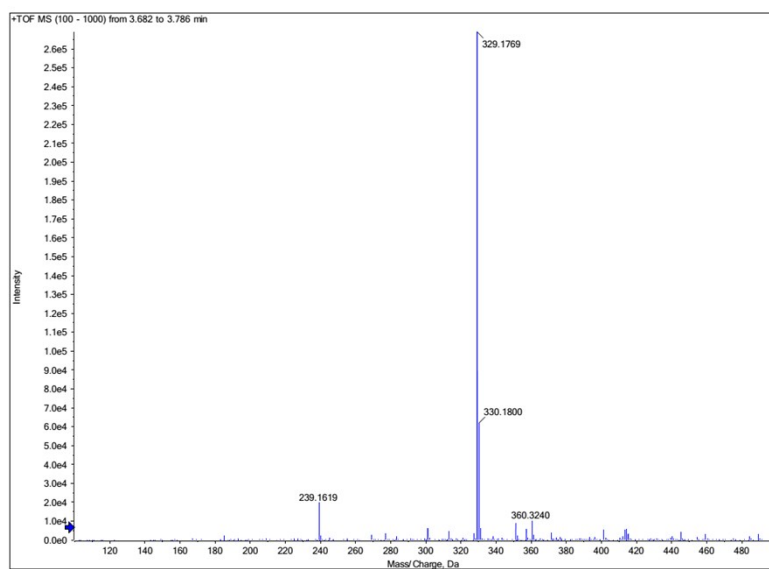
¹³C NMR Spectrum



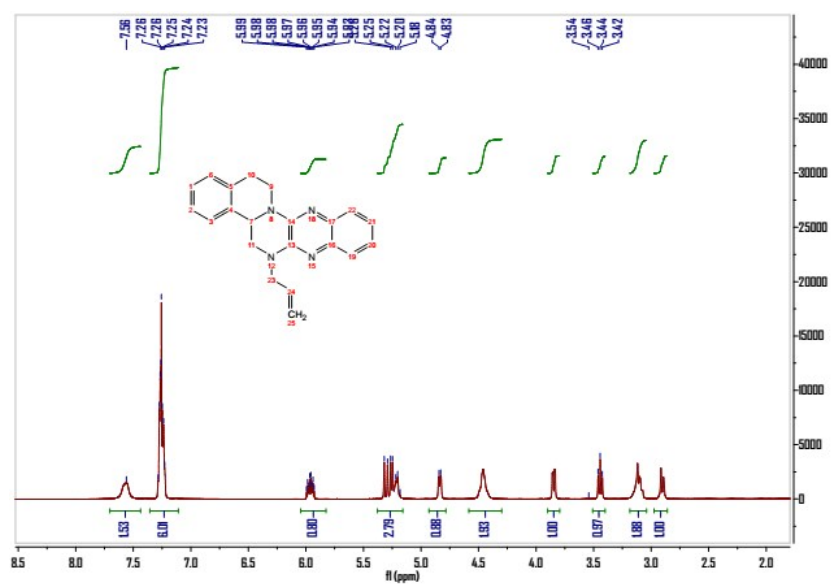
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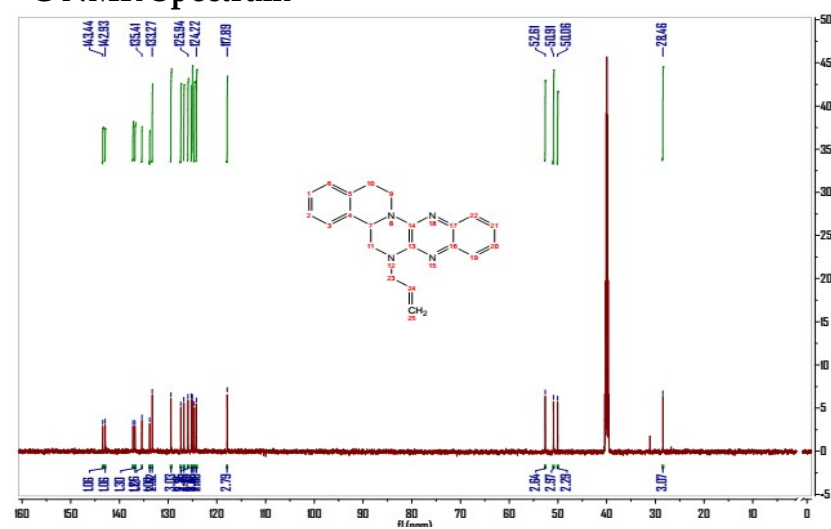
HRMS Spectrum



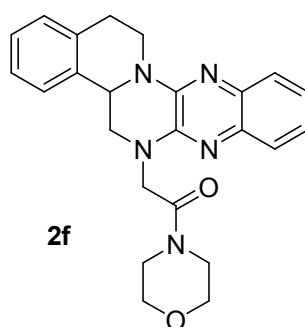
¹H NMR Spectrum



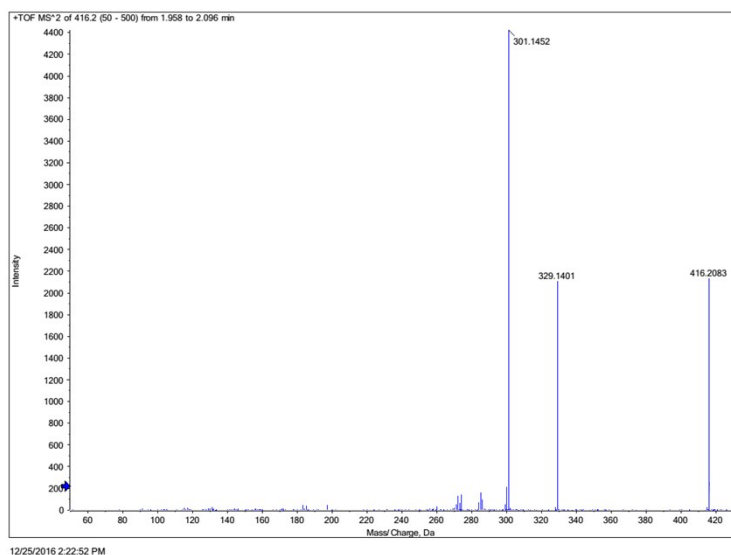
¹³C NMR Spectrum



2j:

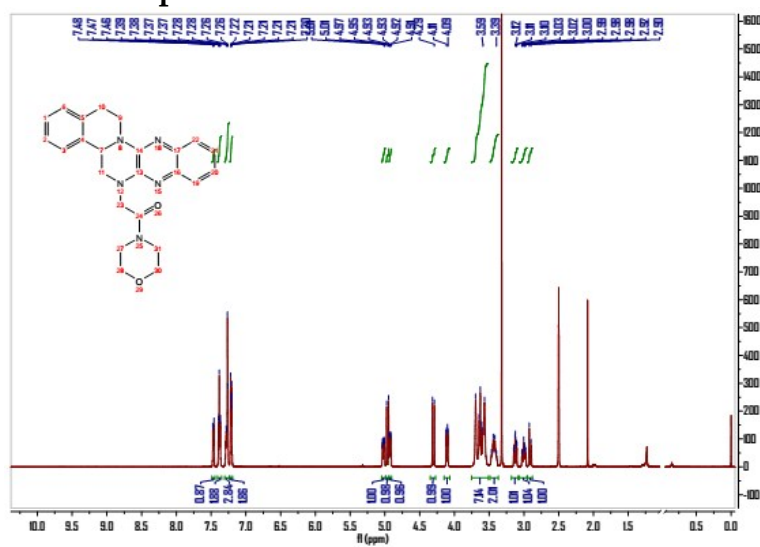


HRMS Spectrum

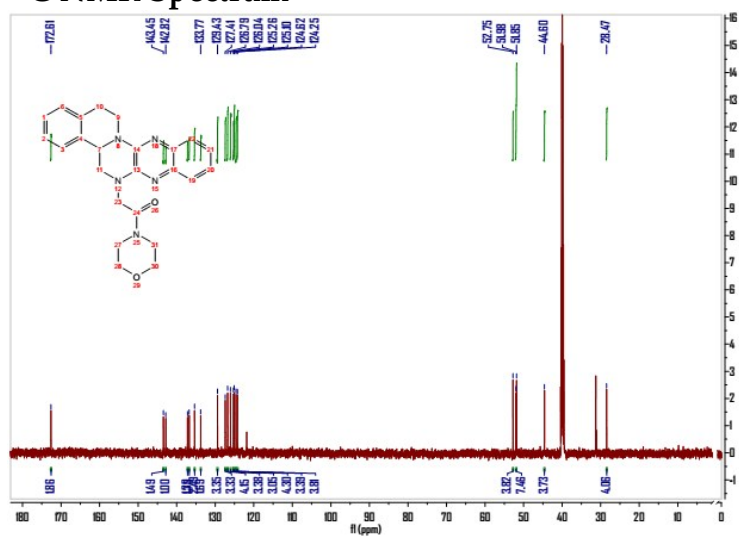


12/25/2016 2:22:52 PM

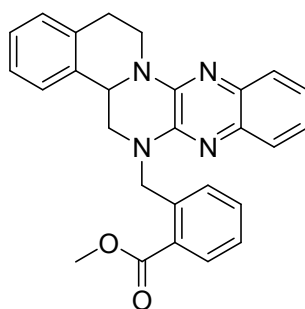
¹H NMR Spectrum



¹³C NMR Spectrum



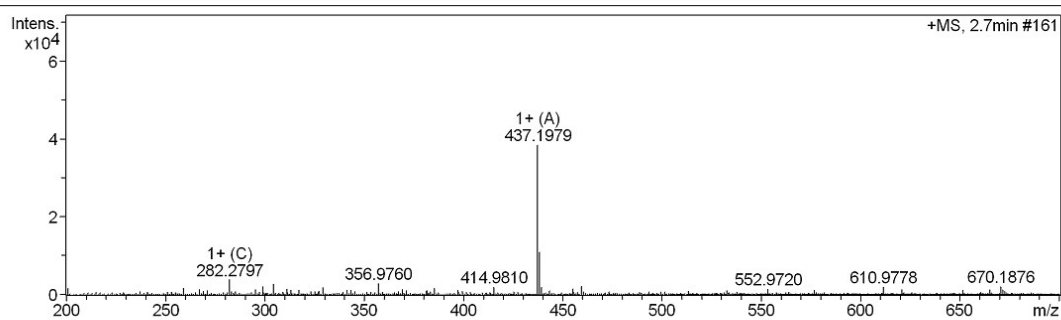
2k:



HRMS Spectrum

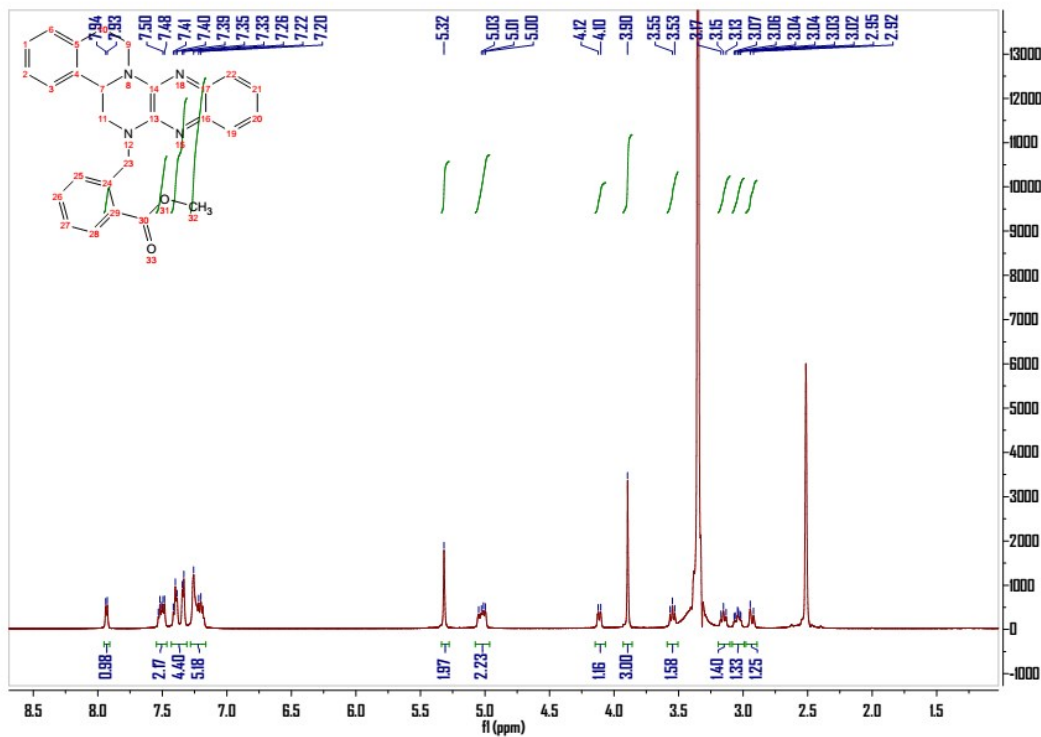
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

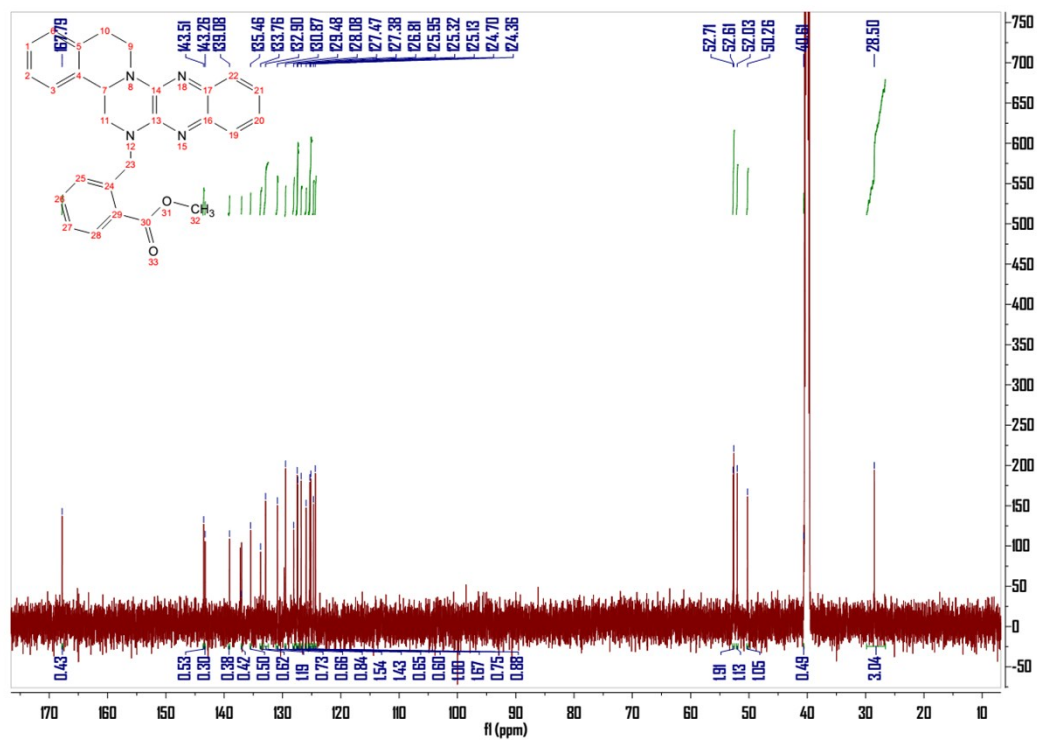


Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
437.1979	1	C ₂₇ H ₂₅ N ₄ O ₂	100.00	437.1972	-1.6	-1.3	10.9	17.5	even	ok

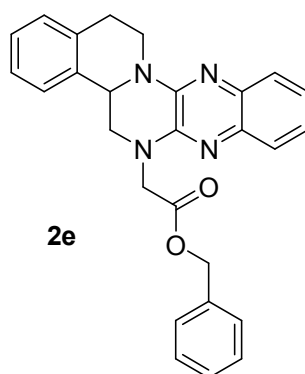
¹H NMR Spectrum



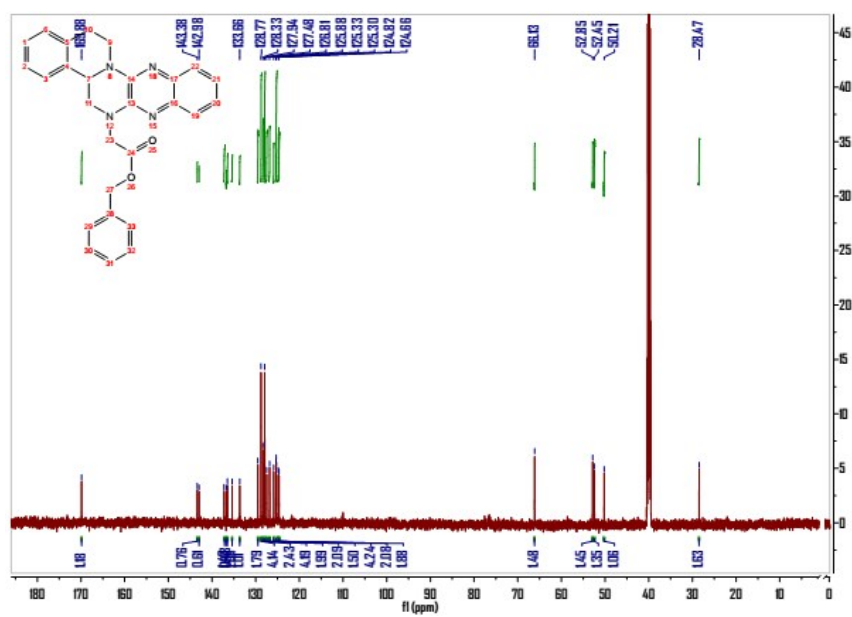
¹³C NMR Spectrum



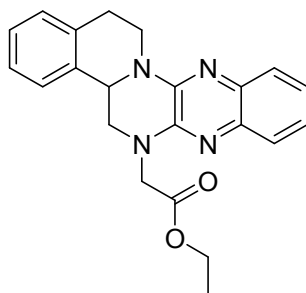
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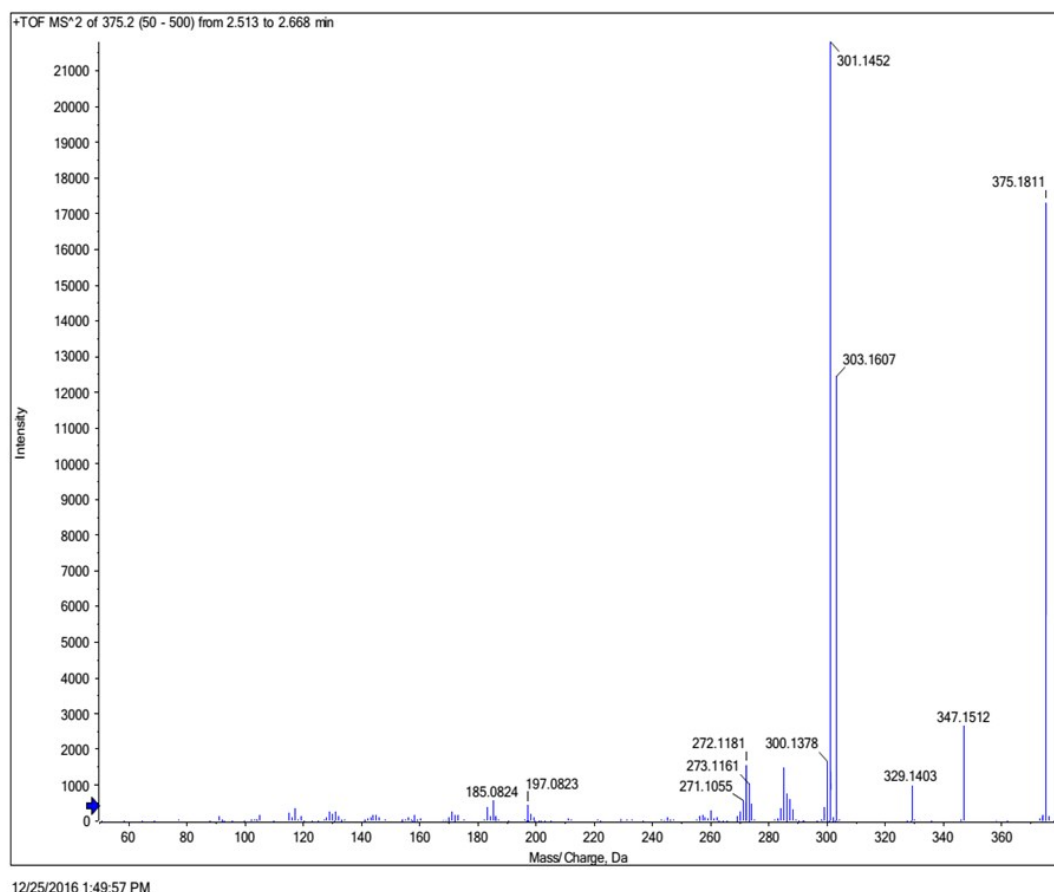
HRMS Spectrum



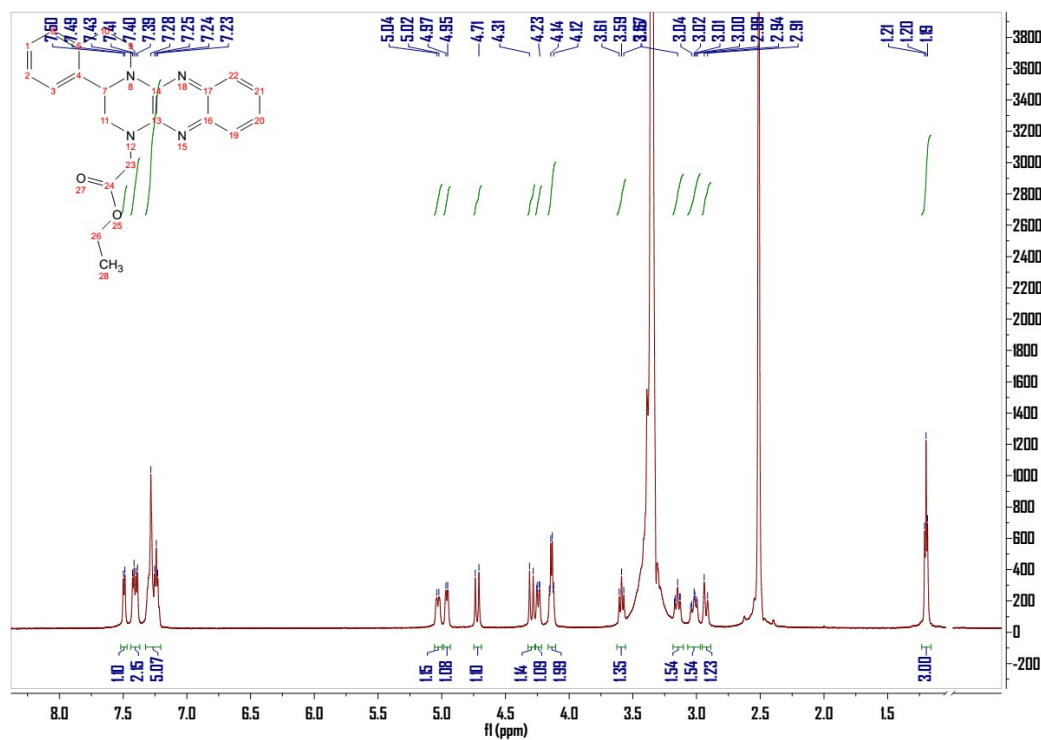
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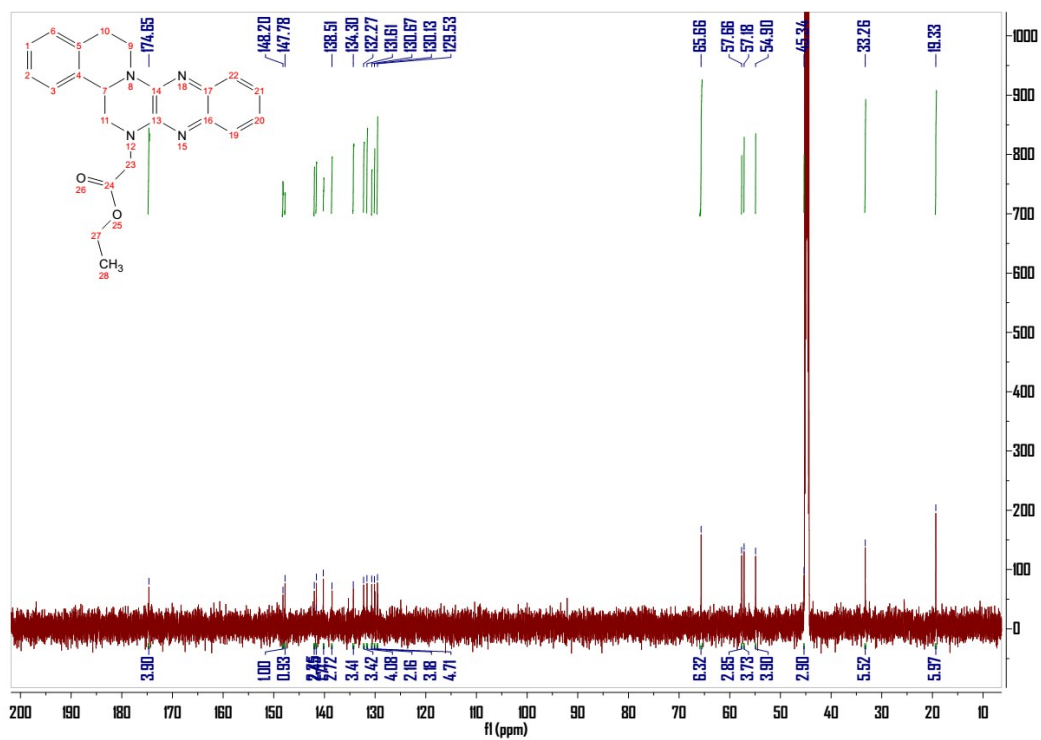


HRMS Spectrum

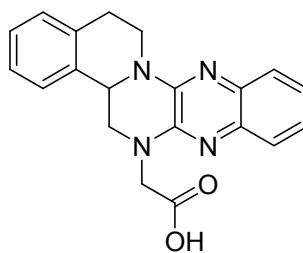


¹H NMR Spectrum

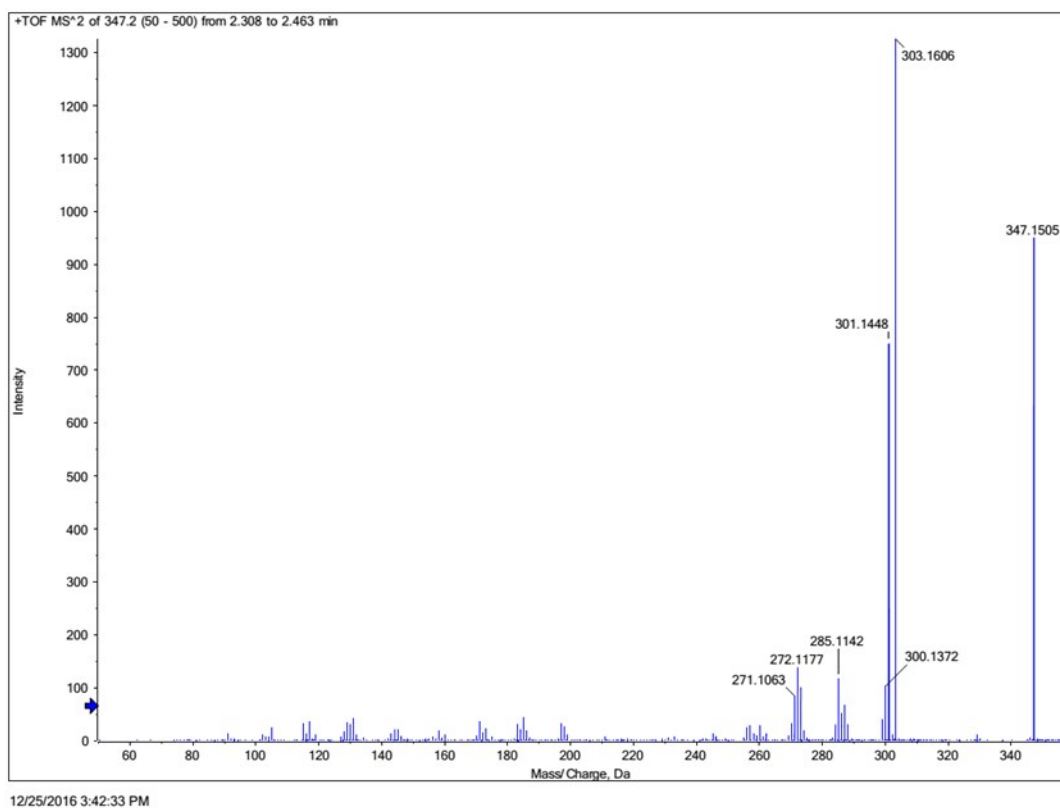




2n:



HRMS Spectrum



¹H NMR Spectrum

