

Supporting Information

Total Synthesis of Calothrixin B via Sequential Sonogashira

Coupling/Copper-Catalyzed Oxidative Cyclization

Nagarajan Ramkumar and Rajagopal Nagarajan*

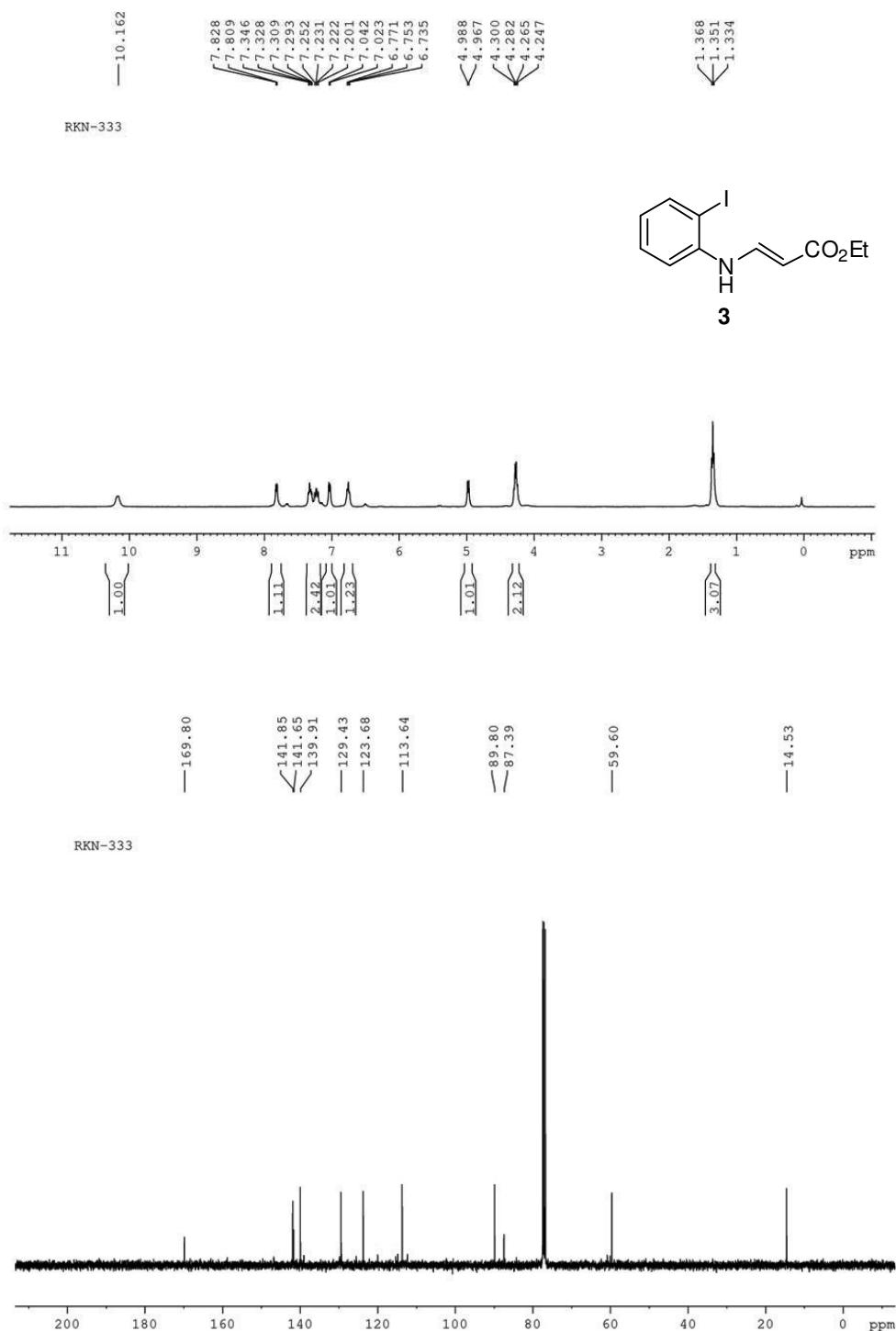
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HRMS of (E)-ethyl 3-((2-iodophenyl)amino)acrylate (3)

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Analysis Info

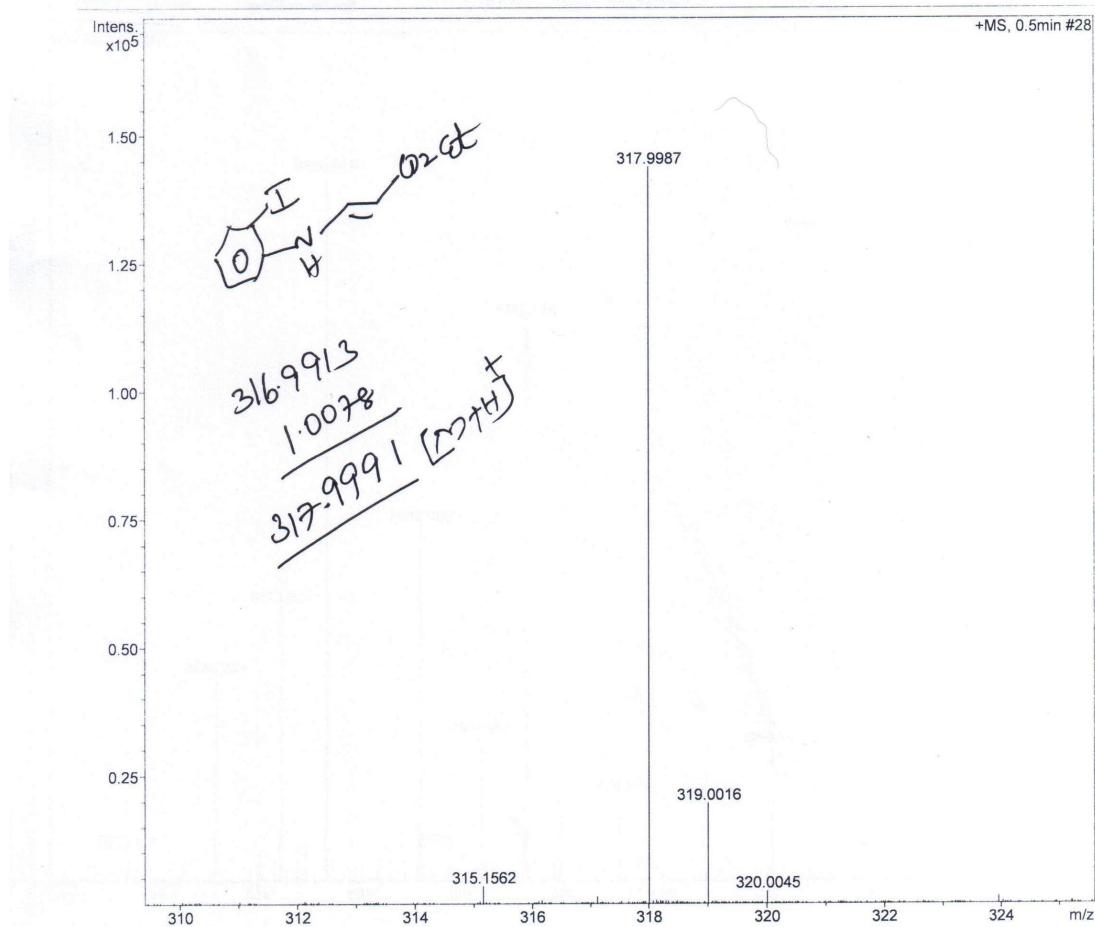
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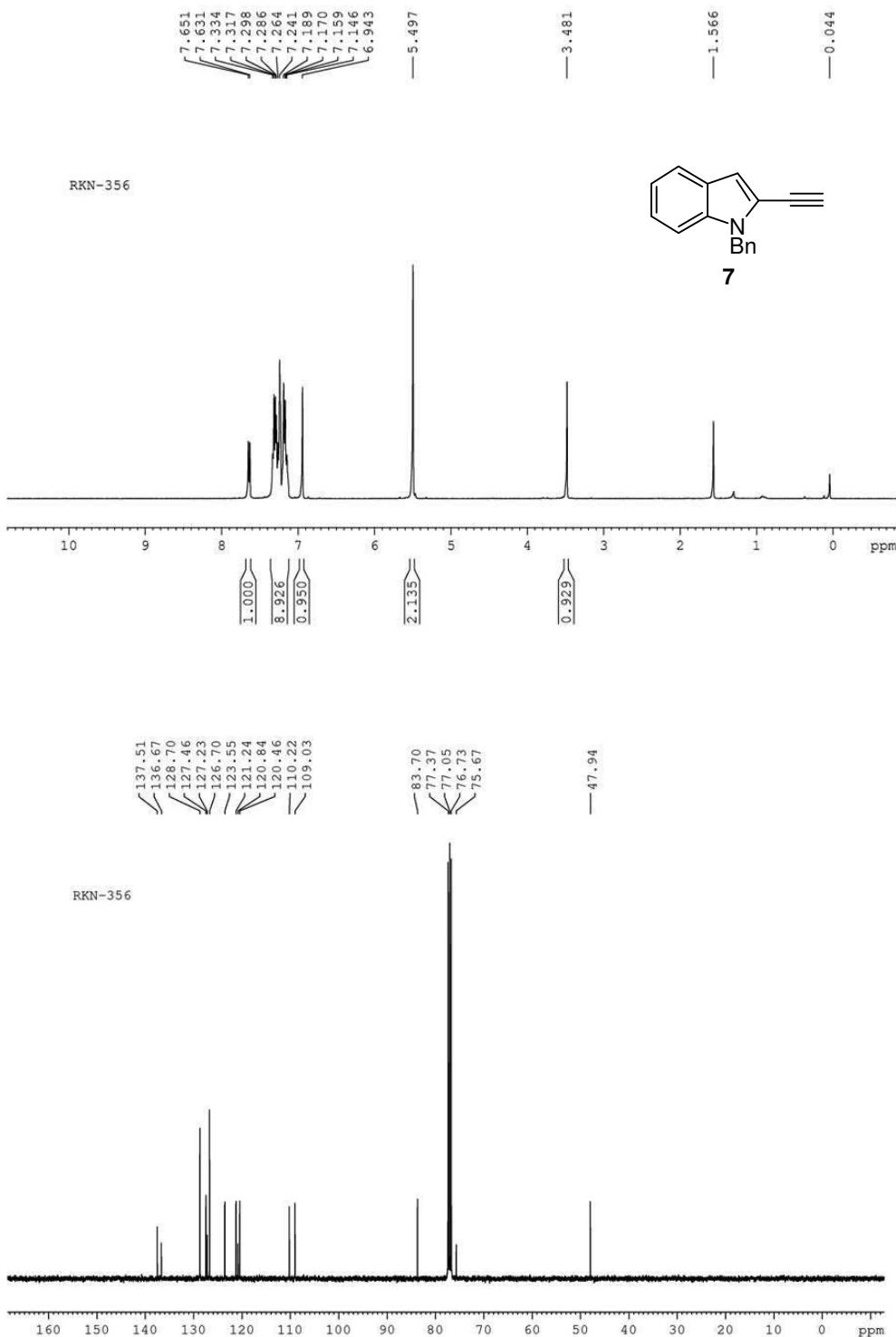
Operator Ramu Sridhar
Instrument maXis 10138

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¹H and ¹³C NMR of 1-benzyl-2-ethynyl-1H-indole (7)



HRMS of 1-benzyl-2-ethynyl-1H-indole (7)

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Analysis Info

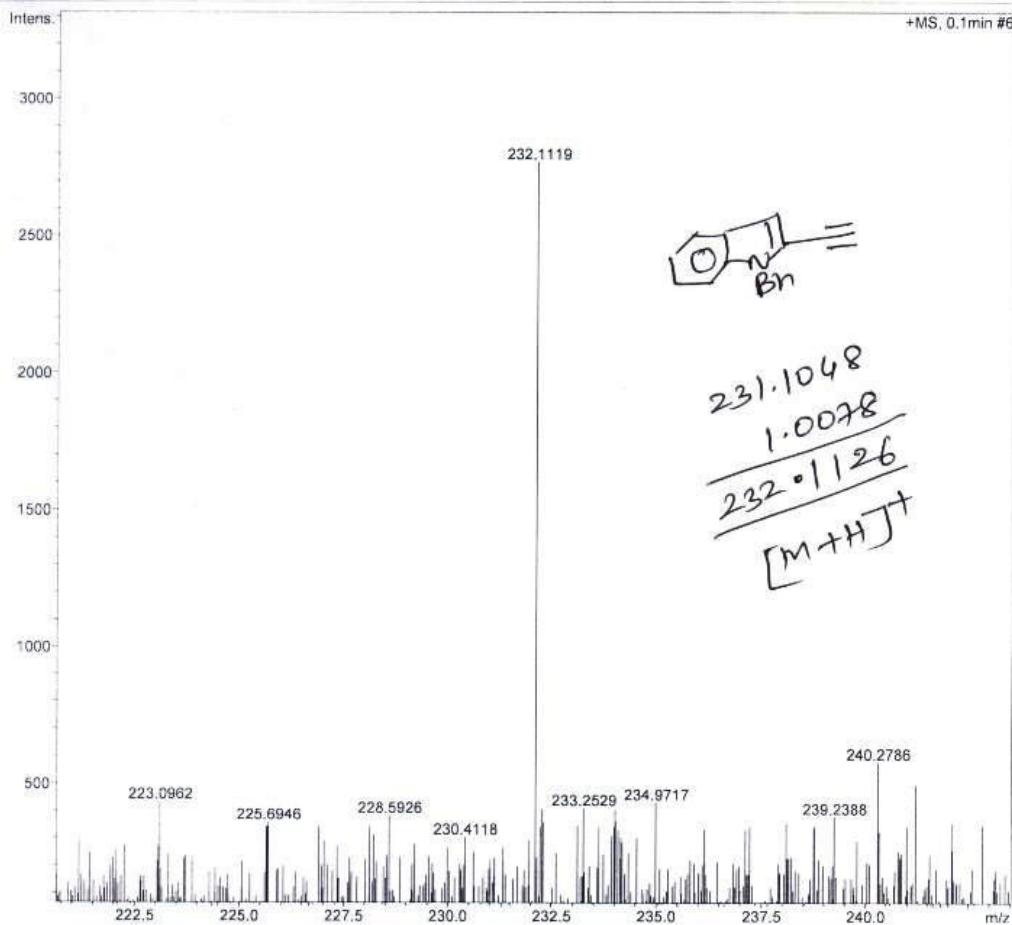
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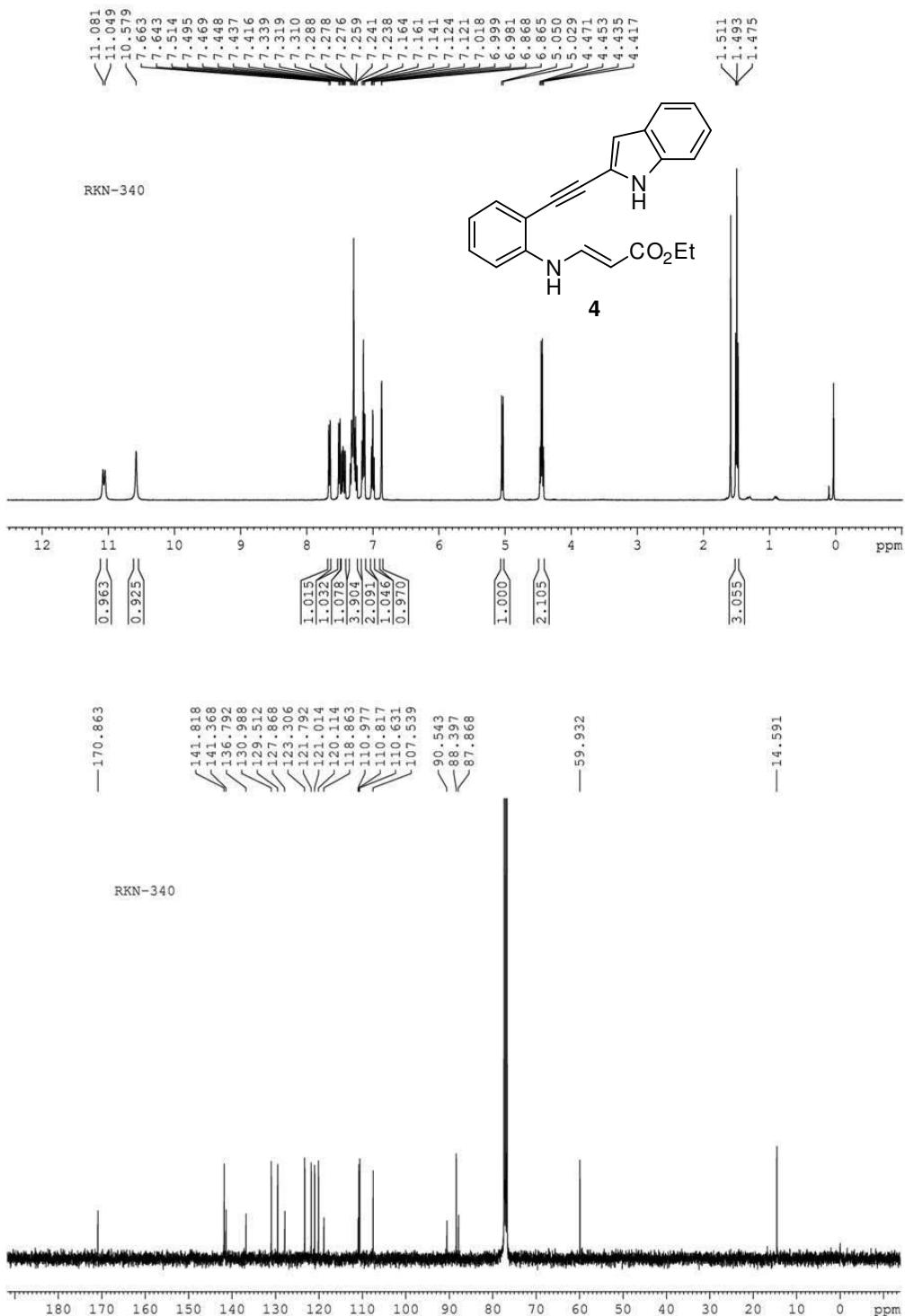
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Instrument maXis 10138

Acquisition Parameter

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Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C NMR of (E)-ethyl 3-((2-((1*H*-indol-2-yl)ethynyl)phenyl)amino)acrylate (4)



HRMS of (*E*-ethyl 3-((2-((1*H*-indol-2-yl)ethynyl)phenyl)amino)acrylate (4)

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Analysis Info

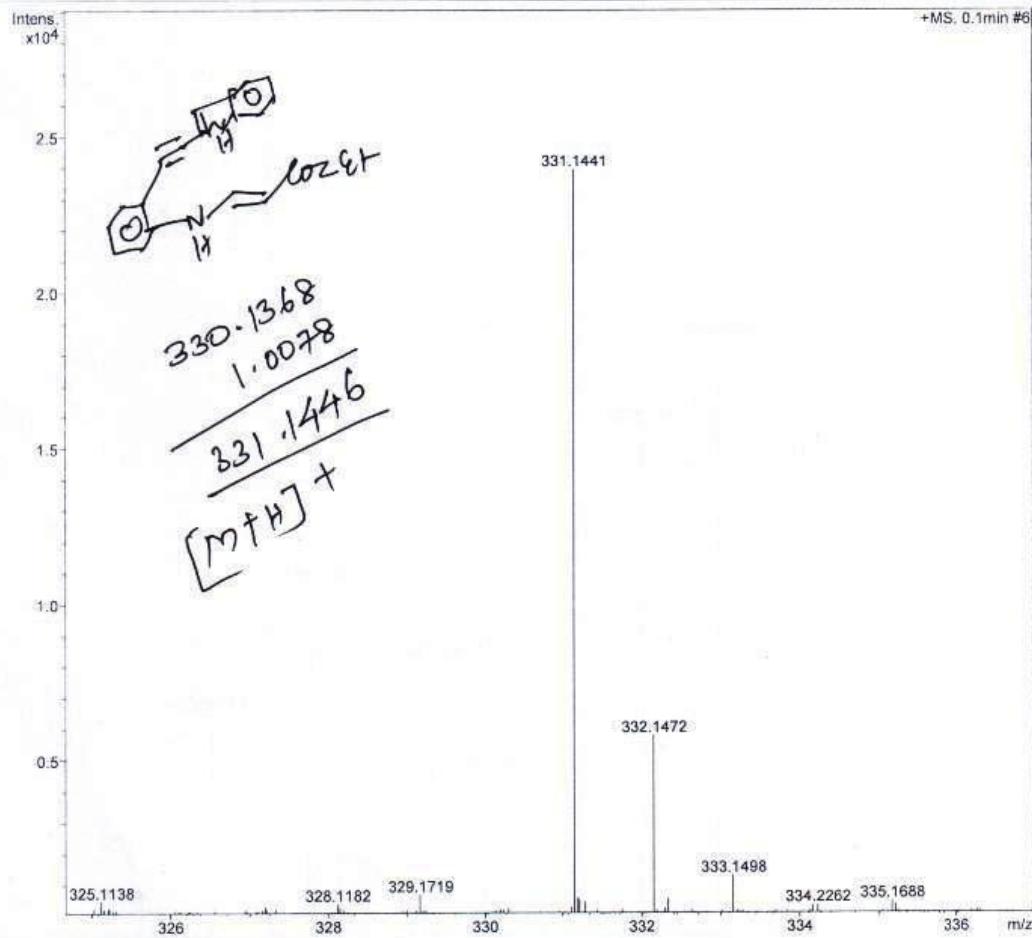
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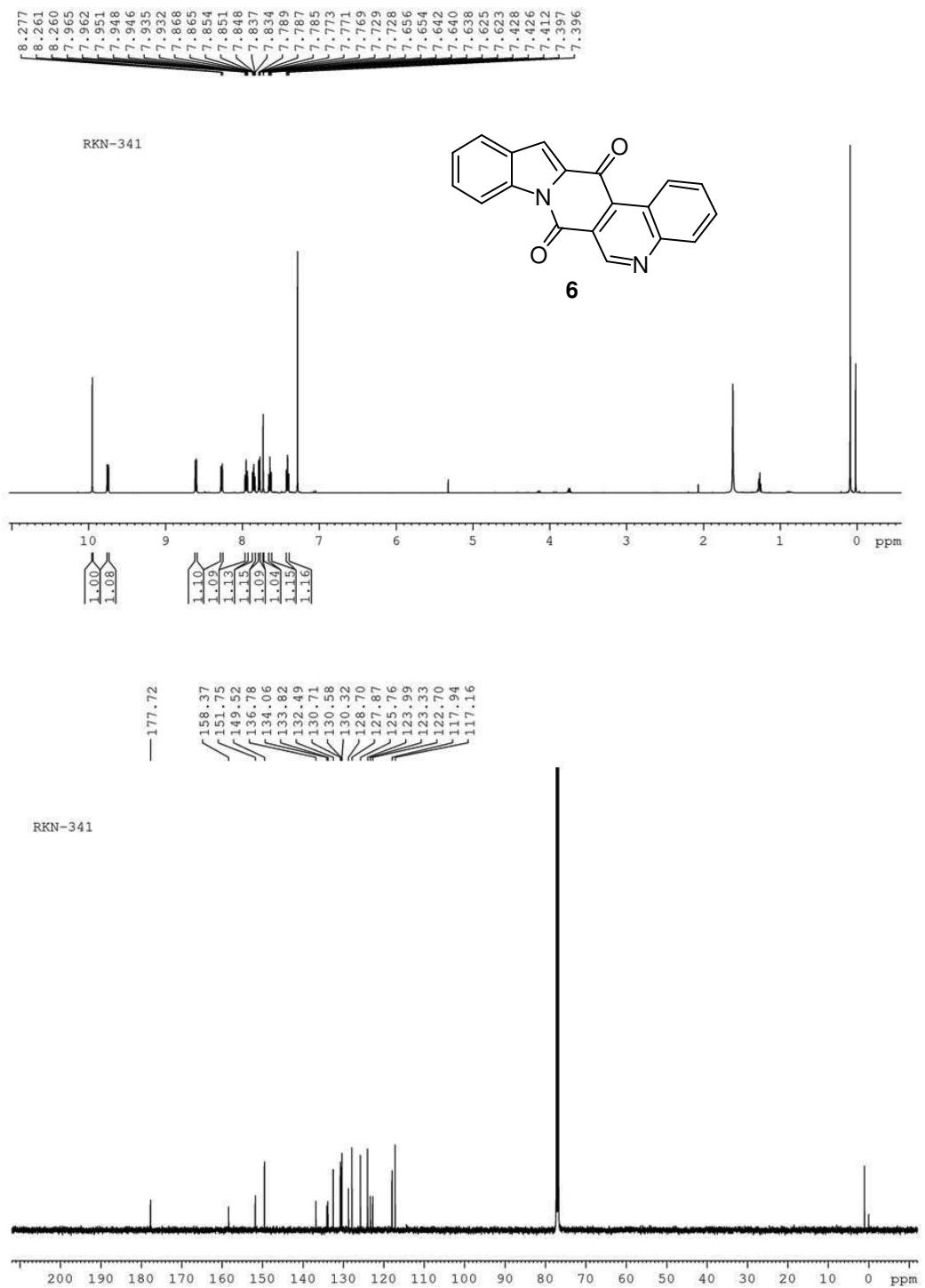
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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¹H and ¹³C NMR of benzo[*f*]indolo[1,2-*b*][2,7]naphthyridine-7,14-dione (6**)**



HRMS of benzo[f]indolo[1,2-b][2,7]naphthyridine-7,14-dione (6)

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Analysis Info

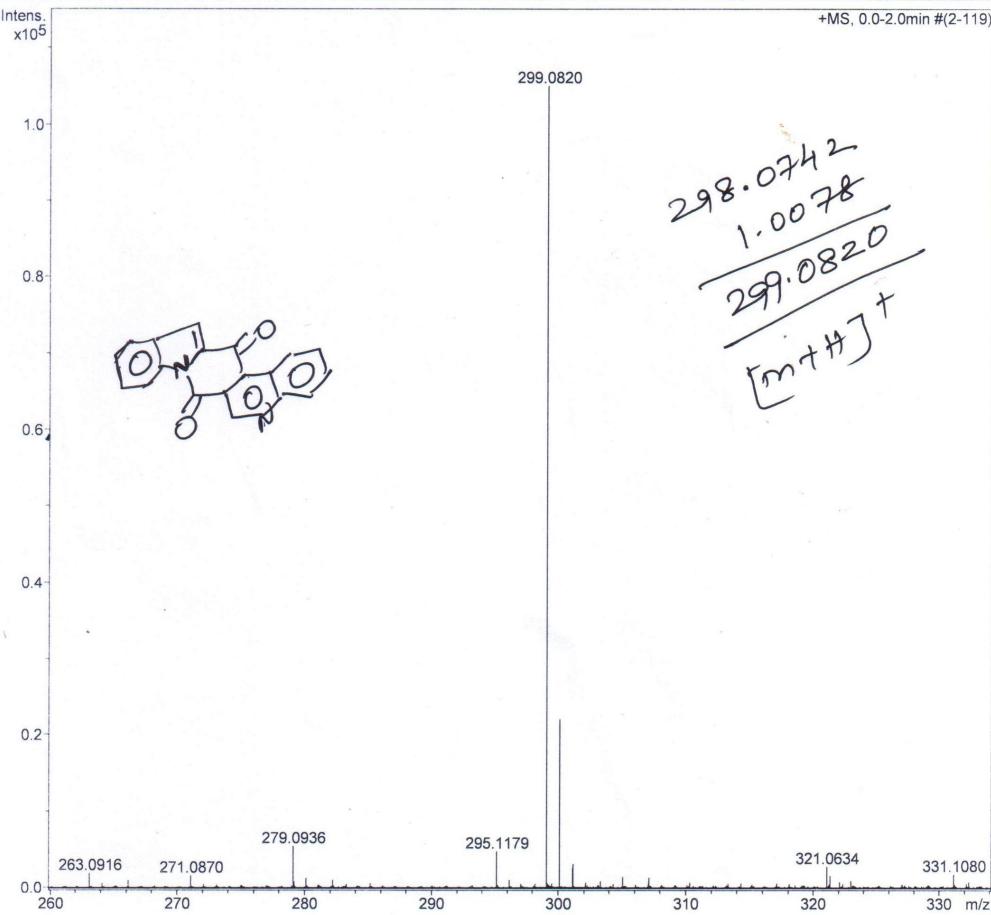
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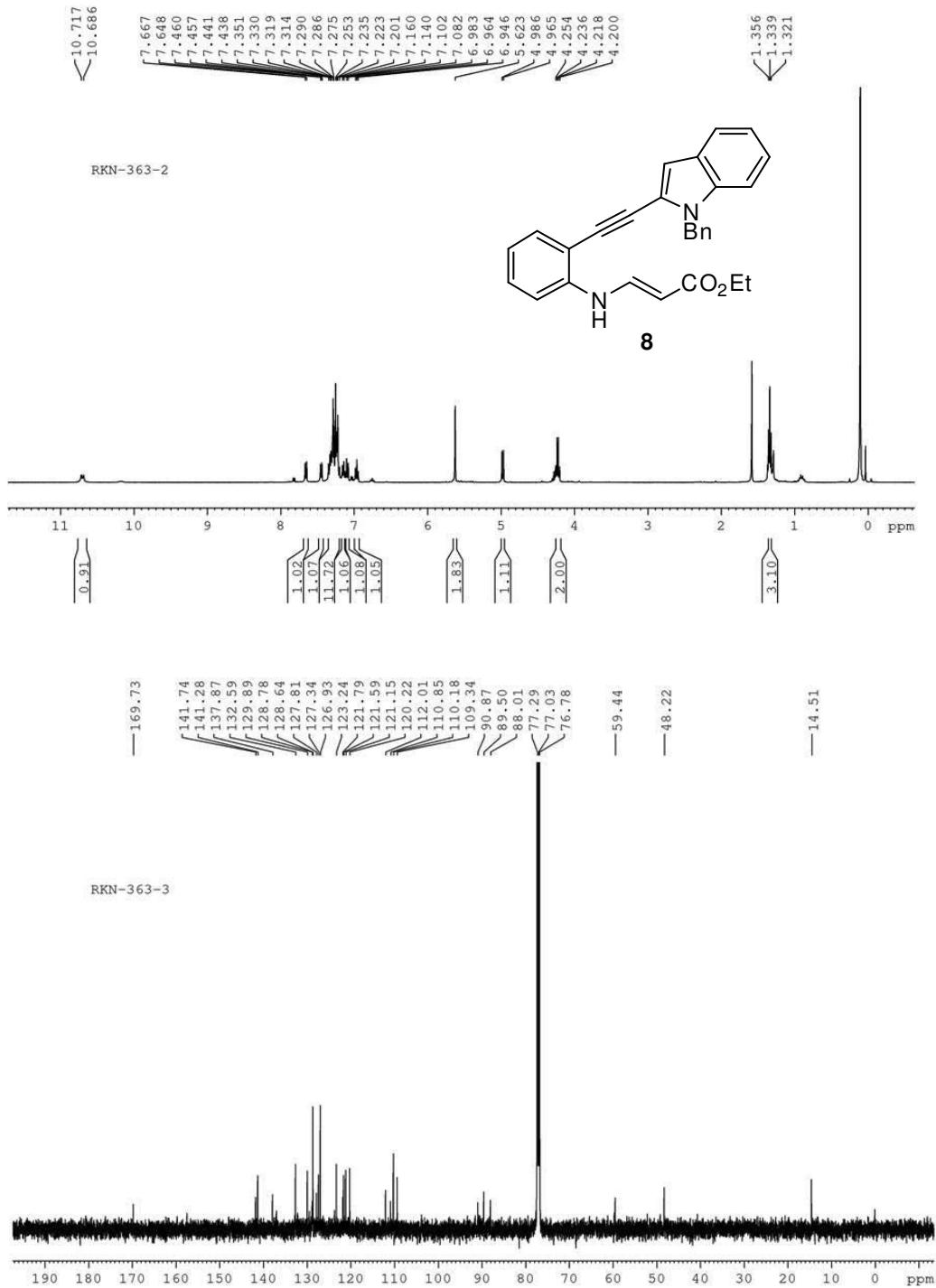
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C NMR of (*E*)-ethyl 3-((2-((1-benzyl-1*H*-indol-2-yl)ethynyl)phenyl)amino)acrylate (8)



HRMS of (*E*-ethyl 3-((2-((1-benzyl-1*H*-indol-2-yl)ethynyl)phenyl)amino)acrylate (8)

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Analysis Info

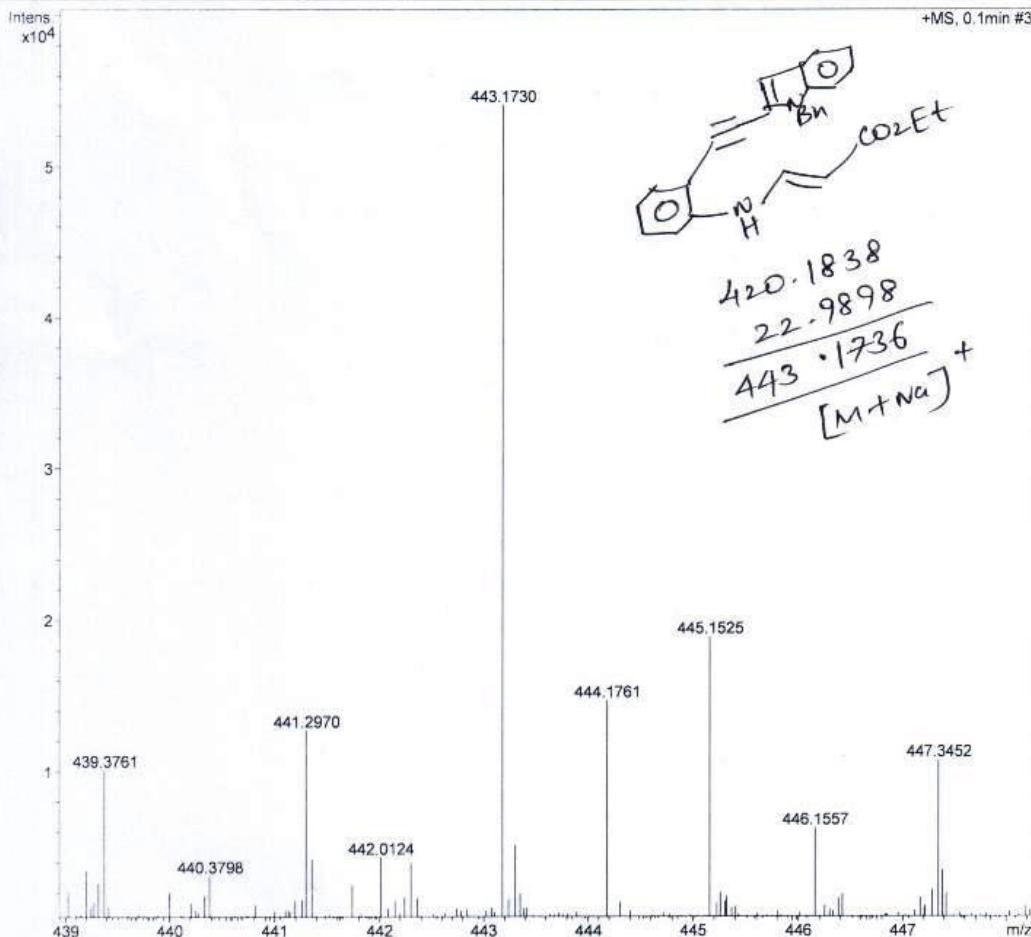
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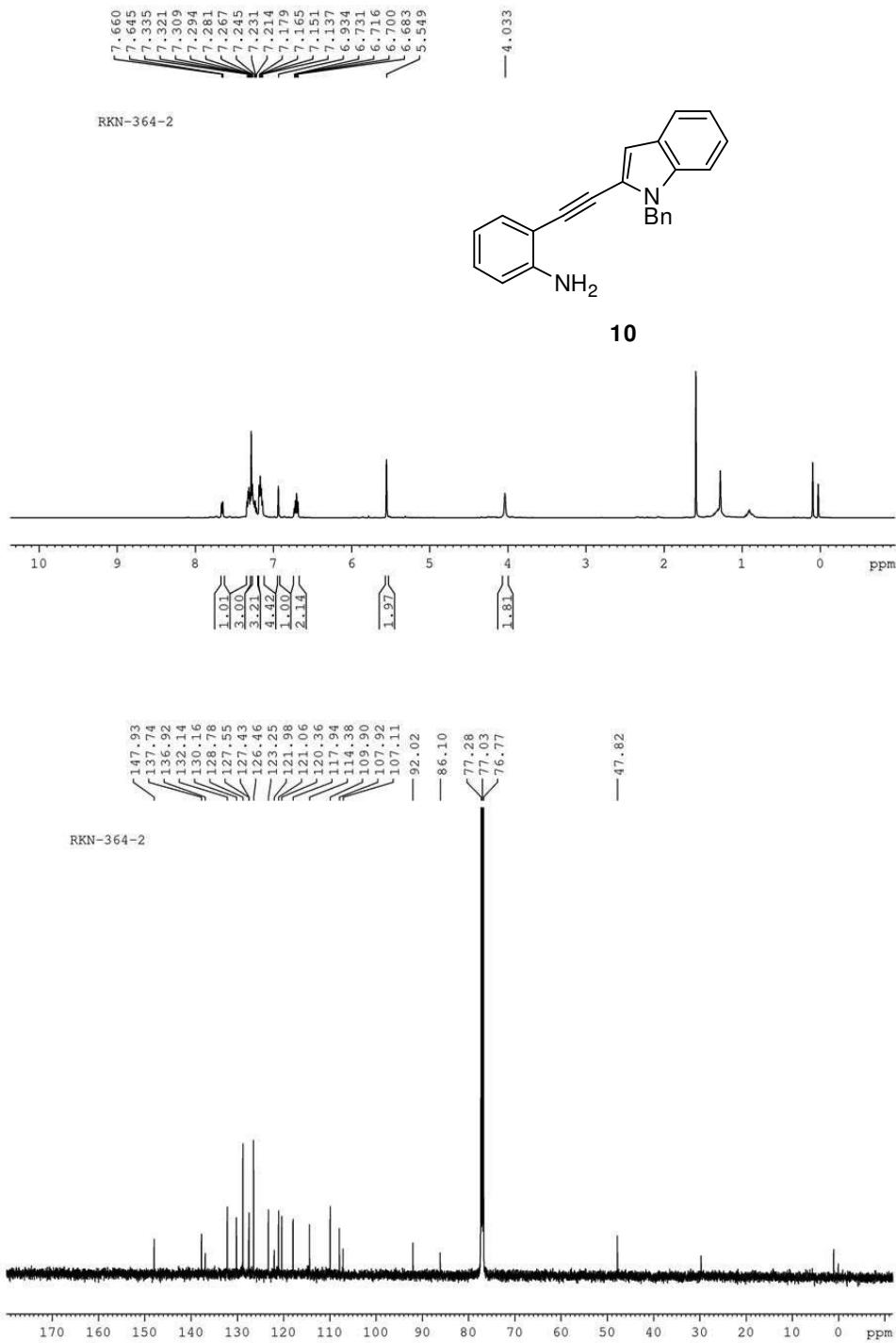
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C NMR of 2-((1-benzyl-1*H*-indol-2-yl)ethynyl)aniline (10**)**



HRMS of 2-((1-benzyl-1H-indol-2-yl)ethynyl)aniline (10)

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Analysis Info

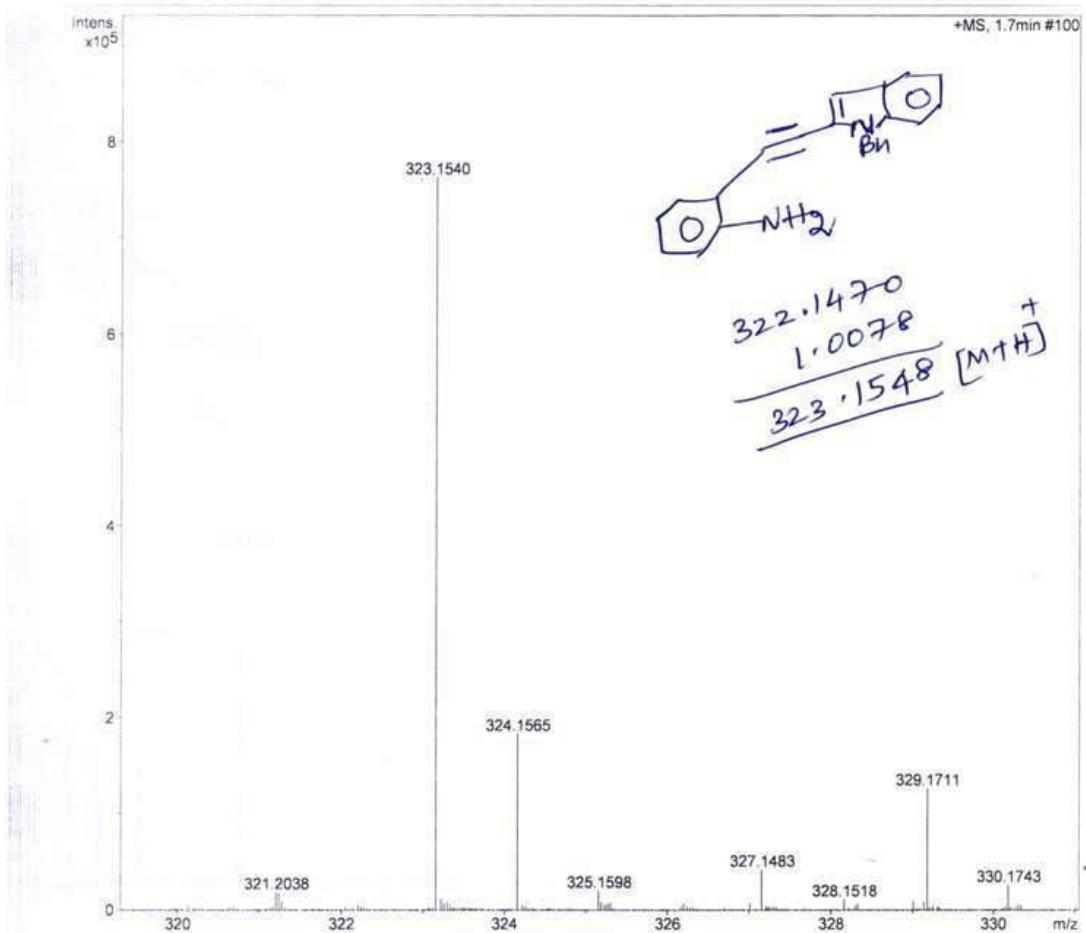
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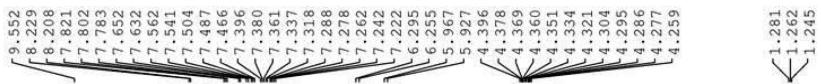
Operator Ramu Sridhar
Instrument maXis 10138

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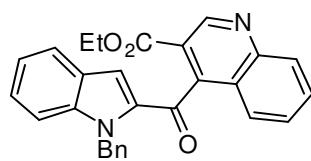
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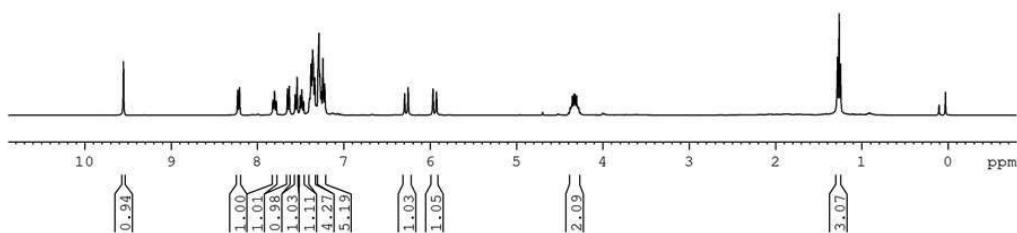
¹H and ¹³C NMR of ethyl 4-(1-benzyl-1*H*-indole-2-carbonyl)quinoline-3-carboxylate (11)



RKN-364

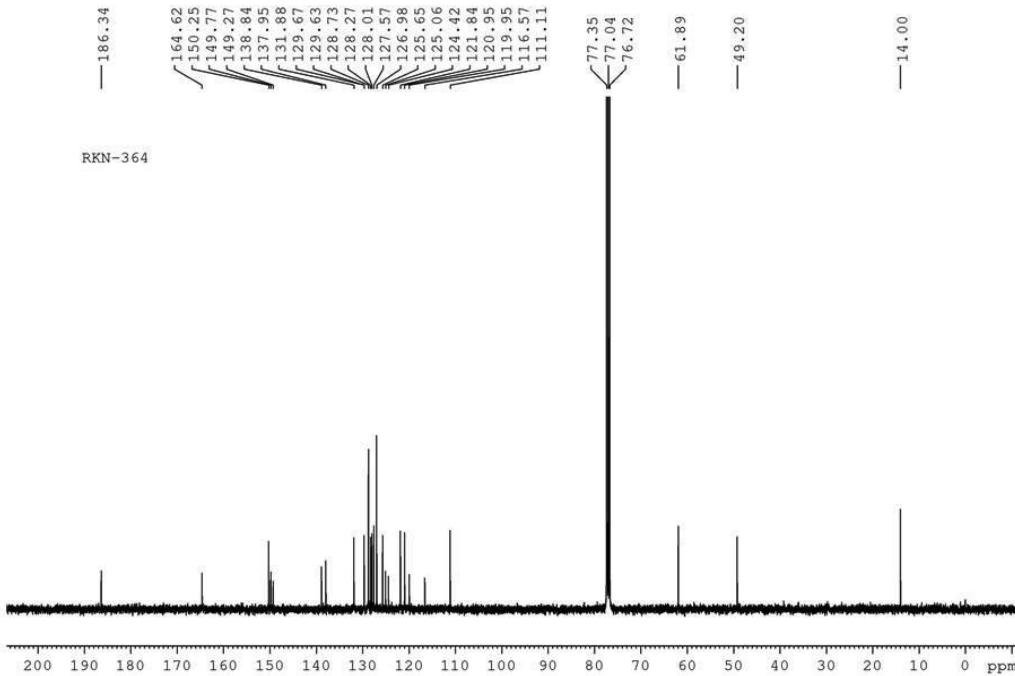


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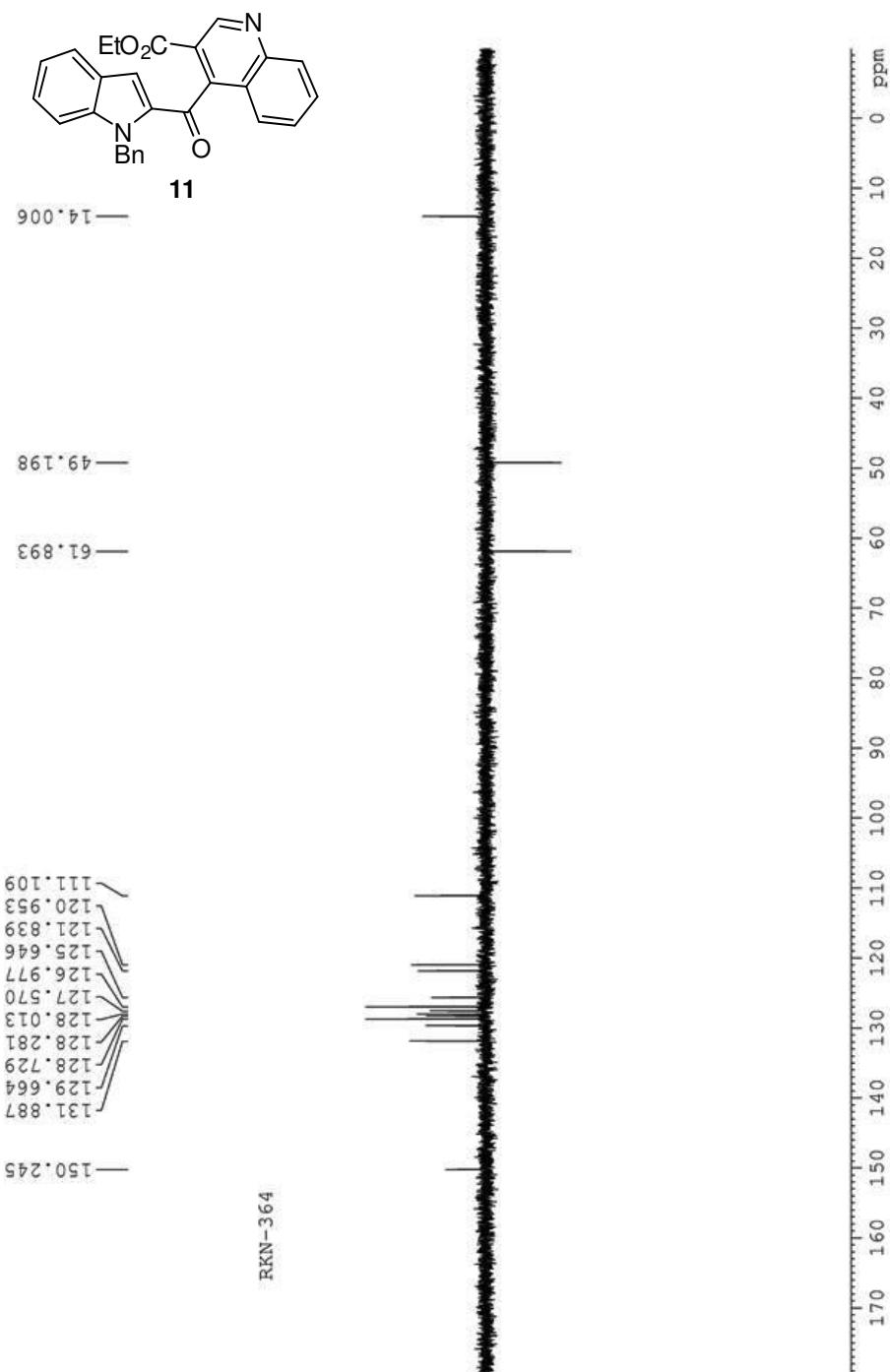


— 186.34

RKN-364



DEPT of ethyl 4-(1-benzyl-1*H*-indole-2-carbonyl)quinoline-3-carboxylate (11)



HRMS of ethyl 4-(1-benzyl-1H-indole-2-carbonyl)quinoline-3-carboxylate (11)

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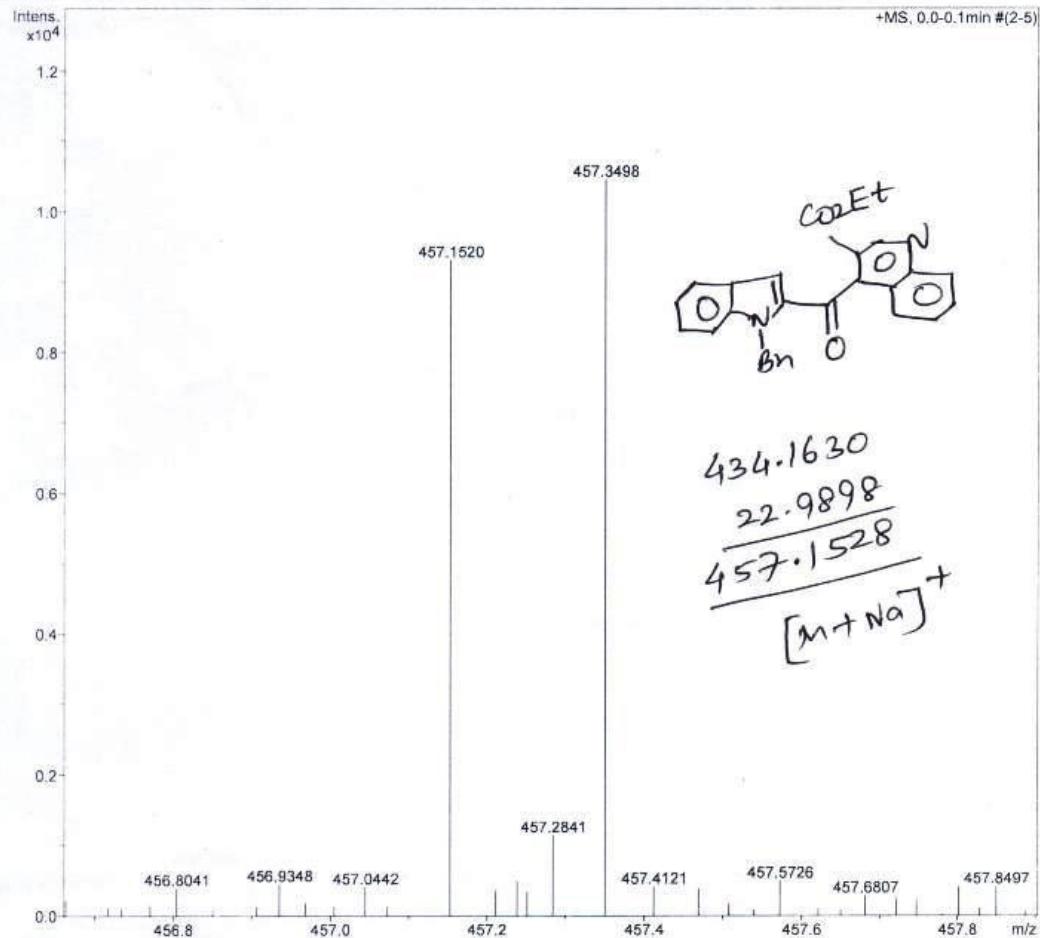
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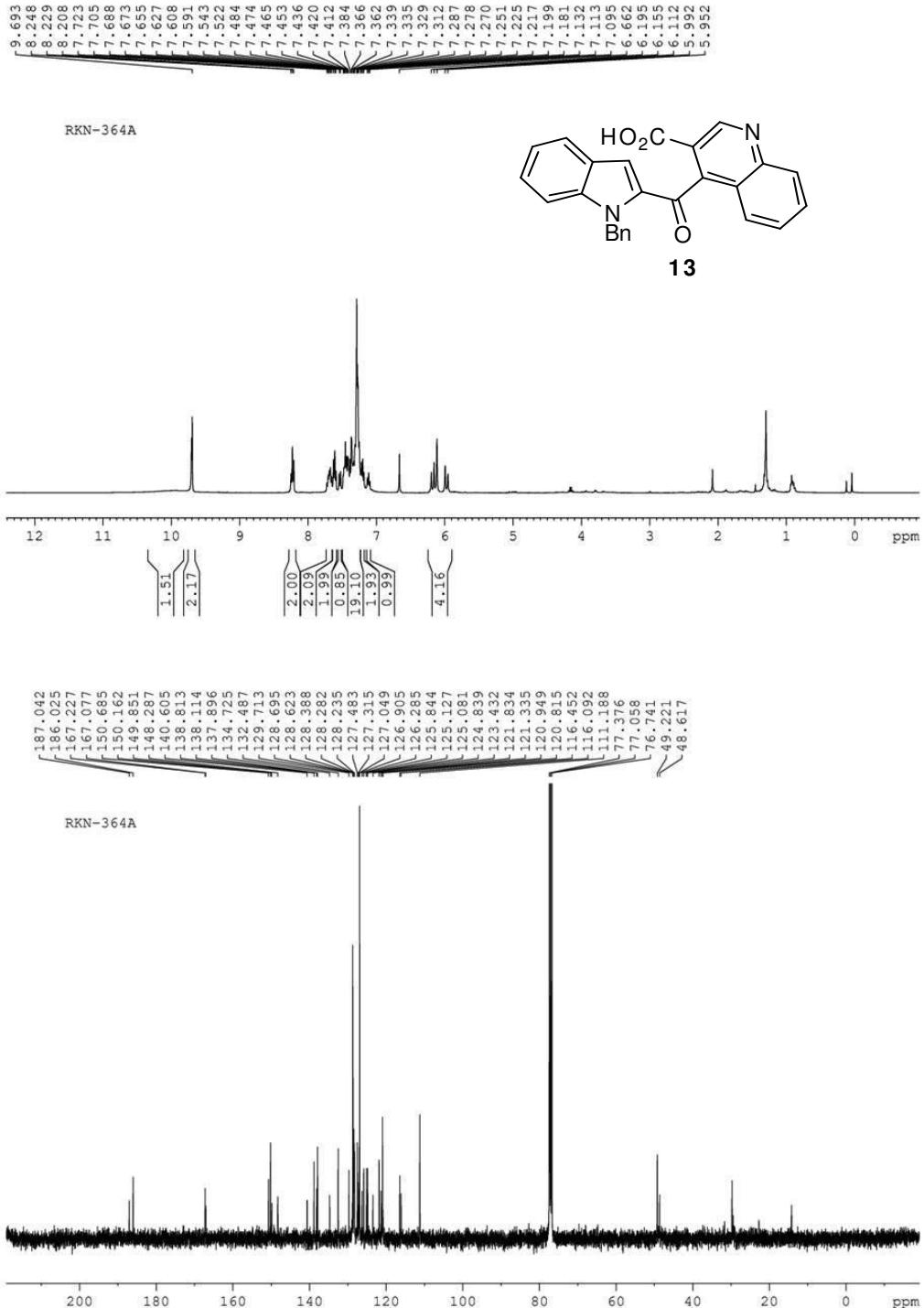
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Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C NMR of 4-(1-benzyl-1*H*-indole-2-carbonyl)quinoline-3-carboxylic acid (13)



HRMS of 4-(1-benzyl-1*H*-indole-2-carbonyl)quinoline-3-carboxylic acid (13)

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Analysis Info

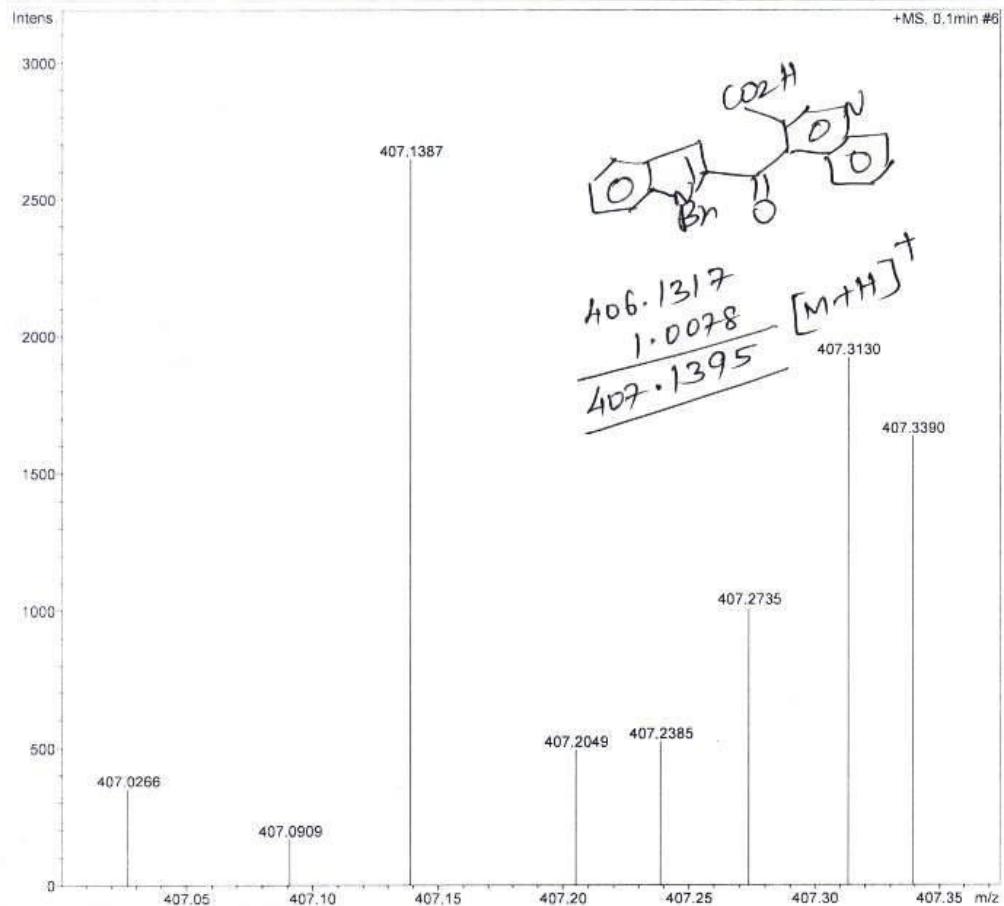
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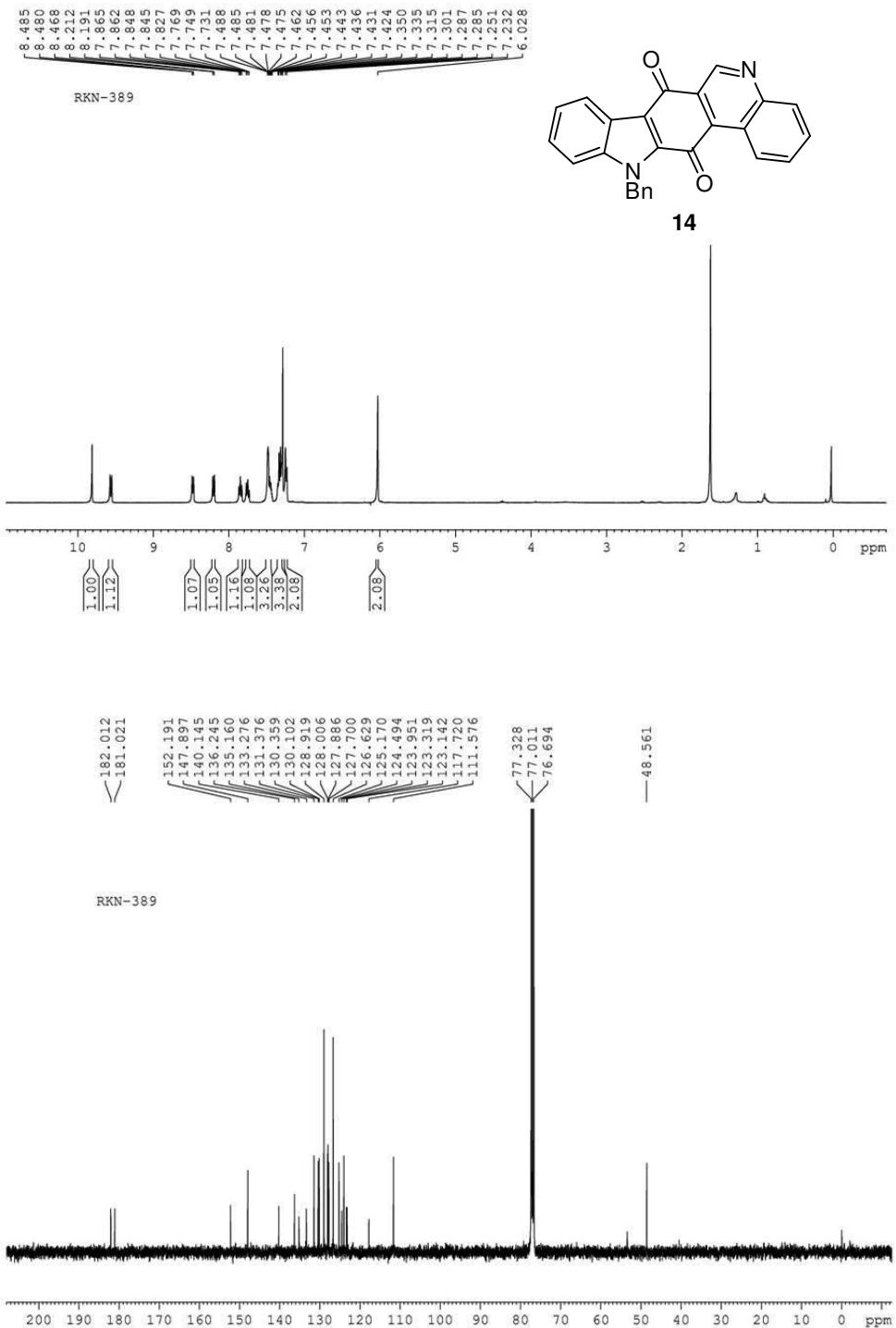
Operator Ramu Sridhar
Instrument maxis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3200 V	Set Dry Heater	180 °C
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Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



¹H and ¹³C NMR of 12-benzyl-7H-indolo[3,2-j]phenanthridine-7,13(12*H*)-dione (14)



HRMS of 12-benzyl-7*H*-indolo[3,2-*j*]phenanthridine-7,13(12*H*)-dione (14)

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Analysis Info

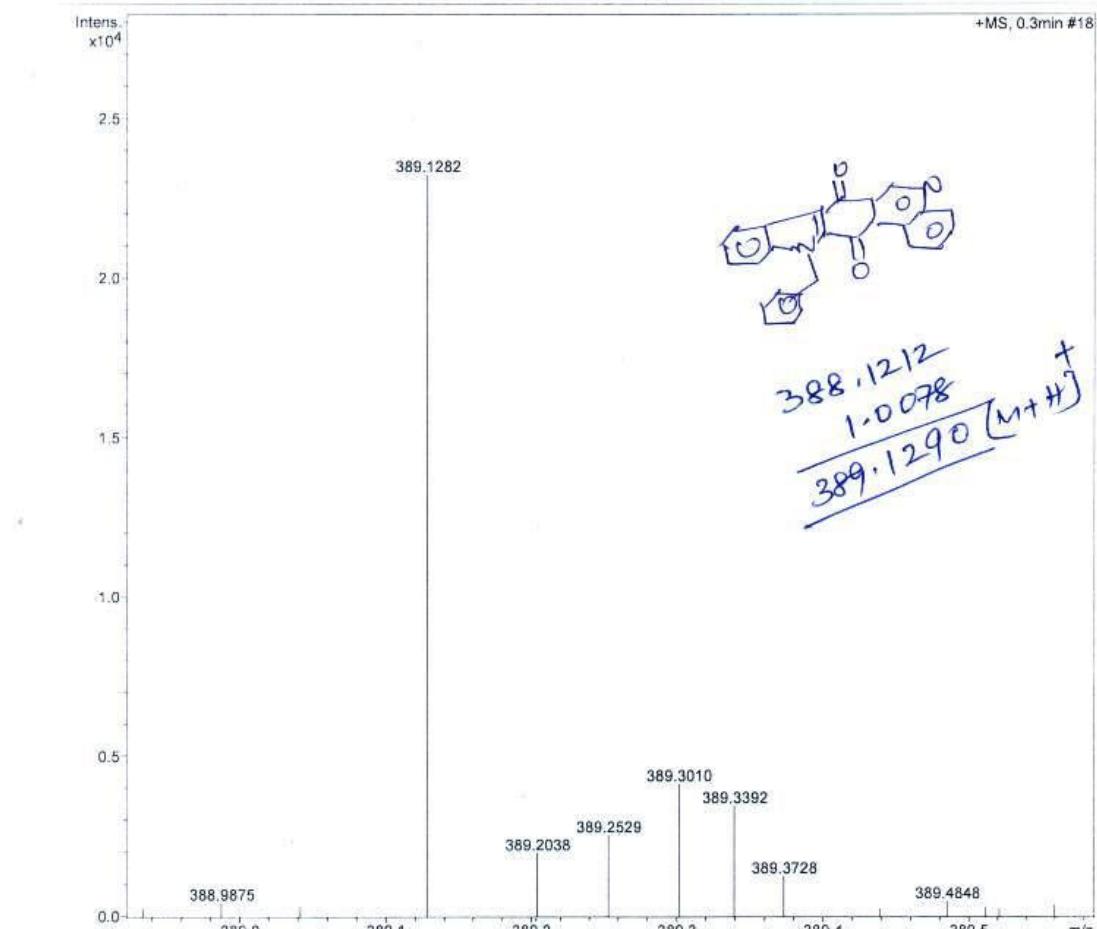
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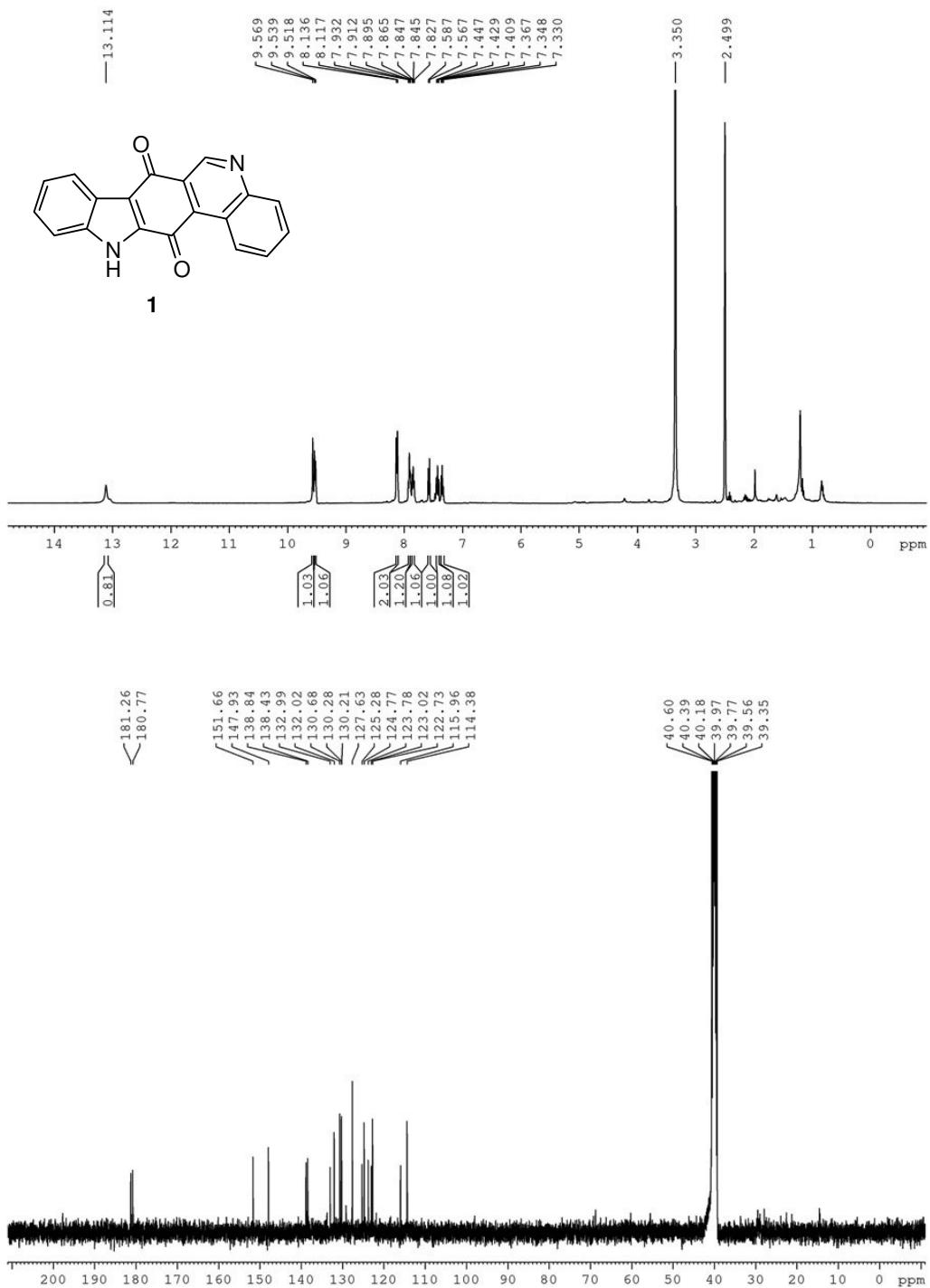
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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Scan End 1700 m/z	Set Collision Cell RF 150.0 Vpp	Set Divert Valve Waste



¹H and ¹³C NMR of 7*H*-indolo[3,2-*j*]phenanthridine-7,13(12*H*)-dione (1)



HRMS of 7H-indolo[3,2-j]phenanthridine-7,13(12H)-dione (1)

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Analysis Info

Analysis Name D:\Data\2015\DrNagarajan\JUNE\RKN-298.d
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Sample Name RKN-298
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Operator Ramu Sridhar
Instrument maXis 10138

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