Electronic Supplementary Information (ESI)

Cyclocondensation reactions of an electron deactivated 2-aminophenyl tethered imidazole with mono/1,2-biselectrophiles: Synthesis and DFT studies on rationalisation of imidazo[1,2-*a*]quinoxaline versus benzo[*f*]imidazo[1,5-*a*][1,3,5]triazepine selectivity switch

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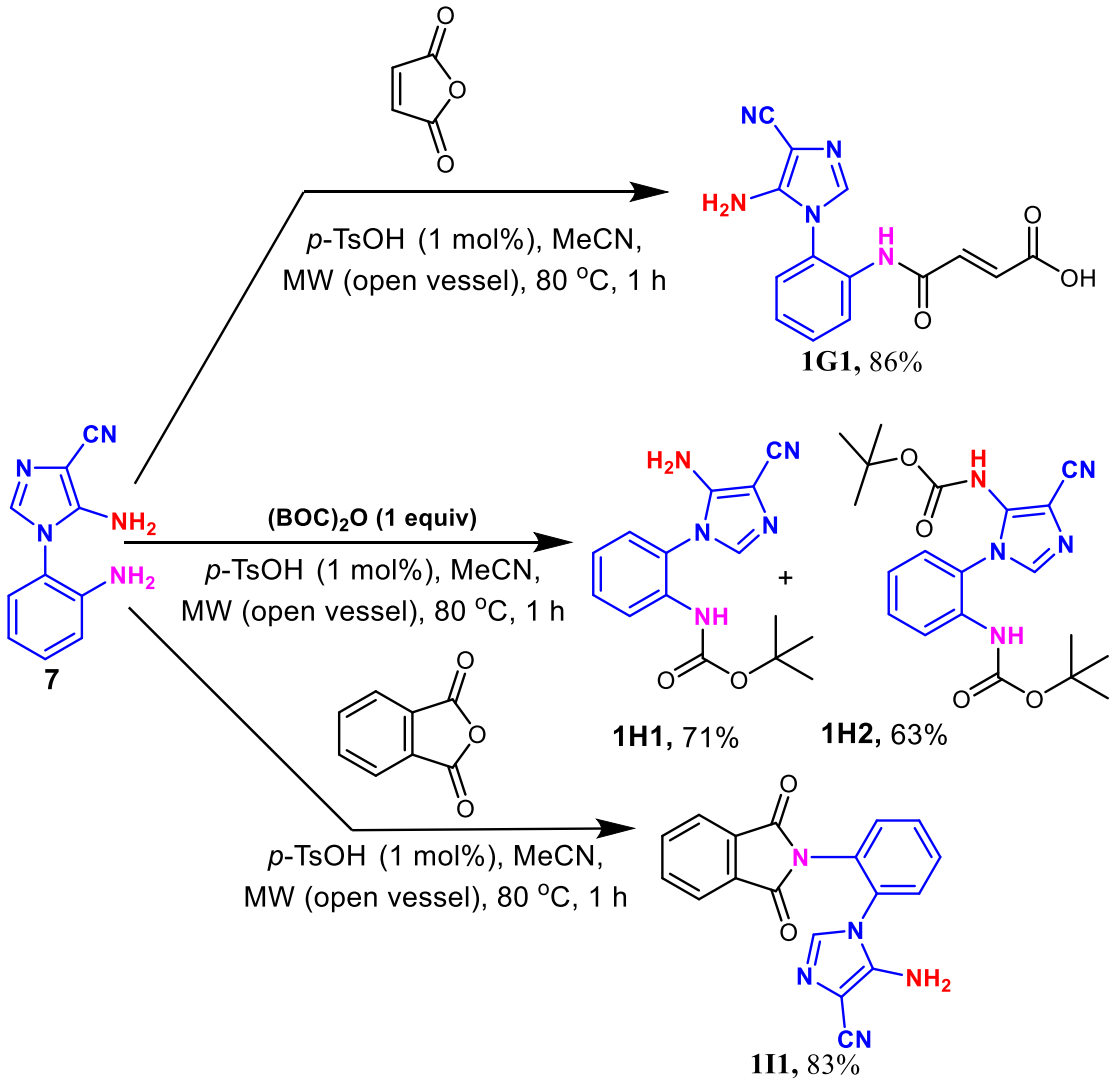
1. Reaction with anhydrides

Reaction of **7** with anhydrides such as acetic, maleic, phthalic and Boc_2O could only yield nucleophilic adducts and fail to afford corresponding PS products.



Scheme S1: Reactions of **7** with anhydrides

2. List of absolute Gibbs Free Energies

Table S1: Absolute Gibbs Free Energy (in Hartree) calculated at B3LYP/6-31+G(d) level of theory.

Cmpd. Code	Absolute Energy
7	-660.104414
CDI	-564.490620
Imidazole	-226.182059
Int-A	-998.425809
Int-A1	-998.779443
Int-A2	-998.393686
2A2	-772.262991
Ts2	-814.790496
Acetaldehyde	-153.809079
Water	-76.419139
Int-B	-815.206435
Int-C	-814.810353
Int-D	-814.813403
1-Me	-814.877372
Paratoluenesulphonic acid	-895.276532
Paratoluenesulphonate	-894.778770
TS1	-1075.148465

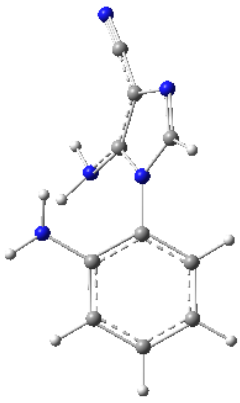
Cartesian Coordinates

List of Cartesian coordinates of all the optimized structures at B3LYP/6-31+G(d) level of theory

7

0 1

C	-3.20822500	-1.24882200	-0.77386600
C	-3.85861700	-0.07474000	-0.38166200
C	-3.14771800	0.95988800	0.22344300
C	-1.76769700	0.84625800	0.45480300
C	-1.11588600	-0.33189100	0.03712200
C	-1.83416300	-1.36710900	-0.56818800
H	-3.75922500	-2.05540200	-1.24760600
H	-4.92737300	0.03696000	-0.54302000
H	-3.66299800	1.86681100	0.53241300
H	-1.29836700	-2.25597300	-0.88883800
N	0.29071800	-0.48023900	0.24669000
C	1.30544000	0.27391200	-0.31496200
C	0.91226700	-1.51141900	0.94893200
C	2.48572900	-0.34191600	0.08955600

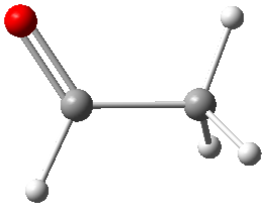


H	0.33153400	-2.23667600	1.50256400
N	2.21111400	-1.45744700	0.87196000
C	3.79023000	0.10283400	-0.24008400
N	4.83264900	0.52861100	-0.54461200
N	1.06128000	1.33360500	-1.16489200
H	0.36797600	1.99728100	-0.82236200
H	1.90949100	1.79761700	-1.47316300
N	-1.03263100	1.90361300	1.01742800
H	-1.60481500	2.59847900	1.48520900
H	-0.26628700	1.61193600	1.61821100

Acetaldehyde

0 1

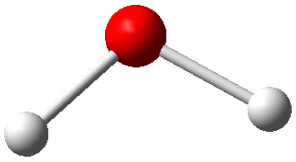
O	-1.23875100	-0.27749500	-0.00000400
C	1.17087300	-0.14860400	-0.00002700
H	1.71158200	0.22213000	0.88158300
H	1.16267900	-1.24152100	-0.00057800
H	1.71195100	0.22327700	-0.88089800
H	-0.31074700	1.50956800	0.00006800
C	-0.23178200	0.39968800	0.00000200



Water

0 1

O	0.00000000	0.00000000	0.11729100
H	0.00000000	0.77129900	-0.46916500
H	0.00000000	-0.77129900	-0.46916500



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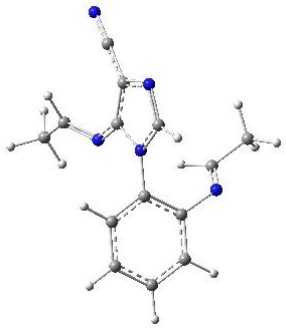

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C	0.33647100	0.93445100	-2.00354600
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N	-0.00665700	0.09794600	-0.96694000
C	-1.33440500	-0.33744100	-0.63609200
C	-2.18346300	0.49343000	0.12203600
C	-1.77861000	-1.57656100	-1.10771900
C	-3.49513400	0.05145400	0.36614000
C	-3.07197600	-2.01368400	-0.82932000
H	-1.09779300	-2.18805800	-1.69346200
C	-3.92839000	-1.19169400	-0.08792900
H	-4.16106200	0.70400400	0.92322700
H	-3.41093800	-2.97852500	-1.19491800
H	-4.94266500	-1.51679900	0.12846000
N	-1.80737300	1.77878200	0.55611100
N	1.62764700	1.14936600	-2.07375200
C	3.56201300	0.41571400	-0.74574200
N	4.69502000	0.40155400	-0.47328700
N	1.13865100	-1.03249100	0.81135000
C	-0.88968800	1.91945000	1.43205300
H	-0.39447300	1.04697800	1.88201700
C	-0.44308600	3.26894400	1.89841600
H	0.62797300	3.40215400	1.69535500
H	-1.00791100	4.06003100	1.39856700
H	-0.57113800	3.35713200	2.98568600
H	-0.41176500	1.34656200	-2.66679800
C	2.11600900	-1.81192600	1.09928800
H	2.96259800	-1.94700300	0.41401600
C	2.15475200	-2.57919700	2.37983400
H	2.25014100	-3.65468200	2.17762800
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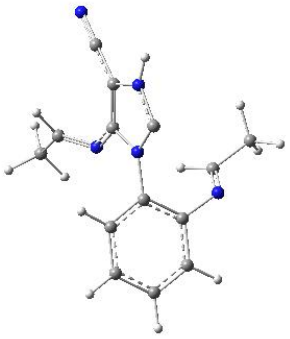
H	1.25441500	-2.39673600	2.97206100

INT_C



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C	-1.31227600	-0.31801800	-0.67724000
C	-2.16908400	0.51455800	0.06864700
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C	-3.47920600	0.06634000	0.31245200
C	-3.04424100	-2.00367000	-0.86551200
H	-1.07185300	-2.16576100	-1.73377900
C	-3.90656200	-1.18224500	-0.13114700
H	-4.15109600	0.72297200	0.85758200
H	-3.37833400	-2.97033500	-1.23127300
H	-4.92074500	-1.50918800	0.08350900
N	-1.81740000	1.80907400	0.49535900
N	1.65428400	0.95571800	-2.07466800
C	3.59926400	0.30632100	-0.66349300
N	4.74143800	0.32462000	-0.42323100
N	1.07456600	-0.91939300	0.91428500
C	-0.90298200	1.98202900	1.36669800
C	-0.49945200	3.34984000	1.82363100
H	0.56889900	3.51496100	1.62886500
H	-1.08391800	4.11768400	1.31011900
H	-0.64032500	3.44660500	2.90878200
C	1.93636400	-1.81833700	1.21656200
H	2.70650900	-2.13139300	0.49797300
C	1.93906900	-2.49190600	2.54856000
H	1.85436000	-3.57989700	2.42441400
H	2.89425400	-2.30832900	3.05933100
H	1.11774100	-2.12978900	3.17176700
H	2.19245400	1.46711700	-2.76040200
H	-0.37979300	1.12945500	1.82294700

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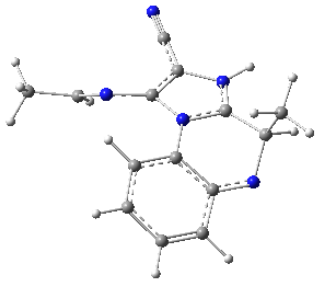

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N	-0.05607800	-0.30949800	0.24650300
C	-1.20489100	0.52602900	0.20127700
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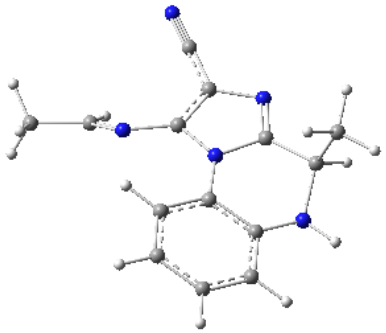
C	-1.19987600	1.85859000	0.64308100
C	-3.37190200	0.84458500	-0.83490800
C	-2.28489800	2.67351900	0.35855500
H	-0.35054400	2.24146500	1.19683600
C	-3.35756500	2.15548200	-0.40820400
H	-4.20572500	0.44549500	-1.40542800
H	-2.30147300	3.70115600	0.70900400
H	-4.19606100	2.80304000	-0.65617700
N	-2.39667200	-1.35978700	-0.85220800
C	-1.55552900	-2.26357800	-0.08579500
H	-1.45238600	-3.20523800	-0.64431400
C	-2.12805500	-2.60089900	1.31087800
H	-1.50905200	-3.34132600	1.83627100
H	-2.20790400	-1.70287400	1.93270700
H	-3.13427000	-3.01164900	1.17552500
N	1.01889800	-2.15376600	-0.25836500
C	3.36576500	-1.40364200	-0.24436400
N	4.50686600	-1.62661100	-0.33571400
N	1.78513100	1.26813800	0.46864400
C	2.71225500	1.78925300	-0.24914600
H	3.06634000	1.29305600	-1.16341100
C	3.34641300	3.09081200	0.10579800
H	4.42733500	2.95398400	0.24612300
H	3.22549800	3.80633900	-0.71869800
H	2.91062500	3.50459700	1.01819100
H	1.21087900	-3.13894500	-0.38077300

1-Me



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C	-0.14259200	-1.61602200	-0.14294900
C	1.95451400	-1.21925200	-0.06363900
C	1.33732100	0.02842800	0.04141000
N	-0.02483500	-0.24812600	0.01392700
C	-1.16611700	0.60901500	0.03459800
C	-2.37771100	0.03604800	-0.41666900
C	-1.12445100	1.93442500	0.47349000
C	-3.52722800	0.84031700	-0.44437600
C	-2.28011700	2.71689400	0.43897700
H	-0.18672100	2.34408900	0.82587600
C	-3.47805100	2.16972400	-0.02922600
H	-4.46232200	0.41029300	-0.79716100
H	-2.23951100	3.74790700	0.77739400
H	-4.38110500	2.77339800	-0.06126500
N	-2.38770600	-1.28334700	-0.87257200
C	-1.49760800	-2.25539200	-0.22024900
H	-1.40774800	-3.12060700	-0.88441000
C	-1.99975600	-2.73054800	1.15872500
H	-1.29832900	-3.45418600	1.58750700
H	-2.10184000	-1.88957900	1.85370000
H	-2.97790900	-3.21707100	1.05778000
H	-3.31714900	-1.64590700	-1.05339100
N	1.01495300	-2.22615100	-0.17820900
C	3.34876600	-1.48382300	-0.00487700
N	4.49713800	-1.67692100	0.04443600
N	1.82918500	1.30332400	0.24672600
C	2.92650700	1.65946900	-0.31491300
H	3.44367100	1.00205200	-1.02541400
C	3.56121300	2.98142000	-0.03478700
H	4.56215700	2.83139500	0.39257800
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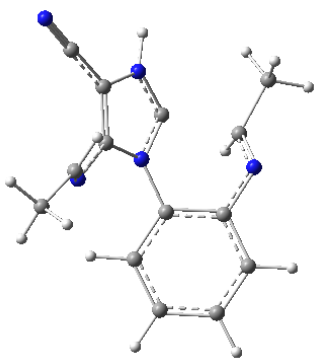
TS_2



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C	0.13207100	1.67303700	-0.68723800
C	-2.02828500	1.08334000	-0.23602100
C	-1.28961700	-0.08018000	-0.31229100
N	0.02573500	0.30308900	-0.60216900
C	1.17463800	-0.54675100	-0.45378300
C	2.23110800	-0.07219600	0.37817400
C	1.19490200	-1.83061800	-1.00639700
C	3.25468500	-0.99120200	0.69751600
C	2.24977800	-2.69265200	-0.71416400
H	0.38380000	-2.15087200	-1.65089300
C	3.26783500	-2.27123200	0.15505100
H	4.04748900	-0.65403500	1.35913200
H	2.27469500	-3.68567600	-1.15363200
H	4.08512800	-2.94651200	0.39736000
N	2.19679600	1.20292900	0.89571000
N	-1.11919900	2.12510400	-0.46040500
C	-3.41355000	1.27147500	-0.05331800
N	-4.55629300	1.45290600	0.09665300
N	-1.69111400	-1.39667600	-0.24245700
C	1.97760100	2.17186700	0.01673500
C	1.85363600	3.58940300	0.52405100
H	1.42445000	4.24893400	-0.23802800
H	1.24704800	3.62786700	1.43422500
H	2.85463700	3.96542000	0.77115900
C	-2.45584400	-1.77614800	0.71279300
H	-2.72704100	-1.08926500	1.52684700
C	-3.00744400	-3.16028700	0.78091400
H	-2.70931500	-3.63896300	1.72325500
H	-4.10531600	-3.12430800	0.77992600
H	-2.66163100	-3.76259400	-0.06242800
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CDI

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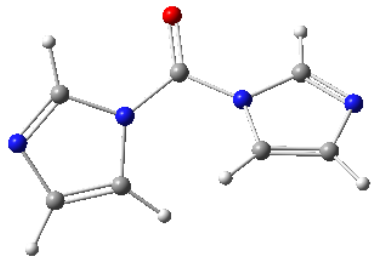

C	-2.41350300	0.71106400	0.41197800
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N	-1.19144600	0.19511400	-0.00856700
H	-2.48289200	1.69955600	0.84285000
H	-3.40611300	-2.10821200	-0.64186700
H	-0.70180700	-1.69685300	-0.96964600
N	-3.38657000	-0.13712000	0.23157000
C	-0.00001400	0.94298000	-0.00008900
O	0.00000700	2.15403500	-0.00022300
N	1.19148800	0.19512500	0.00861900
C	2.41355700	0.71113200	-0.41175600
C	1.46390300	-1.08276300	0.51766500
H	2.48291600	1.69971400	-0.84241400
C	2.80820000	-1.25268600	0.35937300
H	0.70178500	-1.69664100	0.96995700
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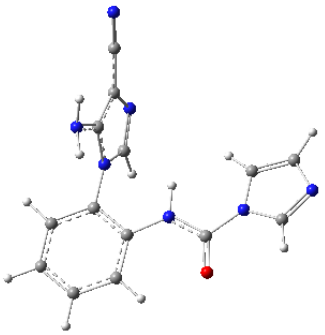
INT_A



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C	-2.18406400	3.64956400	0.09388000
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C	-0.09425800	1.75396800	0.05590500
C	-1.43412900	1.35839700	0.27536300
C	-2.46546600	2.29856700	0.29345000
H	-2.98580800	4.38146700	0.10854200
H	-0.62719400	5.09442600	-0.27519400
H	1.20022700	3.43238900	-0.31435600
H	-3.48112400	1.95428900	0.46495300
N	-1.73351200	-0.02754000	0.48514300
C	-2.17094200	-0.92714400	-0.46723000
C	-1.62520400	-0.74133000	1.68227100
C	-2.29308400	-2.14190800	0.20050600
H	-1.30749500	-0.25499600	2.59489800
N	-1.94795200	-1.99428600	1.53950000
C	-2.70987600	-3.36066000	-0.38991400
N	-3.05246700	-4.32763800	-0.94430900
N	-2.48016600	-0.55828600	-1.75583400
H	-1.95570600	0.21500800	-2.14935900
H	-2.59536800	-1.33058100	-2.40233600
N	0.88866000	0.74548700	0.05717700
H	0.53995100	-0.19021400	0.21937800
C	4.28044200	-0.46559300	-0.43218800
C	3.69529100	-2.36327400	0.37891200
C	2.59331100	-1.56788700	0.51372600
N	2.96550400	-0.32519800	-0.01314200
H	4.81065100	0.35903300	-0.88532600
H	3.80669800	-3.39603400	0.67952100
H	1.63211400	-1.76315800	0.96581400
N	4.73781000	-1.66965600	-0.21479600
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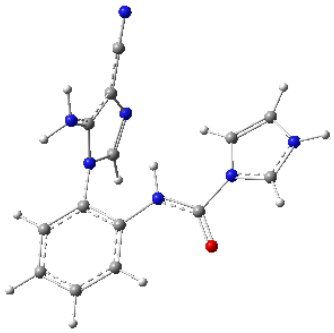
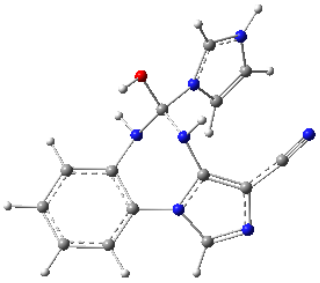
INT_A1



1 1

C	4.26771400	-1.24261300	0.07973800
C	3.53833800	-2.39542000	-0.21605700
C	2.14222700	-2.36866100	-0.29204700
C	1.47311200	-1.16426000	-0.06357400
C	2.20847400	0.00330900	0.23985600
C	3.59806200	-0.03682400	0.30900300
H	5.35102900	-1.27856800	0.13697800
H	4.05524900	-3.33373000	-0.39310700
H	1.58471500	-3.26783100	-0.52123200
H	4.14243900	0.87024600	0.55535300
N	1.47578500	1.20903800	0.50035700
C	0.90233300	2.02277800	-0.46453200
C	0.82400700	1.50391600	1.70134700
C	-0.07009900	2.75993100	0.20426300
H	1.10209800	1.01123400	2.62348400
N	-0.09580400	2.41402100	1.55382400
C	-0.94201900	3.70863600	-0.38795300
N	-1.65745500	4.44687200	-0.93678800
N	1.22153300	1.92165800	-1.79995100
H	2.19456500	1.72985700	-2.01638700
H	0.84509000	2.66762000	-2.37661700
N	0.05805300	-1.02129700	-0.11245100
H	-0.26600800	-0.06345200	-0.18406700
C	-3.30379600	-2.18971100	-0.35321600
C	-4.06460100	-0.24653200	0.42425400
C	-2.70582000	-0.22130500	0.50405000
N	-2.24849800	-1.44279000	0.00556400
H	-3.24444800	-3.19012300	-0.75638900
H	-4.80284100	0.48905200	0.70661000
H	-2.05278600	0.54251400	0.90445700
N	-4.40573700	-1.47835100	-0.11152500
C	-0.87002500	-1.99462600	-0.11067300
O	-0.74765600	-3.19389900	-0.19034400
H	-5.35042000	-1.80139000	-0.29628900

INT_A2



1 1

C	4.25346800	-1.49555700	-0.17278000
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C	1.89290000	-0.93319800	-0.25495000
C	2.23357200	0.42600400	-0.11169900
C	3.56827500	0.81404800	0.02230200
C	4.57975400	-0.14564700	-0.02301600
H	5.03576500	-2.24786500	-0.20018300
H	2.66553400	-2.93850600	-0.38765100
H	3.80914900	1.86278000	0.16800100
H	5.61656300	0.16099300	0.07260100
N	0.53340800	-1.32389100	-0.49647100
N	1.19331400	1.39321700	-0.10225400
C	-0.03115300	1.19245000	0.48959400
C	1.13123100	2.64047300	-0.69748200
H	1.95440600	3.04218300	-1.27217500
N	-0.28091800	0.03418800	1.23176500
H	-0.94673100	0.15755000	1.98957100
C	-0.45638000	-1.20484100	0.53341100
O	-0.55362700	-2.25618400	1.45401000
H	0.47634100	-2.24145400	-0.93121300
C	-0.77542300	2.32982400	0.22859000
N	-0.02509000	3.22644100	-0.50568600
C	-2.13076500	2.50414900	0.62098200
N	-3.24540200	2.50744100	0.95939400
H	0.21682300	-2.21259600	2.04894000
N	-1.80678500	-1.28632400	-0.16788700
C	-2.92338100	-1.79900300	0.36796200
C	-2.12753600	-0.65208500	-1.36120100
H	-2.98328600	-2.34911500	1.29376300
C	-3.47065400	-0.79784700	-1.54370300
H	-1.37803500	-0.16700100	-1.96466500
H	-4.12096200	-0.45653900	-2.33438200
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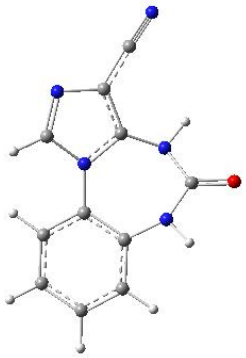
H	-4.90198900	-1.78304400	-0.29594200

2A2



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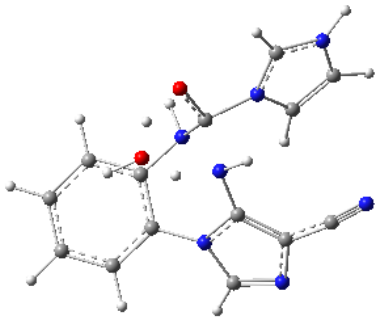
C	3.94044800	-0.18084400	-0.16778300
C	3.06471700	0.84490000	0.18084400
C	1.68348800	0.61833500	0.26810900
C	1.19356000	-0.66882600	-0.00969700
C	2.07078400	-1.68638700	-0.40359700
C	3.44214400	-1.45086700	-0.47041300
H	5.00664800	0.01876000	-0.22126300
H	3.44779100	1.84044500	0.39157800
H	1.67035800	-2.66176500	-0.66141400
H	4.11244100	-2.25068000	-0.76991400
N	0.83878500	1.67929700	0.68050300
N	-0.19047800	-0.95476000	0.12974600
C	-1.23879400	-0.11481800	-0.16193500
C	-0.76125000	-2.15469400	0.53483400
H	-0.15650200	-2.98093300	0.88017300
N	-1.06291800	1.18080500	-0.63789200
H	-1.88669100	1.59366000	-1.06527200
C	-0.28619800	2.15002800	0.00452000
O	-0.57661000	3.33227500	-0.02557500
H	1.32891800	2.46134400	1.10170500
C	-2.39184100	-0.85254200	0.05791700
N	-2.06473200	-2.12709900	0.49064900
C	-3.72150900	-0.39538700	-0.13832700
N	-4.78971000	0.03141000	-0.32269600

TS-1



1 1

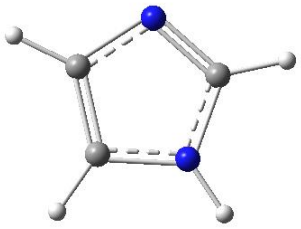
C	4.16797700	-1.33397600	-0.65558100
C	2.83137000	-1.71844900	-0.77842400
C	1.79820000	-0.78229400	-0.62824500
C	2.14626800	0.55033600	-0.32463800
C	3.48184300	0.93106800	-0.16880800
C	4.49595800	-0.01006800	-0.34791700
H	4.95236400	-2.07247900	-0.79197800
H	2.58075400	-2.75047900	-1.01147400
H	3.71977700	1.95882200	0.08995500
H	5.53392600	0.28850500	-0.23973600
N	0.43590100	-1.13051800	-0.87520900
N	1.10301700	1.50850000	-0.19130600
C	-0.09542200	1.26098300	0.42592000
C	1.00446800	2.78695700	-0.71253000
H	1.80541200	3.23136900	-1.28714900
N	-0.32227400	0.04590600	1.11229200
C	-0.48102000	-1.27321200	0.26910200
O	-0.40264700	-2.30411000	1.04086800
H	0.39468300	-2.01333100	-1.38235800
C	-0.86321700	2.40002400	0.26263900
N	-0.15170400	3.34390500	-0.44917700
C	-2.19533600	2.54672400	0.73718400
N	-3.28547900	2.53336700	1.14681600
N	-1.88780800	-1.20872600	-0.36395400
C	-2.90137600	-1.93862500	0.11152800
C	-2.34479900	-0.42785700	-1.41658500
H	-2.82100400	-2.65118100	0.91836500

C	-3.67359900	-0.69594800	-1.56682600
H	-1.68911800	0.22875400	-1.96410000
H	-4.40464100	-0.30523000	-2.25801800
N	-3.99223000	-1.63781200	-0.60367800
H	-4.90869500	-2.04664500	-0.45656600
H	-1.16594300	0.13548600	1.68582300
H	0.59895600	-0.40687400	2.04148300
O	1.05960000	-1.22942500	2.72974300
H	2.02834300	-1.29930000	2.64668200
H	0.59571900	-1.98545700	2.17276900

Imidazole

0 1

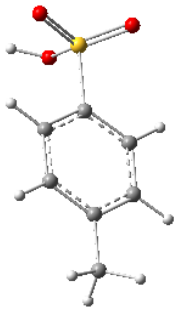
C	0.98904600	-0.54376300	-0.00009300
C	-1.13941200	-0.28077000	-0.00001000
C	-0.61015600	0.98797400	0.00007200
N	0.75913800	0.80523700	0.00005900
H	1.45995600	1.53313000	0.00018300
H	1.98619100	-0.96333400	-0.00016300
H	-2.18194900	-0.56827000	-0.00002400
H	-1.06120400	1.96929000	0.00013800
N	-0.13626000	-1.22687500	-0.00005100



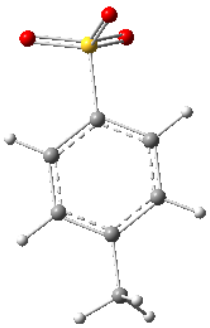
Paratoluenesulphonic acid

0 1

C	1.95974900	-1.20145100	0.00897200
C	2.67592500	0.00733300	0.00988500
C	1.95587400	1.20955300	-0.04566300
C	0.56072500	1.21671900	-0.08981400
C	-0.12053600	-0.00117700	-0.08157600
C	0.56751100	-1.21703200	-0.03872600
H	2.50023300	-2.14481600	0.03771300
H	2.49182400	2.15547700	-0.06269900
H	0.01065500	2.15031100	-0.15139700
H	0.02050500	-2.15411500	-0.05548100
C	4.18463100	0.00569700	0.08081600
H	4.52805700	-0.22307700	1.09844300
H	4.61512800	-0.75153900	-0.58426400
H	4.60081400	0.97900800	-0.19779700
S	-1.90673500	-0.01155600	-0.13194000
O	-2.38367400	1.29701600	-0.58729700
O	-2.35450300	-1.25959600	-0.73245700
O	-2.31075600	-0.12592200	1.46843300
H	-2.57127100	0.76380800	1.77371100



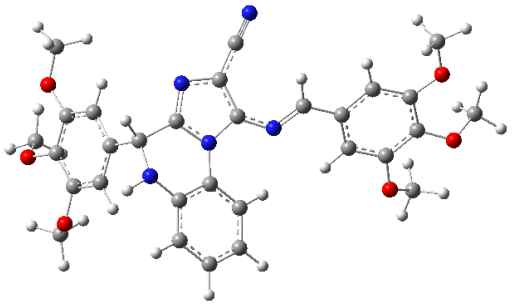
Paratoluenesulphonate



-1 1

C	1.94479900	1.20509700	0.00005600
C	2.66231500	0.00337200	0.00006900
C	1.93340600	-1.19890600	0.00005300
C	0.53923000	-1.19655300	0.00000400
C	-0.16429300	0.01413000	-0.00003000
C	0.54369900	1.21451400	0.00000600
H	2.48651300	2.15099100	0.00009000
H	2.46853600	-2.14888200	0.00008900
H	-0.01460400	-2.13119400	-0.00000700
H	-0.01401800	2.14631200	-0.00000400
C	4.17608200	-0.00966500	-0.00007900
H	4.57722400	-0.52462800	-0.88415900
H	4.58155800	1.00908000	0.00161400
H	4.57737400	-0.52766200	0.88214400
S	-1.99327200	0.00042600	-0.00001000
O	-2.34929000	-0.73188600	1.25090300
O	-2.37410700	1.44300400	-0.00048300
O	-2.34931100	-0.73271400	-1.25042900

1-Me1



Absolute energy: -1885.227952

C	1.70832200	0.89646300	-1.63181500
C	0.07221500	2.12445000	-1.01758600
C	-0.40631600	0.81053800	-0.95484100
N	0.67916900	0.02562000	-1.34051400
C	0.79352700	-1.37914500	-1.56786600
C	1.91104200	-1.79603800	-2.32639500
C	-0.13038300	-2.31296400	-1.09242500
C	2.05008600	-3.16190400	-2.61769400
C	0.02895500	-3.66766700	-1.38762200
H	-0.97326600	-1.96782200	-0.50921300
C	1.11634800	-4.08820800	-2.15832500
H	2.90312500	-3.48990700	-3.20817600
H	-0.69718900	-4.38531300	-1.01785400
H	1.24603200	-5.14051300	-2.39667600
N	2.81479800	-0.85298000	-2.81545300
C	3.05119100	0.38357200	-2.07429800
H	3.44449800	1.12268300	-2.78099800
H	3.65052900	-1.24965300	-3.22878600
N	1.38607400	2.15166800	-1.44246300
C	-0.62141400	3.30638000	-0.64823700
N	-1.20299900	4.27023500	-0.34421600
N	-1.59277300	0.26249400	-0.53622700
C	-2.69680600	0.91181100	-0.70051200
H	-2.72323900	1.85620200	-1.25679000
C	-3.97846200	0.44612400	-0.18232200
C	-5.12595100	1.21258000	-0.46387600
C	-4.09188800	-0.72047300	0.58096600
C	-6.37407800	0.80143300	0.00048400
H	-5.02629800	2.11498000	-1.05654100
C	-5.33580300	-1.13384600	1.06094500
H	-3.21594100	-1.31267100	0.81919900
C	-6.49437600	-0.37734900	0.77792900
C	4.04836300	0.27954700	-0.90579200
C	4.52347100	-0.94130200	-0.44391700
C	4.48989200	1.47035200	-0.30686300
C	5.44018100	-0.99634800	0.62080300
H	4.19866800	-1.88408900	-0.86904200
C	5.40784200	1.42645000	0.74164200
H	4.10576300	2.41797400	-0.66656000
C	5.89217600	0.18524300	1.22768900
O	-5.35254300	-2.32054700	1.73826100

O	-7.71146100	-0.86724900	1.16310100
O	-7.54411600	1.45112800	-0.27242000
O	5.88625900	-2.24924000	0.94368800
O	6.87910700	0.12655100	2.18187200
O	5.92655200	2.53588600	1.34652600
C	5.51736500	3.81830300	0.88022200
H	5.78826700	3.96043800	-0.17346500
H	4.43725900	3.96272600	1.00543400
H	6.05771600	4.53955200	1.49570900
C	6.55576200	0.61435200	3.49140800
H	6.33974600	1.68522300	3.47311800
H	5.69704500	0.06815400	3.90448900
H	7.43952000	0.42340600	4.10473800
C	6.06391700	-2.61915700	2.31416300
H	6.06317100	-3.71196400	2.32189400
H	7.00907600	-2.24247100	2.71132700
H	5.22967600	-2.25283400	2.92590500
C	-6.13742400	-2.46149500	2.92762600
H	-7.18033500	-2.68486500	2.69271900
H	-5.68950100	-3.29567500	3.47302700
H	-6.07865300	-1.55465600	3.54254400
C	-8.52866400	-0.05796200	2.02420600
H	-8.87525900	0.84126900	1.51127600
H	-9.37911500	-0.68729500	2.29505900
H	-7.97207200	0.21845600	2.92914000
C	-7.50190900	2.61166200	-1.09746300
H	-7.10074100	2.37590500	-2.09105300
H	-8.53770500	2.94144900	-1.19226000
H	-6.90413500	3.40743900	-0.63568800

3. X- Ray Crystallography data

Manuscript Text:

Single crystal X-ray analysis confirmed the structure of the compound 1-amino-4-(3,4,5-trimethoxyphenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (**1A2**). Figure S1 represents an ORTEP diagram drawn with 50% probability displacement ellipsoids with atomic labeling.

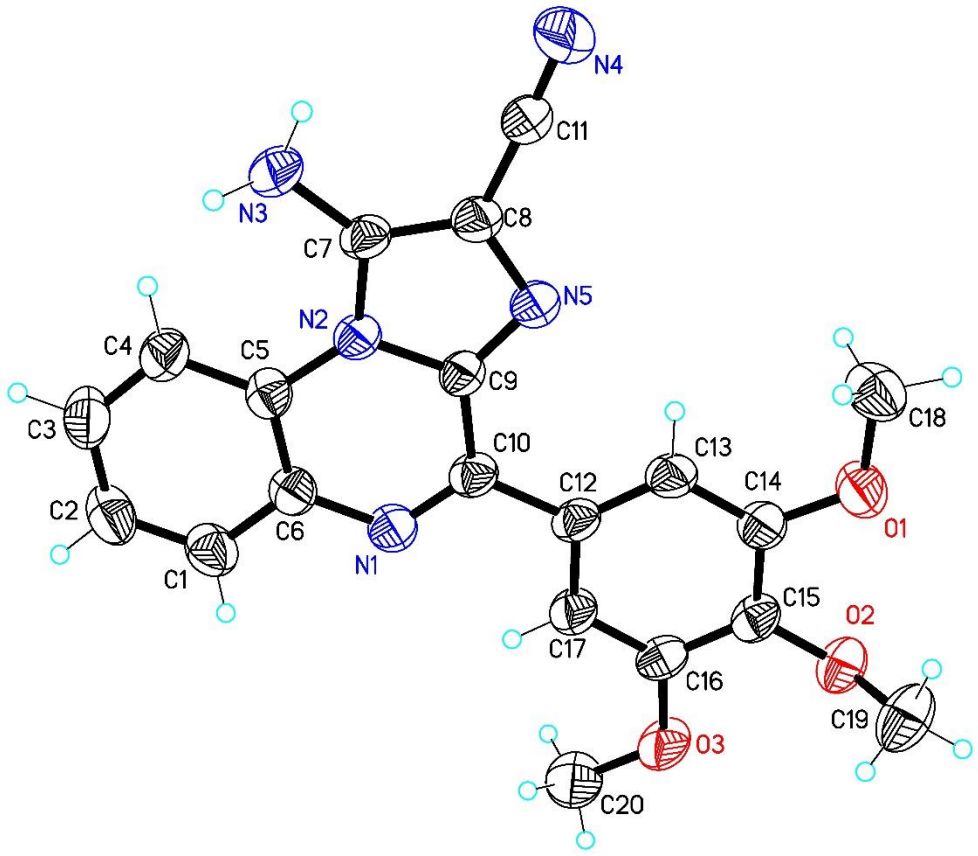


Figure S1: ORTEP diagram for **1A2**

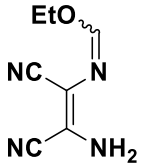
4. Experimental

General considerations: All the reagents were purchased from commercial suppliers. Biotage® Initiator microwave synthesizer (Company: Biotage® Model No. 355301 (Initiator EXPEU)) (used for sealed reactions) and Discover System; Company: CEM; Model No. 908010; Serial No. DU9671) (used for open reflux reactions) were used for carrying out microwave reactions at 200 W power. ^{1}H NMR and ^{13}C NMR spectra were obtained in $CDCl_3$/d_6-DMSO on 400 MHz and 100 MHz Bruker Advance II NMR spectrometer, respectively using TMS ($\delta = 0$) as an internal standard. The physical data of intermediates and final compounds are presented as below:

Synthesis

***N*-(2-amino-1, 2-dicyano-vinyl)-formimydic acid ester (9)**

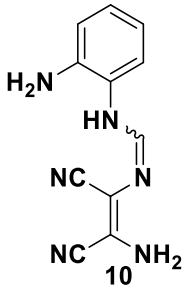
To the reaction mixture of 2,3-diaminomaleonitrile (3 g, 27.75 mmol) in 1,4-dioxane (20 ml), was added $CH(OEt)_3$ (4.5 mL). The mixture was heated at 80 ºC for 6 h (TLC). The reaction mixture was evaporated using rotary evaporator, dark brown solid was extracted with diethyl ether (6 X 20 mL) and kept overnight. Yellow needles (**9**) were formed which were used for next step without further purification. Yield: 81 %; Color: Yellow; m.p: 135 °C (reported 134 - 136 °C)[1] .



9

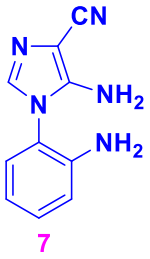
***N*-(2-amino-1,2-dicyano-vinyl)-*N*'-(2-amino-phenyl)formimidine (10)**

To a suspension of **9** (3 g, 21.42 mmol) in methanol (1.5 mL) added *o*-phenylenediamine (1.85 g, 17.14 mmol) and aniline hydrochloride (2.7 mg, 0.021 mmol). The reaction mixture was stirred for 12 h at rt. The precipitate so obtained was filtered, washed with diethyl ether and dried to afford **10**. Yield: 83 %; Color: Brown; m.p: 118 -120 °C.



10

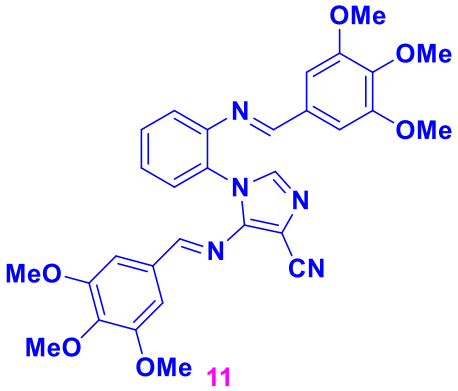
5-Amino-1-(2-amino- phenyl)-1*H*-imidazole-4-carbonitrile (7)



7

To a suspension of **10** (1 g, 4.42 mmol)**,** in water (1 mL) added 1 M aqueous KOH solution (15 mL) which was stirred for 12 h at rt (TLC). The mixture was extracted with EtOAc (10 mL × 3). Organic layer was washed with water, brine, dried over anhydrous Na_2SO_4 and concentrated under vacuum using rotary evaporator to afford the crude product 5-Amino-1-(2-amino-phenyl)-1*H*-imidazole-4-carbonitrile **(7)**. The crude product was recrystallized from EtOAc. Yield: 89 %; Color: Yellowish solid; m.p: 196 - 198 $^{\circ}$C. IR (KBr, cm^{-1}): 3334 (NH_2 stretch), 2211 (CN stretch), 1577 (NH_2 bend). ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.20 - 7.16 (2H, m), 7.00 (1H, d, *J* = 7.32 Hz), 6.85 (1H, d, *J* = 7.92 Hz), 6.66-6.62 (1H, t, *J* = 7.32 Hz), 5.86 (2H, s, NH_2), 5.13 (2H, s, NH_2). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 147.79, 144.72, 132.85, 130.30, 128.42, 118.10, 117.54, 116.54, 116.38, 90.38. HRMS (TOF-ESI) Calcd for $C_{10}H_9N_5$, 199.2200 $[M]^+$; observed: 199.9258 $[M+H]^+$.

5-(((*Z*)-3,4,5-trimethoxybenzylidene)amino)-1-(2-(((*E*)-3,4,5-trimethoxybenzylidene)amino)phenyl)-1*H*-imidazole-4-carbonitrile (11)

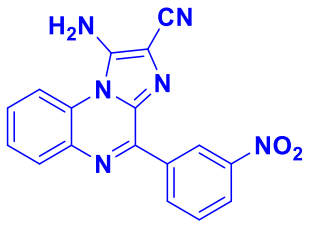


11

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3,4,5-trimthoxybenzaldehyde (199.9 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was stirred 1 h. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 94 %; Color: Yellowish solid; m.p: 181- 183 $^{\circ}$C; IR (KBr, cm^{-1}): 3665 (NH stretch), 2075 (CN stretch), 1454 (C=N).^{1}H NMR (400 MHz,

$CDCl_3$, TMS = 0) δ: 8.59 (1H. s), 8.16 (1H, s), 7.68 (1H, s), 7.53 - 7.47 (2H, m), 7.41 - 7.38 (1H, dd, *J*= 4 Hz), 7.17 (1H, d, *J* = 4 Hz), 6.77 (4H, d, *J* = 4 Hz), 3.90 (3H, s), 3.89 (3H, s), 3.82 (6H, s), 3.79 (6H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 163.13, 161.46, 153.43, 153.32, 148.94, 147.31, 142.08, 141.44, 137.88, 130.82, 130.56, 130.42, 128.22, 127.19, 129.22, 119.08, 116.04, 106.16, 105.69, 61.00, 56.16, 56.14.MS (ESI): m/z: 556.21 $[M+H]^+$. HRMS (TOF-ESI) Calcd for $C_{30}H_{29}N_5O_6$, 555.2118$[M]^+$; observed: 578.2002 $[M+Na]^+$.

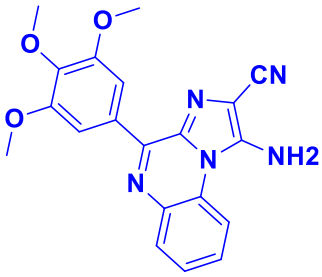
1-amino-4-(3-nitrophenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1A1)



1A1

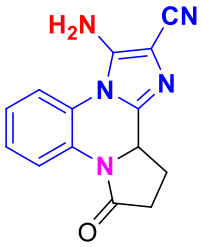
To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3-nitrobenzaldehyde (75.9 mg, 0.502 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 89 %; Colour: Yellow; m.p: 312 ºC (decomposed).IR (KBr, cm^{-1}): 3328 (NH_2 stretch), 2230 (CN stretch), 1455 (NO_2 Symmetric stretch), 1350 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.38 (1H, s), 8.99 (1H, d, *J* = 8 Hz), 8.61 (1H, d, *J* = 8 Hz), 8.39 (1H, d, *J* = 8 Hz), 8.03 (1H, d, *J* = 8 Hz), 7.84 (1H, m), 7.64 (2H, t, m), 7.00 (2H, s, NH_2).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 148.11, 146.93, 145.44, 136.81, 135.98, 135.90, 132.28, 130.34, 130.24, 128.99, 127.98, 127.48, 125.57, 124.20, 116.35, 116.00, 100.00. HRMS (TOF-ESI) Calcd for $C_{17}H_{10}N_6O_2$, 330.0865$[M]^+$; observed: 353.0762$[M+Na]^+$.

1-amino-4-(3,4,5-trimethoxyphenyl)imidazo[1,2-a]quinoxaline-2-carbonitrile (1A2)



To a reaction mixture of **4** (100 mg, 0.502 mmol,) in 1,4-dioxane (1 mL) was added 3,4,5-trimethoxybenzaldehyde (136.5 mg, 0.693 mmol) using *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from the reaction mixture, concentrated under vacuum using rotary evaporator, extracted with ethyl acetate, dried and purified via flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5). Yield: 84 %; Colour: brownish Solid, mp:211-213 ºC. IR (KBr, cm-1) 3318 & 3245 (NH_2 stretch), 2957 (sp^3 hybz C-H stretch), 2216 (CN stretch), 1220 (C-O stretching). ^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 8.53 (1H, d, *J* = 4), 8.14 (1H, d, *J* = 8), 7.96 (2H, s), 7.64-7.60 (2H, m), 4.53 (2H, s; D_2O exchangeable NH_2), 4.03 (6H, s), 3.94 (3H, s). ^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 153.02, 149.63, 142.20, 140.67, 136.57, 133.59, 130.83, 130.40, 128.14, 127.53, 127.45, 114.82, 107.20, 104.19, 61.09, 56.39. HRMS (TOF-ESI) Calcd for $C_{20}H_{17}N_5O_3$, 375.1331$[M]^+$; observed: 376.1349$[M+H]^+$.

3-amino-10-oxo-10,11,12,12a-tetrahydroimidazo[1,2-a]pyrrolo[2,1-c]quinoxaline-2-carbonitrile

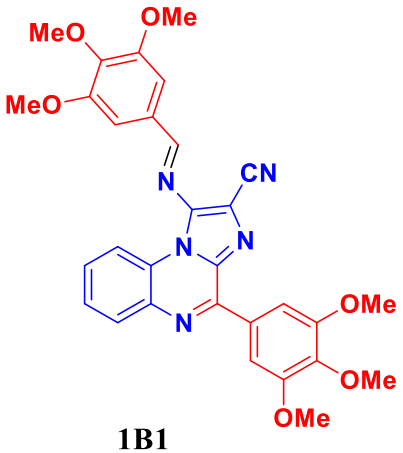


1A3

To a reaction vial, a suspension of **7** (200 mg, 1.005 mmol) in methanol (1 mL) was added Methyl 4-oxobutanoate (116.58 mg, 1.005 mmol) and *p*-TsOH (1mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with ethyl acetate (10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 4 : 6). Yield: 82 %; Colour: Brown; m.p: 202 - 204 ºC**.** IR (KBr, cm-1) 3420 & 3215 (NH_2 stretch), 2979 (sp^3 hybz C-H stretch), 2207 (CN stretch), 1692 (C=C stretch), 1645 (C=O stretch), 1215 (C-O stretching). ^{1}H NMR (400 MHz, d_6-DMSO, TMS = 0) δ: 8.01 (1H, d, *J* = 8.02 Hz), 7.93 (1H, d, *J* = 7.96 Hz), 7.35-7.27 (2H, m), 6.37 (2H, s), 4.87-4.83 (1H, t, *J* = 4.85 Hz), 2.69-2.28 (3H, m). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 173.39, 146.78, 141.11, 128.22,

126.87, 126.72, 125.92, 122.14, 118.46, 117.02, 93.76, 53.84, 30.99, 21.85. HRMS (TOF-ESI) Calcd for $C_{14}H_{11}N_5O$, 265.0964 $[M]^+$; observed: 266.1144 $[M+H]^+$.

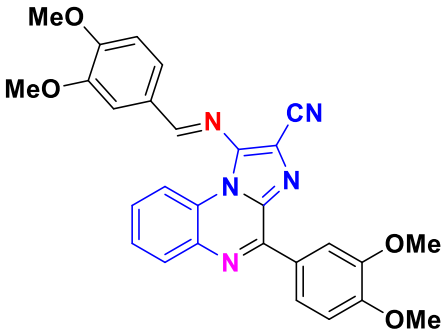
(*E*)-1-((3,4,5-trimethoxybenzylidene)amino)-4-(3,4,5-trimethoxyphenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1B1)



1B1

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3,4,5-trimthoxybenzaldehyde (199.9 mg, 1.004 mmol) and *p*-TsOH (1mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with ethylacetate(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2.5 : 7.5).Yield: 93 %; Colour: yellow; m.p: 142 - 144 ºC**.** IR (KBr, cm^{-1}): 2227 (CN stretch), 1575 (C=N stretch), 1501 (C=C stretch) and 1127 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 8.98 (2H, s), 8.12 - 8.09 (1H, dd, *J* = 4 Hz), 8.03 (2H, s), 7.64 - 7.55 (2H, m), 7.28 (2H, d, *J* = 8 Hz), 4.00 (15H, s), 3.94 (3H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 164.11, 153.74, 152.93, 149.02, 144.79, 143.14, 140.71, 136.87, 135.66, 130.31, 130.13, 130.07, 128.63, 127.50, 117.83, 115.56, 107.27, 106.93, 104.03, 61.19, 60.95, 56.36, 56.27. HRMS (TOF-ESI) Calcd for $C_{30}H_{27}N_5O_6$, 553.1961$[M]^+$; observed: 375.2598 $[M- C_{10}H_{12}O_3]^+$.

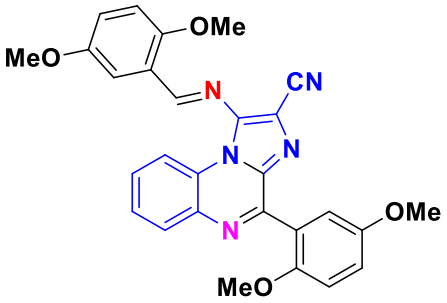
(*E*)-1-((3,4-dimethoxybenzylidene)amino)-4-(3,4-dimethoxy-phenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1B2)



1B2

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3,4-dimethoxybenzaldehyde (166.83 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc (10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 90 %; Colour: yellow; m.p: 141 - 143 ºC**.** IR (KBr, cm^{-1}): 2227 (CN stretch), 1575 (C=N stretch), 1503 (C=C stretch) and 1126 (C-O)**.** ^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.59 (1H, s), 9.09 (1H, d, *J* = 4 Hz) 8.18 (1H, d, *J* = 4 Hz), 7.80 (1H, d, *J* = 4 Hz), 7.69 - 7.65 (2H, m), 7.28 - 7.16 (5H, m), 3.95 (6H, s), 3.93 (6H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 161.24, 155.76, 153.81, 153.74, 152.18, 152.09, 146.01, 130.42, 129.13, 128.15, 127.40, 123.97, 121.97, 118.18, 117.07, 115.70, 113.58, 113.19, 111.26, 104.80, 56.64, 56.49, 55.93, 55.87. HRMS (TOF-ESI) Calcd for $C_{28}H_{23}N_5O_4$, 493.1800 $[M]^+$; observed: 494.25648 $[M+H]^+$.

(*E*)-1-((2,5-dimethoxybenzylidene)amino)-4-(2,5-dimethoxyphenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1B3)

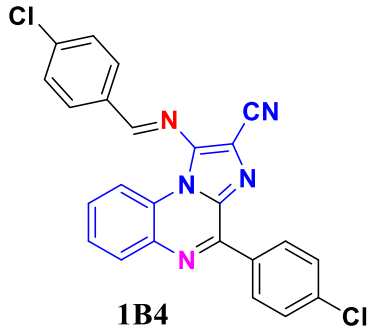


1B3

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 2,5-dimthoxybenzaldehyde (166.83 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using

rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 0.5: 9.5).Yield: 93 %; Colour: Reddish orange; m.p: 140 - 142 ºC.IR (KBr, cm^{-1}): 2233 (CN stretch),, 1496 (C=C stretch) and 1039 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.57 (1H, s), 9.09 - 9.06 (1H, m), 8.20 - 8.19 (1H, m) 7.79 (1H, d, *J* = 3.2 Hz), 7.67 - 7.64 (2H, m), 7.20 - 7.17 (1H, dd, *J*= 8 Hz), 7.15 - 7.14 (1H, m), 7.05 (2H, d, *J*= 4 Hz), 7.02 (1H, d, *J* = 8 Hz), 3.93 (3H, s), 3.91 (3H, s), 3.83 (3H, s), 3.78 (3H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 161.32, 155.81, 153.86, 152.16, 129.15, 127.43, 122.03, 118.18, 117.24, 115.76, 113.63, 113.24, 111.30, 99.99, 56.66, 56.51, 55.93, 55.89. HRMS (TOF-ESI) Calcd for $C_{28}H_{23}N_5O_4$, 493.1750 $[M]^+$; observed: 494.25648 $[M+H]^+$ and 346.1389 $[M-C_9H_{10}O_3]^+$.

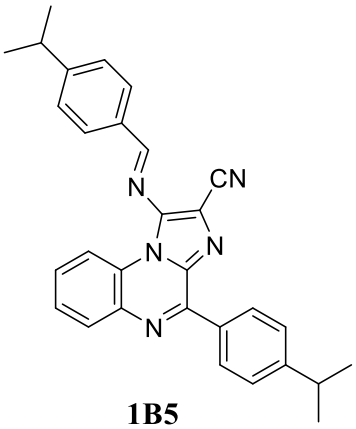
(*E*)-1-((4-chlorobenzylidene)amino)-4-(4-chlorophenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1B4)



1B4

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 4-chlorobenzaldehyde (141.12 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 84 %; Colour: Yellow; m.p: 283 – 285 ºC.IR (KBr, cm^{-1}): 2075 (CN stretch), 1345 (C=N stretch), 772 (C-Cl stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.26 (1H, s), 8.84 (1H, d, *J* = 8 Hz), 8.66-8.56 (4H, m), 8.20 (2H, d, *J* = 8 Hz), 8.13 (1H, d, *J* = 4 Hz), 7.73 (2H, m), 7.68 (2H, *J* = 8 Hz), 7.62 (1H, *J* = 8 Hz), 6.95 (1H, s). HRMS (TOF-ESI) Calcd for $C_{24}H_{13}Cl_2N_5$, 441.0548$[M]^+$; observed: 443.2332$[M+2]^+$.

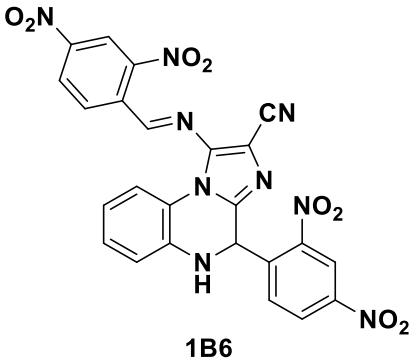
***(E)*-1-((4-isopropylbenzylidene)amino)-4-(4-isopropylphenyl)imidazo[1,2-a]quinoxaline-2-carbonitrile (1B5)**



1B5

To a reaction vial, a suspension of **7** (0.2 g, 1.005 mmol) in methanol (1 mL) was added was added 4-isopropylbenzaldehyde (0.268 g, 1.809 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2.5 : 7.5).Yield: 75 %; Colour: Yellow; m.p: 165-168ºC.IR (KBr, cm^{-1}): 1668 (C=N), 2225 (CN), 1600 (C=C Stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.13 (1H, s), 9.08-9.04 (1H, m), 8.52 (2H, d, *J* = 8 Hz), 8.15-8.13 (1H, m), 8.03 (2H, d, *J* = 8 Hz), 7.63-7.61 (2H, m), 7.47-7.42 (4H, m), 3.08-2.98 (2H, m), 1.24 (12H, m). HRMS (TOF-ESI) Calcd for $C_{30}H_{27}N_5$, 457.2266 [M]+; observed: 458.2122 [M+H]+.

***((E)*-1-((2,4-dinitrobenzylidene)amino)-4-(2,4-dinitrophenyl)imidazo[1,2-a]quinoxaline-2-carbonitrile(1B6)**

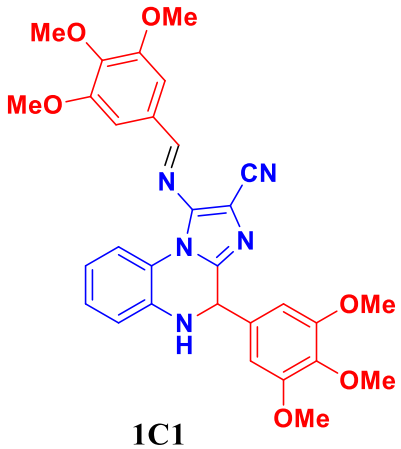


1B6

To a reaction vial, a suspension of **7** (0.2 g, 1.005 mmol) in methanol (1 mL) was added was added 2,4 dinitrobenzaldehyde (0.393 g, 2.001 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (open reflux) at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over

anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 0.5 : 9.5).Yield: 88 %; Colour: Yellow; m.p: 138-140 ºC.IR (KBr, cm^{-1}): 1607 (C=N), 2225 (CN), 1540 (asymmetric stretch NO_2), 1375 (symmetric stretch NO_2).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.64 (1H, s), 8.94-8.89 (3H, m), 8.79-8.76 (2H, m), 8.67 (1H), 8.27-8.16 (2H, m), 7.93-7.80 (2H, m). HRMS (TOF-ESI) Calcd for $C_{24}H_{11}N_9O_8$, 553.0731 [M]+; observed: 378.0890 [M- $C_7H_6N_2O_4$]$^+$.

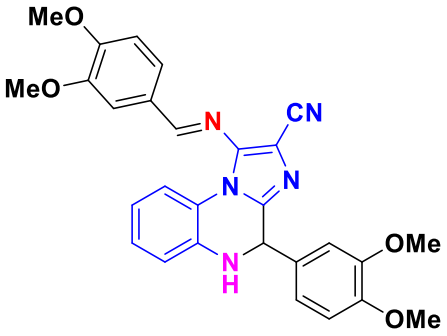
(*E*)-1-((3,4,5-trimethoxybenzylidene)amino)-4-(3,4,5-trimethoxyphenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C1)



1C1

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3,4,5-trimthoxybenzaldehyde (199.9 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 92 %; Colour: yellow; m.p: 389 ºC (decomposed).IR (KBr, cm^{-1}): IR (KBr, cm^{-1}): 2125 (CN stretch), 3285 (NH stretch) cm^{-1}, 1641 (C=N stretch), 1421 (C=C stretch) and 1093 (C-O stretch). ^{1}H NMR (400 MHz, d_6 -DMSO & $CDCl_3$, TMS = 0) δ: 8.93 (1H, s), 8.18- 8.15 (1H, dd, *J* = 4 Hz) 7.64- 7.59 (2H, m), 7.52- 7.49 (1H, dd, *J* = 4 Hz), 7.16- 7.13 (1H, m), 7.08- 7.05 (1H, dd, *J* = 4 Hz), 7.00- 6.96 (3H, m), 6.94- 6.83 (3H, m), 5.59 (1H, s), 3.99 (3H, s), 3.89 (3H, s), 3.86 (6H, s), 3.83 (3H, s), 3.82 (3H, s). HRMS (TOF-ESI) Calcd for $C_{30}H_{29}N_5O_6$, 555.2100 [M]$^+$; observed: 556.1965 [M+H]$^+$.

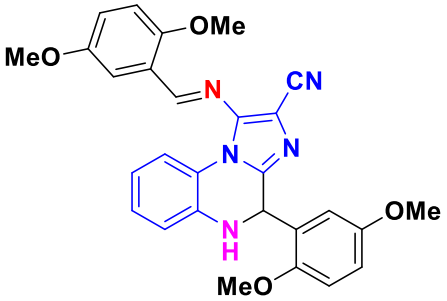
1-((3,4-dimethoxybenzylidene)amino)-4-(3,4-dimethoxyphenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C2)



1C2

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added veratraldehyde (166.83 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 88 %; Colour: yellow; m.p: 387 ºC (decomposed).IR (KBr, cm^{-1}): 2218 (CN stretch), 3333 (NH stretch) cm^{-1}, 1511 (C=N stretch), 1366 (C=C stretch) and 1022 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 8.95 (1H, s), 7.66 - 7.62 (1H, dd, *J*= 4 Hz), 7.54 - 7.52 (1H, m), 7.28 (1H, s), 7.19 - 7.16 (1H, m), 7.11- 6.97 (2H, m), 6.95 - 6.86 (3H, m), 5.61 (1 H, s), 4.01 (1H, s, NH), 3.97 (6H, s), 3.89 (6H, s). ^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 163.24, 153.68, 149.65, 149.38, 149.33, 147.04, 143.63, 136.83, 131.16, 128.32, 127.55, 125.85, 123.02, 119.74, 119.60, 116.15, 115.58, 111.14, 110.87, 110.25, 109.69, 99.68, 56.22, 56.01, 56.88, 56.93, 56.88. HRMS (TOF-ESI) Calcd for $C_{28}H_{25}N_5O_4$, 495.1900 $[M]^+$; observed: 496.3256 $[M+H]^+$.

(*E*)-1-((2,5-dimethoxybenzylidene)amino)-4-(2,5-dimethoxyphenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C3)

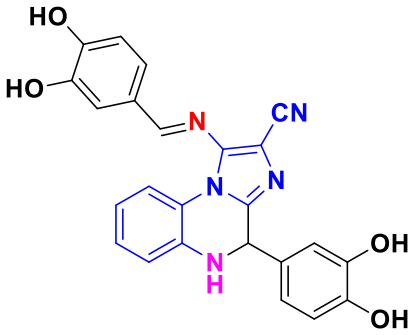


1C3

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 2,5-dimethoxybenzaldehyde (166.83 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was

heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 79 %; Colour: Reddish orange; m.p: 263 - 265 ºC.IR (KBr, cm^{-1}): 2219 (CN stretch), 3333 (NH stretch), 1640 (C=N stretch), 1502 (C=C stretch) and 1127 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 8.92 (1H, s), 8.18 - 8.15 (1H, dd, *J*= 4 Hz), 7.59 (1H, d, *J* = 4 Hz,), 7.52 - 7.49 (1H, dd, *J*= 4 Hz), 7.17 - 7.13 (1H, m), 7.00 - 6.83 (7H, m), 5.59 (1H, s), 3.98 (6H, s), 3.86 (3H, s), 3.83 (3H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 163.27, 153.69, 149.67, 149.41, 149.37, 147.03, 143.59, 136.78, 131.13, 128.33, 127.55, 125.84, 123.04, 119.84, 119.73, 119.63, 115.56, 111.16, 110.87, 110.26, 109.71, 99.67, 56.21, 56.01, 55.93, 55.89.HRMS (TOF-ESI) Calcd for $C_{28}H_{25}N_5O_4$, 495.1907 $[M]^+$; observed: 496.1827 $[M+H]^+$.

(*E*)-1-((3,4-dihydroxybenzylidene)amino)-4-(3,4-dihydroxyphenyl)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1C4)

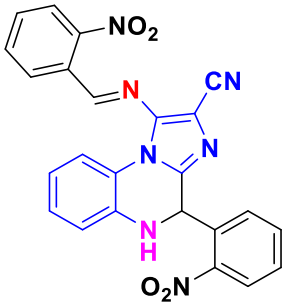


1C4

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3,4-dihydroxybenzaldehyde (138.6 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 77 %; Colour: Yellow; m.p: 286 - 288 ºC.IR (KBr, cm^{-1}): 2221 (CN stretch), 3354 (OH stretch), 3029 (NH stretch), 1633 (C=N stretch), 1367 (C=C stretch) and 1092 (C-O stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 8.16 (2H, m), 7.81 (1H, s), 7.60 (2H, m), 7.46 (1H, d, *J* = 4 Hz), 7.41 (1H, d, *J* = 4 Hz), 7.19 - 7.13 (1H, m), 7.12 - 7.01 (1H, m), 6.97 (1H, m), 6.40 (1H, d, *J* = 4 Hz), 5.85 (1H, t, *J*= 8 Hz).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 149.38, 147.04, 144.15, 138.39, 132.59, 129.74, 127.88, 127.76, 127.70, 123.15, 123.07, 122.86,

121.58, 116.04, 97.38, 74.76. HRMS (TOF-ESI) Calcd for $C_{24}H_{17}N_5O_4$, 439.1281$[M]^+$; observed: 413.2660$[M - CN]^+$.

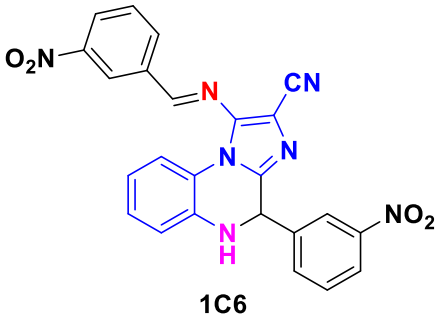
(*E*)-1-((2-nitrobenzylidene)amino)-4-(2-nitrophenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C5)



1C5

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 2-nitrobenzaldehyde (151.72 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether::1 : 9). Yield: 90 %; Colour: Brownish solid; m.p: 216 - 218 ºC. IR (KBr, cm^{-1}): 2075 (CN stretch), 3331 (NH stretch), 1398 (NO_2 Symmetric stretch), 1219 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.34 (1H, s), 8.27 (1H, d, *J* = 8 Hz), 8.16 (1H, d, *J* = 8 Hz), 8.05 (1H, d, *J* = 8 Hz), 7.96 - 7.87 (3H, m), 7.72 (1H, t, *J*= 16 Hz), 7.62 (2H, t, *J*= 16 Hz), 7.14-7.06 (2H, m), 6.97 (1H, d, *J* = 8 Hz), 6.84 (1H, t, *J*= 16 Hz), 6.29 (1H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 161.89, 149.93, 149.04, 146.02, 143.63, 137.94, 134.62, 134.24, 134.16, 133.59, 130.61, 130.35, 128.94, 128.37, 125.58, 125.49, 122.01, 119.56, 119.31, 116.48, 115.59, 100.47, 51.65.MS (ESI): m/z: 465.74 $[M]^+$. HRMS (TOF-ESI) Calcd for $C_{24}H_{15}N_7O_4$, 465.1186$[M]^+$; observed: 488.1083$[M + Na]^+$.

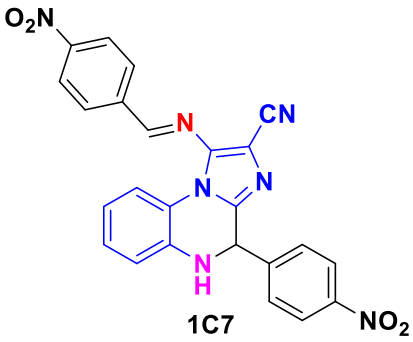
(*E*)-1-((3-nitrobenzylidene)amino)-4-(3-nitrophenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C6)



1C6

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in.methanol (1 mL) was added 3-nitrobenzaldehyde (151.72 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 93 %; Colour: Yellow; m.p: 216 - 218 ºC. IR (KBr, cm^{-1}): 2222 (CN stretch), 1496 (NO_2 Symmetric stretch), 1039 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.21 (1H, s), 8.81 (1H, s), 8.46 (2H, t, *J*= 16 Hz), 8.29 (1H, s), 8.17 (1H, d, *J* = 8 Hz), 7.87 - 7.79 (3H, m), 7.66 (1H, m), 7.36 (1H, s), 7.14 (1H, m), 7.04 (1H, m), 6.81 (1H, m), 6.00 (1H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 164.24, 148.83, 148.29, 146.36, 143.62, 142.04, 137.70, 136.48, 135.38, 134.54, 131.49, 130.71, 128.42, 127.86, 124.47, 123.63, 122.49, 122.04, 119.48, 119.23, 116.37, 115.87, 100.07, 53.96; HRMS (TOF-ESI) Calcd for $C_{24}H_{15}N_7O_4$, 465.1186[M]$^+$; observed: 466.1286 [M + H]$^+$.

(*E*)-1-((4-nitrobenzylidene)amino)-4-(4-nitrophenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C7)

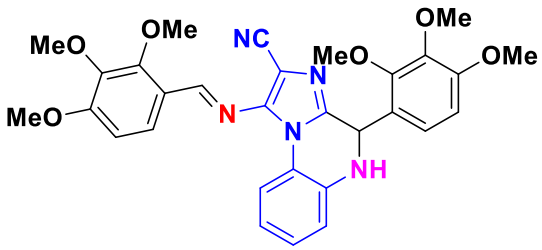


1C7

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 4-nitrobenzaldehyde (151.72 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous

Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.3 : 8.7).Yield: 82 %; Colour: Yellow; m.p: 216 - 218 ºC.IR (KBr, cm^{-1}): 2222 (CN stretch), 3345 (NH stretch), 1522 (NO_2 Symmetric stretch), 1345 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.19 (1H, d, *J* = 1.2 Hz), 8.41 (2H, d, *J* = 8 Hz), 8.29 (2H, d, *J* = 8 Hz), 8.22 - 8.17 (2H, m), 7.94 (1H, d, *J* = 8 Hz), 7.68 (1H, d, *J* = 8 Hz), 7.29 (1H, d, *J* = 8 Hz), 7.17 - 7.13 (1H, m), 7.09 - 7.07 (1H, m), 6.86 - 6.81 (1H, m), 5.93 (1H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 162.32, 149.69, 147.18, 146.60, 145.32, 142.88, 139.86, 136.94, 130.29, 128.21, 127.66, 124.04, 123.37, 121.51, 118.95, 118.55, 115.80, 54.08;

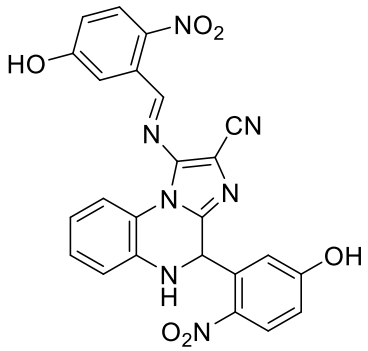
(*E*)-1-((2,3,4-trimethoxybenzylidene)amino)-4-(2,3,4-trimethoxyphenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1C8)



1C8

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 2,3,4-trimthoxybenzaldehyde (199.9 mg, 1.004 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 92 %; Colour: yellow; m.p: 228 - 230 ºC.IR (KBr, cm^{-1}): 2125 (CN stretch), 3285 (NH stretch), 1641 (C=N stretch), 1366 (C=C stretch), 1127 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.13 (1H, s), 8.02 (1H, d, *J* = 8 Hz) 7.91 (1H, d, *J* = 8 Hz), 7.12 - 7.08 (2H, m), 6.91 (2H, m), 6.82- 6.76 (3H, m), 5.82 (1H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 159.82, 158.25, 155.18, 153.50, 151.10, 147.62, 143.38, 141.63, 141.55, 137.76, 127.32, 125.99, 123.01, 122.82, 117.66, 115.31, 109.27, 107.88, 98.29, 60.60, 60.32, 56.31, 55.90, 49.71. HRMS (TOF-ESI) Calcd for $C_{30}H_{29}N_5O_6$, 555.2100 $[M]^+$; observed: 556.1967 $[M+H]^+$.

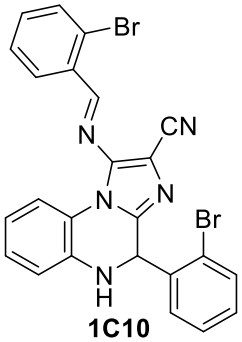
***(E)*-1-((5-hydroxy-2-nitrobenzylidene)amino)-4-(5-hydroxy-2-nitrophenyl)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1C9)**



1C9

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 5-hydroxy-2-nitrobenzaldehyde (0.335 g, 2.010 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.7: 8.3).Yield: 78 %; Colour: brown; m.p: 224-226 ºC.IR (KBr, cm^{-1}): 1611 (C=N), 2225 (CN), 3367 (NH stretch), 1519 (NH bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 11.3 (1H, s), 10.9 (1H, s), 9.44 (1H, s), 8.13 (1H, m), 8.7 (1H, d, *J* = 8.56), 7.93 (1H, d, *J* = 7.32), 7.55 (1H, d, *J* = 3.04), 7.14-7.11 (2H, m), 7.07-6.99 (2H, m), 6.90-6.83 (3H, m), 6.41 (1H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 190.69, 163.06, 162.99, 162.48, 145.88, 143.43, 140.12, 137.93, 137.17, 129.09, 128.83, 128.40, 119.57, 119.33, 116.27, 116.13, 115.34, 100.59, 56.55, 51.55, 51.41, 21.4, 19.08.HRMS (TOF-ESI) Calcd for $C_{24}H_{15}N_7O_6$, 497.1084 [M]+; observed: 498.1112 [M+H]+.

***(E)*-1-((2-bromobenzylidene)amino)-4-(2-bromophenyl)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1C10)**

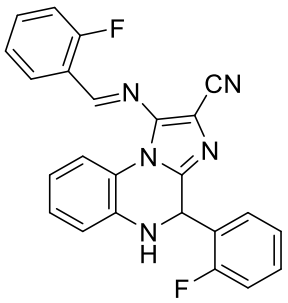


1C10

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added was added 2-bromobenzaldehyde (0.370 g, 2.010 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the

reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 79 %; Colour: yellow; m.p: 155-157 ºC.IR (KBr, cm^{-1}): 2984 (CH stretch) 2221 (CN). ^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.53 (1H, s), 8.28-8.26 (1H, m), 8.13 (1H, d, *J* = 8), 7.71-7.69 (1H, m), 7.62-7.60 (1H, m), 7.50-7.40 (3H, m), 7.20-7.16(1H, m), 7.11-7.07 (1H, m), 6.99-6.97 (1H, m), 6.92-6.89 (1H, m), 6.77 (1H, d, *J* = 4), 6.11 (1H, m), 4.75 (1H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 163.37, 146.39, 142.77, 137.55, 135.91, 134.15, 133.93, 133.75, 133.50, 130.37, 129.24, 129.12, 128.14, 128.07, 127.87, 127.75, 123.26, 122.99, 120.16, 119.81, 116.27, 115.52, 101.15, 55.27.HRMS (TOF-ESI) Calcd for $C_{24}H_{15}Br_2N_5$, 530.9694 $[M]^+$; observed: 533.9792 $[M + 2]^+$ and 535.9767.

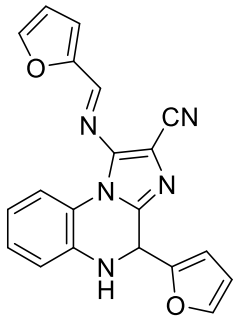
(*E*)-1-((2-Fluorobenzylidene)amino)-4-(2-Fluorophenyl)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1C11)



1C11

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 2-fluorobenzaldehyde (0.248 g, 2.010 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 71 %; Colour: yellow; m.p: 139-141 ºC.IR (KBr, cm^{-1}): 2125 (CN stretch), 3285 (NH stretch), 1641 (C=N stretch), 1366 (C=C stretch), 1127 (C-O stretch).^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.33 (1H, s), 8.19-8.11 (2H, m), 7.60-7.55 (1H, m), 7.34-7.29 (2H, m), 7.26-7.11 (4H, m), 7.06 (1H, d, *J* = 8), 6.92-6.88 (1H, t, *J* = 8), 6.79 (1H, d, *J* = 8), 6.0 (1H, s), 4.47 (1H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 164.76, 161.11 159.24, 157.96, 157.91, 142.44, 136.20, 135.11, 135.02, 130.68, 130.60, 128.79, 128.49, 127.80, 124.92, 124.74, 122.94, 120.13, 119.76, 116.69, 116.48, 116.16, 115.96, 115.57, 50.06. HRMS (TOF-ESI) Calcd for $C_{24}H_{15}F_2N_5$ 411.1296$[M]^+$; observed: 412.1283 $[M + H]^+$.

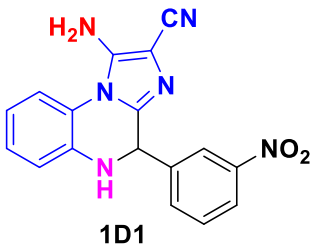
***(E)*-4-(furan-2-yl)-1-((furan-2-ylmethylene)amino)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1C12)**



1C12

To a reaction vial, a suspension of **7** (0.1 g, 0.502 mmol) in methanol (1 mL) was added furan-2-carbaldehyde (0.386 g, 1.005 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2.5 : 7.5).Yield: 73 %; Colour: brown; m.p: 246-248 ºC.IR (KBr, cm^{-1}): 1611 (C=N), 2218 (CN), 1219 (C-O stretch), 1484 (C=C aromatic stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 8.83 (1H, s), 8.25 (1H, d, *J* = 7.32 Hz), 7.75 (1H, d, *J* = 1.24 Hz), 7.35 (1H, d, *J* = 3.68 Hz), 7.22 (1H, d, *J* = 3.68 Hz), 7.11 (1H, t, *J* = 7.32 Hz), 6.93 (1H, t, *J* = 7.36 Hz), 6.84 (1H, d, *J* = 1 Hz), 6.66-6.65 (1H, m), 6.28-6.27 (1H, m), 6.16 (1H, d, *J* = 3.64 Hz), 5.75 (1H, s), 4.54 (1H, s).^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 151.37, 150.26, 157.96, 147.95, 143.20, 135.70, 127.69, 120.41, 119.90, 115.96, 113.28, 110.61, 110.61, 108.03, 49.97. HRMS (TOF-ESI) Calcd for $C_{20}H_{13}N_5O_2$, 355.1069 $[M]^+$; observed: 378.0699 $[M+Na]^+$.

1-amino-4-(3-nitrophenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1D1)

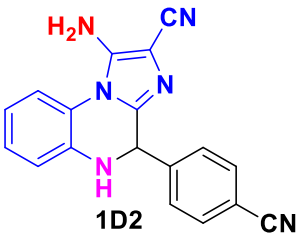


1D1

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3-nitrobenzaldehyde (75.86 mg, 0.502 mmol.) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary

evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 86 %; Colour: Brownish solid; m.p: 374 ºC (decomposed).IR (KBr, cm^{-1}): 3384 (NH stretch), 2226 (CN stretch), 1527 (NO_2 Symmetric stretch), 1366 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 8.17 - 8.13 (2H, m), 7.92-7.65 (3H, m), 7.17- 6.84 (4H, m), 6.34 (2H, NH_2), 5.71 (1H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 148.21, 146.51, 142.37, 139.31, 137.70, 136.10, 134.59, 130.52, 127.56, 127.42, 123.36, 122.89, 122.45, 119.34, 116.61, 93.83, 54.09.HRMS (TOF-ESI) Calcd for $C_{17}H_{12}N_6O_2$, 332.10 $[M]^+$; observed: 333.1169 $[M+H]^+$.

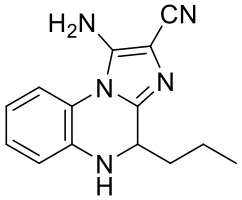
1-amino-4-(4-cyanophenyl)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1D2)



1D2

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added *p*-cyanobenzaldehyde (65.82 mg, 0.502 mmol and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 94 %; Colour: Yellow; m.p: 275 - 277 ºC.IR (KBr, cm^{-1}): 3365 (NH stretch), 2228, 2143 (CN stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 8.77 (2H, d, *J* = 8.24 Hz), 8.65 - 8.62 (1H, dd, *J* = 8 Hz) 8.03 - 7.97 (1H, m), 7.94 - 7.81 (2H, *J* = 8 Hz), 7.64 - 7.57 (2H, m), 6.76 (2H, s), 4.08-4.03 (1H, m). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 147.86, 144.65, 139.05, 135.59, 131.68, 131.50, 129.91, 129.74, 128.08, 127.41, 126.55, 118.22, 115.69, 115.19, 112.94, 100.19, 59.60.

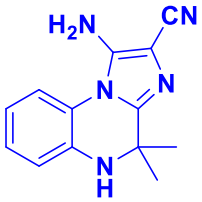
1-amino-4-propyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1D3)



1D3

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added butyraldehyde (0.0724 g, 1.005 mmol) and *p*-TsOH (1 mol %). The mixture was heated under mw irradiation (sealed tube) at 80 ºC for 25 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 88 %; Colour: white; m.p: 132-134 ºC. IR (KBr, cm^{-1}): 3387 (NH_2 stretch) 2227 (CN stretch), 1218 (NH bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.72 (1H, d, *J* = 7.92 Hz), 7.00 (1H, t, *J* = 7.96 Hz), 6.92 (1H, d, *J* = 1.2 Hz), 6.75 (1H, t, *J* = 7.36 Hz), 6.27 (1H, s), 6.13 (2H, s), 4.14 (1H, t, *J* = 6.12 Hz), 1.65-1.54 (2H, m), 1.41-1.36 (2H, m), 0.84 (3H, t, *J* = 7.32 Hz).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 146.2, 141.0, 138.4, 127.1, 122.9, 118.6, 117.6, 117.4, 116.3, 93.6, 51.0, 39.8, 18.4, 14.3.MS (ESI): m/z: 253 [M+], 55 (base peak); HRMS (TOF-ESI) Calcd$C_{14}H_{15}N_5$, 253.1327 [M^+]; observed: 254.1009 [M+H]$^+$.

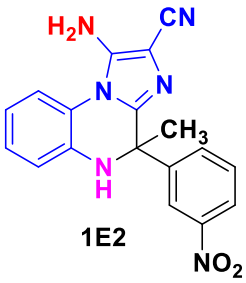
1-amino-4,4-dimethyl-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1E1)



1E1

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) was added acetone (1 equiv.) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), acetone was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.8 : 8.2).Yield: 88 %; Colour: Light Yellow: mp: 213 - 215 ºC**.** ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.80 (1H, d, *J* = 8 Hz), 7.05-7.02 (1H, m), 6.86 (1H, d, *J* = 8 Hz), 6.80 (1H, t, *J* = 8 Hz), 6.28 (1H, NH, s), 6.11 (2H, NH, s), 1.31 (6H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 199.91, 146.94, 144.58, 137.03, 127.25, 121.86, 117.95, 117.74, 115.57, 98.48, 51.40, 28.64, 26.54, 22.84. HRMS (TOF-ESI) Calcd for $C_{13}H_{13}N_5$, 239.1171 [$M]^+$; observed: 262.1062 [M + Na]$^+$.

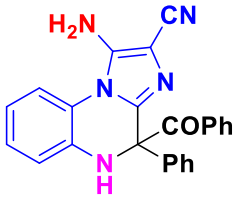
1-amino-4-methyl-4-(3-nitrophenyl)-4,5-dihydroimidazo[1,2*a*]quinoxaline-2-carbonitrile (1E2)



1E2

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added 3-nitro acetophenone (82.90 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 91 %; Colour: Light Yellow: mp: 264 – 266 ºC**.**IR (KBr, cm^{-1}): 3329 (NH stretch), 2212 (CN stretch), 1233 (C-N stretch), 1609 (C=N stretch), 1453 (C=C stretch), 1528 (NO_2 Symmetric stretch), 1376 (NO_2 asymmetric stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 8.10 (1H, s, NH), 7.97 (1H, d, *J* = 8 Hz), 7.64 (1H, d, *J* = 8 Hz), 7.59-7.49 (3H, m), 7.06 (2H, s), 6.70 (1H, s), 6.25 (2H, s, NH_2), 1.79 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 147.88, 146.95, 146.15, 136.71, 132.15, 130.12, 127.02, 122.33, 120.03, 118.91, 117.26, 116.14, 93.28, 57.17, 28.10. HRMS (TOF-ESI) Calcd for $C_{18}H_{14}N_6O_2$, 346.1178 $[M]^+$; observed: 369.1066 $[M + Na]^+$.

1-amino-4-benzoyl-4-phenyl-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1E3)

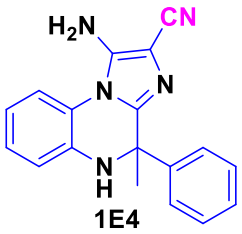


1E3

To a reaction vial, a suspension of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added benzil (105.48 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 95 %; Colour: yellow; m.p: 184 - 186 ^{0}C.IR Spectrum (KBr, cm^{-1}): 3440 (NH stretch), 2206 (CN stretch),

1448 (NH bend), 1670 (C=N stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.74 (2H, t, *J*= 16 Hz), 7.63 (2H, d, *J* = 4 Hz), 7.49 (1H, m), 7.36-7.31 (7H, m), 7.01 (1H, t, *J*= 4 Hz), 6.93 (1H, d, *J* = 4 Hz), 6.78 (1H, m), 6.36 (2H, NH, s)^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 196.26, 139.53, 137.50, 135.80, 134.04, 133.64, 130.22, 128.88, 128.72, 127.65, 127.51, 122.57, 120.19, 117.30, 116.91, 93.51, 69.72. HRMS (TOF-ESI) Calcd for $C_{24}H_{17}N_5O$, 391.1433 $[M]^+$; observed: 414.1319 $[M + Na]^+$.

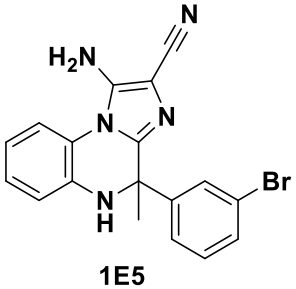
1-amino-4-methyl-4-phenyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E4)



1E4

To a reaction vial, **7** (100 mg, 0.502 mmol) in methanol was added acetophenone (189.04 mg, 1.005 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 92 %; Colour: Light Yellow, m.p: 189-190 ºC.IR Spectrum (KBr, cm^{-1}): 3422 (NH stretch), 2202 (CN stretch), 1371 (CH_3 bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.62 (1H, d, *J* = 8 Hz), 7.33 (1H, s), 7.16 (4H, d, *J* = 4 Hz), 7.01 (2H, d, *J* = 4 Hz), 6.67 (1H, d, *J* = 4 Hz), 6.14 (2H, s), 1.74 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 146.46, 145.10, 142.81, 137.90, 128.76, 127.47, 127.38, 127.26, 125.73, 123.19, 118.85, 117.61, 117.41, 93.71, 52.72, 28.99. HRMS (TOF-ESI) Calcd $C_{18}H_{16}N_5$, 301.1327 [M+]; observed: 302.1330 $[M+H]^{+\cdot}$

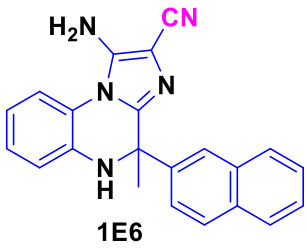
1-amino-4-(3-bromophenyl)-4-methyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E5)



1E5

To a reaction vial, **7** (100 mg, 0.502 mmol) in methanol was added 3-bromoacetophenone (120 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 4 : 6).Yield: 89 %; Colour: Light Yellow, m.p: 244 - 245 ºC.IR Spectrum (KBr, cm^{-1}): 3085 (NH_2 stretch), 2923 (CH stretch), 1460 (CH_3 bend), 785 (Br stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.72 (1H, d, *J* = 8 Hz), 7.40 (1H, t, *J* = 4 Hz), 7.18 - 7.07 (3H, m), 6.98-6.95 (1H, dd, *J* = 4 Hz, J_{34} = 4 Hz), 6.90 - 6.86 (1H, m), 4.63 (1H, s), 4.18 (1H, s), 1.55 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 144.61, 134.85, 129.65, 129.06, 127.41, 126.59, 122.93, 121.67, 119.32, 115.83, 115.46, 114.42, 76.27, 27.69. HRMS (TOF-ESI) Calcd$C_{18}H_{15}BrN_5$, 379.0433 [M^+]; observed: 380.0441 [M+H]$^+$.

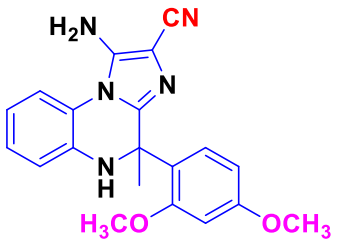
1-amino-4-methyl-4-(naphthalene-2-yl)-4,5-dihydroimidazo-[1,2-a]quinoxaline-2-carbonitrile (1E6)



1E6

To a reaction vial, **7** (200 mg, 1.005 mmol) in methanol was added 2-acetonaphthone (170.87 mg, 1.005 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7). Yield: 93 %; Colour: Light Yellow, m.p. decomposed at 240 ºC.IR Spectrum (KBr, cm^{-1}): 3665 (NH stretch), 3330 (Ar stretch), 2942 (CH stretch), 1020 (Ar bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.82 - 7.77 (2H, m), 7.73 (1H, t, *J* = 8 Hz), 7.67 (1H, d, *J* = 8 Hz), 7.56 - 7.52 (3H, m), 7.43 - 7.41 (2H, m), 7.14 (1H, dd, *J* = 4 Hz), 7.06 (1H, m), 6.66 (1H, m), 6.28 (2H, s), 1.92 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 146.60, 142.66, 137.93, 132.81, 132.44, 128.67, 128.32 127.86, 127.31, 126.88, 126.63, 124.26, 123.27, 118.97, 117.66, 116.65, 93.68, 57.93, 28.73. HRMS (TOF-ESI) Calcd$C_{22}H_{18}N_5$, 351.1484 [M^+]; observed: 352.1240 [M+H]$^+$.

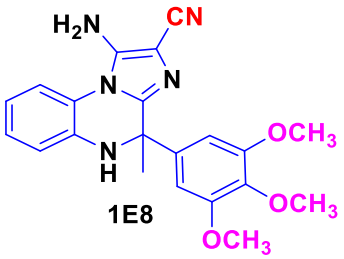
1-amino-4-(2,4-dimethoxyphenyl)-4-methyl-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1E7)



1E7

To a reaction vial, **7** (200 mg, 1.005 mmol,) in methanol was added 2,4--dimethoxyacetophenone (180. mg, 1.005 mmol) the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 86 %; Colour: Light Yellow, m.p: 136 -137 ºC.IR Spectrum (KBr, cm^{-1}): 3300 (NH stretch), 3000 (CH stretch), 1646 (NH bend), 1448 (CH3 stretch) 1330 (CO stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.67 (1H, d, *J* = 8 Hz), 6.97-6.94 (2H, m), 6.74 (1H, t_{13}, *J* = 8 Hz), 6.55 (1H, s), 6.46 (1H, d, *J* = 4 Hz), 6.23 (2H, s), 6.20 (1H, dd, *J* = 4 Hz, J_{34} = 4 Hz), 6.14 (1H, d, *J* = 8 Hz), 3.84 (3H, s), 3.62 (3H, s), 1.86 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 160.31, 158.25, 146.54, 142.82, 138.10, 128.14, 127.01, 123.37, 119.17, 117.42, 116.76, 104.38, 99.96, 93.18, 57.89, 56.17, 55.52, 25.22. HRMS (TOF-ESI) Calcd$C_{20}H_{20}N_5O_2$, 361.1539 [M^+]; observed: 362.1218 [M+H]$^{+\cdot}$

1-amino-4-methyl-(3,4,5-trimethoxyphenyl)-4,5-dihydroimidazo-[1,2-a]quinoxaline-2-carbonitrile (1E8)

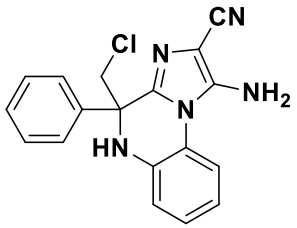


1E8

To a reaction vial, **7** (200 mg, 1.005 mmol,) in methanol was added 3,4,5-trimethoxyacetophenone (211.28 mg, 1.005 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine,

dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2.1: 7.9).Yield: 82 %; Colour: Light Yellow, m.p: 151-152 ºC.IR Spectrum (KBr, cm^{-1}): 3512 (NH stretch),2845, 2994 (CH stretch), 1373 (CH_3 bend),1244 (CH_3 bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.68 (1H, d, *J* = 8 Hz), 7.49 (2H, d, *J* = 8 Hz), 7.25 (1H, s), 7.13-7.06 (5H, m), 6.74 (1H, m), 6.52 (2H, s), 3.57 (6H, s), 3.50 (3H, s), 1.78 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 152.99, 146.45, 145.76, 142.80, 140.64, 138.45, 138.03, 136.64, 128.68, 127.29, 126.01, 123.11, 118.98, 117.71, 116.61, 103.41, 93.48, 60.34, 57.89, 56.23, 29.00, 21.32. HRMS (TOF-ESI) Calcd $C_{21}H_{22}N_5O_3$, 391.1644 [M+]; observed: 392.1251 $[M+H]^+$.

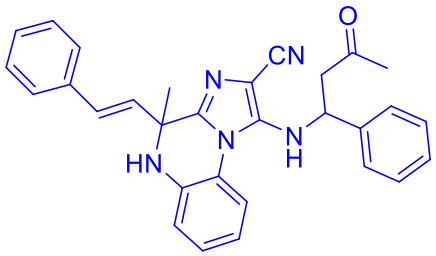
1-amino-4-(chloromethyl)-4-phenyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E9)



1E9

To a reaction mixture of **9** (100 mg, 0.502 mmol,) in methanol was added 2-chloroacetophene (77.6 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1:9). Yield: 74 %; Yield: 62 %; Colour: light brownish, mp: 229-231 ºC .^{1}H NMR (400 MHz, d_6-DMSO, TMS = 0) δ: 7.67 (1H, d, *J* = 8.56), 7.42 (1H, s), 7.32 (2H, d, *J* =7.32), 7.24 (2H, t, *J* = 15.28), 7.18-7.16 (2H, m), 7.05 (1H, t, *J* = 15.28), 6.73 (1H, t, *J* = 15.28), 6.27 (2H, s), 4.32 (1H, d, *J* = 11.6), 4.00 (1H, d, *J* = 11.6). ^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ:146.52, 140.78, 139.34, 136.98, 129.02, 128.56, 127.49, 126.83, 122.34, 119.05, 117.40, 117.20, 116.83, 94.16, 61.87, 50.23. HRMS (TOF-ESI) Calcd for $C_{18}H_{14}ClN_5$, 335.0938 $[M]^+$; observed: 336.0963 $[M + H]^+$.

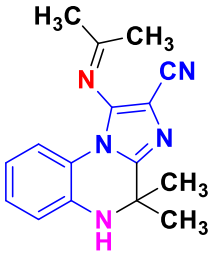
(E)-4-methyl-1-((3-oxo-1-phenylbutyl)amino)-4-styryl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (IE10)



1E10

To a reaction mixture of **7** (200 mg, 1.407 mmol,) in methanol was added benzylideneacetone (205.69 mg, 1.005 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8). Yield: 71 %; Colour: orange Solid, mp:264-266 ºC.^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 7.96 (1H, d, *J* = 6.12), 7.83 (2H, d, *J* = 6.4), 7.60-7.56 (3H, m), 7.46-7.39 (3H, m), 6.99 (1H, t, *J* = 11.24), 6.84 (2H, t, *J* = 11.96), 6.42 (2H, d, *J* = 6.32), 5.99 (1H, s), 4.15-4.12 (1H, q), 3.74-3.63 (2H, m) ^{13}C NMR (100 MHz, $CDCl_3$, TMS = 0) δ: 203.83, 152.59, 145.98, 133.87, 131.38, 130.46, 129.45, 128.66, 128.21, 128.16, 128.13, 127.92, 127.61, 124.75, 123.59, 121.30, 121.30, 116.35, 115.12, 111.34, 99.08, 61.15, 45.63, 43.93, 30.59, 10.77. HRMS (TOF-ESI) Calcd for $C_{30}H_{27}N_5O$, 473.2216 $[M]^+$; observed: 457.1980 $[M - CH_3]^+$.

4,4-dimethyl-1-(propan-2-ylideneamino)-4,5-dihydroimidazo-[1,2-*a*]quinoxaline-2-carbonitrile (1E11)

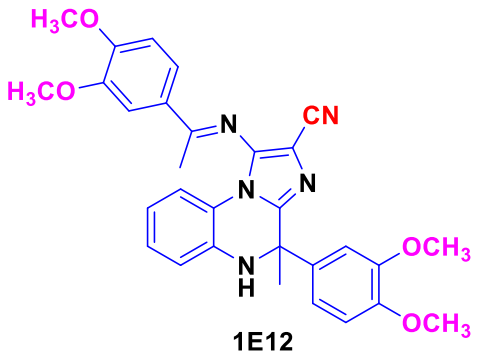


1E11

To a reaction vial, **7**(100 mg, 0.502 mmol) was dissolved in acetone (2 equiv.) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), acetone was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 85 %; Colour: Light Yellow, m.p: 142 -144 ºC. IR Spectrum

(KBr, cm^{-1}): 3322 (NH stretch), 2210 (CN stretch), 1637 (C=N stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.60 (1H, d, *J* = 8 Hz), 7.08 (1H, m), 6.89 (1H, d, *J* = 8 Hz), 6.75 (1H, m), 6.51 (1H, s), 2.34 (3H, s), 2.12 (3H, s), 1.39 (6H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 179.91, 146.95, 144.58, 137.03, 127.25, 121.86, 117.95, 117.74, 115.77, 98.48, 51.40, 28.64, 26.54, 22.84. HRMS (TOF-ESI) Calcd for $C_{24}H_{17}N_5O$, 391.1433 $[M]^+$; observed: 414.1319 $[M + Na]^+$.

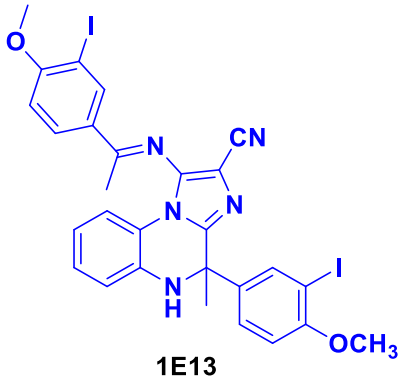
***(E)*-4-(3,4-dimethoxyphenyl)-1((1-(3,4-dimethoxyphenyl)ethylidene)amino)-4-methyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E12)**



1E12

To a reaction vial, **7** (100 mg, 0.502 mmol) in methanol was added 3,4-dimethoxyacetophenone (180.93 mg, 1.004 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2 : 8).Yield: 88 %; Colour: Light Yellow solid, m.p: 170 -171 ºC.IR Spectrum (KBr, cm^{-1}): 3208 (NH stretch), 2966 (CH_3 stretch), 2328 (CN stretch), 1454 (CH_3 bend).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.60 (1H, d, *J* = 7.32 Hz), 6.95-6.80 (2H, m), 6.70-6.68 (1H, m), 6.51 (1H, s), 6.41 (1H, d, *J* = 4 Hz), 6.17-6.15 (2H, m), 6.10 (1H, d, *J* = 8 Hz), 3.83 (3H, s), 3.58 (3H, s), 1.82 (3H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ:160.44, 158.35, 146.44, 142.82, 138.10, 128.35, 127.01, 123.5, 118.92, 117.78, 116.76, 104.67, 100.09, 93.18, 57.89, 56.18, 55.91, 22.45. HRMS (TOF-ESI) Calcd $C_{30}H_{29}N_5O_4$, 523.2220 [M+]; observed: 524.2198 $[M+H]^+$ and 362.2128 $[M - C_{10}H_{12}O_2]^+$

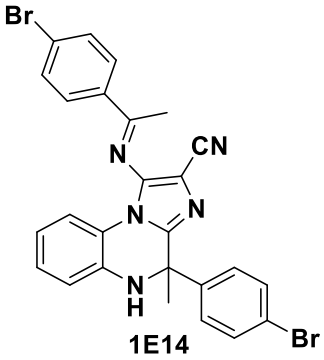
***(E)*-4-(3-iodo-4-methoxyphenyl)-1-((1-(3-iodo-4-methoxyphenyl)ethylidene)amino)-4-methyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E13)**



1E13

To a reaction vial, **7** ((200 mg, 1.005 mmol,) in methanol was added 3-iodo-4-methoxyacetophenone (332.86 mg, 1.206 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.5 : 8.5).Yield: 78 %; Colour: Brownish solid, m.p: 191-192 ºC.IR Spectrum (KBr, cm^{-1}): 3231 (NH stretch), 2230 (CN stretch), 759 (I stretch), 1247 (C-O stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: (400MHz, d_6-DMSO,TMS=0)δ: 7.67(1H, d, *J* = 7.92), 7.60 (1H, d, *J* = 2.44), 7.46 (2H, d, *J* = 8.56), 7.34 (1H, s), 7.11-7.02 (4H, m), 6.85(1H, d, *J* = 8.56), 6.74 (1H, t, *J* = 8.4 Hz), 3.71. (6H, s), 2.28 (3H, s), 1.74 (3H, s). ^{13}C NMR (100 MHz, d_6-DMSO, TMS = 0) δ: 171.61, 157.23, 147.23, 146.49, 142.58, 139.00, 138.22, 137.65, 128.59, 126.01, 127.2, 126.1, 123.11, 119.53, 117.54, 117.43, 116.57, 111.70, 93.65, 86.55, 79.49, 56.81, 29.32, 21.37. HRMS (TOF-ESI) Calcd $C_{28}H_{23}I_2N_5O_2$, 714.9941 [M+]; observed: 458.0117 [M+H-$C_9H_9IO_2$]$^+$.

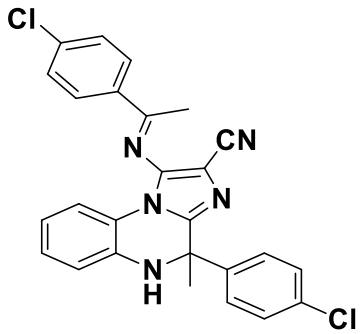
***(E)*-4-(4-bromophenyl)-1-((1-(4-bromophenyl)ethylidene)amino)-4-methyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1E14)**



1E14

To a reaction vial, **7** (100 mg, 0.502 mmol) in methanol was added 4-bromoacetophenone (198.7 mg, 1.004 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc (10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 82 %; Colour: Light Yellow solid, m.p: 230 – 231 ºC.IR Spectrum (KBr, cm^{-1}): 3281 (NH stretch), 2229 (CN stretch), 1394 (CH_3 bend); ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.62 (1H, d, *J* = 8 Hz), 7.44 (2H, d, *J* = 8 Hz), 7.38 (2H, d, *J* = 8 Hz), 7.09 (4H, m), 7.04-6.98 (2H, m), 6.71 - 6.67 (1H, m), 2.24 (3H, s), 1.72 (3H, s).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 146.52, 144.56, 138.33, 131.71, 128.64, 128.12, 127.36, 126.02, 123.12, 123.04, 120.84, 119.10, 117.66, 117.30, 116.62, 93.66, 57.50, 28.62, 21.31. HRMS (TOF-ESI) Calcd $C_{26}H_{19}Br_2N_5$, 559.0007 [M+]; observed: [M+H- C_7H_5BrO] 380.0828, [M+2] .382.0174.

***(E)*-4-(4-chlorophenyl)-1((1-(4-chlorophenyl)ethylidene)amino)-4-methyl-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile(1E15)**

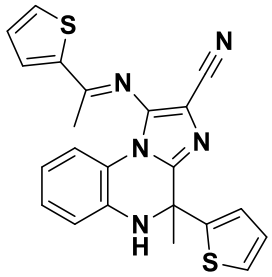


1E15

To a reaction vial, **7** ((100 mg, 0.502 mmol)) in methanol was added *p*-chloroacetophenone (154.63 mg, 1.004 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 2:8).Yield: 89 %; Colour: brown solid, m.p: 210 – 212 ºC. IR (KBr, cm^{-1}): 3253 (NH stretch), 2232 (CN stretch), 1420 (CH_3 bend), 770 (Cl stretch); ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.67 (1H, d, *J* = 8 Hz), 7.49 (2H, d, *J* = 8 Hz), 7.29 - 7.26 (2H, m), 7.22 - 7.19 (2H, m), 7.13 (2H, d, *J* = 8 Hz), 7.06 - 7.04 (2H, m), 6.74 - 6.71 (1H, m), 2.28 (3H, s), 1.77 (3H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 146.52, 145.69, 144.11, 142.37, 138.50, 137.60, 132.26, 128.78, 128.69, 127.76,

127.36, 126.02, 123.11, 119.09, 117.65, 117.30, 116.63, 93.65, 57.45, 28.67, 21.31. HRMS (TOF-ESI) Calcd$C_{26}H_{19}Cl_2N_5$, 471.1008 [M+]; observed: 336.0695 [M- $C_8H_7Cl]^+$., 338.0905 [M- C_8H_7Cl +2] $^+$.

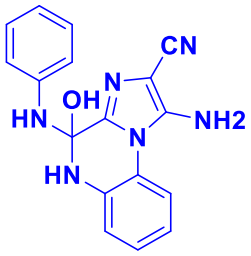
***(E)*-4-methyl-4-(thiophen-2-yl)-1-((1-(thiophen-2-yl)ethylidene)amino)-4,5-dihydroimidazo[1,2-*a*]quinoxaline-2-carbonitrile (1E16)**



1E16

To a reaction vial, **7** (100 mg, 0.502 mmol) in methanol was added 2-acetylthiophene (126.67 mg, 1.004 mmol and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 74 %; Colour: brown solid, m.p: 239 - 240 ºC.IR Spectrum (KBr, cm^{-1}): 3350 (NH stretch), 3000 (CH stretch),2362 (CN stretch), 2880 (SH stretch), 1447 (CH_3 bend); ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.72(1H, d, *J* = 8 Hz), 7.45 (2H, d, *J* = 8), 7.26-7.24(1H, dd, *J* = 4 Hz), 7.08(2H, d, *J* = 8 Hz), 7.03(1H, d, *J* = 8 Hz), 6.97-6.95 (1H,m), 6.78-6.70 (3H, m), 2.25(3H, s), 1.86 (3H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 149.86, 146.43, 145.80, 142.62, 138.42, 137.33, 128.68, 127.34, 127.11, 126.01, 125.79, 124.40, 122.99, 119.17, 117.51, 117.28, 116.69, 93.64, 55.66, 29.05, 21.32. HRMS (TOF-ESI) Calcd $C_{22}H_{18}N_5S_2$, 415.0925[M^+]; observed: 416.1492 [M+H]$^+$.

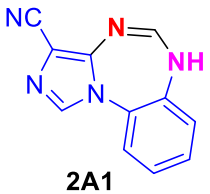
1-amino-4-hydroxy-4-(phenylamino)-4,5-dihydroimidazo[1,2-a]quinoxaline-2-carbonitrile (1F1)



1F1

To a reaction mixture of **4** (150 mg, 0.753 mmol,) in methanol was added phenyl isocyanate (89.69 mg, 0.753 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 5 : 5). Yield: 73 %; Colour: Yellowish Solid, mp: 271 – 273 ºC. ^{1}H NMR (400 MHz, d_6 - DMSO/ $CDCl_3$, TMS = 0) δ: 8.94 (1H, s, D_2O exchangeable NH), 8.21 (1H, d, *J* = 8), 7.73 (1H, s, D_2O exchangeable NH), 7.34 (1H, t, *J* = 8), 7.30 (2H, d, *J* = 8), 7.16-7.03 (3H, m), 6.86 (IH, m), 5.70 (2H, s; D_2O exchangeable NH_2). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 151.02, 146.79, 137.93, 135.10, 130.81, 128.90, 127.32, 127.09, 121.48, 121.11, 120.74, 120.51, 116.92, 115.81, 89.64. HRMS (TOF-ESI) Calcd $C_{17}H_{14}N_6O$, 318.1229, [M^+]; observed: 319.1235 [M+H]$^+$.

4*H*-benzo[*f*]imidazo[1,5-*a*][1,3,5]triazepine-3-carbonitrile (2A1)

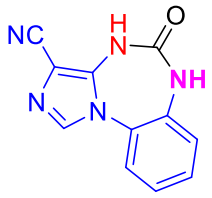


2A1

To a reaction mixture of **9** (100 mg, 0.502 mmol) in acetonitrile (1 mL) was added triethylorthoformate (74.39 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), acetonitrile was evaporated from mixture, washed with water, brine, dried over anhydrous Na_2SO_4, extracted with EtOAc(10 mL × 3), concentrated under vacuum using rotary evaporator, dried and purified *via* flash chromatography (EtOAc: Pet ether:: 2.5 : 7.5).Yield: 89 %; Colour: Yellowish Solid; m.p: 387 ºC (decomposed).IR (KBr, cm^{-1}): 3332 (NH stretch), 2224 (CN stretch), 1642 (C=N stretch).^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.57 (1H, s, NH), 8.07 (1H, s), 7.51 – 7.47 (1H, m), 7.13 - 7.10 (1H, d, *J* = 8 Hz), 6.95 - 6.92 (1H, m), 6.78 – 6.76 (1H, m), 6.64 (1H, d, *J*= 4 Hz). ^{13}C NMR (100 MHz, d_6 -DMSO,

TMS = 0) δ: 147.42, 146.57, 136.27, 133.51, 129.35, 126.51, 124.70, 121.58, 121.22, 115.47, 110.0. HRMS (TOF-ESI) Calcd for $C_{11}H_7N_5$, 209.0700 $[M]^+$; observed: 209.9262 $[M+H]^+$.

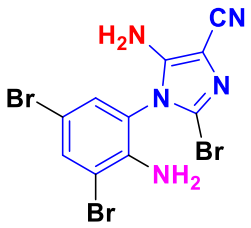
5-oxo-5,6-dihydro-4*H*-benzo[*f*]imidazo[1,5-*a*][1,3,5]triazepine-3-carbonitrile (2A2)



2A2

To a reaction mixture of **7** (100 mg, 0.502 mmol) in methanol (1 mL) was added carbonyldiimidazole (81.39 mg, 0.502 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, washed with water, brine, dried over anhydrous Na_2SO_4, extracted with EtOAc(10 mL × 3), concentrated under vacuum using rotary evaporator, dried and purified *via* flash chromatography (EtOAc: Pet ether:: 1 : 9).Yield: 91 %, Colour: Yellowish Solid, m.p: 309 ºC (decomposed). IR (KBr, cm^{-1}): 3200 (NH stretch), 2350 (CN stretch), 1710 (C=O stretch). ^{1}H NMR (400 MHz, $CDCl_3$, TMS = 0) δ: 9.51 (1H, s, NH), 8.21 (1H, s), 7.73 (1H, s), 7.48 (1H, m), 7.33 (2H, m), 7.09 (1H, m).^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 158.40, 137.32, 133.76, 131.90, 129.25, 125.36, 125.09, 122.46, 122.21, 114.42, 99.06.HRMS (TOF-ESI) Calcd for $C_{11}H_7N_5O$, 225.0700 $[M]^+$; observed: 226.0090 $(M+H)^+$.

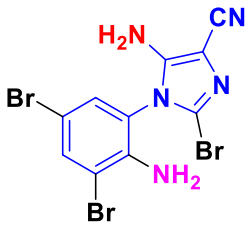
5-amino-1-(2-amino-3,5-dibromophenyl)-2-bromo-1*H*-imidazole-4-carbonitrile (14)



14

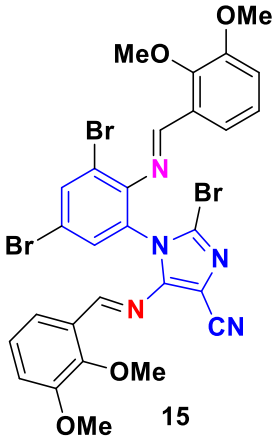
To the reaction vial added **7** (200 mg, 1.005 mmol), and NBS (3 equiv.) in acetonitrile. The reaction mixture was stirred for 1h at rt on. After the completion of the reaction (TLC), acetonitrile was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 1.8 : 8.2).Yield: 91 %; Colour: yellow; m.p: 163 - 165 ºC. IR (KBr, cm^{-1}): 3330 (NH stretch), 2212 (CN stretch), 685 (C-Br stretch). ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 7.70 (1H, d, J = 4 Hz), 7.29 (1H, d, J =

4 Hz) 6.39 (2H, s, NH_2), 5.60 (2H, s, NH_2). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 174.98, 150.23, 143.47, 136.10, 132.16, 118.20, 116.76, 112.61, 109.25, 105.15, 90.43.



14

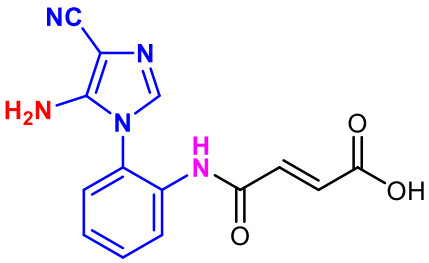
2-bromo-1-(3,5-dibromo-2-(((*E*)-2,3-dimethoxybenzylidene)amino)phenyl)-5-(((*E*)-2,3-dimethoxybenzylidene)amino)-1*H*-imidazole-4-carbonitrile (15)



15

To a reaction vial, a suspension of **16** (200 mg, 0.458 mmol) in methanol (1 mL) was added 2,3-dimethoxybenzaldehyde (152.46 mg, 0.917 mmol) and the mixture was heated under mw irradiation (open reflux) using *p*-TsOH (1 mol %) as catalyst at 80 ºC for 30 min. After the completion of the reaction (TLC), methanol was evaporated from mixture, concentrated under vacuum using rotary evaporator, extracted with EtOAc(10 mL × 3), washed with water, brine, dried over anhydrous Na_2SO_4, and purified *via* flash chromatography (EtOAc: Pet ether:: 3 : 7).Yield: 93 %; Colour: yellow; m.p: 168 - 170 ºC.IR (KBr, cm^{-1}): 3016 (NH stretch), 2349 (CN stretch), 707 (C-Br stretch).^1H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.19 (1H, s), 9.06 (1H, s), 8.46 (1H, d, *J* = 8 Hz), 8.20 (1H, s), 8.00 (1H, d, *J* = 8 Hz), 7.83 (1H, d, *J* = 8 Hz), 7.68 (2H, m), 7.23- 7.15 (2H, dd, *J* = 8 Hz), 3.92 (3H, s), 3.89 (3H, s), 3.84 (6H, s). HRMS (TOF-ESI) Calcd for $C_{28}H_{22}Br_3N_5O_4$, 728.9992 $[M]^+$; observed: 701.4915 $[M +2 – OCH_3]^+$.

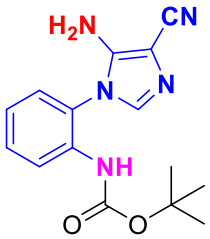
(E)-4-((2-(5-amino-4-cyano-1H-imidazol-1-yl)phenyl)amino)-4-oxobut-2-enoic acid (1G1)



1G1

Yield: 86%; colour: Dark brownish; m. p: 192-194˚C. IR (KBr, cm^{-1}): 3363 & 3310 (NH_2 stretch), 3213 & 3124 (sp^2 hybz C-H stretch), 2936 (Carboxylic Acid O-H Stretch), 2216 (CN), 1703 (C=O of carboxylic acid), 1623 & 1593 (amide peaks), 1495-1446 (aromatic C=C) ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 13.06 (1H, s), 9.95 (1H, s, NH), 7.86 (1H, d, *J* = 7.92 Hz), 7.49-7.45 (1H, m), 7.31 (2H, d, *J* = 4.2 Hz), 7.12 (1H, s), 6.41 (1H, d, *J* = 12.24 Hz), 6.23 (1H, d, *J* = 12.24 Hz), 5.96 (2H, s, NH_2) ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 167.37, 167.28, 164.46, 148.45, 134.52, 133.05, 132.34, 130.31, 128.97, 126.93, 117.88, 91.03. HRMS Calcd for $C_{14}H_{11}N_5O_3$, 297.2740 [M^+]; observed: 298.1044 [M+H]$^+$

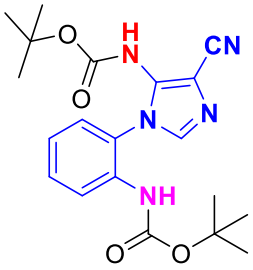
tert-butyl (2-(5-amino-4-cyano-1H-imidazol-1-yl)phenyl)carbamate (IH1)



1H1

Yield 71%; Colour: pale yellow; m. p: 164-166˚C. IR (KBr, cm^{-1}): 3437-3348 (NH_2), 2240 (CN), 1720 (C=O stretch). ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.0 (1H, s, NH), 7.82 (1H, s), 7.15 (1H, t, *J* = 6.72 Hz), 6.90 (1H, d, *J* = 7.92 Hz), 6.82 (1H, d, *J* = 7.32 Hz), 6.60 (1H, t, *J* = 7.32 Hz), 4.99 (2H, s, NH_2), 1.27 (9H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 152.89, 145.08, 138.71, 136.51, 130.93, 128.68, 118.68, 116.78, 116.62, 115.32, 108.60, 81.08, 28.13. HRMS Calcd for $C_{15}H_{17}N_5O_2$, 299.1382 [M^+]; observed: 300.1415 [M+H]$^+$

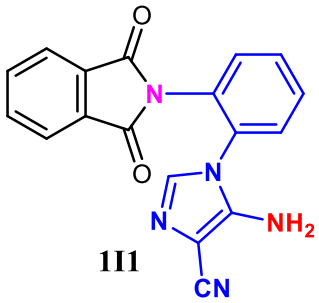
tert-butyl (2-(5-((tert-butoxycarbonyl)amino)-4-cyano-1H-imidazol-1-yl)phenyl)carbamate (IH2)



1H2

Yield 63%; Colour: white; m. p: 136-138˚C. IR (KBr, cm^{-1}): 3390 (NH), 2229 (CN), 1698 (C=O stretch). ^{1}H NMR (400 MHz, d_6 -DMSO, TMS = 0) δ: 9.09 (1H, s, NH), 8.49 (1H, s, NH), 7.76 (1H, s), 7.59 (1H, d, *J* = 7.32 Hz), 7.46 (1H, t, *J* = 5.52 Hz), 7.25 (1H, t, *J* = 6.06 Hz), 7.21 (1H, d, *J* = 6.08 Hz), 1.32 (9H, s), 1.29 (9H, s). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 153.45, 153.14, 138.52, 135.26, 130.72, 129.05, 127.50, 125.90, 125.66, 115.39, 107.73, 81.14, 80.03, 28.37, 28.13

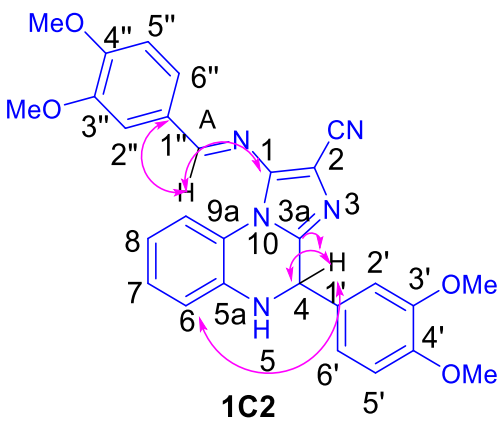
5-amino-1-(2-(1,3-dioxoisoindolin-2-yl)phenyl)-1H-imidazole-4-carbonitrile (1I1)



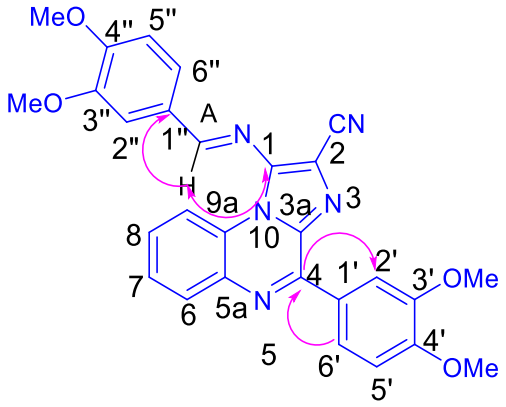
1I1

Yield: 83%; colour: yellowish; m. p: 172-176˚C. IR (KBr, cm^{-1}): 3488 & 3347(NH_2), 2225 (CN), 1715 (aromatic C=C), 1643 (C=O). ^{1}H NMR (400 MHz, d_6-DMSO, TMS = 0) δ: 7.91-7.85 (4H, m), 7.69-7.64 (3H, m), 7.60- 7.58 (1H, m), 7.04 (1H, s), 5.92 (2H, s, NH_2). ^{13}C NMR (100 MHz, d_6 -DMSO, TMS = 0) δ: 166.46, 147.93, 135.51, 132.68, 131.77, 131.73, 131.26, 131.15, 130.89, 129.41, 128.73, 124.23, 117.32. HRMS Calcd for $C_{18}H_{11}N_5O_2$, 329.09 [M^+]; observed: 330.1066 $[M+H]^+$

5. 2D-NMR Correlation Tables



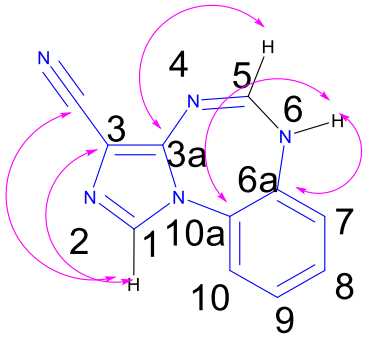
1C2



1B2

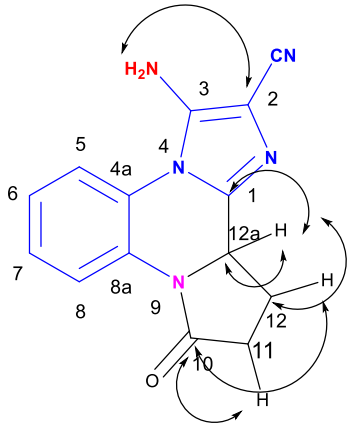
^{13}C NMR **($CDCl_3$)**	1C2	1B2	^{1}H NMR **($CDCl_3$)**	1C2	1B2
C-2	**99.68**	**104.80**	-	-	-
C-3a	**143.63**	**153.74**	-	-	-
C-4	56.22	137.12	**H-4**	5.61	-
C-A	**163.24**	**161.24**	**H-A**	**8.95**	**9.59**

C-2”	**109.69**	**111.26**	**H-2”**	**7.66 - 7.62**	**7.69 -7.65**
C-5”	**119.82**	**113.19**	**H-5”**	**8.17**	**8.18**
C-6”	**125.85**	**113.58**	**H-6”**	**7.54 – 7.52**	**7.28 -7.16**
C-1’	**131.16**	**123.97**	**H-1’**	**-**	**-**
C-2’	**110.25**	**118.18**	**H-2’**	**7.19-7.16**	**9.09**
C-5’	**111.14**	**130.42**	**H-5’**	**7.11-6.97**	**7.28 – 7.16**
C-6’	**119.59**	**111.26**	**H-6’**	**6.95-6.86**	**7.80**



^{13}C NMR (d_6 - DMSO)	**2A1**	**^{1}H NMR (d_6 - DMSO)**	**2A1**
C-1	**136.27**	**H-1**	**8.07**
C-3	**110.0**	**H-3**	**-**
C-3a	**126.51**	**H-3a**	**-**
C-5	**147.42**	**H-5**	**6.64**
NH	**-**	**NH**	**9.57**
C-6a	**146.57**	**H-6a**	**-**
C-7	**121.22**	**H-7**	**6.78 – 6.76**
C-8	**129.35**	**H-8**	**7.13 - 7.10**

C-9	**121.58**	**H-9**	**7.51 – 7.47**
C-10	**124.70**	**H-10**	**6.95 - 6.92**
C-10a	**133.51**	**H-10a**	**-**

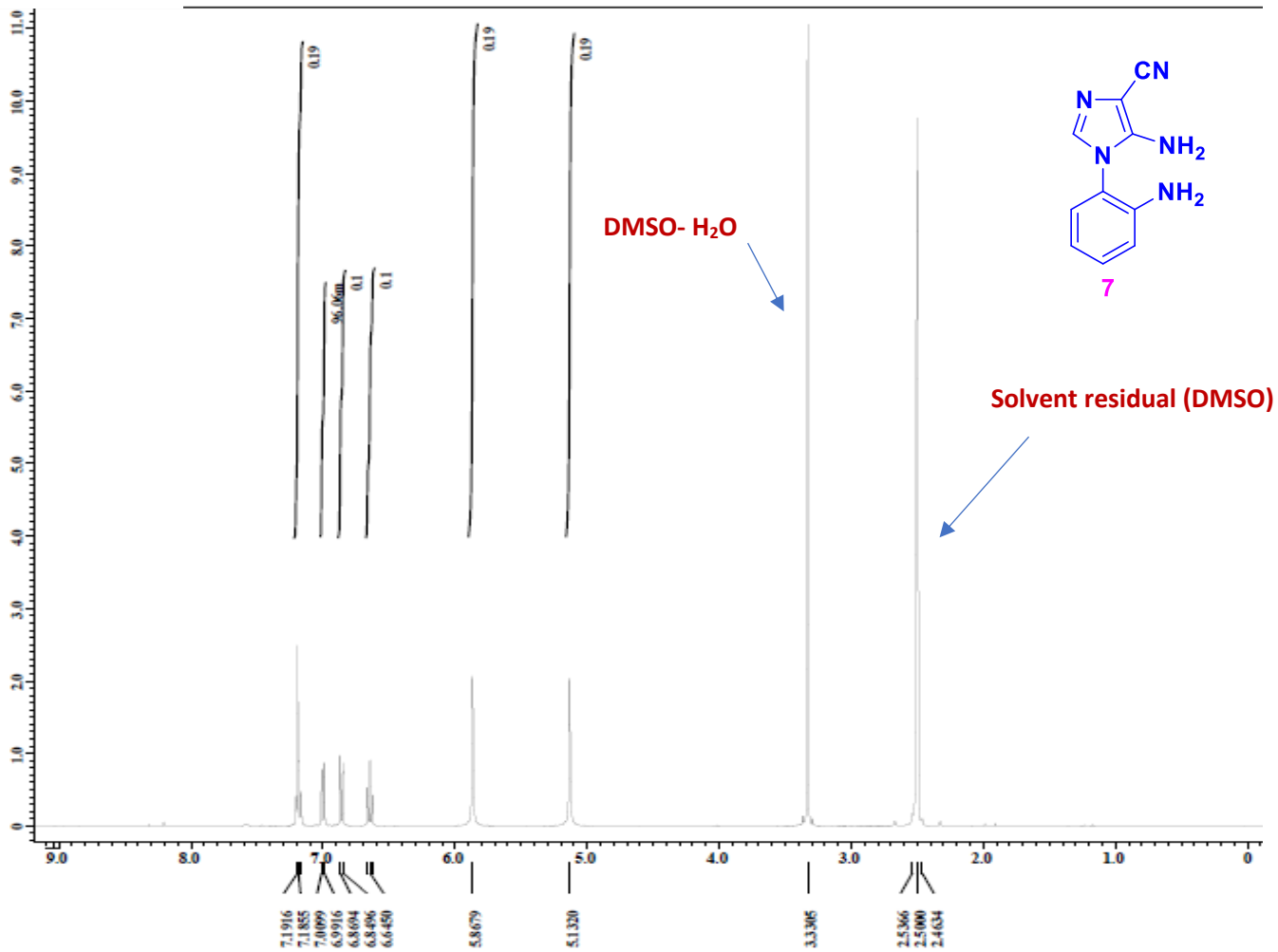


1A3

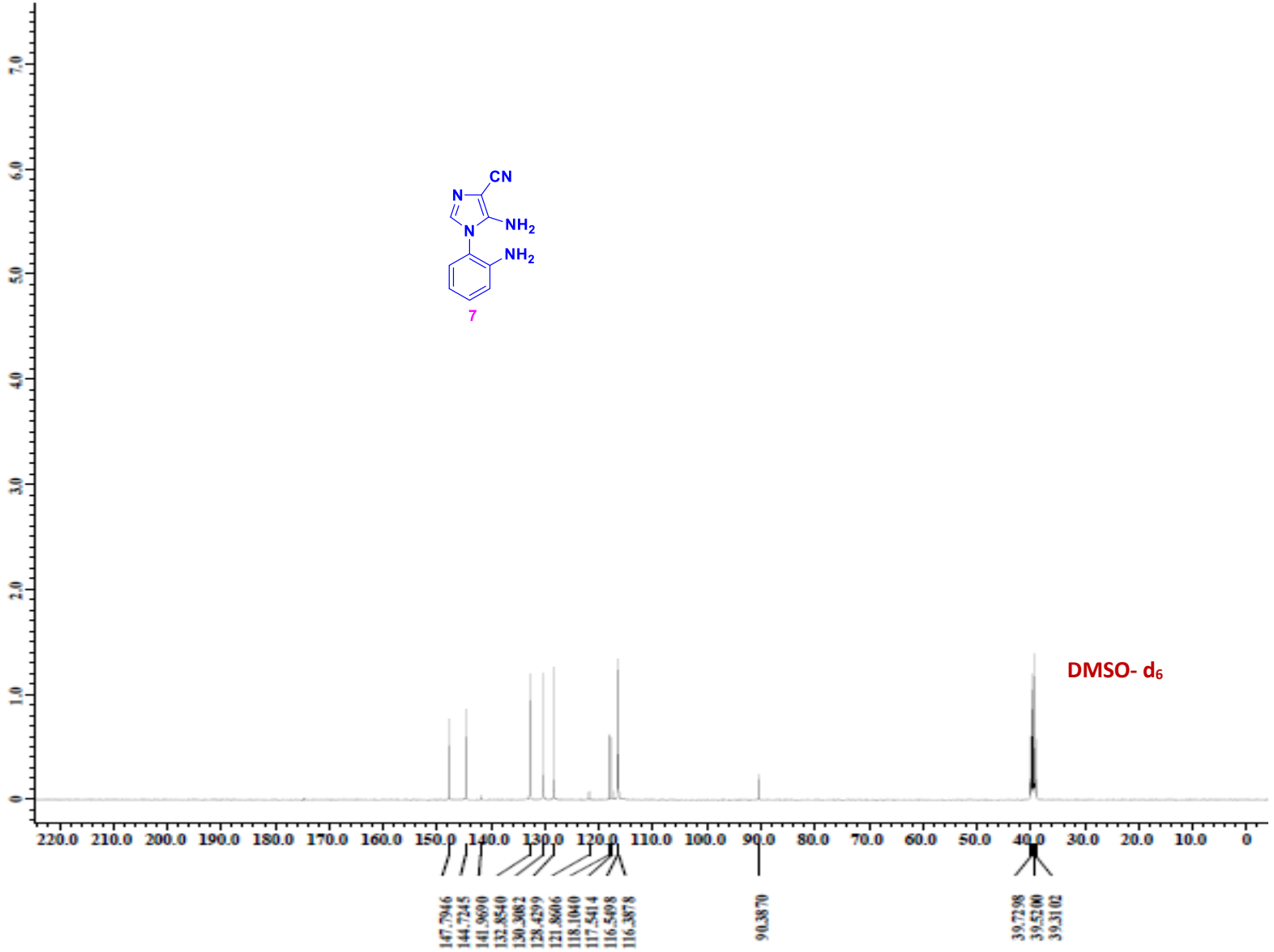
^{13}C NMR	**1A3**	^{1}**H NMR**	**1A3**
C-1	**128.22**	**H-1**	**8.01**
C-2	**93.7**	**H-2**	**-**
C-3	**146.78**	**H-3**	**6.37;**
C-4a	**118.46**	**H-4a**	**7.93; 8.01; 7.35-7.27**
C-5	**122.14**	**H-5**	**8.01; 7.93; 7.35-7.27**
C-6	**125.92**	**H-6**	**8.01, 7.35-7.27**
C-7	**126.72**	**H-7**	**7.35-7.27; 8.01**

C-8	**126.87**	**H-8**	**7.35-7.27; 8.01**
C-8a	**141.11**	**H-8a**	**-**
C-10	**173.79**	**H-10**	**-**
C-11	**30.99**	**H-11**	**2.41-2.28; 2.69-2.46**
C-12	**21.85**	**H-12**	**2.69-2.46; 2.41-2.28; 4.87-4.83**
C-12a	**53.84**	**H-12a**	**4.87-4.83; 2.69-2.46; 2.41-2.28**
-CN	**117.02**		**-**
$-NH_2$		**NH_2**	**6.37**

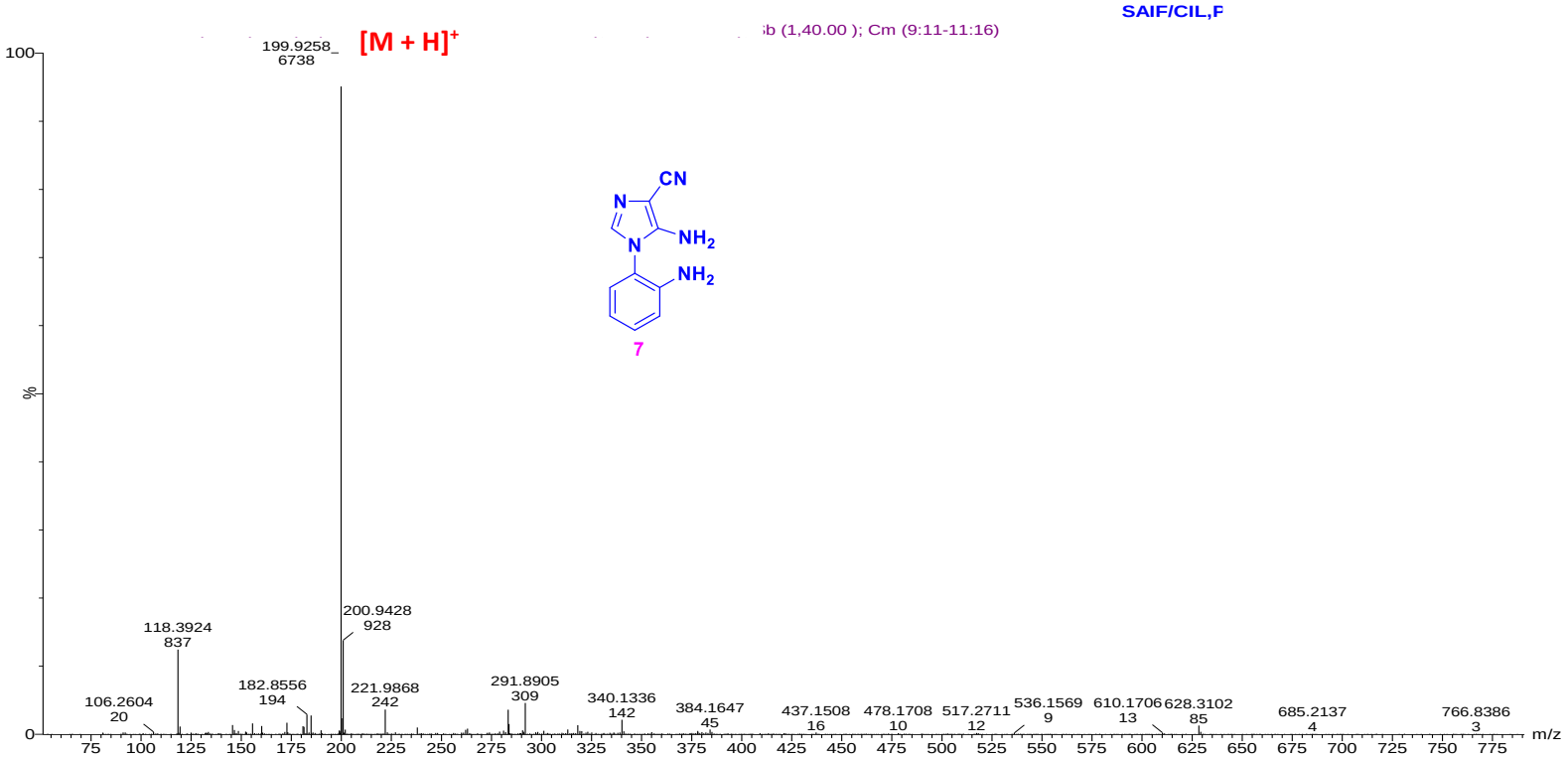
^{1}H NMR



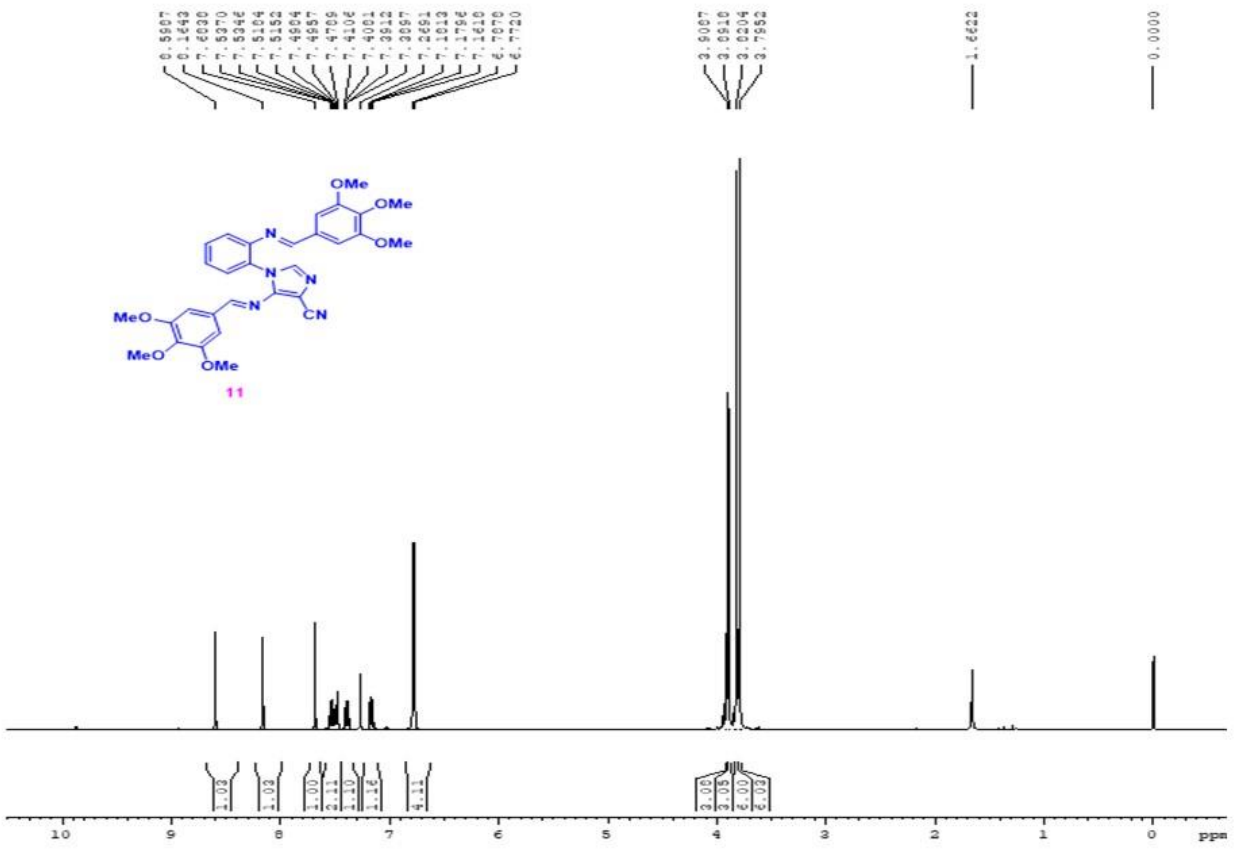
^{13}C NMR


CN
N
NH2
N
NH2
7
DMSO- d6
147.7946
144.7245
141.9690
132.8540
130.3082
128.4299
121.8606
118.1040
117.5414
116.5498
116.3878
90.3870
39.7298
39.5200
39.3102

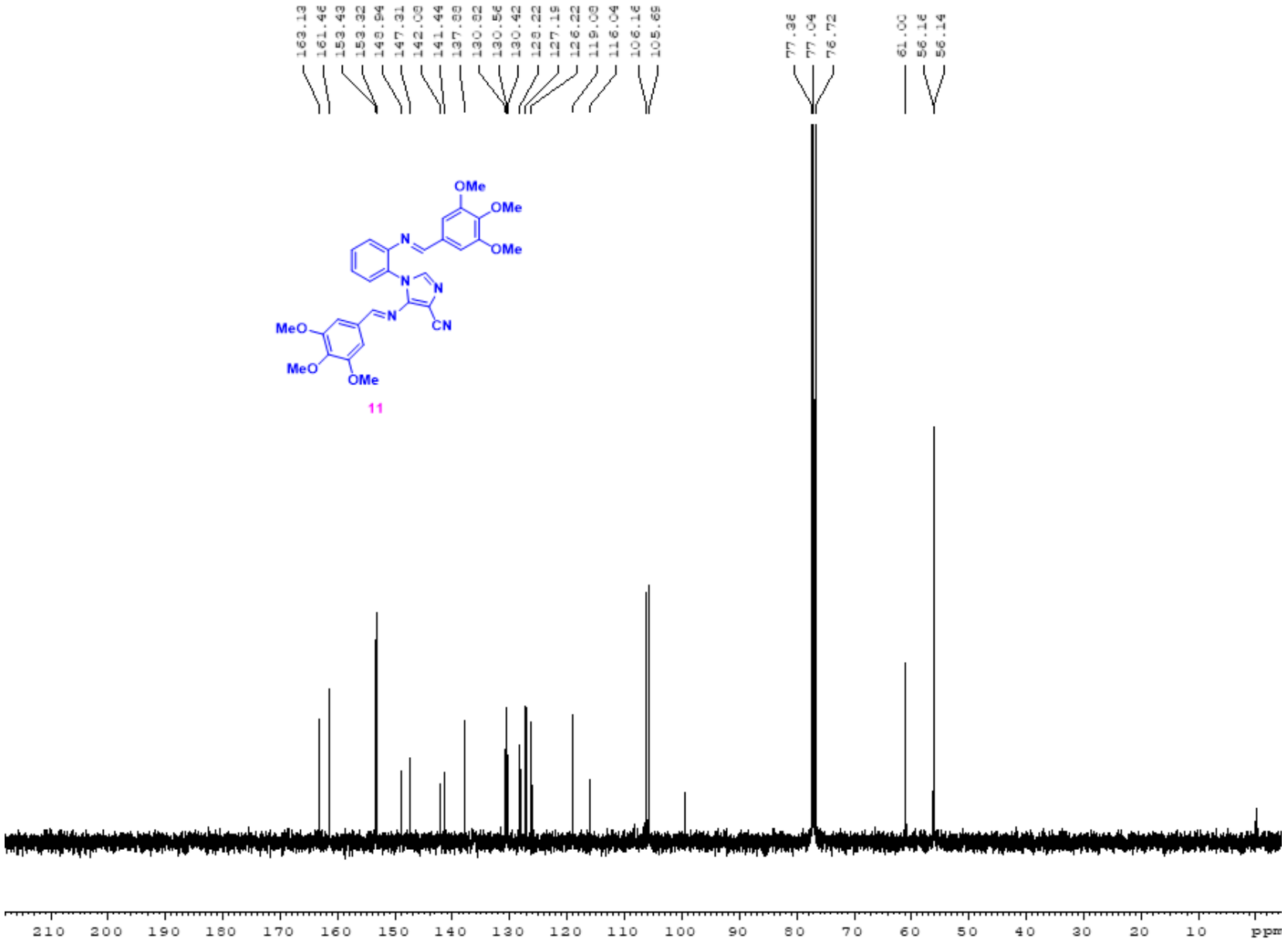
HRMS


SAIF/CIL,F
b (1,40.00); Cm (9:11-11:16)
199.9258
6738
[M + H]+
CN
N
N
NH2
NH2
7
100
%
0
200.9428
928
118.3924
837
106.2604
20
182.8556
194
221.9868
242
291.8905
309
340.1336
142
384.1647
45
437.1508
16
478.1708
10
517.2711
12
536.1569
9
610.1706
13
628.3102
85
685.2137
4
766.8386
3
75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775
m/z

^{1}H NMR


OMe
OMe
OMe
N
N
N
N
CN
MeO
MeO
OMe
11
3.9067
3.8810
3.8204
3.7552
1.6422
0.0000
1.03
1.02
1.00
2.11
1.10
2.16
4.11
2.08
3.05
6.00
6.08
10
9
8
7
6
5
4
3
2
1
0
ppm

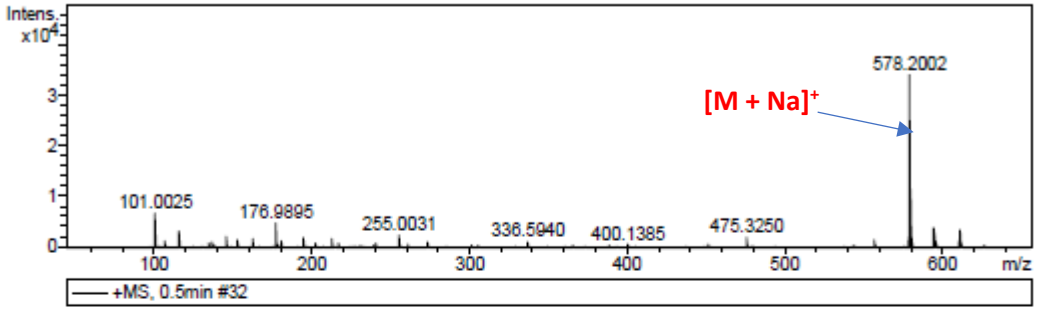
^{13}C NMR


163.13
161.46
153.43
153.32
148.94
147.31
142.08
141.44
137.88
130.82
130.56
130.42
128.22
127.19
126.22
119.08
116.04
106.16
105.69
77.36
77.04
76.72
61.00
56.16
56.14
OMe
OMe
OMe
N
N
N
N
CN
MeO
MeO
OMe
11
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

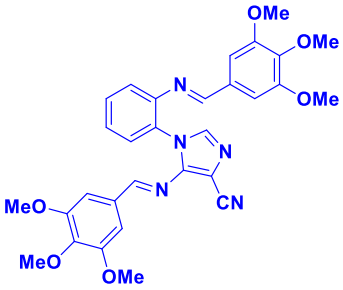
HRMS

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	650 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

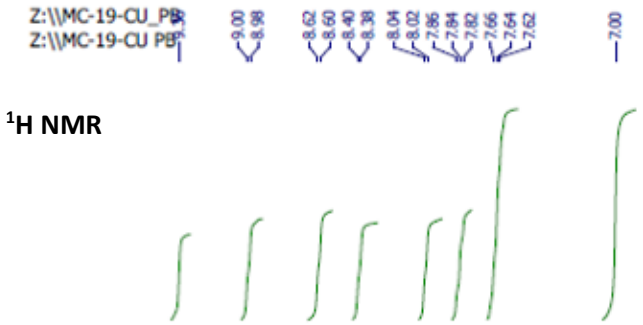


#	m/z	Res.	S/N	I	FWHM
1	101.0025	12713	137.3	6690	0.0079
2	106.9994	13458	23.5	1270	0.0080
3	116.0048	13754	61.1	3252	0.0084
4	134.9789	14539	17.2	884	0.0093
5	137.0016	14226	21.7	1112	0.0096
6	146.0066	14515	45.9	2313	0.0101
7	153.1387	15245	31.4	1618	0.0100
8	162.9737	15123	34.6	1854	0.0108
9	176.9895	16125	85.5	4812	0.0110
10	180.9832	14666	13.6	777	0.0123
11	181.0619	14636	22.8	1300	0.0124
12	194.9999	15969	34.2	1901	0.0122
13	202.1084	16771	18.5	985	0.0121
14	212.9930	16624	35.3	1739	0.0128
15	216.9829	14255	19.8	949	0.0152
16	240.9877	17042	24.0	1015	0.0141
17	255.0031	16823	57.6	2331	0.0152
18	261.1314	17790	18.8	743	0.0147
19	273.1959	17581	29.9	1114	0.0155
20	336.5940	17226	43.4	1235	0.0195
21	451.2217	18717	27.2	730	0.0241
22	475.3250	17992	72.5	2106	0.0264
23	556.2179	20375	46.5	1630	0.0273
24	578.2002	18973	366.4	33910	0.0305
25	579.2033	19005	121.7	11581	0.0305
26	580.2060	19178	23.0	2249	0.0303
27	594.1747	18704	29.3	3913	0.0318
28	595.1778	18889	10.9	1429	0.0315
29	610.2264	19159	39.2	3536	0.0319
30	611.2294	17098	12.8	1121	0.0357



11

^{1}H NMR


Z:\\MC-19-CU_PB
Z:\\MC-19-CU PB
9.00
8.98
8.62
8.60
8.40
8.38
8.04
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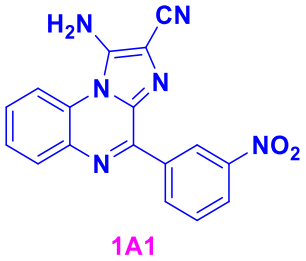
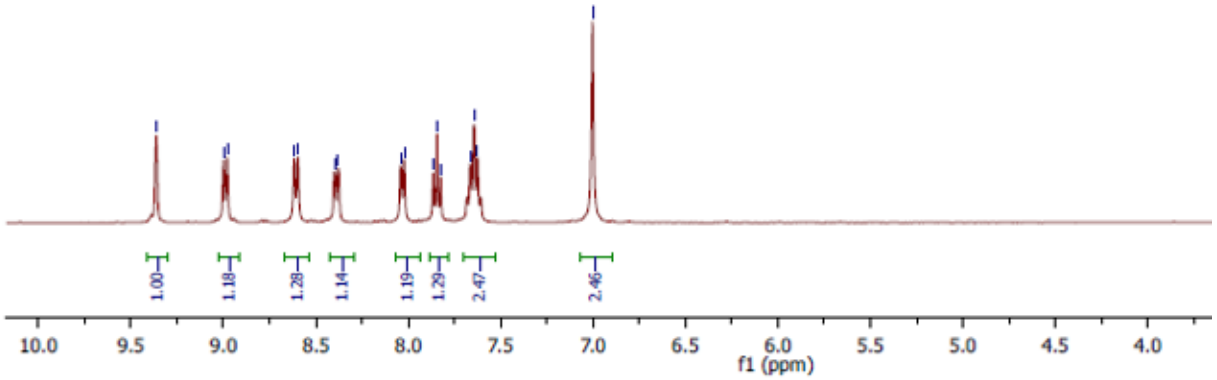
7.86
7.84
7.82
7.66
7.64
7.62
7.00


H2N
CN
N
N
N
NO2

1A1


1.00
1.18
1.28
1.14
1.19
1.29
2.47
2.46
10.0
9.5
9.0
8.5
8.0
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7.0
6.5
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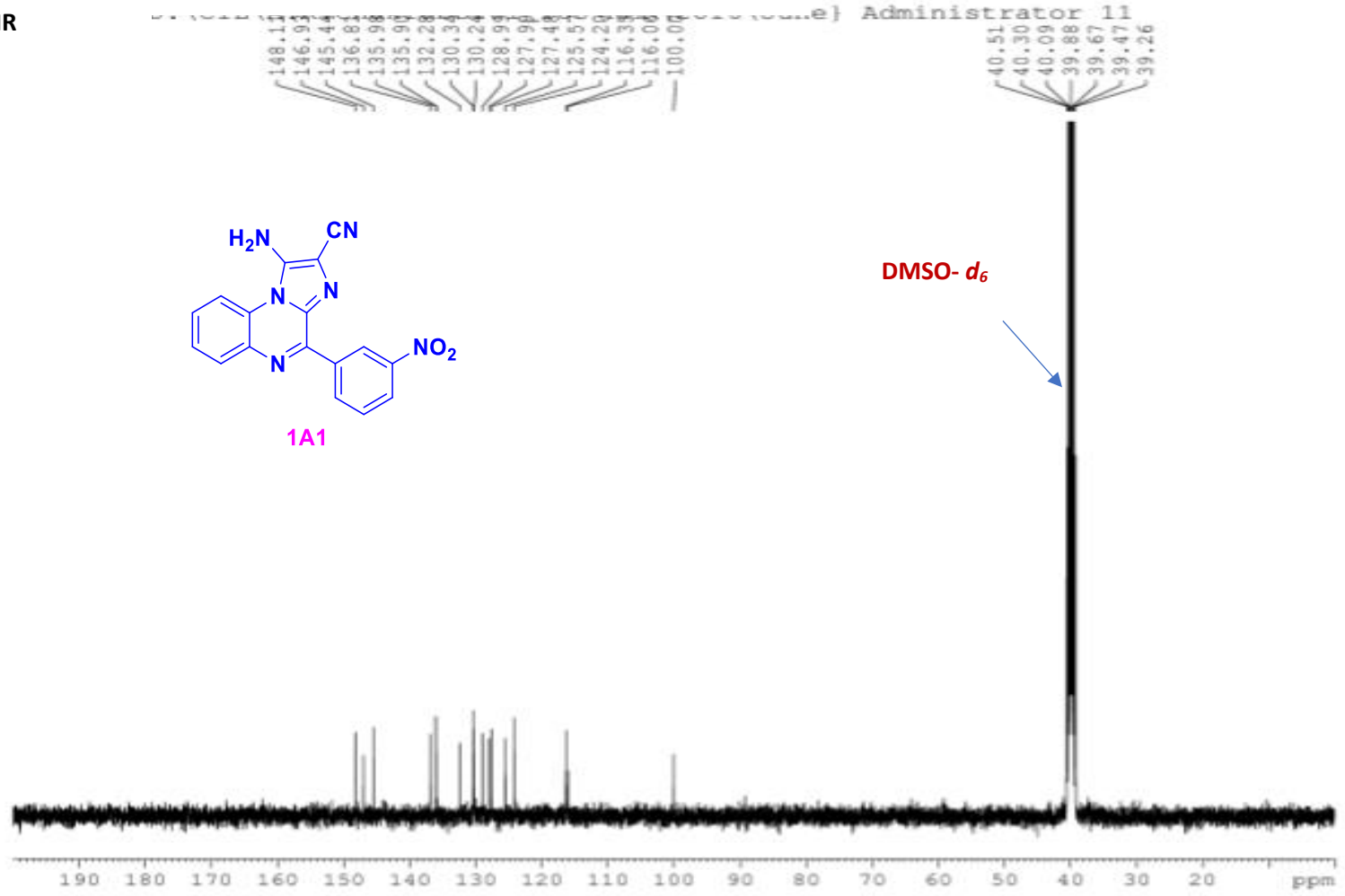
5.5
5.0
4.5
4.0
f1 (ppm)

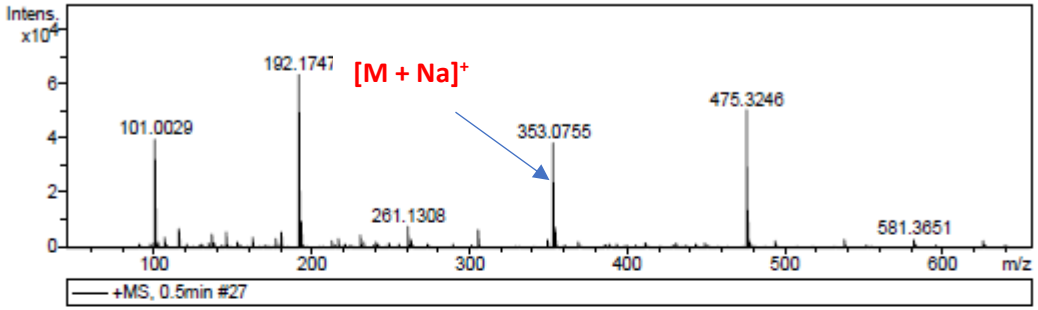
^{13}C NMR


Administrator 11
148.15
146.93
145.44
136.81
135.98
135.90
132.28
130.34
130.24
128.99
127.96
127.48
125.51
124.20
116.38
116.00
100.04
40.51
40.30
40.09
39.88
39.67
39.47
39.26
H2N
CN
N
N
N
NO2
1A1
DMSO- d6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

HRMS

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	650 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
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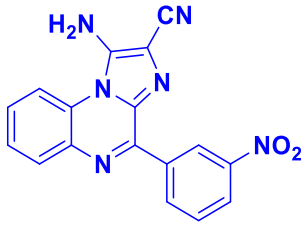
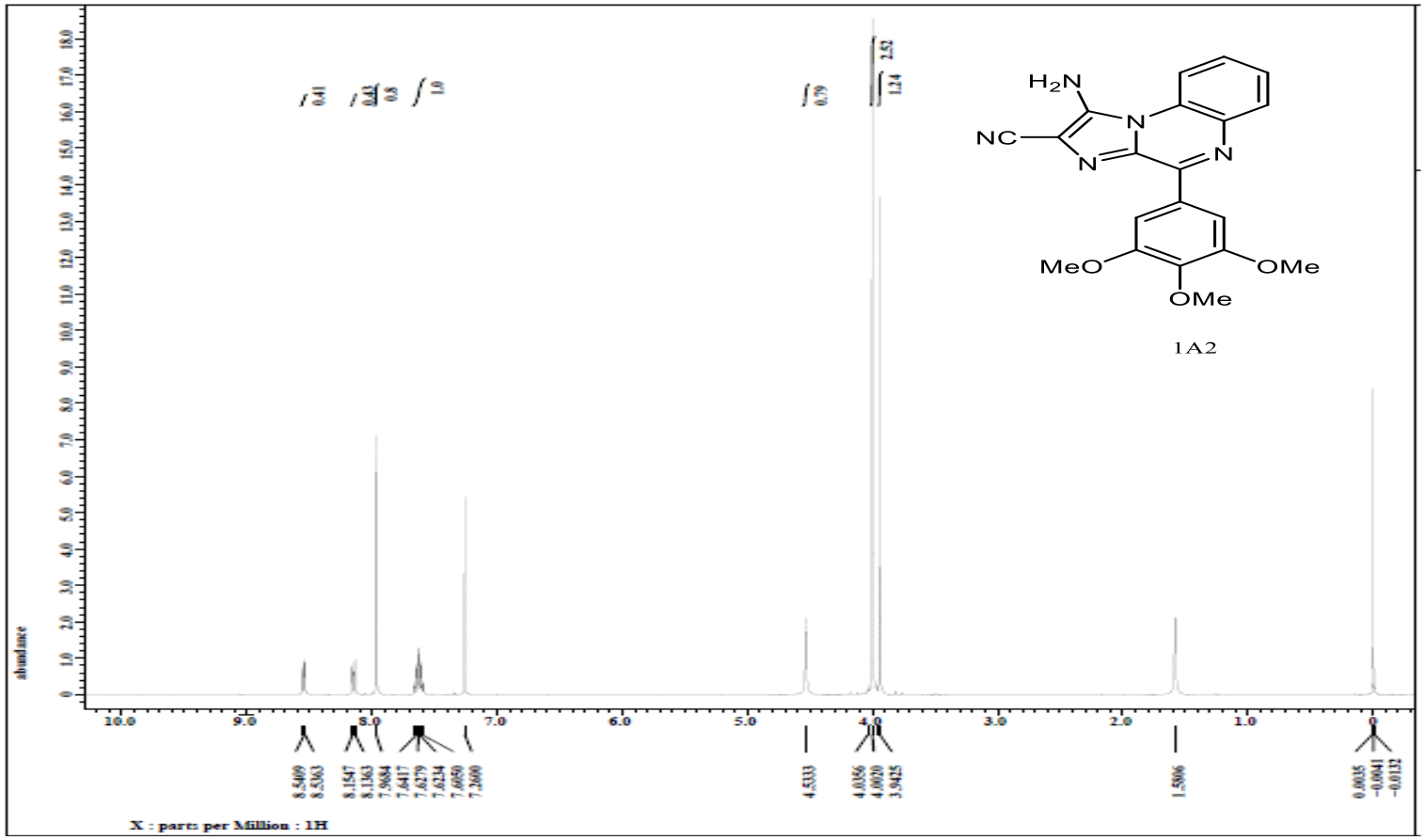
2	102.9989	12807	33.0	2050	0.0080
3	106.9998	13682	55.9	3692	0.0078
4	116.0052	13917	102.4	6806	0.0083
5	137.0017	14437	72.5	4895	0.0095
6	146.0070	14964	86.6	5878	0.0098
7	152.9448	14540	25.7	2016	0.0105
8	162.9738	15471	39.4	3758	0.0105
9	176.9899	15099	26.8	3182	0.0117
10	181.0617	14924	44.6	5605	0.0121
11	192.1747	15652	489.0	63134	0.0123
12	193.1781	15639	75.0	9576	0.0124
13	212.9930	17209	25.9	2582	0.0124
14	216.9893	14890	29.1	2744	0.0146
15	217.1047	15581	35.5	3342	0.0139
16	230.9589	15919	60.0	4695	0.0145
17	261.1308	17398	104.3	7596	0.0150
18	263.0379	17171	42.2	3057	0.0153
19	305.1569	17045	117.2	6504	0.0179
20	349.1830	17204	25.6	2812	0.0203
21	353.0755	18471	359.2	38243	0.0191
22	354.0783	17470	69.4	7284	0.0203
23	369.0493	17558	25.2	2094	0.0210
24	475.3246	18615	345.1	50404	0.0255
25	476.3279	18383	95.4	13670	0.0259
26	477.3304	17742	16.2	2281	0.0269
27	493.3124	19056	27.7	2892	0.0259
28	537.3386	18338	61.3	2881	0.0293
29	581.3651	18876	67.4	2945	0.0308
30	625.3915	18655	64.6	2704	0.0335

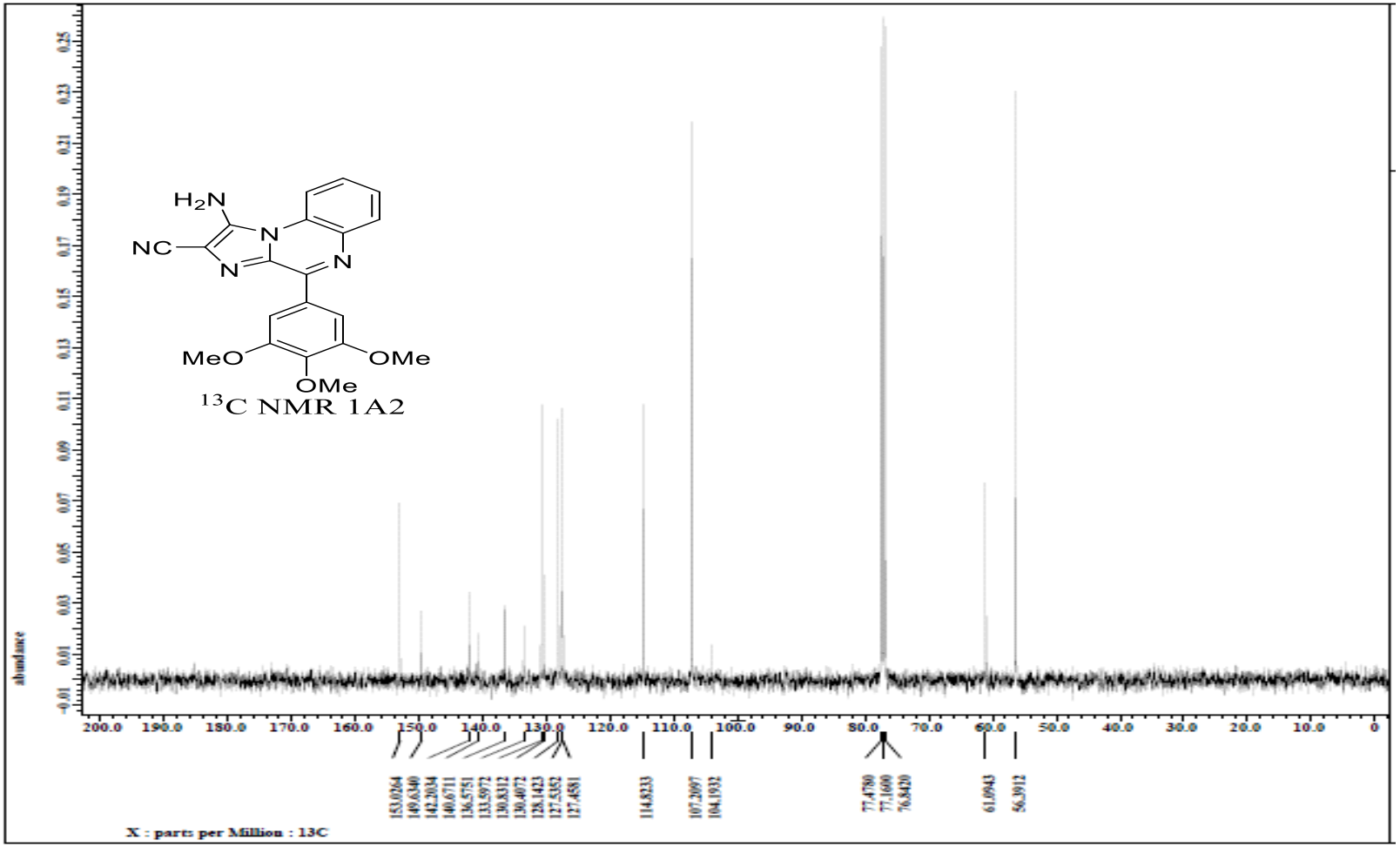


1A1

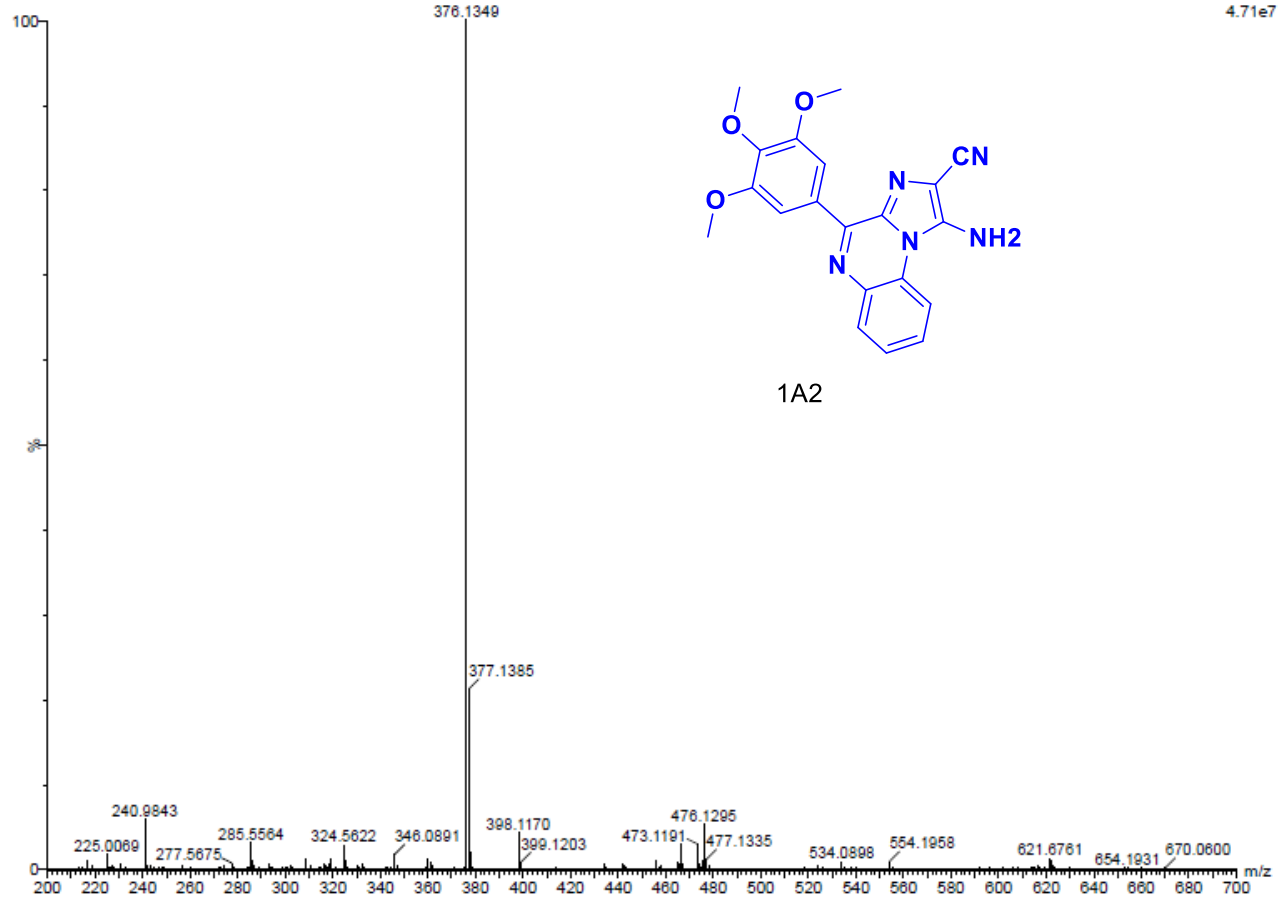
^{1}H NMR



^{13}C NMR


H2N
NC
N
N
N
MeO
OMe
OMe
13C NMR 1A2
abundance
X : parts per Million : 13C
153.0264
149.6340
142.2034
140.6711
136.5751
133.5972
130.8312
130.4072
128.1423
127.5352
127.4581
114.8233
107.2097
104.1932
77.4780
77.1600
76.8420
61.0943
56.3912

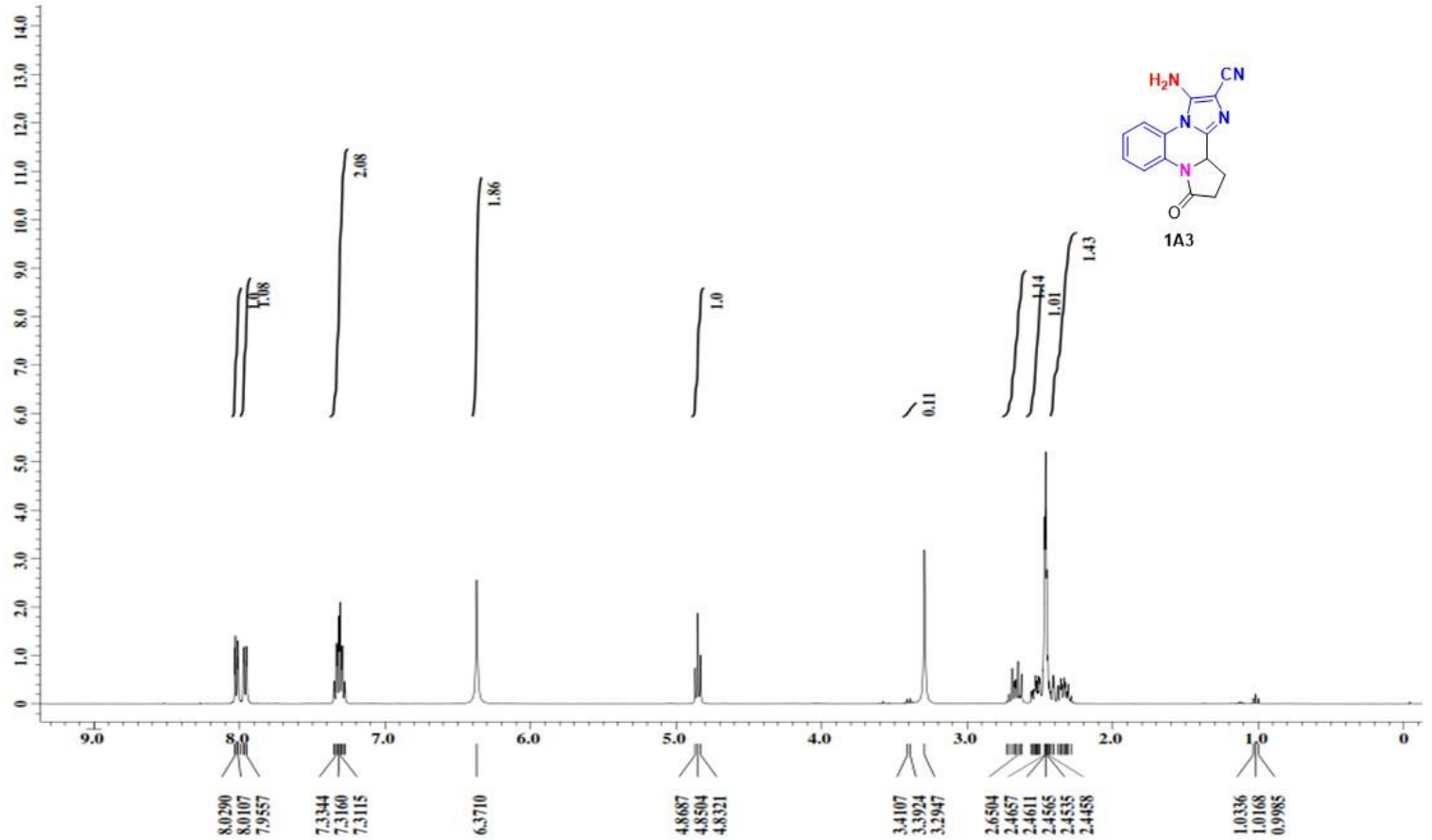
HRMS


376.1349
4.71e7
100
%
0
377.1385
240.9843
225.0069
277.5675
285.5564
324.5622
346.0891
398.1170
399.1203
473.1191
476.1295
477.1335
534.0898
554.1958
621.6761
654.1931
670.0600
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
m/z

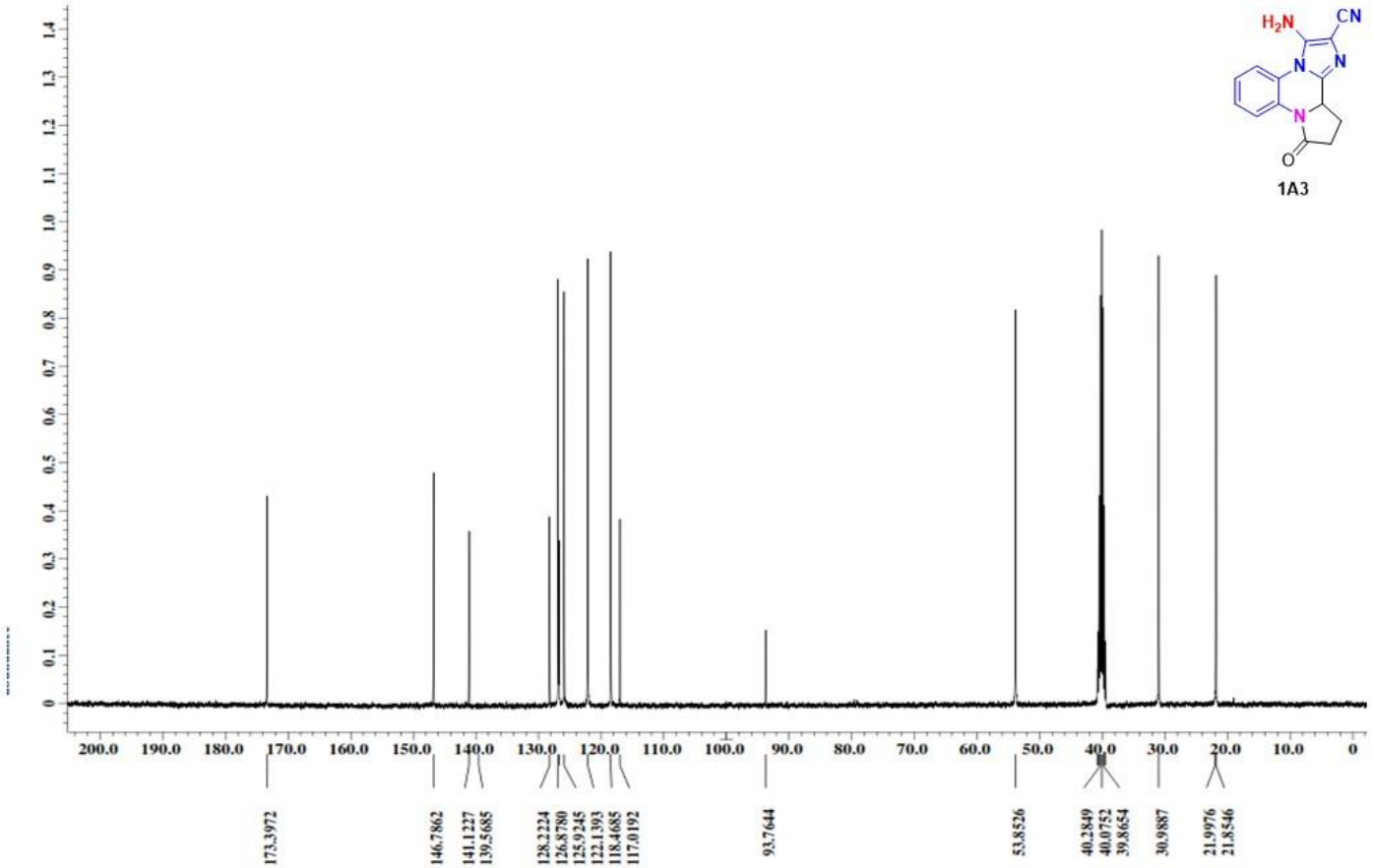
O
O
O
CN
N
N
NH2
N

1A2

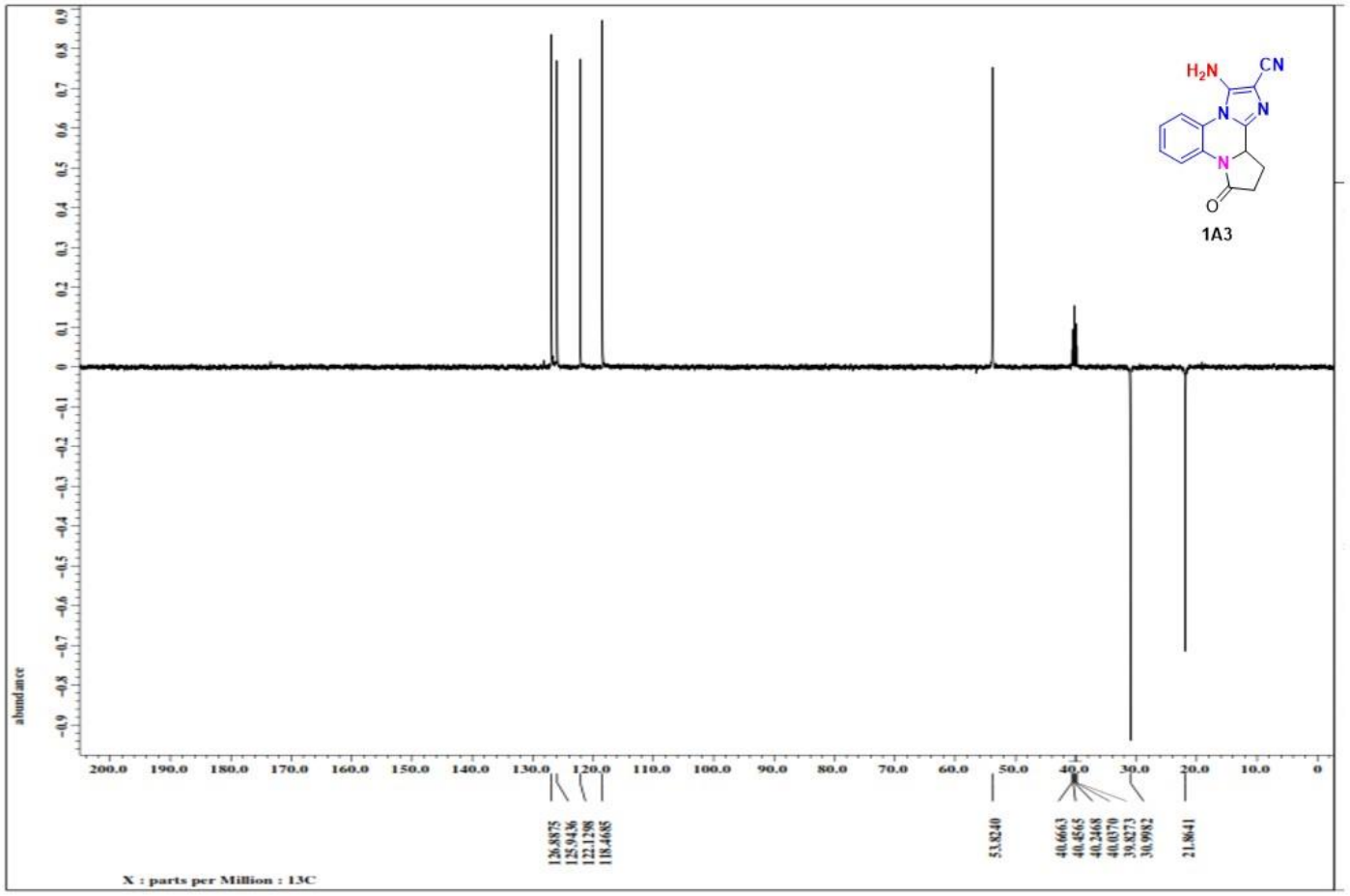
^{1}H NMR


1A3
2.08
1.86
1.08
1.0
1.0
0.11
1.14
1.01
1.43
8.0290
8.0107
7.9557
7.3344
7.3160
7.3115
6.3710
4.8687
4.8504
4.8321
3.4107
3.3924
3.2947
2.6504
2.4657
2.4611
2.4565
2.4535
2.4458
1.0336
1.0168
0.9985

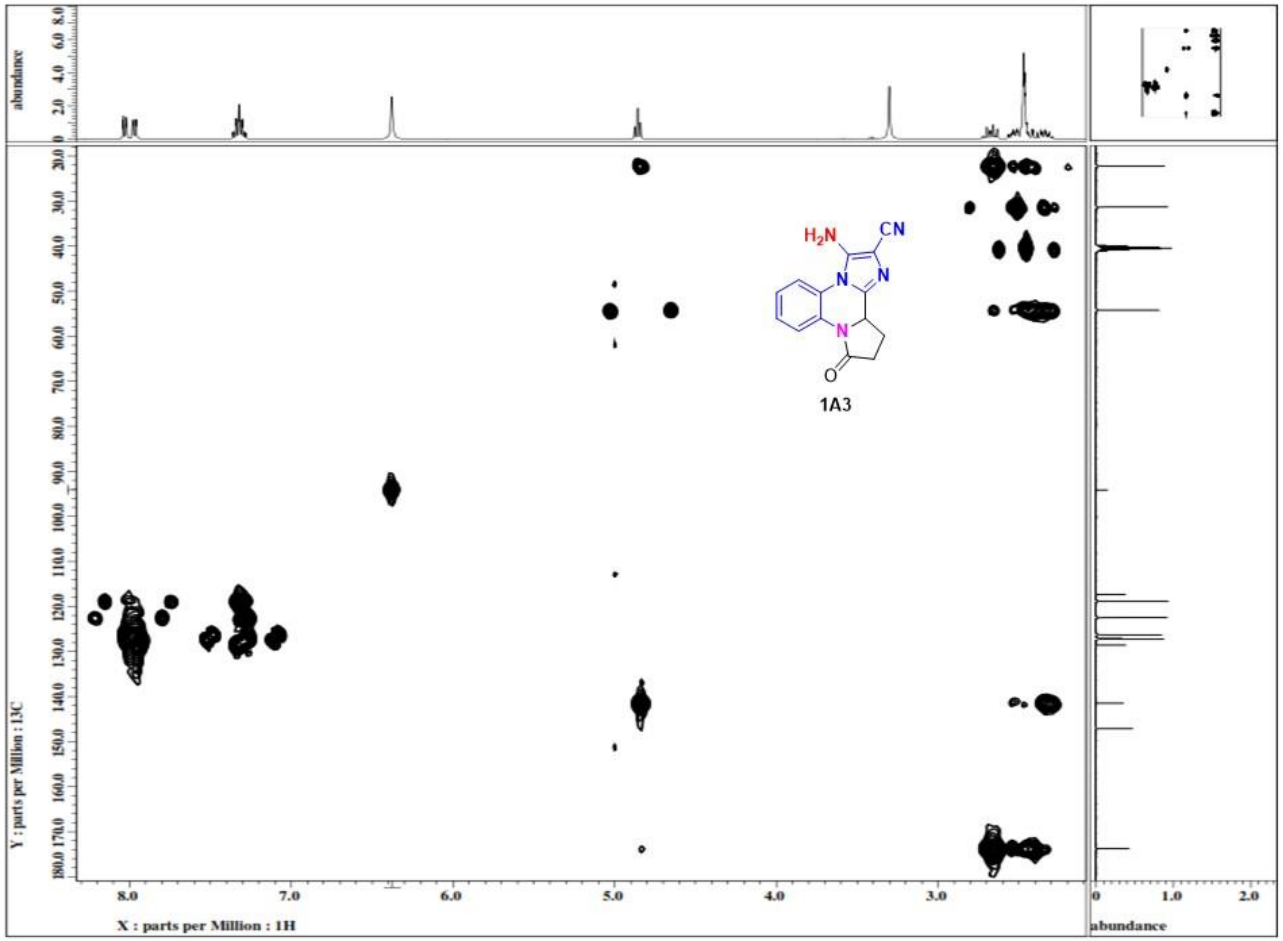
^{13}C NMR


H2N
CN
N
N
N
O
1A3
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
173.3972
146.7862
141.1227
139.5685
128.2224
126.8780
125.9245
122.1393
118.4685
117.0192
93.7644
53.8526
40.2849
40.0752
39.8654
30.9887
21.9976
21.8546

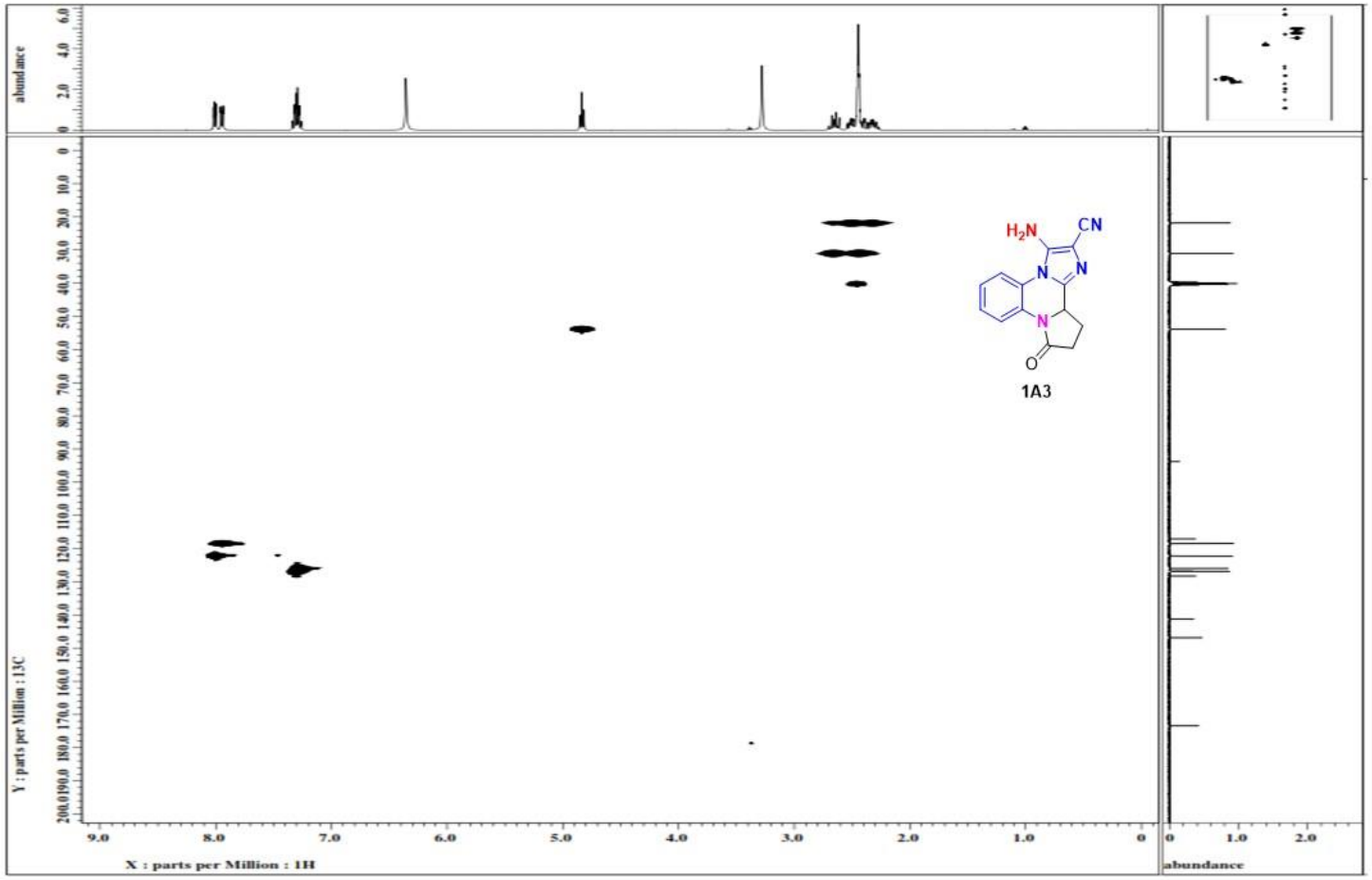
DEPT-135


H2N
CN
N
N
N
O
1A3
abundance
X : parts per Million : 13C
126.8875
125.9436
122.1298
118.4685
53.8240
40.6663
40.4565
40.2468
40.0370
39.8273
30.9982
21.8641

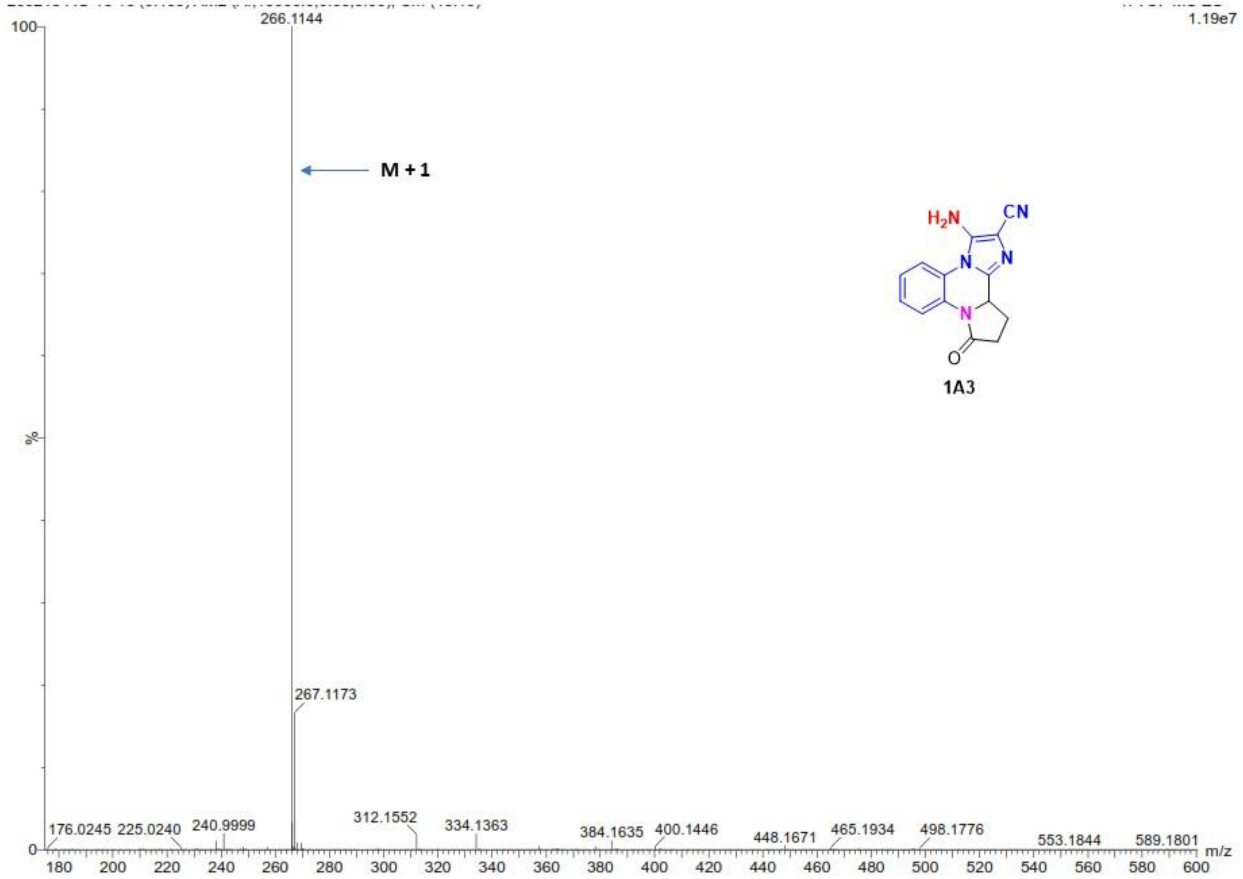
HMBC


abundance
Y : parts per Million : 13C
X : parts per Million : 1H
abundance
H2N
CN
N
N
N
O
1A3

HSQC

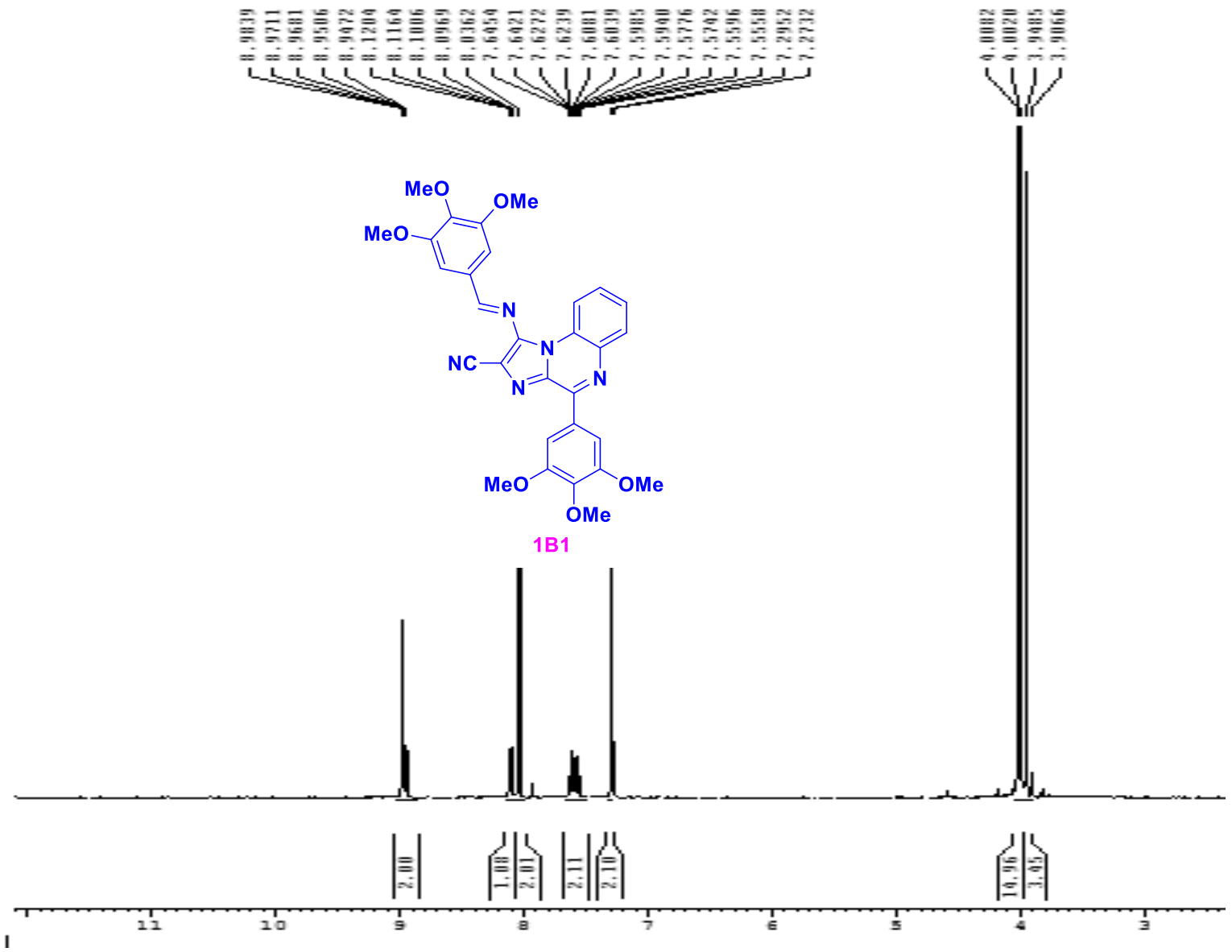

abundance
Y : parts per Million : 13C
X : parts per Million : 1H
abundance
H2N
CN
N
N
N
O
1A3

HRMS

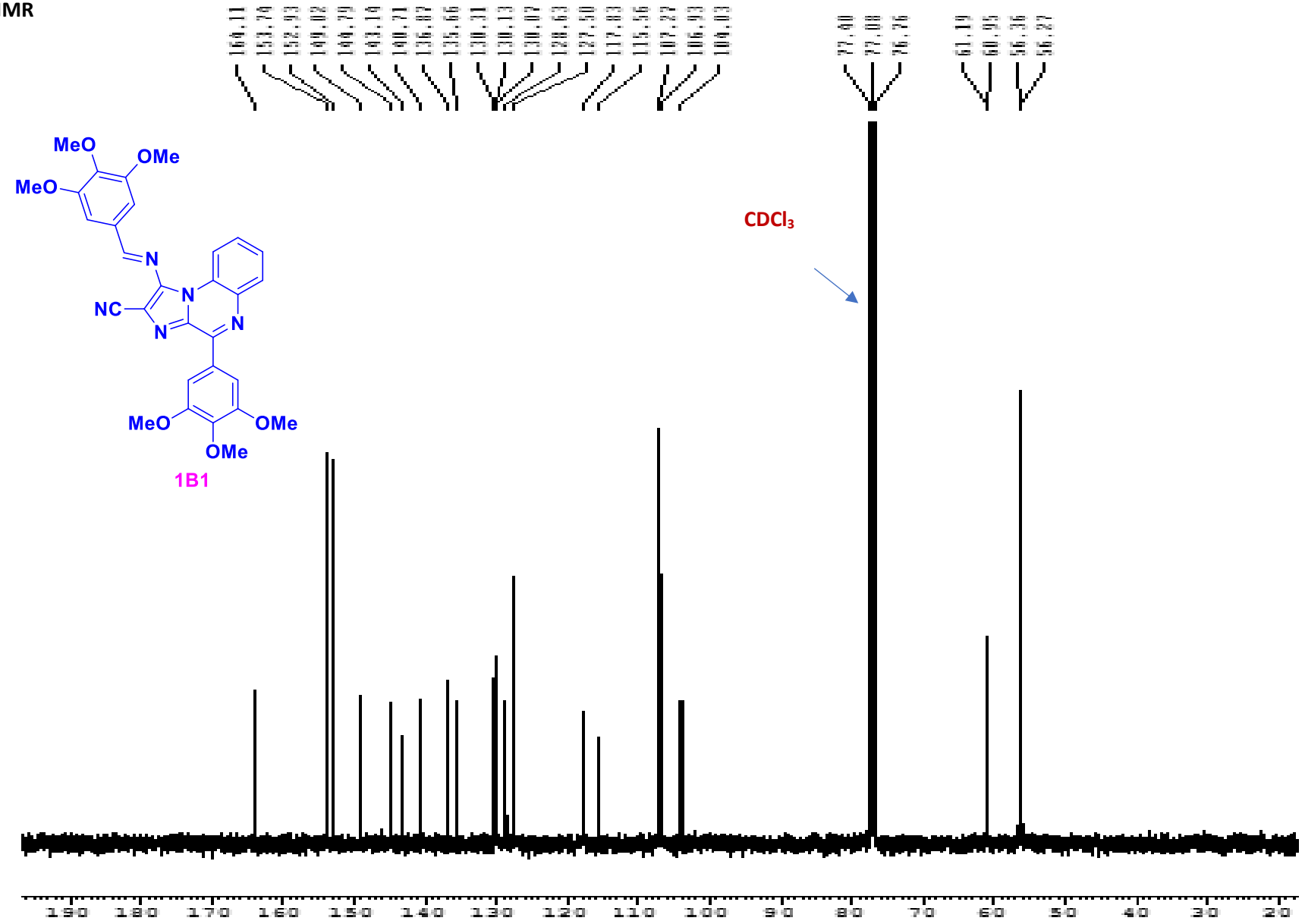

266.1144
1.19e7
100
M + 1
%
267.1173
176.0245
225.0240
240.9999
312.1552
334.1363
384.1635
400.1446
448.1671
465.1934
498.1776
553.1844
589.1801
m/z
0
180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
H2N
CN
N
N
N
O

1A3

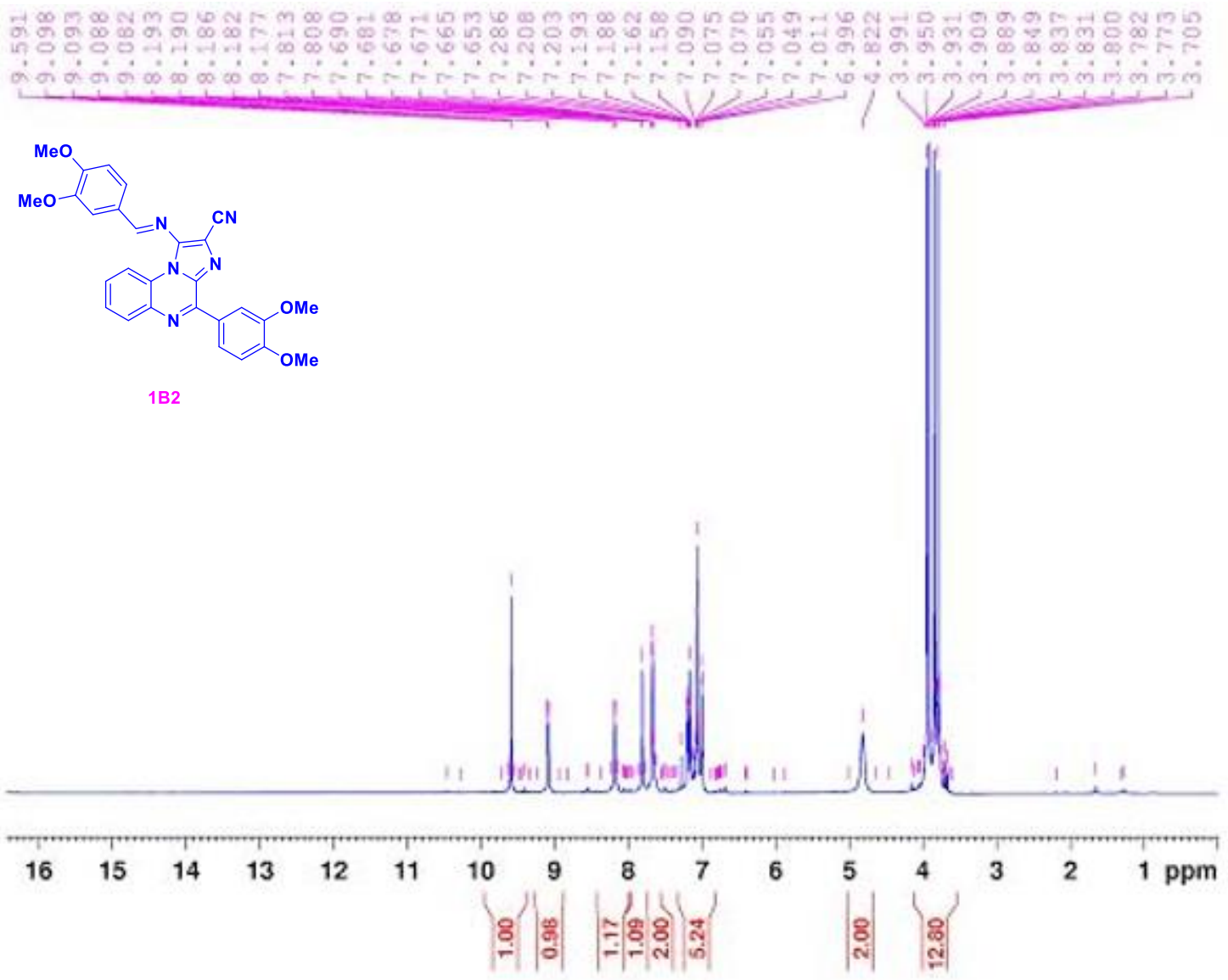
^{1}H NMR

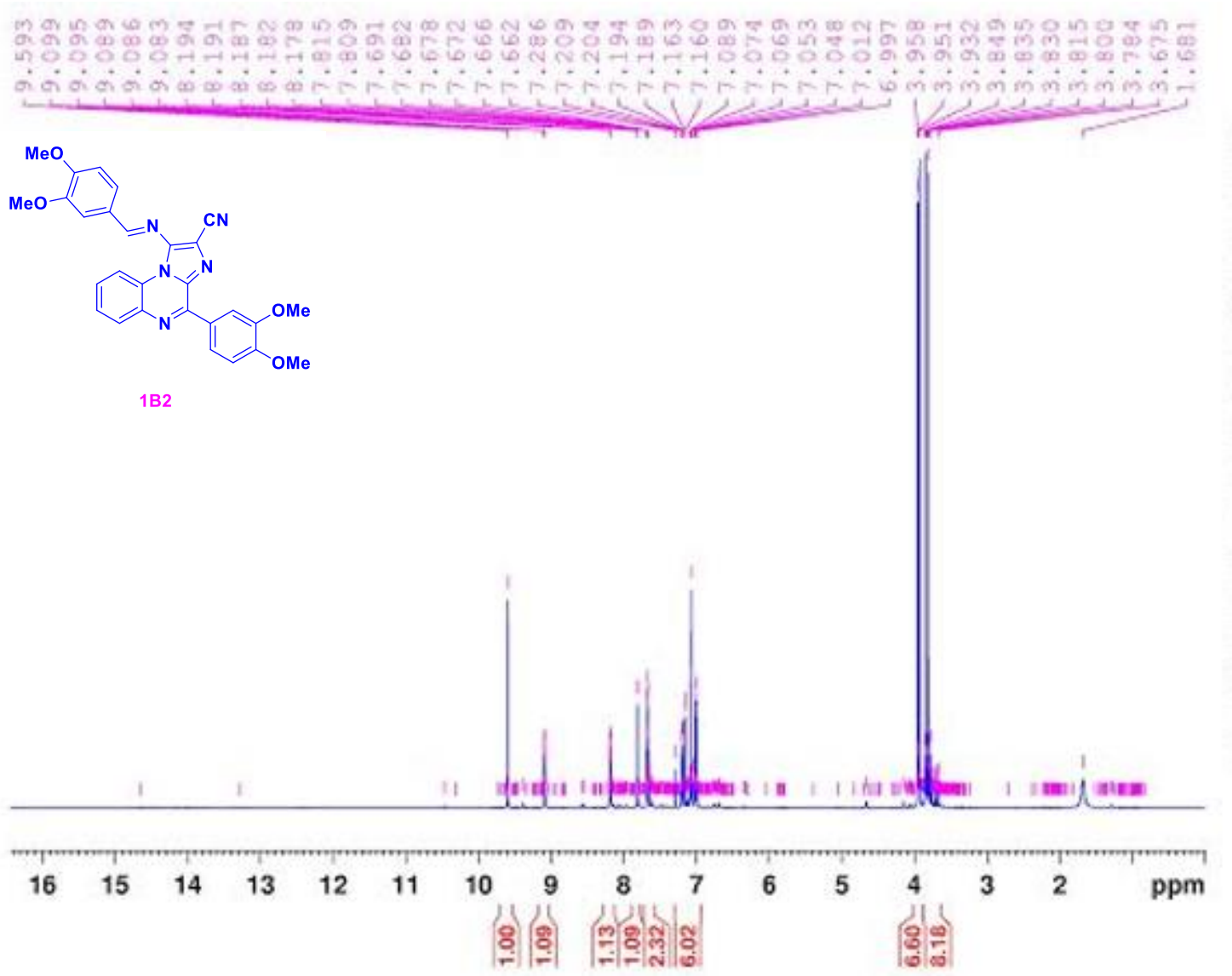

8.9839
8.9711
8.9681
8.9586
8.9472
8.1204
8.1164
8.1086
8.0969
8.0362
7.6459
7.6421
7.6272
7.6239
7.6081
7.6039
7.5985
7.5940
7.5776
7.5742
7.5596
7.5558
7.2952
7.2732
4.0082
4.0020
3.9485
3.9066
MeO
OMe
MeO
N
N
NC
N
N
MeO
OMe
OMe
1B1
2.00
1.08
2.01
2.11
2.10
10.96
3.05
11
10
9
8
7
6
5
4
3

^{13}C NMR

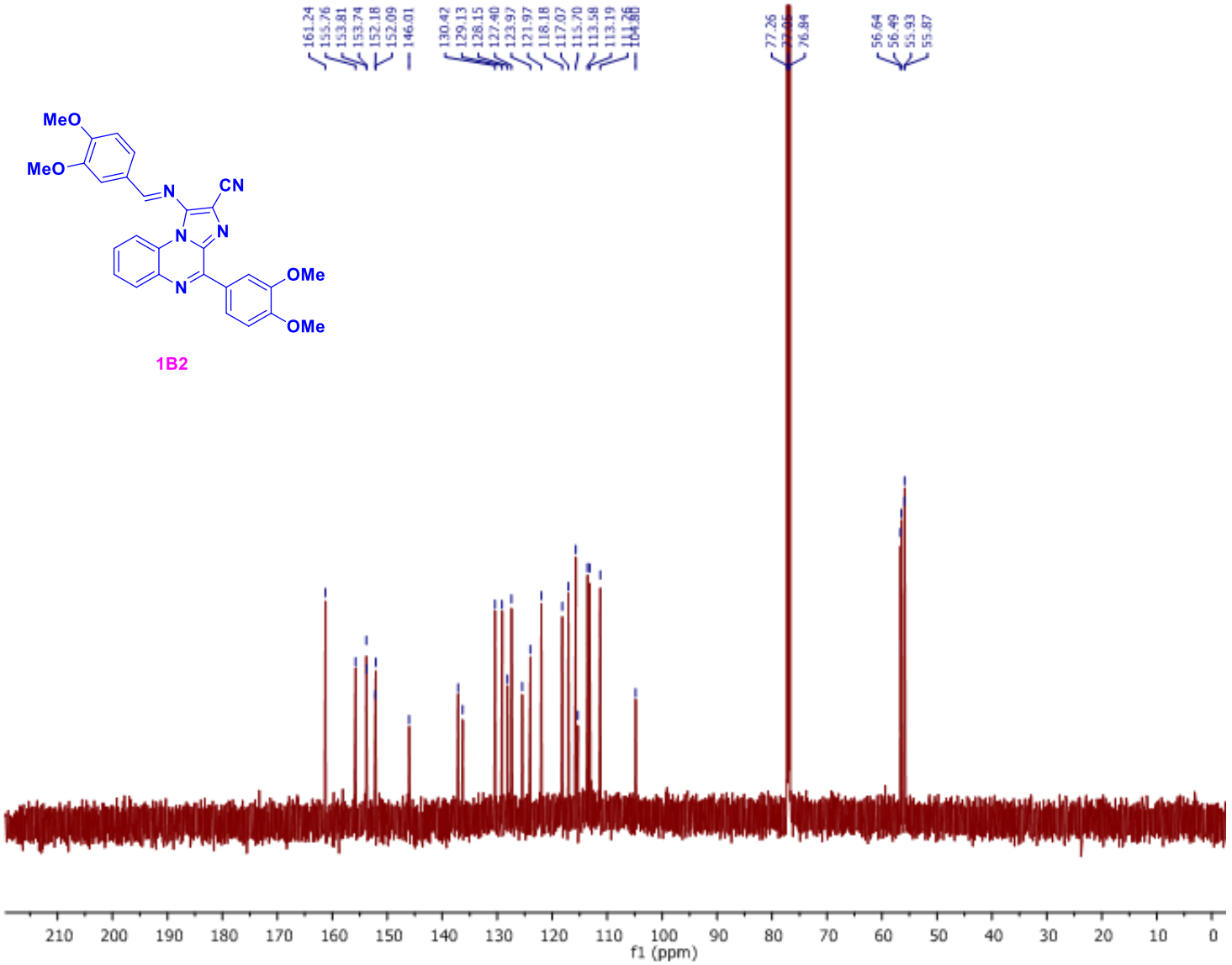

164.11
151.79
152.93
149.02
146.79
141.19
140.71
136.82
135.66
130.71
130.13
130.02
128.63
122.50
117.83
115.56
107.27
106.93
104.03
77.40
77.08
76.76
61.19
60.95
56.36
56.22
MeO
OMe
MeO
N
NC
N
N
MeO
OMe
OMe
1B1
CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20

IH NMR

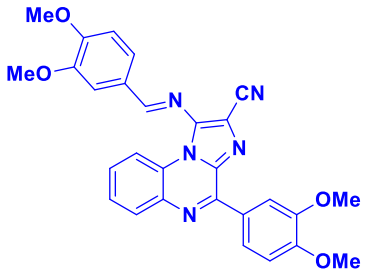

9.591
9.098
9.093
9.088
9.082
8.193
8.190
8.186
8.182
8.177
7.813
7.808
7.690
7.681
7.678
7.671
7.665
7.653
7.286
7.208
7.203
7.193
7.188
7.162
7.158
7.090
7.075
7.070
7.055
7.049
7.011
6.996
4.822
3.991
3.950
3.931
3.909
3.889
3.849
3.837
3.831
3.800
3.782
3.773
3.705
MeO
MeO
N
CN
N
N
N
OMe
OMe
1B2
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
0.98
1.17
1.09
2.00
5.24
2.00
12.80


MeO
MeO
N
CN
N
N
N
OMe
OMe
1B2
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
ppm
1.00
1.09
1.13
1.09
2.32
6.02
6.60
8.16

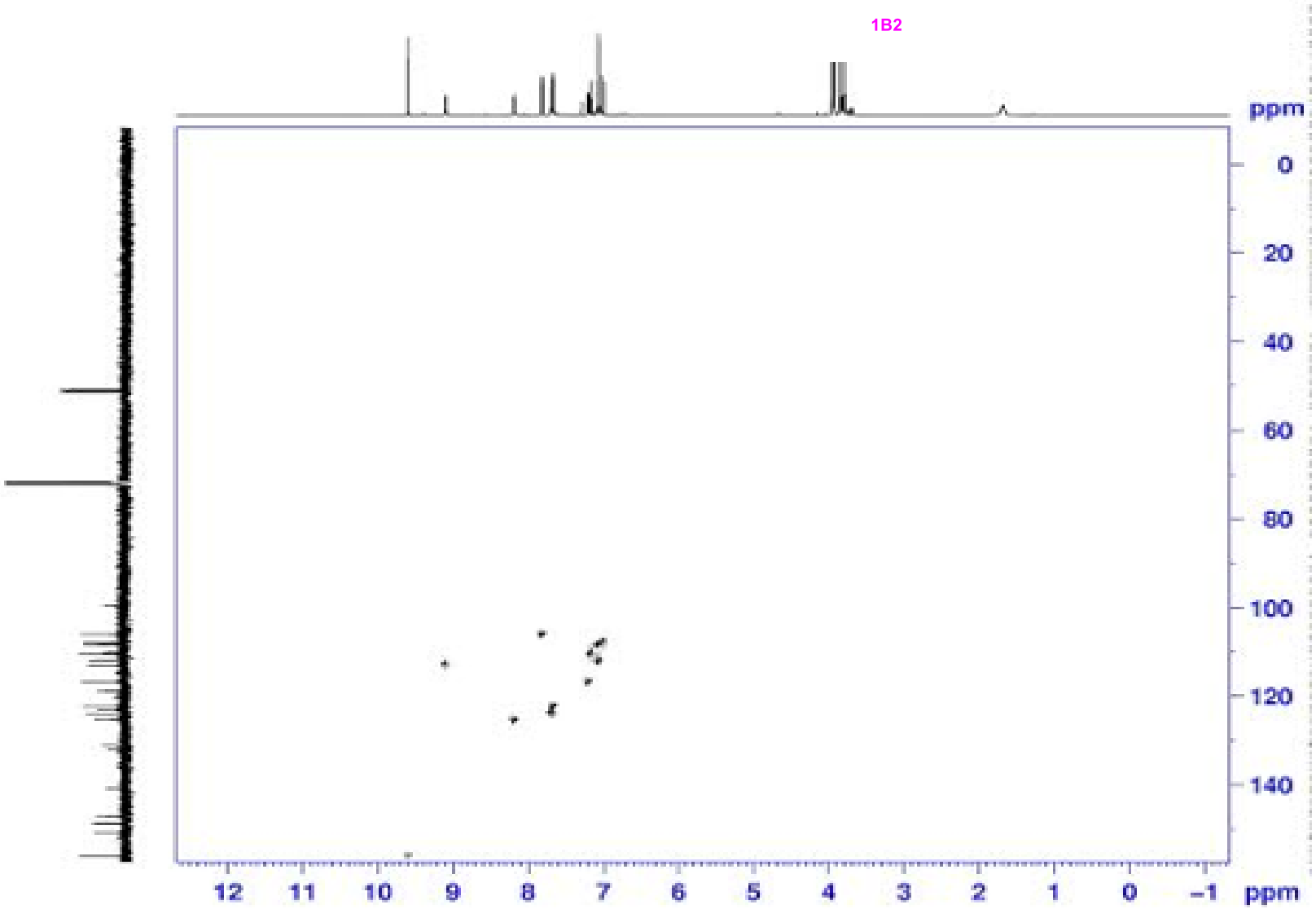
^{13}C NMR


161.24
155.76
153.81
153.74
152.18
152.09
146.01
130.42
129.13
128.15
127.40
123.97
121.97
118.18
117.07
115.70
113.58
113.19
77.26
77.05
76.84
56.64
56.49
55.93
55.87
MeO
MeO
N
CN
N
N
N
OMe
OMe
1B2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

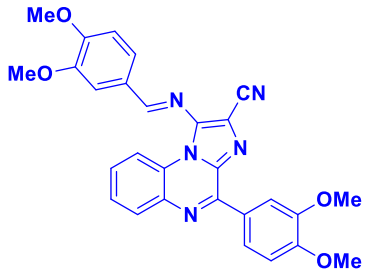
HMQC


MeO
MeO
N
CN
N
N
N
OMe
OMe

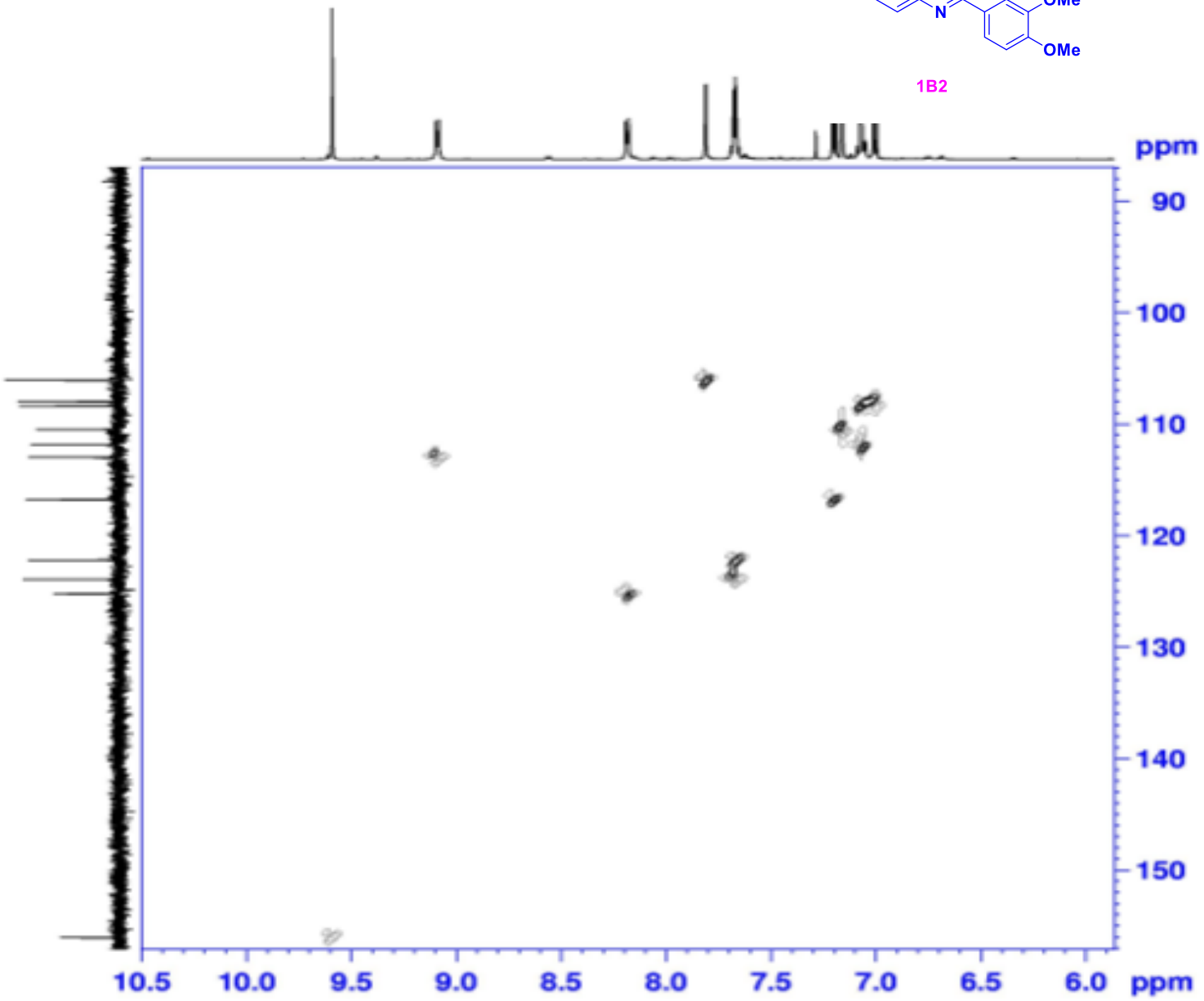
1B2


ppm
0
20
40
60
80
100
120
140
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

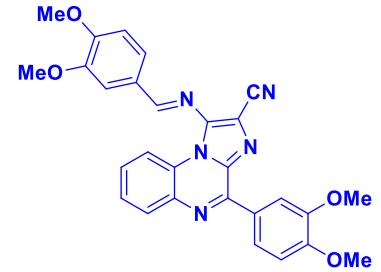
HMQC


MeO
MeO
N
CN
N
N
N
OMe
OMe

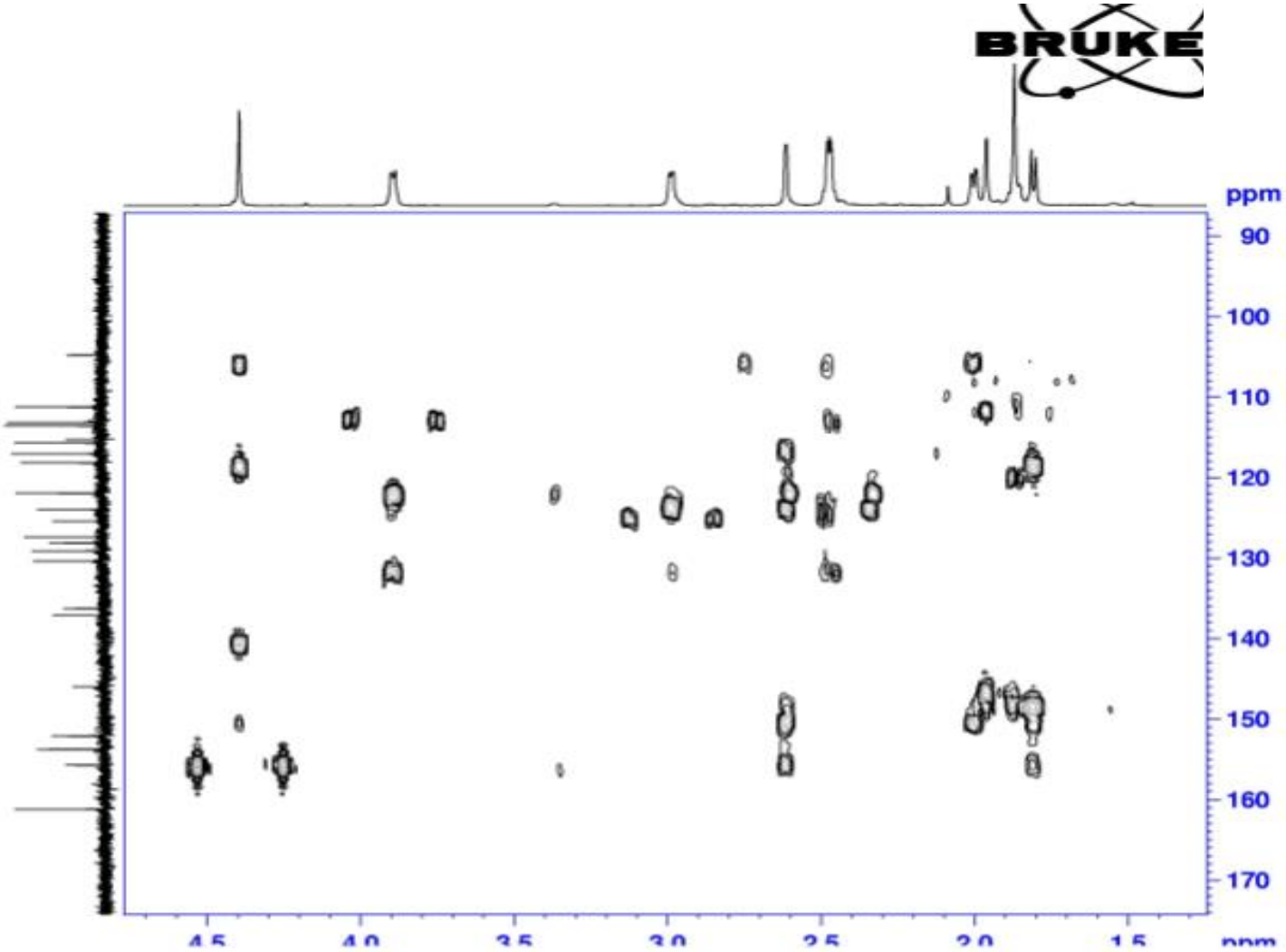
1B2


ppm
90
100
110
120
130
140
150
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
ppm

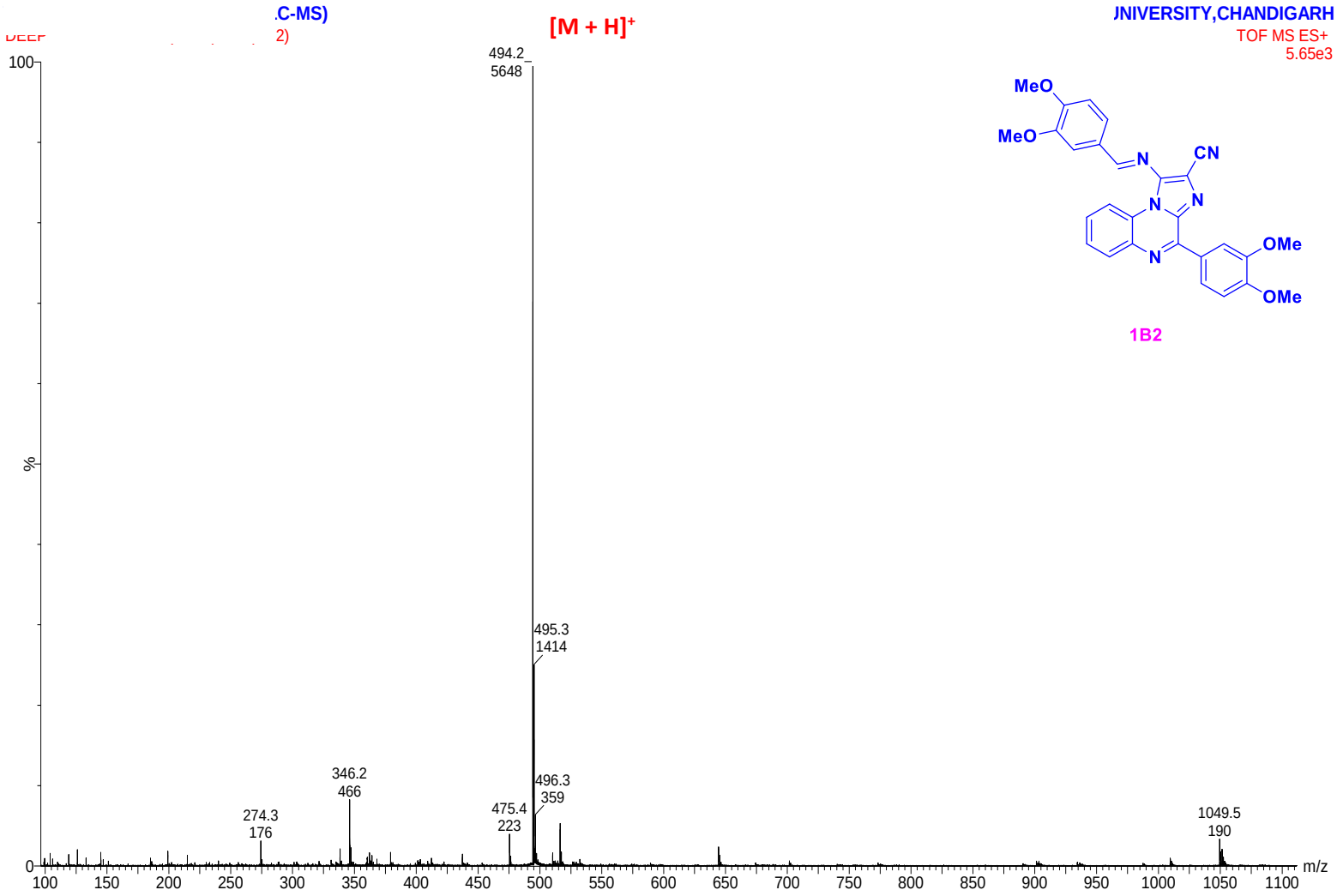
HMBC


MeO
MeO
N
CN
N
N
N
OMe
OMe

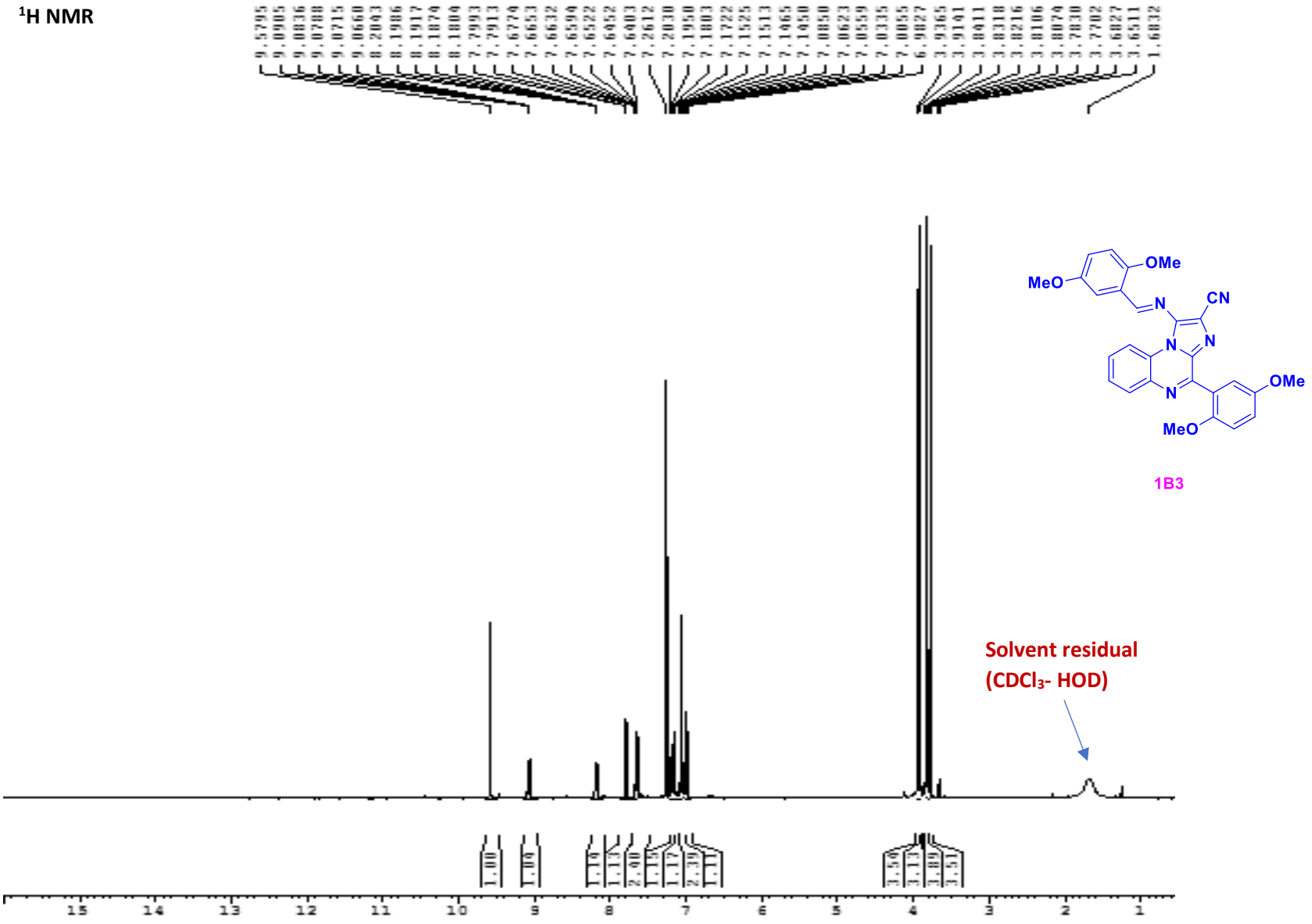
1B2


BRUKE
ppm
90
100
110
120
130
140
150
160
170
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

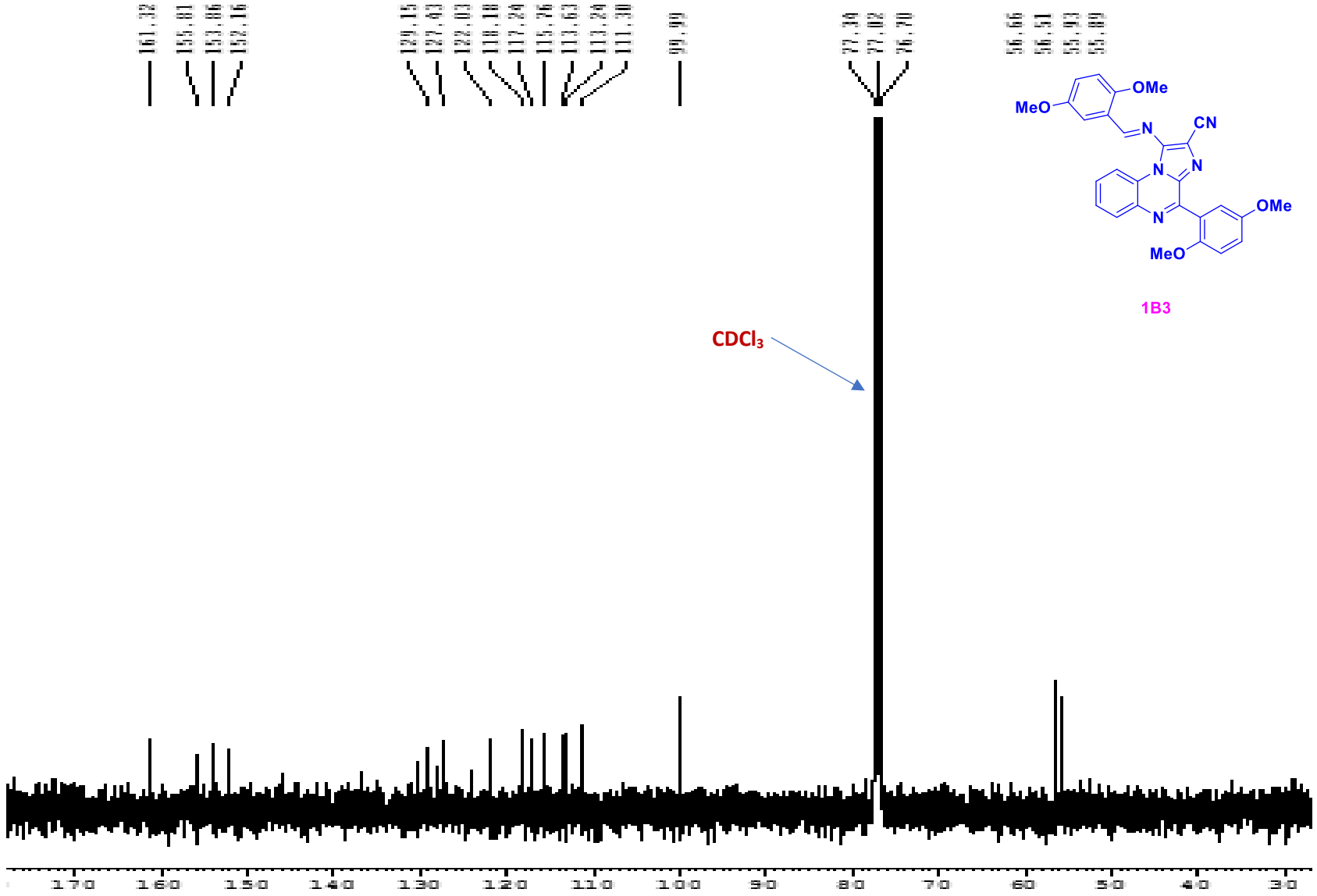
HRMS


.C-MS)
2)
[M + H]+
JNIVERSITY,CHANDIGARH
TOF MS ES+
5.65e3
MeO
MeO
N
CN
N
N
N
OMe
OMe
1B2
494.2
5648
495.3
1414
496.3
359
346.2
466
274.3
176
475.4
223
1049.5
190
100
%
0
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100

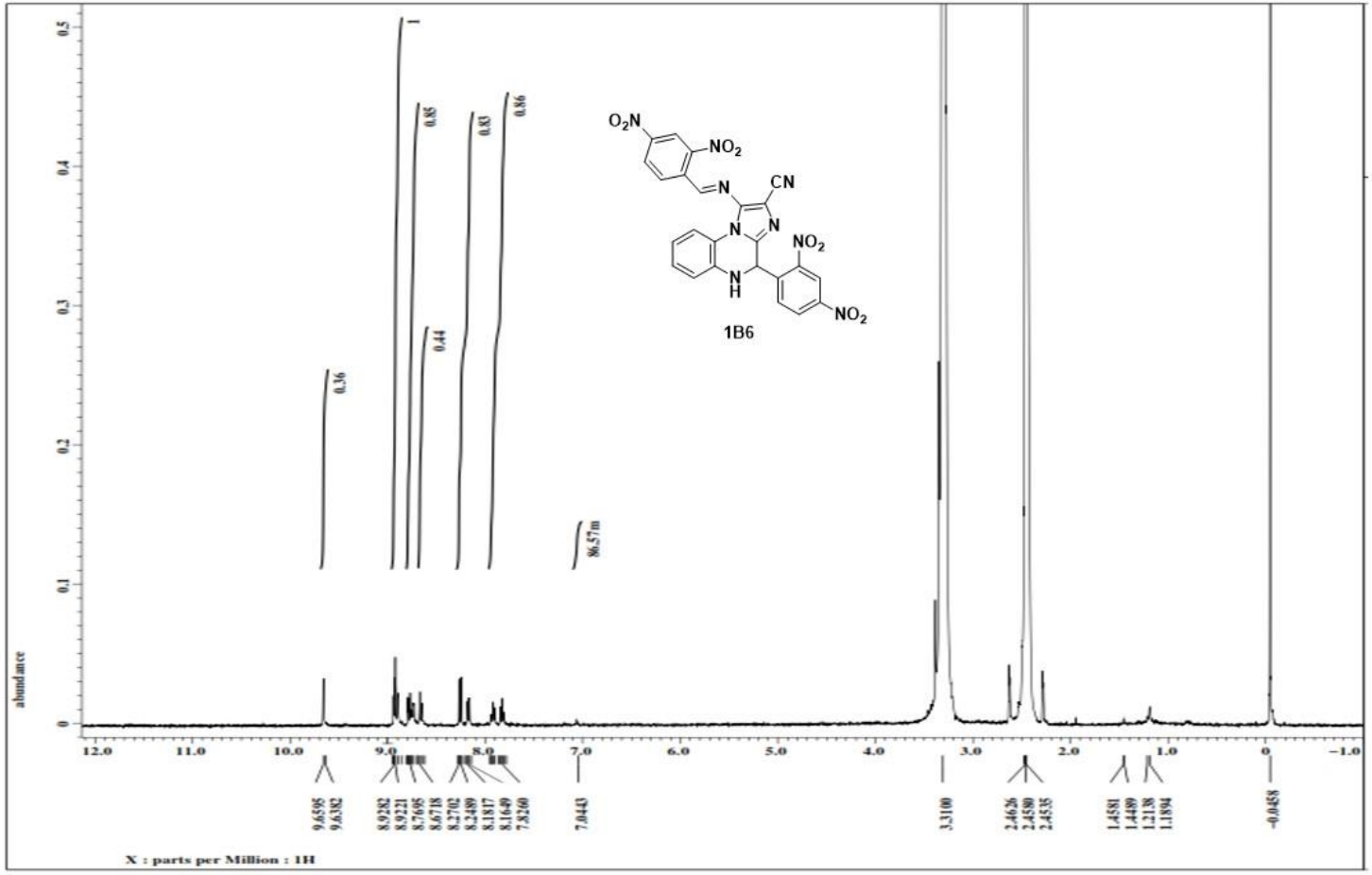
^{1}H NMR


9.5795
9.0905
9.0836
9.0788
9.0715
9.0660
8.2043
8.1986
8.1917
8.1874
8.1804
7.7993
7.7913
7.6774
7.6653
7.6632
7.6599
7.6522
7.6452
7.6403
7.2612
7.2030
7.1958
7.1883
7.1722
7.1525
7.1513
7.1465
7.1458
7.0858
7.0623
7.0559
7.0335
7.0055
6.9827
3.9365
3.9141
3.8411
3.8318
3.8216
3.8106
3.8074
3.7830
3.7702
3.6827
3.6511
1.6832
MeO
OMe
N
CN
N
N
N
OMe
MeO
1B3
Solvent residual
(CDCl3- HOD)
1.00
1.08
1.16
1.13
2.40
1.15
1.11
2.39
1.11
3.50
3.13
3.89
3.51
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1

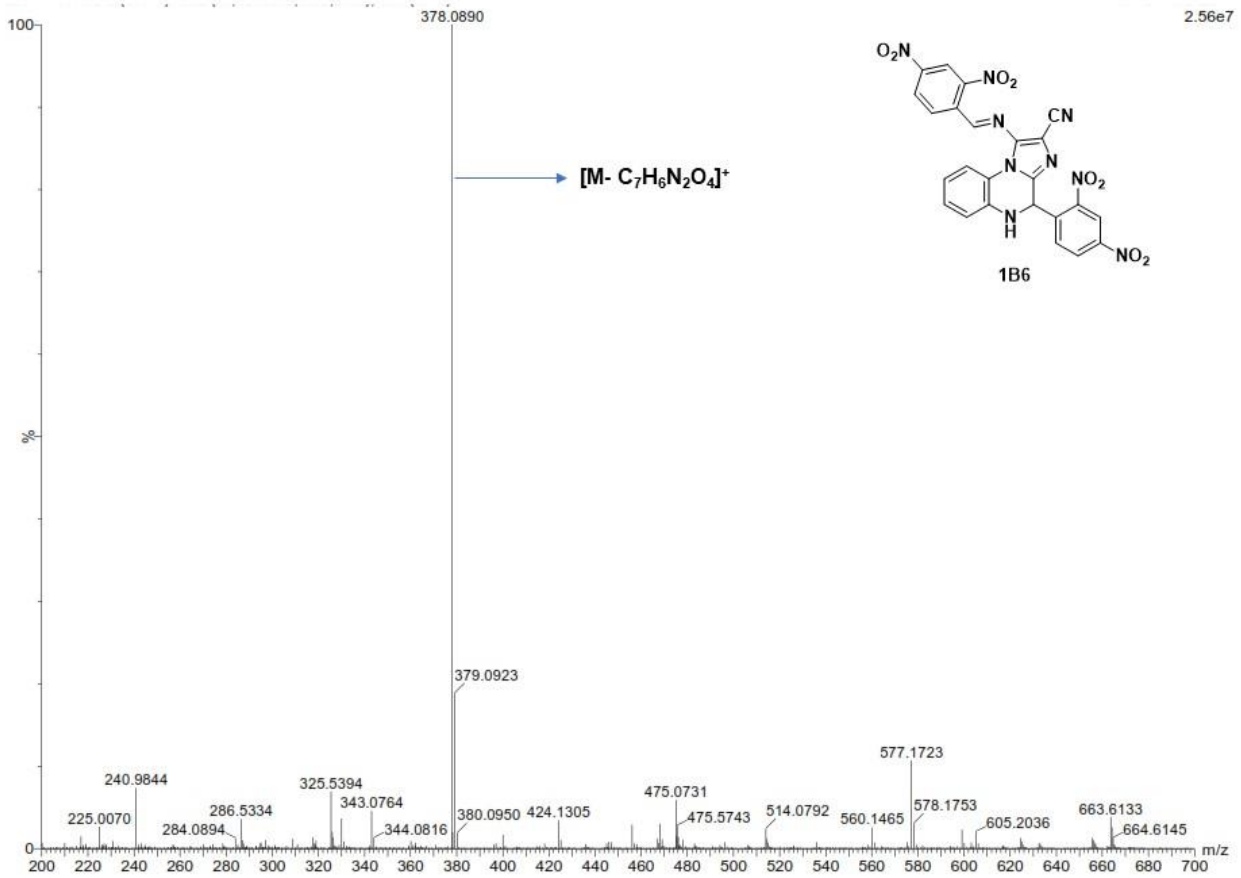
^{13}C NMR


161.32
155.81
153.86
152.16
129.15
122.43
122.03
118.18
117.24
115.26
111.63
111.24
111.20
99.89
77.39
77.02
76.70
56.66
56.51
55.93
55.89
OMe
MeO
N
CN
N
N
N
OMe
MeO
1B3
CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30

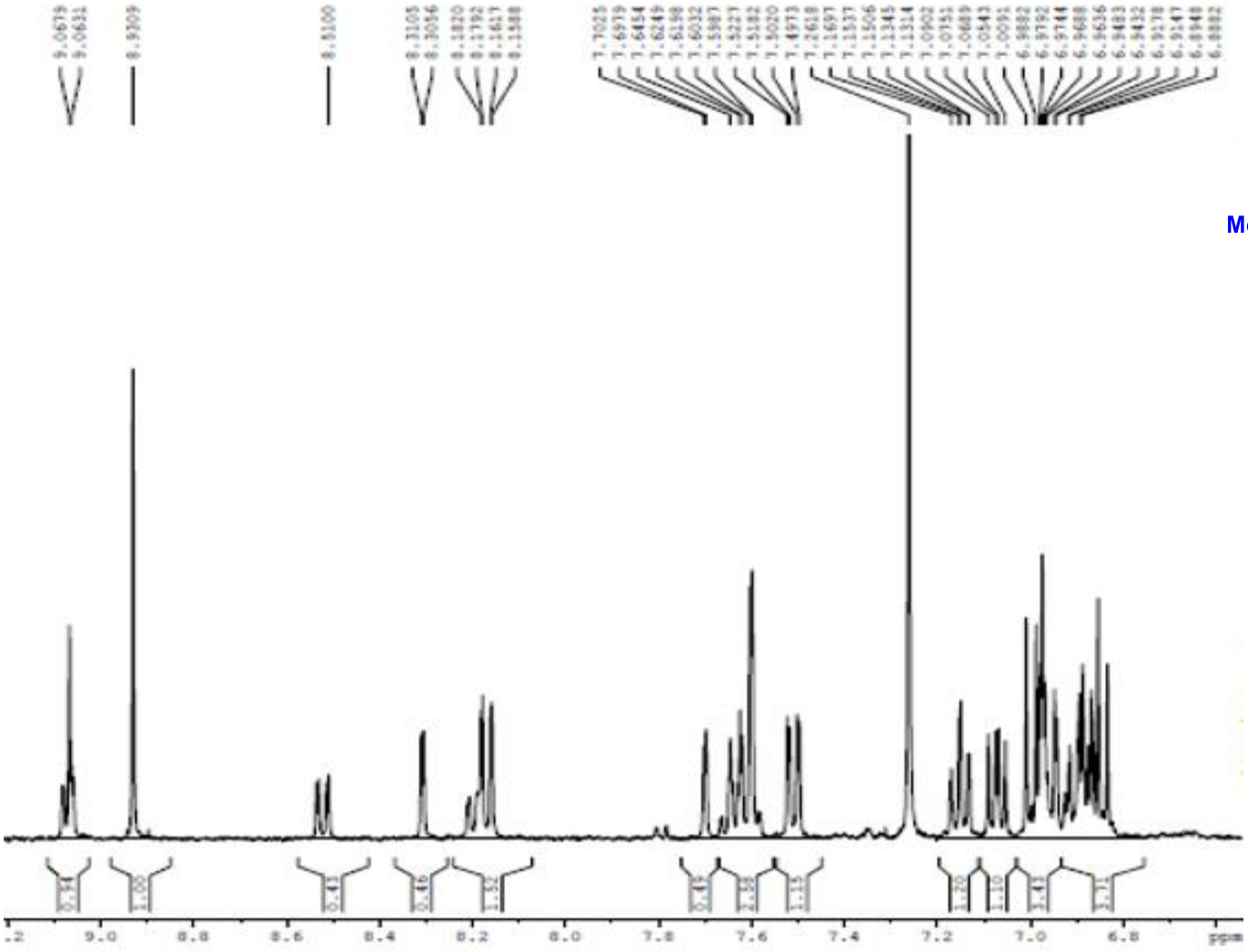
^{1}H NMR

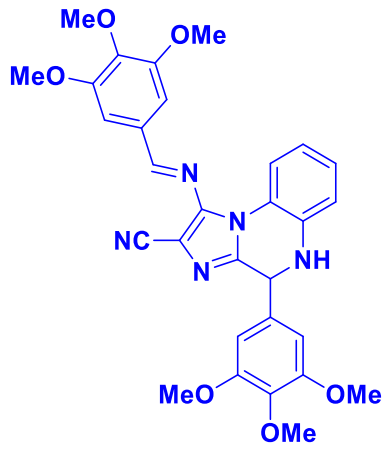

1
0.85
0.83
0.86
0.44
0.36
86.57m
1B6
abundance
X : parts per Million : 1H

HRMS


378.0890
2.56e7
100
%
0
[M- C7H6N2O4]+
379.0923
240.9844
325.5394
343.0764
286.5334
225.0070
284.0894
344.0816
380.0950
424.1305
475.0731
475.5743
514.0792
560.1465
577.1723
578.1753
605.2036
663.6133
664.6145
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
O2N
NO2
N
CN
N
N
NO2
N
H
NO2
1B6

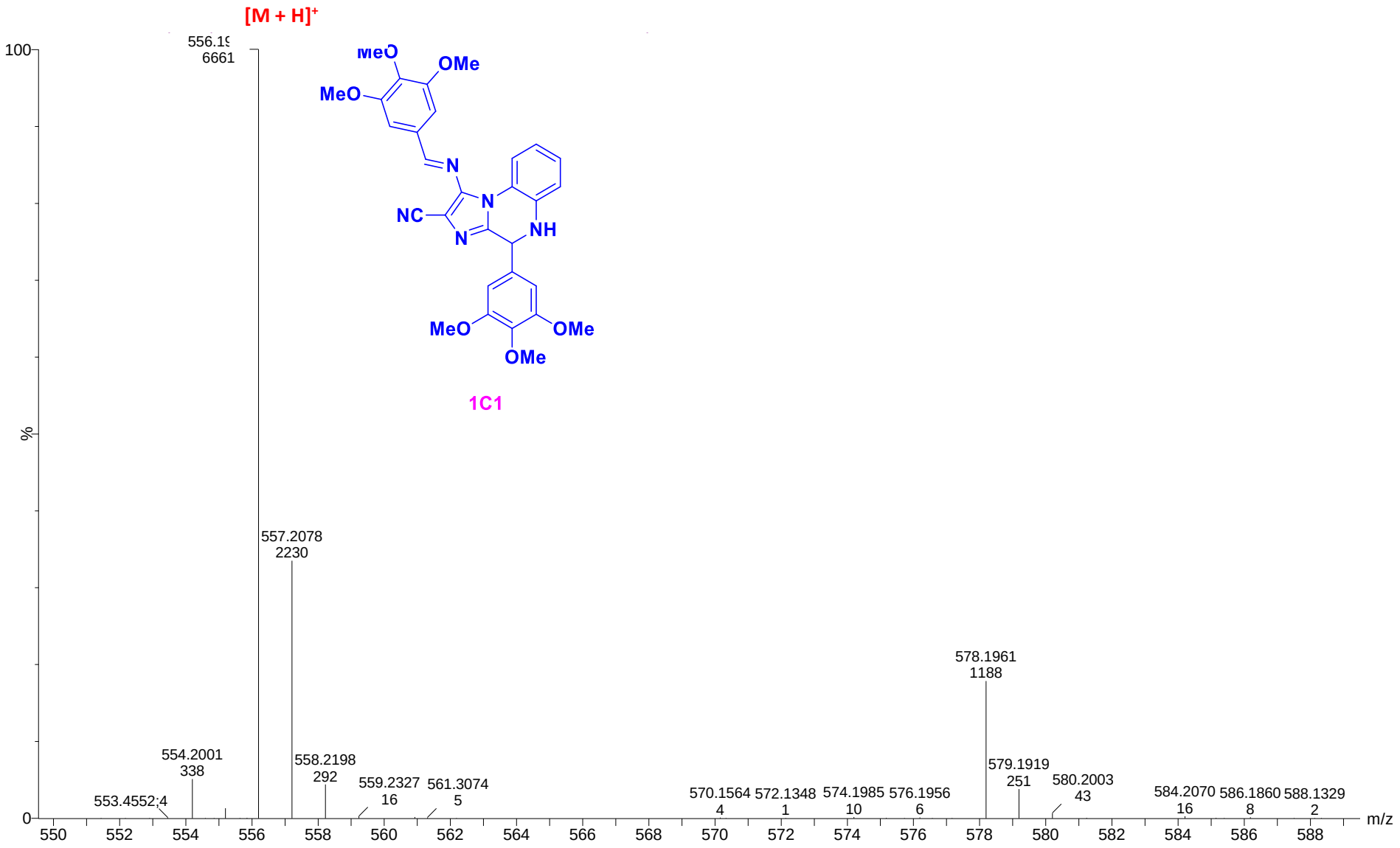
^{1}H NMR



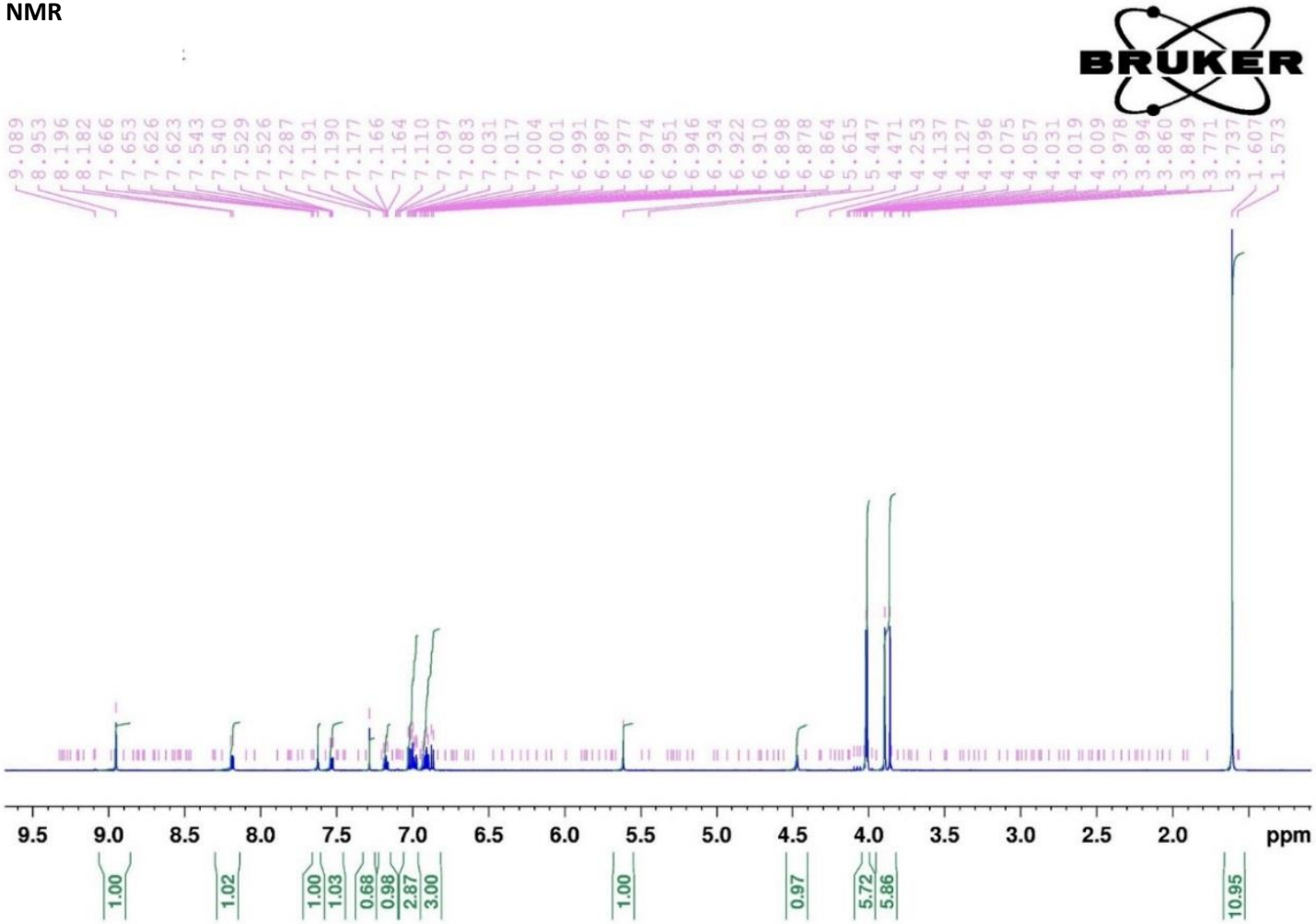


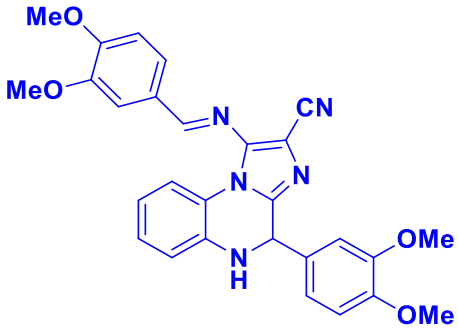
1C1

HRMS


[M + H]+
556.19
6661
MeO
OMe
MeO
N
NC
N
N
NH
MeO
OMe
OMe
1C1
100
%
0
557.2078
2230
554.2001
338
558.2198
292
553.4552
4
559.2327
16
561.3074
5
570.1564
4
572.1348
1
574.1985
10
576.1956
6
578.1961
1188
579.1919
251
580.2003
43
584.2070
16
586.1860
8
588.1329
2
550
552
554
556
558
560
562
564
566
568
570
572
574
576
578
580
582
584
586
588
m/z

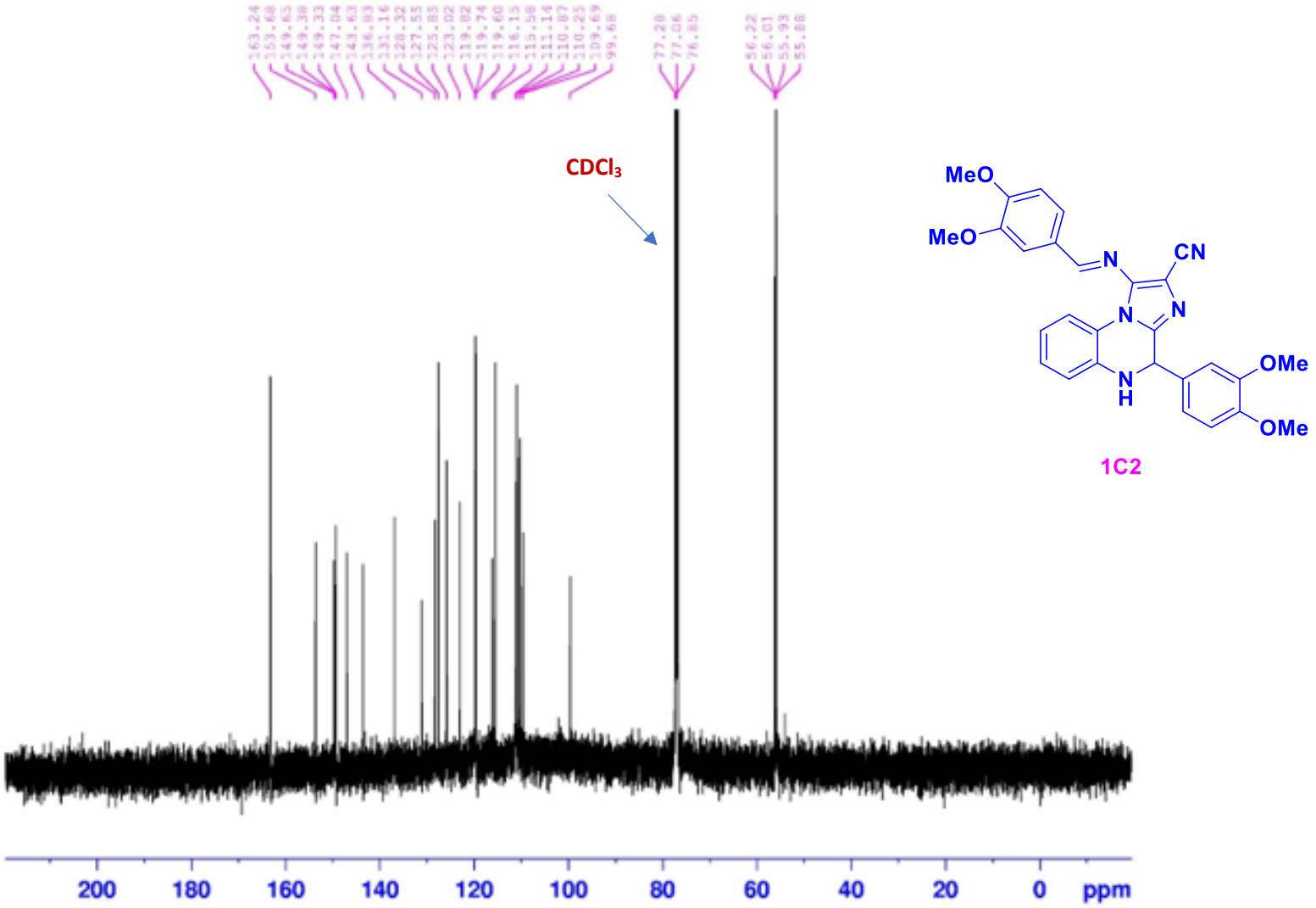
^{1}H NMR


BRUKER
9.089
8.953
8.196
8.182
7.666
7.653
7.626
7.623
7.543
7.540
7.529
7.526
7.287
7.191
7.190
7.177
7.166
7.164
7.110
7.097
7.083
7.031
7.017
7.004
7.001
6.991
6.987
6.977
6.974
6.951
6.946
6.934
6.922
6.910
6.898
6.878
6.864
5.615
5.447
4.471
4.253
4.137
4.127
4.096
4.075
4.057
4.031
4.019
4.009
3.978
3.894
3.860
3.849
3.771
3.737
1.607
1.573
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
1.00
1.02
1.00
1.03
0.68
0.98
2.87
3.00
1.00
0.97
5.72
5.86
10.95

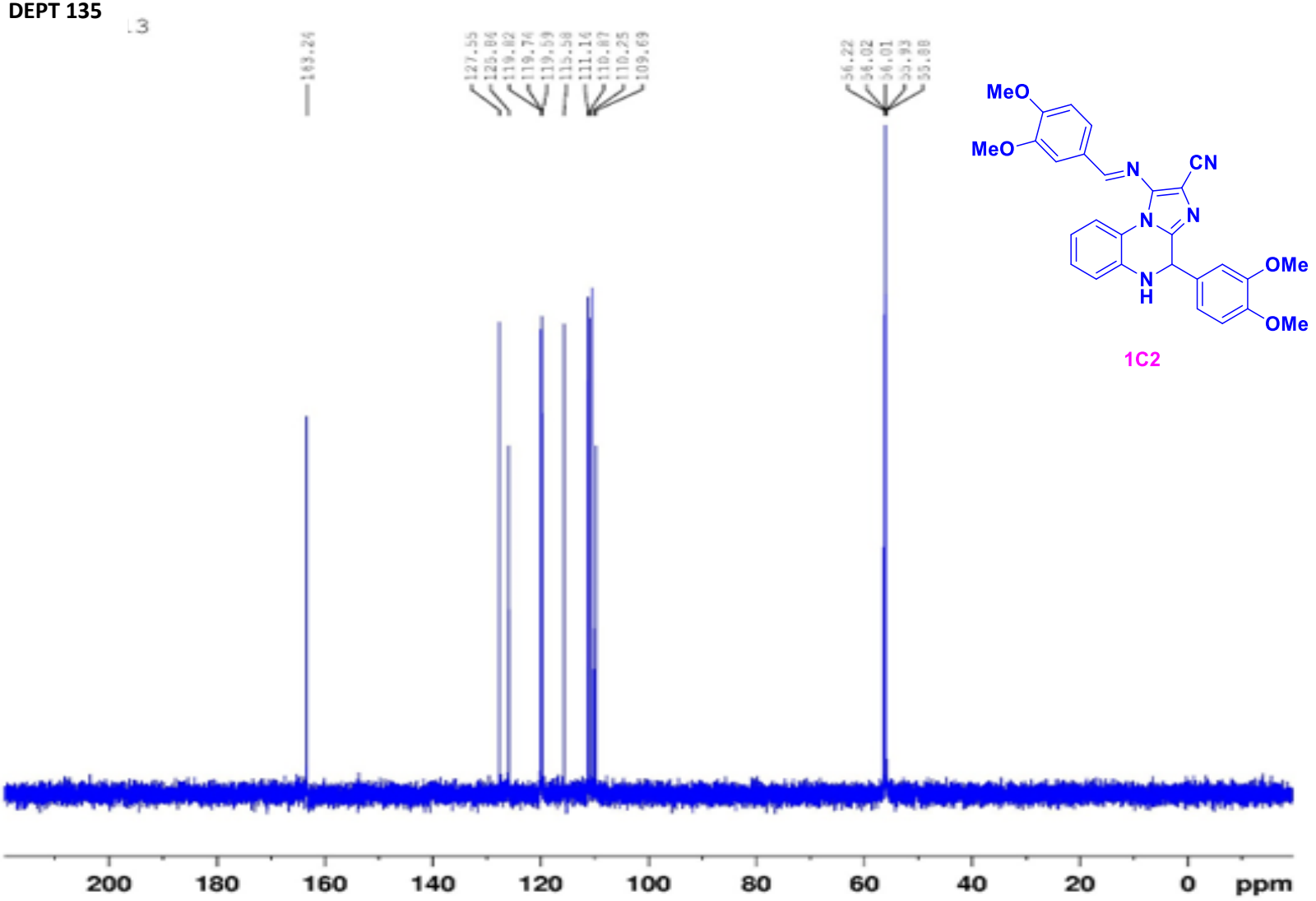

MeO
MeO
N
CN
N
N
N
H
OMe
OMe

1C2

^{13}C NMR

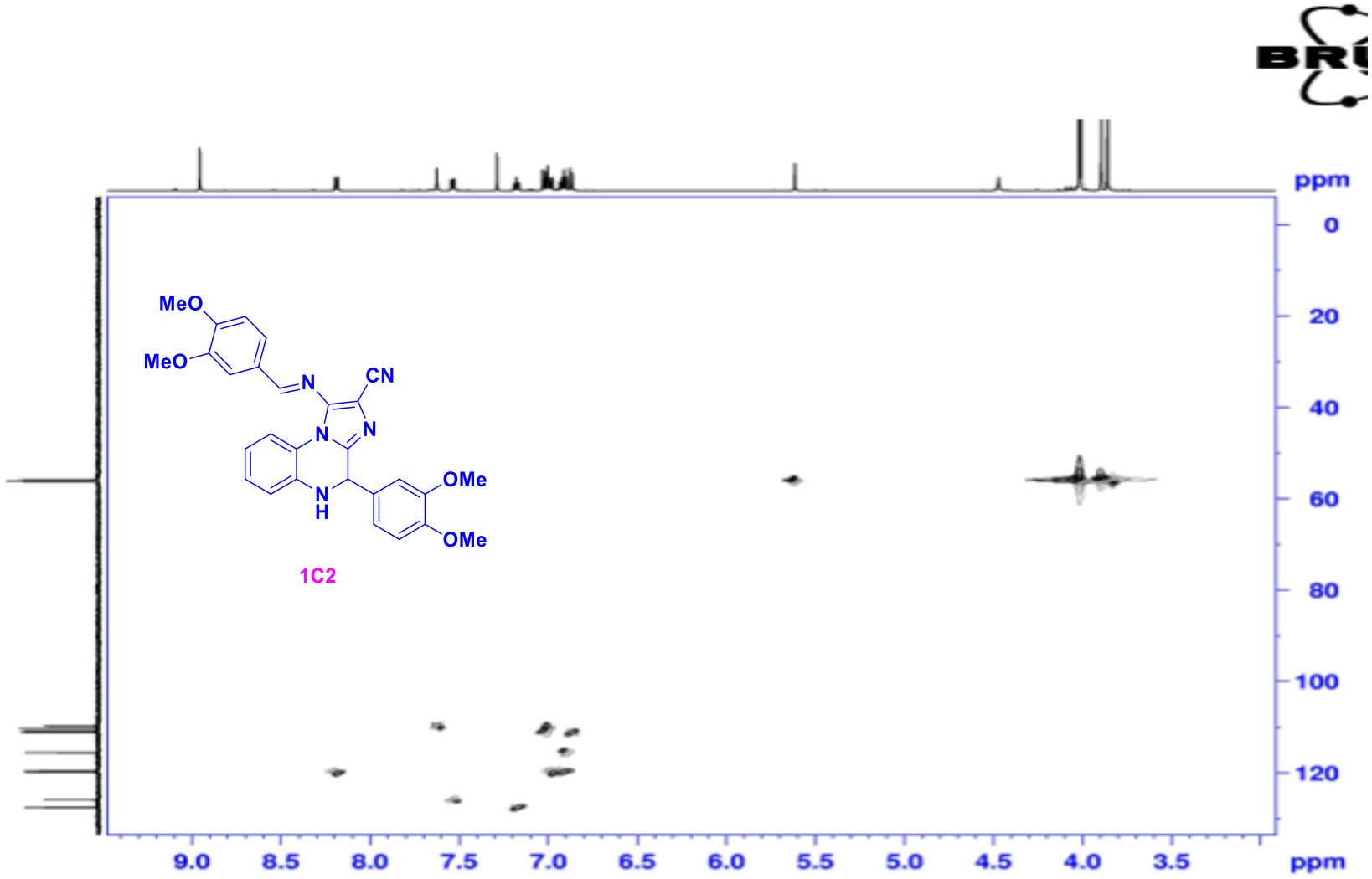

163.24
153.68
149.65
149.38
149.33
147.04
143.63
136.83
131.16
128.32
127.55
125.85
123.02
119.82
119.74
119.60
116.15
115.58
111.14
110.87
110.25
109.69
99.68
77.20
77.04
76.85
56.22
56.01
55.93
55.88
CDCl3
MeO
MeO
N
CN
N
N
N
H
OMe
OMe
1C2
200
180
160
140
120
100
80
60
40
20
0
ppm

DEPT 135

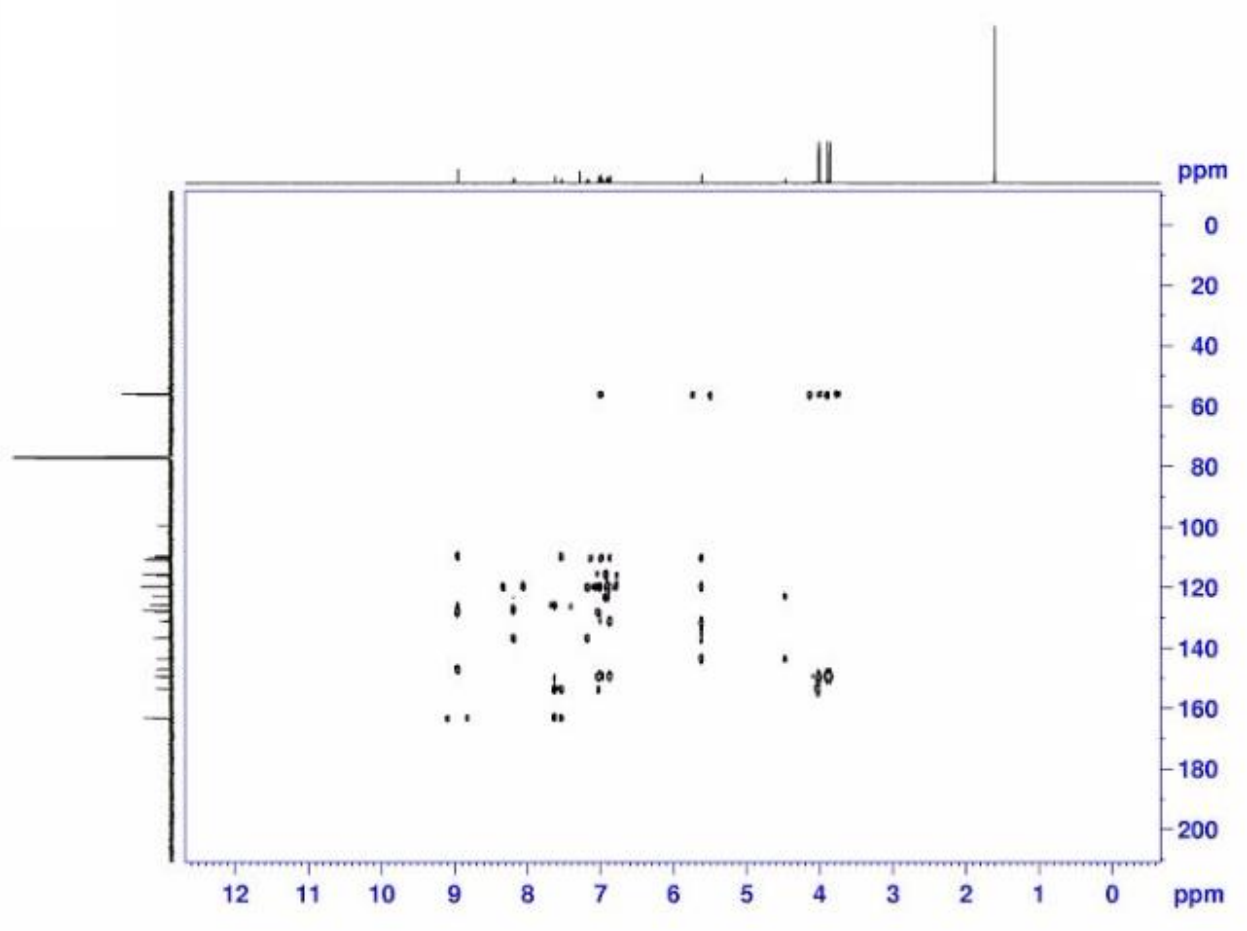

163.26
127.55
125.86
119.82
119.74
119.59
115.58
111.14
110.87
110.25
109.69
56.22
56.02
56.01
55.93
55.80
MeO
MeO
N
CN
N
N
N
H
OMe
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm

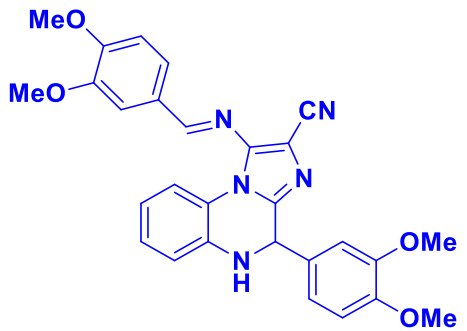
1C2

HMQC


MeO
MeO
N
CN
N
N
N
H
OMe
OMe
1C2
ppm
0
20
40
60
80
100
120
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm

HMBC

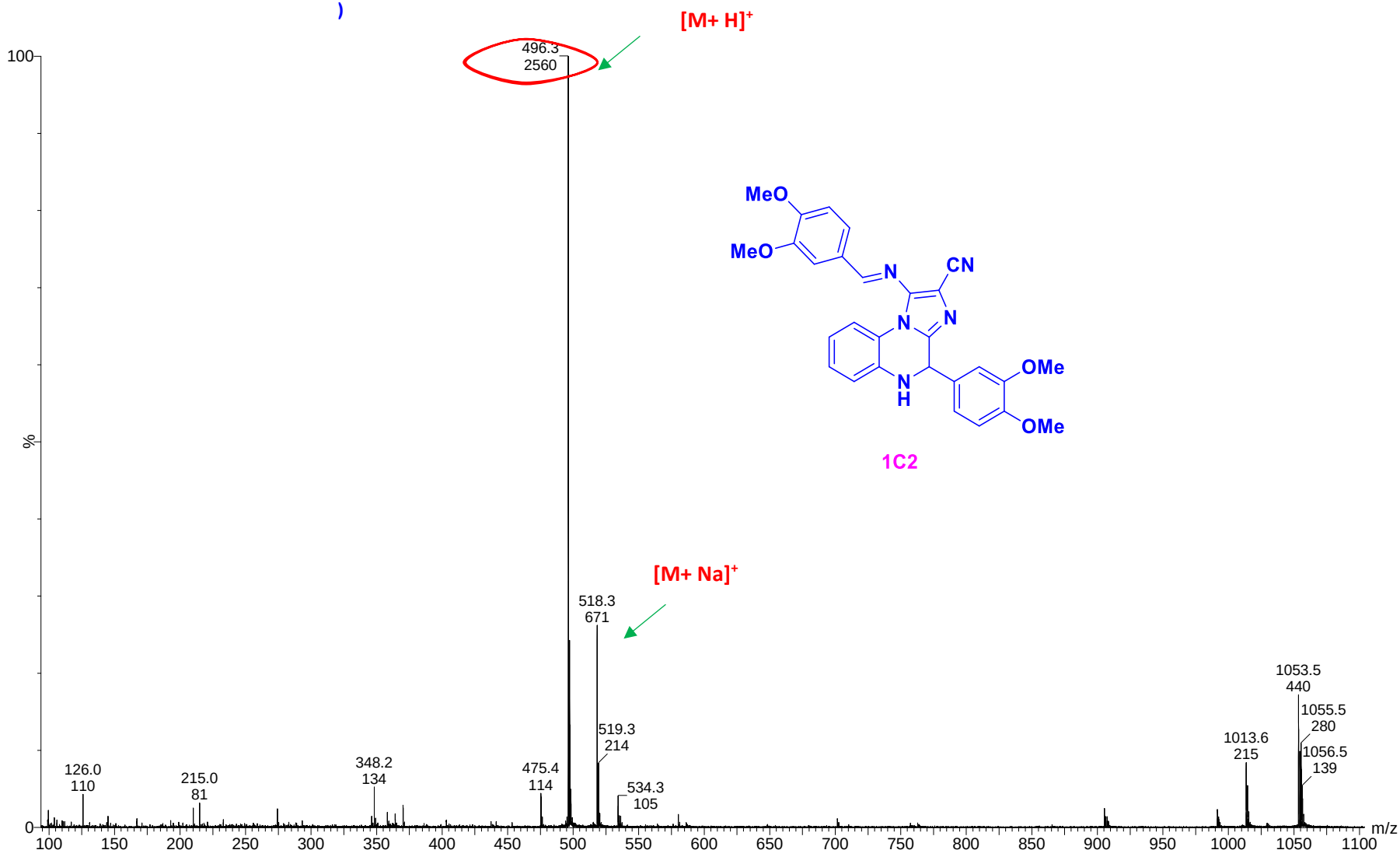

ppm
0
20
40
60
80
100
120
140
160
180
200
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


MeO
MeO
N
CN
N
N
N
H
OMe
OMe

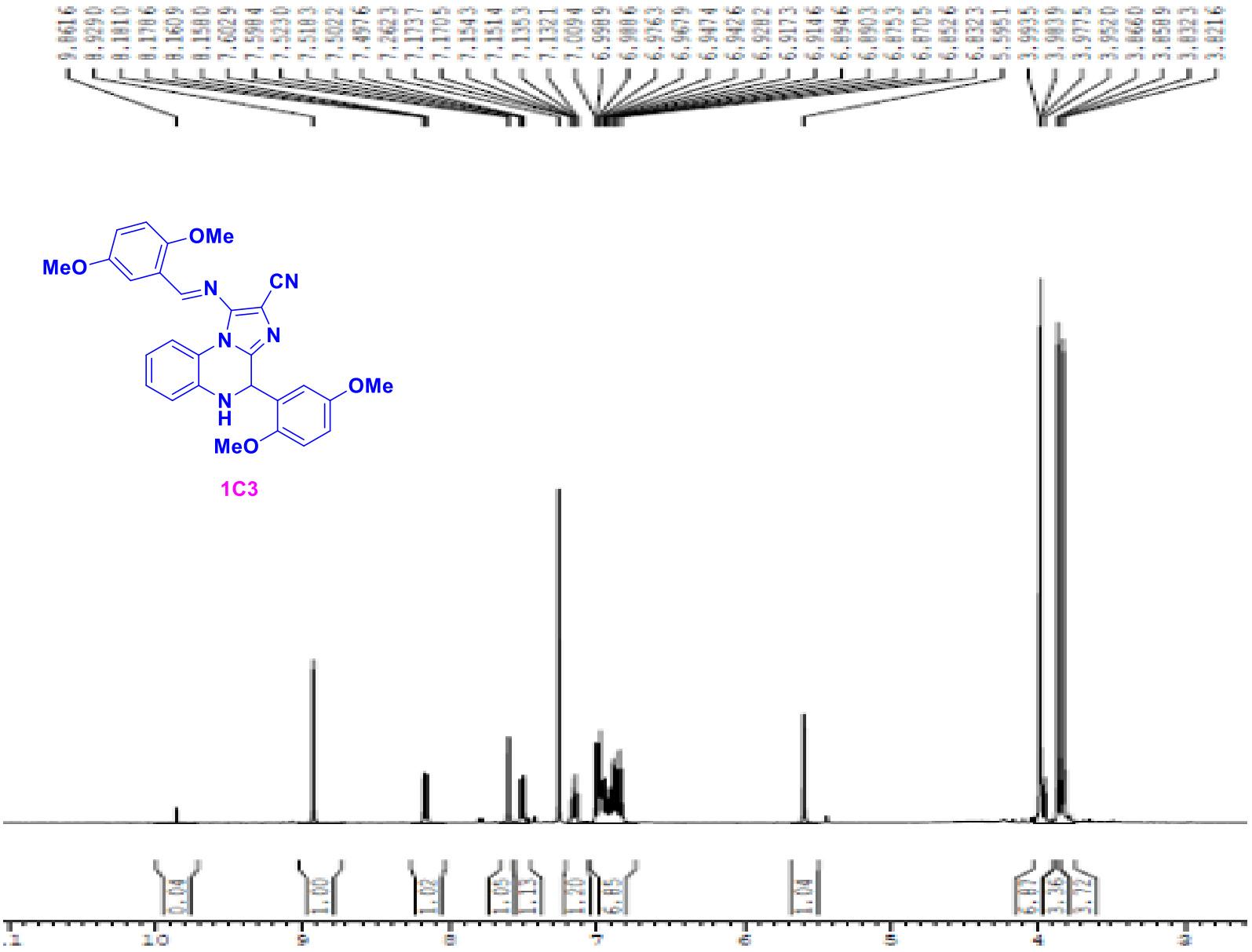
1C2

HRMS

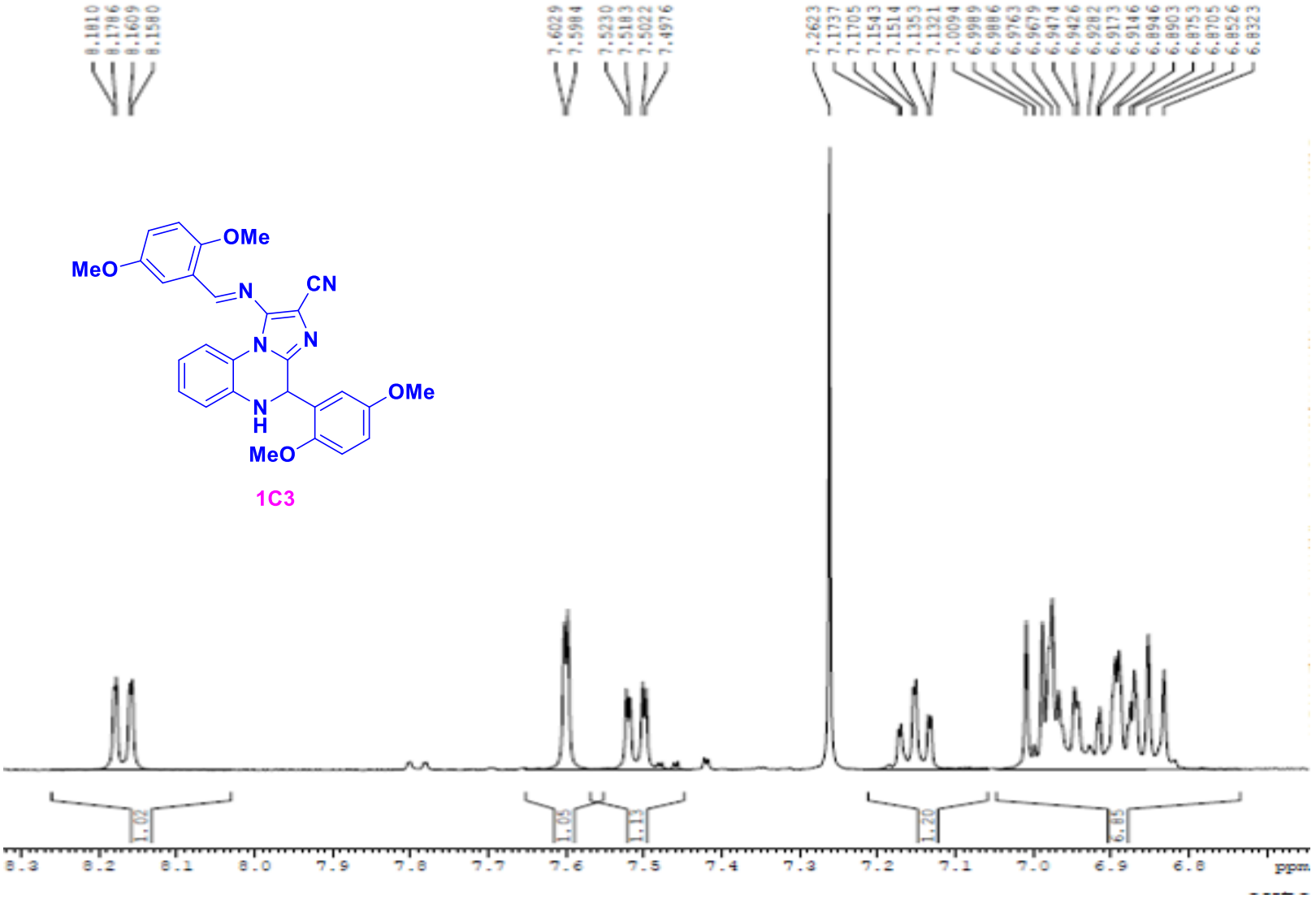
)

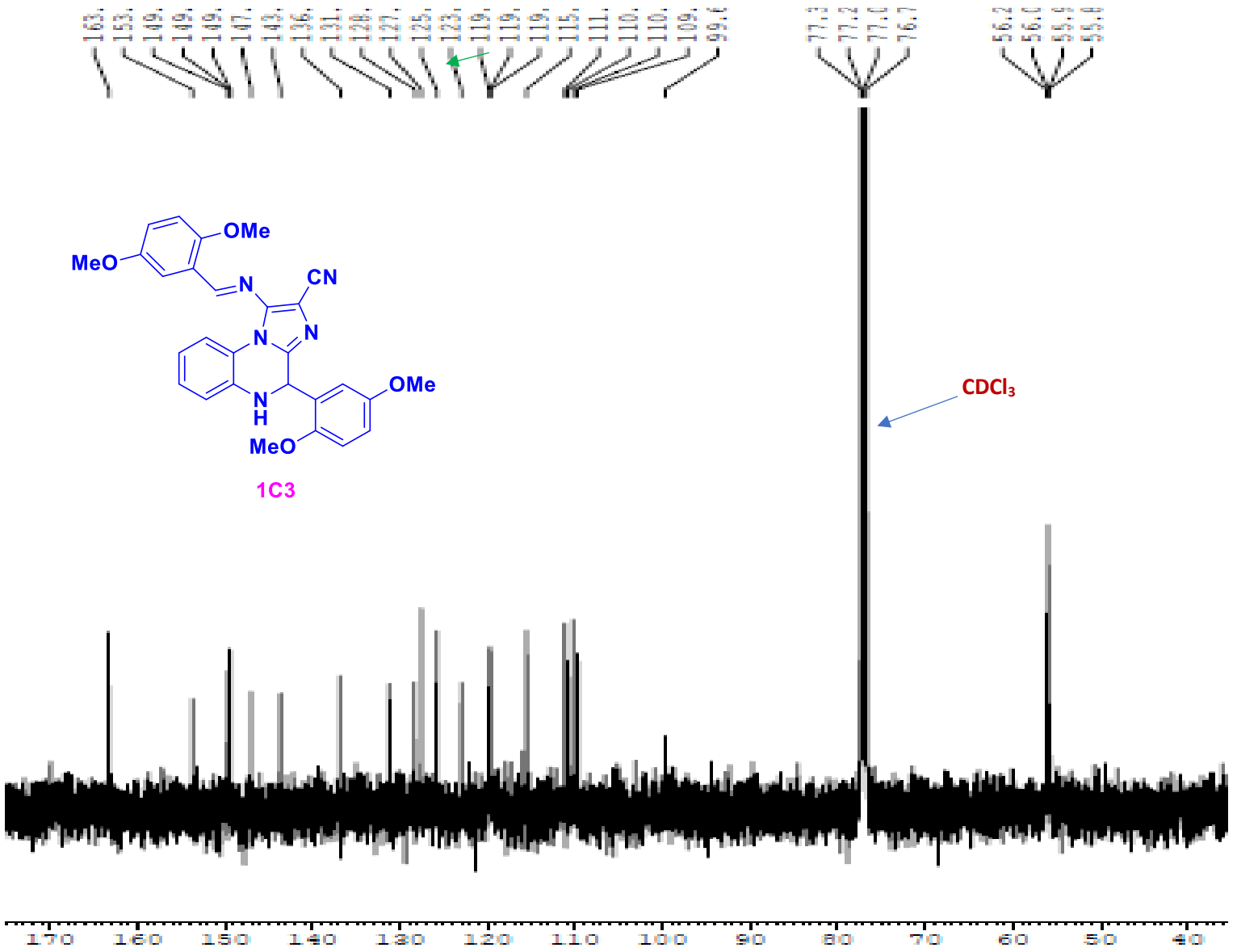

[M+ H]+
496.3
2560
100
%
0
MeO
MeO
N
CN
N
N
N
H
OMe
OMe
1C2
[M+ Na]+
518.3
671
519.3
214
534.3
105
475.4
114
348.2
134
215.0
81
126.0
110
1013.6
215
1053.5
440
1055.5
280
1056.5
139
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100
m/z

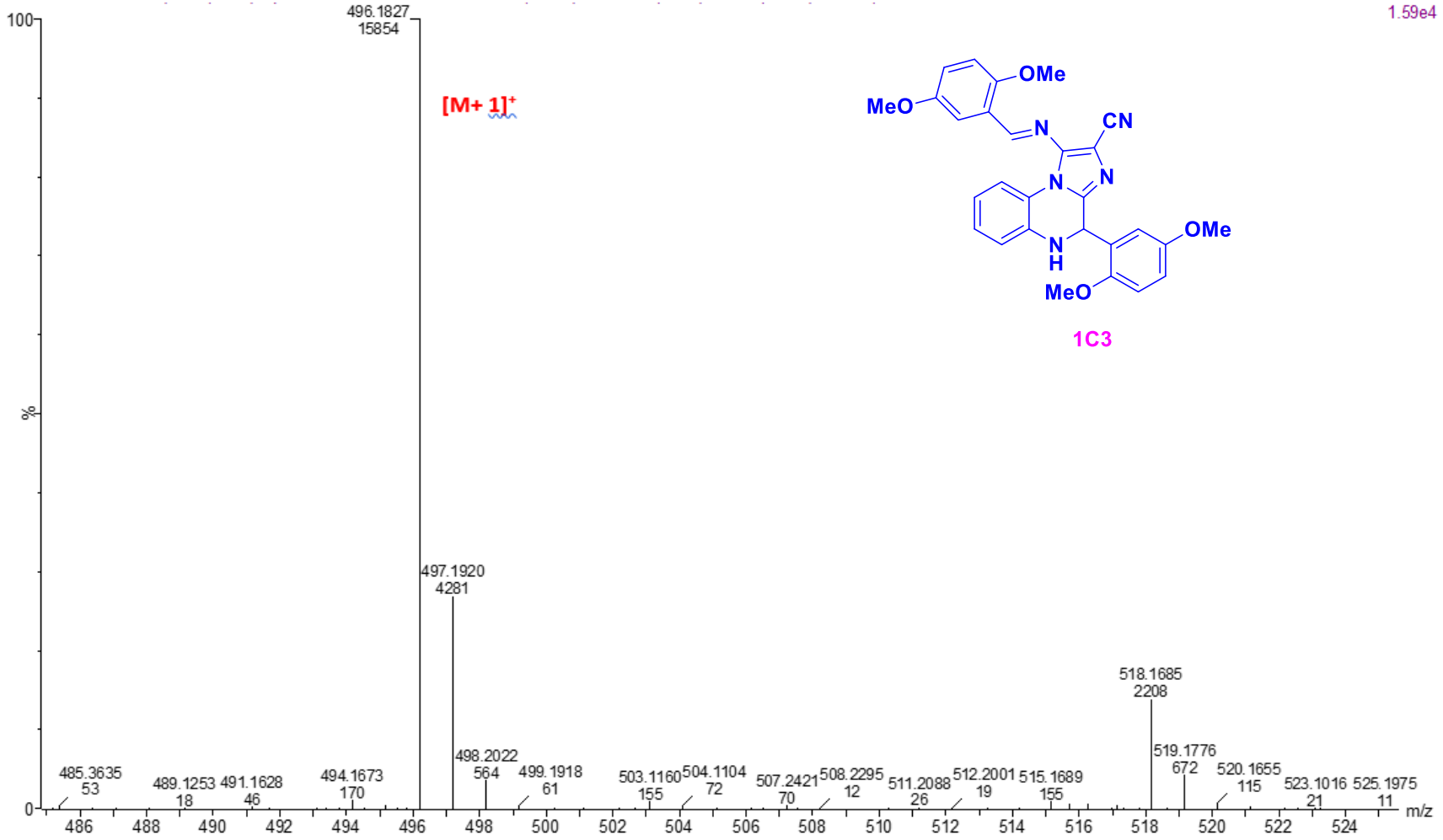
^{1}H NMR


9.8616
8.9290
8.1010
8.1786
8.1609
8.1580
7.6029
7.5984
7.5230
7.5183
7.5022
7.4976
7.2823
7.1737
7.1705
7.1543
7.1514
7.1353
7.1321
7.1094
6.9989
6.9806
6.9763
6.9679
6.9474
6.9426
6.9282
6.9173
6.9146
6.8946
6.8903
6.8753
6.8705
6.8526
6.8323
5.5951
3.9935
3.9839
3.9775
3.9520
3.8660
3.8589
3.8323
3.8216
OMe
MeO
N
CN
N
N
N
H
OMe
MeO
1C3
0.04
1.00
1.02
1.09
1.13
1.20
6.85
1.04
6.87
3.36
3.22
10
9
8
7
6
5
4
3

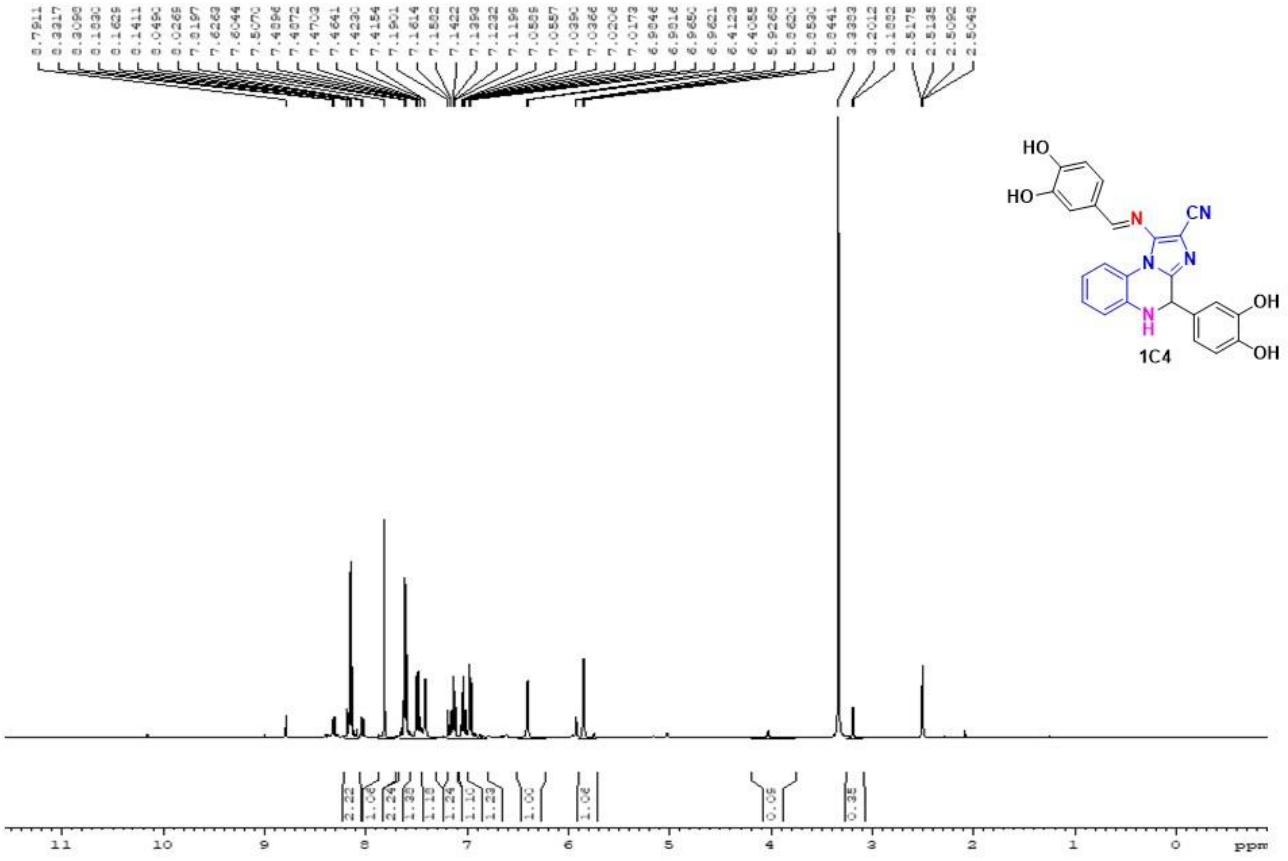
^{1}H NMR


8.1810
8.1786
8.1609
8.1580
7.6029
7.5984
7.5230
7.5183
7.5022
7.4976
7.2623
7.1737
7.1705
7.1543
7.1514
7.1353
7.1321
7.0094
6.9989
6.9886
6.9763
6.9679
6.9474
6.9426
6.9282
6.9173
6.9146
6.8946
6.8903
6.8753
6.8705
6.8526
6.8323
OMe
MeO
N
CN
N
N
N
H
OMe
MeO
1C3
1.02
1.05
1.13
1.20
6.85
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm

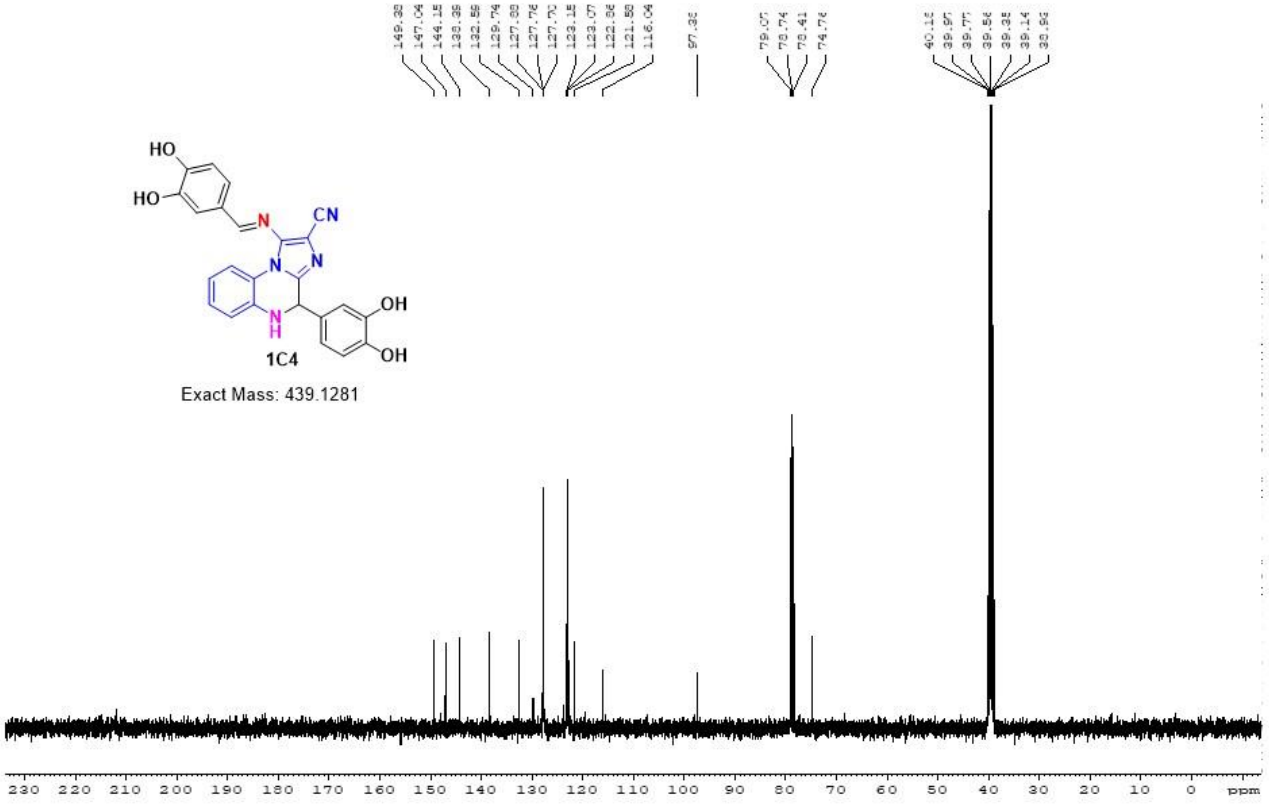

163.
153.
149.
149.
149.
147.
143.
136.
131.
128.
127.
125.
123.
119.
119.
119.
115.
111.
110.
110.
109.
99.8
77.3
77.2
77.1
76.7
56.2
56.0
55.9
55.8
OMe
MeO
N
CN
N
N
N
H
OMe
MeO
1C3
CDCl3
170
160
150
140
130
120
110
100
90
80
70
60
50
40


100
%
0
496.1827
15854
[M+ 1]+
497.1920
4281
498.2022
564
499.1918
61
485.3635
53
489.1253
18
491.1628
46
494.1673
170
503.1160
155
504.1104
72
507.2421
70
508.2295
12
511.2088
26
512.2001
19
515.1689
155
518.1685
2208
519.1776
672
520.1655
115
523.1016
21
525.1975
11
m/z
1.59e4
OMe
MeO
N
CN
N
N
N
H
OMe
MeO
1C3

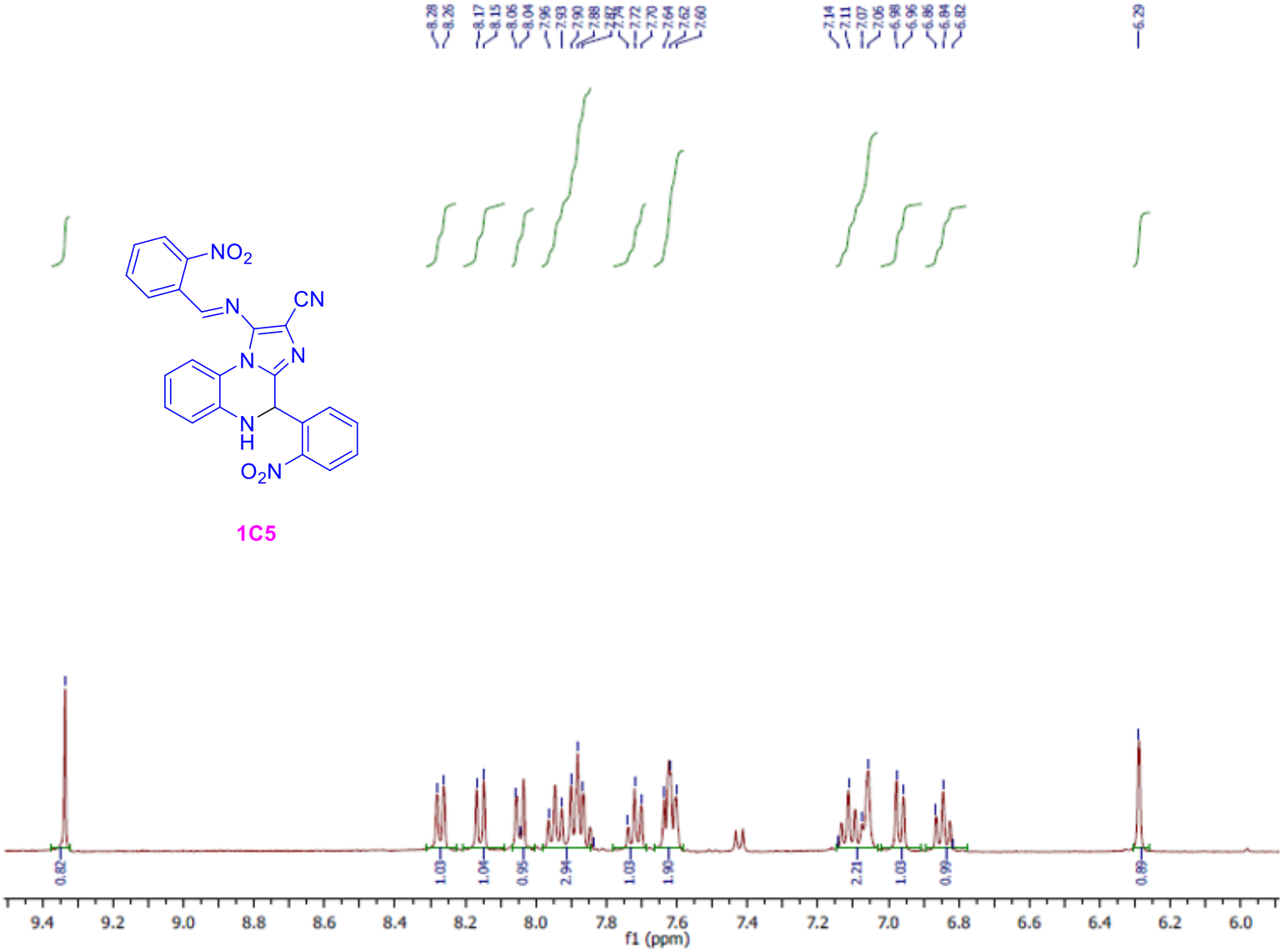
^{1}H NMR



^{13}C NMR

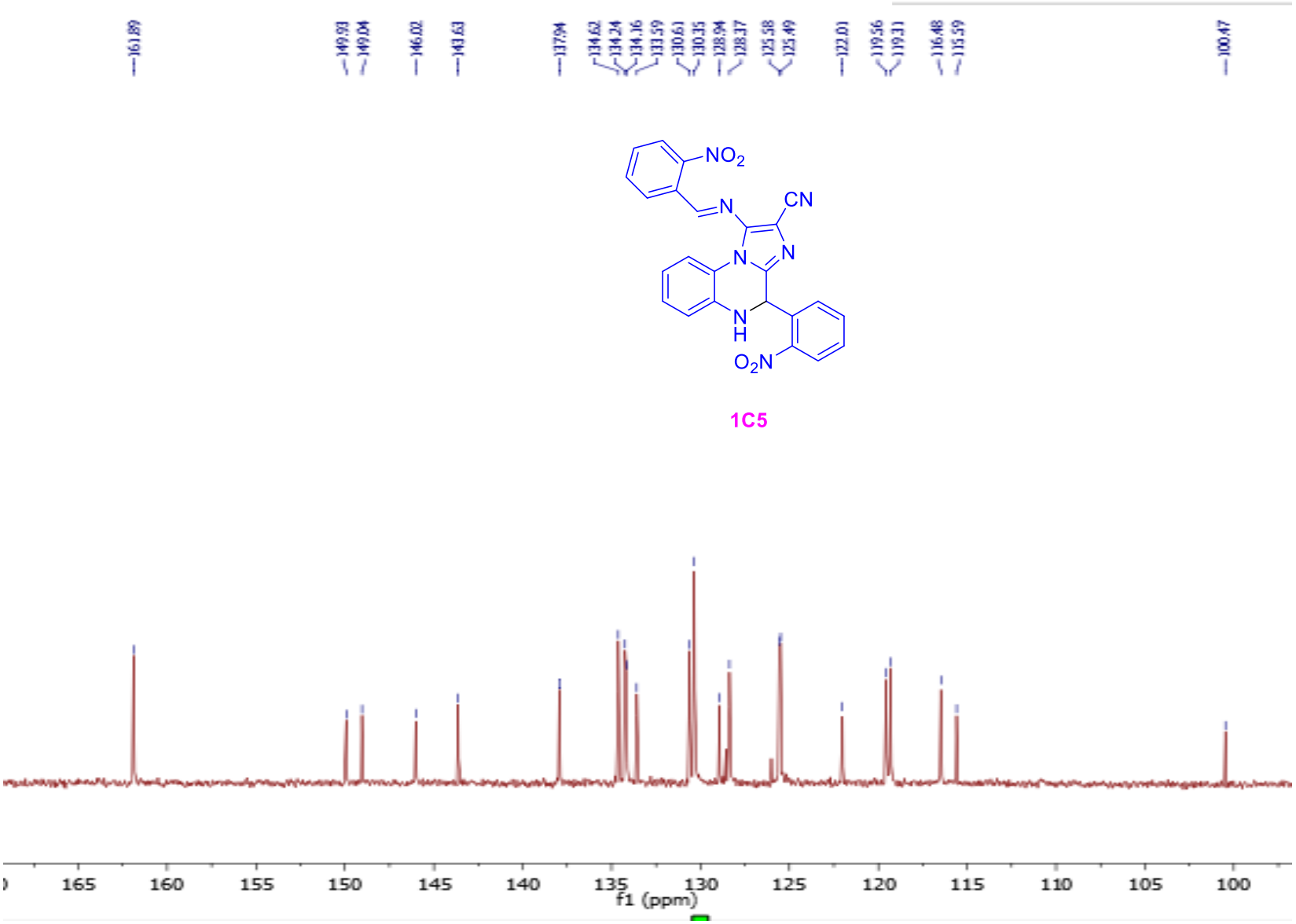

HO
HO
N
CN
N
N
H
OH
OH
1C4
Exact Mass: 439.1281
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{1}H NMR


8.28
8.26
8.17
8.15
8.06
8.04
7.96
7.93
7.90
7.88
7.74
7.72
7.70
7.64
7.62
7.60
7.14
7.11
7.07
7.06
6.98
6.96
6.86
6.84
6.82
6.29
NO2
N
CN
N
N
H
O2N
0.82
1.03
1.04
0.95
2.94
1.03
1.90
2.21
1.03
0.99
0.89
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
f1 (ppm)

1C5

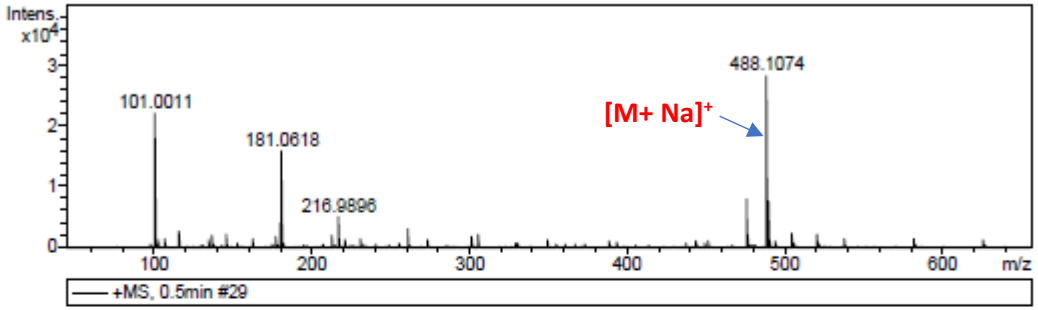
^{13}C NMR


161.89
149.93
149.04
146.02
143.63
137.94
134.62
134.24
134.16
133.59
130.61
130.35
128.94
128.37
125.58
125.49
122.01
119.56
119.31
116.48
115.59
100.47
NO2
N
CN
N
N
N
H
O2N
1C5
165
160
155
150
145
140
135
130
125
120
115
110
105
100
f1 (ppm)

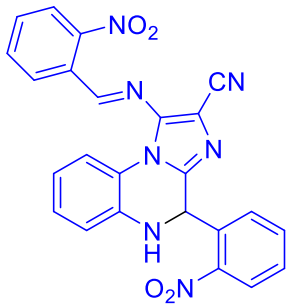
HRMS

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	650 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

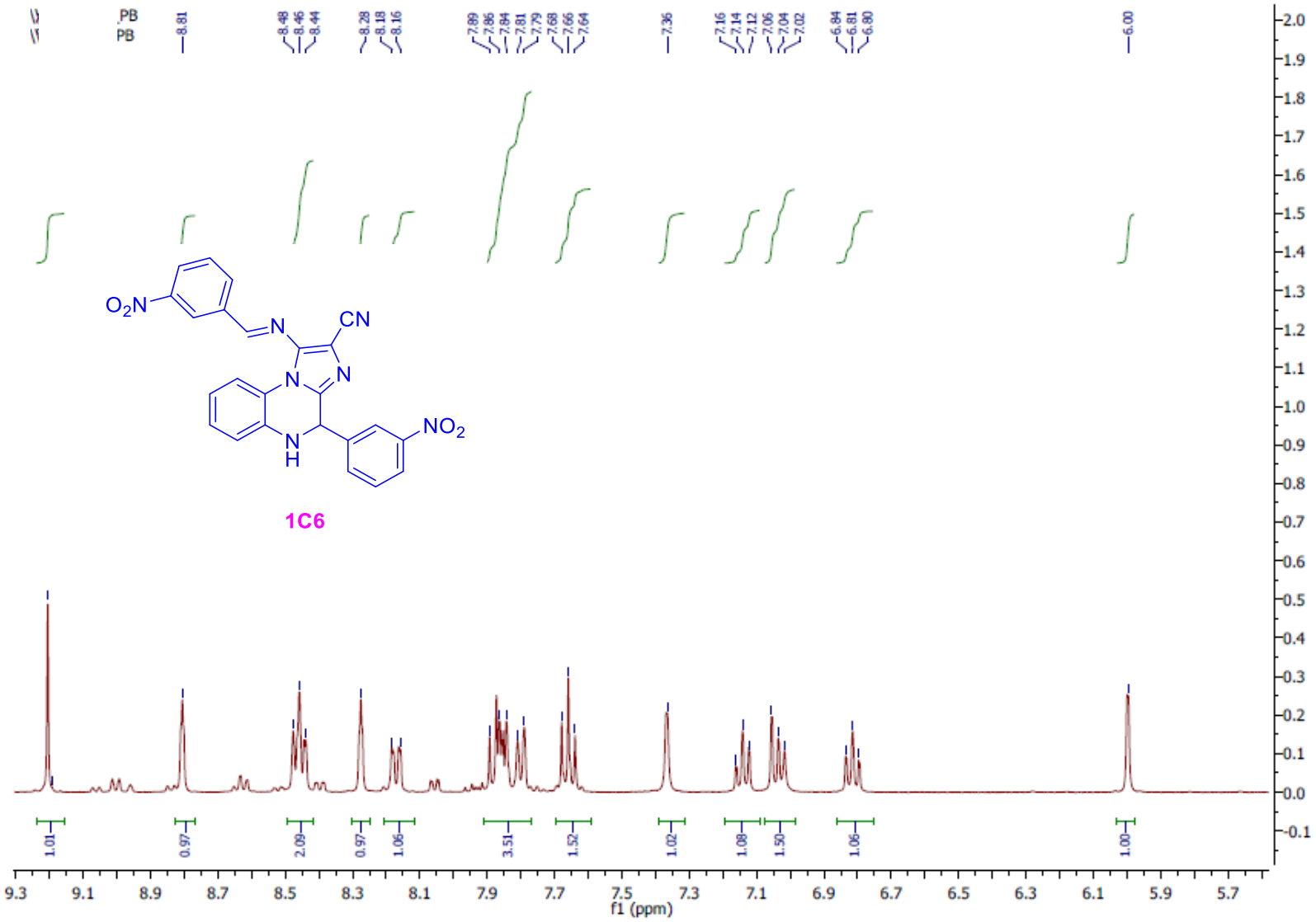


#	m/z	Res.	S/N	I	FWHM
1	101.0011	12819	690.3	22141	0.0079
2	102.9969	12419	39.9	1328	0.0083
3	106.9980	13490	45.1	1587	0.0079
4	116.0037	13859	72.7	2686	0.0084
5	134.9781	14790	33.1	1341	0.0091
6	135.0016	13662	30.6	1242	0.0099
7	137.0009	14174	50.0	2046	0.0097
8	146.0063	15318	52.0	2220	0.0095
9	162.9733	15784	25.0	1449	0.0103
10	176.9889	15246	27.0	1920	0.0116
11	180.0655	14869	54.0	3999	0.0121
12	181.0618	14870	213.0	15960	0.0122
13	212.9929	16212	30.4	2046	0.0131
14	216.9896	15632	78.8	5143	0.0139
15	230.9590	16183	25.0	1455	0.0143
16	261.1309	16963	71.7	3133	0.0154
17	273.1948	15968	32.7	1317	0.0171
18	301.2113	16836	46.0	1880	0.0179
19	305.1574	17043	56.2	2306	0.0179
20	349.1840	16984	34.6	1306	0.0206
21	475.3250	18972	75.9	8031	0.0251
22	476.3281	18546	21.7	2263	0.0257
23	488.1074	18773	331.7	28416	0.0260
24	489.1102	17652	91.5	7695	0.0277
25	490.1129	19378	16.9	1398	0.0253
26	504.0819	18967	40.2	2431	0.0266
27	520.1335	18312	50.8	2214	0.0284
28	537.3396	19544	41.9	1499	0.0275
29	581.3656	18664	54.4	1491	0.0311
30	625.3923	17994	46.9	1267	0.0348

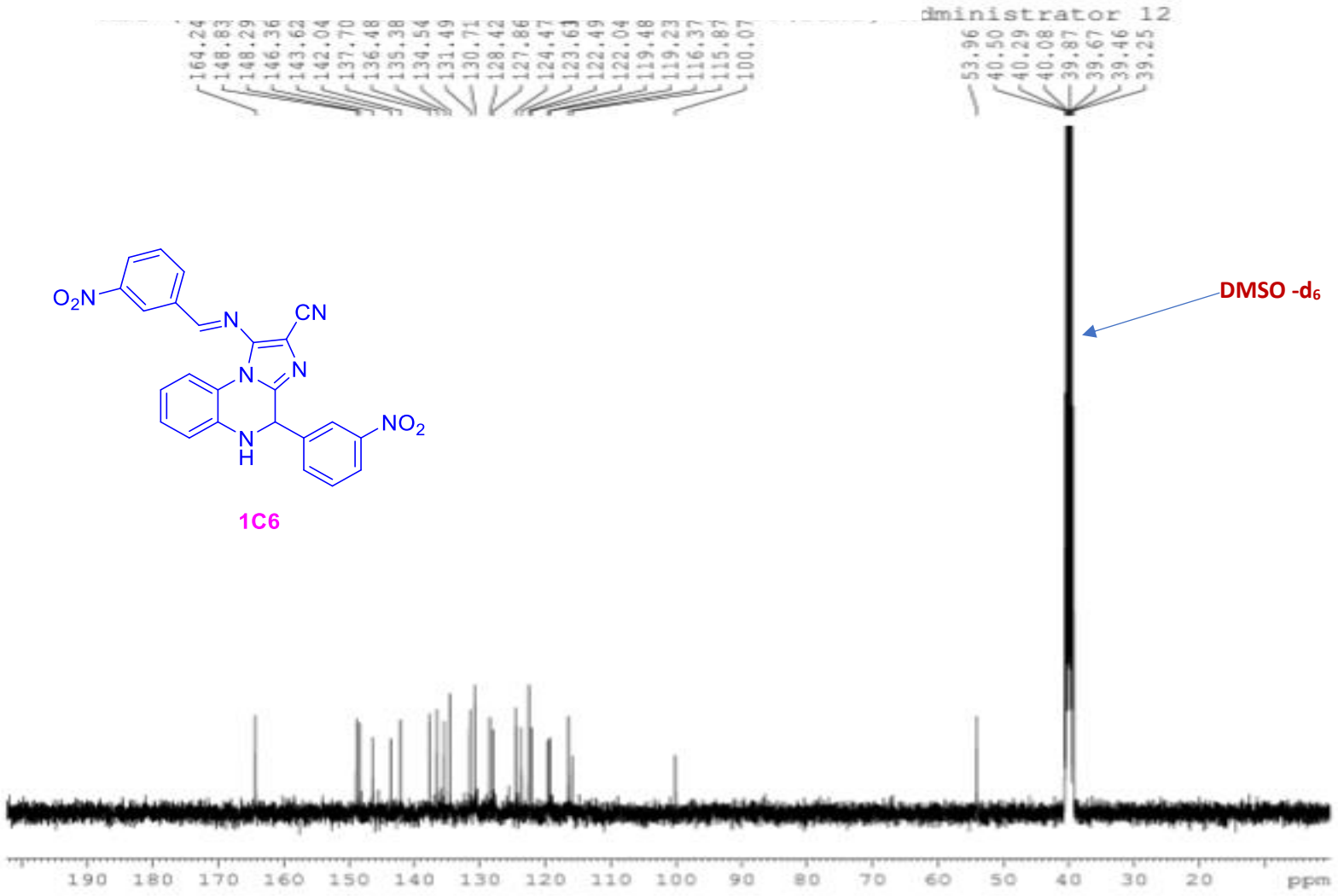


1C5

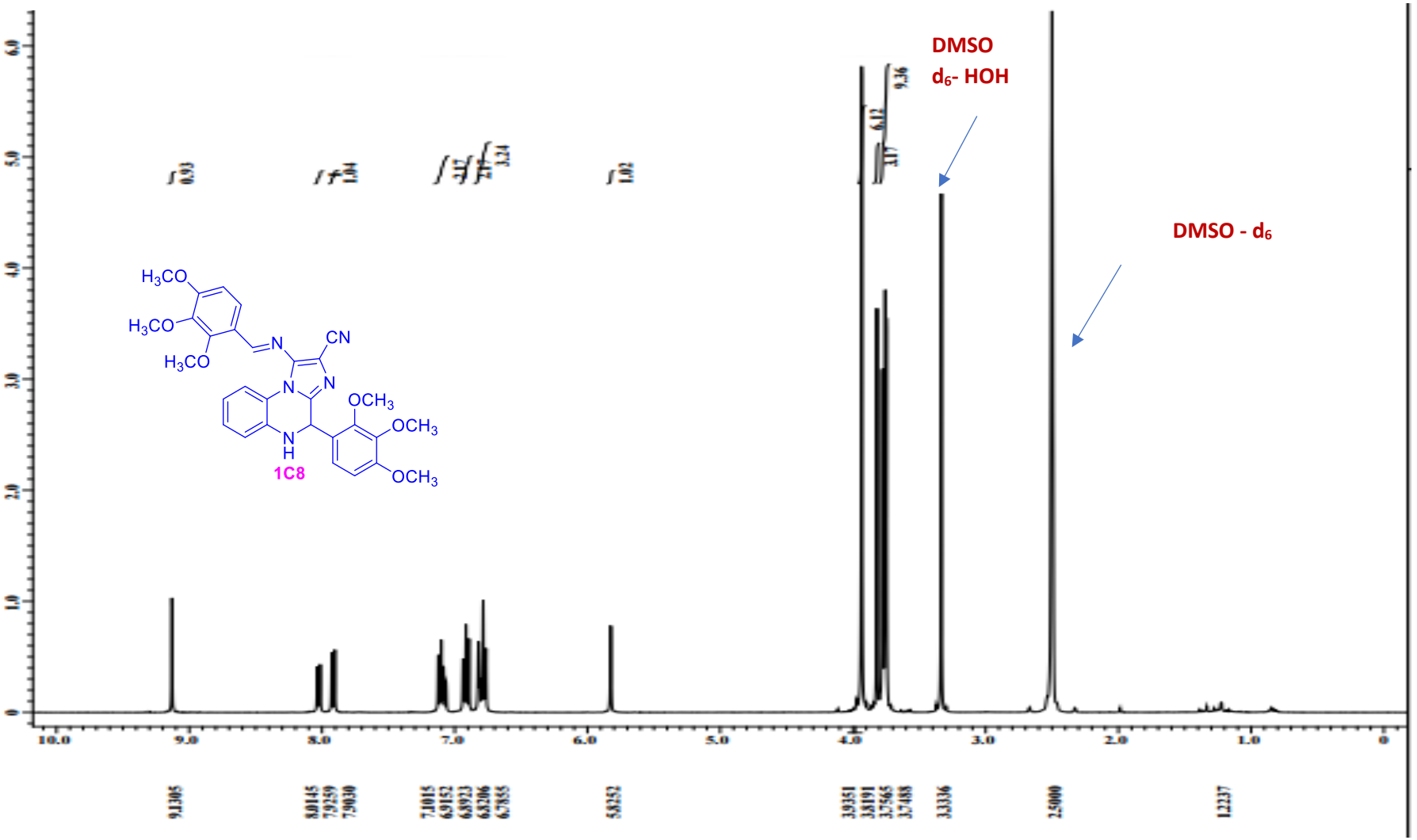
^{1}H NMR

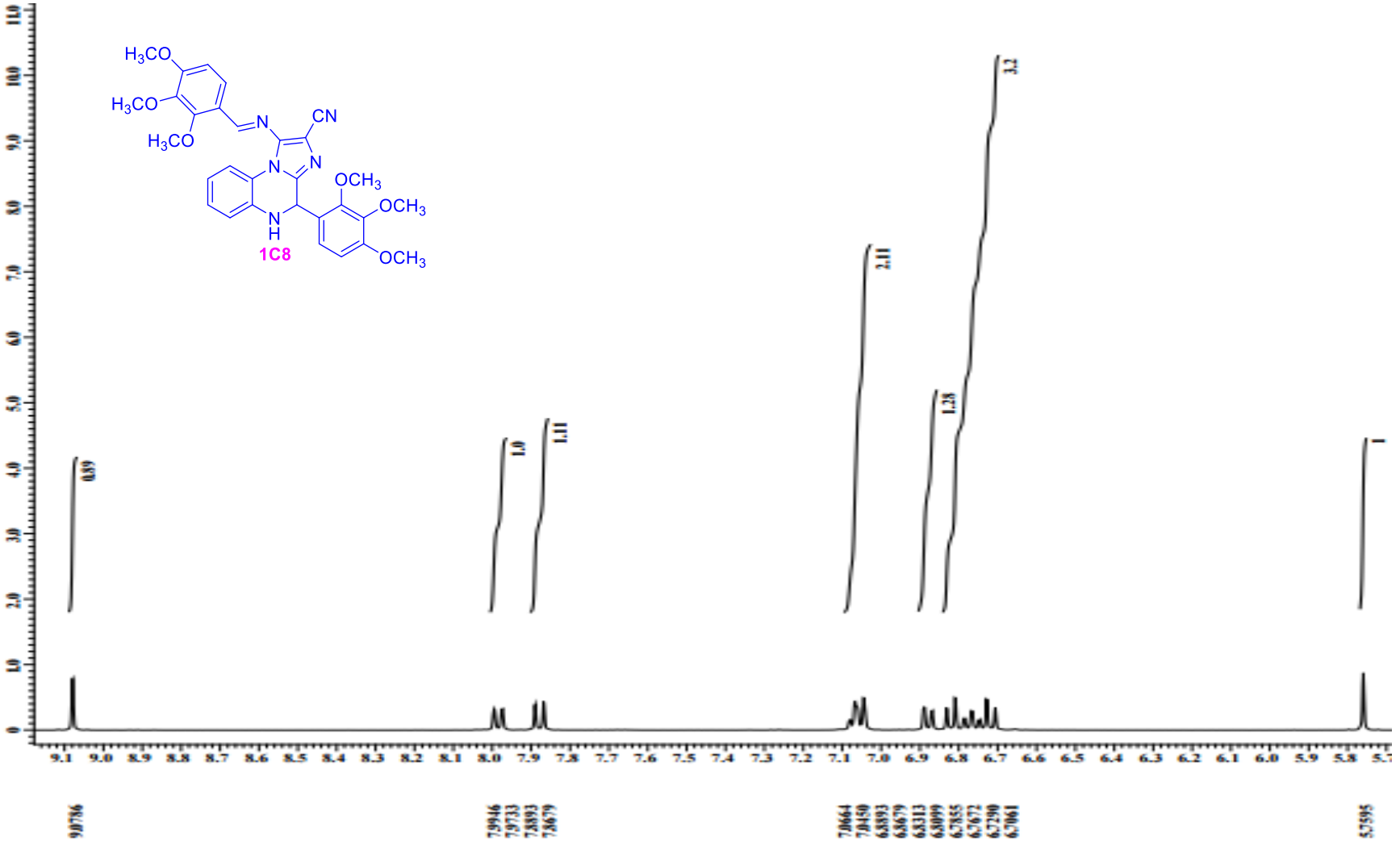

PB
PB
8.81
8.48
8.46
8.44
8.28
8.18
8.16
7.89
7.86
7.84
7.81
7.79
7.68
7.66
7.64
7.36
7.16
7.14
7.12
7.06
7.04
7.02
6.84
6.81
6.80
6.00
O2N
N
CN
N
N
H
NO2
1C6
1.01
0.97
2.09
0.97
1.06
3.51
1.52
1.02
1.08
1.50
1.06
1.00
f1 (ppm)

^{13}C NMR

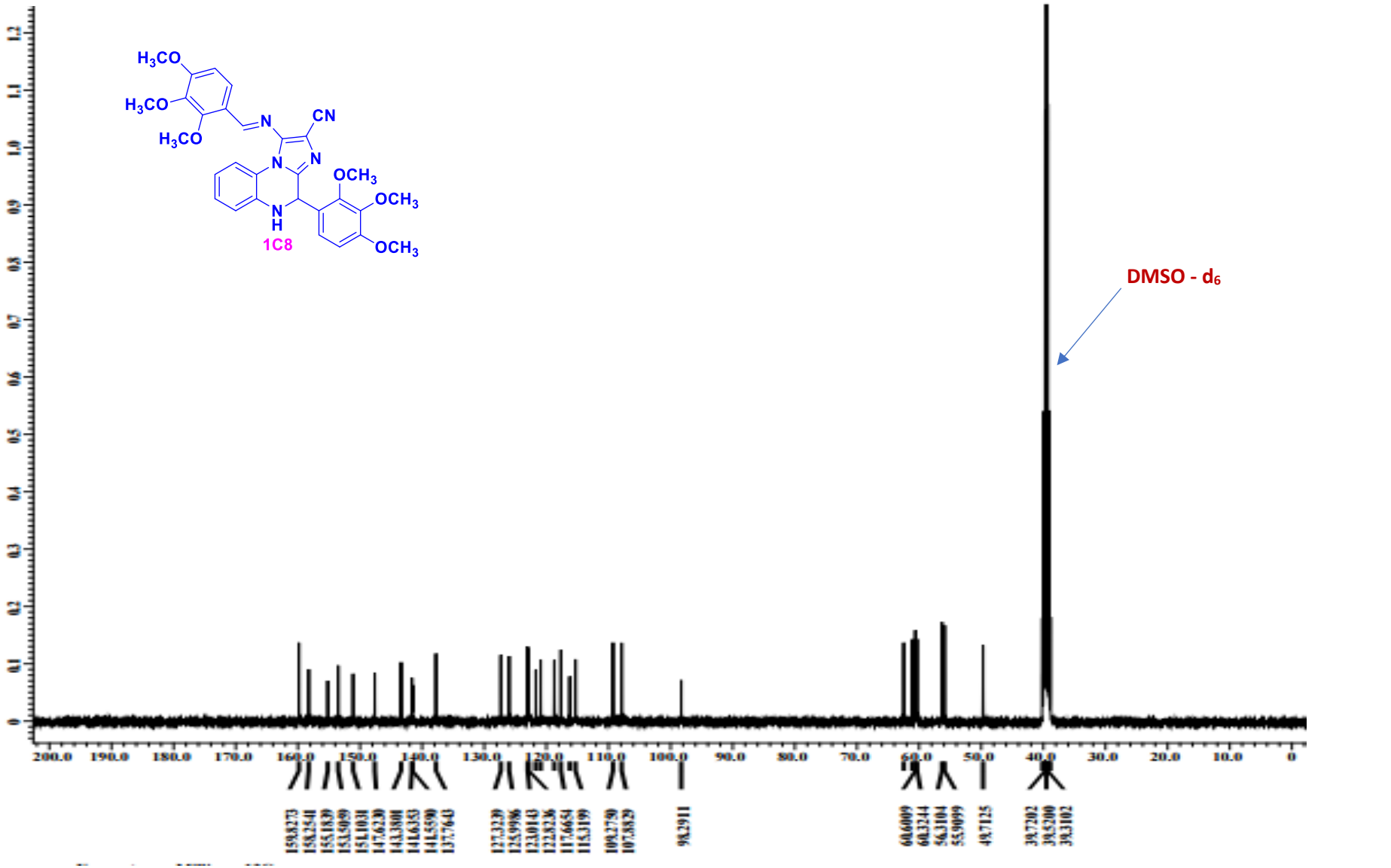

dministrator 12
164.24
148.83
148.29
146.36
143.62
142.04
137.70
136.48
135.38
134.54
131.49
130.71
128.42
127.86
124.47
123.61
122.49
122.04
119.48
119.23
116.37
115.87
100.07
53.96
40.50
40.29
40.08
39.87
39.67
39.46
39.25
DMSO -d6
O2N
N
CN
N
N
N
H
NO2
1C6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

^{1}H NMR

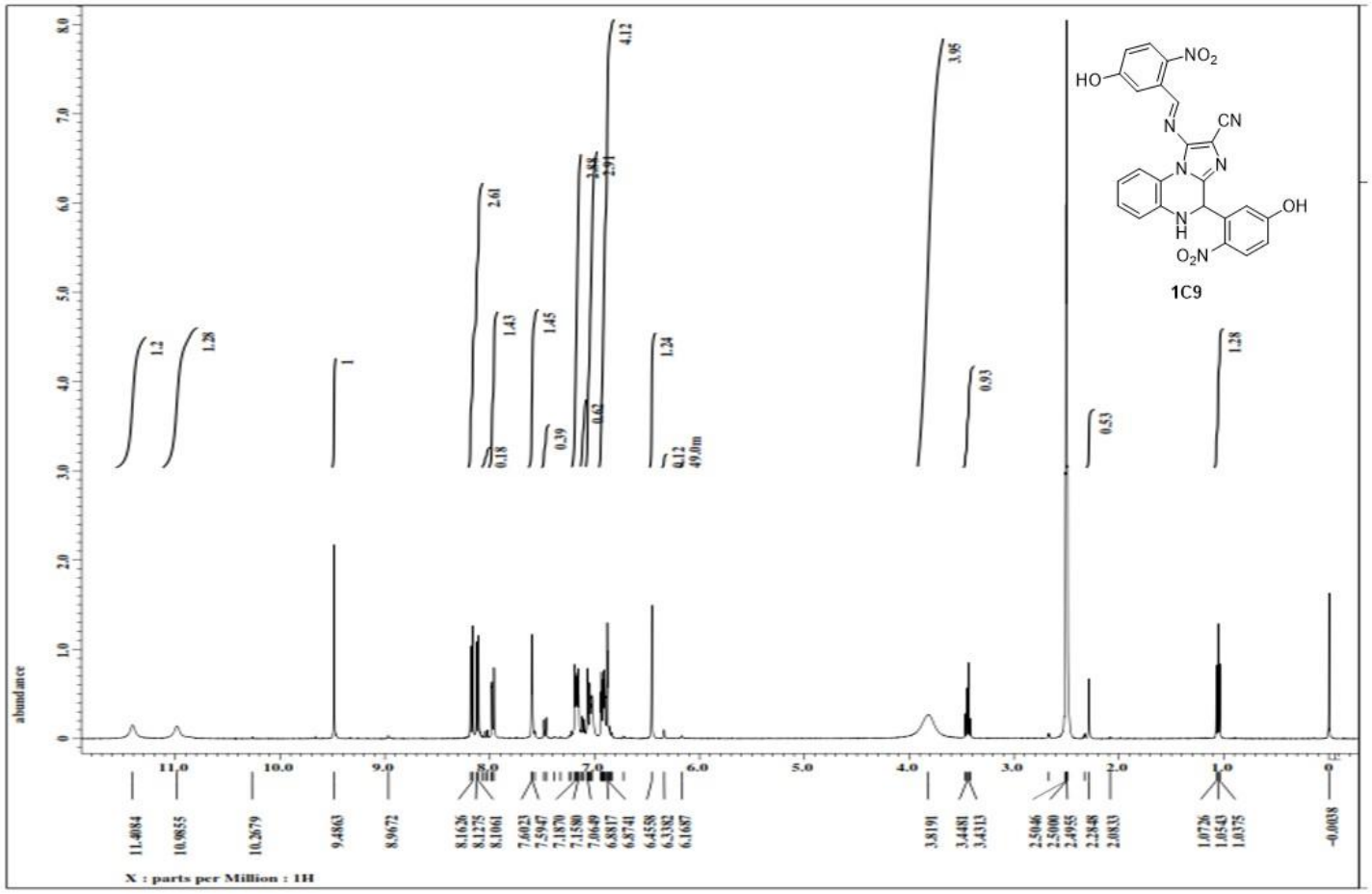

DMSO
d6- HOH
DMSO - d6
H3CO
H3CO
H3CO
N
CN
N
N
OCH3
OCH3
OCH3
N
H
1C8
9.36
6.12
3.17
3.24
1.02
1.04
0.93
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.1305
8.0145
7.9259
7.9030
7.1015
6.9152
6.8923
6.8206
6.7855
5.8252
3.9351
3.8191
3.7565
3.7488
3.3336
2.5000
1.2237


H3CO
H3CO
H3CO
N
CN
N
N
OCH3
OCH3
OCH3
N
H
1C8
0.89
1.0
1.11
2.11
1.28
3.2
1
9.0786
7.9946
7.9733
7.8893
7.8679
7.0664
7.0450
6.8893
6.8679
6.8313
6.8099
6.7855
6.7672
6.7290
6.7061
5.7595

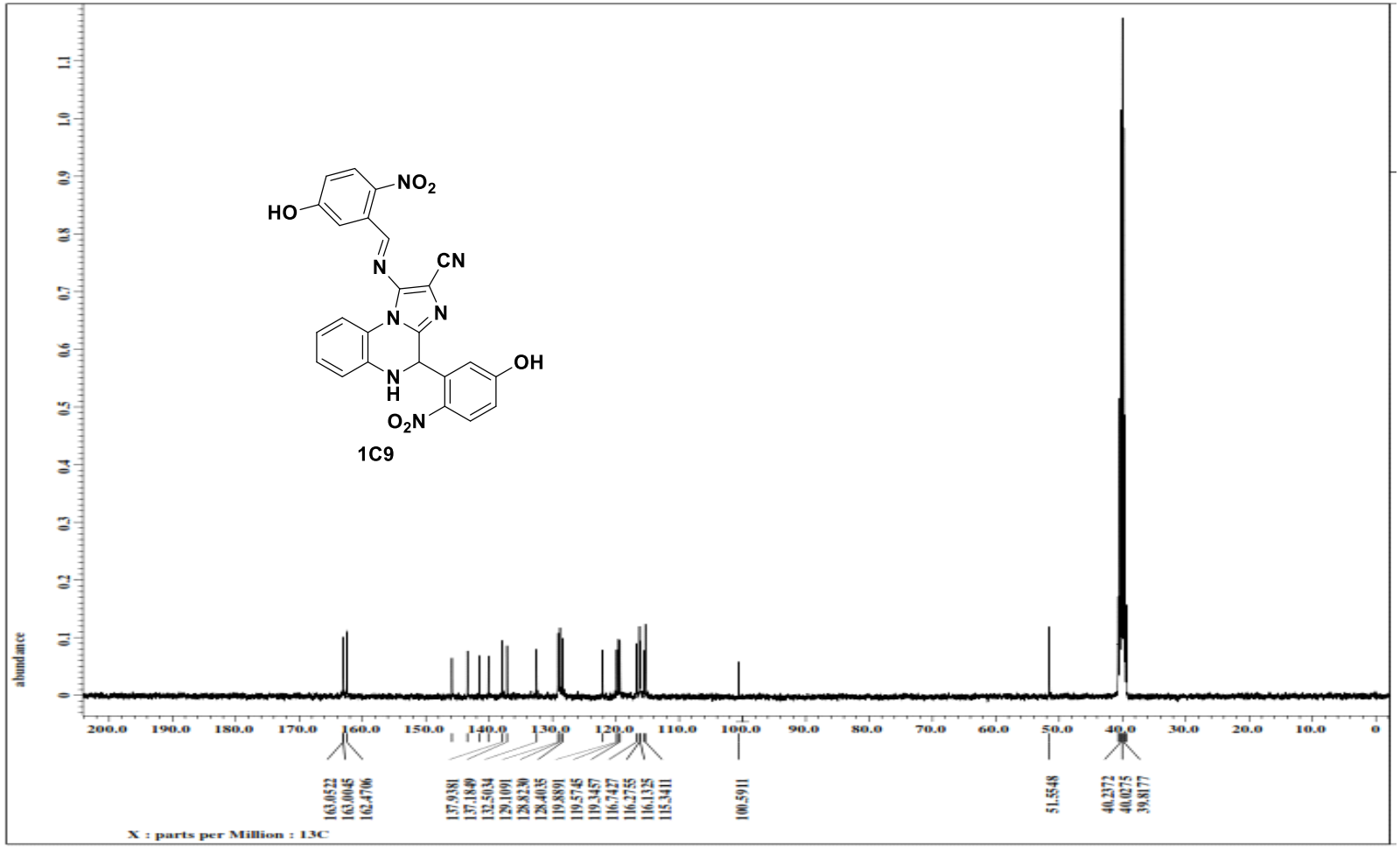
^{13}C NMR


H3CO
H3CO
H3CO
N
CN
N
N
OCH3
OCH3
OCH3
N
H
1C8
DMSO - d6
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
159.8273
158.2541
155.1839
153.5089
151.1031
147.6230
143.3801
141.6353
141.5590
137.7643
127.3329
125.9986
123.0143
122.8336
117.6654
115.3199
109.2750
107.3829
98.2911
60.6009
60.3244
56.3104
55.9099
48.7125
39.7202
39.5200
39.3102

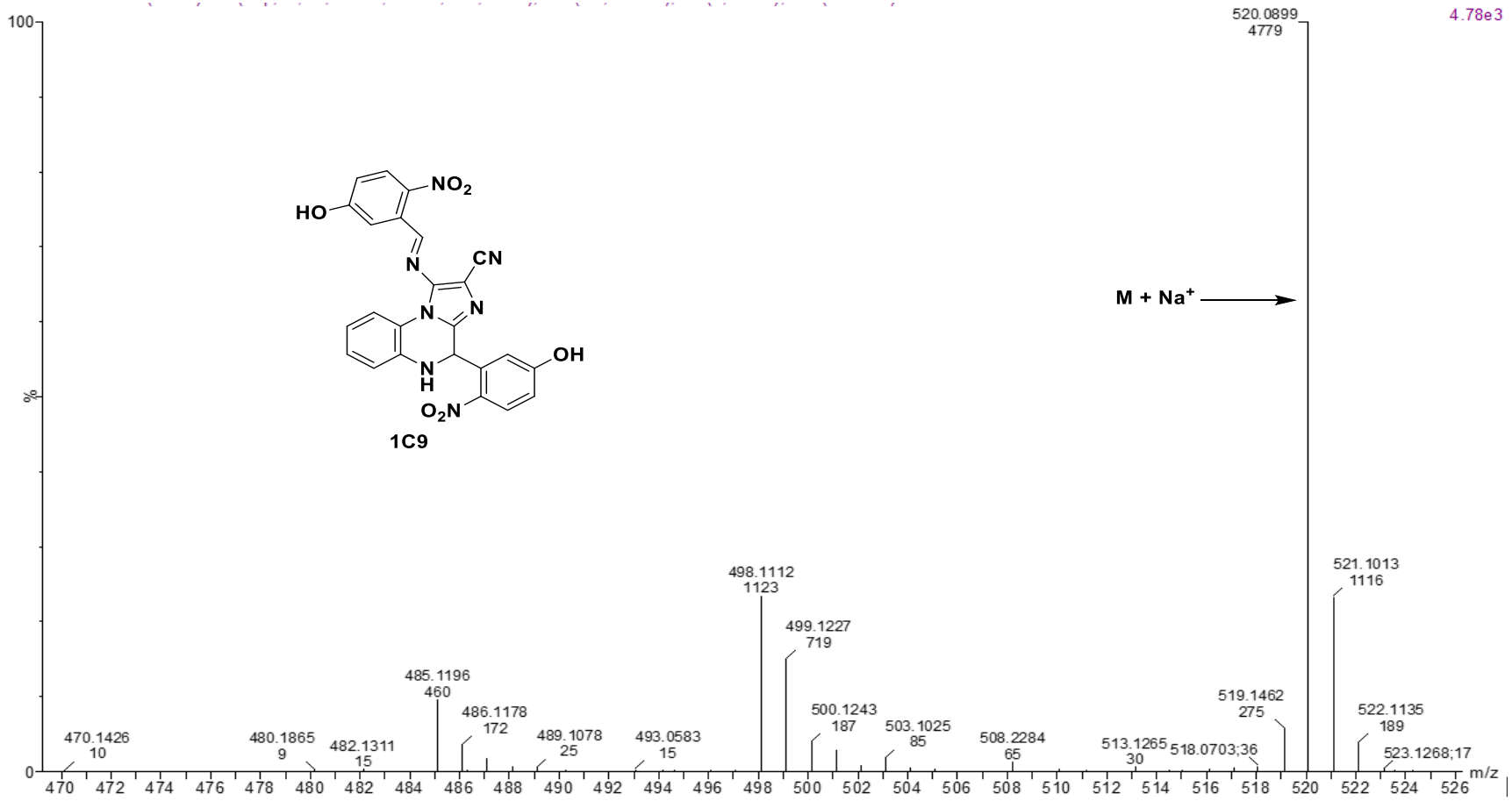
^{1}H NMR



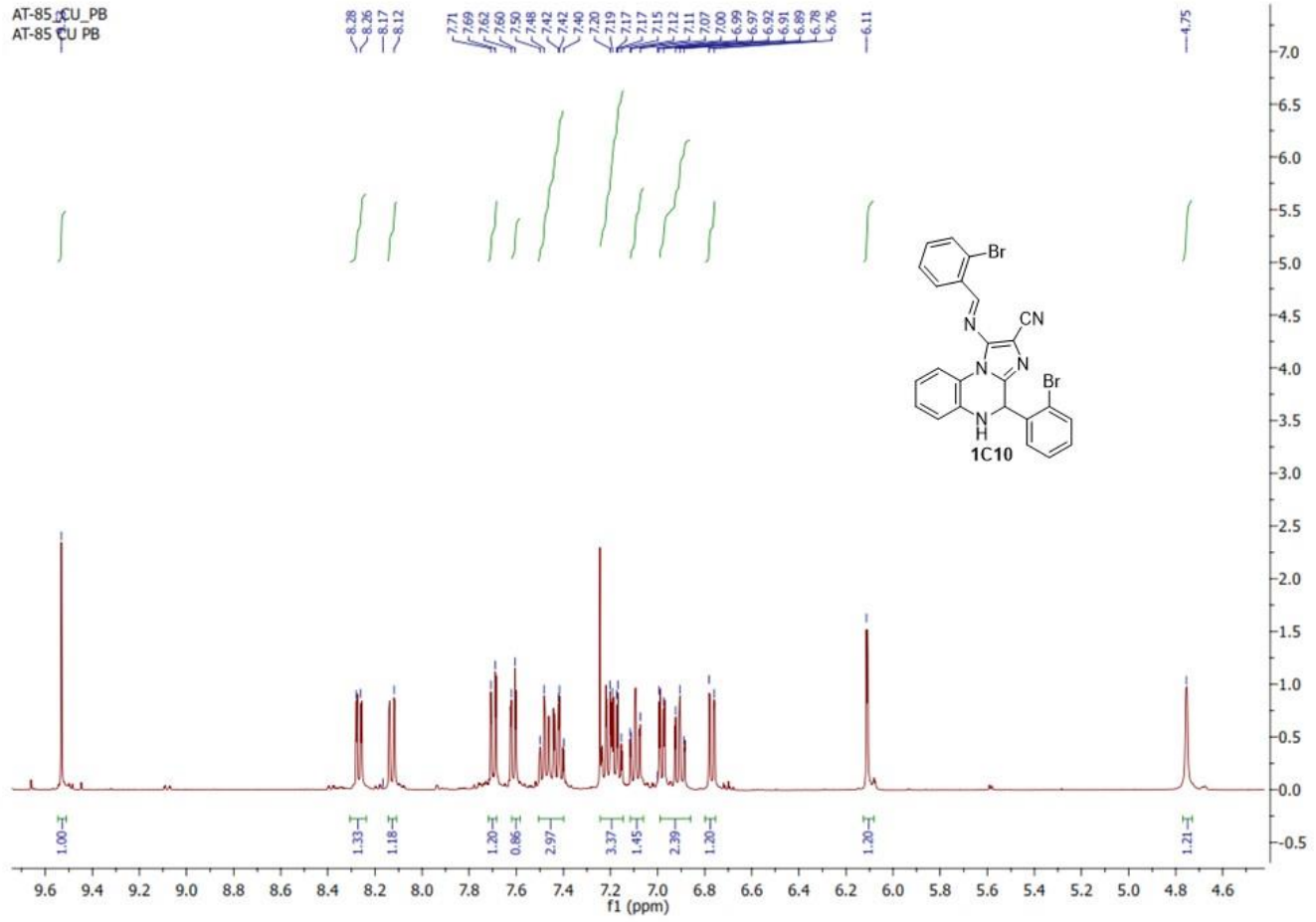
^{13}C NMR


NO2
HO
N
CN
N
N
N
H
OH
O2N
1C9
abundance
X : parts per Million : 13C
163.0522
163.0045
162.4706
137.9381
137.1849
132.5034
129.1091
128.8230
128.4035
119.8891
119.5745
119.3457
116.7427
116.2755
116.1325
115.3411
100.5911
51.5548
40.2372
40.0275
39.8177

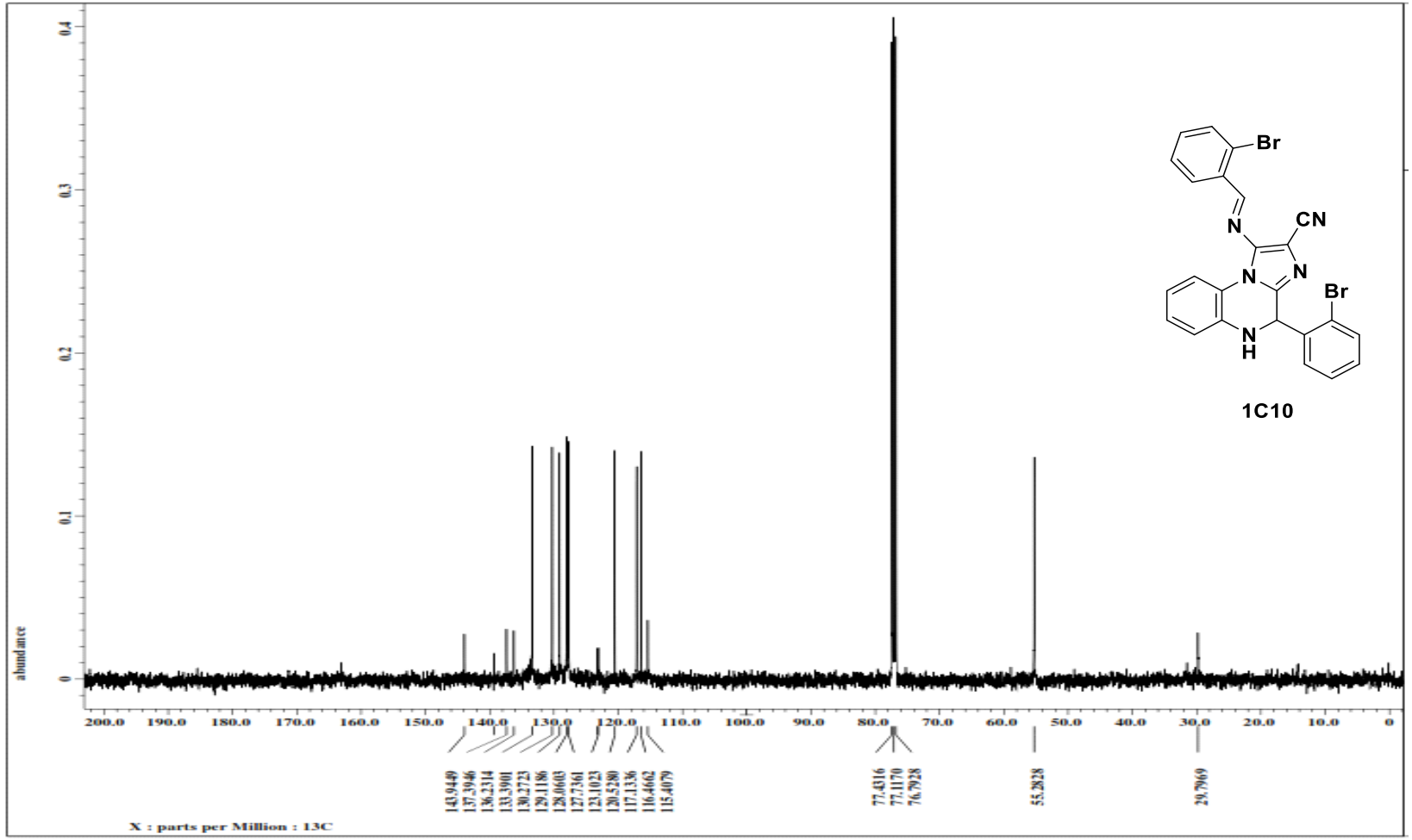
HRMS


100
%
0
520.0899
4779
4.78e3
M + Na+
498.1112
1123
521.1013
1116
499.1227
719
485.1196
460
519.1462
275
486.1178
172
500.1243
187
522.1135
189
503.1025
85
489.1078
25
470.1426
10
480.1865
9
482.1311
15
493.0583
15
508.2284
65
513.1265
30
518.0703;36
523.1268;17
m/z
470 472 474 476 478 480 482 484 486 488 490 492 494 496 498 500 502 504 506 508 510 512 514 516 518 520 522 524 526
HO
NO2
N
CN
N
N
N
H
OH
O2N
1C9

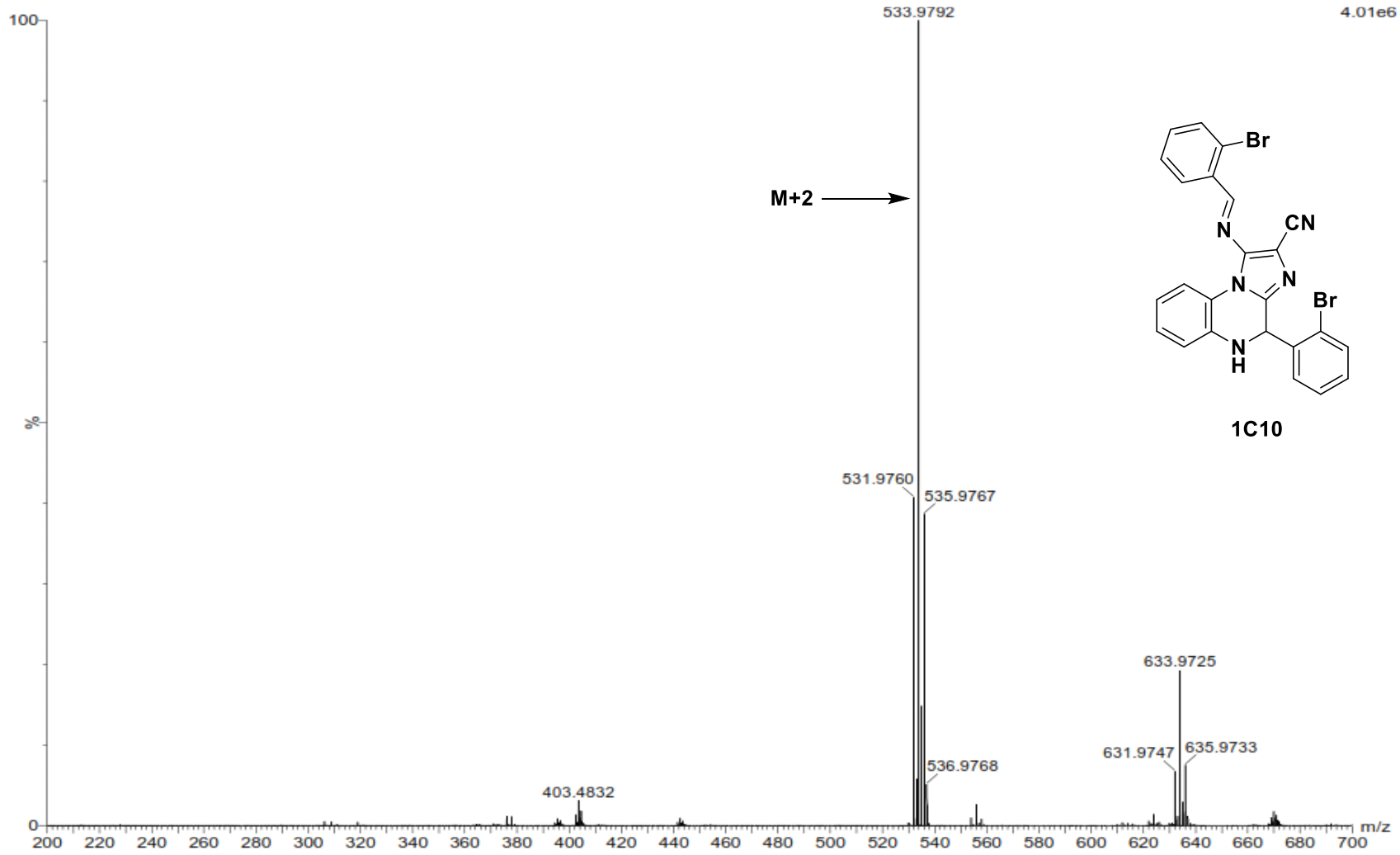
^{1}H NMR


AT-85 CU_PB
AT-85 CU PB
8.28
8.26
8.17
8.12
7.71
7.69
7.62
7.60
7.50
7.48
7.42
7.42
7.40
7.20
7.19
7.17
7.17
7.15
7.12
7.11
7.07
7.00
6.99
6.97
6.92
6.91
6.89
6.78
6.76
6.11
4.75
Br
N
CN
N
N
Br
N
H
1C10
1.00
1.33
1.18
1.20
0.86
2.97
3.37
1.45
2.39
1.20
1.20
1.21
f1 (ppm)

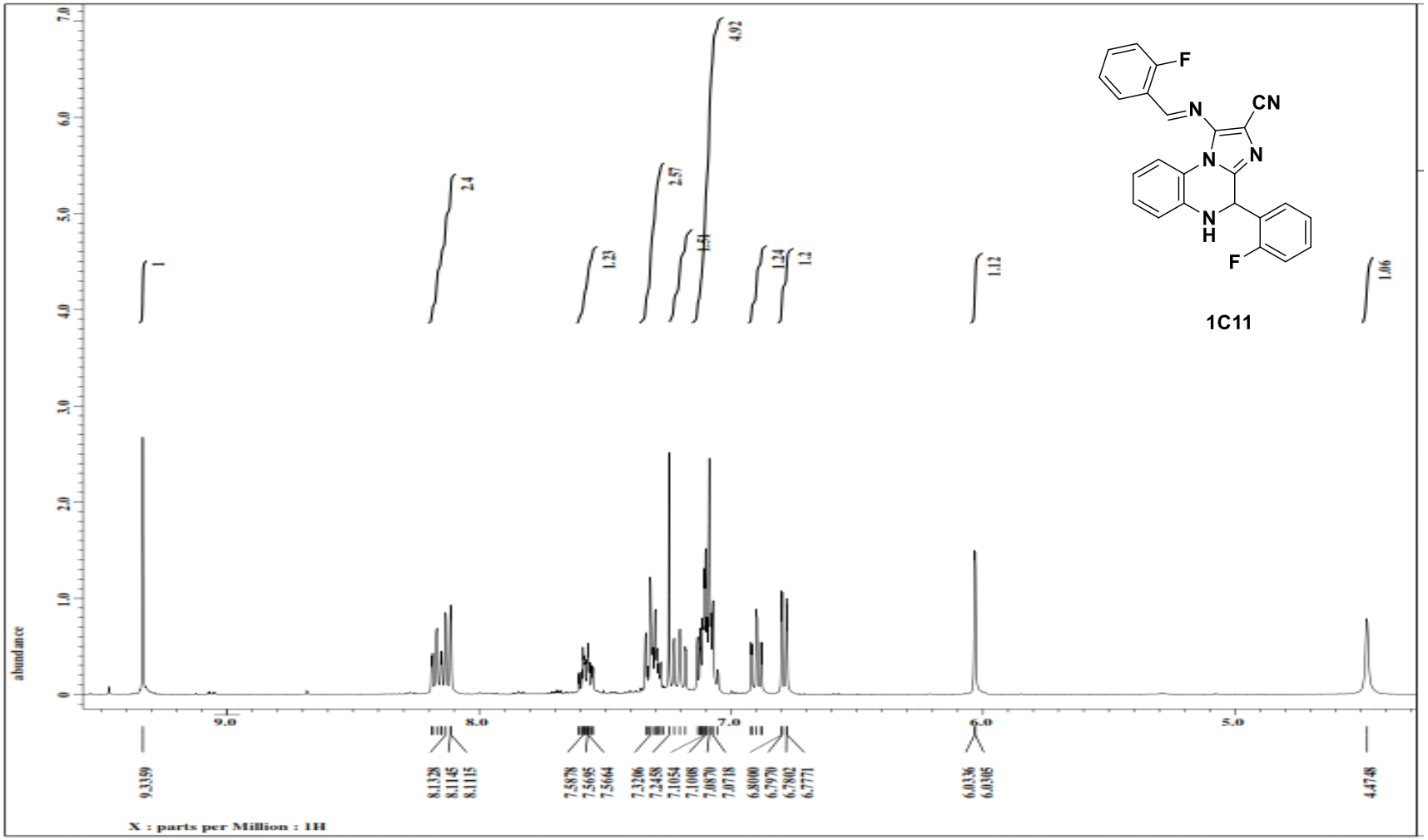
^{13}C NMR


abundance
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.9449
137.3946
136.2314
133.3901
130.2723
129.1186
128.0603
127.7361
123.1023
120.5280
117.1336
116.4662
115.4079
77.4316
77.1170
76.7928
55.2828
29.7969
X : parts per Million : 13C
Br
N
CN
N
N
Br
N
H
1C10

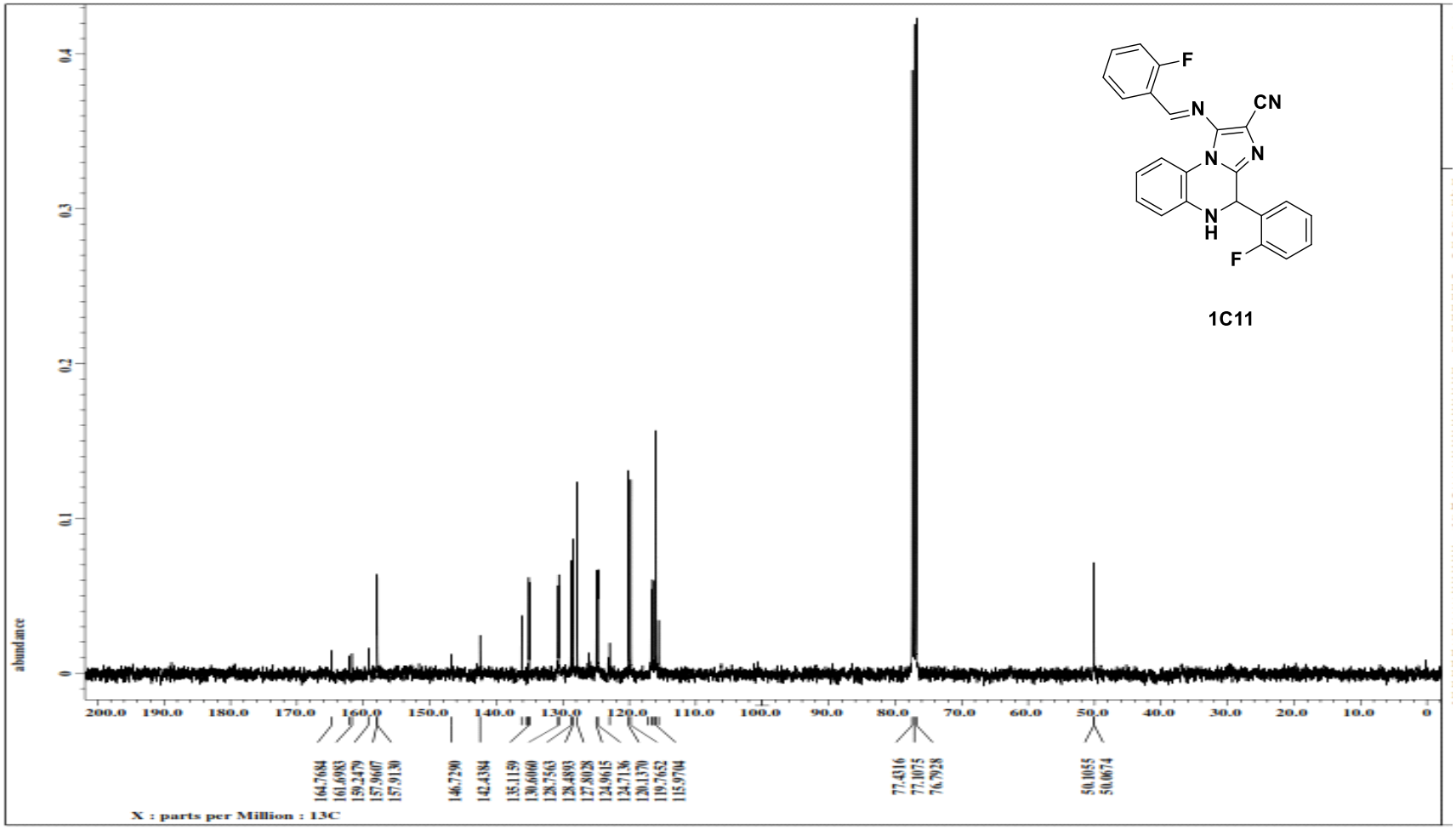
HRMS


533.9792
4.01e6
100
%
0
M+2
Br
N
CN
N
N
Br
N
H
1C10
531.9760
535.9767
633.9725
631.9747
635.9733
536.9768
403.4832
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
m/z

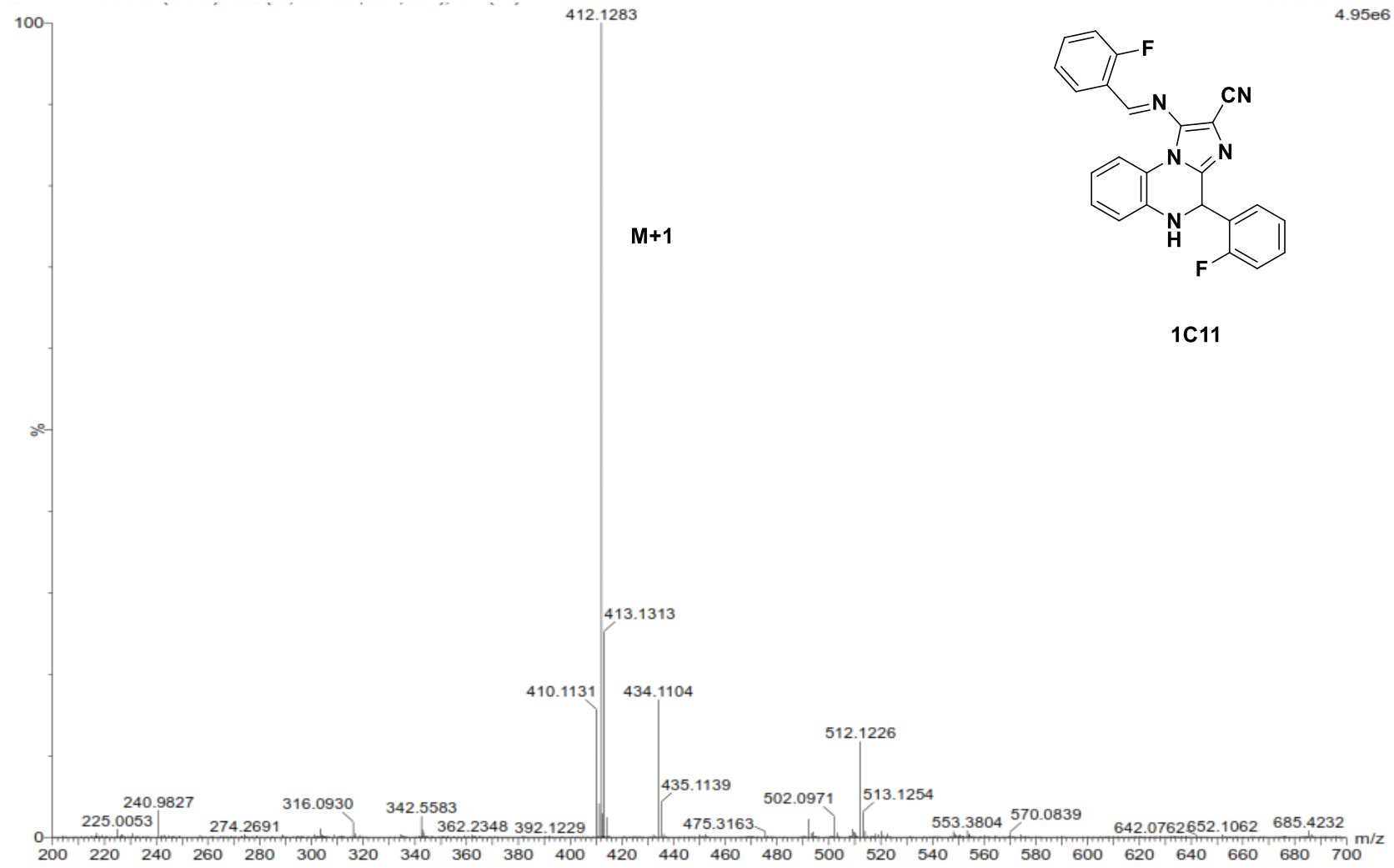
^{1}H NMR



^{13}C NMR


F
N
CN
N
N
N
H
F
1C11
abundance
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
164.7684
161.6983
159.2479
157.9607
157.9130
146.7290
142.4384
135.1159
130.6060
128.7563
128.4893
127.8028
124.9615
124.7136
120.1370
119.7652
115.9704
77.4316
77.1075
76.7928
50.1055
50.0674
X : parts per Million : 13C

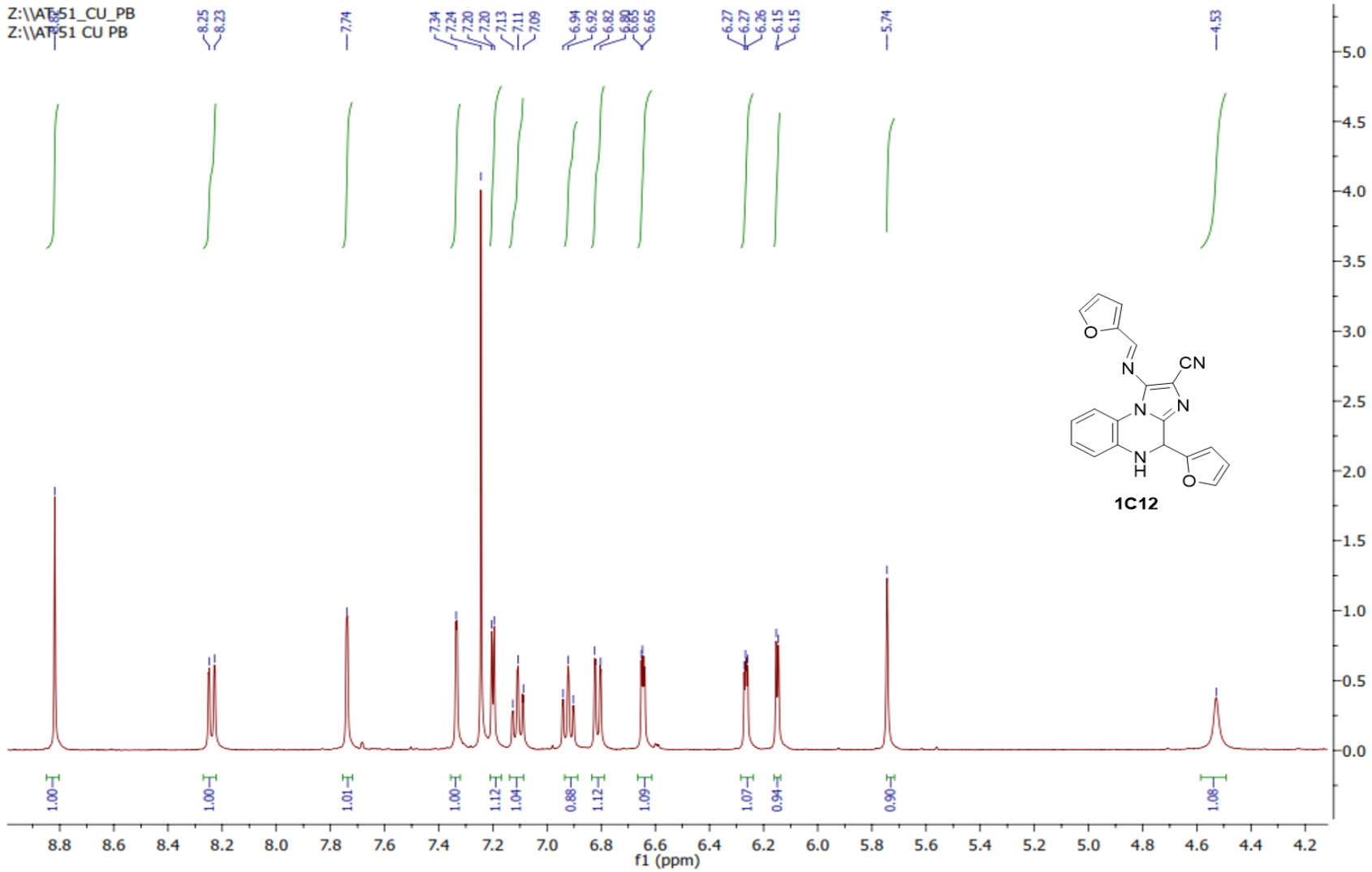
HRMS


412.1283
4.95e6
100
%
0
M+1
413.1313
410.1131
434.1104
512.1226
435.1139
240.9827
316.0930
342.5583
225.0053
274.2691
362.2348
392.1229
475.3163
502.0971
513.1254
553.3804
570.0839
642.0762
652.1062
685.4232
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700

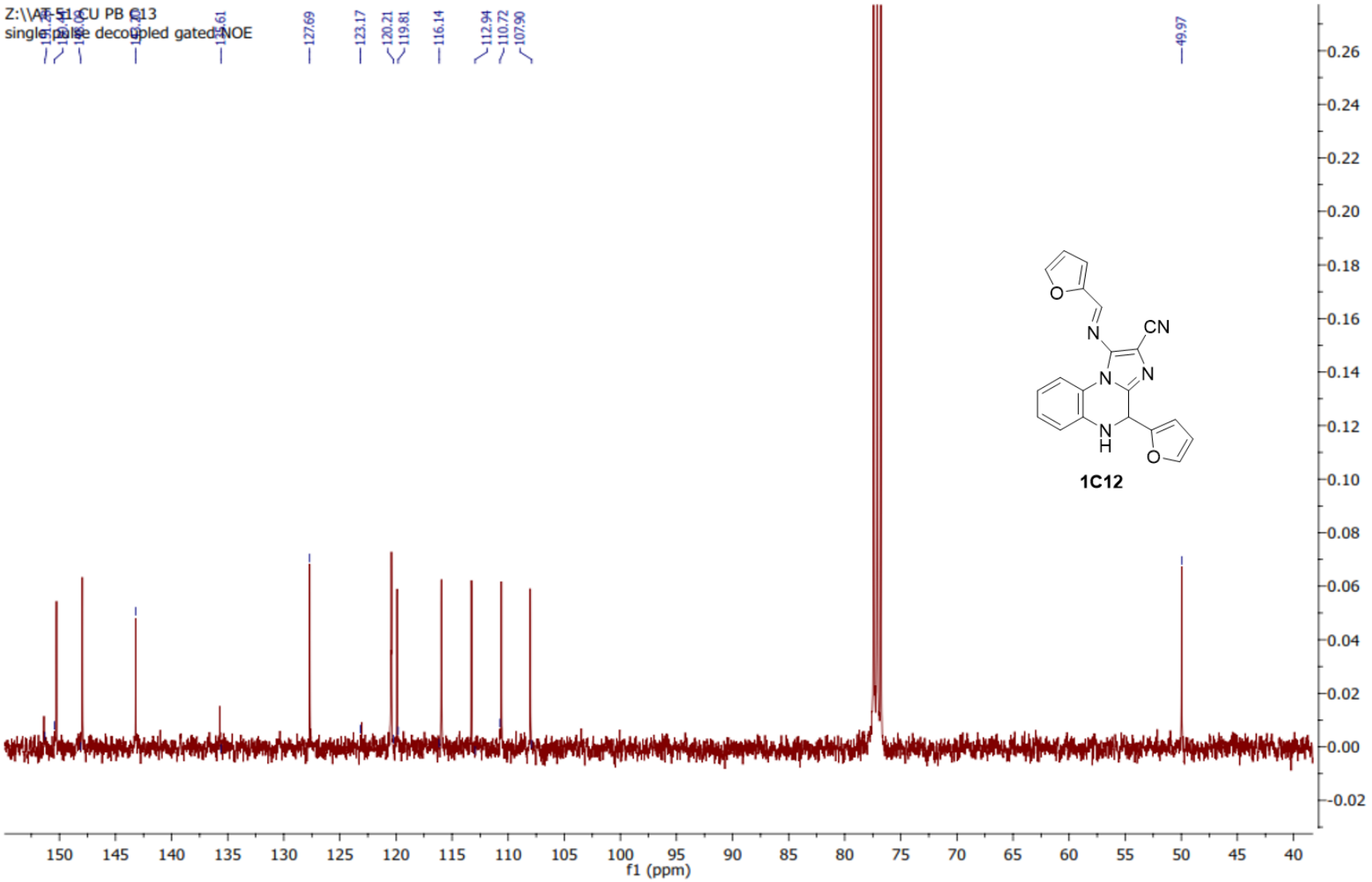
F
N
CN
N
N
N
H
F

1C11

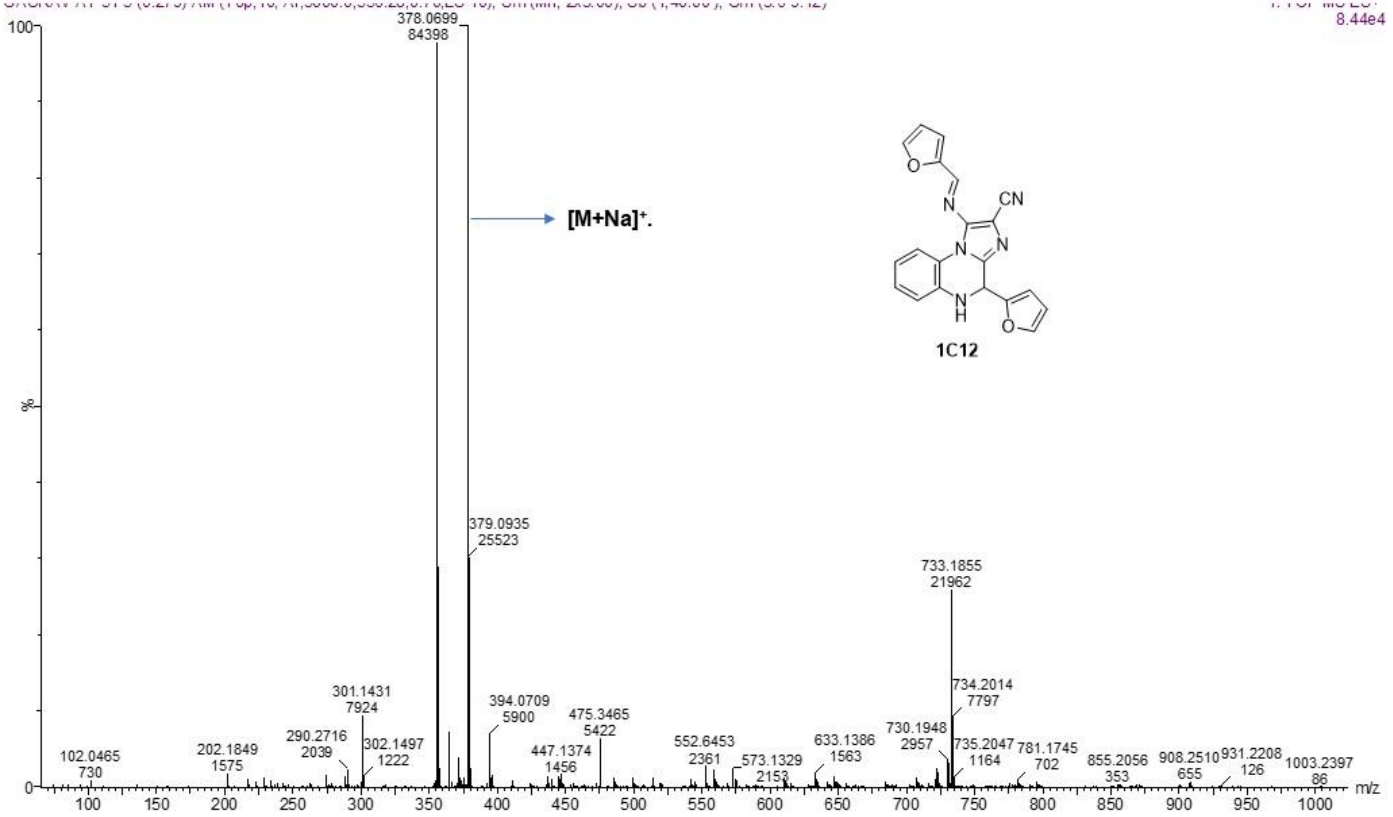
^{1}H NMR


Z:\\AT-51_CU_PB
Z:\\AT-51 CU PB
8.25
8.23
7.74
7.34
7.24
7.20
7.20
7.13
7.11
7.09
6.94
6.92
6.82
6.80
6.65
6.27
6.27
6.26
6.15
6.15
5.74
4.53
1.00
1.00
1.01
1.00
1.12
1.04
0.88
1.12
1.09
1.07
0.94
0.90
1.08
f1 (ppm)
1C12

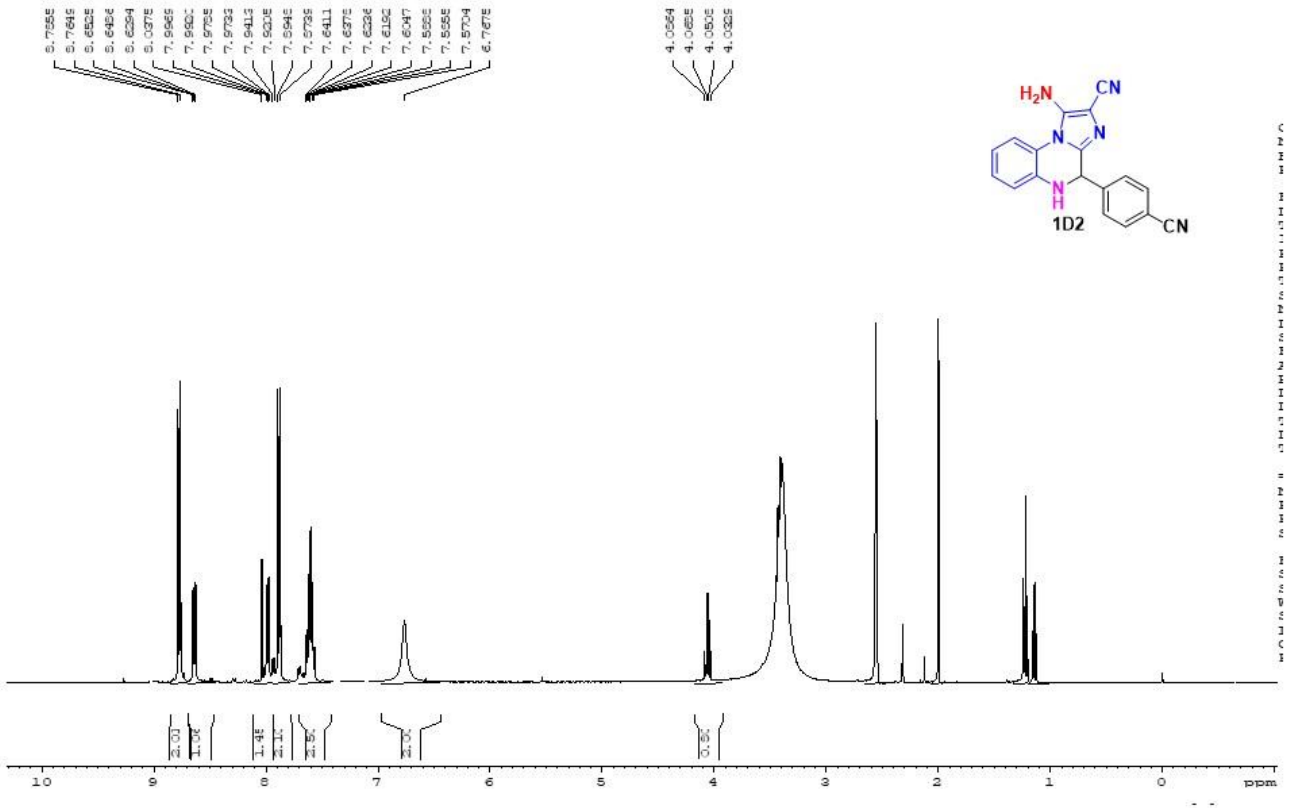
^{13}C NMR


Z:\\AT-51-CU PB C13
single pulse decoupled gated NOE
127.69
123.17
120.21
119.81
116.14
112.94
110.72
107.90
49.97
CN
N
N
N
H
O
O
1C12
f1 (ppm)

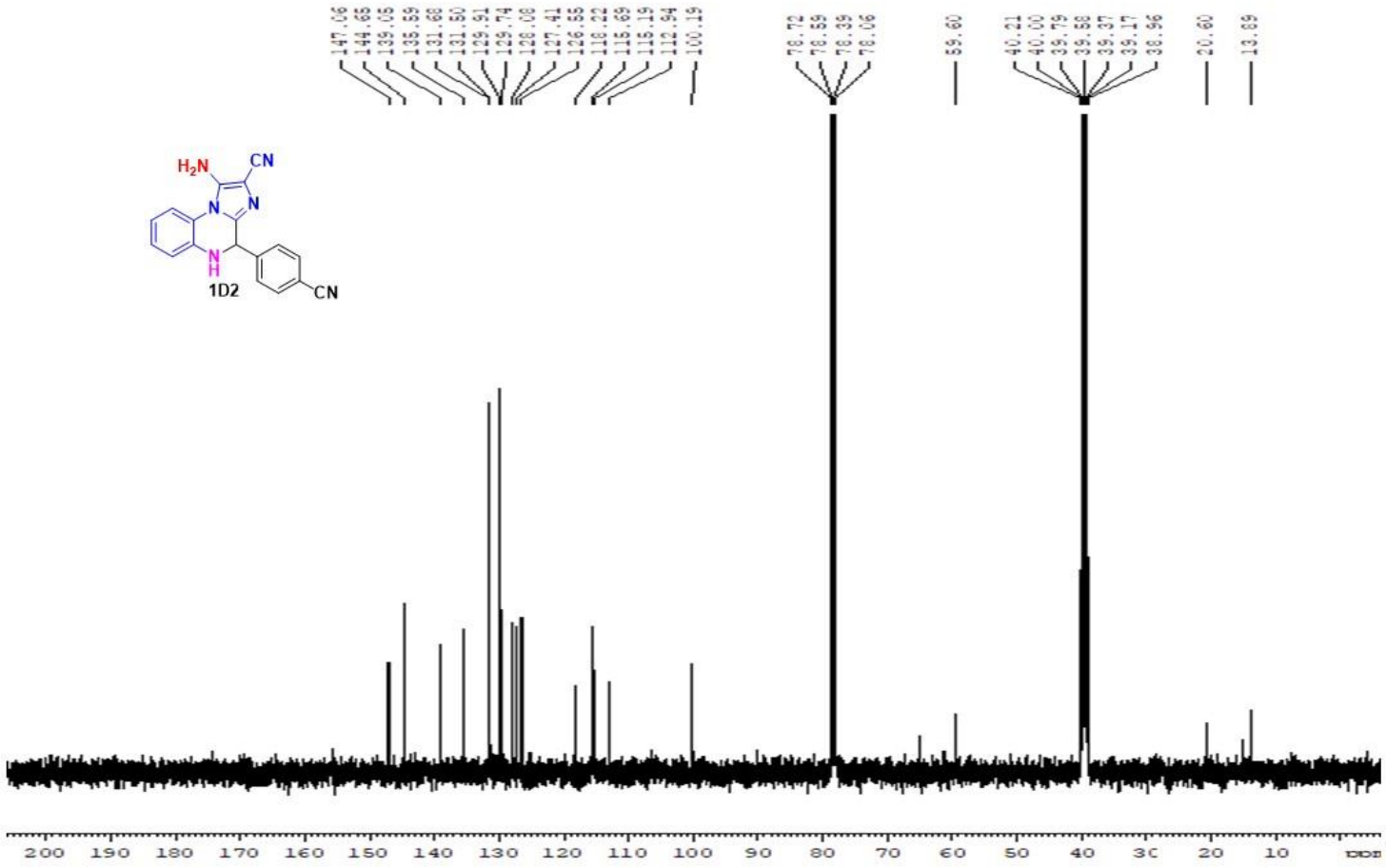
HRMS


8.44e4
100
%
0
378.0699
84398
[M+Na]+.
379.0935
25523
733.1855
21962
734.2014
7797
301.1431
7924
394.0709
5900
475.3465
5422
290.2716
2039
302.1497
1222
102.0465
730
202.1849
1575
447.1374
1456
552.6453
2361
573.1329
2153
633.1386
1563
730.1948
2957
735.2047
1164
781.1745
702
855.2056
353
908.2510
655
931.2208
126
1003.2397
86
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
CN
N
O
N
N
H
O
1C12

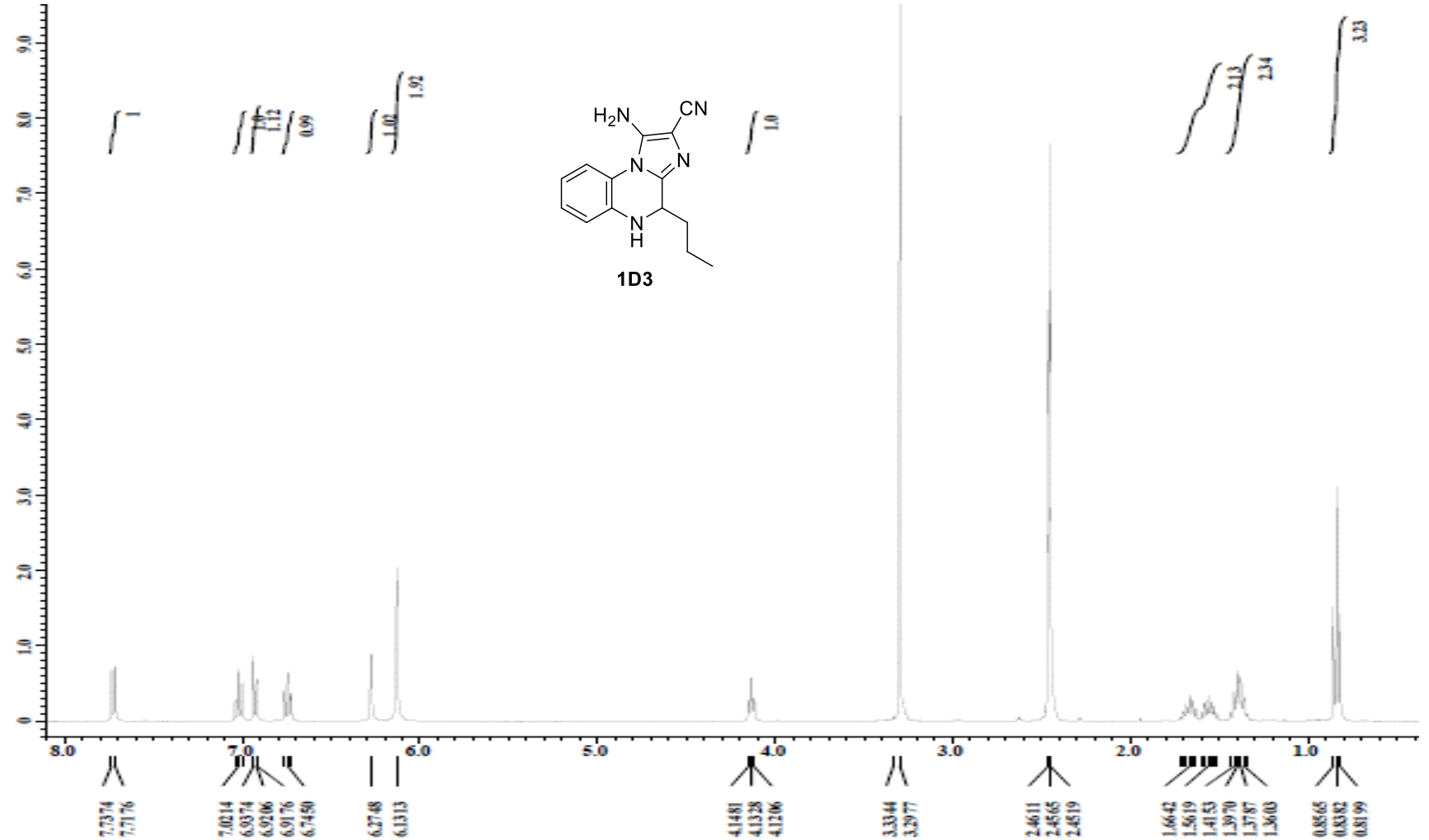
^{1}H NMR


8.7655
8.7645
8.6528
8.6484
8.6294
8.0375
7.9965
7.9901
7.9758
7.9733
7.9413
7.9208
7.8943
7.8738
7.6411
7.6375
7.6236
7.6192
7.6047
7.5565
7.5558
7.5704
6.7675
4.0564
4.0468
4.0503
4.0325
H2N
CN
N
N
N
H
1D2
CN
2.00
1.02
1.48
2.10
2.15
2.10
0.85
10
9
8
7
6
5
4
3
2
1
0
ppm

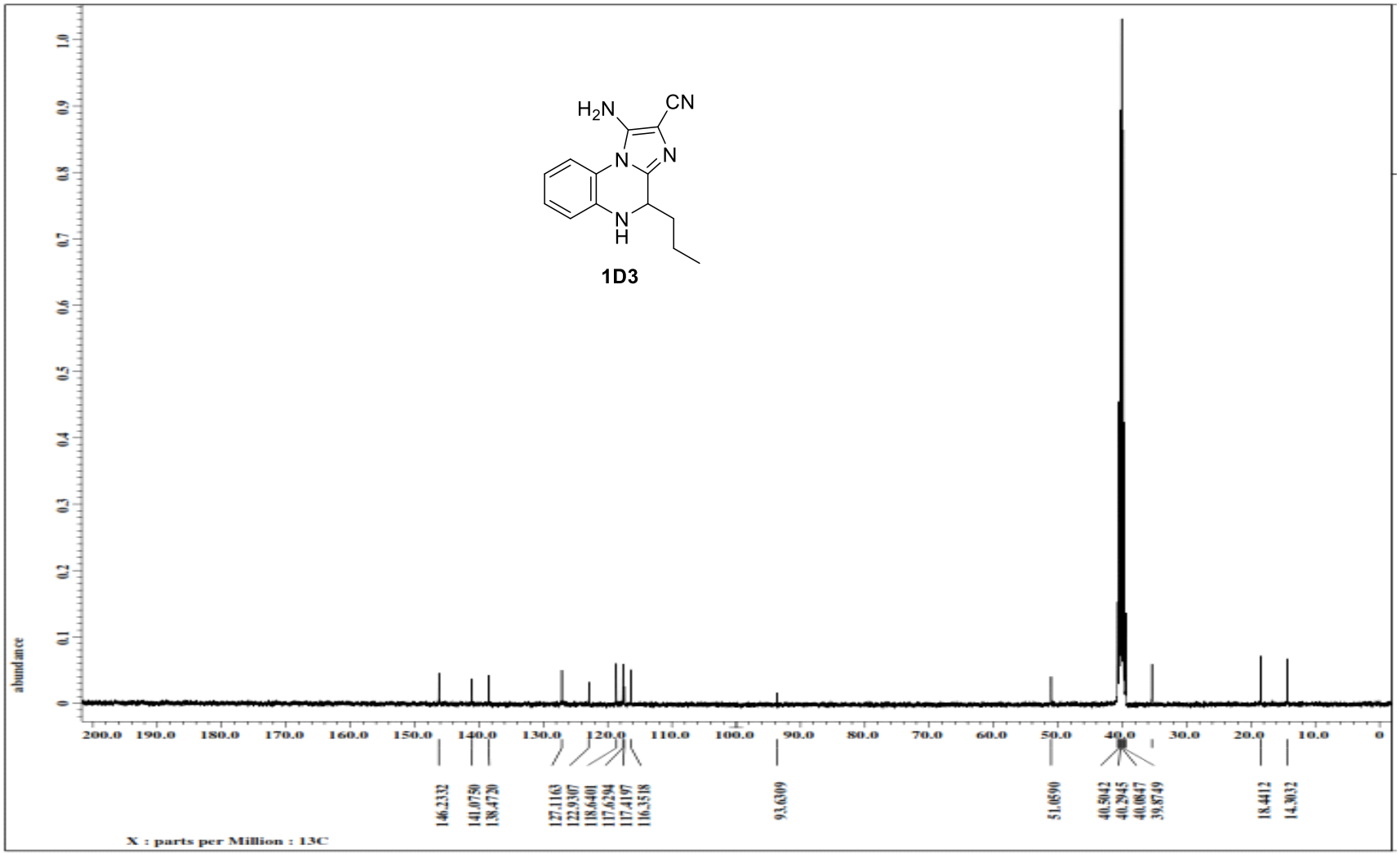
^{13}C NMR


147.06
144.65
139.08
135.59
131.68
131.50
129.91
129.74
128.08
127.41
126.85
118.22
115.69
115.19
112.94
100.19
78.72
78.59
78.39
78.06
59.60
40.21
40.00
39.79
39.58
39.37
39.17
38.96
20.60
13.69
H2N
CN
N
N
H
1D2
CN
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

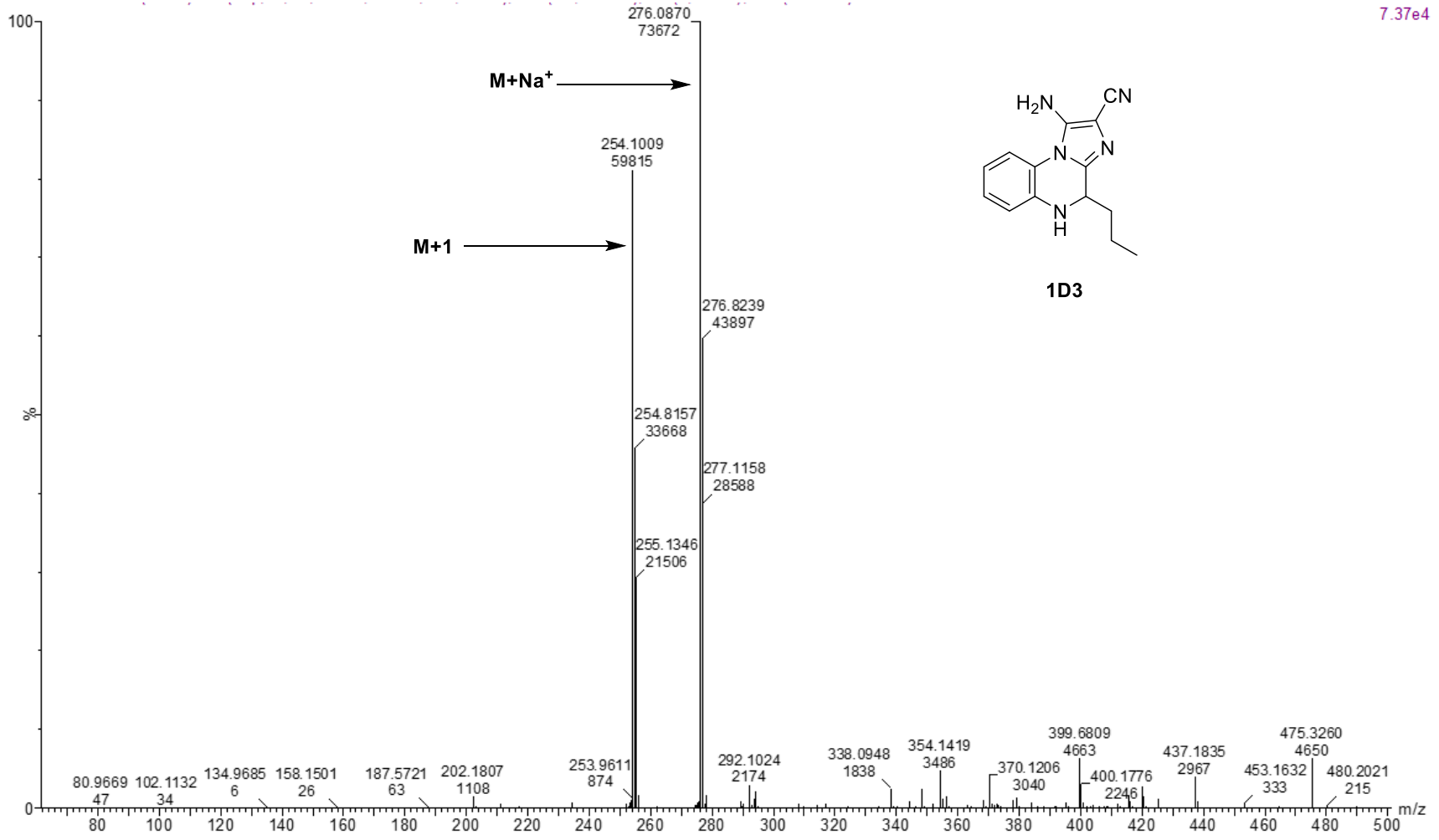
^{1}H NMR


1
1.12
0.99
1.02
1.92
1.0
2.13
2.14
3.33
H2N
CN
N
N
N
H
1D3
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.7374
7.7176
7.0214
6.9374
6.9206
6.9176
6.7450
6.2748
6.1313
4.1481
4.1328
4.1206
3.3344
3.2977
2.4611
2.4565
2.4519
1.6642
1.5619
1.4153
1.3970
1.3787
1.3603
0.8565
0.8382
0.8199

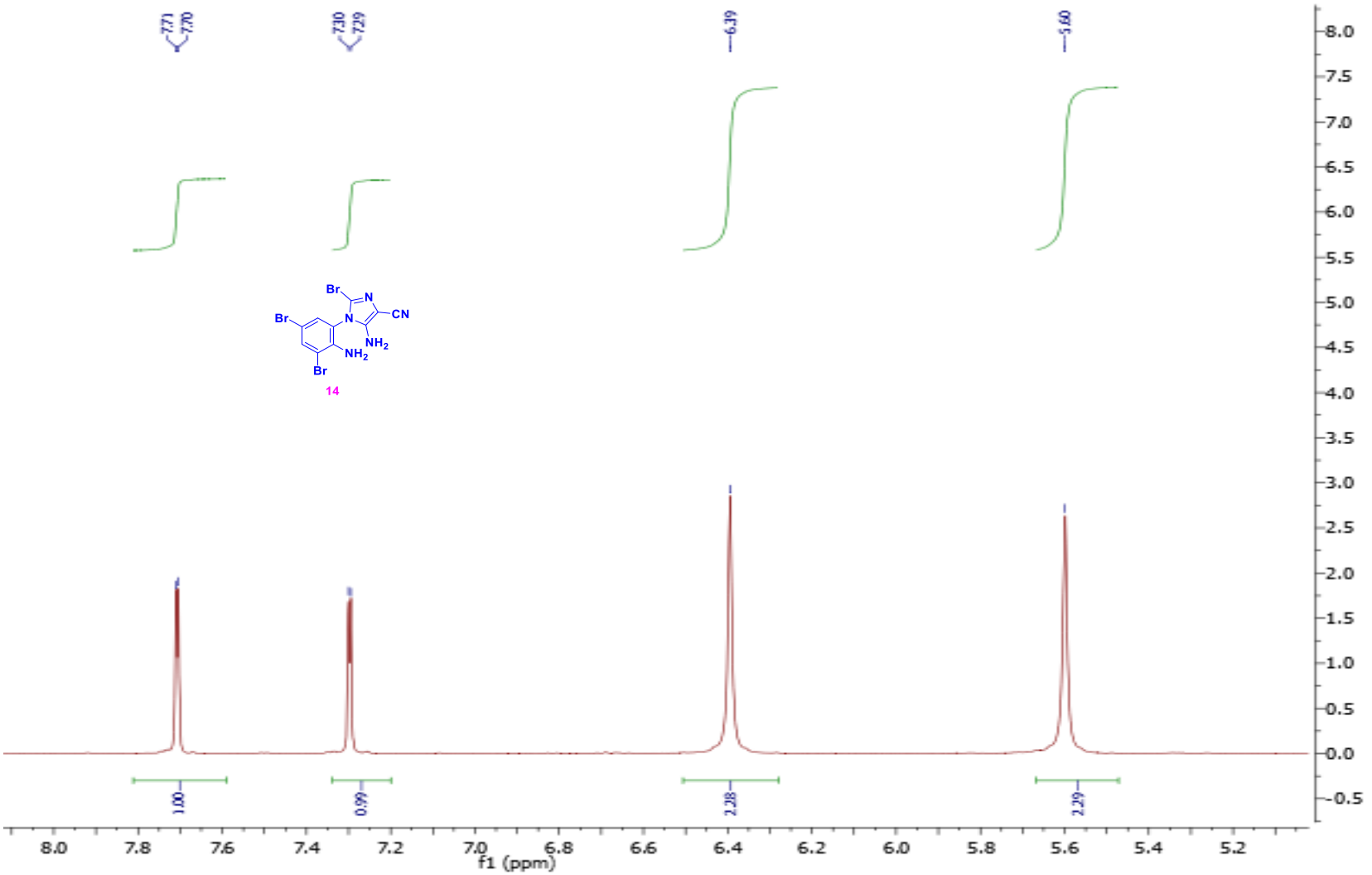
^{13}C NMR


H2N
CN
N
N
N
H
1D3
abundance
X : parts per Million : 13C
146.2332
141.0750
138.4720
127.1163
122.9307
118.6401
117.6294
117.4197
116.3518
93.6309
51.0590
40.5042
40.2945
40.0847
39.8749
18.4412
14.3032

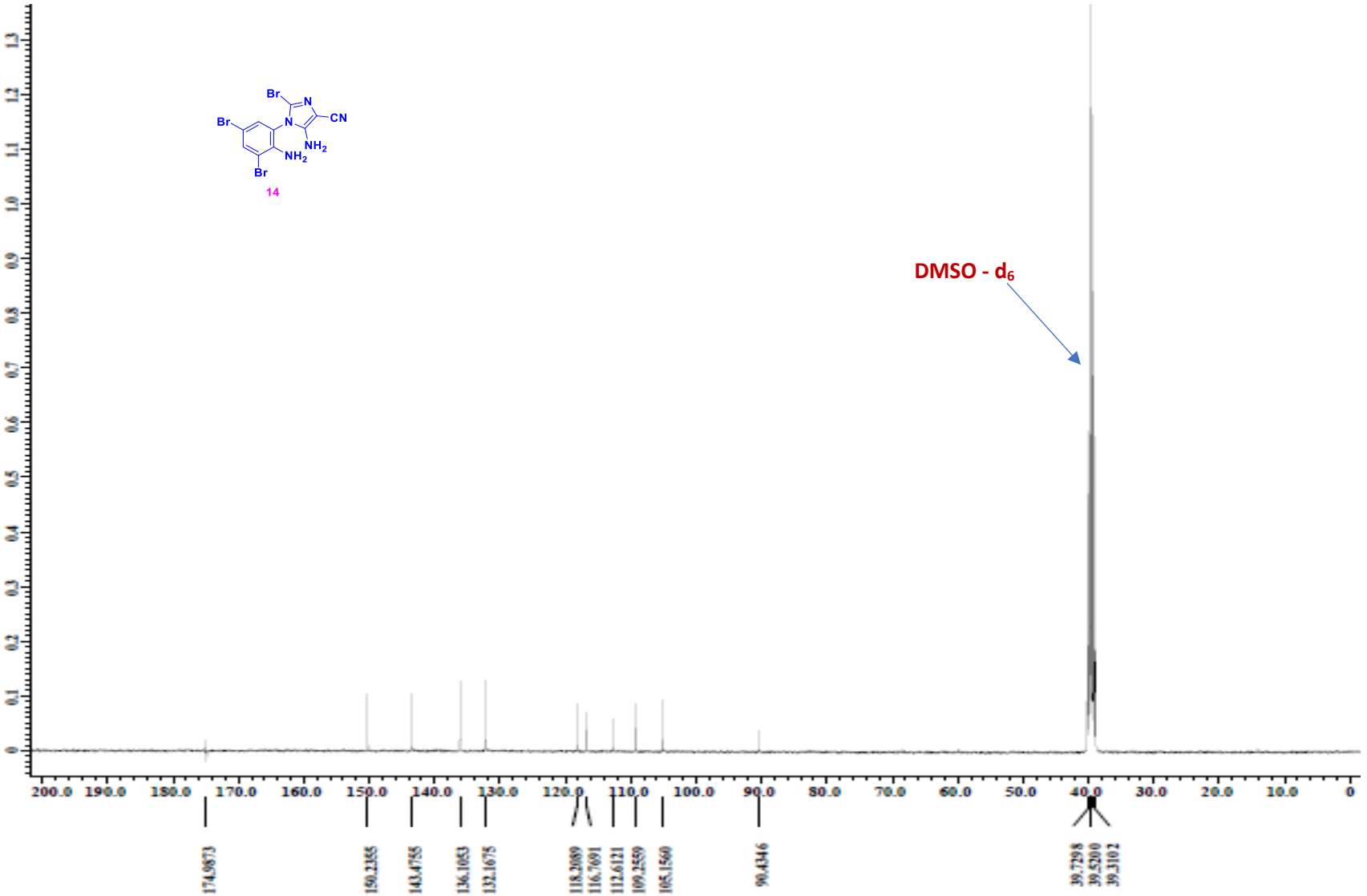
HRMS


276.0870
73672
M+Na+
254.1009
59815
M+1
276.8239
43897
254.8157
33668
277.1158
28588
255.1346
21506
80.9669
47
102.1132
34
134.9685
6
158.1501
26
187.5721
63
202.1807
1108
253.9611
874
292.1024
2174
338.0948
1838
354.1419
3486
370.1206
3040
399.6809
4663
400.1776
2246
437.1835
2967
453.1632
333
475.3260
4650
480.2021
215
7.37e4
100
%
0
m/z
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
H2N
CN
N
N
N
H
1D3

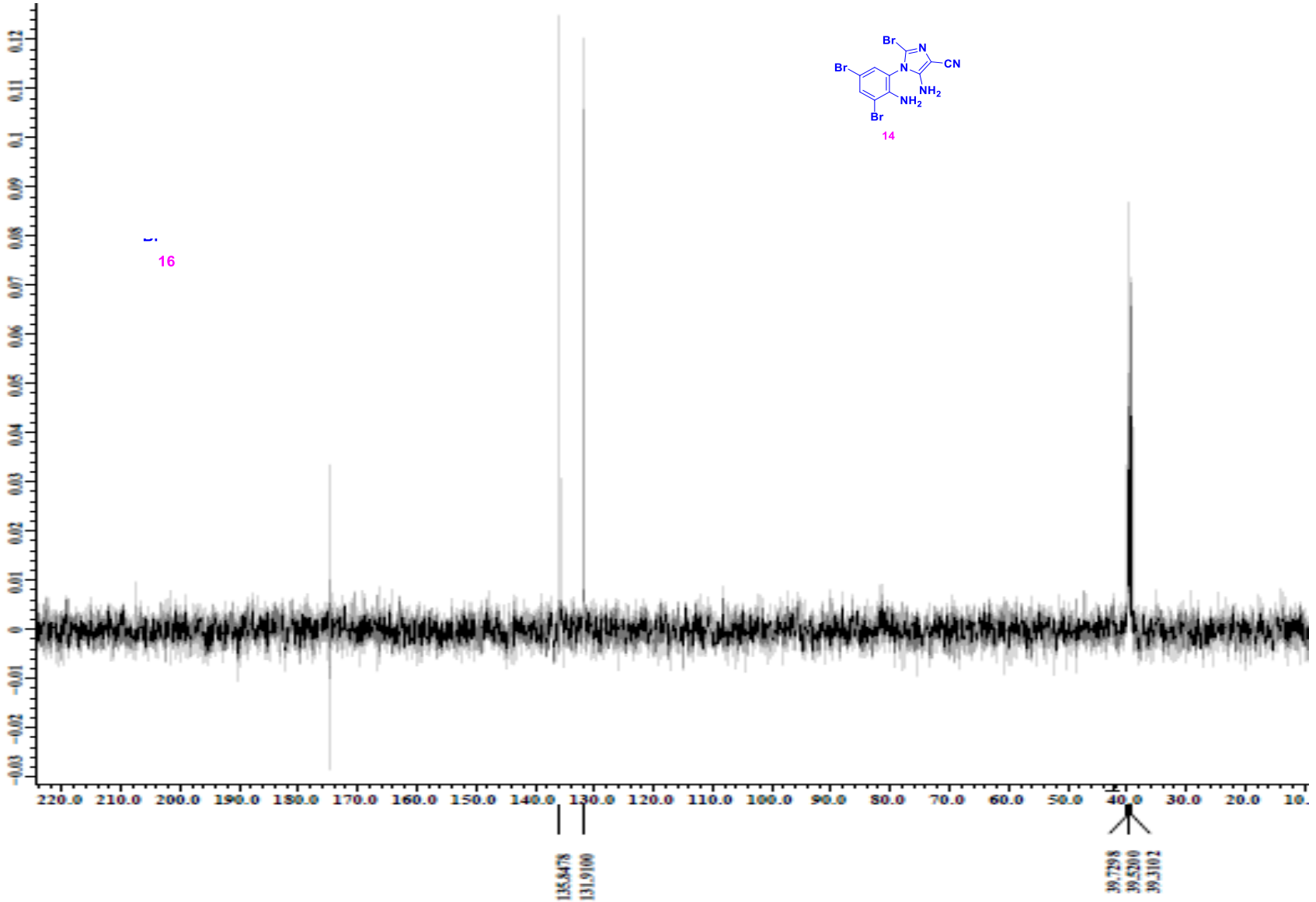
^{1}H NMR


7.71
7.70
7.30
7.29
6.39
5.60
Br
N
CN
Br
N
NH2
NH2
Br
14
1.00
0.99
2.28
2.29
f1 (ppm)

^{13}C NMR

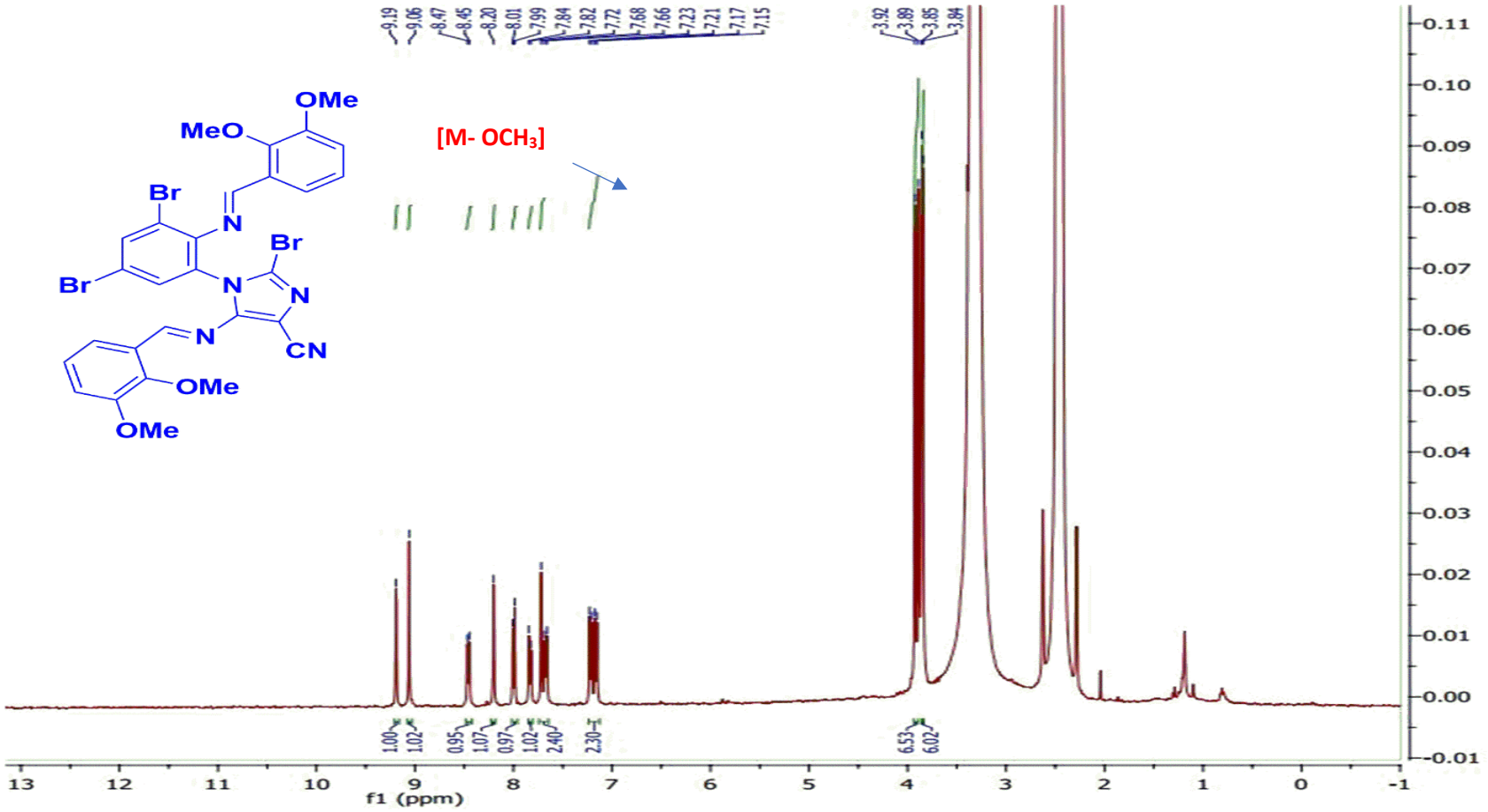

Br
N
CN
Br
N
NH2
NH2
Br
14
DMSO - d6
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
174.9873
150.2355
143.4755
136.1053
132.1675
118.2089
116.7691
112.6121
109.2559
105.1560
90.4346
39.7298
39.5200
39.3102

DEPT Experiment

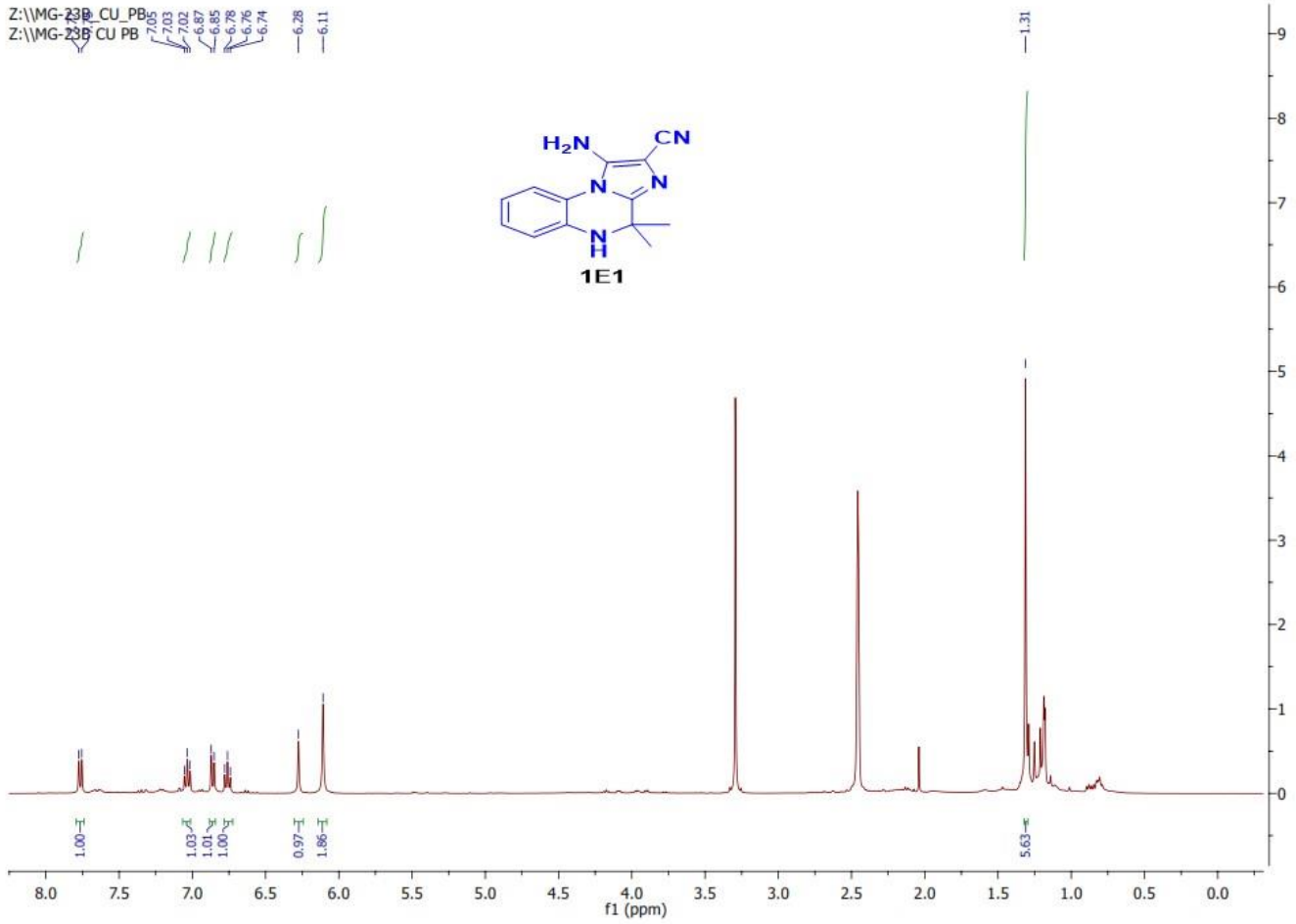


HRMS

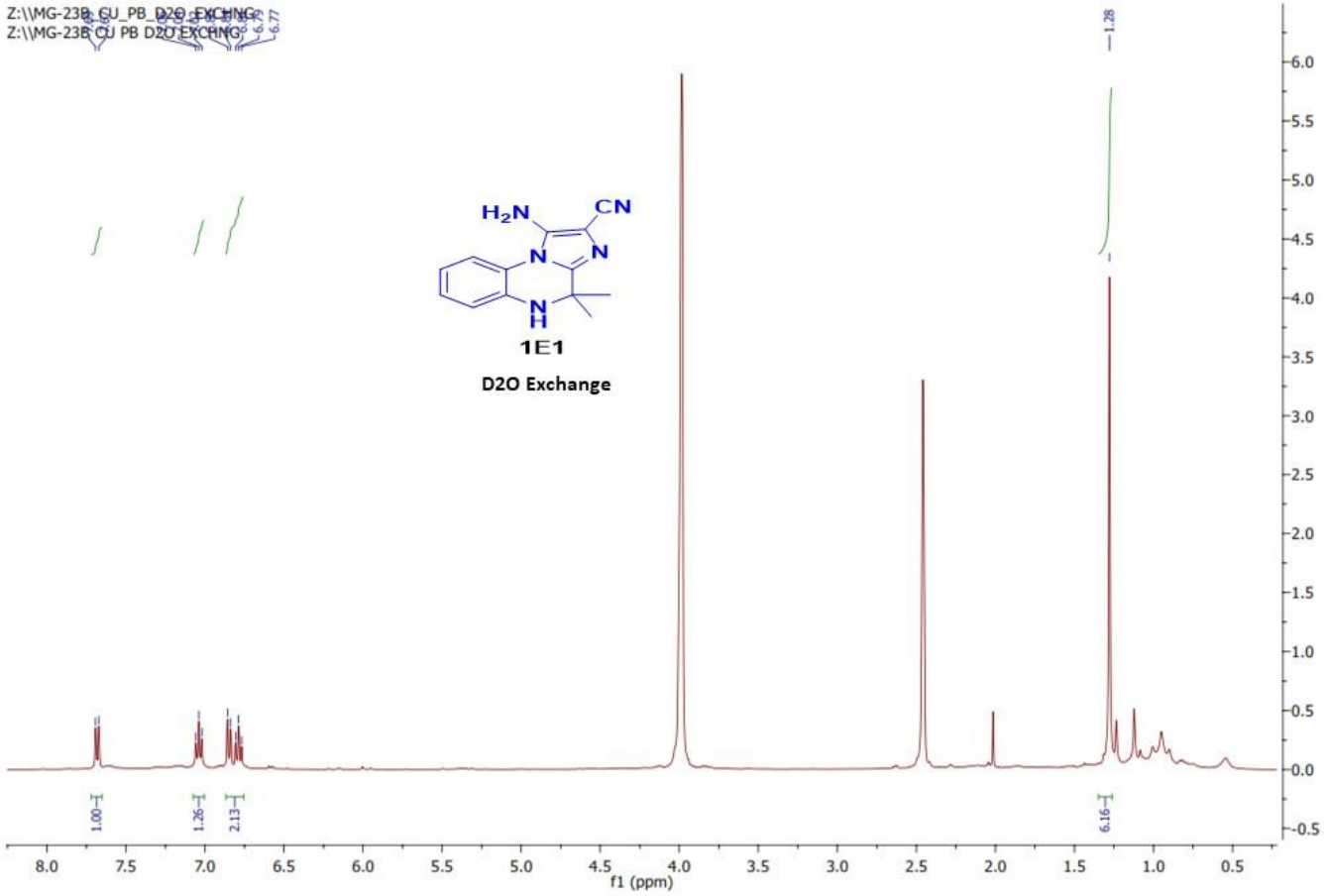
15


OMe
MeO
Br
N
Br
Br
N
N
N
CN
OMe
OMe
[M- OCH3]
9.19
9.06
8.47
8.45
8.20
8.01
7.99
7.84
7.82
7.72
7.68
7.66
7.23
7.21
7.17
7.15
3.92
3.89
3.85
3.84
1.00
1.02
0.95
1.07
0.97
1.02
2.40
2.30
6.53
6.02
f1 (ppm)

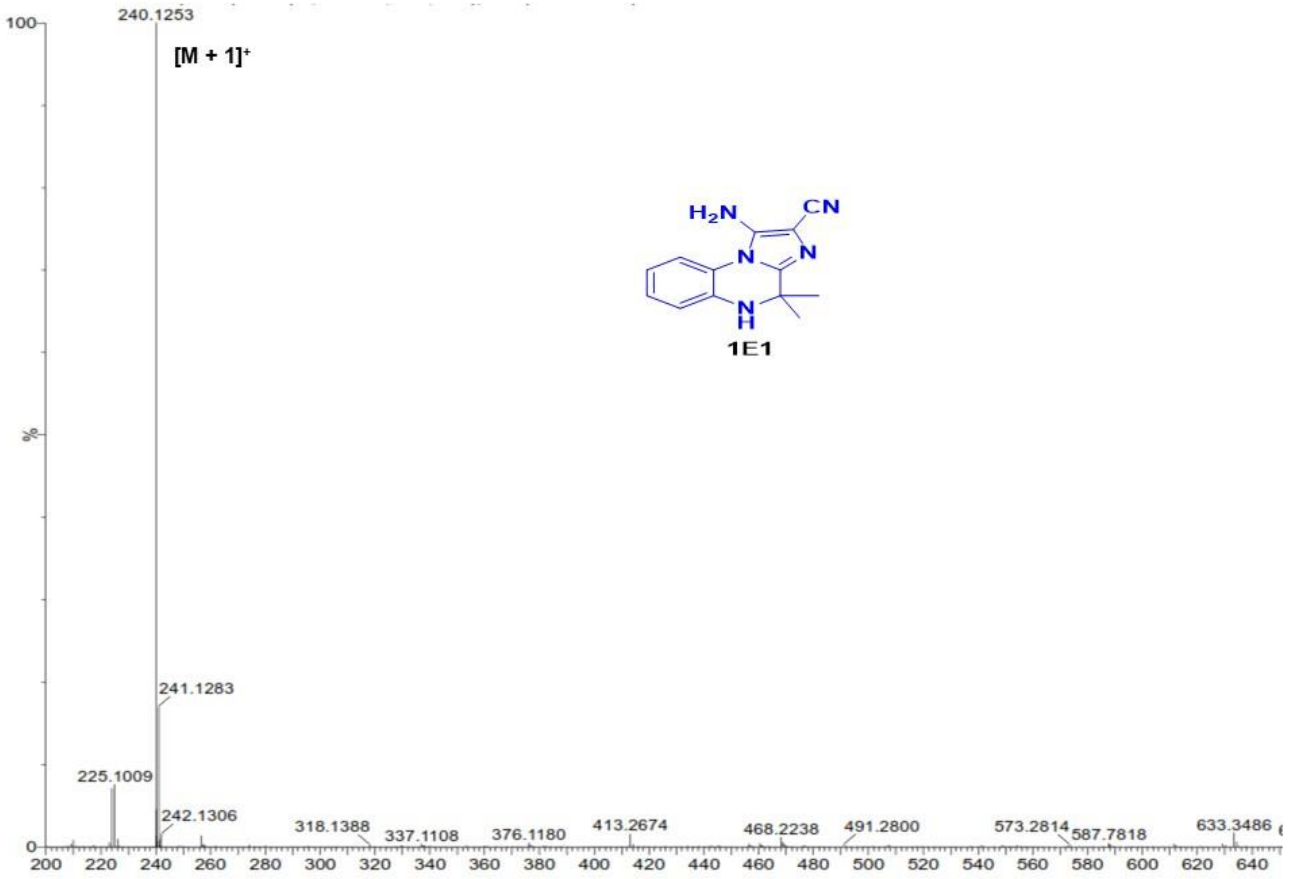
^{1}H NMR

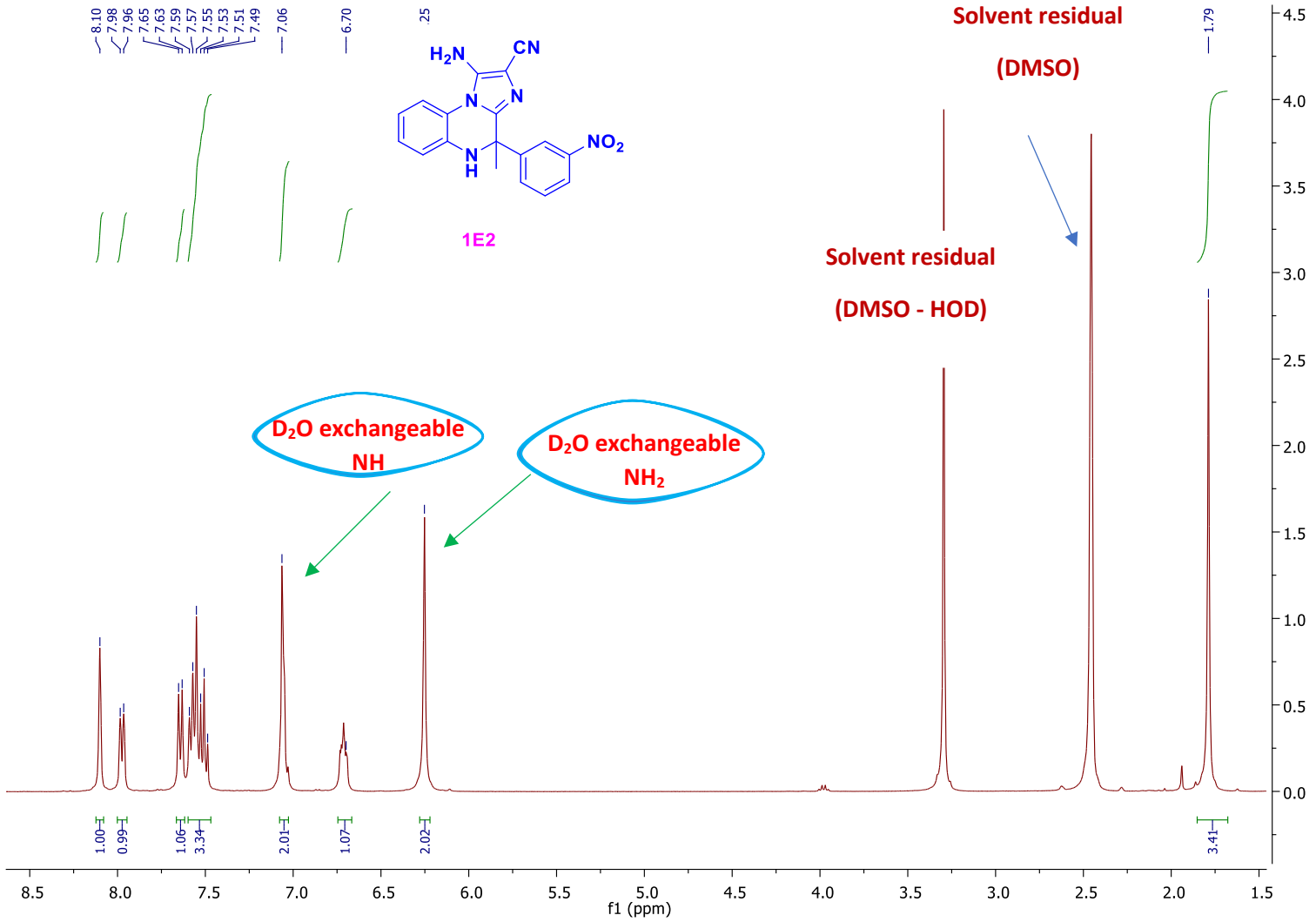

Z:\\MG-23B_CU_PB
Z:\\MG-23B CU PB
7.05
7.03
7.02
6.87
6.85
6.78
6.76
6.74
6.28
6.11
1.31
H2N
CN
N
N
N
H
1E1
1.00
1.03
1.01
1.00
0.97
1.86
5.63
f1 (ppm)

D_2O exchange NMR

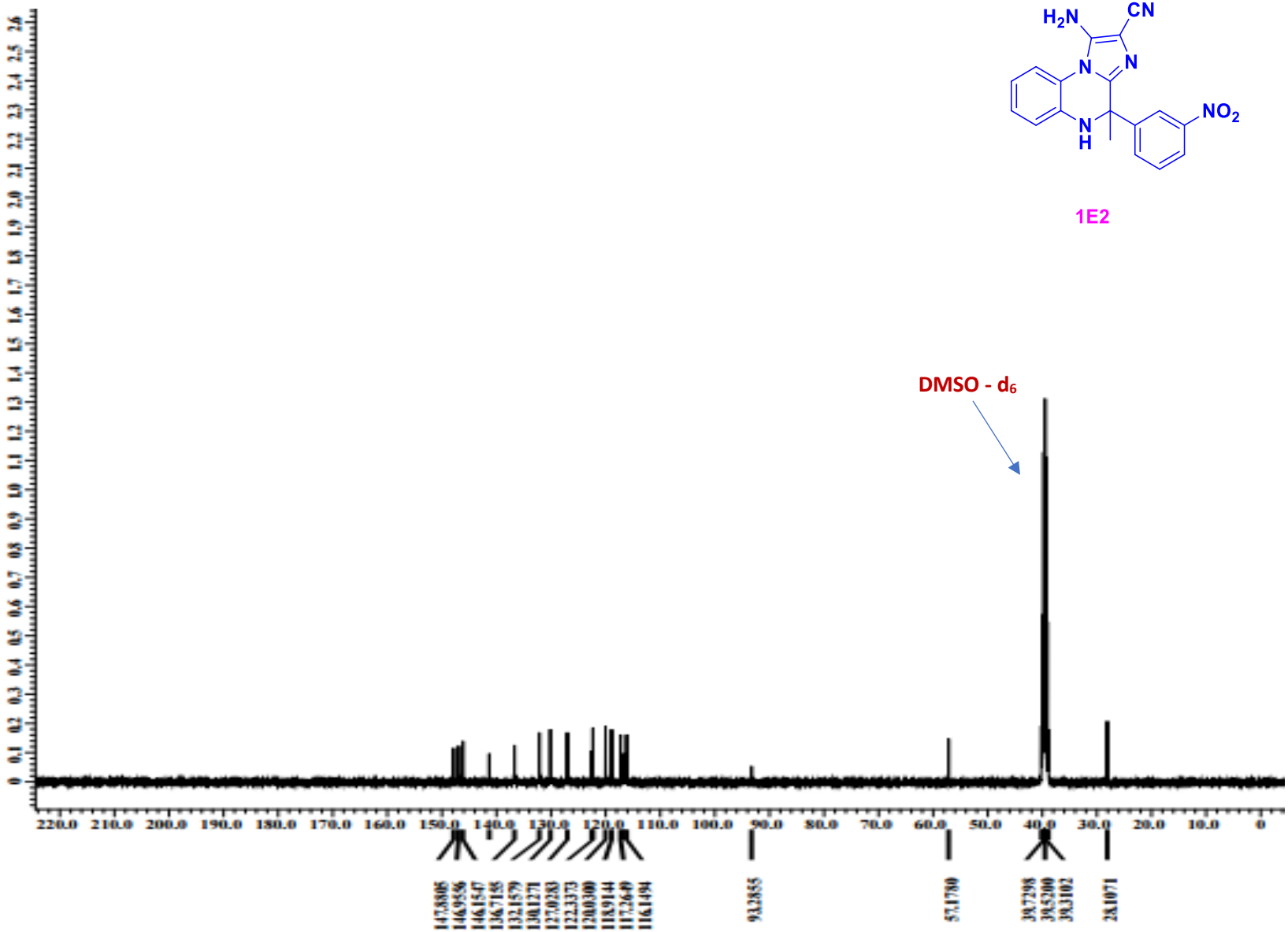


HRMS


240.1253
[M + 1]+
100
%
0
241.1283
225.1009
242.1306
318.1388
337.1108
376.1180
413.2674
468.2238
491.2800
573.2814
587.7818
633.3486
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640
H2N
CN
N
N
N
H
1E1


8.10
7.98
7.96
7.65
7.63
7.59
7.57
7.55
7.53
7.51
7.49
7.06
6.70
1.79
H2N
CN
N
N
N
H
NO2
1E2
Solvent residual
(DMSO)
Solvent residual
(DMSO - HOD)
D2O exchangeable
NH
D2O exchangeable
NH2
1.00
0.99
1.06
3.34
2.01
1.07
2.02
3.41
f1 (ppm)

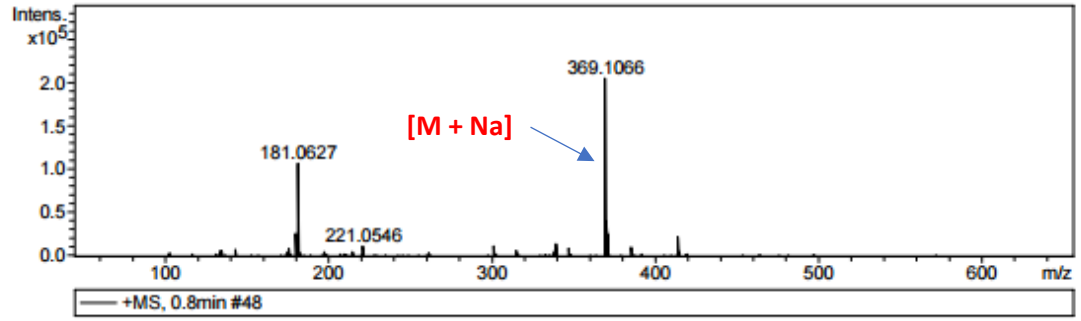
^{13}C NMR


H2N
CN
N
N
N
H
NO2
1E2
DMSO - d6
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
147.3805
146.9556
146.1547
136.7185
132.1579
130.1271
127.0283
122.3373
120.0300
118.9144
117.2649
116.1494
93.2855
57.1780
39.7298
39.5300
39.3102
28.1071

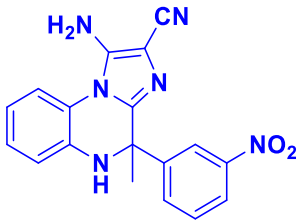
HRMS

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	650 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

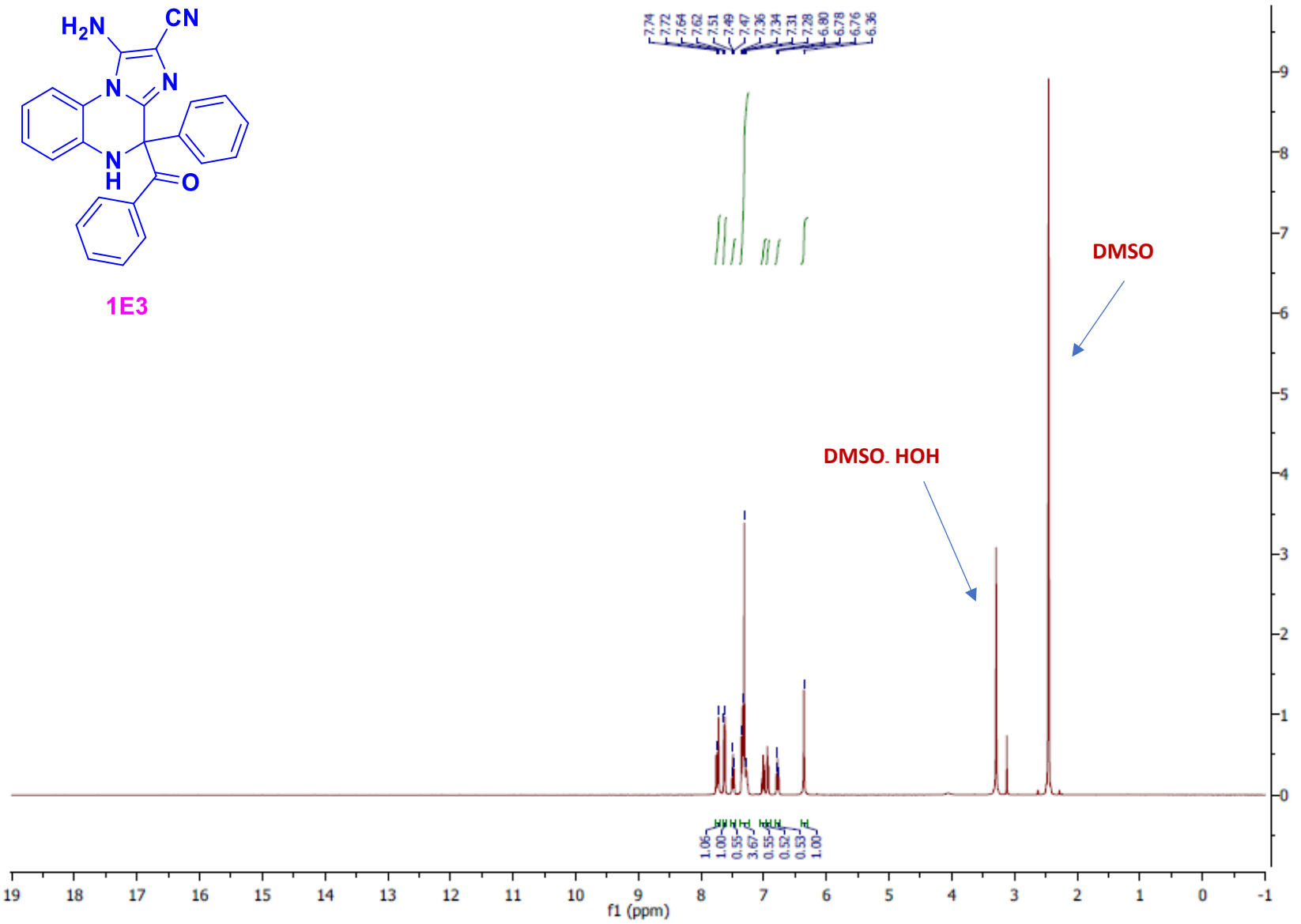


#	m/z	Res.	S/N	I	FWHM
1	102.9780	13203	146.4	4189	0.0078
2	131.0082	13503	36.9	2569	0.0097
3	133.0782	13685	48.7	3544	0.0097
4	134.0738	14135	92.5	6884	0.0095
5	135.0062	14151	88.1	6687	0.0095
6	142.9696	15245	98.0	8668	0.0094
7	175.0134	15629	119.9	5029	0.0112
8	176.1192	15479	246.9	9851	0.0114
9	180.0663	15386	826.0	26960	0.0117
10	181.0627	15124	3472.6	106970	0.0120
11	182.0667	14970	172.6	5003	0.0122
12	197.0363	15681	301.9	5549	0.0126
13	207.0409	15590	149.8	2587	0.0133
14	210.0526	15742	181.9	3079	0.0133
15	215.0051	16289	306.6	5014	0.0132
16	220.0582	15751	200.5	3167	0.0140
17	221.0546	16462	791.1	12391	0.0134
18	261.0471	17133	330.0	4271	0.0152
19	301.1408	17114	821.0	12109	0.0176
20	302.1430	16041	168.7	2505	0.0188
21	315.1565	17448	367.7	6476	0.0181
22	338.1380	18301	277.4	7353	0.0185
23	339.1346	17366	536.1	14409	0.0195
24	347.1241	16603	333.0	9981	0.0209
25	369.1066	18256	8610.2	204774	0.0202
26	370.1096	17233	1752.8	41033	0.0215
27	371.1120	17094	202.3	4669	0.0217
28	385.0807	17733	573.3	10196	0.0217
29	413.2660	17615	1394.9	22088	0.0235
30	414.2692	18408	375.4	5953	0.0225

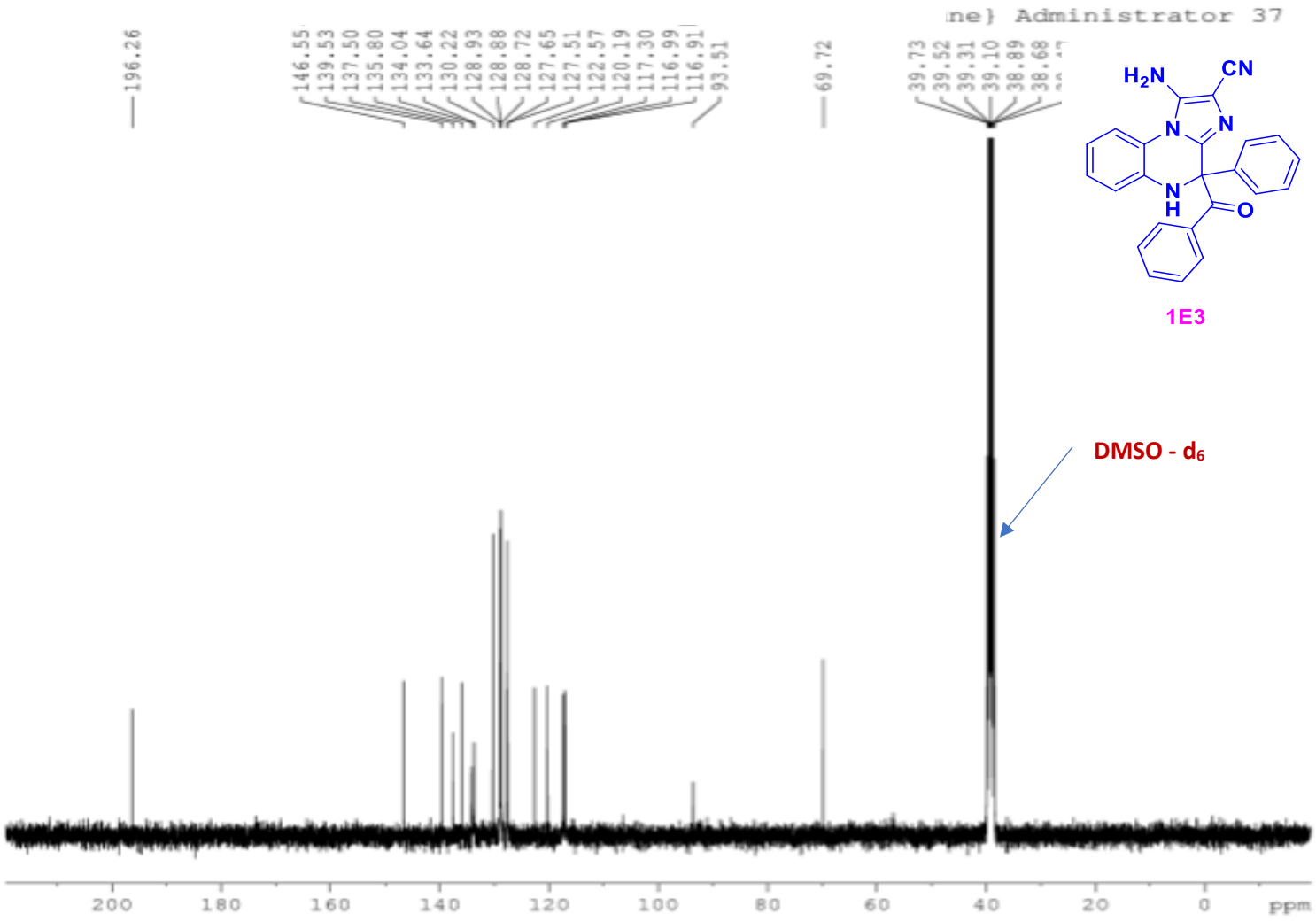


1E2

^{1}H NMR


H2N
CN
N
N
N
H
O
1E3
7.74
7.72
7.64
7.62
7.51
7.49
7.47
7.36
7.34
7.31
7.28
6.80
6.78
6.76
6.36
DMSO
DMSO. HOH
1.06
1.00
0.55
3.67
0.55
0.52
0.53
1.00
f1 (ppm)

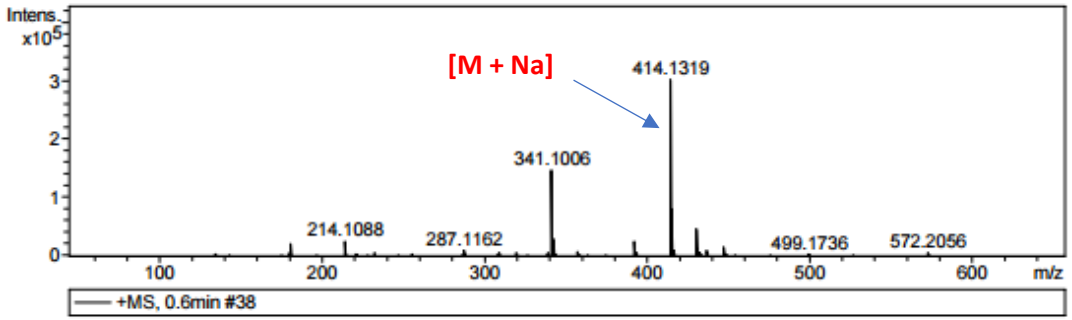
^{13}C NMR

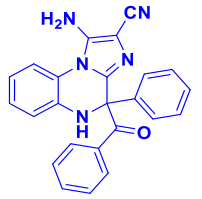

ne} Administrator 37
196.26
146.55
139.53
137.50
135.80
134.04
133.64
130.22
128.93
128.88
128.72
127.65
127.51
122.57
120.19
117.30
116.99
116.91
93.51
69.72
39.73
39.52
39.31
39.10
38.89
38.68
H2N
CN
N
N
N
H
O
1E3
DMSO - d6
200
180
160
140
120
100
80
60
40
20
0
ppm

HRMS

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	650 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

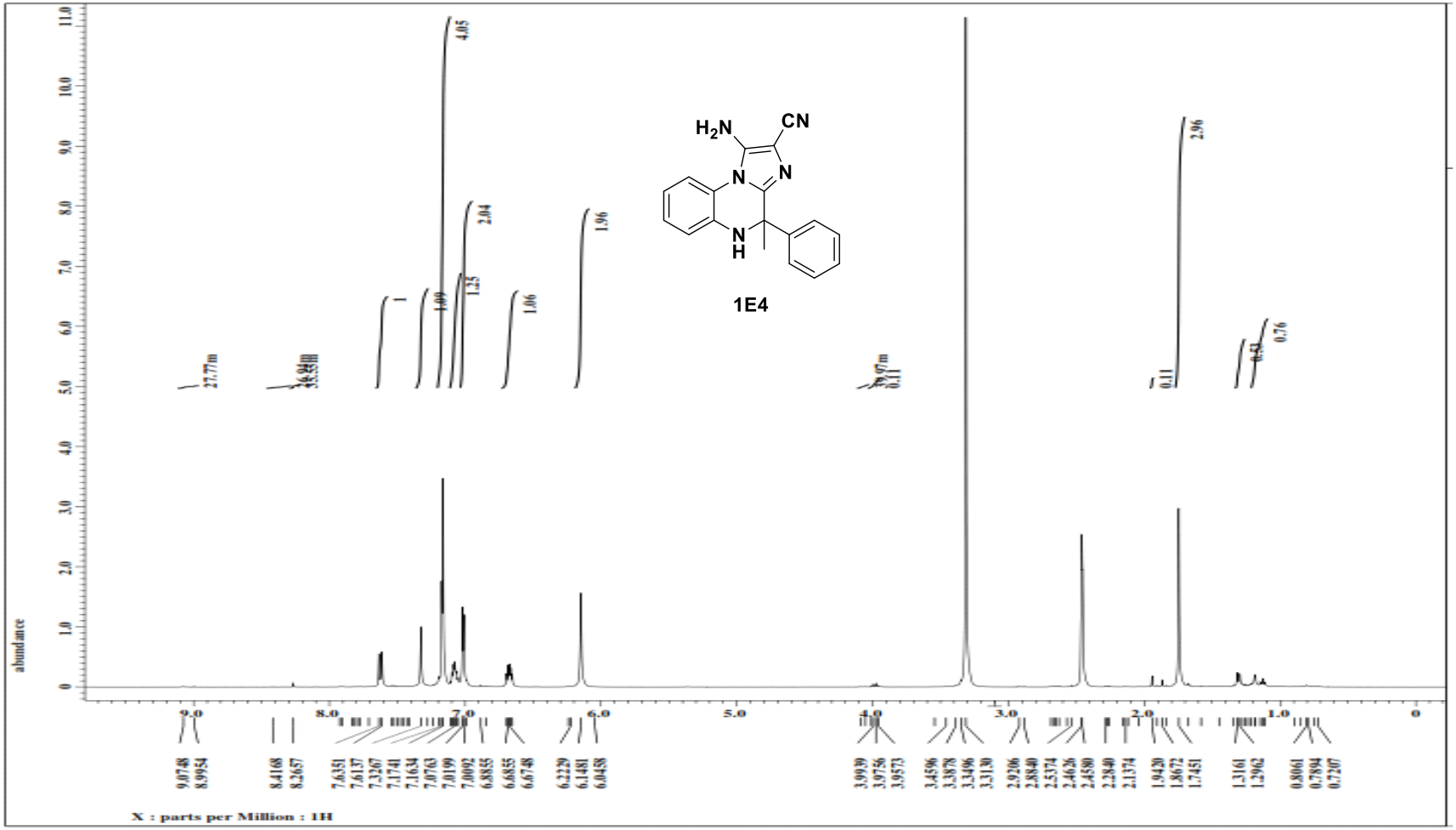




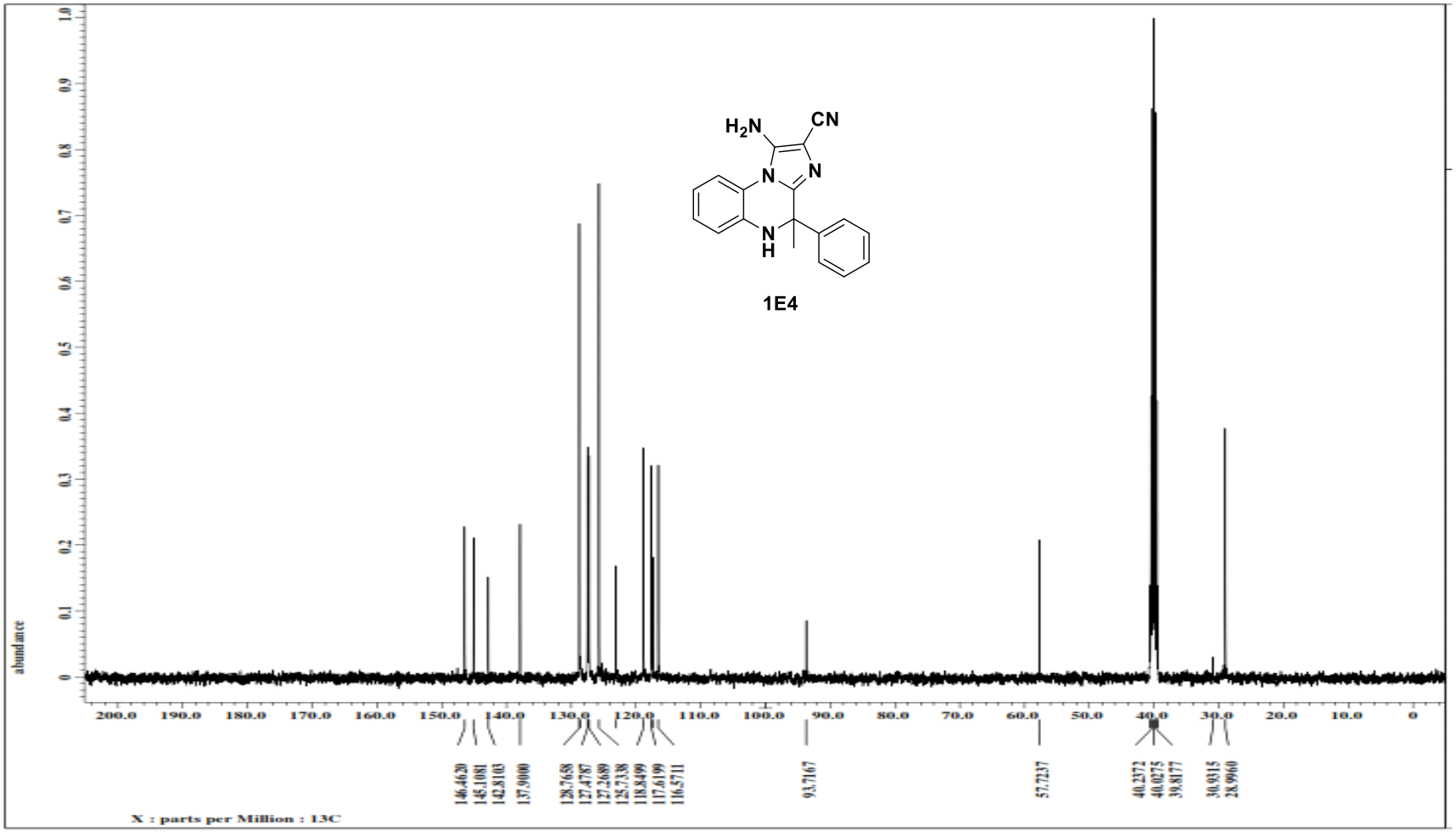
1E3

#	m/z	Res.	S/N	I	FWHM
1	135.0029	14350	96.1	3939	0.0094
2	180.0655	15392	71.9	5541	0.0117
3	181.0620	15274	285.1	22209	0.0119
4	214.1088	16307	698.8	25858	0.0131
5	215.1108	15620	95.5	3374	0.0138
6	221.0547	16673	148.8	3736	0.0133
7	232.0593	16470	524.6	6878	0.0141
8	255.0854	16374	335.0	4151	0.0156
9	287.1162	17451	808.7	10431	0.0165
10	308.0905	17205	316.2	4424	0.0179
11	309.0978	16500	492.2	6907	0.0187
12	319.1189	17013	382.6	6061	0.0188
13	339.1344	17483	283.3	5528	0.0194
14	341.1006	17642	7468.1	148143	0.0193
15	342.1037	17511	1476.6	29569	0.0195
16	343.1060	17176	177.4	3594	0.0200
17	357.0750	18404	420.1	8617	0.0194
18	392.1503	18282	1563.5	25925	0.0214
19	393.1533	17574	404.1	6905	0.0224
20	414.1319	18274	11090.4	302781	0.0227
21	415.1352	18390	2871.3	79806	0.0226
22	416.1383	17436	364.2	10314	0.0239
23	430.1061	18793	1309.6	45974	0.0229
24	431.1093	17698	333.5	11881	0.0244
25	432.1374	16420	193.4	7058	0.0263
26	436.1143	18507	267.2	10727	0.0236
27	447.1426	18125	326.6	16424	0.0247
28	448.1452	18651	93.7	4804	0.0240
29	499.1736	18293	150.0	4861	0.0273
30	572.2056	17981	131.5	5556	0.0318

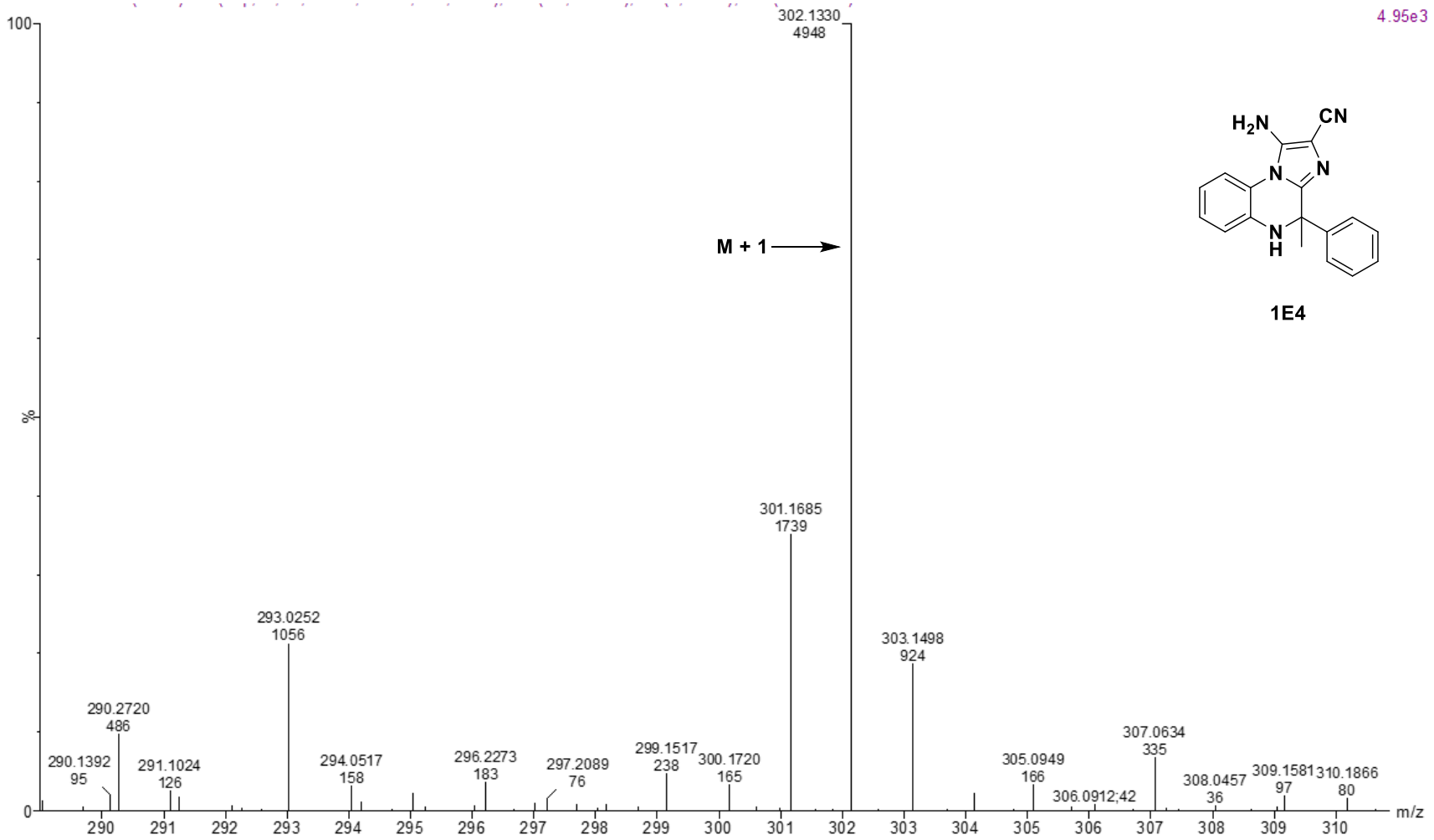
^{1}H NMR



^{13}C NMR

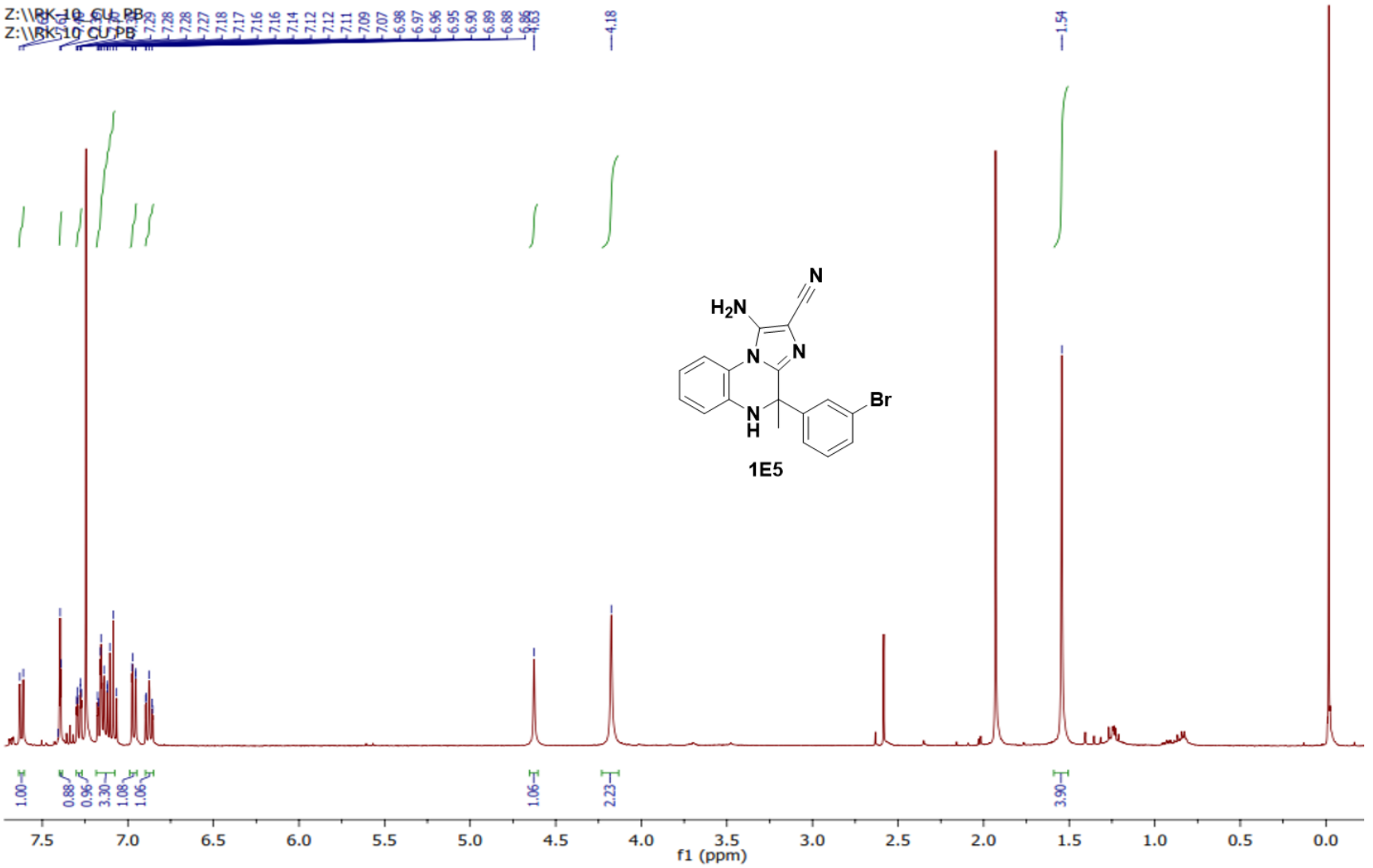

H2N
CN
N
N
N
H
1E4
abundance
X : parts per Million : 13C
146.4620
145.1081
142.8103
137.9000
128.7658
127.4787
127.2689
125.7338
118.8499
117.6199
116.5711
93.7167
57.7237
40.2372
40.0275
39.8177
30.9315
28.9960

HRMS

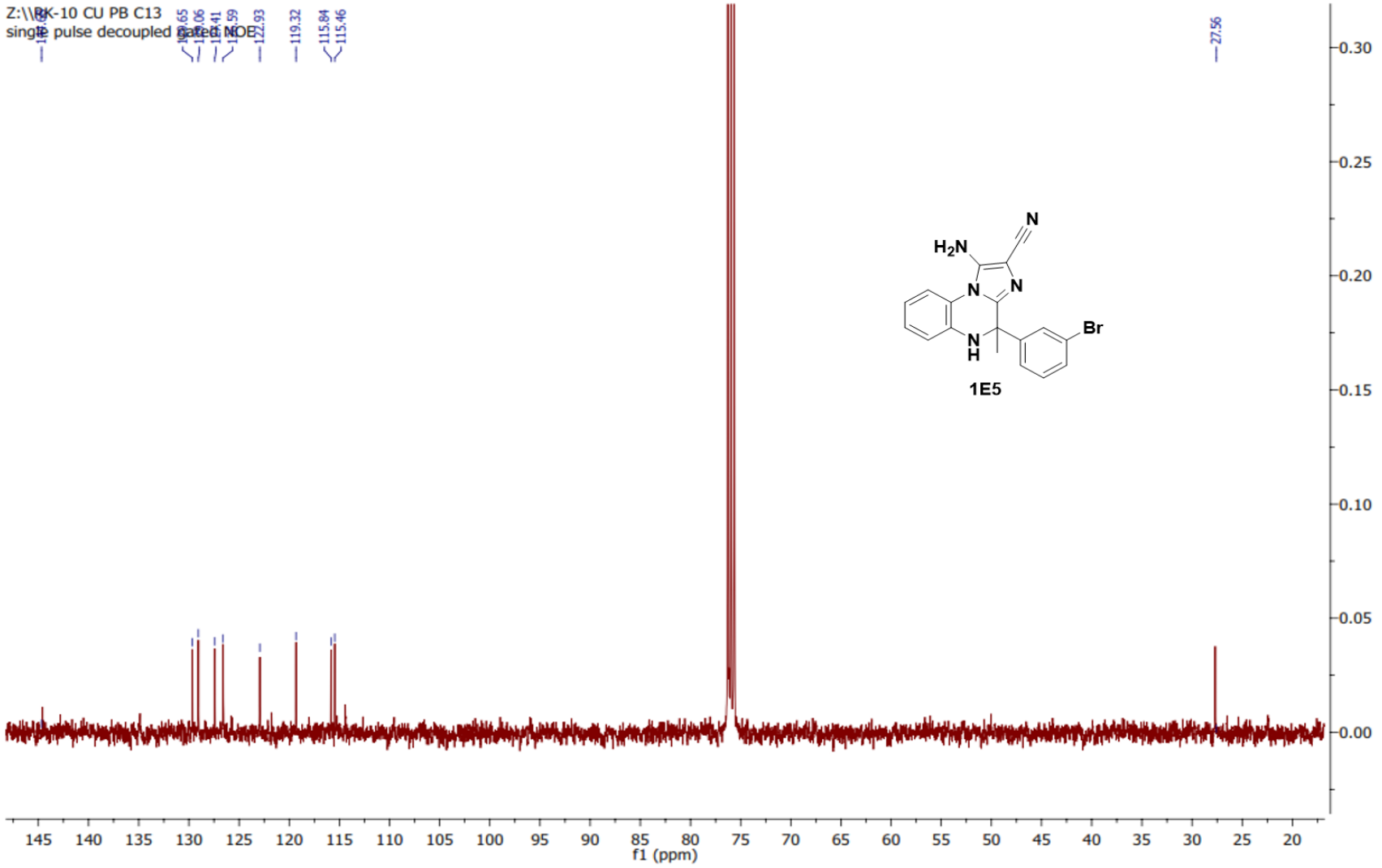

4.95e3
100
%
0
302.1330
4948
M + 1
301.1685
1739
293.0252
1056
303.1498
924
290.2720
486
290.1392
95
291.1024
126
294.0517
158
296.2273
183
297.2089
76
299.1517
238
300.1720
165
305.0949
166
306.0912;42
307.0634
335
308.0457
36
309.1581
97
310.1866
80
m/z
290
291
292
293
294
295
296
297
298
299
300
301
302
303
304
305
306
307
308
309
310
H_2N
CN
N
N
N
H

1E4

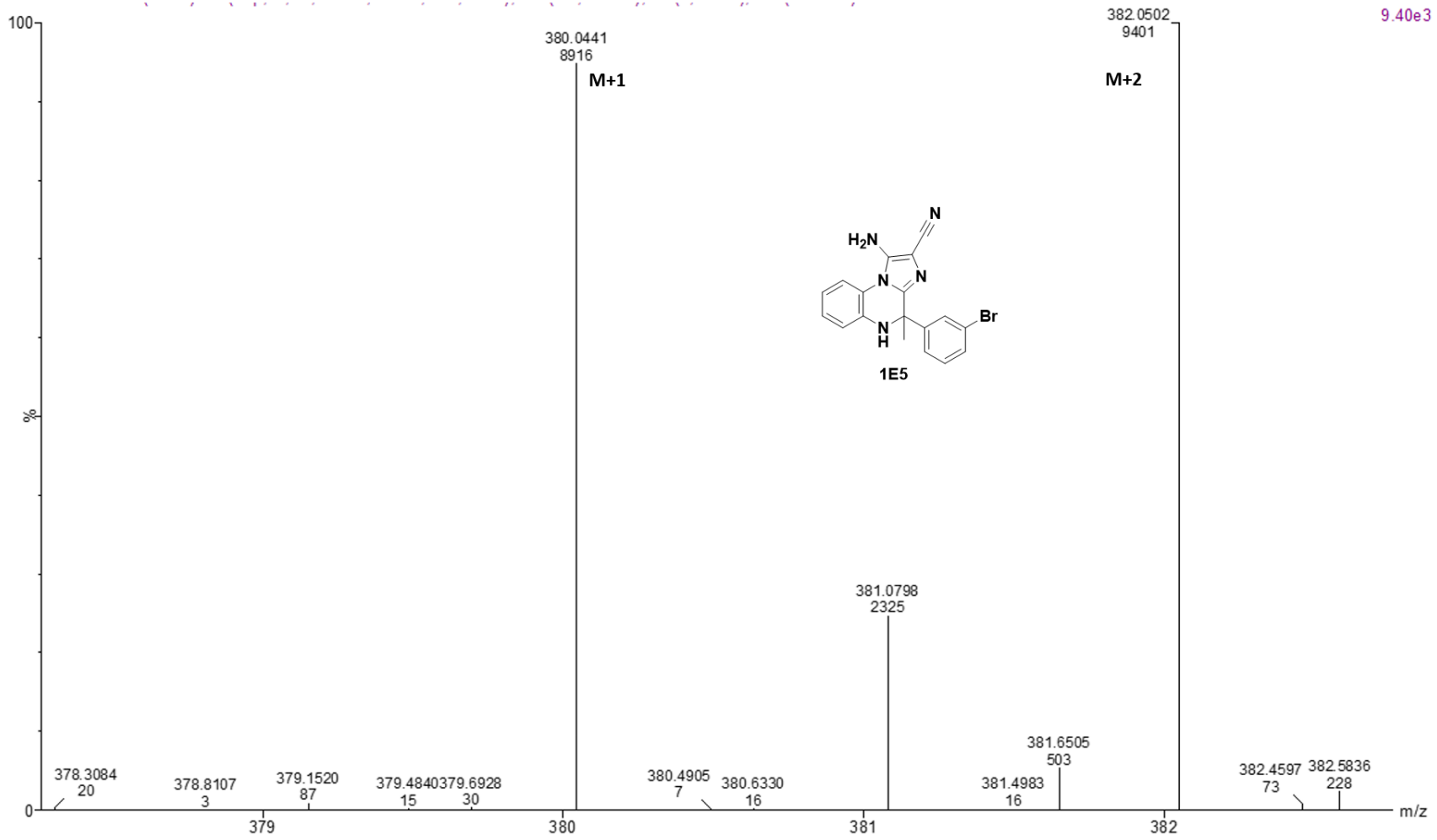
^{1}H NMR


Z:\\RK-10-CU-PB
Z:\\RK-10-CU-PB
4.18
1.54
N
H2N
N
N
N
H
Br
1E5
1.00
0.88
0.96
3.30
1.08
1.06
1.06
2.23
3.90
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

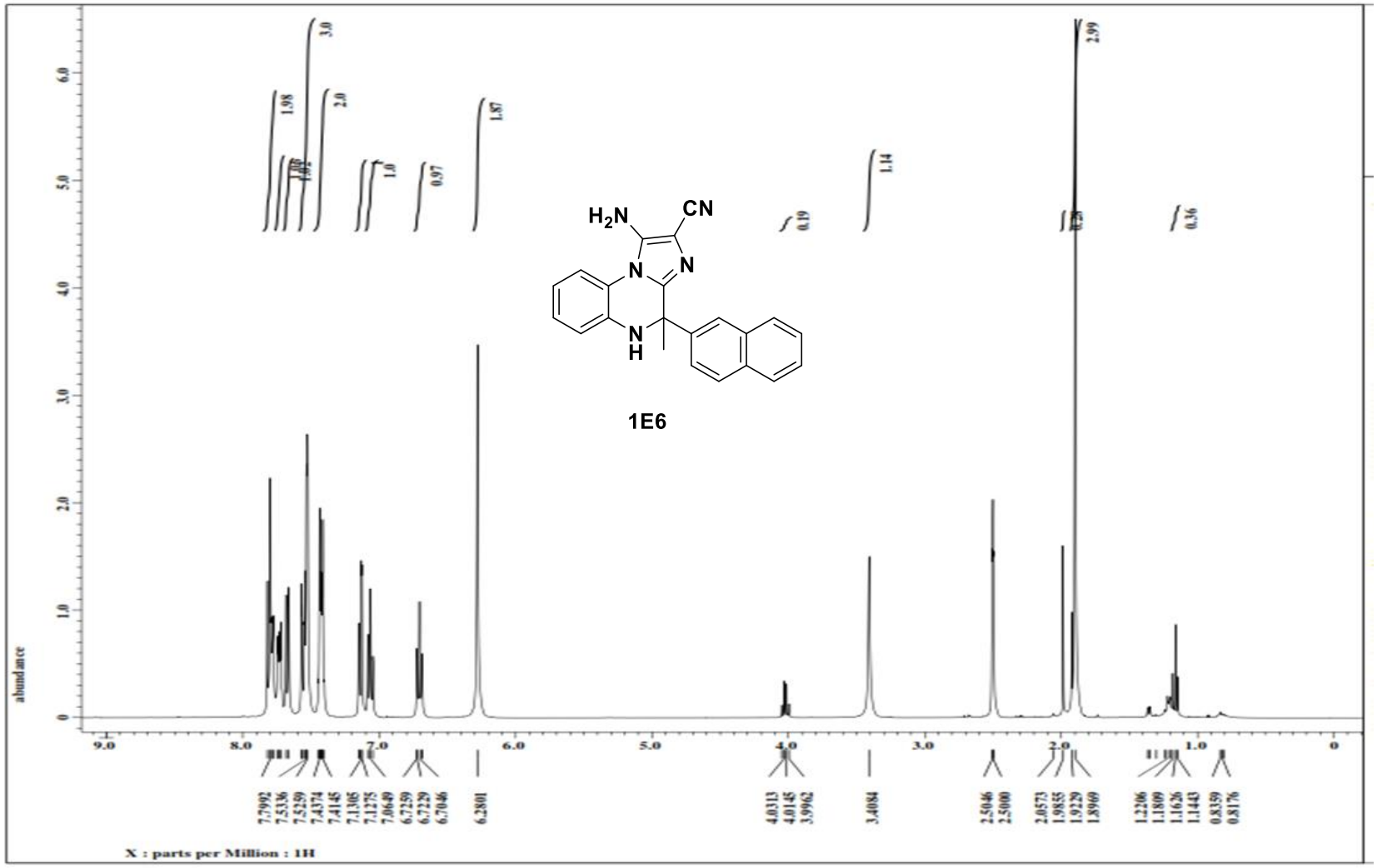
13C NMR


Z:\\BK-10 CU PB C13
single pulse decoupled gated NOE
122.93
119.32
115.84
115.46
27.56
1E5
Br
N
H2N
N
N
N
H
0.30
0.25
0.20
0.15
0.10
0.05
0.00
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)

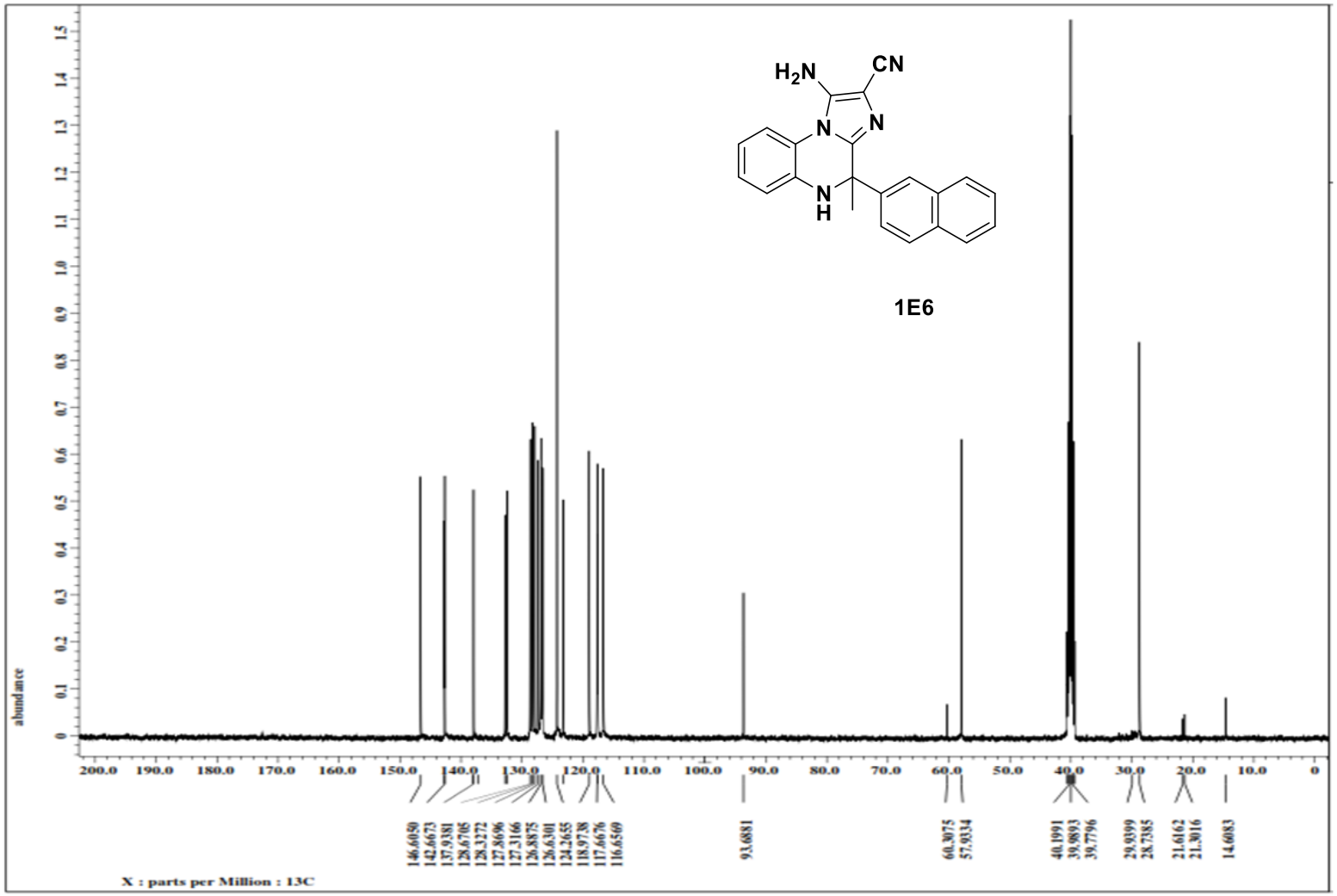
HRMS


9.40e3
100
%
0
380.0441
8916
M+1
382.0502
9401
M+2
381.0798
2325
381.6505
503
378.3084
20
378.8107
3
379.1520
87
379.4840
15
379.6928
30
380.4905
7
380.6330
16
381.4983
16
382.4597
73
382.5836
228
379
380
381
382
m/z
N
H2N
N
N
N
H
Br
1E5

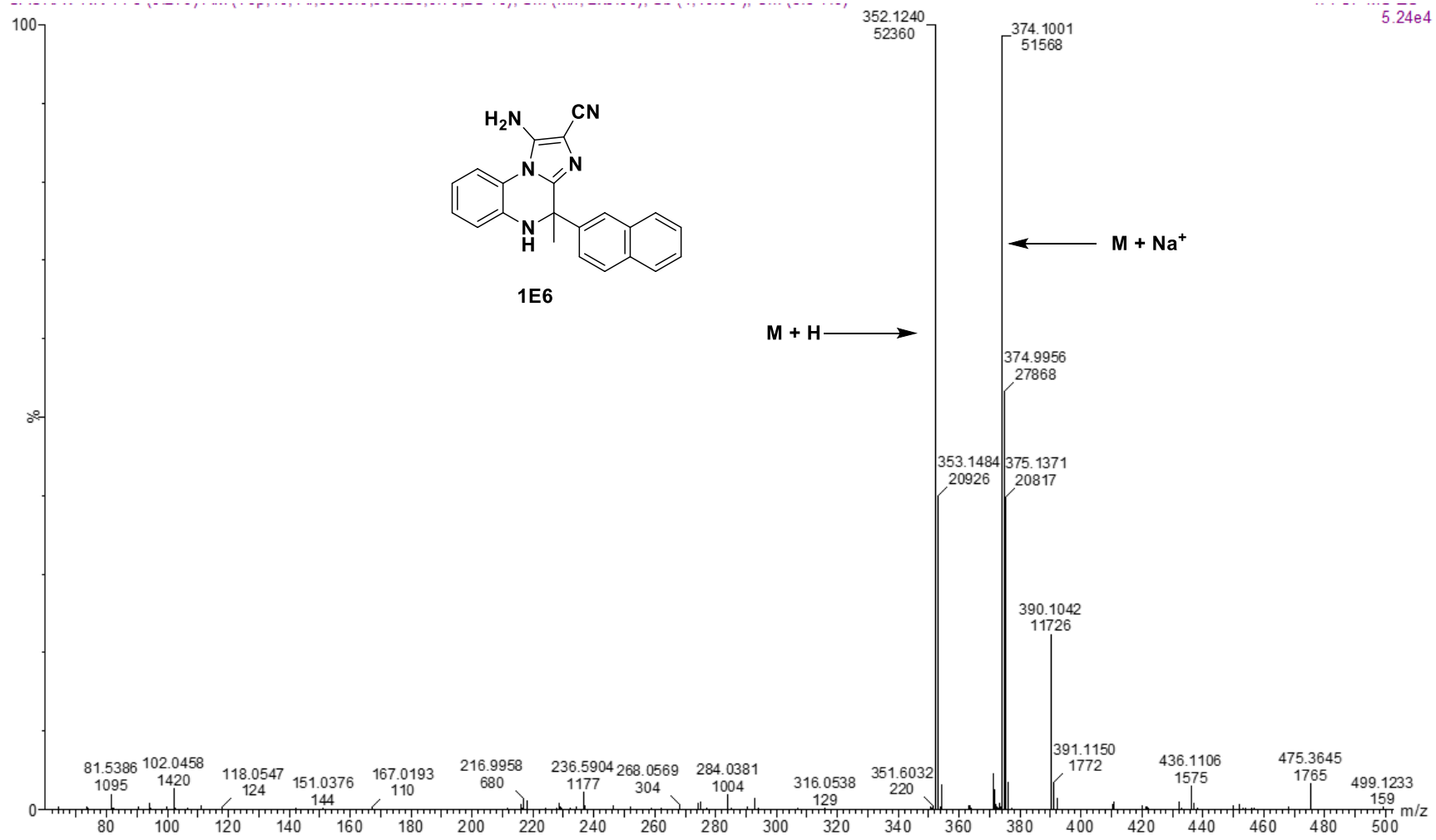
^{1}H NMR



^{13}C NMR

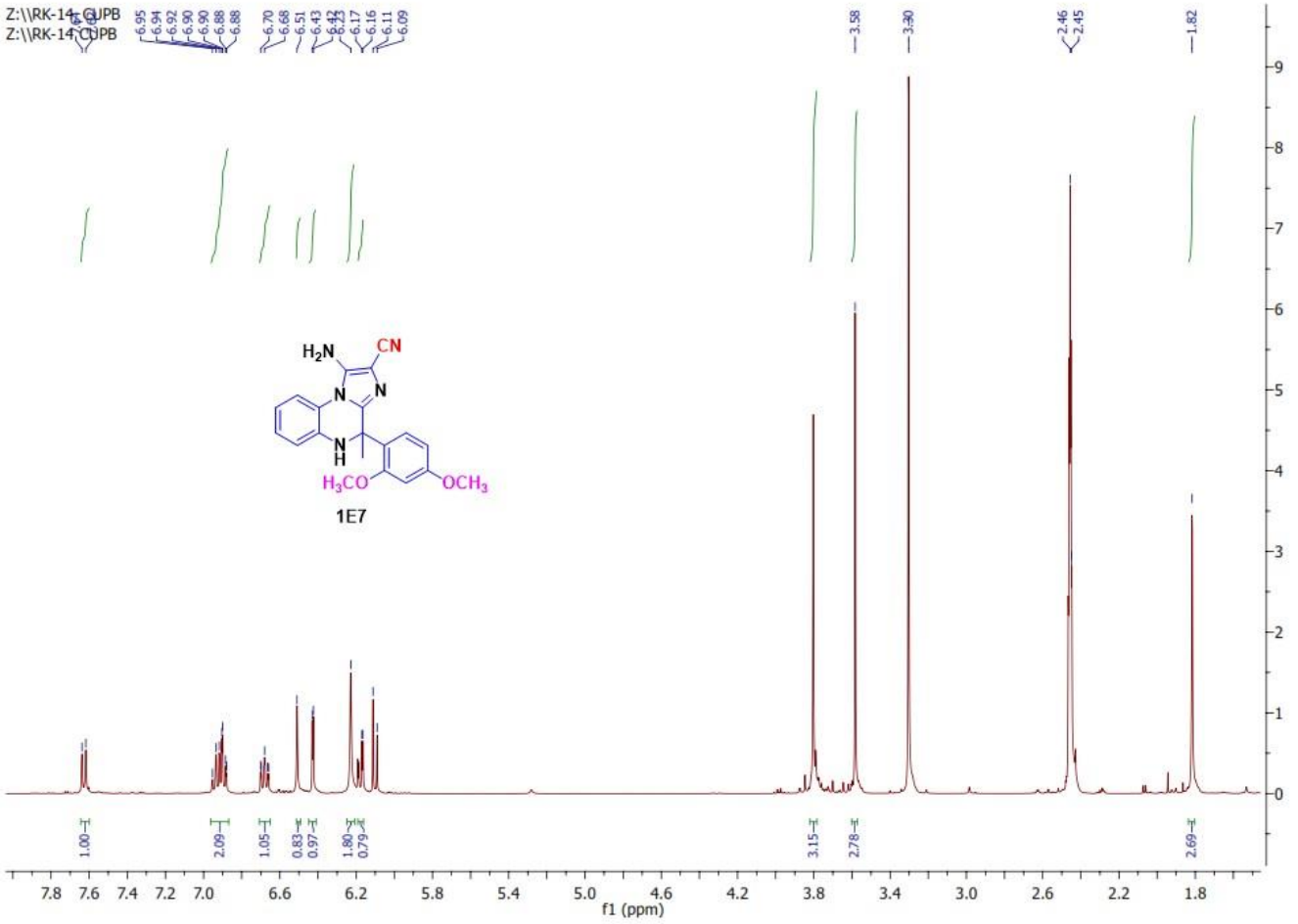

H2N
CN
N
N
N
H
1E6
abundance
X : parts per Million : 13C
146.6050
142.8673
137.9381
128.6705
128.3272
127.8696
127.3166
126.8875
126.6301
124.2655
118.9738
117.4676
116.6569
93.6881
60.3075
57.9334
40.1991
39.9893
39.7796
29.9399
28.7385
21.6162
21.3016
14.6083

HRMS

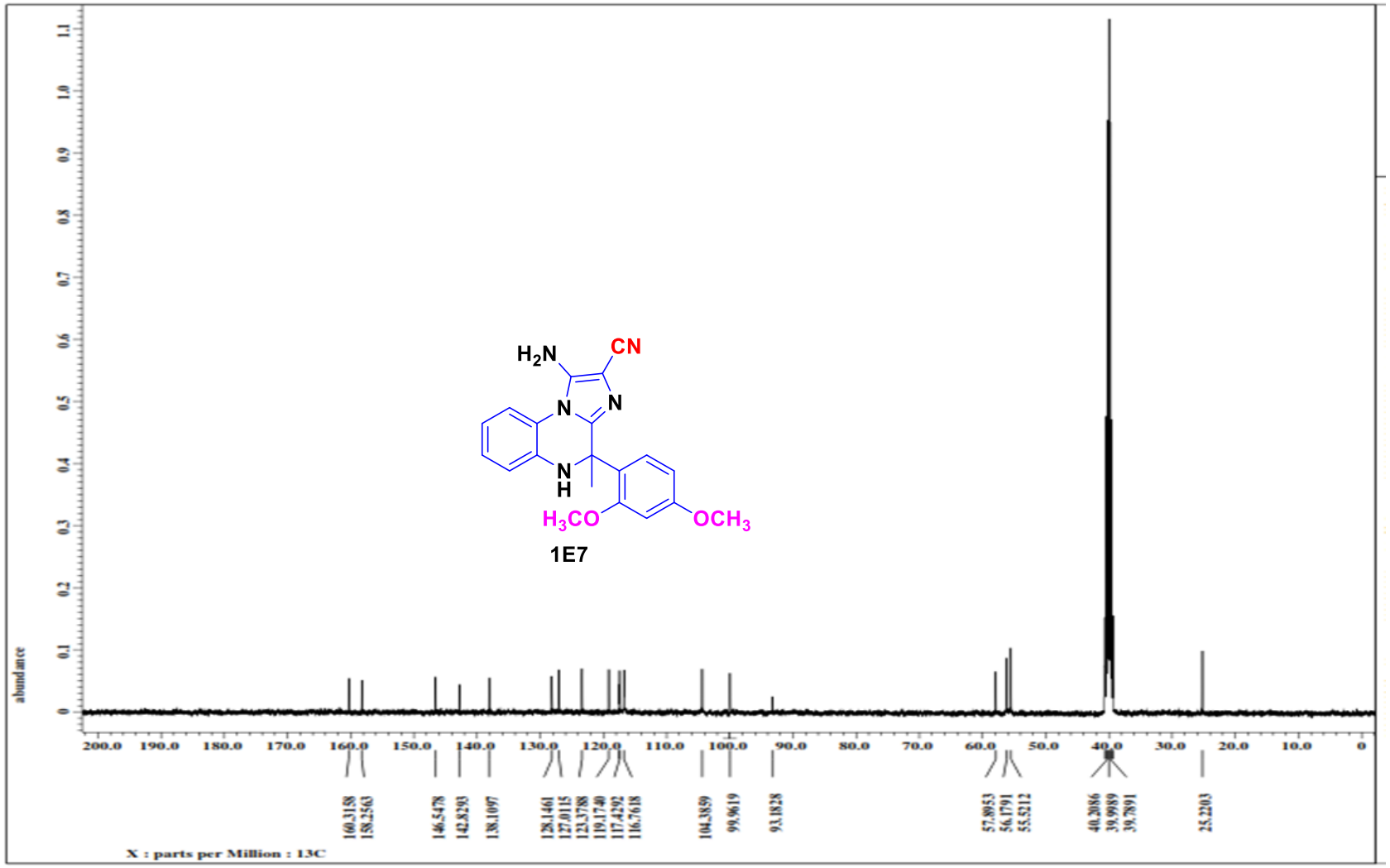

5.24e4
100
%
0
352.1240
52360
374.1001
51568
M + Na+
M + H
374.9956
27868
353.1484
20926
375.1371
20817
390.1042
11726
391.1150
1772
436.1106
1575
475.3645
1765
499.1233
159
81.5386
1095
102.0458
1420
118.0547
124
151.0376
144
167.0193
110
216.9958
680
236.5904
1177
268.0569
304
284.0381
1004
316.0538
129
351.6032
220
m/z
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500

1E6

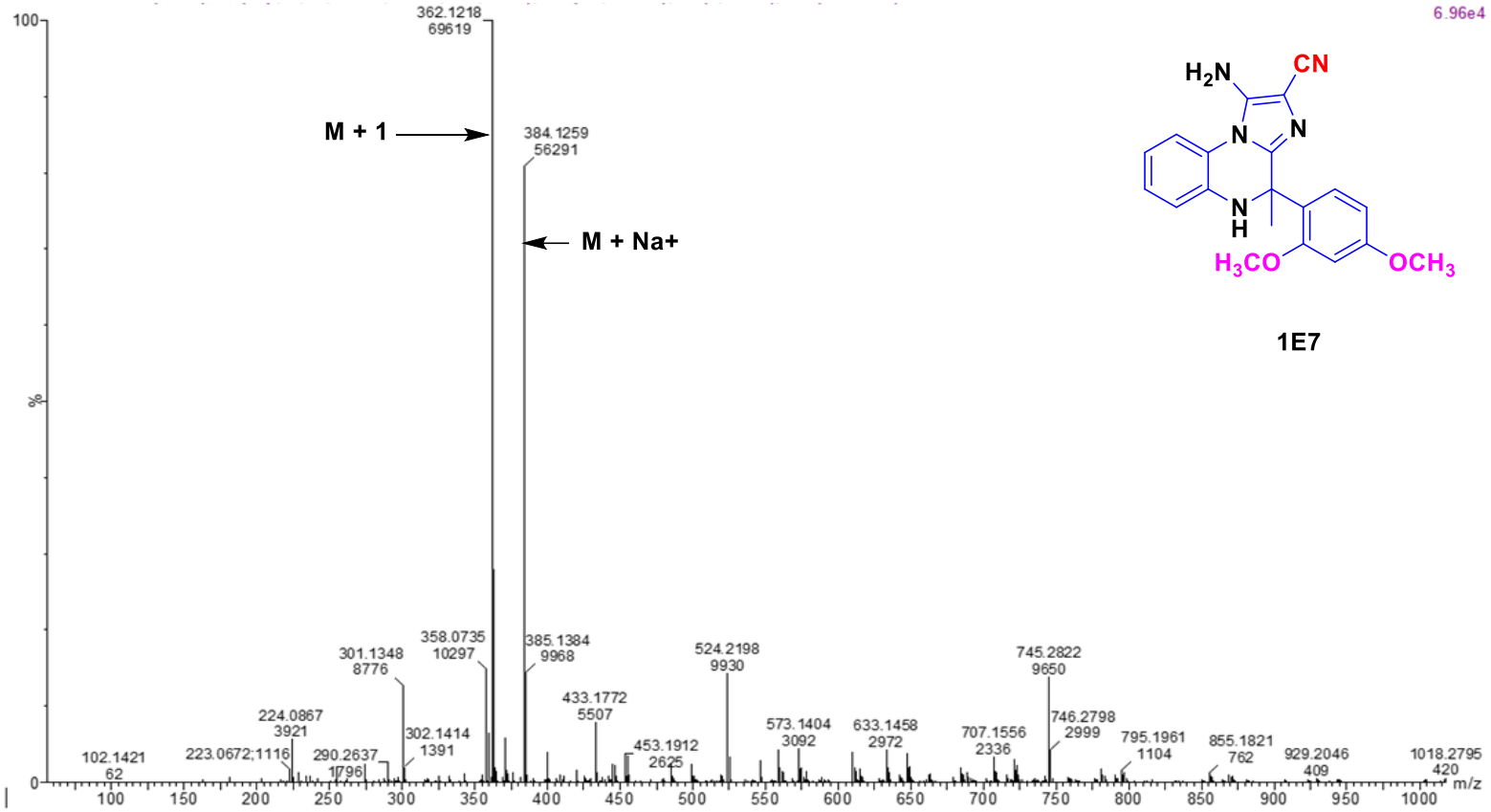
^{1}H NMR


Z:\\RK-14-CUPB
Z:\\RK-14-CUPB
6.95
6.94
6.92
6.90
6.90
6.88
6.88
6.70
6.68
6.51
6.43
6.42
6.23
6.17
6.16
6.11
6.09
3.58
3.30
2.46
2.45
1.82
H2N
CN
N
N
N
H
H3CO
OCH3
1E7
1.00
2.09
1.05
0.83
0.97
1.80
0.79
3.15
2.78
2.69
7.8
7.6
7.4
7.2
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
2.6
2.2
1.8
f1 (ppm)

^{13}C NMR


H2N
CN
N
N
N
H
H3CO
OCH3
1E7
abundance
X : parts per Million : 13C
160.3158
158.2563
146.5478
142.8293
138.1097
128.1461
127.0115
123.3788
119.1740
117.4292
116.7618
104.3859
99.9619
93.1828
57.8953
56.1791
55.5212
40.2086
39.9989
39.7891
25.2203

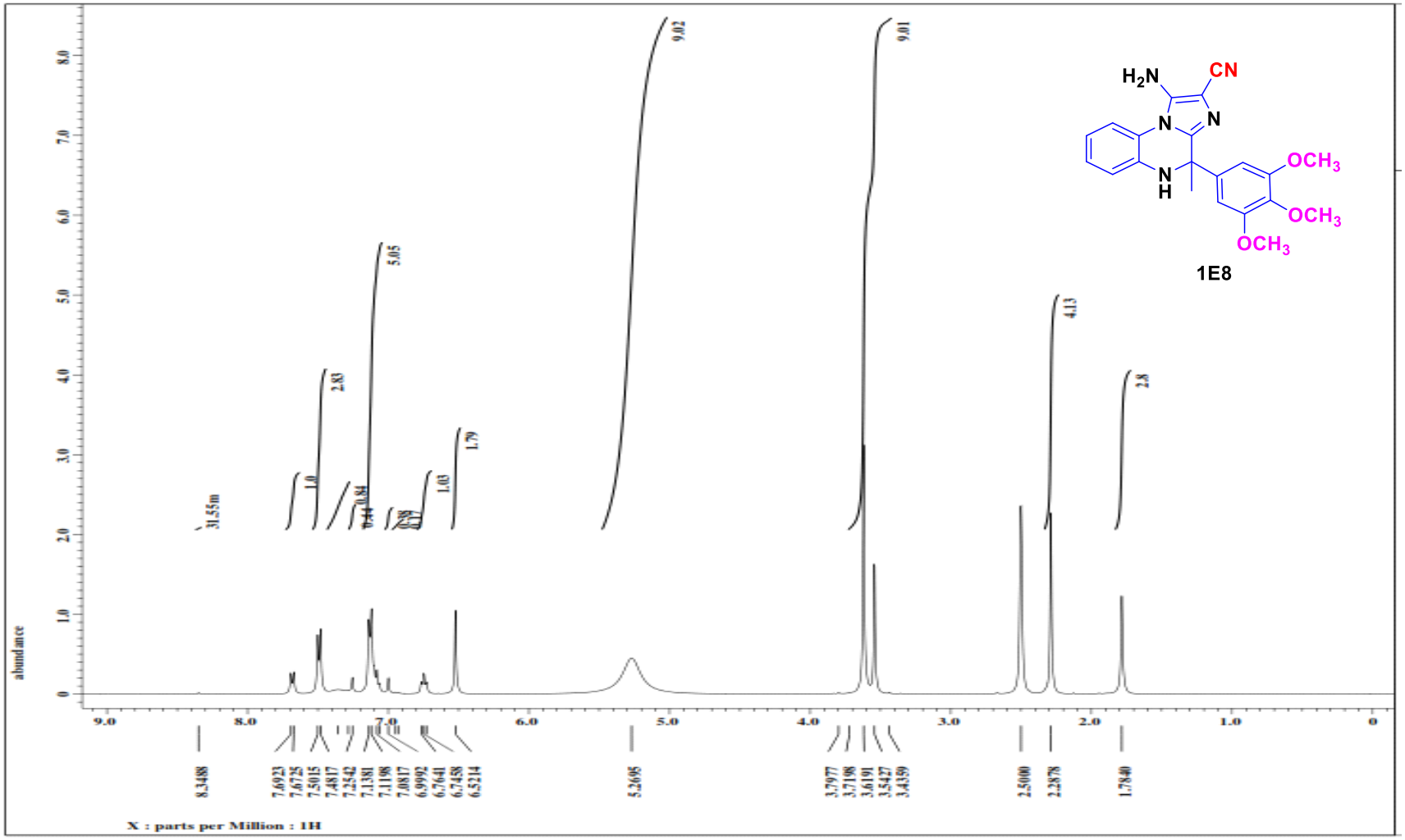
HRMS


6.96e4
100
%
0
362.1218
69619
M + 1
384.1259
56291
M + Na+
358.0735
10297
385.1384
9968
301.1348
8776
524.2198
9930
745.2822
9650
433.1772
5507
224.0867
3921
746.2798
2999
573.1404
3092
633.1458
2972
707.1556
2336
795.1961
1104
855.1821
762
929.2046
409
1018.2795
420
302.1414
1391
453.1912
2625
102.1421
62
223.0672;1116
290.2637
1796
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

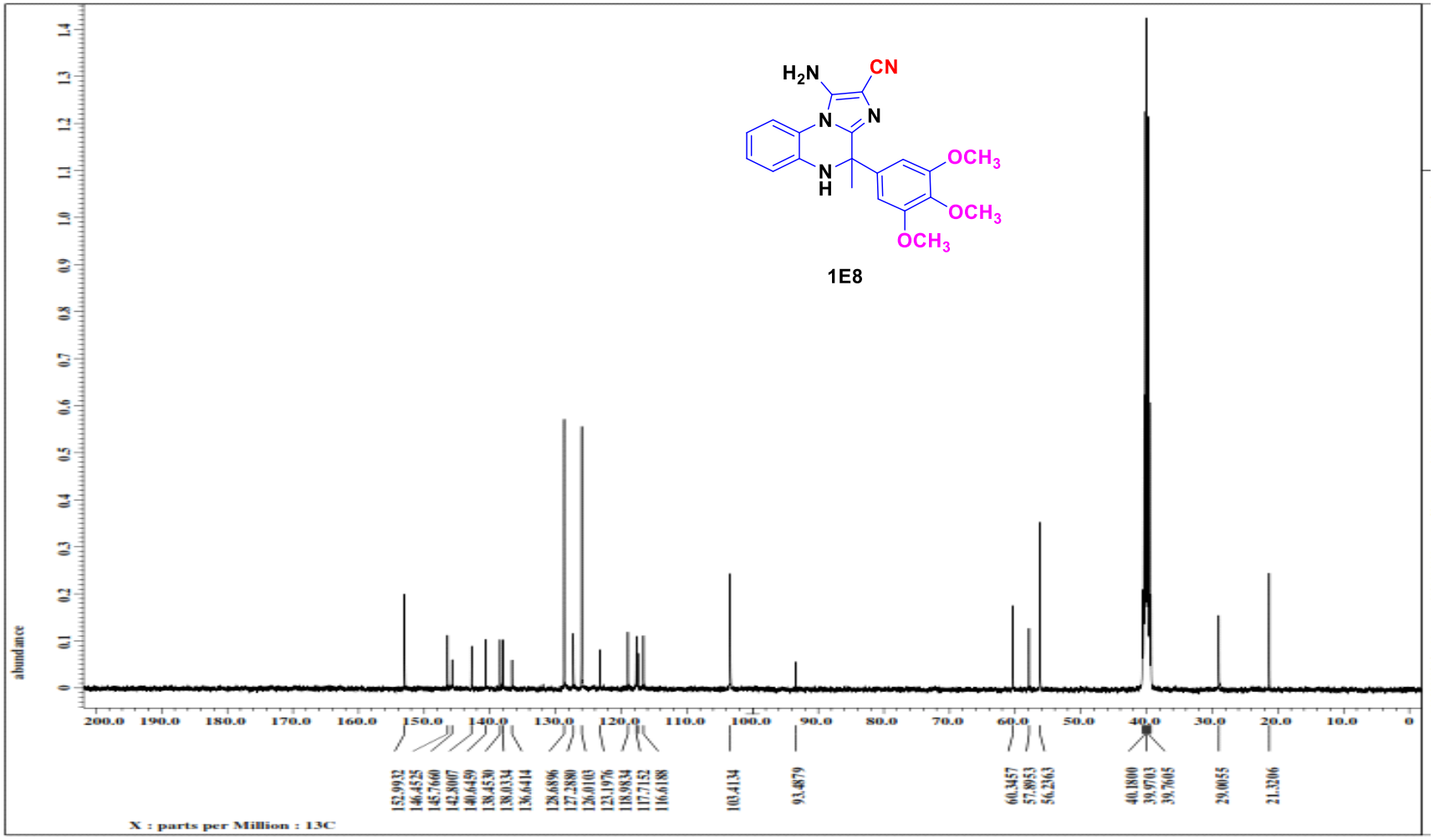
H2N
CN
N
N
N
H
H3CO
OCH3

1E7

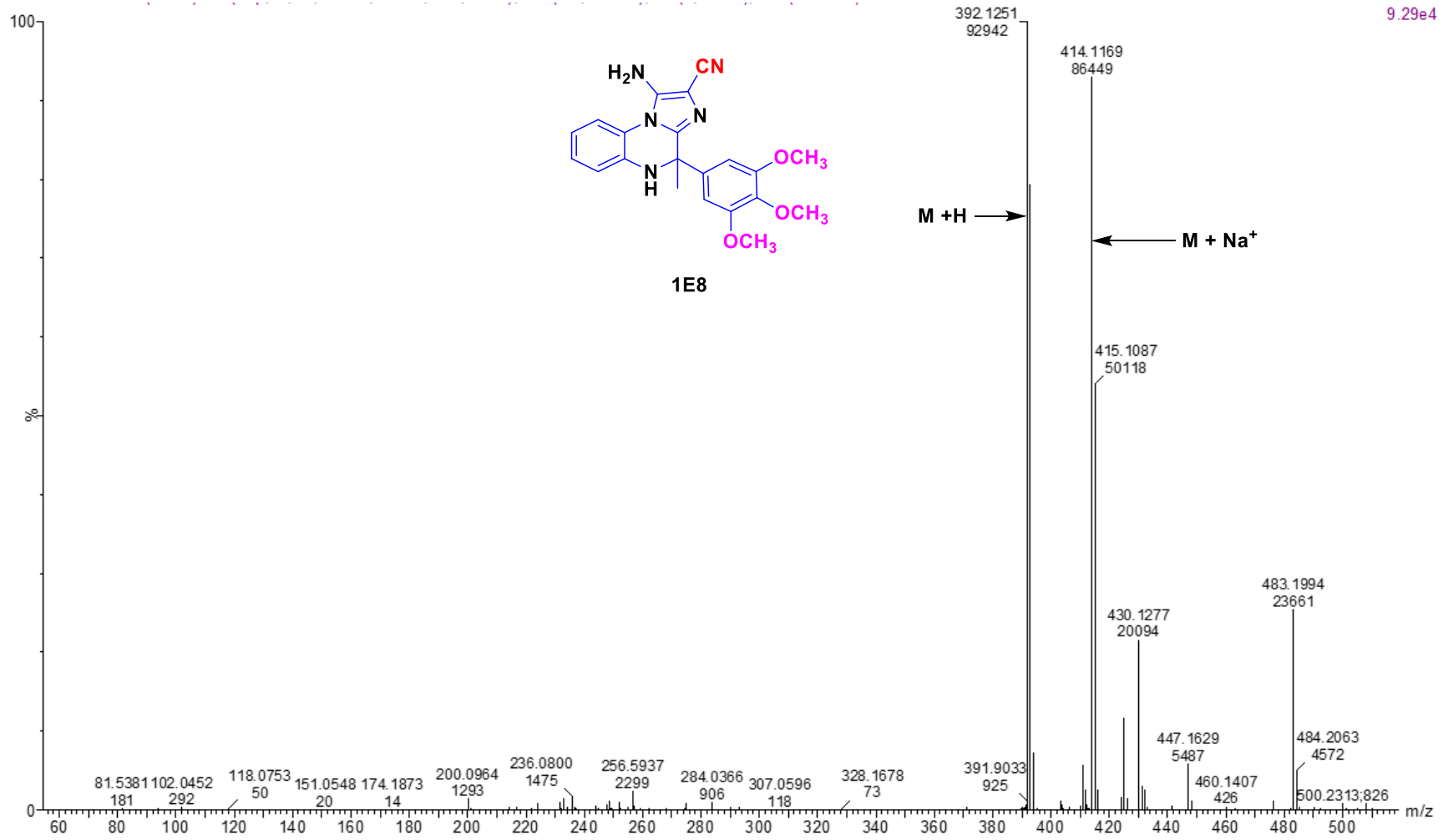
^{1}H NMR


9.02
9.01
5.05
4.13
2.83
2.8
1.79
1.03
1.0
31.55m
abundance
X : parts per Million : 1H
8.3488
7.6923
7.6728
7.5015
7.4817
7.2542
7.1381
7.1198
7.0817
6.9992
6.7641
6.7458
6.5214
5.2695
3.7977
3.7198
3.6191
3.5427
3.4359
2.5000
2.2878
1.7840
1E8

^{13}C NMR

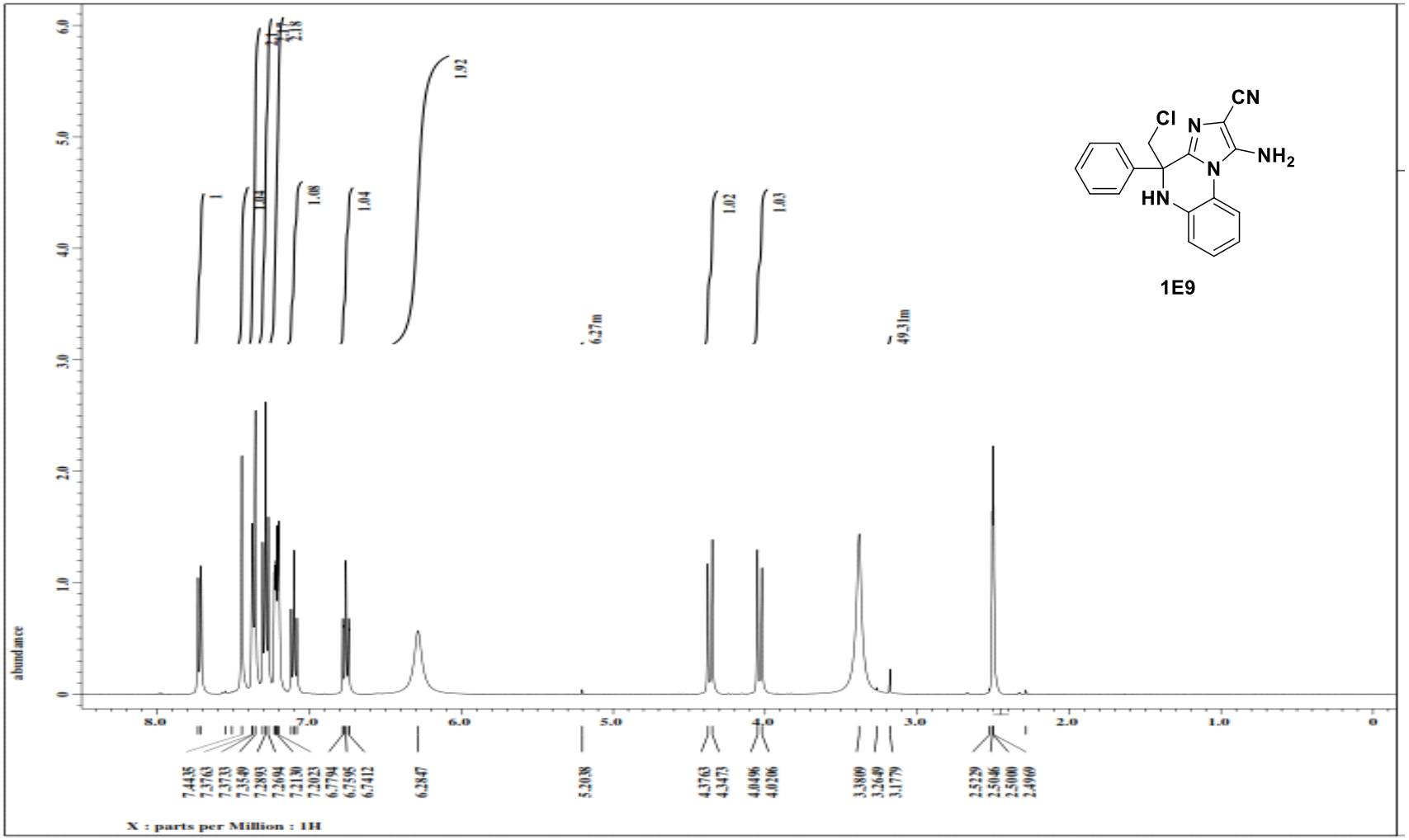

H2N
CN
N
N
N
H
OCH3
OCH3
OCH3
1E8
abundance
X : parts per Million : 13C
152.9932
146.4525
145.7660
142.8007
140.6459
138.4530
138.0334
136.6414
128.6896
127.2880
126.0103
123.1976
118.9834
117.7152
116.6188
103.4134
93.4879
60.3457
57.8053
56.2263
40.1800
39.9703
39.7605
29.0055
21.3206

HRMS

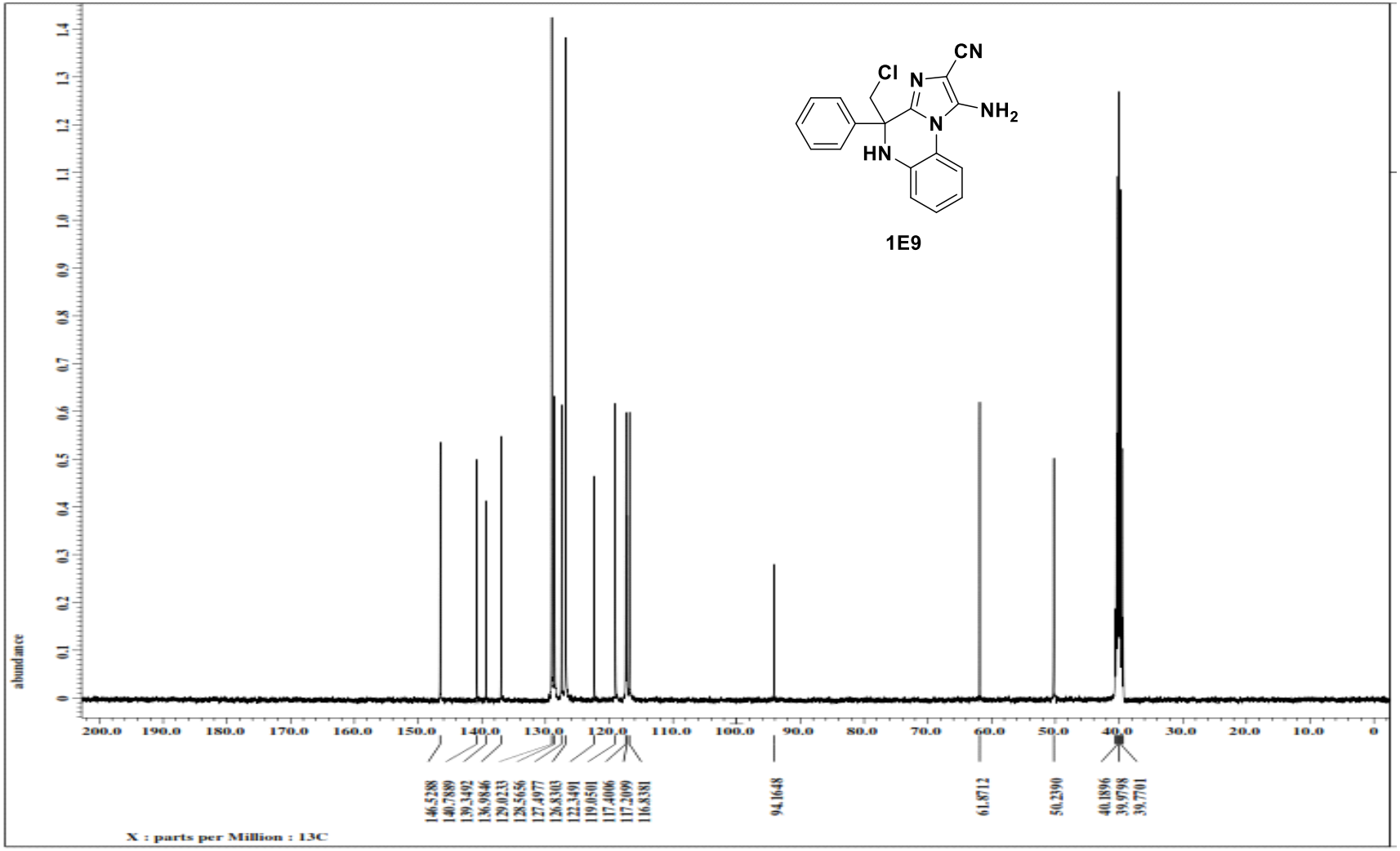

392.1251
92942
9.29e4
414.1169
86449
M +H
M + Na+
415.1087
50118
483.1994
23661
430.1277
20094
447.1629
5487
484.2063
4572
460.1407
426
500.2313;826
391.9033
925
328.1678
73
307.0596
118
284.0366
906
256.5937
2299
236.0800
1475
200.0964
1293
174.1873
14
151.0548
20
118.0753
50
102.0452
292
81.5381
181
100
%
0
m/z
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
H2N
CN
N
N
N
H
OCH3
OCH3
OCH3

1E8

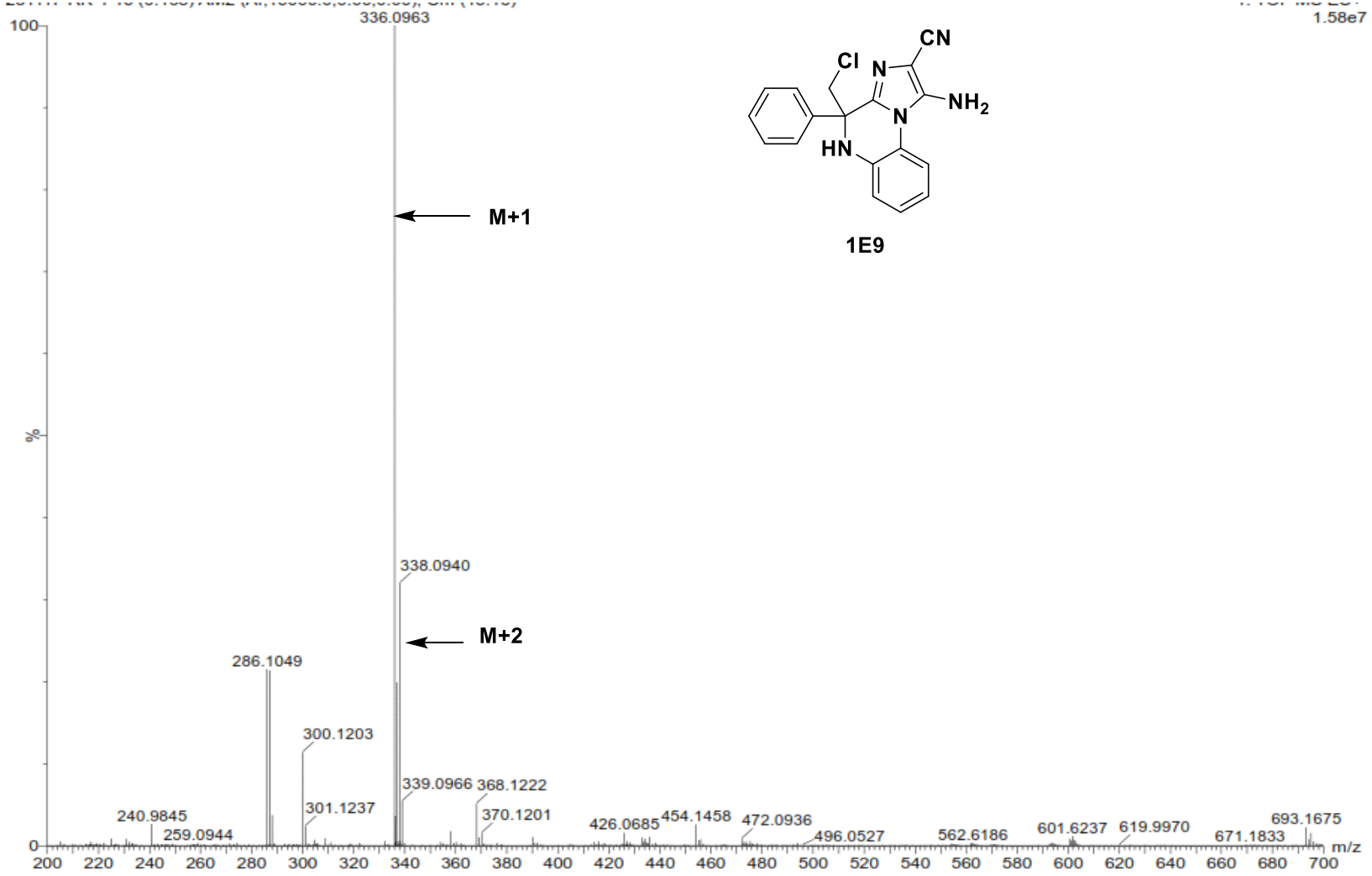
^{1}H NMR


1
1.04
1.08
1.04
1.92
6.27m
1.02
1.03
49.31m
abundance
X : parts per Million : 1H
7.4435
7.3763
7.3733
7.3549
7.2893
7.2694
7.2130
7.2023
6.7794
6.7595
6.7412
6.2847
5.2038
4.3763
4.3473
4.0496
4.0206
3.3809
3.2649
3.1779
2.5229
2.5046
2.5000
2.4969
Cl
CN
N
NH2
N
HN
1E9

^{13}C NMR


CN
Cl
N
NH2
N
HN
1E9
abundance
X : parts per Million : 13C
146.5288
140.7889
139.3492
136.9846
129.0233
128.5656
127.4977
126.8303
122.3491
119.0501
117.4006
117.2099
116.8381
94.1648
61.8712
50.2190
40.1896
39.9798
39.7701

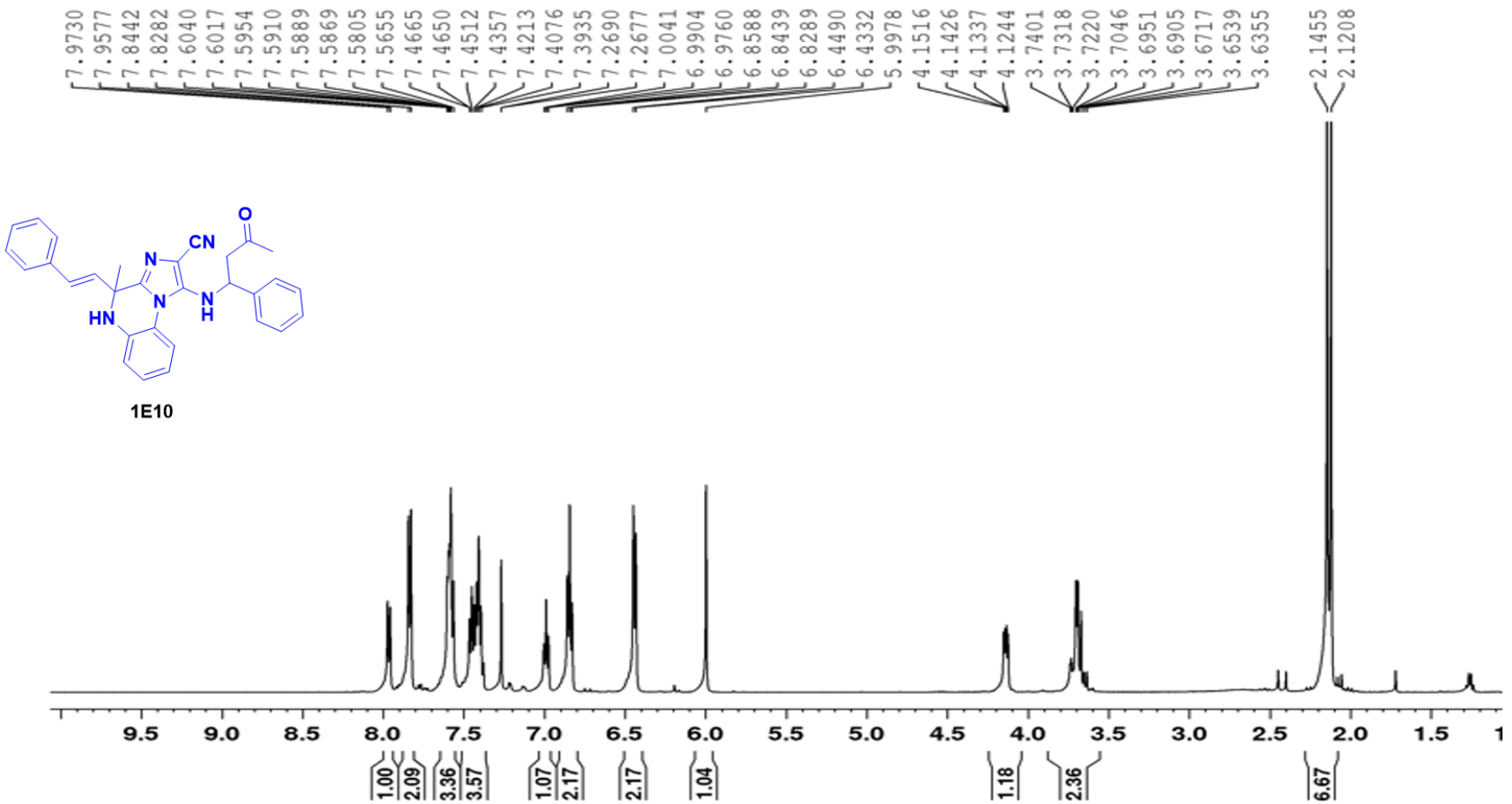
HRMS

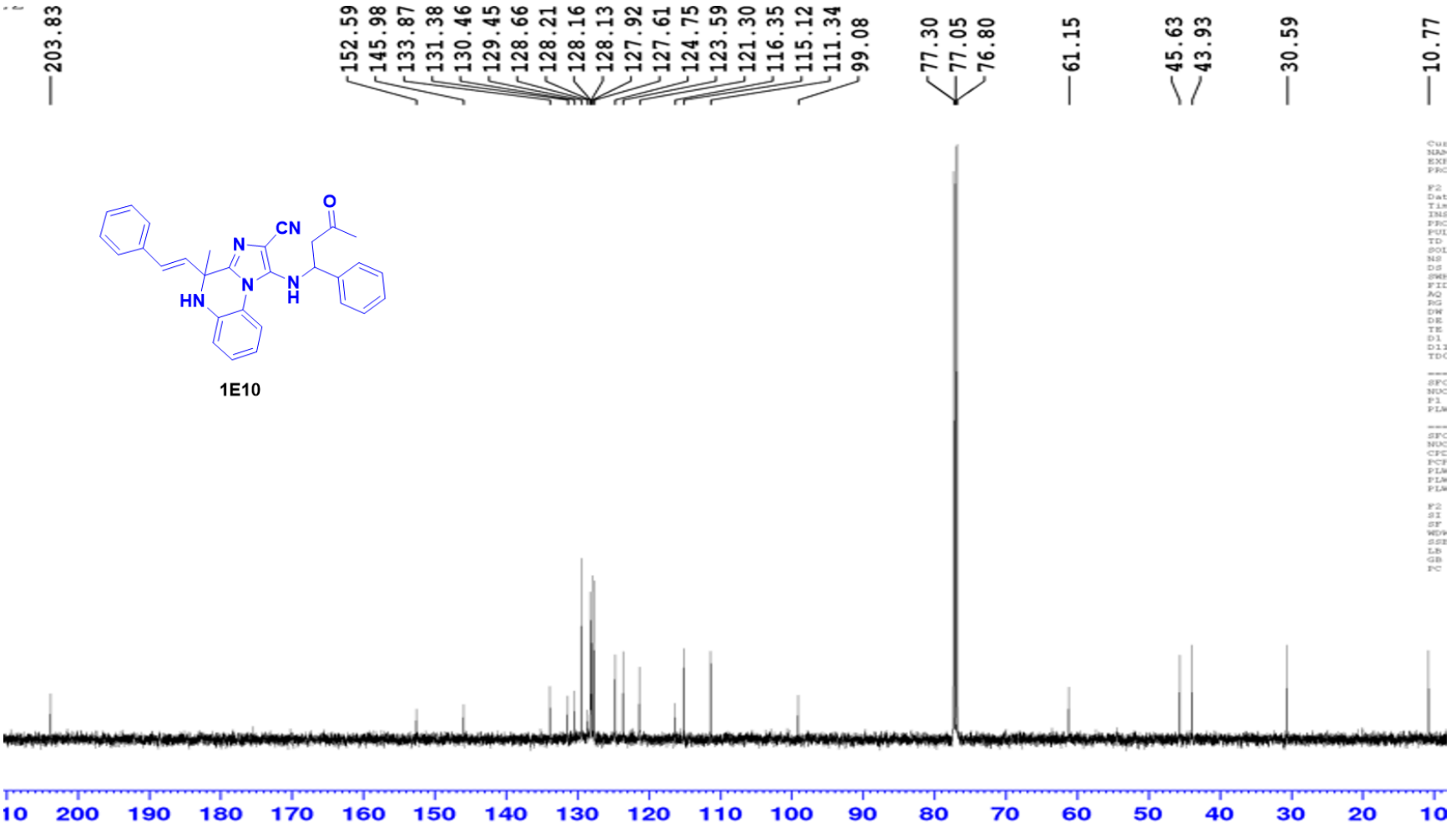

336.0963
1.58e7
100
%
0
M+1
338.0940
M+2
286.1049
300.1203
339.0966
368.1222
301.1237
370.1201
240.9845
259.0944
426.0685
454.1458
472.0936
496.0527
562.6186
601.6237
619.9970
671.1833
693.1675
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700

Cl
N
CN
NH2
N
HN

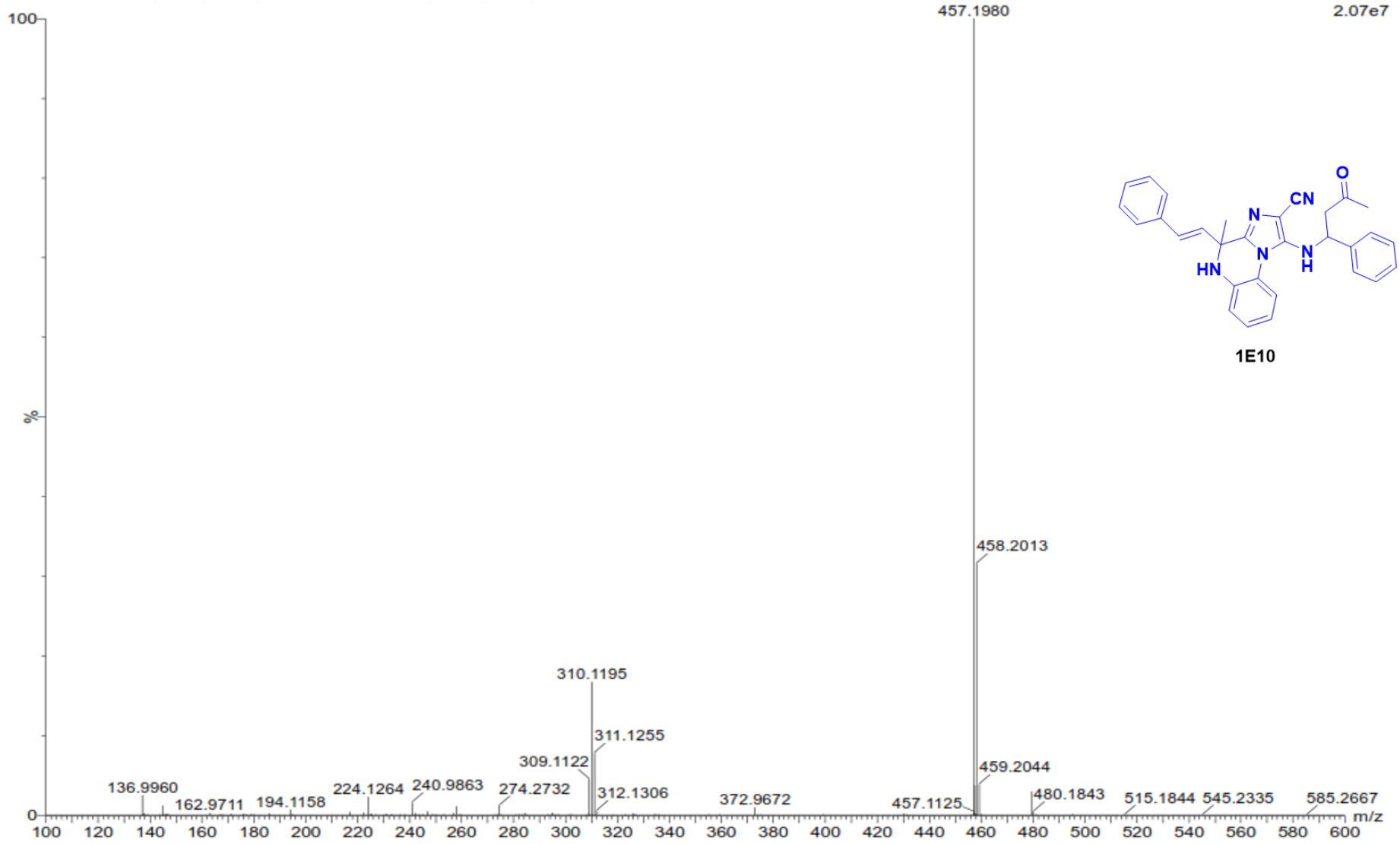
1E9

1H NMR


7.9730
7.9577
7.8442
7.8282
7.6040
7.6017
7.5954
7.5910
7.5889
7.5869
7.5805
7.5655
7.4665
7.4650
7.4512
7.4357
7.4213
7.4076
7.3935
7.2690
7.2677
7.0041
6.9904
6.9760
6.8588
6.8439
6.8289
6.4490
6.4332
5.9978
4.1516
4.1426
4.1337
4.1244
3.7401
3.7318
3.7220
3.7046
3.6951
3.6905
3.6717
3.6539
3.6355
2.1455
2.1208
O
CN
N
N
N
H
HN
1E10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.00
2.09
3.36
3.57
1.07
2.17
2.17
1.04
1.18
2.36
6.67

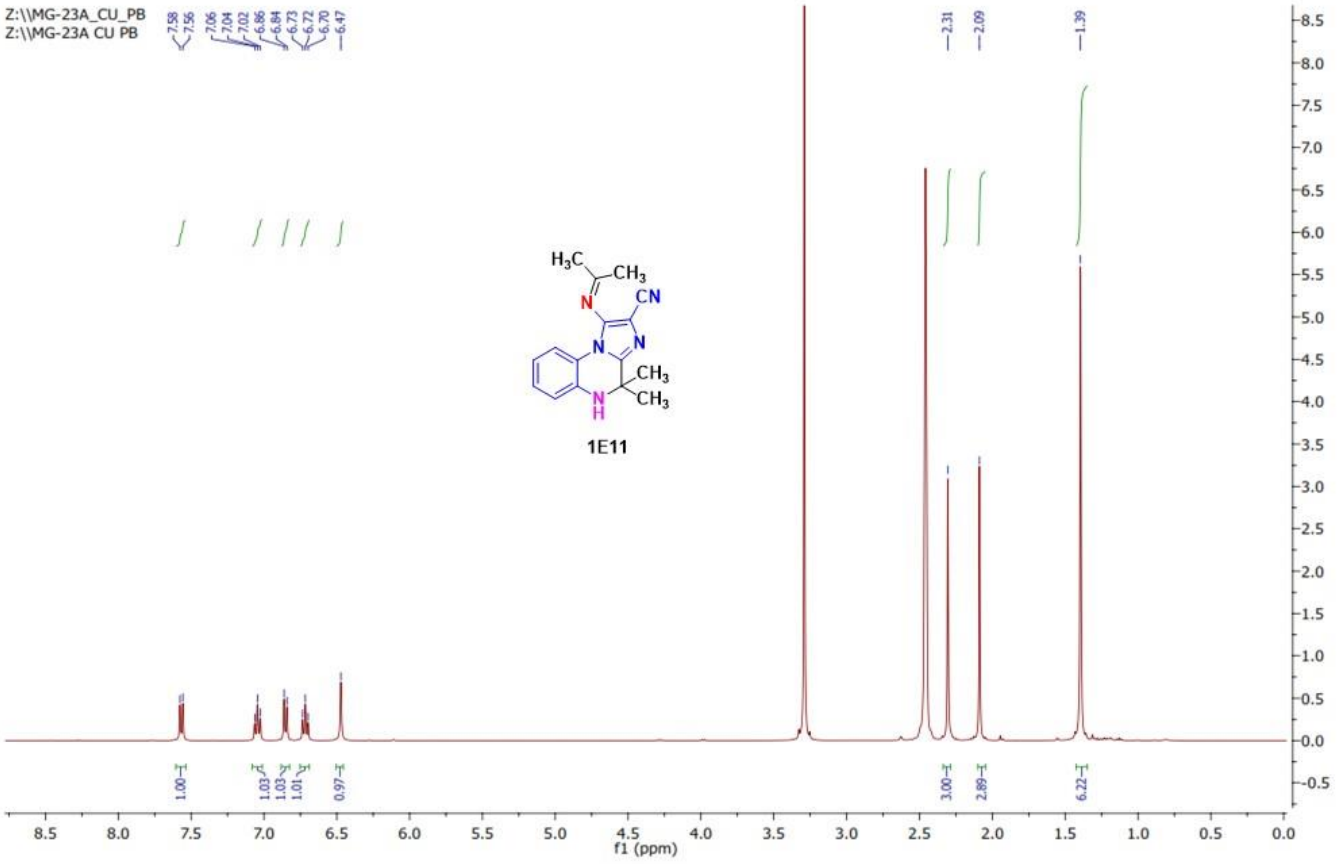

203.83
152.59
145.98
133.87
131.38
130.46
129.45
128.66
128.21
128.16
128.13
127.92
127.61
124.75
123.59
121.30
116.35
115.12
111.34
99.08
77.30
77.05
76.80
61.15
45.63
43.93
30.59
10.77
O
CN
N
N
N
H
HN
1E10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

HRMS

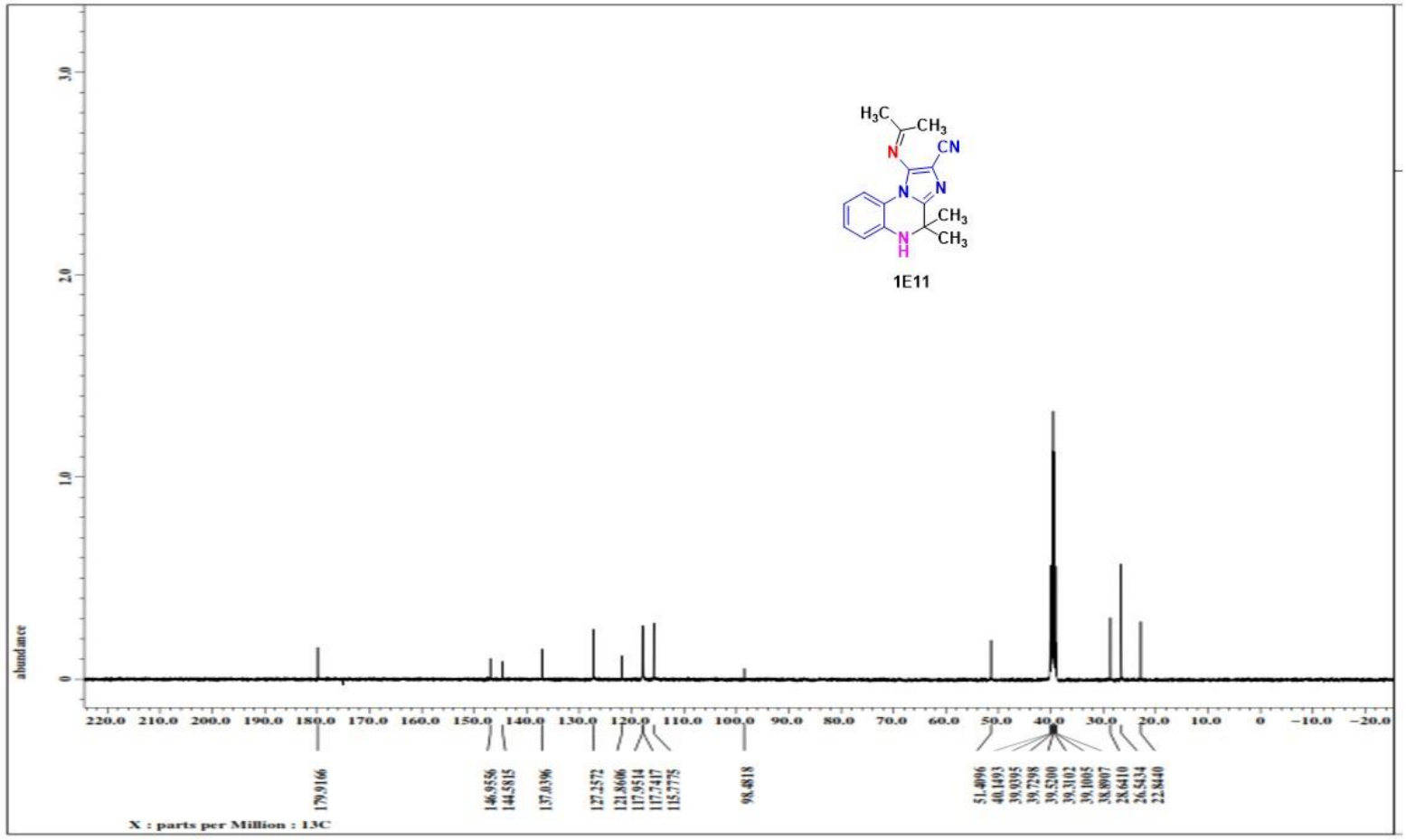

457.1980
2.07e7
100
%
0
458.2013
310.1195
311.1255
309.1122
459.2044
136.9960
162.9711
194.1158
224.1264
240.9863
274.2732
312.1306
372.9672
457.1125
480.1843
515.1844
545.2335
585.2667
m/z
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
O
CN
N
N
HN
N
H

1E10

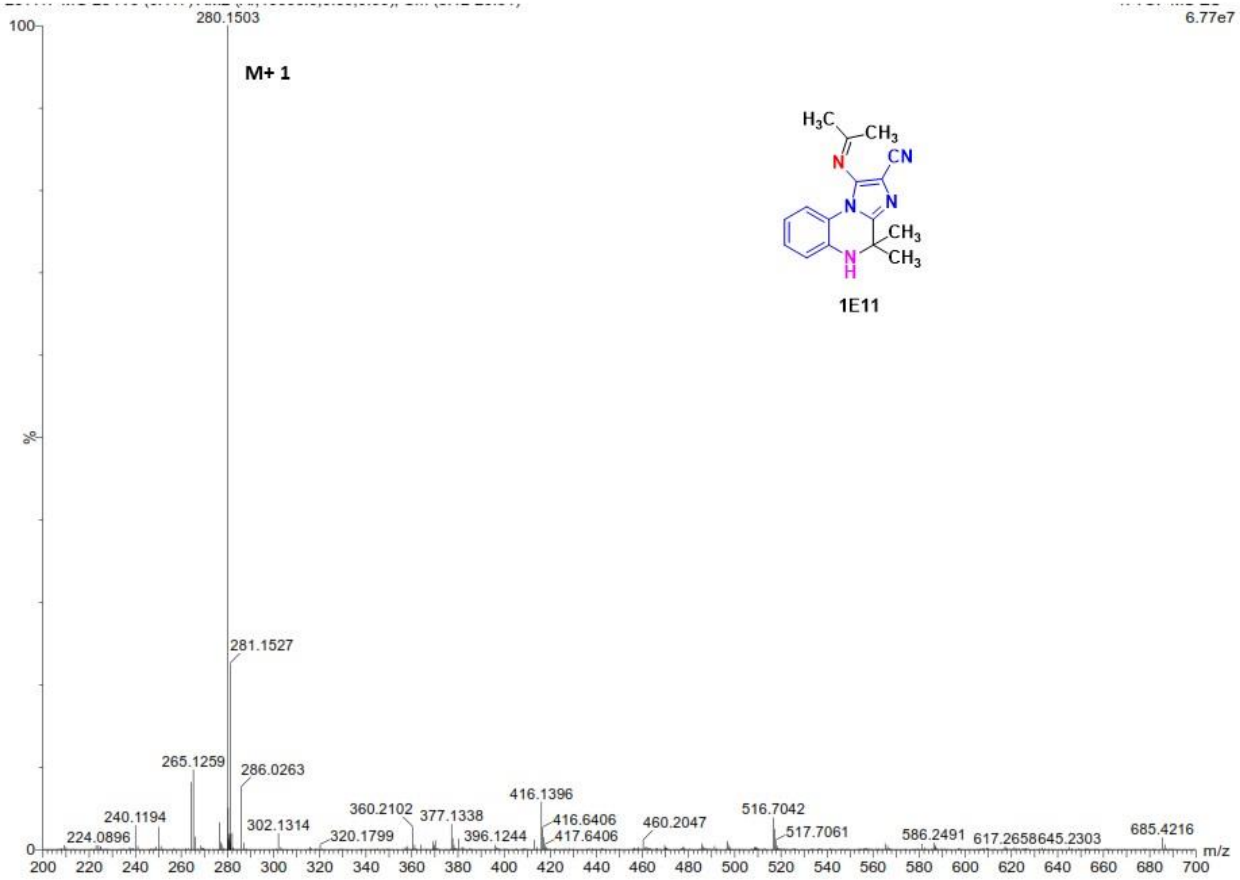
^{1}H NMR


Z:\\MG-23A_CU_PB
Z:\\MG-23A CU PB
7.58
7.56
7.06
7.04
7.02
6.86
6.84
6.73
6.72
6.70
6.47
2.31
2.09
1.39
1E11
1.00
1.03
1.03
1.01
0.97
3.00
2.89
6.22
f1 (ppm)

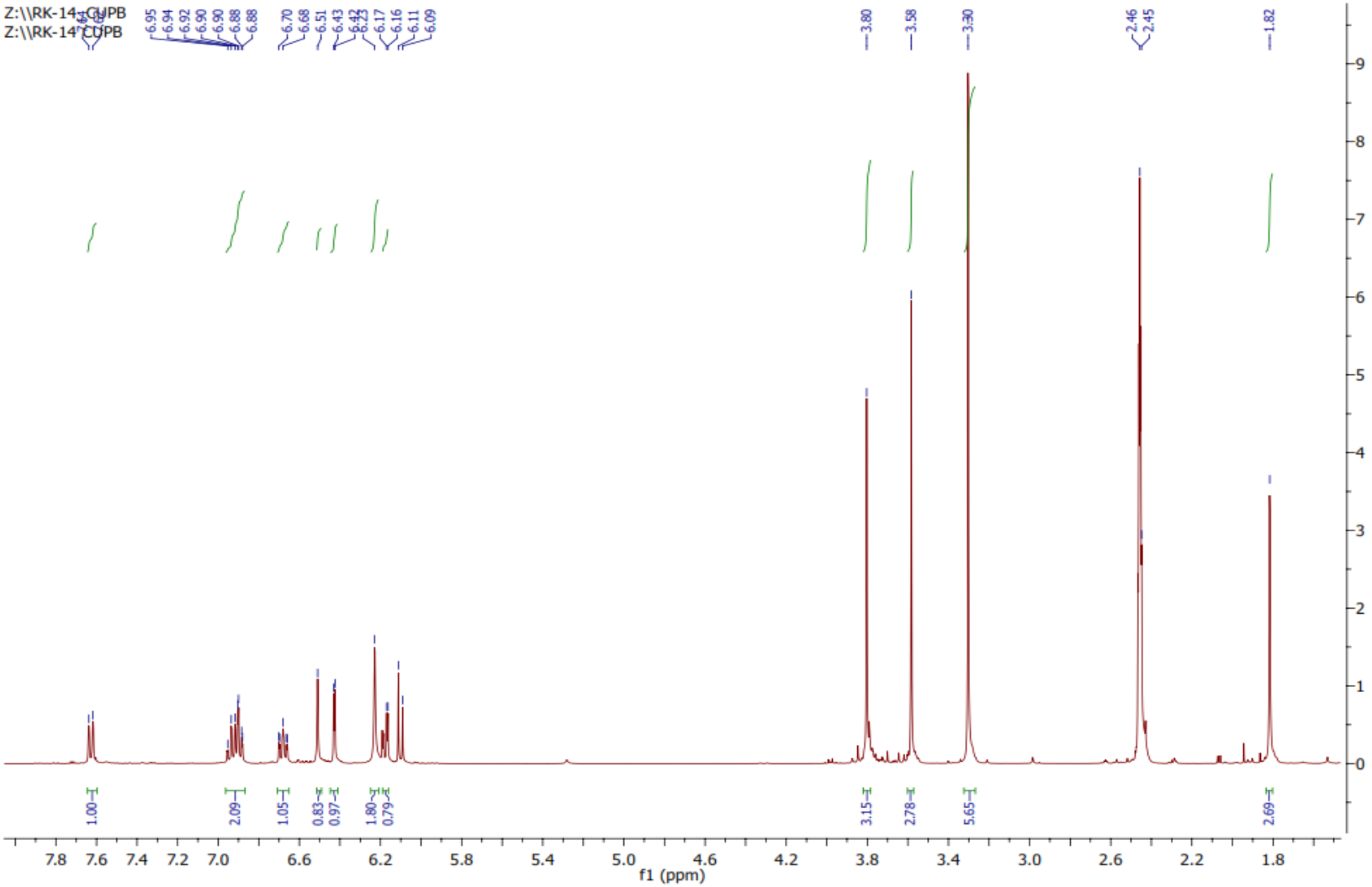
^{13}C NMR


1E11
abundance
X : parts per Million : 13C
179.9166
146.9556
144.5815
137.0396
127.2572
121.8606
117.9514
117.7417
115.7775
98.4818
51.4096
40.1493
39.9395
39.7298
39.5200
39.3102
39.1005
38.8907
28.6410
26.5434
22.8440

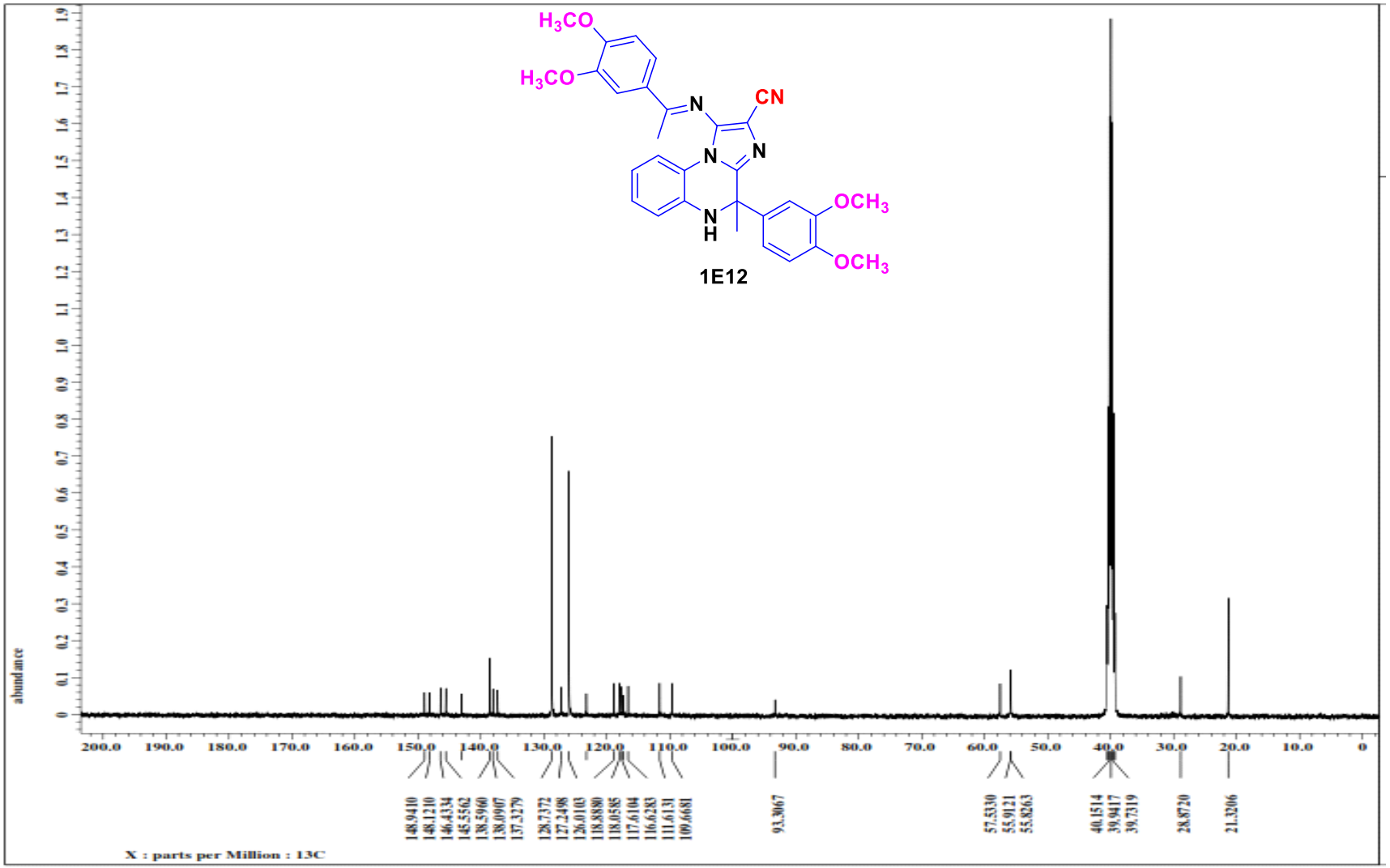
HRMS


280.1503
6.77e7
100
M+ 1
%
0
281.1527
265.1259
286.0263
240.1194
224.0896
302.1314
320.1799
360.2102
377.1338
396.1244
416.1396
416.6406
417.6406
460.2047
516.7042
517.7061
586.2491
617.2658645.2303
685.4216
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
H3C
CH3
N
CN
N
N
CH3
CH3
N
H
1E11

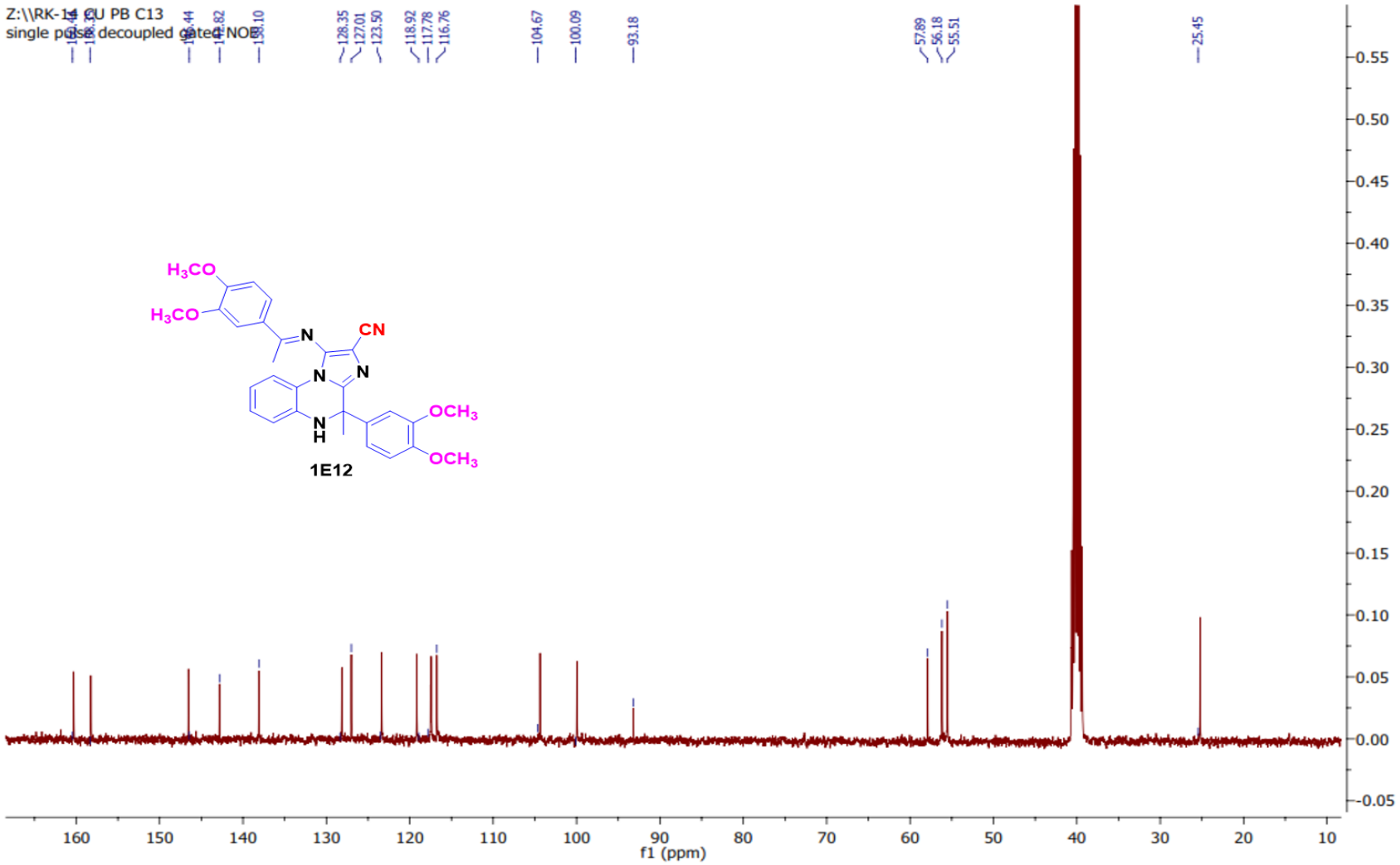
^{1}H NMR


Z:\\RK-14-CUPB
Z:\\RK-14'CUPB
6.95
6.94
6.92
6.90
6.90
6.88
6.88
6.70
6.68
6.51
6.43
6.42
6.23
6.17
6.16
6.11
6.09
3.80
3.58
3.30
2.46
2.45
1.82
1.00
2.09
1.05
0.83
0.97
1.80
0.79
3.15
2.78
5.65
2.69
f1 (ppm)

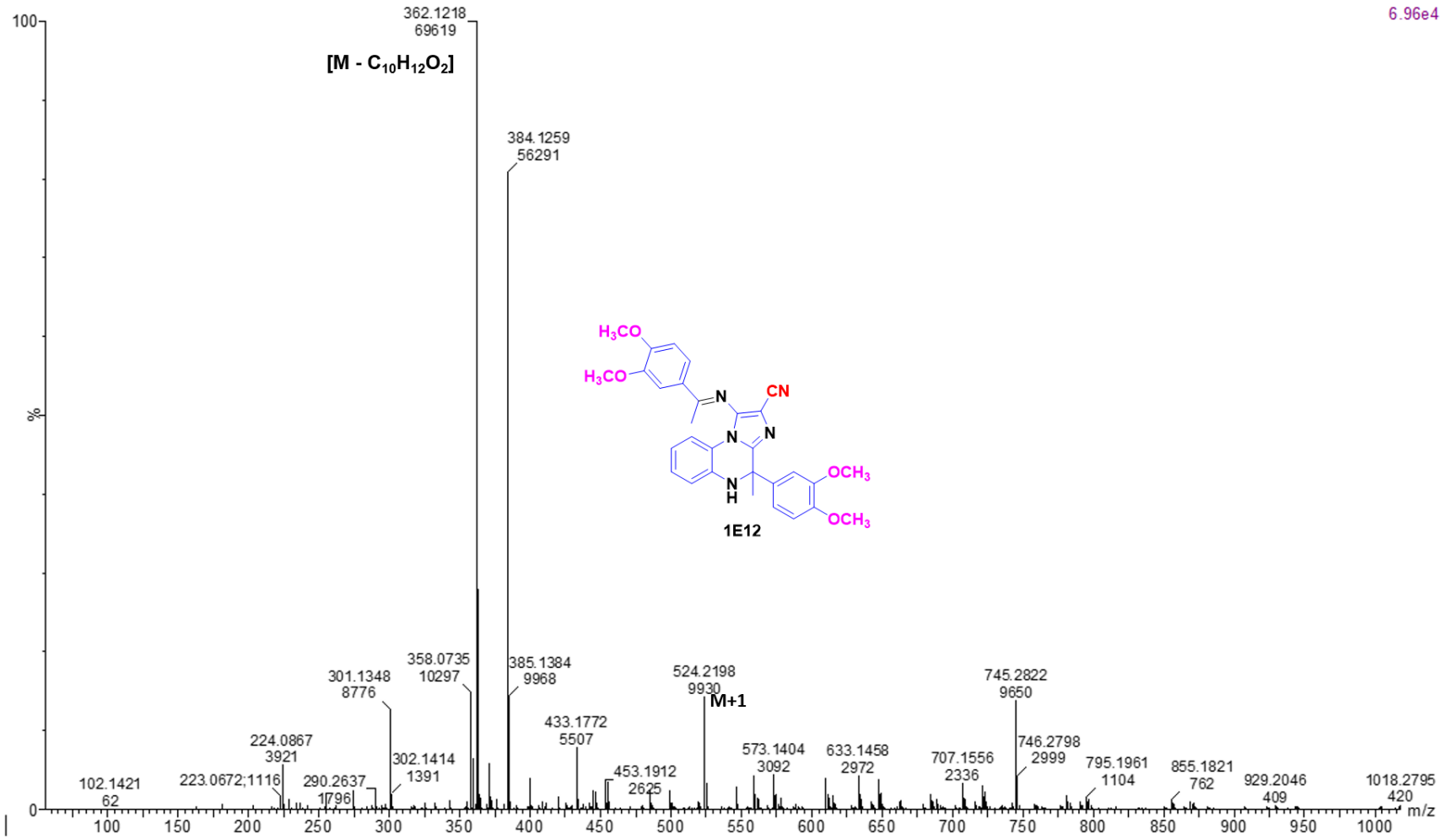
^{13}C NMR


H3CO
H3CO
N
CN
N
N
N
H
OCH3
OCH3
1E12
abundance
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
148.9410
148.1210
146.4334
145.5562
138.5960
138.0907
137.3279
128.7372
127.2498
126.0103
118.8880
118.0585
117.6104
116.6283
111.6131
109.6681
93.3067
57.5330
55.9121
55.8263
40.1514
39.9417
39.7319
28.8720
21.3206
X : parts per Million : 13C

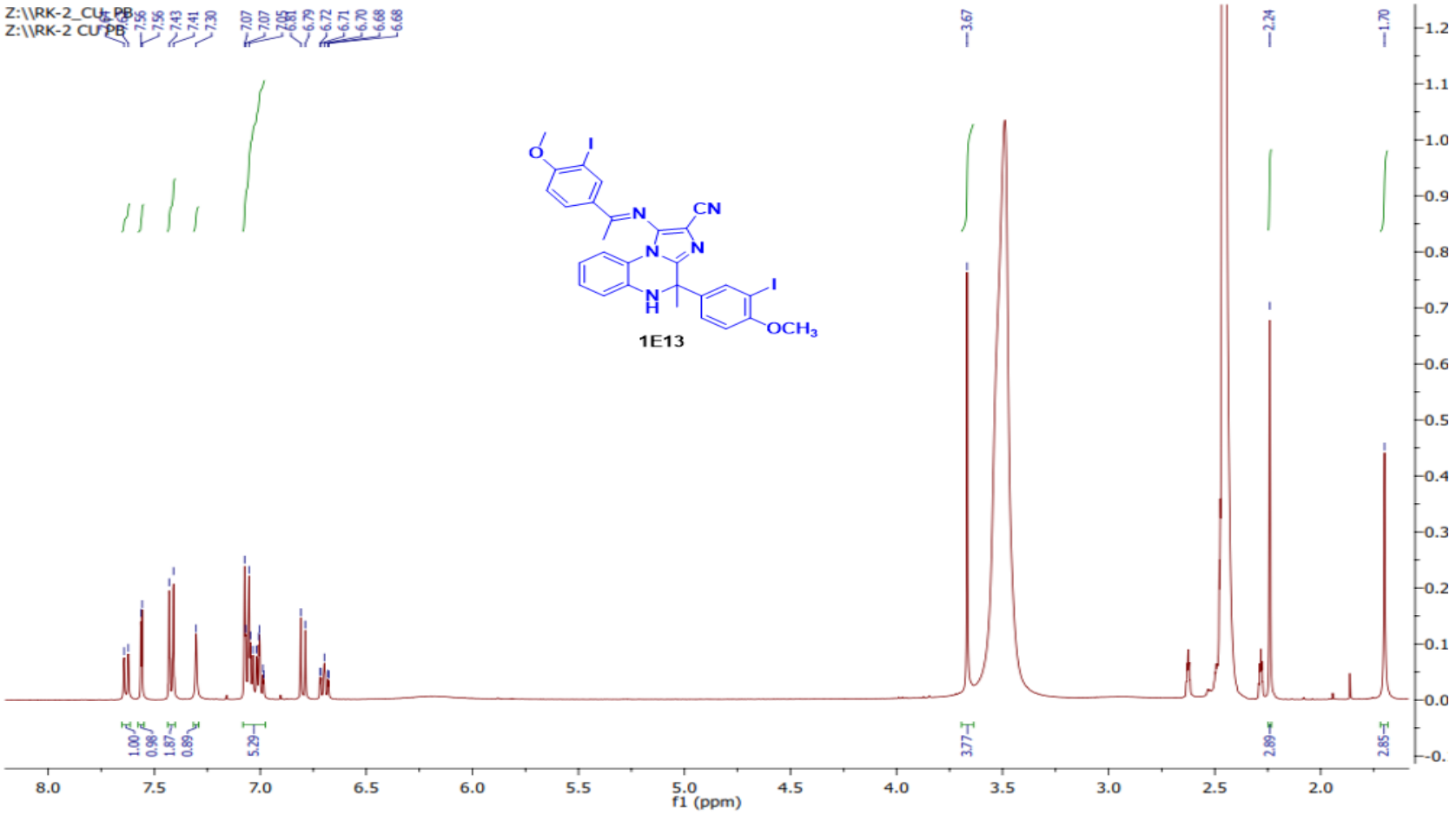
13C NMR


Z:\\RK-14 CU PB C13
single pulse decoupled gated NOE
128.35
127.01
123.50
118.92
117.78
116.76
104.67
100.09
93.18
57.89
56.18
55.51
25.45
H3CO
H3CO
CN
N
N
N
N
H
OCH3
OCH3
1E12
f1 (ppm)

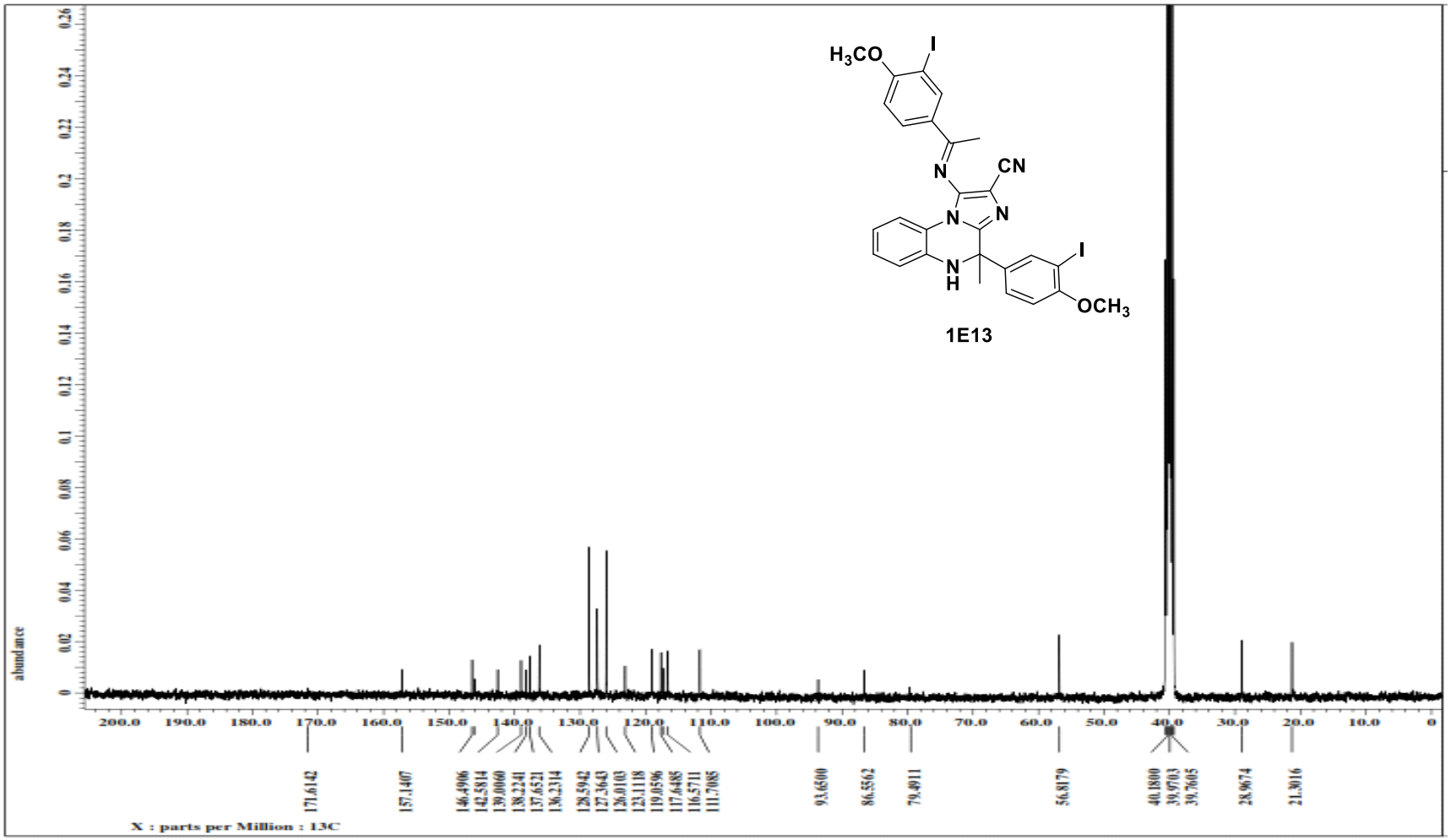
HRMS


362.1218
69619
[M - C10H12O2]
384.1259
56291
6.96e4
100
%
0
H3CO
H3CO
N
CN
N
N
N
H
OCH3
OCH3
1E12
358.0735
10297
385.1384
9968
301.1348
8776
524.2198
9930
M+1
745.2822
9650
433.1772
5507
224.0867
3921
573.1404
3092
633.1458
2972
746.2798
2999
707.1556
2336
795.1961
1104
855.1821
762
302.1414
1391
453.1912
2625
929.2046
409
1018.2795
420
102.1421
62
223.0672;1116
290.2637
1796
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000

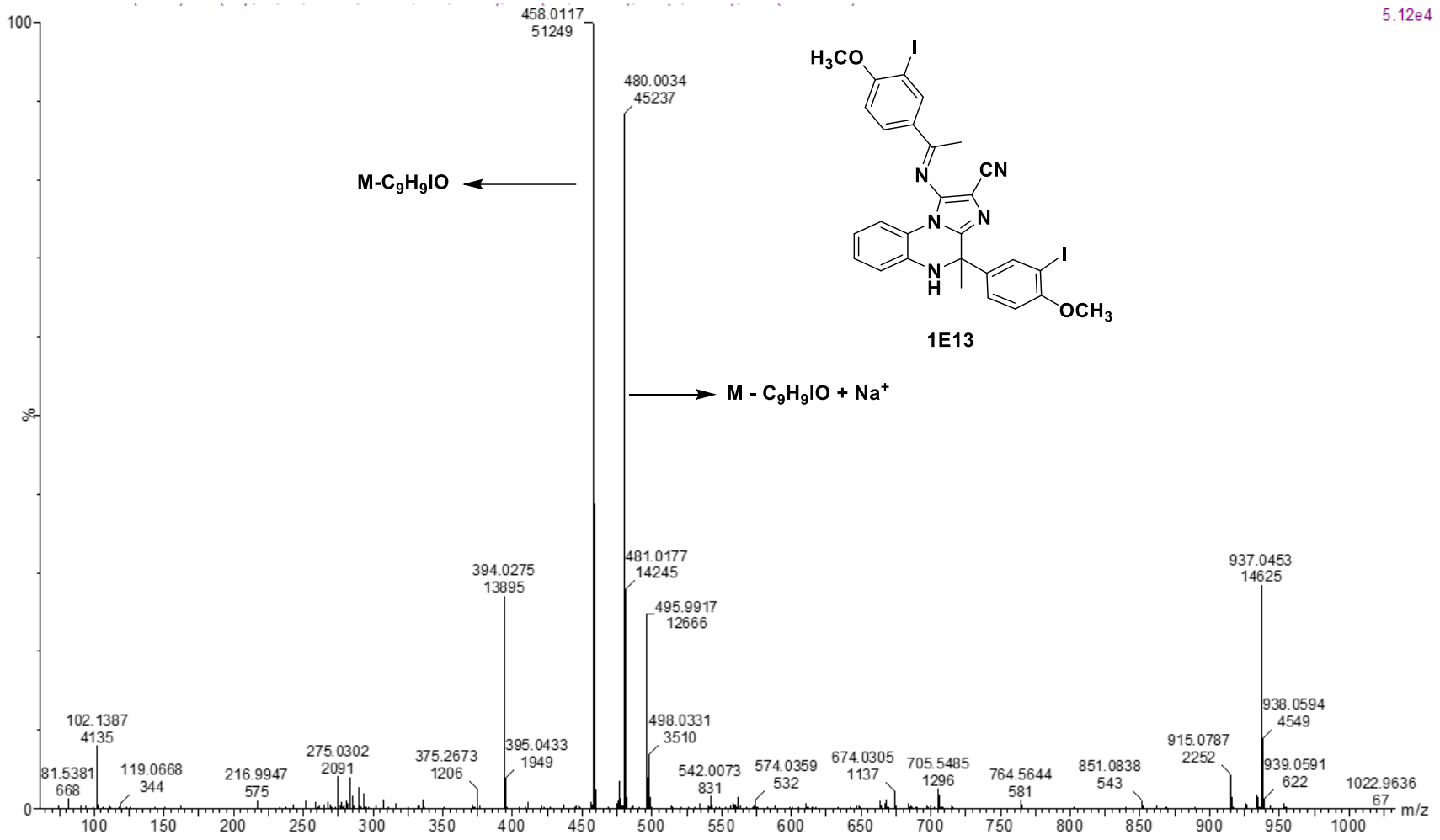
^{1}H NMR



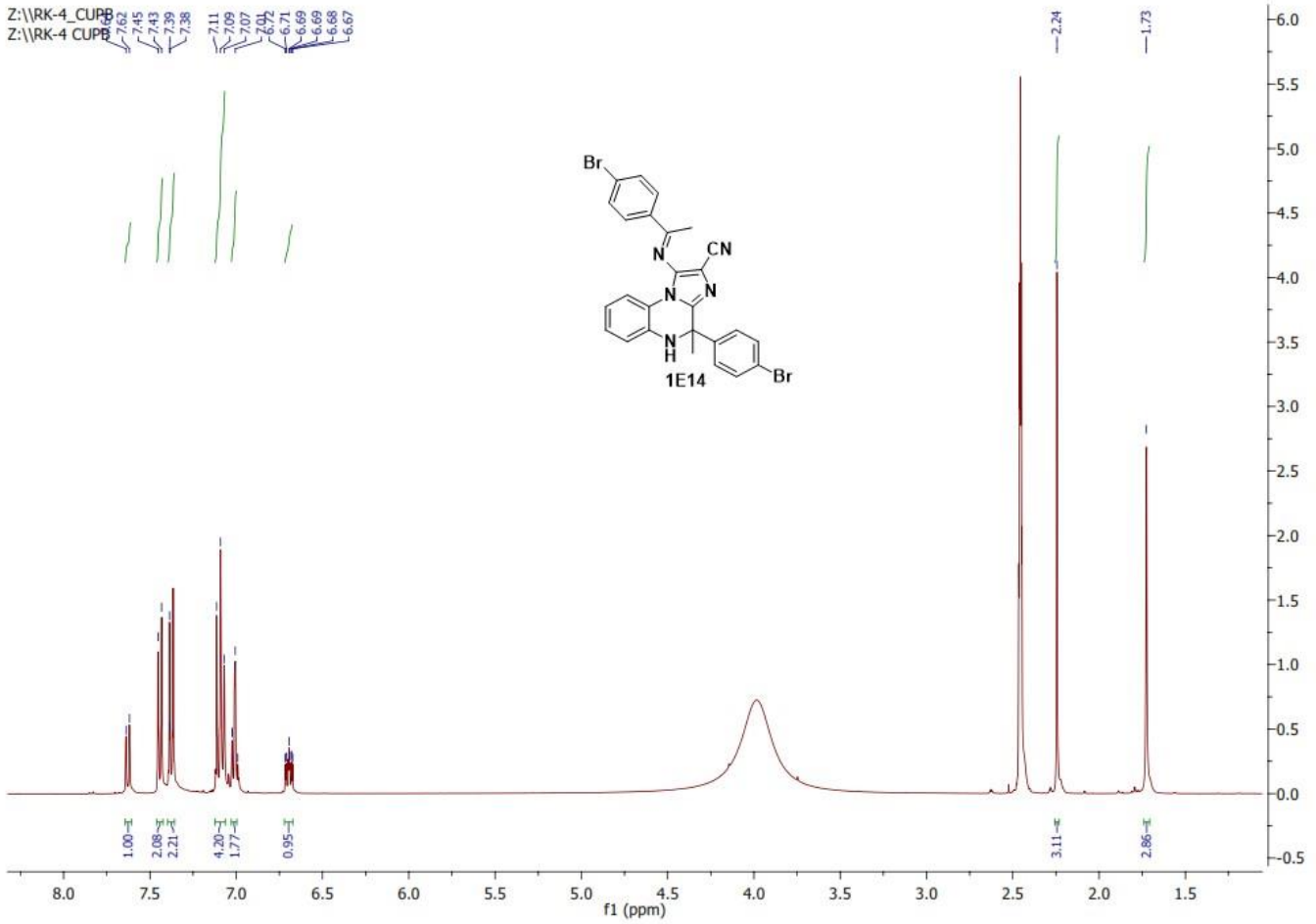
^{13}C NMR


H3CO
I
N
CN
N
N
N
H
I
OCH3
1E13
abundance
X : parts per Million : 13C
171.6142
157.1407
146.4906
142.5814
139.0060
138.2241
137.6521
136.2314
128.5942
127.3643
126.0103
123.1118
119.0596
117.6485
116.5711
111.7085
93.6600
86.5562
79.4911
56.8179
40.1800
39.9703
39.7605
28.9674
21.3016

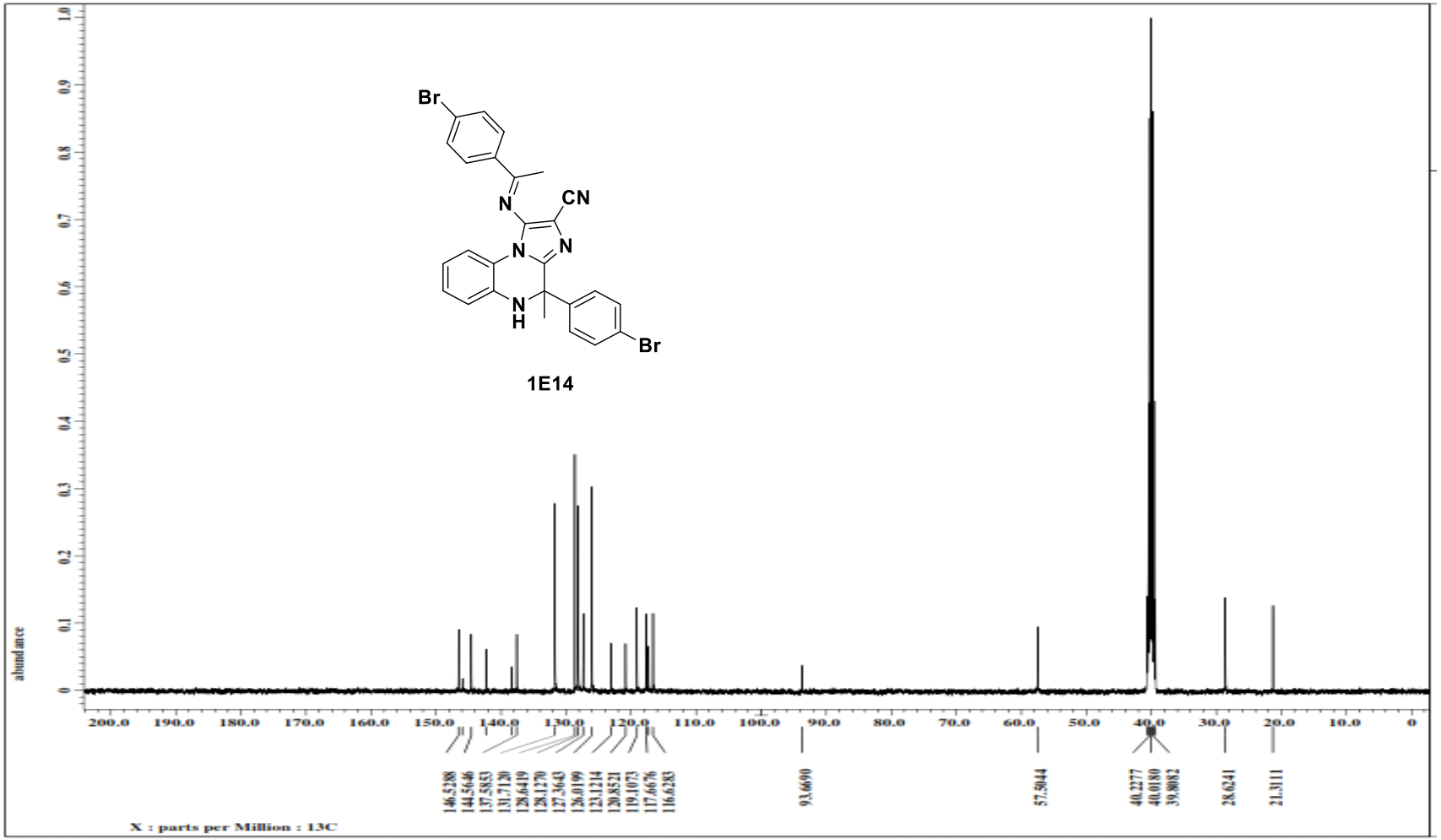
HRMS


5.12e4
100
%
0
458.0117
51249
480.0034
45237
M-C9H9IO
M - C9H9IO + Na+
481.0177
14245
394.0275
13895
495.9917
12666
498.0331
3510
937.0453
14625
938.0594
4549
939.0591
622
915.0787
2252
102.1387
4135
81.5381
668
119.0668
344
216.9947
575
275.0302
2091
375.2673
1206
395.0433
1949
542.0073
831
574.0359
532
674.0305
1137
705.5485
1296
764.5644
581
851.0838
543
1022.9636
67
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
H3CO
I
N
CN
N
N
N
H
I
OCH3
1E13

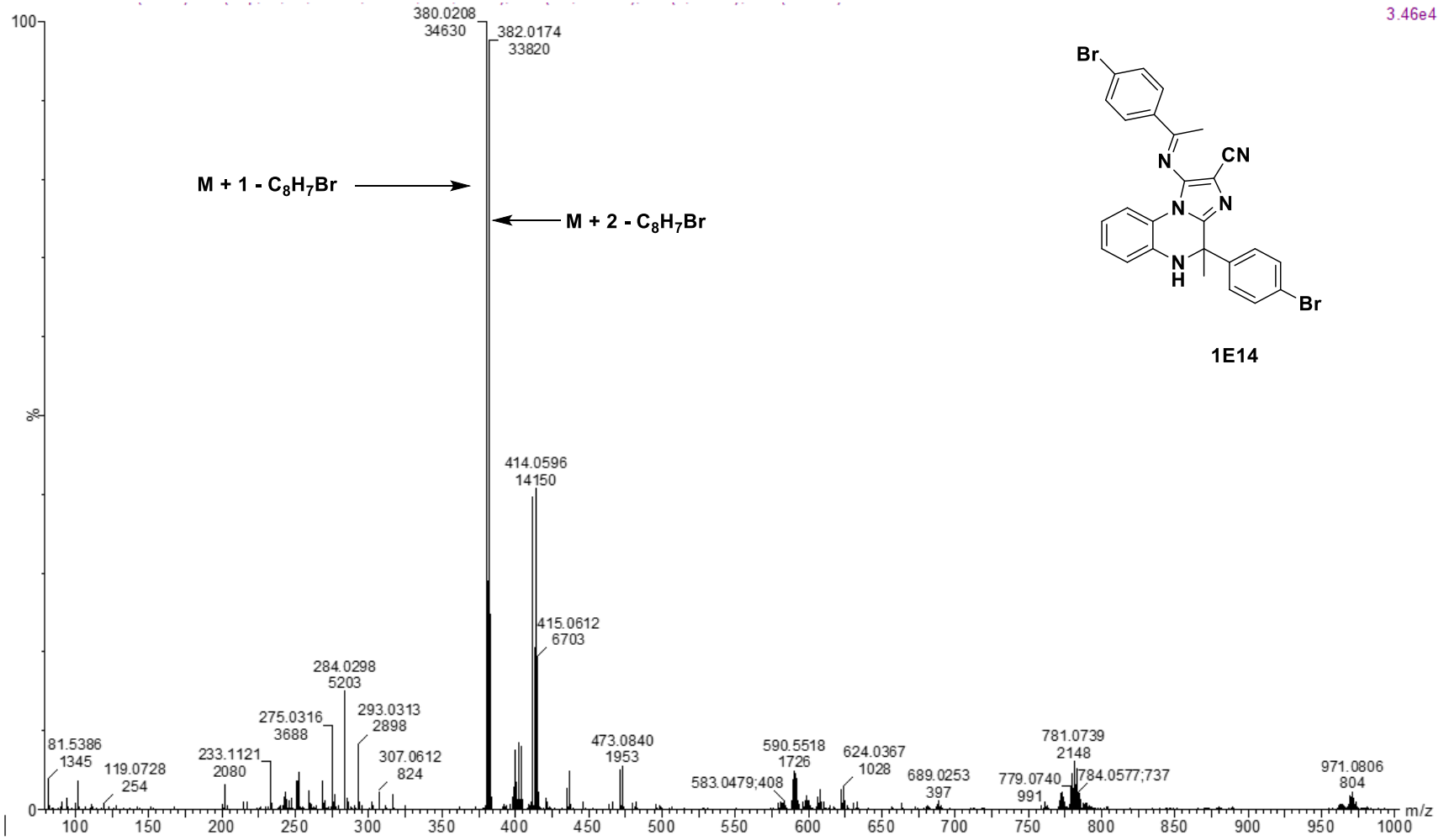
^{1}H NMR


Z:\\RK-4_CUPB
Z:\\RK-4 CUPB
7.62
7.45
7.43
7.39
7.38
7.11
7.09
7.07
7.01
6.72
6.71
6.69
6.69
6.68
6.67
2.24
1.73
Br
N
CN
N
N
N
H
Br
1E14
1.00
2.08
2.21
4.20
1.77
0.95
3.11
2.86
f1 (ppm)

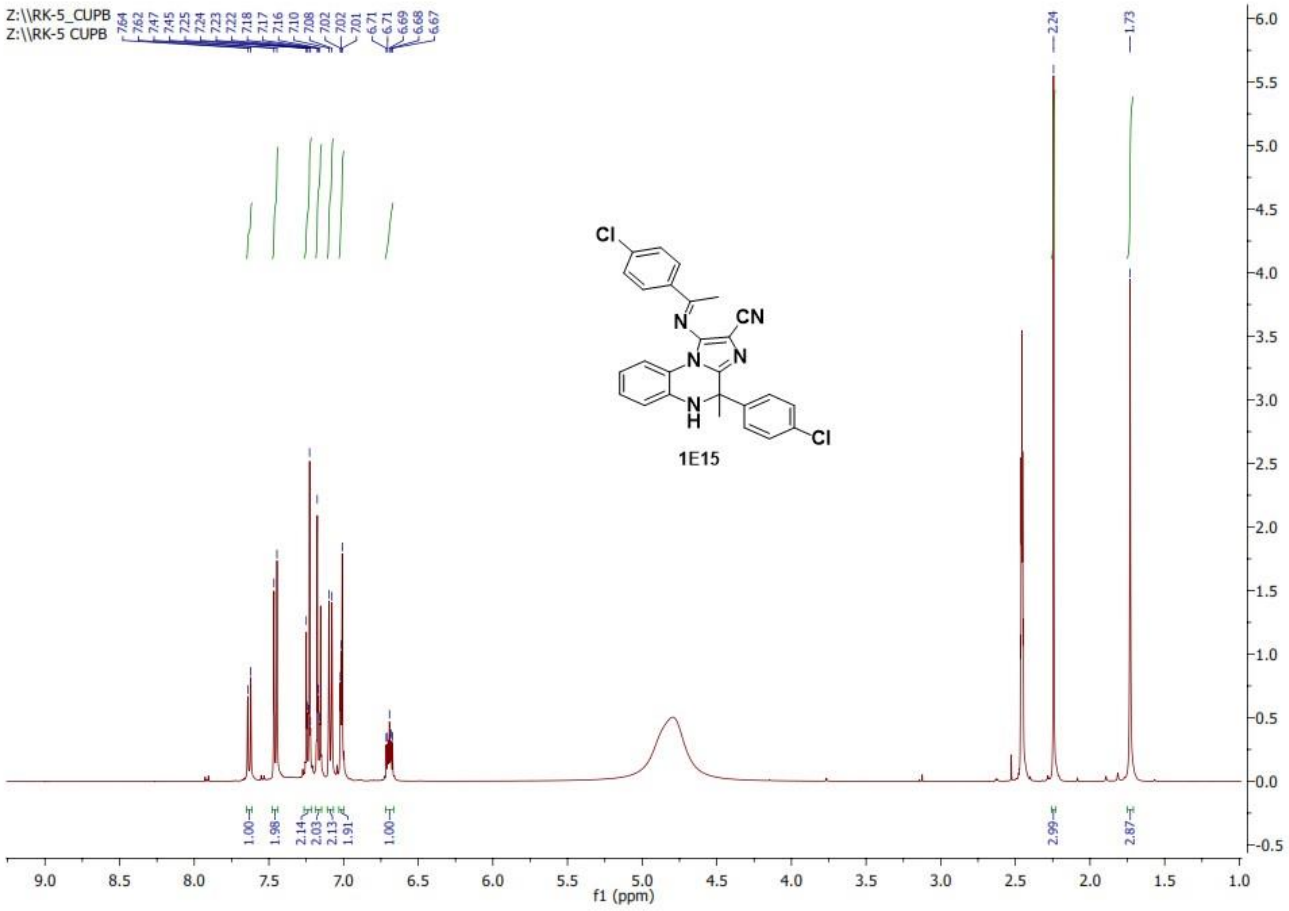
^{13}C NMR


Br
N
CN
N
N
N
H
Br
1E14
abundance
X : parts per Million : 13C
146.5288
144.5646
137.5853
131.7120
128.6419
128.1270
127.3643
126.0199
123.1214
120.8521
119.1073
117.6676
116.6283
93.6690
57.5044
40.2277
40.0180
39.8082
28.6241
21.3111

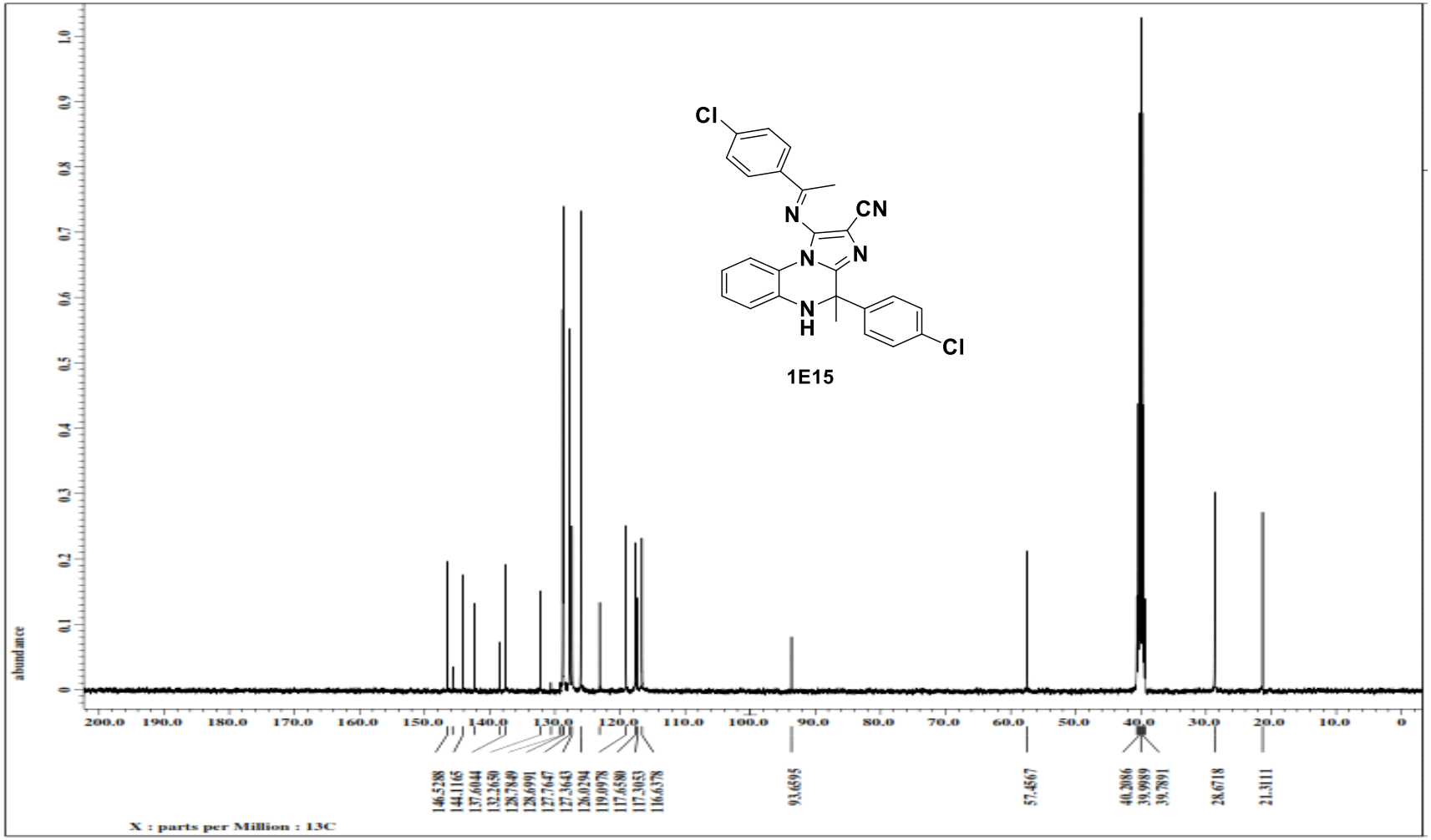
HRMS


3.46e4
100
%
0
380.0208
34630
382.0174
33820
M + 1 - C8H7Br
M + 2 - C8H7Br
414.0596
14150
415.0612
6703
284.0298
5203
293.0313
2898
275.0316
3688
307.0612
824
233.1121
2080
81.5386
1345
119.0728
254
473.0840
1953
590.5518
1726
583.0479;408
624.0367
1028
689.0253
397
779.0740
991
781.0739
2148
784.0577;737
971.0806
804
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
Br
N
CN
N
N
N
H
Br
1E14

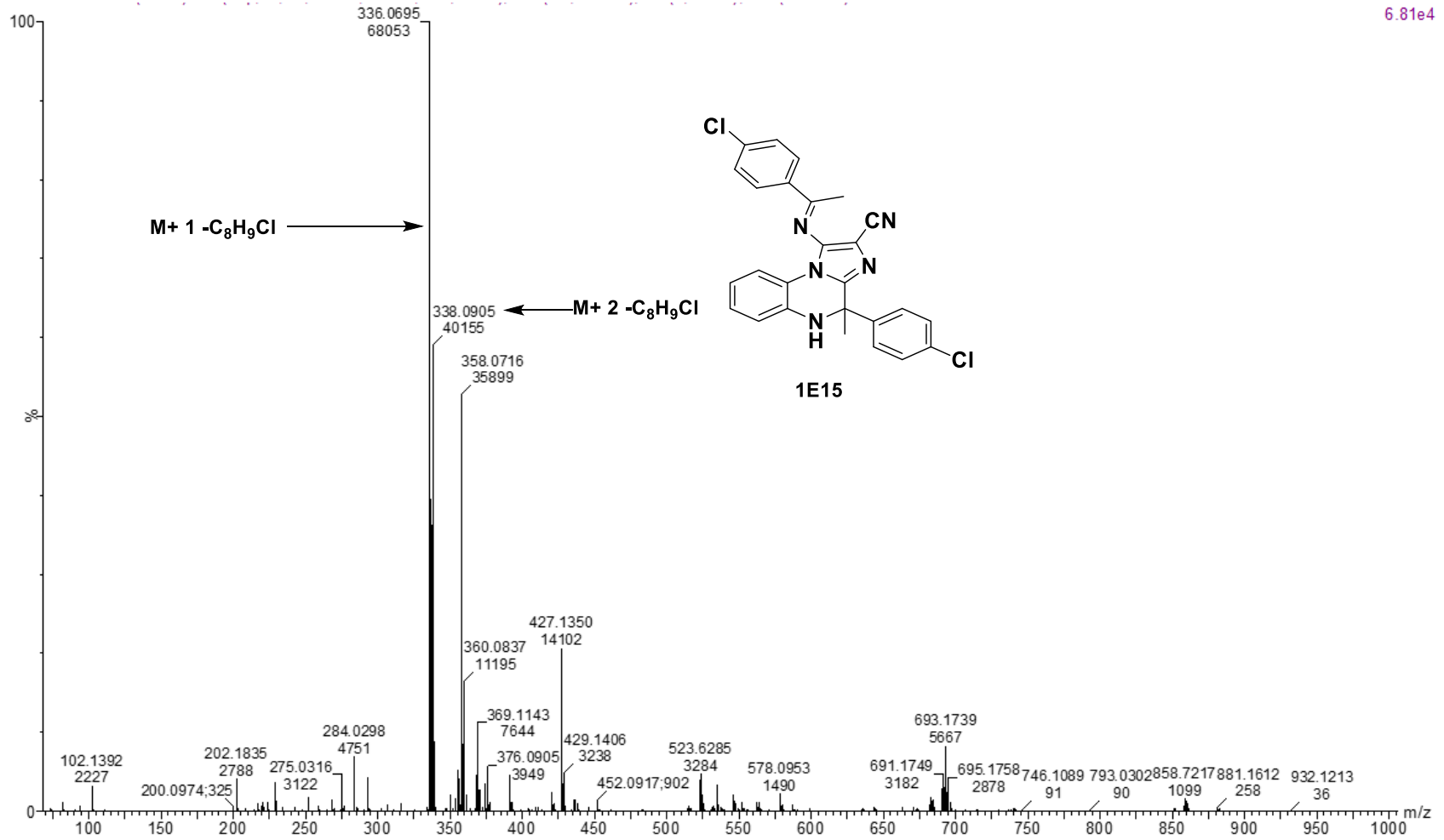
^{1}H NMR


Z:\\RK-5_CUPB
Z:\\RK-5 CUPB
7.64
7.62
7.47
7.45
7.25
7.24
7.23
7.22
7.18
7.17
7.16
7.10
7.08
7.02
7.02
7.02
7.01
6.71
6.71
6.69
6.68
6.67
2.24
1.73
Cl
N
CN
N
N
N
H
Cl
1E15
1.00
1.98
2.14
2.03
2.13
1.91
1.00
2.99
2.87
f1 (ppm)

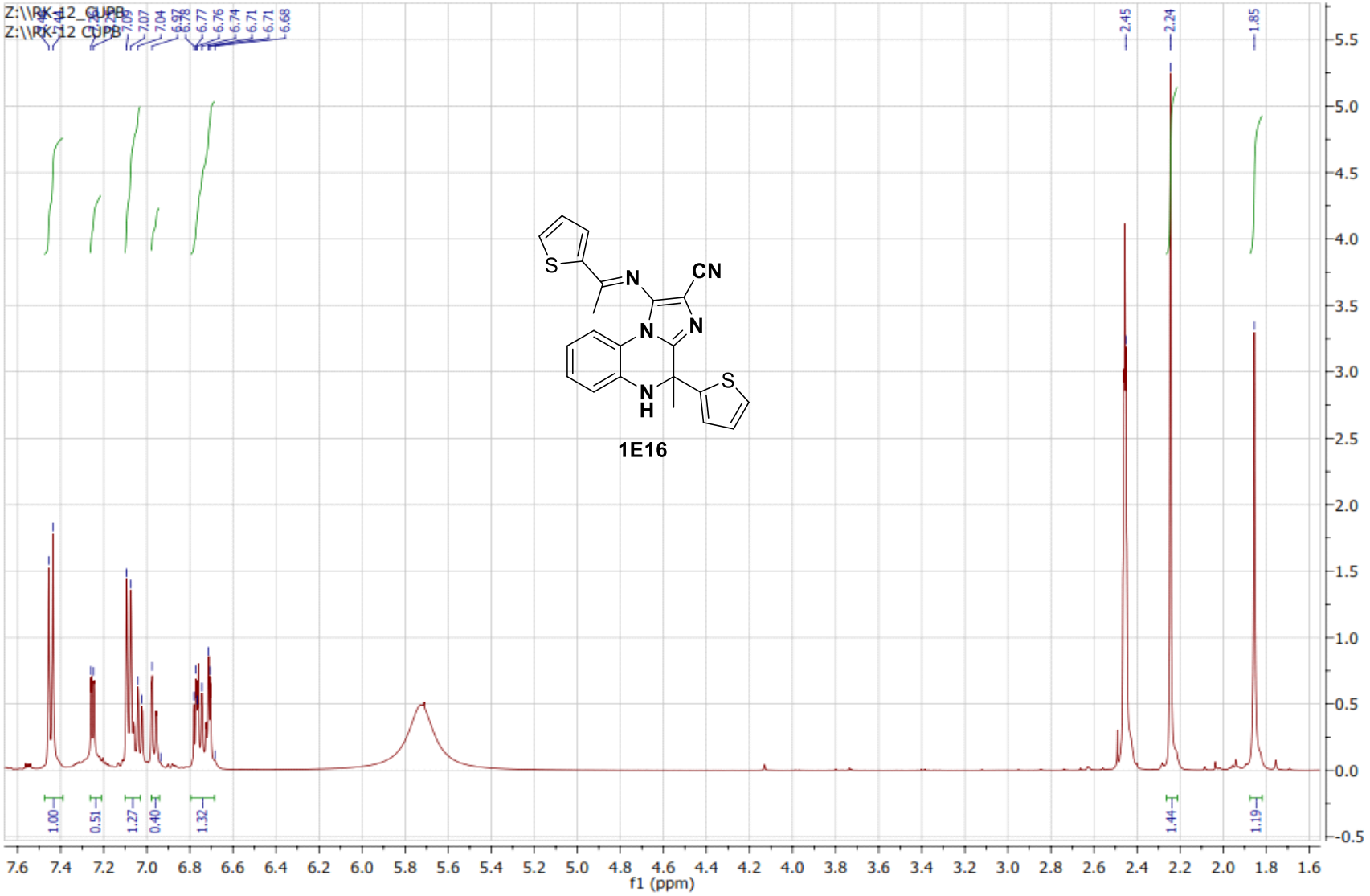
^{13}C NMR


Cl
N
CN
N
N
N
H
Cl
1E15
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
146.5288
144.1165
137.6044
132.2650
128.7840
128.6991
127.7647
127.3643
126.0294
119.0978
117.6580
117.3053
116.6378
93.6695
57.4567
40.2086
39.9989
39.7891
28.6718
21.3111
X : parts per Million : 13C

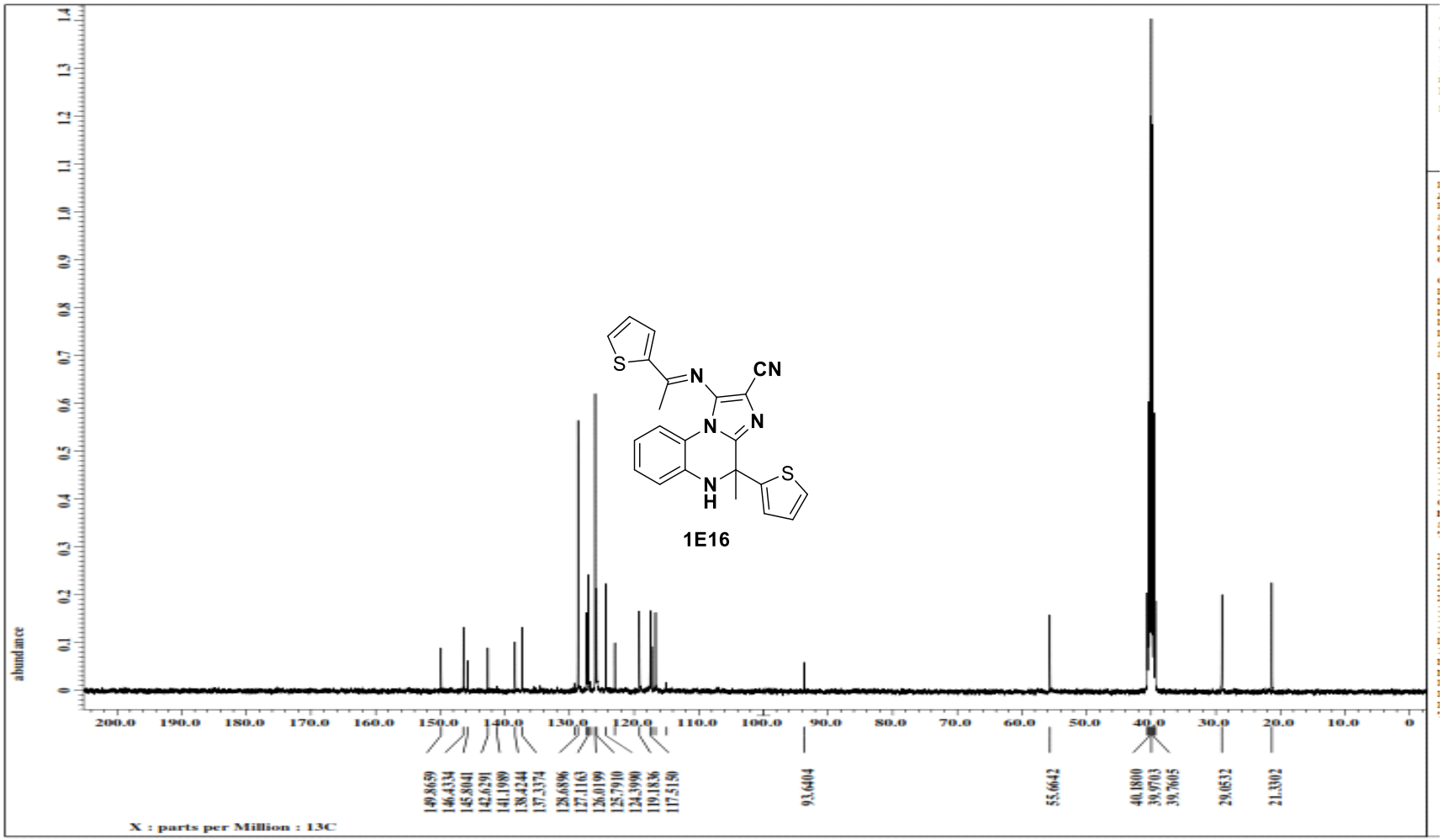
HRMS


6.81e4
100
%
0
336.0695
68053
M+ 1 -C8H9Cl
338.0905
40155
M+ 2 -C8H9Cl
358.0716
35899
427.1350
14102
360.0837
11195
369.1143
7644
429.1406
3238
376.0905
3949
284.0298
4751
202.1835
2788
275.0316
3122
102.1392
2227
200.0974;325
452.0917;902
523.6285
3284
578.0953
1490
693.1739
5667
691.1749
3182
695.1758
2878
746.1089
91
793.0302
90
858.7217
1099
881.1612
258
932.1213
36
Cl
CN
N
N
N
H
Cl
1E15
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

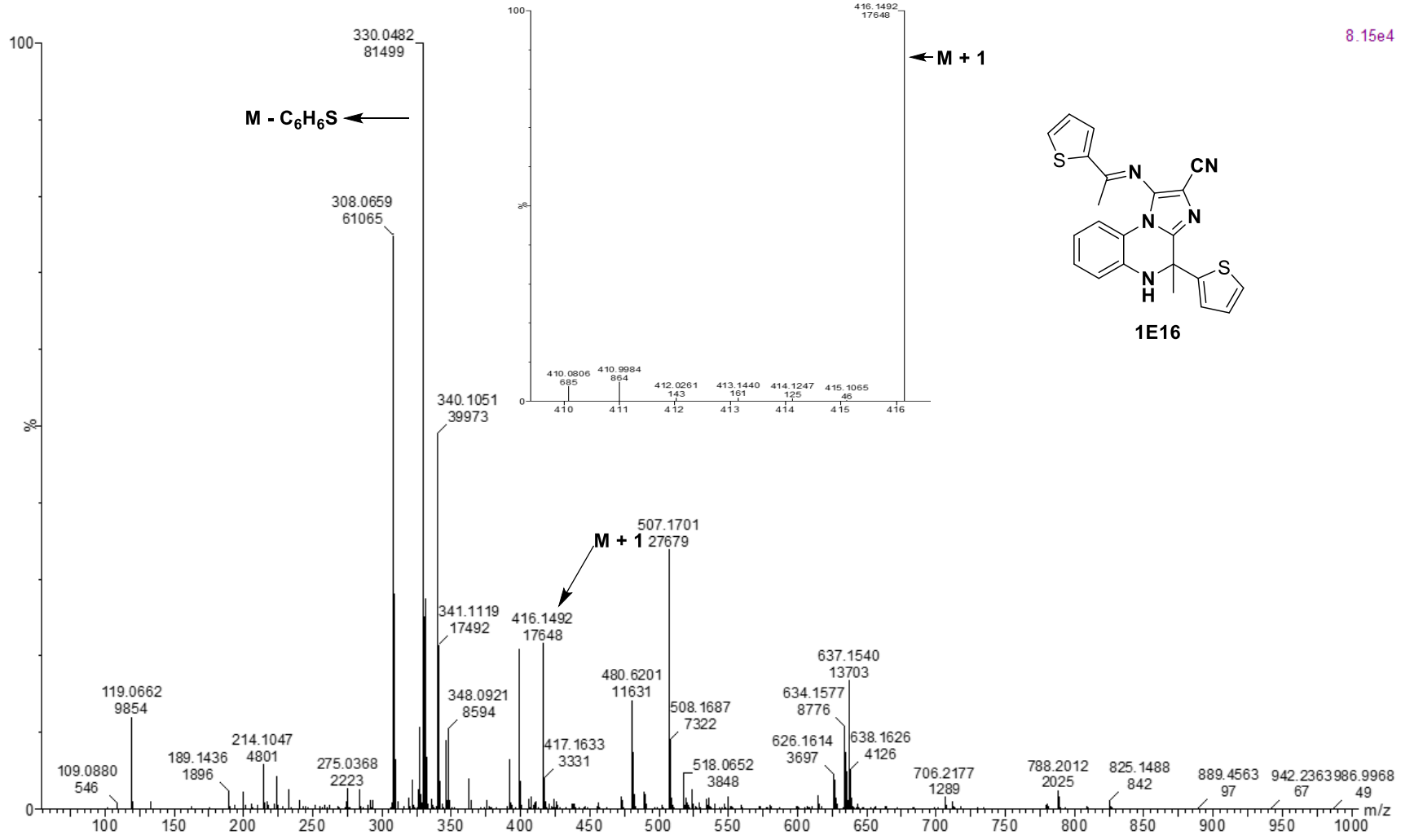
^{1}H NMR


Z:\\RK-12_CUPB
Z:\\RK-12 CUPB
7.69
7.07
7.04
6.97
6.78
6.77
6.76
6.74
6.71
6.71
6.68
2.45
2.24
1.85
S
N
CN
N
N
N
H
S
1E16
1.00
0.51
1.27
0.40
1.32
1.44
1.19
f1 (ppm)

^{13}C NMR


abundance
1E16
149.8659
146.4334
145.8041
142.6291
141.1989
138.4244
137.3374
128.6896
127.1163
126.0199
125.7910
124.3990
119.1836
117.5150
93.6404
55.6642
40.1800
39.9703
39.7605
29.0832
21.3302
X : parts per Million : 13C

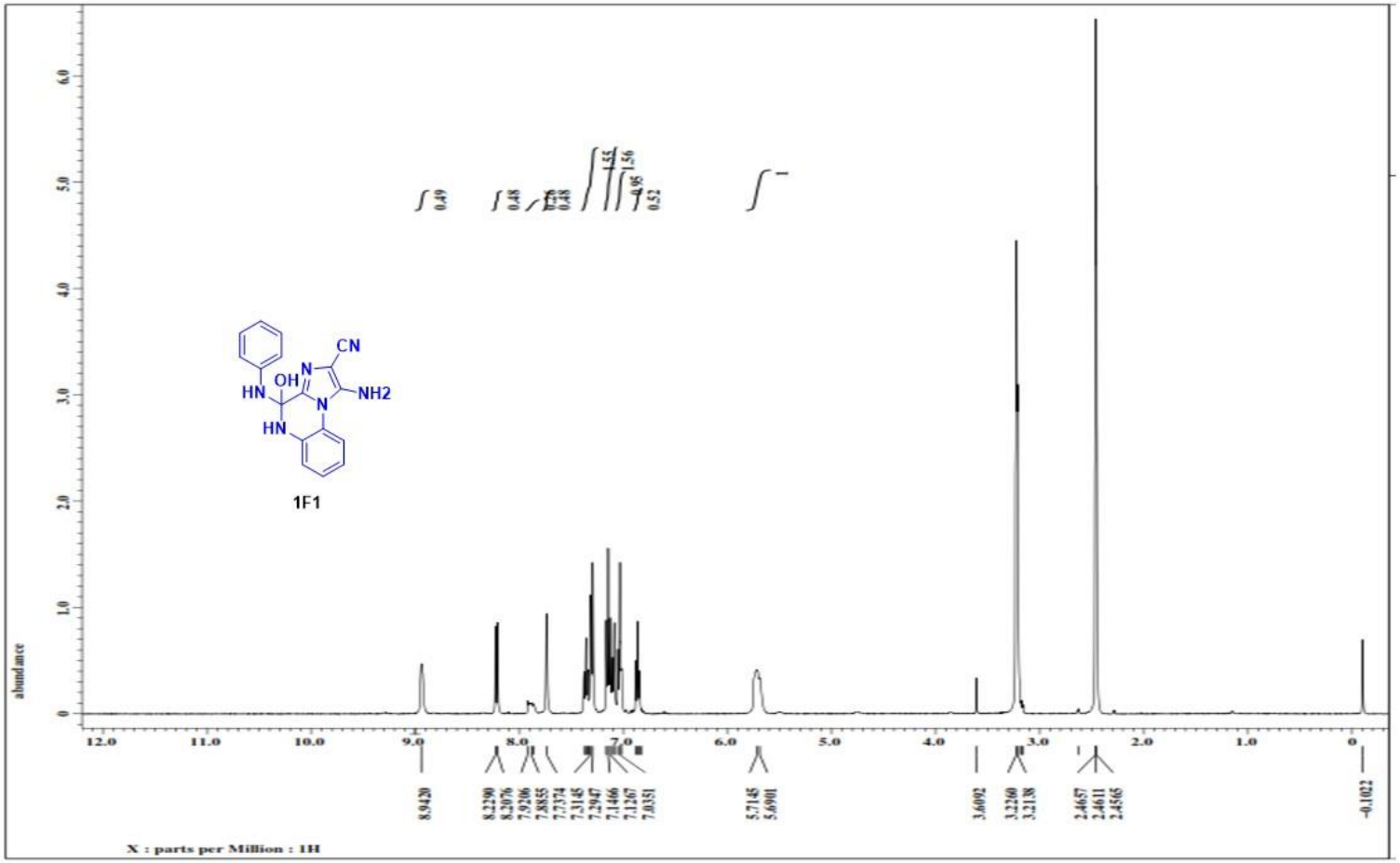
HRMS


M - C6H6S
M + 1
M + 1
330.0482
81499
308.0659
61065
340.1051
39973
341.1119
17492
416.1492
17648
507.1701
27679
480.6201
11631
637.1540
13703
634.1577
8776
638.1626
4126
626.1614
3697
508.1687
7322
348.0921
8594
417.1633
3331
518.0652
3848
214.1047
4801
189.1436
1896
119.0662
9854
109.0880
546
275.0368
2223
706.2177
1289
788.2012
2025
825.1488
842
889.4563
97
942.2363
67
986.9968
49
416.1492
17648
410.0806
685
410.9984
864
412.0261
143
413.1440
161
414.1247
125
415.1065
46
8.15e4
m/z
%

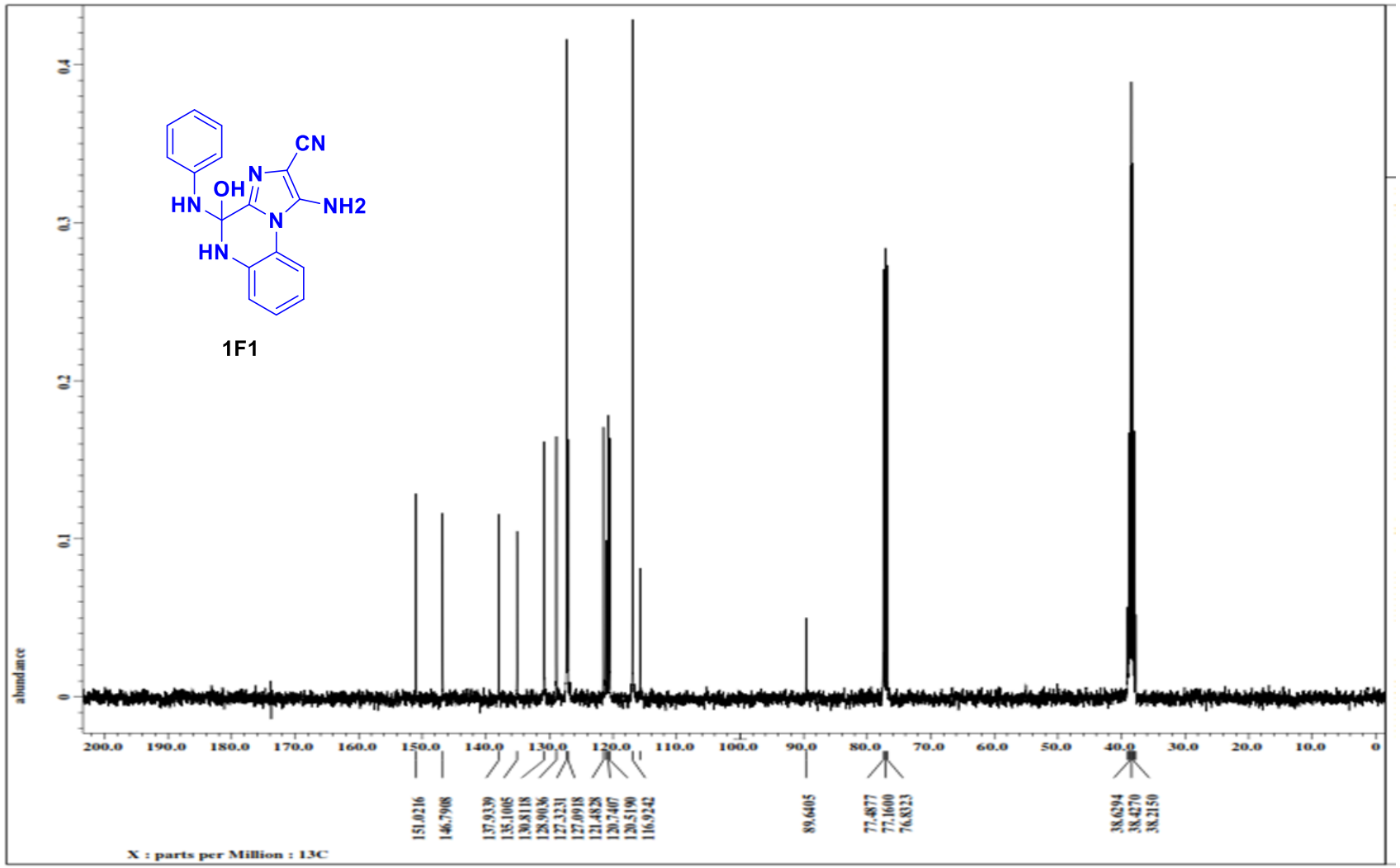
S
N
CN
N
N
N
H
S

1E16

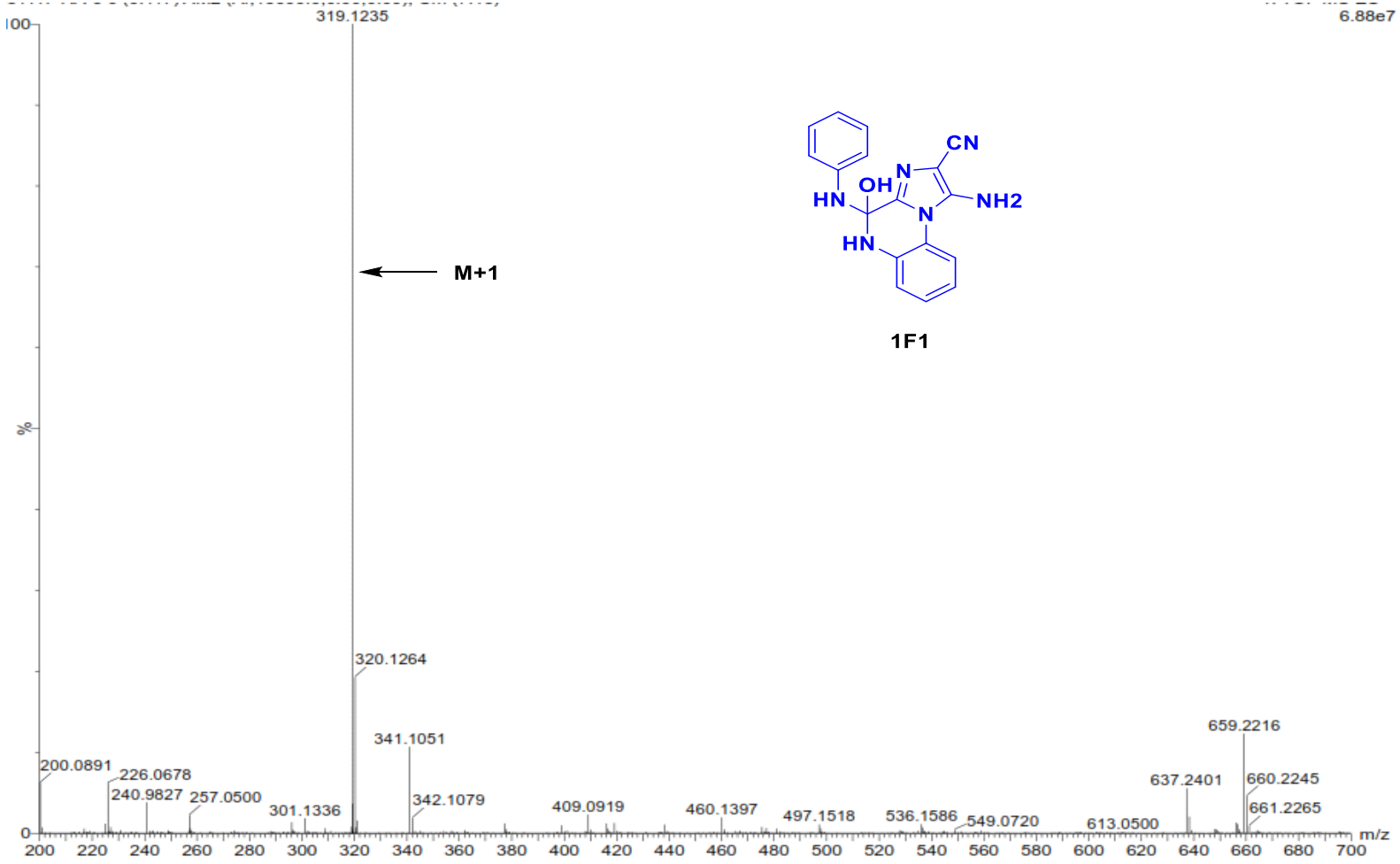
^{1}H NMR



^{13}C NMR


CN
N
OH
HN
NH2
N
HN
1F1
abundance
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
151.0216
146.7908
137.9339
135.1005
130.8118
128.9036
127.3231
127.0918
121.4828
120.7407
120.5190
116.9242
89.6405
77.4877
77.1600
76.8323
38.6294
38.4270
38.2150
X : parts per Million : 13C

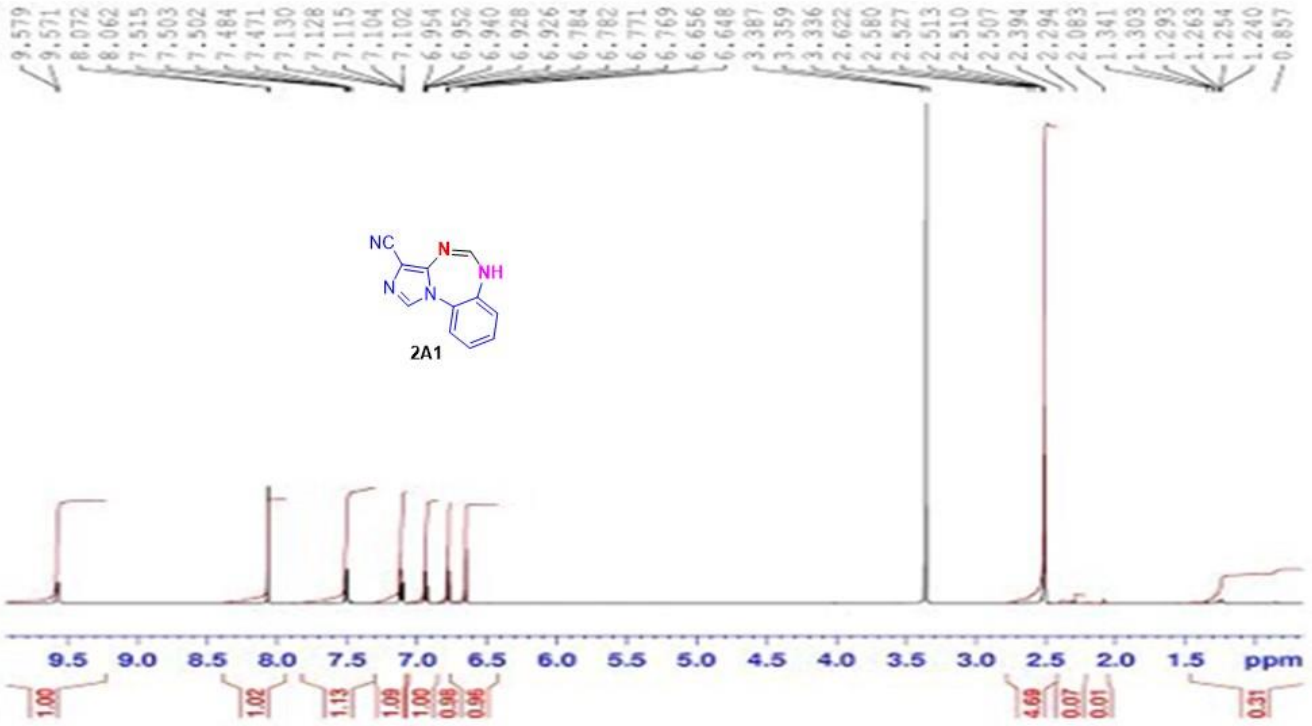
HRMS


319.1235
6.88e7
100
%
0
M+1
320.1264
341.1051
342.1079
200.0891
226.0678
240.9827
257.0500
301.1336
409.0919
460.1397
497.1518
536.1586
549.0720
613.0500
637.2401
659.2216
660.2245
661.2265
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
m/z

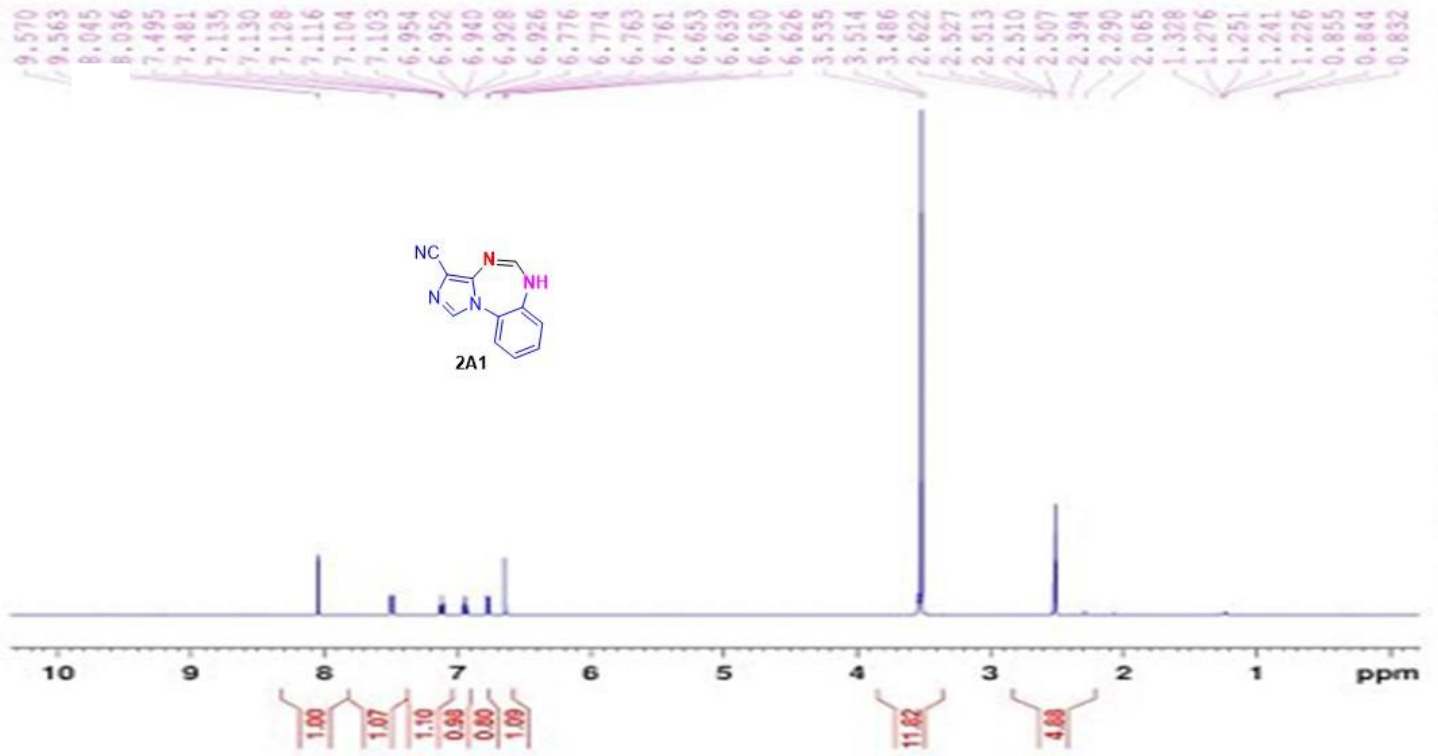
CN
N
OH
HN
NH2
N
HN

1F1

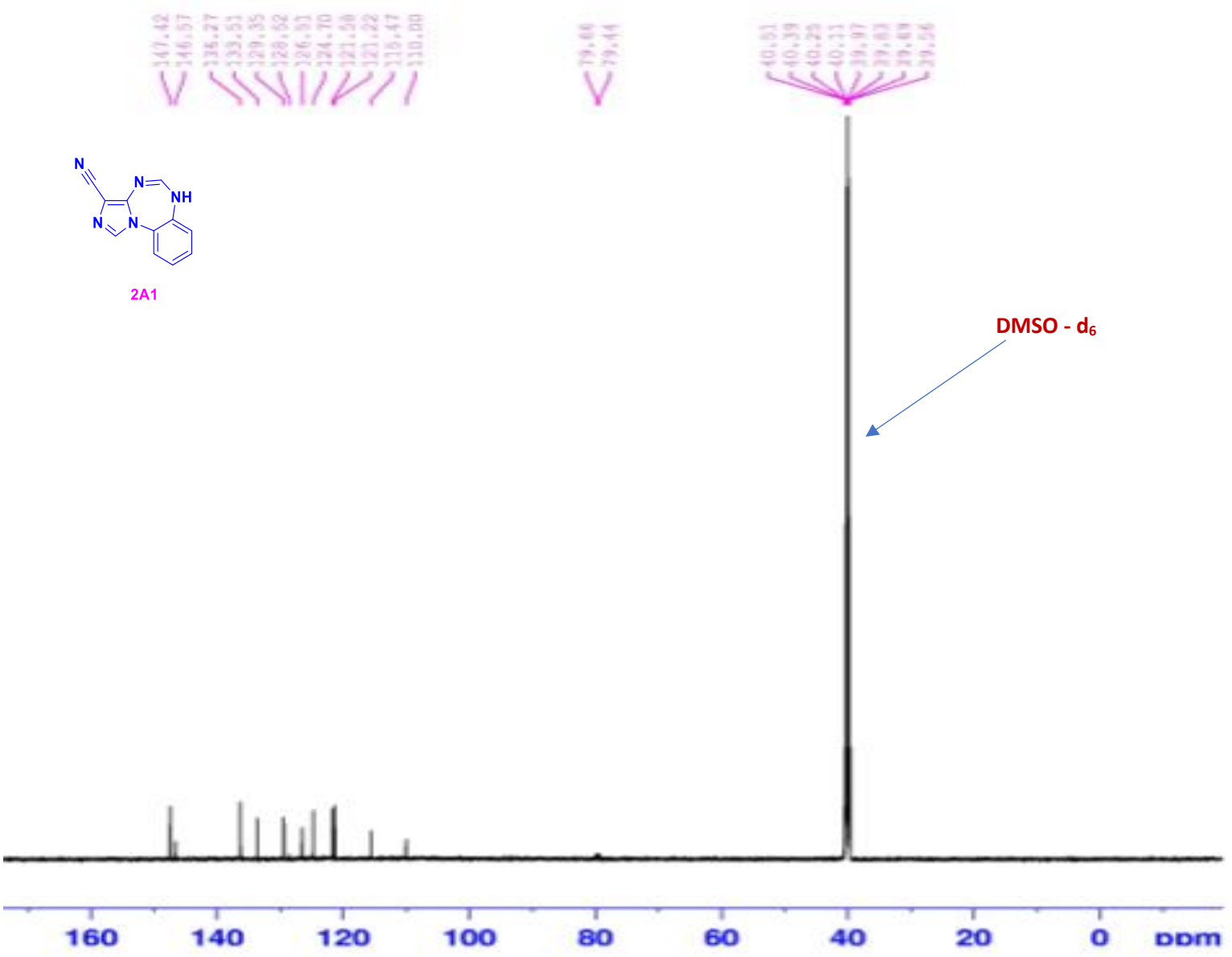
^{1}H NMR


9.579
9.571
8.072
8.062
7.515
7.503
7.502
7.484
7.471
7.130
7.128
7.115
7.104
7.102
6.954
6.952
6.940
6.928
6.926
6.784
6.782
6.771
6.769
6.656
6.648
3.387
3.359
3.336
2.622
2.580
2.527
2.513
2.510
2.507
2.394
2.294
2.083
1.341
1.303
1.293
1.263
1.254
1.240
0.857
NC
N
NH
N
N
2A1
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.00
1.02
1.13
1.09
1.00
0.98
0.96
4.69
0.07
0.01
0.31

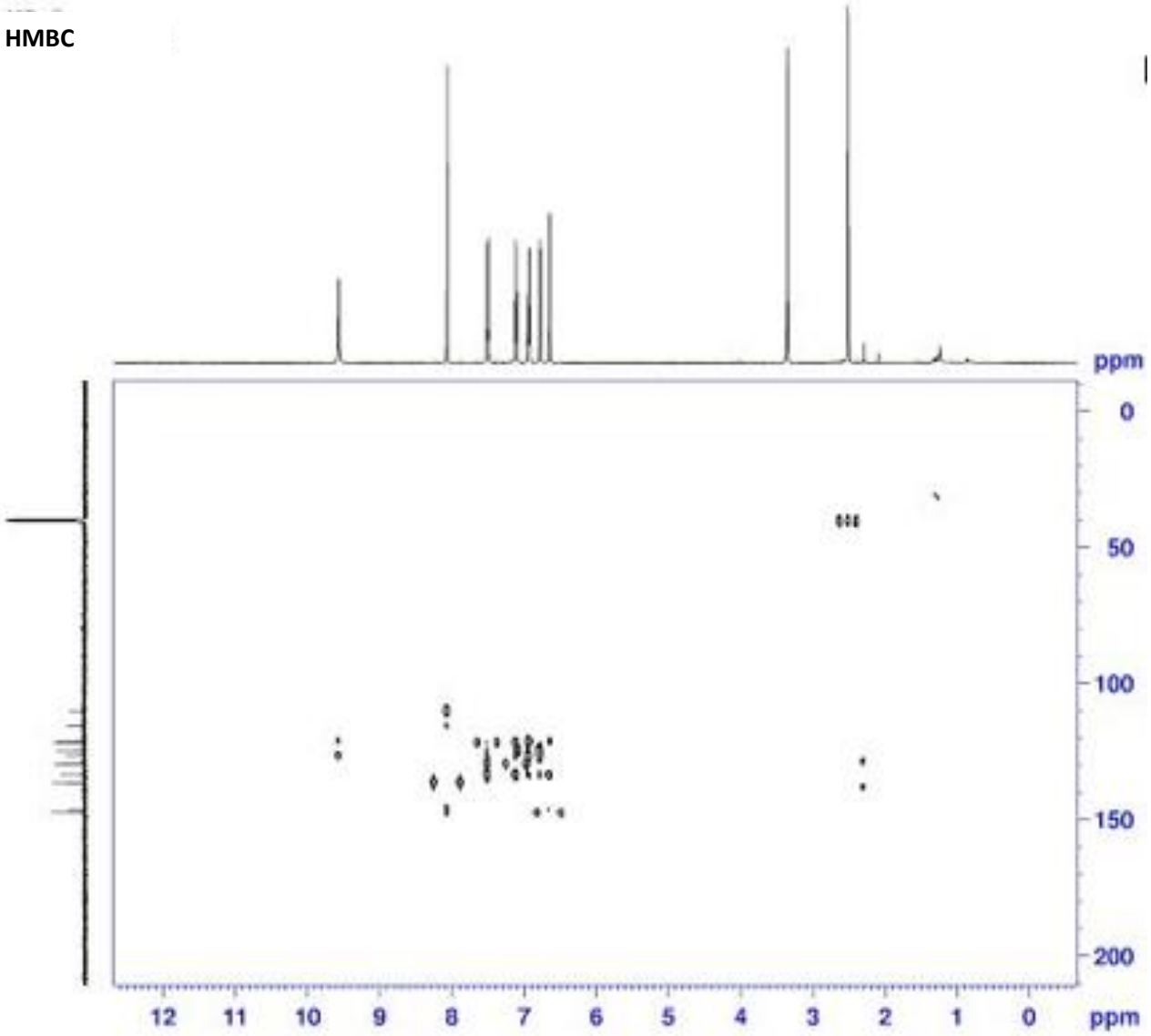
D_20 Experiment

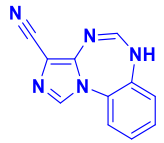


^{13}C NMR

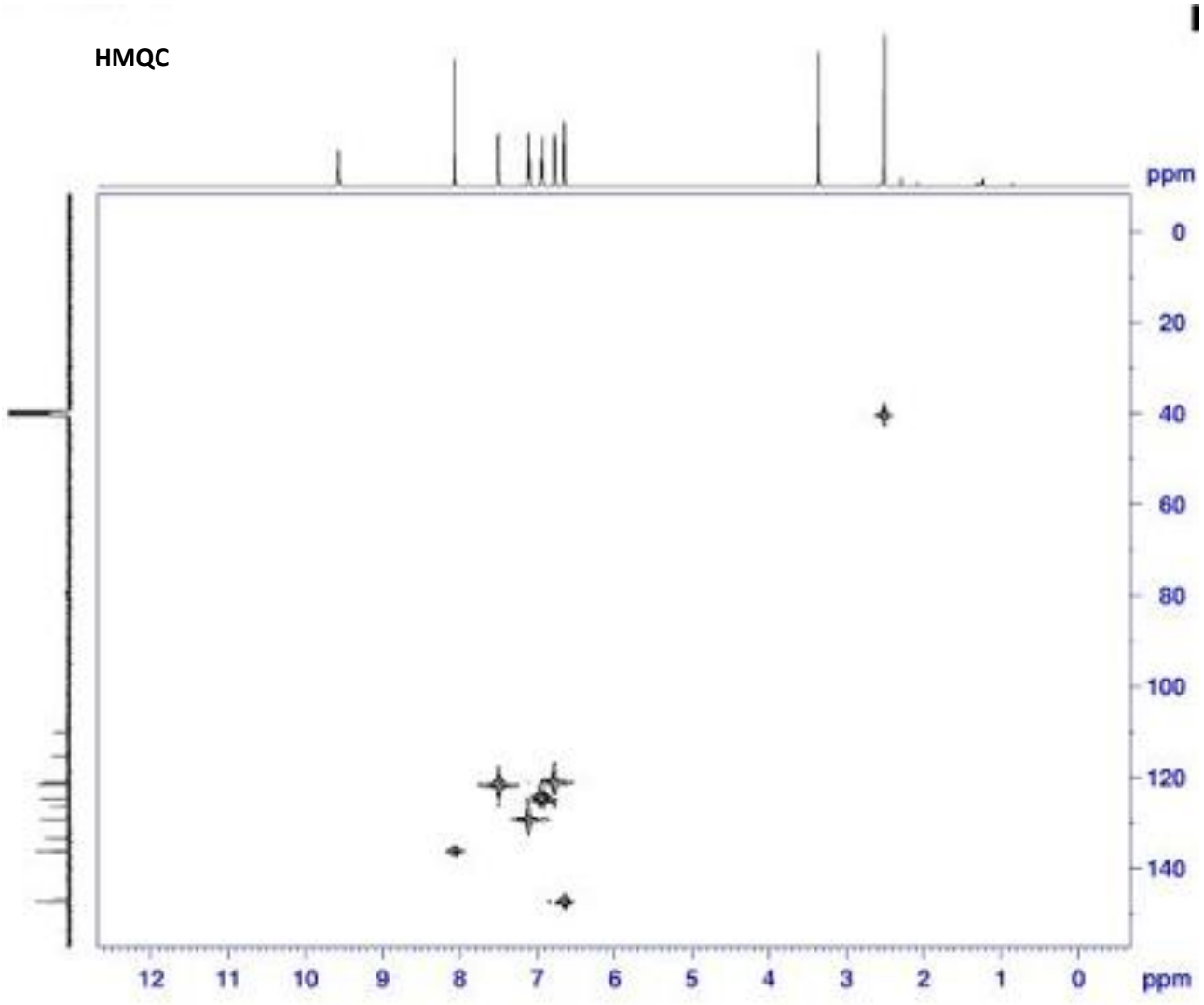

147.42
146.57
136.27
133.51
129.35
128.52
126.51
124.70
121.50
121.22
116.47
110.08
29.46
29.44
40.51
40.39
40.28
40.11
39.97
39.83
39.69
39.54
N
N
NH
N
N
2A1
DMSO - d6
160
140
120
100
80
60
40
20
0
ppm

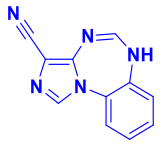
HMBC





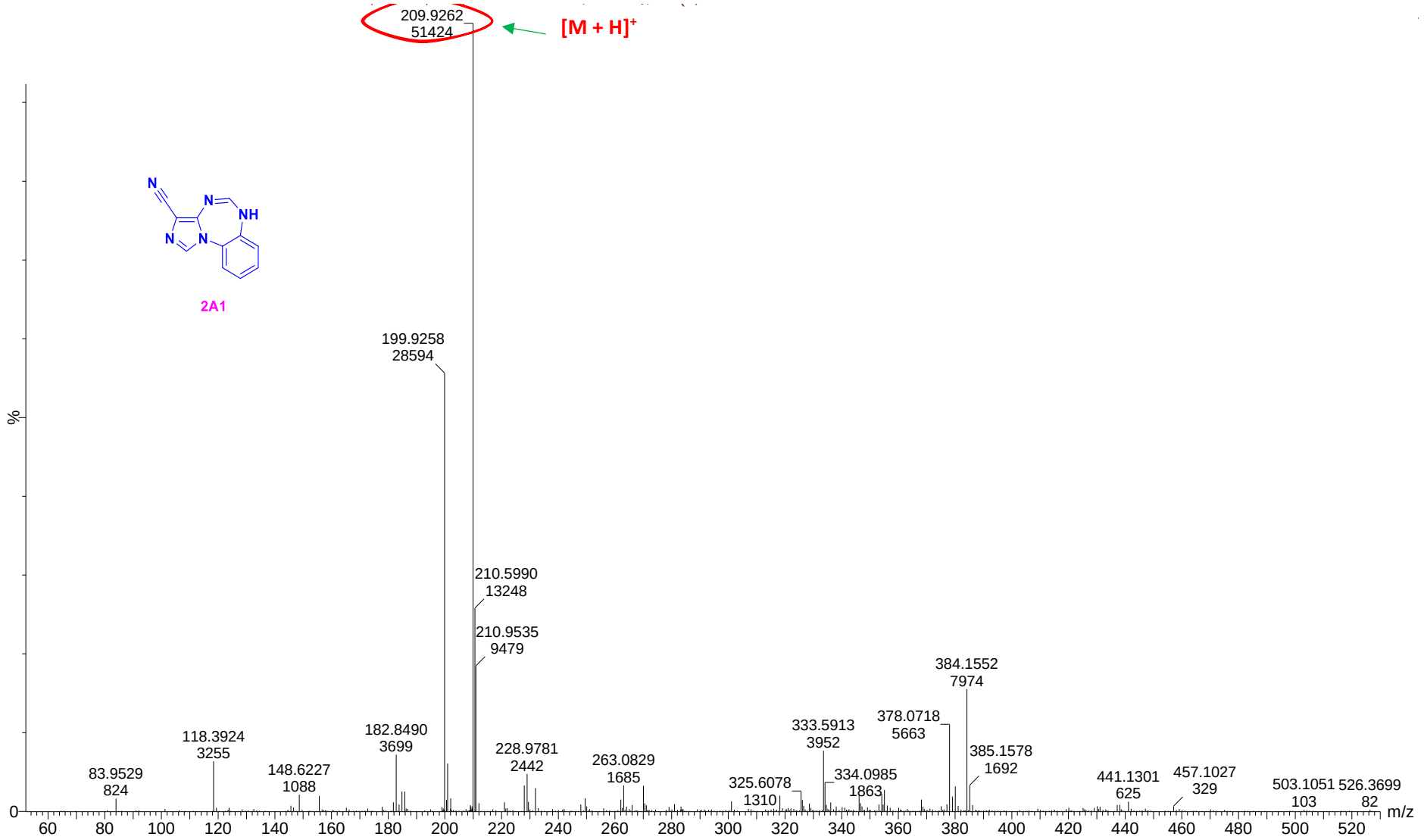
2A1

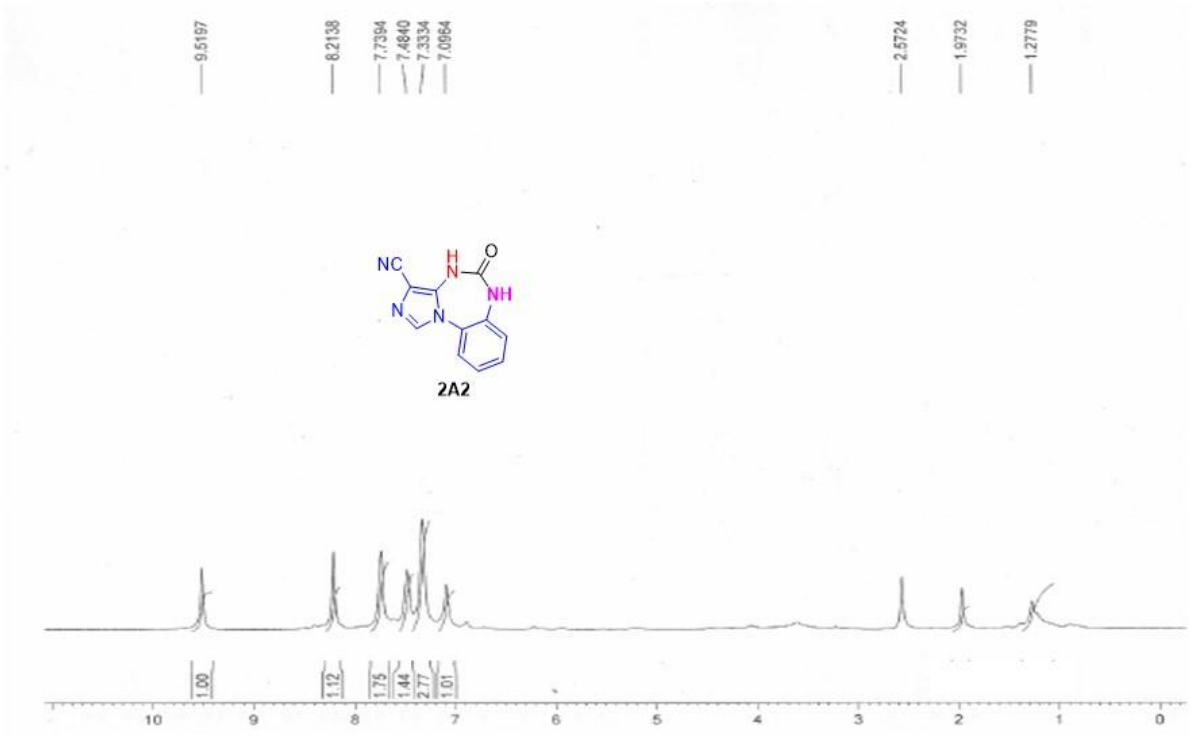

HMQC
ppm
0
20
40
60
80
100
120
140
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


N
N
NH
N
N

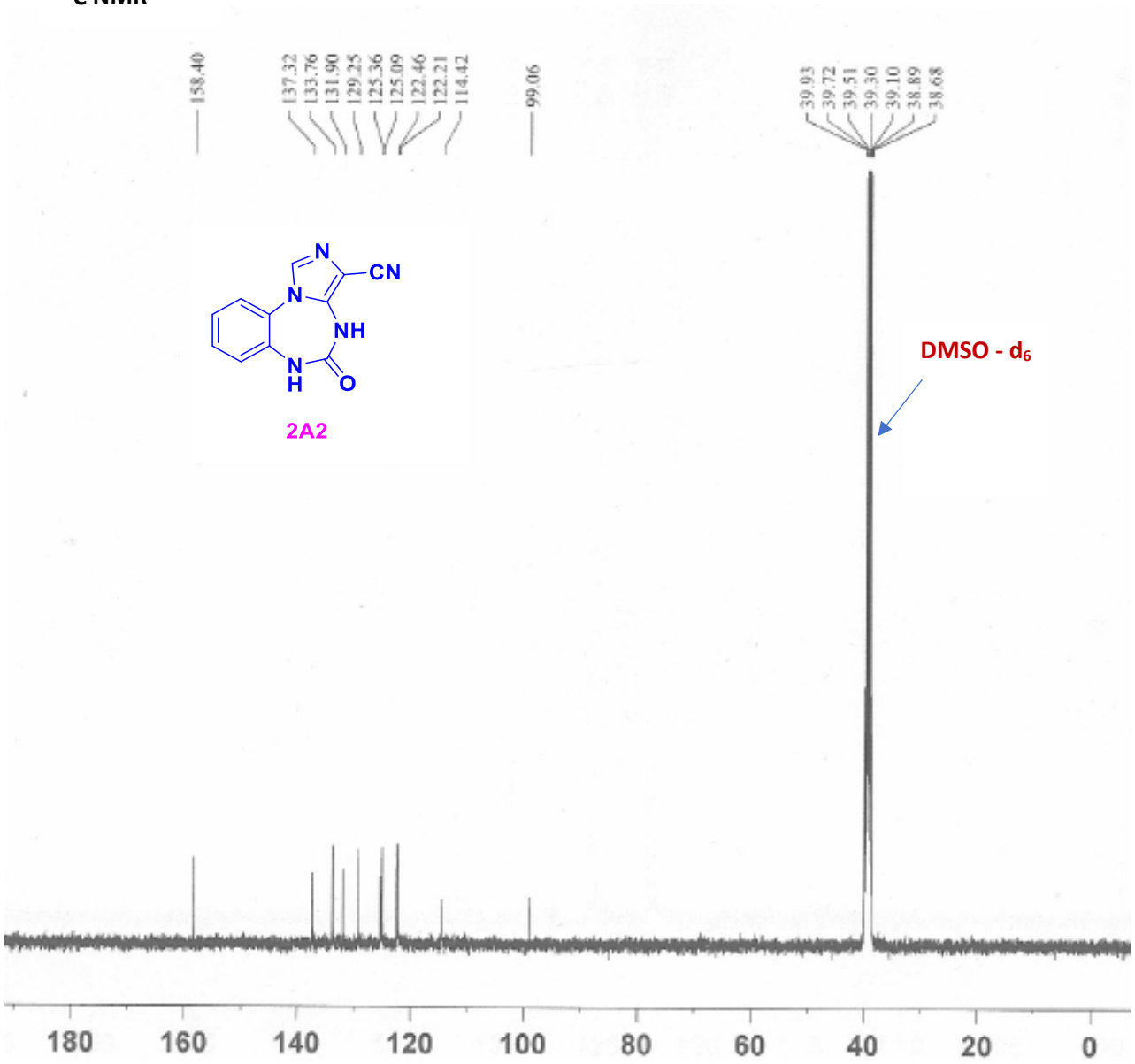
2A1

HRMS

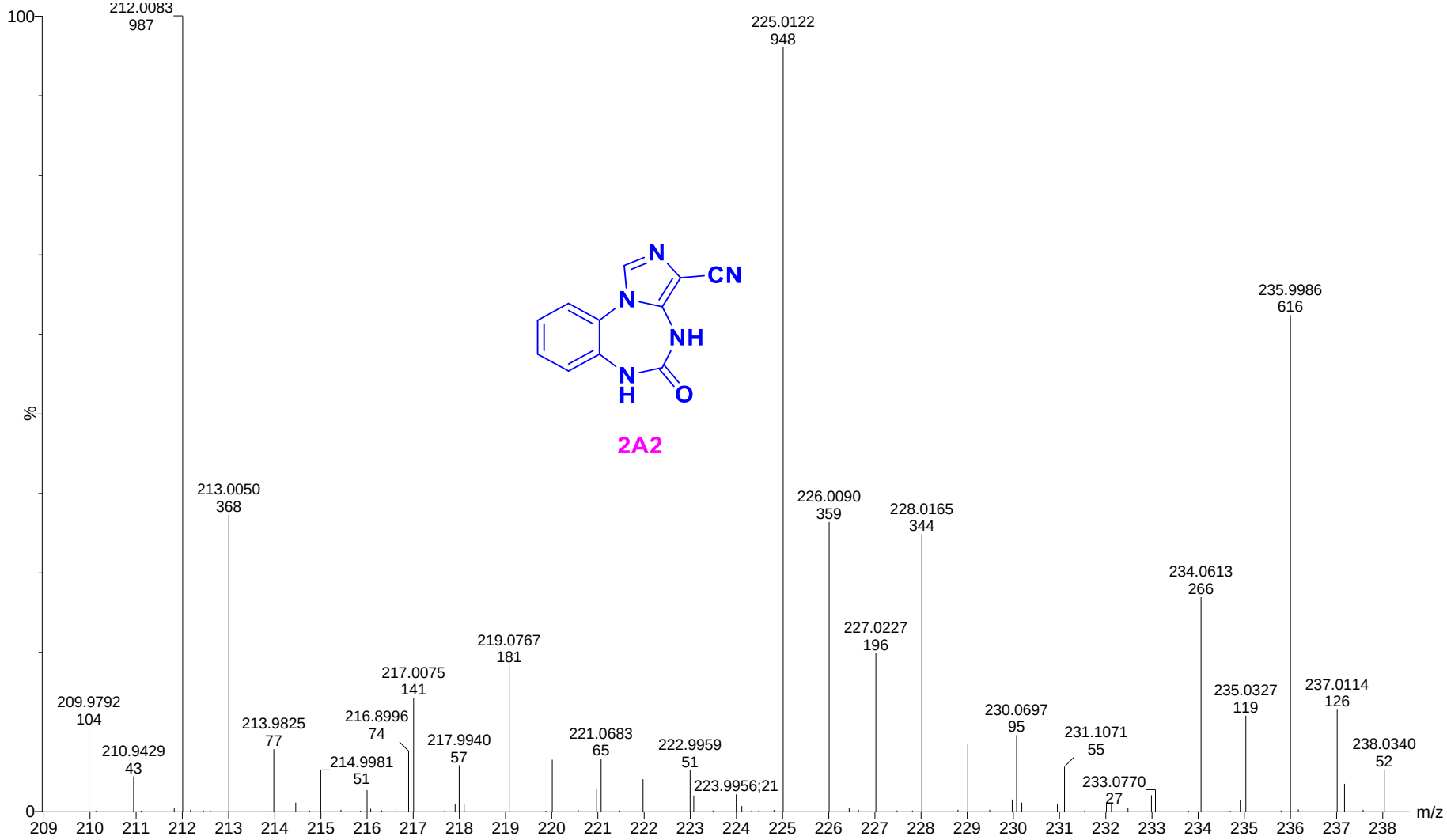

209.9262
51424
[M + H]+
199.9258
28594
210.5990
13248
210.9535
9479
384.1552
7974
378.0718
5663
333.5913
3952
385.1578
1692
334.0985
1863
118.3924
3255
182.8490
3699
228.9781
2442
263.0829
1685
148.6227
1088
83.9529
824
325.6078
1310
441.1301
625
457.1027
329
503.1051
103
526.3699
82
%
0
m/z
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
2A1


9.5197
8.2138
7.7394
7.4840
7.3334
7.0964
2.5724
1.9732
1.2779
NC
H
N
O
NH
N
N
2A2
1.00
1.12
1.75
1.44
2.77
1.01
10
9
8
7
6
5
4
3
2
1
0

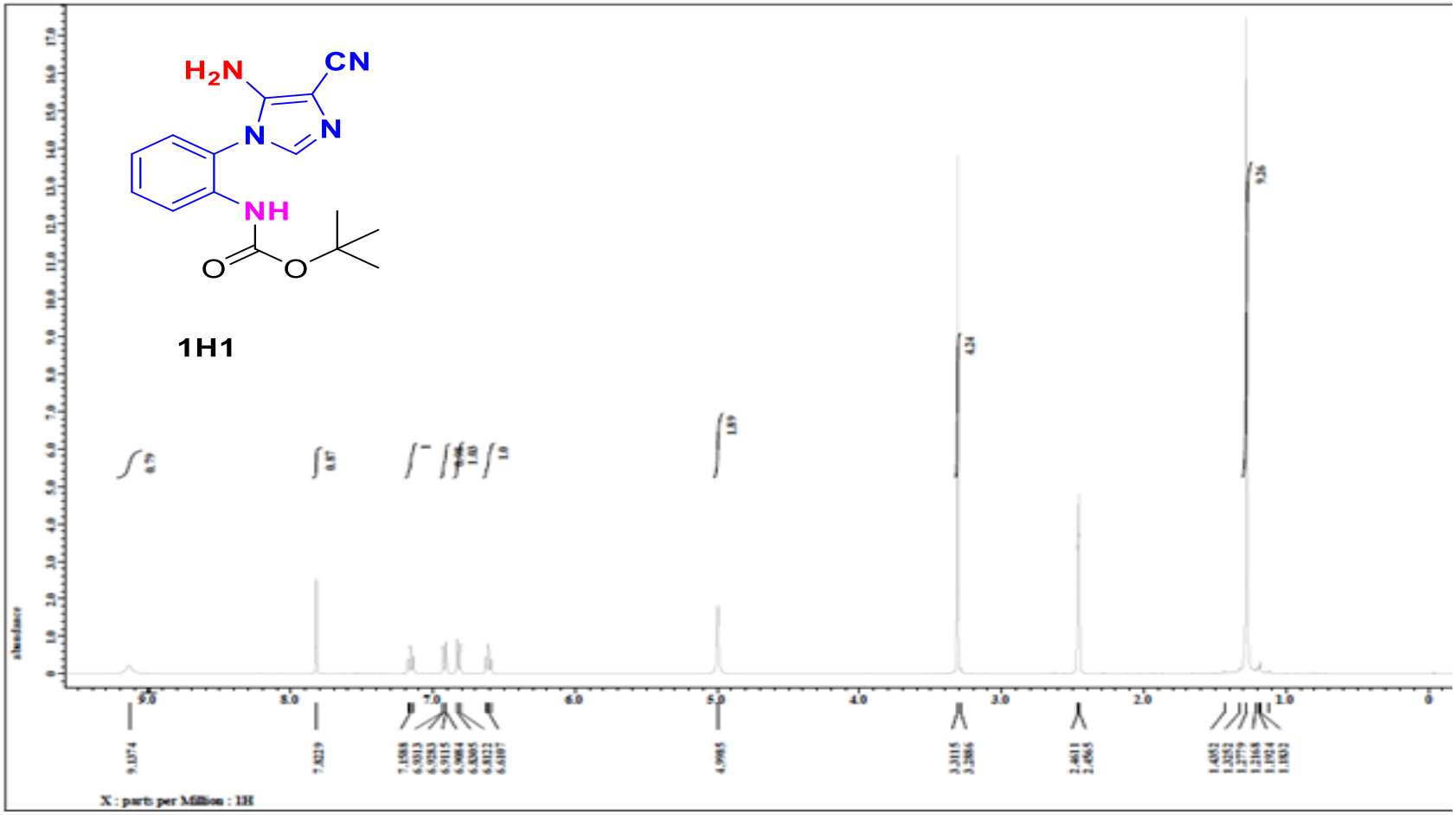
^{13}C NMR


158.40
137.32
133.76
131.90
129.25
125.36
125.09
122.46
122.21
114.42
99.06
39.93
39.72
39.51
39.30
39.10
38.89
38.68
N
CN
N
NH
N
H
O
2A2
DMSO - d6
180
160
140
120
100
80
60
40
20
0

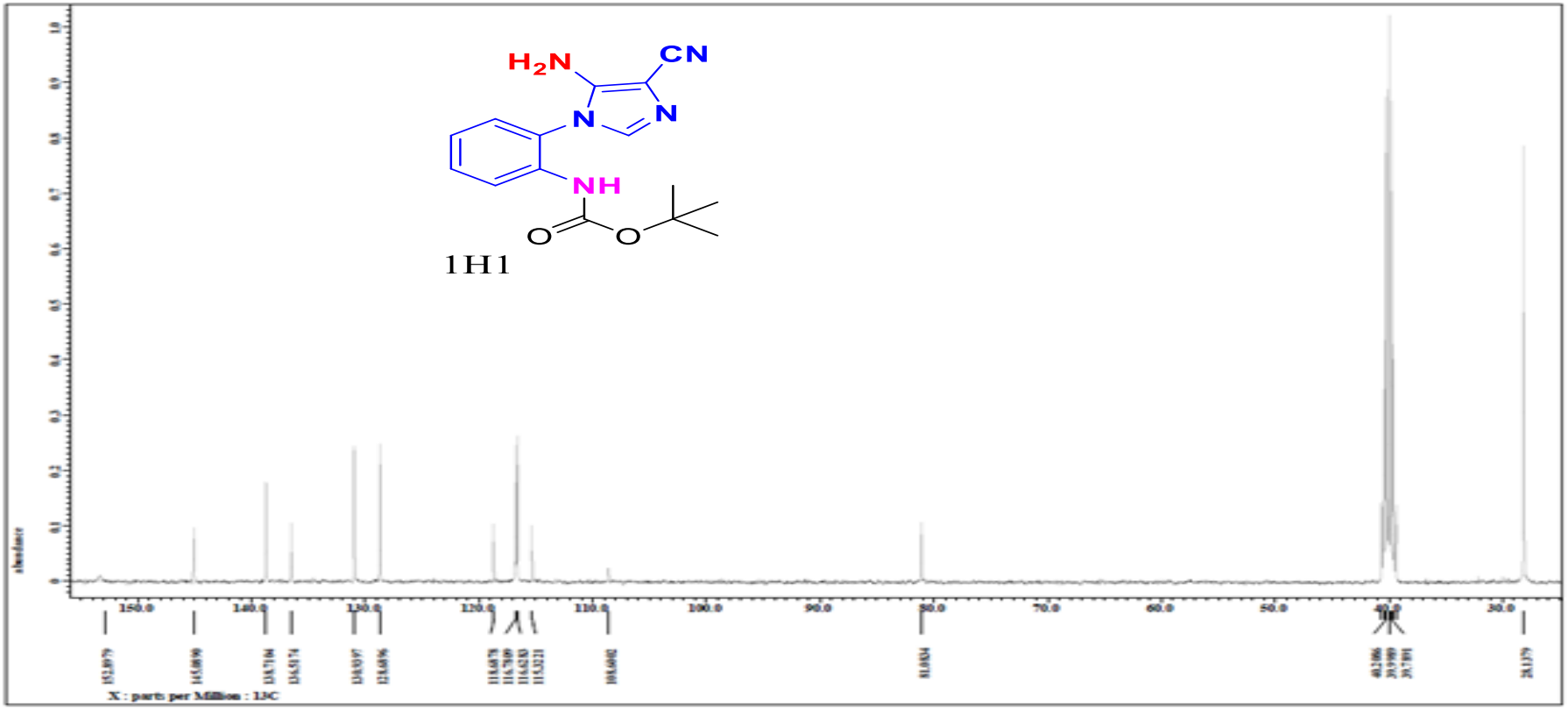
HRMS


212.0083
987
225.0122
948
235.9986
616
213.0050
368
226.0090
359
228.0165
344
234.0613
266
227.0227
196
219.0767
181
217.0075
141
235.0327
119
237.0114
126
209.9792
104
230.0697
95
216.8996
74
213.9825
77
231.1071
55
217.9940
57
238.0340
52
210.9429
43
221.0683
65
222.9959
51
214.9981
51
233.0770
27
223.9956;21
100
%
0
m/z
209
210
211
212
213
214
215
216
217
218
219
220
221
222
223
224
225
226
227
228
229
230
231
232
233
234
235
236
237
238
N
CN
N
NH
N
H
O
2A2

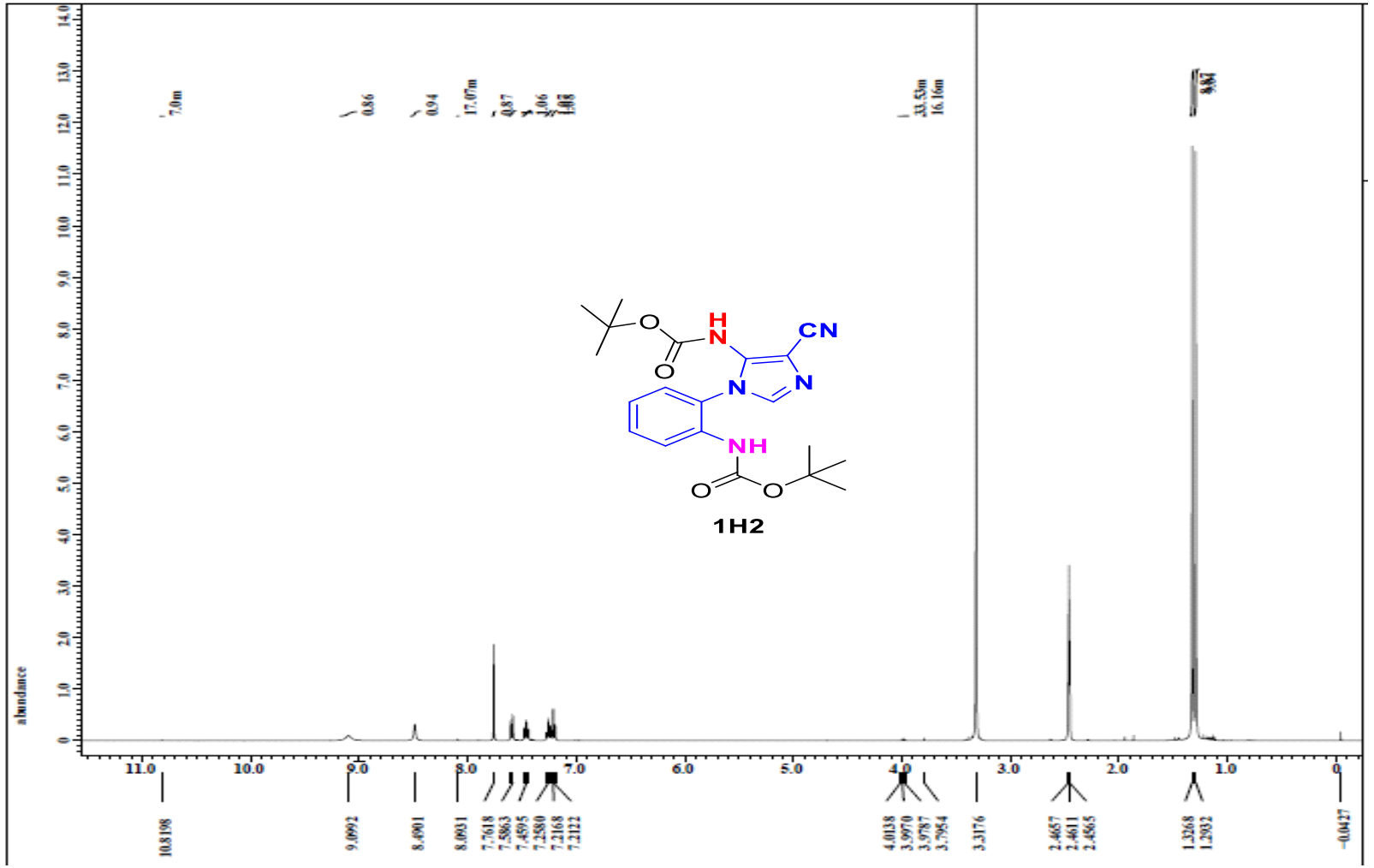
^{1}H NMR



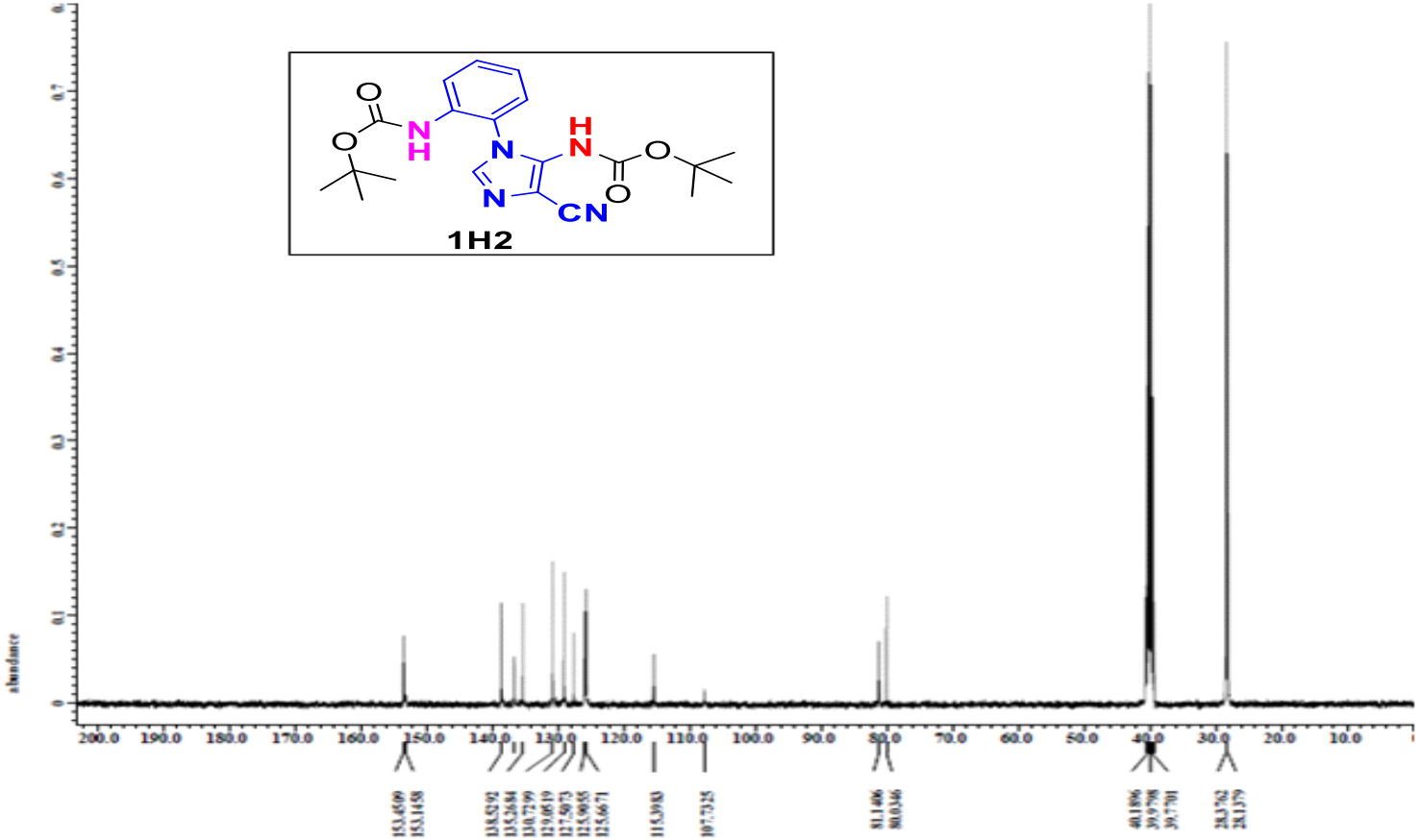
^{13}C NMR



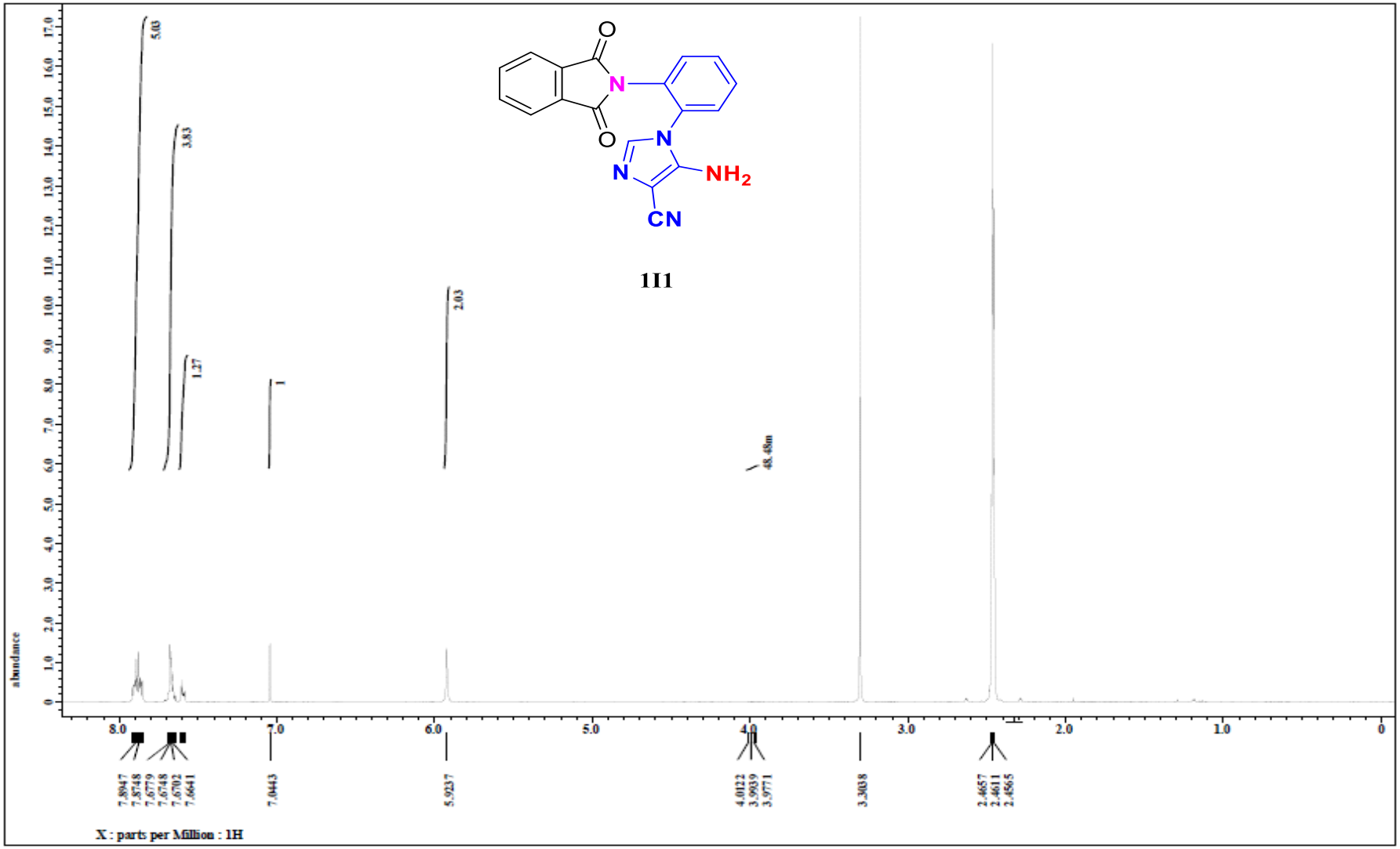
^{1}H NMR


abundance
1H2
CN
NH
10.8198
9.0092
8.4901
8.0031
7.7618
7.5863
7.4595
7.2580
7.2168
7.2122
4.0138
3.9970
3.9787
3.7954
3.3176
2.4657
2.4611
2.4565
1.3268
1.2932
-0.0427

^{13}C NMR

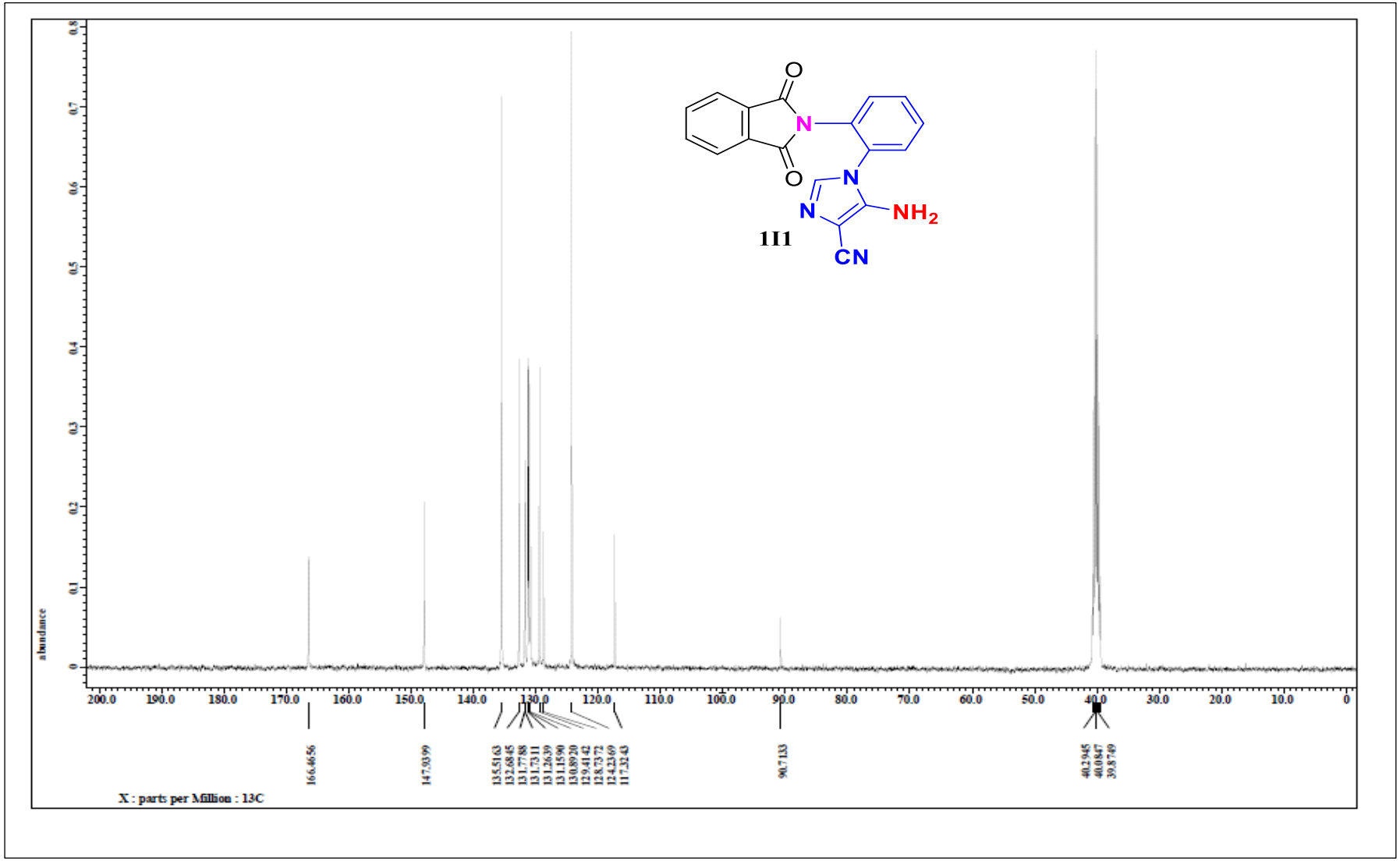

1H2
abundance
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
153.4509
153.1458
138.5192
135.2684
130.7299
129.0619
127.5073
125.9055
125.6671
115.3983
107.7325
81.1406
80.0346
40.1896
39.9798
39.7701
28.3762
28.1379

^{1}H NMR

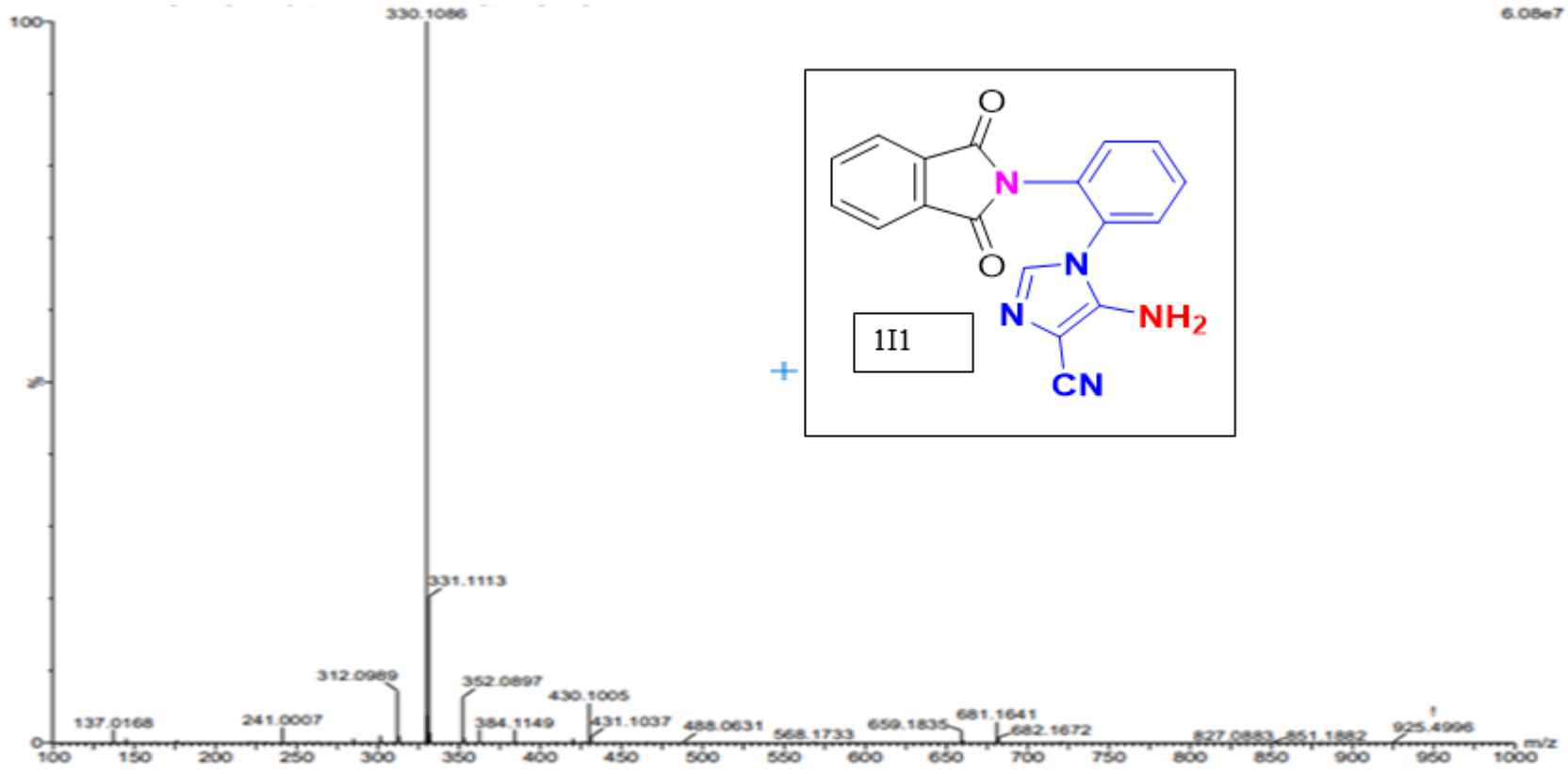

5.03
3.83
1.27
1
2.03
48.48m
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8947
7.8748
7.6779
7.6748
7.6702
7.6641
7.0443
5.9237
4.0122
3.9939
3.9771
3.3038
2.4657
2.4611
2.4565
X : parts per Million : 1H

111

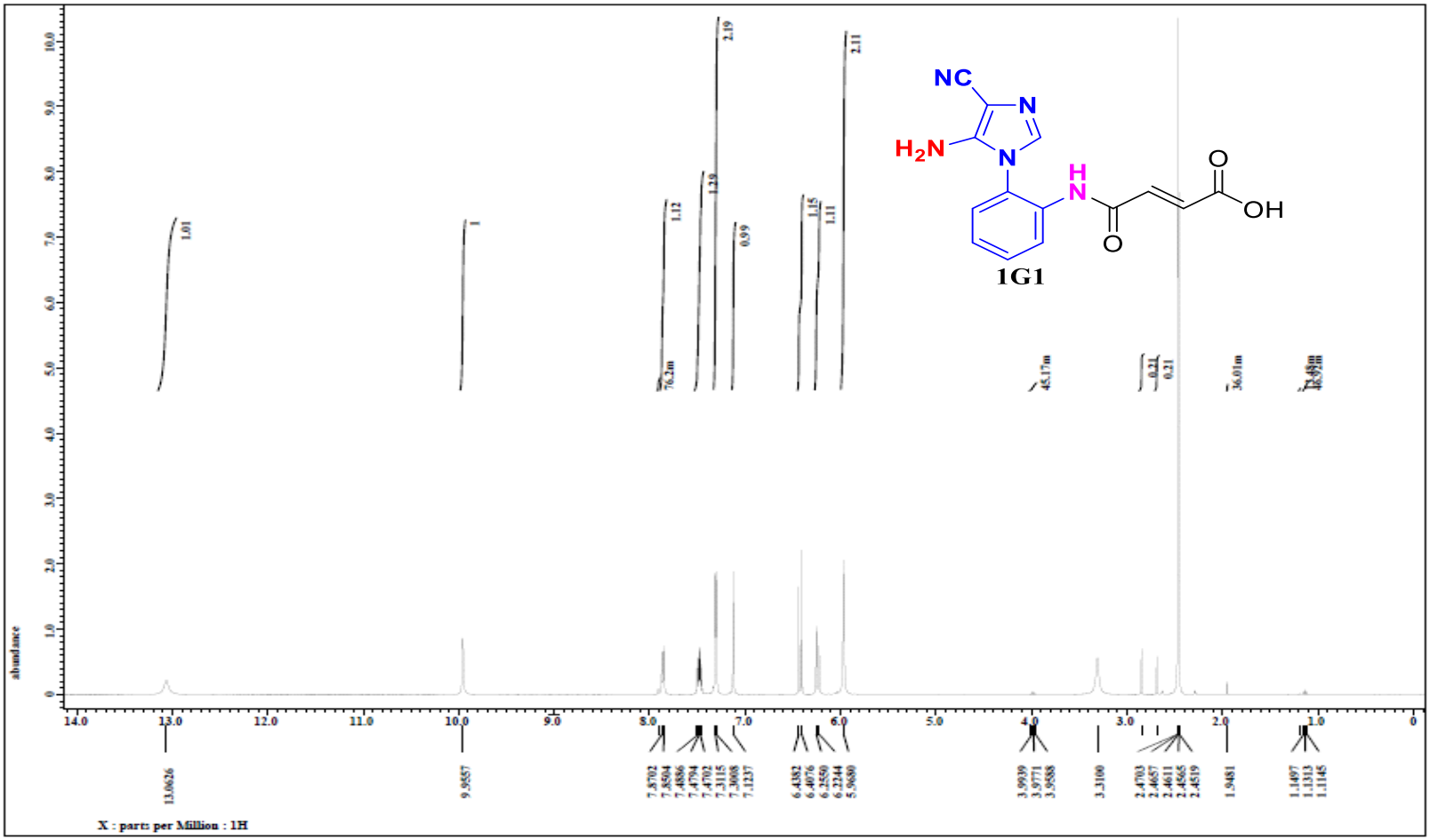
^{13}C NMR


O
N
O
N
N
NH2
CN
111
abundance
X : parts per Million : 13C
166.4656
147.9399
135.5163
132.6845
131.7788
131.7311
131.2639
131.1590
130.8920
129.4142
128.7372
124.2369
117.3243
90.7133
40.2945
40.0847
39.8749

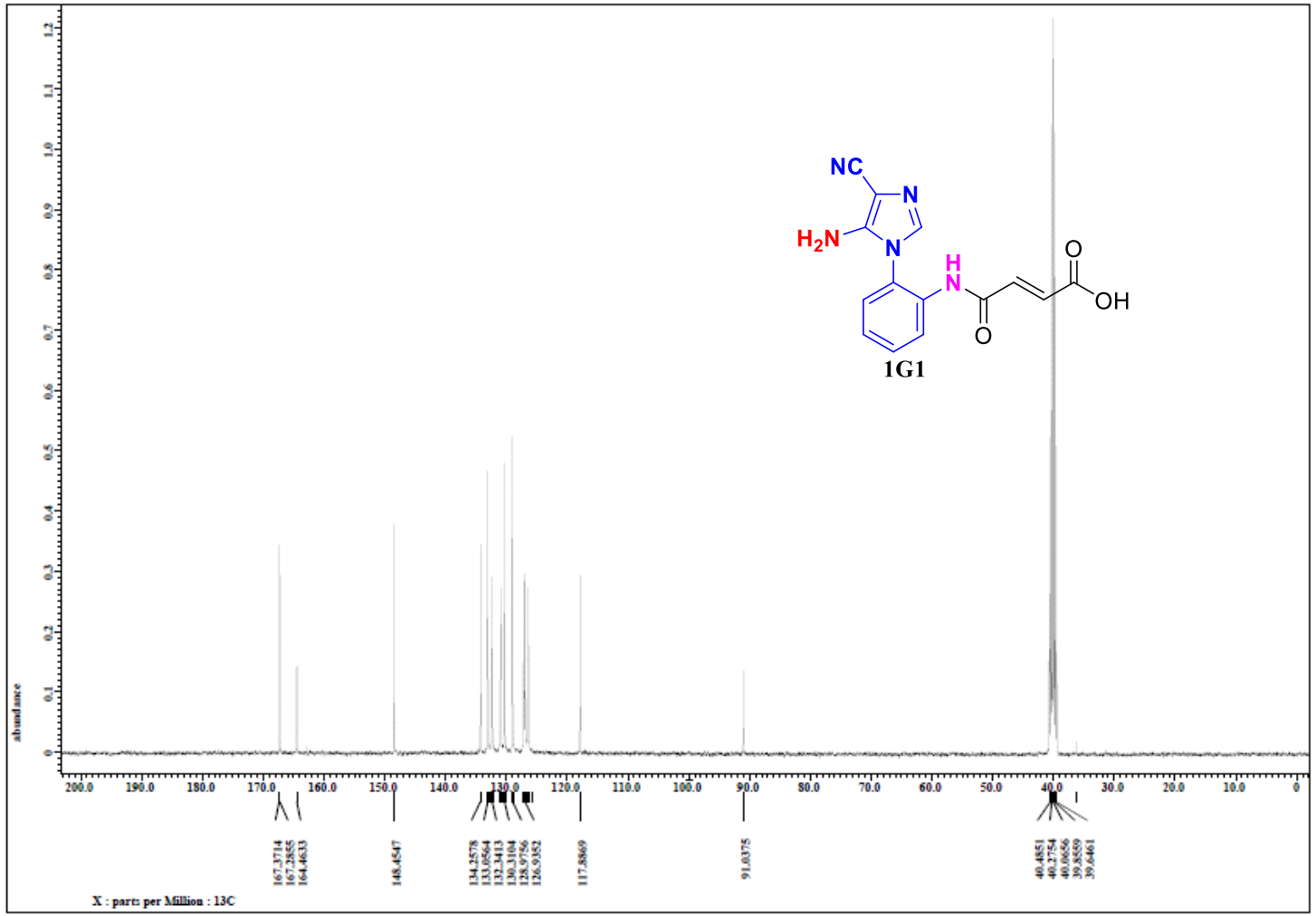
HRMS


330.1086
6.08e7
331.1113
312.0989
352.0897
430.1005
137.0168
241.0007
384.1149
431.1037
488.0631
568.1733
659.1835
681.1641
682.1672
925.4996
m/z
1I1
O
N
O
N
N
NH2
CN

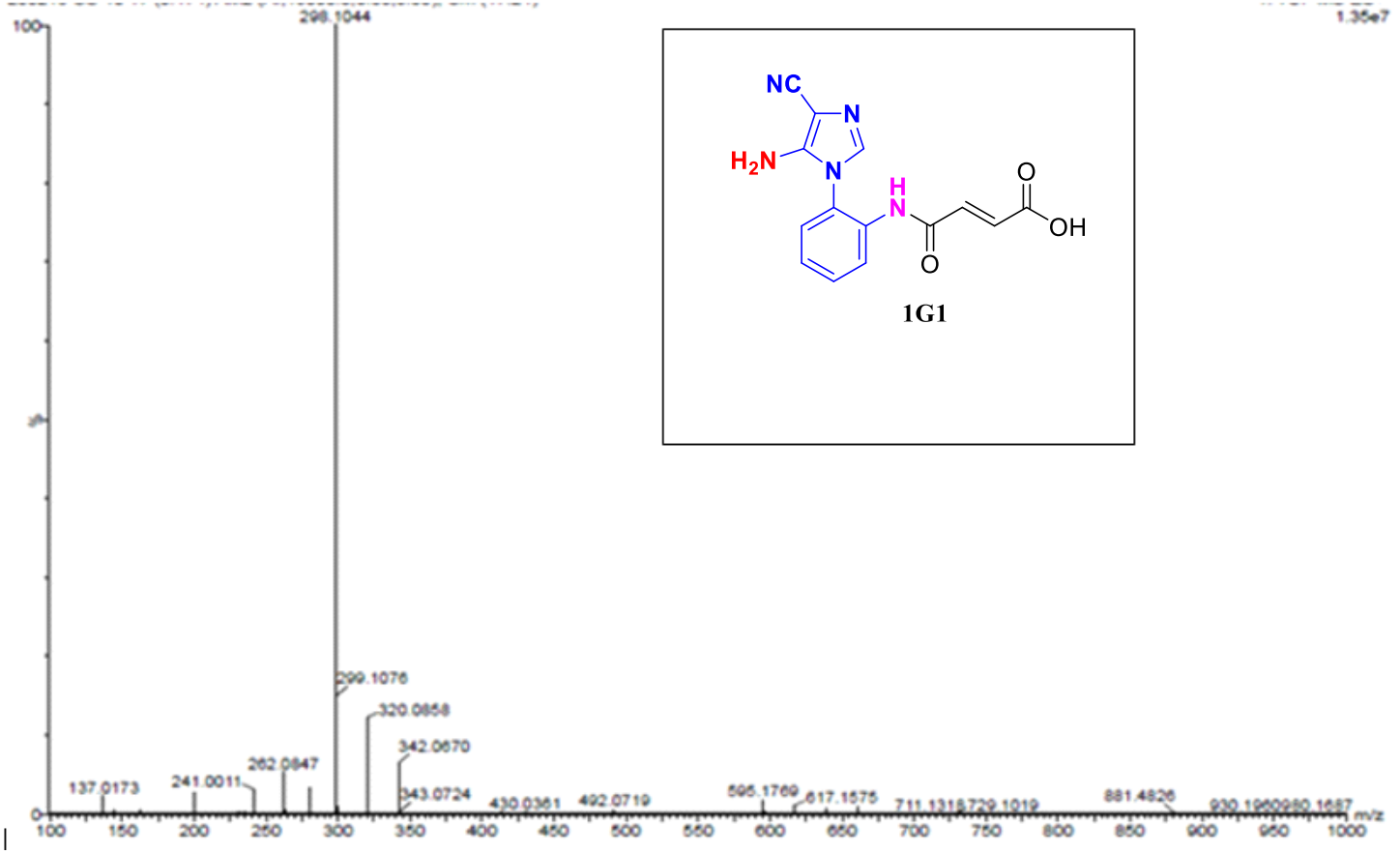
^{1}H NMR



^{13}C NMR



HRMS


298.1044
1.35e7
100
%
0
299.1076
320.0858
342.0670
262.0847
241.0011
137.0173
343.0724
430.0361
492.0719
595.1769
617.1575
711.1318
729.1019
881.4826
930.1960
980.1687
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000

NC
N
H2N
N
H
N
O
OH
O

1G1

6. References

1. R. Kumar, R. K. Ujjinamatada and R. S. Hosmane, *Org. Lett.*, 2008, **10**, 4681-4684.