Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Photocatalyst-, metal- and additive- free, direct C-H arylation of quinoxalin-2(1*H*)-ones with aryl acyl peroxides induced by visible light †

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Supporting Information

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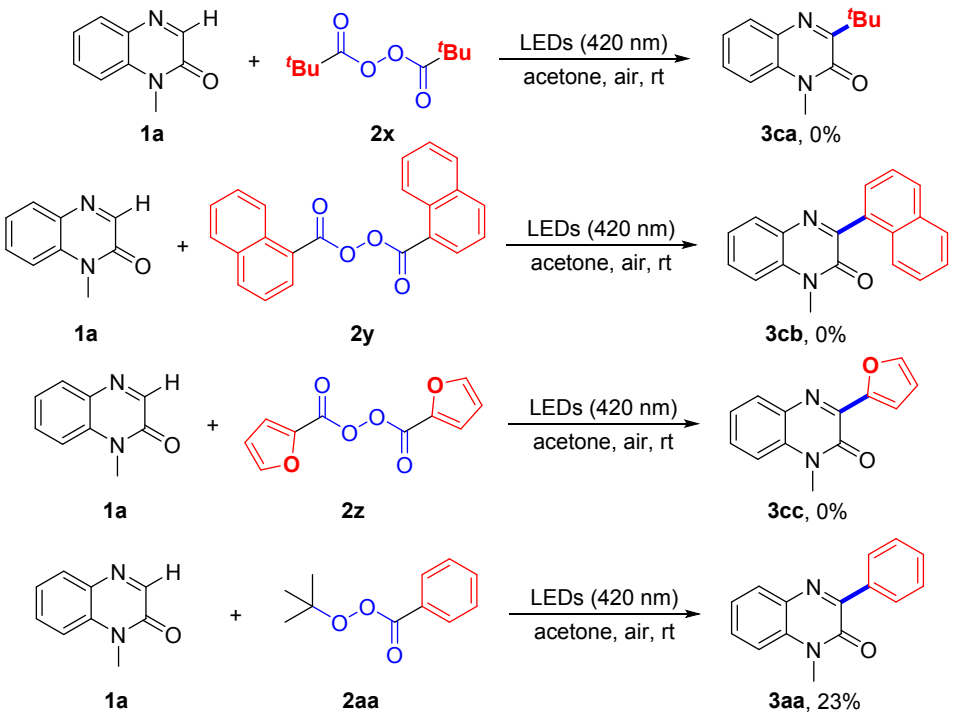
1. Ineffective transformations



2. Fluorescence quenching experiment

The fluorescence quenching experiments were carried out, and the results were shown in Figure 1. In a typical experiment, to a 2.0 mL solution of 1-methyl-3-phenylquinoxalin-2(1*H*)-one (**3aa**) in acetone (2.0×10^{-6} mol/L) was added different amounts of BPO (**2a**). It was found that the emission intensity of 1-methyl-3-phenylquinoxalin-2(1*H*)-one has been decreased along with the increasing of the amount of BPO.

3. Computational details

Geometry optimizations of all stationary points were carried out at the M06-2X[1]/6-311G(d,p) level. Vibrational frequency calculations were performed to identify that each of the species was a local minimum (no imaginary frequencies) or a transition state (one imaginary frequency). To confirm that each transition state connects the desired reactants and products along the reaction path, intrinsic reaction coordinate (IRC) calculations were conducted at the same level of theory. In order to obtain more accurate energies, single point energies were computed at the M06-2X/def2-TZVPP[2] level. The solvent effect of acetone was considered with SMD solvation model.[3] All calculations were performed using the Gaussian 16 C.01 package.[4]

Cartesian coordinates of the optimized structures

A

O	-2.43321200	-1.02213500	-0.00066200
C	-1.70639000	-0.00001000	0.00002800
O	-2.43321100	1.02214100	0.00076400
C	-0.23964800	0.00000100	0.00000200
C	0.44465300	-1.21516900	0.00039000
C	0.44465000	1.21516900	-0.00041100
C	1.83266100	-1.21103400	0.00037900
H	-0.10763500	-2.14842400	0.00073800
C	1.83266100	1.21103300	-0.00045000
H	-0.10763000	2.14842900	-0.00074100
C	2.52234200	0.00000100	-0.00004700
H	2.37739600	-2.14713500	0.00071100
H	2.37739300	2.14713600	-0.00080200
H	3.60628800	0.00000100	-0.00006600

TS_{A-B}

O	2.35326600	1.14239500	0.12358000
C	2.03821200	0.00000000	0.00000000
O	2.35326600	-1.14239500	-0.12358100
C	0.17224700	0.00000000	0.00000000
C	-0.44883400	1.22653600	-0.05050000
C	-0.44883500	-1.22653600	0.05050000
C	-1.84559600	1.20736700	-0.05268500
H	0.10859900	2.15228400	-0.08315500
C	-1.84559600	-1.20736700	0.05268500
H	0.10859900	-2.15228400	0.08315500
C	-2.53538500	0.00000000	0.00000000
H	-2.38392000	2.14733500	-0.09181100
H	-2.38392100	-2.14733400	0.09181100
H	-3.61888400	0.00000000	0.00000000

B

C	0.00000000	1.39583600	0.00000000
C	-1.22265200	0.76868800	0.00015300
C	1.22265200	0.76868800	-0.00015300
C	-1.21077300	-0.63038900	-0.00016000
H	-2.15636800	1.32011100	0.00013500
C	1.21077300	-0.63038900	0.00016000
H	2.15636800	1.32011100	-0.00013500
C	0.00000000	-1.32010400	0.00000000
H	-2.14849700	-1.17517100	-0.00011600
H	2.14849700	-1.17517100	0.00011600
H	0.00000000	-2.40387000	0.00000000

Int1

C	2.08780000	-2.22172400	-1.10108700
C	1.57419300	-0.99137300	-1.47487000
C	1.41640900	0.01820400	-0.51398700
C	1.78528200	-0.23912800	0.82139800
C	2.30605500	-1.49011300	1.17339300
C	2.45715300	-2.48135000	0.22339700
H	2.20082200	-2.99369400	-1.85331900
H	1.28965400	-0.81968000	-2.50387400
H	2.57649000	-1.64651500	2.21132200
H	2.85678300	-3.44918600	0.49937900
C	1.10481500	1.83676200	1.49148900
C	0.64661600	2.20826200	0.13487600
H	0.96126500	2.60237500	2.24972600
N	1.62890700	0.71577100	1.81785000
N	0.87414700	1.25566300	-0.83370400
C	0.42208800	1.52270500	-2.19563400
H	1.25093900	1.40335400	-2.89411900
H	-0.38392900	0.83435400	-2.46038300
H	0.05667700	2.54398100	-2.23068300
O	0.11018200	3.28113000	-0.08812600
C	-1.50374100	-0.10626000	0.57122400
C	-1.54553900	-1.47266800	0.42544800
C	-2.56198500	0.75427600	0.40236800
C	-2.78499400	-2.02814700	0.09103900
H	-0.66533100	-2.09408500	0.56045000
C	-3.79096700	0.17598000	0.06584000
H	-2.45761200	1.82770000	0.51998700
C	-3.89636100	-1.20534700	-0.08556900
H	-2.87698100	-3.10146900	-0.03382300
H	-4.66044200	0.80789900	-0.07798400
H	-4.85211600	-1.64459600	-0.34664200

$TS_{1\text{-}C}$

C	3.43434200	-1.11032000	-1.19908100
C	2.67835700	0.04859500	-1.25897800
C	1.74219900	0.32518000	-0.25262300
C	1.58181200	-0.58769300	0.81402400
C	2.36579600	-1.75101500	0.85141200
C	3.28535200	-2.01625300	-0.14298100
H	4.15200200	-1.31099900	-1.98578700
H	2.81411600	0.73453300	-2.08399700
H	2.21752900	-2.42651000	1.68624500
H	3.88486900	-2.91743500	-0.10853000
C	-0.10730200	0.65915500	1.72052100
C	0.04953400	1.74139400	0.71807900
H	-0.79605400	0.88872800	2.52891700
N	0.66500400	-0.37863100	1.82608700
N	0.98019900	1.48836000	-0.26353700
C	1.16895600	2.47515900	-1.32286700
H	2.20133900	2.82771800	-1.32656000
H	0.93030600	2.03159000	-2.29099900
H	0.49907600	3.30595600	-1.12620500
O	-0.61196800	2.76486400	0.77110400
C	-1.89164200	-0.17809900	0.43223000
C	-1.85869500	-1.54579400	0.31282600
C	-2.84677700	0.65697200	-0.09517900
C	-2.89568200	-2.13314800	-0.41916700
H	-1.07228600	-2.14236200	0.76358700
C	-3.87497500	0.04566100	-0.82046800
H	-2.80265000	1.73262200	0.03695800
C	-3.89442900	-1.33885700	-0.97908700
H	-2.91939800	-3.20973300	-0.54754200
H	-4.65611500	0.65583200	-1.26055200
H	-4.69449000	-1.80258500	-1.54418000

C

C	-3.87757300	-0.86095500	0.71035000
C	-3.05504500	0.25217400	0.84410200
C	-1.85556100	0.33389600	0.13930700
C	-1.45985700	-0.75232500	-0.72119900
C	-2.34916700	-1.86606700	-0.84051200
C	-3.52702400	-1.92230200	-0.14145100
H	-4.80385300	-0.90039800	1.27053900
H	-3.35967800	1.05691100	1.49899200
H	-2.03620700	-2.66577400	-1.50158100

H	-4.18291800	-2.77862300	-0.23920300
C	0.61772500	0.28576300	-1.19638700
C	0.13304600	1.55051800	-0.49413500
H	0.97722700	0.61610800	-2.17566900
N	-0.32202400	-0.78976000	-1.39856600
N	-1.04401300	1.46082000	0.21606900
C	-1.48278100	2.61685800	0.99375600
H	-2.43815200	2.98432900	0.61489600
H	-1.58897600	2.34063400	2.04391500
H	-0.72945500	3.39136700	0.89502800
O	0.79329400	2.56644700	-0.53869300
C	1.83281100	-0.21716200	-0.41589500
C	1.65937700	-1.01966300	0.71149400
C	3.11742300	0.15844900	-0.80353000
C	2.76415500	-1.44258700	1.44397000
H	0.66162900	-1.31721300	1.01719300
C	4.22165900	-0.26583900	-0.07045500
H	3.25070200	0.78271700	-1.68033400
C	4.04703800	-1.06724400	1.05417500
H	2.62262600	-2.06703900	2.31863400
H	5.21833800	0.02685600	-0.38045500
H	4.90726800	-1.39994200	1.62350900

Int2

C	-2.47496800	-1.88490400	-1.67042800
C	-1.56785100	-2.38107800	-0.78027900
C	-0.44817500	-1.59296300	-0.41279800
C	-0.30531200	-0.24720200	-1.02340000
C	-1.30721900	0.19049600	-1.99269600
C	-2.35301500	-0.59525500	-2.29986500
H	-3.33582600	-2.49565100	-1.92041200
H	-1.71698000	-3.35690400	-0.34218500
H	-1.15752600	1.17511500	-2.41830300
H	-3.11211300	-0.27814900	-3.00266600
C	1.59625400	0.21327900	0.27236200
C	1.52169800	-1.17078500	0.88327100
H	1.29450600	0.89120500	1.09757700
N	0.66120100	0.54688100	-0.76113600
N	0.48947400	-2.03787100	0.41083500
C	0.40576700	-3.37641300	1.00413700
H	-0.44695600	-3.41114200	1.68429800
H	0.29530600	-4.11692200	0.21385200
H	1.32210900	-3.55627200	1.55462300

O	2.28967000	-1.55291700	1.71797500
C	3.01793400	0.54410700	-0.14387300
C	3.42942900	0.34009100	-1.45967500
C	3.92333400	1.02399800	0.80027700
C	4.74146300	0.61869900	-1.82971300
H	2.72551300	-0.03391700	-2.19555300
C	5.23529900	1.29818700	0.42887400
H	3.59798400	1.18483400	1.82192000
C	5.64597100	1.09664500	-0.88617700
H	5.05629900	0.46104100	-2.85478200
H	5.93512900	1.67507700	1.16565600
H	6.66777600	1.31395400	-1.17504600
O	-0.80313500	-0.18014300	2.04534000
C	-1.11649900	0.96812100	1.65321900
O	-0.40926400	1.99485400	1.69990900
C	-2.47910000	1.09416600	0.96600200
C	-3.38887400	0.03859600	0.99896600
C	-2.79528300	2.24304600	0.23873500
C	-4.59448800	0.12254400	0.30834200
H	-3.12868900	-0.85012600	1.56206300
C	-3.99534100	2.32934600	-0.46042100
H	-2.07874400	3.05626400	0.22560000
C	-4.89621100	1.26632600	-0.42927200
H	-5.29798400	-0.70264300	0.34014000
H	-4.22948200	3.22155700	-1.03073700
H	-5.83209100	1.33098100	-0.97326800

TS_{2-3}

C	-2.70634300	1.63229500	1.73520900
C	-1.80222100	2.24425900	0.91482800
C	-0.59136600	1.58140100	0.59888200
C	-0.34518900	0.25074600	1.18829300
C	-1.34230500	-0.31477700	2.08623200
C	-2.48766100	0.34583000	2.33866900
H	-3.63834900	2.14525800	1.94671800
H	-2.02117400	3.21440100	0.49424800
H	-1.11617900	-1.29032700	2.49915800
H	-3.25078500	-0.07221000	2.98192700
C	1.60326500	-0.00897100	-0.07422900
C	1.51304100	1.41886100	-0.55025700
H	1.17553100	-0.59801800	-0.95960800
N	0.71195500	-0.43567800	0.94299200
N	0.34034300	2.13478600	-0.16892900
C	0.13105300	3.45897700	-0.76135300

H	-0.71351400	3.39831700	-1.44940900
H	-0.06526400	4.18659200	0.02437300
H	1.03016600	3.73072000	-1.30198700
O	2.33789700	1.94003400	-1.24609700
C	3.02387200	-0.47291800	0.14680300
C	3.52542000	-0.61883200	1.43867900
C	3.84122600	-0.74869400	-0.94877500
C	4.83744100	-1.04007800	1.63350700
H	2.88938600	-0.40535700	2.29089300
C	5.15270300	-1.16611100	-0.75198100
H	3.44582000	-0.64143800	-1.95273600
C	5.65287100	-1.31309500	0.53947400
H	5.22182900	-1.15277200	2.64067000
H	5.78215000	-1.38312300	-1.60719300
H	6.67447200	-1.64159000	0.69196600
O	-0.84448700	0.50229400	-2.10253500
C	-0.99269800	-0.67079000	-1.71173800
O	-0.11032200	-1.56789500	-1.70163700
C	-2.34288500	-1.03990000	-1.09744900
C	-3.40082200	-0.13278500	-1.12636900
C	-2.50896500	-2.26189500	-0.44349000
C	-4.60871400	-0.43727500	-0.50481800
H	-3.25605900	0.81517900	-1.63158100
C	-3.71254600	-2.56876100	0.18346400
H	-1.67630000	-2.95543700	-0.42734000
C	-4.76411600	-1.65473800	0.15577300
H	-5.42835000	0.27259700	-0.53276100
H	-3.83183800	-3.51711500	0.69560700
H	-5.70269700	-1.89138900	0.64463200

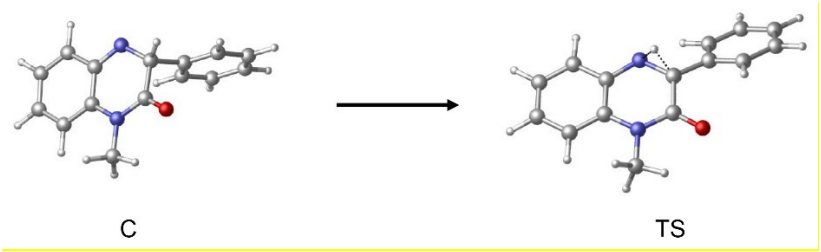
Int3

C	-3.76453600	1.44340700	1.15673600
C	-2.87558900	2.06508600	0.29516800
C	-1.52146700	1.70190200	0.31626300
C	-1.08452200	0.70920200	1.21171300
C	-2.00473300	0.08651700	2.06487500
C	-3.33702900	0.45163800	2.04605300
H	-4.80815600	1.73481300	1.13476400
H	-3.23021200	2.82910100	-0.38293400
H	-1.63243000	-0.68270300	2.73201300
H	-4.04584600	-0.02935100	2.70883300
C	1.10218100	0.86752900	0.48446900
C	0.75813200	1.97917600	-0.45643100

H	2.31219400	-1.95399200	-1.06674400
N	0.23504400	0.30085600	1.25036600
N	-0.58407500	2.28873200	-0.52142000
C	-1.01157500	3.31905300	-1.46530500
H	-1.78479300	2.91613200	-2.12073900
H	-1.40310700	4.18359300	-0.92613200
H	-0.14946300	3.61560400	-2.05283300
O	1.59402100	2.57410400	-1.11272900
C	2.50705300	0.39046500	0.55727300
C	2.96781800	-0.13893500	1.76778900
C	3.35146500	0.37170400	-0.55995100
C	4.24465200	-0.67579400	1.86407400
H	2.31303300	-0.12658100	2.63061200
C	4.62410100	-0.18302300	-0.46234700
H	3.00255400	0.76656400	-1.50253400
C	5.07585300	-0.70407700	0.74696300
H	4.59117700	-1.07413300	2.81060100
H	5.26476600	-0.20509300	-1.33643600
H	6.07121300	-1.12711700	0.81940800
O	0.80080300	-0.66052700	-2.19986200
C	0.51542900	-1.52371100	-1.40531900
O	1.43700500	-2.28168700	-0.80125700
C	-0.87542100	-1.85270900	-0.99209600
C	-1.91605000	-1.10246900	-1.54132300
C	-1.14527800	-2.85692600	-0.06208700
C	-3.22766800	-1.36261000	-1.16667700
H	-1.68367900	-0.31818900	-2.25292400
C	-2.46032600	-3.11751100	0.30626600
H	-0.33173700	-3.42679400	0.36873200
C	-3.49949300	-2.37309400	-0.24596300
H	-4.03732600	-0.77887400	-1.58883500
H	-2.67387900	-3.89880700	1.02601500
H	-4.52369400	-2.57533600	0.04644200

[1,2]-H shift

We have also calculated the [1,2]-H shift step and the structure of the transition state is shown in the following figure. The reaction barrier is calculated to be 36.9 kcal/mol.



Cartesian coordinates of the transition state

C	-4.33804200	-0.79431800	0.13678600
C	-3.56199200	0.35821700	0.20042700
C	-2.17669600	0.28734900	0.03298200
C	-1.57616800	-0.97061000	-0.19379900
C	-2.37807100	-2.11730200	-0.26312900
C	-3.74980300	-2.03640700	-0.09672900
H	-5.41019600	-0.71517400	0.27092100
H	-4.04227200	1.30963700	0.38204800
H	-1.88372100	-3.06507000	-0.44317500
H	-4.35805200	-2.93112000	-0.14747400
C	0.59783400	0.05744500	-0.29400200
C	0.00529600	1.38757000	-0.01897400
H	0.20490100	-0.50388500	-1.37207200
N	-0.20881000	-1.13122900	-0.34275500
N	-1.37475600	1.43504500	0.07794100
C	-2.00632200	2.72983000	0.30624800
H	-2.74852100	2.92274100	-0.47037300
H	-2.49316600	2.74801600	1.28385000
H	-1.23628000	3.49278700	0.27120700
O	0.68718700	2.38920700	0.10511300
C	2.04679800	-0.16964000	-0.11000700
C	2.48700700	-1.36725000	0.46892300
C	3.00164400	0.76702100	-0.53396800
C	3.84477600	-1.61615500	0.63322100
H	1.75635700	-2.09690300	0.79465100
C	4.35618300	0.51069400	-0.36770000
H	2.67775300	1.69026400	-0.99339200
C	4.78548000	-0.67912800	0.21706700
H	4.16698000	-2.54428900	1.09151200
H	5.08205300	1.24266700	-0.70324600
H	5.84409000	-0.87394700	0.34426100

4. References

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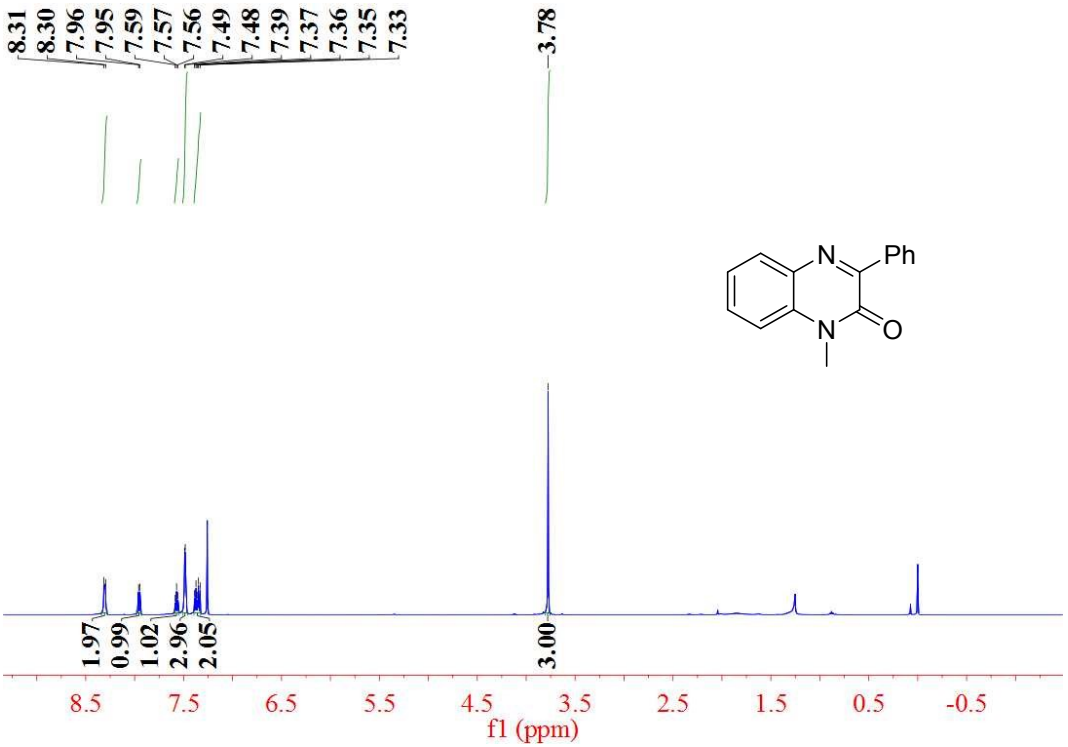
4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16 Rev. C.01., Wallingford, CT, 2016.

5. Copies of NMR spectra

3aa ^{1}H NMR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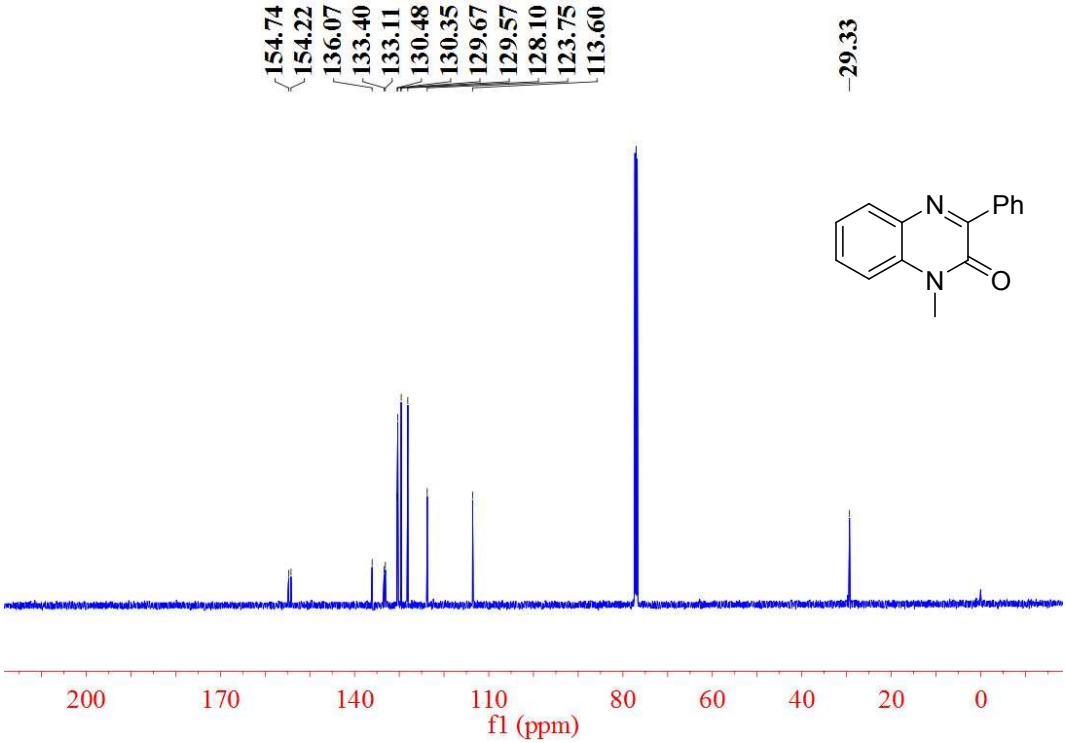
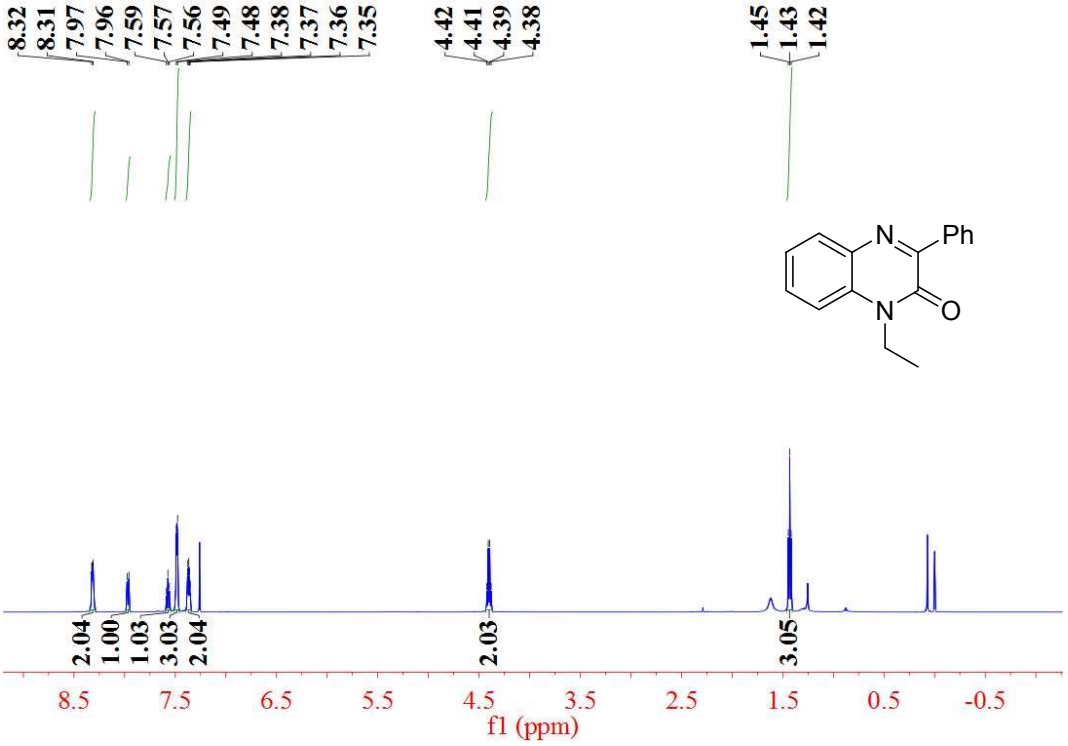
8.30
7.96
7.95
7.59
7.57
7.56
7.49
7.48
7.39
7.37
7.36
7.35
7.33
3.78
N
Ph
N
O
1.97
0.99
1.02
2.96
2.05
3.00
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

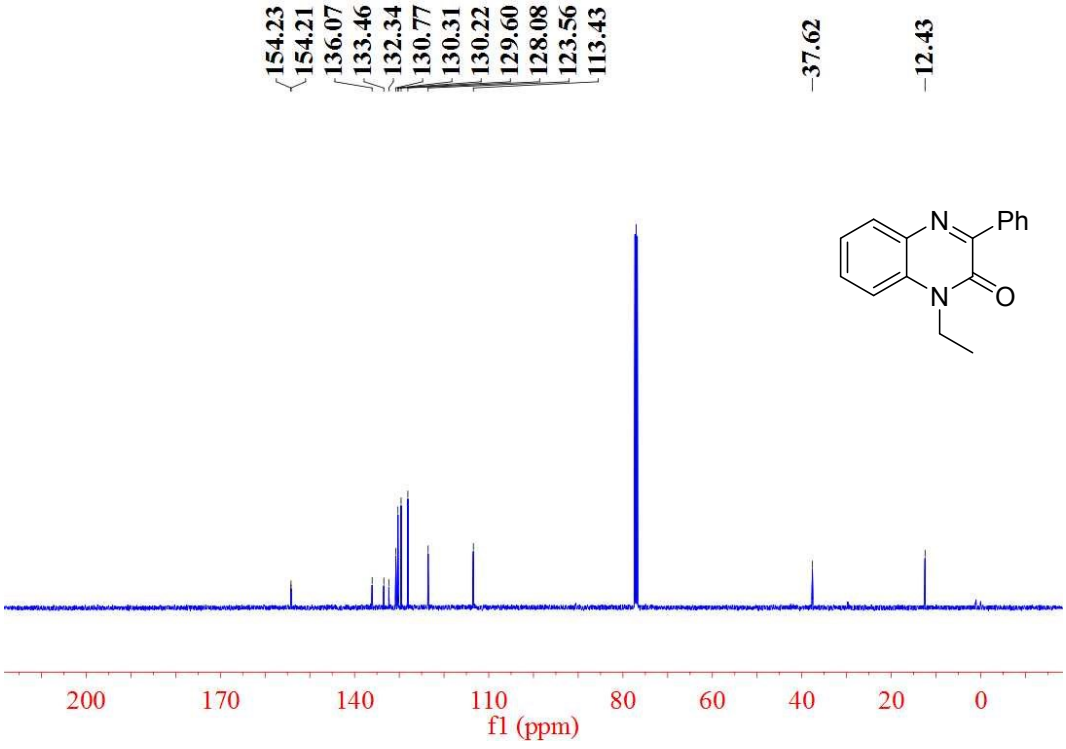
3aa ^{13}C NMR


154.74
154.22
136.07
133.40
133.11
130.48
130.35
129.67
129.57
128.10
123.75
113.60
29.33
N
Ph
N
O
200
170
140
110
80
60
40
20
0
f1 (ppm)

3ab ^{1}H NMR



3ab ^{13}C NMR



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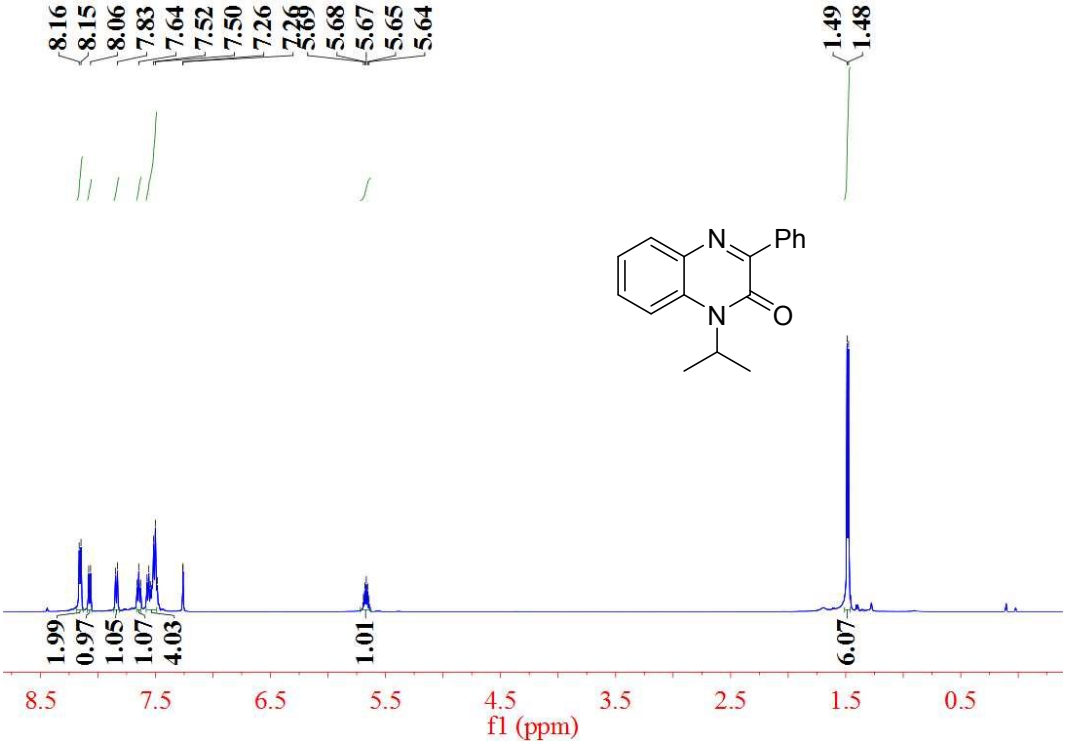

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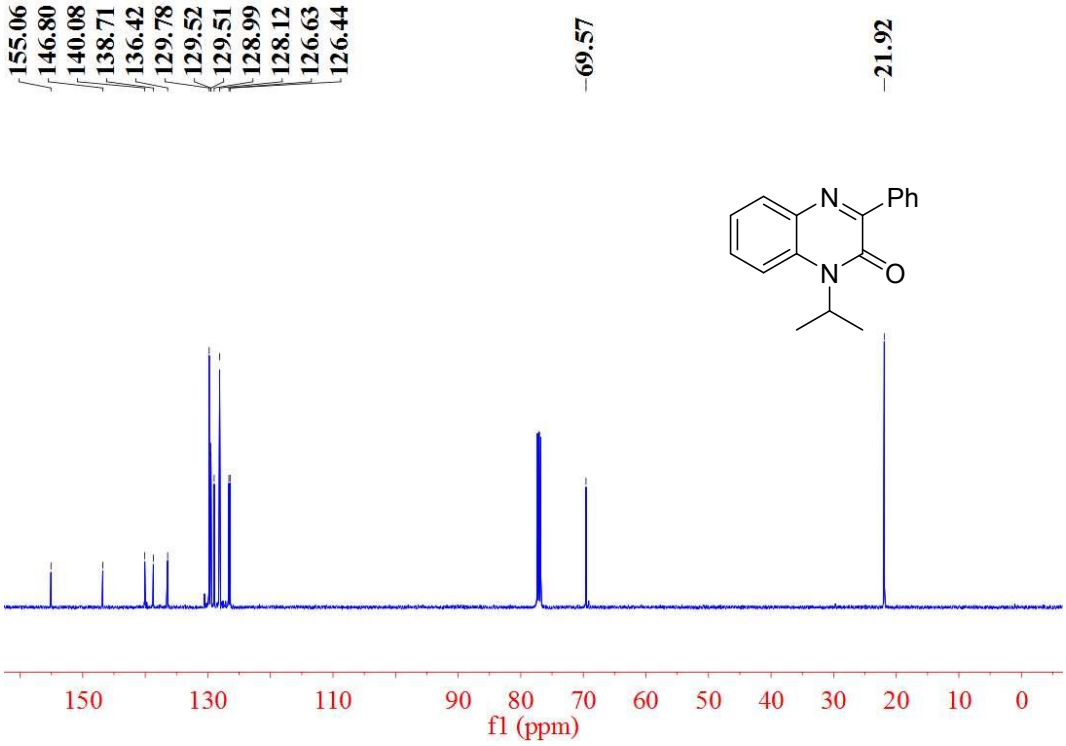

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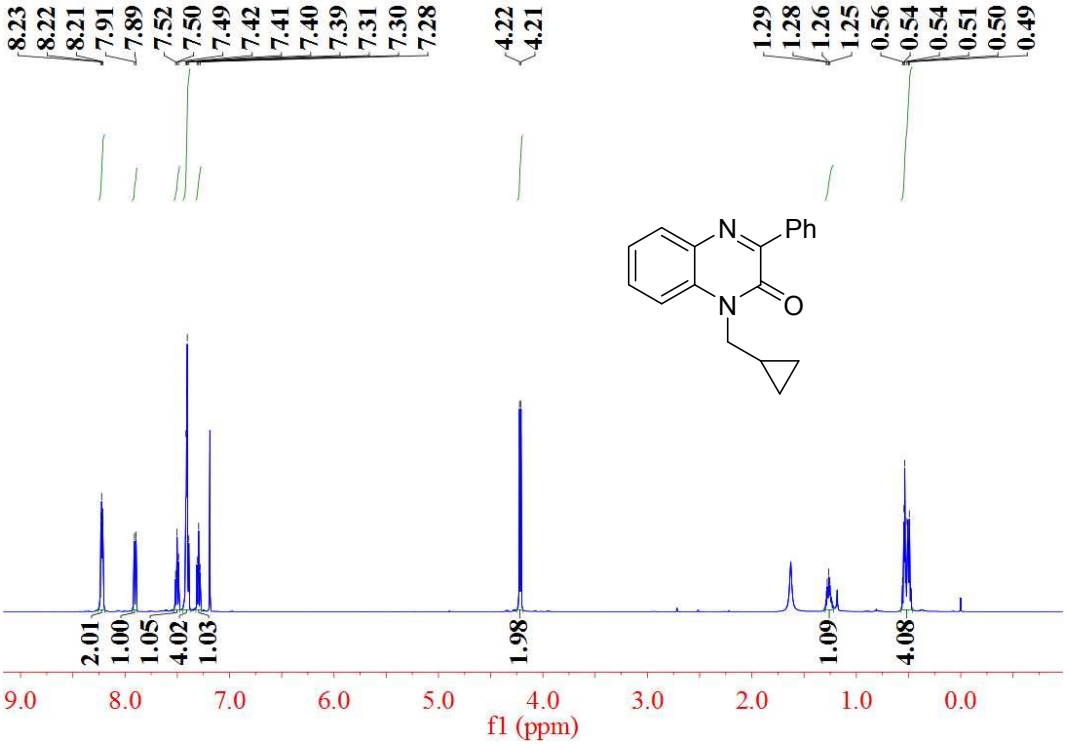

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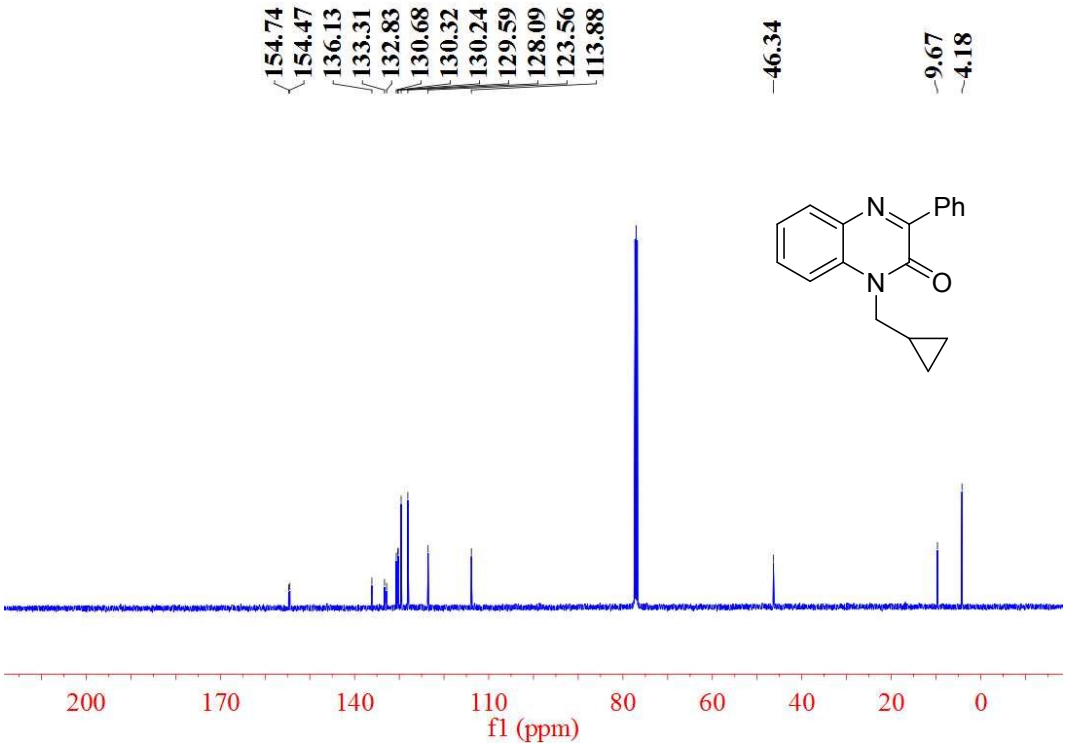

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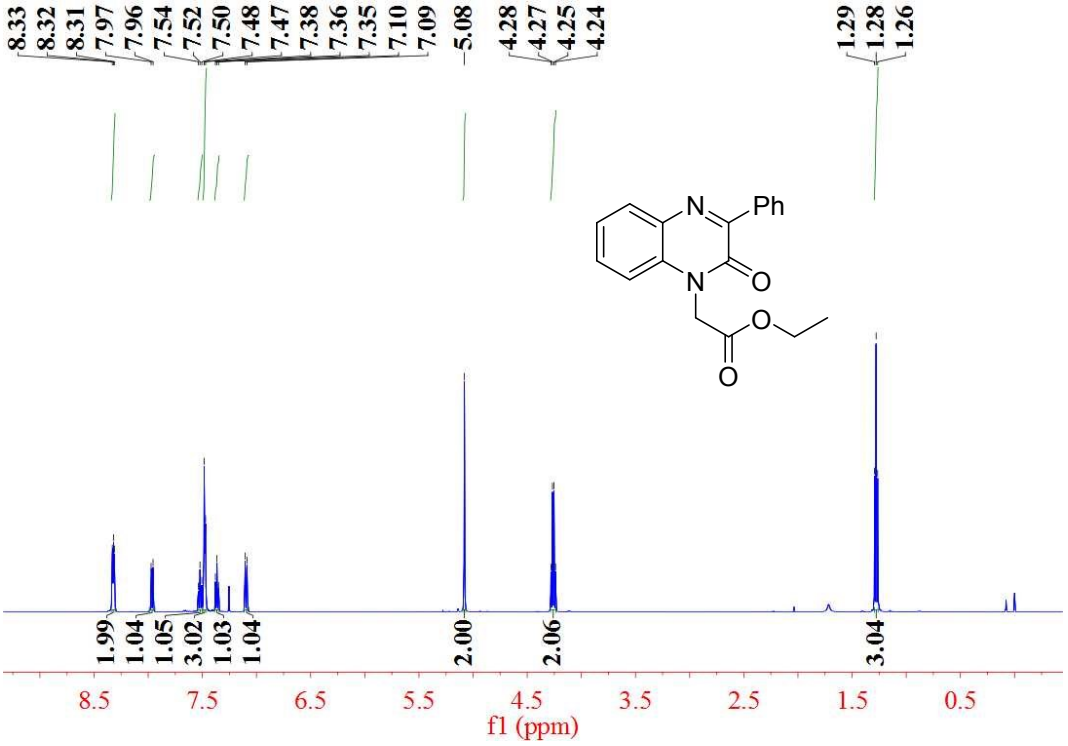

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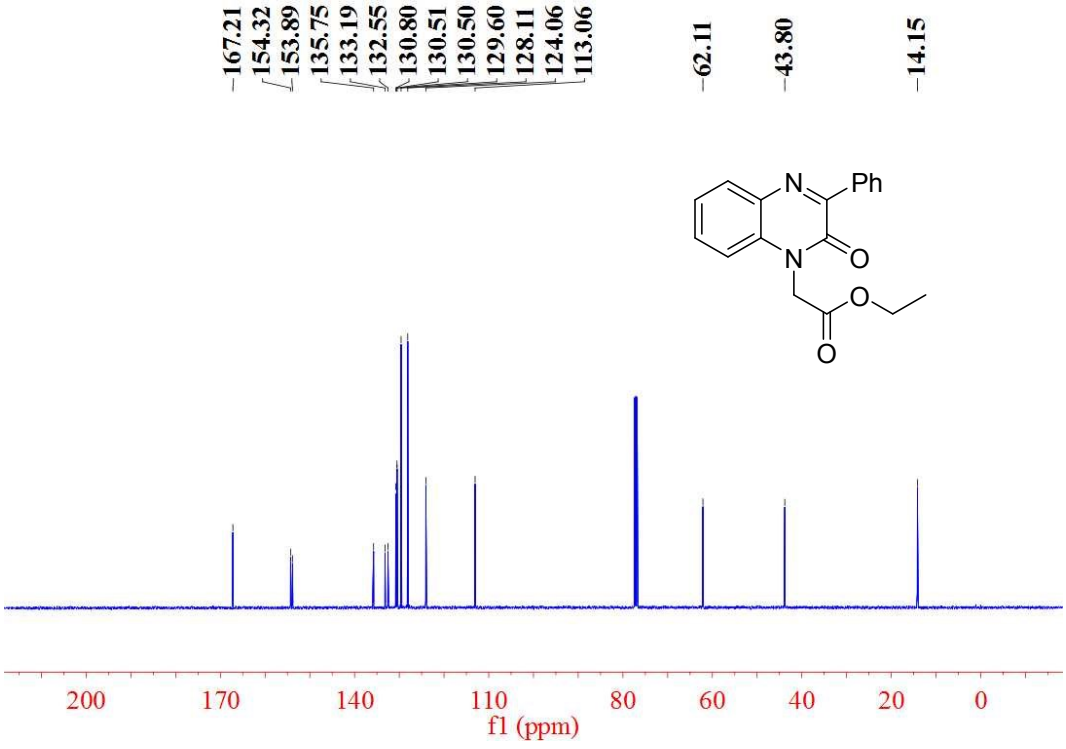

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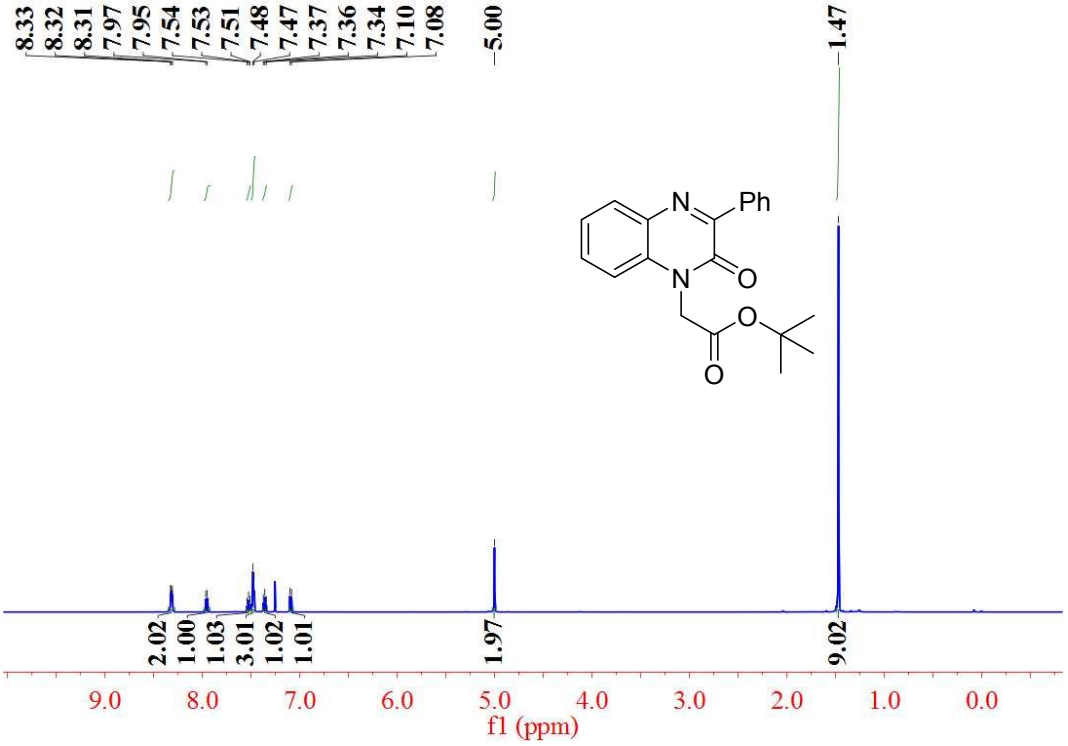

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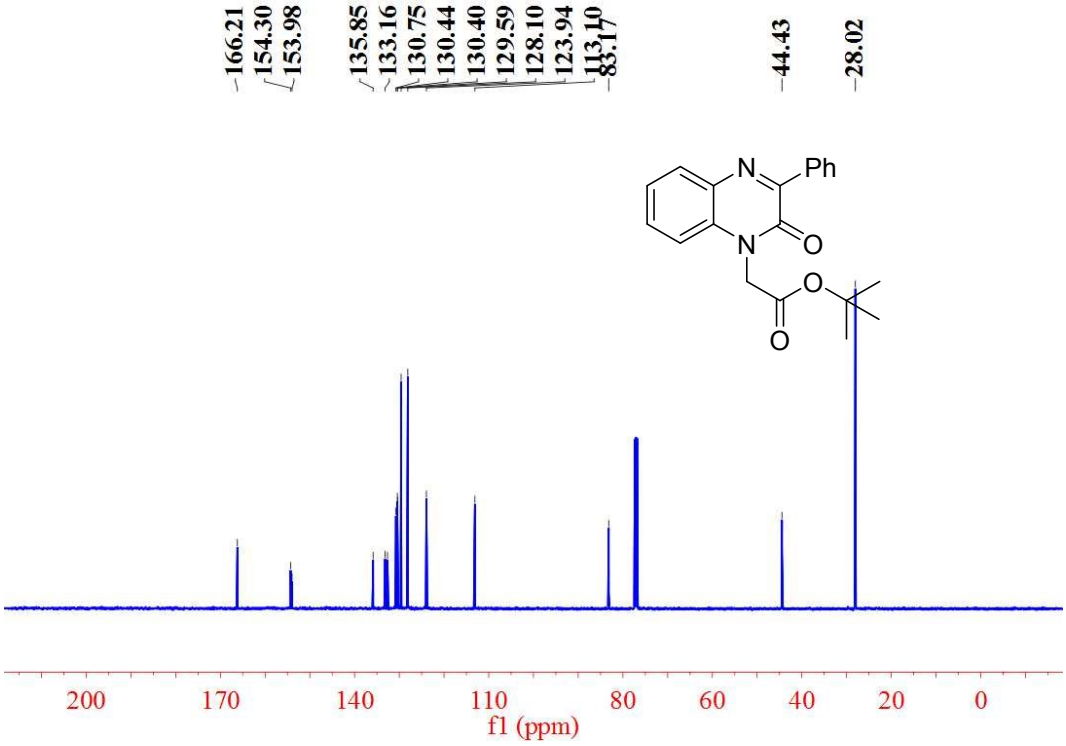

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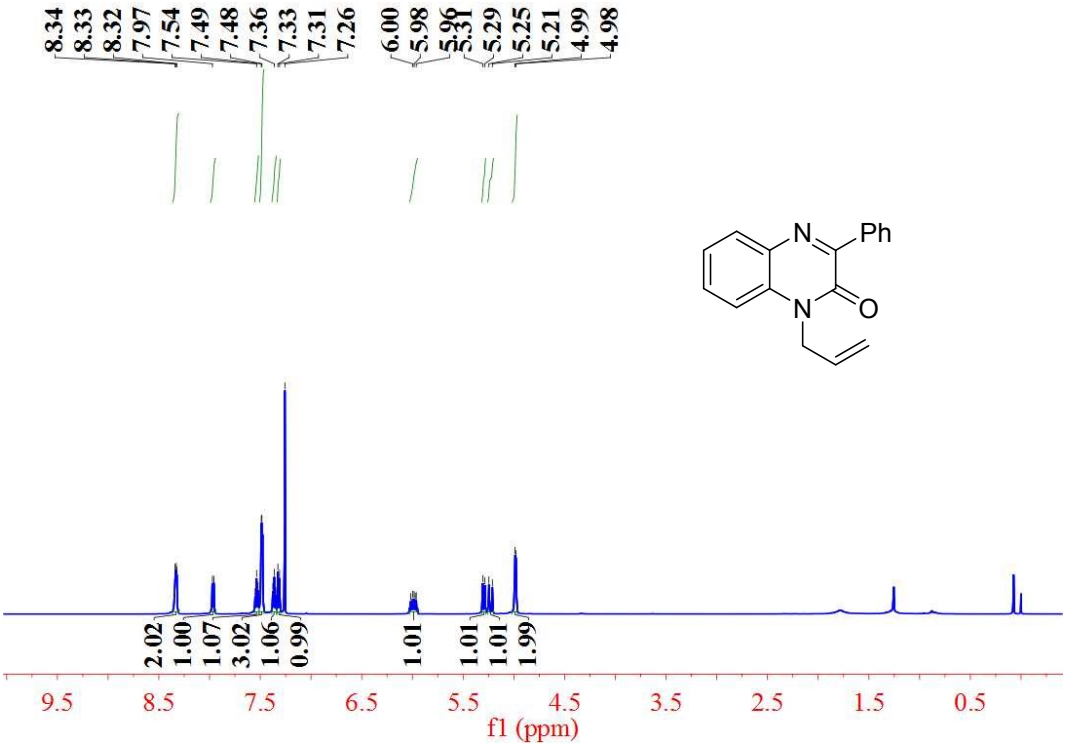

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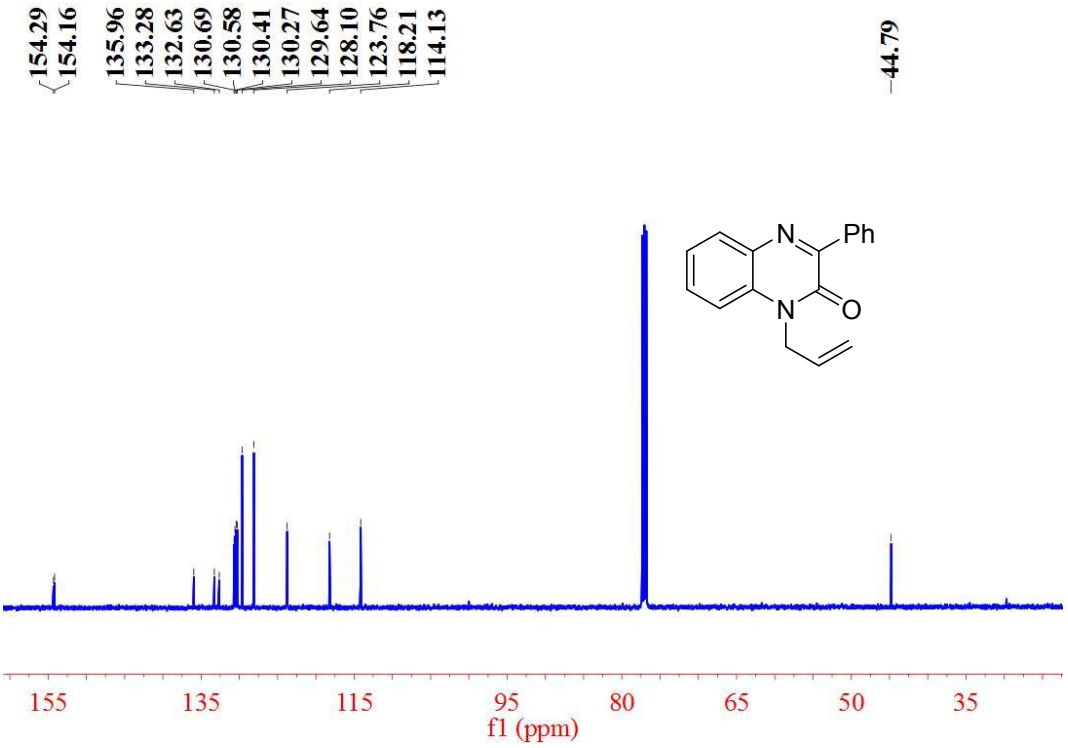

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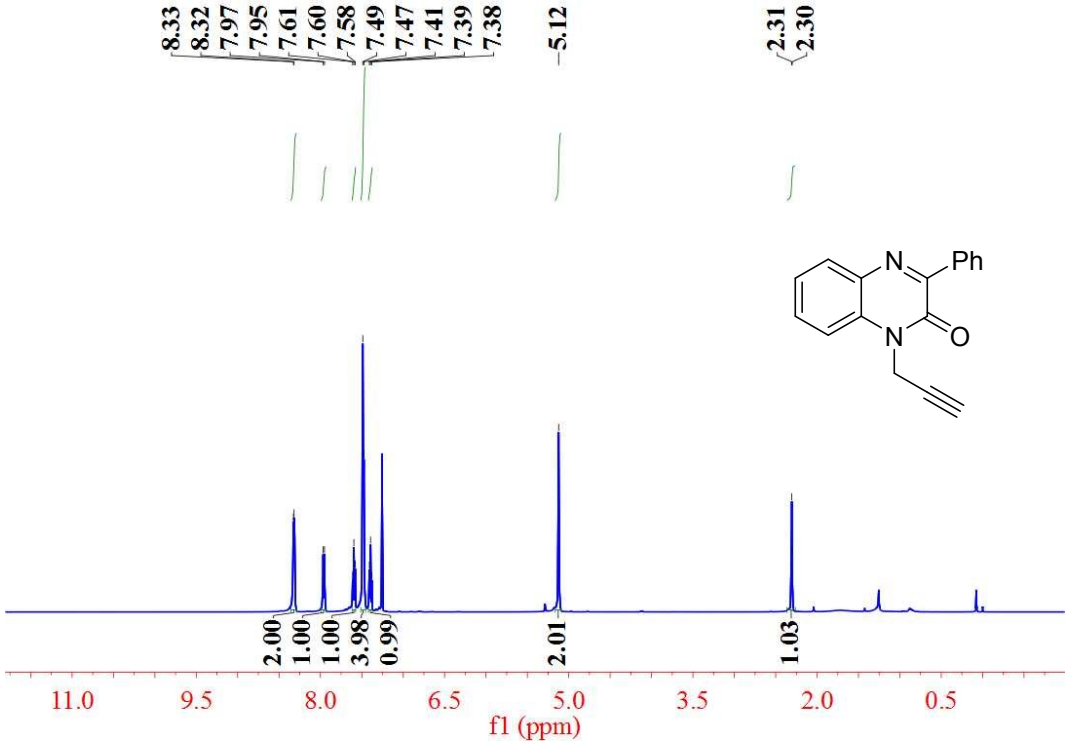

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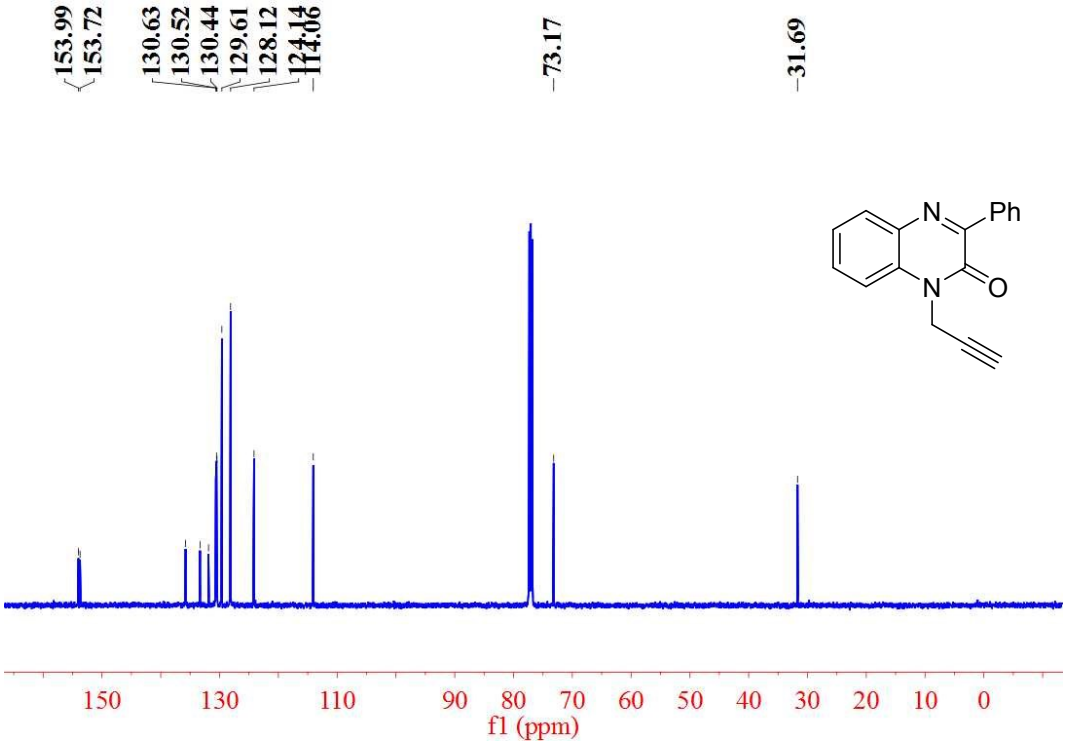

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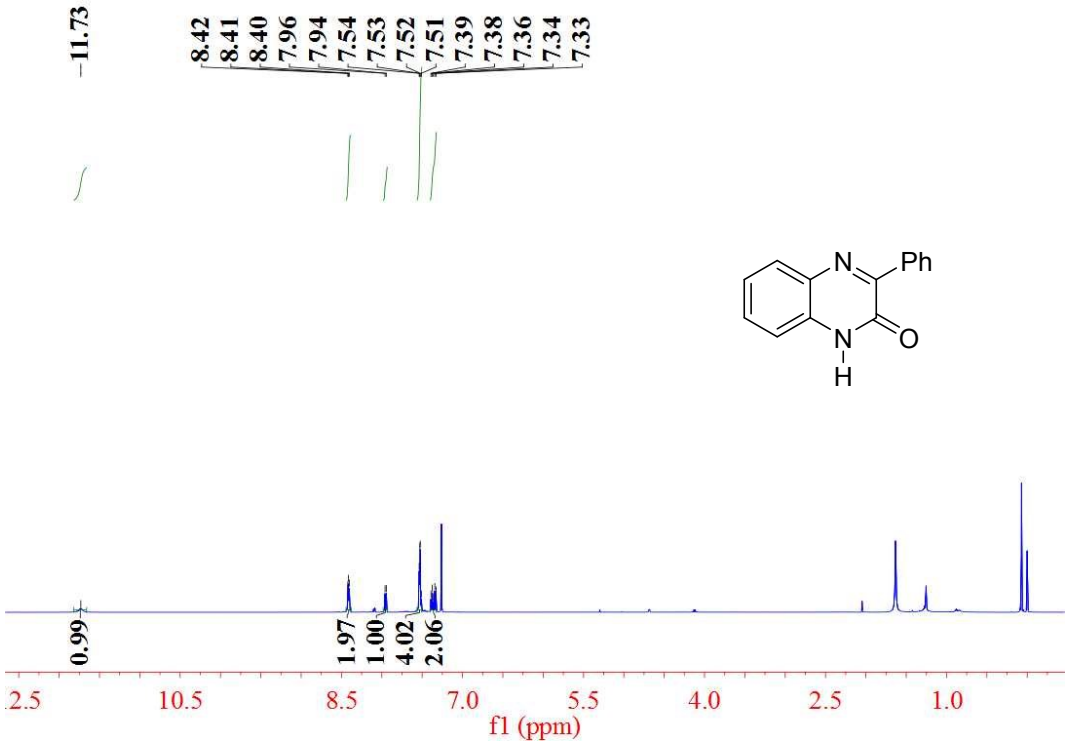

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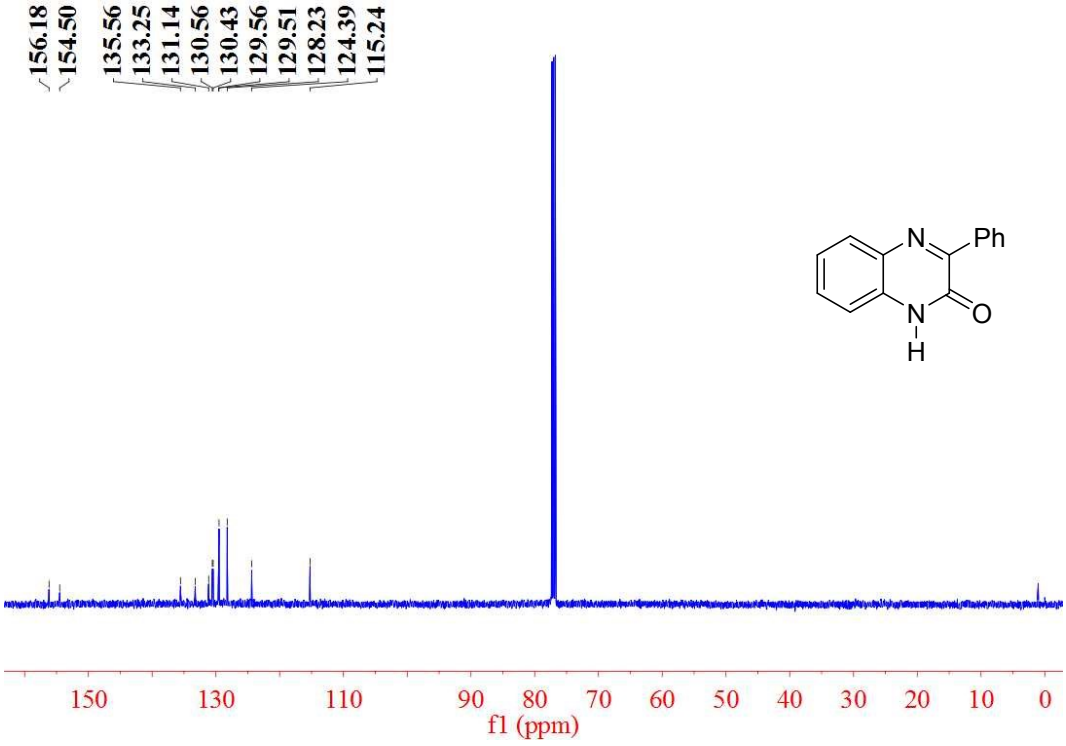

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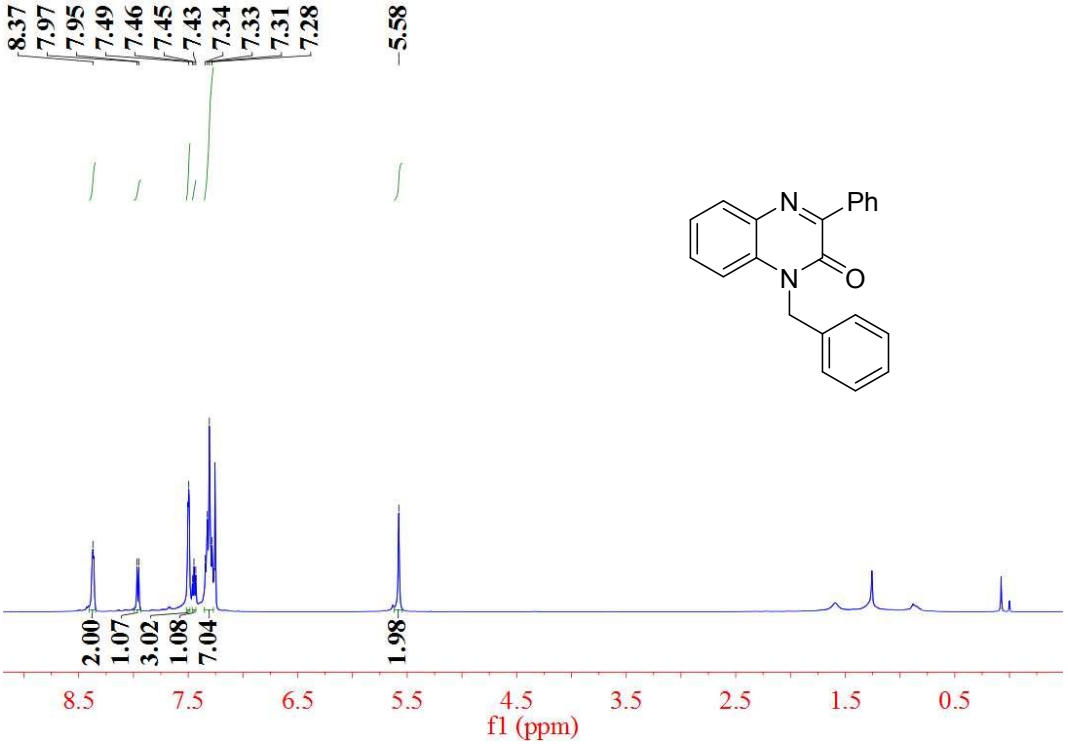

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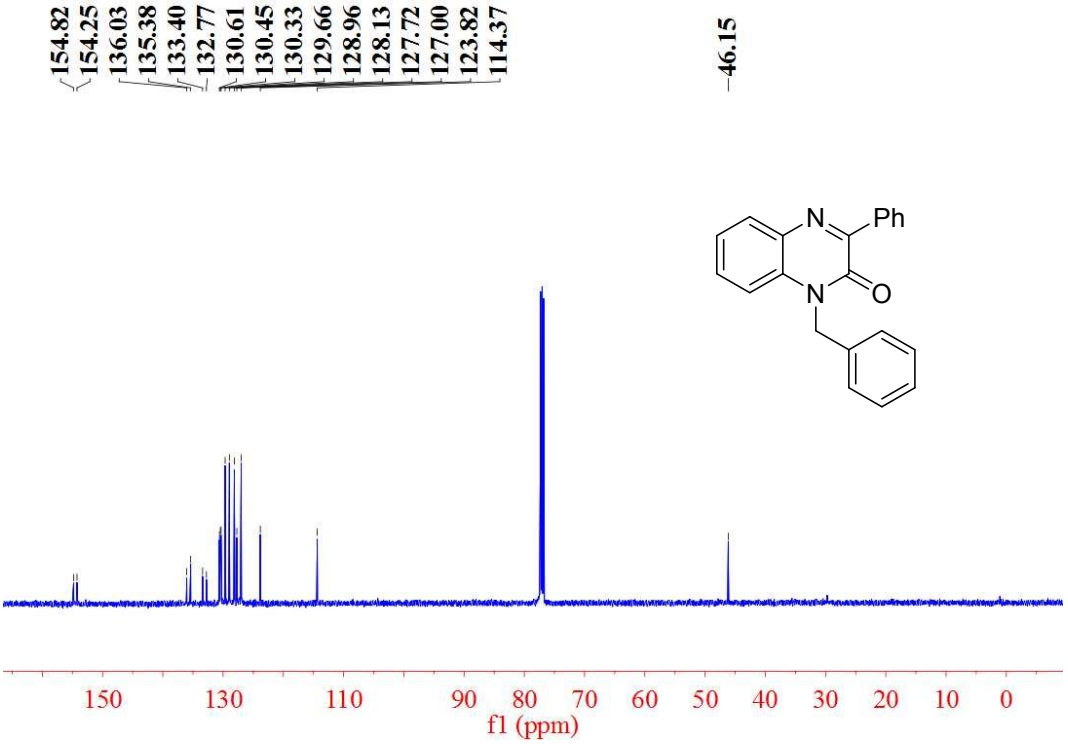

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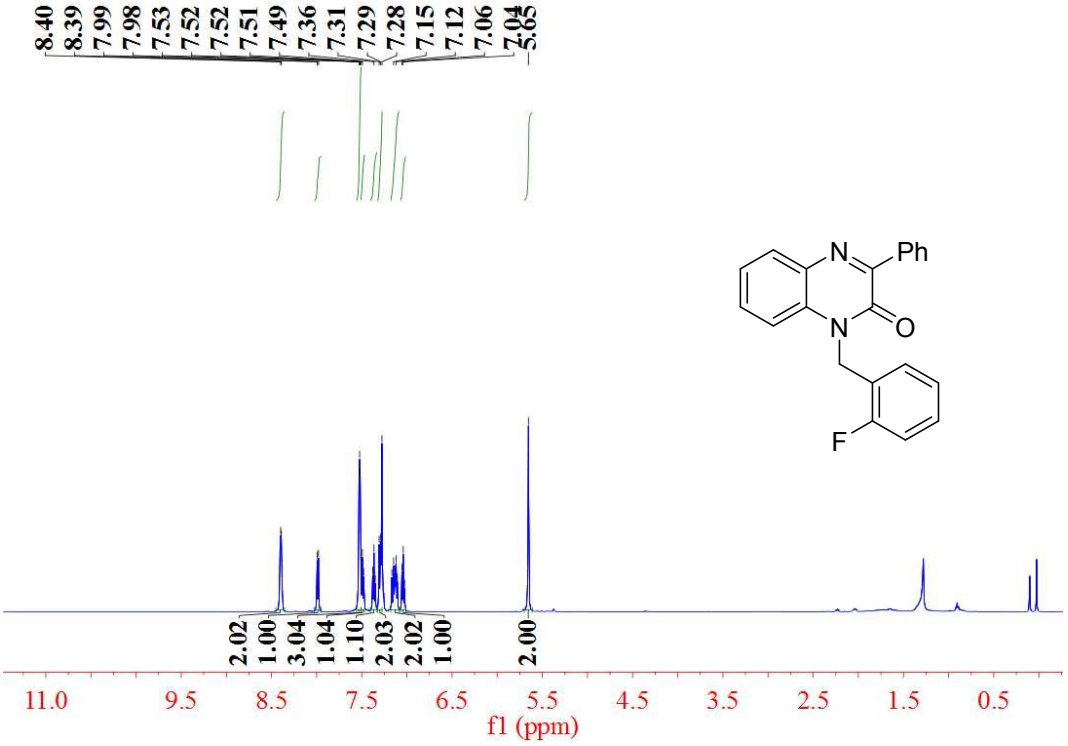

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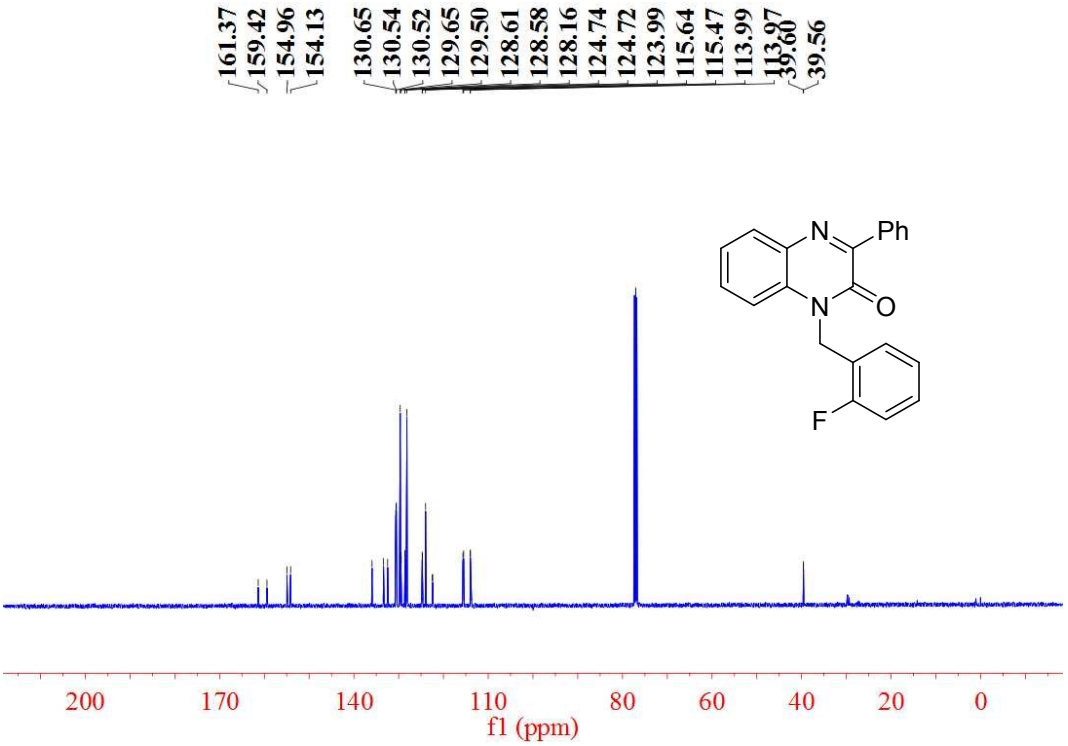

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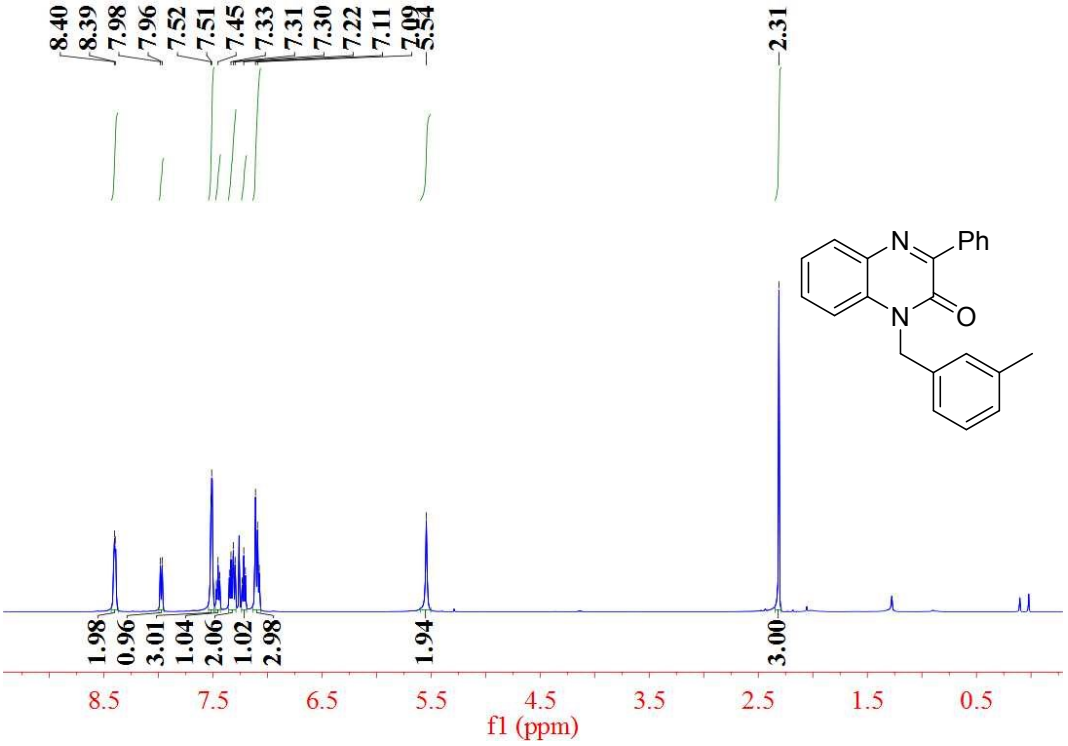

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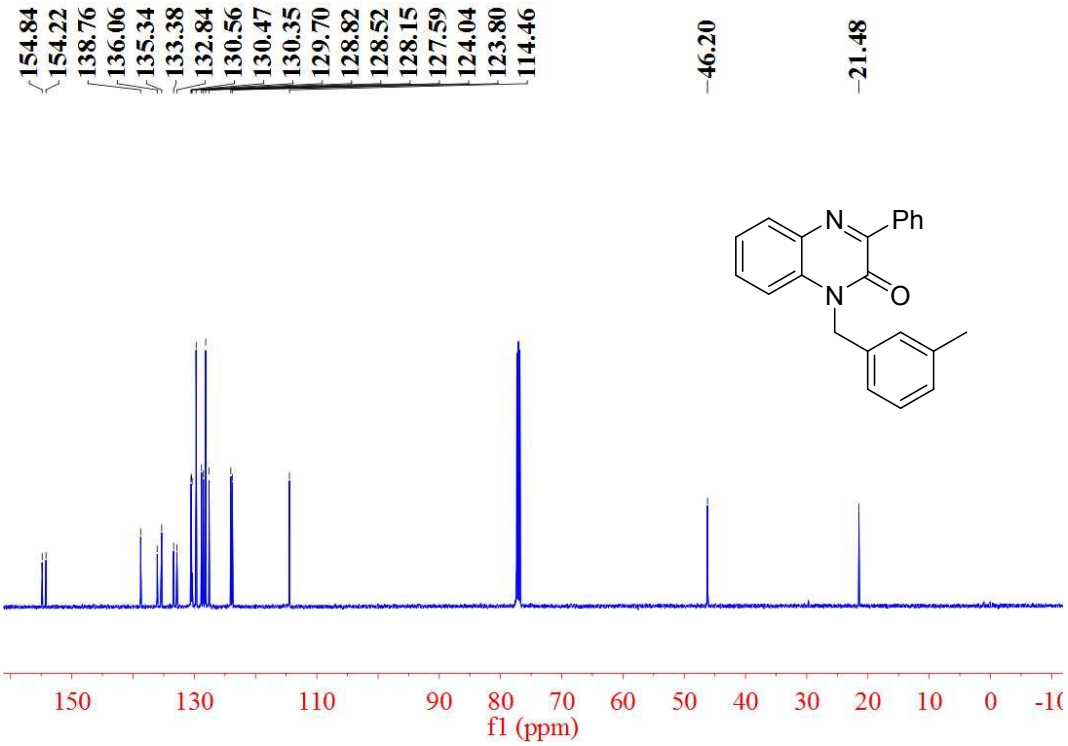

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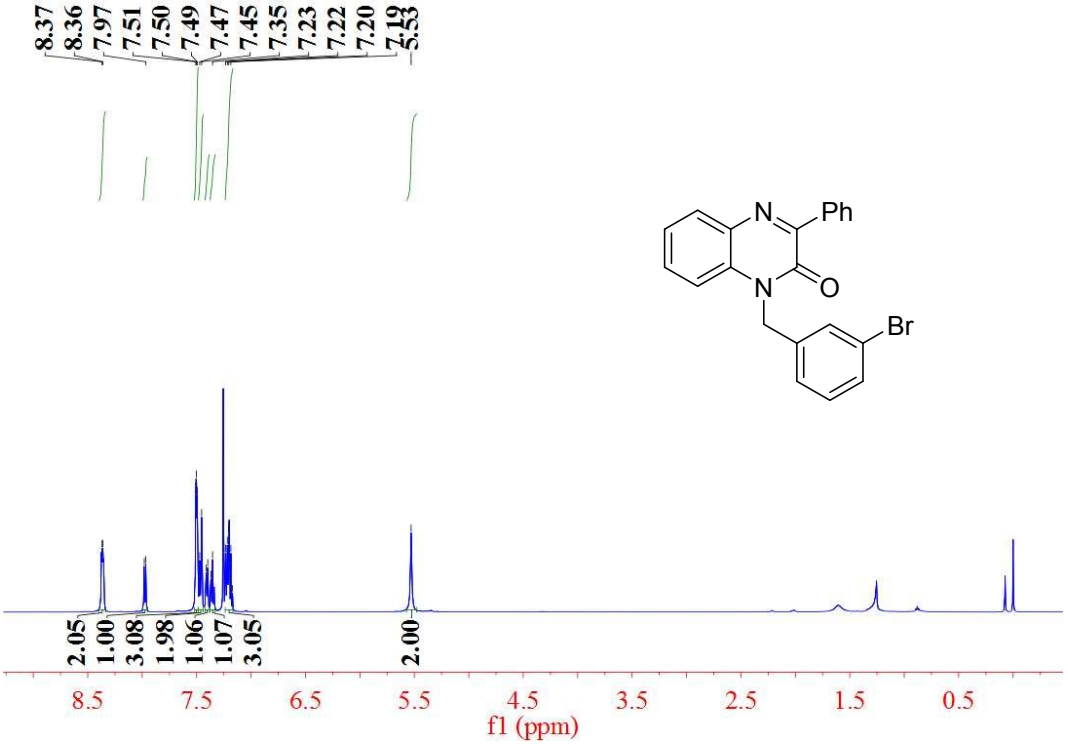

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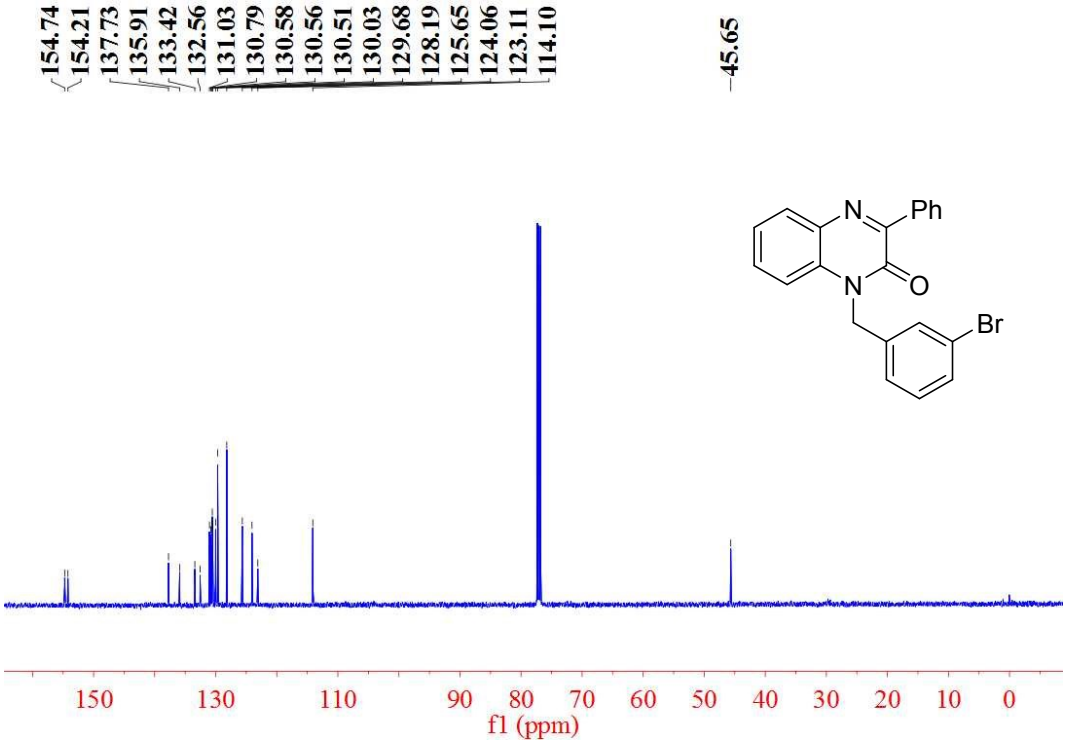

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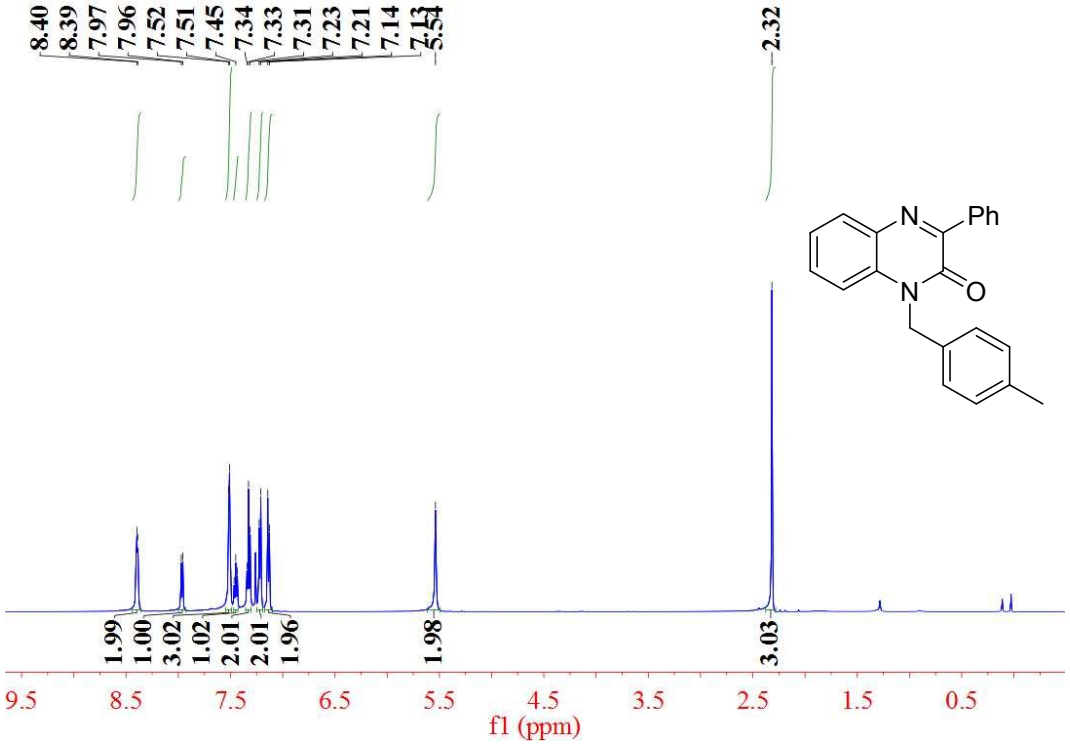

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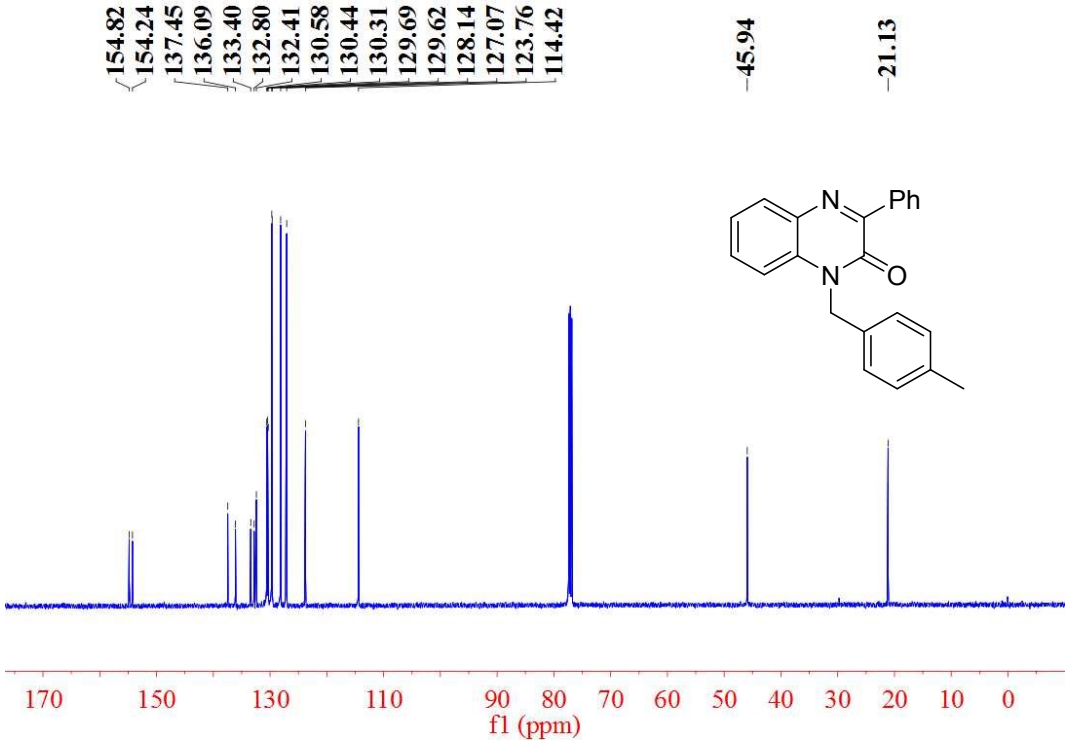

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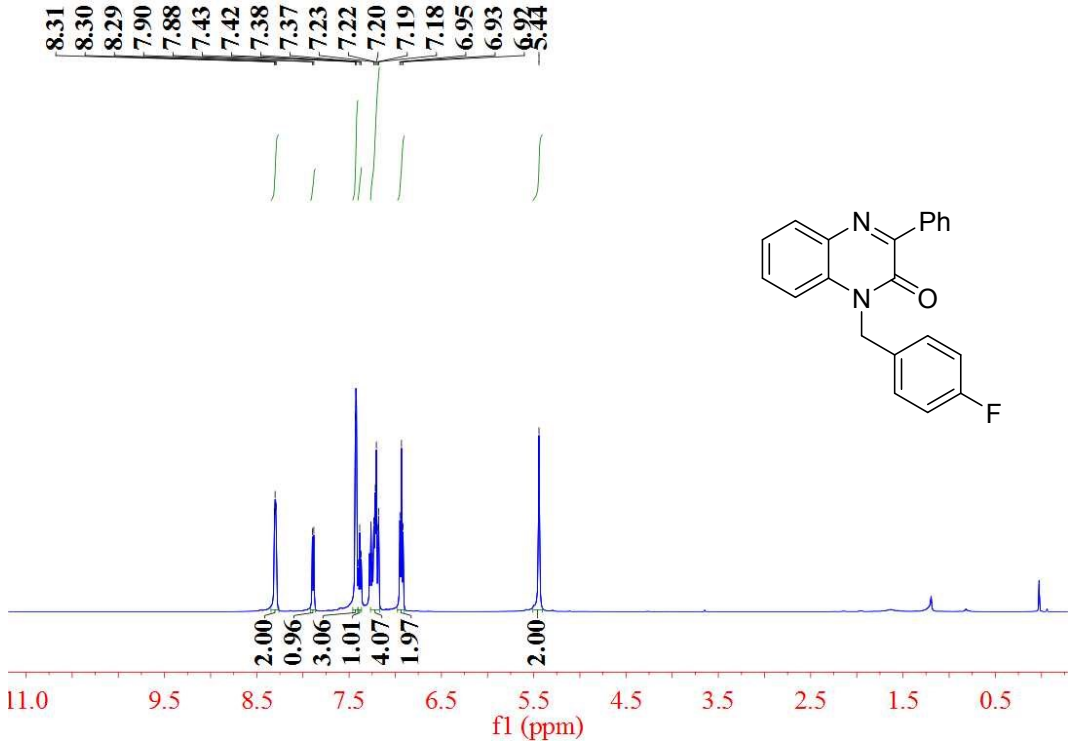

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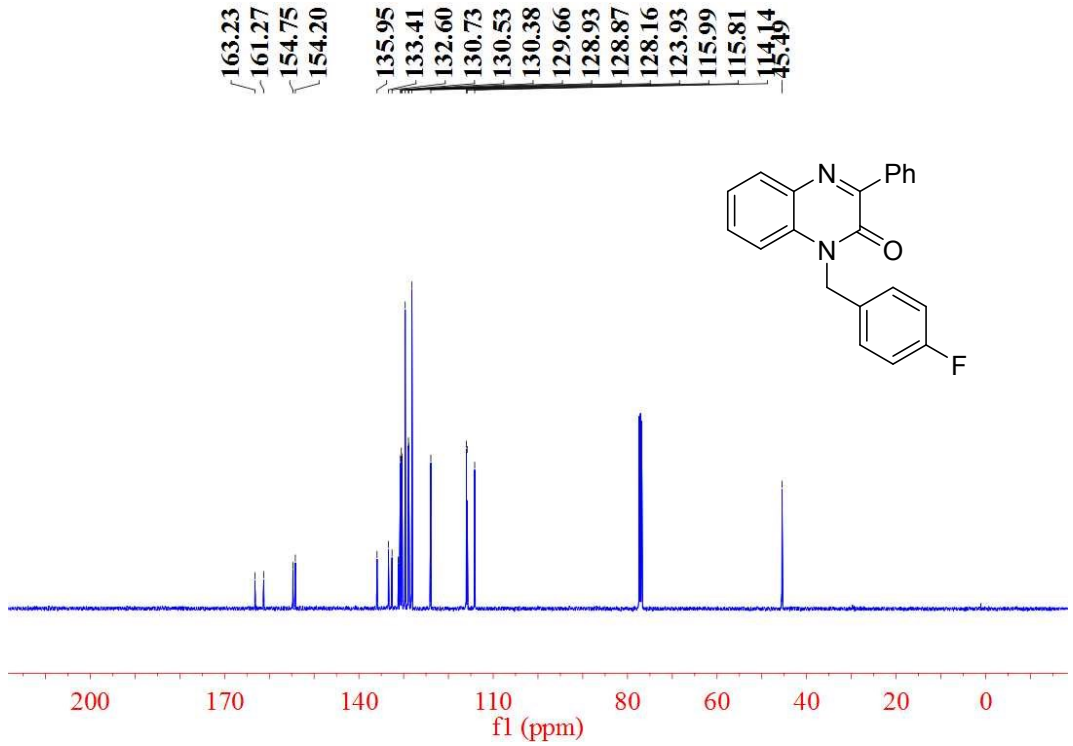

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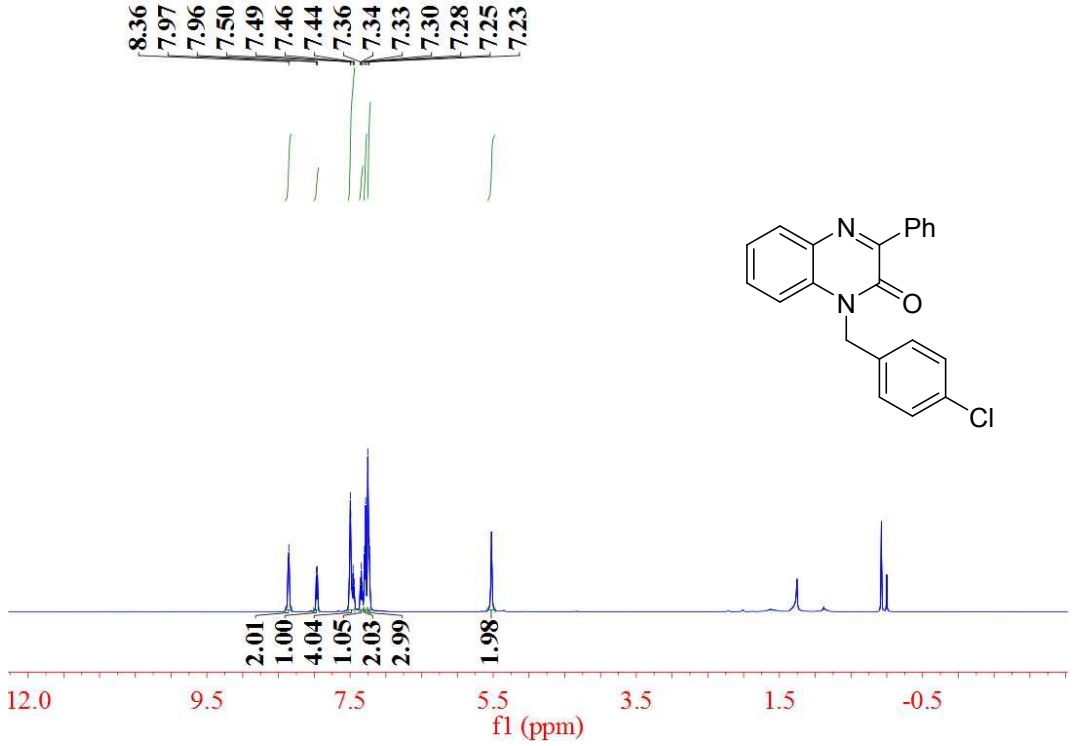

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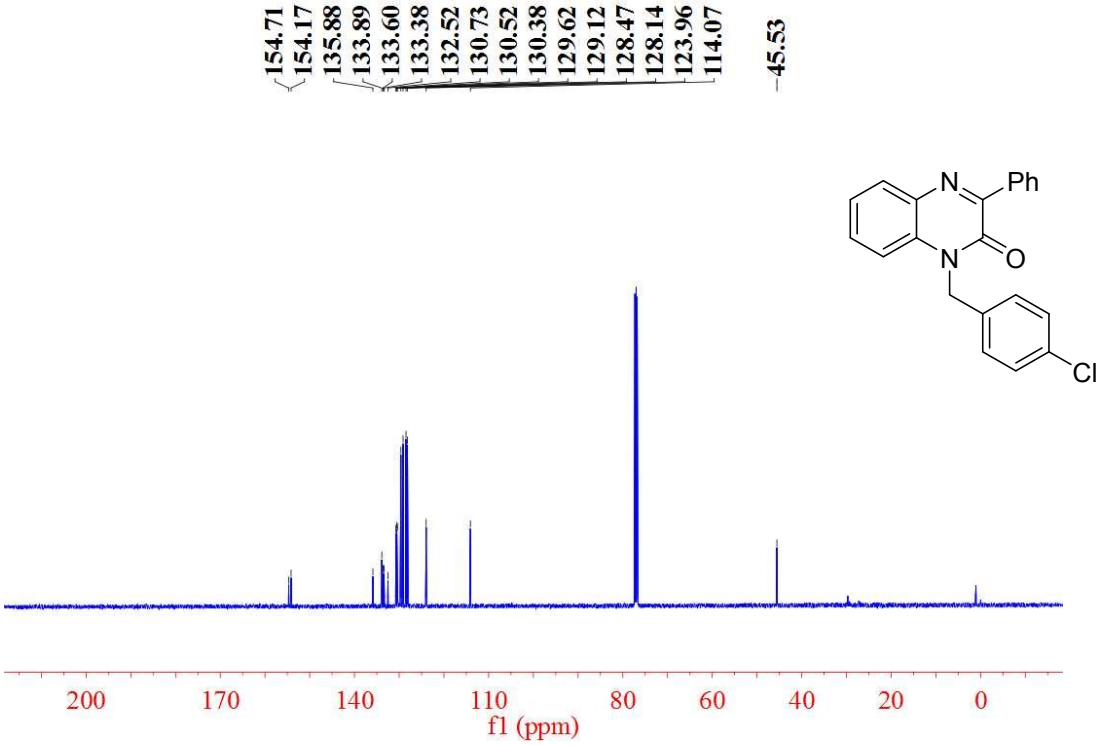

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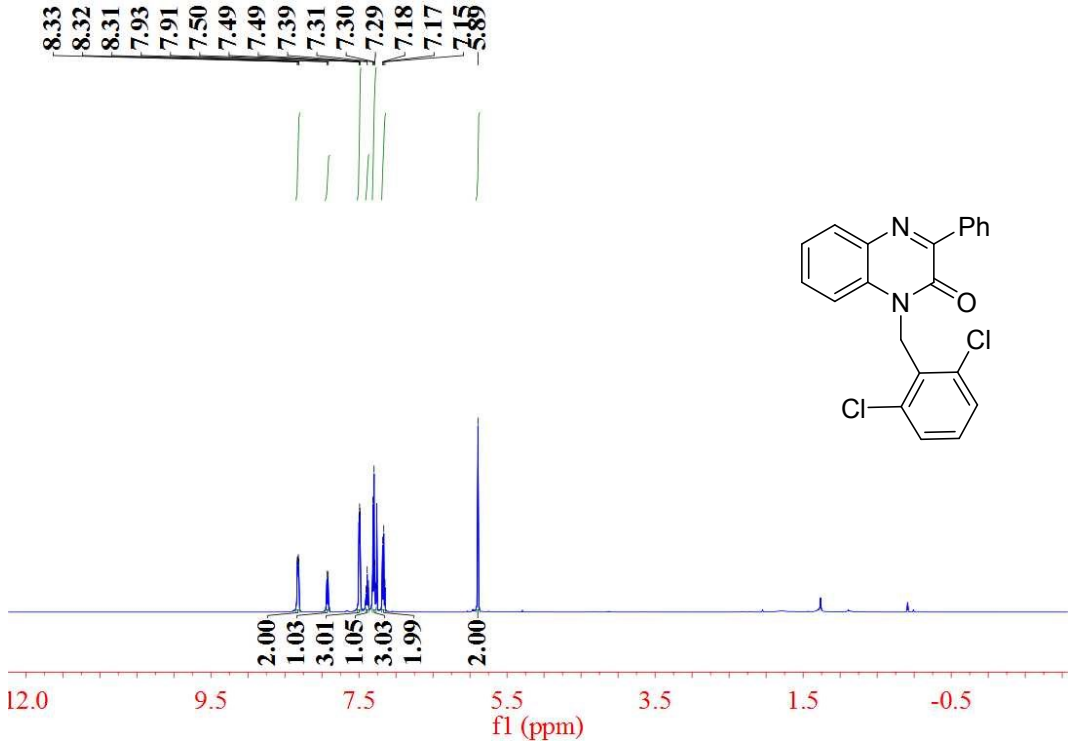

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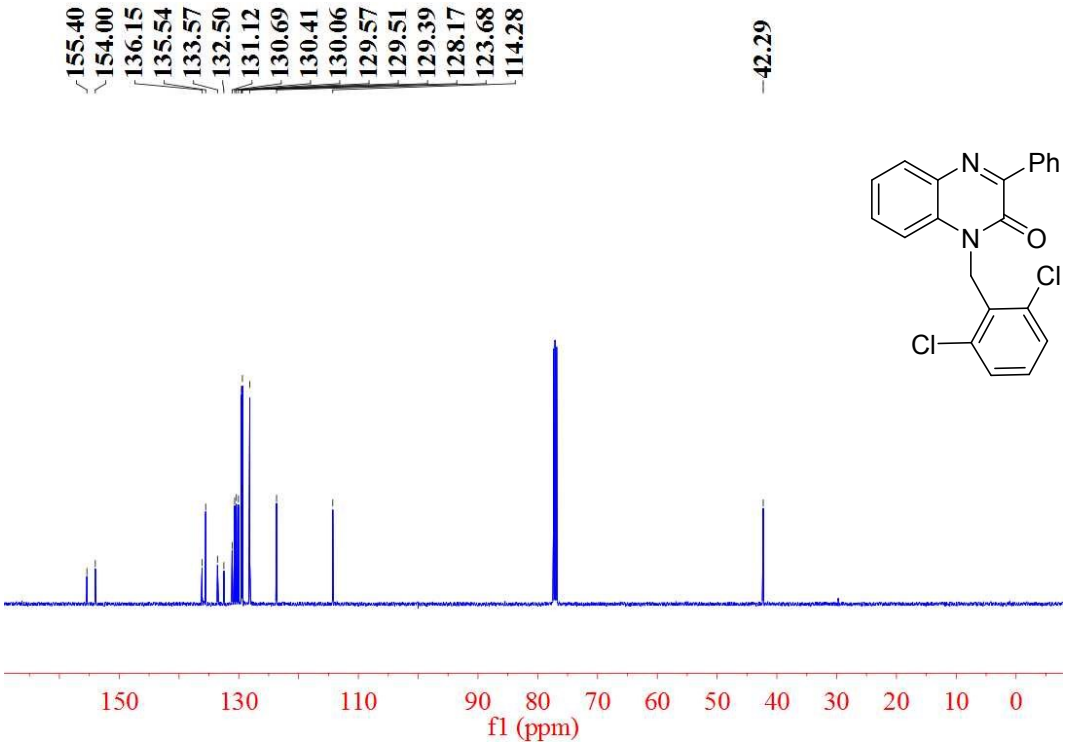

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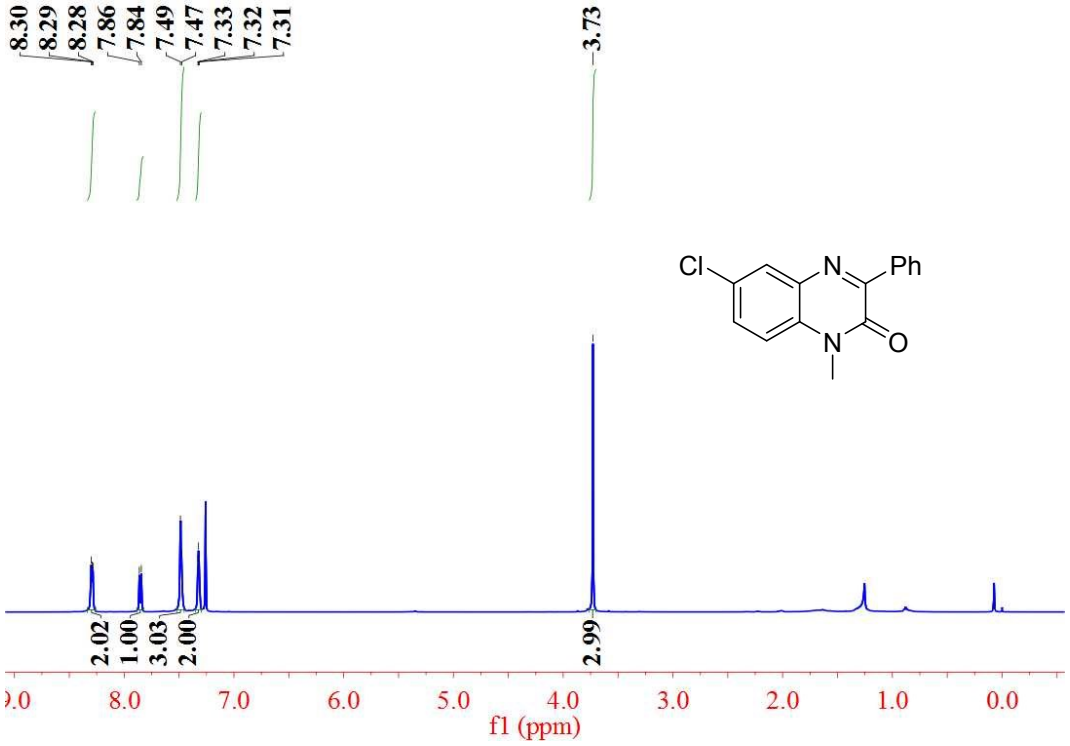

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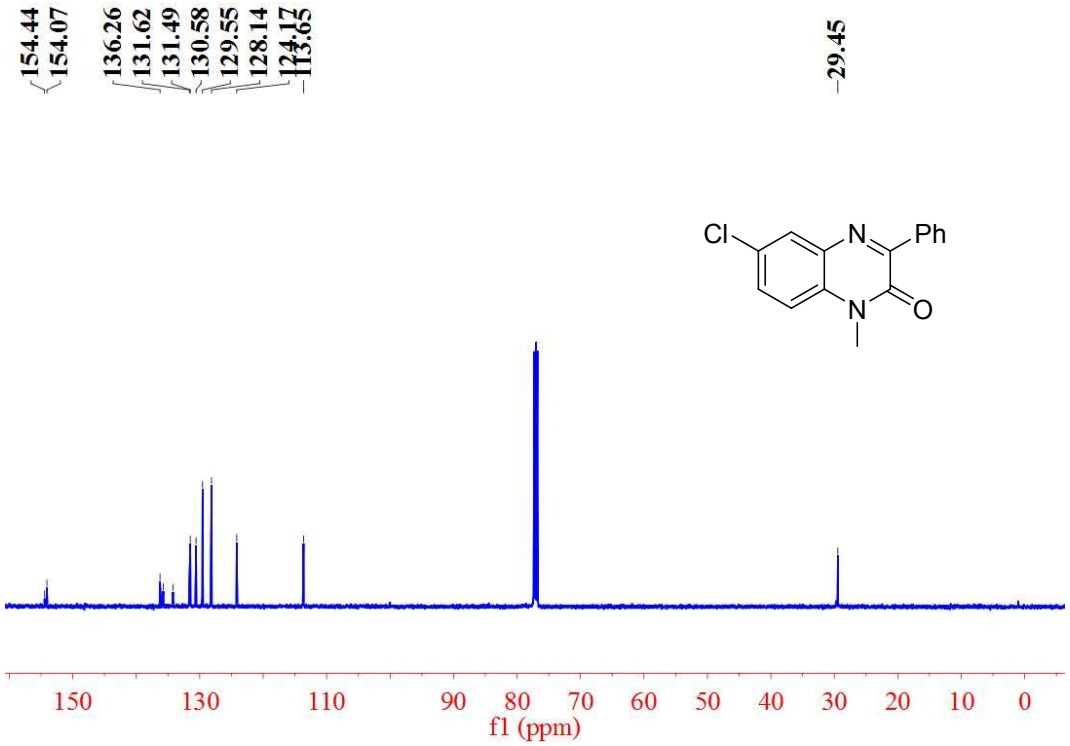

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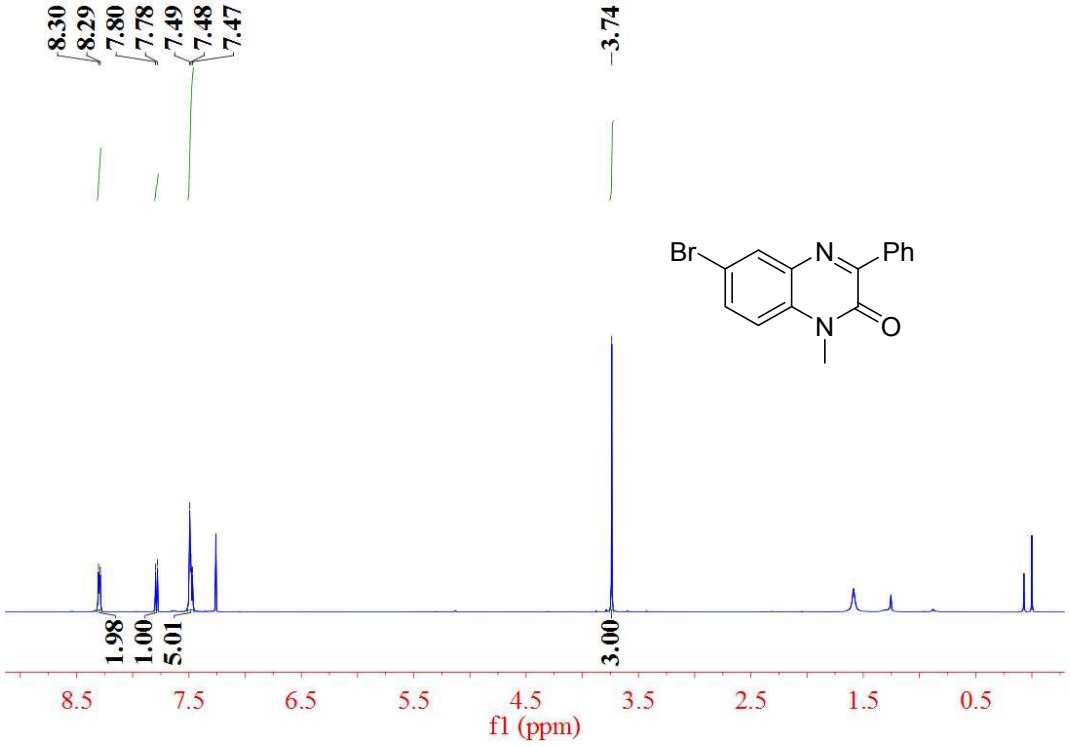

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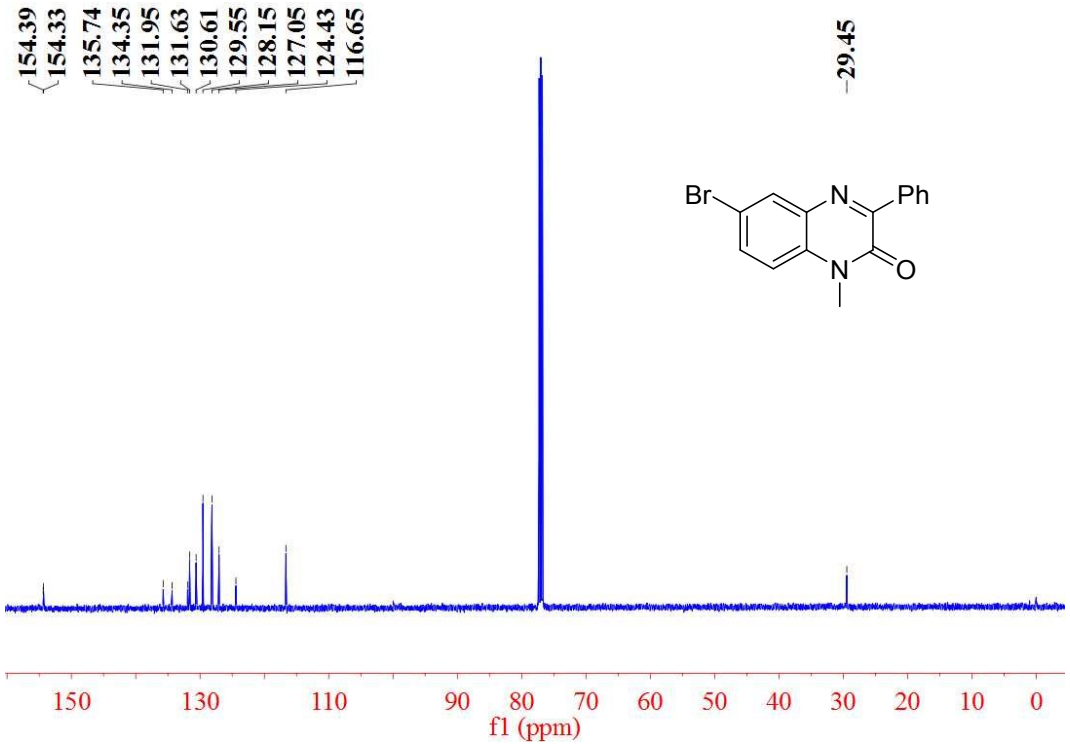

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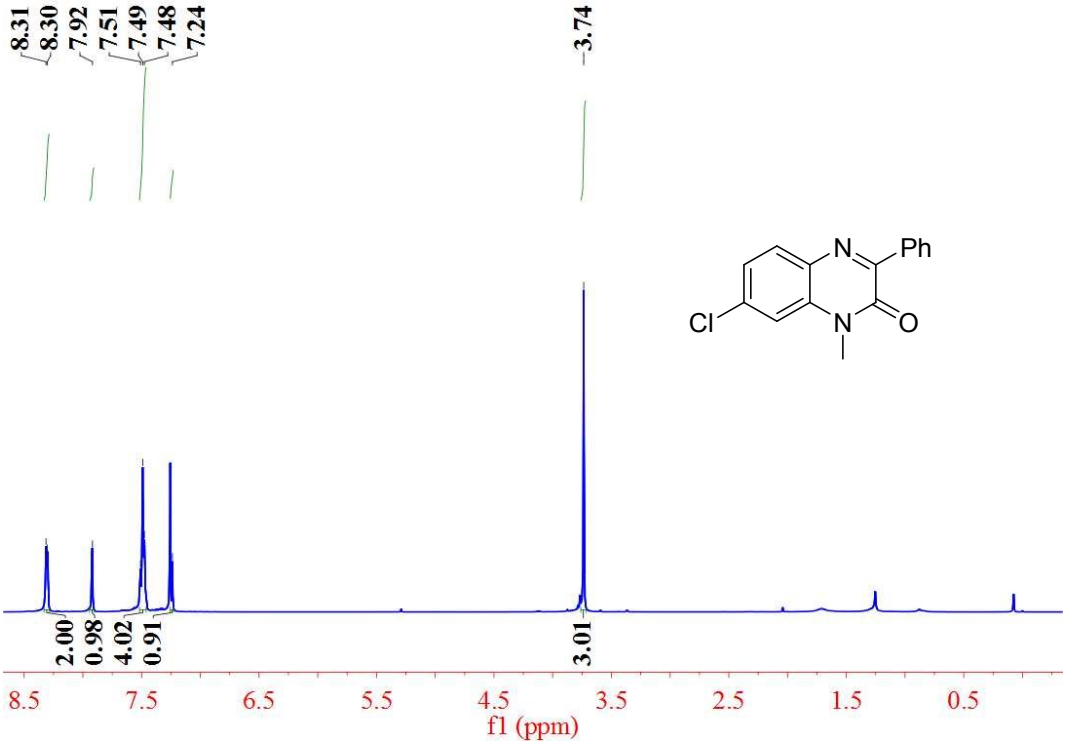

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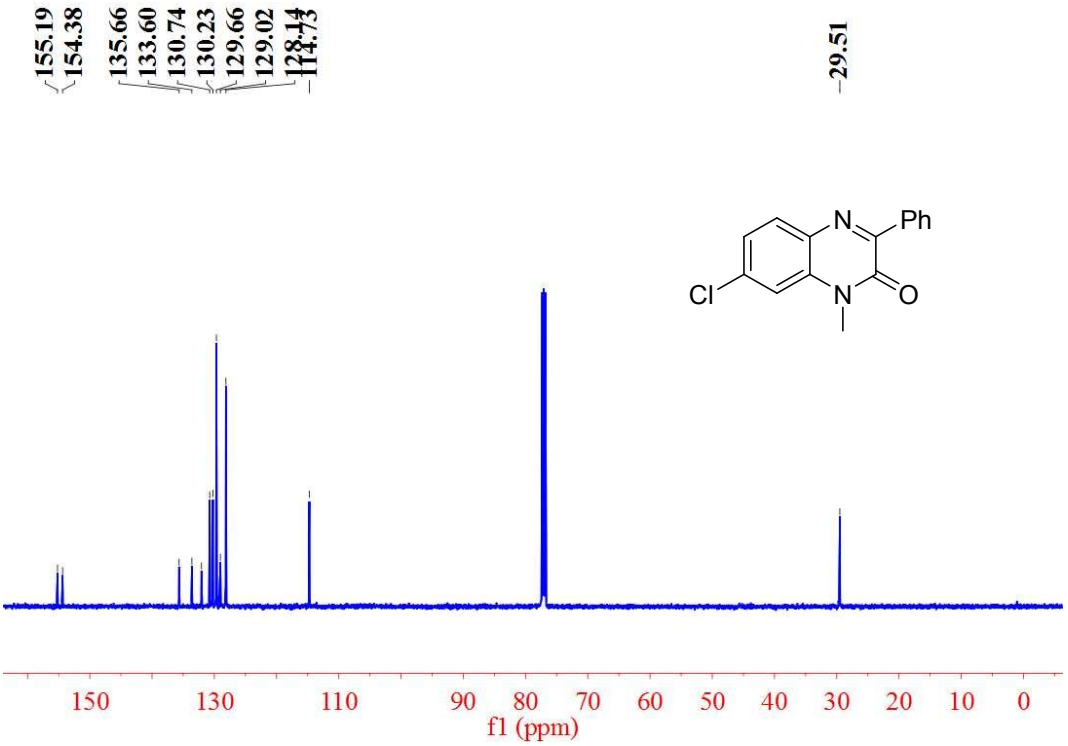

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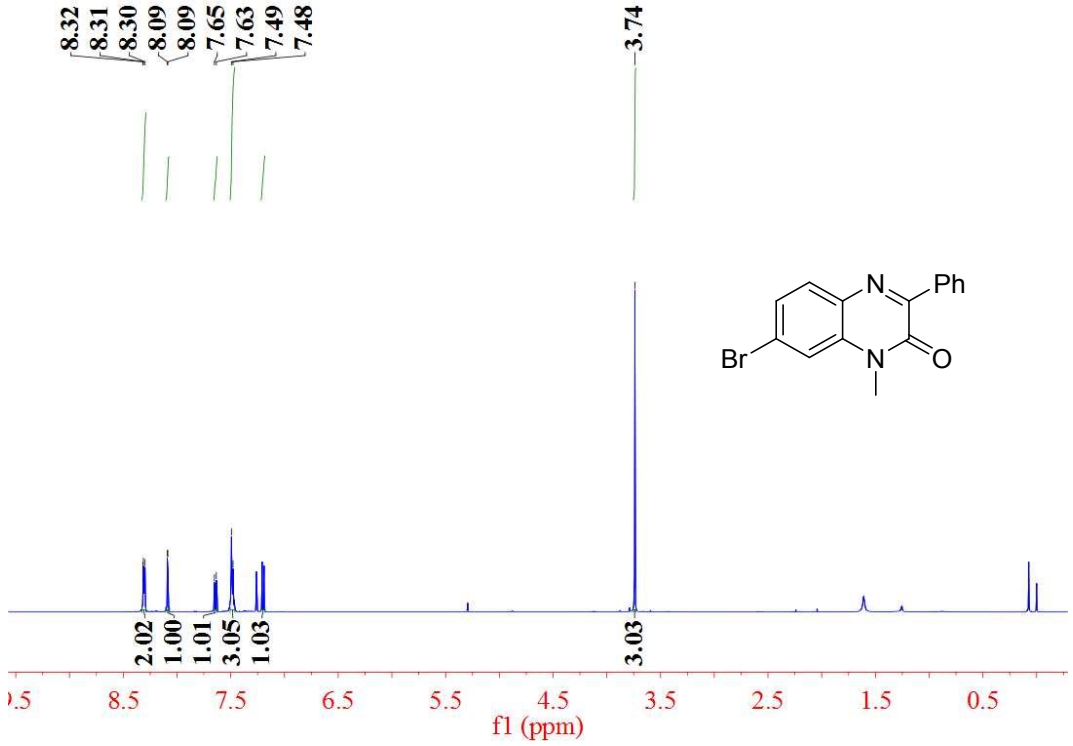

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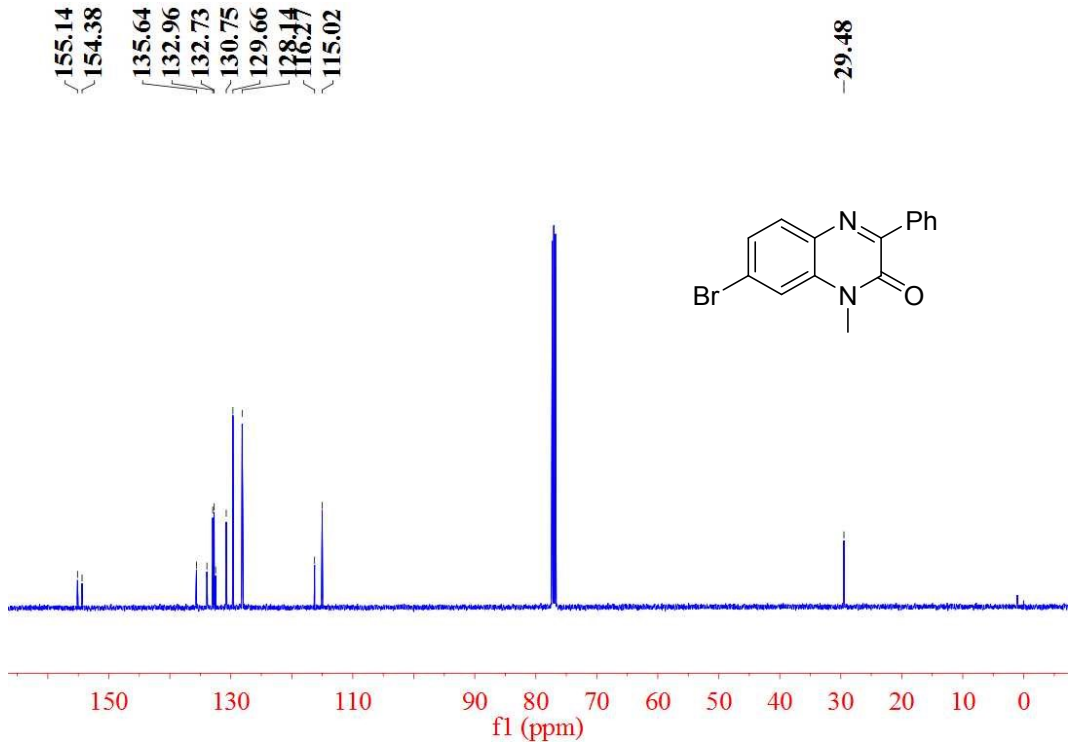

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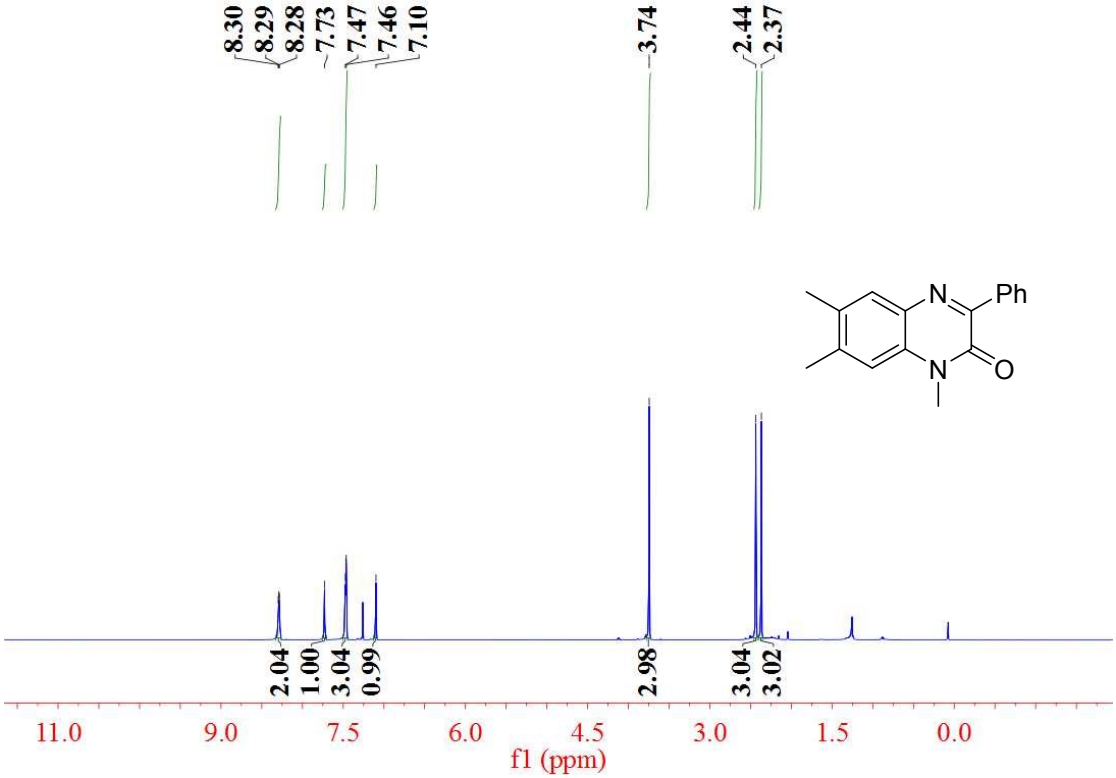

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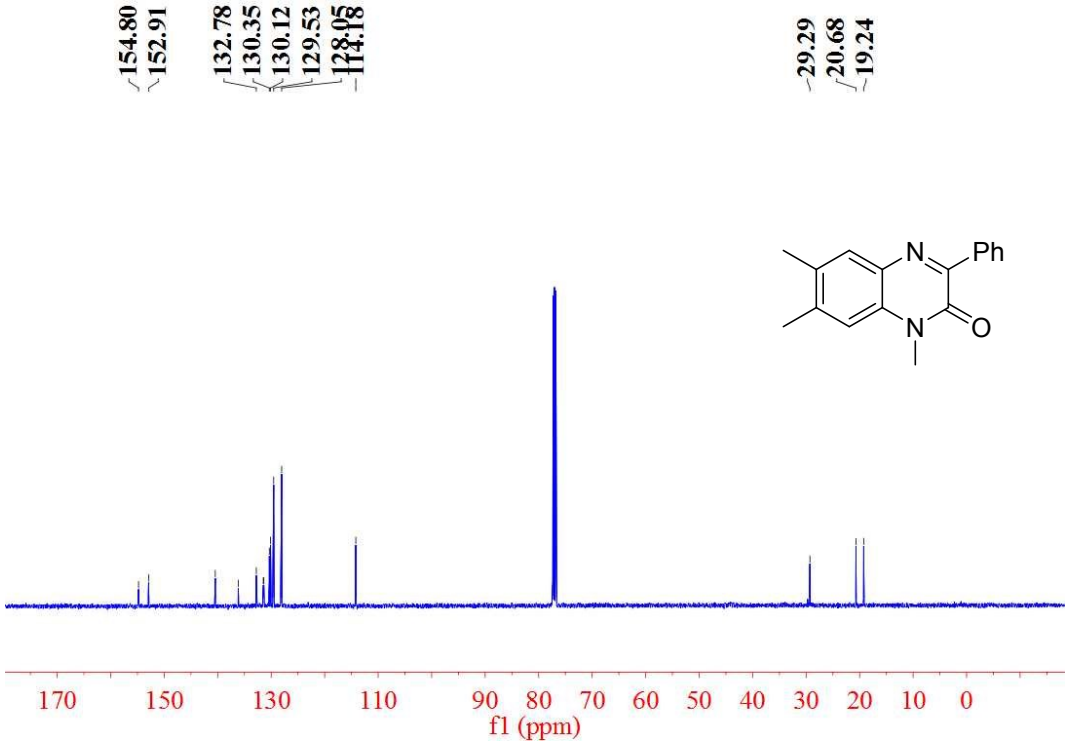

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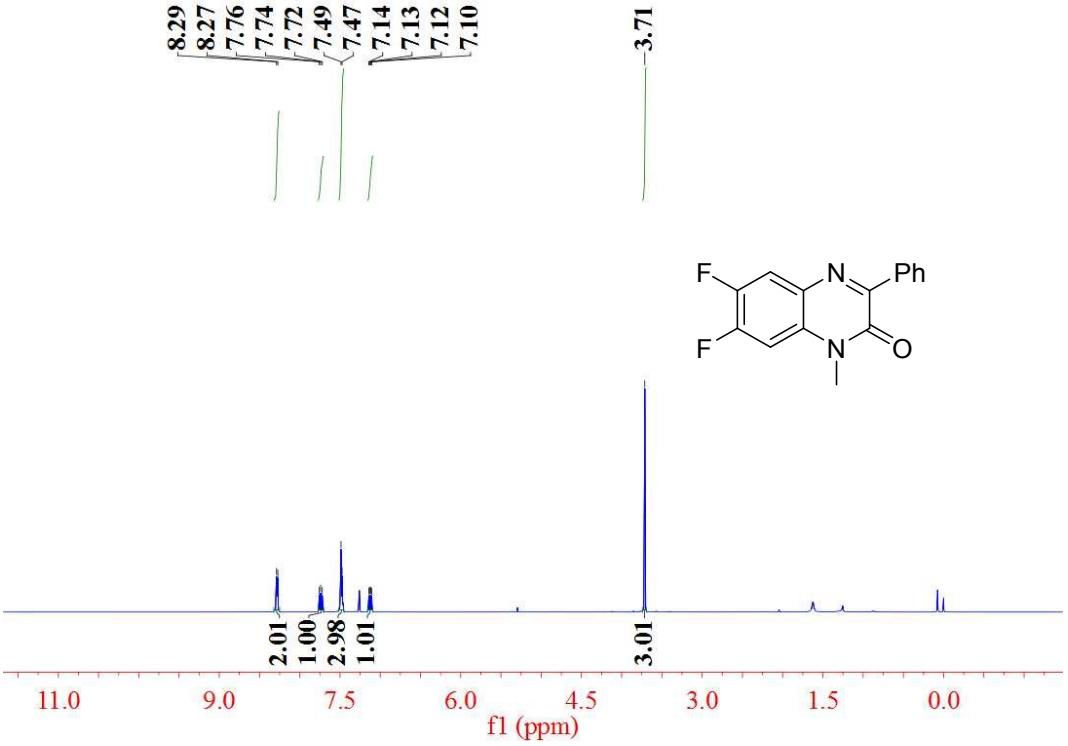

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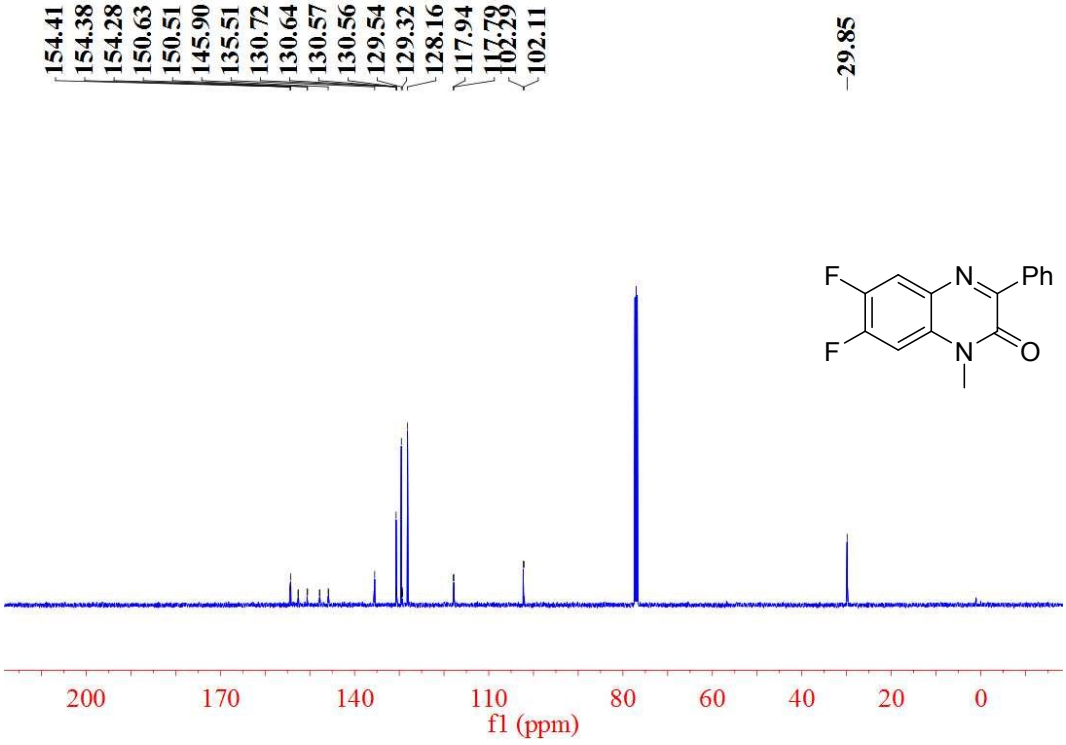

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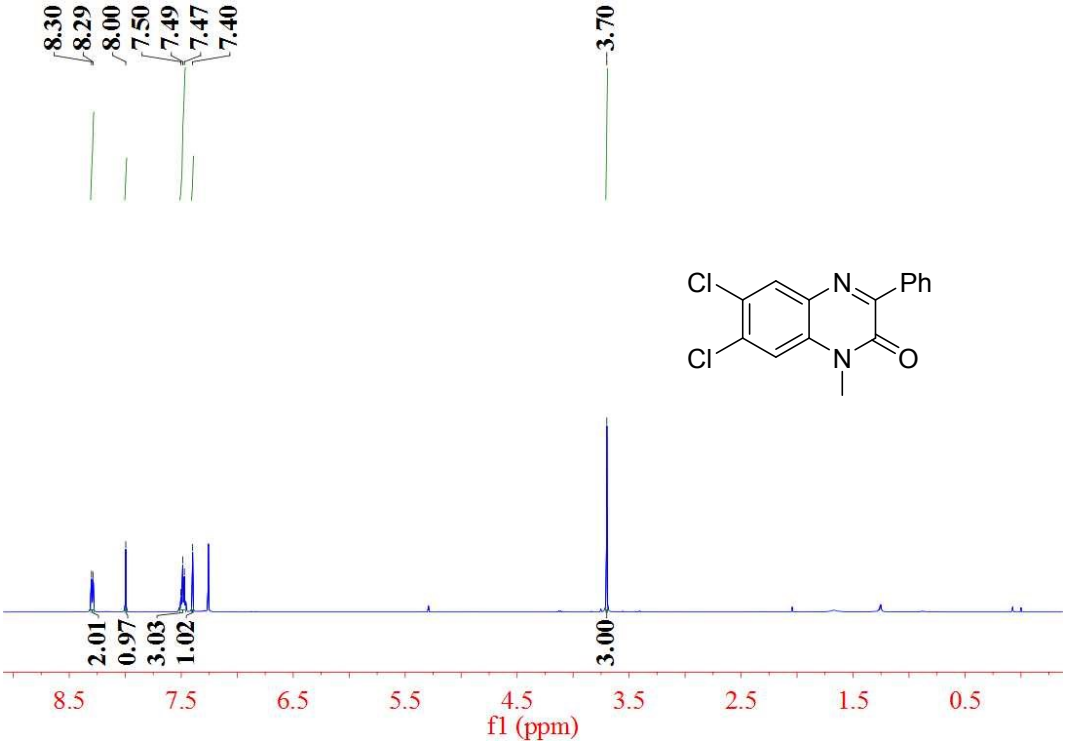

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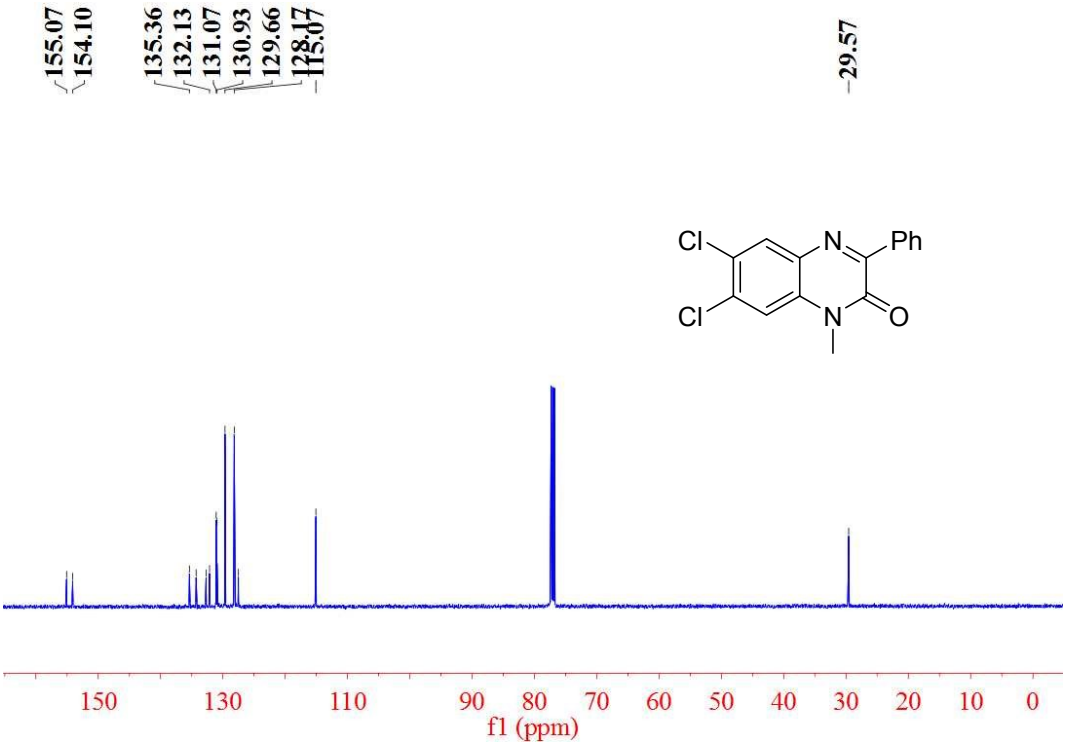

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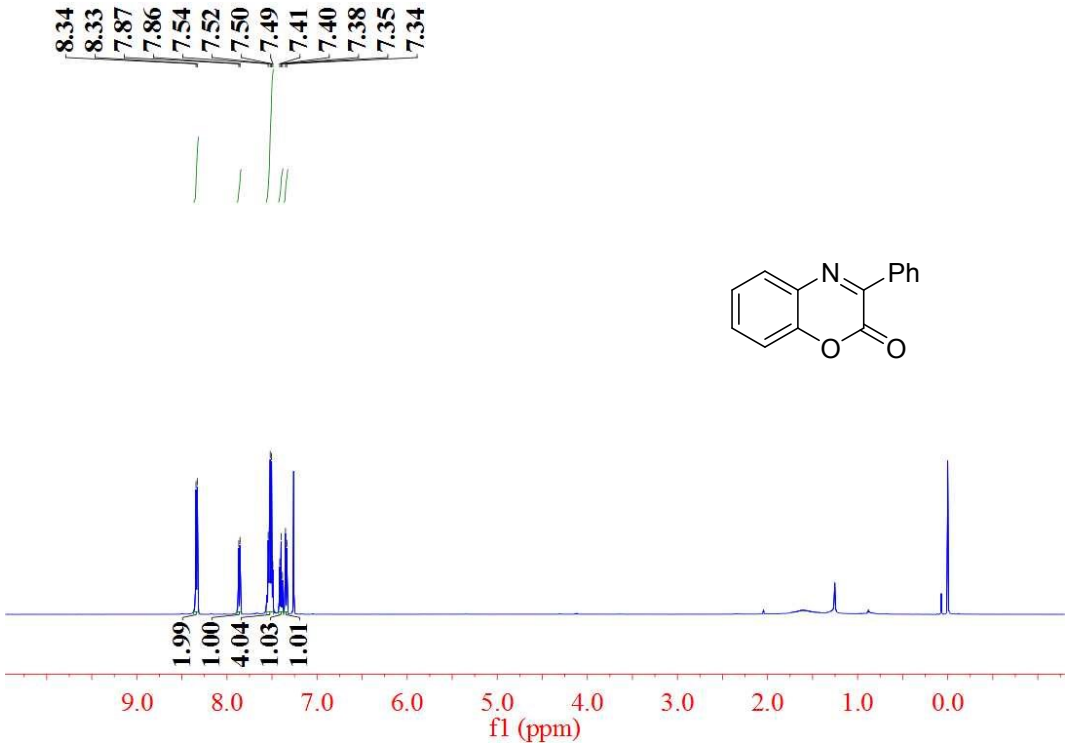

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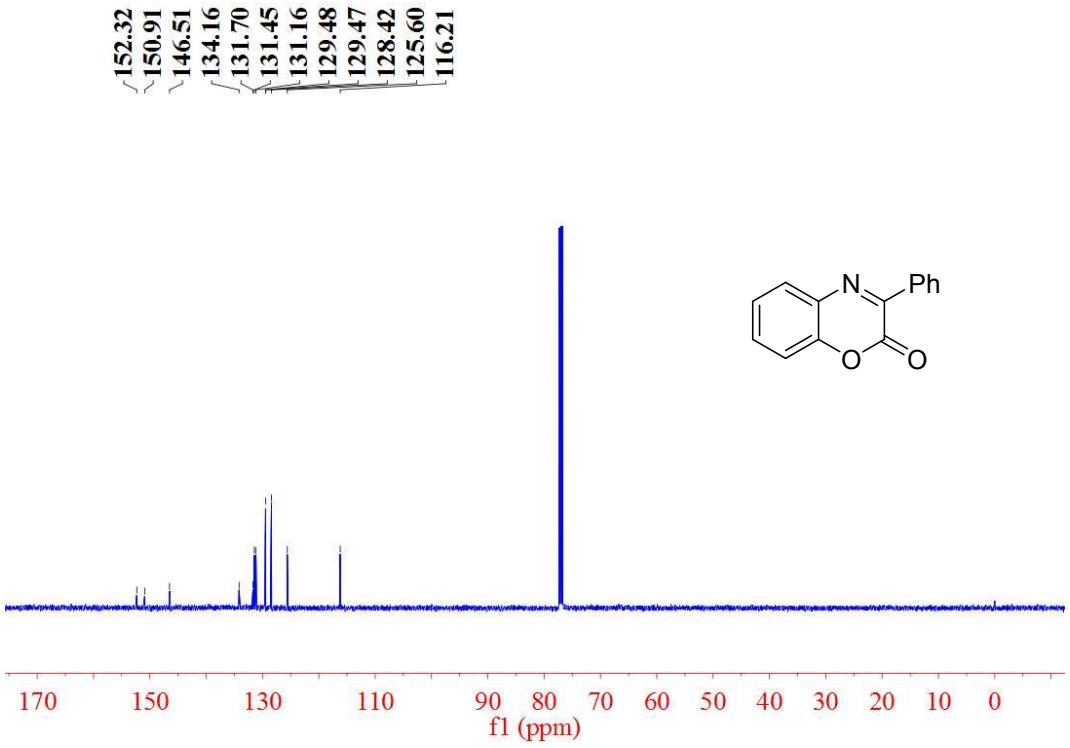

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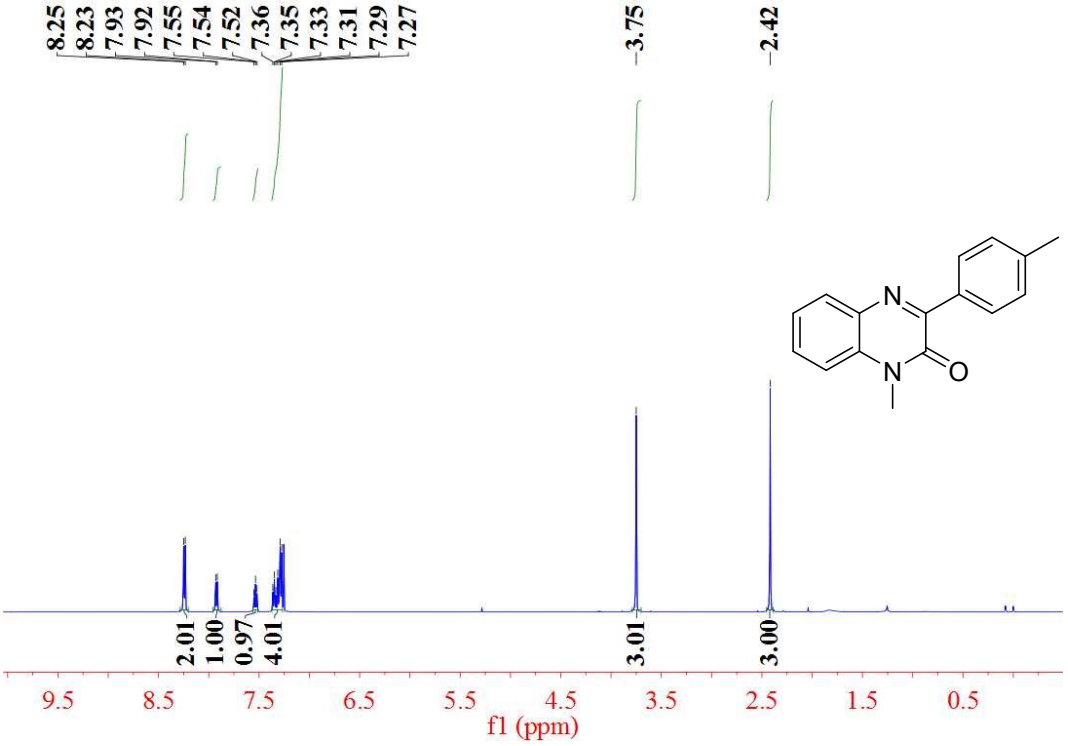
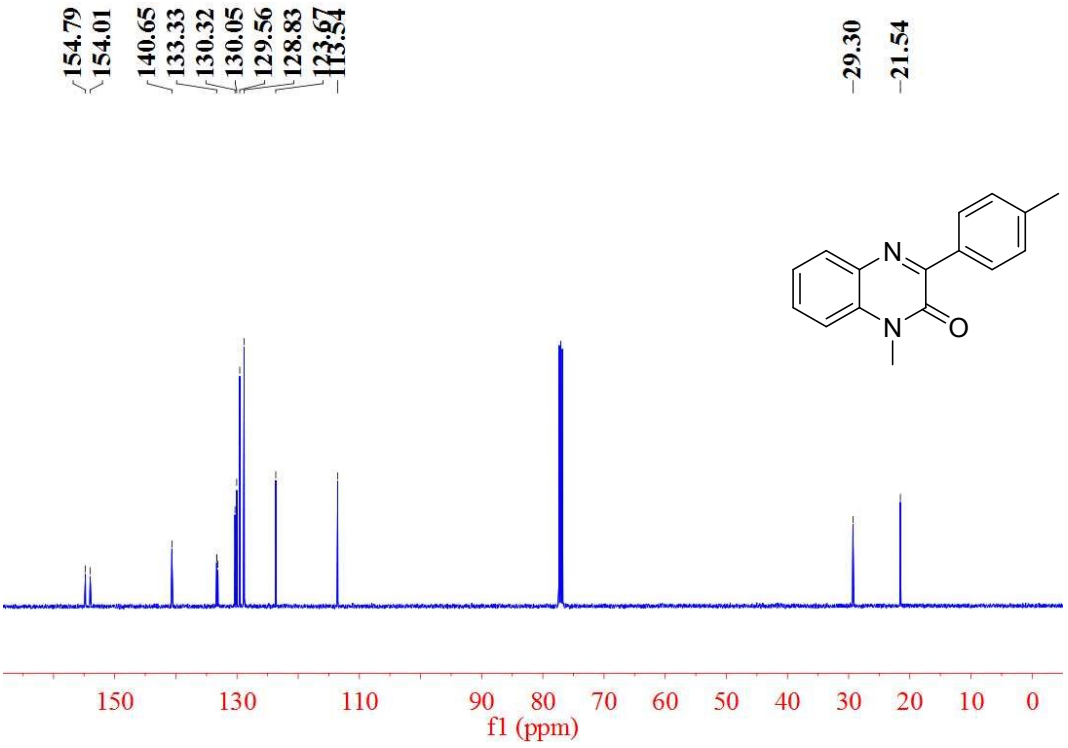
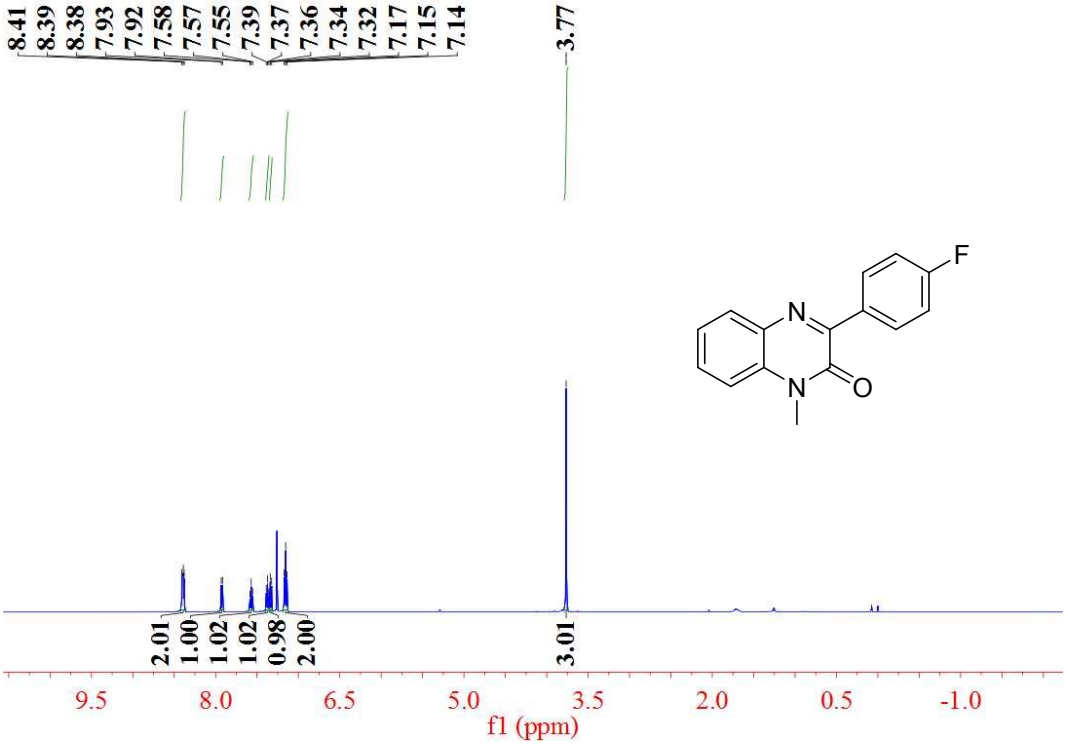


3bb ^{13}C NMR



3bc ^{1}H NMR



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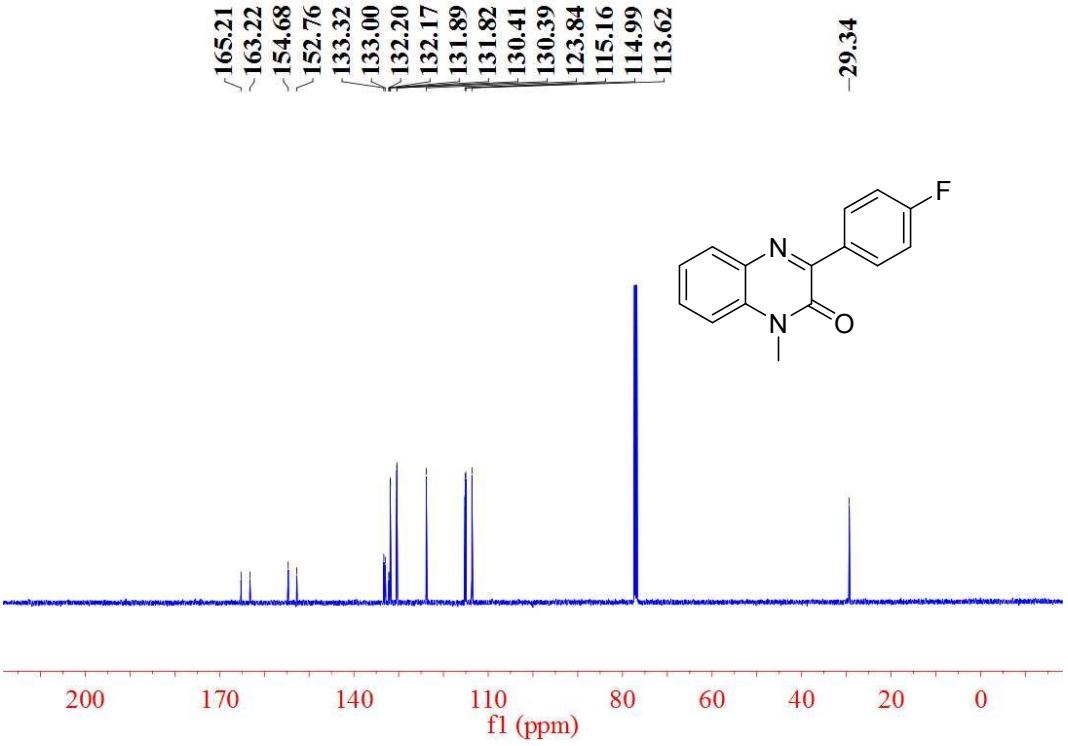

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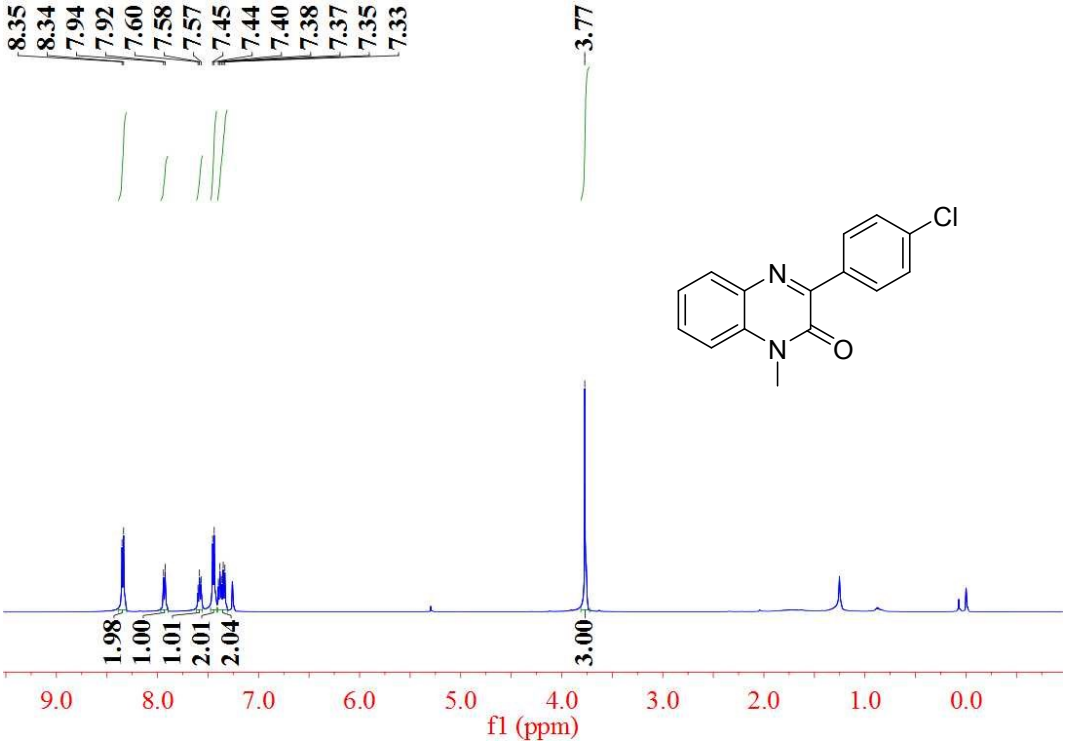

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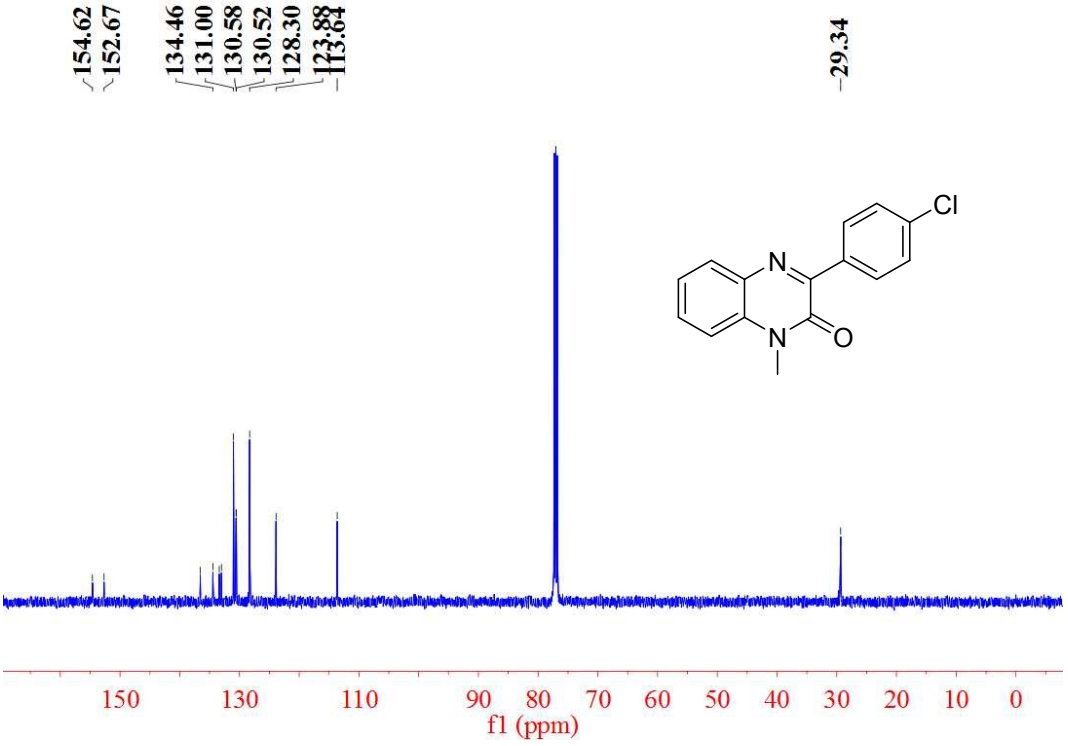

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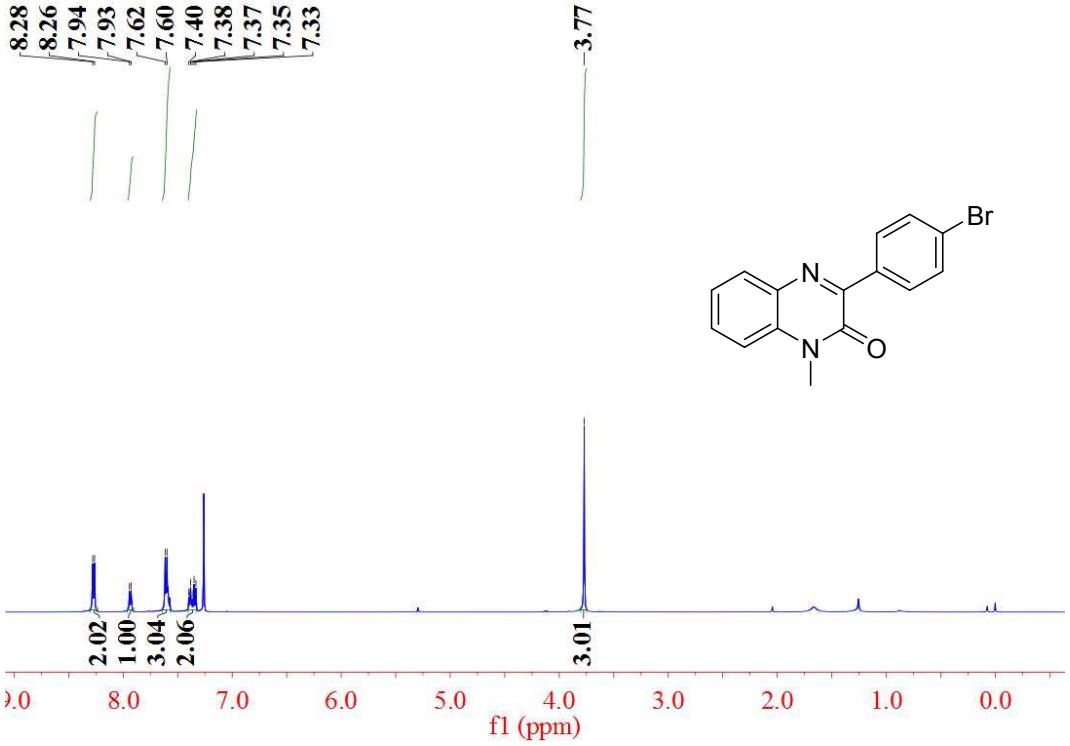

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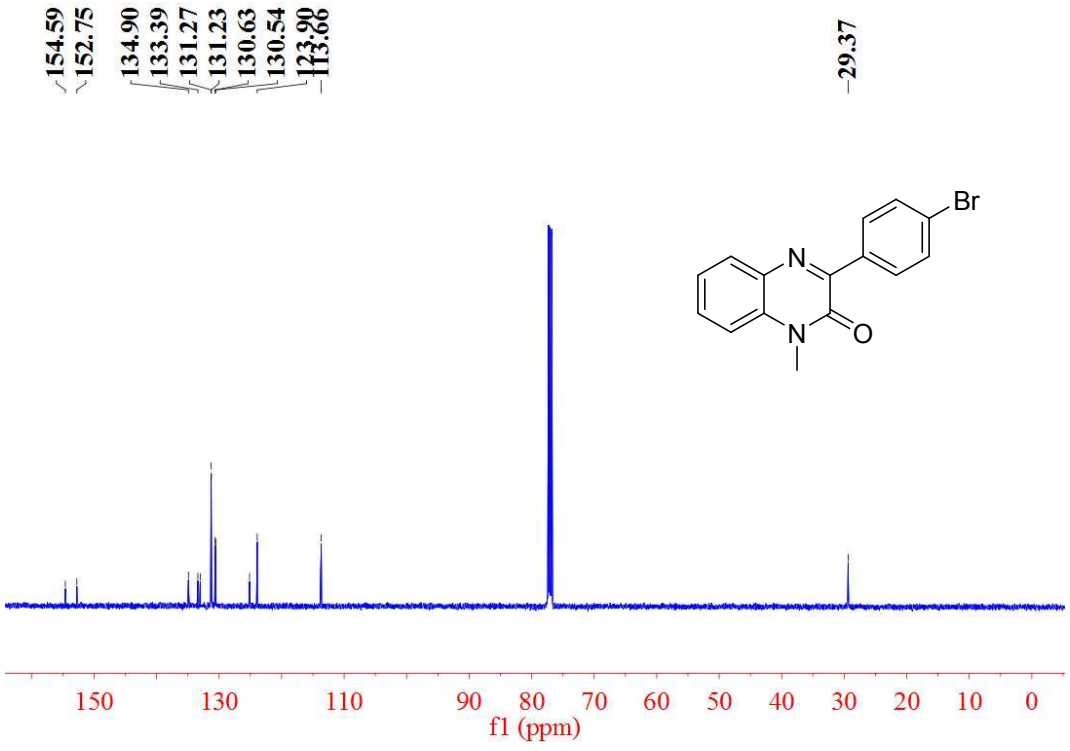

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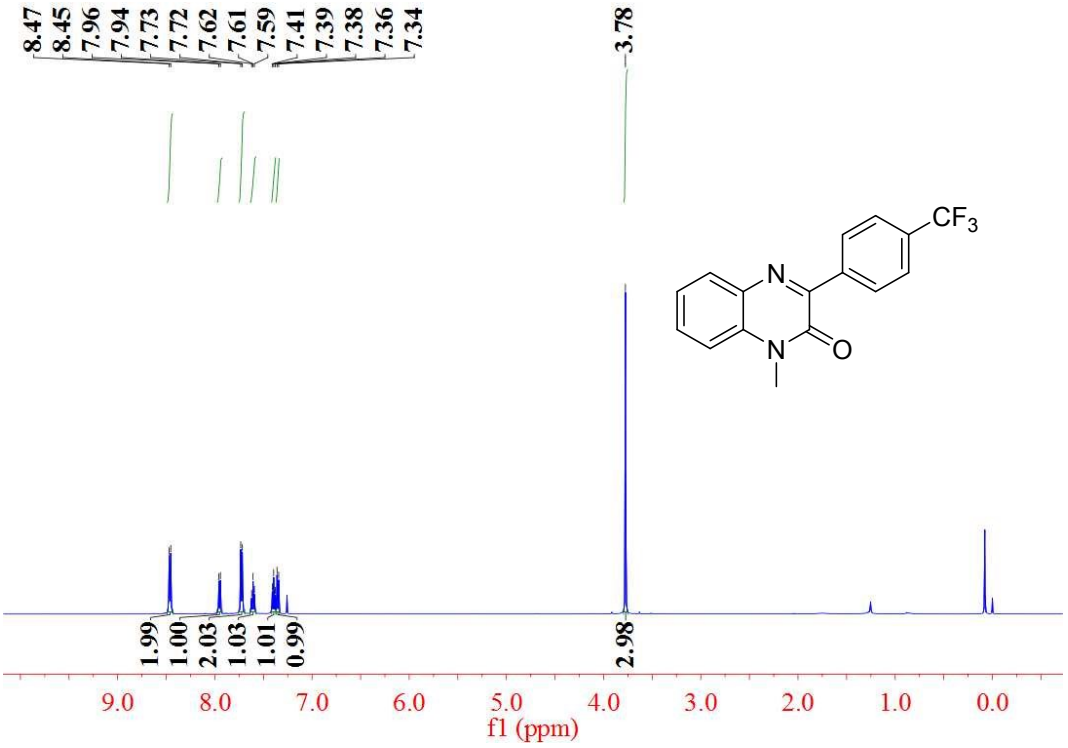

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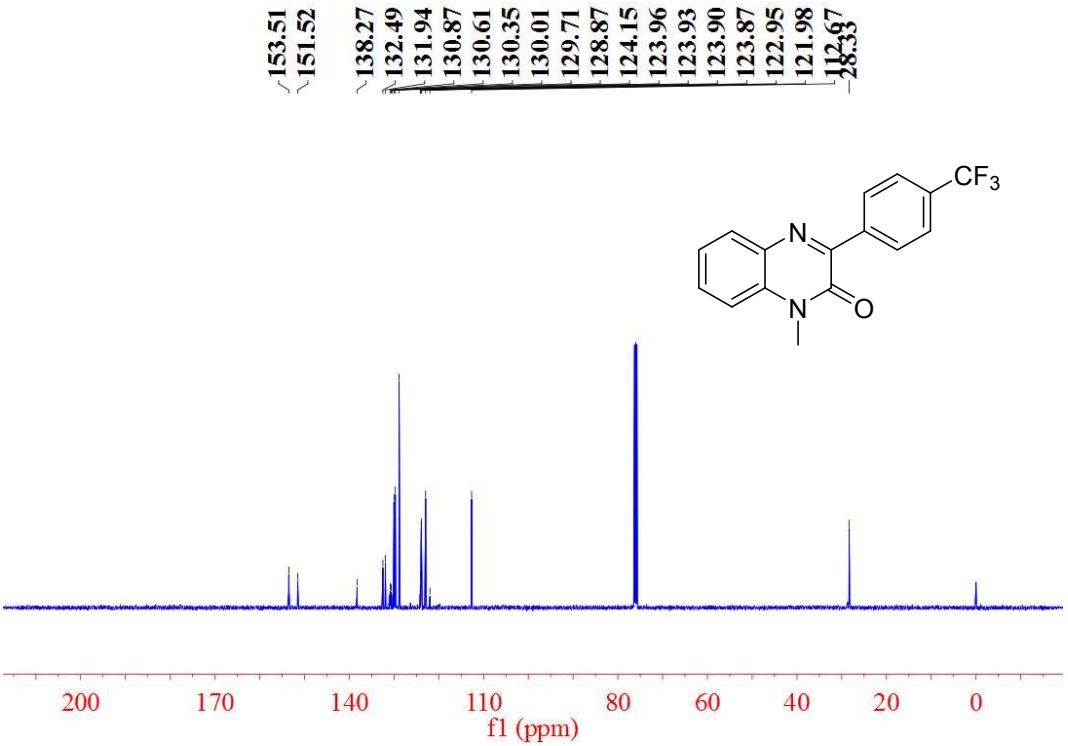

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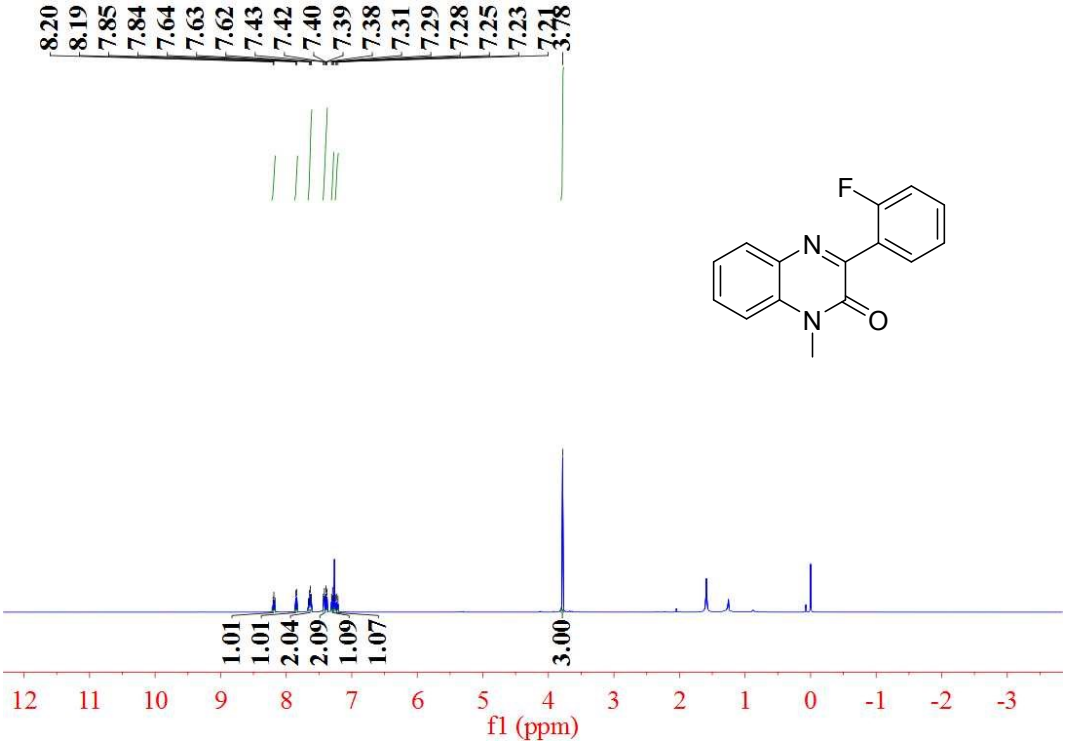

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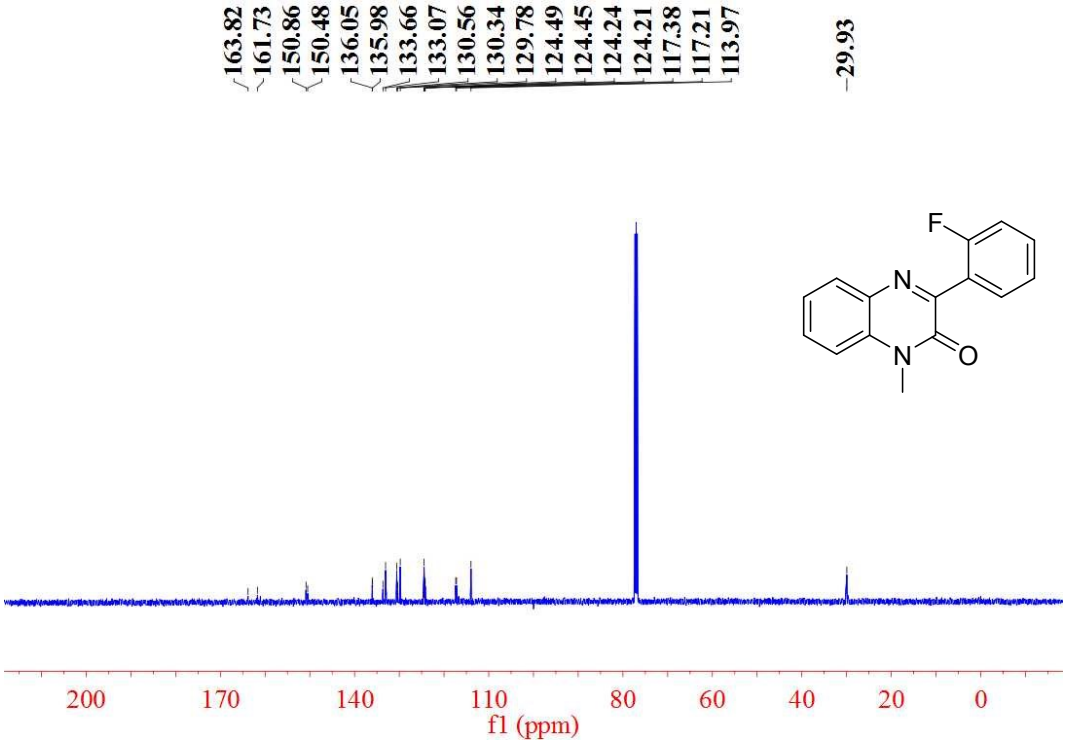

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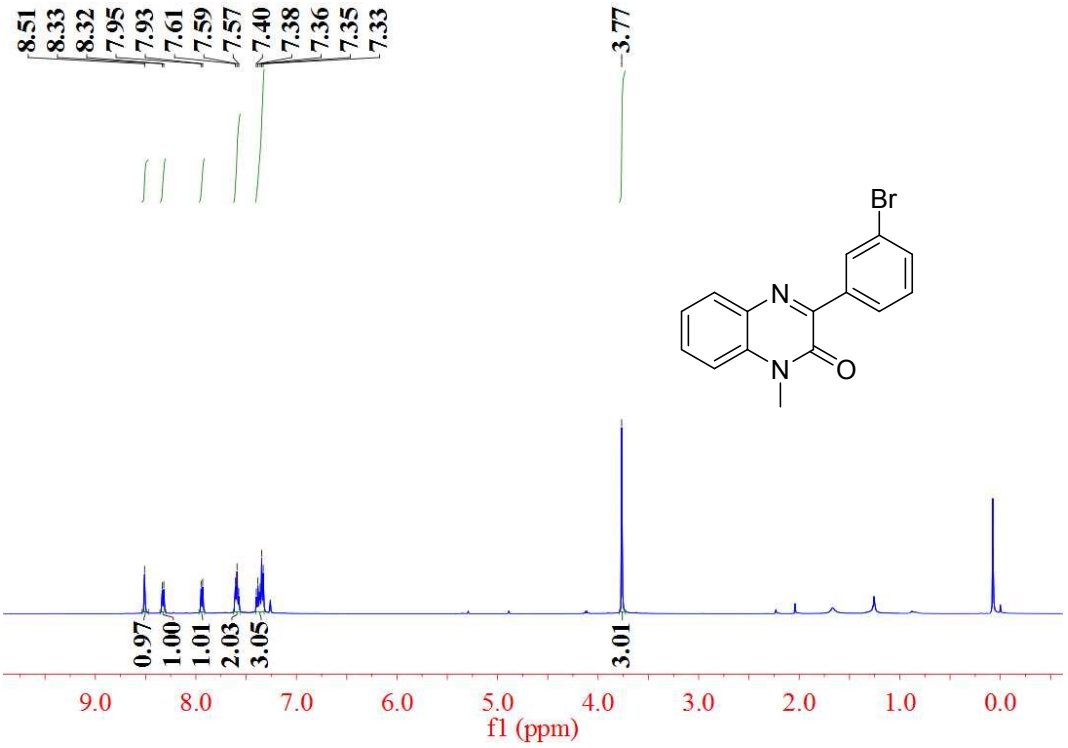
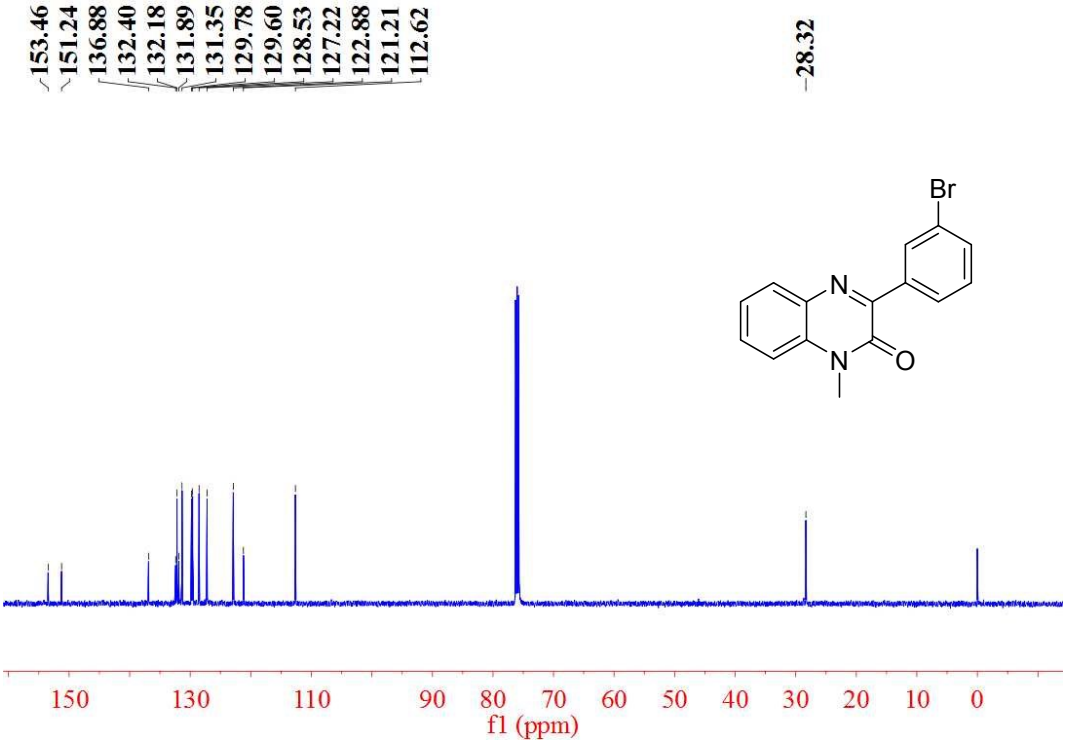


3bh ^{13}C NMR



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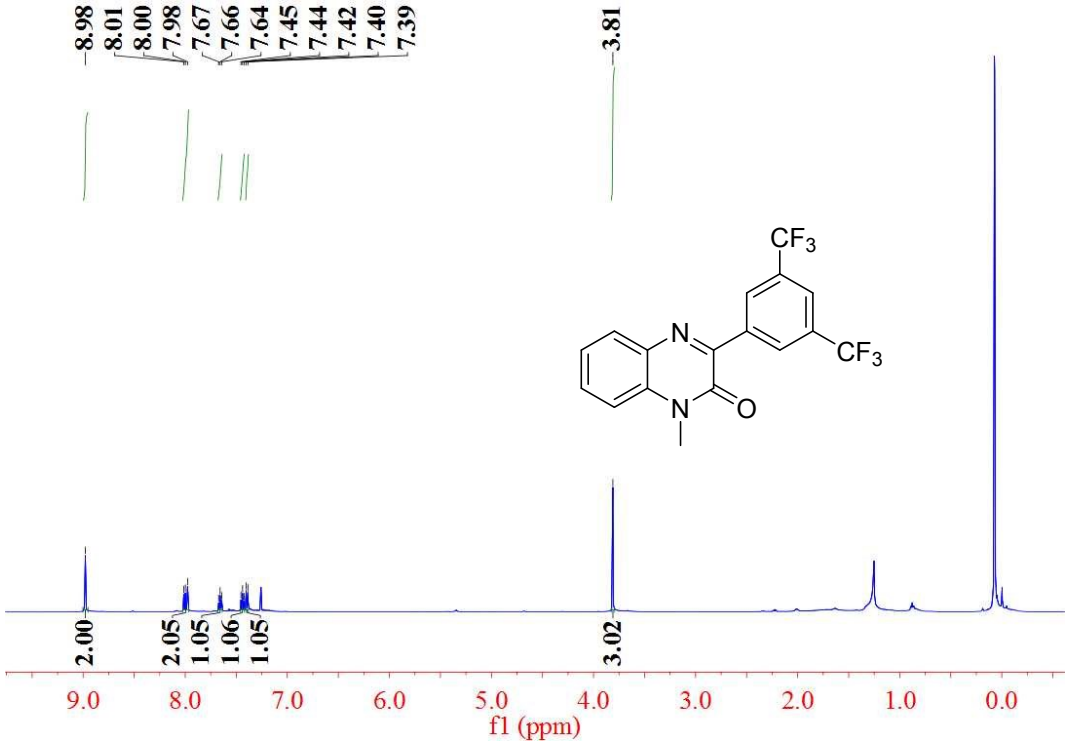

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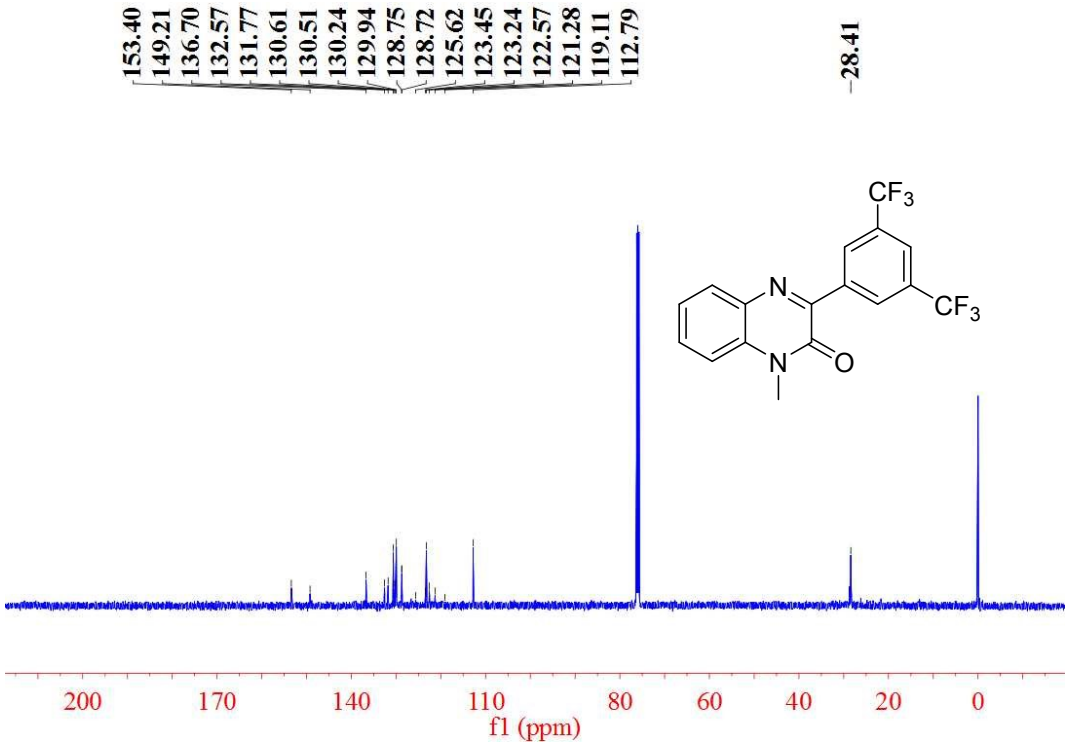

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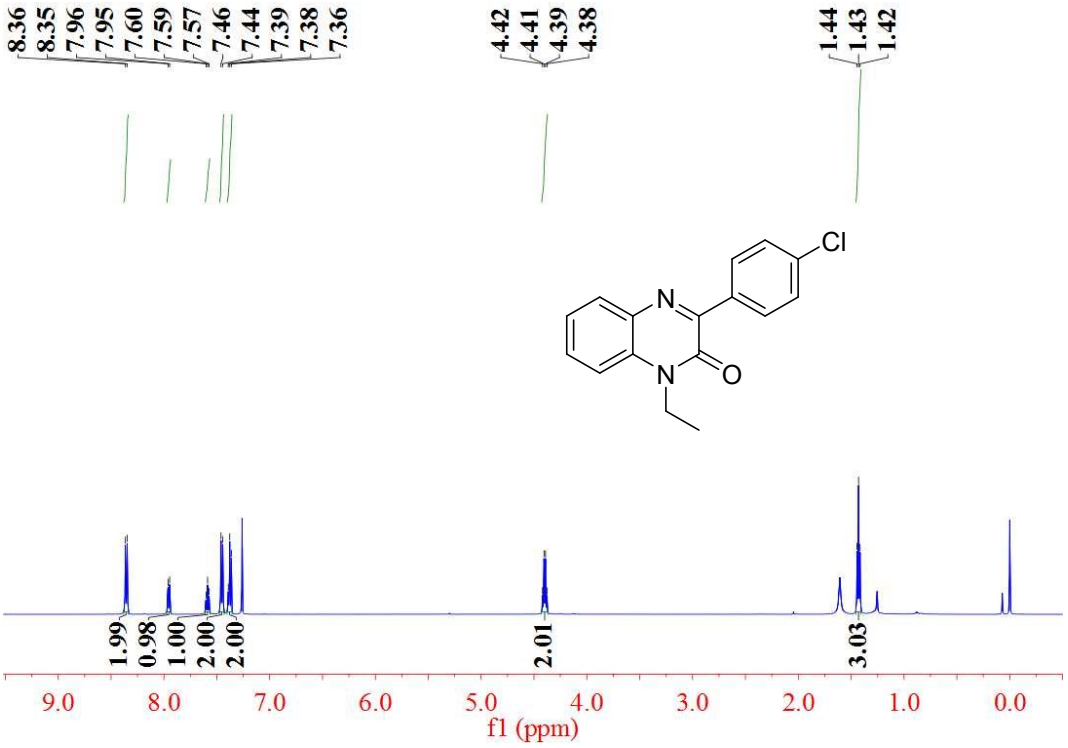

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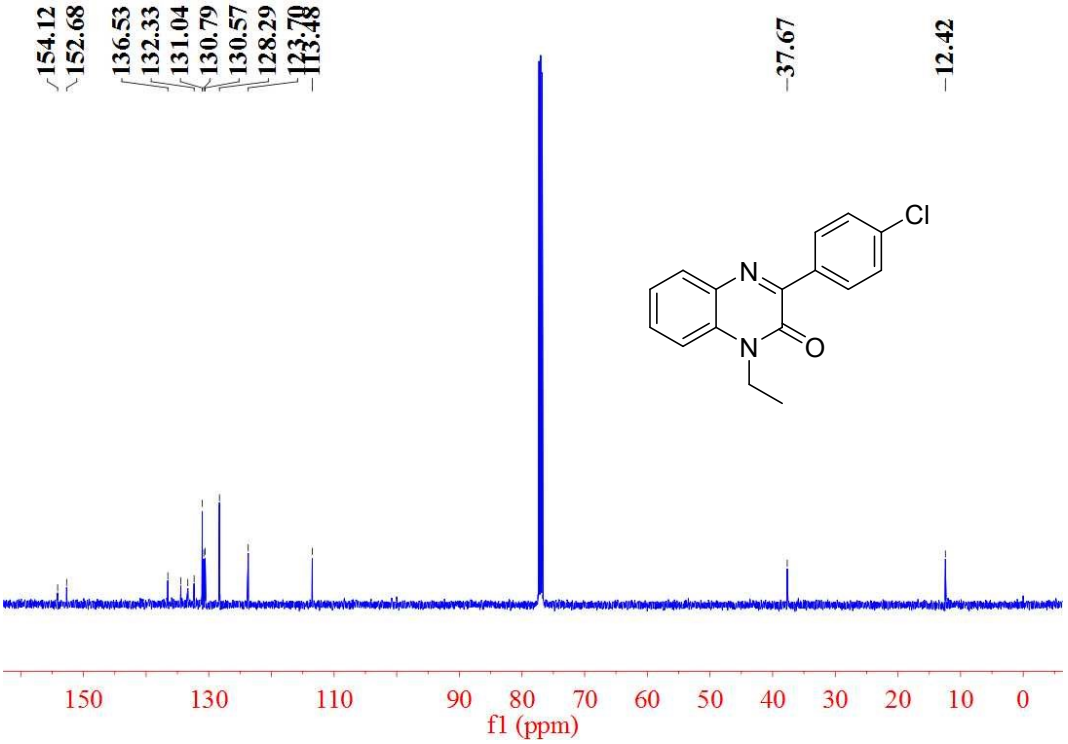
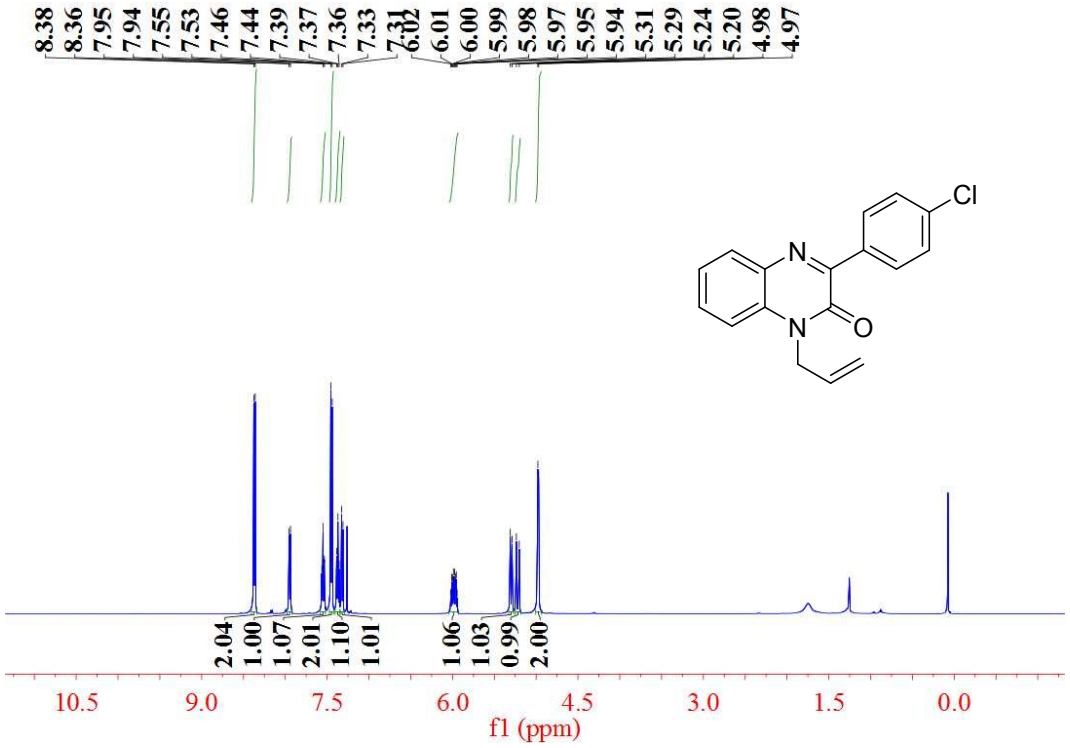


3bk ^{1}H NMR



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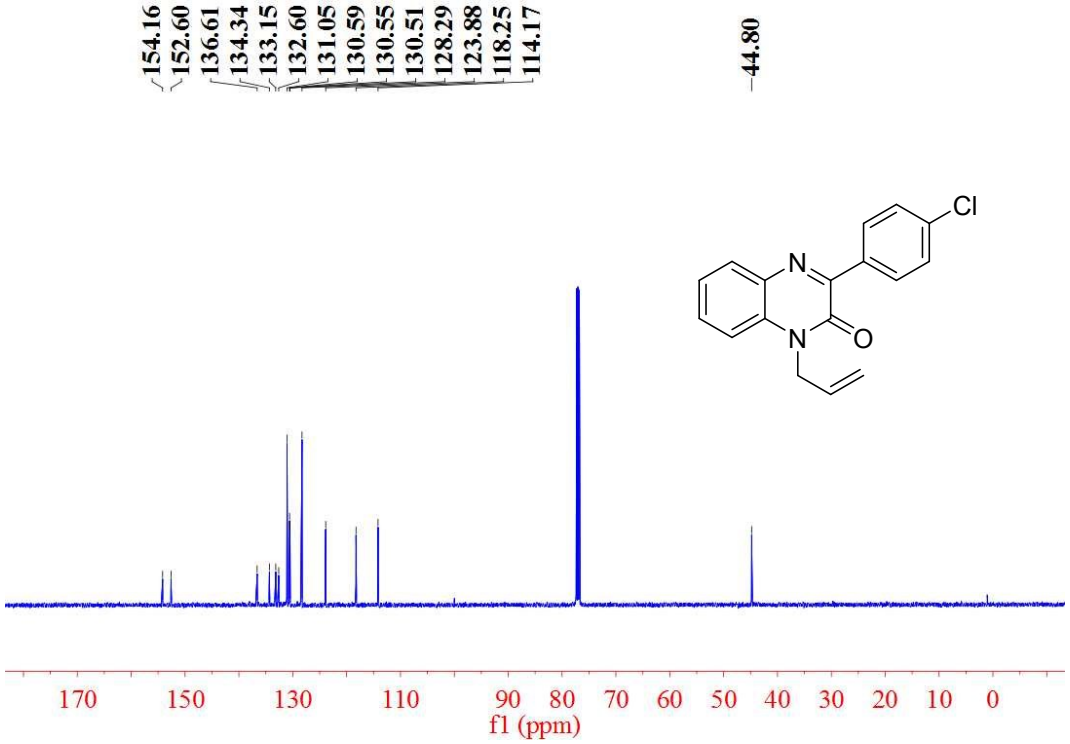

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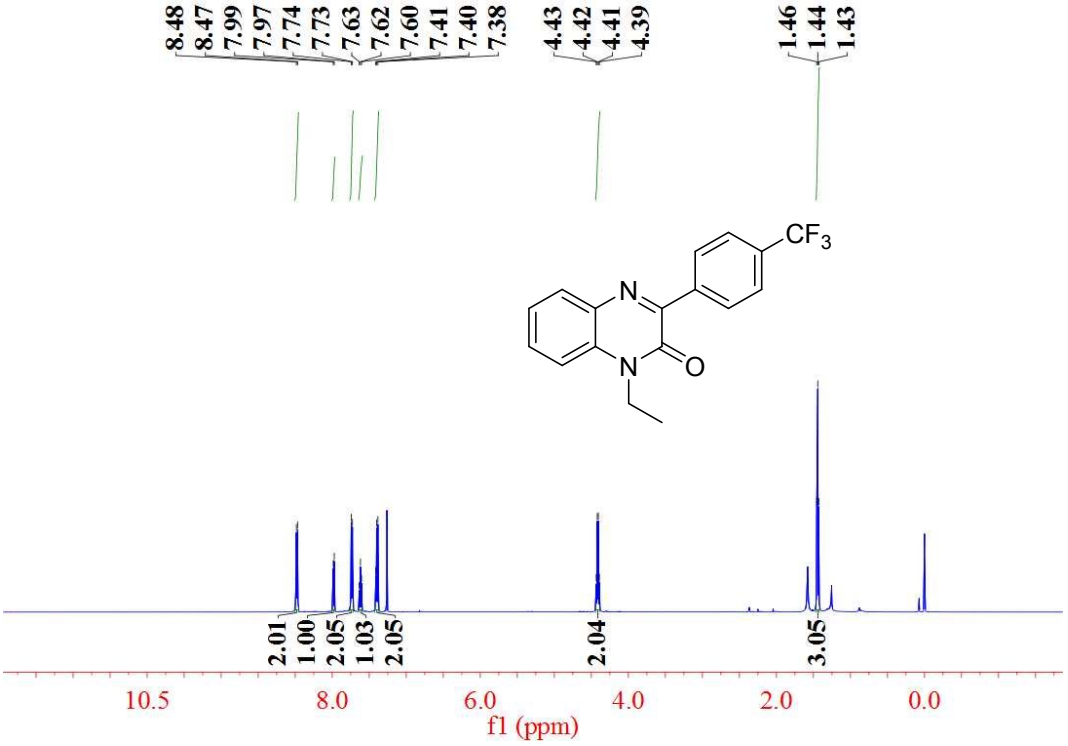

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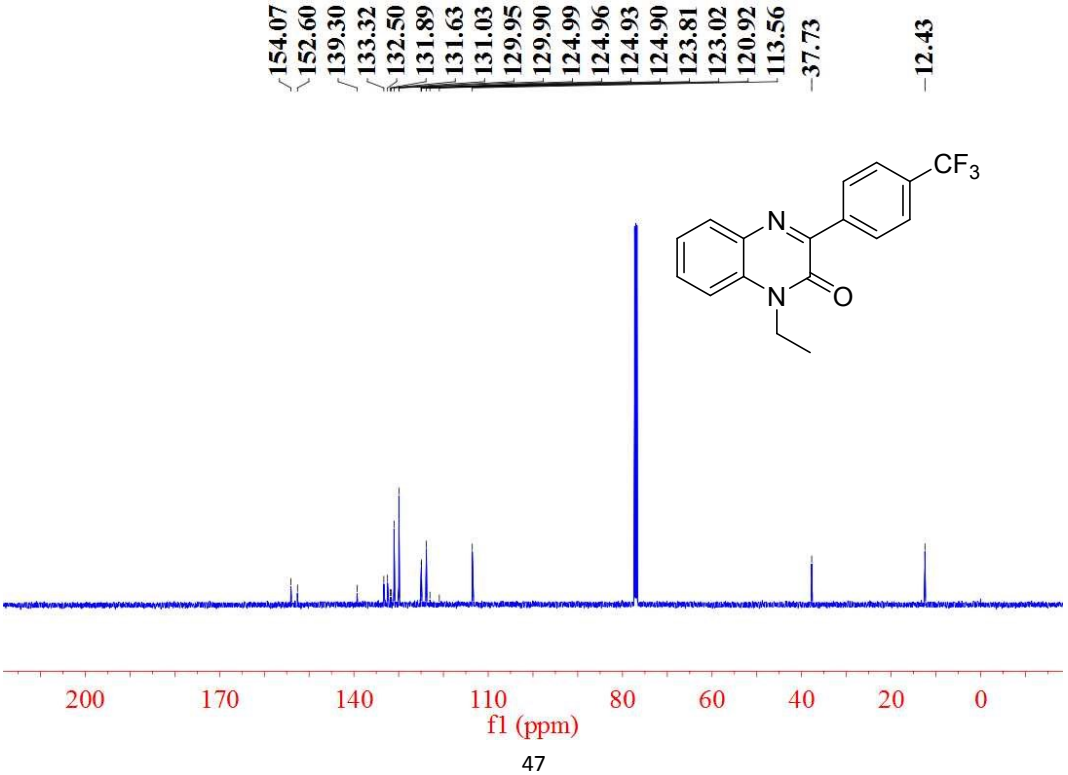

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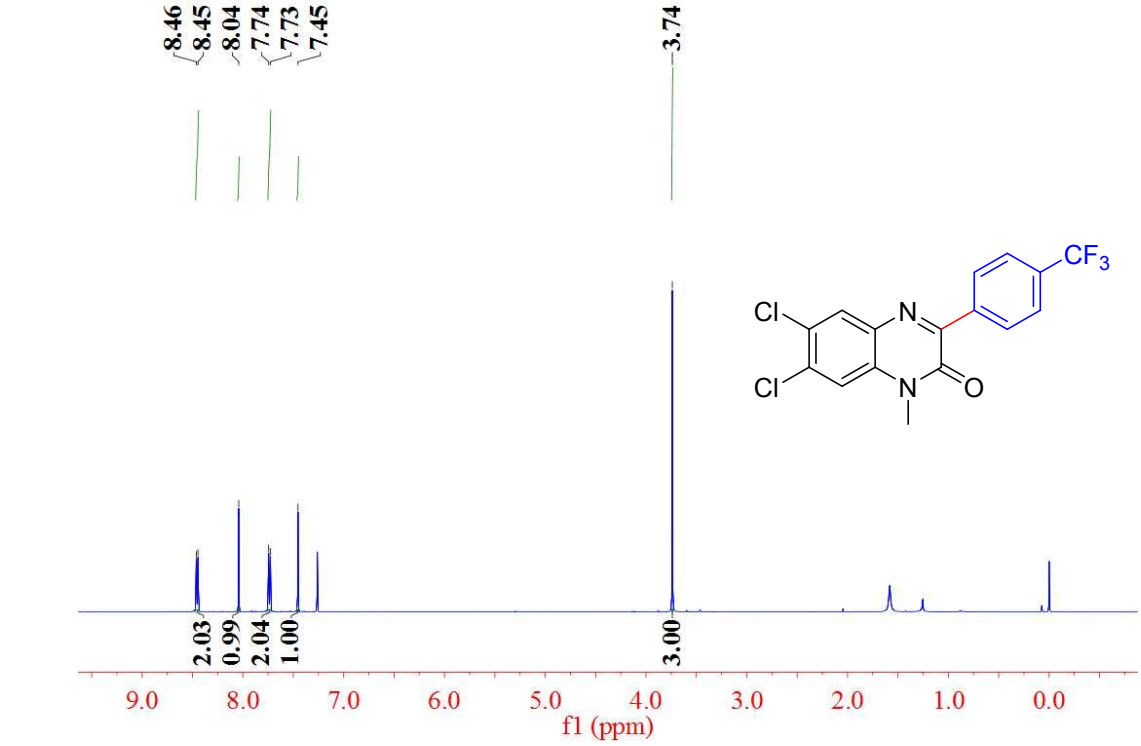

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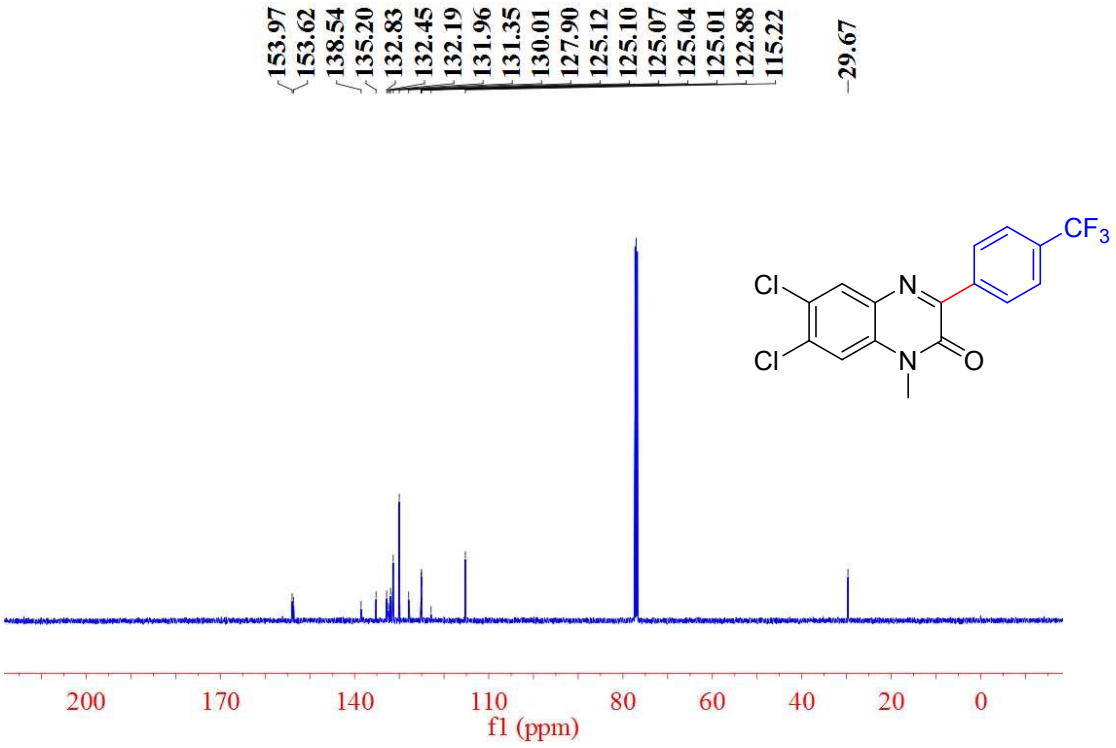

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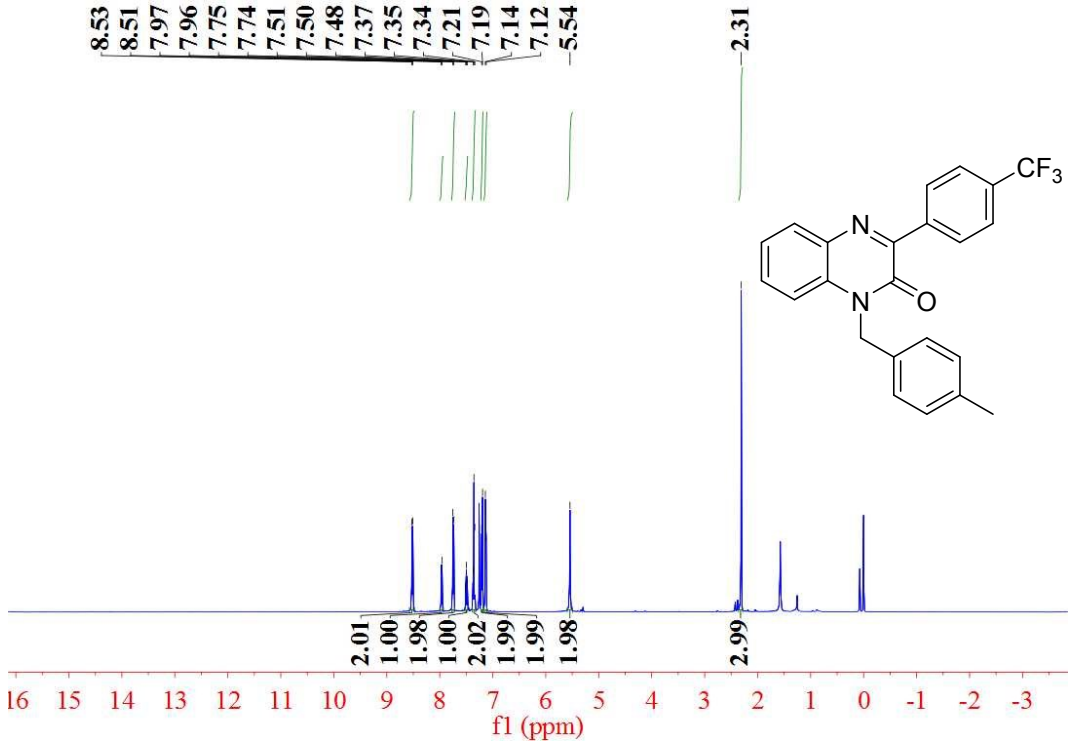
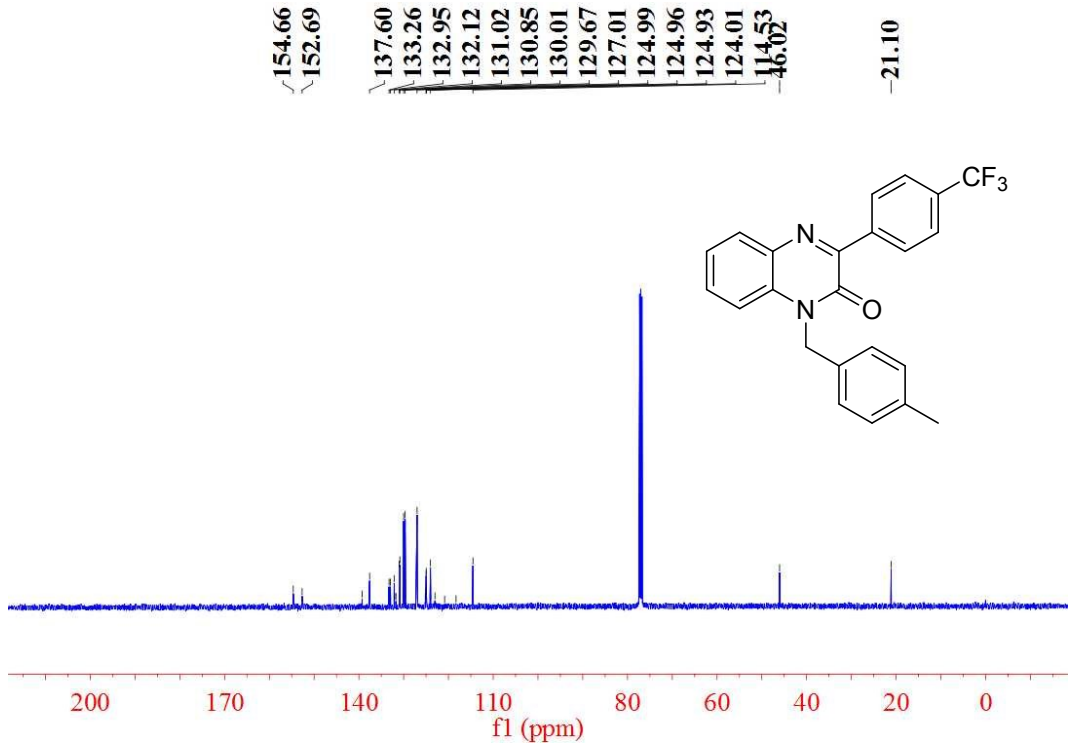


3bn ^{13}C NMR



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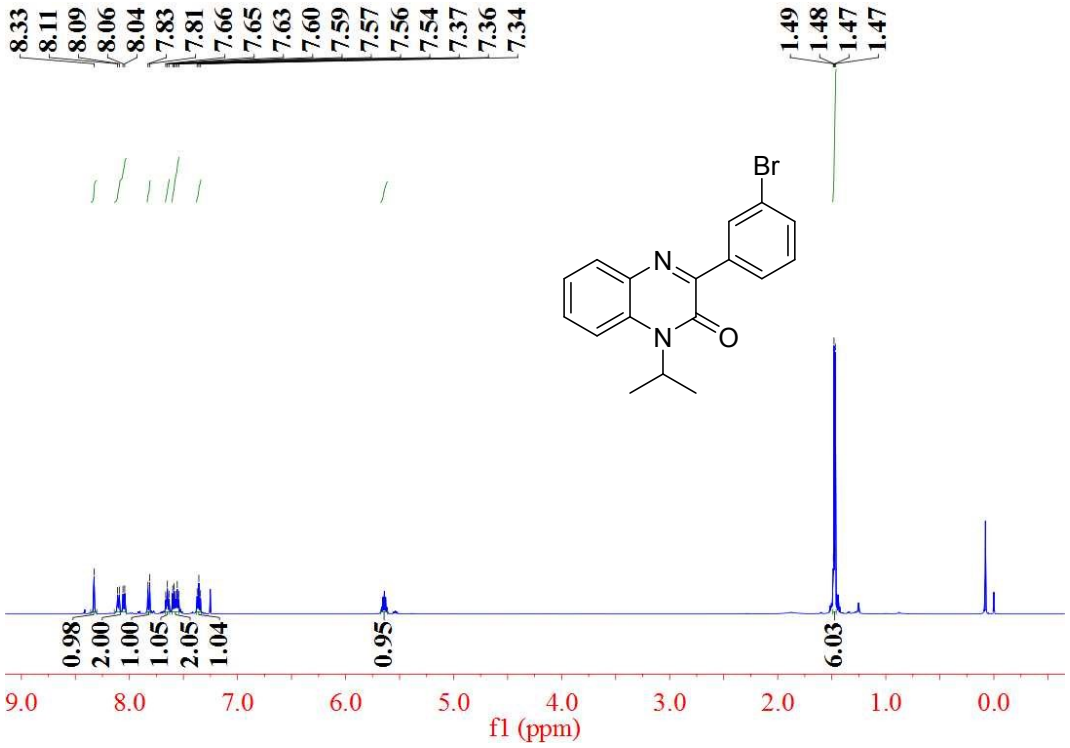

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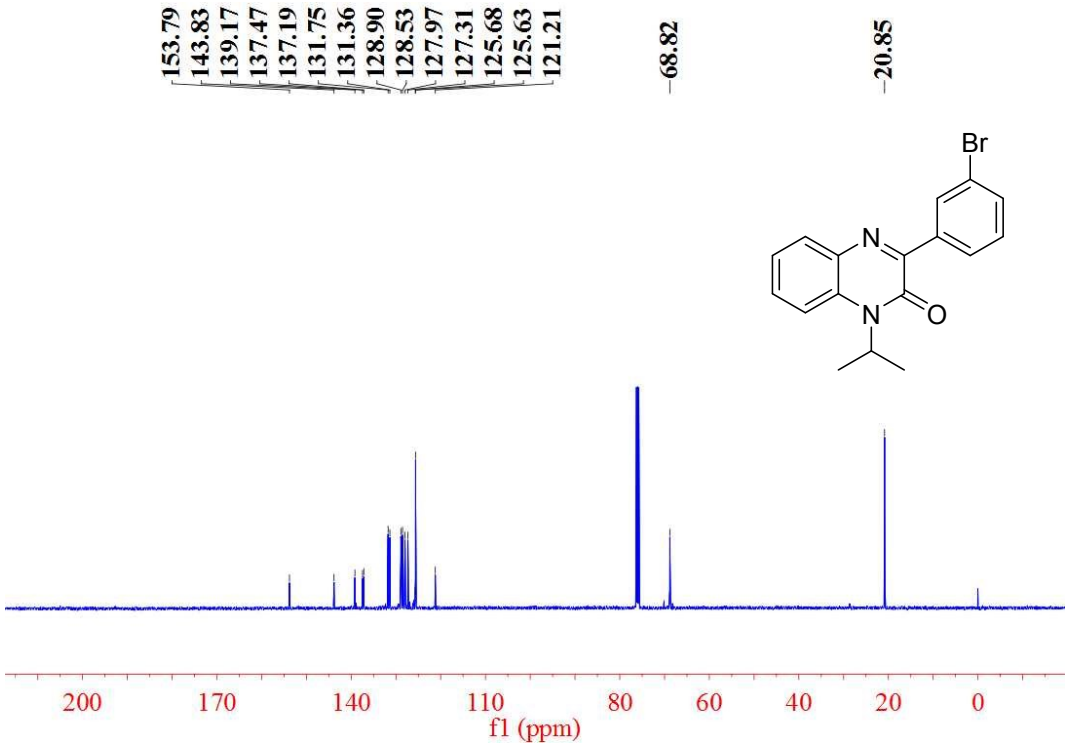

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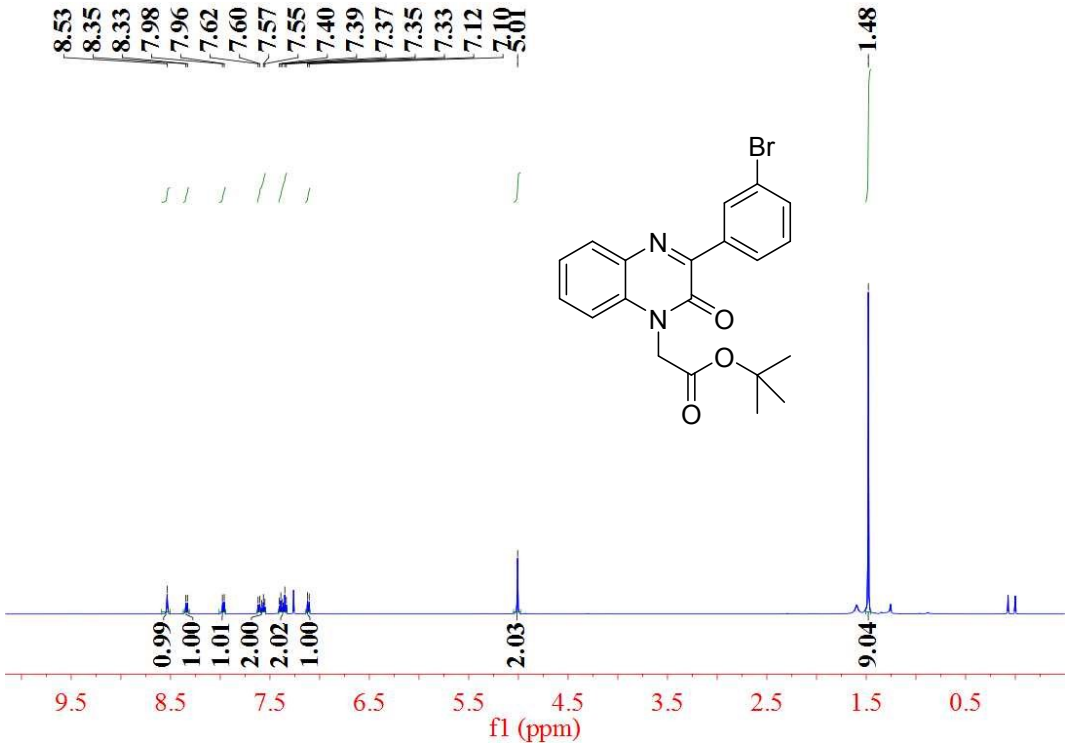
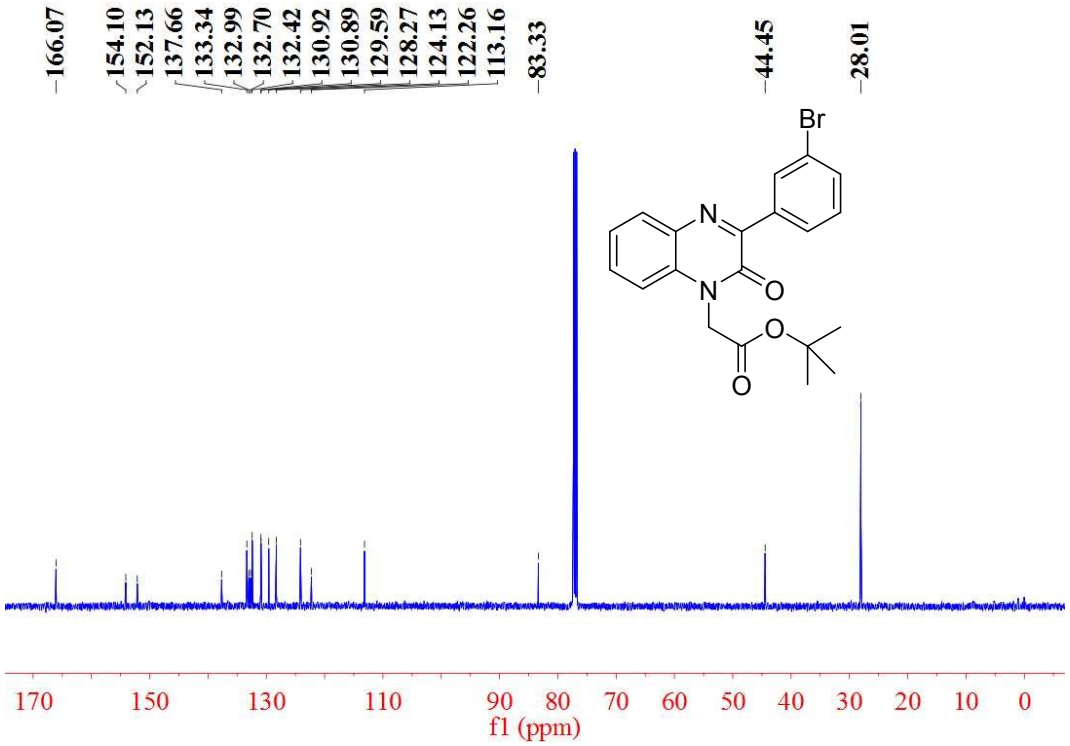
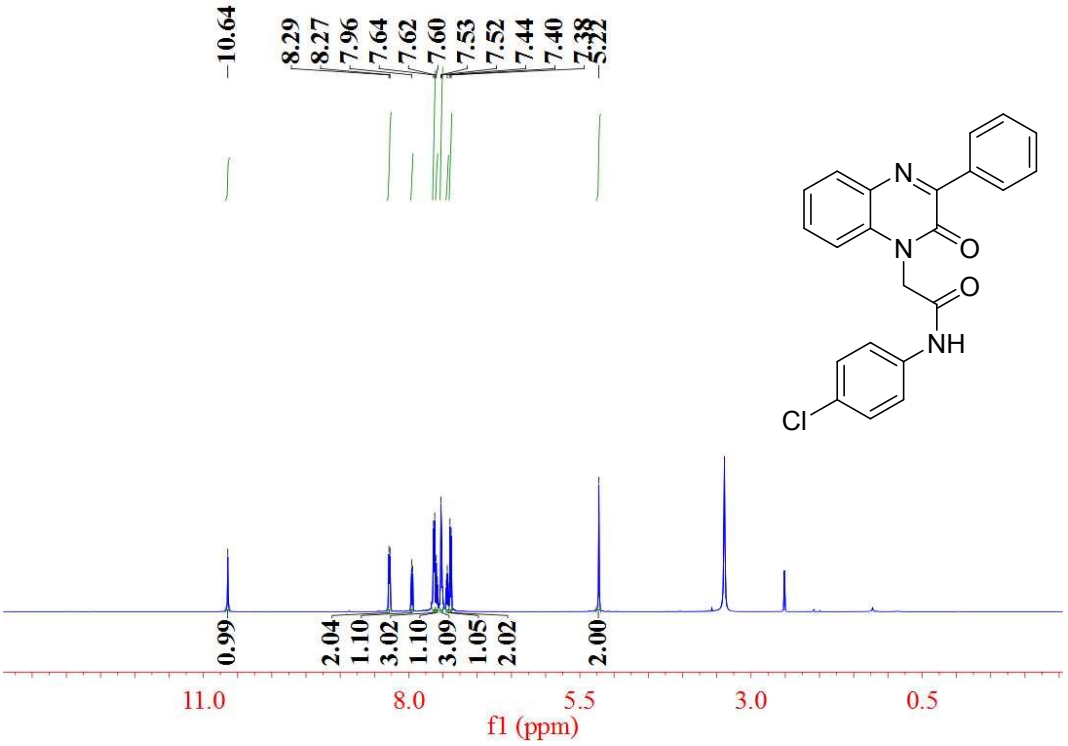


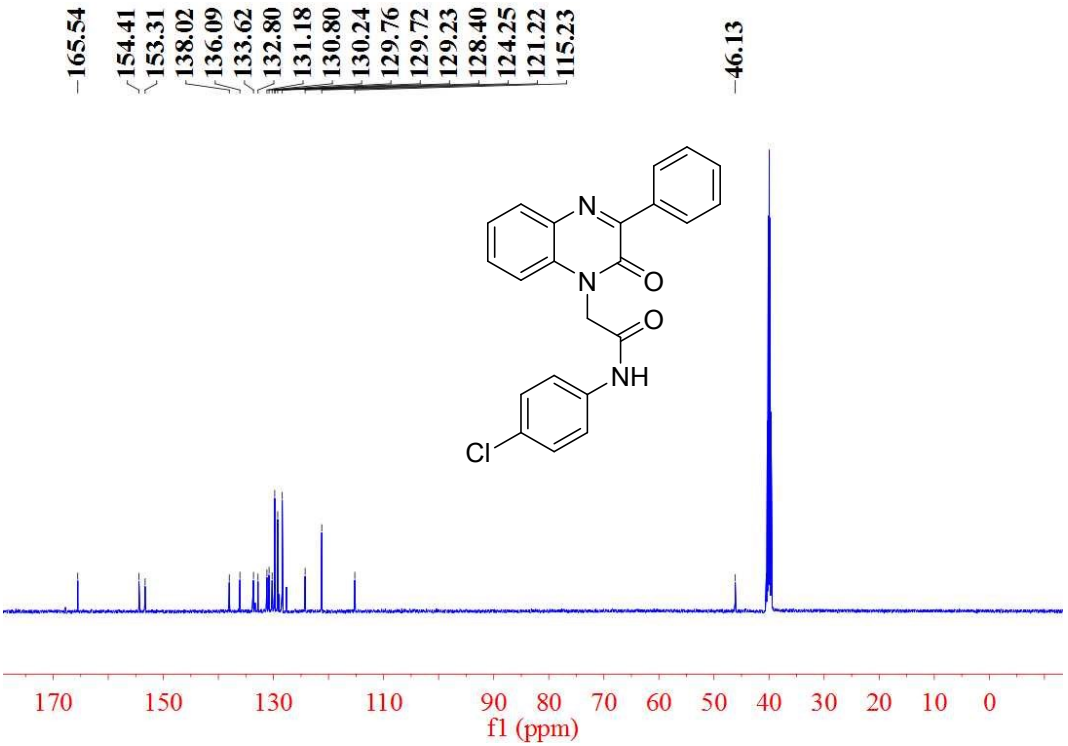
3bp ^{13}C NMR



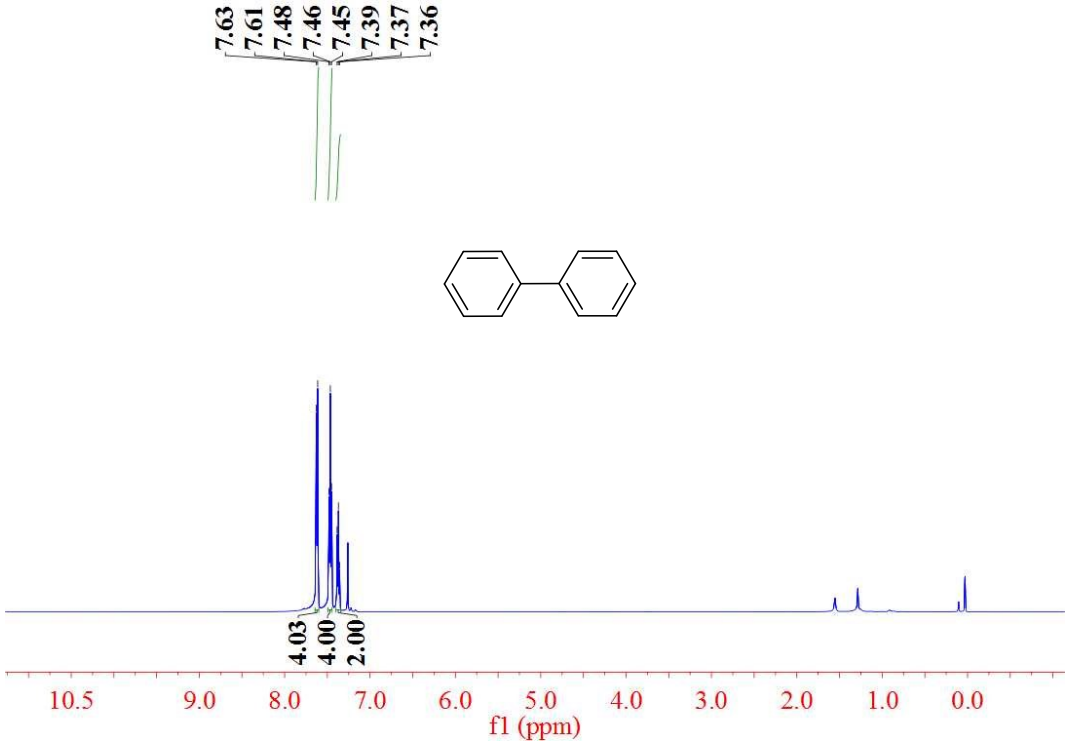
3bq ^{1}H NMR



3bq ^{13}C NMR



7 ^{1}H NMR



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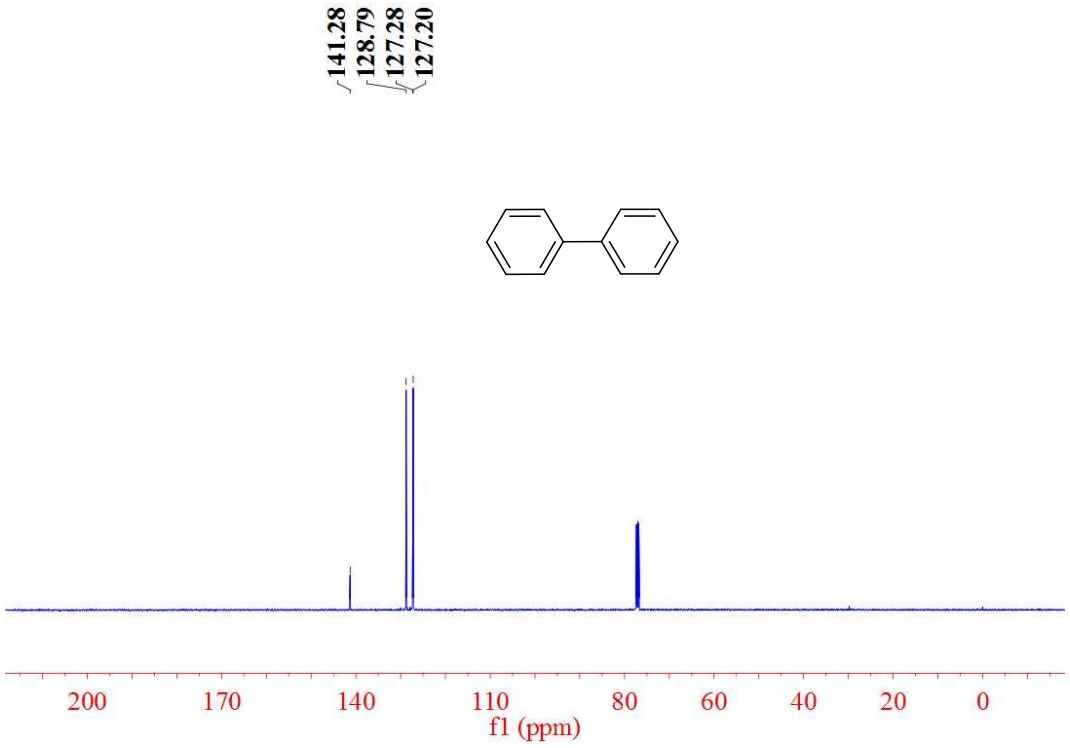

6. GC-MS spectra of benzoic acid