Electronic Supplementary Material (ESI) for New Journal of Chemistry.

[TEATNM] and [TEATCM] as novel catalysts for the synthesis of pyridine-3,5-dicarbonitriles *via* anomeric based oxidation

Saeed Baghery,* Mohammad Ali Zolfigol,* Farahnaz Maleki

Department of Organic Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan 6517838683, Iran

**Corresponding Author: Fax: +988138380709*

E-mail: zolfi@basu.ac.ir and mzolfigol@yahoo.com (M.A. Zolfigol); saadybaghery@yahoo.com (S. Baghery).

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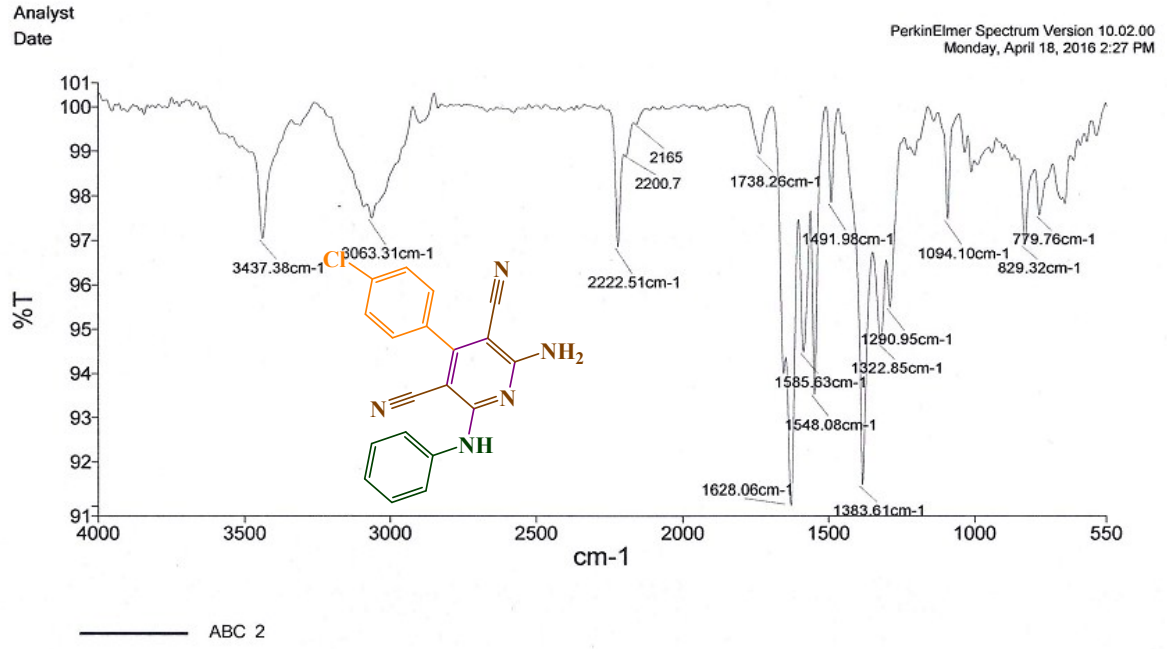

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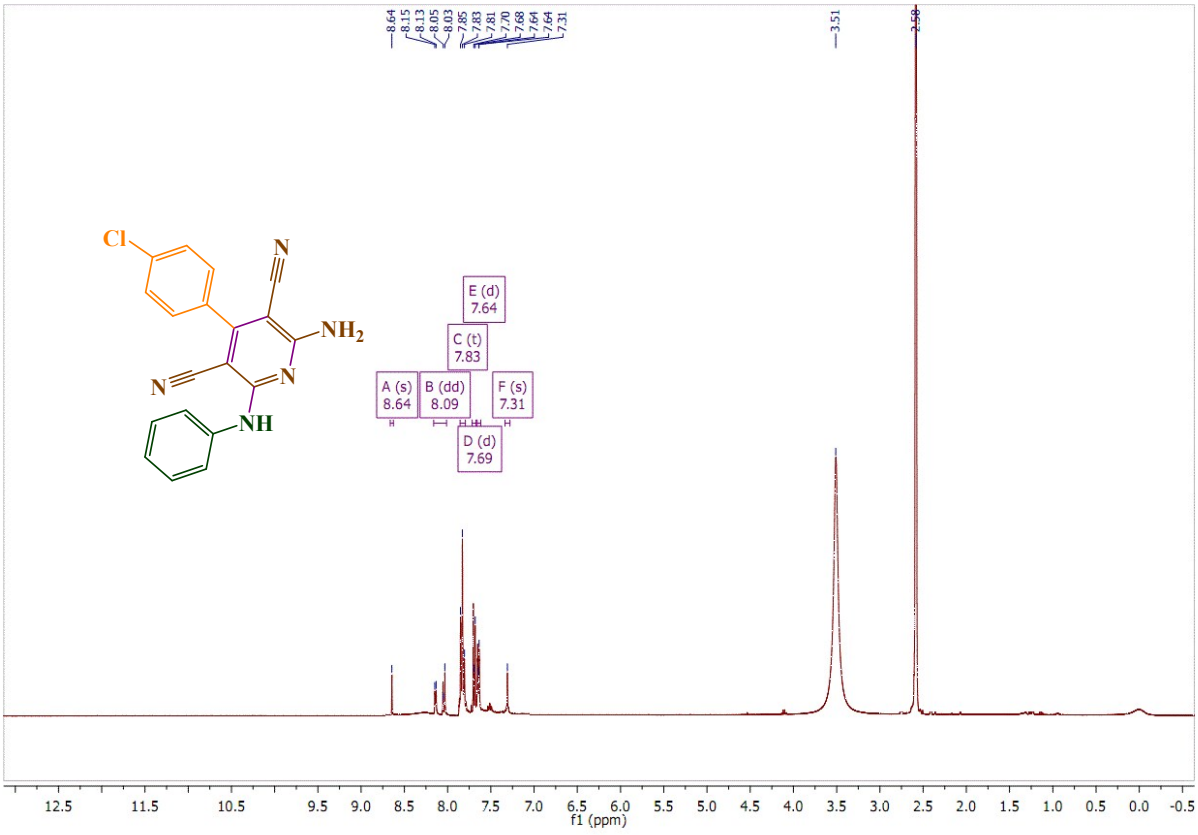

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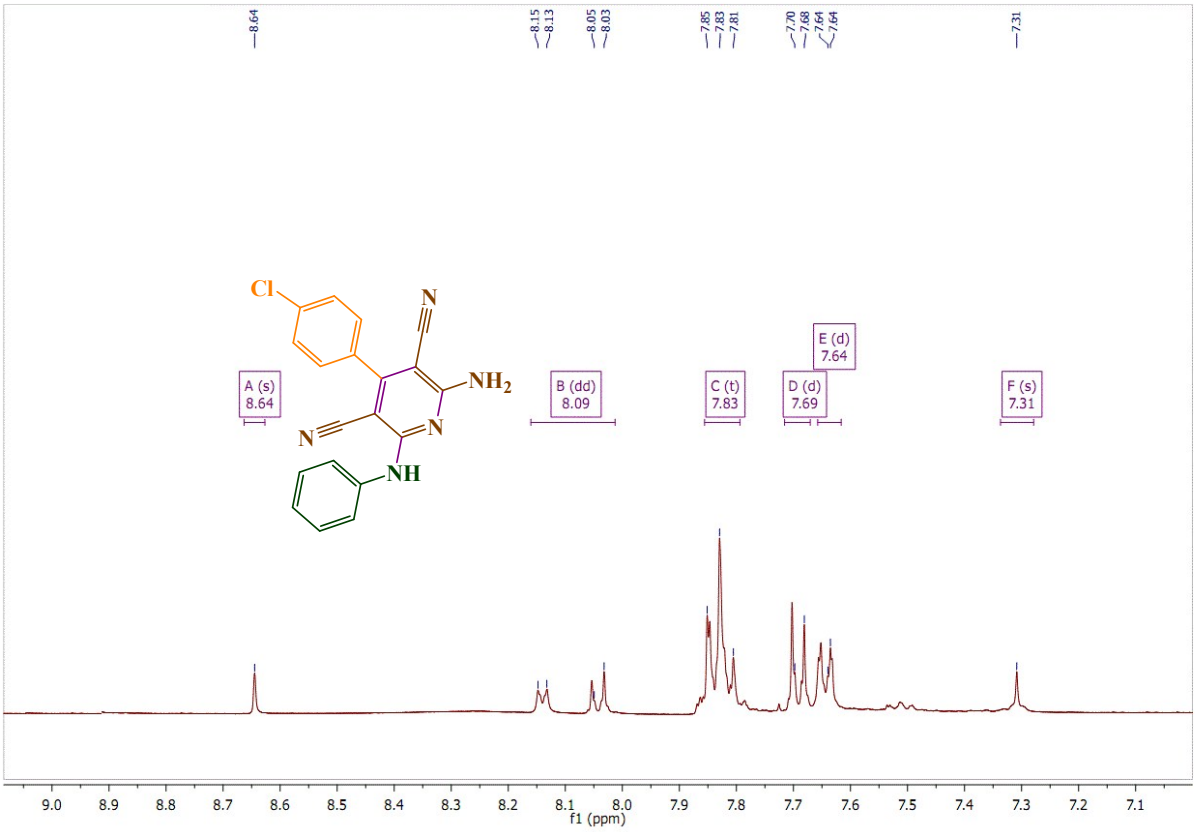

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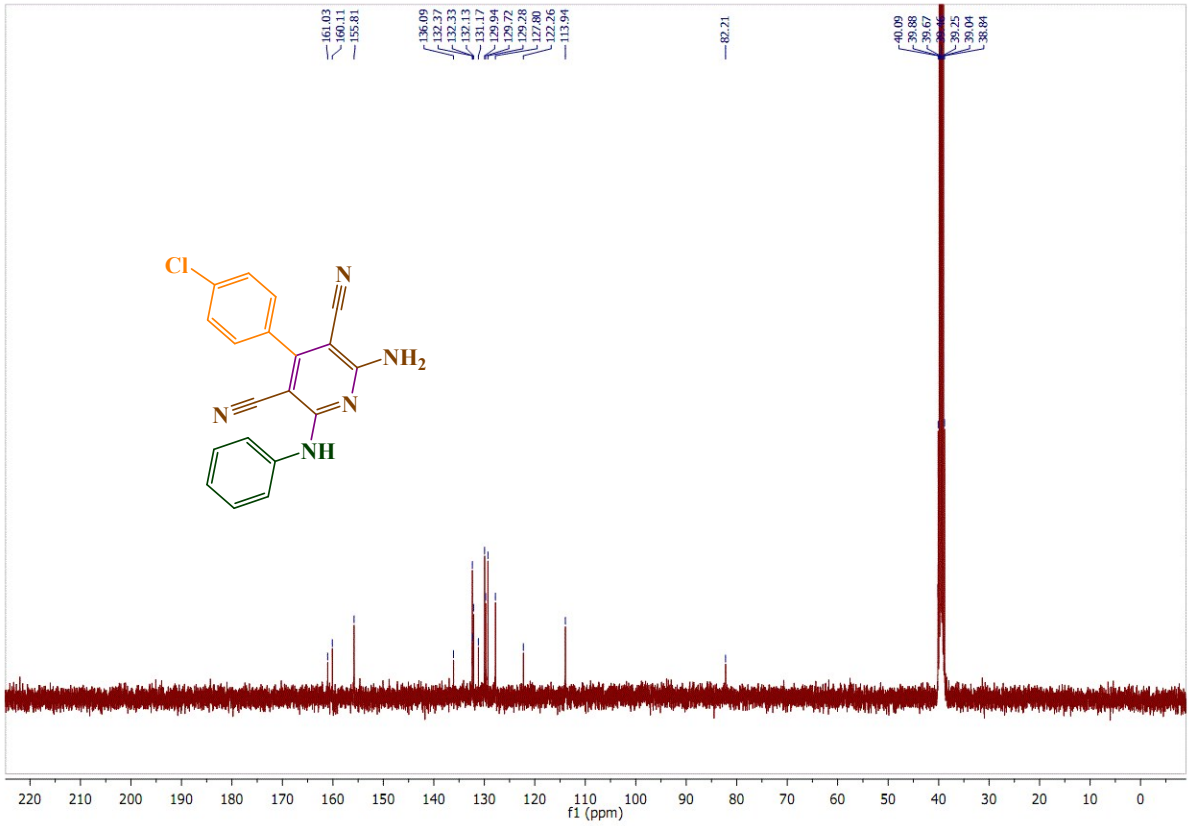

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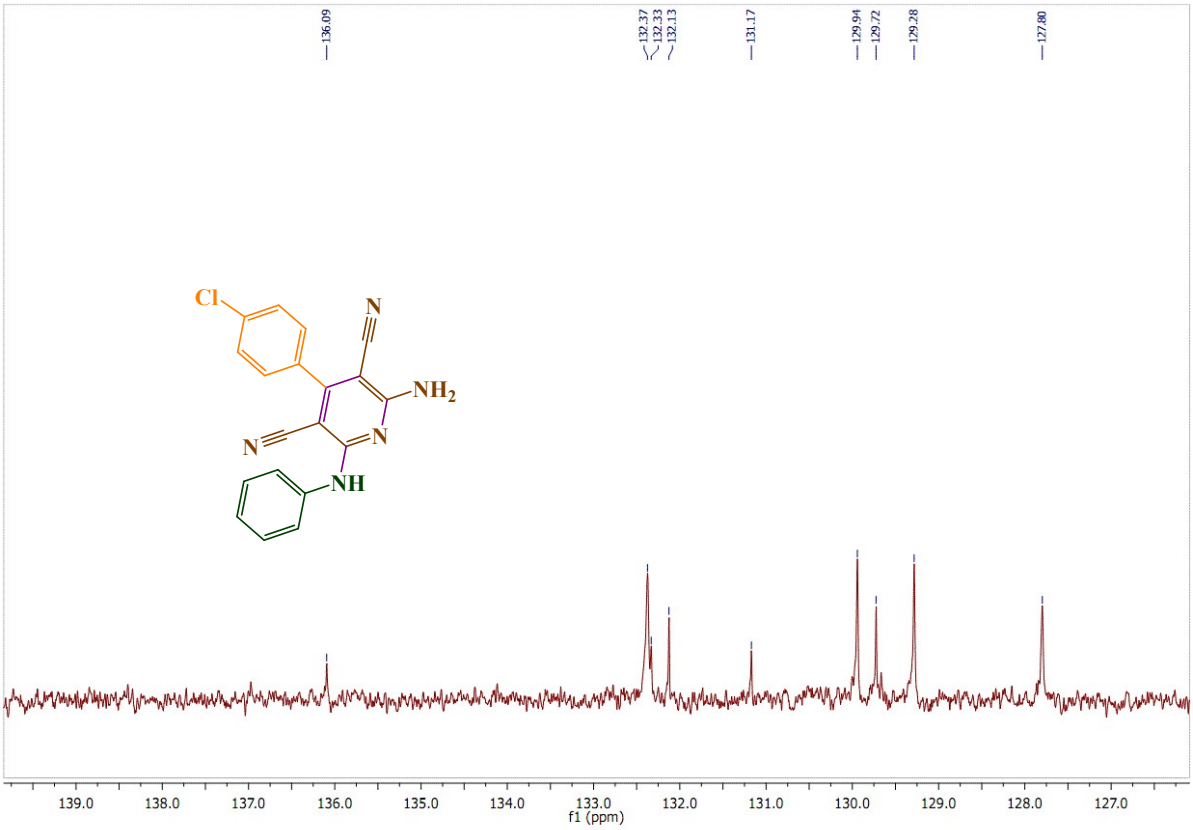

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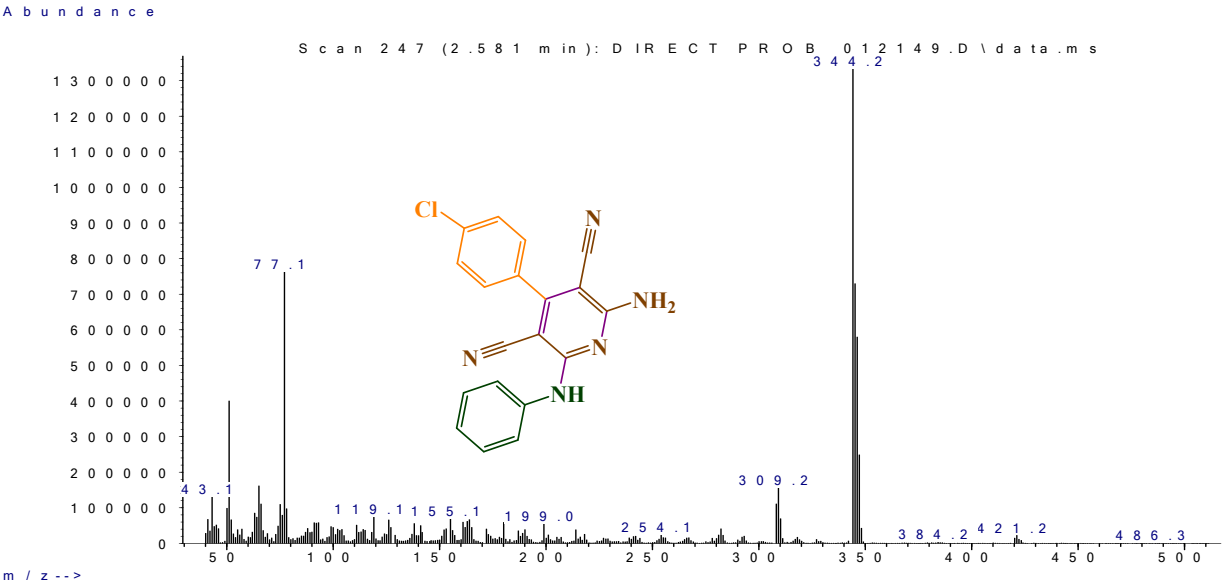

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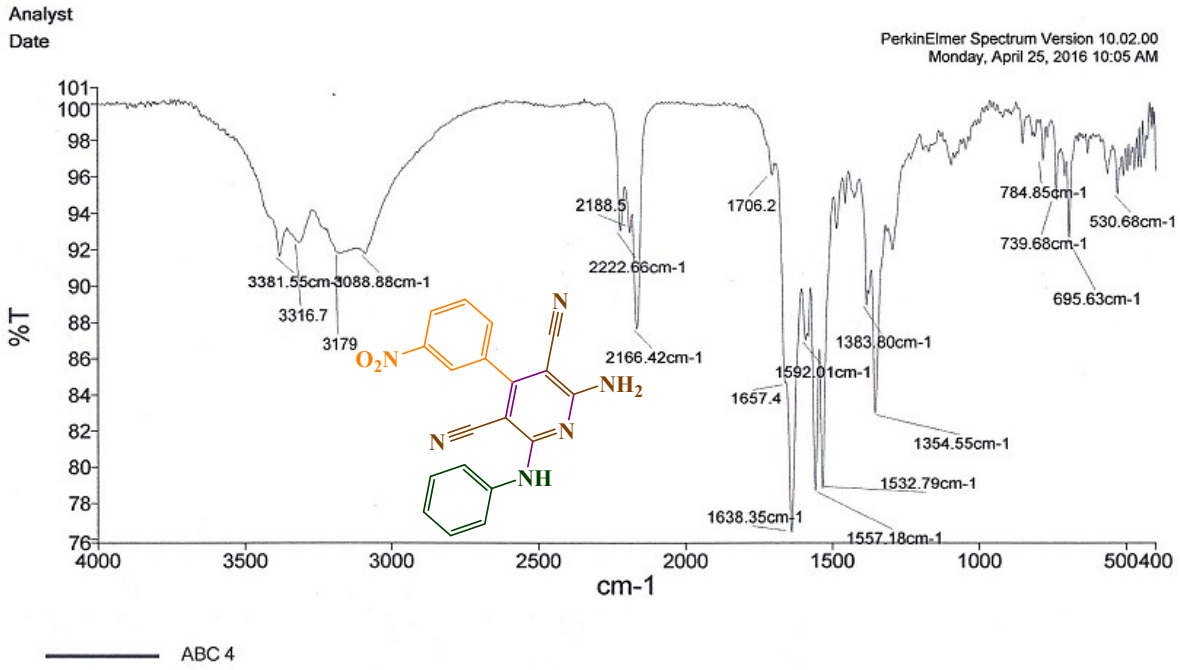

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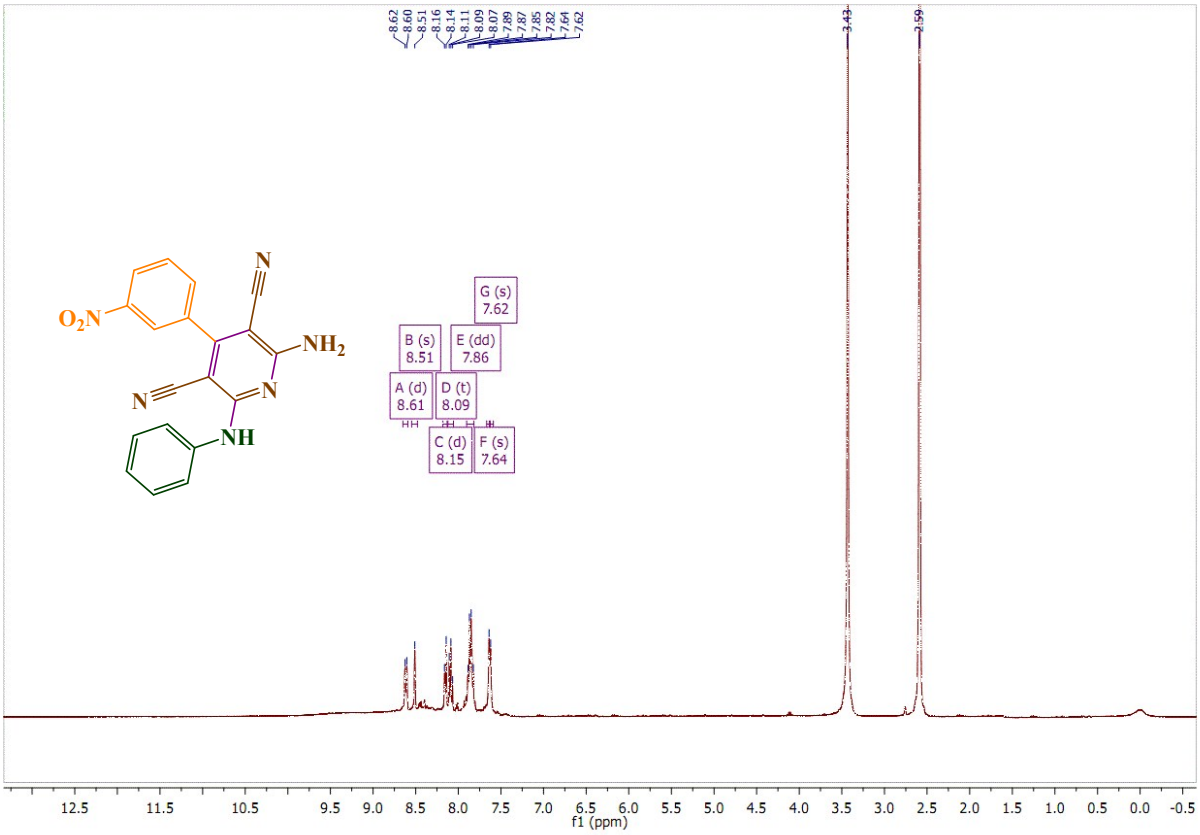

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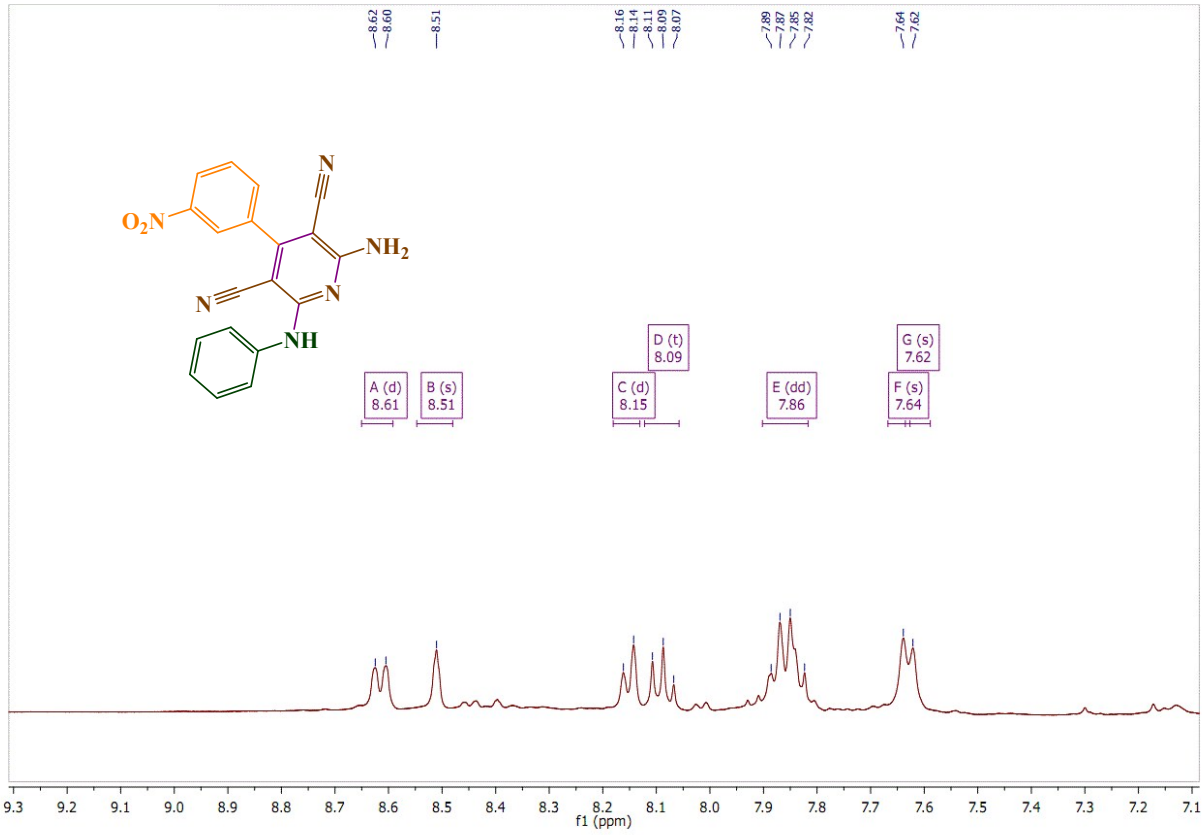

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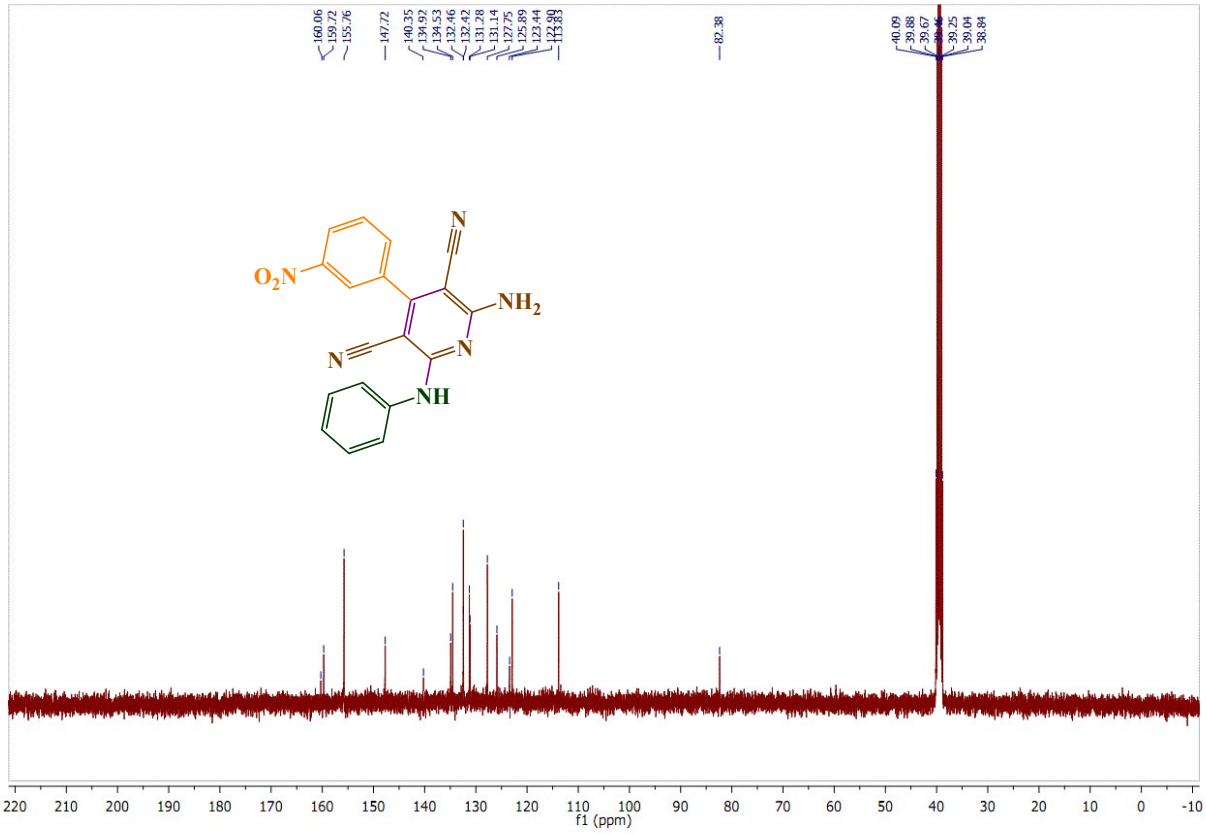

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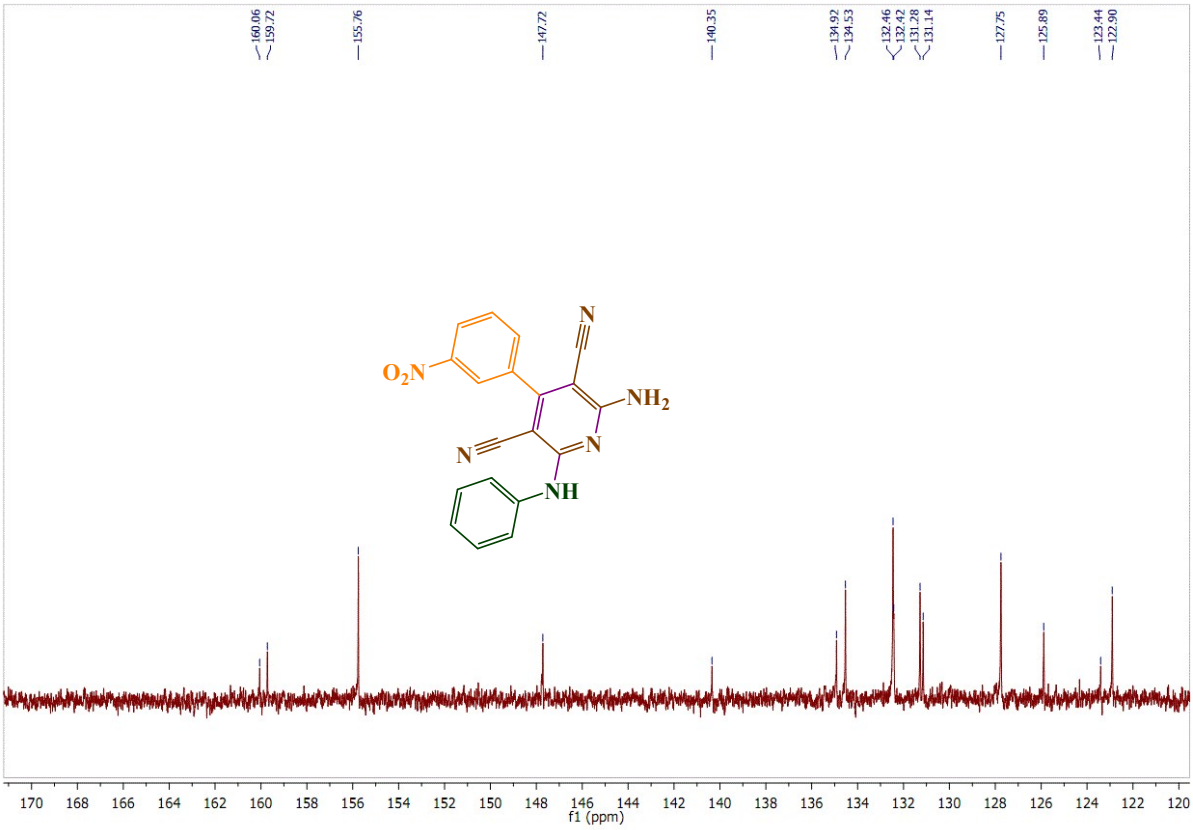

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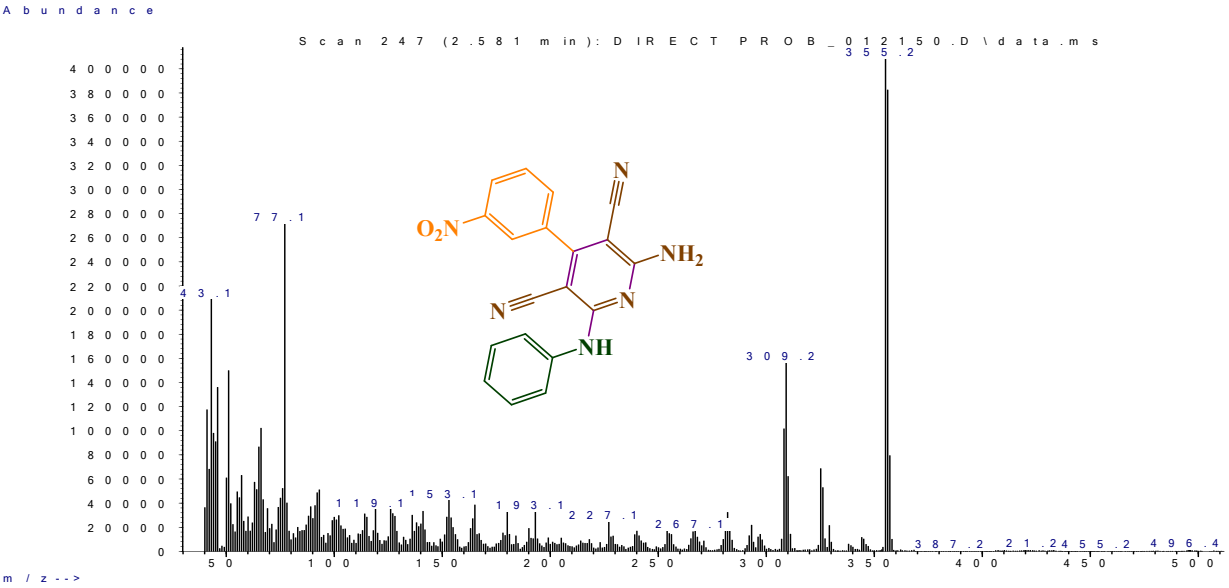

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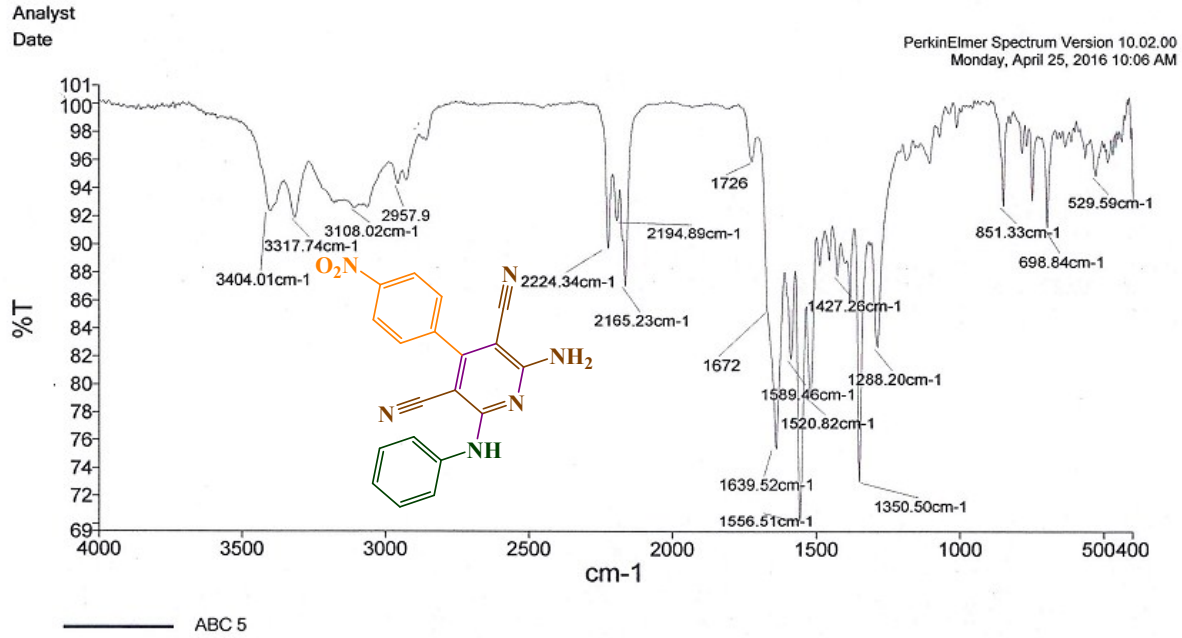

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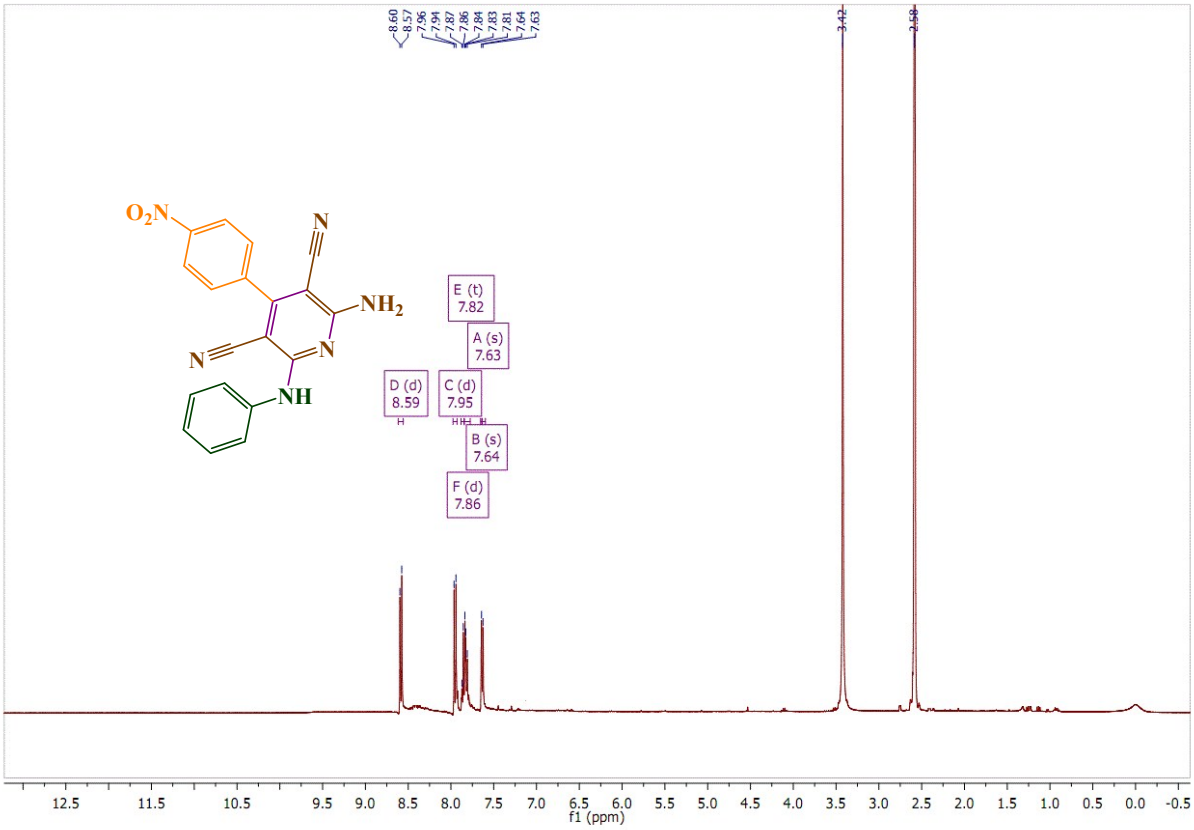

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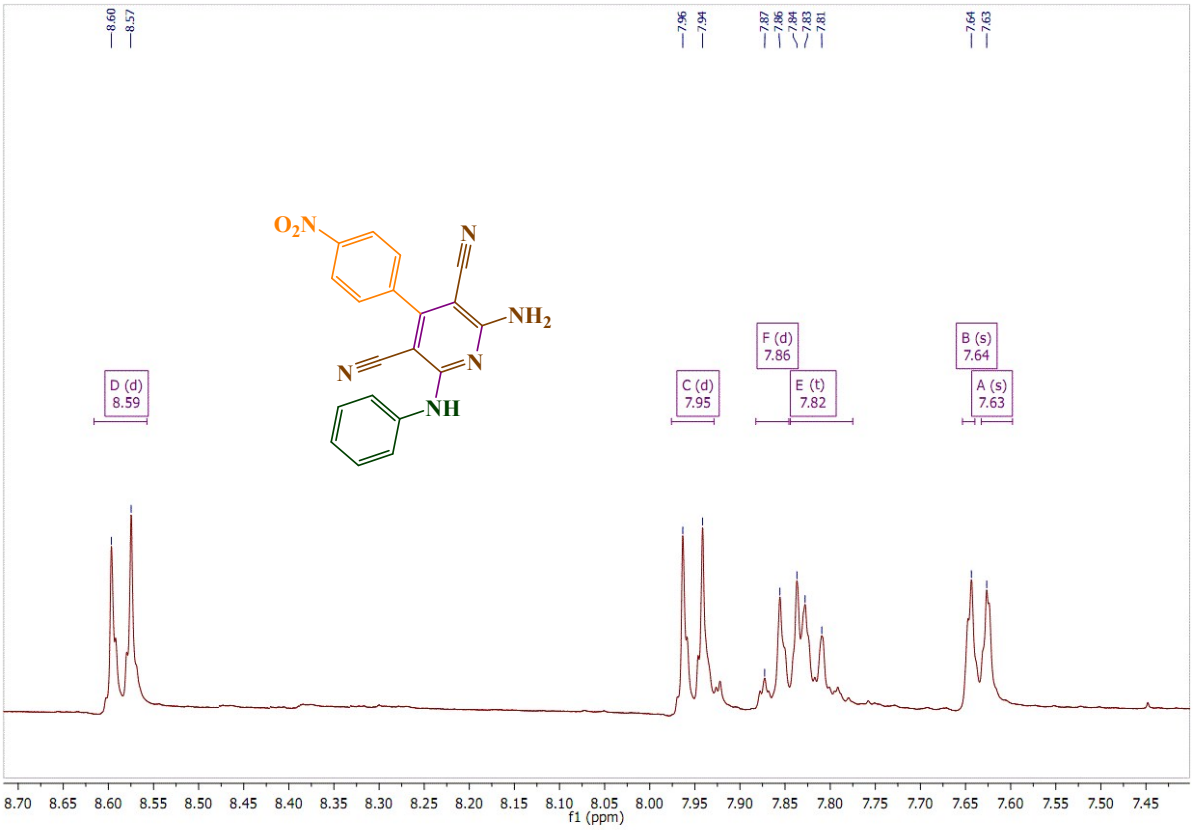

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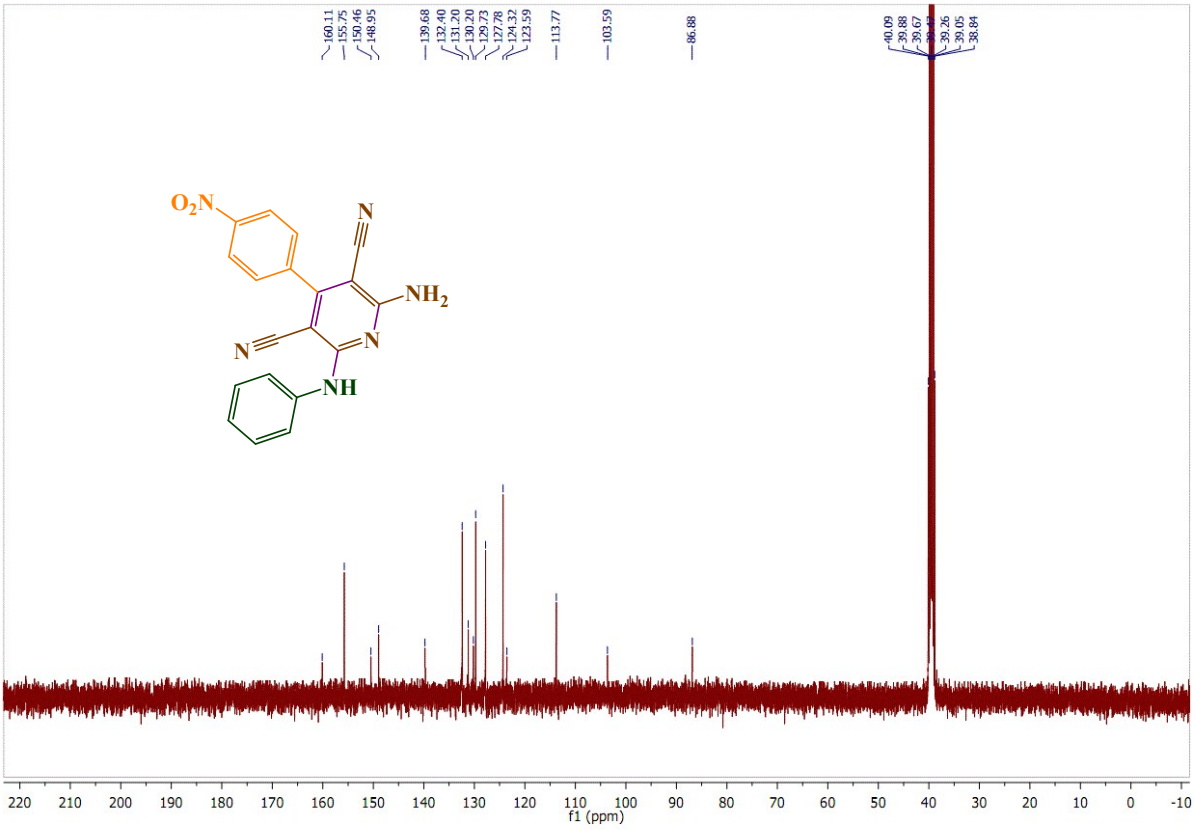

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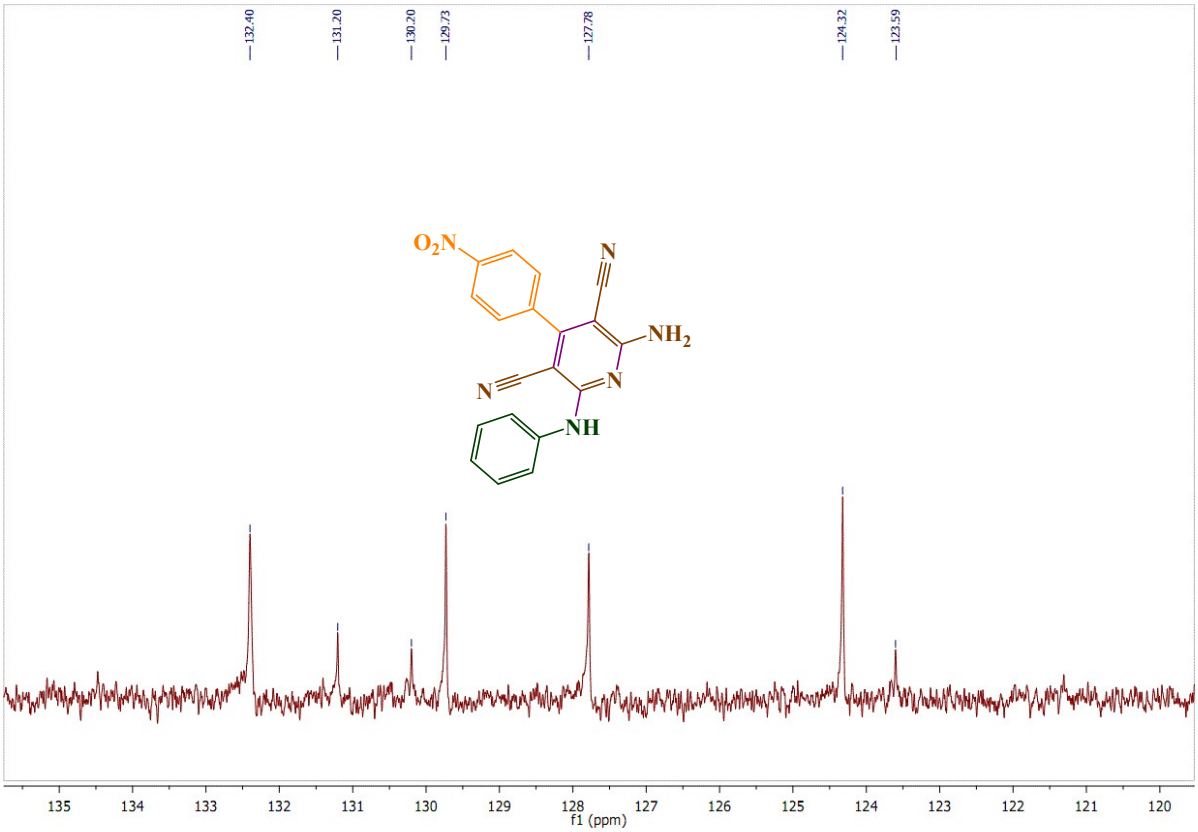

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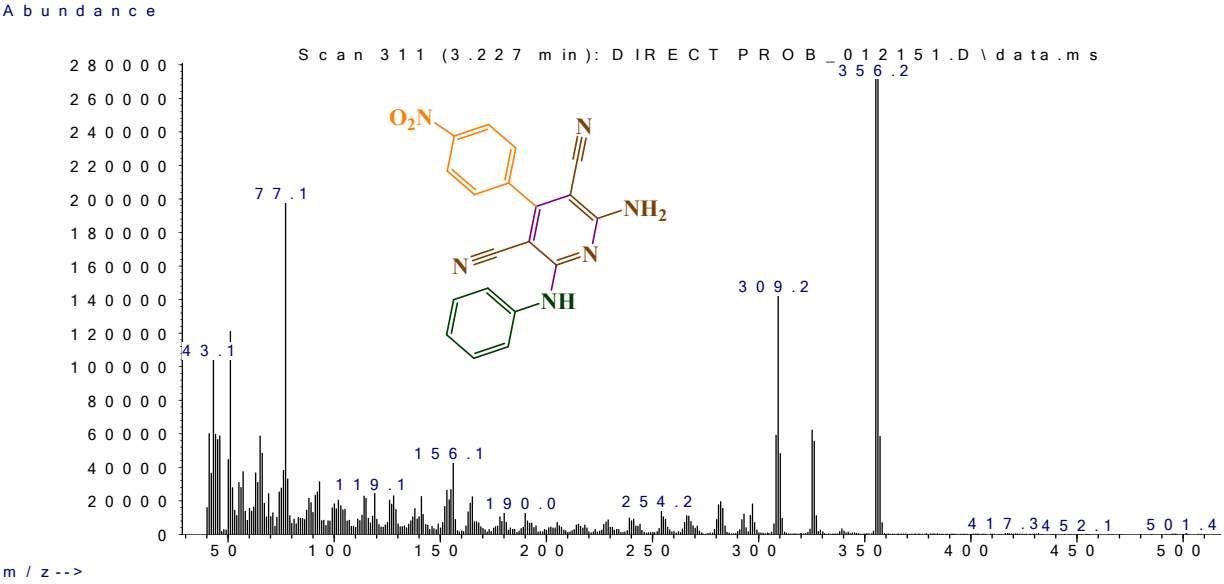

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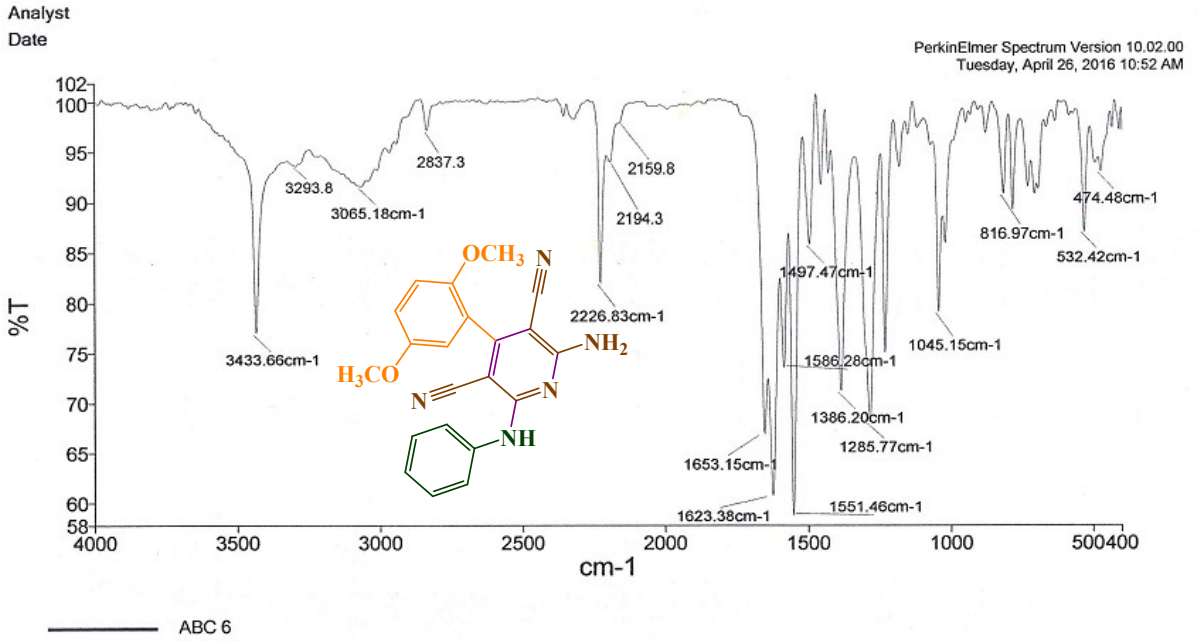

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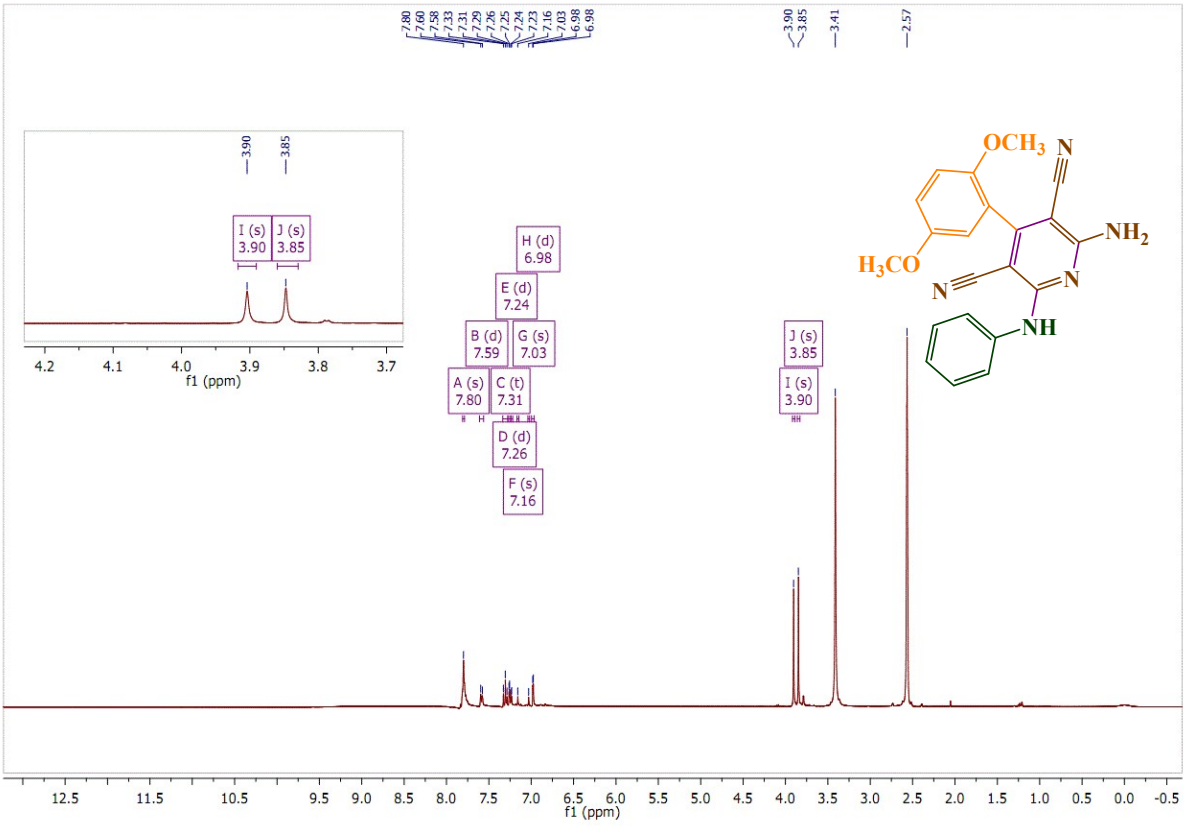

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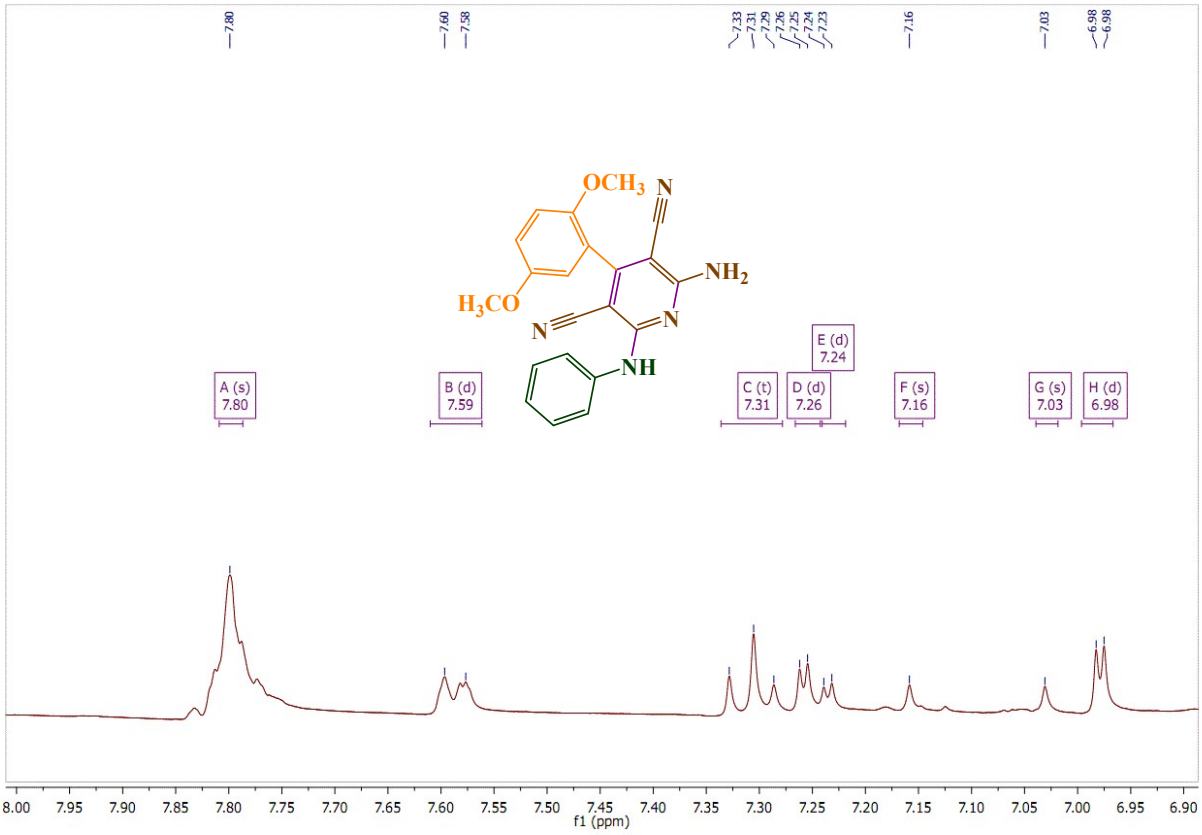

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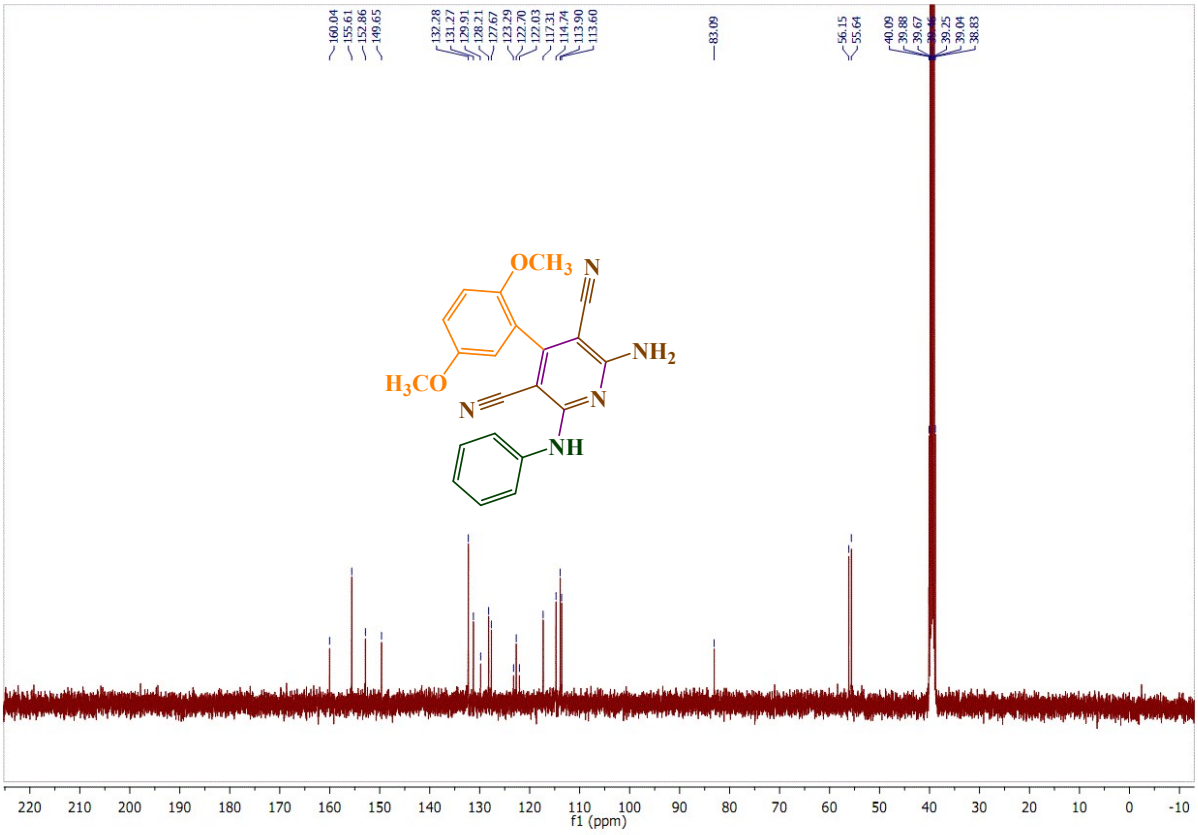

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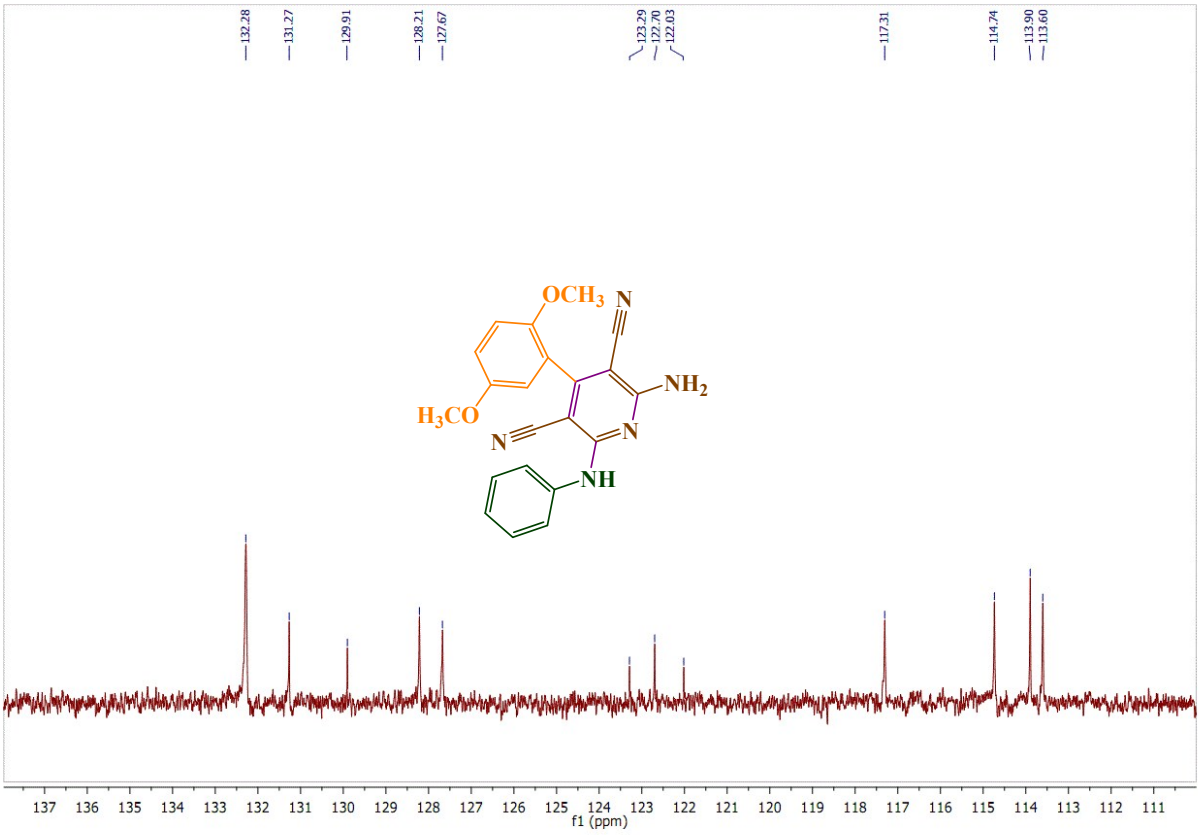

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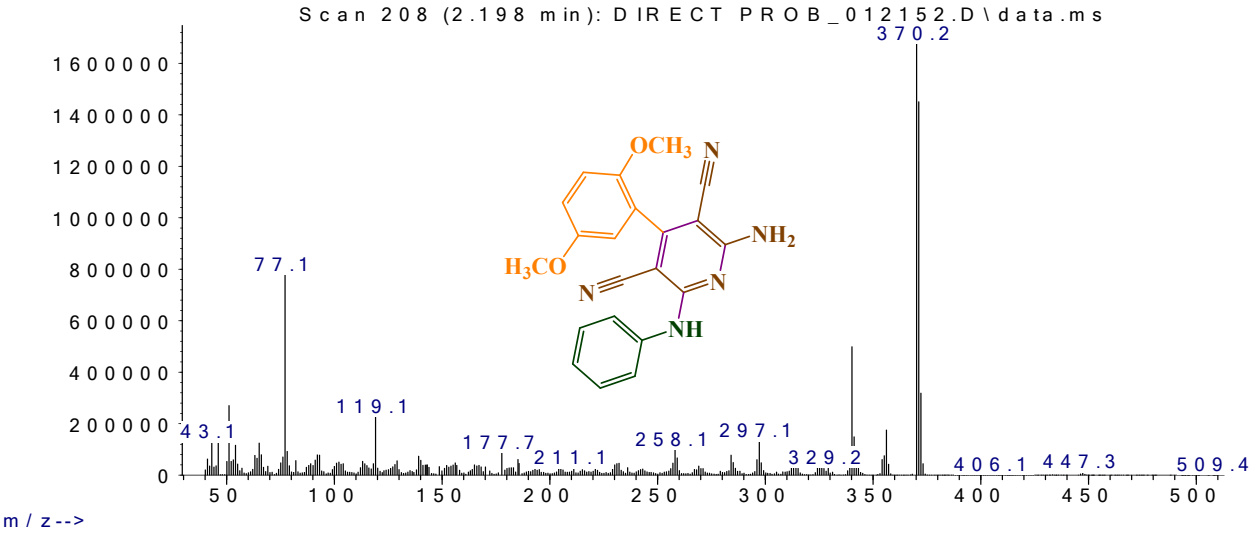

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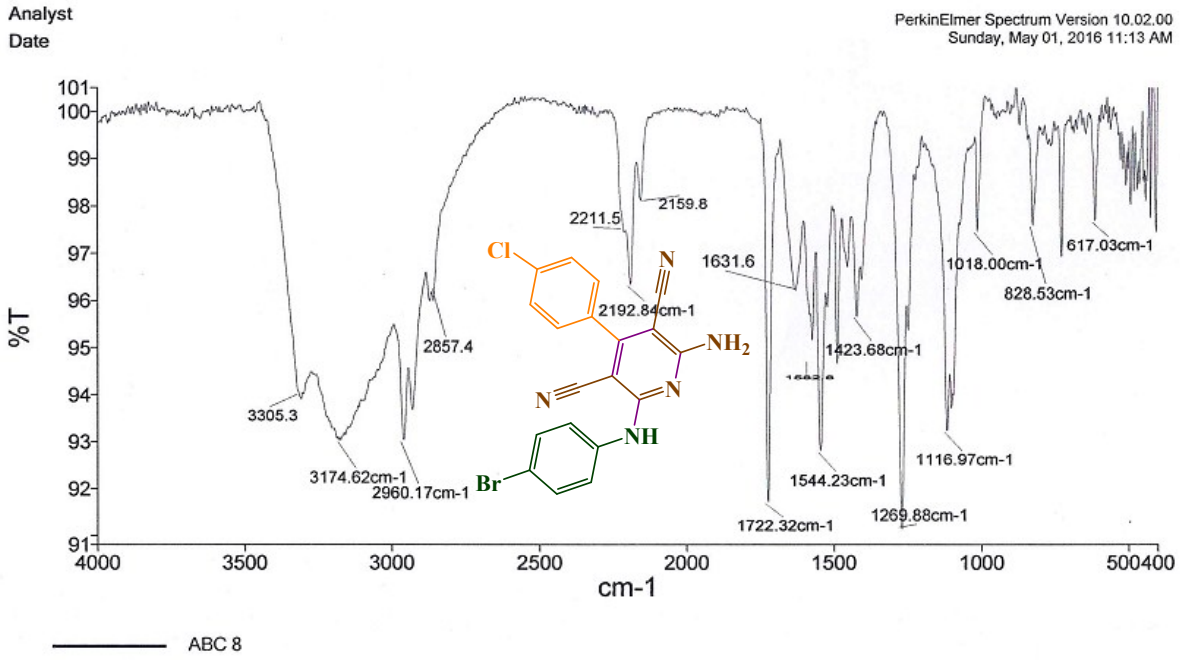

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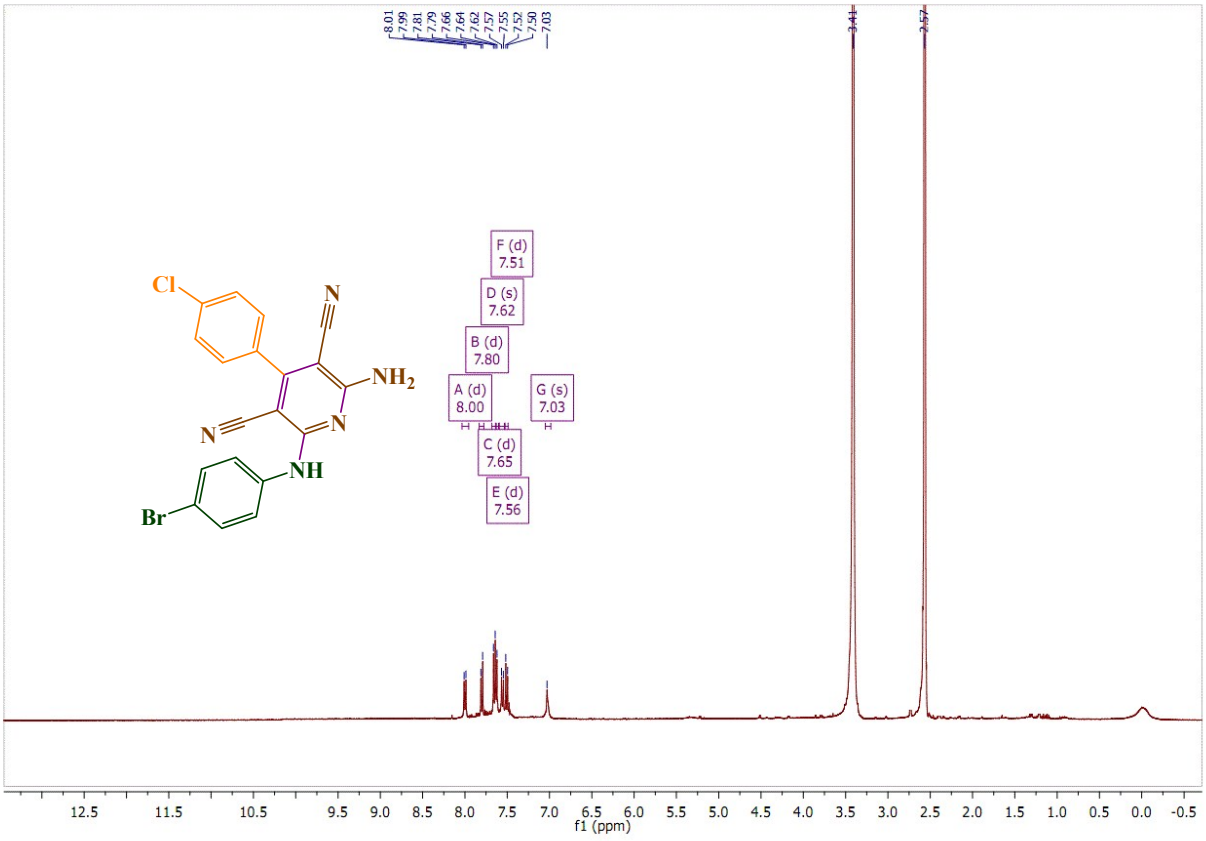

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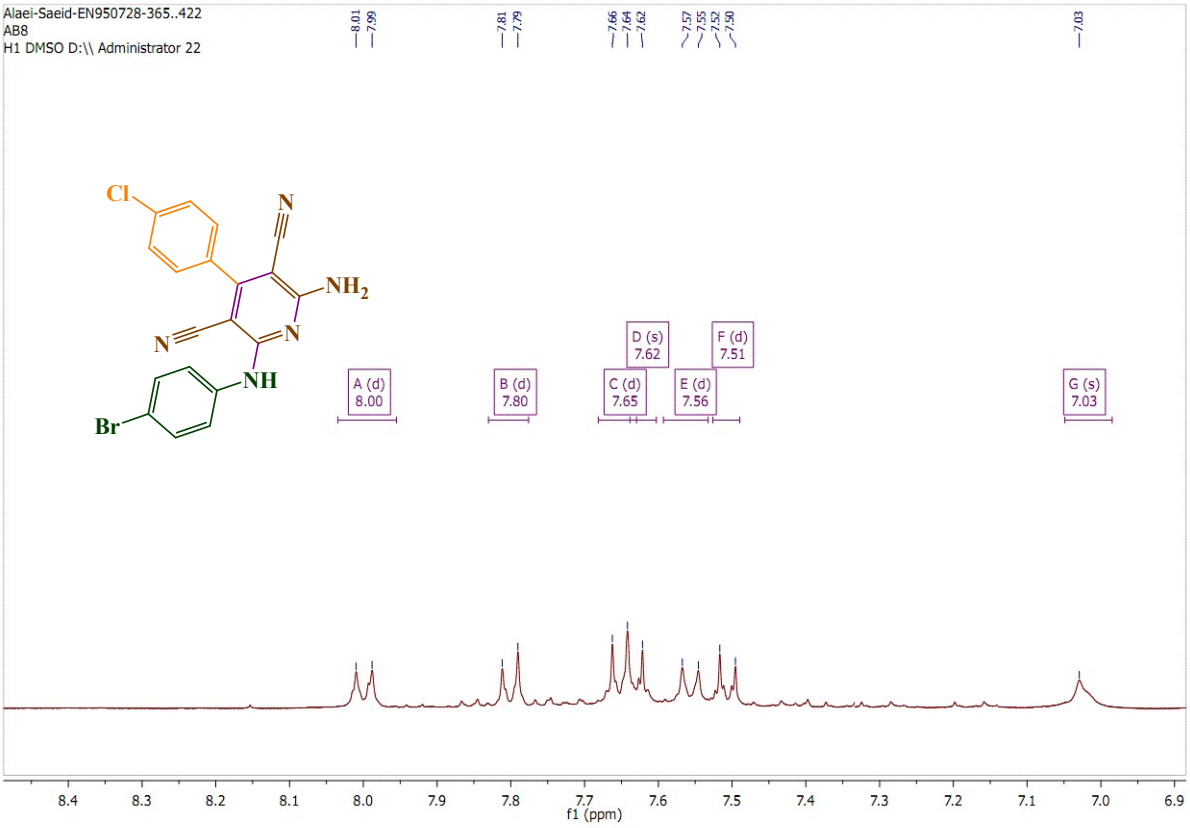

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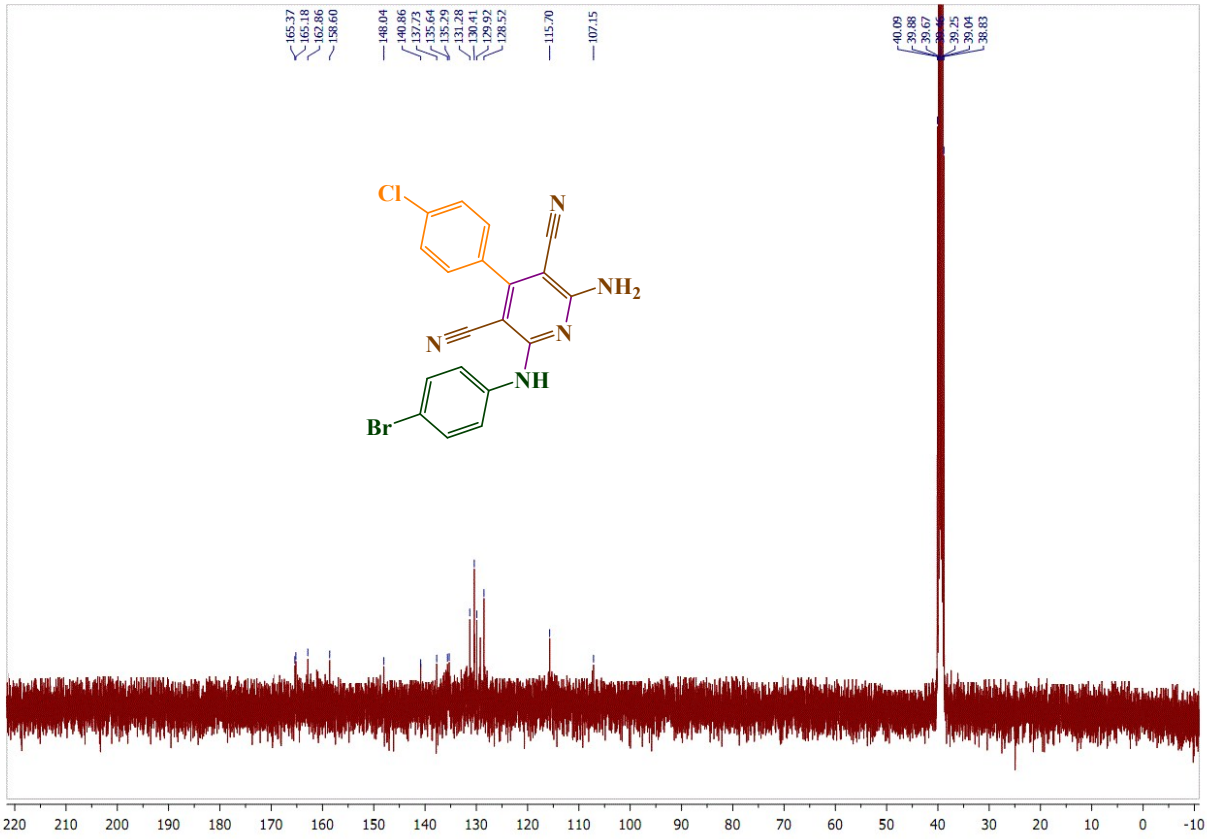

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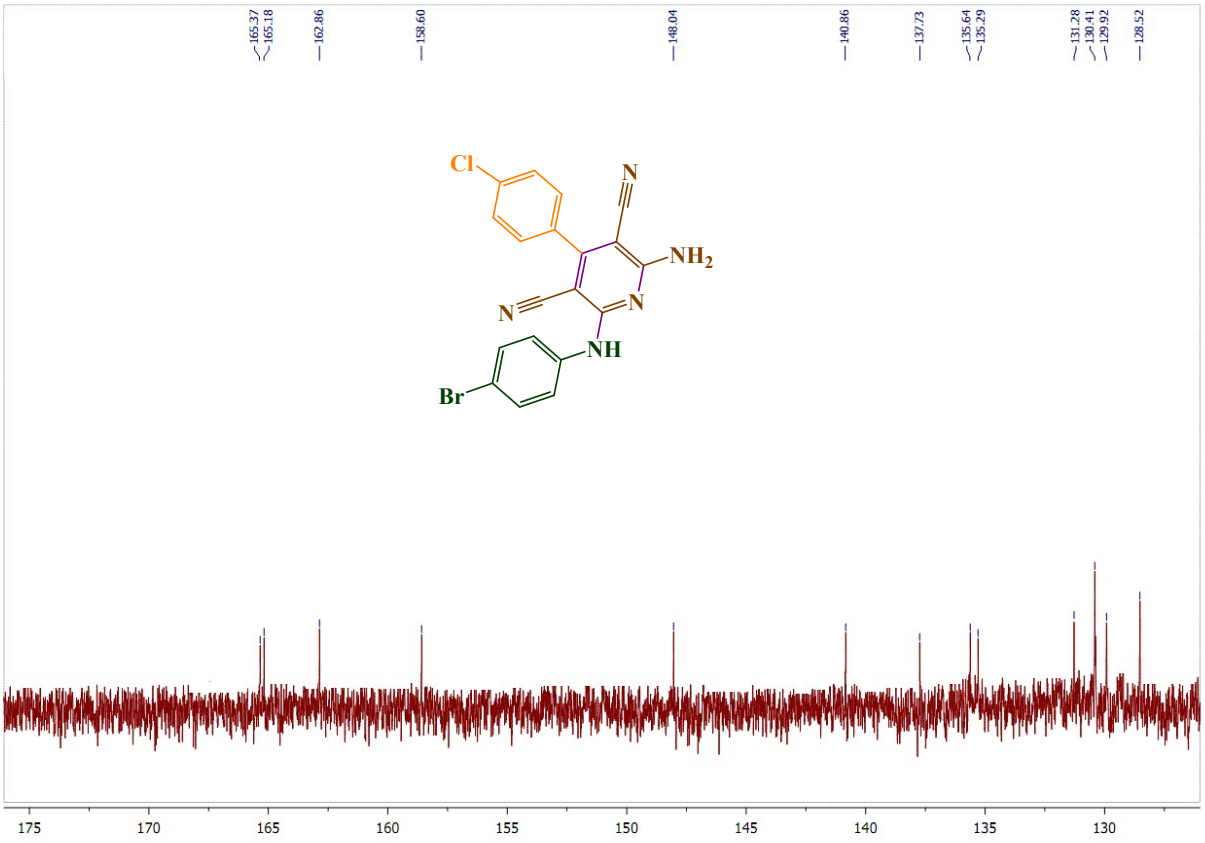

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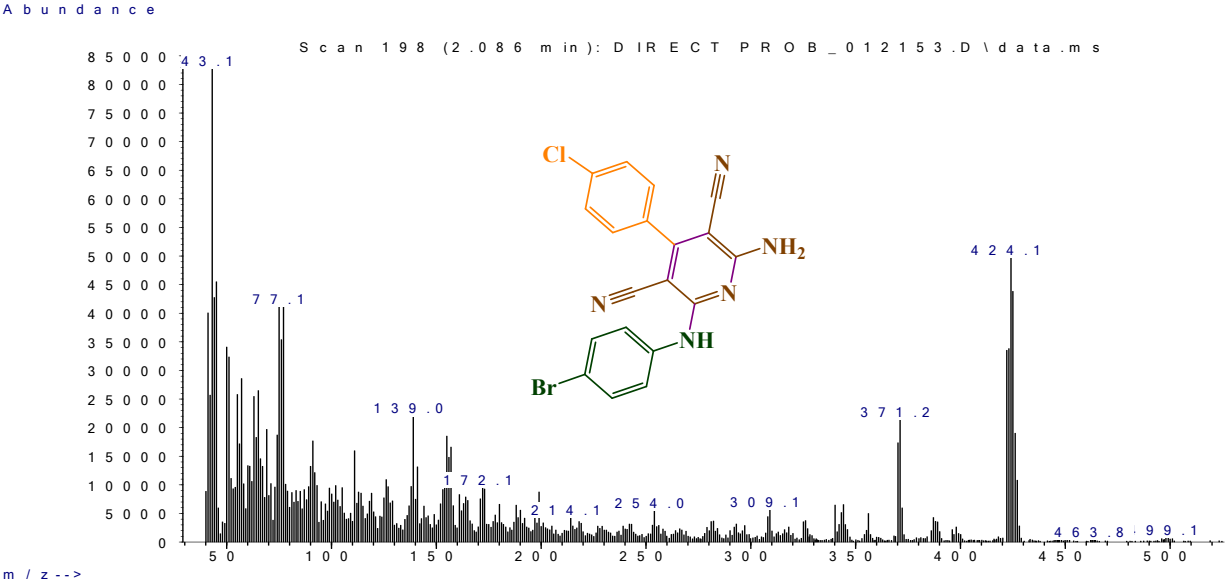

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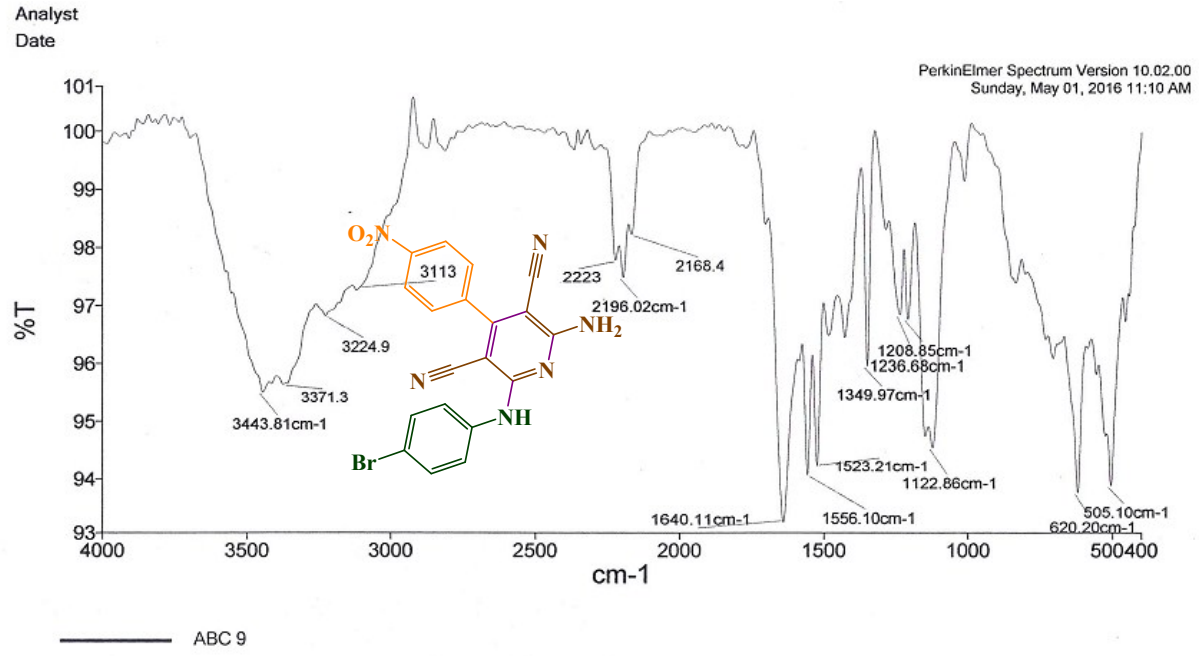

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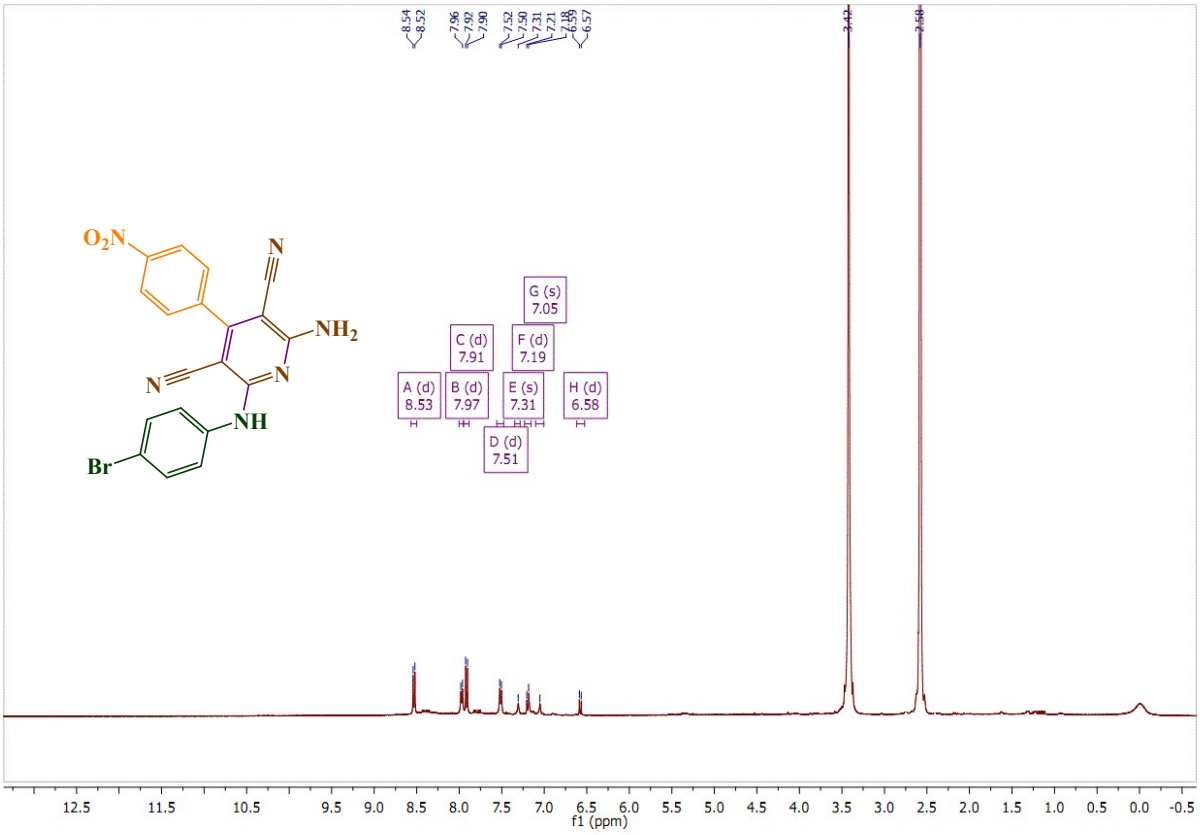

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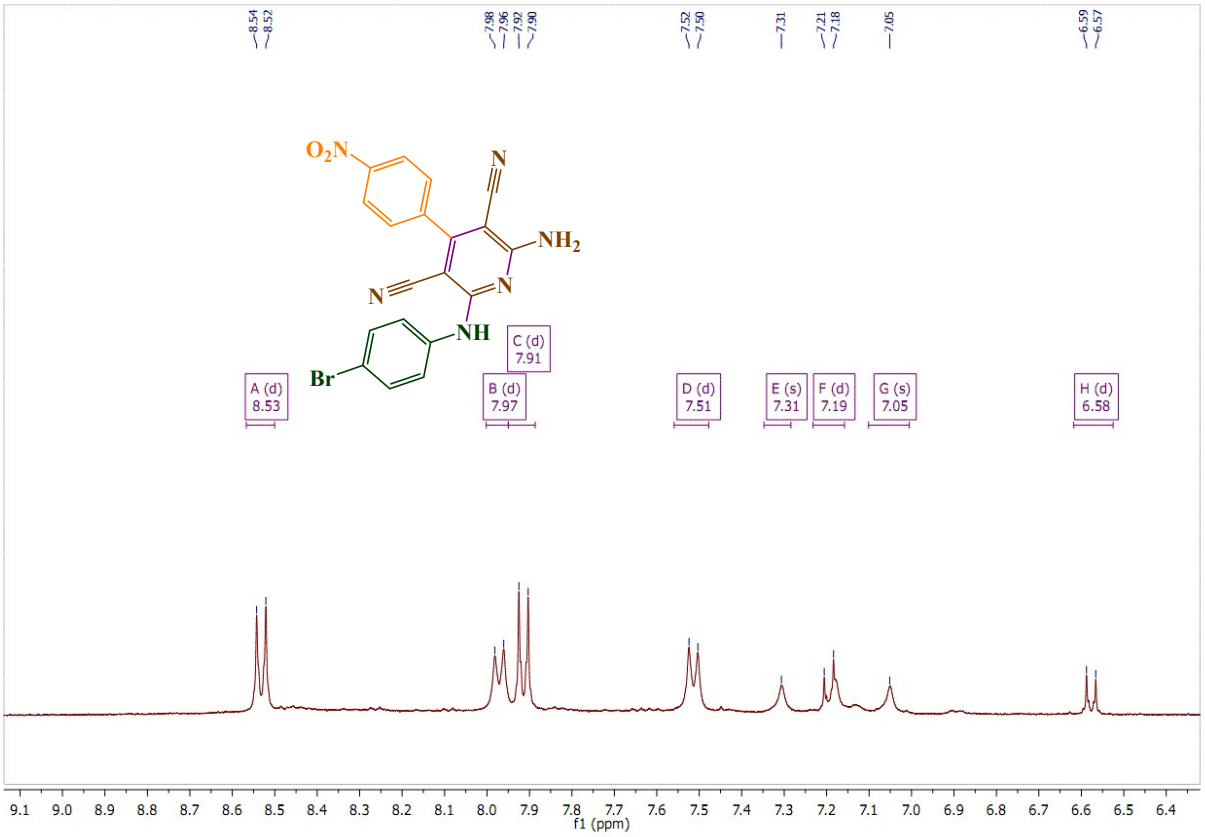

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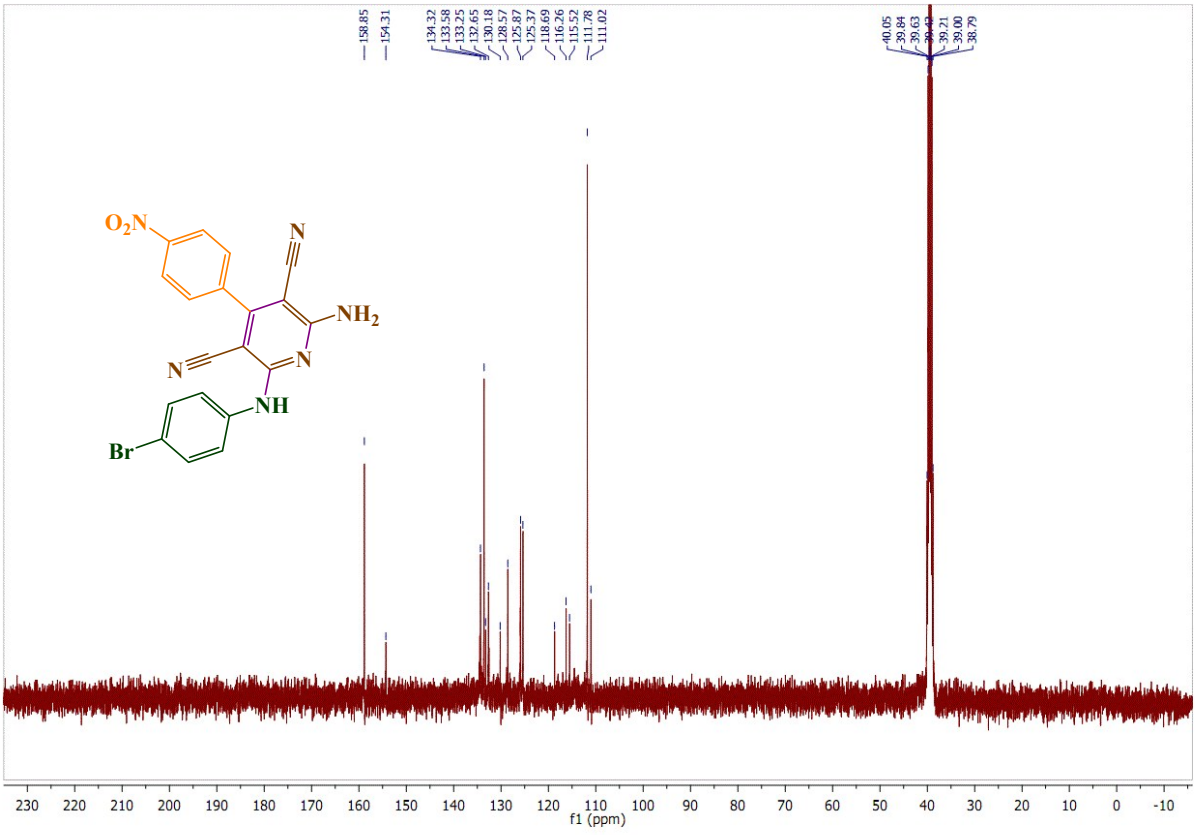

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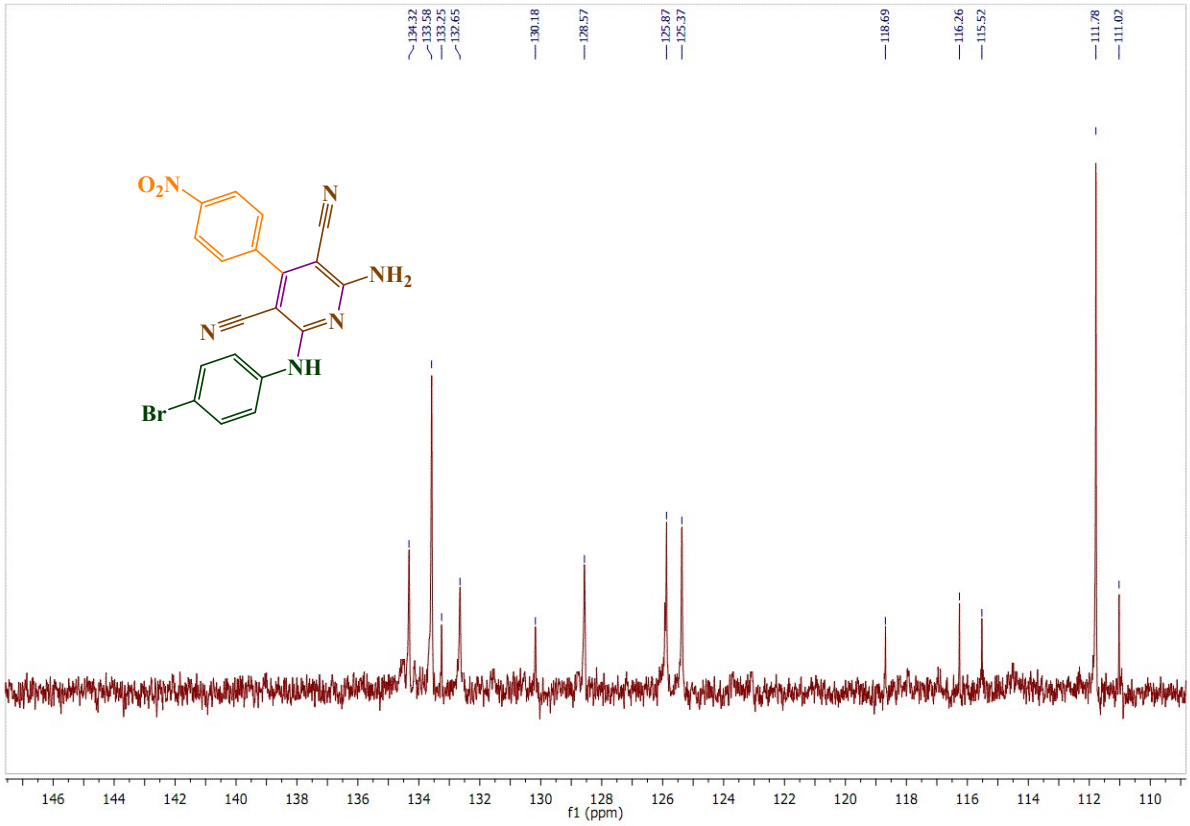

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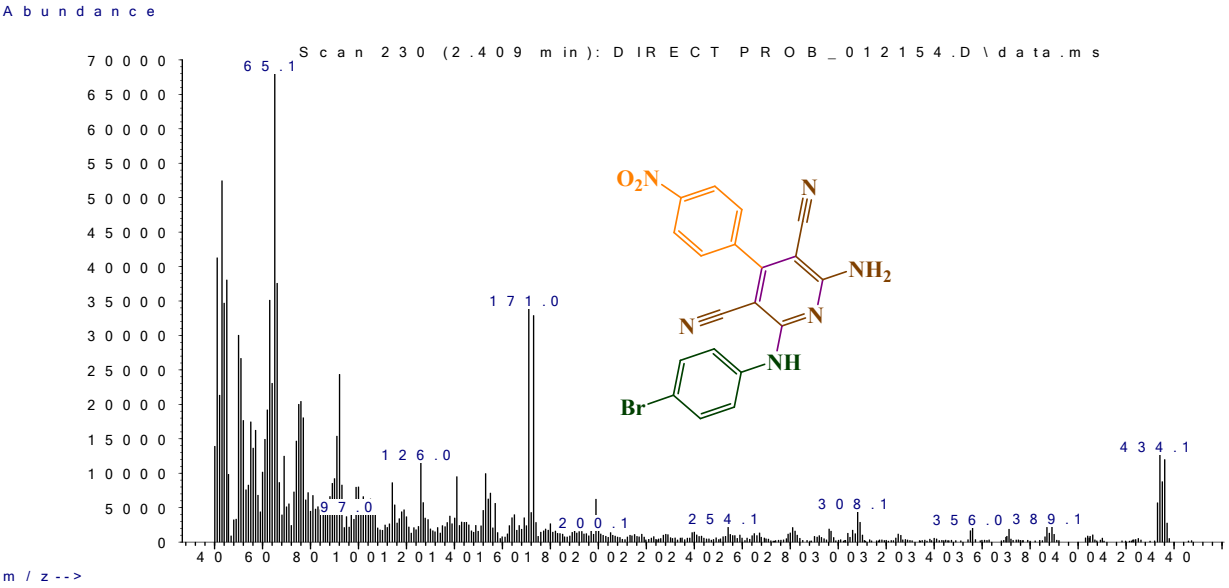

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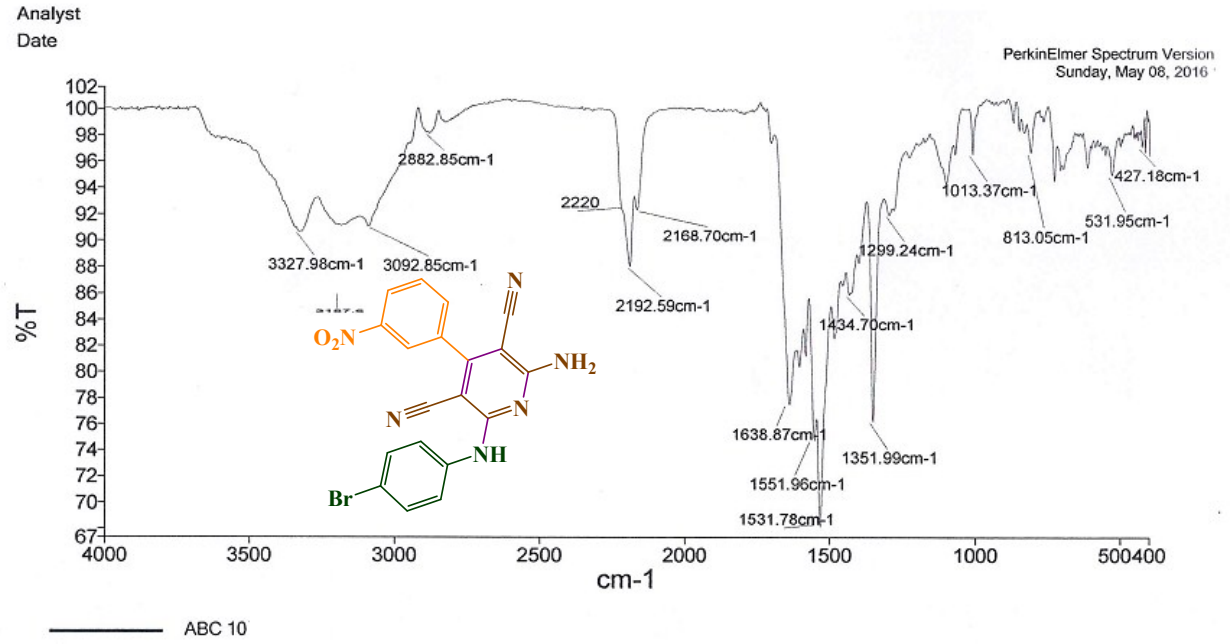

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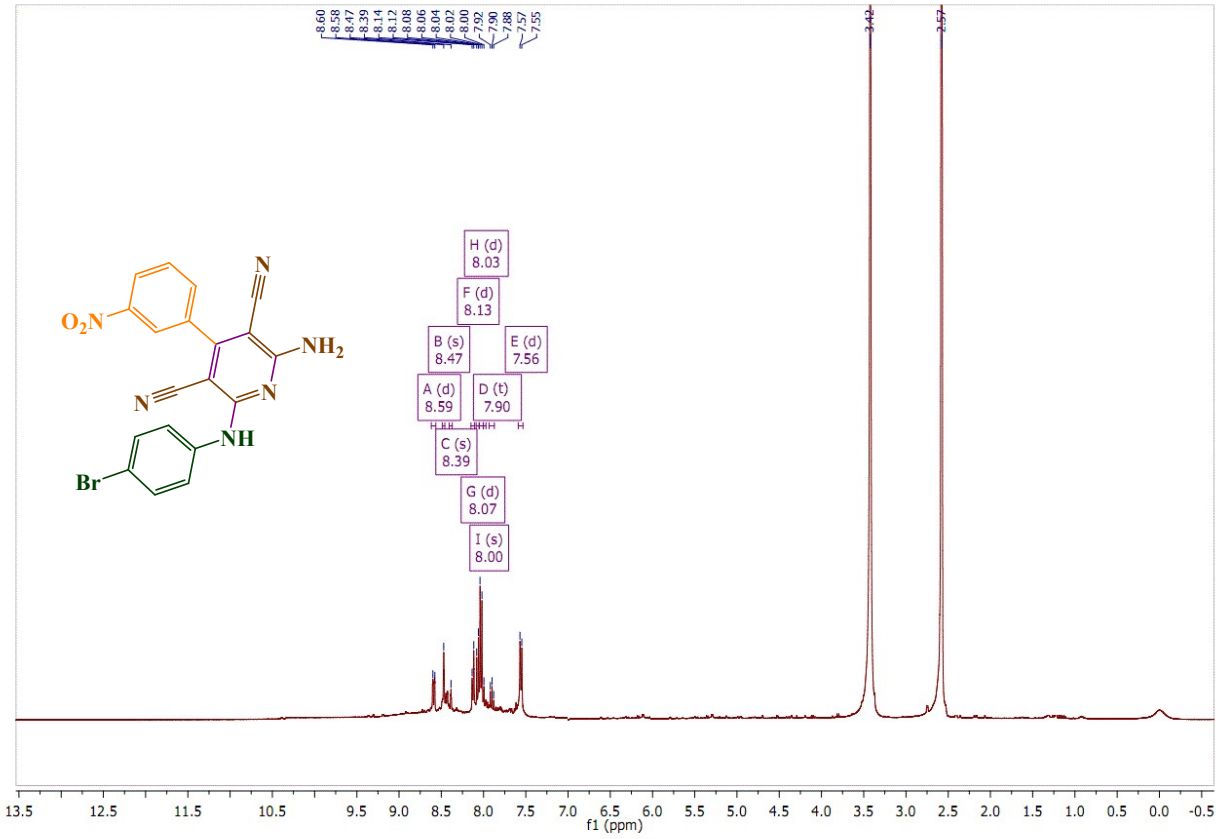

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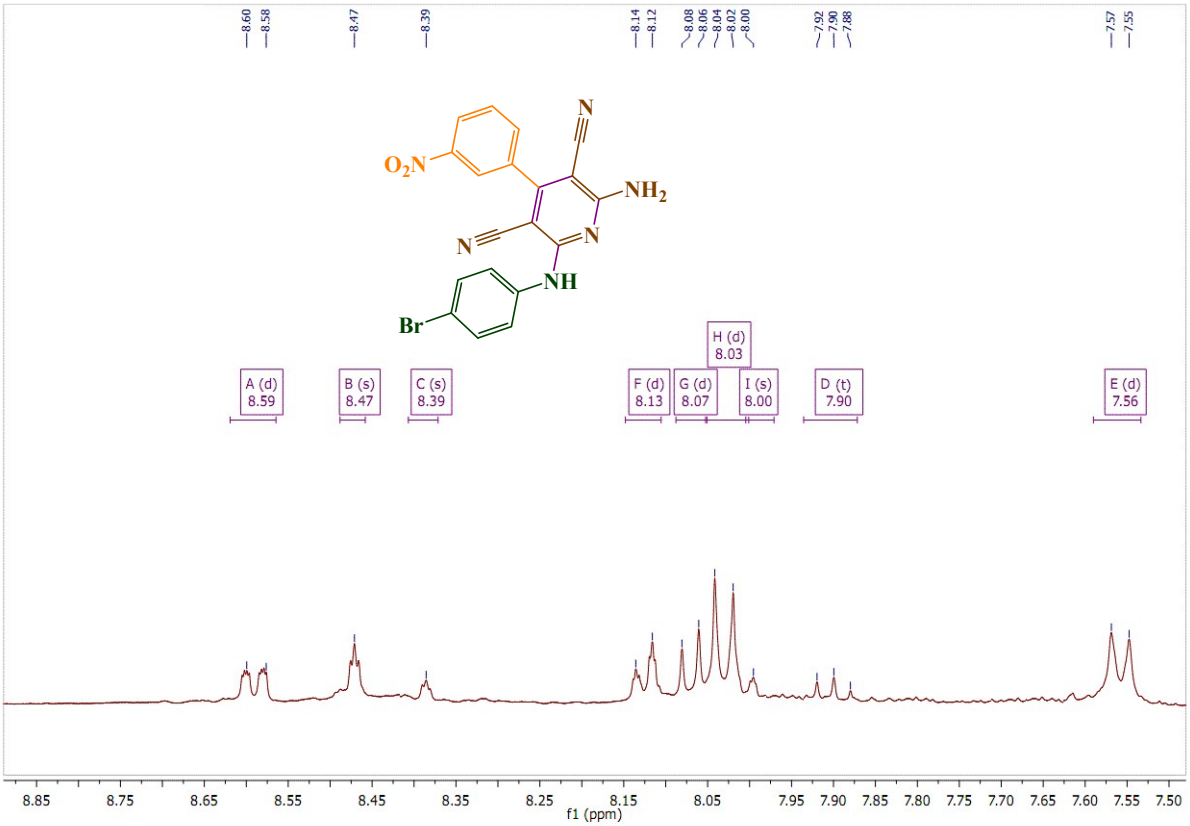

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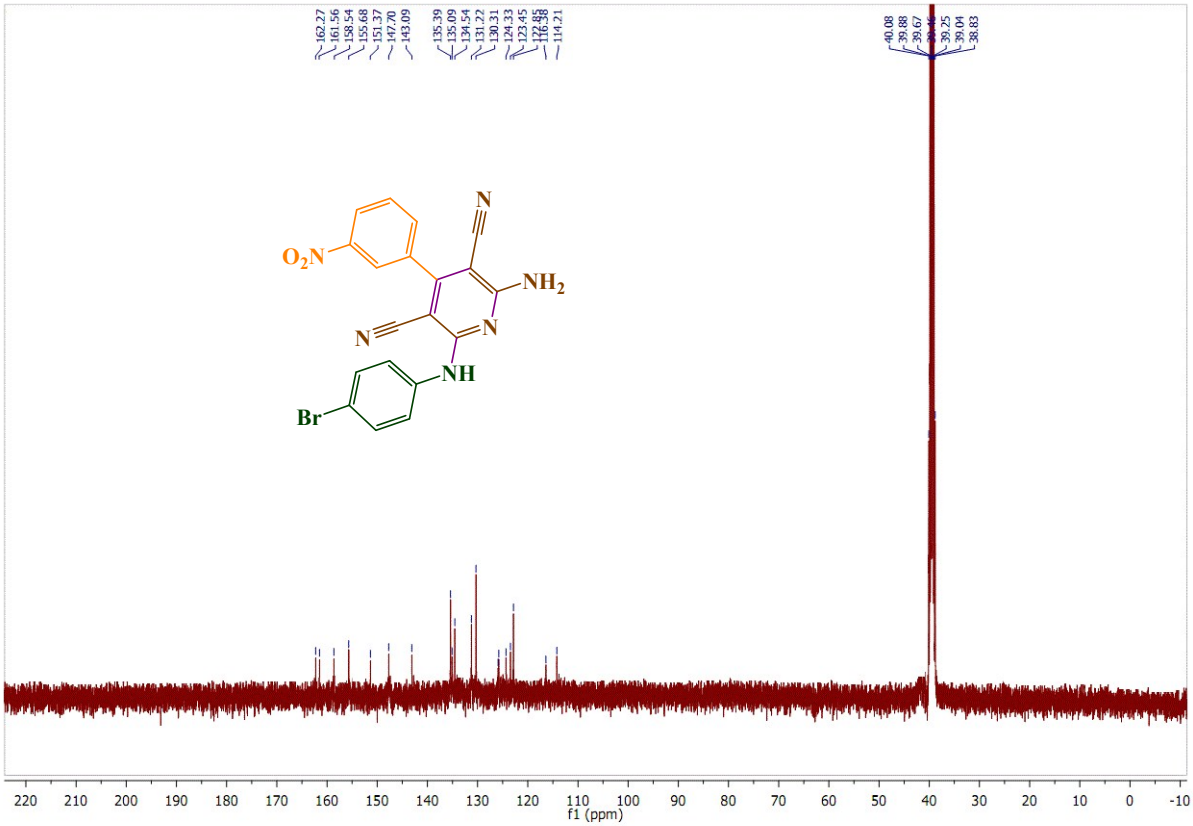

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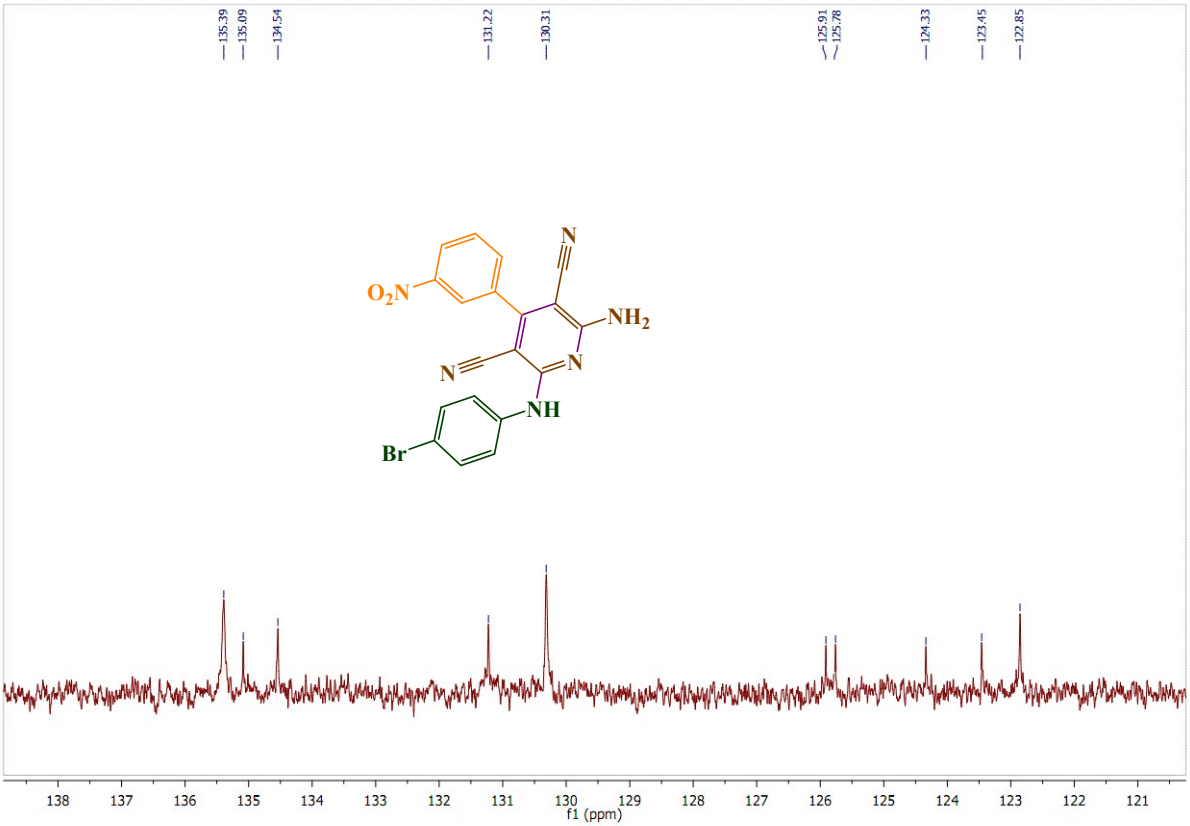

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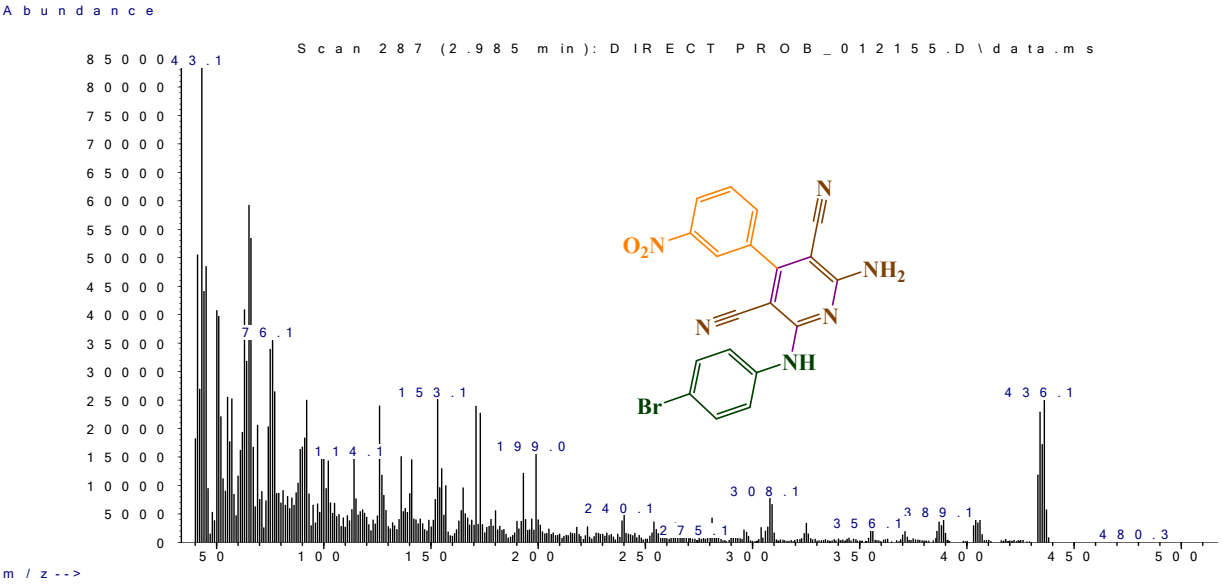

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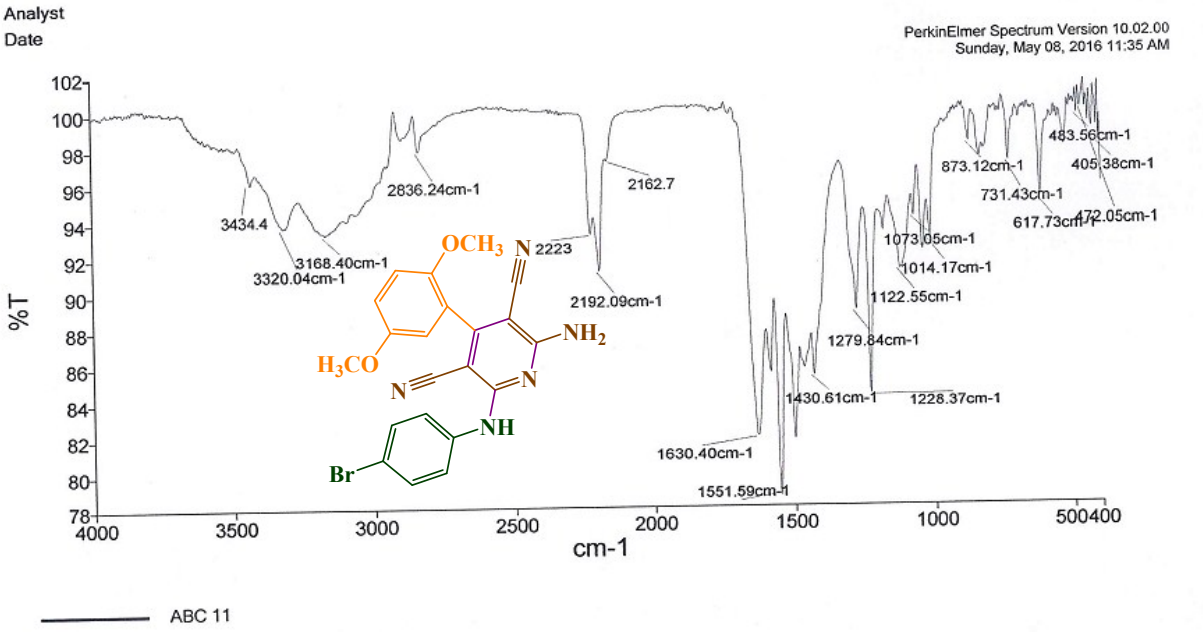


Fig S44. The ^{1}H NMR spectrum of 2-amino-6-((4-bromophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 11)

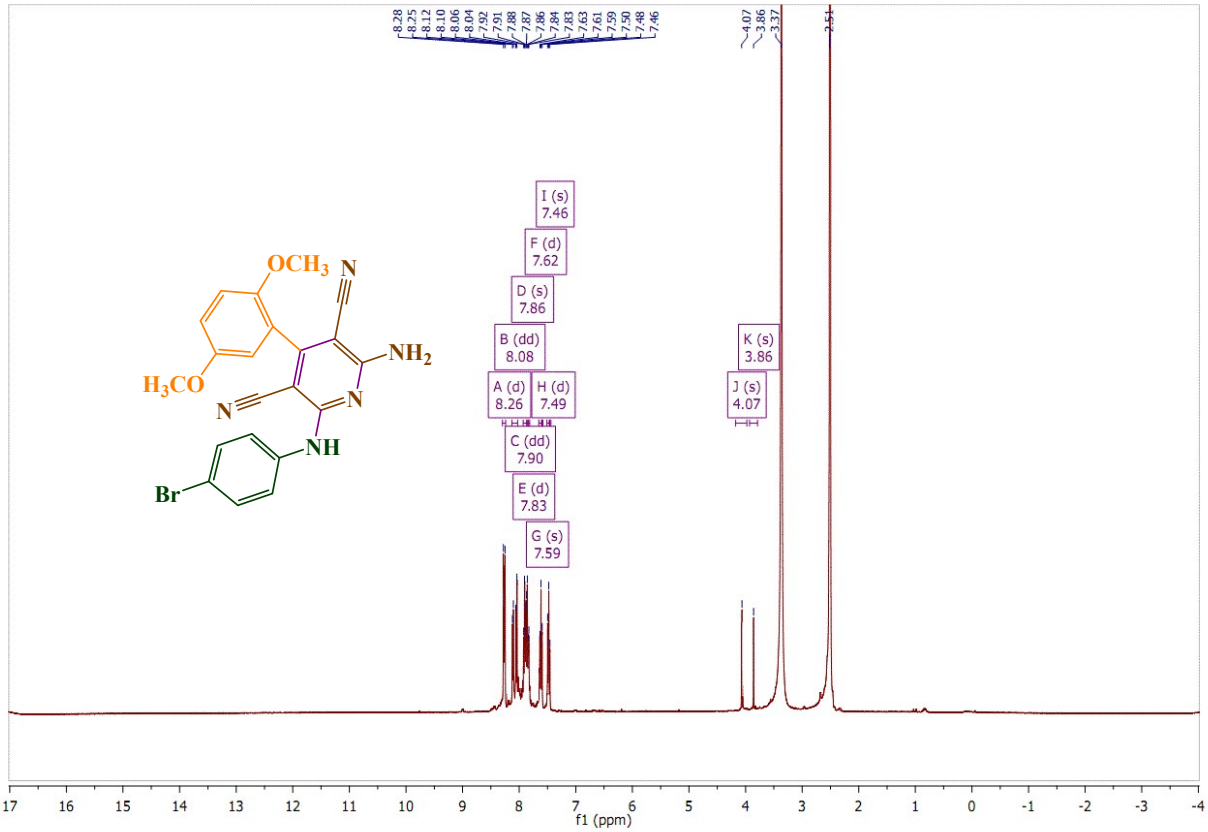


Fig S45. The ^{1}H NMR spectrum of 2-amino-6-((4-bromophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 11)

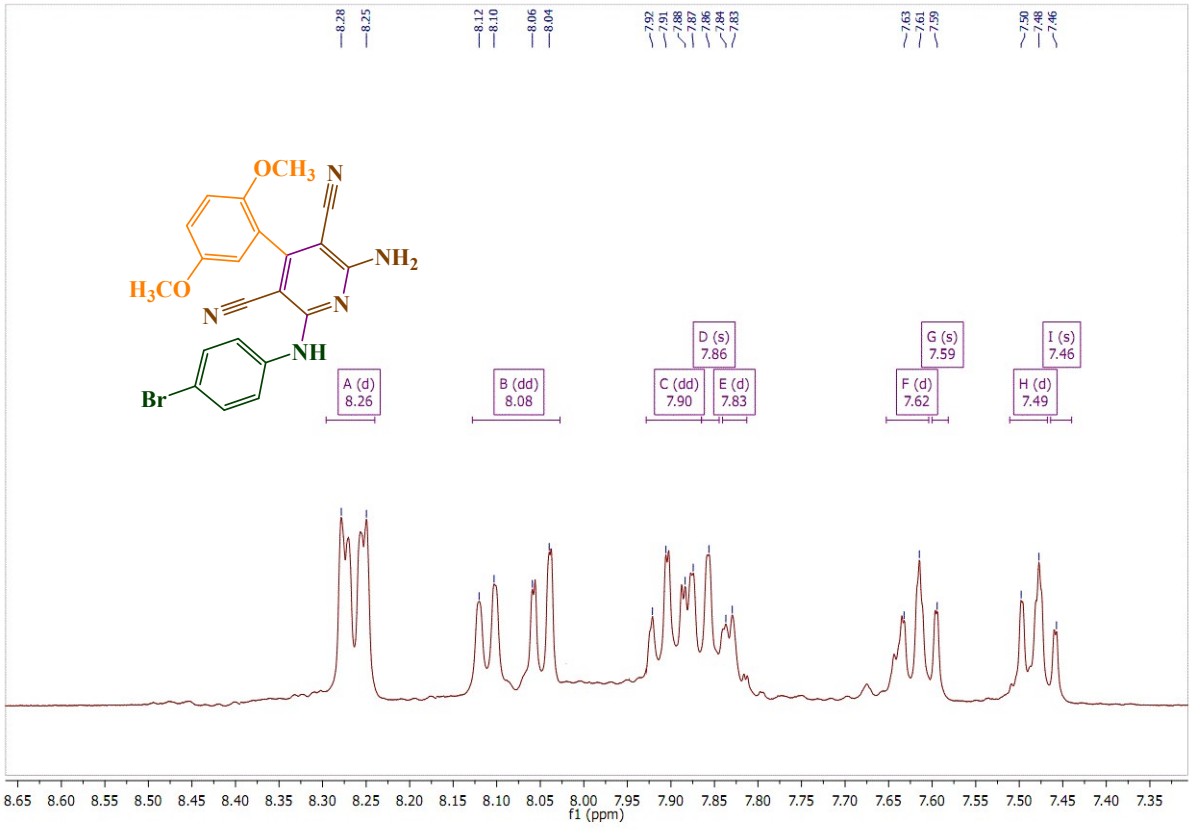


Fig S46. The ^{13}C NMR spectrum of 2-amino-6-((4-bromophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 11)

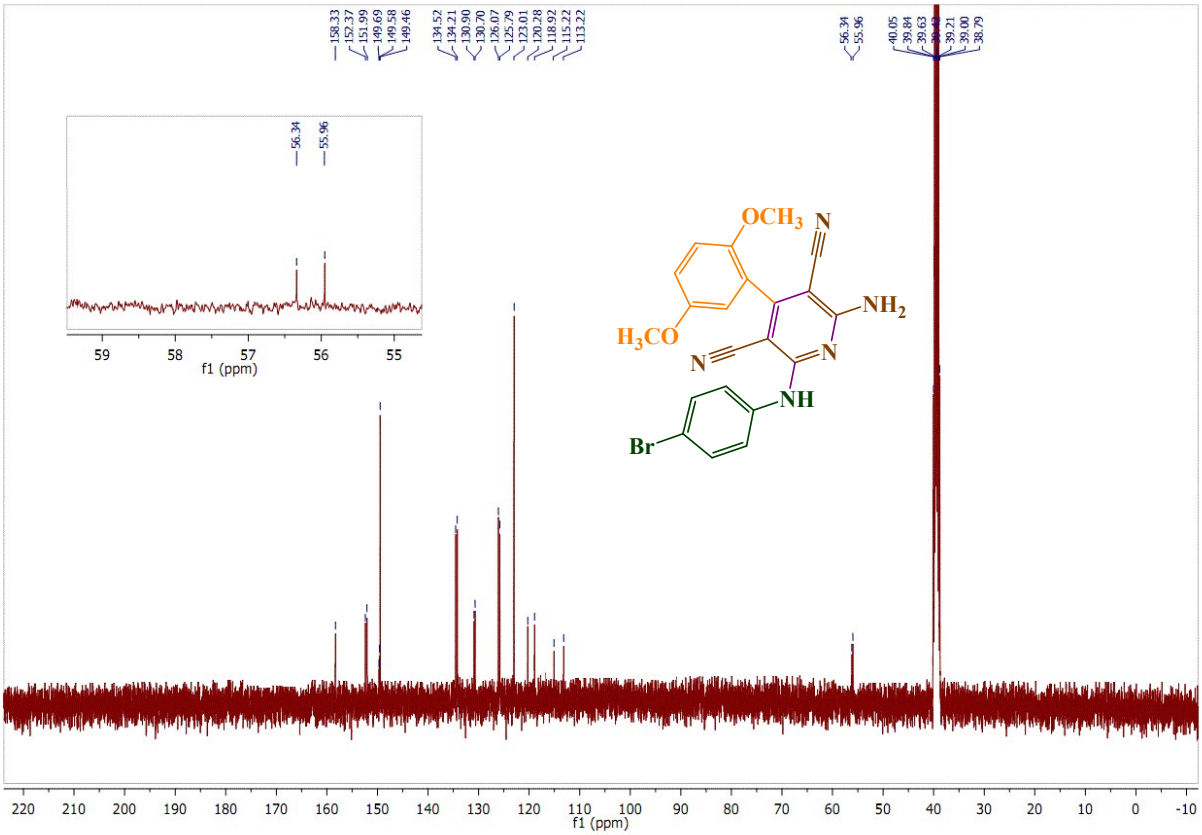


Fig S47. The ^{13}C NMR spectrum of 2-amino-6-((4-bromophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 11)

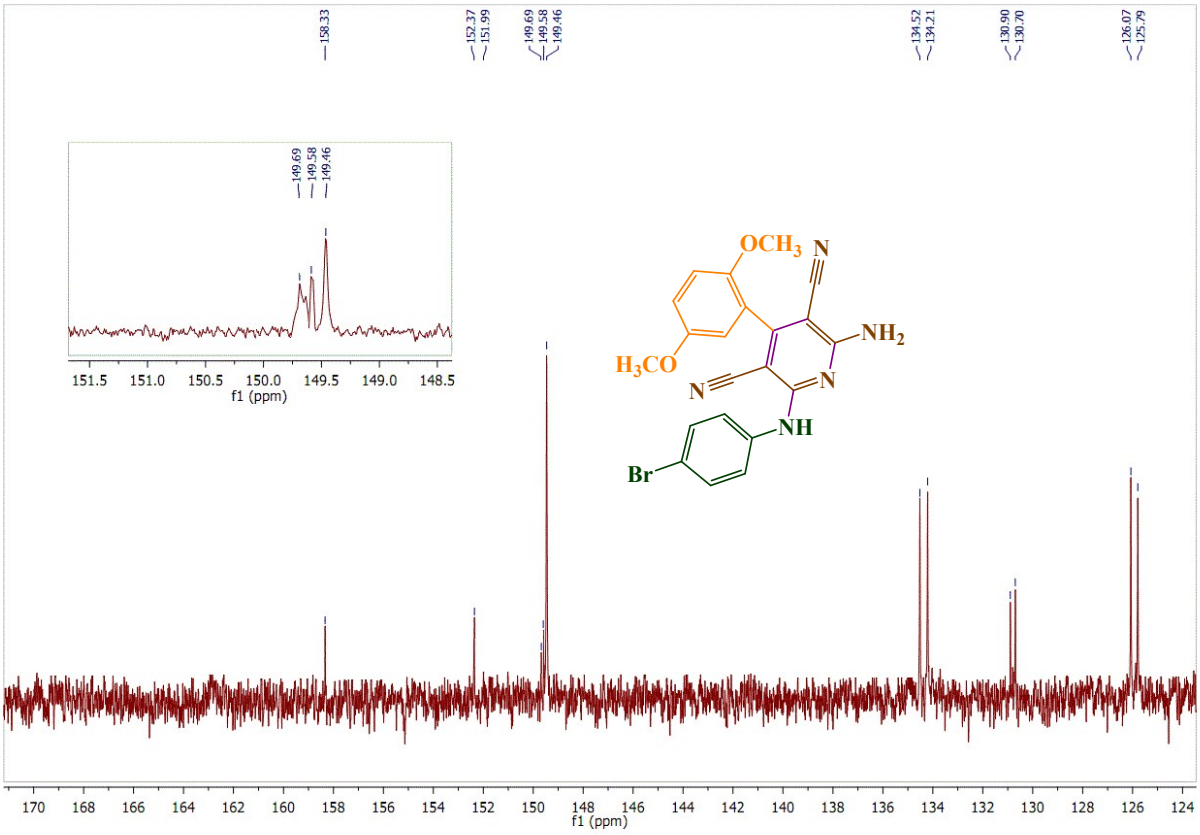


Fig S48. The mass spectrum of 2-amino-6-((4-bromophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 11)

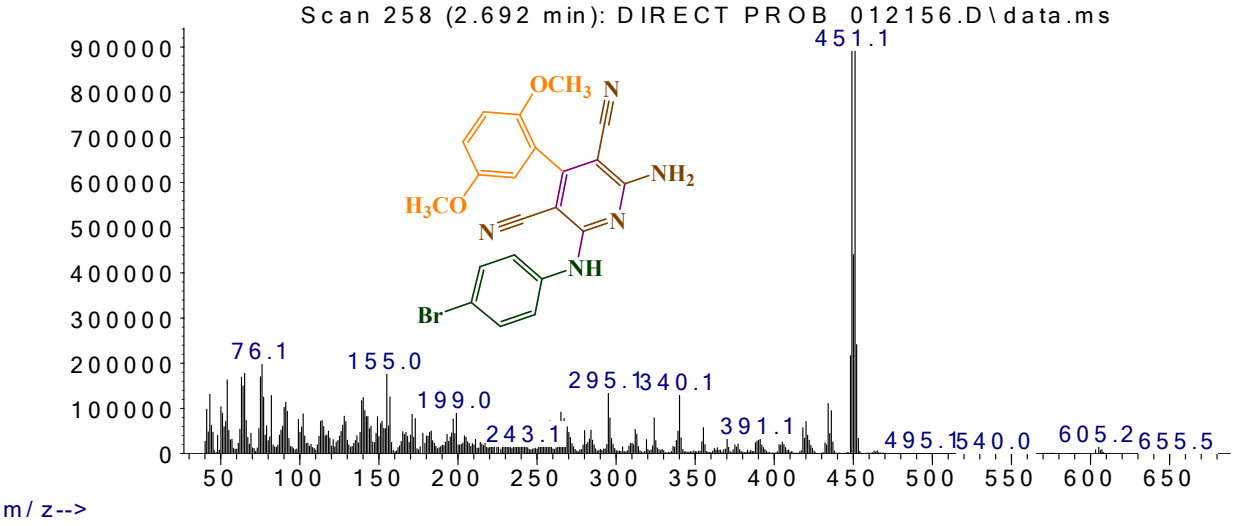


Fig S49. The FT-IR spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

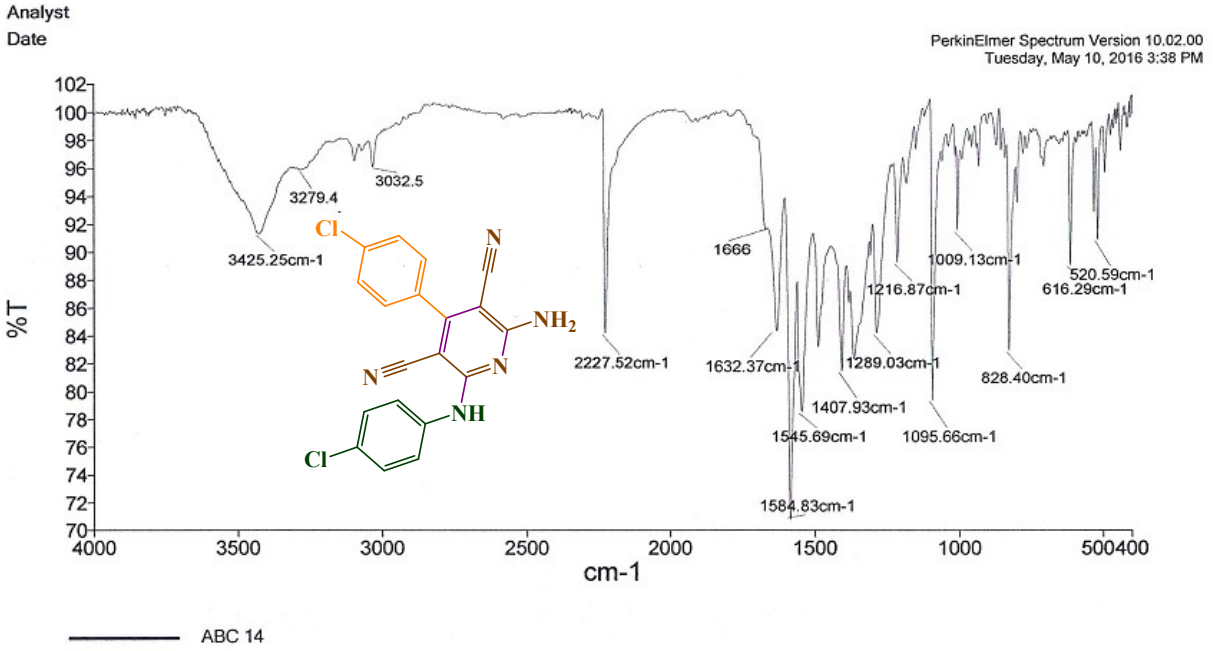


Fig S50. The ^{1}H NMR spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

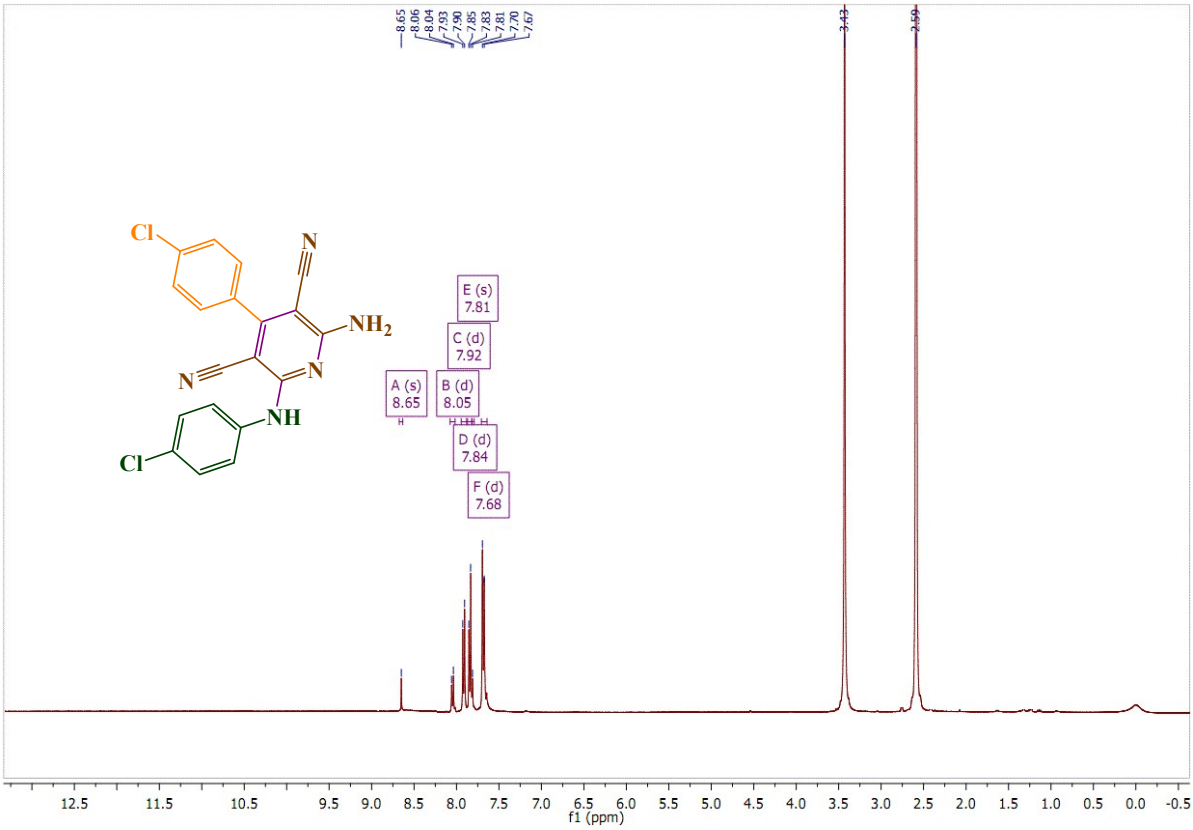


Fig S51. The ^{1}H NMR spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

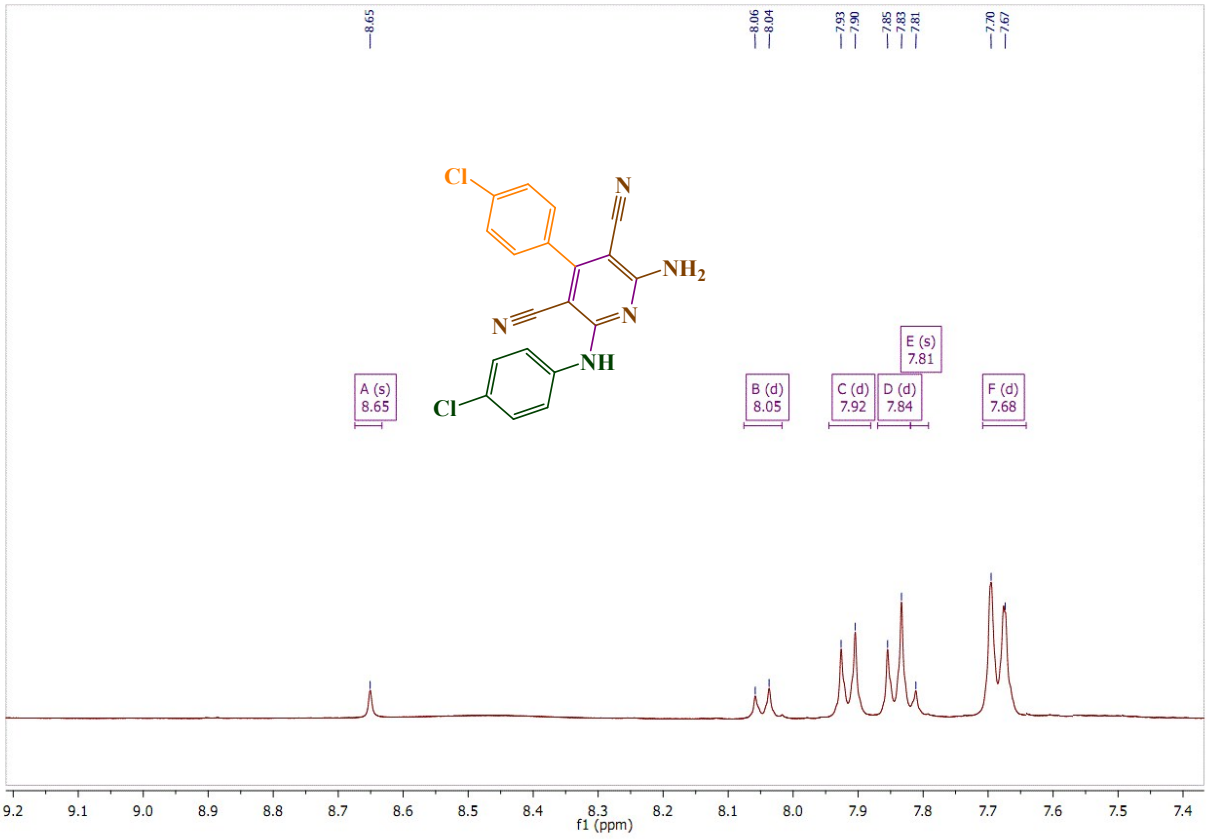


Fig S52. The ^{13}C NMR spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

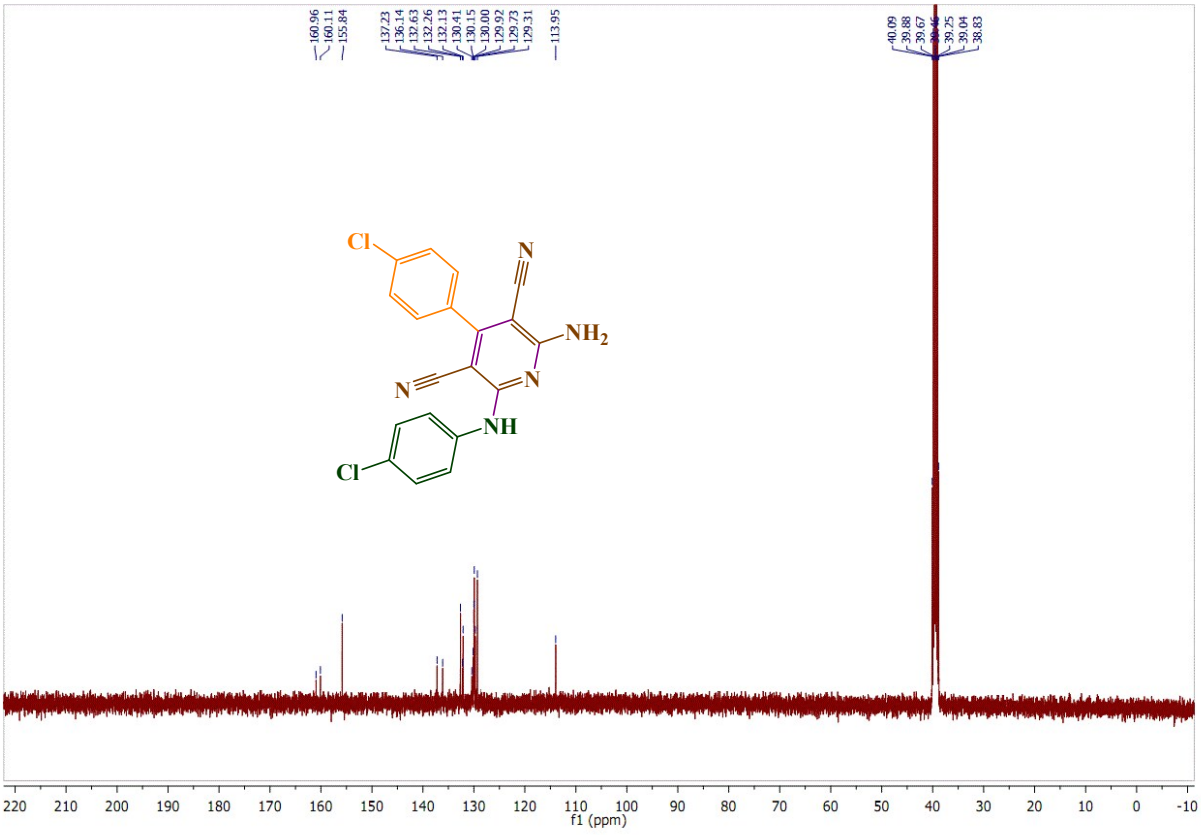


Fig S53. The ^{13}C NMR spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

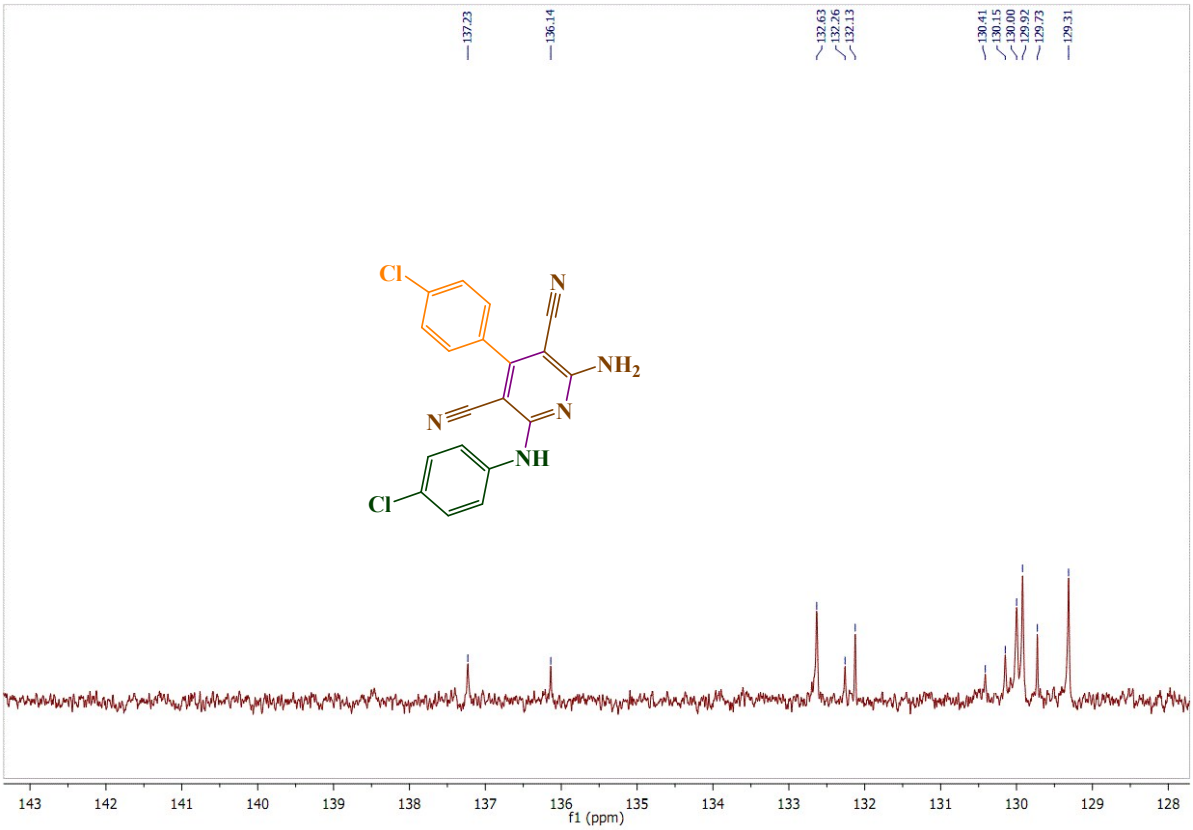


Fig S54. The mass spectrum of 2-amino-4-(4-chlorophenyl)-6-((4-chlorophenyl)amino)pyridine-3,5-dicarbonitrile (Table 4, entry 14)

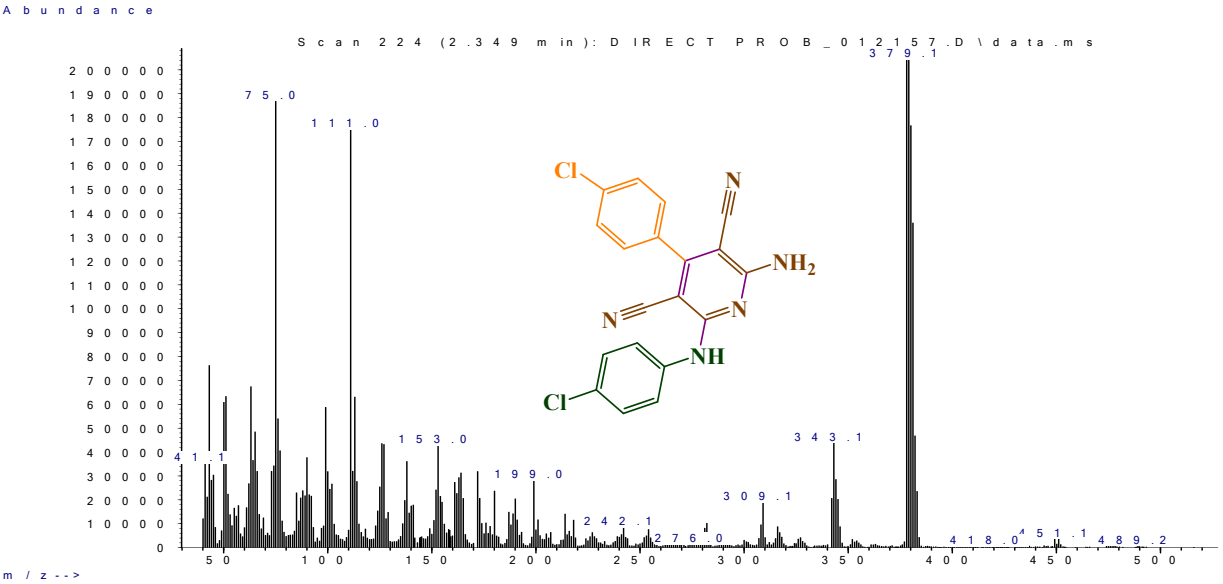


Fig S55. The FT-IR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

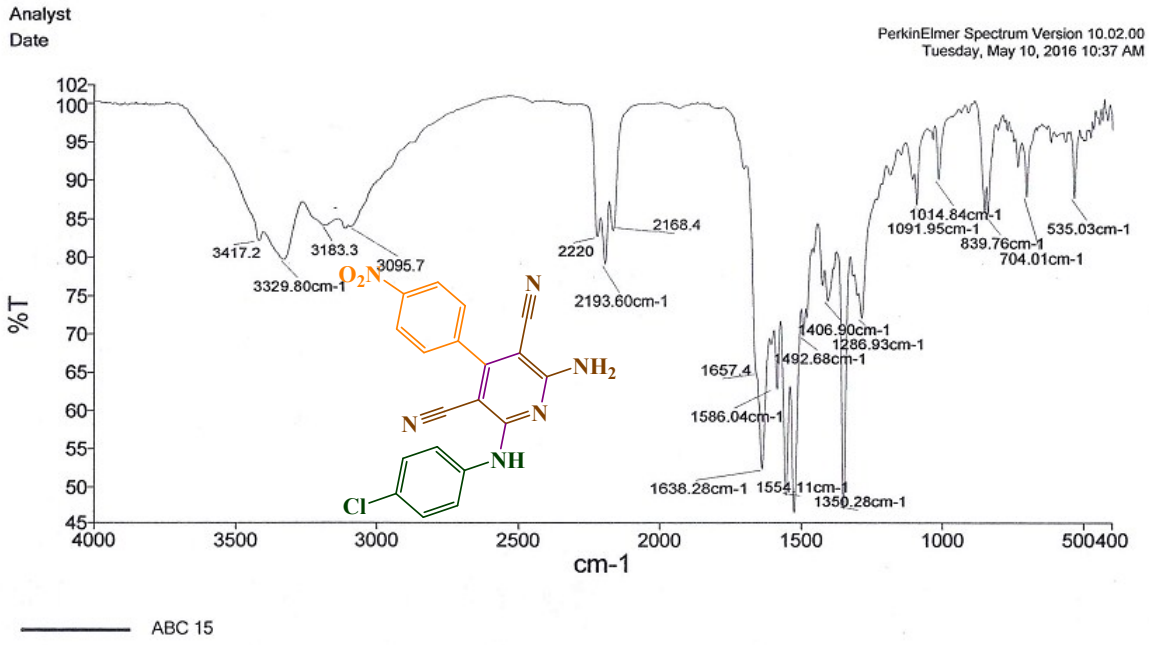


Fig S56. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

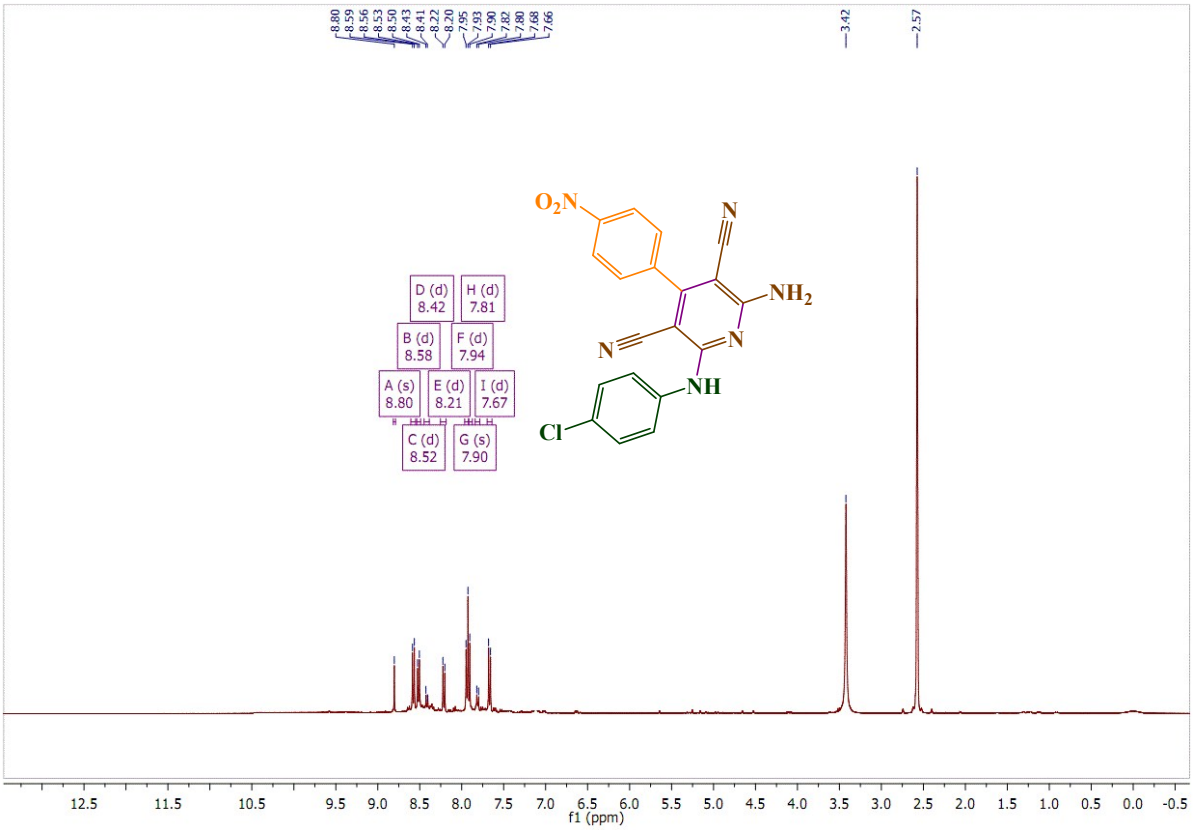


Fig S57. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

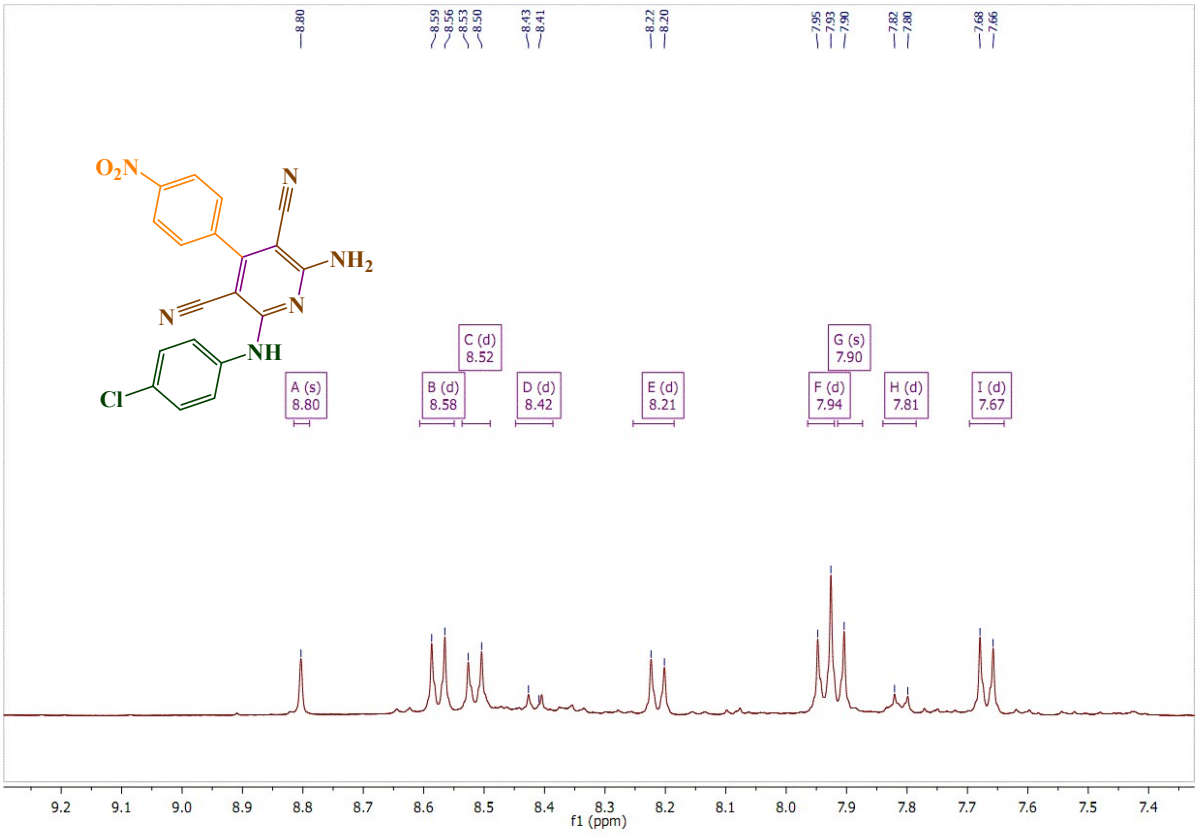


Fig S58. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

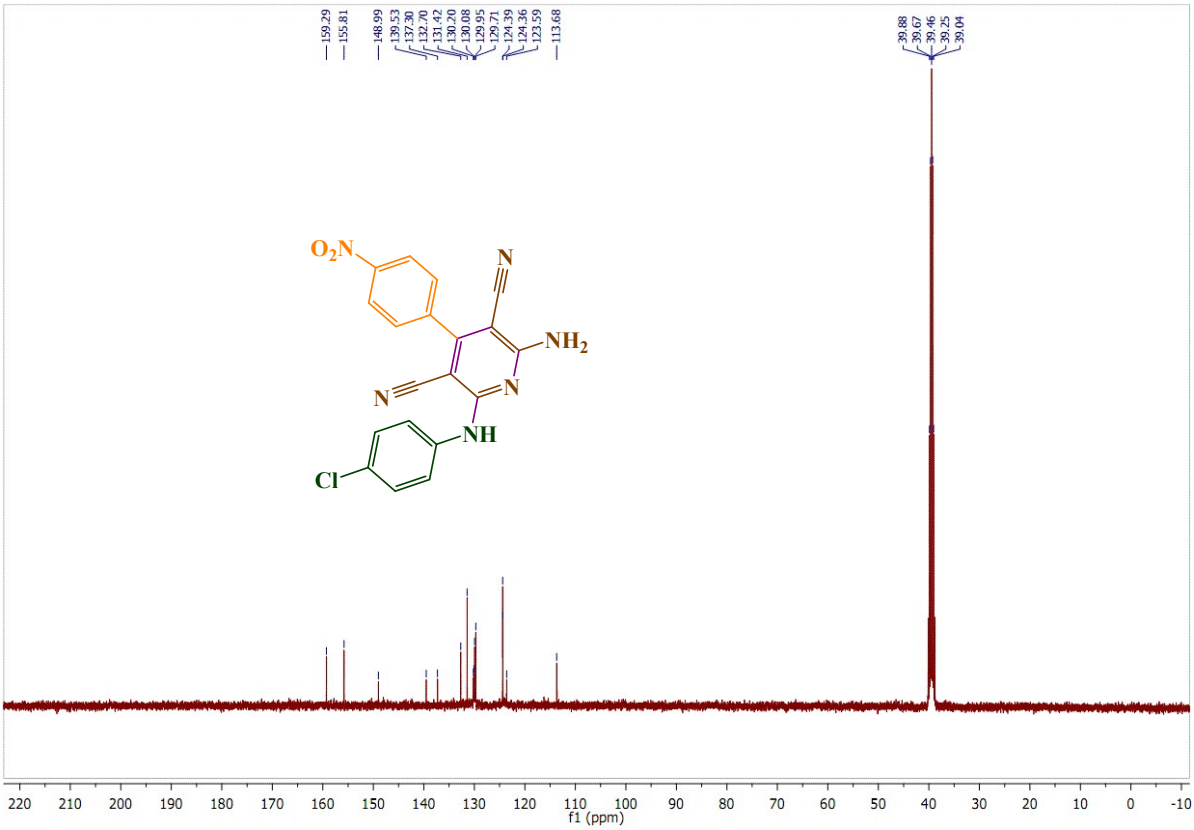


Fig S59. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

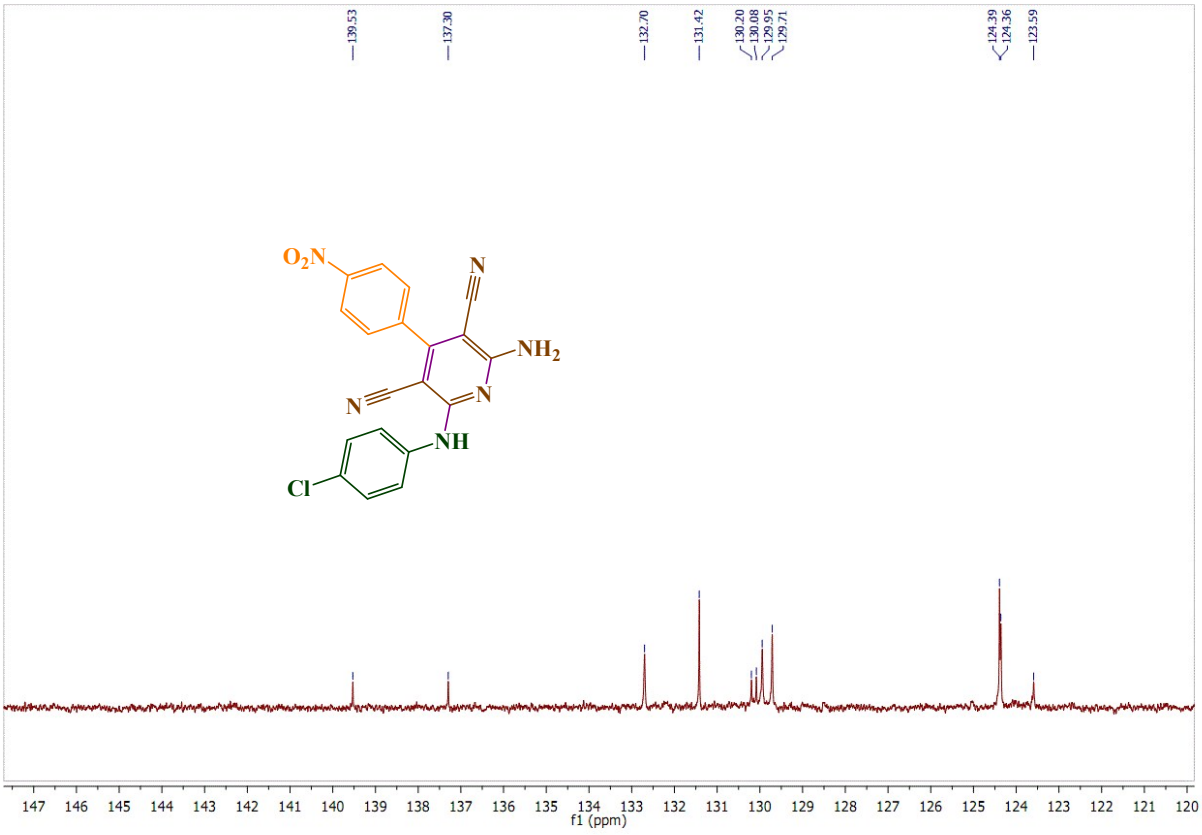


Fig S60. The mass spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(4-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 15)

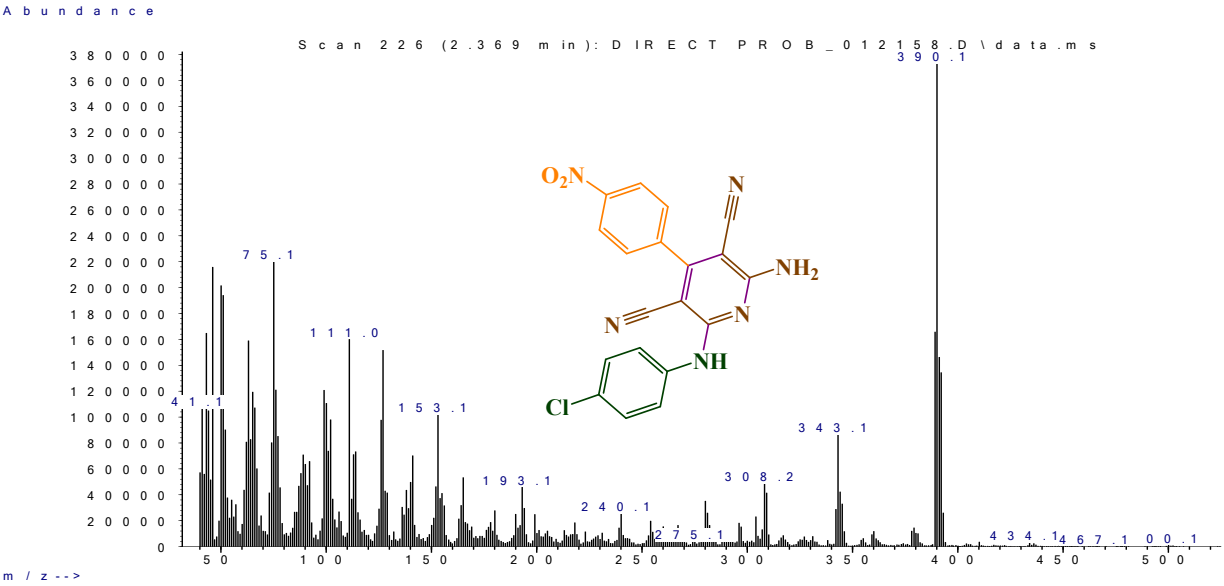


Fig S61. The FT-IR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

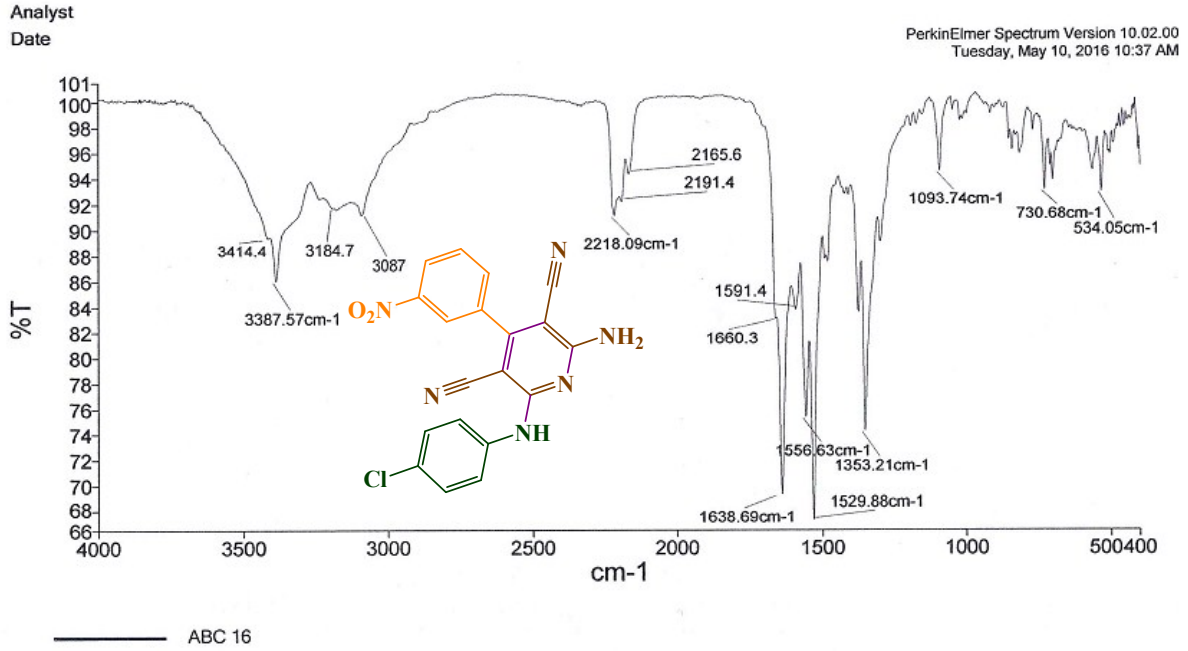


Fig S62. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

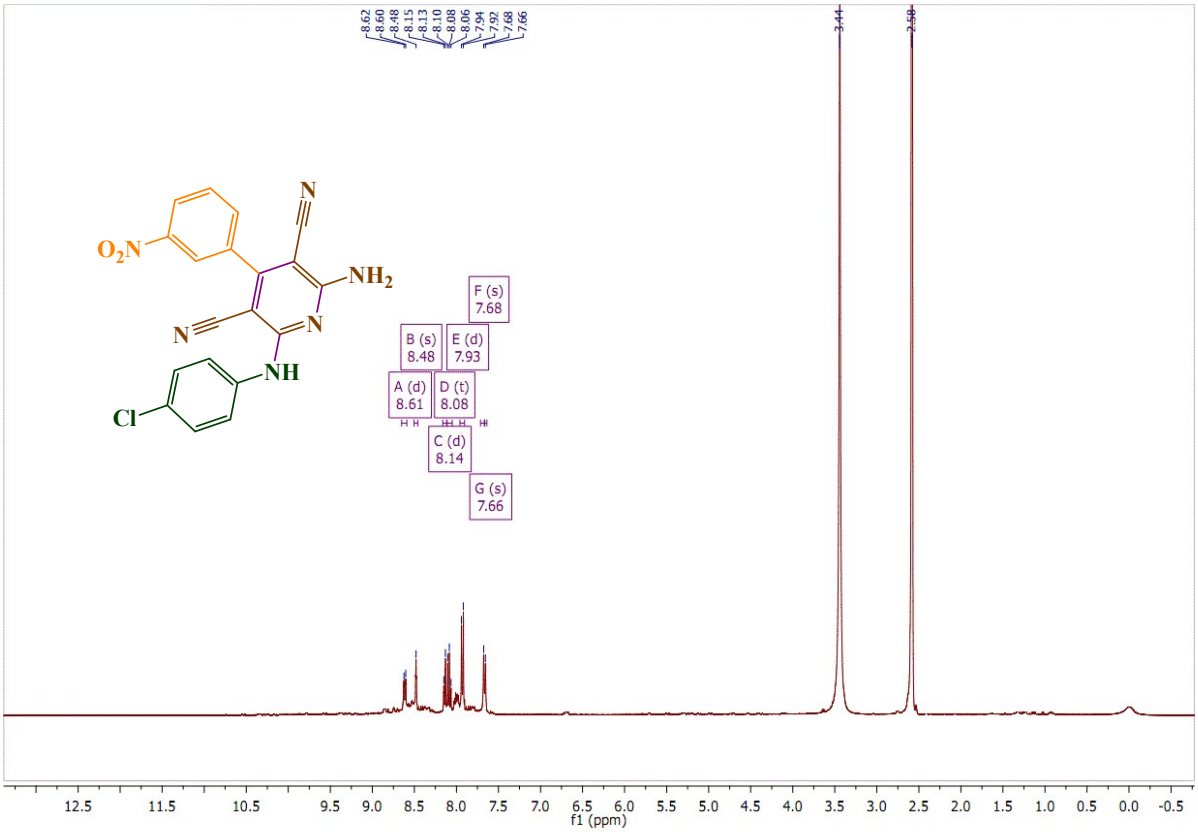


Fig S63. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

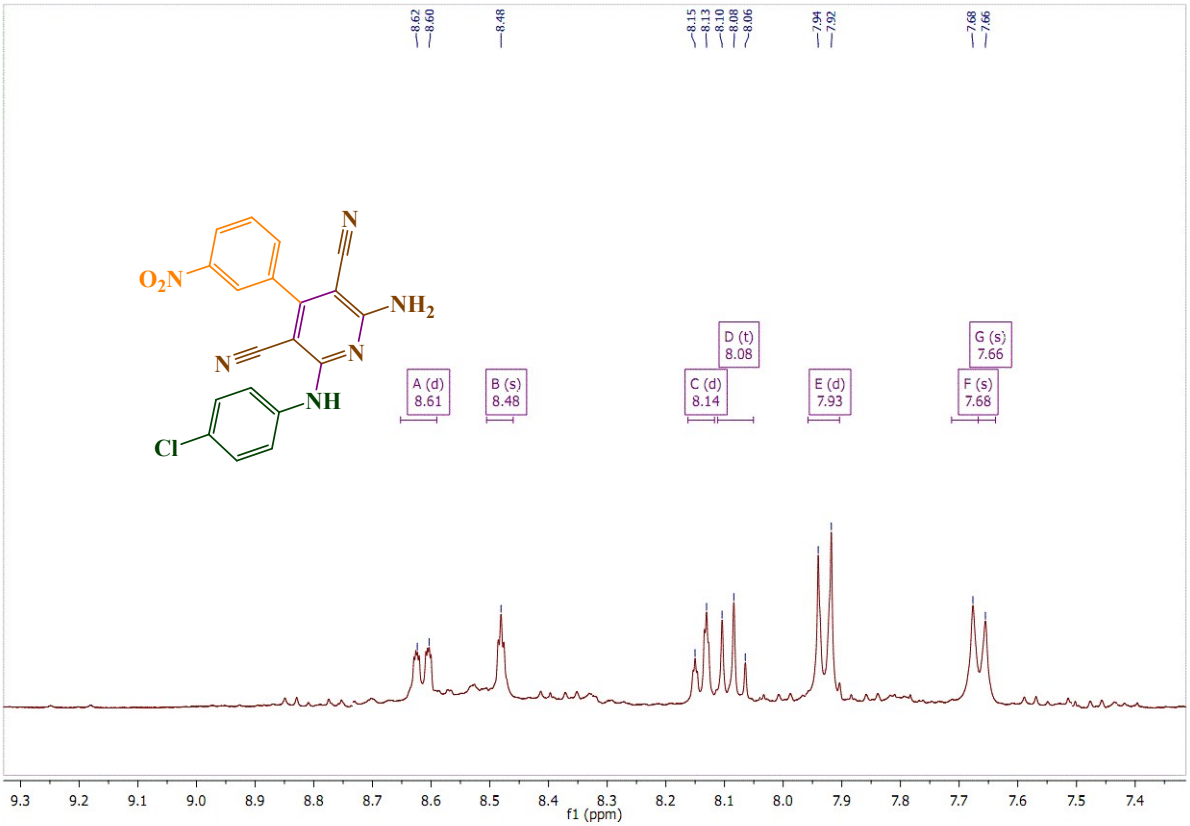


Fig S64. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

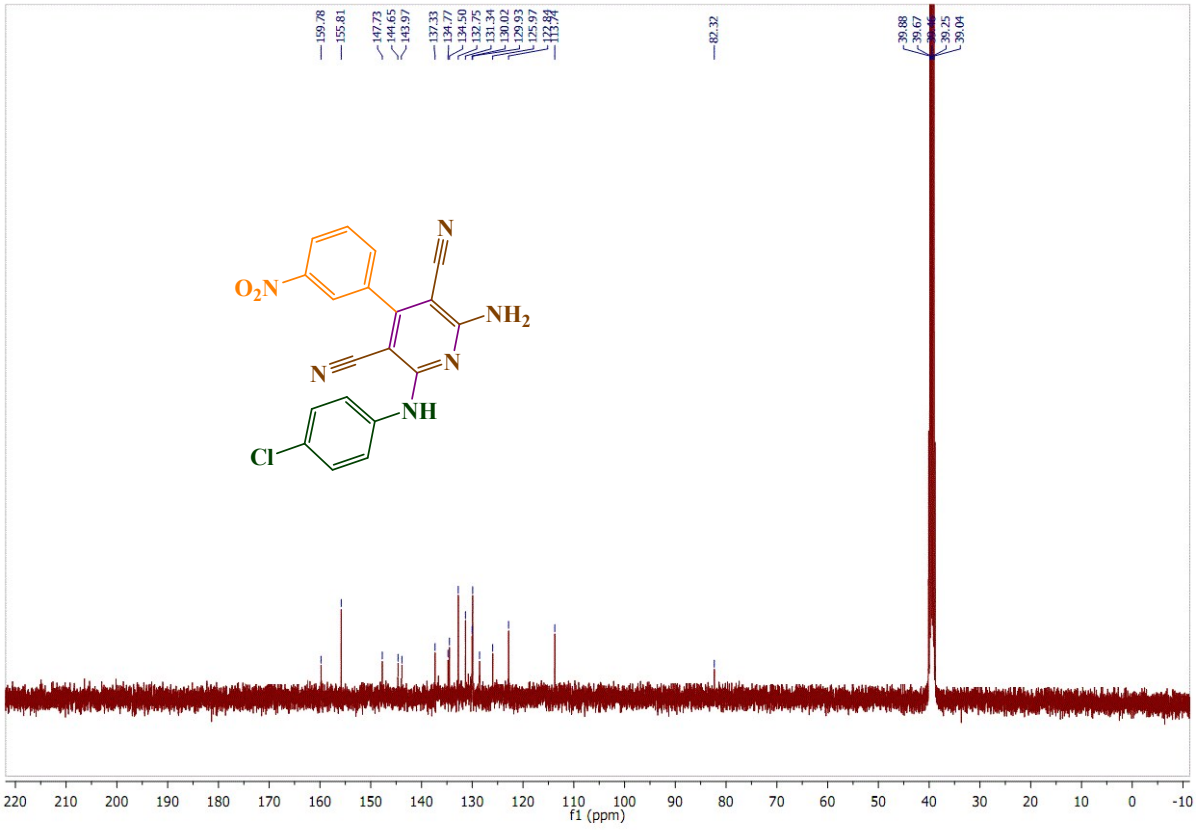


Fig S65. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

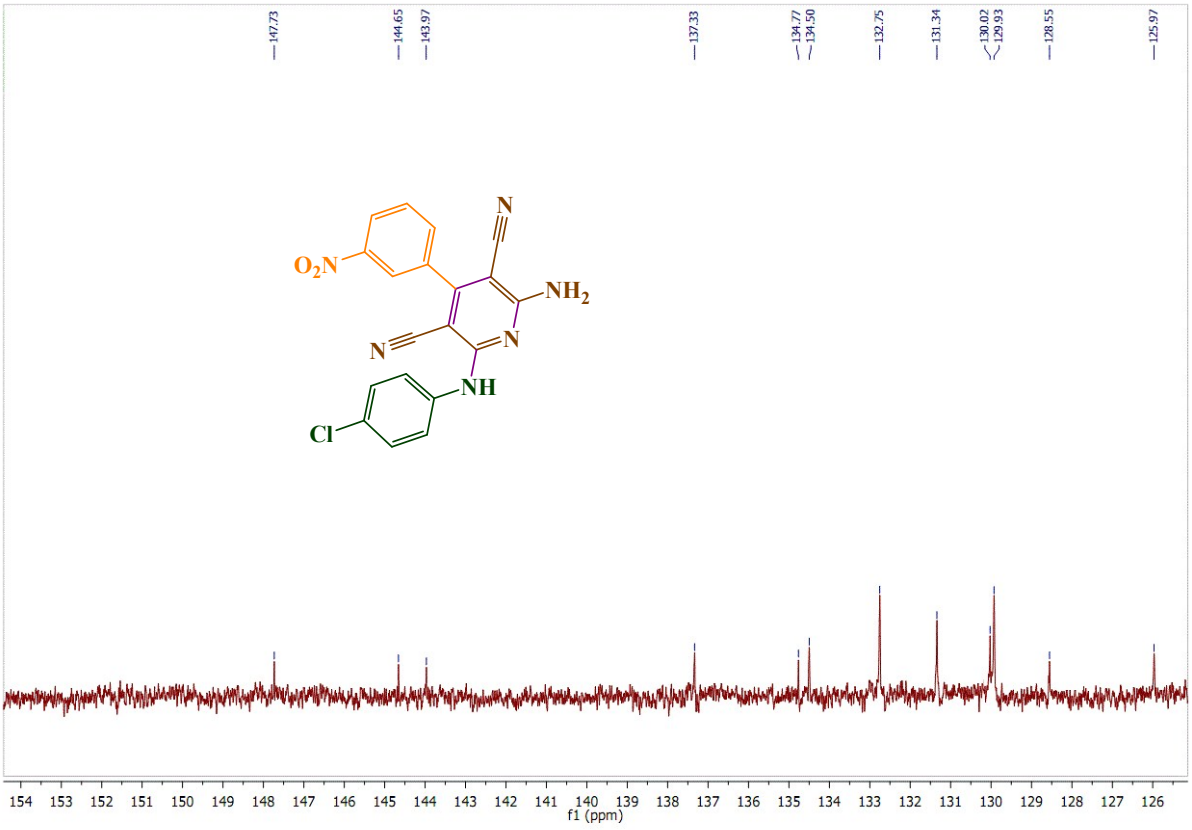


Fig S66. The mass spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(3-nitrophenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 16)

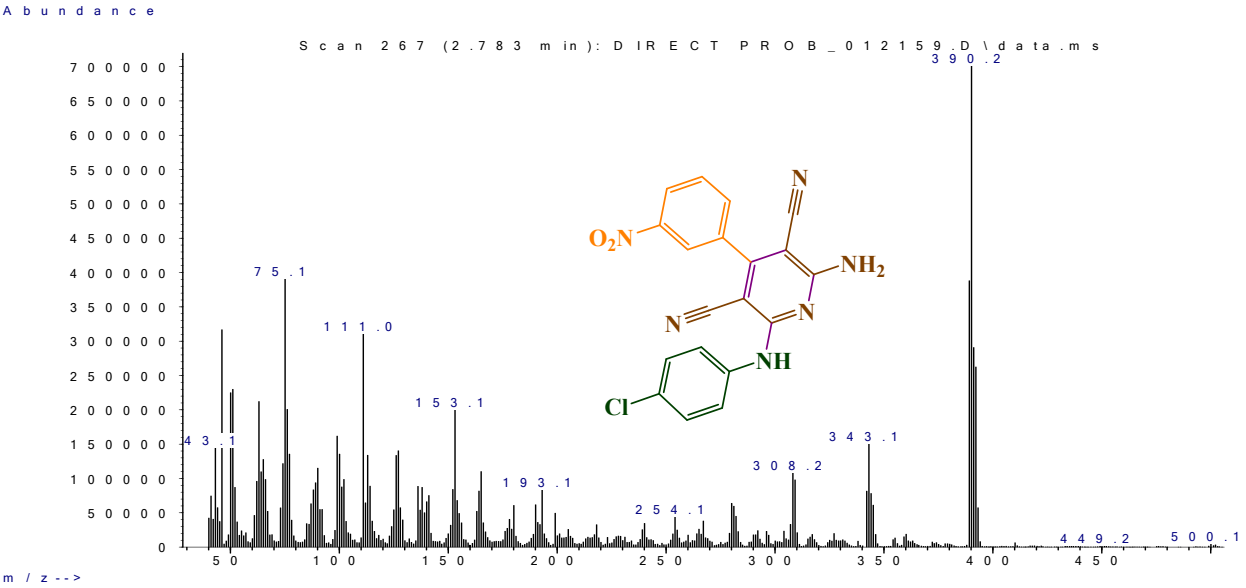


Fig S67. The FT-IR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

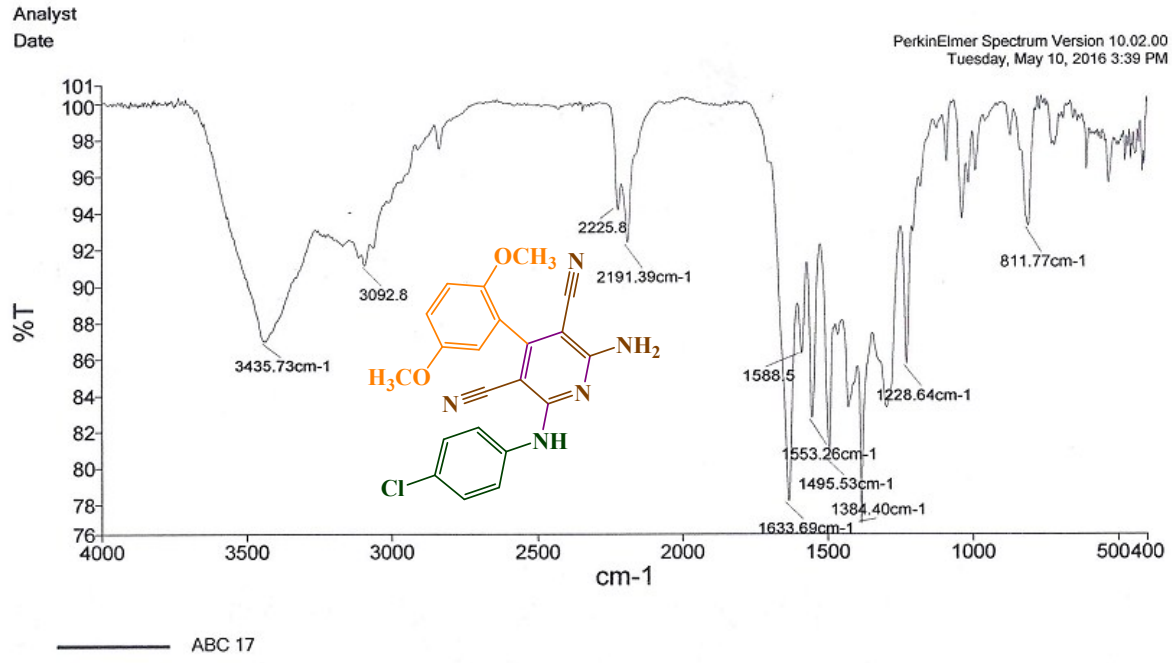


Fig S68. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

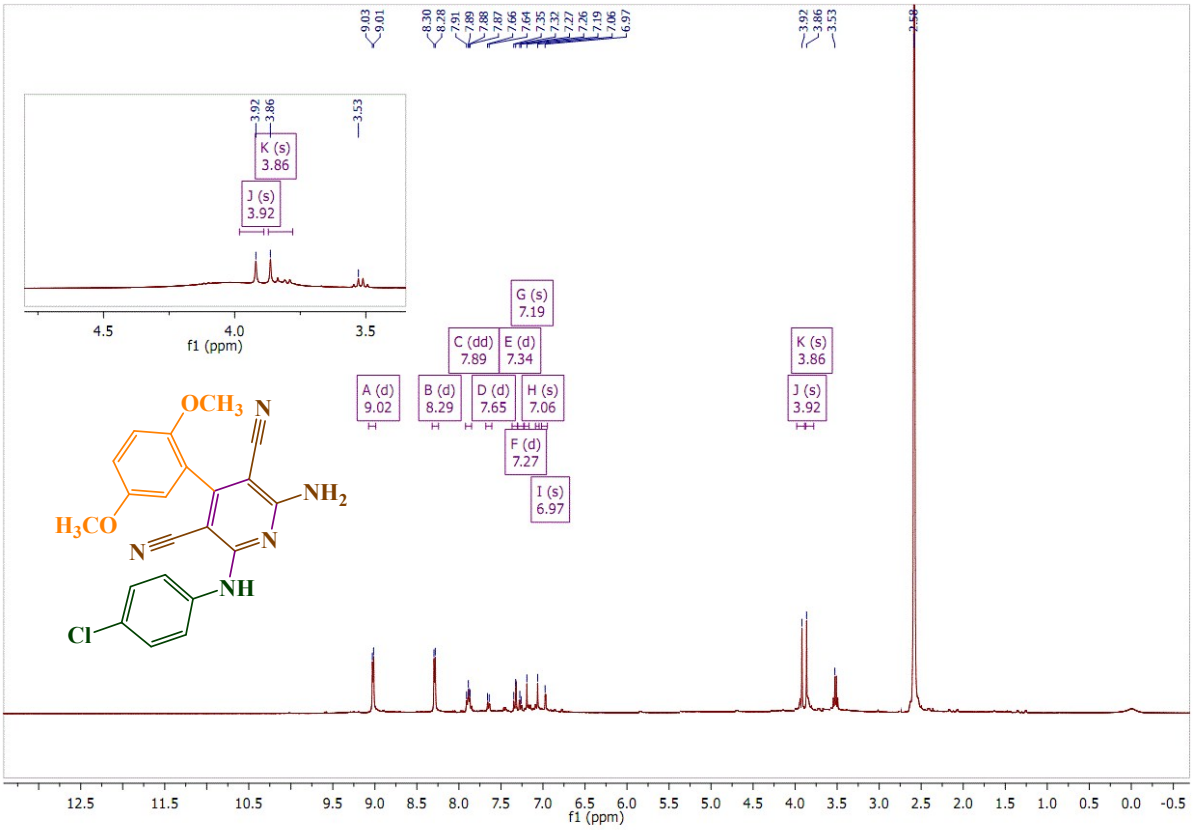


Fig S69. The ^{1}H NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

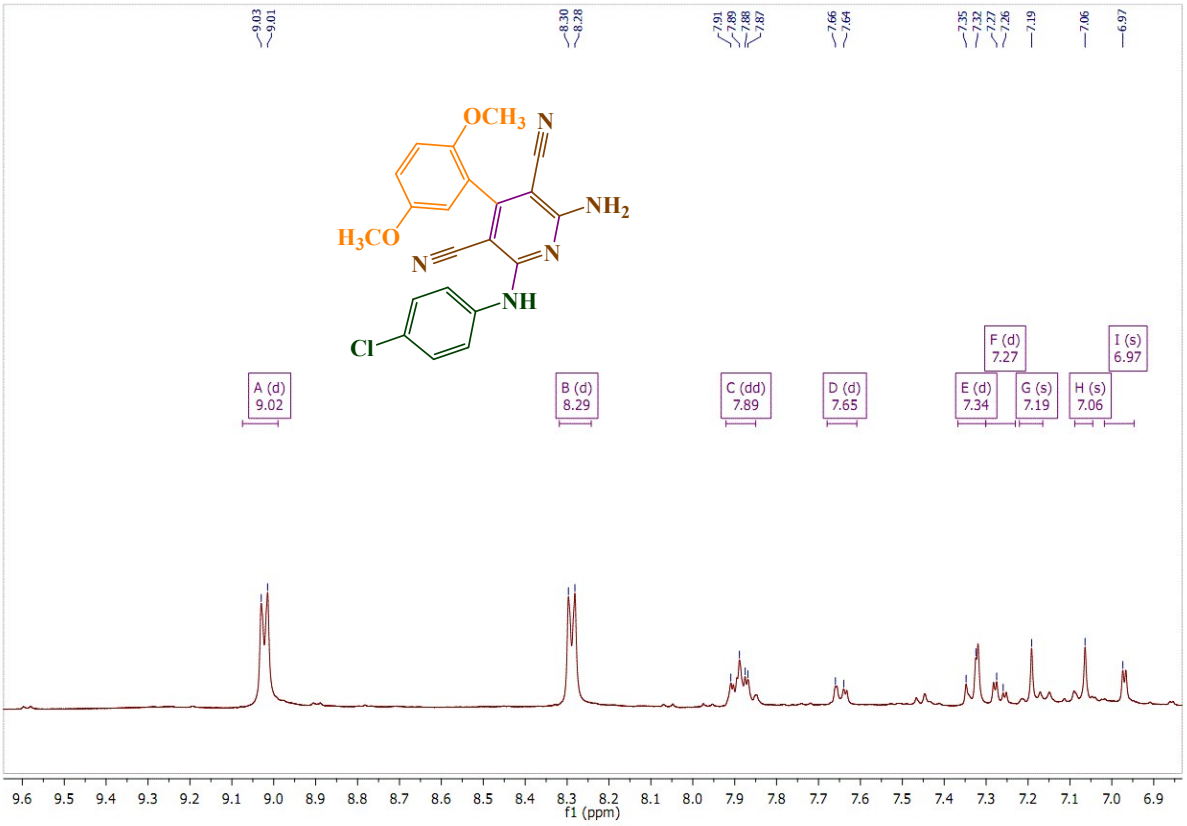


Fig S70. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

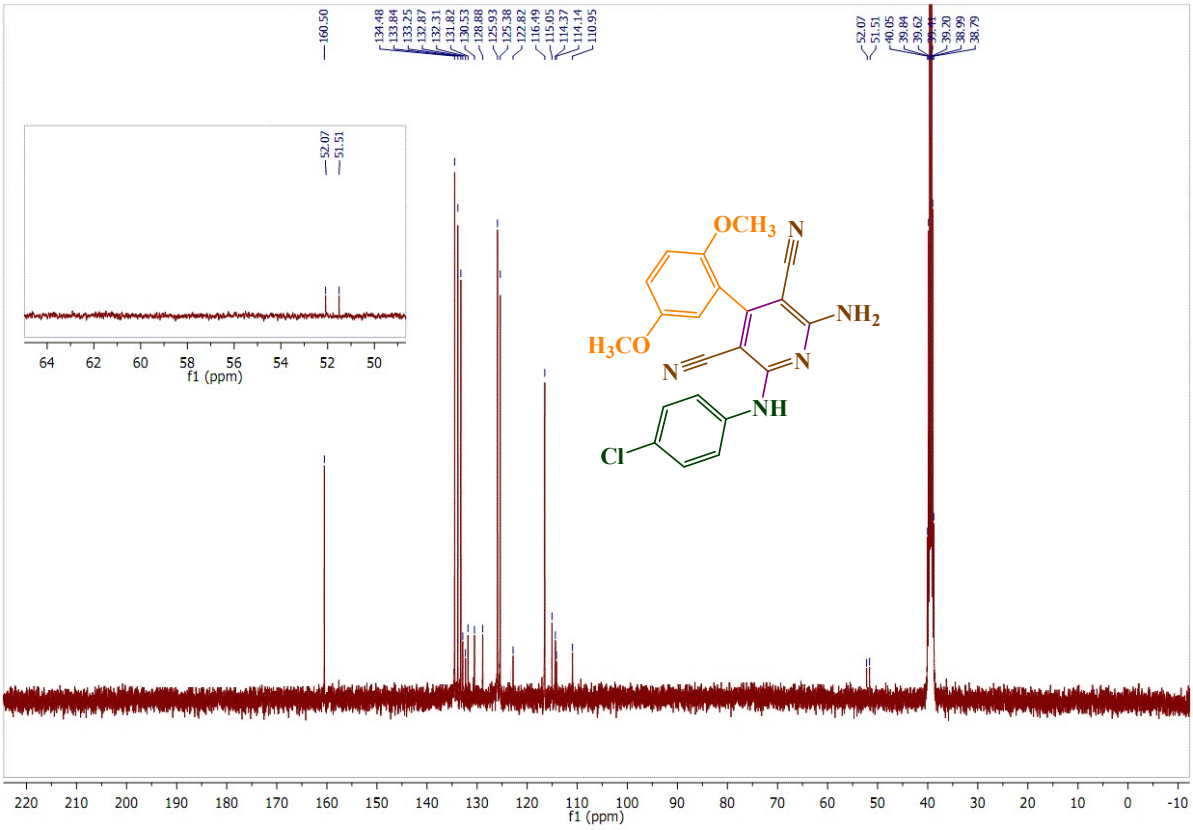


Fig S71. The ^{13}C NMR spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

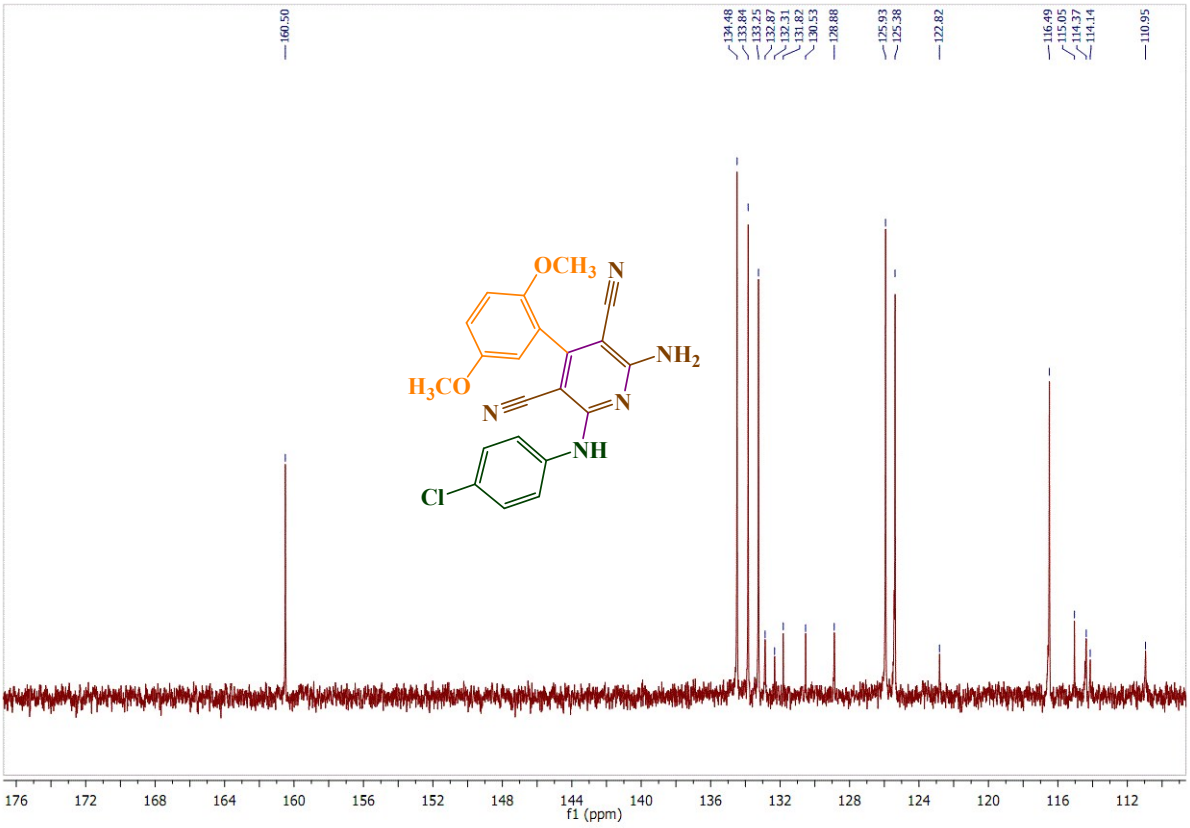
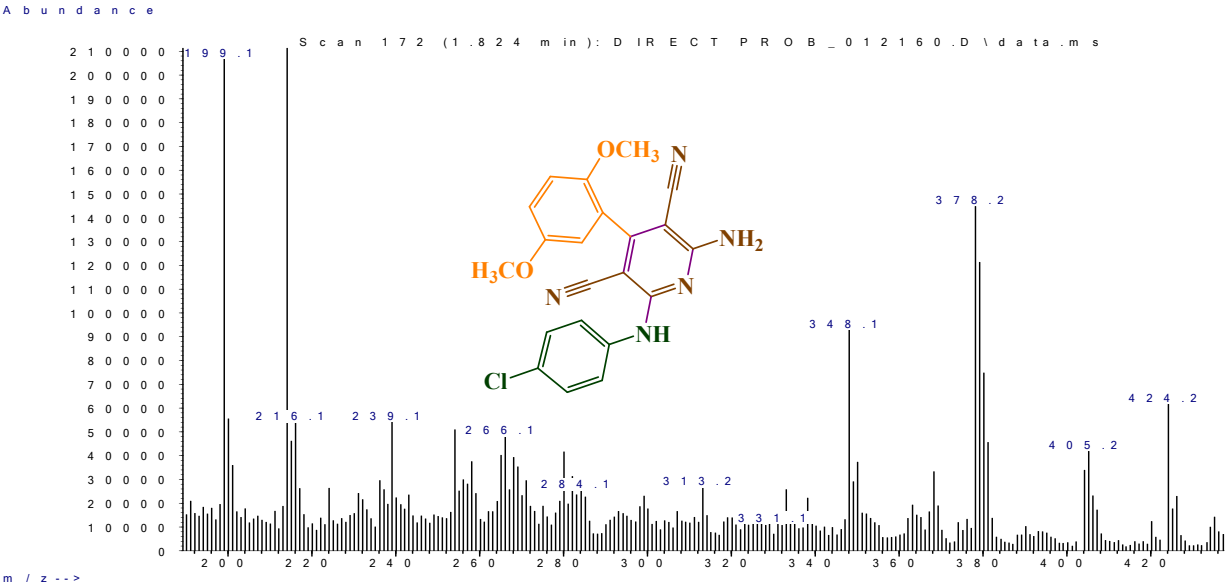
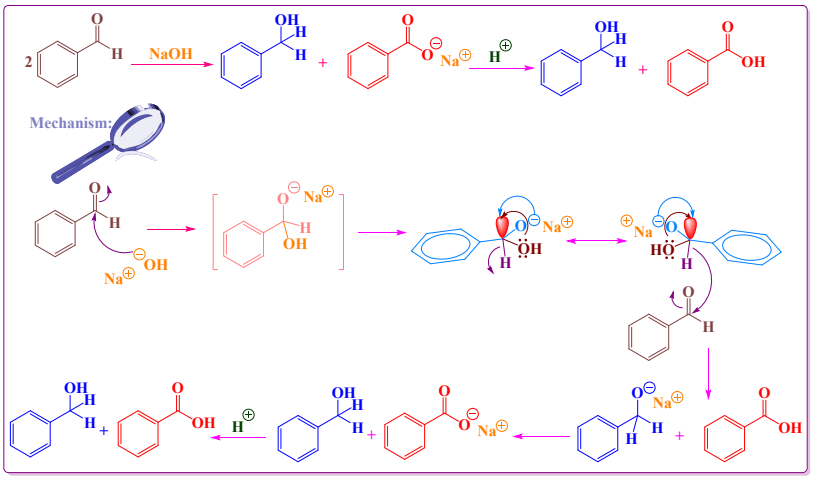
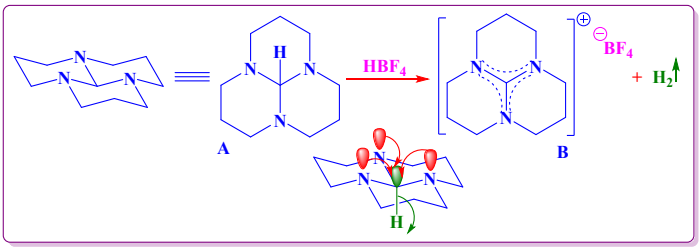


Fig S72. The mass spectrum of 2-amino-6-((4-chlorophenyl)amino)-4-(2,5-dimethoxyphenyl)pyridine-3,5-dicarbonitrile (Table 4, entry 17)

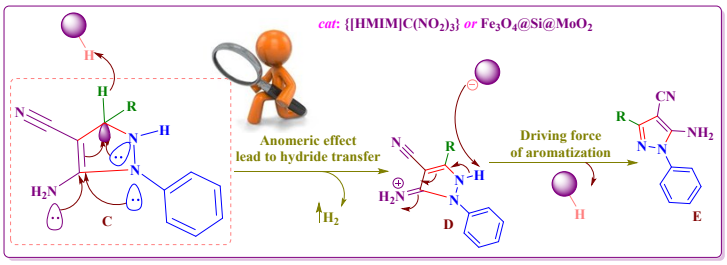




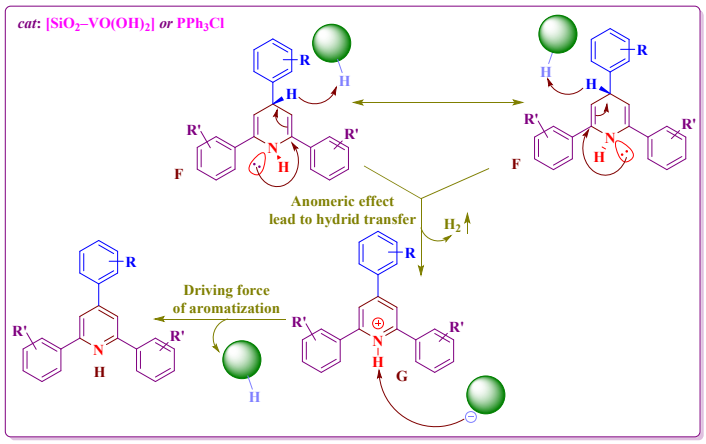
Scheme S1. The suggested mechanism for the in-situ oxidation-reduction in Cannizzaro reaction by uncommon hydride transfer *via* ABO mechanism.[25]



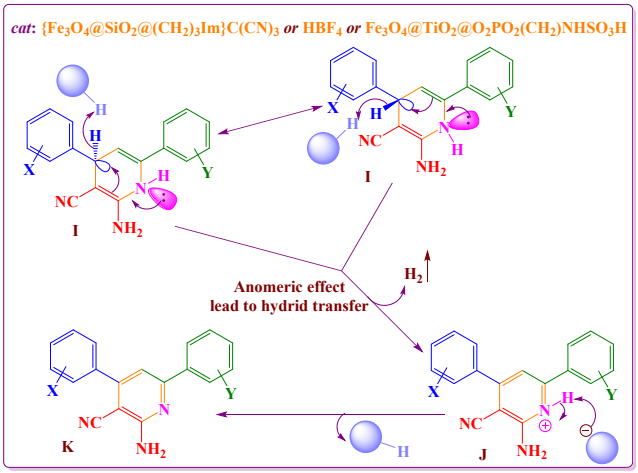
Scheme S2. A striking example which had been detected for an unusual hydride transfer from tricyclic orthoamide (A) by ABO mechanism.[26]



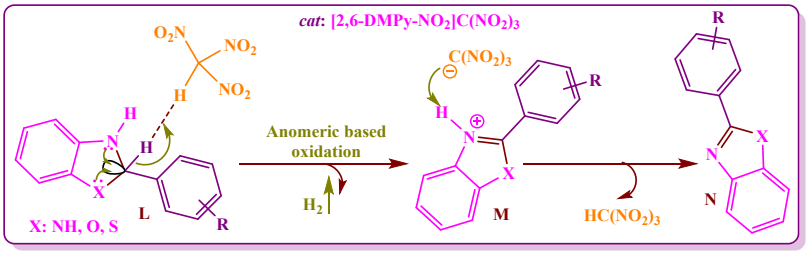
Scheme S3. Synthesis of 1,4-dihydropyrano-[2,3-*c*]-pyrazole derivatives *via* ABO mechanism.[23a,b]



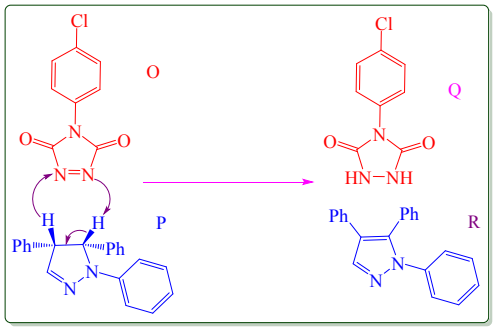
Scheme S4. Synthesis of 2,4,6-triarylpyridines by ABO mechanism.[23c,d]



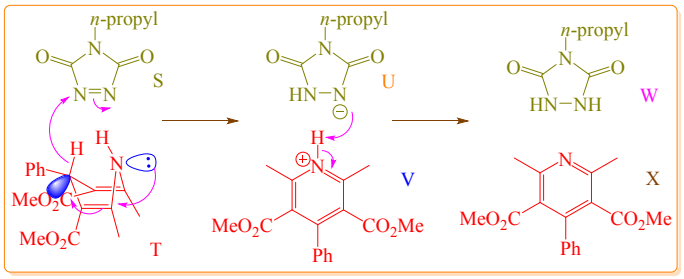
Scheme S5. Synthesis of 2-amino-3-cyanopyridines *via* ABO mechanism.[23e-g]



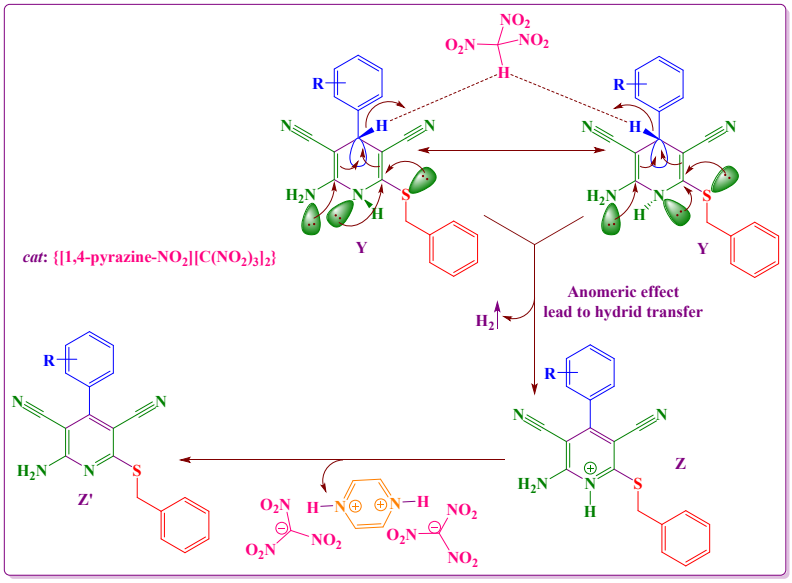
Scheme S6. Synthesis of 2-sbstituted benz-(imida, oxa and othia)-zole derivatives by ABO mechanism.[23h]



Scheme S7. Concerted oxidation *via* hydrogen abstraction-addition mechanism for the synthesis of 1,3,5-trisubstituted pyrazolines.[23i]



Scheme S8. Stepwise ABO mechanism for the aromatization of dihydropyridines.[23i]



Scheme S9. The synthesis of 2-amino-3,5-dicarbonitrile-6-sulfanylpyridines by ABO mechanism.[23j]

Supplementary data

Table S1. Electronic energy, zero point energy and corrected electronic energy at B3LYP/SVP level of theory

Compounds	Eel	ZPE	E_0
Stereoisomer 8A	-1006.0560552	0.3045152	-1005.751540
Stereoisomer 8B	-1006.0556538	0.3042918	-1005.751362
9-($CH(CN)_3$)	-1321.8489381	0.2615111	-1321.587427
9-($CH(NO_2)_3$)	-1658.3500469	0.3384009	-1658.011646
4	-1004.891294	0.281852	-1004.609442
10	-1156.3323528	0.3109338	-1156.021419
TS-($CH(CN)_3$)	-1322.9589092	0.2774572	-1322.681452
TS-($CH(NO_2)_3$)	-1659.4723295	0.3519455	-1659.120384
TS1-O_2	-1156.2208459	0.3035729	-1155.917273
TS2-O_2	-1156.2506771	0.3079281	-1155.942749
$CH(CN)_3$	-316.94853	0.012175	-316.936355
$CH(NO_2)_3$	-653.4685789	0.0555679	-653.413011
H_2O_2	-151.4230926	0.0263706	-151.396722
O_2	-150.2047989	0.0038669	-150.200932
H_2	-1.1737901	0.0099631	-1.163827

Fig. S73. Total Energy along IRC of **TS-(CH(CN)$_3$)**

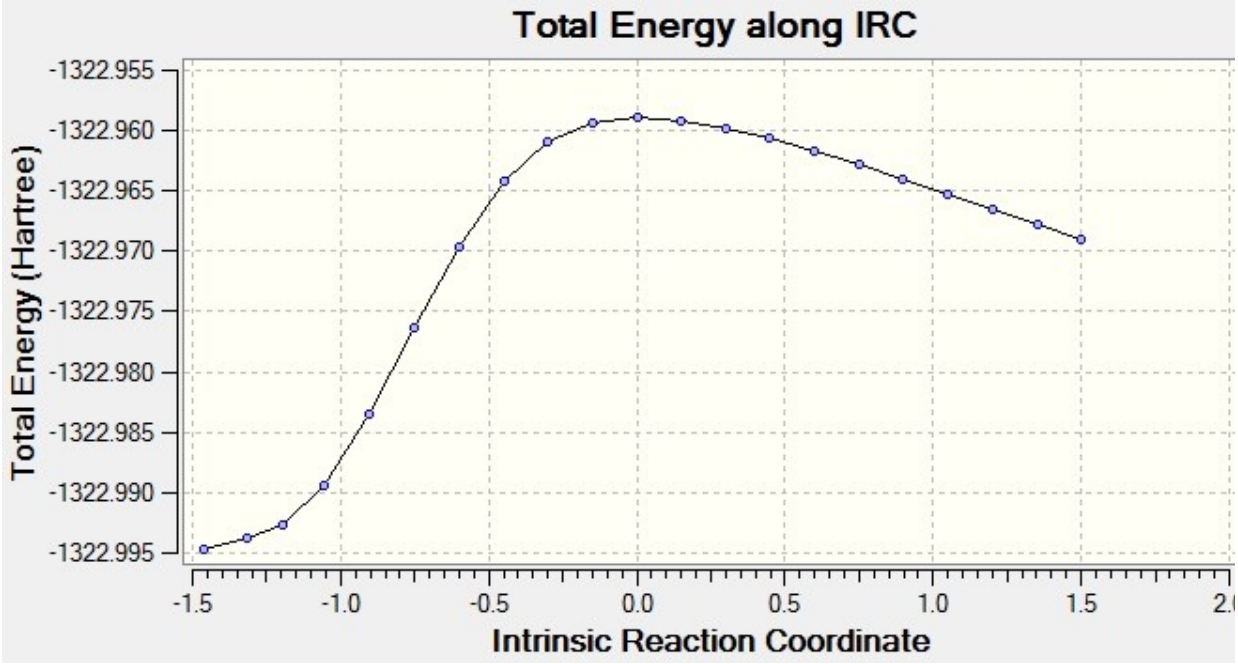


Fig. S74. Total Energy along IRC of **TS-(CH(NO$_2$)$_3$)**

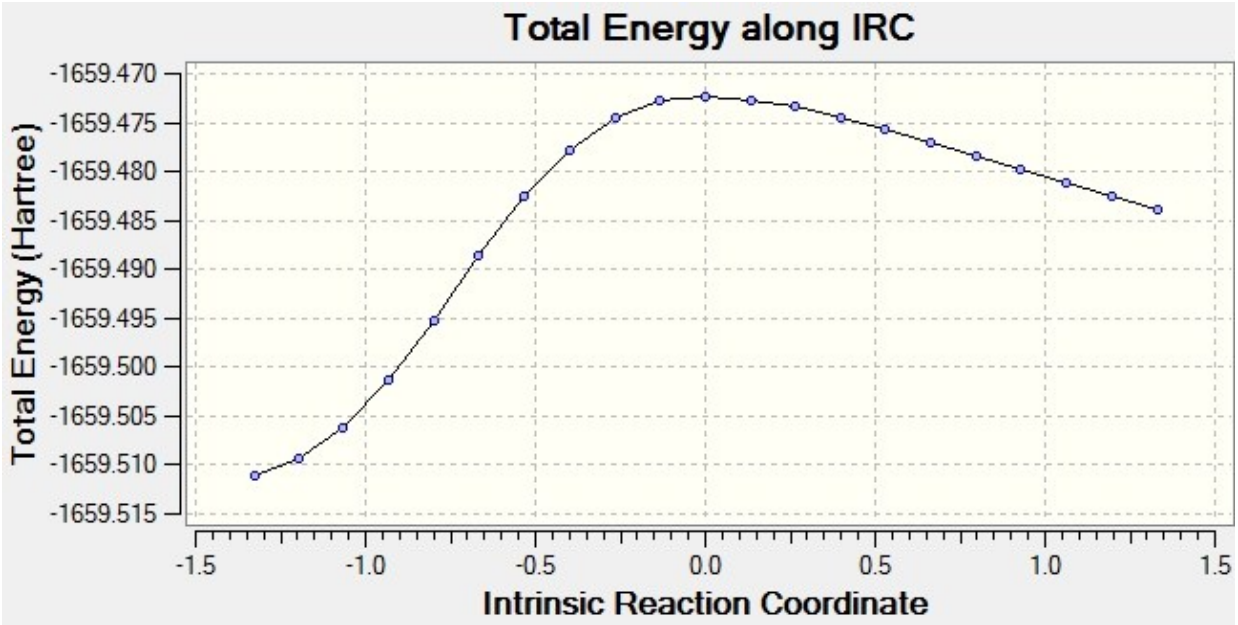
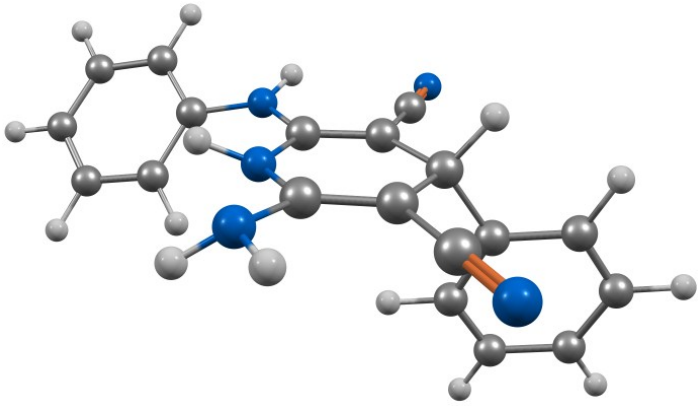
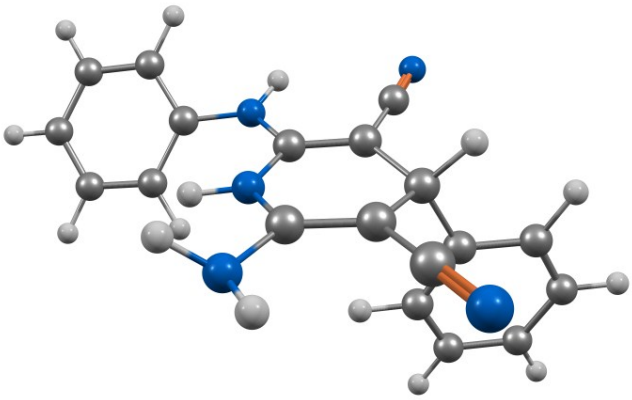


Fig. S75. The optimized structure of all compounds involved in conversion of **1** to **3** according to the mechanism suggested in Figure 1.

Stereoisomer 8A

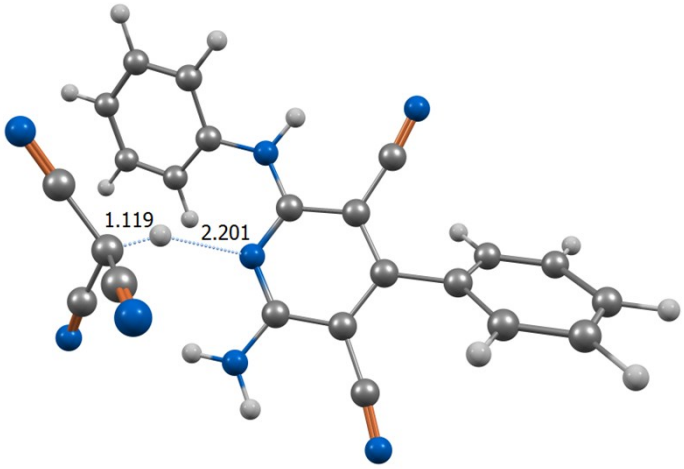


Stereoisomer 8B

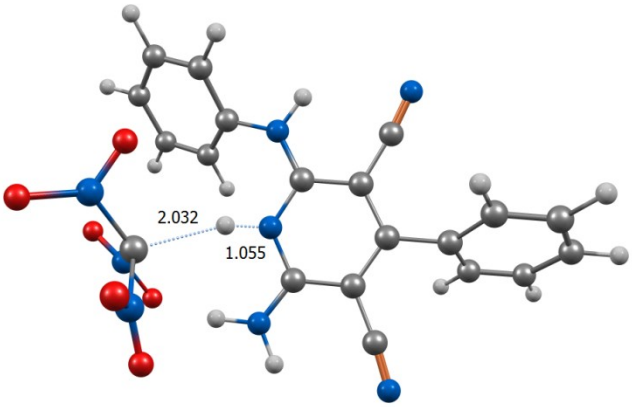


9-($CH(CN)_3$)

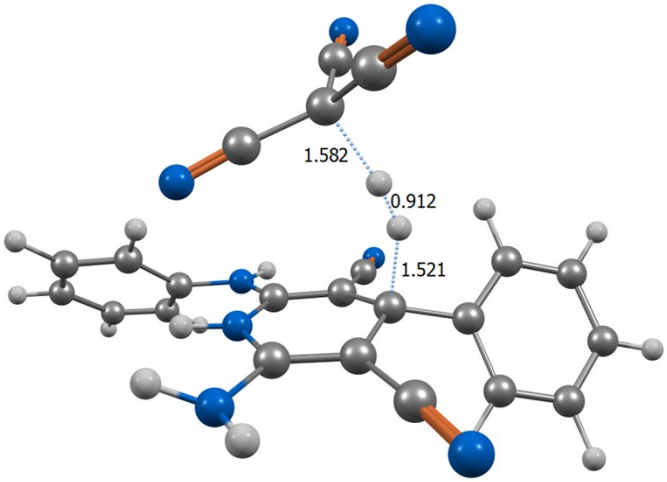
9-($CH(NO_2)_3$)



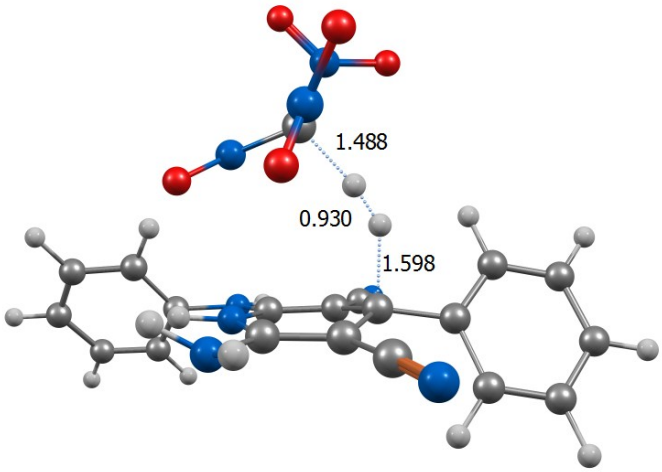
TS-($CH(CN)_3$)



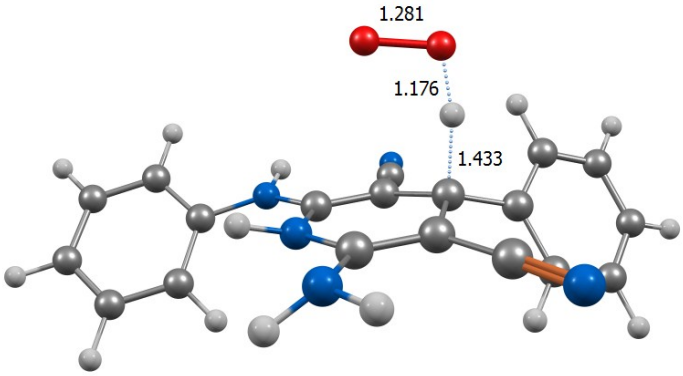
TS-($CH(NO_2)_3$)



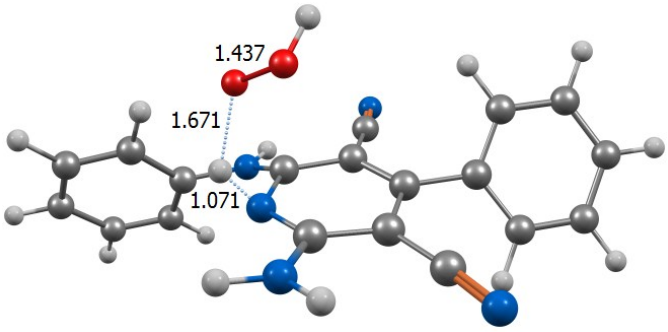
TS1-O_2



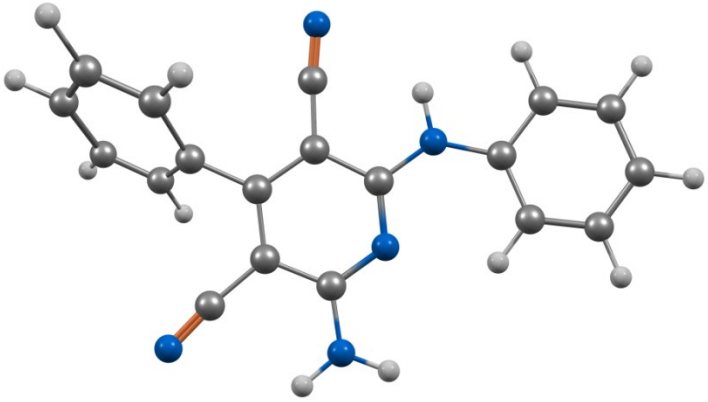
TS2-O_2

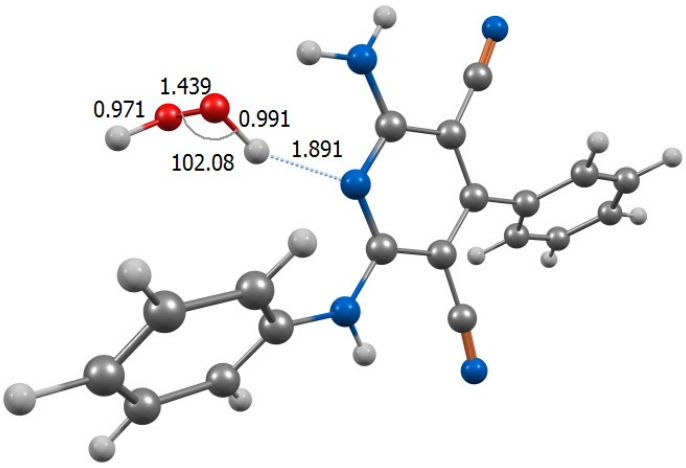


4



10





Cartesian atomic coordinates of calculated structures at B3LYP/SVP level of theory

"Stereoisomer 8A"

C	-0.848156000	-0.094690000	-0.611117000
C	0.365421000	-0.646867000	-0.944626000
C	1.673181000	0.140056000	-0.944933000
C	1.404657000	1.599813000	-0.586693000
C	0.160569000	2.076611000	-0.271906000
N	-0.943433000	1.234342000	-0.223321000
N	-2.031704000	-0.793147000	-0.698659000
H	-1.964676000	-1.663186000	-1.218552000
N	-0.141831000	3.401026000	-0.034823000
H	-0.795530000	3.578178000	0.723213000
H	0.659277000	4.025903000	-0.018498000
C	0.385617000	-2.012374000	-1.335422000
C	2.489761000	2.518341000	-0.567218000
N	3.349851000	3.304325000	-0.553028000
N	0.351931000	-3.127133000	-1.674542000
C	2.716955000	-0.487543000	-0.013518000
C	2.452634000	-0.657507000	1.354062000
C	3.958307000	-0.896630000	-0.515175000
C	3.407774000	-1.223848000	2.199342000
H	1.486047000	-0.345184000	1.759050000
C	4.918960000	-1.464398000	0.328591000
H	4.177218000	-0.770271000	-1.579352000
C	4.645927000	-1.629583000	1.687948000
H	3.186626000	-1.351509000	3.262327000
H	5.882729000	-1.778518000	-0.080208000
H	5.394152000	-2.074106000	2.349160000
C	-3.275185000	-0.528747000	-0.093674000
C	-4.436736000	-1.003195000	-0.732827000
C	-3.403112000	0.148225000	1.134297000
C	-5.691833000	-0.801868000	-0.160715000
H	-4.345233000	-1.530510000	-1.686095000
C	-4.669255000	0.363576000	1.685654000
H	-2.514275000	0.480881000	1.671036000
C	-5.818967000	-0.107456000	1.047219000
H	-6.579950000	-1.183389000	-0.670631000
H	-4.750685000	0.888698000	2.640924000
H	-6.803927000	0.057120000	1.489440000
H	-1.849566000	1.676513000	-0.345046000
H	2.104979000	0.101989000	-1.961886000

"Stereoisomer 8B"

C	-0.787220000	-0.127159000	-0.597690000
C	0.412226000	-0.605372000	-1.073377000
C	1.720293000	0.176087000	-0.945663000
C	1.413408000	1.635411000	-0.622835000
C	0.190777000	2.042711000	-0.156997000
N	-0.865627000	1.151044000	-0.076723000
N	-1.958966000	-0.848431000	-0.672608000
H	-1.903396000	-1.677361000	-1.257339000
N	-0.100560000	3.312712000	0.297348000
H	0.665357000	3.975171000	0.211139000
H	-0.986813000	3.704408000	-0.012211000
C	0.426398000	-1.889680000	-1.674881000
C	2.428304000	2.615422000	-0.789462000
N	3.236861000	3.443703000	-0.925833000
N	0.392404000	-2.941797000	-2.176940000
C	2.682838000	-0.472017000	0.056720000
C	2.410897000	-0.460137000	1.433671000
C	3.848658000	-1.105804000	-0.391621000
C	3.282964000	-1.066954000	2.338716000
H	1.507921000	0.034299000	1.802365000
C	4.725246000	-1.716306000	0.511731000
H	4.074726000	-1.122235000	-1.461691000
C	4.444672000	-1.698437000	1.879539000
H	3.058014000	-1.046276000	3.408412000
H	5.630649000	-2.205364000	0.143218000
H	5.128561000	-2.172925000	2.587936000
C	-3.205023000	-0.576418000	-0.078085000
C	-4.377628000	-0.864599000	-0.801263000
C	-3.320839000	-0.069369000	1.231063000
C	-5.630914000	-0.641607000	-0.232410000
H	-4.295126000	-1.260288000	-1.816758000
C	-4.582911000	0.177325000	1.780282000
H	-2.427631000	0.088276000	1.839294000
C	-5.742775000	-0.106257000	1.055833000
H	-6.529801000	-0.876857000	-0.807793000
H	-4.654077000	0.570249000	2.797710000
H	-6.726259000	0.077396000	1.493834000
H	-1.734720000	1.461014000	0.340358000
H	2.227579000	0.148814000	-1.924820000

"9-($CH(CN)_3$)"

C	0.012676000	-0.859995000	-0.269828000
C	-1.376127000	-1.109237000	0.007438000
C	-2.313237000	-0.079786000	-0.212382000
C	-1.838767000	1.152061000	-0.707110000
C	-0.432708000	1.313429000	-0.932703000
N	0.447131000	0.329883000	-0.693756000
N	0.911793000	-1.863380000	-0.060292000
N	0.058582000	2.485319000	-1.391328000
C	-1.730807000	-2.384648000	0.538759000
C	-2.692879000	2.243058000	-1.046586000
N	-3.294683000	3.188839000	-1.358287000
N	-1.900822000	-3.452622000	0.969255000
C	-3.760206000	-0.287092000	0.059053000
C	-4.444001000	-1.384133000	-0.495101000
C	-4.466305000	0.615003000	0.875373000
C	-5.803989000	-1.569656000	-0.242056000
C	-5.823040000	0.418050000	1.136361000
C	-6.495537000	-0.671895000	0.576289000
C	2.297466000	-1.923942000	-0.335624000
C	3.078600000	-2.775051000	0.466550000
C	2.906403000	-1.228789000	-1.395727000

C	4.442615000	-2.925479000	0.218074000
C	4.276196000	-1.381649000	-1.627624000
C	5.051324000	-2.225112000	-0.827229000
H	0.529380000	-2.692484000	0.385903000
H	1.026960000	2.549549000	-1.682145000
H	-0.563885000	3.255797000	-1.602923000
H	-3.914405000	-2.086400000	-1.141807000
H	-3.947723000	1.465307000	1.322610000
H	-6.324786000	-2.420706000	-0.687150000
H	-6.356367000	1.121256000	1.780285000
H	-7.559217000	-0.821519000	0.777403000
H	2.609961000	-3.317657000	1.292331000
H	2.309678000	-0.584977000	-2.038569000
H	5.033895000	-3.587940000	0.854482000
H	4.737821000	-0.837322000	-2.455407000
H	6.121318000	-2.335462000	-1.015675000
H	2.216066000	0.974735000	0.446980000
C	2.918514000	1.738589000	0.864751000
C	3.301767000	2.566562000	-0.295791000
C	2.169844000	2.524844000	1.865629000
C	4.076172000	1.050375000	1.466292000
N	3.528766000	3.181664000	-1.249045000
N	4.973203000	0.499931000	1.945261000
N	1.555668000	3.119622000	2.644309000

"9-($CH(NO_2)_3$)"

C	0.483941000	1.056309000	-0.067205000
C	1.893515000	1.169316000	0.106479000
C	2.730563000	0.050239000	-0.118853000
C	2.148276000	-1.157424000	-0.549779000
C	0.728948000	-1.256904000	-0.696653000
N	-0.039343000	-0.162637000	-0.388188000
N	-0.321171000	2.121542000	0.072804000
N	0.114590000	-2.356263000	-1.097198000
C	2.399926000	2.465915000	0.421774000
C	2.899392000	-2.341398000	-0.816054000
N	3.420599000	-3.351724000	-1.058879000
N	2.704198000	3.558223000	0.680174000
C	4.198820000	0.165924000	0.065133000
C	5.083241000	-0.213786000	-0.961209000
C	4.722579000	0.659052000	1.274780000
C	6.461640000	-0.094754000	-0.781181000
C	6.102344000	0.758133000	1.455318000
C	6.973803000	0.386079000	0.427436000
C	-1.661622000	2.340043000	-0.361852000
C	-2.444298000	3.233569000	0.380865000
C	-2.176782000	1.749070000	-1.523861000
C	-3.743484000	3.524089000	-0.031601000
C	-3.487099000	2.032523000	-1.915739000
C	-4.272651000	2.918866000	-1.175300000
H	-1.055474000	-0.355314000	-0.180268000
H	0.136019000	2.937300000	0.475704000
H	-0.918264000	-2.414769000	-1.222822000
H	0.656150000	-3.207878000	-1.209326000
H	4.693632000	-0.583905000	-1.911305000
H	4.049897000	0.944487000	2.086018000
H	7.137899000	-0.381189000	-1.589753000
H	6.497147000	1.128852000	2.403923000
H	8.053995000	0.470943000	0.568568000
H	-2.041636000	3.680006000	1.293110000
H	-1.568923000	1.078225000	-2.132736000
H	-4.351653000	4.214704000	0.556766000
H	-3.892855000	1.548908000	-2.806073000
H	-5.297533000	3.132274000	-1.485873000
C	-2.686691000	-1.354337000	0.506810000
N	-2.218223000	-2.527742000	1.216439000
O	-2.130947000	-2.400140000	2.432046000
O	-1.889995000	-3.530039000	0.595438000
N	-3.258127000	-1.519045000	-0.788300000
O	-4.272796000	-0.901503000	-1.070502000
O	-2.615794000	-2.189049000	-1.620016000
N	-3.523971000	-0.520026000	1.418465000
O	-4.614695000	-0.938905000	1.741287000
O	-3.022578000	0.530627000	1.788121000

"4"

C	0.955728000	-0.000148000	-0.003022000
C	-0.343825000	-0.628763000	0.020589000
C	-1.495271000	0.180276000	-0.013454000
C	-1.321101000	1.578465000	-0.063326000
C	0.013036000	2.105027000	-0.076009000
N	1.095124000	1.322117000	-0.049088000
N	2.055539000	-0.806520000	0.031256000
H	1.837476000	-1.797948000	0.070977000
N	0.222857000	3.438578000	-0.124805000
H	-0.549657000	4.090969000	-0.159626000
H	1.173771000	3.780881000	-0.150953000
C	-0.402212000	-2.049924000	0.121382000
C	-2.401147000	2.505492000	-0.144989000
N	-3.200862000	3.348659000	-0.213066000
N	-0.330025000	-3.209197000	0.203146000
C	-2.856524000	-0.420291000	0.003135000
C	-3.217143000	-1.401011000	-0.937929000
C	-3.803933000	-0.014492000	0.959916000
C	-4.496832000	-1.958320000	-0.923863000
H	-2.497432000	-1.718459000	-1.695043000
C	-5.078699000	-0.582801000	0.978158000
H	-3.536973000	0.738651000	1.703854000
C	-5.429305000	-1.553362000	0.035392000
H	-4.765235000	-2.713055000	-1.666918000
H	-5.801162000	-0.264310000	1.733425000
H	-6.429378000	-1.993900000	0.048045000
C	3.437579000	-0.537067000	0.031496000
C	4.289862000	-1.658357000	0.093439000
C	4.006100000	0.747689000	-0.027027000
C	5.673731000	-1.501203000	0.096734000
H	3.857207000	-2.662432000	0.139812000
C	5.396496000	0.888609000	-0.022512000
H	3.354979000	1.614857000	-0.074792000
C	6.239471000	-0.223271000	0.038689000
H	6.313268000	-2.386097000	0.145429000
H	5.824055000	1.893801000	-0.068389000

H	7.324571000	-0.097709000	0.041286000

"10"

C	0.576631000	-0.463156000	-0.055838000
C	-0.792932000	-0.900870000	-0.019356000
C	-1.820514000	0.064343000	-0.032339000
C	-1.452805000	1.422075000	-0.078193000
C	-0.058441000	1.769006000	-0.095916000
N	0.905926000	0.828684000	-0.088122000
N	1.559437000	-1.409693000	-0.048160000
N	0.332586000	3.054571000	-0.112749000
C	-1.045262000	-2.304124000	-0.018374000
C	-2.396277000	2.491050000	-0.048279000
N	-3.079084000	3.433237000	-0.026748000
N	-1.136576000	-3.464801000	-0.010883000
C	-3.251559000	-0.341075000	-0.001463000
C	-4.147806000	0.129924000	-0.977426000
C	-3.730310000	-1.199609000	1.004205000
C	-5.489153000	-0.254978000	-0.950498000
C	-5.075187000	-1.571880000	1.035025000
C	-5.956948000	-1.103651000	0.056760000
C	2.959426000	-1.258656000	-0.186254000
C	3.791706000	-2.080648000	0.592669000
C	3.535718000	-0.374309000	-1.111881000
C	5.178377000	-2.013418000	0.453388000
C	4.925388000	-0.300204000	-1.229525000
C	5.752933000	-1.115926000	-0.452249000
H	2.556561000	1.710449000	0.180853000
H	1.239528000	-2.359160000	0.119766000
H	1.329561000	3.264500000	-0.017121000
H	-0.355088000	3.795477000	-0.060443000
H	-3.790615000	0.788836000	-1.771234000
H	-3.050644000	-1.565337000	1.776346000
H	-6.171490000	0.111826000	-1.720968000
H	-5.434460000	-2.231870000	1.828202000
H	-7.008584000	-1.400109000	0.079485000
H	3.343617000	-2.770132000	1.313086000
H	2.899271000	0.247108000	-1.740857000
H	5.812529000	-2.661433000	1.063463000
H	5.361906000	0.397029000	-1.948854000
H	6.838930000	-1.058038000	-0.556620000
H	4.430197000	2.316949000	1.551086000
O	3.493893000	2.568932000	1.606956000
O	3.119214000	2.525637000	0.218507000

"TS-($CH(CN)_3$)"

C	-1.069451000	-0.840674000	-0.003060000
C	0.233467000	-1.140227000	-0.416169000
C	1.379130000	-0.552930000	0.268285000
C	1.092963000	-0.013241000	1.593921000
C	-0.218768000	0.283101000	1.955980000
N	-1.249512000	-0.112360000	1.141888000
N	-2.169676000	-1.262293000	-0.677208000
N	-0.569750000	0.939855000	3.088753000
C	0.371900000	-1.949619000	-1.577756000
C	2.121521000	0.455444000	2.460054000
N	2.892792000	0.863375000	3.229991000
N	0.375778000	-2.623832000	-2.526832000
C	2.728918000	-1.174590000	0.011849000
C	3.288180000	-2.030702000	0.975494000
C	3.410559000	-0.973215000	-1.198226000
C	4.507290000	-2.667423000	0.732129000
C	4.628709000	-1.610385000	-1.438086000
C	5.181134000	-2.458208000	-0.473595000
C	-3.538708000	-1.058290000	-0.348827000
C	-4.043885000	0.221542000	-0.059762000
C	-4.403256000	-2.164507000	-0.364675000
C	-5.400959000	0.373896000	0.244748000
C	-5.759558000	-1.993417000	-0.085805000
C	-6.261480000	-0.726347000	0.230563000
H	-2.198726000	0.148933000	1.393259000
H	-1.972523000	-1.872897000	-1.466967000
H	-1.436936000	1.467508000	3.086097000
H	0.184766000	1.358639000	3.625000000
H	2.765439000	-2.209012000	1.917331000
H	2.992246000	-0.302758000	-1.952054000
H	4.931191000	-3.328188000	1.492108000
H	5.150316000	-1.437622000	-2.382278000
H	6.137501000	-2.952524000	-0.660914000
H	-3.396279000	1.101477000	-0.104438000
H	-4.005872000	-3.156405000	-0.593639000
H	-5.787134000	1.371277000	0.468113000
H	-6.426302000	-2.858739000	-0.106709000
H	-7.322507000	-0.597042000	0.455560000
H	1.604650000	0.731786000	-0.514339000
H	1.340450000	1.571723000	-0.752164000
C	0.656934000	2.972757000	-1.024354000
C	1.635416000	3.882580000	-0.481642000
C	0.535959000	2.917968000	-2.460486000
C	-0.572457000	2.864527000	-0.290616000
N	2.445528000	4.576874000	-0.022844000
N	0.455338000	2.813080000	-3.614489000
N	-1.549300000	2.698958000	0.323063000

"TS-($CH(NO_2)_3$)"

C	-1.092851000	-1.300663000	-0.060132000
C	0.211251000	-1.624119000	-0.460318000
C	1.344872000	-1.065990000	0.250381000
C	1.067893000	-0.565519000	1.583287000
C	-0.237193000	-0.205616000	1.920437000
N	-1.263202000	-0.548194000	1.072278000
N	-2.193259000	-1.706642000	-0.733020000
N	-0.577626000	0.468817000	3.042761000
C	0.354675000	-2.415863000	-1.633112000
C	2.110188000	-0.176845000	2.472575000
N	2.909103000	0.149134000	3.252267000
N	0.363498000	-3.075614000	-2.592091000
C	2.706668000	-1.628760000	-0.058496000
C	3.257009000	-2.591459000	0.804596000
C	3.409896000	-1.265480000	-1.217154000
C	4.488991000	-3.179087000	0.510180000
C	4.642207000	-1.853968000	-1.506198000

C	5.184539000	-2.811801000	-0.644750000
C	-3.557735000	-1.453453000	-0.397170000
C	-4.039068000	-0.139099000	-0.279563000
C	-4.425108000	-2.542665000	-0.224405000
C	-5.383691000	0.071418000	0.044423000
C	-5.770017000	-2.317340000	0.073062000
C	-6.250217000	-1.011055000	0.217564000
H	-2.208132000	-0.252058000	1.305167000
H	-2.009622000	-2.296954000	-1.541414000
H	-1.404295000	1.057766000	2.984479000
H	0.195009000	0.924830000	3.523110000
H	2.717043000	-2.889450000	1.705923000
H	2.999079000	-0.502180000	-1.881537000
H	4.906425000	-3.925594000	1.190139000
H	5.182702000	-1.555549000	-2.407428000
H	6.151110000	-3.268450000	-0.871255000
H	-3.373207000	0.705570000	-0.473764000
H	-4.039700000	-3.560483000	-0.321234000
H	-5.756607000	1.094354000	0.135489000
H	-6.443876000	-3.167685000	0.201623000
H	-7.302014000	-0.838384000	0.457132000
H	1.540460000	0.332050000	-0.498129000
H	1.215880000	1.201771000	-0.546548000
C	0.514716000	2.512270000	-0.484045000
N	1.120187000	3.291639000	0.601671000
O	1.804078000	4.247461000	0.279223000
O	0.953482000	2.881040000	1.740123000
N	-0.882287000	2.196727000	-0.355180000
O	-1.393743000	1.704783000	-1.362125000
O	-1.467827000	2.322771000	0.719925000
N	0.822303000	3.130982000	-1.819473000
O	0.048701000	3.966368000	-2.238232000
O	1.844882000	2.750460000	-2.353065000

"TS1-O_2"

C	1.002164000	-0.226586000	0.029655000
C	-0.287898000	-0.737785000	0.026923000
C	-1.467996000	0.137896000	0.217254000
C	-1.157719000	1.578129000	0.055036000
C	0.147112000	2.036272000	0.064521000
N	1.202085000	1.140677000	0.046052000
N	2.115903000	-1.021111000	0.042577000
N	0.512647000	3.352991000	0.134290000
C	-0.410203000	-2.152511000	-0.061988000
C	-2.174756000	2.575078000	0.030361000
N	-2.940260000	3.452515000	0.005595000
N	-0.425719000	-3.315712000	-0.122316000
C	-2.795606000	-0.374907000	-0.269939000
C	-3.390860000	0.126812000	-1.441699000
C	-3.461058000	-1.395890000	0.433214000
C	-4.614297000	-0.373859000	-1.892233000
C	-4.681569000	-1.899158000	-0.020732000
C	-5.264367000	-1.388377000	-1.184014000
C	3.456281000	-0.678477000	-0.232750000
C	4.474222000	-1.340371000	0.477602000
C	3.808514000	0.263605000	-1.217598000
C	5.814342000	-1.061412000	0.211811000
C	5.154773000	0.550746000	-1.458317000
C	6.163523000	-0.106809000	-0.749405000
H	2.102954000	1.473050000	0.377460000
H	1.939978000	-1.988645000	0.298852000
H	1.348539000	3.639977000	-0.364637000
H	-0.243722000	4.030257000	0.118022000
H	-2.889028000	0.909821000	-2.014050000
H	-3.022751000	-1.795194000	1.350850000
H	-5.059368000	0.029900000	-2.805318000
H	-5.181591000	-2.691066000	0.542390000
H	-6.222141000	-1.779018000	-1.536975000
H	4.204903000	-2.071787000	1.243870000
H	3.033926000	0.746898000	-1.814786000
H	6.592106000	-1.588161000	0.770084000
H	5.414698000	1.281795000	-2.228173000
H	7.213768000	0.116233000	-0.949514000
H	-1.581742000	0.057516000	1.643628000
O	-1.430120000	0.023064000	2.808978000
O	-0.168721000	0.123003000	3.005859000

"TS2-O_2"

C	0.878501000	-0.240517000	0.097597000
C	-0.470184000	-0.751447000	0.102878000
C	-1.550636000	0.109107000	-0.144122000
C	-1.303762000	1.486194000	-0.388097000
C	0.024230000	1.974063000	-0.255276000
N	1.073051000	1.130377000	-0.099538000
N	1.905100000	-1.081554000	-0.167708000
N	0.302192000	3.287945000	-0.276246000
C	-0.621625000	-2.160925000	0.247470000
C	-2.325947000	2.451018000	-0.609381000
N	-3.077982000	3.320610000	-0.795428000
N	-0.638062000	-3.320359000	0.352107000
C	-2.941367000	-0.414458000	-0.173824000
C	-3.778611000	-0.165533000	-1.276432000
C	-3.440806000	-1.167677000	0.904015000
C	-5.080770000	-0.666992000	-1.302111000
C	-4.748251000	-1.654829000	0.880469000
C	-5.569952000	-1.409413000	-0.223447000
C	3.290368000	-0.776019000	-0.310885000
C	4.009101000	-0.075142000	0.670750000
C	3.948247000	-1.249453000	-1.457047000
C	5.371785000	0.171096000	0.477266000
C	5.313694000	-1.016161000	-1.627945000
C	6.028204000	-0.296842000	-0.664587000
H	1.684236000	1.345866000	0.753128000
H	1.660866000	-2.069046000	-0.164925000
H	1.256179000	3.612495000	-0.189006000
H	-0.451178000	3.965302000	-0.280237000
H	-3.404144000	0.408705000	-2.125957000
H	-2.807050000	-1.357374000	1.772310000
H	-5.716143000	-0.474578000	-2.169881000
H	-5.125523000	-2.229877000	1.729400000
H	-6.591930000	-1.796090000	-0.242807000
H	3.496167000	0.243808000	1.581417000

H	3.379765000	-1.794214000	-2.214768000
H	5.928713000	0.717825000	1.242568000
H	5.818312000	-1.390507000	-2.522084000
H	7.096178000	-0.109385000	-0.800414000
H	-0.025550000	0.516929000	3.237966000
O	0.354534000	1.135425000	2.596656000
O	1.477679000	0.386397000	2.105498000

"H_2O_2"

O	0.000000000	0.720966000	-0.052570000
H	0.829293000	0.896268000	0.420563000
O	0.000000000	-0.720966000	-0.052570000
H	-0.829293000	-0.896268000	0.420563000

"O_2"

O	0.000000000	0.000000000	0.599983000
O	0.000000000	0.000000000	-0.599983000

"H_2"

H	0.000000000	0.000000000	0.380387000
H	0.000000000	0.000000000	-0.380387000

"$CH(CN)_3$"

C	-0.000091000	-0.000207000	0.496194000
H	-0.000127000	-0.000357000	1.603780000
C	-1.299414000	-0.551912000	0.056130000
C	1.127617000	-0.849293000	0.056089000
C	0.171792000	1.401013000	0.056289000
N	2.014742000	-1.516881000	-0.266272000
N	-2.321388000	-0.985704000	-0.266319000
N	0.306746000	2.502979000	-0.266266000

"$CH(NO_2)_3$"

H	0.000024000	-0.000056000	-1.639653000
C	0.000002000	0.000007000	-0.546011000
N	1.181420000	-0.809748000	-0.044744000
O	2.207641000	-0.599250000	-0.652033000
O	0.996156000	-1.544003000	0.895952000
N	-1.291956000	-0.618277000	-0.044678000
O	-1.834940000	-0.090882000	0.896269000
O	-1.622968000	-1.612068000	-0.652149000
N	0.110518000	1.428018000	-0.044799000
O	0.839409000	1.634786000	0.895594000
O	-0.585286000	2.211426000	-0. 651725000

Fig. S76. The SEM (a) and TEM (b and c) images of [TEATCM] after recycling.