Supplementary Material

Abnormal Strecker Reaction of 3-Formylindole and Aniline

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1. Cartesian Coordinates and Energies

Formylindole.log
Energy (E) = -477.006195219 Hartree
Enthalpy (H) = -476.855504 Hartree
Gibbs free energy (G) = -476.897769 Hartree
Charge = 0, Spin = 1
C 0.118294 -0.349332 -0.000109
C 0.807634 0.881872 0.000022
C 2.200836 0.967199 0.000115
C 2.906653 -0.224536 0.000085
C 2.241865 -1.465054 -0.000048
C 0.858917 -1.540421 -0.000148
C -1.292269 -0.030365 -0.000203
C -1.384756 1.347271 -0.000172
H 2.707623 1.926442 0.000227
H 3.991407 -0.201381 0.000171
H 2.827064 -2.378902 -0.000068
H 0.361380 -2.505007 -0.000253
H -2.268684 1.967402 -0.000229
H 0.056285 2.876195 0.000341
N -0.142645 1.888632 0.000037
C -2.420146 -0.940086 -0.000337
H -2.155773 -2.016993 0.000555
O -3.592870 -0.595932 0.000471

PhNH2.log
Energy (E) = -287.522023948 Hartree
Enthalpy (H) = -287.396740 Hartree
Gibbs free energy (G) = -287.432479 Hartree
Charge = 0, Spin = 1
C 0.937825 0.000001 -0.010395
C 0.221318 -1.205602 -0.005538
C 0.221318 1.205602 -0.005536
C -1.168750 -1.199567 0.003526
H 0.761960 -2.148264 -0.010890
C -1.168752 1.199567 0.003526
H 0.761956 2.148267 -0.010884
C -1.877308 -0.000000 0.008125
H -1.702116 -2.145553 0.009007
H -1.702117 2.145552 0.009008
H -2.962008 -0.000001 0.016275
H 2.769951 0.833398 0.284931
N 2.329787 -0.000002 -0.077811
H 2.769950 -0.833384 0.284975

HCN.log
Energy (E) = -93.3926522795 Hartree
Enthalpy (H) = -93.372517 Hartree
Gibbs free energy (G) = -93.395340 Hartree
Charge = 0, Spin = 1
C -0.000000 0.000000 0.500595
H -0.000000 0.000000 1.571369
N 0.000000 -0.000000 -0.653563

AcOH.log
Energy (E) = -229.025238682 Hartree
Enthalpy (H) = -228.957158 Hartree
Gibbs free energy (G) = -228.989833 Hartree
Charge = 0, Spin = 1
C -1.392204 -0.109516 -0.000011
H -1.911499 0.846910 -0.000125
H -1.676349 -0.689220 -0.881579
H -1.676494 -0.689083 0.881602
C 0.092371 0.119763 0.000117
O 0.642797 1.197939 -0.000046
O 0.775507 -1.037553 -0.000011
H 1.716912 -0.813177 -0.000079

AcO.log
Energy (E) = -228.517926800 Hartree
Enthalpy (H) = -228.463470 Hartree
Gibbs free energy (G) = -228.495450 Hartree
Charge = -1, Spin = 1
C 1.349164 -0.000454 -0.003982
H 1.750762 -0.895625 -0.487613
H 1.751020 0.893735 -0.489229
H 1.702888 0.000523 1.034478
C -0.201949 0.000007 -0.013403
O -0.755993 -1.126732 0.002919
O -0.755002 1.127238 0.002915

H2O.log
Energy (E) = -76.4036713265 Hartree
Enthalpy (H) = -76.378096 Hartree
Gibbs free energy (G) = -76.399519 Hartree
Charge = 0, Spin = 1
O -0.000000 0.000000 0.118721
H 0.000000 0.755689 -0.474884
H -0.000000 -0.755689 -0.474884

INT1.log
Energy (E) = -570.417352124 Hartree
Enthalpy (H) = -570.242107 Hartree
Gibbs free energy (G) = -570.290390 Hartree
Charge = 0, Spin = 1
C -0.641181 -0.218981 -0.104589
C -1.400348 0.959992 0.065224
C -2.797873 0.947463 0.098335
C -3.424945 -0.278709 -0.042953
C -2.685330 -1.466459 -0.208390
C -1.301934 -1.449668 -0.236811
C 0.742724 0.177354 -0.091915
C 0.766229 1.534658 0.087202

H -3.366883 1.861862 0.229700
H -4.508907 -0.326587 -0.022391
H -3.213318 -2.409016 -0.310317
H -0.734604 -2.368104 -0.347899
H 1.610392 2.206658 0.146261
H -0.763505 2.976054 0.300510
N -0.514693 2.008523 0.178632
C 1.902439 -0.759935 -0.235411
H 1.827314 -1.310516 -1.179795
H 1.776979 -1.316749 1.611978
C 3.183487 -0.006510 -0.285288
N 4.185694 0.572034 -0.300832
O 1.951990 -1.751592 0.769365

INT2.log
Energy (E) = -781.495149610 Hartree
Enthalpy (H) = -781.221363 Hartree
Gibbs free energy (G) = -781.285066 Hartree
Charge = 0, Spin = 1
C -2.156798 -0.447694 0.000246
C -3.360409 0.284257 -0.000049
C -4.615953 -0.314021 -0.000531
C -4.653497 -1.700388 -0.000713
C -3.471203 -2.455361 -0.000381
C -2.224796 -1.845599 0.000117
C -1.090146 0.543034 0.000869
C -1.710152 1.799513 0.000835
H -5.523470 0.279473 -0.000737
H -5.611619 -2.208342 -0.001107
H -3.532681 -3.538194 -0.000488
H -1.335985 -2.467361 0.000521
H -1.229669 2.773730 0.000924
H -3.703801 2.395783 0.000115
N -3.035255 1.639969 0.000245
C 0.307926 0.479297 0.001043
H 0.841745 1.441180 0.001868
C 2.453214 -0.687703 0.000009
C 3.247862 0.460266 -0.000532
C 3.025789 -1.958273 0.000397
C 4.630204 0.309081 -0.000627
H 2.813820 1.459140 -0.000859
C 4.409839 -2.088121 0.000238
H 2.395674 -2.843093 0.000886
C 5.216700 -0.954701 -0.000272
H 5.254165 1.196401 -0.001022
H 4.852981 -3.077990 0.000522
H 6.296690 -1.054163 -0.000389
H 0.558564 -1.511485 -0.000888
N 1.031652 -0.616898 0.000117
C 1.298281 3.453668 -0.000309
N 0.586806 4.389985 -0.000560

TS1.log
Energy (E) = -781.484038806 Hartree
Enthalpy (H) = -781.211367 Hartree
Gibbs free energy (G) = -781.273403 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -89.3538
C -2.070057 -0.322823 -0.065058
C -3.323669 0.158593 -0.495674
C -4.529637 -0.452175 -0.159848
C -4.464797 -1.580169 0.641579
C -3.231711 -2.071680 1.100341
C -2.037897 -1.455350 0.760464
C -1.080993 0.580324 -0.624197
C -1.782646 1.549677 -1.326578
H -5.477085 -0.055678 -0.507851
H -5.380699 -2.085747 0.927400
H -3.214225 -2.946547 1.741184
H -1.111110 -1.847240 1.165976
H -1.400484 2.404394 -1.865405
H -3.818433 1.860645 -1.685088
N -3.100376 1.295630 -1.259077
C 0.334119 0.582085 -0.581321
H 0.869602 1.379511 -1.075401
C 2.470429 -0.497422 -0.140269
C 3.218927 0.665503 0.024291
C 3.085809 -1.741554 -0.273347
C 4.607686 0.572917 0.029769
H 2.706269 1.605238 0.208775
C 4.472954 -1.817103 -0.257912
H 2.485998 -2.637857 -0.399083
C 5.237001 -0.660211 -0.114250
H 5.198168 1.472983 0.163970
H 4.956934 -2.781957 -0.364393
H 6.319894 -0.722875 -0.106044
H 0.564968 -1.253313 0.187445
N 1.050610 -0.441951 -0.170852
C 0.682317 2.505590 1.195972
N 0.303080 3.362211 1.904891

INT3.log
Energy (E) = -781.540387645 Hartree
Enthalpy (H) = -781.266255 Hartree
Gibbs free energy (G) = -781.326586 Hartree
Charge = 0, Spin = 1
C -2.084305 -0.042179 0.041217
C -3.310290 0.399701 -0.505664
C -4.457803 -0.398292 -0.503338
C -4.355600 -1.657701 0.062085
C -3.144598 -2.116000 0.616725
C -2.010875 -1.322890 0.613063
C -1.144410 1.033215 -0.140782
C -1.815336 2.048419 -0.764553
H -5.390707 -0.043227 -0.928211
H -5.226845 -2.304259 0.081035

H -3.104219 -3.107055 1.056531
H -1.085620 -1.681976 1.054242
H -1.457338 3.020168 -1.072003
H -3.814535 2.250529 -1.421629
N -3.113676 1.674638 -0.985813
C 0.308539 1.029575 0.230568
H 0.712390 2.035461 0.067869
C 2.418811 -0.110248 -0.440787
C 3.246510 0.820655 0.199679
C 3.001009 -1.258405 -1.000079
C 4.620817 0.603682 0.266758
H 2.833596 1.715517 0.652071
C 4.370947 -1.462356 -0.924636
H 2.368291 -1.988256 -1.497705
C 5.195124 -0.532538 -0.291173
H 5.243873 1.337222 0.769000
H 4.797835 -2.358707 -1.363880
H 6.265682 -0.695612 -0.231346
H 0.518520 -0.752369 -0.797833
N 1.044109 0.083309 -0.582849
C 0.457624 0.748907 1.690240
N 0.578439 0.509380 2.816651

INT4.log
Energy (E) = -1239.63235137 Hartree
Enthalpy (H) = -1239.217545 Hartree
Gibbs free energy (G) = -1239.306788 Hartree
Charge = 0, Spin = 1
C -0.720864 1.511574 0.878064
C -2.072653 1.174460 1.105116
C -3.125927 1.949422 0.612156
C -2.797248 3.067178 -0.135297
C -1.454266 3.415577 -0.380369
C -0.414195 2.652651 0.120828
C 0.064018 0.493768 1.522226
C -0.813873 -0.395338 2.081333
H -4.158565 1.679517 0.807167
H -3.589600 3.689161 -0.539181
H -1.235501 4.298730 -0.971544
H 0.617963 2.929432 -0.074672
H -0.615265 -1.307206 2.626141
H -2.918609 -0.540537 1.999242
N -2.095699 0.023624 1.856835
C 1.552729 0.364367 1.405481
H 2.023598 1.349797 1.536181
C 3.148674 0.111965 -0.496825
C 4.277803 0.395016 0.273668
C 3.256172 0.081222 -1.891824
C 5.496294 0.651663 -0.352227
H 4.226735 0.405584 1.356972
C 4.475697 0.336048 -2.503457
H 2.378110 -0.143571 -2.491027
C 5.604545 0.625251 -1.737632
H 6.366272 0.871332 0.258164
H 4.542688 0.312093 -3.586370
H 6.556150 0.826120 -2.217655
H 1.123472 -0.006216 -0.556662
N 1.892466 -0.191034 0.084339
C 2.088545 -0.505063 2.474278
N 2.511373 -1.188318 3.306803
H 1.308931 -1.916902 0.087890
C -0.410505 -2.457121 -0.478671
C -1.456036 -3.521209 -0.351744
H -2.391901 -3.040386 -0.053203
H -1.614979 -3.975131 -1.333582
H -1.164025 -4.288895 0.362866
O -0.576414 -1.425448 -1.127029
O 0.713414 -2.710473 0.161133
C -3.979198 -0.657425 -1.110781
C -5.213776 0.054481 -1.594364
H -6.029061 -0.090358 -0.887382
H -4.996426 1.119808 -1.704851
H -5.500550 -0.327792 -2.577225
O -3.928177 -1.306219 -0.078381
O -2.957142 -0.498922 -1.936293
H -2.135494 -0.916902 -1.572292

TS2.log
Energy (E) = -1239.59270388 Hartree
Enthalpy (H) = -1239.178359 Hartree
Gibbs free energy (G) = -1239.267019 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -126.7674
C -0.799866 2.130097 0.436740
C -2.087149 1.575589 0.432751
C -3.159409 2.165265 -0.219727
C -2.906564 3.361729 -0.883201
C -1.627624 3.933785 -0.888488
C -0.560232 3.326666 -0.233438
C 0.031541 1.196249 1.184275
C -0.851036 0.139439 1.585413
H -4.141393 1.707319 -0.217456
H -3.714022 3.859329 -1.409051
H -1.466615 4.866860 -1.417573
H 0.427359 3.776482 -0.250996
H -0.601222 -0.755838 2.139984
H -2.920139 -0.338405 1.147818
N -2.065310 0.372136 1.156403
C 1.393444 1.199455 1.319360
H 1.979329 2.071134 1.053075
C 3.596500 -0.057090 -0.664763
C 3.977584 -1.340718 -0.254609
C 4.578398 0.883926 -0.995901
C 5.325463 -1.673323 -0.189026
H 3.210367 -2.064653 0.000143
C 5.922492 0.537955 -0.927616

H 4.283863 1.881945 -1.308937
C 6.304271 -0.740136 -0.523614
H 5.611524 -2.671891 0.125584
H 6.676308 1.272828 -1.191899
H 7.354683 -1.005790 -0.471269
H 1.996901 1.036676 -1.310403
N 2.241502 0.294880 -0.666051
C 2.065274 0.220973 2.117734
N 2.612847 -0.567739 2.766577
H 1.589295 -0.496723 -0.729411
C -0.612407 -2.058264 -0.658830
C -1.479819 -3.190642 -0.167342
H -2.158190 -2.817219 0.606742
H -2.101187 -3.573268 -0.980070
H -0.854406 -3.983135 0.239156
O -1.208732 -1.066061 -1.278340
O 0.599081 -2.040683 -0.470444
C -4.430267 -1.439537 -0.191836
C -5.809487 -2.043751 -0.368785
H -6.489135 -1.696405 0.410456
H -6.207244 -1.811355 -1.357293
H -5.724458 -3.132023 -0.283605
O -4.066138 -1.184095 0.997444
O -3.732973 -1.265267 -1.224563
H -2.231441 -1.137966 -1.240855

INT5_2.log
Energy (E) = -1239.60542281 Hartree
Enthalpy (H) = -1239.192896 Hartree
Gibbs free energy (G) = -1239.282804 Hartree
Charge = 0, Spin = 1
C 0.378660 1.429532 0.914066
C -1.009443 1.356144 0.739004
C -1.735942 2.398059 0.193725
C -1.029830 3.548855 -0.166117
C 0.349768 3.642224 0.026735
C 1.073516 2.580822 0.575102
C 0.770830 0.128724 1.456576
C -0.506706 -0.599378 1.584761
H -2.805623 2.316594 0.037299
H -1.564548 4.386477 -0.600849
H 0.867753 4.552837 -0.253852
H 2.145606 2.654319 0.720245
H -0.616402 -1.609405 1.964568
H -3.162259 -0.236360 1.174376
N -1.511401 0.097677 1.175551
C 1.999193 -0.347402 1.721717
H 2.893181 0.246622 1.551149
C 2.821924 0.049260 -1.409322
C 3.214079 -1.250913 -1.040231
C 3.669656 1.118861 -1.072959
C 4.400960 -1.462296 -0.348927
H 2.564116 -2.085065 -1.286170
C 4.848426 0.895286 -0.369224
H 3.394731 2.127116 -1.370237
C 5.225147 -0.394252 0.004690
H 4.673830 -2.474809 -0.066989
H 5.481091 1.740775 -0.114980
H 6.145761 -0.564026 0.552337
H 1.239338 1.172660 -2.006933
N 1.650486 0.256344 -2.109553
C 2.203636 -1.669304 2.221259
N 2.372641 -2.739319 2.635415
H 0.966534 -0.494153 -2.046000
C -1.307102 -1.740722 -1.460368
C -2.366283 -2.663116 -0.909617
H -2.664227 -2.327587 0.087903
H -3.255848 -2.647285 -1.543519
H -1.969331 -3.674286 -0.844221
O -1.675993 -0.499257 -1.745896
O -0.154281 -2.088603 -1.641454
C -4.764223 -0.219332 0.096958
C -6.257398 -0.339896 0.186963
H -6.642682 0.389582 0.903105
H -6.705329 -0.179065 -0.791657
H -6.518184 -1.333939 0.558905
O -4.156753 -0.390444 1.250145
O -4.178594 0.012847 -0.957576
H -2.597821 -0.307195 -1.444868

INT5.log
Energy (E) = -1239.61004274 Hartree
Enthalpy (H) = -1239.198143 Hartree
Gibbs free energy (G) = -1239.288291 Hartree
Charge = 0, Spin = 1
C 2.884265 -0.518121 0.262124
C 2.054469 -1.647401 0.253822
C 2.361708 -2.772267 -0.490161
C 3.543375 -2.746059 -1.234671
C 4.381684 -1.628875 -1.224075
C 4.060407 -0.497911 -0.471747
C 2.205405 0.454870 1.120497
C 0.979227 -0.247883 1.547385
H 1.705561 -3.635543 -0.496047
H 3.815658 -3.610125 -1.831669
H 5.293524 -1.639691 -1.811461
H 4.710169 0.371318 -0.474292
H 0.198505 0.161964 2.177055
H -0.443397 -2.332882 1.088311
N 0.908866 -1.442442 1.067475
C 2.583267 1.702658 1.447659
H 3.504005 2.133609 1.069212
C 1.809379 2.523916 2.321071
N 1.196482 3.192732 3.044393
C -0.076802 2.845575 -0.315029
C 1.097566 3.208046 -0.973956

C 1.706672 2.283813 -1.823791
C 1.161092 1.022389 -2.010316
C -0.021450 0.649487 -1.346486
C -0.625345 1.581671 -0.481129
H -0.559834 3.548013 0.356972
H 1.524068 4.195920 -0.836179
H 2.621850 2.547218 -2.345932
H 1.651519 0.305791 -2.663337
H -1.523905 1.299426 0.056559
N -0.550798 -0.614756 -1.487525
H -0.241488 -1.134542 -2.294473
H -1.546900 -0.693692 -1.311440
C -2.335607 -2.088949 1.173161
C -3.663857 -2.738392 0.912961
H -3.604314 -3.821639 1.010889
H -4.415125 -2.330927 1.590449
H -3.955112 -2.482802 -0.110576
O -1.305562 -2.876872 1.026244
O -2.224069 -0.896632 1.471171
C -4.167458 0.543273 -0.763679
C -5.113618 1.507936 -1.422390
H -5.273582 1.222404 -2.460589
H -6.062815 1.533759 -0.883164
H -4.682967 2.512275 -1.381050
O -3.555030 -0.324460 -1.367408
O -4.058060 0.744948 0.540576
H -3.401793 0.098891 0.928202

TS3.log
Energy (E) = -1239.60413698 Hartree
Enthalpy (H) = -1239.182534 Hartree
Gibbs free energy (G) = -1239.267839 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -367.6887
C -2.743235 0.596866 0.181121
C -1.913355 1.727972 0.286095
C -2.230046 2.943915 -0.313775
C -3.417579 3.006318 -1.030208
C -4.263152 1.889536 -1.137950
C -3.939079 0.681876 -0.535769
C -2.071794 -0.466525 0.906729
C -0.873850 0.105839 1.393256
H -1.573164 3.801882 -0.222639
H -3.700135 3.935926 -1.512885
H -5.185910 1.975630 -1.702116
H -4.599313 -0.175142 -0.628401
H -0.075268 -0.350508 1.959752
H 0.053704 1.991516 1.228682
N -0.796598 1.383211 1.039746
C -2.455135 -1.816452 0.987934
H -3.470475 -2.069350 0.696209
C -1.969406 -2.612573 2.084055
N -1.580141 -3.259497 2.963817
C -0.175739 -2.802471 -0.195931
C -1.538463 -2.908837 -0.612387
C -1.972902 -2.063980 -1.681707
C -1.247288 -0.968417 -2.030392
C 0.010468 -0.711591 -1.394132
C 0.564231 -1.708340 -0.523850
H 0.229575 -3.546137 0.481143
H -2.056776 -3.848704 -0.452338
H -2.935918 -2.247255 -2.146241
H -1.612238 -0.267630 -2.773702
H 1.561627 -1.559713 -0.127110
N 0.672882 0.414984 -1.620661
H 0.303639 1.104545 -2.256298
H 1.635863 0.524797 -1.294815
C 2.340311 1.965664 1.273508
C 3.757547 2.470641 1.066921
H 3.826500 3.537176 1.279582
H 4.457670 1.914807 1.694992
H 4.036351 2.290971 0.023737
O 1.415401 2.801770 1.394993
O 2.152760 0.705186 1.284949
C 4.189368 -0.561764 -0.802141
C 5.347105 -1.355436 -1.350619
H 5.457913 -1.173941 -2.418543
H 6.264364 -1.073315 -0.827555
H 5.181448 -2.420068 -1.167550
O 3.516168 0.191269 -1.502346
O 3.980840 -0.757077 0.476331
H 3.218144 -0.118998 0.829819

INT6.log
Energy (E) = -1239.61122606 Hartree
Enthalpy (H) = -1239.199618 Hartree
Gibbs free energy (G) = -1239.283391 Hartree
Charge = 0, Spin = 1
C 3.017477 0.393512 -0.117460
C 2.409684 1.653854 -0.335377
C 2.957936 2.838335 0.166319
C 4.130739 2.742605 0.896025
C 4.751801 1.498291 1.121531
C 4.208189 0.326857 0.622720
C 2.168885 -0.579327 -0.750292
C 1.121570 0.114493 -1.302014
H 2.477273 3.794934 -0.010506
H 4.582190 3.643013 1.300306
H 5.672779 1.461315 1.694682
H 4.701752 -0.624684 0.802224
H 0.248972 -0.245964 -1.825047
H 0.517349 2.127703 -1.239052
N 1.268863 1.450263 -1.072984
C 2.296909 -2.068739 -0.624572
H 3.307302 -2.316393 -0.282054
C 2.116311 -2.760055 -1.907738

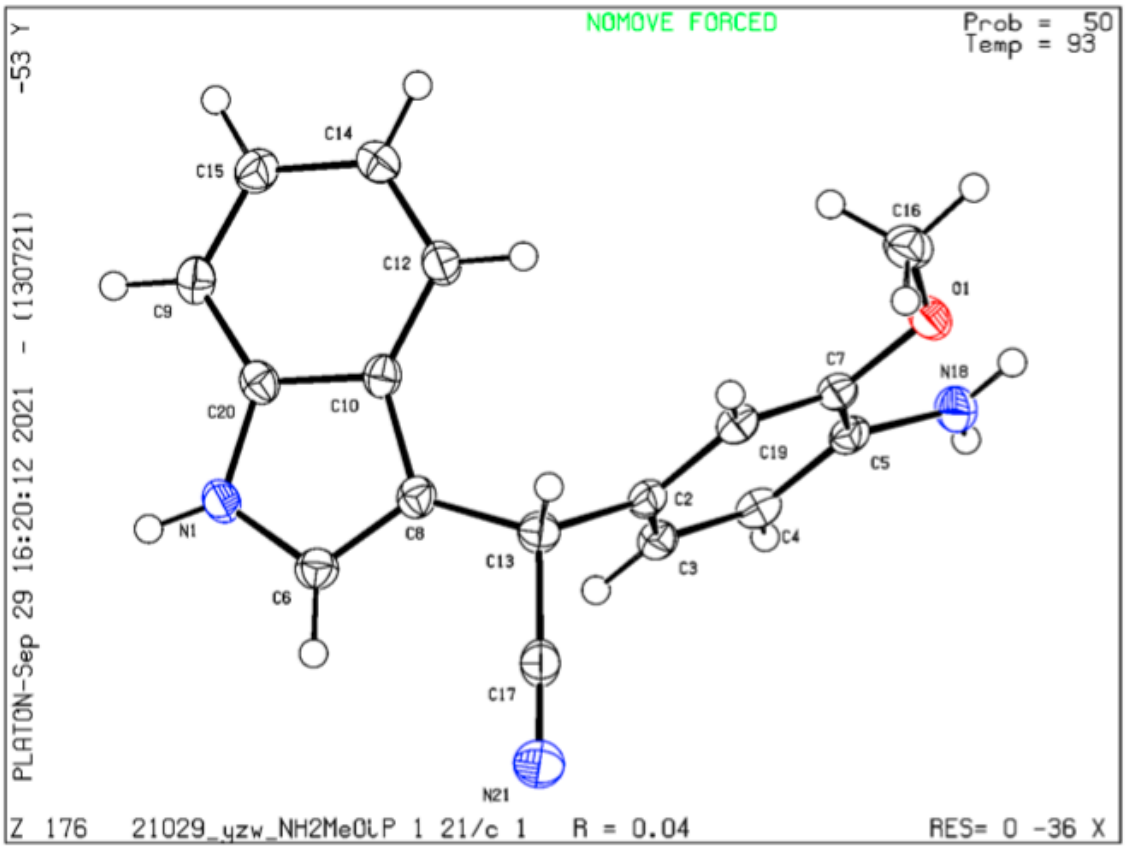
N 1.952346 -3.310634 -2.912911
C -0.113574 -2.592368 -0.038690
C 1.293022 -2.668091 0.452567
C 1.517412 -1.936371 1.732357
C 0.607040 -1.113478 2.266517
C -0.685332 -0.941045 1.626766
C -1.035496 -1.780040 0.493624
H -0.367188 -3.197582 -0.904056
H 1.569296 -3.722372 0.583763
H 2.488635 -2.046161 2.205085
H 0.812543 -0.556824 3.174400
H -2.034642 -1.694580 0.077698
N -1.536961 -0.065650 2.069599
H -1.281643 0.514521 2.858918
H -2.522847 0.041164 1.672715
C -2.037829 2.239075 -1.017408
C -3.438166 2.709501 -0.710984
H -3.474573 3.797309 -0.714265
H -4.135963 2.306529 -1.449552
H -3.742310 2.321297 0.265768
O -1.106458 3.018156 -1.187397
O -1.848380 0.940924 -1.086905
C -4.537740 -0.367796 0.299109
C -5.997774 -0.778784 0.271277
H -6.131382 -1.662450 -0.355446
H -6.372647 -0.964581 1.278075
H -6.580602 0.033323 -0.175100
O -4.066589 0.077419 1.377898
O -3.894182 -0.472734 -0.788532
H -2.705545 0.379937 -0.930655

PD.log
Energy (E) = -781.555429587 Hartree
Enthalpy (H) = -781.281315 Hartree
Gibbs free energy (G) = -781.341947 Hartree
Charge = 0, Spin = 1

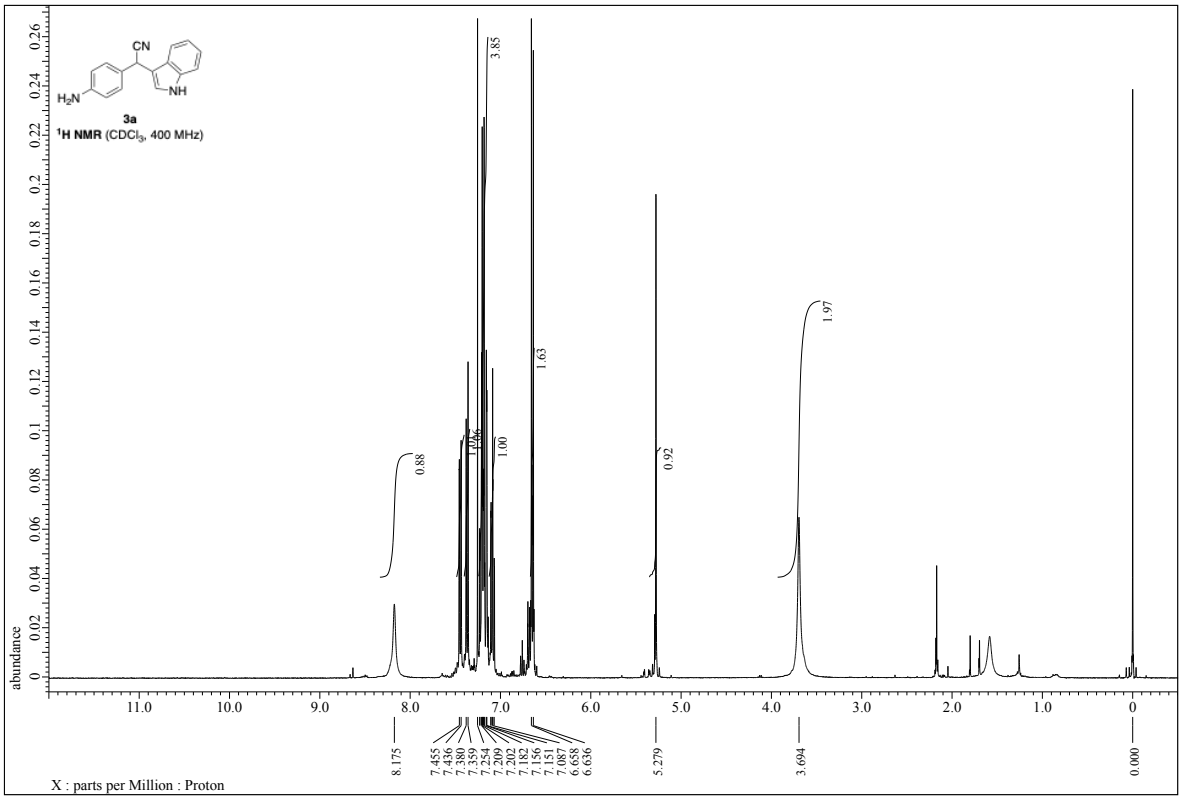
C 1.730348 -0.218763 -0.299687
C 2.939766 -0.165151 0.430198
C 3.808893 -1.257595 0.510112
C 3.441141 -2.413750 -0.157031
C 2.237488 -2.488911 -0.885452
C 1.379626 -1.405586 -0.961357
C 1.106107 1.070078 -0.162729
C 1.929781 1.826329 0.623291
H 4.734499 -1.200718 1.073564
H 4.092375 -3.281020 -0.115857
H 1.980944 -3.414310 -1.391030
H 0.447201 -1.471797 -1.513609
H 1.814726 2.847800 0.956141
H 3.789407 1.426439 1.553786
N 3.033457 1.090962 0.981125
C -0.209883 1.462119 -0.784571
H -0.120309 1.392134 -1.876678
C -0.517112 2.873189 -0.494975
N -0.761973 3.979038 -0.253510
C -1.557599 0.234380 0.987074
C -1.375379 0.573532 -0.353729
C -2.278960 0.082380 -1.293238
C -3.339283 -0.729570 -0.910846
C -3.525381 -1.069126 0.436248
C -2.613830 -0.571805 1.381422
H -0.853255 0.596604 1.730704
H -2.154080 0.330349 -2.344135
H -4.030373 -1.105398 -1.659737
H -2.738151 -0.826336 2.430084
N -4.613504 -1.834339 0.834574
H -5.003577 -2.432915 0.121495
H -4.499610 -2.320951 1.711558

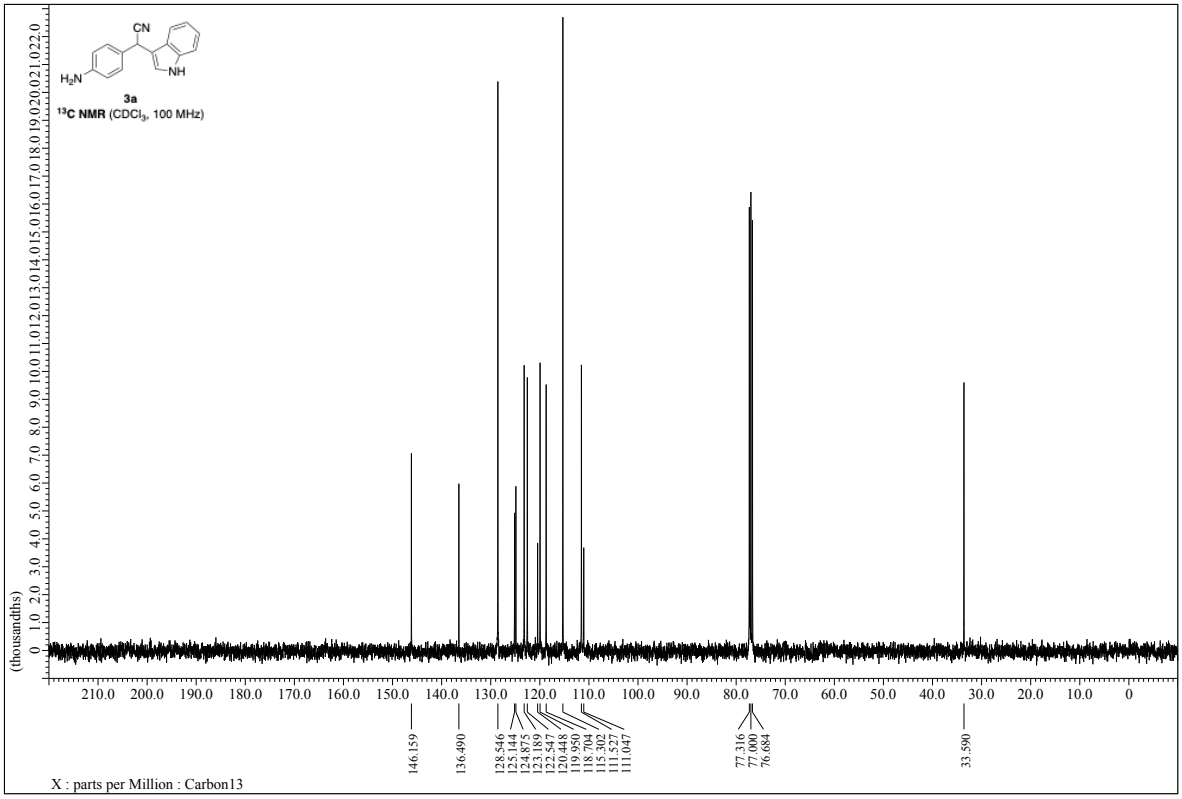
2. Structural figures of X-ray crystallographic analysis

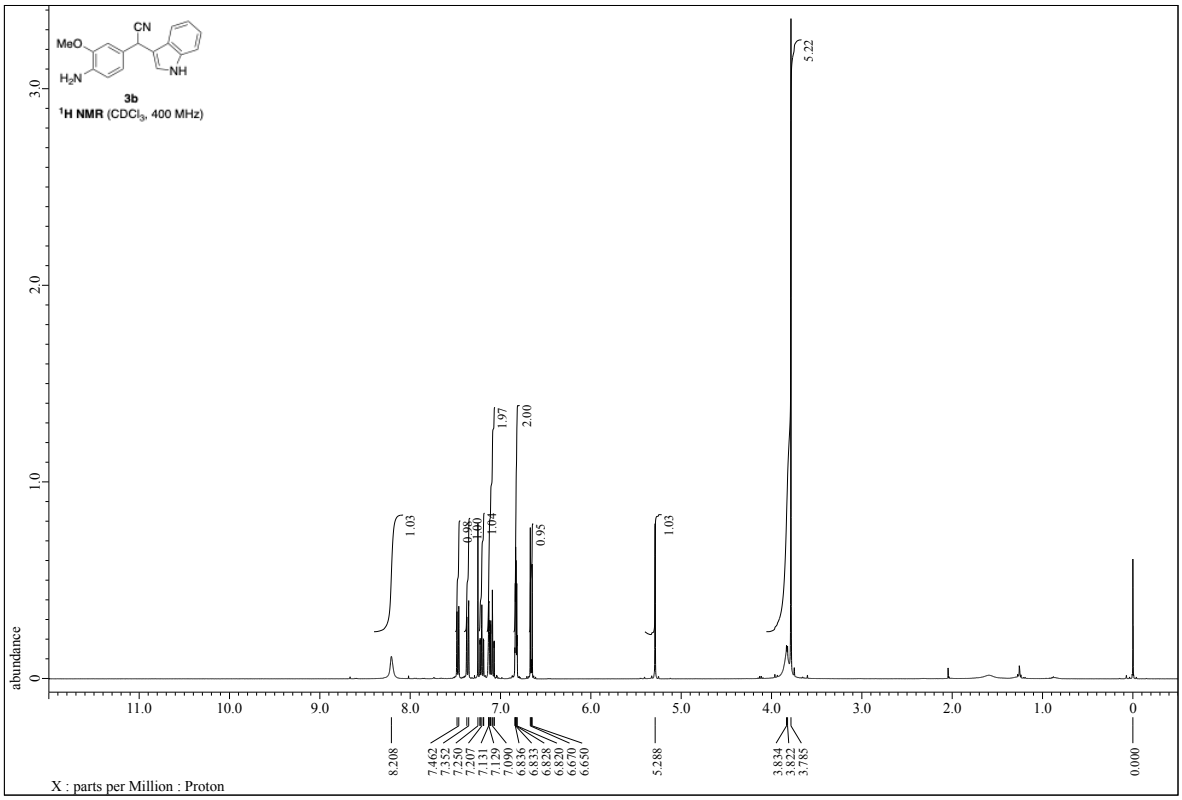
Datablock 21029_yzw_NH2MeOindoleCN - ellipsoid plot

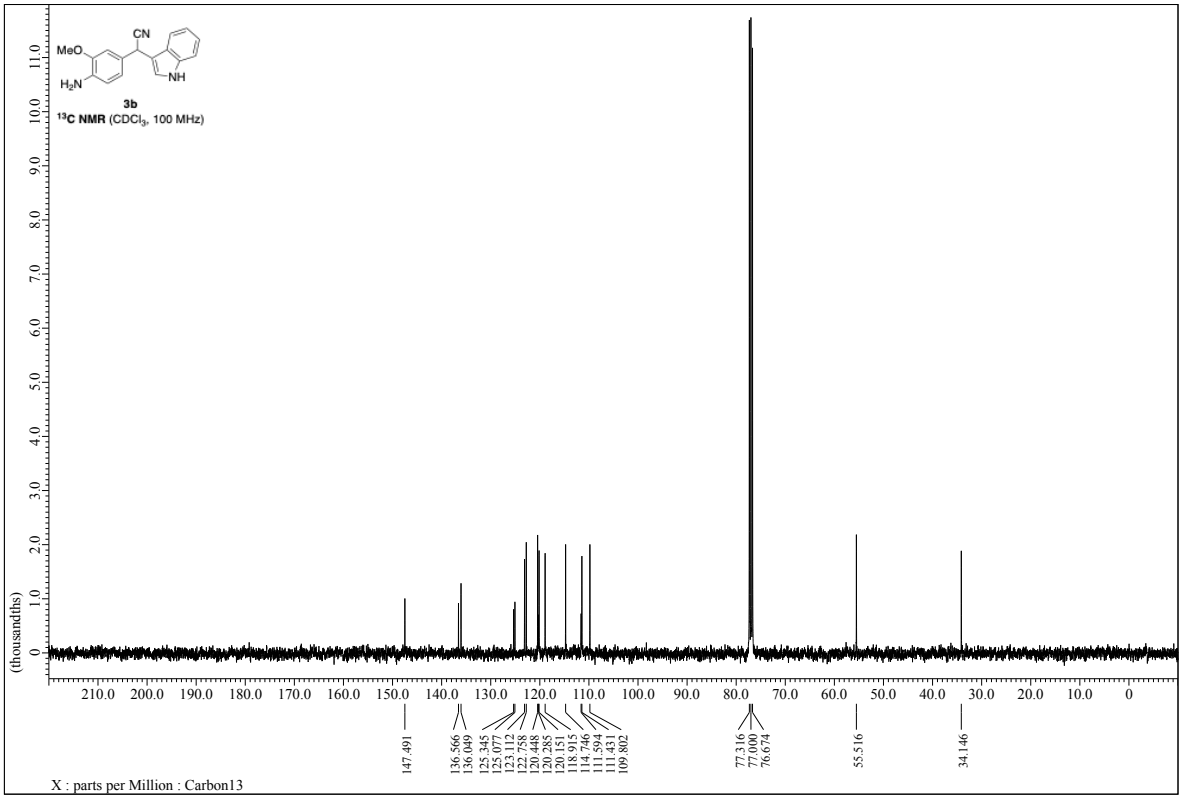


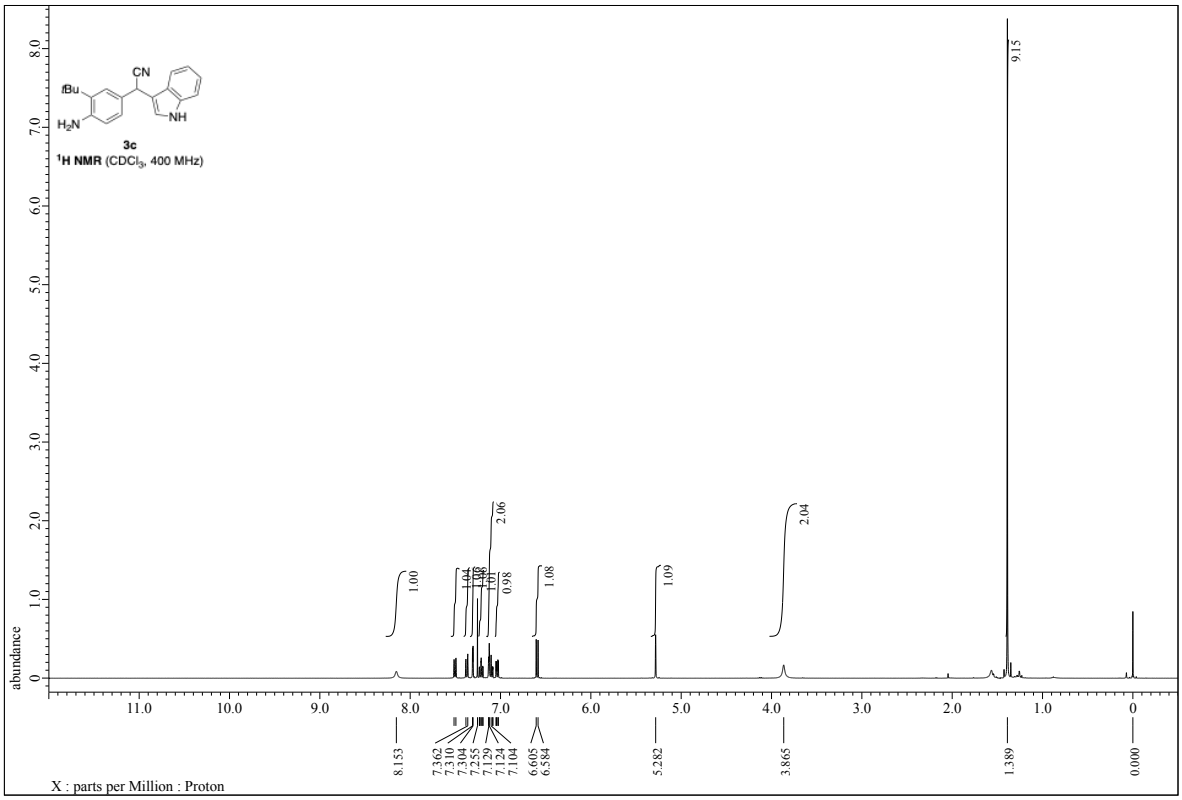
3. ^{1}H and ^{13}C NMR Spectra of new compounds

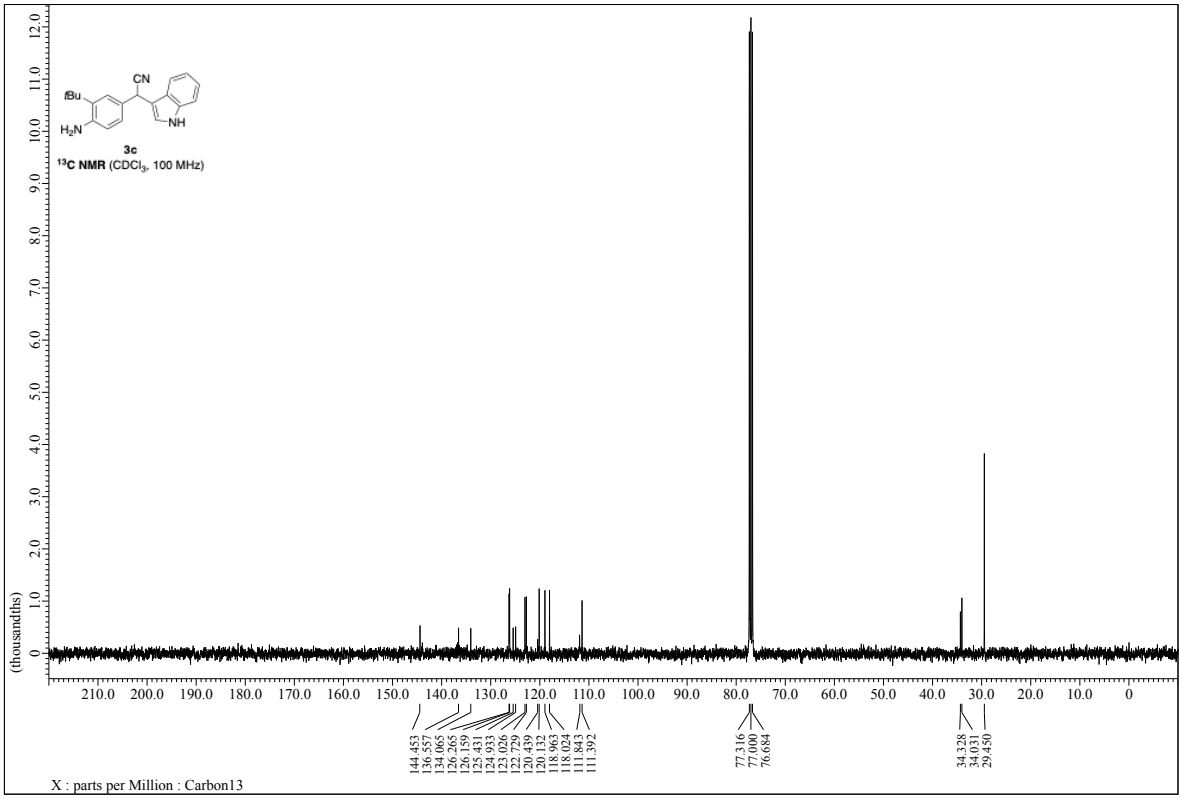


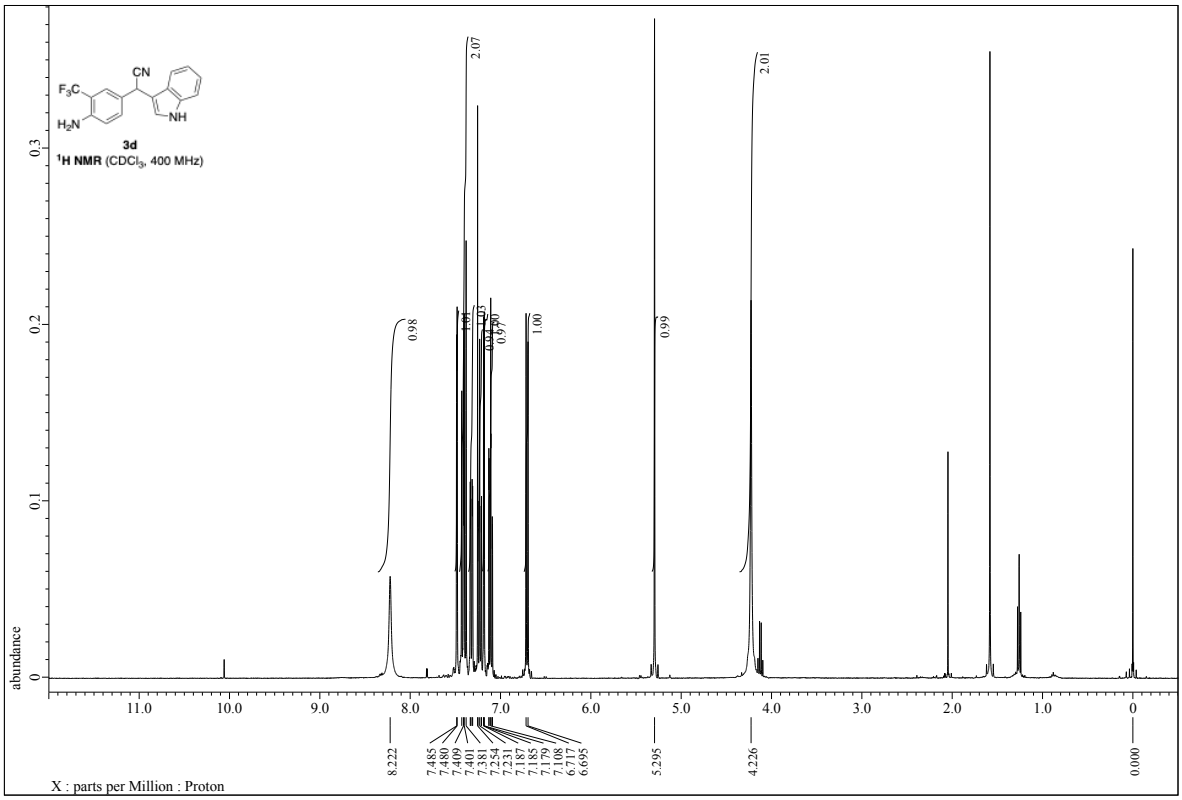


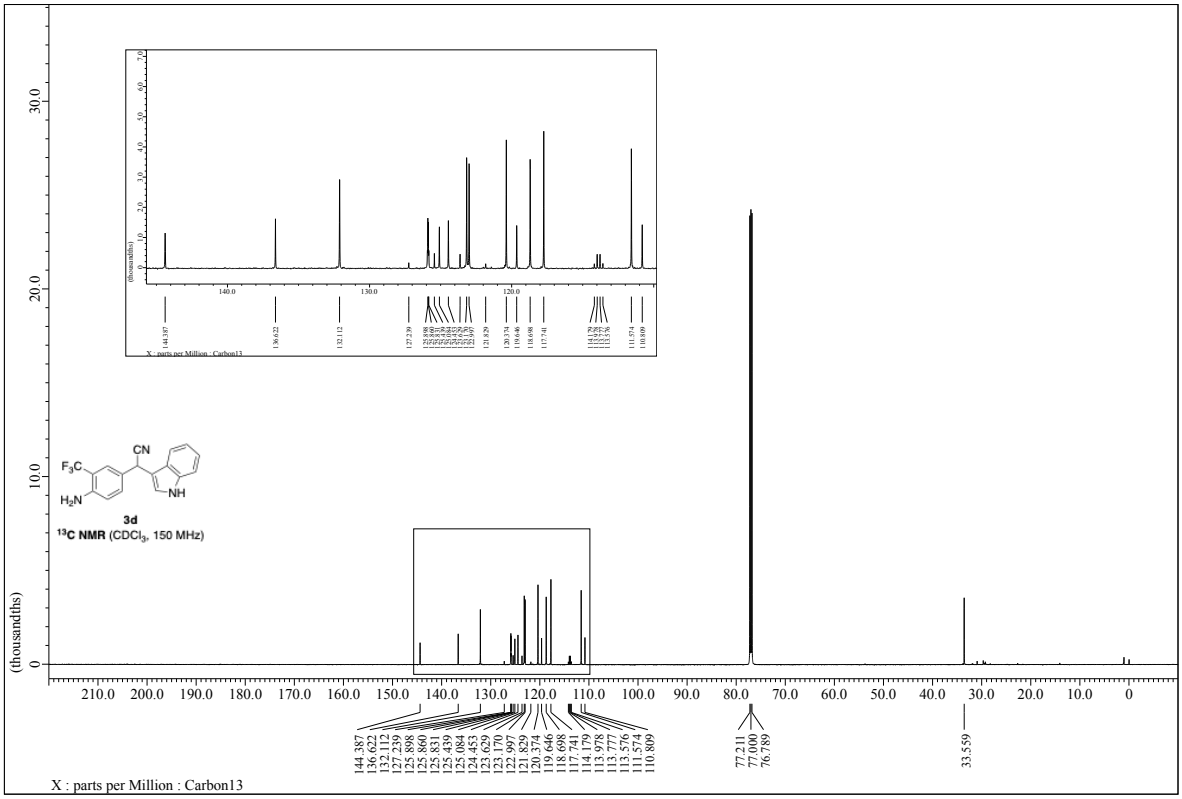

MeO
CN
NH
H2N
3b
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

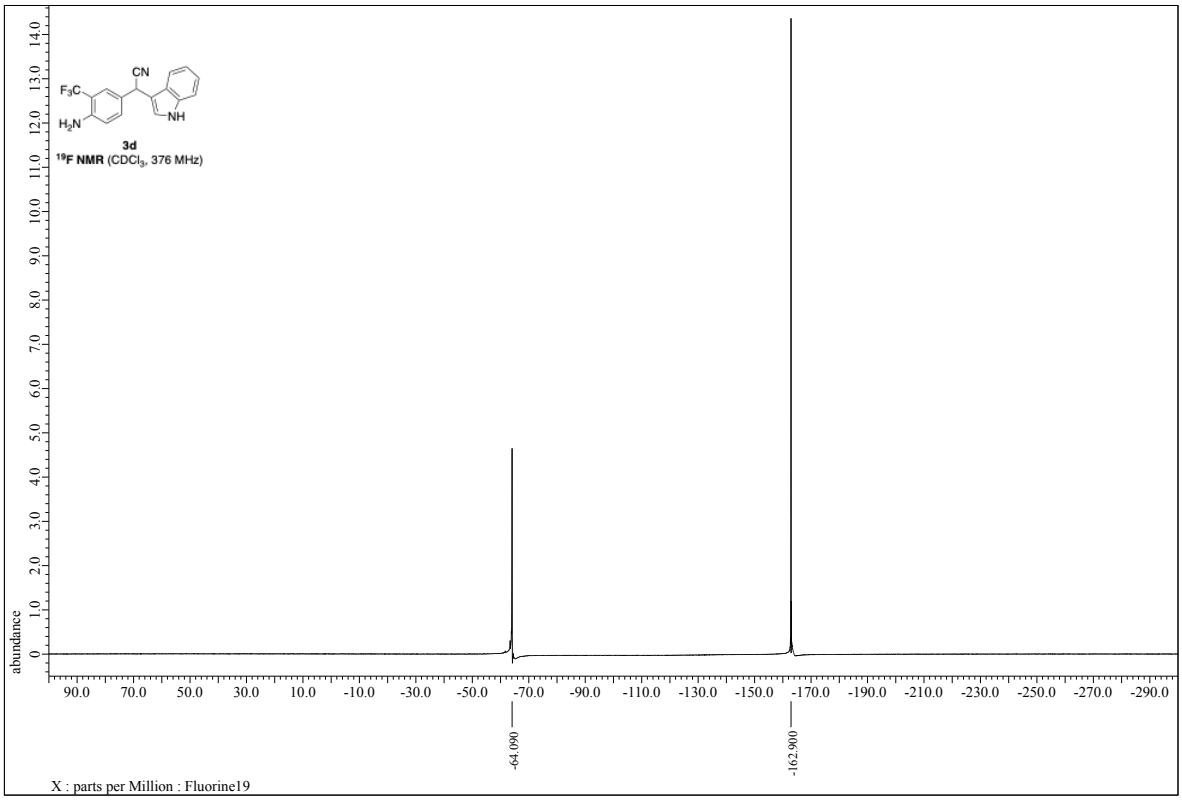

MeO
CN
NH
H2N
3b
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

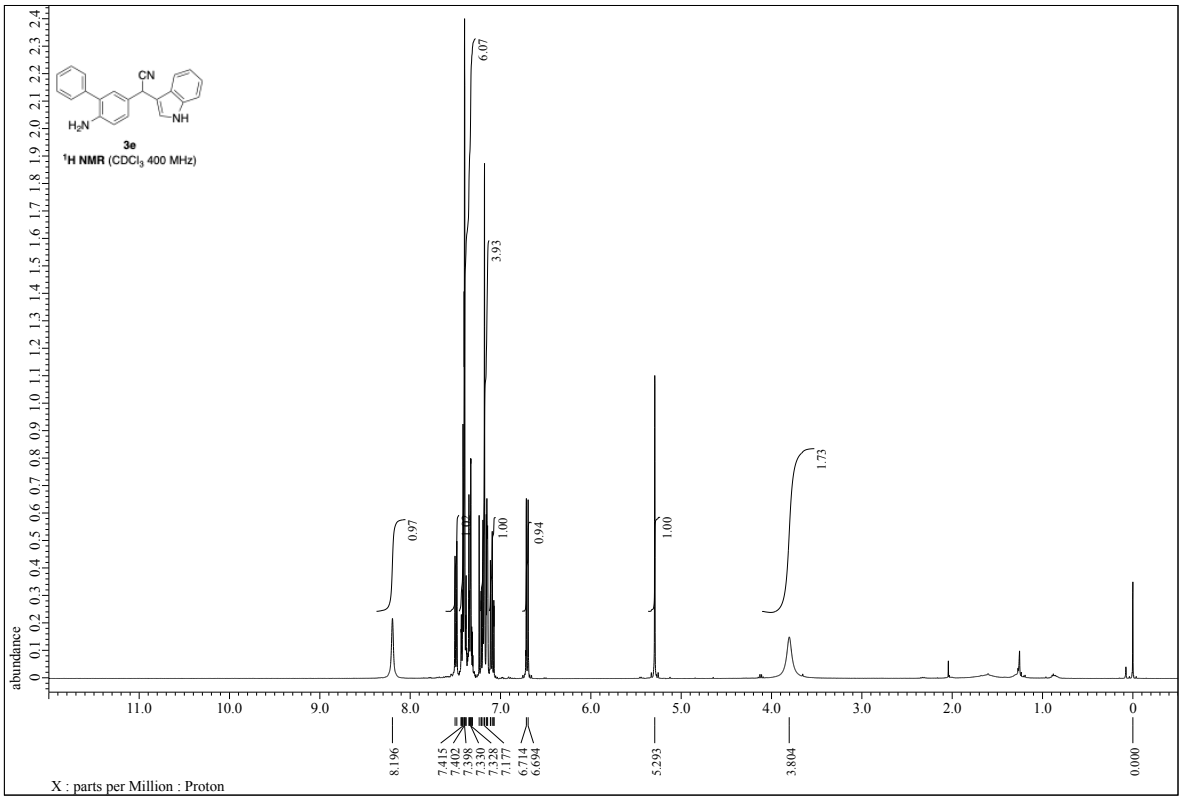

CN
tBu
H2N
NH
3c
1H NMR (CDCl3, 400 MHz)
abundance
9.15
2.06
2.04
1.00
1.04
1.08
1.01
0.98
1.08
1.09
8.153
7.362
7.310
7.304
7.255
7.129
7.124
7.104
6.605
6.584
5.282
3.865
1.389
0.000
X : parts per Million : Proton

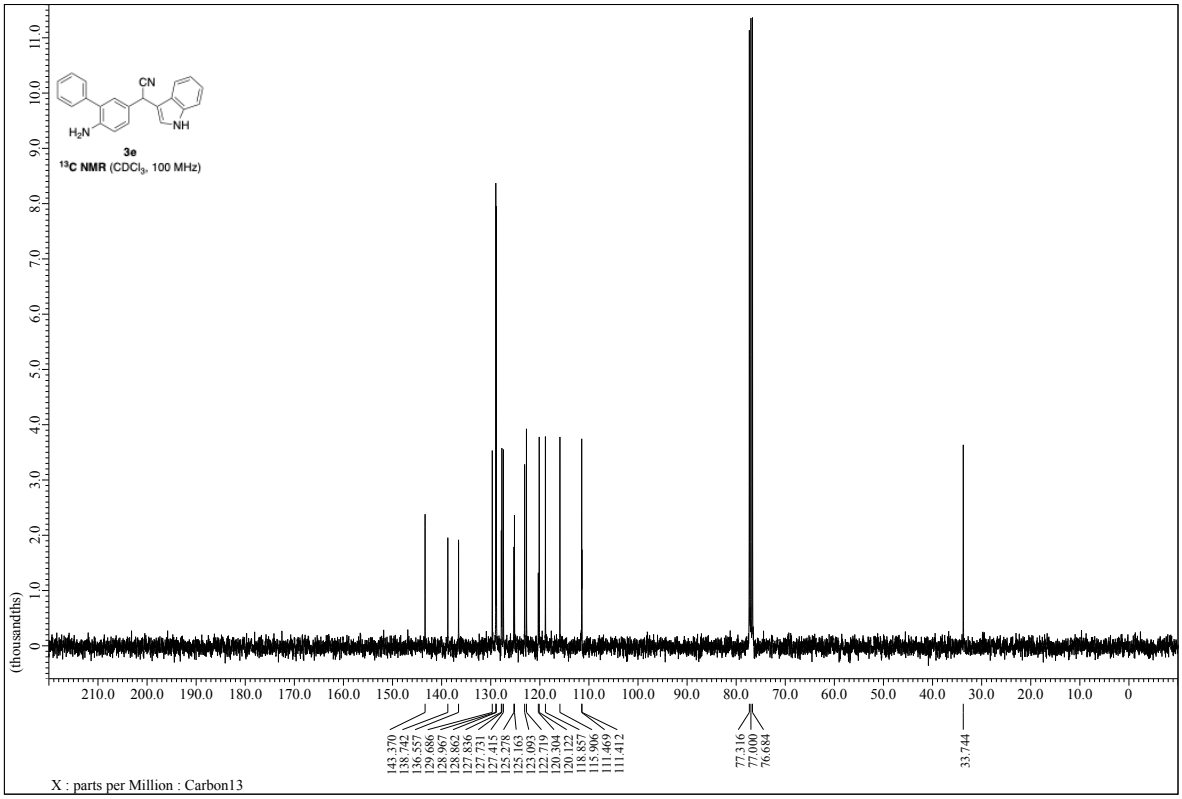

CN
tBu
H2N
NH
3c
13C NMR (CDCl3, 100 MHz)
(thousandths)
144.453
136.557
134.065
126.265
126.159
125.431
124.933
123.026
122.729
120.432
120.132
118.963
118.024
111.843
111.392
77.316
77.000
76.684
34.328
34.031
29.450
X : parts per Million : Carbon13

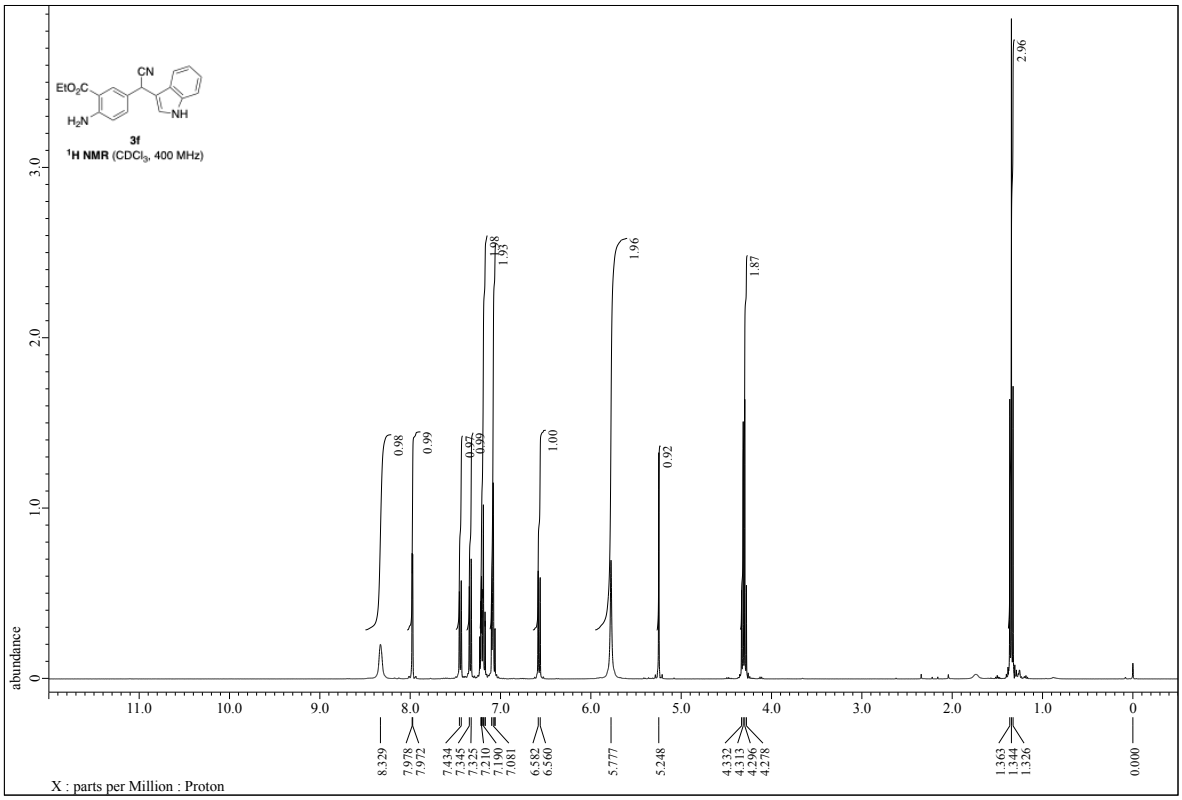

3d
^{1}H NMR (CDCl$_3$, 400 MHz)
abundance
X : parts per Million : Proton

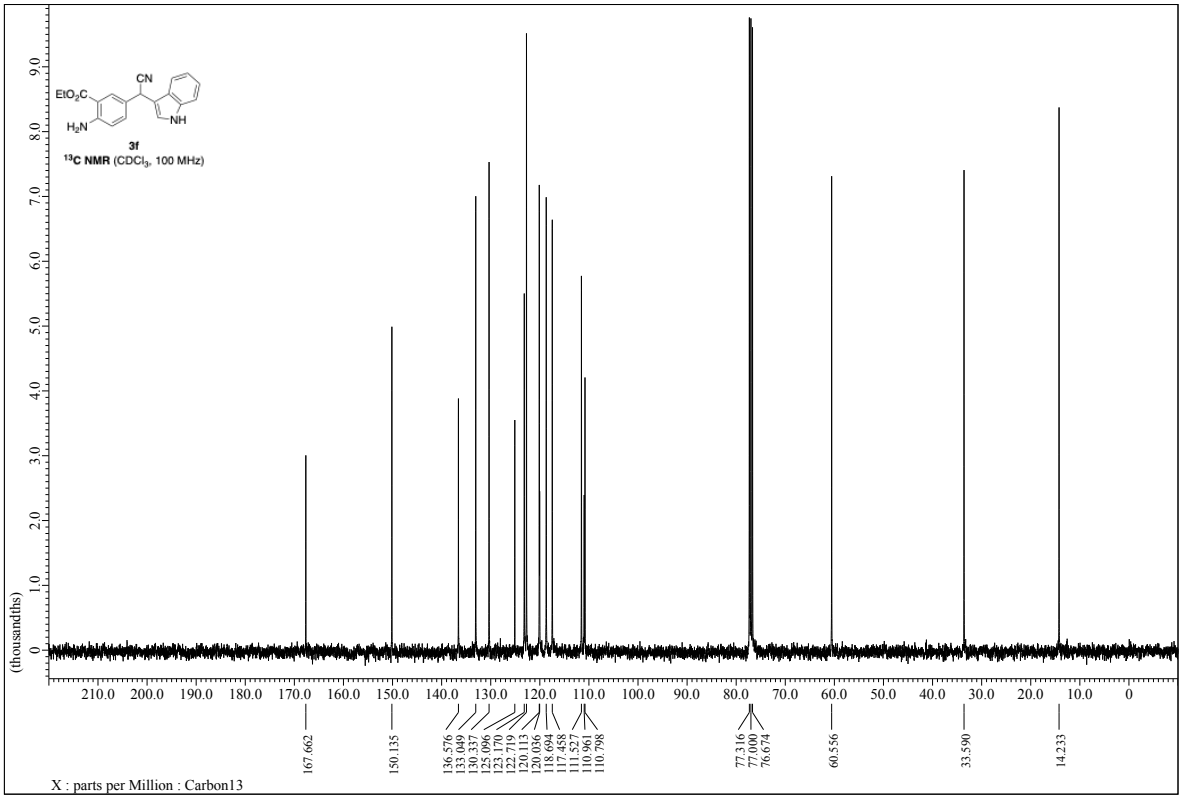

3d
^{13}C NMR (CDCl$_3$, 150 MHz)
(thousandths)
X : parts per Million : Carbon13

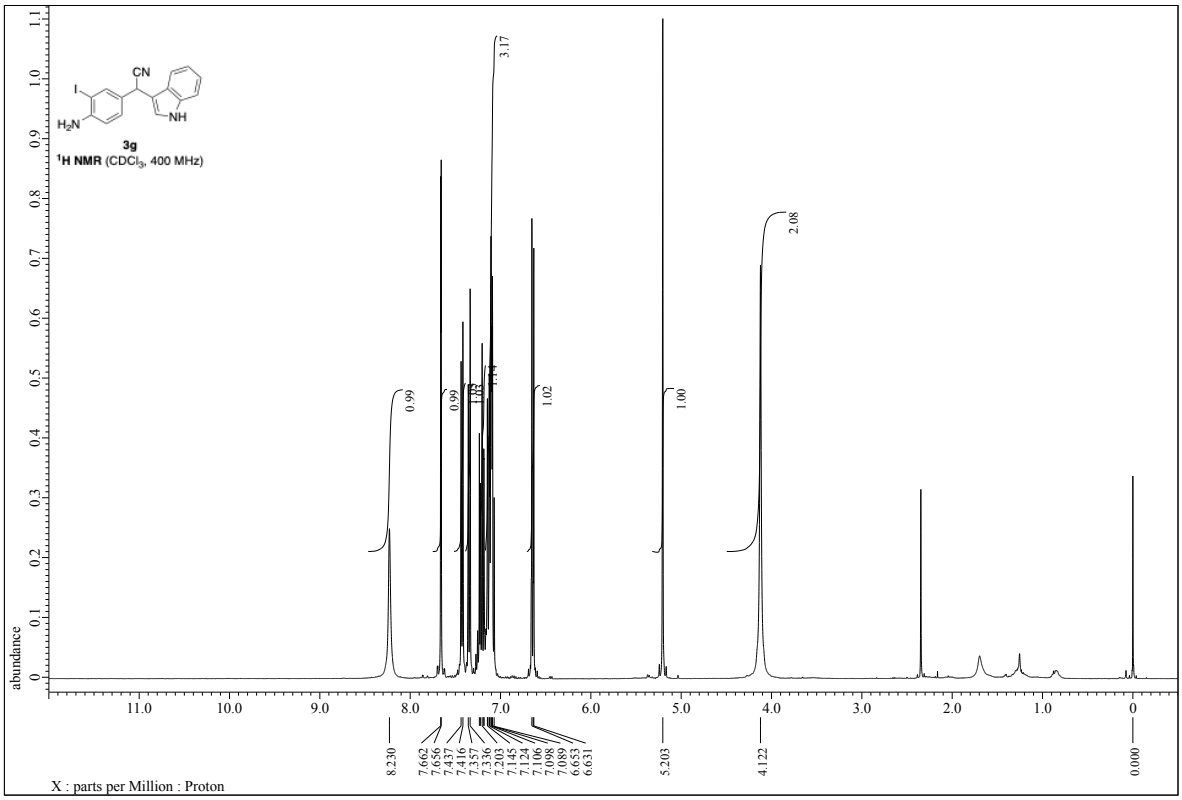

CN
F3C
H2N
NH
3d
19F NMR (CDCl3, 376 MHz)
abundance
-64.090
-162.900
X : parts per Million : Fluorine19

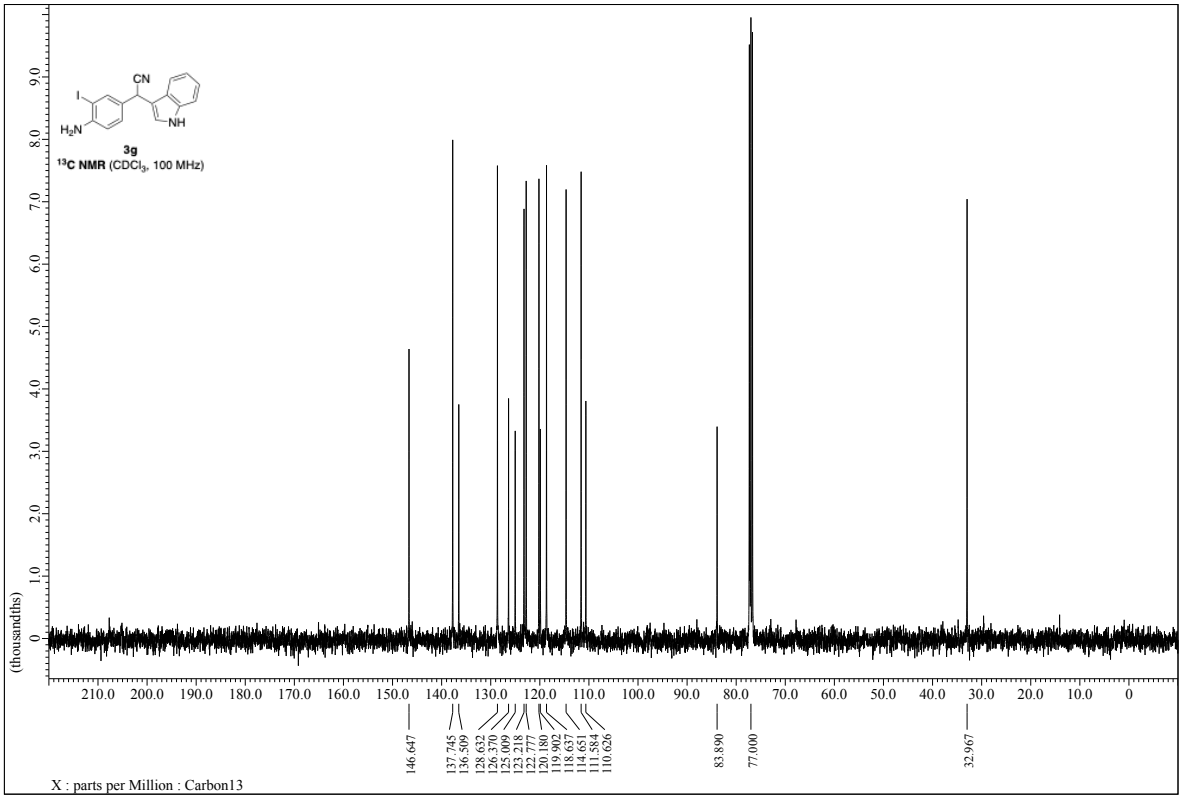

3e
^{1}H NMR (CDCl$_3$ 400 MHz)
abundance
X : parts per Million : Proton
8.196
7.415
7.402
7.398
7.330
7.328
7.177
6.714
6.694
5.293
3.804
0.000
0.97
1.16
1.00
0.94
1.00
1.73
6.07
3.93

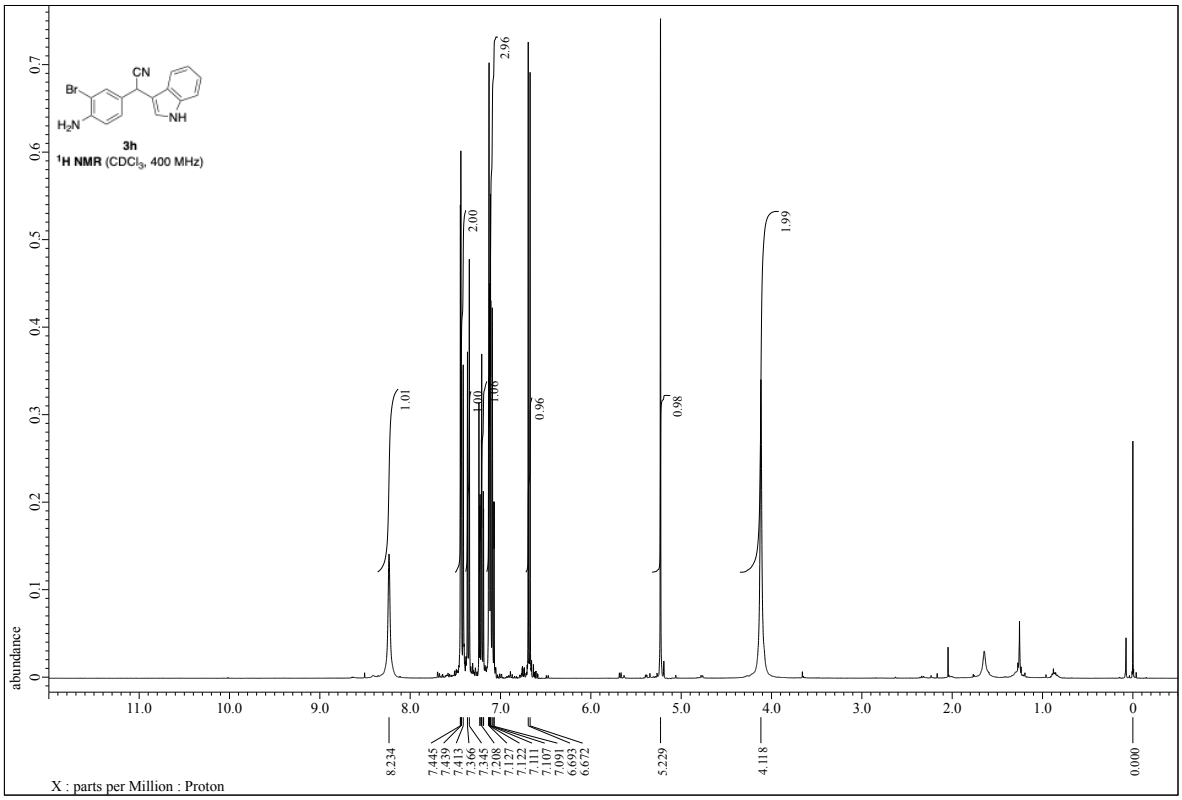

3e
^{13}C NMR (CDCl$_3$, 100 MHz)
(thousandths)
X : parts per Million : Carbon13
143.370
138.742
136.557
129.606
128.967
128.862
127.836
127.731
127.415
125.278
125.163
123.093
122.719
120.394
120.122
118.857
115.906
111.469
111.412
77.316
77.000
76.684
33.744

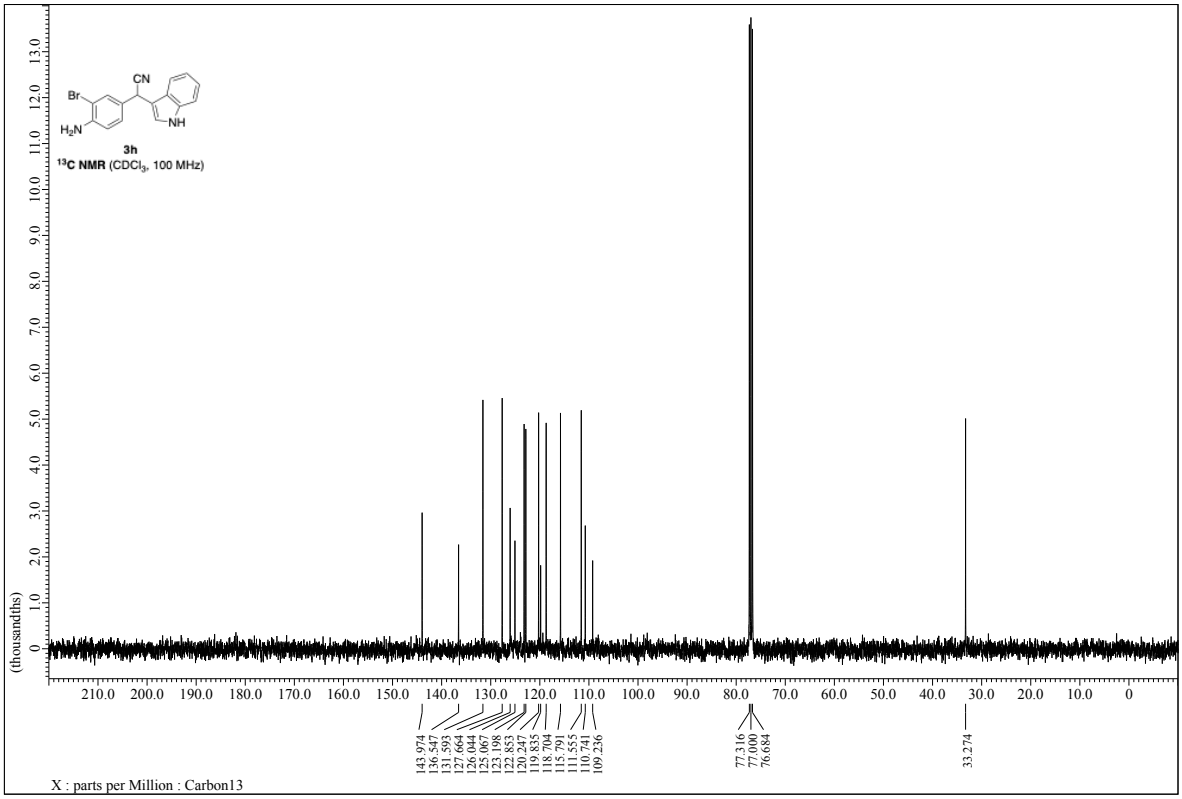

3f
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

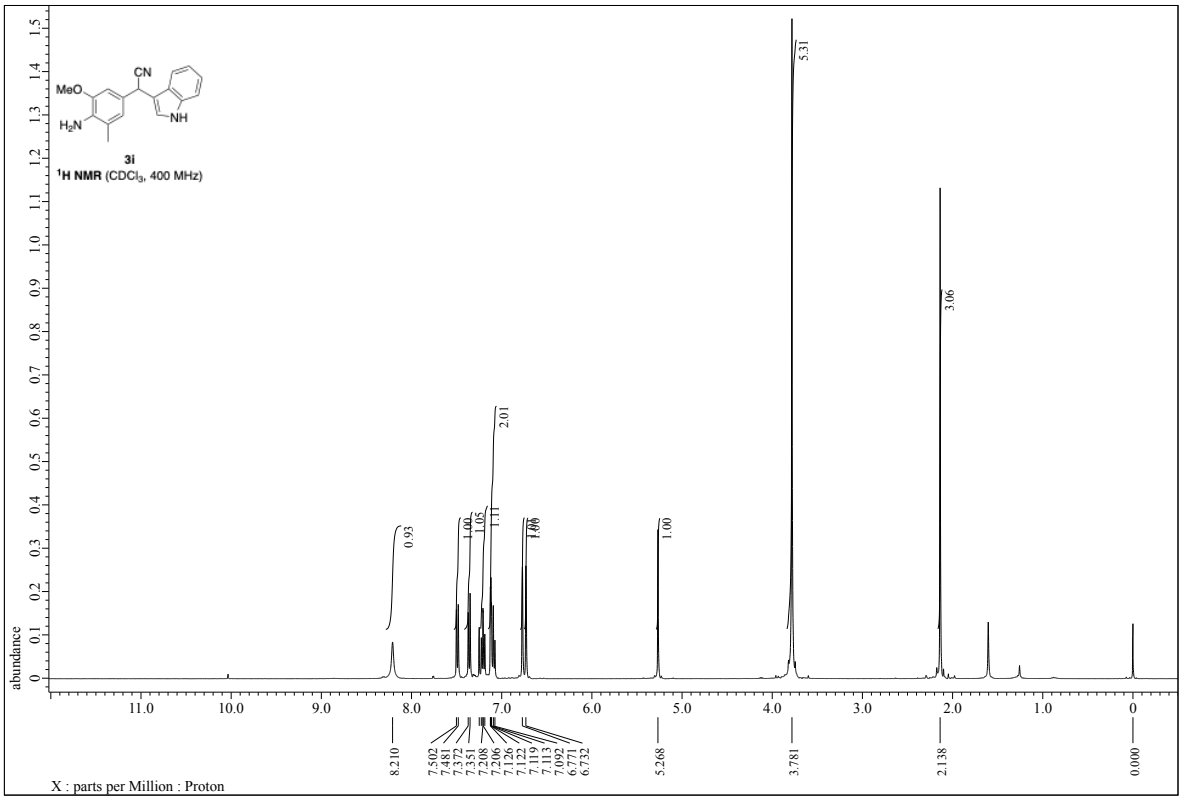

3f
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

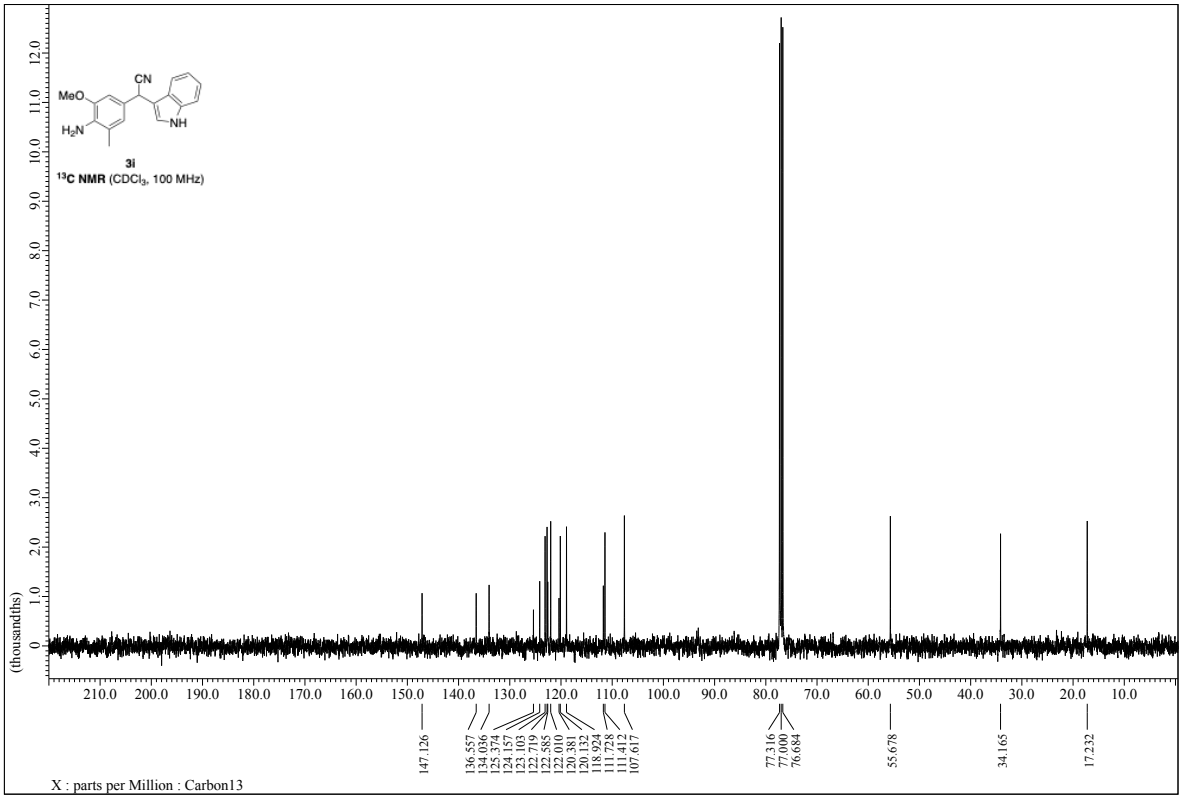

3g
¹H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

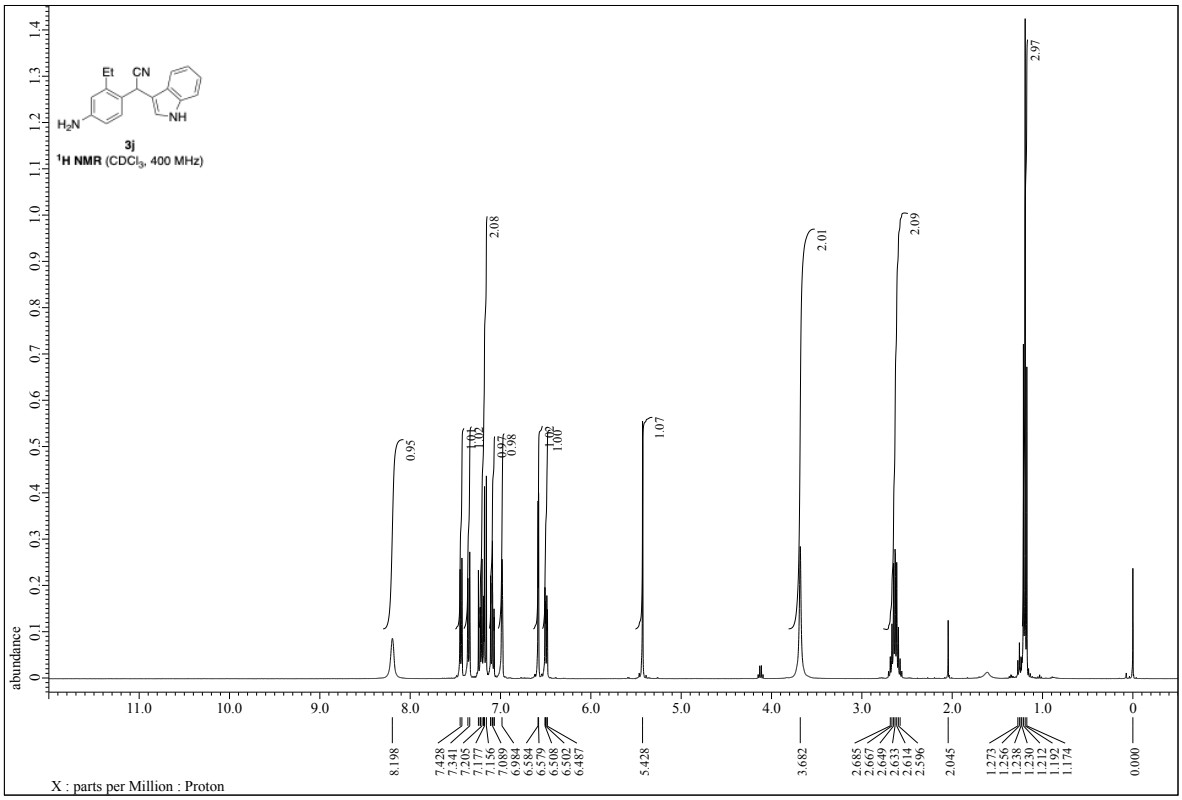

3g
¹³C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

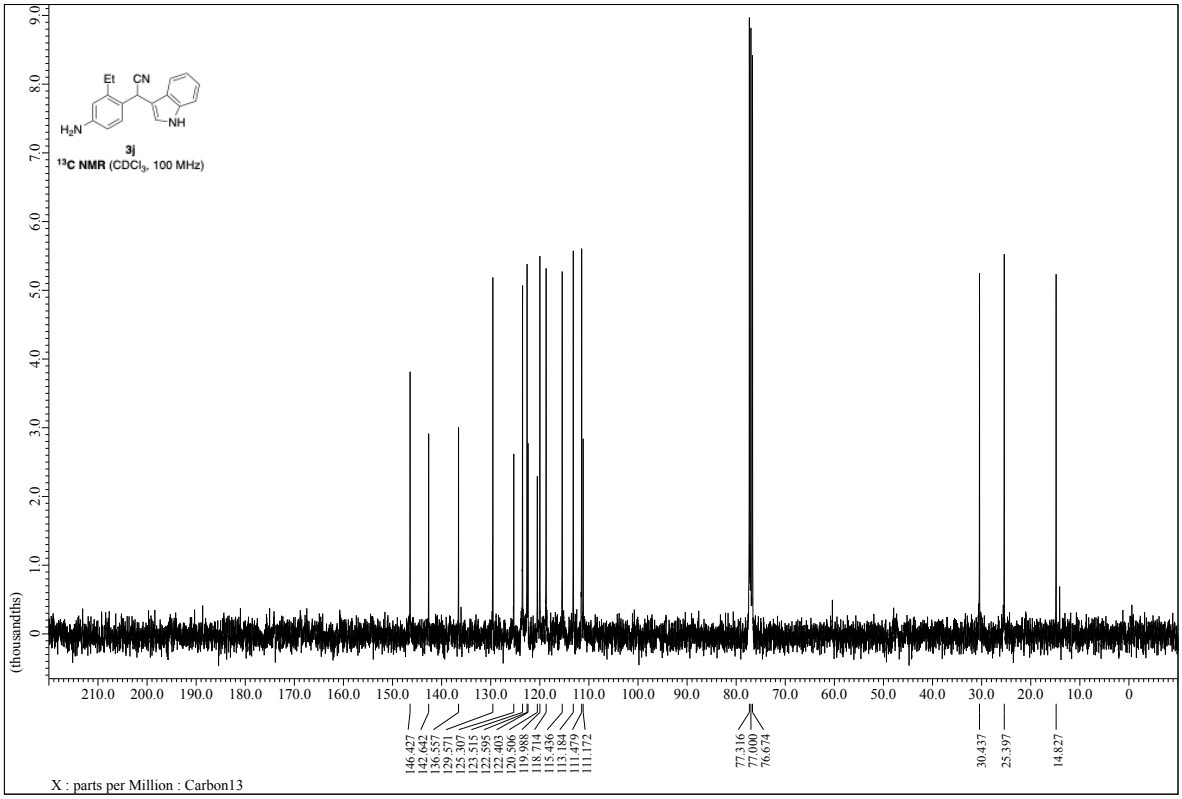

3h
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

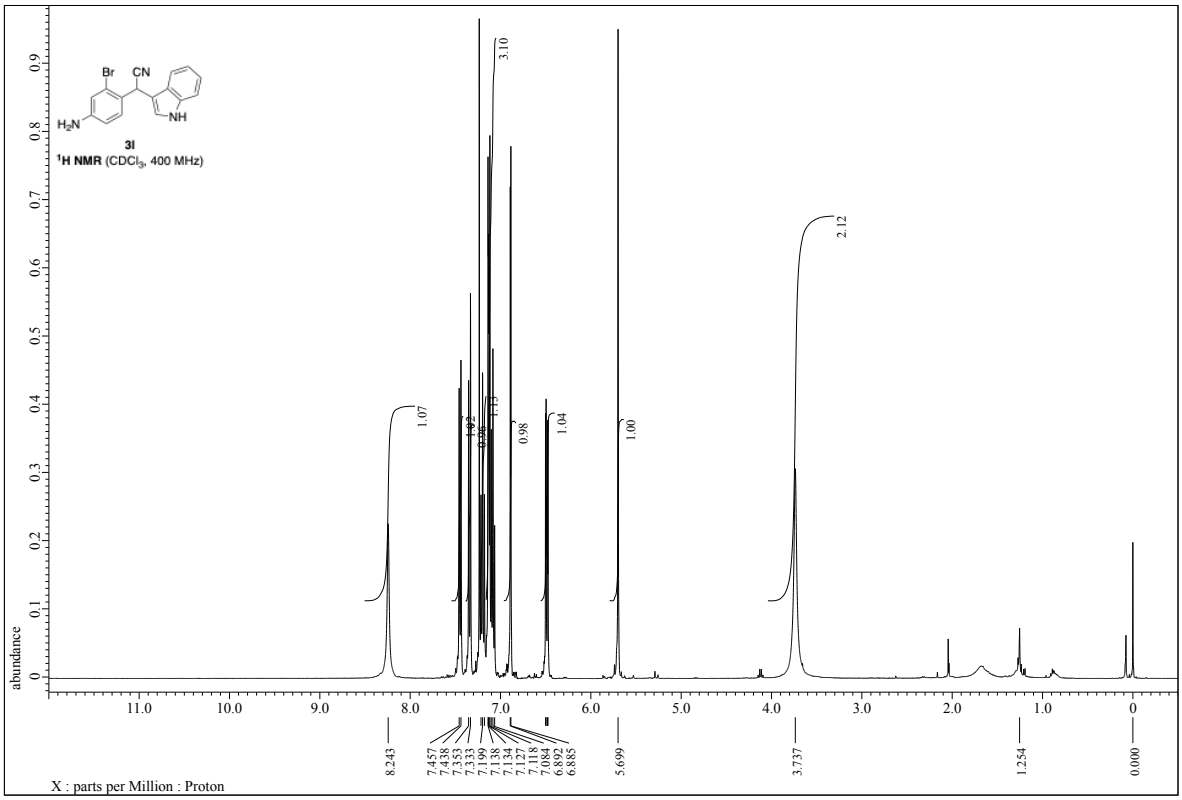

3h
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

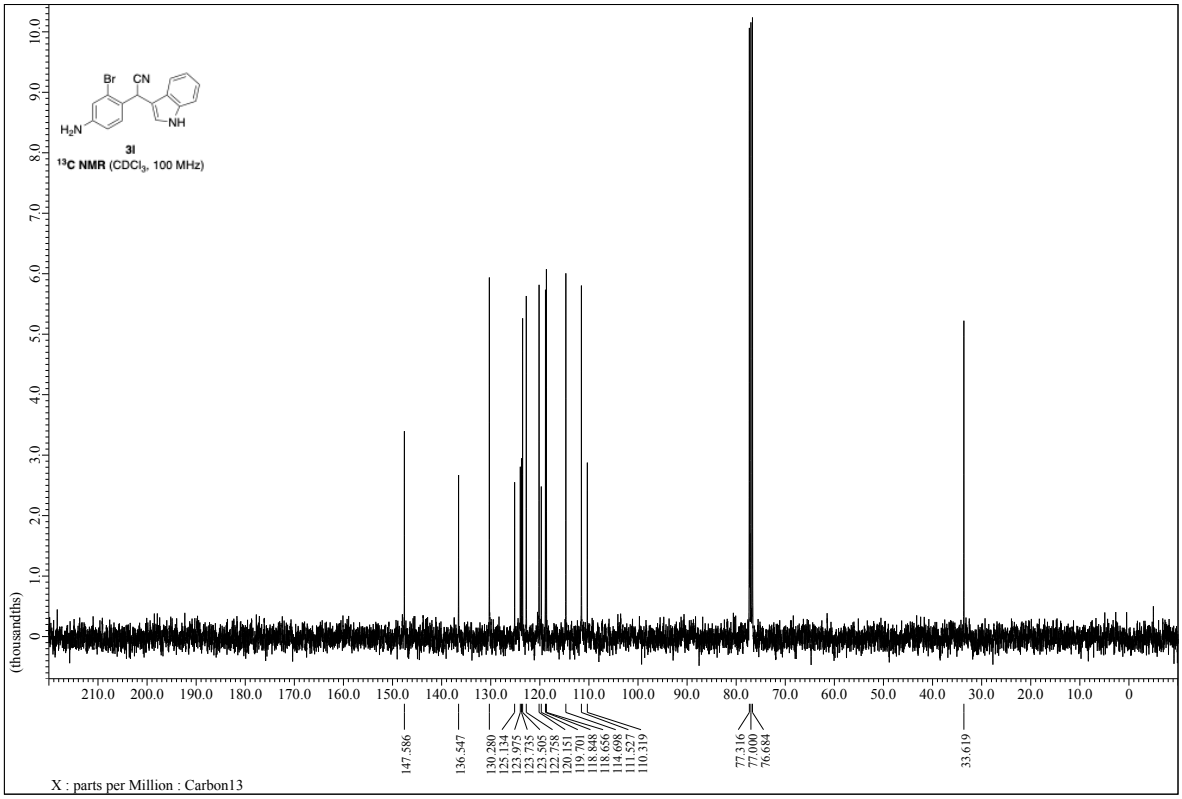

MeO
CN
NH
H2N
3i
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

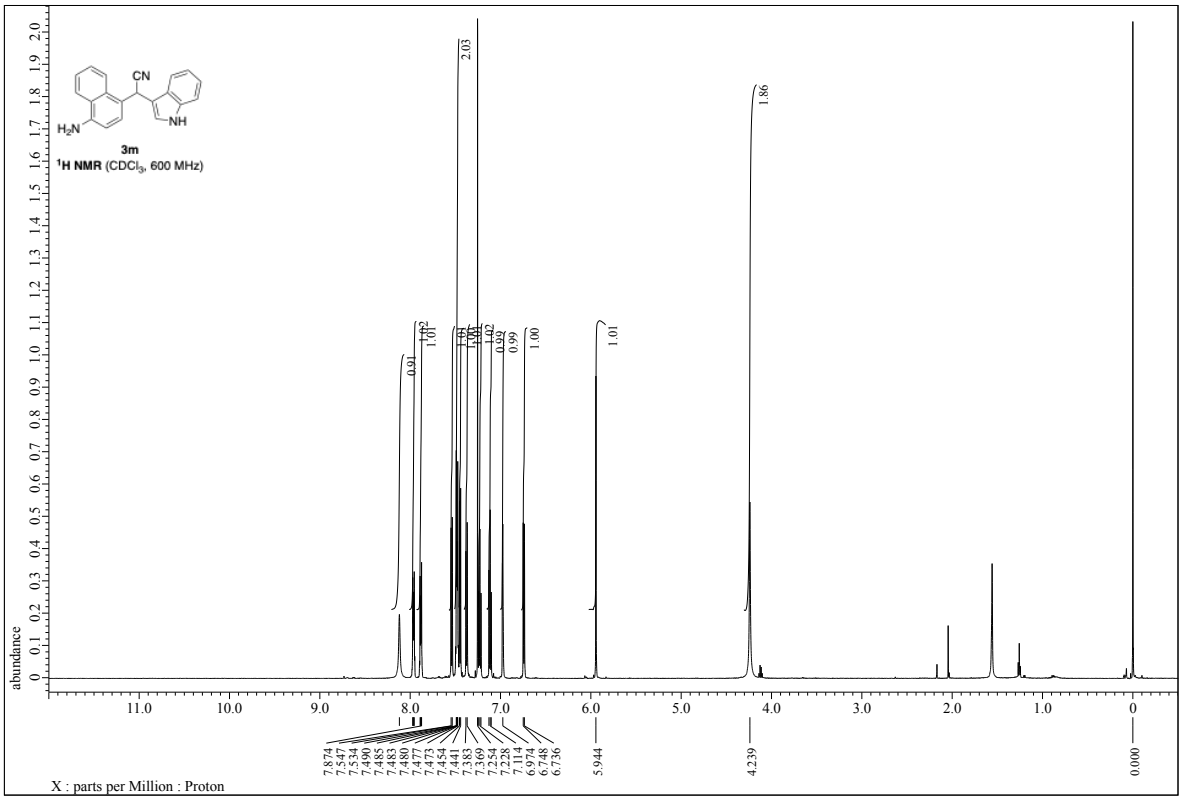

MeO
CN
NH
H2N
3i
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

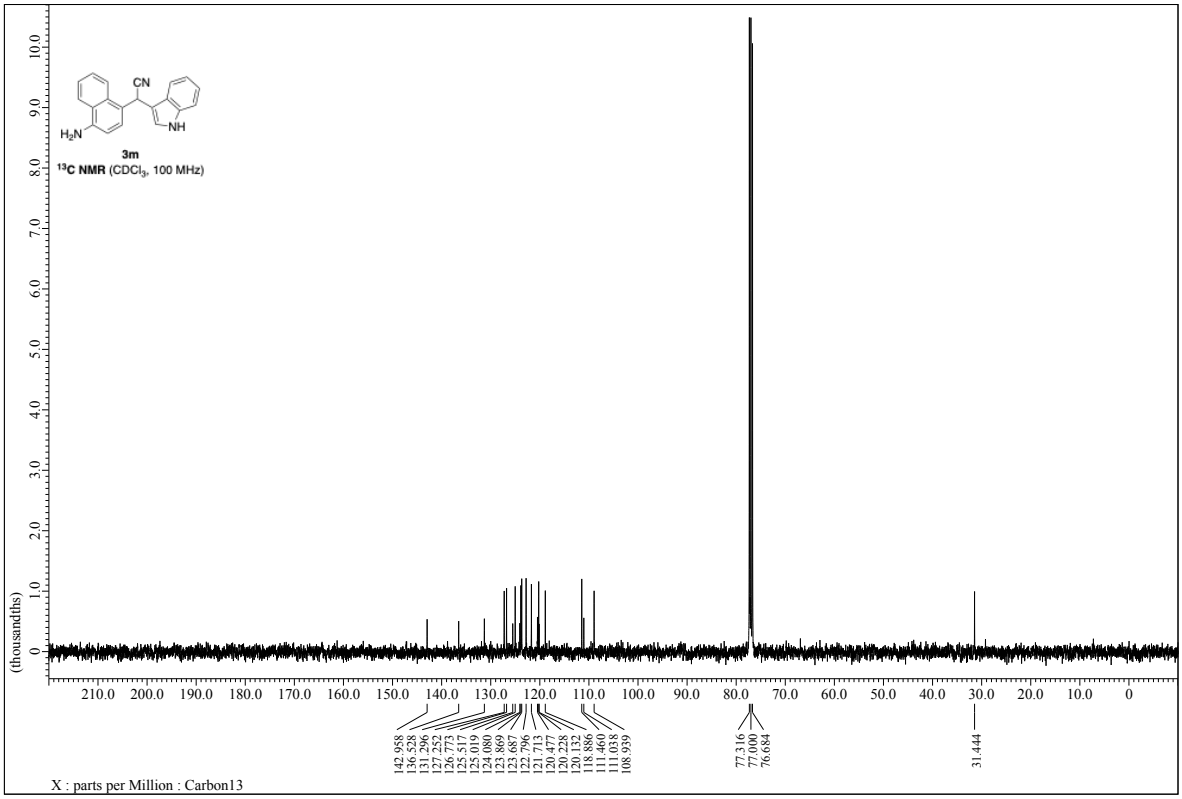

Et
CN
H_2N
NH
3j
^{1}H NMR ($CDCl_3$, 400 MHz)
abundance
X : parts per Million : Proton

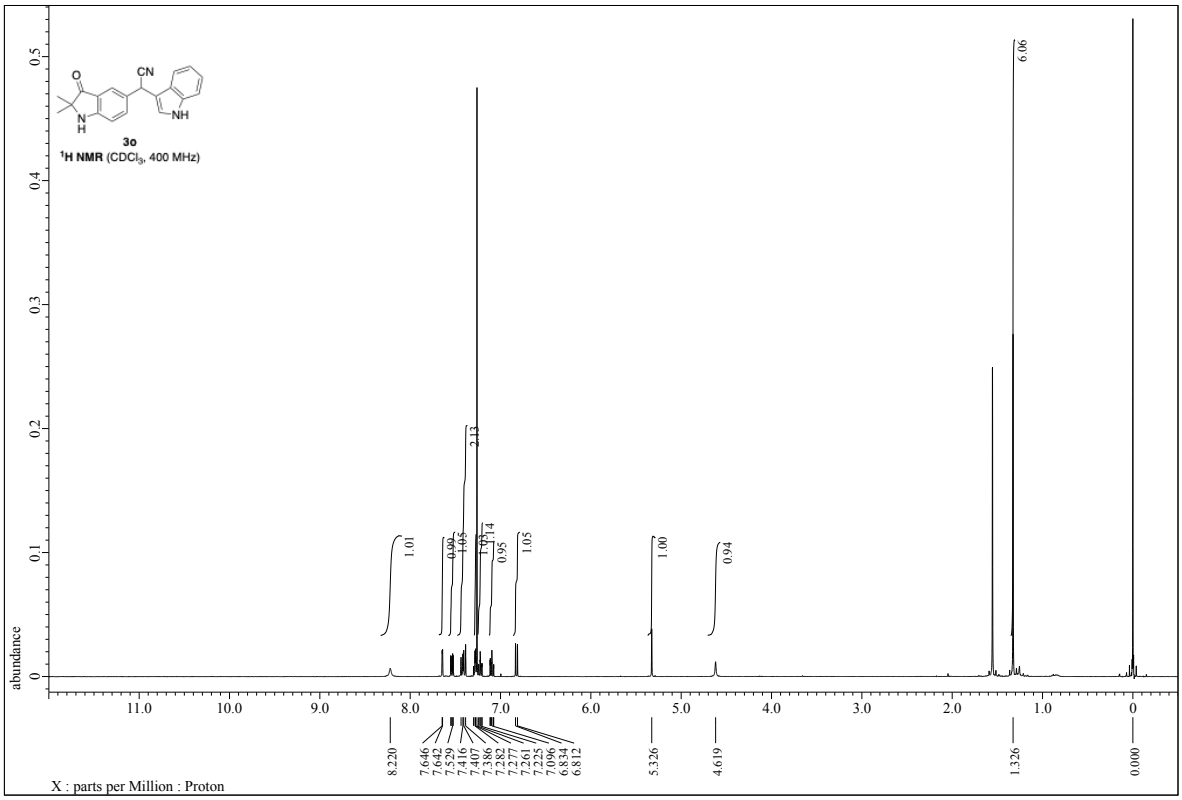

Et
CN
H_2N
NH
3j
^{13}C NMR ($CDCl_3$, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

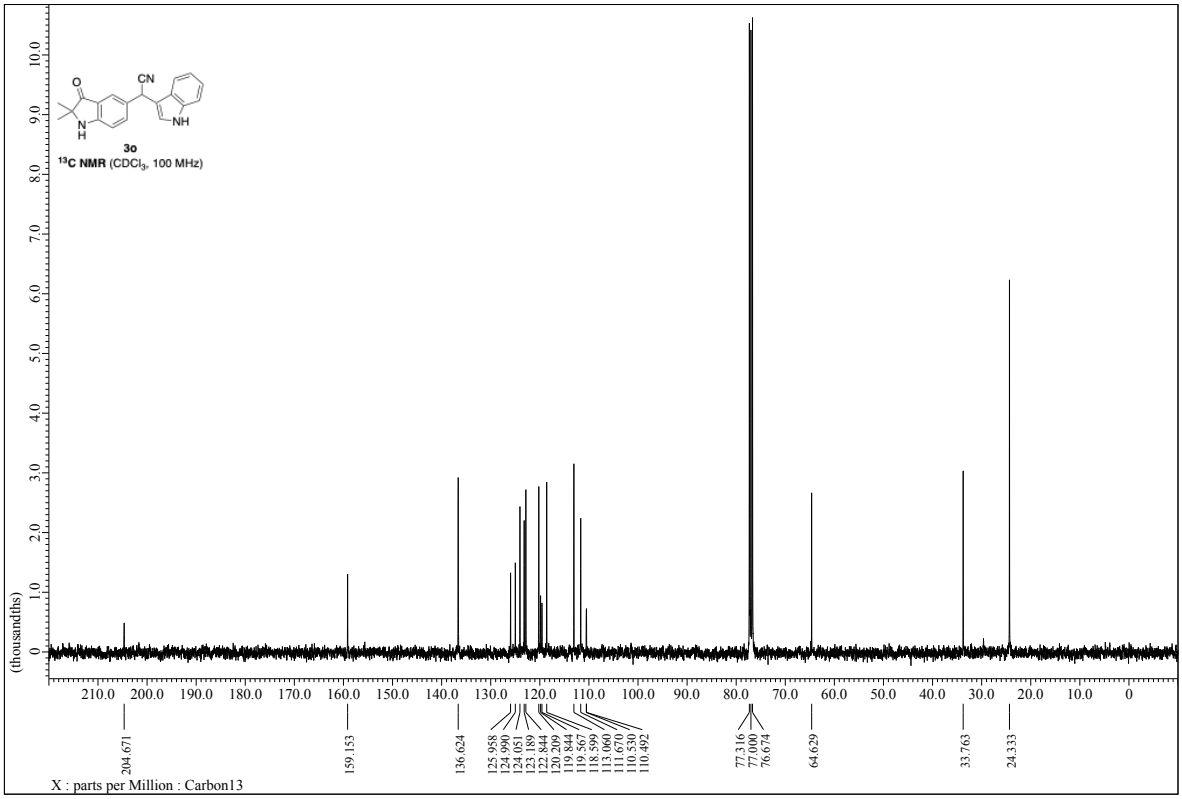

Br
CN
H2N
NH
3l
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

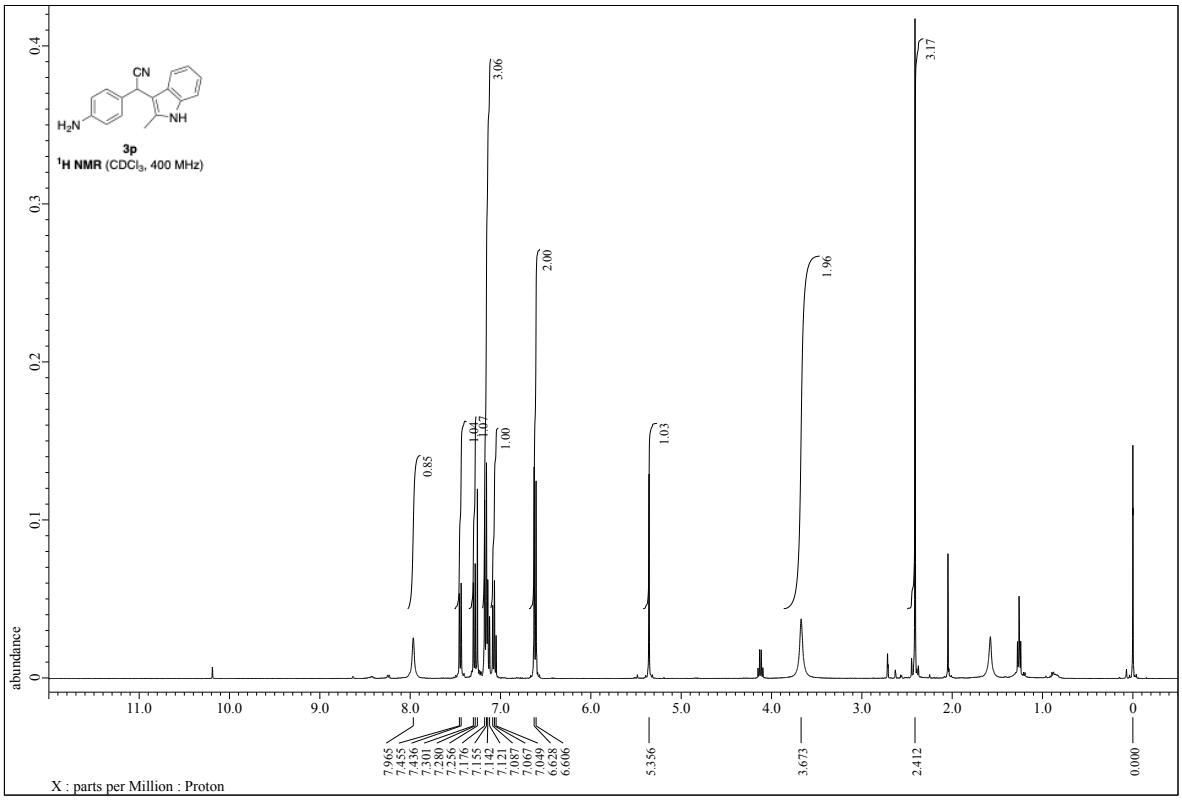

Br
CN
H2N
NH
3l
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

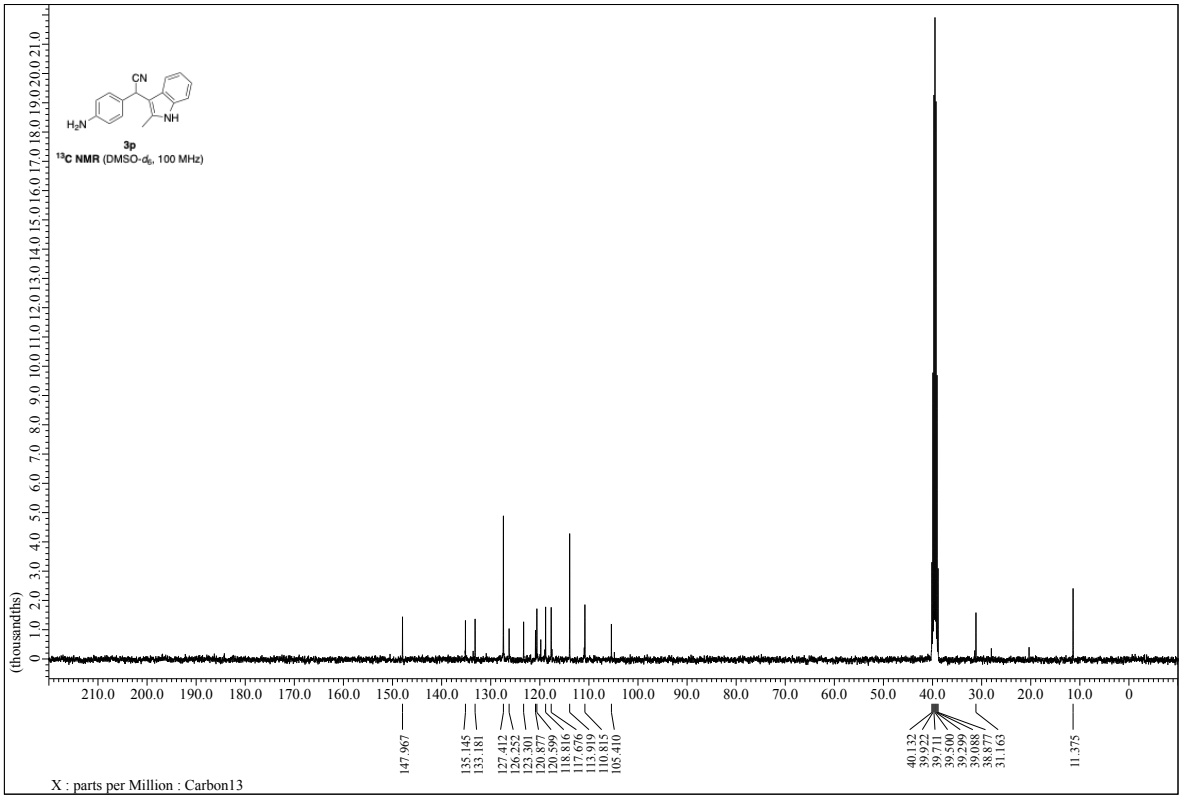

CN
NH
H2N
3m
1H NMR (CDCl3, 600 MHz)
abundance
X : parts per Million : Proton

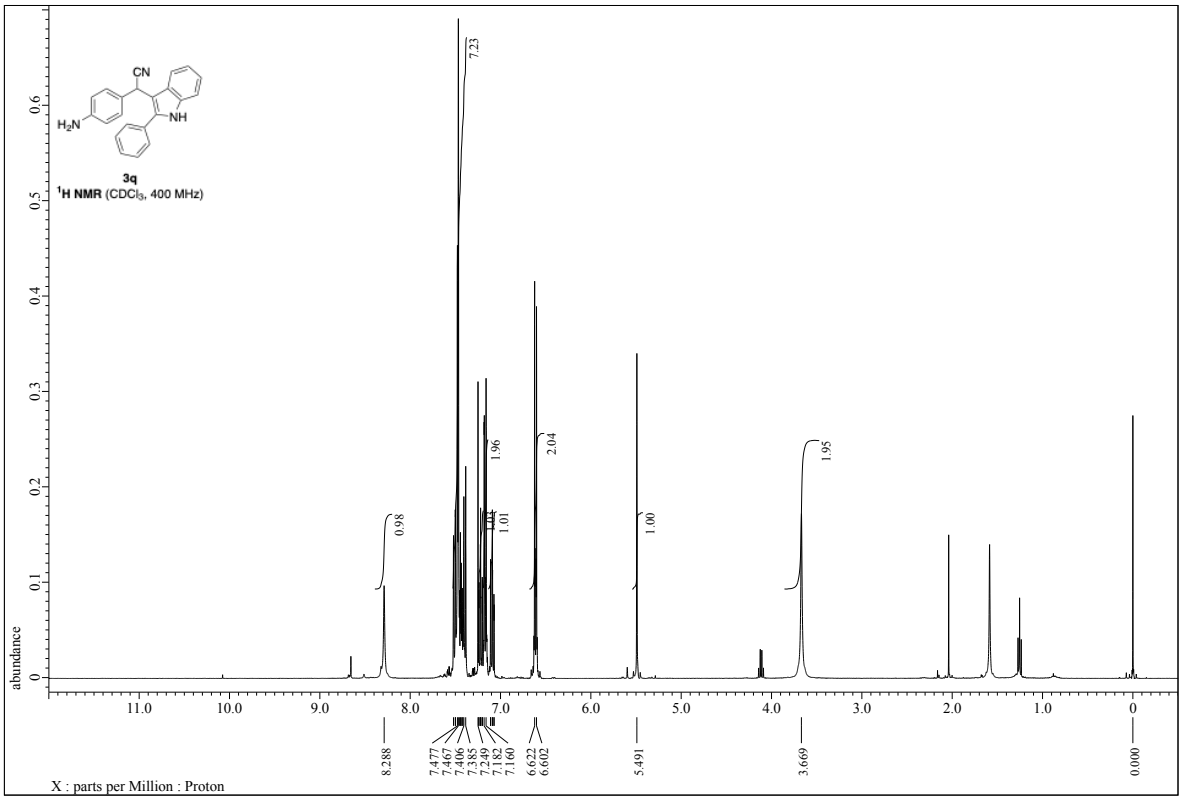

CN
NH
H2N
3m
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

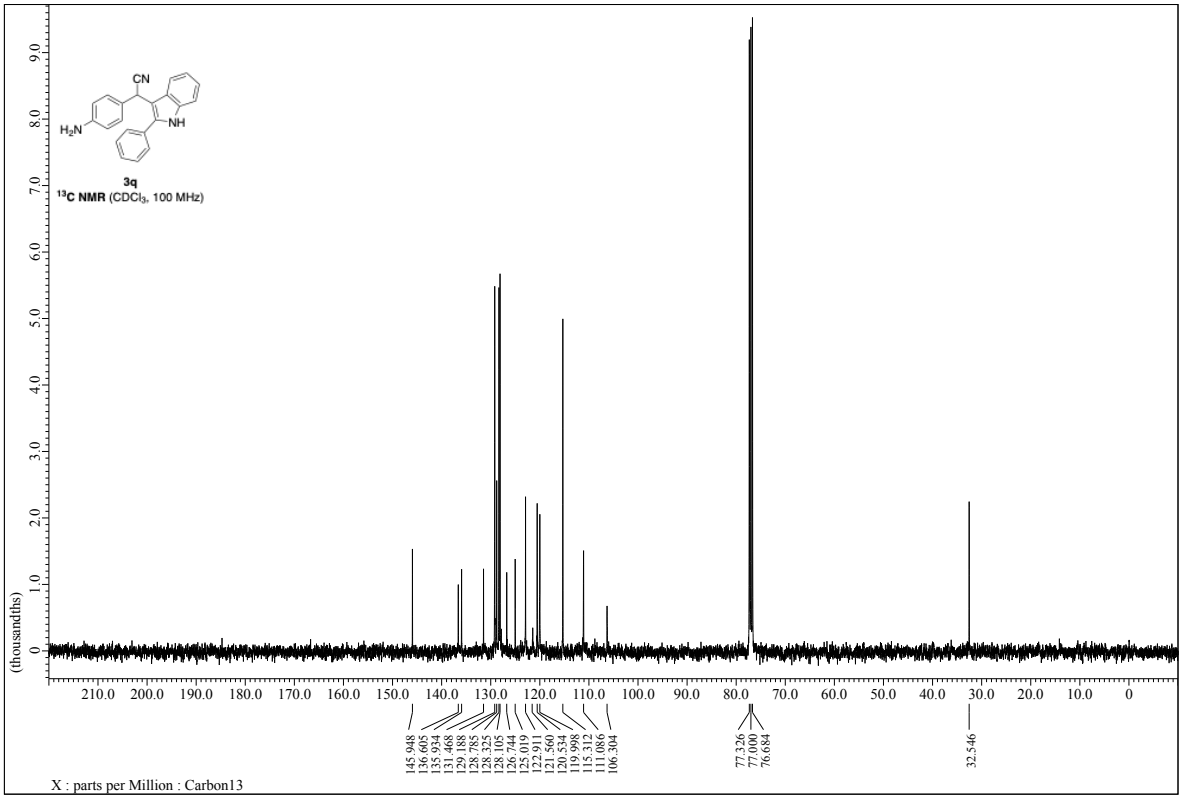

3o
^{1}H NMR (CDCl$_3$, 400 MHz)
abundance
X : parts per Million : Proton

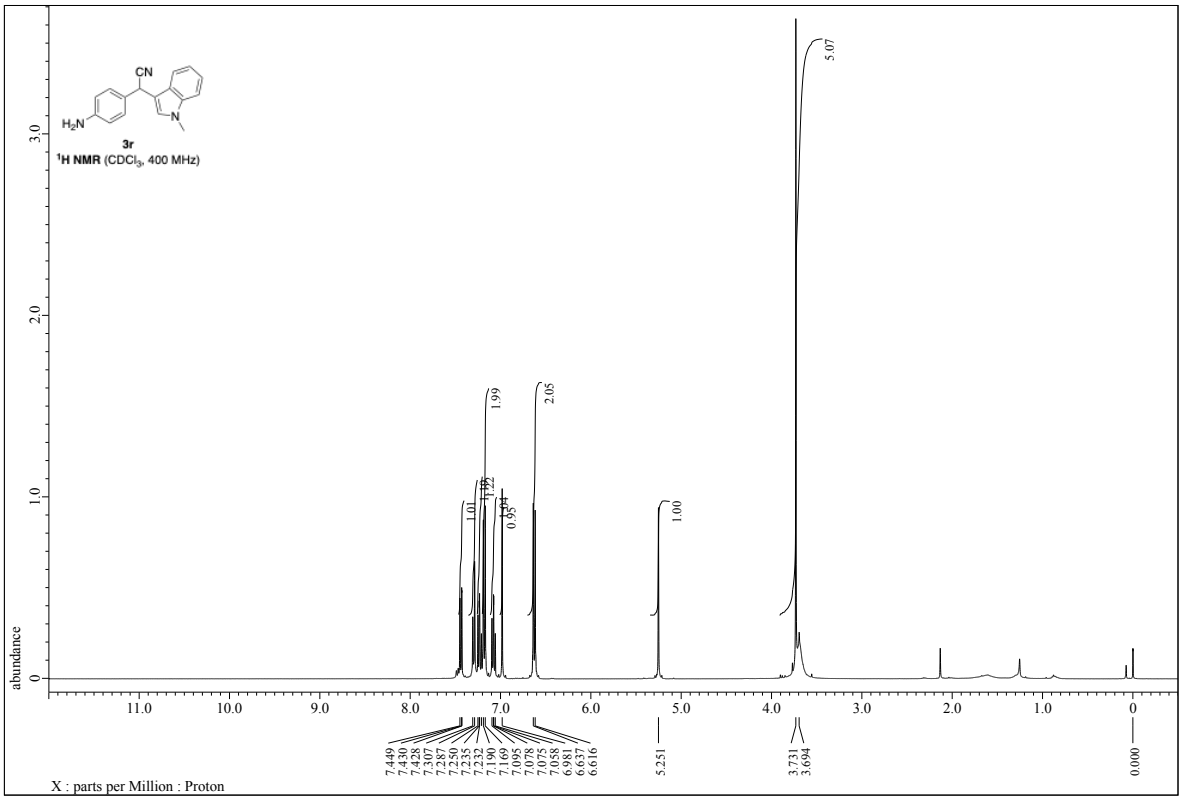

3o
^{13}C NMR (CDCl$_3$, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

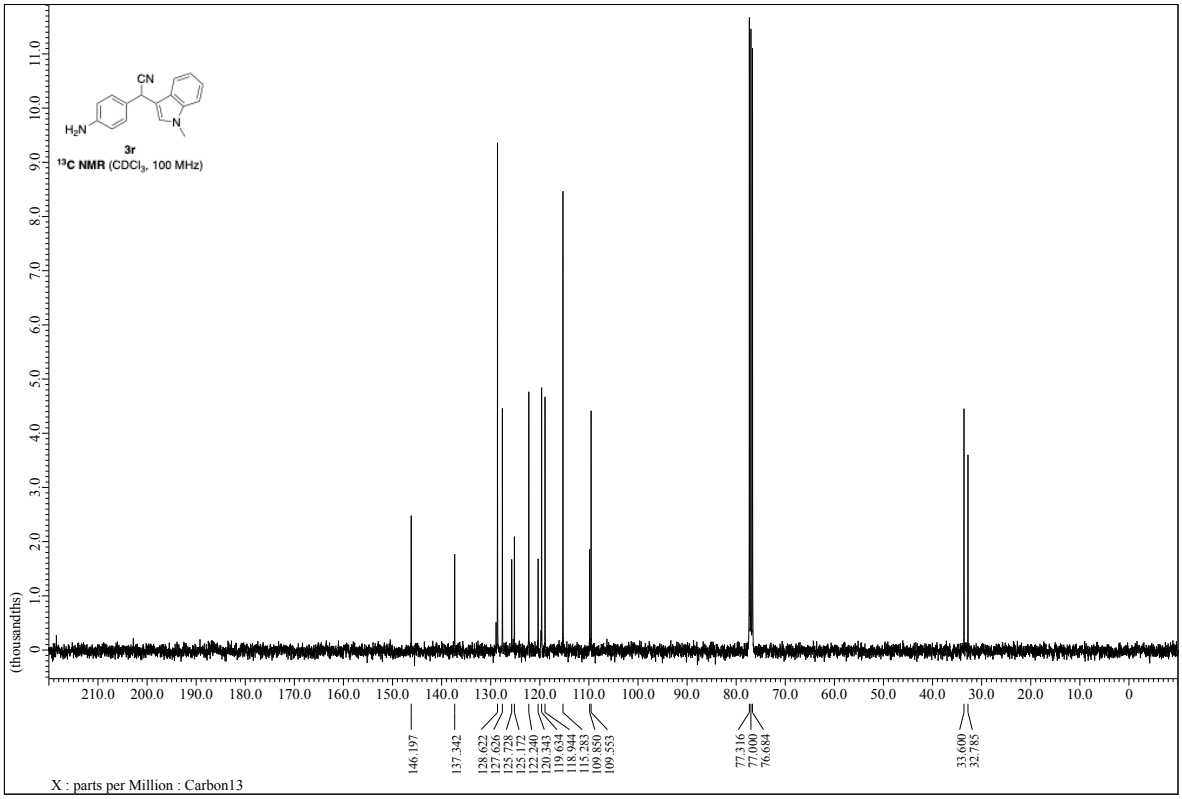

CN
H2N
NH
3p
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

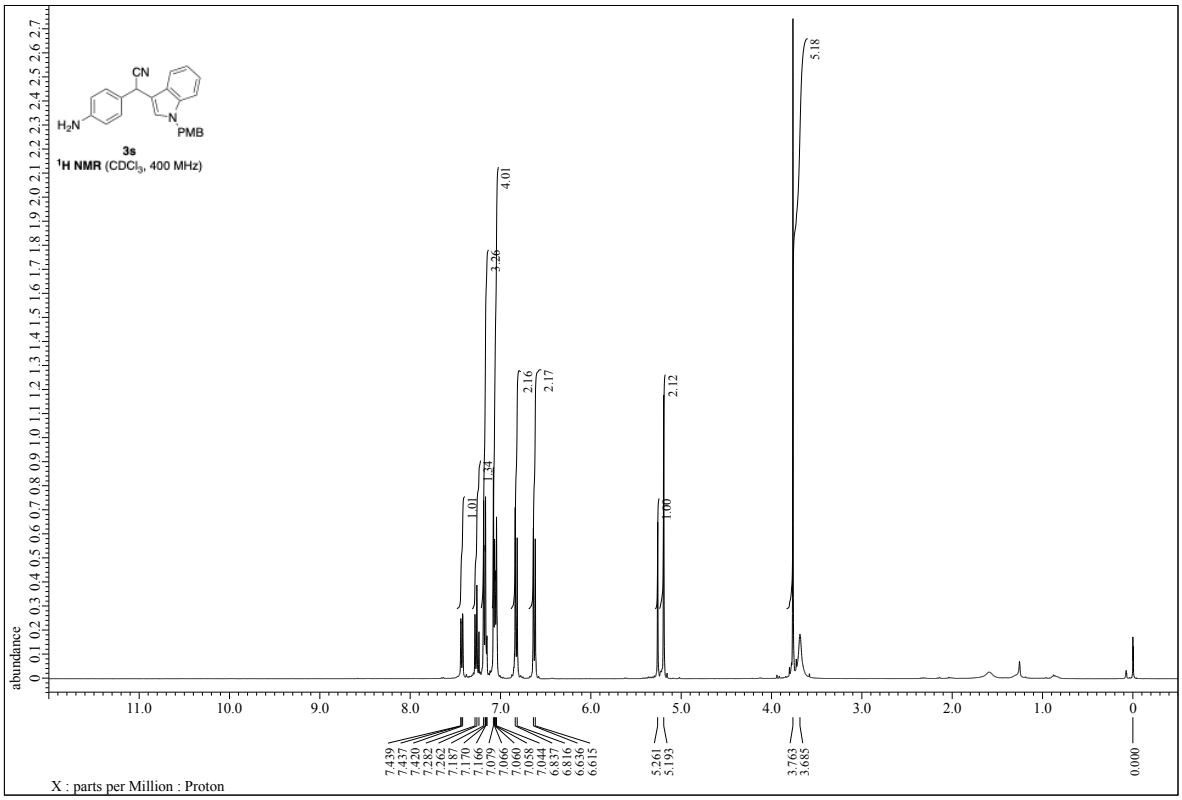

CN
H2N
NH
3p
13C NMR (DMSO-d6, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

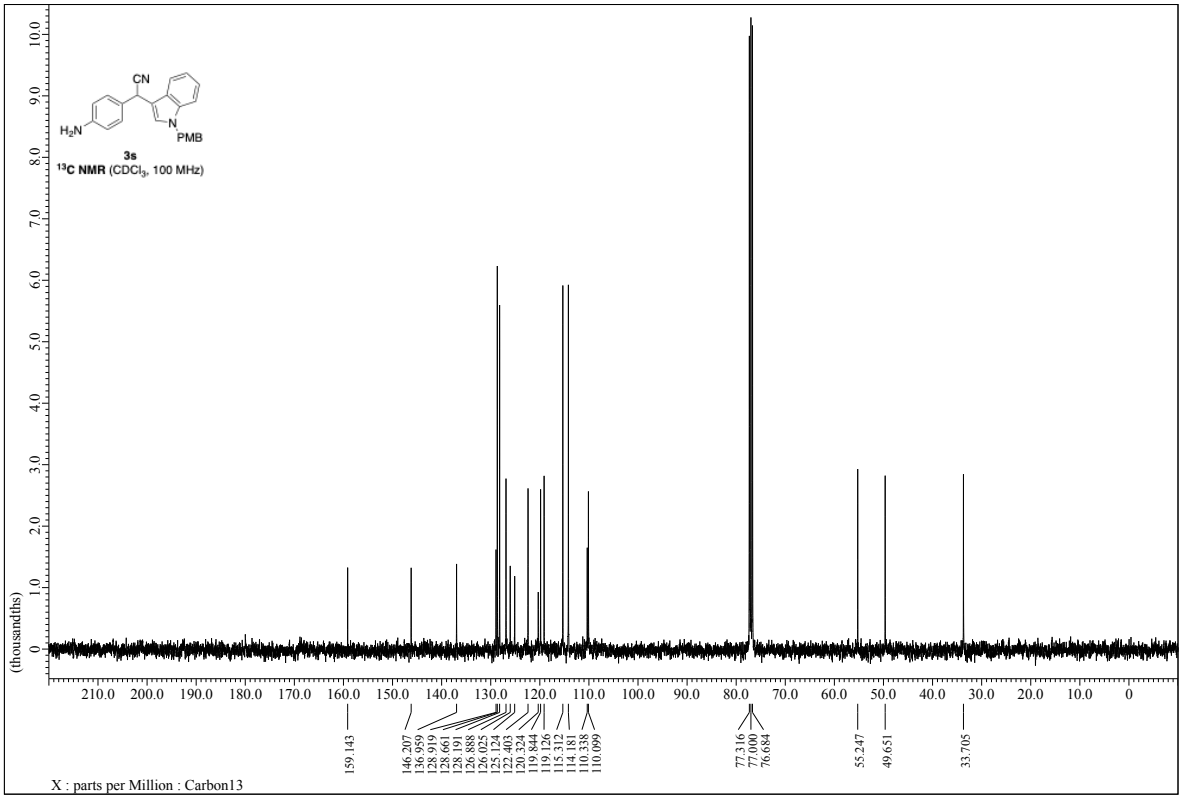

CN
H2N
NH
3q
1H NMR (CDCl3, 400 MHz)
abundance
7.23
1.96
2.04
1.95
0.98
1.04
1.01
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.288
7.477
7.467
7.406
7.385
7.249
7.182
7.160
6.622
6.602
5.491
3.669
0.000
X : parts per Million : Proton

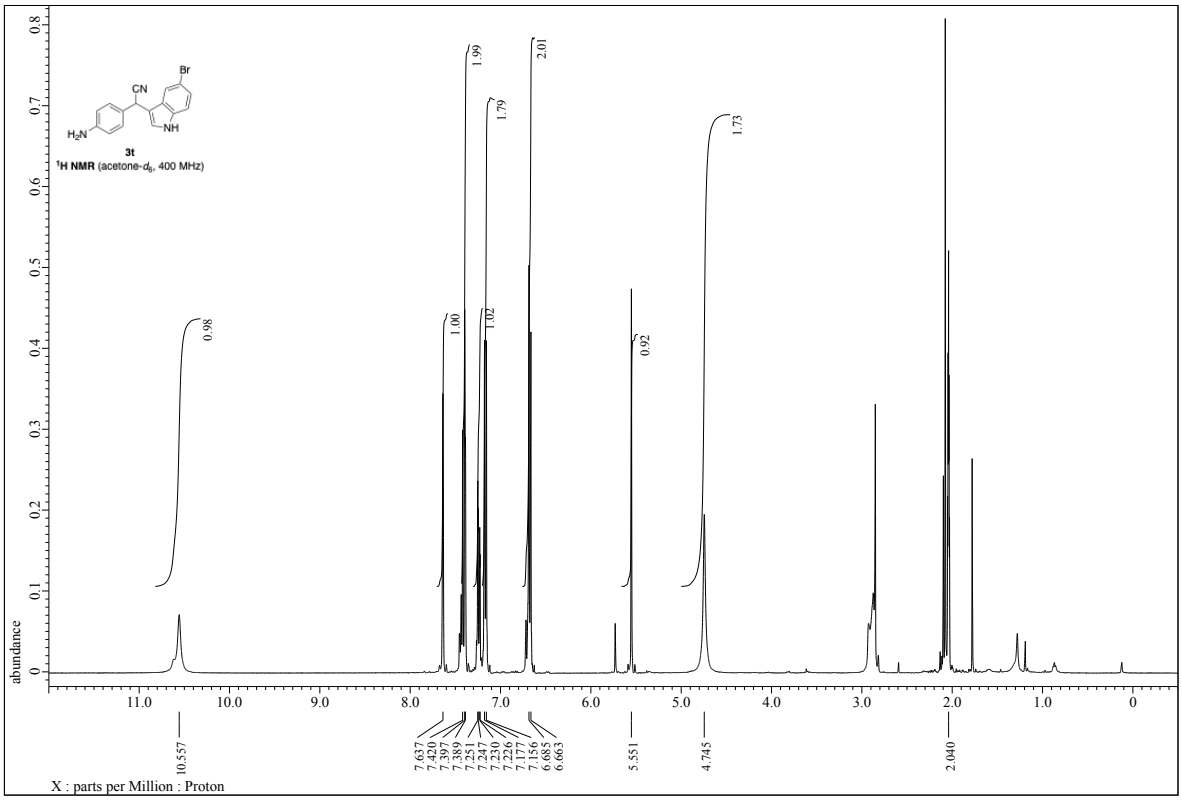

CN
H2N
NH
3q
13C NMR (CDCl3, 100 MHz)
(thousandths)
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
145.948
136.605
135.934
131.468
129.188
128.785
128.325
128.105
126.744
125.019
122.911
121.560
120.534
119.998
115.312
111.086
106.304
77.326
77.000
76.684
32.546
X : parts per Million : Carbon13

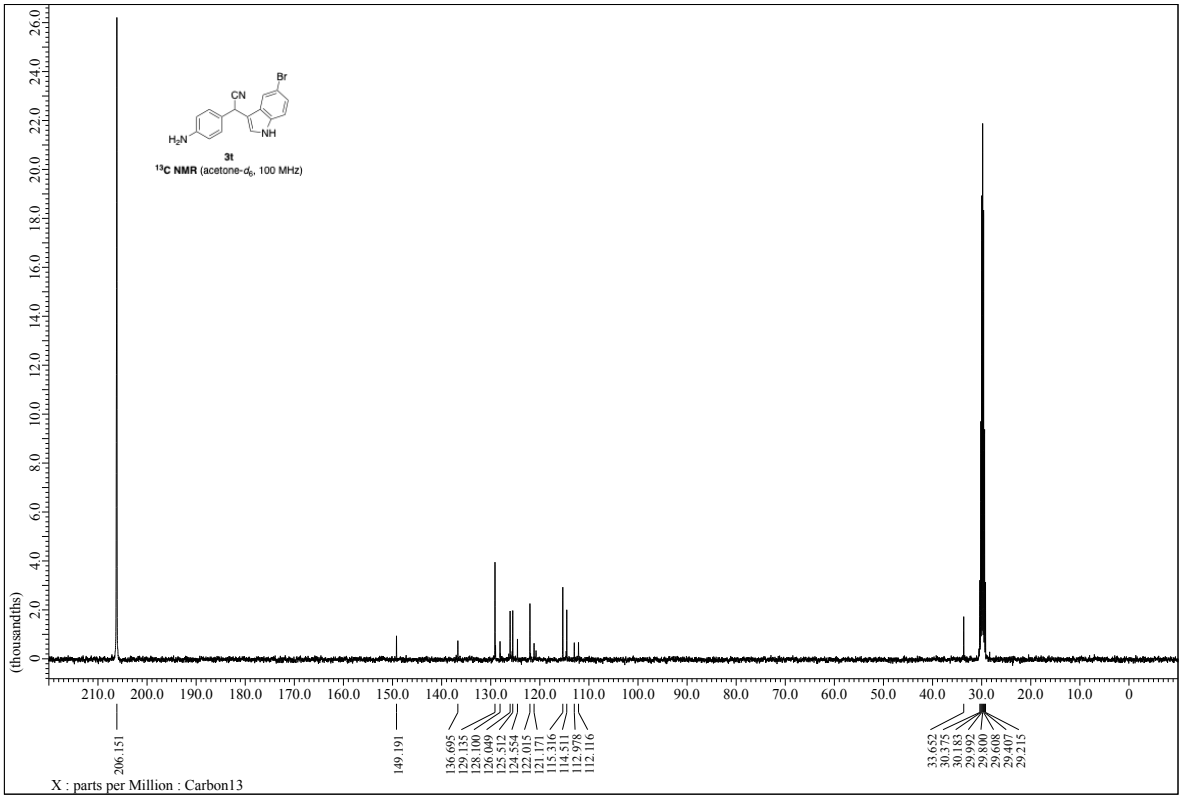

CN
H2N
N
3r
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton

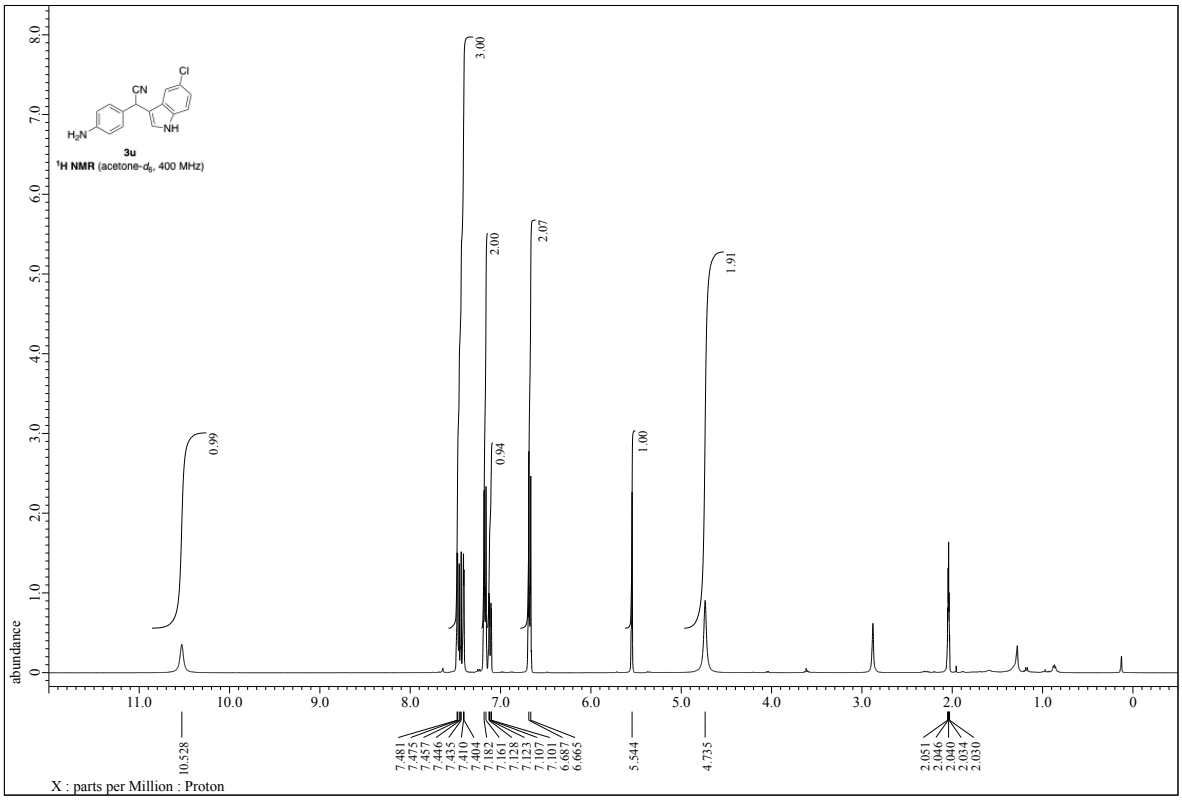

CN
H2N
N
3r
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13

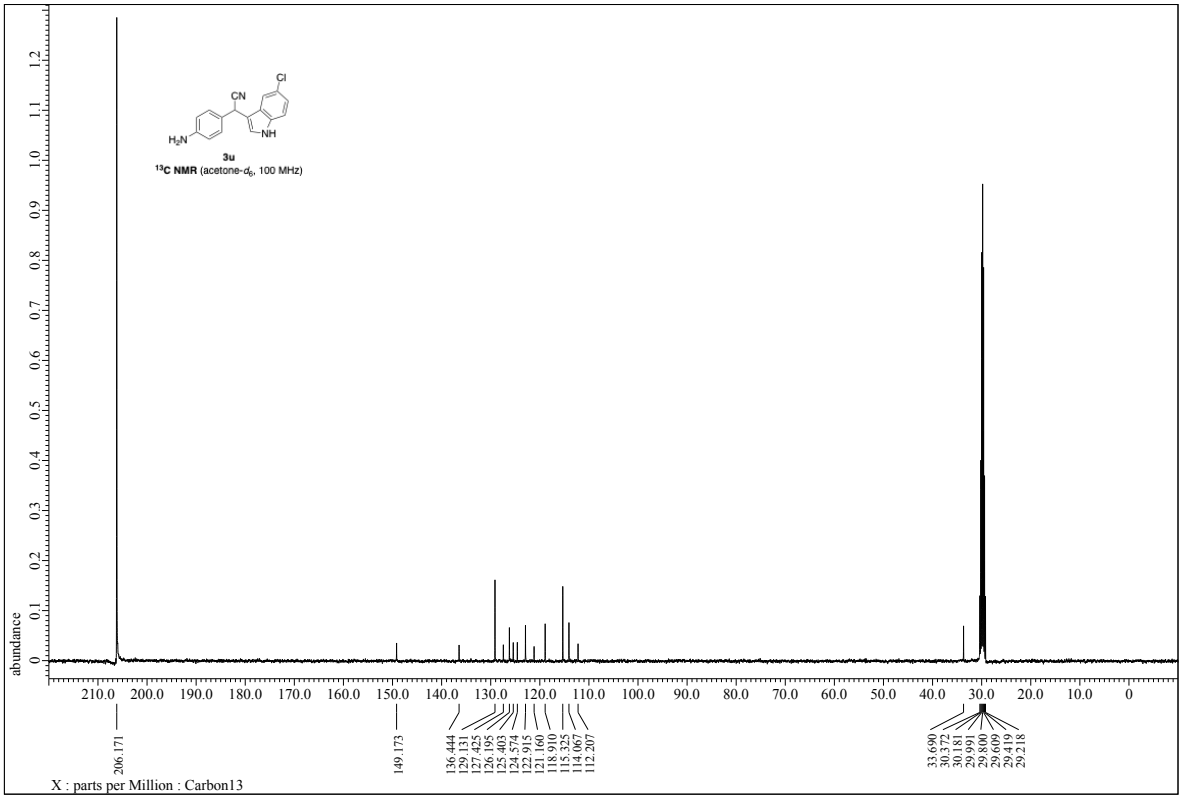

CN
H2N
N
PMB
3s
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton
7.439
7.437
7.430
7.282
7.262
7.187
7.170
7.166
7.079
7.066
7.060
7.038
7.044
6.837
6.816
6.636
6.615
5.261
5.193
3.763
3.685
0.000

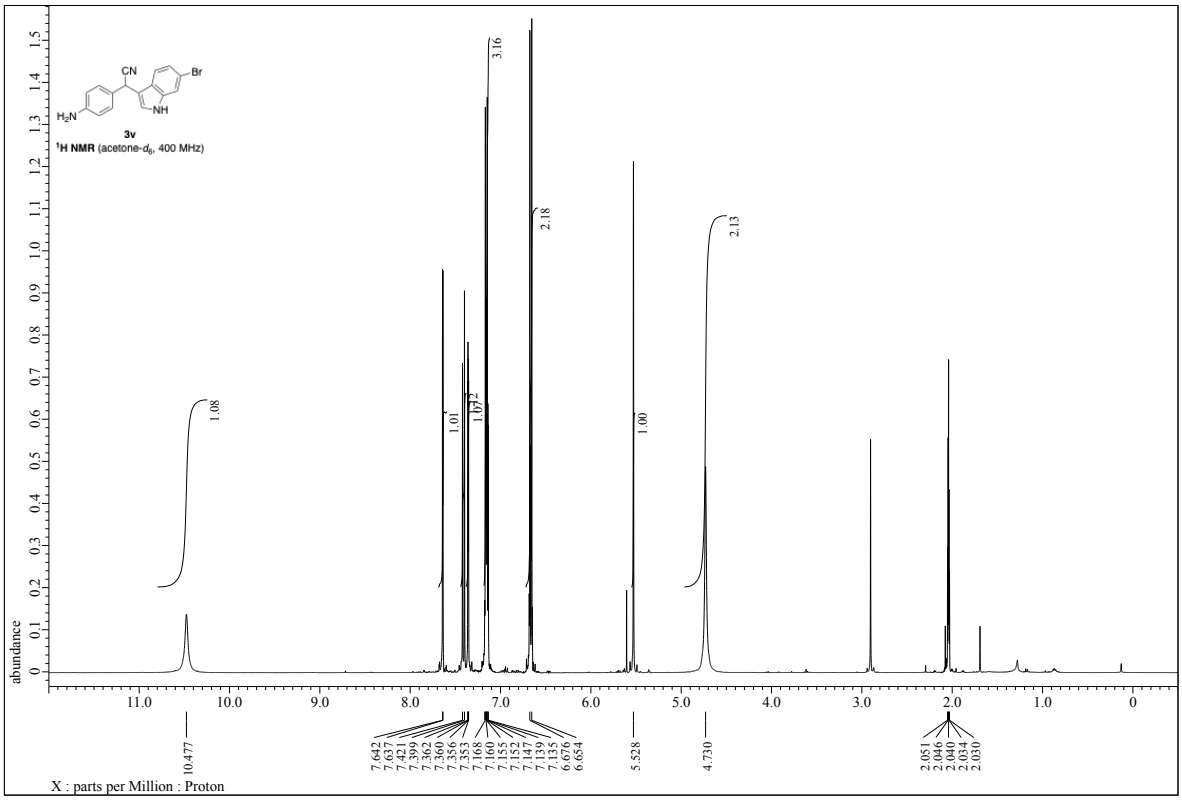

CN
H2N
N
PMB
3s
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13
159.143
146.207
136.959
128.919
128.661
128.310
126.888
126.025
125.124
122.403
120.324
119.844
119.126
115.312
114.181
110.338
110.099
77.316
77.000
76.684
55.247
49.651
33.705

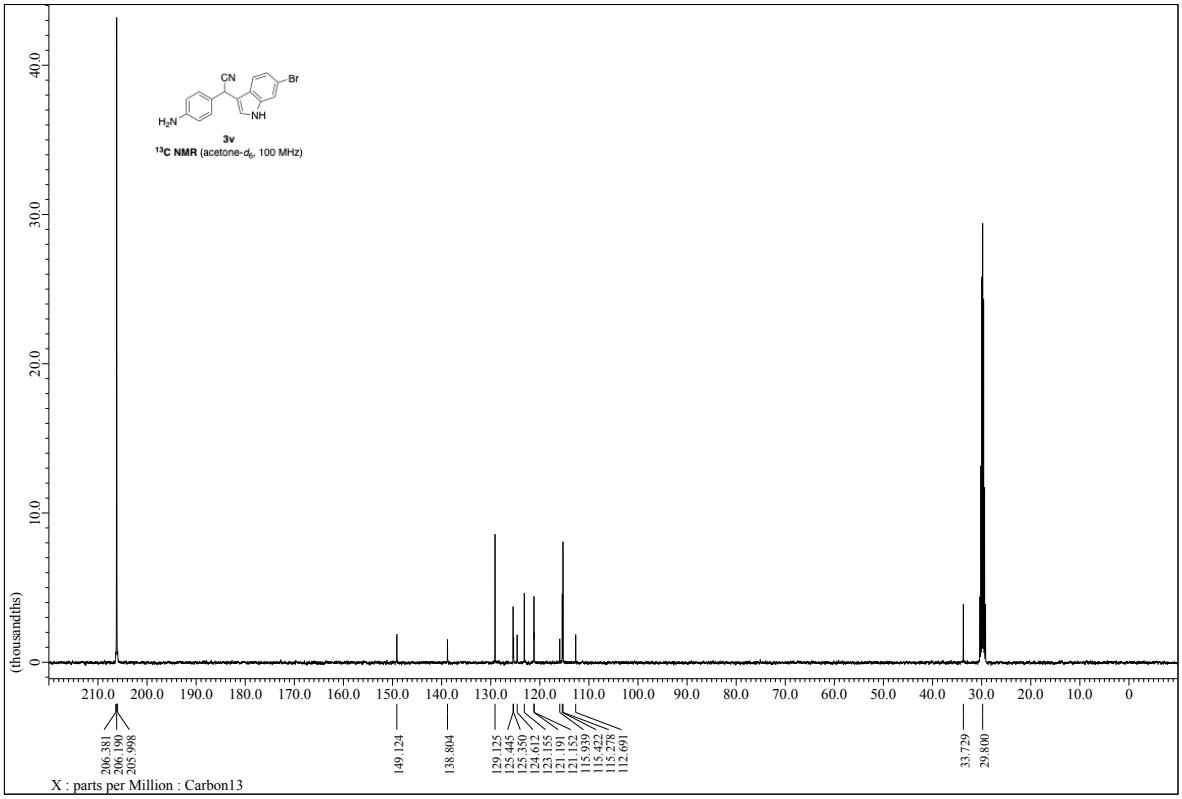

3t
¹H NMR (acetone-d6, 400 MHz)
abundance
0.98
1.00
1.02
1.99
1.79
2.01
0.92
1.73
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.557
7.637
7.420
7.390
7.251
7.247
7.230
7.226
7.177
7.156
6.685
6.663
5.551
4.745
2.040
X : parts per Million : Proton

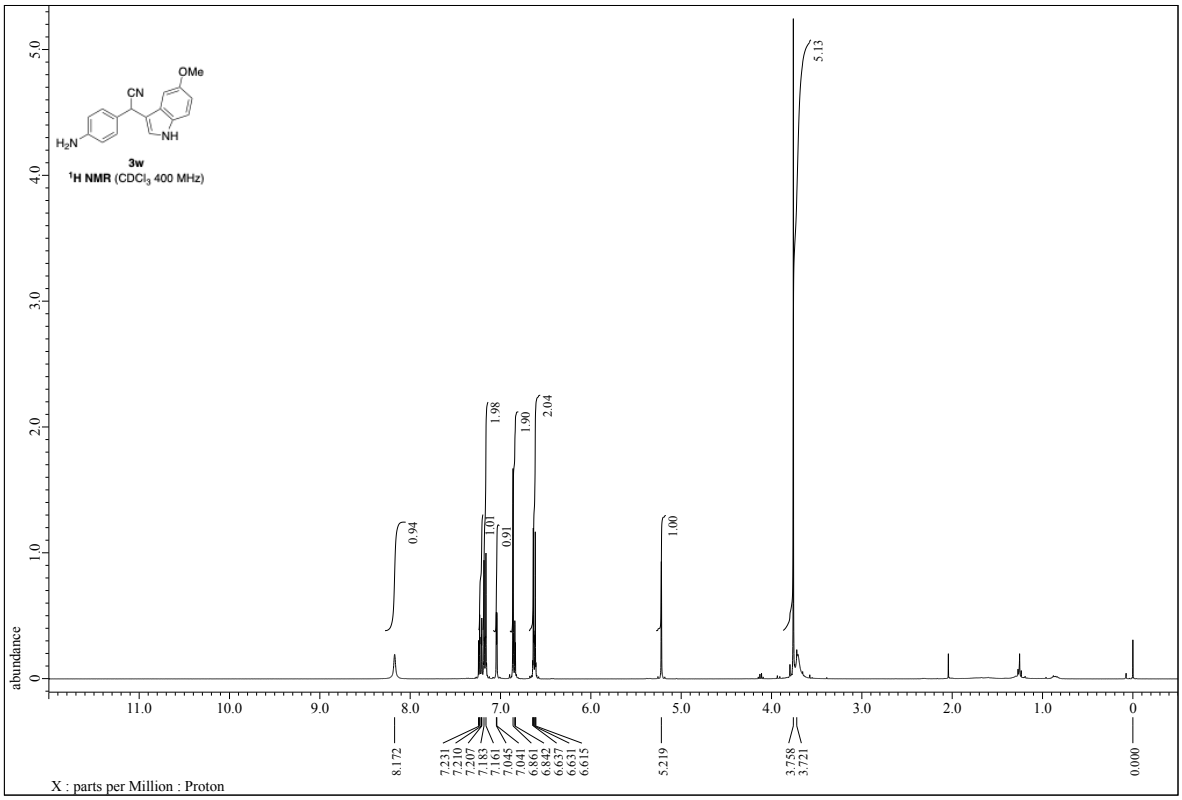

3t
¹³C NMR (acetone-d6, 100 MHz)
(thousandths)
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
206.151
149.191
136.695
129.135
128.100
126.049
125.512
124.554
122.015
121.171
115.316
114.511
112.978
112.116
33.652
30.375
30.183
29.992
29.800
29.608
29.407
29.215
X : parts per Million : Carbon13

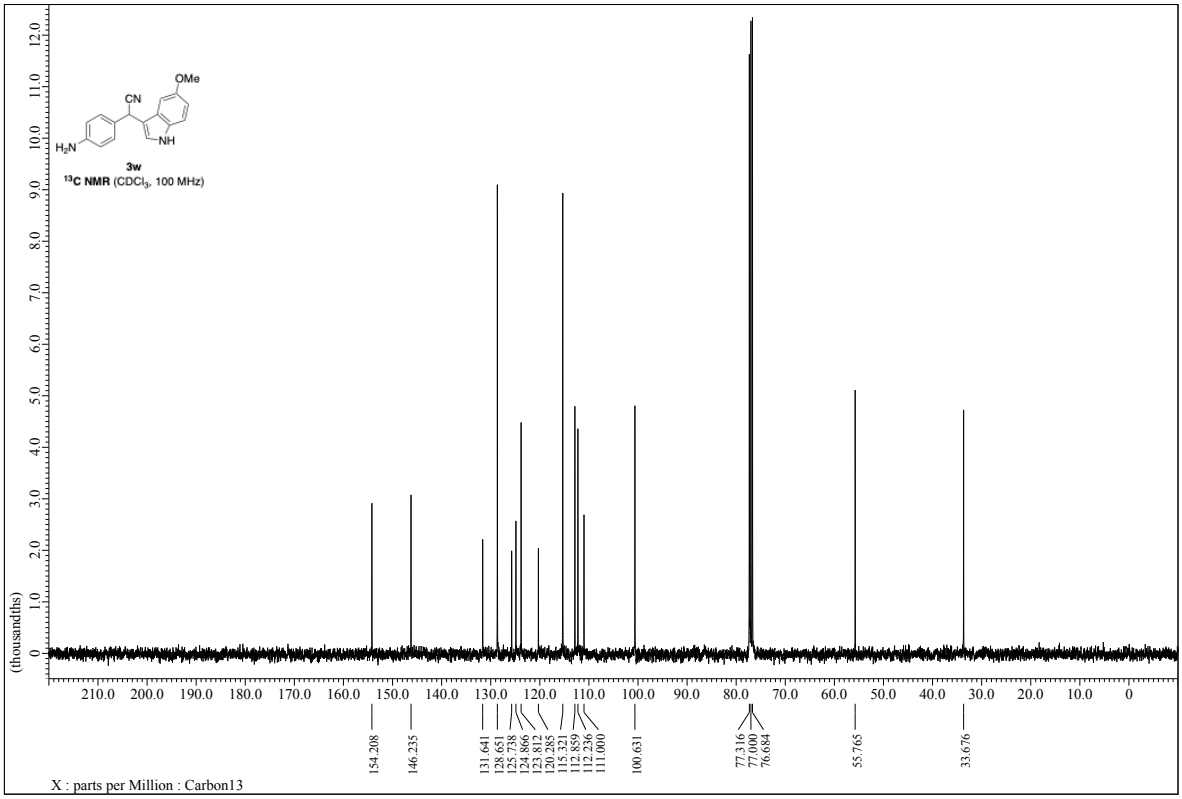

3u
¹H NMR (acetone-d6, 400 MHz)
abundance
X : parts per Million : Proton


3u
¹³C NMR (acetone-d6, 100 MHz)
abundance
X : parts per Million : Carbon13


3v
¹H NMR (acetone-d_6, 400 MHz)
abundance
X : parts per Million : Proton


3v
¹³C NMR (acetone-d_6, 100 MHz)
(thousandths)
X : parts per Million : Carbon13


OMe
CN
NH
H2N
3w
1H NMR (CDCl3 400 MHz)
abundance
X : parts per Million : Proton


OMe
CN
NH
H2N
3w
13C NMR (CDCl3, 100 MHz)
(thousandths)
X : parts per Million : Carbon13