Green Chemistry

Electronic Supporting Information

Thiazolyl-phosphine hydrochloride salts: Effective auxiliary ligands for ruthenium-catalyzed nitrile hydration reactions and related amide bond forming processes in water

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An ORTEP plot of the structure of tris(5-(2-aminothiazolyl))phosphine trihydrochloride (6), with selected bonding parameters listed in the caption, and copies of the NMR spectra of selected amides synthesized in this work.

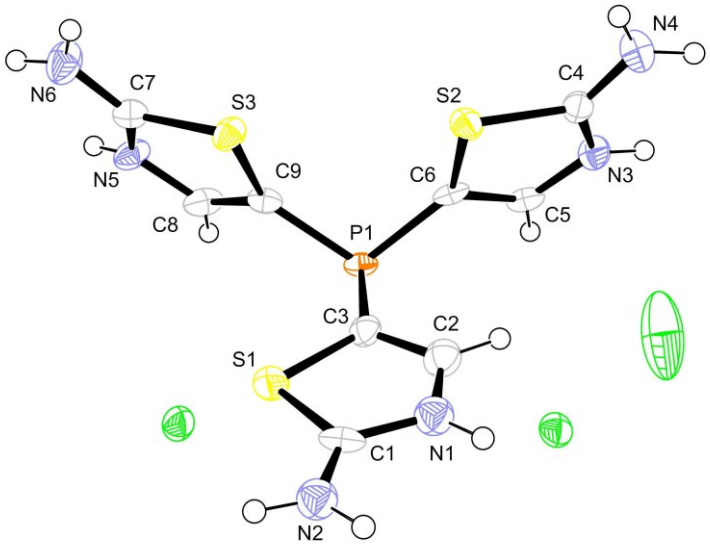
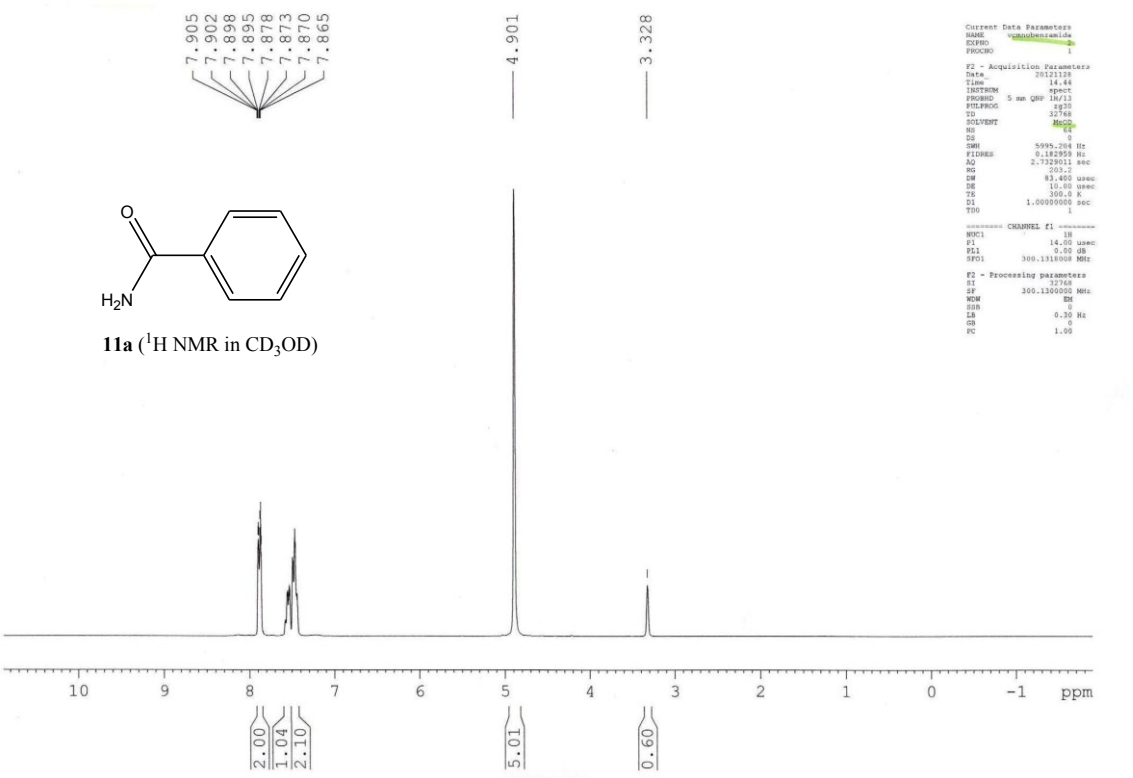
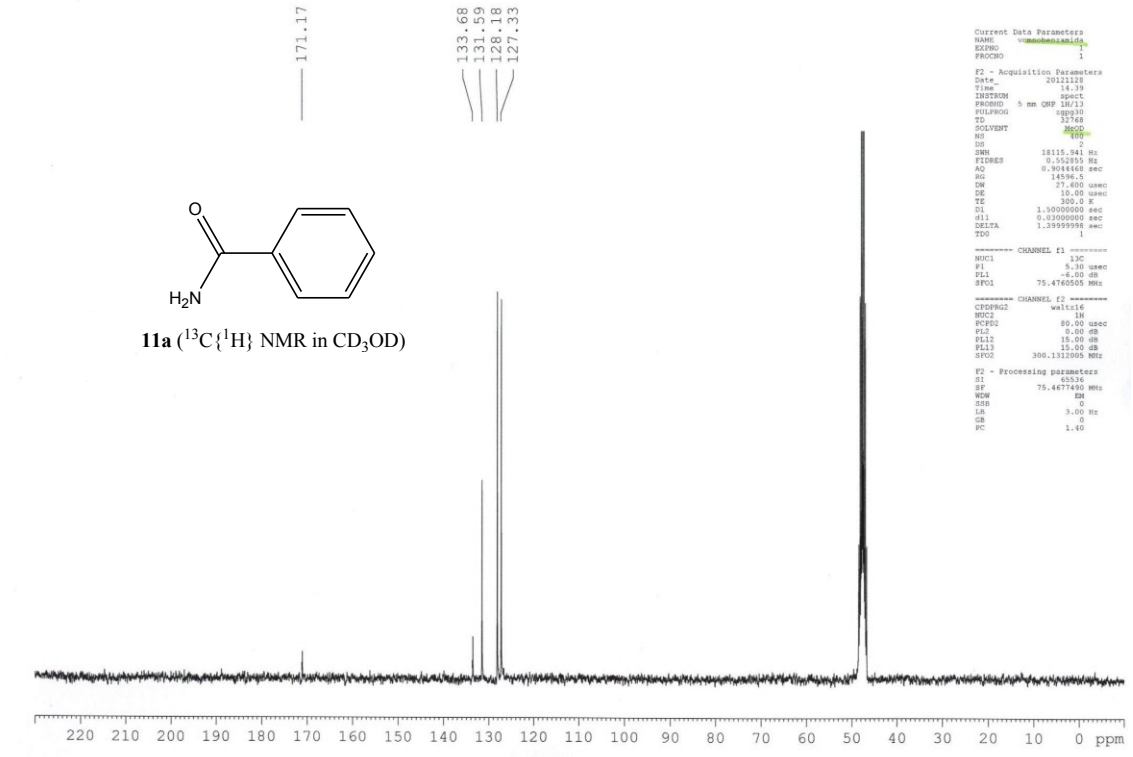


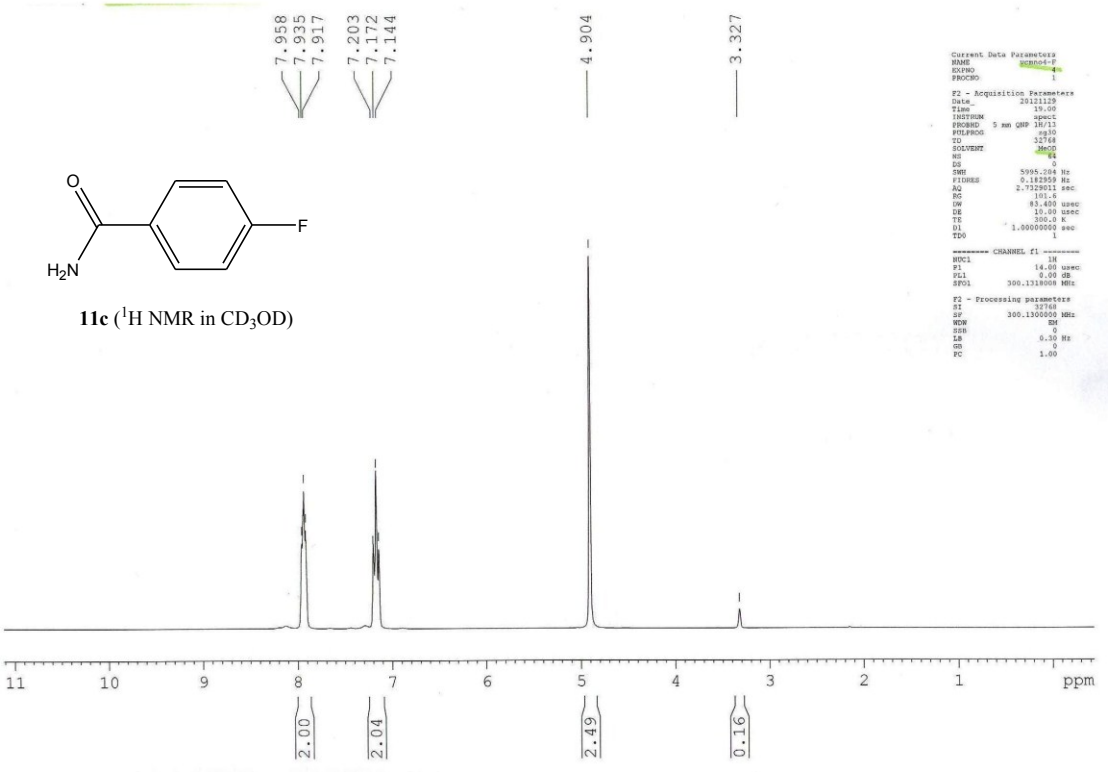
Fig. S1 ORTEP-type view of the structure of tris(5-(2-aminothiazolyl))phosphine trihydrochloride (**6**) showing the crystallographic labeling scheme. Thermal ellipsoids are drawn at 20% probability level. Selected bond lengths (Å): P(1)-C(3) = 1.825(7); P(1)-C(6) = 1.805(7); P(1)-C(9) = 1.793(7); C(1)-N(1) = 1.350(9); C(1)-N(2) = 1.307(9); N(1)-C(2) = 1.315(9); C(2)-C(3) = 1.345(9); C(3)-S(1) = 1.753(6); S(1)-C(1) = 1.709(7); Selected bond angles (º): C(3)-P(1)-C(6) = 95.2(3); C(3)-P(1)-C(9) = 102.3(3); C(6)-P(1)-C(9) = 105.9(3); N(1)-C(1)-N(2) = 121.9(7); C(1)-N(1)-C(2) = 114.3(6); N(1)-C(2)-C(3) = 116.8(7); C(2)-C(3)-S(1) = 107.5(5); C(3)-S(1)-C(1) = 91.3(3); S(1)-C(1)-N(2) = 127.9(6).



11a (^{1}H NMR in CD_3OD)



11a ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



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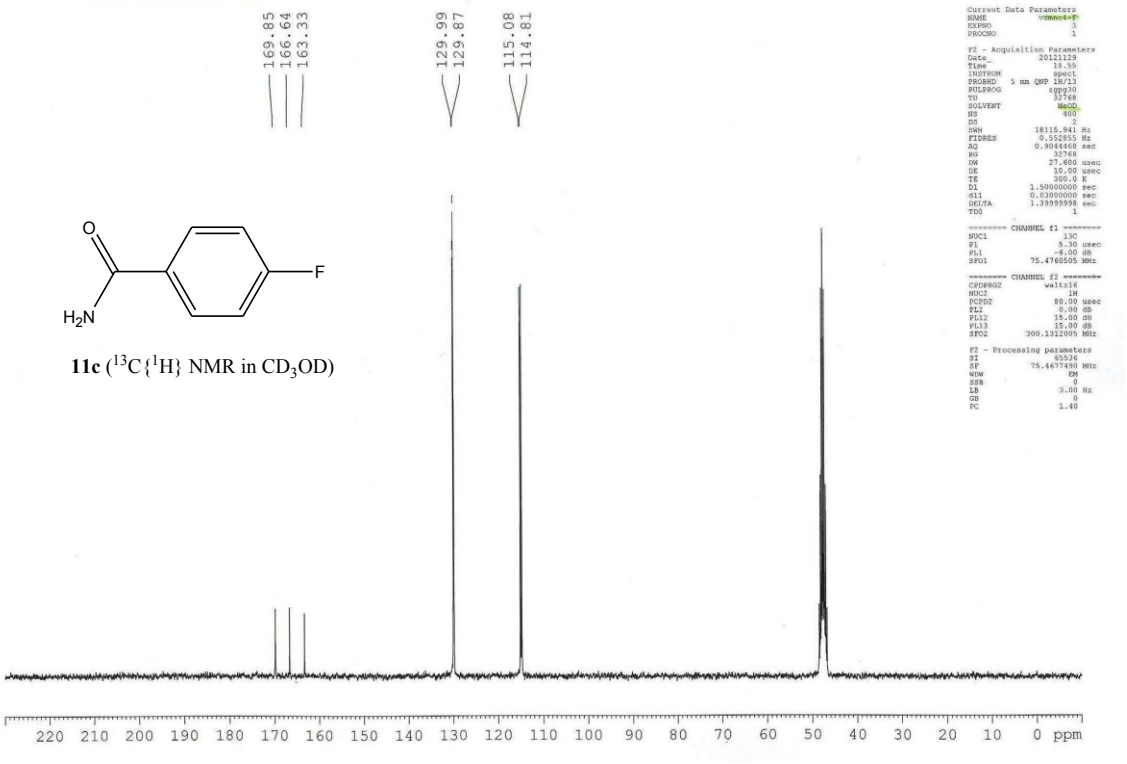

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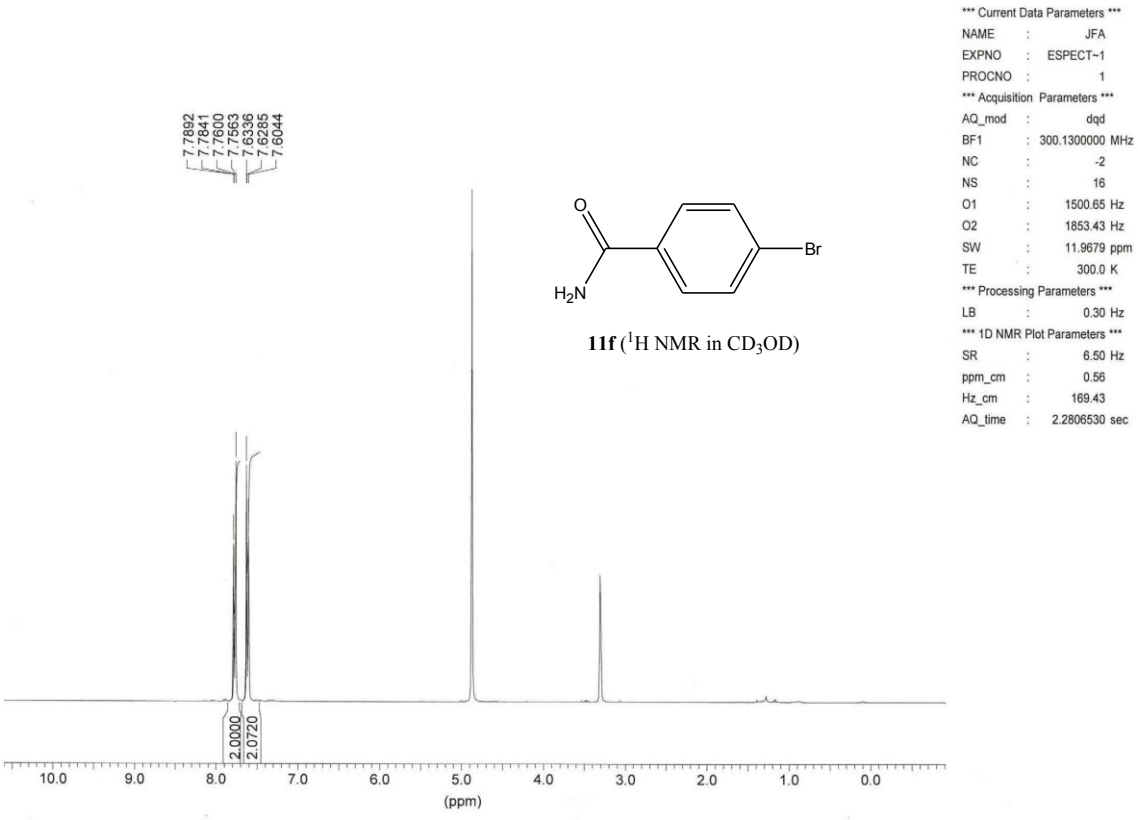

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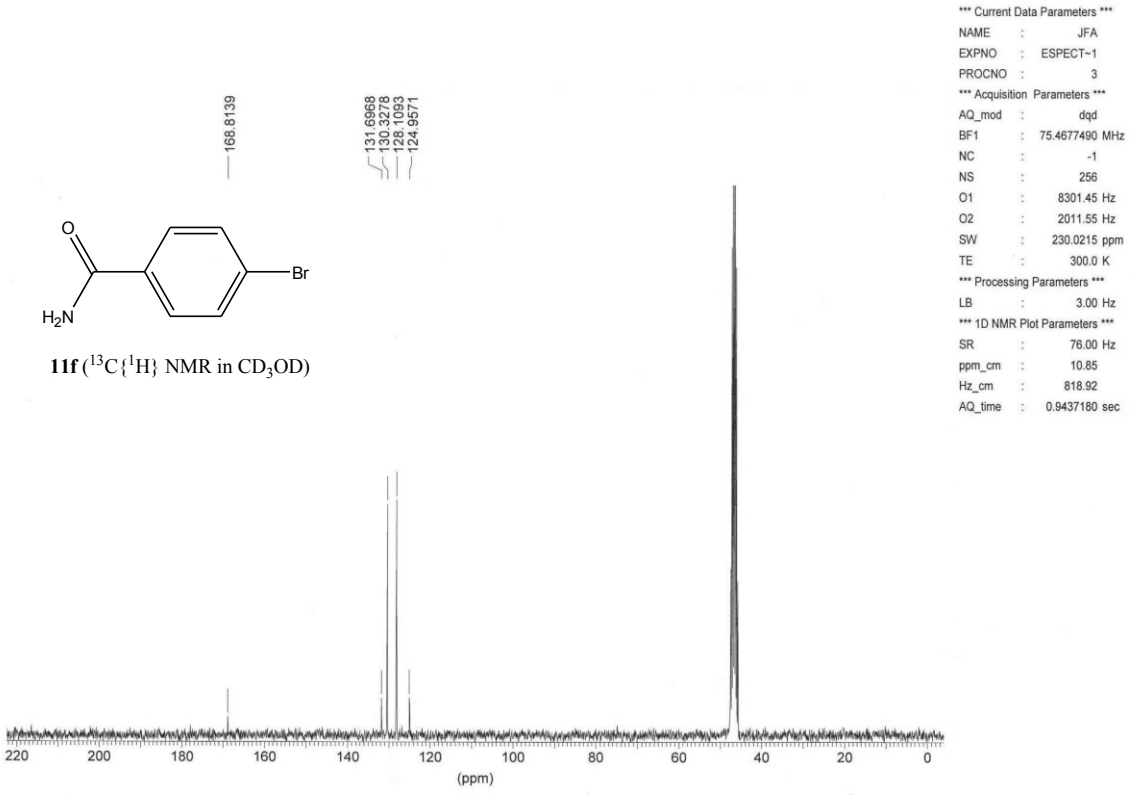
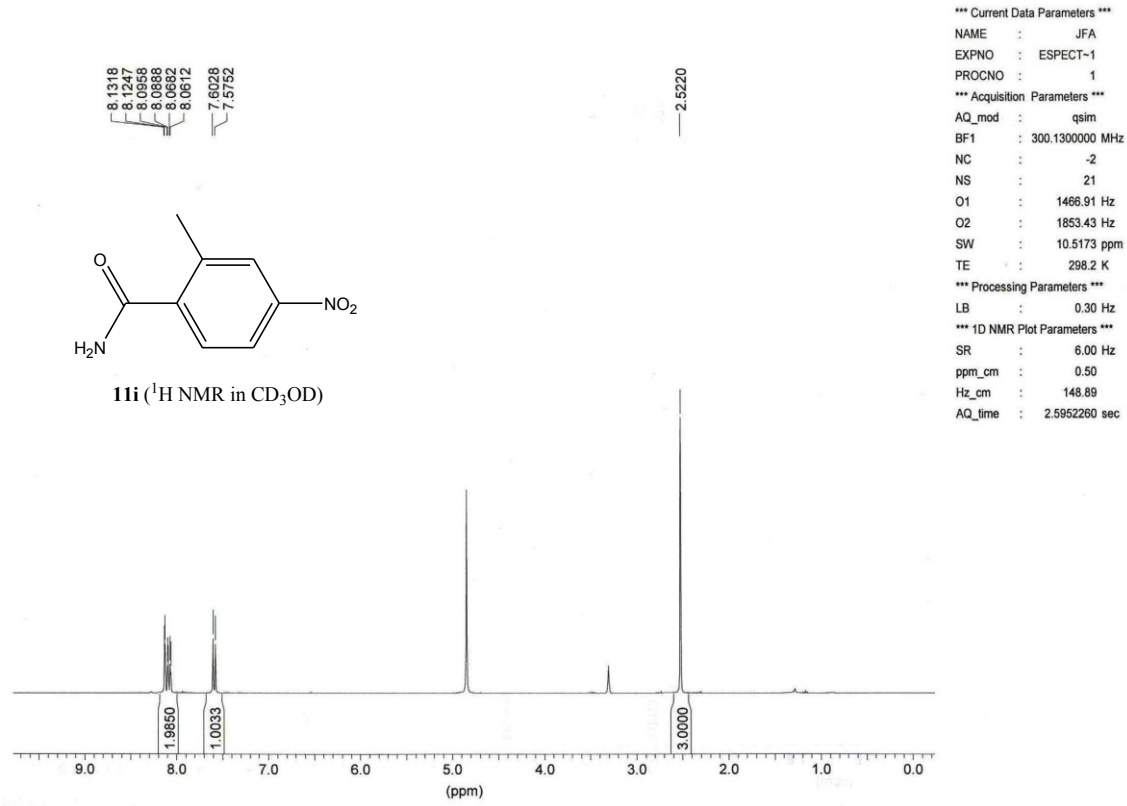
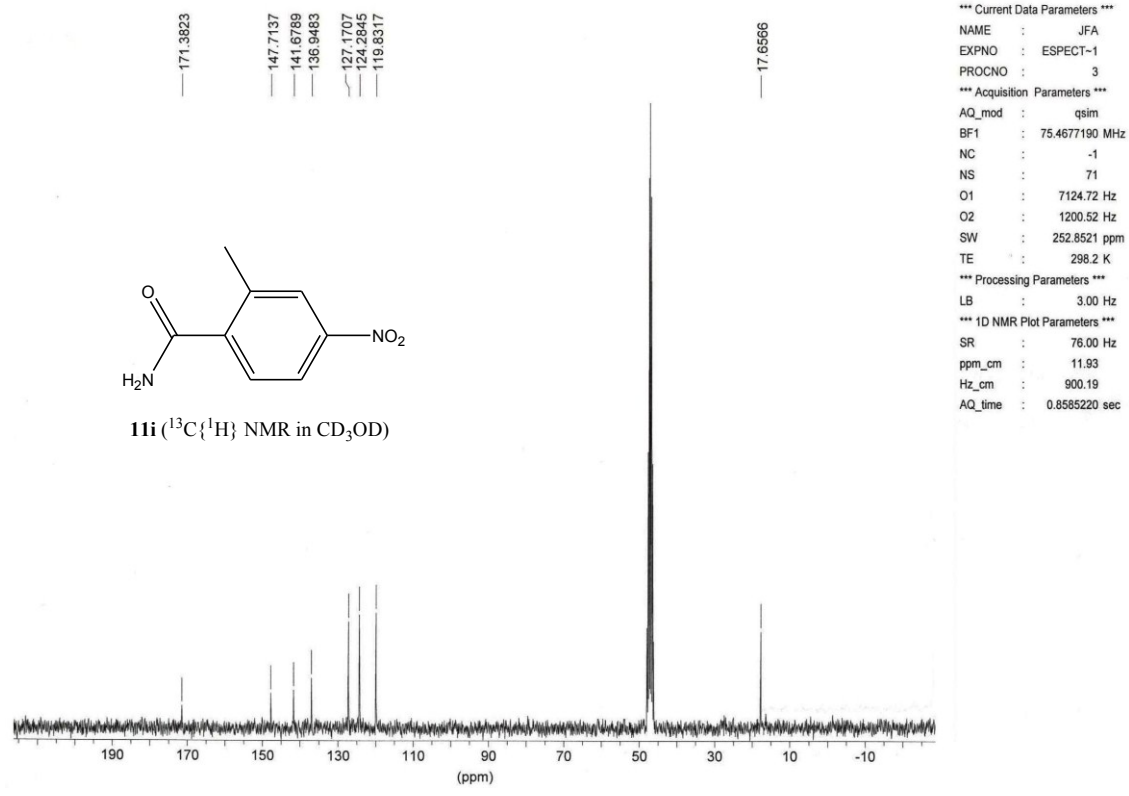


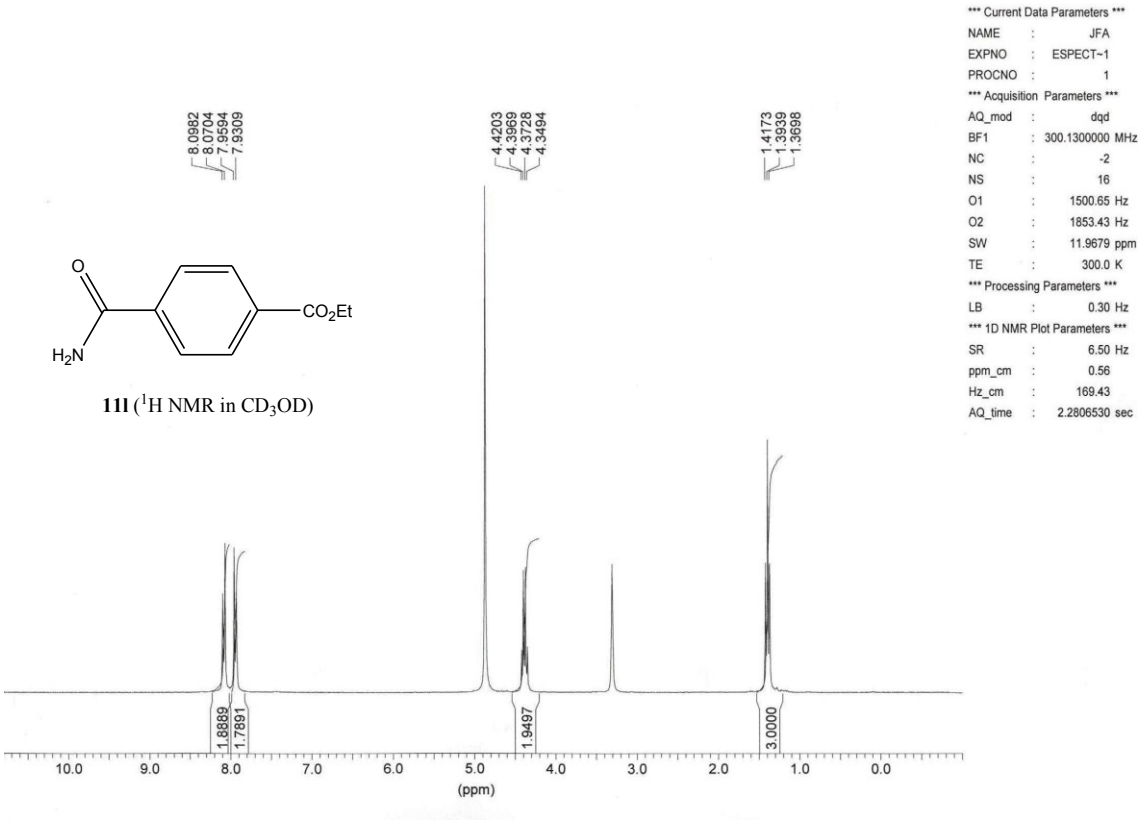
11f ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



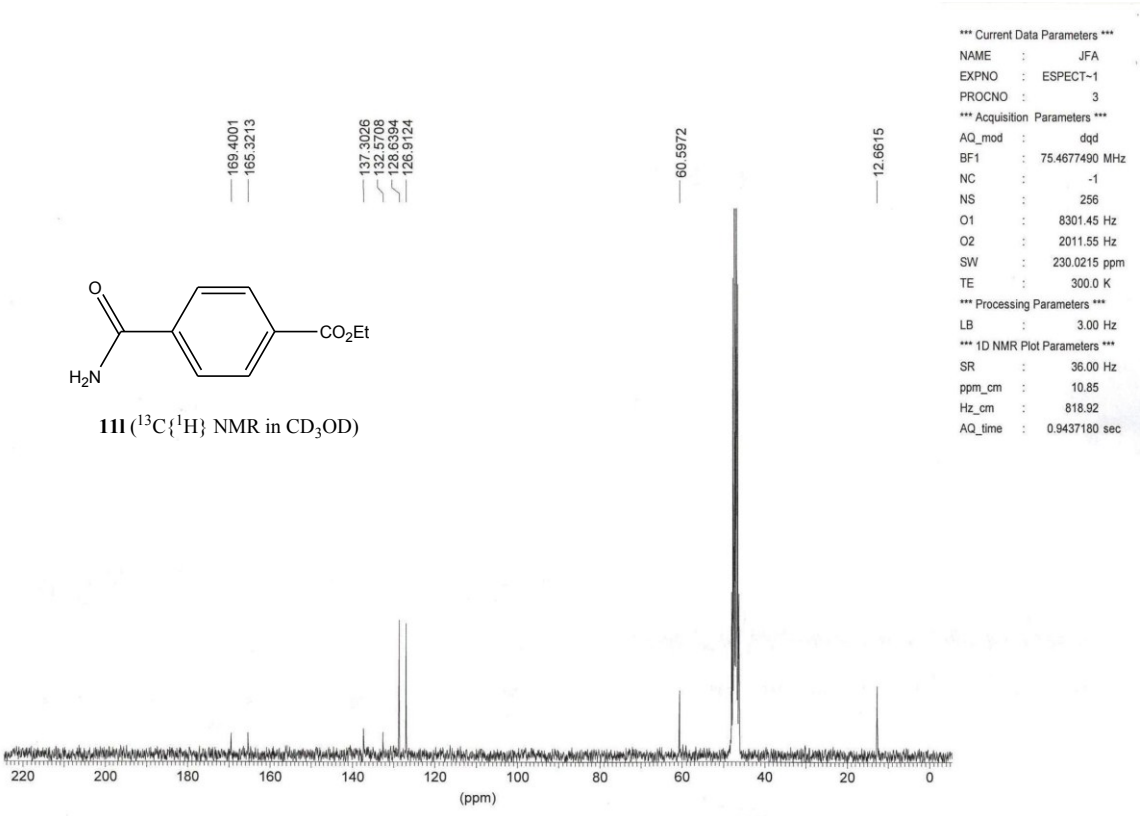
11i (^{1}H NMR in CD_3OD)



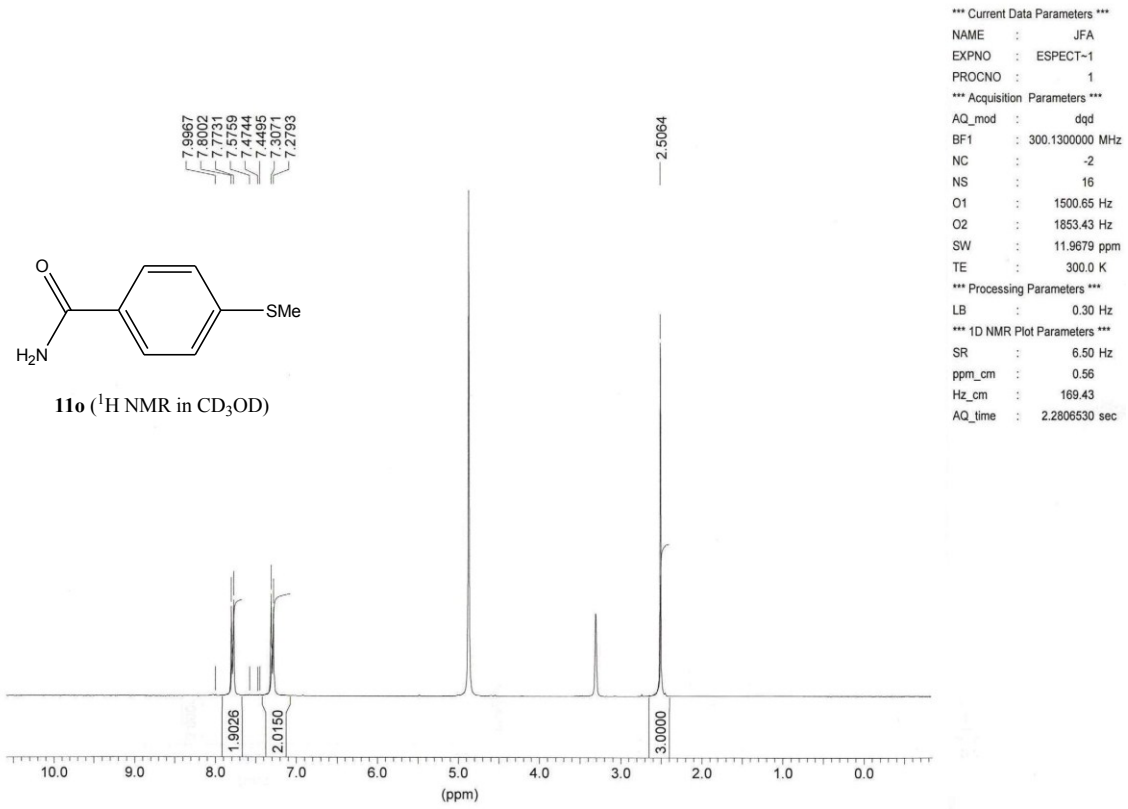
11i ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



11l (^{1}H NMR in CD_3OD)



11l ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



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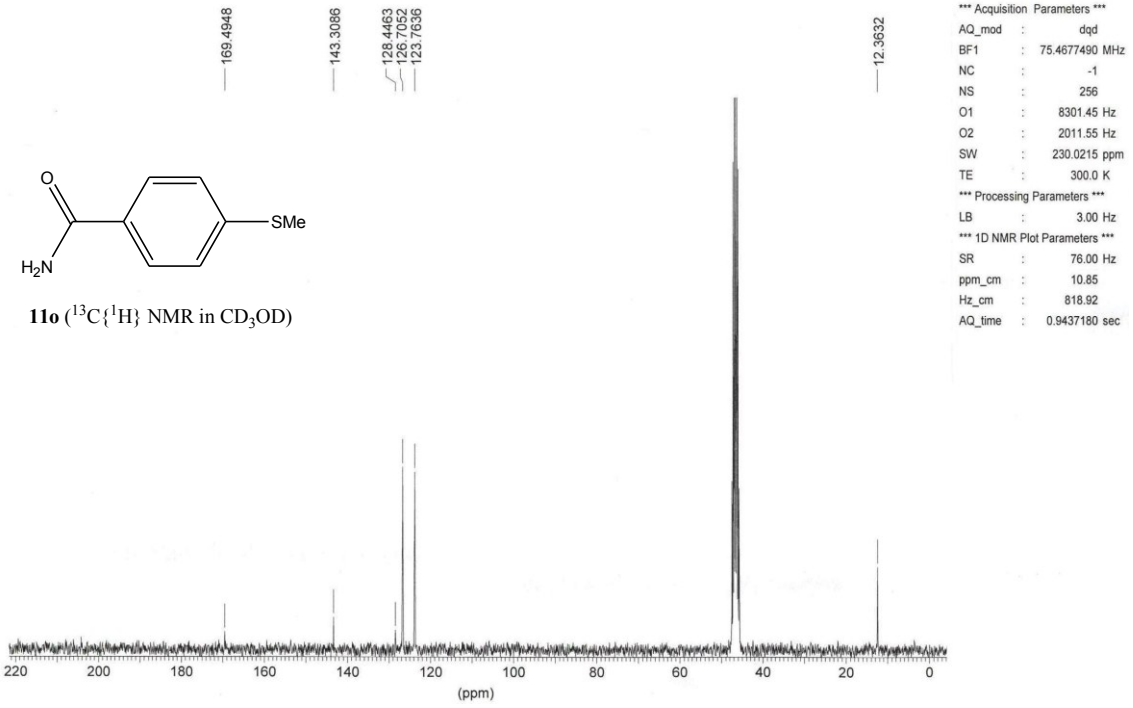
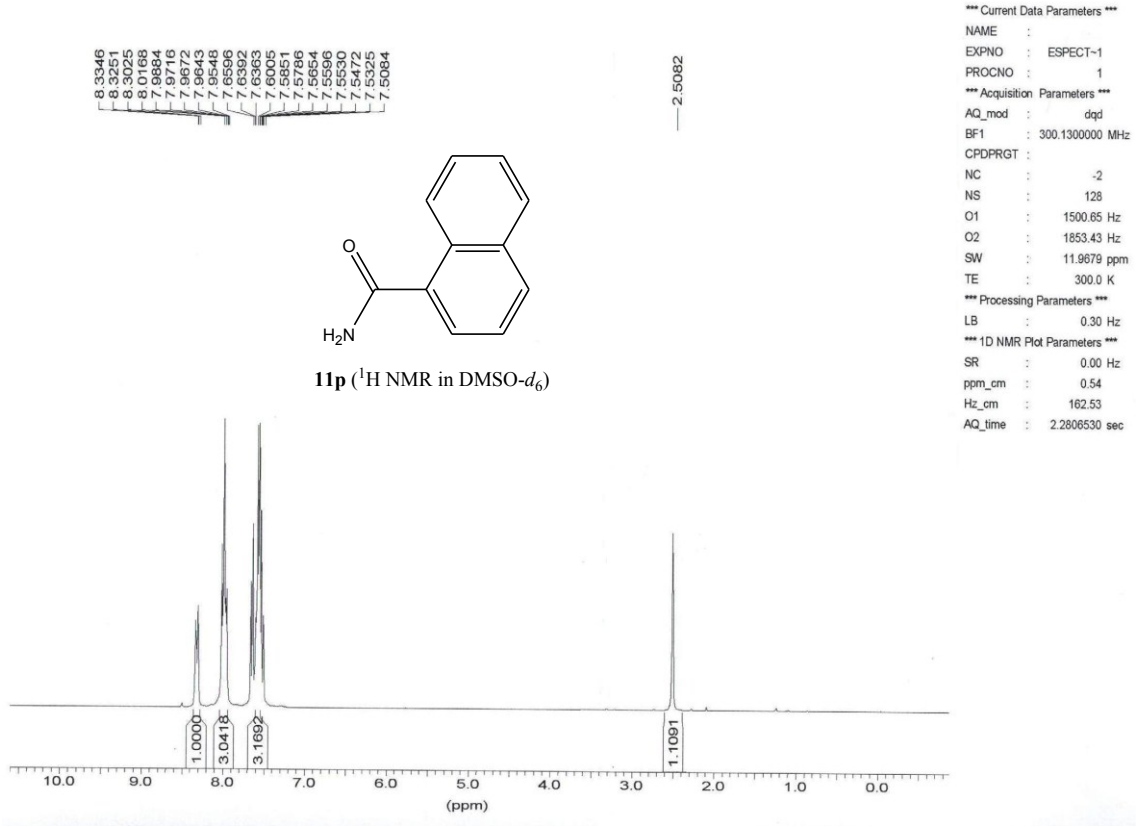
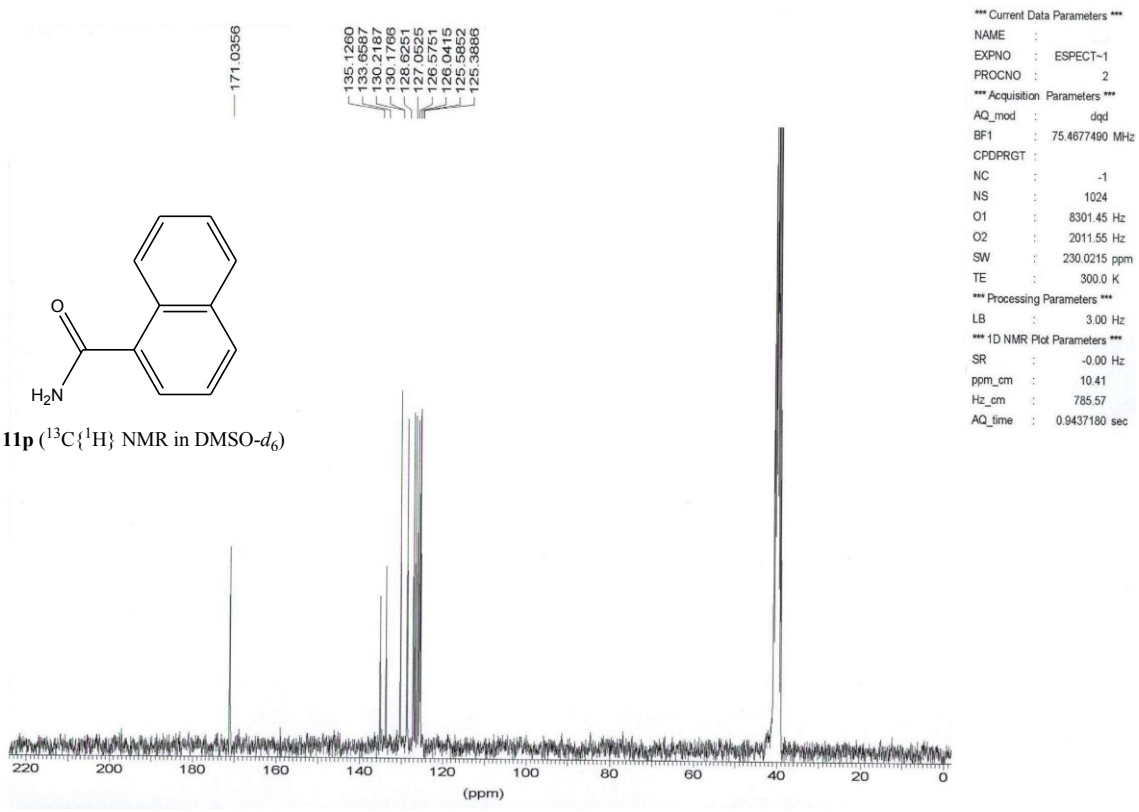


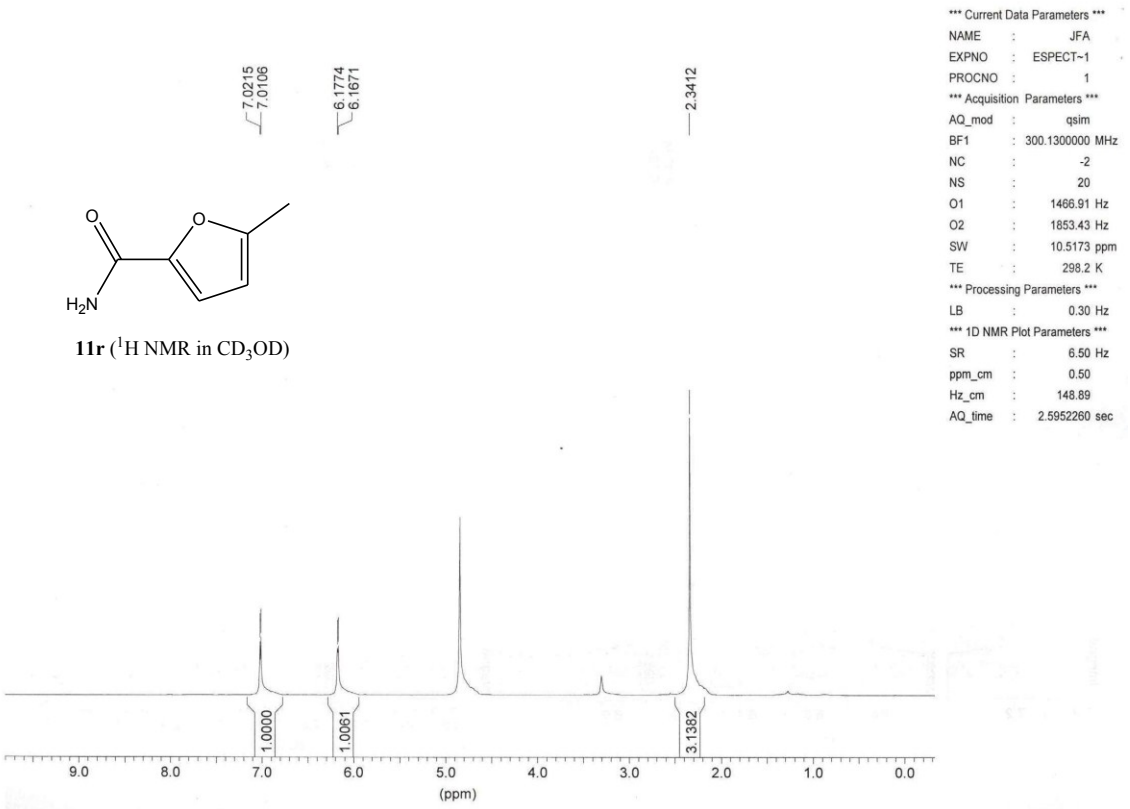
11o ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



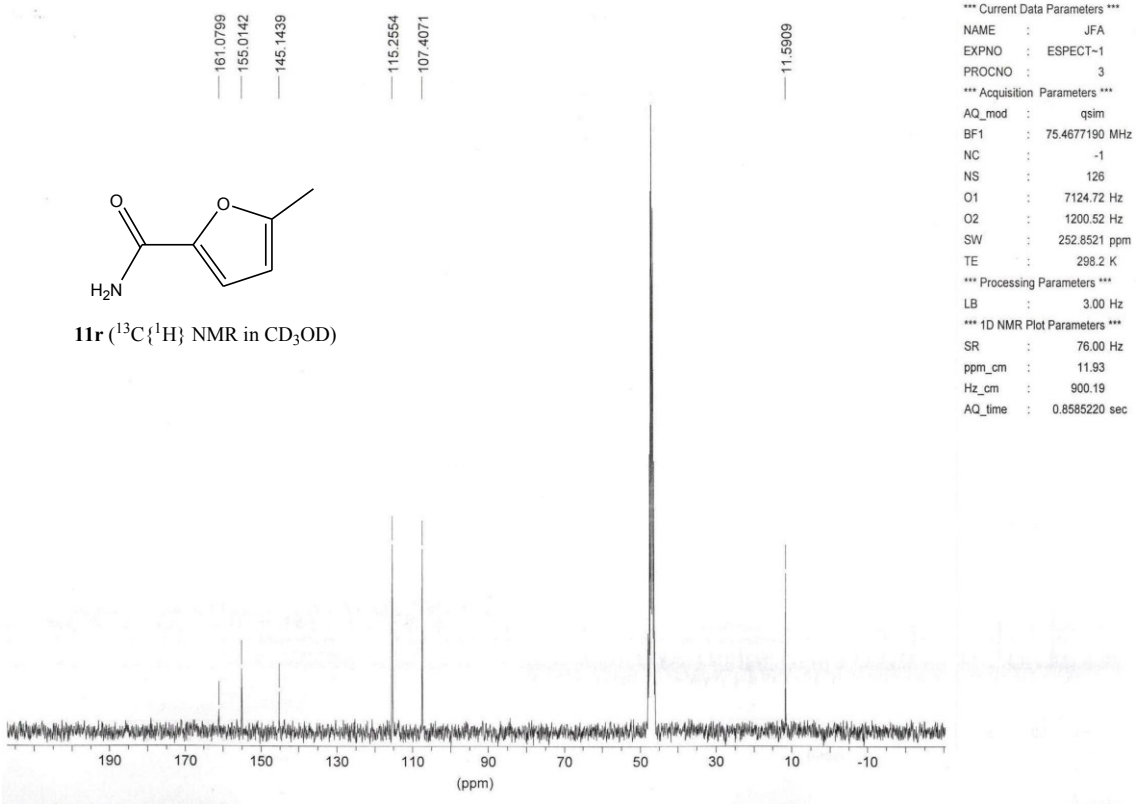
11p (^{1}H NMR in DMSO-d_6)



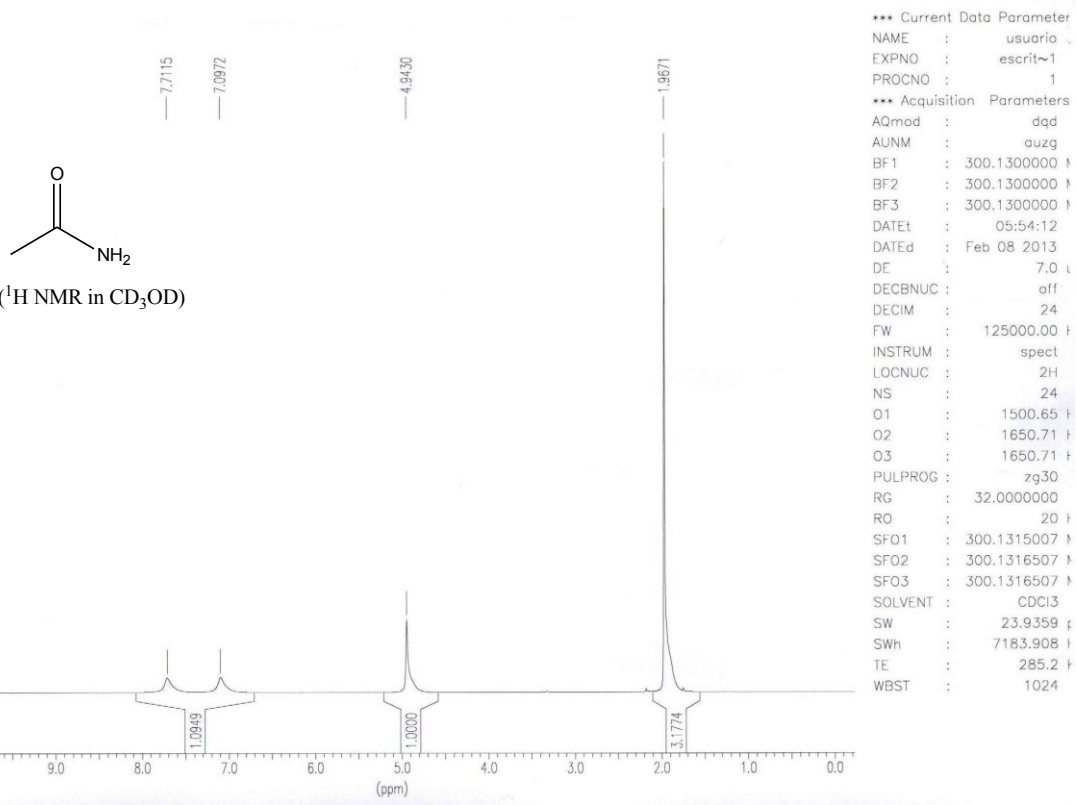
11p (^{13}C{^{1}H} NMR in DMSO-d_6)



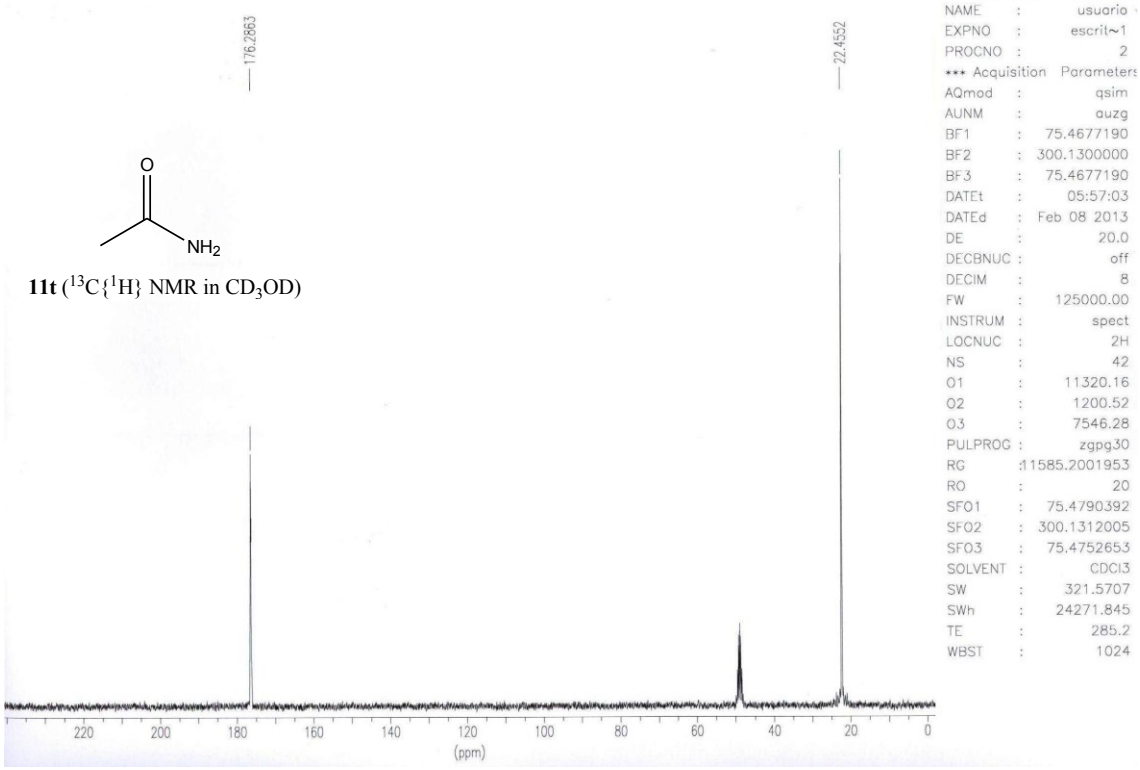
11r (^{1}H NMR in CD_3OD)



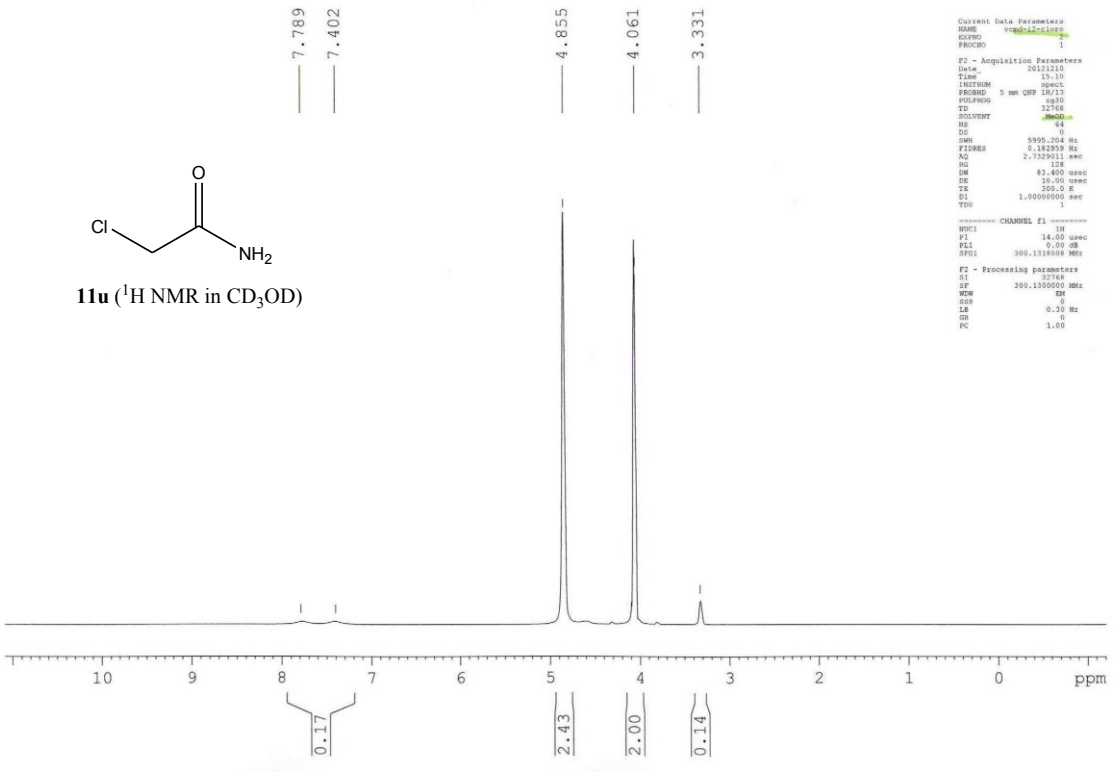
11r ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



11t (^{1}H NMR in CD_3OD)



11t (^{13}C{^{1}H} NMR in CD_3OD)



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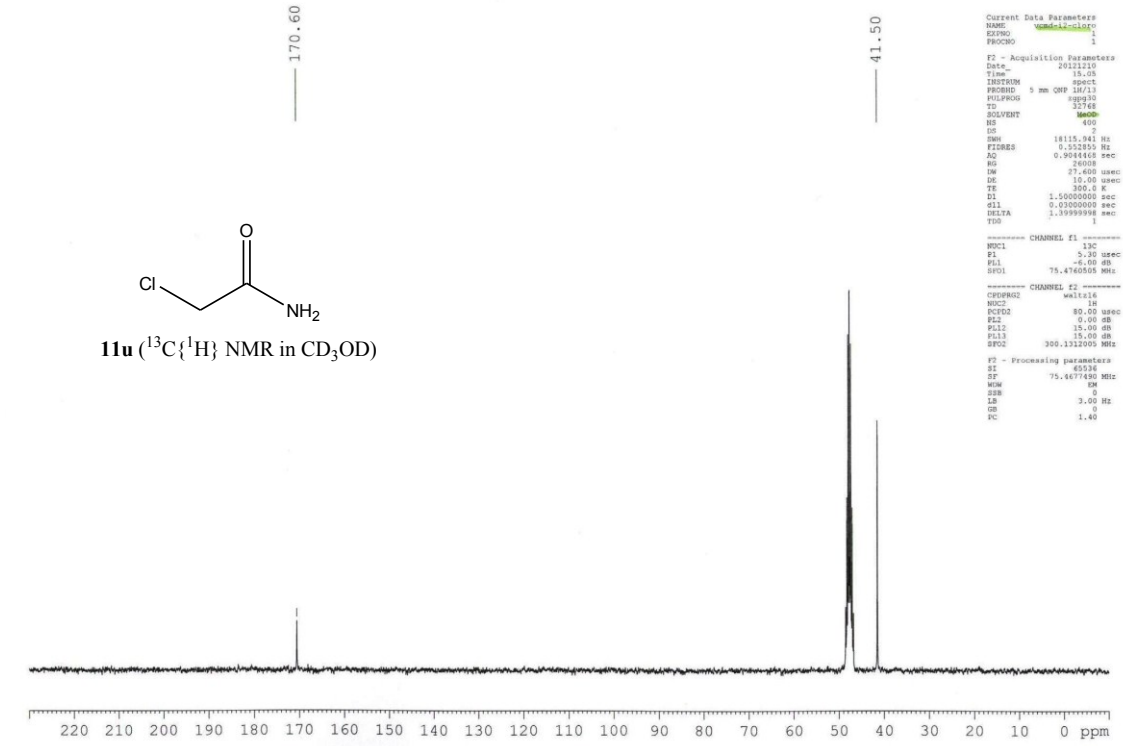
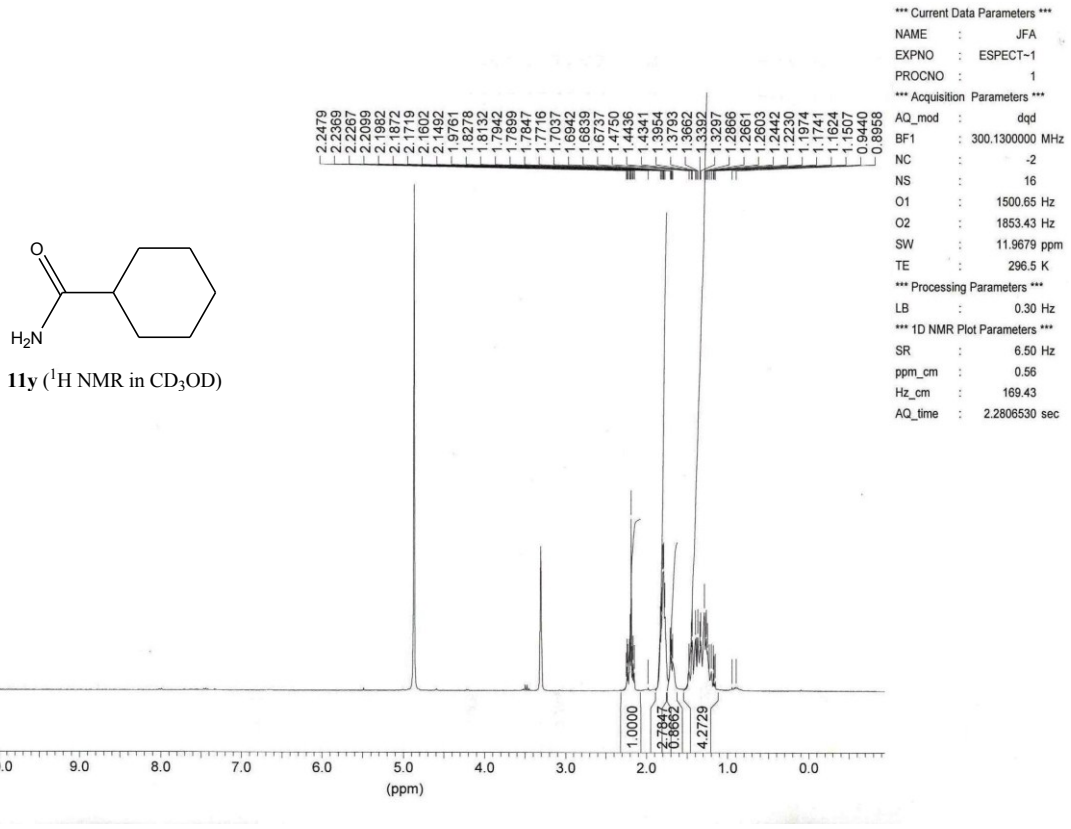
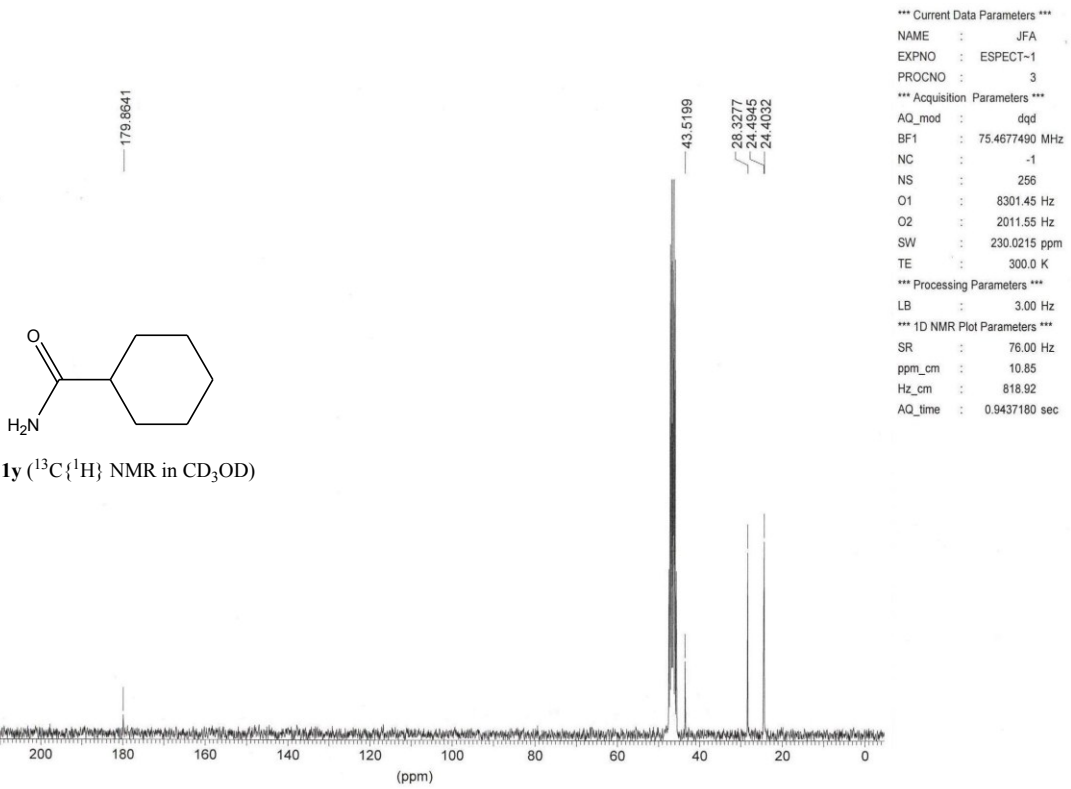


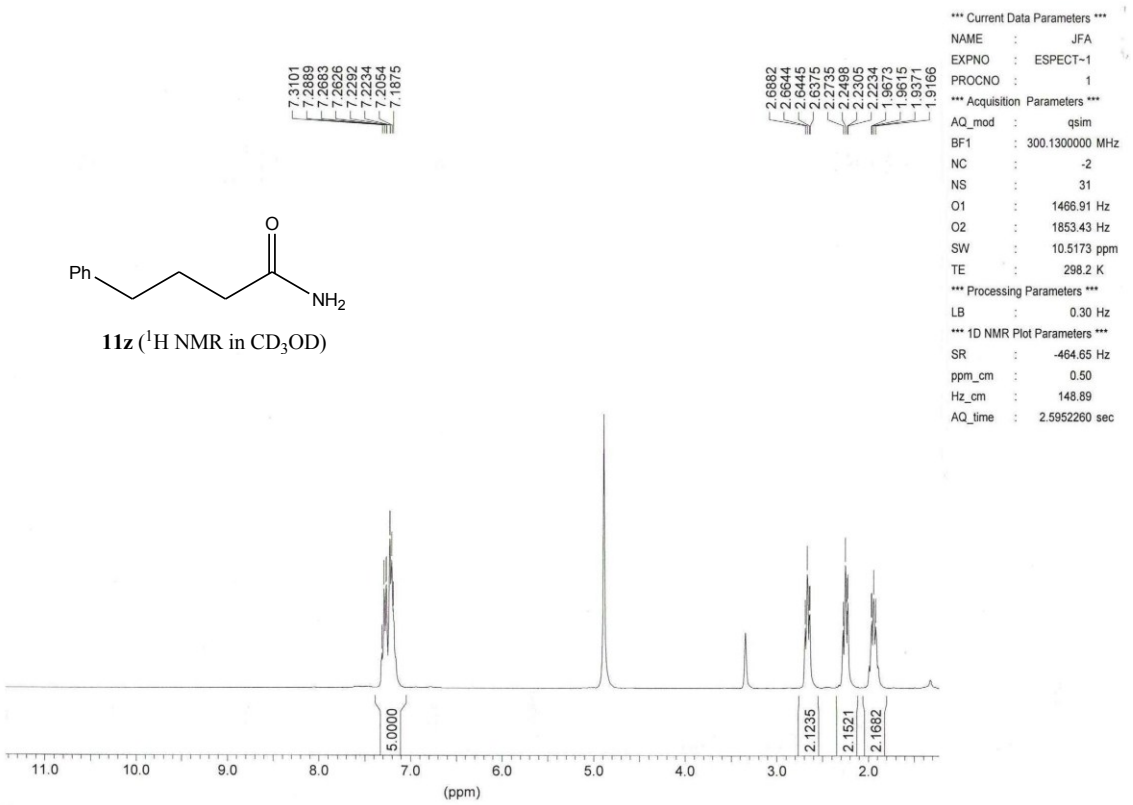
11u (^{13}C{^{1}H} NMR in CD_3OD)



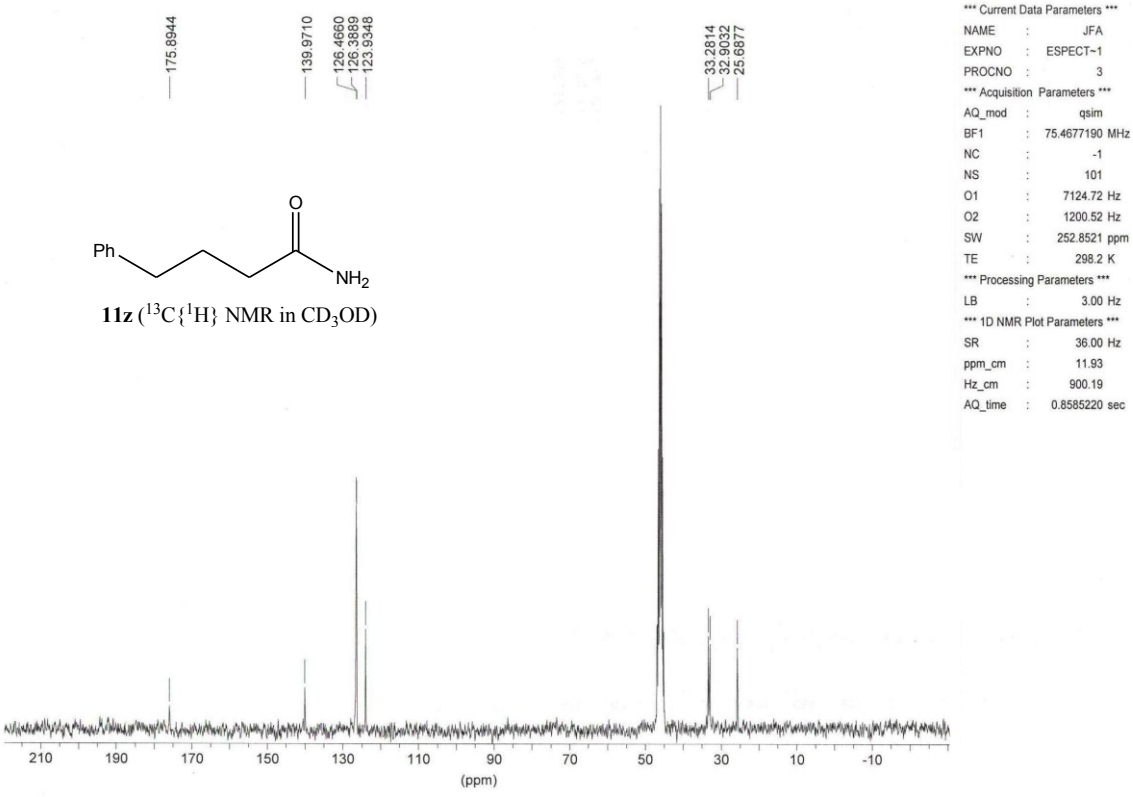
11y (^{1}H NMR in CD_3OD)



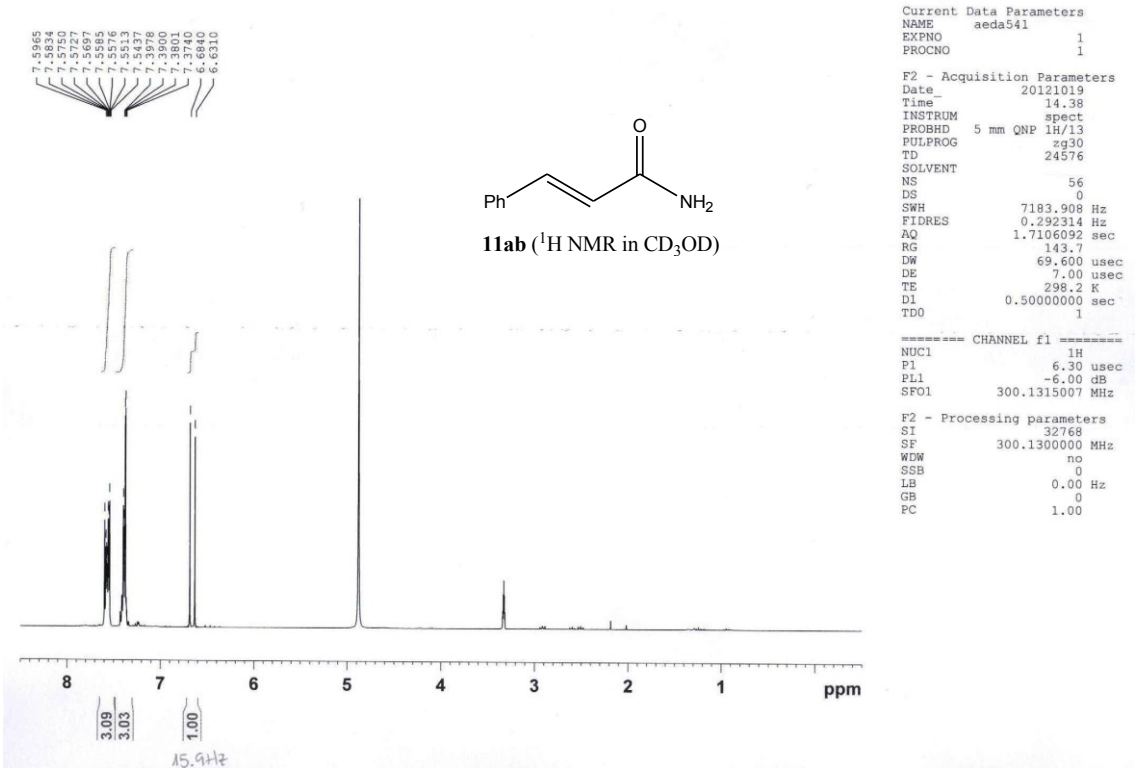
11y ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



11z (^{1}H NMR in CD_3OD)



11z ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



11ab (^{1}H NMR in CD_3OD)

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DE               7.00 usec
TE              298.2 K
D1           0.50000000 sec
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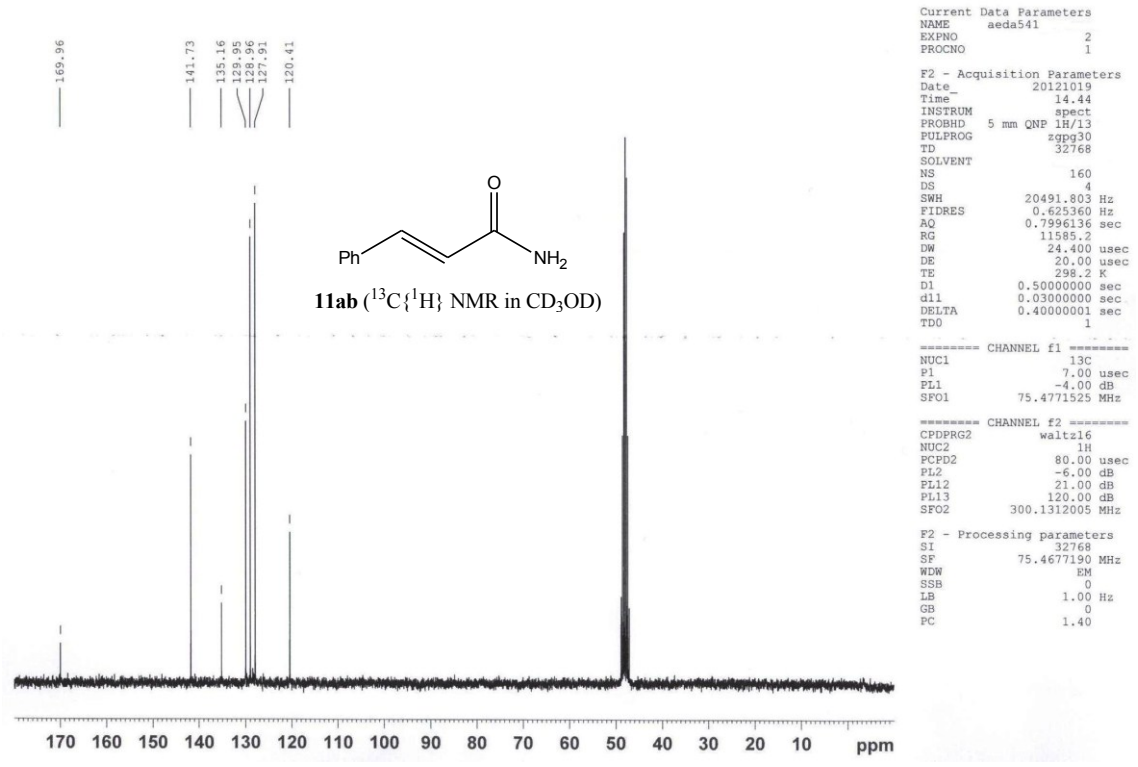

11ab ($^{13}C\{^{1}H\}$ NMR in CD_3OD)

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PL1            -4.00 dB
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PL12           21.00 dB
PL13          120.00 dB
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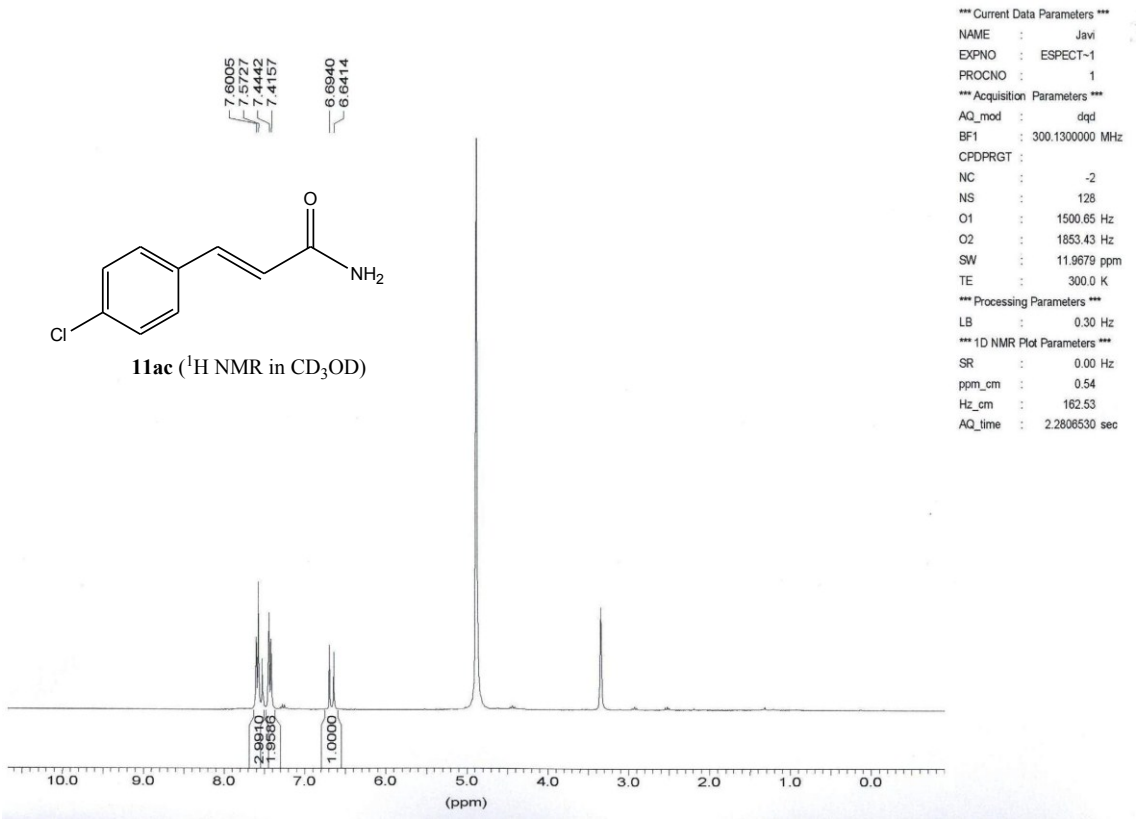

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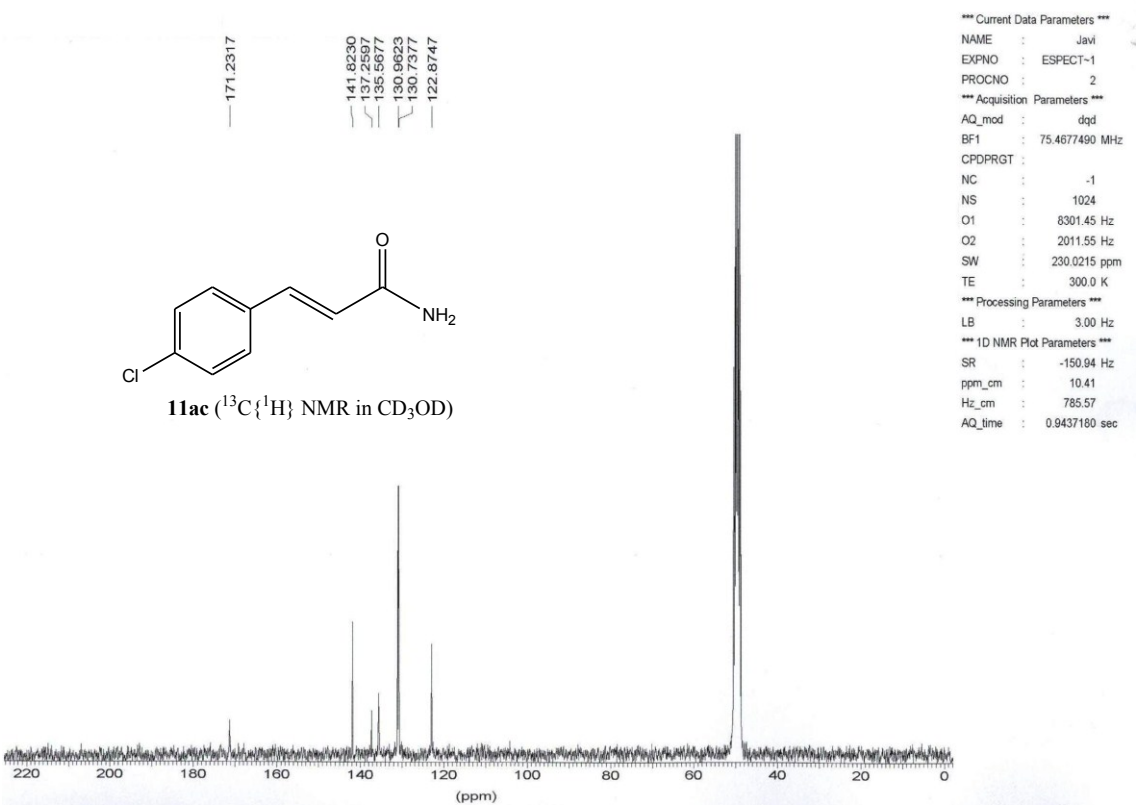

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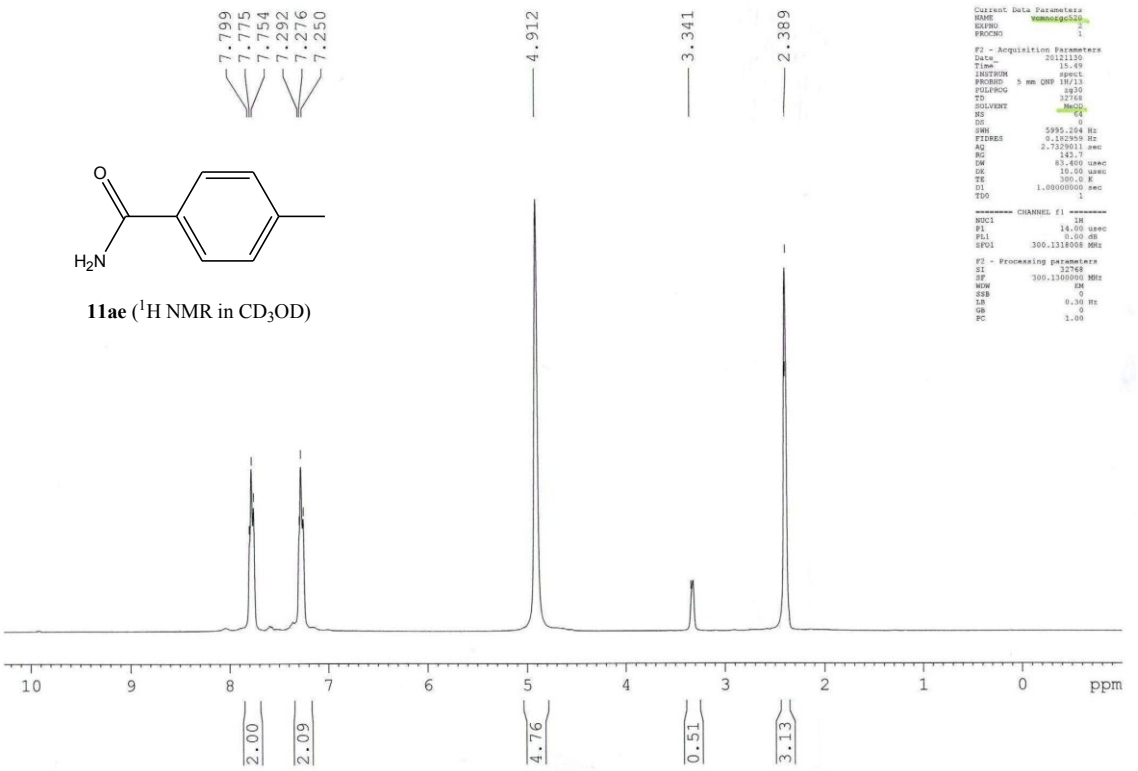

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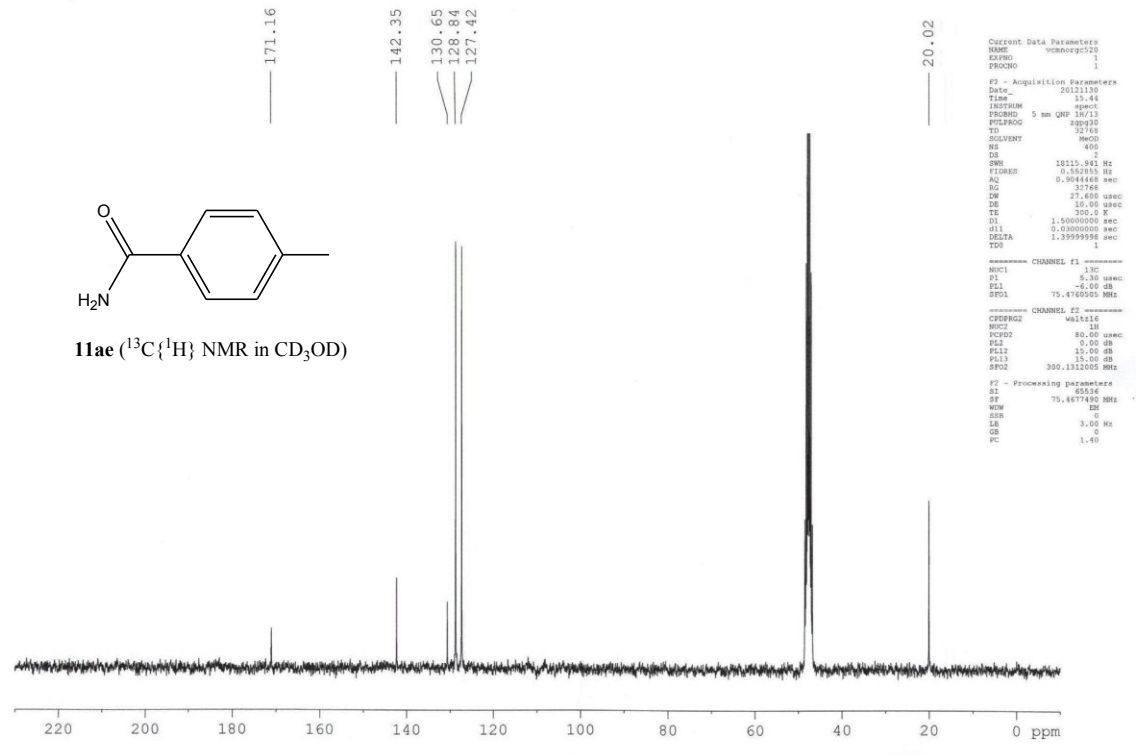
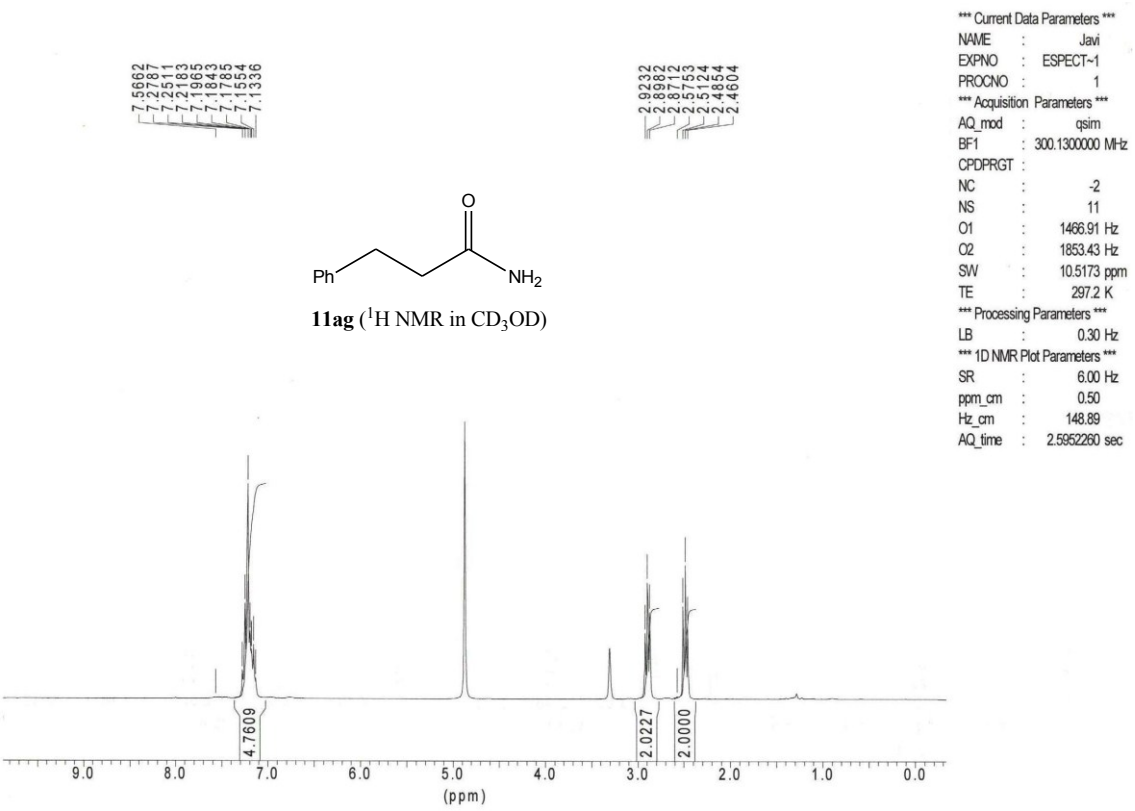


11ae ($^{13}C\{^{1}H\}$ NMR in CD_3OD)



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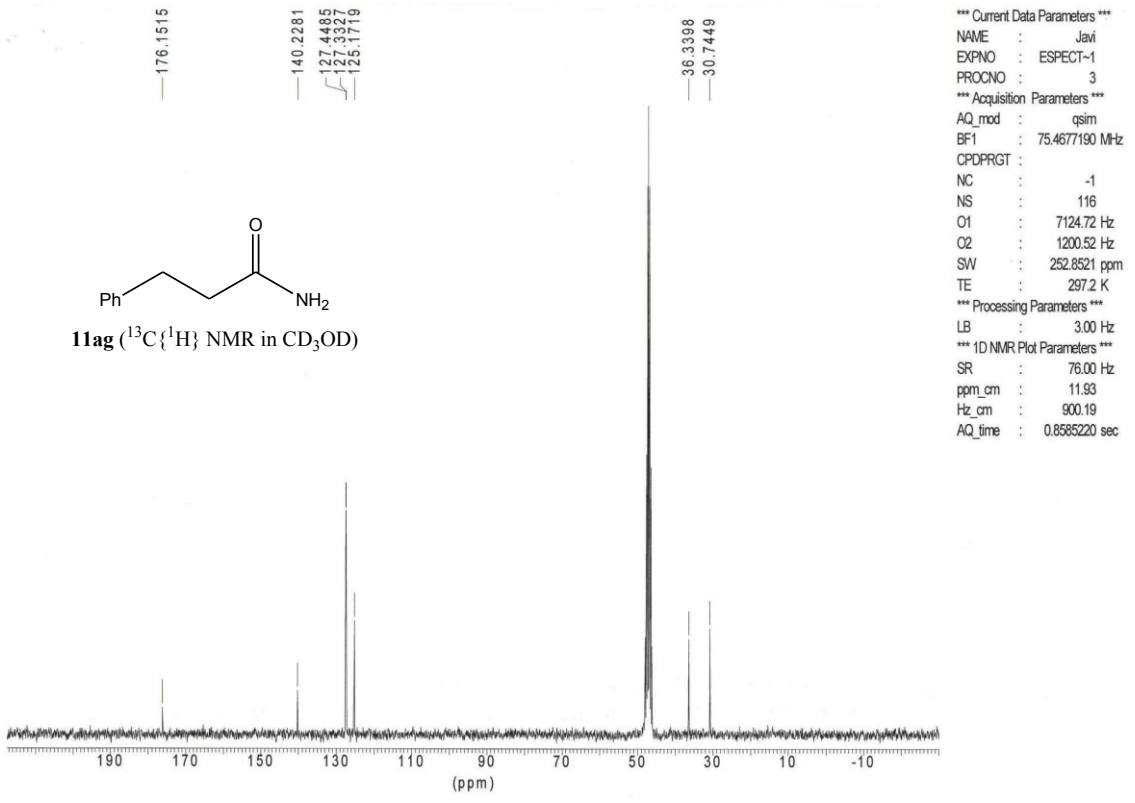

11ag ($^{13}C\{^{1}H\}$ NMR in CD_3OD)