

Design and Synthesis of Meldrum's acid Based 7-Azaindole Anchored 1,2,3-Triazole Hybrids as Anticancer Agents

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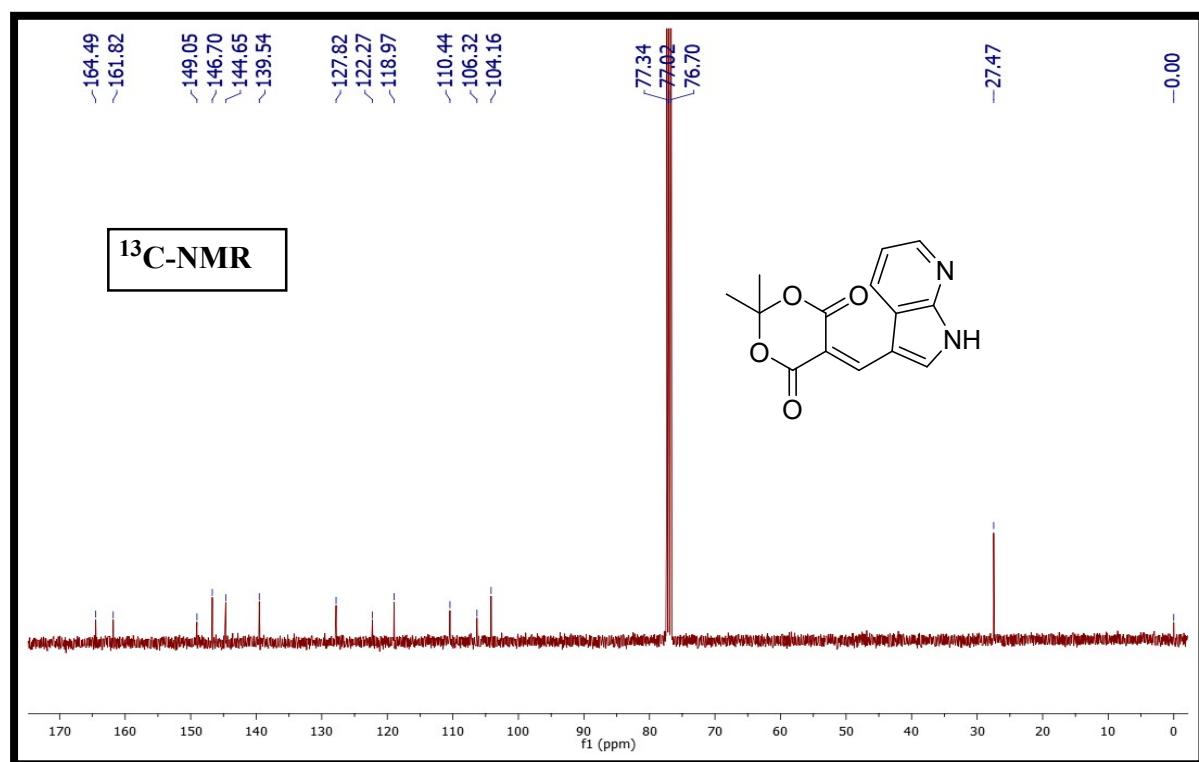
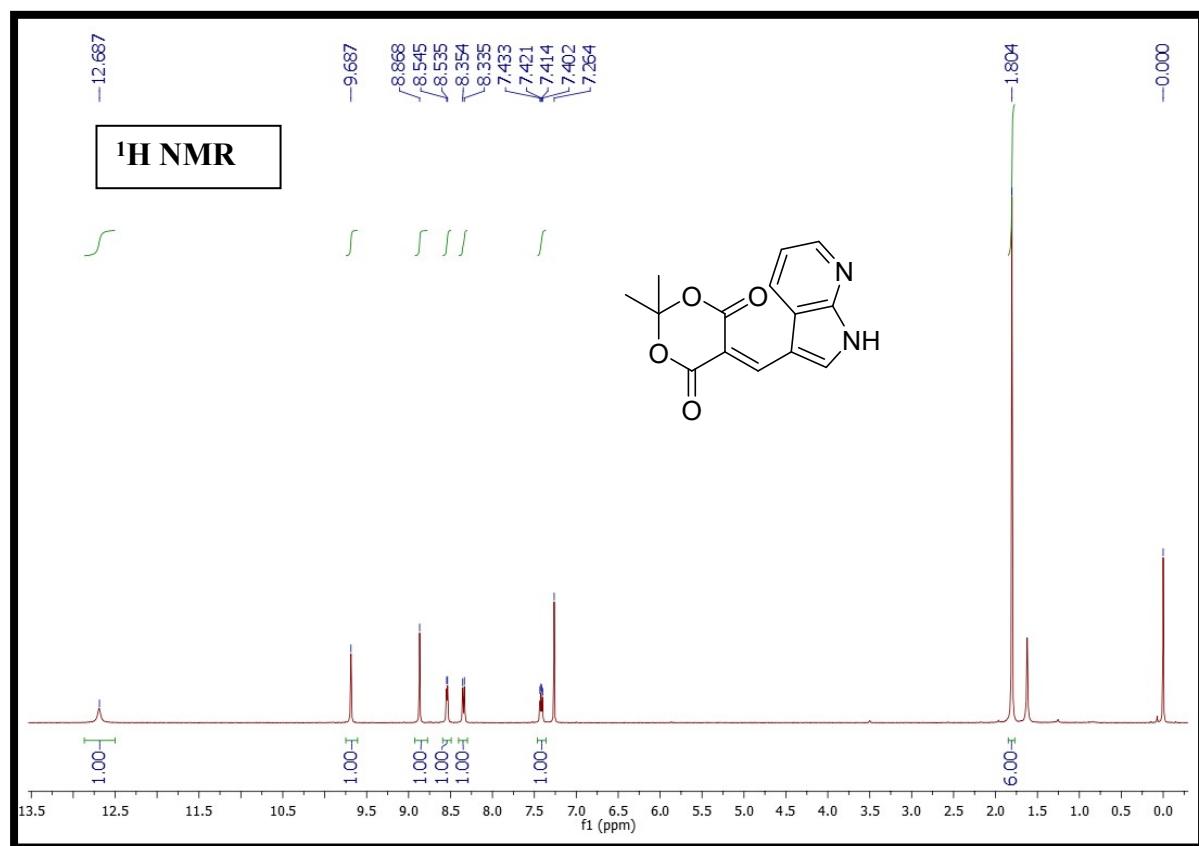
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^dTelangana Mahila Viswavidyalayam, Hyderabad – 500095, Telangana Hyderabad, India

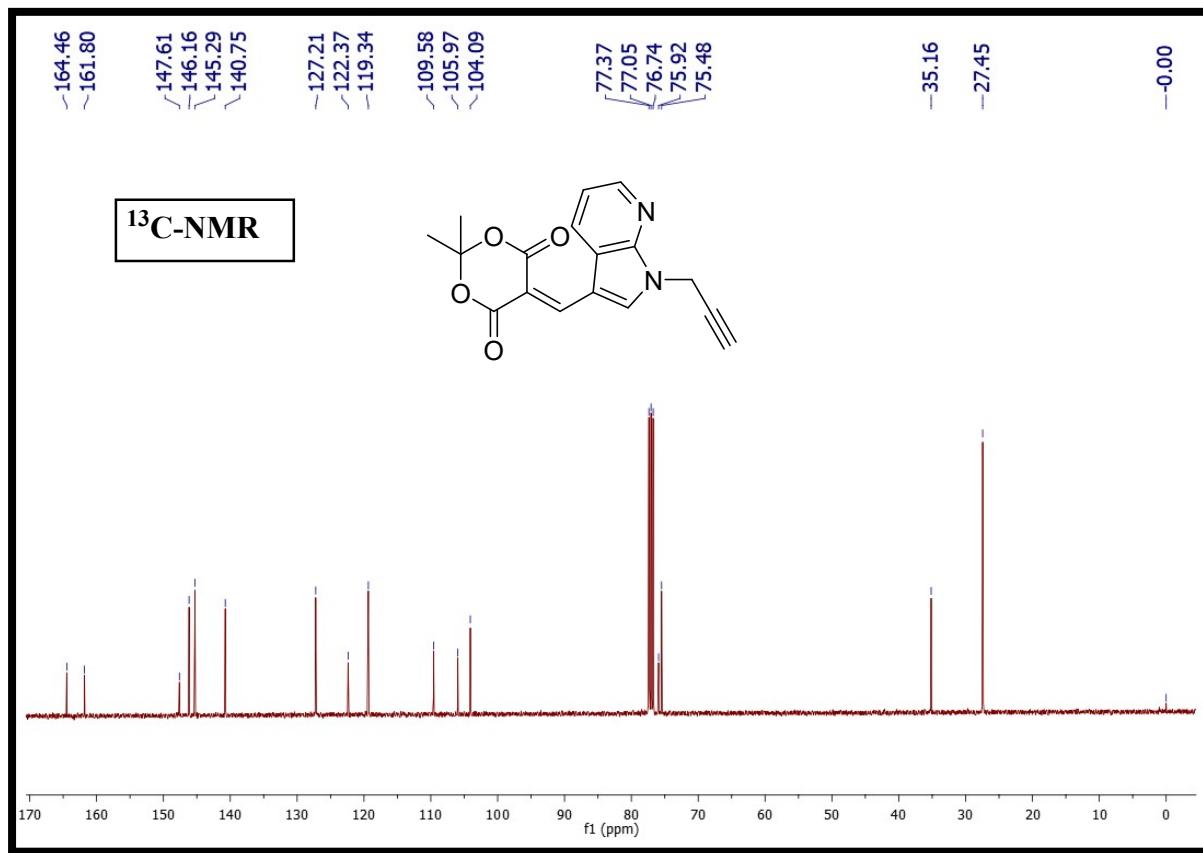
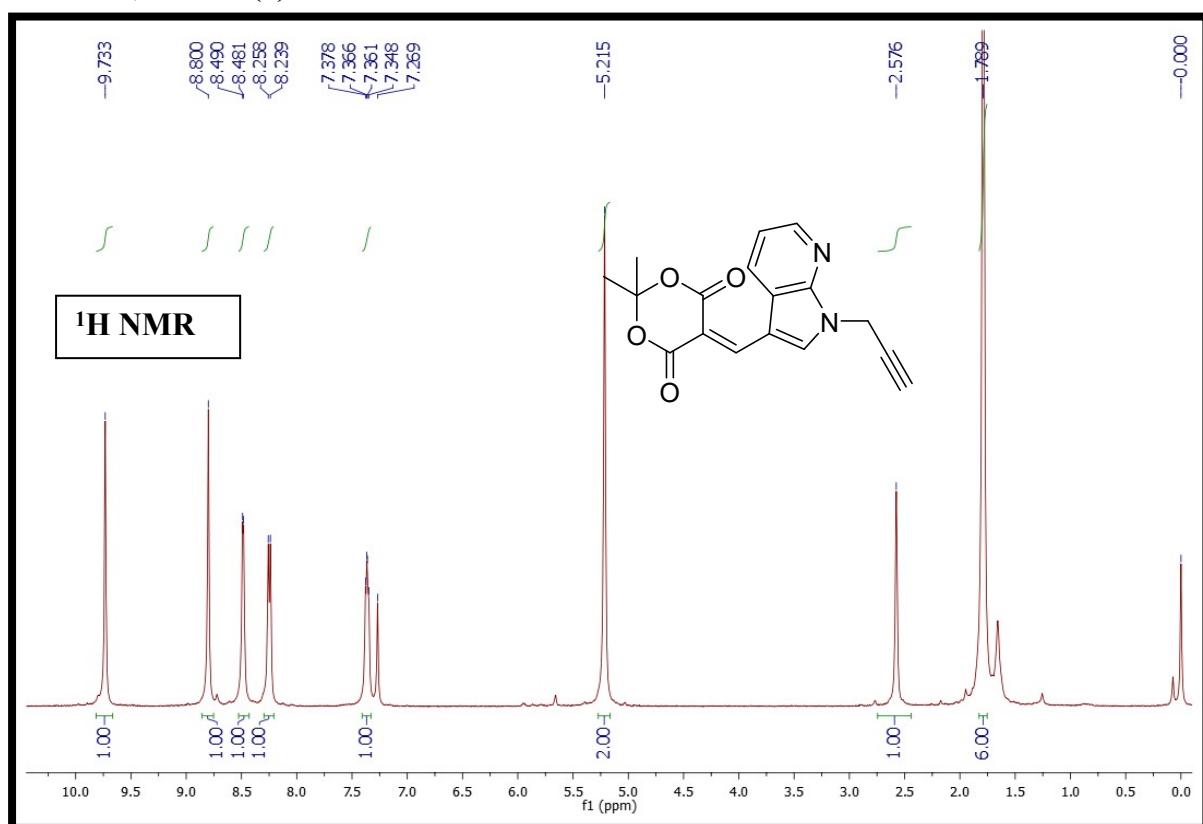
Supplementary Information

- 1. ^1H NMR & ^{13}C NMR SPECTRA COPIES**
- 2. HRMS/ESI-MS COPIES**

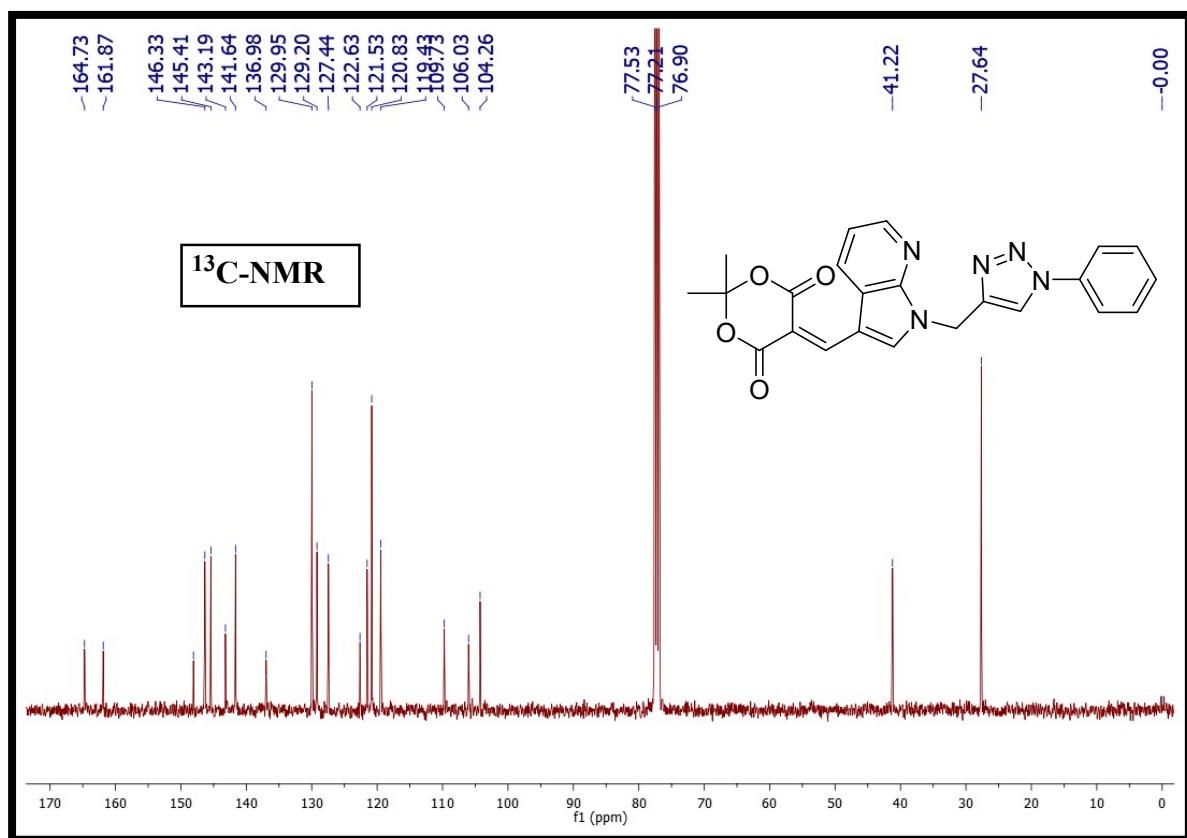
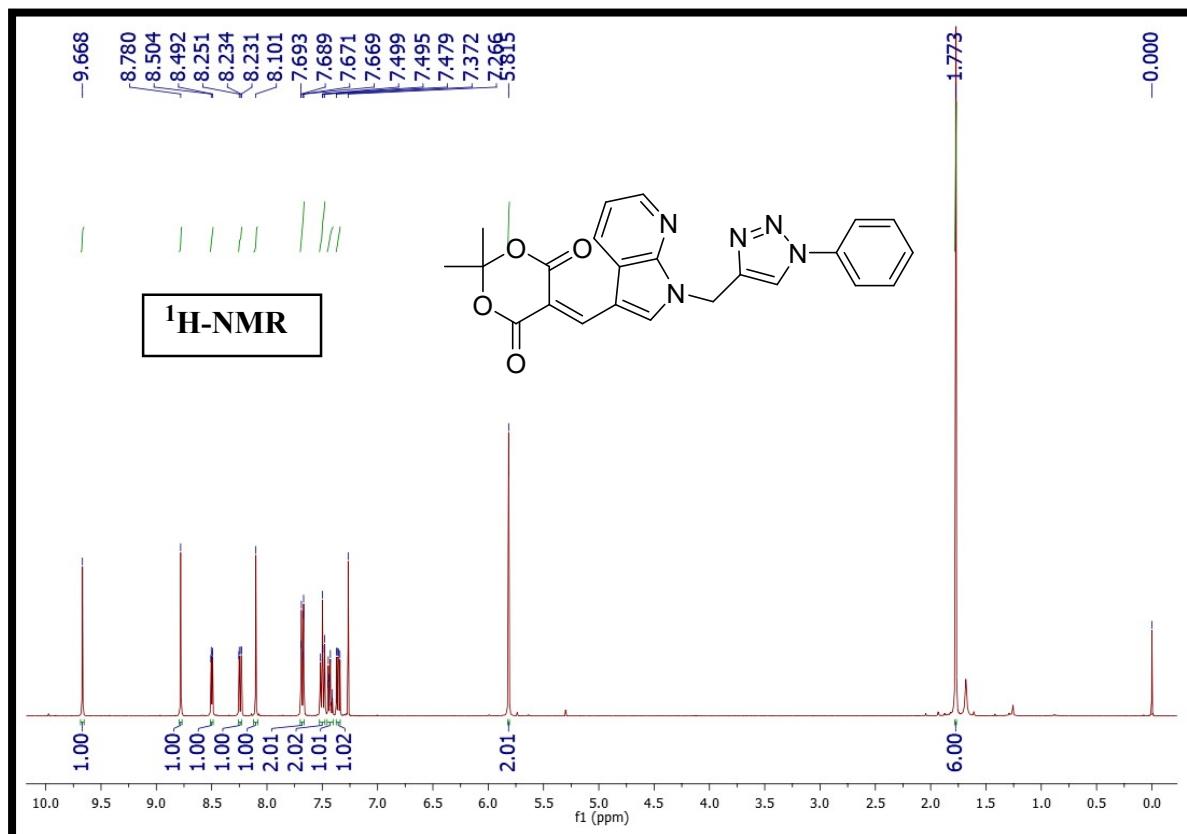
5-((1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (3):



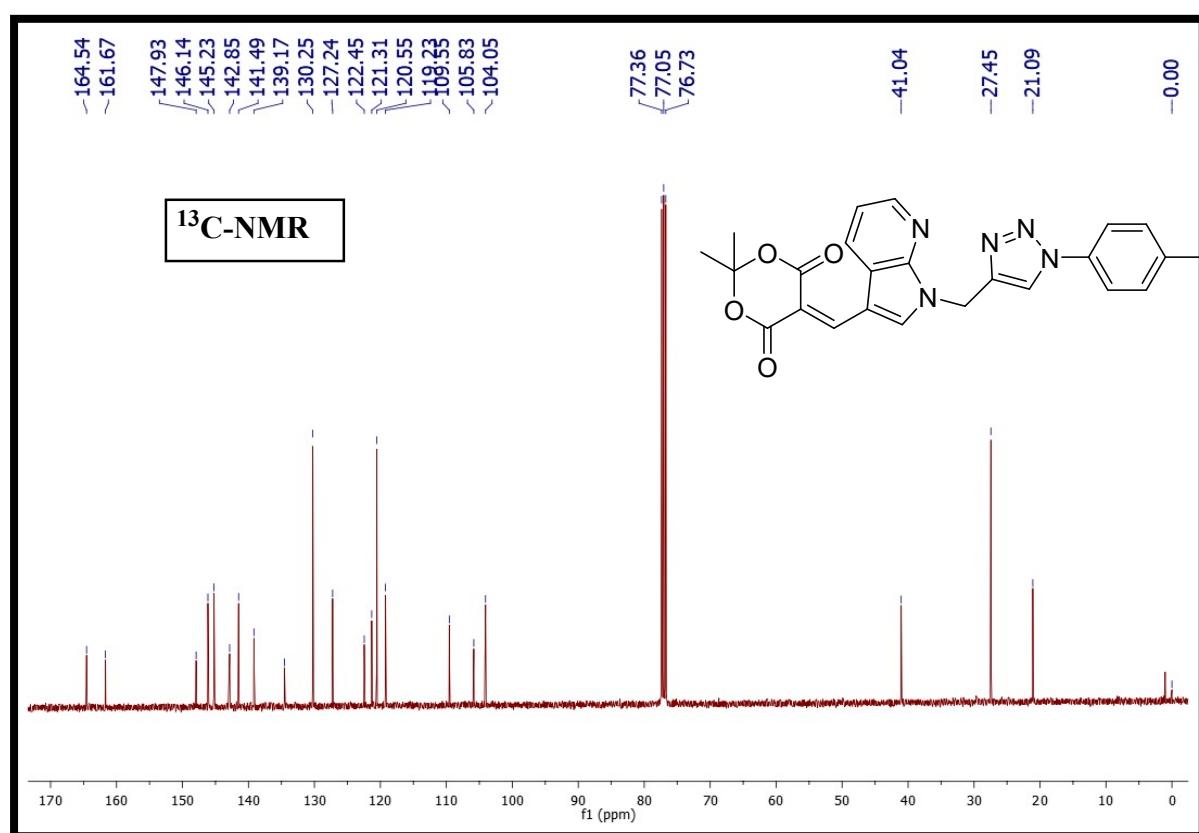
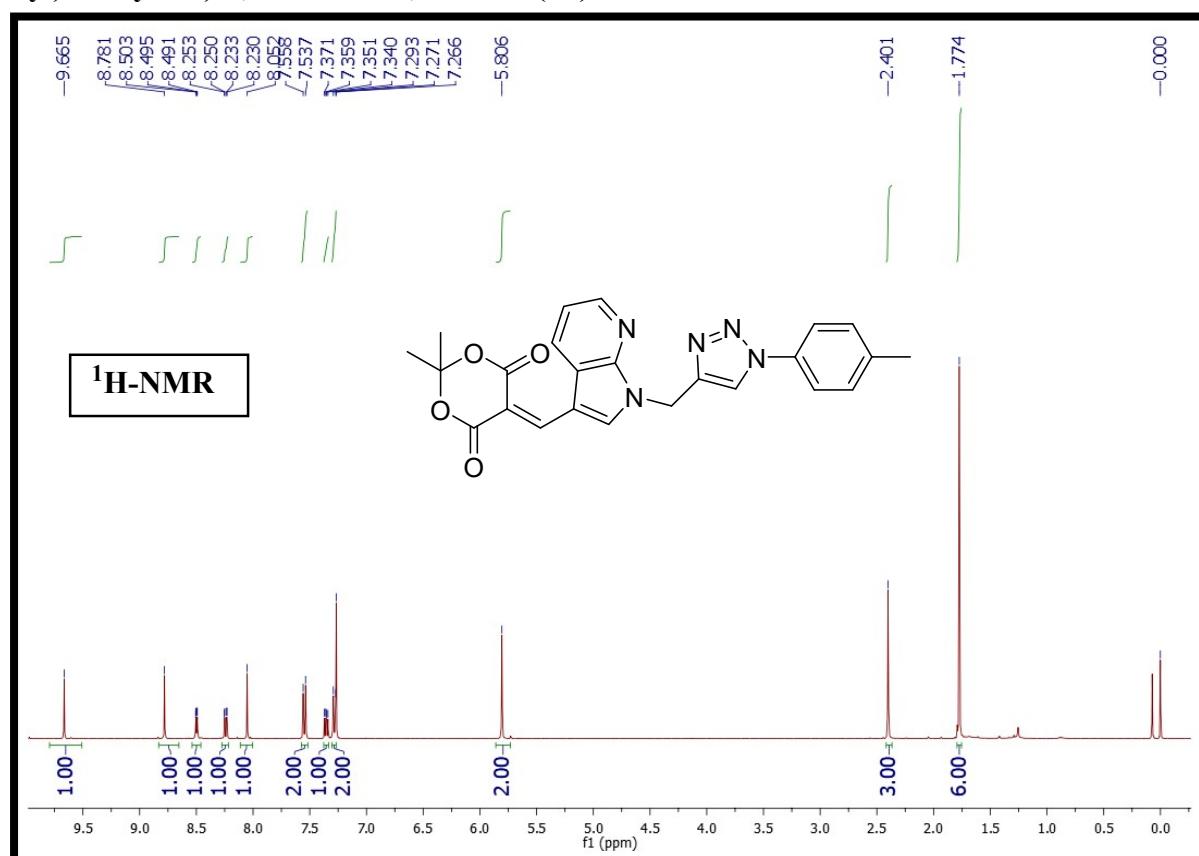
2,2-dimethyl-5-((1-(prop-2-yn-1-yl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-1,3-dioxane-4,6-dione (4):



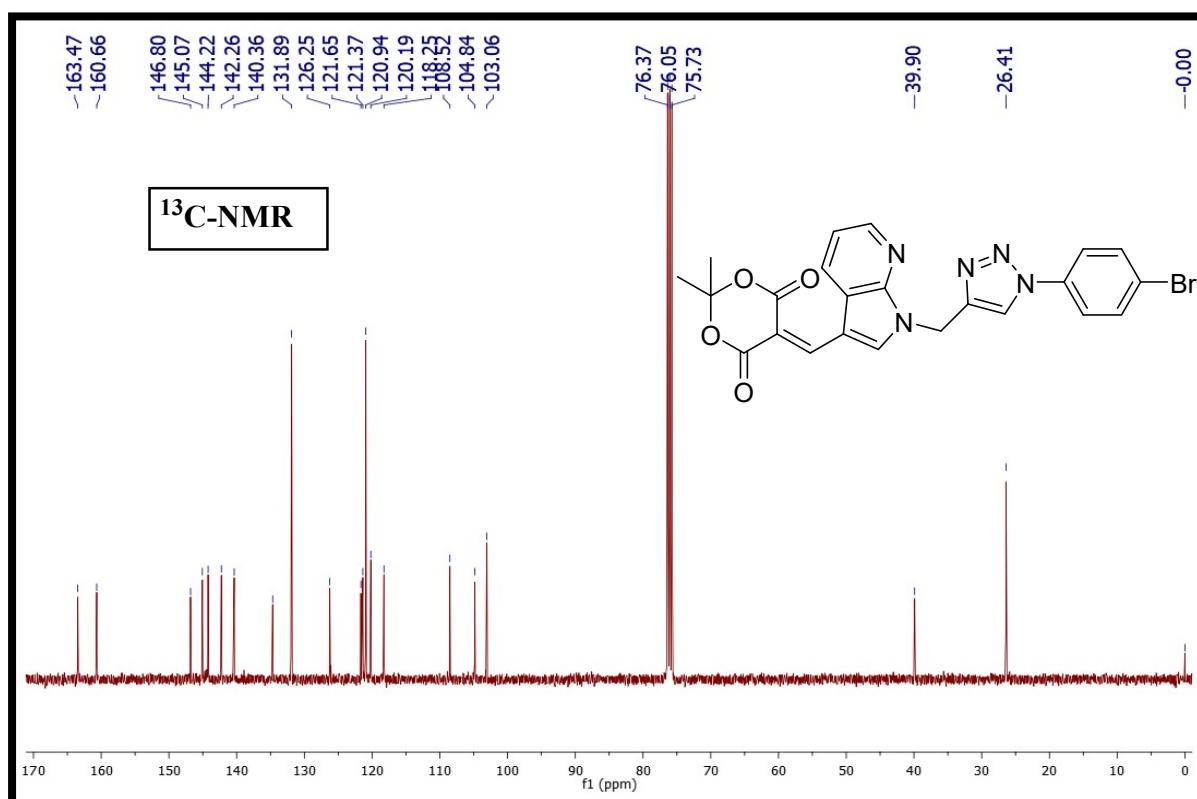
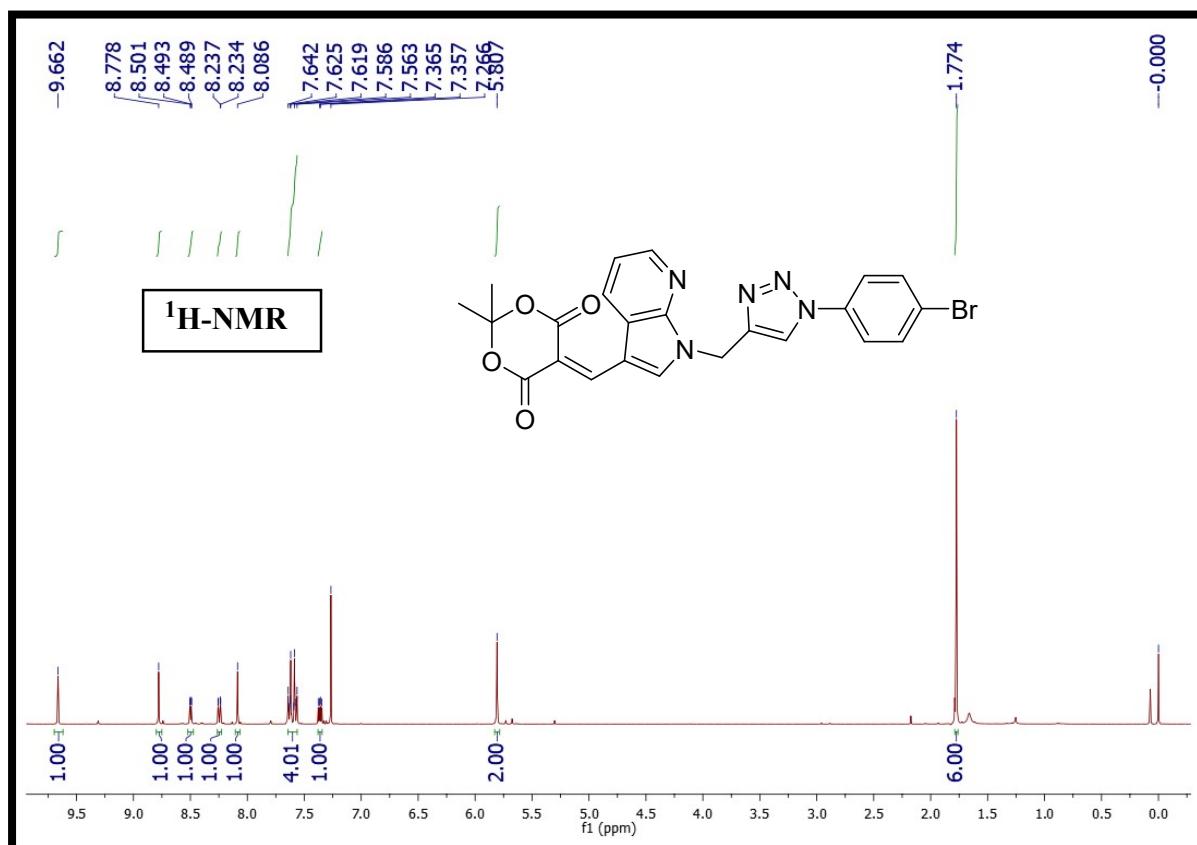
2,2-dimethyl-5-((1-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-1,3-dioxane-4,6-dione (6a):



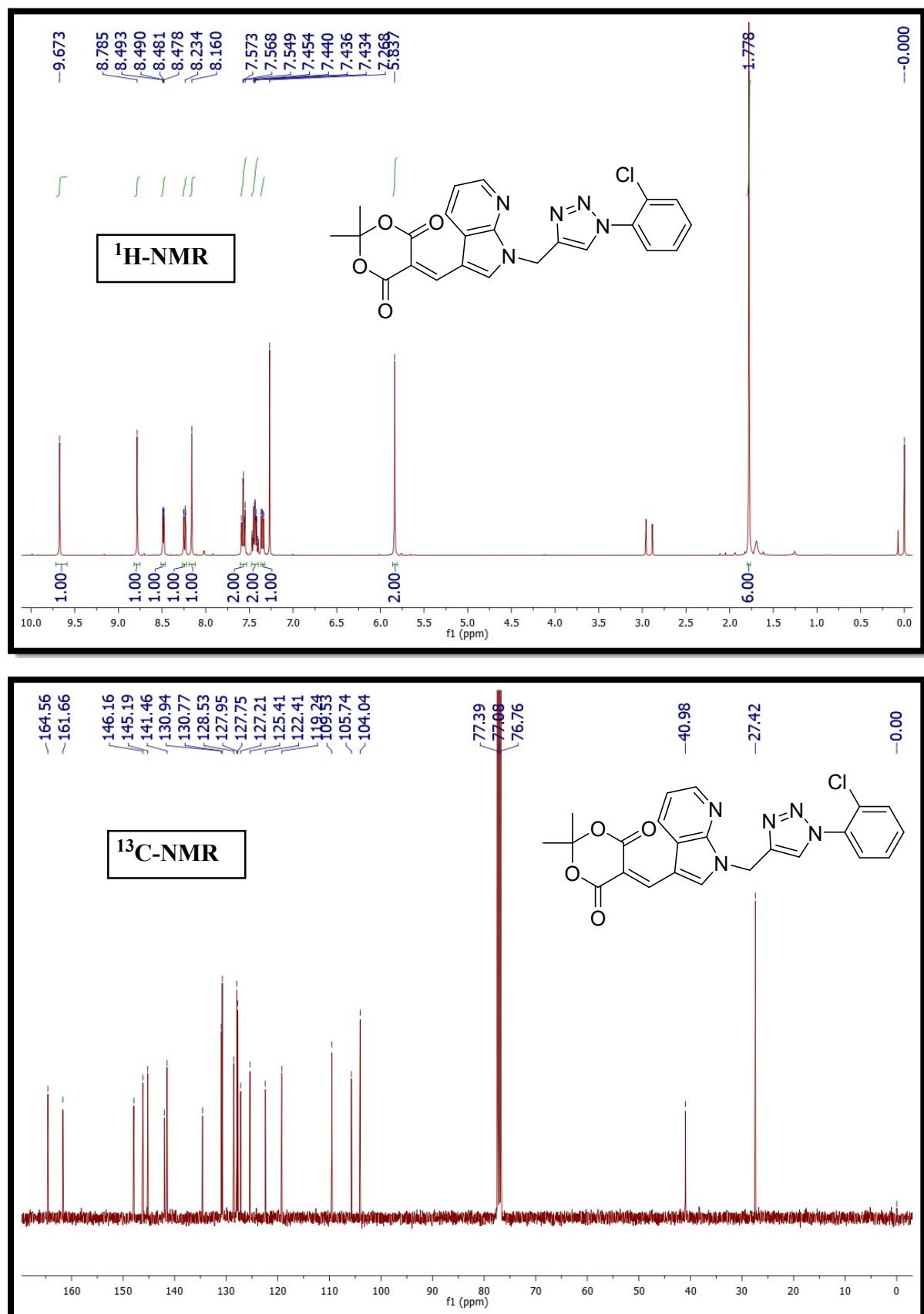
2,2-dimethyl-5-((1-((1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-1,3-dioxane-4,6-dione (6b):



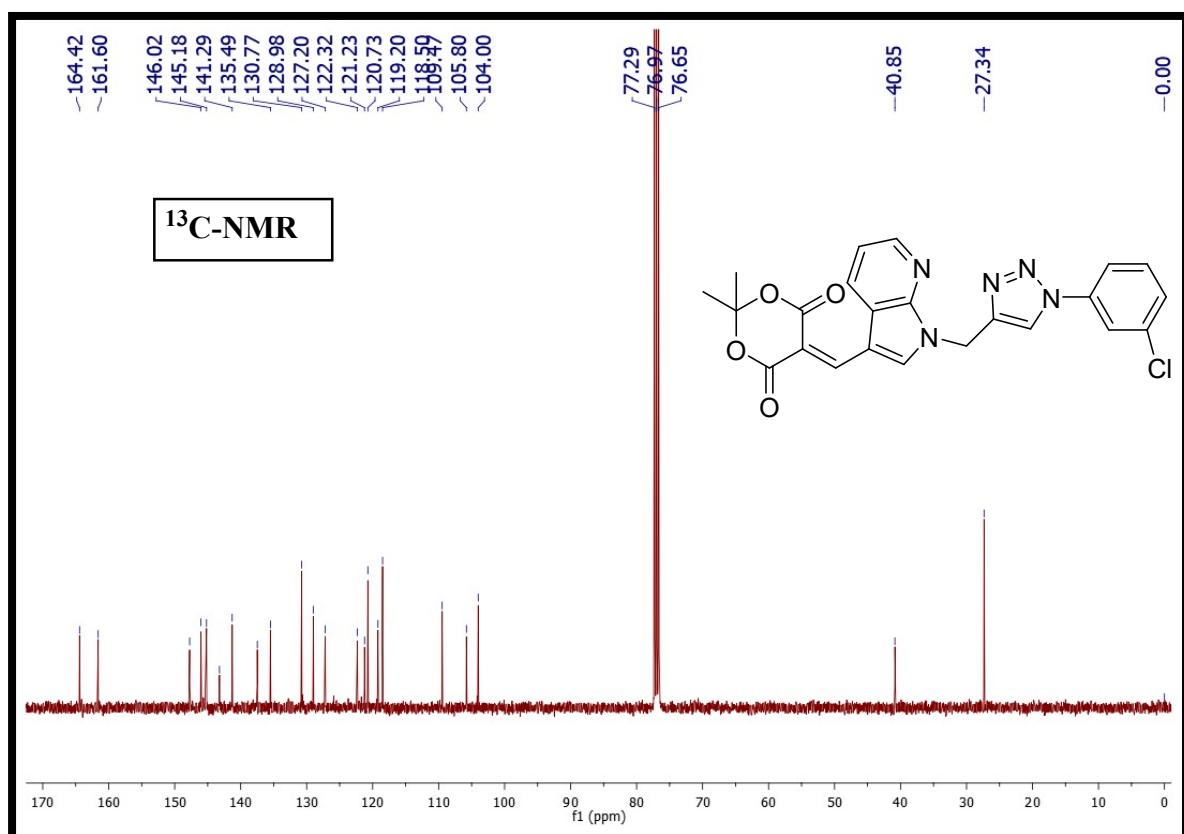
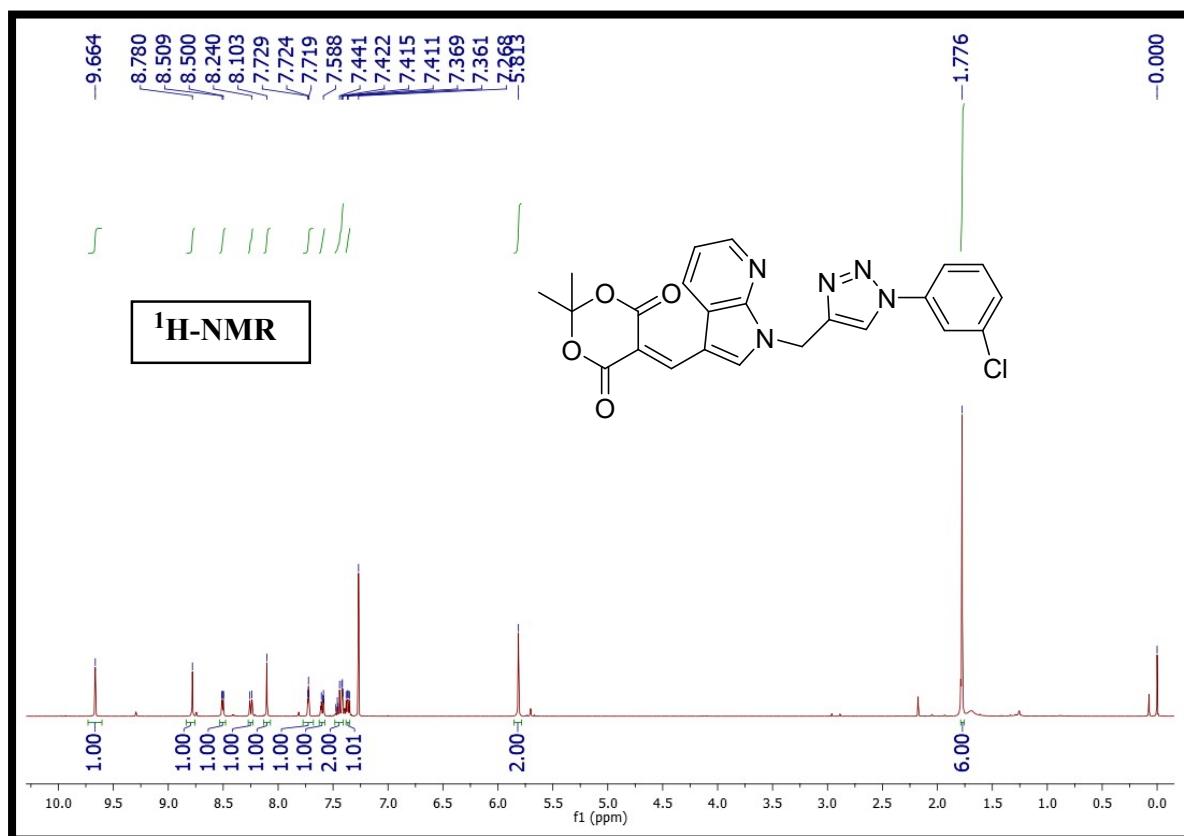
5-((1-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6c):



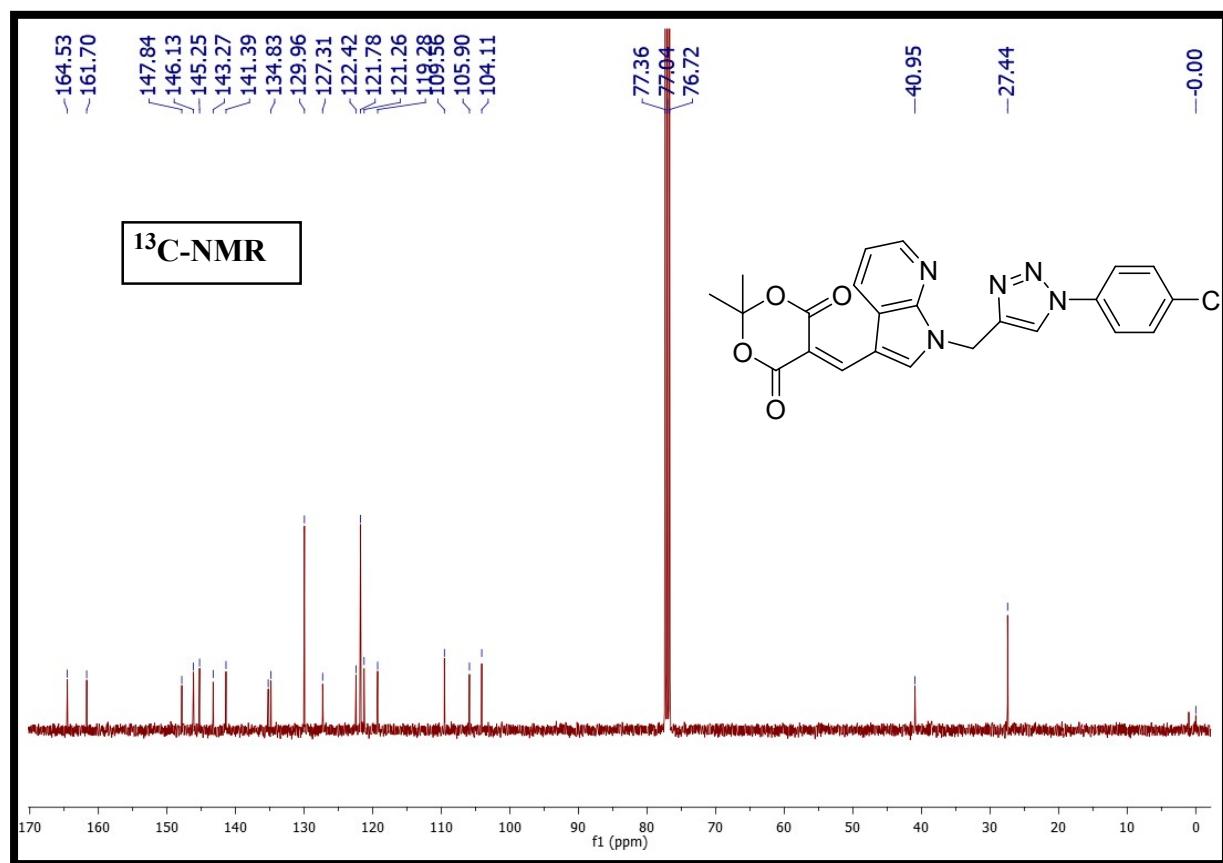
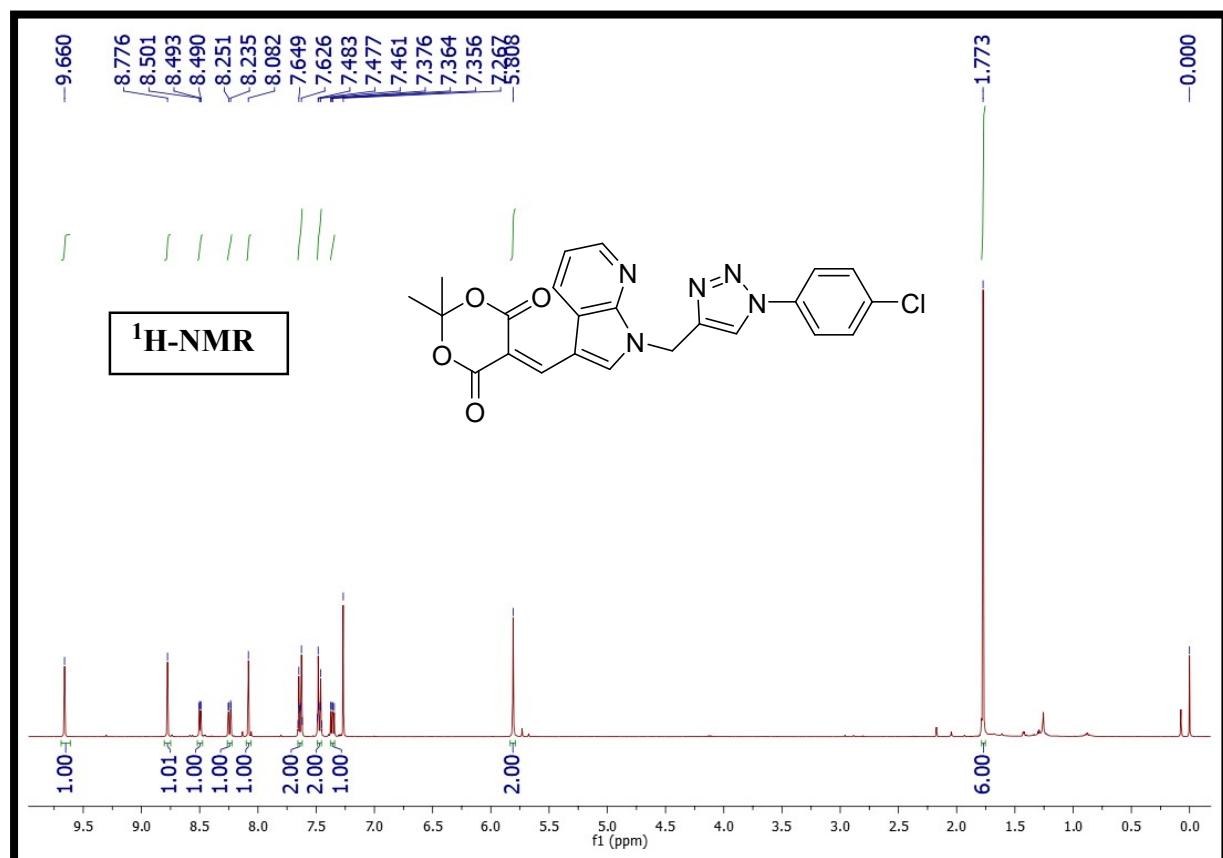
5-((1-((1-(2-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6d):



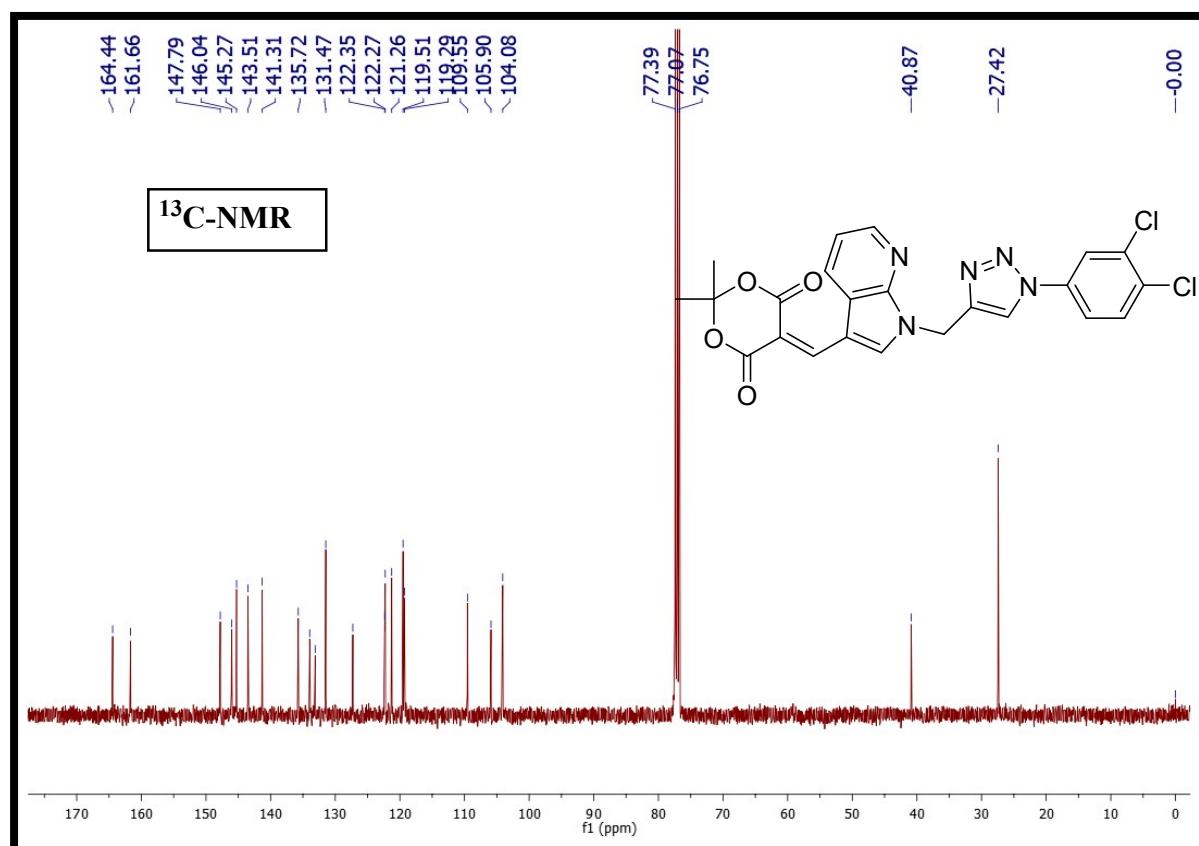
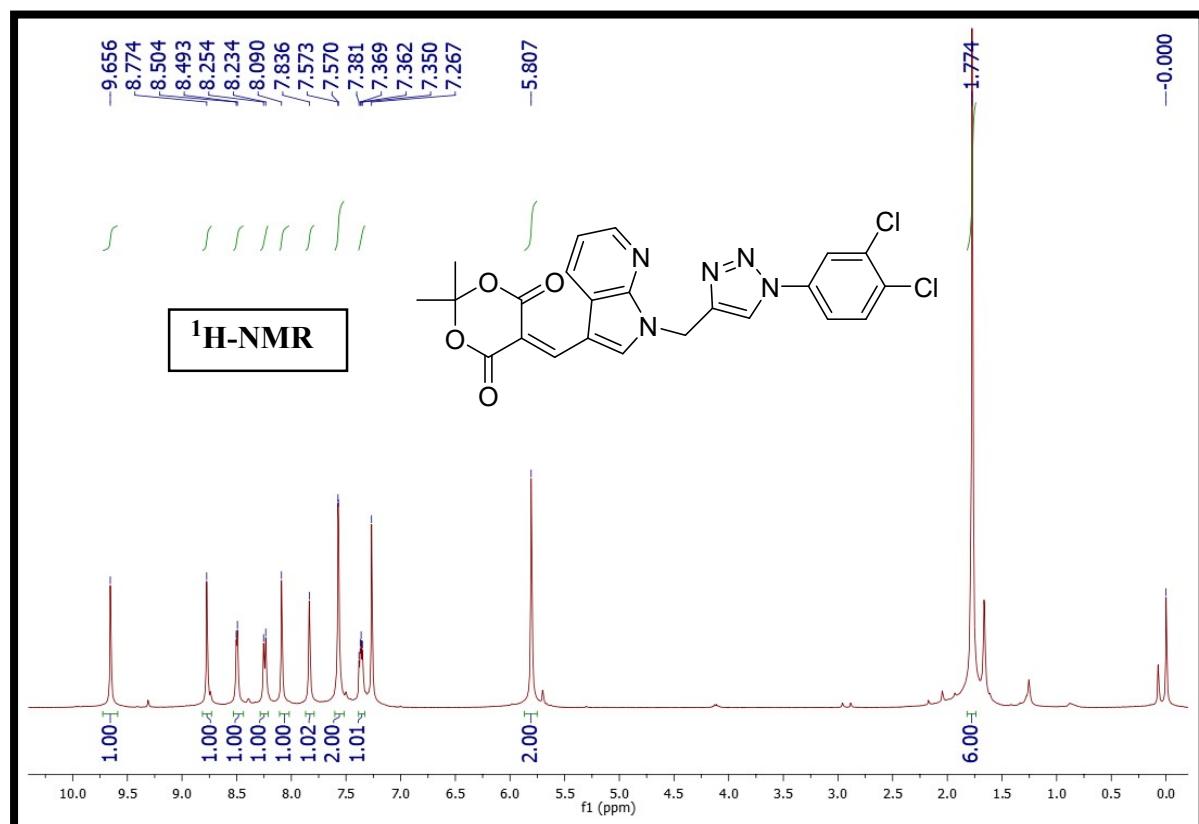
5-((1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6e):



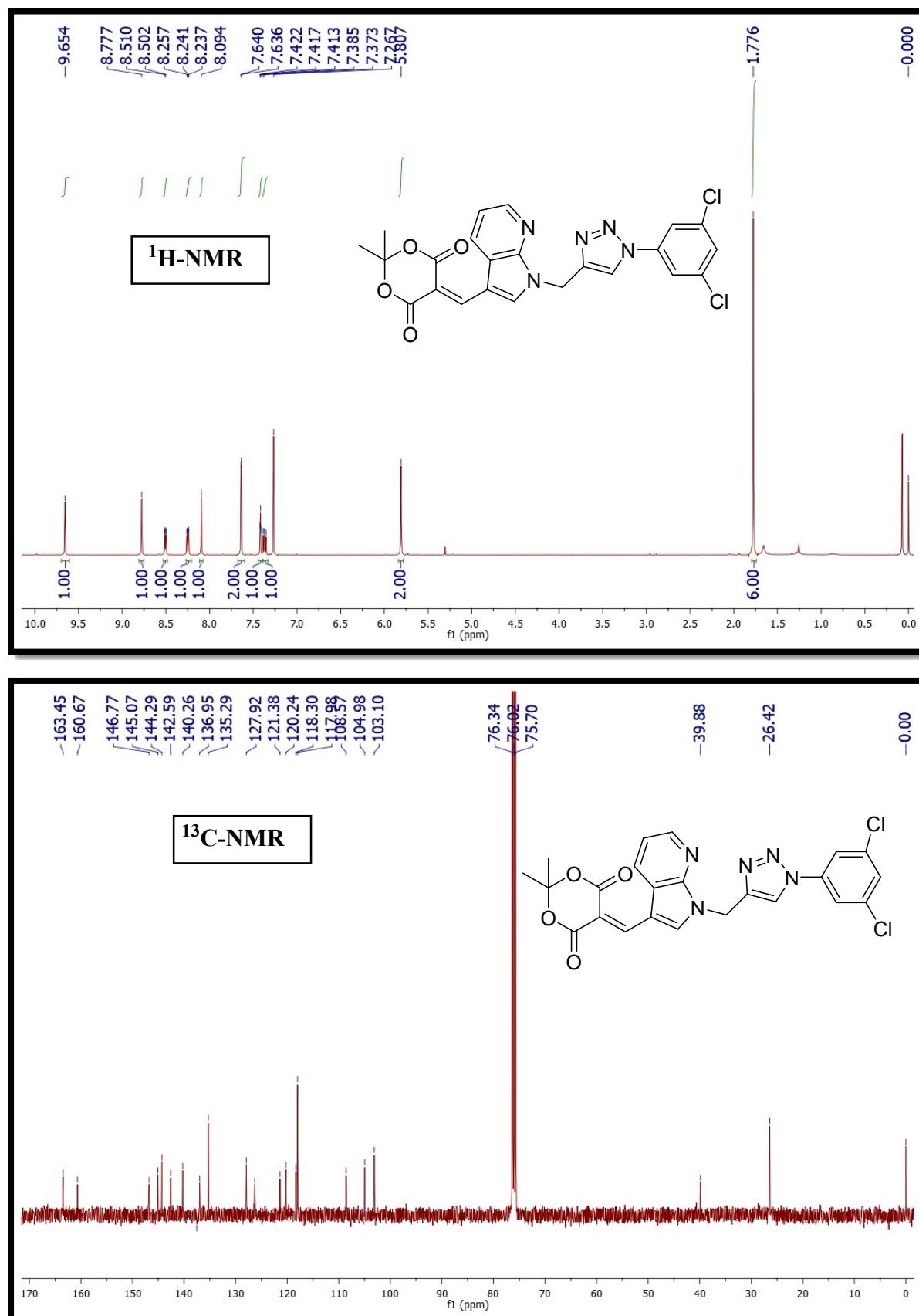
5-((1-((1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6f):



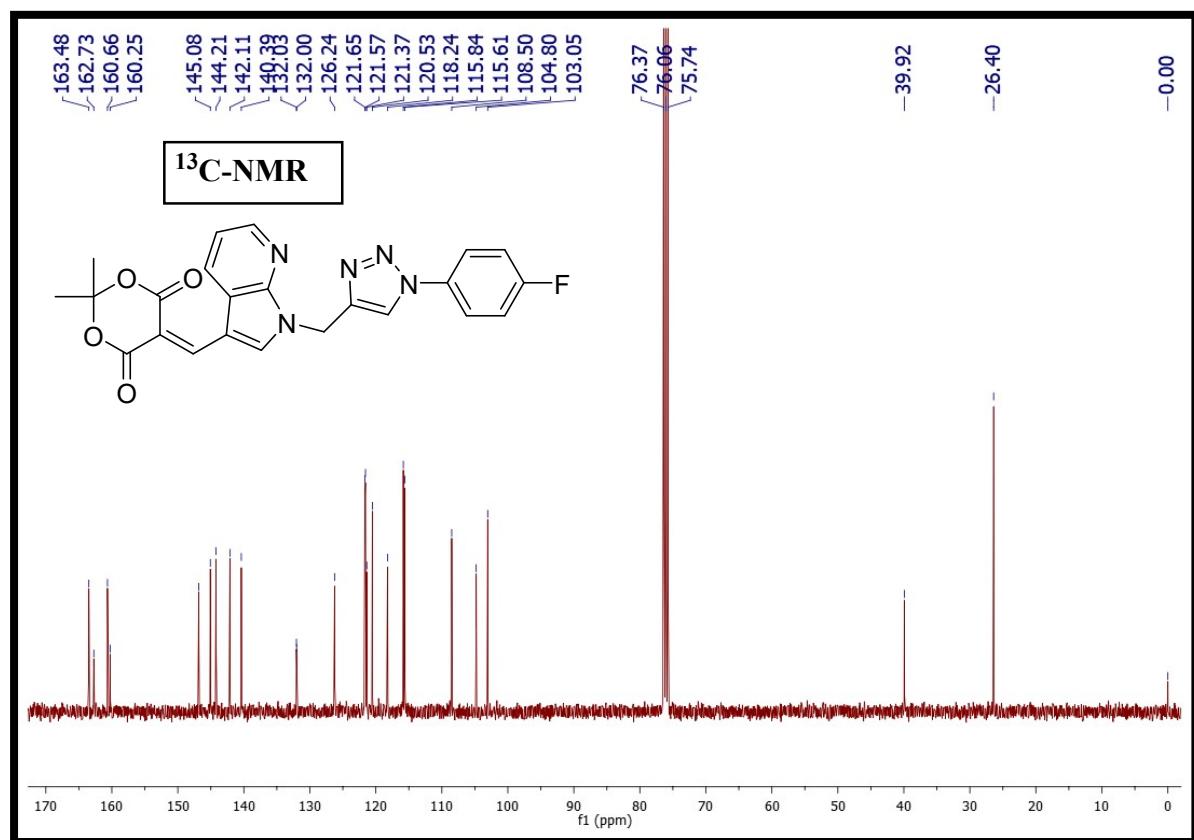
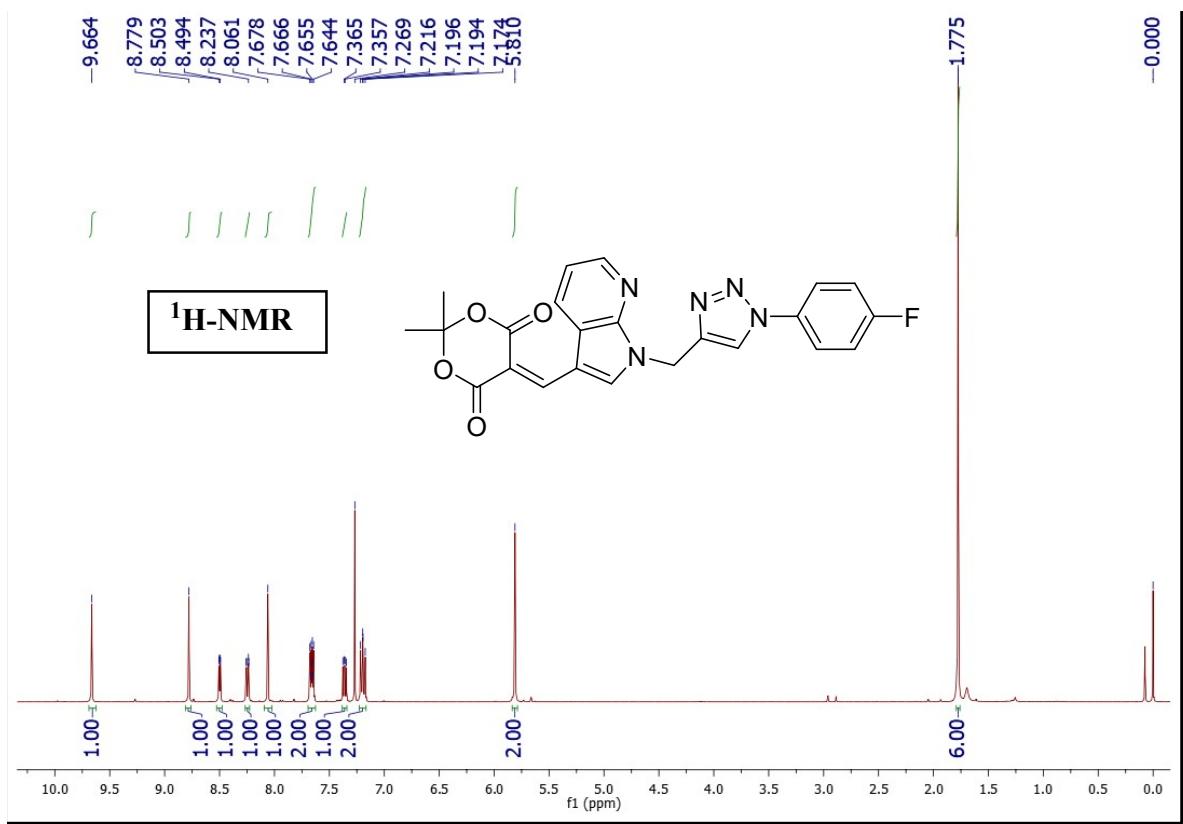
5-((1-((1-(3,4-dichlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6g):



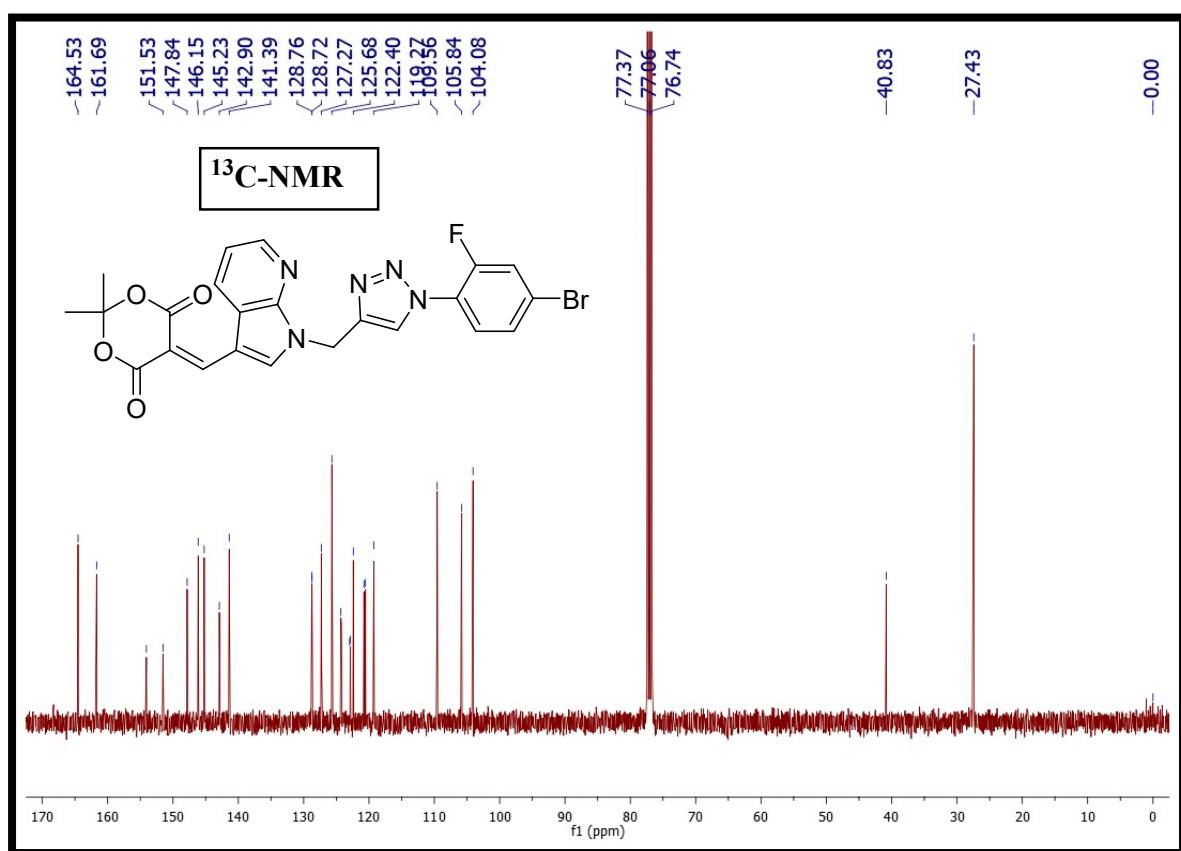
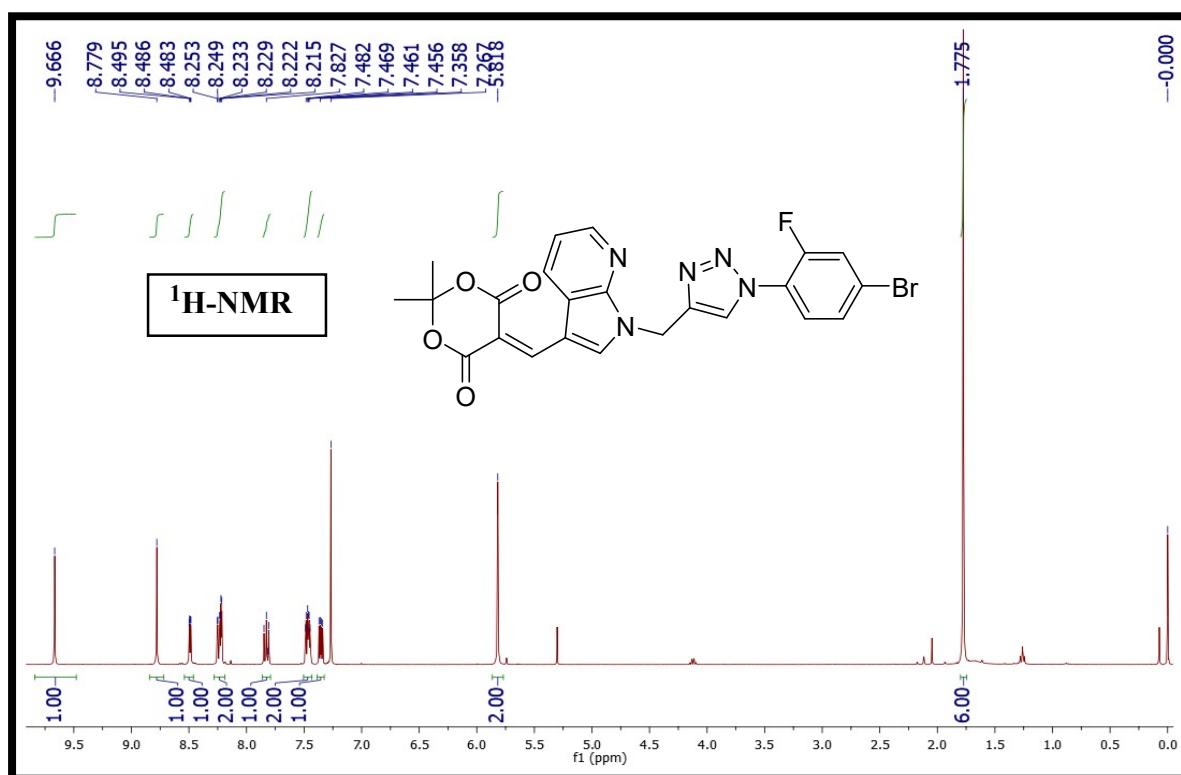
5-((1-((1-(3,5-dichlorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6h):



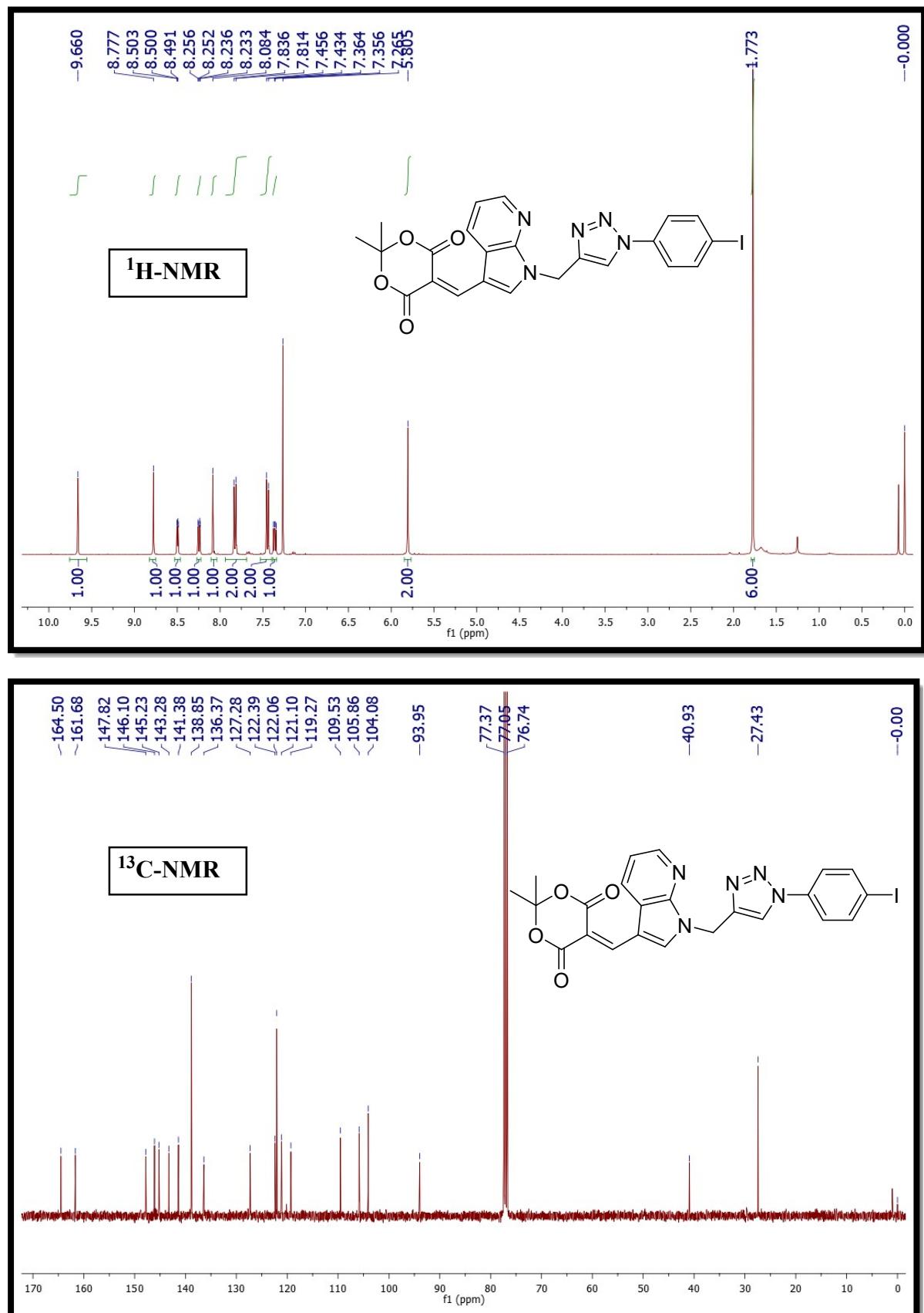
5-((1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6i):



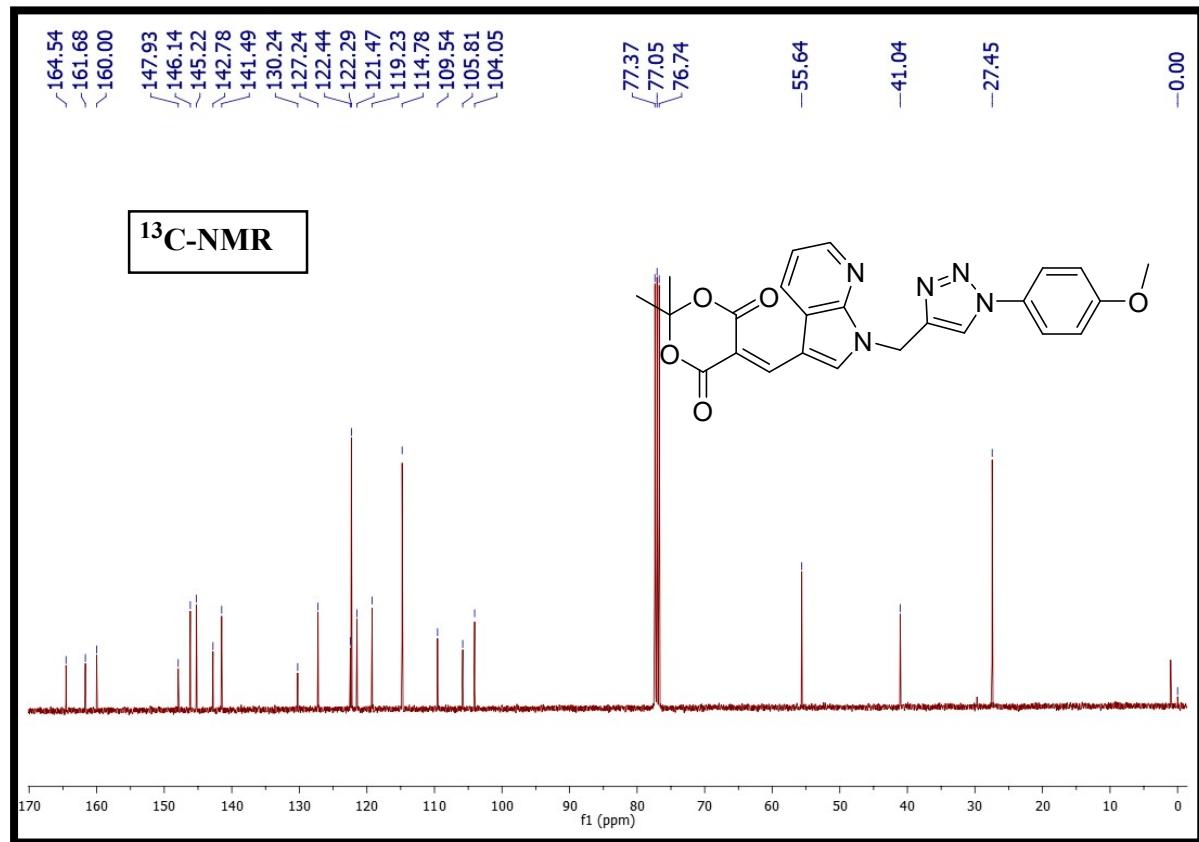
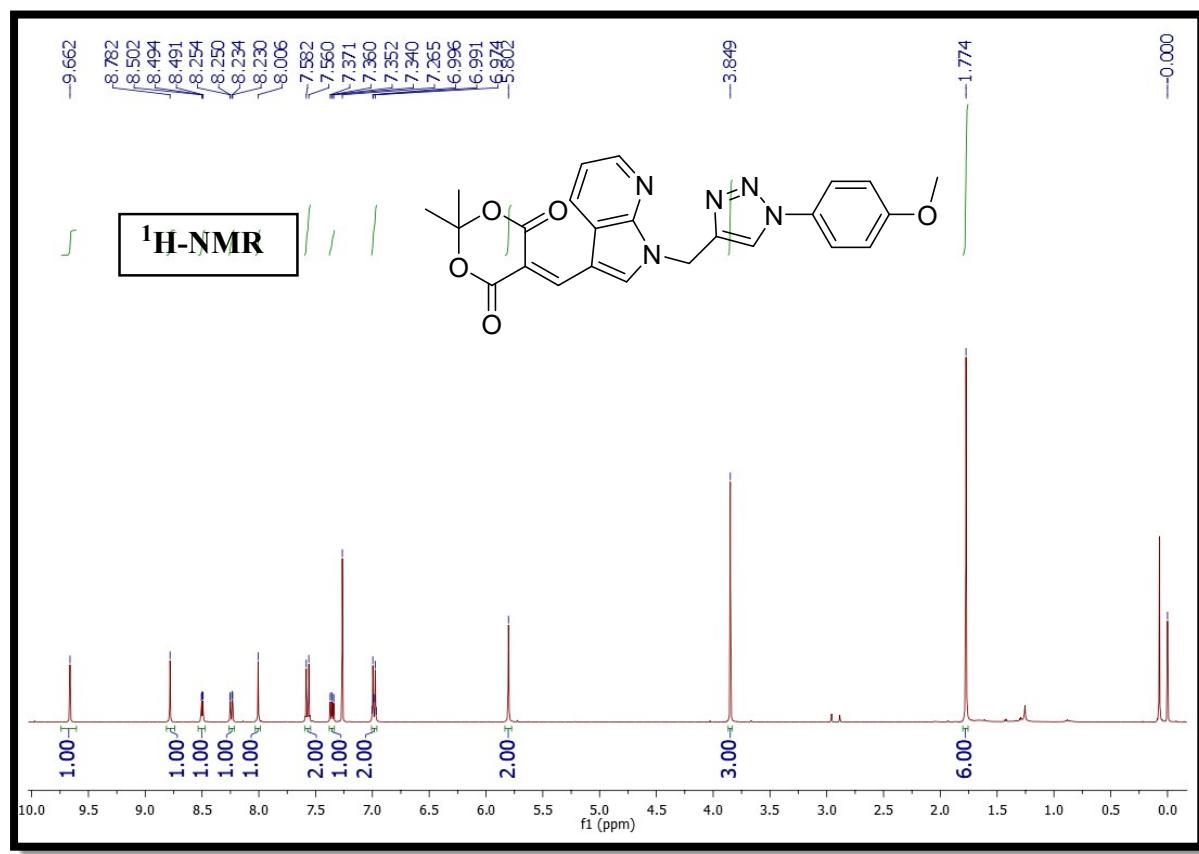
5-((1-((1-(4-bromo-2-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6j):



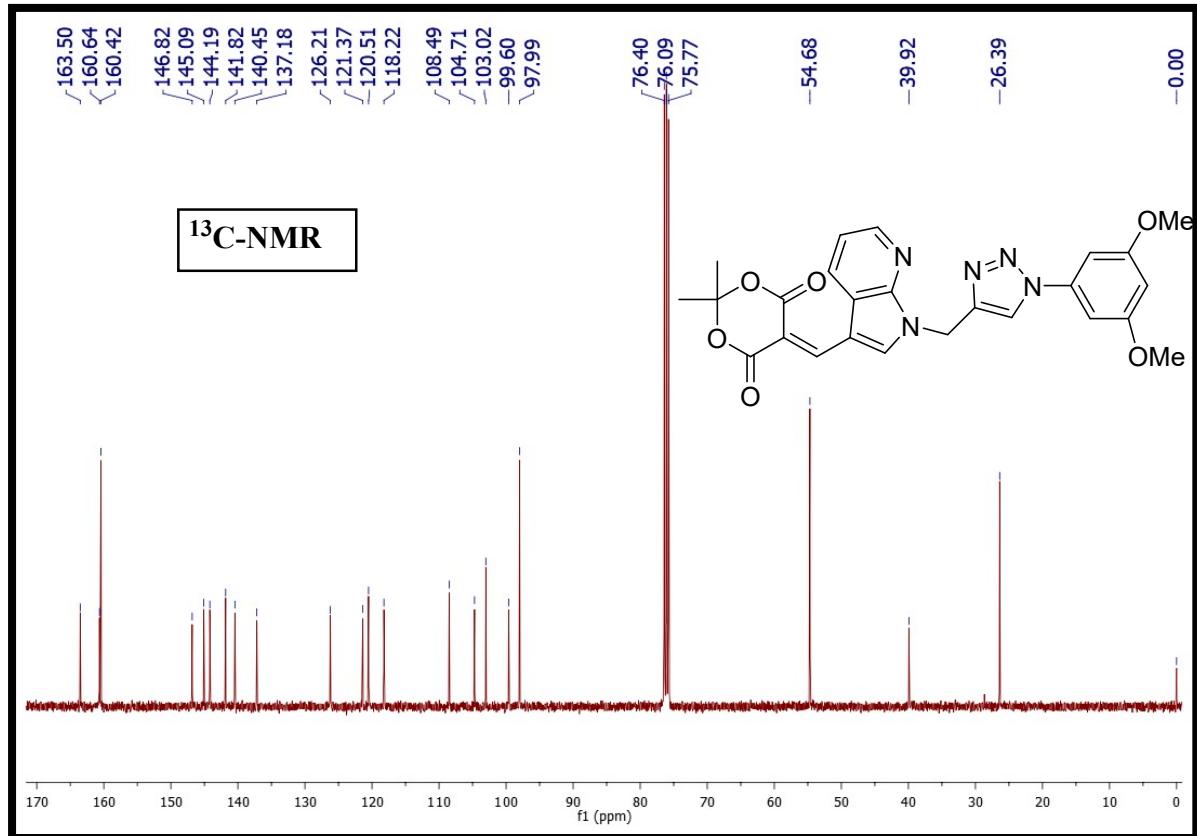
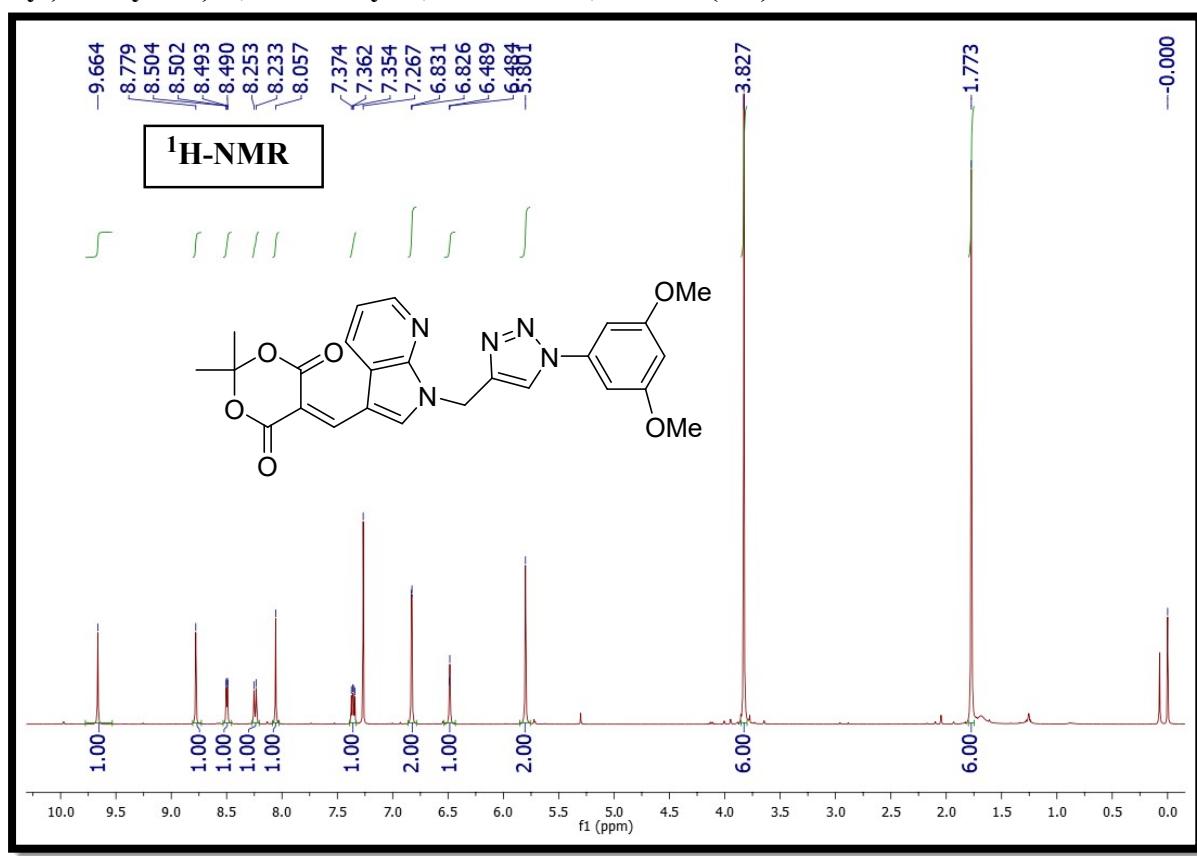
5-((1-((1-(4-iodophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6k):



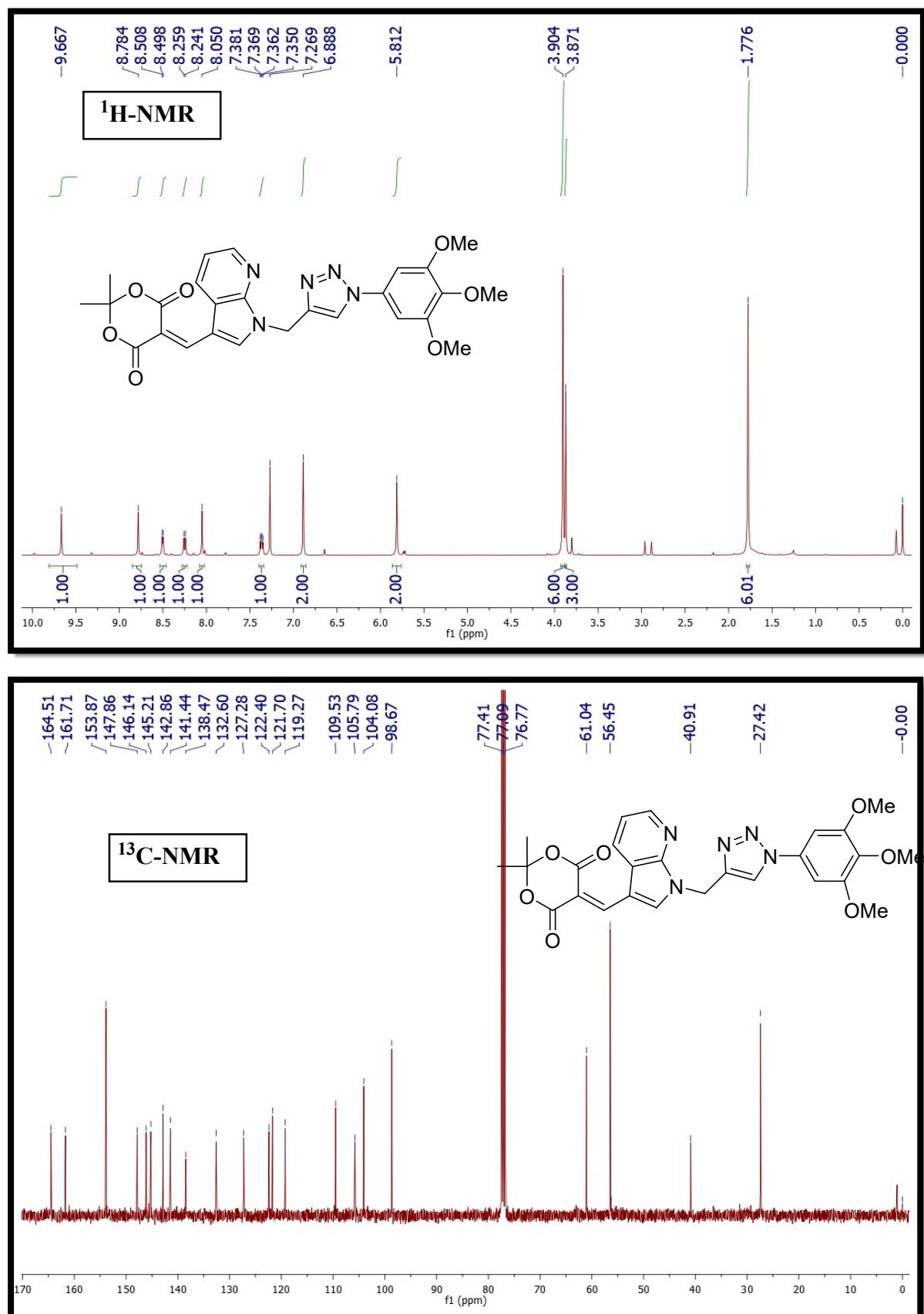
5-((1-((1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6l):



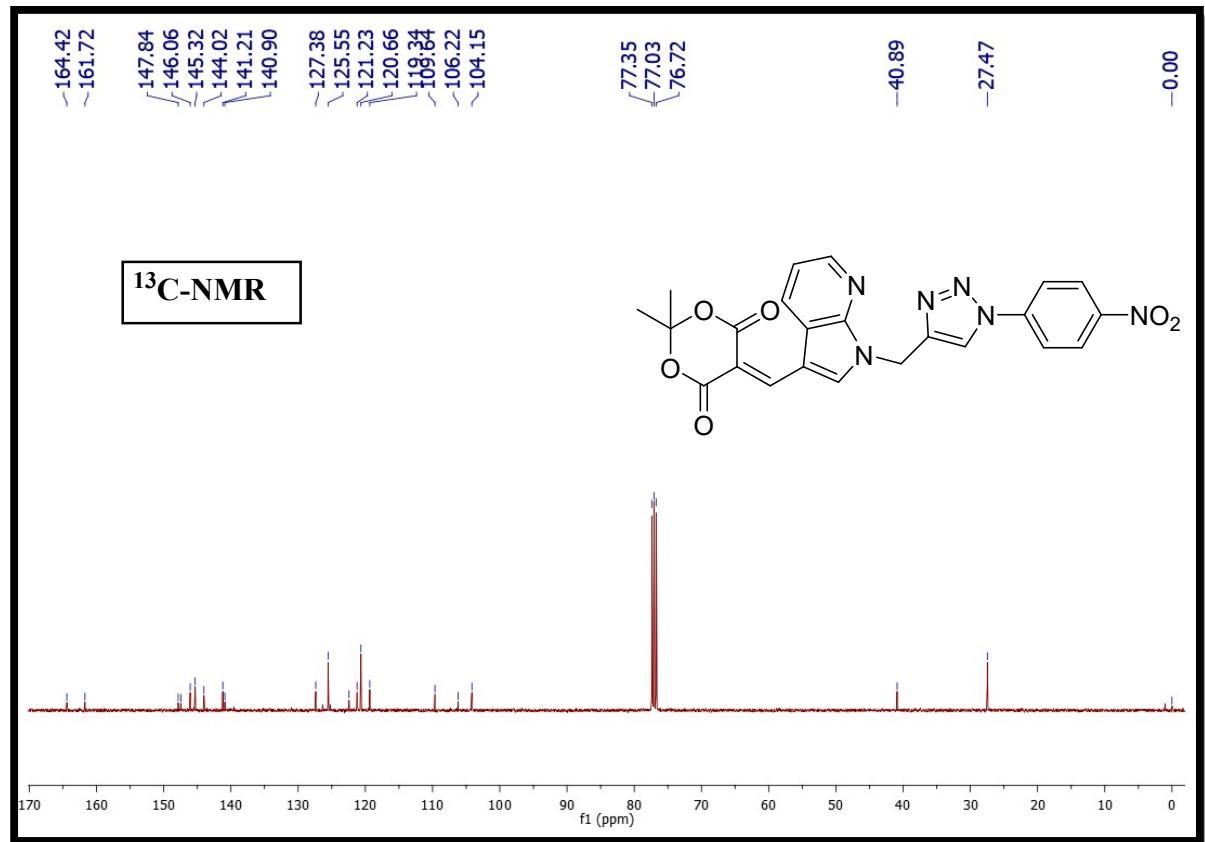
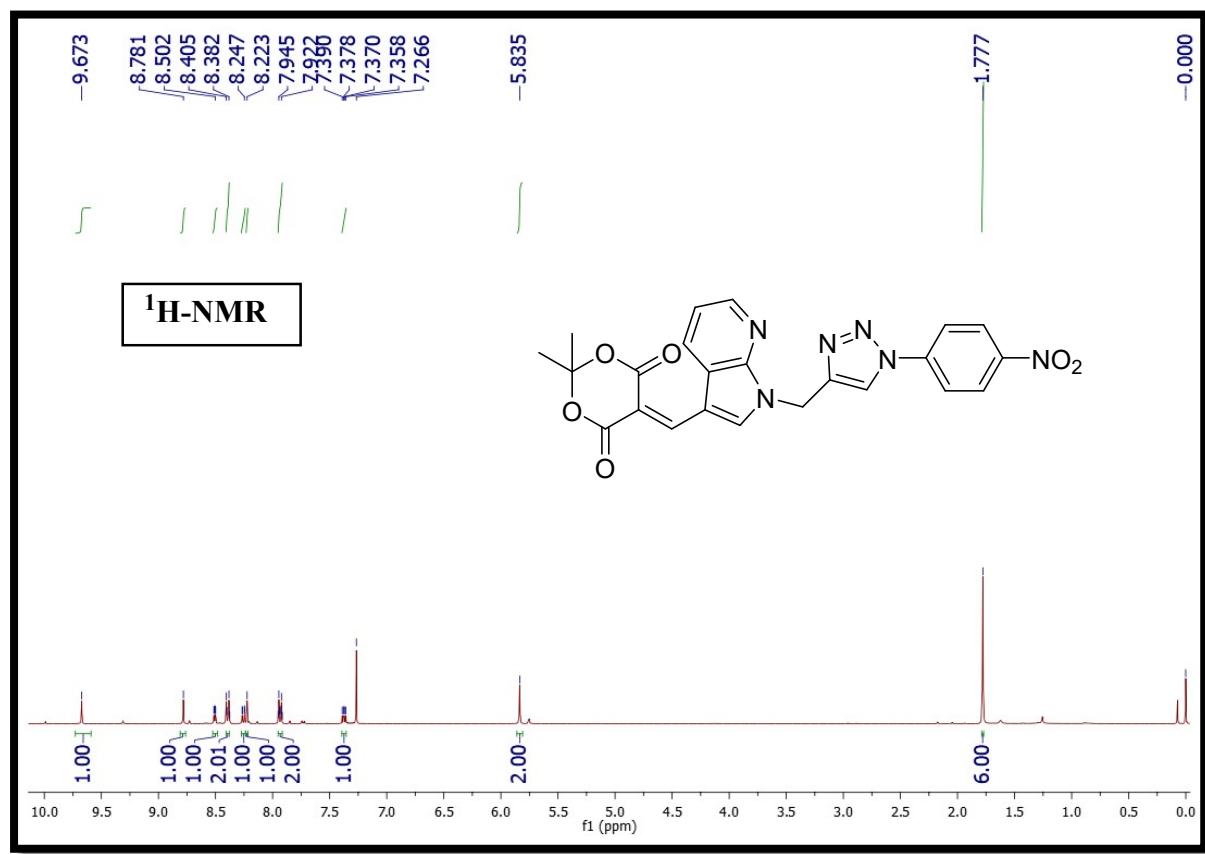
5-((1-((1-(3,5-dimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (6m):

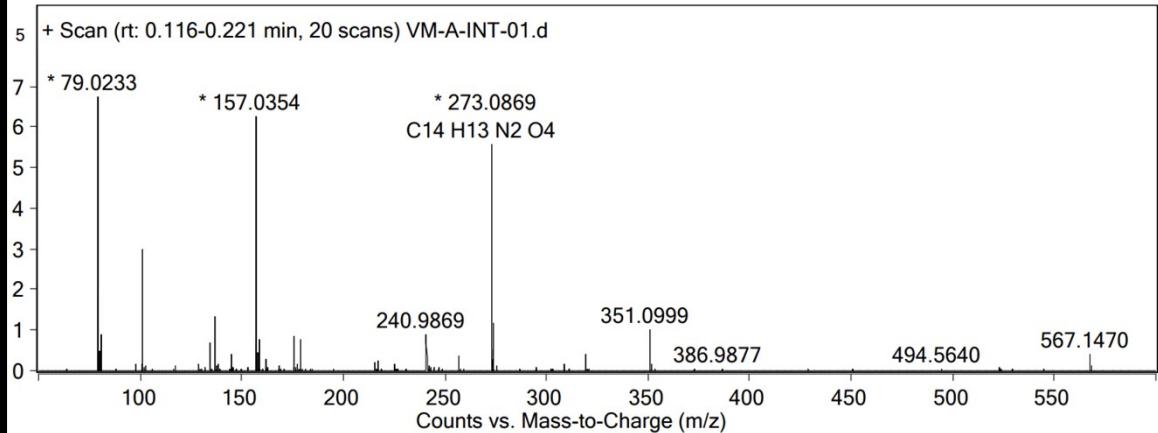


2,2-dimethyl-5-((1-((1-(3,4,5-trimethoxyphenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-1,3-dioxane-4,6-dione (6n):

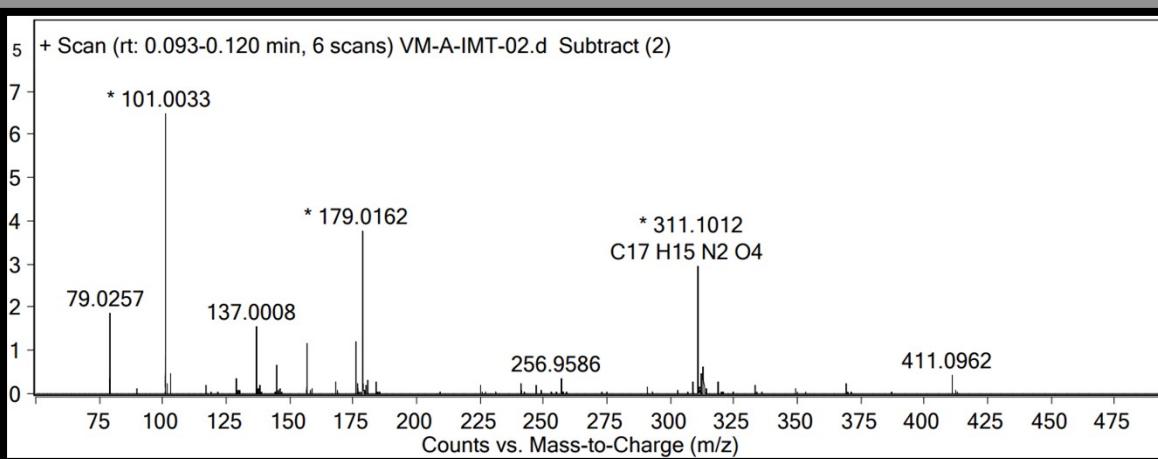


2,2-dimethyl-5-((1-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-1,3-dioxane-4,6-dione (6o):



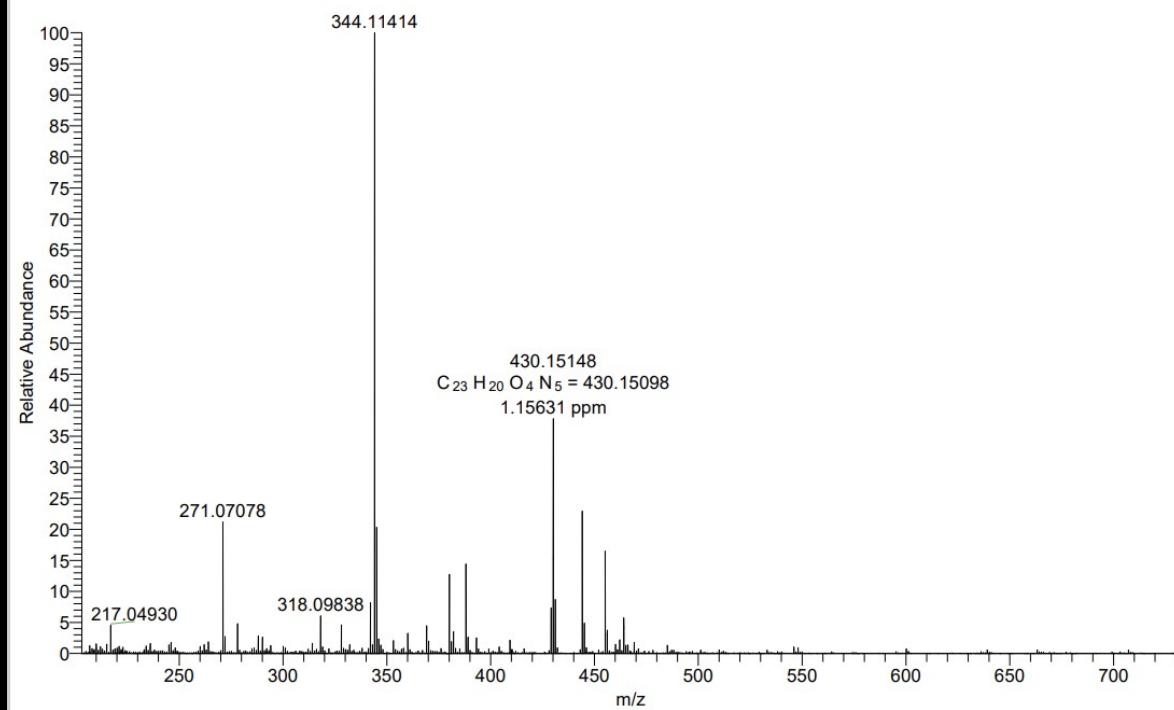


HRMS of compound 3



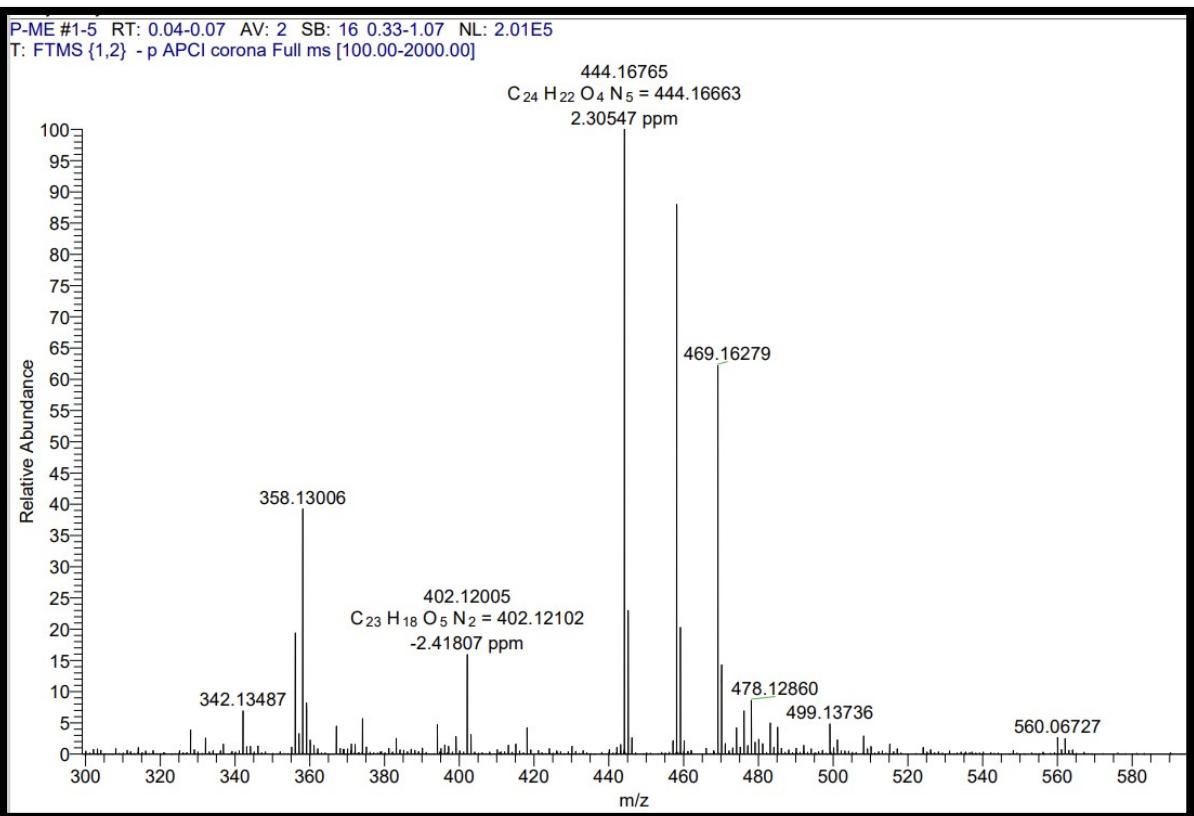
HRMS of compound 4

SIMPLE #3-10 RT: 0.06-0.15 AV: 4 SB: 18 0.32-1.07 NL: 4.73E5
T: FTMS {1,2} - p APCI corona Full ms [100.00-2000.00]

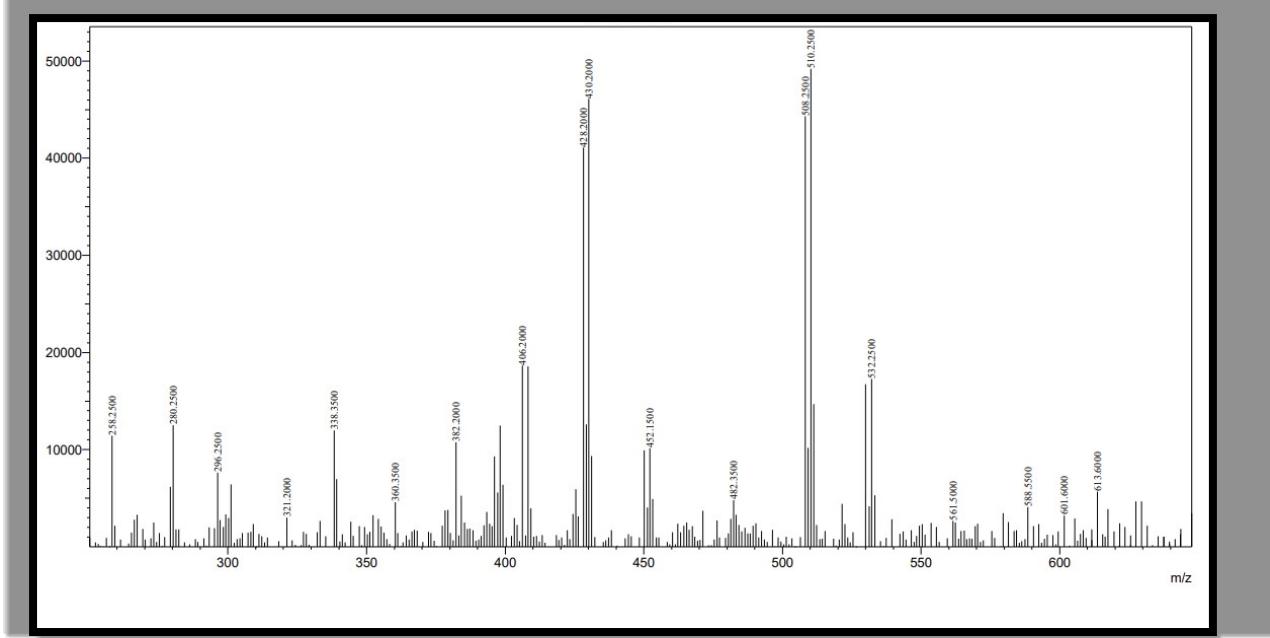


HRMS of compound 6a

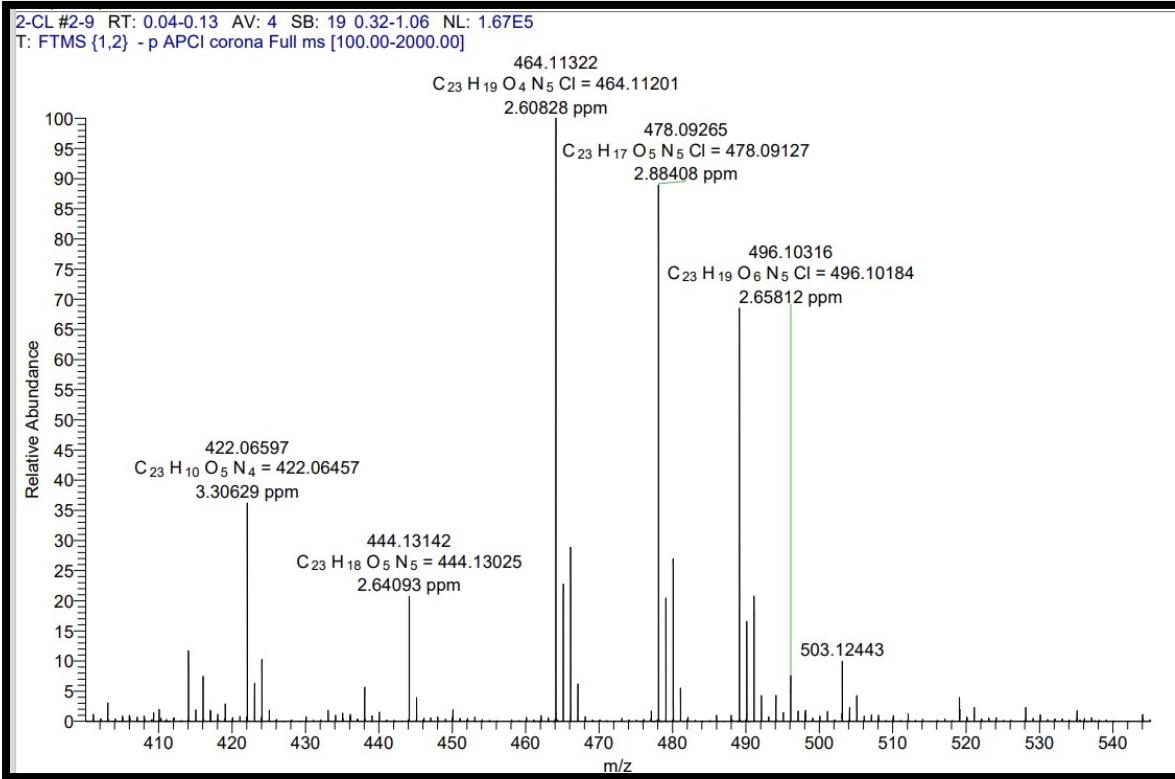
P-ME #1-5 RT: 0.04-0.07 AV: 2 SB: 16 0.33-1.07 NL: 2.01E5
T: FTMS {1,2} - p APCI corona Full ms [100.00-2000.00]



HRMS of compound 6b

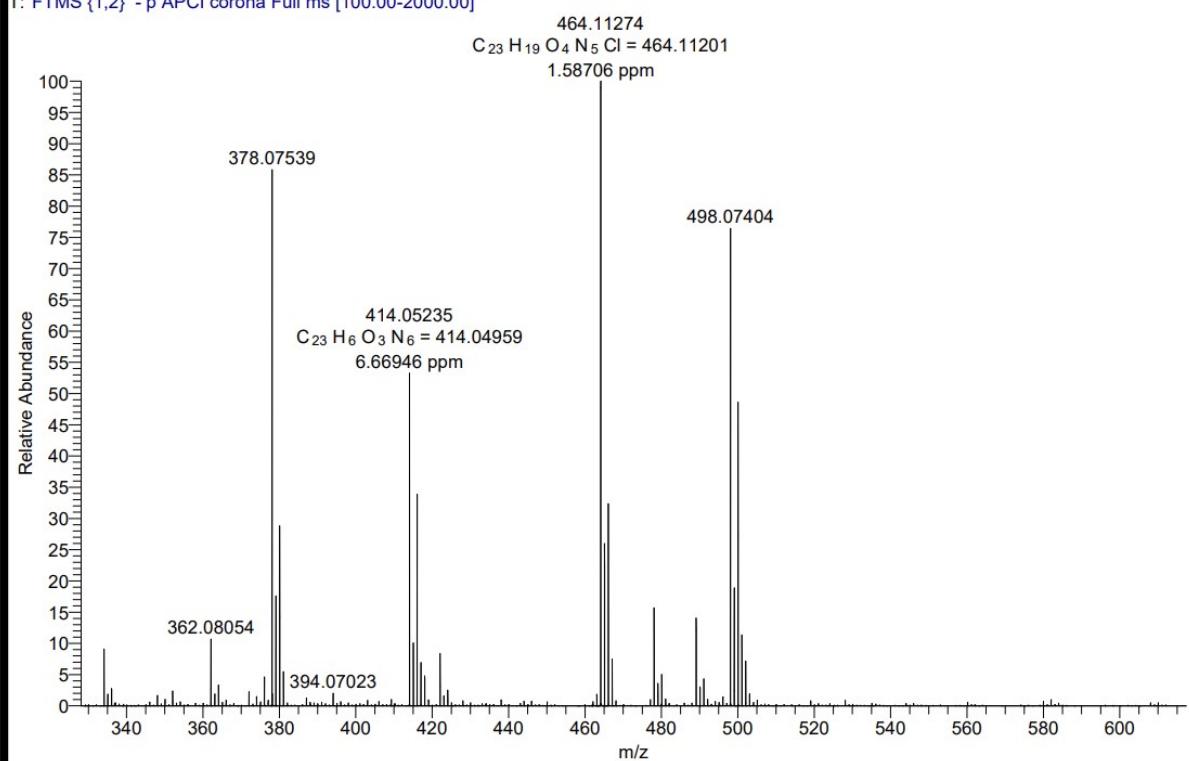


ESI Mass of 6c



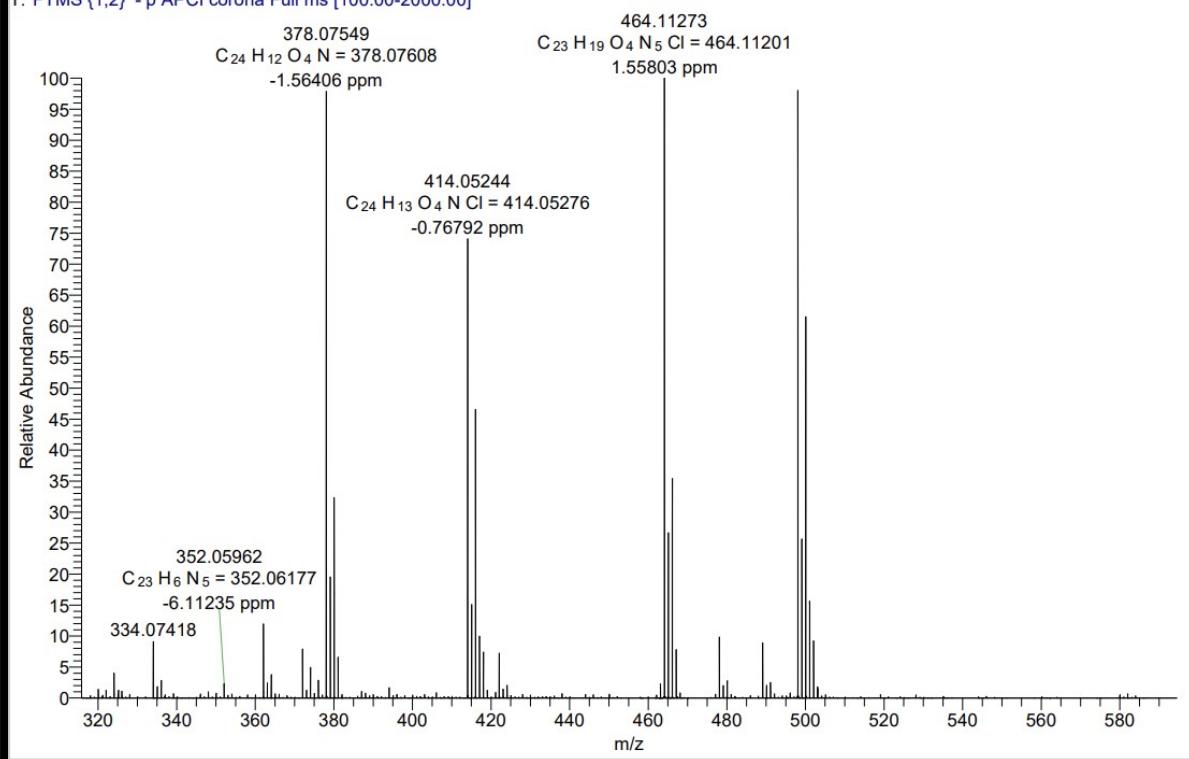
HRMS of compound 6d

3-CL #1-9 RT: 0.03-0.11 AV: 4 SB: 19 0.32-1.08 NL: 1.61E6
T: FTMS {1,2} - p APCI corona Full ms [100.00-2000.00]

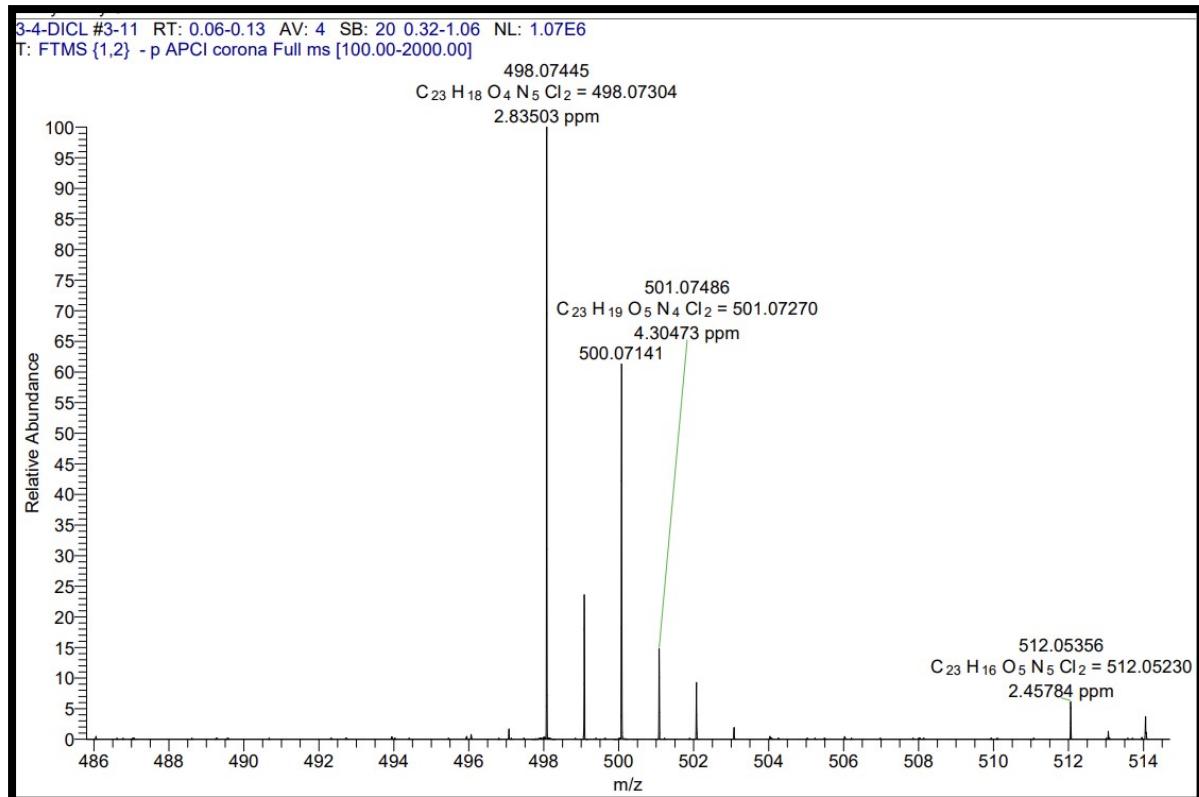


HRMS of compound 6e

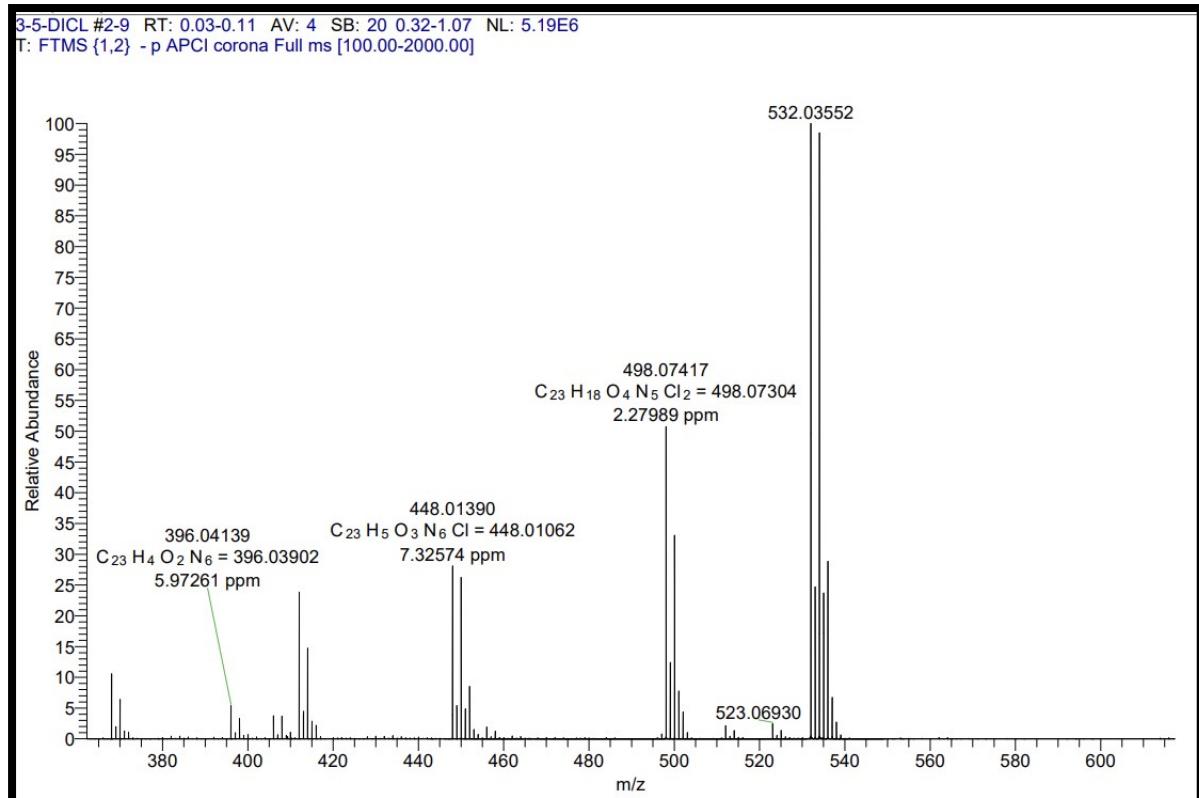
P-CL #1-6 RT: 0.03-0.08 AV: 3 SB: 21 0.32-1.04 NL: 3.79E6
T: FTMS {1,2} - p APCI corona Full ms [100.00-2000.00]



HRMS of compound 6f

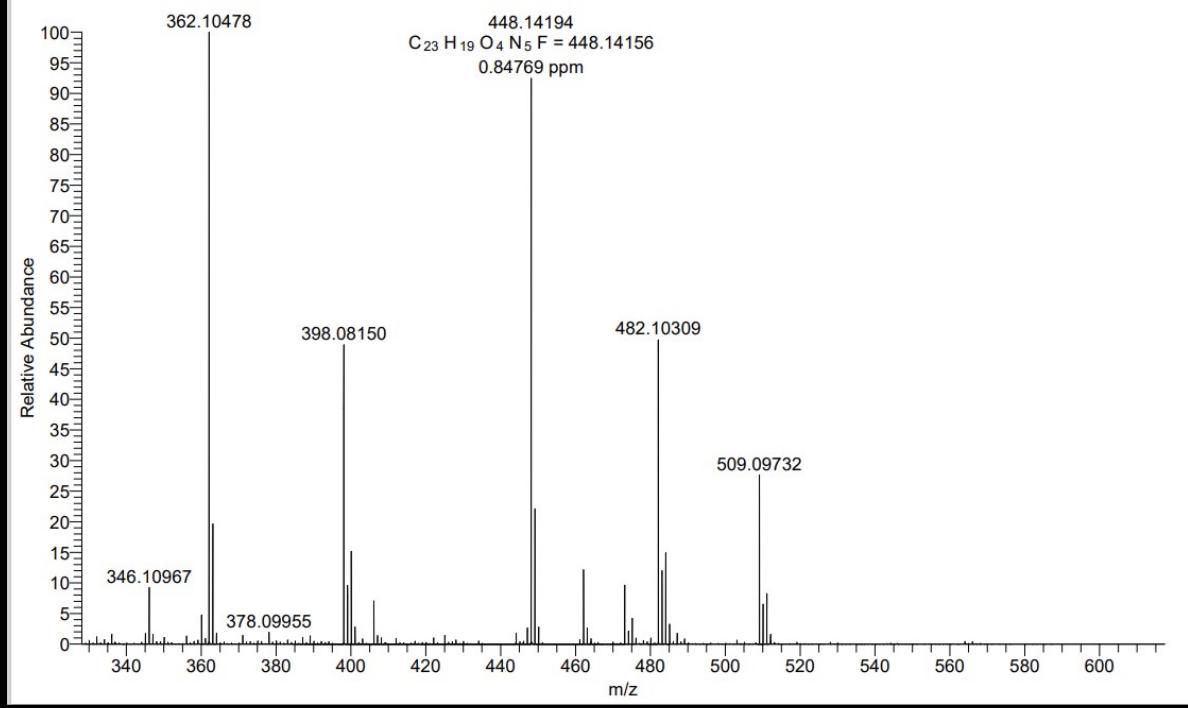


HRMS of compound 6g

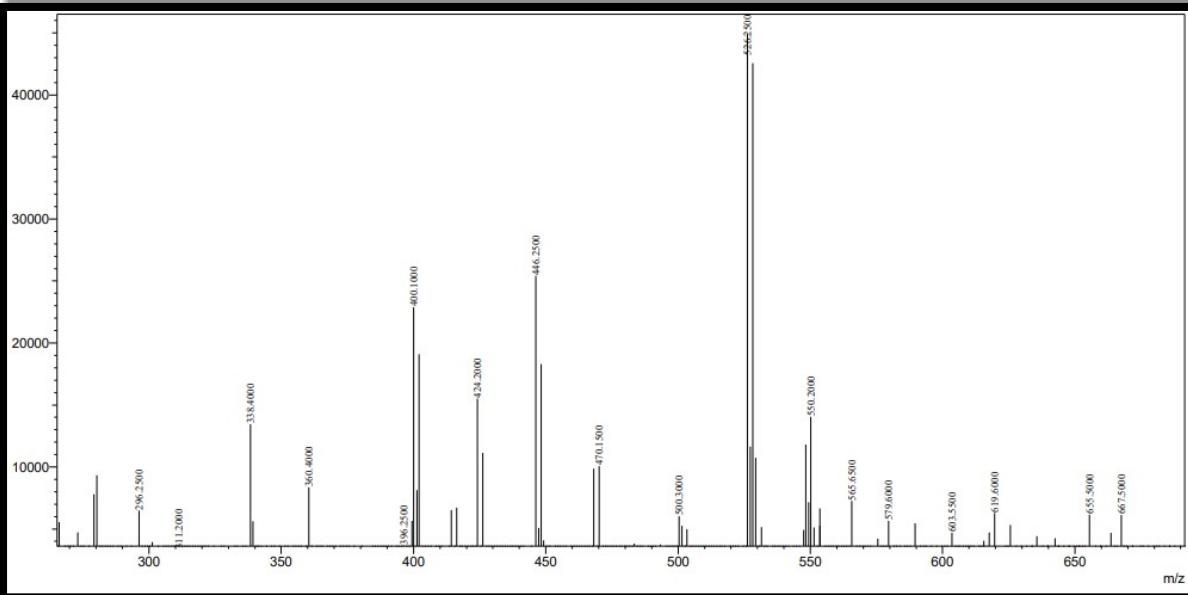


HRMS of compound 6h

4-F #1-8 RT: 0.04-0.12 AV: 4 SB: 20 0.32-1.08 NL: 1.38E6
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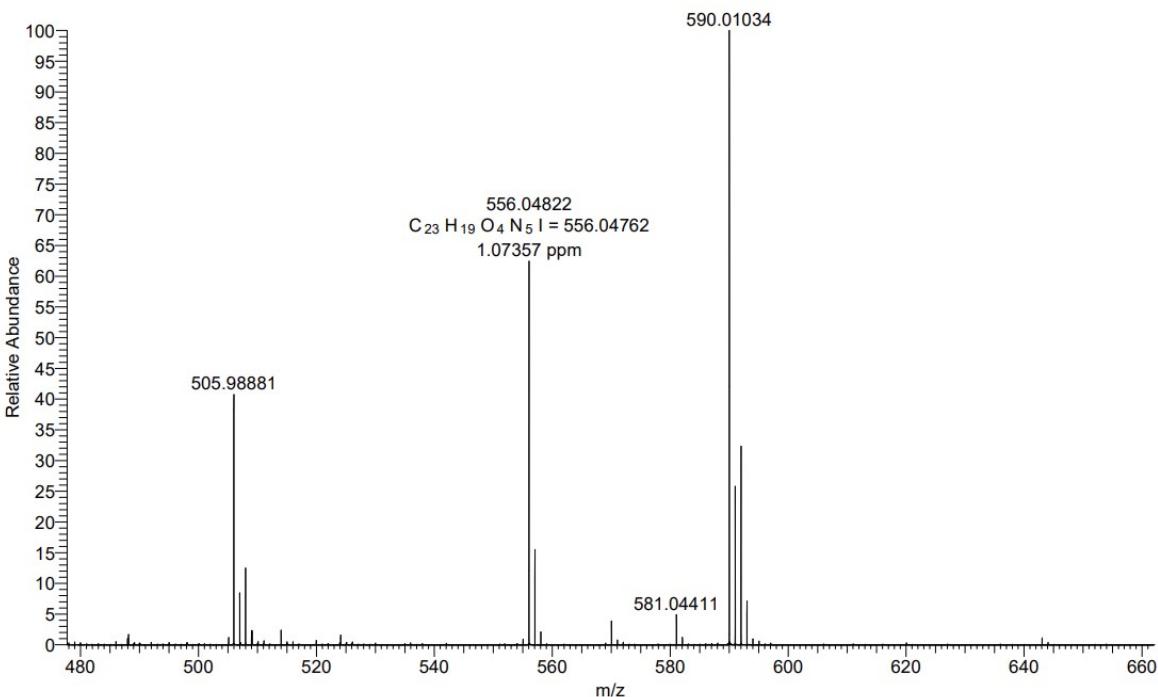


HRMS of compound 6i



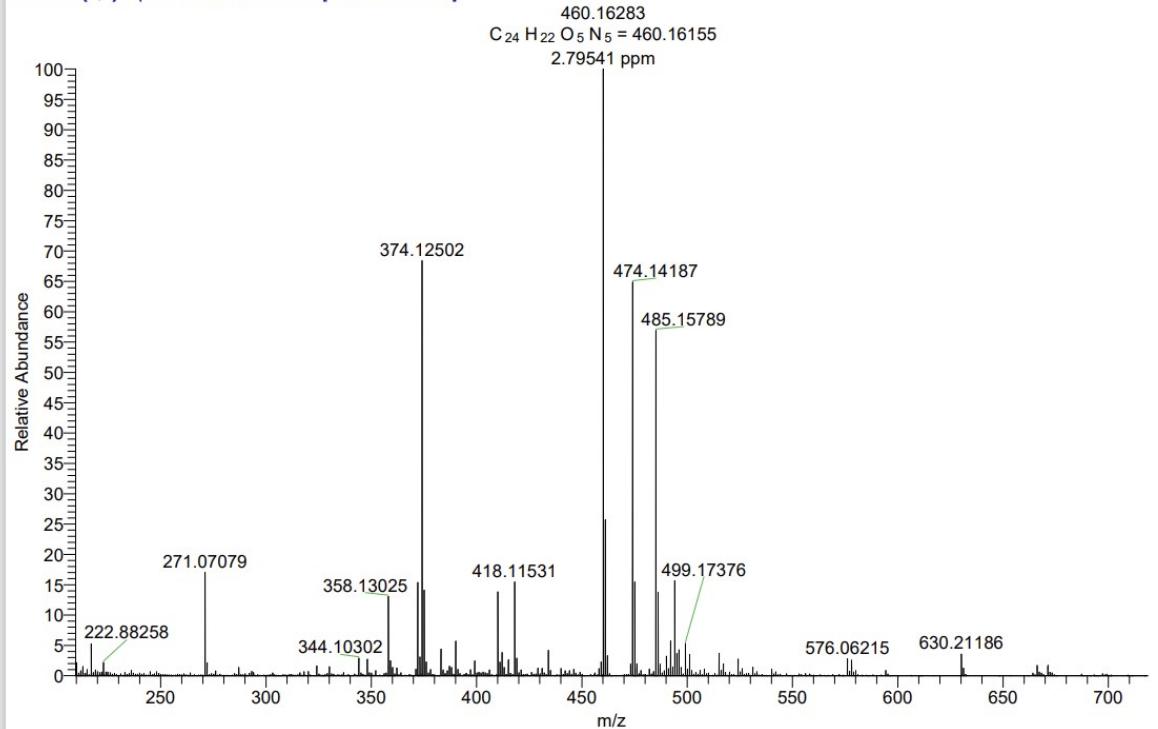
ESI Mass of 6j

P-I #2-8 RT: 0.03-0.11 AV: 4 SB: 18 0.33-1.04 NL: 2.51E6
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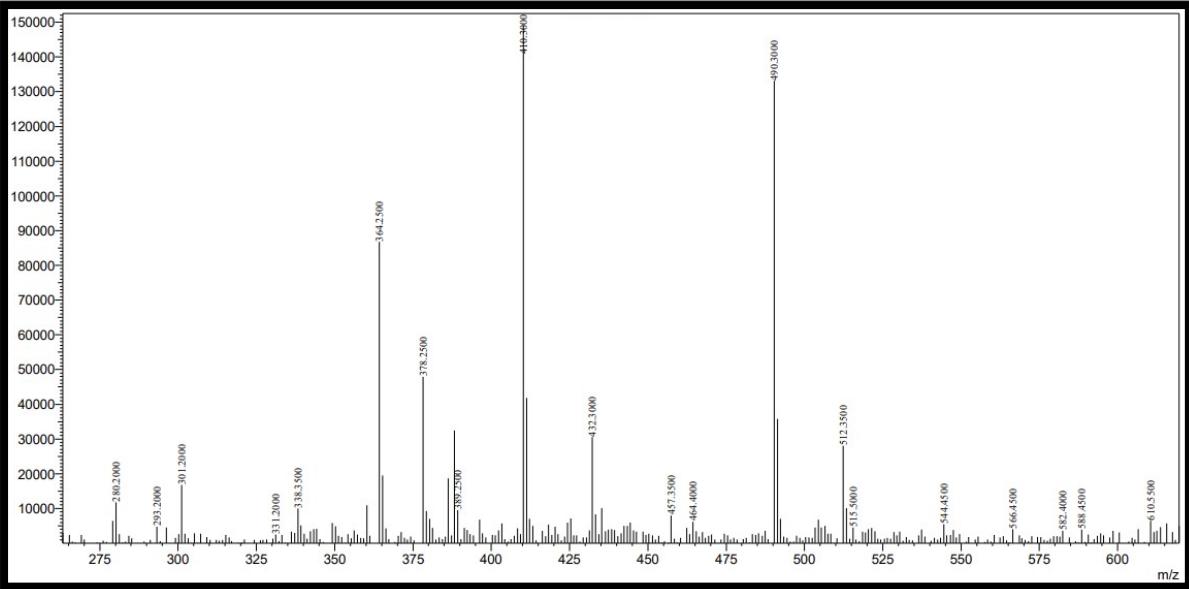


HRMS of compound 6k

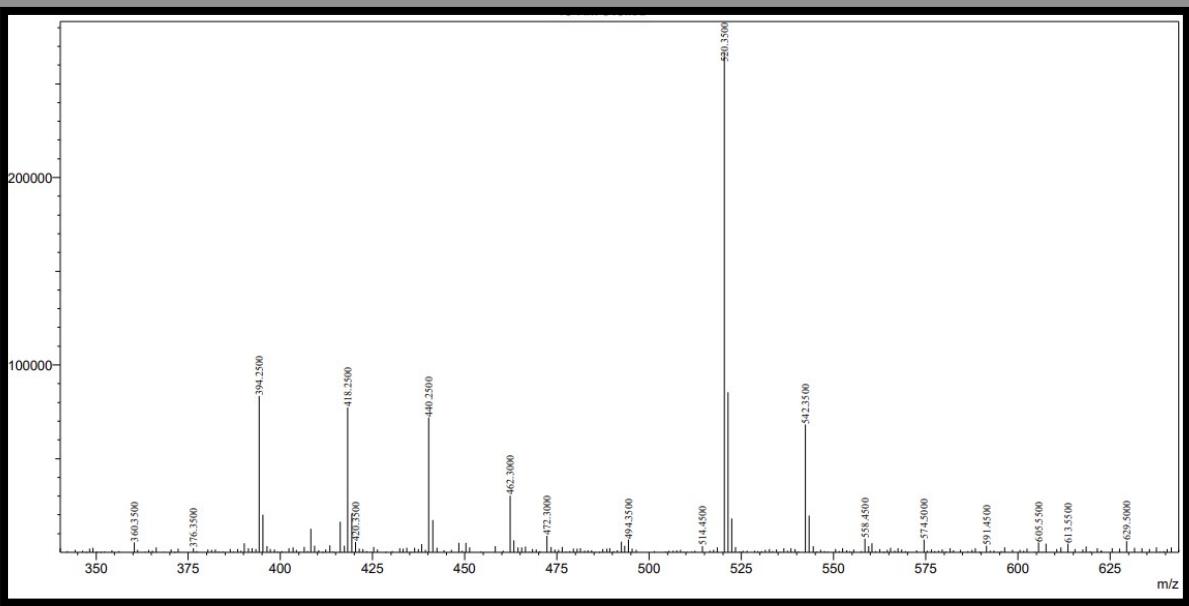
P-OME #2-6 RT: 0.03-0.09 AV: 3 SB: 17 0.33-1.07 NL: 3.48E5
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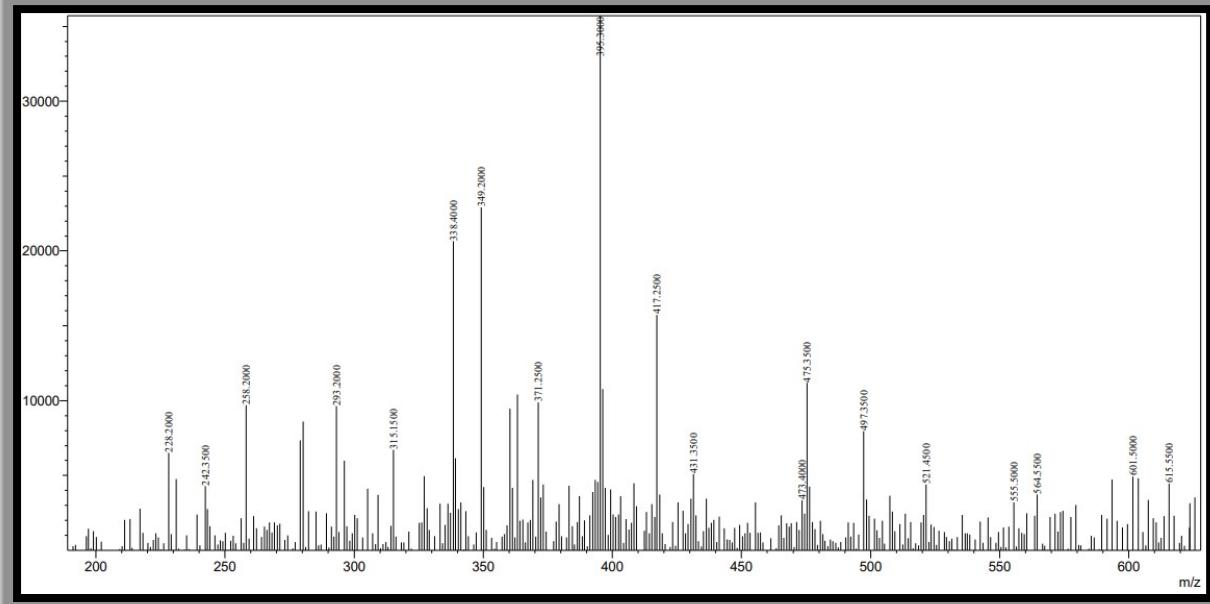
HRMS of compound 6l



ESI Mass of 6m



ESI Mass of 6n



ESI Mass of 6o