

**Molecular diversity of three-component reaction of α -amino acids, dialkyl
acetylenedicarboxylates and N-substituted maleimides**

Liang Chen, Jing Sun*, Ju Xie, Chao-Guo Yan*

Supporting Information

Figures of single crystal structures	2-4
^1H and ^{13}C NMR, HRMS spectra of the compounds	5-43

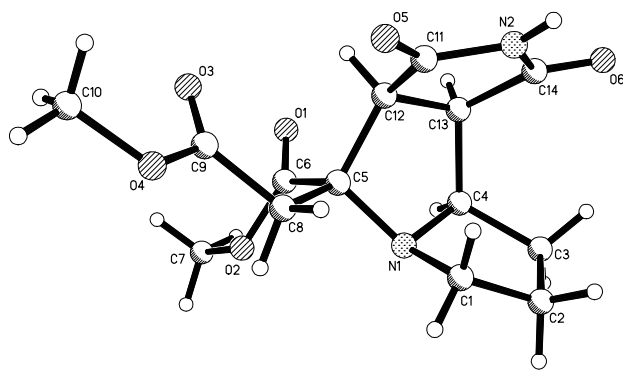


Fig. s1 ORTEP-drawing of the crystal structure of **1a**

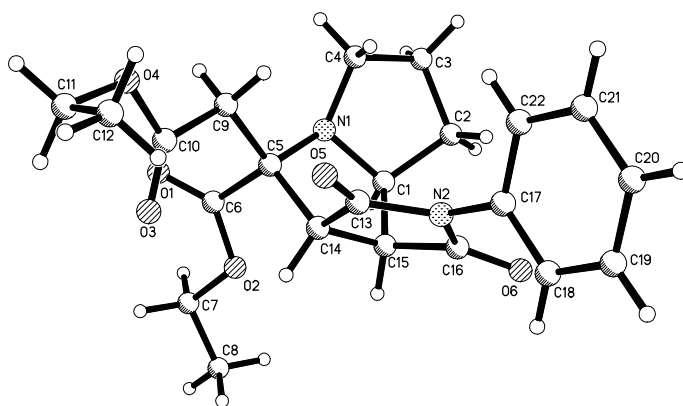


Fig. s2 ORTEP-drawing of the crystal structure of **1g**

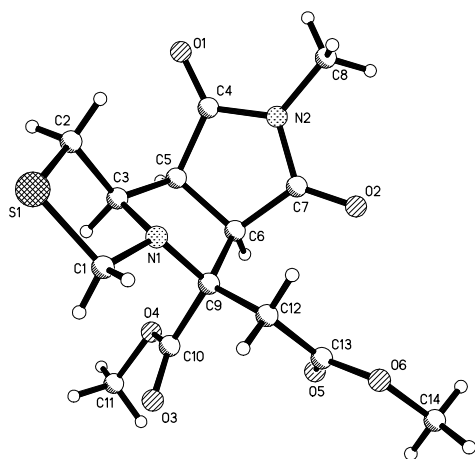


Fig. s3 ORTEP-drawing of the crystal structure of **2b**

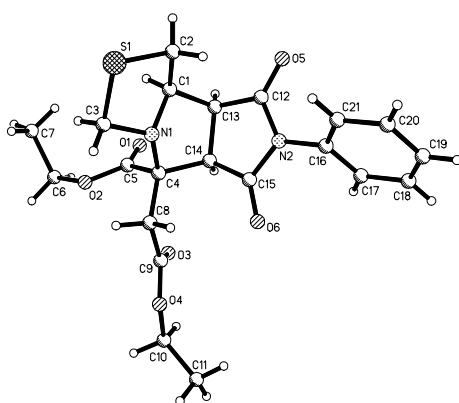


Fig. s4 ORTEP-drawing of the crystal structure of **2g**

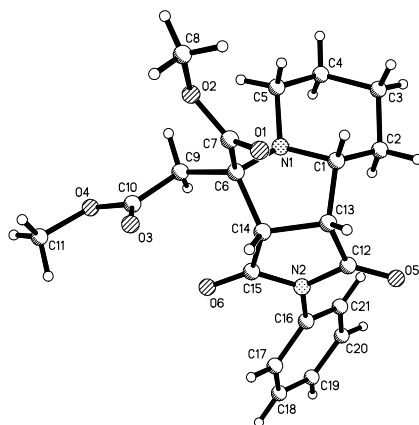


Fig. s5 ORTEP-drawing of the crystal structure of **3a**

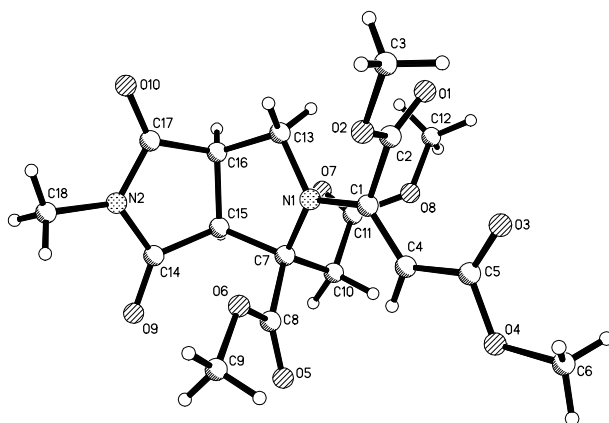


Fig. s6 ORTEP-drawing of the crystal structure of **4a**

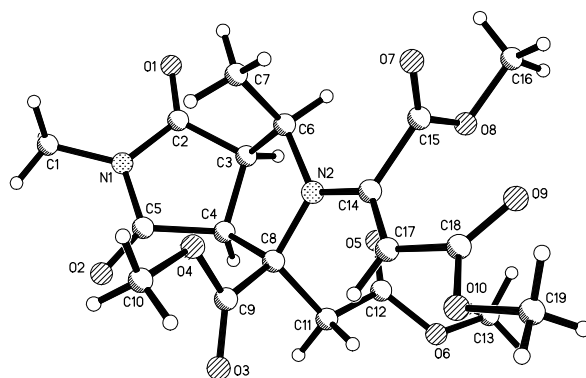


Fig. s7 ORTEP-drawing of the crystal structure of **4d**

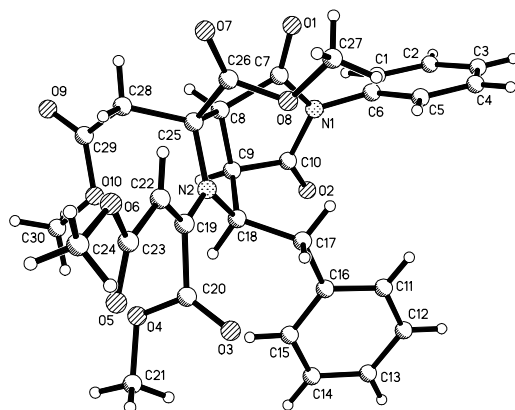


Fig. s8 ORTEP-drawing of the crystal structure of **4k**

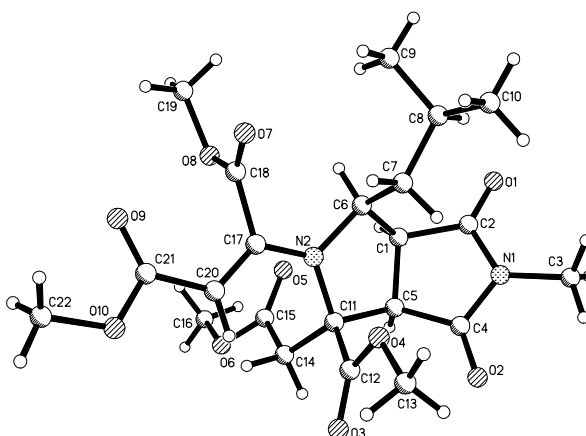
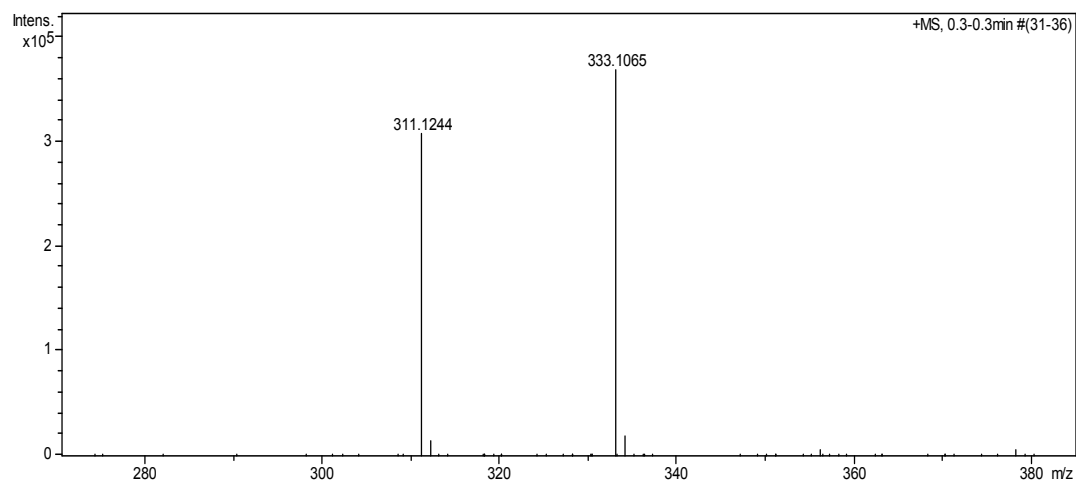
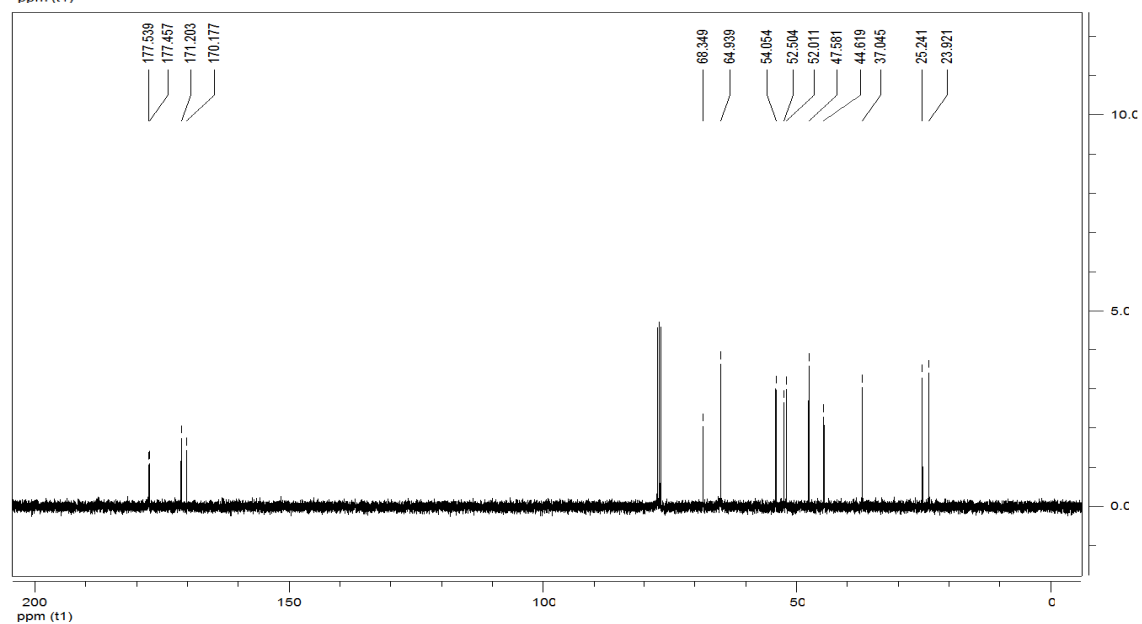
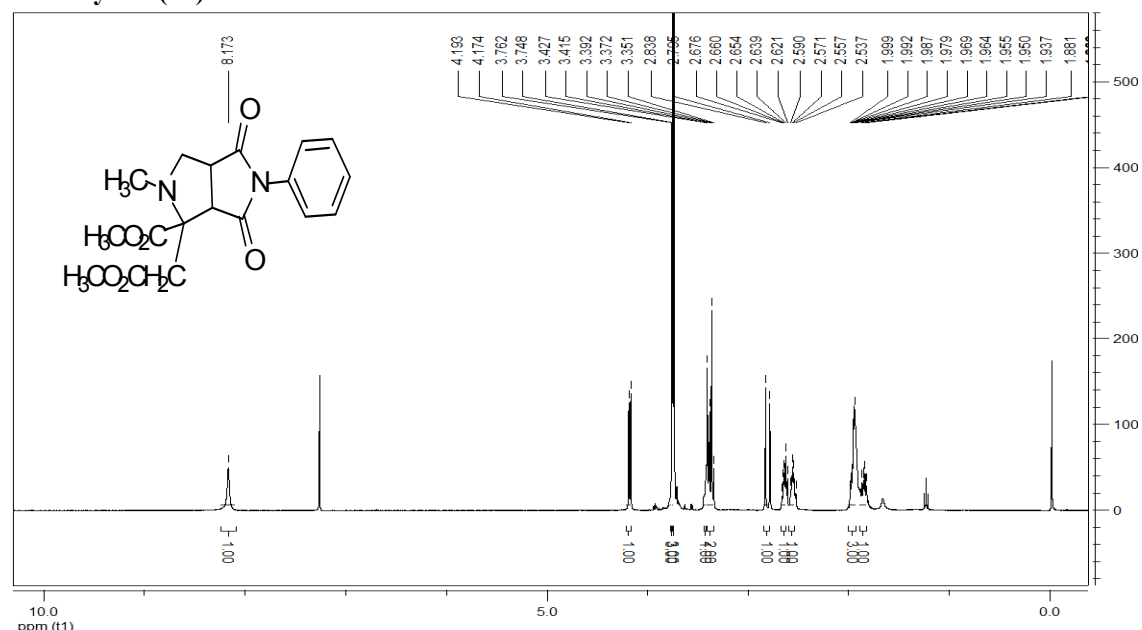
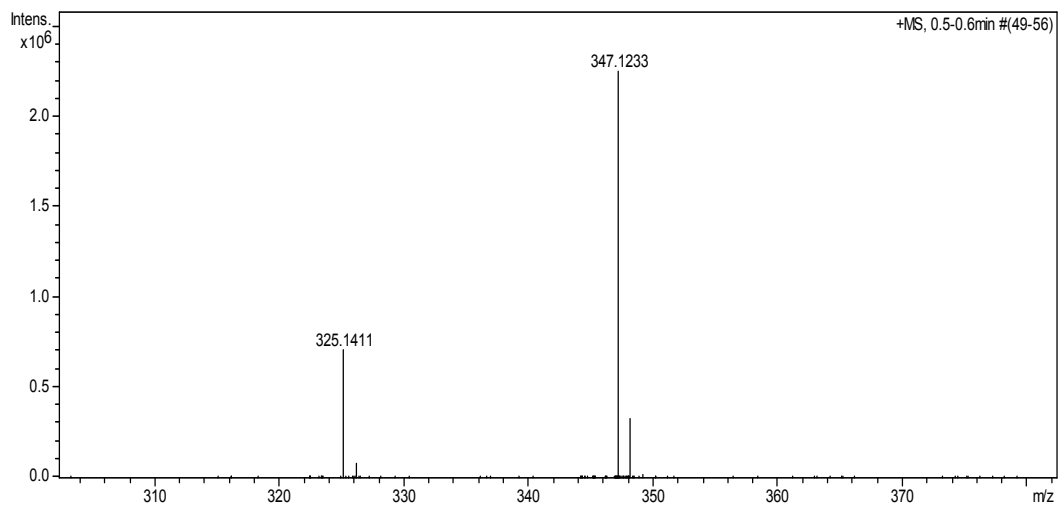
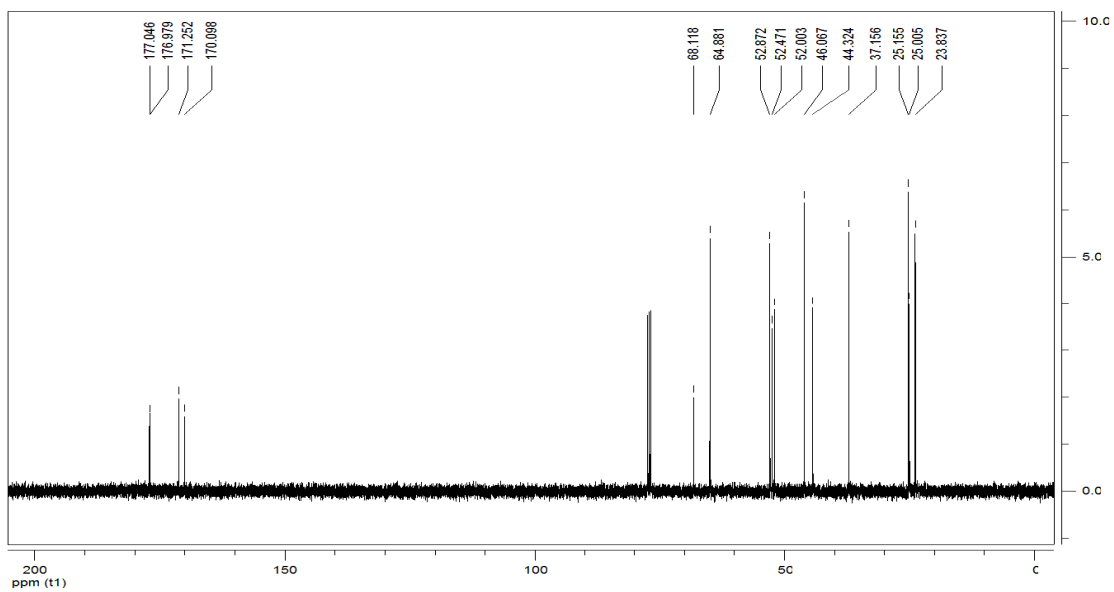
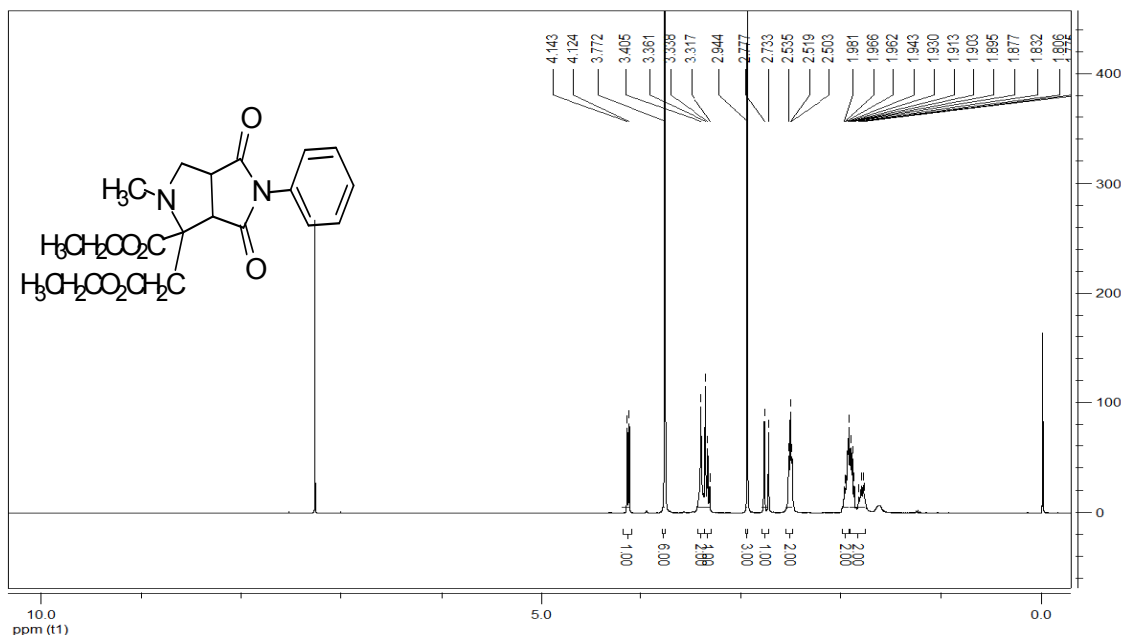


Fig. s9 ORTEP-drawing of the crystal structure of **4m**

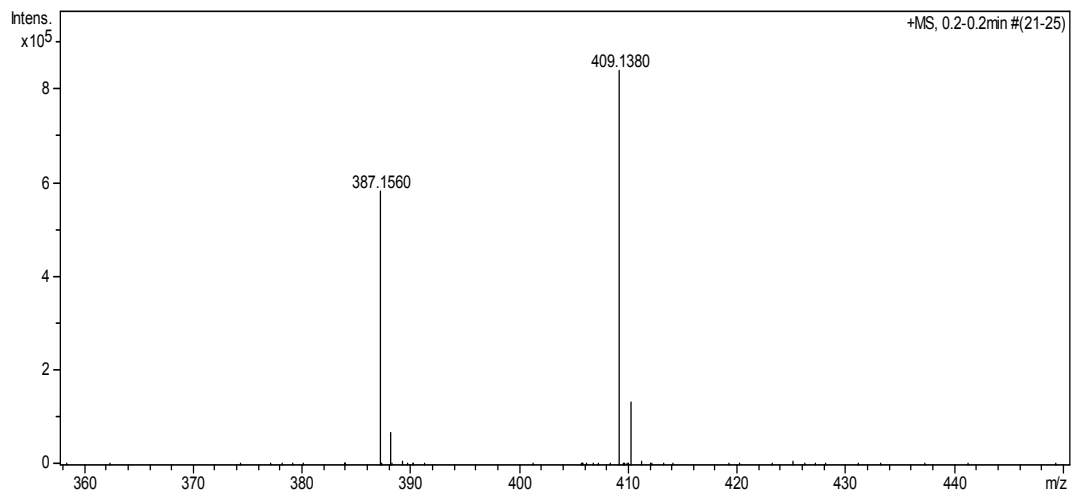
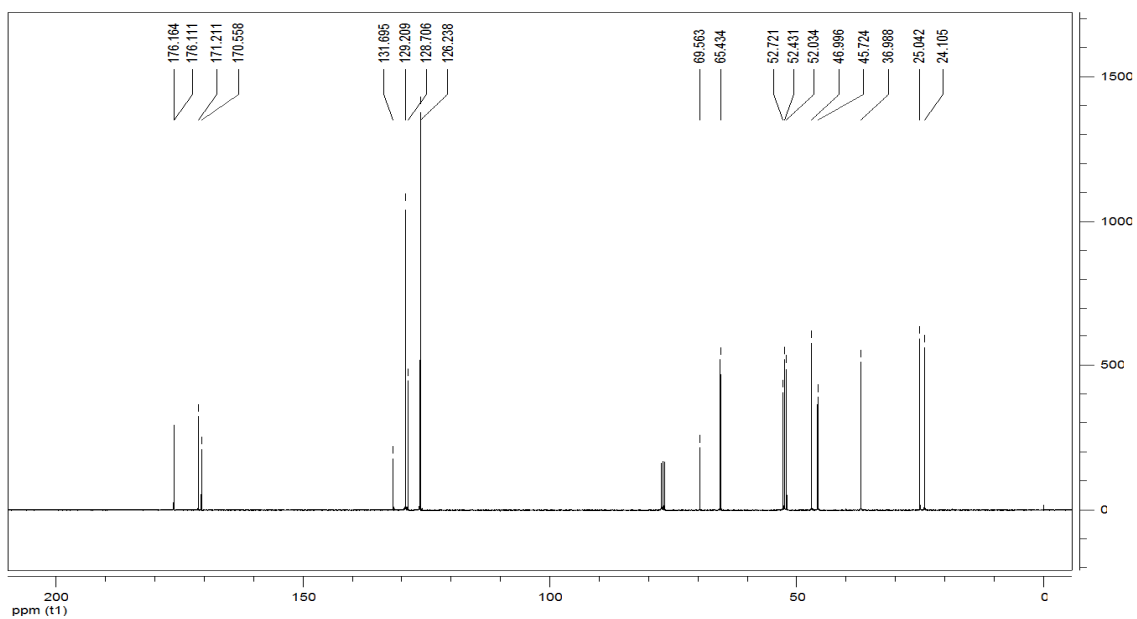
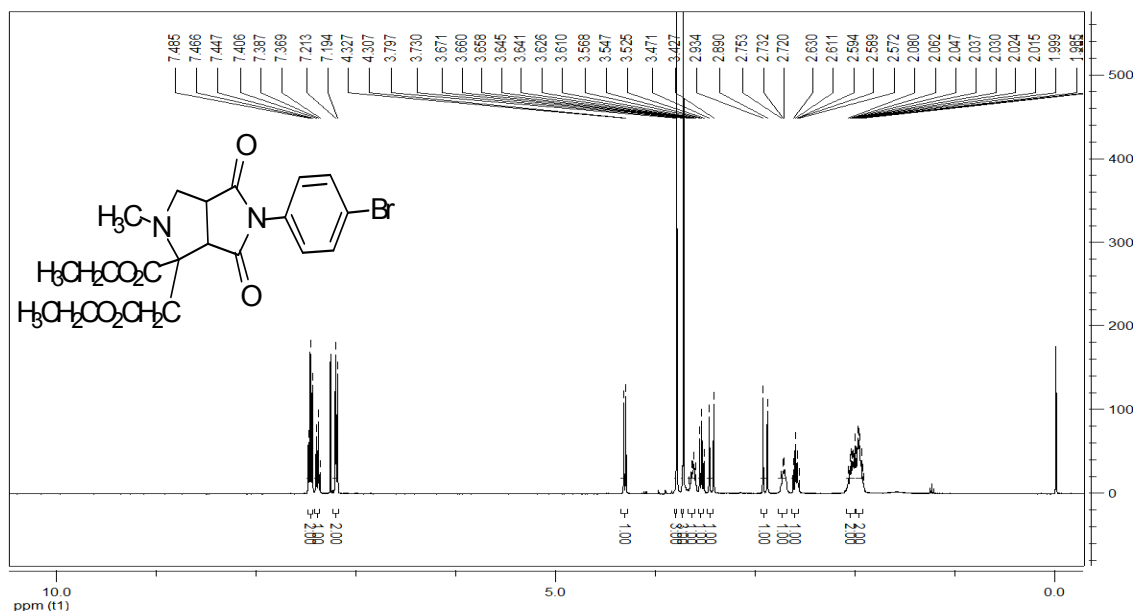
Methyl 4-(2-methoxy-2-oxoethyl)-1,3-dioxodecahydropyrrolo[3,4-a]pyrrolizine-4-carboxylate (1a):



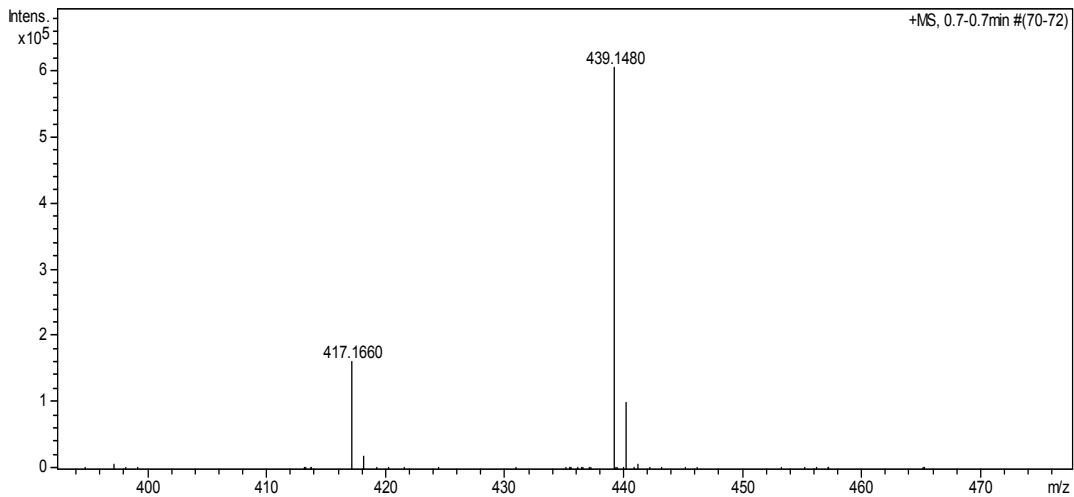
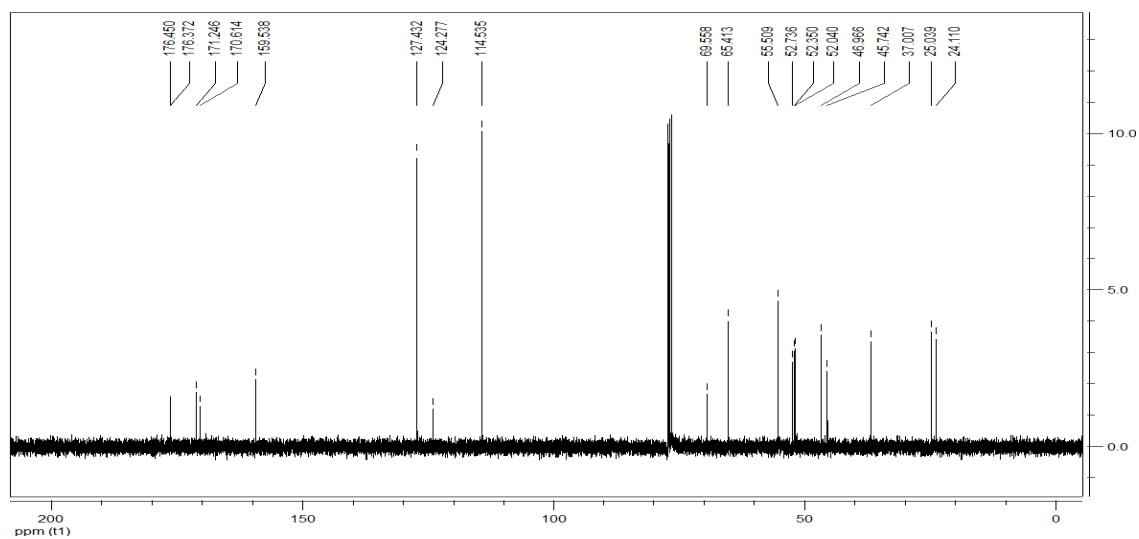
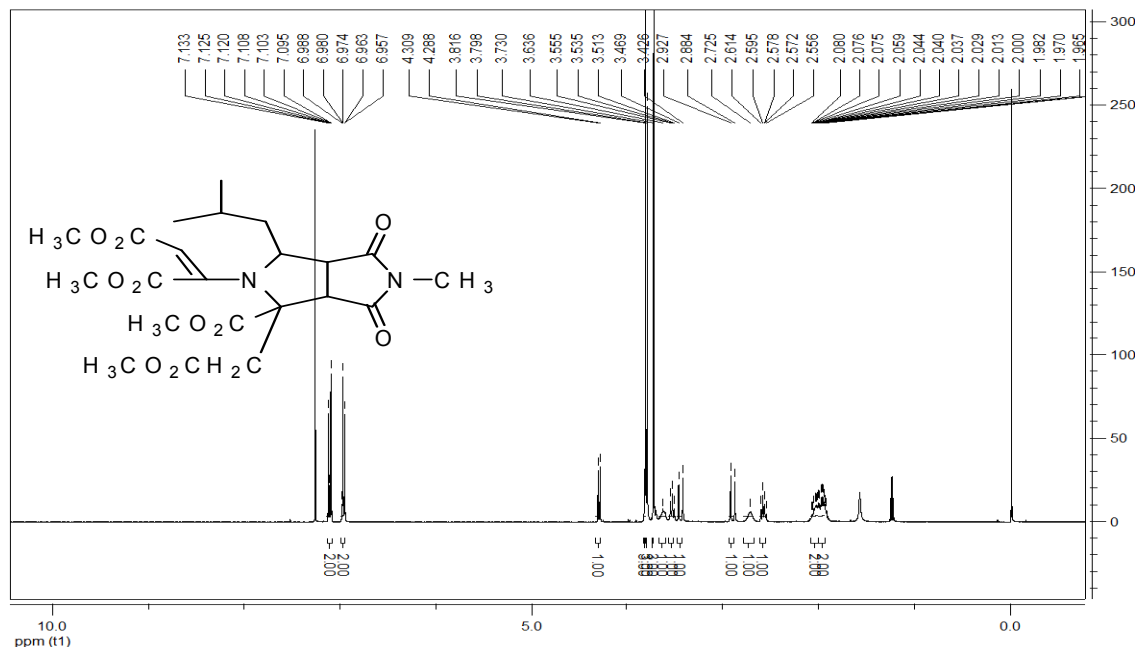
Methyl 4-(2-methoxy-2-oxoethyl)-2-methyl-1,3-dioxodecahydropyrrolo[3,4-a]pyrrolizine- 4-carboxylate(1b):



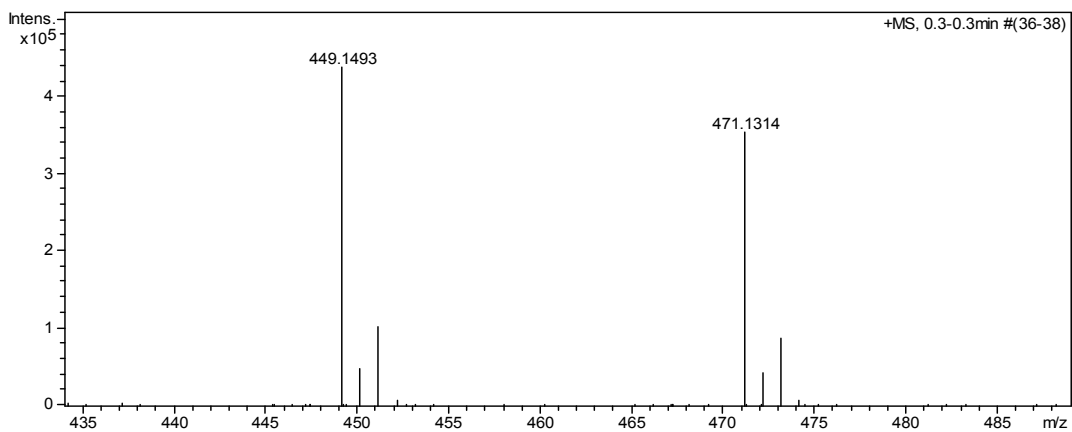
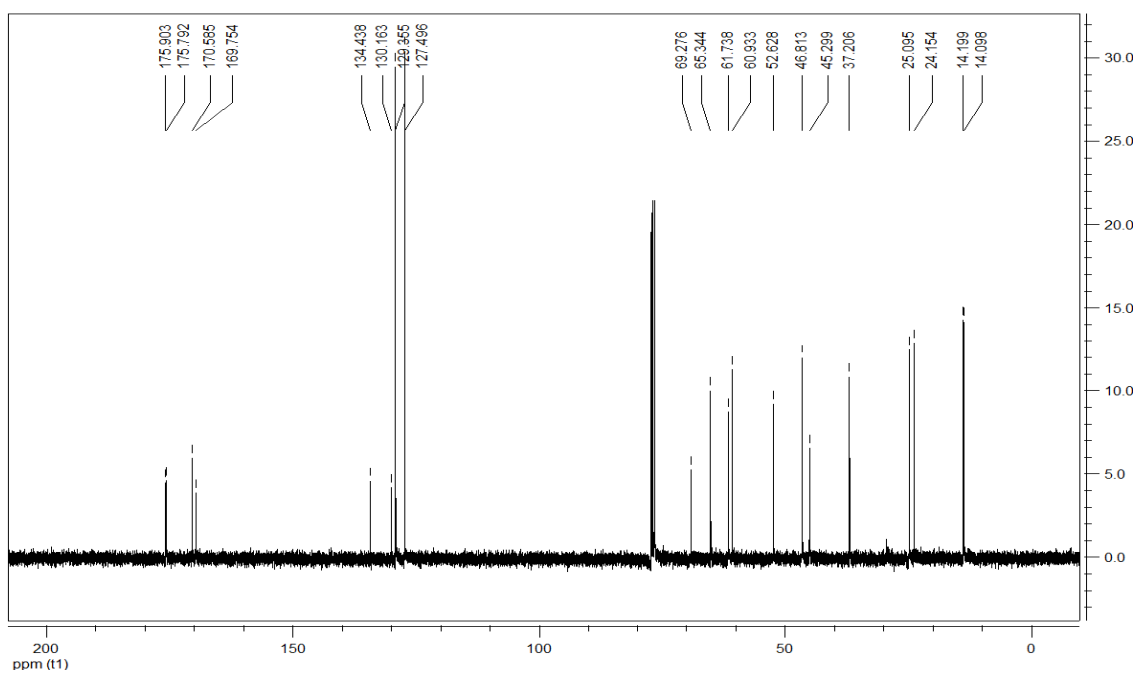
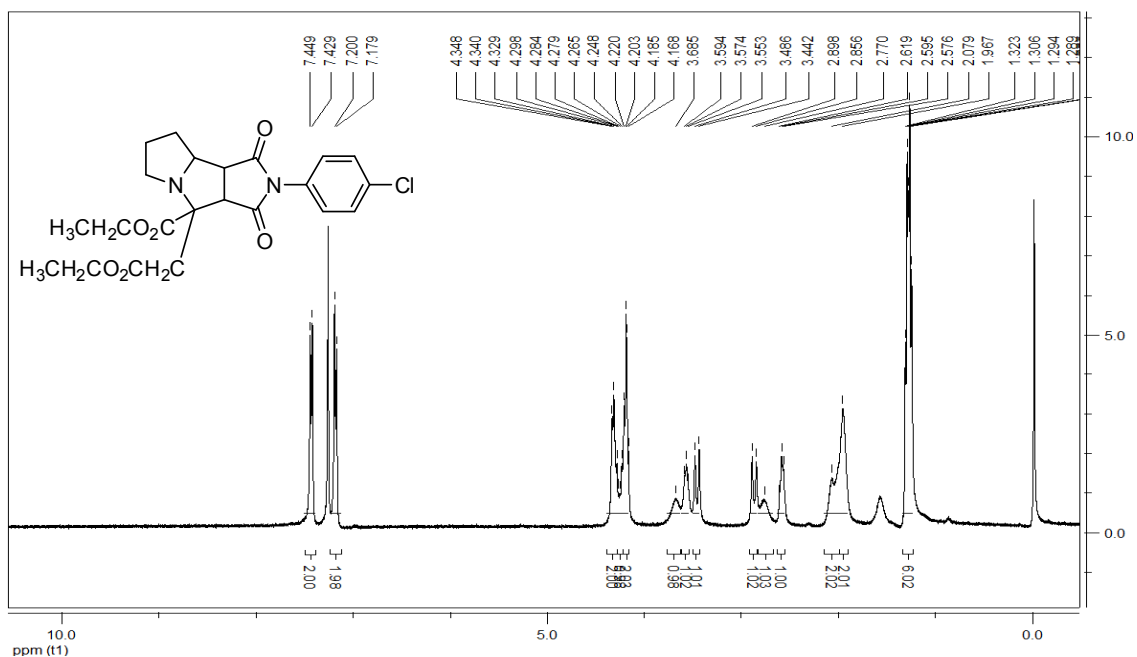
Methyl 4-(2-methoxy-2-oxoethyl)-1,3-dioxo-2-phenyldecahydropyrrolo[3,4-a]pyrrolizine-4-carboxylate (1c):



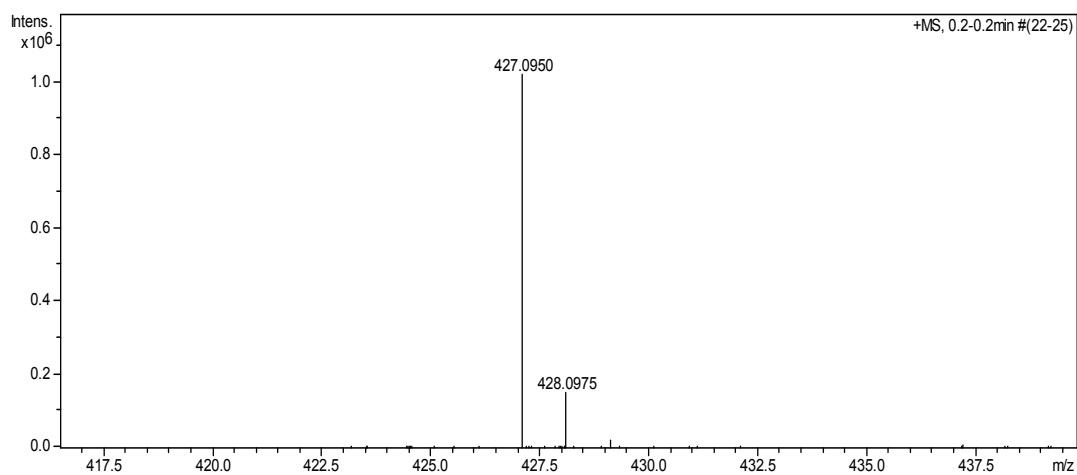
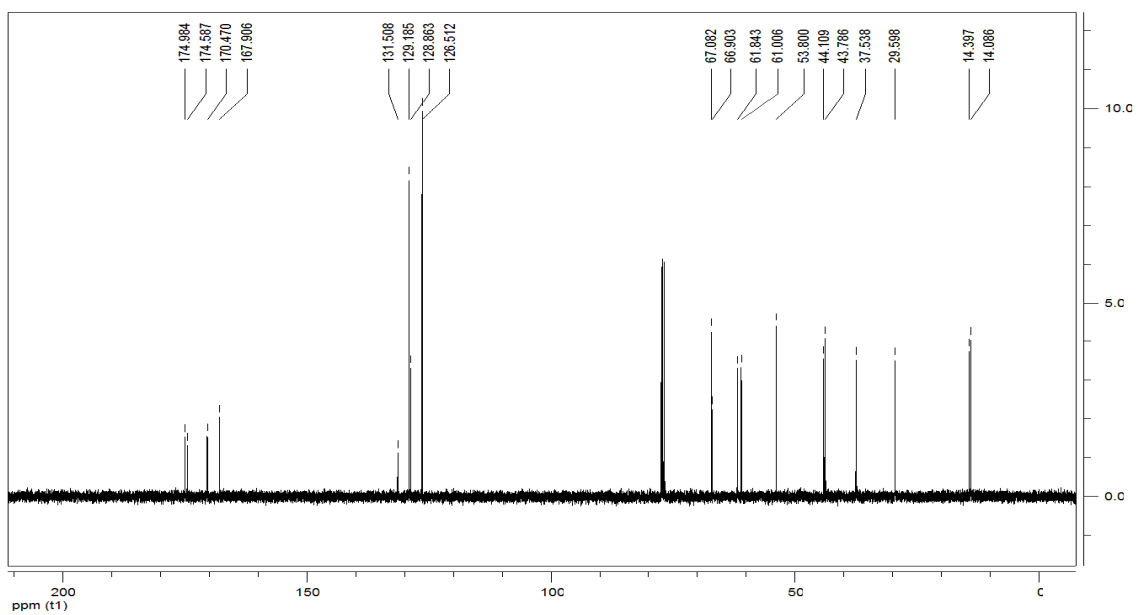
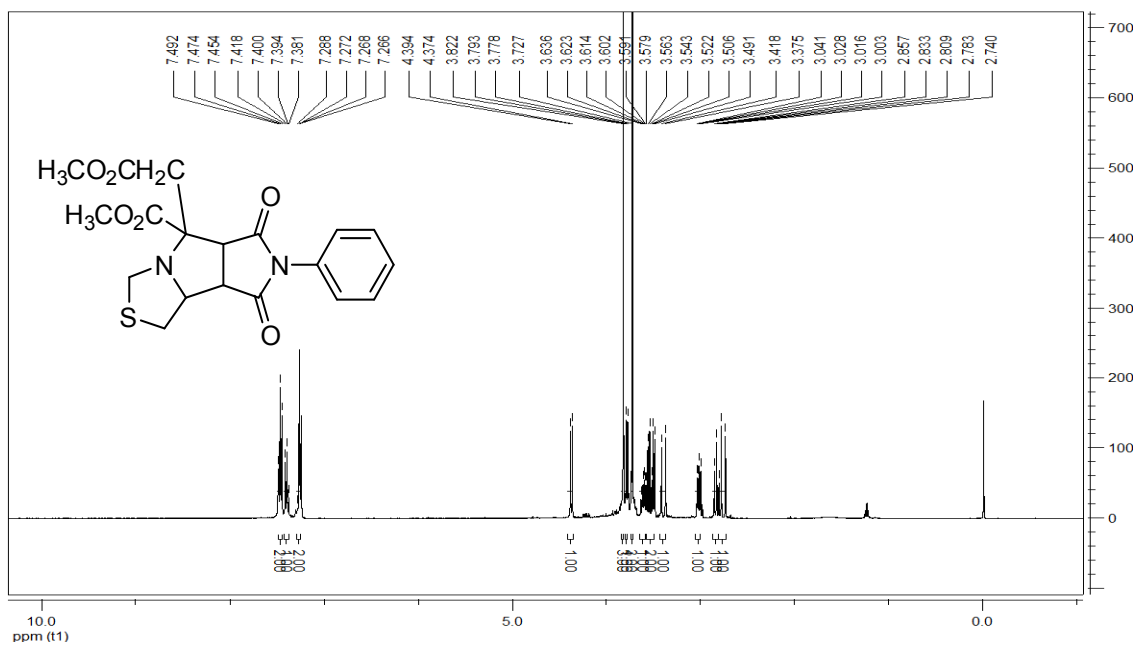
Methyl 4-(2-methoxy-2-oxoethyl)-2-(4-methoxyphenyl)-1,3-dioxodecahydropyrrolo[3,4-a]pyrrolizine-4-carboxylate (1d):



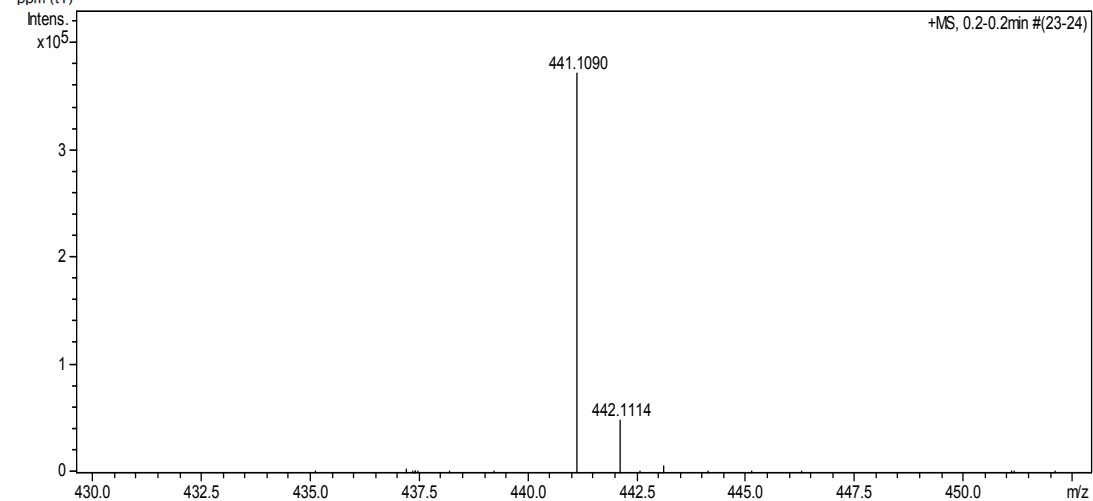
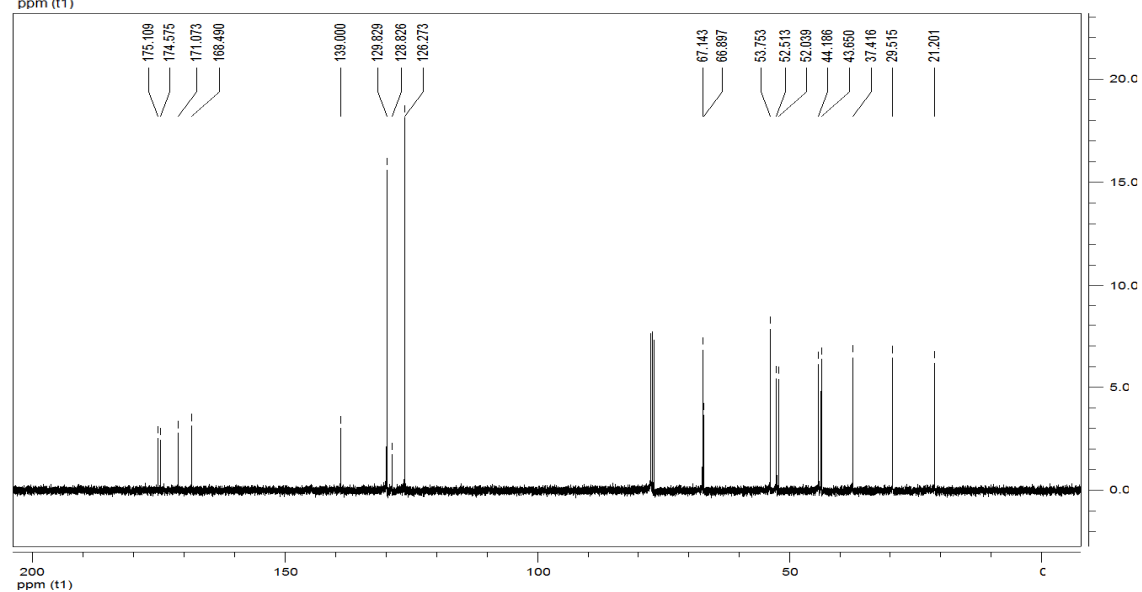
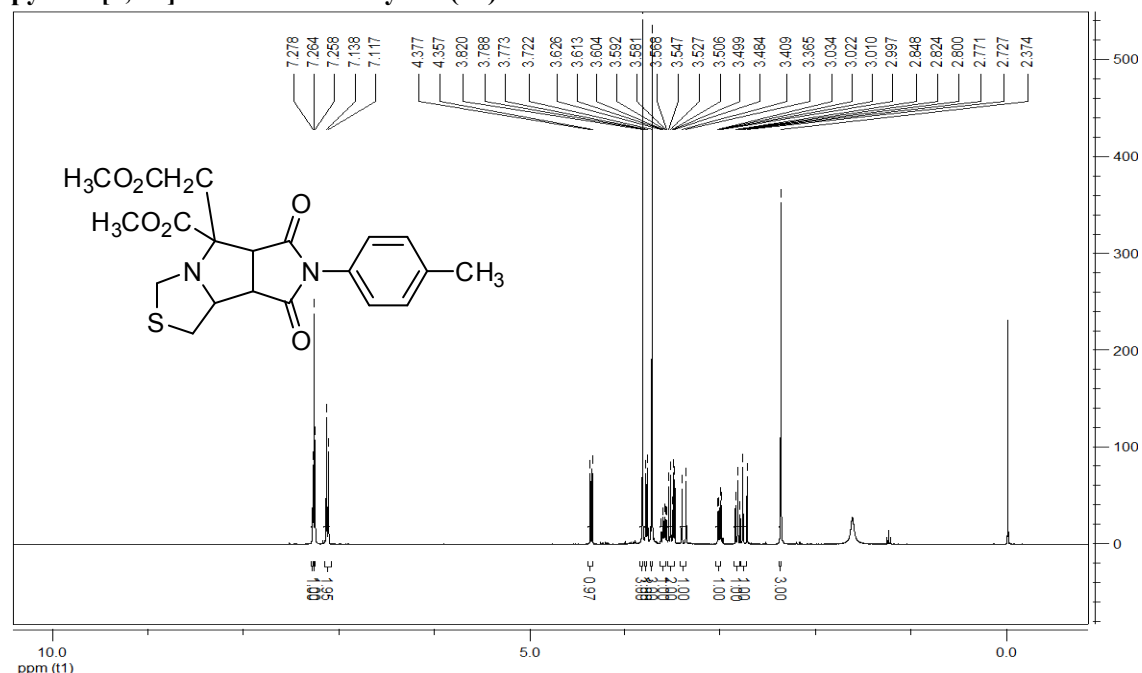
Ethyl 2-(4-chlorophenyl)-4-(2-ethoxy-2-oxoethyl)-1,3-dioxodecahydropyrrolo[3,4-a]pyrrolizine-4-carboxylate (1h):



Methyl 5-(2-methoxy-2-oxoethyl)-6,8-dioxo-7-phenyloctahydro-1H-pyrrolo[3',4':3,4]-pyrrolo[1,2-c]thiazole-5-carboxylate (2c):

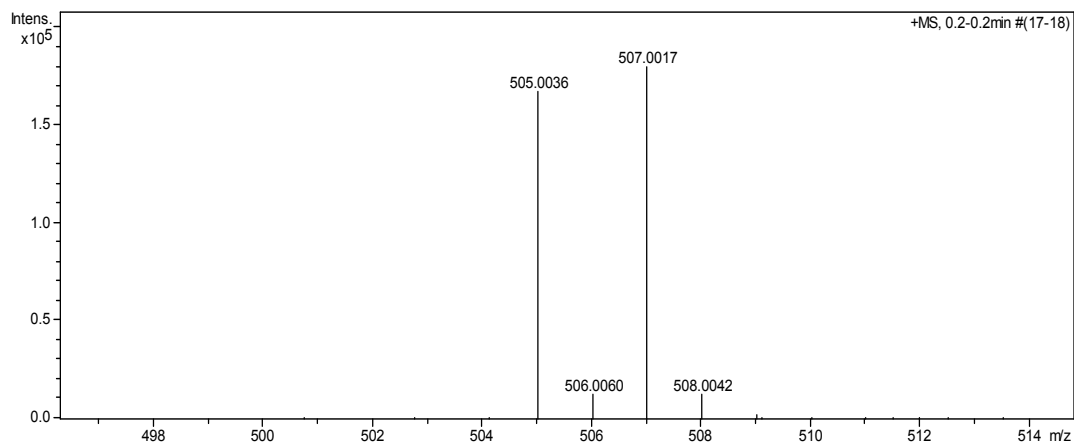
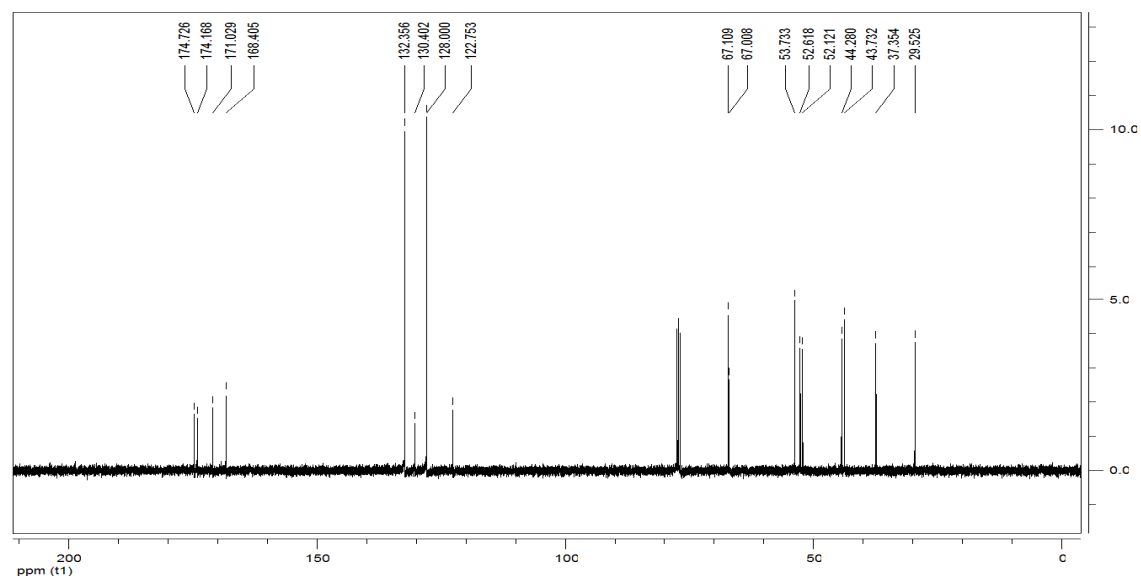
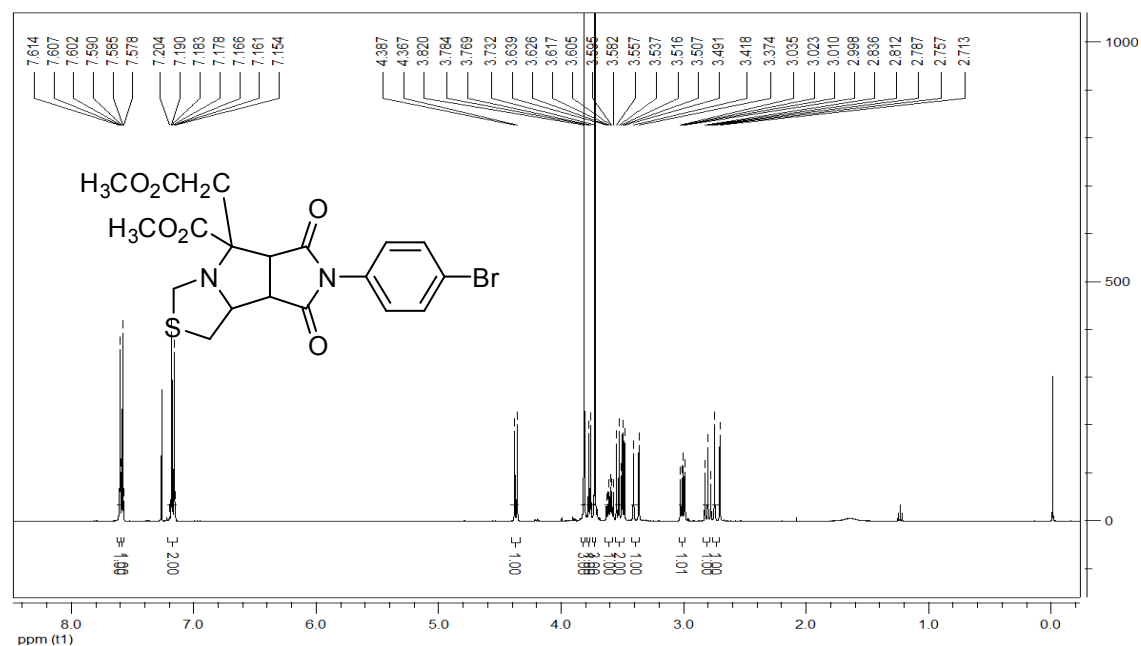


Methyl 5-(2-methoxy-2-oxoethyl)-6,8-dioxo-7-(p-tolyl)octahydro-1H-pyrrolo[3',4':3,4]-pyrrolo[1,2-c]thiazole-5-carboxylate (2d):

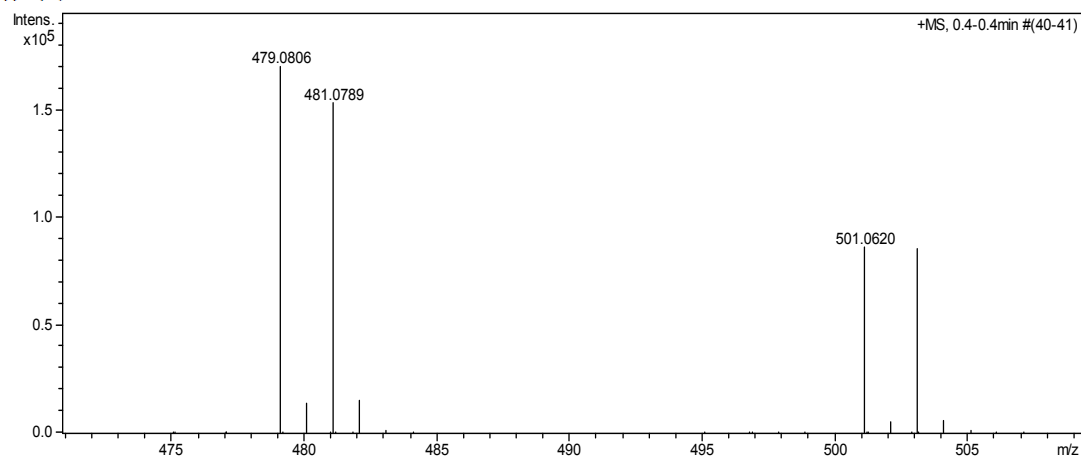
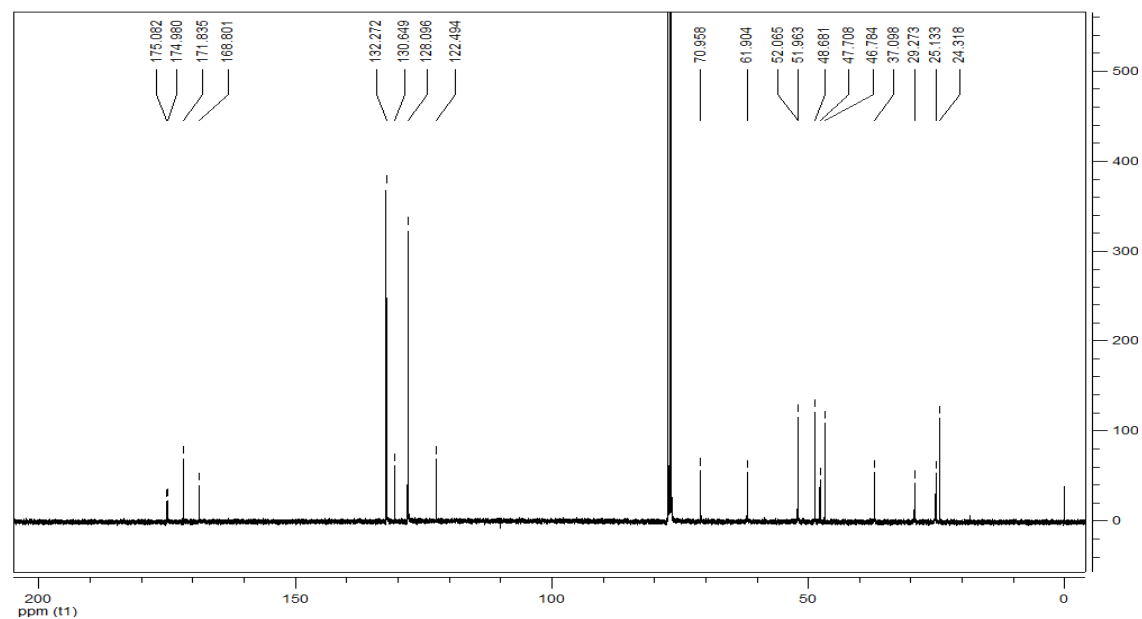
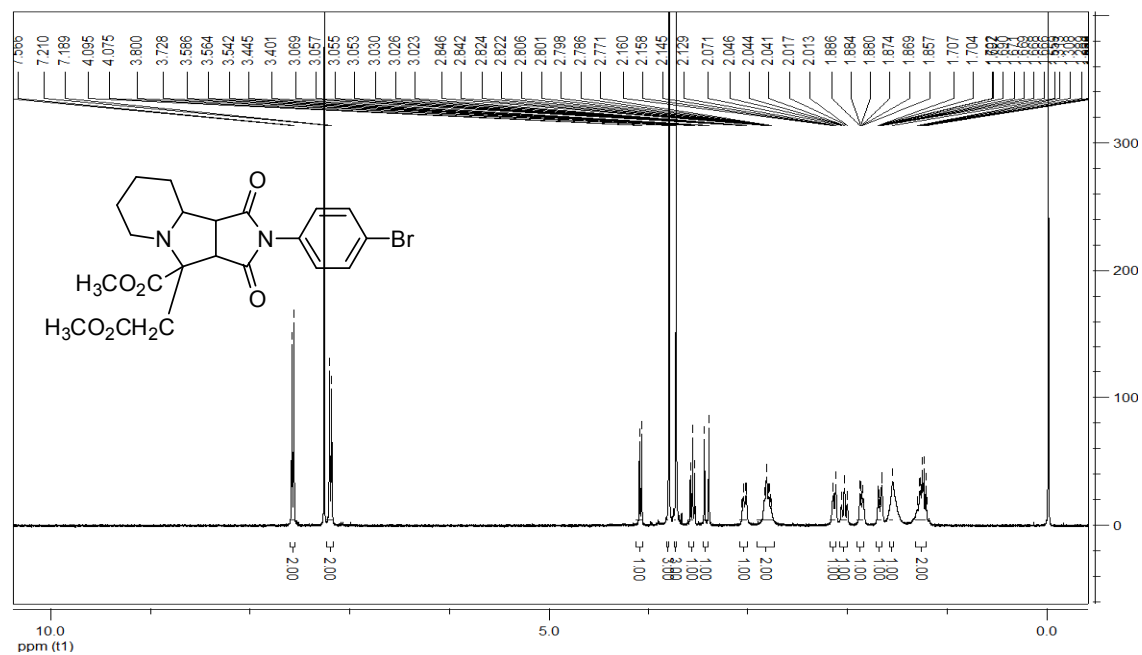


Methyl

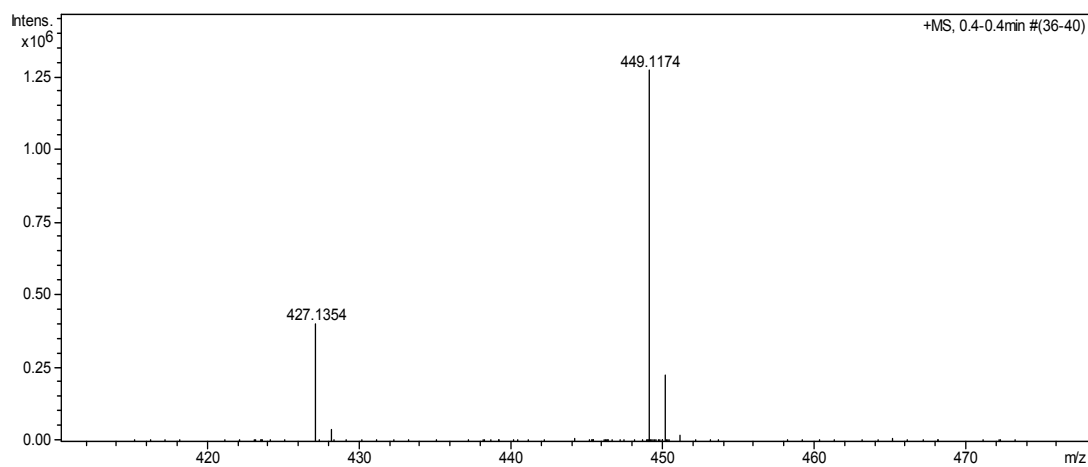
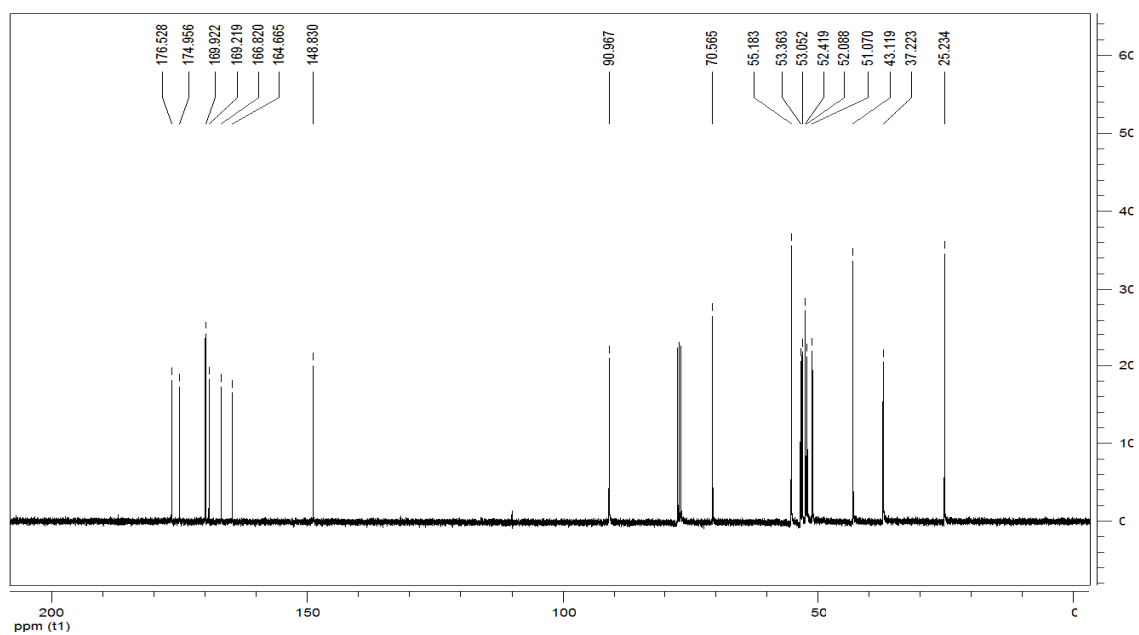
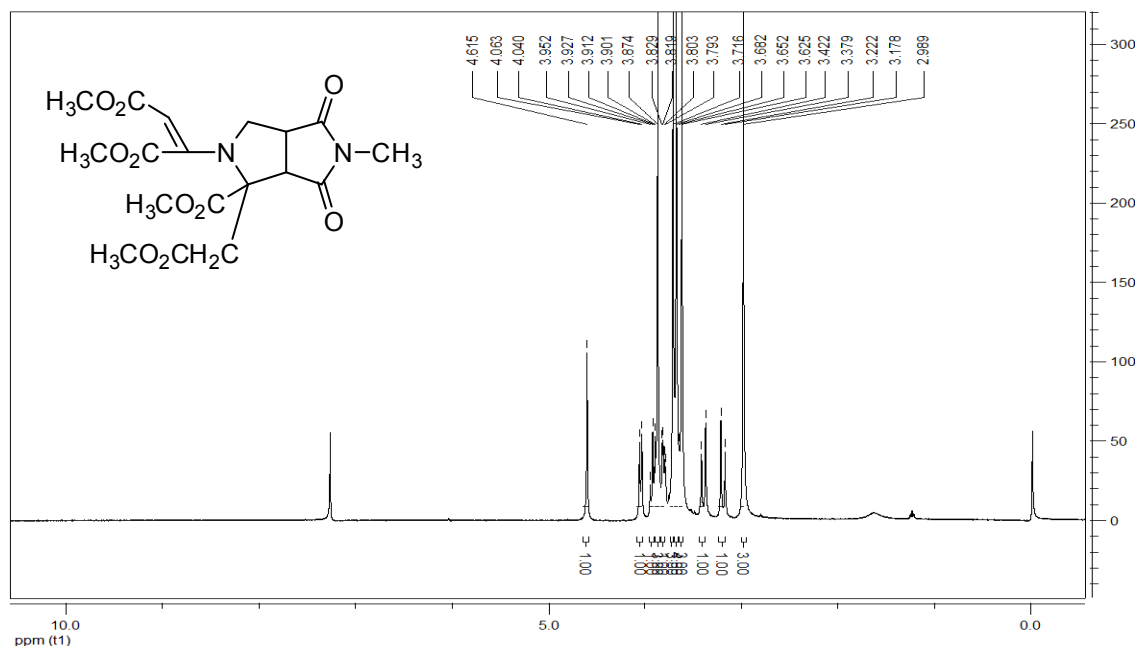
7-(4-bromophenyl)-5-(2-methoxy-2-oxoethyl)-6,8-dioxooctahydro-1H-pyrrolo[3',4':3,4]pyrrolo[1,2-c]thiazole-5-carboxylate (2f):



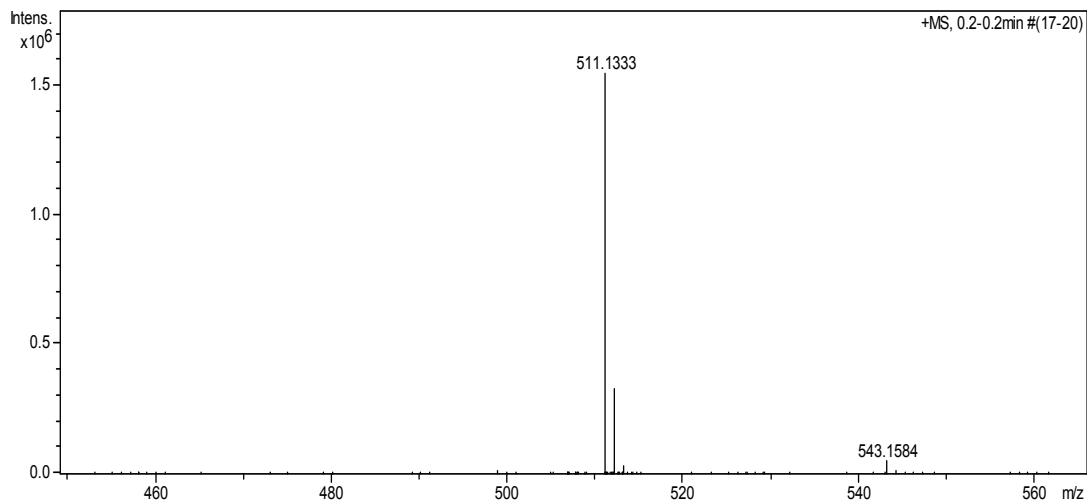
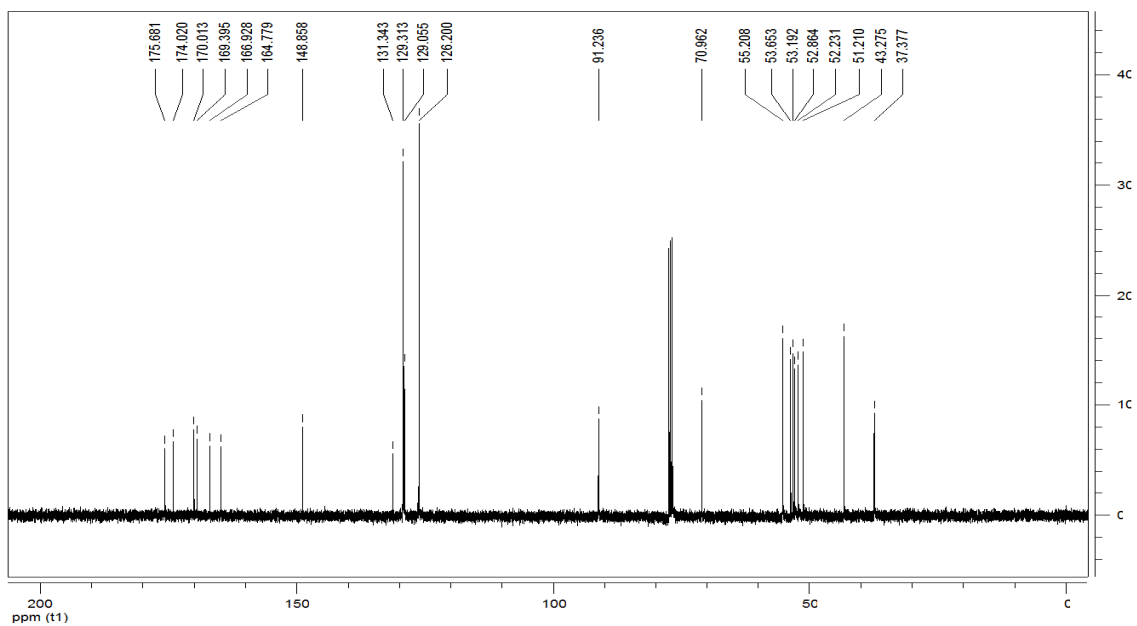
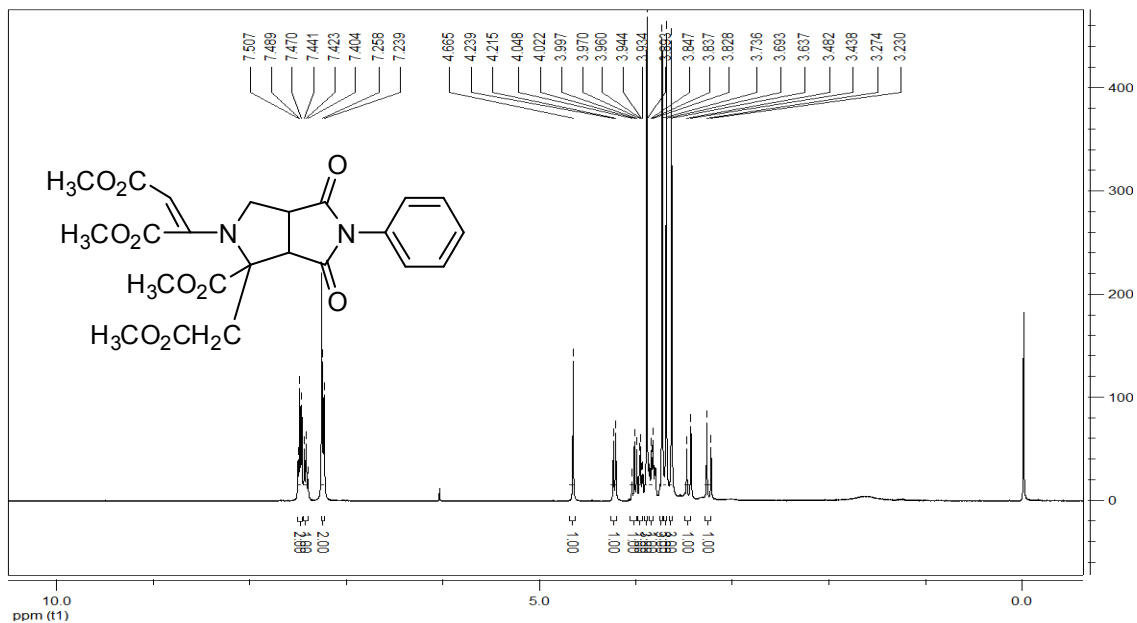
Methyl 2-(4-bromophenyl)-4-(2-methoxy-2-oxoethyl)-1,3-dioxodecahydro-1H-pyrrolo[3,4-a]indolizine-4-carboxylate (3b):



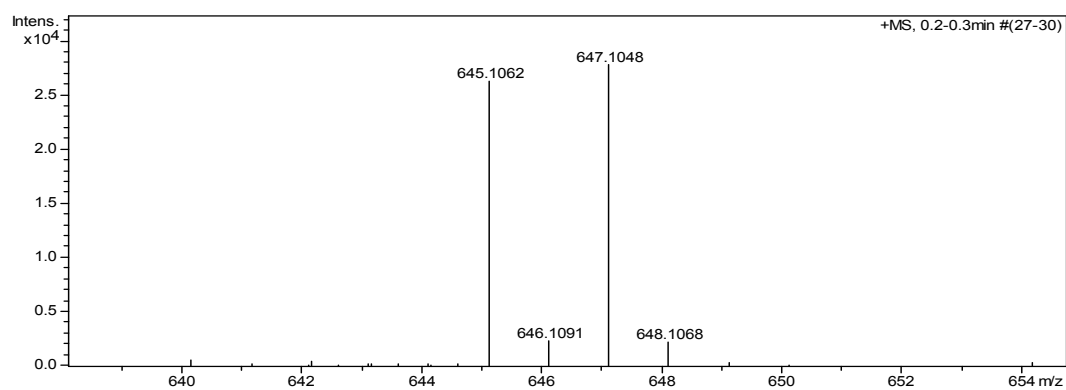
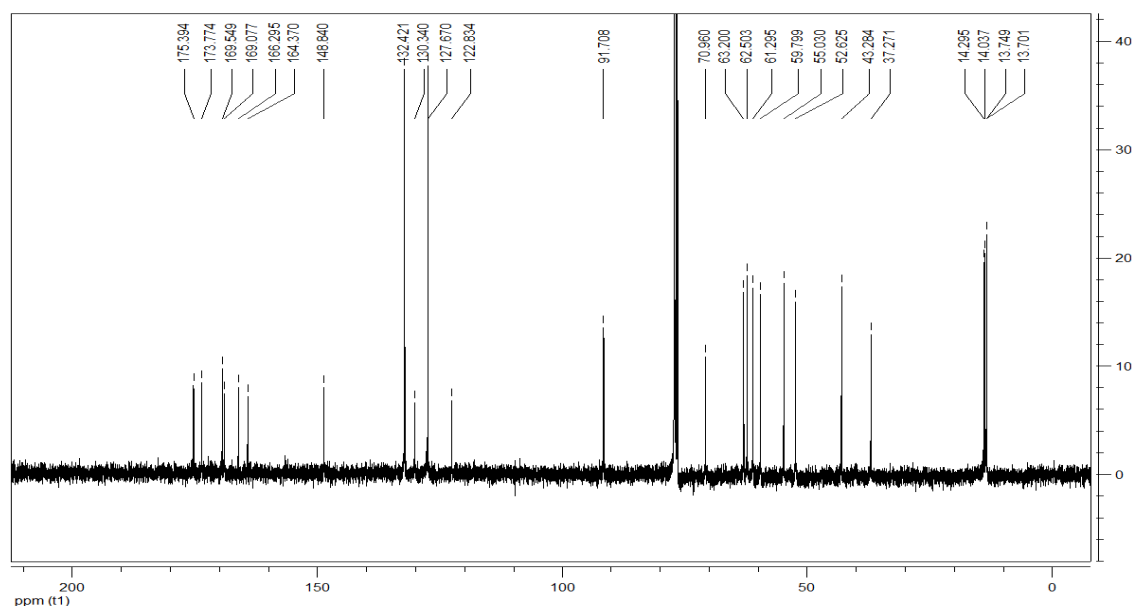
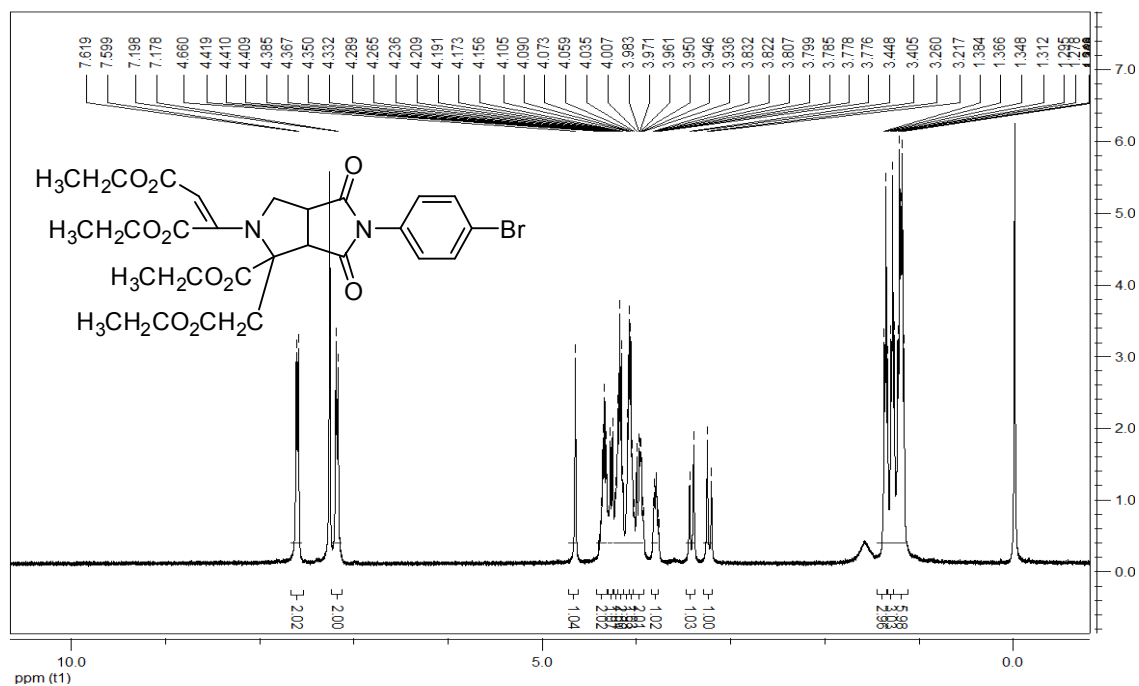
Dimethyl 2-(1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-5-methyl-4,6-dioxohexahydro-pyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4a):



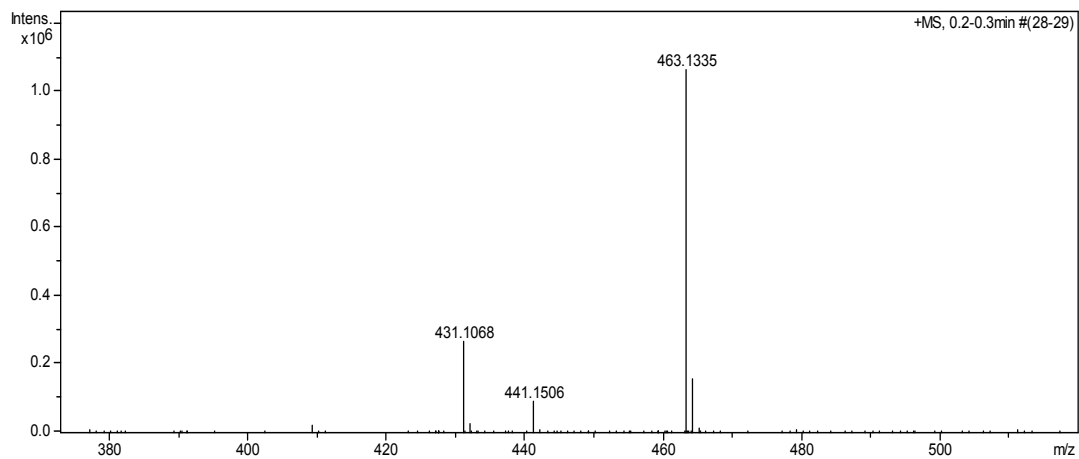
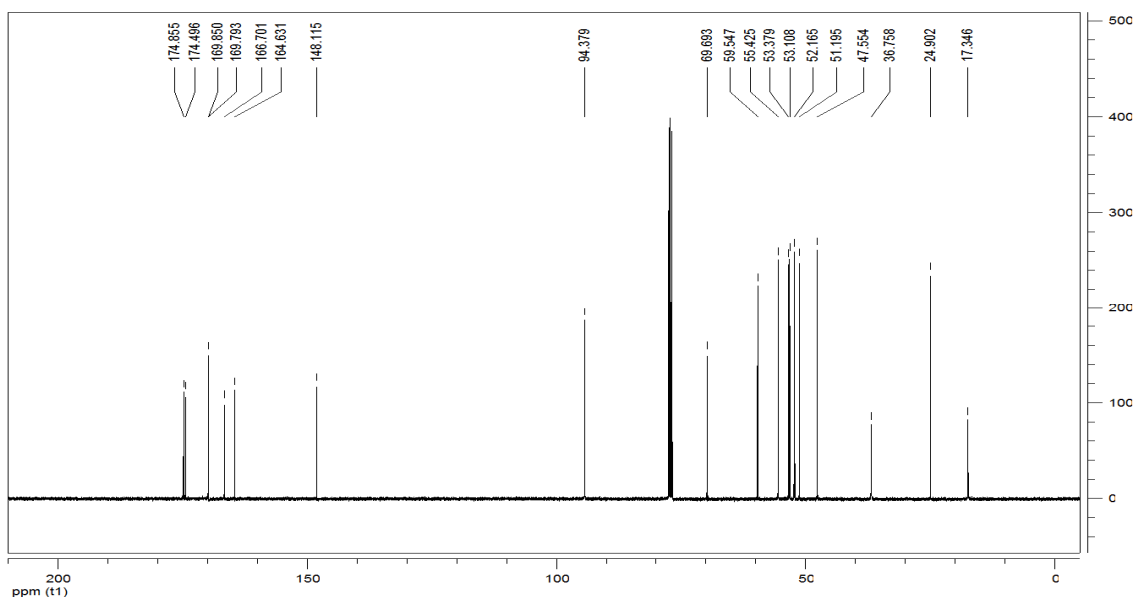
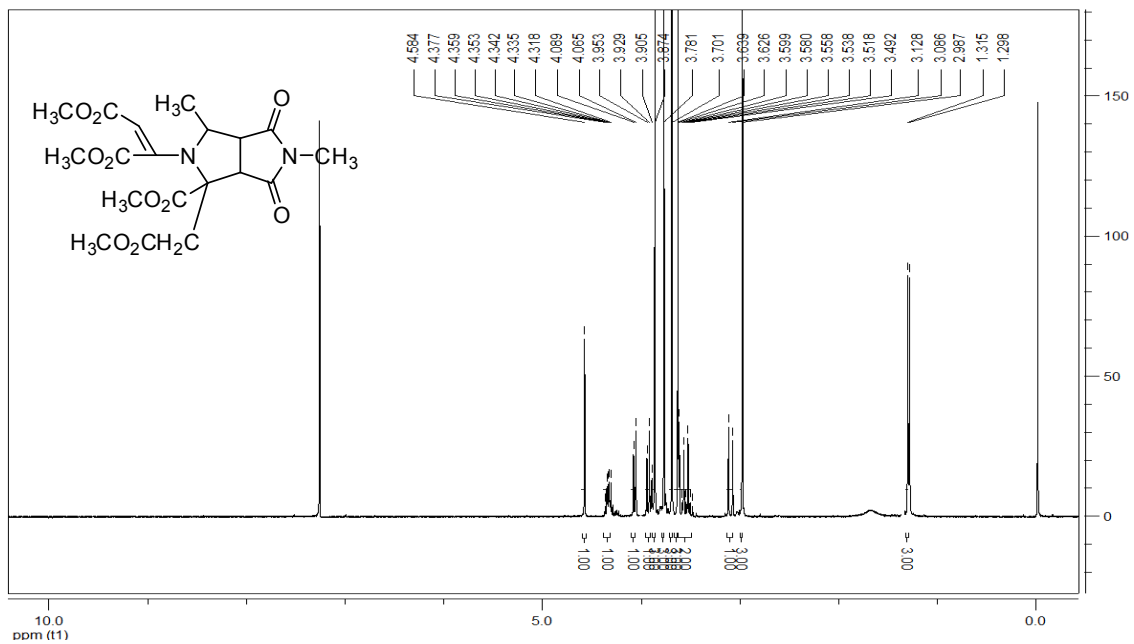
Dimethyl 2-(1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-4,6-dioxo-5-phenylhexahydro-pyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4b):



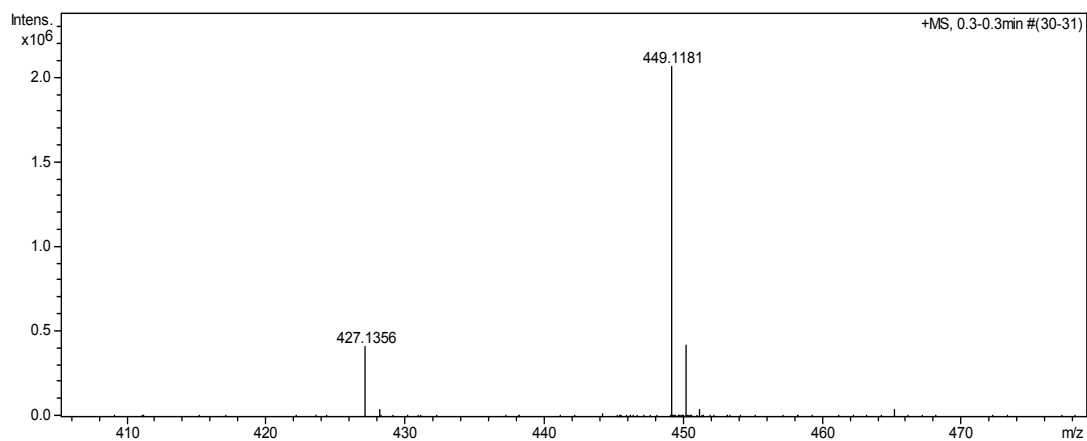
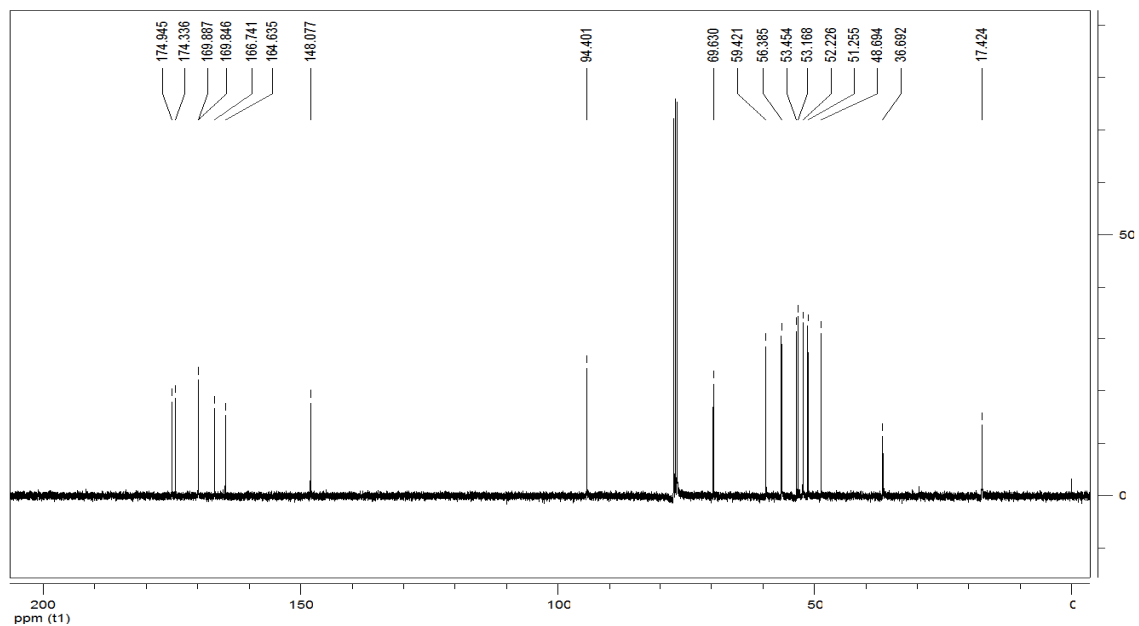
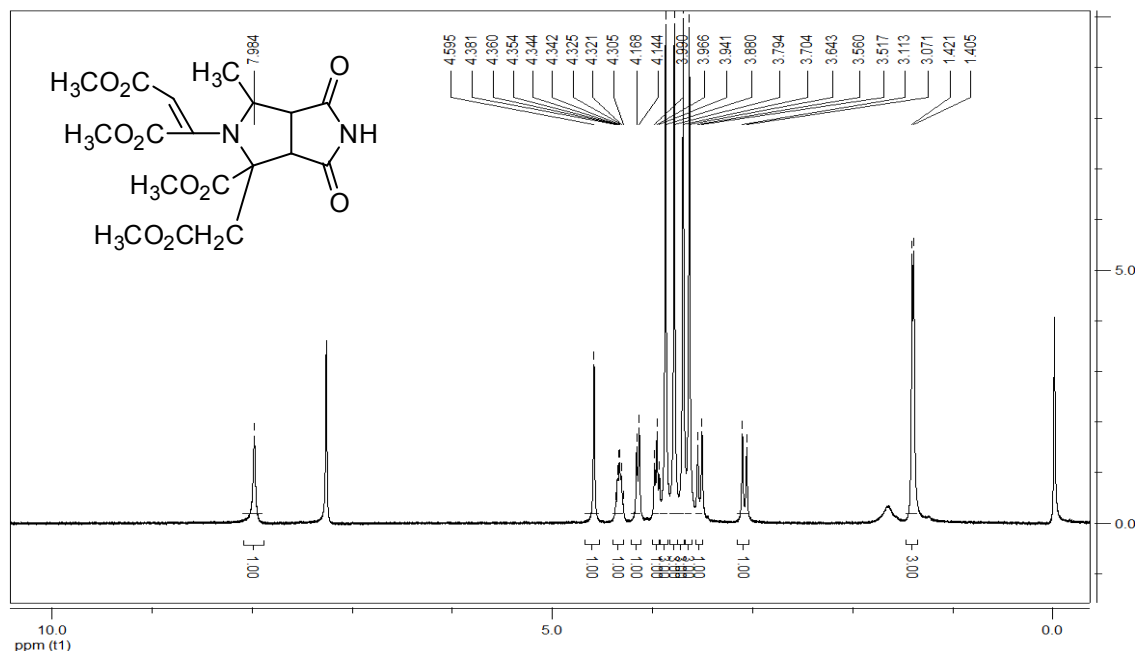
Diethyl 2-(5-(4-bromophenyl)-1-(2-ethoxy-2-oxoethyl)-1-(ethoxycarbonyl)-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4c):



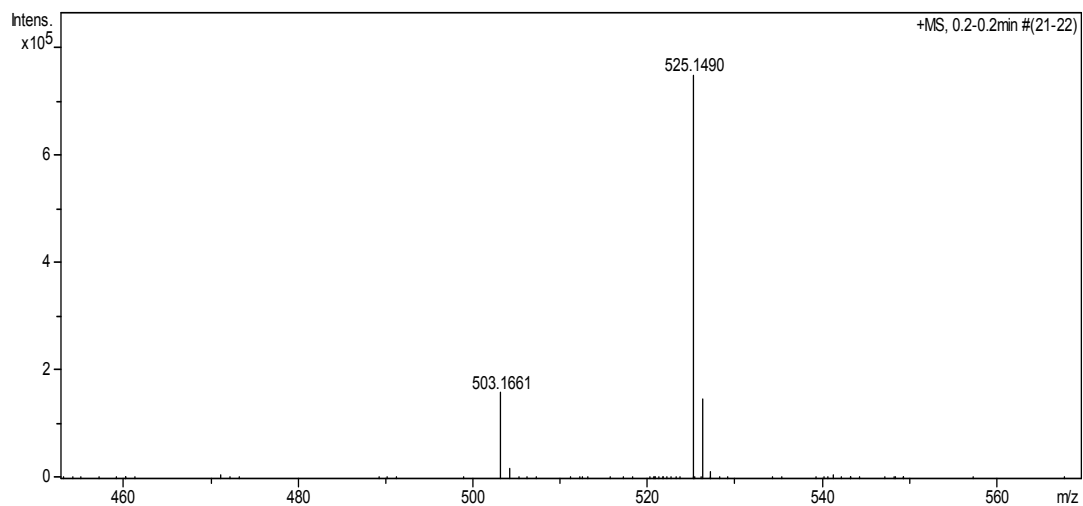
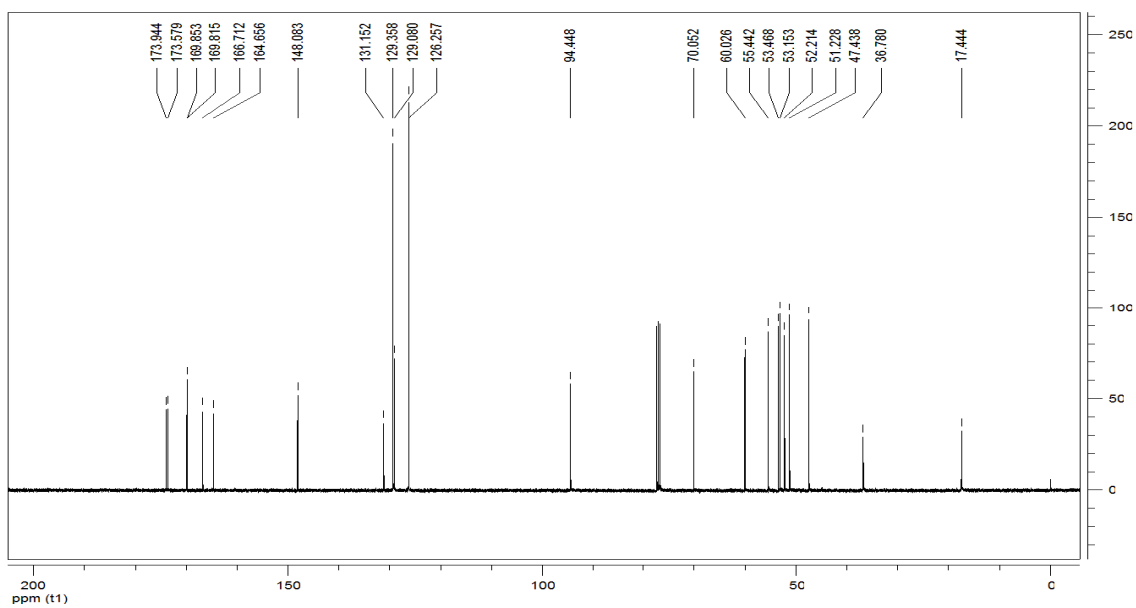
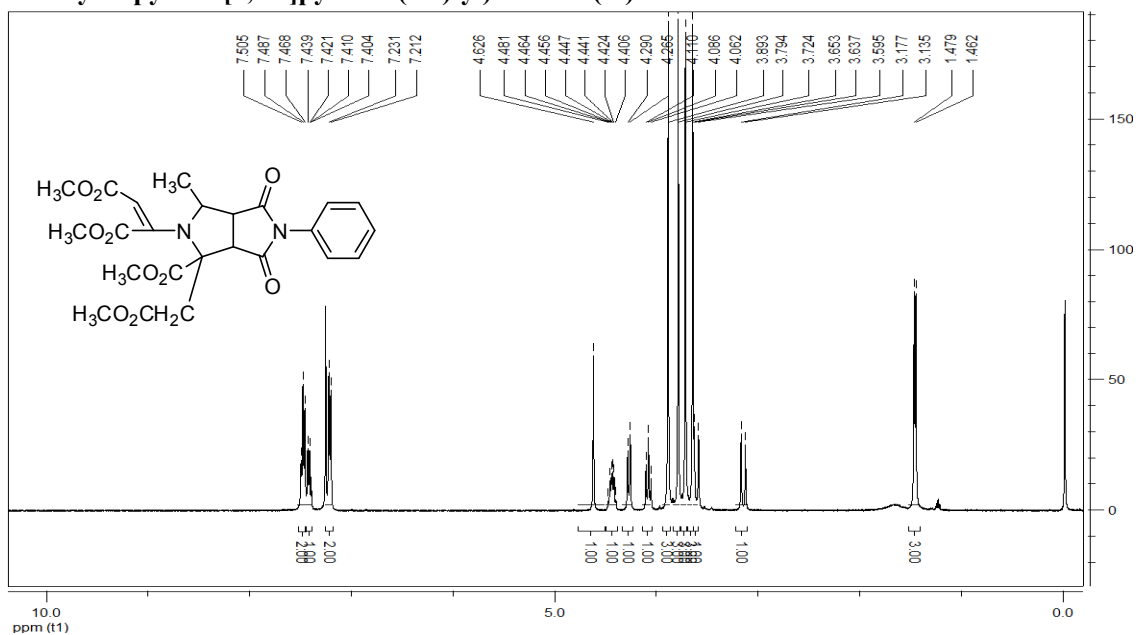
Dimethyl 2-(1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-3,5-dimethyl-4,6-dioxohexa-hydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4d):



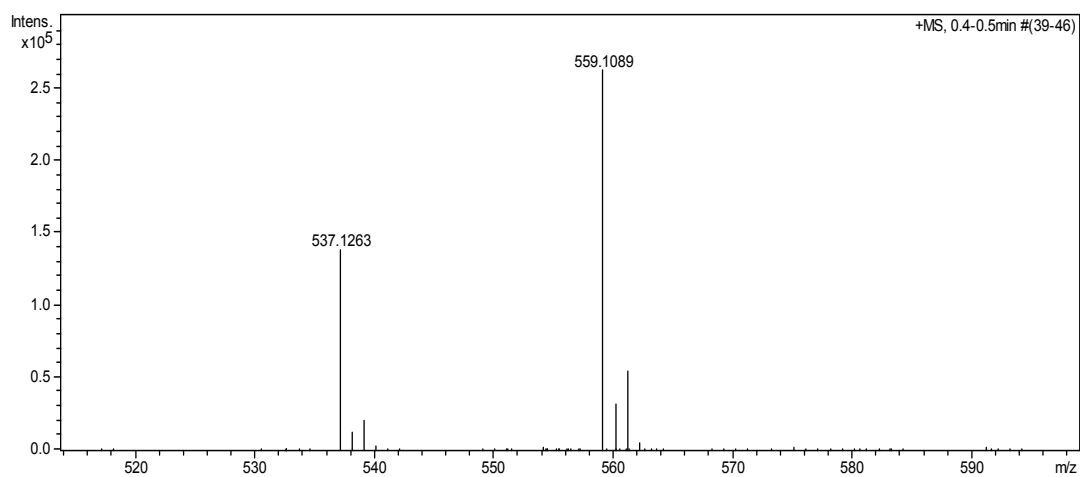
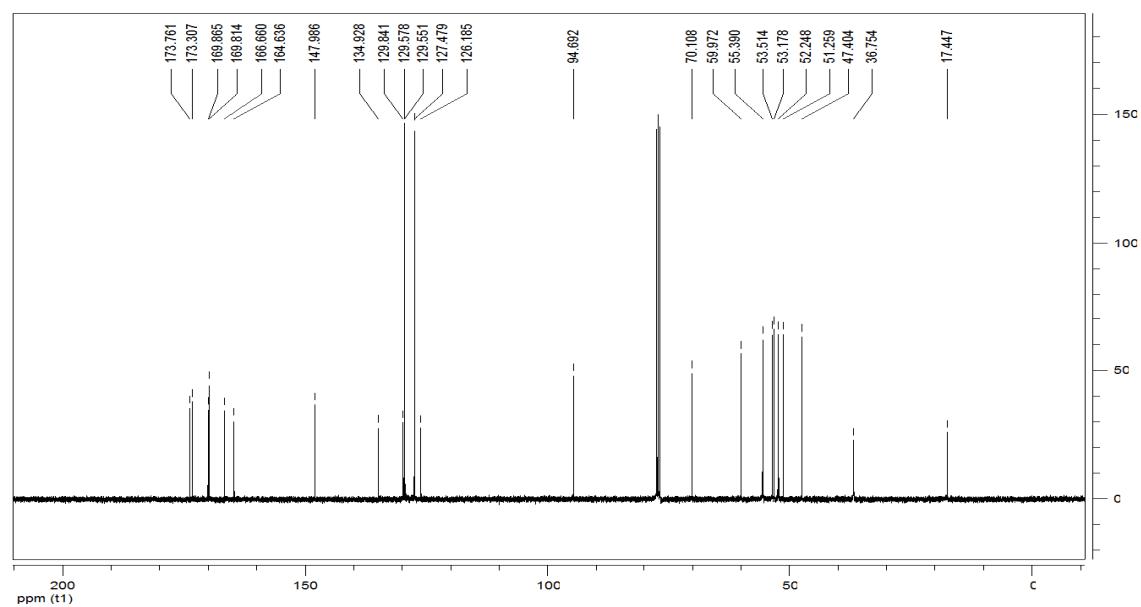
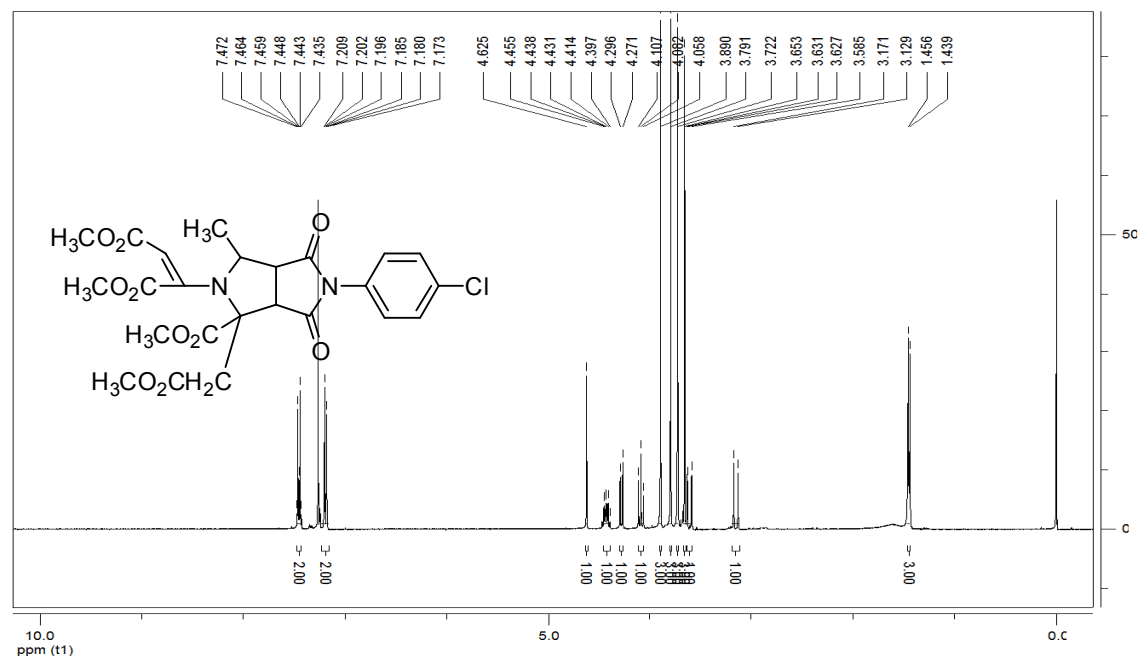
Dimethyl 2-(1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-3-methyl-4,6-dioxohexahydro-pyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4e):



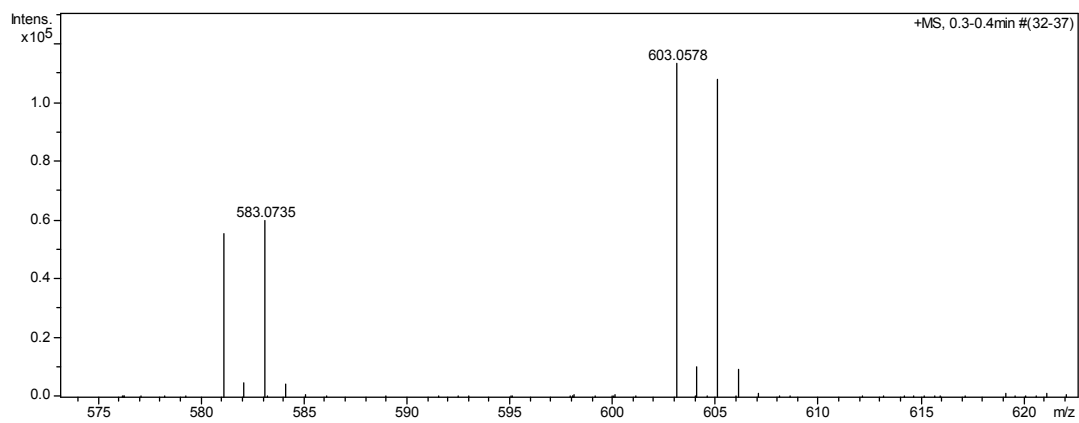
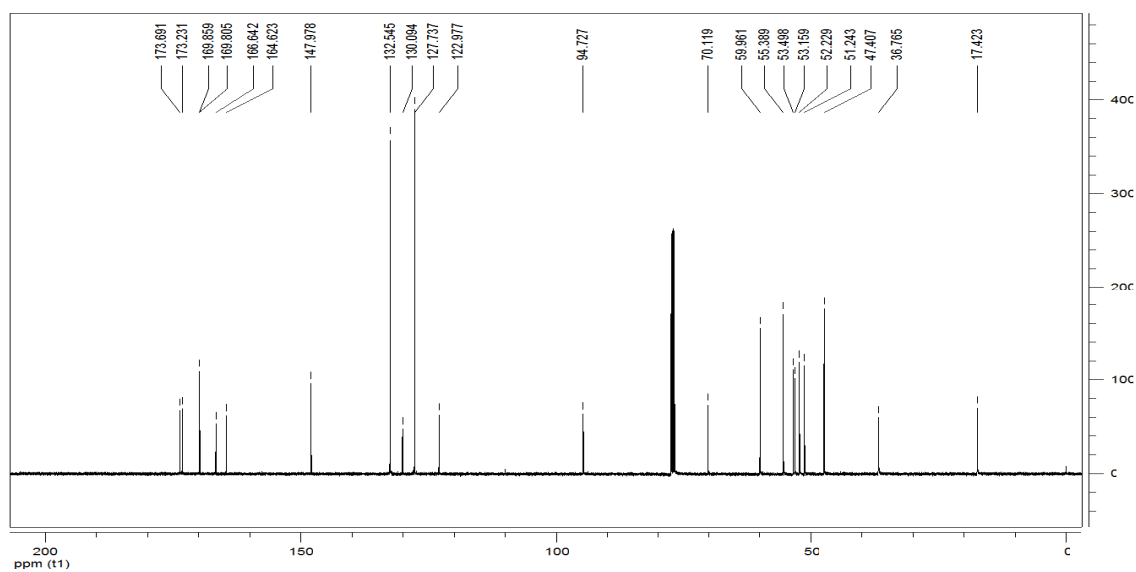
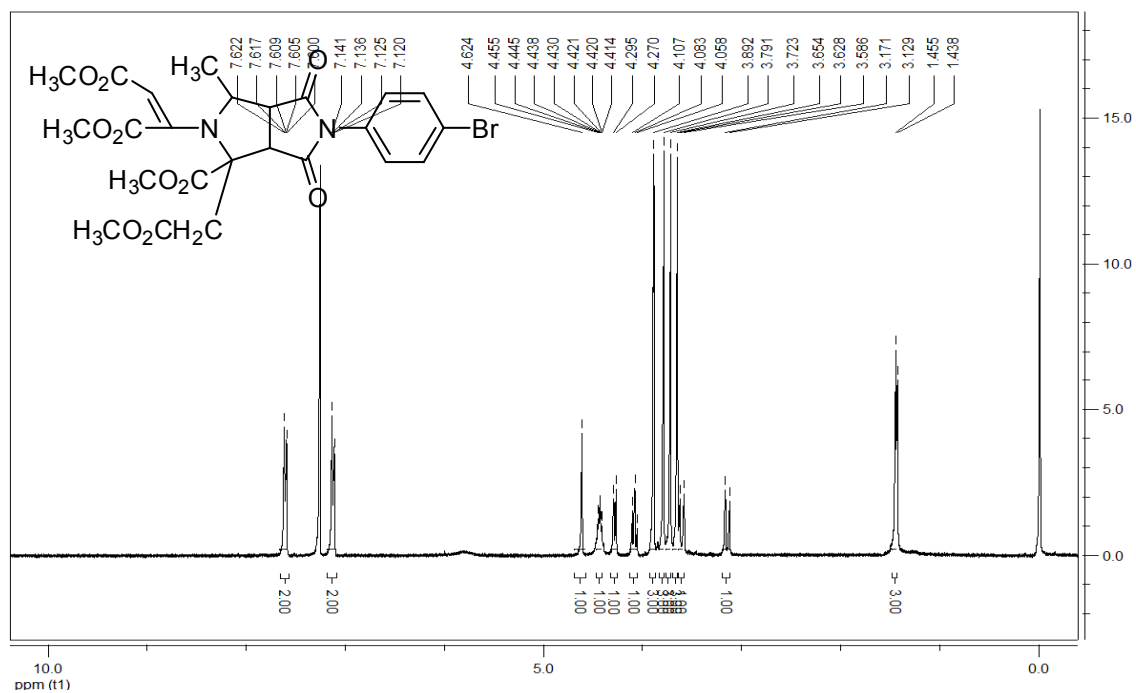
Dimethyl 2-(1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-3-methyl-4,6-dioxo-5-phenyl-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4f):



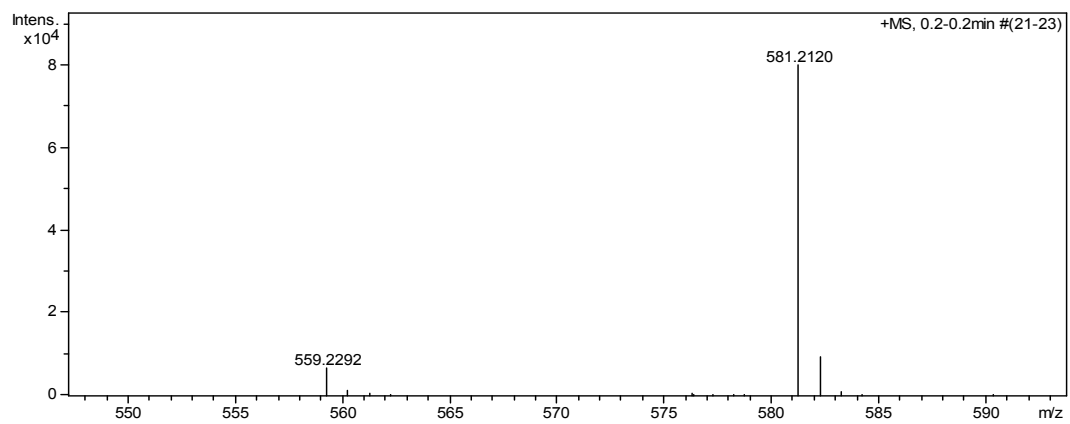
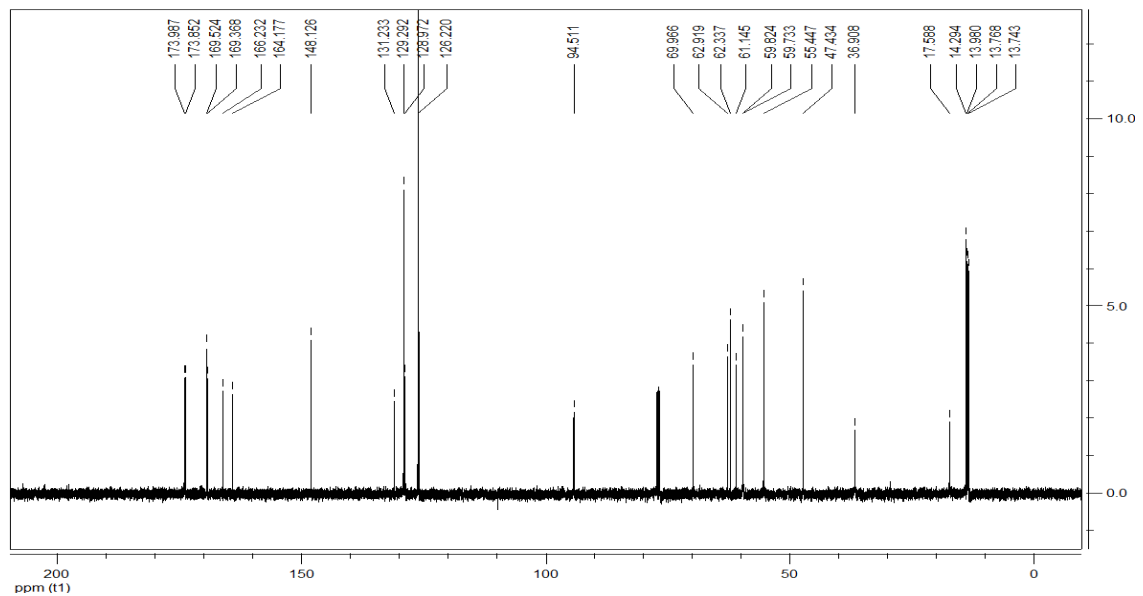
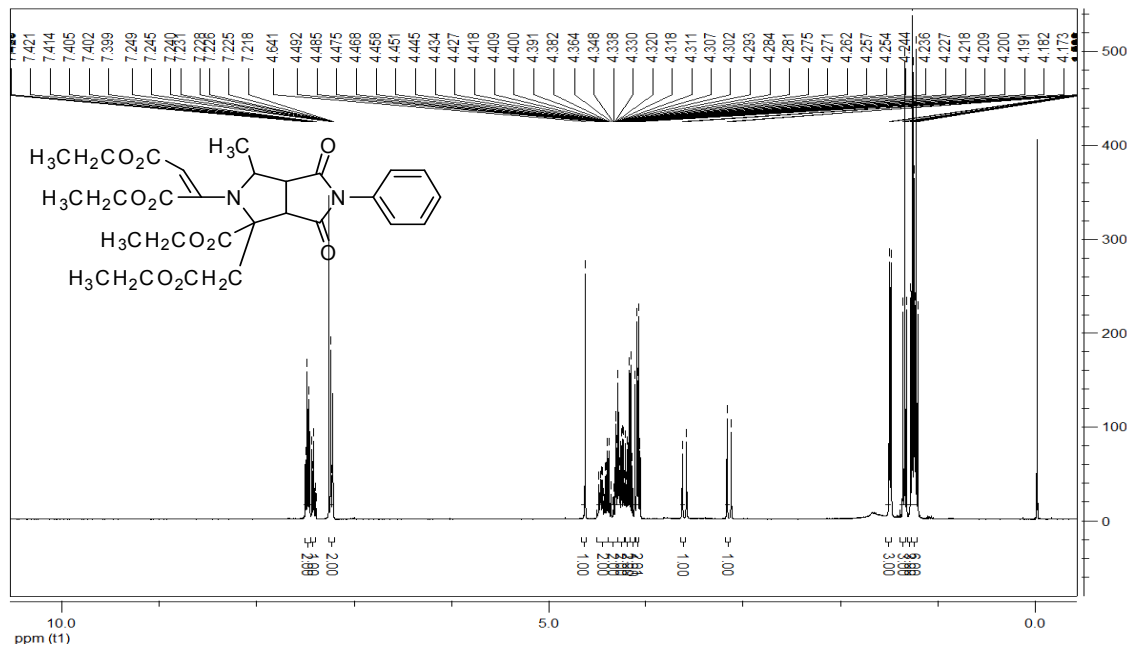
Dimethyl 2-(5-(4-chlorophenyl)-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-3-methyl-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4g):



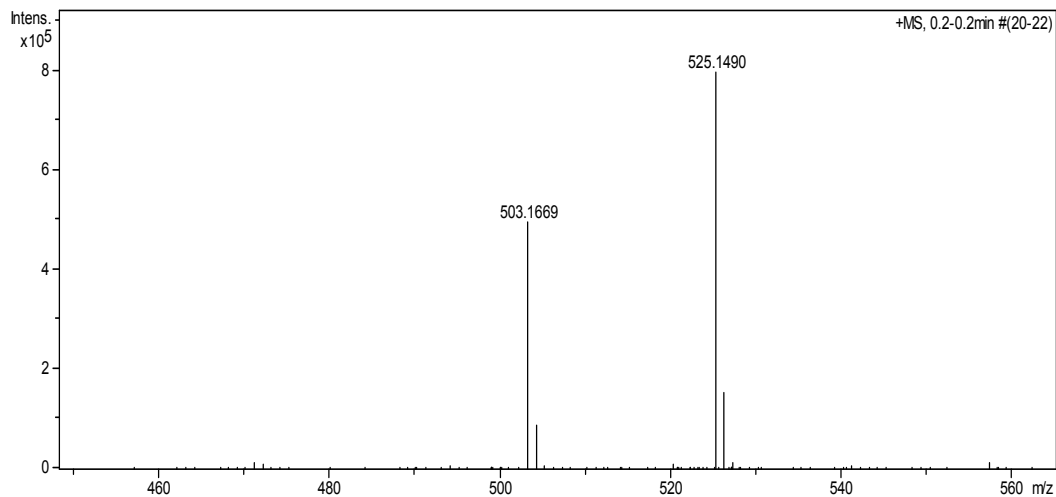
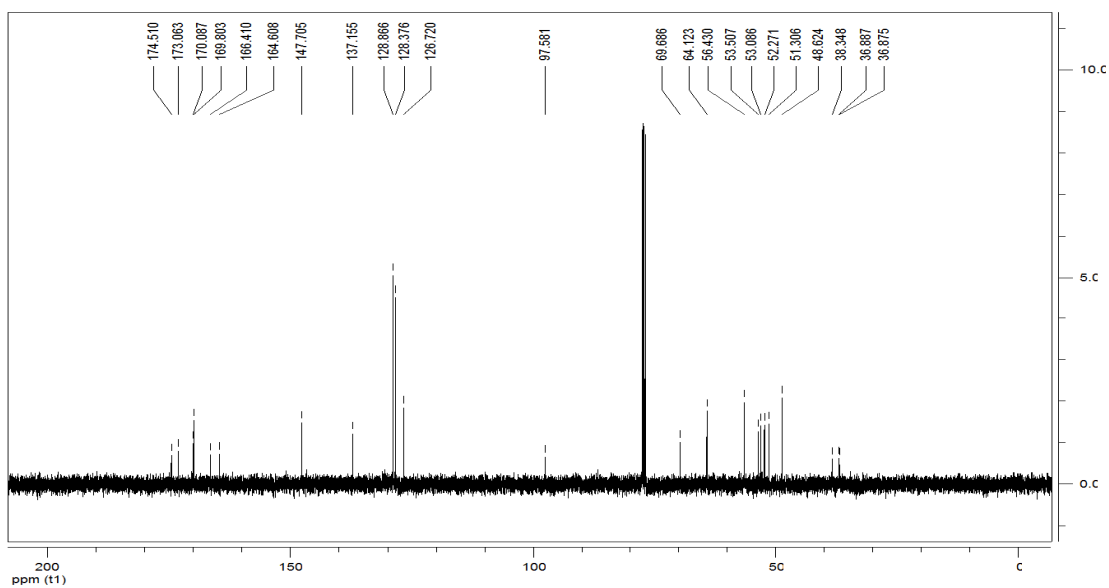
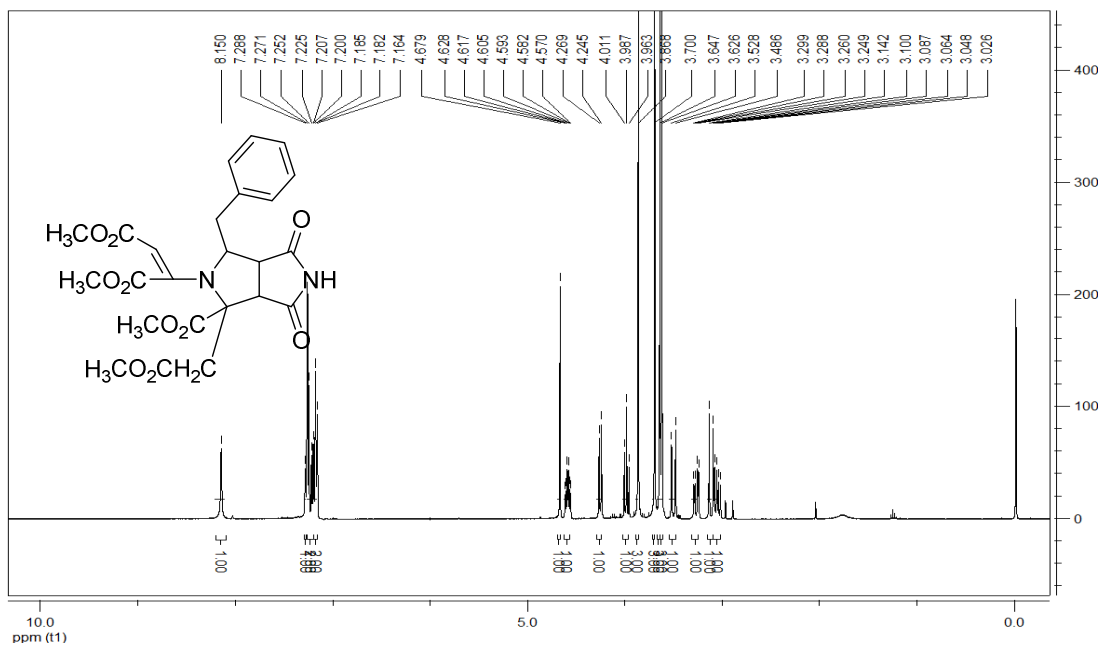
Dimethyl 2-(5-(4-bromophenyl)-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-3-methyl-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4h):



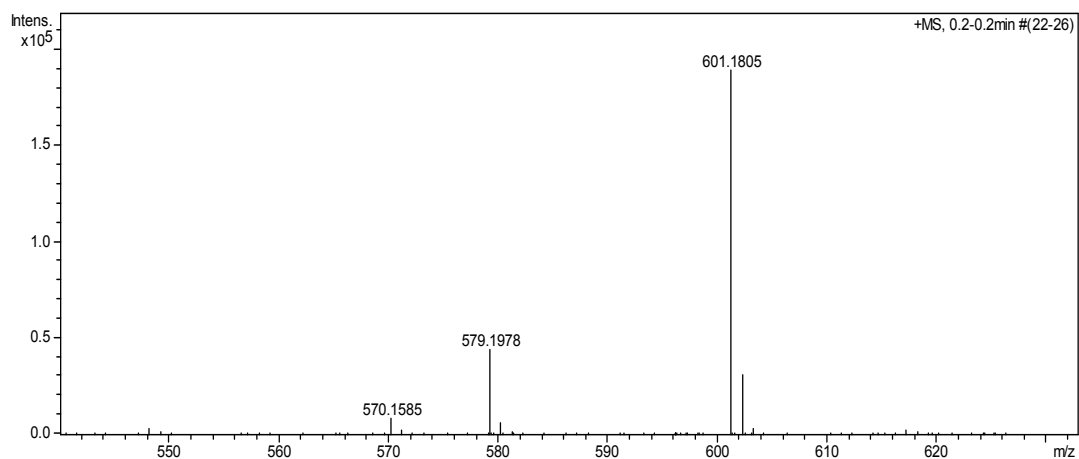
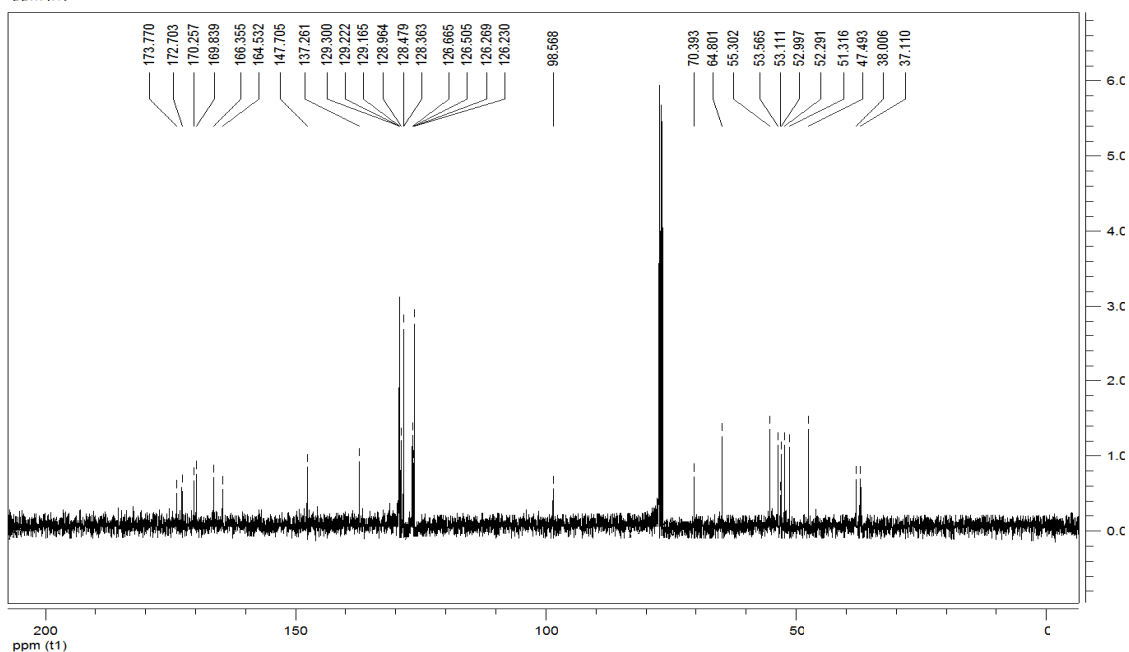
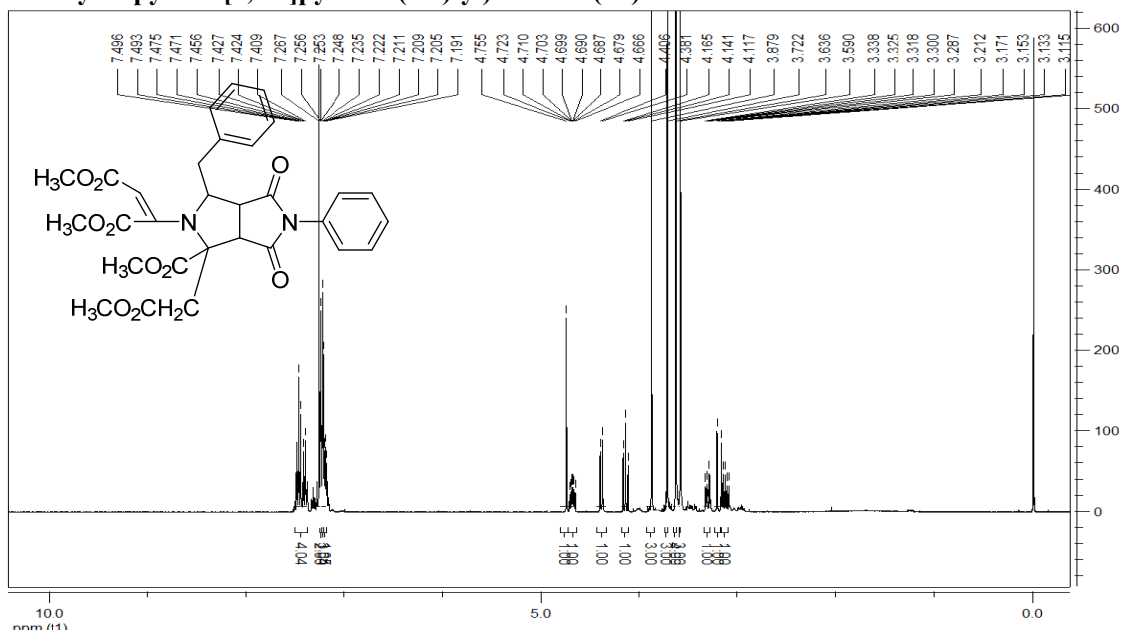
Diethyl 2-(1-(2-ethoxy-2-oxoethyl)-1-(ethoxycarbonyl)-3-methyl-4,6-dioxo-5-phenyl-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4i):



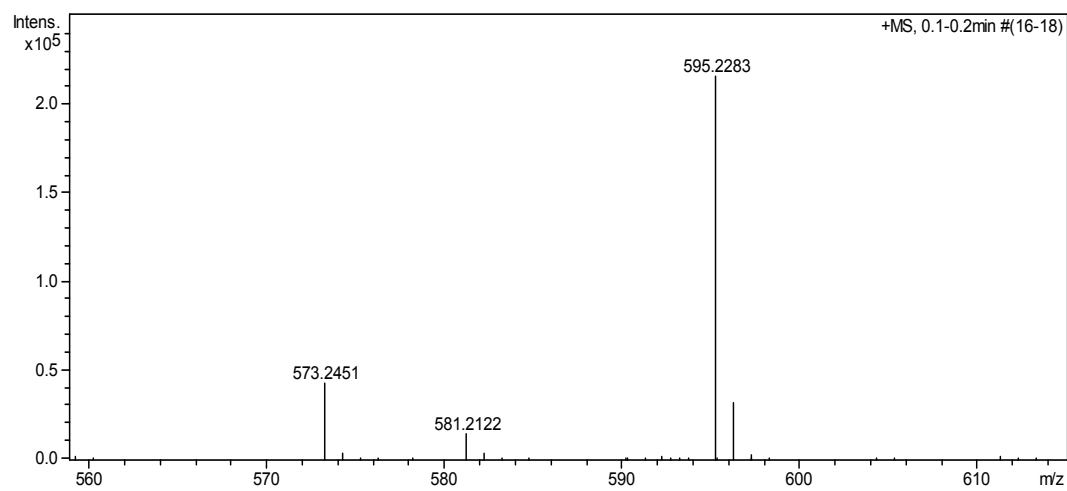
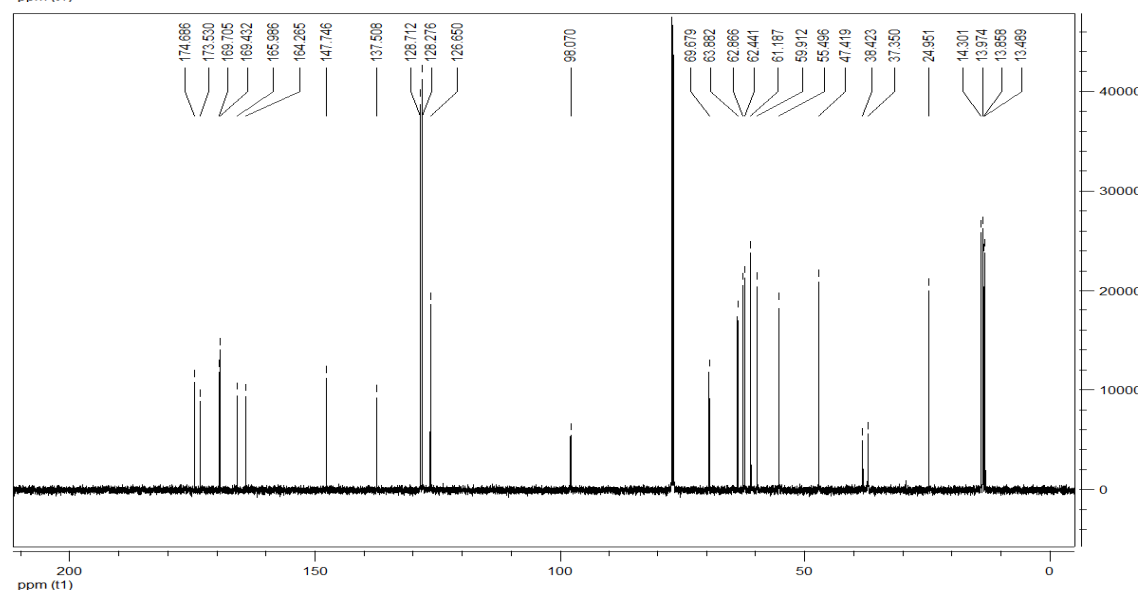
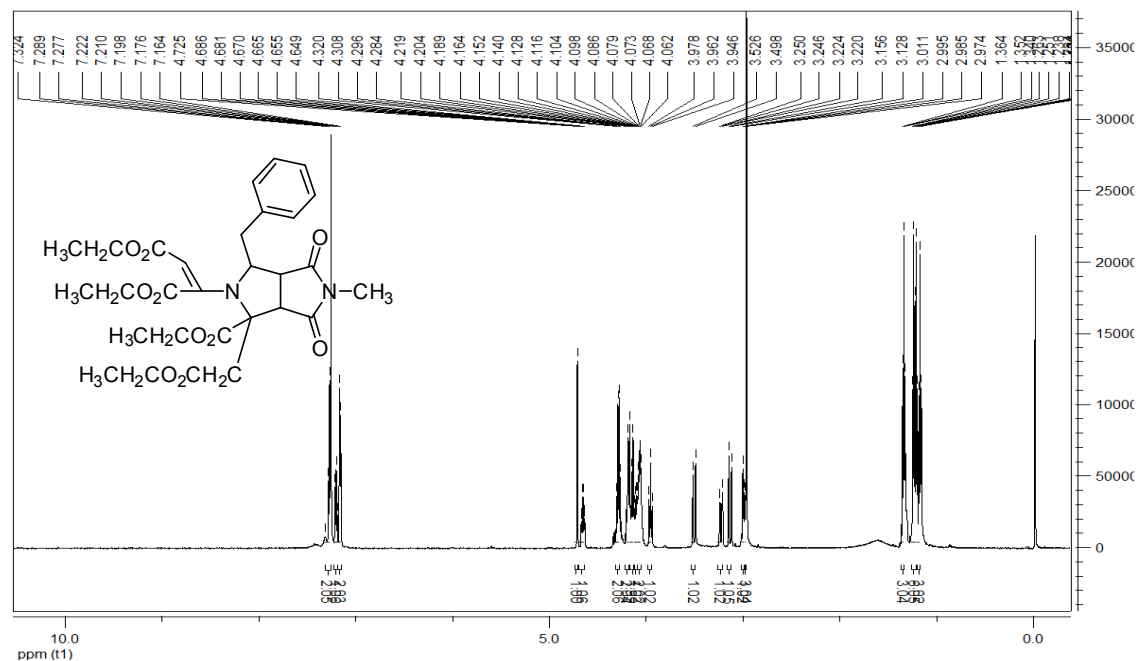
Dimethyl 2-(3-benzyl-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-4,6-dioxohexahydro-pyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4j):



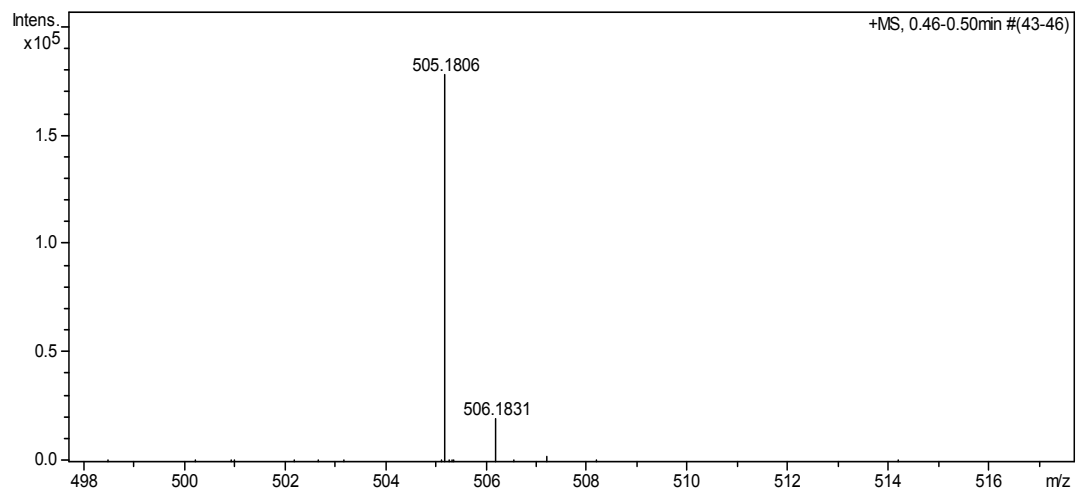
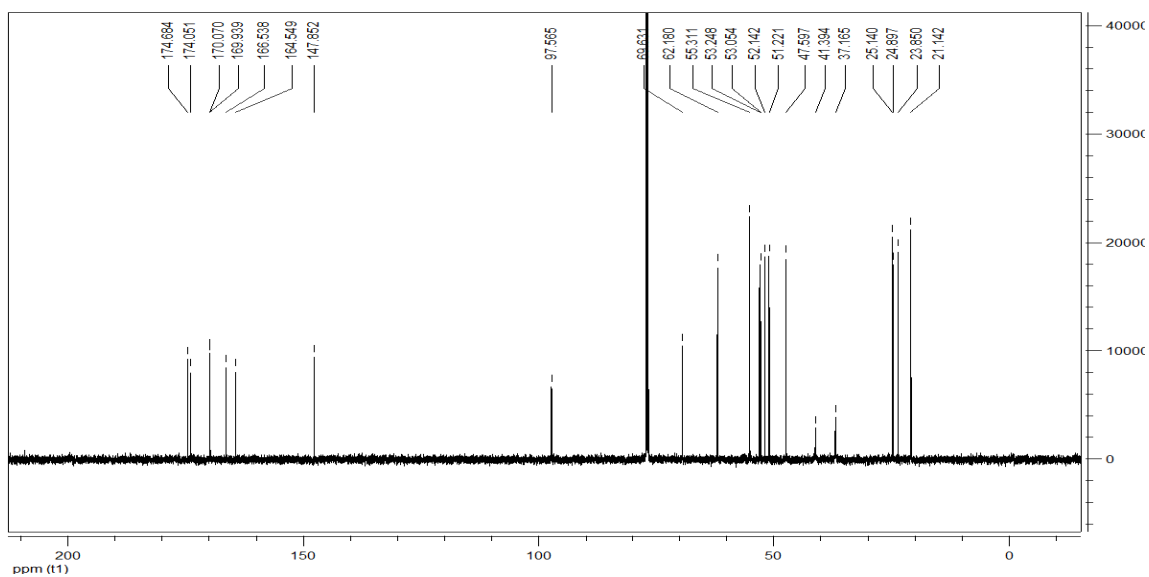
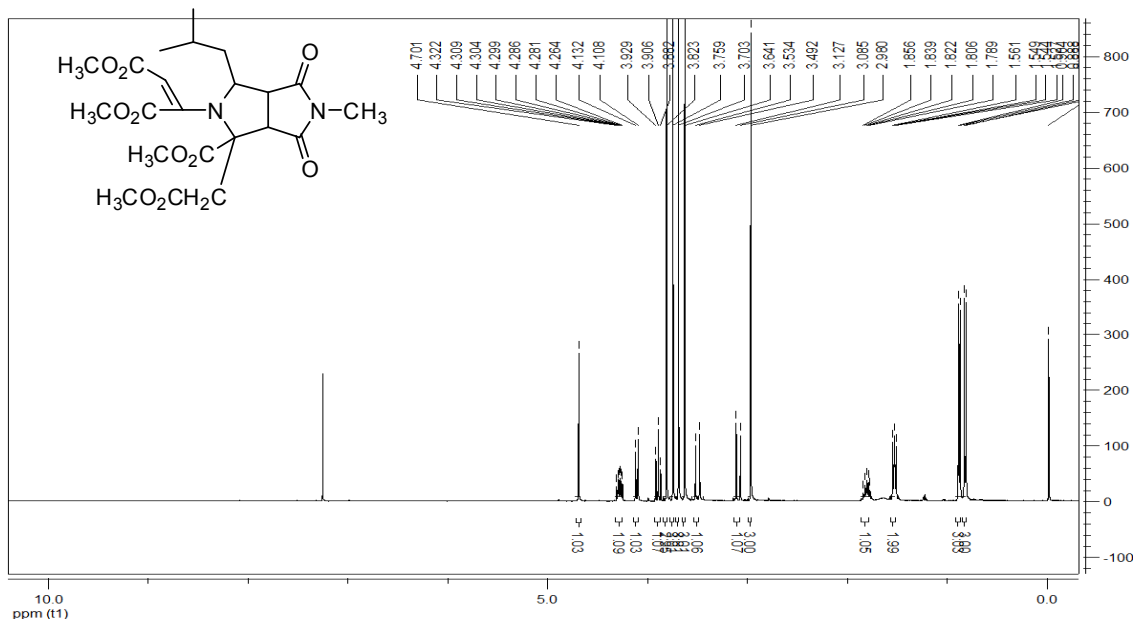
**Dimethyl 2-(3-benzyl-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-4,6-dioxo-5-phenylp
hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4k):**



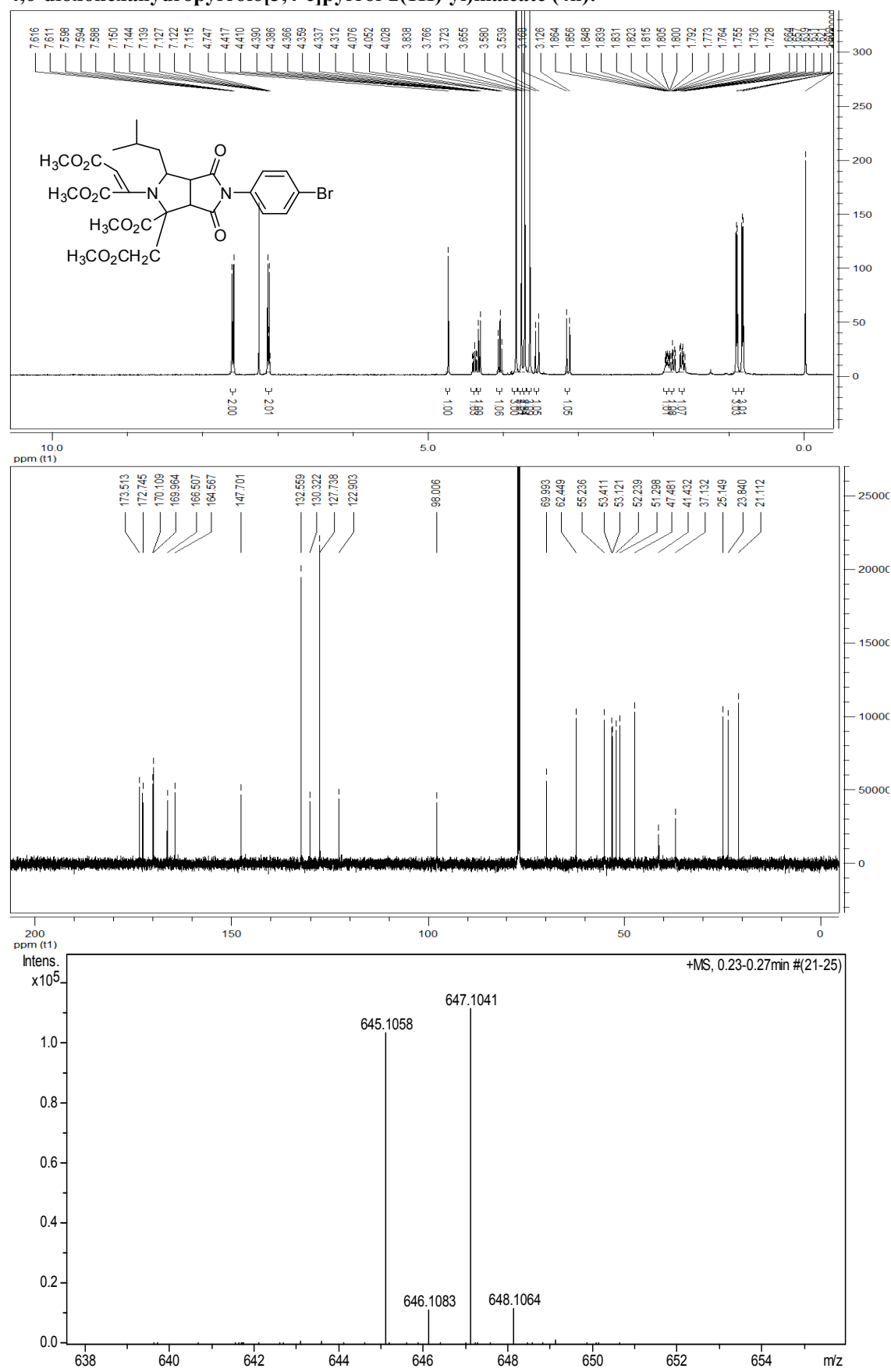
Diethyl 2-(3-benzyl-1-(2-ethoxy-2-oxoethyl)-1-(ethoxycarbonyl)-5-methyl-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4l):



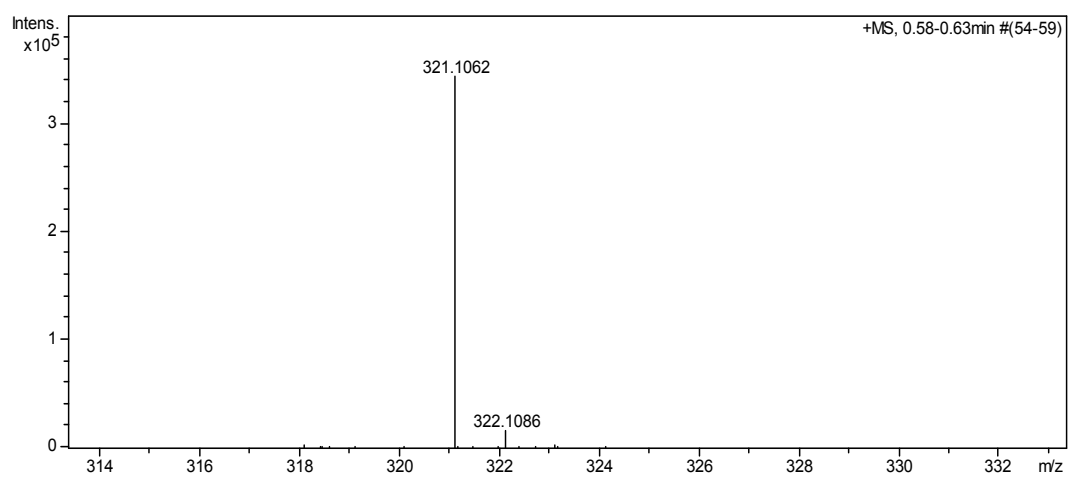
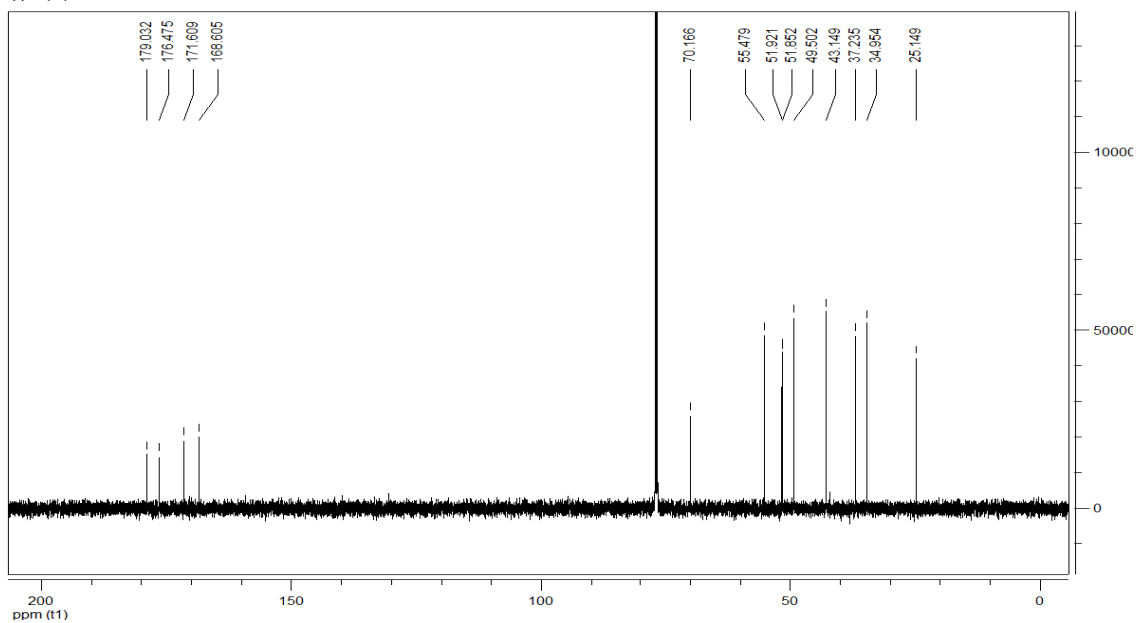
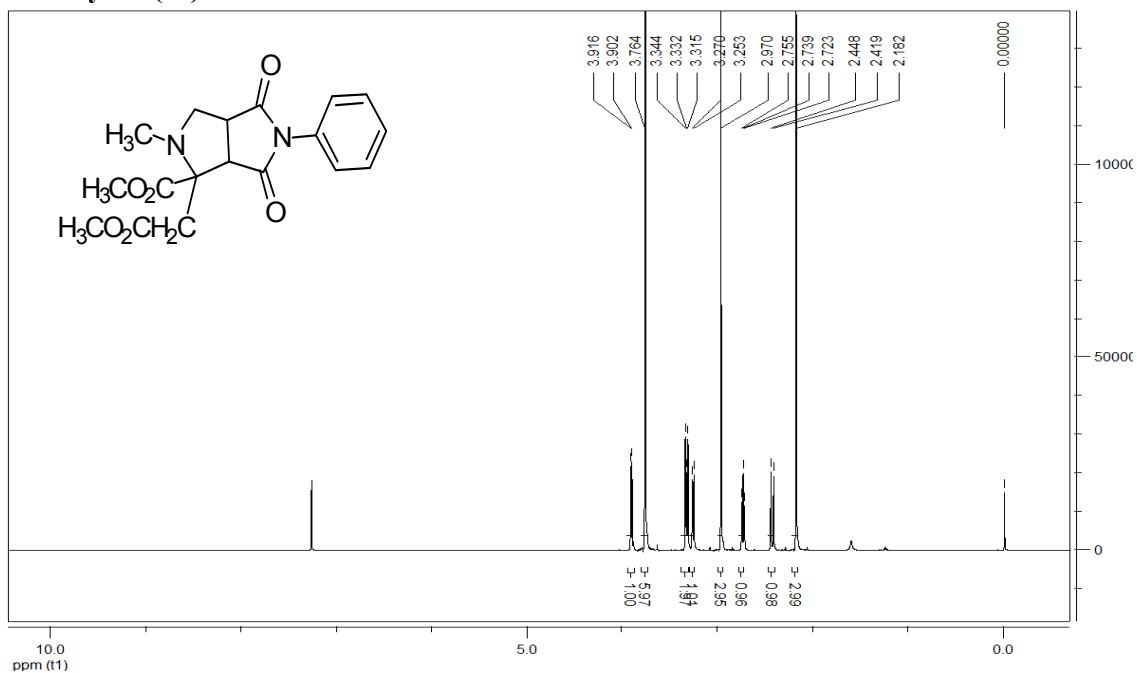
Dimethyl 2-(3-isobutyl-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-5-methyl-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4m):



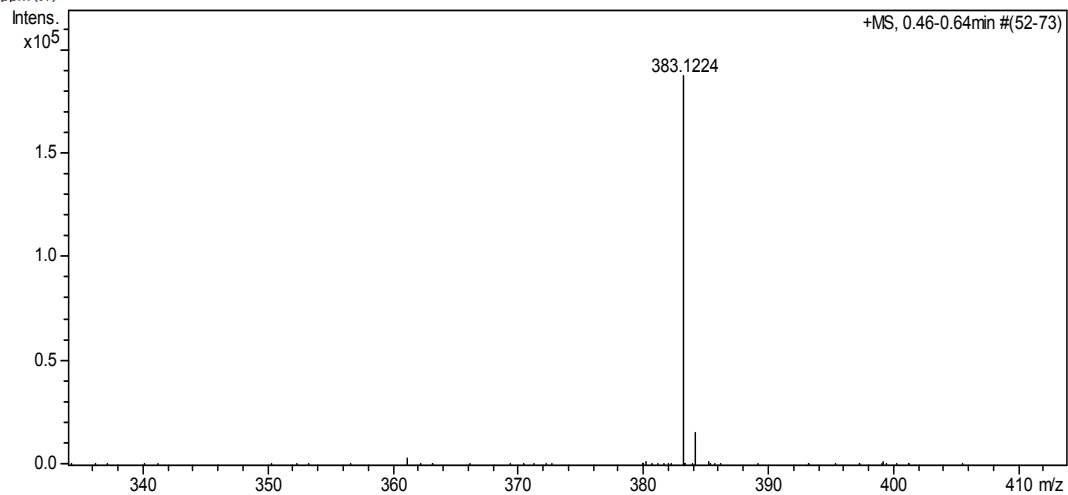
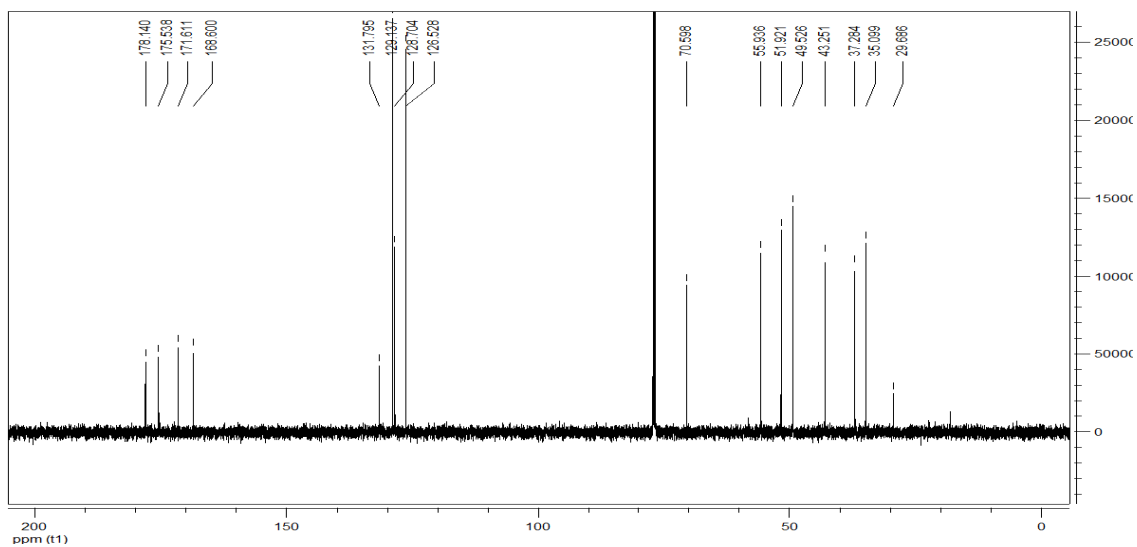
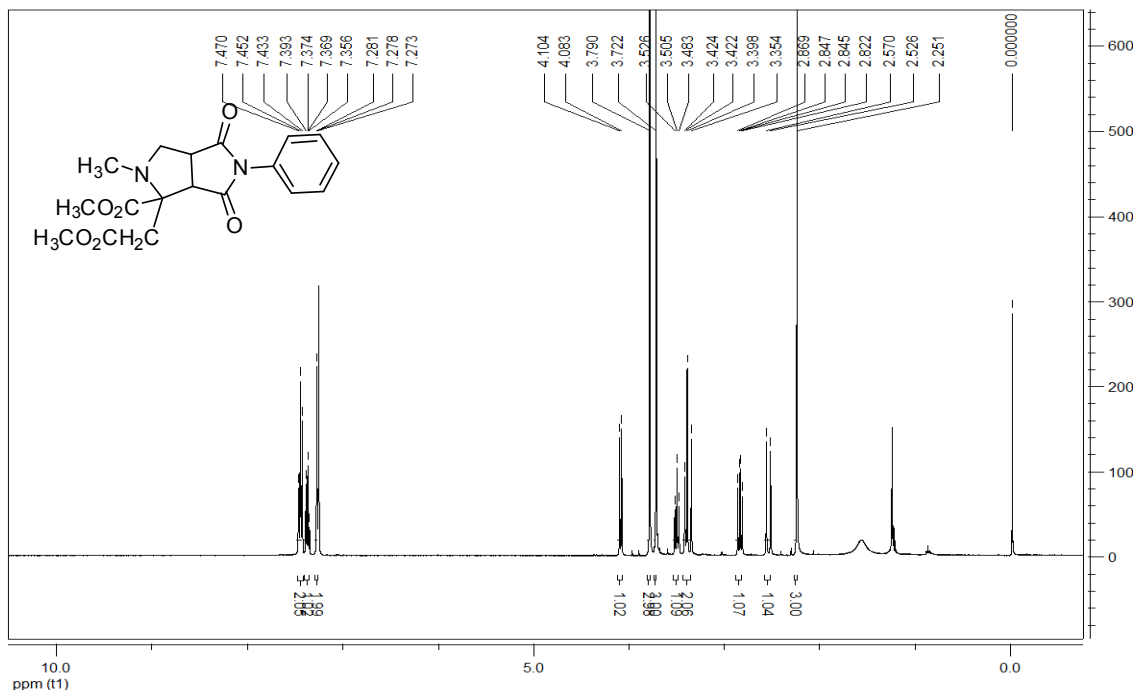
Dimethyl 2-(5-(4-bromophenyl)-3-isobutyl-1-(2-methoxy-2-oxoethyl)-1-(methoxycarbonyl)-4,6-dioxohexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)maleate (4n):



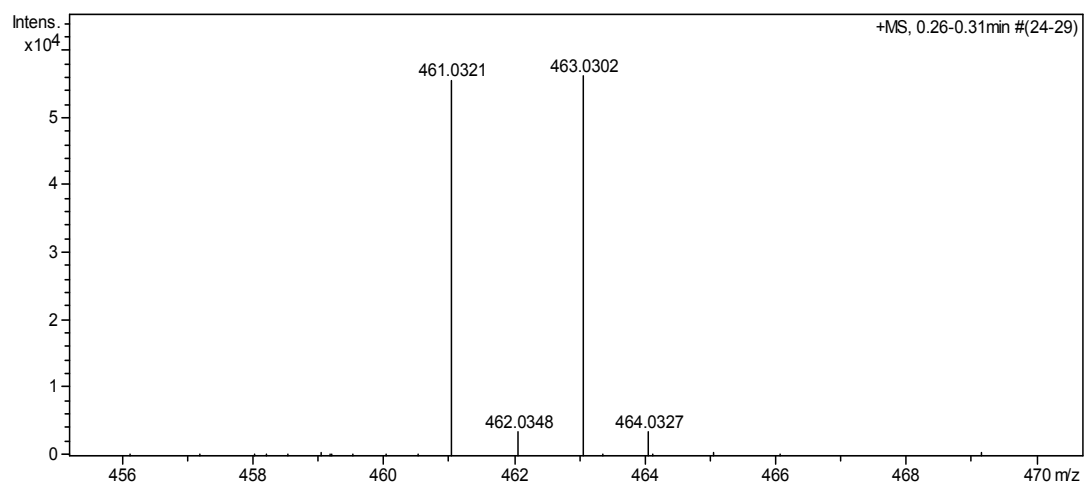
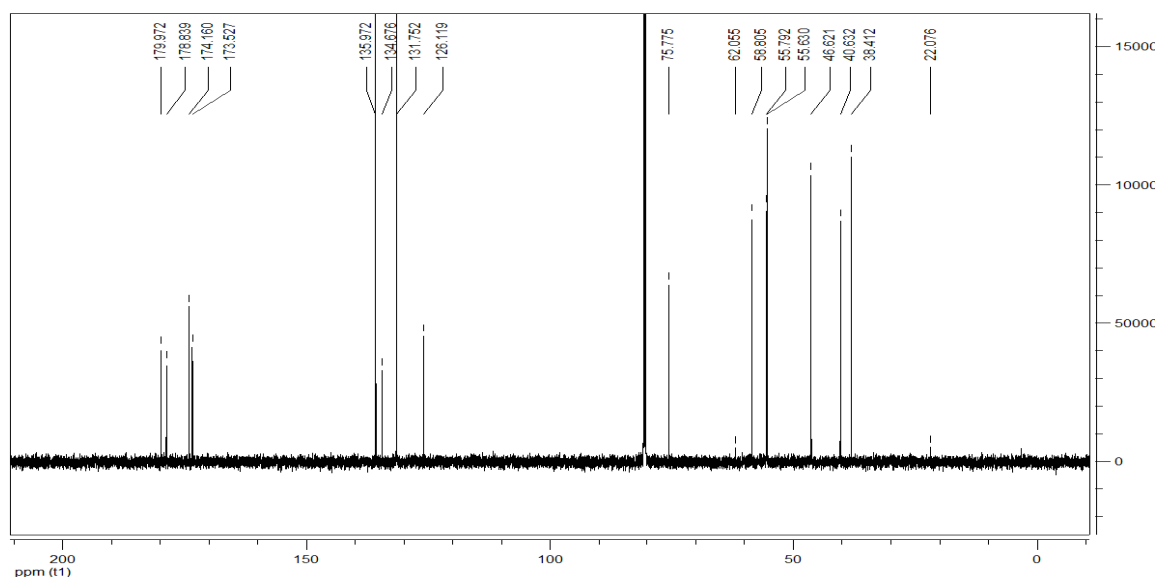
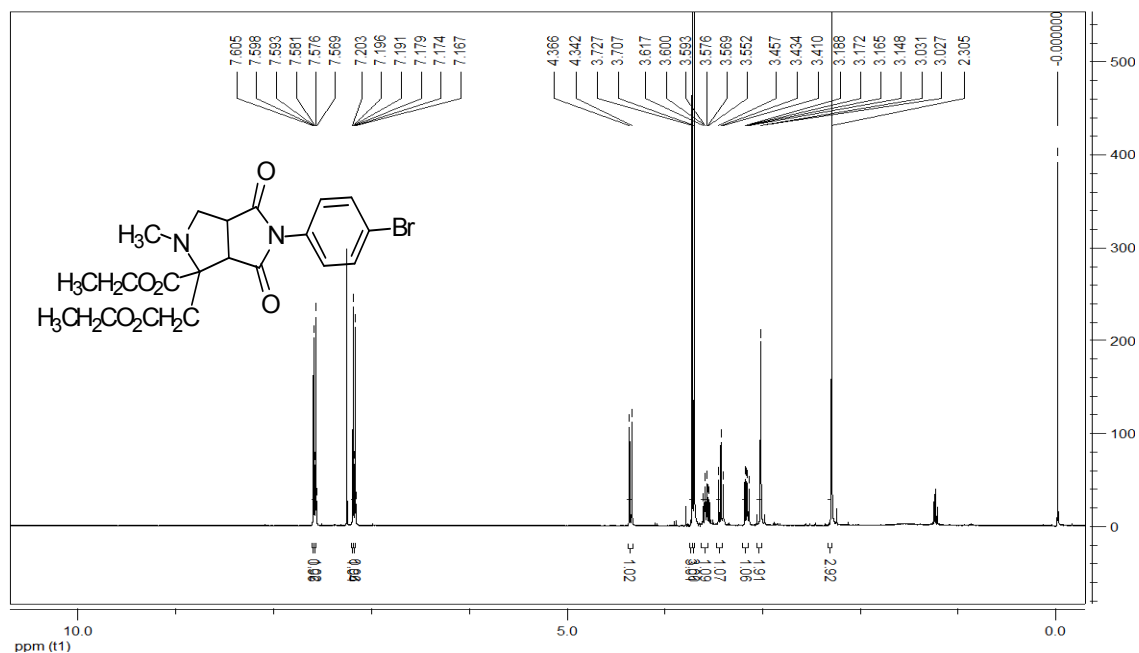
Methyl 1-(2-methoxy-2-oxoethyl)-2,5-dimethyl-4,6-dioxo-octahydropyrrolo[3,4-c]pyrrole-1-carboxylate (5a):



Methyl 1-(2-methoxy-2-oxoethyl)-2-methyl-4,6-dioxo-5-phenyloctahydropyrrolo[3,4-c]-pyrrole-1-carboxylate (5b):

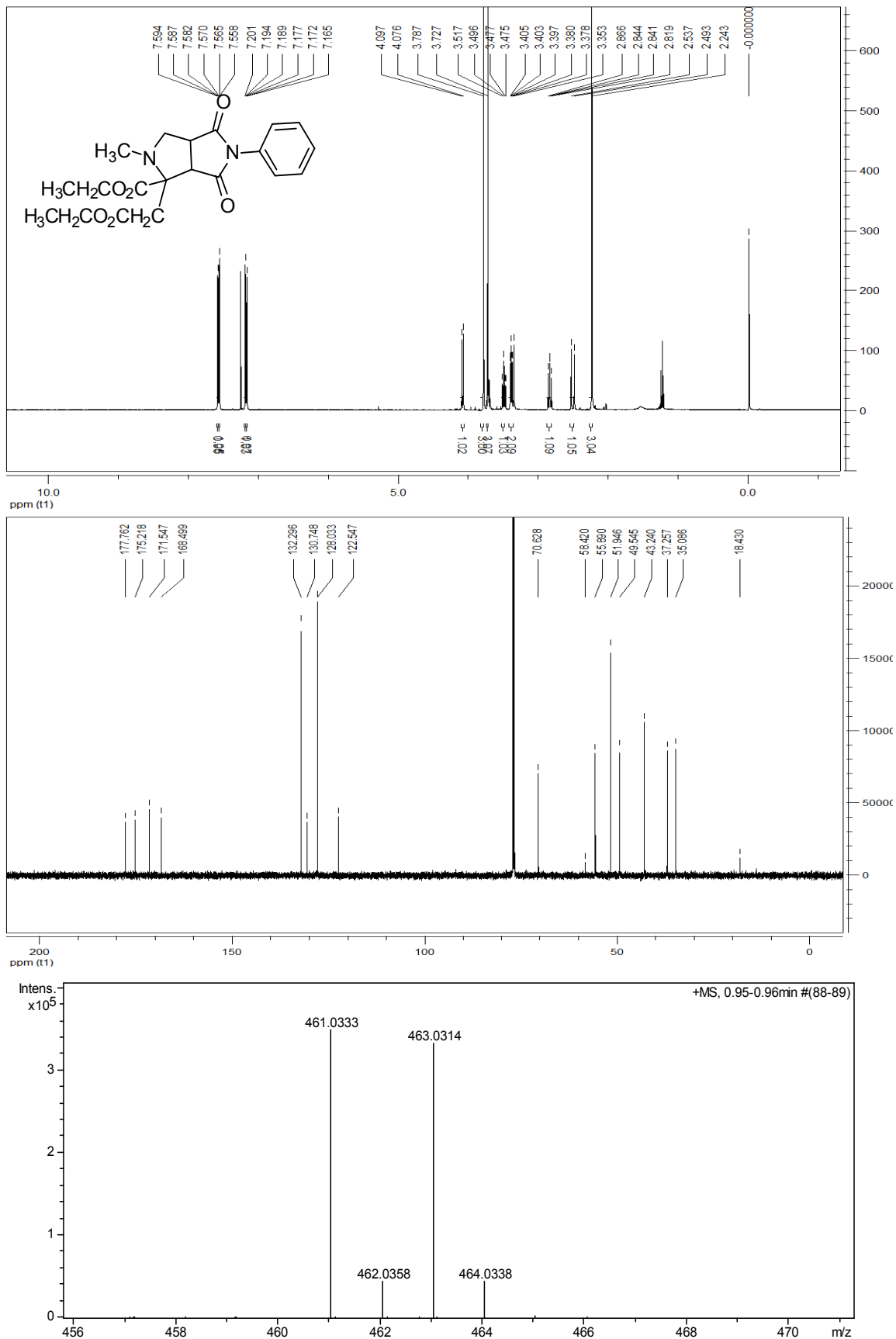


Methyl 5-(4-bromophenyl)-1-(2-methoxy-2-oxoethyl)-2-methyl-4,6-dioxooctahydropyrrolo-[3,4-c]pyrrole-1-carboxylate (5c):

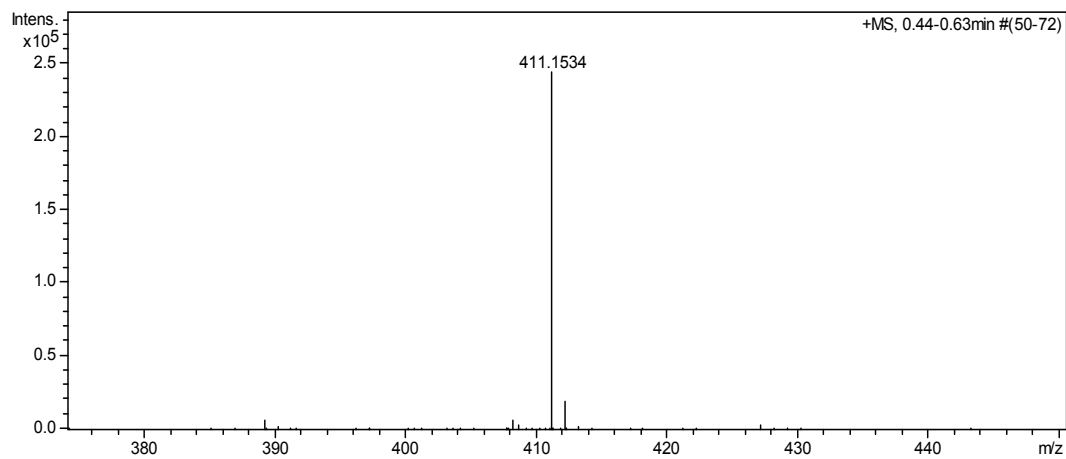
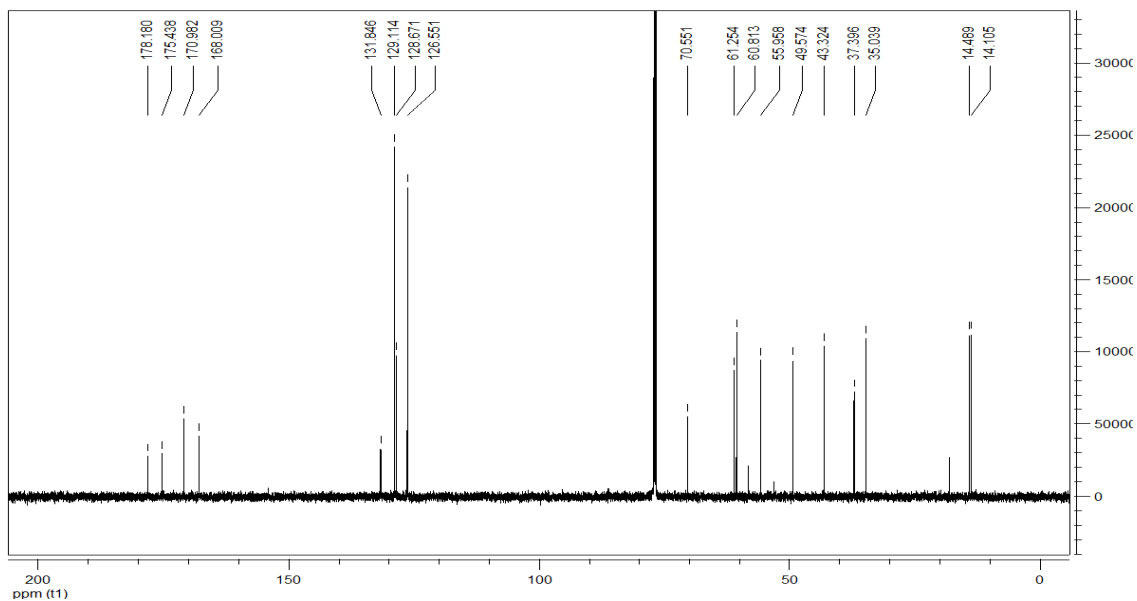
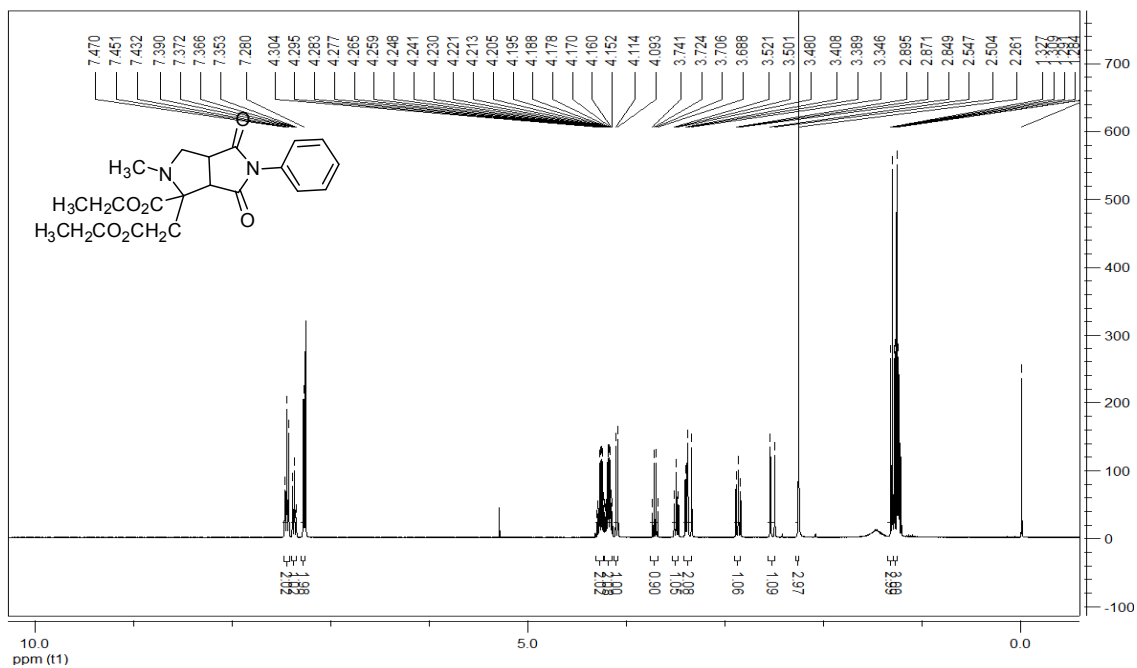


methyl

5-(4-bromophenyl)-1-(2-methoxy-2-oxoethyl)-2-methyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate (5c')



Ethyl 1-(2-ethoxy-2-oxoethyl)-2-methyl-4,6-dioxo-5-phenyloctahydropyrrolo[3,4-c]-pyrrole-1-carboxylate (5d):



Ethyl 5-(4-bromophenyl)-1-(2-ethoxy-2-oxoethyl)-2-methyl-4,6-dioxooctahydropyrrolo-[3,4-c]-pyrrole-1-carboxylate (5e):

