Electronic Supplementary Material (ESI) for RSC Advances.

Convenient synthesis of functionalized pyrrolo[3,4-*b*]pyridines and pyrrolo[3,4-*b*]quinolines via three-component reactions

Yan-Hong Jiang, Man Xiao, Chao-Guo Yan*

Supporting Information

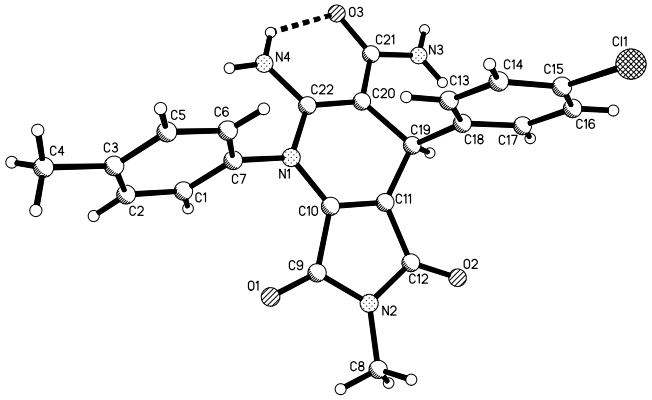


Fig. s1 ORTEP-drawings of the crystal structures of **1p**

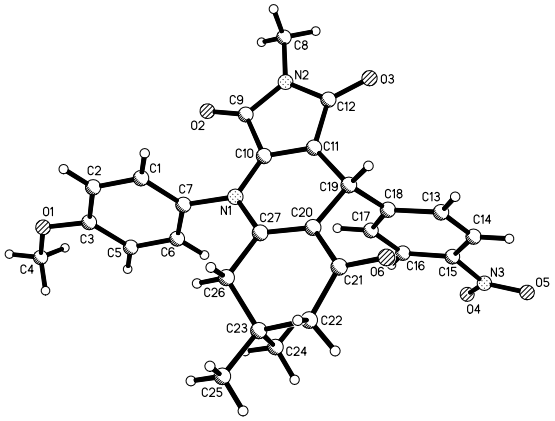


Fig. s2 ORTEP-drawings of the crystal structures of **3g**

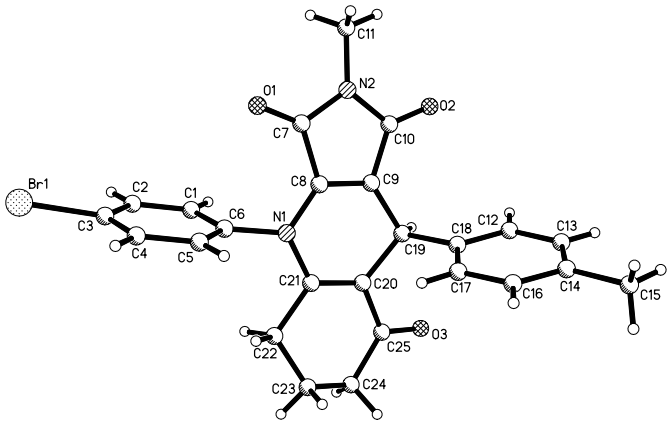
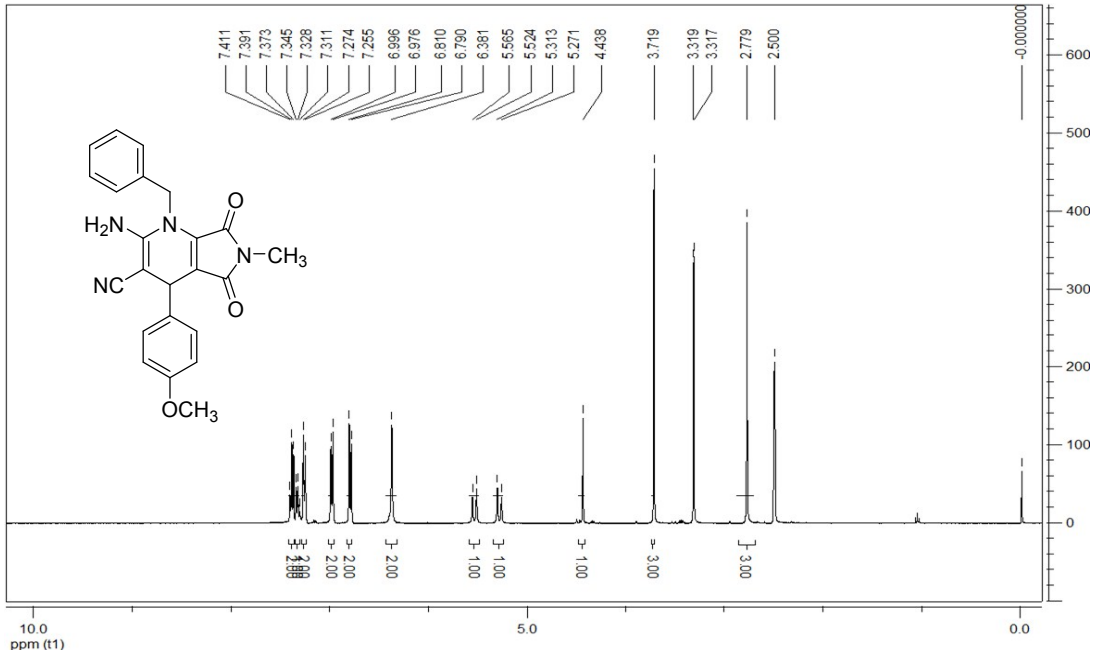
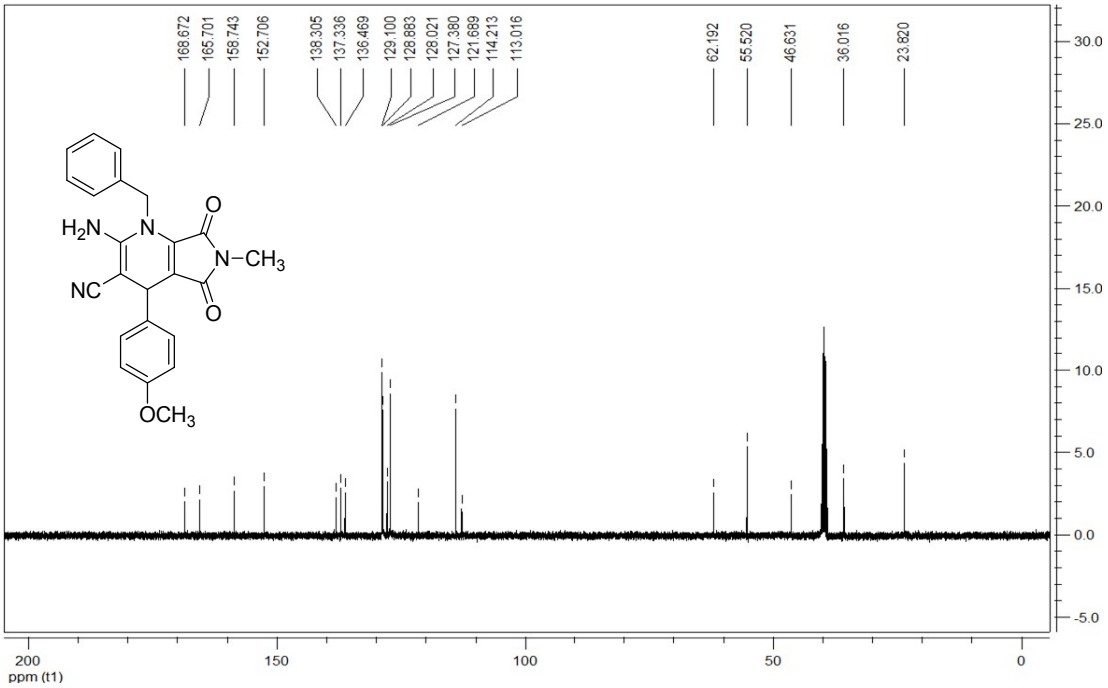
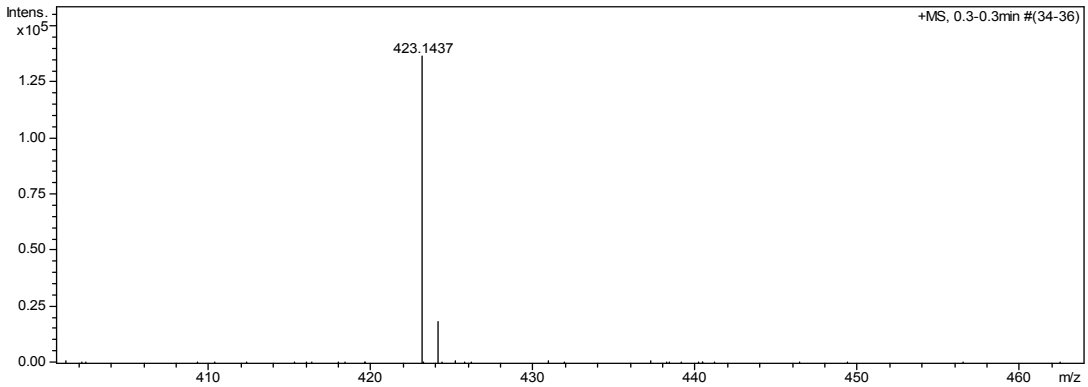


Fig. s3 ORTEP-drawings of the crystal structures of **3j**

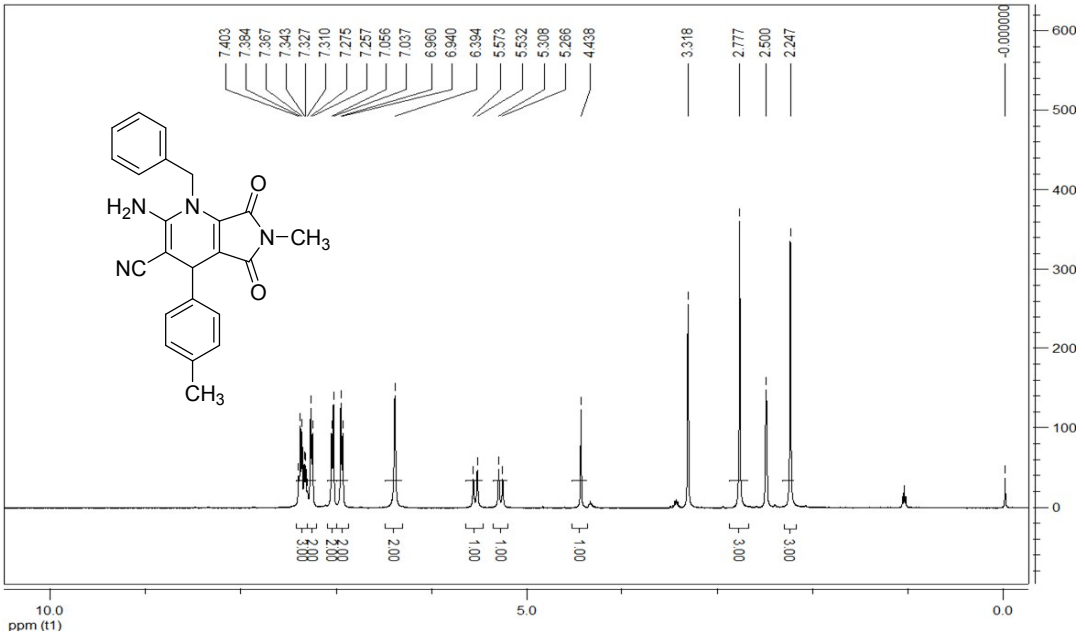
2-Amino-1-benzyl-4-(4-methoxyphenyl)-6-methyl-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1a):

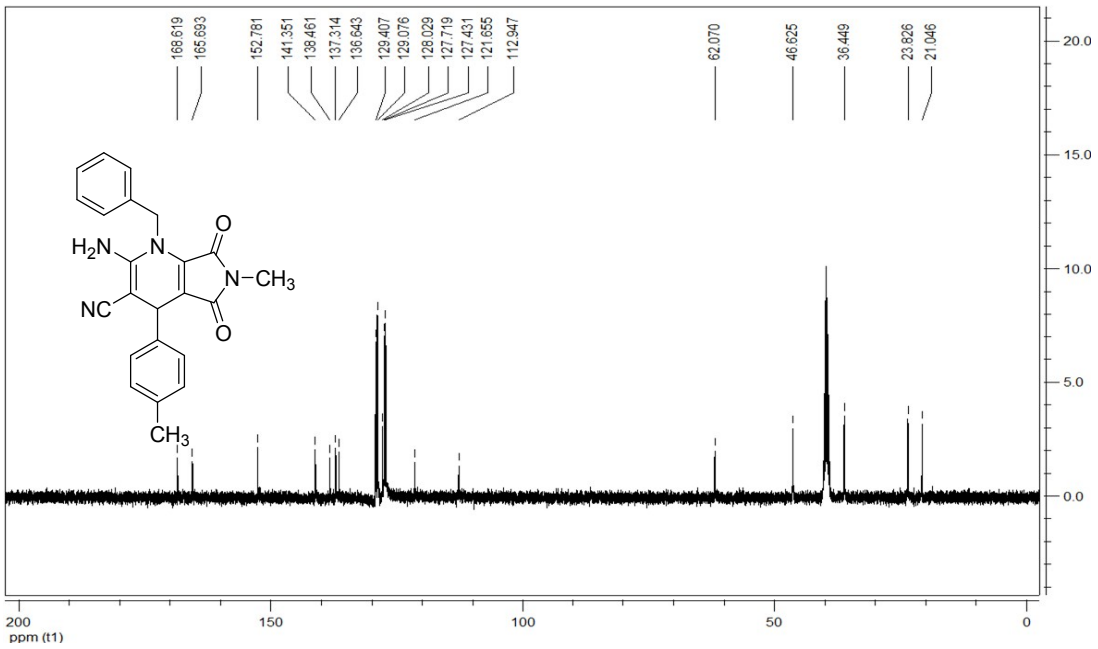


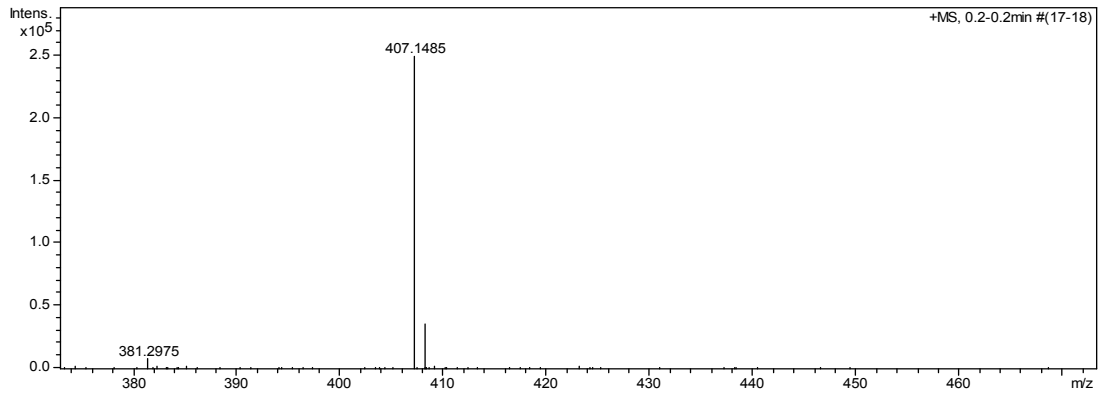




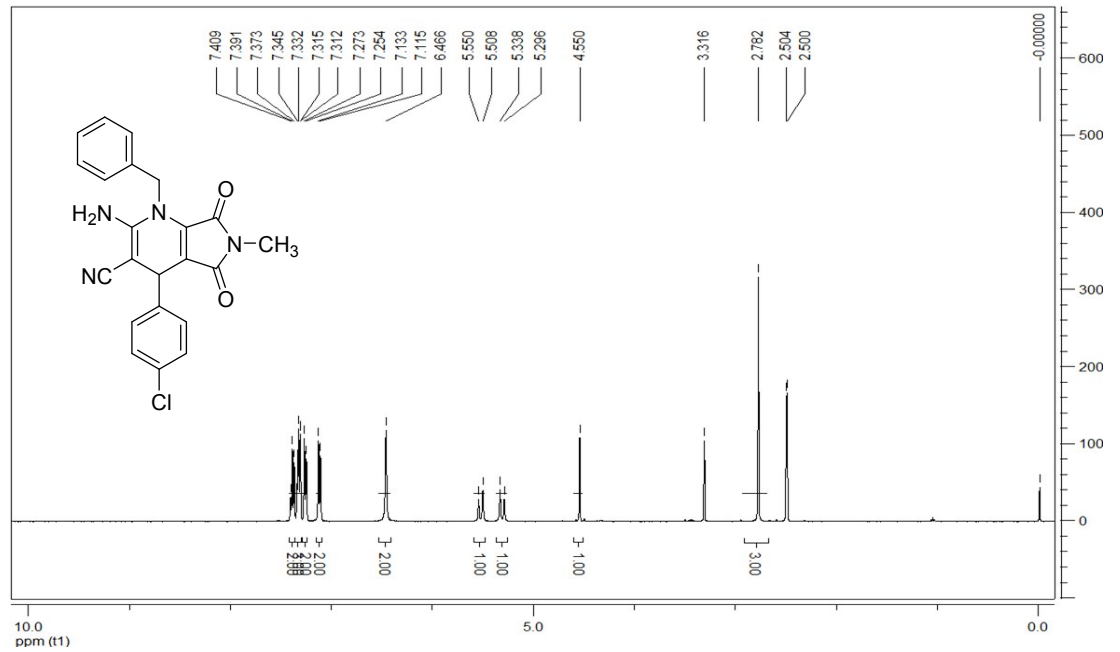
2-Amino-1-benzyl-6-methyl-5,7-dioxo-4-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1b):

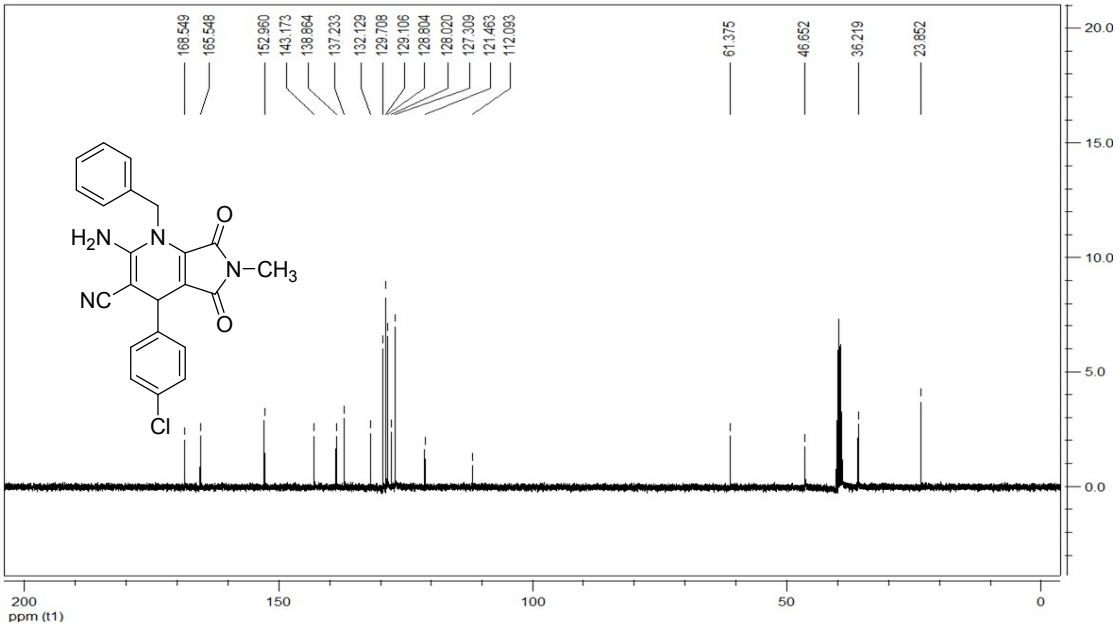


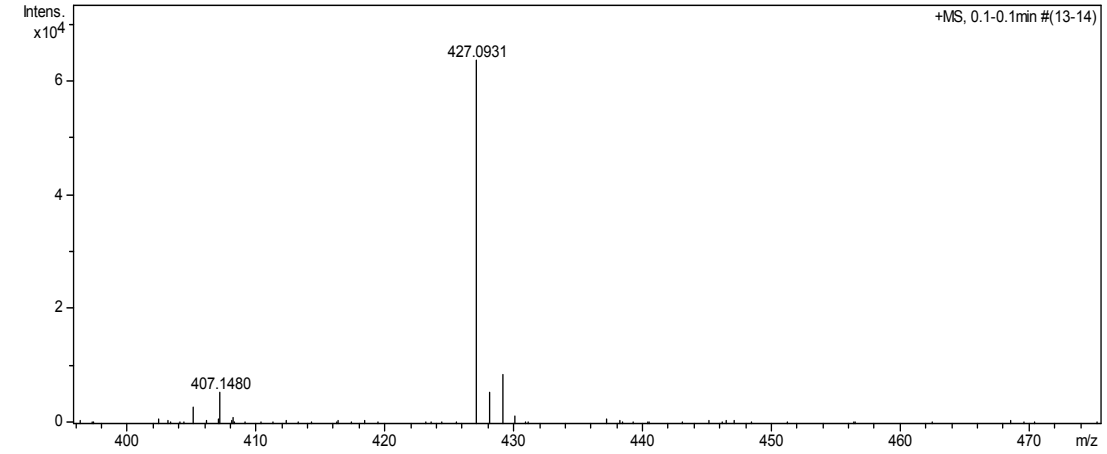




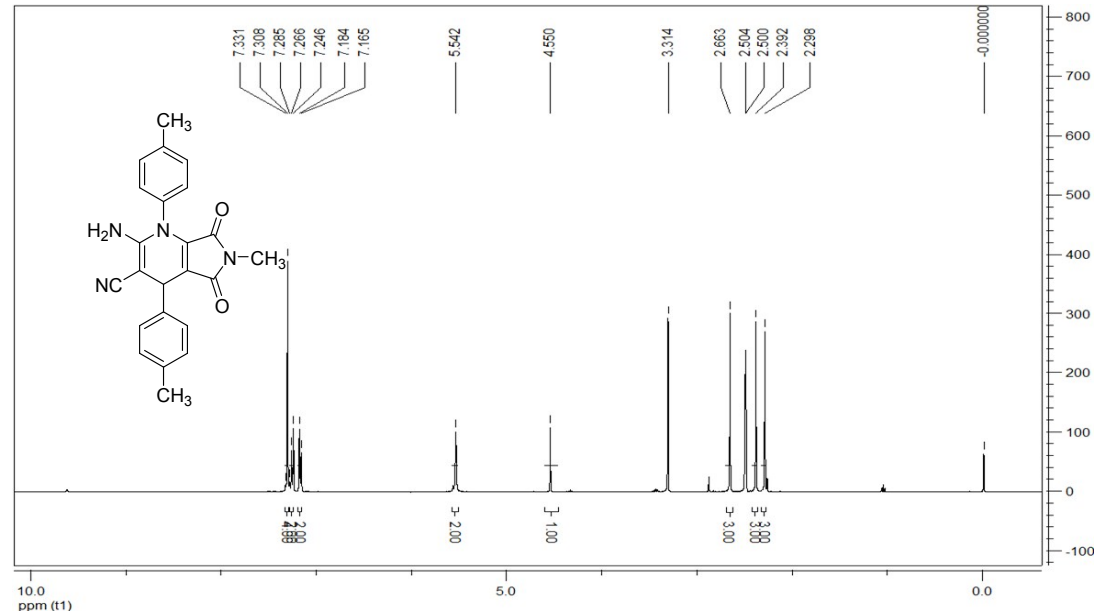
2-Amino-1-benzyl-4-(4-chlorophenyl)-6-methyl-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1c):

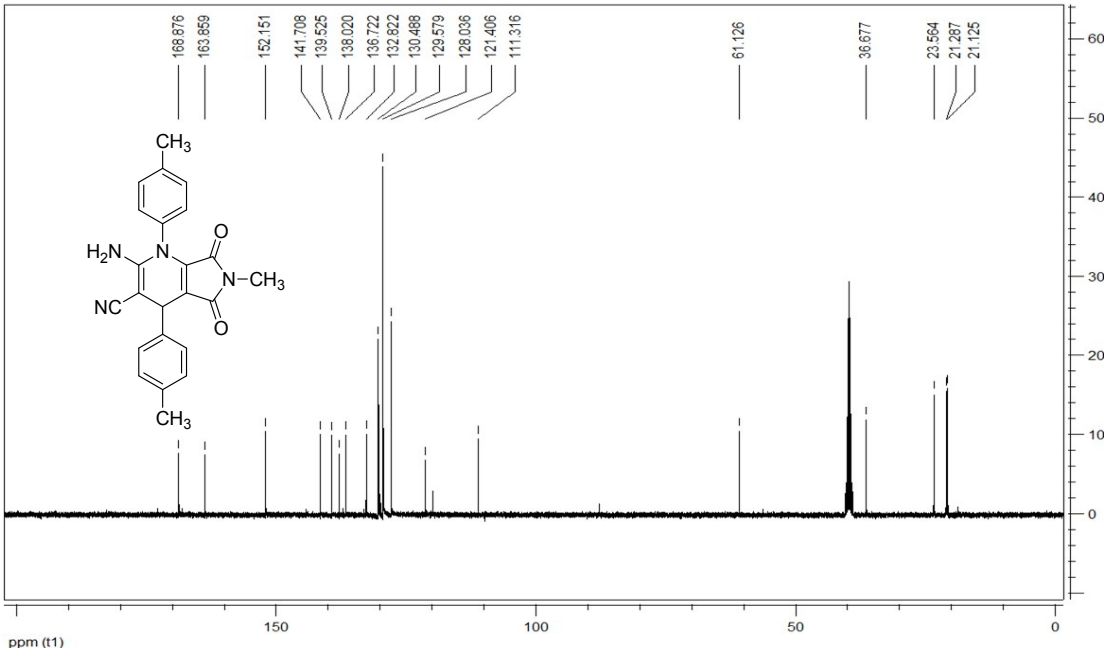


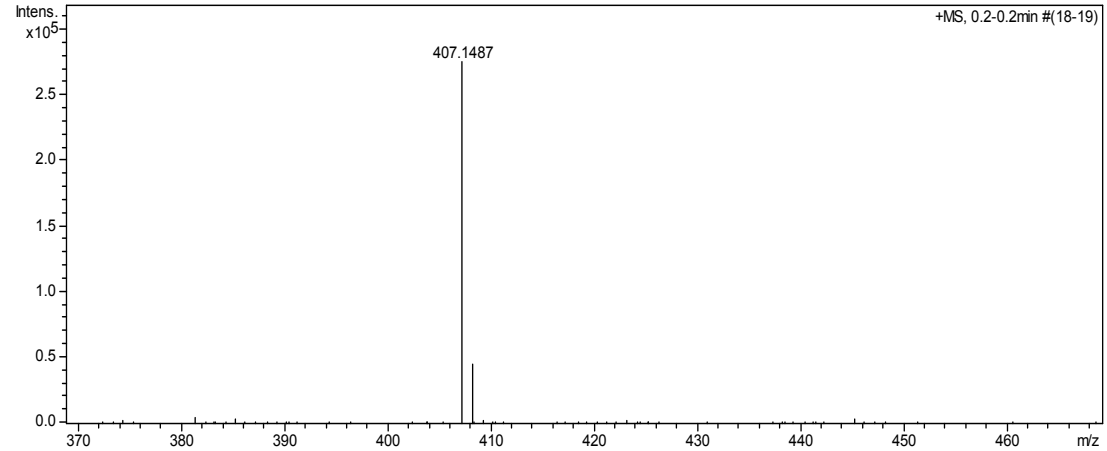




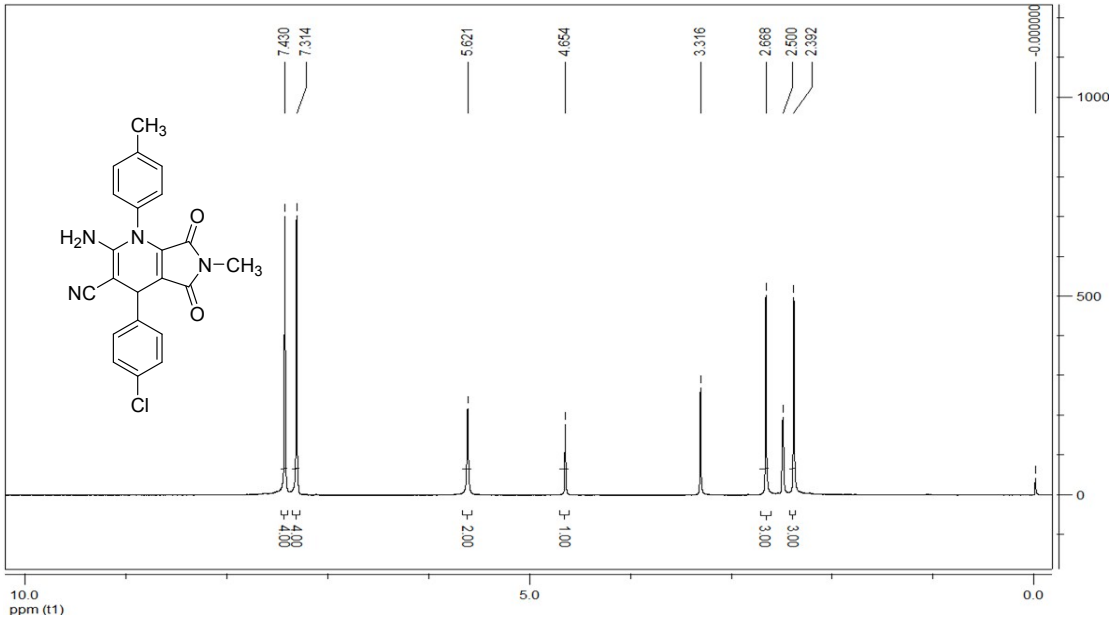
2-Amino-6-methyl-5,7-dioxo-1,4-di-p-tolyl-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1d):

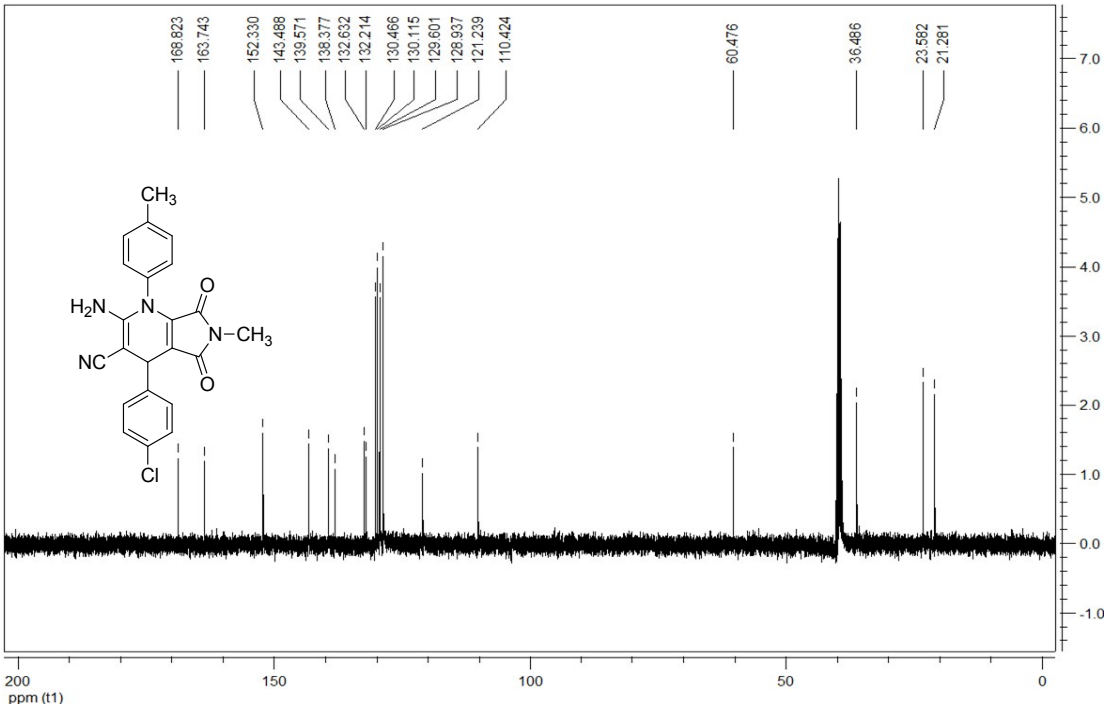


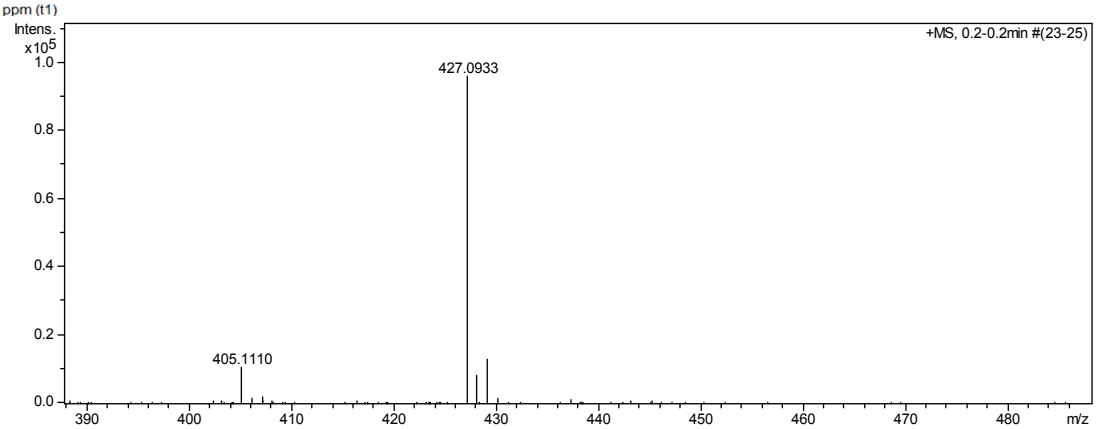




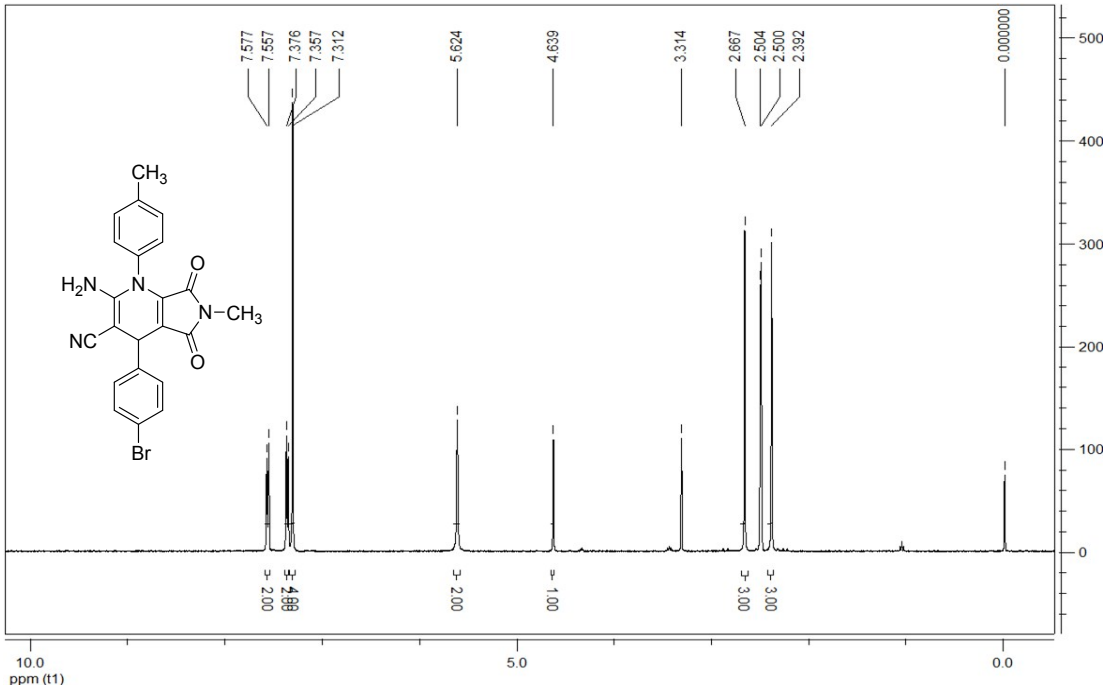
2-Amino-4-(4-chlorophenyl)-6-methyl-5,7-dioxo-1-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1e):

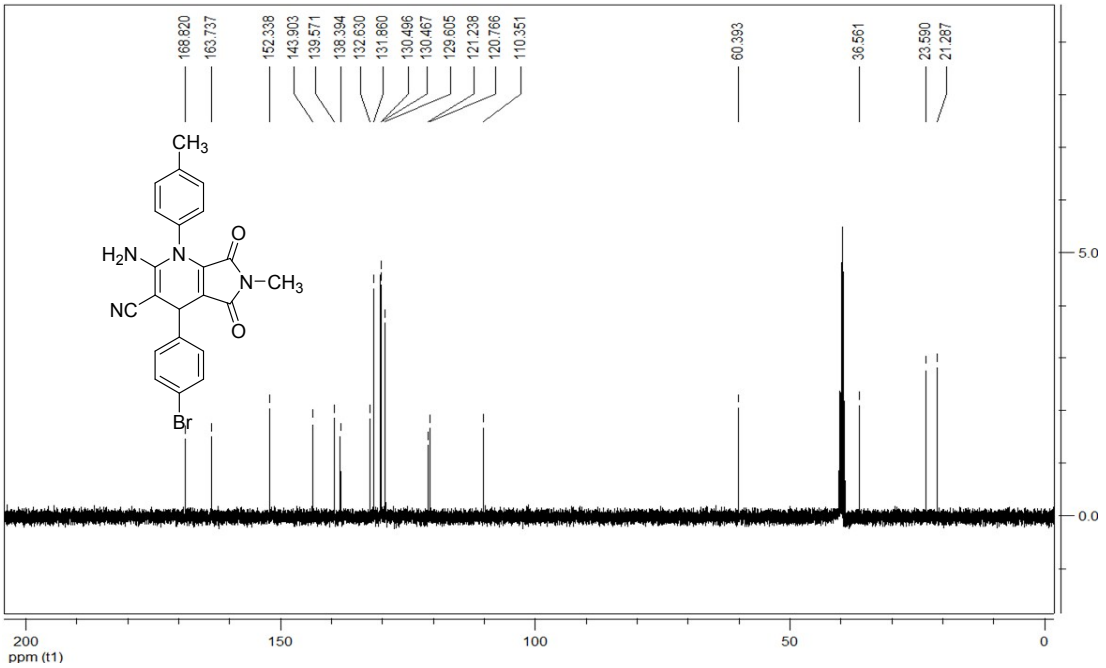


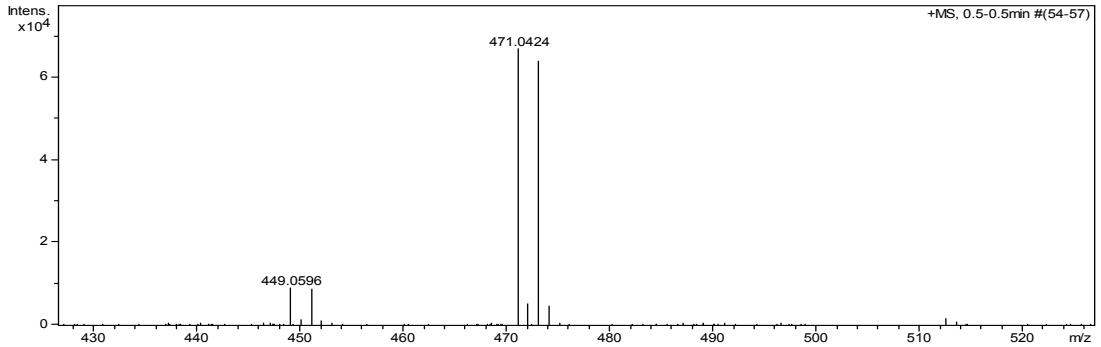




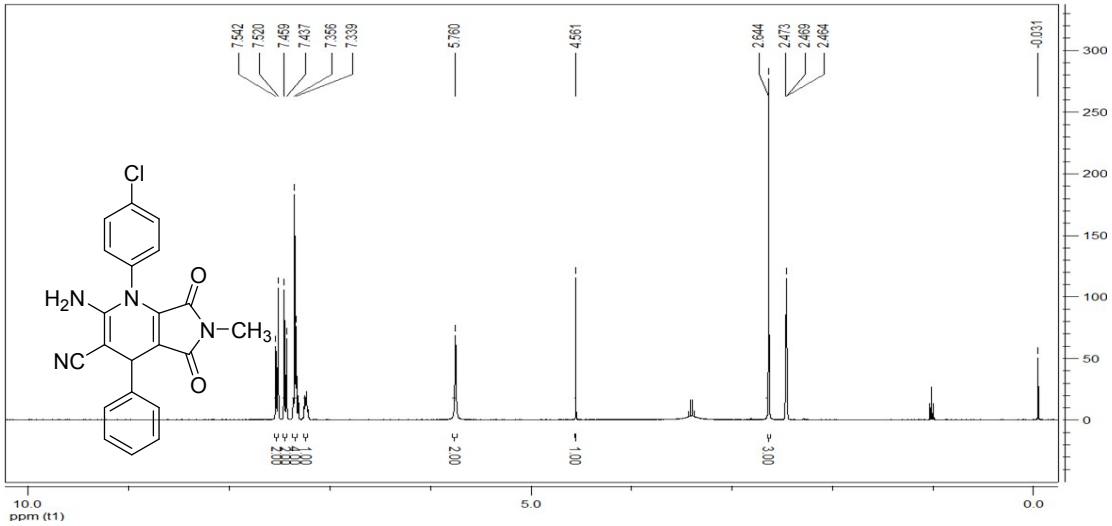
2-Amino-4-(4-bromophenyl)-6-methyl-5,7-dioxo-1-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1f):

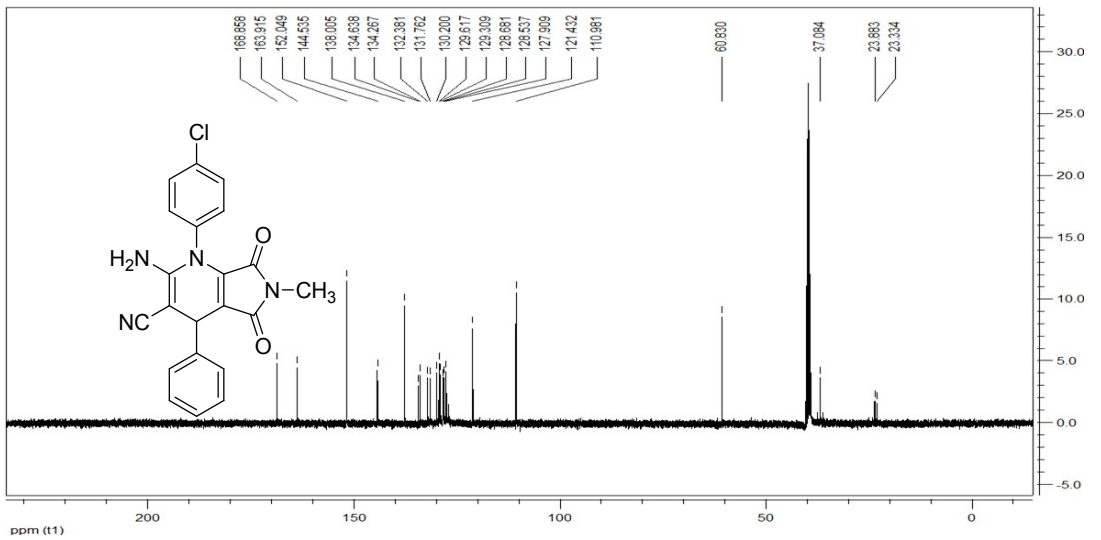


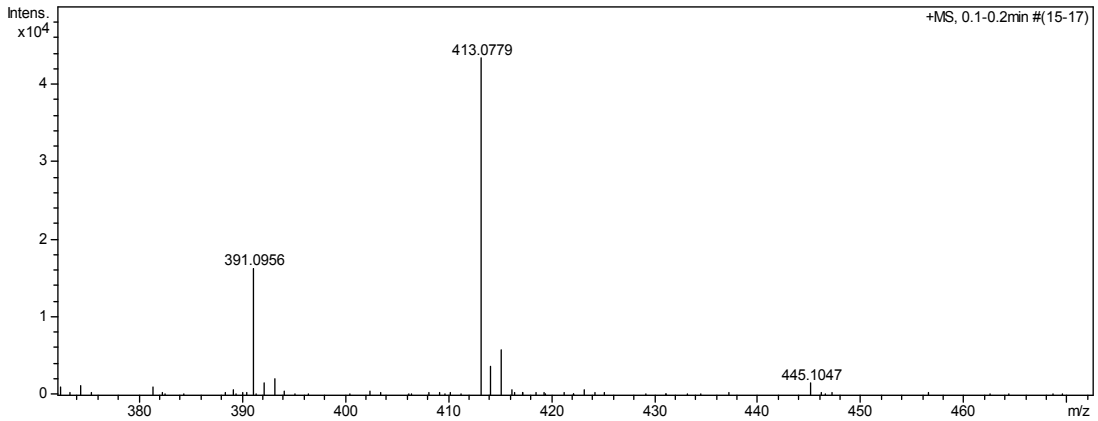




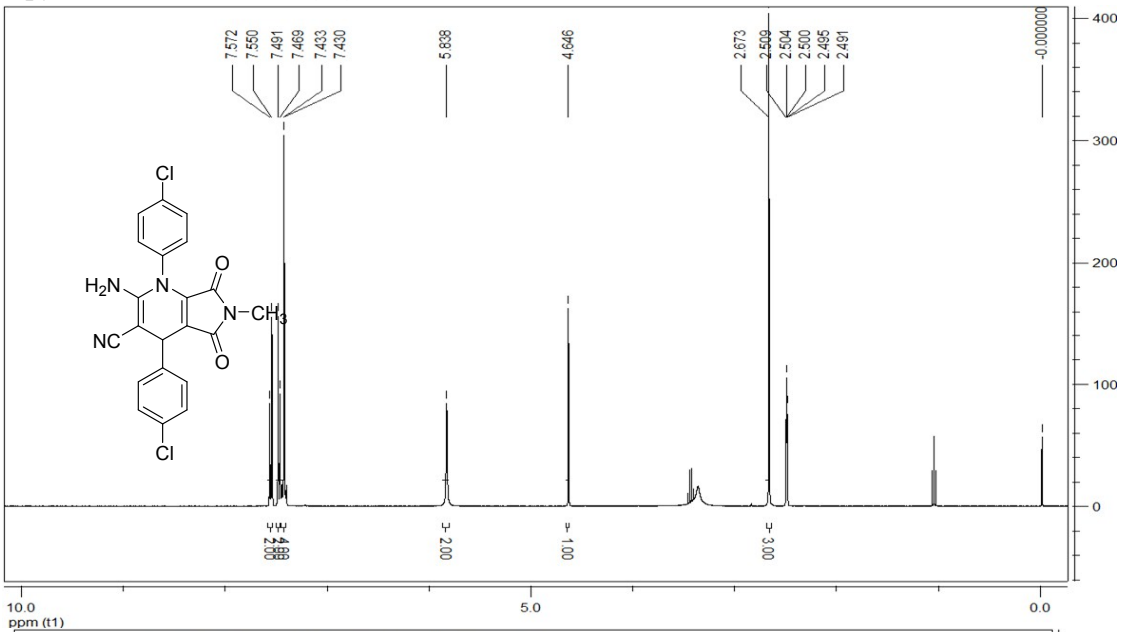
2-Amino-1-(4-chlorophenyl)-6-methyl-5,7-dioxo-4-phenyl-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1g): Yellow solid, 72%, m.p. 240~242℃; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.56 (d, J = 8.8 Hz, 2H, ArH), 7.48 (d, J = 8.8 Hz, 2H, ArH), 7.40-7.35 (m, 4H, ArH), 7.29-7.25 (m, 1H, ArH), 5.79 (s, 2H, NH_2), 4.59 (s, 1H, CH), 2.67 (s, 3H CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 168.9, 163.9, 152.0, 144.5, 138.0, 134.6, 134.3, 132.4, 131.8, 130.2, 129.6, 128.7, 128.5, 121.4, 110.0, 60.8, 37.0, 23.9, 23.3; IR (KBr) υ: 3452, 3098, 2941, 2876, 2184, 1771, 1716, 1676, 1626, 1559, 1489, 1417, 1379, 1280, 1181, 1079, 980, 839, 758 cm^{-1}; MS (*m*/*z*): HRMS (ESI) Calcd. for $C_{21}H_{15}ClN_4NaO_2$ ([M+Na]$^+$): 413.0776. Found: 413.0779.

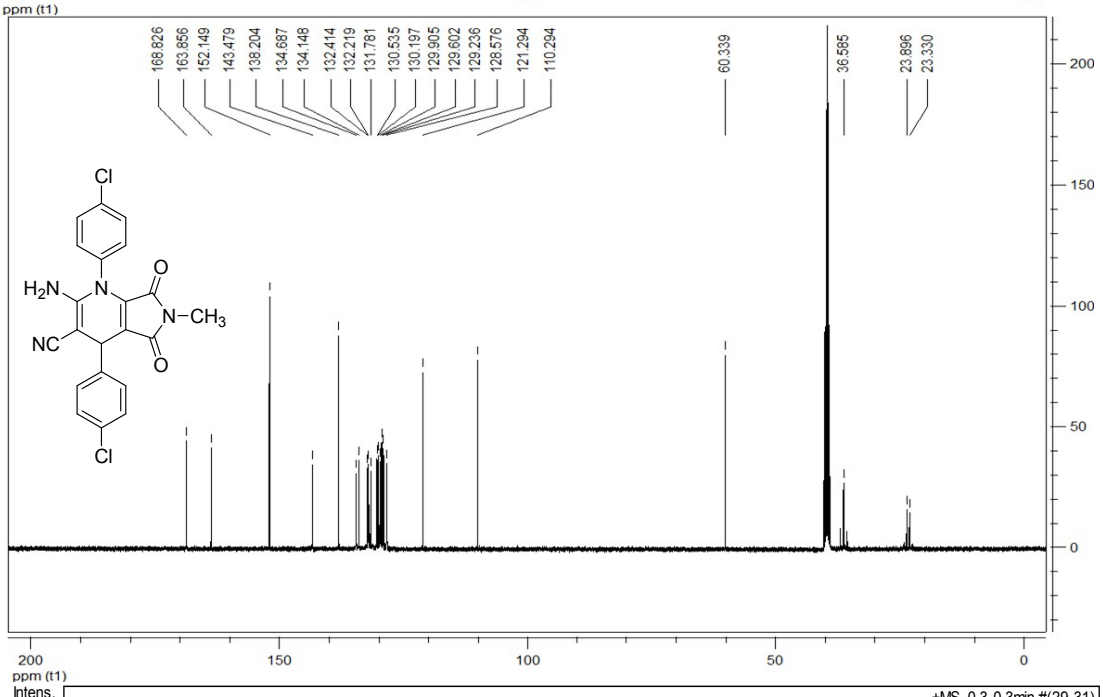


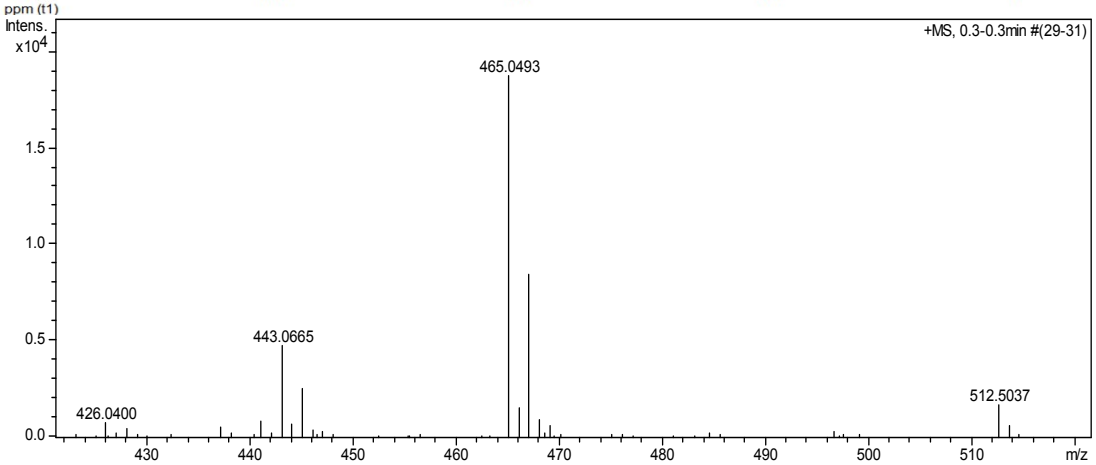




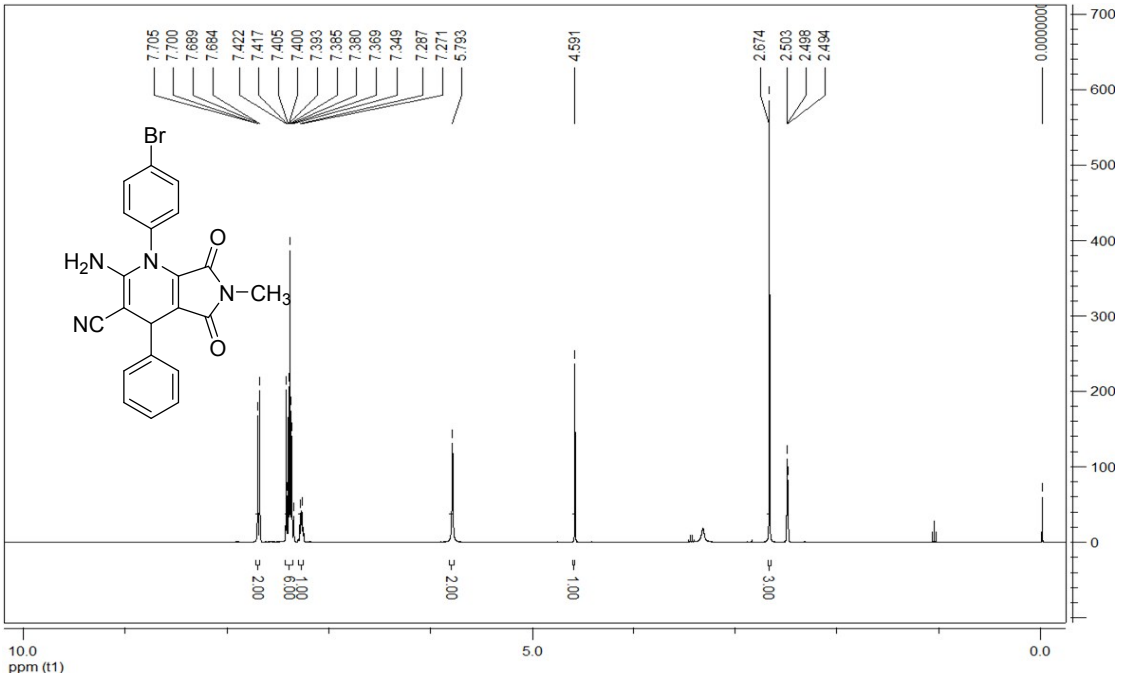
2-Amino-1,4-bis(4-chlorophenyl)-6-methyl-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carbonitrile (1h):

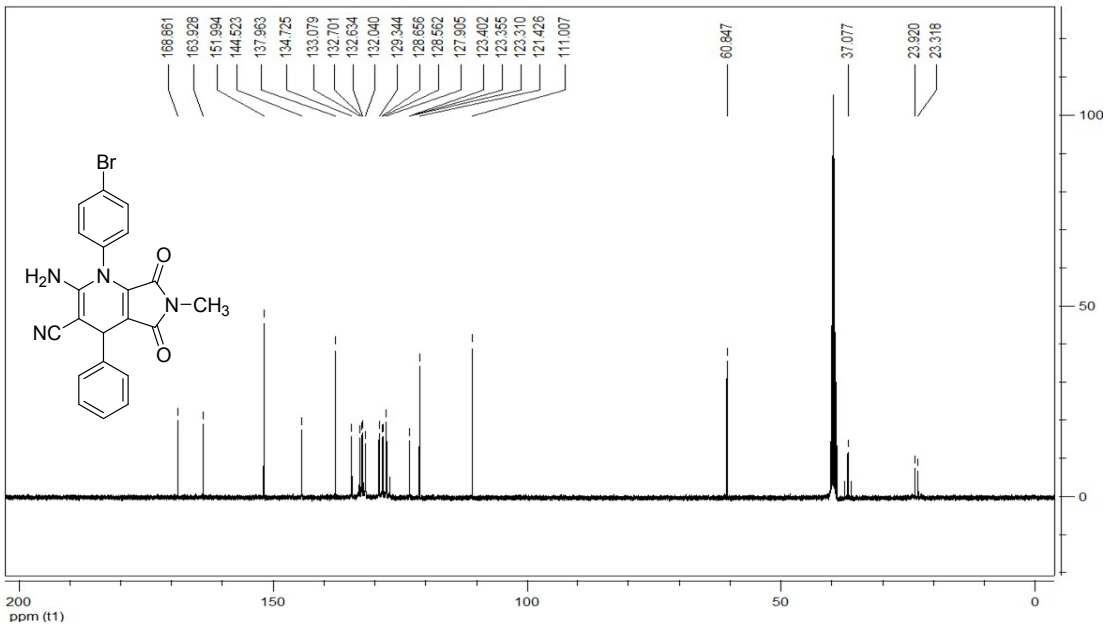


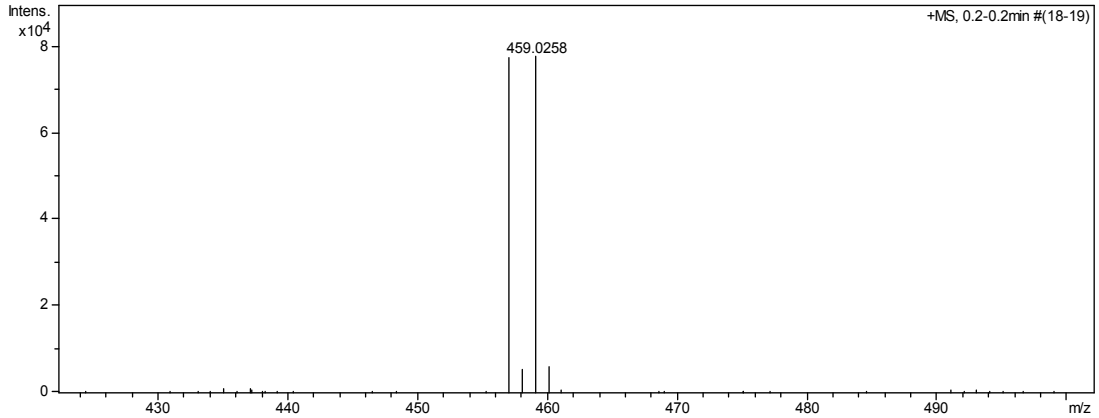




2-Amino-1-(4-bromophenyl)-6-methyl-5,7-dioxo-4-phenyl-4,5,6,7-tetrahydro-1H-pyrrolo[3,4-b]pyridine-3-carbonitrile (1i):







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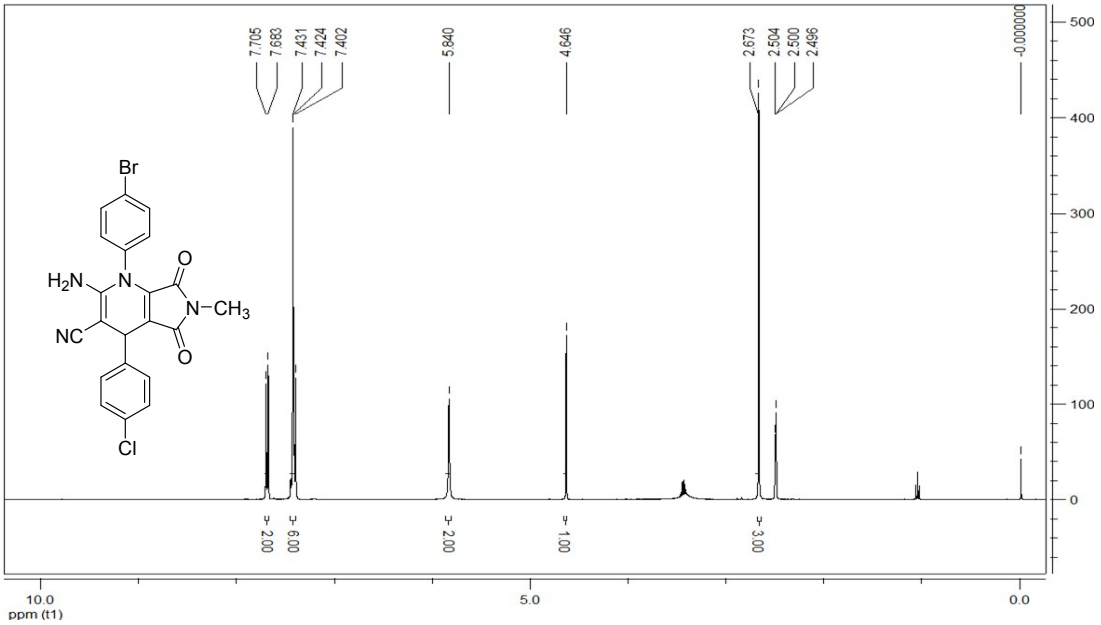
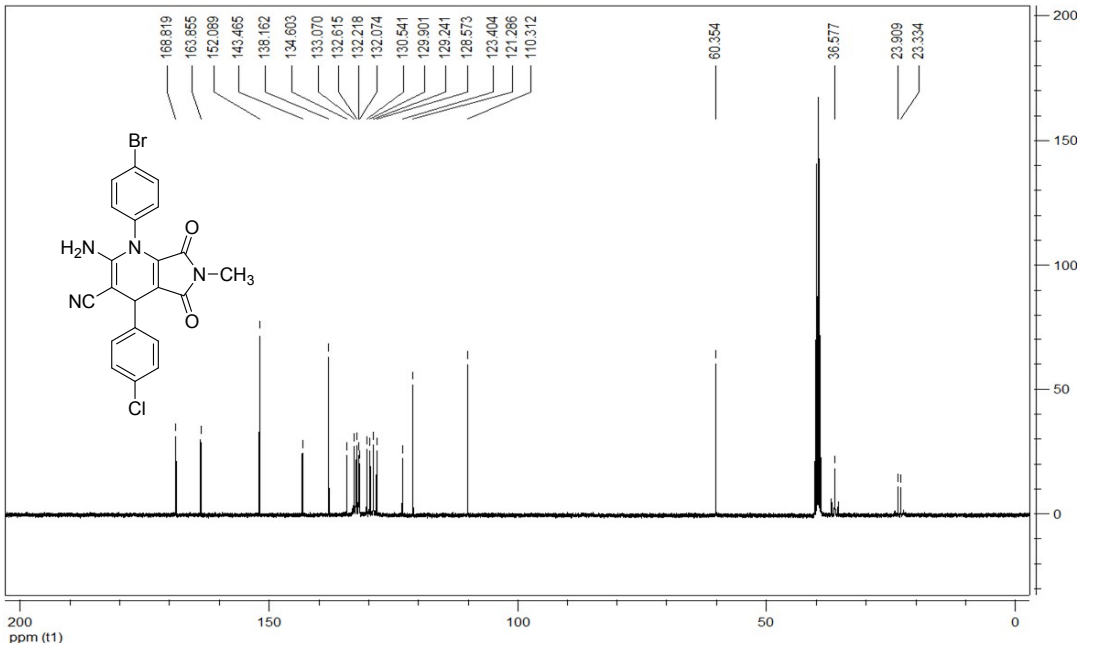
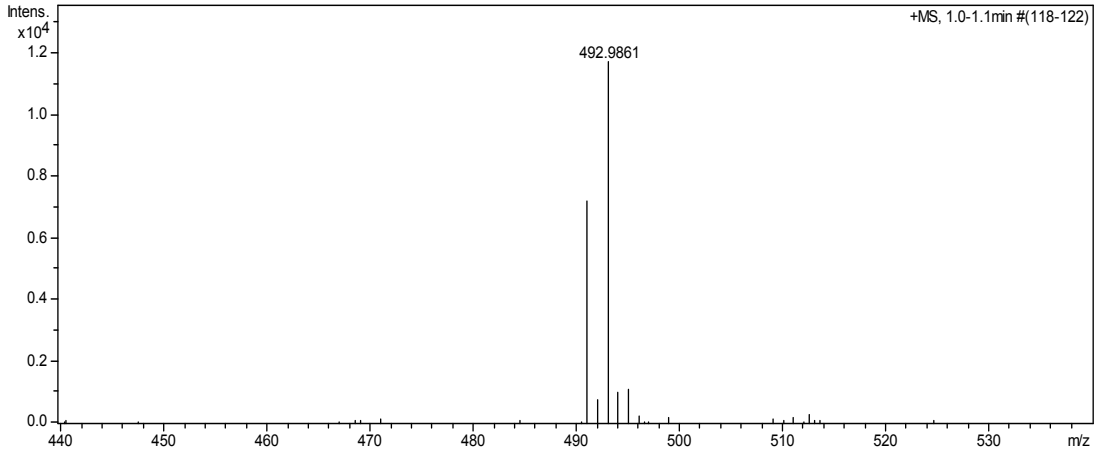
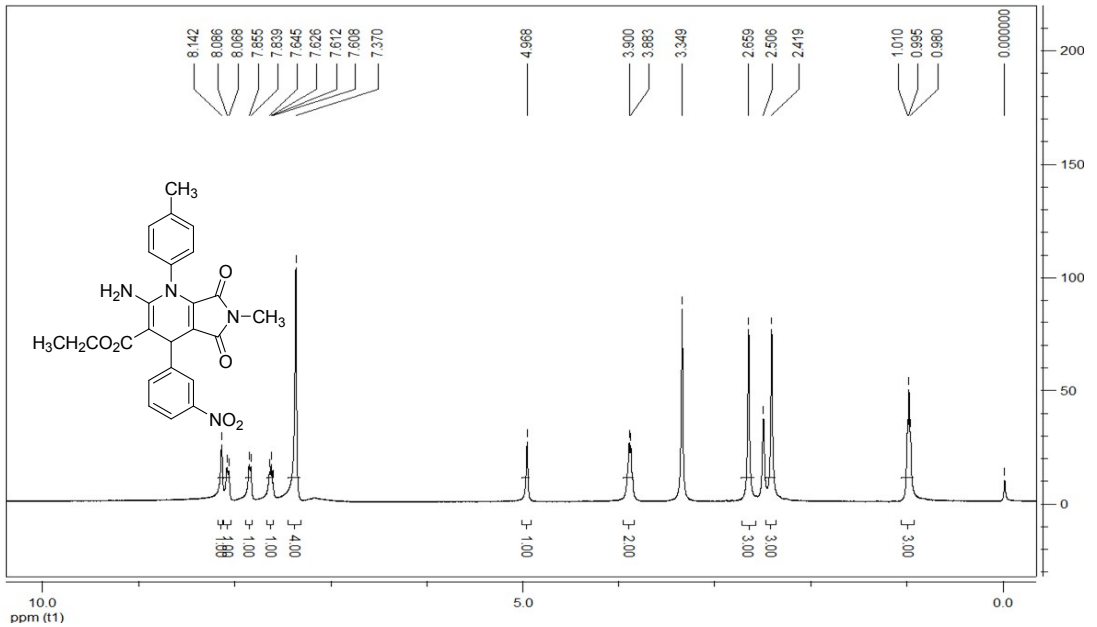
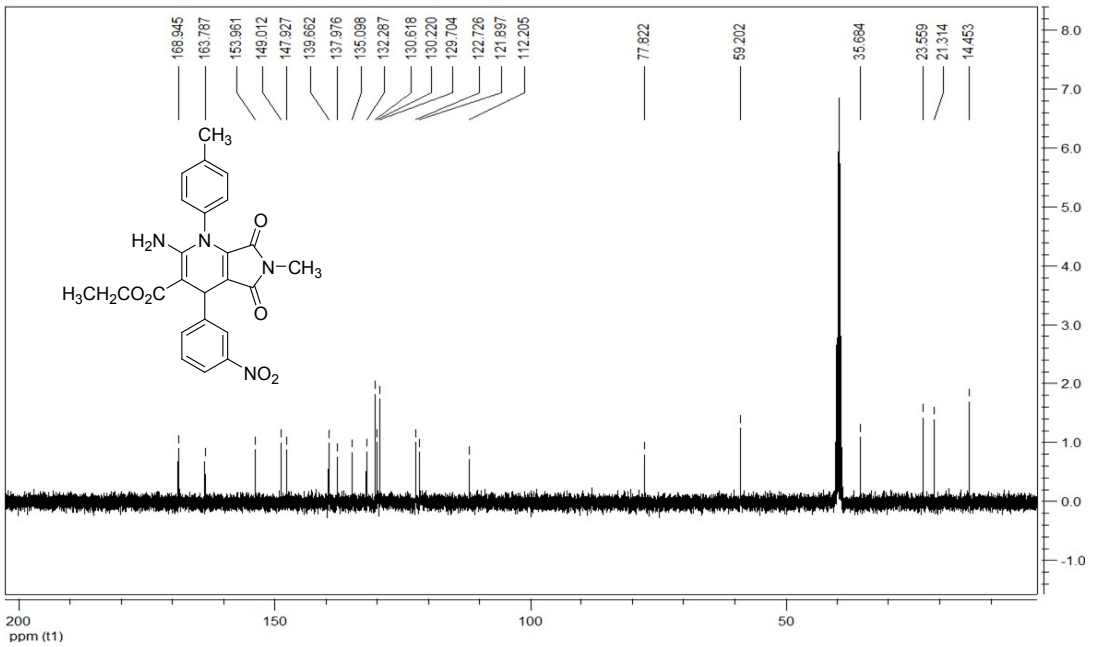


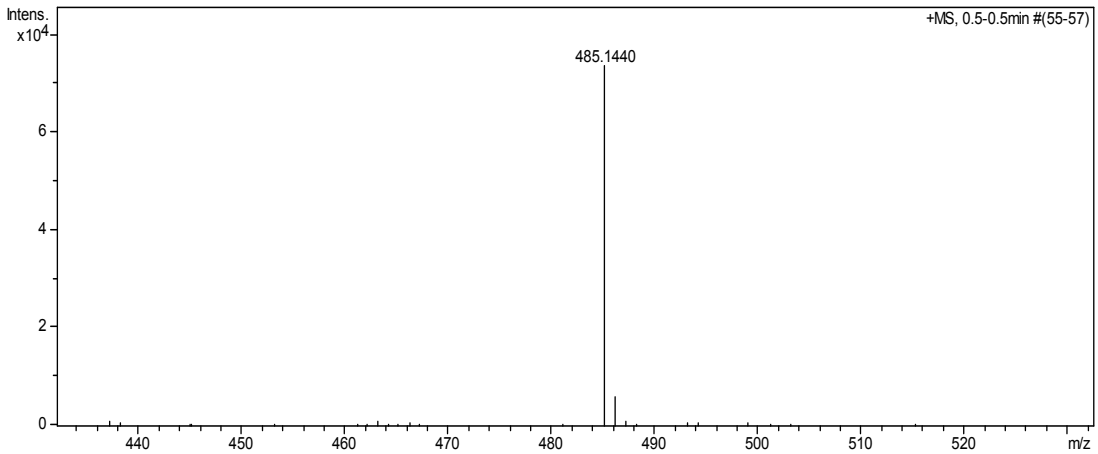




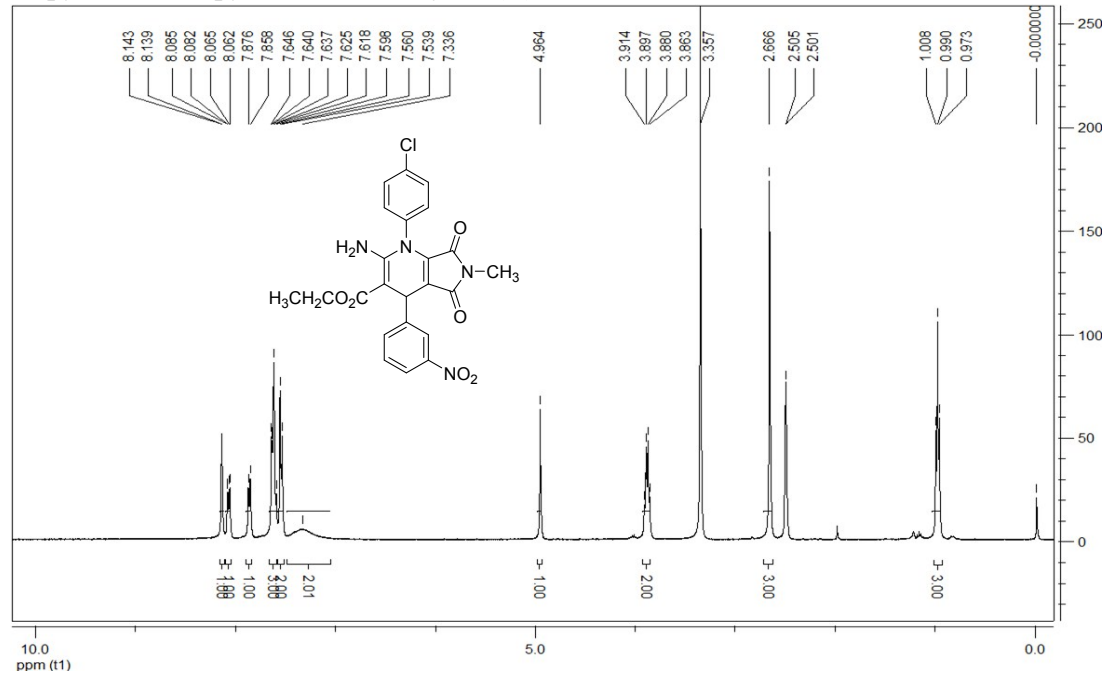
Ethyl-2-amino-6-methyl-4-(3-nitrophenyl)-5,7-dioxo-1-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxylate (1k):

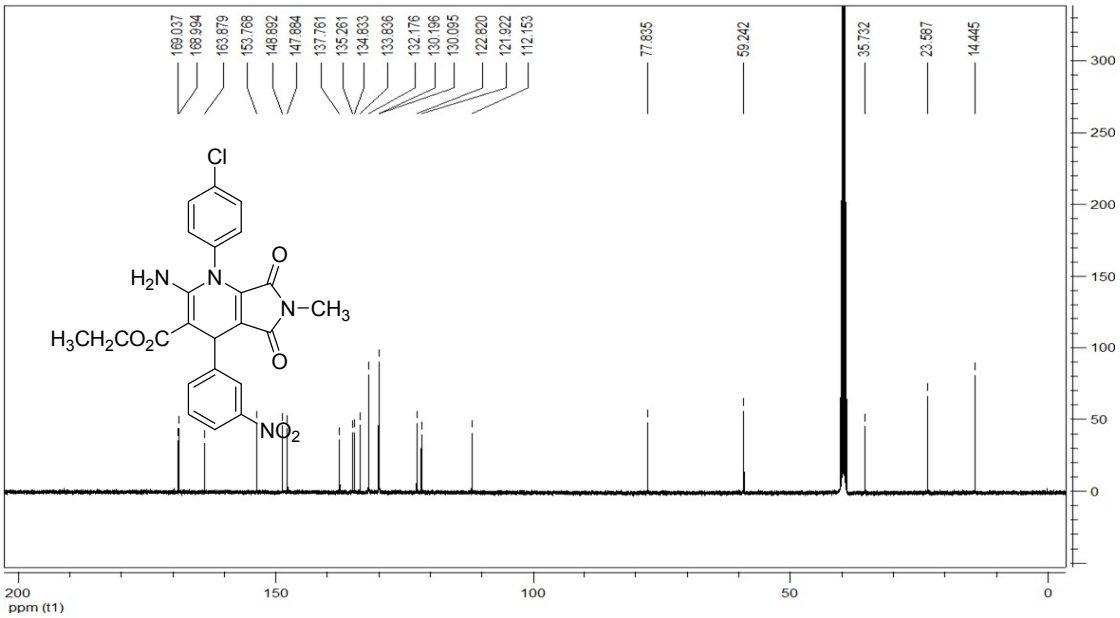


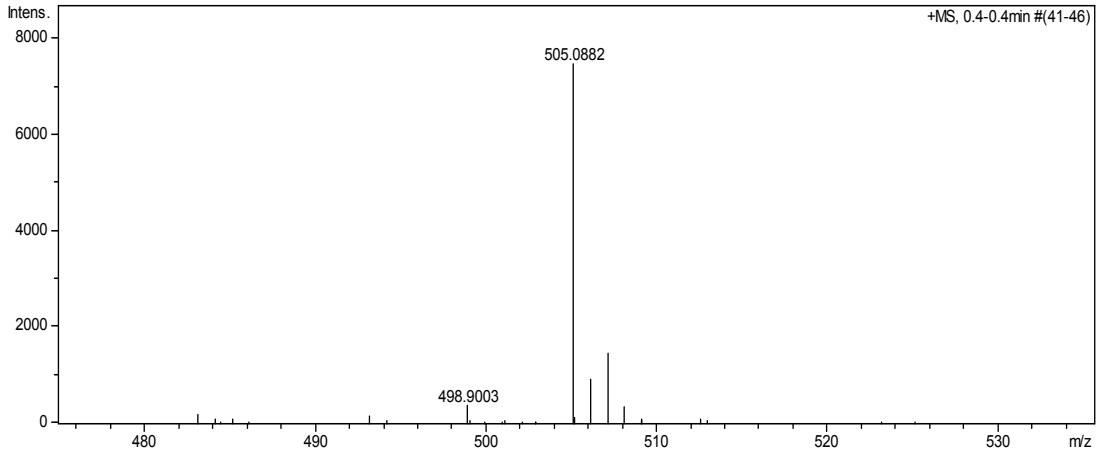




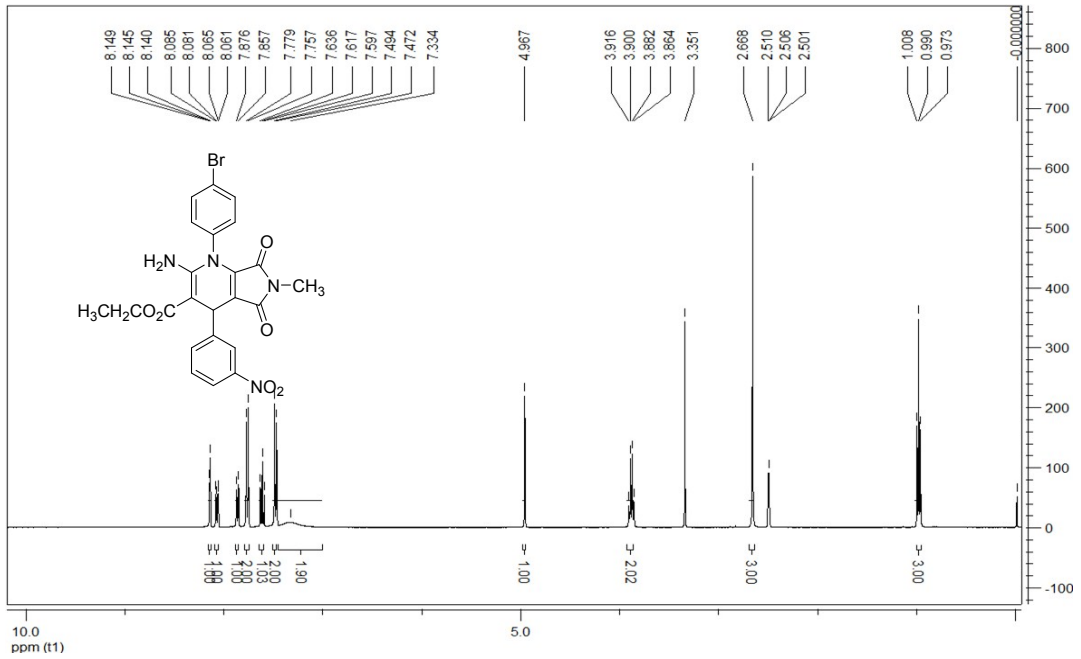
Ethyl-2-amino-1-(4-chlorophenyl)-6-methyl-4-(3-nitrophenyl)-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxylate (1l):

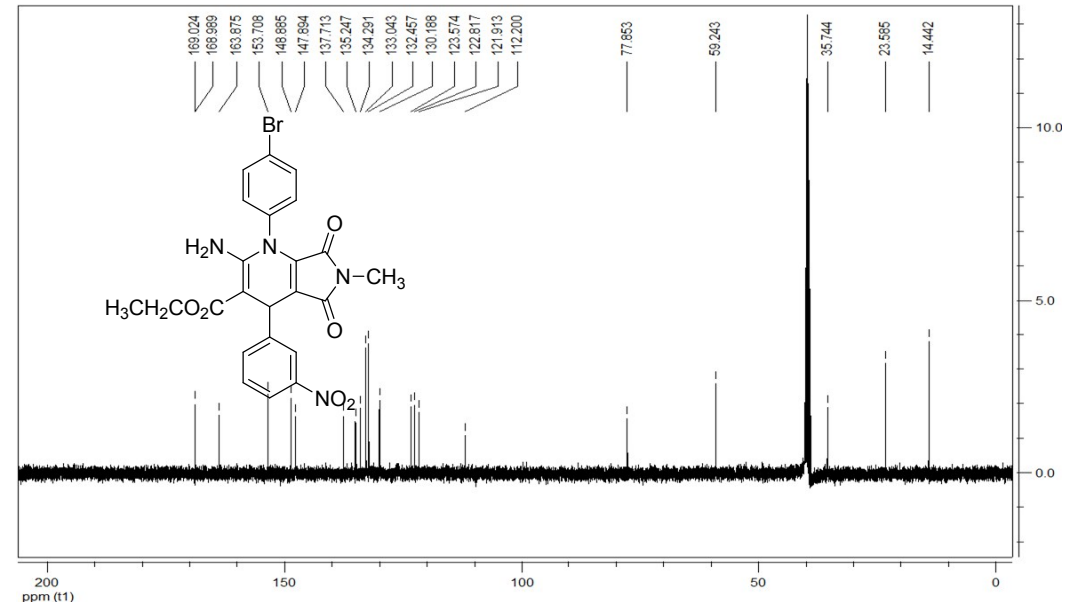


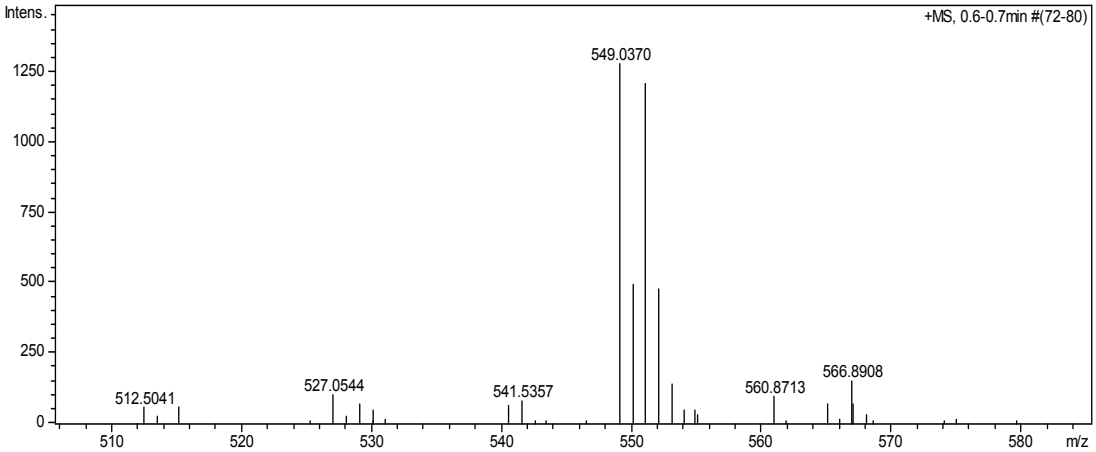




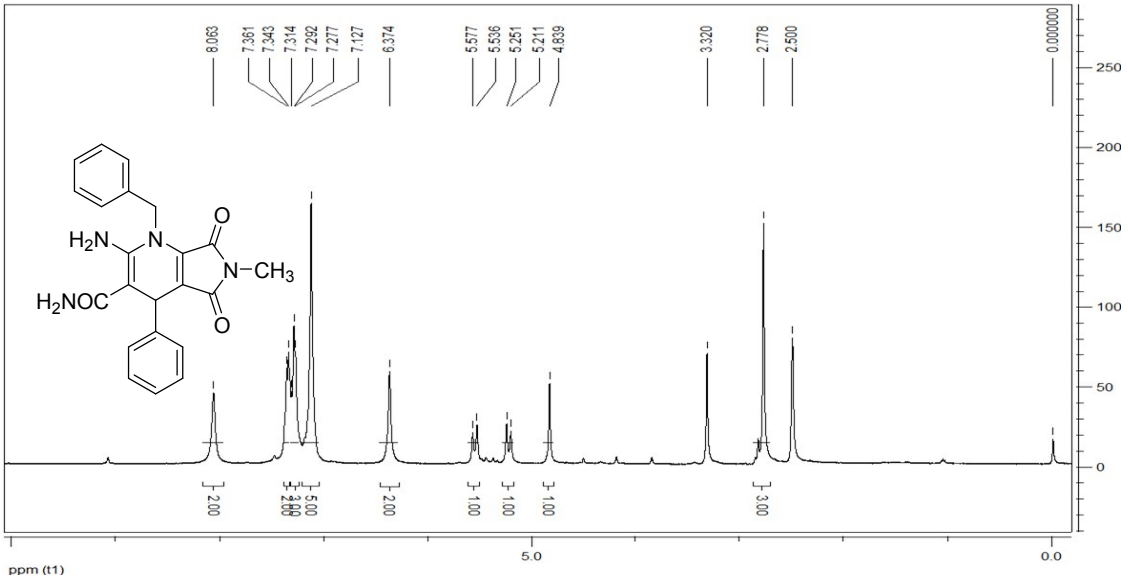
Ethyl-2-amino-1-(4-bromophenyl)-6-methyl-4-(3-nitrophenyl)-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxylate (1m):

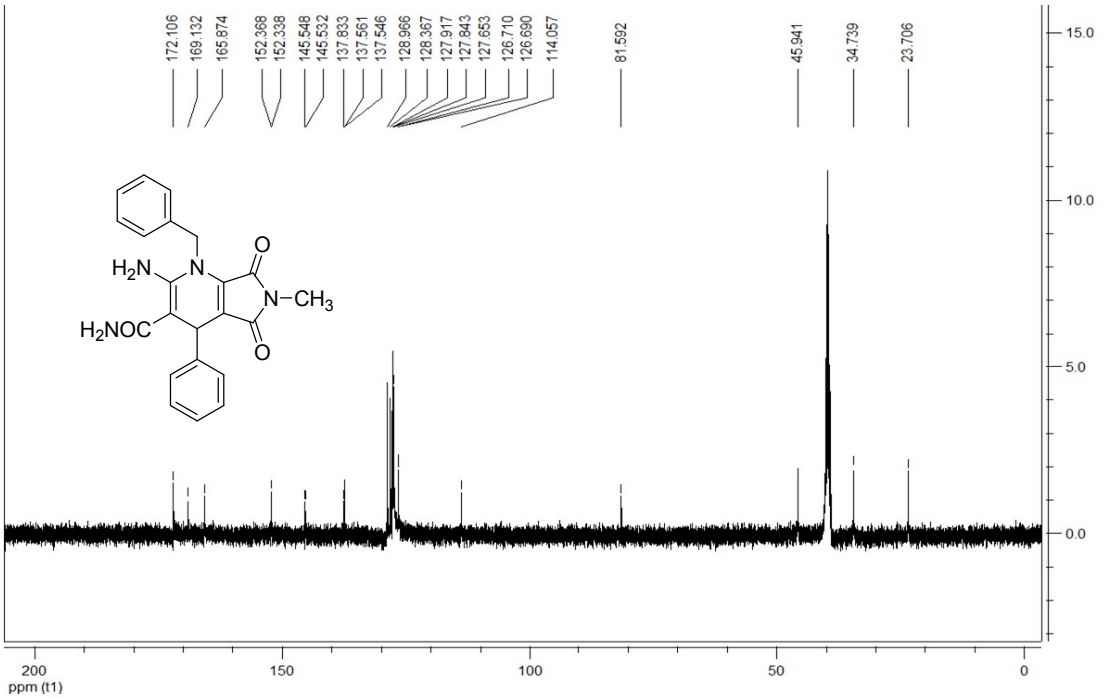


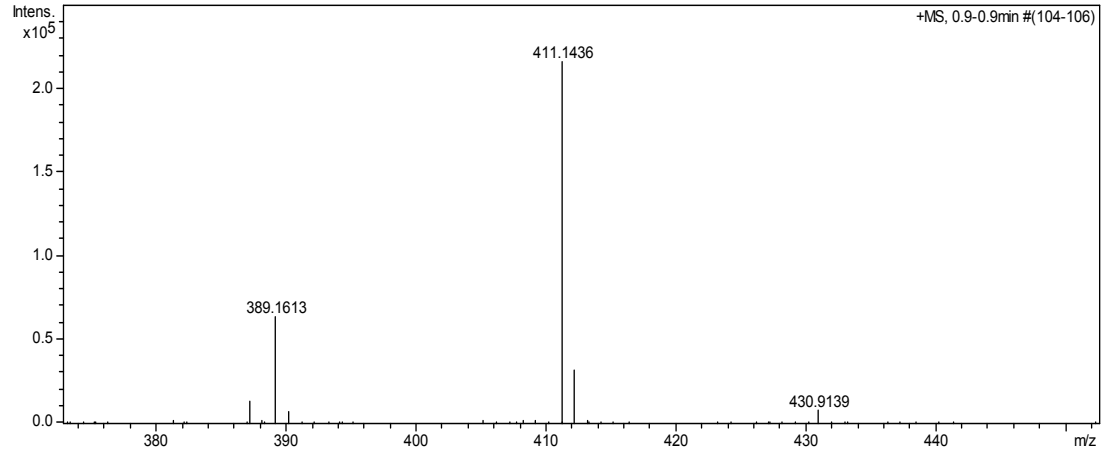




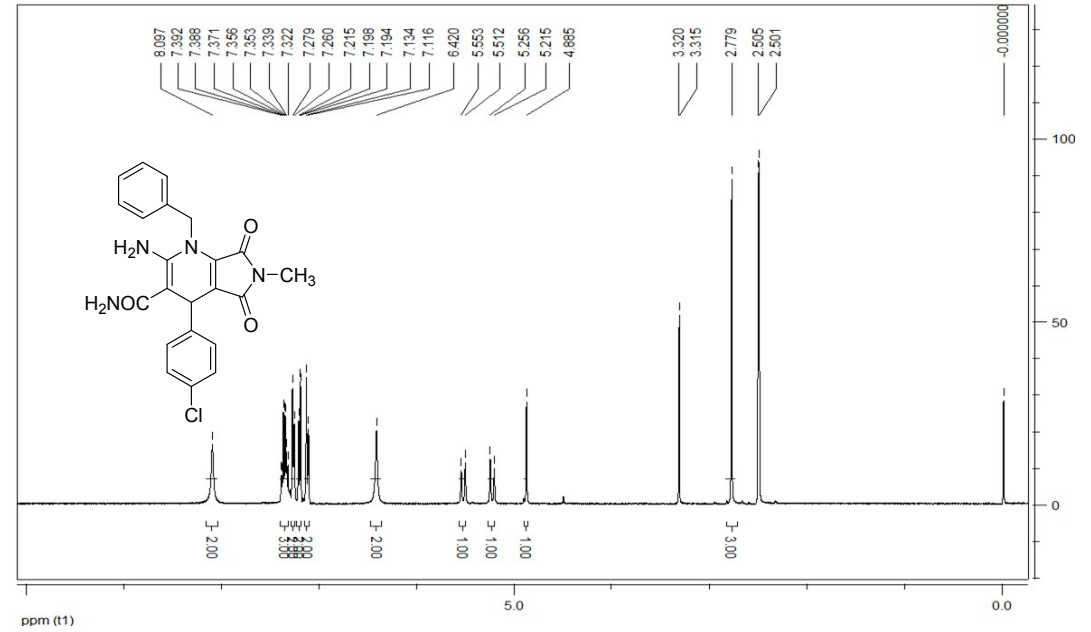
2-Amino-1-benzyl-6-methyl-5,7-dioxo-4-phenyl-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxamide (1n):

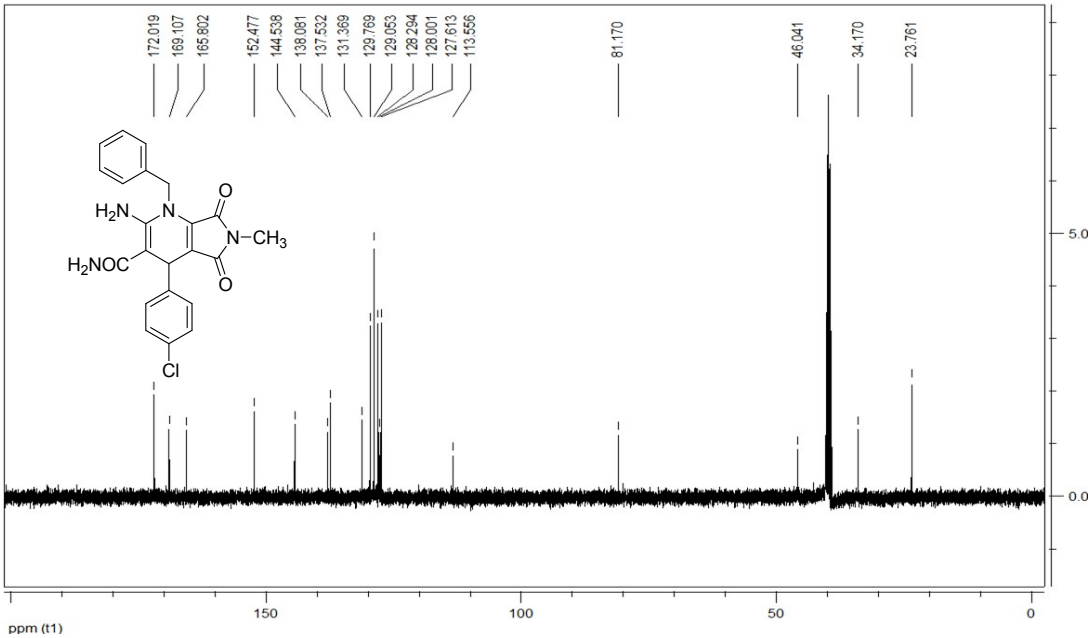


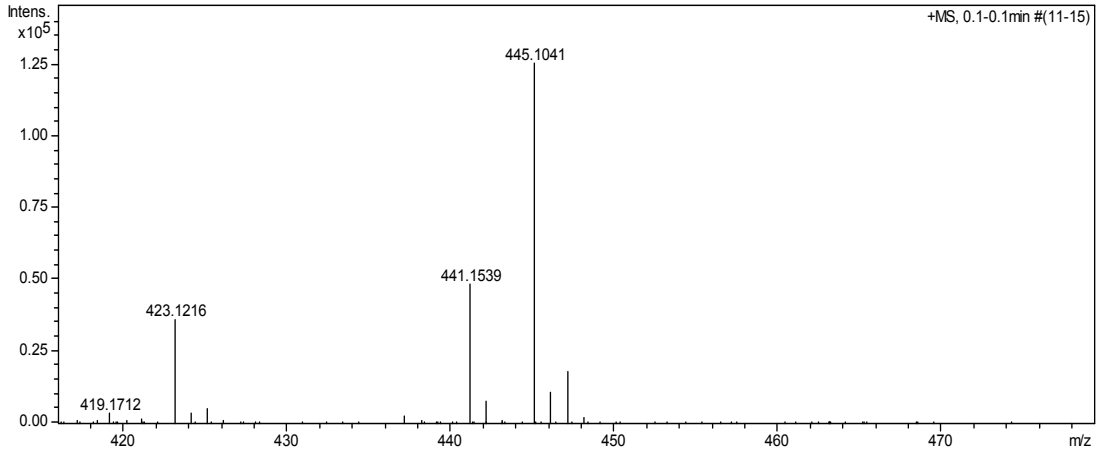




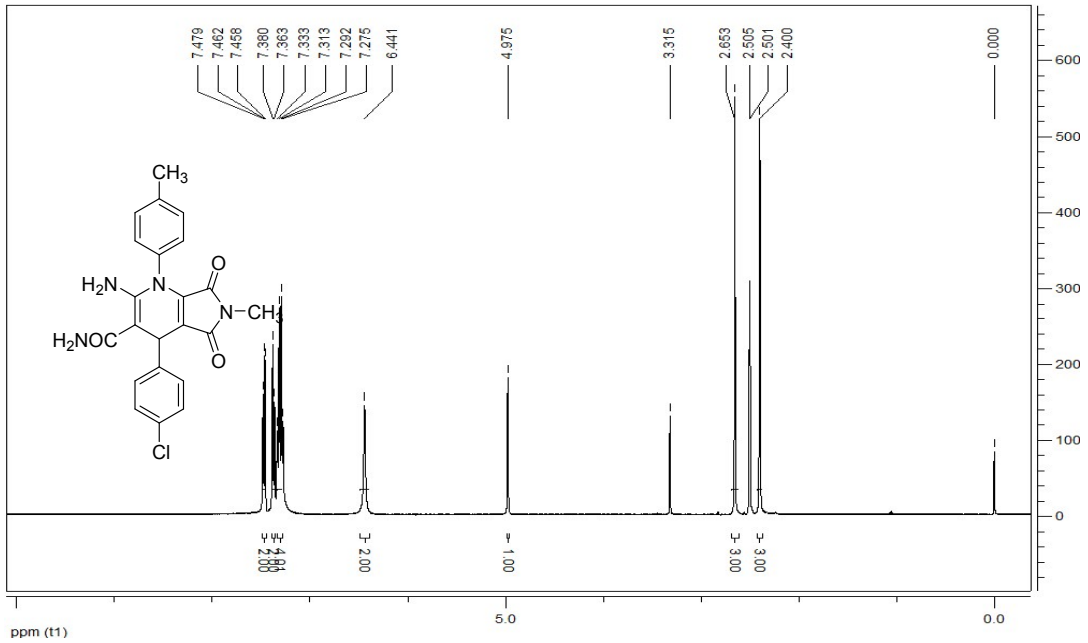
2-Amino-1-benzyl-4-(4-chlorophenyl)-6-methyl-5,7-dioxo-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxamide (1o):

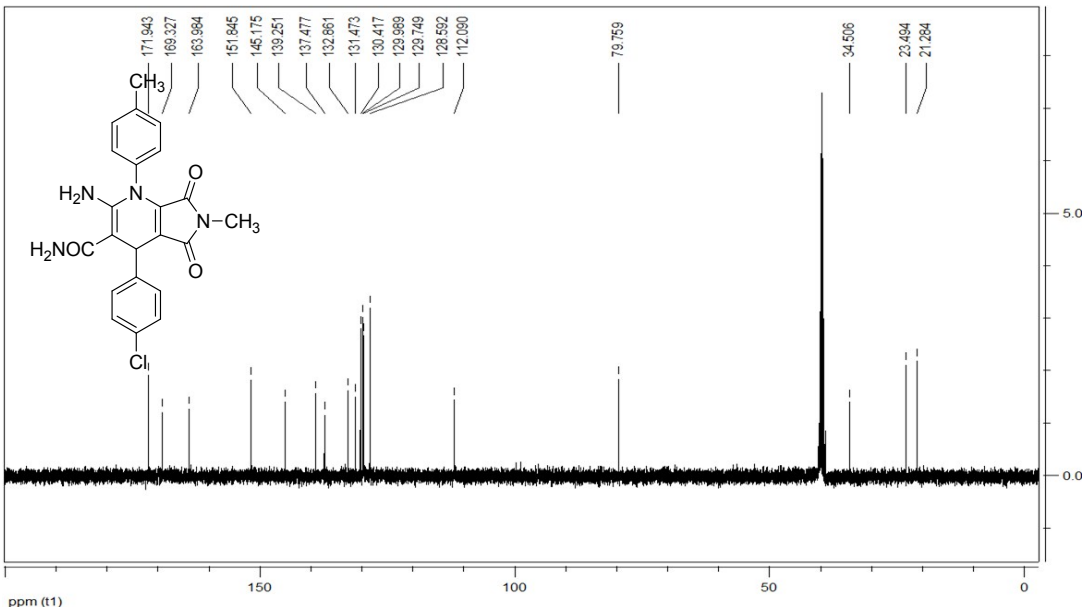


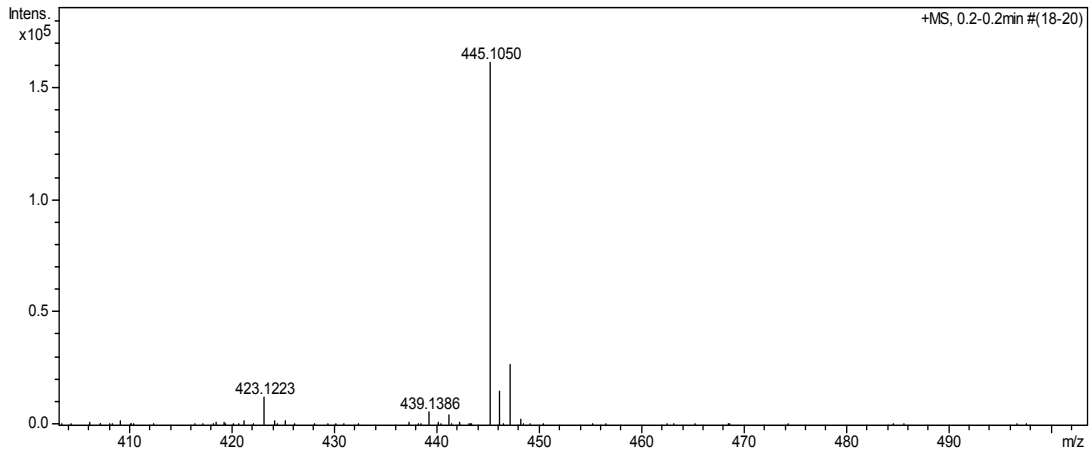




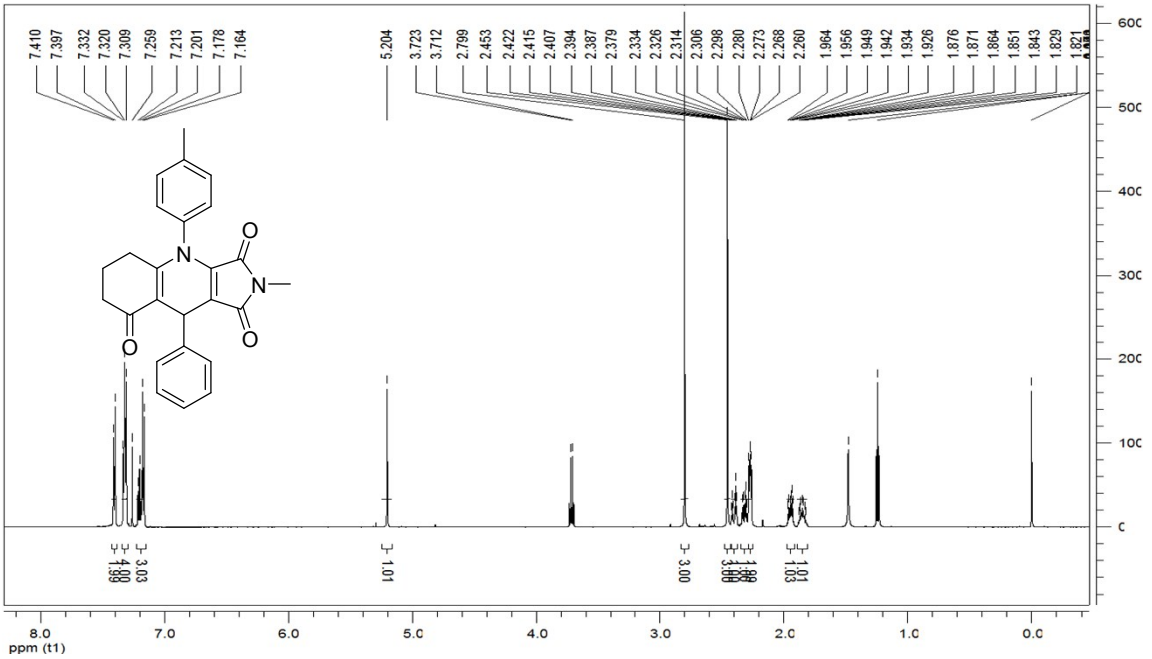
2-Amino-4-(4-chlorophenyl)-6-methyl-5,7-dioxo-1-(*p*-tolyl)-4,5,6,7-tetrahydro-1*H*-pyrrolo[3,4-*b*]pyridine-3-carboxamide (1p):

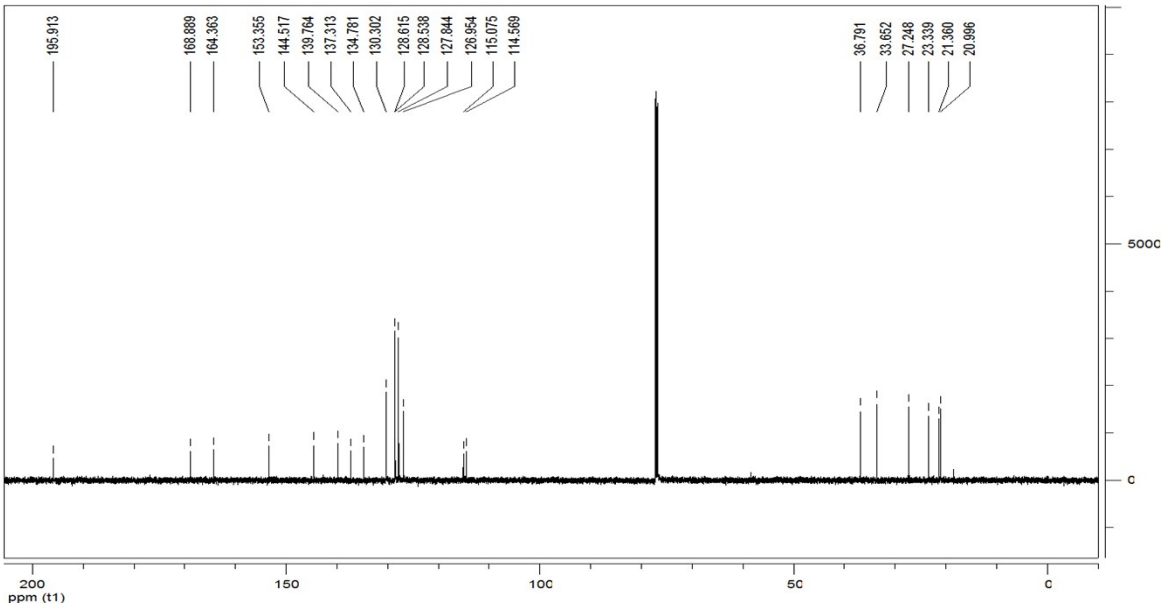


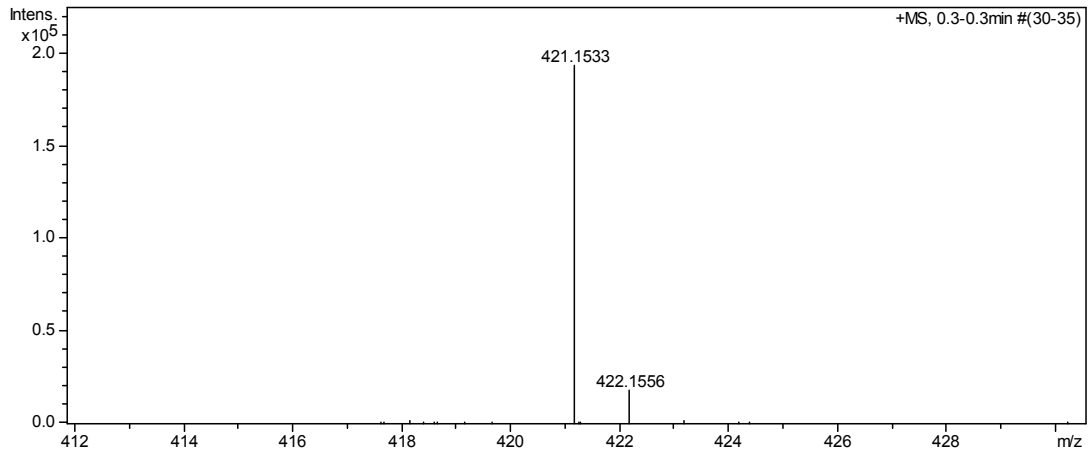




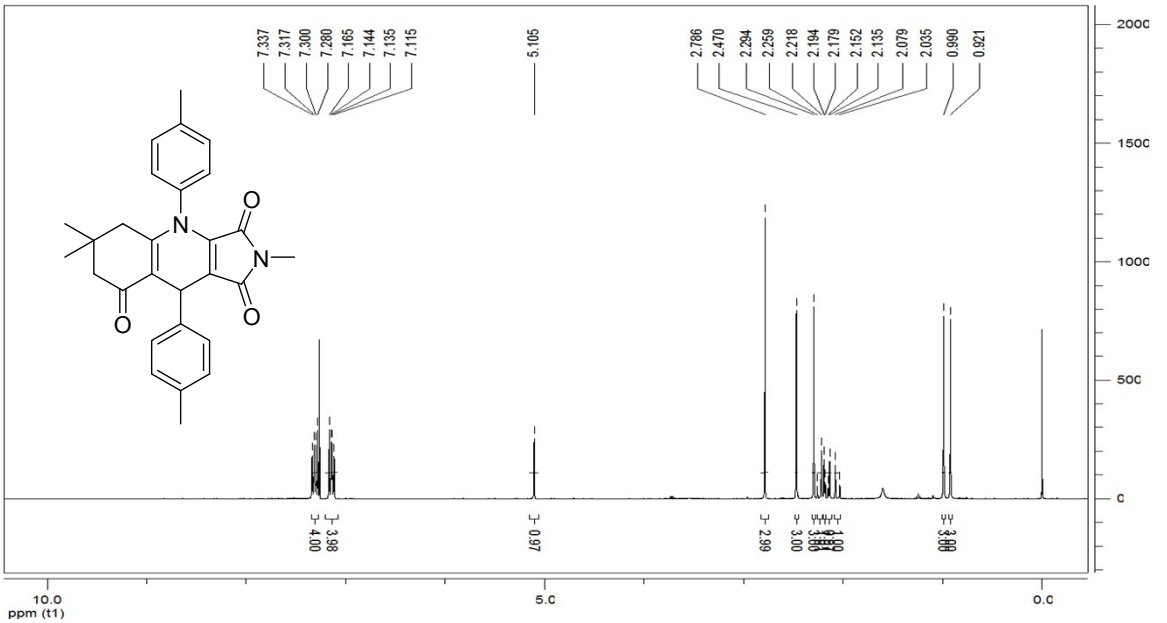
2-Methyl-9-phenyl-4-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3a):

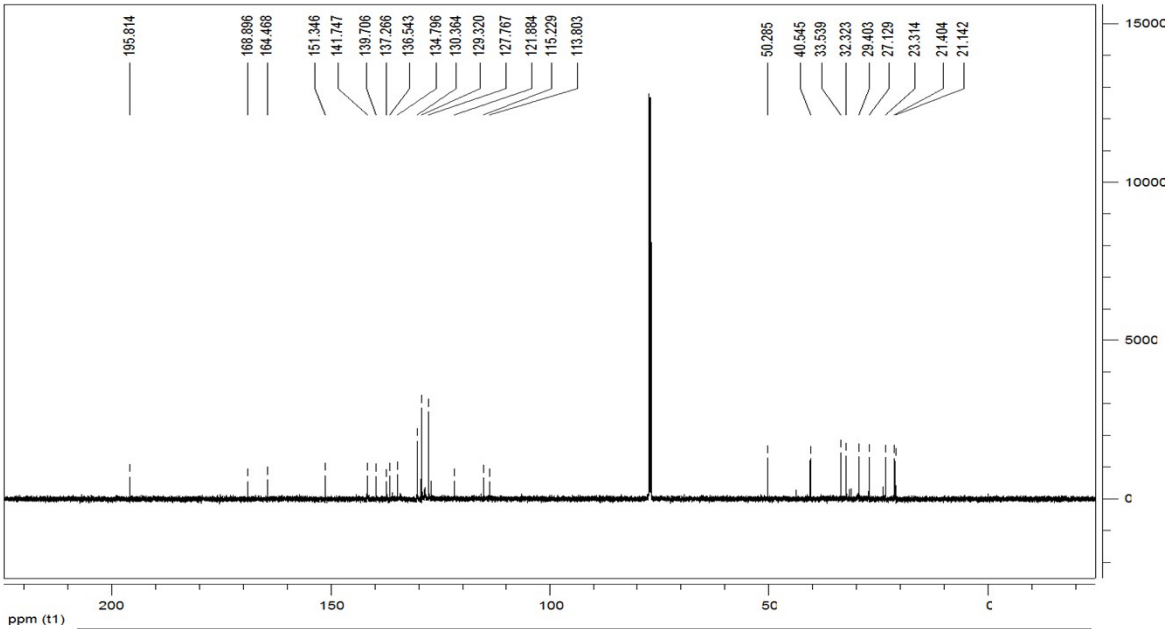


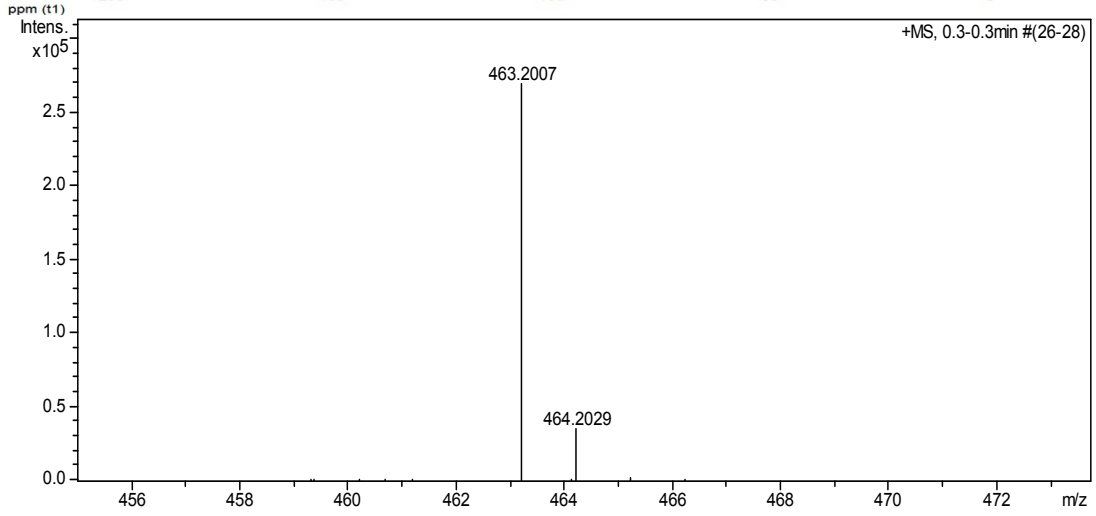




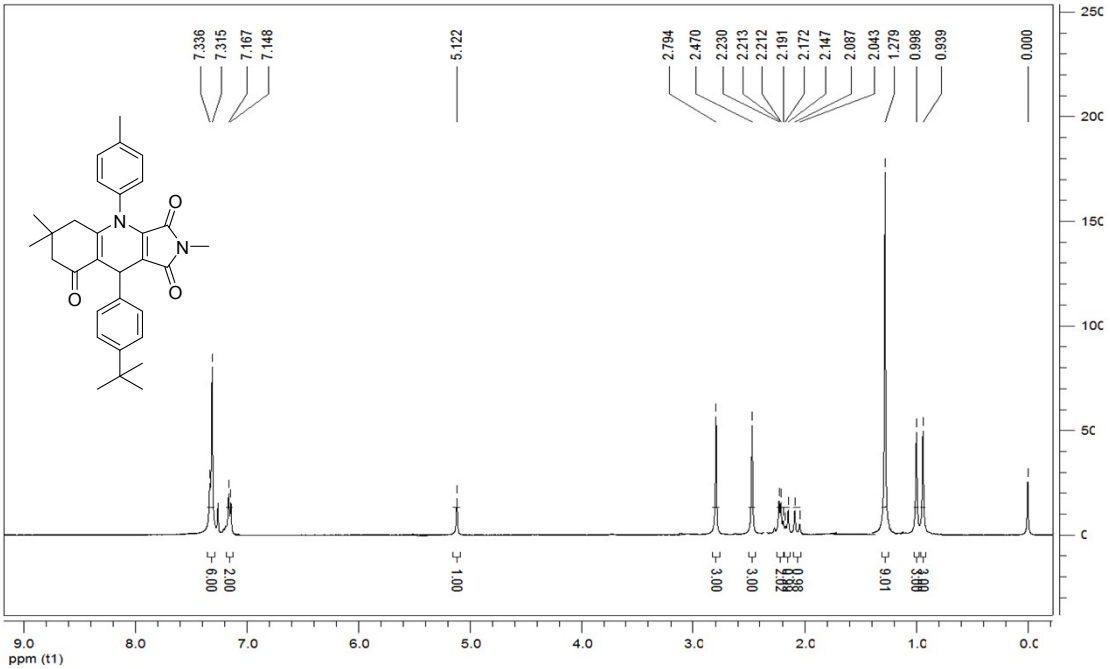
2,7,7-Trimethyl-4,9-di-p-tolyl-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3b):

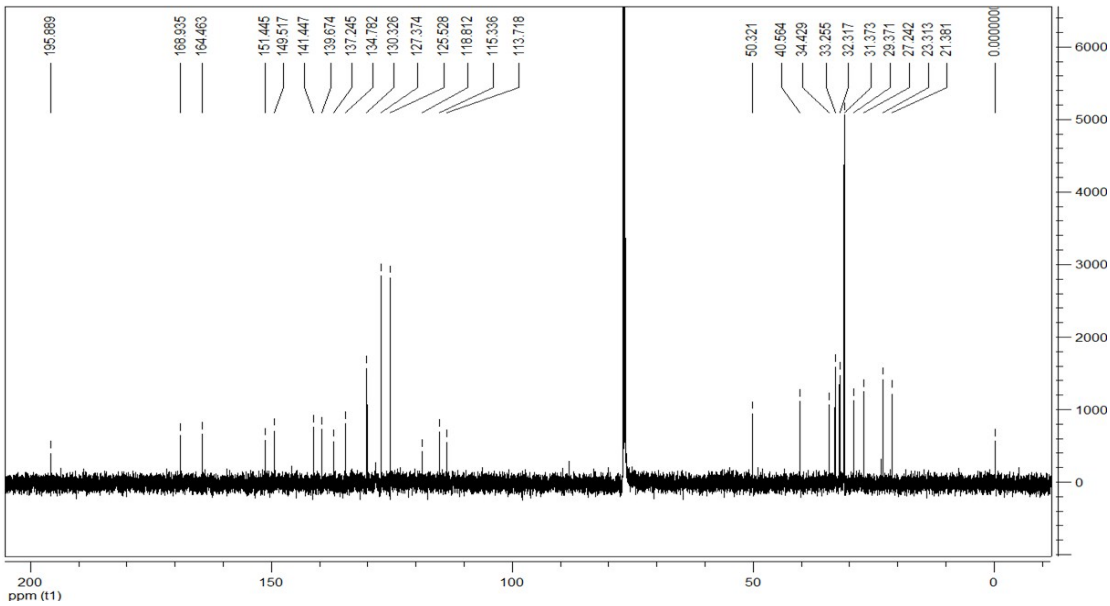


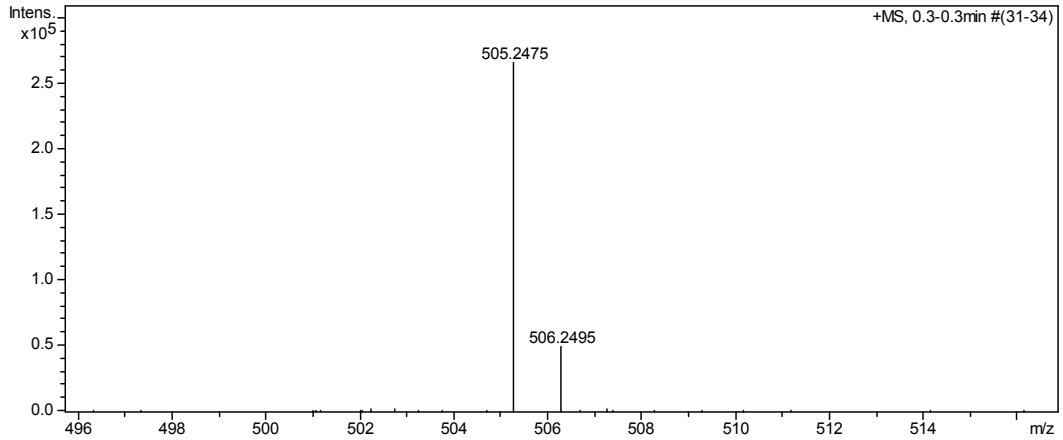




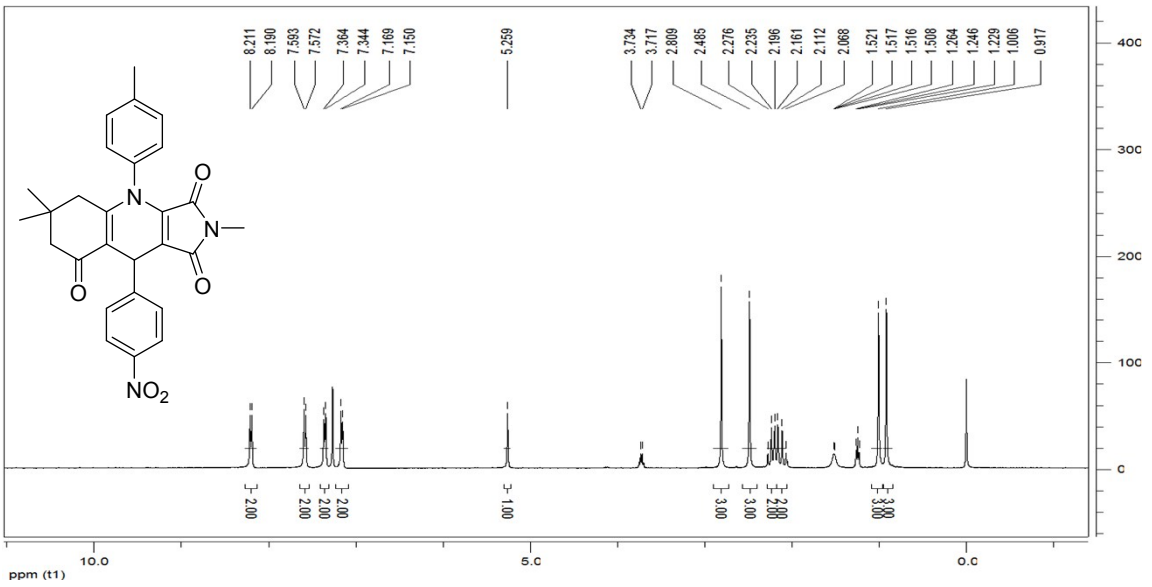
9-(4-(tert-Butyl)phenyl)-2,7,7-trimethyl-4-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3c):

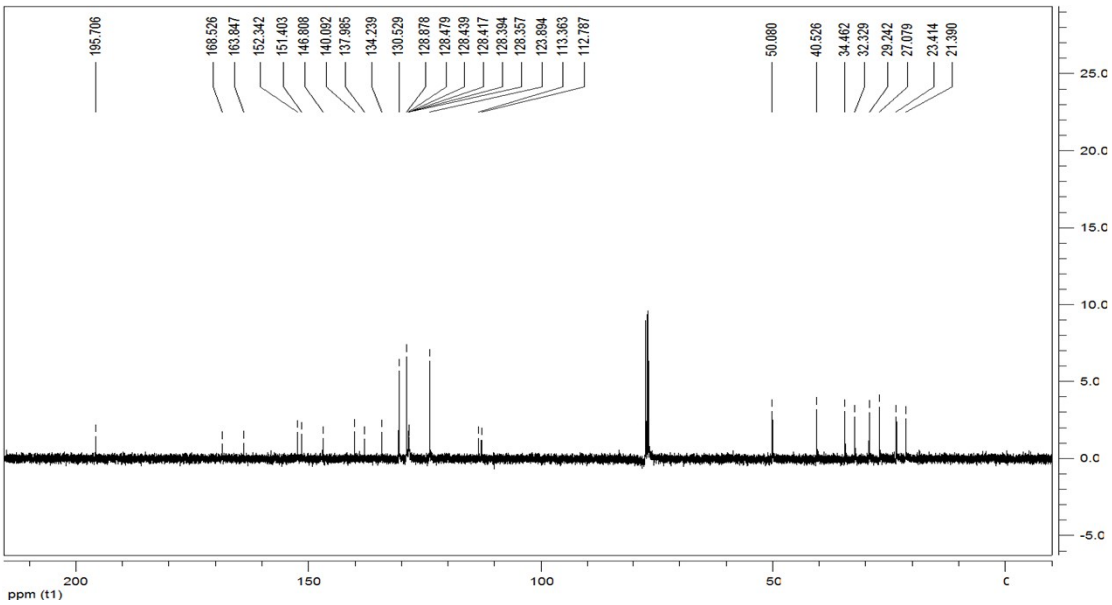


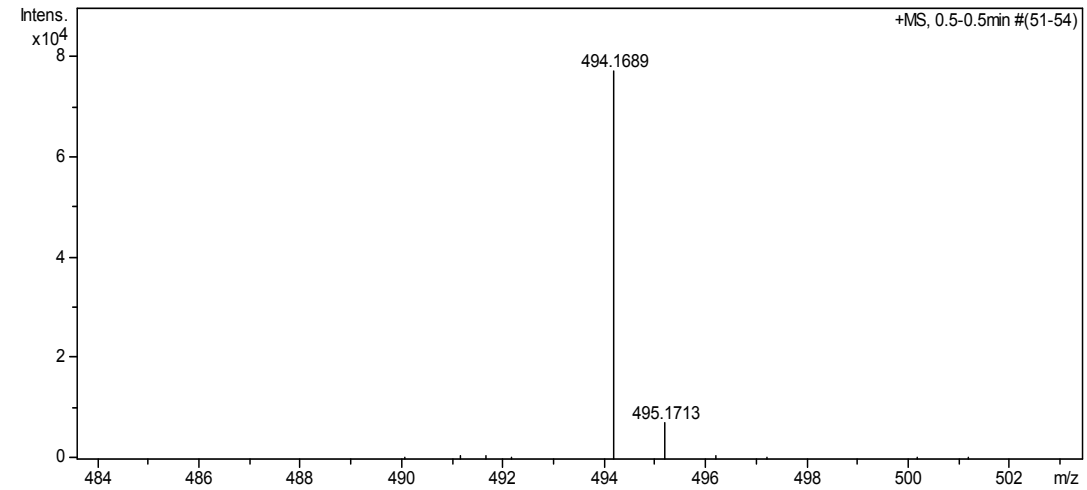




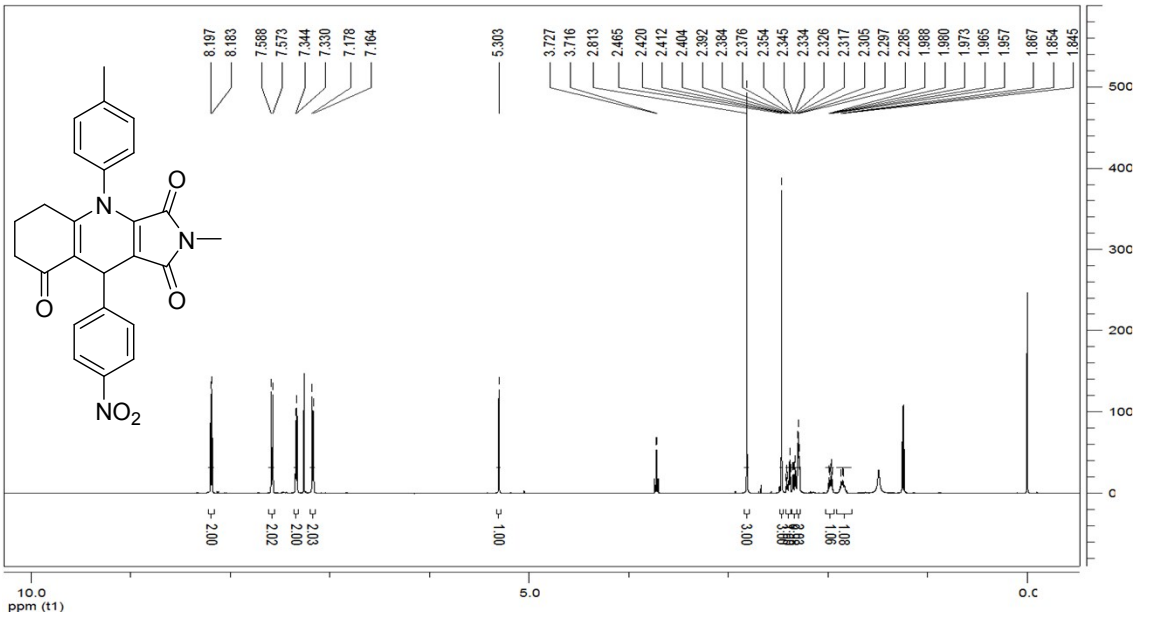
2,7,7-Trimethyl-9-(4-nitrophenyl)-4-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3d):.

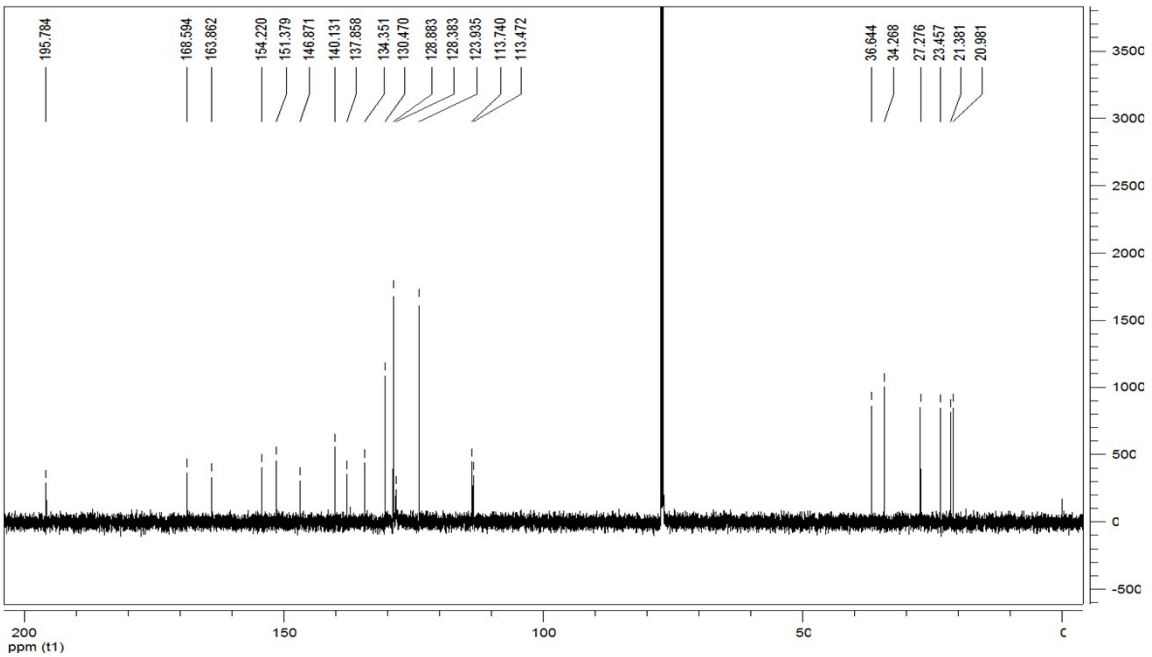


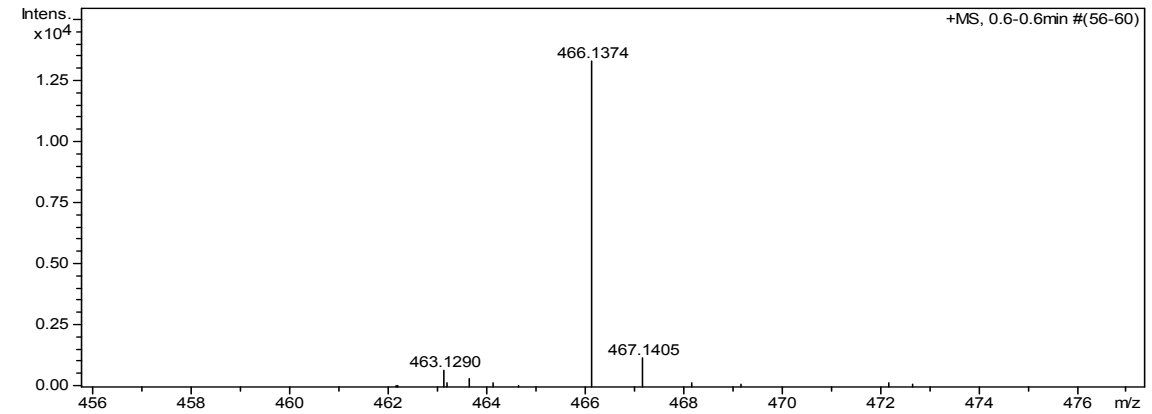




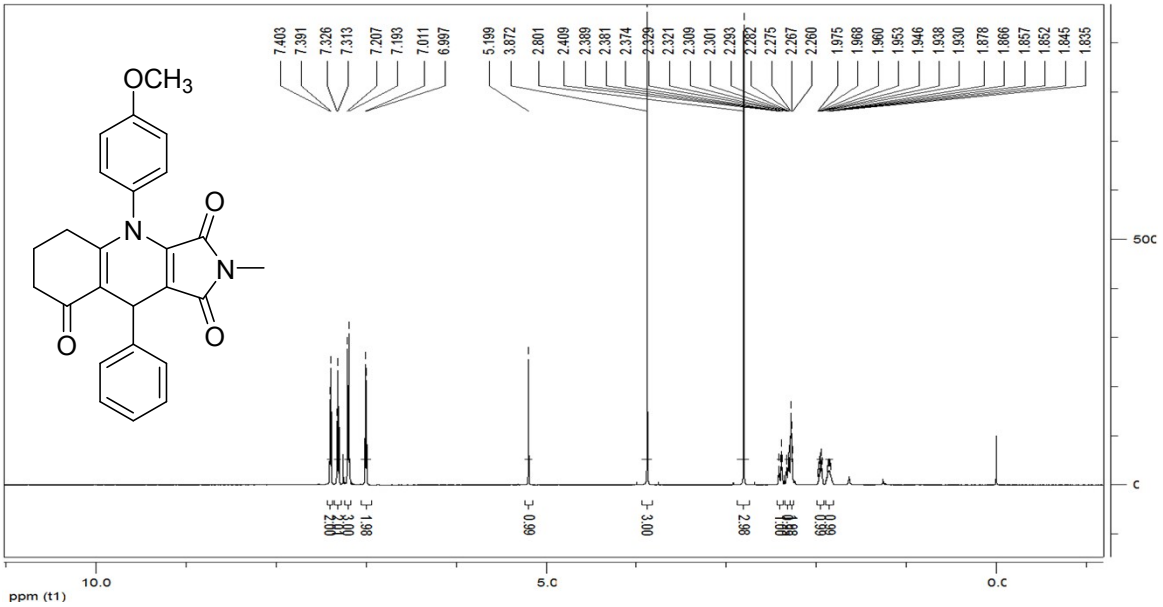
2-Methyl-9-(4-nitrophenyl)-4-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3e):

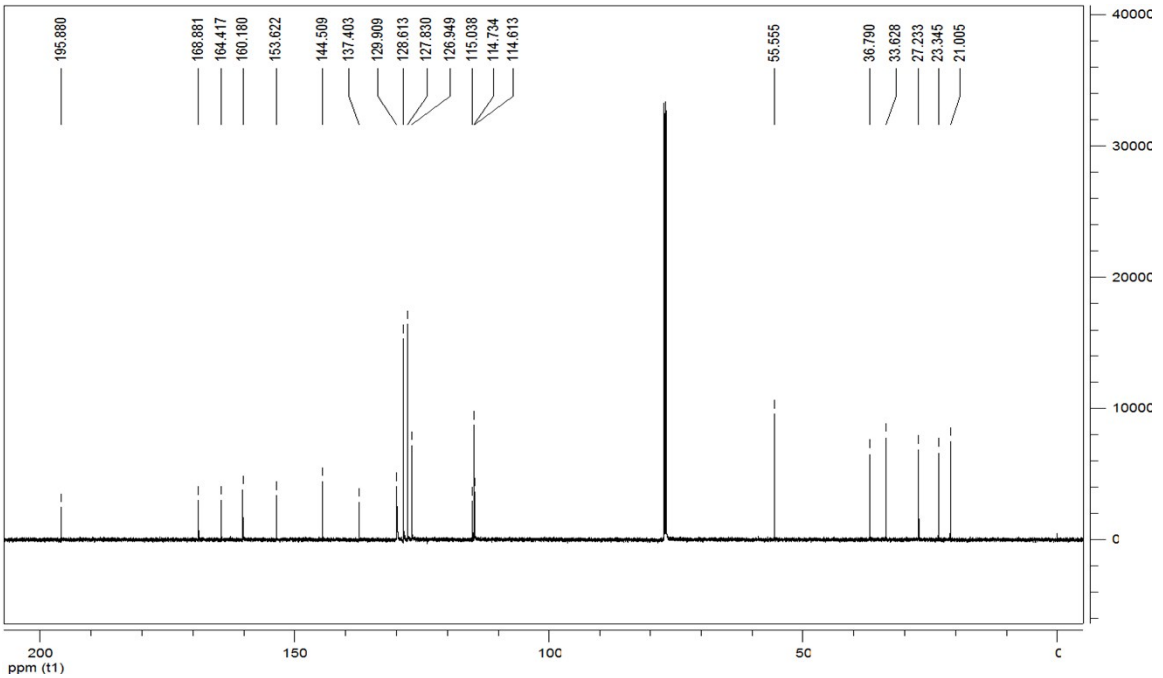


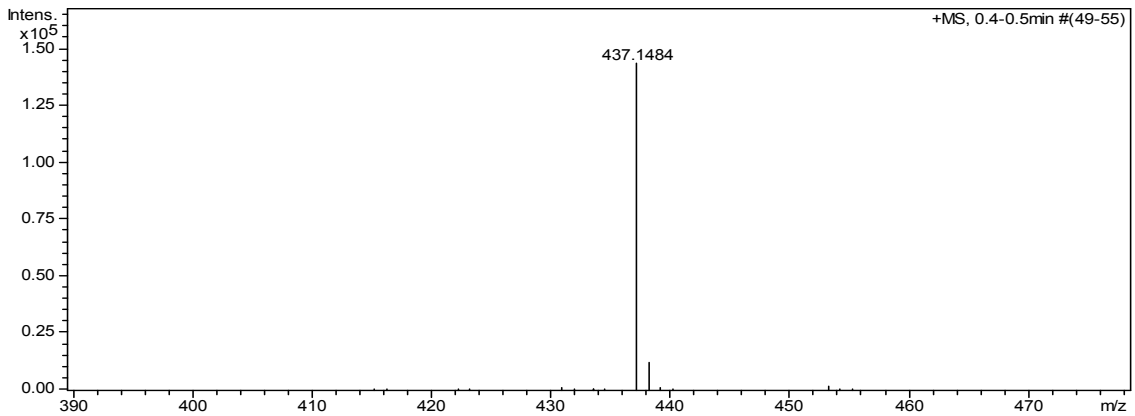




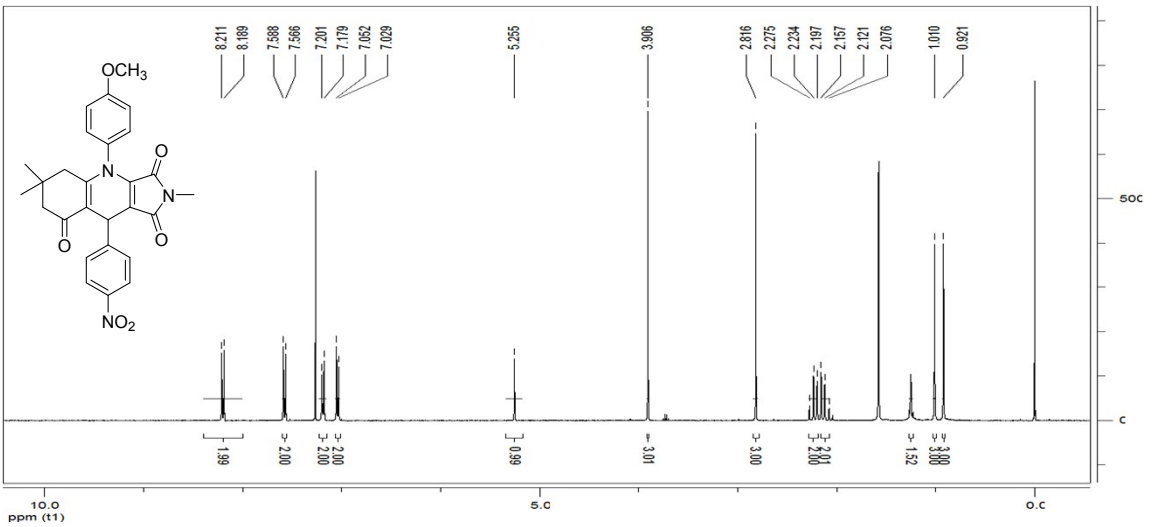
2-Methyl-9-(4-methoxyphenyl)-4-phenyl-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3f):

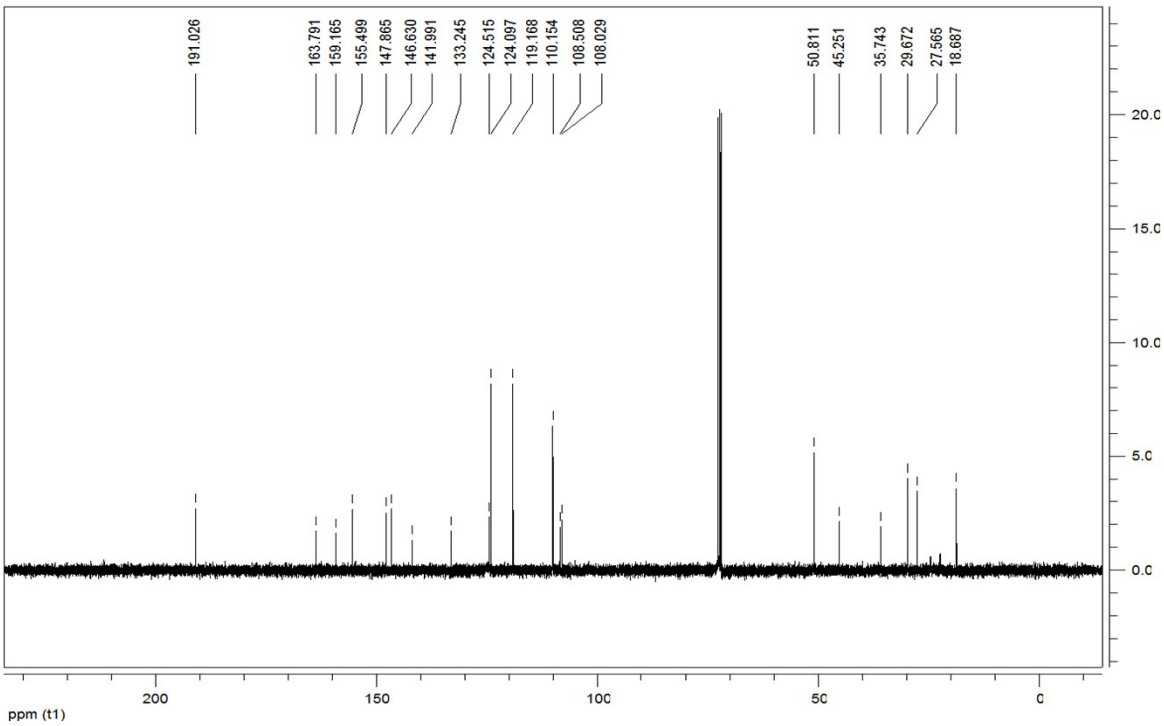


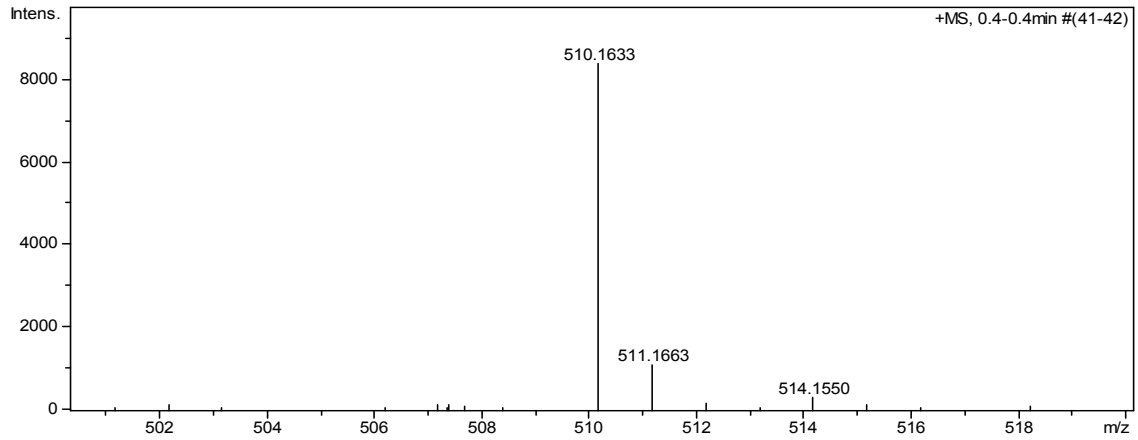




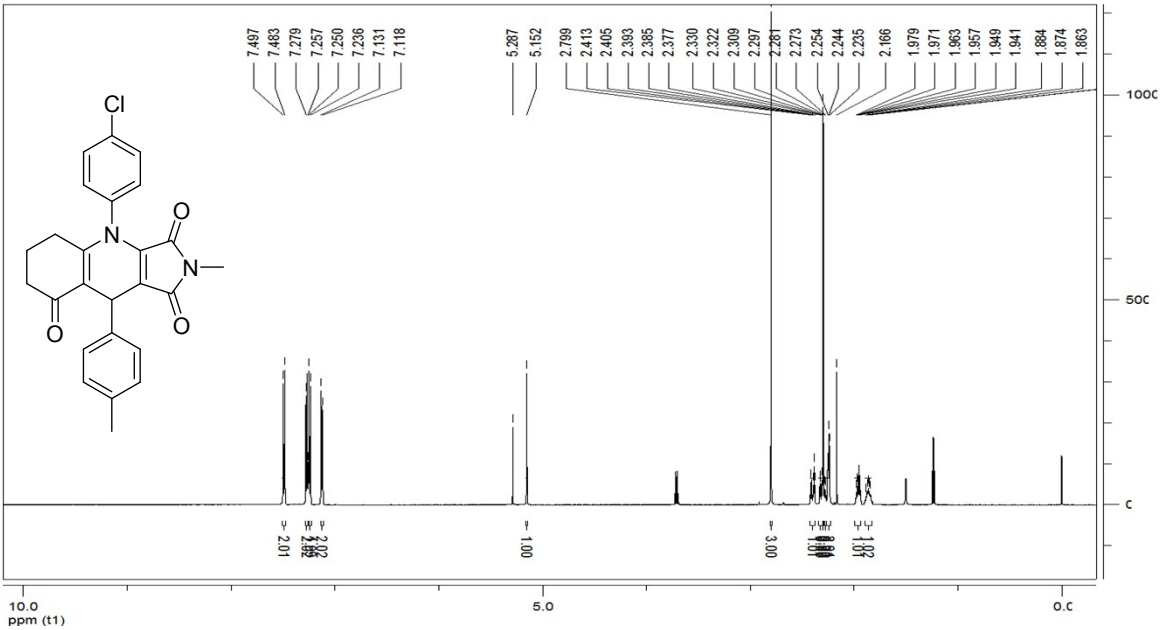
4-(4-Methoxyphenyl)-2,7,7-trimethyl-9-(4-nitrophenyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*] quinoline-1,3,5(2*H*,4*H*)-trion (3g):

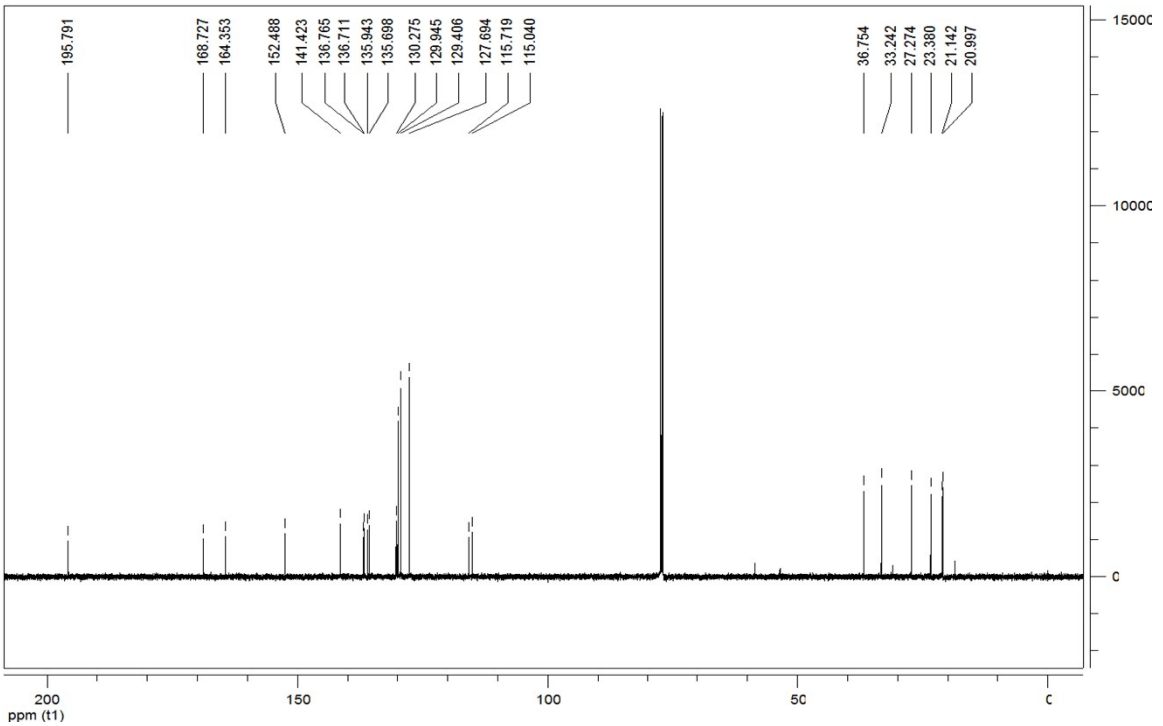


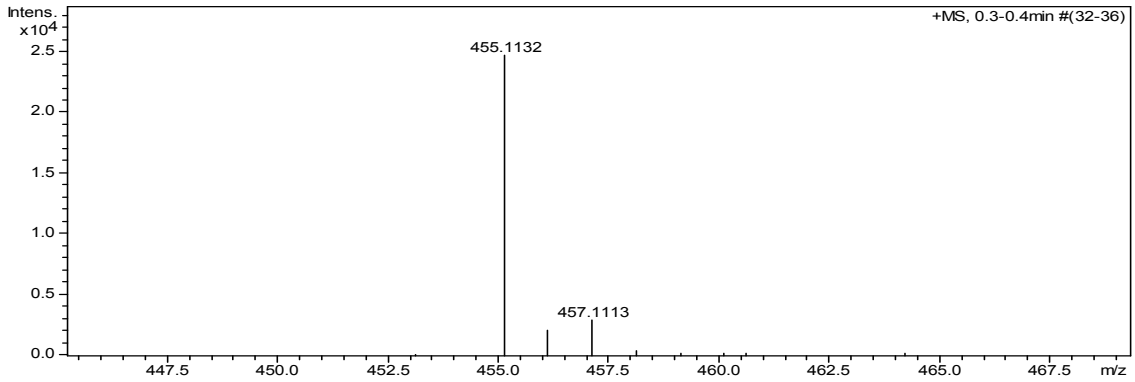




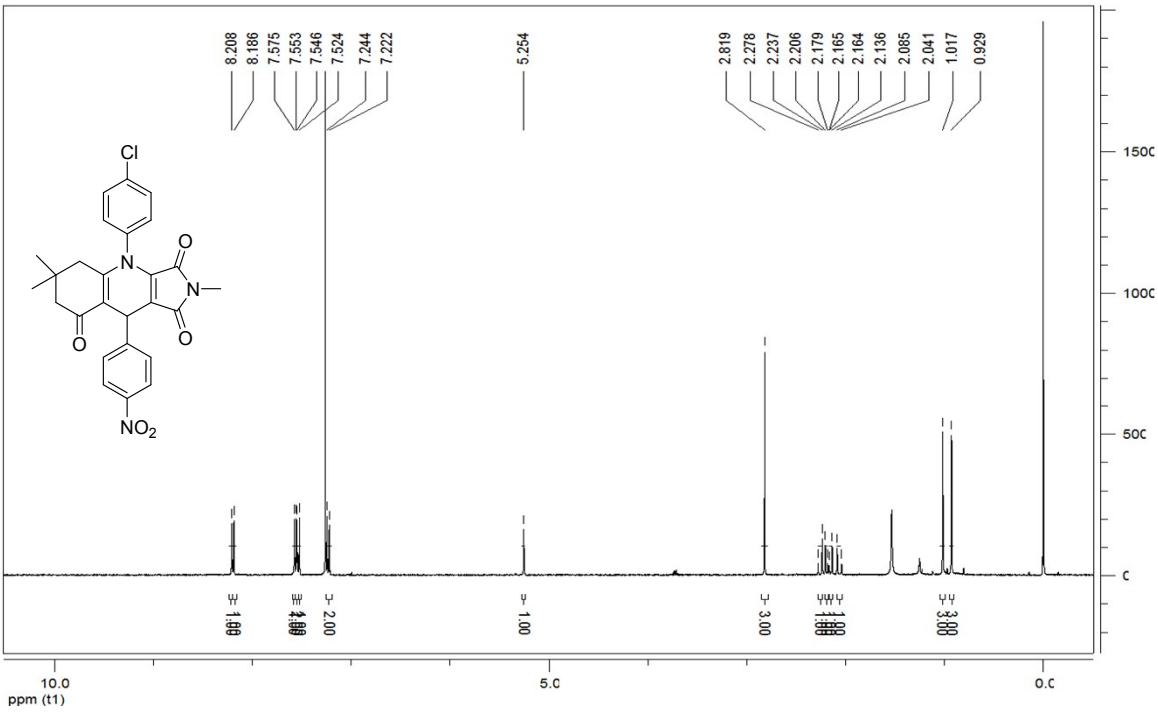
4-(4-Chlorophenyl)-2-methyl-9-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3h):

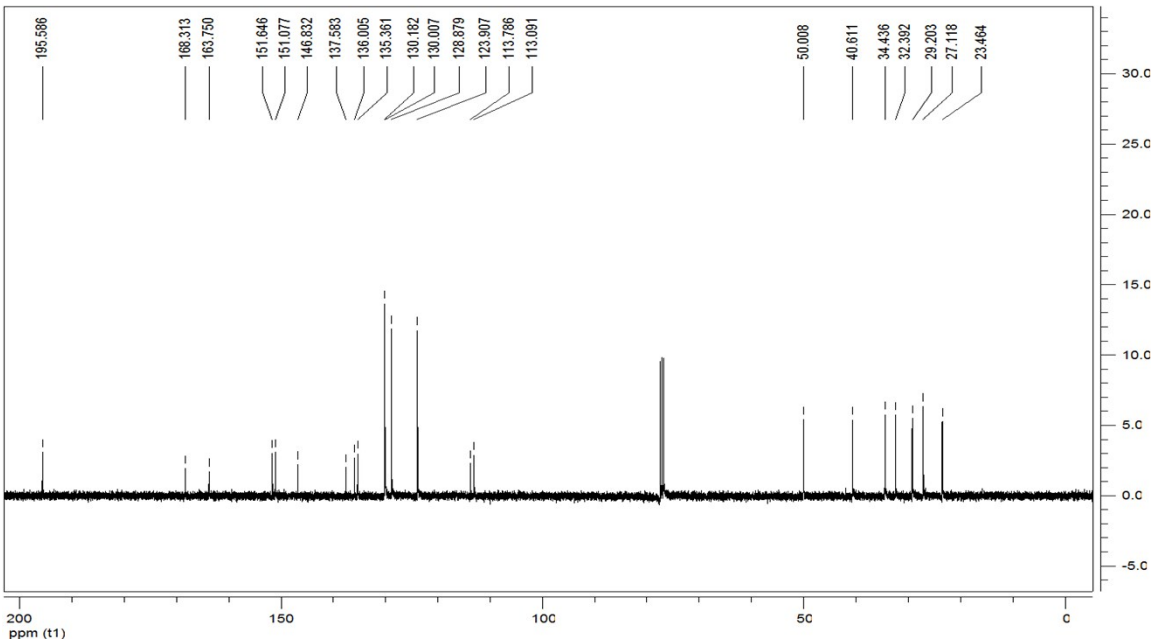


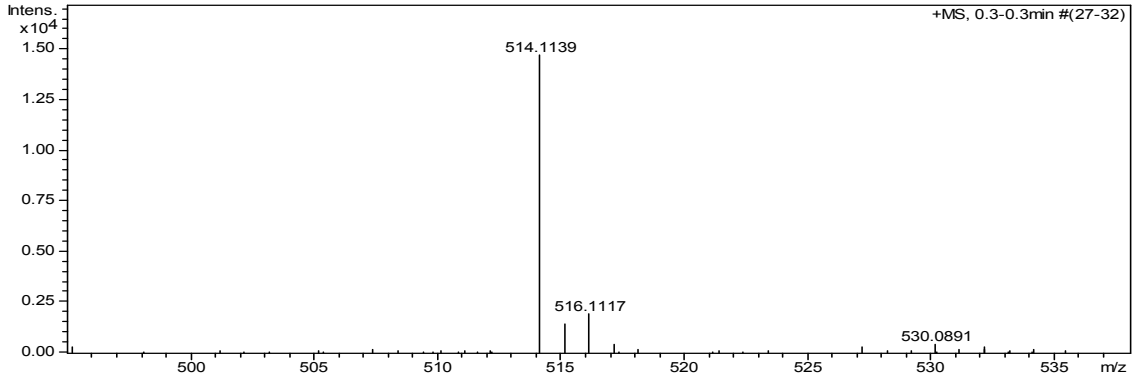




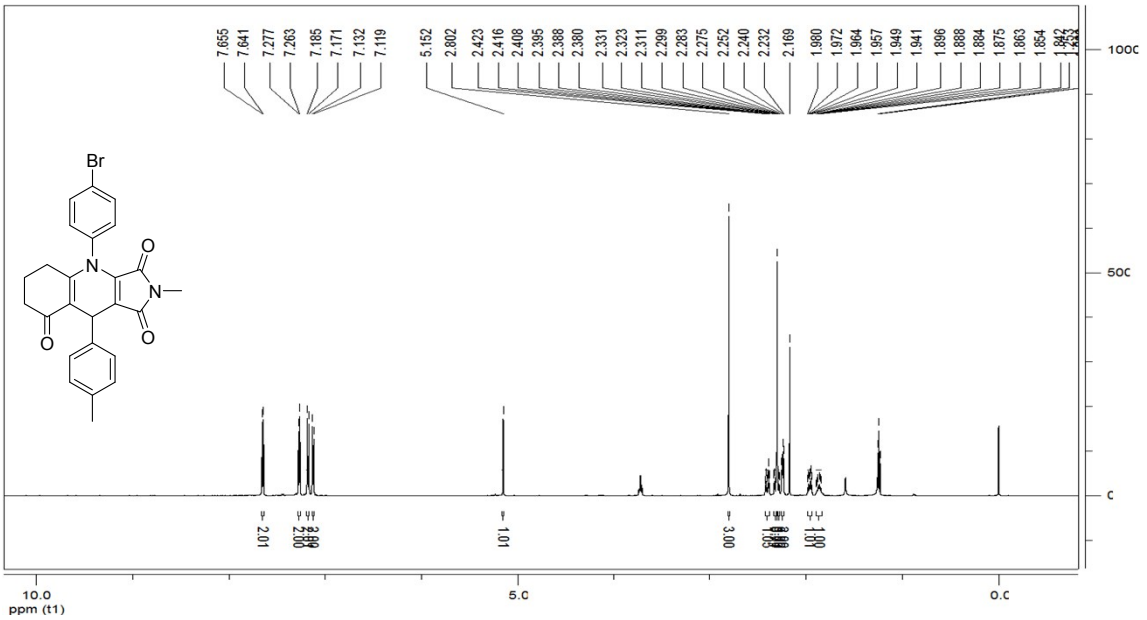
4-(4-Chlorophenyl)-2,7,7-trimethyl-9-(4-nitrophenyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (**3i**):

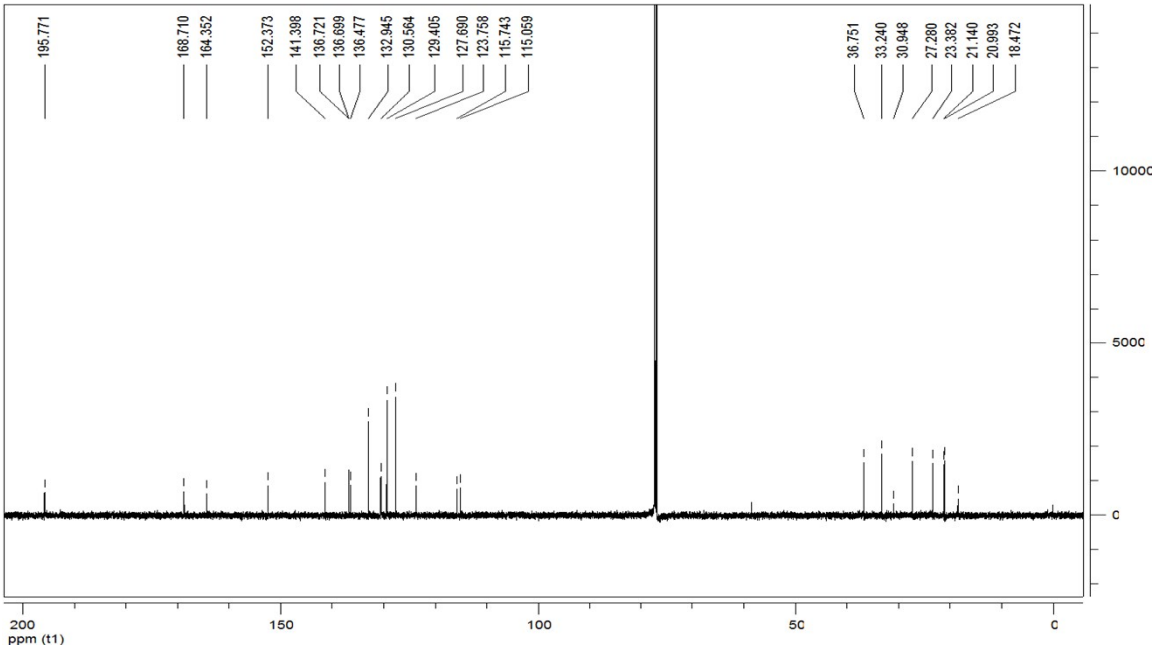


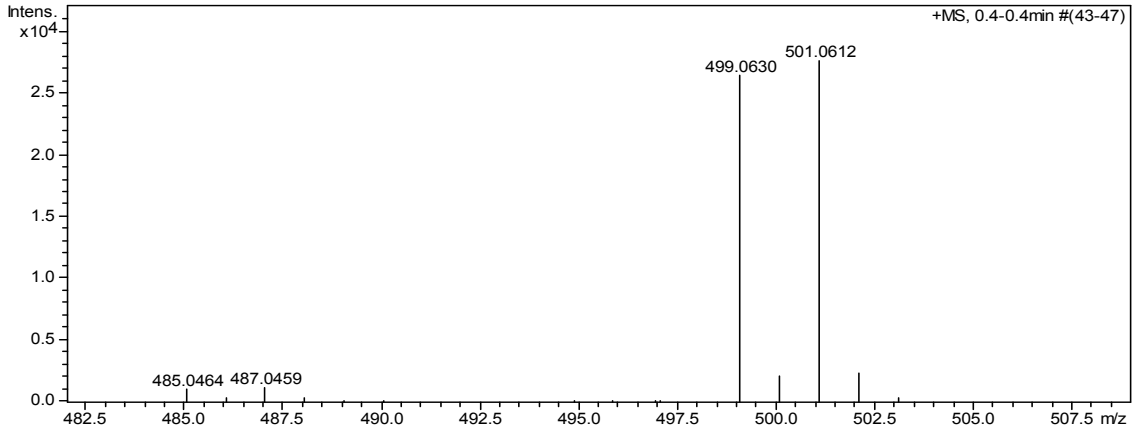




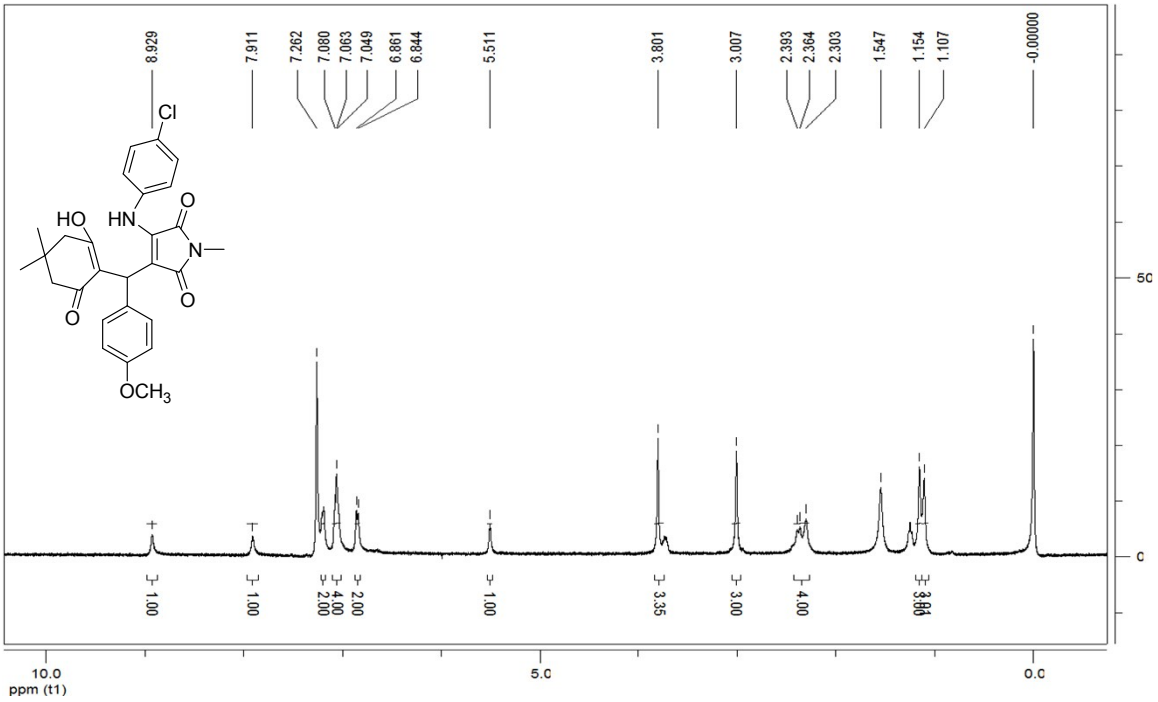
4-(4-Bromophenyl)-2-methyl-9-(*p*-tolyl)-6,7,8,9-tetrahydro-1*H*-pyrrolo[3,4-*b*]quinoline-1,3,5(2*H*,4*H*)-trione (3j):

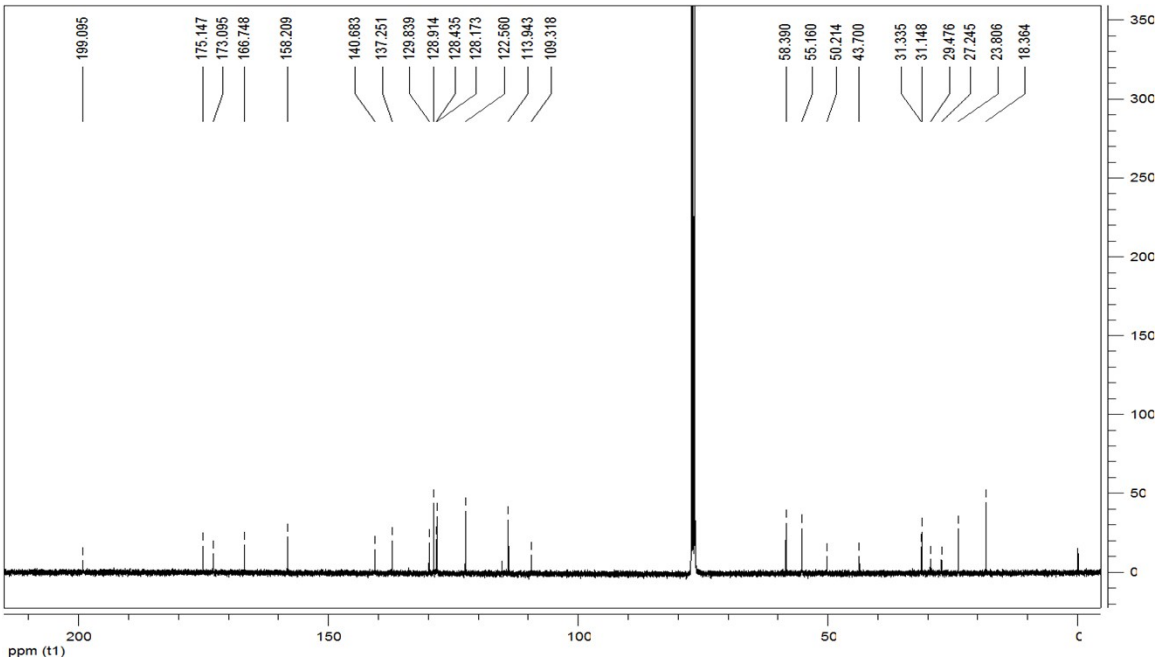


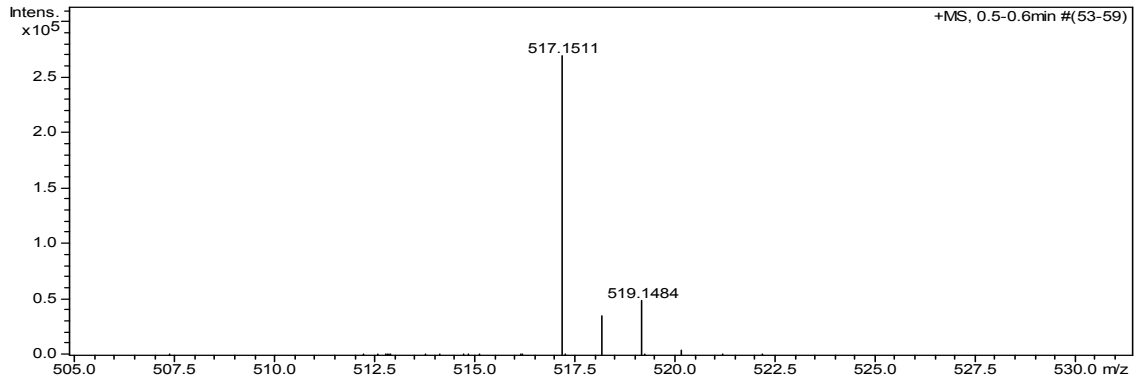




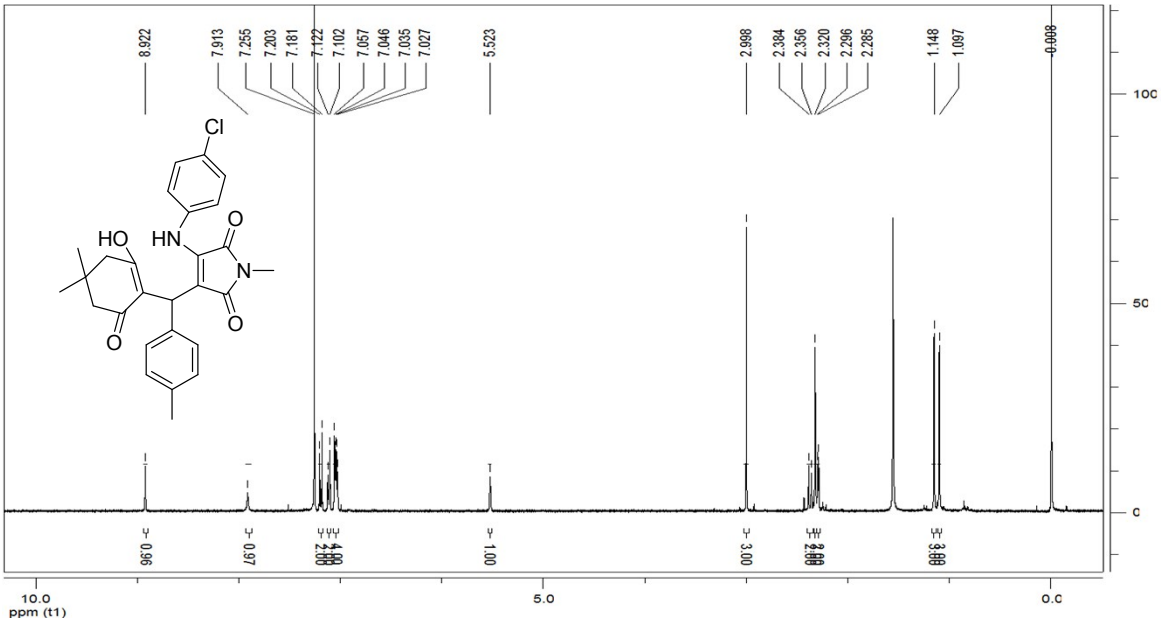
3-((4-Chlorophenyl)amino)-4-((2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-en-1-yl)(4-methoxyphenyl)methyl)-1-methyl-1*H*-pyrrole-2,5-dione (2a):

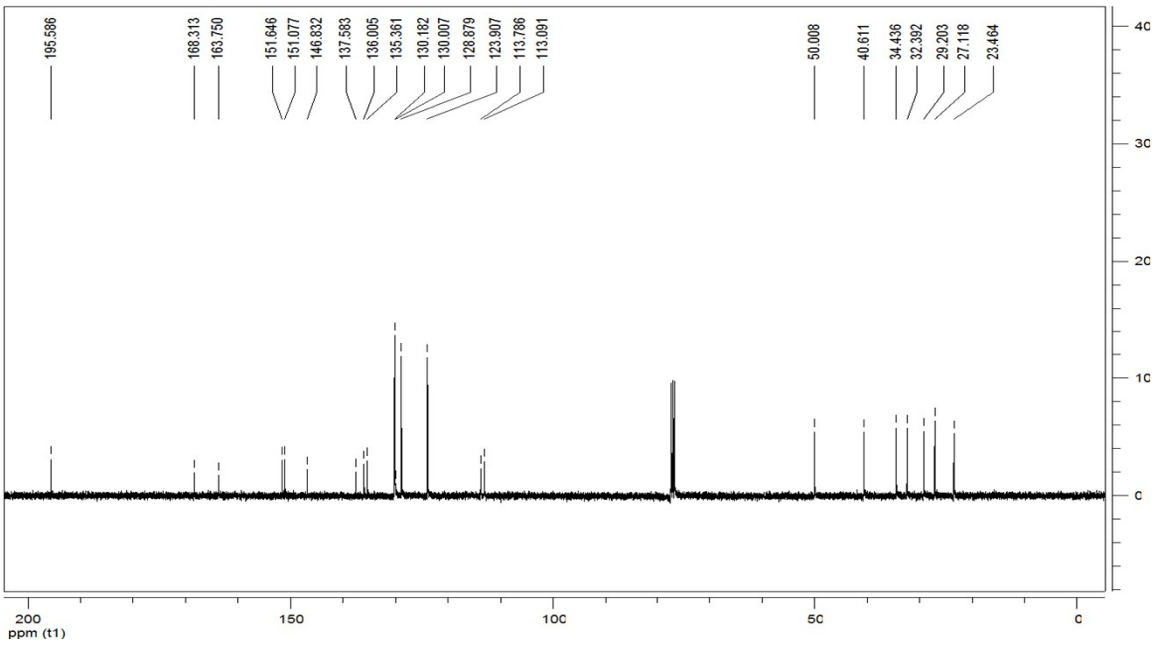


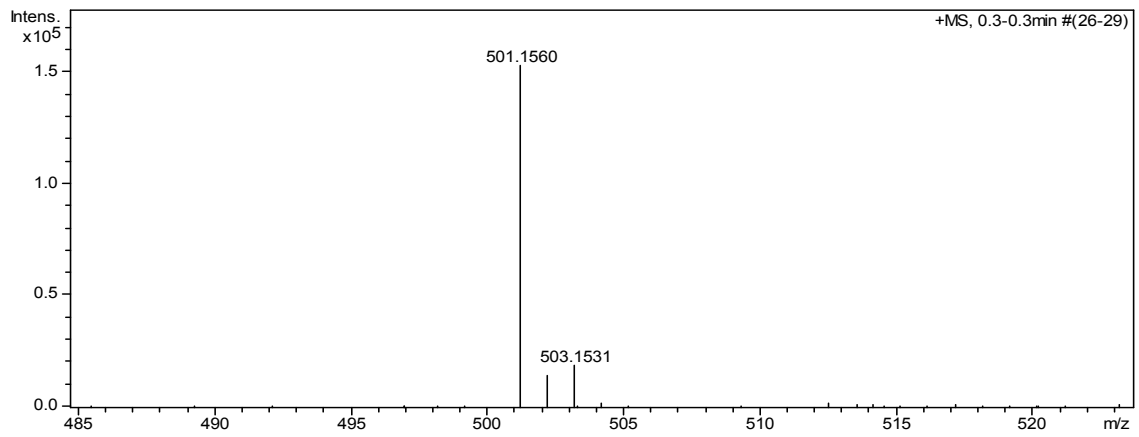




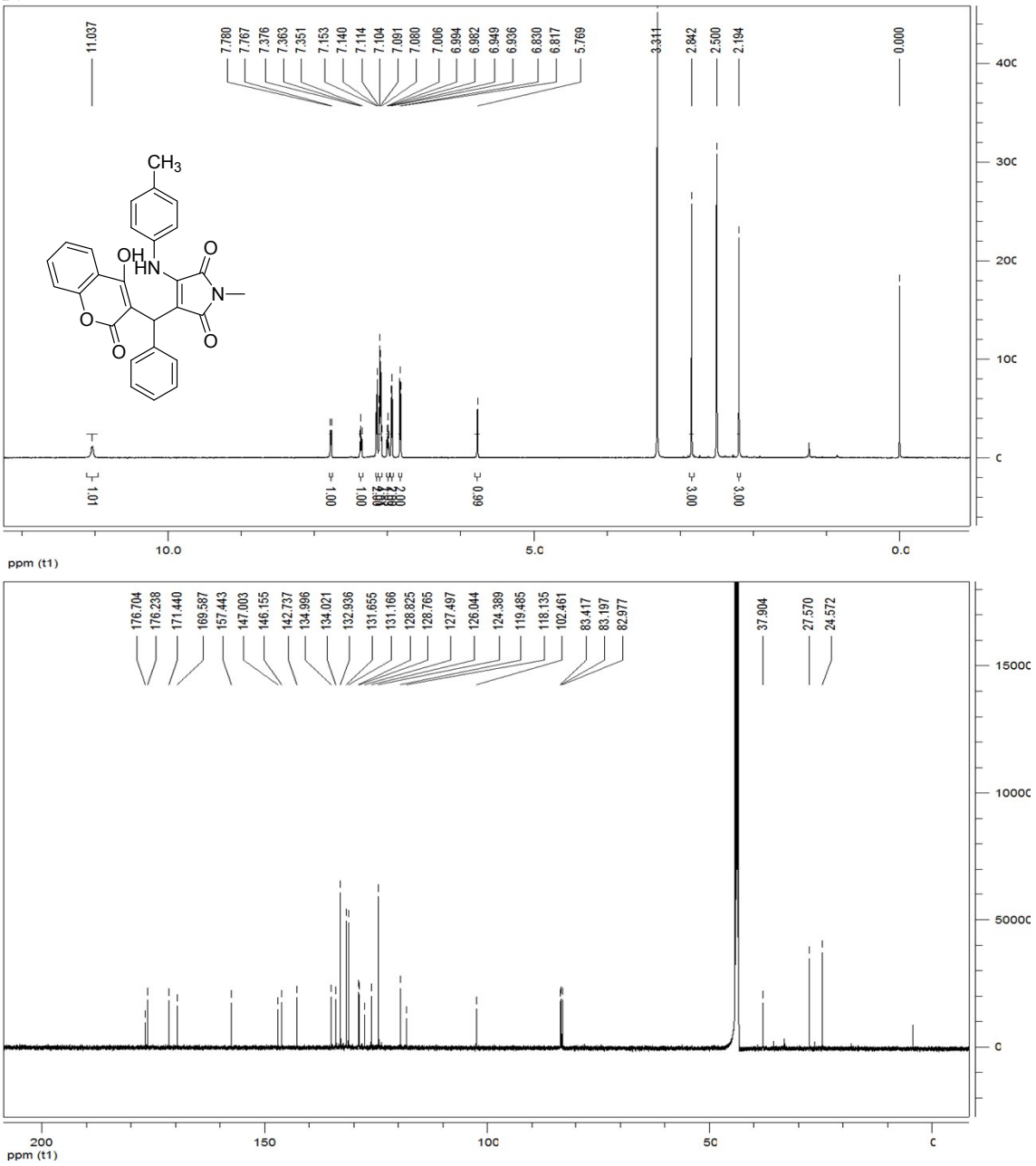
3-((4-Chlorophenyl)amino)-4-((2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-en-1-yl)(*p*-tolyl)methyl)-1-methyl-1*H*-pyrrole-2,5-dione (2b):

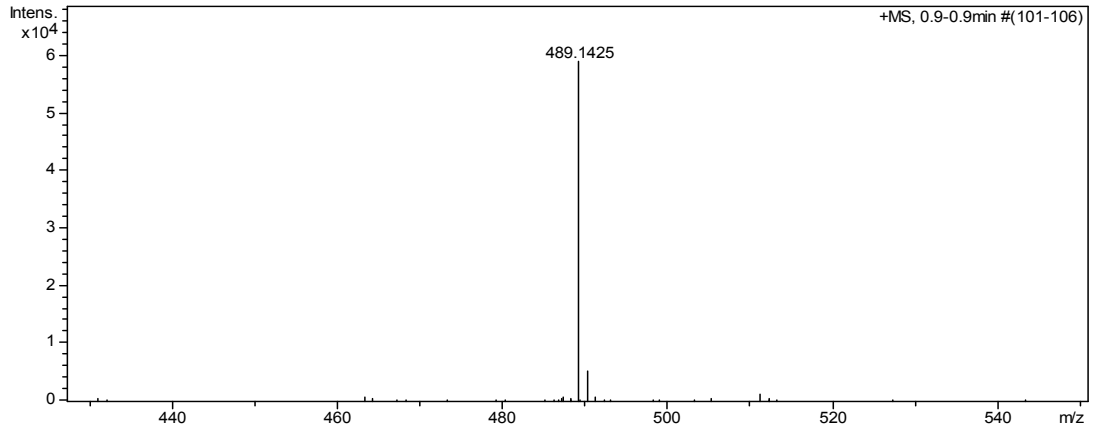






3-((4-hydroxy-2-oxo-2H-chromen-3-yl)(phenyl)methyl)-1-methyl-4-(p-tolylamino)-1*H*-pyrrole-2,5-dione (4a):





3-((4-hydroxy-2-oxo-2*H*-chromen-3-yl)(4-nitrophenyl)methyl)-1-methyl-4-(p-tolylamino)-1*H*-pyrrole-2,5-dione (4b):