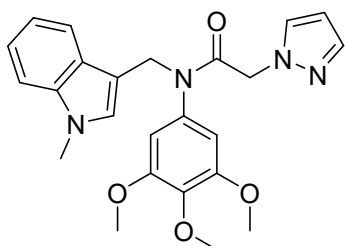


Supporting Information

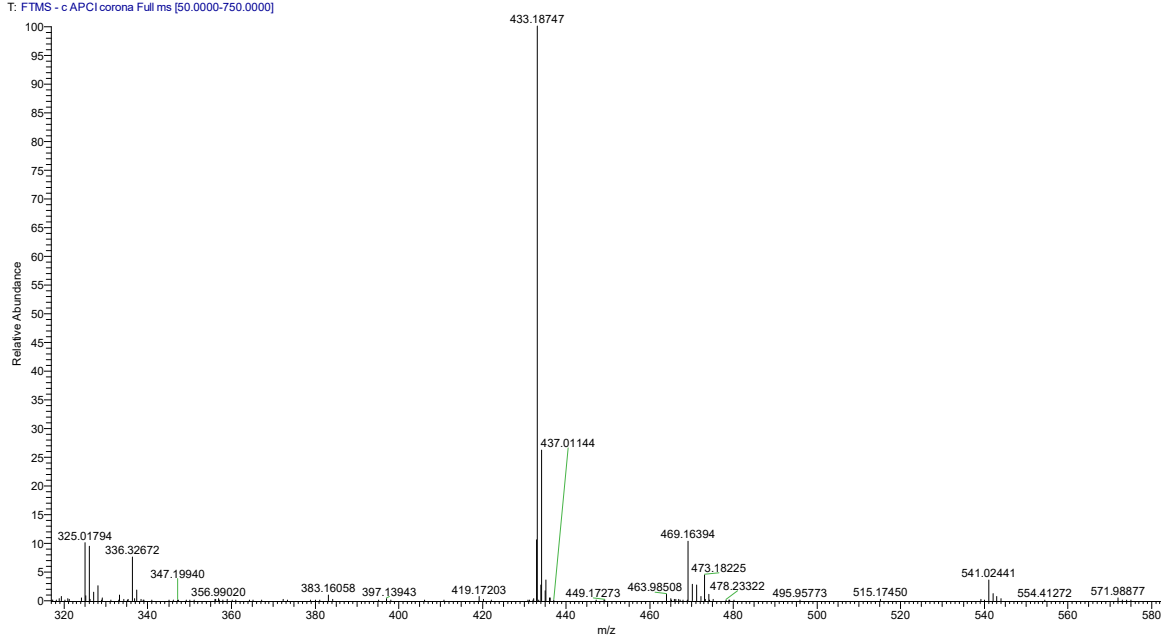
Synthesis and bioactive evaluation of N-((1-methyl-1H-indol-3-yl)methyl)-N-(3,4,5-trimethoxyphenyl)acetamide derivatives as agents for inhibiting tubulin polymerization

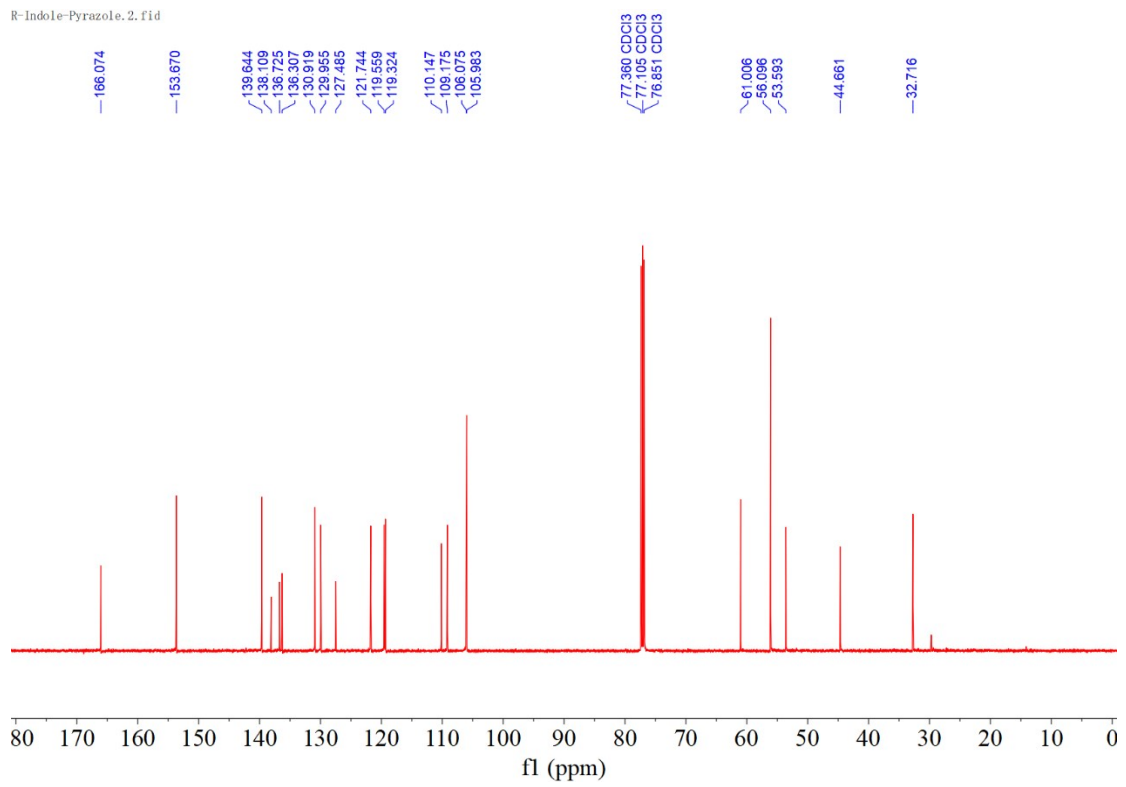
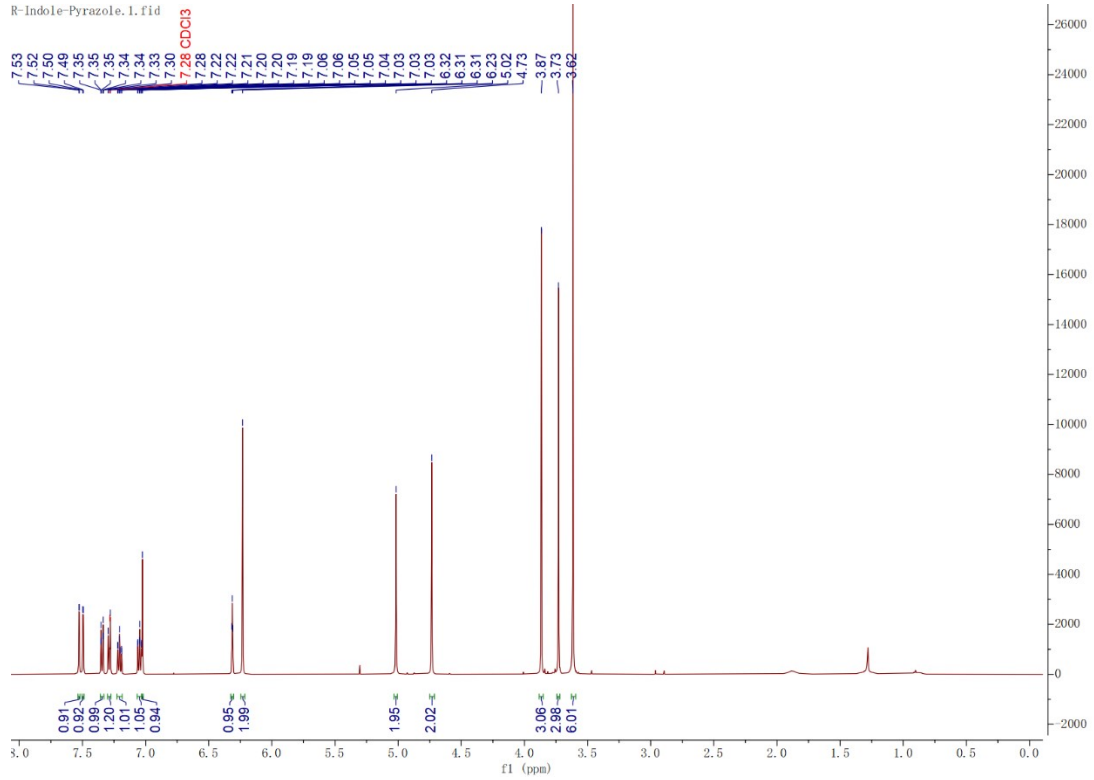
MS, ^1H NMR and ^{13}C NMR spectrum of Compounds 7a-7r

7a :

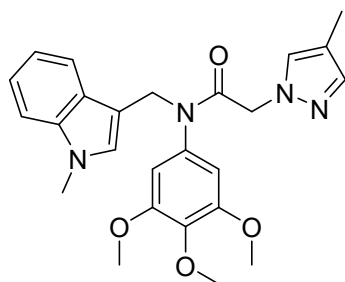


1 #14 RT: 0.15 AV: 1 NL: 9.23E6
T: FTMS - c APCI corona Full ms [50.0000-750.0000]

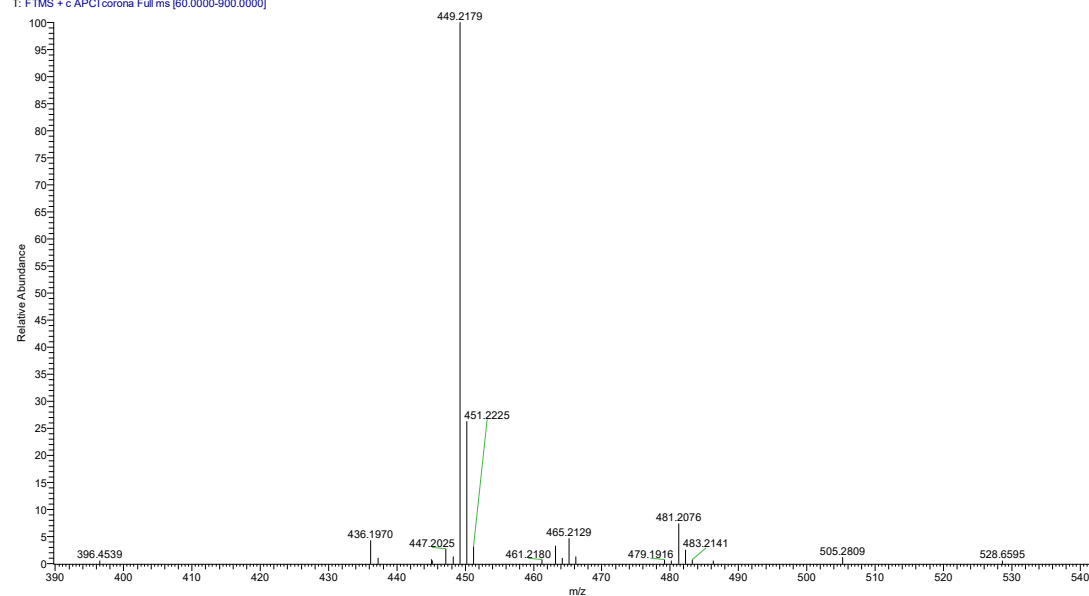




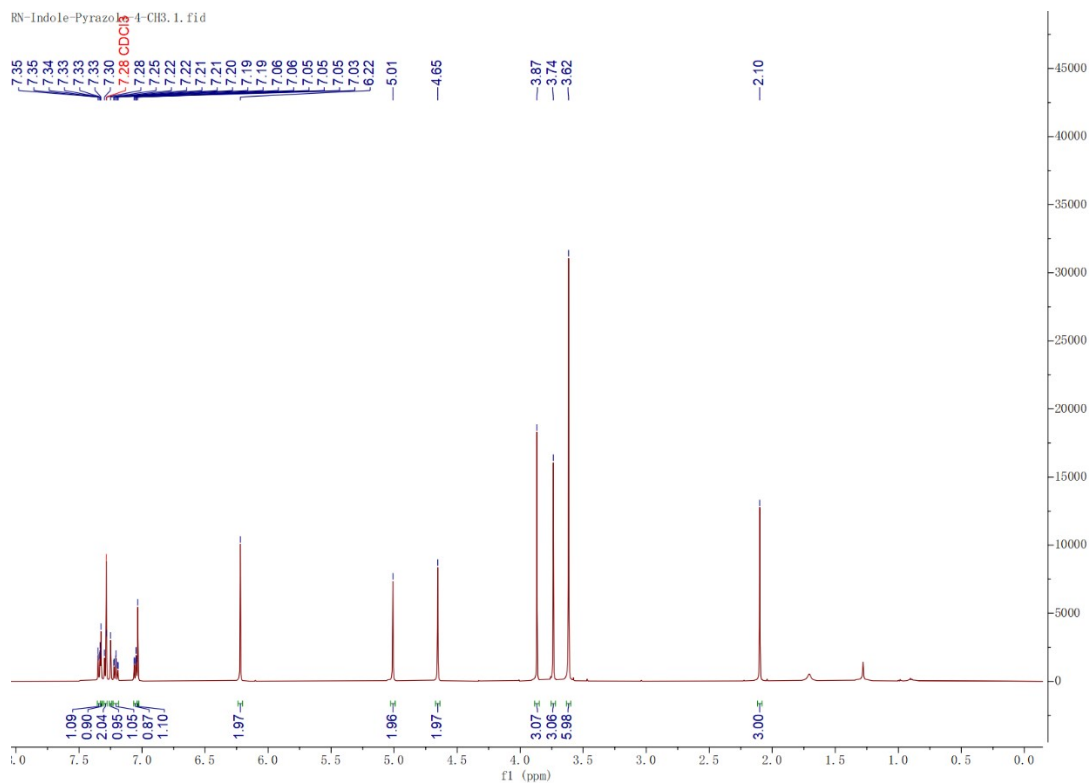
7b :



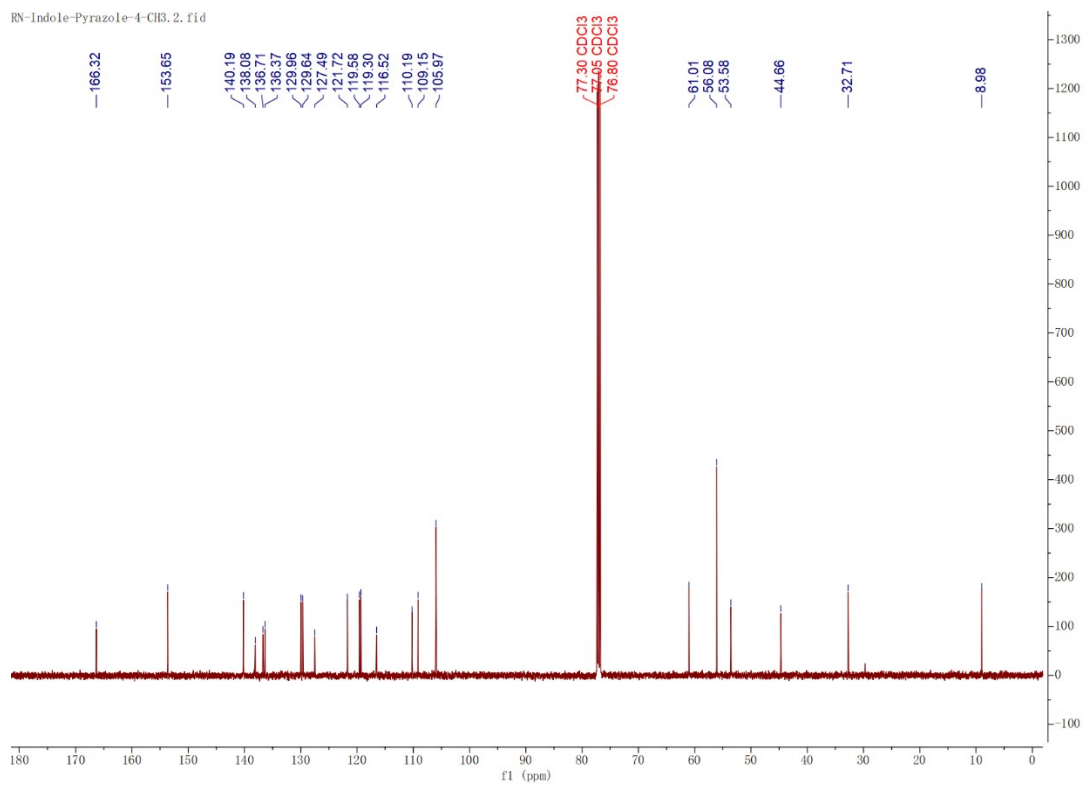
7 #21 RT: 0.21 AV: 1 NL: 6.54E7
T: FTMS + c APCI corona Full ms [60.0000-900.0000]



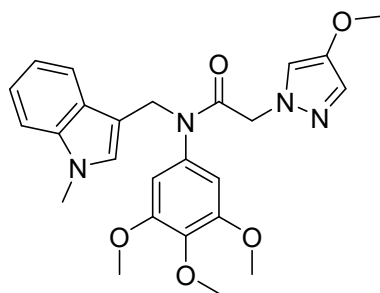
RN-Indole-Pyrazolo[4-CH3]. 1. fid



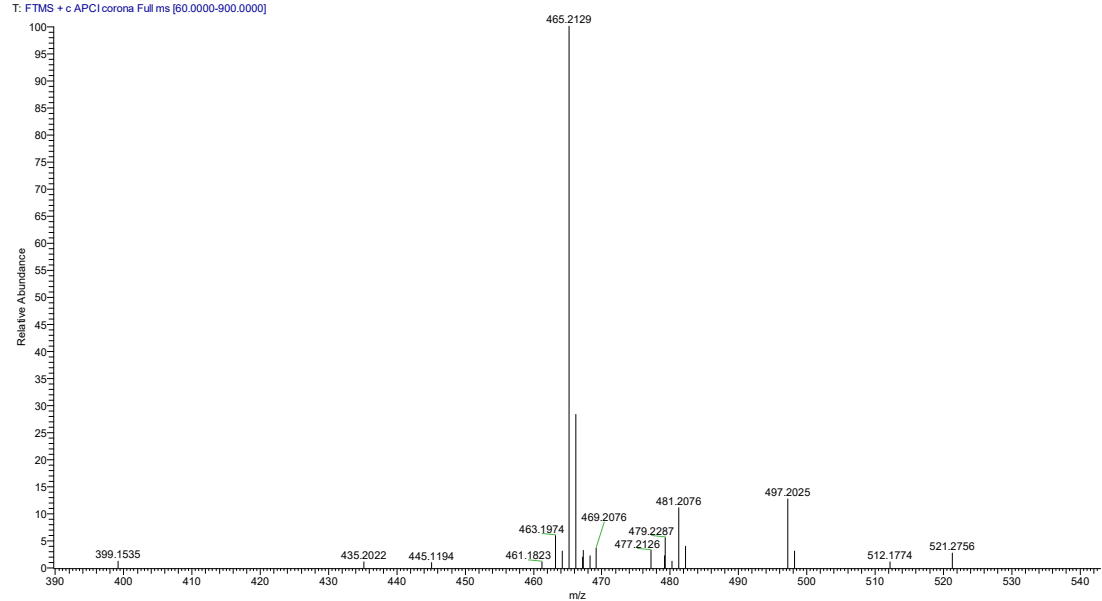
RN-Indole-Pyrazole-4-CH3. 2. fid



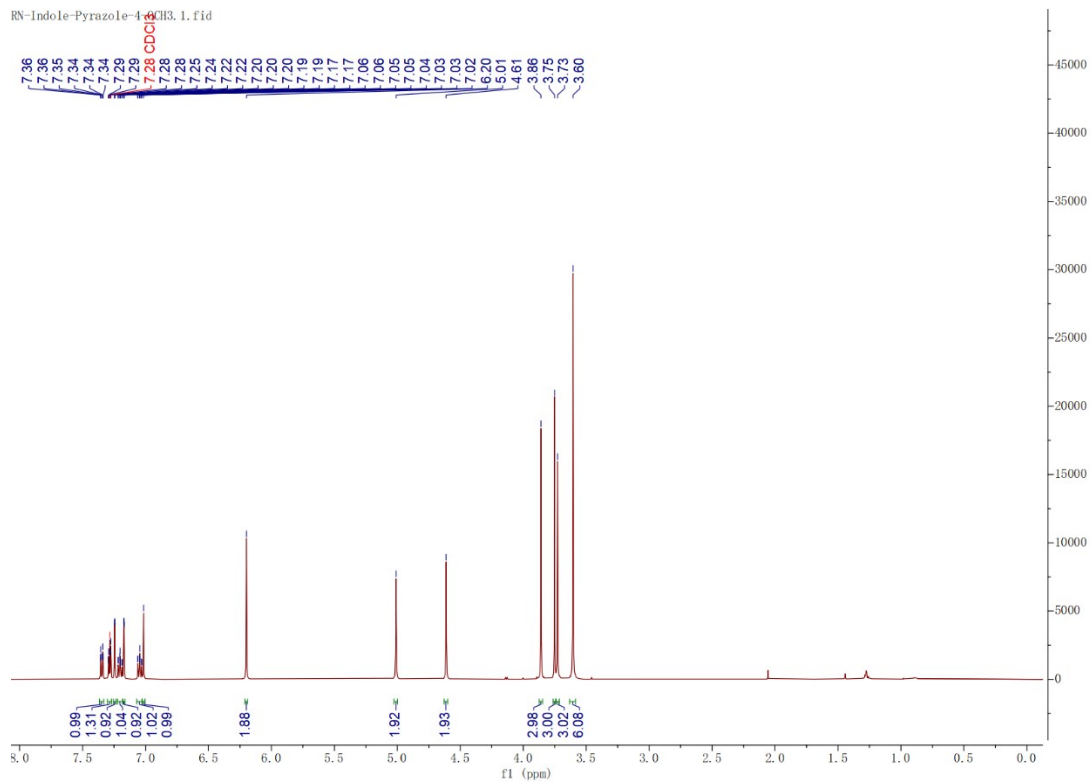
7c :



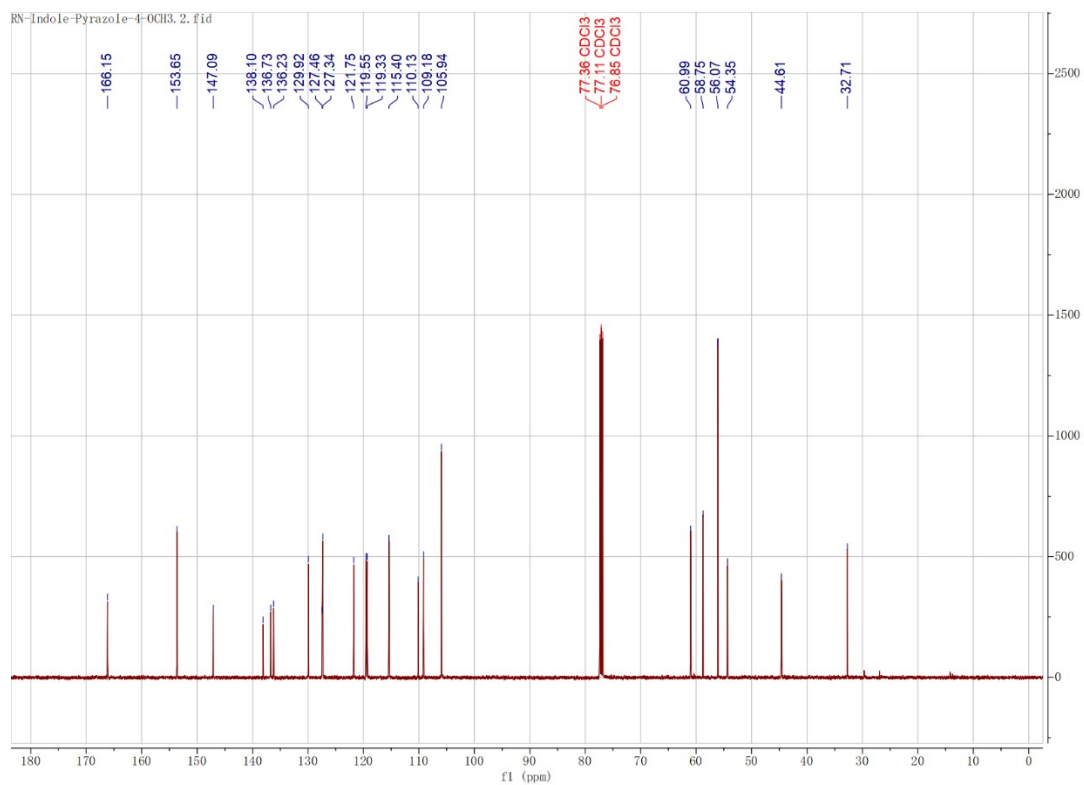
21 RT: 0.21 AV: 1 NL: 4.22E7
T: FTMS + c-APCI corona Full ms [80.0000-900.0000]



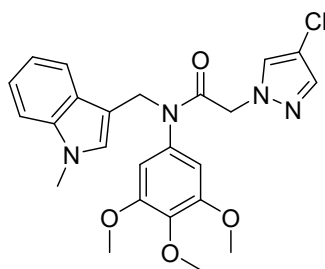
RN-Indole-Pyrazole-4-OCH3. 1. fid



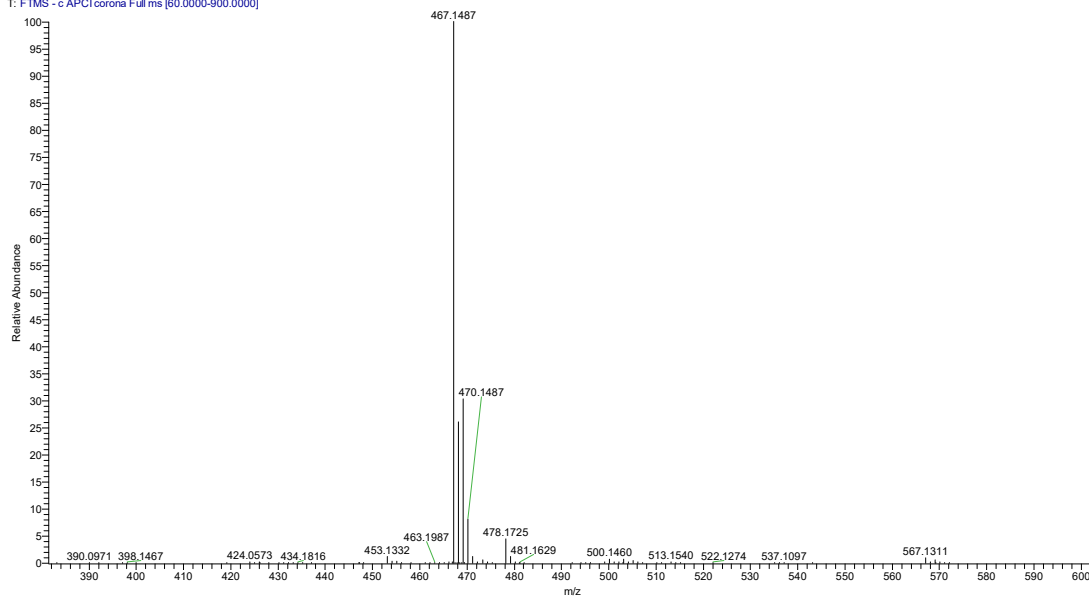
RN-Indole-Pyrazole-4-OCH3. 2. fid



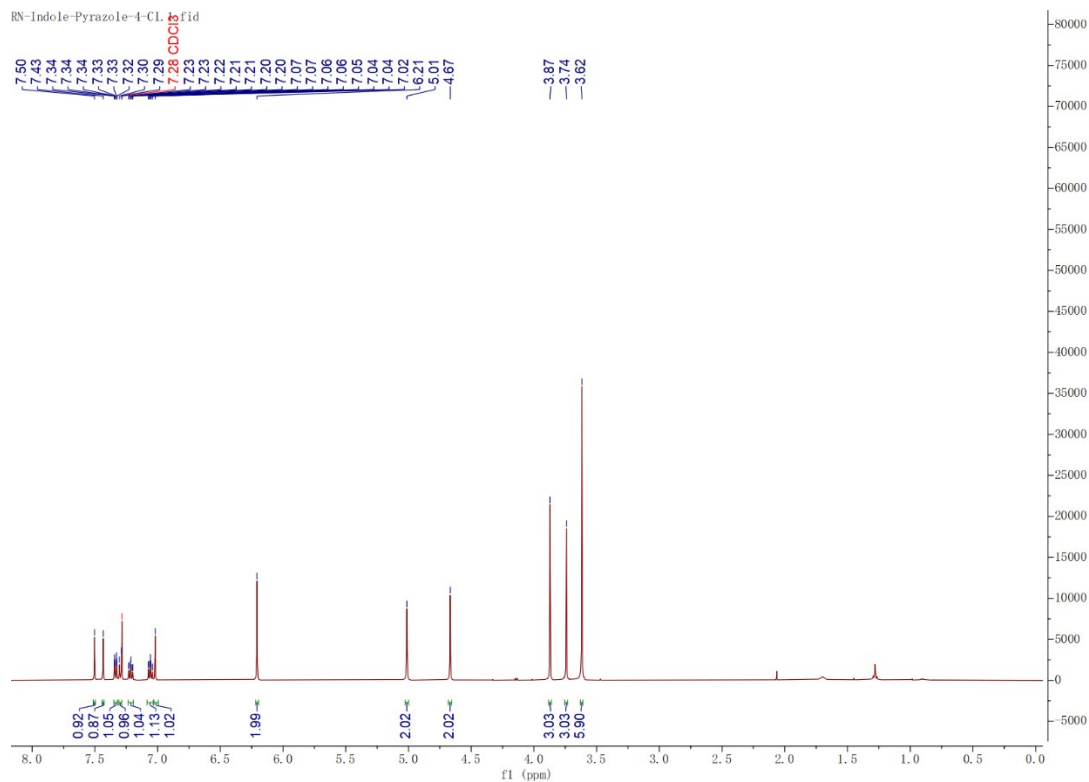
7d :



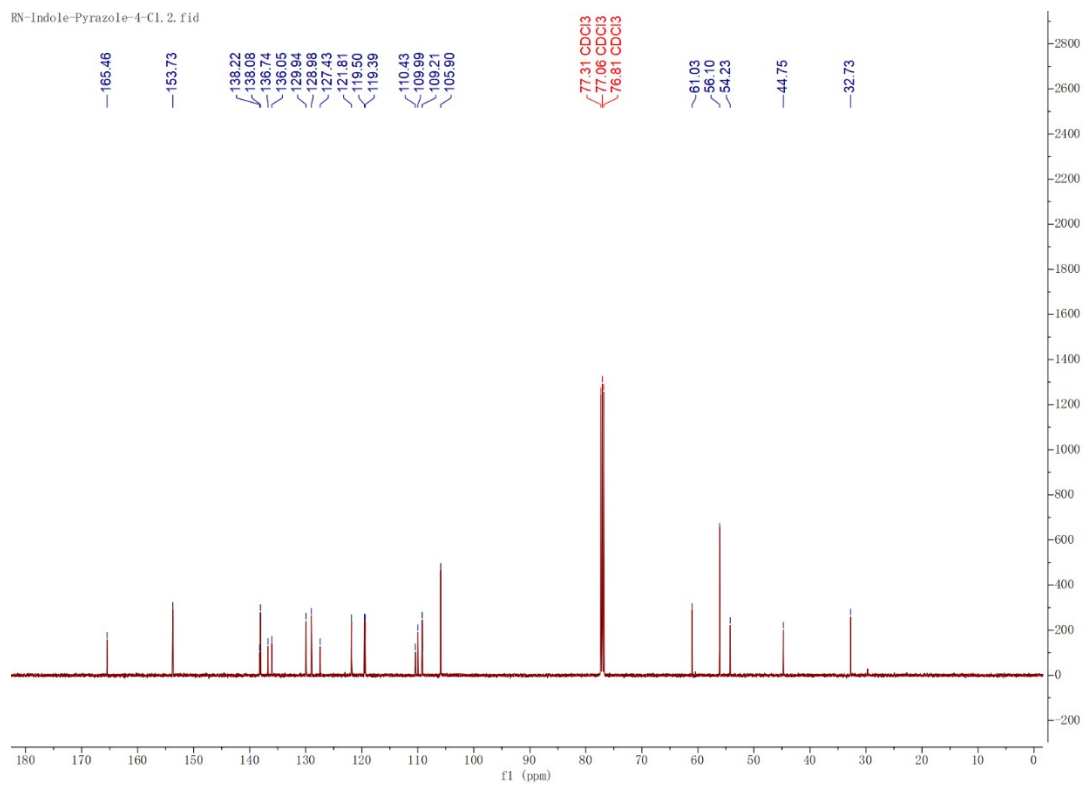
12 #12 RT: 0.12 AV: 1 NL: 1.05E8
T: FTMS - c APCI corona Full ms [60.0000-900.0000]



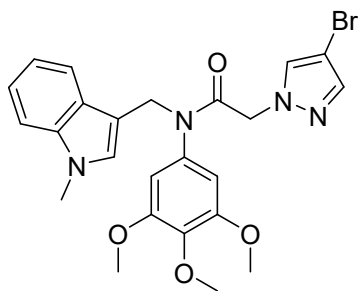
RN-Indole-Pyrazole-4-Cl. F1d



RN-Indole-Pyrazole-4-Cl. 2. fid

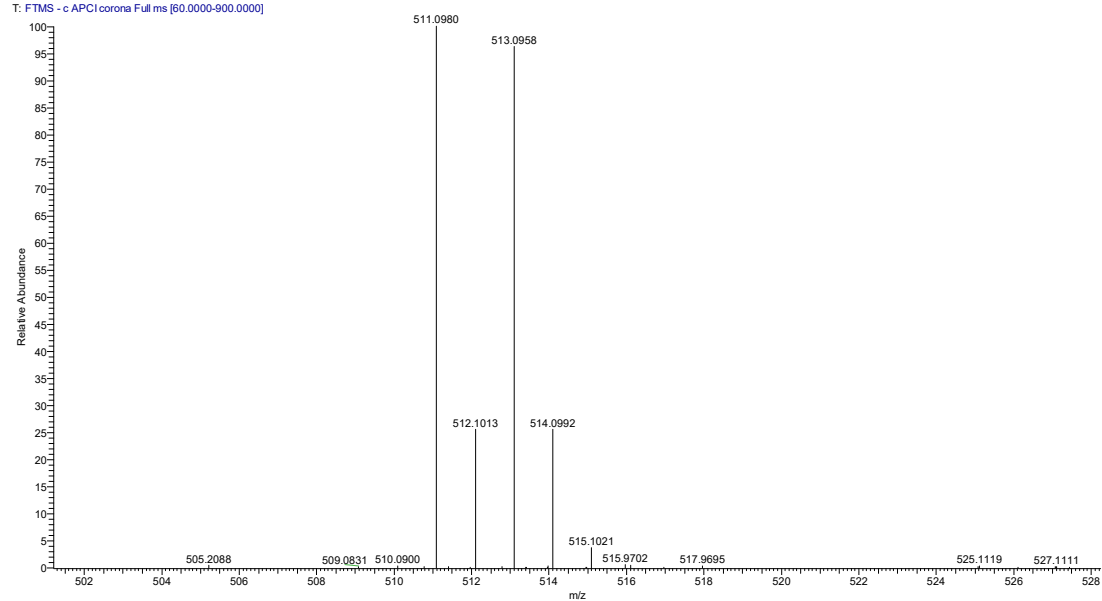


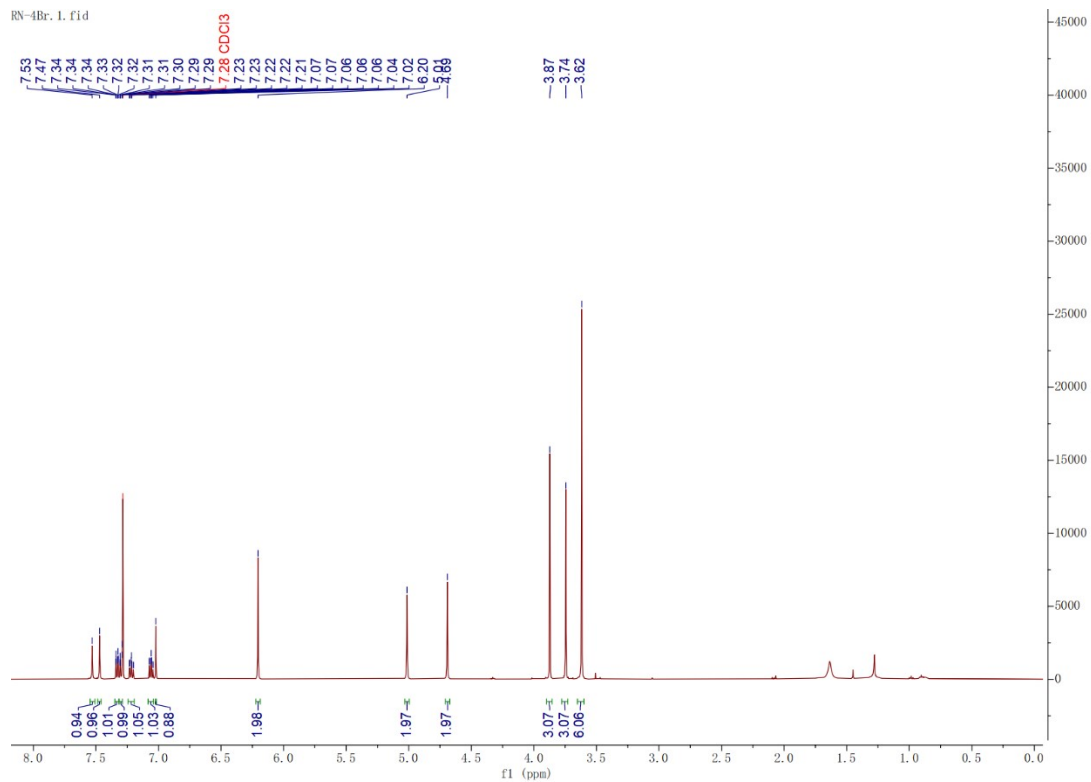
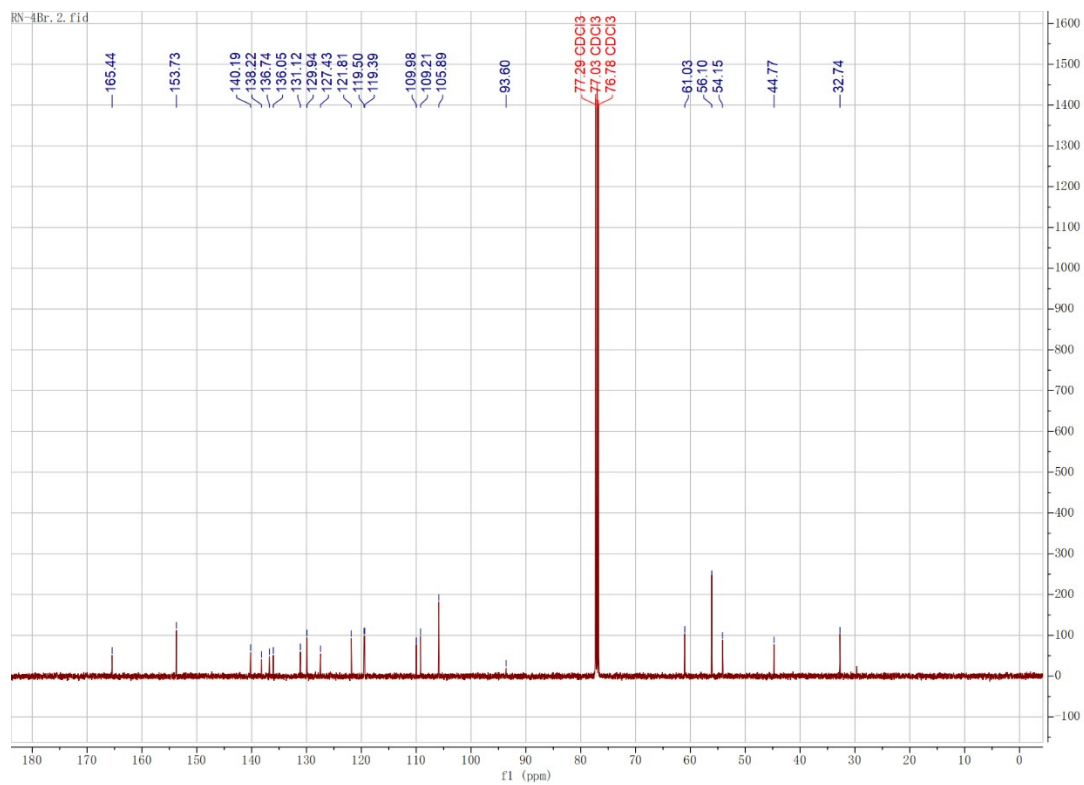
7e :



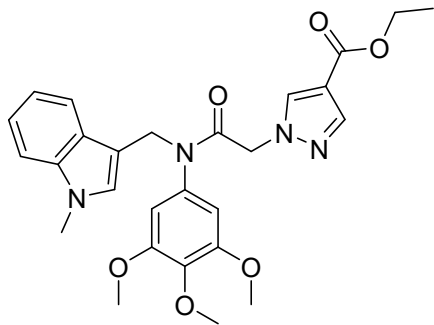
9 #20 RT: 0.20 AV: 1 NL: 9.67E7

T: FTMS - c APCI corona Fullms [60.0000-900.0000]

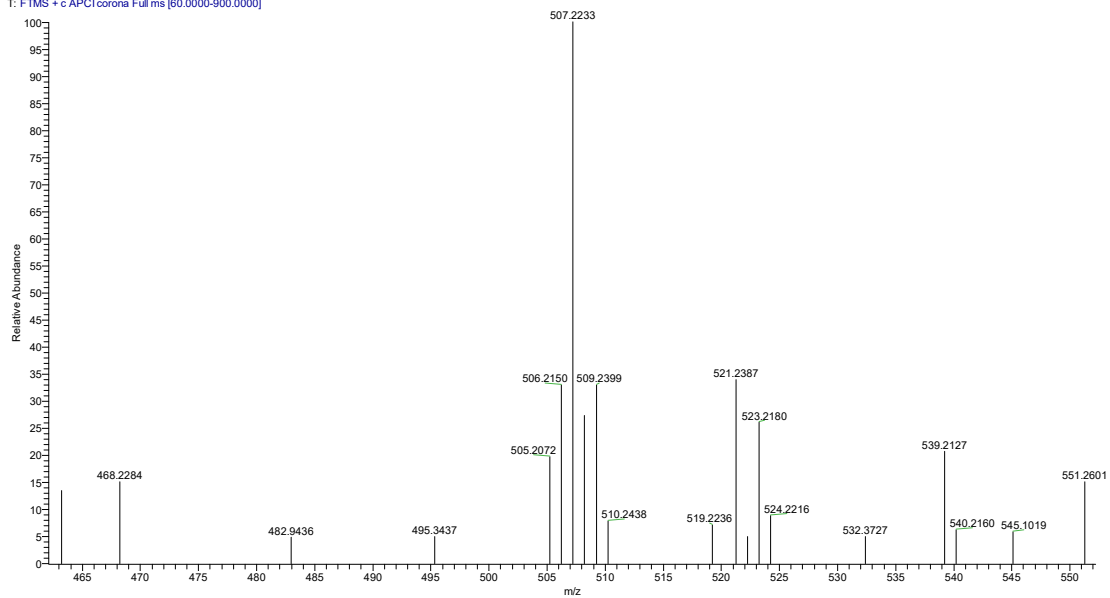




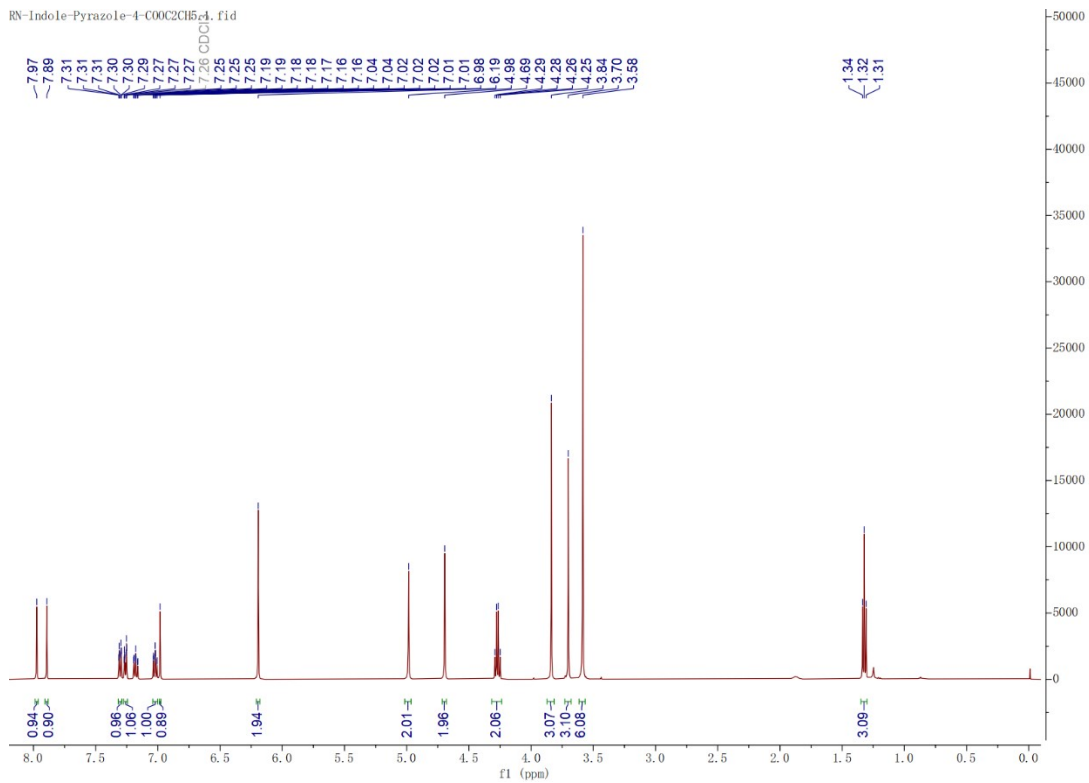
7f :



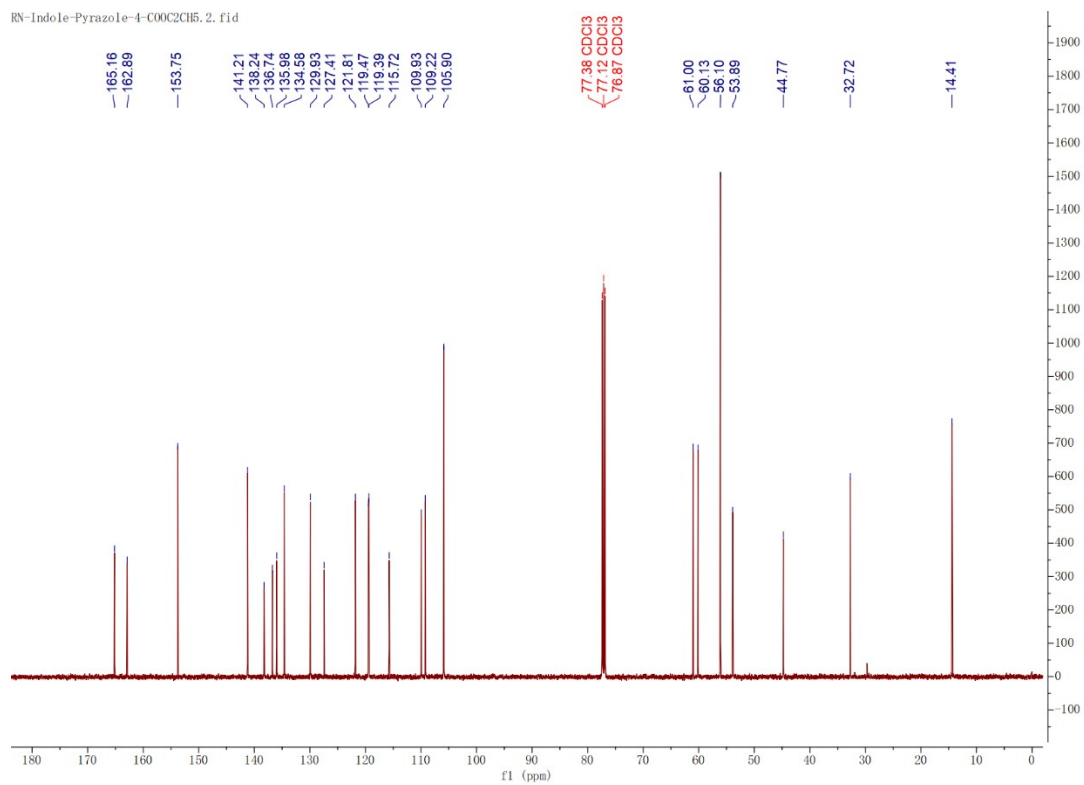
6 #15 RT: 0.15 AV: 1 NL: 1.54E7
T: FTMS + c APCI corona Full ms [60.0000-900.0000]



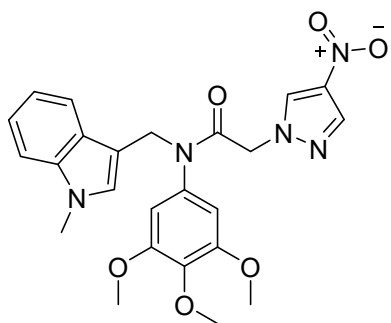
RN-Indole-Pyrazole-4-COOC2H5.c1.fid



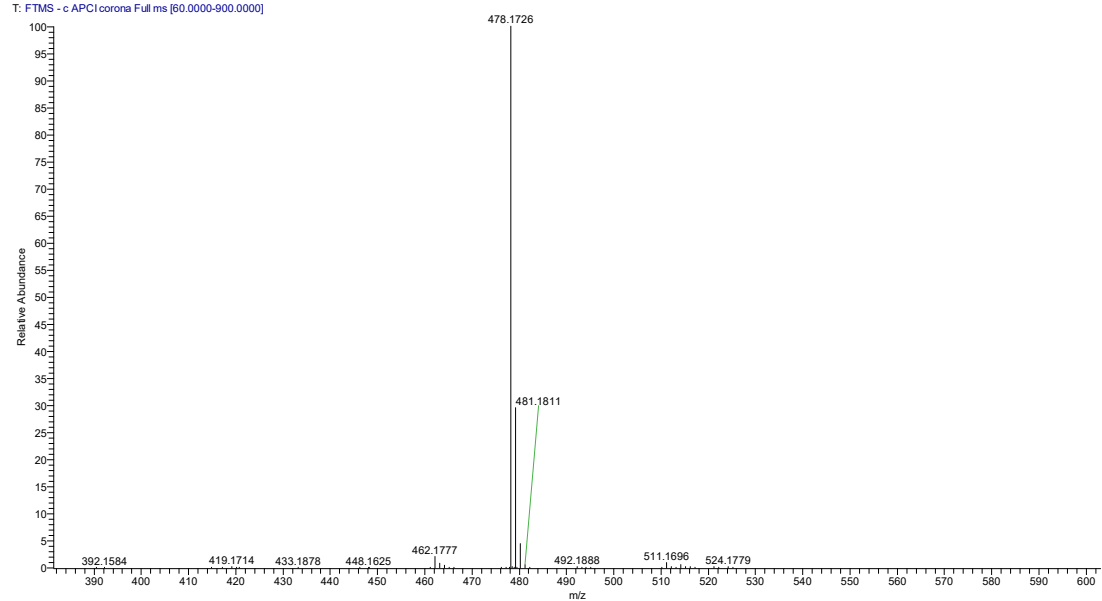
RN-Indole-Pyrazole-4-COOC2H5. 2. fid

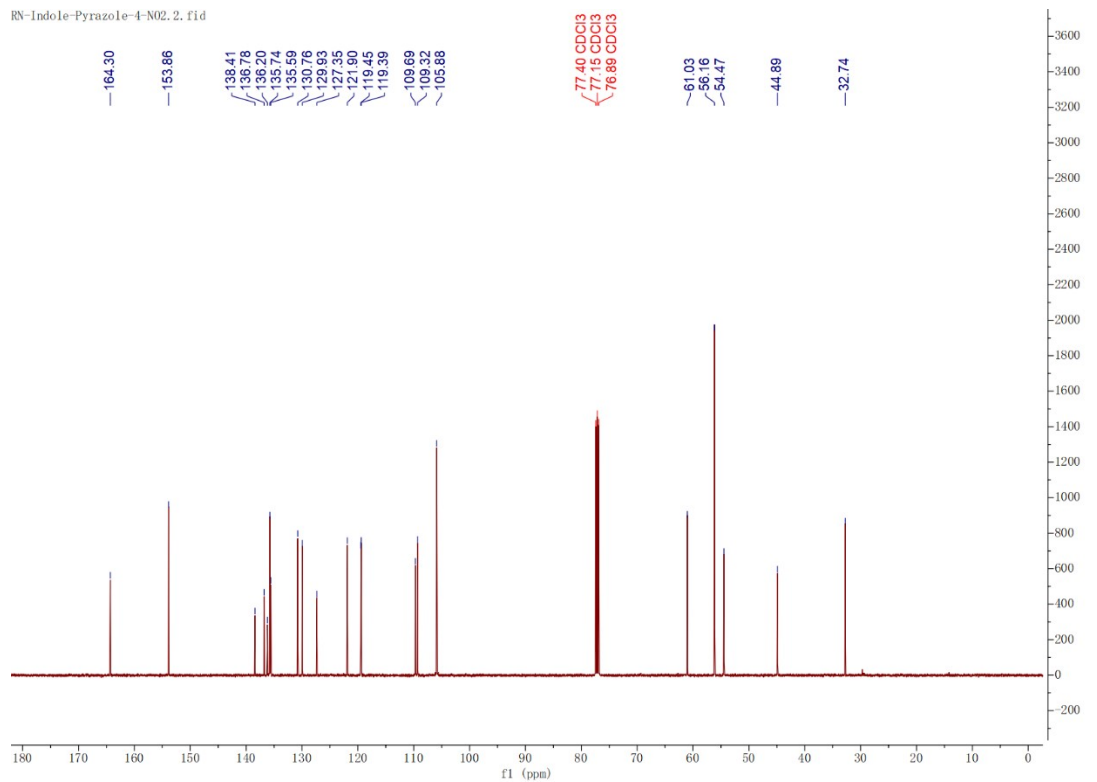
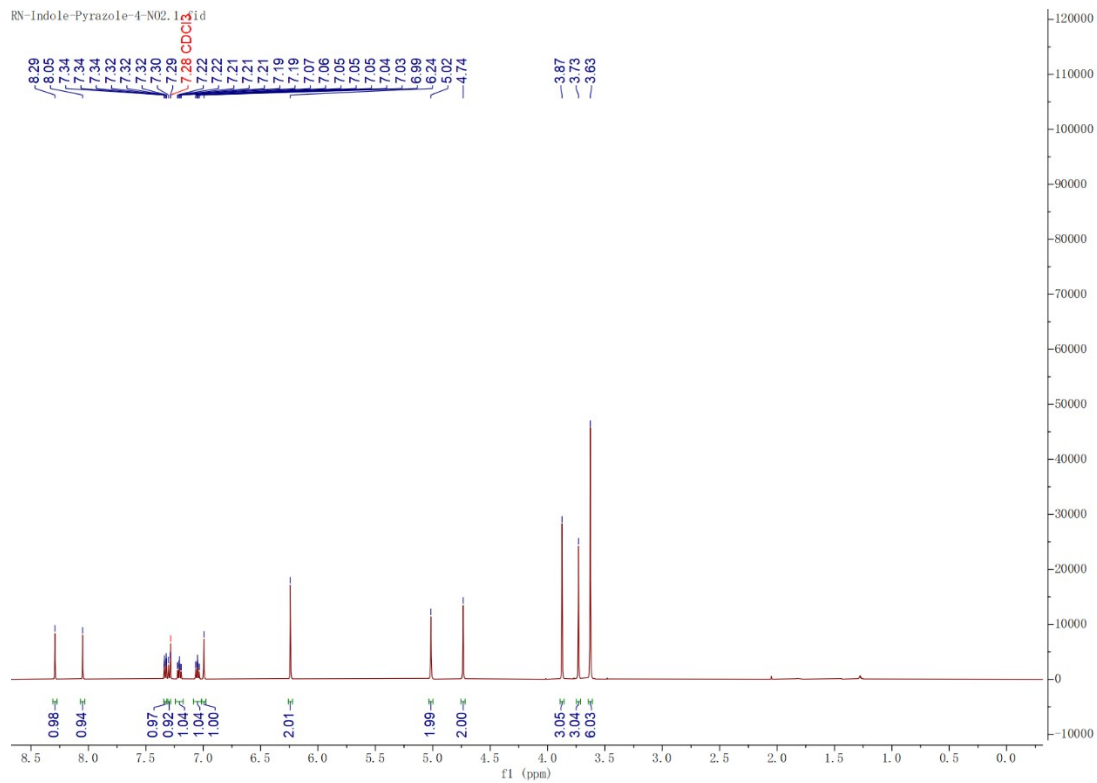


7g :

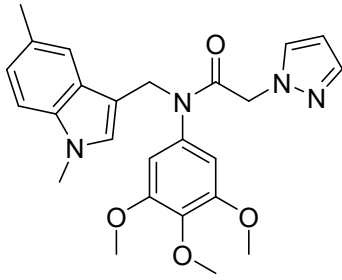


11#12 RT: 0.12 AV: 1 NL: 2.53E9
T: FTMS - c APCI corona Full ms [0.0000-900.0000]

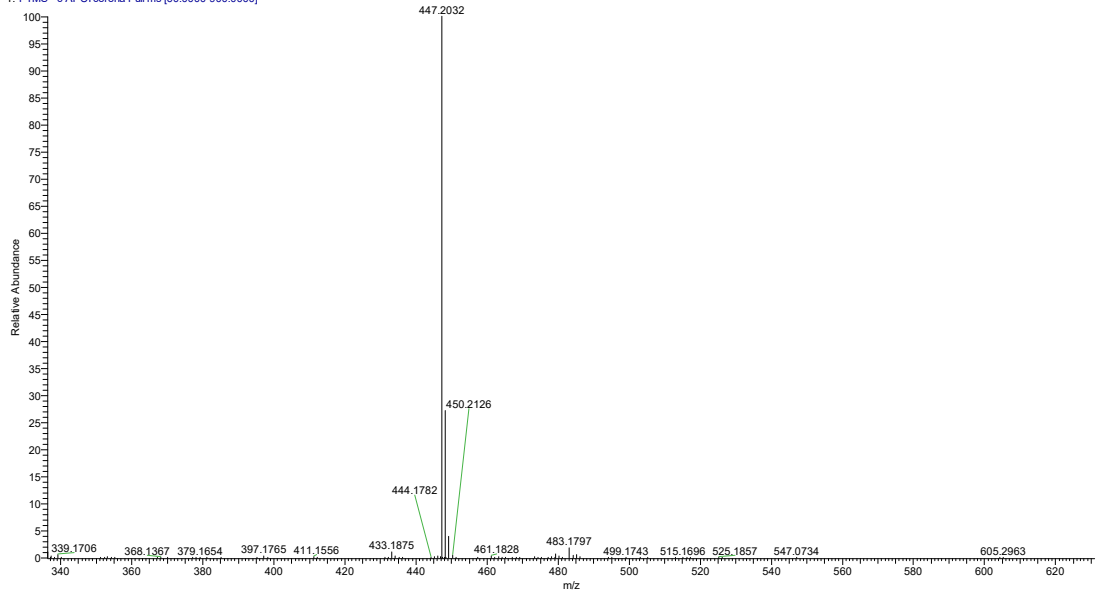




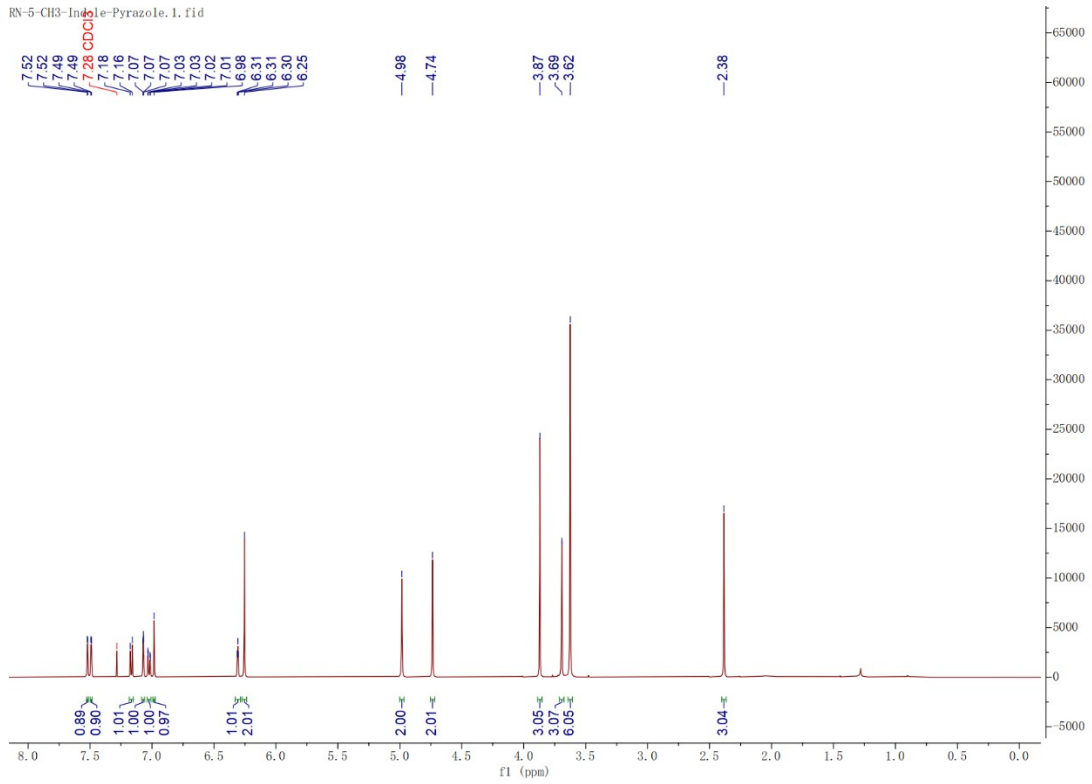
7h :



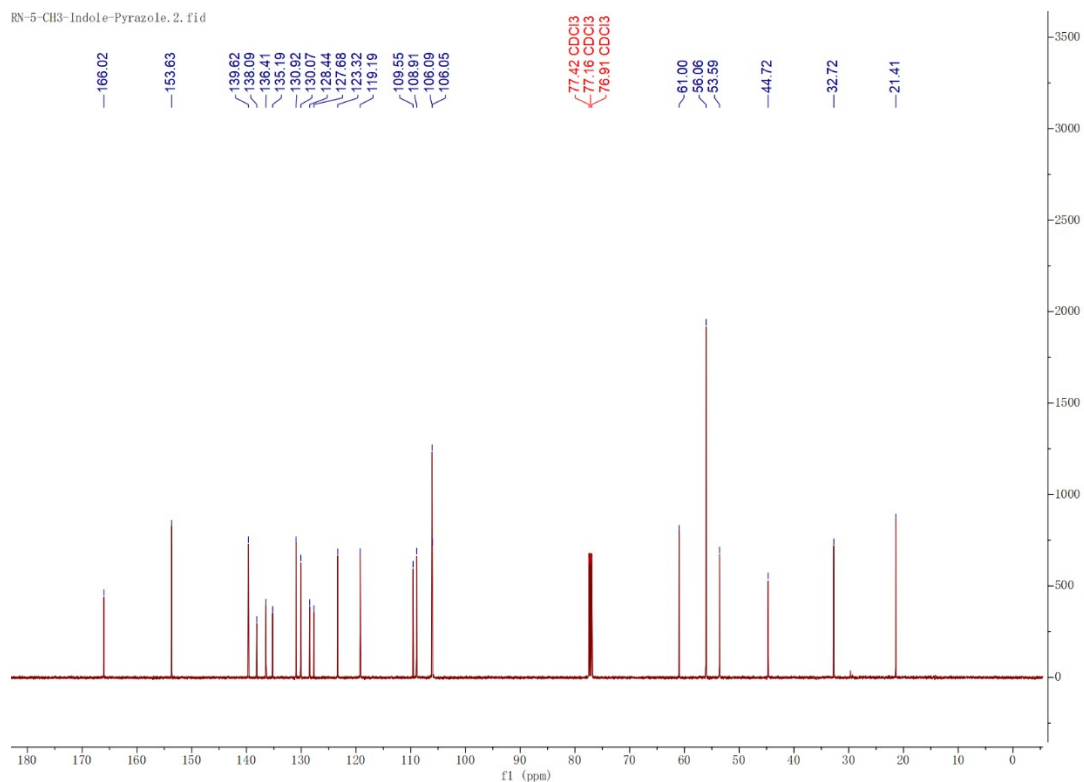
16 #20 RT: 0.20 AV: 1 NL: 3.19E8
 T: FTMS - c APCI corona Full ms [60.0000-900.0000]



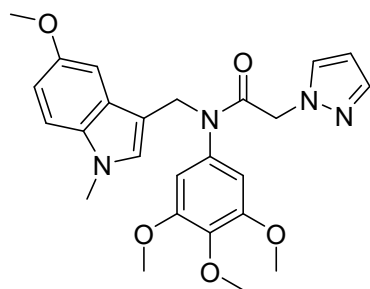
RN-5-CH3-Indole-Pyrazole.1.fid



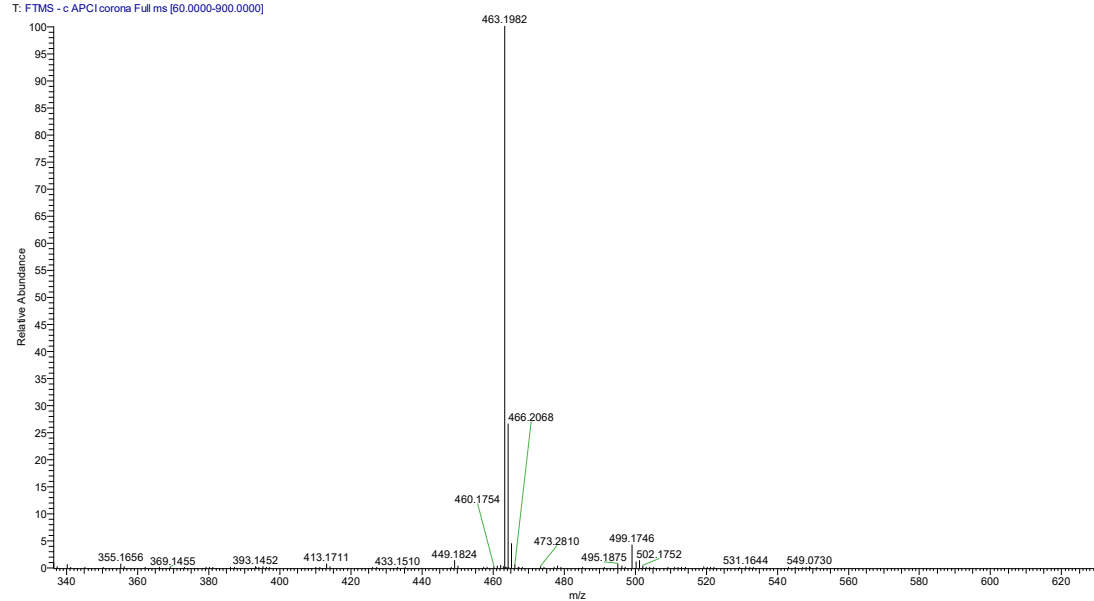
RN-5-CH3-Indole-Pyrazole.2.fid



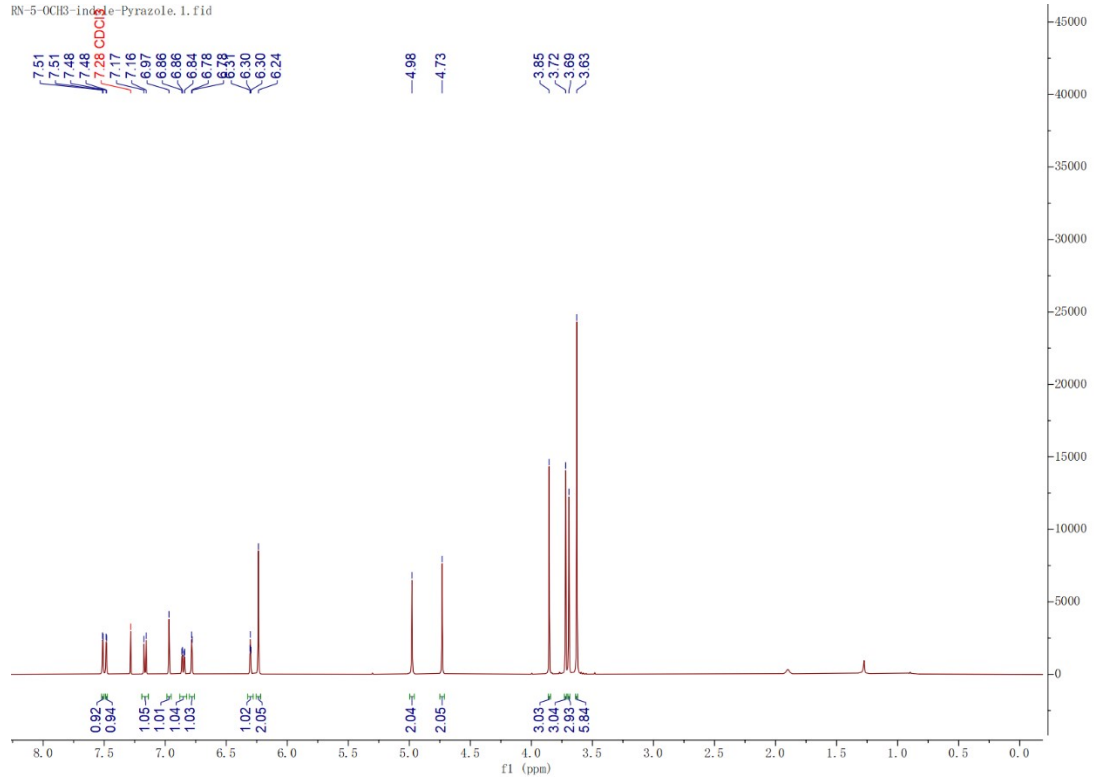
7i :



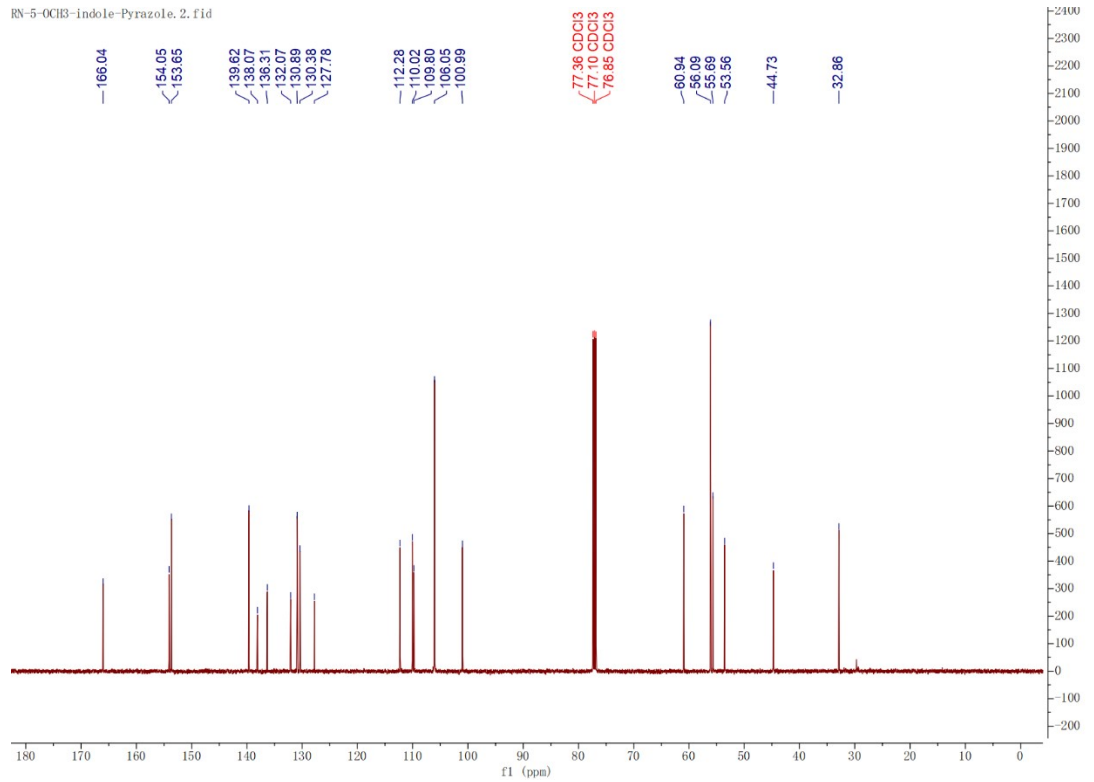
15 #20 RT: 0.20 AV: 1 NL: 5.50E8
T: FTMS - c APCLcorona Full.ms [60.0000-900.0000]



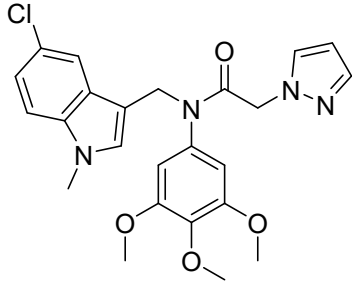
RN-5-OCH3-indole-Pyrazole. 1. fid



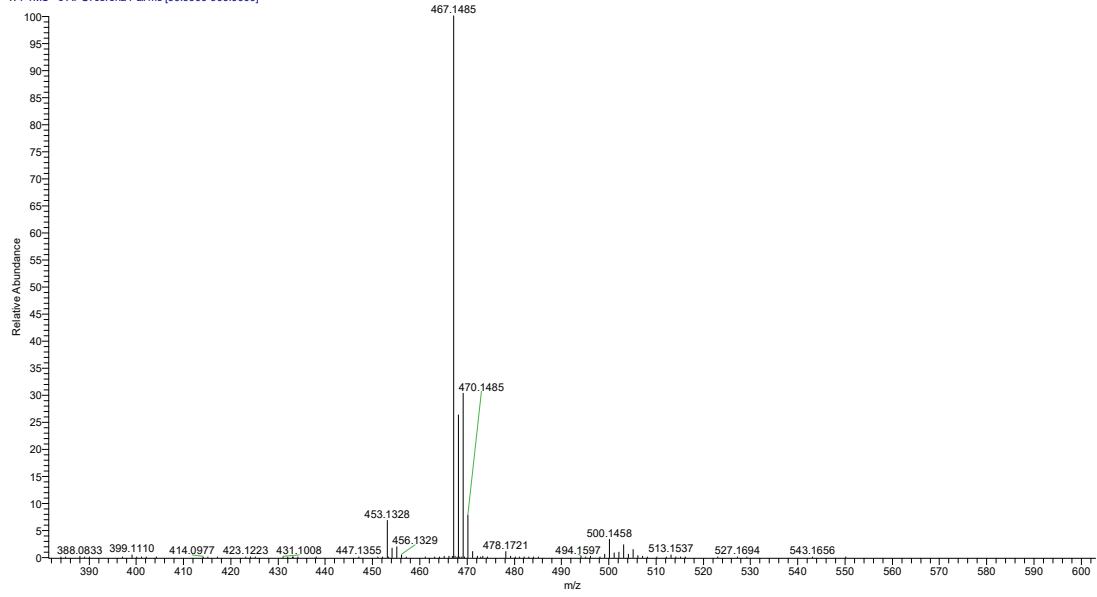
RN-5-OCH3-indole-Pyrazole. 2. fid



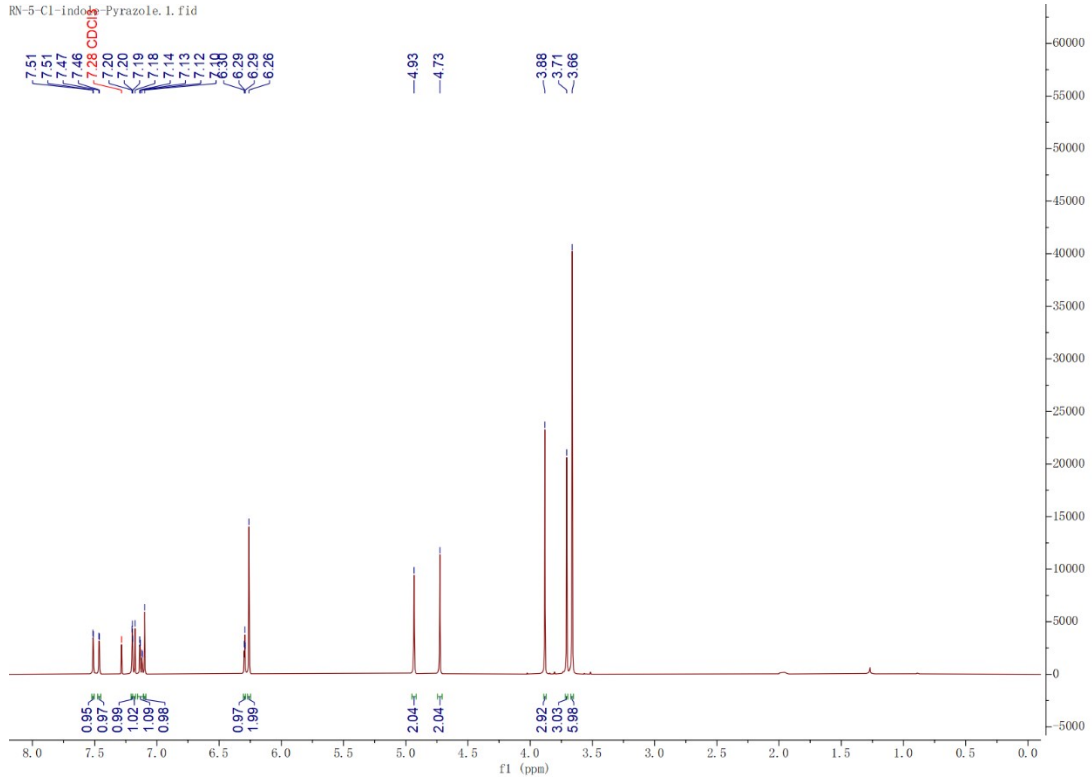
7j :



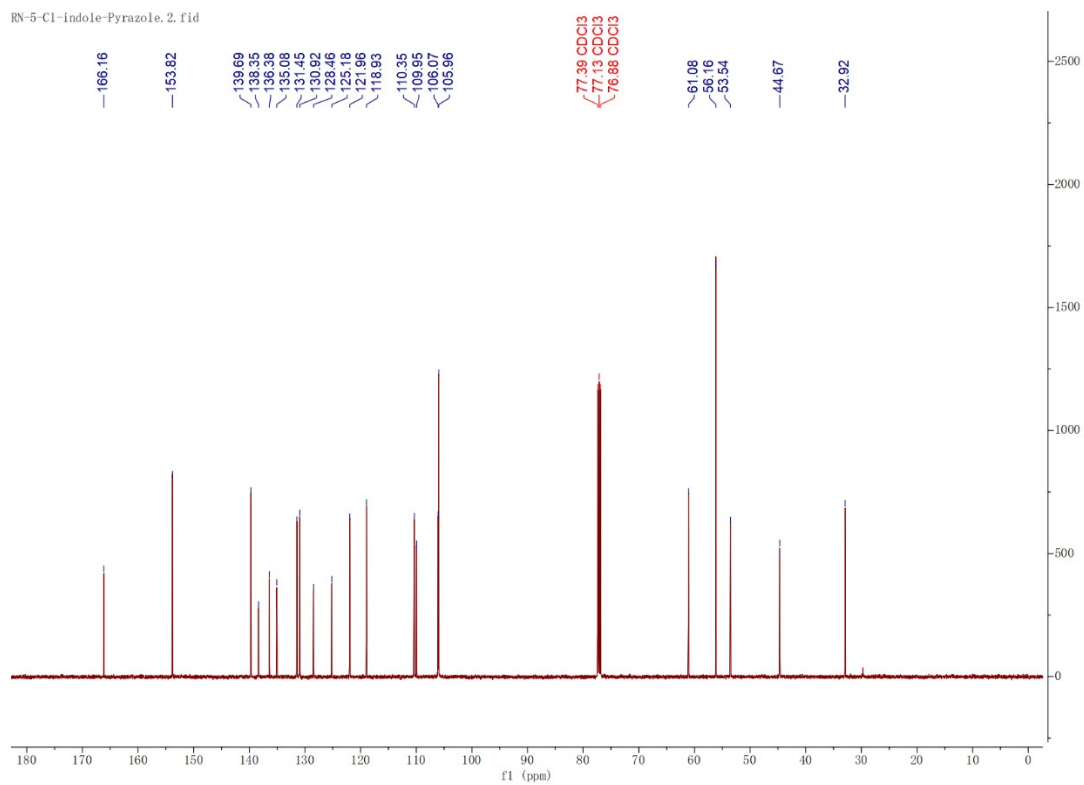
13 #12 RT: 0.12 AV: 1 NL: 2.30E8
T: FTMS - c APCI corona Full ms [60.0000-900.0000]



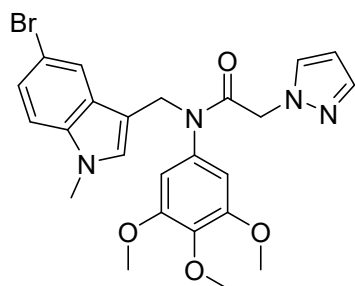
RN-5-Cl-indole-Pyrazole. 1. fid



RN-5-Cl-indole-Pyrazole. 2. fid

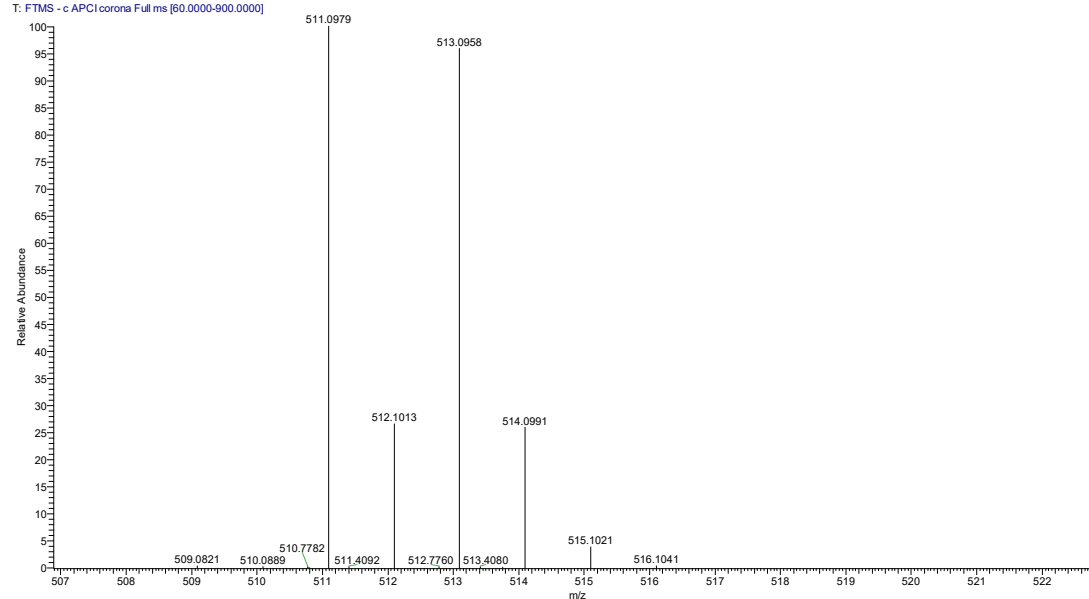


7k :

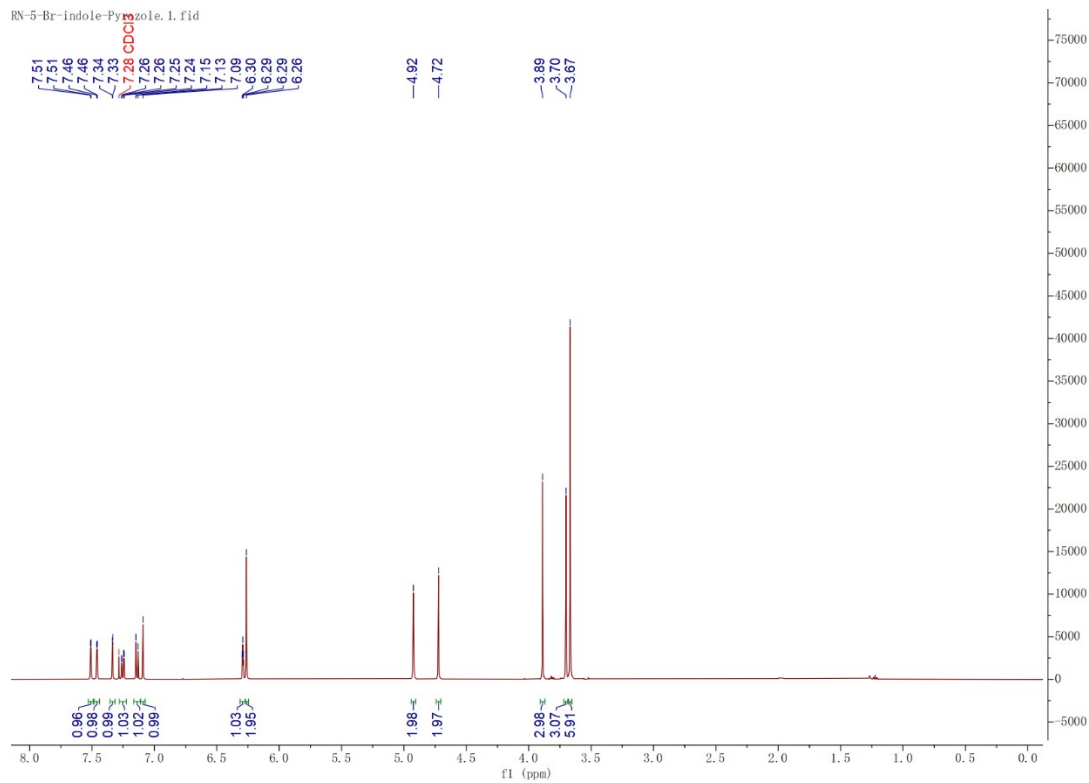


14 #20 RT: 0.20 AV: 1 NL: 2.03E8

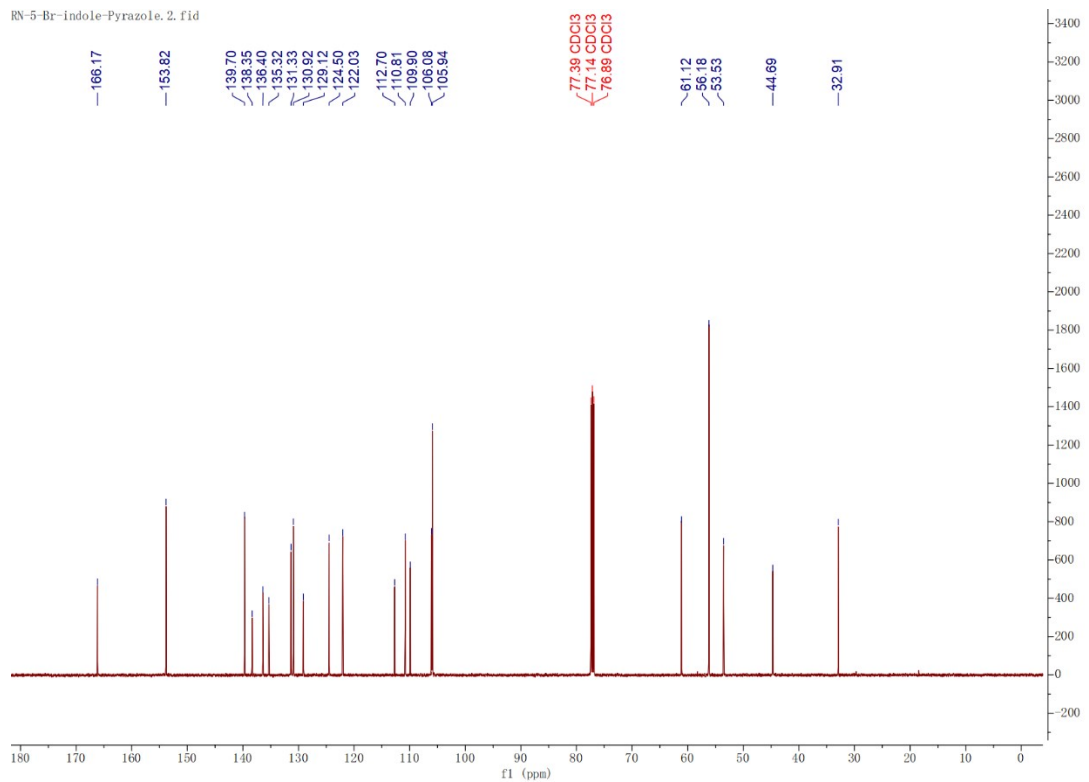
T: FTMS - c APCLcorona Full.ms [60.0000-900.0000]



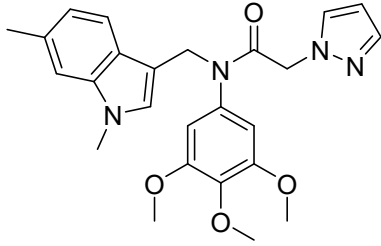
RN-5-Br-indole-Pyrazole. 1. fid



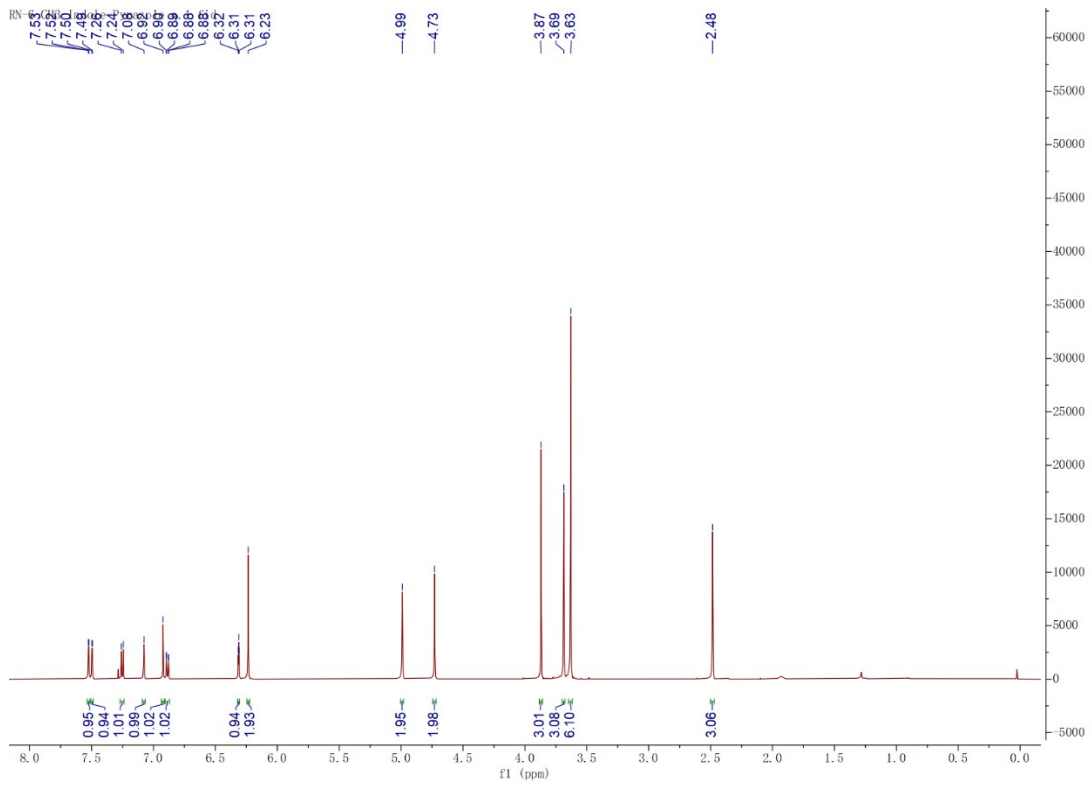
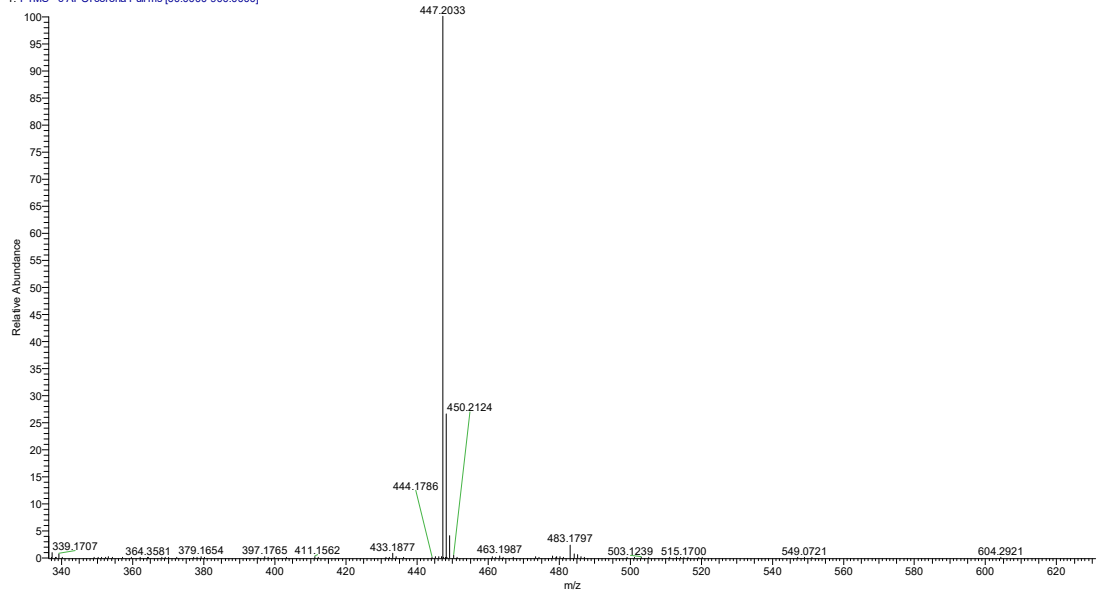
RN-5-Br-indole-Pyrazole. 2. fid



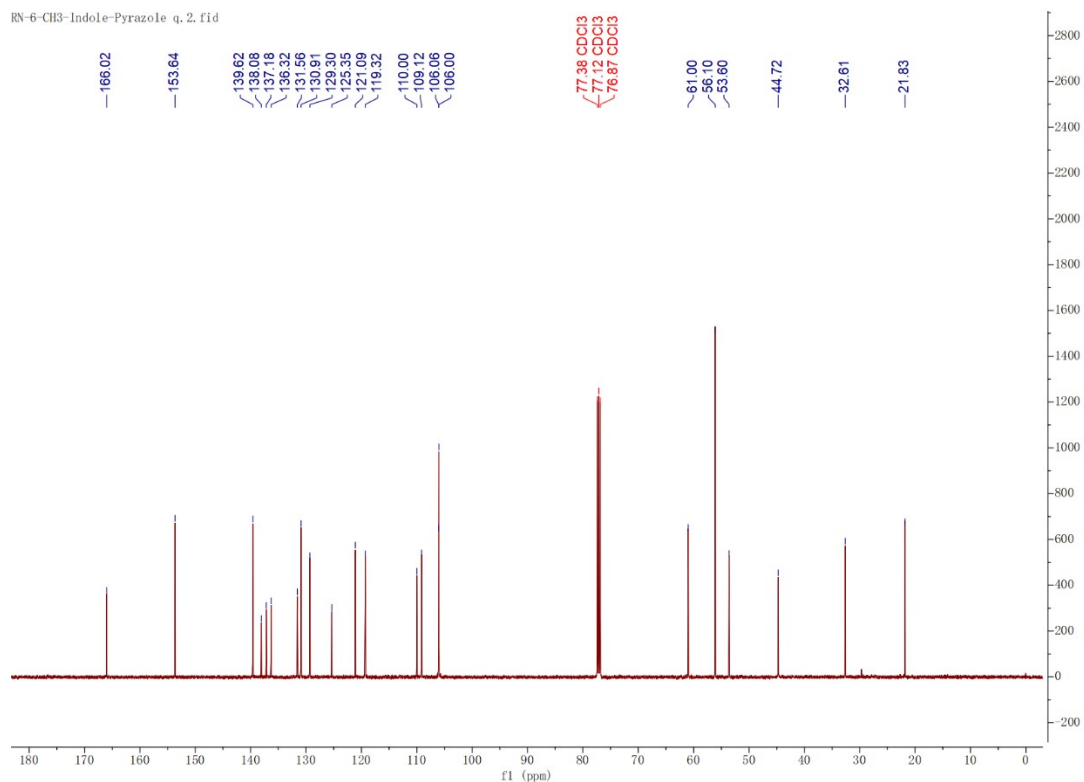
71 :



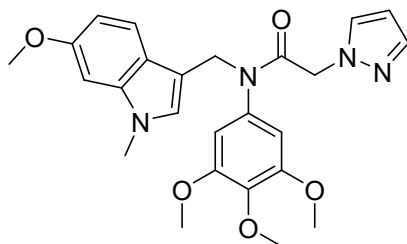
17 #20 RT: 0.20 AV: 1 NL: 1.03E8
 T: FTMS - c APCI corona Full ms [60.0000-900.0000]



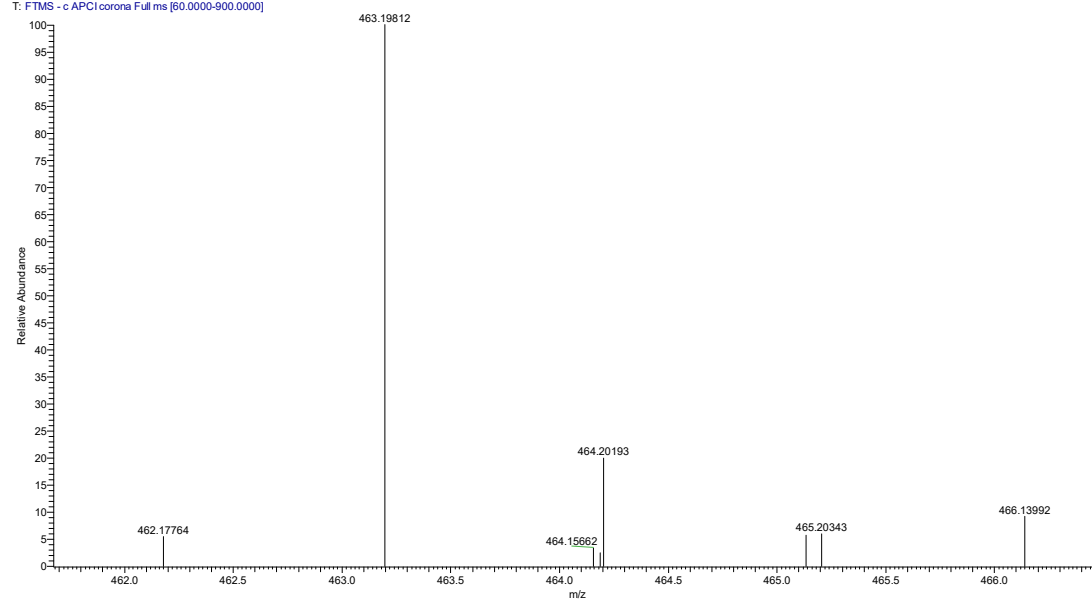
RN-6-CH3-Indole-Pyrazole q.2.fid



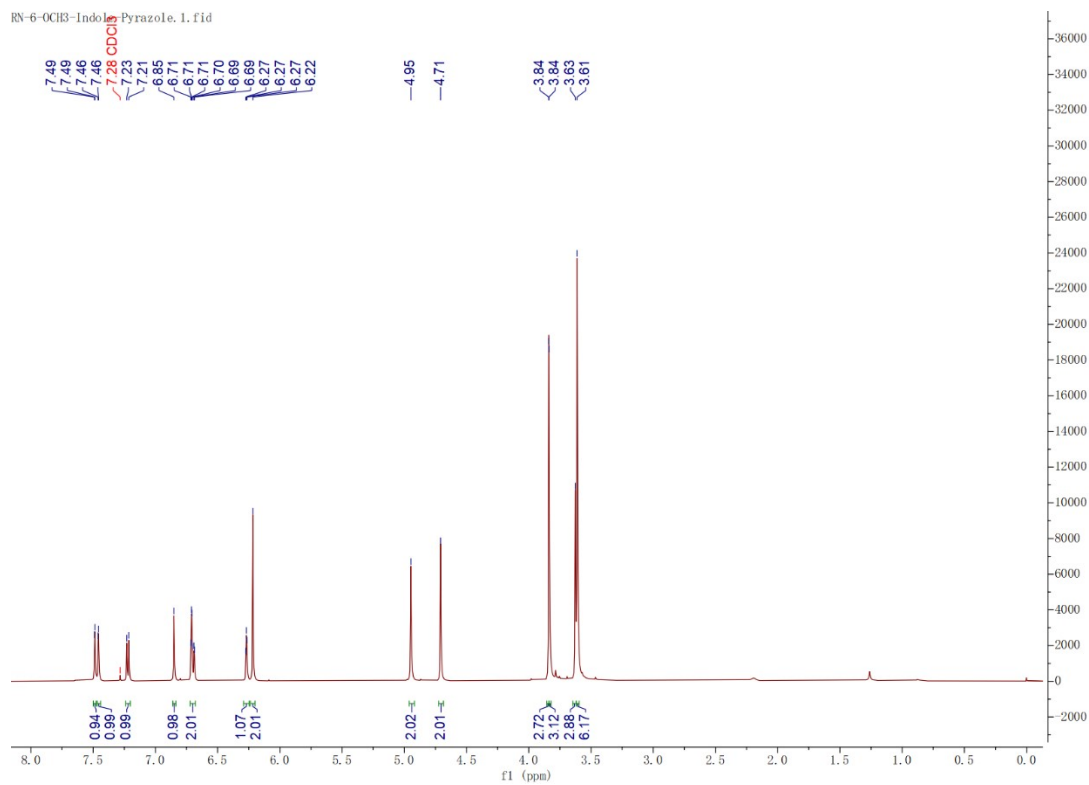
7m :



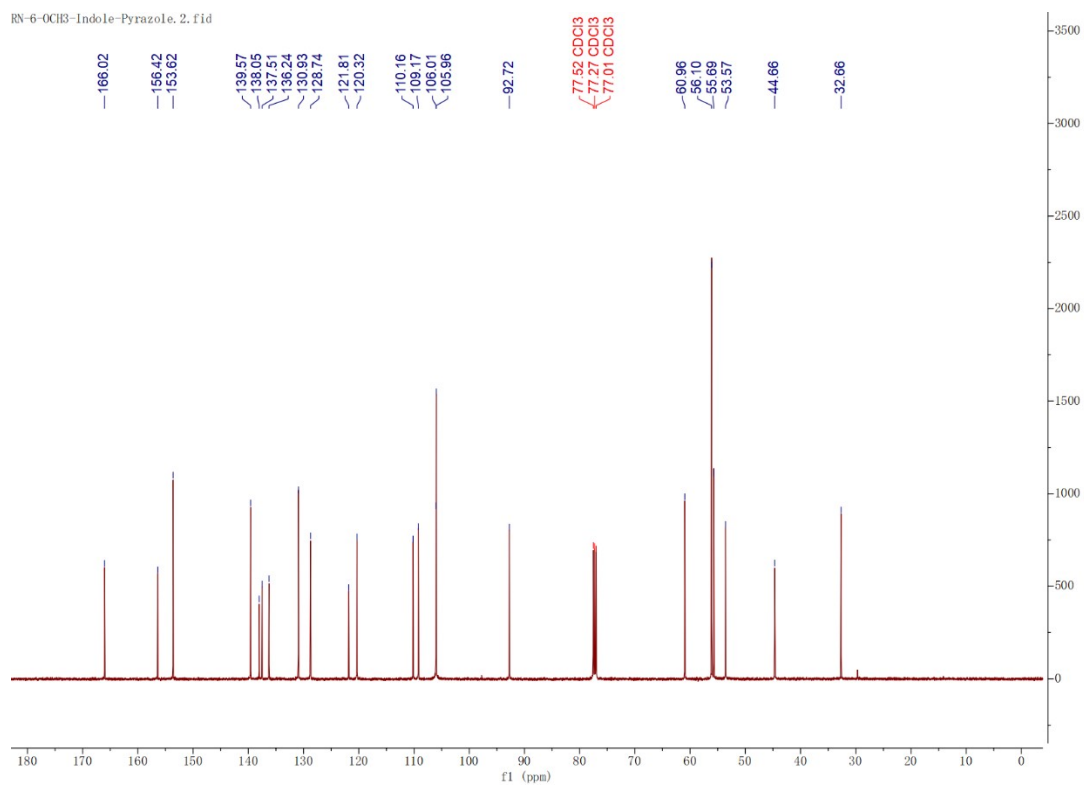
20 #18 RT: 0.19 AV: 1 NL: 9.73E4
T: FTMS - c APCI corona Full ms [60.0000-900.0000]



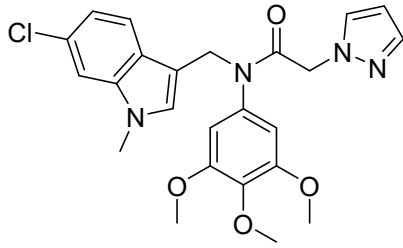
RN-6-OCH3-Indole-Pyrazole.1.fid



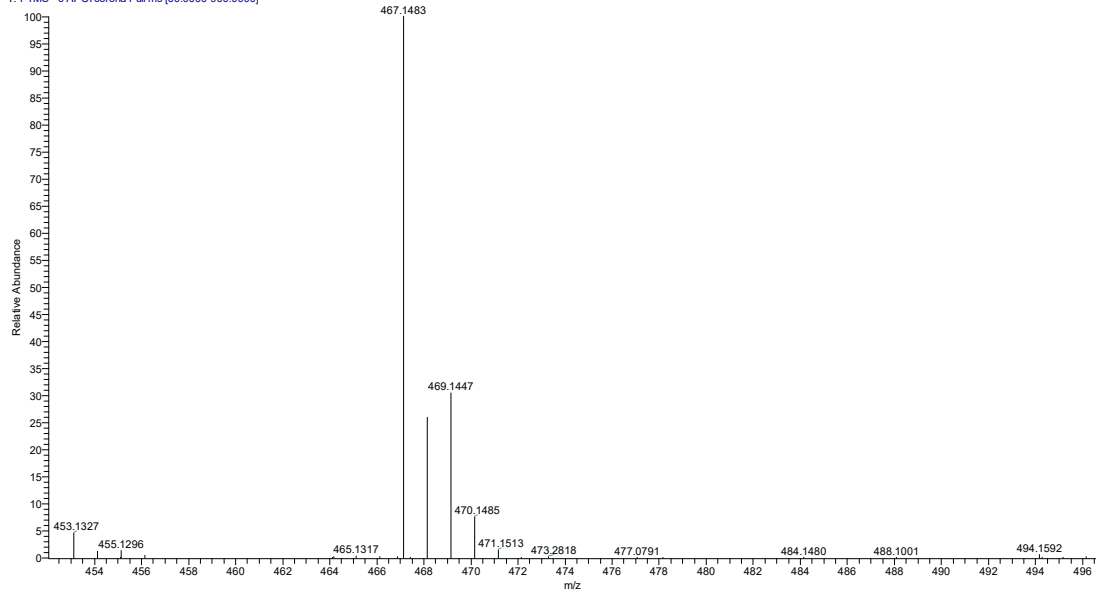
RN-6-OCH3-Indole-Pyrazole.2.fid



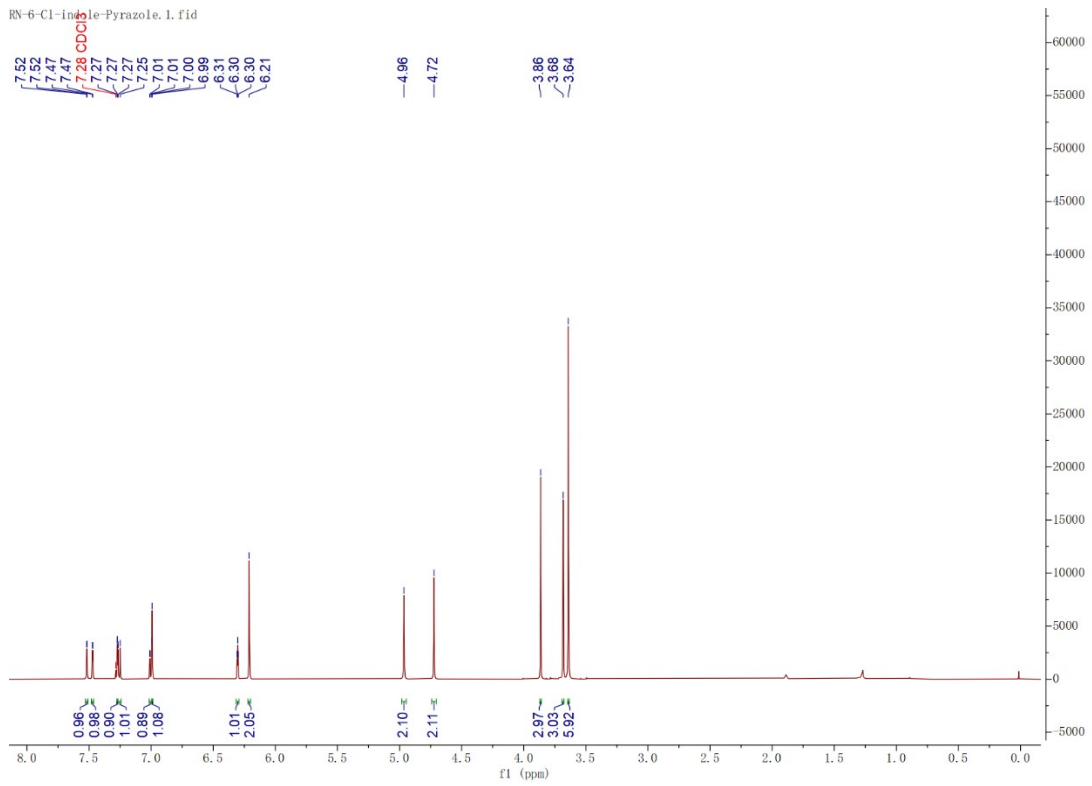
7n :



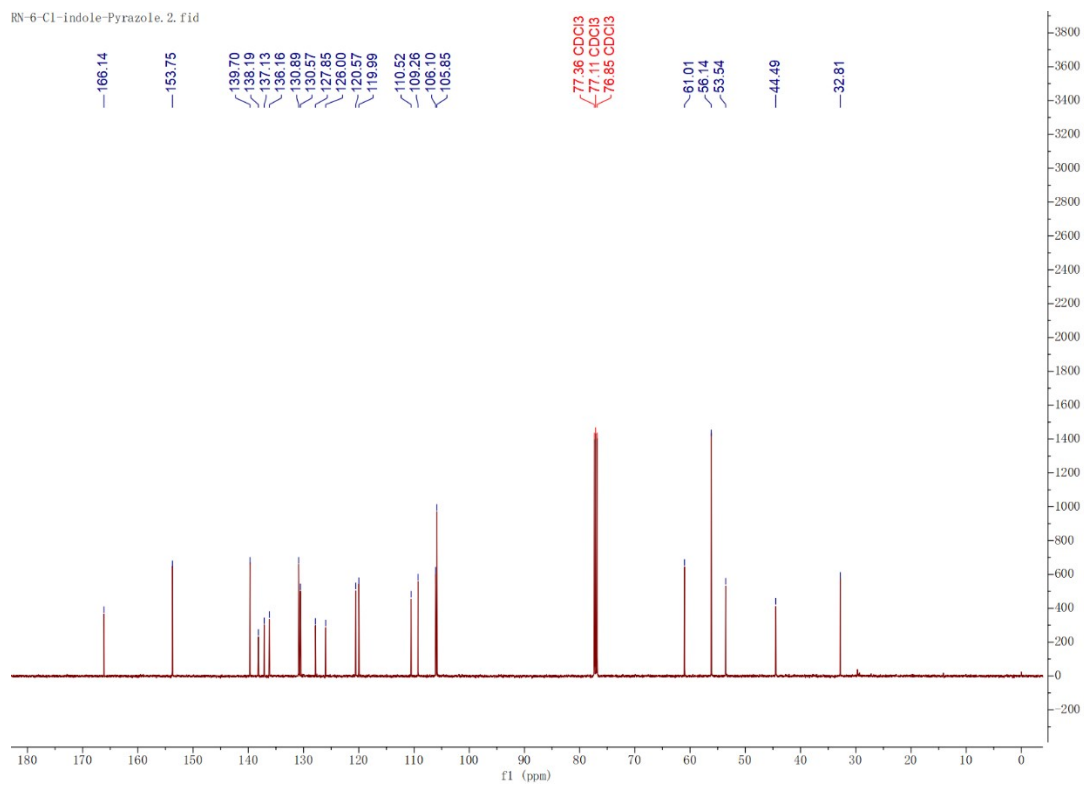
19 #20 RT: 0.20 AV: 1 NL: 2.49E8
 T: FTMS - c APCI corona Full ms [60.0000-900.0000]



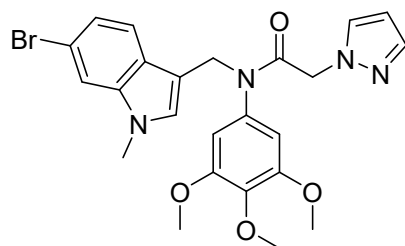
RN-6-Cl-imidazole-Pyrazole. 1. fid



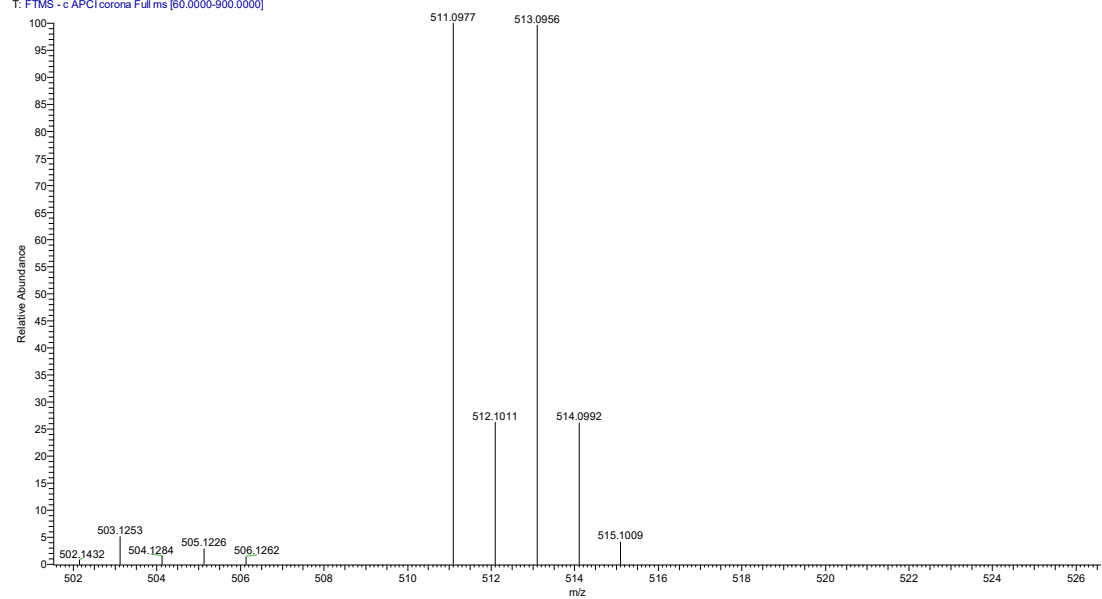
RN-6-Cl-indole-Pyrazole. 2. fid



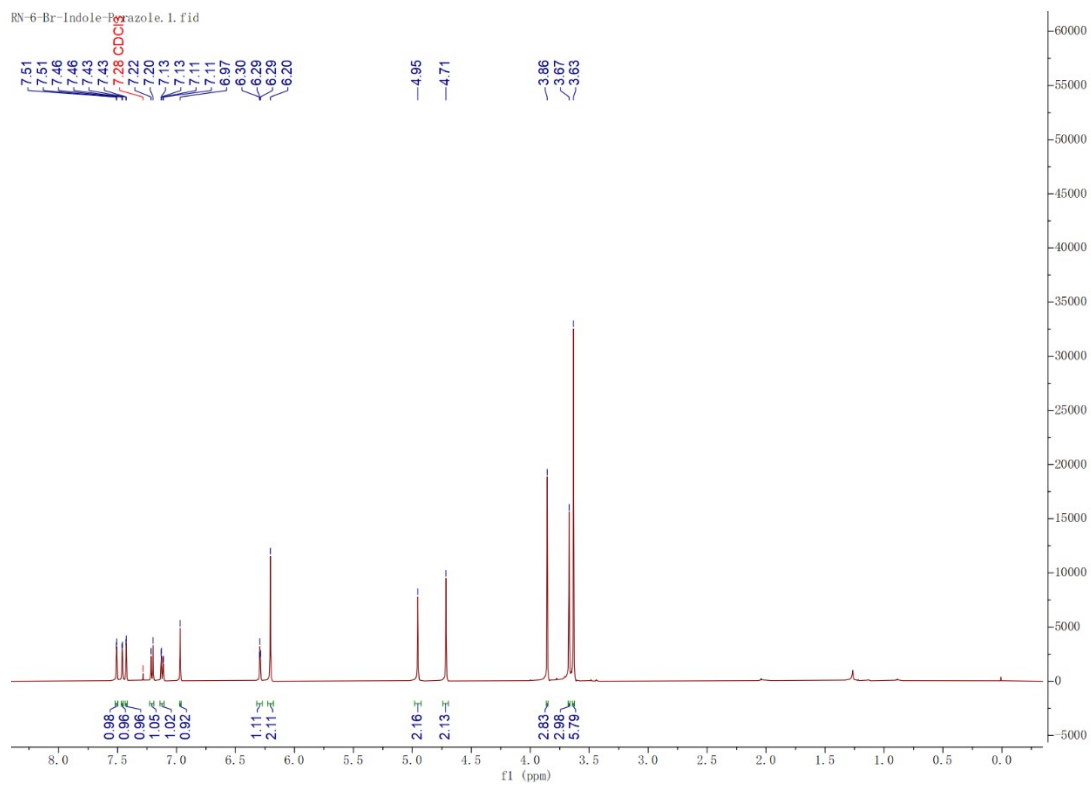
7o :



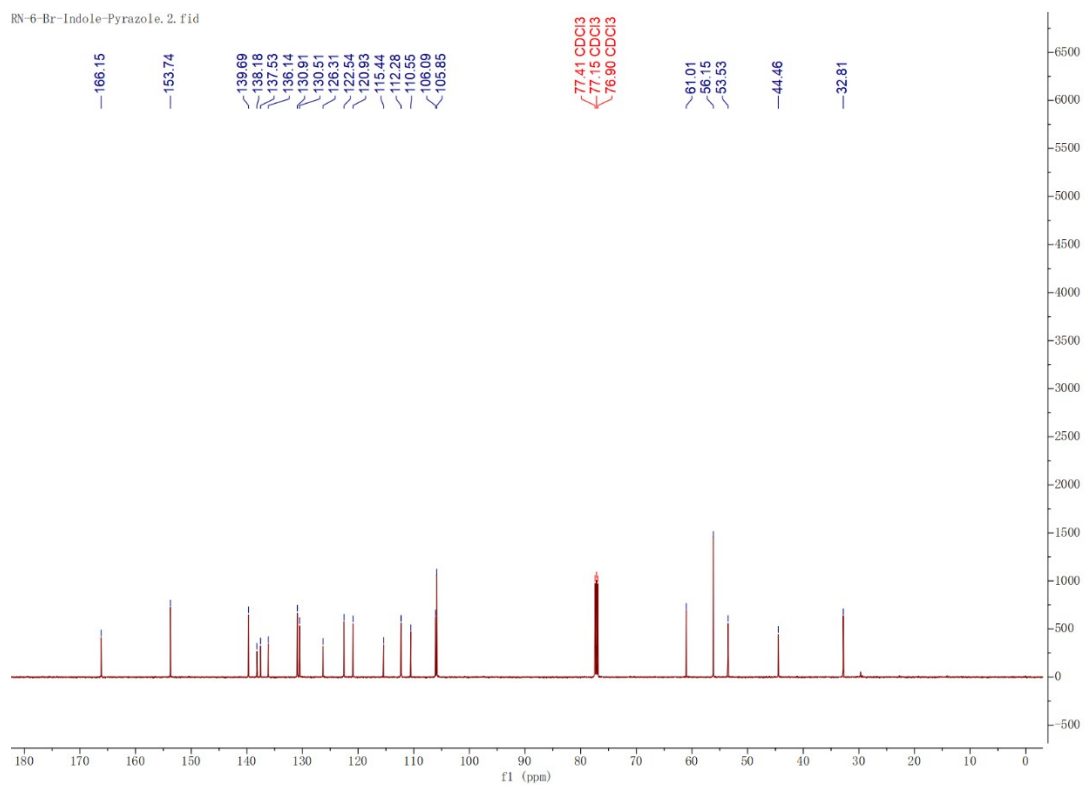
18 #16 RT: 0.16 AV: 1 NL: 8.84E7
T: FTMS - c APCI corona Full ms [60.0000-900.0000]



RN-6-Br-Indole-Pyrazole. 1. fid

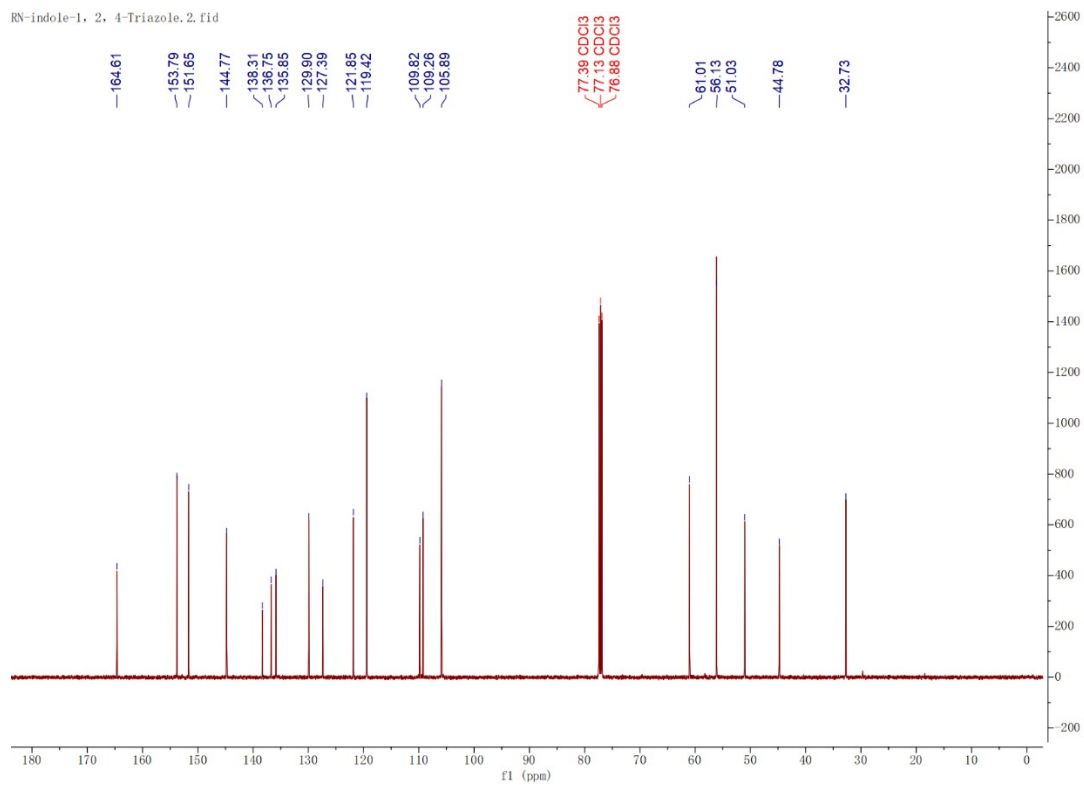


RN-6-Br-Indole-Pyrazole. 2. fid

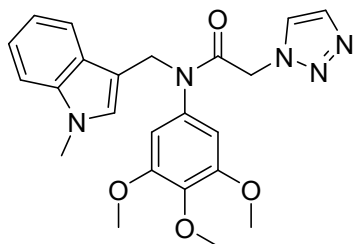


7p :

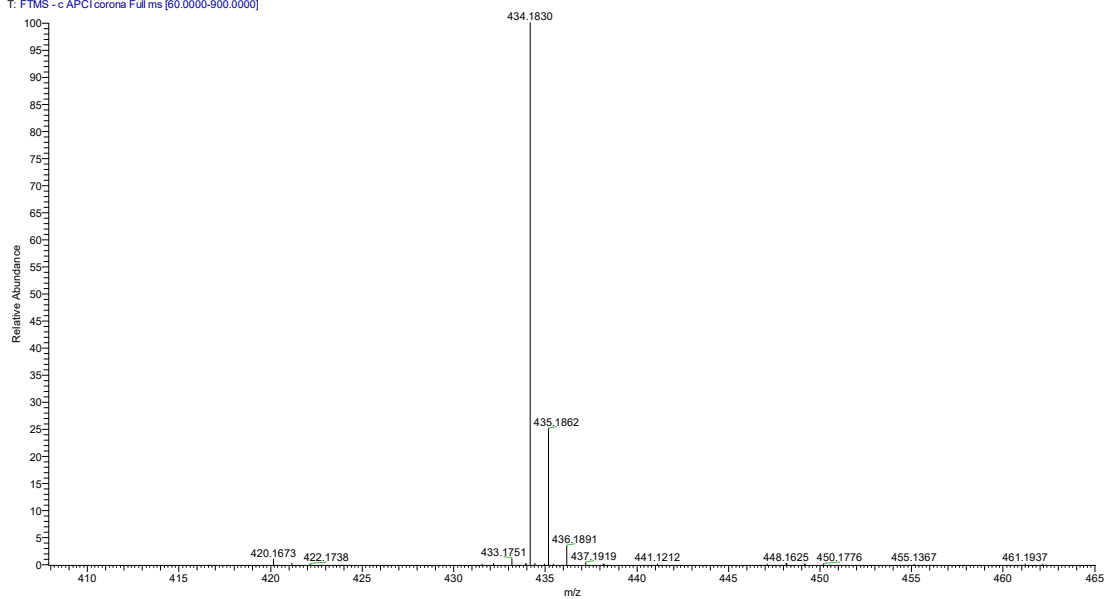
RN-indole-1, 2, 4-Triazole.2.fid

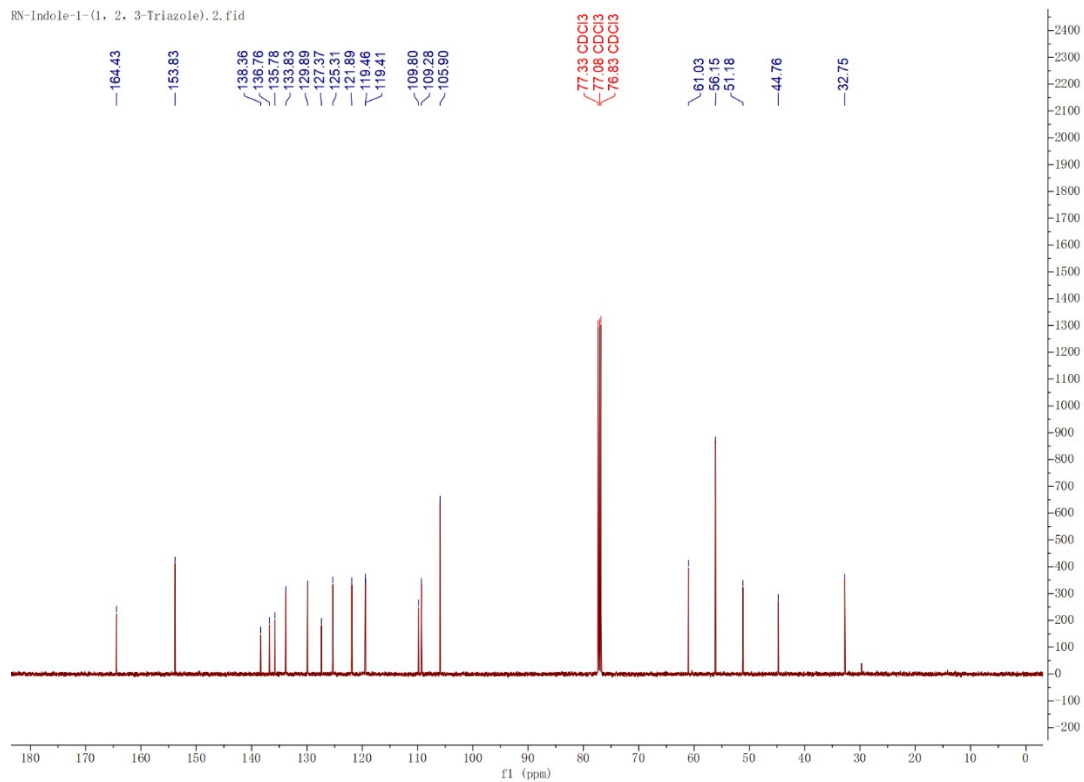
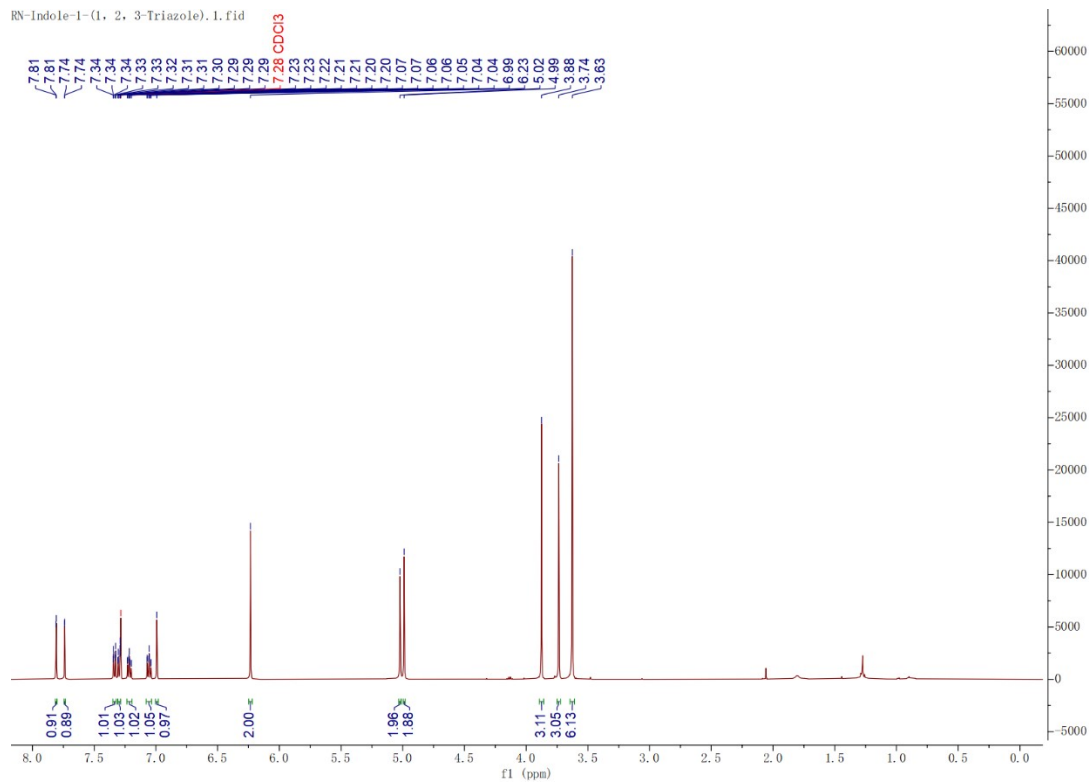


7q :

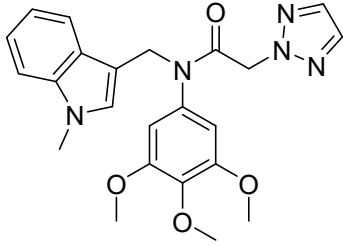


1 #20 RT: 0.20 AV: 1 NL: 3.43E8
T: FTMS - c APCI corona Full ms [60.0000-900.0000]

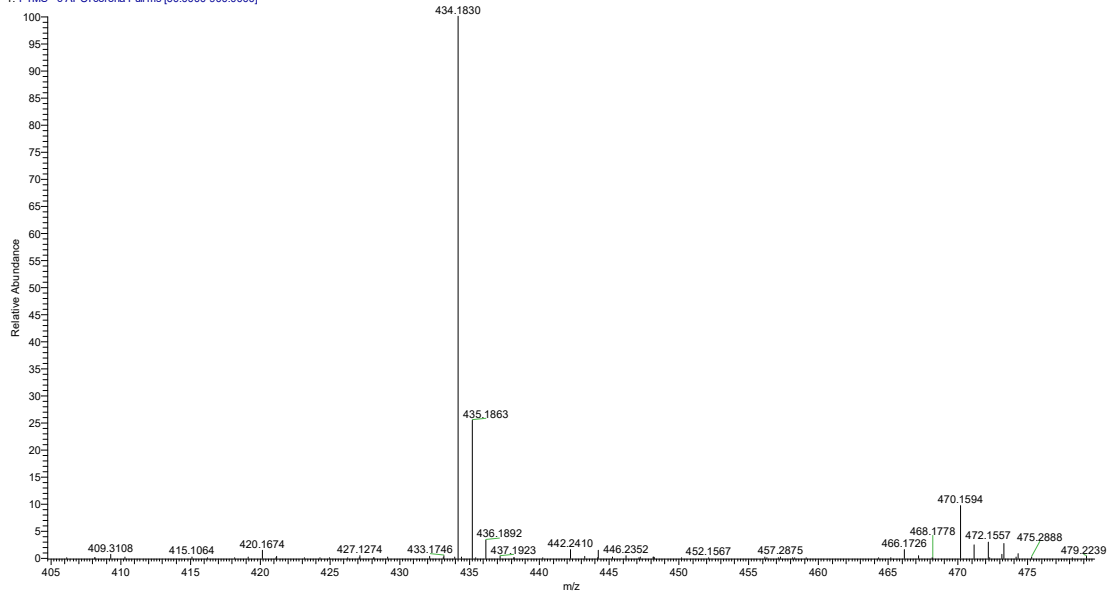




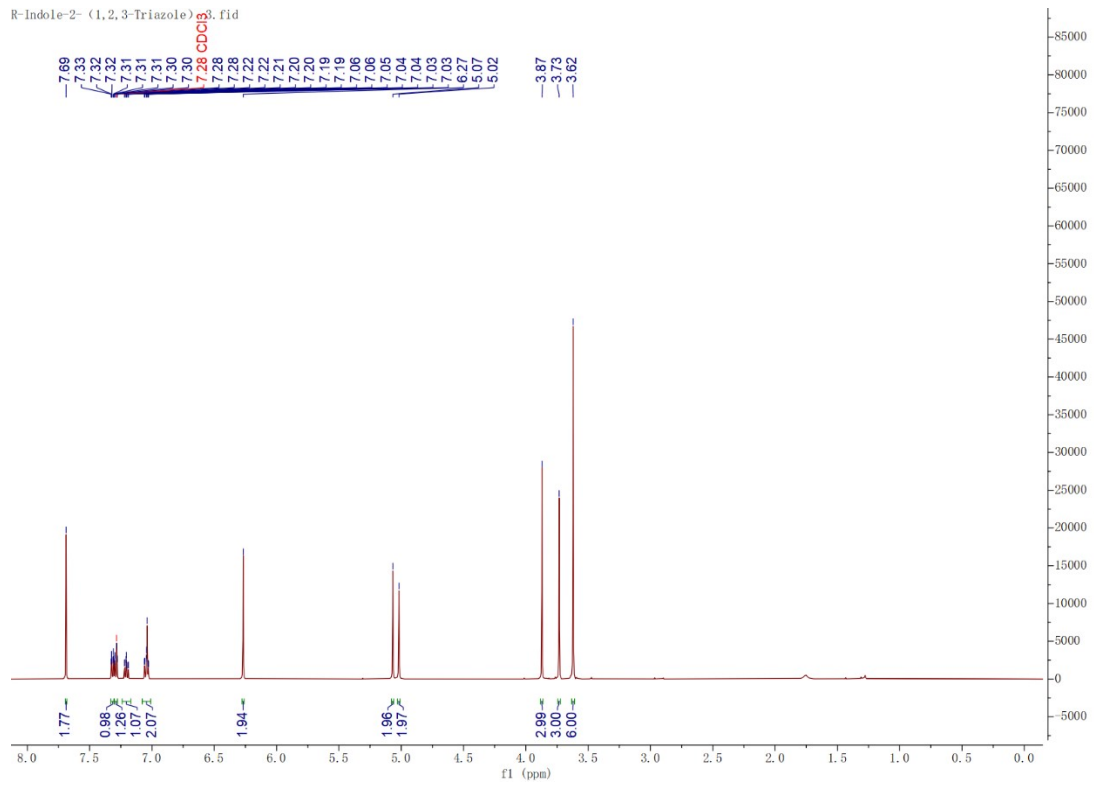
7r :



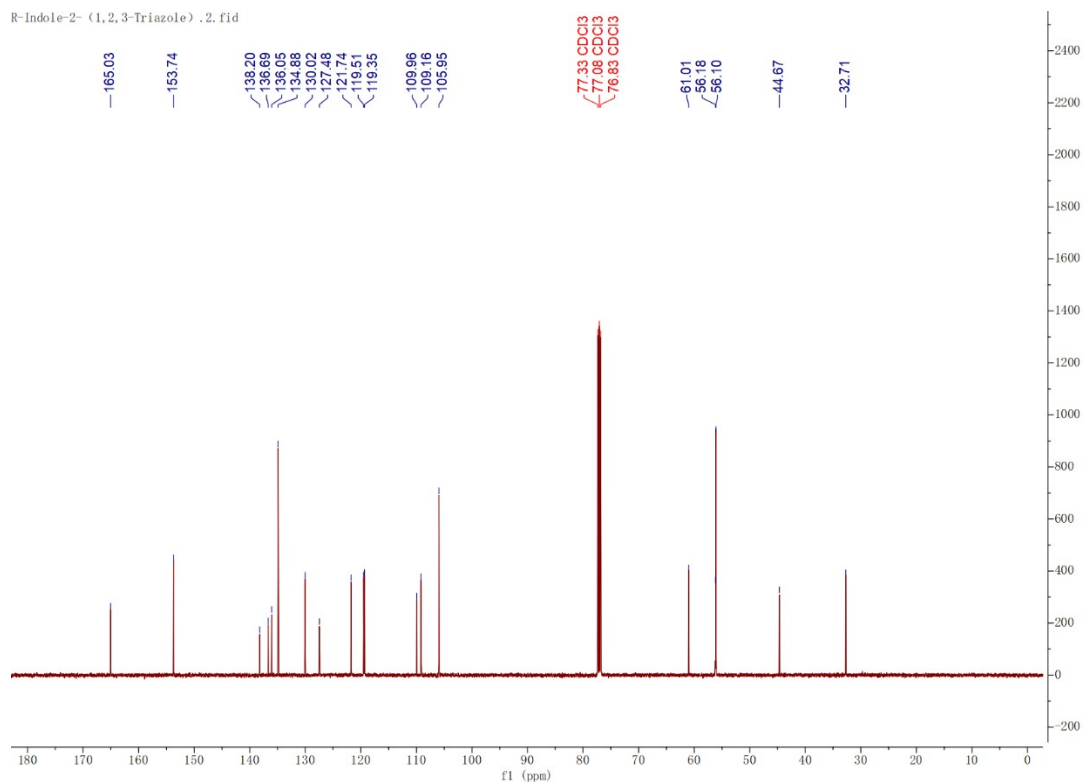
2 #16 RT: 0.16 AV: 1 NL: 2.51E8
T: FTMS - c APCI corona Full ms [60.0000-900.0000]



R-Indole-2-(1,2,3-Triazole)3.fid



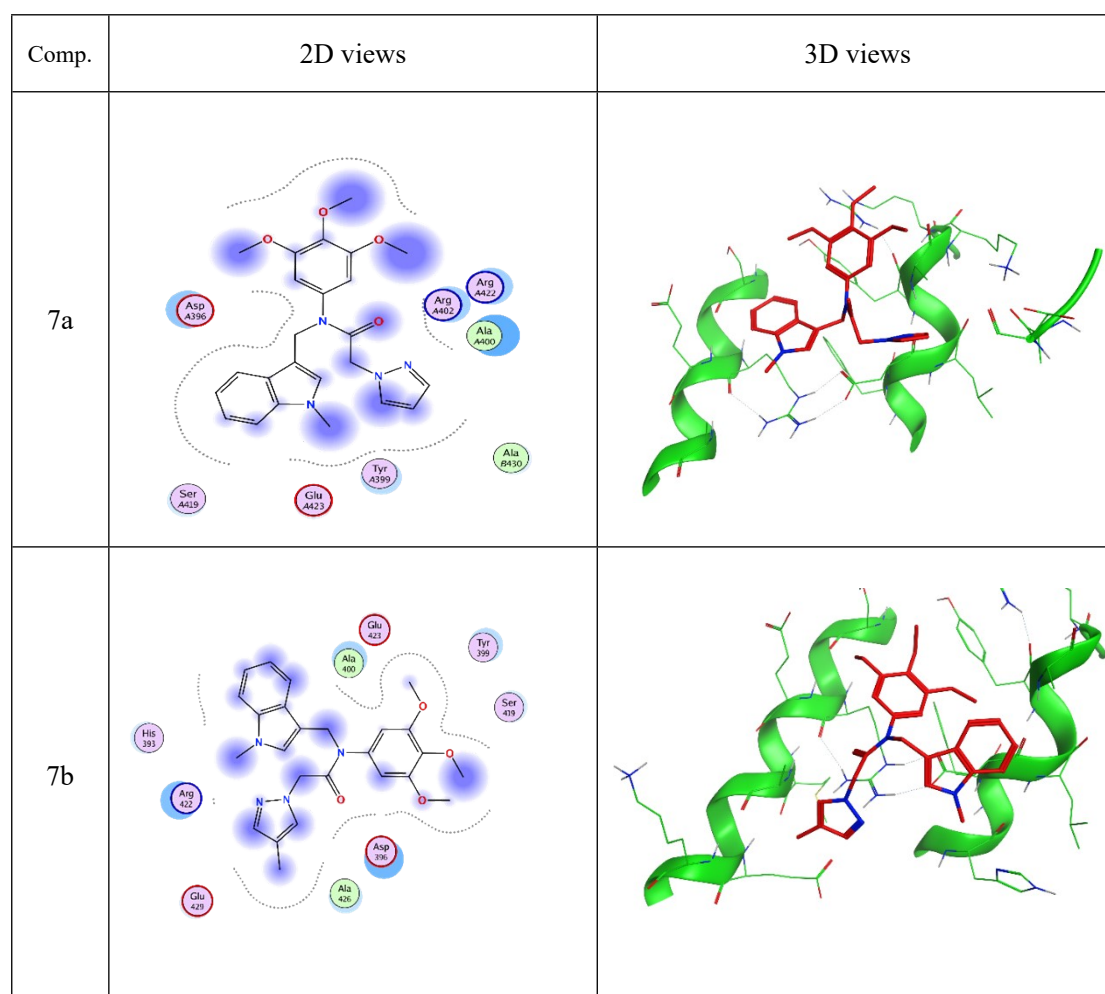
R-Indole-2- (1,2,3-Triazole) .2. fid

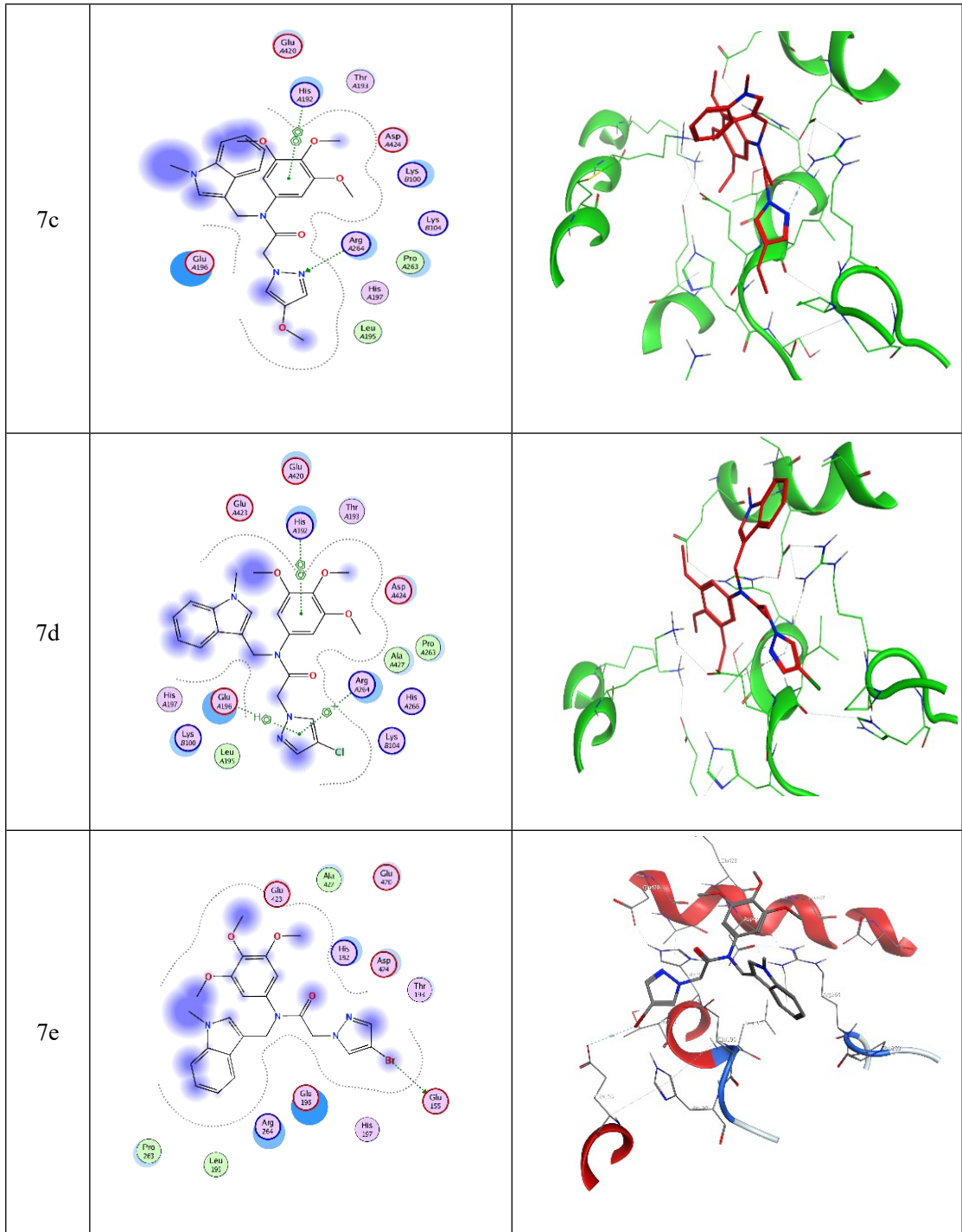


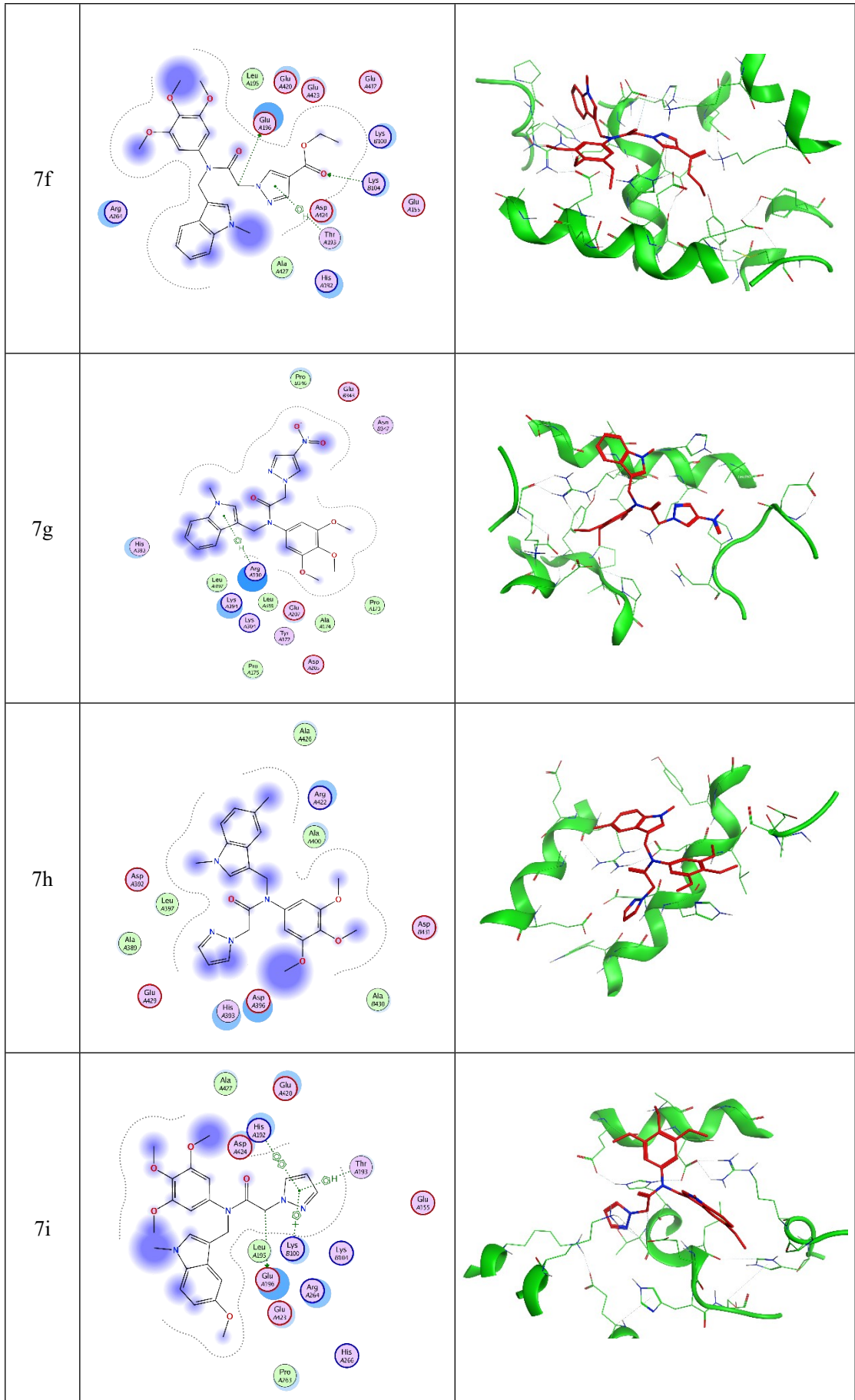
Molecular docking study of 7a-7r

Compounds	S- score (kcal/m ol)	Interactions	Amino acids involved	Atoms/fragment involved in ligand
7a	-5.90	-	-	-
7b	-6.08	-	-	-
7c	-6.74	H-acceptor, pi-pi	ARG 264, HIS 192	N 29, 6-ring
7d	-7.16	pi-H, pi-cation, pi-pi	GLU 196 ARG 264 HIS 192	5-ring, 6-ring, 6-ring
7e	-6.64	H-donor	GLU 155	Br 33
7f	-7.36	H-donor, H- acceptor, pi-H	GLU 196, LYS 104, THR 193	C 16, O 34, 5-ring
7g	-6.22	pi-H	ARG 390	5-ring
7h	-6.25	-	-	-
7i	-7.02	H-acceptor, pi-H	GLU 196, THR 193, LYS 100, HIS 192	C 27, 5-ring, 5-ring, 5-ring

7j	-6.95	pi-cation, pi-pi	ARG 264, HIS 100	5-ring, 6-ring
7k	-6.57	pi-cation, pi-pi	THR 193, ARG 264	5-ring, 6-ring
7l	-5.75	pi-H	LYS 304	5-ring
7m	-6.77	H-acceptor, pi-H, pi-cation	LYS 394, ARG 390	O 14, 5-ring
7n	-6.78	H-donor	ASP 199	Cl 33
7o	-6.53	pi-H, pi-H	GLU 196, LYS 100	5-ring, 6-ring
7p	-5.71	-	-	-
7q	-5.71	-	-	-
7r	-5.8294	-	-	-







7j		
7k		
7l		
7m		

