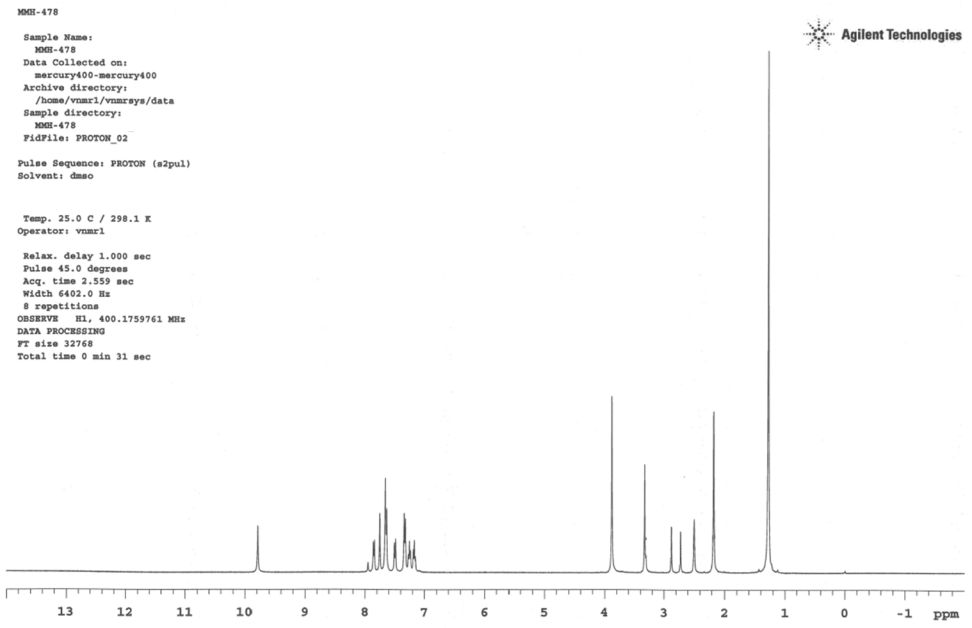
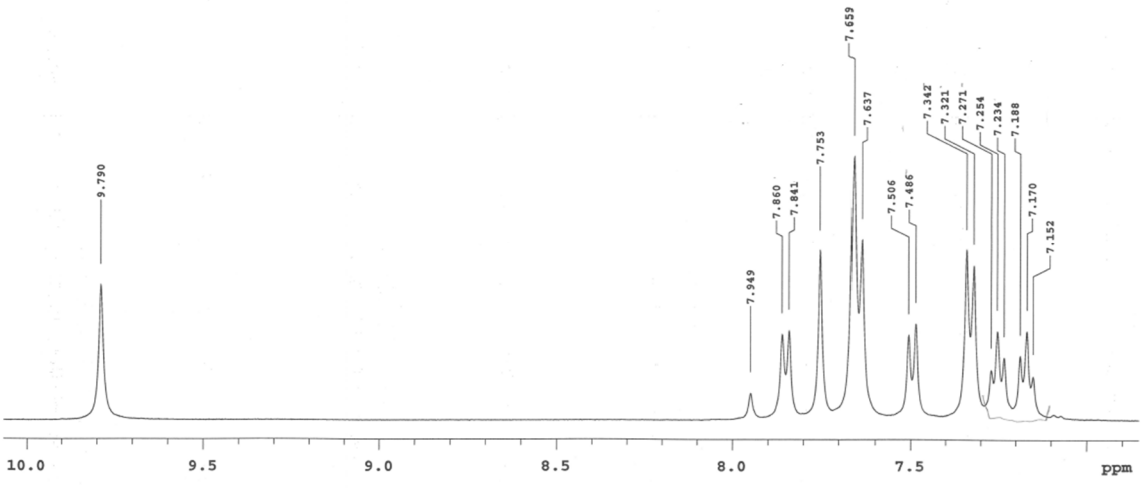
Enzyme-Targeted Antiproliferative Effects of Novel Indole–Acrylamide Xenobiotics Acting on Cyclooxygenase Pathways

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(S.N.B.)

Figure S1(a):NMR spectrum of (E)-N-(4-(tert-butyl)phenyl)-2-methyl-3-(1-methyl-1H-indol-3-yl)acrylamide, 6a





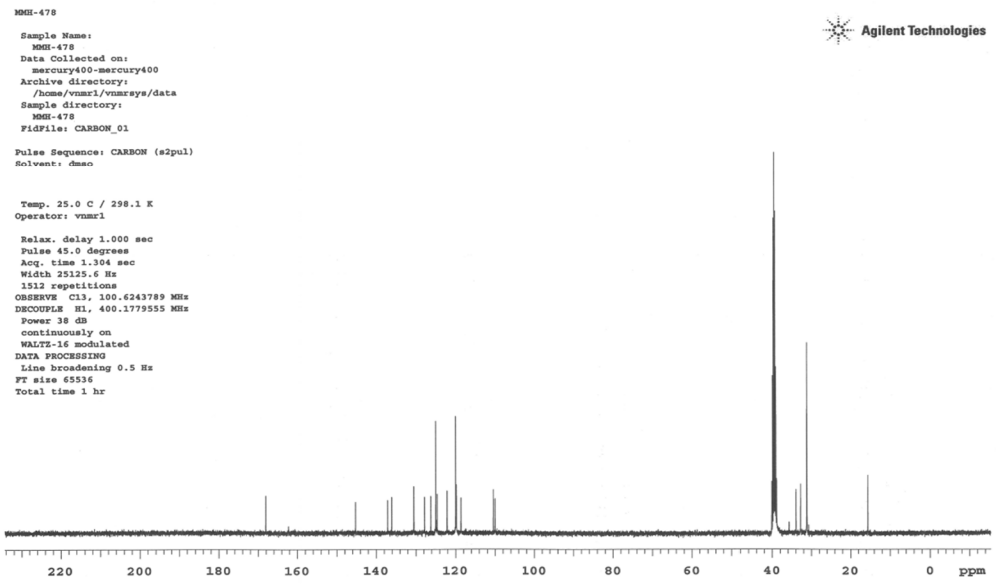
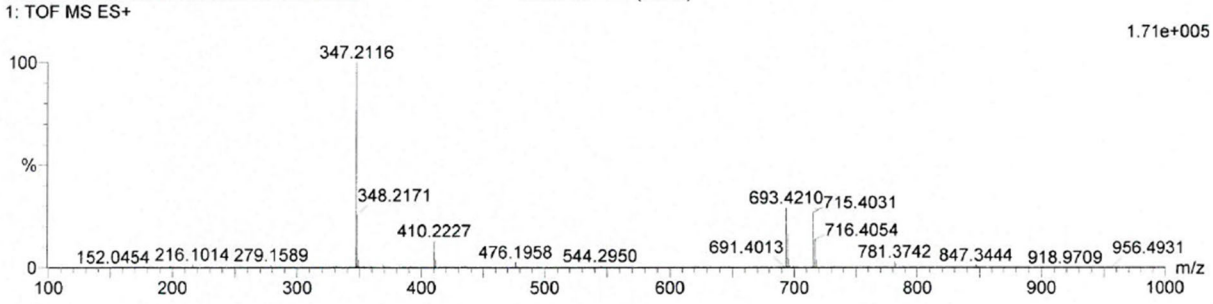


Figure S1(b): HRMS spectrum of (E)-N-(4-(tert-butyl)phenyl)-2-methyl-3-(1-methyl-1H-indol-3-yl)acrylamide, 6a

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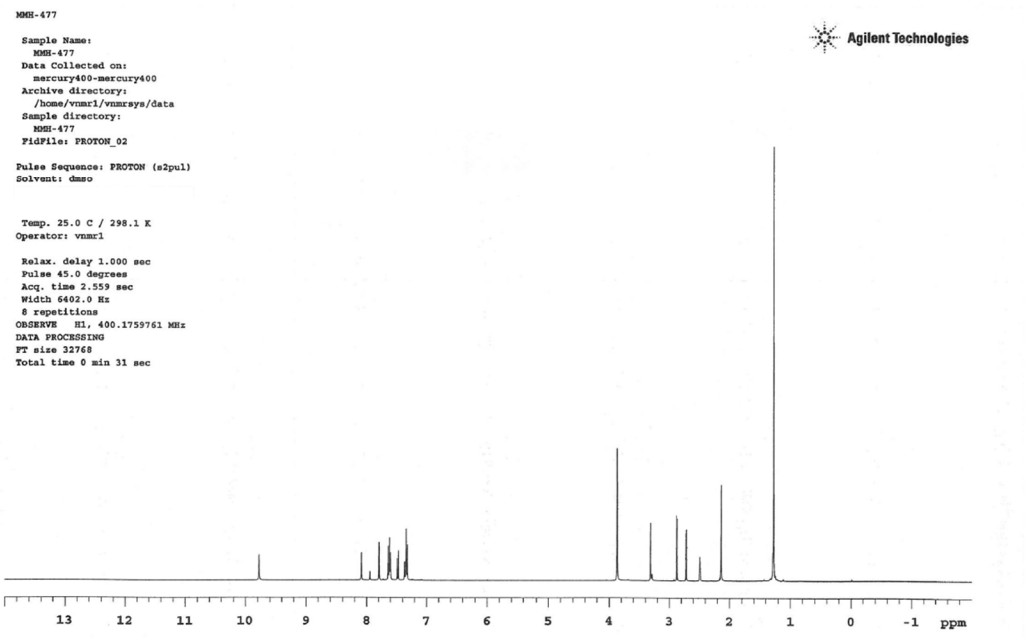
Single Mass Analysis
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Element prediction: Off
Number of isotope peaks used for i-FIT = 3

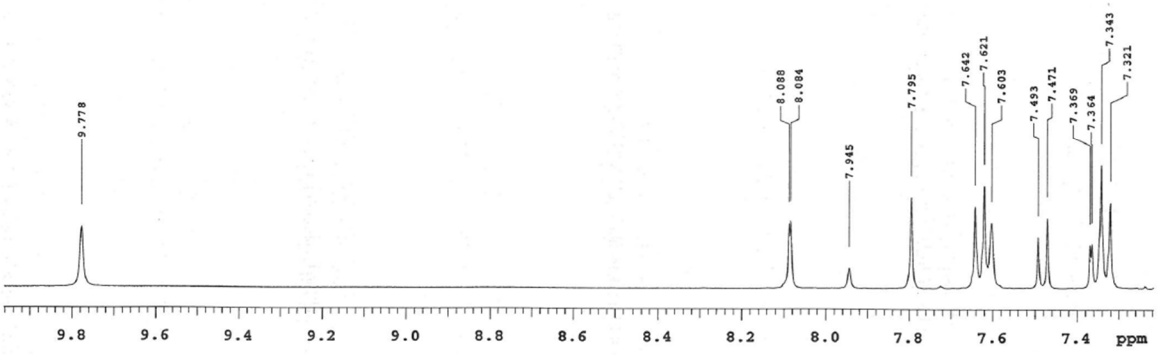
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-24 H: 1-28 N: 1-3 O: 1-2
G.U. Eczacilik Fakultesi Merkez Laboratuvari MMH478 154 (6.023)
1: TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
347.2116	347.2123	-0.7	-2.0	11.5	415.7	0.0	C23 H27 N2 O

Figure S2(a):NMR spectrum of (E)-3-(5-bromo-1-methyl-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6b





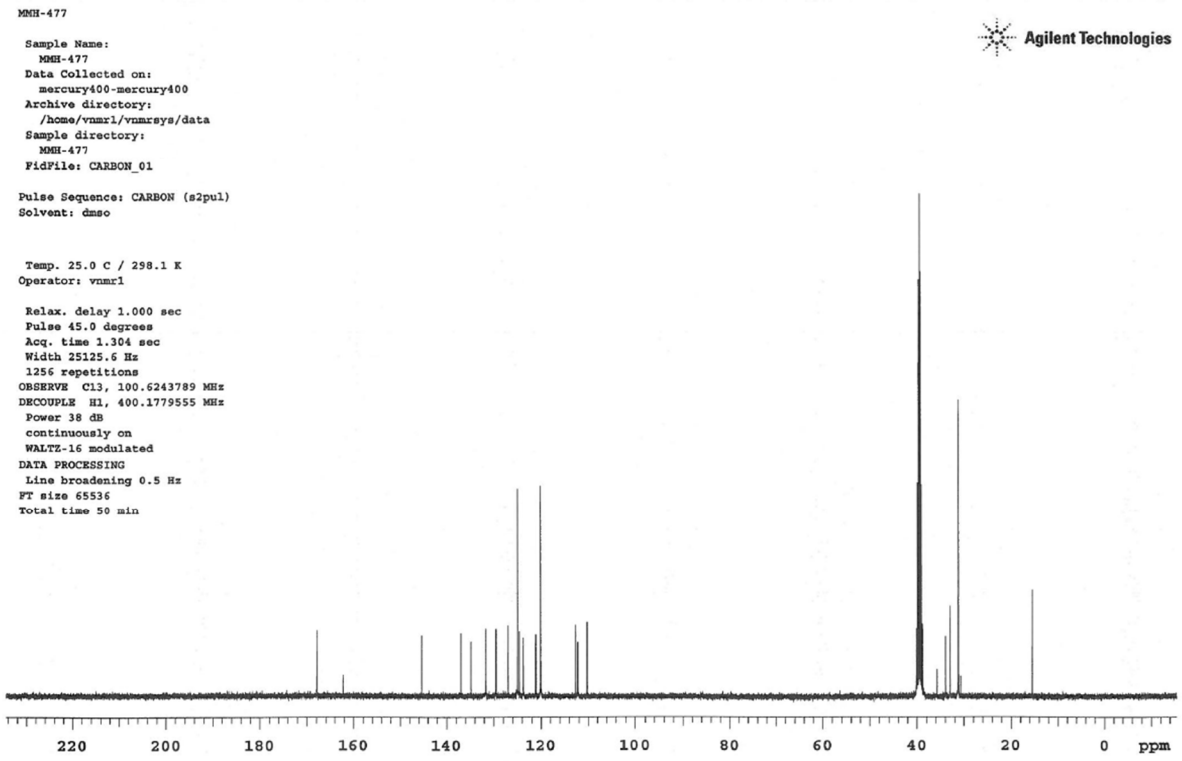


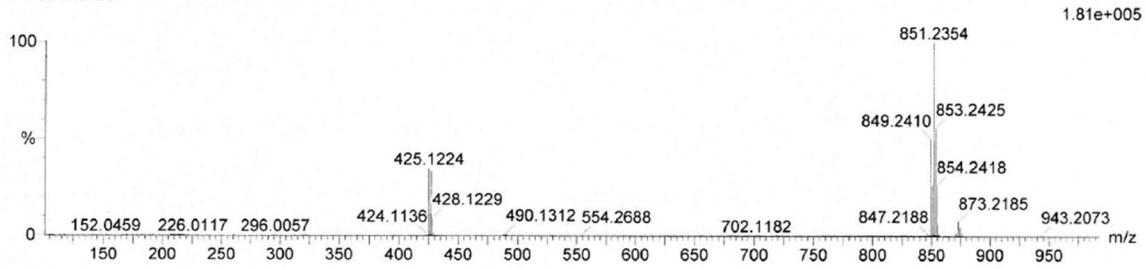
Figure S2(b): HRMS spectrum of (E)-3-(5-bromo-1-methyl-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6b

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Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

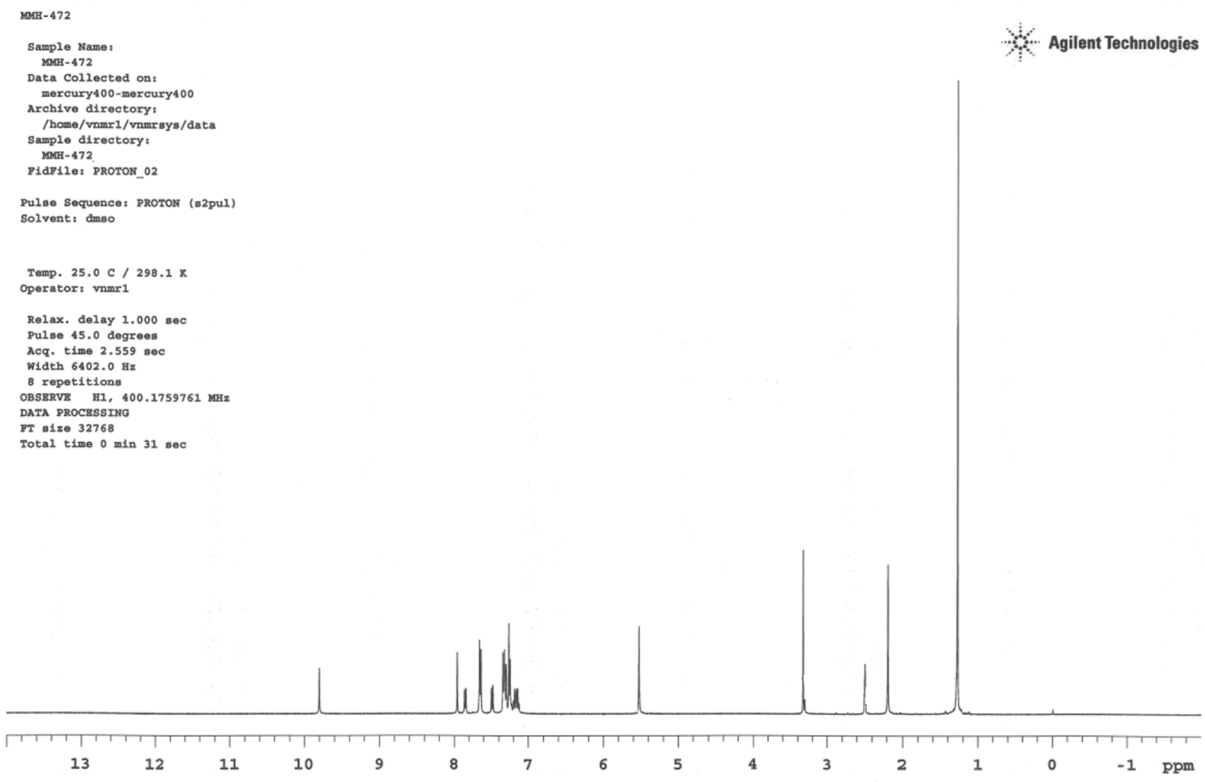
Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-24 H: 1-27 N: 1-3 O: 1-2 Br: 1-1

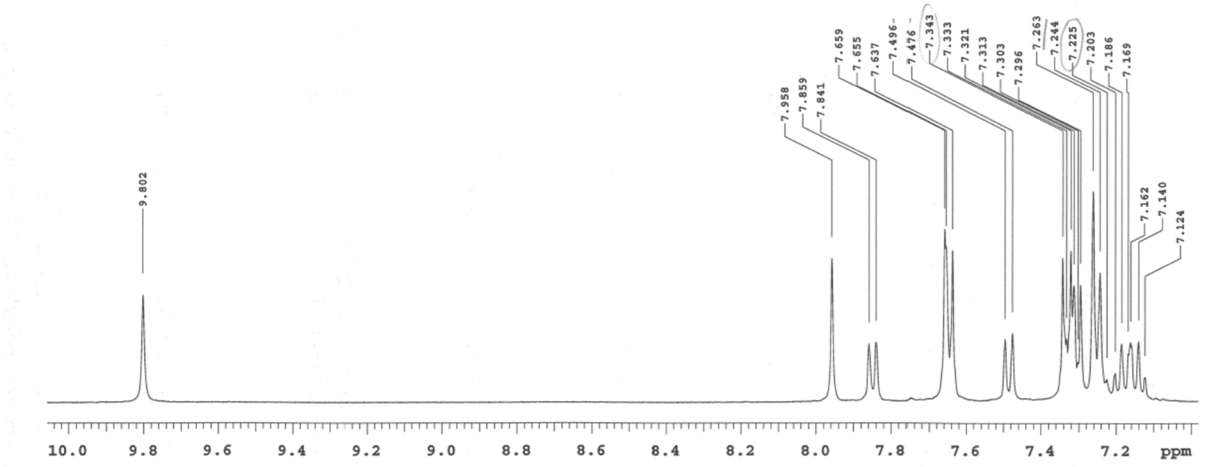
G.U. Eczacilik Fakultesi Merkez Laboratuvari MMH477_SOL 162 (6.337)
1: TOF MS ES+



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
425.1224	425.1228	-0.4	-0.9	11.5	263.7	0.0	C23 H26 N2 O Br

Figure S3(a): NMR spectrum of (E)-3-(1-benzyl-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6c





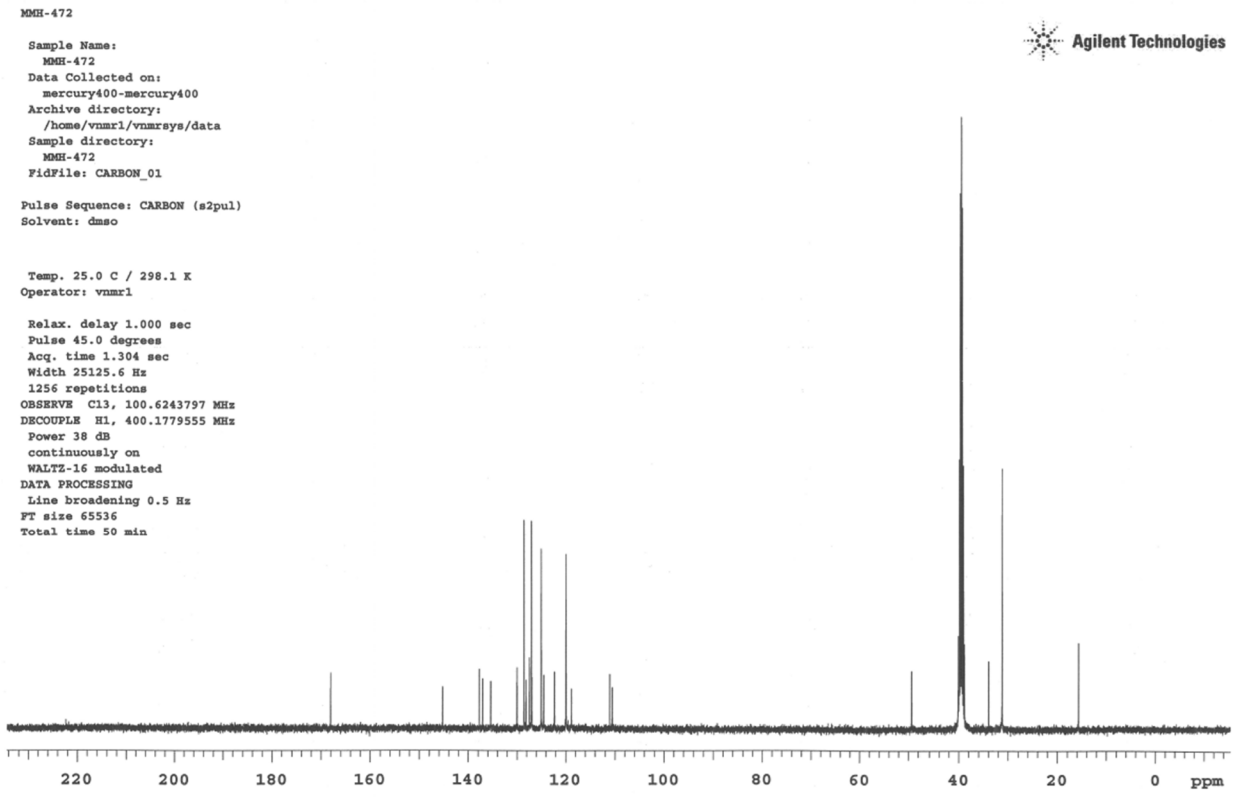


Figure S3(b): HRMS spectrum of (E)-3-(1-benzyl-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6c

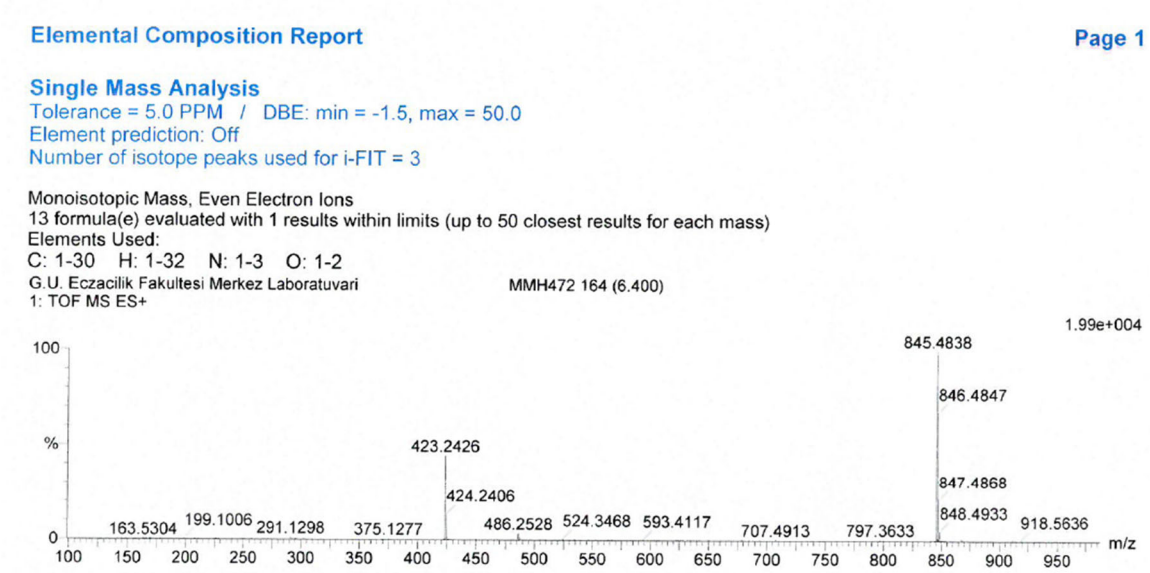
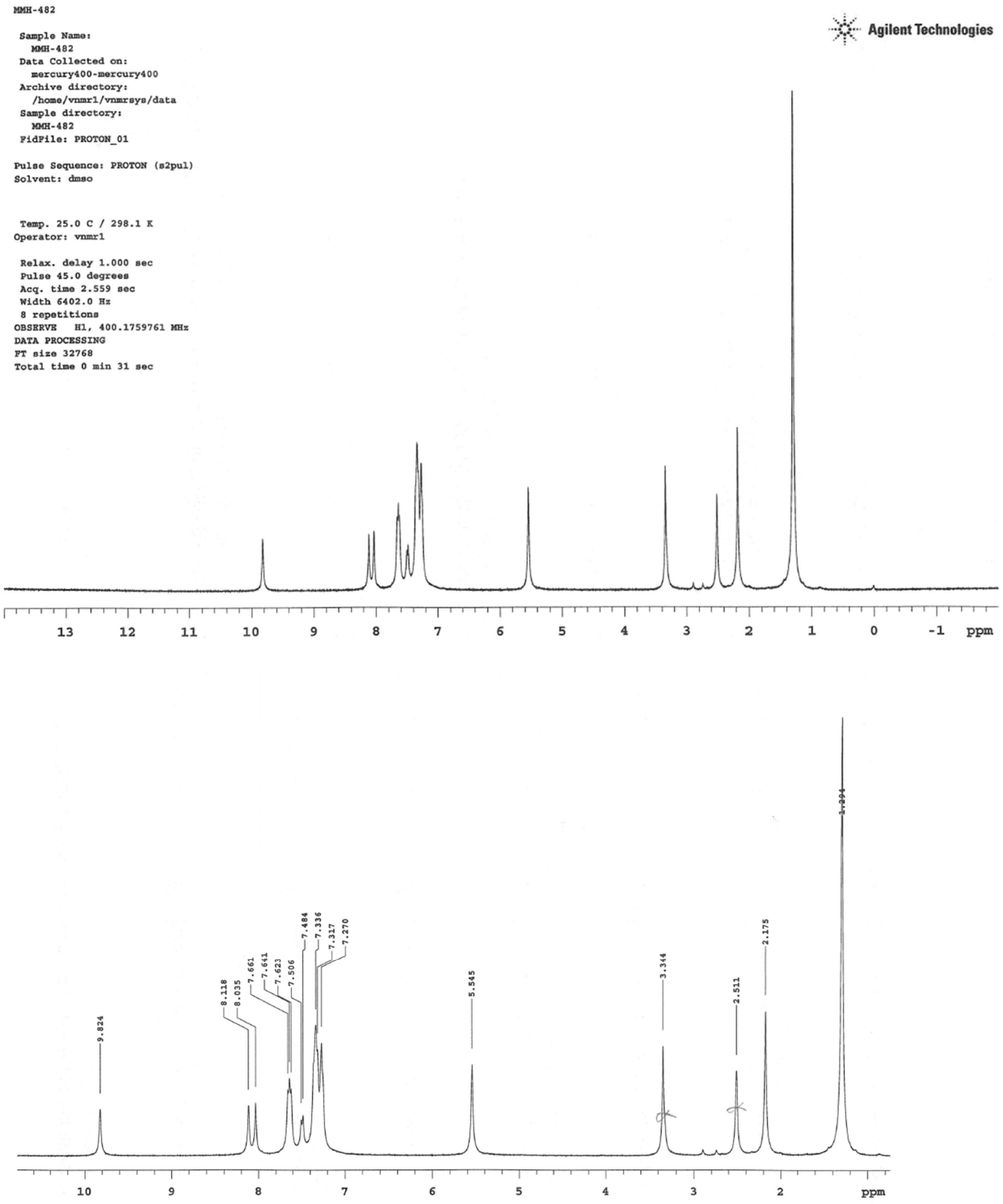


Figure S4(a): NMR spectrum of (E)-3-(1-benzyl-5-bromo-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6d



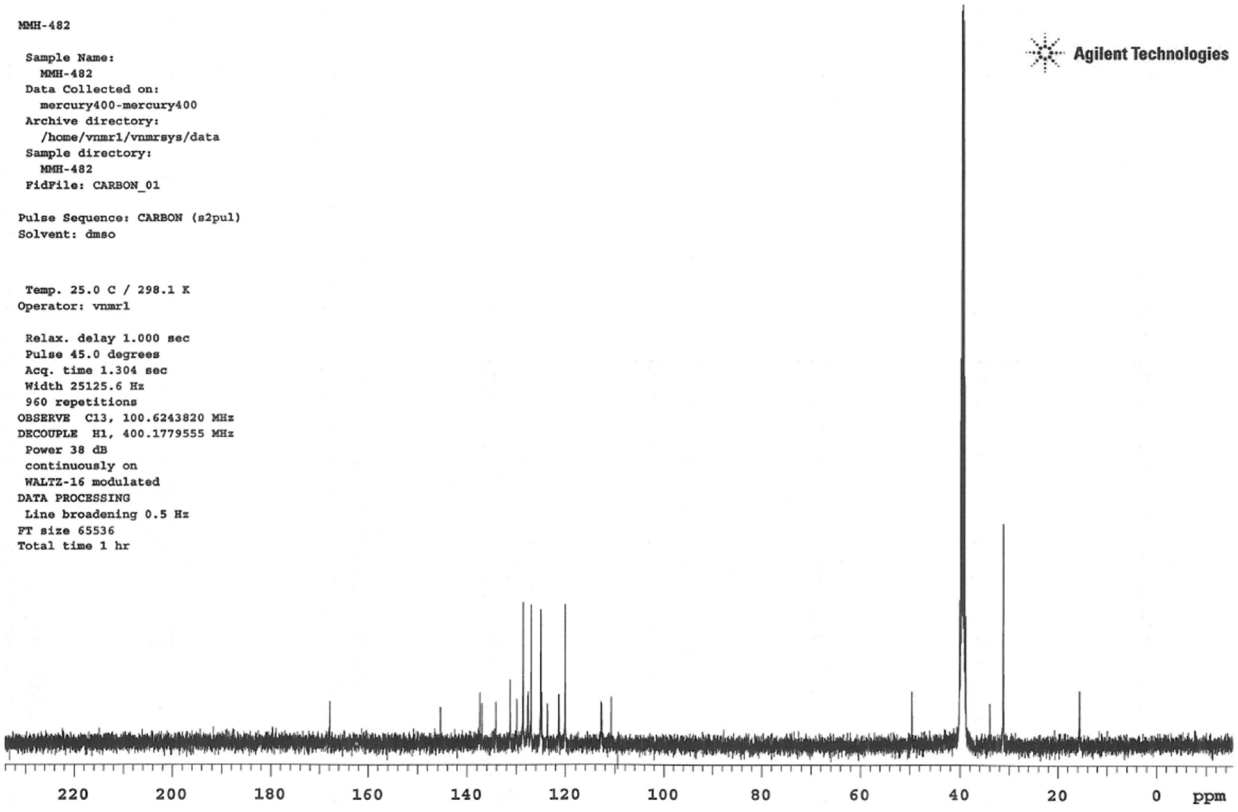


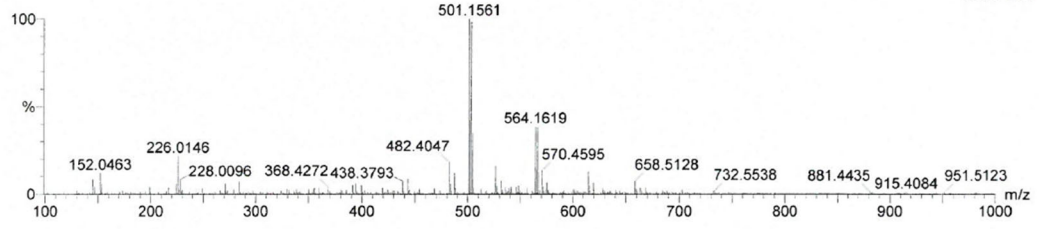
Figure S4(b):HRMS spectrum of (E)-3-(1-benzyl-5-bromo-1H-indol-3-yl)-N-(4-(tert-butyl)phenyl)-2-methylacrylamide, 6d

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 1-30 H: 1-31 N: 1-3 O: 1-2 Br: 1-1

G.U. Eczacilik Fakultesi Merkez Laboratuvari MMH482 184 (7.198)
1: TOF MS ES+
6.09e+003



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
501.1561	501.1541	2.0	4.0	15.5	45.3	0.0	C29 H30 N2 O Br