Supplementary material

Structure-activity relationships reveal a 2-furoyloxychalcone as a potent cytotoxic and apoptosis inducer for human U-937 and HL-60 leukaemia cells

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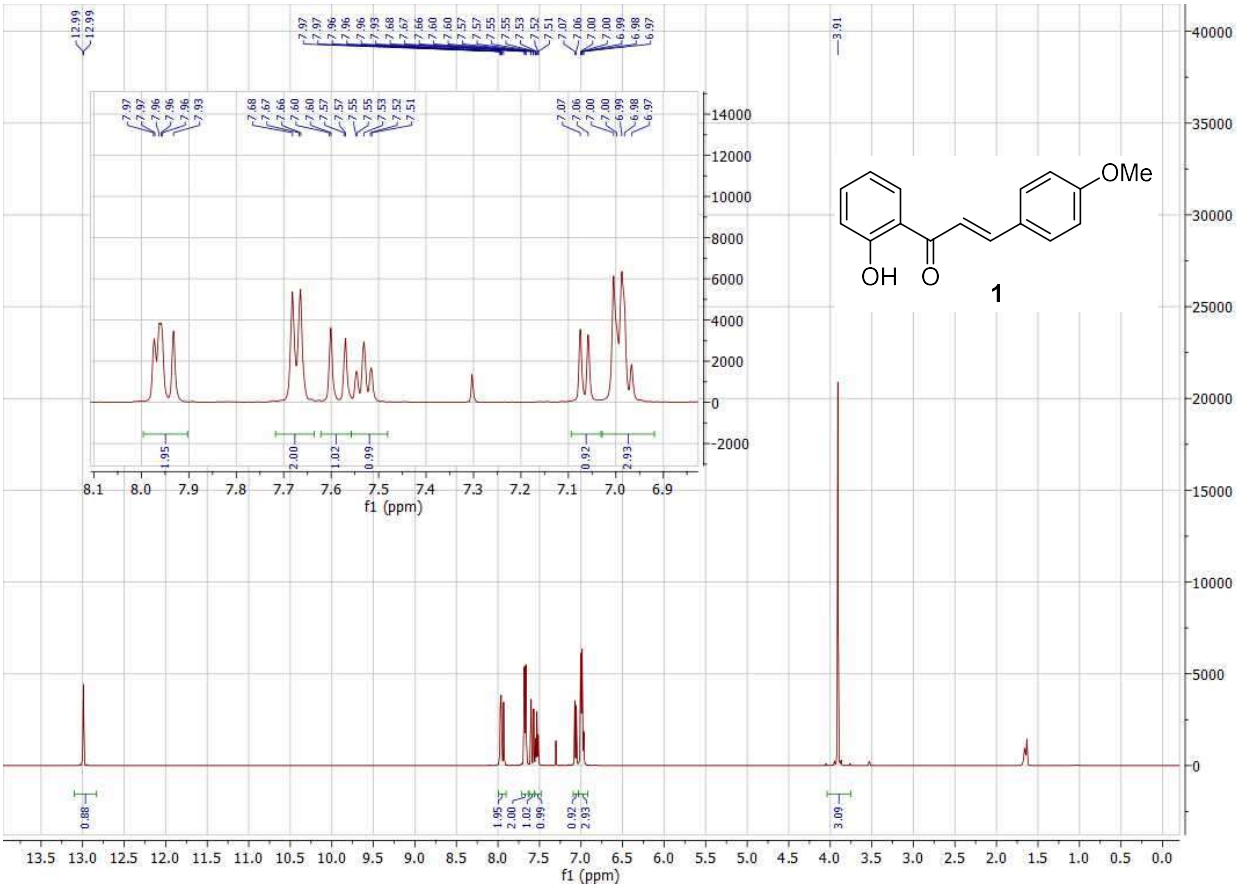


Figure S1: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **1.**

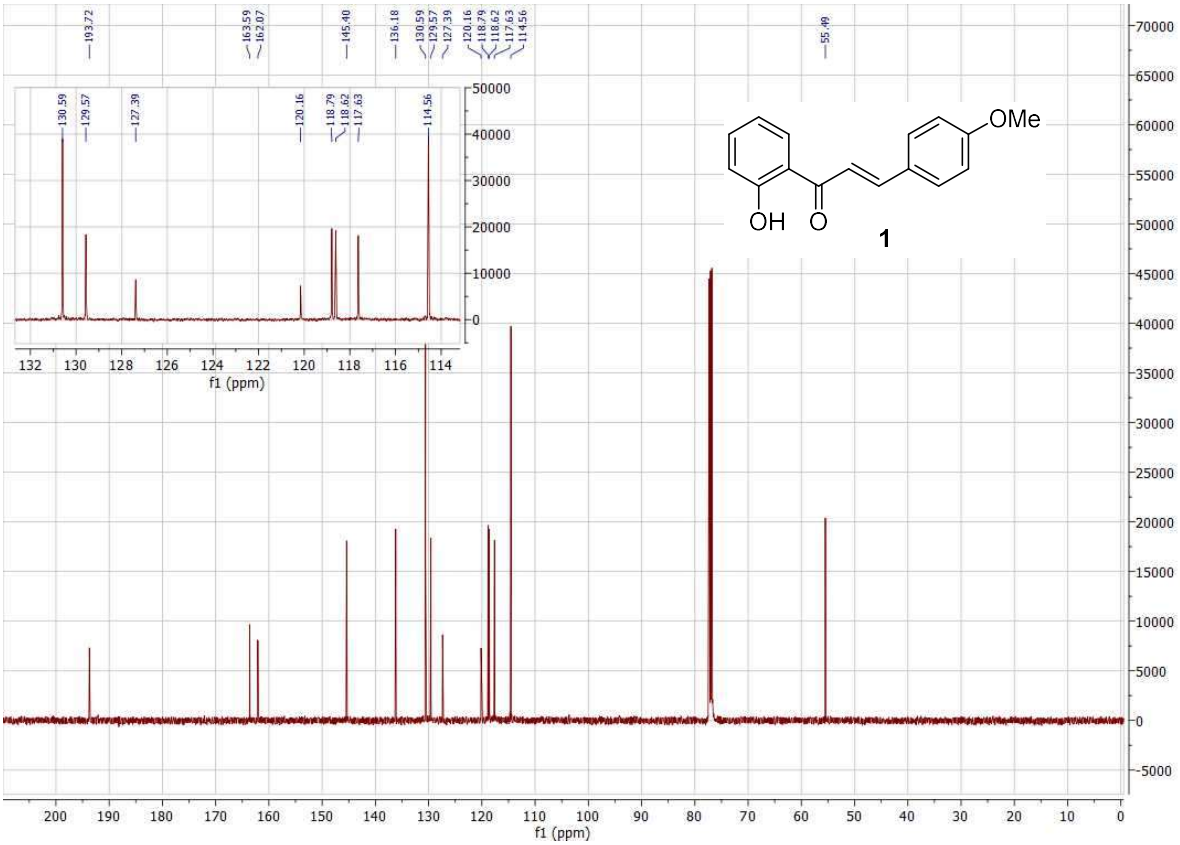


Figure S2: ^{13}C-NMR (126 MHz, $CDCl_3$) Spectrum of Compound **1**

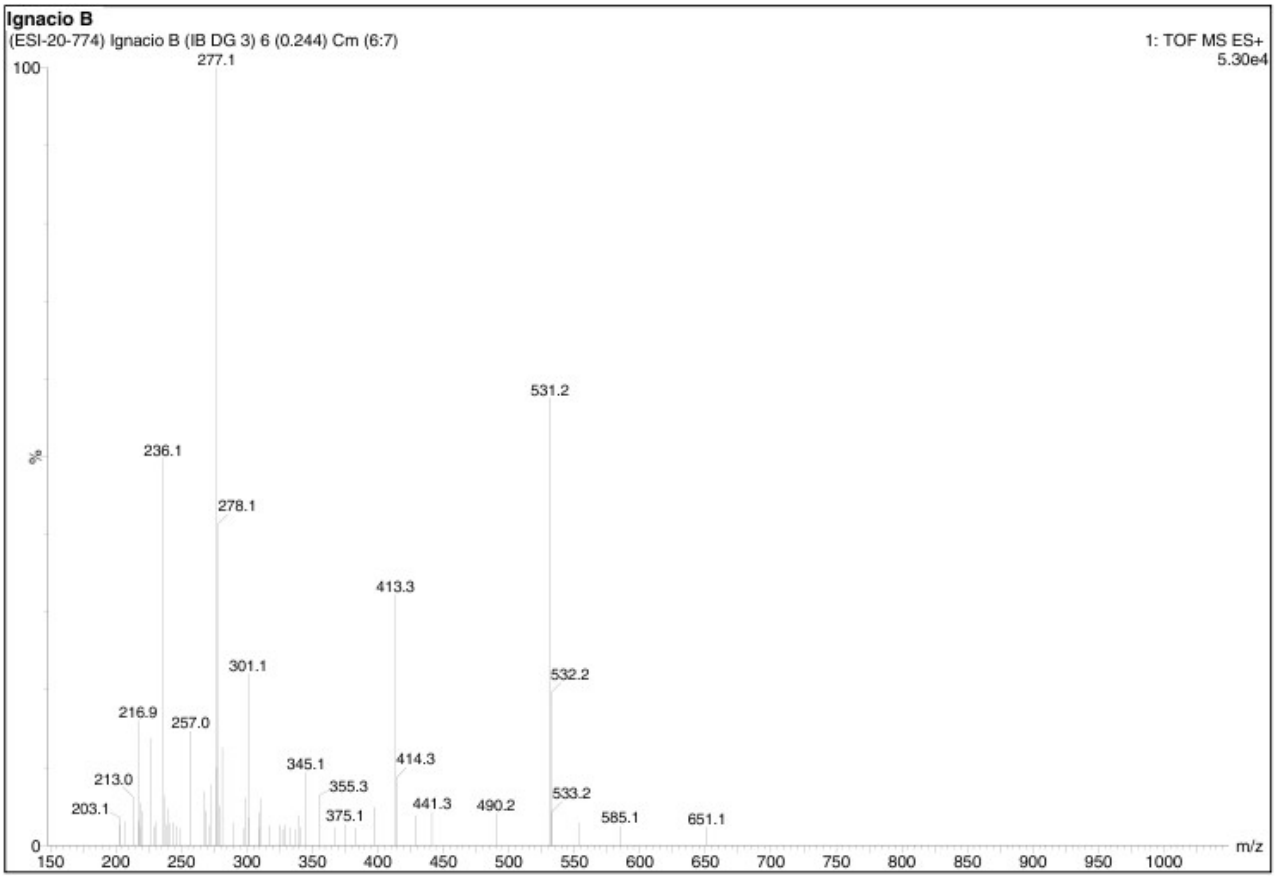


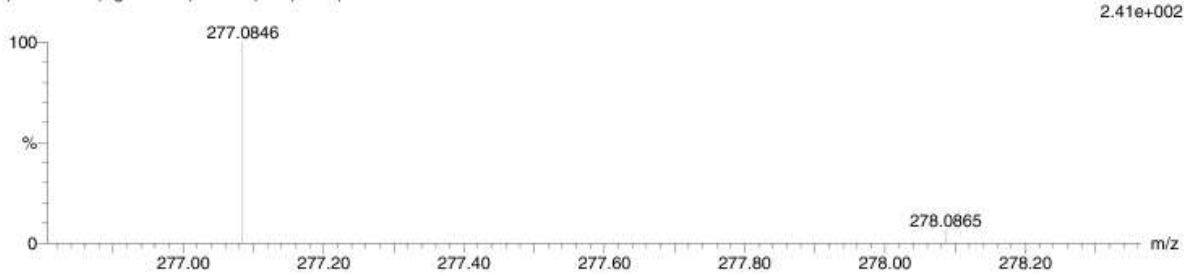
Figure S3: ESI-MS Spectrum of Compound **1**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
172 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-44 H: 0-52 O: 0-4 Na: 0-1 79Br: 0-4 81Br: 0-4

Ignacio B
(ESI-20-774) Ignacio B (IB DG 3) 27 (0.889)



Minimum:	50.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
277.0846	100.00	277.0841	0.5	1.8	9.5	13.6	2.9	C16 H14 O3 Na
		277.0837	0.9	3.2	-2.5	10.7	0.1	C9 H24 O4 81Br

Figure S4: HRHRESI-MS Spectrum of Compound **1**

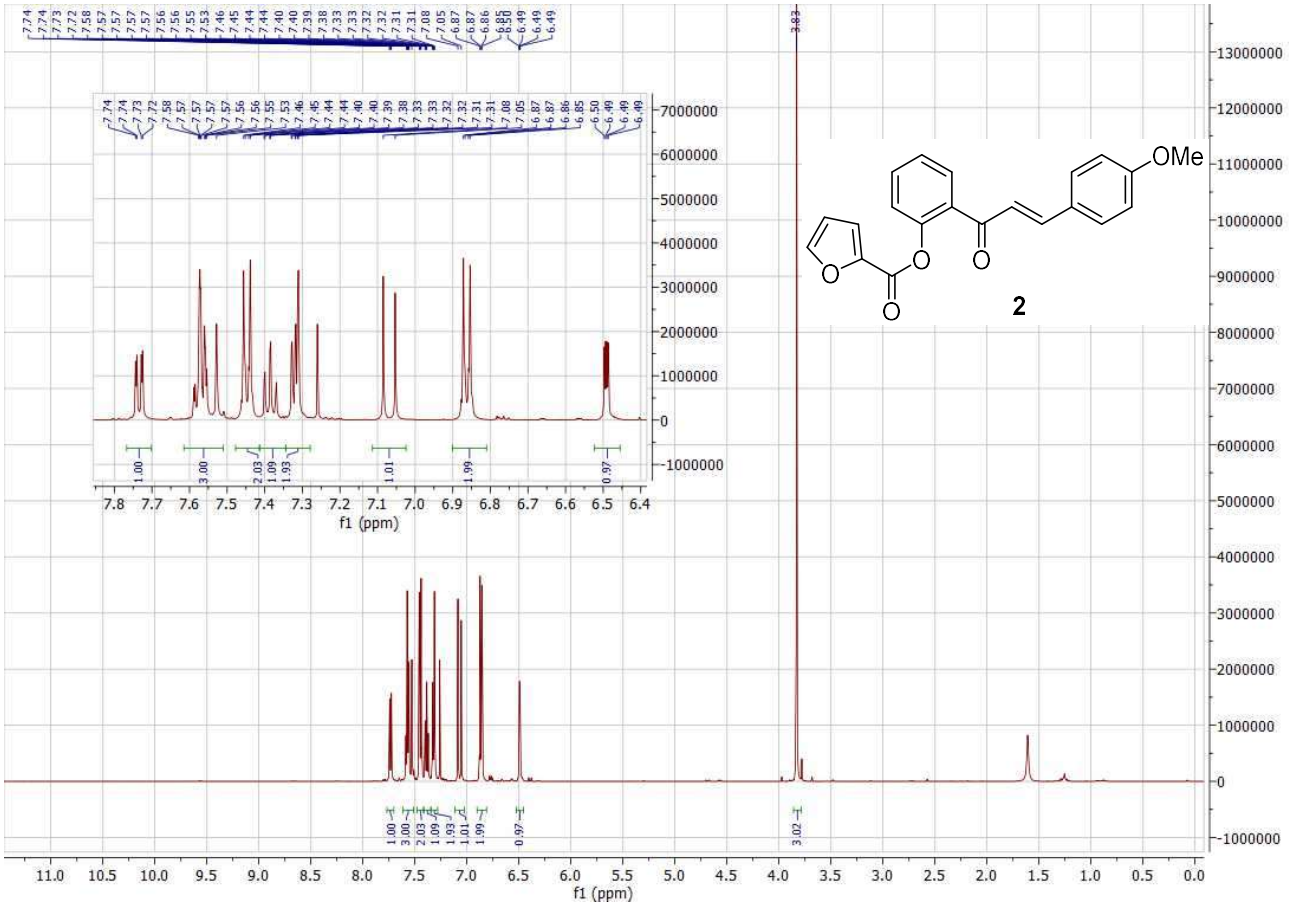


Figure S5: ^{1}H -NMR (500 MHz, $CDCl_3$) Spectrum of Compound **2.**

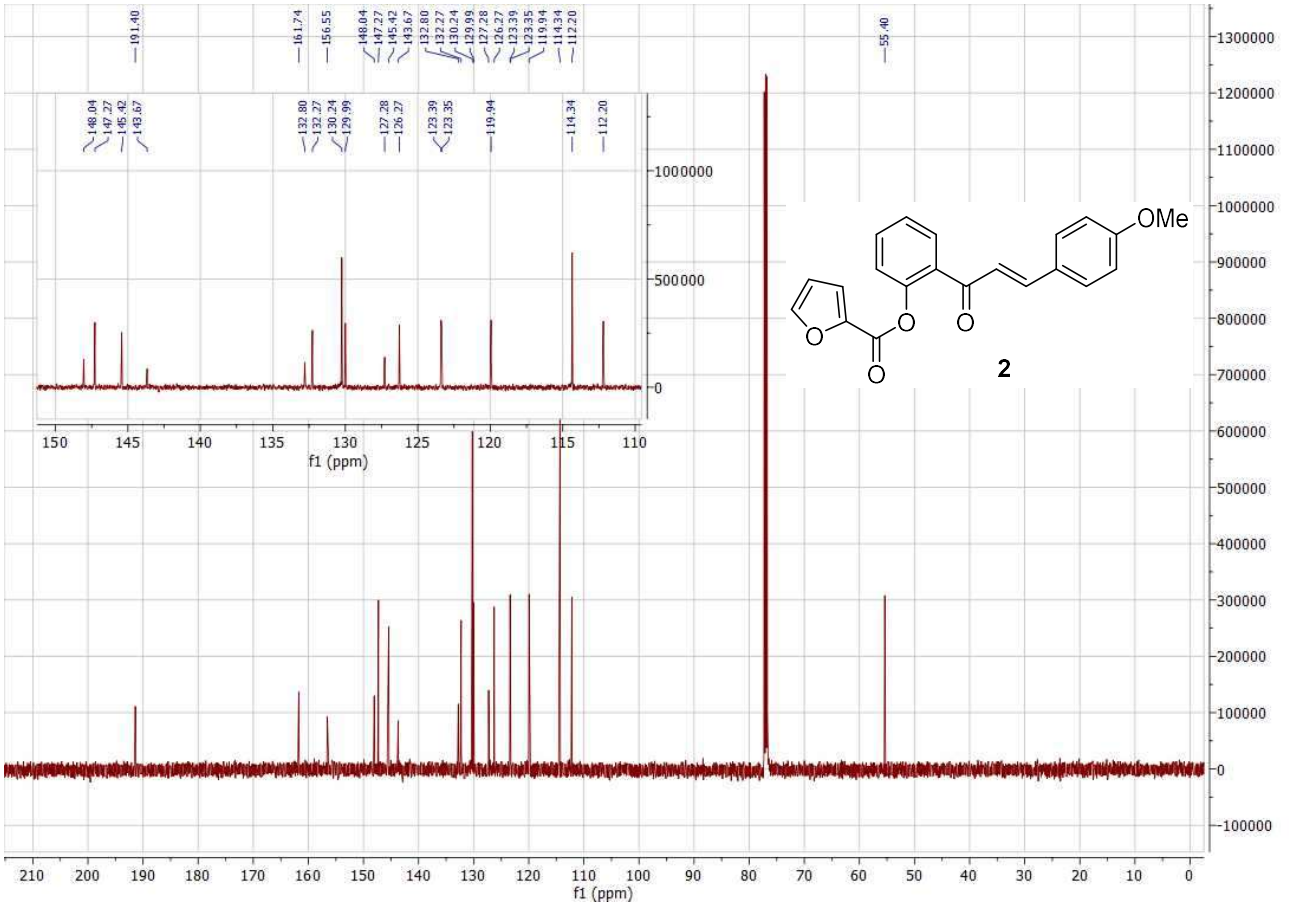


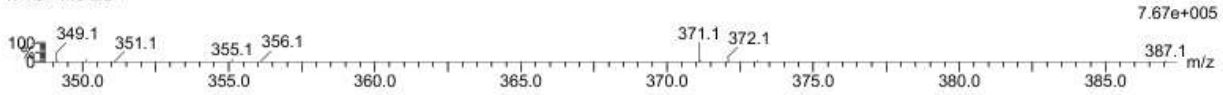
Figure S6: ^{13}C-NMR (126 MHz, $CDCl_3$) Spectrum of Compound **2**

Figure S7: ESI-MS Spectrum of Compound **2**

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 3 mass(es) processed
Tolerance = 5.0 PPM / DBE: min = -20.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1534 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-2 O: 0-10 Na: 0-2
Synapt (ESI 21-143) Ignacio B (DG-12) 139 (1.021)
1: TOF MS ES+



Minimum:	16.00				-20.0				
Maximum:	100.00		5.0	5.0	300.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
349.1077	45.30	349.1076	0.1	0.3	13.5	32.7	0.000	100.00	C21 H17 O5
		349.1087	-1.0	-2.9	-1.5	47.8	15.086	0.00	C10 H23 O10 Na2
371.0897	100.00	371.0895	0.2	0.5	13.5	55.6	0.000	100.00	C21 H16 O5 Na
		371.0879	1.8	4.9	12.5	65.7	10.086	0.00	C18 H15 N2 O7
372.0929	23.49	372.0931	-0.2	-0.5	7.5	52.5	n/a	n/a	C15 H18 N O10

Figure S8: HRESI-MS Spectrum of Compound **2**

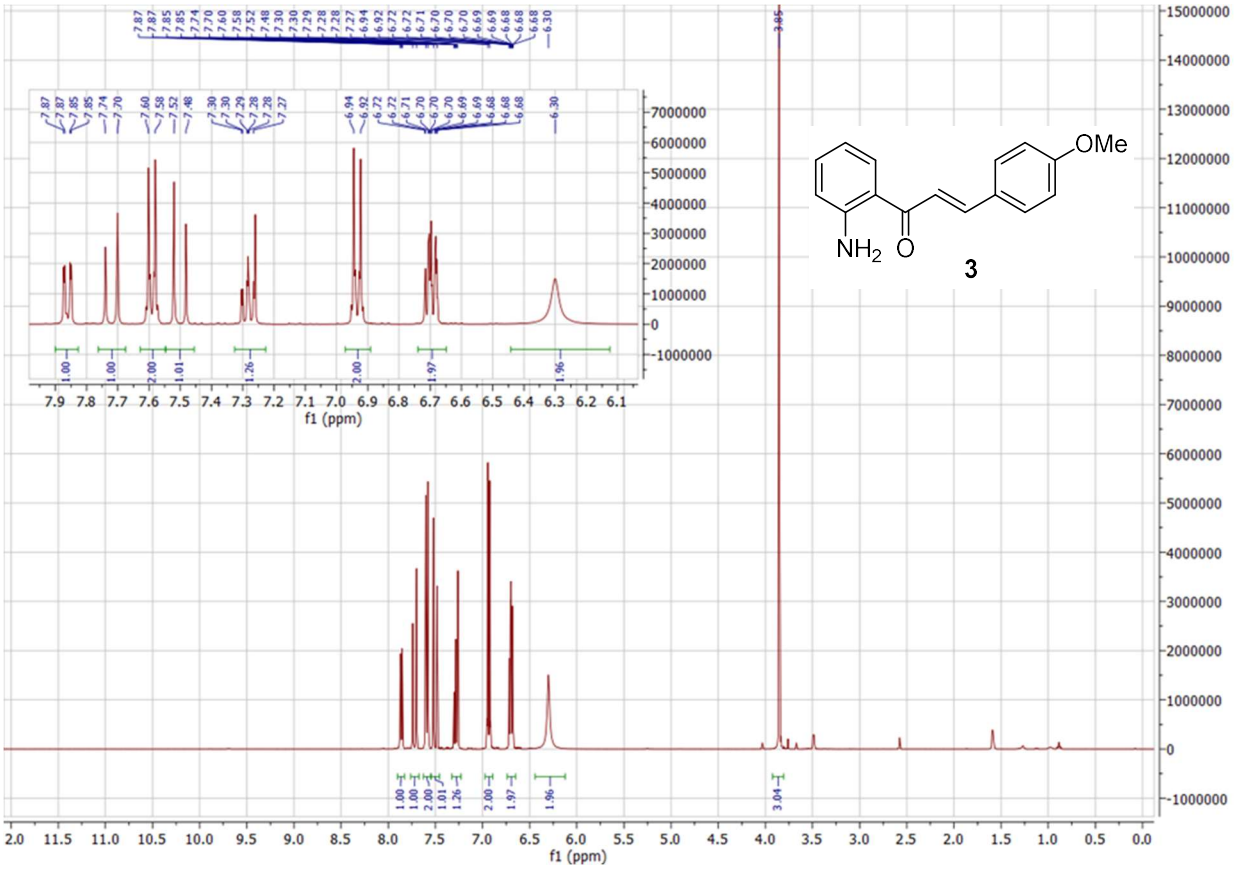


Figure S9: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3**

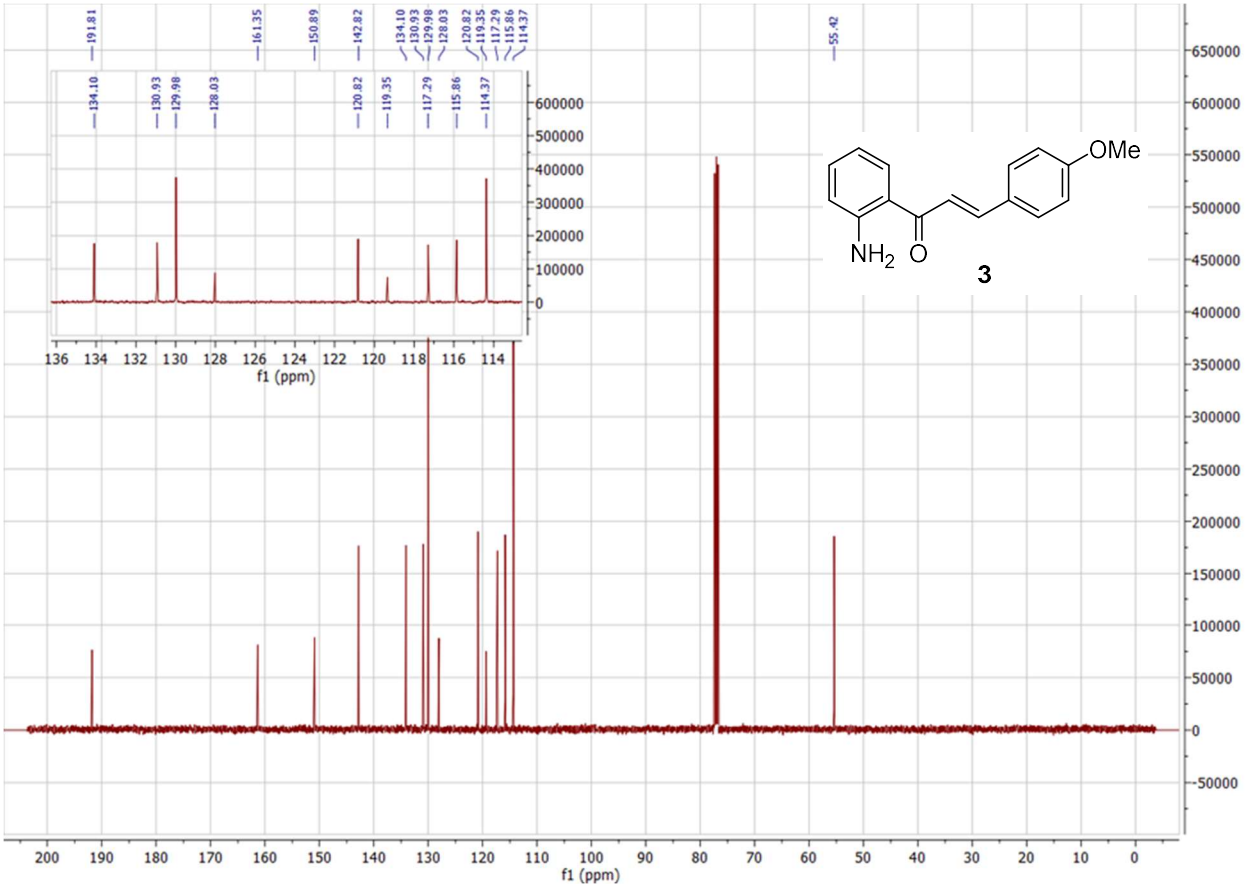


Figure S10: ^{13}C-NMR (101 MHz, CDCl3) Spectrum of Compound **3**

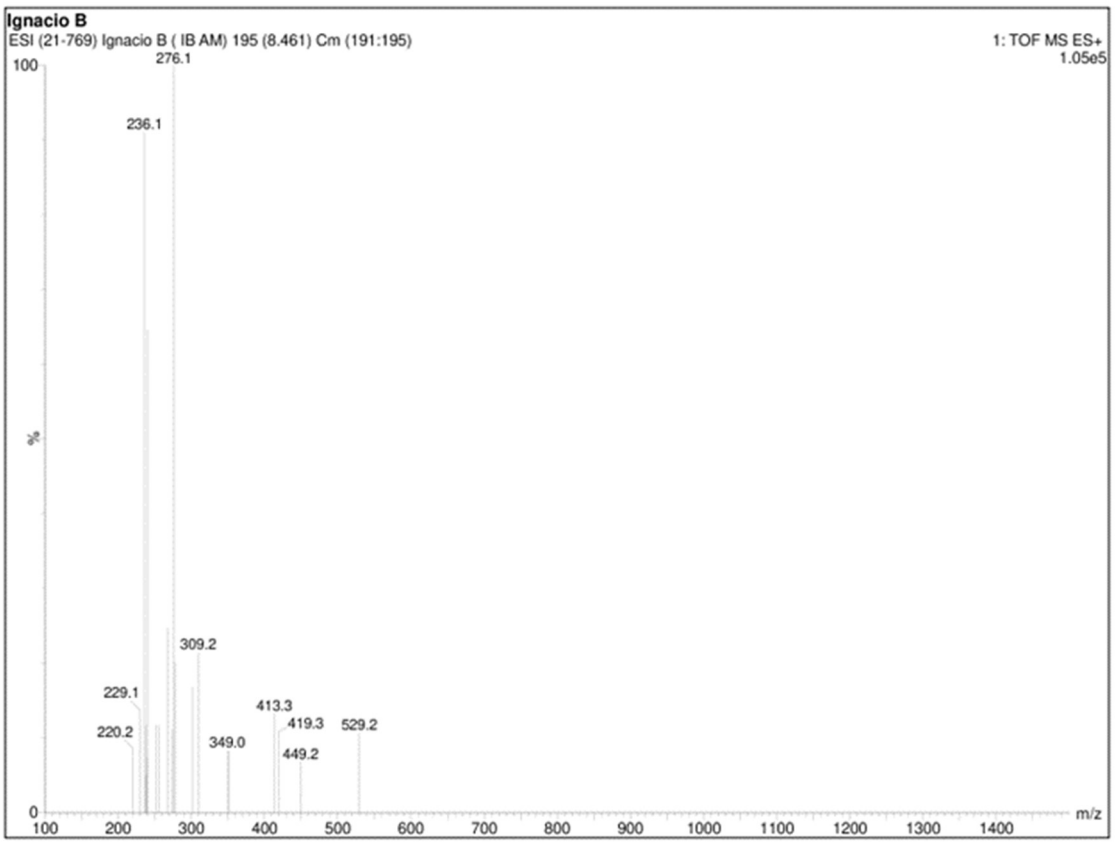
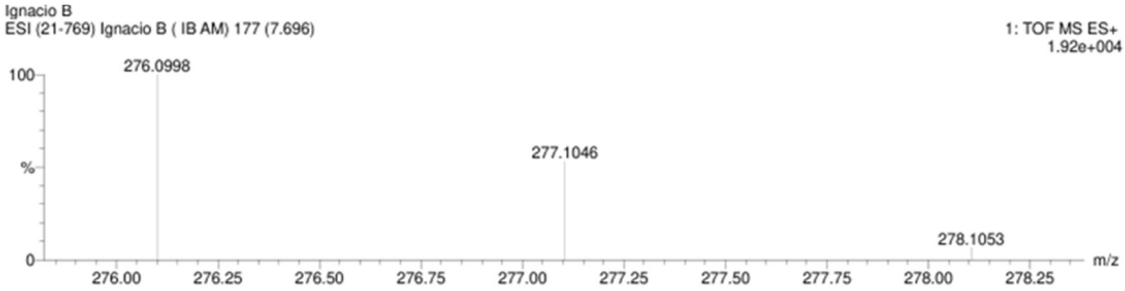


Figure S11: ESI-MS Spectrum of Compound **3**

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1474 formula(e) evaluated with 23 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-90 H: 0-140 N: 0-2 O: 0-10 Na: 0-2 S: 0-2



Minimum:	50.00				-1.5			
Maximum:	100.00		5.0	20.0	100.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
276.0998	100.00	276.1025	-2.7	-9.8	12.5	24.4	0.9	C18 H14 N O2
		276.1000	-0.2	-0.7	9.5	24.6	1.1	C16 H15 N O2 Na
		276.0976	2.2	8.0	6.5	25.1	1.5	C14 H16 N O2 Na2
		276.1034	-3.6	-13.0	4.5	28.6	5.1	C13 H19 N O2 Na S
		276.1010	-1.2	-4.3	1.5	29.1	5.6	C11 H20 N O2 Na2 S

Figure S12: HRESI-MS Spectrum of Compound **3**

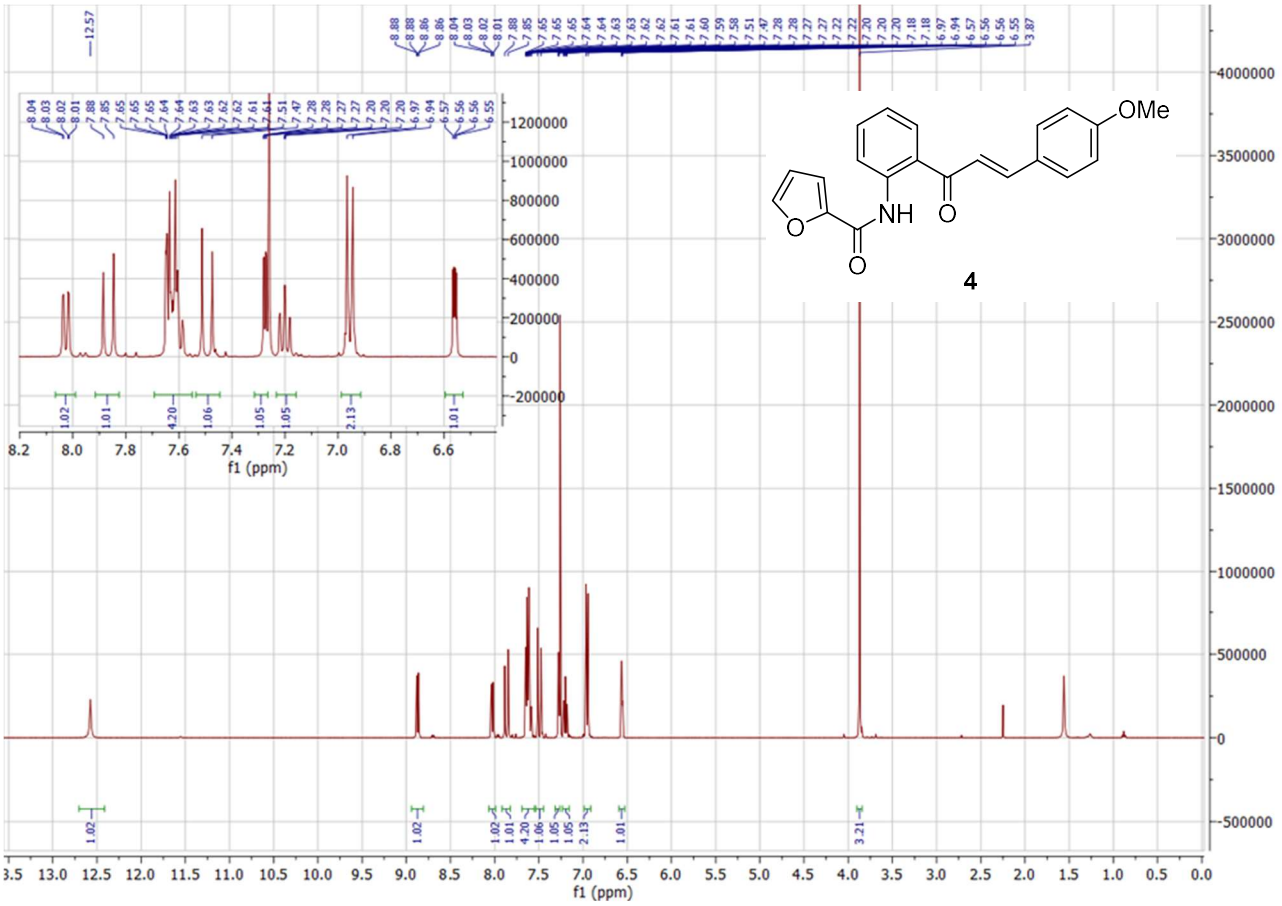


Figure S13: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4**

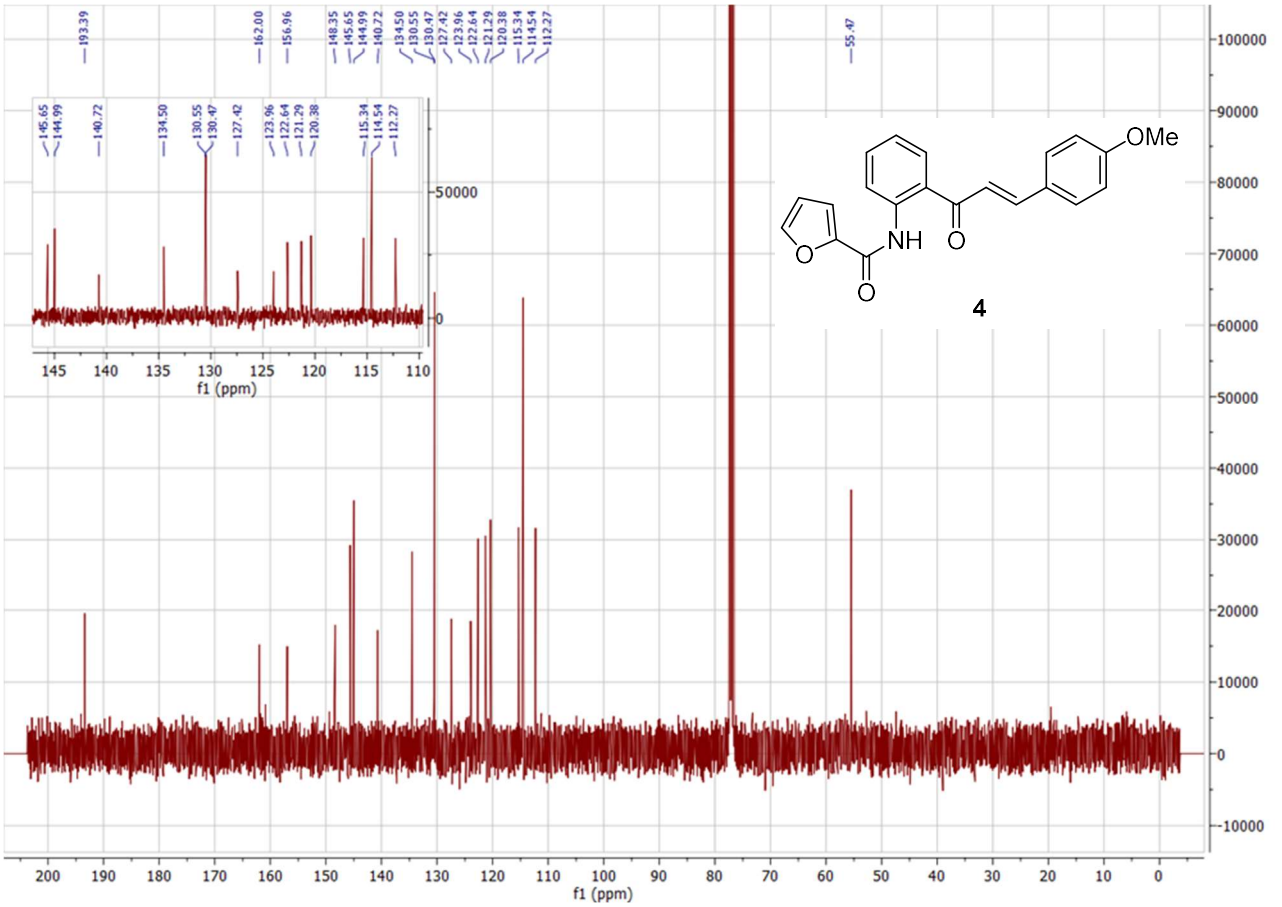


Figure S14: ^{13}C-NMR (101 MHz, $CDCl_3$) Spectrum of Compound **4**

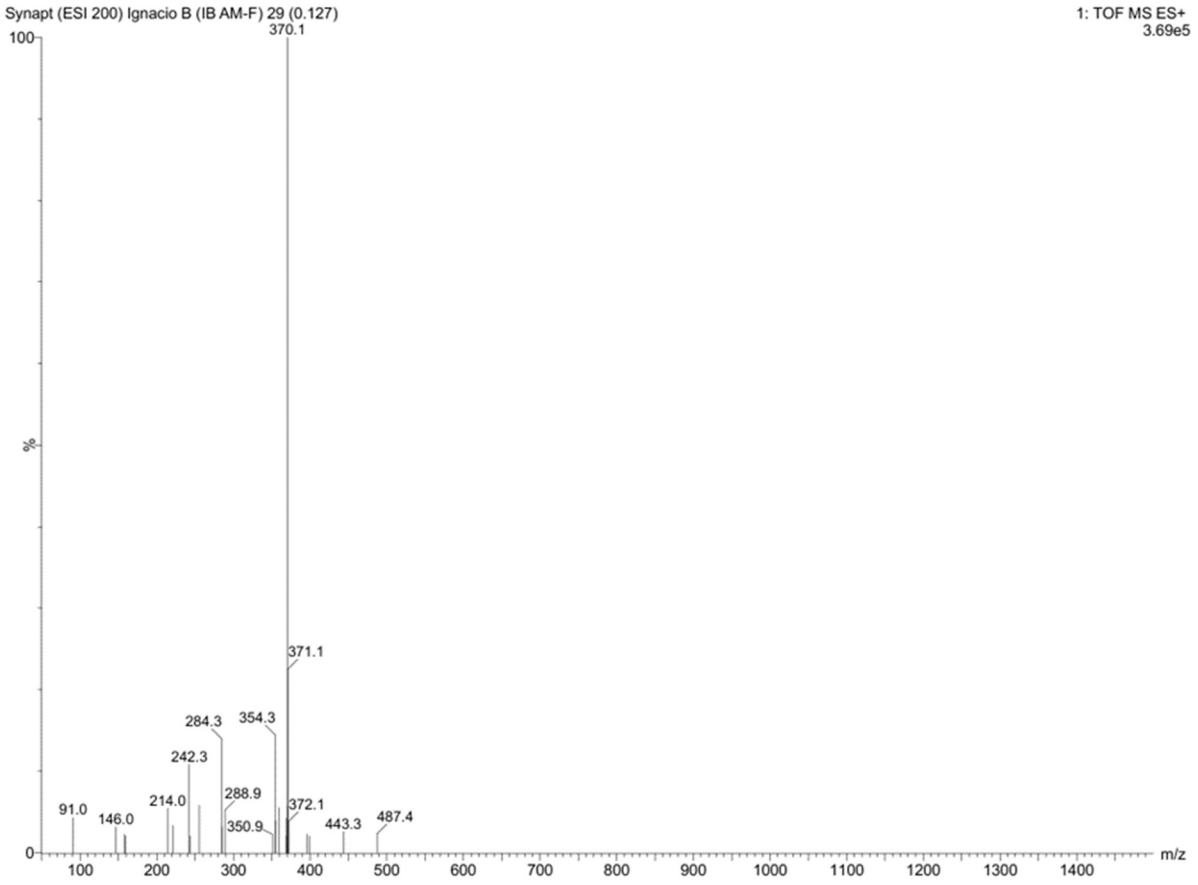
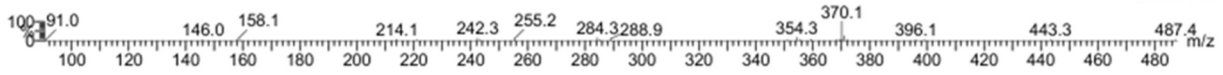


Figure S15: ESI-MS Spectrum of Compound 4

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 5.0 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
1539 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-80 N: 0-5 O: 0-10 Na: 0-2
Synapt (ESI 200) Ignacio B (IB AM-F) 29 (0.127)
1: TOF MS ES+
3.70e+005



Minimum:	20.00				-1.5				
Maximum:	100.00		5.0	5.0	50.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
370.1053	100.00	370.1055	-0.2	-0.5	13.5	36.8	0.016	98.40	C21 H17 N O4 Na
		370.1039	1.4	3.8	12.5	41.5	4.785	0.84	C18 H16 N3 O6
		370.1045	0.8	2.2	15.5	42.1	5.358	0.47	C20 H14 N5 Na2
		370.1069	-1.6	-4.3	18.5	42.6	5.816	0.30	C22 H13 N5 Na
371.1086	22.46	371.1083	0.3	0.8	5.5	31.6	0.958	38.38	C16 H21 O7 Na2
		371.1091	-0.5	-1.3	7.5	31.7	1.099	33.32	C15 H19 N2 O9
		371.1096	-1.0	-2.7	10.5	32.1	1.518	21.91	C17 H17 N4 O3 Na2
		371.1072	1.4	3.8	20.5	33.3	2.749	6.40	C27 H15 O2

Figure S16: HRESI-MS Spectrum of Compound **4**

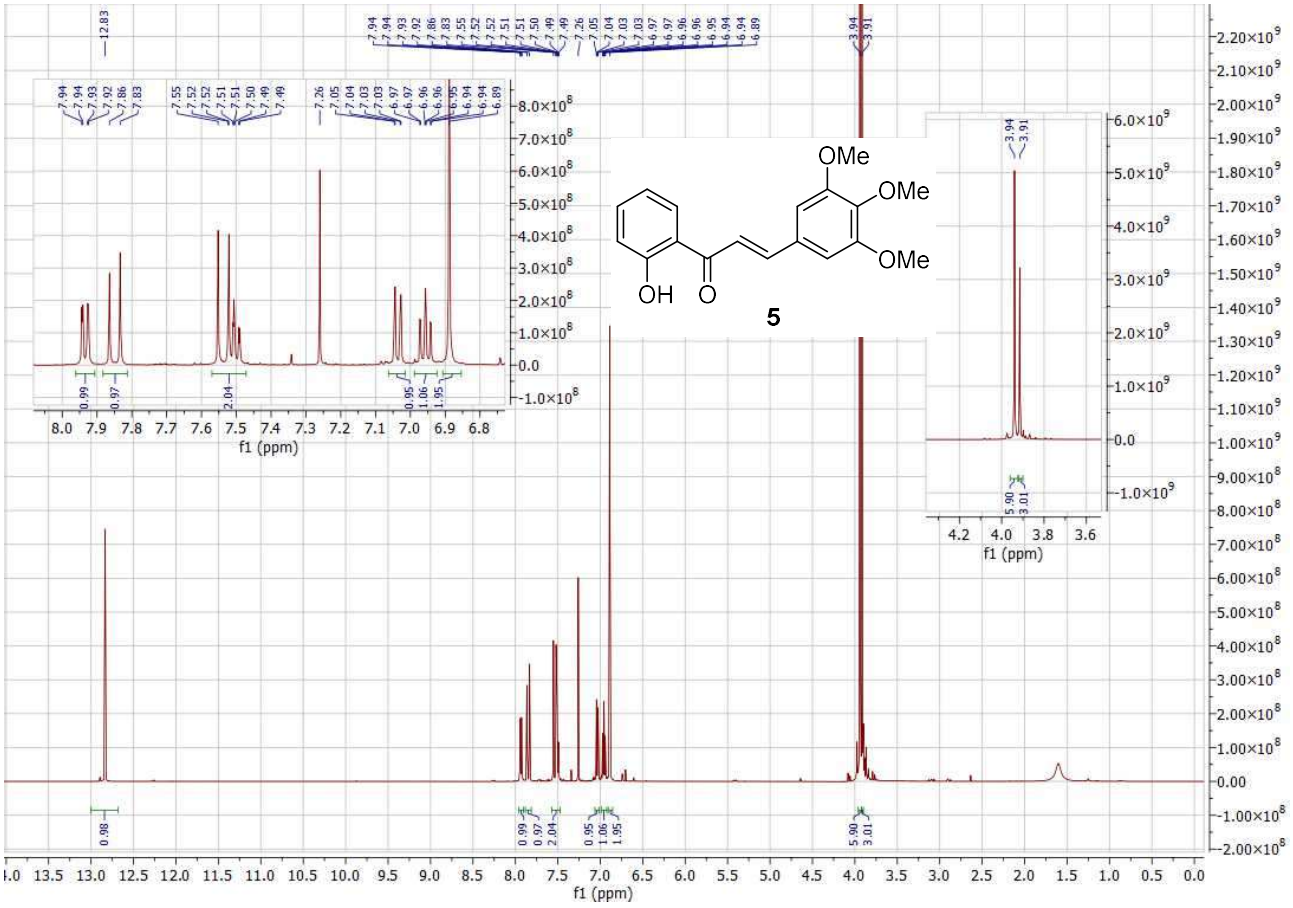


Figure S17: ^{1}H -NMR (500 MHz, $CDCl_3$) Spectrum of Compound **5**

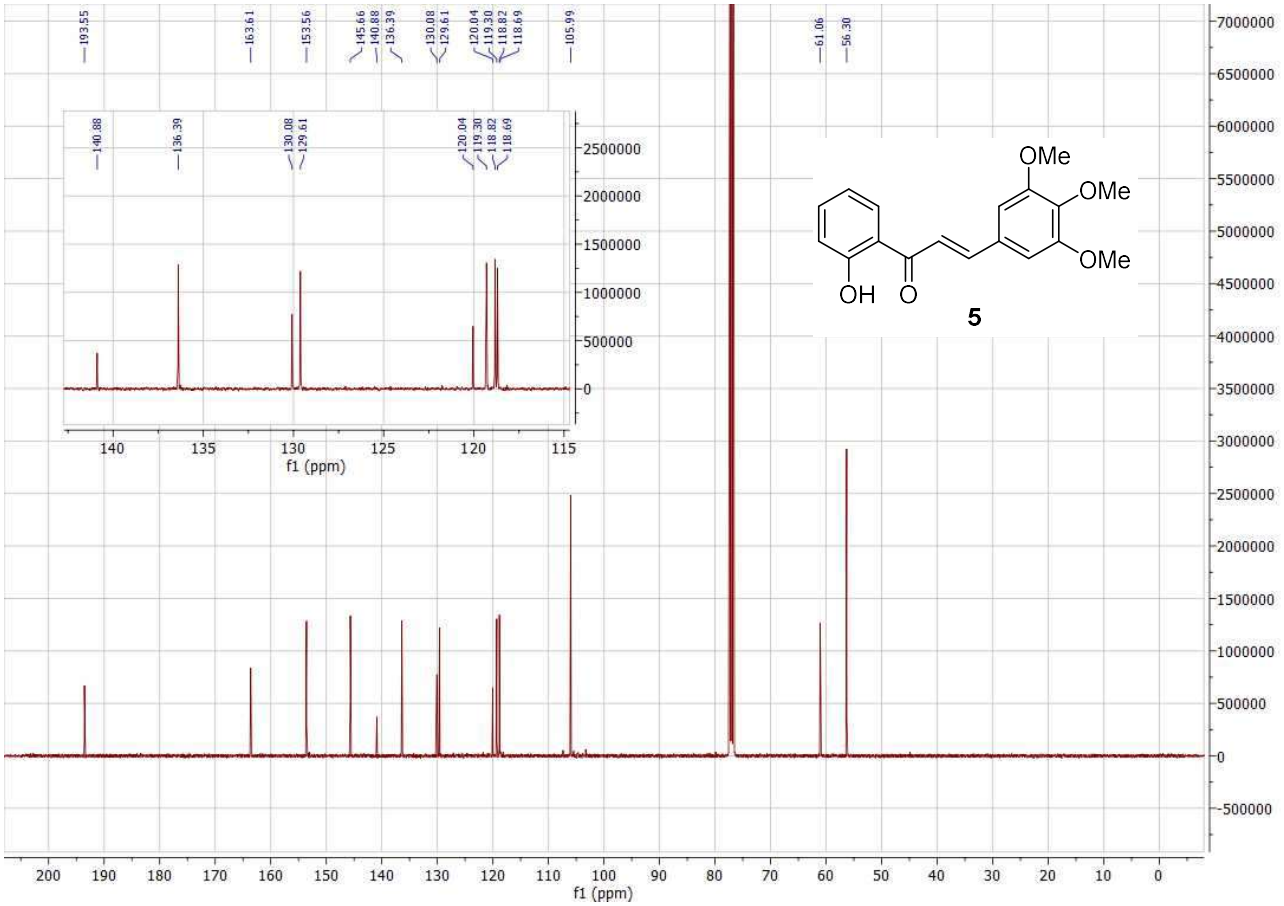


Figure S18: ^{13}C -NMR (101 MHz, $CDCl_3$) Spectrum of Compound **5**

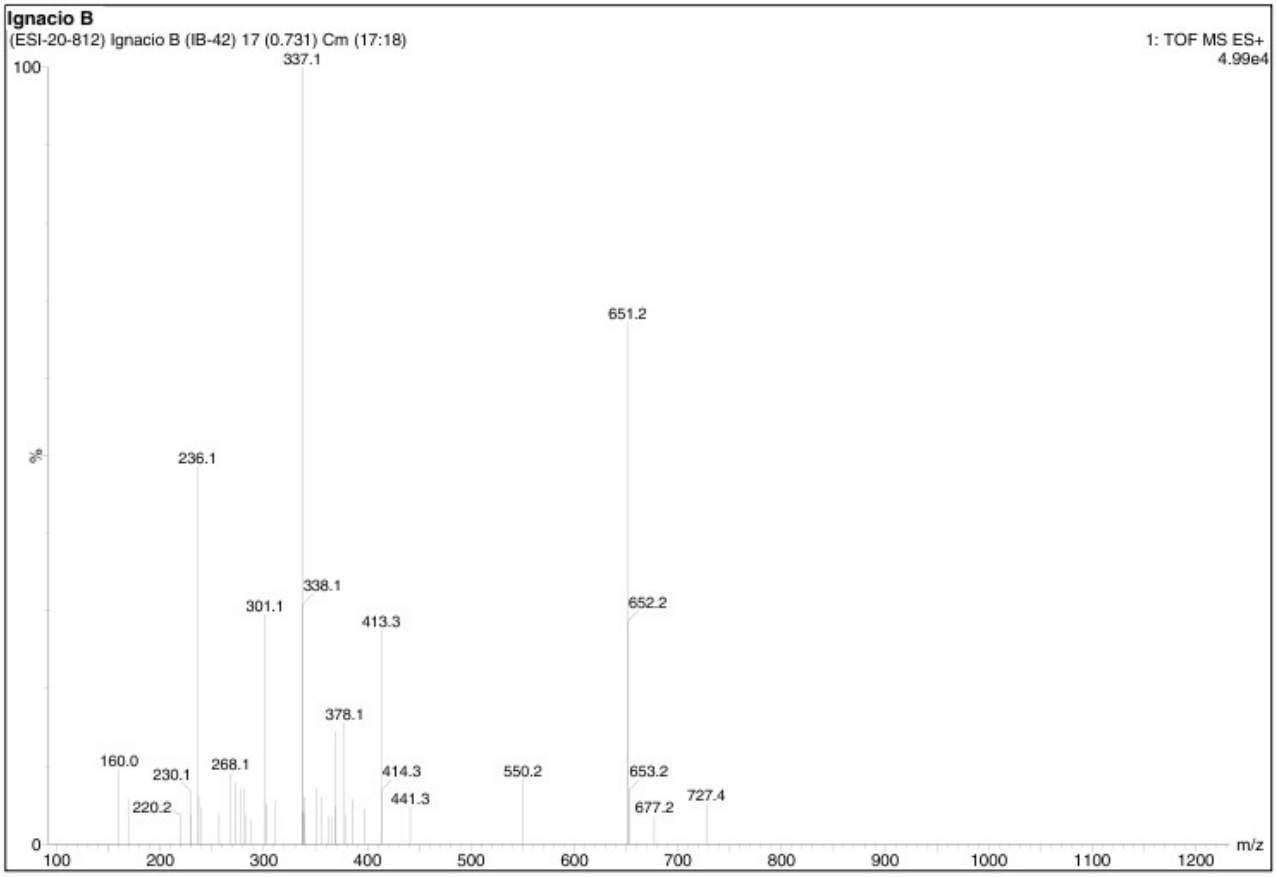


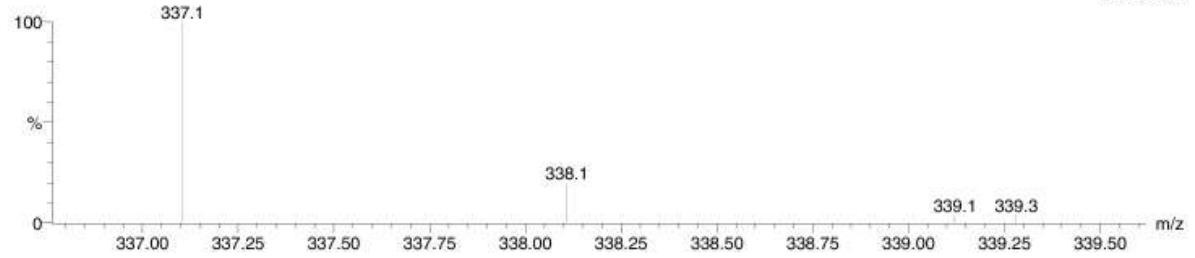
Figure S19: ESI-MS Spectrum of Compound **5**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
394 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-70 H: 0-100 N: 0-3 O: 0-12 Na: 0-1
Ignacio B
(ESI-20-812) Ignacio B (IB-42) 22 (0.940)

1: TOF MS ES+
5.59e+003



Minimum:	30.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
337.1046	100.00	337.1052	-0.6	-1.8	9.5	24.6	0.2	C18 H18 O5 Na
		337.1036	1.0	3.0	8.5	25.9	1.6	C15 H17 N2 O7

Figure S20: HRESI-MS Spectrum of Compound **5**

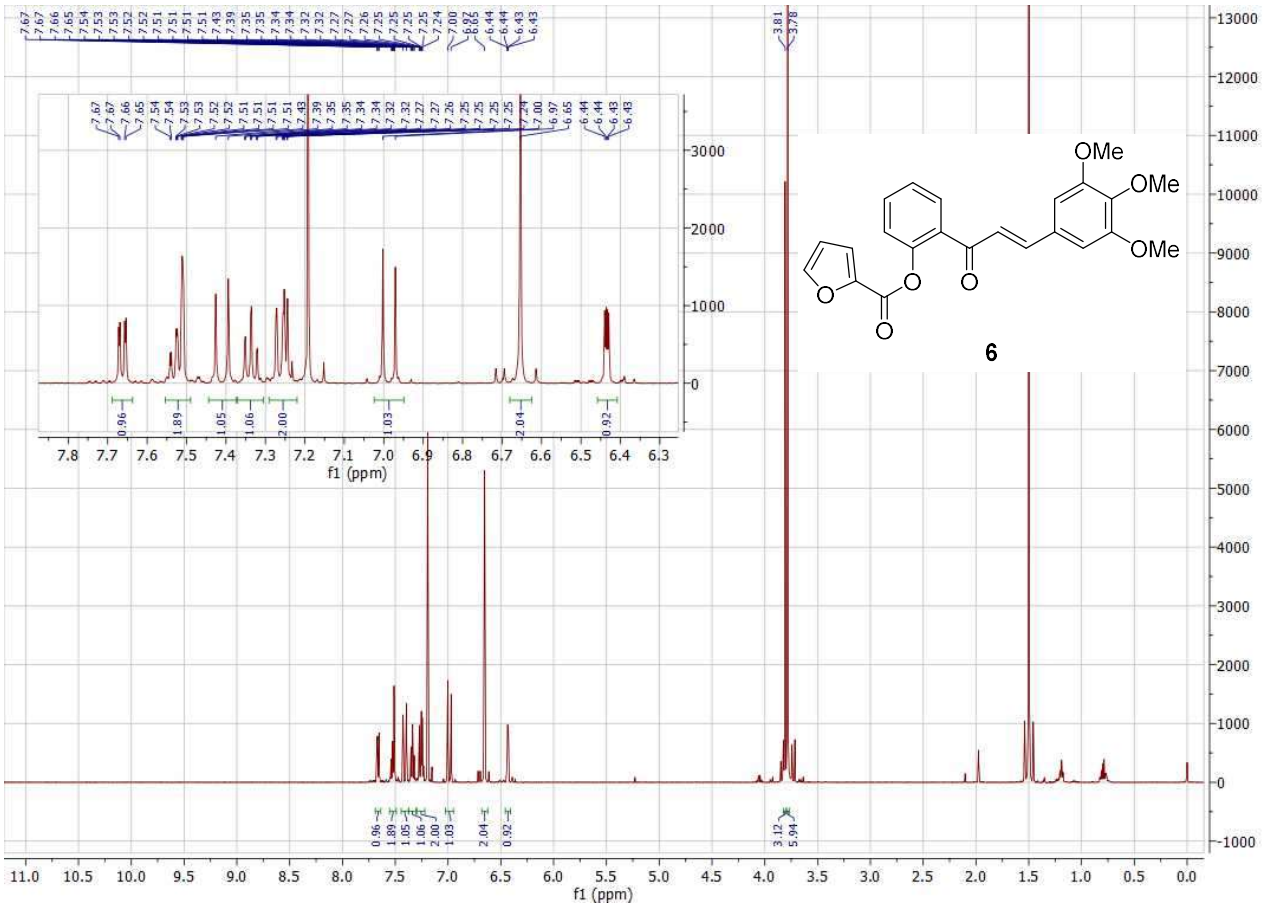


Figure S21: ^{1}H -NMR (500 MHz, $CDCl_3$) Spectrum of Compound **6**

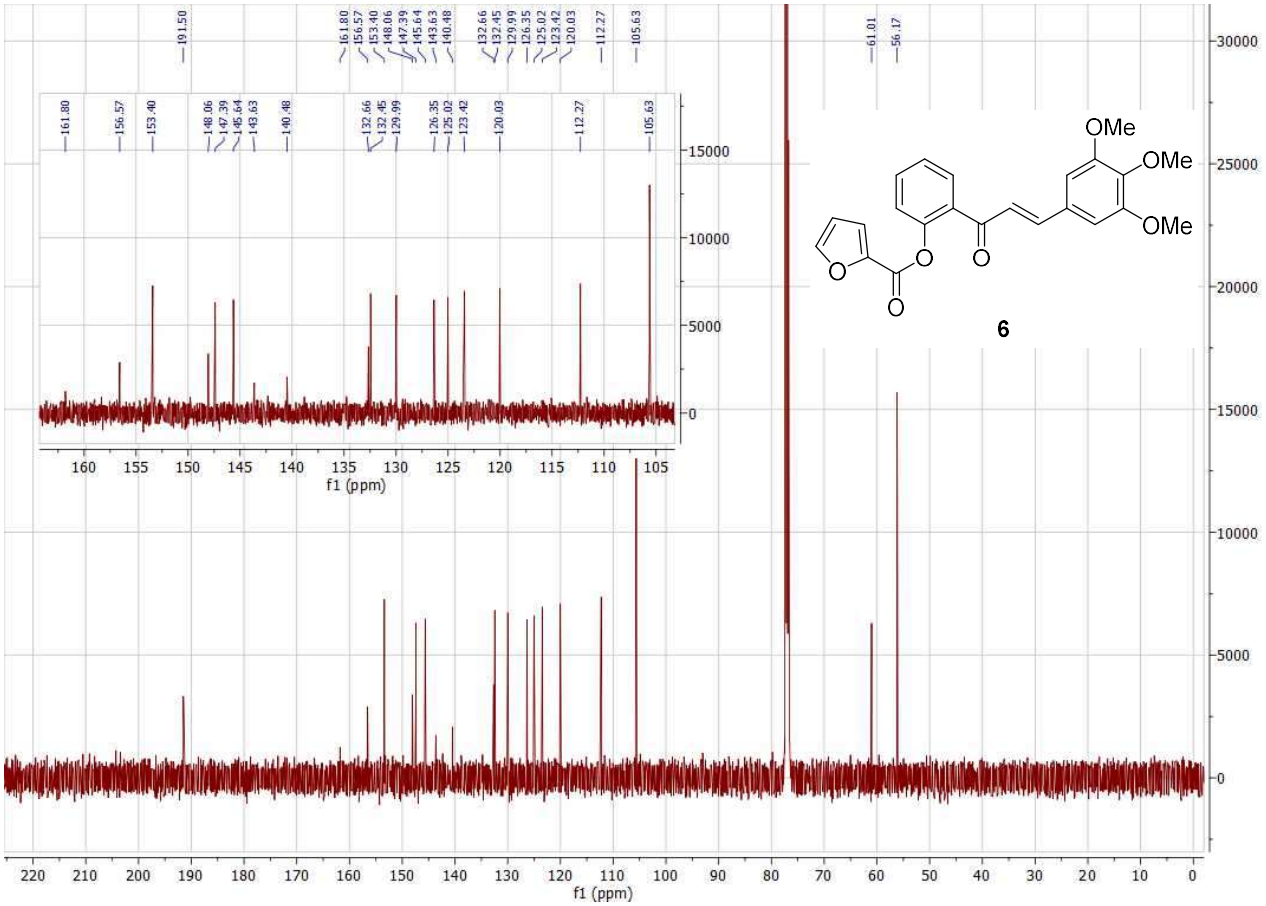


Figure S22: ^{13}C -NMR (126 MHz, $CDCl_3$) Spectrum of Compound **6**

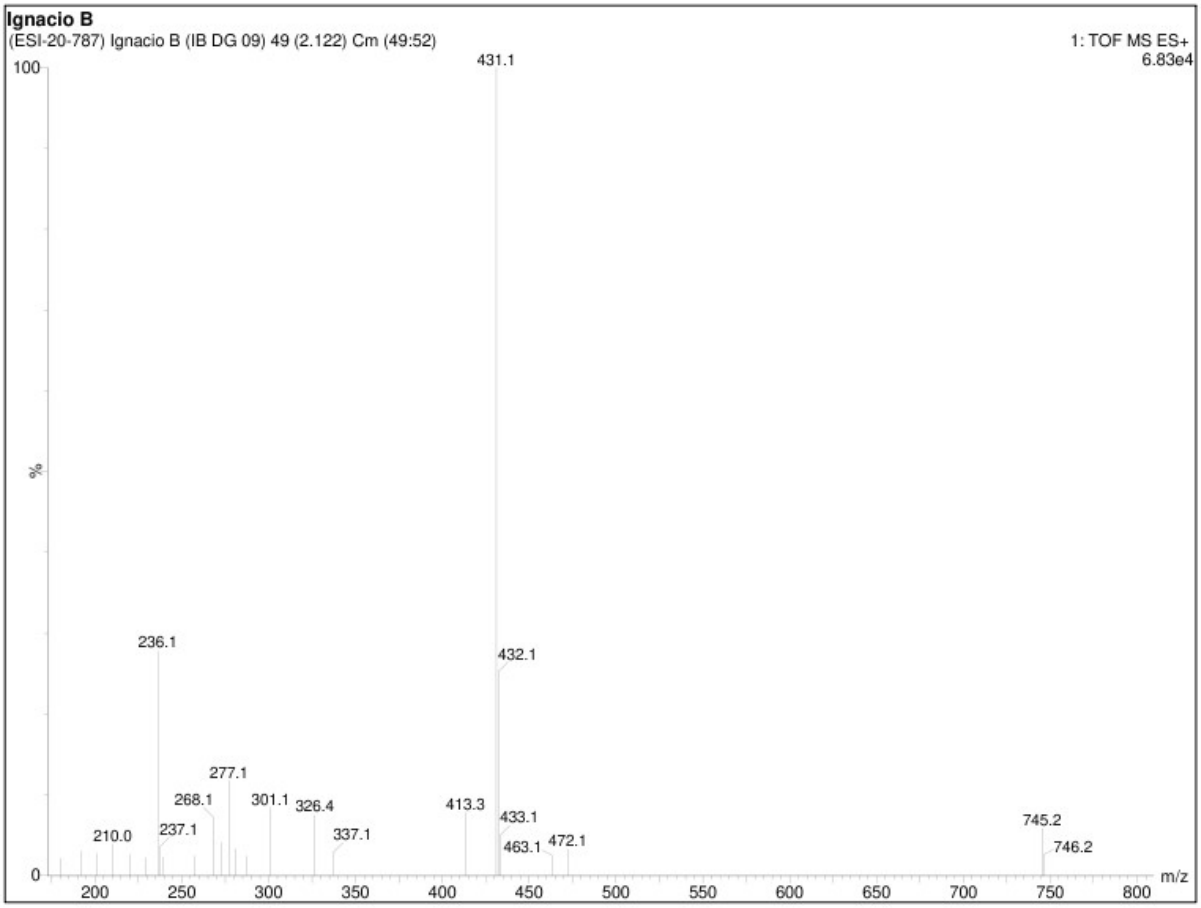


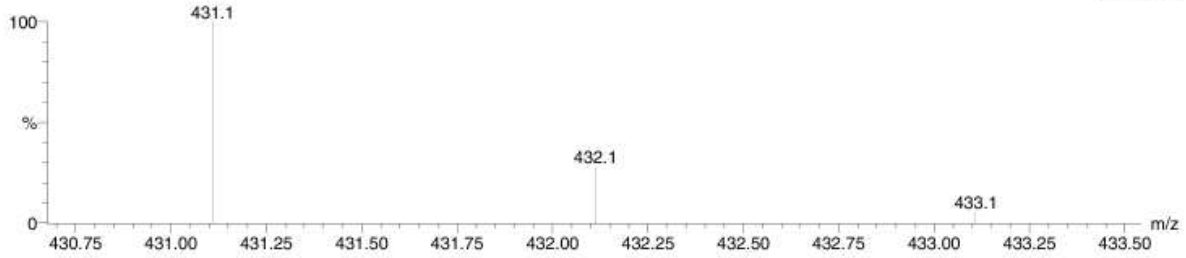
Figure S23: ESI-MS Spectrum of Compound **6**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
491 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-44 H: 0-52 N: 0-4 O: 0-10 Na: 0-1
Ignacio B
(ESI-20-787) Ignacio B (IB DG 09) 65 (2.819)

1: TOF MS ES+
3.29e+003



Minimum:	50.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
431.1093	100.00	431.1091	0.2	0.5	12.5	11.9	1.5	C20 H19 N2 O9
		431.1107	-1.4	-3.2	13.5	10.7	0.3	C23 H20 O7 Na
		431.1072	2.1	4.9	25.5	15.7	5.2	C32 H15 O2

Figure S24: HRESI-MS Spectrum of Compound **6**

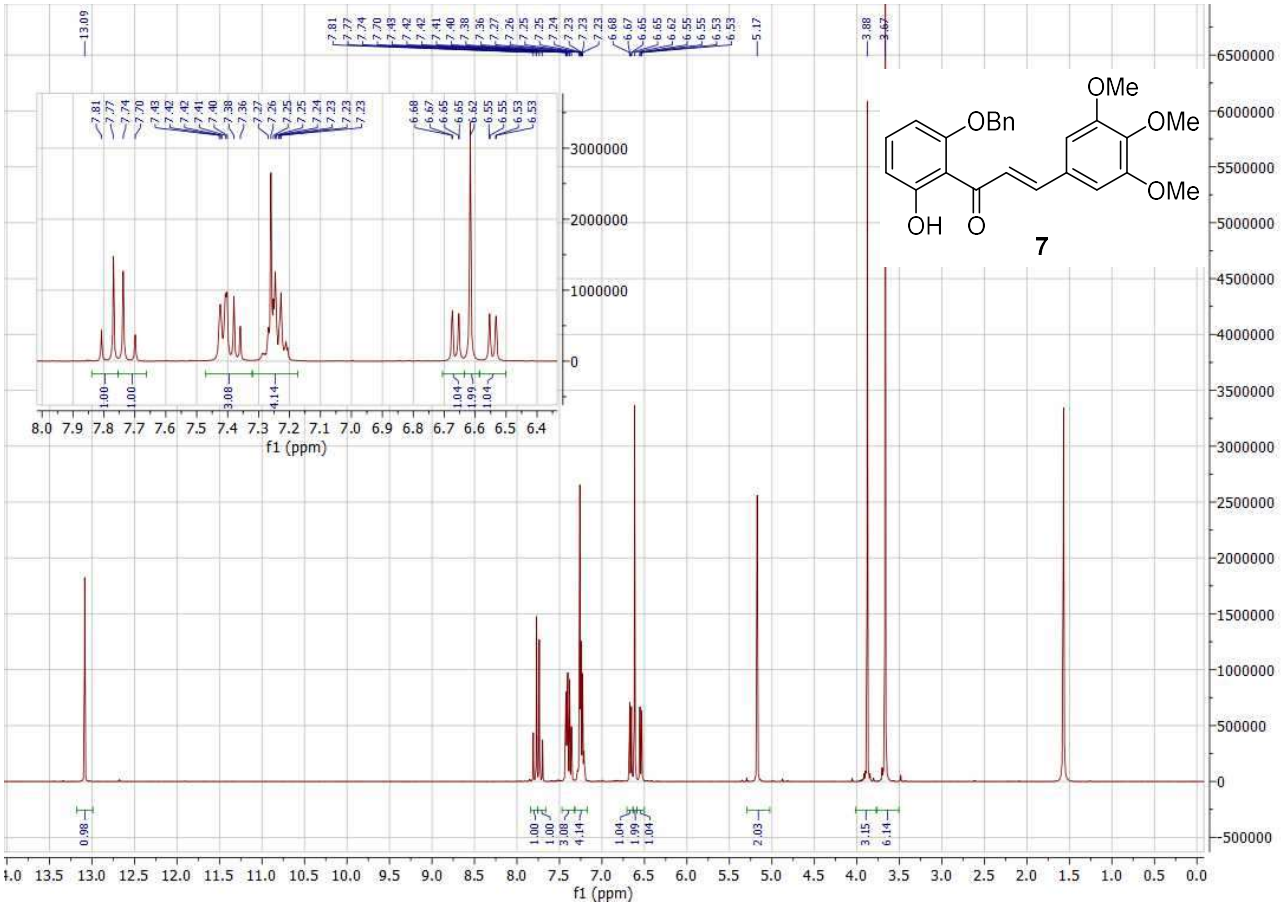


Figure S25: ^{1}H -NMR (400 MHz, $CDCl_3$) Spectrum of Compound **7**

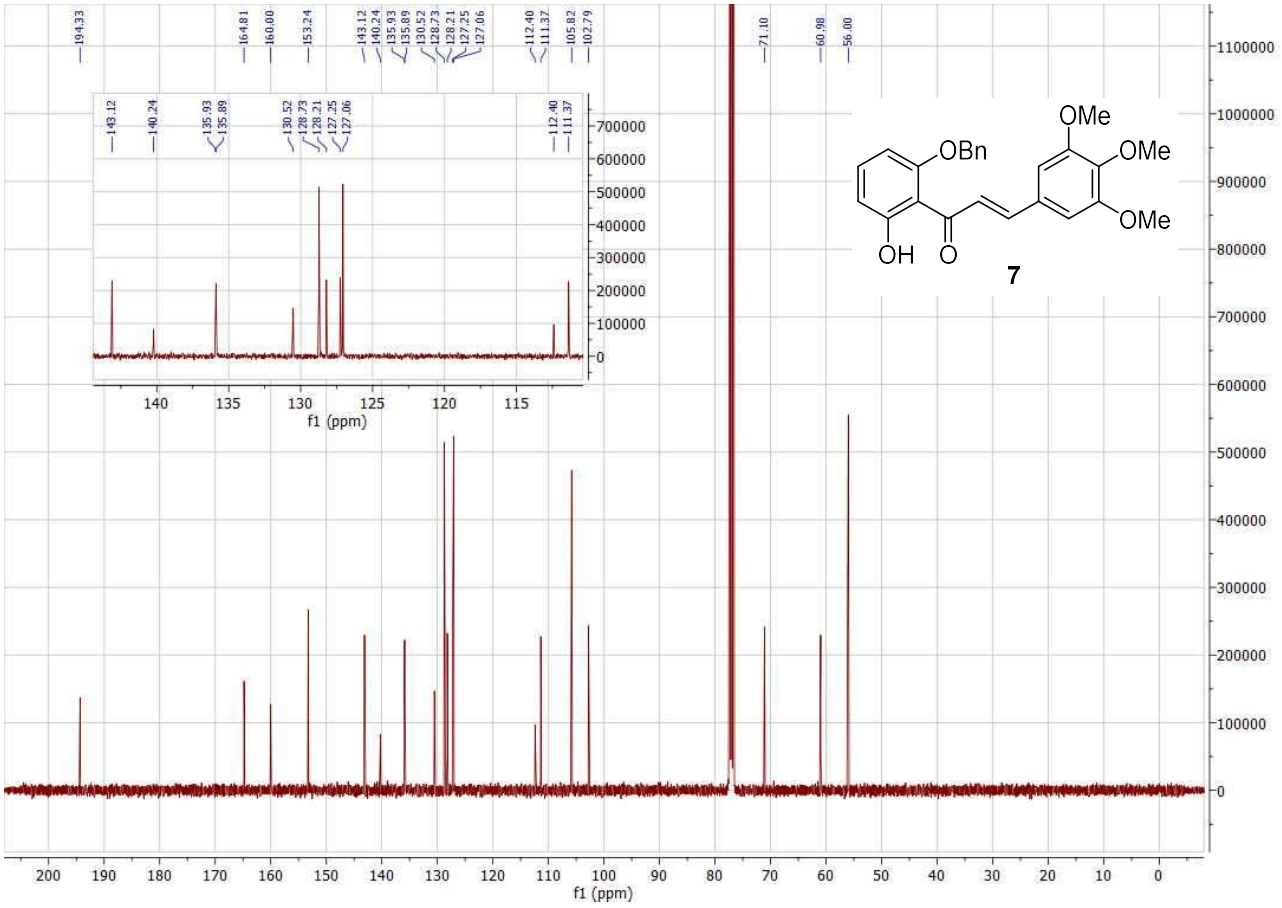


Figure S26: ^{13}C -NMR (101 MHz, $CDCl_3$) Spectrum of Compound **7**

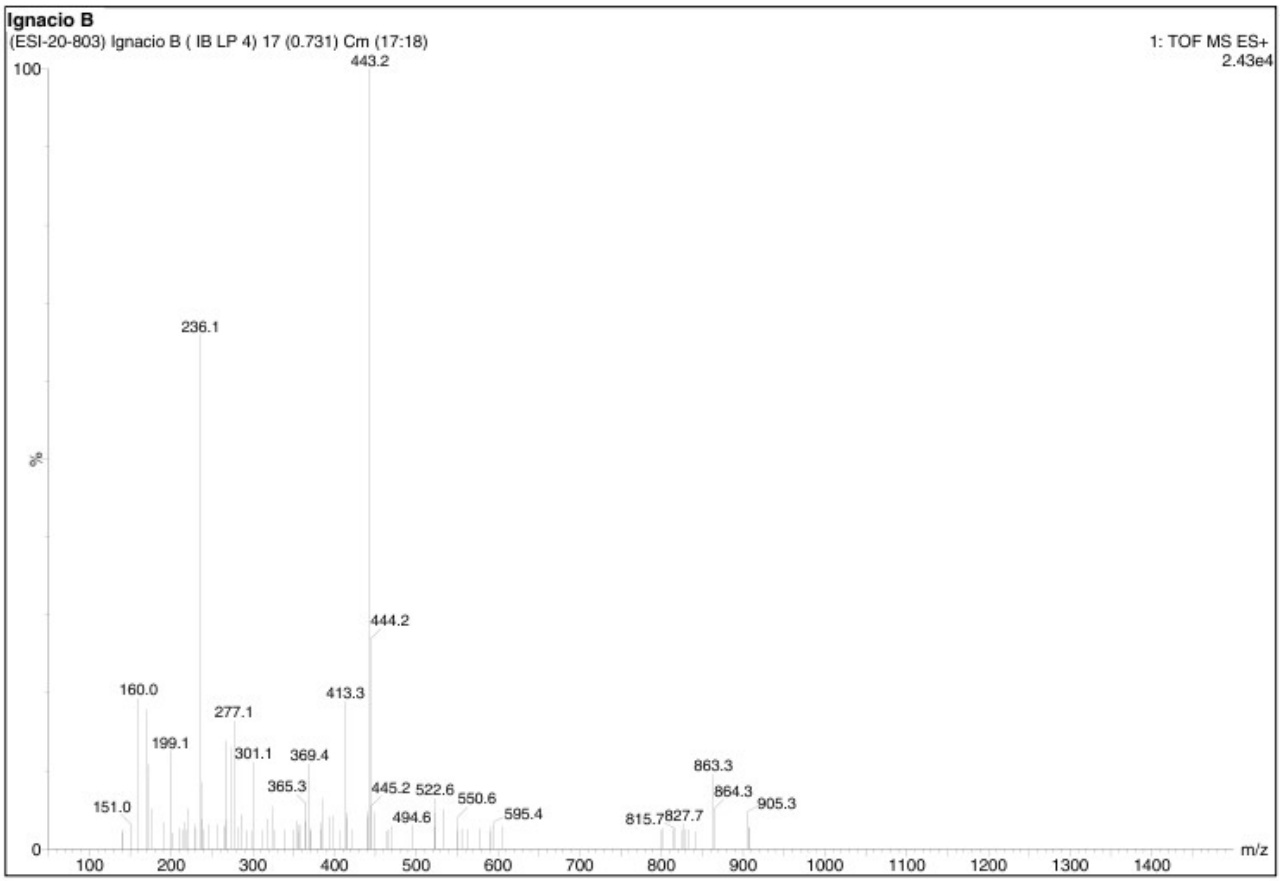


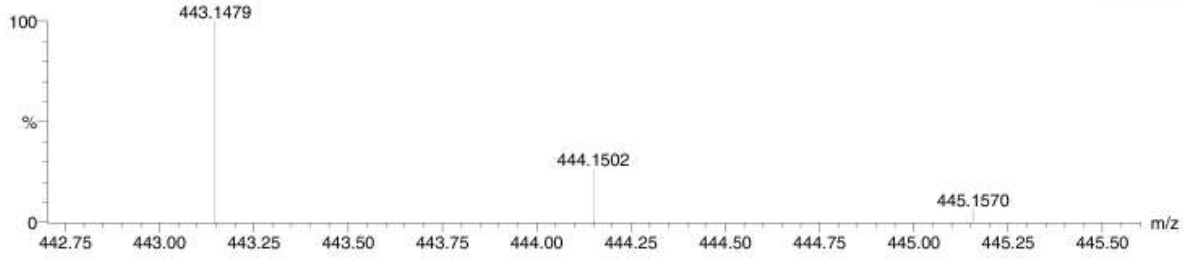
Figure S27: ESI-MS Spectrum of Compound **7**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
717 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-3 O: 0-20 Na: 0-1
Ignacio B
(ESI-20-803) Ignacio B (IB LP 4) 30 (1.288)

1: TOF MS ES+
3.93e+003



Minimum:	30.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
443.1479	100.00	443.1471	0.8	1.8	13.5	9.6	0.1	C25 H24 O6 Na
		443.1489	-1.0	-2.3	0.5	16.8	7.3	C13 H28 N2 O13 Na
		443.1495	-1.6	-3.6	16.5	12.3	2.8	C27 H23 O6

Figure S28: HRESI-MS Spectrum of Compound **7**

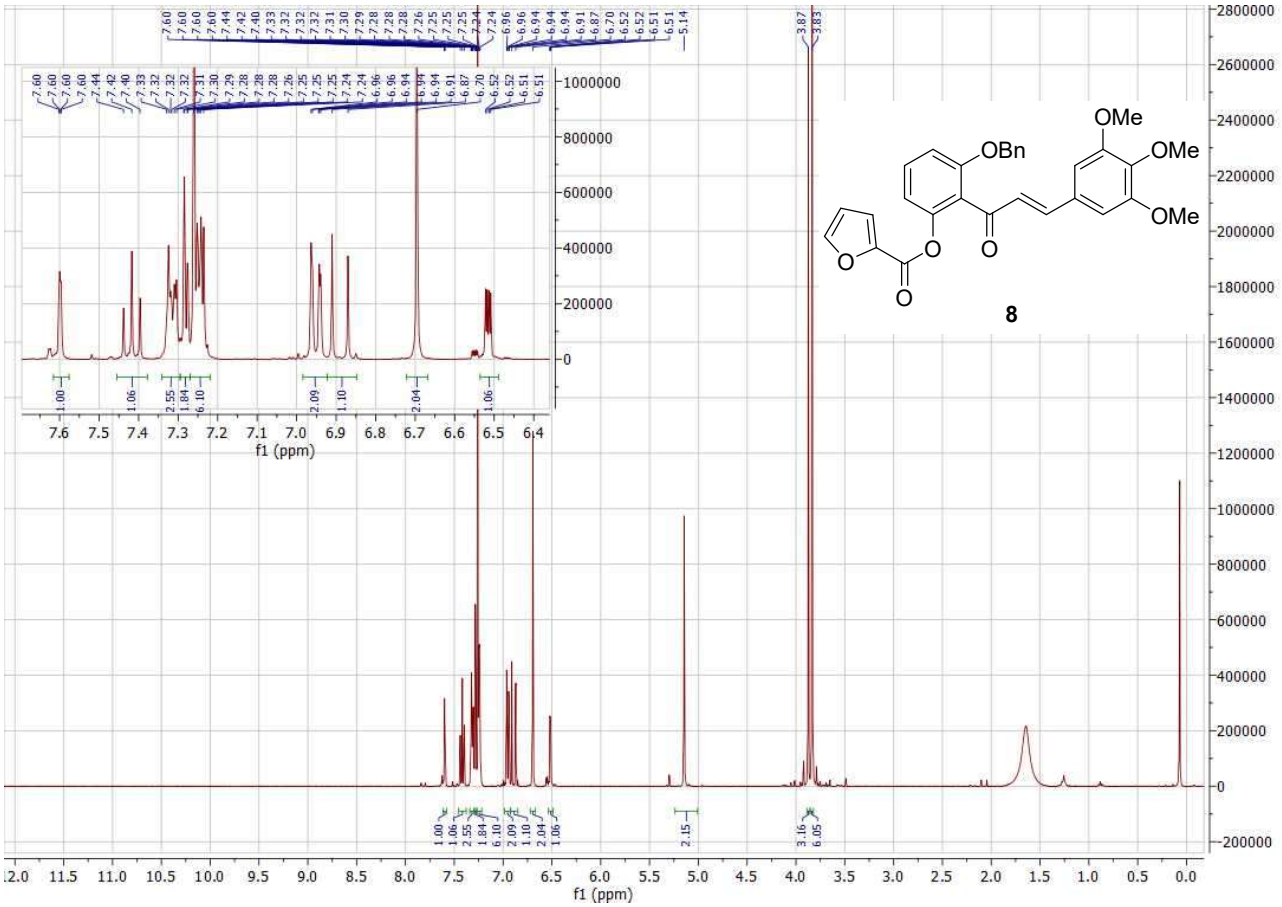


Figure S29: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **8**

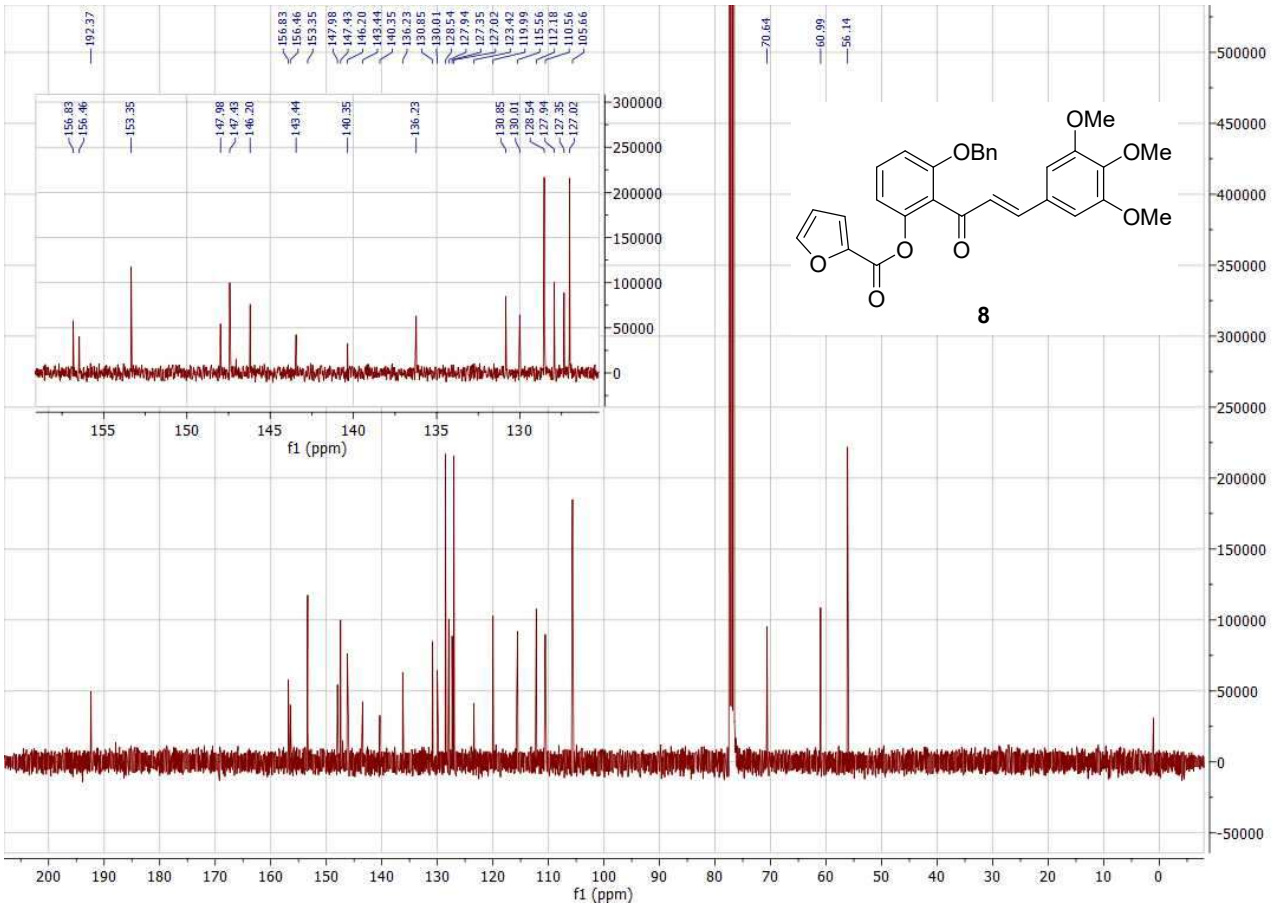


Figure S30: ^{13}C-NMR (101 MHz, $CDCl_3$) Spectrum of Compound **8**

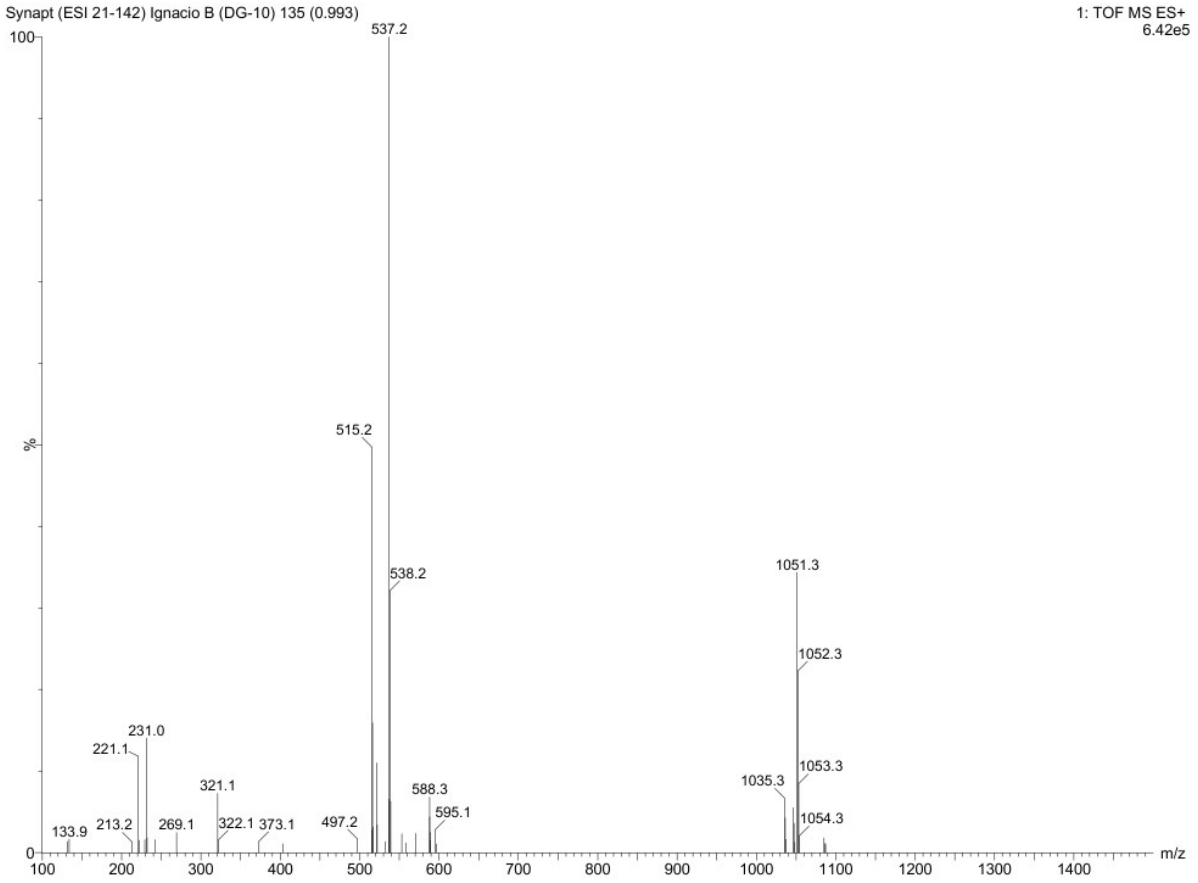
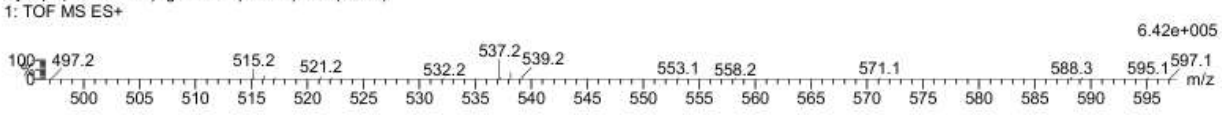


Figure S31: ESI-MS Spectrum of Compound **8**

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 3 mass(es) processed
Tolerance = 5.0 PPM / DBE: min = -20.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1533 formula(e) evaluated with 9 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-2 O: 0-10 Na: 0-2
Synapt (ESI 21-142) Ignacio B (DG-10) 135 (0.993)
1: TOF MS ES+



Minimum:	16.00				-20.0				
Maximum:	100.00		5.0	5.0	300.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
515.1707	49.70	515.1706	0.1	0.2	17.5	37.1	0.350	70.44	C30 H27 O8
		515.1682	2.5	4.9	14.5	38.1	1.368	25.47	C28 H28 O8 Na
		515.1711	-0.4	-0.8	20.5	40.0	3.197	4.09	C32 H25 N2 O2 Na2
537.1528	100.00	537.1525	0.3	0.6	17.5	41.0	0.248	78.02	C30 H26 O8 Na
		537.1501	2.7	5.0	14.5	42.6	1.869	15.42	C28 H27 O8 Na2
		537.1509	1.9	3.5	16.5	43.5	2.770	6.27	C27 H25 N2 O10
		537.1549	-2.1	-3.9	20.5	46.6	5.851	0.29	C32 H25 O8
538.1563	32.08	538.1572	-0.9	-1.7	30.5	36.6	0.602	54.77	C40 H21 N Na
		538.1548	1.5	2.8	27.5	36.8	0.793	45.23	C38 H22 N Na2

Figure S32: HRESI-MS Spectrum of Compound **8**

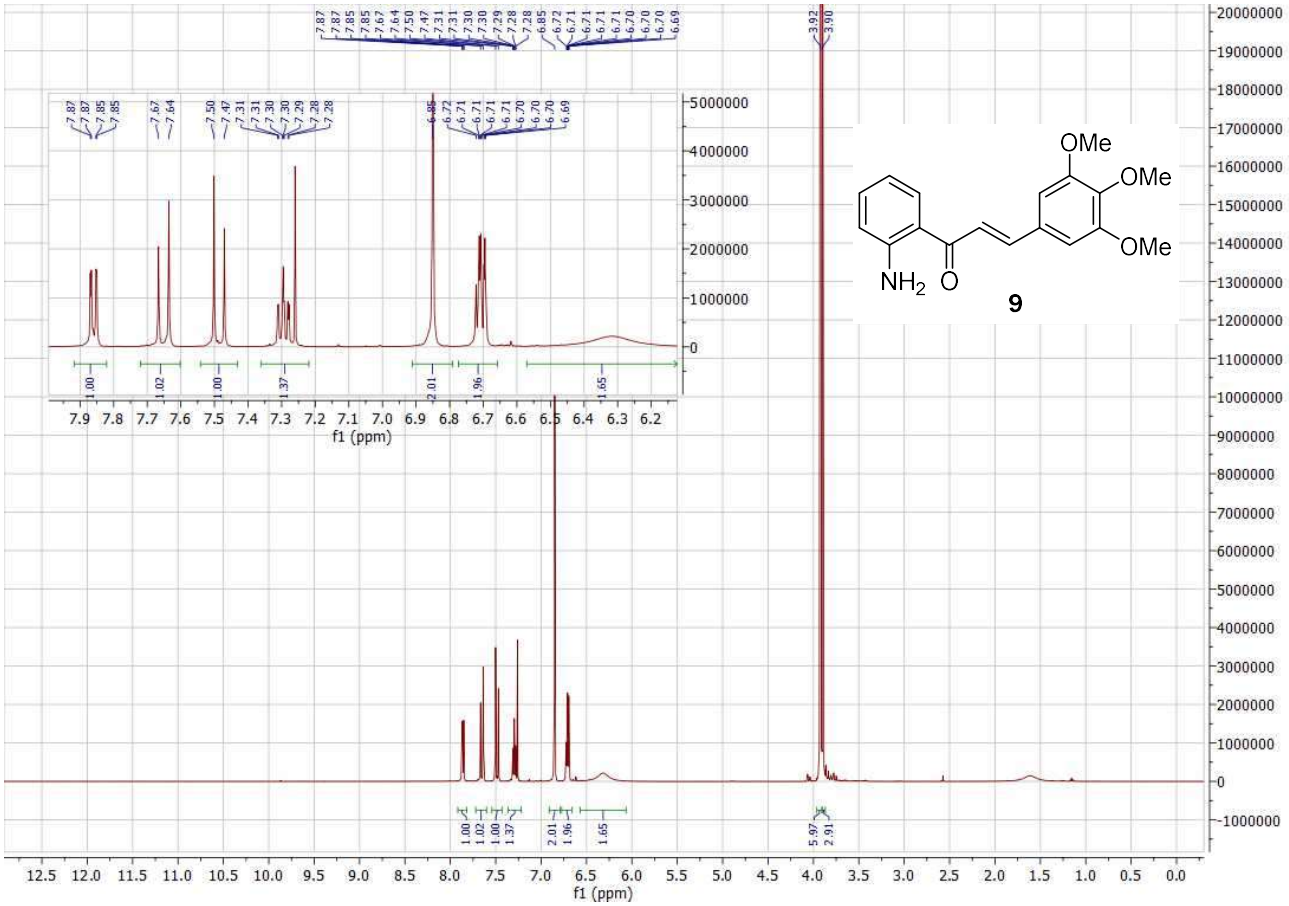


Figure S33: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **9**

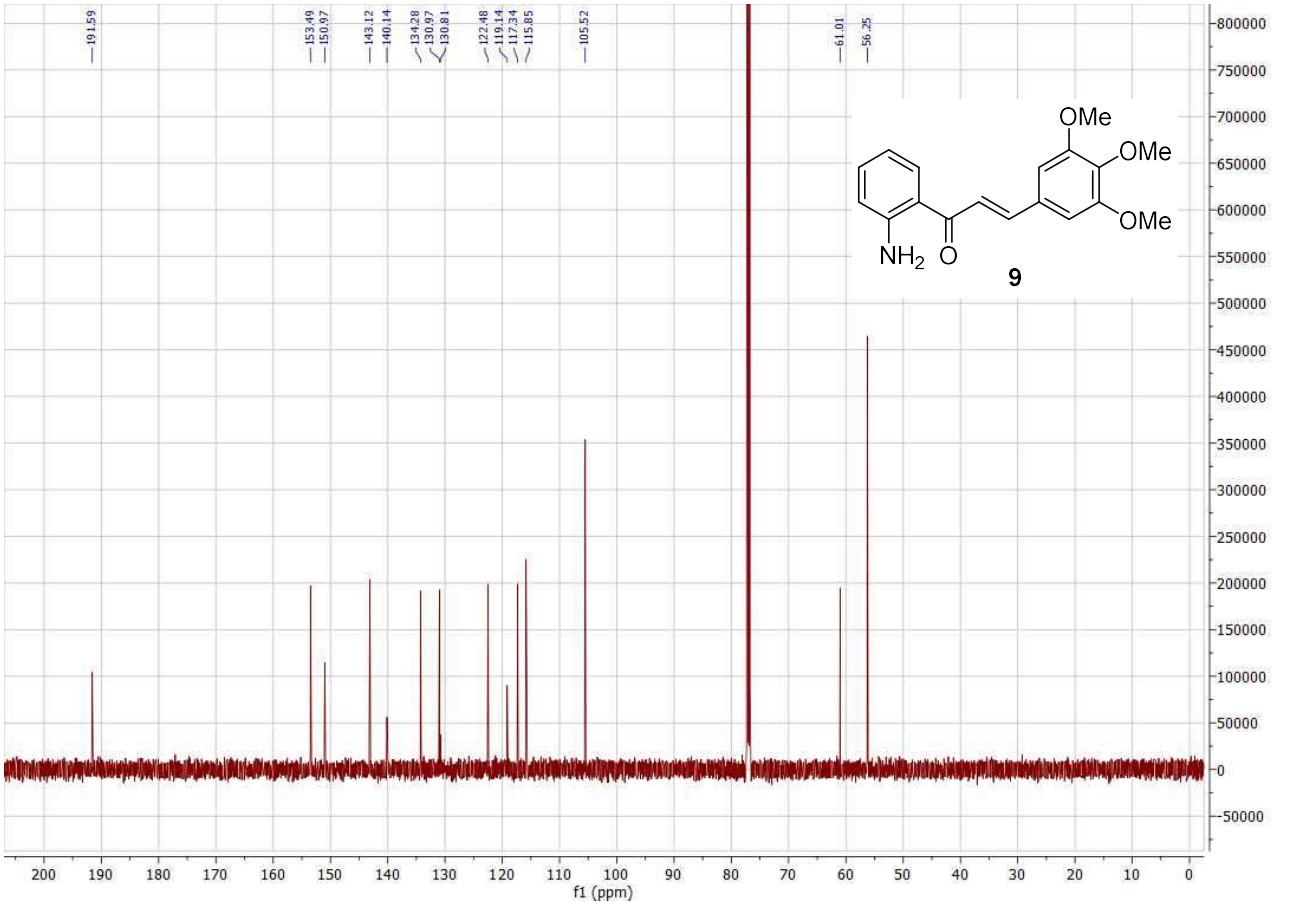


Figure S34: ^{13}C-NMR (126 MHz, $CDCl_3$) Spectrum of Compound **9**

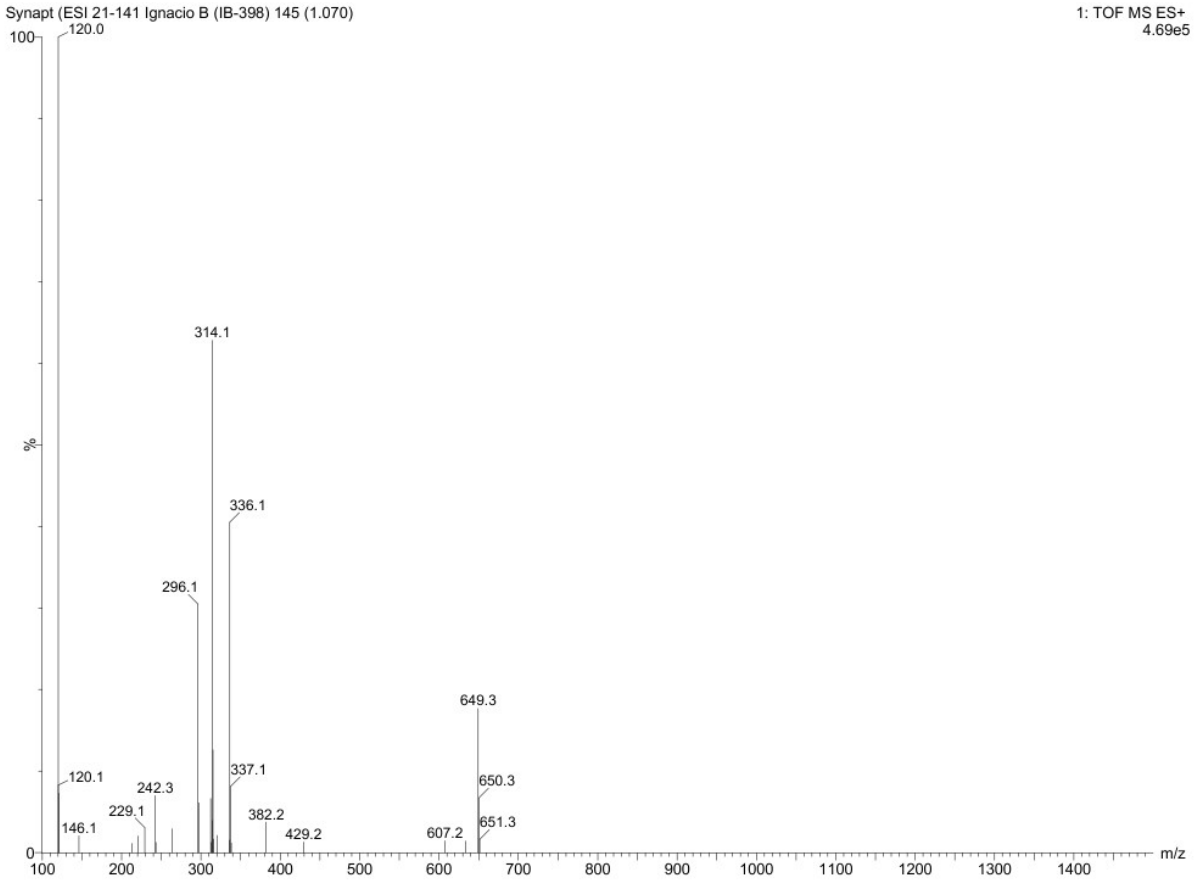
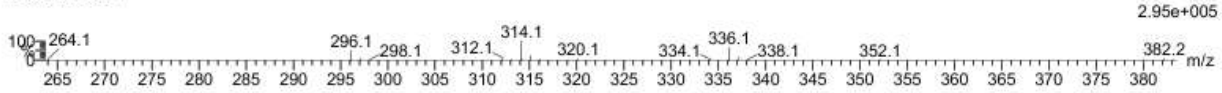


Figure S35: ESI-MS Spectrum of Compound **9**

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 4 mass(es) processed
Tolerance = 5.0 PPM / DBE: min = -20.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2035 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-2 O: 0-10 Na: 0-2
Synapt (ESI 21-141 Ignacio B (IB-398) 145 (1.070)
1: TOF MS ES+



Minimum:	16.00				-20.0				
Maximum:	100.00		5.0	5.0	300.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
296.1288	48.47	296.1287	0.1	0.3	10.5	27.1	0.000	100.00	C18 H18 N O3
		296.1297	-0.9	-3.0	-4.5	43.1	16.031	0.00	C7 H24 N O8 Na2
314.1394	100.00	314.1392	0.2	0.6	9.5	30.7	0.000	100.00	C18 H20 N O4
		314.1403	-0.9	-2.9	-5.5	48.5	17.730	0.00	C7 H26 N O9 Na2
315.1427	20.04	315.1420	0.7	2.2	1.5	30.9	n/a	n/a	C13 H24 O7 Na
336.1212	64.46	336.1212	0.0	0.0	9.5	26.4	n/a	n/a	C18 H19 N O4 Na

Figure S36: HRESI-MS Spectrum of Compound **9**

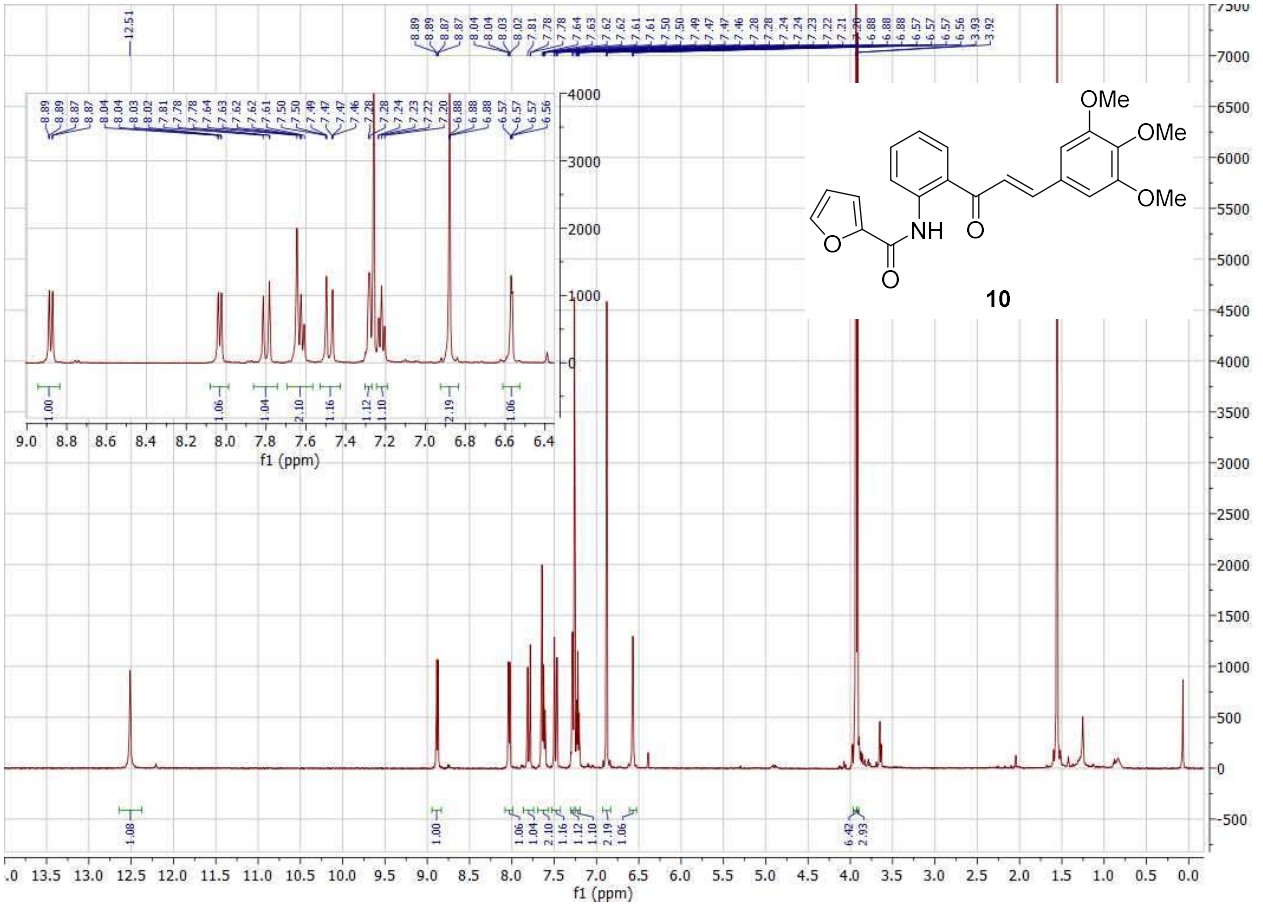


Figure S37: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **10**

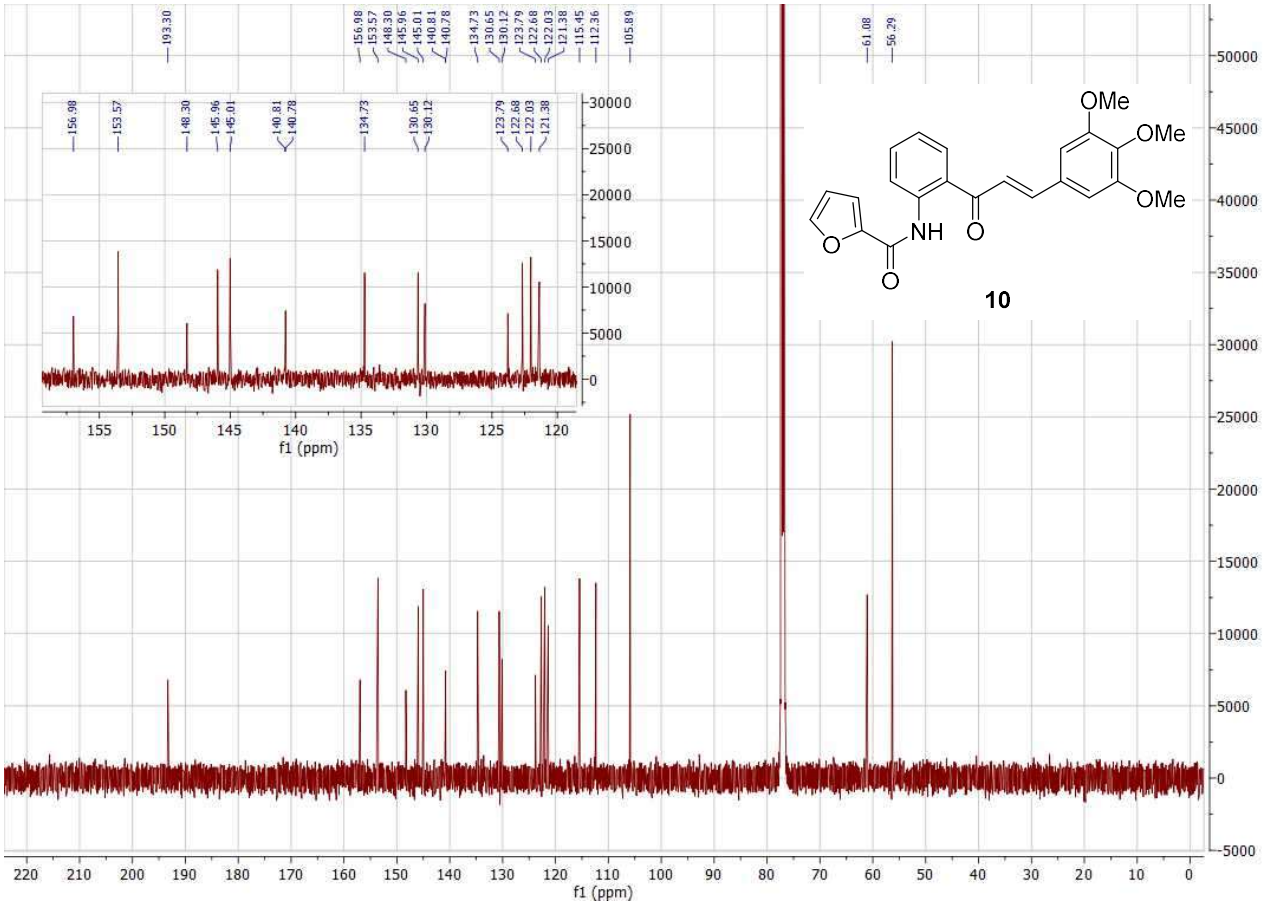


Figure S38: ^{13}C-NMR (126 MHz, $CDCl_3$) Spectrum of Compound **10**

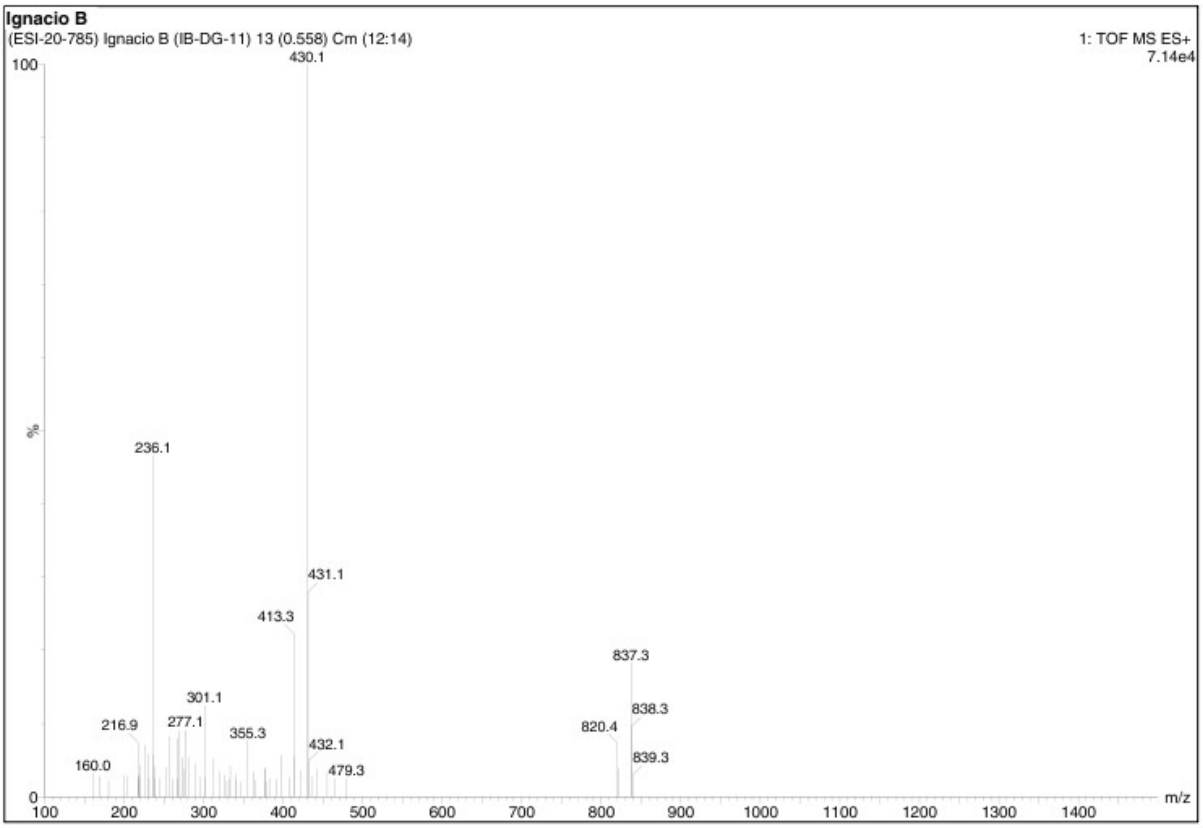


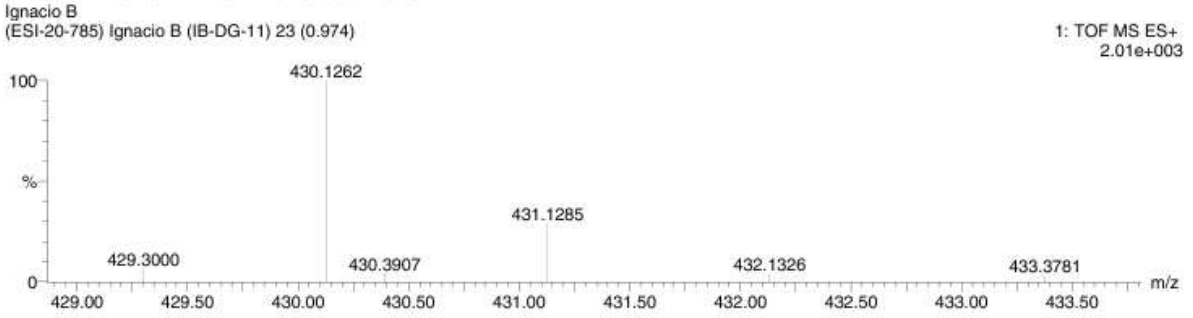
Figure S39: ESI-MS Spectrum of Compound **10**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
487 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-44 H: 0-52 N: 0-4 O: 0-10 Na: 0-1

Ignacio B
(ESI-20-785) Ignacio B (IB-DG-11) 23 (0.974)



Minimum:	50.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
430.1262	100.00	430.1267	-0.5	-1.2	13.5	16.8	0.2	C23 H21 N O6 Na
		430.1250	1.2	2.8	12.5	18.5	1.9	C20 H20 N3 O8

Figure S40: HRESI-MS Spectrum of Compound **10**

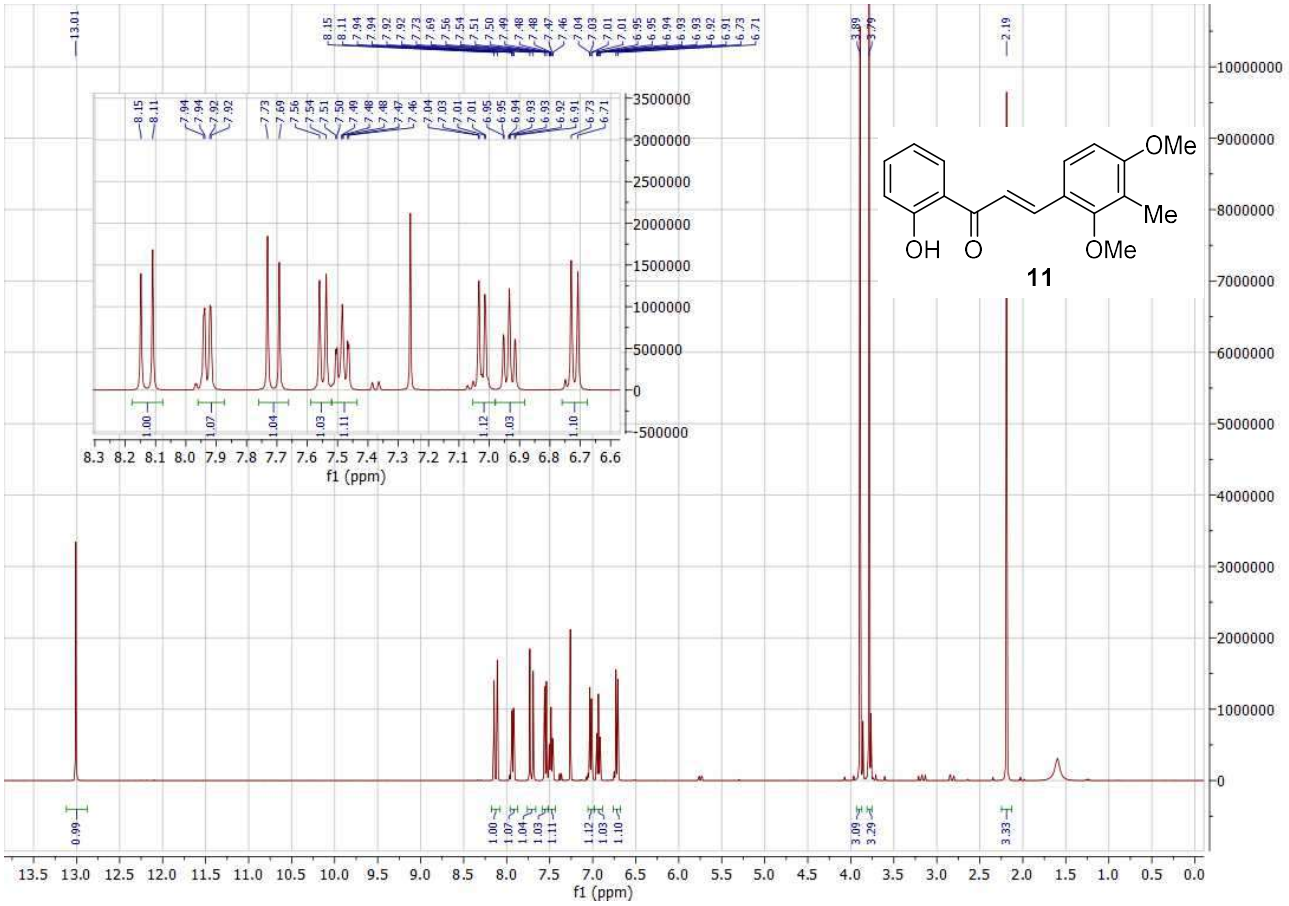


Figure S41: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **11**

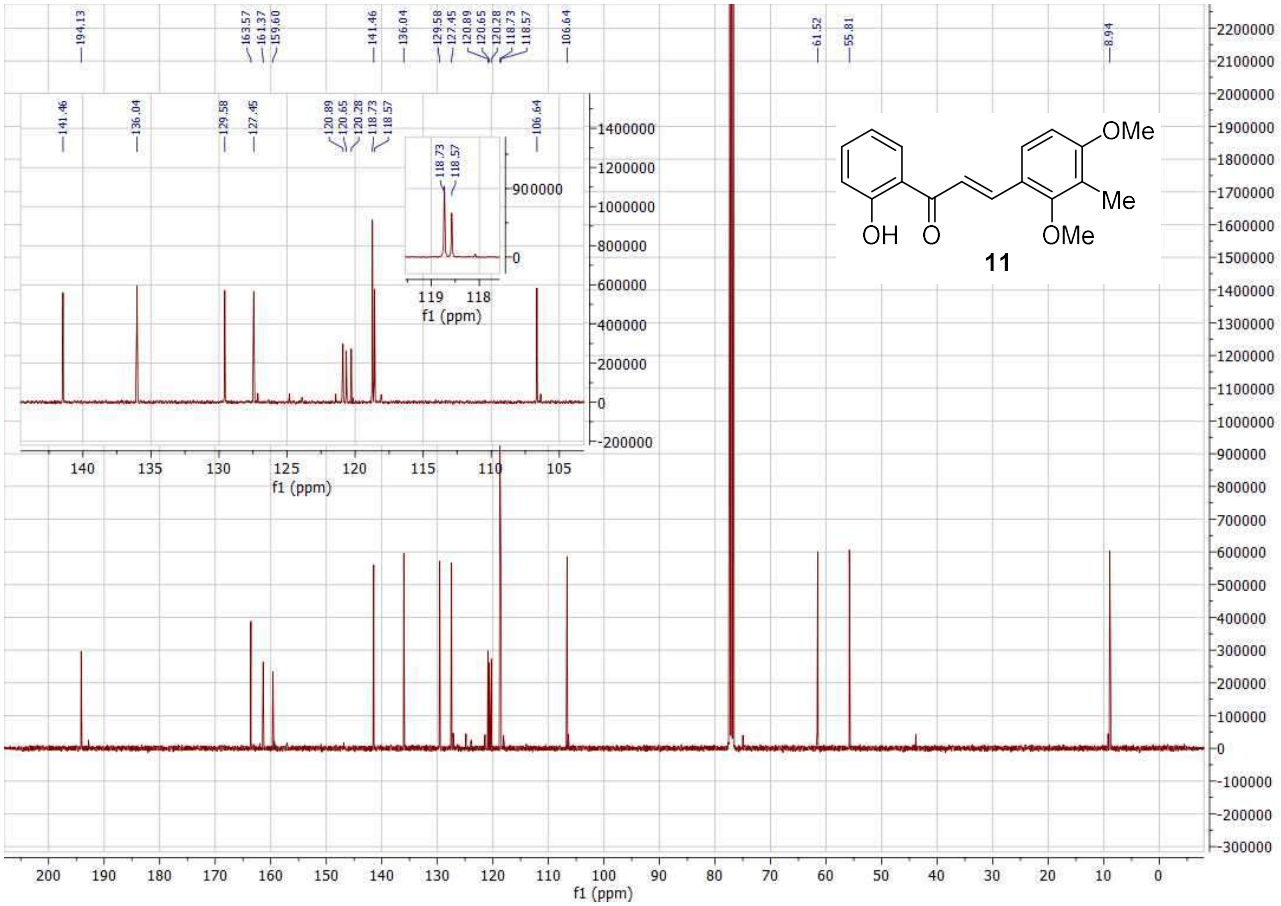


Figure S42: ^{13}C-NMR (101 MHz, $CDCl_3$) Spectrum of Compound **11**

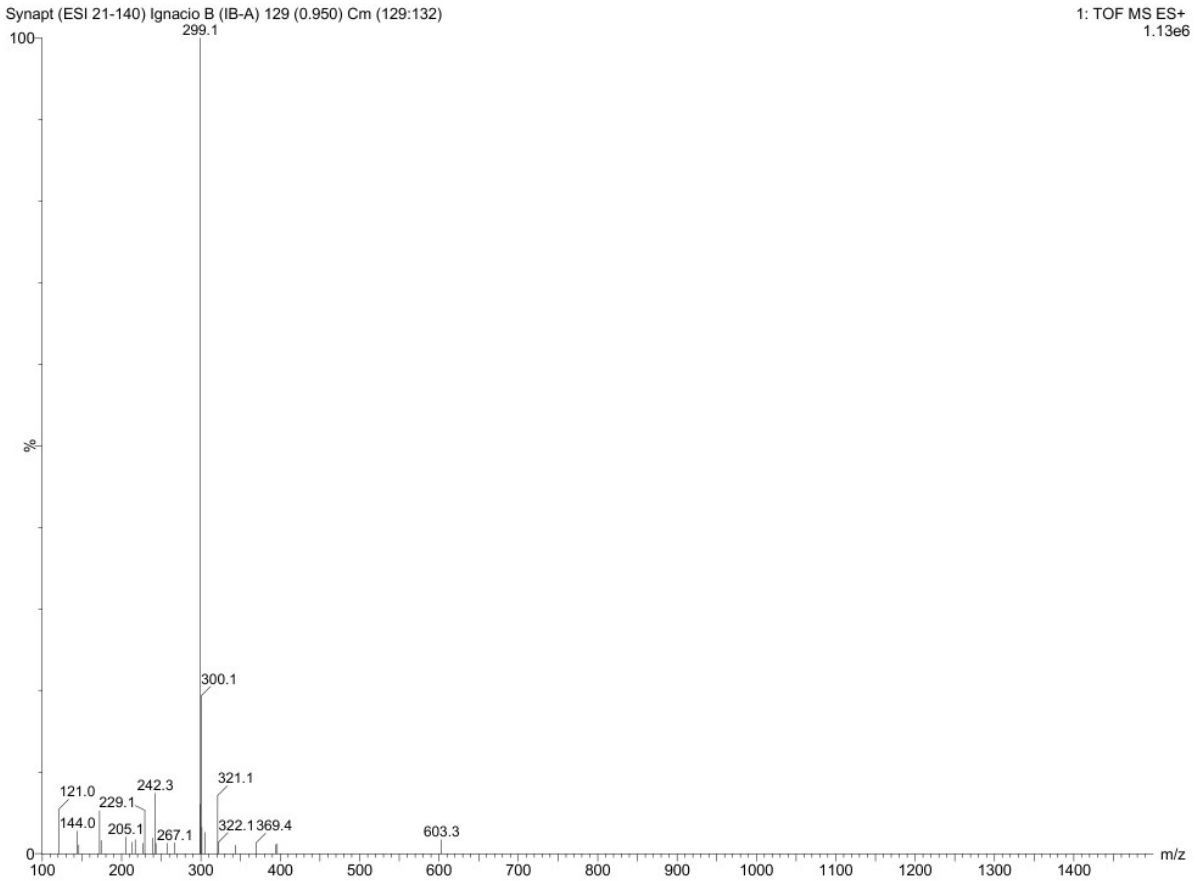


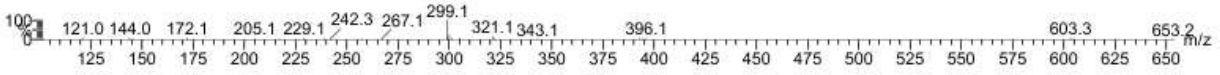
Figure S43: ESI-MS Spectrum of Compound **11**

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 5.0 PPM / DBE: min = -20.0, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1013 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-60 N: 0-2 O: 0-10 Na: 0-2
Synapt (ESI 21-140) Ignacio B (IB-A) 120 (0.885)
1: TOF MS ES+

5.36e+005



Minimum:	16.00				-20.0				
Maximum:	100.00		5.0	5.0	300.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
299.1284	100.00	299.1283	0.1	0.3	9.5	30.5	0.000	100.00	C18 H19 O4
		299.1294	-1.0	-3.3	-5.5	52.8	22.291	0.00	C7 H25 O9 Na2
300.1318	19.91	---							

Figure S44: HRESI-MS Spectrum of Compound **11**

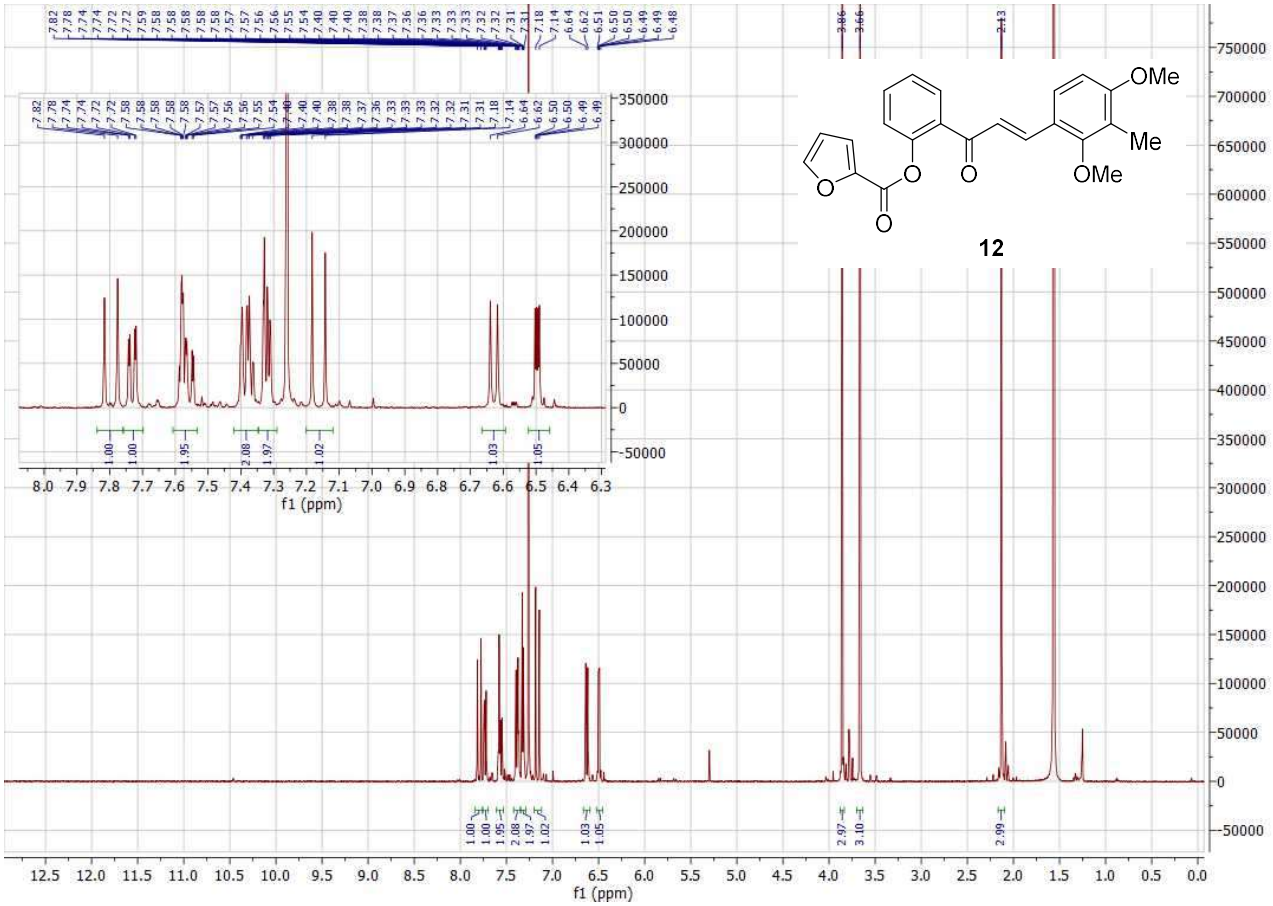


Figure S45: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **12**

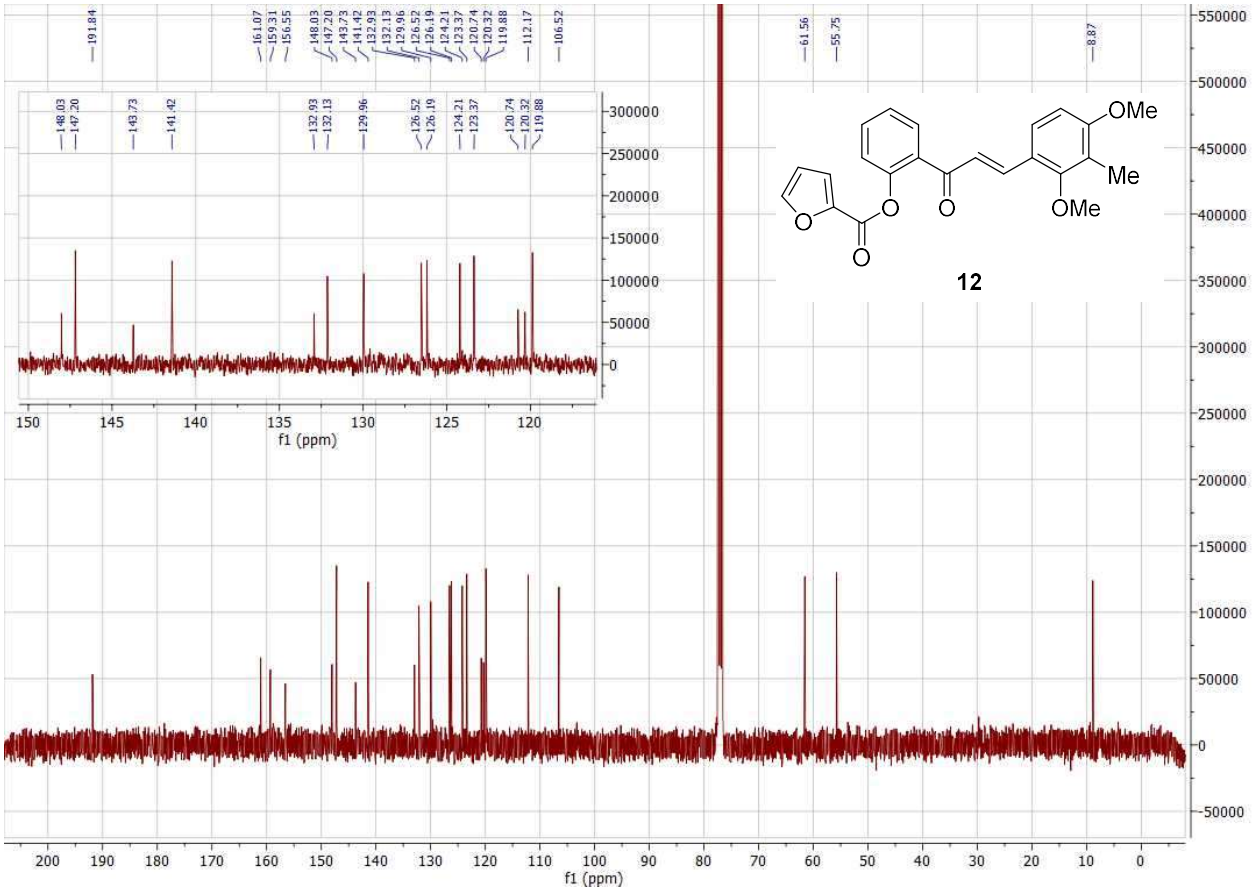


Figure S46: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **12**

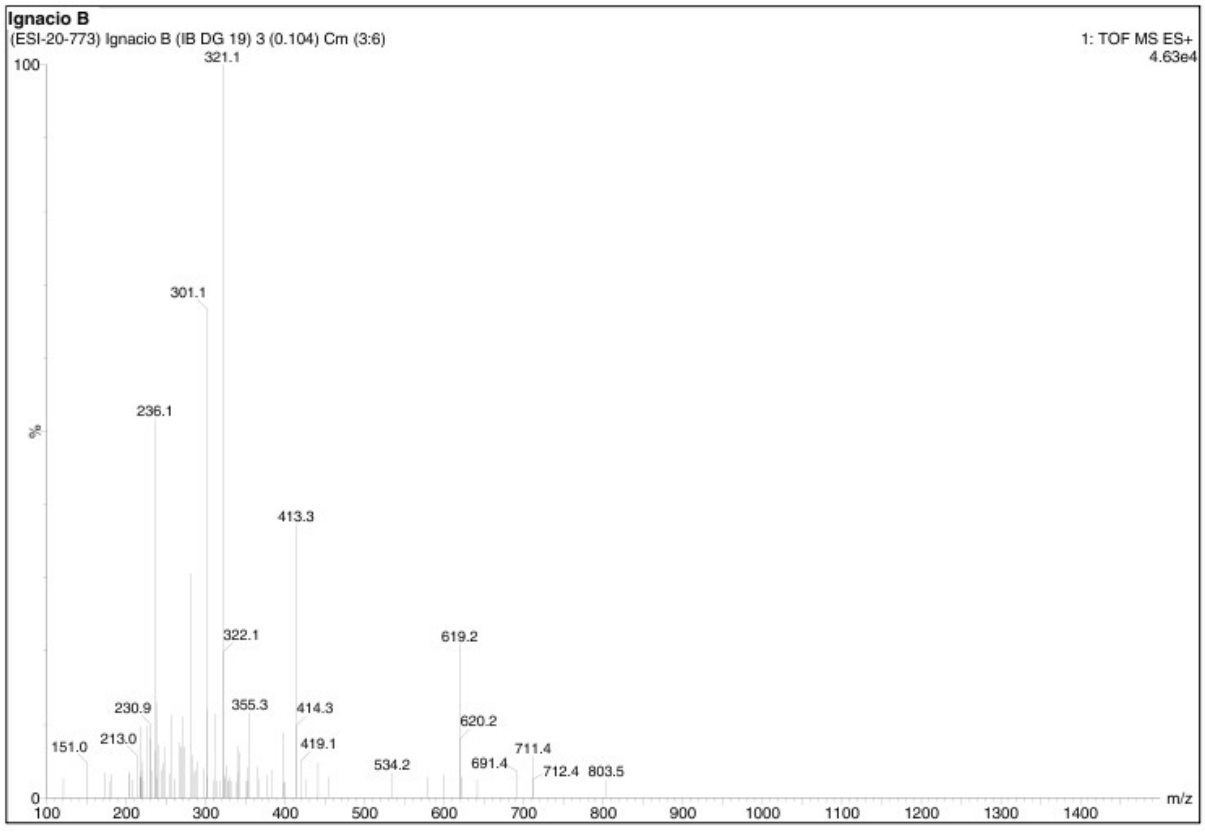


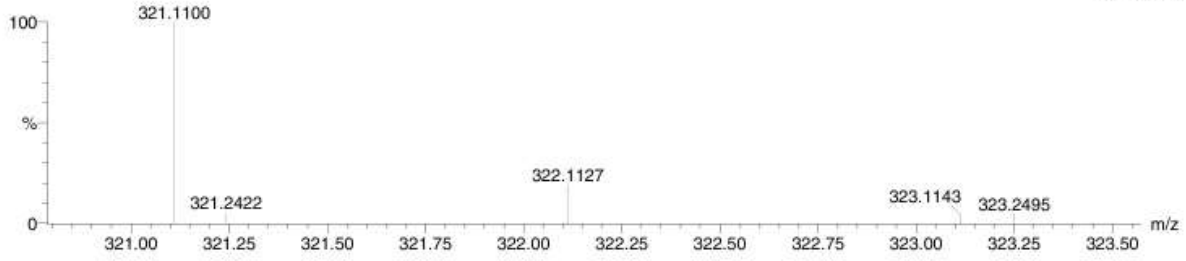
Figure S47: ESI-MS Spectrum of Compound **12**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
372 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-70 H: 0-100 N: 0-3 O: 0-12 Na: 0-1
Ignacio B
(ESI-20-773) Ignacio B (IB DG 19) 26 (1.114)

1: TOF MS ES+
2.90e+003



Minimum:	30.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
321.1100	100.00	321.1103	-0.3	-0.9	9.5	27.9	0.3	C18 H18 O4 Na
		321.1087	1.3	4.0	8.5	29.0	1.3	C15 H17 N2 O6

Figure S48: HRESI-MS Spectrum of Compound **12**

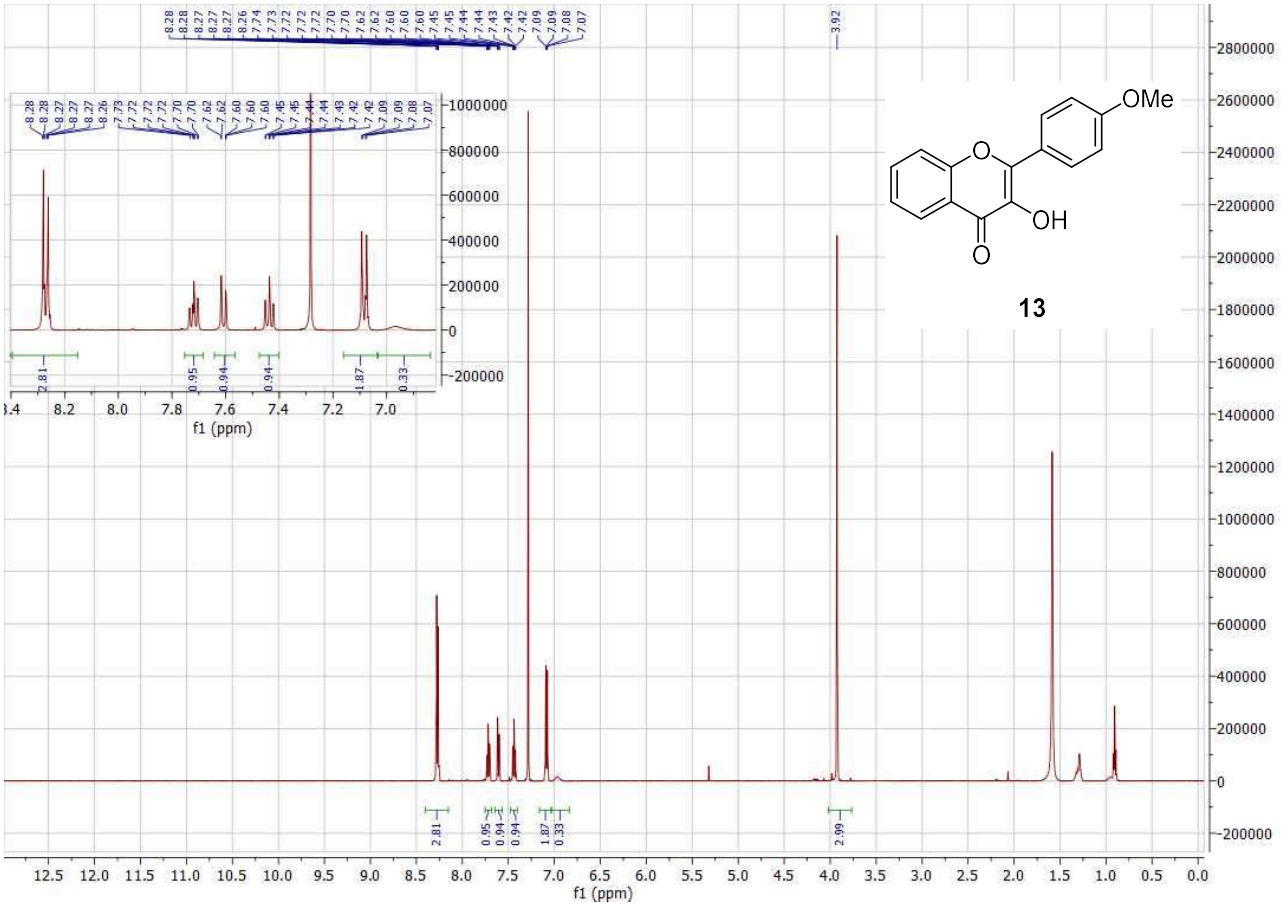


Figure S49: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **13**

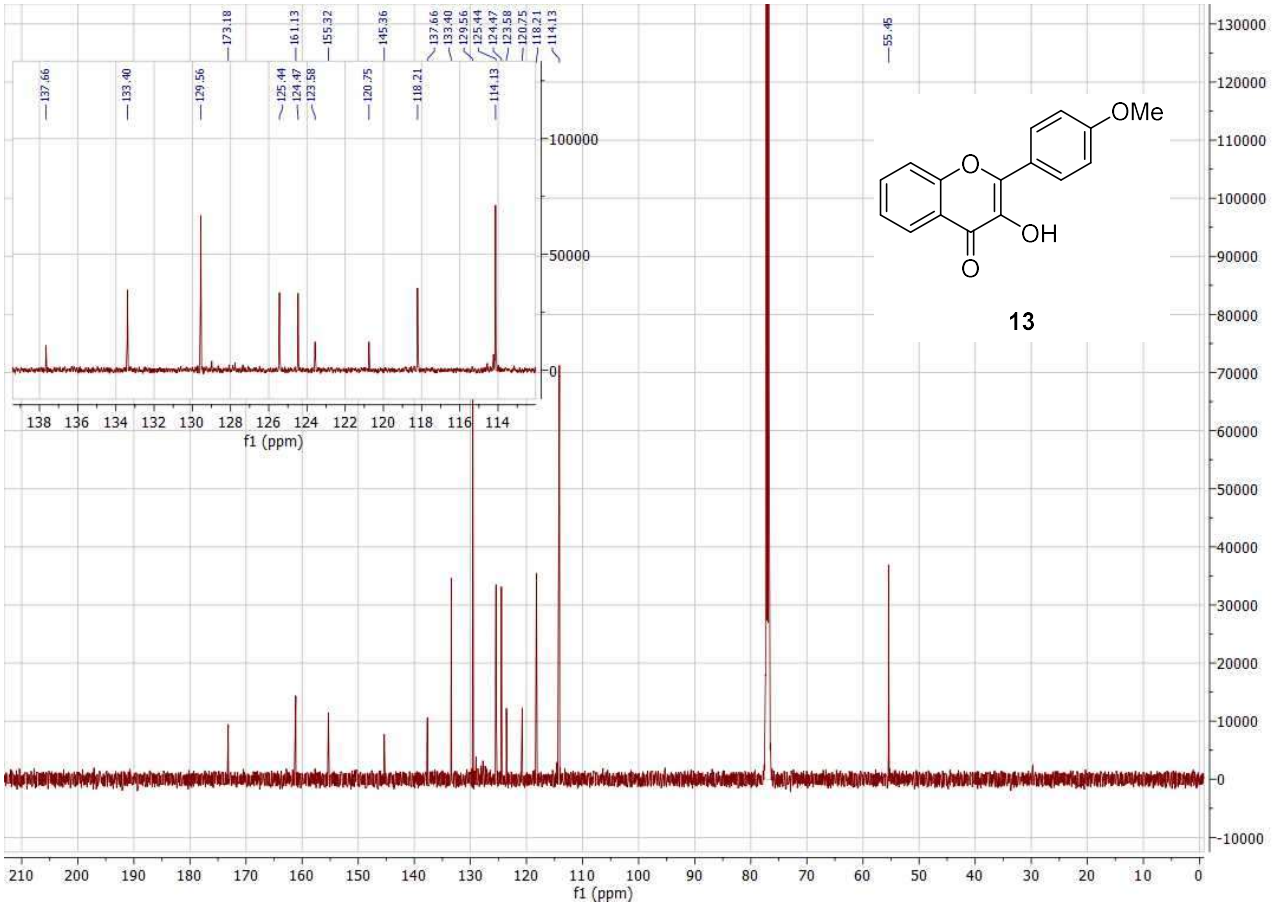


Figure S50: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **13**

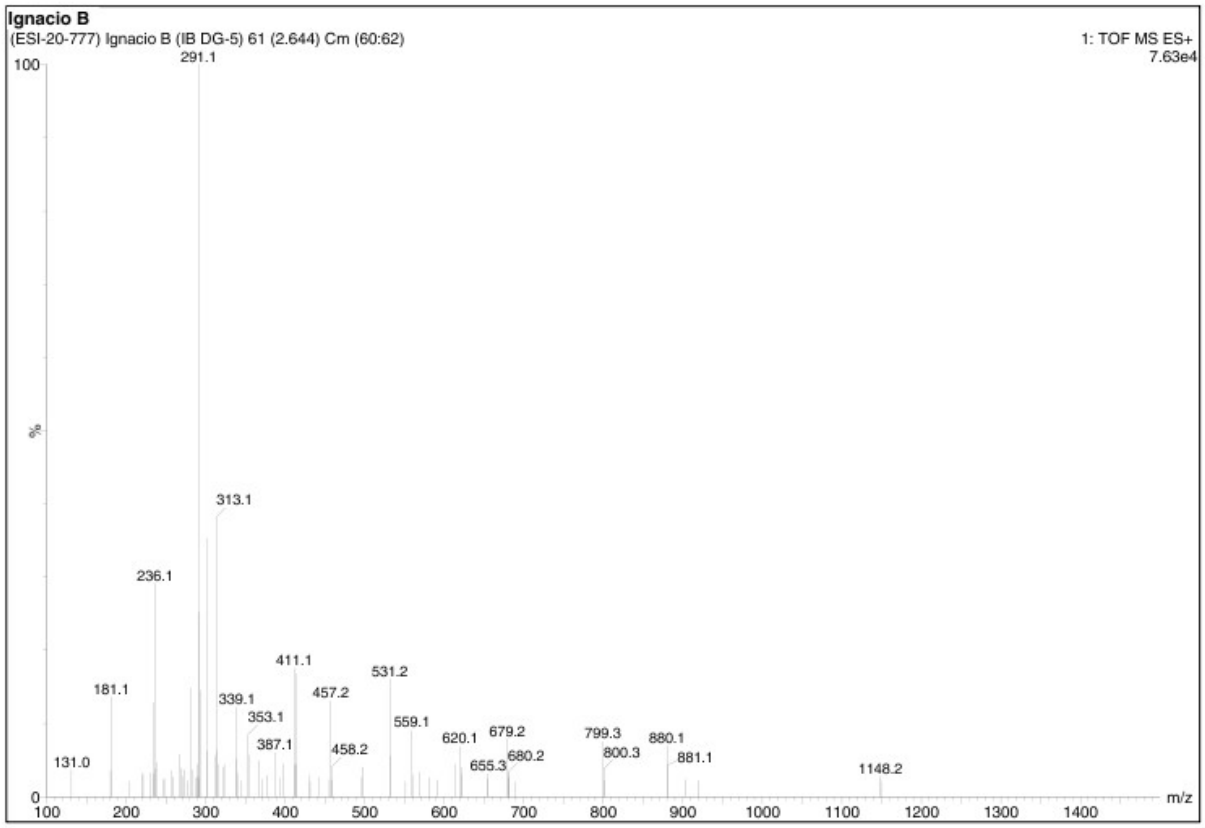


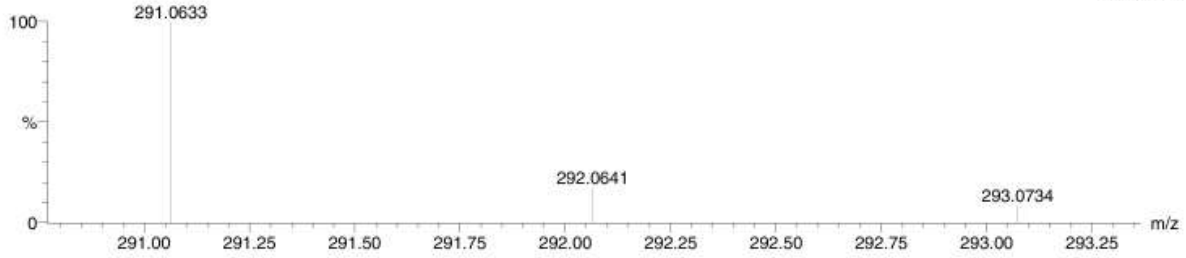
Figure S51: ESI-MS Spectrum of Compound **13**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-44 H: 0-52 O: 0-4 Na: 0-1
Ignacio B
(ESI-20-777) Ignacio B (IB DG-5) 1 (0.036)

1: TOF MS ES+
9.66e+003



Minimum:	50.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
291.0633	100.00	291.0633	0.0	0.0	10.5	21.9	0.0	C16 H12 O4 Na

Figure S52: HRESI-MS Spectrum of Compound **13**

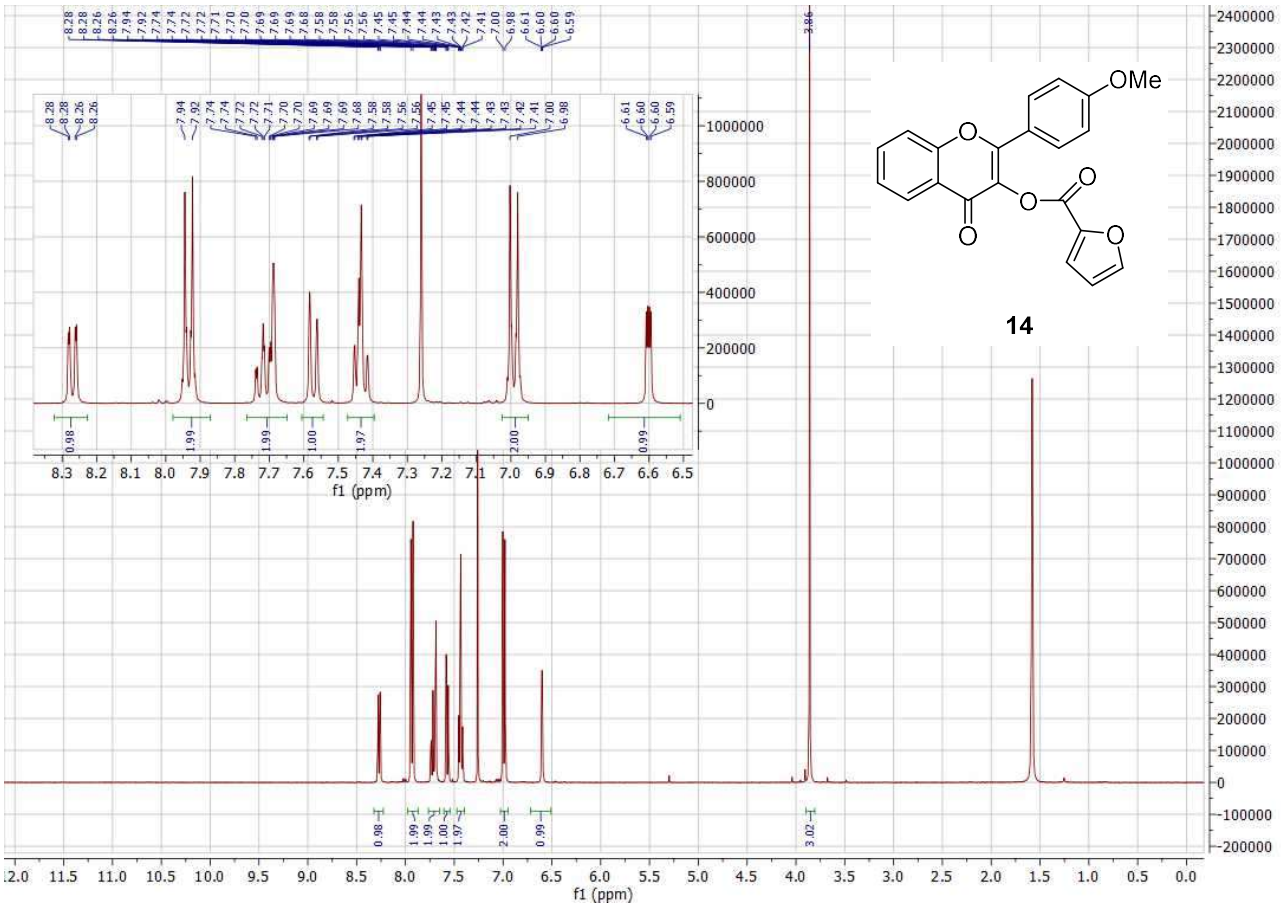


Figure S53: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **14**

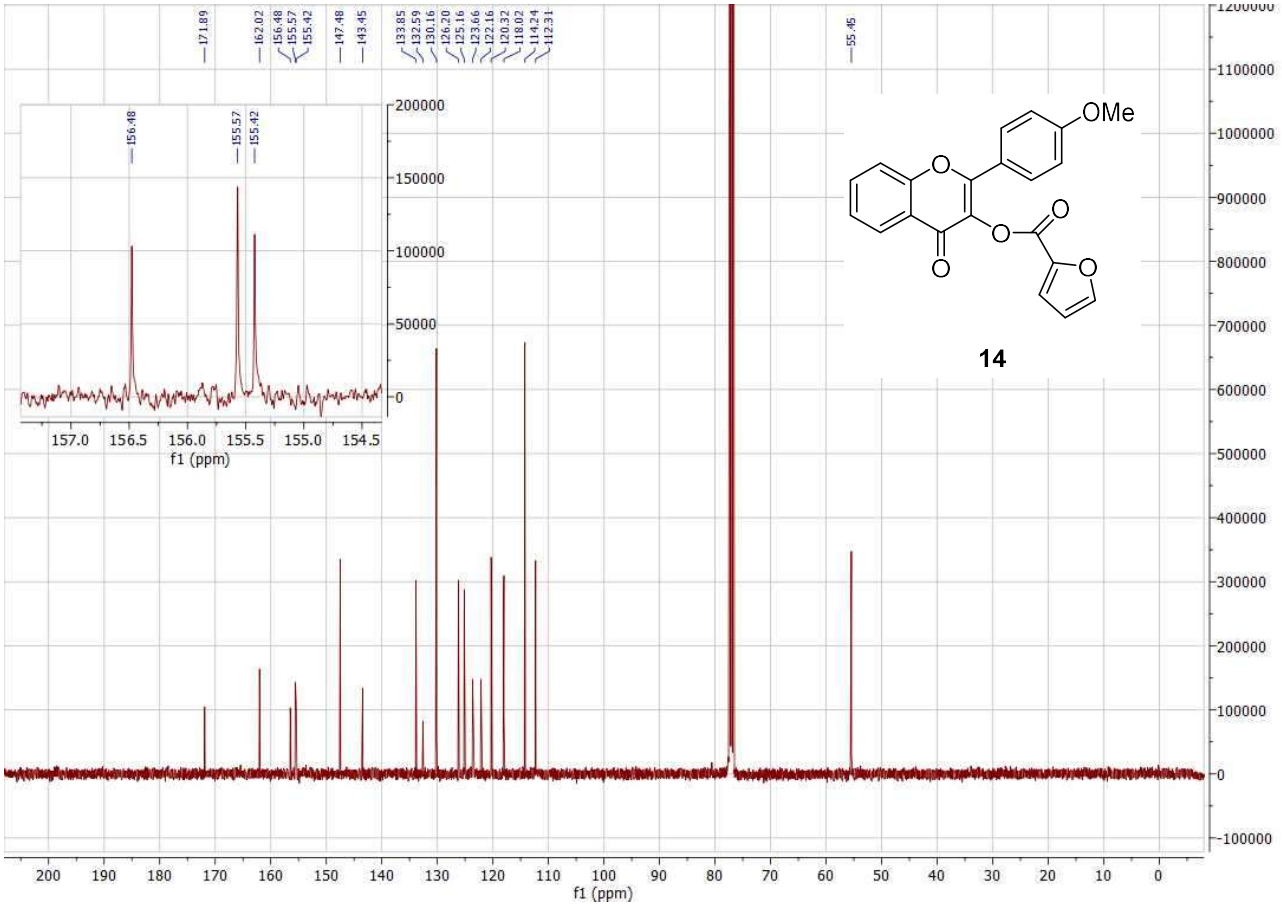


Figure S54: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **14**

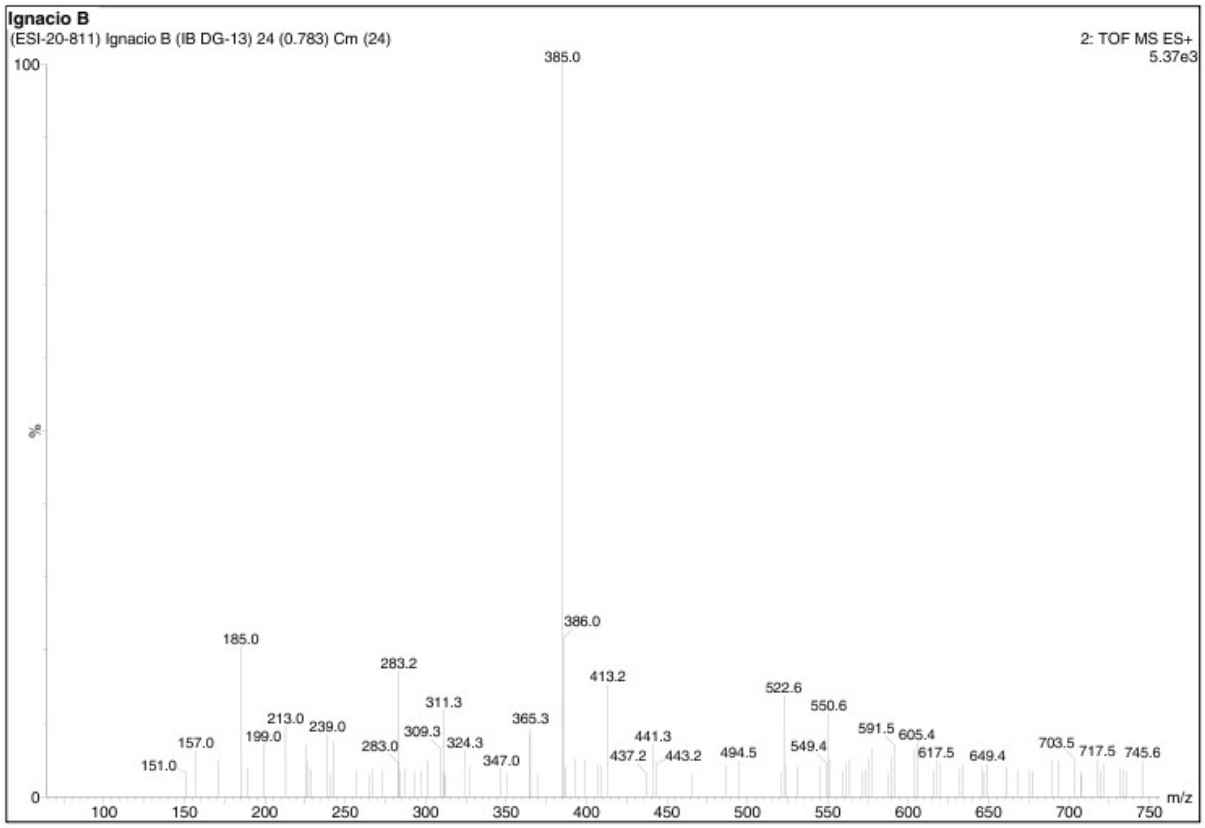


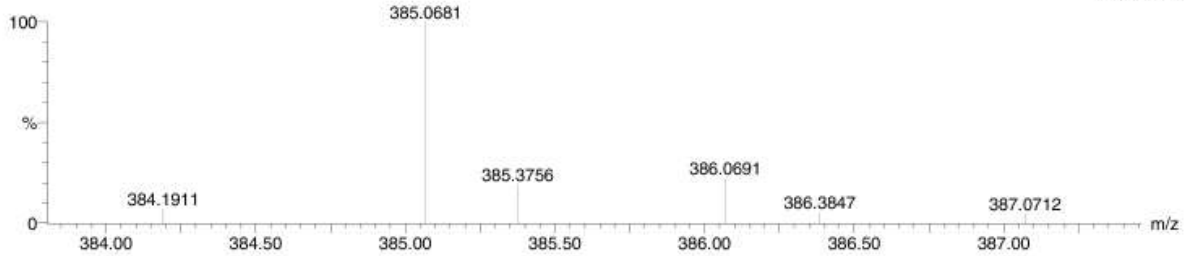
Figure S55: ESI-MS Spectrum of Compound **14**

Elemental Composition Report **Page 1**

Tolerance = 5.0 PPM / DBE: min = -3.0, max = 120.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
452 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-70 H: 0-100 N: 0-3 O: 0-12 Na: 0-1
Ignacio B
(ESI-20-811) Ignacio B (IB DG-13) 23 (0.974)

1: TOF MS ES+
7.75e+003



Minimum:	30.00				-3.0			
Maximum:	100.00		5.0	5.0	120.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
385.0681	100.00	385.0688	-0.7	-1.8	14.5	40.1	1.6	C21 H14 O6 Na
		385.0672	0.9	2.3	13.5	38.8	0.2	C18 H13 N2 O8

Figure S56: HRESI-MS Spectrum of Compound **14**