Supplementary Information

Antimicrobial, Anti-Inflammatory and Antioxidant Activities of Polyoxygenated Chalcones

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NMR spectra of chalcones **11**-**19**

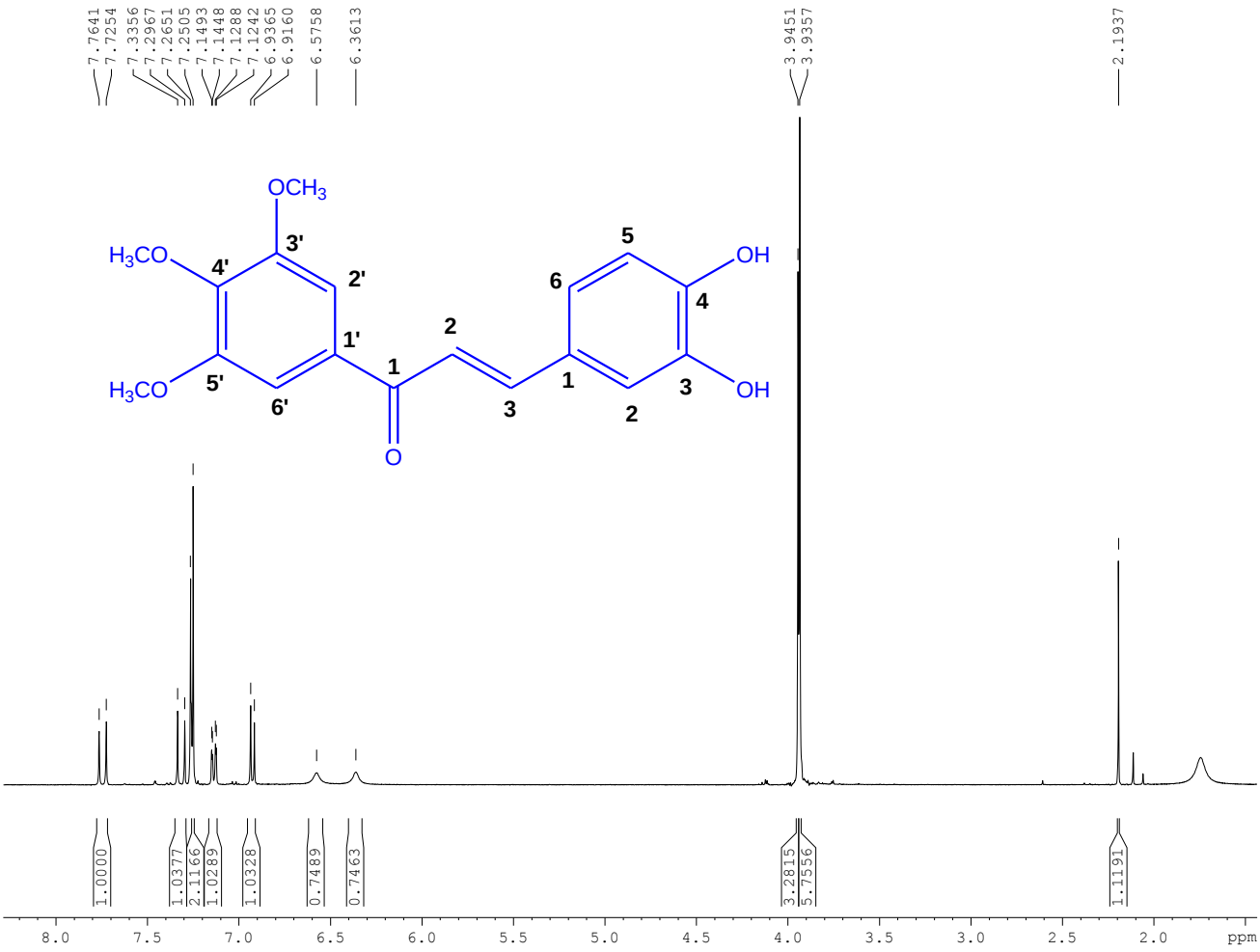


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11**.

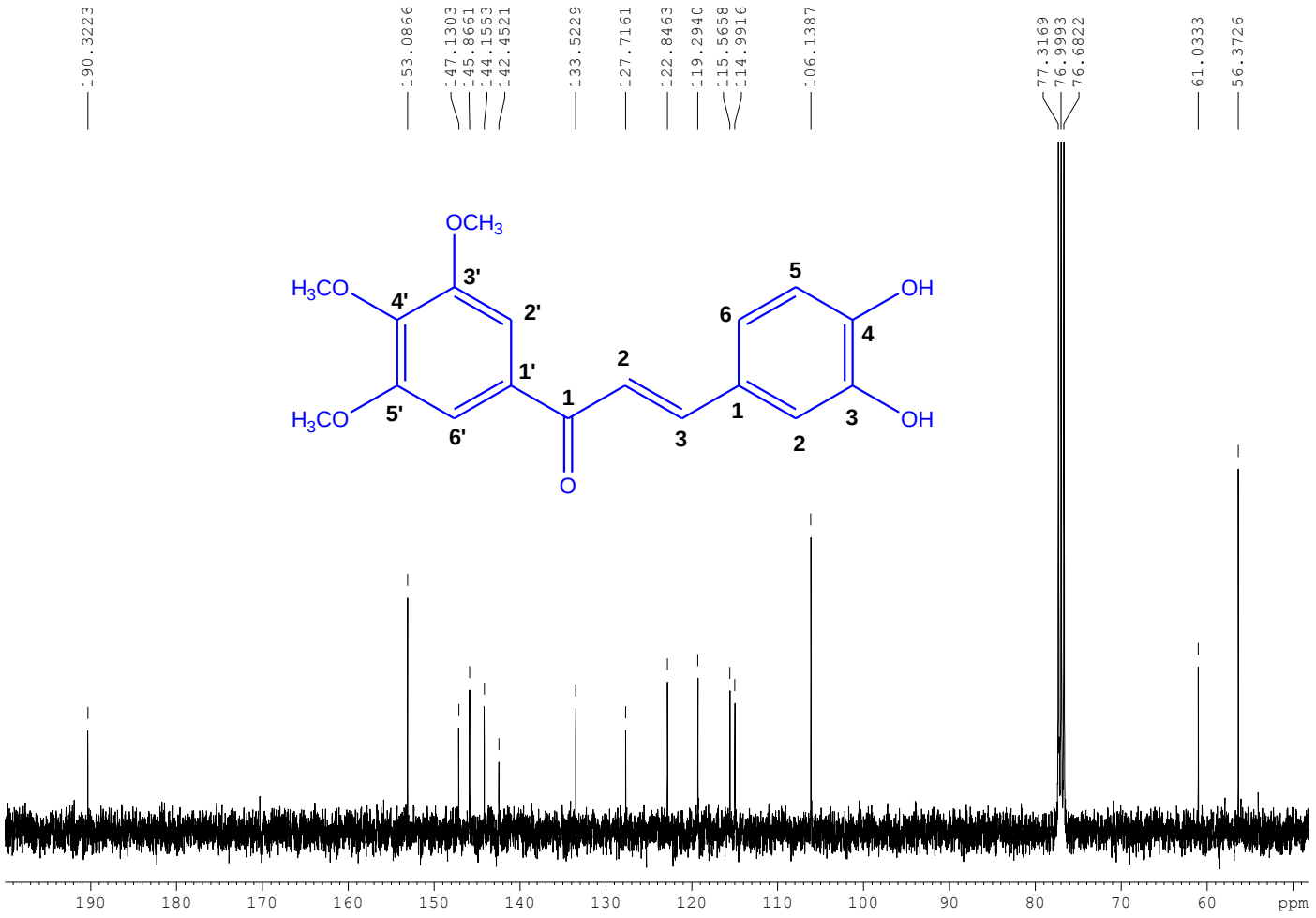


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **11**.

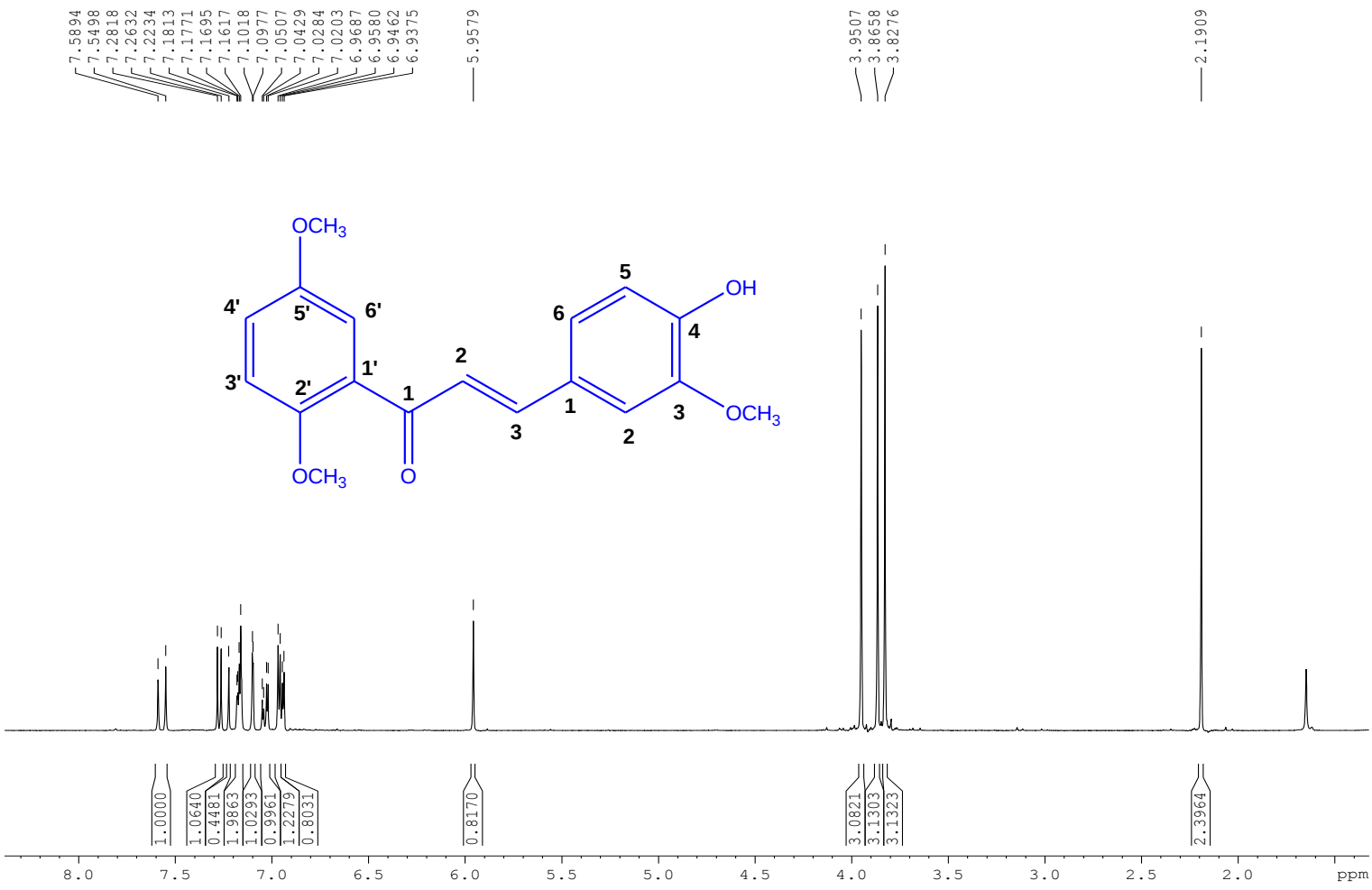


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **12**.

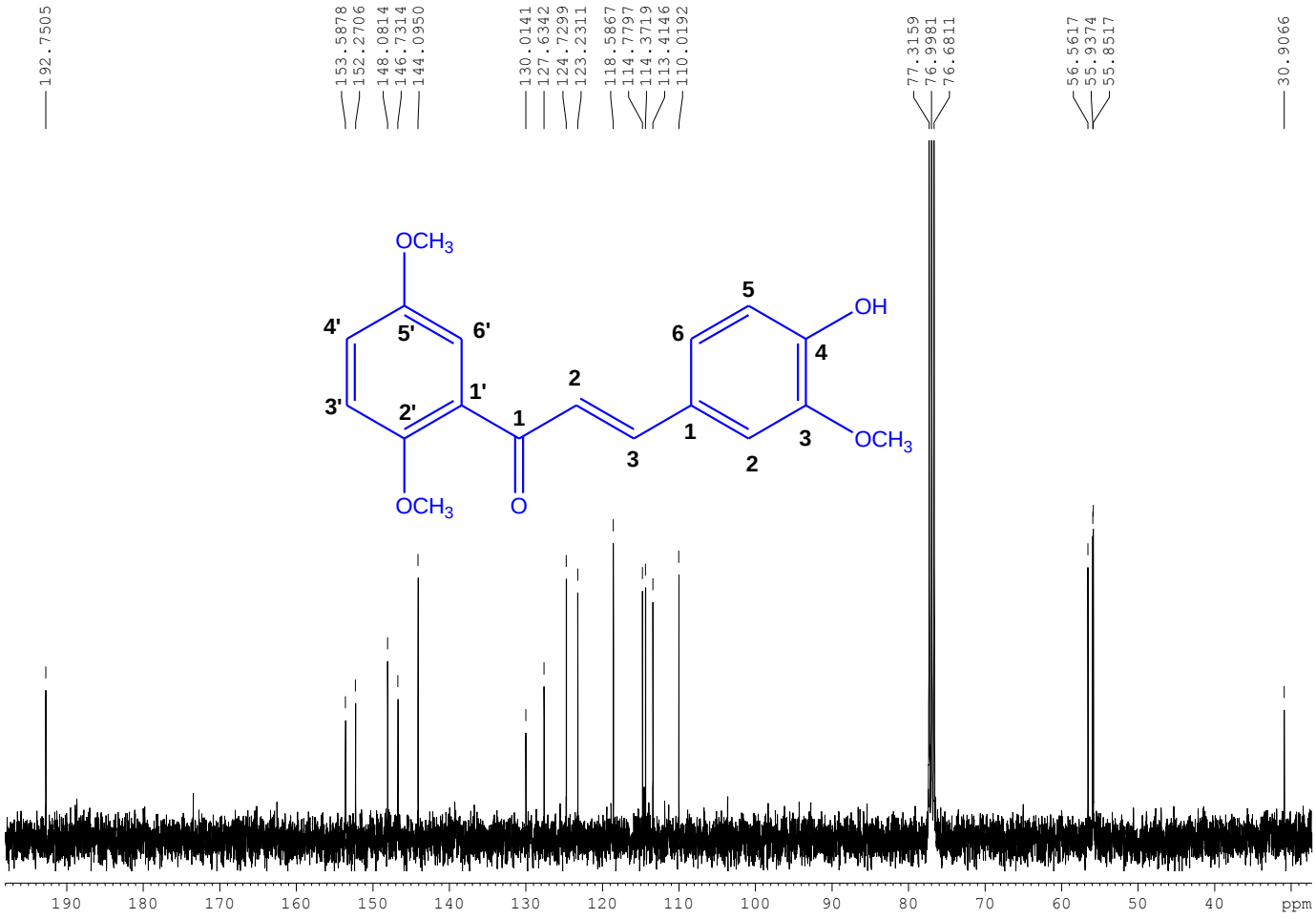


Figure S4. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **12**.

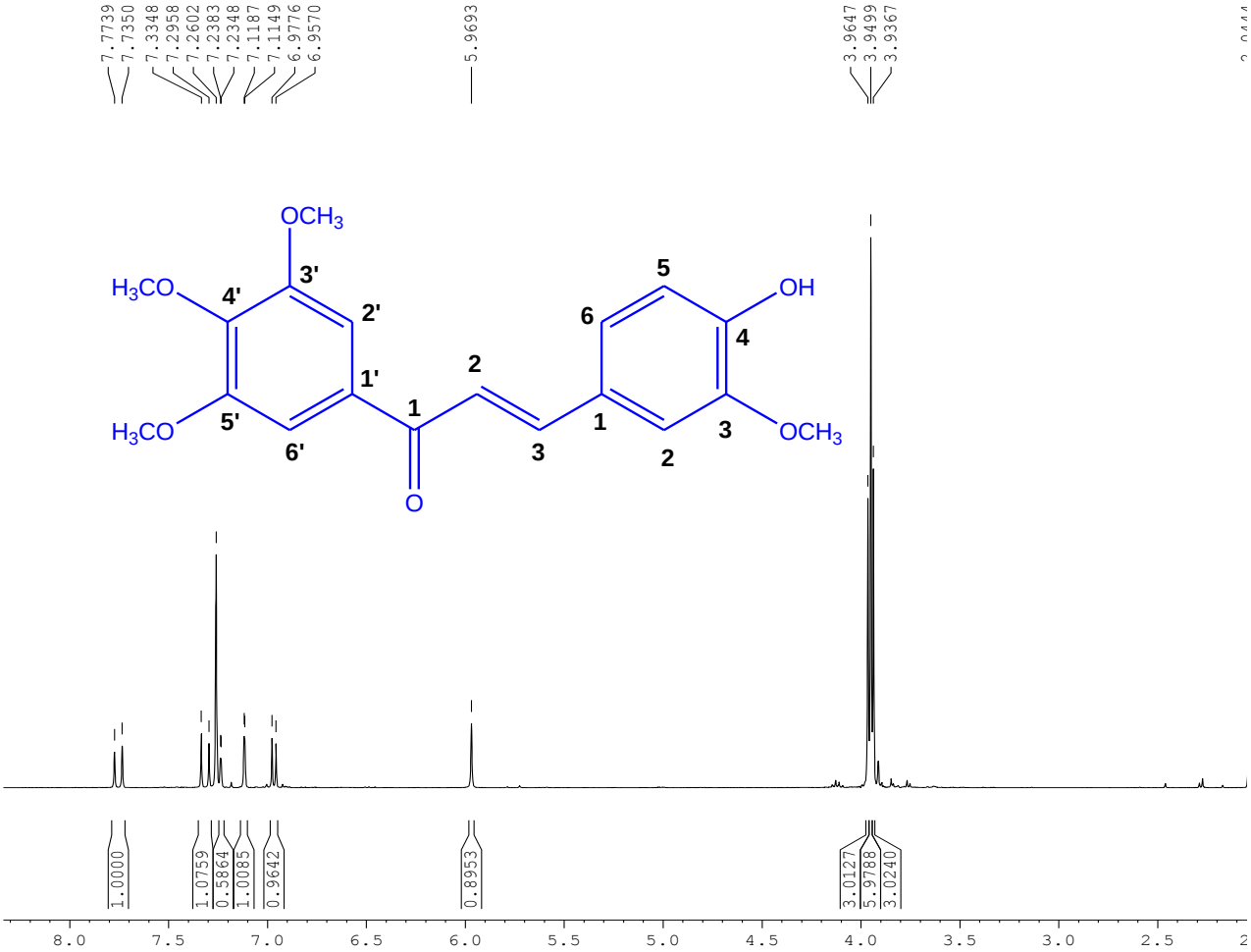


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **13**.

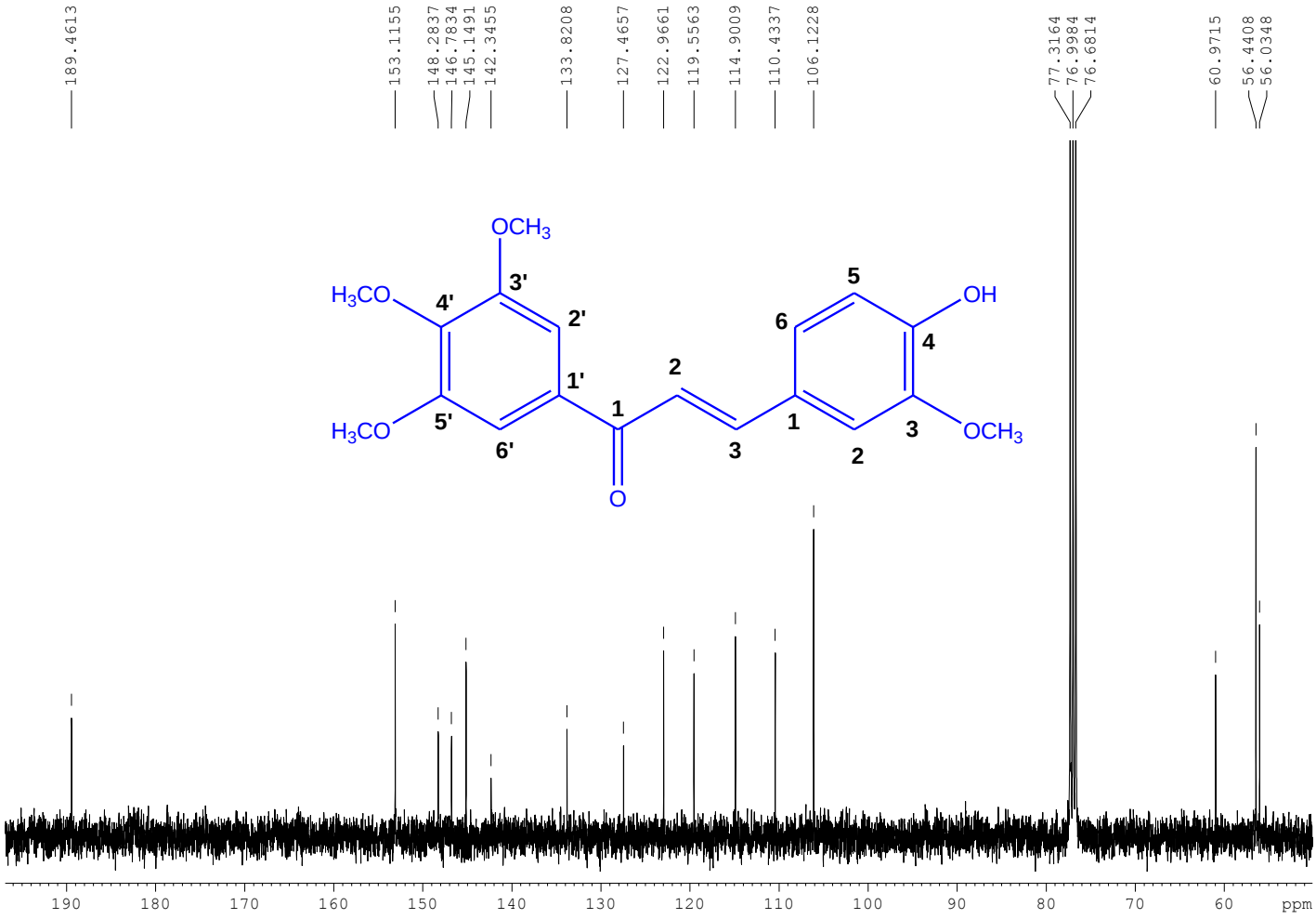


Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **13**.

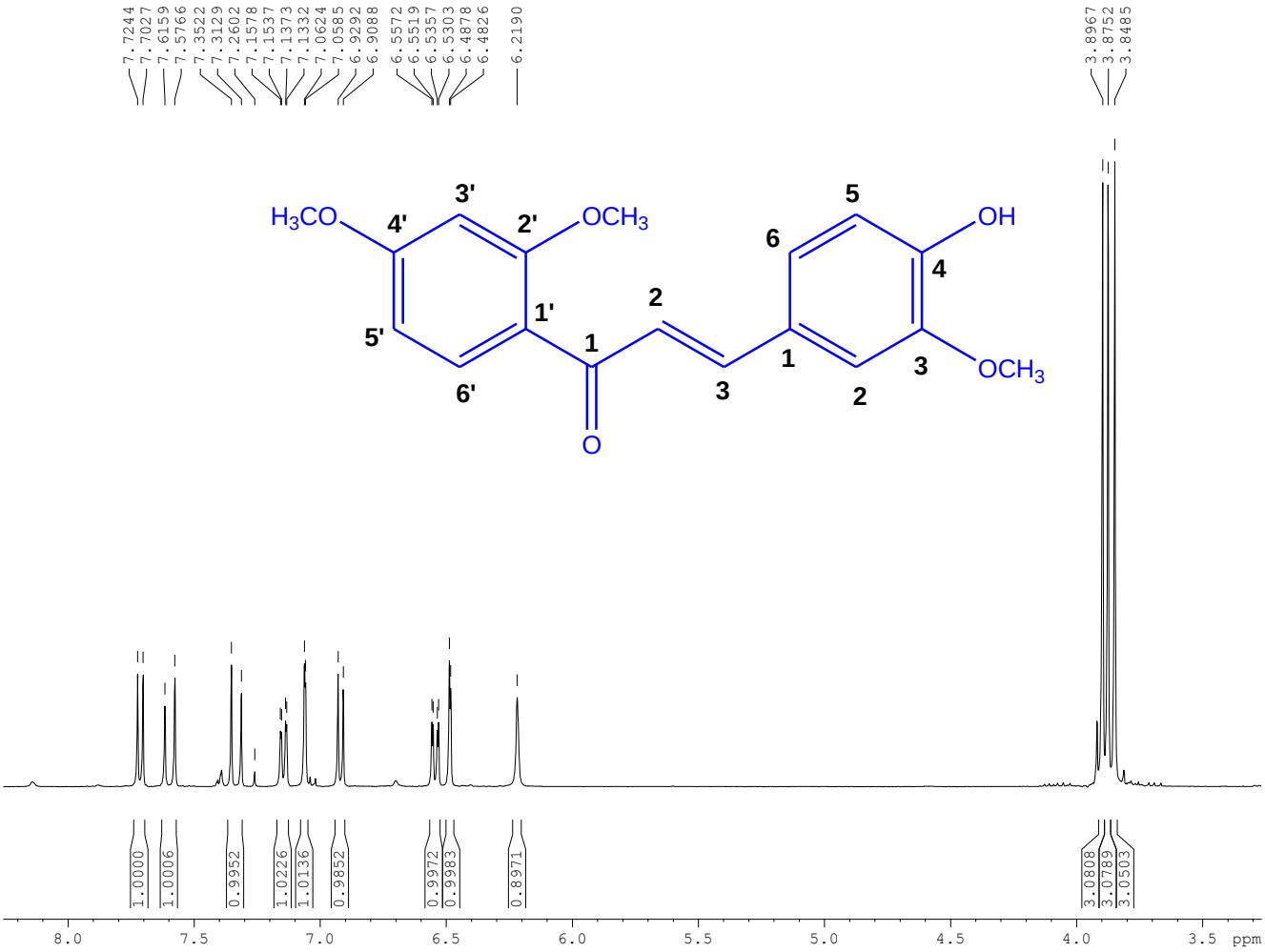


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **14**.

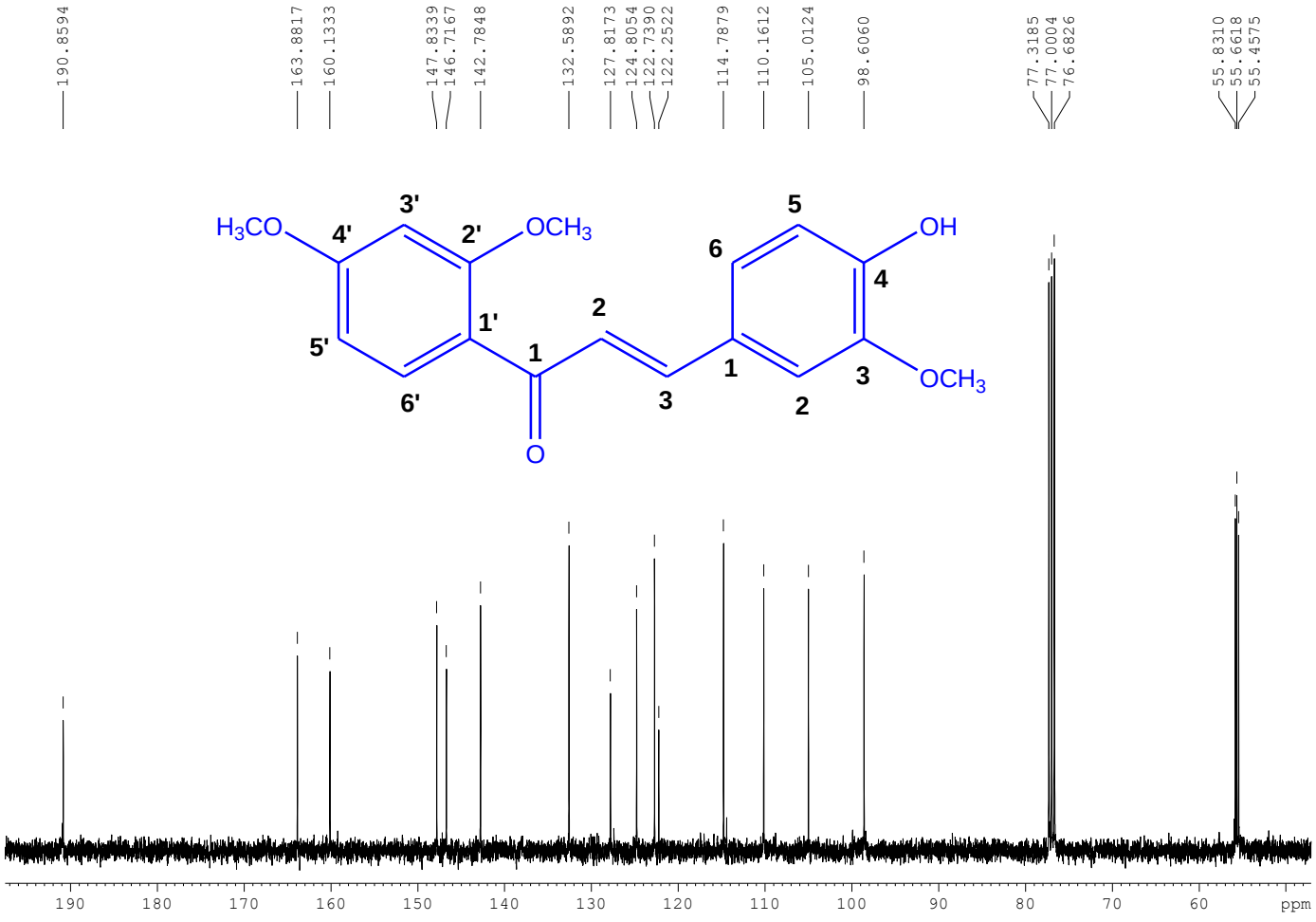


Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **14**.

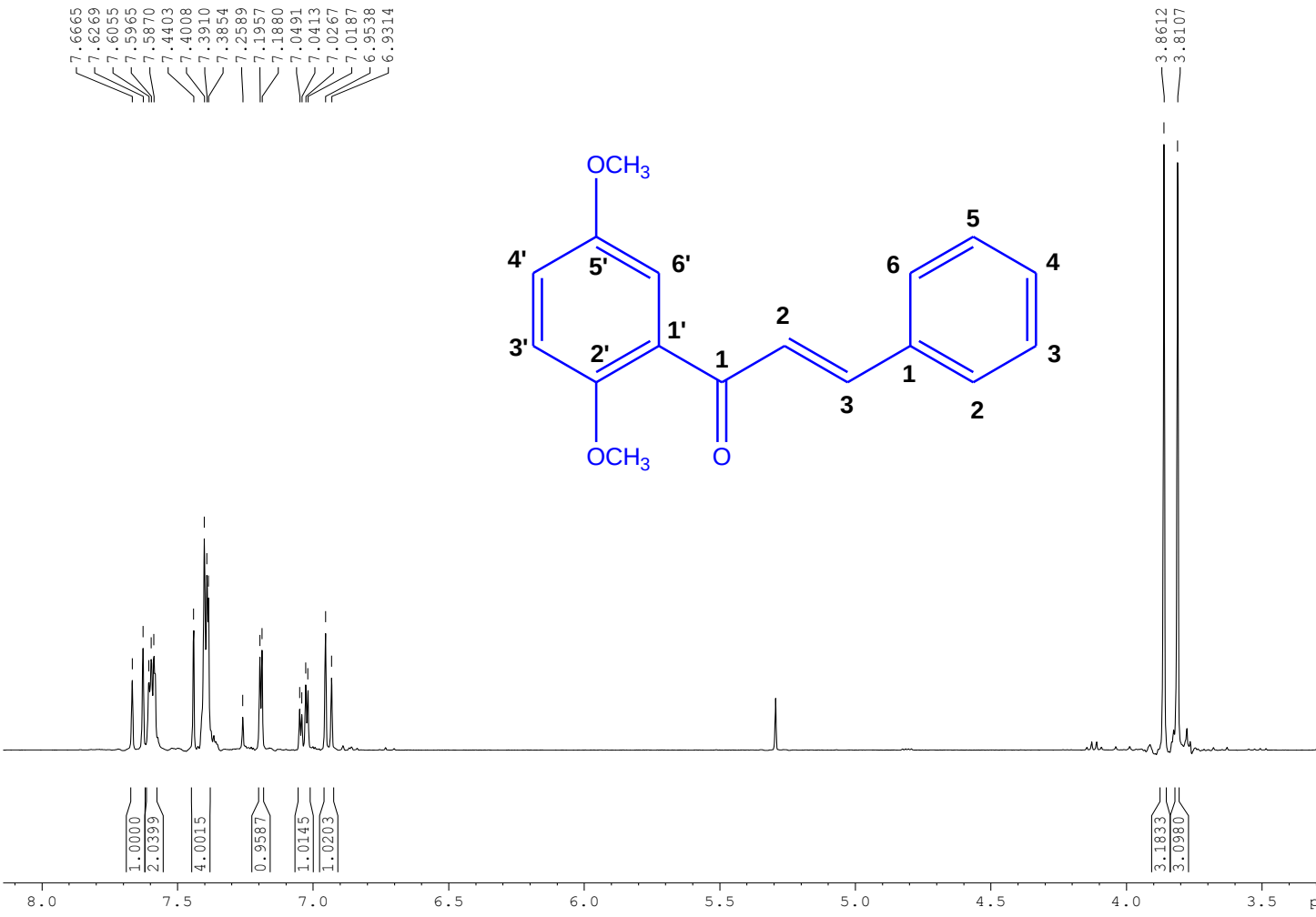


Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **15**.

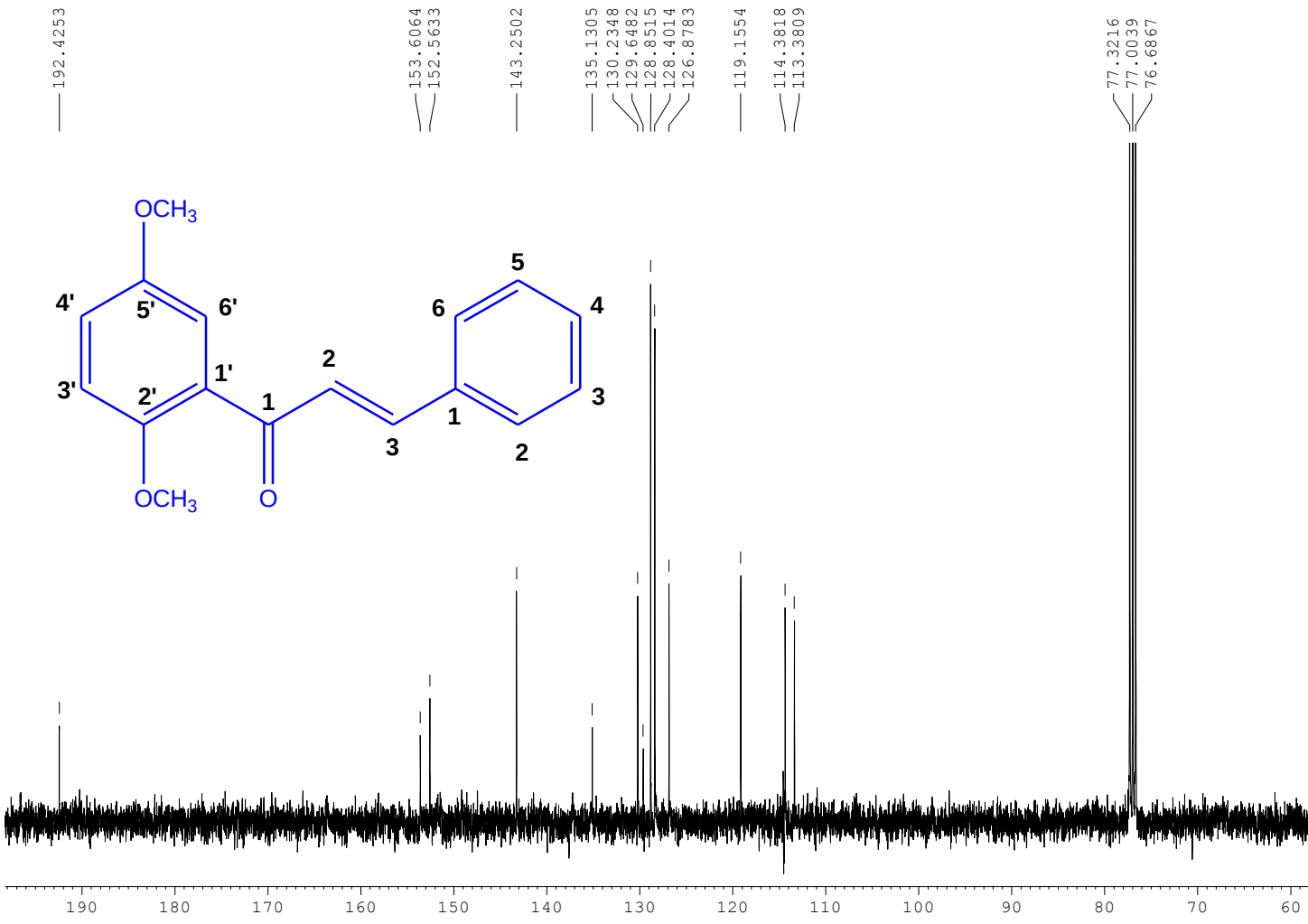


Figure S10. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **15**.

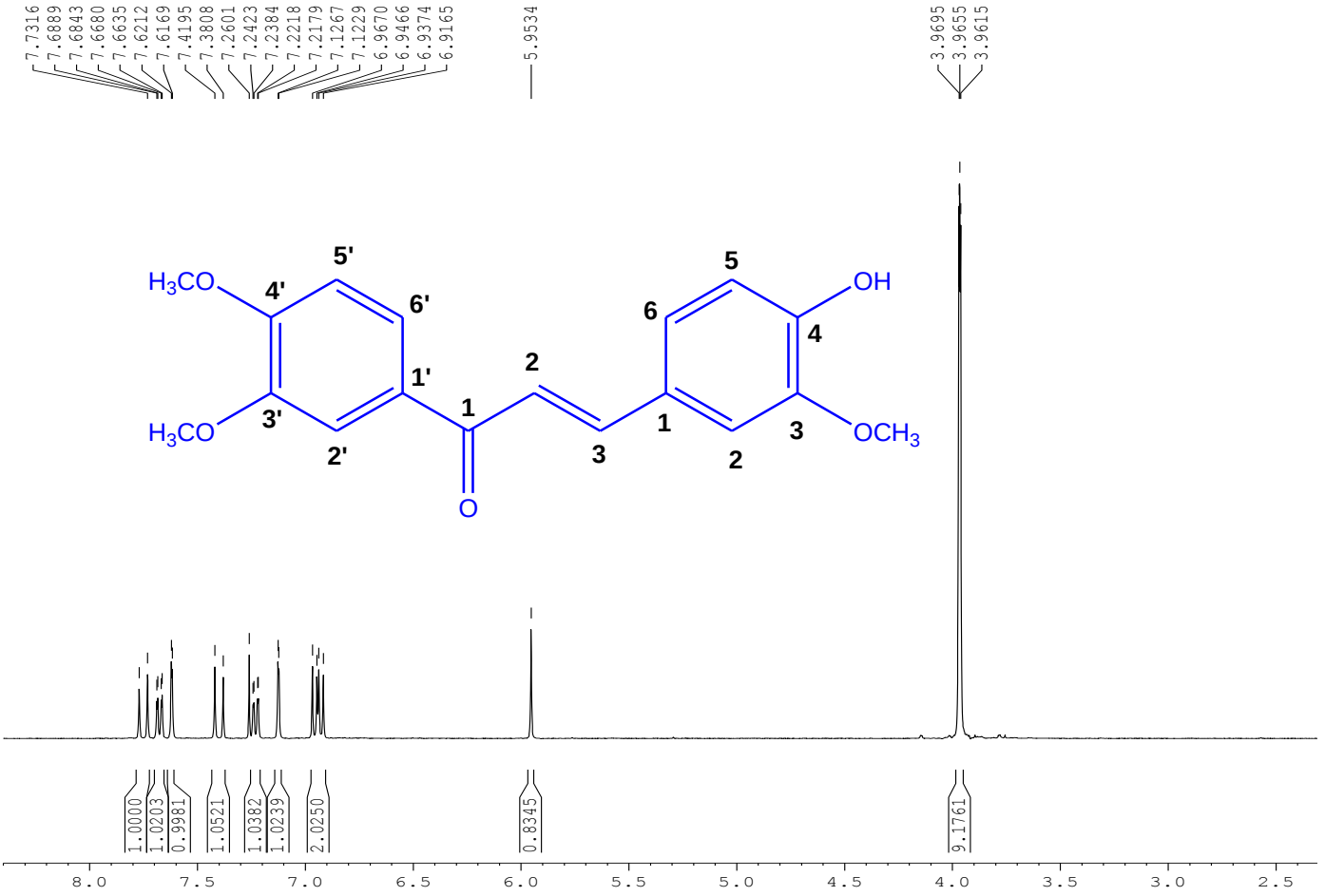


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **16**.

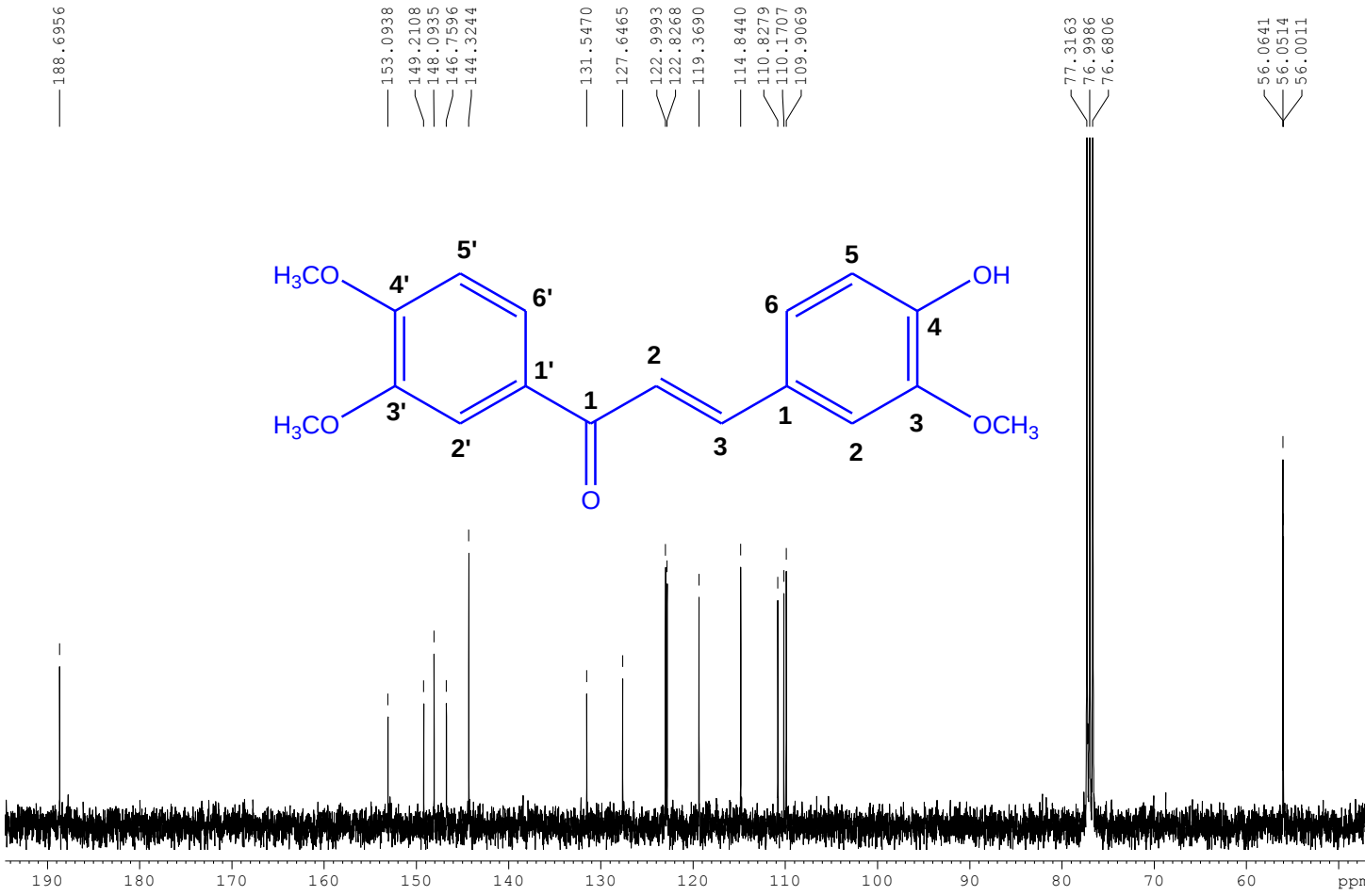


Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **16**.

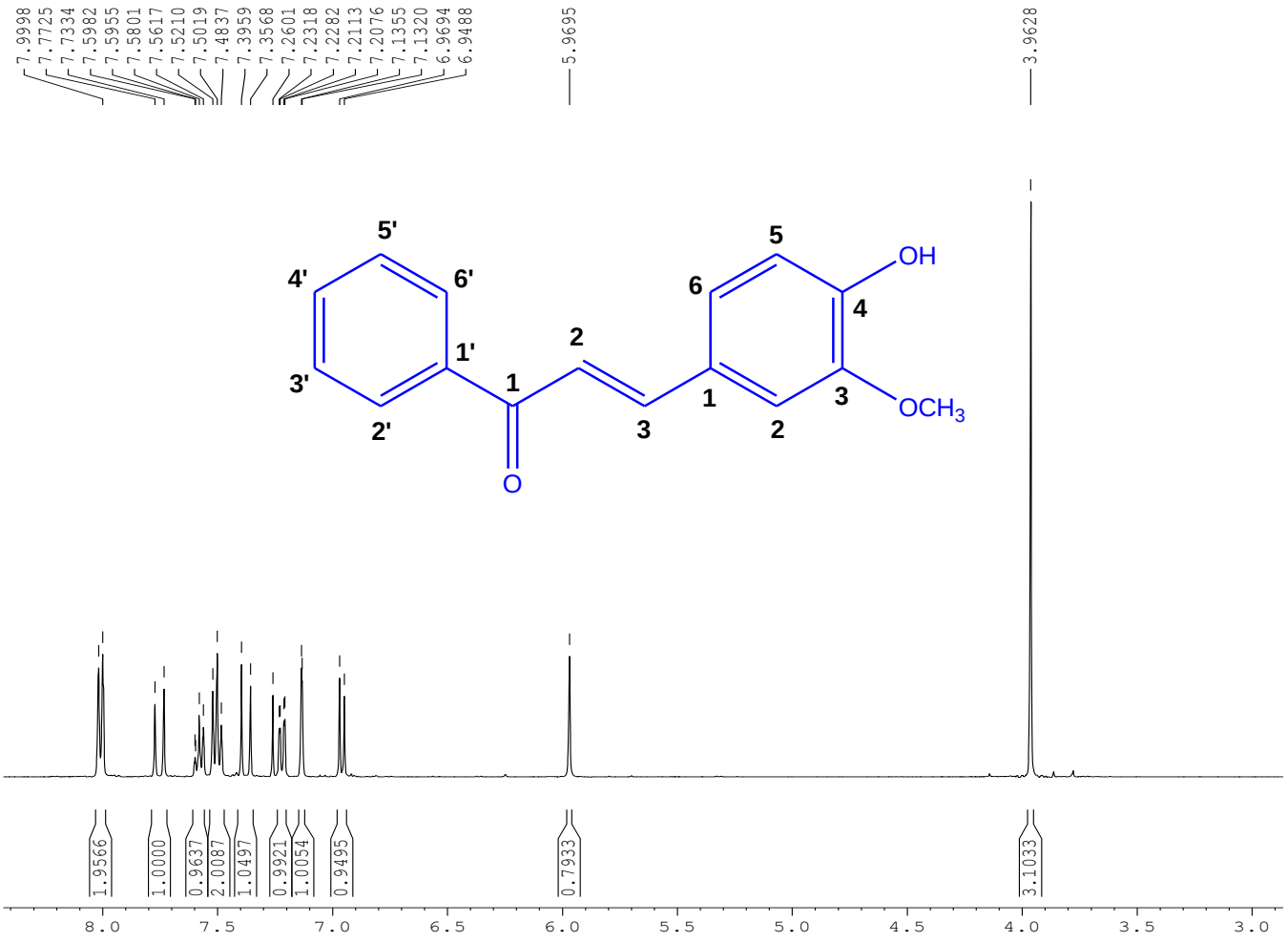


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **17**.

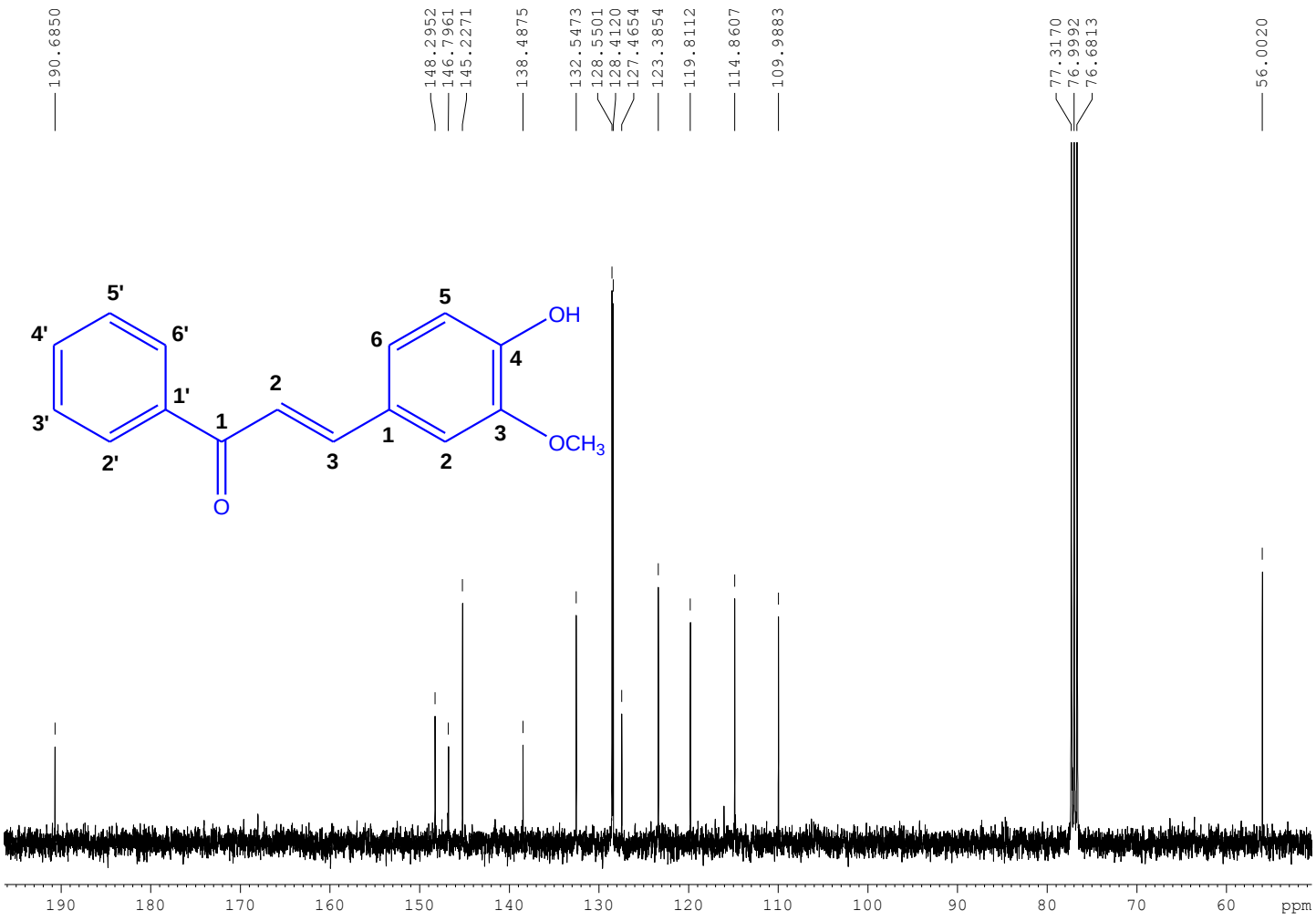


Figure S14. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **17**.

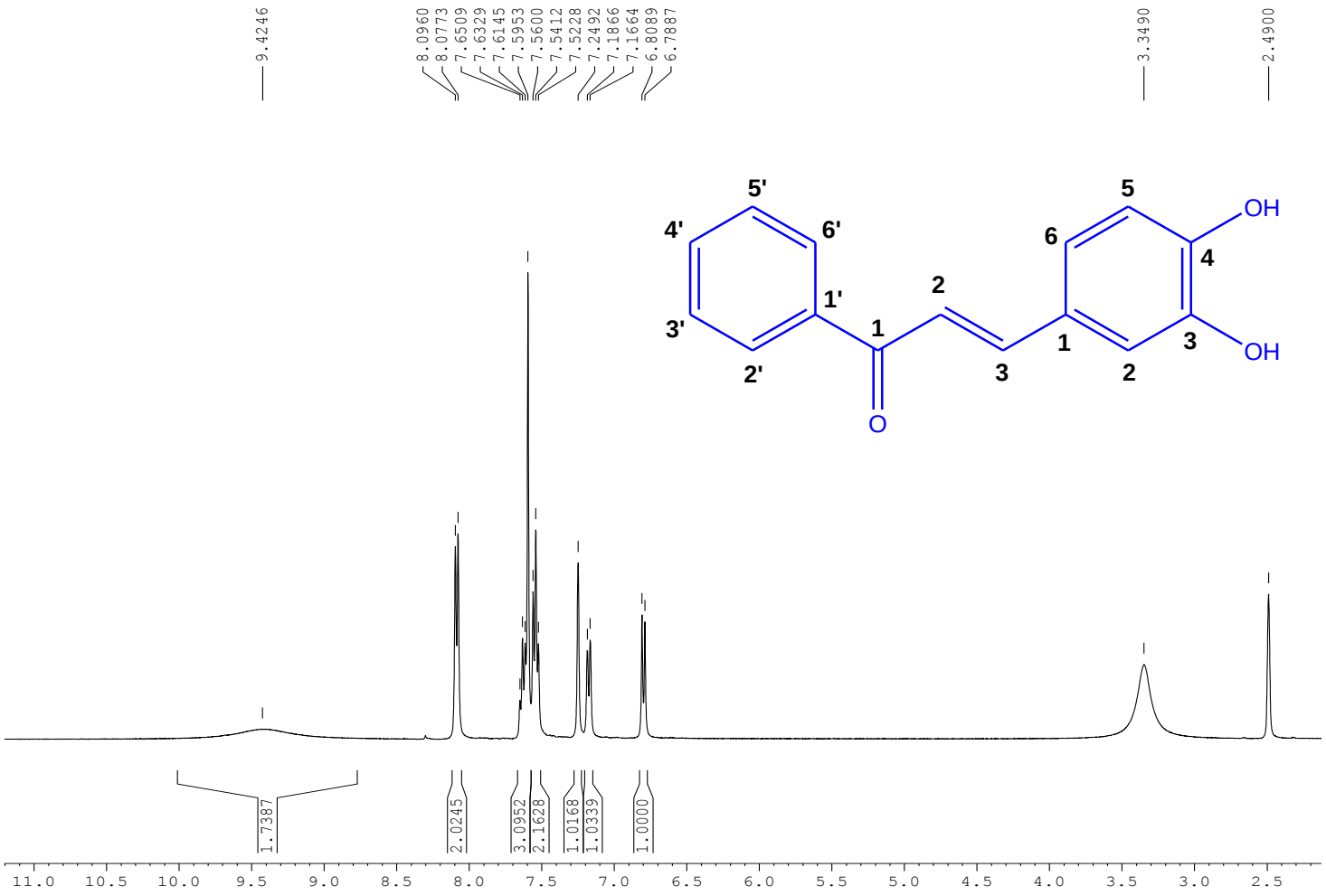


Figure S15. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **18**.

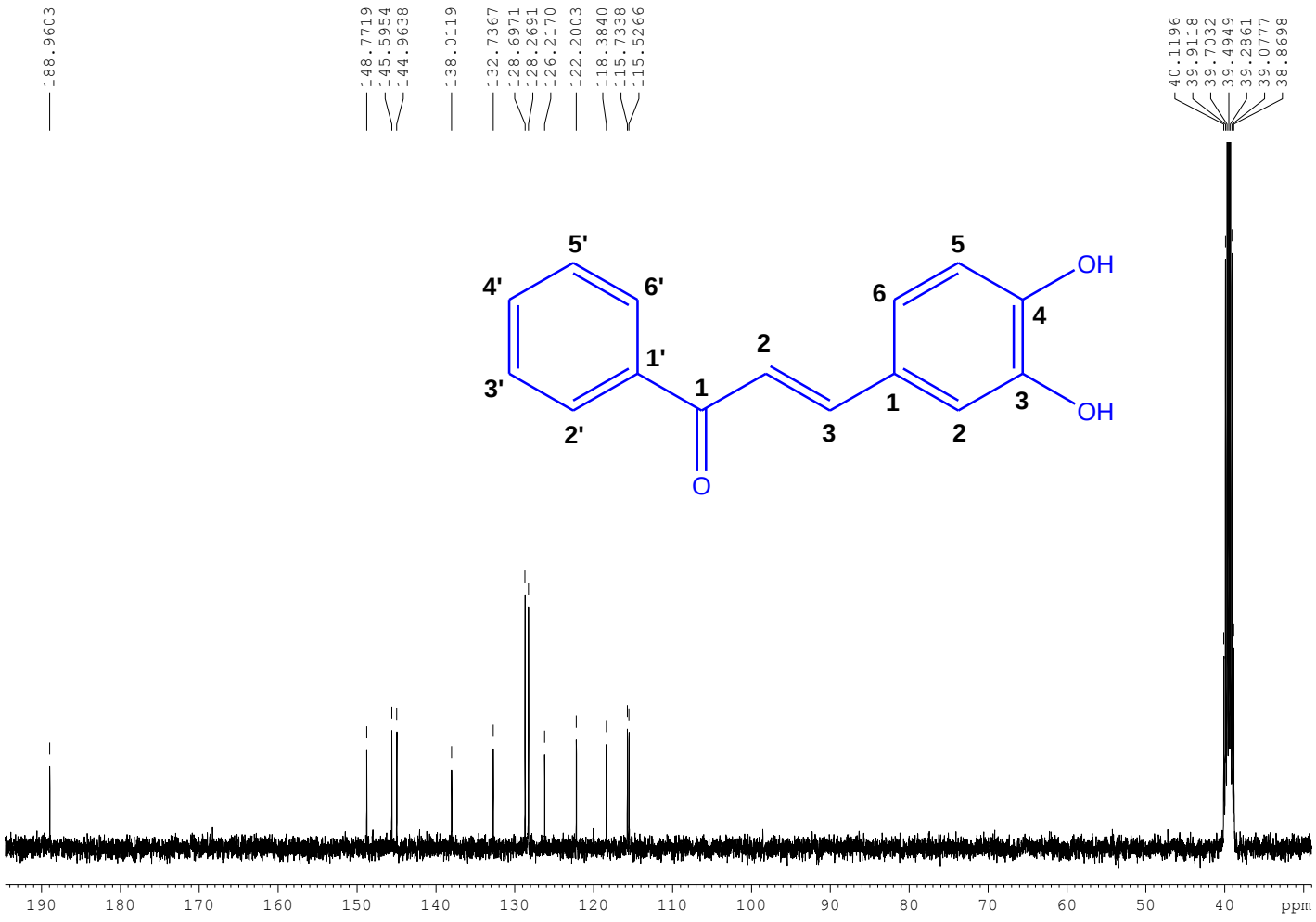


Figure S16. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **18**.

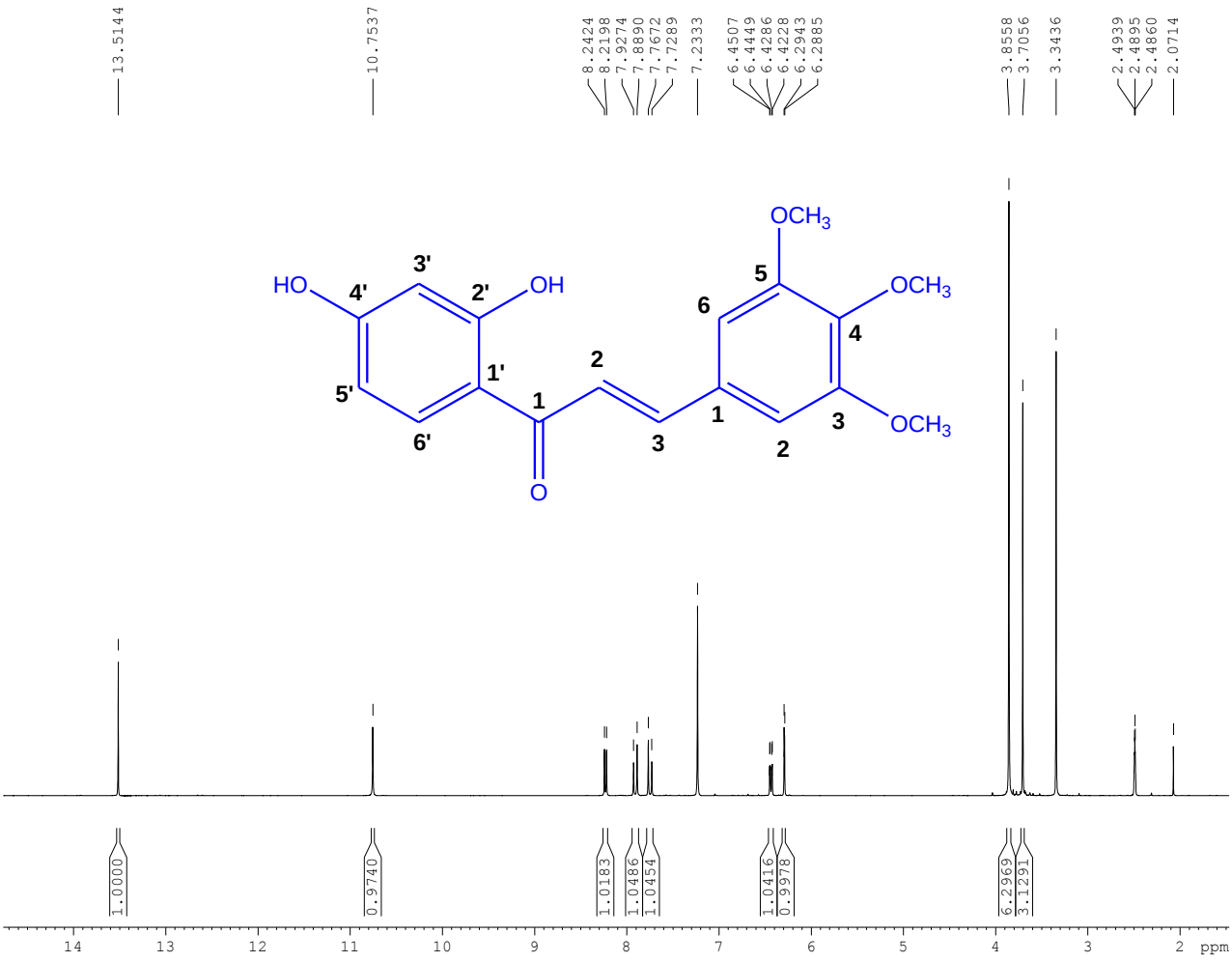


Figure S17. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **19**.

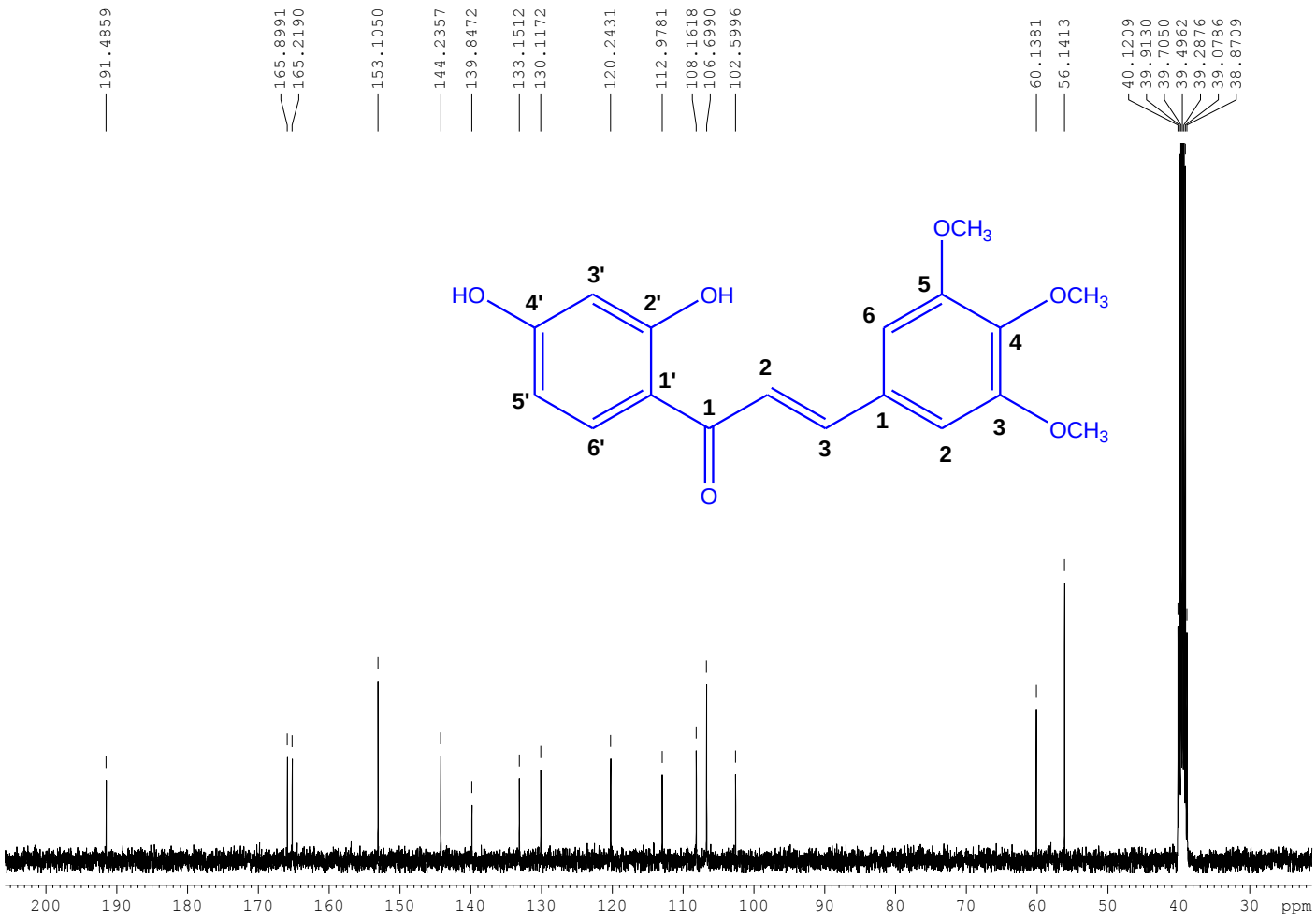


Figure S18. ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **19**.

IR spectra of chalcones **11**-**19**

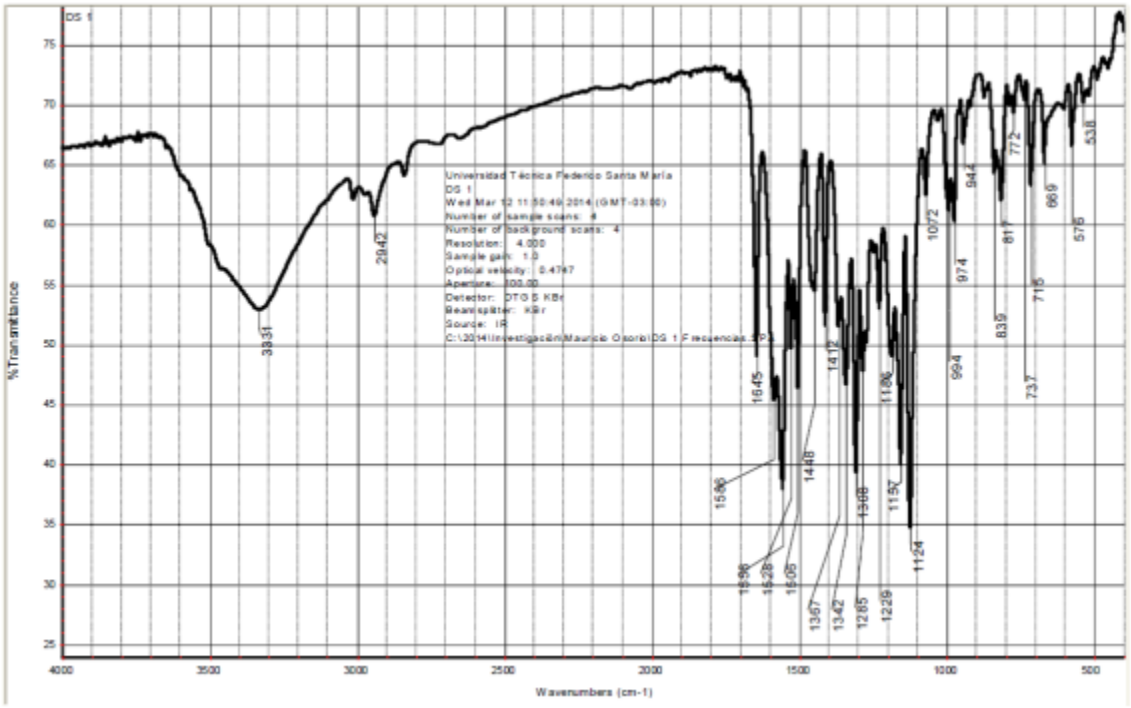


Figure S19. IR (KBr) spectrum of **11**: ν / cm^{-1} 3331 (st. O–H), 2942 (st. C–H alcane), 1645 (st. C=O), 1586, 1558 (ring st. C=C).

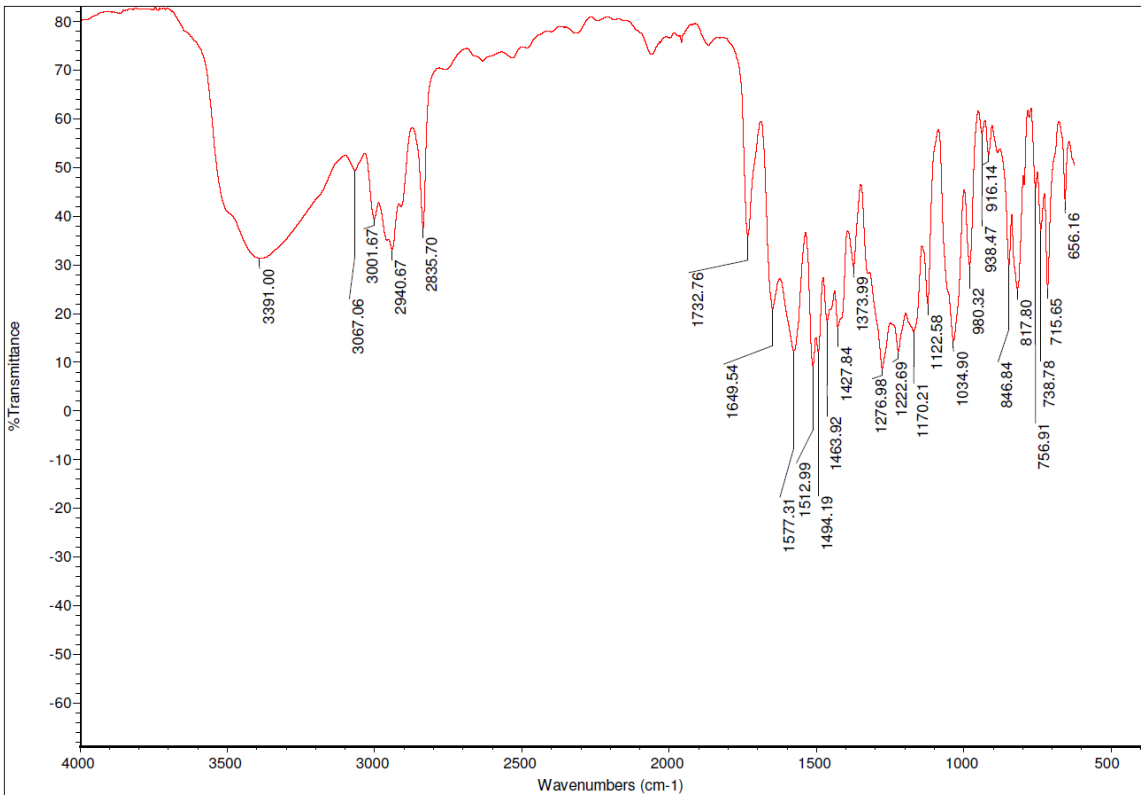


Figure S20. IR (film) spectrum of **12**: ν / cm^{-1} 3391 (st. O–H), 3067, 3002 (aromatic st. C–H), 2941, 2836 (st. alcane C–H), 1650 (st. C=O), 1577, 1513 (ring st. C=C).

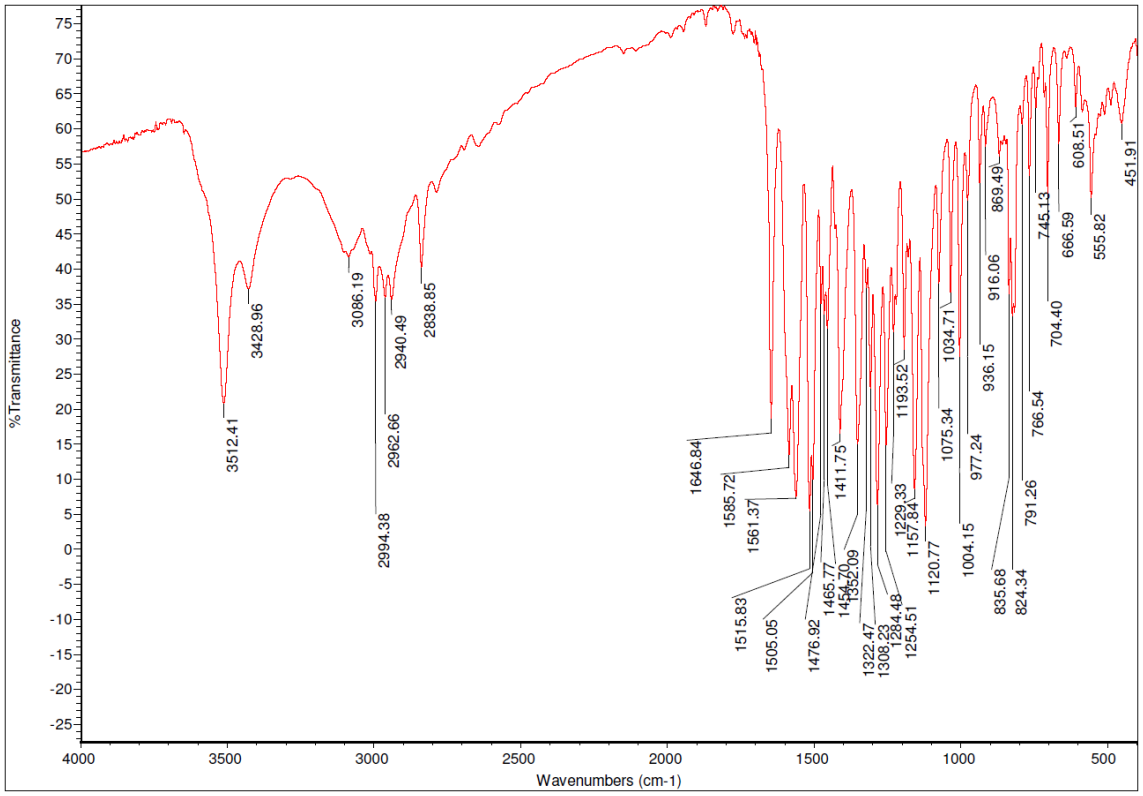


Figure S21. IR (KBr) spectrum of **13**: ν / cm^{-1} 3512, 3429 (st. O–H), 3086 (aromatic st. C–H), 2994, 2963, 2941, 2839 (st. alcane C–H), 1647 (st. C=O), 1586, 1561, 1516 (ring st. C=C).

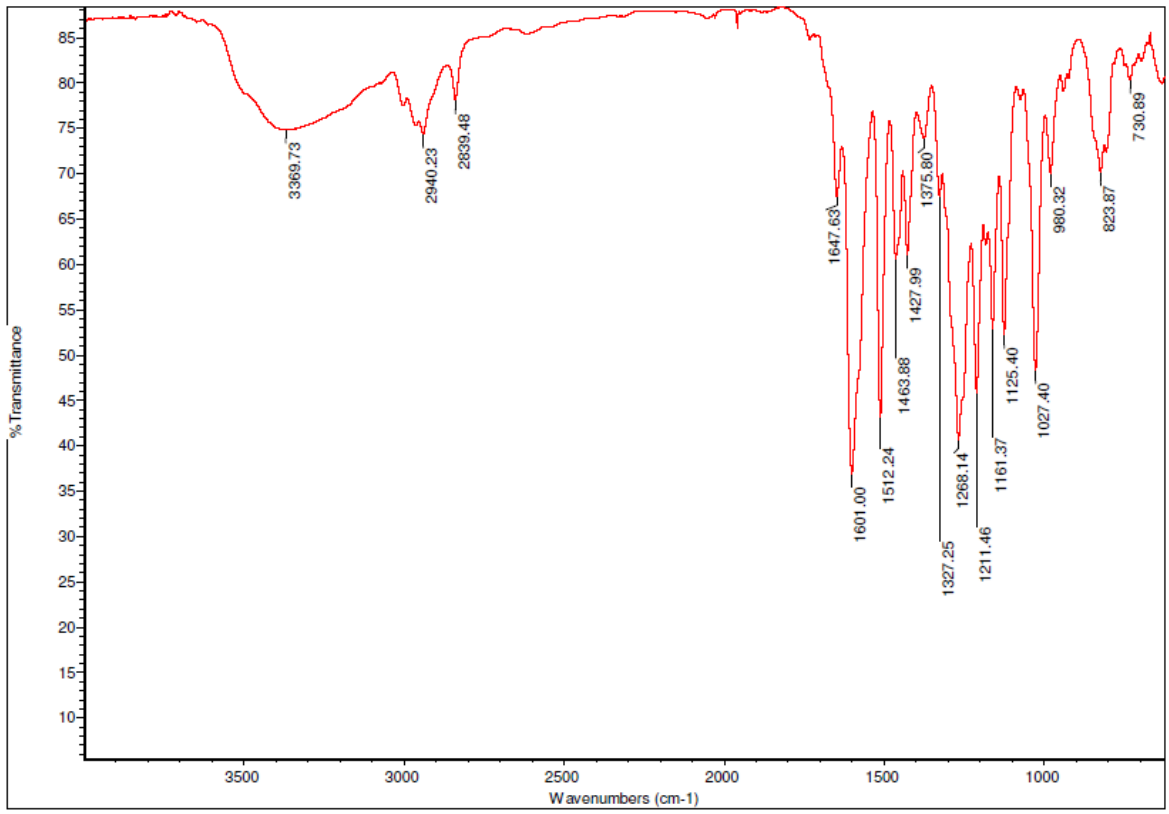


Figure S22. IR (film) spectrum of **14**: ν / cm^{-1} 3370 (st. O–H), 2940, 2840 (st. alcane C–H), 1648 (st. C=O), 1601, 1512 (ring st. C=C).

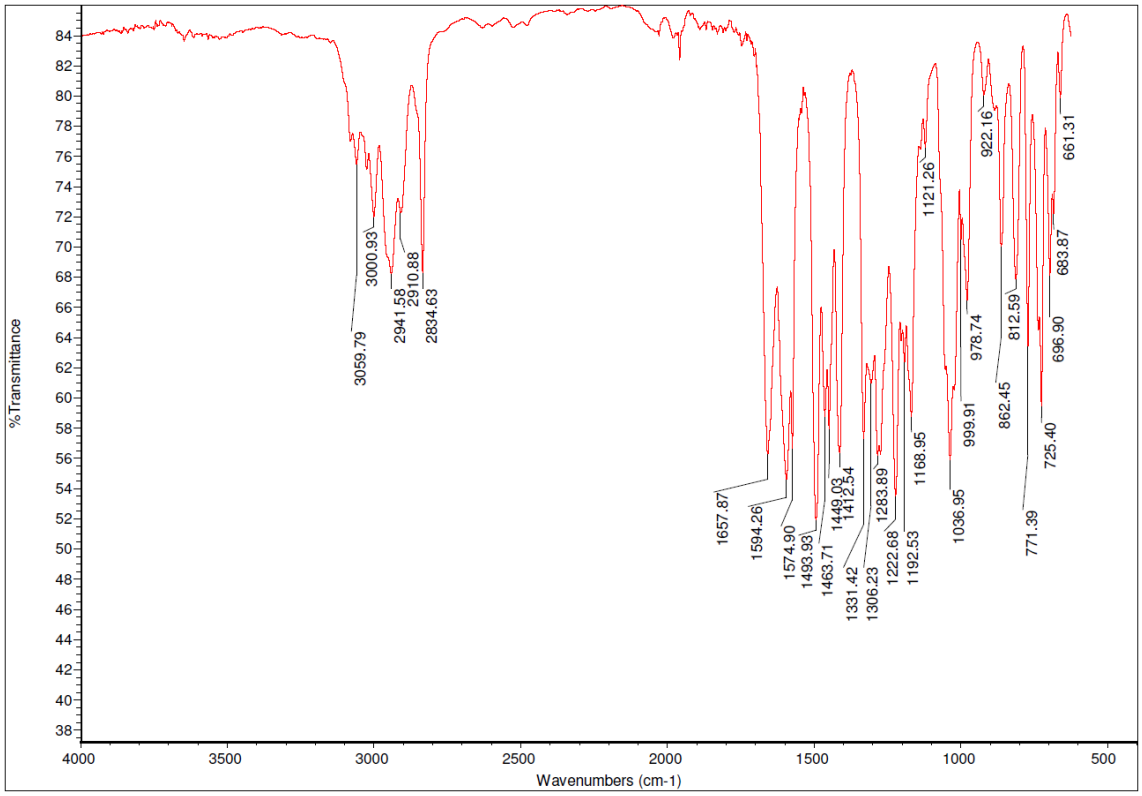


Figure S23. IR (film) spectrum of **15**: ν / cm^{-1} 3060, 3001 (aromatic st. C–H), 2942, 2911, 2835 (st. alcane C–H), 1658 (st. C=O), 1594, 1575 (ring st. C=C).

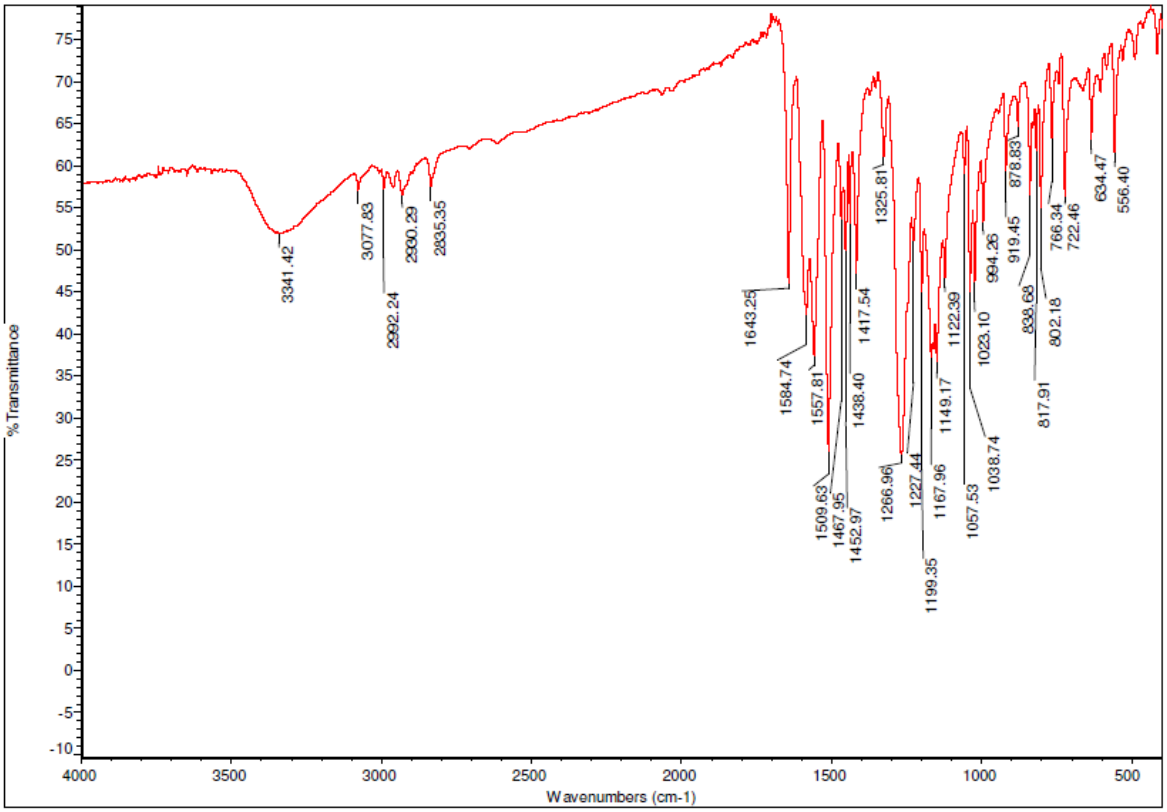


Figure S24. IR (KBr) spectrum of **16**: ν / cm^{-1} 3341 (st. O–H), 3078 (aromatic st. C–H), 2992, 2930, 2835 (st. alcane C–H), 1643 (st. C=O), 1585, 1557, 1510 (ring st. C=C).

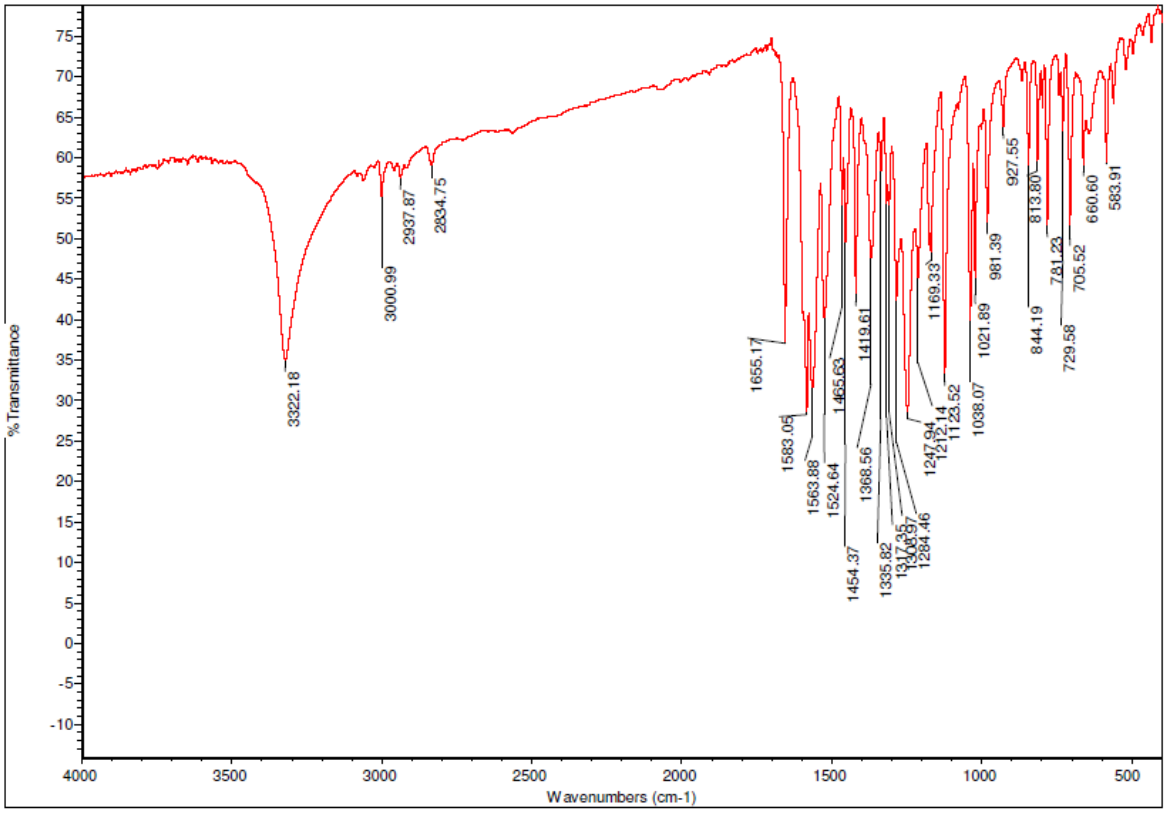


Figure S25. IR (KBr) spectrum of **17**: ν / cm^{-1} 3322 (st. O–H), 3001 (aromatic st. C–H), 2938, 2835 (st. alcane C–H), 1655 (st. C=O), 1583, 1564, 1525 (ring st. C=C).

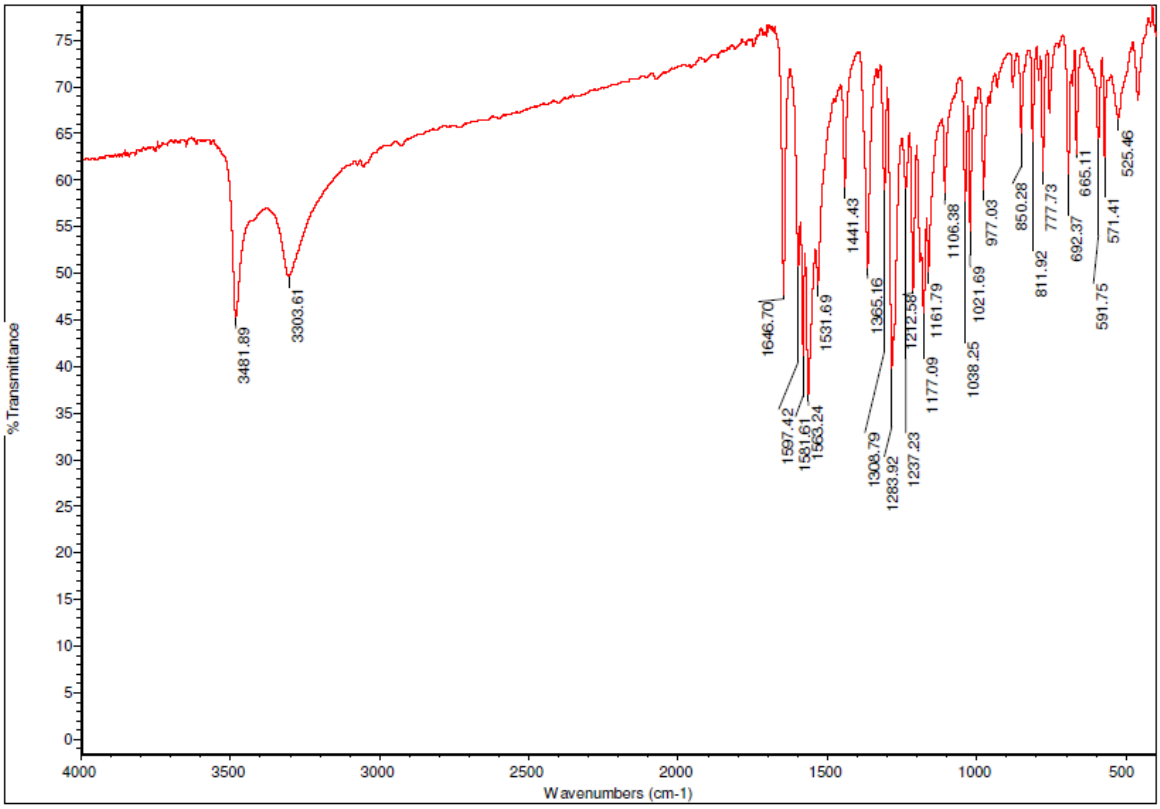


Figure S26. IR (KBr) spectrum of **18**: ν / cm^{-1} 3482, 3304 (st. O–H), 1647 (st. C=O), 1582, 1563 (ring st. C=C).

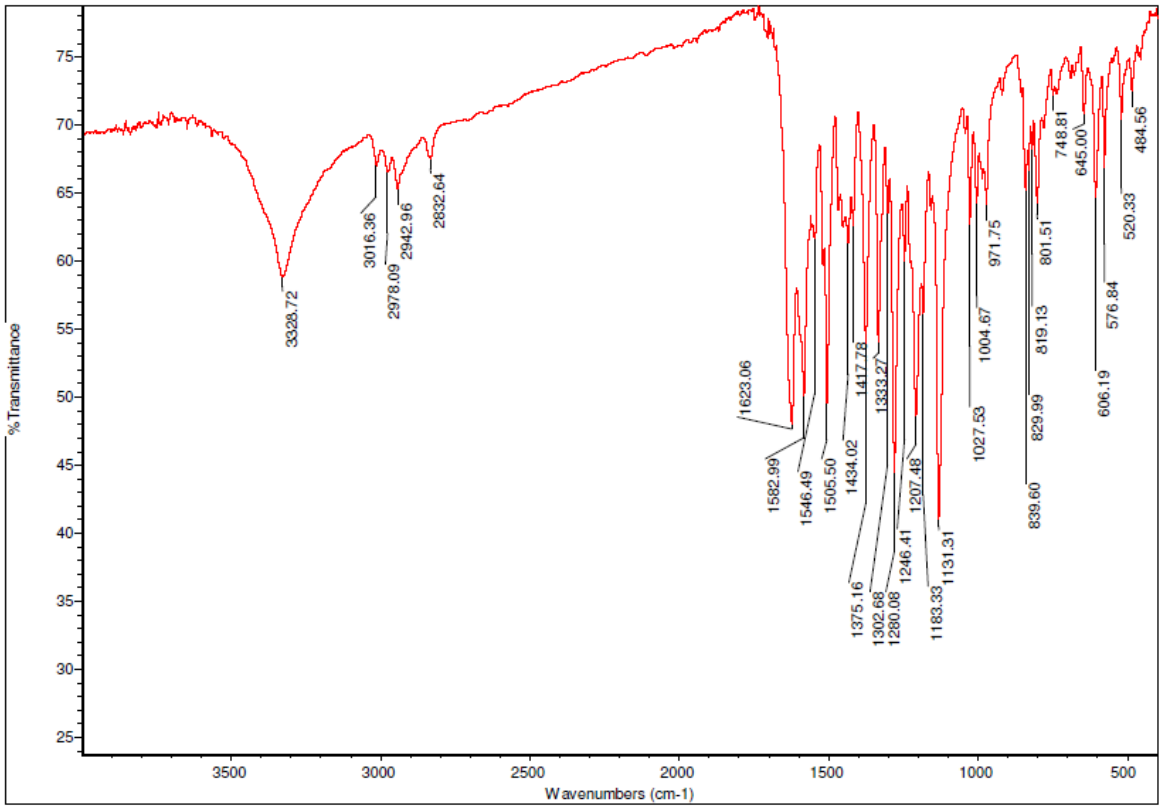
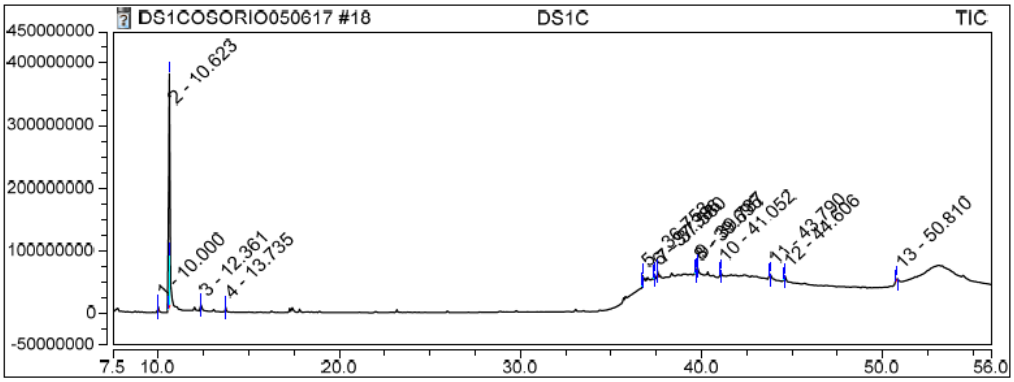


Figure S27. IR (KBr) spectrum of **19**: ν / cm^{-1} 3329 (st. O–H), 3016 (aromatic st. C–H), 2978, 2943, 2833 (st. alcane C–H), 1655 (st. C=O), 1583, 1506 (ring st. C=C).

Chromatograms and MS spectra of chalcones **11**-**19**

Injection Details			
Injection Name:	**DS1C**	*Run Time (min):*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**20/Jun/17 17:01**	*Sample Weight:*	**1.0000**



No.	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	10.000	Cyclooctasiloxane, hexadecamethyl-	130246	556-68-3	819	0.56
2	10.623	Ethanone, 1-(3,4,5-trimethoxyphenyl)	21162714	1136-86-3	918	90.96
3	12.361	Benzoic acid, 3,4,5-trimethoxy-	125674	118-41-2	853	0.54
4	13.735	Cyclononasiloxane, octadecamethyl-	101835	556-71-8	755	0.44
5	36.753	11H-Dibenzo[b,e][1,4]dioxepin-7-carb	336243	4723-32-4	681	1.45
6	37.386	11a-Hydroxyprogesterone, trimethyls	115975	0	571	0.50
7	37.580	Tetracosane, 11-decyl-	139483	55429-84-0	680	0.60
8	39.695	trans-4-Ethoxy-2',3',4'-trimethoxychal	101218	0	609	0.44
9	39.787	Tetratriacontane	225546	14167-59-0	697	0.97
10	41.052	trans-3',4',5'-Trimethoxy-4-(methylthi	115519	121646-13-7	578	0.50
11	43.790	Demecolcine	114413	477-30-5	521	0.49
12	44.606	Trimetozine	208278	635-41-6	553	0.90
13	50.810	Olean-12-en-29-oic acid, 3-hydroxy-1	389073	1477-44-7	492	1.67

Figure S28. Chromatogram of compound **11**: it shows degradative decomposition fragments only.

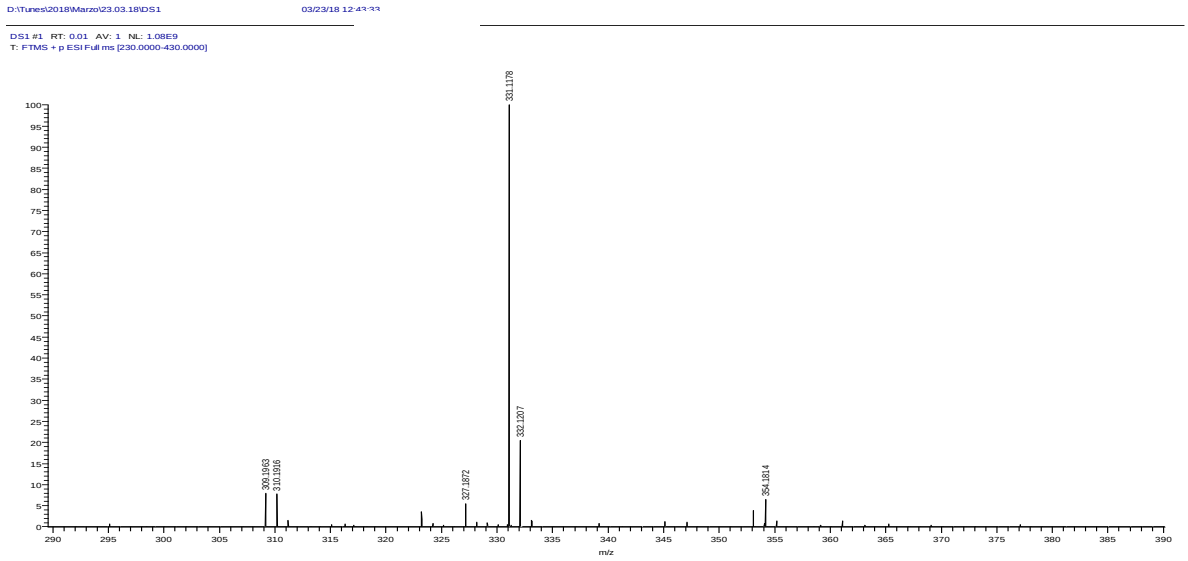
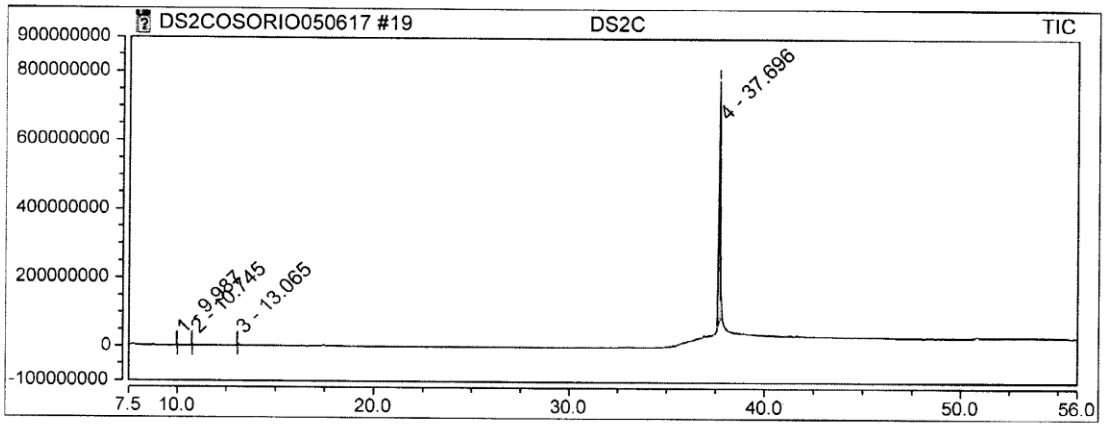


Figure S29. HRMS of compound **11**.

Injection Details

Injection Name:	**DS2C**	*Run Time (min):*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**20/Jun/17 18:00**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	9.987	Cyclooctasiloxane, hexadecamethyl-	76804	556-68-3	684	0.16
2	10.745	Heptadecane	131505	629-78-7	865	0.28
3	13.065	Octadecane	70024	593-45-3	824	0.15
4	37.696	Alpha-(3,4-dimethoxybenzylidene)-2-	47319578	10493-06-8	689	99.42

Figure S30. Chromatogram of compound **12**: peak No. 4 was selected to mass spectrum.

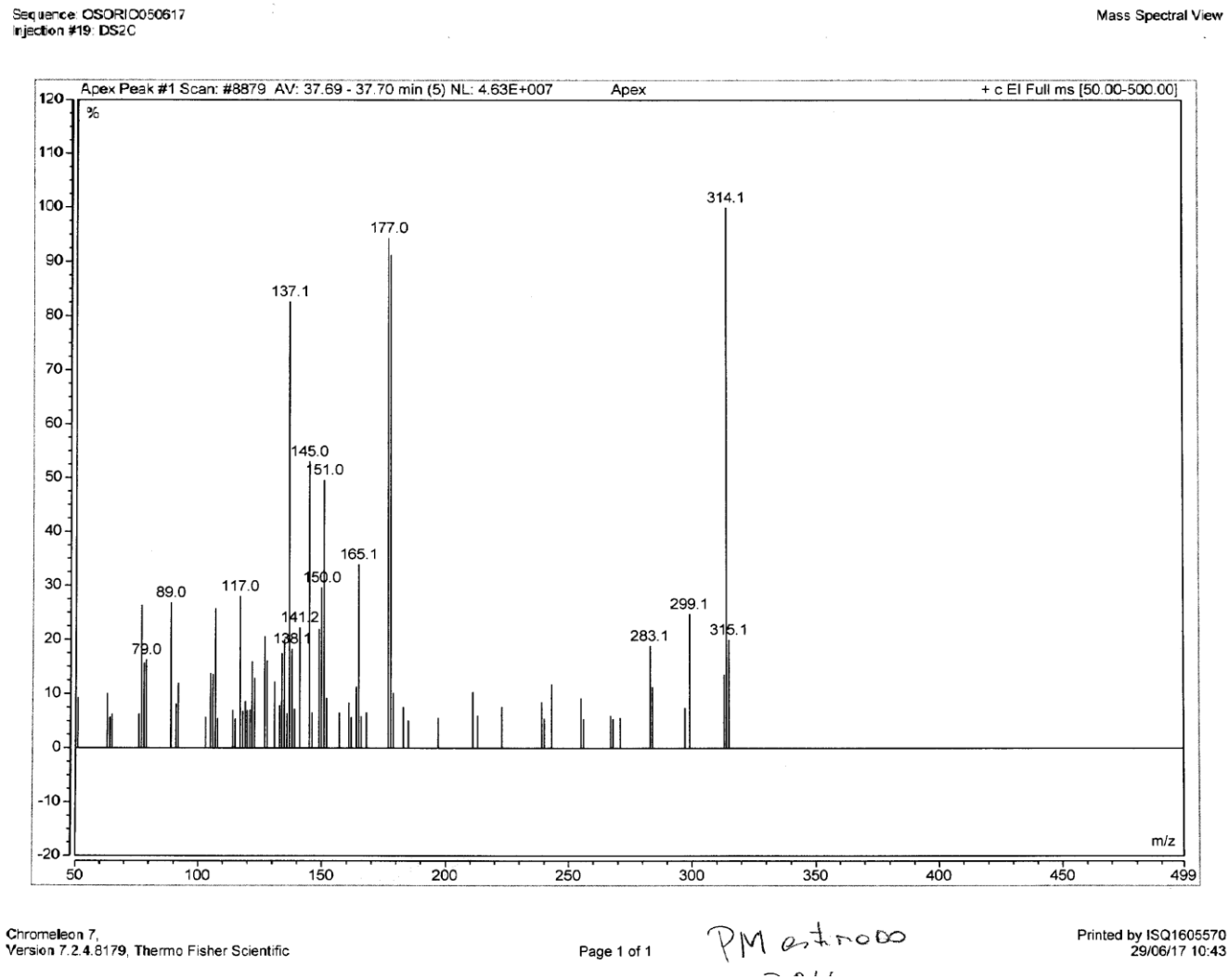


Figure S31. Mass spectrum of compound **12**.

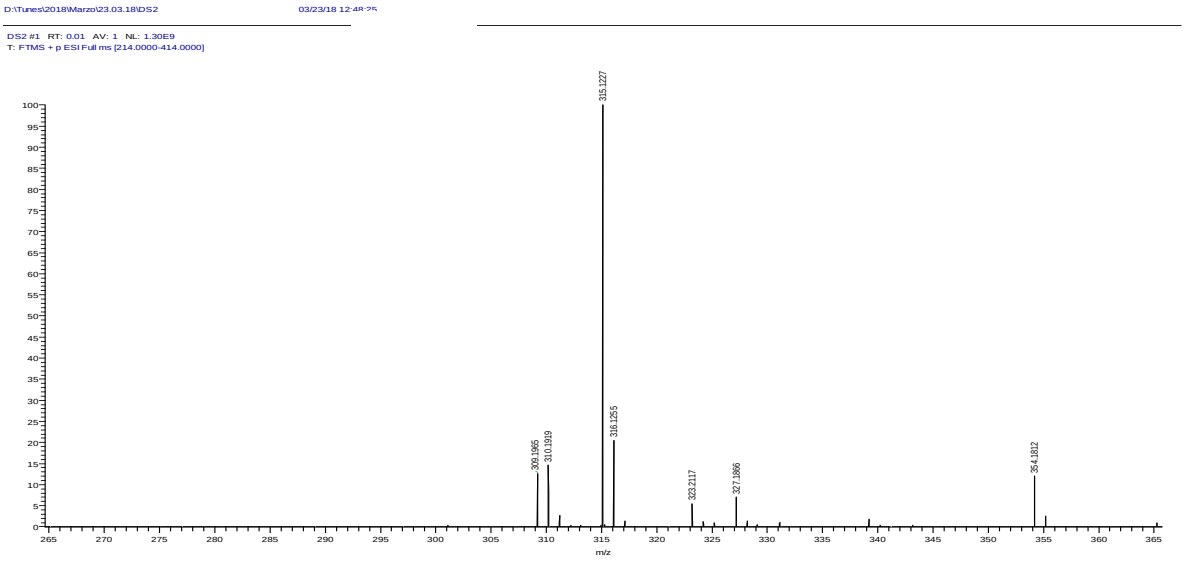
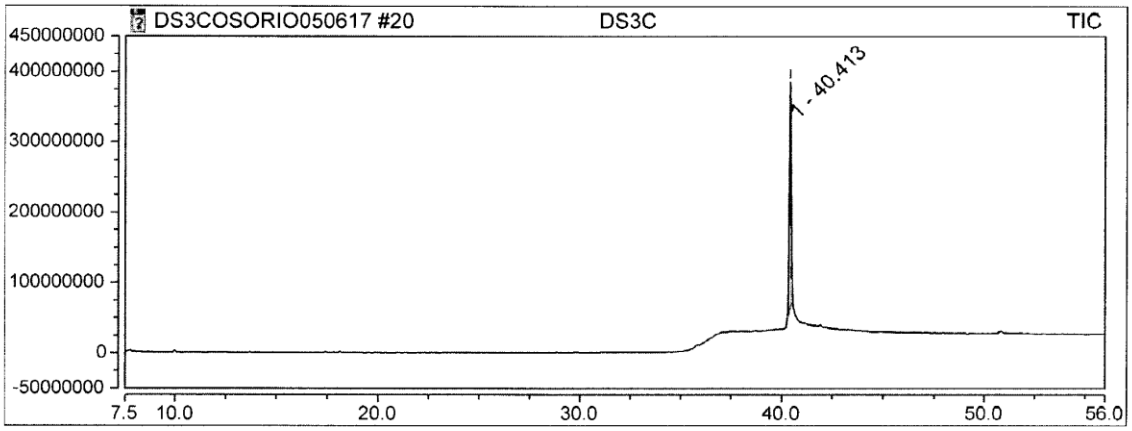


Figure S32. HRMS of compound **12**.

Injection Details			
Injection Name:	**DS3C**	*Run Time (min):*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**20/Jun/17 19:00**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	40.413	trans-3',4',5'-Trimethoxy-4-(methylthi	24736160	121646-13-7	788	100.00

Figure S33. Chromatogram of compound **13**: peak No. 1 was selected to mass spectrum.

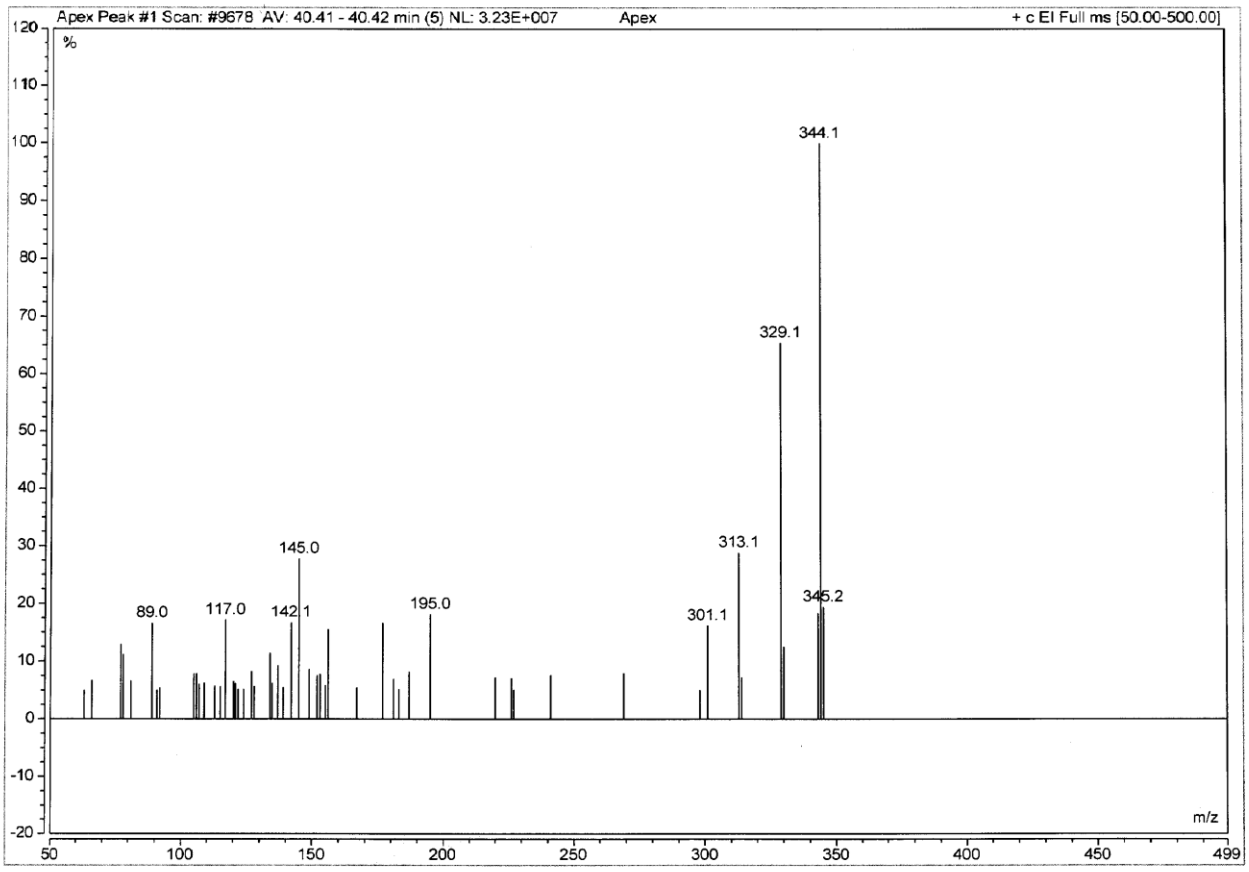
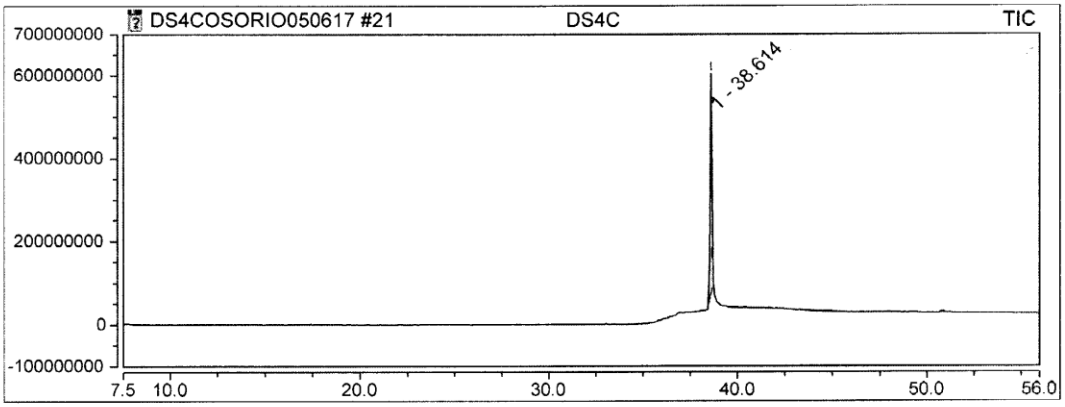


Figure S34. Mass spectrum of compound **13**.

Injection Details			
Injection Name:	**DS4C**	*Run Time (min):*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**20/Jun/17 19:59**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	38.614	Alpha-(3,4-dimethoxybenzylidene)-2-	42027284	10493-06-8	714	100.00

Figure S35. Chromatogram of compound **14**: peak No. 1 was selected to mass spectrum.

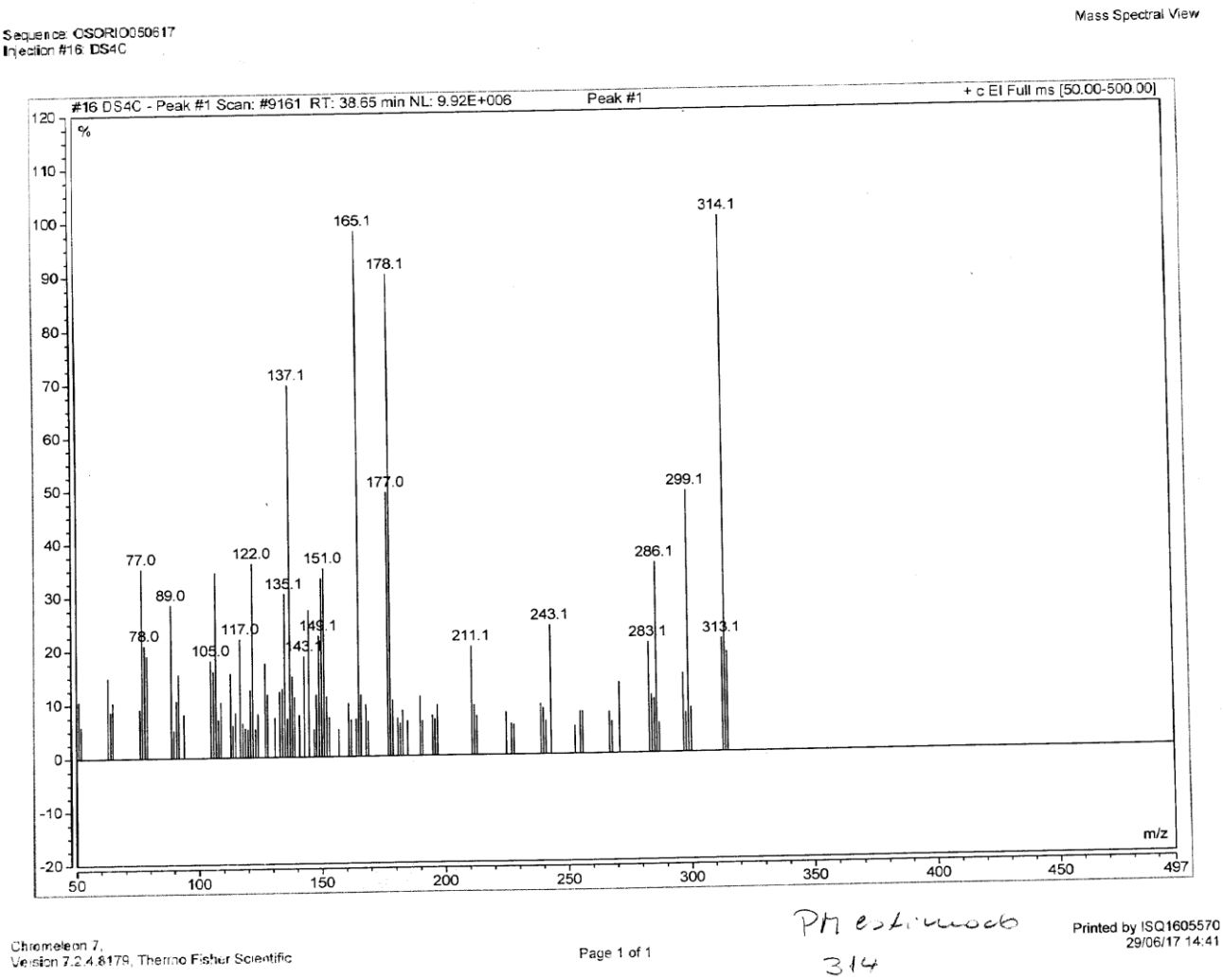
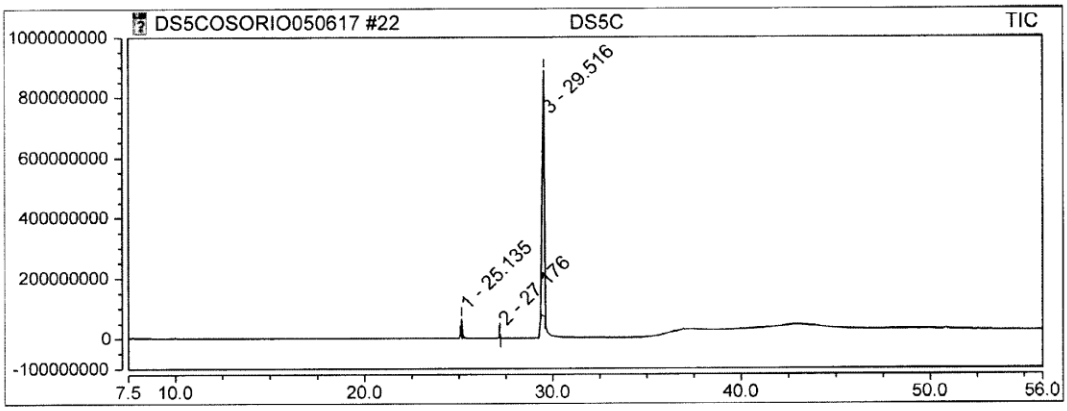


Figure S36. Mass spectrum of compound **14**.

Injection Details			
Injection Name:	**DS5C**	*Run Time (min).*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**20/Jun/17 20:58**	*Sample Weight:*	**1.0000**



No.	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	25.135	3,4-Dimethoxychalcone	3205527	53744-28-8	694	3.29
2	27.176	m-Methoxyphenylacetamide	486930	18463-71-3	657	0.50
3	29.516	3,4-Dimethoxychalcone	93884439	53744-28-8	690	96.22

Figure S37. Chromatogram of compound **15**: peak No. 3 was selected to mass spectrum.

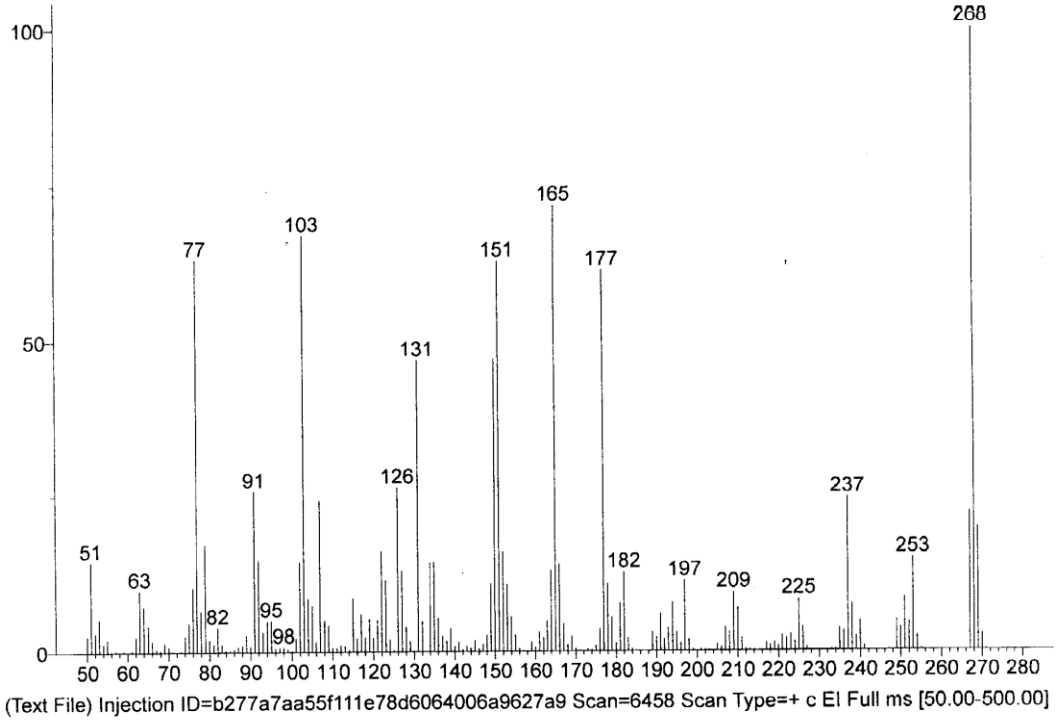
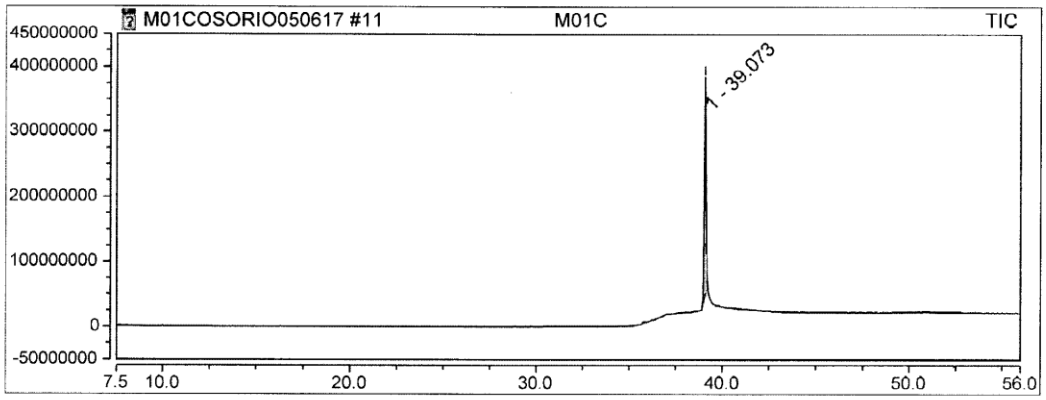


Figure S38. Mass spectrum of compound **15**.

Injection Details			
Injection Name:	**M01C**	*Run Time (min).*	**48.49**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**09/Jun/17 14:45**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	39.073	trans-3',4'-Dimethoxy-4-(methylthio)c	22065178	131316-20-6	771	100.00

Figure S39. Chromatogram of compound **16**: peak No. 1 was selected to mass spectrum.

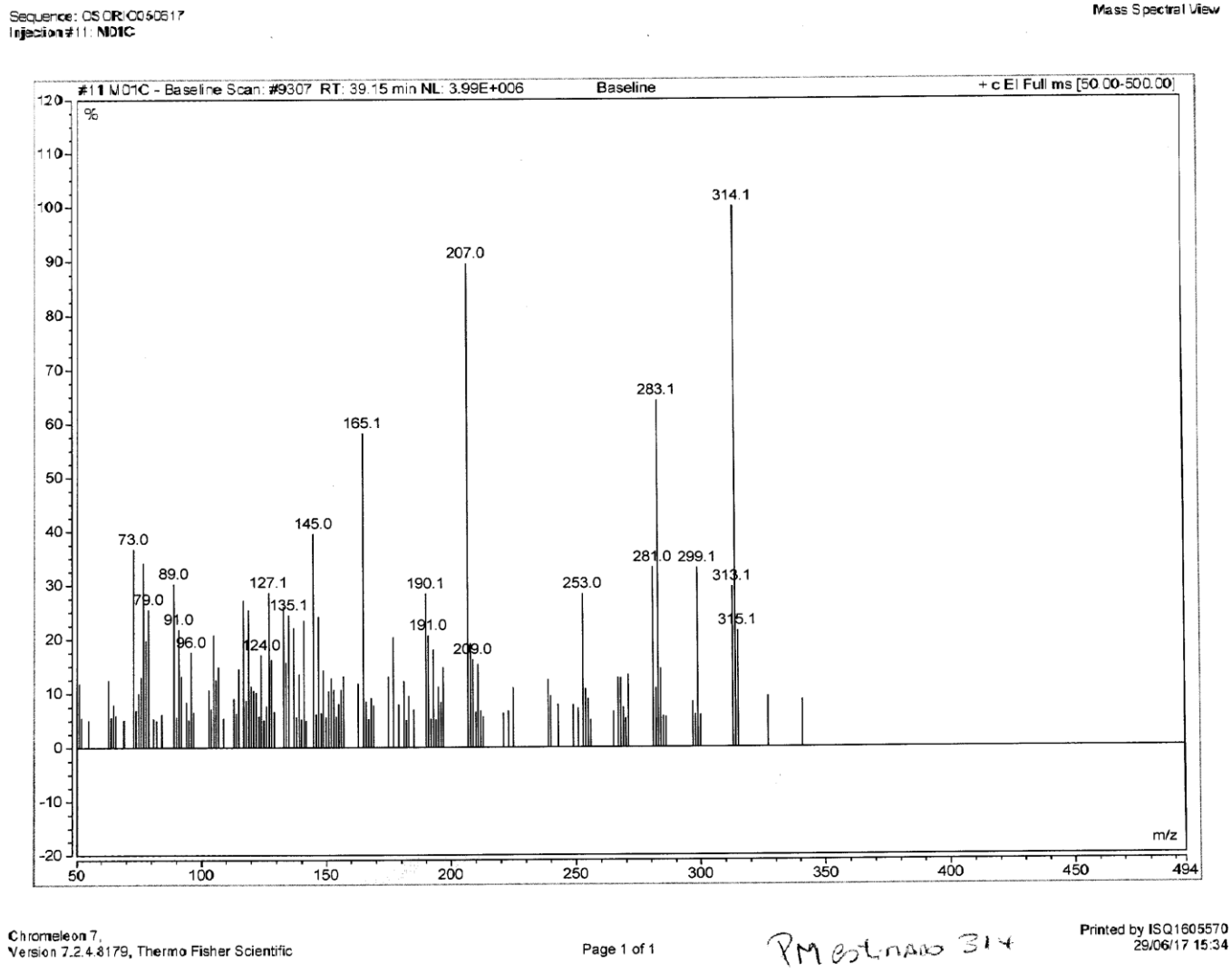
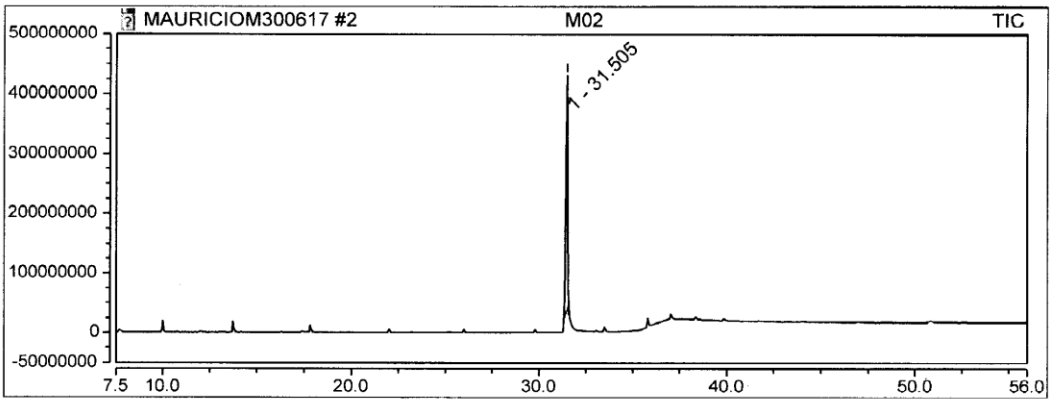


Figure S40. Mass spectrum of compound **16**.

Injection Details			
Injection Name:	**M02**	*Run Time (min).*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**30/Jun/17 14:20**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	31.505	Propenone, 3-(3,4-dimethoxyphenyl)-	39623379	0	691	100.00

Figure S41. Chromatogram of compound **17**: peak No. 1 was selected to mass spectrum.

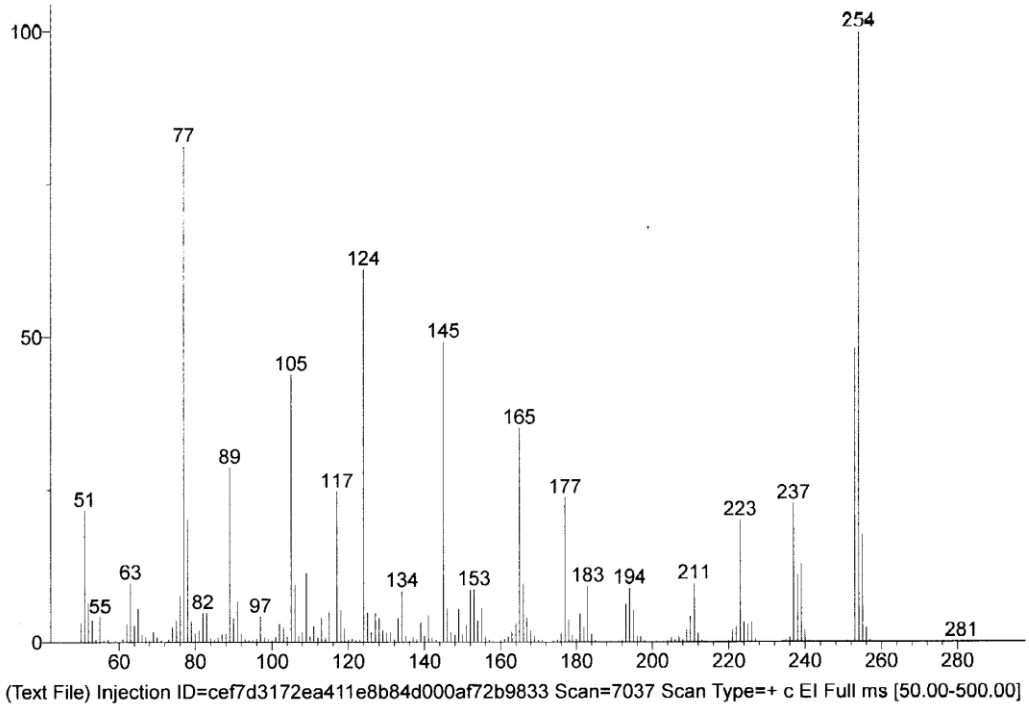
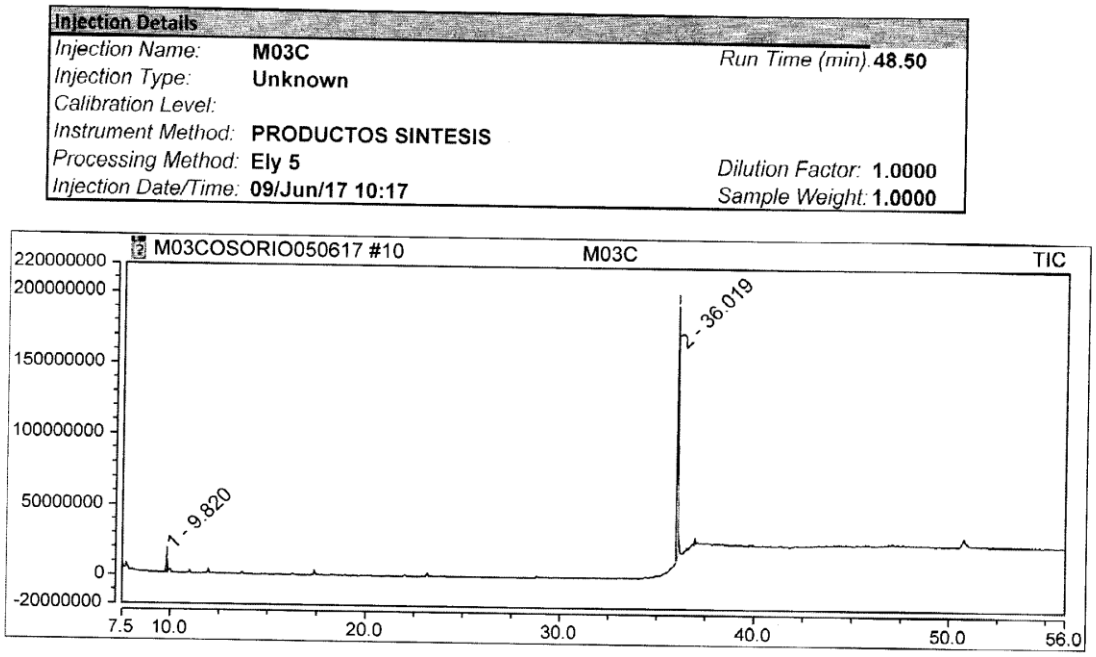


Figure S42. Mass spectrum of compound **17**.



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	9.820	Acetamide, N-(1,2-dihydro-4,6-dimet	193072	0	772	3.31
2	36.019	2,3-Naphthalenediol, 1,4-di-2-propen	5633189	68873-16-5	664	96.69

Figure S43. Chromatogram of compound **18**: peak No. 2 was selected to mass spectrum.

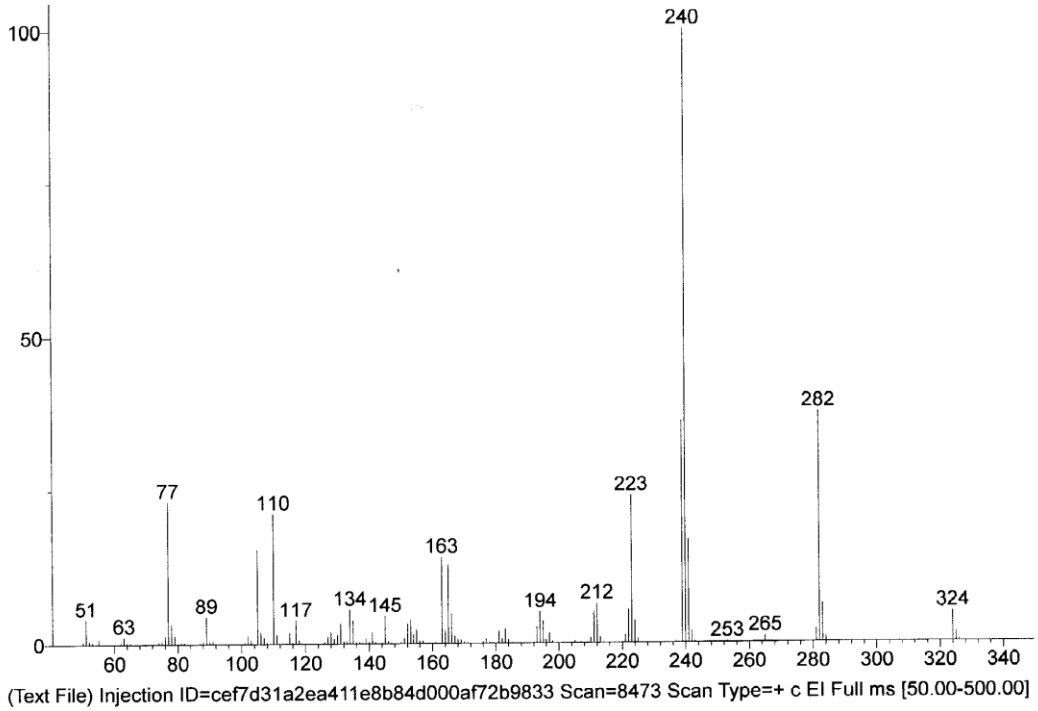


Figure S44. Mass spectrum of compound **18**.

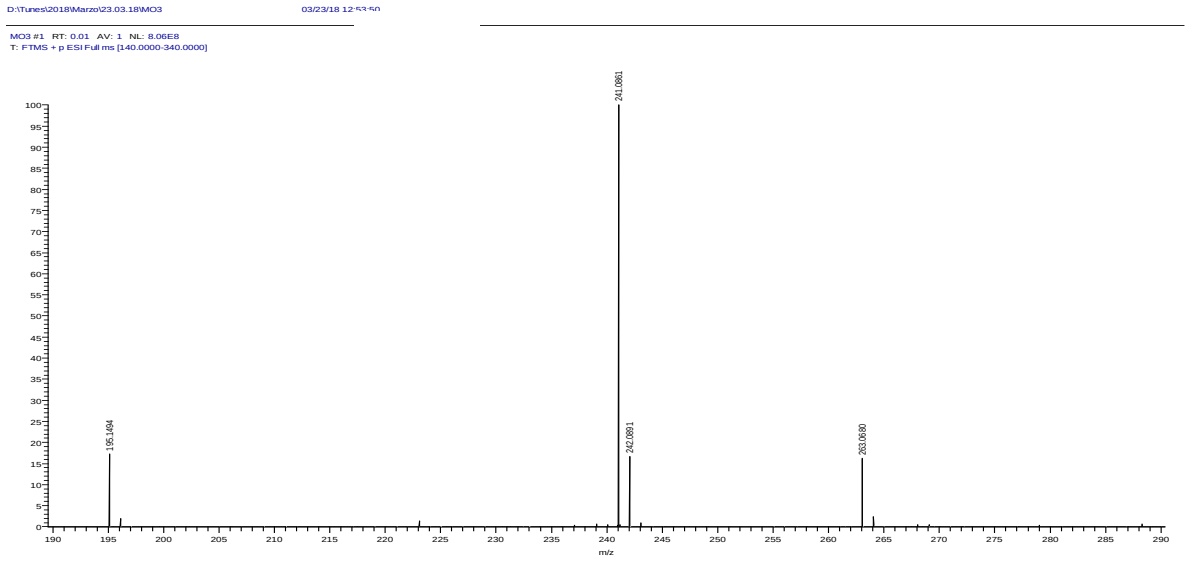
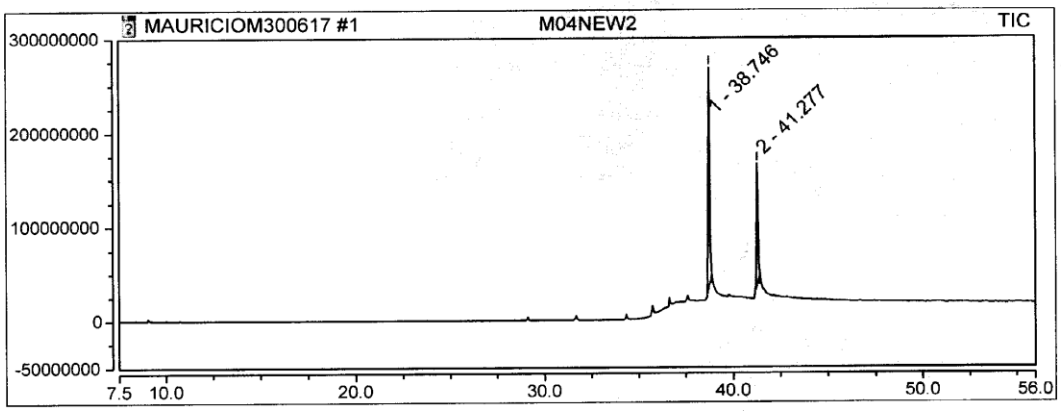


Figure S45. HRMS of compound **18**.

Injection Details			
Injection Name:	**M04NEW2**	*Run Time (min).*	**48.50**
Injection Type:	**Unknown**		
Calibration Level:			
Instrument Method:	**PRODUCTOS SINTESIS**		
Processing Method:	**Ely 5**	*Dilution Factor:*	**1.0000**
Injection Date/Time:	**30/Jun/17 12:18**	*Sample Weight:*	**1.0000**



No	Ret. Time min	Peak Name	Area counts*min	CAS Number	SI	Rel.Area %
1	38.746	1-(2-Hydroxy-4-methoxyphenyl)-3-(3,	16119804	13745-26-1	651	59.78
2	41.277	4a,7a-Epoxy-5H-cyclopenta[a]cyclop	10843738	51906-04-8	637	40.22

Figure S46. Chromatogram of compound **19**: peak No. 1 was selected to mass spectrum.

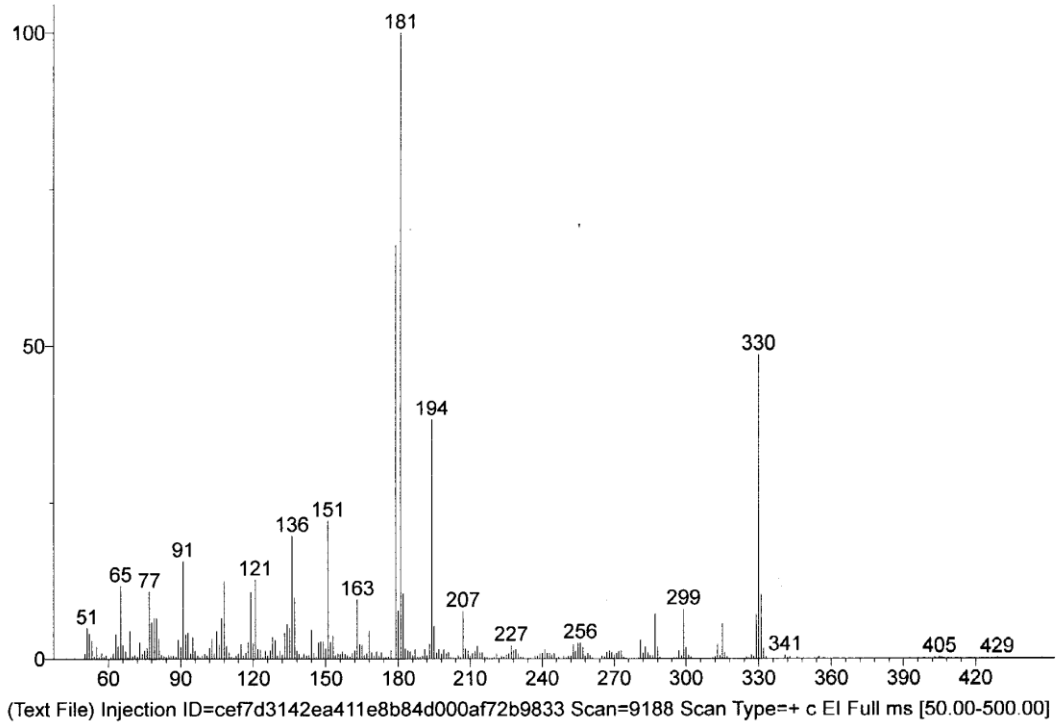


Figure S47. HRMS of compound **19**.