

Synthesis and NLRP3-inflammasome inhibitory activity of the naturally occurring Velutone F and of its non-natural regioisomeric chalconoids

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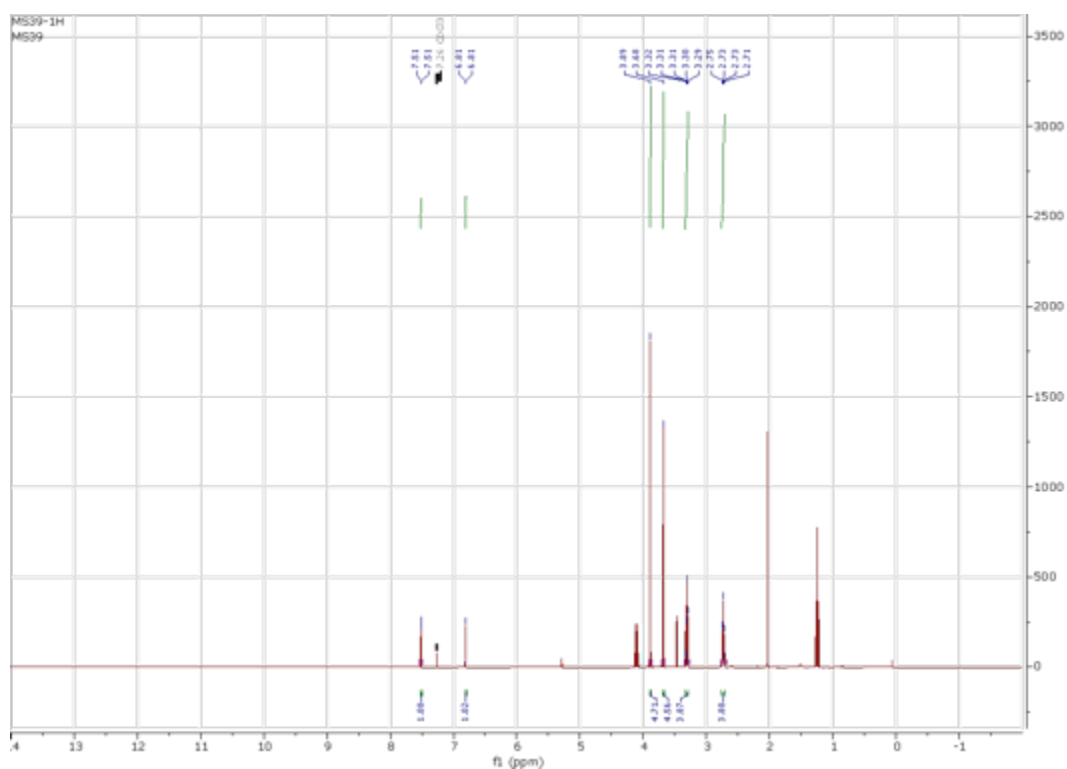
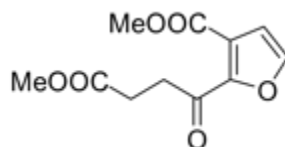
§Both the authors contributed equally

Summary

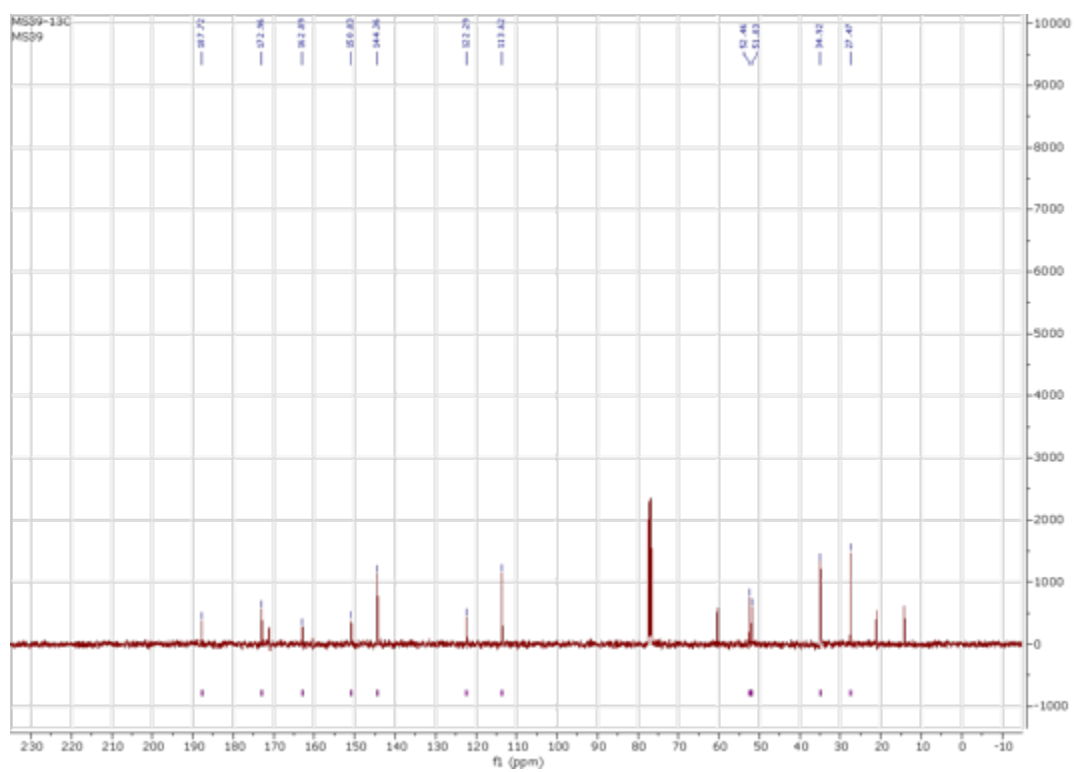
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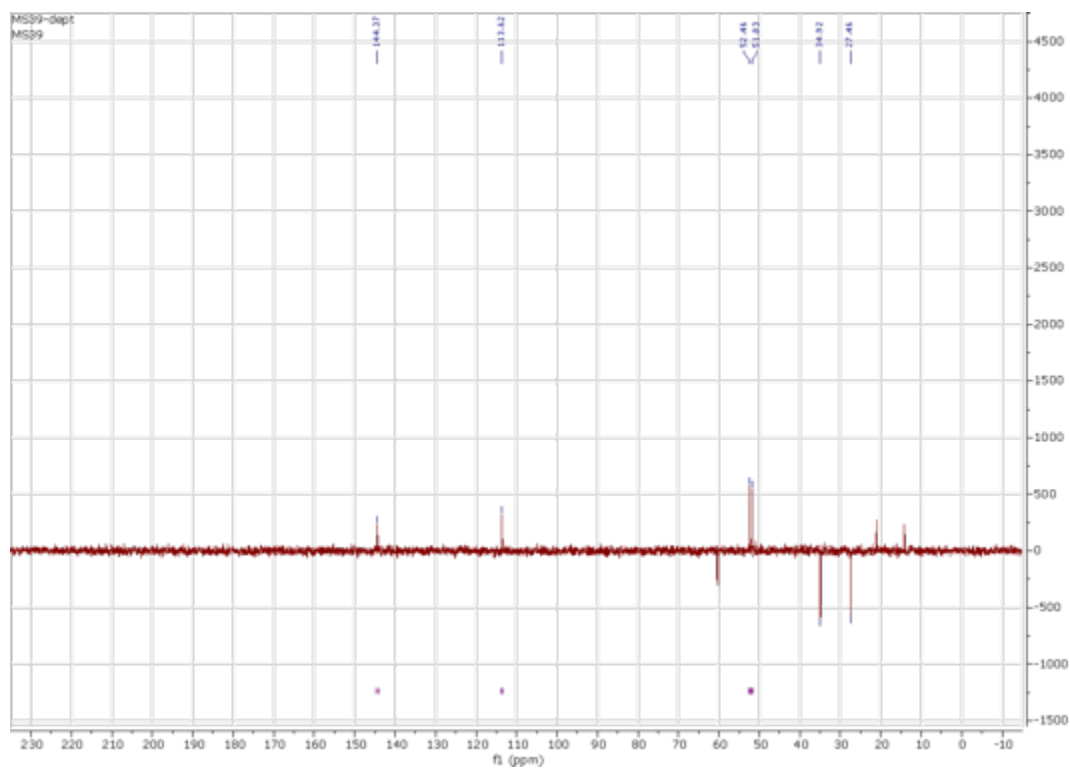
methyl 3-(4-methoxy-4-oxobutanoyl)furan-2-carboxylate (**3**)



^1H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, J = 1.7 Hz, 1H), 6.81 (d, J = 1.7 Hz, 1H), 3.89 (s, 3H), 3.68 (s, 3H), 3.31 (t, J = 6.7 Hz, 2H), 2.73 (t, J = 6.6 Hz, 2H).

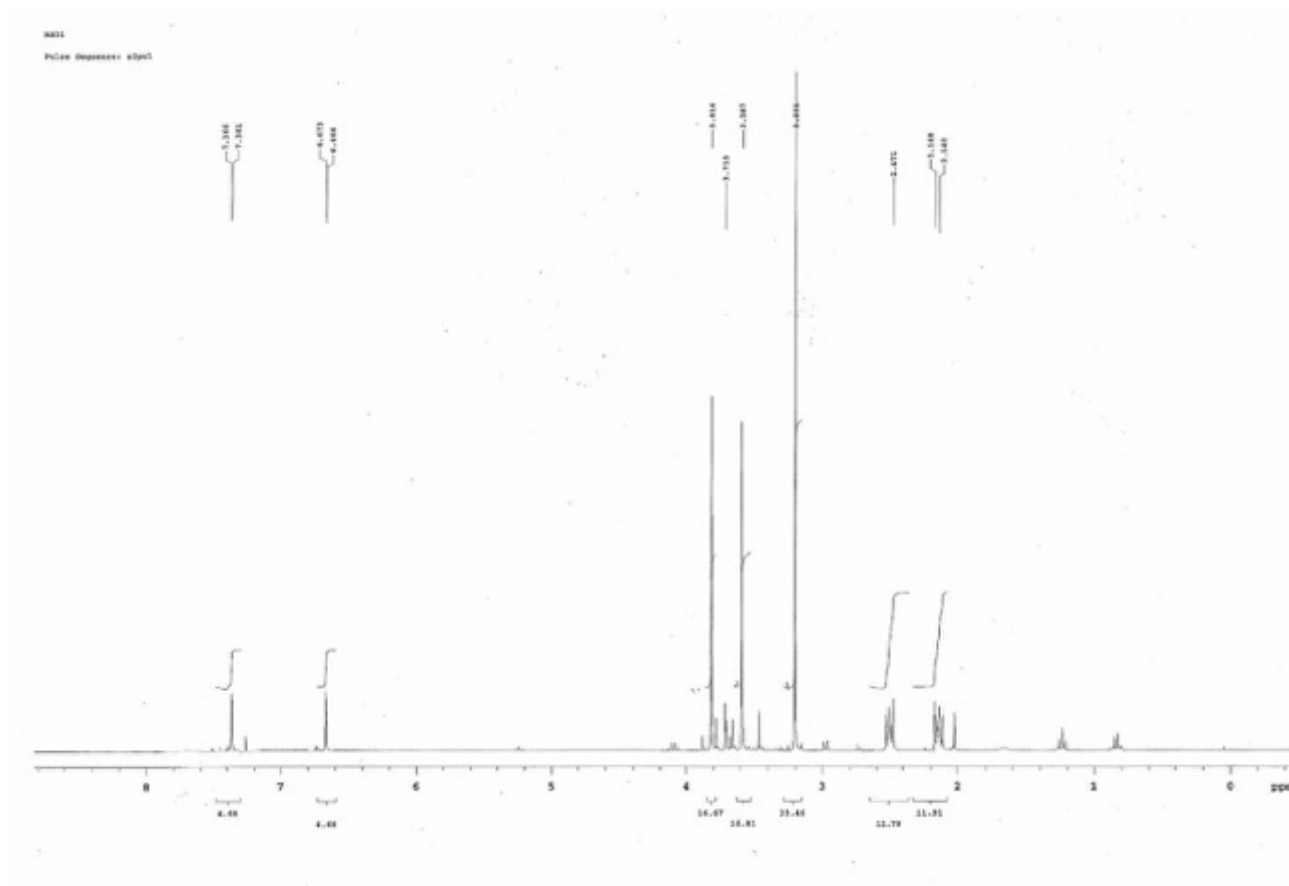
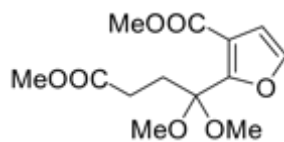


¹³C NMR (101 MHz, Chloroform-d) δ 187.72, 172.96, 162.89, 150.83, 144.36, 122.29, 113.62, 52.46, 51.83, 34.92, 27.47.

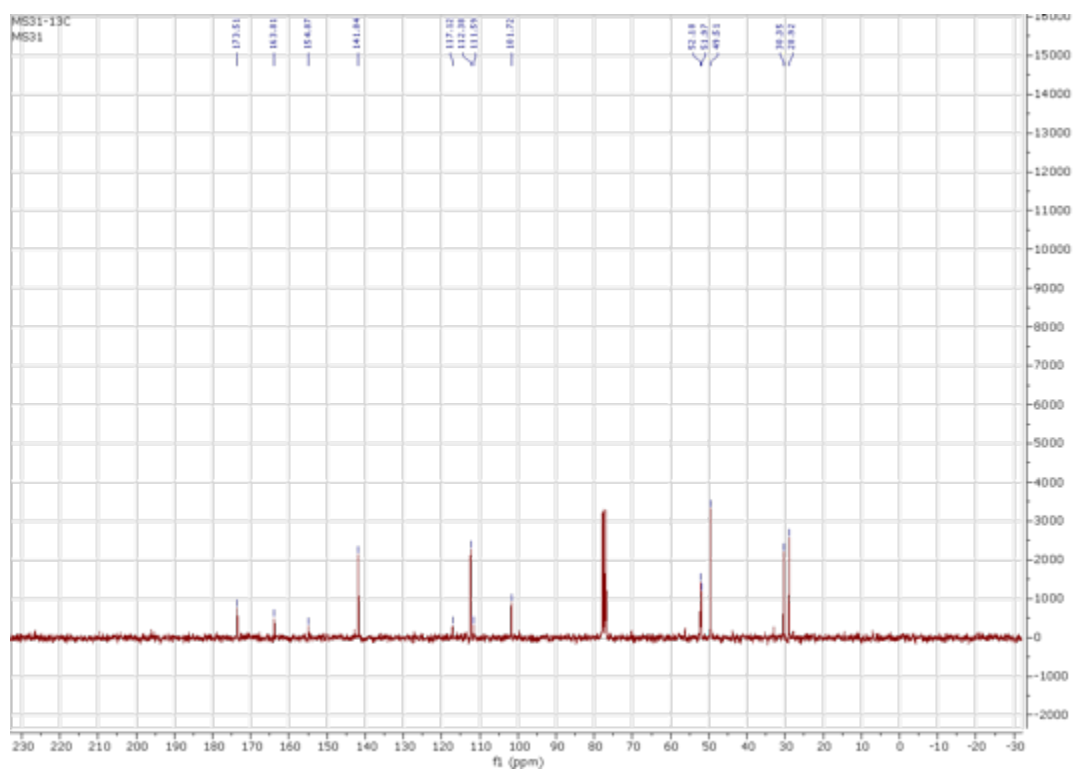


¹³C NMR (101 MHz, Chloroform-d) δ 144.37, 113.62, 52.46, 51.83, 34.92, 27.46.

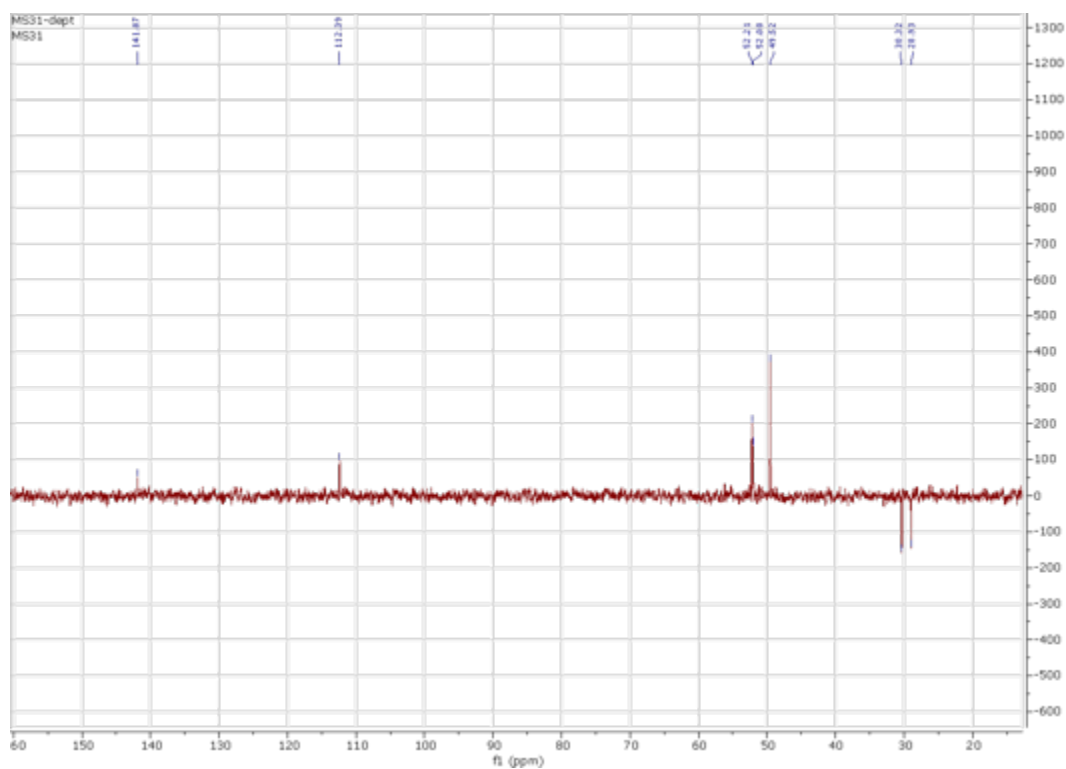
methyl 3-(1,1,4-trimethoxy-4-oxobutyl)furan-2-carboxylate (**4**)



^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 (d, J = 1.7 Hz, 1H), 6.66 (d, J = 1.7 Hz, 1H), 3.81 (s, 3H), 3.58 (s, 3H), 3.20 (s, 6H), 2.47 (t, J = 6.7 Hz, 2H), 2.16 (t, J = 6.6 Hz, 2H).

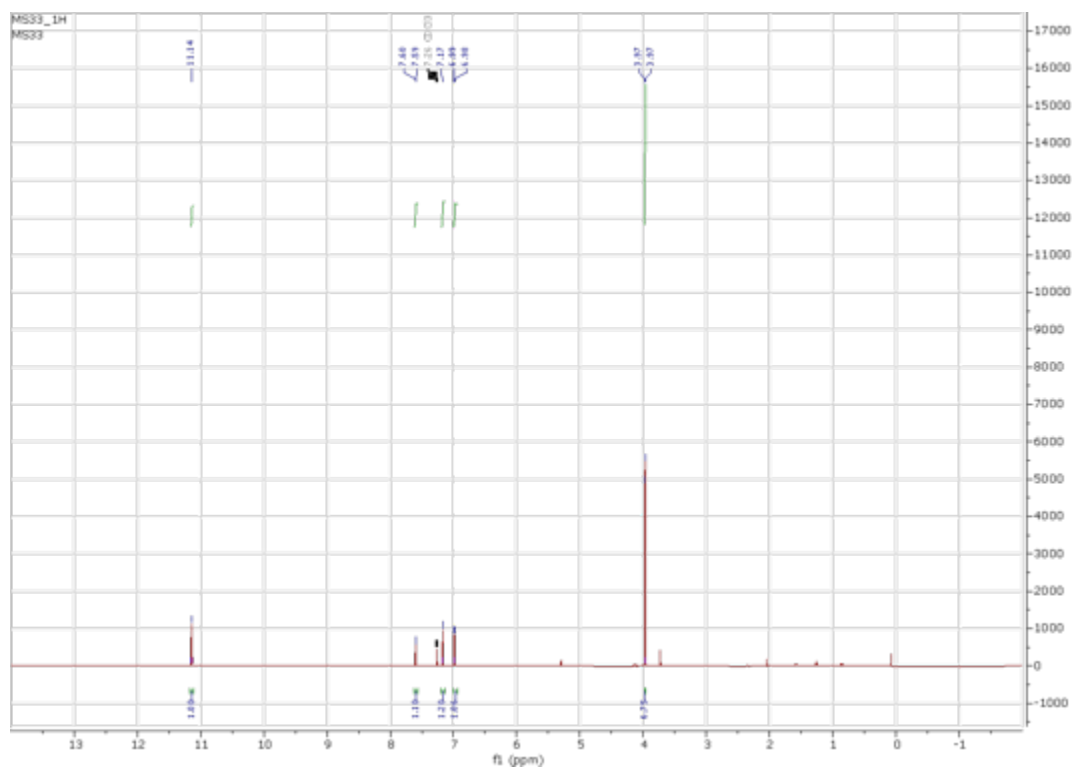
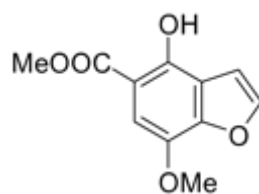


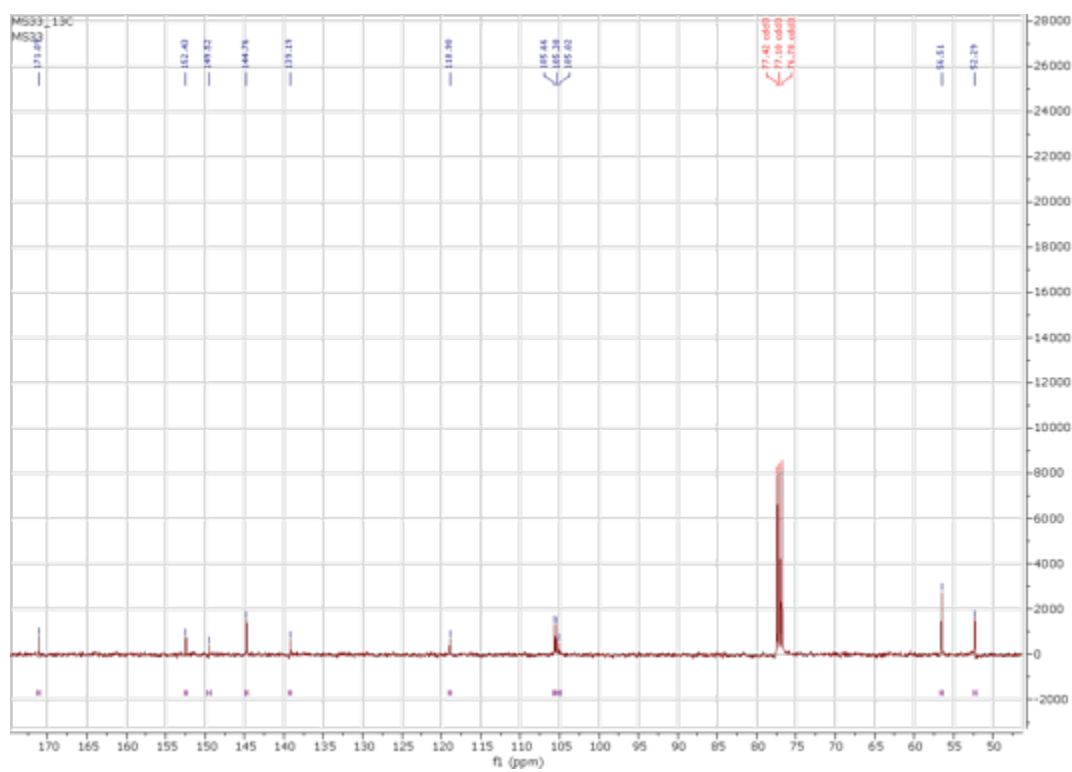
^{13}C NMR (75 MHz, Chloroform-d) δ 173.51, 163.81, 154.87, 141.84, 117.12, 112.38, 111.59, 101.72, 52.18, 51.97, 49.51, 30.35, 28.92.



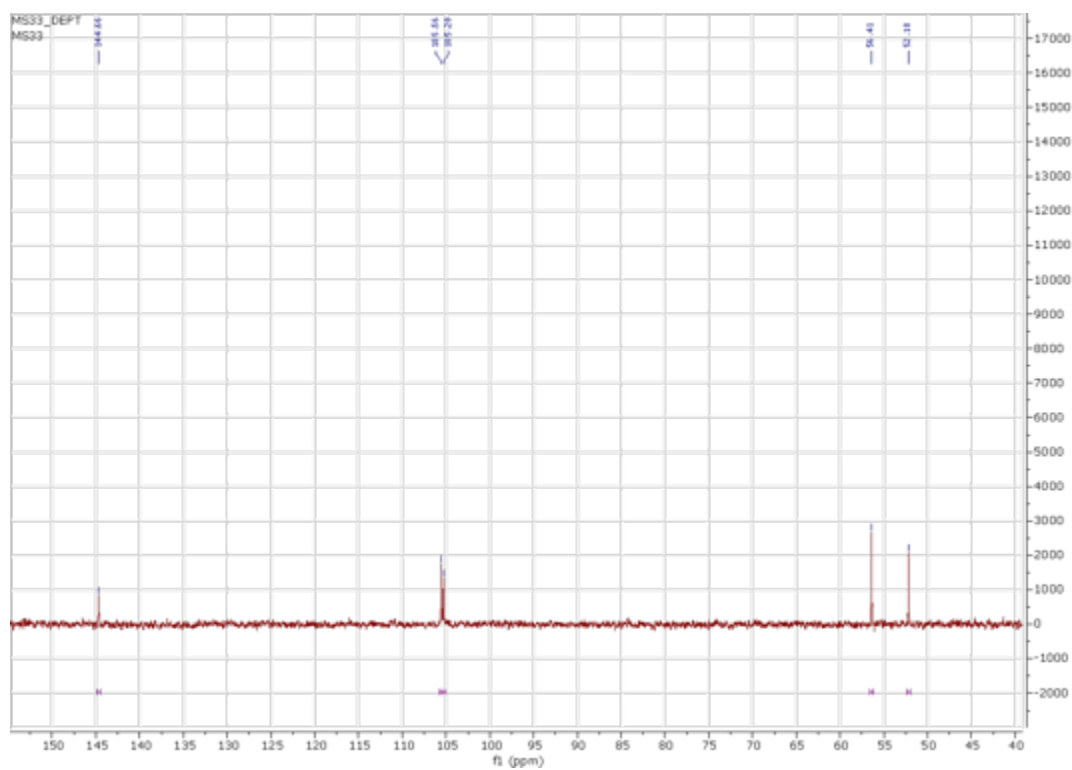
^{13}C NMR (75 MHz, Chloroform-d) δ 141.87, 112.39, 52.21, 52.00, 49.52, 30.32, 28.93.

methyl 4-hydroxy-7-methoxybenzofuran-5-carboxylate (**5**)



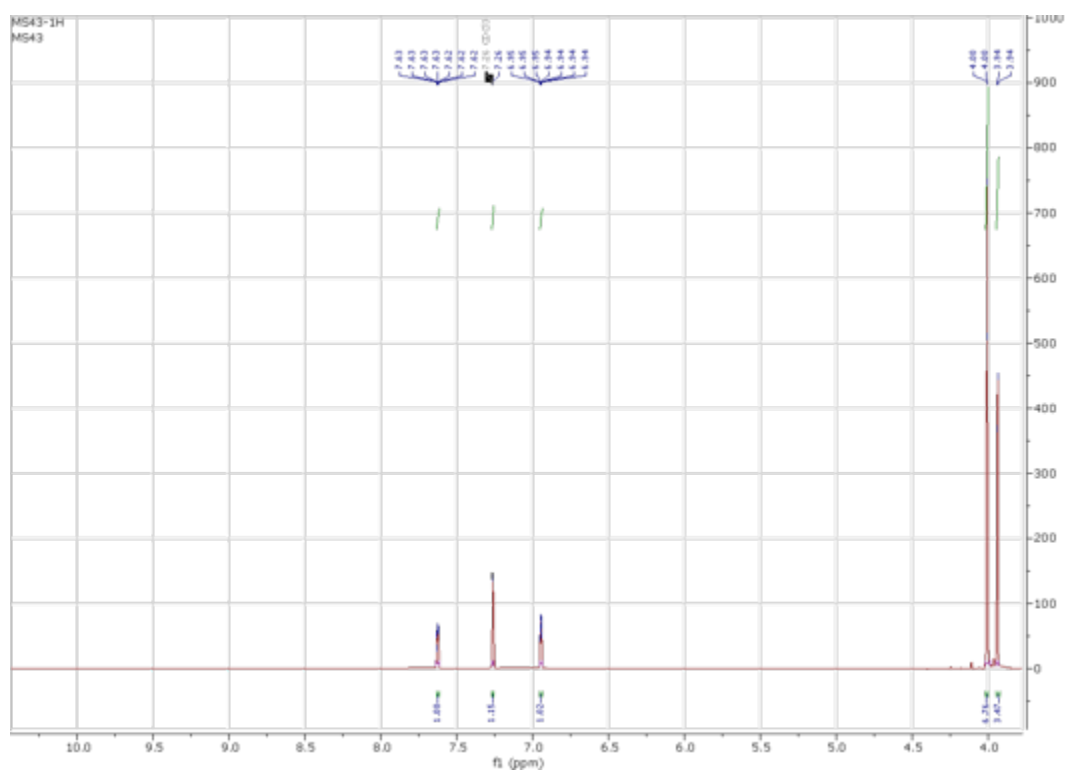
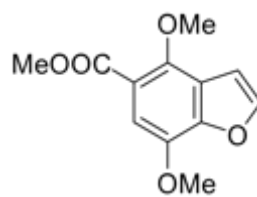


¹³C NMR (101 MHz, Chloroform-d) δ 171.09, 152.43, 149.52, 144.76, 139.19, 118.90, 105.66, 105.38, 105.02, 56.51, 52.29.

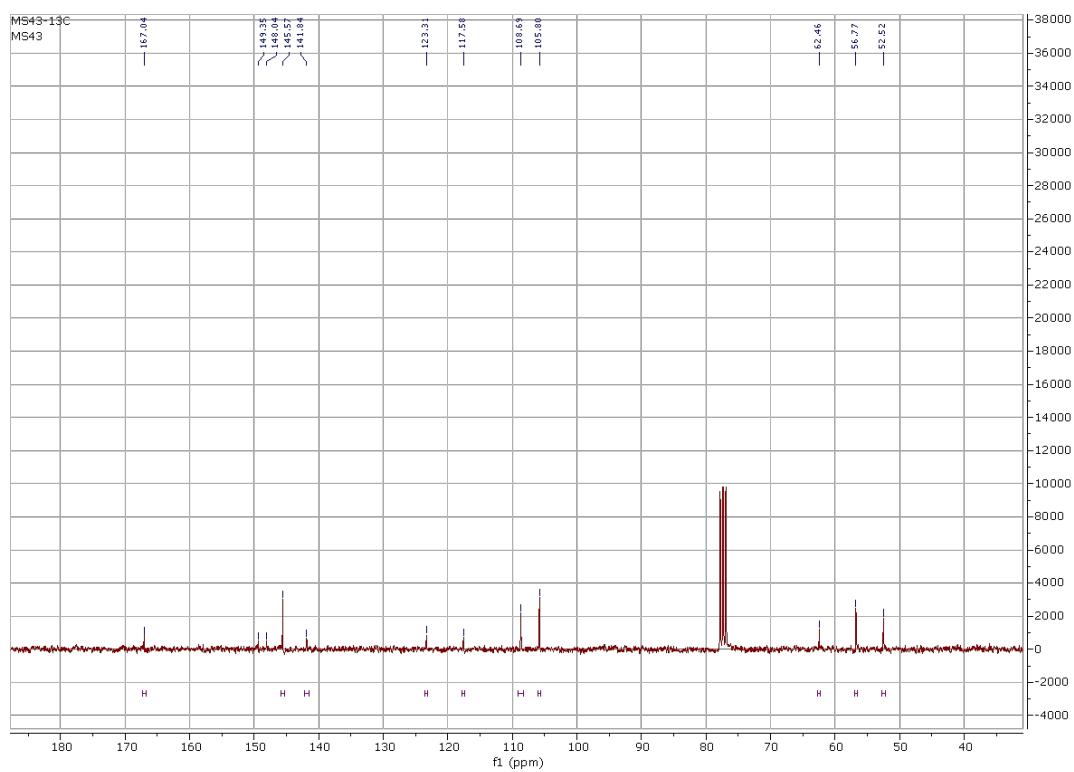


¹³C NMR (101 MHz, Chloroform-d) δ 144.66, 105.56, 105.28, 56.41, 52.18.

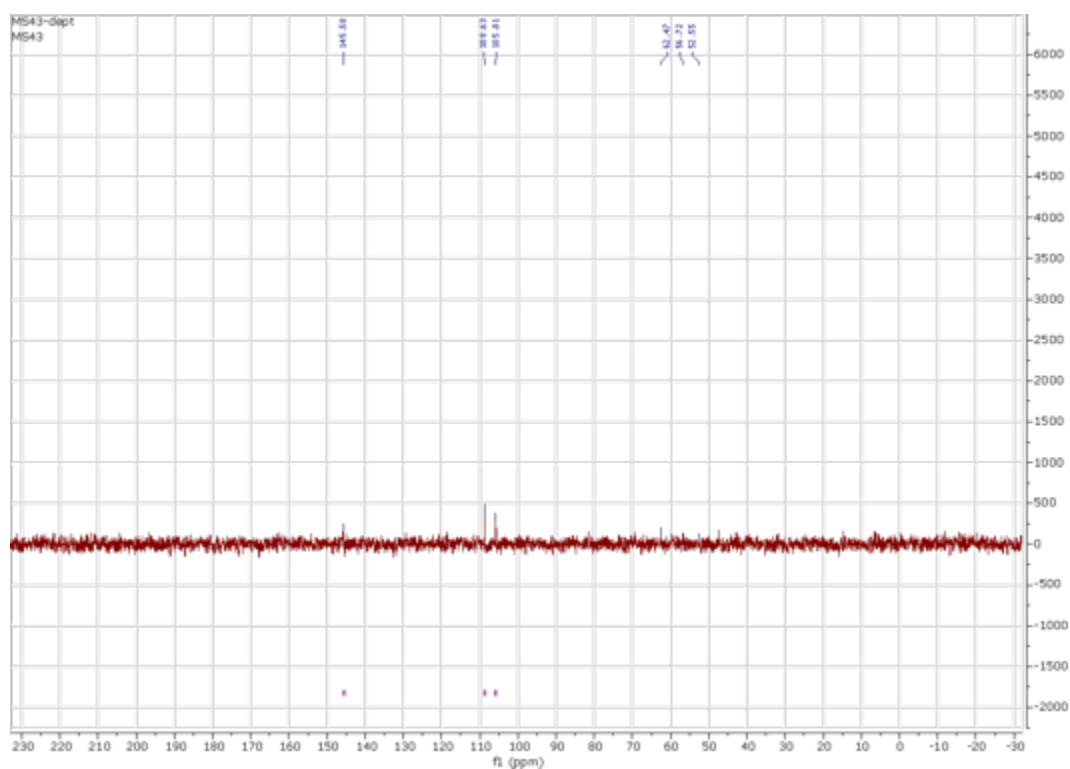
methyl 4,7-dimethoxybenzofuran-5-carboxylate (**6**)



^1H NMR (300 MHz, Chloroform-*d*) δ 7.63 – 7.61 (m, 1H), 7.26 (s, 1H), 6.95 – 6.94 (m, 1H), 4.00 (d, J = 0.8 Hz, 6H), 3.94 (d, J = 0.8 Hz, 3H).

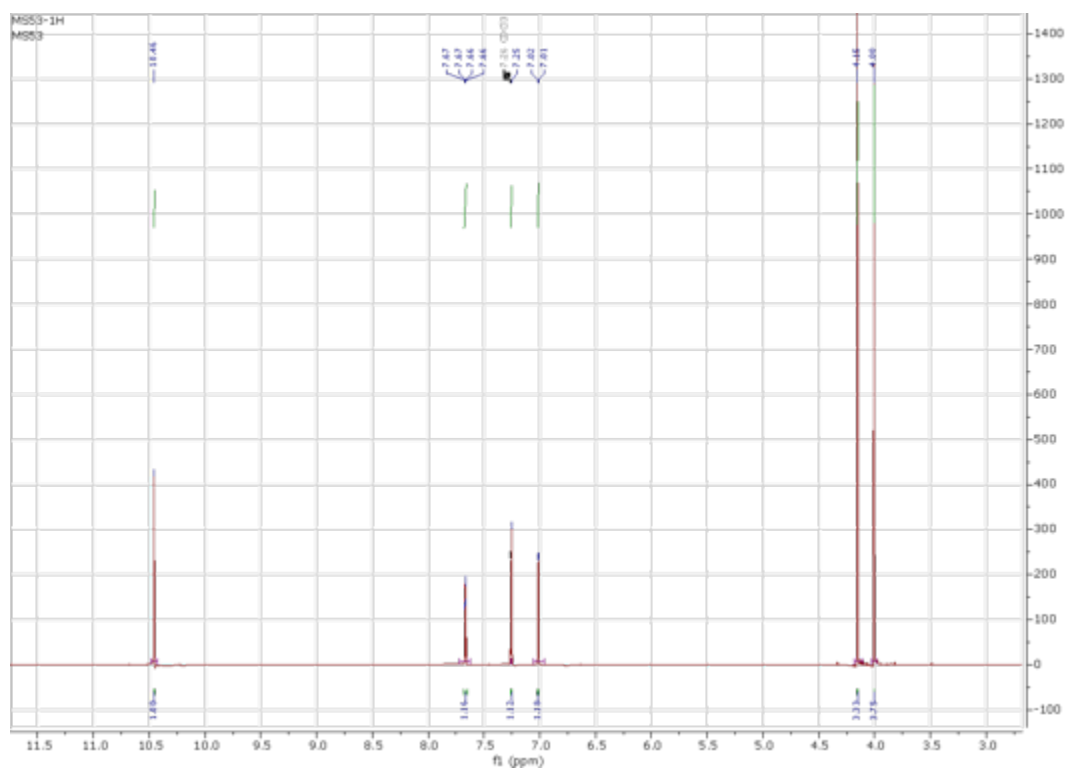
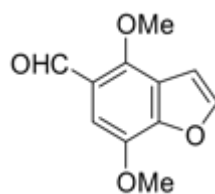


^{13}C NMR (75 MHz, Chloroform- d) δ 167.04, 149.35, 148.04, 145.57, 141.84, 123.31, 117.58, 108.69, 105.80, 62.46, 56.77, 52.52.

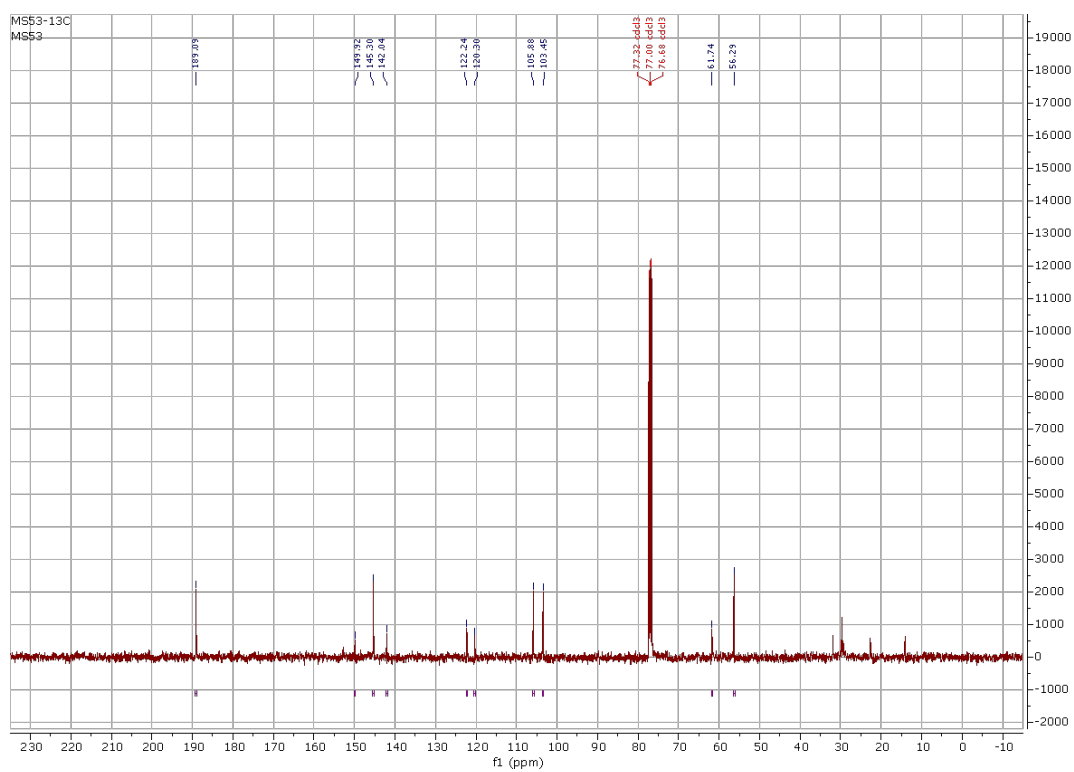


^{13}C NMR (75 MHz, Chloroform- d) δ 145.58, 108.63, 105.81, 62.47, 56.72, 52.55.

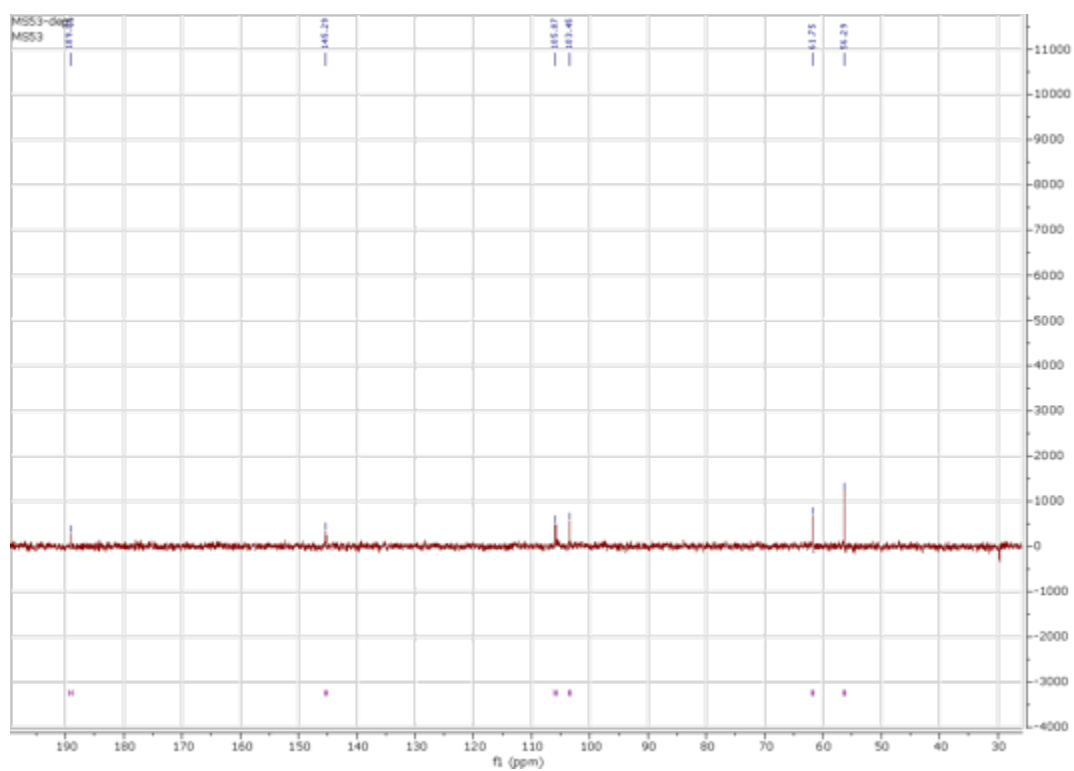
4,7-dimethoxybenzofuran-5-carbaldehyde (7)



¹H NMR (400 MHz, Chloroform-*d*) δ 10.46 (s, 1H), 7.67 (dd, $J = 2.3, 0.4$ Hz, 1H), 7.25 (s, 1H), 7.02 (d, $J = 2.3$ Hz, 1H), 4.15 (s, 3H), 4.00 (s, 3H).

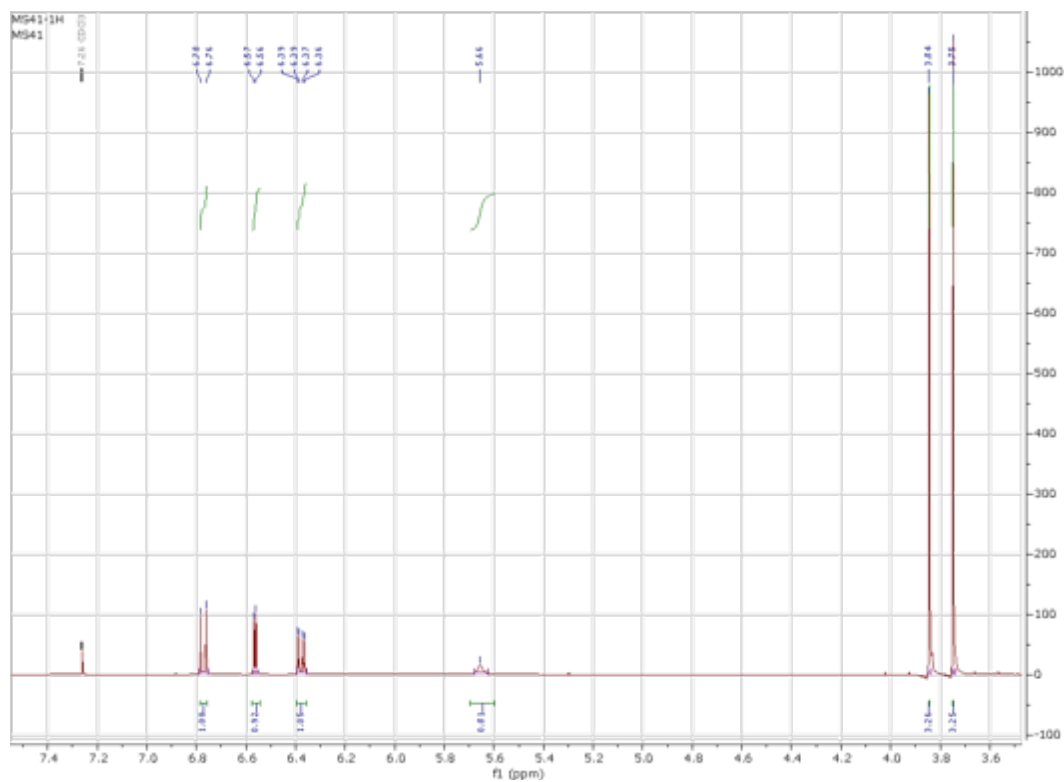
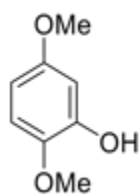


¹³C NMR (101 MHz, Chloroform-d) δ 189.09, 149.92, 145.30, 142.04, 122.24, 120.30, 105.88, 103.45, 61.74, 56.29.

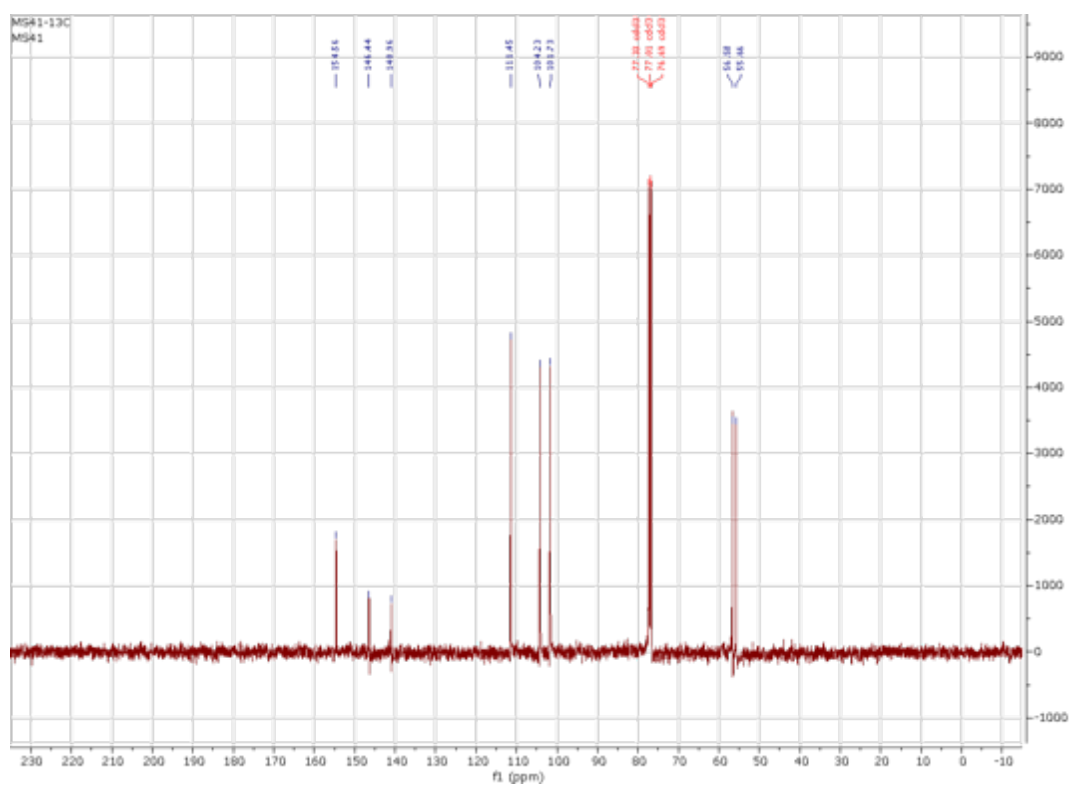


¹³C NMR (101 MHz, Chloroform-d) δ 189.09, 145.29, 105.87, 103.45, 61.75, 56.29.

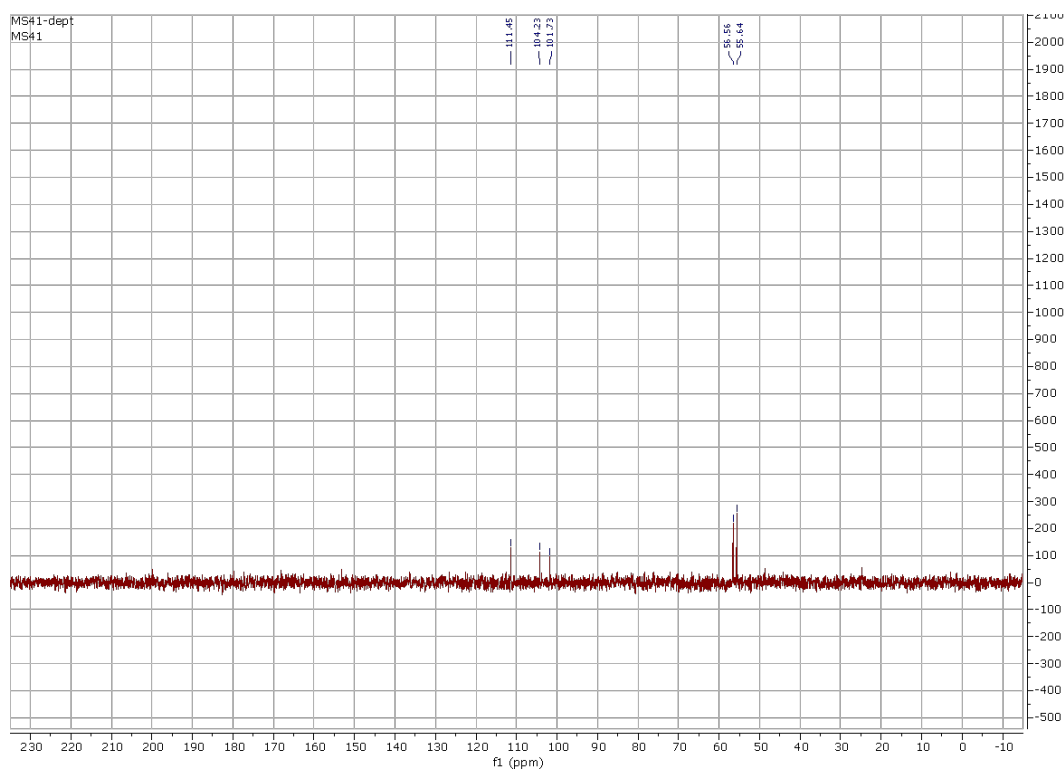
2,5-dimethoxyphenol (9)



¹H NMR (400 MHz, Chloroform-d) δ 6.77 (d, J = 8.8 Hz, 1H), 6.56 (d, J = 2.9 Hz, 1H), 6.38 (dd, J = 8.8, 2.9 Hz, 1H), 5.66 (s, 1H), 3.84 (s, 3H), 3.75 (s, 3H).

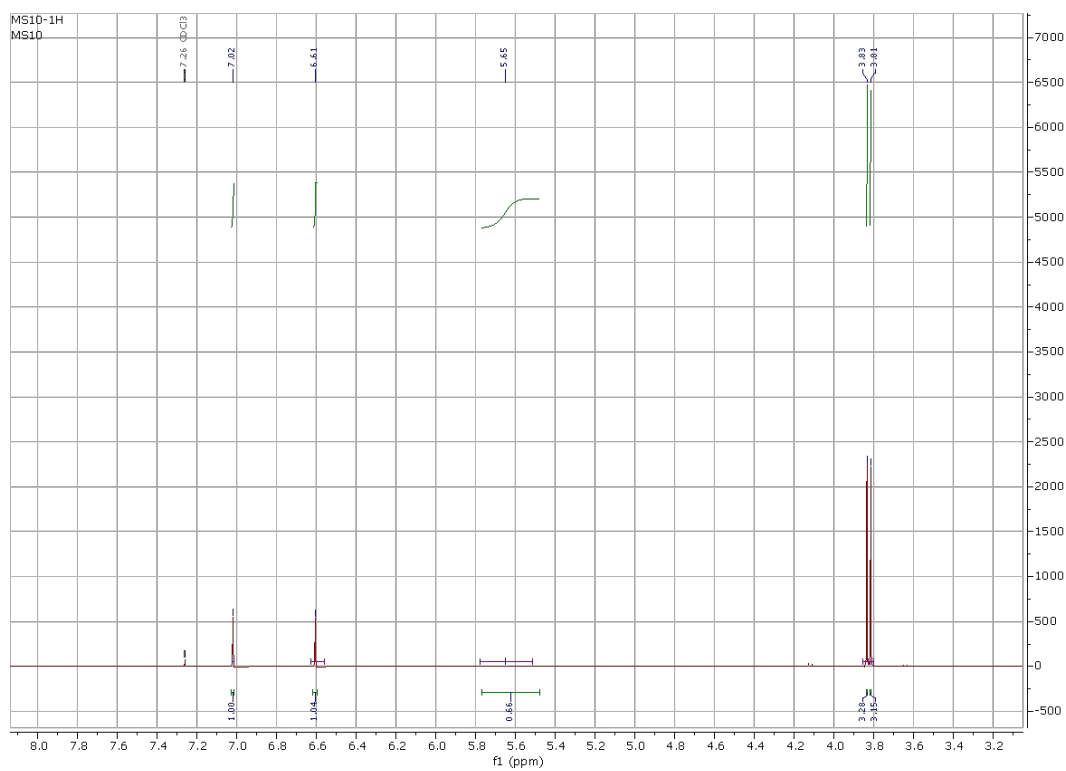
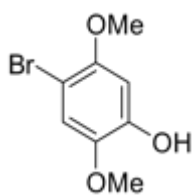


^{13}C NMR (101 MHz, Chloroform-d) δ 154.56, 146.44, 140.96, 111.45, 104.23, 101.73, 56.58, 55.66.

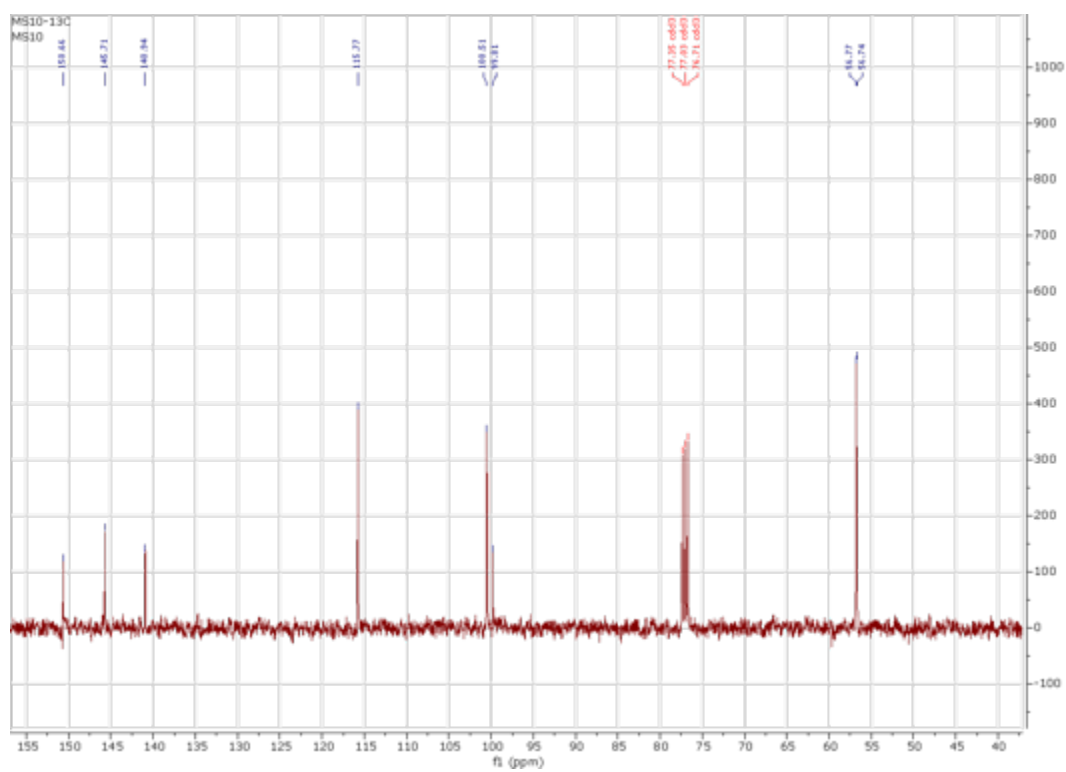


^{13}C NMR (101 MHz, Chloroform-d) δ 111.45, 104.23, 101.73, 56.56, 55.64.

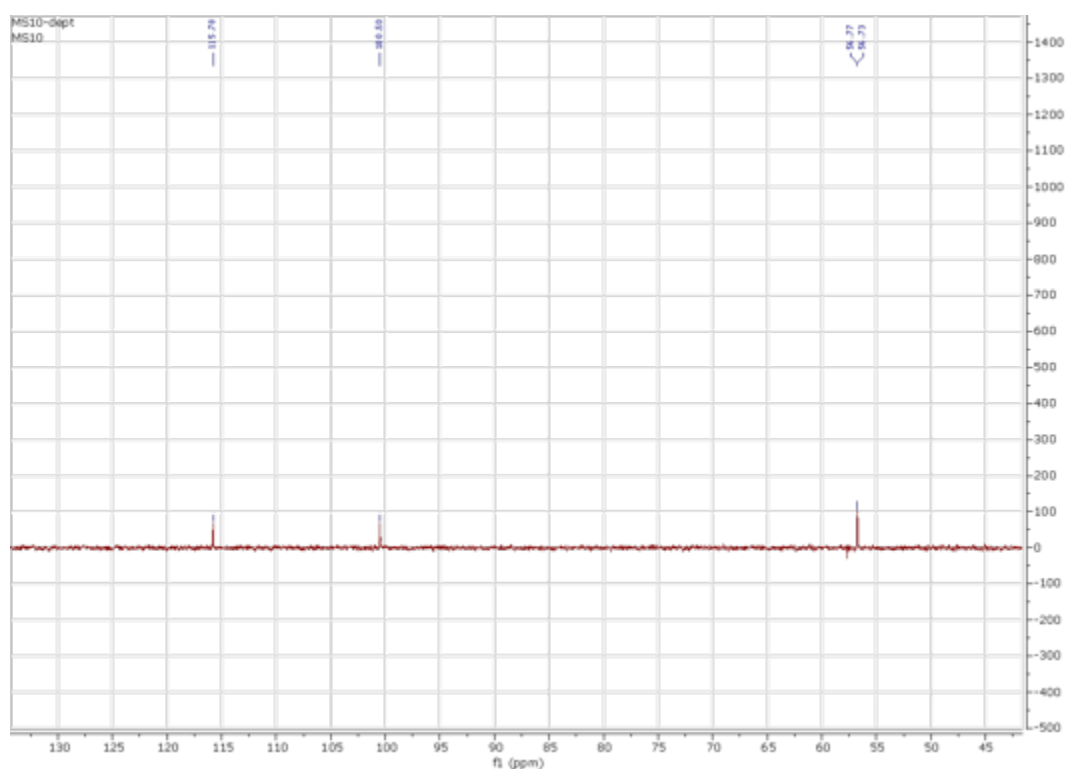
4-bromo-2,5-dimethoxyphenol (**10**)



^1H NMR (400 MHz, Chloroform- d) δ 7.02 (s, 1H), 6.61 (s, 1H), 5.65 (s, 1H), 3.83 (s, 3H), 3.81 (s, 3H).

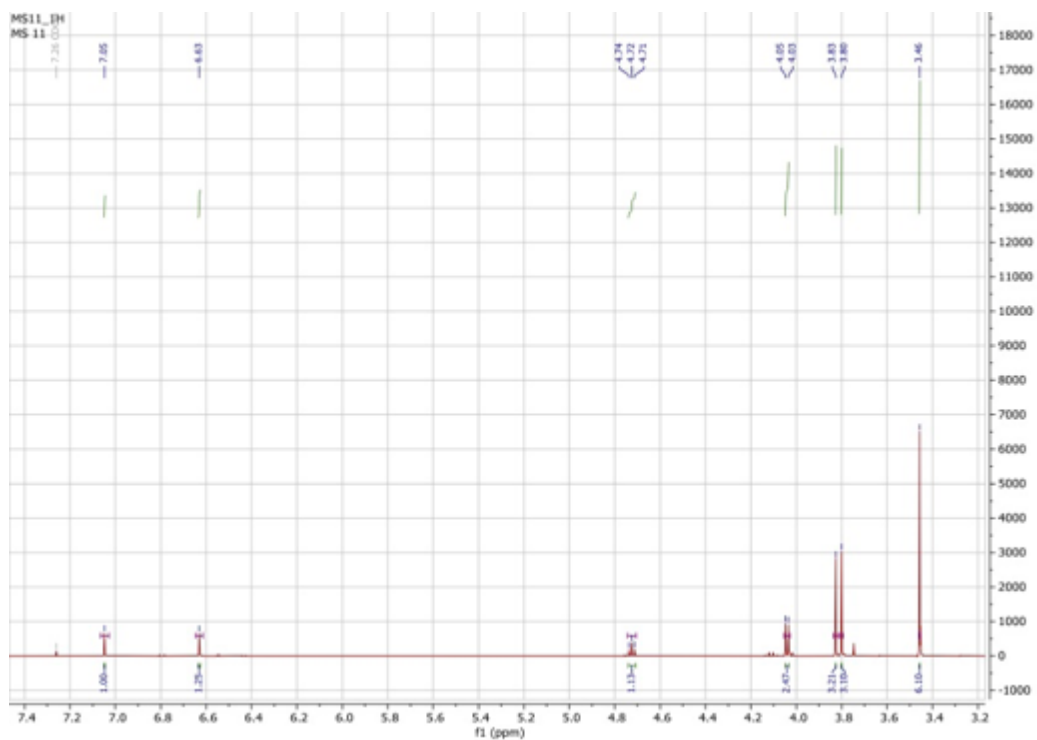
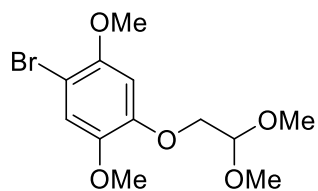


^{13}C NMR (101 MHz, Chloroform-d) δ 150.66, 145.71, 140.94, 115.77, 100.51, 99.81, 56.77, 56.74.

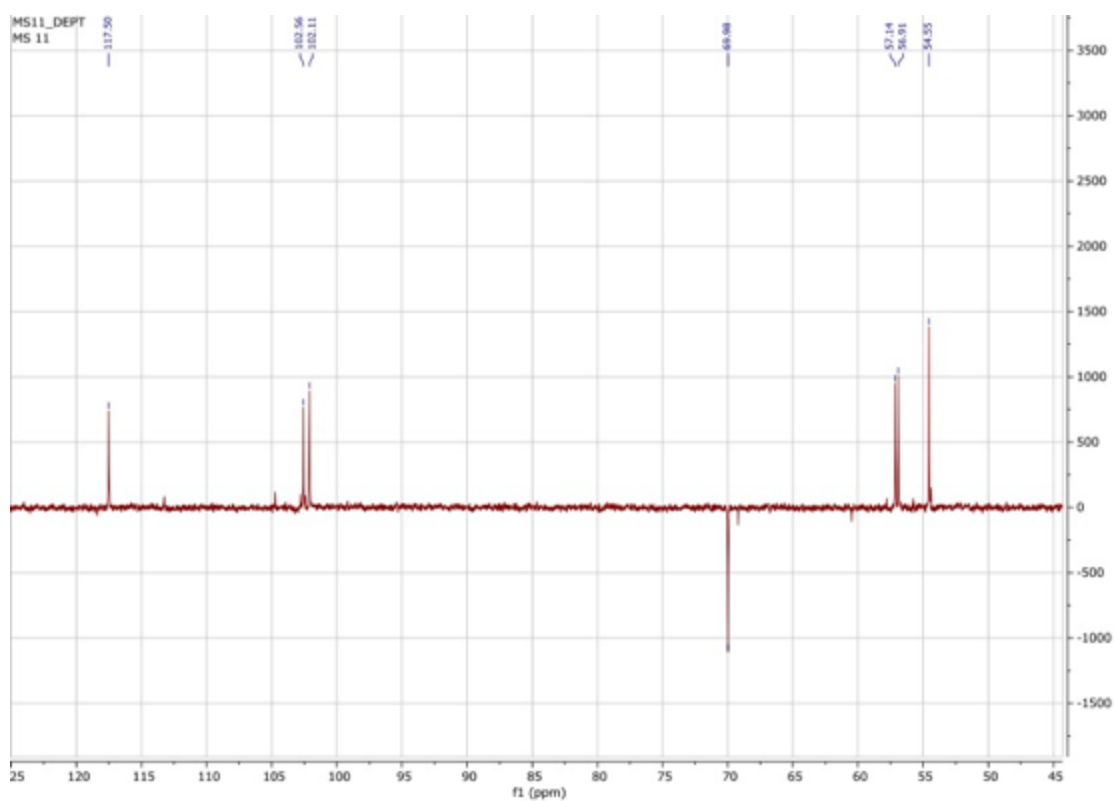
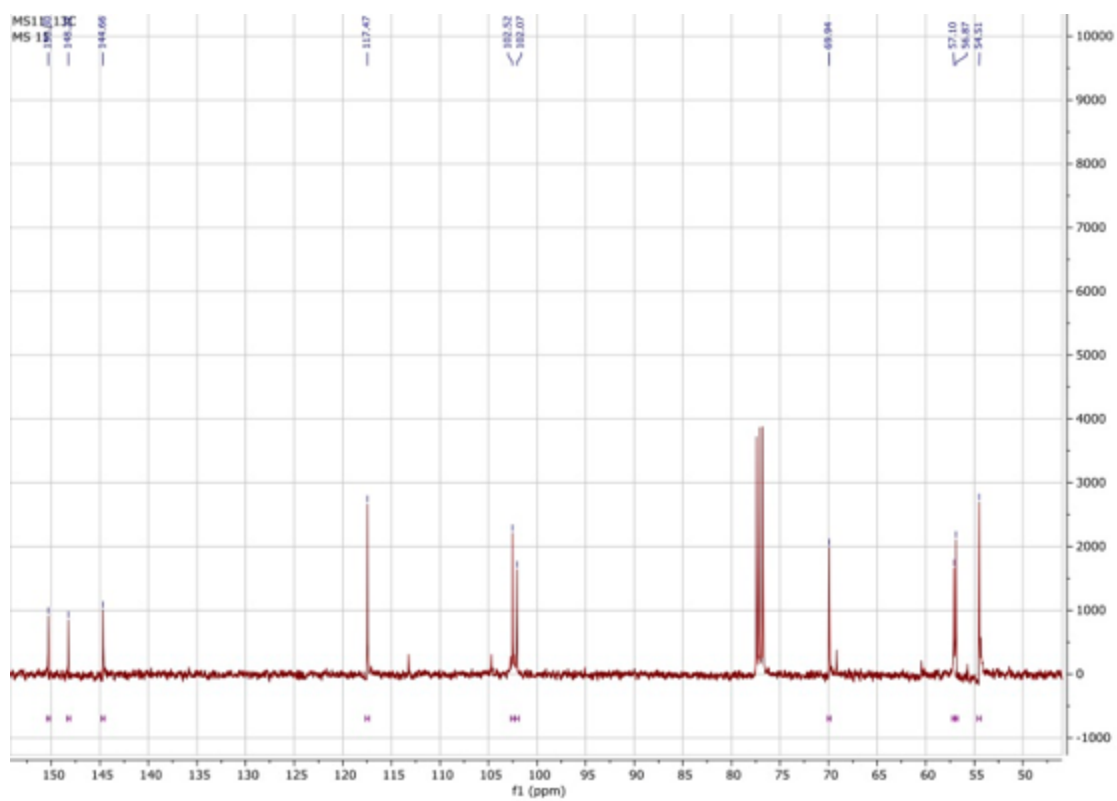


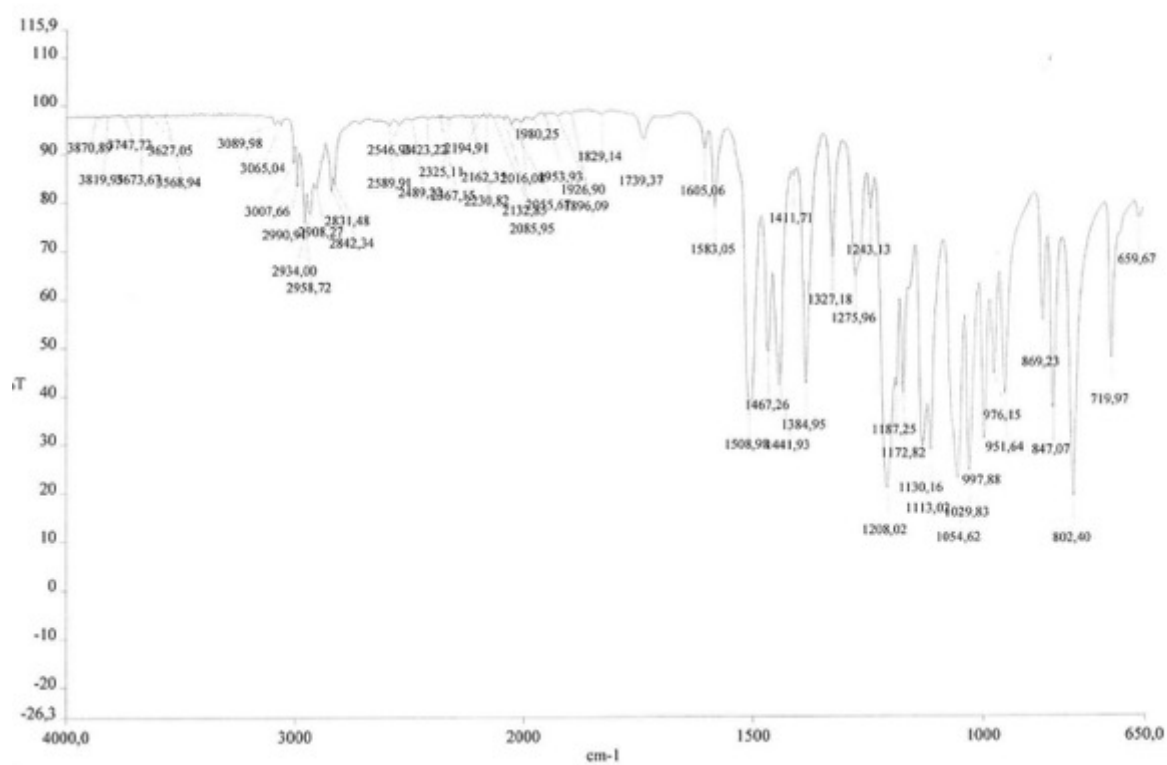
^{13}C NMR (101 MHz, Chloroform-d) δ 115.78, 100.50, 56.77, 56.73.

1-bromo-4-(2,2-dimethoxyethoxy)-2,5-dimethoxybenzene (**11**)

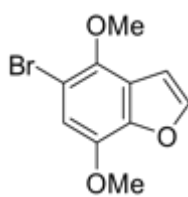


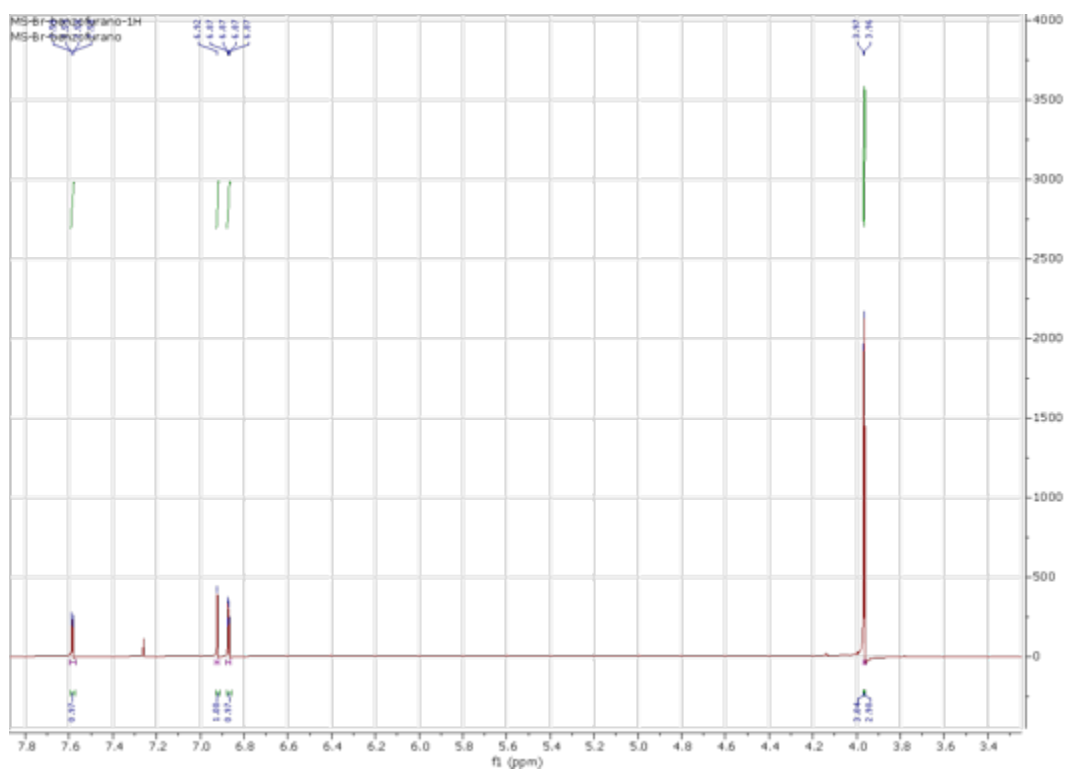
^1H NMR (400 MHz, Chloroform- d) δ 7.05 (s, 1H), 6.63 (s, 1H), 4.72 (t, J = 5.2 Hz, 1H), 4.04 (d, J = 5.2 Hz, 2H), 3.83 (s, 3H), 3.80 (s, 3H), 3.46 (s, 6H).



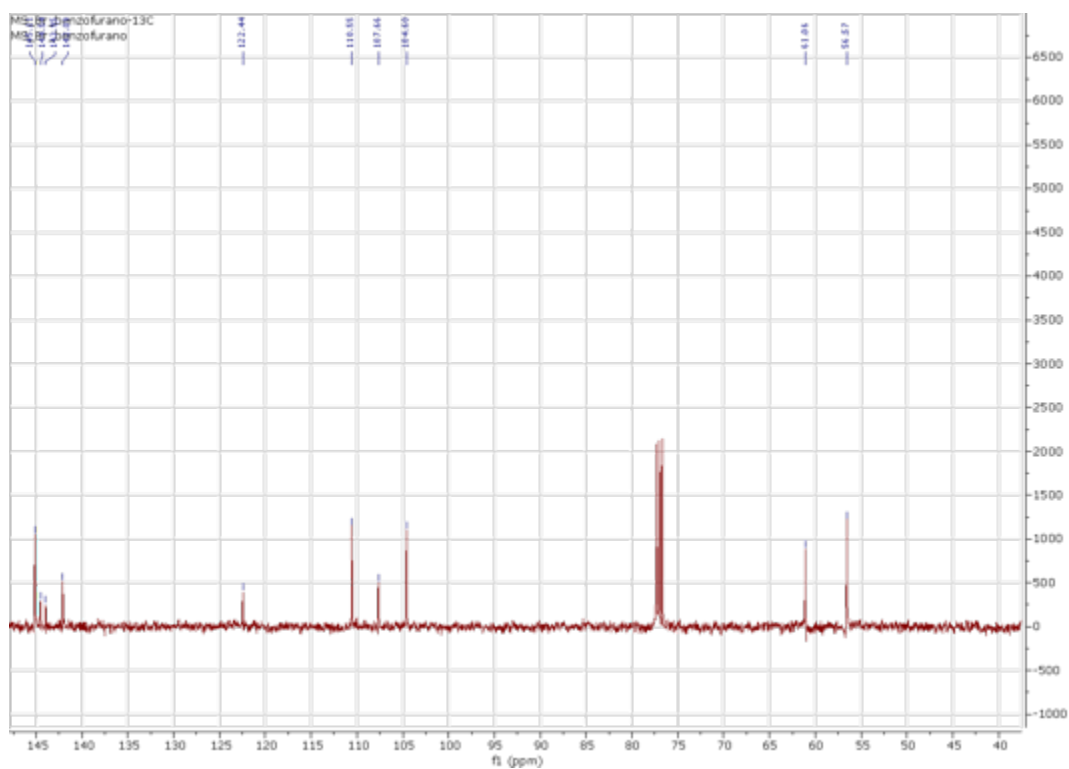


5-bromo-4,7-dimethoxybenzofuran (12)

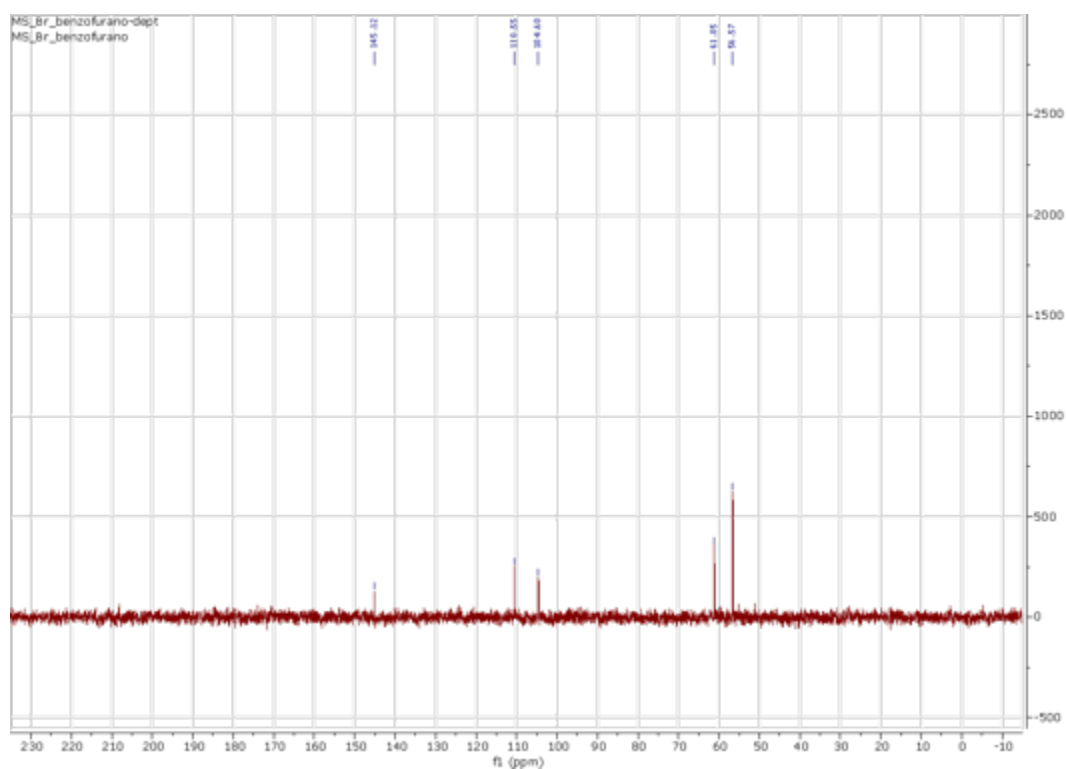




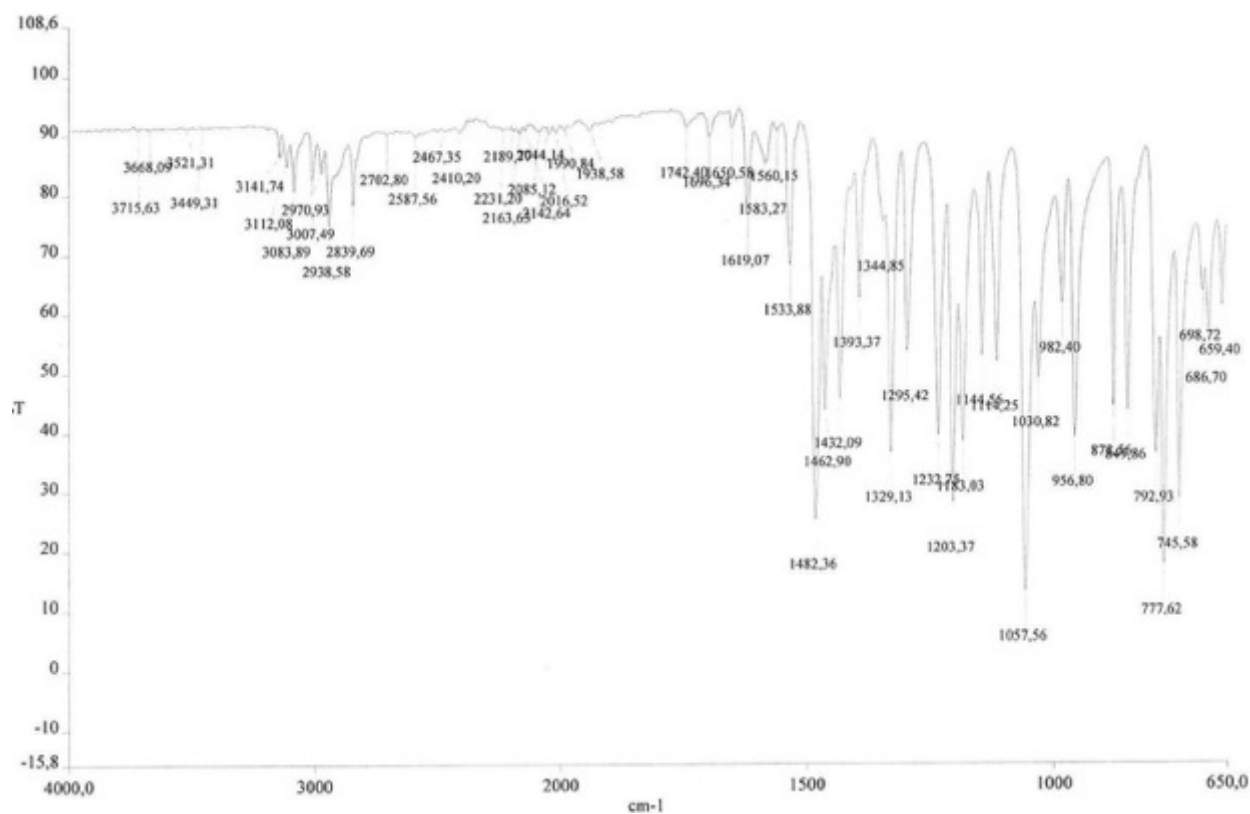
^1H NMR (400 MHz, Chloroform- d) δ 7.59 (dd, $J = 2.2, 0.5$ Hz, 1H), 6.92 (s, 1H), 6.87 (dd, $J = 2.1, 0.4$ Hz, 1H), 3.97 (d, $J = 1.7$ Hz, 6H).



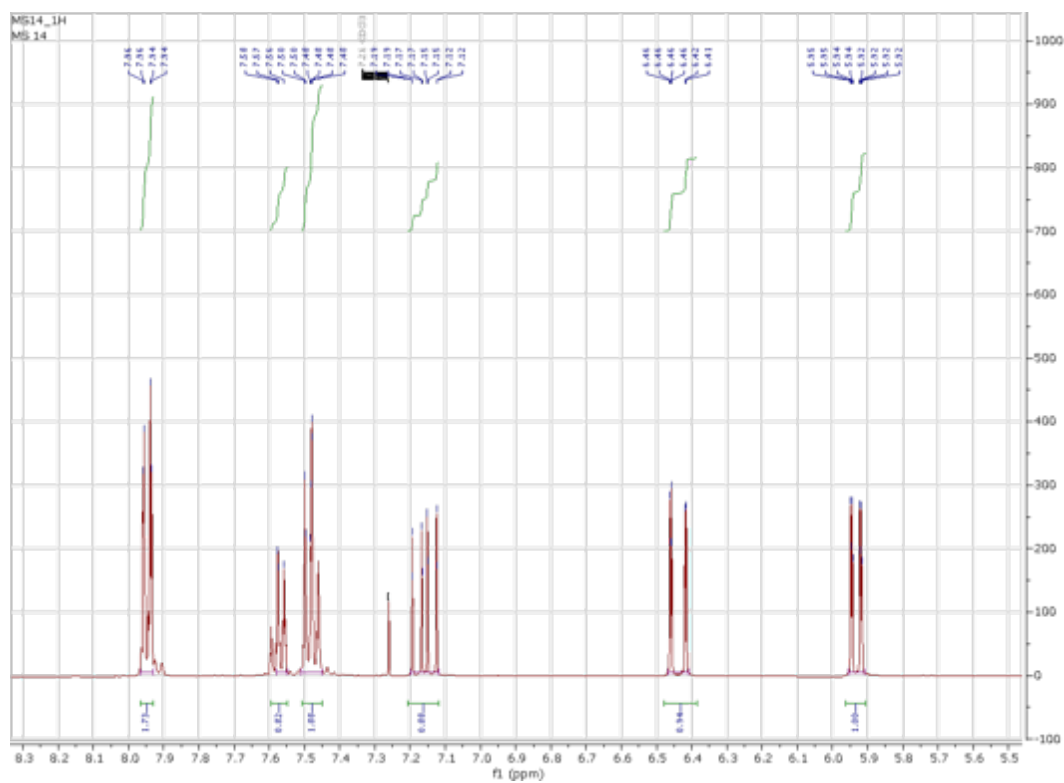
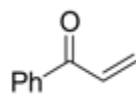
^{13}C NMR (101 MHz, Chloroform- d) δ 145.11, 144.54, 143.95, 142.09, 122.44, 110.55, 107.66, 104.60, 61.06, 56.57.



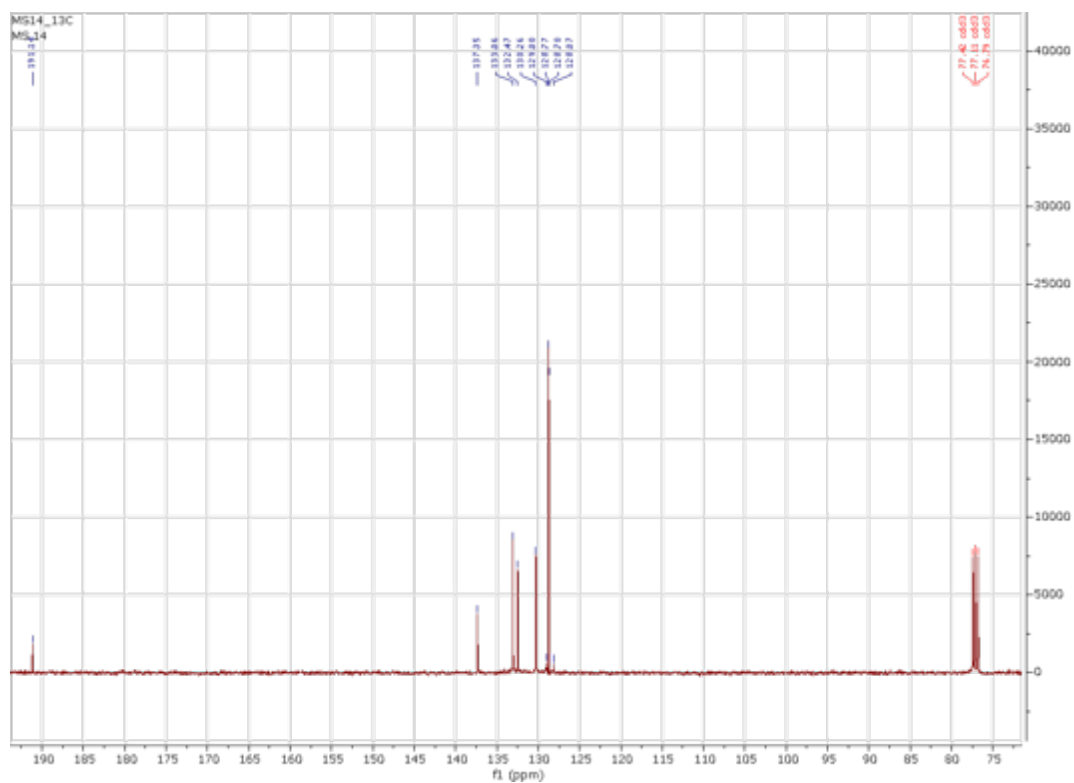
^{13}C NMR (101 MHz, Chloroform-d) δ 145.12, 110.55, 104.60, 61.05, 56.57.



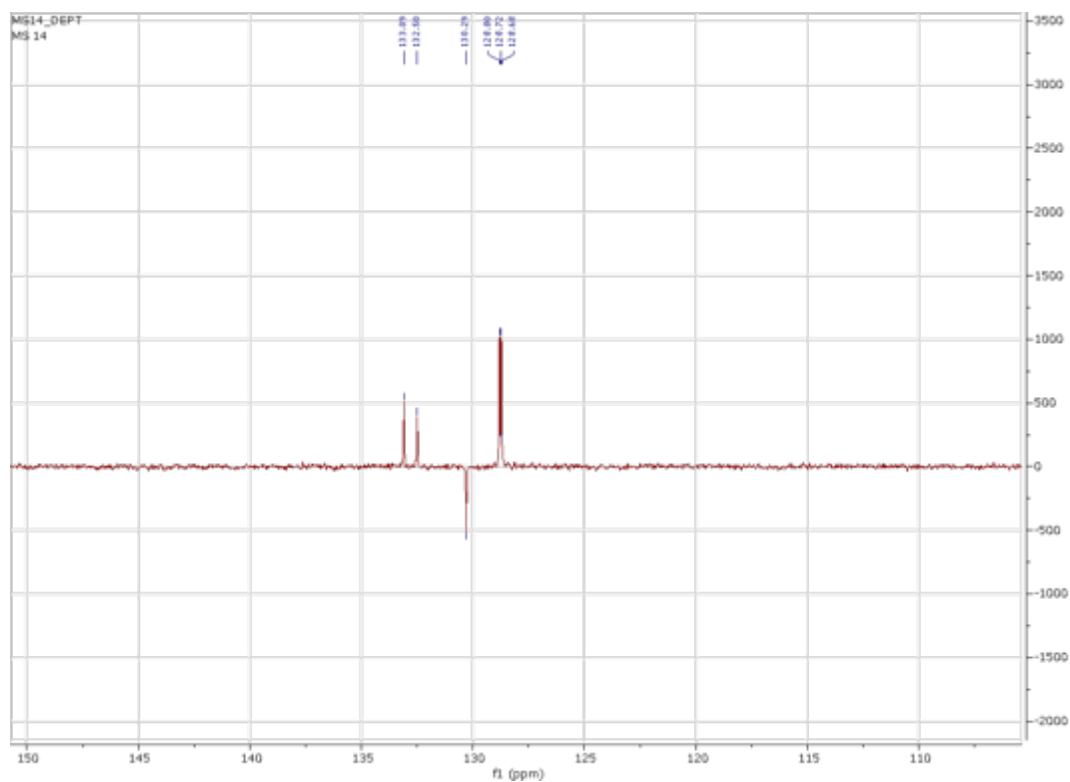
1-phenylprop-2-en-1-one (13)



¹H NMR (400 MHz, Chloroform-d) δ 7.97 – 7.93 (m, 2H), 7.58 – 7.55 (m, 1H), 7.51 – 7.45 (m, 2H), 7.16 (ddd, J = 17.2, 10.6, 0.6 Hz, 1H), 6.44 (dd, J = 17.2, 1.7 Hz, 1H), 5.95 – 5.91 (m, 1H).

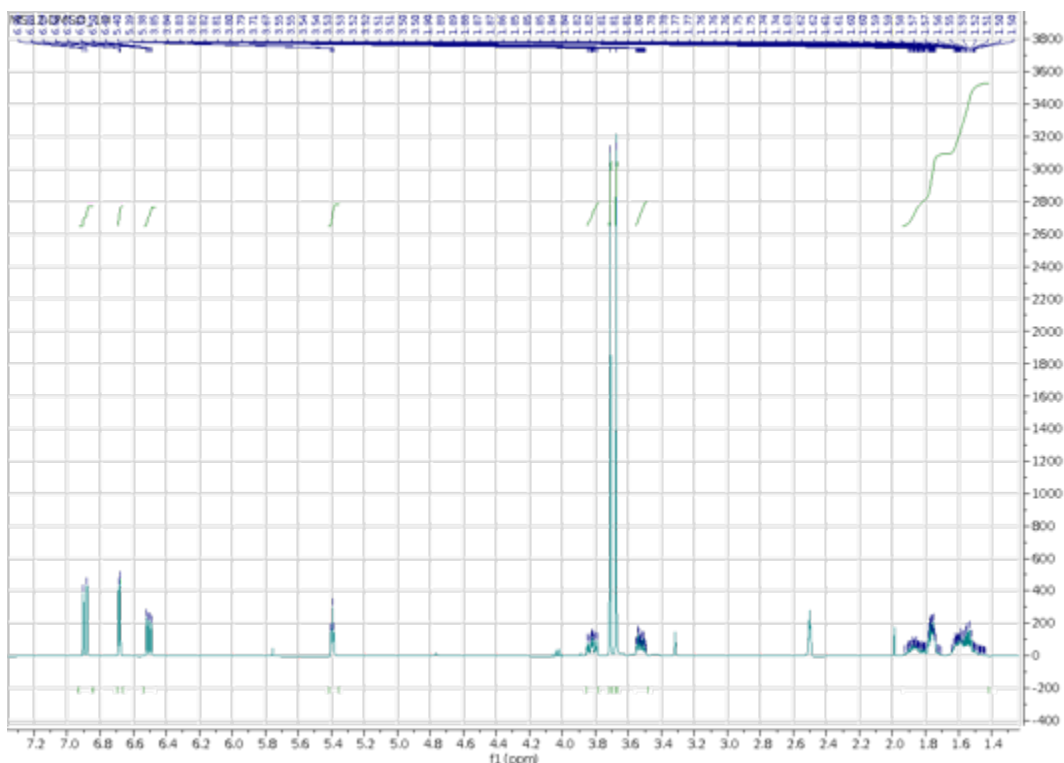
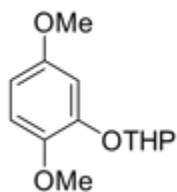


^{13}C NMR (101 MHz, Chloroform-d) δ 191.14, 137.35, 133.06, 132.47, 130.26, 129.00, 128.77, 128.70, 128.07.



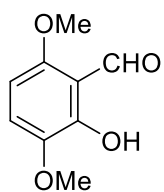
^{13}C NMR (101 MHz, Chloroform-d) δ 133.09, 132.50, 130.29, 128.80, 128.72, 128.68.

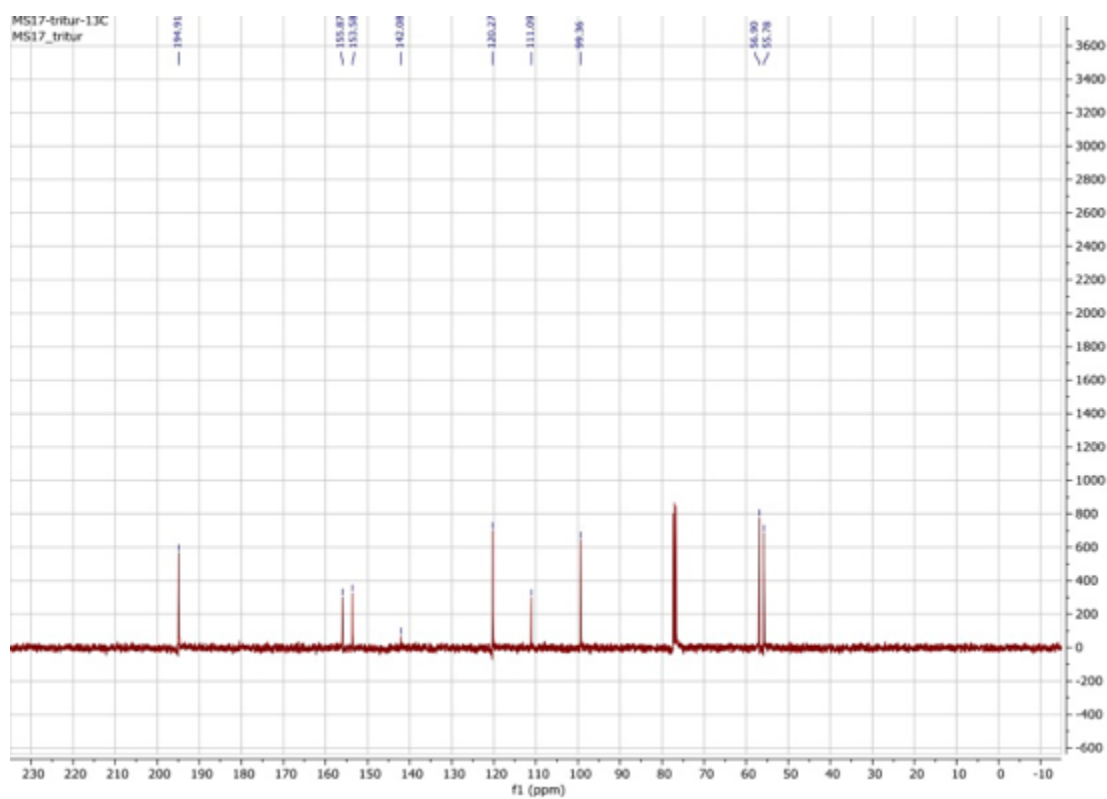
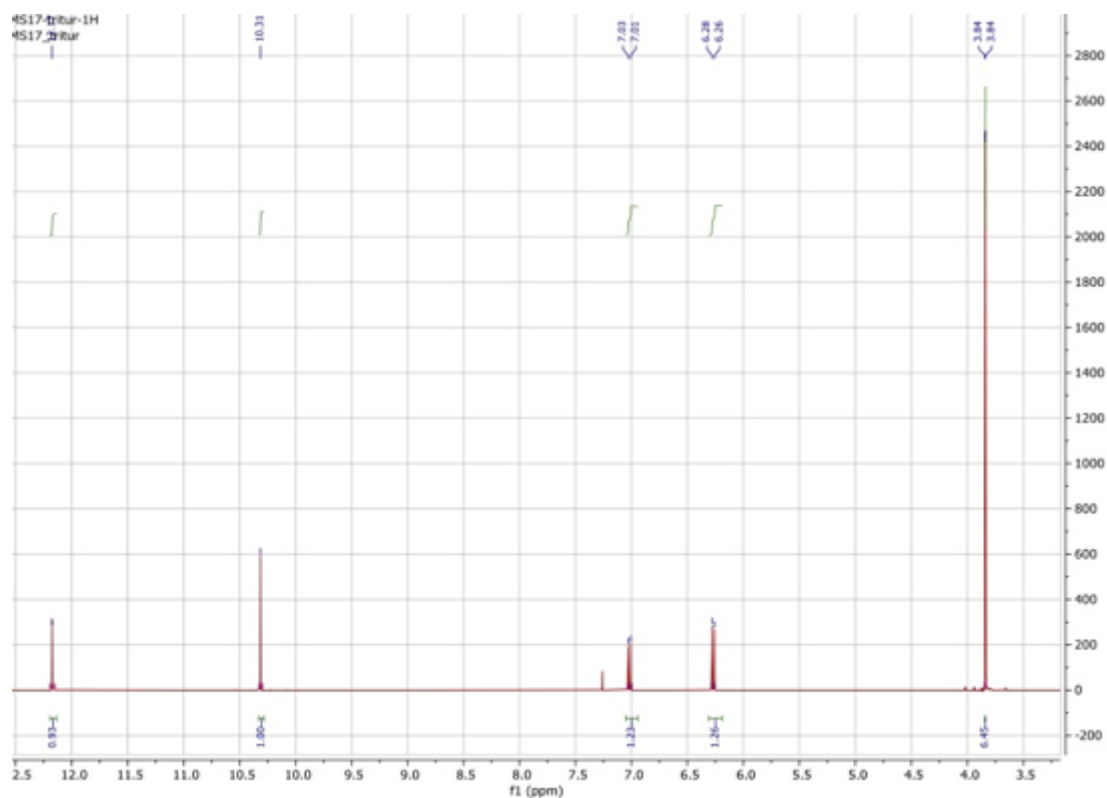
2-(2,5-dimethoxyphenoxy)tetrahydro-2H-pyran (14)

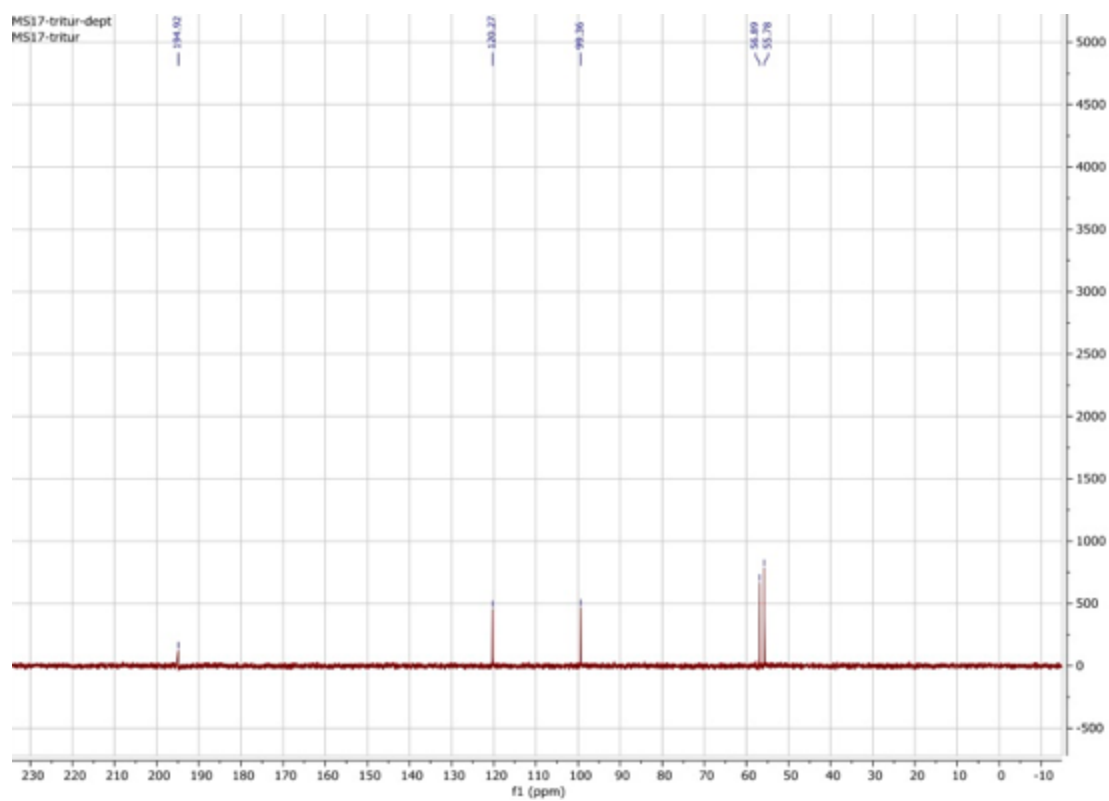


^1H NMR (400 MHz, dmsO) δ 6.89 (d, $J = 8.8$ Hz, 1H), 6.68 (d, $J = 2.9$ Hz, 1H), 6.50 (dd, $J = 8.9, 2.9$ Hz, 1H), 5.39 (t, $J = 3.3$ Hz, 1H), 3.82 (ddd, $J = 11.1, 8.9, 3.8$ Hz, 1H), 3.71 (s, 3H), 3.67 (s, 3H), 3.53 (dtd, $J = 11.5, 4.3, 1.2$ Hz, 1H), 1.94 – 1.38 (m, 7H).

2-hydroxy-3,6-dimethoxybenzaldehyde (15)

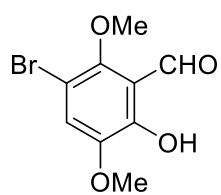


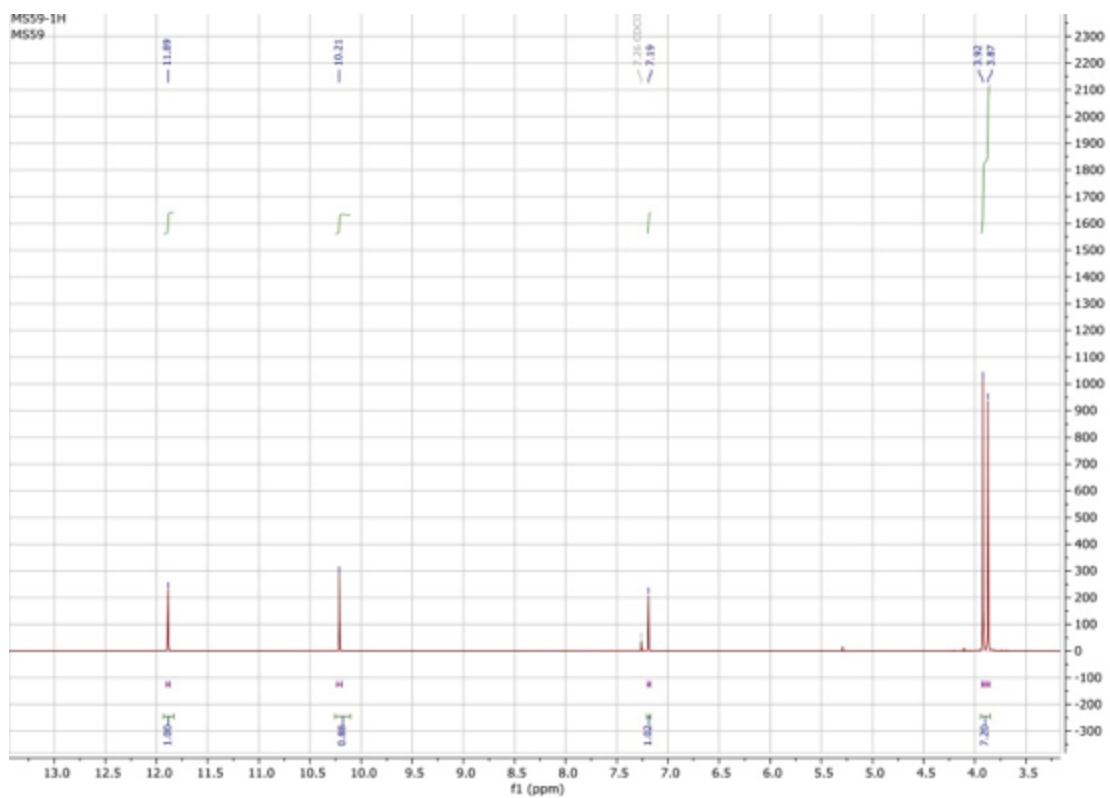




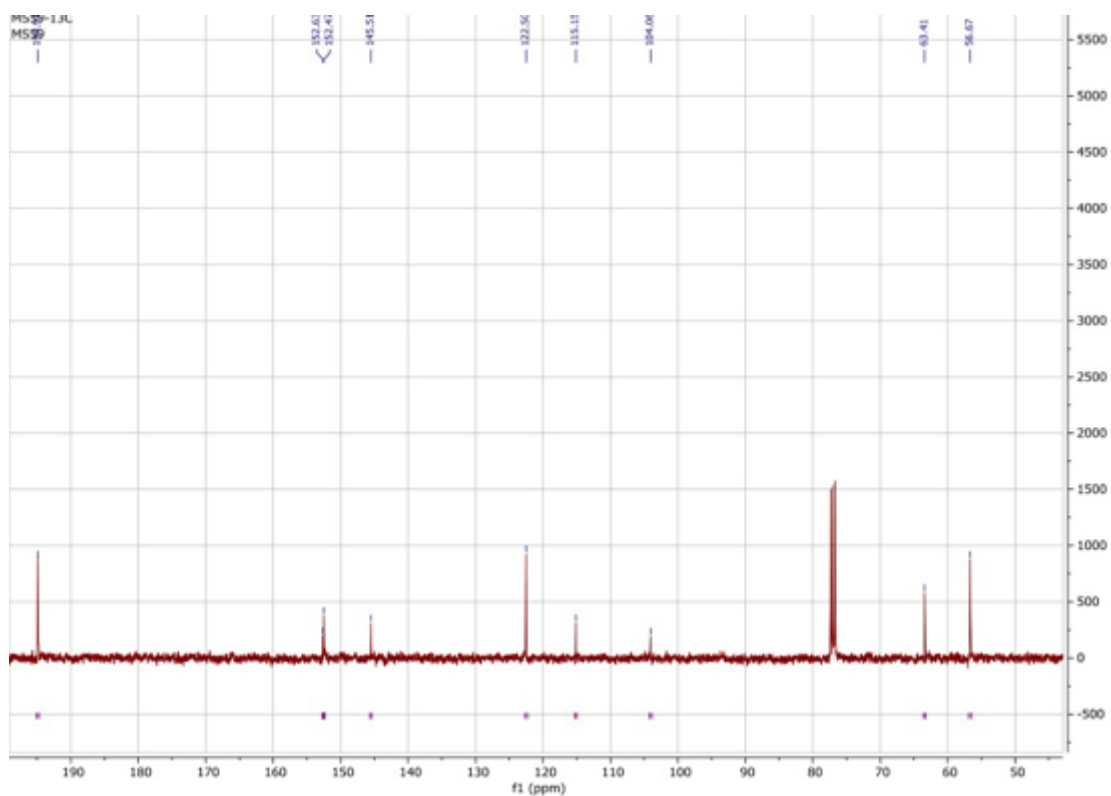
^{13}C NMR (101 MHz, Chloroform-d) δ 194.92, 120.27, 99.36, 56.89, 55.78.

3-bromo-6-hydroxy-2,5-dimethoxybenzaldehyde (**16**)

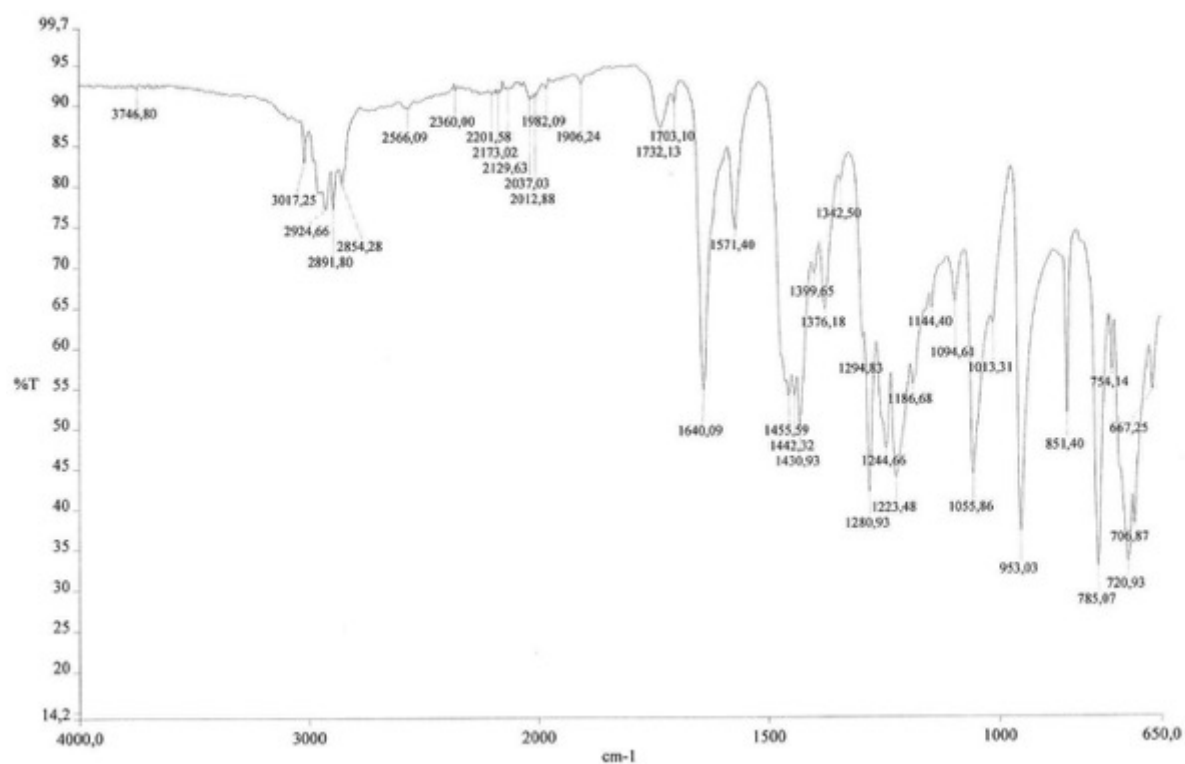
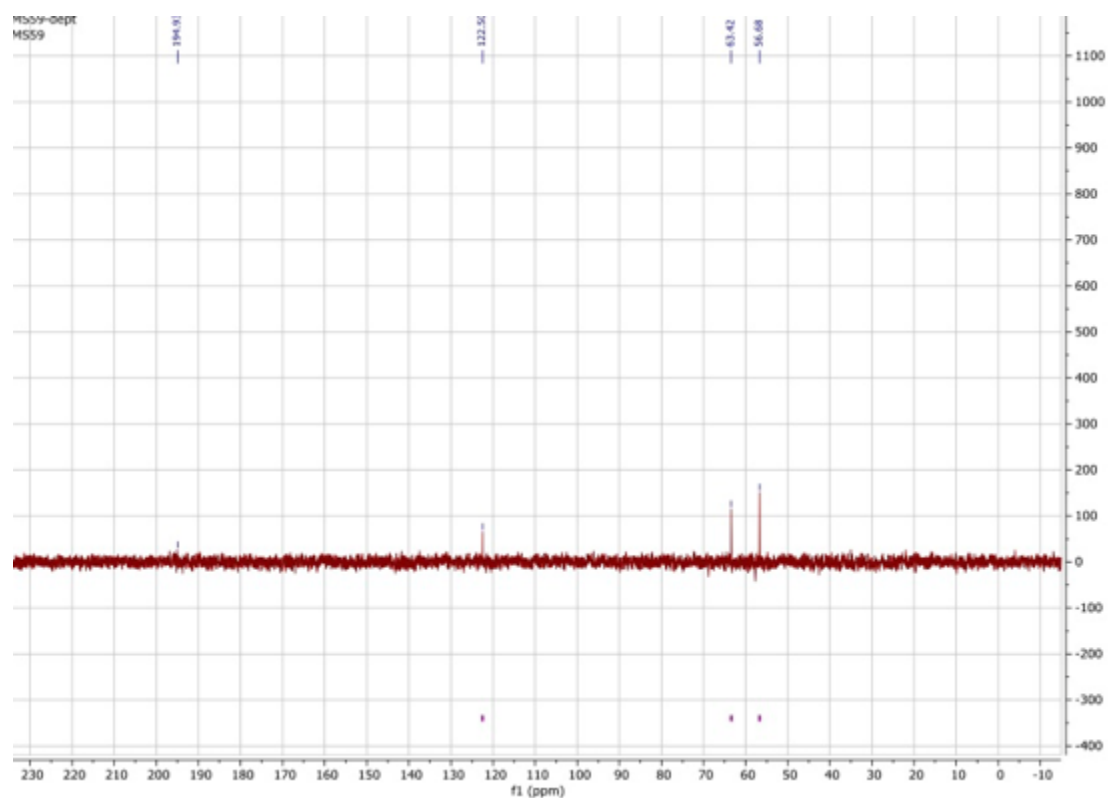




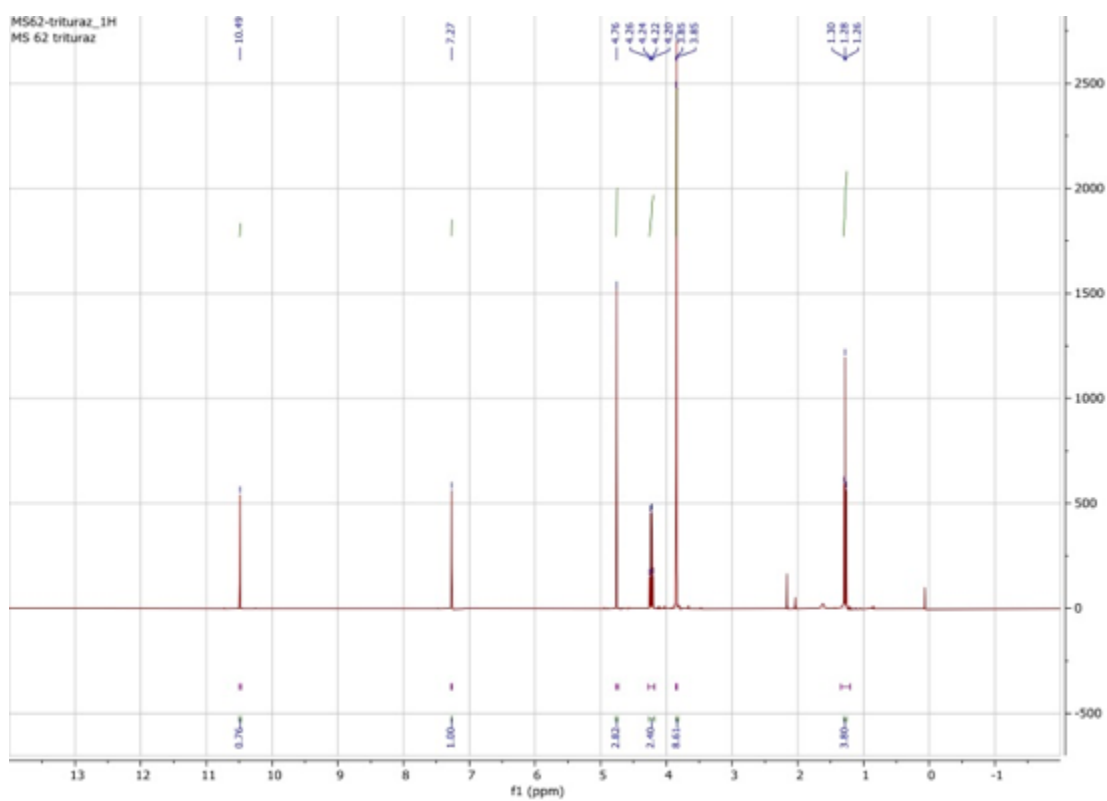
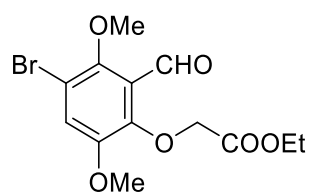
¹H NMR (400 MHz, Chloroform-*d*) δ 11.89 (s, 1H), 10.21 (s, 1H), 7.19 (s, 1H), 3.92 (s, 3H), 3.87 (s, 3H).



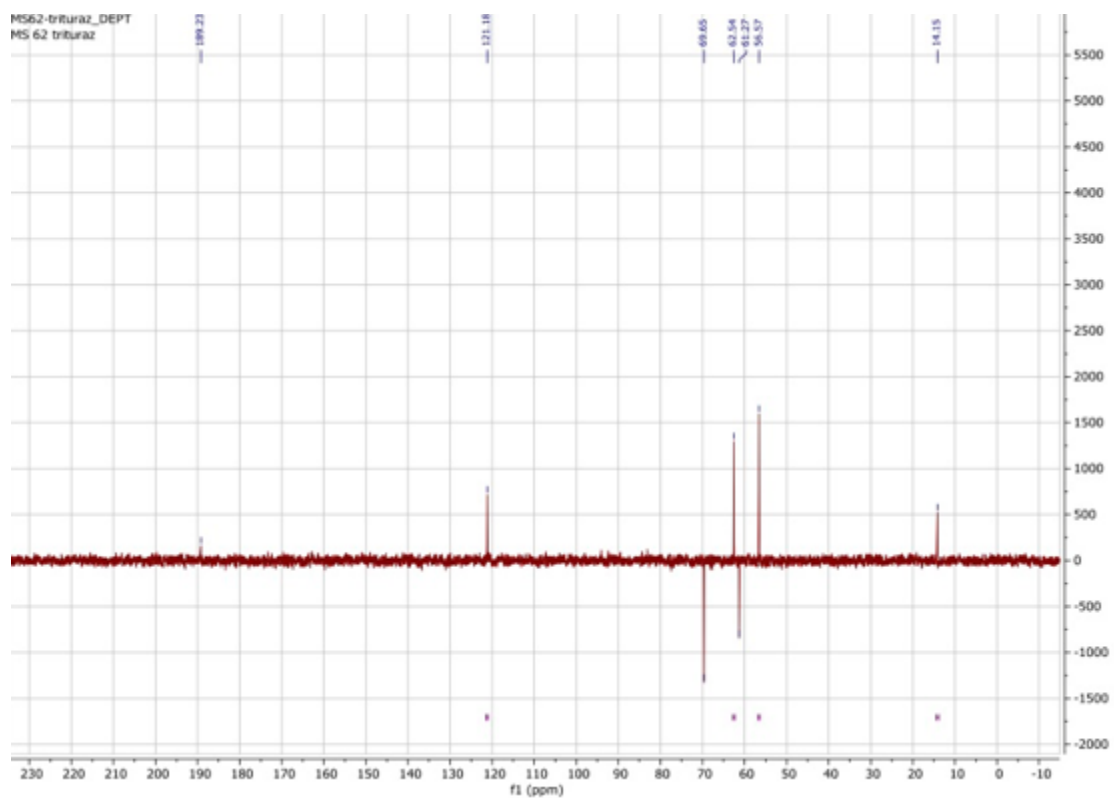
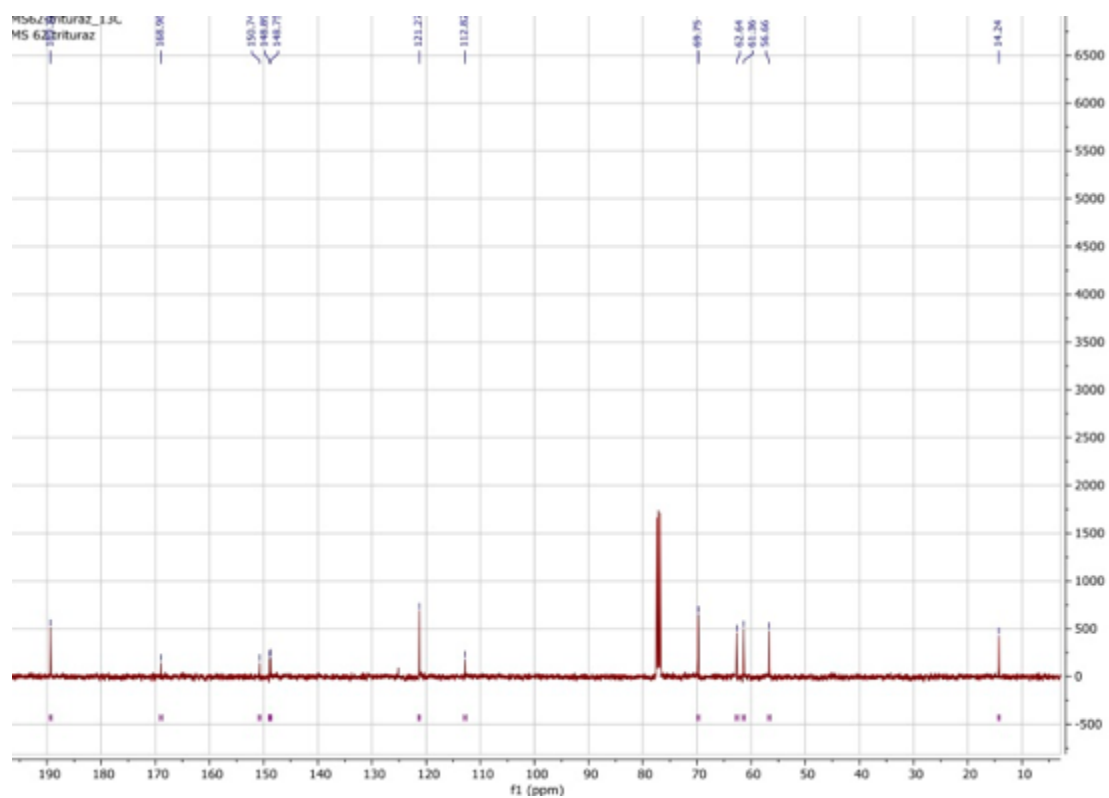
¹³C NMR (101 MHz, Chloroform-*d*) δ 194.91, 152.63, 152.47, 145.51, 122.50, 115.15, 104.06, 63.41, 56.67.

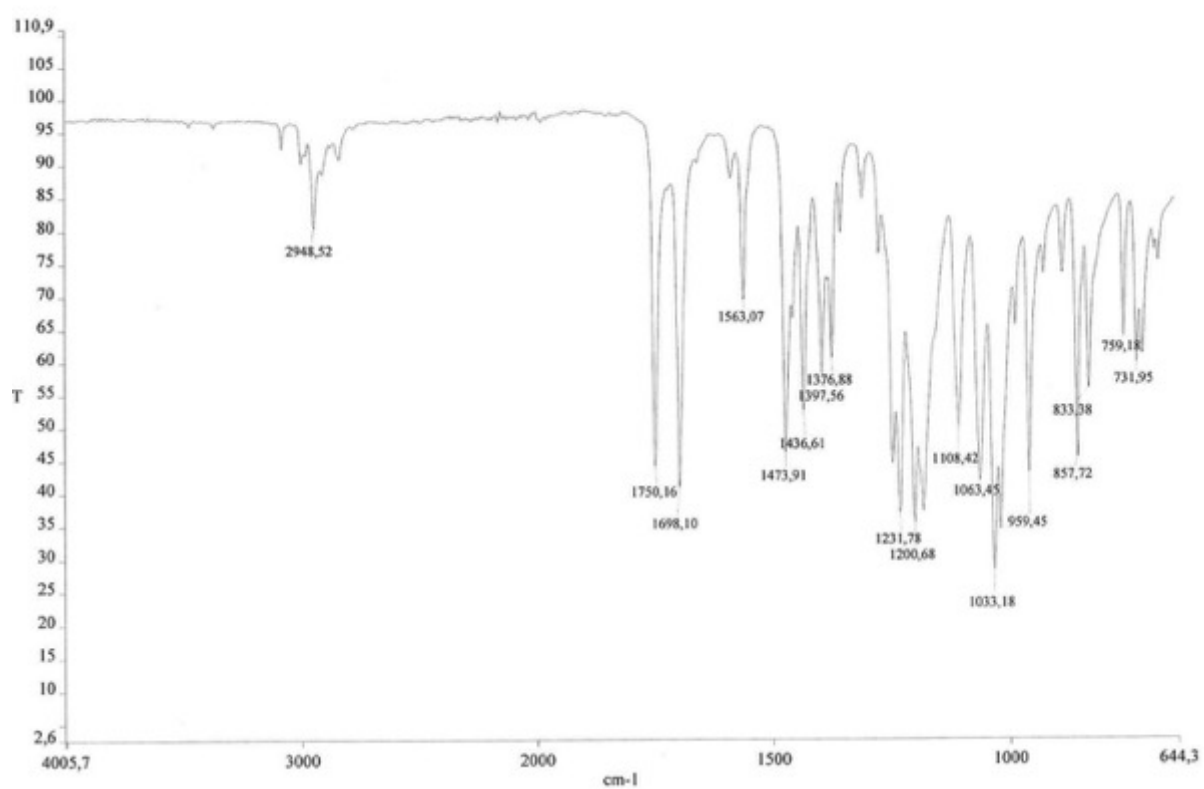


ethyl 2-(4-bromo-2-formyl-3,6-dimethoxyphenoxy)acetate (**17**)

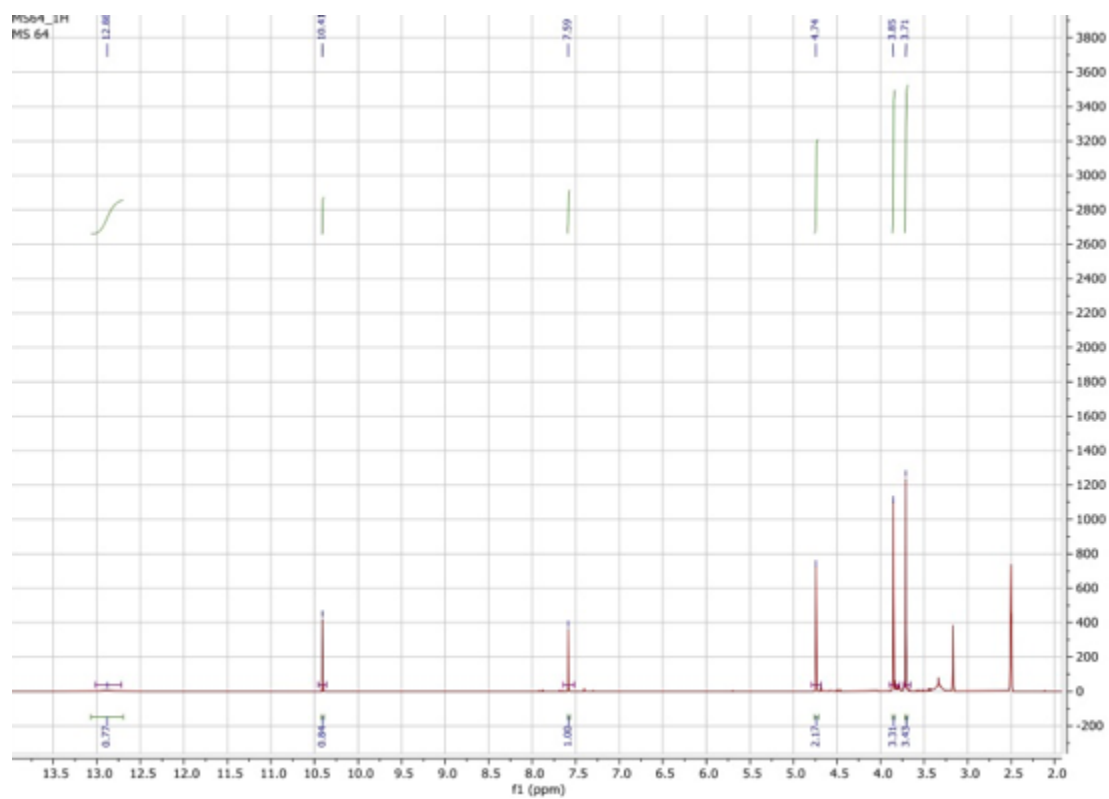
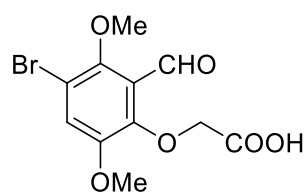


^1H NMR (400 MHz, Chloroform- d) δ 10.49 (s, 1H), 7.27 (s, 1H), 4.76 (s, 2H), 4.23 (q, $J = 7.1$ Hz, 2H), 3.85 (d, $J = 2.1$ Hz, 6H), 1.28 (t, $J = 7.1$ Hz, 3H).

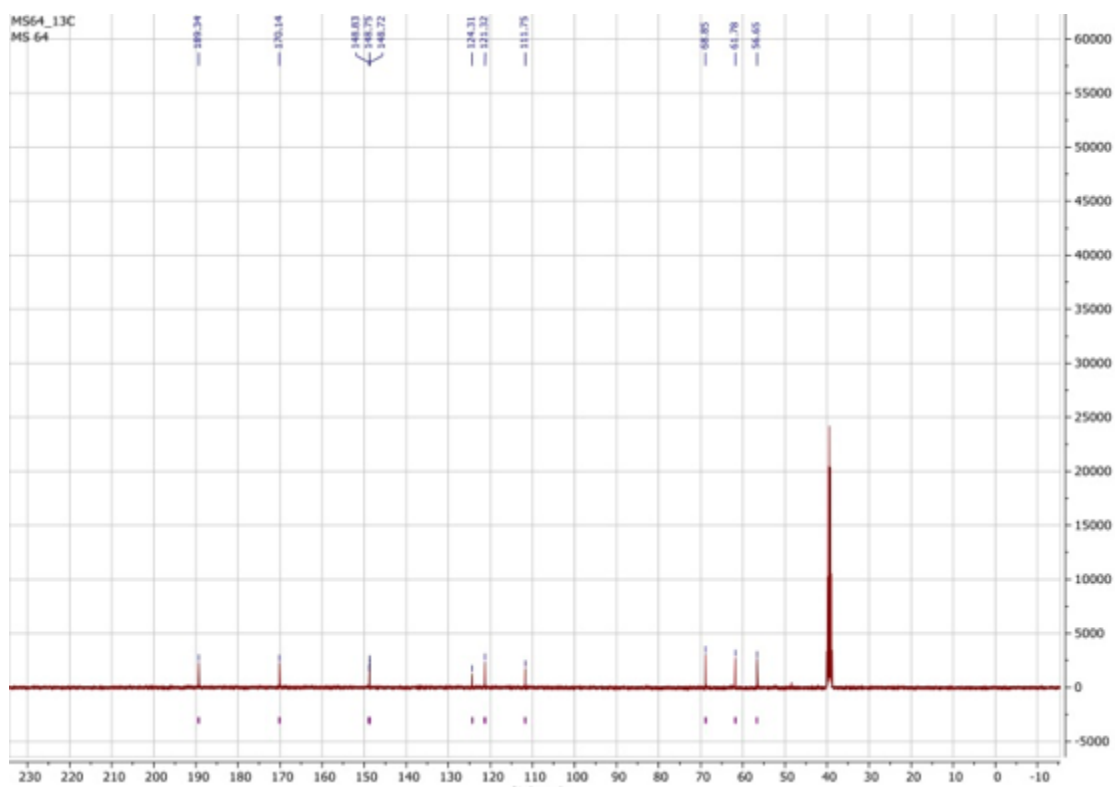




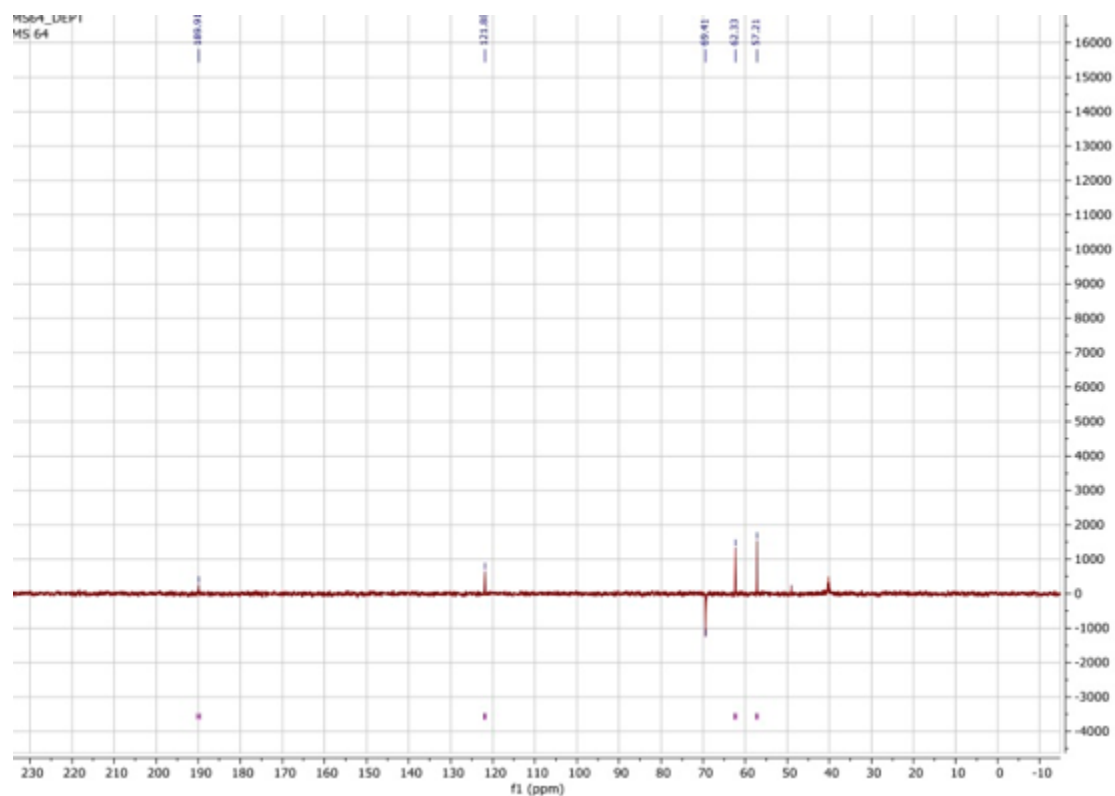
2-(3-bromo-6-formyl-2,5-dimethoxyphenoxy)acetic acid



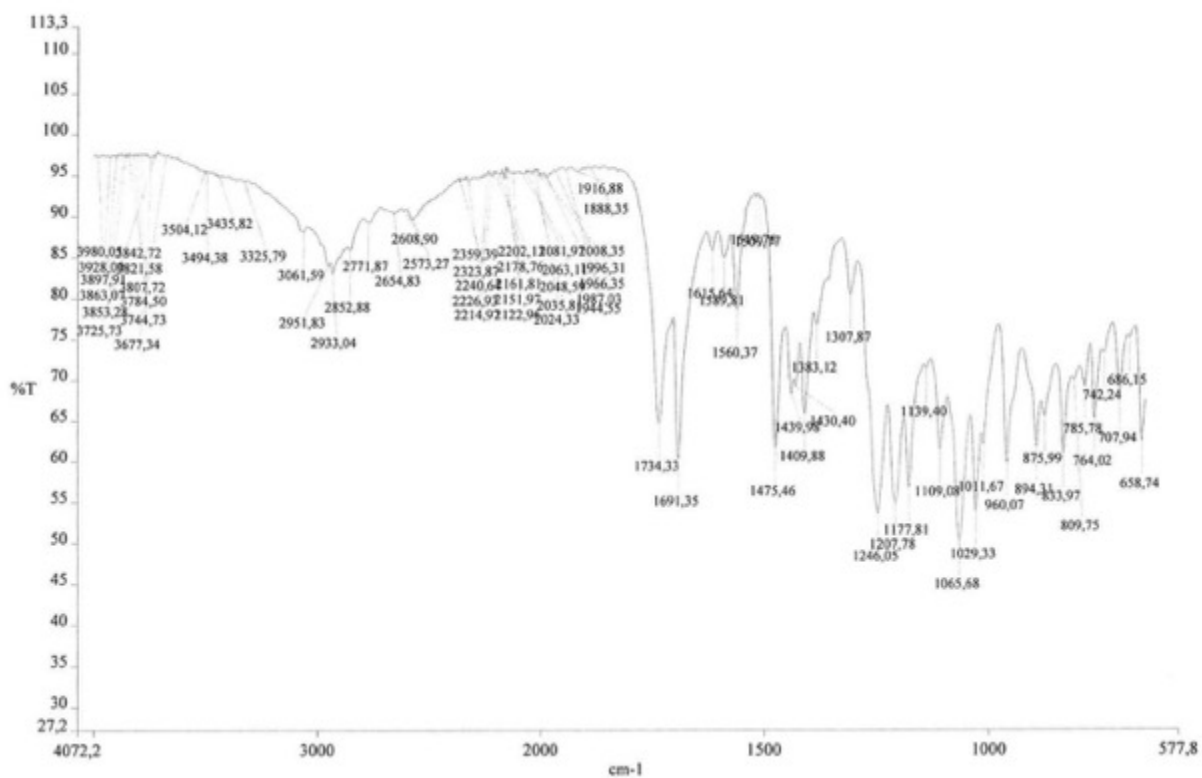
¹H NMR (400 MHz, DMSO-*d*₆) δ 12.88 (s, 1H), 10.41 (s, 1H), 7.59 (s, 1H), 4.74 (s, 2H), 3.85 (s, 3H), 3.71 (s, 3H).



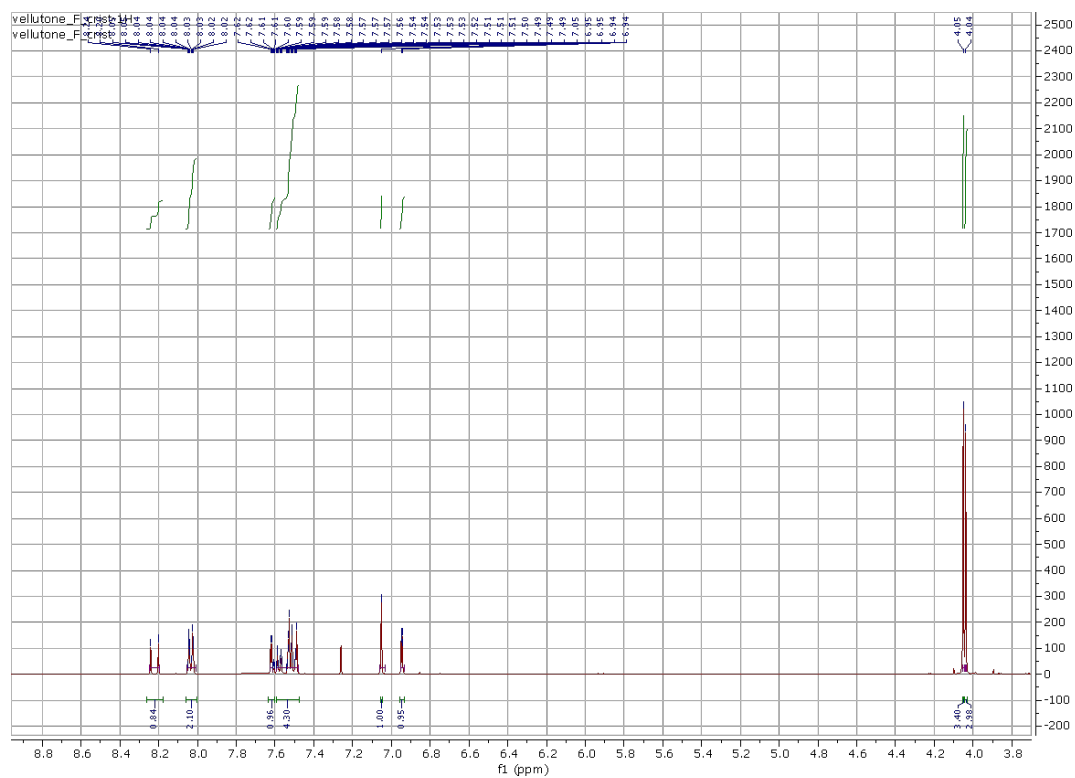
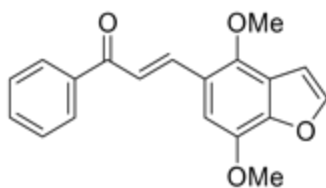
^{13}C NMR (101 MHz, dmso) δ 189.34, 170.14, 148.83, 148.75, 148.72, 124.31, 121.32, 111.75, 68.85, 61.78, 56.65.



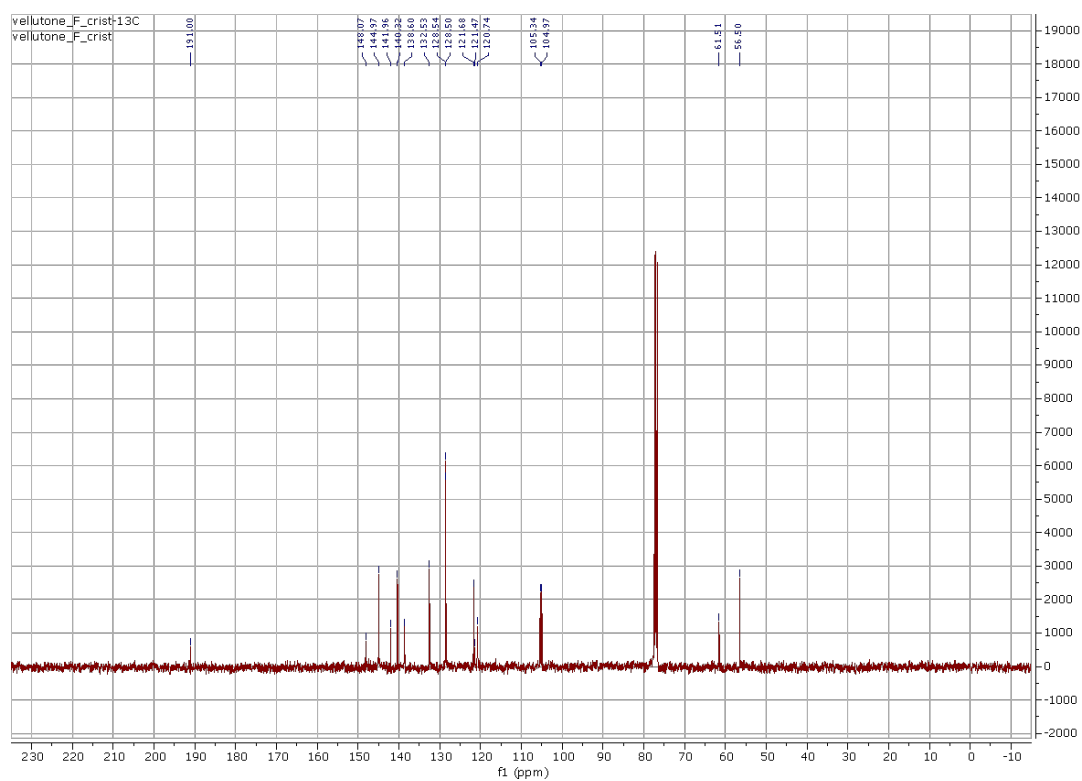
^{13}C NMR (101 MHz, dmso) δ 189.91, 121.88, 69.41, 62.33, 57.21.



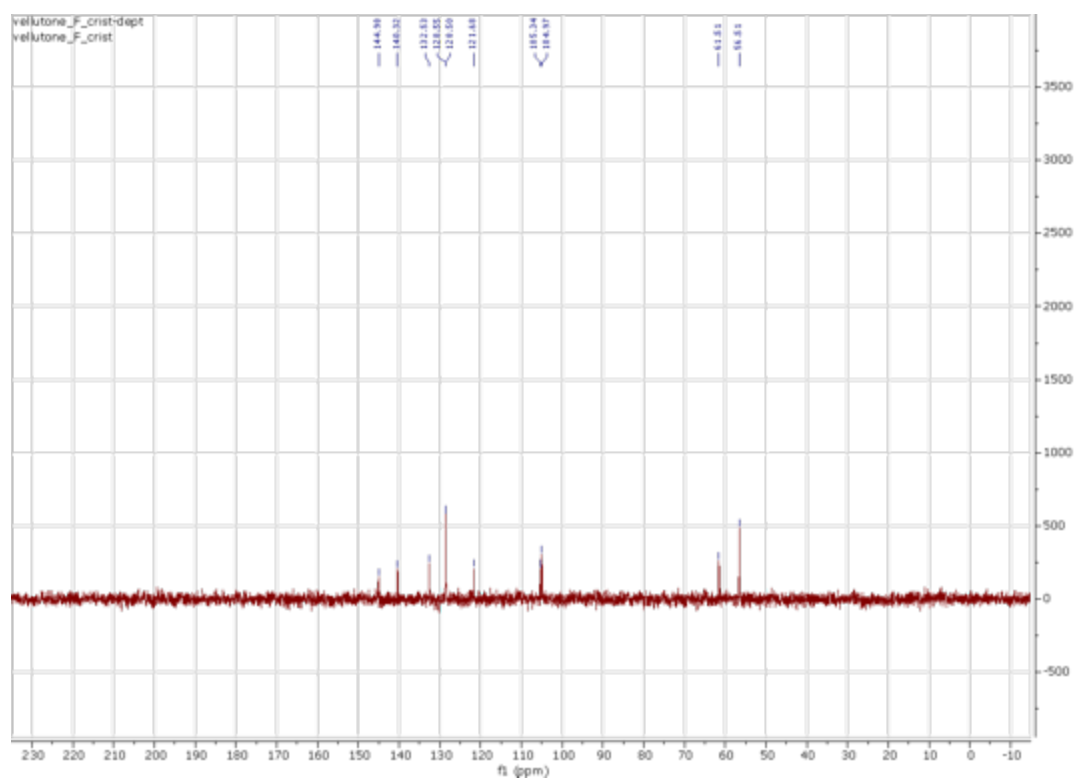
(E)-3-(4,7-dimethoxybenzofuran-5-yl)-1-phenylprop-2-en-1-one (**1**)



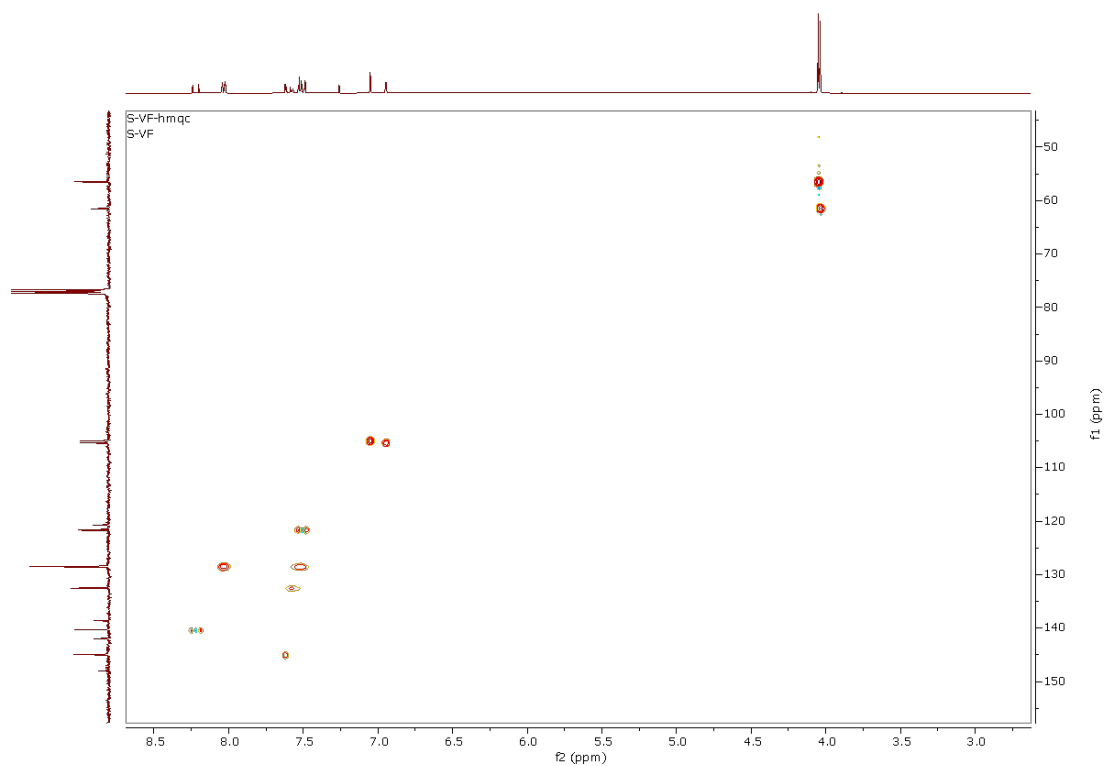
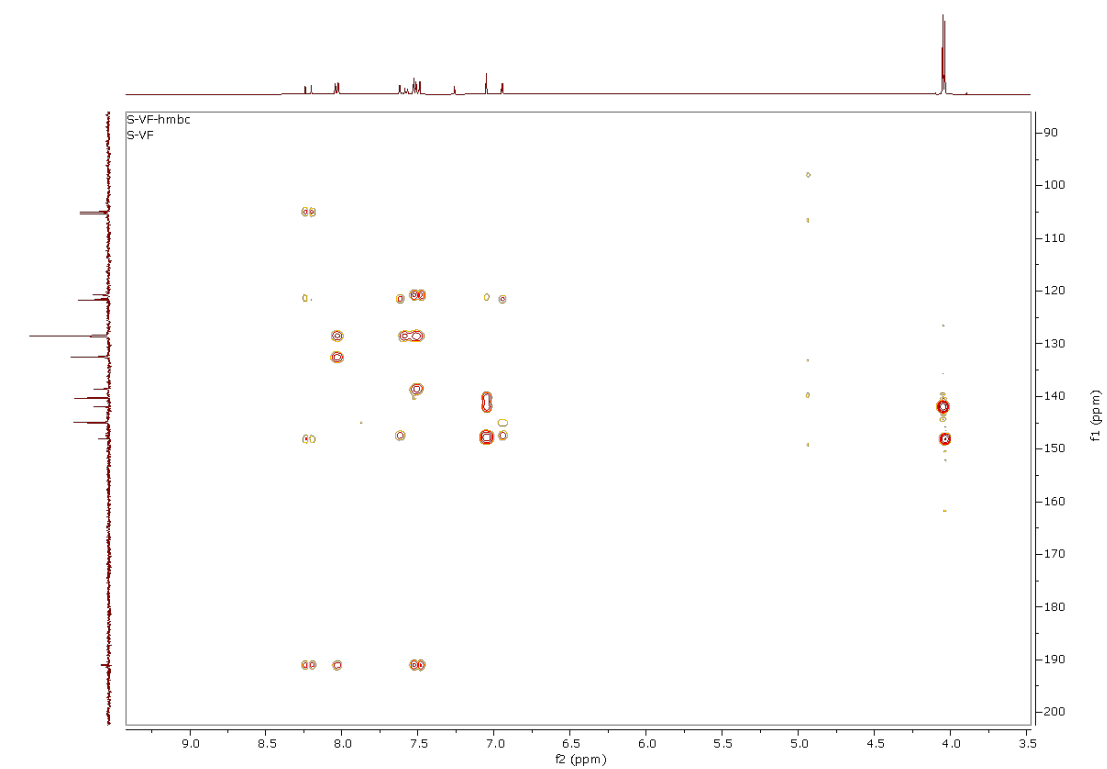
^1H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, J = 15.8 Hz, 1H), 8.05 – 8.01 (m, 2H), 7.62 (d, J = 2.2 Hz, 1H), 7.59 – 7.48 (m, 4H), 7.05 (s, 1H), 6.95 (dd, J = 2.2, 0.6 Hz, 1H), 4.05 (s, 3H), 4.04 (s, 3H).



^{13}C NMR (101 MHz, Chloroform-d) δ 191.00, 148.07, 144.97, 141.96, 140.32, 138.60, 132.53, 128.54, 128.50, 121.68, 121.47, 120.74, 105.34, 104.97, 61.51, 56.50.



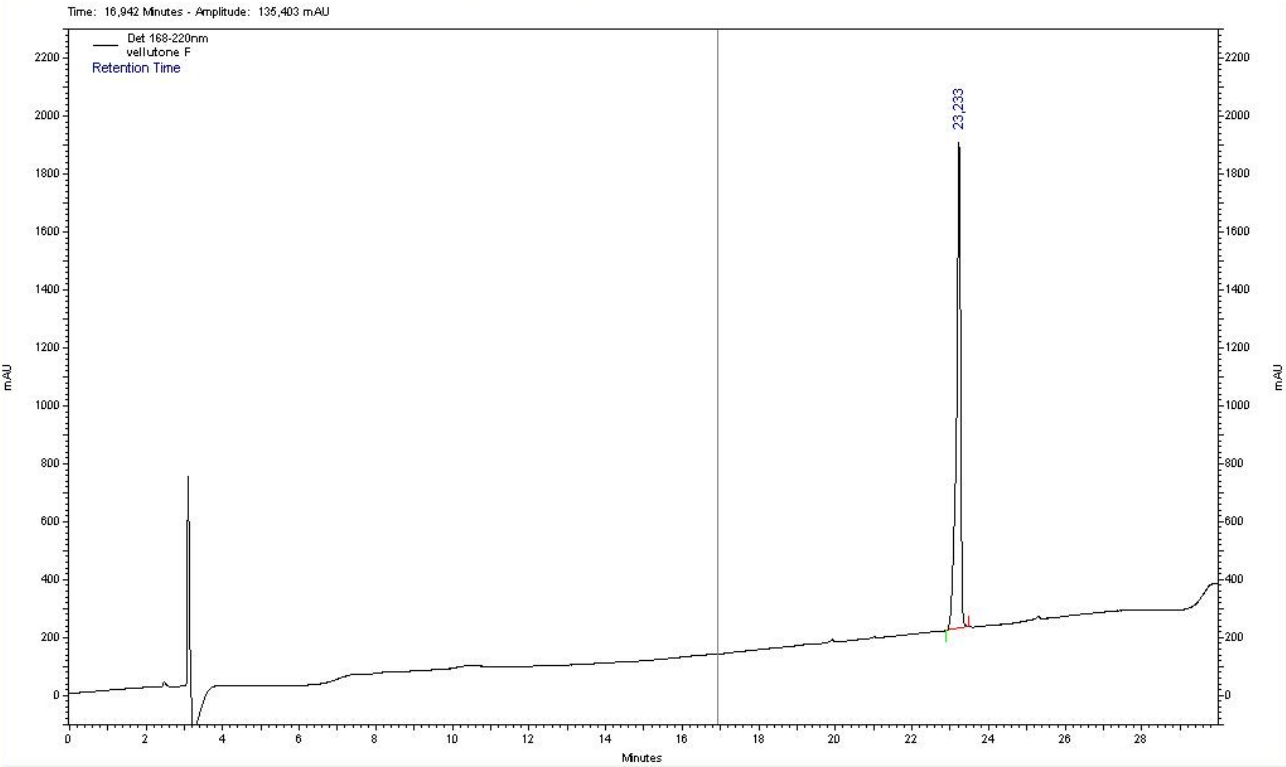
^{13}C NMR (101 MHz, Chloroform-d) δ 144.98, 140.32, 132.53, 128.55, 128.50, 121.68, 105.34, 104.97, 61.51, 56.51.



Area % Report

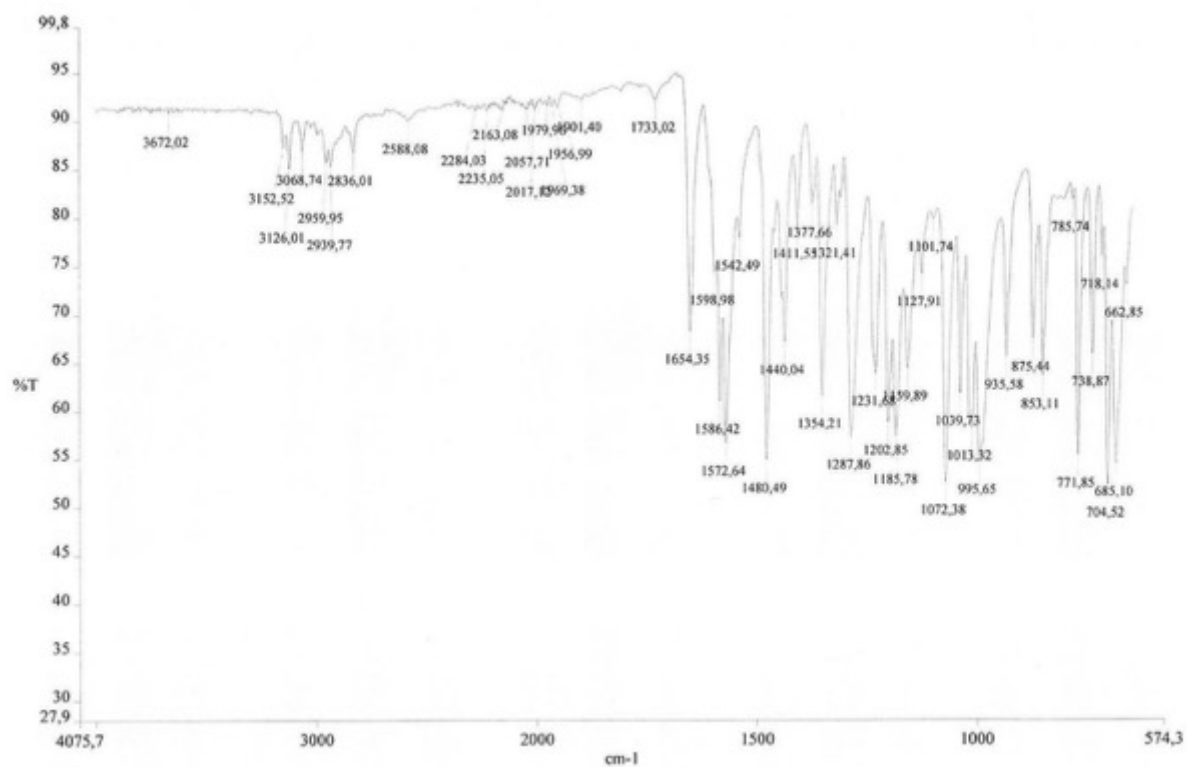
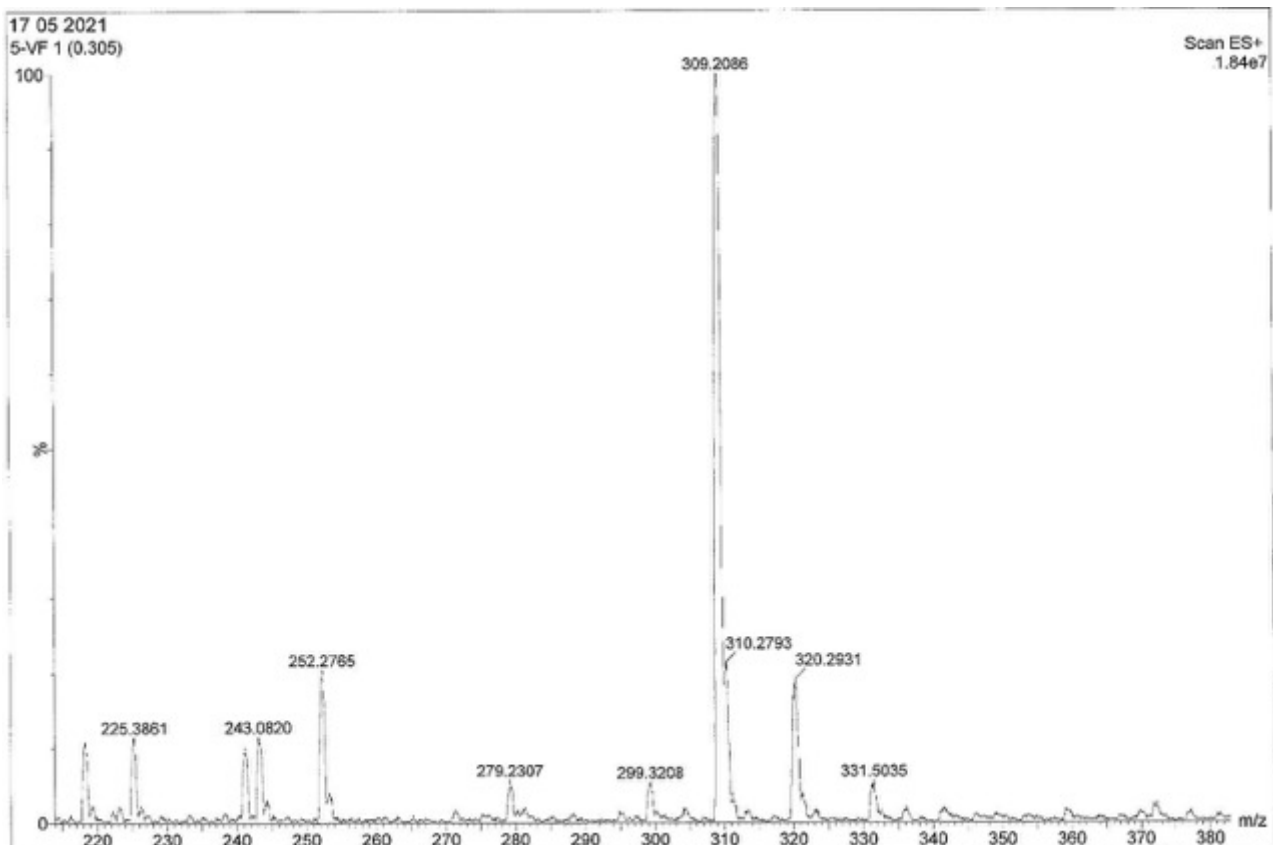
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 Method: C:\32Karat\Projects\Default\Method\standard 0.7 ml.met

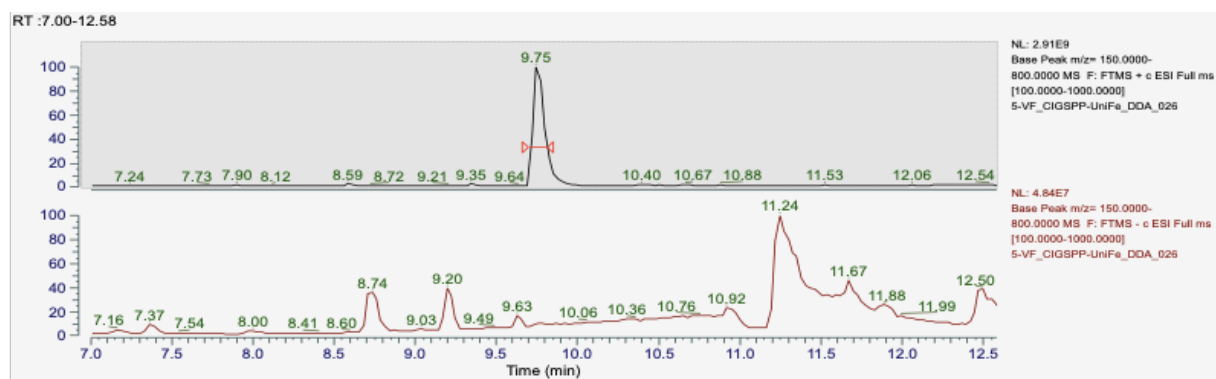
Acquired: 05/05/2021 17.37.21
Printed: 04/08/2022 13.15.03



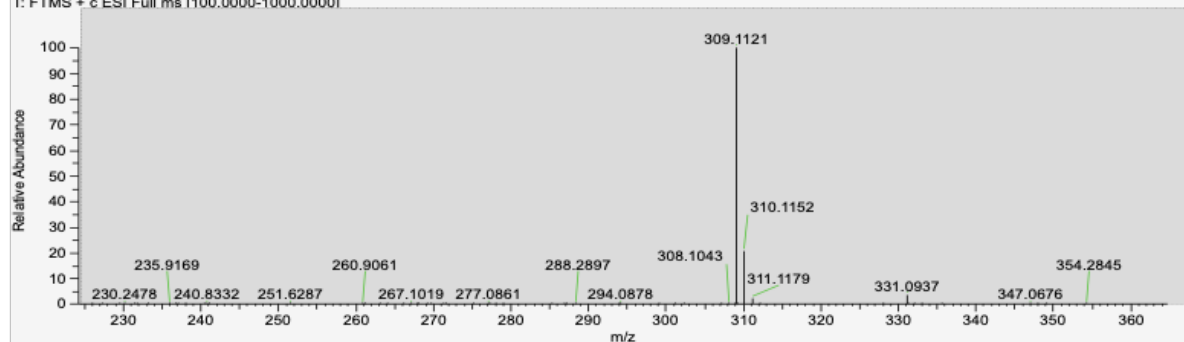
Det 168-220nm
Results

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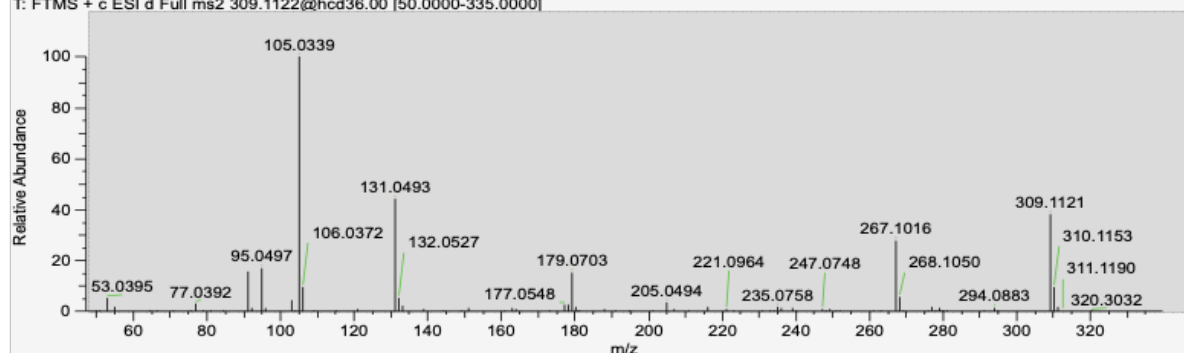


5-VF_CIGSPP-UniFe_DDA_026 #2089-2113 RT: 9.7-9.81 AV: 4 SB: 6 9.50-9.65 NL: 2.01E+009
T: FTMS + c ESI Full ms [100.0000-1000.0000]

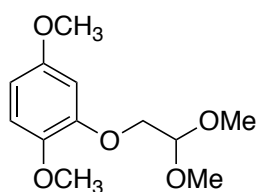


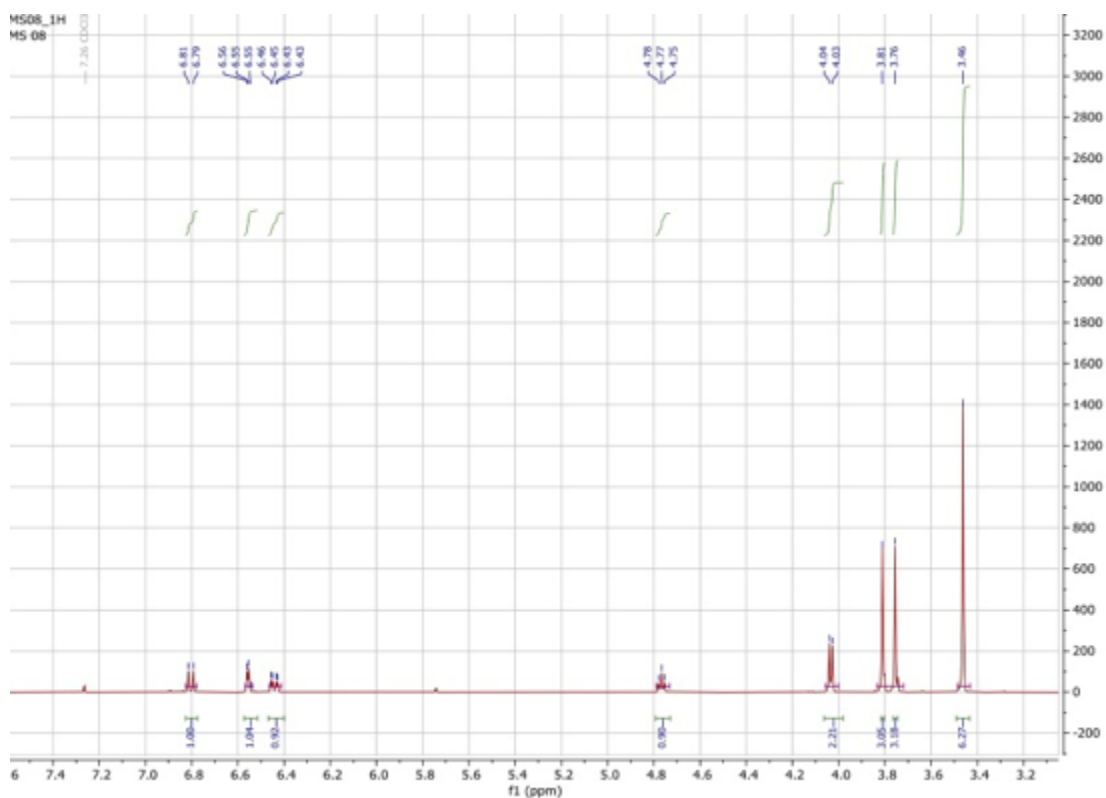
Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
309,1121	C ₁₉ H ₁₇ O ₄	24,8937856024	11,5	-0,15	309,11214	1	95,99	4	4	99,93	98,96
331,0937	C ₁₉ H ₁₆ O ₄ ²³ Na	17,1572498096	11,5	-1,02	331,09408	3	95,46	3	5	99,81	98,83

5-VF_CIGSPP-UniFe_DDA_026 #2095 RT: 9.73 AV: 1 NL: 1.94E+008
T: FTMS + c ESI d Full ms2 309.1122@hcd36.00 [50.0000-335.0000]

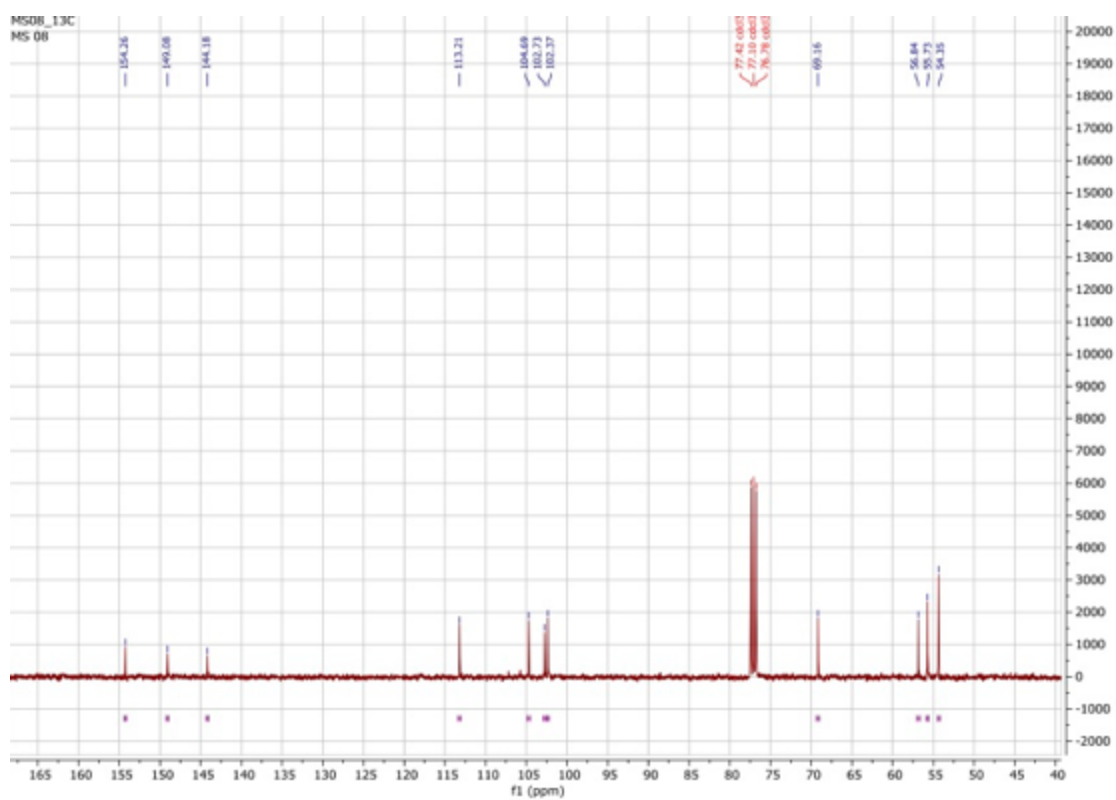


2-(2,2-dimethoxyethoxy)-1,4-dimethoxybenzene (**18**)

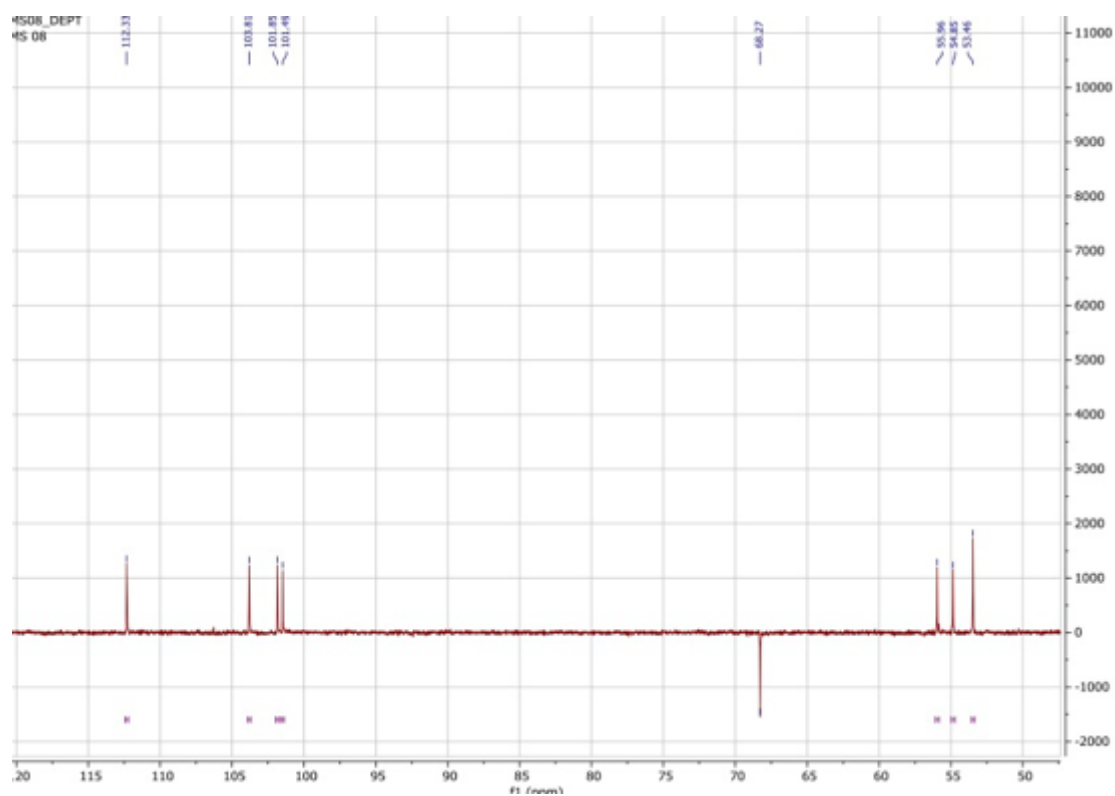




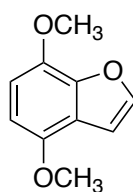
¹H NMR (400 MHz, Chloroform-*d*) δ 6.80 (d, *J* = 8.8 Hz, 1H), 6.56 (d, *J* = 2.9 Hz, 1H), 6.44 (dd, *J* = 8.8, 2.8 Hz, 1H), 4.77 (t, *J* = 5.2 Hz, 1H), 4.03 (d, *J* = 5.2 Hz, 2H), 3.78 (d, *J* = 21.9 Hz, 6H), 3.46 (s, 6H).

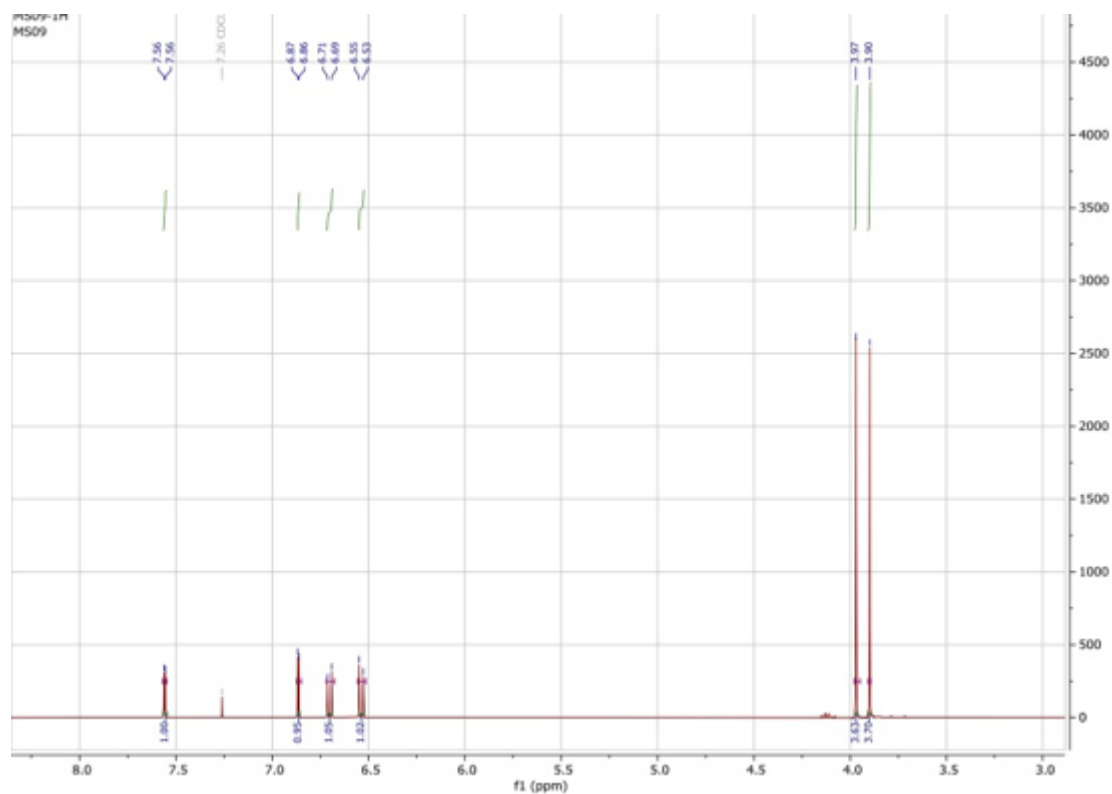


¹³C NMR (101 MHz, Chloroform-*d*) δ 154.26, 149.08, 144.18, 113.21, 104.69, 102.73, 102.37, 69.16, 56.84, 55.73, 54.35.

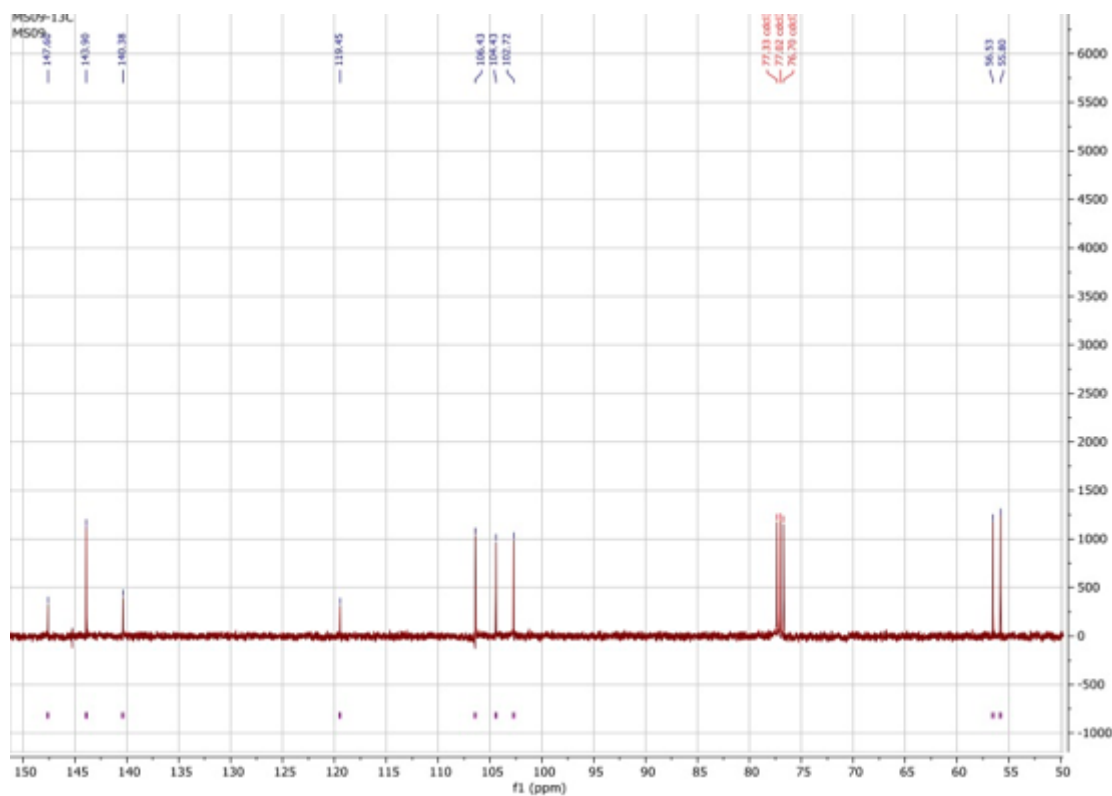


4,7-dimethoxybenzofuran (19)

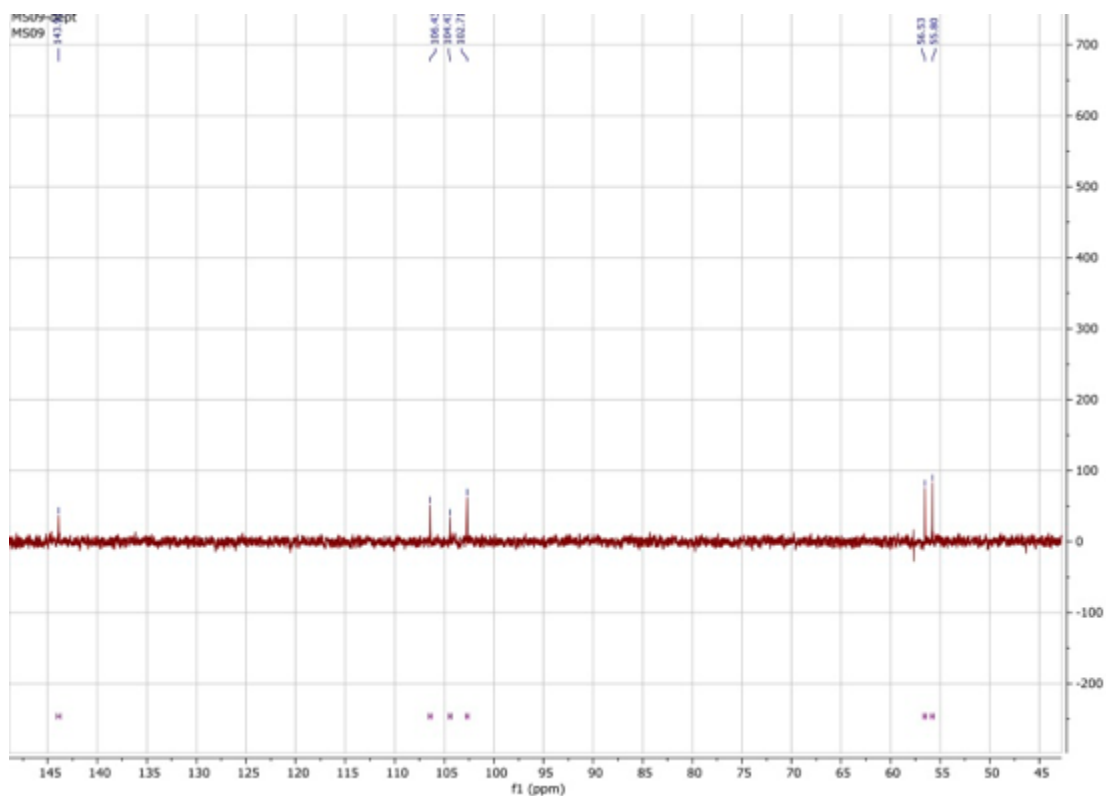




¹H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, J = 2.1 Hz, 1H), 6.86 (d, J = 2.1 Hz, 1H), 6.70 (d, J = 8.5 Hz, 1H), 6.54 (d, J = 8.5 Hz, 1H), 3.97 (s, 3H), 3.90 (s, 3H).

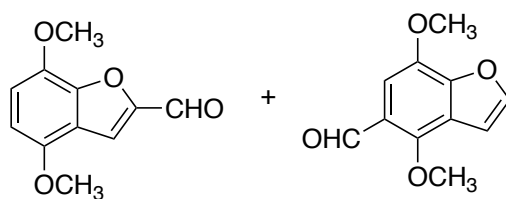


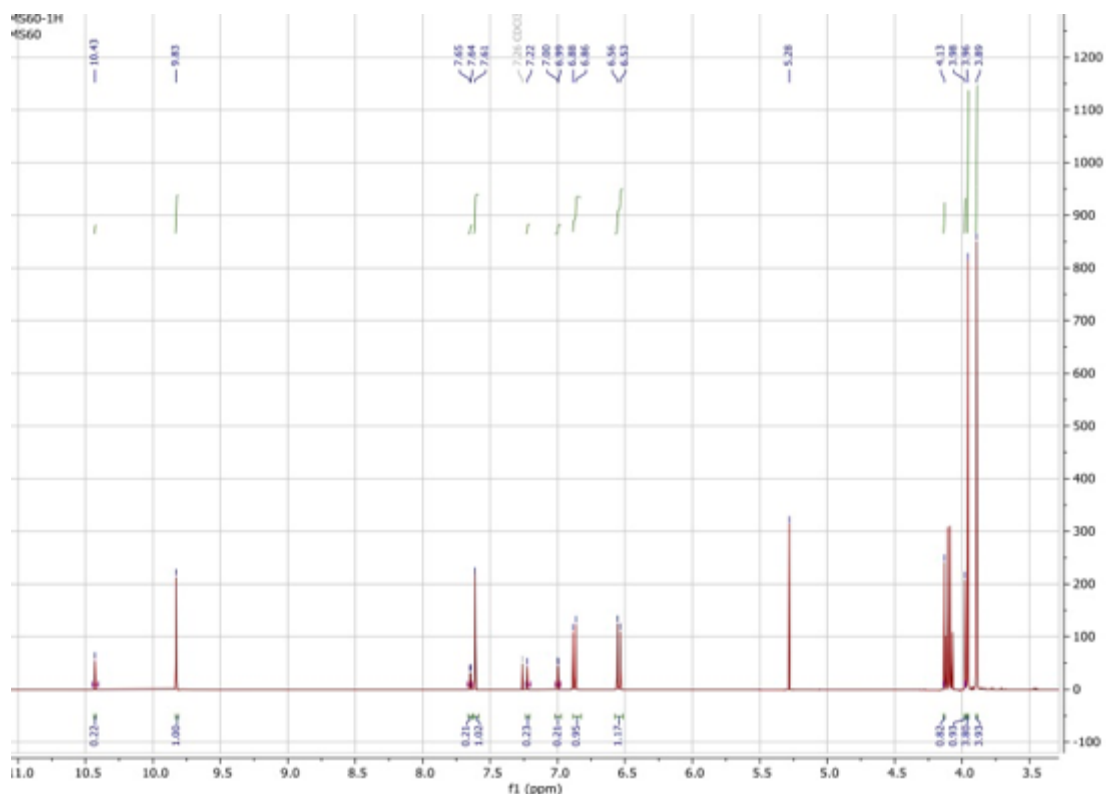
¹³C NMR (101 MHz, Chloroform-*d*) δ 147.60, 143.90, 140.38, 119.45, 106.43, 104.43, 102.72, 56.53, 55.80.



^{13}C NMR (101 MHz, Chloroform- d) δ 143.91, 106.43, 104.43, 102.71, 56.53, 55.80.

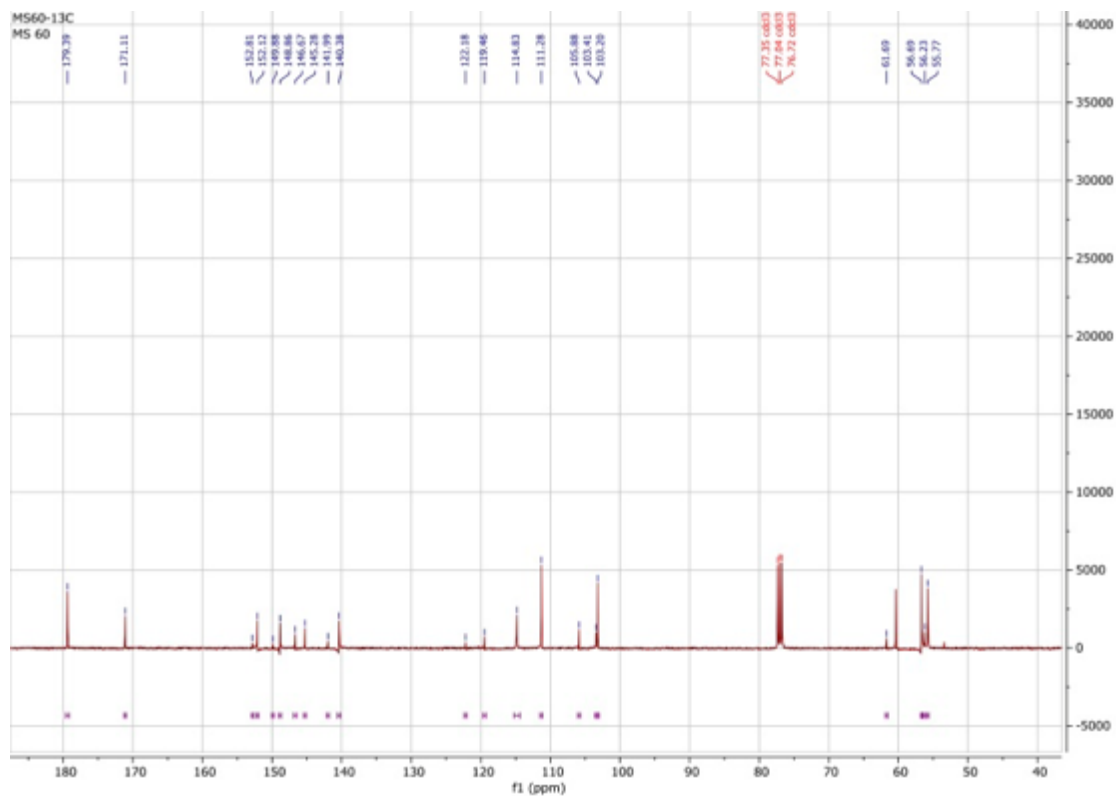
4,7-dimethoxybenzofuran-2-carbaldehyde (**20**) + 4,7-dimethoxybenzofuran-5-carbaldehyde (**7**)



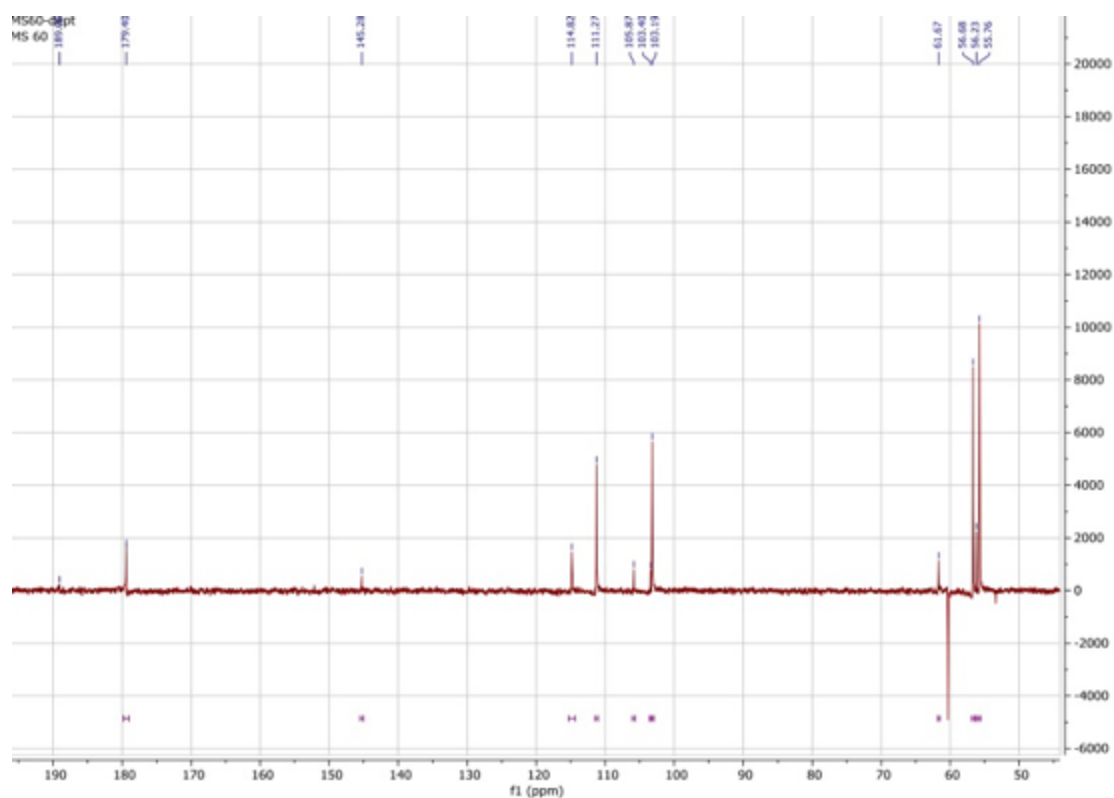


15 ¹H NMR (400 MHz, Chloroform-*d*) δ 10.43 (s, 1H), 7.65 (d, *J* = 2.3 Hz, 1H), 7.22 (s, 1H), 7.00 (d, *J* = 2.3 Hz, 1H), 4.13 (s, 3H), 3.98 (s, 3H).

16 ¹H NMR (400 MHz, Chloroform-*d*) δ 9.83 (s, 1H), 7.61 (s, 1H), 6.87 (d, *J* = 8.5 Hz, 1H), 6.54 (d, *J* = 8.6 Hz, 1H), 3.96 (s, 3H), 3.89 (s, 3H).



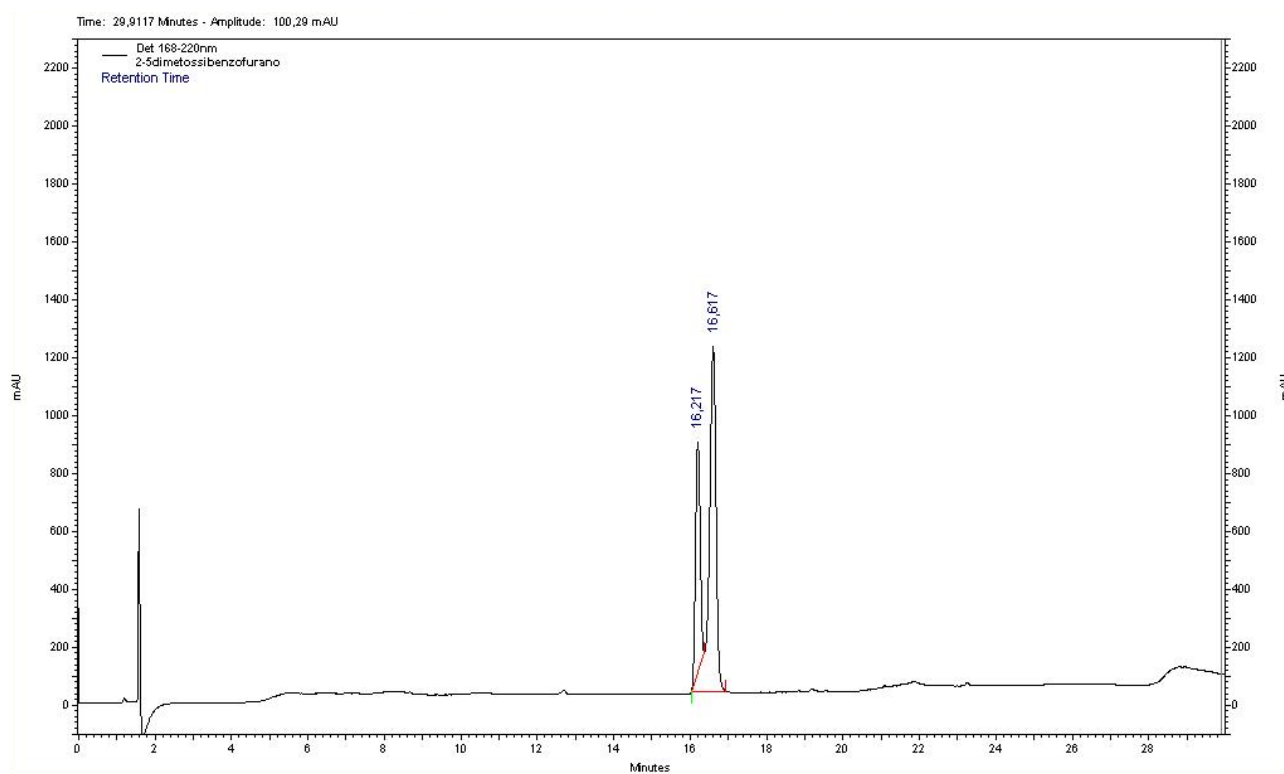
^{13}C NMR (101 MHz, Chloroform- d) δ 189.05, 179.39, 171.11, 152.81, 152.12, 149.88, 148.86, 146.67, 145.28, 141.99, 140.38, 122.18, 119.46, 114.83, 111.28, 105.88, 103.41, 103.20, 77.35, 77.04, 76.72, 61.69, 56.69, 56.23, 55.77.



^{13}C NMR (101 MHz, Chloroform- d) δ 189.06, 179.40, 145.28, 114.82, 111.27, 105.87, 103.40, 103.19, 61.67, 56.68, 56.23, 55.76.

Area % Report

Data File: C:\32Karat\Projects\Default\Data\delia\Martina\2-5dimetossibenzofurano.dat
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 Printed: 04/08/2022 13.17.44

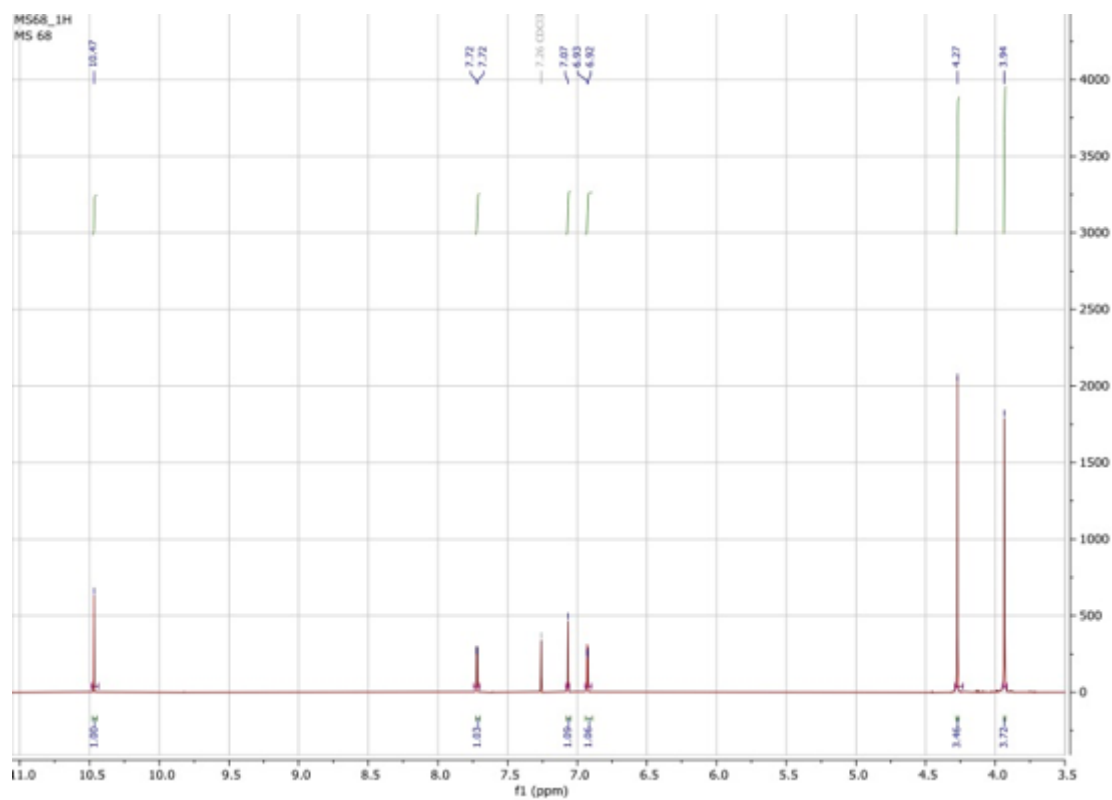
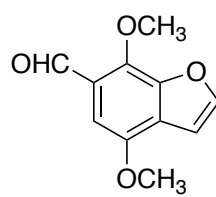


**Det 168-220nm
Results**

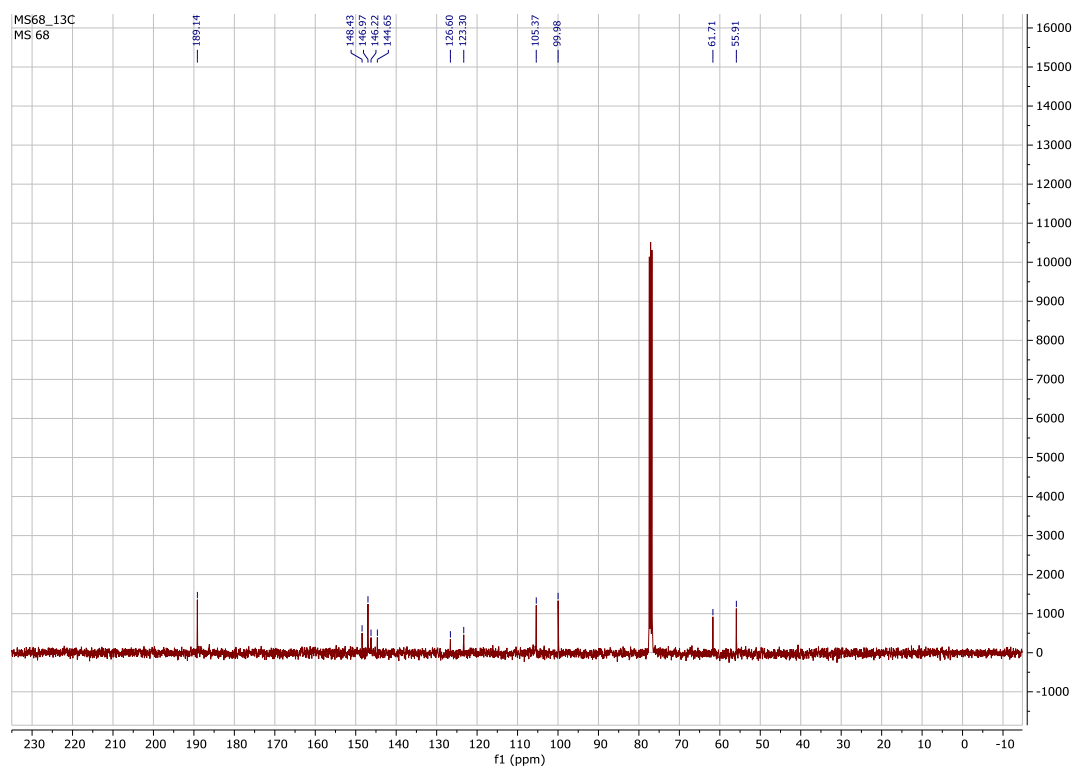
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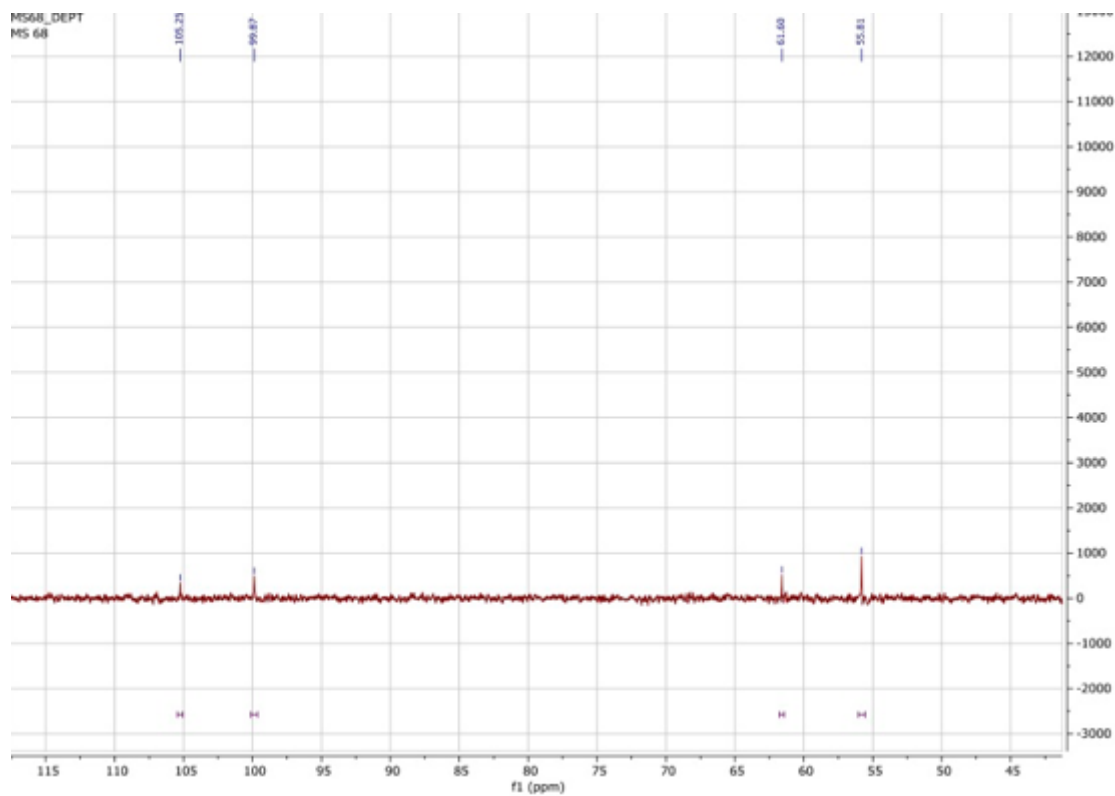
4,7-dimethoxybenzofuran-6-carbaldehyde (21)



¹H NMR (400 MHz, Chloroform-*d*) δ 10.47 (s, 1H), 7.72 (d, *J* = 2.1 Hz, 1H), 7.07 (s, 1H), 6.92 (d, *J* = 2.1 Hz, 1H), 4.27 (s, 3H), 3.94 (s, 3H).

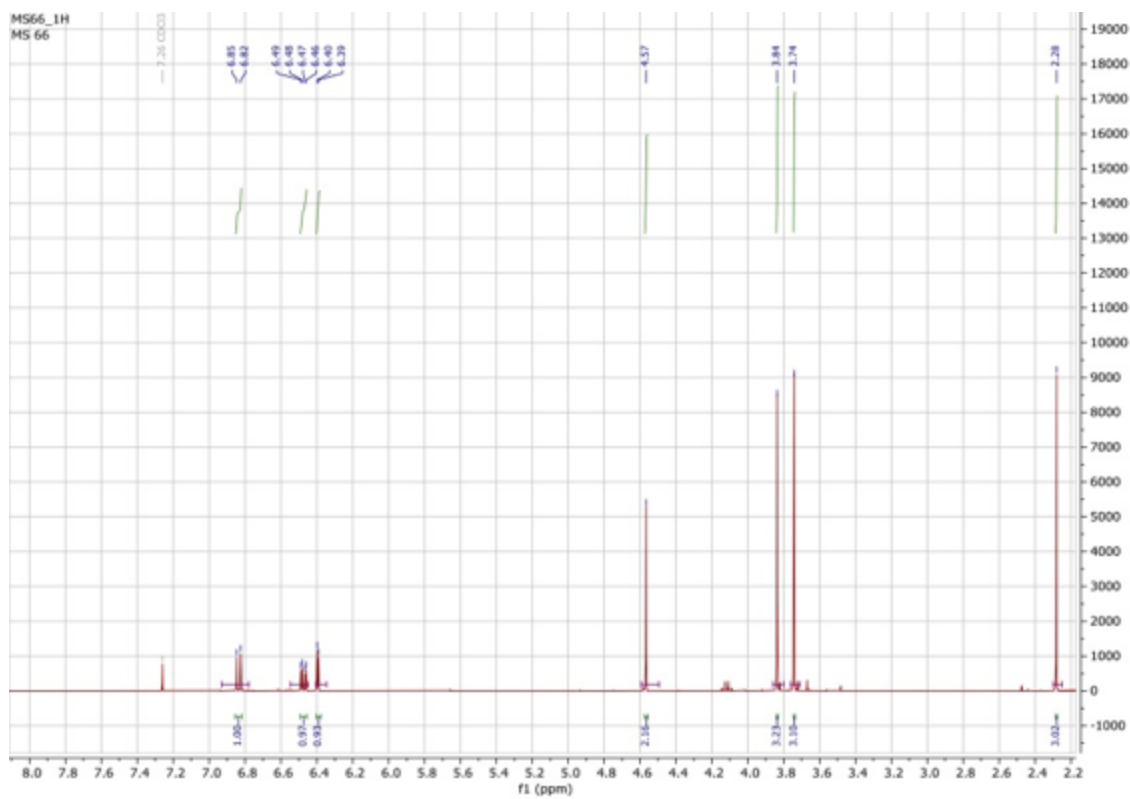
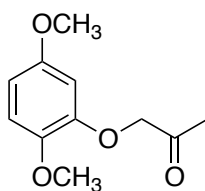


^{13}C NMR (101 MHz, Chloroform-d) δ 189.14, 148.43, 146.97, 146.22, 144.65, 126.60, 123.30, 105.37, 99.98, 61.71, 55.91.

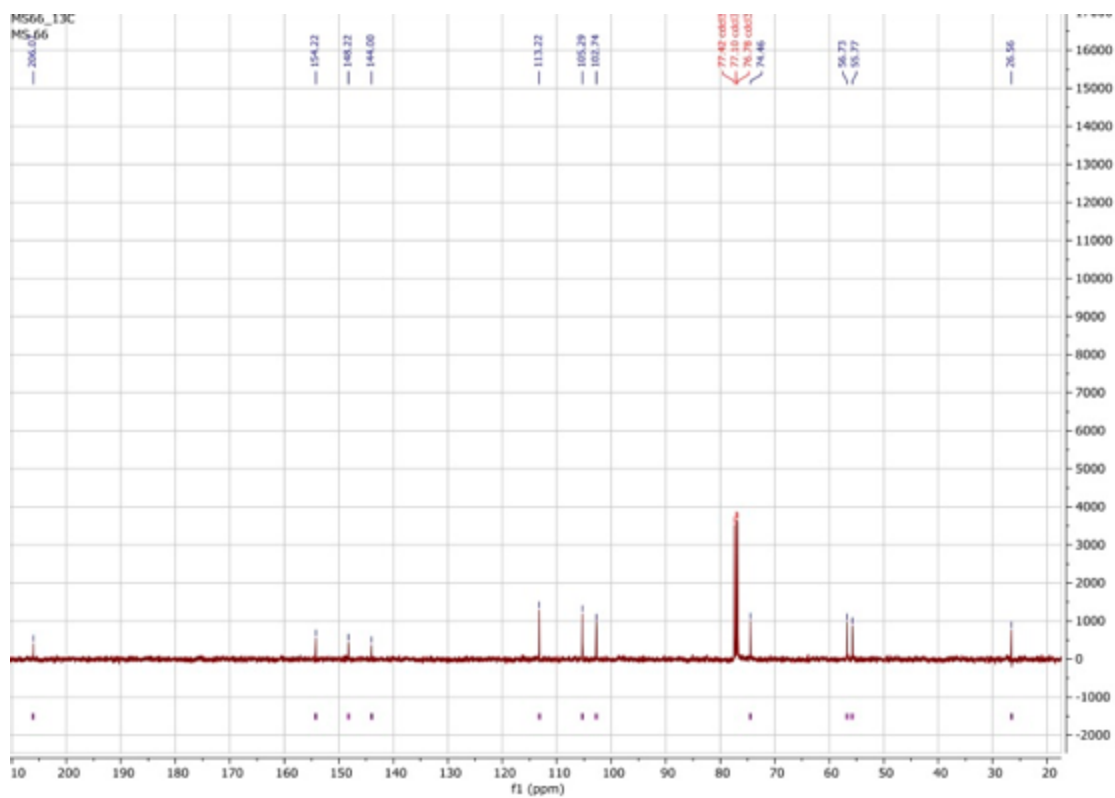


^{13}C NMR (101 MHz, Chloroform-d) δ 105.25, 99.87, 61.60, 55.81.

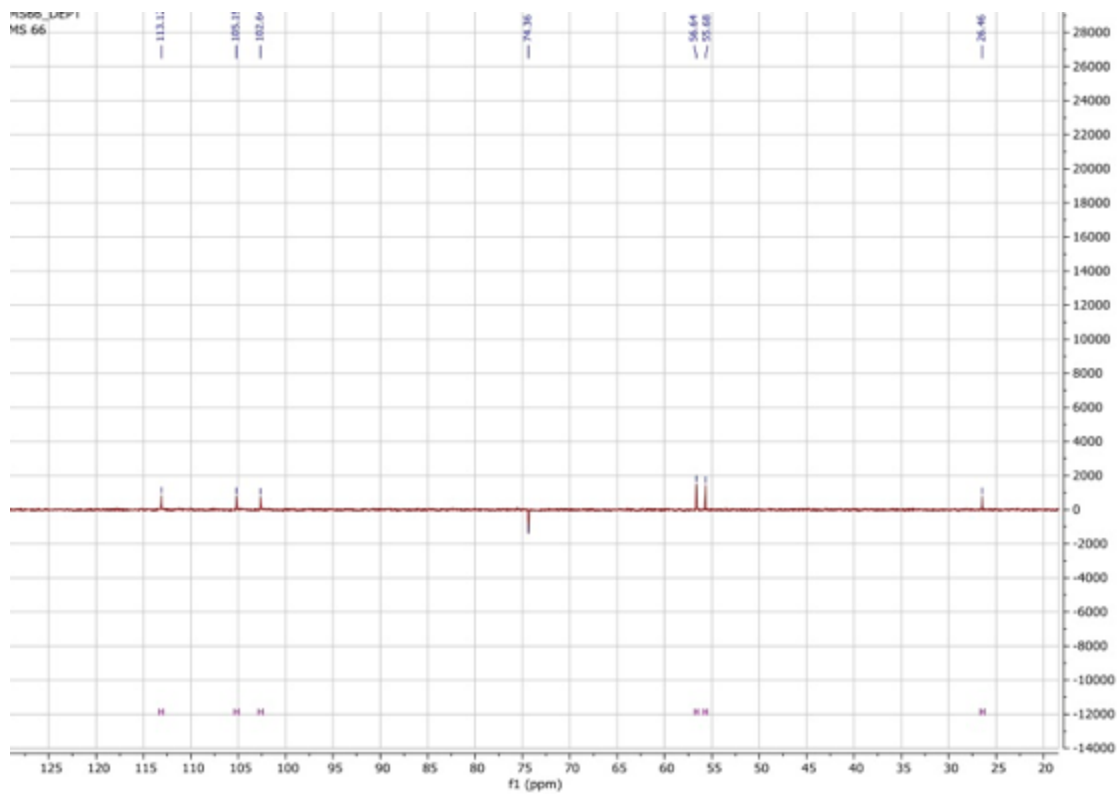
1-(2,5-dimethoxyphenoxy)propan-2-one (24)



^1H NMR (400 MHz, Chloroform- d) δ 6.83 (d, $J = 8.8$ Hz, 1H), 6.47 (dd, $J = 8.8, 2.8$ Hz, 1H), 6.39 (d, $J = 2.8$ Hz, 1H), 4.57 (s, 2H), 3.84 (s, 3H), 3.74 (s, 3H), 2.28 (s, 3H).

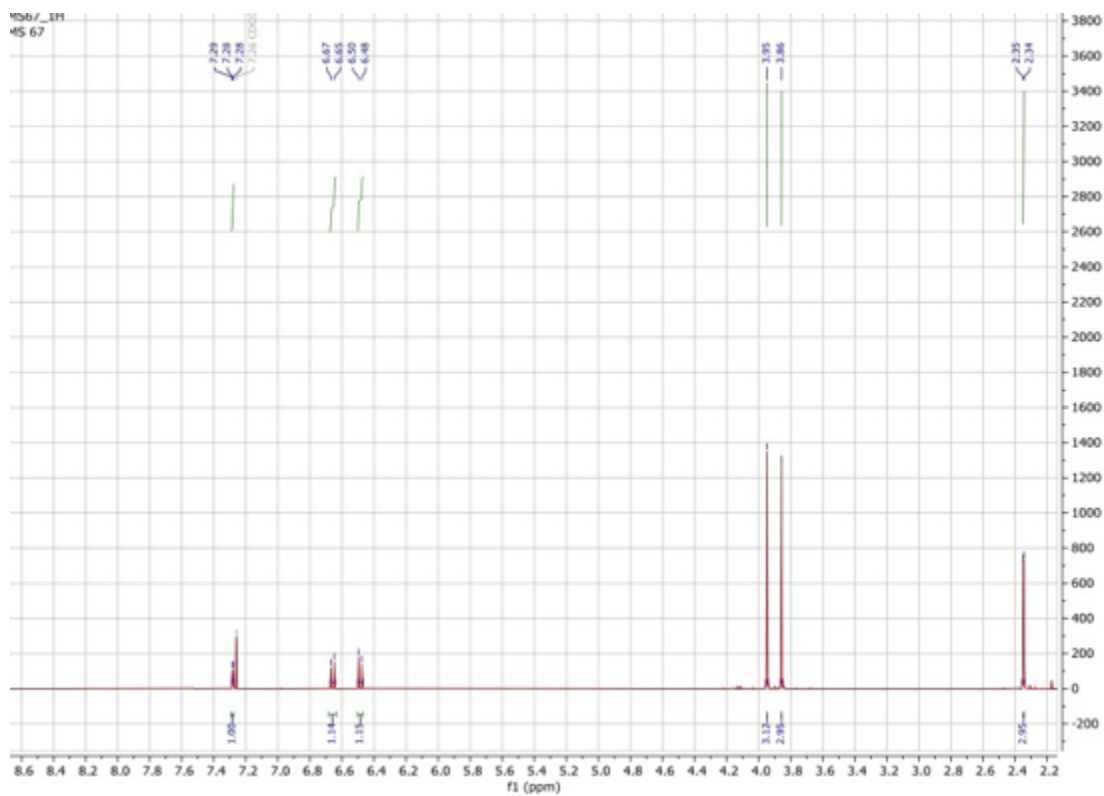
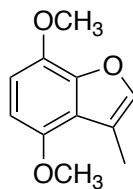


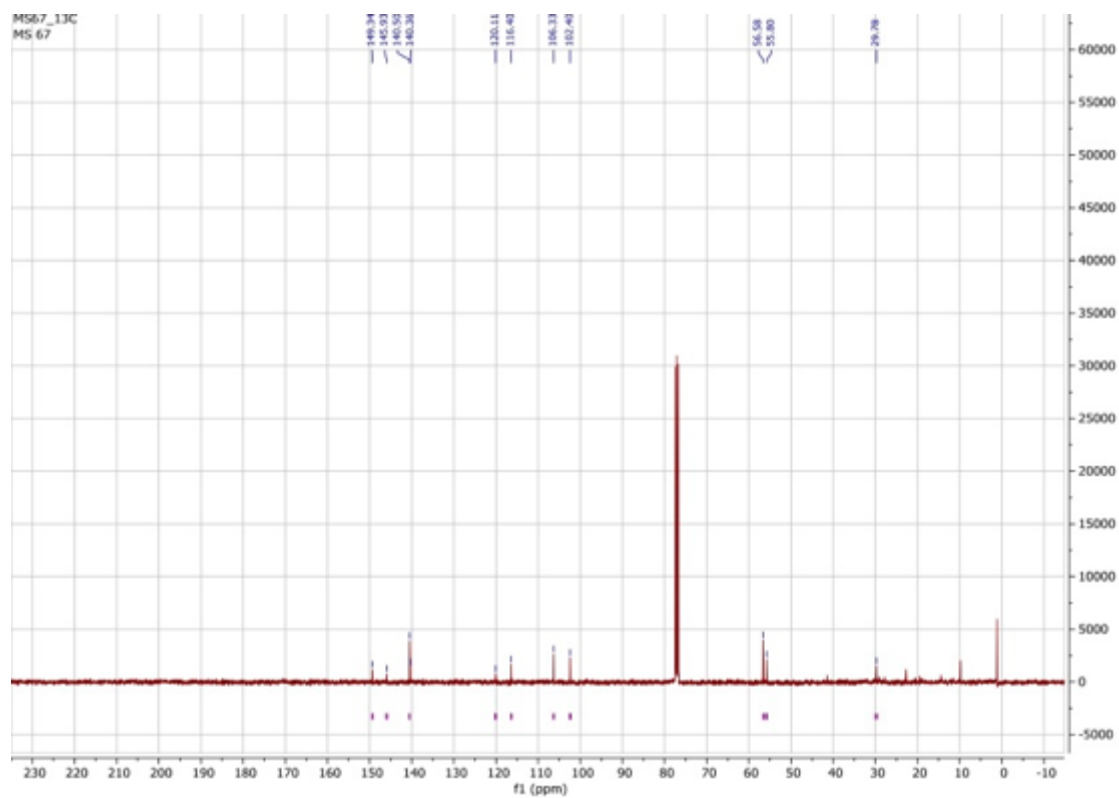
¹³C NMR (101 MHz, Chloroform-d) δ 206.07, 154.22, 148.22, 144.00, 113.22, 105.29, 102.74, 74.46, 56.73, 55.77, 26.56.



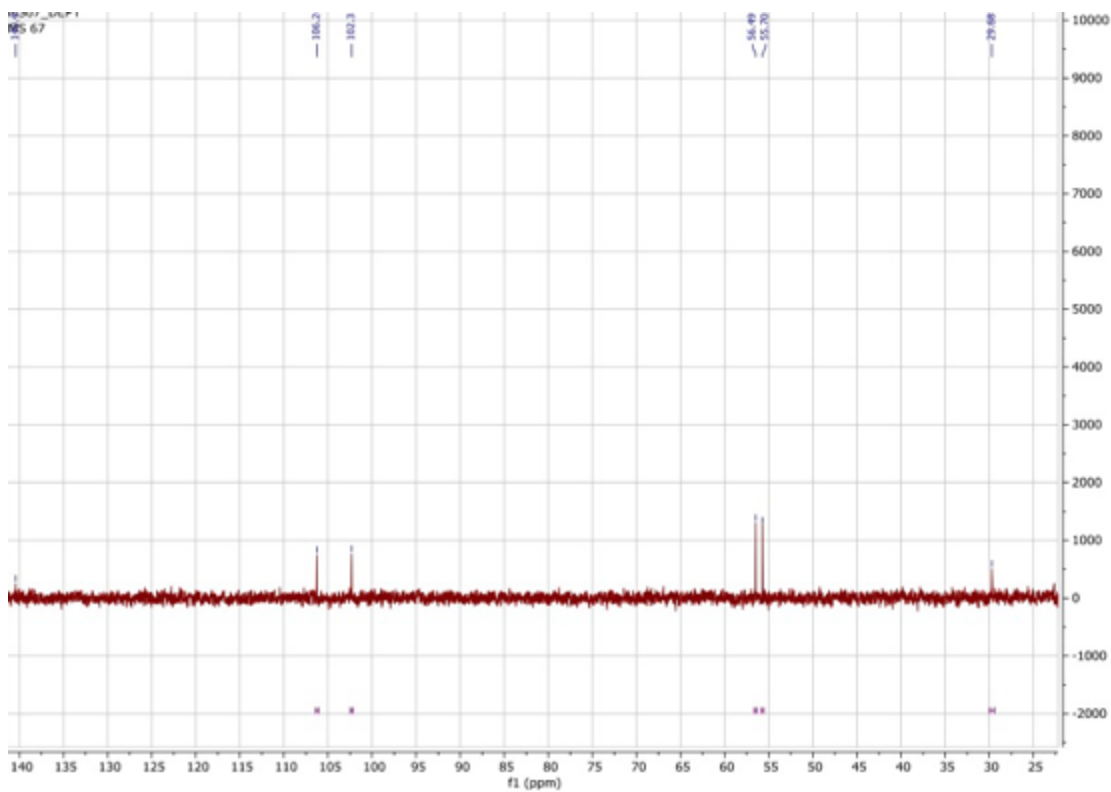
¹³C NMR (101 MHz, Chloroform-d) δ 113.12, 105.19, 102.64, 74.36, 56.64, 55.68, 26.46.

4,7-dimethoxy-3-methylbenzofuran (25)

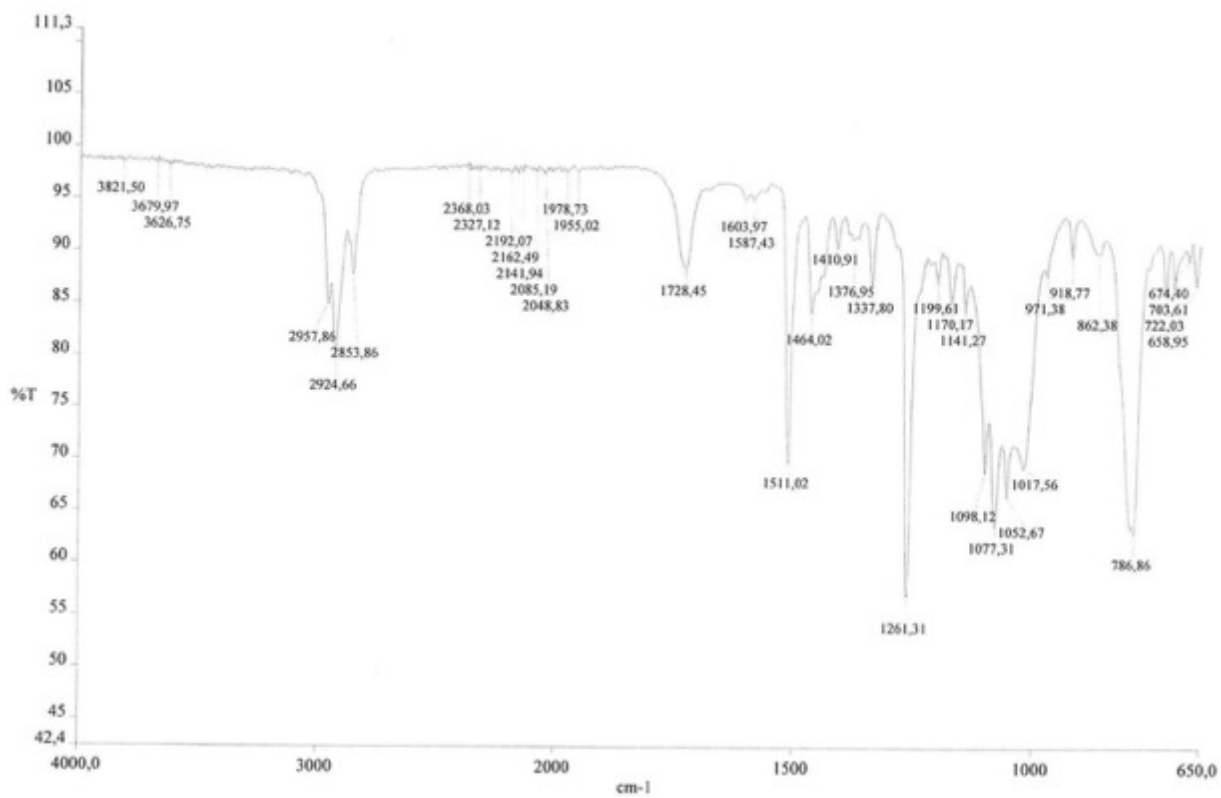




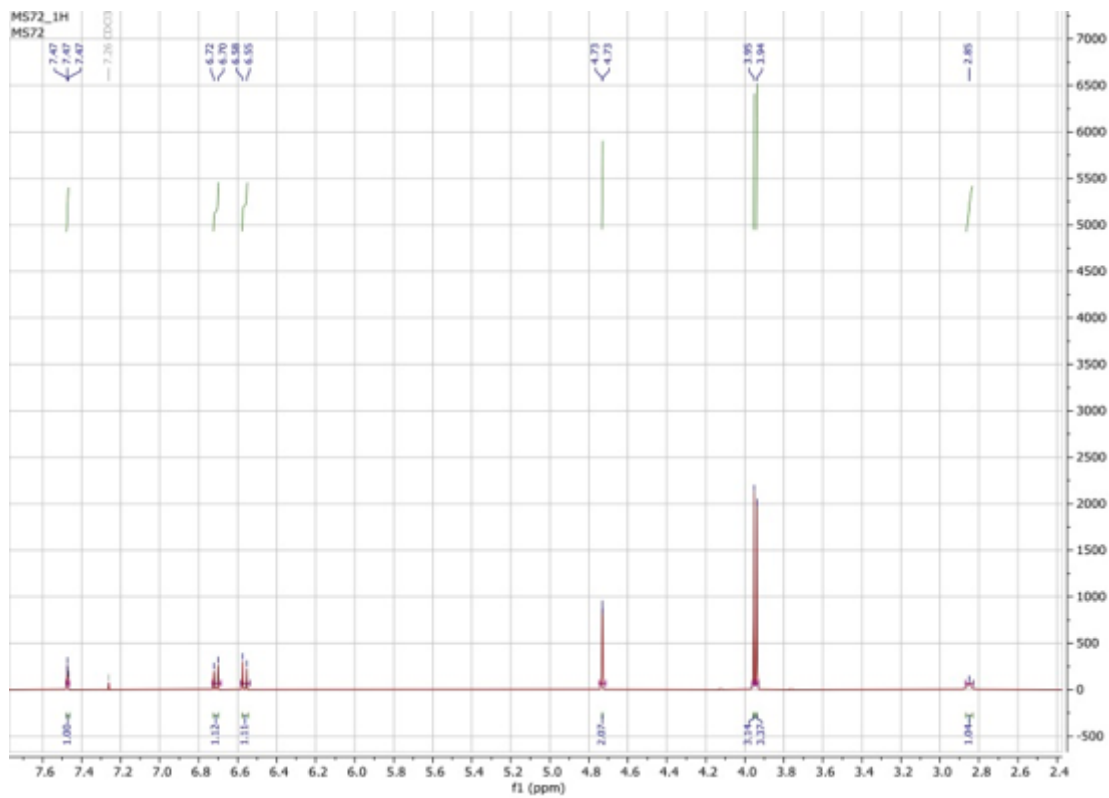
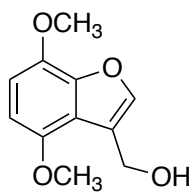
¹³C NMR (101 MHz, Chloroform-d) δ 149.34, 145.93, 140.50, 140.36, 120.11, 116.40, 106.33, 102.40, 56.58, 55.80, 29.78.



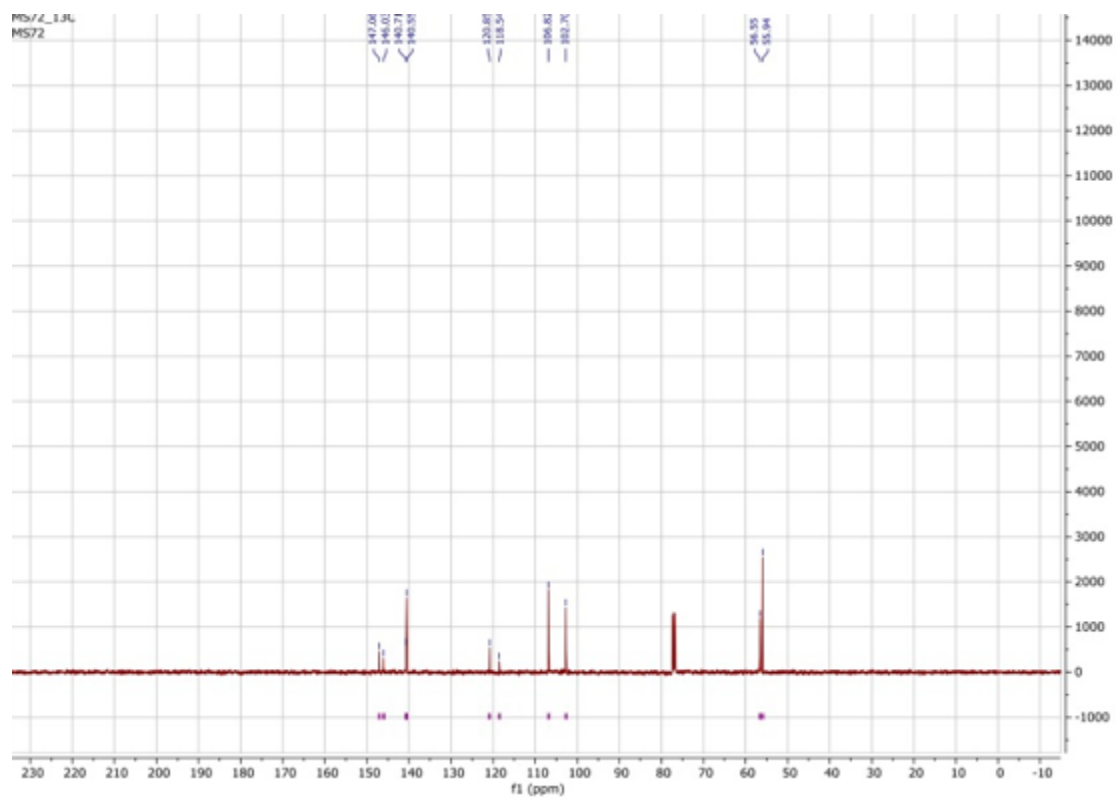
¹³C NMR (101 MHz, Chloroform-d) δ 140.41, 106.24, 102.31, 56.49, 55.70, 29.68.



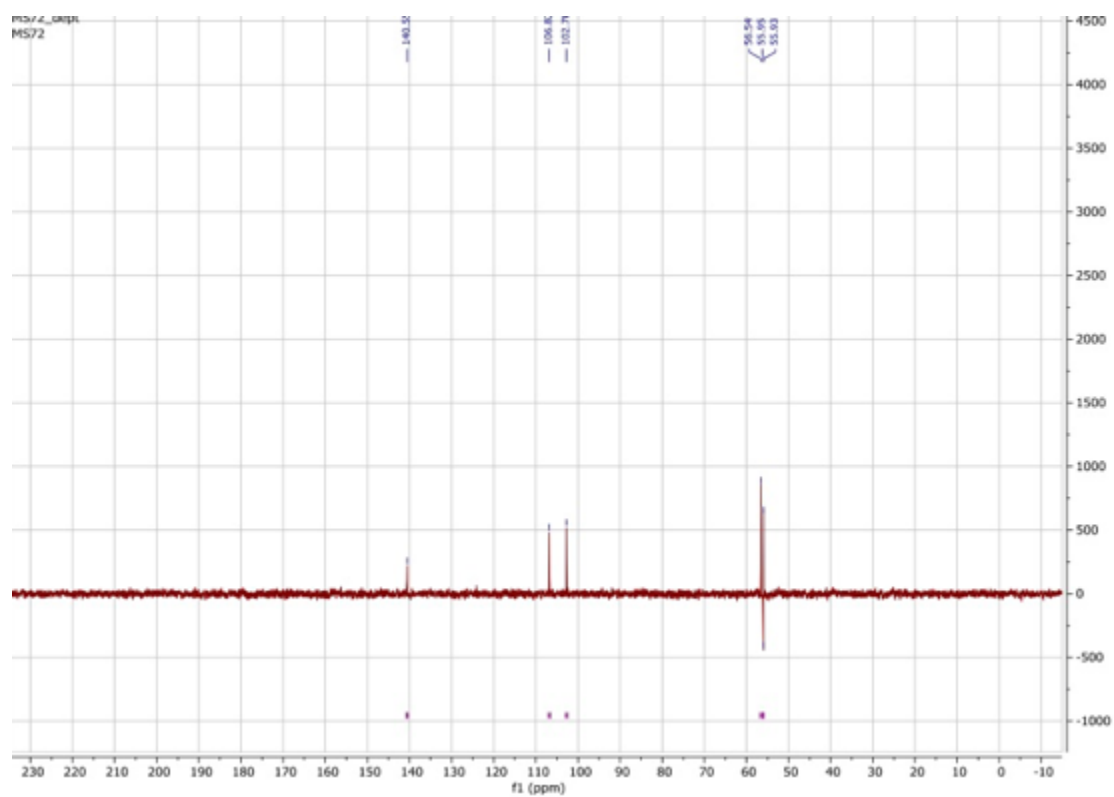
(4,7-dimethoxybenzofuran-3-yl)methanol (26)



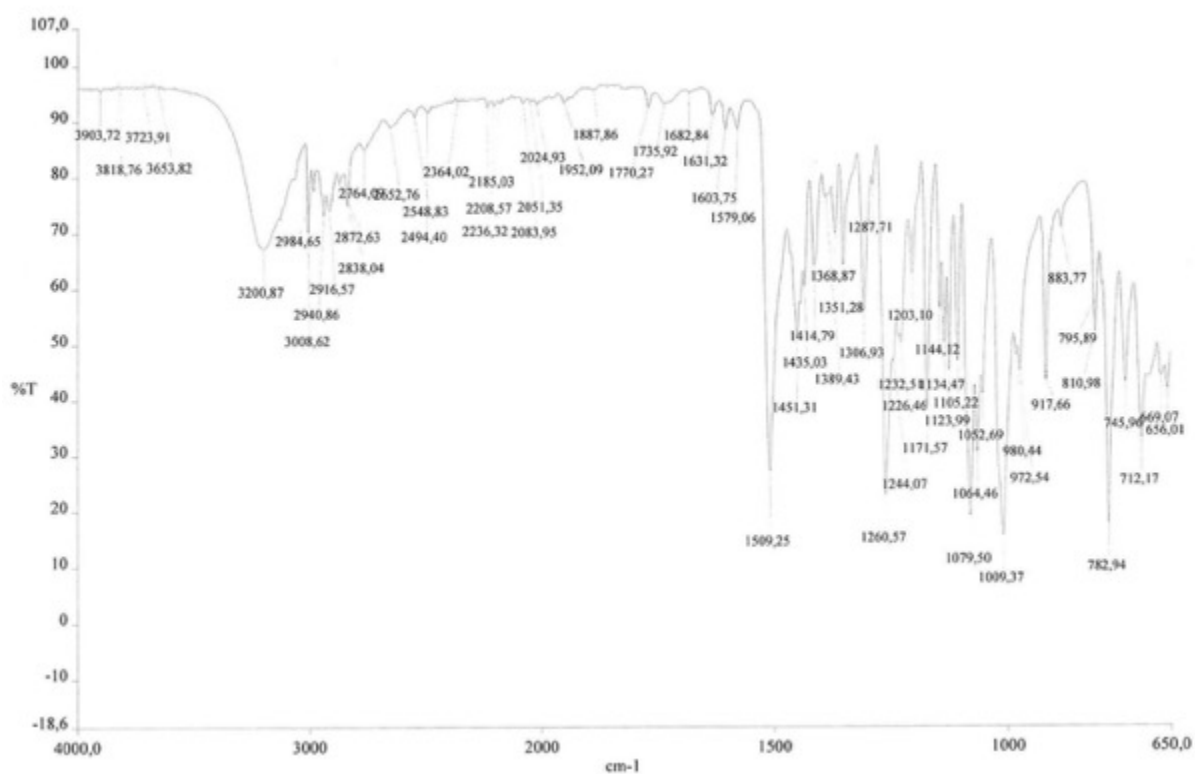
^1H NMR (400 MHz, Chloroform-d) δ 7.47 (d, J = 1.0 Hz, 1H), 6.71 (d, J = 8.6 Hz, 1H), 6.56 (d, J = 8.6 Hz, 1H), 4.73 (d, J = 0.9 Hz, 2H), 3.95 (s, 3H), 3.94 (s, 3H), 2.85 (s, 1H).



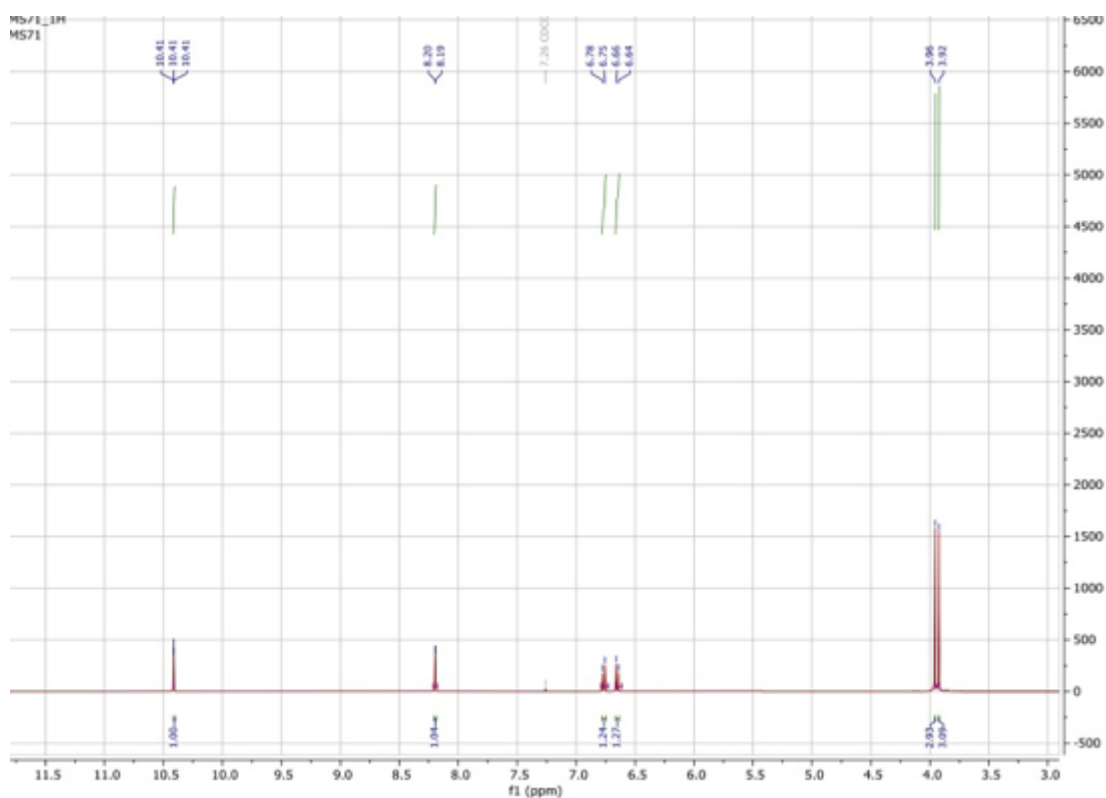
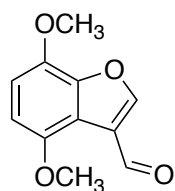
¹³C NMR (101 MHz, Chloroform-d) δ 147.06, 146.03, 140.71, 140.55, 120.85, 118.54, 106.82, 102.70, 56.55, 55.94.

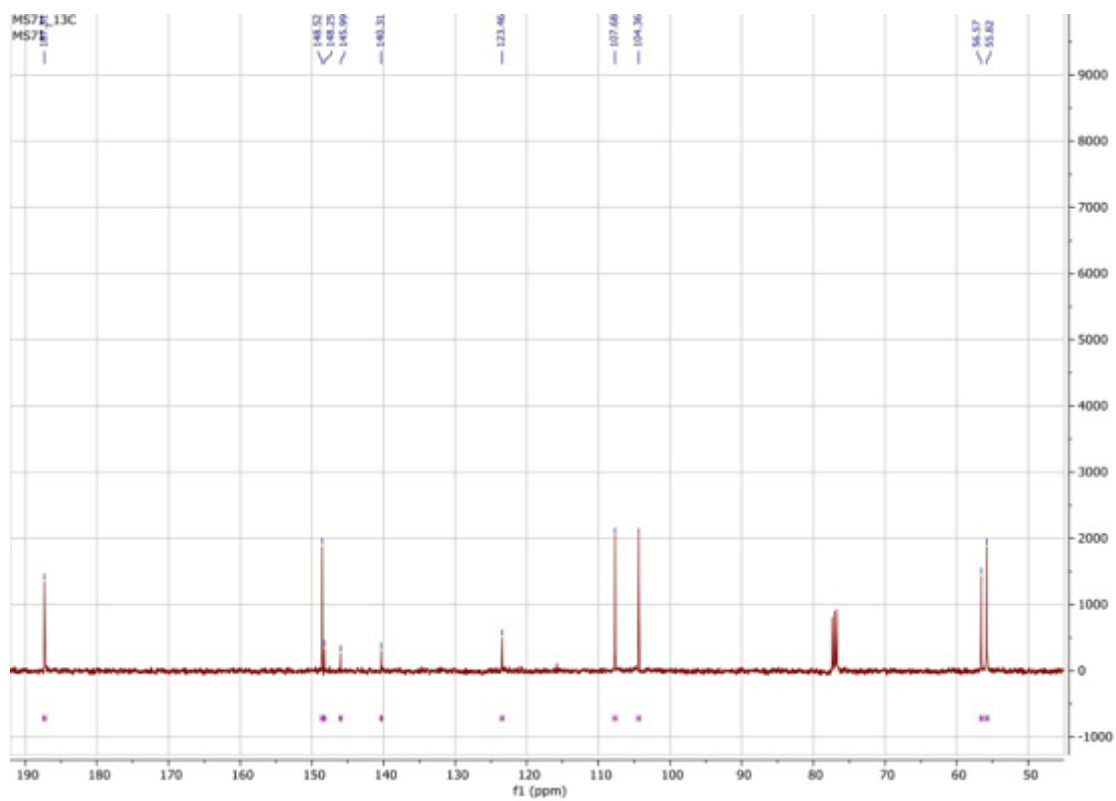


¹³C NMR (101 MHz, Chloroform-d) δ 140.55, 106.82, 102.70, 56.54, 55.95, 55.93.

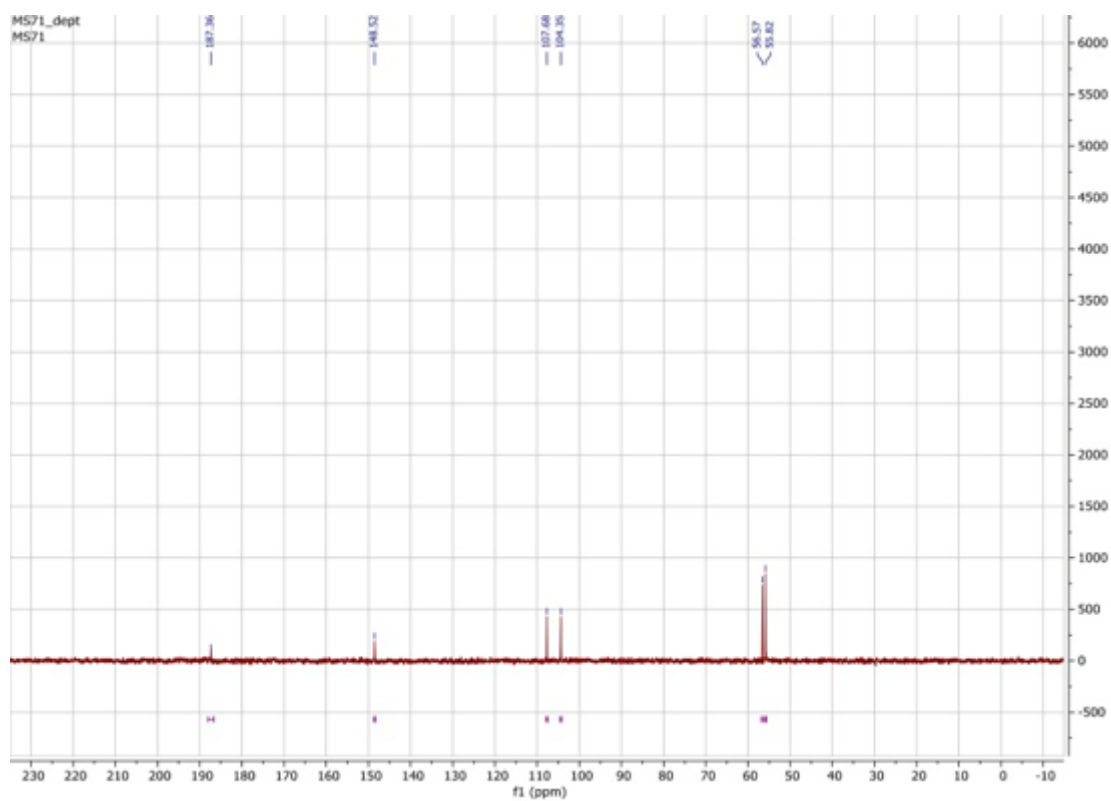


4,7-dimethoxybenzofuran-3-carbaldehyde (27)

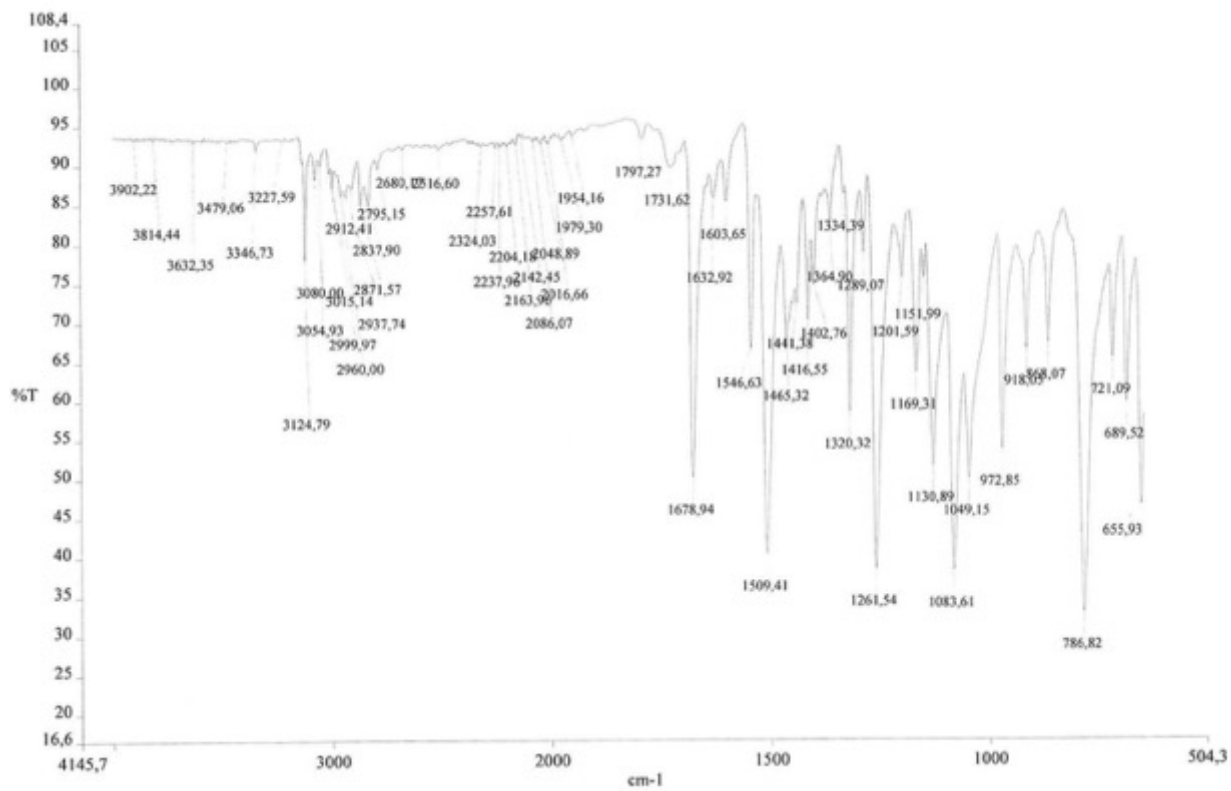




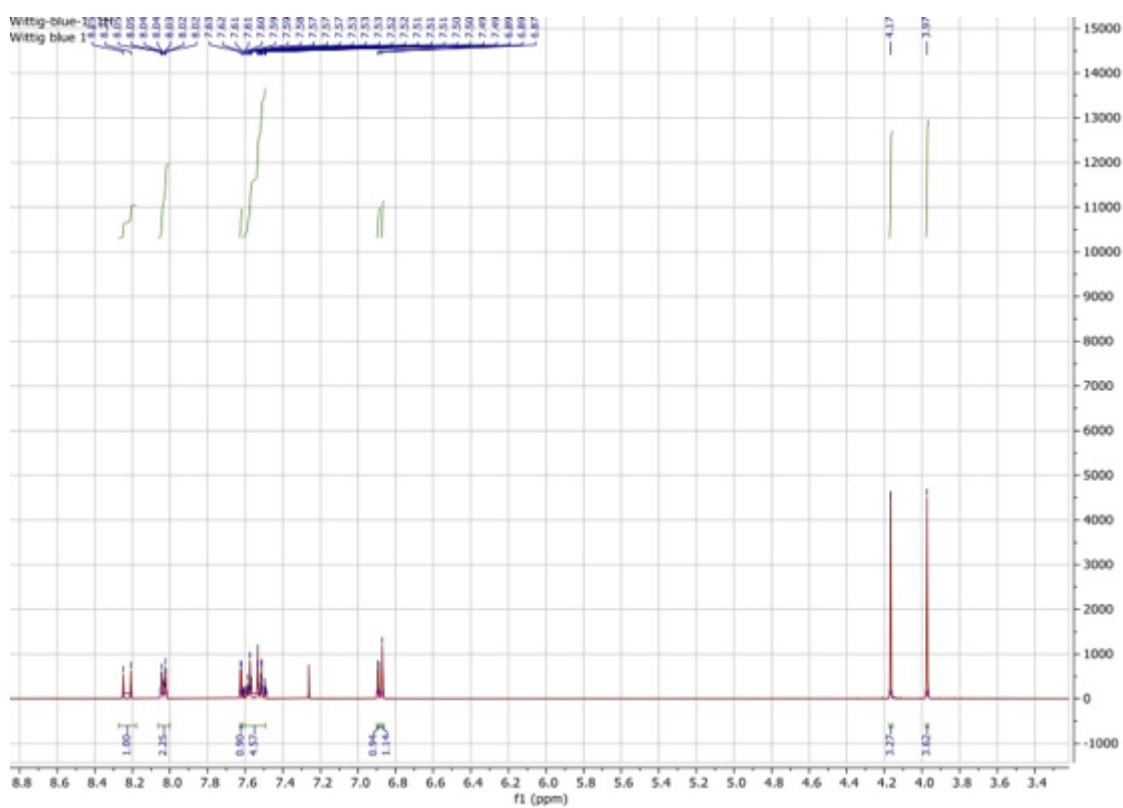
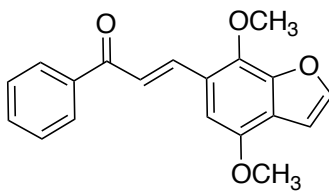
^{13}C NMR (101 MHz, Chloroform-d) δ 187.31, 148.52, 148.25, 145.99, 140.31, 123.46, 107.68, 104.36, 56.57, 55.82.



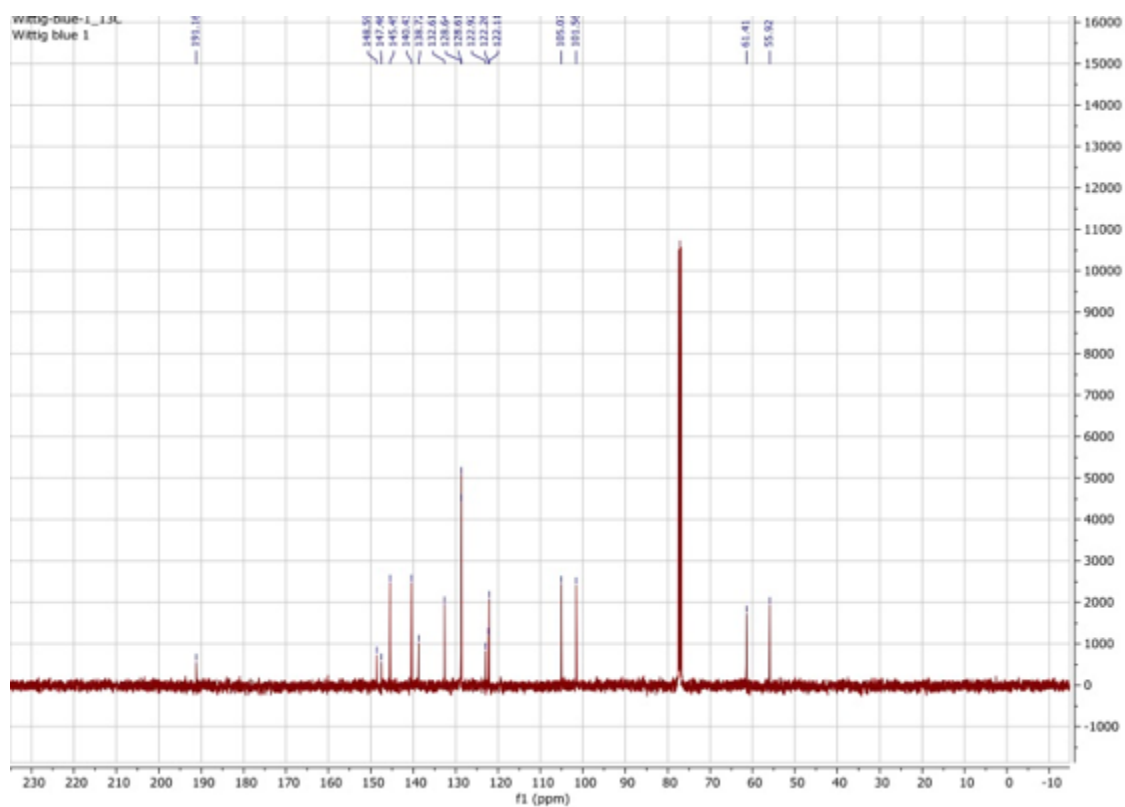
^{13}C NMR (101 MHz, Chloroform-d) δ 187.36, 148.52, 107.68, 104.35, 56.57, 55.82.



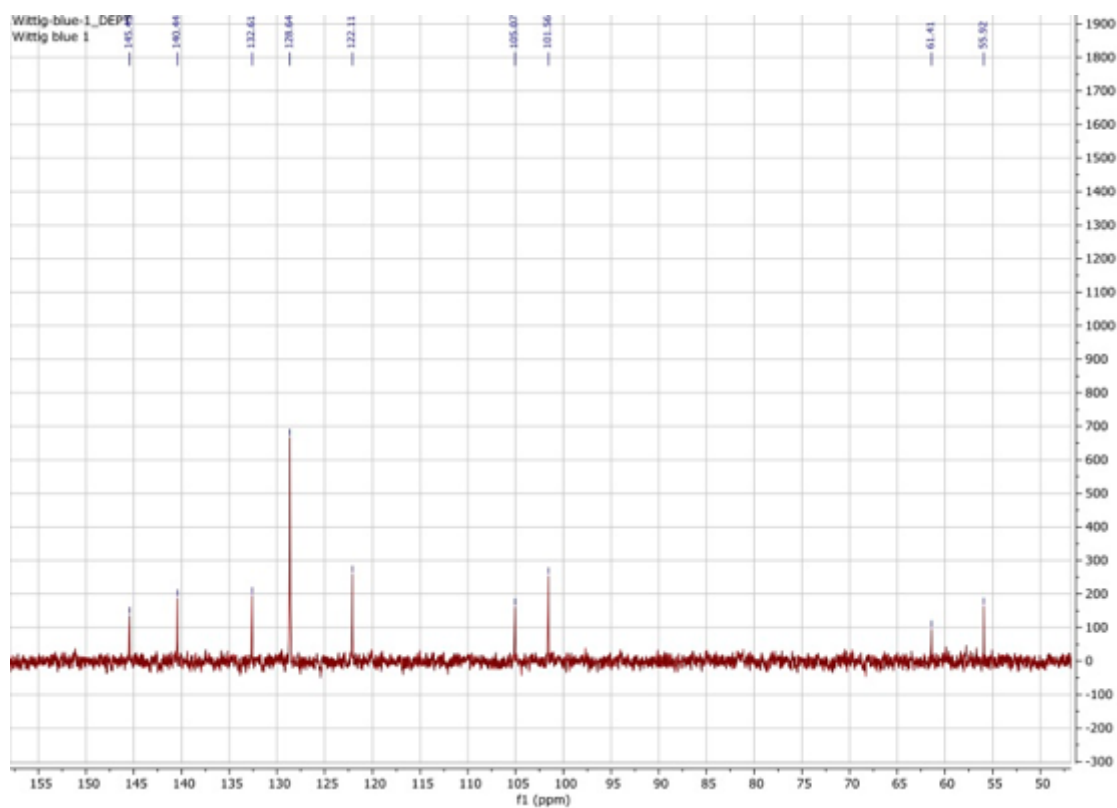
(*E*)-3-(4,7-dimethoxybenzofuran-6-yl)-1-phenylprop-2-en-1-one (23)



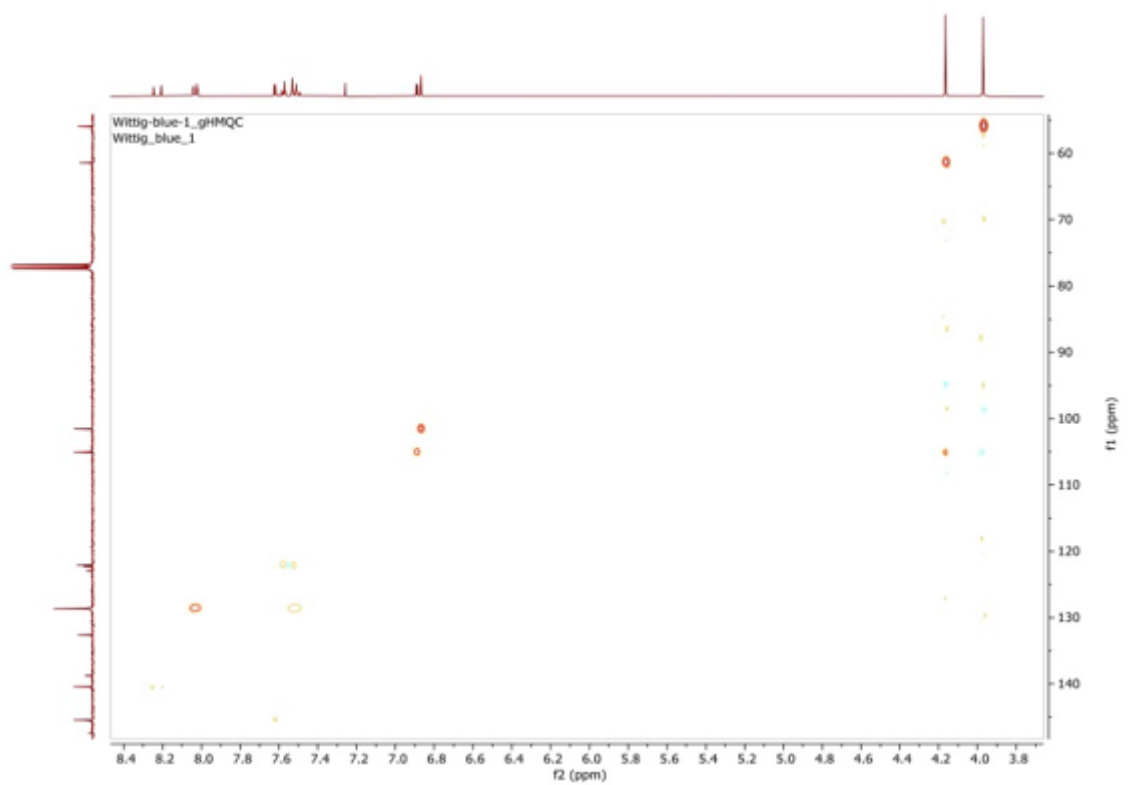
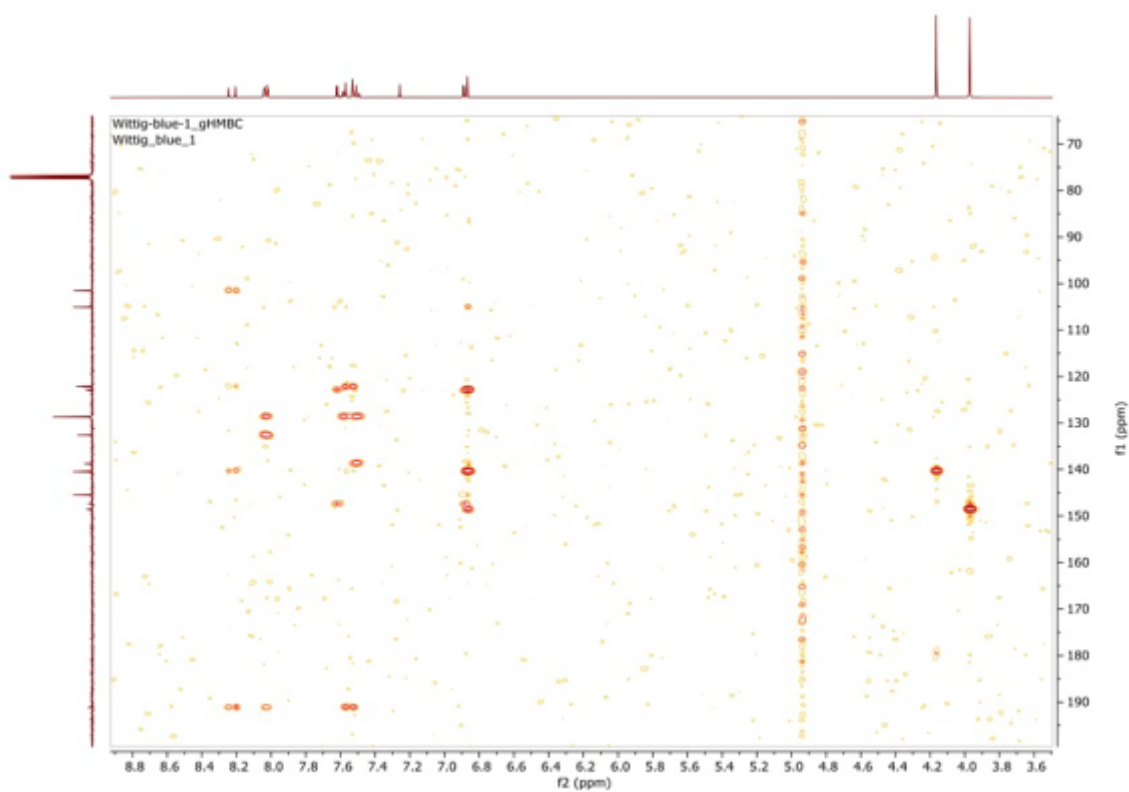
^1H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, $J = 15.9$ Hz, 1H), 8.05 – 8.02 (m, 2H), 7.62 (d, $J = 2.1$ Hz, 1H), 7.61 – 7.49 (m, 4H), 6.89 (d, $J = 2.1$ Hz, 1H), 6.87 (s, 1H), 4.17 (s, 3H), 3.97 (s, 3H).

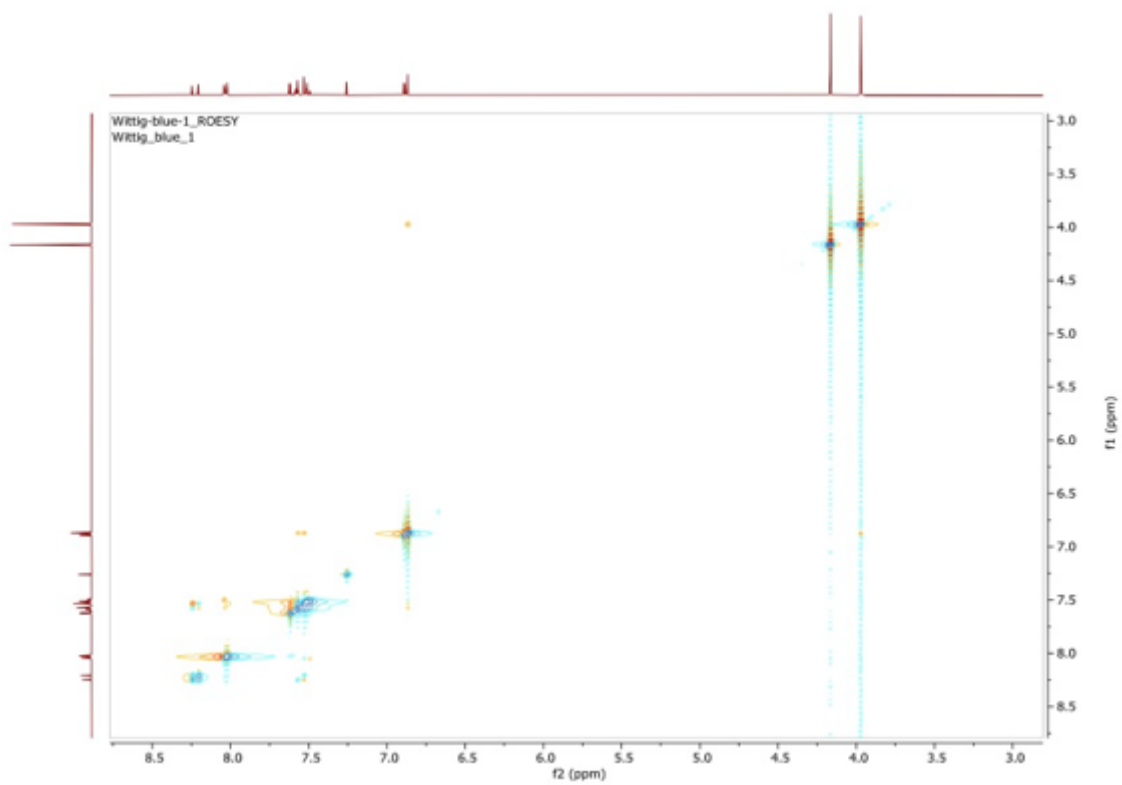
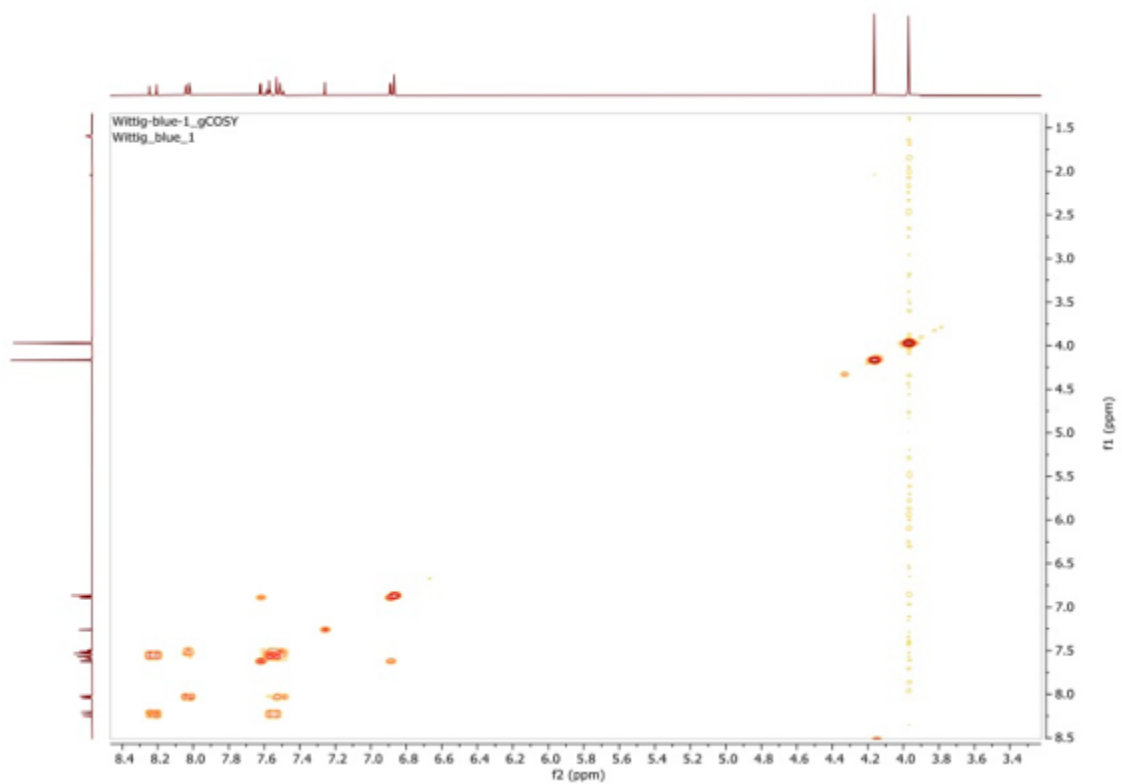


^{13}C NMR (101 MHz, Chloroform-d) δ 191.16, 148.59, 147.46, 145.45, 140.43, 138.72, 132.61, 128.64, 128.61, 122.92, 122.26, 122.11, 105.07, 101.56, 61.41, 55.92.



^{13}C NMR (101 MHz, Chloroform-d) δ 145.45, 140.44, 132.61, 128.64, 122.11, 105.07, 101.56, 61.41, 55.92.





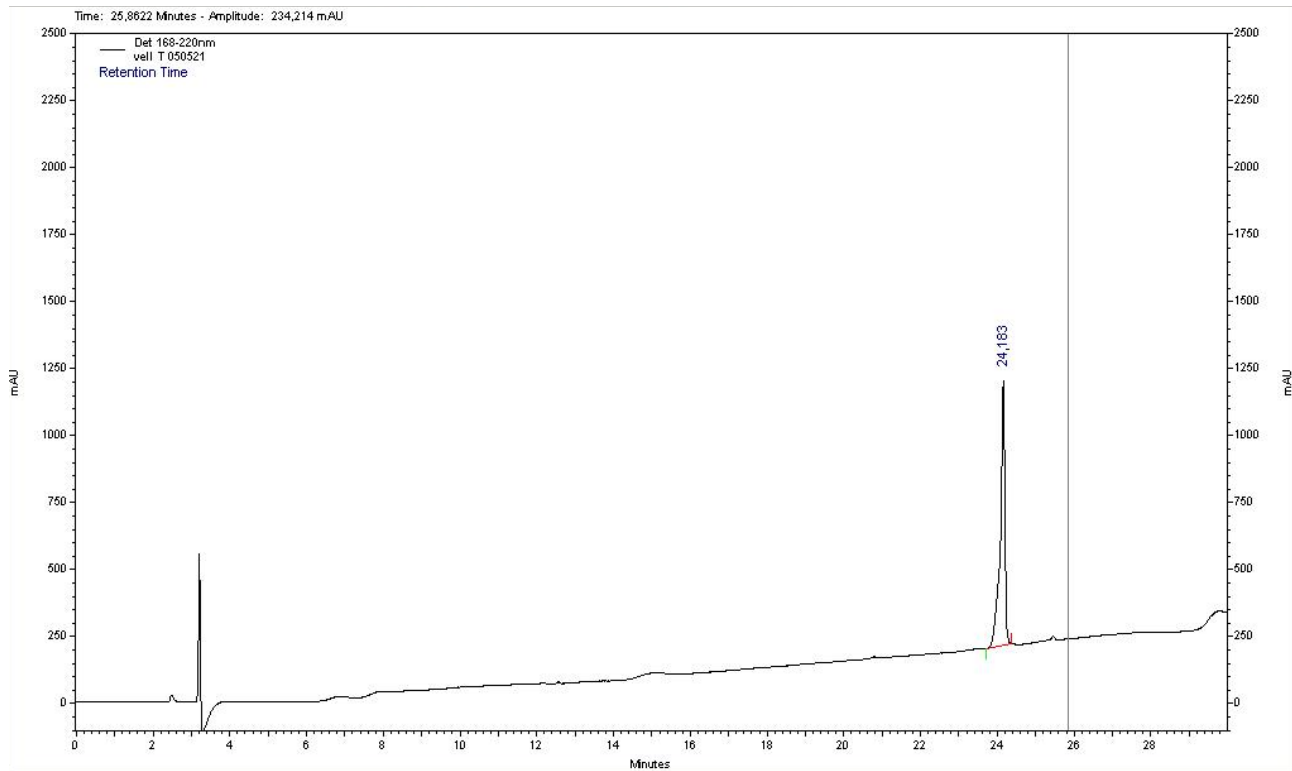
Area % Report

Data File: C:\32Karat\Projects\Default\Data\delia\Martina\vell T 050521.dat

Method: C:\32Karat\Projects\Default\Method\standard 0.7 ml.met

Acquired: 05/05/2021 15.47.23

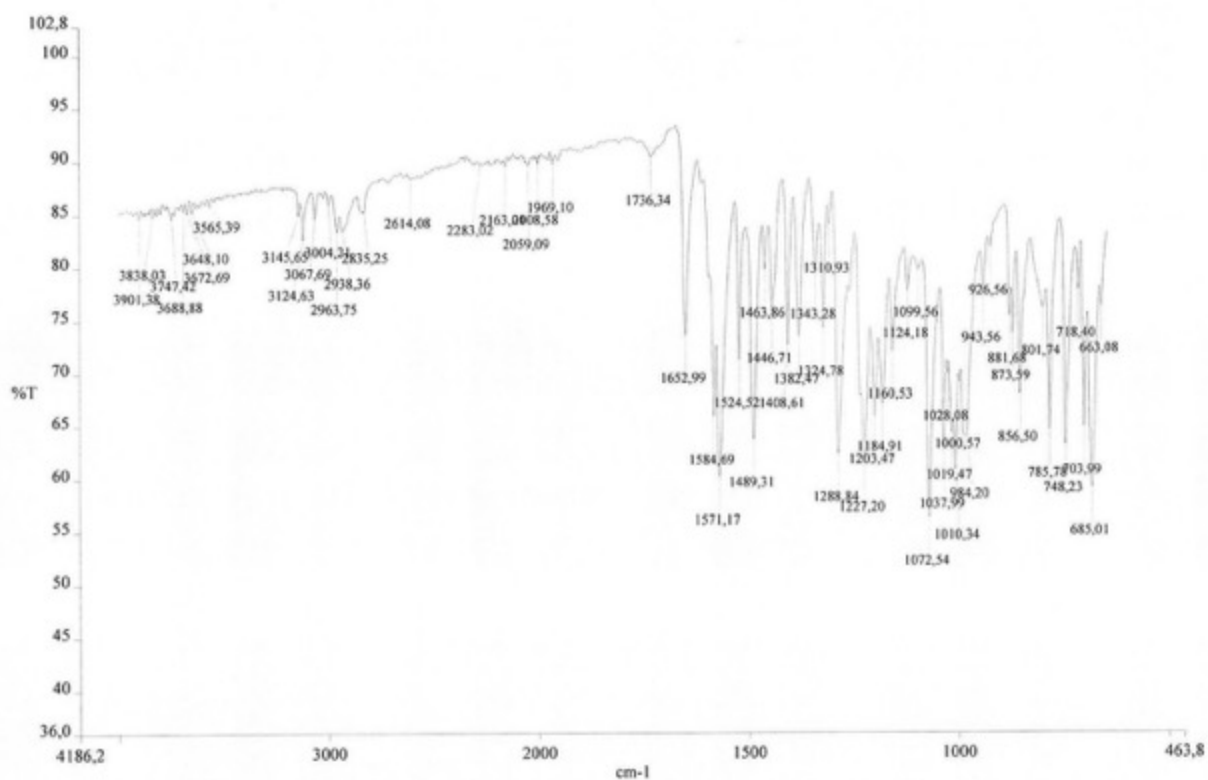
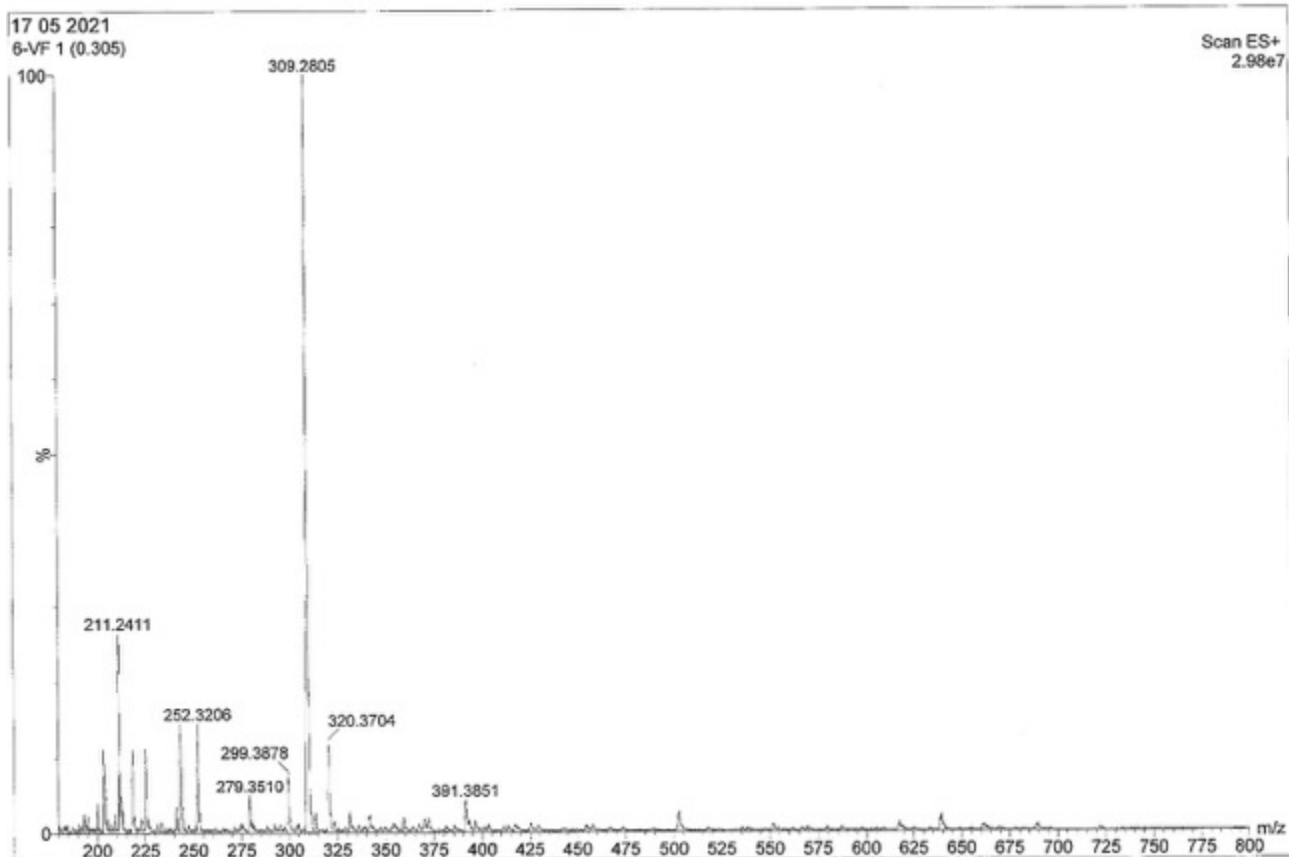
Printed: 04/08/2022 13.20.32



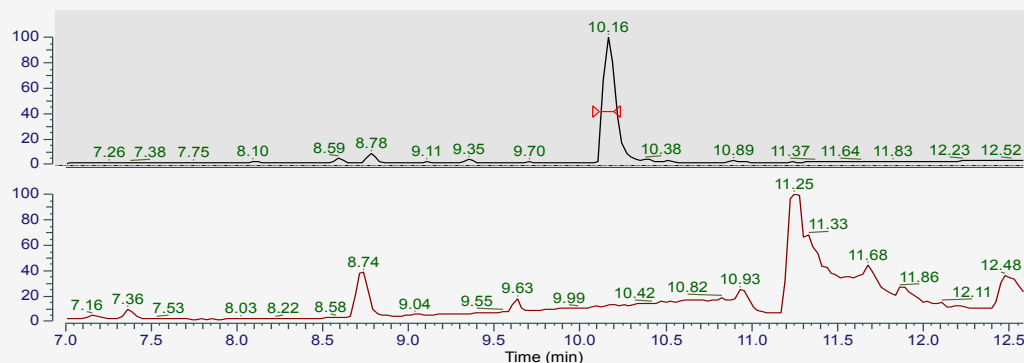
Det 168-220nm

Results

Time	Area	Area %	Height	Height %
24,183	8149082	100,00	987191	100,00
Totals	8149082	100,00	987191	100,00



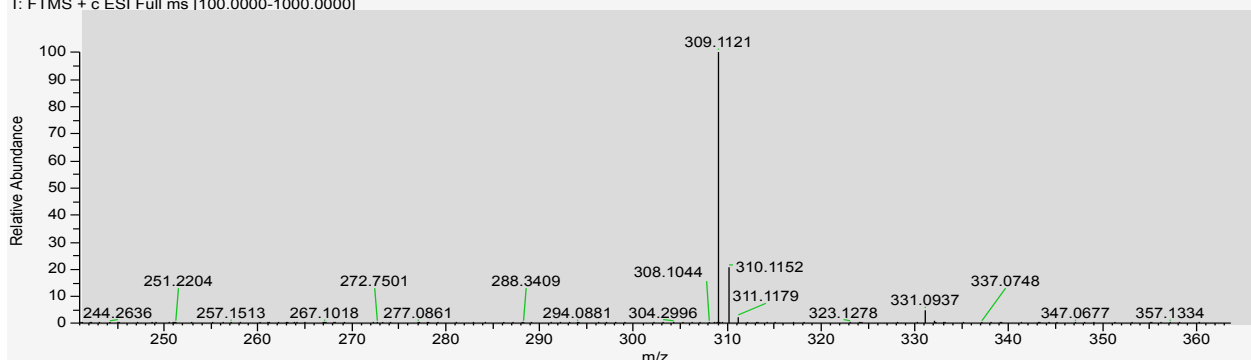
RT : 7.00-12.58



NL: 1.60E9
Base Peak m/z= 150.0000-
800.0000 MS F: FTMS + c ESI Full ms
[100.0000-1000.0000]
6-VF_CIGSPP-UniFe_DDA_027

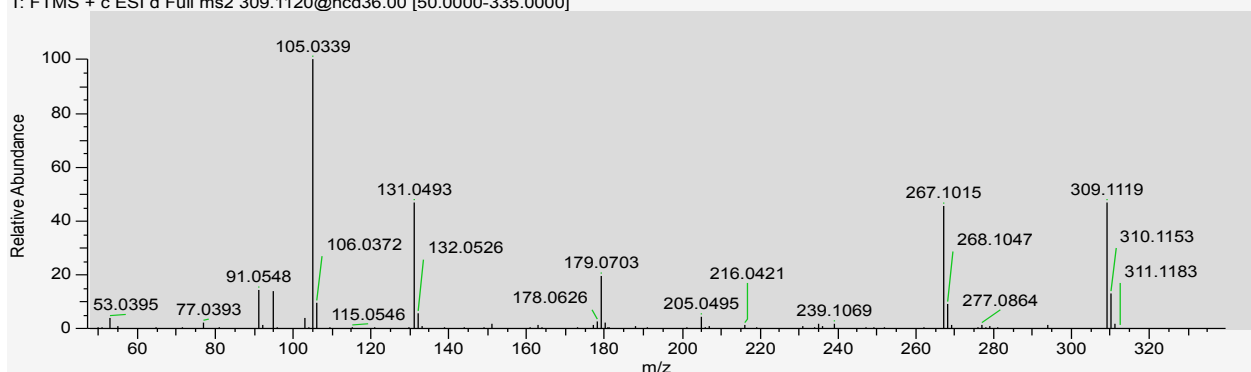
NL: 4.73E7
Base Peak m/z= 150.0000-
800.0000 MS F: FTMS - c ESI Full ms
[100.0000-1000.0000]
6-VF_CIGSPP-UniFe_DDA_027

6-VF_CIGSPP-UniFe_DDA_027 #2177-2198 RT: 10.11-10.2 AV: 4 SB: 7 9.85-10.03 NL: 9.90E+008
T: FTMS + c ESI Full ms [100.0000-1000.0000]

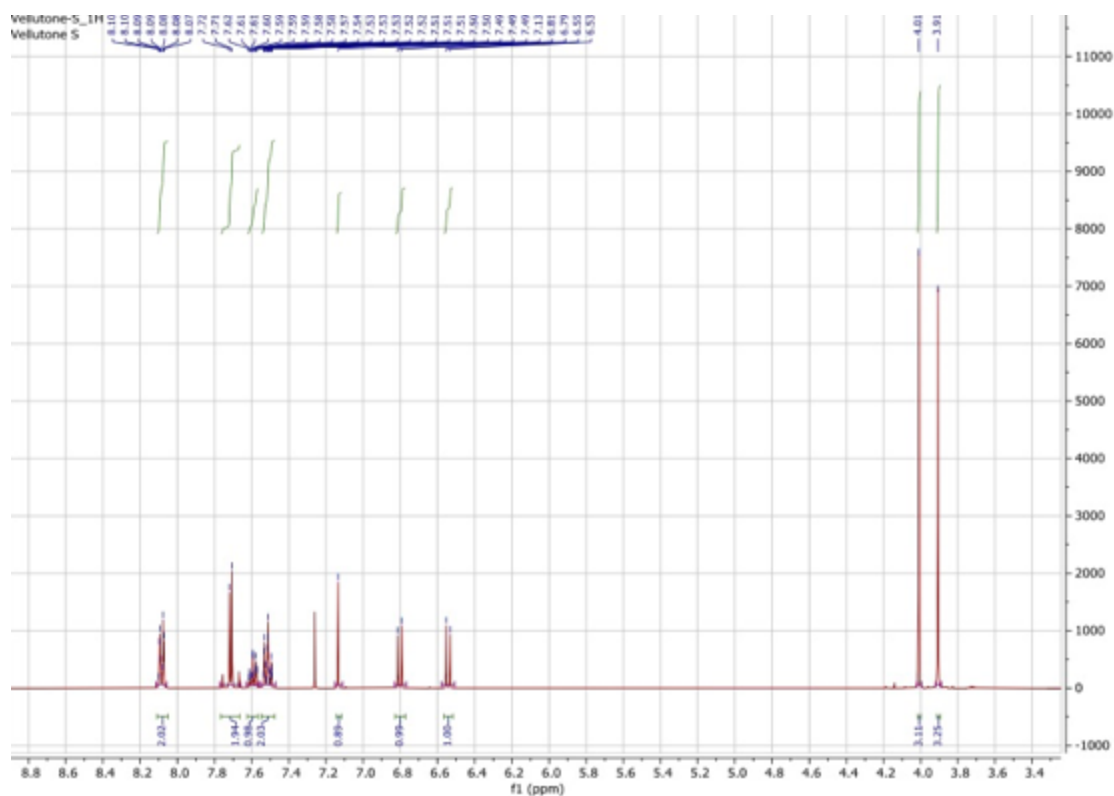
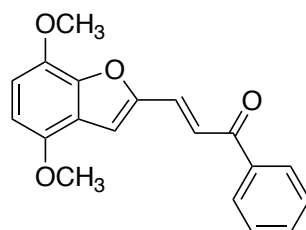


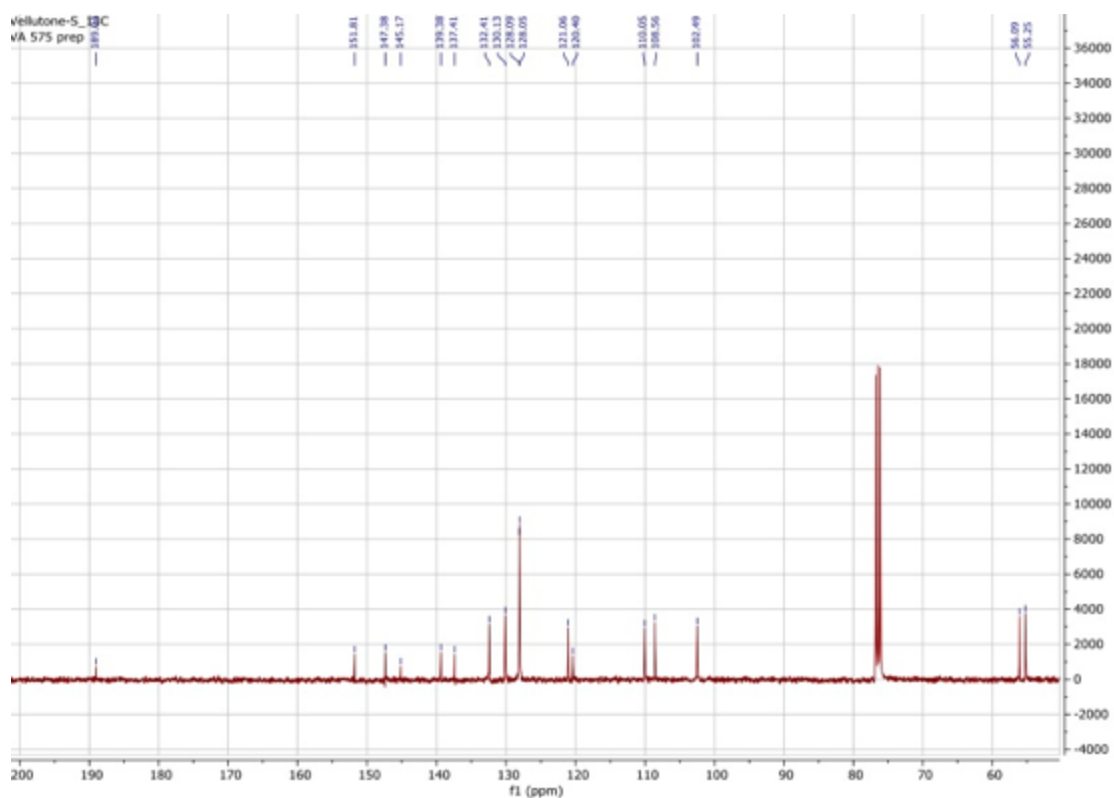
Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
309,1121	C ₁₉ H ₁₇ O ₄	18,7690501150057	11,5	-0,21	309,11214	1	95,49	4	4	99,75	98,82
331,0937	C ₁₉ H ₁₆ O ₄ ²³ Na	12,9725080889243	11,5	-1,02	331,09408	7	93,67	2	6	98,15	97,22

6-VF_CIGSPP-UniFe_DDA_027 #2184 RT: 10.14 AV: 1 NL: 1.30E+008
T: FTMS + c ESI d Full ms2 309.1120@hcd36.00 [50.0000-335.0000]

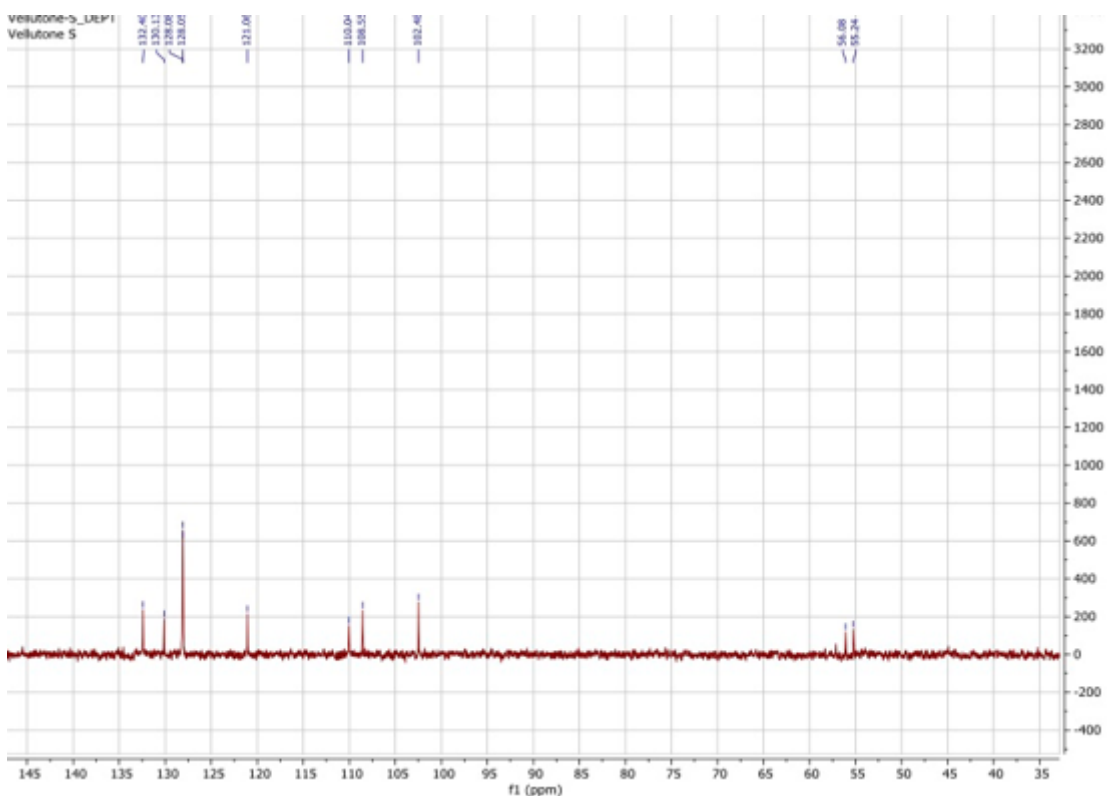


(*E*)-3-(4,7-dimethoxybenzofuran-2-yl)-1-phenylprop-2-en-1-one (22)





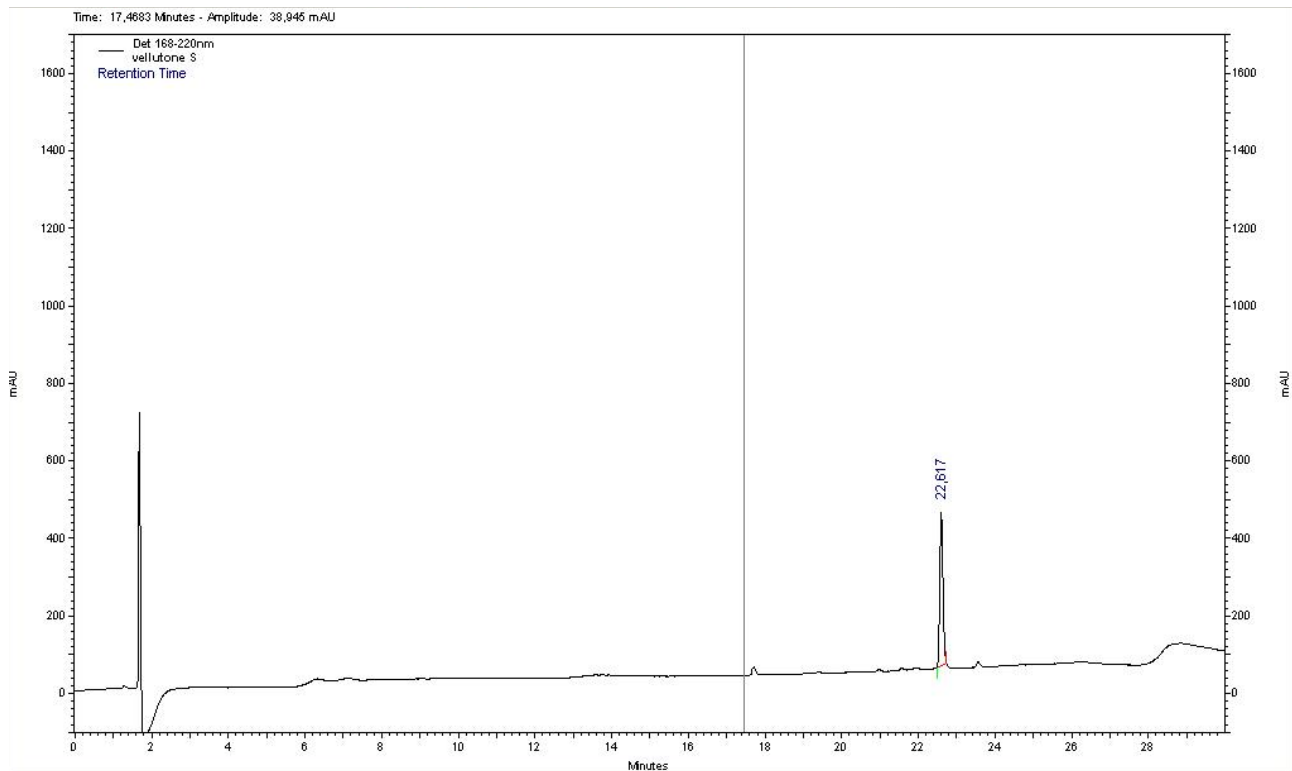
^{13}C NMR (101 MHz, Chloroform-d) δ 189.04, 151.81, 147.38, 145.17, 139.38, 137.41, 132.41, 130.13, 128.09, 128.05, 121.06, 120.40, 110.05, 108.56, 102.49, 56.09, 55.25.



^{13}C NMR (101 MHz, Chloroform-d) δ 132.40, 130.13, 128.08, 128.05, 121.06, 110.04, 108.55, 102.48, 56.08, 55.24.

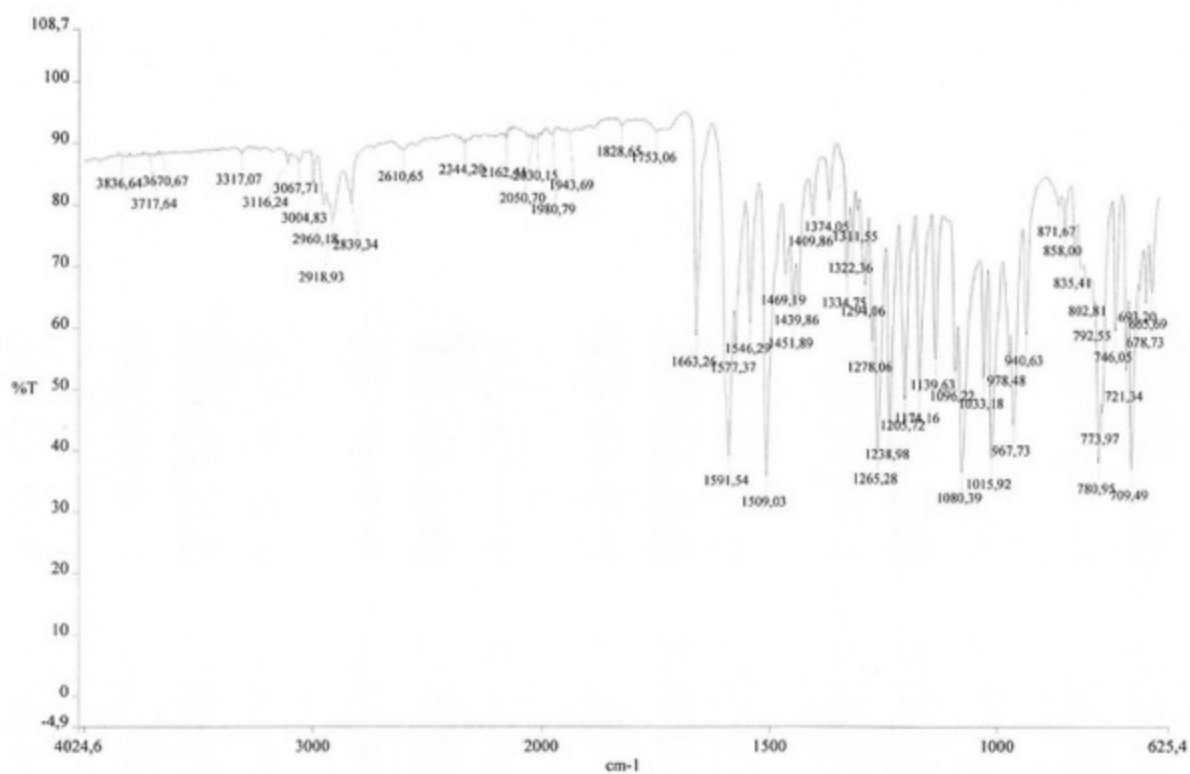
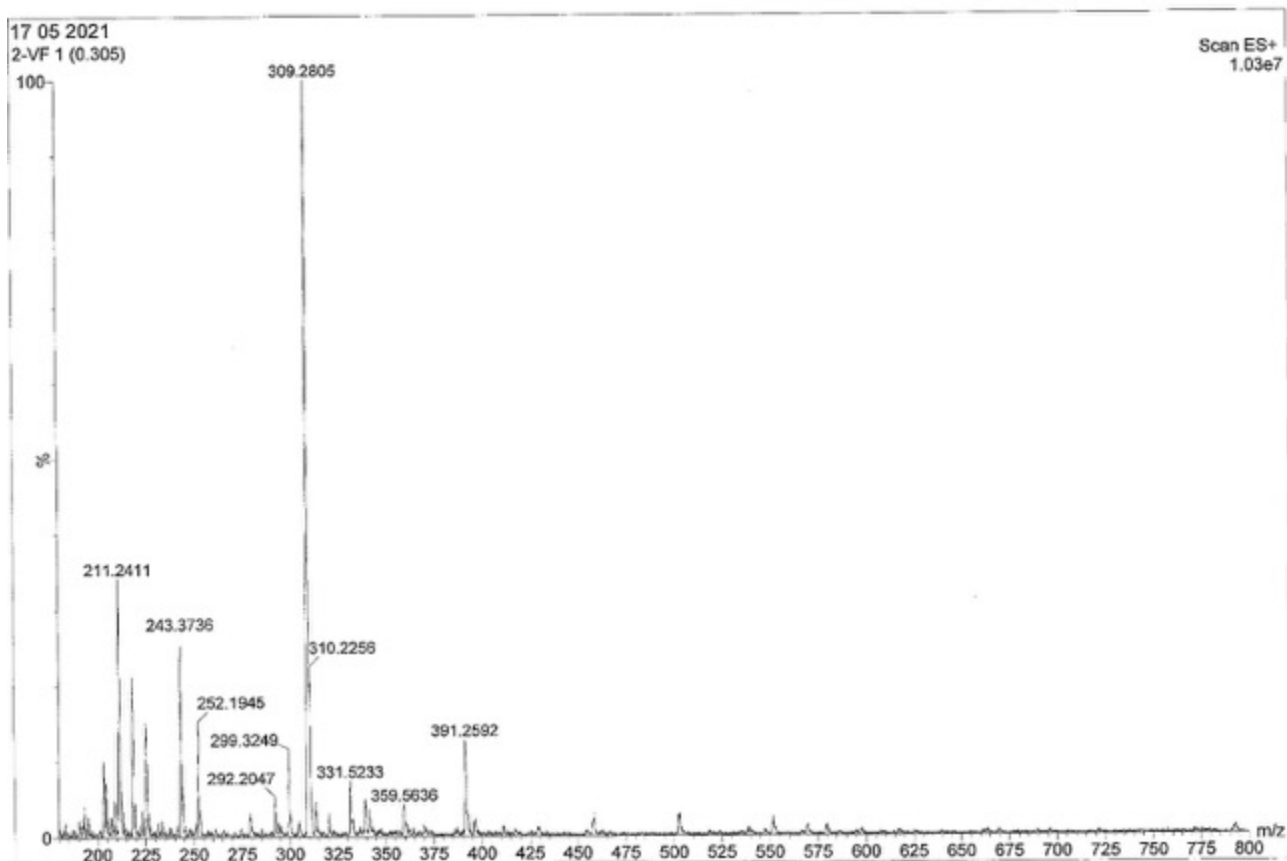
Area % Report

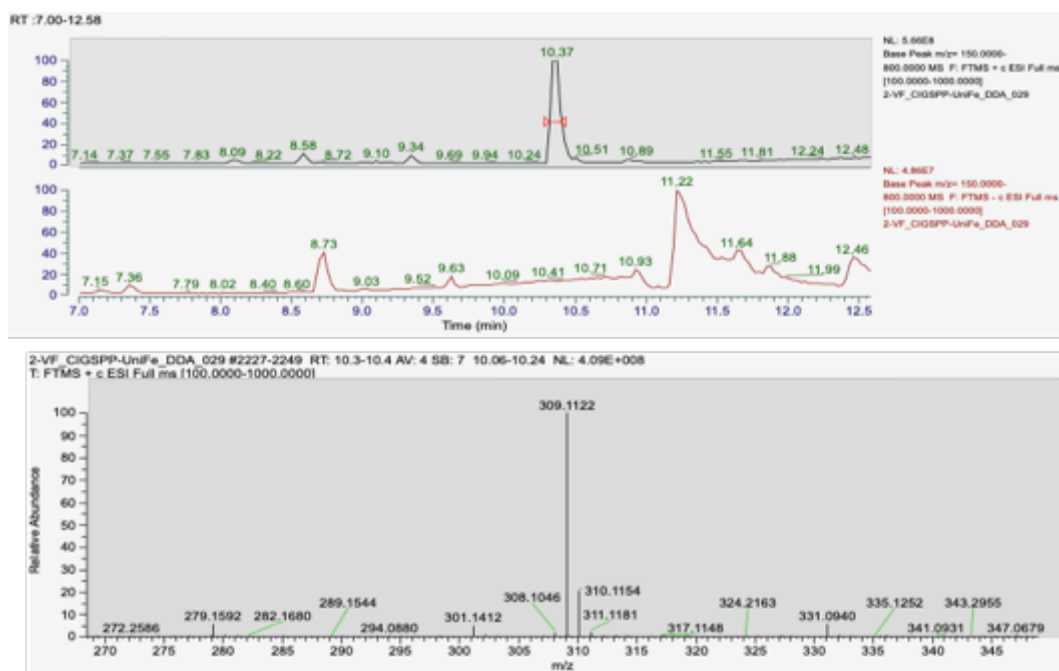
Data File: C:\32Karat\Projects\Default\Data\delia\Martina\vellutone S.dat
 Method: C:\32Karat\Projects\Default\Method\standard 0.7 ml.met
 Acquired: 15/04/2021 15.58.12
 Printed: 04/08/2022 13.12.03



**Det 168-220nm
Results**

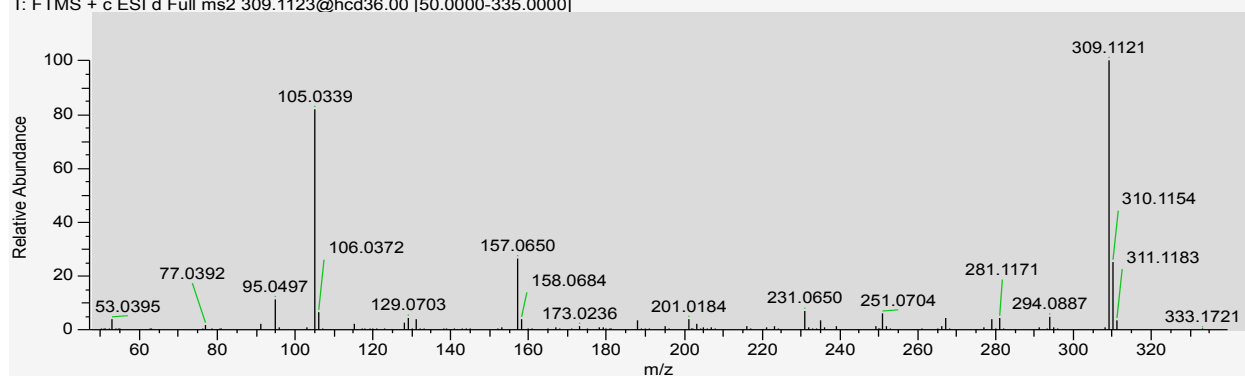
Time	Area	Area %	Height	Height %
22,617	2249606	100,00	392360	100,00
Totals	2249606	100,00	392360	100,00



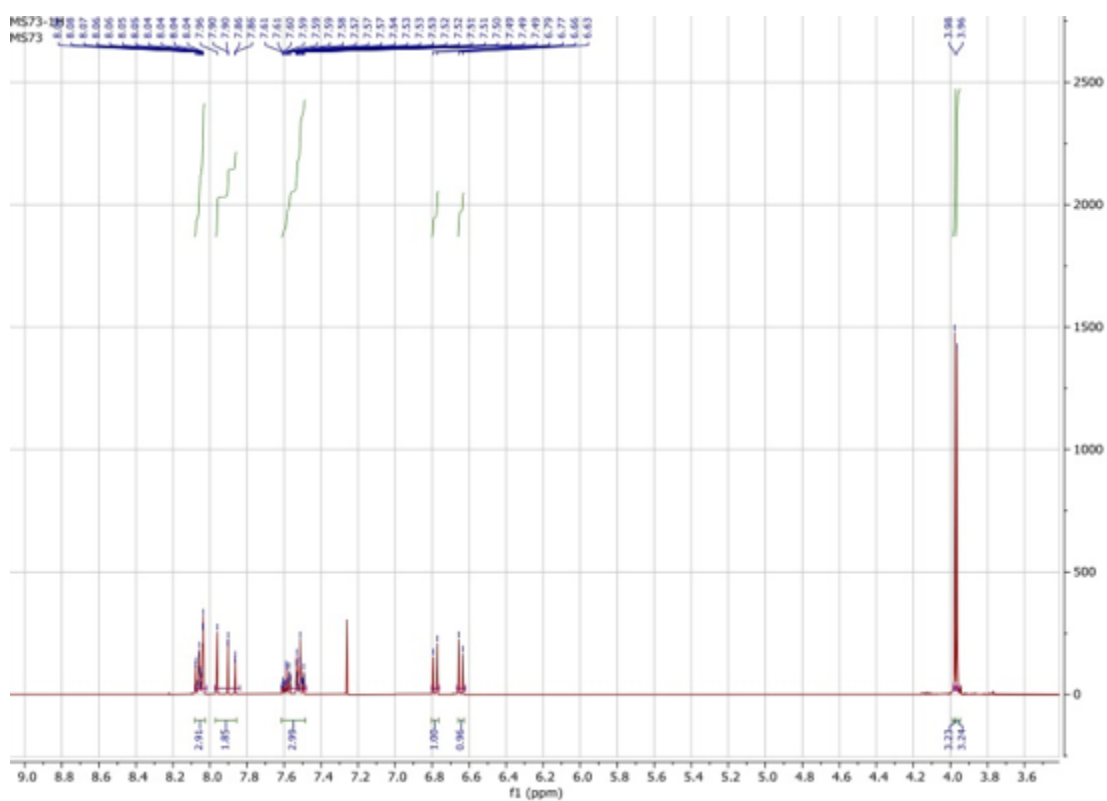
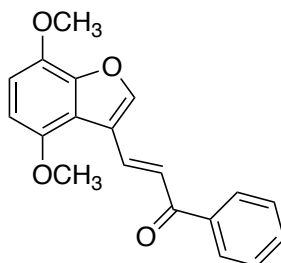


Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
309,1122	C ₁₉ H ₁₇ O ₄	25,1421183814927	11,5	0,19	309,11214	1	95,94	4	4	99,87	98,96
331,094	C ₁₉ H ₁₆ O ₄ ²³ Na	17,8402298795552	11,5	-0,37	331,09408	3	95,07	3	5	99,37	98,83

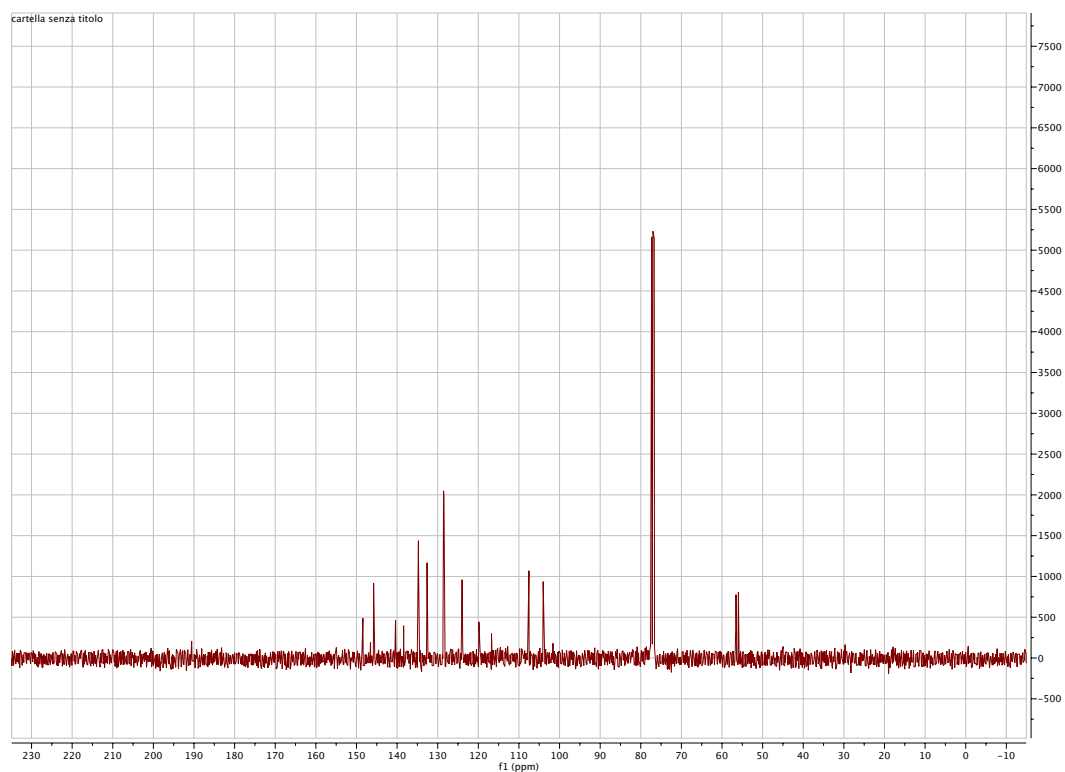
2-VF_CIGSPP-UniFe_DDA_029 #2233 RT: 10.33 AV: 1 NL: 3.71E+007
 T: FTMS + c ESI d Full ms2 309.1123@hcd36.00 [50.0000-335.0000]



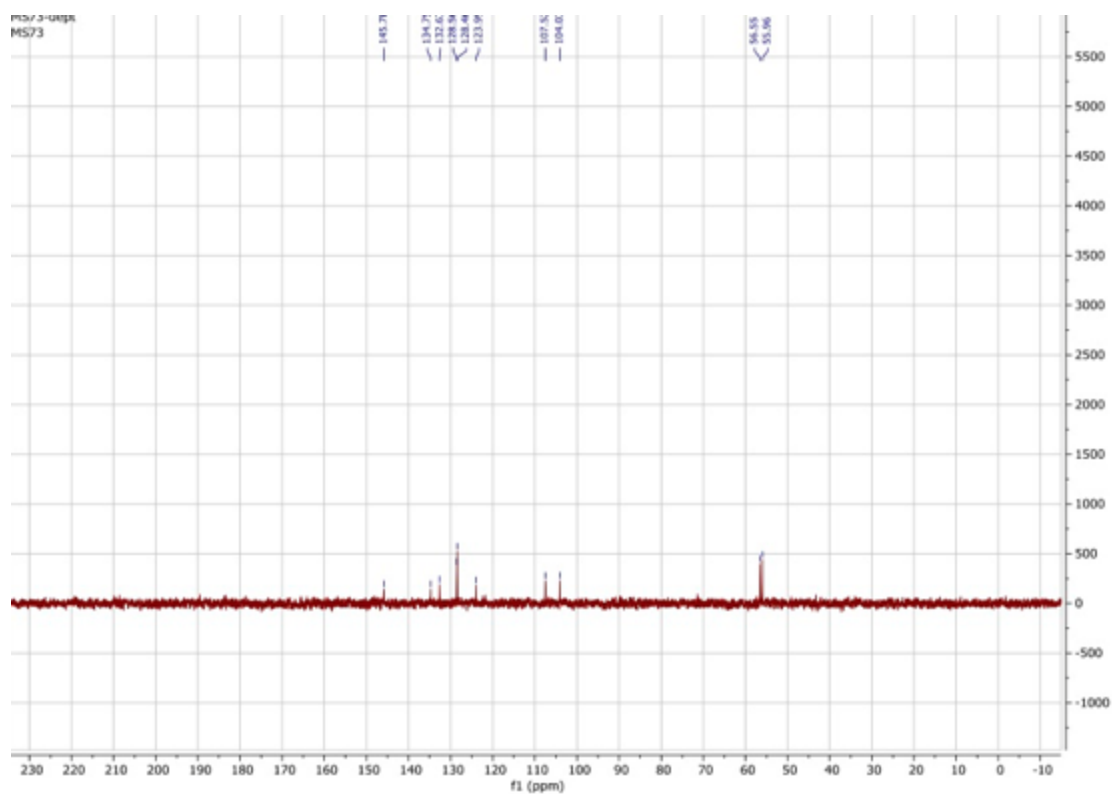
(*E*)-3-(4,7-dimethoxybenzofuran-3-yl)-1-phenylprop-2-en-1-one (28)



^1H NMR (400 MHz, Chloroform-*d*) δ 8.08 – 8.02 (m, 3H), 7.97 – 7.84 (m, 2H), 7.61 – 7.48 (m, 3H), 6.78 (d, J = 8.6 Hz, 1H), 6.65 (d, J = 8.7 Hz, 1H), 3.98 (s, 3H), 3.96 (s, 3H).



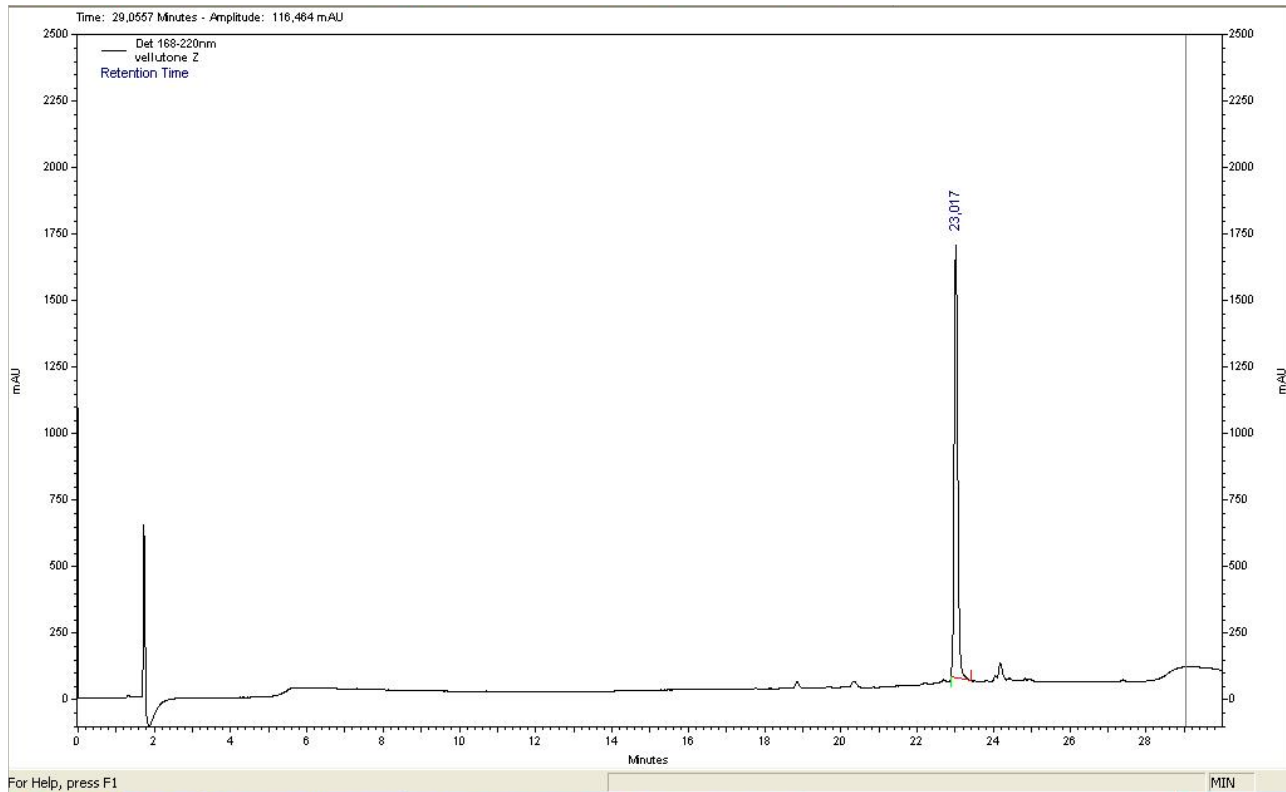
^{13}C NMR (101 MHz, Chloroform-d) δ 190.58, 148.41, 146.56, 145.78, 140.38, 138.38, 134.75, 132.62, 128.56, 128.46, 124.00, 119.85, 116.75, 107.53, 104.04, 56.56, 55.96.



^{13}C NMR (101 MHz, Chloroform-d) δ 145.78, 134.75, 132.63, 128.56, 128.46, 123.99, 107.52, 104.03, 56.55, 55.96.

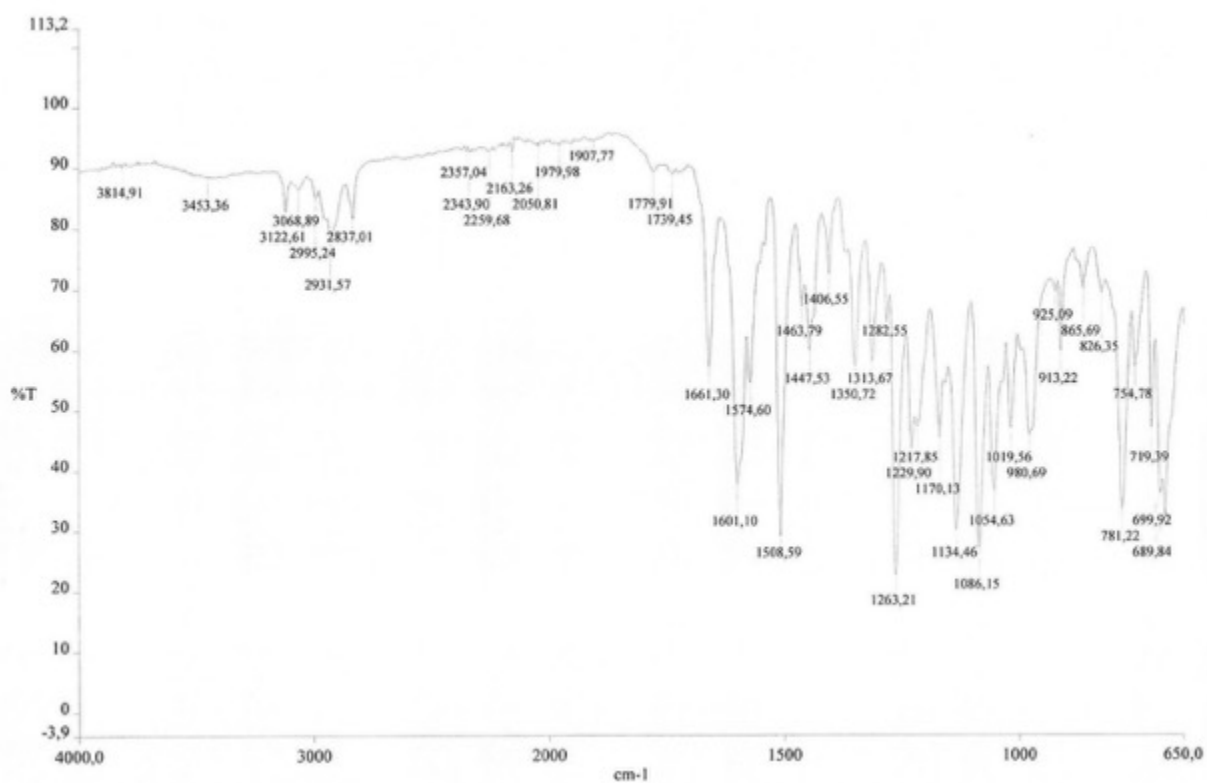
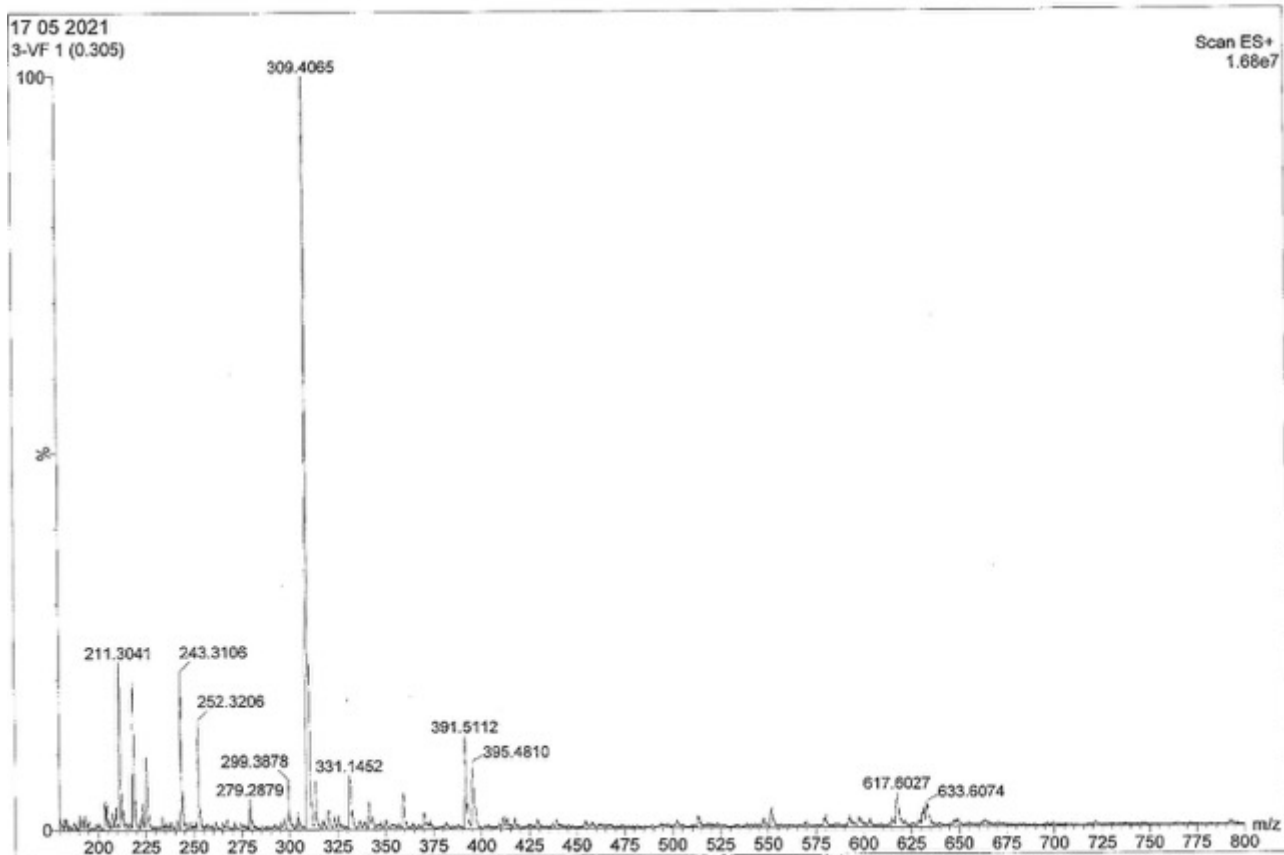
Area % Report

Data File: C:\32Karat\Projects\Default\Data\delia\Martina\vellutone Z.dat
 Method: C:\32Karat\Projects\Default\Method\standard 0.7 ml.met
 Acquired: 16/04/2021 8.50.00
 Printed: 04/08/2022 13.22.32

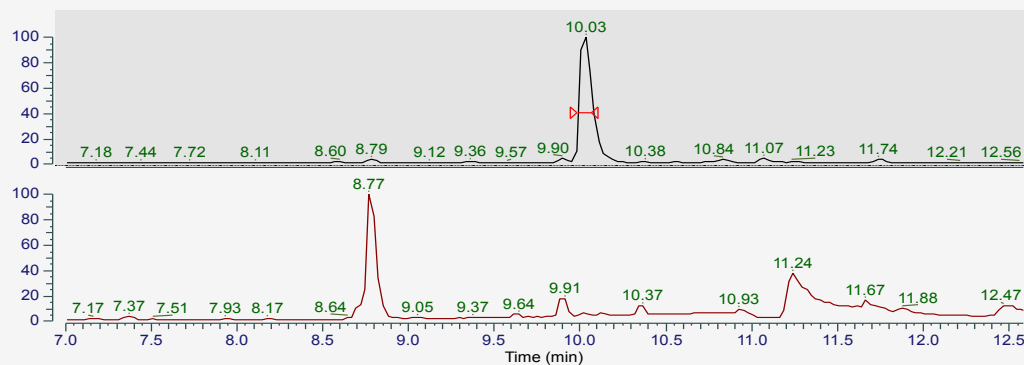


Det 168-220nm Results

Time	Area	Area %	Height	Height %
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Totals	10467135	100,00	1624633	100,00



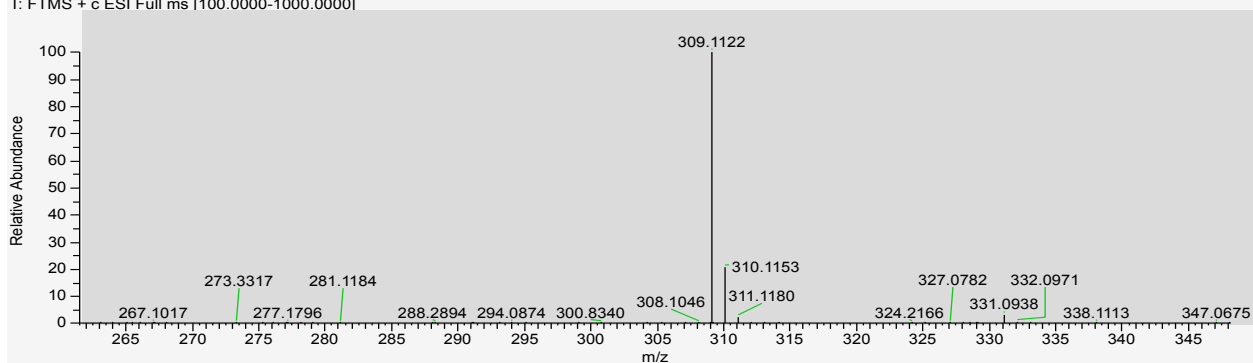
RT :7.00-12.58



NL: 4.88E9
Base Peak m/z= 150.0000-
800.0000 MS F: FTMS + c ESI Full ms
[100.0000-1000.0000]
3-VF_CIGSPP-UniFe_DDA_030

NL: 1.33E8
Base Peak m/z= 150.0000-
800.0000 MS F: FTMS - c ESI Full ms
[100.0000-1000.0000]
3-VF_CIGSPP-UniFe_DDA_030

3-VF_CIGSPP-UniFe_DDA_030 #2158-2183 RT: 9.97-10.08 AV: 5 SB: 5 9.81-9.94 NL: 2.93E9
T: FTMS + c ESI Full ms [100.0000-1000.0000]



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
309,1122	C ₁₉ H ₁₇ O ₄	23,7200377676601	11,5	0,2	309,11214	1	95,94	4	4	99,96	98,96
331,0938	C ₁₉ H ₁₆ O ₄ ^{2,3} Na	15,094285170234	11,5	-0,81	331,09408	5	93,79	2	5	98,16	97,31