

## Differential production of phytotoxins from *Phomopsis* sp. from grapevine plants showing esca symptoms.

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# HRESI MS of phomopsolide B (1)



FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

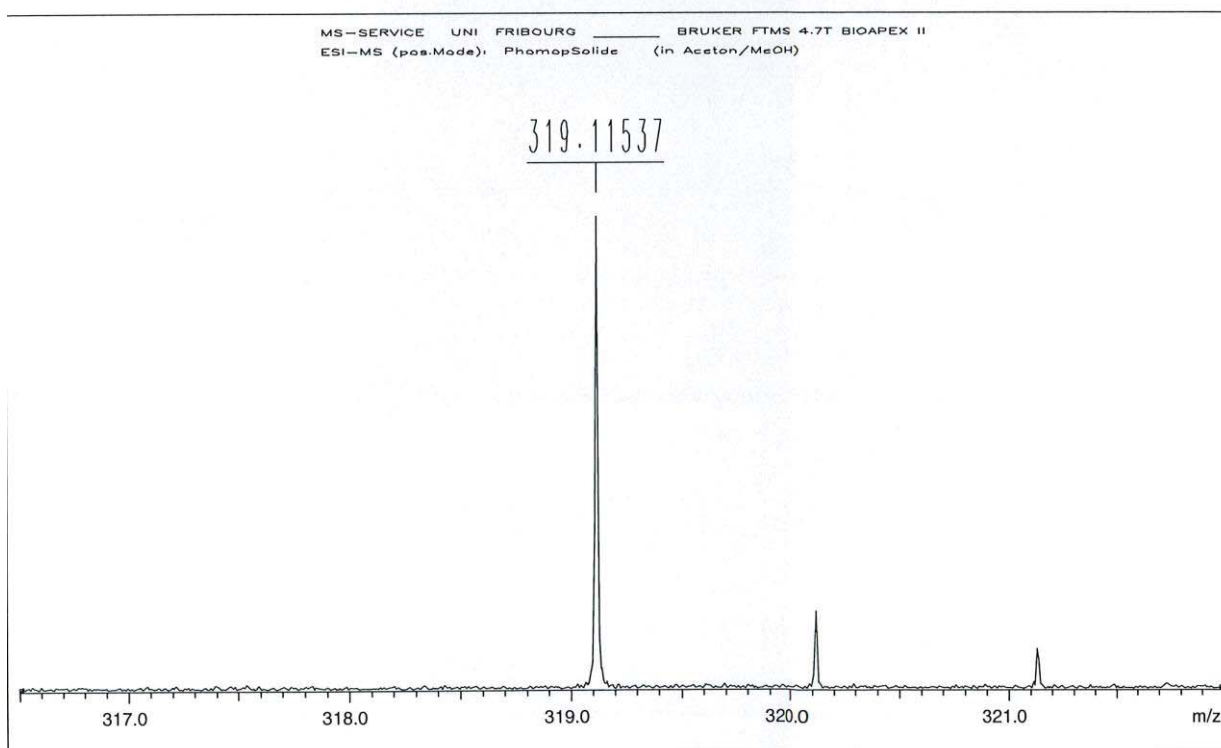
ESI-MS: PhomopSolide

XMASS Mass Analysis for /Data/UNI\_NE/ABOU1325\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 319.1153690

Charge = +1

#	C	H	O	Na	mass	DBE	error
*** Mass Analysis for mass 319.1153690							
1	15	20	6	1	319.1152095	5.5	1.595e-04
2	17	19	6	0	319.1176148	8.5	2.246e-03
3	24	15	1	0	319.1117415	17.5	3.627e-03
4	22	16	1	1	319.1093362	14.5	6.033e-03
5	10	23	11	0	319.1234880	-0.5	8.119e-03
6	13	19	9	0	319.1023586	4.5	1.301e-02
7	19	20	3	1	319.1304656	9.5	1.510e-02
8	11	20	9	1	319.0999533	1.5	1.542e-02
9	21	19	3	0	319.1328709	12.5	1.750e-02
10	20	15	4	0	319.0964854	13.5	1.888e-02



# HRESI MS of Phomopsolidone A (2)



FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

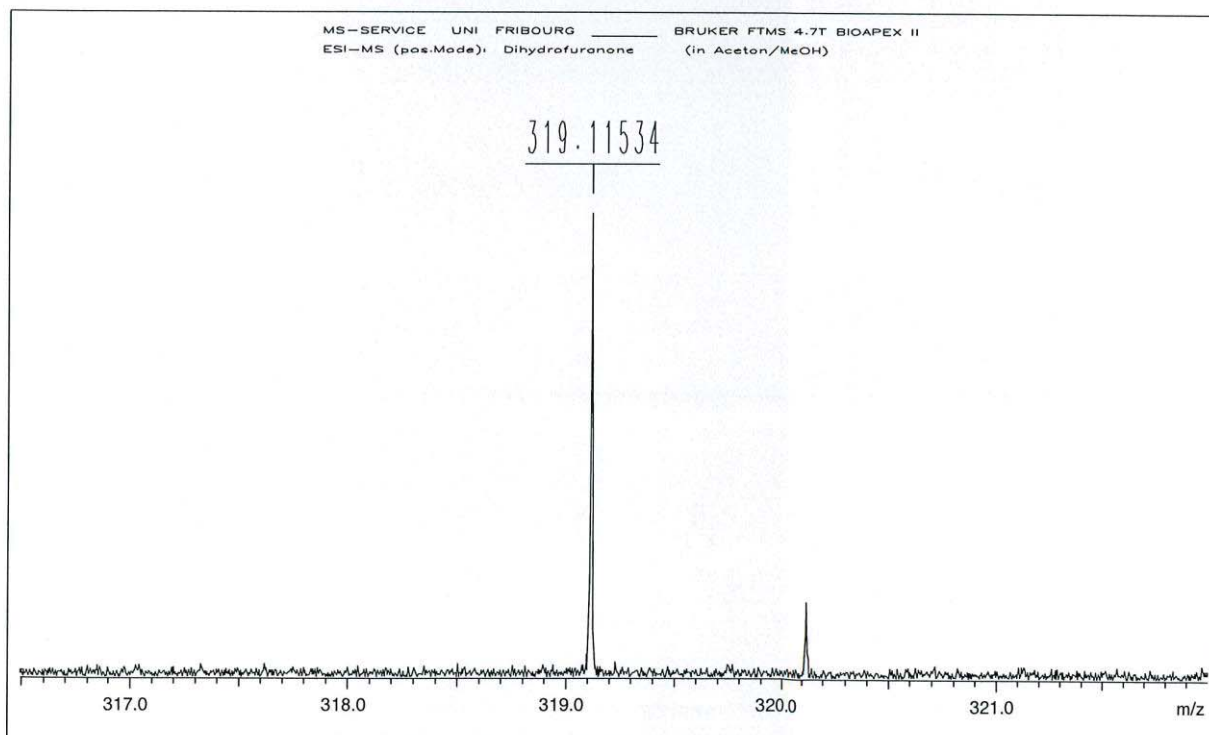
ESI-MS: Dihydrofuranone

XMASS Mass Analysis for /Data/UNI\_NE/ABOU1326\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

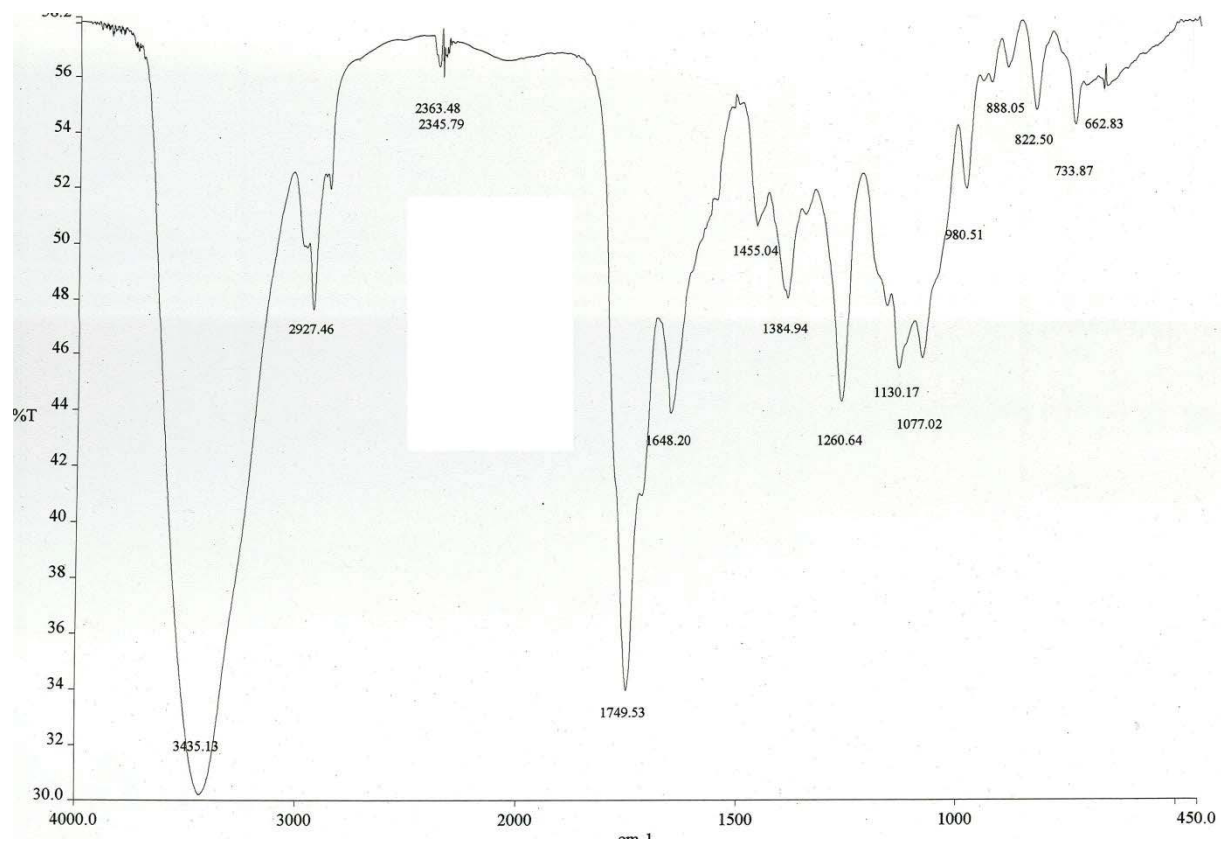
Ion mass = 319.1153360

Charge = +1

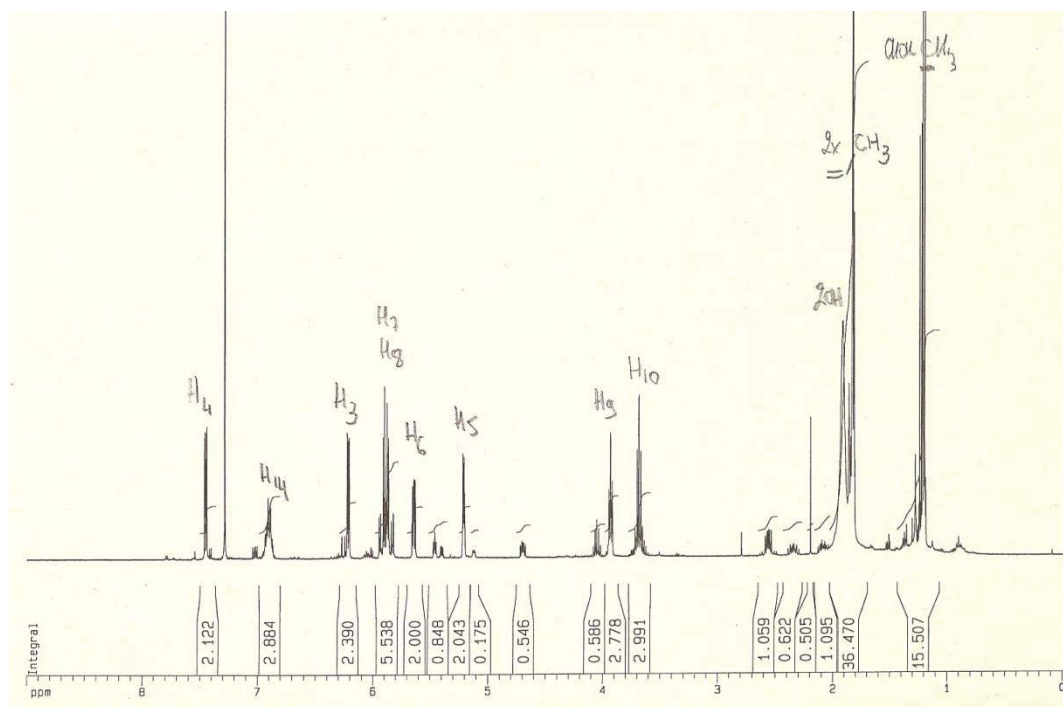
#	C	H	O	Na	mass	DBE	error
*** Mass Analysis for mass 319.1153360							
1	15	20	6	1	319.1152095	5.5	1.265e-04
2	17	19	6	0	319.1176148	8.5	2.279e-03
3	24	15	1	0	319.1117415	17.5	3.594e-03
4	22	16	1	1	319.1093362	14.5	6.000e-03
5	10	23	11	0	319.1234880	-0.5	8.152e-03
6	13	19	9	0	319.1023586	4.5	1.298e-02
7	19	20	3	1	319.1304656	9.5	1.513e-02
8	11	20	9	1	319.0999533	1.5	1.538e-02
9	21	19	3	0	319.1328709	12.5	1.753e-02
10	20	15	4	0	319.0964854	13.5	1.885e-02



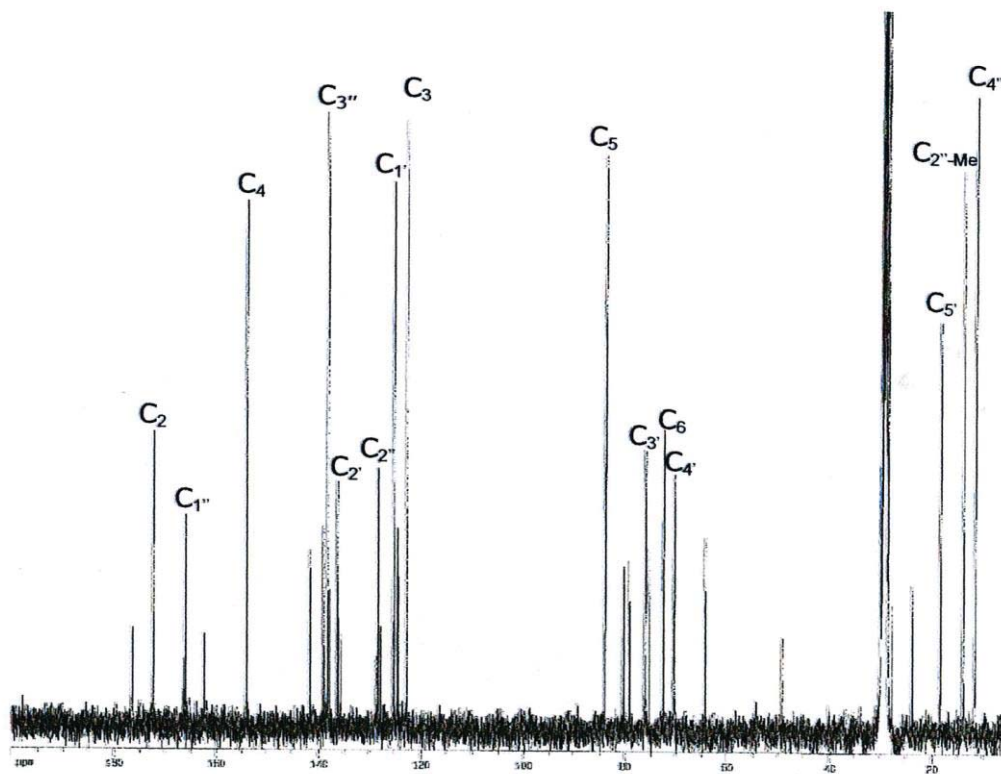
# IR spectra of phomopsolidone A (2)



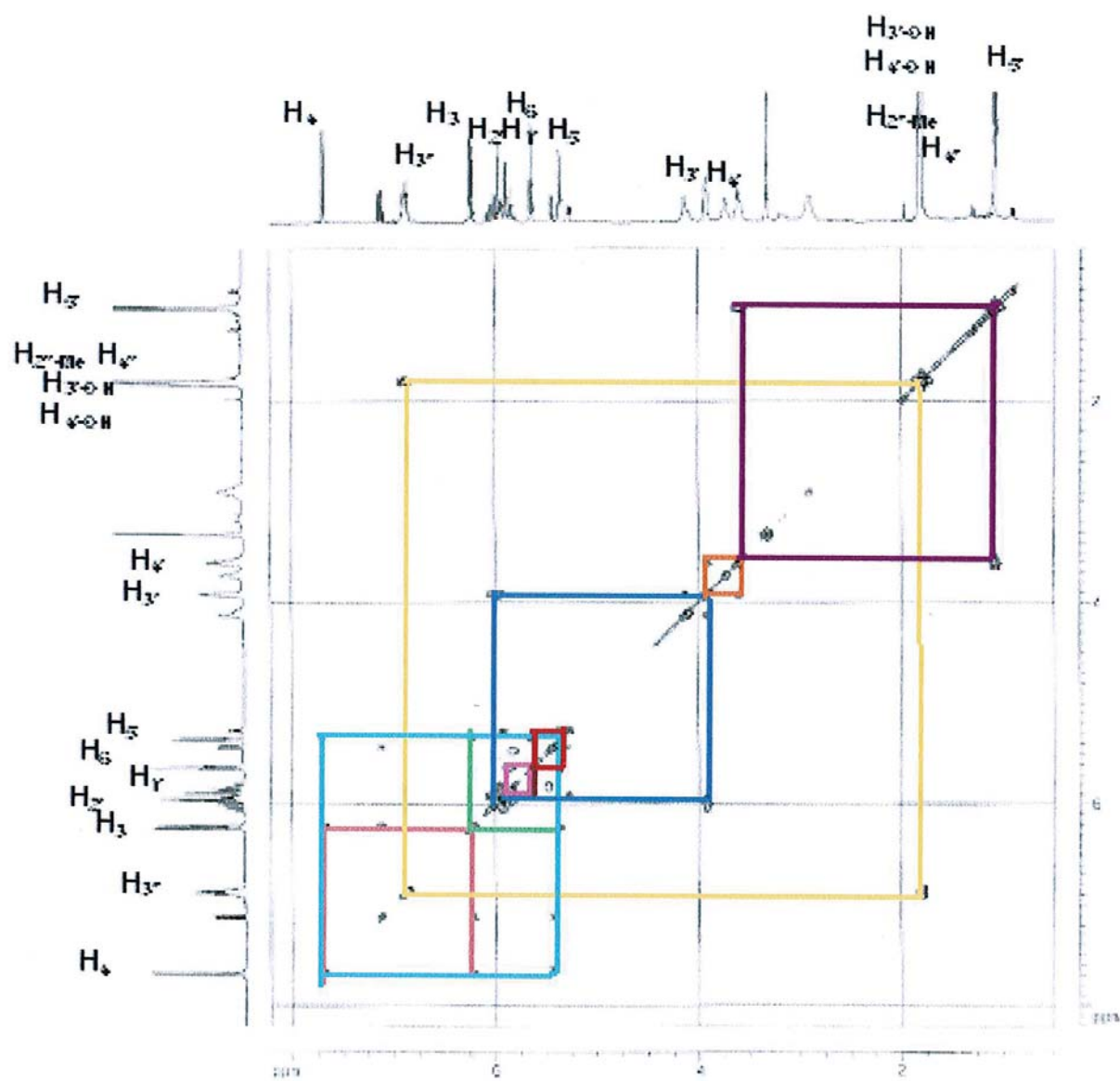
### **<sup>1</sup>H NMR of phomopsolidone A (2)**



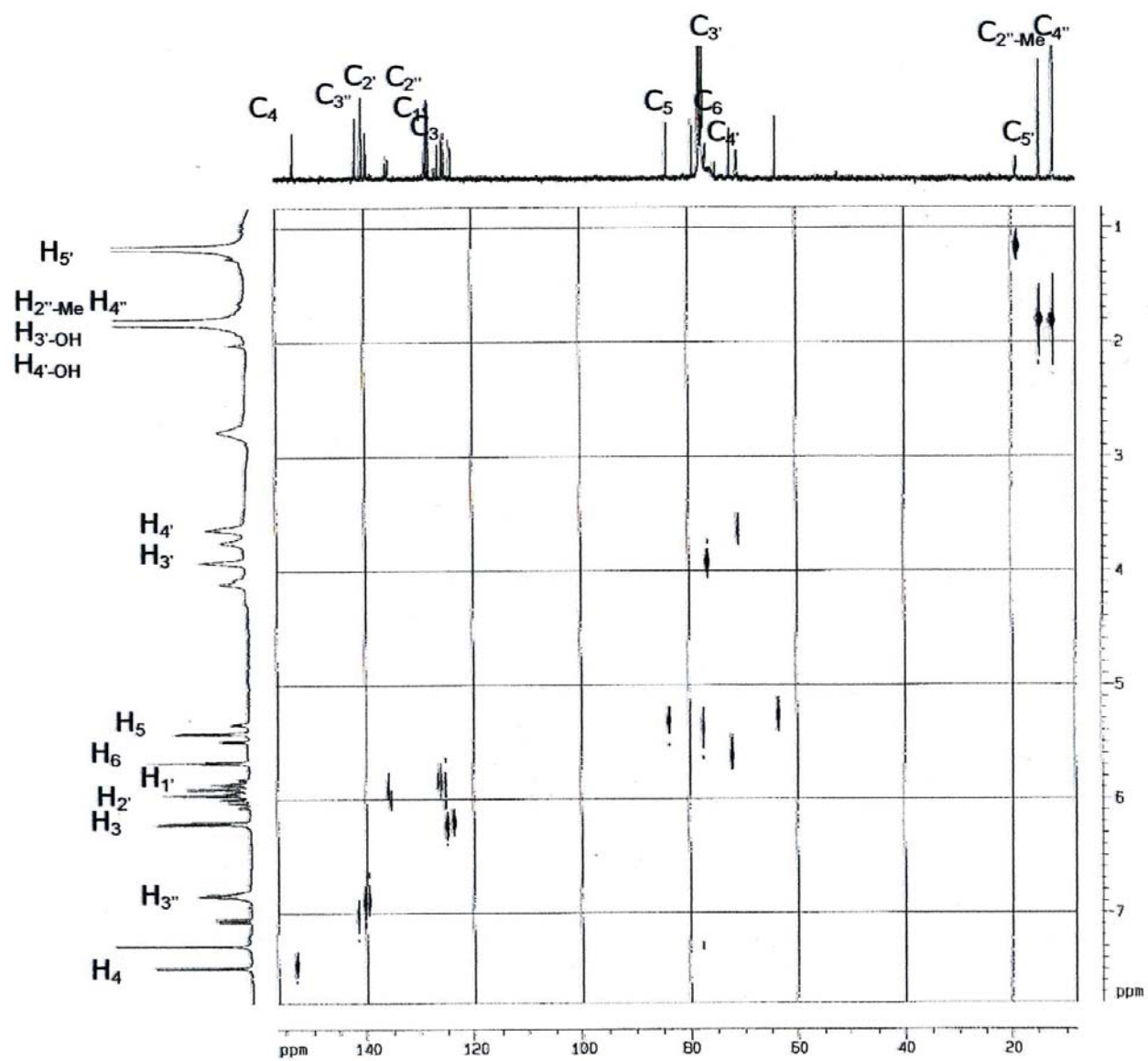
### **<sup>13</sup>C NMR of phomopsolidone A (2)**



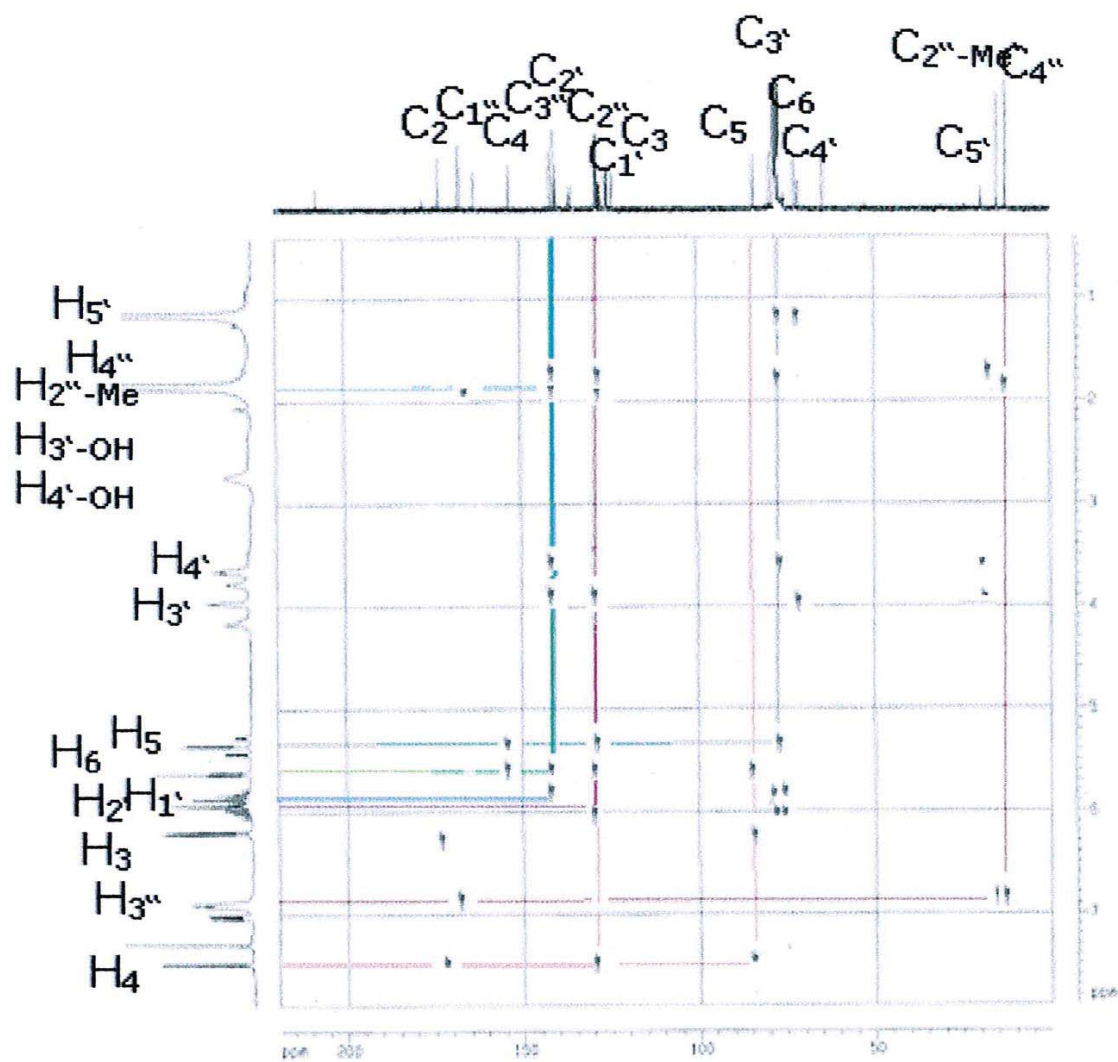
COSY of phomopsolidone A (2)



# HSQC ( $^1\text{H}$ - $^{13}\text{C}$ ) of phomopsolidone A (2)



HMBC ( $^1\text{H}$ - $^{13}\text{C}$ ) of phomopsolidone A (2)





# HR ESI MS of phomopsolidone B (3)



FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

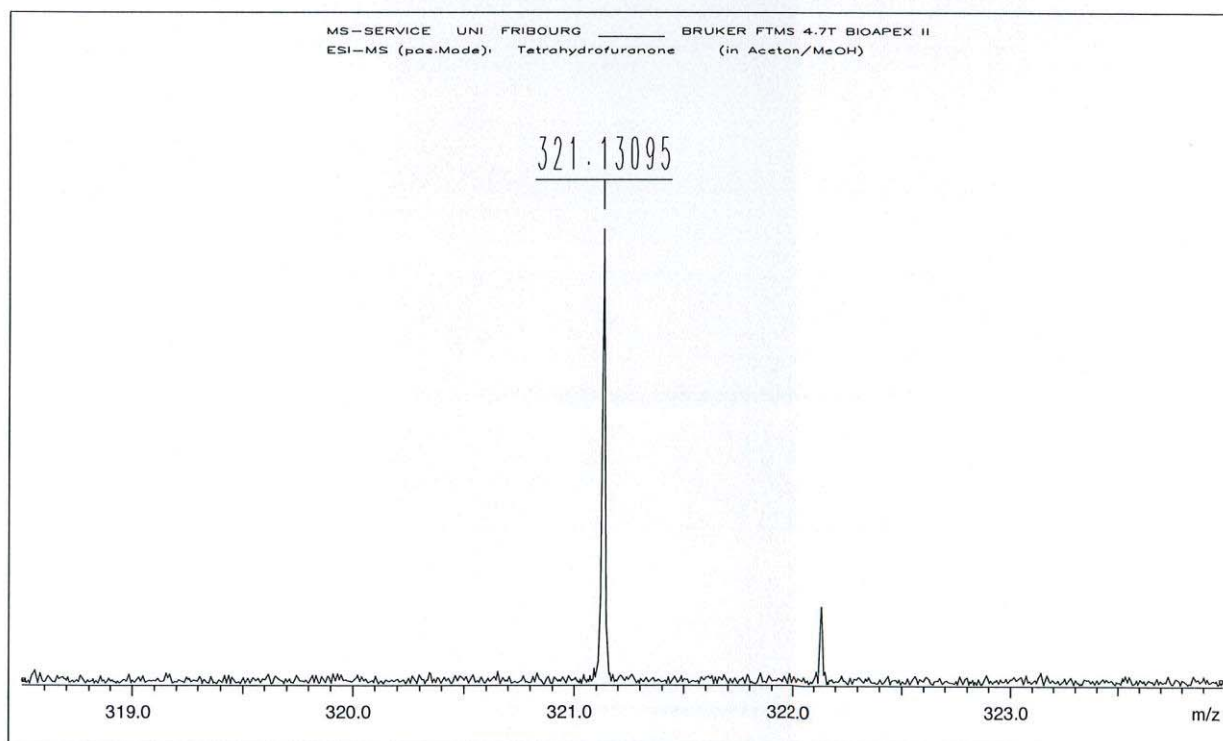
ESI-MS: Tetrahydrofuranone

XMASS Mass Analysis for /Data/UNI\_NE/ABOU1327\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

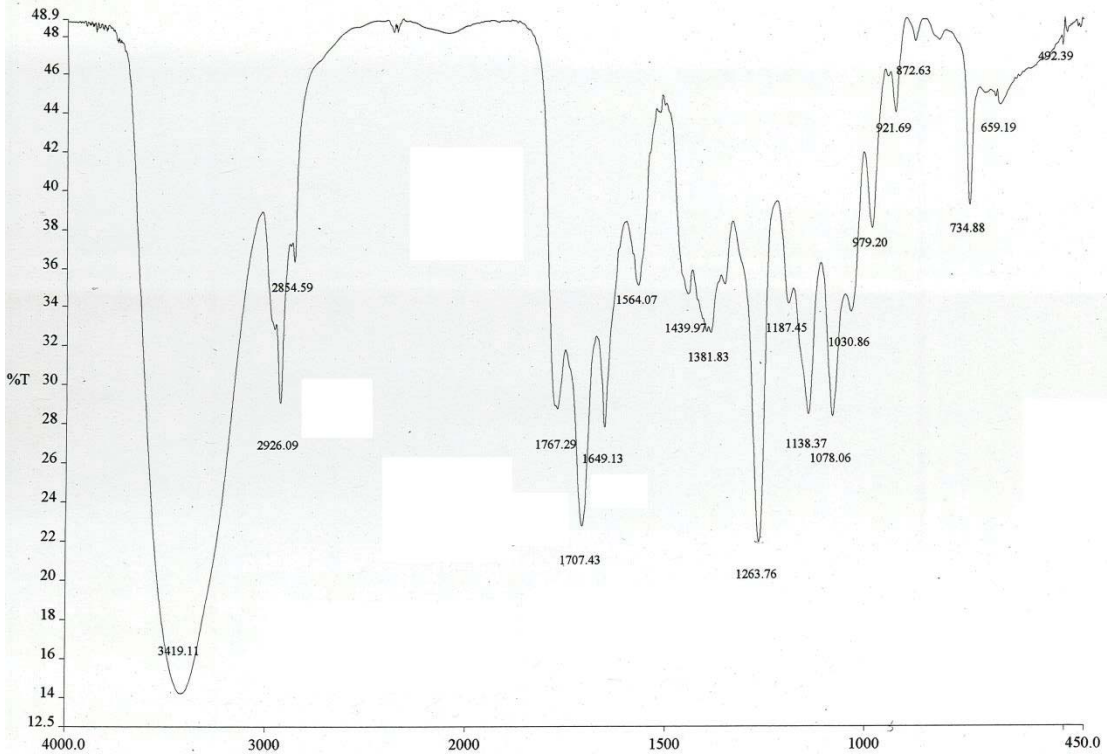
Ion mass = 321.1309550

Charge = +1

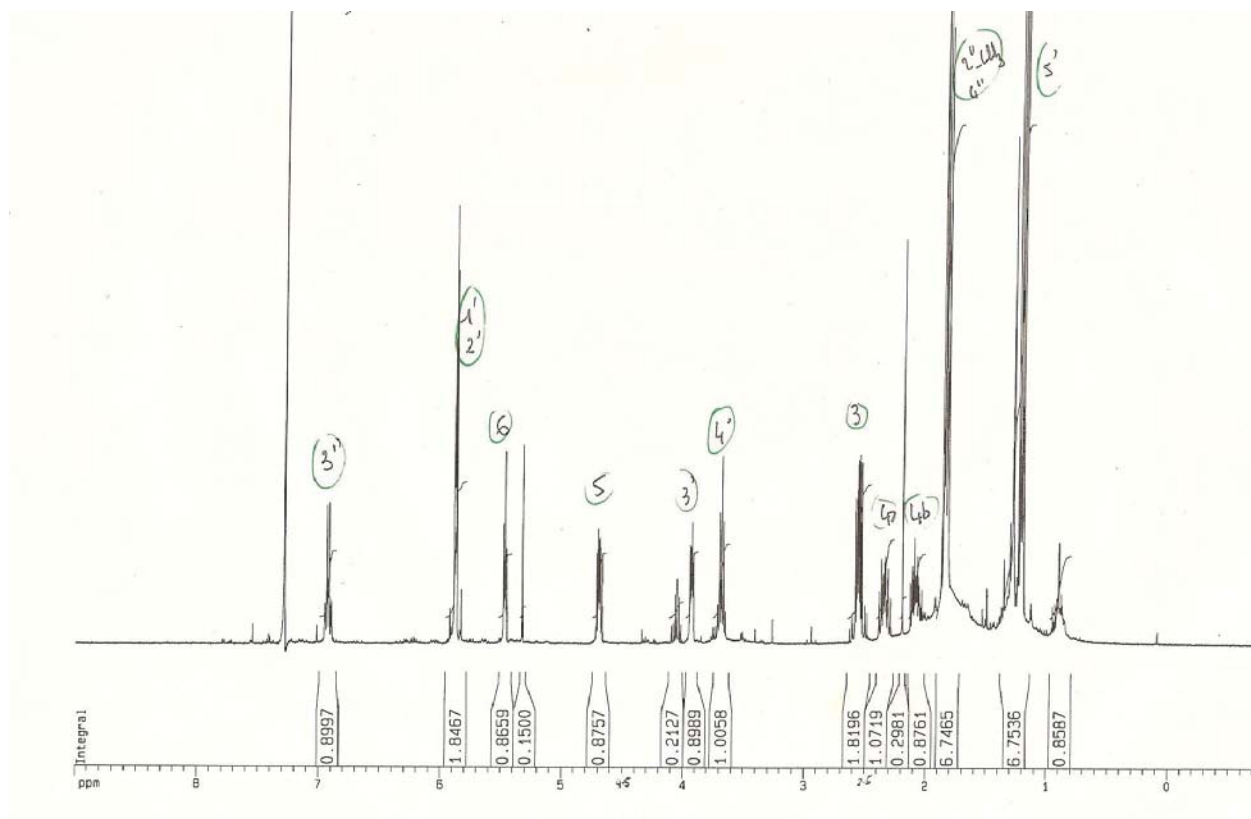
#	C	H	O	Na	mass	DBE	error
*** Mass Analysis for mass 321.1309550							
1	15	22	6	1	321.1308595	4.5	9.547e-05
2	17	21	6	0	321.1332648	7.5	2.310e-03
3	24	17	1	0	321.1273916	16.5	3.563e-03
4	22	18	1	1	321.1249863	13.5	5.969e-03
5	10	25	11	0	321.1391381	-1.5	8.183e-03
6	13	21	9	0	321.1180087	3.5	1.295e-02
7	19	22	3	1	321.1461157	8.5	1.516e-02
8	11	22	9	1	321.1156034	0.5	1.535e-02
9	21	21	3	0	321.1485210	11.5	1.757e-02
10	20	17	4	0	321.1121355	12.5	1.882e-02



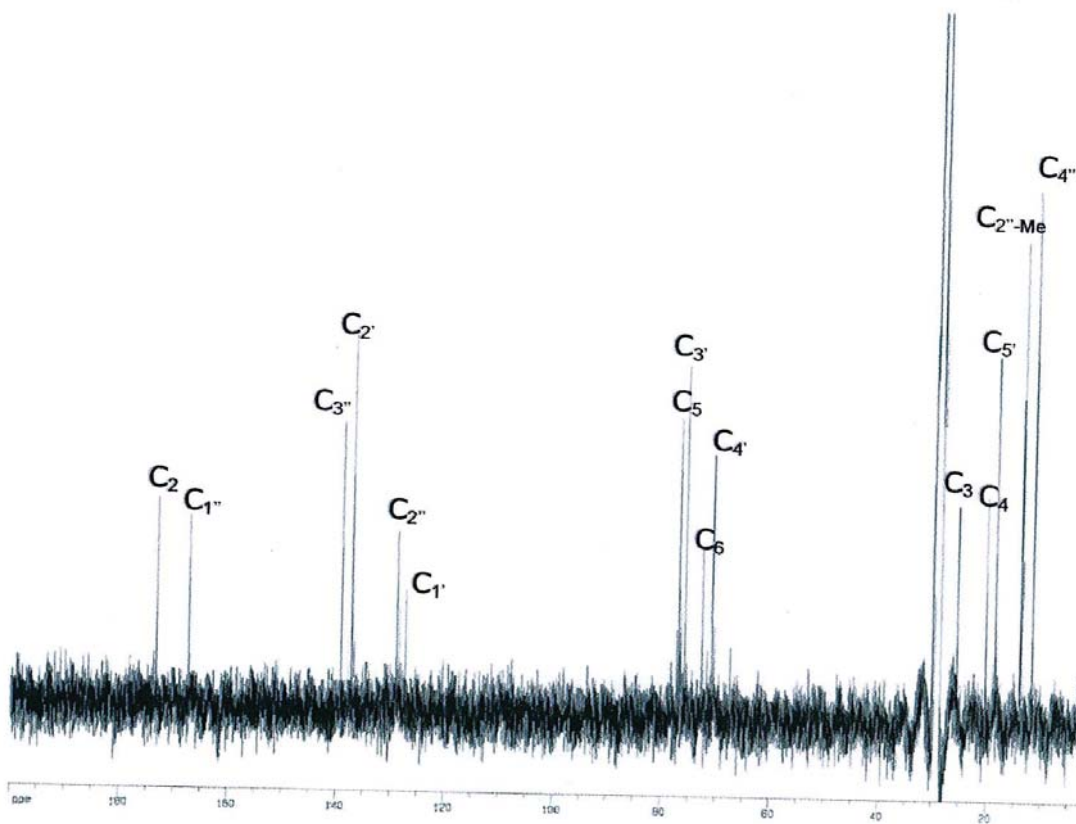
# IR spectra of phomopsolidone B (3)



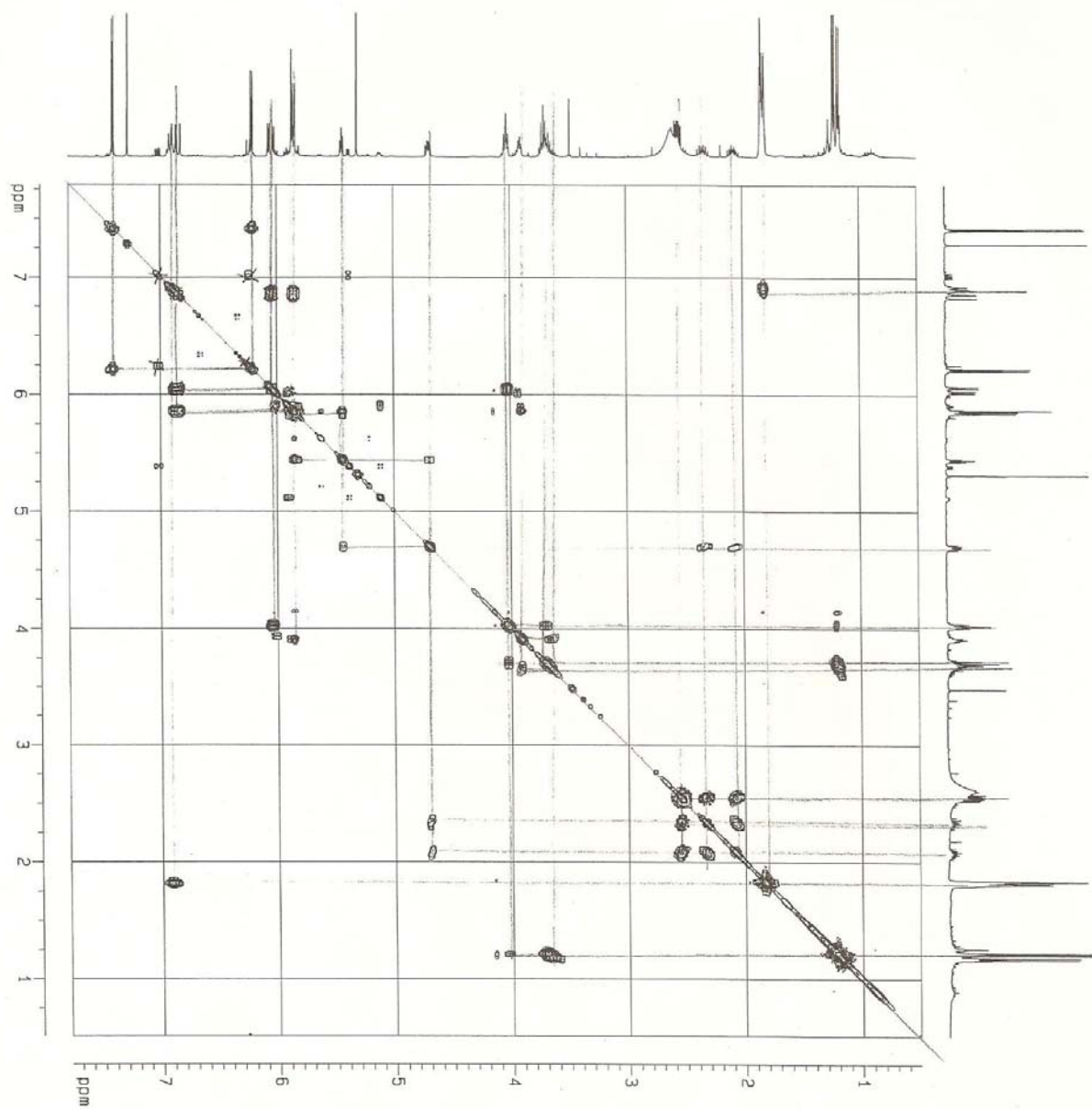
### $^1\text{H}$ NMR of phomopsolidone B (3)



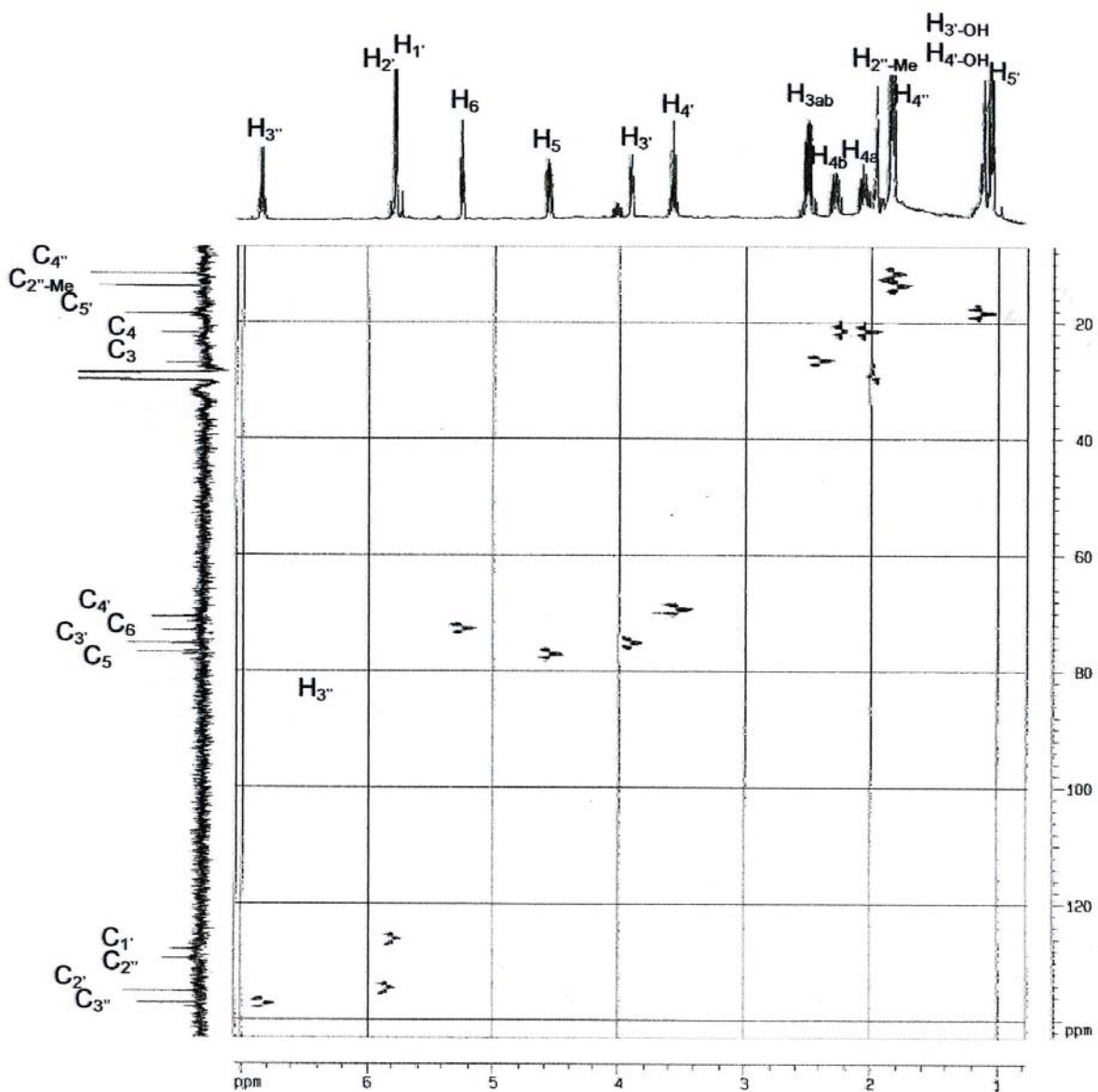
### $^{13}\text{C}$ NMR of phomopsolidone B (3)



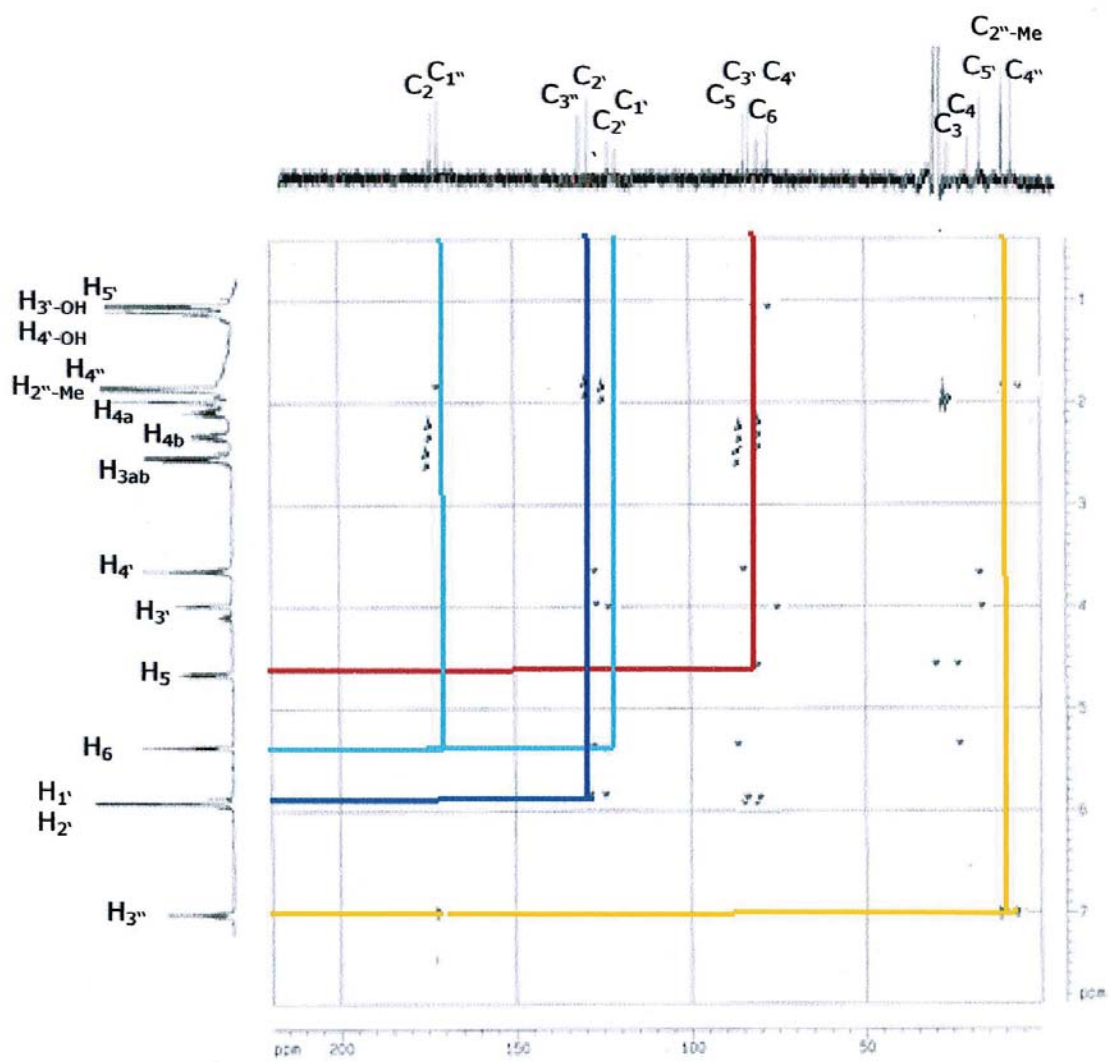
COSY of phomopsilidone B (3)



# HSQC of phomopsolidone B (3)

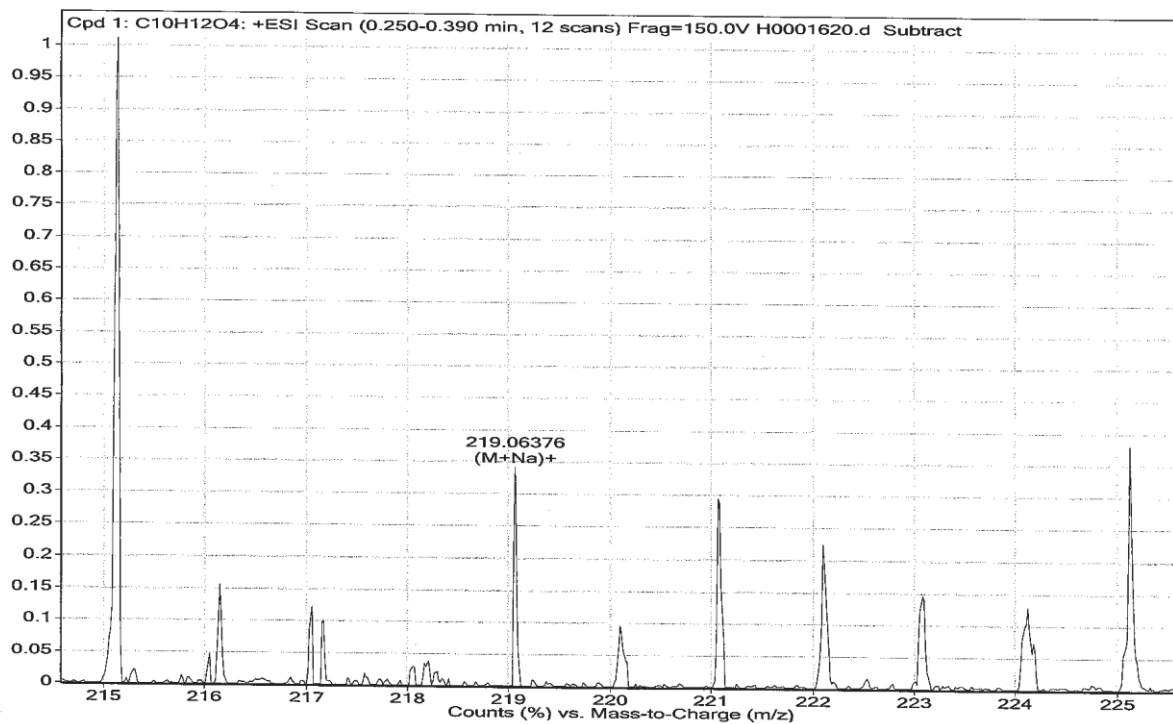


# HMBC phomopsolidone B (3)



# HRESI MS of Phomopsolidones C (4) and D (5)

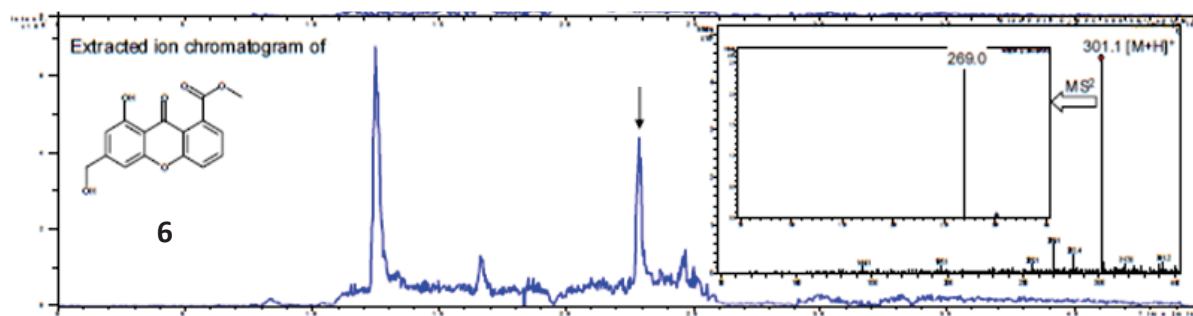
Sample Name	Furanone	Position	Vial 51	Instrument Name	Instrument 1	User Name	CJ
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	H0001620.d	ACQ Method	ESIPisoTOF1500.m	Comment	C10H12O4	Acquired Time	7/1/2014 5:15:15 PM



## MS Spectrum Peak List

<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
219.06376	219.06278	4.48	1	434	C10 H12 Na O4	(M+Na)+

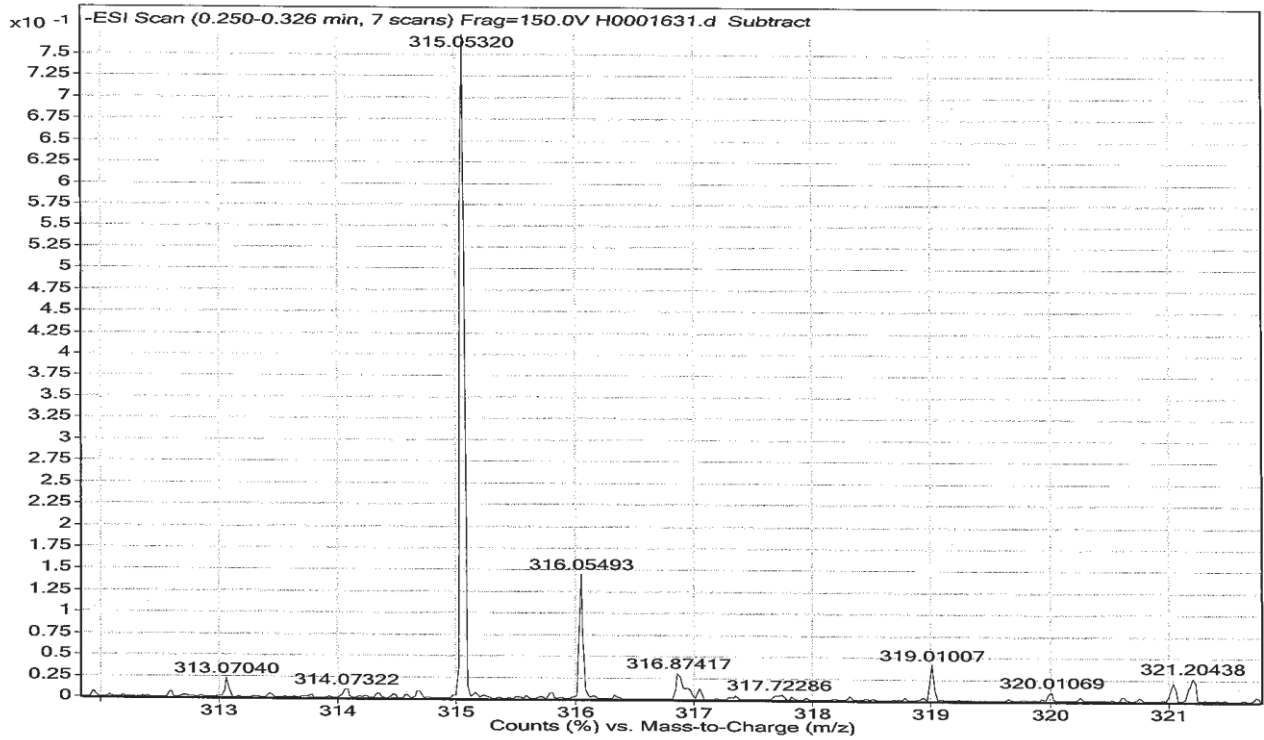
# ESI MS of sydowninin (6)





# HRESI MS of sydowninol (7)

Sample Name	Phomopsis Nicolas	Position	Vial 56	Instrument Name	Instrument 1	User Name	CJ
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	H0001631.d	ACQ Method	ESInIsoTOF1500.m	Comment	C16H12O6 ET C16H13O7	Acquired Time	7/4/2014 12:19:31 PM



# HRESI MS of Cytosporon B (8)



ESI-MS: CYTOSPORON

XMASS Mass Analysis for /Data/UNI\_NE/MANS2636\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 345.1674970

Charge = +1

#	C	H	O	Na	mass	DBE	error
*** Mass Analysis for mass 345.1674970							
1	18	26	5	1	345.1672450	5.5	2.520e-04
2	20	25	5	0	345.1696503	8.5	2.153e-03
3	13	29	10	0	345.1755236	-0.5	8.027e-03
4	16	25	8	0	345.1543942	4.5	1.310e-02
5	22	26	2	1	345.1825012	9.5	1.500e-02
6	14	26	8	1	345.1519889	1.5	1.551e-02
7	24	25	2	0	345.1849065	12.5	1.741e-02
8	23	21	3	0	345.1485210	13.5	1.898e-02
9	15	30	7	1	345.1883744	0.5	2.088e-02
10	21	22	3	1	345.1461157	10.5	2.138e-02

