ELECTRONIC SUPPORTING INFORMATION (ESI)

Chrysomycins A-C, antileukemic naphthocoumarins from *Streptomyces sporoverrucosus*

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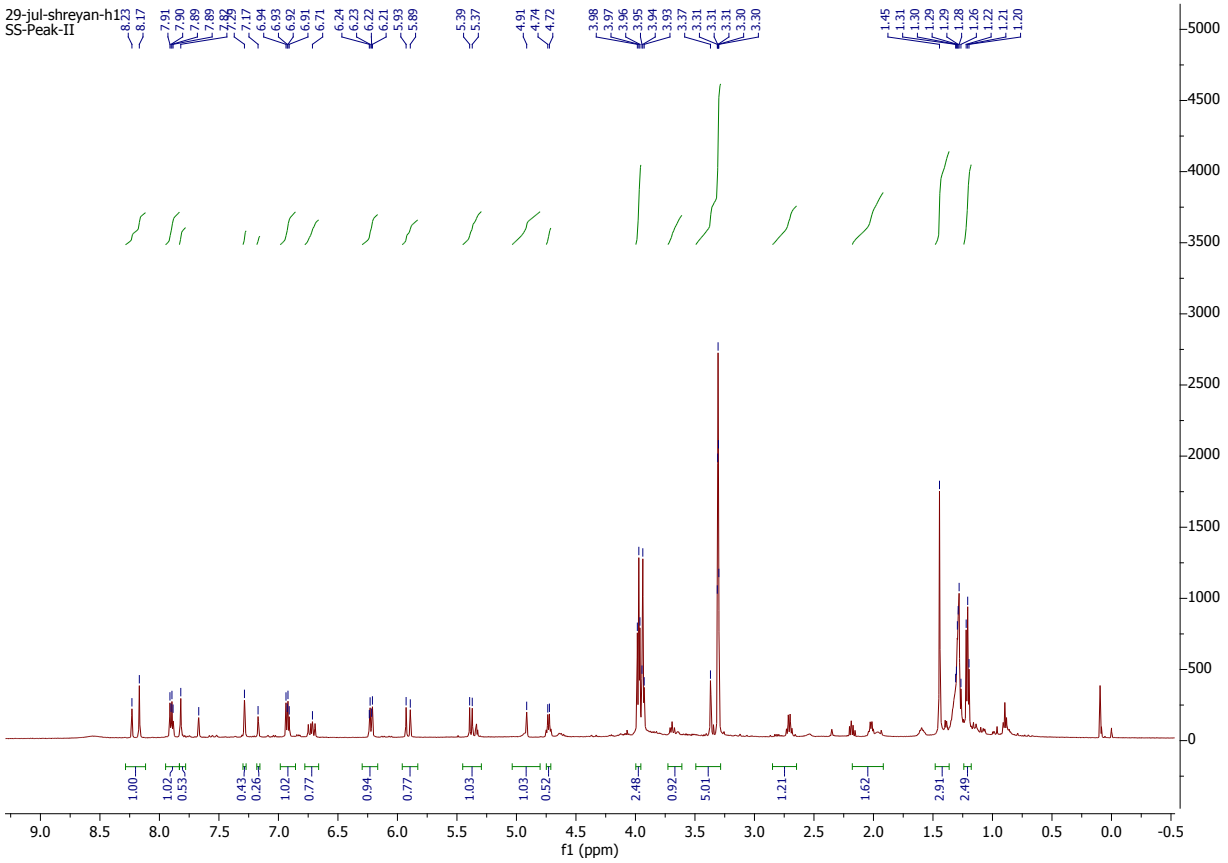
CONTENTS

S1 ^{1}H -NMR Spectrum of chrysomycin A (**1**) in CD_3OD



S2. HRMS Spectrum of chrysomycin A (**1**)

Qualitative Compound Report

Data File	SS.d	**Sample Name**	SS
Sample Type	Sample	**Position**	Vial 71
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 8:53:39
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

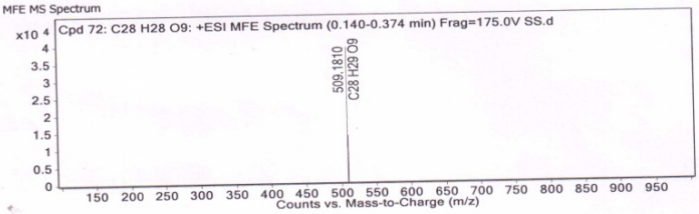
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 72: C28 H28 O9	0.201	508.1737	C28 H28 O9	C28 H28 O9	-0.74	C28 H28 O9

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 72: C28 H28 O9	509.181	0.201	Find by Molecular Feature	508.1737

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
509.181	1	39252.06	C28 H29 O9	(M+H)+
510.1844	1	13827.81	C28 H29 O9	(M+H)+

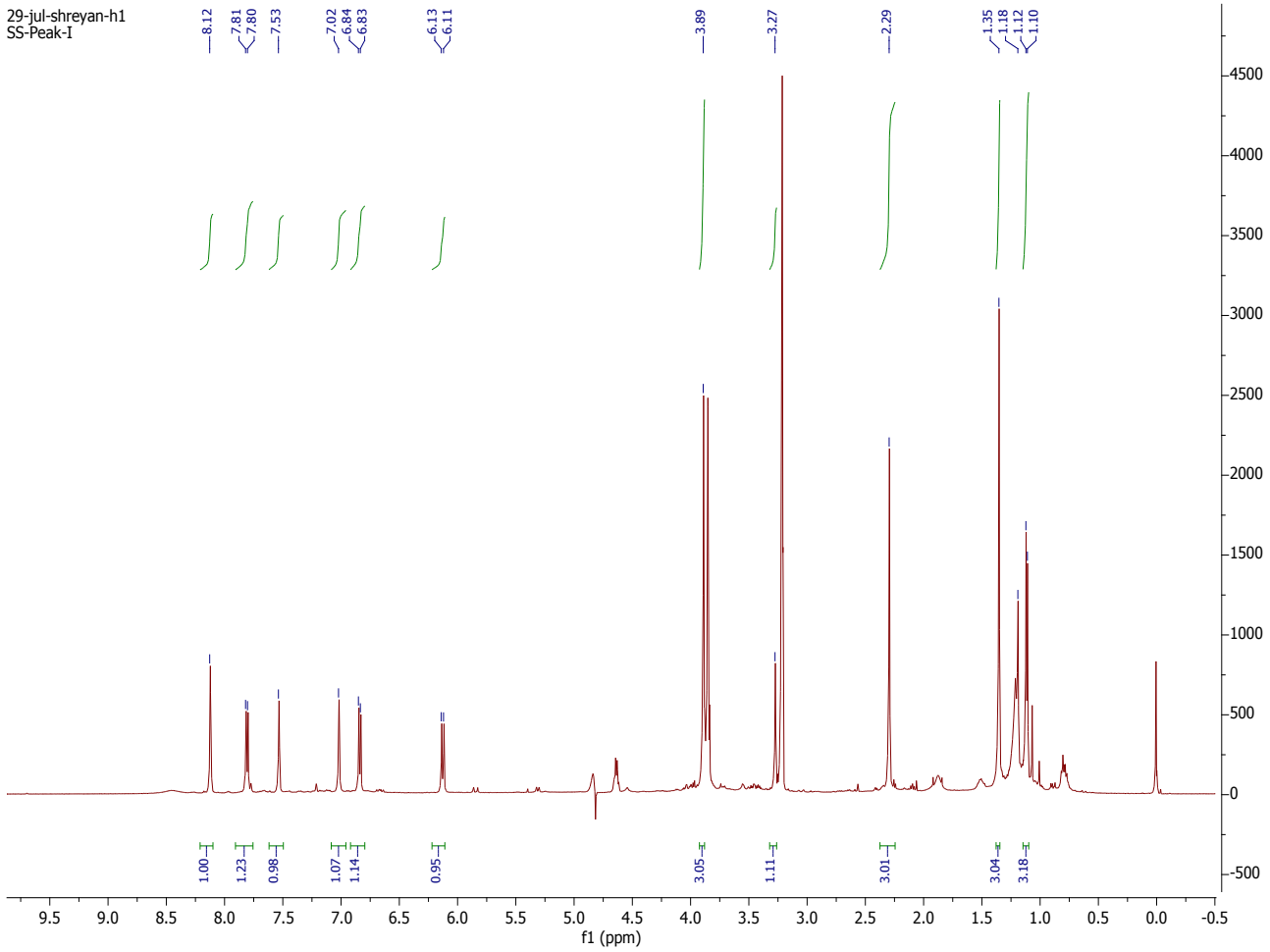
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	509.181	509.1806	-0.73	100	100	73.95	76.36
2	510.1844	510.184	-0.77	35.23	30.96	26.05	23.64

--- End Of Report ---

Page 1 of 1 Printed at: 9:01 PM on:16-07-2013

S3 ^{1}H -NMR Spectrum of chrysomycin B (**2**) in CD_3OD



S4. HRMS Spectrum of chrysomycin B (**2**)

Formula — **Qualitative Compound Report** — Molecular Formula

Data File	SS.d	**Sample Name**	SS
Sample Type	Sample	**Position**	Vial 71
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 8:53:39
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

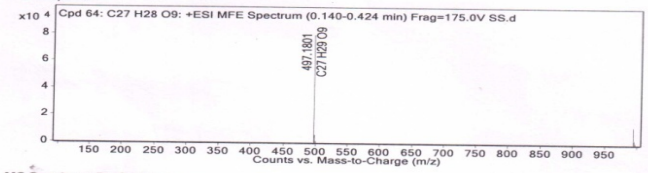
Sample Group — **Info.**
Acquisition SW Version — 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 64: C27 H28 O9	0.2	496.1728	C27 H28 O9	C27 H28 O9	1.07	C27 H28 O9

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 64: C27 H28 O9	497.1801	0.2	Find by Molecular Feature	496.1728

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
497.1801	1	79574.78	C27 H29 O9	(M+H)+
498.1832	1	24610.64	C27 H29 O9	(M+H)+
499.186	1	6021.46	C27 H29 O9	(M+H)+
500.1914	1	1421.38	C27 H29 O9	(M+H)+
993.3522	1	12668.3		(2M+H)+
994.3552	1	7721.12		(2M+H)+
995.3567	1	3137.06		(2M+H)+
996.3617	1	1285.23		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	497.1801	497.1806	0.99	100	100	71.29	73
2	498.1832	498.184	1.56	30.93	29.88	22.05	21.81
3	499.186	499.1866	1.28	7.57	6.16	5.39	4.49
4	500.1914	500.1893	-4.24	1.79	0.95	1.27	0.69

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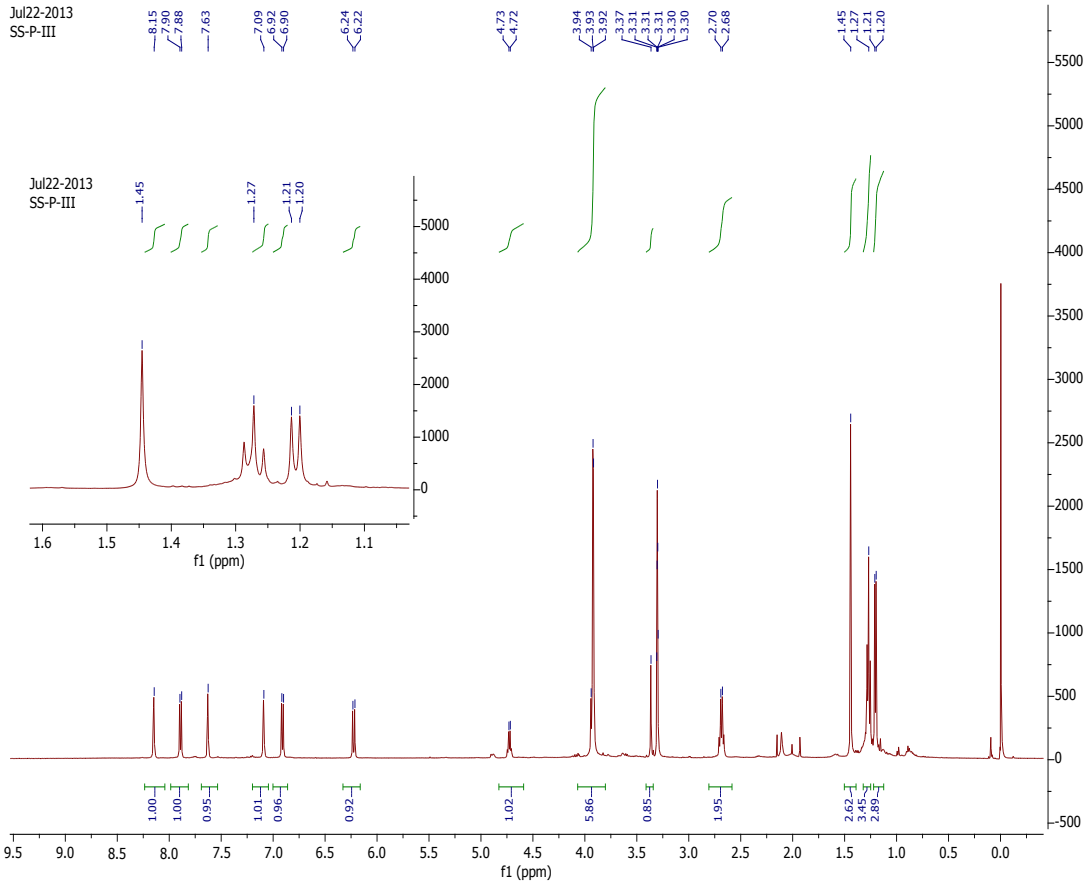
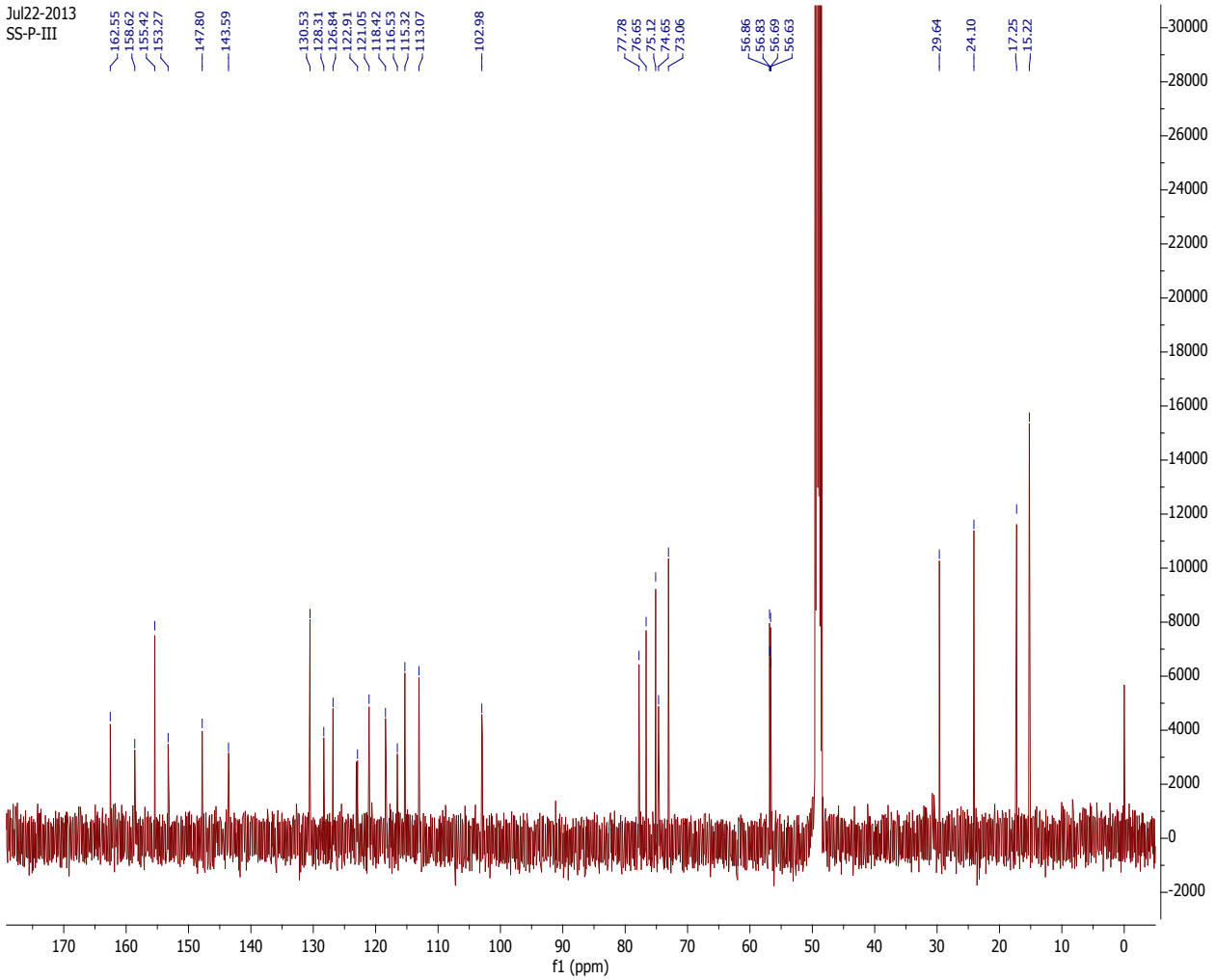
Agilent Technologies — Page 1 of 1 — Printed at: 8:58 PM on:16-07-2013

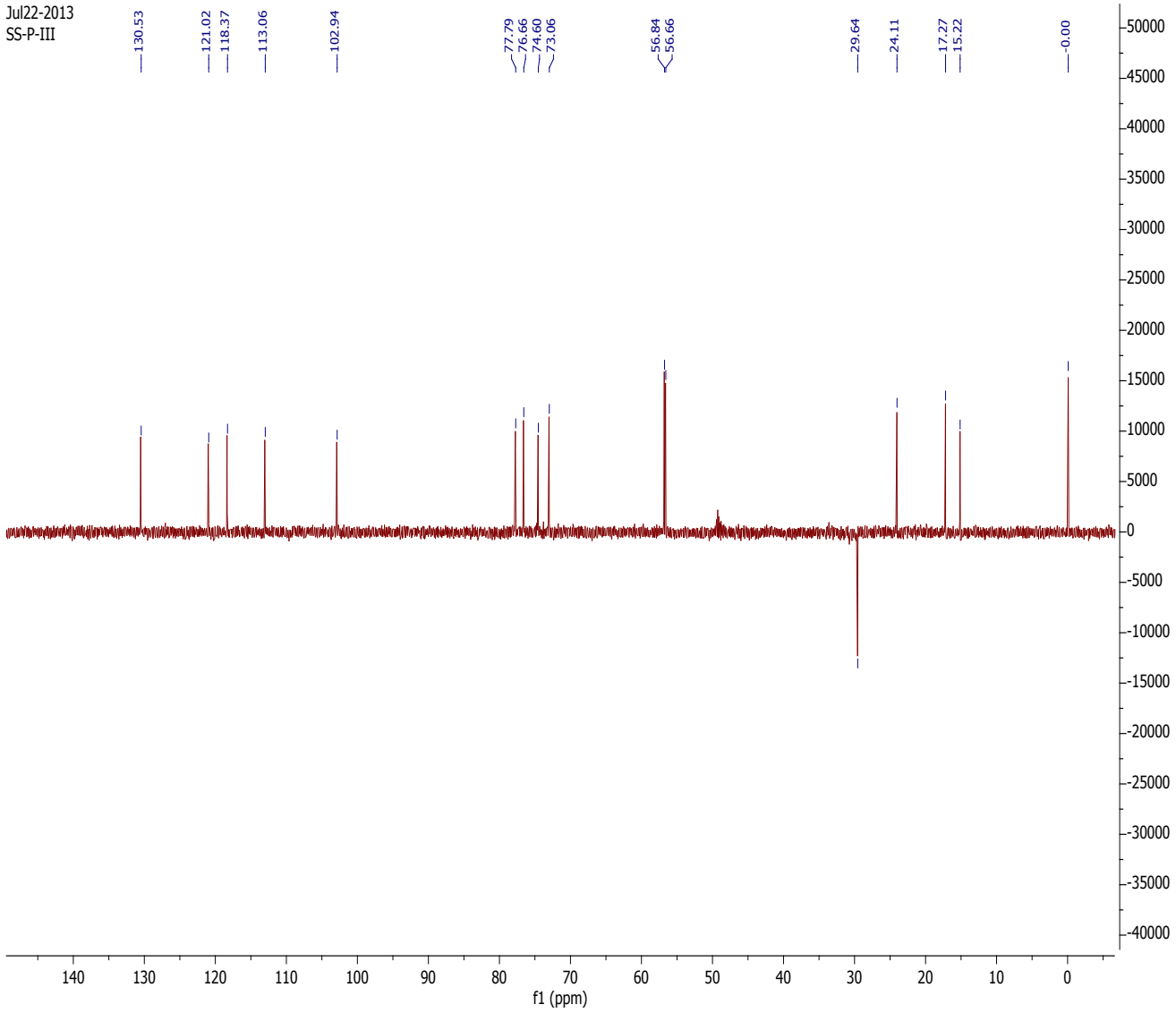
S5 ^{1}H -NMR Spectrum of chrysomycin C(**3**) in CD_3OD



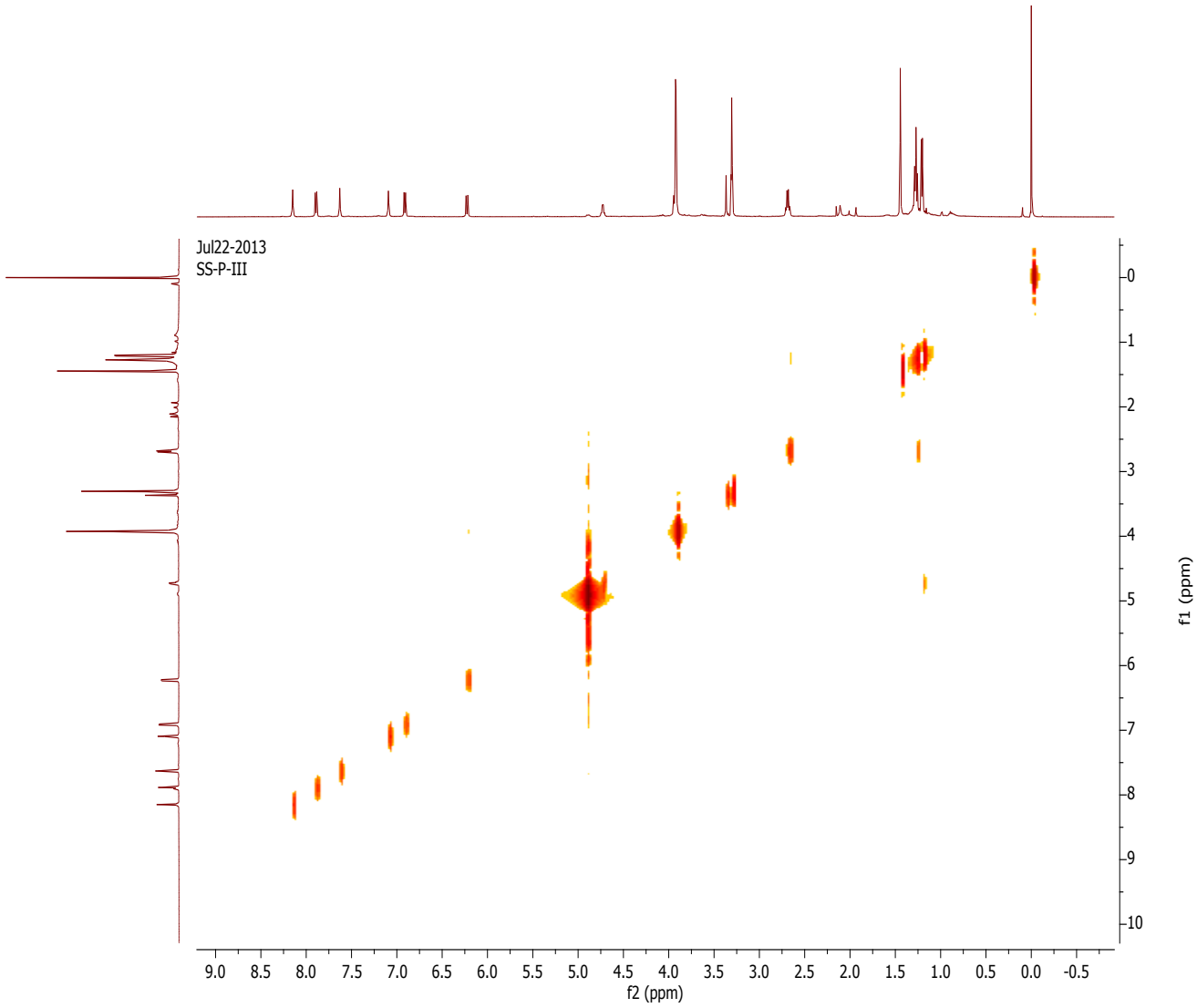
S6. ^{13}C NMR Spectrum of chrysomycin C (**3**) in CD_3OD



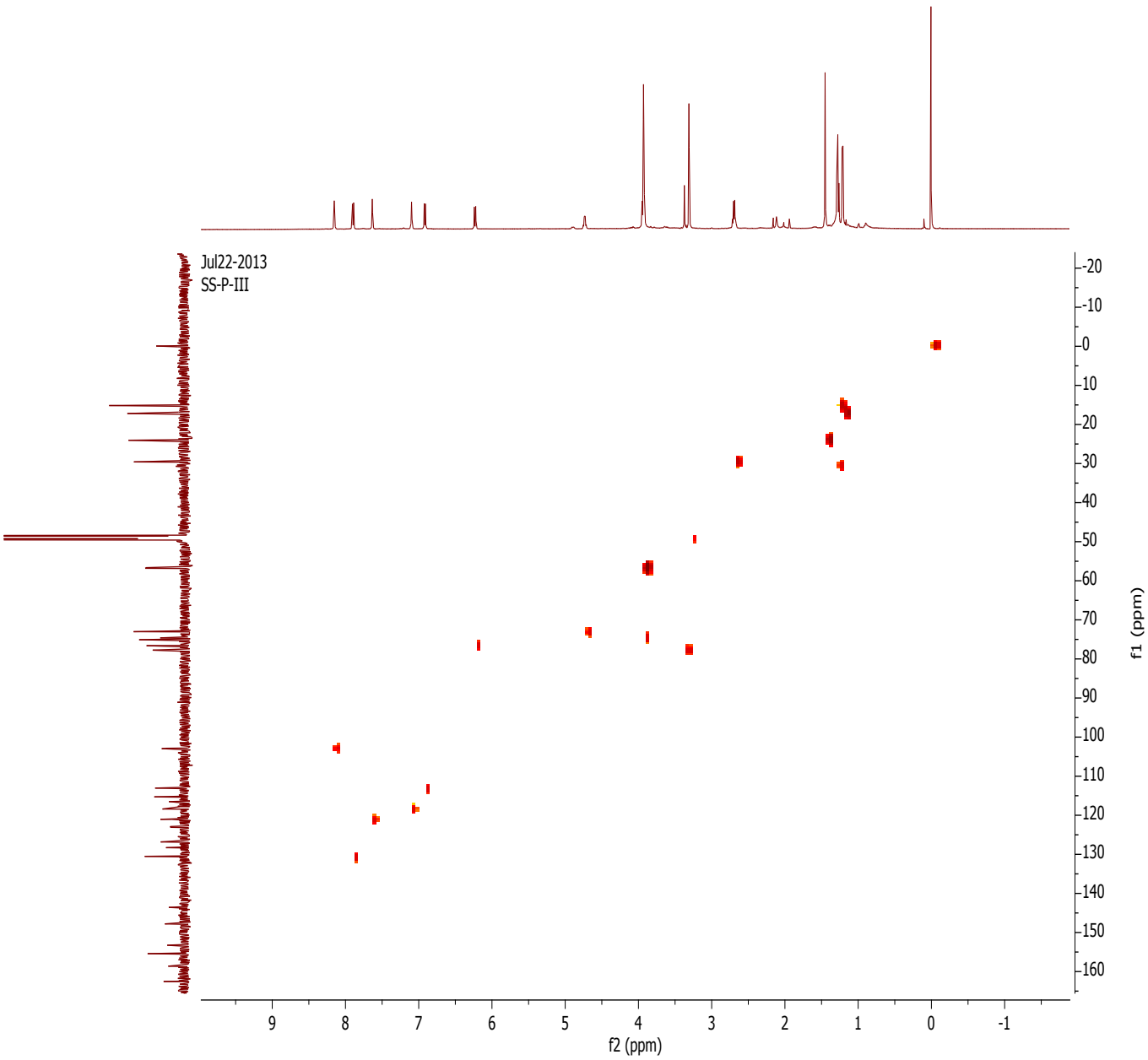
S7. DEPT 135 Spectrum of chrysomycin C (**3**) in CD_3OD



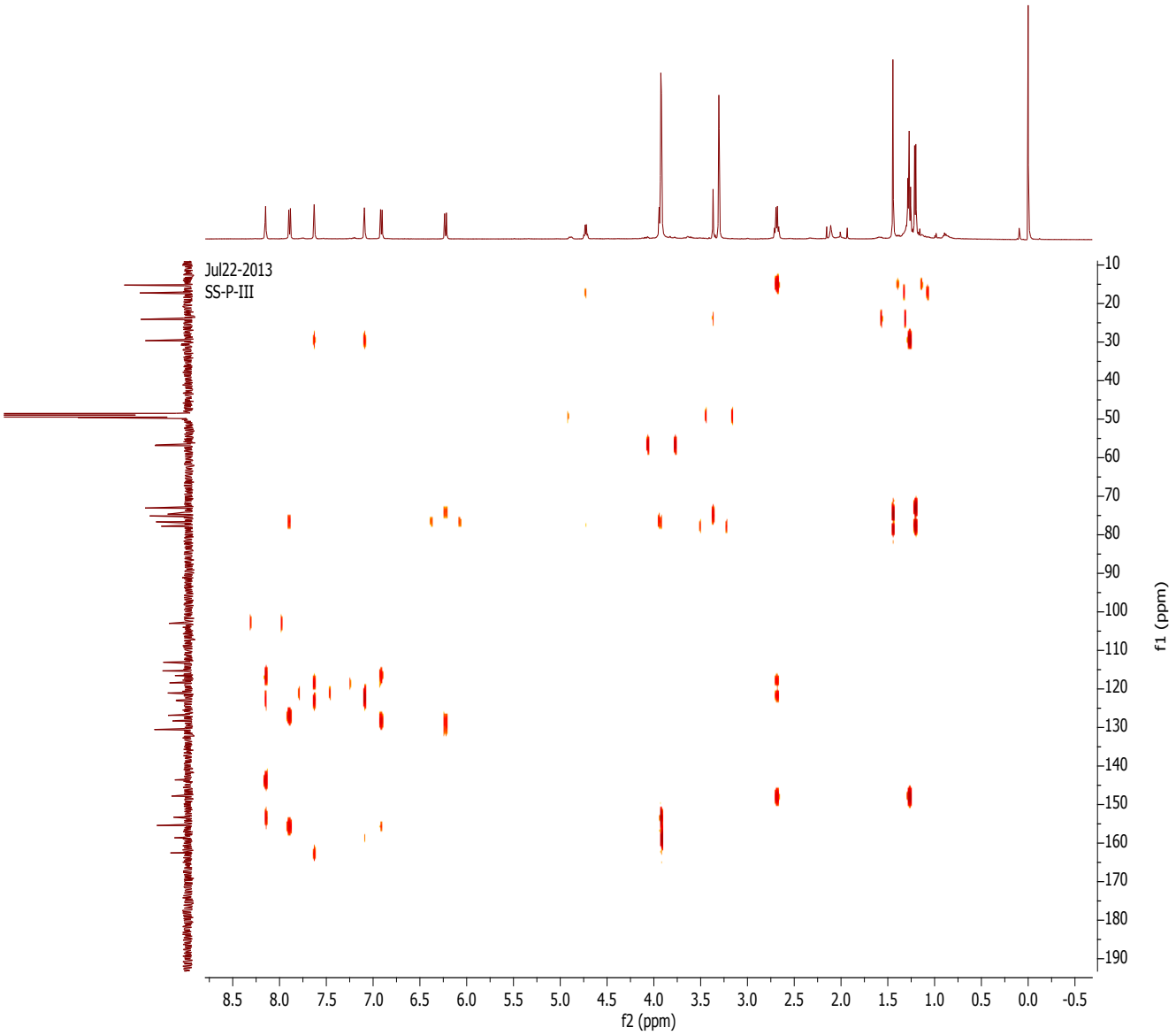
S8. COSY Spectrum of chrysomycin C (**3**) in CD_3OD



S9. HSQC Spectrum of chrysomycin C (**3**) in CD_3OD



S10. HMBC spectrum of chrysomycin C (**3**) in CD_3OD



S11. HRMS of chrysomycin C (**3**)

Qualitative Compound Report

Data File	SS.d	**Sample Name**	SS
Sample Type	Sample	**Position**	Vial 71
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	16-07-2013 PM 8:53:39
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

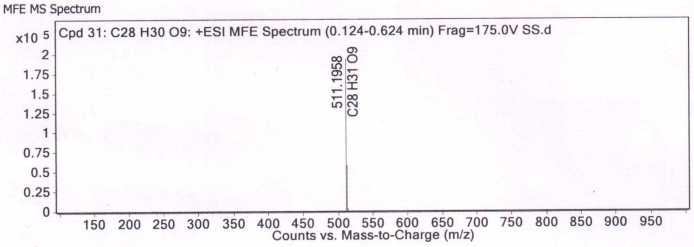
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C28 H30 O9	0.197	510.1881	C28 H30 O9	C28 H30 O9	1.68	C28 H30 O9

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 31: C28 H30 O9	511.1958	0.197	Find by Molecular Feature	510.1881

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
511.1958	1	193471.98	C28 H31 O9	(M+H)+
512.199	1	57939.72	C28 H31 O9	(M+H)+
513.1973	1	14553.15	C28 H31 O9	(M+H)+
514.1945	1	3195.54	C28 H31 O9	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	511.1958	511.1963	0.88	100	100	71.88	72.21
2	512.199	512.1997	1.24	29.95	30.98	21.53	22.37
3	513.1973	513.2023	9.84	7.52	6.49	5.41	4.68
4	514.1945	514.205	20.44	1.65	1.02	1.19	0.74

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Agilent Technologies Page 1 of 1 Printed at: 8:59 PM on:16-07-2013

S12. HRMS of chrysomycin D (**4**)

Qualitative Compound Report

Data File	SS-529.d	**Sample Name**	SS-529
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	22-07-2013 PM 12:09:50
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

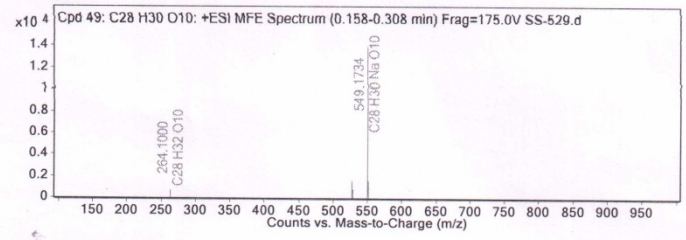
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 49: C28 H30 O10	0.196	526.1835	C28 H30 O10	C28 H30 O10	0.81	C28 H30 O10

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 49: C28 H30 O10	549.1734	0.196	Find by Molecular Feature	526.1835

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
264.1	2	703.24	C28 H32 O10	(M+2H)+2
264.5994	2	231.03	C28 H32 O10	(M+2H)+2
527.1856	1	1568.04		(M+H)+
528.1903	1	770.16		(M+H)+
549.1734	1	13959.3	C28 H30 Na O10	(M+Na)+
550.1752	1	4834.88	C28 H30 Na O10	(M+Na)+
551.1753	1	1597.78	C28 H30 Na O10	(M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	264.1	264.0992	-2.75	100	100	75.27	76.32
2	264.5994	264.6009	5.71	32.85	31.03	24.73	23.68

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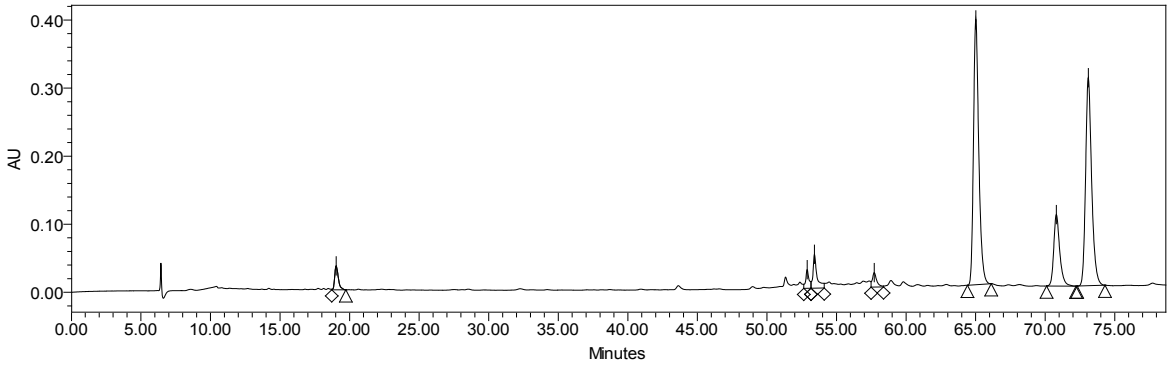
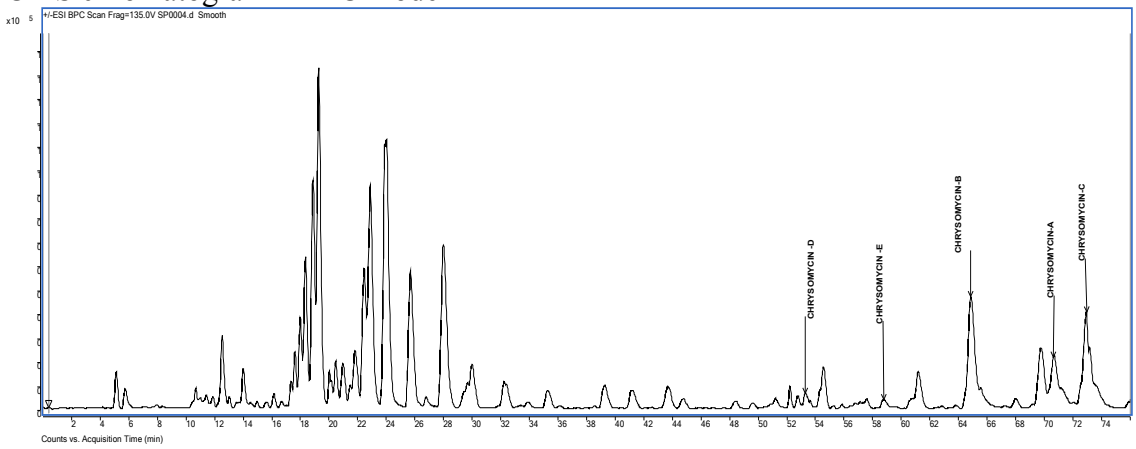
Agilent Technologies Page 1 of 1 Printed at: 12:32 PM on:22-07-2013

13. LCMS of active fraction

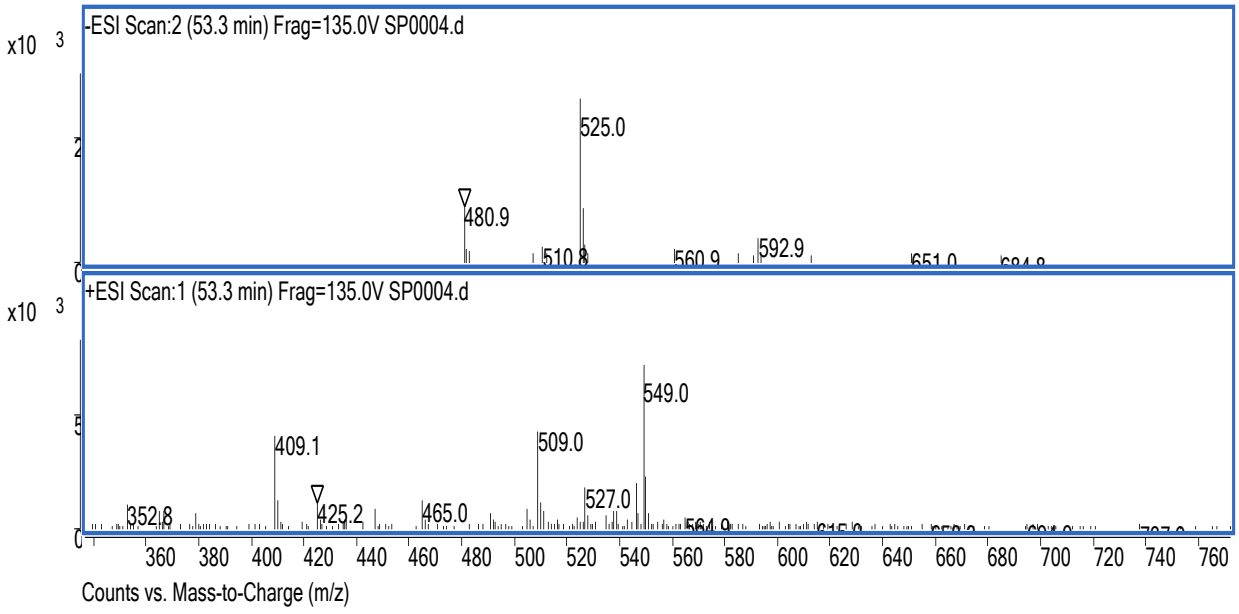
13.1 LC chromatogram at 280 nm

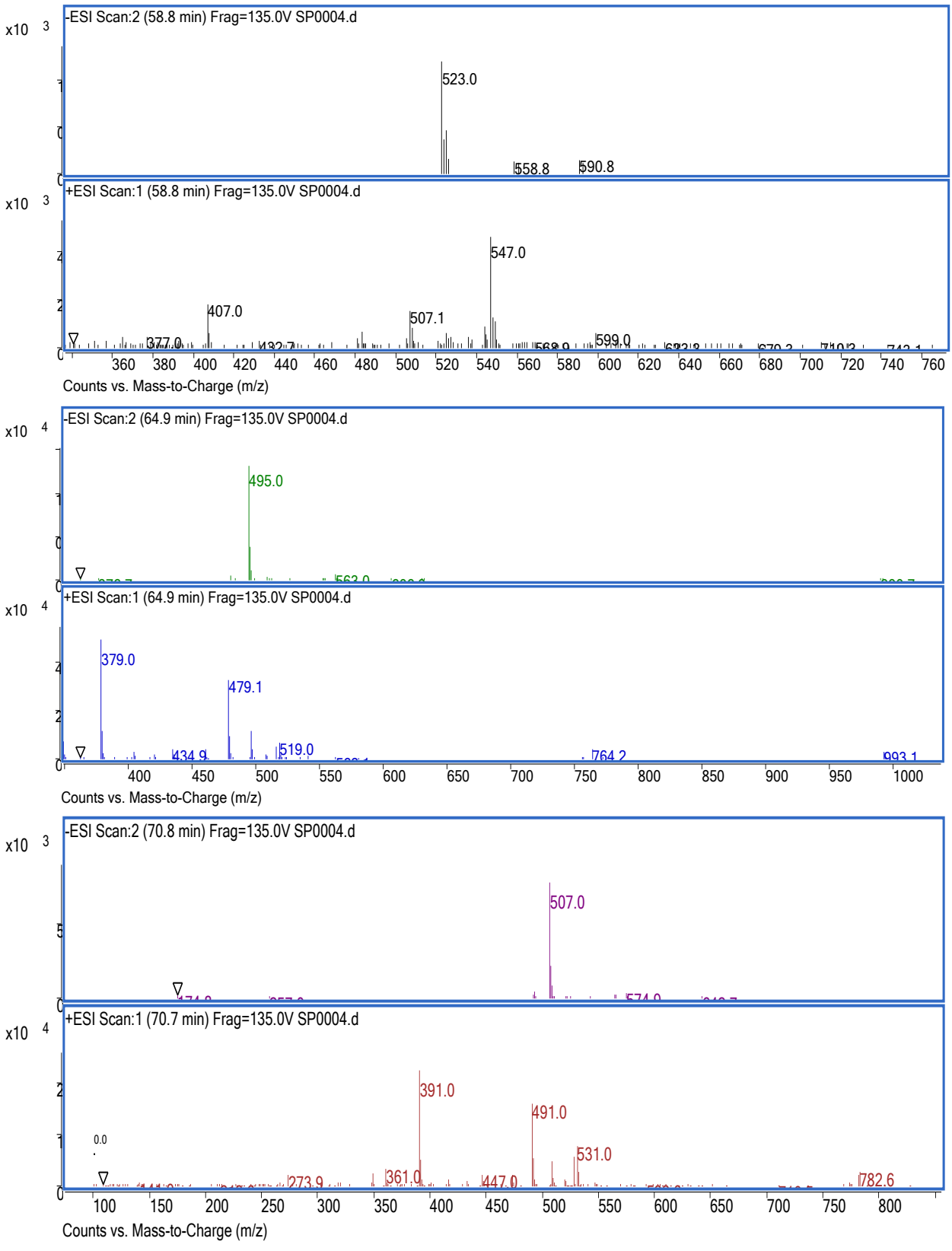


13.2. LCMS chromatogram in TIC mode

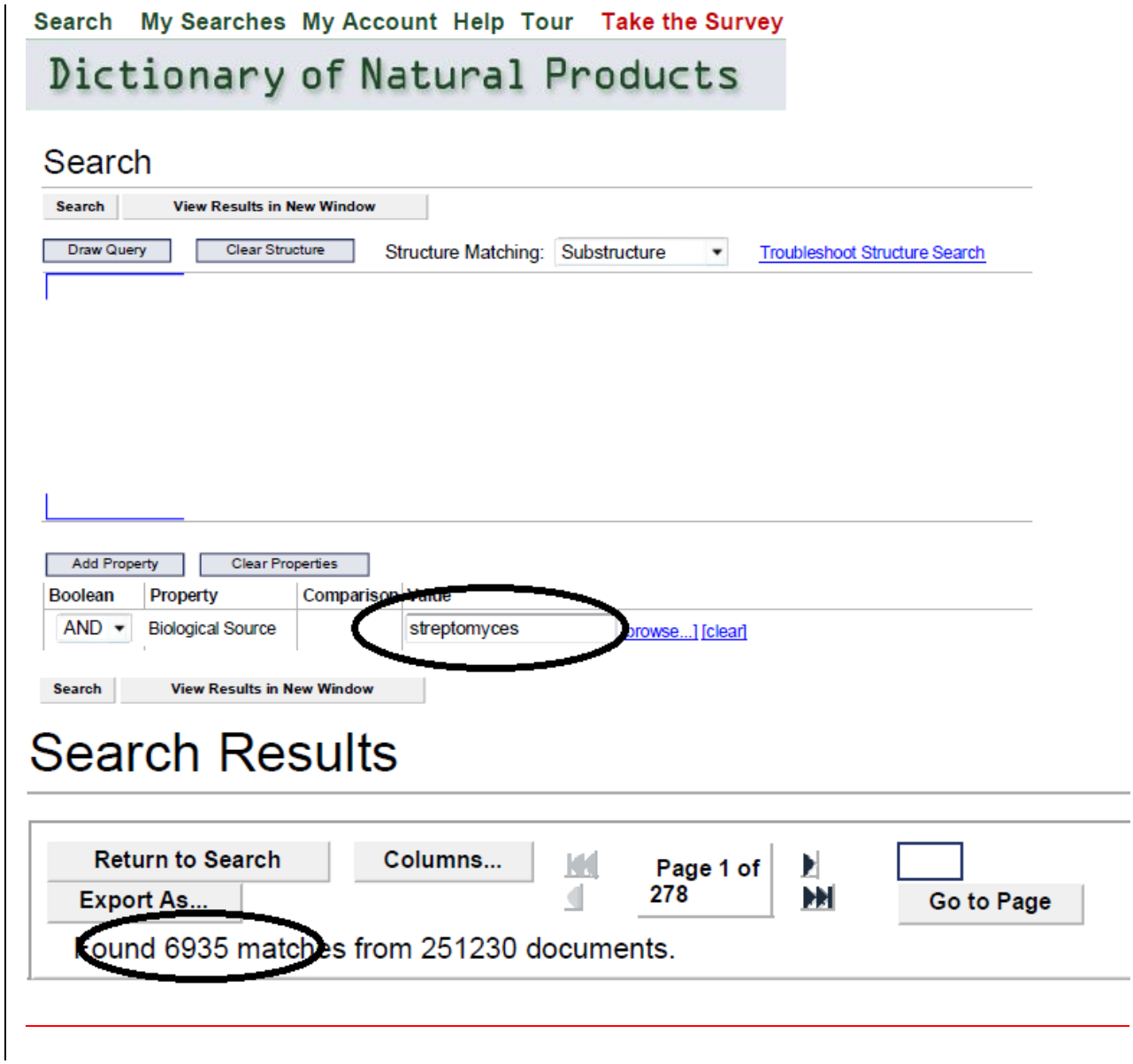


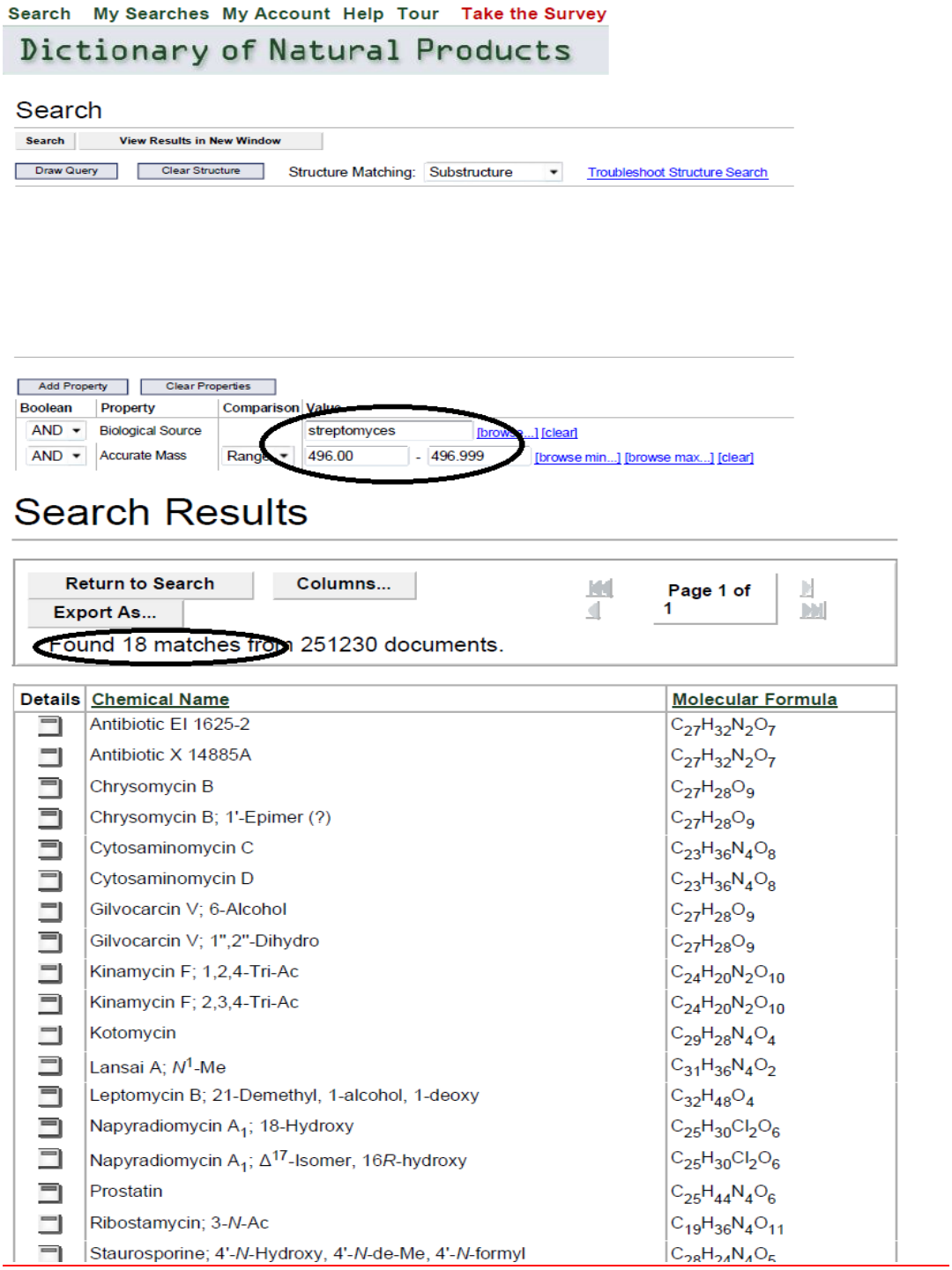
13.3. MS spectras of chrysomycins A-E

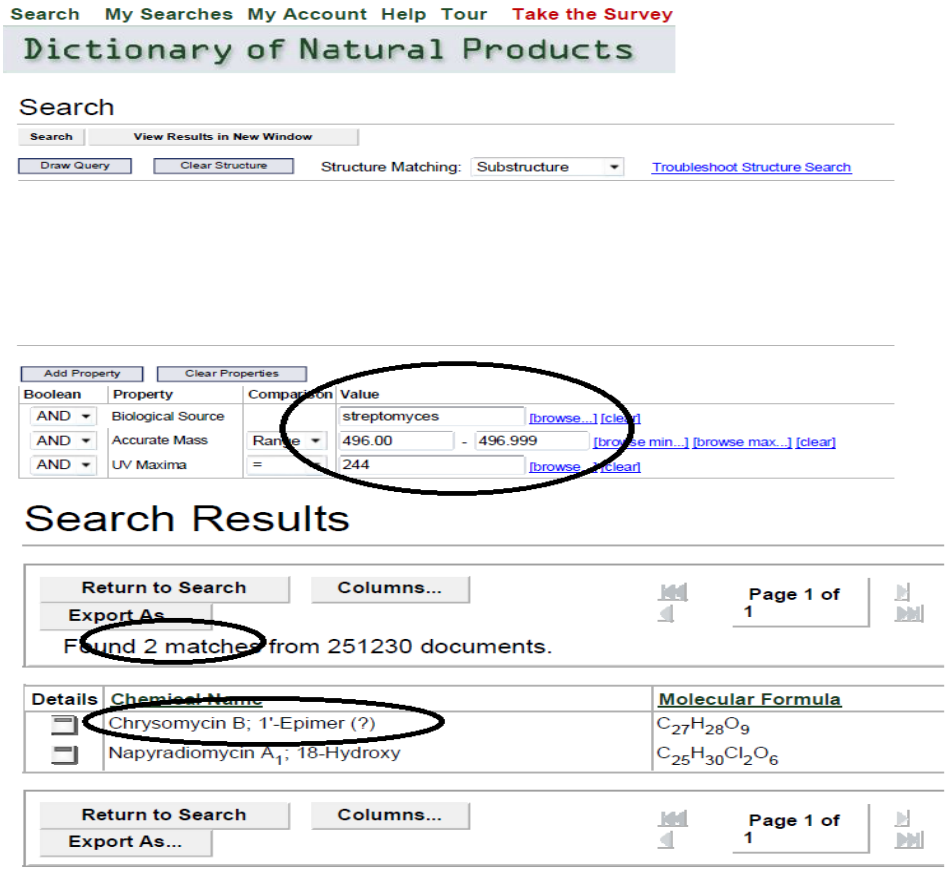




S14. Screenshots of DNP database search during dereplication







S15. Screenshots of DNP substructure search using basic naphthocoumarin skeleton