

ELECTRONIC SUPPORTING INFORMATION (ESI)

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

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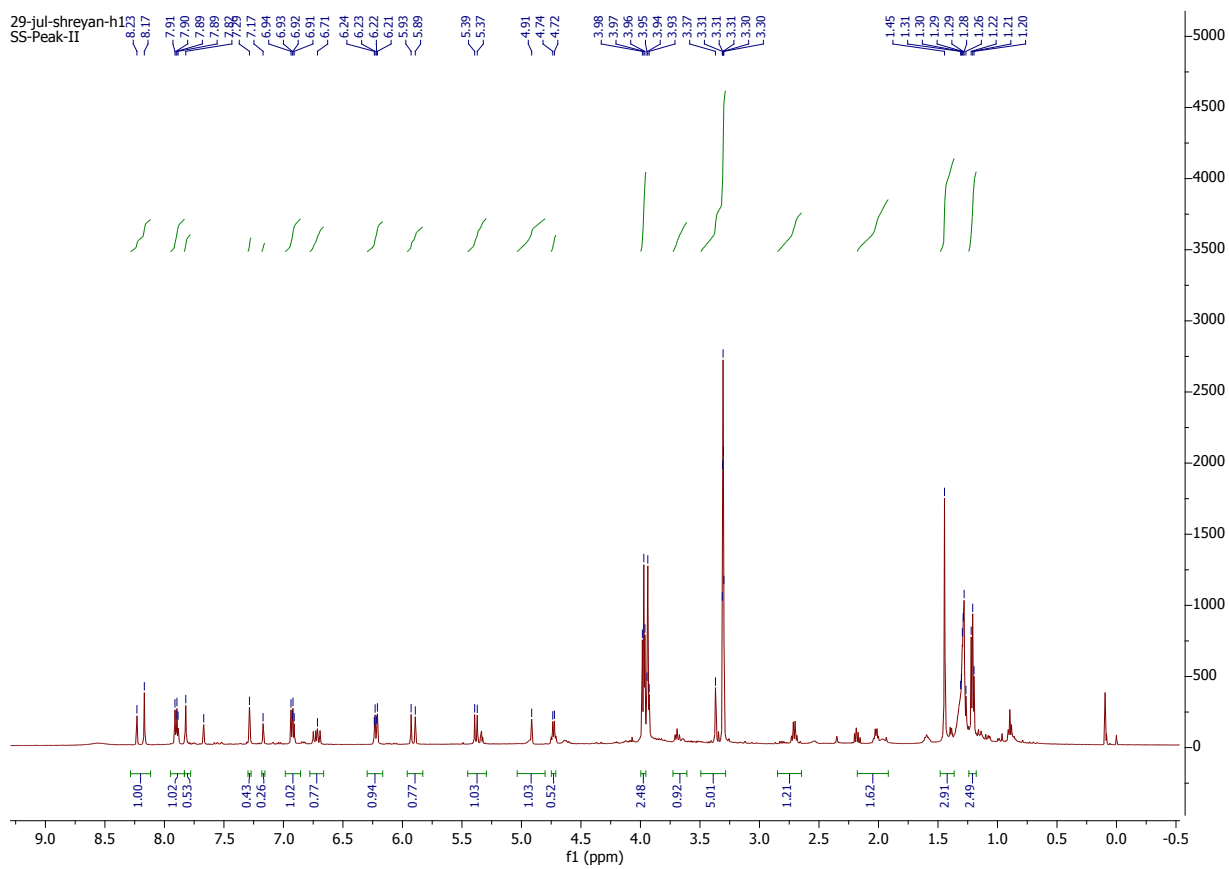
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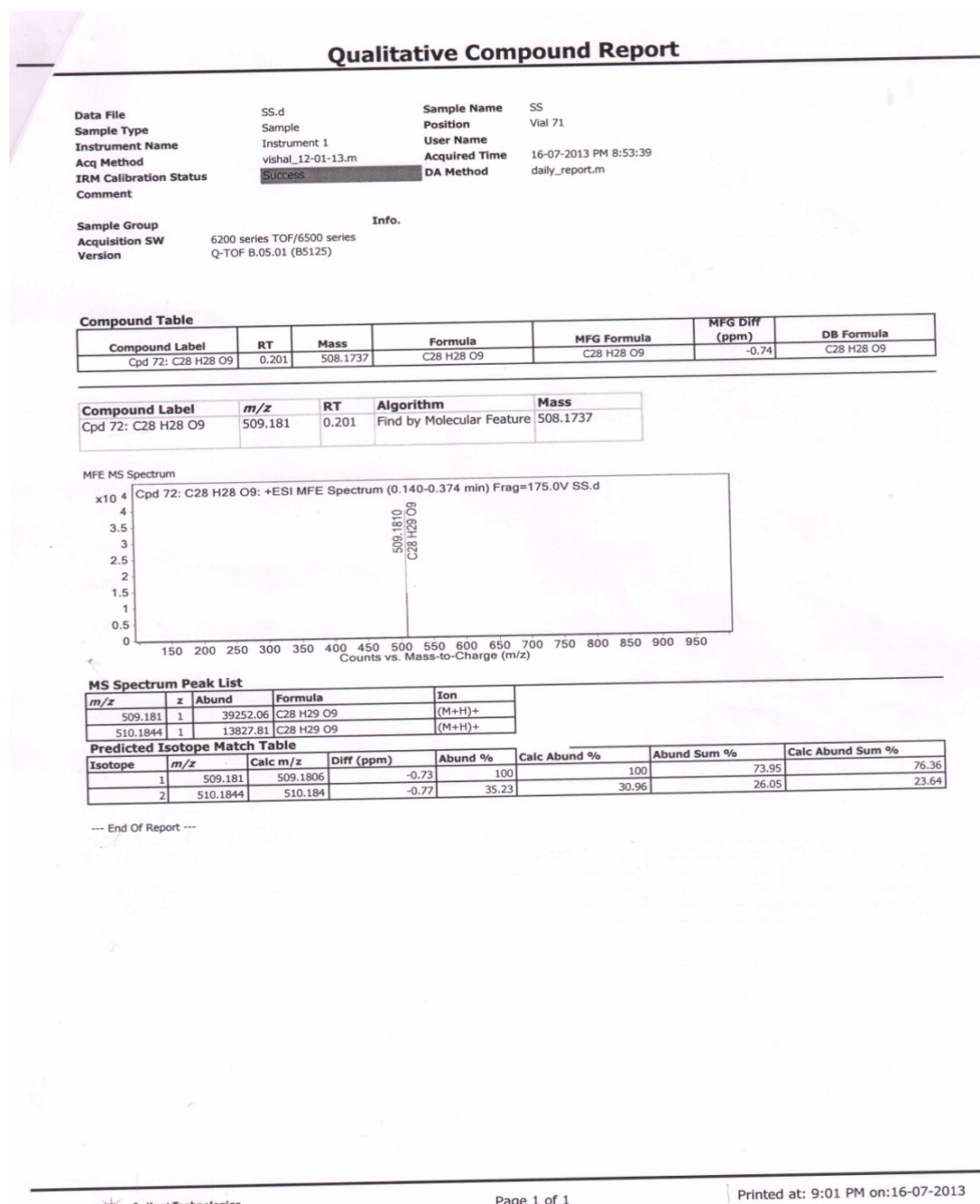
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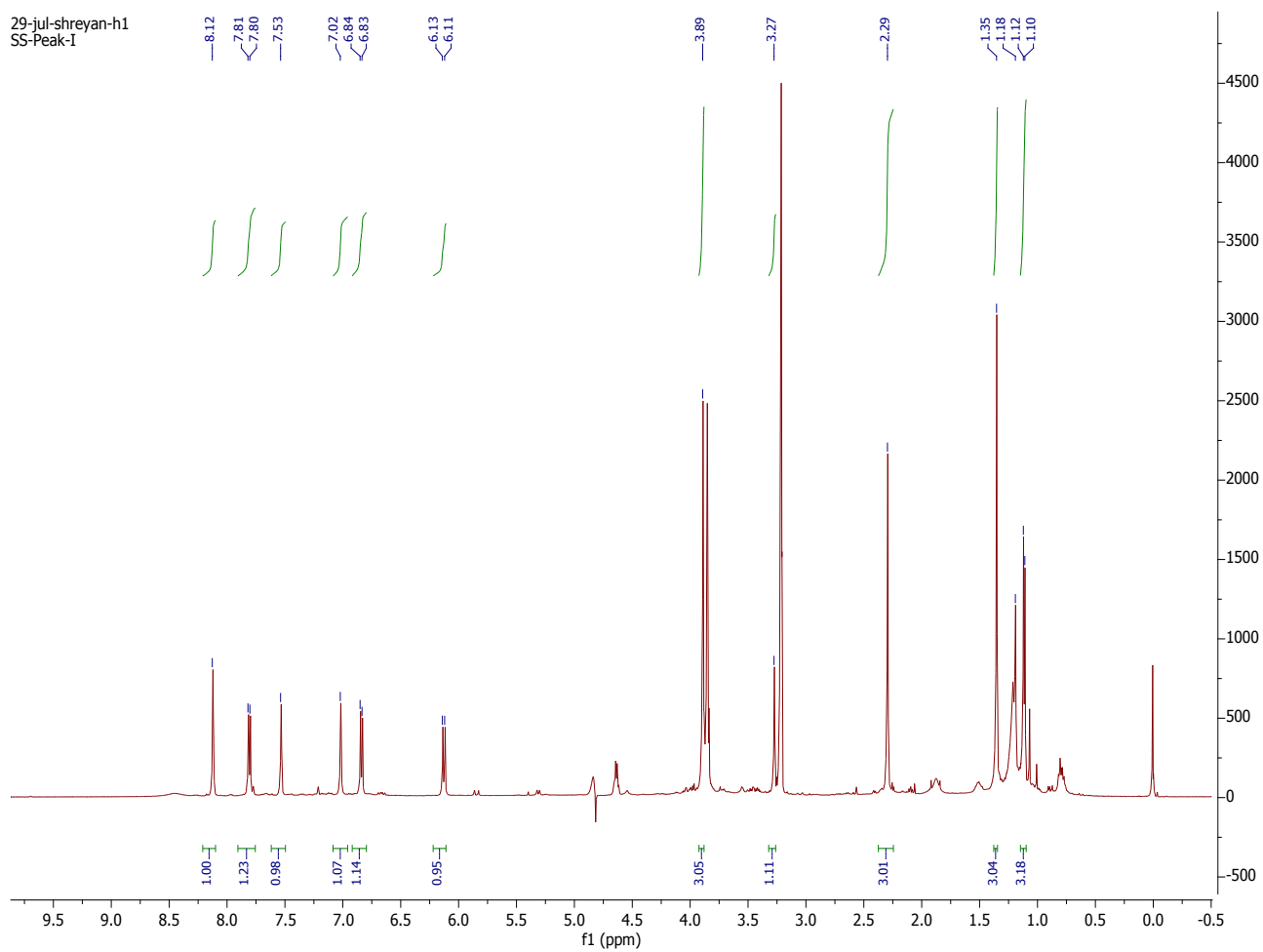
S1 ^1H -NMR Spectrum of chrysomycin A (1) in CD_3OD



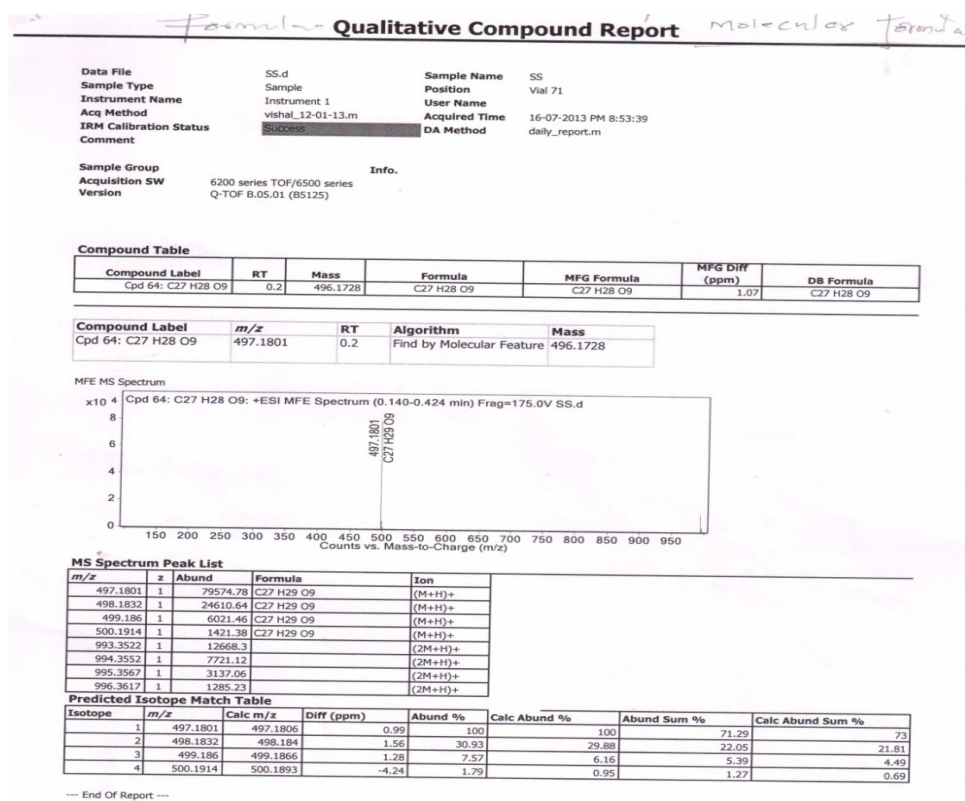
S2. HRMS Spectrum of chrysomycin A (1)



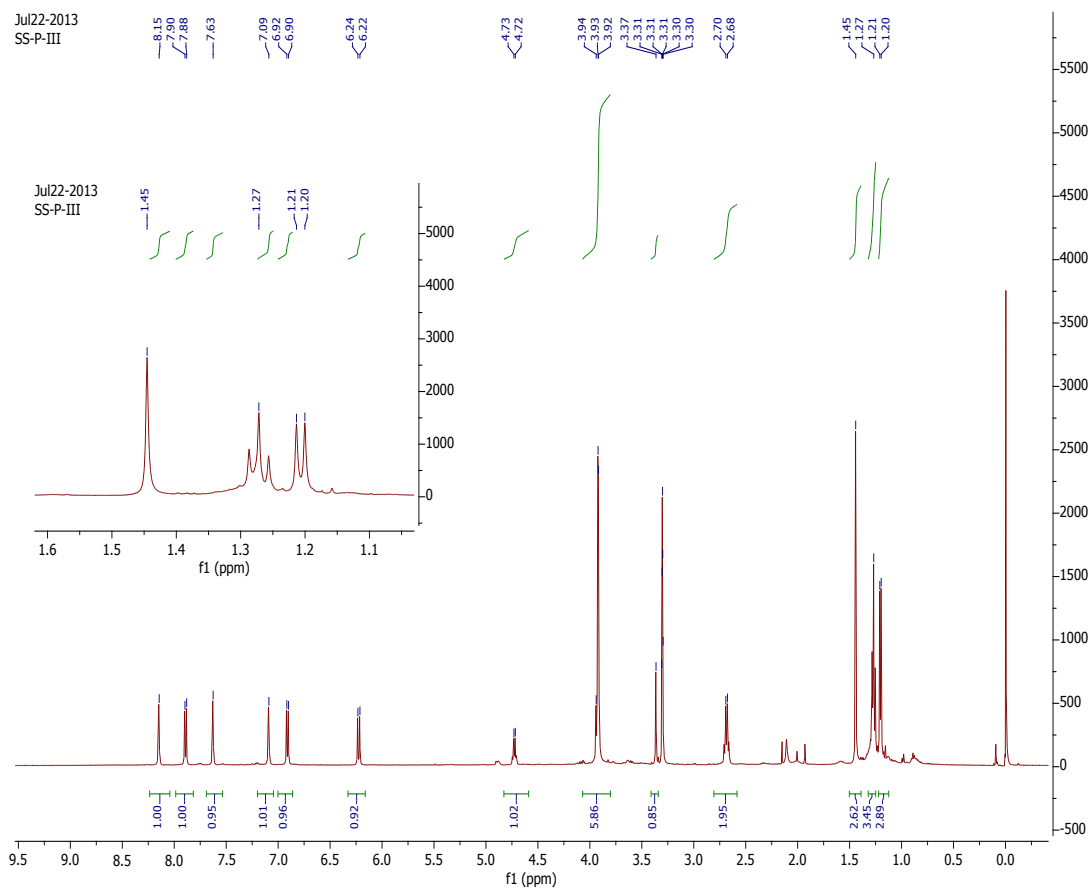
S3 ^1H -NMR Spectrum of chrysomycin B (2) in CD_3OD



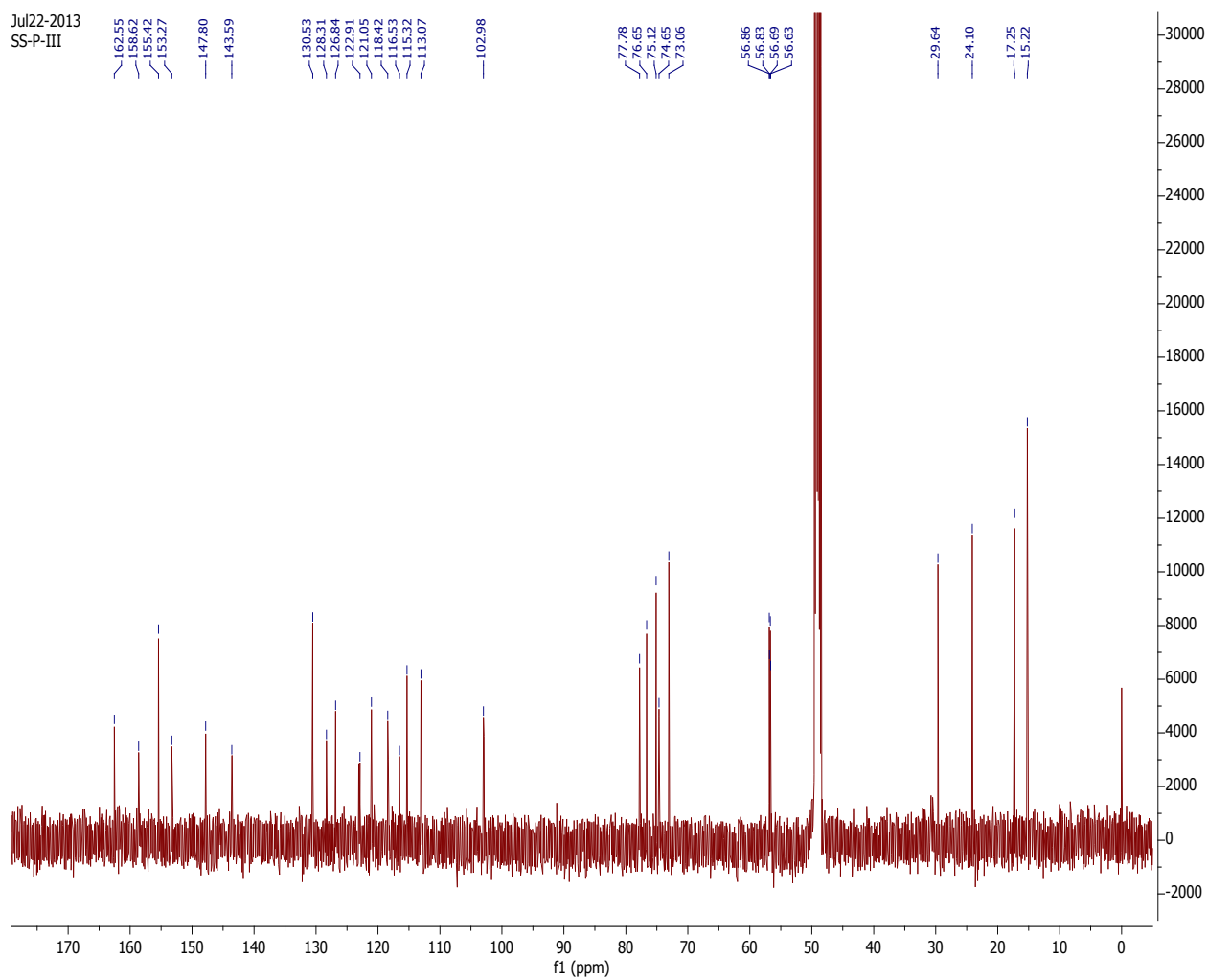
S4. HRMS Spectrum of chrysomycin B (2)



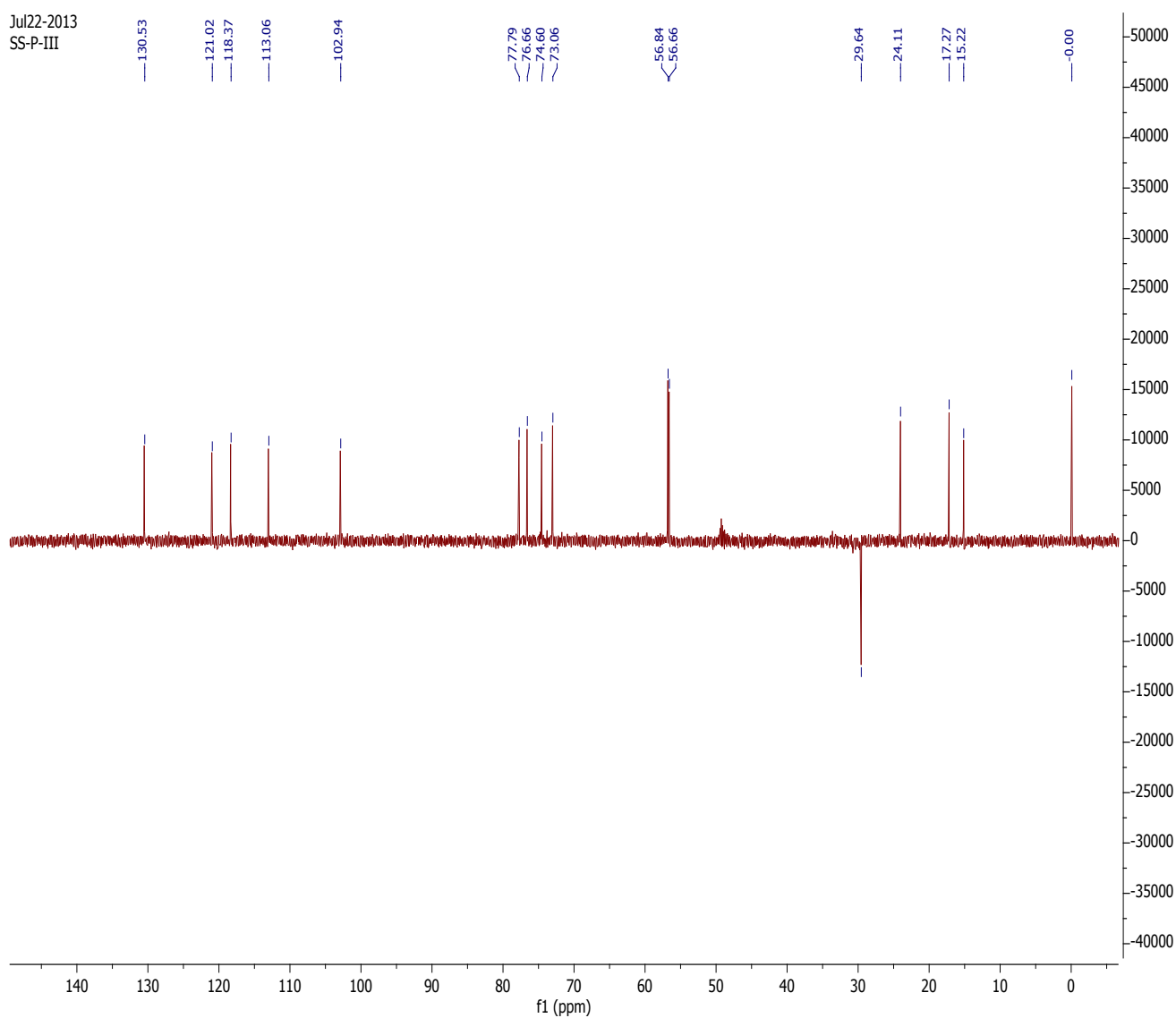
S5 ^1H -NMR Spectrum of chrysomycin C(3) in CD_3OD



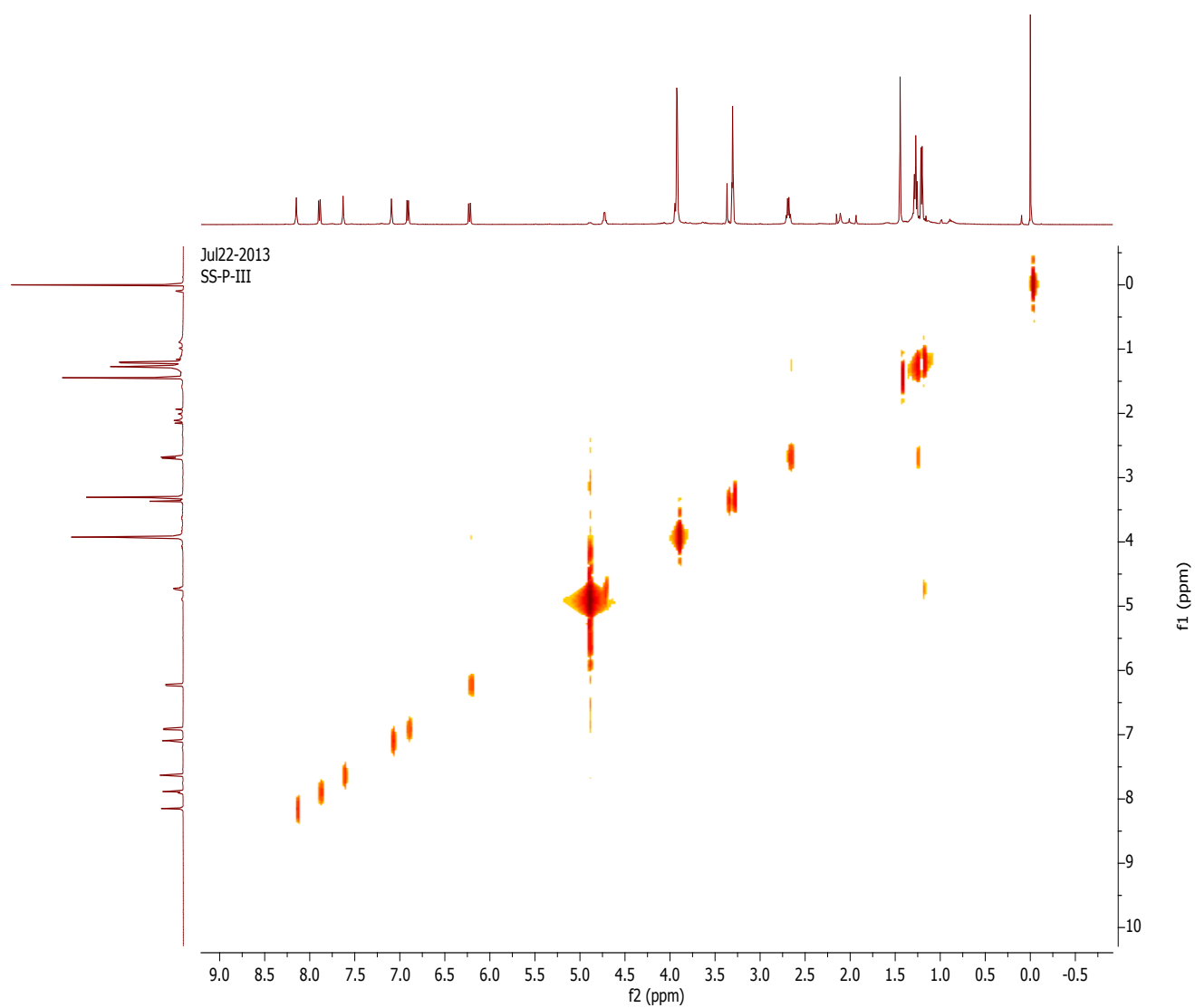
S6. ^{13}C NMR Spectrum of chrysomycin C (**3**) in CD_3OD



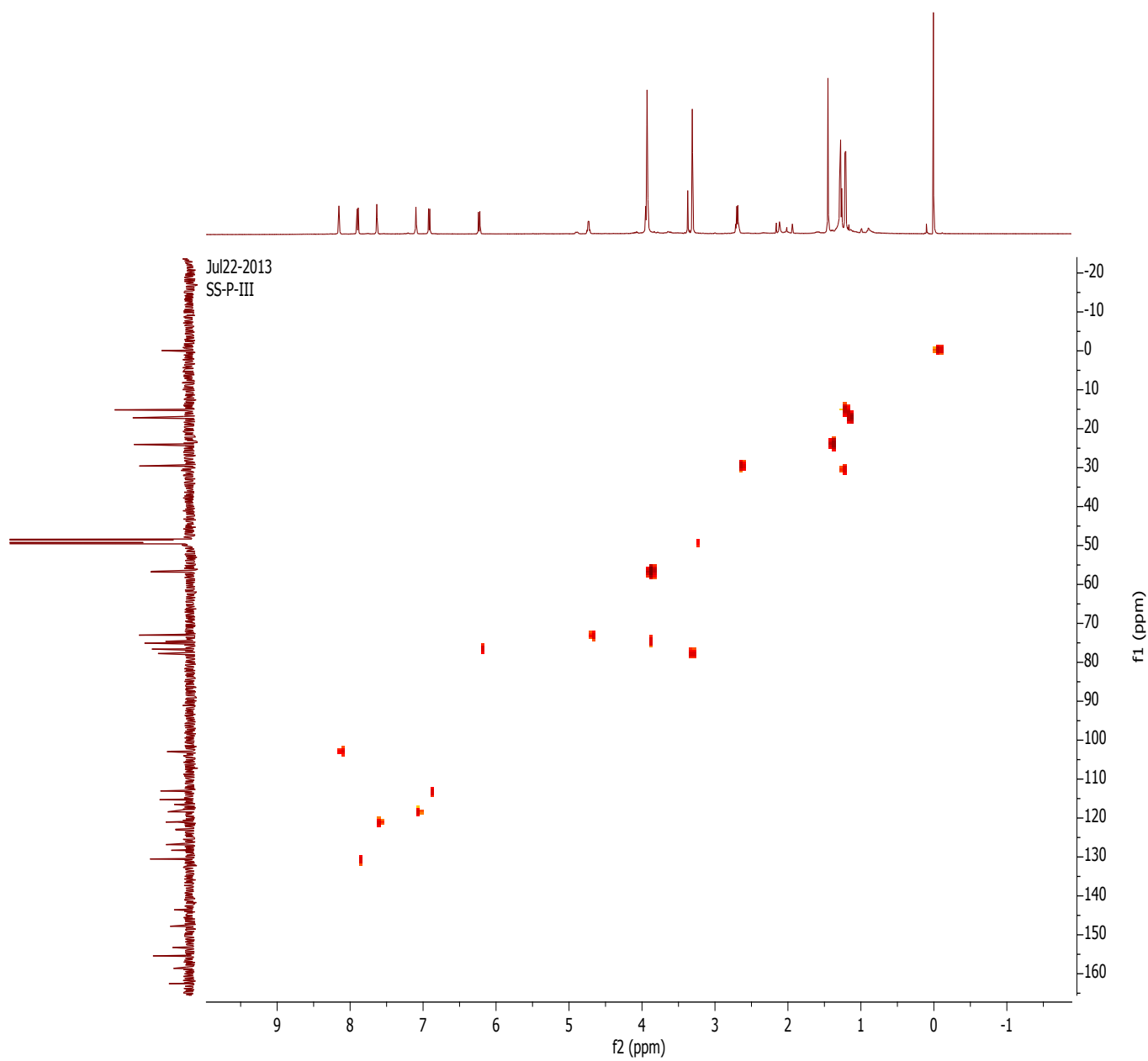
S7. DEPT 135 Spectrum of chryso mycin C (**3**) in CD₃OD



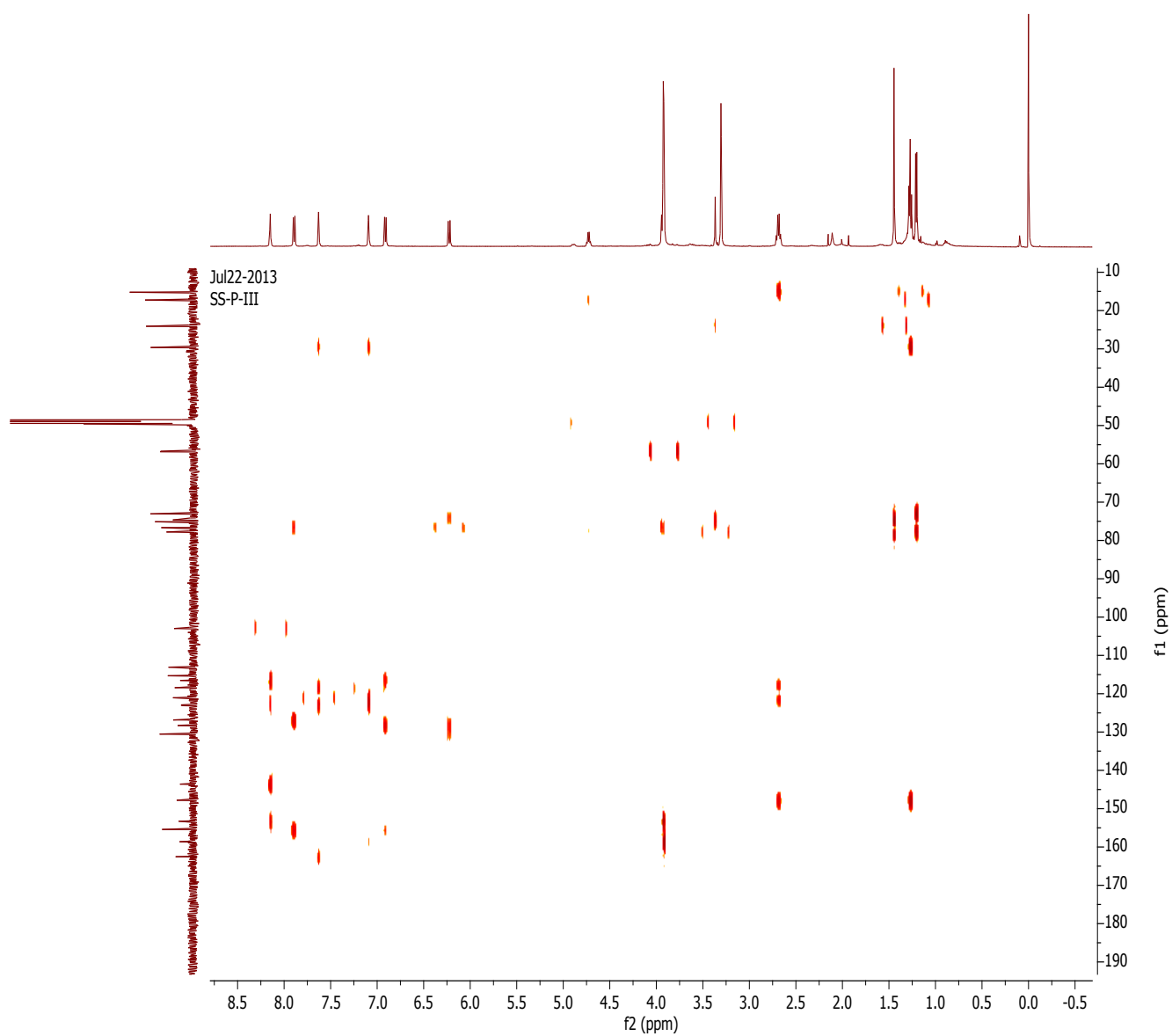
S8. COSY Spectrum of chrysomycin C (**3**) in CD₃OD



S9. HSQC Spectrum of chrysomycin C (3) in CD₃OD



S10. HMBC spectrum of chrysomycin C (**3**) in CD₃OD



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

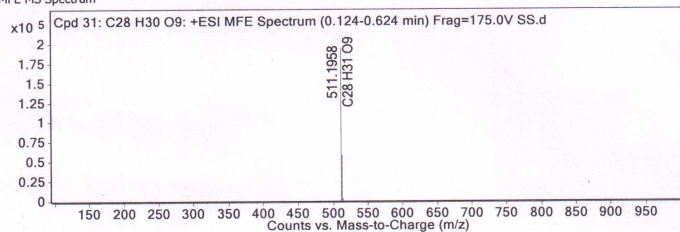
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 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

--- End Of Report ---

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			

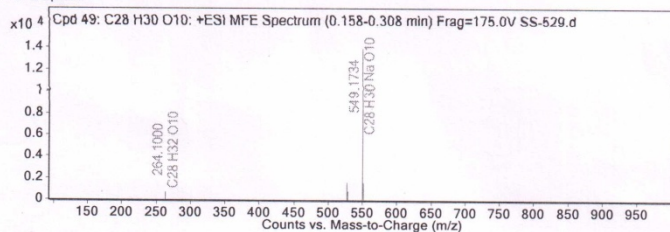
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

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)+

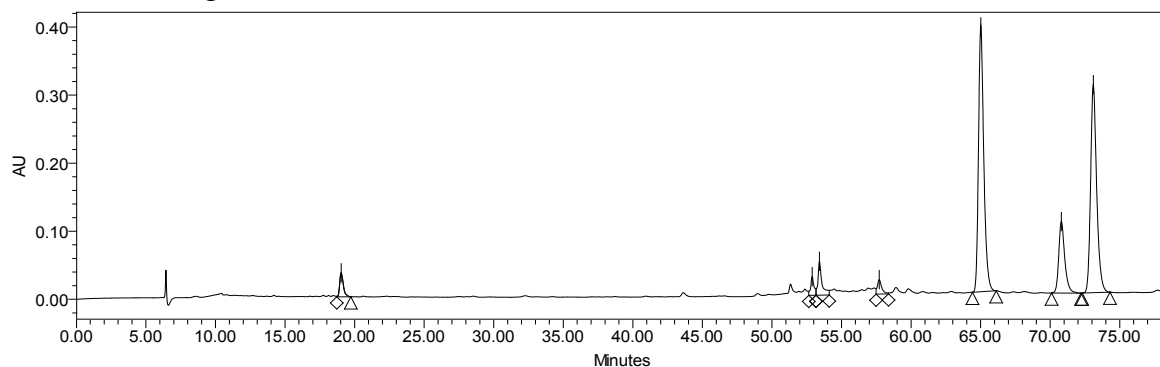
Predicted Isotope Match Table

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

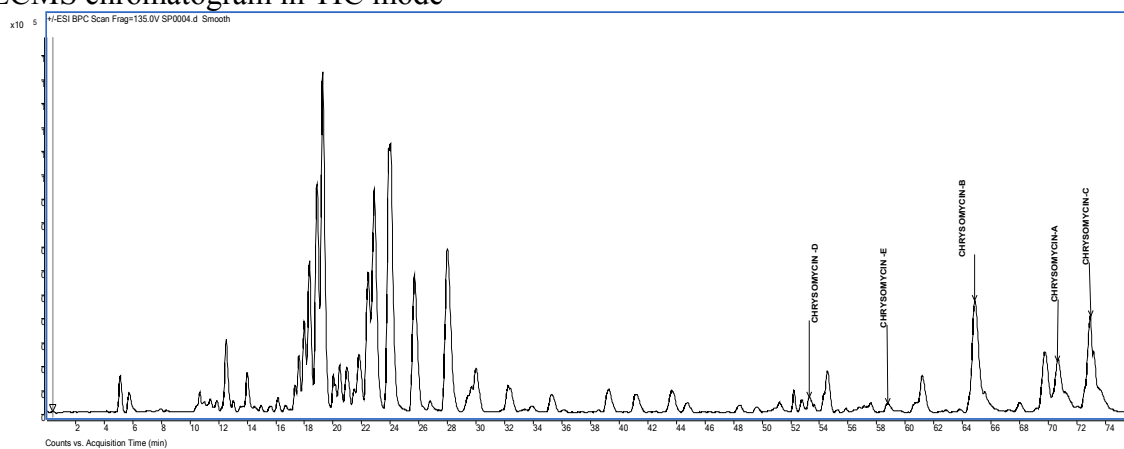
--- End Of Report ---

13. LCMS of active fraction

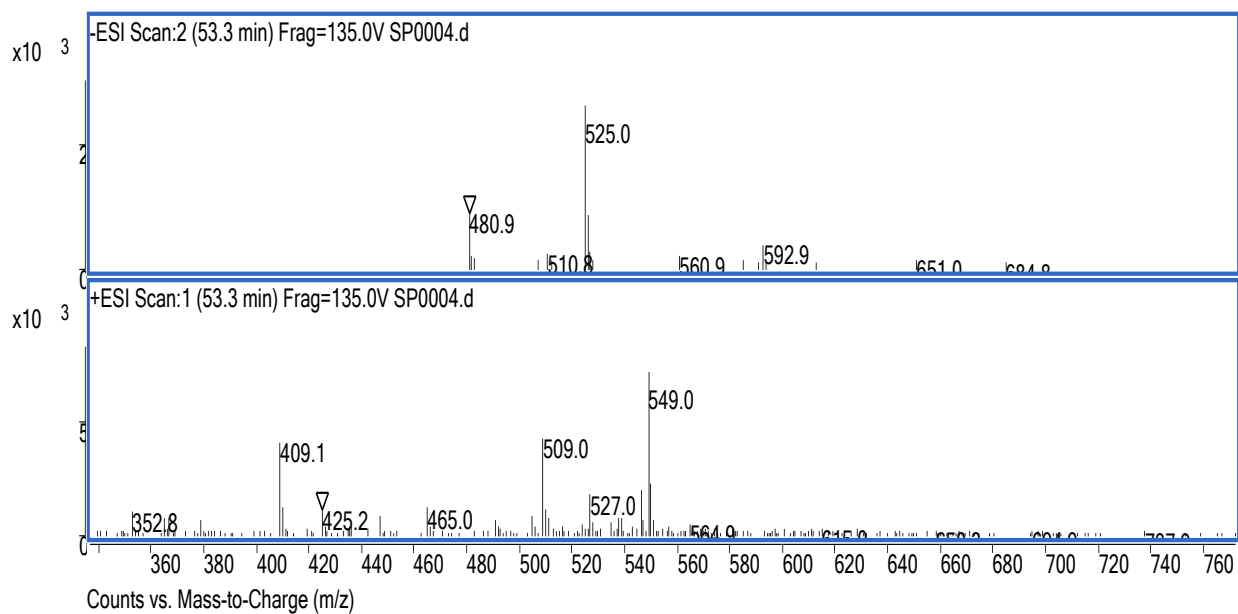
13.1 LC chromatogram at 280 nm

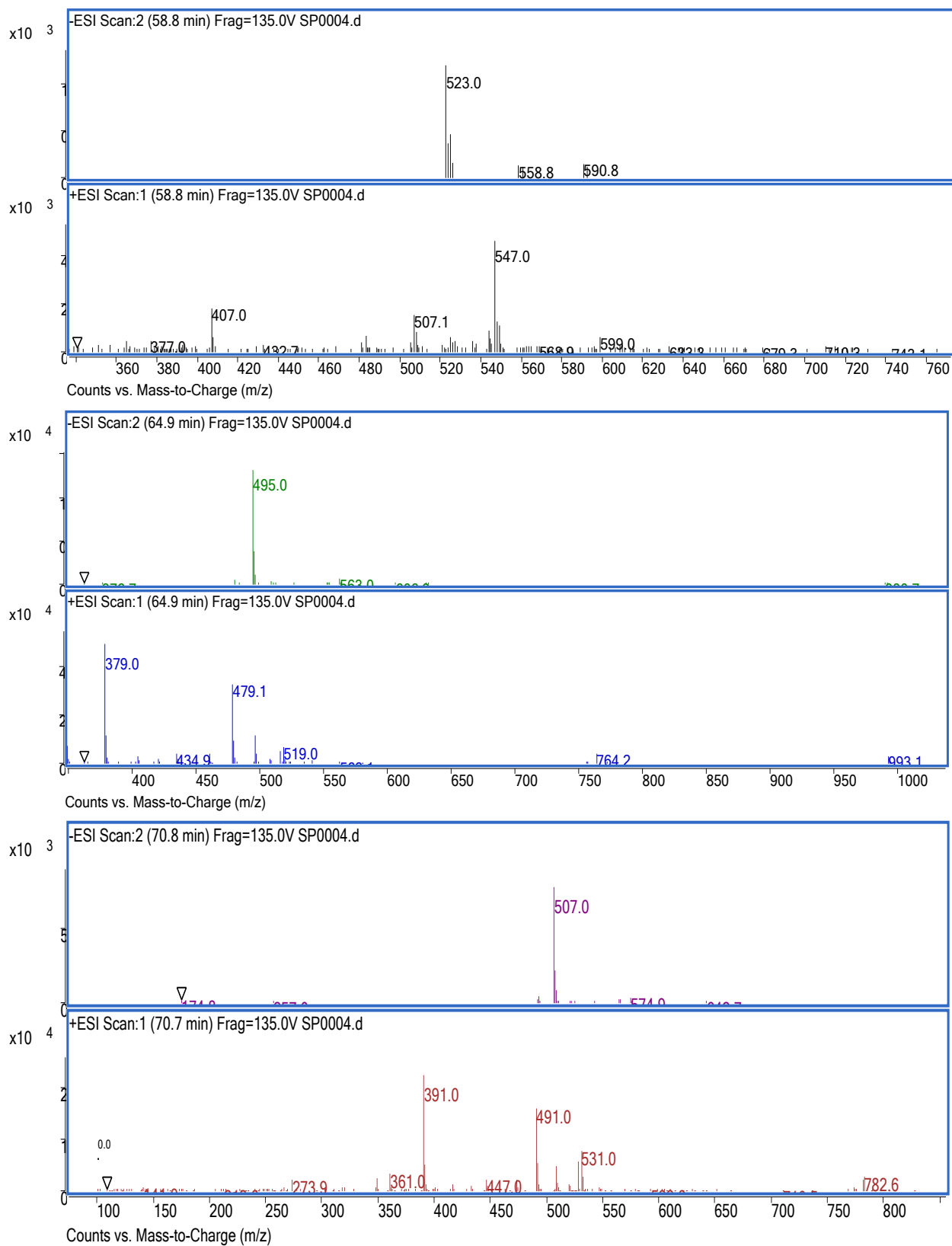


13.2. LCMS chromatogram in TIC mode



13.3. MS spectras of chrysomycins A-E





S14. Screenshots of DNP database search during dereplication

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Draw Query Clear Structure Structure Matching: Substructure [Troubleshoot Structure Search](#)

Add Property Clear Properties

Boolean	Property	Comparison	Value
AND	Biological Source		streptomyces browse... clear

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Structure Matching: [Troubleshoot Structure Search](#)

Boolean	Property	Comparison	Value
AND	Biological Source		streptomyces [browse...] [clear]
AND	Accurate Mass	Range	496.00 - 496.999 [browse min...] [browse max...] [clear]

Search Results

Page 1 of 1

Found 18 matches from 251230 documents.

Details	Chemical Name	Molecular Formula
<input type="checkbox"/>	Antibiotic EI 1625-2	C ₂₇ H ₃₂ N ₂ O ₇
<input type="checkbox"/>	Antibiotic X 14885A	C ₂₇ H ₃₂ N ₂ O ₇
<input type="checkbox"/>	Chrysomycin B	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Chrysomycin B; 1'-Epimer (?)	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Cytosaminomycin C	C ₂₃ H ₃₆ N ₄ O ₈
<input type="checkbox"/>	Cytosaminomycin D	C ₂₃ H ₃₆ N ₄ O ₈
<input type="checkbox"/>	Gilvocarcin V; 6-Alcohol	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Gilvocarcin V; 1",2"-Dihydro	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Kinamycin F; 1,2,4-Tri-Ac	C ₂₄ H ₂₀ N ₂ O ₁₀
<input type="checkbox"/>	Kinamycin F; 2,3,4-Tri-Ac	C ₂₄ H ₂₀ N ₂ O ₁₀
<input type="checkbox"/>	Kotomycin	C ₂₉ H ₂₈ N ₄ O ₄
<input type="checkbox"/>	Lansai A; N ¹ -Me	C ₃₁ H ₃₆ N ₄ O ₂
<input type="checkbox"/>	Leptomycin B; 21-Demethyl, 1-alcohol, 1-deoxy	C ₃₂ H ₄₈ O ₄
<input type="checkbox"/>	Napyradiomycin A ₁ ; 18-Hydroxy	C ₂₅ H ₃₀ Cl ₂ O ₆
<input type="checkbox"/>	Napyradiomycin A ₁ ; Δ ¹⁷ -Isomer, 16R-hydroxy	C ₂₅ H ₃₀ Cl ₂ O ₆
<input type="checkbox"/>	Prostatin	C ₂₅ H ₄₄ N ₄ O ₆
<input type="checkbox"/>	Ribostamycin; 3-N-Ac	C ₁₉ H ₃₆ N ₄ O ₁₁
<input type="checkbox"/>	Staurosporine; 4'-N-Hydroxy, 4'-N-de-Me, 4'-N-formyl	C ₂₈ H ₂₄ N ₄ O ₅

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[Add Property](#) [Clear Properties](#)

Boolean	Property	Comparison	Value
AND	Biological Source		<input type="text" value="streptomyces"/> [browse...] [clear]
AND	Accurate Mass	Range	<input type="text" value="496.00"/> - <input type="text" value="496.999"/> [browse min...] [browse max...] [clear]
AND	UV Maxima	=	<input type="text" value="244"/> [browse...] [clear]

Search Results

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Details	Chemical Name	Molecular Formula
<input type="checkbox"/>	Chrysomycin B; 1'-Epimer (?)	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Napyradiomycin A ₁ ; 18-Hydroxy	C ₂₅ H ₃₀ Cl ₂ O ₆

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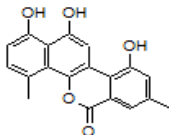
S15. Screenshots of DNP substructure search using basic naphthocoumarin skeleton

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[Add Property](#) [Clear Properties](#)

Boolean	Property	Comparison	Value	Delete
AND	Chemical Name		<input type="text"/> [browse...] [clear]	<input type="checkbox"/>
AND	Molecular Formula		<input type="text"/> [browse...] [clear]	<input type="checkbox"/>
AND	Molecular Formula by Element	= C	<input type="text"/> [clear]	<input type="checkbox"/>
AND	CAS Registry Nos.		<input type="text"/> [browse...] [clear]	<input type="checkbox"/>
AND	All Text		<input type="text"/> [browse...] [clear]	<input type="checkbox"/>
AND	Melting Point	=	<input type="text"/> [browse...] [clear]	<input type="checkbox"/>
AND	Boiling Point	=	<input type="text"/> [browse...] [clear]	<input type="checkbox"/>

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Details	Chemical Name	Molecular Formula
<input type="checkbox"/>	Chrysoycin A	C ₂₈ H ₃₂ O ₉
<input type="checkbox"/>	Chrysoycin A; 1'-Epimer(?)	C ₂₈ H ₃₂ O ₉
<input type="checkbox"/>	Chrysoycin B	C ₂₇ H ₃₀ O ₉
<input type="checkbox"/>	Chrysoycin B; 1'-Epimer(?)	C ₂₇ H ₃₀ O ₉
<input type="checkbox"/>	Gilvocarcin M	C ₂₆ H ₂₈ O ₉
<input type="checkbox"/>	Gilvocarcin M; 4'-Hydroxy	C ₂₆ H ₂₈ O ₁₀
<input type="checkbox"/>	Gilvocarcin M; 1'-Oxo	C ₂₆ H ₂₄ O ₁₀
<input type="checkbox"/>	Gilvocarcin V	C ₂₇ H ₂₈ O ₉
<input type="checkbox"/>	Gilvocarcin V; 1',2'-Dihydro	C ₂₇ H ₃₀ O ₉
<input type="checkbox"/>	Gilvocarcin V; 4'-Hydroxy	C ₂₇ H ₂₈ O ₁₀
<input type="checkbox"/>	Gilvocarcin V; 4'-Hydroxy, 1',2'-dihydro	C ₂₇ H ₃₀ O ₁₀
<input type="checkbox"/>	Ravidomycin	C ₃₁ H ₃₃ NO ₉
<input type="checkbox"/>	Ravidomycin; O-De-Ac	C ₂₉ H ₃₁ NO ₈
<input type="checkbox"/>	Ravidomycin; O-De-Ac, N-oxide	C ₂₉ H ₃₁ NO ₉
<input type="checkbox"/>	Ravidomycin; N-De-Me, O-de-Ac, N-Ac	C ₃₀ H ₃₁ NO ₉
<input type="checkbox"/>	Ravidomycin; N-De-Me, O-de-Ac	C ₂₈ H ₂₉ NO ₉
<input type="checkbox"/>	Ravidomycin; N-De-Me	C ₃₀ H ₃₁ NO ₉
<input type="checkbox"/>	Ravidomycin; Di-Ac	C ₃₅ H ₃₇ NO ₁₁
<input type="checkbox"/>	Ravidomycin; N,N-Di-de-Me, N-Ac	C ₃₁ H ₃₁ NO ₁₀
<input type="checkbox"/>	Ravidomycin; 1',2'-Dihydro	C ₃₁ H ₃₃ NO ₉
<input type="checkbox"/>	Ravidomycin; 1',2'-Dihydro, O-de-Ac	C ₂₉ H ₃₃ NO ₈
<input type="checkbox"/>	Ravidomycin; 1',2'-Dihydro, di-Ac	C ₃₅ H ₃₉ NO ₁₁
<input type="checkbox"/>	Ravidomycin; 1',2'-Dihydro, 1'-hydroxy	C ₃₁ H ₃₅ NO ₁₀
<input type="checkbox"/>	Ravidomycin; 1',2'-Epoxide	C ₃₁ H ₃₃ NO ₁₀
<input type="checkbox"/>	Ravidomycin; N-Oxide	C ₃₁ H ₃₃ NO ₁₀
<input type="checkbox"/>	Ravidomycin M	C ₃₀ H ₃₃ NO ₉
<input type="checkbox"/>	Ravidomycin M; O-De-Ac	C ₂₈ H ₃₁ NO ₈