Article

Loseolamycins: a group of new bioactive alkylresorcinols produced after heterologous expression of a type III PKS from *Micromonospora endolithica*

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Received: date; Accepted: date; Published: date

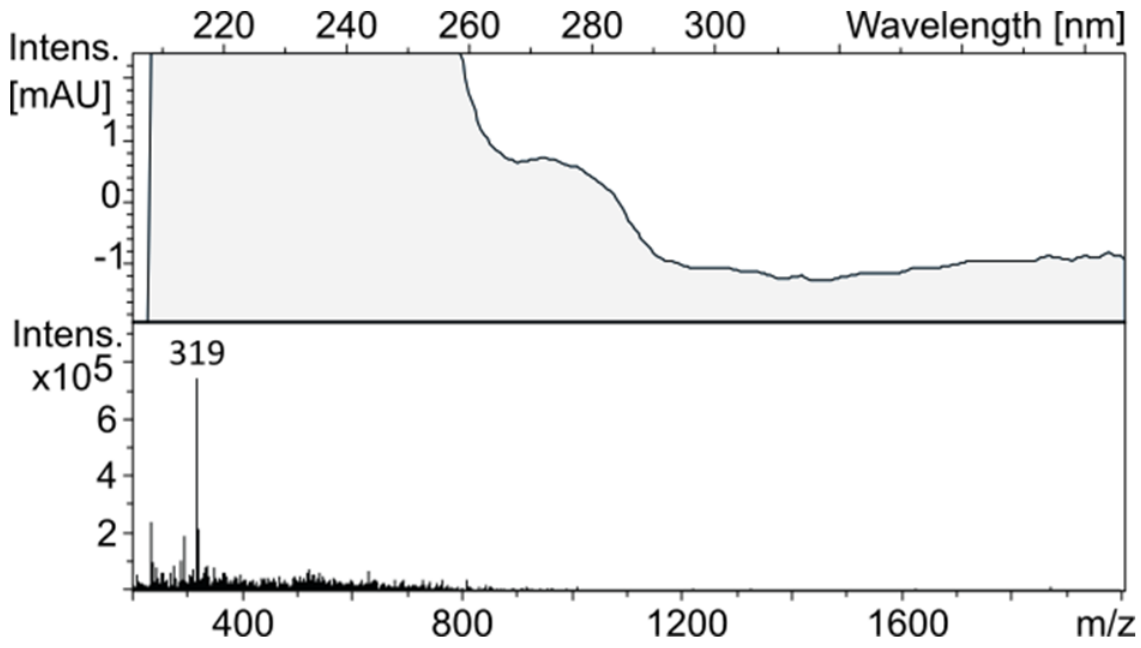

Figure S1. *UV/Vis spectrum of loseolamycin A1.*

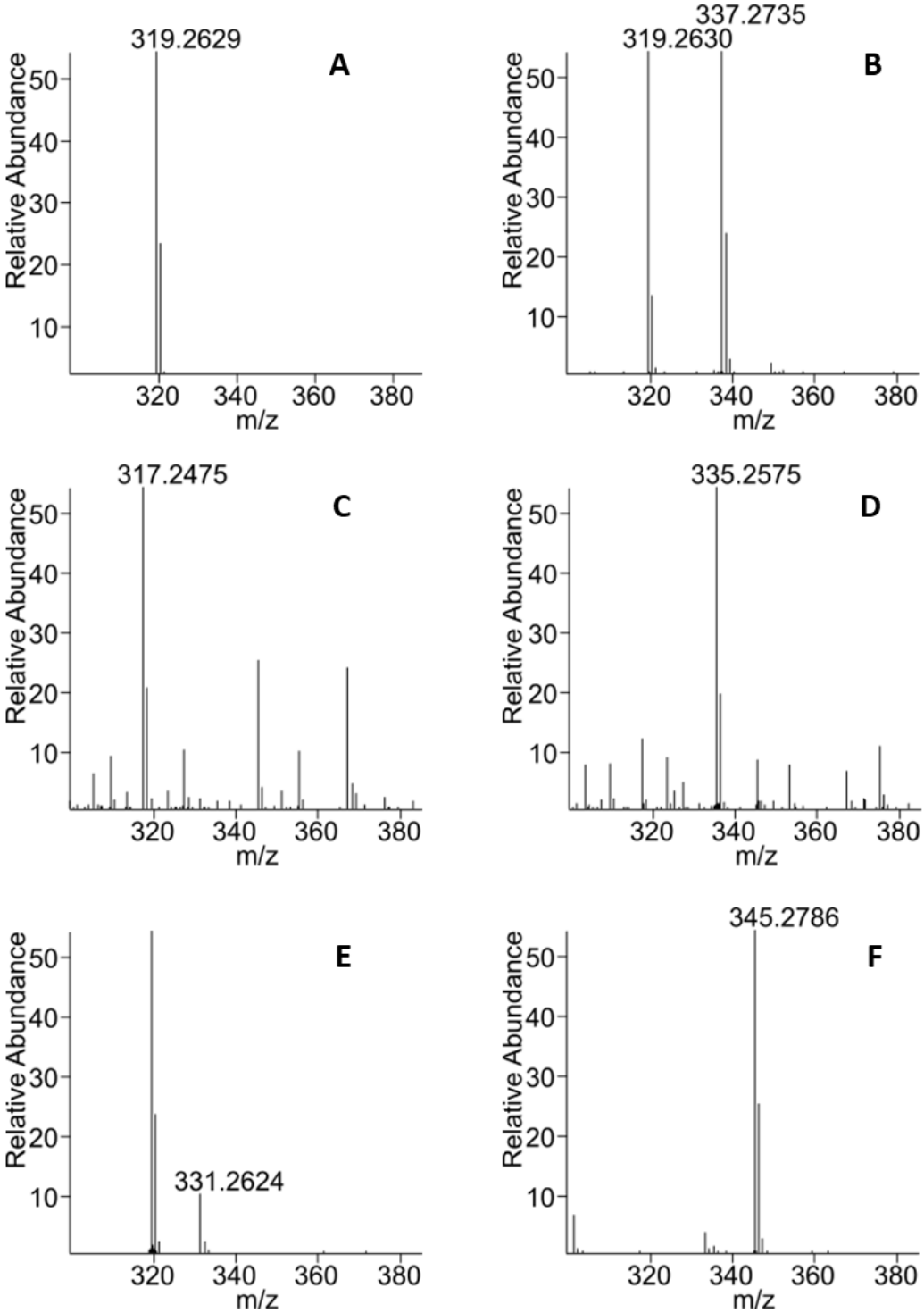

Figure S2. *Mass spectra of loseolamycins using positive ionization mode. A - compound* ***1****, B – compound* ***2****, C – compound* ***3****, D – compound* ***4****, E – compound* ***5****, F – compound* ***6****.*

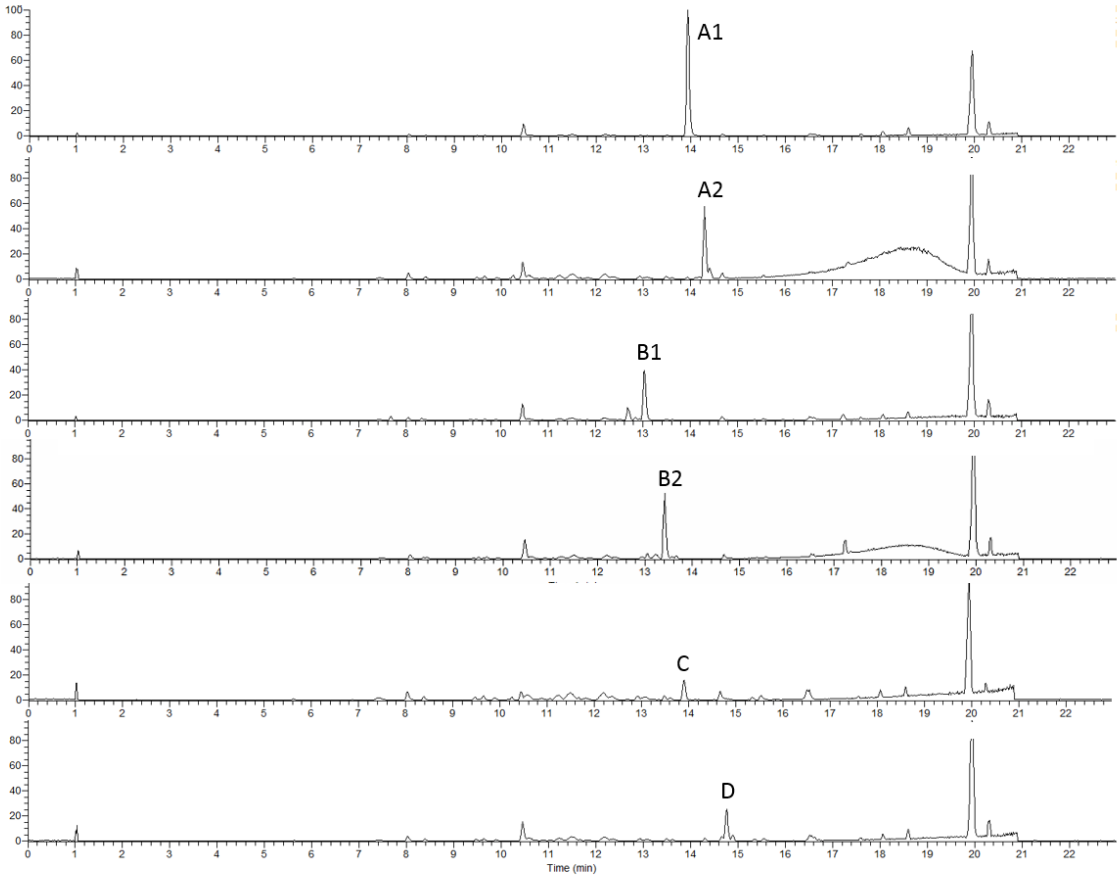

Figure S3. *Purity of the isolated loseolamycin derivatives A1 (compound **1**), A2 (compound **2**), B1 (compound **3**), B2 (compound **4**), C (compound **5**) and D (compound **6**) after two chromatographic steps. Base Peak Chromatograms (BPC) are shown.*

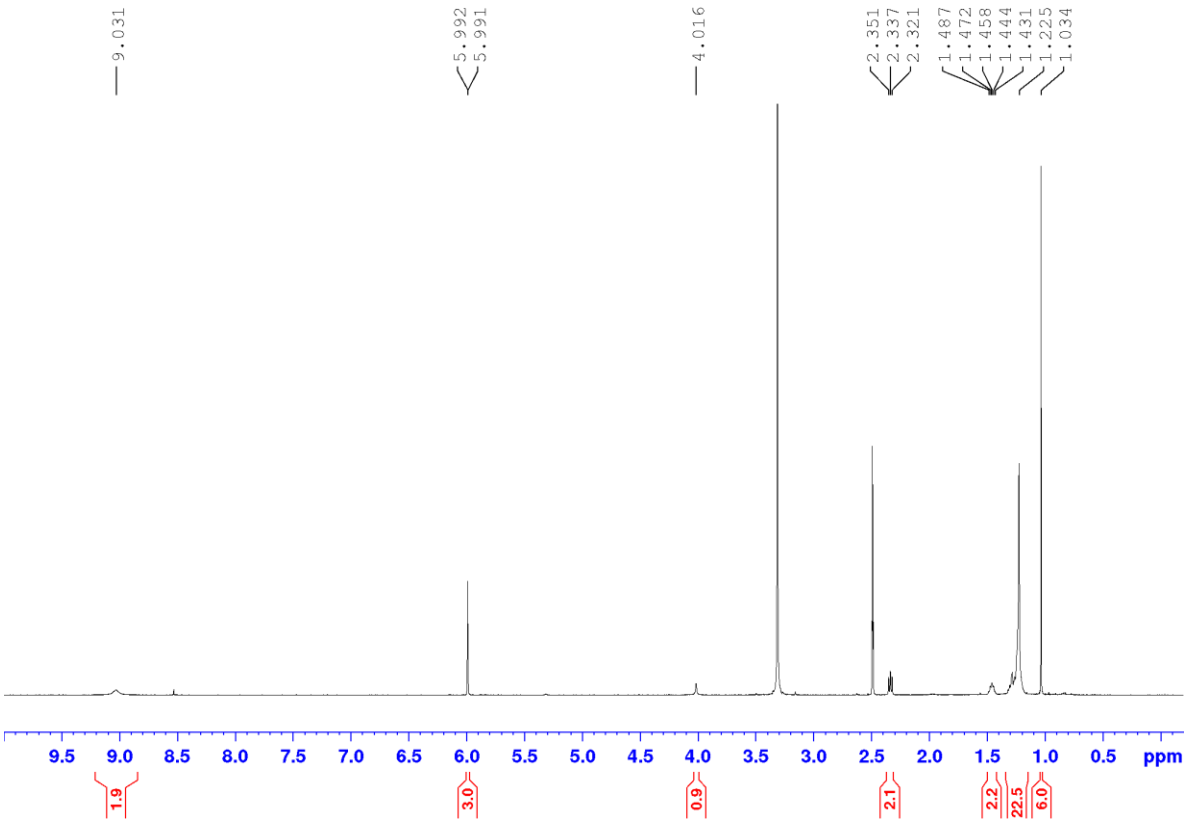

Figure S4. *^{1}H-NMR spectrum (500 MHz, DMSO-d6) of loseolamycin A1, complete spectrum.*

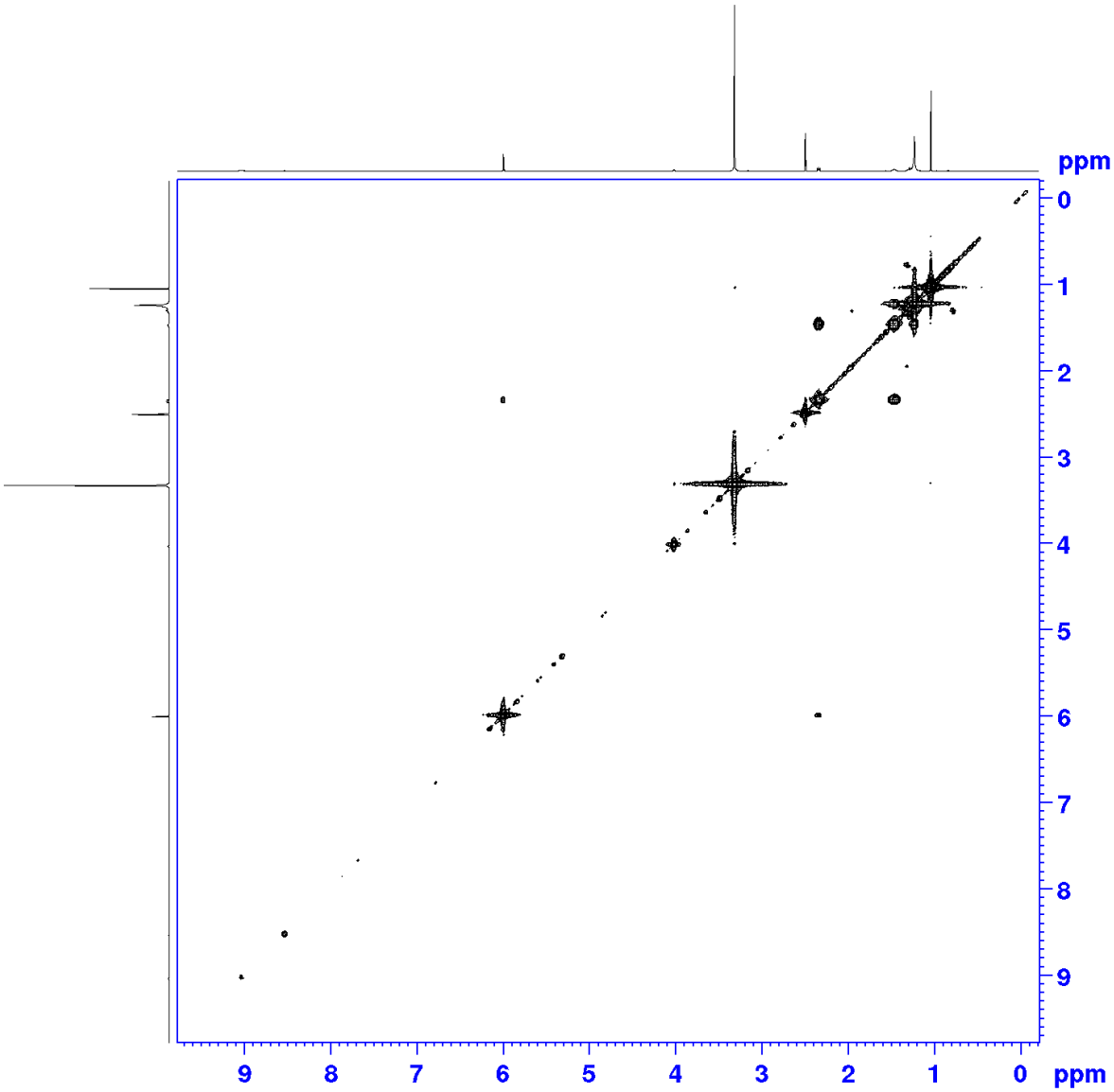

Figure S5. *^{1}H-^{1}H-COSY spectrum (500 MHz, DMSO-d6) of loseolamycin A1, complete spectrum.*

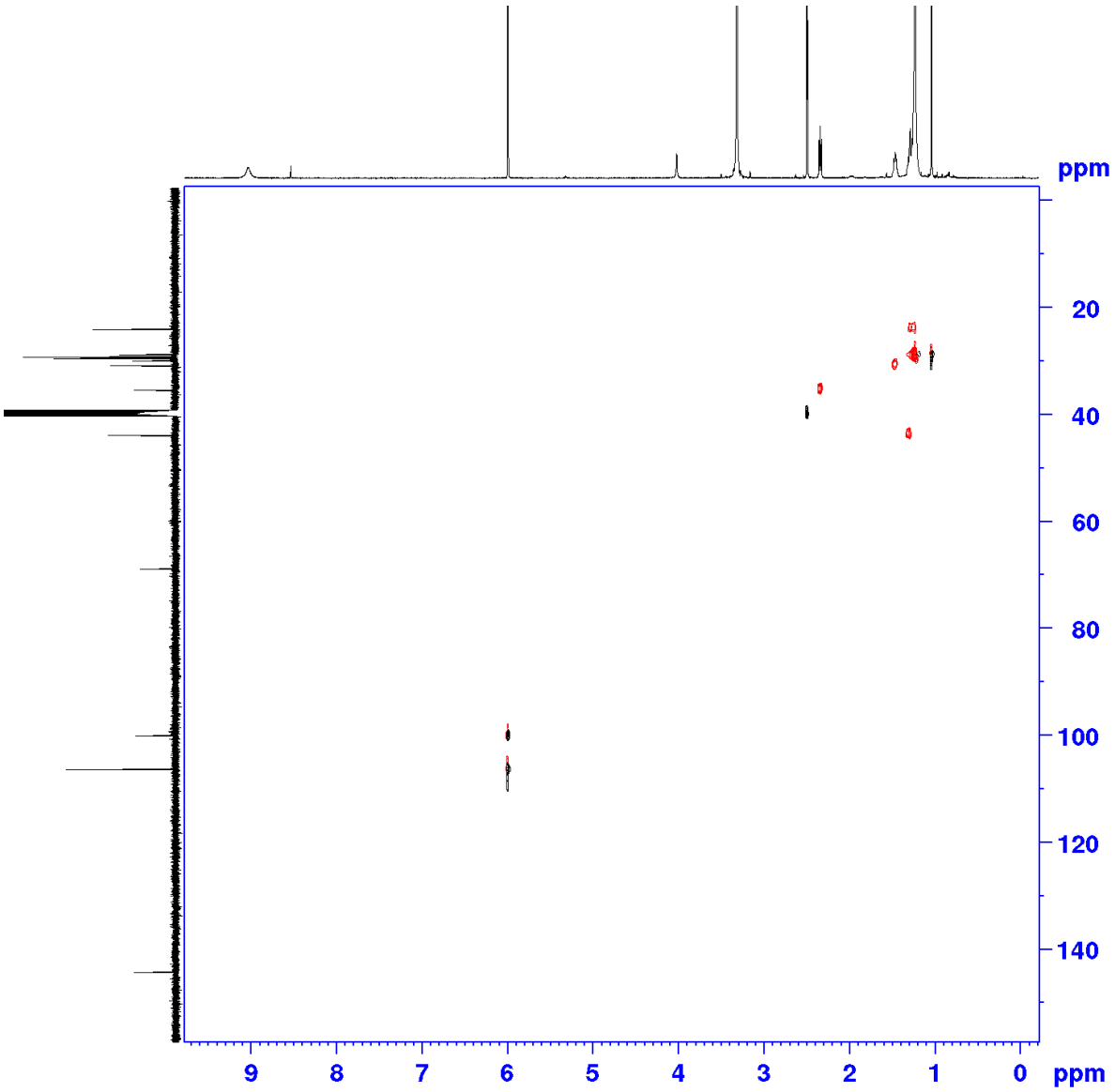

Figure S6. *HSQC-spectrum (500 MHz; 125 MHz, DMSO-d6) of loseolamycin A1, complete spectrum.*

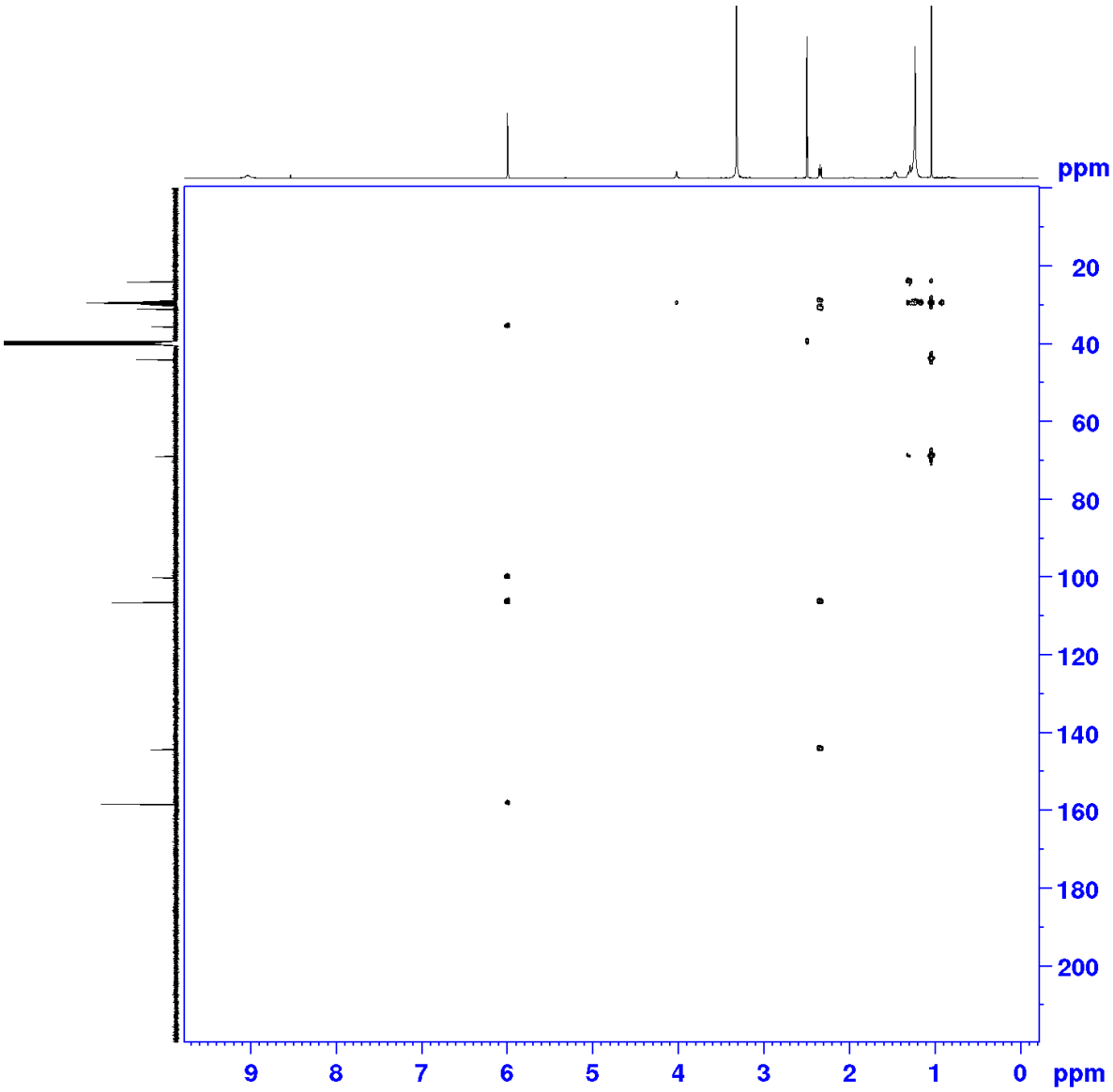

Figure S7. *HMBC-spectrum (500 MHz; 125 MHz, DMSO-d6) of loseolamycin A1, complete spectrum.*

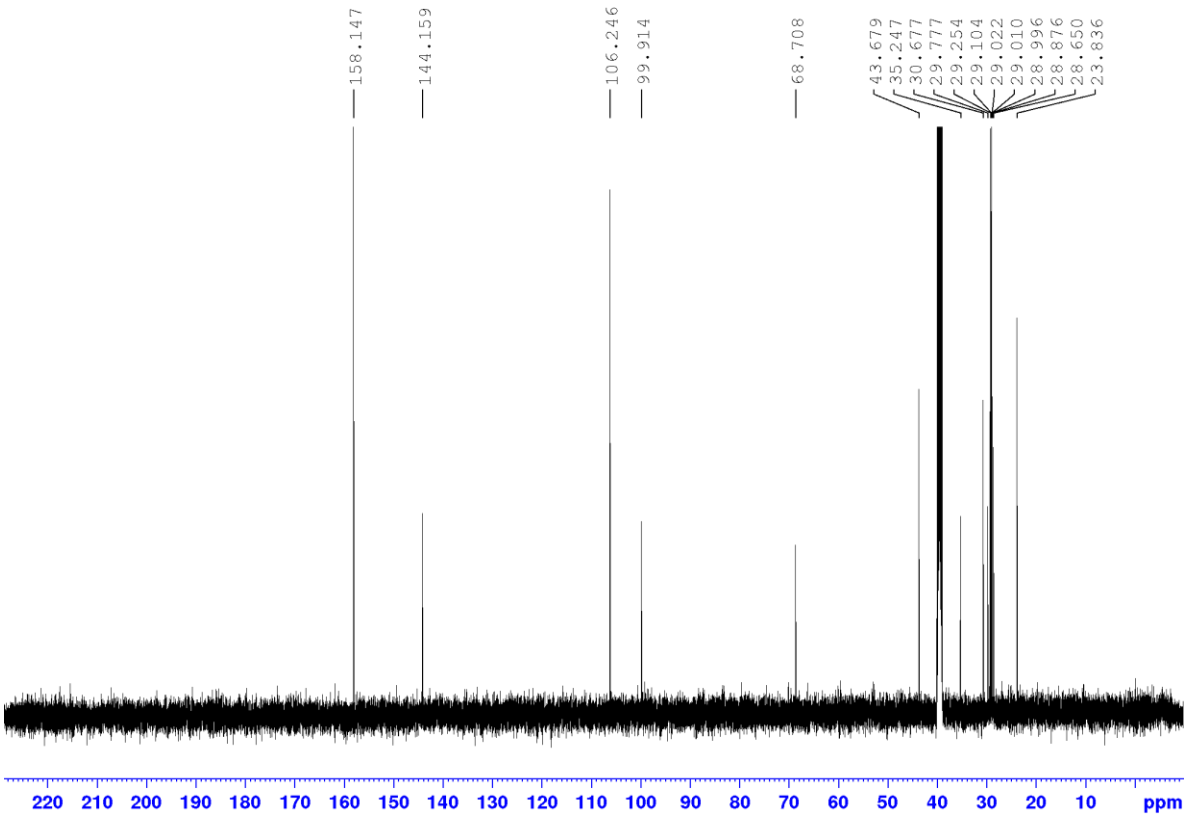

Figure S8. *^{13}C-spectrum (125 MHz, DMSO-d6) of loseolamycin A1, complete spectrum.*

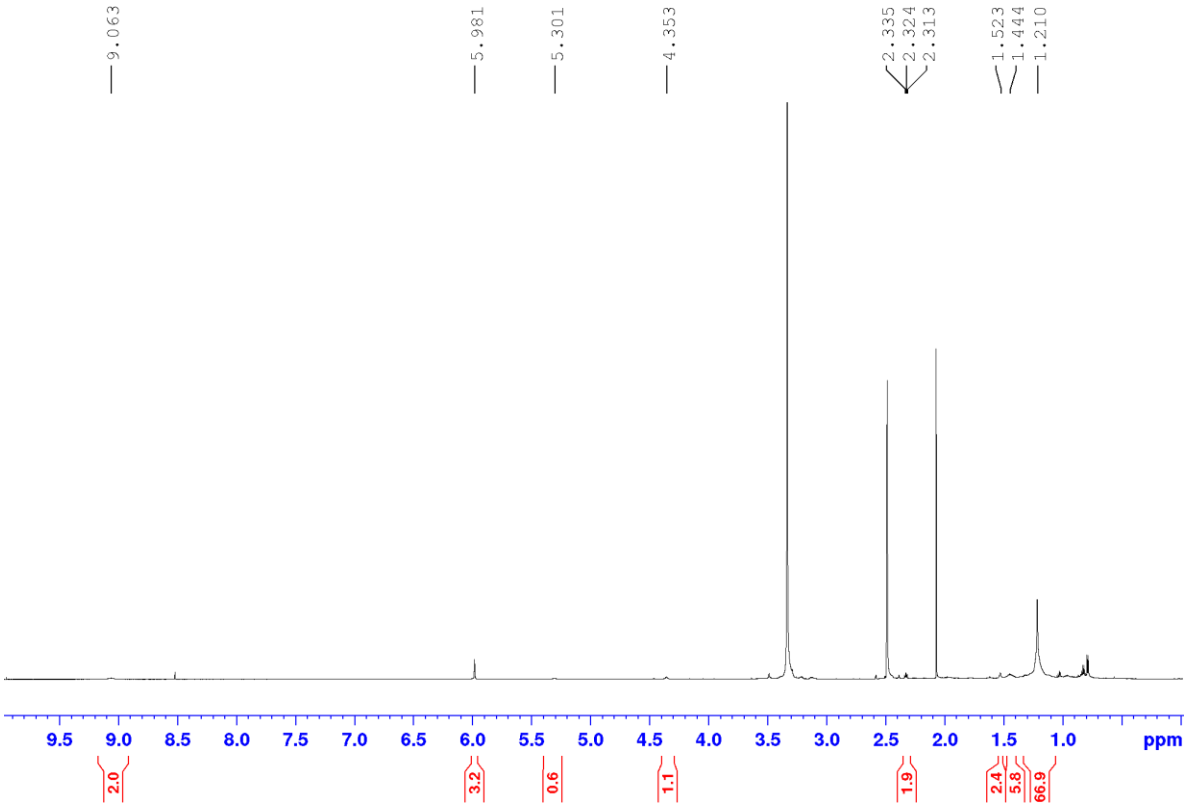

Figure S9. *^{1}H-NMR spectrum (500 MHz, DMSO-d6) of loseolamycin A2, complete spectrum.*

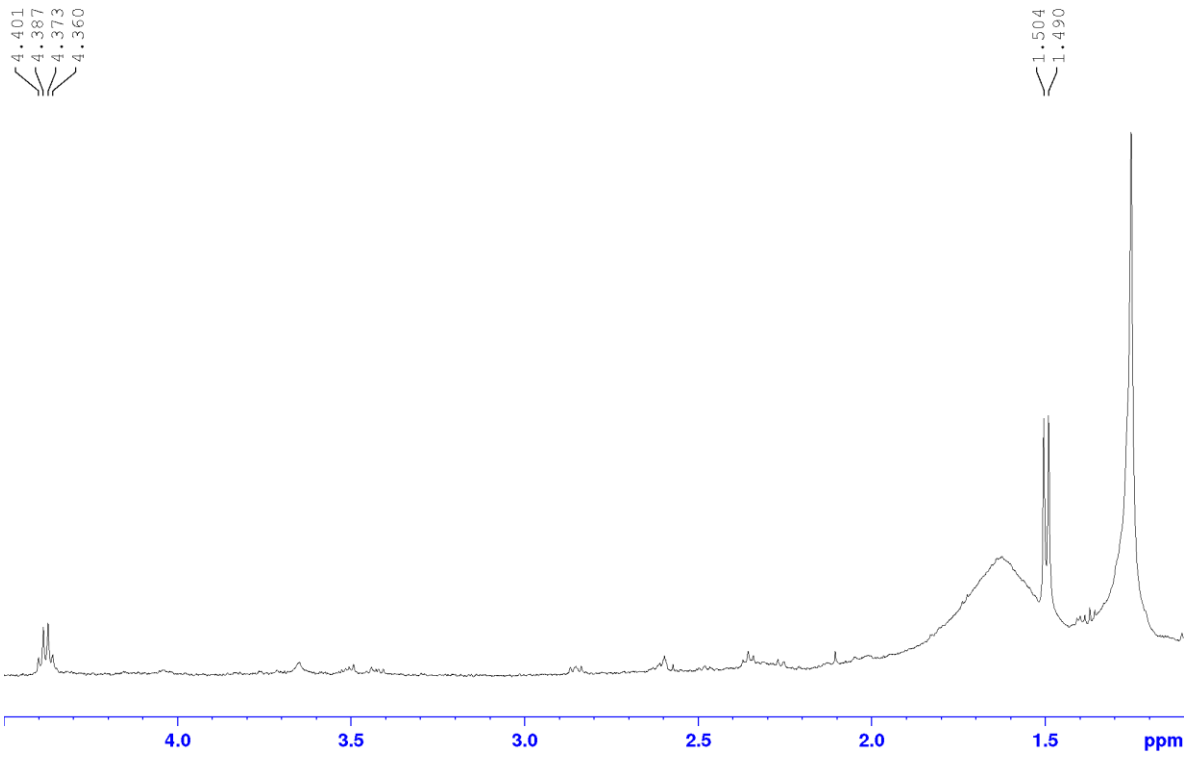

Figure S10. *^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of loseolamycin A2, zoomed from 1.0 – 4.5 ppm.*

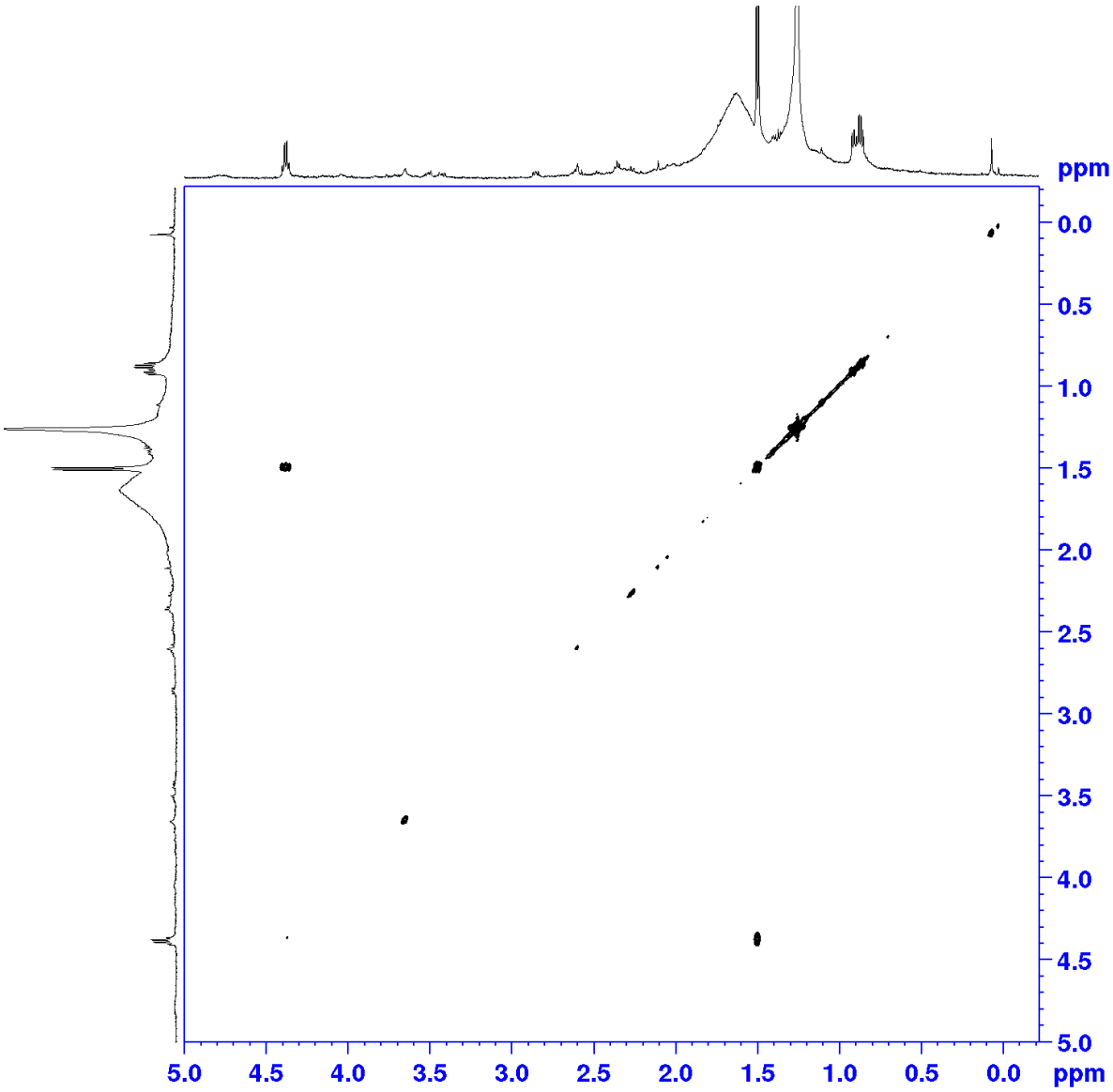

Figure S11. *^{1}H-^{1}H -COSY (500 MHz, $CDCl_3$) of loseolamycin A2, zoomed from 1.0 – 4.5 ppm.*

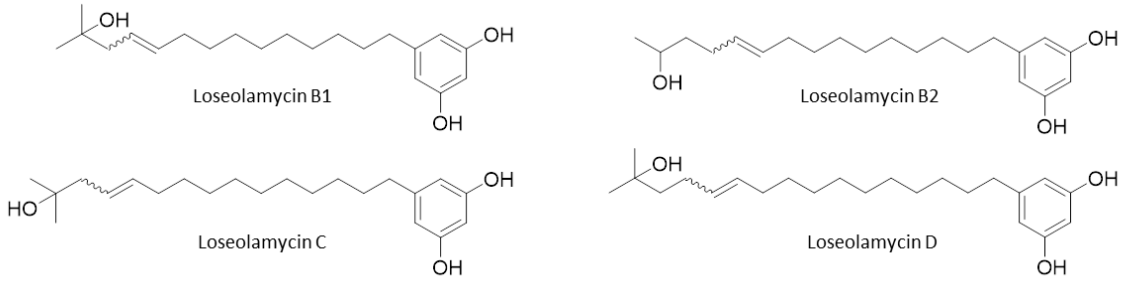

Figure S12. *Proposed structures of loseolamycins B1 (compound **3**), B2 (compound **4**), C (compound **5**) and D (compound **6**) based on MS/MS experiments.*

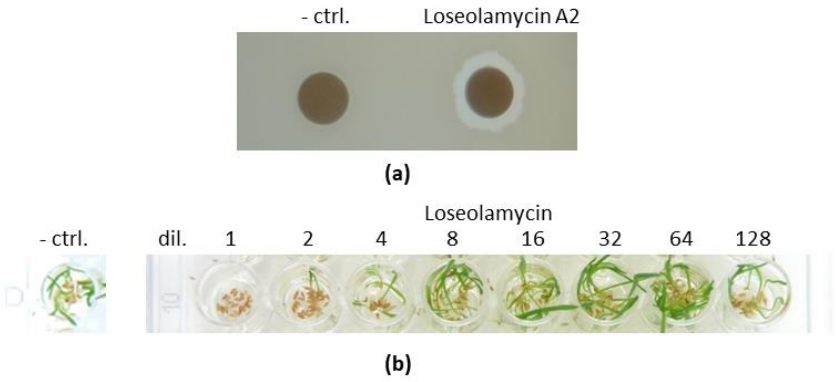

Figure S13. *Antibacterial and herbicidal activity. (a) Loseolamycin A2 on a filter disc inhibits the growth of B. subtilis. The sample's solvent methanol was used as negative control (- ctrl) and shows no inhibition zone. (b) A mixture of loseolamycin derivatives inhibits germination of the weed Agrostis stolonifera. The phytotoxic effect was reproduced once and is concentration dependent. Methanol in plant medium was used as negative control (- ctrl) and shows no inhibition of seed germination.*

Table S1. *Organisms, BACs, plasmids and primer used in this work.*

Material	Purpose
A. Organisms	
Micromonospora endolithica LU17765	originating strain of type III PKS [BASF]
Streptomyces albus Del14	optimized heterologous host [1]
Escherichia coli GB05 RedCC	cloning host [Helmholtz-Institut für Pharmazeutische Forschung Saarland (HIPS)]
Escherichia coli ET12567 pUB307	alternate host intergeneric conjugation [2]
Escherichia coli GB 2005	bioactivity test
Pseudomonas putida KT2440	bioactivity test
Bacillus subtilis ATCC 6633	bioactivity test
Agrostis stolonifera	bioactivity test
B. BACs	
I7 [IG652BAC1-2]	heterologous expression of type III PKS [GenBank: MT904273]
I7act	heterologous expression of promoter activated type III PKS
C. Plasmids	
pUC19	promoter TS61 / ampicillin resistance marker
D. PCR primer	
20180710_02_fw [I7act]	TGAATCAGATTTGCGAGTCCCGCAGTCGCGAACGGACCGGACTCGTTGGTCGTCAGGTGGCACTTTTCG
20180710_02_rev [I7act]	CACCGGCACGCCCATGTCCCCCACCTCTCGTCCCCGATCCCCCACGCTTCGCGGATATCCTACTATGCCGAGGTATAATGTAGCCAGCGTGTTACCAATGCTTAATCAGTG

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[2] F. Flett, V. Mersinias, C.P. Smith, High efficiency intergeneric conjugal transfer of plasmid DNA from Escherichia coli to methyl DNA-restricting streptomycetes, FEMS Microbiol. Lett. 155 (2006) 223–229. https://doi.org/10.1111/j.1574-6968.1997.tb13882.x.