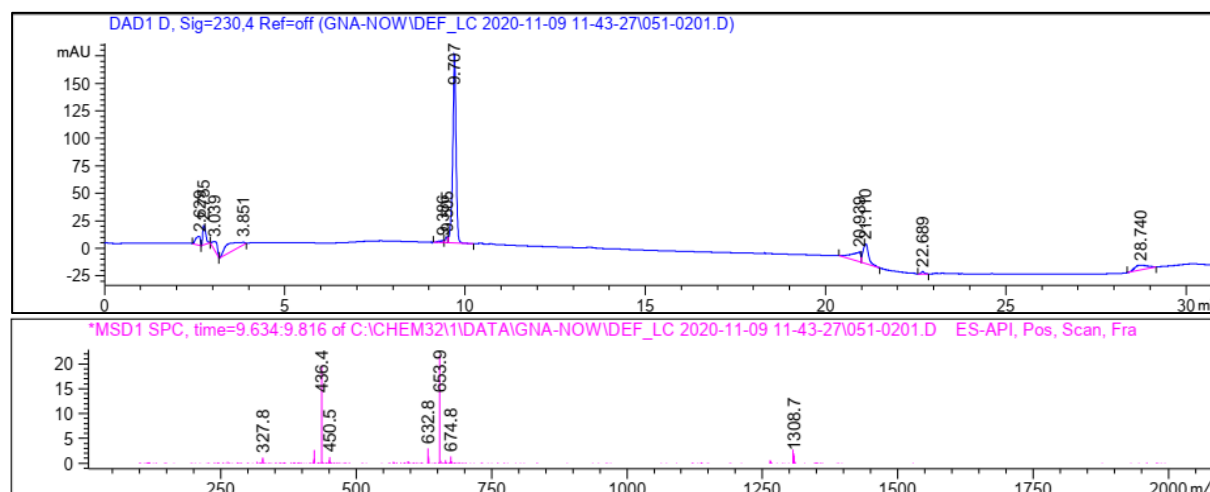


Fig. S4. LC-MS analysis of NOSO-95C and acetylated derivatives after *in vitro* acetylation (see Materials and Methods) at different times of reaction (15 min, 4h, or 24h) with Acetyl-CoA (**B**), or Odilorhabdin acetyltransferase A (OatA) (**C**), or both (**A**). For each tested condition, a table and corresponding LC-MS chromatograms present observed ions with retention time, peak area and suggested compounds. LC-MS were performed on an Agilent 1260 Infinity HPLC system with a Waters Symmetry analytical C18 column (5 μm , 4.6 mm \times 150 mm). We injected 10 μL of reaction mixture into the apparatus, the flow rate was set to 0.7 mL/min and UV detection was performed at 220, 230 and 250 nm. The following mobile phases were used: A: 0.1% trifluoroacetic acid in water; B: acetonitrile. The following gradient was used: 2 to 30% of B in A from 0 to 15 min. ESI-LC-MS data were obtained in positive mode on an Agilent 1260 Infinity system (Agilent 6120 Quadrupole LC/MS, 1260 Quaternary Pump, 1260 ALS, 1260 TCC, 1260 DAD VL, 1260 FC-AS).

A: Odilorhabdin acetyltransferase A (OatA) + acetyl-CoA + NOSO-95C (400 $\mu\text{g}/\text{mL}$)

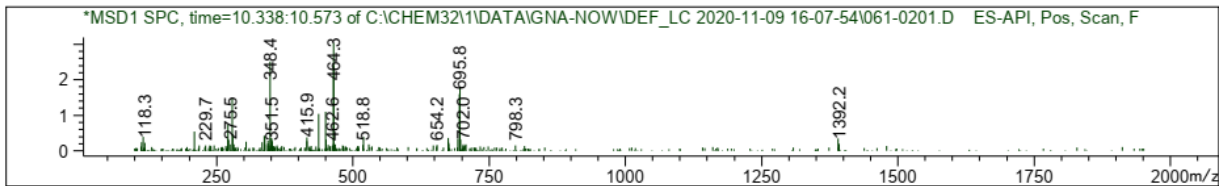
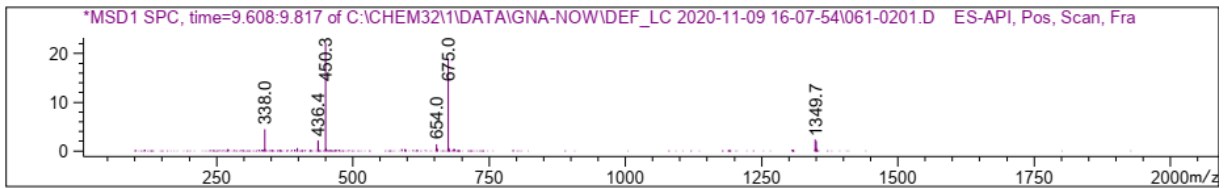
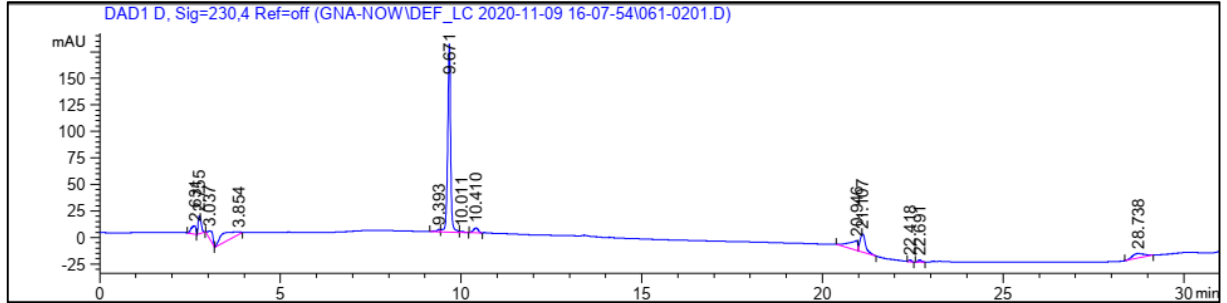
- Incubation time: 15 min

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.71	1106	[M+H] ⁺ : 1308.7 [M+2H] ²⁺ : 632.8 [M+2H] ²⁺ : 653.9 [M+2H] ²⁺ : 674.8	Mono-Acetylated NOSO-95C NOSO-95C Mono-Acetylated NOSO-95C Bi-acetylated NOSO-95C



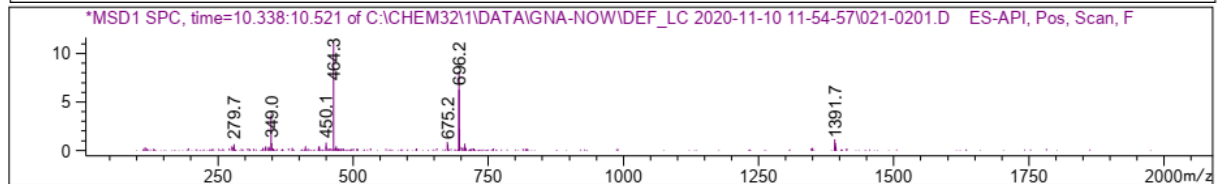
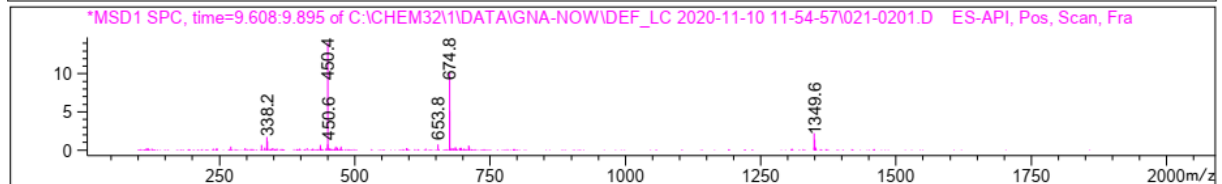
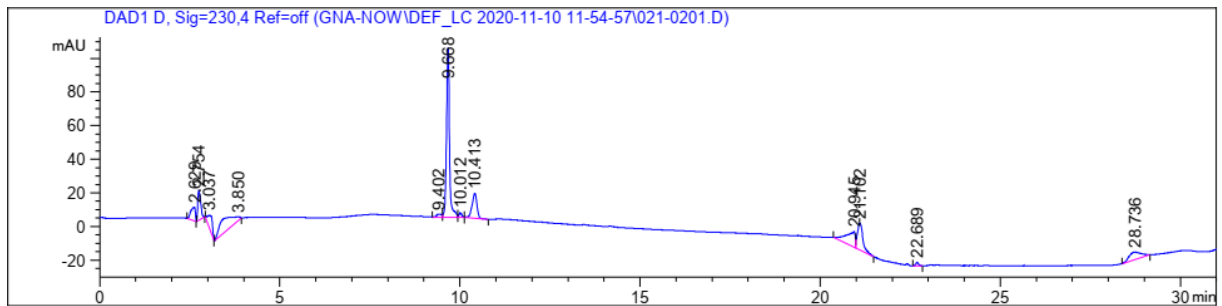
- Incubation time : 4h

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.67	1001	[M+H] ⁺ : 1349.7 [M+2H] ²⁺ : 654.0 [M+2H] ²⁺ : 675.0	Bi-Acetylated NOSO-95C Mono-Acetylated NOSO-95C Bi-Acetylated NOSO-95C
10.41	40	[M+H] ⁺ : 1392.2 [M+2H] ²⁺ : 695.8	Tri-Acetylated NOSO-95C Tri-Acetylated NOSO-95C



- Incubation time : 24h

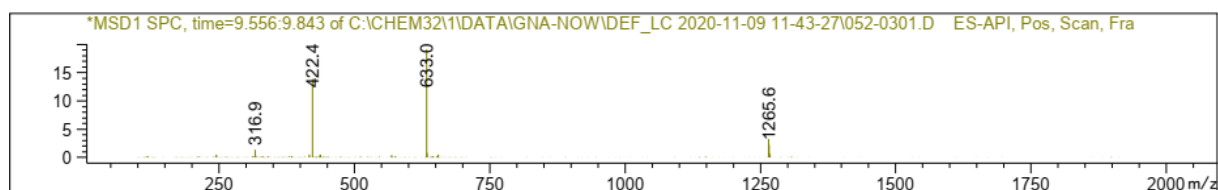
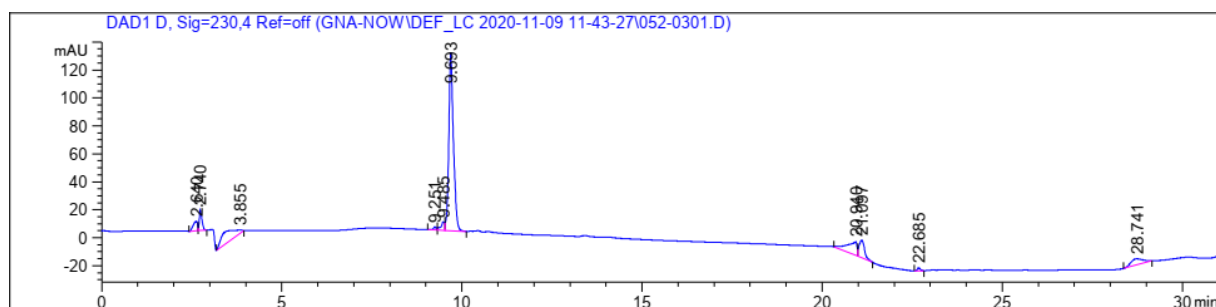
Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.67	579	[M+H] ⁺ : 1349.6 [M+2H] ²⁺ : 674.8	Bi-Acetylated NOSO-95C Bi-Acetylated NOSO-95C
10.41	137	[M+H] ⁺ : 1391.7 [M+2H] ²⁺ : 696.2	Tri-Acetylated NOSO-95C Tri-Acetylated NOSO-95C



B: Acetyl-CoA + NOSO-95C (400 µg/mL)

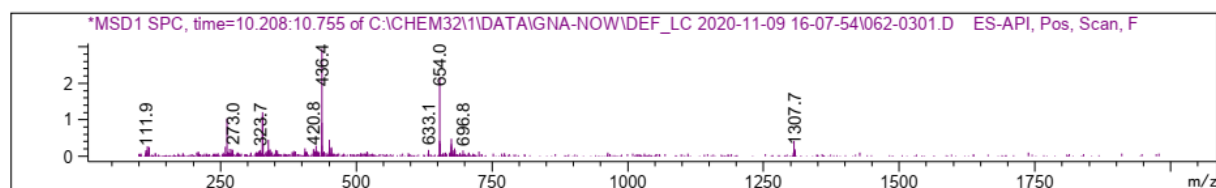
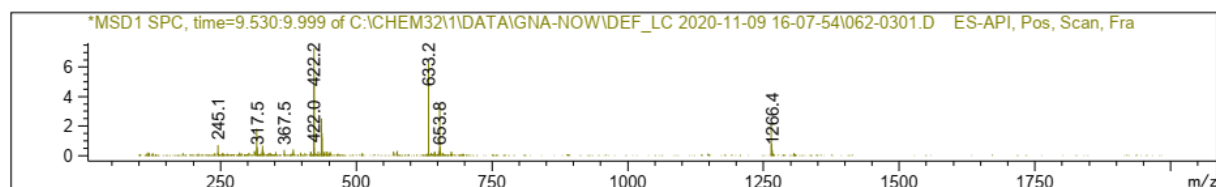
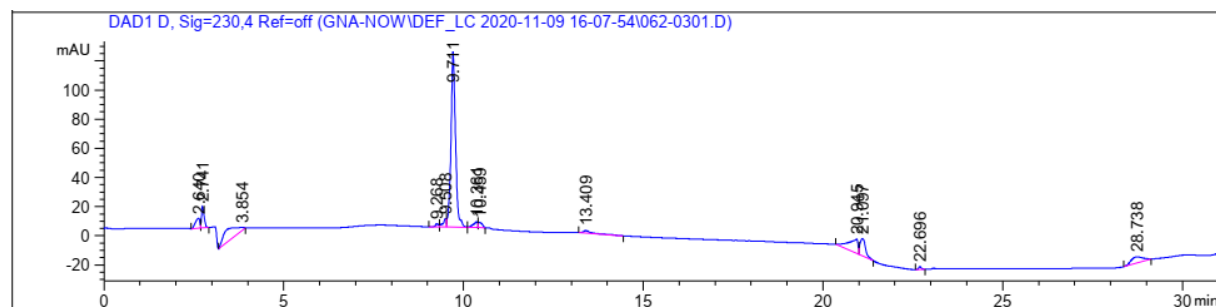
- Incubation time: 15 min

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.71	1139	[M+H] ⁺ : 1265.6 [M+2H] ²⁺ : 633.0	NOSO-95C NOSO-95C



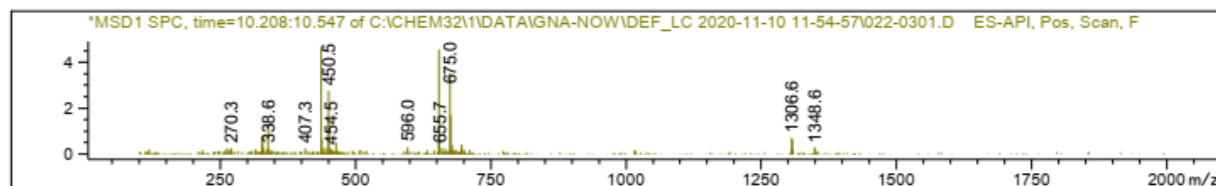
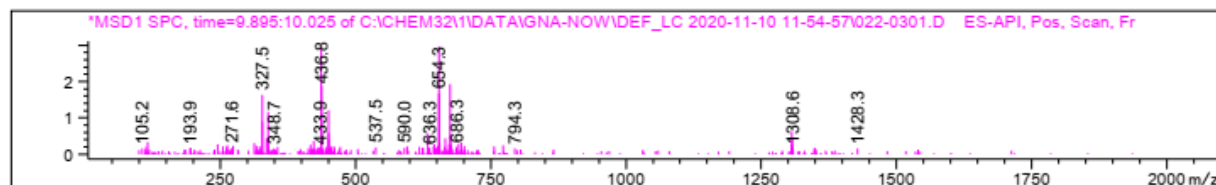
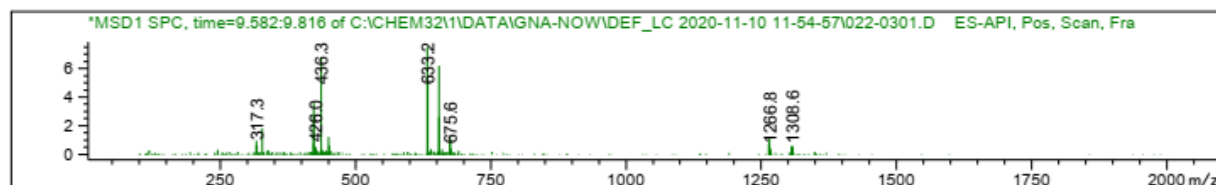
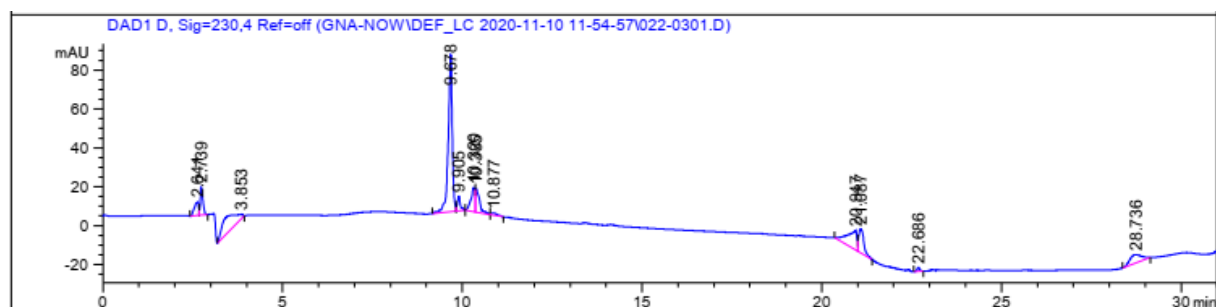
- Incubation time: 4h

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.71	1062	[M+H] ⁺ : 1266.4 [M+2H] ²⁺ : 633.2 [M+2H] ²⁺ : 653.8	NOSO-95C NOSO-95C Mono-Acetylated NOSO-95C
10.36	33	[M+H] ⁺ : 1307.7 [M+2H] ²⁺ : 654.0	Mono-Acetylated NOSO-95C Mono-Acetylated NOSO-95C



- Incubation time: 24h

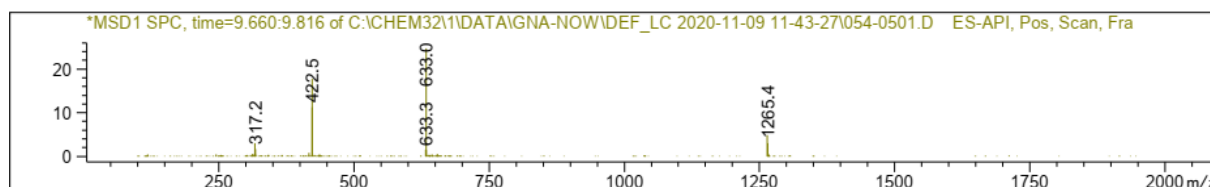
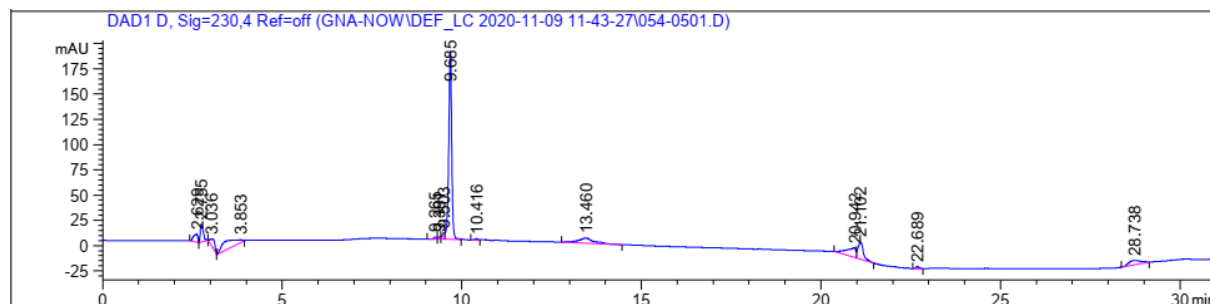
Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.68	625	[M+H] ⁺ : 1266.8 [M+H] ⁺ : 1308.6 [M+2H] ²⁺ : 633.2 [M+2H] ²⁺ : 654.0	NOSO-95C NOSO-95C Mono-Acetylated NOSO-95C Mono-Acetylated NOSO-95C
9.91	43	[M+H] ⁺ : 1308.6 [M+2H] ²⁺ : 654.3	Mono-Acetylated NOSO-95C Mono-Acetylated NOSO-95C
10.33	190	[M+H] ⁺ : 1306.6 [M+H] ⁺ : 1348.6 [M+2H] ²⁺ : 655.7 [M+2H] ²⁺ : 675.0	Mono-Acetylated NOSO-95C Bi-Acetylated NOSO-95C Mono-Acetylated NOSO-95C Bi-Acetylated NOSO-95C



C: Odilorhabdin acetyltransferase A (OatA)+ NOSO-95C (400 µg/mL)

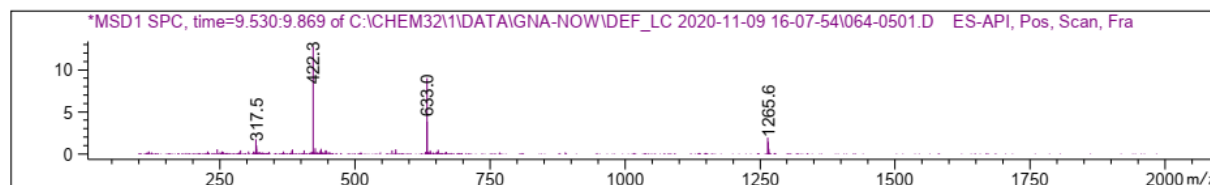
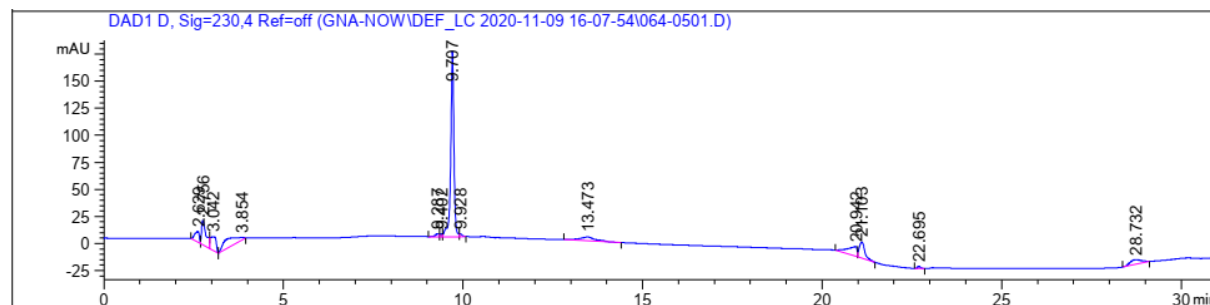
- Incubation time: 15 min

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.68	1084	[M+H] ⁺ : 1265.4 [M+2H] ²⁺ : 633.0	NOSO-95C NOSO-95C



- Incubation time: 4h

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.70	1071	[M+H] ⁺ : 1265.6 [M+2H] ²⁺ : 633.0	NOSO-95C NOSO-95C



- Incubation time: 24h

Retention time (min)	Peak Area (230 nm)	Ion mass	Proposed compound
9.64	964	[M+H] ⁺ : 1265.6 [M+2H] ²⁺ : 633.2	NOSO-95C

