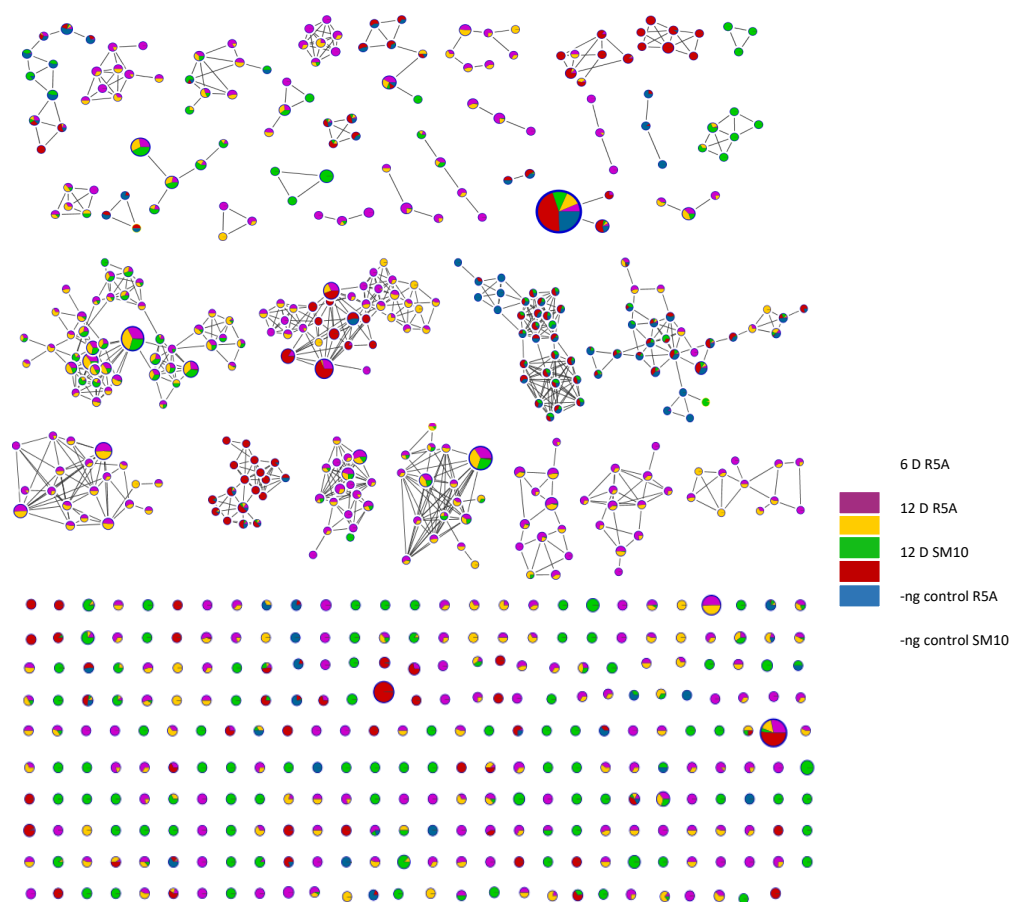


# Metabolomic Profiling and Molecular Networking of Nudibranch-Associated *Streptomyces* sp. SCSIO 001680

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**Figure S1.** Molecular network of metabolites produced by *Streptomyces* sp. SCSIO 001680 generated by Cytoscape 3.7.2.

**Table S1.** Spectral information (LC-MS/MS data) for compounds identified through GNPS. For all compounds: Ion source: LC-ESI; MS-Level: MS2; Instrument: qTOF; Ionization mode: Positive; MS Category: Experimental

Compound	MoNA ID	Exact Mass	Precursor Type	Precursor m/z	Top 5 peaks
Marineosin A	CCMSLIB00000001623	409.2837	M+H	410.2909	393.2656 361.2434 333.2522 319.2020 291.2099
Desferrioxamine E	CCMSLIB00000001622	600.348	M+Na	623.339	601.3568 201.1657 183.1604 102.1711 84.1714
Desferrioxamine D2	CCMSLIB00004698381	586.3326	[M+Na] <sup>+</sup>	609.322	509.31 409.22 309.21 223.14 123.09
Deferoxamine	CCMSLIB00005435927	560.353	M+H	561.3634	561.3634 319.2555 243.1670 201.1656 102.1716
Bisucaberin	CCMSLIB00005724304	400.232	M+H	401.25	401.2513 301.1620 201.1663 165.1553 102.1715

**Table S2.** Spectral information for compounds dereplicated on Marinlit. For all compounds: Ion source: LC-ESI; MS-Level: MS2; Instrument: qTOF; Ionization mode: Positive; MS Category: Experimental.

Compound	Energy level	Precursor Type	Precursor m/z	Exact Mass	Top 5 peaks
Halichoblelide	2	[M+H] <sup>+</sup>	1039.5786	1038.5763	1039.5786 1021.5662 955.5907 977.5794 959.5669
Streptodepsipeptide P11B	2	[M+H] <sup>+</sup>	1083.6068	1082.5999	1083.6068 1065.5952 1039.6166 1021.6066 1003.5950
Alternarin A	0	[M+H] <sup>+</sup>	495.2402	494.2338	495.2402 309.1772 189.1803 126.1707 84.1720
Alexandrolide	0	[M+H] <sup>+</sup>	528.3527	527.3458	528.3527 510.3418 212.1471 196.1563 156.1374
Pachastrelloside A	1	[M+H] <sup>+</sup>	783.4519	782.4452	721.4529 407.2175 331.2093 137.1232
Didemnaketal F	0	[M+H] <sup>+</sup>	853.4938	852.4871	835.4829 725.4085 707.3994 675.3744 319.2104