

Anti-Infective Discorhabdins from a Deep-Water Alaskan Sponge of the genus *Latrunculia*[†]

MinKyun Na,^{‡,§} Yuanqing Ding,[‡] Bin Wang,[‡] Babu L. Tekwani,[‡] Raymond F. Schinazi,[⊥] Scott Franzblau,^{||} Michelle Kelly,[▽] Robert Stone,[◦] Xing-Cong Li,[‡] Daneel Ferreira,[‡] and Mark T. Hamann^{‡,*}

Department of Pharmacognosy and the National Center for Natural Products Research (NCNPR), School of Pharmacy, The University of Mississippi, University, MS 38677, USA, College of Pharmacy, Yeungnam University, Gyeongsan, Gyeongbuk 712-749, South Korea, Department of Pediatrics, Emory University/VA Medical Center, Decatur, GA 30033, USA, Institute for Tuberculosis Research, College of Pharmacy, University of Illinois at Chicago, Chicago, Illinois 60607, USA, National Centre for Aquatic Biodiversity and Biosecurity, National Institute of Water and Atmospheric Research (NIWA), Private Bag 109695, Auckland, New Zealand, Auke Bay Laboratories, Alaska Fisheries Science Center, NOAA Fisheries, 17109 Point Lena Loop Road, Juneau, AK 99801, USA

[†] Dedicated to the late Dr. John W. Daly of NIDDK, NIH, Bethesda, Maryland and to the late Dr. Richard E. Moore of the University of Hawaii at Manoa for their pioneering work on bioactive natural products.

* To whom correspondence should be addressed. Tel: +1-662-915-5730. Fax: +1-662-915-6975. E-mail: mthamann@olemiss.edu.

[‡] The University of Mississippi.

[§] Yeungnam University.

[⊥] Emory University/VA Medical Center.

^{||} University of Illinois at Chicago.

[▽] NIWA.

[◦] Alaska Fisheries.

Table 1: Important Thermodynamic Parameters (TPs) and Frequencies (Frs) of Discorhabdin Y (**2**) Salt.

	E	$E'=E+ZPE$	H	G	E''
TPs(a.u.)	-3582.376781	-3582.047298	-3582.026993	-3582.095583	-3584.916614
Frs(cm^{-1})	32 37 44 76 109 120 149 170 179 203 215 226 237 269 277 311 320 327 330 388 409 416 426 466 495 517 528 558 568 597 604 625 633 649 656 666 716 727 731 732 738 759 771 812 816 833 864 891 906 939 947 964 970 1001 1010 1034 1051 1065 1074 1092 1113 1128 1142 1149 1187 1198 1217 1224 1255 1265 1269 1282 1303 1313 1350 1356 1364 1373 1374 1385 1389 1394 1423 1454 1472 1476 1492 1497 1500 1506 1515 1518 1533 1581 1607 1641 1655 1662 1774 1813 3044 3044 3047 3053 3058 3071 3101 3113 3117 3127 3132 3139 3173 3280 3512 3552 3643 1503 1505 1513 1514 1516 1519 1523 1534 1541 1630 1708 1742 2962 2973 2994 3007 3013 3026 3035 3041 3044 3050 3060 3061 3068 3073 3082 3085 3089 3102 3106 3113 3115 3132 3143 3148 3148 3172 3180 3224 3595 3709				
<i>E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at B3LYP/6-31G** level; E'': single point energy in the gas phase at B3LYP/aug-cc-pVDZ//B3LYP/6-31G** level.</i>					

Table 2. Optimized Z-Matrixes of Discorhabdin Y (**2**) Salt in the Gas Phase (Å).

C	-0.057589	-0.059232	-0.024237
C	-0.076179	-0.091181	1.358988
C	1.104373	-0.098876	2.192999
C	2.384285	0.006103	1.587858
C	2.413548	0.083805	0.182846
C	1.175978	0.027050	-0.747425
C	3.706382	0.080531	2.374401
C	4.867175	-0.369568	1.434769
C	4.852476	0.333887	0.078901
N	3.529553	0.211243	-0.519776
C	3.913899	1.523033	2.916587
C	4.985880	1.614907	4.010270
C	4.711353	0.671425	5.171951
C	4.102309	-0.643227	4.774316
C	3.687870	-0.914814	3.524316

C	-1.405170	-0.052048	1.808199
C	-1.668732	0.034039	3.283556
C	-0.481662	-0.591557	4.041589
N	0.845189	-0.198416	3.502787
N	-1.363884	-0.020464	-0.435750
C	-2.190597	-0.012719	0.656716
O	1.332575	0.089045	-1.959456
O	4.991731	0.933355	6.320887
B	3.942241	-1.939575	6.151275
H	4.791468	-1.449871	1.270070
H	5.828654	-0.191318	1.922036
H	5.107682	1.397223	0.172017
H	5.581107	-0.117368	-0.599399
H	3.399579	0.251277	-1.529717
H	2.961842	1.879416	3.327025
H	3.325703	-1.914286	3.292010
H	-2.581547	-0.488686	3.582779
H	-1.791682	1.084248	3.576932
H	-0.499376	-0.295515	5.091622
H	-0.548614	-1.686179	4.000194
H	1.629732	-0.288018	4.140020
H	-1.663772	-0.000817	-1.401516
H	-3.263838	0.021617	0.538835
H	5.060081	2.628267	4.412133
H	4.154169	2.202218	2.092487
H	5.978286	1.360668	3.614119