

Electronic Supplementary Information

An elastic siderophore synthetase and rubbery substrates assemble multimeric linear and macrocyclic hydroxamic acid metal chelators

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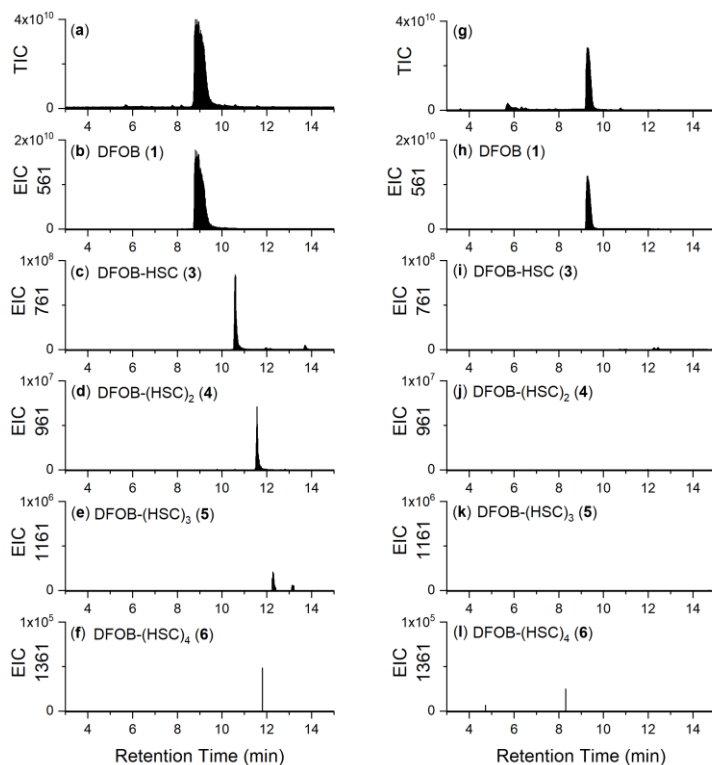


Fig S1. LC-MS traces from (a–f) commercial **1**, or (g–l) HPLC-purified **1**, as detected by total ion current (TIC) (a, g), or shown as an extracted ion chromatogram (EIC) with values set to report the $[M+H]^+$ adducts of (b, h) **1**, (c, i) **3**, (d, j) **4**, (e, k) **5**, or (f, l) **6**.

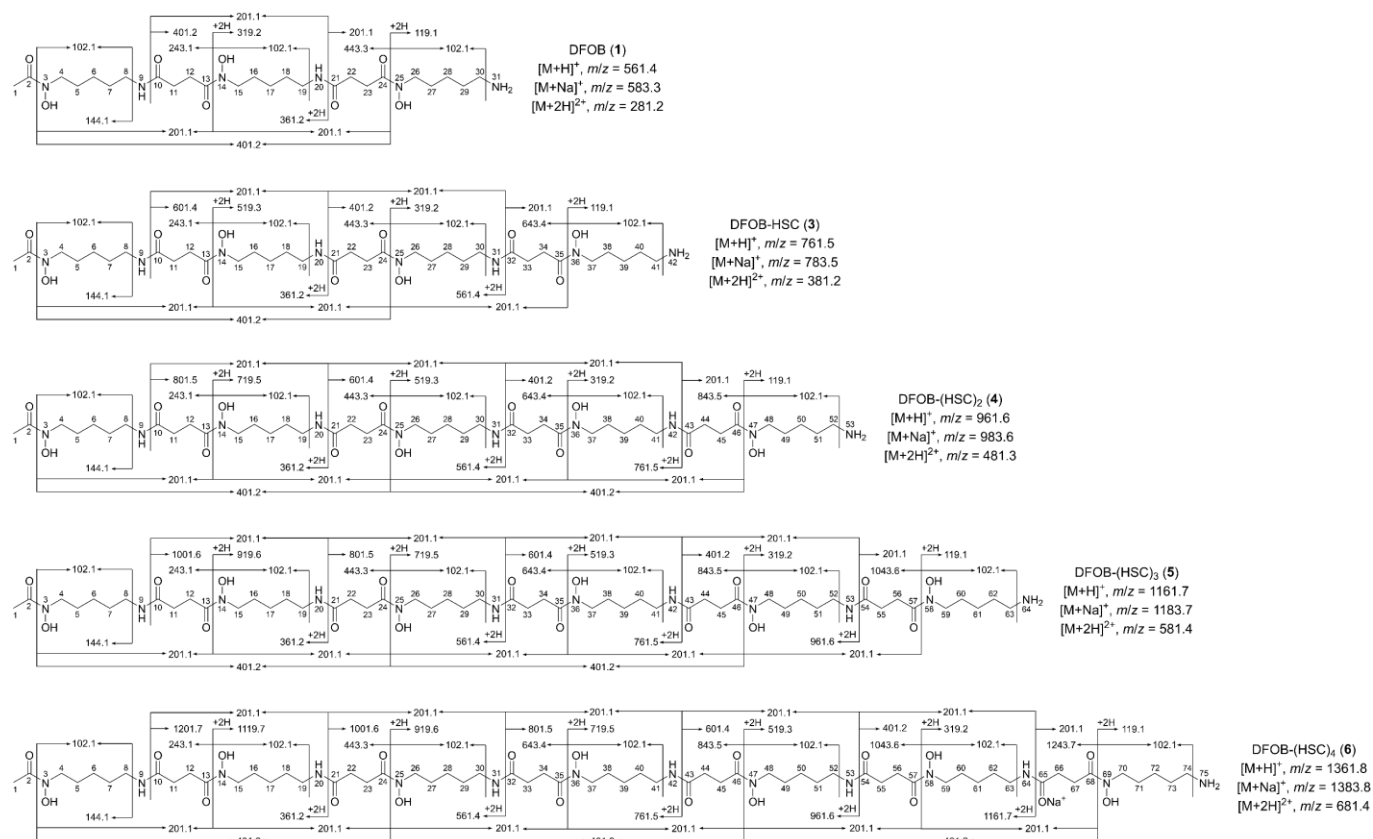


Fig. S2. Theoretical MS/MS fragmentation patterns of **1**, **3**–**6**.

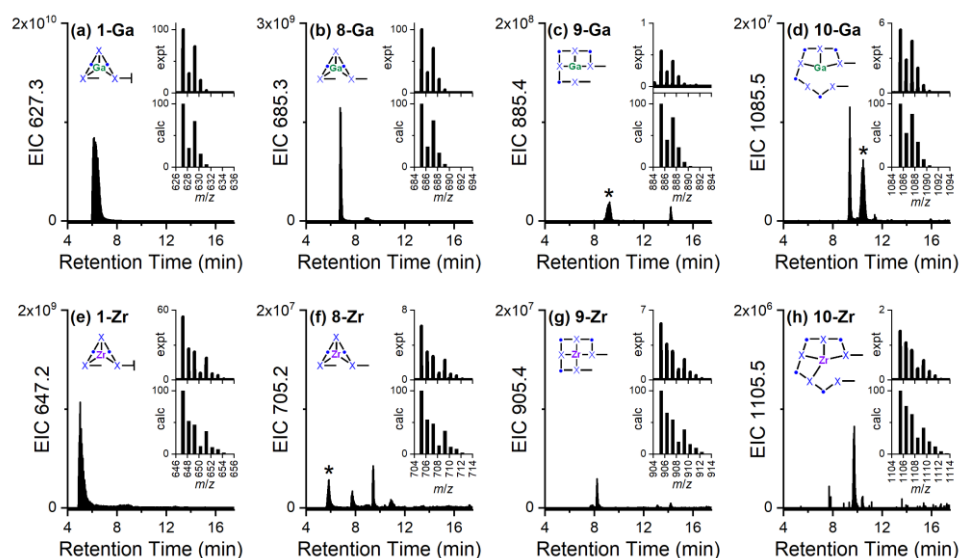


Fig. S3. EIC traces from chelators with excess Ga(III) or Zr(IV) with EIC values set to report Ga(III) (a-d) or Zr(IV) (e-h) complexes with **1** or **8–10**, with isotope patterns (upper: experiment; lower: calculated) from the major or asterisked peak in the inset, and the relevant species as a cartoon.

WP_012013773.1 pdbj 7TGK A	-----MTPGDAVTHLTTPARWEQANRLLVLRKALAEFAHERLLTPEPLPAEPGRYT	49
	MGSSHHHHHSSGLVPRGSHMSLTDVAVAHLSPERWEANRLLVLRKALAEFAHERLFTPEPADGQDGRYV	69
WP_012013773.1 pdbj 7TGK A	VRSDDGTV EYRFTARLLALDHWQIDPDSITRHGESSGQLPVDAGDFCL ELRGALGLSDRVLPVYLEEITA	118
	VRSDDGLTSYRFTAVRRALDHWQVDAGSITRTRDGAELPLAALDFI ELRHTLGLSDEILPVYLEEISS	138
WP_012013773.1 pdbj 7TGK A	TLAGSAYKYLARGGPAAEKLV AADFQTVESAMTEGHPCFVANNRGLGFSSEDEYHRYAPEAAAPVRLIWL A	187
	TLSGTCYKLT KPQVTAAGLLEGGFQALESGMTEGHPCFVANNRGLGFGVDEYLAYAPETAHPVRLVWLA	207
WP_012013773.1 pdbj 7TGK A	AHRDHSTFSCSAELDYDTLIRTELDEQTRARFAATLAGLGLDLADHHLIPVHPQWWHKL SVTFAGEVA	256
	AHRSRAAFATAGAGIDYASFVRQELGEETVERFDGVL RGRGLDPADYLLIPVHPQWWNKLSVTFAAEVA	276
WP_012013773.1 pdbj 7TGK A	RRHLVCLGEGPDDYRAQQSIRTFNLT E P SRHYVKTALSVLNMGFMRGLSAAYMAATPAINDWLANLID	325
	RQNLVCLGESDDEYLAQQSIRTFNATHPEKHVYKTALSVLNMGFMRGLSAAYMEATPAINDWLDRLID	345
WP_012013773.1 pdbj 7TGK A	GDEVFRSTGLTILRERAAVGYRHRQYEAATDRYS PYRKMLAALWRESPAQGLEPGRRLATMASLLHVDP	394
	NDPVLKSTGLSII RERAAVGYRHL EYEAATDRYS PYRKMLAALWRESPVPALRDGESLTTMAALVHVDH	414
WP_012013773.1 pdbj 7TGK A	EGRSHTAALIAASGLTFAAWLRRYLDAYLVFL LHA FYAHDLAFMPHGENVILVLHEGVVERVIFKDI AE	463
	EGRSVAGELIARSGLAPTAWLRHYLRAYYTPLLHSFYAYDLAFMPHGENTILVLKDGVVQR AVYKDI AE	483
WP_012013773.1 pdbj 7TGK A	EIVVMSADAPLP PAVERI RADVP EQMRLLSIF TDV I DCFLRHLNAVLVEAGVCP EETFWQTVAES AAGY	532
	EIVVMDPDAVLPPEVRRVRAEVPEDMKLLSIF TDV FDCFFRFLAAGLATEEVLAEEDDFWRTVAEVTREY	552
WP_012013773.1 pdbj 7TGK A	LDRVPHLAERARRYDLFAPEFALSCLNRLQLRDNQ QMVLDLADPAGALQLVGTLANPLAPYRPGT	596
	QEAHPELDDRFRQYDLFAPEFALSCLNRLQLRDNRQ QMVLDLADPSAALQLVGTLRNPLAGL - - -	612

Fig. S4. Sequence alignment (UniProt Blast)¹ between DesD from *Streptomyces griseoflavus* DSM 40698² (PDB: 7TGK_A) and *Salinispora tropica* CNB-440 (NCBI Reference Sequence: WP_012013773.1) showing the two conserved residues (*S. griseoflavus* DSM 40698 numbering: R303, D497) that interact with the substrate.

References

1. The UniProt Consortium. UniProt: the Universal Protein Knowledgebase in 2023. Nucl Acids Res. 2023;51(D1):D523–D31. <https://doi.org/10.1093/nar/gkac1052>.
2. Yang J, Banas VS, Patel KD, Rivera GSM, Mydy LS, Gulick AM, Wenciewicz TA. An acyl-adenylate mimic reveals the structural basis for substrate recognition by the iterative siderophore synthetase DesD. J Biol Chem. 2022;298(8):102166. 10.1016/j.jbc.2022.102166.