



**Table S2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for sea21mo. U(eq) is defined as one third of the trace of the orthogonalized.

U <sup>ij</sup> Tensor	x	y	z	U(eq)
Br(1)	3438(1)	2823(1)	4472(1)	17(1)
Br(2)	1810(1)	3577(1)	5436(1)	20(1)
O(1)	4634(2)	643(2)	7605(1)	14(1)
O(2)	1769(2)	447(2)	4370(1)	17(1)
O(3)	2509(2)	2208(2)	7374(1)	16(1)
N(1)	1932(2)	4026(2)	8057(1)	17(1)
C(1)	3240(3)	516(2)	6989(1)	10(1)
C(2)	3643(3)	1621(2)	6226(1)	13(1)
C(3)	3133(2)	1307(2)	5396(1)	12(1)
C(4)	2239(2)	200(2)	5125(1)	11(1)
C(5)	1861(3)	1367(2)	5881(1)	11(1)
C(6)	3105(3)	1248(2)	6667(1)	11(1)
C(7)	1560(2)	1078(2)	7456(1)	11(1)
C(8)	1760(3)	2737(2)	7798(1)	12(1)

**Table S3.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for sea21mo.

Bond	Bond length (Angle)
Br(1)–C(3)	1.8848(17)
Br(2)–C(5)	1.9423(18)
O(1)–C(1)	1.425(2)
O(1)–H(1)	0.72(2)
O(2)–C(4)	1.212(2)
O(3)–C(6)	1.405(2)
O(3)–H(3)	0.70(2)
N(1)–C(8)	1.141(2)
C(1)–C(2)	1.499(3)
C(1)–C(6)	1.538(3)
C(1)–C(7)	1.547(3)
C(2)–C(3)	1.335(3)
C(2)–H(2)	0.9300
C(3)–C(4)	1.480(3)
C(4)–C(5)	1.519(3)
C(5)–C(6)	1.526(3)
C(5)–H(5)	0.9800
C(6)–H(6)	0.9800
C(7)–C(8)	1.470(3)
C(7)–H(7A)	0.9700
C(7)–H(7B)	0.9700
C(1)–O(1)–H(1)	114(2)
C(6)–O(3)–H(3)	112(2)
O(1)–C(1)–C(2)	107.31(16)

**Table S3.** *Cont.*

O(1)–C(1)–C(6)	109.05(16)
C(2)–C(1)–C(6)	110.33(15)
O(1)–C(1)–C(7)	108.41(14)
C(2)–C(1)–C(7)	109.89(15)
C(6)–C(1)–C(7)	111.73(16)
C(3)–C(2)–C(1)	122.58(18)
C(3)–C(2)–H(2)	118.7
C(1)–C(2)–H(2)	118.7
C(2)–C(3)–C(4)	123.92(17)
C(2)–C(3)–Br(1)	121.68(14)
C(4)–C(3)–Br(1)	114.36(13)
O(2)–C(4)–C(3)	122.68(18)
O(2)–C(4)–C(5)	122.65(18)
C(3)–C(4)–C(5)	114.57(16)
C(4)–C(5)–C(6)	114.77(16)
C(4)–C(5)–Br(2)	109.87(12)
C(6)–C(5)–Br(2)	109.91(13)
C(4)–C(5)–H(5)	107.3
C(6)–C(5)–H(5)	107.3
Br(2)–C(5)–H(5)	107.3
O(3)–C(6)–C(5)	110.18(16)
O(3)–C(6)–C(1)	108.45(15)
C(5)–C(6)–C(1)	110.37(15)
O(3)–C(6)–H(6)	109.3
C(5)–C(6)–H(6)	109.3
C(1)–C(6)–H(6)	109.3
C(8)–C(7)–C(1)	110.49(16)
C(8)–C(7)–H(7A)	109.6
C(1)–C(7)–H(7A)	109.6
C(8)–C(7)–H(7B)	109.6
C(1)–C(7)–H(7B)	109.6
H(7A)–C(7)–H(7B)	108.1
N(1)–C(8)–C(7)	179.2(2)

Symmetry transformations used to generate equivalent atoms.

**Table S4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for sea21mo. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 (h^2 a^{*2} U11 + \dots + 2h k a^* b^* U12)$ .

	U11	U22	U33	U23	U13	U12
Br(1)	23(1)	17(1)	11(1)	3(1)	2(1)	-6(1)
Br(2)	29(1)	11(1)	19(1)	-4(1)	-2(1)	-3(1)
O(1)	12(1)	20(1)	11(1)	-1(1)	-2(1)	0(1)
O(2)	21(1)	20(1)	10(1)	-2(1)	-1(1)	-3(1)
O(3)	23(1)	13(1)	13(1)	4(1)	2(1)	5(1)
N(1)	13(1)	18(1)	19(1)	-2(1)	1(1)	1(1)
C(1)	10(1)	11(1)	10(1)	-1(1)	-1(1)	1(1)
C(2)	11(1)	12(1)	15(1)	-3(1)	3(1)	0(1)
C(3)	13(1)	10(1)	13(1)	2(1)	5(1)	0(1)
C(4)	7(1)	14(1)	12(1)	0(1)	3(1)	2(1)
C(5)	15(1)	8(1)	11(1)	-4(1)	1(1)	-2(1)
C(6)	14(1)	10(1)	10(1)	1(1)	2(1)	-1(1)
C(7)	11(1)	11(1)	10(1)	-2(1)	-2(1)	-1(1)
C(8)	9(1)	18(1)	10(1)	1(1)	1(1)	2(1)

**Table S5.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for sea21mo.

	x	y	z	U(eq)
H(2)	4272	2561	6335	15
H(5)	699	-1116	6104	14
H(6)	4253	-1628	6483	14
H(7A)	604	1043	7038	13
H(7B)	1295	349	7943	13
H(1)	4430(30)	360(30)	8047(16)	23(8)
H(3)	2990(30)	-2930(30)	7412(15)	20(8)