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Supplementary data for 3-iodo-2-(4-methoxyphenyl)-1-methylsulfonyl-2,3-dihydroquinolin-4(1*H*)-one 2e

Supplementary Table 1 Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for compound **2e**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Esd's are given in parentheses.

	x/a	*y/b*	*z/c*	*U*(eq)
I(1)	–1151(1)	4181(1)	8628(1)	55(1)
S(2)	1758(1)	1559(1)	9475(1)	48(1)
C(6)	2043(2)	5753(3)	9331(2)	35(1)
C(1)	2445(2)	4350(3)	9564(2)	34(1)
C(2)	3461(3)	4152(4)	10248(2)	48(1)
C(8)	365(2)	4737(3)	8135(2)	36(1)
N(1)	1823(2)	3190(2)	9088(1)	35(1)
O(1)	570(2)	7236(2)	8438(2)	63(1)
C(15)	3118(3)	2808(3)	7758(2)	44(1)
O(4)	917(3)	766(2)	8839(2)	74(1)
O(3)	2956(3)	1004(3)	9799(2)	73(1)
C(13)	4067(3)	4355(3)	6968(2)	48(1)
C(5)	2682(3)	6916(3)	9770(2)	49(1)
C(7)	957(3)	6032(3)	8624(2)	38(1)
C(10)	2222(2)	3808(3)	7749(1)	33(1)
C(14)	4041(3)	3061(3)	7366(2)	48(1)
C(3)	4057(3)	5311(5)	10671(2)	59(1)
C(9)	1246(2)	3489(3)	8197(1)	31(1)
C(11)	2260(3)	5086(3)	7321(2)	47(1)
C(4)	3692(3)	6711(4)	10434(2)	60(1)
C(17)	1122(4)	1828(4)	10312(2)	60(1)
O(2)	4949(2)	4758(3)	6594(2)	69(1)
C(16)	5856(4)	3779(5)	6542(3)	77(1)
C(12)	3171(3)	5355(4)	6943(2)	57(1)

Supplementary Table 2 Bond lengths (Å) and angles (º) for compound **2e**. Esd's are given in parentheses.

I(1)-C(8)	2.164(3)	S(2)-O(3)	1.422(3)
S(2)-O(4)	1.430(3)	S(2)-N(1)	1.660(2)
S(2)-C(17)	1.759(3)	C(6)-C(5)	1.398(4)
C(6)-C(1)	1.405(4)	C(6)-C(7)	1.485(4)
C(1)-C(2)	1.403(4)	C(1)-N(1)	1.414(3)
C(2)-C(3)	1.367(5)	C(2)-H(2)	0.9300
C(8)-C(7)	1.510(4)	C(8)-C(9)	1.520(4)
C(8)-H(8)	0.9800	N(1)-C(9)	1.485(3)
O(1)-C(7)	1.214(3)	C(15)-C(10)	1.378(4)
C(15)-C(14)	1.399(4)	C(15)-H(15)	0.9300
C(13)-O(2)	1.370(4)	C(13)-C(12)	1.373(5)
C(13)-C(14)	1.381(5)	C(5)-C(4)	1.380(5)
C(5)-H(5)	0.9300	C(10)-C(11)	1.396(4)
C(10)-C(9)	1.527(3)	C(14)-H(14)	0.9300
C(3)-C(4)	1.394(6)	C(3)-H(3)	0.9300
C(9)-H(9)	0.9800	C(11)-C(12)	1.374(4)
C(11)-H(11)	0.9300	C(4)-H(4)	0.9300

Supplementary Table 2 (cont.)

C(17)-H(17A)	0.9600	C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600	O(2)-C(16)	1.398(5)
C(16)-H(16A)	0.9600	C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600	C(12)-H(12)	0.9300
O(3)-S(2)-O(4)	118.42(18)	O(3)-S(2)-N(1)	110.06(15)
O(4)-S(2)-N(1)	105.92(12)	O(3)-S(2)-C(17)	107.78(17)
O(4)-S(2)-C(17)	109.27(19)	N(1)-S(2)-C(17)	104.53(14)
C(5)-C(6)-C(1)	119.4(3)	C(5)-C(6)-C(7)	119.1(3)
C(1)-C(6)-C(7)	121.5(2)	C(2)-C(1)-C(6)	118.9(2)
C(2)-C(1)-N(1)	122.5(2)	C(6)-C(1)-N(1)	118.6(2)
C(3)-C(2)-C(1)	120.3(3)	C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9	C(7)-C(8)-C(9)	112.6(2)
C(7)-C(8)-I(1)	105.63(17)	C(9)-C(8)-I(1)	111.64(17)
C(7)-C(8)-H(8)	109.0	C(9)-C(8)-H(8)	109.0
I(1)-C(8)-H(8)	109.0	C(1)-N(1)-C(9)	116.19(19)
C(1)-N(1)-S(2)	123.22(17)	C(9)-N(1)-S(2)	120.56(16)
C(10)-C(15)-C(14)	121.9(3)	C(10)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1	O(2)-C(13)-C(12)	115.4(3)
O(2)-C(13)-C(14)	124.9(3)	C(12)-C(13)-C(14)	119.6(3)
C(4)-C(5)-C(6)	121.2(3)	C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4	O(1)-C(7)-C(6)	122.1(3)
O(1)-C(7)-C(8)	121.4(3)	C(6)-C(7)-C(8)	116.5(2)
C(15)-C(10)-C(11)	117.2(3)	C(15)-C(10)-C(9)	119.8(2)
C(11)-C(10)-C(9)	123.0(2)	C(13)-C(14)-C(15)	119.3(3)
C(13)-C(14)-H(14)	120.4	C(15)-C(14)-H(14)	120.4
C(2)-C(3)-C(4)	121.5(3)	C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2	N(1)-C(9)-C(8)	108.48(19)
N(1)-C(9)-C(10)	110.2(2)	C(8)-C(9)-C(10)	111.7(2)
N(1)-C(9)-H(9)	108.8	C(8)-C(9)-H(9)	108.8
C(10)-C(9)-H(9)	108.8	C(12)-C(11)-C(10)	121.5(3)
C(12)-C(11)-H(11)	119.2	C(10)-C(11)-H(11)	119.2
C(5)-C(4)-C(3)	118.6(3)	C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7	S(2)-C(17)-H(17A)	109.5
S(2)-C(17)-H(17B)	109.5	H(17A)-C(17)-H(17B)	109.5
S(2)-C(17)-H(17C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5	C(13)-O(2)-C(16)	119.6(3)
O(2)-C(16)-H(16A)	109.5	O(2)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5	O(2)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(16B)-C(16)-H(16C)	109.5
C(13)-C(12)-C(11)	120.6(3)	C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7		

Supplementary Table 3 Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **2e**. The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12})$. Esd's are given in parentheses.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	45(1)	64(1)	63(1)	–7(1)	26(1)	–4(1)
S(2)	81(1)	28(1)	37(1)	3(1)	21(1)	4(1)
C(6)	43(1)	35(1)	34(1)	–5(1)	20(1)	–6(1)
C(1)	39(1)	38(1)	27(1)	–3(1)	14(1)	–3(1)
C(2)	47(2)	61(2)	34(1)	–4(1)	8(1)	1(1)
C(8)	39(1)	39(1)	31(1)	2(1)	12(1)	1(1)
N(1)	49(1)	29(1)	26(1)	0(1)	11(1)	–2(1)
O(1)	84(2)	37(1)	64(1)	6(1)	15(1)	14(1)
C(15)	48(2)	39(1)	47(2)	1(1)	18(1)	3(1)
O(4)	136(3)	33(1)	48(1)	–3(1)	18(2)	–22(1)
O(3)	103(2)	58(2)	62(2)	18(1)	28(1)	39(1)
C(13)	50(2)	58(2)	40(1)	–7(1)	18(1)	–10(1)
C(5)	63(2)	42(2)	54(2)	–14(1)	35(1)	–17(1)
C(7)	50(2)	30(1)	39(1)	1(1)	20(1)	4(1)
C(10)	40(1)	35(1)	25(1)	–4(1)	11(1)	–2(1)
C(14)	44(2)	50(2)	53(2)	–10(1)	18(1)	4(1)
C(3)	48(2)	86(3)	40(2)	–14(2)	7(1)	–9(2)
C(9)	41(1)	30(1)	23(1)	–2(1)	10(1)	–2(1)
C(11)	59(2)	43(2)	46(2)	10(1)	27(1)	6(1)
C(4)	58(2)	75(2)	53(2)	–32(2)	27(2)	–28(2)
C(17)	88(2)	51(2)	48(2)	9(1)	32(2)	–4(2)
O(2)	65(2)	75(2)	81(2)	0(1)	45(1)	–6(1)
C(16)	63(2)	78(3)	103(3)	–25(2)	49(2)	–15(2)
C(12)	72(2)	51(2)	58(2)	14(2)	37(2)	4(2)

Supplementary Table 4 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for compound **2e**. Esd's are given in parentheses.

	x	y	z	U(eq)
H(2)	3731	3229	10414	58
H(8)	48	5010	7551	43
H(15)	3110	1942	8032	53
H(5)	2422	7845	9611	59
H(14)	4629	2365	7373	58
H(3)	4722	5162	11128	71
H(9)	784	2639	7945	37
H(11)	1654	5771	7290	56
H(4)	4120	7491	10717	72
H(17A)	1654	2426	10720	89
H(17B)	1023	919	10556	89
H(17C)	341	2286	10117	89
H(16A)	5484	2906	6290	115
H(16B)	6363	3576	7089	115
H(16C)	6346	4181	6212	115
H(12)	3181	6221	6669	68

Supplementary Table 5 Torsion angles (°) for compound **2e**. Esd's are given in parentheses.

C(5)-C(6)-C(1)-C(2)	1.7(4)	C(7)-C(6)-C(1)-C(2)	–178.7(3)
C(5)-C(6)-C(1)-N(1)	–177.0(2)	C(7)-C(6)-C(1)-N(1)	2.6(4)
C(6)-C(1)-C(2)-C(3)	–0.9(4)	N(1)-C(1)-C(2)-C(3)	177.8(3)
C(2)-C(1)-N(1)-C(9)	–149.3(3)	C(6)-C(1)-N(1)-C(9)	29.3(3)
C(2)-C(1)-N(1)-S(2)	28.8(4)	C(6)-C(1)-N(1)-S(2)	–152.6(2)
O(3)-S(2)-N(1)-C(1)	–58.7(2)	O(4)-S(2)-N(1)-C(1)	172.1(2)
C(17)-S(2)-N(1)-C(1)	56.8(3)	O(3)-S(2)-N(1)-C(9)	119.3(2)
O(4)-S(2)-N(1)-C(9)	–9.8(3)	C(17)-S(2)-N(1)-C(9)	–125.2(2)
C(1)-C(6)-C(5)-C(4)	–0.8(4)	C(7)-C(6)-C(5)-C(4)	179.6(3)
C(5)-C(6)-C(7)-O(1)	–3.5(4)	C(1)-C(6)-C(7)-O(1)	176.9(3)
C(5)-C(6)-C(7)-C(8)	175.4(2)	C(1)-C(6)-C(7)-C(8)	–4.2(4)
C(9)-C(8)-C(7)-O(1)	154.4(3)	I(1)-C(8)-C(7)-O(1)	–83.5(3)
C(9)-C(8)-C(7)-C(6)	–24.6(3)	I(1)-C(8)-C(7)-C(6)	97.5(2)
C(14)-C(15)-C(10)-C(11)	0.8(4)	C(14)-C(15)-C(10)-C(9)	–179.1(2)
O(2)-C(13)-C(14)-C(15)	177.0(3)	C(12)-C(13)-C(14)-C(15)	–1.9(5)
C(10)-C(15)-C(14)-C(13)	1.0(4)	C(1)-C(2)-C(3)-C(4)	–1.0(5)
C(1)-N(1)-C(9)-C(8)	–56.9(3)	S(2)-N(1)-C(9)-C(8)	124.9(2)
C(1)-N(1)-C(9)-C(10)	65.8(3)	S(2)-N(1)-C(9)-C(10)	–112.4(2)
C(7)-C(8)-C(9)-N(1)	52.9(3)	I(1)-C(8)-C(9)-N(1)	–65.8(2)
C(7)-C(8)-C(9)-C(10)	–68.9(3)	I(1)-C(8)-C(9)-C(10)	172.50(15)
C(15)-C(10)-C(9)-N(1)	57.7(3)	C(11)-C(10)-C(9)-N(1)	–122.3(3)
C(15)-C(10)-C(9)-C(8)	178.4(2)	C(11)-C(10)-C(9)-C(8)	–1.6(3)
C(15)-C(10)-C(11)-C(12)	–1.8(4)	C(9)-C(10)-C(11)-C(12)	178.2(3)
C(6)-C(5)-C(4)-C(3)	–1.0(4)	C(2)-C(3)-C(4)-C(5)	1.9(5)
C(12)-C(13)-O(2)-C(16)	–176.0(3)	C(14)-C(13)-O(2)-C(16)	5.1(5)
O(2)-C(13)-C(12)-C(11)	–178.0(3)	C(14)-C(13)-C(12)-C(11)	1.0(5)
C(10)-C(11)-C(12)-C(13)	0.9(5)		

Supplementary data for 3-bromo-2-(4-bromophenyl)-1-methylsulfonyl-2,3-dihydroquinolin-4(1*H*)-one 3d

Supplementary Table 6 Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for compound **3d**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Esd's are given in parentheses.

	x/a	y/b	z/c	U(eq)
Br(1)	–1151(1)	4352(1)	8571(1)	54(1)
S(3)	1528(1)	1572(1)	9479(1)	38(1)
C(3)	4016(2)	5241(3)	10669(2)	47(1)
C(6)	2041(2)	5728(2)	9308(1)	30(1)
C(9)	1166(2)	3451(2)	8205(1)	30(1)
O(2)	629(2)	818(2)	8855(1)	55(1)
O(3)	2730(2)	907(2)	9808(1)	56(1)
C(13)	4169(2)	3777(3)	6972(2)	46(1)
C(10)	2213(2)	3622(2)	7760(1)	29(1)
N(1)	1729(2)	3161(2)	9079(1)	30(1)
C(7)	991(2)	6041(3)	8586(1)	35(1)
C(12)	4064(3)	2600(3)	7438(2)	55(1)
C(1)	2396(2)	4309(2)	9550(1)	28(1)
C(14)	3293(3)	4863(3)	6879(2)	52(1)
C(8)	311(2)	4753(2)	8123(1)	33(1)
O(1)	666(2)	7259(2)	8370(1)	54(1)
C(5)	2714(2)	6869(3)	9748(2)	39(1)
C(16)	841(3)	1976(3)	10284(2)	52(1)
C(15)	2318(2)	4784(3)	7275(2)	42(1)
C(2)	3397(2)	4082(3)	10244(1)	38(1)
C(4)	3690(2)	6631(3)	10425(2)	47(1)
C(11)	3097(3)	2525(3)	7830(2)	50(1)
Br(2)	5529(1)	3888(1)	6458(1)	81(1)

Supplementary Table 7 Bond lengths (Å) and angles (º) for compound **3d**. Esd's are given in parentheses.

Br(1)-C(8)	1.959(2)	C(10)-C(11)	1.386(3)
S(3)-O(3)	1.4262(19)	N(1)-C(1)	1.417(3)
S(3)-O(2)	1.4298(17)	C(7)-O(1)	1.215(3)
S(3)-N(1)	1.6614(18)	C(7)-C(8)	1.517(3)
S(3)-C(16)	1.749(2)	C(12)-C(11)	1.378(4)
C(3)-C(2)	1.374(3)	C(12)-H(12)	0.9300
C(3)-C(4)	1.375(4)	C(1)-C(2)	1.403(3)
C(3)-H(3)	0.9300	C(14)-C(15)	1.389(3)
C(6)-C(5)	1.394(3)	C(14)-H(14)	0.9300
C(6)-C(1)	1.406(3)	C(8)-H(8)	0.9800
C(6)-C(7)	1.477(3)	C(5)-C(4)	1.370(3)
C(9)-N(1)	1.477(3)	C(5)-H(5)	0.9300
C(9)-C(8)	1.511(3)	C(16)-H(16A)	0.9600
C(9)-C(10)	1.521(3)	C(16)-H(16B)	0.9600
C(9)-H(9)	0.9800	C(16)-H(16C)	0.9600
C(13)-C(12)	1.370(4)	C(15)-H(15)	0.9300
C(13)-C(14)	1.370(4)	C(2)-H(2)	0.9300
C(13)-Br(2)	1.895(2)	C(4)-H(4)	0.9300
C(10)-C(15)	1.378(3)	C(11)-H(11)	0.9300

O(3)-S(3)-O(2)	117.72(12)	C(2)-C(1)-C(6)	118.9(2)
O(3)-S(3)-N(1)	110.06(11)	C(2)-C(1)-N(1)	122.5(2)
O(2)-S(3)-N(1)	105.69(10)	C(6)-C(1)-N(1)	118.59(19)
O(3)-S(3)-C(16)	108.48(13)	C(13)-C(14)-C(15)	119.8(3)
O(2)-S(3)-C(16)	109.56(13)	C(13)-C(14)-H(14)	120.1
N(1)-S(3)-C(16)	104.54(11)	C(15)-C(14)-H(14)	120.1
C(2)-C(3)-C(4)	121.6(2)	C(9)-C(8)-C(7)	112.08(19)
C(2)-C(3)-H(3)	119.2	C(9)-C(8)-Br(1)	110.57(15)
C(4)-C(3)-H(3)	119.2	C(7)-C(8)-Br(1)	106.68(15)
C(5)-C(6)-C(1)	119.3(2)	C(9)-C(8)-H(8)	109.1
C(5)-C(6)-C(7)	119.1(2)	C(7)-C(8)-H(8)	109.1
C(1)-C(6)-C(7)	121.6(2)	Br(1)-C(8)-H(8)	109.1
N(1)-C(9)-C(8)	109.21(18)	C(4)-C(5)-C(6)	121.1(2)
N(1)-C(9)-C(10)	109.97(18)	C(4)-C(5)-H(5)	119.4
C(8)-C(9)-C(10)	112.94(18)	C(6)-C(5)-H(5)	119.4
N(1)-C(9)-H(9)	108.2	S(3)-C(16)-H(16A)	109.5
C(8)-C(9)-H(9)	108.2	S(3)-C(16)-H(16B)	109.5
C(10)-C(9)-H(9)	108.2	H(16A)-C(16)-H(16B)	109.5
C(12)-C(13)-C(14)	120.0(2)	S(3)-C(16)-H(16C)	109.5
C(12)-C(13)-Br(2)	119.6(2)	H(16A)-C(16)-H(16C)	109.5
C(14)-C(13)-Br(2)	120.4(2)	H(16B)-C(16)-H(16C)	109.5
C(15)-C(10)-C(11)	117.9(2)	C(10)-C(15)-C(14)	121.0(2)
C(15)-C(10)-C(9)	124.1(2)	C(10)-C(15)-H(15)	119.5
C(11)-C(10)-C(9)	118.0(2)	C(14)-C(15)-H(15)	119.5
C(1)-N(1)-C(9)	116.74(17)	C(3)-C(2)-C(1)	119.7(2)
C(1)-N(1)-S(3)	122.80(14)	C(3)-C(2)-H(2)	120.1
C(9)-N(1)-S(3)	120.42(14)	C(1)-C(2)-H(2)	120.1
O(1)-C(7)-C(6)	122.6(2)	C(5)-C(4)-C(3)	119.3(2)
O(1)-C(7)-C(8)	120.9(2)	C(5)-C(4)-H(4)	120.3
C(6)-C(7)-C(8)	116.5(2)	C(3)-C(4)-H(4)	120.3
C(13)-C(12)-C(11)	120.0(3)	C(12)-C(11)-C(10)	121.2(3)
C(13)-C(12)-H(12)	120.0	C(12)-C(11)-H(11)	119.4
C(11)-C(12)-H(12)	120.0	C(10)-C(11)-H(11)	119.4

Supplementary Table 8 Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **3d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12})$. Esd's are given in parentheses.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	38(1)	65(1)	63(1)	–2(1)	19(1)	1(1)
S(3)	55(1)	24(1)	36(1)	1(1)	14(1)	–4(1)
C(3)	38(2)	61(2)	35(2)	–7(1)	0(1)	–7(1)
C(6)	37(1)	28(1)	29(1)	–2(1)	12(1)	–1(1)
C(9)	33(1)	28(1)	26(1)	–2(1)	3(1)	–5(1)
O(2)	81(2)	34(1)	47(1)	–5(1)	11(1)	–24(1)
O(3)	72(1)	37(1)	57(1)	13(1)	13(1)	17(1)
C(13)	38(2)	61(2)	42(2)	–24(1)	15(1)	–15(1)
C(10)	34(1)	31(1)	22(1)	–6(1)	4(1)	–2(1)
N(1)	40(1)	23(1)	25(1)	1(1)	5(1)	–4(1)
C(7)	41(2)	34(2)	32(1)	2(1)	13(1)	6(1)
C(12)	51(2)	59(2)	60(2)	–7(2)	20(2)	14(2)
C(1)	31(1)	29(1)	25(1)	–1(1)	10(1)	–3(1)
C(14)	57(2)	52(2)	52(2)	2(1)	25(2)	–11(2)
C(8)	32(1)	39(2)	27(1)	2(1)	6(1)	2(1)
O(1)	72(1)	34(1)	51(1)	6(1)	5(1)	16(1)
C(5)	46(2)	31(2)	44(2)	–6(1)	19(1)	–5(1)
C(16)	70(2)	45(2)	48(2)	5(1)	28(2)	–9(1)
C(15)	44(2)	41(2)	44(2)	3(1)	16(1)	4(1)
C(2)	38(2)	40(2)	33(1)	4(1)	3(1)	0(1)
C(4)	45(2)	49(2)	45(2)	–16(1)	11(1)	–14(1)
C(11)	60(2)	41(2)	54(2)	5(1)	25(2)	12(1)
Br(2)	58(1)	108(1)	93(1)	–48(1)	46(1)	–34(1)

Supplementary Table 9 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for compound **3d**.

	x/a	*y*/b	*z/c*	*U*(eq)
H(3)	4671	5082	11133	56
H(9)	643	2622	7972	36
H(12)	4646	1850	7489	66
H(14)	3350	5652	6552	62
H(8)	6	5003	7544	39
H(5)	2497	7808	9580	47
H(16A)	725	1105	10561	78
H(16B)	32	2430	10072	78
H(16C)	1389	2615	10659	78
H(15)	1727	5526	7212	50
H(2)	3641	3151	10415	45
H(4)	4127	7401	10717	56
H(11)	3037	1724	8147	60

Supplementary Table 10 Torsion angles (°) for compound **3d**. Esd's are given in parentheses.

N(1)-C(9)-C(10)-C(15)	–127.4(2)	C(9)-N(1)-C(1)-C(6)	27.9(3)
C(8)-C(9)-C(10)-C(15)	–5.1(3)	S(3)-N(1)-C(1)-C(6)	–149.98(17)
N(1)-C(9)-C(10)-C(11)	54.3(3)	C(12)-C(13)-C(14)-C(15)	1.7(4)
C(8)-C(9)-C(10)-C(11)	176.6(2)	Br(2)-C(13)-C(14)-C(15)	–178.51(19)
C(8)-C(9)-N(1)-C(1)	–55.0(2)	N(1)-C(9)-C(8)-C(7)	53.3(2)
C(10)-C(9)-N(1)-C(1)	69.4(2)	C(10)-C(9)-C(8)-C(7)	–69.4(2)
C(8)-C(9)-N(1)-S(3)	122.91(17)	N(1)-C(9)-C(8)-Br(1)	–65.5(2)
C(10)-C(9)-N(1)-S(3)	–112.63(18)	C(10)-C(9)-C(8)-Br(1)	171.75(14)
O(3)-S(3)-N(1)-C(1)	–62.2(2)	O(1)-C(7)-C(8)-C(9)	152.8(2)
O(2)-S(3)-N(1)-C(1)	169.73(17)	C(6)-C(7)-C(8)-C(9)	–27.9(3)
C(16)-S(3)-N(1)-C(1)	54.1(2)	O(1)-C(7)-C(8)-Br(1)	–86.1(2)
O(3)-S(3)-N(1)-C(9)	119.99(17)	C(6)-C(7)-C(8)-Br(1)	93.2(2)
O(2)-S(3)-N(1)-C(9)	–8.1(2)	C(1)-C(6)-C(5)-C(4)	–1.8(3)
C(16)-S(3)-N(1)-C(9)	–123.70(18)	C(7)-C(6)-C(5)-C(4)	179.5(2)
C(5)-C(6)-C(7)-O(1)	–1.8(3)	C(11)-C(10)-C(15)-C(14)	–1.0(4)
C(1)-C(6)-C(7)-O(1)	179.6(2)	C(9)-C(10)-C(15)-C(14)	–179.3(2)
C(5)-C(6)-C(7)-C(8)	178.9(2)	C(13)-C(14)-C(15)-C(10)	–0.3(4)
C(1)-C(6)-C(7)-C(8)	0.3(3)	C(4)-C(3)-C(2)-C(1)	–0.9(4)
C(14)-C(13)-C(12)-C(11)	–1.7(4)	C(6)-C(1)-C(2)-C(3)	–0.4(3)
Br(2)-C(13)-C(12)-C(11)	178.4(2)	N(1)-C(1)-C(2)-C(3)	179.3(2)
C(5)-C(6)-C(1)-C(2)	1.8(3)	C(6)-C(5)-C(4)-C(3)	0.5(4)
C(7)-C(6)-C(1)-C(2)	–179.6(2)	C(2)-C(3)-C(4)-C(5)	0.9(4)
C(5)-C(6)-C(1)-N(1)	–177.99(19)	C(13)-C(12)-C(11)-C(10)	0.4(4)
C(7)-C(6)-C(1)-N(1)	0.6(3)	C(15)-C(10)-C(11)-C(12)	1.0(4)
C(9)-N(1)-C(1)-C(2)	–151.8(2)	C(9)-C(10)-C(11)-C(12)	179.4(2)
S(3)-N(1)-C(1)-C(2)	30.3(3)		