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Supporting information for article:

Synthesis, crystal structure and docking studies of tetracyclic 10-iodo-1,2-dihydroisoquinolino[2,1-*b*][1,2,4]benzothiadiazine 12,12-dioxide and its precursors

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Computing details

For structures **6**, **7** and 8, data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: SHELXT2018/2 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ShelXle* (Hübschle *et al.*, 2011); software used to prepare material for publication: *ORTEP-3* (Farrugia, 2012), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

N-(*o*-Nitrobenzene sulfonyl)-1,3,4-trihydroisoquinoline (6)

Crystal data

$C_{15}H_{14}N_2O_4S$
$M_r = 318.34$
Monoclinic, $P2_1/n$ (No. 14)
$a = 10.048$ (2) Å
$b = 13.802$ (3) Å
$c = 10.543$ (2) Å
$\beta = 90.487$ (10)º
$V = 1462.1$ (5) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.446$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9277 reflections
$\theta = 2.4$–28.3º
$\mu = 0.241$ mm^{-1}
$T = 296$ K
Block, colorless
0.71 × 0.44 × 0.37 mm

Data collection

Bruker Apex II CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ϕ and ω scans
Absorption correction: numerical (*SADABS* V2008/1; Bruker, 2012)
$T_{min} = 0.953$, $T_{max} = 1.000$
88246 measured reflections
3655 independent reflections
3186 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.4$º, $\theta_{min} = 2.4$º
$h = -13\rightarrow13$
$k = -18\rightarrow18$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.0337$
$wR(F^2) = 0.0993$
$S = 1.05$
3655 reflections
200 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighboring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.3875P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: *SHELXL2018*/3 (Sheldrick 2015b),
$F_c^* = kF_c[1 + 0.001\ x\ F_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0196 (17)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are considered individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 U_{eq}(C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22434 (3)	0.26068 (2)	0.60528 (3)	0.04245 (12)
O1	0.50587 (11)	0.20404 (9)	0.77057 (11)	0.0604 (3)
O2	0.38599 (13)	0.11032 (8)	0.88638 (13)	0.0684 (3)
O3	0.08662 (11)	0.26975 (10)	0.57400 (11)	0.0639 (3)
O4	0.28485 (13)	0.16783 (7)	0.60442 (10)	0.0601 (3)
N1	0.40900 (12)	0.18751 (8)	0.83468 (11)	0.0447 (3)
N2	0.30384 (11)	0.32965 (8)	0.50775 (10)	0.0387 (2)
C11	0.23944 (12)	0.30865 (9)	0.76181 (12)	0.0378 (3)
C12	0.31513 (12)	0.26713 (9)	0.85821 (12)	0.0382 (3)
C13	0.30676 (14)	0.29842 (12)	0.98299 (13)	0.0512 (3)
H13	0.354690	0.267156	1.046770	0.061*
C14	0.22664 (16)	0.37633 (13)	1.01123 (16)	0.0595 (4)
H14	0.220668	0.398329	1.094359	0.071*
C15	0.15540 (17)	0.42156 (12)	0.91610 (17)	0.0609 (4)
H15	0.104449	0.475901	0.934740	0.073*
C16	0.15893 (14)	0.38686 (11)	0.79286 (15)	0.0507 (3)
H16	0.106949	0.416177	0.730354	0.061*
C21	0.24900 (13)	0.42650 (10)	0.48524 (13)	0.0429 (3)
H21A	0.267296	0.467345	0.558201	0.052*
H21B	0.153214	0.422111	0.474512	0.052*
C22	0.30903 (13)	0.47152 (9)	0.36841 (11)	0.0383 (3)
C23	0.24522 (16)	0.55062 (11)	0.31337 (14)	0.0503 (3)
H23	0.166312	0.573547	0.347718	0.060*
C24	0.29830 (19)	0.59550 (12)	0.20775 (15)	0.0596 (4)
H24	0.255336	0.648539	0.171586	0.071*
C25	0.41473 (18)	0.56144 (12)	0.15648 (14)	0.0576 (4)
H25	0.450102	0.591103	0.085093	0.069*
C26	0.47847 (15)	0.48399 (11)	0.21043 (13)	0.0508 (3)
H26	0.557377	0.461662	0.175409	0.061*
C27	0.42689 (13)	0.43775 (9)	0.31754 (12)	0.0405 (3)
C28	0.49646 (14)	0.35160 (11)	0.37493 (14)	0.0506 (3)
H28A	0.591487	0.363952	0.377085	0.061*
H28B	0.481158	0.295572	0.321219	0.061*
C29	0.45009 (13)	0.32842 (10)	0.50848 (13)	0.0450 (3)
H29A	0.482405	0.265121	0.534232	0.054*
H29B	0.484281	0.376232	0.567793	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0496 (2)	0.04094 (18)	0.03662 (18)	−0.01290 (13)	−0.00905 (13)	0.00428 (12)
O1	0.0539 (6)	0.0632 (7)	0.0643 (7)	0.0073 (5)	0.0114 (5)	0.0065 (5)
O2	0.0834 (8)	0.0445 (6)	0.0772 (8)	−0.0024 (5)	0.0016 (6)	0.0179 (5)
O3	0.0494 (6)	0.0888 (8)	0.0534 (6)	−0.0281 (6)	−0.0163 (5)	0.0193 (6)
O4	0.0991 (9)	0.0331 (5)	0.0480 (6)	−0.0088 (5)	−0.0127 (5)	−0.0023 (4)
N1	0.0480 (6)	0.0434 (6)	0.0427 (6)	−0.0013 (5)	−0.0067 (5)	0.0030 (5)
N2	0.0410 (5)	0.0378 (5)	0.0373 (5)	0.0013 (4)	0.0002 (4)	0.0046 (4)
C11	0.0372 (6)	0.0376 (6)	0.0385 (6)	−0.0076 (5)	0.0000 (5)	0.0033 (5)
C12	0.0347 (6)	0.0399 (6)	0.0401 (6)	−0.0081 (5)	−0.0030 (5)	−0.0001 (5)
C13	0.0447 (7)	0.0685 (9)	0.0401 (7)	−0.0084 (6)	−0.0060 (5)	−0.0058 (6)
C14	0.0539 (8)	0.0724 (10)	0.0523 (8)	−0.0098 (7)	0.0060 (7)	−0.0202 (8)
C15	0.0570 (9)	0.0538 (9)	0.0722 (11)	0.0028 (7)	0.0166 (8)	−0.0105 (8)
C16	0.0465 (7)	0.0501 (8)	0.0558 (8)	0.0045 (6)	0.0063 (6)	0.0078 (6)

C21	0.0434 (6)	0.0421 (7)	0.0433 (7)	0.0072 (5)	0.0078 (5)	0.0080 (5)
C22	0.0425 (6)	0.0371 (6)	0.0355 (6)	−0.0017 (5)	0.0018 (5)	0.0015 (5)
C23	0.0571 (8)	0.0464 (7)	0.0474 (7)	0.0071 (6)	0.0025 (6)	0.0077 (6)
C24	0.0815 (11)	0.0471 (8)	0.0500 (8)	−0.0018 (7)	−0.0031 (7)	0.0138 (6)
C25	0.0770 (10)	0.0560 (9)	0.0400 (7)	−0.0201 (8)	0.0061 (7)	0.0071 (6)
C26	0.0529 (8)	0.0571 (8)	0.0425 (7)	−0.0127 (6)	0.0103 (6)	−0.0050 (6)
C27	0.0435 (6)	0.0408 (6)	0.0371 (6)	−0.0045 (5)	0.0038 (5)	−0.0036 (5)
C28	0.0464 (7)	0.0524 (8)	0.0530 (8)	0.0102 (6)	0.0112 (6)	0.0002 (6)
C29	0.0412 (6)	0.0474 (7)	0.0464 (7)	0.0065 (5)	−0.0024 (5)	0.0024 (6)

Geometric parameters (Å², º)

S1—O4	1.4185 (12)	C21—C22	1.5099 (17)
S1—O3	1.4254 (12)	C21—H21A	0.9700
S1—N2	1.6172 (11)	C21—H21B	0.9700
S1—C11	1.7835 (13)	C22—C27	1.3849 (18)
O1—N1	1.2114 (16)	C22—C23	1.3905 (18)
O2—N1	1.2197 (16)	C23—C24	1.385 (2)
N1—C12	1.4707 (18)	C23—H23	0.9300
N2—C21	1.4645 (16)	C24—C25	1.376 (3)
N2—C29	1.4696 (17)	C24—H24	0.9300
C11—C12	1.3880 (18)	C25—C26	1.368 (2)
C11—C16	1.3898 (19)	C25—H25	0.9300
C12—C13	1.3878 (19)	C26—C27	1.4005 (18)
C13—C14	1.377 (2)	C26—H26	0.9300
C13—H13	0.9300	C27—C28	1.5039 (19)
C14—C15	1.377 (3)	C28—C29	1.521 (2)
C14—H14	0.9300	C28—H28A	0.9700
C15—C16	1.386 (2)	C28—H28B	0.9700
C15—H15	0.9300	C29—H29A	0.9700
C16—H16	0.9300	C29—H29B	0.9700
O4—S1—O3	119.55 (8)	N2—C21—H21B	109.5
O4—S1—N2	108.28 (7)	C22—C21—H21B	109.5
O3—S1—N2	106.56 (6)	H21A—C21—H21B	108.1
O4—S1—C11	107.95 (6)	C27—C22—C23	119.69 (12)
O3—S1—C11	104.85 (7)	C27—C22—C21	121.76 (11)
N2—S1—C11	109.35 (6)	C23—C22—C21	118.53 (12)
O1—N1—O2	124.76 (13)	C24—C23—C22	120.49 (14)
O1—N1—C12	118.22 (11)	C24—C23—H23	119.8
O2—N1—C12	116.94 (12)	C22—C23—H23	119.8
C21—N2—C29	112.72 (10)	C25—C24—C23	119.85 (15)
C21—N2—S1	116.94 (8)	C25—C24—H24	120.1
C29—N2—S1	119.29 (9)	C23—C24—H24	120.1
C12—C11—C16	117.68 (12)	C26—C25—C24	120.03 (13)
C12—C11—S1	124.49 (10)	C26—C25—H25	120.0
C16—C11—S1	117.46 (10)	C24—C25—H25	120.0
C13—C12—C11	121.90 (13)	C25—C26—C27	121.09 (14)
C13—C12—N1	115.88 (12)	C25—C26—H26	119.5
C11—C12—N1	122.22 (11)	C27—C26—H26	119.5
C14—C13—C12	119.21 (14)	C22—C27—C26	118.85 (13)
C14—C13—H13	120.4	C22—C27—C28	120.42 (11)
C12—C13—H13	120.4	C26—C27—C28	120.72 (12)
C15—C14—C13	119.85 (14)	C27—C28—C29	113.19 (11)
C15—C14—H14	120.1	C27—C28—H28A	108.9
C13—C14—H14	120.1	C29—C28—H28A	108.9
C14—C15—C16	120.61 (15)	C27—C28—H28B	108.9
C14—C15—H15	119.7	C29—C28—H28B	108.9
C16—C15—H15	119.7	H28A—C28—H28B	107.8
C15—C16—C11	120.59 (14)	N2—C29—C28	107.87 (11)

C15—C16—H16	119.7	N2—C29—H29A	110.1
C11—C16—H16	119.7	C28—C29—H29A	110.1
N2—C21—C22	110.82 (10)	N2—C29—H29B	110.1
N2—C21—H21A	109.5	C28—C29—H29B	110.1
C22—C21—H21A	109.5	H29A—C29—H29B	108.4

O4—S1—N2—C21	174.25 (10)	C14—C15—C16—C11	−3.1 (2)
O3—S1—N2—C21	44.45 (12)	C12—C11—C16—C15	0.1 (2)
C11—S1—N2—C21	−68.37 (11)	S1—C11—C16—C15	173.41 (12)
O4—S1—N2—C29	−44.33 (11)	C29—N2—C21—C22	51.67 (15)
O3—S1—N2—C29	−174.13 (11)	S1—N2—C21—C22	−164.46 (9)
C11—S1—N2—C29	73.05 (11)	N2—C21—C22—C27	−18.59 (17)
O4—S1—C11—C12	8.80 (13)	N2—C21—C22—C23	163.18 (12)
O3—S1—C11—C12	137.28 (11)	C27—C22—C23—C24	0.3 (2)
N2—S1—C11—C12	−108.79 (11)	C21—C22—C23—C24	178.59 (14)
O4—S1—C11—C16	−164.02 (11)	C22—C23—C24—C25	0.3 (2)
O3—S1—C11—C16	−35.55 (12)	C23—C24—C25—C26	−0.6 (2)
N2—S1—C11—C16	78.38 (11)	C24—C25—C26—C27	0.3 (2)
C16—C11—C12—C13	3.29 (19)	C23—C22—C27—C26	−0.57 (19)
S1—C11—C12—C13	−169.52 (10)	C21—C22—C27—C26	−178.78 (12)
C16—C11—C12—N1	−176.67 (11)	C23—C22—C27—C28	−179.31 (13)
S1—C11—C12—N1	10.51 (17)	C21—C22—C27—C28	2.48 (19)
O1—N1—C12—C13	−113.75 (14)	C25—C26—C27—C22	0.2 (2)
O2—N1—C12—C13	63.11 (16)	C25—C26—C27—C28	178.98 (14)
O1—N1—C12—C11	66.22 (16)	C22—C27—C28—C29	−17.28 (19)
O2—N1—C12—C11	−116.92 (14)	C26—C27—C28—C29	164.01 (13)
C11—C12—C13—C14	−3.6 (2)	C21—N2—C29—C28	−67.02 (14)
N1—C12—C13—C14	176.35 (13)	S1—N2—C29—C28	150.04 (10)
C12—C13—C14—C15	0.5 (2)	C27—C28—C29—N2	47.28 (16)
C13—C14—C15—C16	2.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O3^{i}	0.9300	2.4000	3.1093 (19)	133.00
C21—H21*A*···O2^{ii}	0.9700	2.5700	3.1843 (18)	121.00
C21—H21*B*···O3	0.9700	2.4500	2.8713 (17)	106.00
C29—H29*A*···O4	0.9700	2.5100	2.9532 (18)	108.00

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2.
*No classical hydrogen bonds found.

***N*-(*o*-Aminobenzene sulfonyl)-1,3,4-trihydroisoquinoline (7)**

Crystal data

$C_{15}H_{16}N_2O_2S$	F(000) = 608
M_r = 288.36	D_x = 1.358 Mg m^{-3}
Monoclinic, $P2_1/n$ (No. 14)	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 10.3376 (5) Å	Cell parameters from 9944 reflections
b = 12.6151 (5) Å	θ = 2.5–28.1º
c = 10.8850 (5) Å	μ = 0.232 mm^{-1}
β = 96.590 (2)º	T = 296 K
V = 1410.13 (11) Å^3	Platelet, colorless
Z = 4	0.70 × 0.63 × 0.25 mm

Data collection

Bruker Apex II CCD diffractometer	24938 measured reflections
	3524 independent reflections
Radiation source: sealed tube	2860 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.023

Detector resolution: 8.3333 pixels mm^{-1}
ϕ and ω scans
Absorption correction: numerical
(*SADABS* V2008/1; Bruker, 2012)
T_{min} = 0.938, T_{max} = 1.000

θ_{max} = 28.4º, θ_{min} = 2.5º
h = −13→13
k = −16→16
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.0350
$wR(F^2)$ = 0.1029
S = 1.07
3524 reflections
189 parameters
0 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.3199P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = –0.36 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are considered individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 U_{eq}(C). The nitrogen-bound H atoms were located on a difference map and refined freely.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.36887 (3)	0.30805 (3)	0.41884 (3)	0.03528 (11)
O1	0.34861 (12)	0.19583 (8)	0.41677 (10)	0.0495 (3)
O2	0.49141 (10)	0.34827 (10)	0.47555 (9)	0.0479 (3)
N1	0.19007 (18)	0.22126 (15)	0.19078 (17)	0.0631 (4)
N2	0.25856 (11)	0.35848 (9)	0.49702 (10)	0.0349 (3)
C1	0.25700 (14)	0.47423 (11)	0.50735 (13)	0.0380 (3)
H1A	0.214333	0.504656	0.431445	0.046*
H1B	0.345581	0.500824	0.519821	0.046*
C2	0.06877 (16)	0.33107 (13)	0.60393 (16)	0.0501 (4)
H2A	−0.024753	0.320862	0.589619	0.060*
H2B	0.103838	0.277716	0.662725	0.060*
C3	0.12588 (14)	0.31450 (13)	0.48327 (15)	0.0447 (3)
H3A	0.128283	0.239482	0.464112	0.054*
H3B	0.072729	0.350037	0.416401	0.054*
C11	0.34692 (13)	0.35721 (11)	0.26712 (12)	0.0356 (3)
C12	0.25866 (14)	0.31072 (12)	0.17451 (13)	0.0417 (3)
C13	0.24247 (17)	0.36177 (16)	0.05937 (14)	0.0549 (4)
H13	0.183682	0.334057	−0.003531	0.066*
C14	0.31081 (19)	0.45126 (17)	0.03702 (16)	0.0628 (5)
H14	0.297303	0.483392	−0.040281	0.075*
C15	0.39995 (19)	0.49467 (15)	0.12815 (17)	0.0588 (5)
H15	0.447519	0.554593	0.111808	0.071*

C16	0.41707 (15)	0.44793 (13)	0.24301 (15)	0.0455 (3)
H16	0.475807	0.476966	0.305053	0.055*
C21	0.18557 (13)	0.50654 (12)	0.61447 (12)	0.0370 (3)
C22	0.09610 (13)	0.43882 (12)	0.65963 (13)	0.0400 (3)
C23	0.03411 (16)	0.47287 (15)	0.76068 (15)	0.0529 (4)
H23	−0.026015	0.428583	0.792175	0.063*
C24	0.06035 (16)	0.57013 (17)	0.81395 (15)	0.0581 (5)
H24	0.018948	0.590748	0.881572	0.070*
C25	0.14736 (17)	0.63706 (16)	0.76791 (16)	0.0584 (5)
H25	0.164088	0.703503	0.803229	0.070*
C26	0.21007 (16)	0.60530 (14)	0.66878 (15)	0.0492 (4)
H26	0.269526	0.650614	0.637909	0.059*
H1C	0.140 (2)	0.1999 (17)	0.134 (2)	0.072 (7)*
H1D	0.208 (2)	0.1835 (16)	0.255 (2)	0.067 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03212 (18)	0.0394 (2)	0.03337 (17)	0.00473 (13)	−0.00013 (12)	0.00224 (13)
O1	0.0616 (7)	0.0373 (6)	0.0492 (6)	0.0098 (5)	0.0046 (5)	0.0044 (4)
O2	0.0306 (5)	0.0674 (7)	0.0438 (6)	0.0037 (5)	−0.0041 (4)	0.0023 (5)
N1	0.0664 (10)	0.0648 (10)	0.0532 (9)	−0.0158 (8)	−0.0148 (8)	−0.0044 (8)
N2	0.0312 (6)	0.0366 (6)	0.0373 (6)	−0.0041 (5)	0.0055 (4)	−0.0011 (5)
C1	0.0374 (7)	0.0385 (7)	0.0395 (7)	−0.0049 (6)	0.0102 (5)	−0.0018 (5)
C2	0.0397 (8)	0.0495 (9)	0.0634 (10)	−0.0062 (7)	0.0153 (7)	0.0086 (7)
C3	0.0339 (7)	0.0452 (8)	0.0544 (9)	−0.0095 (6)	0.0029 (6)	−0.0032 (6)
C11	0.0336 (7)	0.0415 (7)	0.0318 (6)	0.0079 (6)	0.0043 (5)	0.0011 (5)
C12	0.0370 (7)	0.0504 (8)	0.0372 (7)	0.0100 (6)	0.0028 (6)	−0.0046 (6)
C13	0.0491 (9)	0.0798 (13)	0.0343 (7)	0.0148 (9)	−0.0021 (6)	−0.0016 (7)
C14	0.0605 (11)	0.0862 (14)	0.0429 (9)	0.0230 (10)	0.0114 (8)	0.0203 (9)
C15	0.0608 (11)	0.0597 (11)	0.0587 (10)	0.0051 (9)	0.0197 (8)	0.0181 (8)
C16	0.0422 (8)	0.0490 (8)	0.0460 (8)	0.0016 (7)	0.0080 (6)	0.0029 (6)
C21	0.0307 (6)	0.0451 (8)	0.0350 (6)	0.0006 (6)	0.0035 (5)	−0.0014 (5)
C22	0.0307 (7)	0.0527 (9)	0.0369 (7)	0.0024 (6)	0.0049 (5)	0.0069 (6)
C23	0.0391 (8)	0.0785 (12)	0.0427 (8)	0.0048 (8)	0.0115 (6)	0.0114 (8)
C24	0.0443 (9)	0.0918 (14)	0.0385 (8)	0.0128 (9)	0.0059 (6)	−0.0123 (8)
C25	0.0457 (9)	0.0737 (12)	0.0548 (9)	0.0033 (9)	0.0019 (7)	−0.0257 (9)
C26	0.0409 (8)	0.0544 (9)	0.0525 (9)	−0.0055 (7)	0.0065 (7)	−0.0139 (7)

Geometric parameters (Å², º)

S1—O1	1.4309 (11)	C11—C12	1.408 (2)
S1—O2	1.4366 (11)	C12—C13	1.402 (2)
S1—N2	1.6285 (12)	C13—C14	1.368 (3)
S1—C11	1.7542 (13)	C13—H13	0.9300
N1—C12	1.355 (2)	C14—C15	1.387 (3)
N1—H1C	0.81 (2)	C14—H14	0.9300
N1—H1D	0.84 (2)	C15—C16	1.375 (2)
N2—C1	1.4648 (18)	C15—H15	0.9300
N2—C3	1.4712 (17)	C16—H16	0.9300
C1—C21	1.5062 (19)	C21—C22	1.390 (2)
C1—H1A	0.9700	C21—C26	1.390 (2)
C1—H1B	0.9700	C22—C23	1.402 (2)
C2—C22	1.502 (2)	C23—C24	1.371 (3)
C2—C3	1.515 (2)	C23—H23	0.9300
C2—H2A	0.9700	C24—C25	1.370 (3)
C2—H2B	0.9700	C24—H24	0.9300
C3—H3A	0.9700	C25—C26	1.380 (2)
C3—H3B	0.9700	C25—H25	0.9300

C11—C16	1.396 (2)	C26—H26	0.9300
O1—S1—O2	118.45 (7)	N1—C12—C13	119.26 (15)
O1—S1—N2	106.54 (6)	N1—C12—C11	124.01 (14)
O2—S1—N2	105.86 (6)	C13—C12—C11	116.73 (15)
O1—S1—C11	109.40 (7)	C14—C13—C12	121.80 (16)
O2—S1—C11	106.98 (7)	C14—C13—H13	119.1
N2—S1—C11	109.34 (6)	C12—C13—H13	119.1
C12—N1—H1C	118.6 (16)	C13—C14—C15	120.86 (15)
C12—N1—H1D	120.6 (14)	C13—C14—H14	119.6
H1C—N1—H1D	120 (2)	C15—C14—H14	119.6
C1—N2—C3	111.43 (11)	C16—C15—C14	119.11 (17)
C1—N2—S1	116.37 (9)	C16—C15—H15	120.4
C3—N2—S1	120.00 (10)	C14—C15—H15	120.4
N2—C1—C21	109.87 (11)	C15—C16—C11	120.47 (16)
N2—C1—H1A	109.7	C15—C16—H16	119.8
C21—C1—H1A	109.7	C11—C16—H16	119.8
N2—C1—H1B	109.7	C22—C21—C26	119.79 (14)
C21—C1—H1B	109.7	C22—C21—C1	120.85 (13)
H1A—C1—H1B	108.2	C26—C21—C1	119.35 (13)
C22—C2—C3	113.64 (12)	C21—C22—C23	118.14 (15)
C22—C2—H2A	108.8	C21—C22—C2	121.03 (13)
C3—C2—H2A	108.8	C23—C22—C2	120.81 (14)
C22—C2—H2B	108.8	C24—C23—C22	121.32 (16)
C3—C2—H2B	108.8	C24—C23—H23	119.3
H2A—C2—H2B	107.7	C22—C23—H23	119.3
N2—C3—C2	108.14 (12)	C25—C24—C23	120.22 (15)
N2—C3—H3A	110.1	C25—C24—H24	119.9
C2—C3—H3A	110.1	C23—C24—H24	119.9
N2—C3—H3B	110.1	C24—C25—C26	119.60 (17)
C2—C3—H3B	110.1	C24—C25—H25	120.2
H3A—C3—H3B	108.4	C26—C25—H25	120.2
C16—C11—C12	121.00 (13)	C25—C26—C21	120.91 (16)
C16—C11—S1	116.94 (11)	C25—C26—H26	119.5
C12—C11—S1	122.00 (11)	C21—C26—H26	119.5
O1—S1—N2—C1	−177.66 (10)	C11—C12—C13—C14	1.2 (2)
O2—S1—N2—C1	55.39 (11)	C12—C13—C14—C15	0.4 (3)
C11—S1—N2—C1	−59.54 (11)	C13—C14—C15—C16	−1.4 (3)
O1—S1—N2—C3	−38.45 (12)	C14—C15—C16—C11	0.8 (3)
O2—S1—N2—C3	−165.39 (11)	C12—C11—C16—C15	0.9 (2)
C11—S1—N2—C3	79.68 (12)	S1—C11—C16—C15	−176.48 (13)
C3—N2—C1—C21	56.94 (15)	N2—C1—C21—C22	−22.43 (18)
S1—N2—C1—C21	−160.49 (9)	N2—C1—C21—C26	157.38 (13)
C1—N2—C3—C2	−68.32 (15)	C26—C21—C22—C23	−0.7 (2)
S1—N2—C3—C2	150.63 (11)	C1—C21—C22—C23	179.12 (13)
C22—C2—C3—N2	42.95 (18)	C26—C21—C22—C2	−179.23 (14)
O1—S1—C11—C16	−151.08 (11)	C1—C21—C22—C2	0.6 (2)
O2—S1—C11—C16	−21.61 (13)	C3—C2—C22—C21	−11.2 (2)
N2—S1—C11—C16	92.59 (12)	C3—C2—C22—C23	170.24 (14)
O1—S1—C11—C12	31.61 (14)	C21—C22—C23—C24	0.0 (2)
O2—S1—C11—C12	161.08 (11)	C2—C22—C23—C24	178.59 (15)
N2—S1—C11—C12	−84.72 (12)	C22—C23—C24—C25	0.8 (3)
C16—C11—C12—N1	178.24 (16)	C23—C24—C25—C26	−1.0 (3)
S1—C11—C12—N1	−4.6 (2)	C24—C25—C26—C21	0.4 (3)
C16—C11—C12—C13	−1.8 (2)	C22—C21—C26—C25	0.5 (2)
S1—C11—C12—C13	175.35 (11)	C1—C21—C26—C25	−179.33 (15)
N1—C12—C13—C14	−178.85 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O2^{i}	0.81 (2)	2.26 (2)	3.0612 (19)	176 (2)
N1—H1*D*···O1	0.84 (2)	2.16 (2)	2.813 (2)	134.0 (18)
C1—H1*B*···O2	0.9700	2.5200	2.9512 (18)	107.00
C1—H1*B*···O2^{ii}	0.9700	2.5400	3.4207 (18)	151.00
C3—H3*A*···O1	0.9700	2.4500	2.9067 (19)	108.00
C16—H16···O2	0.9300	2.4600	2.8516 (19)	106.00
C23—H23···O1^{iii}	0.9300	2.5300	3.441 (2)	168.00

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1/2, −*y*+1/2, *z*+1/2.

10-iodo-1,2-dihydroisoquinolino[2,1-*b*][1,2,4]benzothiadiazine 12,12-dioxide (8)

Crystal data

$C_{15}H_{11}IN_2O_2S$
M_r = 410.22
Monoclinic, $P2_1/c$ (No. 14)
a = 10.9586 (6) Å
b = 10.2679 (6) Å
c = 12.9392 (8) Å
β = 93.624 (3)º
V = 1453.03 (15) Å^3
Z = 4
F(000) = 800
D_x = 1.875 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 7151 reflections
θ = 2.5–28.0º
μ = 2.352 mm^{-1}
T = 296 K
Platelet, yellow
0.49 × 0.36 × 0.06 mm

Data collection

Bruker Apex II CCD
Diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ϕ and ω scans
Absorption correction: numerical (*SADABS* V2008/1; Bruker, 2012)
T_{min} = 0.763, T_{max} = 1.000
19964 measured reflections
3628 independent reflections
2871 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 28.5º, θ_{min} = 1.9º
h = −14→14
k = −13→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.0444
$wR(F^2)$ = 0.1498
S = 1.03
3628 reflections
190 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighboring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0905P)^2 + 2.0774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.86 e Å^{-3}
$\Delta\rho_{min}$ = –1.09 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are considered individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 U_{eq}(C). Two reflections with large differences between their observed and calculated intensities were omitted. This is due to obstruction by the beam stop.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	1.01660 (3)	0.46280 (3)	0.16942 (3)	0.06583 (18)
S1	0.70749 (8)	0.75401 (9)	0.41931 (8)	0.0379 (2)
O1	0.8074 (3)	0.7664 (4)	0.4940 (3)	0.0613 (9)
O2	0.6731 (4)	0.8659 (3)	0.3584 (3)	0.0624 (9)
N1	0.5073 (3)	0.5693 (3)	0.3420 (2)	0.0324 (6)
N2	0.5882 (3)	0.7021 (3)	0.4798 (2)	0.0335 (6)
C1	0.4936 (3)	0.6383 (3)	0.4240 (2)	0.0290 (6)
C2	0.5695 (4)	0.7534 (4)	0.5854 (3)	0.0407 (8)
H2A	0.636382	0.810999	0.607258	0.049*
H2B	0.568488	0.681763	0.634225	0.049*
C3	0.4510 (4)	0.8261 (4)	0.5847 (3)	0.0448 (9)
H3A	0.456633	0.905008	0.543989	0.054*
H3B	0.434757	0.850892	0.654831	0.054*
C11	0.6227 (3)	0.5507 (3)	0.3062 (2)	0.0293 (6)
C12	0.7255 (3)	0.6235 (3)	0.3372 (2)	0.0302 (7)
C13	0.8396 (3)	0.6004 (3)	0.2992 (3)	0.0354 (7)
H13	0.907117	0.650186	0.321468	0.042*
C14	0.8503 (4)	0.5020 (4)	0.2277 (3)	0.0361 (7)
C15	0.7487 (4)	0.4288 (4)	0.1941 (3)	0.0400 (8)
H15	0.756778	0.362938	0.145654	0.048*
C16	0.6363 (4)	0.4529 (4)	0.2319 (3)	0.0372 (8)
H16	0.568830	0.403990	0.208068	0.045*
C21	0.3706 (3)	0.6515 (3)	0.4628 (3)	0.0310 (7)
C22	0.3482 (3)	0.7433 (4)	0.5396 (3)	0.0369 (8)
C23	0.2295 (4)	0.7573 (5)	0.5695 (3)	0.0489 (10)
H23	0.213387	0.818906	0.619466	0.059*
C24	0.1357 (4)	0.6830 (5)	0.5274 (4)	0.0562 (12)
H24	0.056878	0.694086	0.548763	0.067*
C25	0.1585 (4)	0.5911 (5)	0.4528 (4)	0.0534 (11)
H25	0.094778	0.539973	0.424588	0.064*
C26	0.2745 (4)	0.5745 (4)	0.4199 (3)	0.0413 (8)
H26	0.289054	0.512725	0.369543	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0549 (2)	0.0607 (3)	0.0861 (3)	−0.00008 (14)	0.03780 (19)	−0.01542 (16)
S1	0.0315 (4)	0.0329 (4)	0.0506 (5)	−0.0050 (3)	0.0134 (4)	−0.0122 (4)
O1	0.0339 (15)	0.082 (2)	0.068 (2)	−0.0142 (15)	0.0099 (14)	−0.0392 (18)
O2	0.074 (2)	0.0292 (14)	0.088 (2)	0.0057 (14)	0.0405 (19)	0.0050 (15)
N1	0.0285 (14)	0.0386 (15)	0.0301 (13)	−0.0017 (12)	0.0031 (11)	−0.0050 (11)
N2	0.0280 (14)	0.0397 (16)	0.0335 (14)	−0.0027 (12)	0.0088 (11)	−0.0097 (12)
C1	0.0267 (15)	0.0305 (15)	0.0300 (15)	0.0007 (12)	0.0024 (12)	0.0012 (12)
C2	0.0400 (19)	0.047 (2)	0.0350 (17)	−0.0013 (17)	0.0056 (14)	−0.0137 (15)
C3	0.047 (2)	0.044 (2)	0.045 (2)	0.0035 (18)	0.0142 (17)	−0.0107 (17)
C11	0.0282 (16)	0.0322 (16)	0.0278 (14)	0.0005 (12)	0.0045 (12)	−0.0015 (12)
C12	0.0314 (16)	0.0281 (15)	0.0316 (15)	0.0006 (12)	0.0071 (13)	−0.0036 (12)
C13	0.0300 (16)	0.0329 (17)	0.0442 (18)	−0.0014 (14)	0.0109 (14)	−0.0042 (14)
C14	0.0364 (18)	0.0358 (17)	0.0374 (17)	0.0019 (15)	0.0137 (14)	−0.0024 (14)

C15	0.047 (2)	0.0387 (18)	0.0351 (17)	−0.0001 (17)	0.0121 (15)	−0.0073 (15)
C16	0.0377 (19)	0.0404 (19)	0.0339 (17)	−0.0048 (15)	0.0050 (14)	−0.0097 (14)
C21	0.0259 (15)	0.0332 (16)	0.0345 (16)	0.0051 (13)	0.0058 (12)	0.0061 (13)
C22	0.0364 (18)	0.0411 (19)	0.0338 (16)	0.0095 (15)	0.0087 (14)	0.0043 (14)
C23	0.041 (2)	0.061 (3)	0.046 (2)	0.015 (2)	0.0143 (17)	0.0056 (19)
C24	0.031 (2)	0.079 (3)	0.060 (3)	0.014 (2)	0.0143 (18)	0.020 (2)
C25	0.0276 (18)	0.066 (3)	0.067 (3)	−0.0008 (19)	0.0033 (18)	0.012 (2)
C26	0.0298 (17)	0.045 (2)	0.049 (2)	0.0005 (16)	0.0018 (15)	0.0051 (17)

Geometric parameters (Å², º)

I1—C14	2.055 (4)	C12—C13	1.393 (5)
S1—O1	1.419 (3)	C13—C14	1.379 (5)
S1—O2	1.430 (4)	C13—H13	0.9300
S1—N2	1.653 (3)	C14—C15	1.391 (6)
S1—C12	1.729 (3)	C15—C16	1.376 (6)
N1—C1	1.293 (4)	C15—H15	0.9300
N1—C11	1.388 (4)	C16—H16	0.9300
N2—C1	1.389 (4)	C21—C26	1.403 (5)
N2—C2	1.491 (4)	C21—C22	1.403 (5)
C1—C21	1.474 (5)	C22—C23	1.388 (6)
C2—C3	1.498 (6)	C23—C24	1.365 (7)
C2—H2A	0.9700	C23—H23	0.9300
C2—H2B	0.9700	C24—C25	1.384 (8)
C3—C22	1.500 (6)	C24—H24	0.9300
C3—H3A	0.9700	C25—C26	1.376 (6)
C3—H3B	0.9700	C25—H25	0.9300
C11—C12	1.389 (5)	C26—H26	0.9300
C11—C16	1.405 (5)		
O1—S1—O2	117.9 (2)	C14—C13—C12	118.6 (3)
O1—S1—N2	107.81 (19)	C14—C13—H13	120.7
O2—S1—N2	109.33 (19)	C12—C13—H13	120.7
O1—S1—C12	112.00 (19)	C13—C14—C15	120.3 (3)
O2—S1—C12	108.68 (19)	C13—C14—I1	120.3 (3)
N2—S1—C12	99.50 (16)	C15—C14—I1	119.4 (3)
C1—N1—C11	120.3 (3)	C16—C15—C14	120.6 (3)
C1—N2—C2	120.1 (3)	C16—C15—H15	119.7
C1—N2—S1	119.5 (2)	C14—C15—H15	119.7
C2—N2—S1	118.6 (2)	C15—C16—C11	120.5 (3)
N1—C1—N2	124.3 (3)	C15—C16—H16	119.8
N1—C1—C21	119.0 (3)	C11—C16—H16	119.8
N2—C1—C21	116.7 (3)	C26—C21—C22	119.9 (3)
N2—C2—C3	109.9 (3)	C26—C21—C1	119.6 (3)
N2—C2—H2A	109.7	C22—C21—C1	120.5 (3)
C3—C2—H2A	109.7	C23—C22—C21	118.4 (4)
N2—C2—H2B	109.7	C23—C22—C3	121.8 (4)
C3—C2—H2B	109.7	C21—C22—C3	119.7 (3)
H2A—C2—H2B	108.2	C24—C23—C22	121.8 (4)
C2—C3—C22	110.5 (3)	C24—C23—H23	119.1
C2—C3—H3A	109.6	C22—C23—H23	119.1
C22—C3—H3A	109.6	C23—C24—C25	119.6 (4)
C2—C3—H3B	109.6	C23—C24—H24	120.2
C22—C3—H3B	109.6	C25—C24—H24	120.2
H3A—C3—H3B	108.1	C26—C25—C24	120.8 (4)
N1—C11—C12	124.6 (3)	C26—C25—H25	119.6
N1—C11—C16	117.7 (3)	C24—C25—H25	119.6
C12—C11—C16	117.6 (3)	C25—C26—C21	119.5 (4)
C11—C12—C13	122.4 (3)	C25—C26—H26	120.2
C11—C12—S1	118.2 (3)	C21—C26—H26	120.2

C13—C12—S1	119.3 (3)		
O1—S1—N2—C1	−157.1 (3)	C11—C12—C13—C14	0.4 (5)
O2—S1—N2—C1	73.5 (3)	S1—C12—C13—C14	−175.2 (3)
C12—S1—N2—C1	−40.2 (3)	C12—C13—C14—C15	0.5 (6)
O1—S1—N2—C2	38.2 (3)	C12—C13—C14—I1	−179.7 (3)
O2—S1—N2—C2	−91.1 (3)	C13—C14—C15—C16	−0.3 (6)
C12—S1—N2—C2	155.1 (3)	I1—C14—C15—C16	179.9 (3)
C11—N1—C1—N2	2.5 (5)	C14—C15—C16—C11	−0.9 (6)
C11—N1—C1—C21	−177.3 (3)	N1—C11—C16—C15	−179.4 (3)
C2—N2—C1—N1	−166.0 (4)	C12—C11—C16—C15	1.8 (5)
S1—N2—C1—N1	29.6 (5)	N1—C1—C21—C26	9.3 (5)
C2—N2—C1—C21	13.8 (5)	N2—C1—C21—C26	−170.5 (3)
S1—N2—C1—C21	−150.6 (3)	N1—C1—C21—C22	−168.6 (3)
C1—N2—C2—C3	−46.8 (5)	N2—C1—C21—C22	11.6 (5)
S1—N2—C2—C3	117.8 (3)	C26—C21—C22—C23	−1.5 (5)
N2—C2—C3—C22	52.9 (4)	C1—C21—C22—C23	176.4 (3)
C1—N1—C11—C12	−15.1 (5)	C26—C21—C22—C3	−179.5 (3)
C1—N1—C11—C16	166.1 (3)	C1—C21—C22—C3	−1.7 (5)
N1—C11—C12—C13	179.7 (3)	C2—C3—C22—C23	150.6 (4)
C16—C11—C12—C13	−1.5 (5)	C2—C3—C22—C21	−31.4 (5)
N1—C11—C12—S1	−4.7 (5)	C21—C22—C23—C24	1.1 (6)
C16—C11—C12—S1	174.1 (3)	C3—C22—C23—C24	179.1 (4)
O1—S1—C12—C11	142.0 (3)	C22—C23—C24—C25	−0.1 (7)
O2—S1—C12—C11	−85.9 (3)	C23—C24—C25—C26	−0.6 (7)
N2—S1—C12—C11	28.3 (3)	C24—C25—C26—C21	0.2 (7)
O1—S1—C12—C13	−42.3 (4)	C22—C21—C26—C25	0.8 (6)
O2—S1—C12—C13	89.8 (3)	C1—C21—C26—C25	−177.0 (4)
N2—S1—C12—C13	−156.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O1	0.9700	2.4900	2.934 (5)	107.00

*No classical hydrogen bonds found.