Electronic Supplementary Information for

Planar Blatter radicals through Bu_3SnH and TMS_3SiH–assisted cyclization of aryl iodides: Azaphilic radical addition

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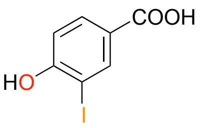
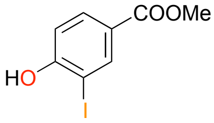
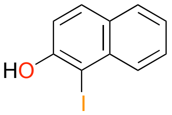
1. Additional synthetic details



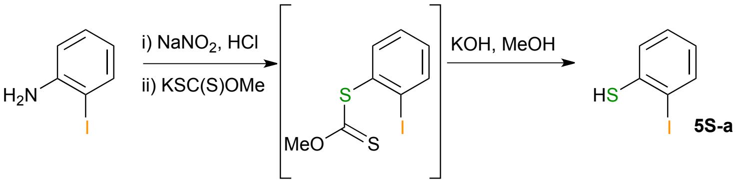
Synthesis of 4-hydroxy-3-iodobenzoic acid.[1] 4-Hydroxy-3-iodobenzoic acid was obtained according to a general literature procedure.[2] Thus, a 15% solution of iodine in 20% KI (40 mL) was added dropwise to a stirred solution of 4-hydroxybenzoic acid (1.99 g, 14.4 mmol) in 30 mL 2N $NaOH_{(aq)}$. The reaction mixture was stirred for 3 h at room temperature and then acidified with acetic acid to pH 3. The resulting suspension was filtered and the precipitate was washed well with water and dried giving 2.13 g (56% yield) as grey crystals: mp 139–141 °C (lit.[1] 172–175 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, J = 2.0 Hz, 1H), 7.85 (dd, J_1 = 8.6 Hz, J_2 = 2.0 Hz, 1H), 6.86 (d, J = 8.6 Hz, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 168.5, 162.4, 142.5, 132.6, 124.7, 115.0, 83.9; IR (KBr) *v* 1683, 1575, 1434, 1369, 1295, 1245, 1199, 769, 668 cm^{-1}; MS (ESI) *m/z* 263 (100, $[M-H]^-$). Anal. Calcd for $C_7H_5IO_3$: C, 31.85; H, 1.91. Found: C, 31.67; H, 2.03.



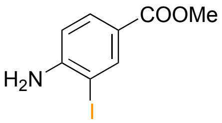
Methyl 4-ydroxy-3-iodobenzoate (5O-b).[3] Esterification of 4-hydroxy-3-iodobenzoic acid (*vide supra*) with MeOH in the presence of H_2SO_4 gave 1.25 g (66% yield) of methyl 4-hydroxy-3-iodobenzoate (**5O-b**) as grey crystals: mp 147–148 °C (lit.[3] 159 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (s, 1H), 7.93 (dd, J_1 = 8.4 Hz, J_2 = 1.7 Hz, 1H), 7.01 (d, J = 8.1 Hz, 1H), 3.89 (s, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 165.6, 158.9, 140.4, 132.1, 124.5, 114.8, 85.3, 52.4; IR (KBr) *v* 1690, 1596, 1439, 1408, 1270, 967, 765, 670, 630 cm^{-1}; MS (ESI) *m/z* 279 (100, $[M+H]^+$). Anal. Calcd for $C_8H_7IO_3$: C, 34.56; H, 2.54. Found: C, 34.58; H, 2.55.



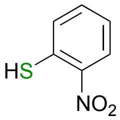
1-Iodonaphth-2-ol (5O-d).[4] 1-Iodonaphth-2-ol was obtained according to the same procedure as for 4-hydroxy-3-iodobenzoic acid giving 3.62 g (93 % yield) as grey crystals: mp 84–87 °C (lit.[4] 87–88 °C); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, J = 8.5 Hz, 1H), 7.76–7.71 (m, 2H), 7.55 (t, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 1H), 7.25 (t, J = 9.0 Hz, 1H), 5.82 (bs, 2H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 153.9, 134.9, 130.7, 130.4, 129.8, 128.4, 128.3, 124.3, 116.6, 86.3; IR (KBr) *v* 1622, 1496, 1431, 1346, 1302, 1232, 974, 923, 807, 745 cm^{-1}; MS (ESI) *m/z* 269 (100, $[M-H]^-$). Anal. Calcd for $C_{10}H_7IO$: C, 44.47; H, 2.61. Found: C, 44.31; H, 2.58.



Synthesis of 2-iodobenzenethiol (5S-a).[5] Following a literature procedure,[5] a solution of $NaNO_2$ (0.704 g, 0.01 mol) in water (2 mL) was added during 30 min to an ice cooled solution of *o*-iodoaniline (0.01 mol) in 35% aqueous HCl (1.67 mL, 0.02 mol) containing ice (2.0 g). After 45 min of stirring 20% aqueous solution of sodium acetate was added until the pH of the solution was 4-5. Next potassium methyl xanthate[6] (1.46 g, 0.01 mol) in water (2 mL) was added. The reaction mixture was slowly warmed up to room temperature and the resulting mixture was dissolved in CH_2Cl_2. The organic phase was separated, dried ($MgSO_4$) and evaporated to dryness. The residue was dissolved in MeOH (10 mL) containing KOH (3.0 g, 0.046 mol) and refluxed for 10 h. The reaction mixture was cooled and neutralized with 10% HCl (15 mL), and extracted with ether (3×10 mL). The combined organic phases were dried ($MgSO_4$) and evaporated to afford crude *o*-iodothiophenol, which was purified by column chromatography using silica gel (eluent, hexane/ethyl acetate = 5:1) giving 467 mg (20% yield) of **5S-a** as colorless oil: ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 7.40 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.21 (td, J_1 = 7.5 Hz, J_2 = 1.1 Hz, 1H), 6.81 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 4.14 (s, 1H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 1139.8, 138.4, 128.9, 128.6, 126.7, 98.3; MS (ESI) *m/z* 235 (100, $[M-H]^-$). Anal. Calcd for C_6H_5IS: C, 30.53; H, 2.13; S, 13.58. Found: C, 30.43; H, 2.29; S, 13.42.



Methyl 4-amino-2-iodobenzoate (7).[7] Methyl 4-aminobenzoate (0.525 g, 3.47 mmol) and pyridinium iodine monochloride[8] (0.841 g, 3.47 mmol) were dissolved in methanol (30 mL) and stirred at ambient temperature. After 2h, when the substrate was no longer present in the reaction mixture (TLC control), saturated aqueous solution of $Na_2S_2O_3$ was added dropwise until the color change from red to yellow. Then, the reaction mixture was concentrated to 2/3 volume, extracted with CH_2Cl_2, dried over $MgSO_4$ and evaporated to dryness. A pale yellow residue was purified by column chromatography (~10% AcOEt/pet. ether) and crystalized from pet. ether/CH_2Cl_2 giving 816 mg (85% yield) of methyl 4-amino-2-iodobenzoate (**7**) as pale crystals: mp 90–92 ^oC (MeOH/H_2O, 9:1; lit.[7] 90 ^oC); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, *J* = 1.6 Hz, 1H), 7.80 (dd, J_1 = 8.7 Hz, J_2 = 1.6 Hz, 1H), 6.69 (d, *J* = 8.7 Hz, 1H), 4.54 (s, 2H), 3.85 (s, 3H); $^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$) δ 165.9, 150.8, 141.1, 131.3, 121.3, 113.2, 82.2, 52.0; HRMS (ESI-TOF) *m/z* 278 $[M+H]^+$. Anal. Calcd for $C_8H_8INO_2$: C, 34.68; H, 2.91; N, 5.05. Found: C, 34.61; H, 2.95; N, 5.27.



Synthesis of 2-nitrobenzenethiol.[9] 2-Nitrobenzenethiol was obtained in a nearly quantitative yield from commercial 1,2-bis(2-nitrophenyl)disulfane by reduction with $NaBH_4$ in THF at reflux in the presence of MeOH according to the literature procedure,[9] and used to the next step without further purification. Pale yellow oil; MS (ESI) *m/z* 154 $[M-H]^-$.

2. NMR spectra

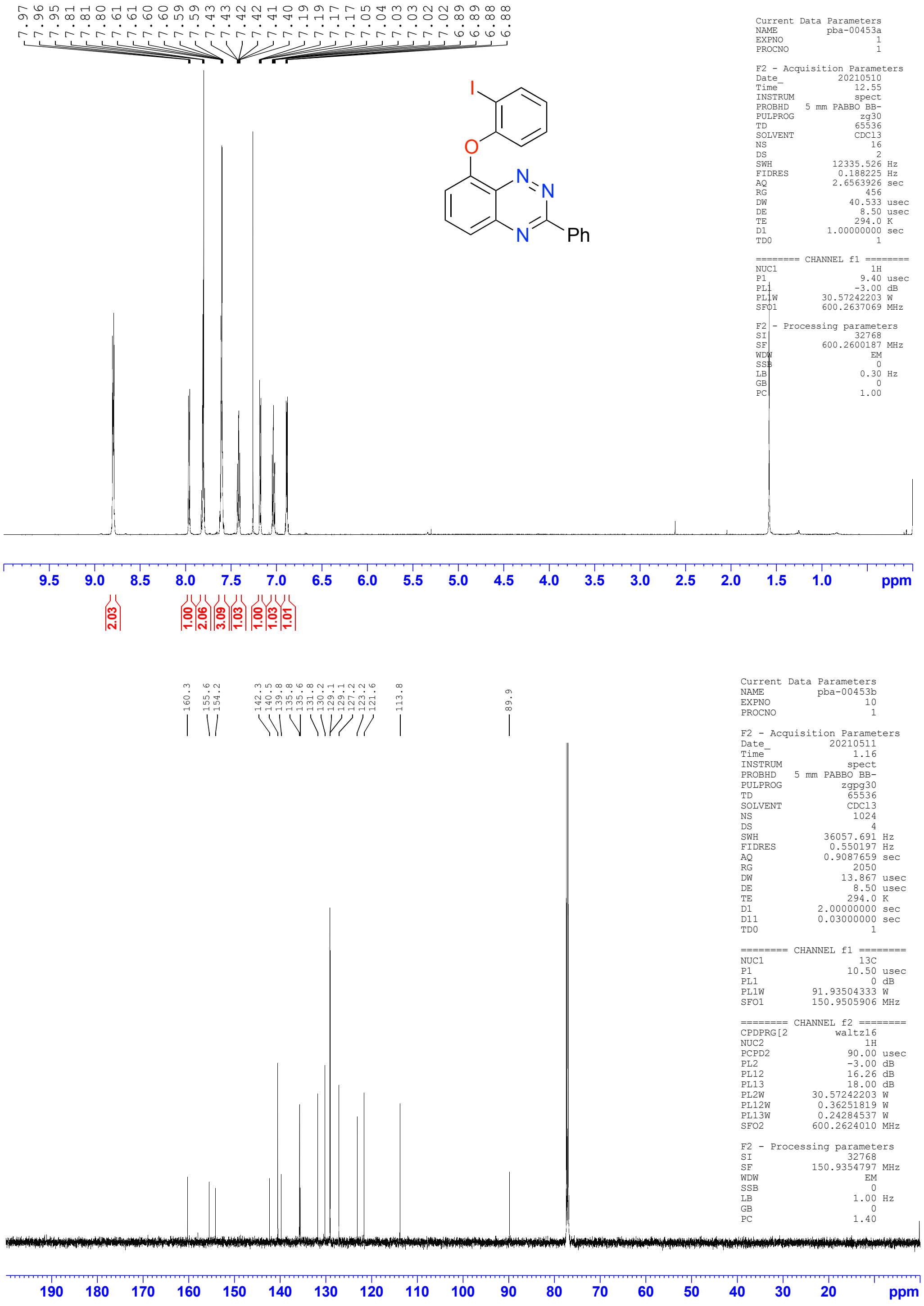


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Figure S1. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(2-iodophenoxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2O-a**) recorded in CDCl$_3$ at 600 and 151 MHz, respectively.

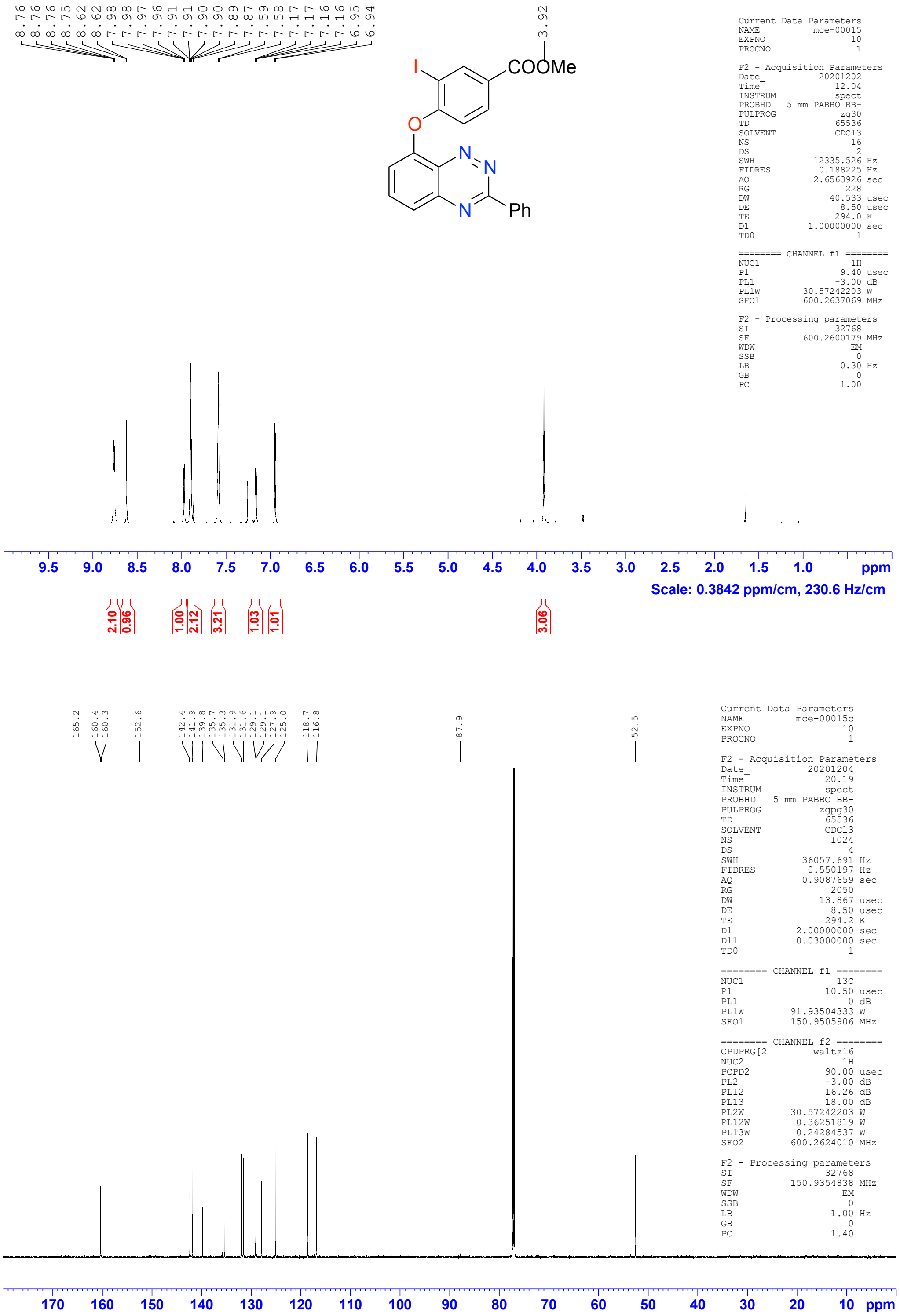

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Figure S2. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(2-iodo-3-methoxycarbonylphenoxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2O-b**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

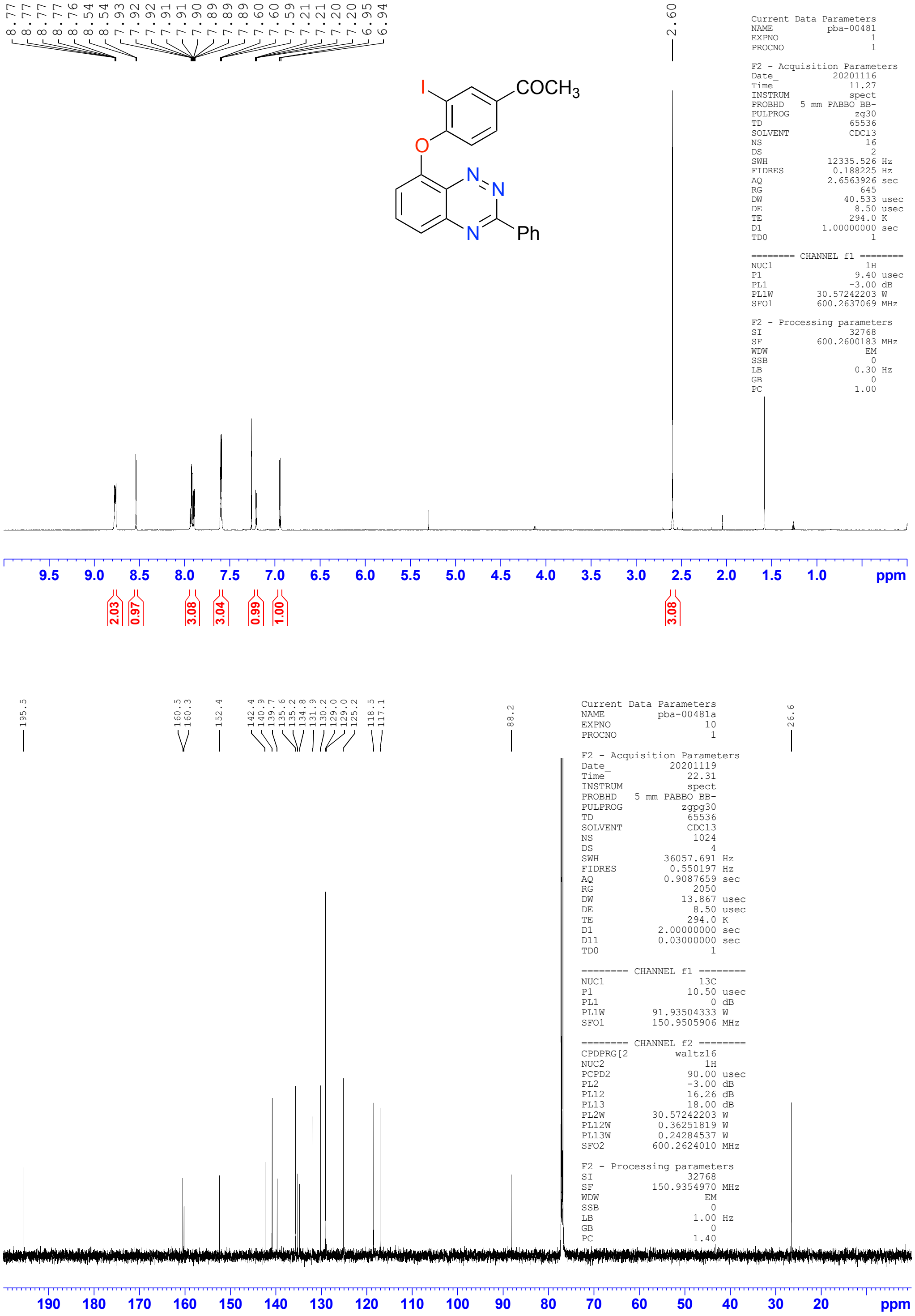

Figure S3. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(4-acetyl-2-iodophenyloxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2O-c**) recorded in CDCl$_3$ at 600 and 151 MHz, respectively.

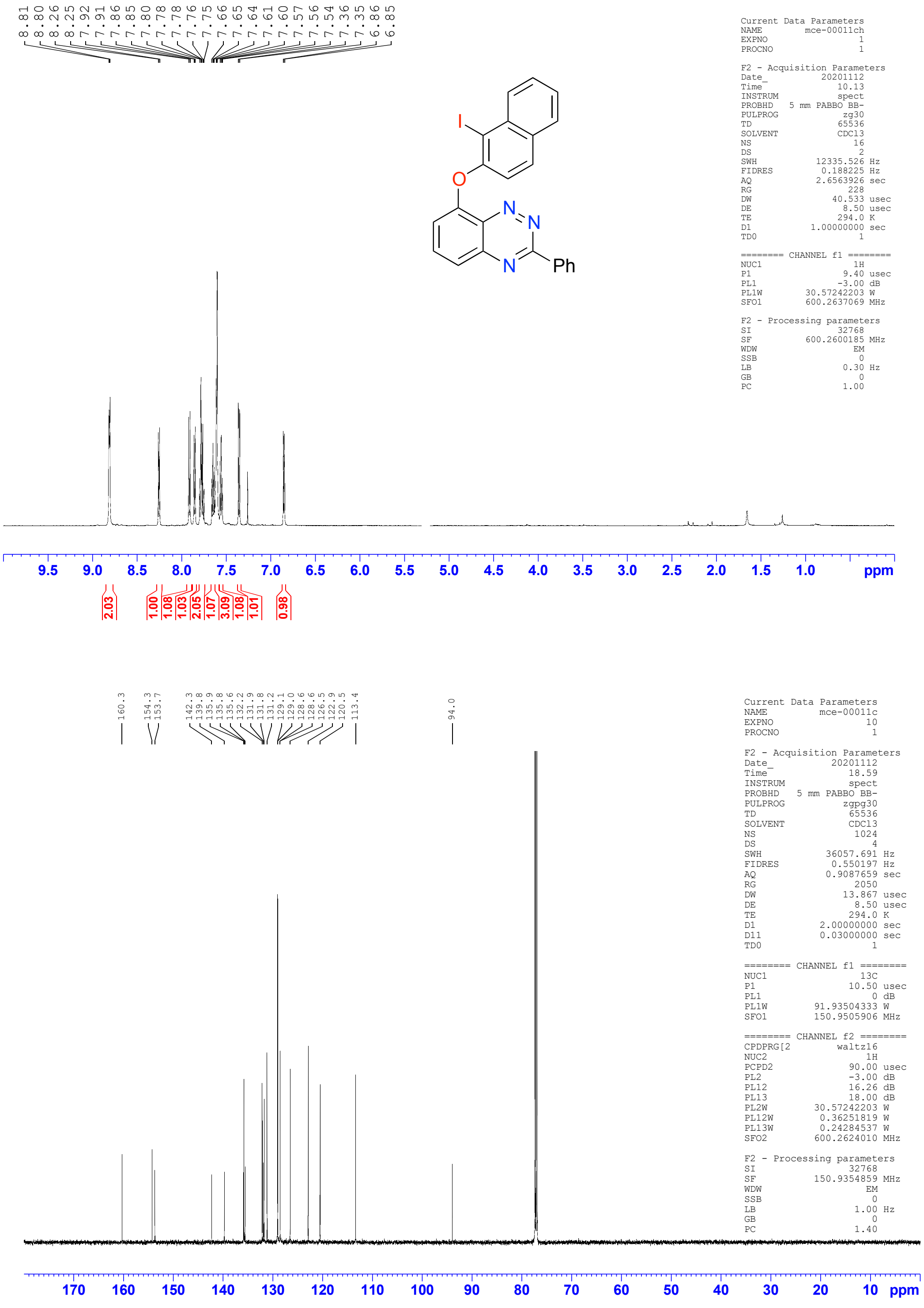

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Figure S4. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for 8-((1-Iodonaphthalen-2-yl)oxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2O-d**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

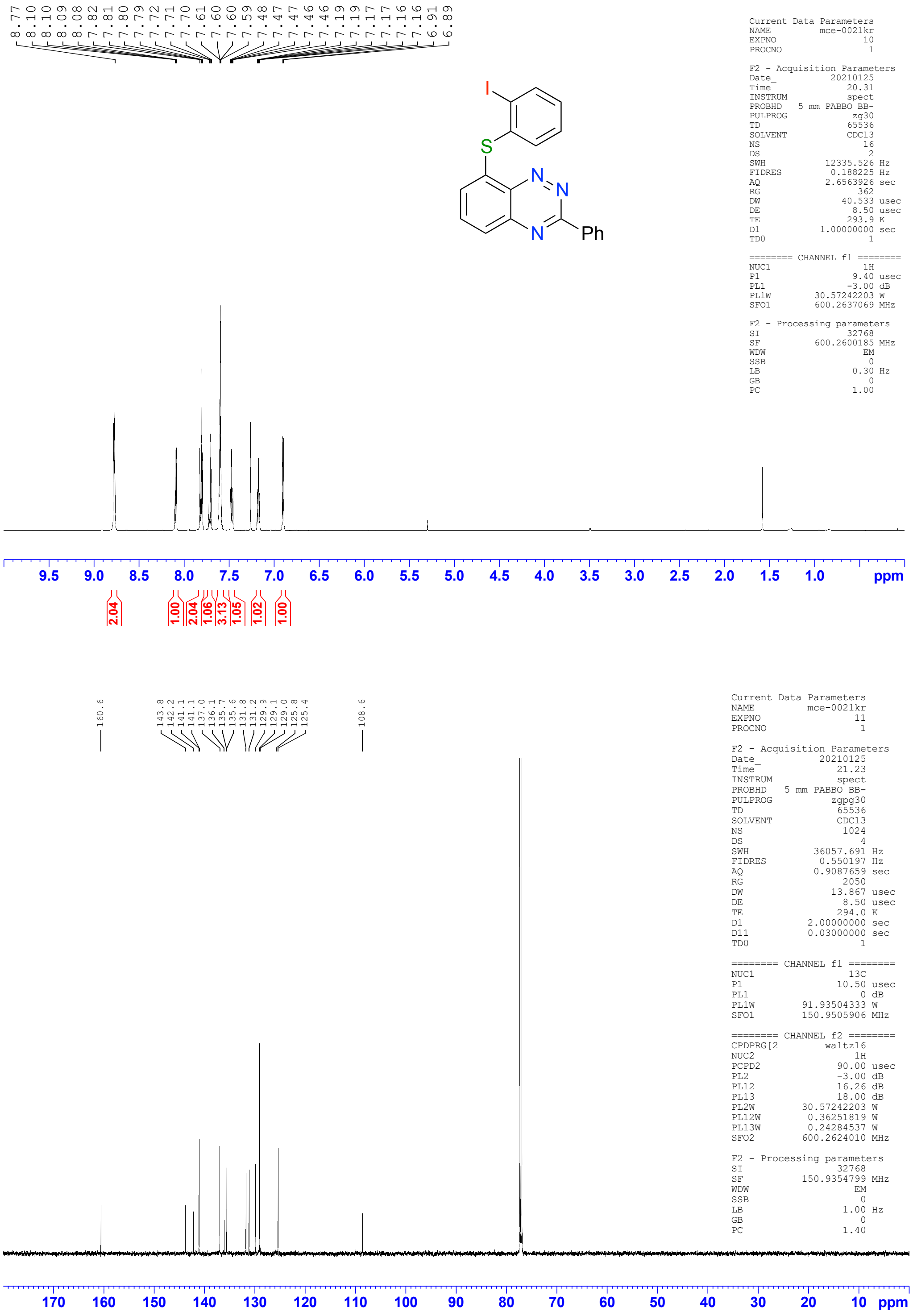

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Figure S5. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(2-iodophenylsulfanyl)-3-phenylbenzo[*e*][1,2,4]triazine (**2S-a**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

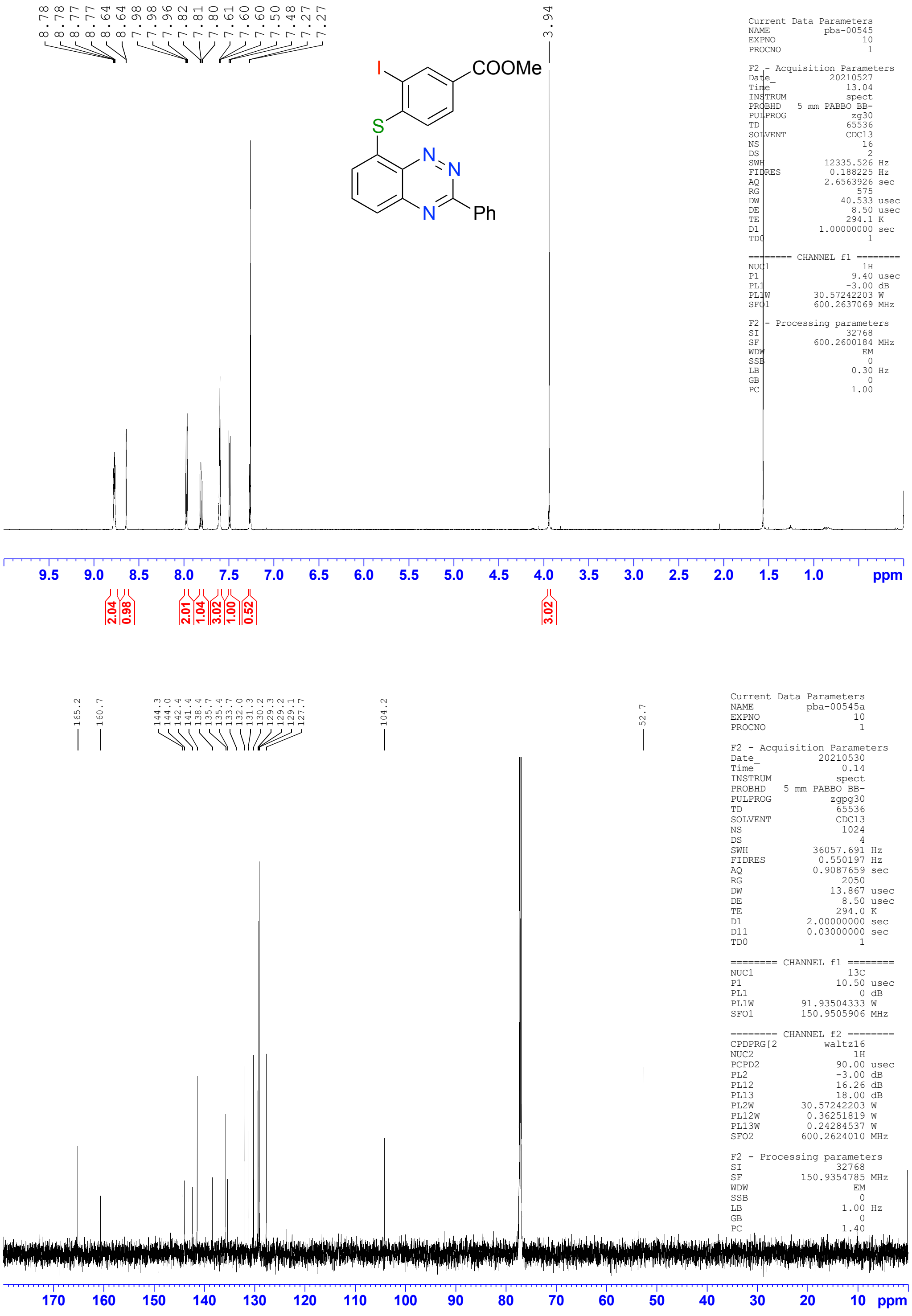
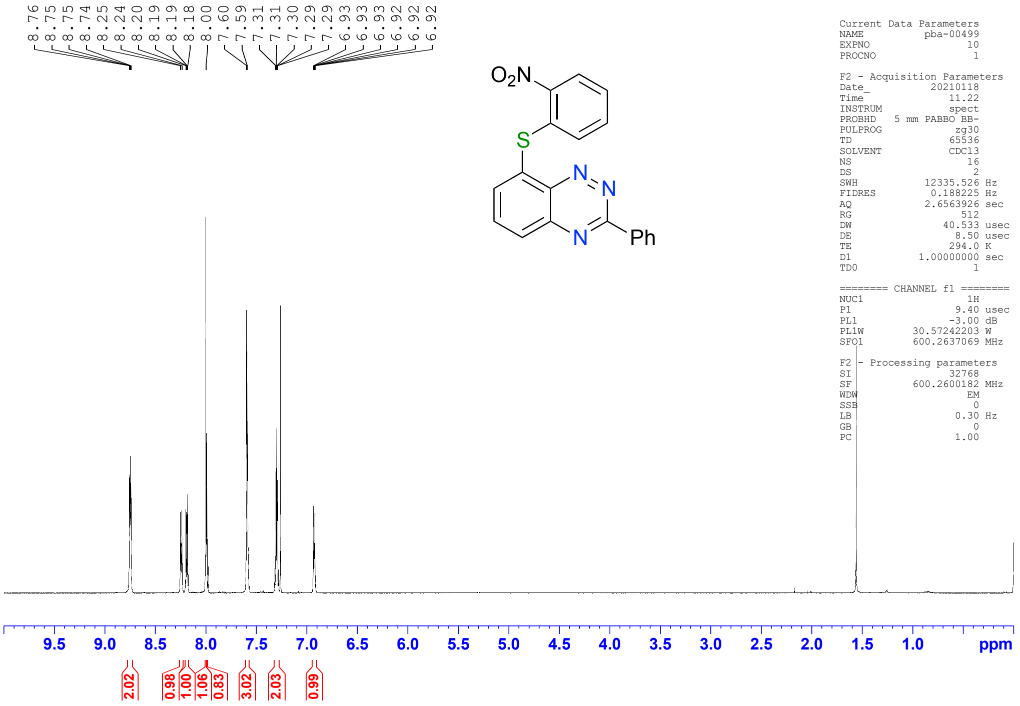


Figure S6. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(3-iodo-4-methoxycarbonylphylsulfanyl)-3-phenylbenzo[*e*][1,2,4]triazine (**2S-b**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.



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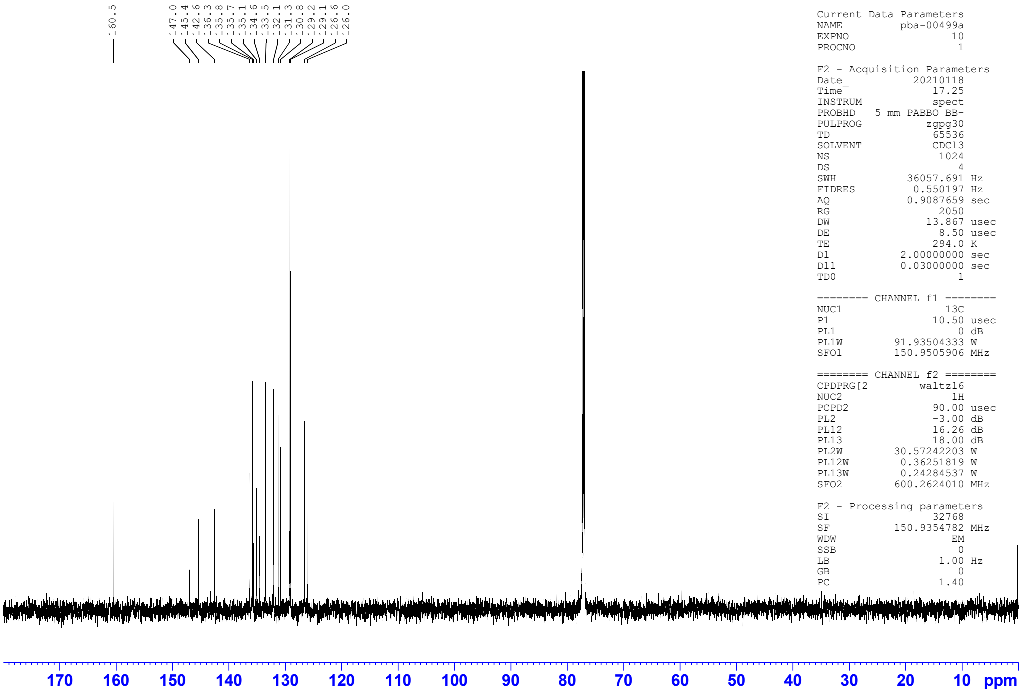

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NUC1                13C
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PL1W        91.93504333 W
SFO1        150.9505906 MHz

======== CHANNEL f2 ========
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PL13W        0.24284537 W
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```

Figure S7. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for 8-(2-nitrophenylsulfanyl)-3-phenylbenzo[*e*][1,2,4]triazine (**3S**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

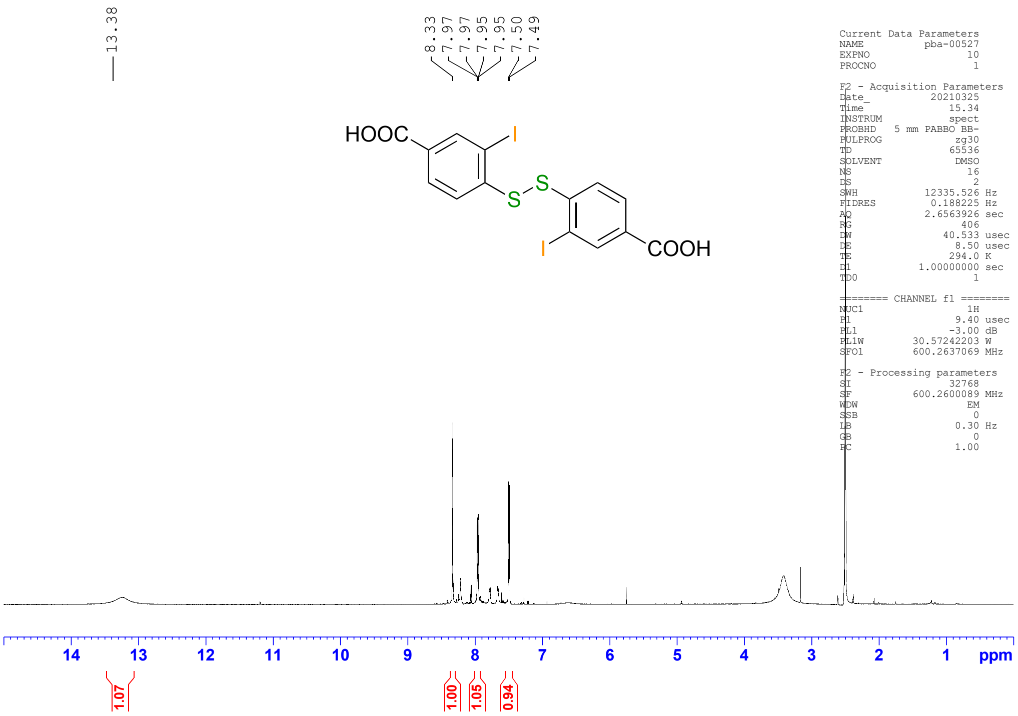
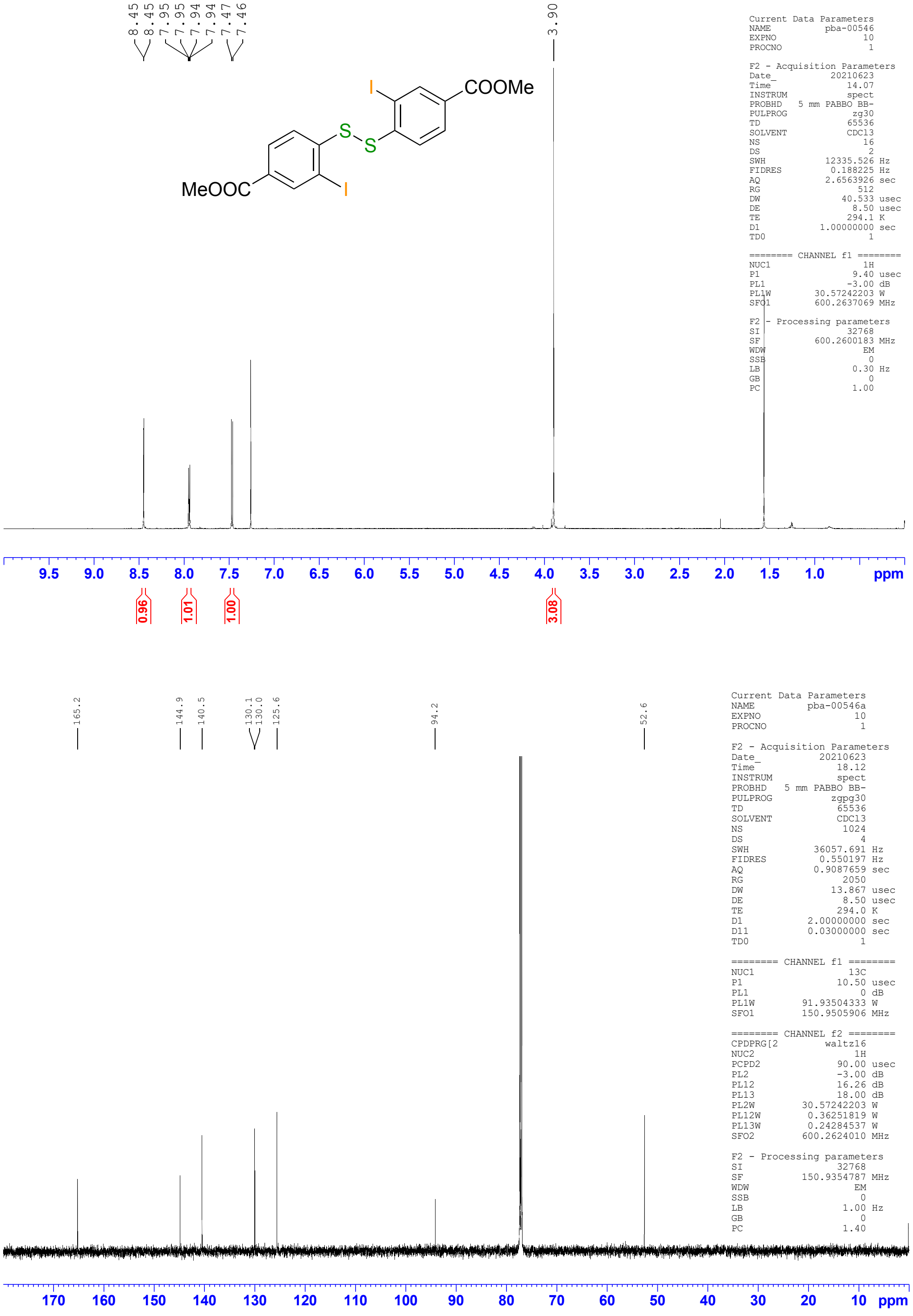


Figure S8. ^{1}H NMR spectrum for 4,4'-disulfanediylbis(3-iodobenzoic acid) (**8**) recorded in DMSO-d_6 at 600 MHz.



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PROCNO                  1

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FIDRES           0.188225 Hz
AQ              2.6563926 sec
RG                    512
DW                 40.533 usec
DE                   8.50 usec
TE                  294.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.40 usec
PL1                 -3.00 dB
PL1W          30.57242203 W
SFO1          600.2637069 MHz

F2 - Processing parameters
SI                  32768
SF            600.2600183 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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PROCNO                  1

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PULPROG            zgpg30
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NS                   1024
DS                      4
SWH             36057.691 Hz
FIDRES           0.550197 Hz
AQ              0.9087659 sec
RG                   2050
DW                 13.867 usec
DE                   8.50 usec
TE                  294.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
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P1                  10.50 usec
PL1                     0 dB
PL1W          91.93504333 W
SFO1          150.9505906 MHz

======== CHANNEL f2 ========
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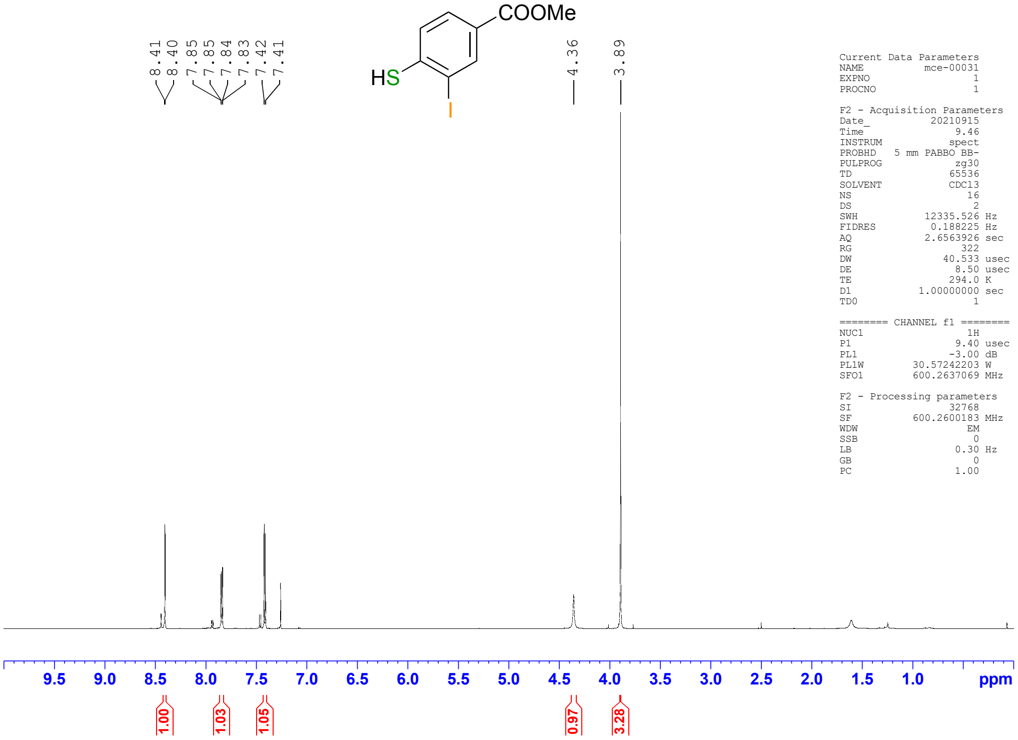
NUC2                   1H
PCPD2               90.00 usec
PL2                 -3.00 dB
PL12                16.26 dB
PL13                18.00 dB
PL2W          30.57242203 W
PL12W          0.36251819 W
PL13W          0.24284537 W
SFO2          600.2624010 MHz

F2 - Processing parameters
SI                  32768
SF            150.9354787 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

Figure S9. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for dimethyl ester of 4,4'-disulfanediylbis(3-iodobenzoic acid) (**9**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.



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PROCNO                1

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PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ            2.6563926 sec
RG                  322
DW               40.533 usec
DE                 8.50 usec
TE                294.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 9.40 usec
PL1               -3.00 dB
PL1W        30.57242203 W
SFO1        600.2637069 MHz

F2 - Processing parameters
SI                32768
SF          600.2600183 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
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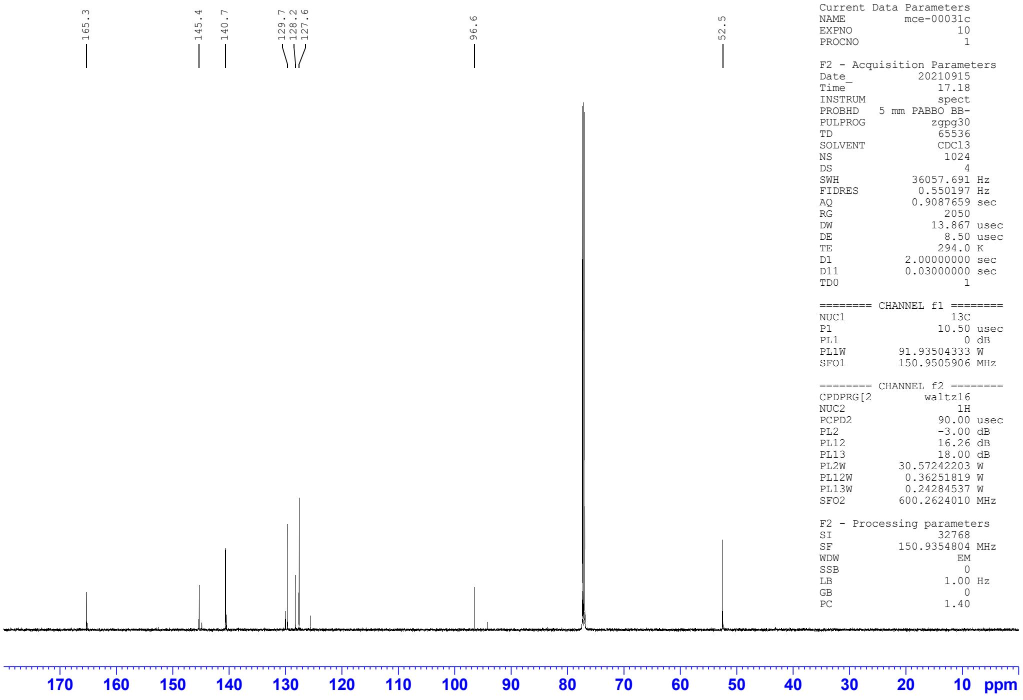

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PROCNO                 1

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PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            36057.691 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                  2050
DW                13.867 usec
DE                  8.50 usec
TE                 294.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.50 usec
PL1                    0 dB
PL1W         91.93504333 W
SFO1         150.9505906 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               16.26 dB
PL13               18.00 dB
PL2W         30.57242203 W
PL12W         0.36251819 W
PL13W         0.24284537 W
SFO2         600.2624010 MHz

F2 - Processing parameters
SI                 32768
SF           150.9354804 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Figure S10. ^{1}H and ^{13}C{^{1}H} NMR spectra for methyl 3-iodo-4-mercaptobenzoate (**5S-b**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

3. XRD data collection and refinement

Single-crystal XRD measurement for **1O-c** was performed with a Rigaku XtalAB Synergy, Pilatus 300K diffractometer. The measurements were conducted at 278(2) K using the CuK_α radiation (λ=1.54184 Å). The data was integrated using CrysAlisPro program.[10] Intensities for absorption were corrected using multi-scan method as in SCALE3 ABSPACK scaling algorithm implemented in CrysAlisPro program.[10] Additional crystal and refinement information are listed in Table S1.

CCDC: File 2107124 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S1. Selected structural data for 1O-c

	CCDC: 2107124
Formula	$C_{21}H_{14}N_3O_2$
Formula Weight	340.35
Crystal System	Triclinic
Space Group	$P\bar{1}$
a/Å	7.22150(10)
b/Å	13.01330(10)
c/Å	17.3541(2)
α/°	79.6460(10)
β/°	85.7900(10)
γ/°	89.4150(10)
Volume/$Å^3$	3022.76(5)
Z	4
2θ range for data collection/°	6.906 to 157.498
Index ranges	$-9 \leq h \leq 8$, $-15 \leq k \leq 16$, $-21 \leq l \leq 21$
No. of measured, independent, and observed [$I>2\sigma(I)$] reflections	46239, 6489, 5717
Rint	0.0245
Goodness-of-fit on F^2	1.060
Final R indexes [$F^2 > 2\sigma(F^2)$]	R_1=0.0371, w$R2$=0.1062
Final R indexes [all data]	R_1=0.0410, w$R2$= 0.1093
Data/restraints/parameters	6489/0/472
Largest diff. peak/hole $Å^{-3}$	0.23/-0.16

Structure solution and refinement

The structures were solved with the ShelXT[11] structure solution program using Intrinsic Phasing and refined in the ShelXle by the full-matrix least-squares minimization on F^2 with the ShelXL[12] refinement package. All non-hydrogen atoms were refined anisotropically and C–H hydrogens were generated geometrically using the HFIX command as in ShelXL. Hydrogen atoms were refined isotropically and constrained to ride on their parent atoms. The crystal data and structure refinement descriptors are presented in Table S1. Partial packing diagrams for **1O-c**, is shown in Figures S11 and S12, while selected geometrical parameters are listed in Table S2 and compared to those of **1O-a**.[13]

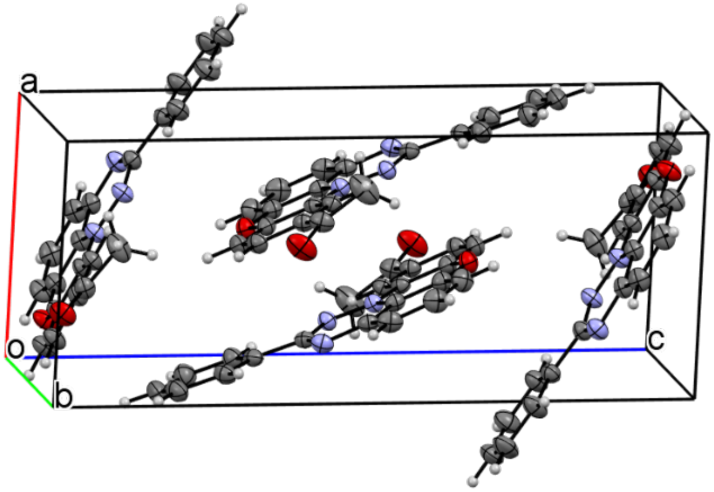


Figure S11. Unit cell packing diagram for **1O-c**.

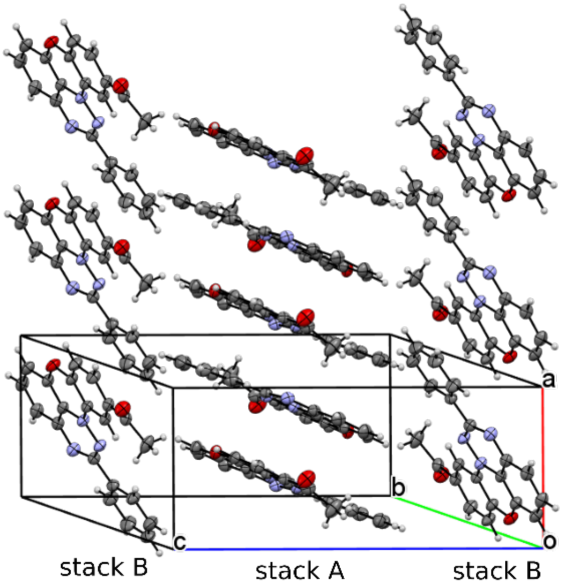


Figure S12. Slipped stacks of **1O-c**. Angle between the adjacent stacks is 36.5°.

Close contacts within the stacks:

Stack A

C(2)···C(7a) 3.228 Å (-0.172 Å inside VDW separation)

C(2)···C(8) 3.313 Å (-0.087 Å inside VDW separation)

C(3a)···C(11) 3.372 Å (-0.028 Å inside VDW separation)

C(8)…C(Ph) 3.365 Å (-0.035 Å inside VDW separation)

C(11a)…C(Ph) 3.319 Å (-0.081 Å inside VDW separation)

Stack B

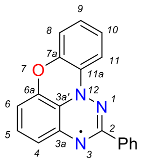
C(7a)···C(Ph) 3.381 Å (-0.019 Å inside VDW separation)

Close contacts between the stacks:

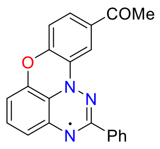
O8···H-C(Me) 2.634 Å (-0.086 Å inside VDW separation)

Slippage angles - of 27.0° (for stack A) and 62.2° (for stack B) were calculated as an angles defined by O(7)···O(7)···N(12) minus 90°. The two oxygen atoms used for the measurements were for two molecules in the stack with the same orientation.

Table S2. Selected interatomic distances and angles for planar benzo[*e*][1,2,4]triazin-4-yl radicals.[a]



1a



1c

	1O-a [b]	**1O-c**
$d_{\text{N1–N12}}$	1.35(1)	1.360(1) 1.359(1)
$d_{\text{N1–C2}}$	1.32(1)	1.341(1) 1.341(1)
$d_{\text{C2–N3}}$	1.364(9)	1.334(1) 1.335(1)
$d_{\text{N3–C3a}}$	1.38(1)	1.374(2) 1.372(2)
$d_{\text{C3a–C3a'}}$	1.38(1)	1.401(2) 1.401(2)
$d_{\text{C3a'–C6a}}$	1.36(1)	1.395(2) 1.396(2)
$d_{\text{C6a–O7}}$	1.39(1)	1.376(1) 1.382(1)
$d_{\text{O7-C7a}}$	1.381(9)	1.376(1) 1.373(1)
$d_{\text{N12–C11a}}$	1.42(1)	1.399(1) 1.400(1)
$d_{\text{C2-Ph}}$	1.50(1)	1.489(2) 1.487(2)
$\alpha_{\text{N12-N1-C2}}$	114.1(6)	114.93(8) 114.92(9)
$\alpha_{\text{N1-C2-N3}}$	130.2(7)	128.5(1) 128.1(1)
$\alpha_{\text{C7a-O7-C6a}}$	118.5(6)	117.82(9) 117.66(9)
$\alpha_{\text{C3a'-N12-C11a}}$	118.6(6)	118.99(8) 118.79(9)
$\theta_{\text{N12-N1-C2-N3}}$	1(1)	-0.2(2) 1.6(2)
$\theta_{\text{C3a'-C6a-O7-C7a}}$	0(1)	-0.4(2) 4.6(2)
$\beta_{\text{triazine-(C2)Ph}}$	2.9	4.2 5.3

[a] *d* - interatomic distance, α - interatomic angle, θ - dihedral angle, β - inter-ring angle. [b] Ref.[13]

The intramolecular inter-ring angle was calculated as the angle between two planes: one was defined by all seventeen C and N atoms of the heterocyclic core and the second by six C atom of the Ph substituent. The mean plane of the heterocyclic core (defined by seventeen C and N atoms) was used to measure the intermolecular separation within the stack and also to measure the angle between the two neighboring stacks.

4. Electronic absorption spectroscopy

Electronic absorption spectra for radicals **1** were recorded in spectroscopic grade CH_2Cl_2 at concentrations in a range 1.5–10× 10^{-5} M and fitted to the Beer–Lambert law. Results are shown in Figures S13 and S14.

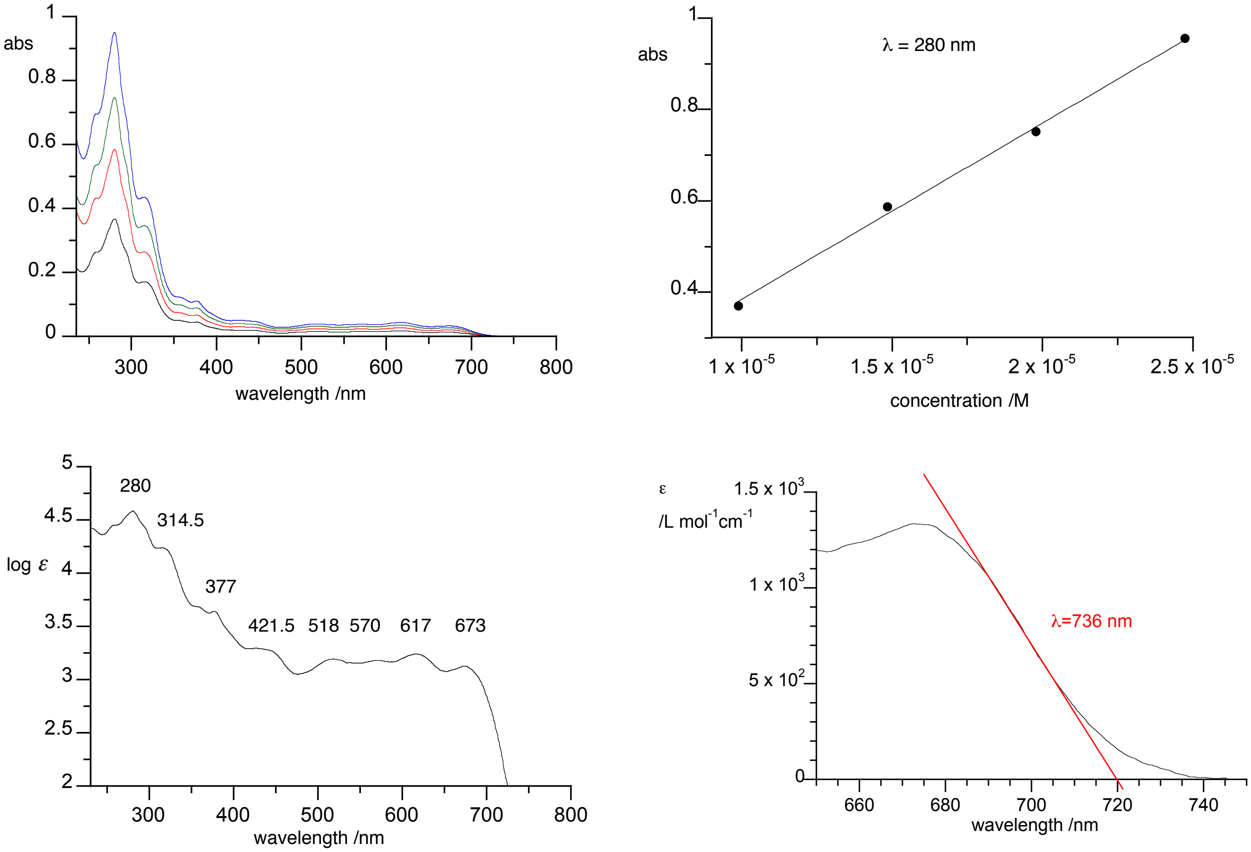


Figure S13. Clockwise: electronic absorption spectra for **1O-c** in CH_2Cl_2 for four concentrations, determination of molar extinction coefficient ε at λ = 280 nm (best fit function: ε = 38495×conc, r^2 = 0.9974), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

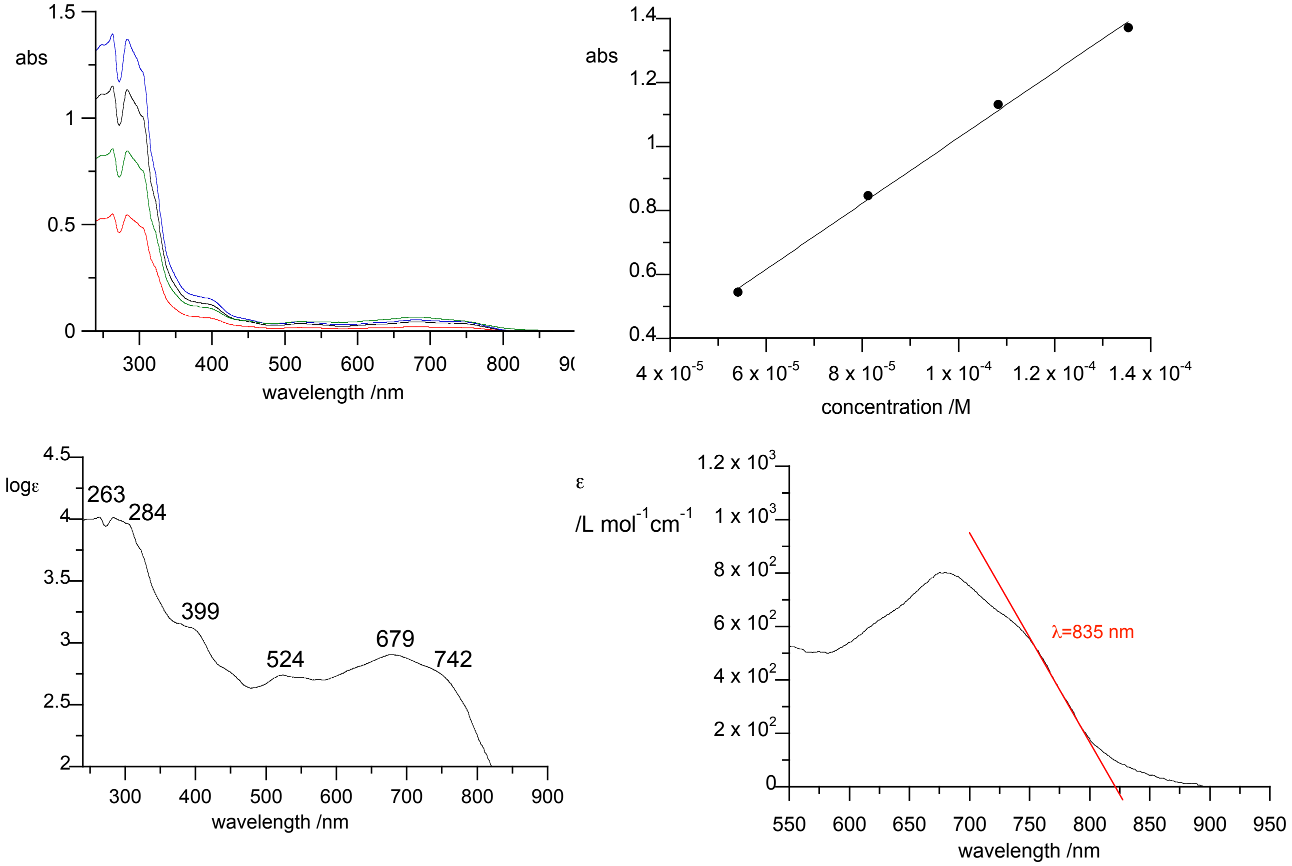


Figure S14. Clockwise: electronic absorption spectra for **1S-b** in CH_2Cl_2 for four concentrations, determination of molar extinction coefficient ε at λ = 284 nm (best fit function: ε = 10275×conc, r^2 = 0.9973), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

5. Electrochemical results

The electrochemical characterization of selected radicals was conducted using Autolab PGSTAT128N potentiostat/galvanostat instrument in dry and degassed CH_2Cl_2 (concentration 0.5 mM) in the presence of $[n\text{-Bu}_4N]^+[PF_6]^-$ as an electrolyte (concentration 50 mM) using glassy carbon as the working electrode and Ag/AgCl as the reference electrode with a scan rate of 50 mV s^{-1} at *ca.* 20 °C. In the end of each measurement decamethylferrocene ($FcMe_{10}$) was added and the peak potentials were referenced to the $FcMe_{10}/FcMe_{10}^+$ couple. The oxidation potential for the $FcMe_{10}/FcMe_{10}^+$ couple was established at –0.56 V *vs* the Fc/Fc^+ couple (–0.10 V *vs* SCE).[14]

Cyclic voltammetry (CV) plots are shown in Figures S15–S18 and numerical result are shown in Table 1 in the main text.

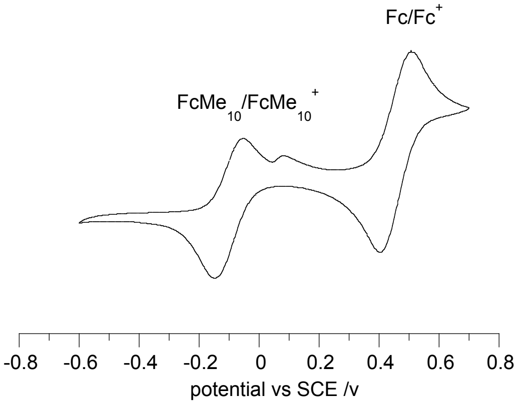
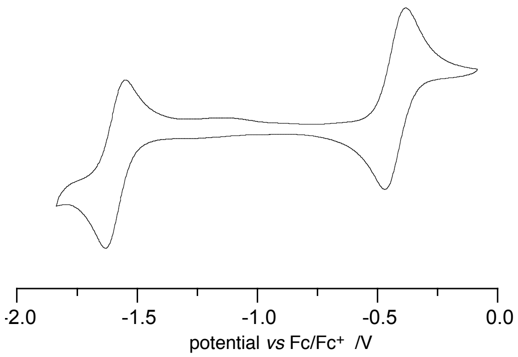


Figure S15. Cyclic voltammogram for ferrocene (Fc) and decamethylferrocene ($FeMe_{10}$). The small peak at about 0.05 V is related to some impurity in the commercial $FeMe_{10}$.



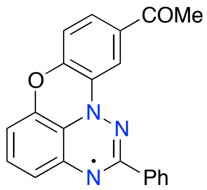
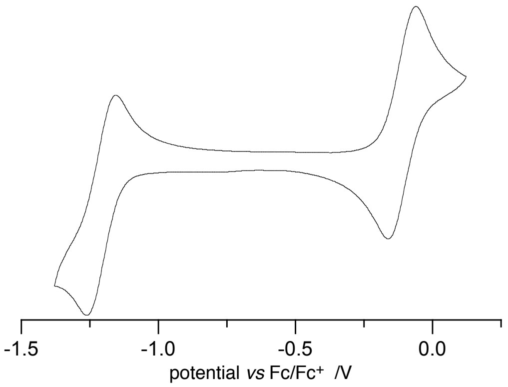


Figure S16. Cyclic voltammogram for **1O-c**.



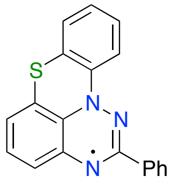
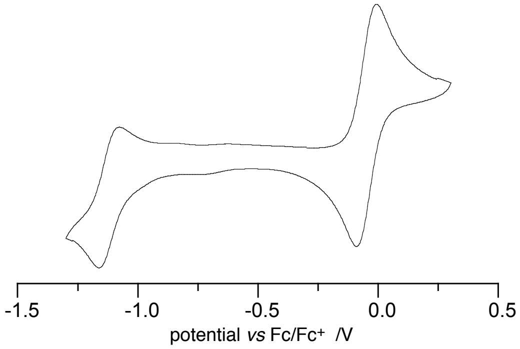


Figure S17. Cyclic voltammogram for **1S-a**.



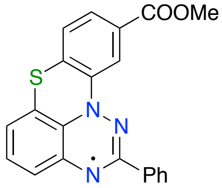


Figure S18. Cyclic voltammogram for **1S-b**.

6. EPR spectrscopy

EPR spectra for radicals **1** were recorded on an X-band EMX-Nano EPR spectrometer at ambient temperature on dilute and degassed solutions in distilled benzene in a concentration range of $2\text{-}5\times10^{-4}$ M. The microwave power was set with the Power Sweep program below the saturation of the signal, modulation frequency of 100 kHz, modulation amplitude of 0.5 G_{pp} and spectral width of 100 G. Accurate *g*-values were obtained using TEMPO as EMX-Nano internal standard.

Simulations of the spectra were performed with the EasySpin (Matlab) using all EPR-active nuclei and DFT results as the starting point for simulations. The chemically equivalent nuclei (H in the Ph substituent) were treated as a group of 2 identical nuclei. The resulting *hfcc* values were perturbed several times until a global minimum for the fit was achieved. Experimental and simulated spectra are shown in Figures S19 and S20 and resulting *hfcc* are listed in Table S3. The *hfcc* values were assigned to the nitrogen nuclei in **1** on the basis of trends in DFT results.

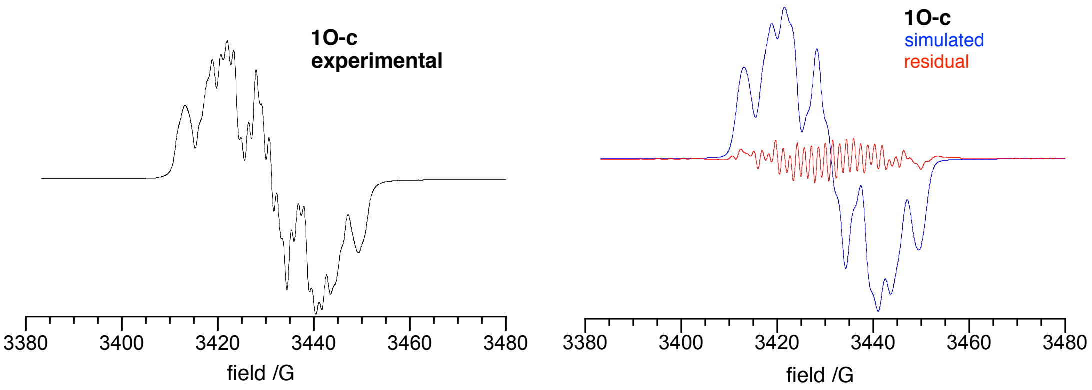


Figure S19. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1O-c** recorded in benzene at *ca* 20 °C.

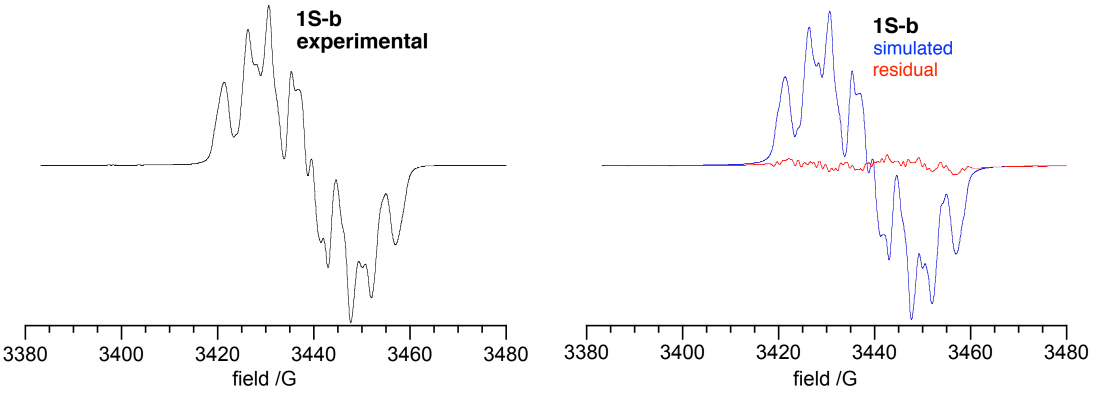


Figure S20. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1S-b** recorded in benzene at *ca* 20 °C.

Table S3. Experimental hyperfine coupling constants (G) for radicals in series **1** in benzene at *ca*. 20 ^{o}C.

atom	**1O-a**	**1O-b**	**1O-c**	**1O-d**	**1S-a**	**1S-b**
$a_{N(12)}$	7.51	7.29	7.24	7.60	7.54	7.08
$a_{N(1)}$	4.28	4.44	4.41	4.18	4.47	4.44
$a_{N(3)}$	4.42	4.52	4.52	4.18	4.49	4.52
a_H	1.94	0.87	2.02	0.30	1.18	1.78
a_H	1.11	1.84	1.61	0.30	0.76	1.47
a_H	0.72	1.98	0.78	0.30	0.74	1.36
a_H	0.60	1.13	0.44	0.30	0.72	0.74
a_H	0.39	0.62	0.40	0.30	0.71	0.86
a_H	0.29	0.23	0.30	0.30	0.69	0.28
a_H	0.11	0.27	0.20	0.30	0.53	0.35
a_H	0.10	0.33	0.14	0.30	0.40	0.06
a_H	0.09	0.37	0.05	-	0.31	0.11
a_H	0.03	-	-	-	0.26	-
g	2.0036	2.0037	2.0039	2.0034	2.0039	2.0043

7. Archive for UB3LYP/6-31G(2d,p) geometry optimization results.

1S-b

```
1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H14N3O2S1(2)\PIOTR\24-Se
 p-2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
  Geom=(NoDistance,NoAngle) fcheck\\C(8)-S-Ph(N1) benzotrazinyl (phenaz
 inoBT), C1 with the COOMe\\0,2\N,0.5742767674,-0.2057798294,0.05937430
 26\N,-1.4344632562,1.6680168647,-0.2228103953\C,-1.6511610441,0.367039
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 ,-6.3725185083,-1.3217524964\H,0.0675590439,-6.7214122426,-2.268856664
 4\H,-0.0894404701,-7.0862158222,-0.53683641\H,-1.4321052707,-6.2635353
 315,-1.3971120493\\Version=ES64L-G09RevD.01\State=2-A\HF=-1521.5923273
 \S2=0.766375\S2-1=0.\S2A=0.750201\RMSD=2.307e-09\RMSF=1.021e-06\Dipole
 =-0.0480508,0.3278178,-0.0825013\Quadrupole=3.9429498,3.3525403,-7.295
 49,11.2721957,1.6217214,-0.6176343\PG=C01 [X(C21H14N3O2S1)]\\@
```

1O-a

```
1\1\GINC-LOCALHOST\SP\UB3LYP\6-311++G(2d,p)\C19H12N3O1(2)\PIOTR\14-Sep
 -2021\0\\#P UB3LYP/6-311++G(2d,p) SCF=tight SCF=Direct #P Geom=(NoDist
 ance,NoAngle) SCRF(Solvent=benzene)\\Parent C(8)-O-Ph(N1) benzotraziny
 l (phenazinoBT), Cs opt\\0,2\N,0,-0.2279945082,0.,-0.7068912291\N,0,1.
 6342308182,0.,1.3147774172\C,0,0.3141730381,0.,1.5107475896\N,0,-0.651
 1944713,0.,0.5772813358\C,0,2.8747587314,0.,-2.6901553245\C,0,1.525294
 733,0.,-2.3786764485\C,0,1.1192429656,0.,-1.0420625687\C,0,2.056303327
 2,0.,0.0130670541\C,0,3.4227100243,0.,-0.320281521\C,0,3.8144680324,0.
 ,-1.6500459807\C,0,-1.1799195482,0.,-1.7366863092\C,0,-0.7265516782,0.
 ,-3.0685289936\C,0,-1.6343949522,0.,-4.1176431627\C,0,-3.0025964506,0.
 ,-3.8542738611\C,0,-3.4580568847,0.,-2.5364763795\C,0,-2.5535440658,0.
 ,-1.48031653\C,0,-0.1674933344,0.,2.9170571338\C,0,-1.5355202766,0.,3.
 2213939115\C,0,-1.9627296157,0.,4.5448686804\C,0,-1.0320885266,0.,5.58
 34203093\C,0,0.3304717827,0.,5.2886511585\C,0,0.7611634188,0.,3.966122
 5371\O,0,0.607802556,0.,-3.3994557106\H,0,4.1444354867,0.,0.4875266765
 \H,0,-1.2474203049,0.,-5.1300423865\H,0,-4.5217388028,0.,-2.3262246262
 \H,0,-2.8822307131,0.,-0.4505760941\H,0,-2.2557347868,0.,2.4132296866\
 H,0,-3.0252780726,0.,4.7664014926\H,0,1.0608349088,0.,6.0915258161\H,0
 ,1.8160583604,0.,3.7224448829\H,0,4.8703351187,0.,-1.898622529\H,0,3.1
 753691985,0.,-3.7308245809\H,0,-3.7063464888,0.,-4.6790512891\H,0,-1.3
 674420192,0.,6.615759843\\Version=ES64L-G09RevD.01\State=2-A"\HF=-970.
 9653337\S2=0.764573\S2-1=0.\S2A=0.750168\RMSD=3.879e-09\Dipole=-0.3799
 885,0.,-0.9682011\Quadrupole=6.3262081,-11.9067033,5.5804952,0.,-0.727
 6571,0.\PG=CS [SG(C19H12N3O1)]\\@
```

10O-a

```
1\1\GINC-LOCALHOST\SP\UB3LYP\6-311++G(2d,p)\C19H12N3O1(2)\PIOTR\28-Oct
 -2021\0\\#P UB3LYP/6-311++G(2d,p) SCF=tight SCF=Direct #P Geom=(NoDist
 ance,NoAngle) SCRF(Solvent=benzene)\\C(8)-O-Ph(N1) Formation of the fl
 at Blatter, Ph radical before add opt at DFT\\0,2\N,0,-0.0753185307,0.
 6644308986,0.1267804261\N,0,1.1731731663,-1.8110720007,0.2102417086\C,
 0,-0.1365862117,-1.6412804423,0.2211192194\N,0,-0.7752395804,-0.421247
 1685,0.195025128\C,0,3.4390079435,1.6662461791,0.042014589\C,0,2.06961
 76326,1.7623161301,0.0164172928\C,0,1.2807923849,0.5765416327,0.087363
```

```
 0818\C,0,1.9247365651,-0.6897222057,0.1505315515\C,0,3.339117296,-0.76
 30018849,0.1637999211\C,0,4.068933131,0.3995663089,0.1179759226\C,0,0.
 7817804274,2.7573403342,-2.2967000911\C,0,0.7480098485,3.386480542,-1.
 0699615188\C,0,-0.0516522148,4.5270908497,-0.9543528743\C,0,-0.7759032
 713,4.9751411832,-2.0568869\C,0,-0.7224900533,4.3036623618,-3.27825700
 46\C,0,0.0758778061,3.1570541979,-3.4035847494\C,0,-1.0159355998,-2.82
 84103657,0.2740653257\C,0,-2.4111217636,-2.6873522612,0.2968316298\C,0
 ,-3.2277257638,-3.8122745297,0.347505444\C,0,-2.6659036529,-5.08779088
 9,0.375185368\C,0,-1.2786102593,-5.2350691088,0.3519625057\C,0,-0.4580
 174448,-4.1148279799,0.3019782794\O,0,1.4869485182,3.0039641913,0.0242
 631806\H,0,3.8057572271,-1.7395123834,0.2171020746\H,0,-0.094655105,5
 .0396221455,0.001148369\H,0,-1.2931347791,4.6607916779,-4.1291616779\H
 ,0,0.1334108229,2.6156455286,-4.3426296396\H,0,-2.8379253918,-1.692847
 2248,0.274777690 9\H,0,-4.3060721012,-3.6920971327,0.365227559\H,0,-0.8
 362628127,-6.22582748,0.3732323538\H,0,0.6202185814,-4.2166570679,0.28
 45359814\H,0,5.1531241717,0.3583836822,0.1327389077\H,0,4.0268543147,2
 .5757721994,0.0030788405\H,0,-1.3951847999,5.8601714558,-1.9556167\H,0
 ,-3.305478896,-5.963842544,0.4144881444\\Version=ES64L-G09RevD.01\Stat
 e=2-A\HF=-970.8752639\S2=0.757399\S2-1=0.\S2A=0.750032\RMSD=8.319e-09\
 Dipole=0.8157744,-0.2283447,-0.2889001\Quadrupole=4.8733313,2.9382992,
 -7.8116305,1.2856908,2.7283462,-2.4323524\PG=C01 [X(C19H12N3O1)]\\@
```

10O-a to 1O-a transition state

```
1\1\GINC-LOCALHOST\SP\UB3LYP\6-311++G(2d,p)\C19H12N3O1(2)\PIOTR\28-Oct
 -2021\0\\#P UB3LYP/6-311++G(2d,p) SCF=tight SCF=Direct #P Geom=(NoDist
 ance,NoAngle) SCRF(Solvent=benzene)\\BT-O-Ph TS for N1 cycl, opt at B3
 LYP/6-31G(2d,p)\\0,2\N,0,-0.1231668471,-0.2665868394,-1.1284873918\N,0
 ,-1.8400632338,1.3741383308,0.2834570853\C,0,-2.1918559228,0.215465291
 6,-0.2405384669\N,0,-1.3562021418,-0.6108560611,-0.9596014687\C,0,2.11
 374657,2.4982253051,-0.2798554945\C,0,1.6995644979,1.2791515146,-0.772
 1851095\C,0,0.3362856166,0.8971149976,-0.5983445372\C,0,-0.5541701315,
 1.7562629505,0.1079425641\C,0,-0.0959771044,2.9959838492,0.6074060707\
 C,0,1.2166058945,3.3504093688,0.4010981208\C,0,1.963726636,-1.65758122
 56,-0.6460371696\C,0,2.8131661306,-0.7992429676,-1.3032777737\C,0,3.99
 24512061,-1.3243944902,-1.8385246146\C,0,4.2589594449,-2.6862930345,-1
 .7087679254\C,0,3.3687977425,-3.5312385331,-1.0461245899\C,0,2.1846060
 646,-3.0068197097,-0.5084647477\C,0,-3.5811235191,-0.260453233l,-0.072
 7980399\C,0,-3.992634384,-1.4823215573,-0.6246500736\C,0,-5.3030822157
 ,-1.9187282247,-0.4599133009\C,0,-6.2164675525,-1.1453755471,0.2548648
 423\C,0,-5.8132861241,0.0710783436,0.8067955256\C,0,-4.5055778548,0.51
 20776051,0.6451589361\O,0,2.6168695091,0.5590708505,-1.4783529303\H,0,
 -0.7956162981,3.633295926,1.1345948563\H,0,4.6794046687,-0.6572167548,
 -2.3493642626\H,0,3.5846822583,-4.5904781913,-0.9498958304\H,0,1.47031
 20657,-3.648227132,-0.0014992111\H,0,-3.2765493583,-2.075525103,-1.178
 7965098\H,0,-5.6117256697,-2.8654128725,-0.8912900599\H,0,-6.520620858
 4,0.6767035727,1.3640900996\H,0,-4.1807373243,1.4546806371,1.068454320
 1\H,0,1.5852851094,4.3003496595,0.7741572058\H,0,3.1472782072,2.787998
 965,-0.4283417789\H,0,5.1731183125,-3.0885640045,-2.1324480531\H,0,-7.
 2384000442,-1.4882616861,0.3818401331\\Version=ES64L-G09RevD.01\State=
 2-A\HF=-970.8722517\S2=0.761042\S2-1=0.\S2A=0.750086\RMSD=6.890e-09\Di
 pole=0.1220641,0.6422344,0.5302761\Quadrupole=6.2582413,4.6985666,-10.
 9568079,3.9496398,-3.0175888,3.2043671\PG=C01 [X(C19H12N3O1)]\\@
```

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