Electronic Supplementary Information for

Substituent effects on the electronic structure of the flat Blatter radical: Correlation analysis of experimental and computational data

Paulina Bartos,[†] Aniket A. Hande,[†,§] Anna Pietrzak,[¶] Anna Chrostowska[§] and Piotr Kaszyński,[†,d,e]*

[†] Faculty of Chemistry, University of Łódź, 91-403 Łódź, Poland
[§] Université de Pau et des Pays de l'Adour E2S UPPA, CNRS, IPREM 64000, Pau, France
[¶] Faculty of Chemistry, Łódź University of Technology, Żeromskiego 116, 90-024, Łódź, Poland
[‡] Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, 90-363 Łódź, Poland
[⊥] Department of Chemistry, Middle Tennessee State University, Murfreesboro, TN, 37132, USA

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1. Additional synthetic details

Preparation of intermediates

2-Amino-4-iodophenol.[1] 2-Amino-4-iodophenol was obtained according to literature procedure.[2] Thus, *to* the solution of 4-iodo-2-nitrophenol (1.068 g, 4.0 mmol) in EtOH (20 mL), $SnCl_2$ (4.513 g, 20 mmol) was added in one portion and the reaction mixture was stirred for 1.5 hr at 70 °C under ambient atmosphere. The reaction mixture was poured into sat. $NaHCO_3$ (100 mL), filtered through Celite, which was washed well with EtOAc. The organic layer was separated, washed with H_2O (2×30 mL) and dried (Na_2SO_4). The solvent was removed under vacuum to give 760 mg (3.2 mmol) of 4-iodo-2-aminophenol as brownish solid, which was used for the next step without further purification: mp 126–128 °C (lit.[1] mp 139 °C); ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.27 (bs, 1H), 6.87 (d, J = 2.1 Hz, 1H), 6.65 (dd, J_1 = 8.2 Hz, J_2 = 2.1 Hz, 1H), 6.43 (d, J = 8.2 Hz, 1H), 4.74 (bs, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 143.0, 139.2, 124.3, 121.8, 116.4, 81.7; IR (ATR) ν 3381, 3207, 3191, 1581, 1492, 1443, 1257, 1198, 905, 853, 769 cm^{-1}; HRMS (ESI-TOF) $[M+H]^+$ *m/z* calcd for C_6H_7INO: 235.9572; found: 235.9574. Anal. Calcd for C_6H_6INO: C, 30.66; H, 2.57; N, 5.96. Found C, 30.71; H, 2.52; N, 6.03.

2-Amino-4-benzyloxyphenol.[3] The phenol was obtained in 69% yield as grey powder by reduction of 4-benzyloxy-2-nitrophenol with Zn in AcOH according to a literature procedure[3] and used in the next step without further purification: ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.50 (s, 1H), 7.39 (d, J = 7.2 Hz, 2H), 7.37 (t, J = 7.4 Hz, 2H), 7.30 (t, J = 6.7 Hz, 1H), 6.50 (d, J = 8.6 Hz, 1H), 6.27 (d, J = 2.8 Hz, 1H), 6.03 (dd, J_1 = 8.5 Hz, J_2 = 2.8 Hz, 1H), 4.90 (s, 2H), 4.54 (bs, 2H); IR (KBr) ν 3384, 3293, 1521, 1233, 1182, 1017, 734, 695 cm^{-1}; HRMS (ESI-TOF) $[M+H]^+$ *m/z* calcd for $C_{13}H_{14}NO_2$: 216.1025; found: 216.1026.

3-Amino-4-hydroxyphenyl acetate. It was obtained in 87% yield as a brown solid by catalytic reduction of 4-hydroxy-3-nitrophenyl acetate in a THF–EtOH mixture (1:1) at ambient temperature in the presence of 10% Pd/C at 2 bars and used to the next step without further purification: ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.01 (s, 1H), 6.57 (d, J = 8.3 Hz, 1H), 6.29 (d, J = 2.3 Hz, 1H), 6.08 (dd, J_1 = 8.3 Hz, J_2 = 2.3 Hz, 1H), 4.68 (bs, 2H), 2.17 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 169.5, 143.4, 141.5, 137.4, 113.9, 108.2, 107.4, 20.8; IR (KBr) ν

3384, 3293, 1601, 1521, 1233, 1183, 1017, 794, 734, 695 cm^{-1}. Anal. Calcd for $C_8H_9NO_3$: C, 57.48; H, 5.43; N, 8.38. Found C, 57.49; H, 5.72; N, 8.17.

4-Iodo-2-nitrophenol.[4] 4-Iodo-2-nitrophenol was obtained according to a literature procedure.[5] Thus, $NaNO_2$ (4.56 g, 66.0 mmol) dissolved in H_2O (24 mL) was added dropwise *to a* suspension of *4*-amino-2-nitro*phenol* (9.25 g, 60 mmol) in 32 mL conc. HCl (32 mL) at 0 °C. After 20 min of stirring, KI (100 g, 600 mmol) dissolved in H_2O (140 mL) was added and the reaction mixture, which was allowed to warm up to room temperature. The stirring was continued for 12 hrs. H_2O (200 mL) was added to the reaction mixture and the resulting mixture was extracted with EtOAc (3×100 mL). The organic extracts were dried (Na_2SO_4) and concentrated under vacuum to give crude product which was purified by column chromatography (SiO_2, pet. ether/CH_2Cl_2 1:1), giving 9.82 g (62% yield) of the phenol as yellow crystals: mp 78–79 °C (lit.[4] mp 81 °C); ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.3 (bs, 1H), 8.12 (d, J = 2.1 Hz, 1H), 7.80 (dd, J_1 = 8.7 Hz, J_2 = 2.1 Hz, 1H), 6.94 (d, J = 8.7 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 152.1, 143.5, 138.7, 133.2, 121.8, 80.4; IR (ATR) v 1605, 1567, 1513, 1465, 1404, 1228, 1158, 831, 655, 610, 538 cm^{-1}; HRMS (ESI-TOF) $[M-H]^+$ *m/z* calcd for $C_6H_3INO_3$ 263.9158; found: 263.9158. Anal. Calcd for $C_6H_4INO_3$: C, 27.19; H, 1.52; N, 5.29. Found C, 27.15 H, 1.46; N, 15.31.

4-Benzyloxy-2-nitrophenol.[6] It was obtained as yellow crystals in 85% yield by selective debenzylation of 1,4-dibenzyloxy-2-nitrobenzene with TFA in CH_2Cl_2 according to a literature procedure:[7] mp 65–66 °C (EtOH, lit.[6] mp 68–70); ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.35 (s, 1H), 7.60 (d, J = 3.1 Hz, 1H), 7.43 (t, J = 6.8 Hz, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.34 (t, J = 7.0 Hz, 1H), 7.29 (dd, J_1 = 9.2 Hz, J_2 = 3.1 Hz, 1H), 7.09 (d, J = 9.2 Hz, 1H), 5.06 (s, 2H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 151.7, 150.3, 136.0, 133.1, 128.9, 128.5, 128.0, 127.8, 121.0, 107.3, 71.0; IR (KBr) v 3235, 1537, 1485, 1431, 1330, 1248, 1022, 747, 700 cm^{-1}; HRMS (ESI-TOF) $[M-2H]^-$ *m/z* calcd for $C_{13}H_9NO_4$: 243.0532; found: 243.0534. Anal. Calcd for $C_{13}H_{11}NO_4$: C, 63.67; H, 4.52; N, 5.71. Found C, 63.73; H, 4.76; N, 5.45.

4-Hydroxy-3-nitrophenyl acetate.[8] It was obtained as yellow crystals in 53% yield by nitration of 4-acetoxyphenol[9] with HNO_3 in AcOH according to a literature procedure:[9] mp 79–80 °C

(MeOH, lit.[8] mp 84 °C); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.74 (s, 1H), 7.36 (d, J = 8.8 Hz, 1H), 7.16 (d, J = 8.8 Hz, 1H), 2.27 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 169.3, 149.8, 141.6, 136.2, 129.1, 119.6, 118.2, 20.7; IR (KBr) v 3301, 1757, 1537, 1430, 1196, 950, 915 cm^{-1}. Anal. Calcd for $C_8H_7NO_5$: C, 48.74; H, 3.58; N, 7.10. Found C, 48.51; H, 3.63; N, 7.22.

1,4-Dibenzyloxy-2-nitrobenzene.[10] It was obtained as yellow crystals in 94% yield by nitration of 1,4-di(benzyloxy)benzene with conc. HNO_3 in AcOH according to a literature procedure:[7] mp 77–78 °C (MeOH; lit.[10] mp 80–81 °C); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.49 (d, J = 3.0 Hz, 1H), 7.45 (d, J = 7.4 Hz, 2H), 7.37–7.42 (m, 6H), 7.31–7.36 (m, 2H), 7.13 (dd, J_1 = 9.1 Hz, J_2 = 3.0 Hz, 1H), 7.05 (d, J = 9.1 Hz, 1H), 5.18 (s, 2H), 5.05 (s, 2H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 152.4, 146.5, 140.4, 136.1, 136.0, 128.9, 128.8, 128.5, 128.3, 127.7, 127.3, 121.6, 117.4, 111.3, 72.2, 71.1; IR (KBr) v 1522, 1451, 1386, 1341, 1227, 1016, 756, 733, 694 cm^{-1}; HRMS (ESI-TOF) [M+Na]$^+$ m/z calcd for $C_{20}H_{17}NO_4Na$: 358.1055; found: 358.1051. Anal. Calcd for $C_{20}H_{17}NO_4$: C, 71.63; H, 5.11; N, 4.18. Found C, 71.60; H, 5.06; N, 4.32.

1,4-Di(benzyloxy)benzene.[10] It was obtained in 47% yield as yellow crystals by benzylation of hydroquinone with benzyl bromide in DMF according to a literature procedure:[7] mp 127–128 °C (EtOH) (lit.[10] mp 127-128 °C); ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.43 (d, J = 7.4 Hz, 4H), 7.39 (t, J = 7.5 Hz, 4H), 7.32 (t, J = 7.2 Hz, 2H), 6.91 (s, 4H), 5.02 (s, 4H); ^{13}C{^{1}H} NMR (151 MHz, DMSO-d_6) δ 153.3, 137.4, 128.7, 128.0, 127.6, 115.9, 70.8; IR (KBr) v 2902, 1509, 1238, 1018, 813, 733, 696 cm^{-1}; HRMS (ESI-TOF) [M]$^+$ m/z calcd for $C_{20}H_{18}O_2$: 290.1307; found: 290.1312. Anal. Calcd for $C_{20}H_{18}O_2$: C, 82.73; H, 6.27. Found C, 82.78; H, 6.28.

2. NMR spectra

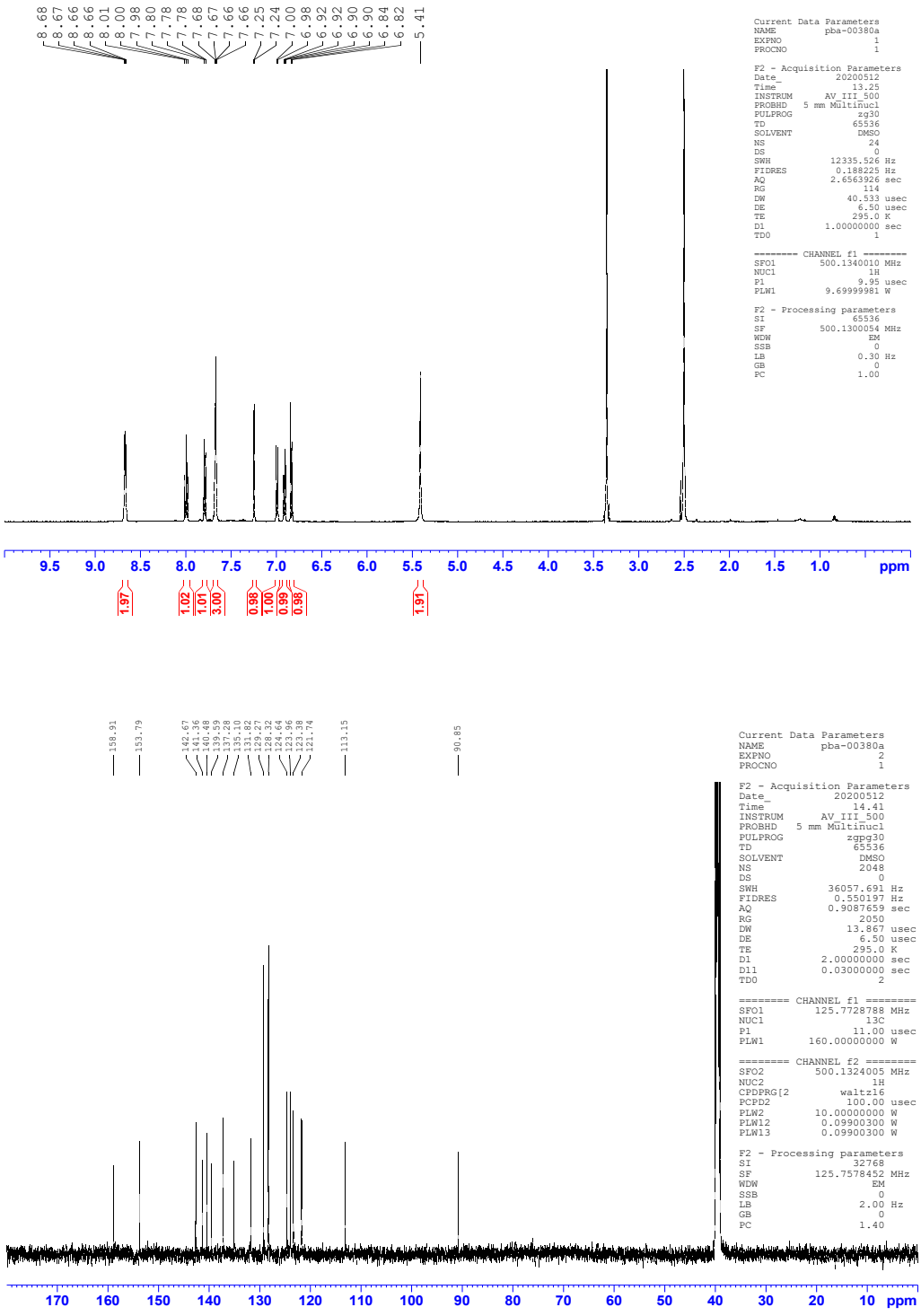


Figure S1. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for 8-(2-amino-4-iodo-1-phenyloxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2n**) recorded in DMSO-*d6* at 500 and 125 MHz, respectively.

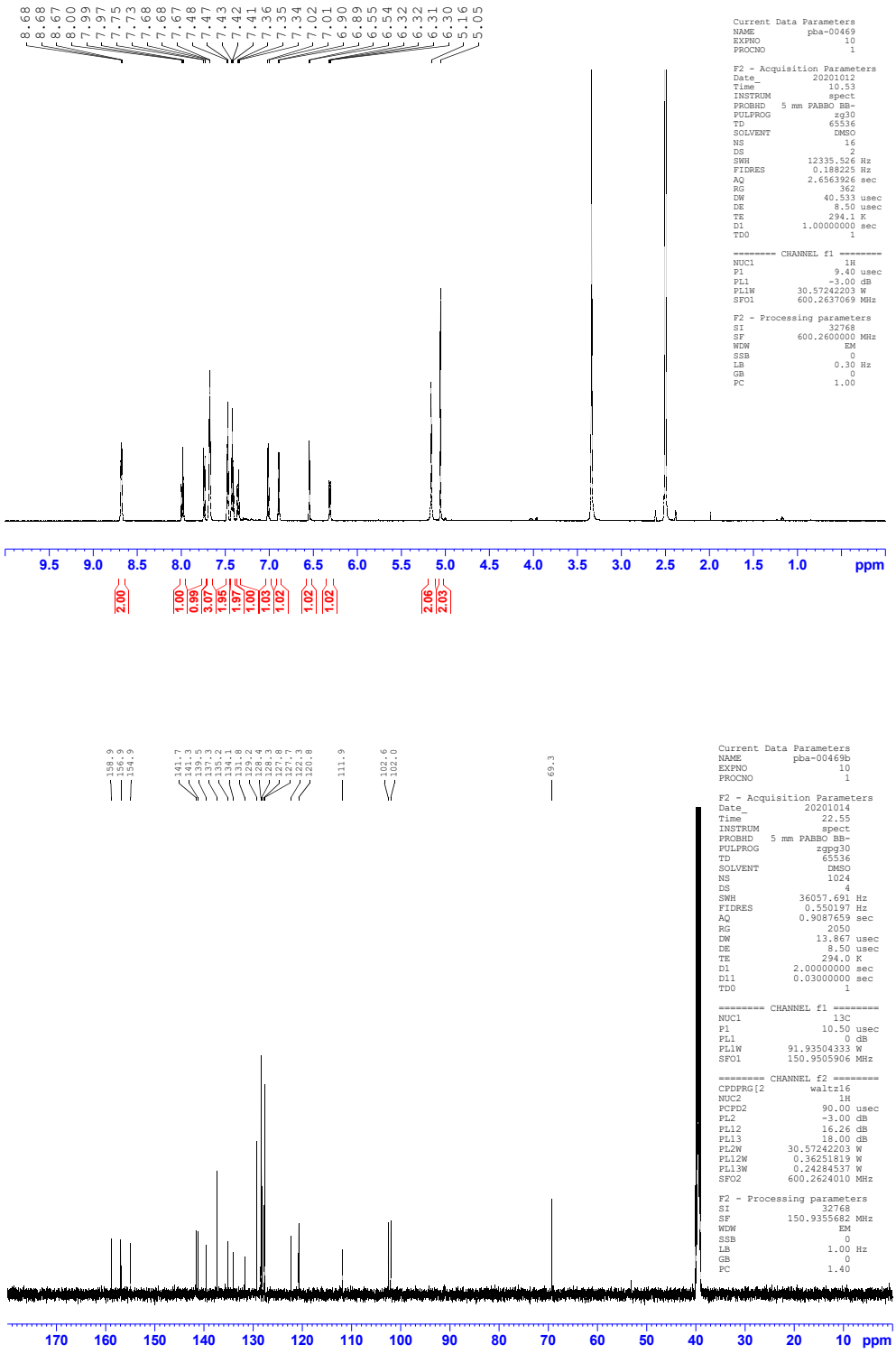


Figure S2. ^{1}H and ^{13}C{^{1}H} NMR spectra for 8-(2-amino-4-benzyloxy-1-phenyloxy)-3-phenylbenzo[*e*][1,2,4]triazine (**2p**) recorded in DMSO-*d6* at 600 and 151 MHz, respectively.

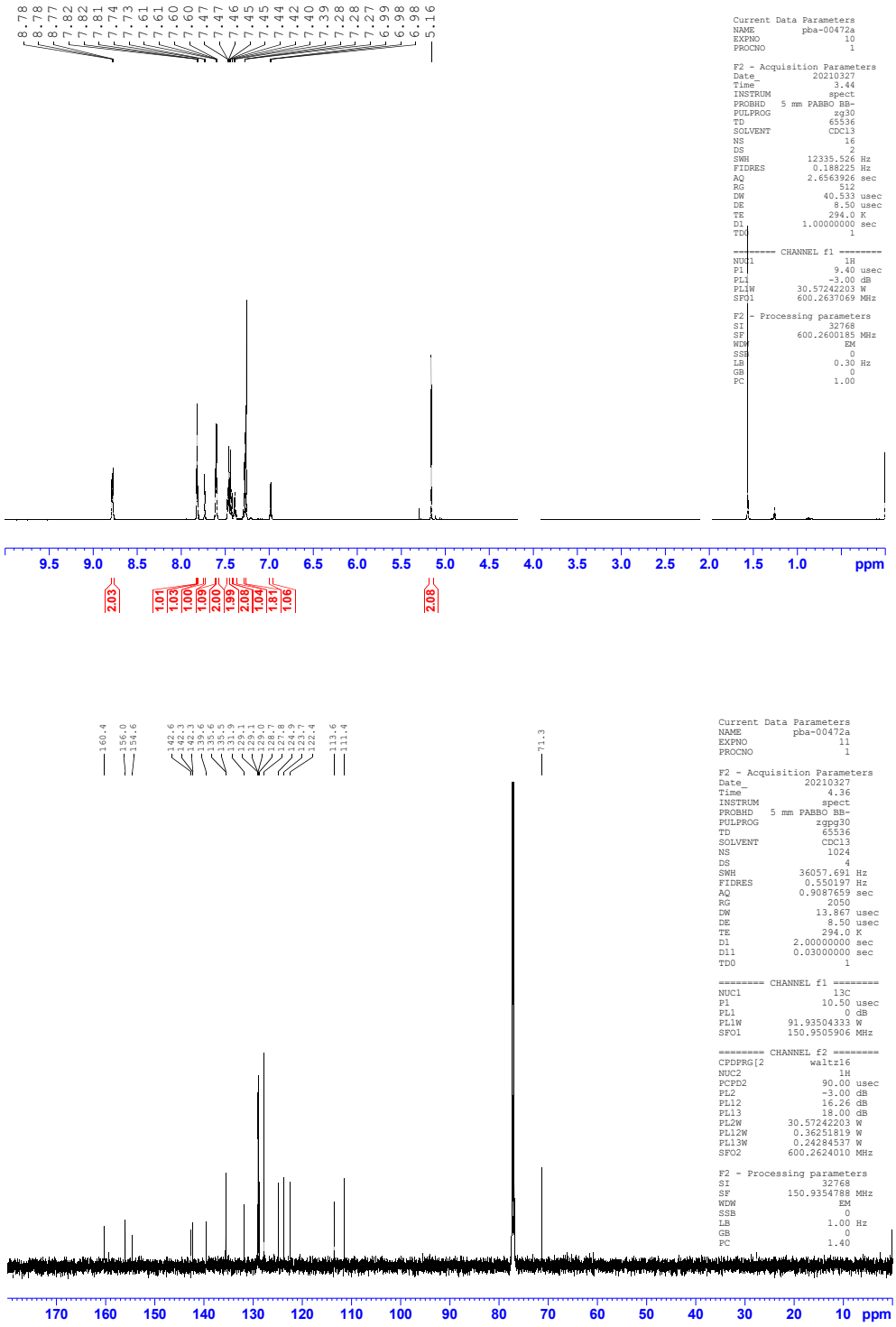


Figure S3. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for 8-(2-nitro-4-benzyloxy-1-phenyloxy)-3-phenylbenzo[*e*][1,2,4]triazine (**5p**) recorded in $CDCl_3$ at 600 and 151 MHz, respectively.

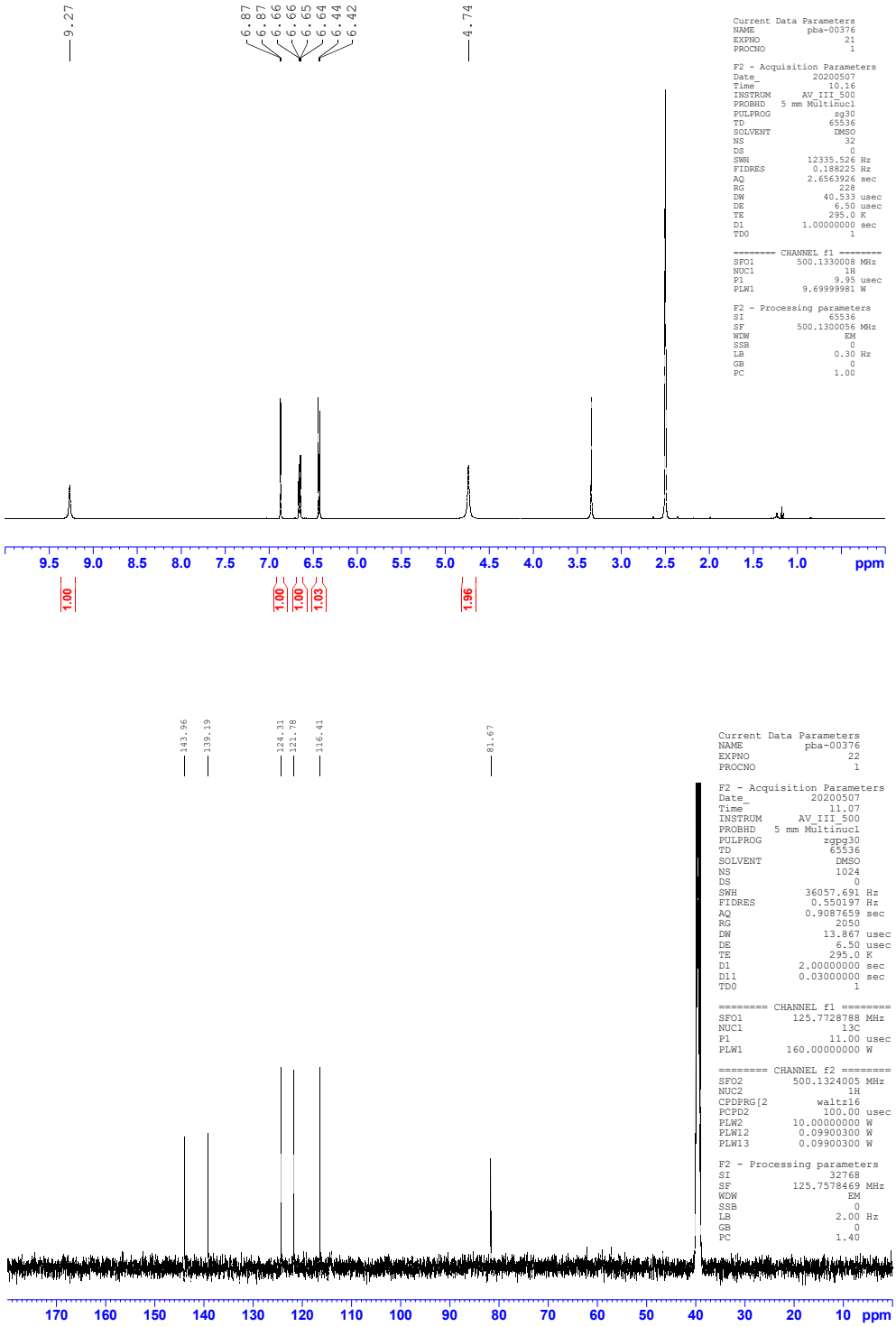


Figure S4. ^{1}H and ^{13}C{^{1}H} NMR spectra for 2-amino-4-iodophenol recorded in DMSO-*d6* at 500 and 125 MHz, respectively.

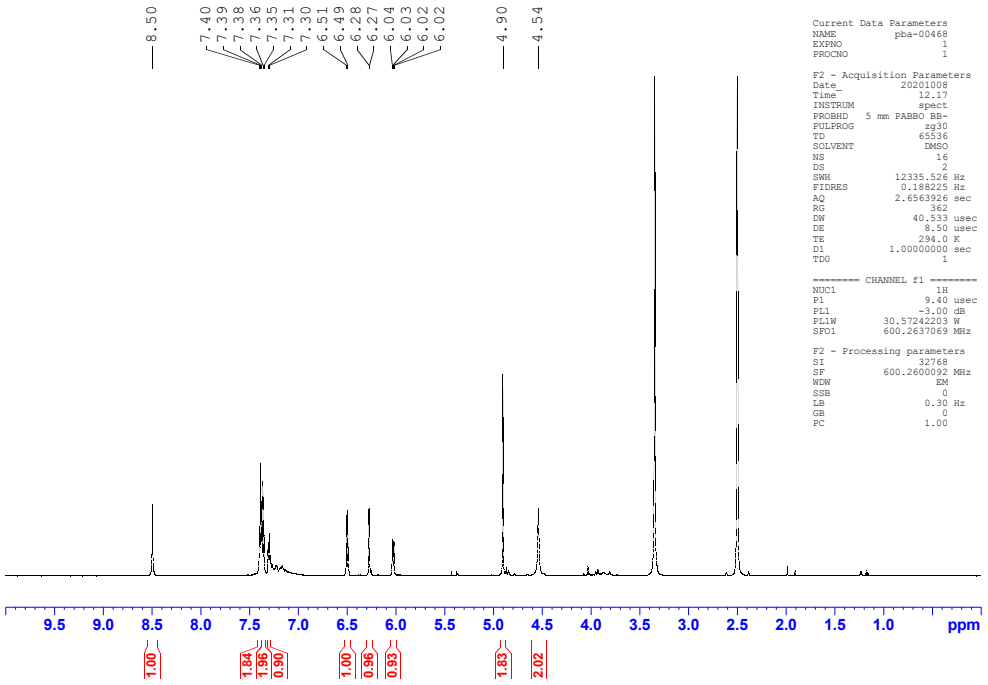


Figure S5. ^{1}H NMR spectrum for 2-amino-4-benzyloxyphenol recorded in DMSO-d_6 at 600 MHz.

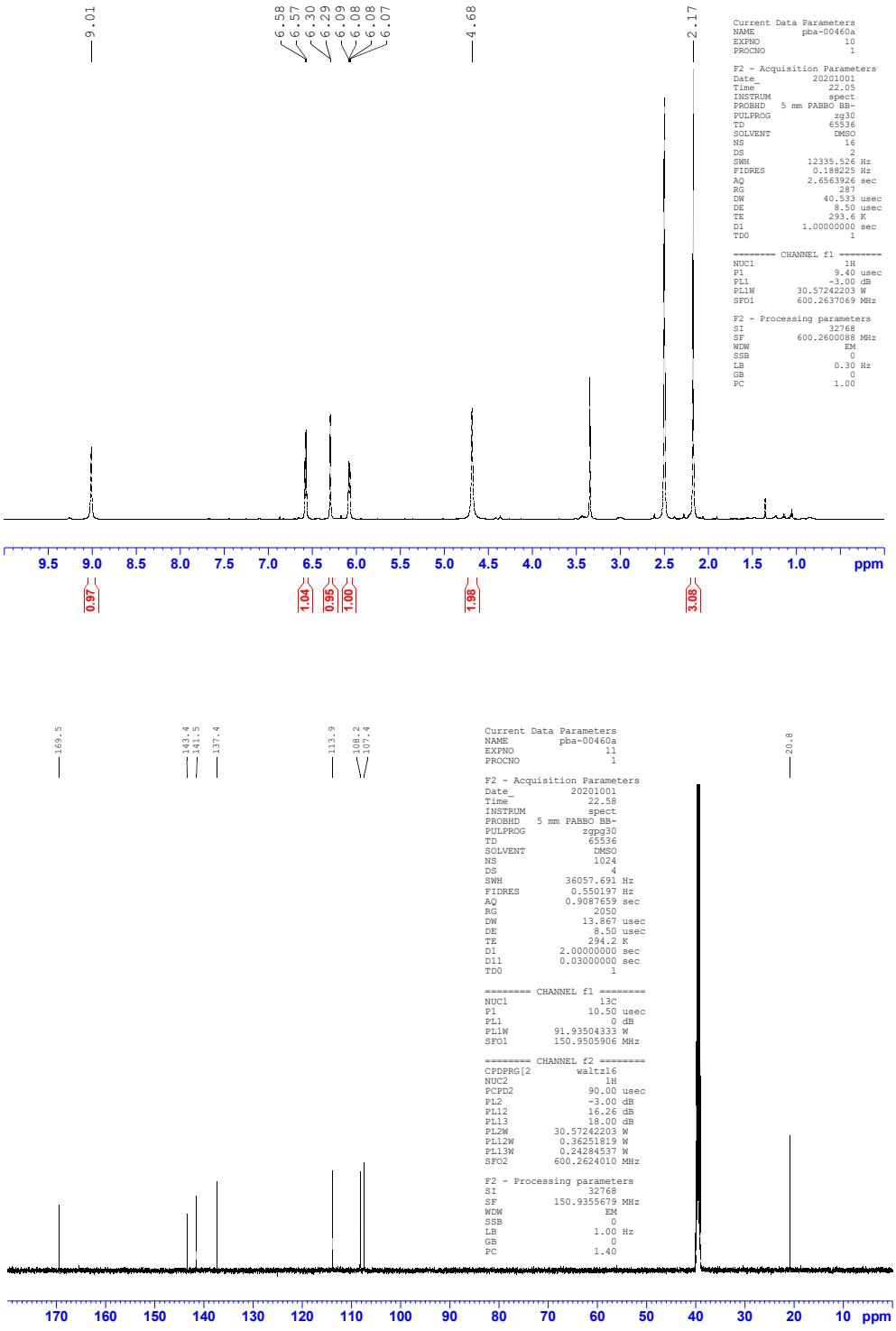


Figure S6. ^{1}H and ^{13}C{^{1}H} NMR spectra for 3-amino-4-hydroxyphenyl acetate recorded in DMSO-d_6 at 600 and 151 MHz, respectively.

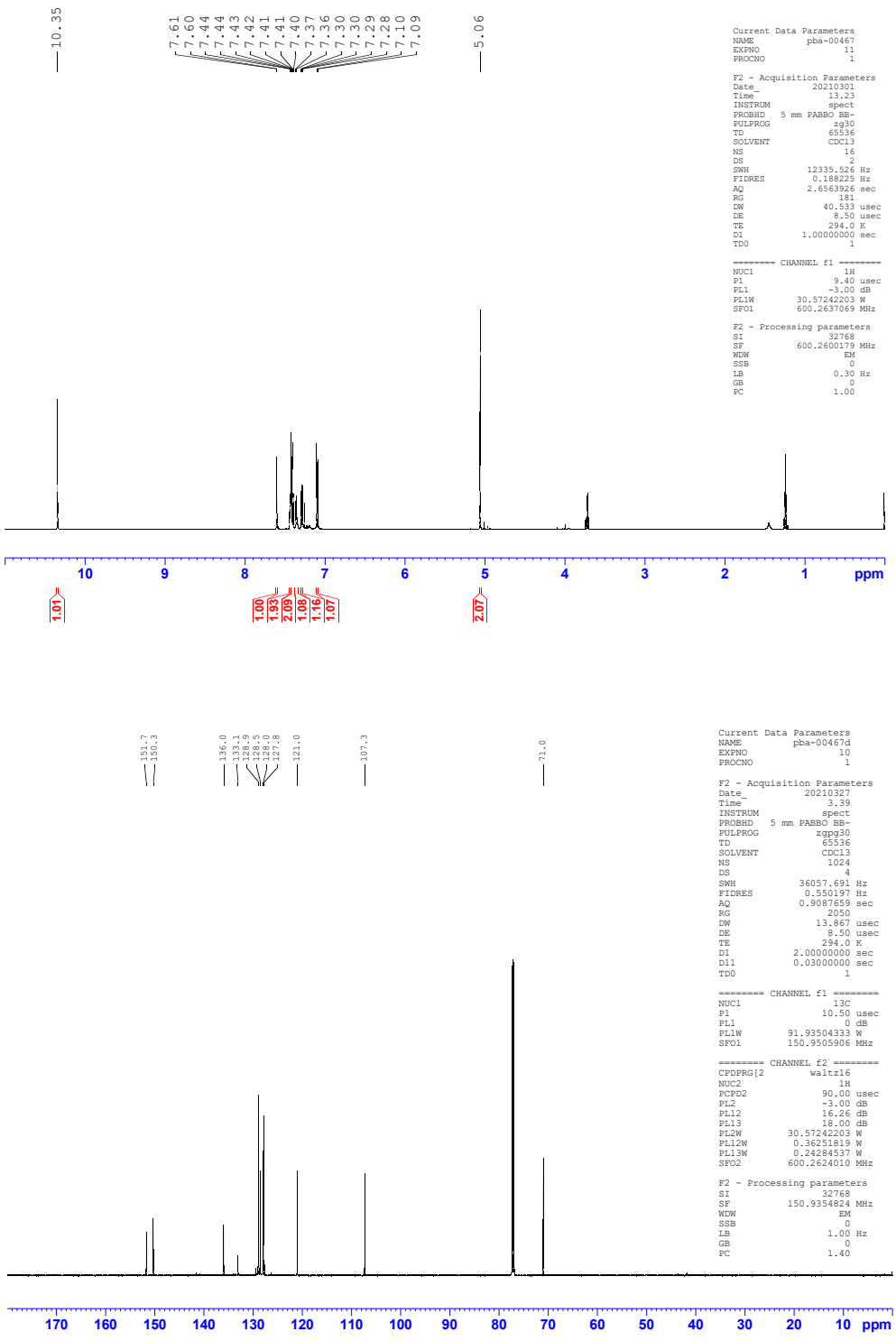


Figure S7. ^{1}H and ^{13}C{^{1}H} NMR spectra for 4-benzyloxy-2-nitrophenol recorded in DMSO-d_6 at 600 and 151 MHz, respectively.

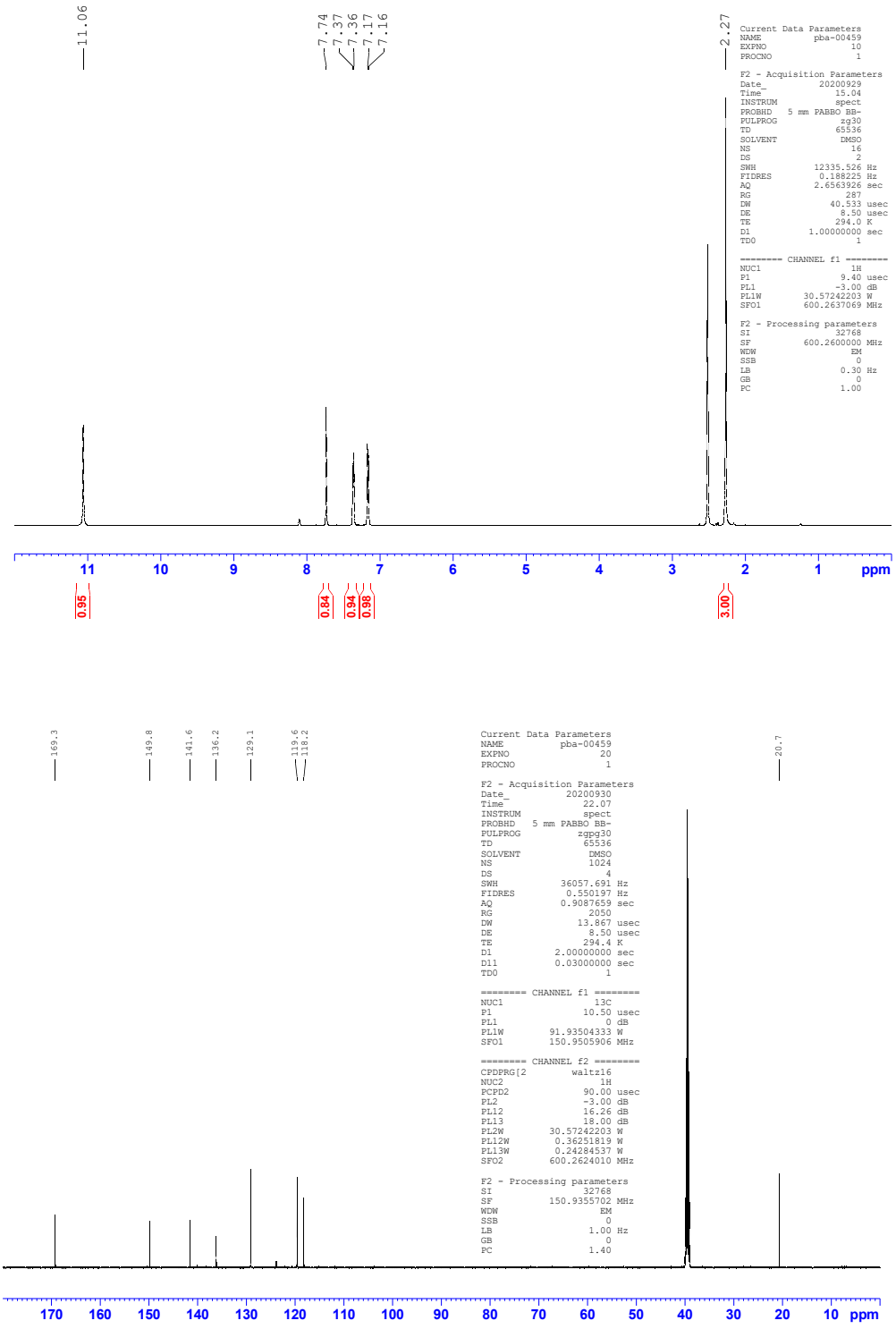


Figure S8. ^{1}H and ^{13}C{^{1}H} NMR spectra for 4-hydroxy-3-nitrophenyl acetate recorded in DMSO-d_6 at 600 and 151 MHz, respectively.

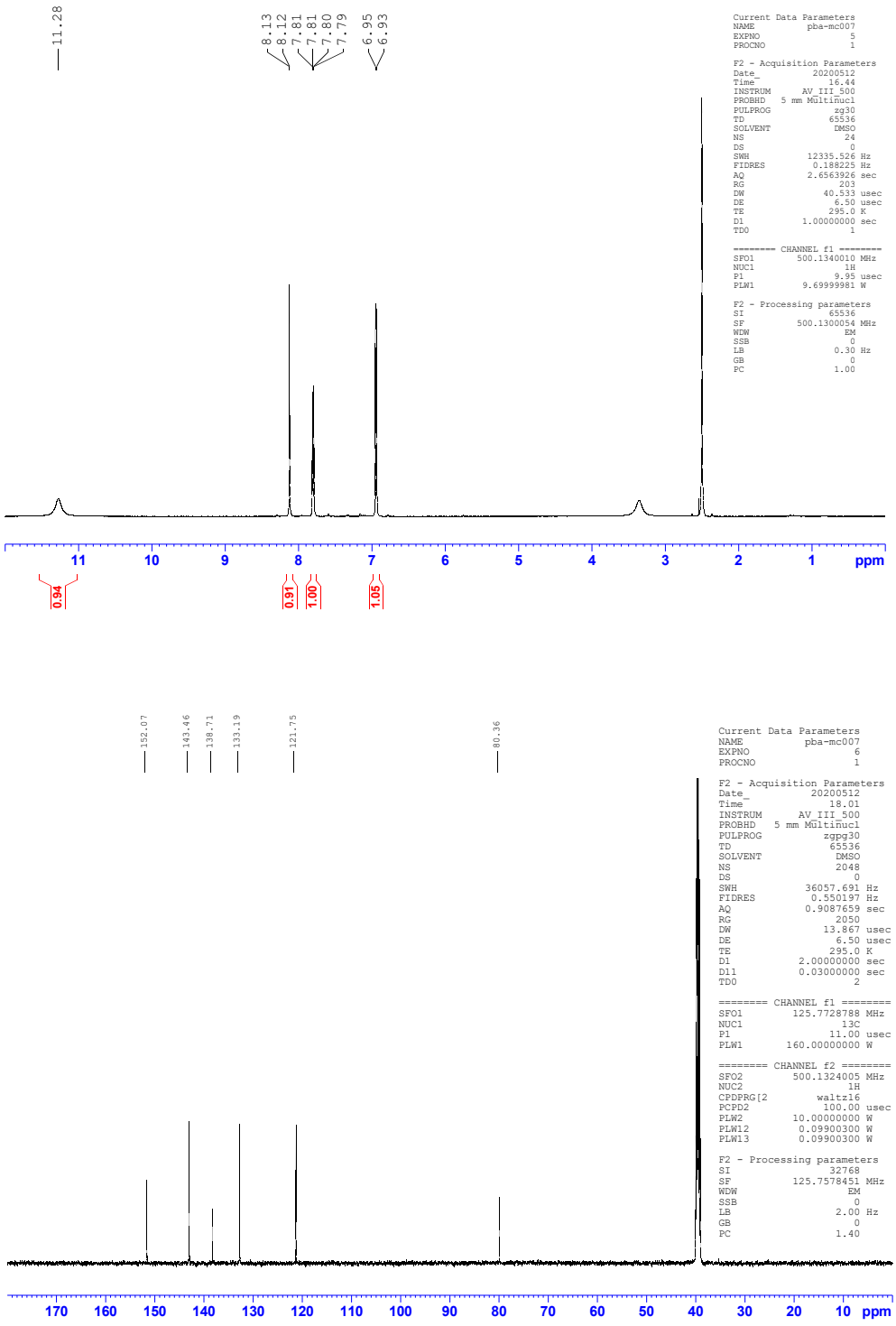


Figure S9. ^{1}H and ^{13}C{^{1}H} NMR spectra for 4-iodo-2-nitrophenol recorded in DMSO-d_6 at 500 and 125 MHz, respectively.

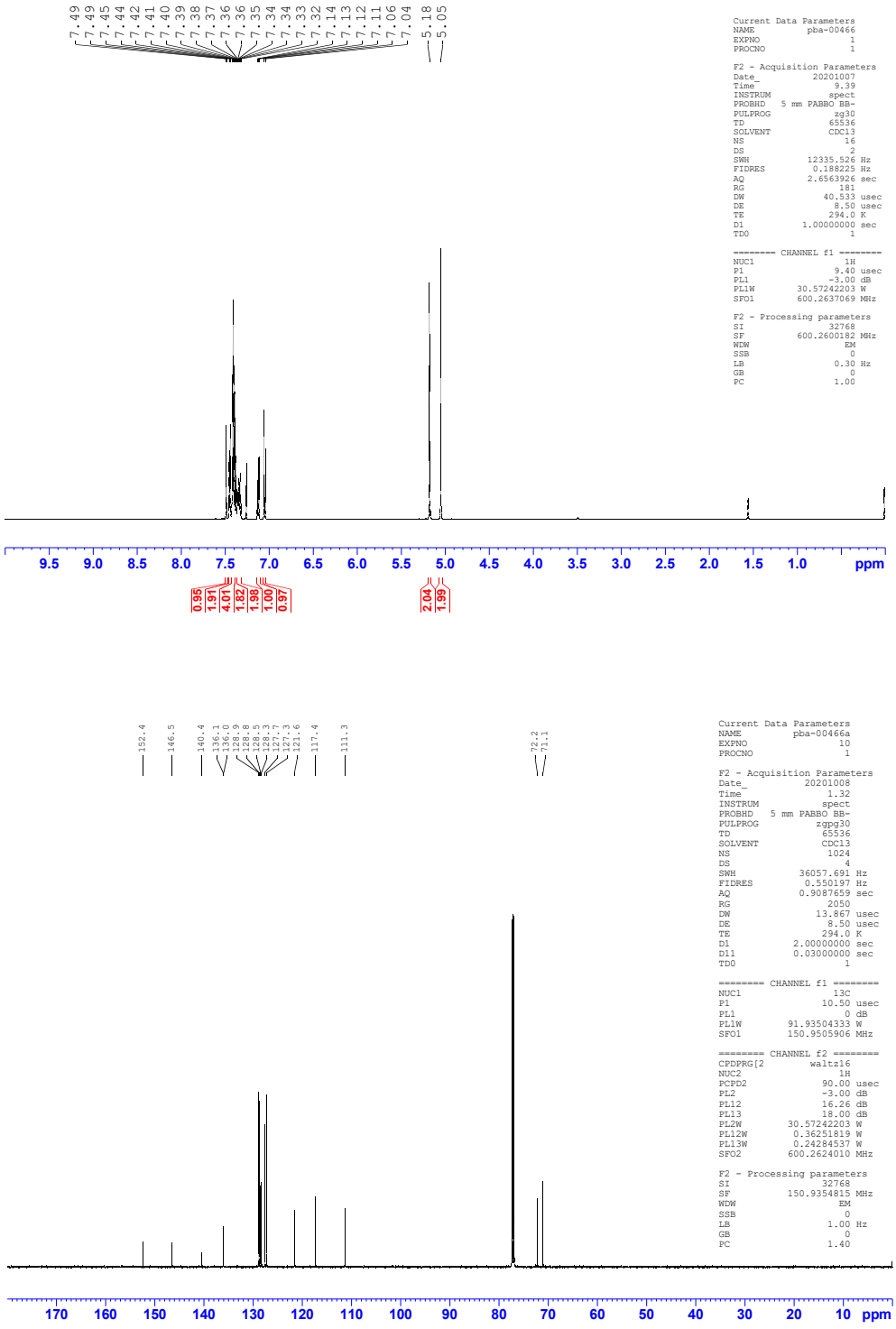


Figure S10. ^{1}H and ^{13}C{^{1}H} NMR spectra for 2-nitrohydroquinone dibenzyl ether recorded in DMSO-d_6 at 600 and 151 MHz, respectively.

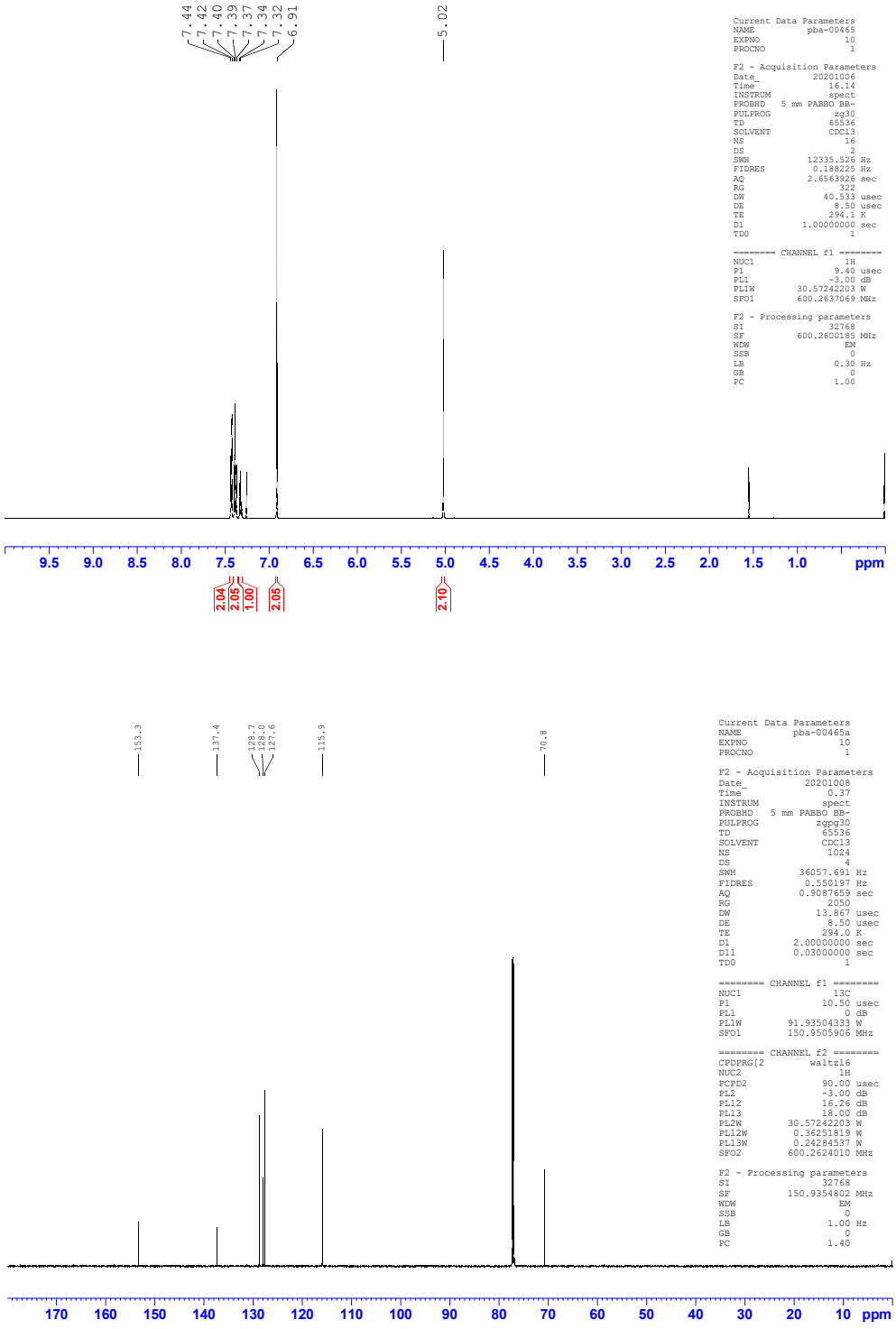


Figure S11. ^{1}H and ^{13}C{^{1}H} NMR spectra for 1,4-di(benzyloxy)benzene recorded in DMSO-d_6 at 600 and 151 MHz, respectively.

3. XRD data collection and refinement

Single-crystal XRD measurements for **1n**, **1q**, and **1s** were performed with a Rigaku XtalAB Synergy, Pilatus 300K diffractometer. The measurements were conducted at 100.0(1) K using the CuK_α radiation (λ=1.54184 Å). The data was integrated using CrysAlisPro program.[11] Intensities for absorption were corrected using multi-scan method as in SCALE3 ABSPACK scaling algorithm implemented in CrysAlisPro program.[11] Additional crystal and refinement information are listed in Table S1.

CCDC: Files 2007763-2007765 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 1n, 1q and 1s

	1n CCDC: 2007765	**1q** CCDC: 2007764	**1s** CCDC: 2007763
Formula	$C_{19}H_{11}IN_3O$	$C_{25}H_{16}N_3O$	$C_{27}H_{16}N_3O$
Formula Weight	424.21	374.41	398.43
Crystal System	Orthorhombic	Monoclinic	Monoclinic
Space Group	*P*ccn	$P2_1/c$	$P2_1/c$
a/Å	28.8753(2)	21.5515(6)	18.3724(7)
b/Å	13.0456(1)	5.0208(1)	13.2094(5)
c/Å	8.0244(1)	18.0754(5)	8.0305(3)
α/°	90	90	90
β/°	90	113.476(3)	97.937(4)
γ/°	90	90	90
Volume/Å^3	3022.76(5)	1793.97(9)	1930.2(1)
Z	8	4	4
2θ range for data collection/°	7.436 to 157.34	8.948 to 140.106	8.272 to 134.146
Index ranges	-28 ≤ h ≤ 36, -16 ≤ k ≤ 16, -10 ≤ l ≤ 9	-25 ≤ h ≤ 26, -6 ≤ k ≤ 6, -22 ≤ l ≤ 21	-21 ≤ h ≤ 21, -15 ≤ k ≤ 13, -9 ≤ l ≤ 9
No. of measured, independent, and observed [$I>2\sigma(I)$] reflections	34519, 3242, 3014	32411, 3393, 2842	17388, 3441, 2334
*R*int	0.0376	0.0440	0.0385
Goodness-of-fit on F^2	1.097	1.060	1.235
Final *R* indexes [$F^2 > 2\sigma(F^2)$]	R_1=0.0234, w*R*2=0.0632	R_1=0.0637, *wR2*=0.1753	R_1=0.0655, wR_2=0.1685
Final *R* indexes [all data]	R_1=0.0252, w*R*2= 0.0642	R_1=0.0724, *wR2*= 0.1824	R_1=0.0973, wR_2=0.1923
Data/restraints/parameters	3242/0/217	3393/151/287	3441/0/274
Largest diff. peak/hole Å^{-3}	0.98/-0.44	0.41/-0.40	0.65/-0.26

Structure solution and refinement

The structures were solved with the ShelXT[12] structure solution program using Intrinsic Phasing and refined in the ShelXle by the full-matrix least-squares minimization on F^2 with the ShelXL[13] 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 phenyl group in **1q** is disordered over two orientations with occupancy ratio 0.524(4):0.476(4). The phenyl ring of the first component of disordered structure is rotated around 59.8° with respect to the orientation of the first component. Sums of occupancies of relevant sites were set equal to 1 and refined using free variables. PART instruction was applied to exclude bonding between equivalent disordered atoms. Anisotropic displacement parameters of neighboring disordered atoms were restrained using SIMU and RIGU procedures as in ShelXL. The crystal data and structure refinement descriptors are presented in Table S1. Partial packing diagrams for **1n**, **1q** and **1s** are shown in Figures S12–S17, while selected geometrical parameters are listed in Table S2 and compared to those of **1a**,[14] **1d**,[15] and **1e**.[16]

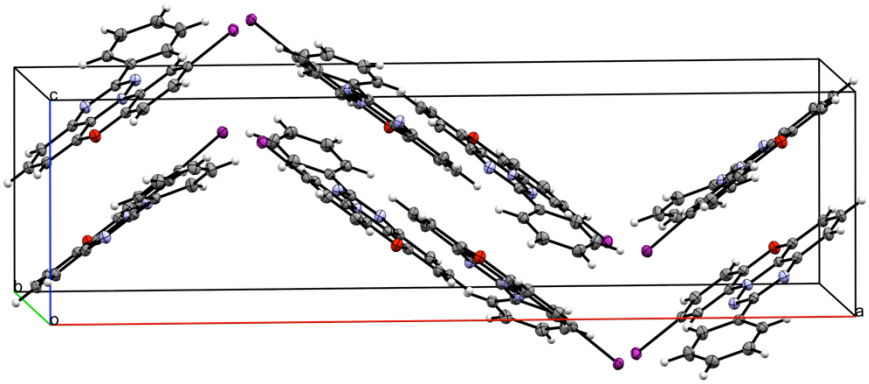


Figure S12. Unit cell packing diagram for **1n**.

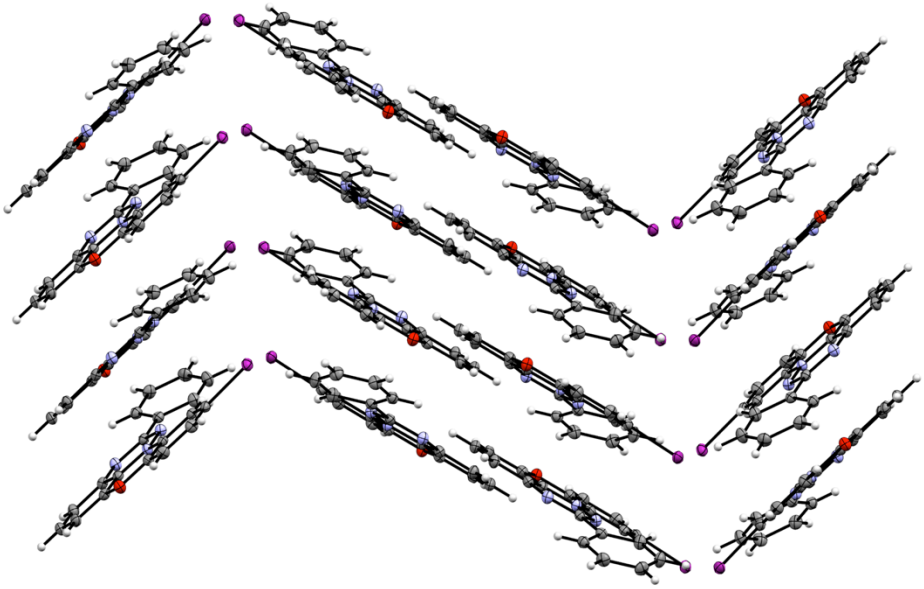


Figure S13. Slipped stacks of **1n**. Angles between the adjacent stacks are 74.8 and 8.7°.

Close contacts within the stacks:

C(11)···C(6a) 3.262 Å (-0.138 Å inside VDW separation)

C(3a')···C(6) 3.386 Å (-0.014 Å inside VDW separation)

Close contacts between the stacks:

I···H-C(Ph) 3.140 Å (-0.040 Å inside VDW separation)

C(4)-H···O(7) 2.563 Å (-0.157 Å inside VDW separation)

C(5)-H···C(Ph) 3.383 Å (-0.017 Å inside VDW separation)

Slippage angle - of 23.1° was calculated as an angle 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 same orientation.

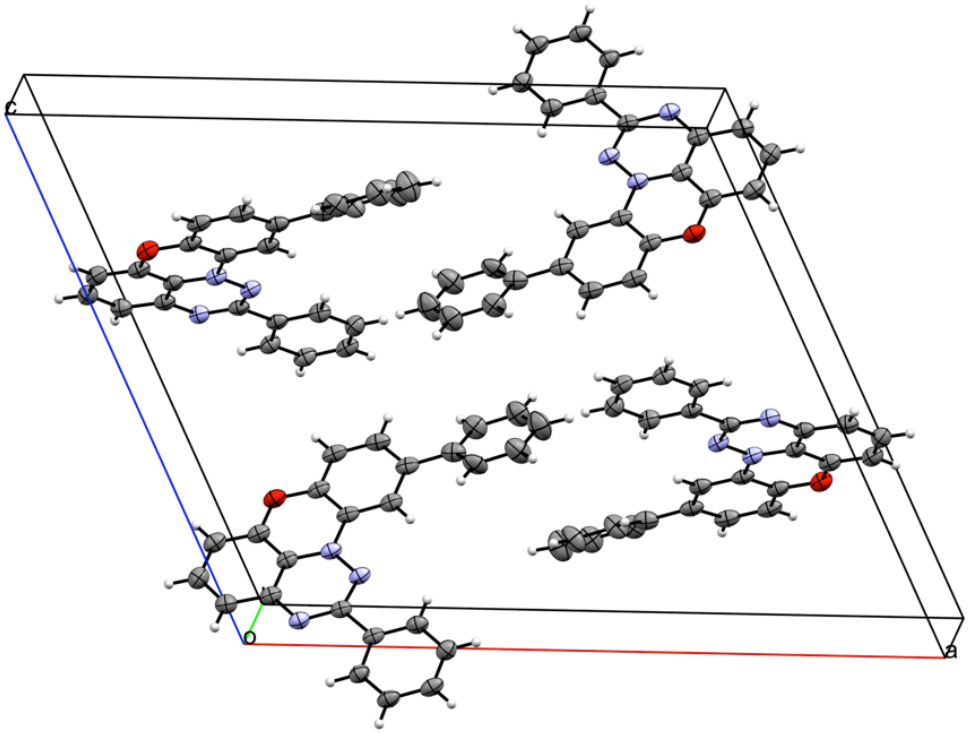


Figure S14. Unit cell packing diagram for **1q**.

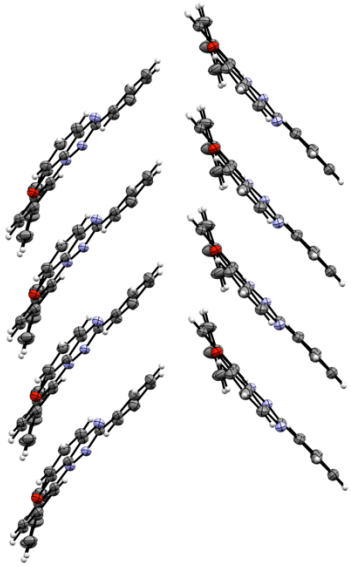


Figure S15. Two slipped stacks of **1q**. The angle between the stacks is 80.6°.

Close contacts within the stacks:

Close contacts between the heterocyclic cores

C(2)···C(11a) 3.281 Å (-0.119 Å inside VDW separation)

C(3a)···O(7) 3.386 Å (-0.051 Å inside VDW separation)

Close contacts between the C(10)–Ph groups

C(*m*)-H···C(*m*') 2.773 Å (-0.627 Å inside VDW separation)

C(*o*)-H···C(*o*') 2.184 Å (-0.716 Å inside VDW separation)

C(*m*')-H···C(*m*) 2.183 Å (-0.717 Å inside VDW separation)

C(*o*')-H···C(*o*) 2.122 Å (-0.778 Å inside VDW separation)

Slippage angle - of 36.8° was calculated as an angle 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 same orientation.

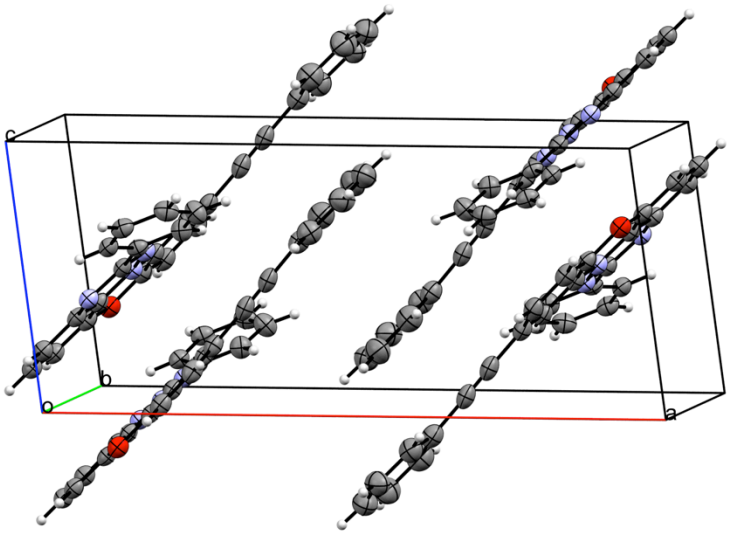


Figure S16. Packing diagram for unit cell of **1s**.

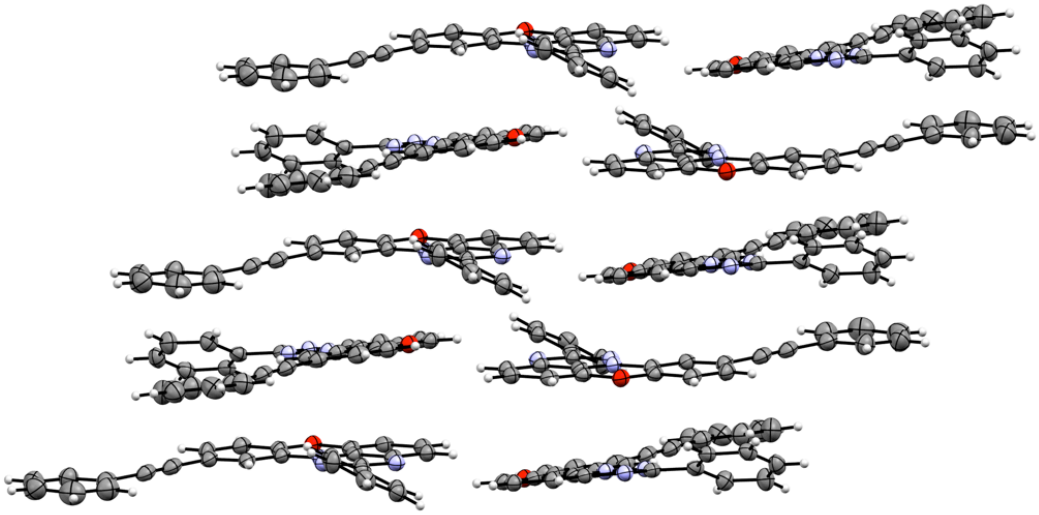


Figure S17. Two slipped stacks of **1s**. Angle between the stacks is 0°.

Close contacts within the stacks:

C(6a)···C(11a) 3.207 Å (-0.193 Å inside VDW separation)

C(11a)···C(11) 3.336 Å (-0.064 Å inside VDW separation)

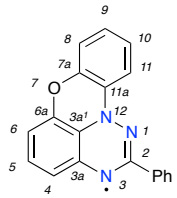
C(7a)-H···C(11) 3.369 Å (-0.031 Å inside VDW separation)

Close contacts between the stacks:

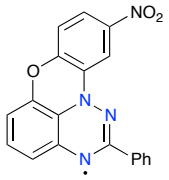
C(4)-H···O(7) 2.577 Å (-0.143 Å inside VDW separation)

Slippage angle - of 23.1° was calculated as an angle 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 same orientation.

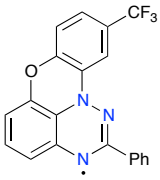
Table S2. Selected interatomic distances and angles for planar benzo[*e*][1,2,4]triazin-4-yl radicals.[a]



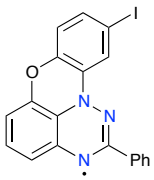
1a



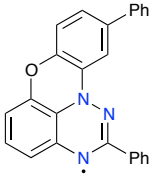
1d



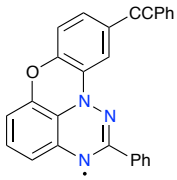
1e



1n



1q



1s

	1a [b]	**1d** [c]	**1e** [d]	**1n**	**1q**	**1s**
$d_{N1–N12}$	1.35(1)	1.358(2)	1.354(1)	1.356(3)	1.360(2)	1.360(3)
$d_{N1–C2}$	1.32(1)	1.343(2)	1.343(1)	1.343(3)	1.346(3)	1.340(3)
$d_{C2–N3}$	1.364(9)	1.340(2)	1.337(1)	1.340(3)	1.326(3)	1.346(4)
$d_{N3–C3a}$	1.38(1)	1.373(2)	1.375(1)	1.376(3)	1.378(3)	1.382(3)
$d_{C3a–C3a'}$	1.38(1)	1.409(2)	1.407(1)	1.407(3)	1.410(3)	1.404(4)
$d_{C3a'–C6a}$	1.36(1)	1.392(2)	1.393(2)	1.396(3)	1.402(3)	1.391(4)
$d_{C6a–O7}$	1.39(1)	1.382(2)	1.381(1)	1.380(3)	1.389(3)	1.384(3)
d_{O7-C7a}	1.381(9)	1.367(2)	1.379(1)	1.381(3)	1.371(3)	1.388(4)
$d_{N12–C11a}$	1.42(1)	1.398(2)	1.401(1)	1.400(3)	1.405(3)	1.399(3)
d_{C2-Ph}	1.50(1)	1.491(2)	1.485(1)	1.486(3)	1.489(3)	1.479(4)
$d_{C10-NO2}$		1.465(2)				
$\alpha_{N12-N1-C2}$	114.1(6)	114.8(1)	115.06(1)	114.9(2)	114.4(2)	115.5(2)
$\alpha_{N1-C2-N3}$	130.2(7)	128.7(1)	128.47(9)	128.7(2)	128.7(2)	128.1(3)
$\alpha_{C7a-O7-C6a}$	118.5(6)	117.8(1)	117.67(8)	118.1(2)	117.7 (2)	117.8(2)
$\alpha_{C3a'-N12-C11a}$	118.6(6)	118.8(1)	119.09(1)	119.0(2)	119.8(2)	119.4(2)
$\theta_{N12-N1-C2-N3}$	1(1)	0.8(2)	2.6(1)	0.0(3)	-0.4(3)	1.1(4)
$\theta_{C3a'-C6a-O7-C7a}$	0(1)	–1.1(2)	5.5(1)	–1.0(3)	–3.0(3)	2.0(4)
$\beta_{triazine-(C2)Ph}$	2.9	4.7	4.0	22.3	2.95	25.8

[a] *d* - interatomic distance, α - interatomic angle, θ - dihedral angle, β - inter-ring angle. [b] Ref [14]. [c] Ref [15]. [d] Ref [16].

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 S18–S24.

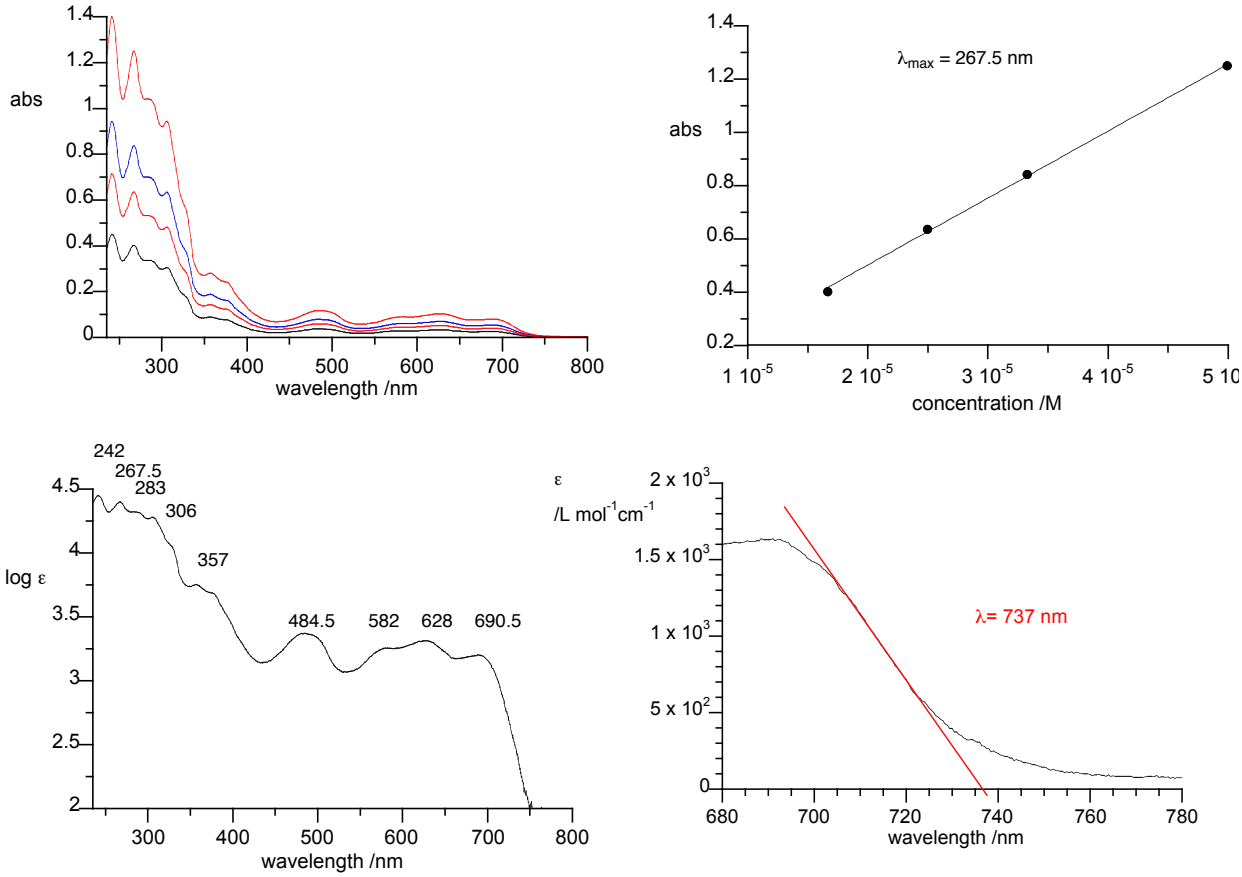


Figure S18. Clockwise: electronic absorption spectra for **1n** (X = I) in CH_2Cl_2 for four concentrations, determination of molar extinction coefficient ε at λ = 267.5 nm (best fit function: ε = 25111×conc, r^2 = 0.9991), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

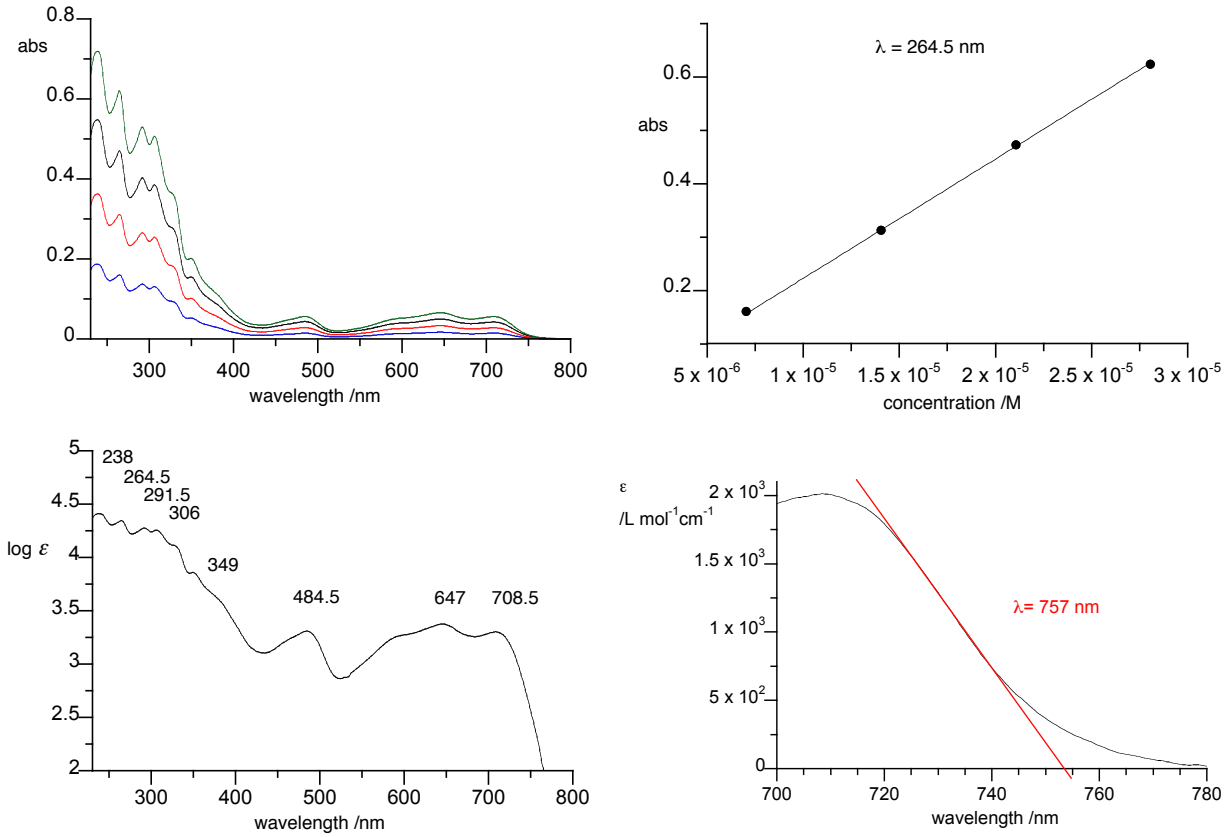
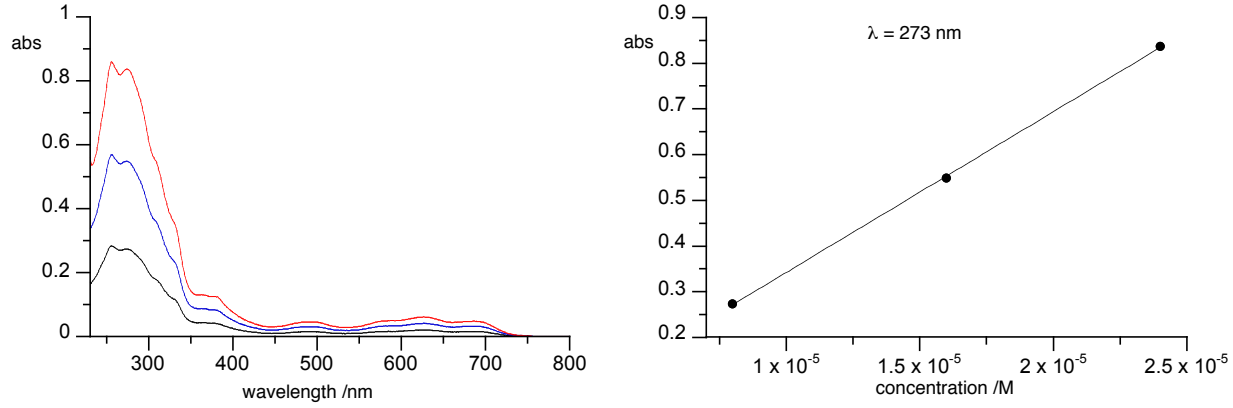


Figure S19. Clockwise: electronic absorption spectra for **1p** (X = OBn) in CH_2Cl_2 for three concentrations, determination of molar extinction coefficient ε at λ = 264.5 nm (best fit function: ε = 22313×conc, r^2 = 0.9997), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).



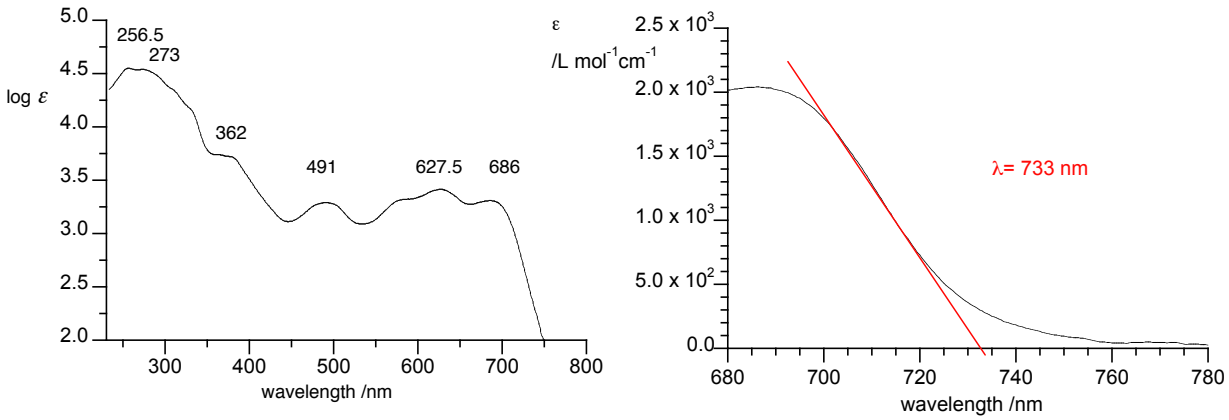


Figure S20. Clockwise: electronic absorption spectra for **1q** (X = Ph) in CH_2Cl_2 for three concentrations, determination of molar extinction coefficient ε at λ = 273 nm (best fit function: ε = 35137×conc, r^2 = 0.9998), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

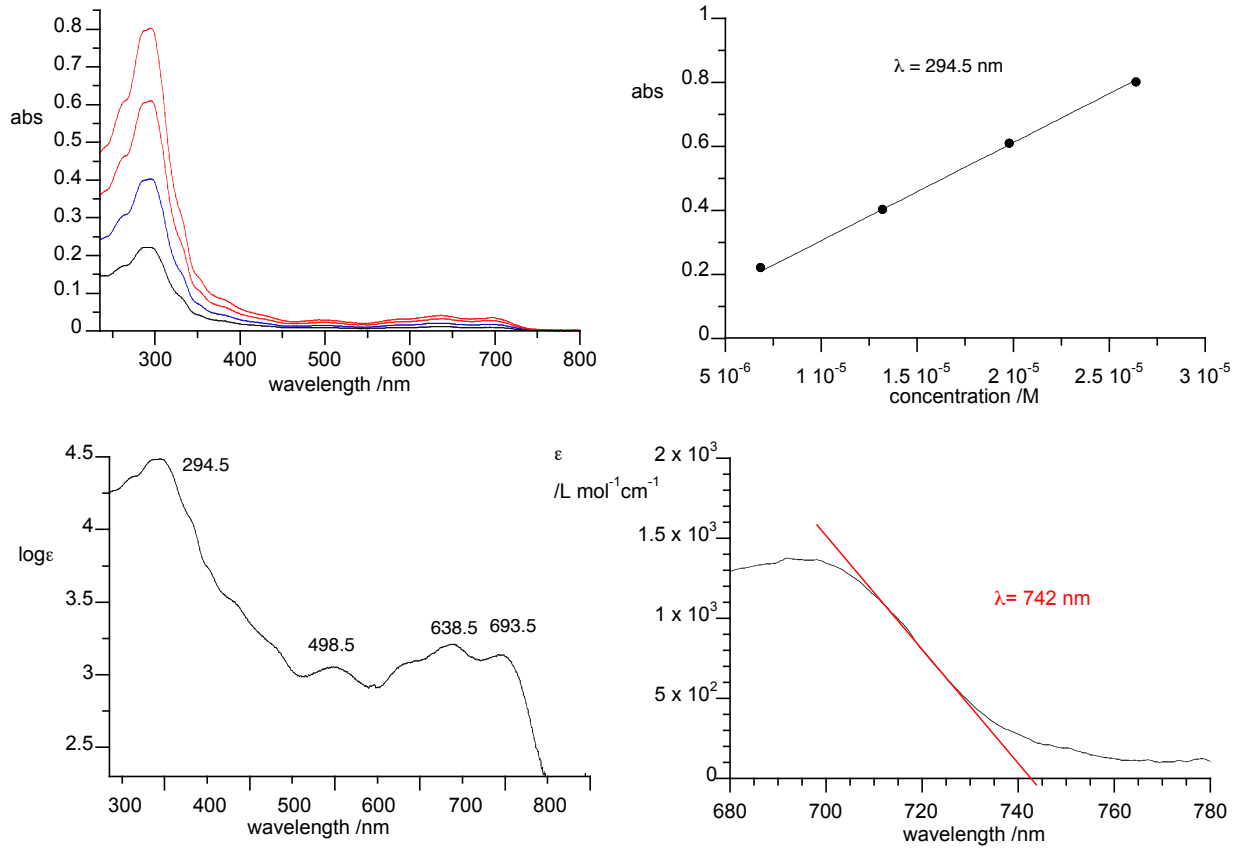


Figure S21. Clockwise: electronic absorption spectra for **1r** (X = 2-thienyl) in CH_2Cl_2 for four concentrations, determination of molar extinction coefficient ε at λ = 294.5 nm (best fit function: ε = 30573×conc, r^2 = 0.9989), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

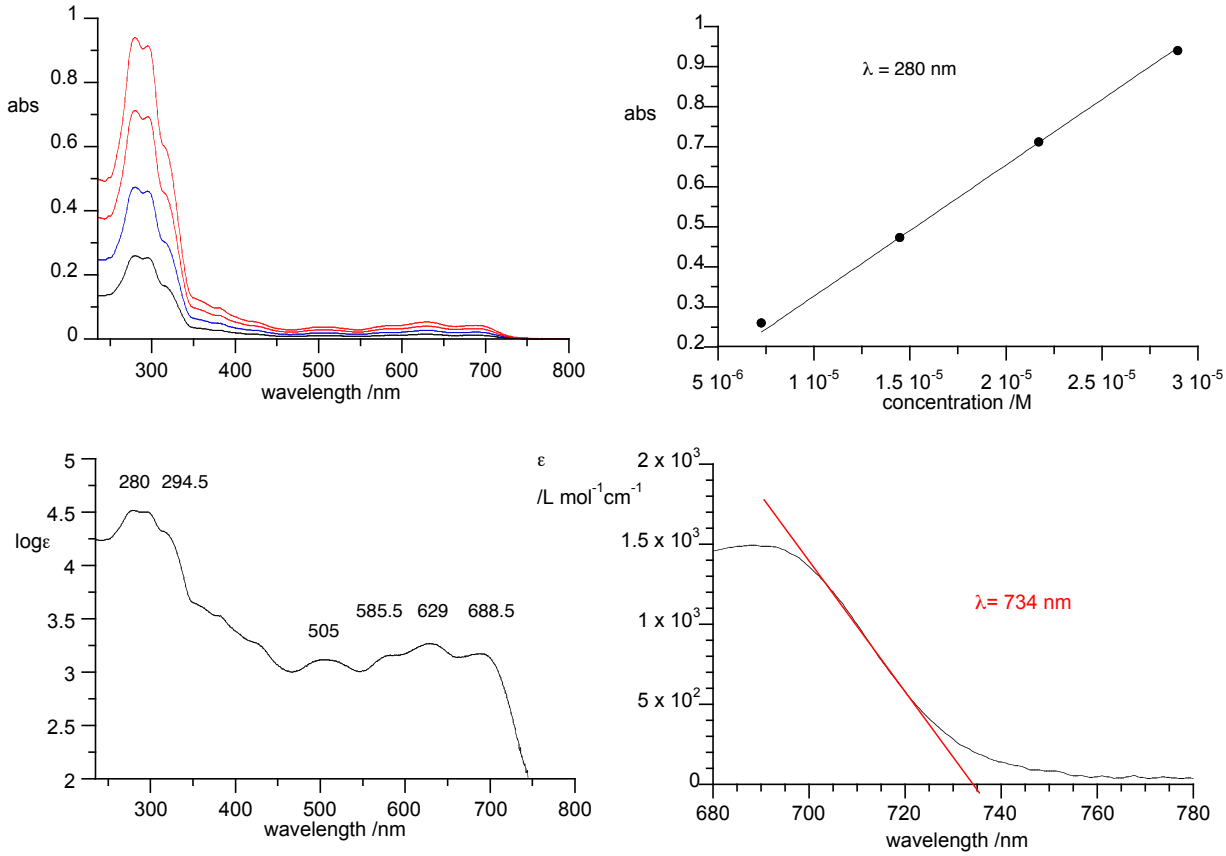
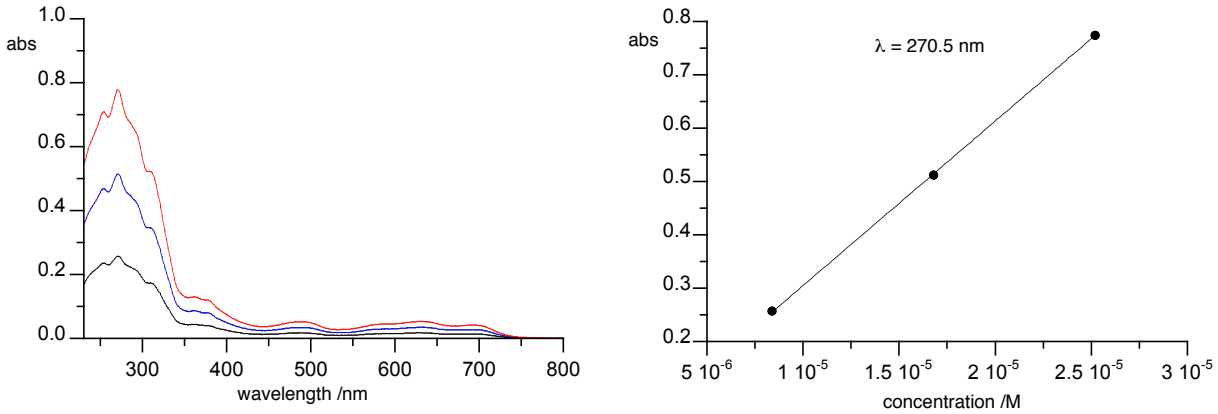


Figure S22. Clockwise: electronic absorption spectra for **1s** (X = CCPh) in CH_2Cl_2 for four concentrations, determination of molar extinction coefficient ε at λ = 280 nm (best fit function: ε = 32701×conc, r^2 = 0.9978), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).



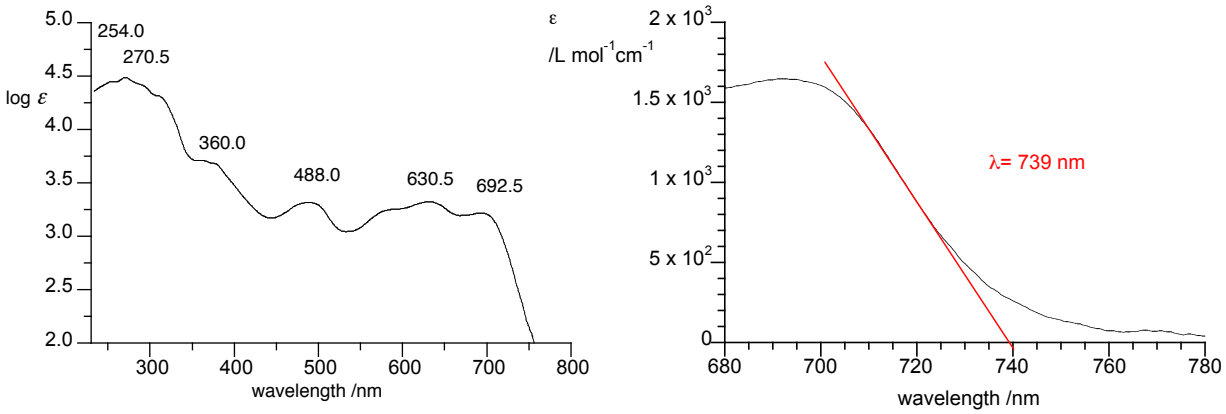


Figure S23. Clockwise: electronic absorption spectra for **1u** (X = $NHCOCF_3$) in CH_2Cl_2 for three concentrations, determination of molar extinction coefficient ε at λ = 270.5 nm (best fit function: ε = 30788×conc, r^2 = 0.9999), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

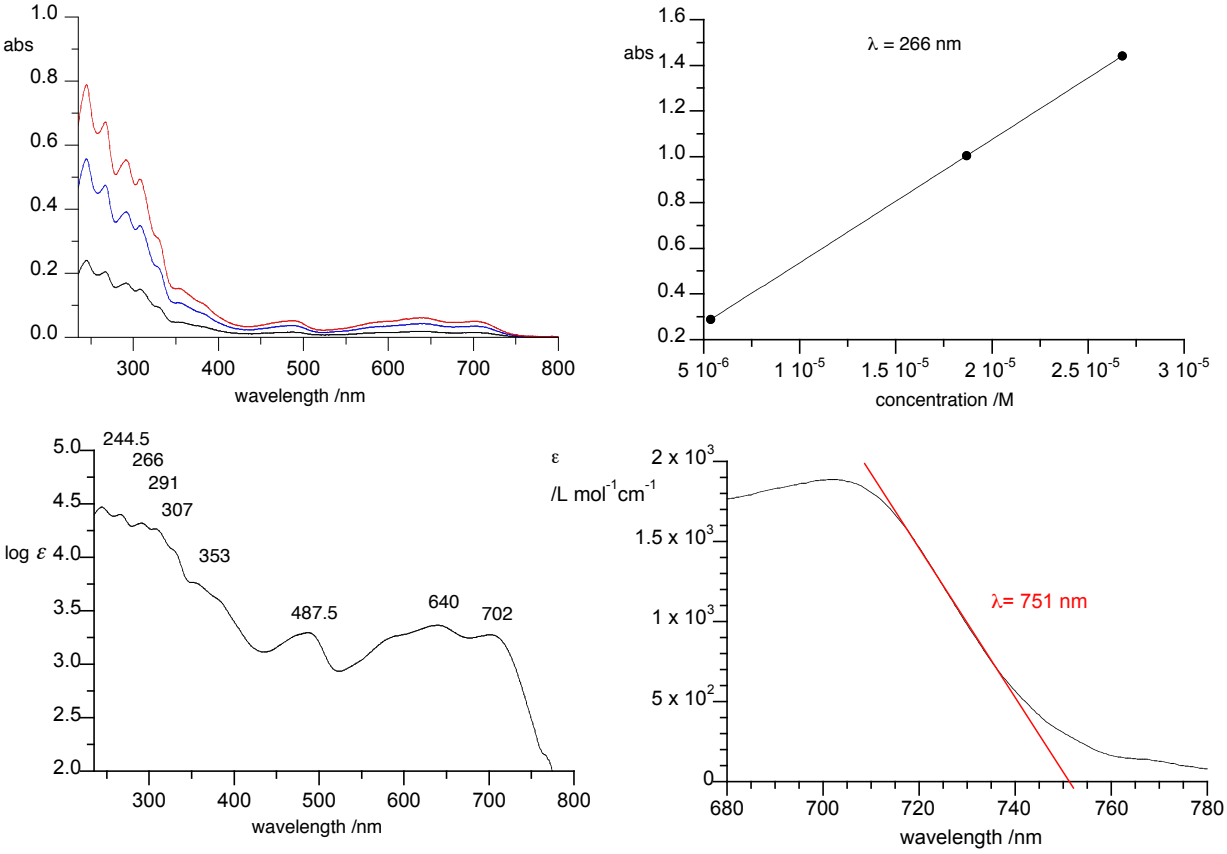


Figure S24. Clockwise: electronic absorption spectra for **1v** (X = NHCOOMe) in CH_2Cl_2 for three concentrations, determination of molar extinction coefficient ε at λ = 266 nm (best fit function: ε = 53718×conc, r^2 = 0.9999), molar extinction *log* (ε) plot, and onset of absorption (optical band-gap).

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 ^oC. 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.[17]

Cyclic voltammetry (CV) plots are shown in Figures S25–S32 and numerical result are shown in Table 3 in the main text.

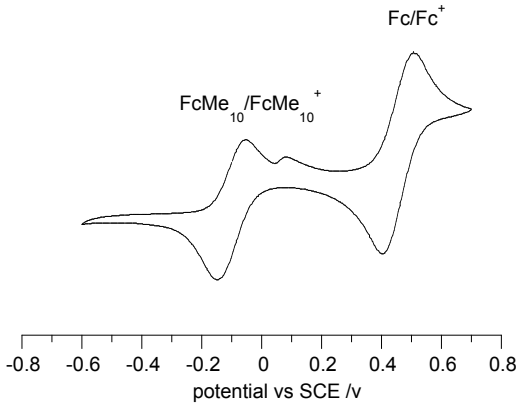
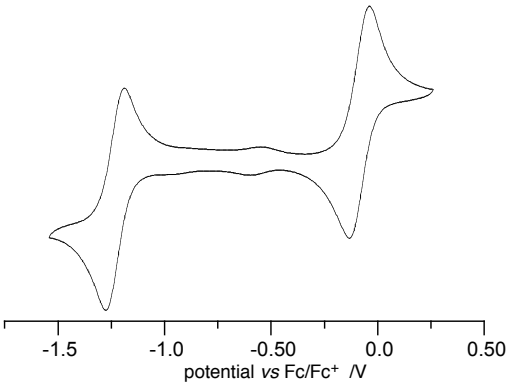


Figure S25. Cyclic voltammogram for ferrocene (Fc) and decamethylferrocene ($FeMe_{10}$). The small peak at about 0.05 V is related to some impurity in the commercial $FeMe_{10}$.



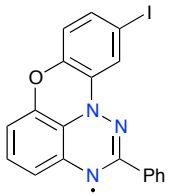
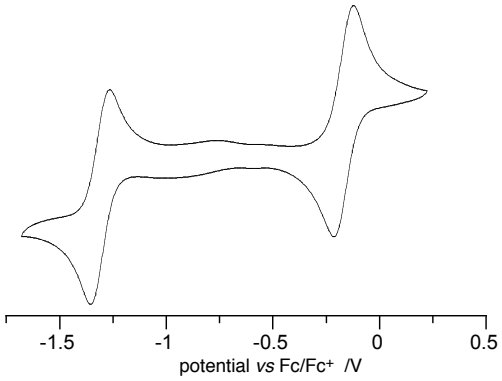


Figure S26. Cyclic voltammogram for **1n**.



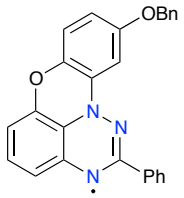
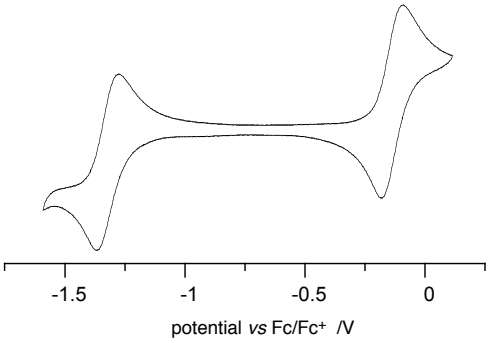


Figure S27. Cyclic voltammogram for **1p**.



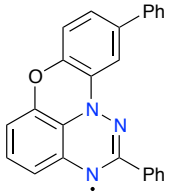
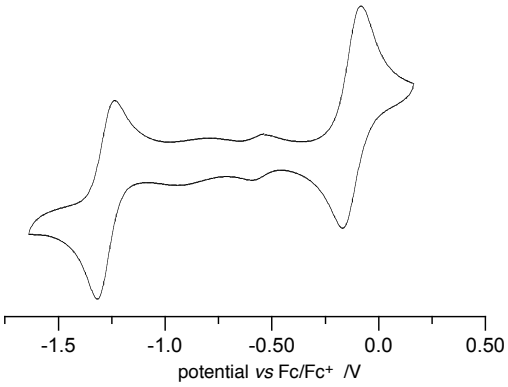


Figure S28. Cyclic voltammogram for **1q**.



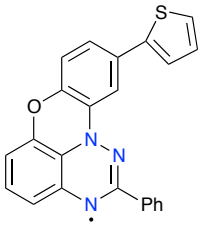
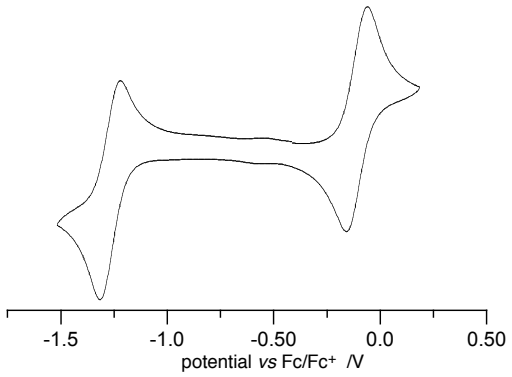


Figure S29. Cyclic voltammogram for **1r**.



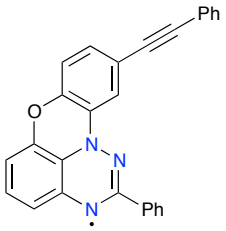
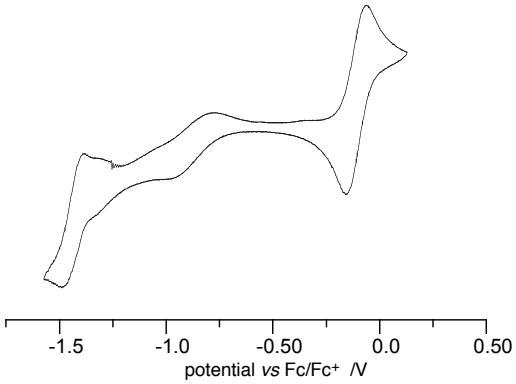


Figure S30. Cyclic voltammogram for **1s**.



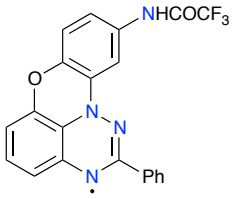
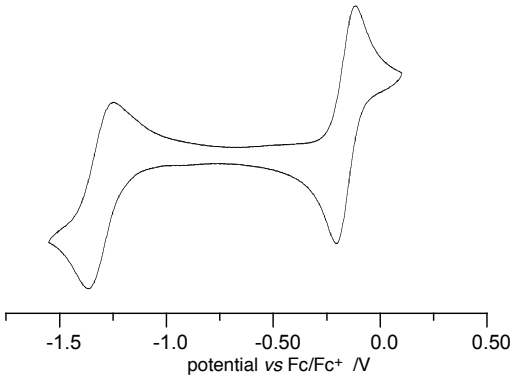


Figure S31. Cyclic voltammogram for **1u**.



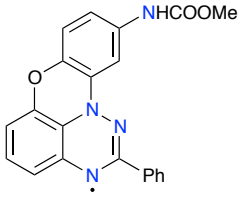


Figure S32. Cyclic voltammogram for **1v**.

6. EPR spectra

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 2–5×10^{-4} M. Acid **1f** showed insufficient solubility to record its isotropic EPR spectrum. 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 S33–S39 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 (section 7.b; *vide infra*).

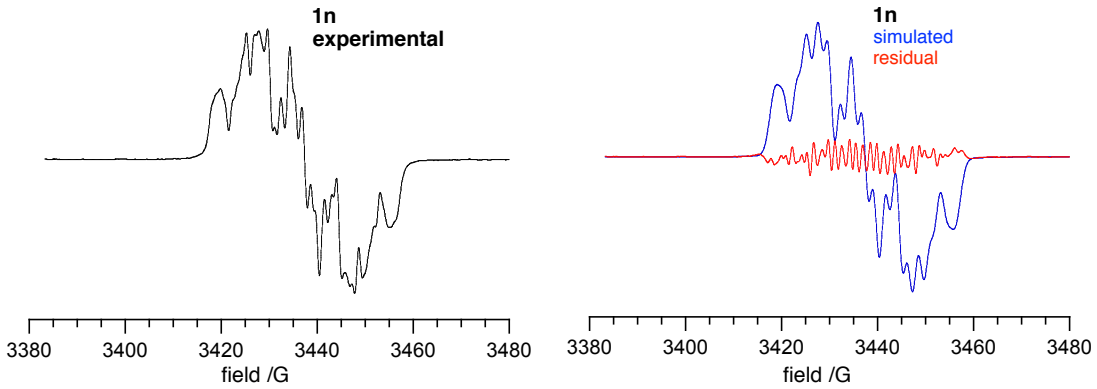


Figure S33. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1n** (X = I) recorded in benzene at *ca* 20 ºC.

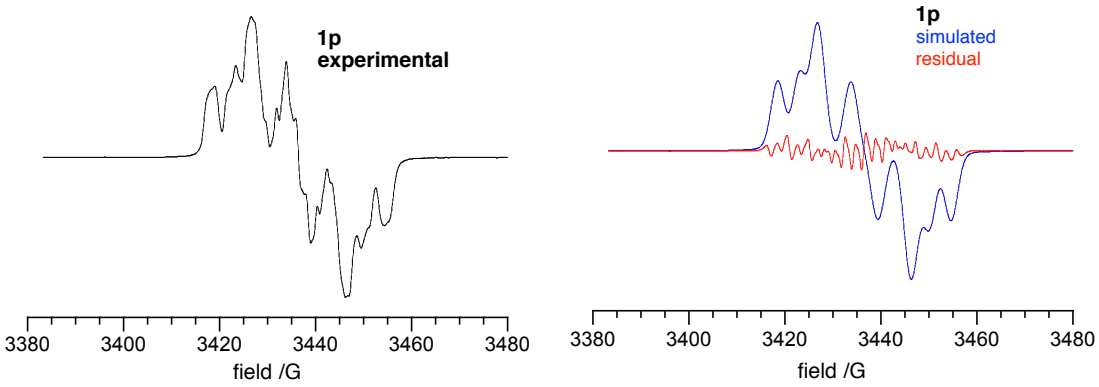


Figure S34. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1p** (X = OBn) recorded in benzene at *ca* 20 ºC.

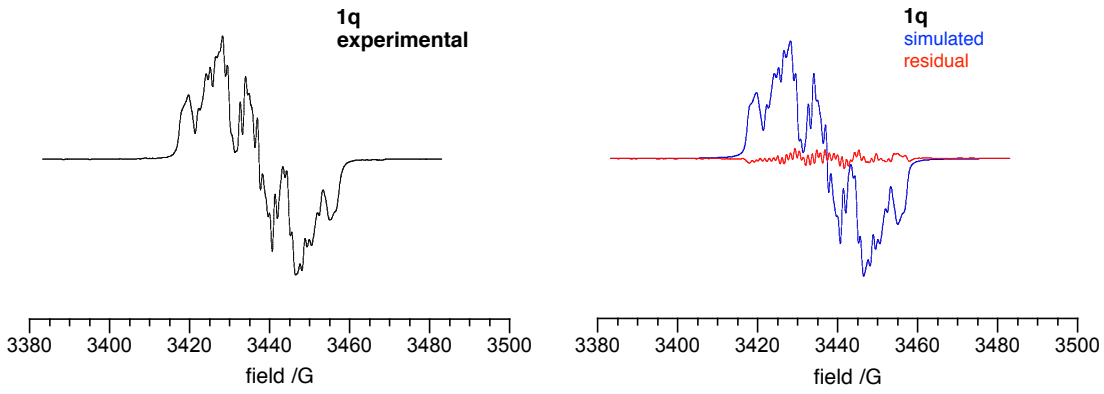


Figure S35. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1q** (X = Ph) recorded in benzene at *ca* 20 ºC.

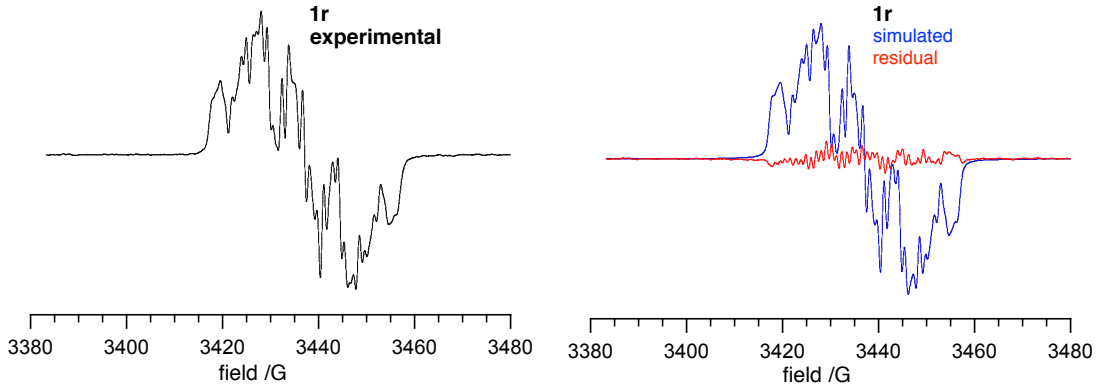


Figure S36. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1r** (X = 2-thienyl) recorded in benzene at *ca* 20 ºC.

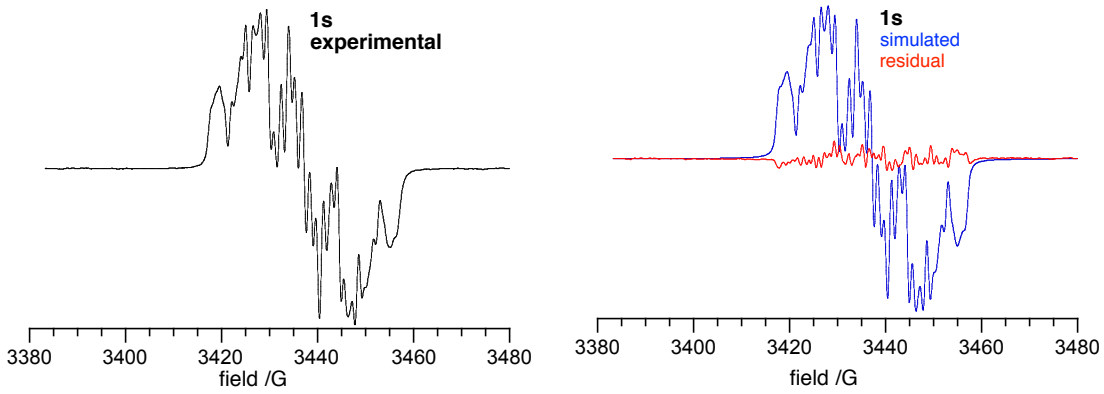


Figure S37. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1s** (X = CCPh) recorded in benzene at *ca* 20 ºC.

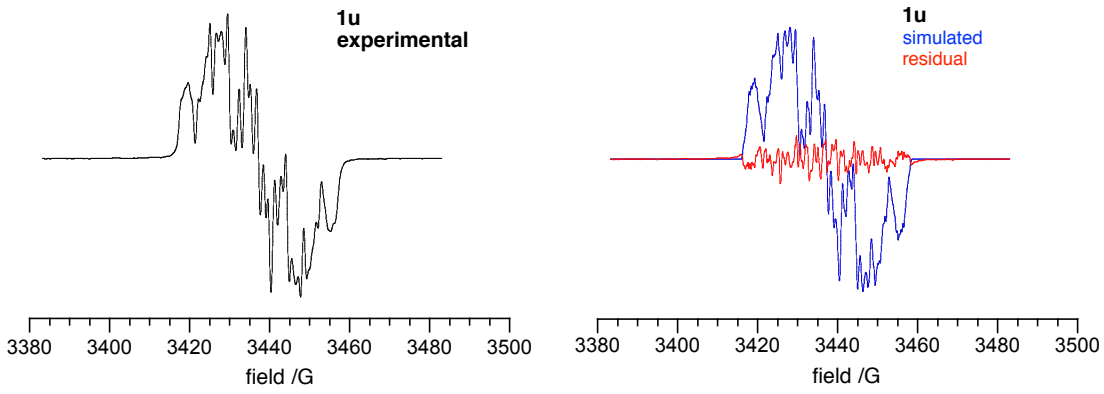


Figure S38. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1u** (X = $NHCOCF_3$) recorded in benzene at *ca* 20 ºC.

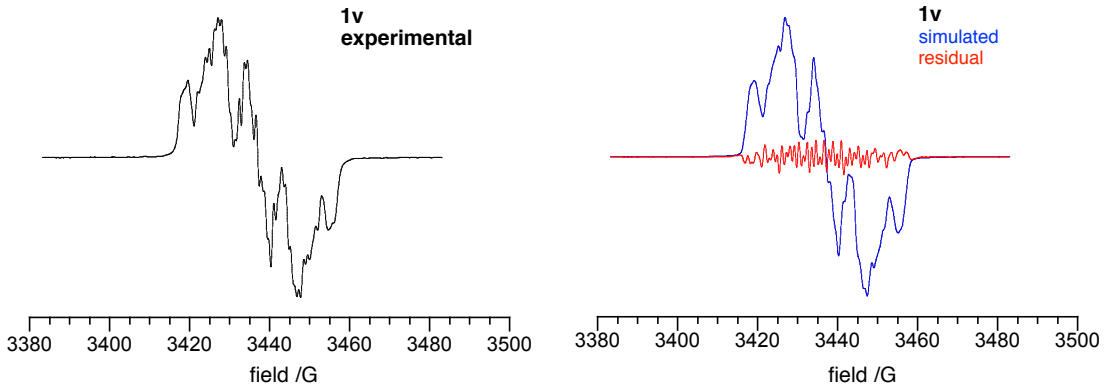


Figure S39. Experimental (black, left), simulated (blue, right) and difference (red, right) spectra for **1v** (X = NHCOOMe) recorded in benzene at *ca* 20 ºC.

Table S3. Experimental hyperfine coupling constants (G) and *g* values for radicals in series **1** recorded in benzene at 22 ºC.

atom	**1a** H	**1b** COOMe	**1c** CN	**1d** NO_2	**1e** CF_3	**1f** OMe	**1g** F	**1h** Cl	**1i** Br	**1j** Ac
$a_{N(12)}$	7.51	7.29	7.03	6.95	7.11	7.37	7.15	7.15	7.15	7.24
$a_{N(1)}$	4.28	4.44	4.50	4.55	4.50	4.29	4.40	4.46	4.42	4.41
$a_{N(3)}$	4.42	4.52	4.70	4.66	4.53	4.37	4.44	4.54	4.48	4.52
a_N	–	-	1.81	1.06	-	-	-	-	-	-
$a_{H/F}$	-	-	-	-	2.04	-	2.02	-	-	-
a_H	1.94	0.87	1.51	2.07	1.58	2.14	1.76	2.08	1.98	2.02
a_H	1.11	1.84	1.49	0.78	1.04	1.57	1.39	1.76	1.76	1.61
a_H	0.72	1.98	1.44	0.96	0.82	1.12	0.75	1.49	1.01	0.78
a_H	0.60	1.13	0.67	0.67	0.44	0.71	0.57	1.44	0.89	0.44
a_H	0.39	0.62	0.57	0.34	0.41	0.71	0.44	0.71	0.31	0.40
a_H	0.29	0.23	0.39	0.41	0.23	0.37	0.13	0.45	0.18	0.30
a_H	0.11	0.27	0.17	0.32	0.07	0.33	0.10	0.29	0.17	0.20
a_H	0.10	0.33	0.10	0.17	0.00	0.23	0.08	0.05	0.08	0.14
a_H	0.09	0.37	0.07	0.66	0.05	0.09	0.03	0.01	0.28	0.05
g	2.0036	2.0037	2.0035	2.0039	2.0039	2.0038	2.0035	2.0038	2.0034	2.0039

Table S3. Continues

atom	**1l** NH_2	**1m** NHAc	**1n** I	**1p** OBn	**1q** Ph	**1r** Thienyl	**1s** CCPh	**1u** $NHCOCF_3$	**1v** NHCOOMe
$a_{N(12)}$	7.26	7.43	7.15	7.60	7.42	7.35	7.18	7.22	7.34
$a_{N(1)}$	4.18	4.32	4.46	4.15	4.30	4.39	4.30	4.42	4.30
$a_{N(3)}$	4.34	4.35	4.54	4.33	4.35	4.42	4.35	4.50	4.53
a_N	1.52	1.32	-	-	-	-	-	1.36	1.38
$a_{H/F}$	-	-	-	-	-	-	-	-	-
a_H	1.43	0.71	2.08	1.99	1.92	1.70	1.82	1.77	1.50
a_H	1.05	0.73	1.76	1,00	1.84	1.93	1.80	0.57	1.06
a_H	0.74	0.75	1.49	0.90	1.11	0.85	1.06	0.51	0.76
a_H	0.71	0.40	1.44	0.65	0.71	0.14	0.71	0.69	0.67
a_H	0.75	1.08	0.71	0.50	0.79	0.40	0.72	0.69	0.73
a_H	0.68	0.36	0.45	0.31	0.59	0.39	0.30	0.69	0.73
a_H	0.41	0.41	0.29	0.40	0.42	0.28	0.37	0.40	0.69
a_H	0.27	0.38	0.01	0.18	0.32	0.27	0.36	0.23	0.46
a_H	0.40	0.31	0.05	0.07	0.30	0.42	0.17	0.52	0.42
g	2.035	2.0039	2.0036	2.0040	2.0037	2.0035	2.0034	2.0036	2.0036

7. Computational details and results

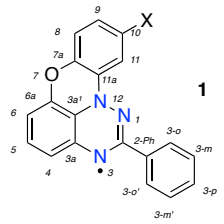
a) geometry optimization

Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs.[18] Geometry optimizations were undertaken at the UB3LYP/6-31G(2d,p) level of theory for radicals and at the B3LYP/6-31G(2d,p) level for closed-shell systems using tight convergence limits and appropriate symmetry constraints (C_1 or C_s). For derivatives containing COR, OR, NHCOR, 2-thienyl and OAc at least two orientations of the functional group relative to the heterocyclic ring were tested in an attempt at location of the global minimum. Vibrational frequencies were used to characterize the nature of the stationary points and to obtain thermodynamic parameters.

For all calculations involving Br and I atoms LANL2DZdp basis set and ECP were used (available from Basis Set Exchange v 1.2.2) requested with the *gen* keyword.

Selected bond lengths for radicals in series **1** are listed in Table S4.

Table S4. Selected interatomic distances for radicals in series **1**.[a]



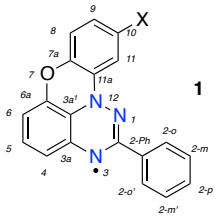
	N12–N1 /Å	N1–C2 /Å	C2–N3 /Å	N12-C3a' /Å	C6a–O7 /Å	O7–C7a /Å	C11a–N12 /Å
1a, X=H	1.3521	1.3429	1.3345	1.3883	1.3725	1.3748	1.4024
1b, X=COOMe	1.3518	1.3432	1.3349	1.3876	1.3758	1.3688	1.4034
1c, X=CN	1.35165	1.3443	1.3349	1.38785	1.3775	1.3669	1.4005
1d, X=NO_2	1.3513	1.3444	1.3353	1.38745	1.3787	1.3648	1.4005
1e, X=CF_3	1.3517	1.3438	1.3348	1.3882	1.37575	1.3699	1.4009
1f, X=OMe	1.3527	1.3429	1.3338	1.3896	1.3697	1.3781	1.4007
1g, X=F	1.3519	1.3435	1.3344	1.3890	1.3718	1.3759	1.3993
1h, X=Cl	1.3518	1.3436	1.3345	1.3888	1.3737	1.3730	1.4000
1i, X=Br	1.3516	1.3439	1.3349	1.3888	1.3731	1.3715	1.4002
1j, X=COMe	1.3522	1.3436	1.3346	1.3876	1.3758	1.3685	1.4032
1l, X=NH_2	1.3527	1.3426	1.3338	1.3894	1.3683	1.3793	1.4010
1m, X=NHAc	1.3527	1.3432	1.3338	1.3887	1.3704	1.3763	1.4009
1n, X=I	1.3515	1.3438	1.3349	1.3885	1.3736	1.3712	1.4005
1o, X=OH	1.3527	1.3432	1.3338	1.3894	1.3694	1.3784	1.3996
1p, X=OBn	1.3527	1.3430	1.3338	1.3897	1.3698	1.3778	1.4007
1q, X=Ph	1.3521	1.3429	1.3345	1.3884	1.3726	1.3736	1.4027
1r, X=Thioph	1.3520	1.3431	1.3344	1.3884	1.3729	1.3729	1.4026
1s, X=CCPh	1.3521	1.3430	1.33475	1.3881	1.3737	1.37165	1.4027
1t, X=OAc	1.3520	1.3433	1.3343	1.3887	1.3723	1.3749	1.4005
1u, X=$NHCOCF_3$	1.3525	1.3439	1.3339	1.3886	1.3725	1.3734	1.3997
1v, X=NHCOOMe	1.3525	1.3432	1.3338	1.3890	1.3703	1.3766	1.4006

[a] UB3LYP/6-31G(2d,p) level of theory in vacuum.

b) hfcc calculations

Isotropic Fermi contact coupling constants for radicals **1** were calculated using the UCAM-B3LYP/EPR-III // UB3LYP/6-31G(2d,p) method in benzene dielectric medium requested with the SCRF(Solvent=Benzene) keyword (PCM model[19]). For calculations involving heavier elements two different basis sets were requested with the *gen* keyword: EPR-III for light elements (H–F) and triple zeta for heaver elements. Thus, 6-311+G(2df) basis set for Cl and S atoms and LANL2DZdp basis set and ECP for Br and I atoms. The resulting *hfcc* values are shown in Table S5 and spin densities are listed in Table S6.

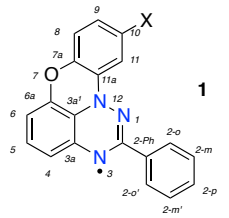
Table S5. Calculated hyperfine coupling constants (G) for radicals in series **1** in benzene.[a]



hfcc /G	**1a** [b] H	**1b** COOMe	**1c** CN	**1d** NO_2	**1e** CF_3	**1f** OMe	**1g** F	**1h** Cl	**1i** Br	**1j** COMe
$a_{N(12)}$	6.13	5.98	5.64	5.55	5.77	6.19	5.84	5.83	5.84	6.02
$a_{N(1)}$	3.95	4.08	4.26	4.31	4.18	3.85	4.07	4.10	4.10	4.07
$a_{N(3)}$	4.16	4.23	4.28	4.31	4.25	4.09	4.20	4.22	4.22	4.20
$a_{H(4)}$	-0.49	-0.59	-0.69	-0.73	-0.63	-0.39	-0.53	-0.56	-0.57	-0.56
$a_{H(5)}$	-0.92	-0.85	-0.73	-0.70	-0.78	-0.93	-0.83	-0.81	-0.81	-0.88
$a_{H(6)}$	-0.80	-0.95	-1.09	-1.15	-1.00	-0.68	-0.88	-0.92	-0.93	-0.92
$a_{H(8)}$	1.05	0.95	0.92	0.85	0.96	1.11	1.03	1.02	1.02	0.96
$a_{H(9)}$	-2.43	-2.17	-2.22	-2.05	-2.29	-2.85	-2.60	-2.52	-2.51	-2.19
$a_{H(10)}$	1.11	–	–	–	–	–	–	–	–	–
$a_{H(11)}$	-2.46	-2.60	-2.68	-2.74	-2.59	-2.05	-2.39	-2.52	-2.55	-2.53
$a_{H(2\text{-}o)\ avrg}$	0.52	0.54	0.57	0.58	0.56	0.50	0.54	0.55	0.55	0.54
$a_{H(2\text{-}m)avrg}$	-0.31	-0.32	-0.34	-0.34	-0.33	-0.31	-0.32	-0.32	-0.32	-0.32
$a_{H(2\text{-}p)}$	0.44	0.46	0.49	0.50	0.48	0.42	0.46	0.46	0.46	0.46
a_N	–	–	-0.12	0.21	–	–	–	–	-	–
a_F					-1.00 avg	-	-2.63	-	-	

[a] CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium.

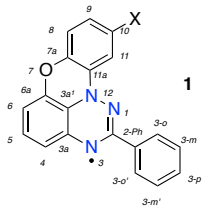
Table S5. Continues



hfcc /G	**1l** [b] NH_2	**1m** [b] NHAc	**1n** I	**1o** OH	**1p** OBn	**1q** Ph	**1r** Thioph	**1s** PhCC	**1t** OAc	**1u** NH $COCF_3$	**1v** NH CO_2Me
$a_{N(12)}$	6.16	6.09	5.86	6.07	6.17	6.12	6.06	6.00	6.00	5.86	606
$a_{N(1)}$	3.84	3.94	4.08	3.92	3.87	3.96	3.99	4.03	4.01	4.09	3.95
$a_{N(3)}$	4.10	4.14	4.22	4.12	4.09	4.17	4.18	4.20	4.18	4.19	4.14
$a_{H(4)}$	-0.39	-0.44	-0.56	-0.41	-0.39	-0.49	-0.51	-0.55	-0.50	-0.53	-0.44
$a_{H(5)}$	-0.95	-0.94	-0.83	-0.92	-0.93	-0.91	-0.89	-0.86	-0.88	-0.85	-0.92
$a_{H(6)}$	-0.67	-0.76	-0.92	-0.73	-0.69	-0.81	-0.84	-0.89	-0.83	-0.89	-0.77
$a_{H(8)}$	1.08	1.03	1.02	1.08	1.11	1.05	1.04	1.04	1.05	0.99	1.04
$a_{H(9)}$	-2.77	-2.60	-2.50	-2.76	-2.85	-2.45	-2.46	-2.44	-2.51	-2.50	-2.63
$a_{H(10)}$	–	–	–	–	-	–	–	–	–	–	–
$a_{H(11)}$	-2.15	-2.31	-2.56	-2.14	-2.05	-2.45	-2.51	-2.58	-2.40	-2.43	-2.30
$a_{H(2\text{-}o)\ avrg}$	0.50	0.52	0.55	0.52	0.51	0.52	0.52	0.53	0.50	0.55	0.52
$a_{H(2\text{-}m)avrg}$	-0.30	-0.31	-0.32	-0.30	-0.30	-0.31	-0.31	-0.31	-0.29	-0.32	-0.31
$a_{H(2\text{-}p)}$	0.42	0.44	0.46	0.43	0.42	0.44	0.44	0.45	0.45	0.46	0.44
a_N	-0.35	0.05	-	–	–	-	-	-	–	0.13	0.04
$a_{H(10\text{-}o)\ avrg}$			-			0.18	0.33	0.13		-	-
$a_{H(10\text{-}m)avrg}$			-			-0.09	-0.10	-0.07		-	-
$a_{H(10\text{-}p)}$			-			0.16	0.21	0.14		-	-

[a] CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium.

Table S6. DFT calculated spin densities for radicals in series **1**.[a]



Spin density	**1a** H	**1b** COOMe	**1c** CN	**1d** NO_2	**1e** CF_3	**1f** OMe	**1g** F	**1h** Cl	**1k** Br	**1j** Ac
$\rho_{N(12)}$	0.241	0.233	0.225	0.221	0.228	0.241	0.231	0.231	0.230	0.235
$\rho_{N(1)}$	0.280	0.290	0.298	0.302	0.295	0.273	0.286	0.287	0.288	0.288
$\rho_{C(2)}$	-0.056	-0.058	-0.065	-0.064	-0.064	-0.056	-0.060	-0.061	-0.058	-0.060
$\rho_{N(3)}$	0.280	0.285	0.289	0.291	0.286	0.275	0.283	0.284	0.284	0.283
$\rho_{C(3a)}$	0.014	0.014	0.012	0.008	0.013	0.017	0.012	0.012	0.010	0.016
$\rho_{C(4)}$	0.004	0.008	0.011	0.014	0.009	-0.001	0.006	0.008	0.009	0.006
$\rho_{C(5)}$	0.029	0.027	0.022	0.022	0.025	0.031	0.026	0.026	0.026	0.028
$\rho_{C(6)}$	0.020	0.026	0.032	0.034	0.029	0.016	0.023	0.025	0.025	0.025
$\rho_{C(6a)}$	0.027	0.022	0.017	0.015	0.018	0.028	0.022	0.022	0.020	0.023
$\rho_{C(3a')}$	0.073	0.071	0.077	0.076	0.076	0.078	0.080	0.078	0.075	0.073
$\rho_{O(7)}$	0.027	0.026	0.024	0.023	0.025	0.031	0.027	0.026	0.026	0.026
$\rho_{C(7a)}$	0.087	0.080	0.080	0.073	0.080	0.107	0.091	0.089	0.090	0.082
$\rho_{C(8)}$	-0.053	-0.045	-0.043	-0.041	-0.046	-0.054	-0.052	-0.050	-0.050	-0.047
$\rho_{C(9)}$	0.089	0.077	0.076	0.069	0.081	0.102	0.096	0.090	0.087	0.076
$\rho_{C(10)}$	-0.047	-0.038	-0.040	-0.035	-0.044	-0.045	-0.047	-0.046	-0.044	-0.036
$\rho_{C(11)}$	0.082	0.076	0.087	0.083	0.078	0.062	0.077	0.081	0.084	0.077
$\rho_{C(11a)}$	-0.065	-0.056	-0.062	-0.056	-0.060	-0.070	-0.068	-0.068	-0.067	-0.059
$\rho_{C(2\text{-}Ph)}$	0.006	0.007	0.008	0.008	0.007	0.006	0.007	0.008	0.007	0.006
$\rho_{C(2\text{-}o)\ avrg}$	-0.022	-0.023	-0.024	-0.024	-0.023	-0.021	-0.023	-0.023	-0.024	-0.023
$\rho_{C(2\text{-}m)\ avrg}$	0.011	0.013	0.013	0.013	0.012	0.011	0.012	0.012	0.013	0.012
$\rho_{C(2\text{-}p)}$	-0.018	-0.019	-0.020	-0.020	-0.019	-0.017	-0.018	-0.019	-0.019	-0.018
ρ_{X} [b]		0.001 (C)	-0.014 (N)	0.005 (N)	0.003 (CF_3)	-0.003 (O)	-0.001 (F)	-0.002 (Cl)	-	0.004 (C=O)

[a] CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium. Densities on the hydrogen atoms summed up to the adjacent carbon atoms. [b] Density of atom at the C(10) position.

Table S6. Continuation

Spin density	**1l** NH_2	**1m** NHAc	**1n** I	**1o** OH	**1p** OBn	**1q** Ph	**1r** Thioph	**1s** CCPh	**1t** OAc	**1u** NH $COCF_3$	**1v** NH CO_2Me
$\rho_{N(12)}$	0.240	0.237	0.232	0.238	0.240	0.237	0.236	0.236	0.234	0.230	0.236
$\rho_{N(1)}$	0.274	0.281	0.287	0.277	0.272	0.282	0.284	0.285	0.284	0.289	0.281
$\rho_{C(2)}$	-0.058	-0.058	-0.058	-0.056	-0.061	-0.060	-0.061	-0.058	-0.060	-0.060	-0.057
$\rho_{N(3)}$	0.276	0.278	0.284	0.277	0.276	0.280	0.281	0.283	0.281	0.283	0.278
$\rho_{C(3a)}$	0.017	0.018	0.011	0.014	0.018	0.017	0.017	0.014	0.016	0.015	0.016
$\rho_{C(4)}$	0.001	0.000	0.008	0.002	0.001	0.002	0.003	0.004	0.004	0.002	0.002
$\rho_{C(5)}$	0.033	0.031	0.027	0.031	0.032	0.030	0.029	0.028	0.028	0.027	0.032
$\rho_{C(6)}$	0.015	0.019	0.025	0.018	0.016	0.021	0.022	0.025	0.022	0.024	0.019
$\rho_{C(6a)}$	0.027	0.023	0.021	0.026	0.026	0.025	0.024	0.024	0.023	0.020	0.023
$\rho_{C(3a')}$	0.077	0.074	0.077	0.080	0.076	0.072	0.073	0.074	0.076	0.076	0.077
$\rho_{O(7)}$	0.029	0.028	0.026	0.029	0.031	0.027	0.027	0.027	0.027	0.026	0.028
$\rho_{C(7a)}$	0.101	0.094	0.088	0.101	0.105	0.087	0.088	0.089	0.091	0.088	0.092
$\rho_{C(8)}$	-0.056	-0.049	-0.050	-0.056	-0.054	-0.049	-0.049	-0.049	-0.049	-0.047	-0.049
$\rho_{C(9)}$	0.105	0.090	0.086	0.098	0.104	0.091	0.090	0.086	0.091	0.085	0.090
$\rho_{C(10)}$	-0.045	-0.036	-0.045	-0.044	-0.046	-0.043	-0.041	-0.041	-0.045	-0.035	-0.039
$\rho_{C(11)}$	0.067	0.070	0.085	0.071	0.057	0.071	0.074	0.081	0.074	0.074	0.070
$\rho_{C(11a)}$	-0.067	-0.063	-0.068	-0.071	-0.065	-0.058	-0.058	-0.064	-0.063	-0.061	-0.065
$\rho_{C(2\text{-}Ph)}$	0.006	0.007	0.007	0.007	0.005	0.006	0.006	0.006	0.007	0.007	0.006
$\rho_{C(2\text{-}o)\ avrg}$	-0.022	-0.022	-0.023	-0.023	-0.020	-0.022	-0.022	-0.022	-0.022	-0.022	-0.022
$\rho_{C(2\text{-}m)\ avrg}$	0.011	0.012	0.012	0.012	0.012	0.019	0.012	0.011	0.011	0.011	0.011
$\rho_{C(2\text{-}p)}$	-0.017	-0.018	-0.018	-0.017	-0.017	-0.018	-0.018	-0.018	-0.018	-0.018	-0.017
ρ_x [b]	-0.005 (N)	0.0002 (N)	-	-0.004 (O)	-0.001 (O)	0.008 (C)	0.012 (C)	0.014 (C)	0.001 (O)	0.005 (N)	0.001 (N)

[a] CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium. Densities on the hydrogen atoms summed up to the adjacent carbon atoms. [b] Density of the atom at the C(10) position.

c) spin delocalization

Spin delocalization parameter RDV (Radical Delocalization Value) was calculated according to the formula Eq S1:[20]

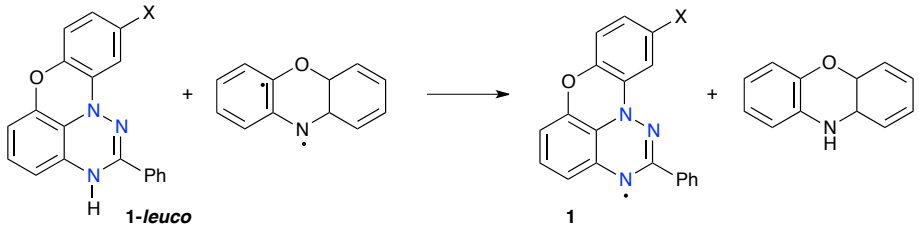
$$RDV = \sum_{i=1}^{n} (\rho_i)^2 \qquad \text{eq S1}$$

where spin concentration ρ_i on each heavy atoms *i* (hydrogen atoms summed up to heavy atoms) is obtained with the CAM-B3LYP/EPR-III // UB3LYP/6-31G(2d,p) method in benzene dielectric medium using the PCM model[19] [keywords: SCRF(Solvent=benzene)].

For the purpose of this work, the inverse is reported: $RDV^{-1} = 1/RDV$, since now the larger value corresponds to the greater delocalization. A graphical correlation of the calculated RDV^{-1} values with the σ_m substituent parameters is shown in Figure S40.

d) N–H bond dissociation energy and resonance stabilization

The N–H bond dissociation enthalpy (BDE) in the *leuco* form (**1-*leuco***) of the radicals was calculated at the (U)B3LYP/6-311++G(2d,p) // (U)B3LYP/6-31G(2d,p) level of theory in benzene dielectric medium (requested with the SCRF(Solvent=benzene) keyword; PCM model[19]) as a change of enthalpy ΔH in an isodesmic reaction with the structurally similar phenoxazin-10-yl radical (Scheme S1) and referenced to the experimental C–H *BDE* of phenoxazine in benzene (77.2±0.3 kcal mol^{-1}).[21] The thermodynamic parameters for radicals **1**, *leuco* forms **1-*leuco***, phenoxazin-10-yl and phenoxazine in benzene were obtained at the (U)B3LYP/6-31G(2d,p) level of theory in vacuum, as described above. Results are shown in Table S7.



Scheme S1. Isodesmic reaction to calculate the N–H BDE in **1-*leuco***.

Resonance stabilization energy (RSE, Table S7) was obtained by comparing BDE in **1-*leuco*** to that in CH_3–H (104.9 kcal mol^{-1})[22] in vacuum according to formula Eq S2.

$$RSE = BDE_{CH4} - BDE_{\mathbf{1}\text{-}leuco} \qquad \text{eq S2}$$

e) oxidation potentials for radicals 1

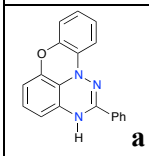
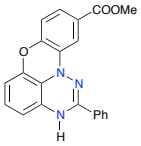
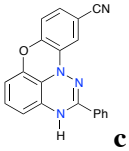
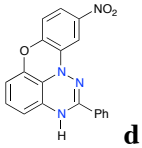
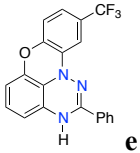
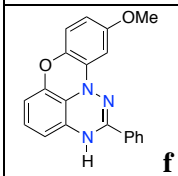
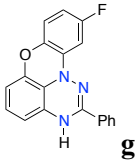
The oxidation potential $E_{1/2}^{0/+1}$ for radicals **1** was calculated at the (U)B3LYP/6-31++G(2d,p) // (U)B3LYP/6-31G(2d,p) level of theory in CH_2Cl_2 dielectric medium (single point calculations) using the following process and equation S3:

$$\mathbf{1} \rightarrow \mathbf{1}^+ \qquad E_{1/2}^{0/+1} = \Delta G_{298}/23.016 - (4.44V + 0.71V) \qquad \text{eq S3}$$

where ΔG_{298} is the free energy change in kcal mol^{-1}, 23.016 is conversion of kcal mol^{-1} to eV, 4.44±0.02 V is the absolute potential of standard H^+/H electrode, (SHE),[23] and 0.71 V is the relative standard potential of the Fc/Fc^+ electrode (*vs* SHE).

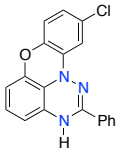
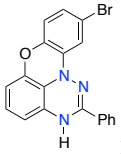
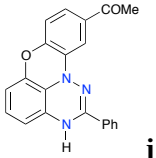
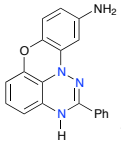
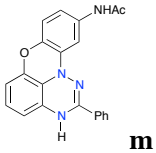
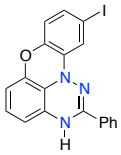
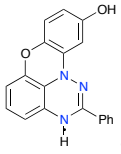
Thermodynamic corrections were obtained at the (U)B3LYP/6-31G(2d,p) level of theory in vacuum. The results are shown in Table S7.

Table S7. Bond dissociation enthalpy (BDE) for **1-*leuco***, resonance stabilization energy (*RSE*) and radical delocalization value (RDV) in radicals **1**, and oxidation potential $E_{1/2}^{0/+1}$ for **1** *vs* SCE.

1-*leuco*	*BDE* in ***1-leuco*** [a] /kcal mol^{-1}	*RSE* in **1** [a] /kcal mol^{-1}	RDV^{-1} in **1** [b] /1	$E_{1/2}^{0/+1}$ in **1** [c] /V
 **a**	68.521	36.38	3.8579	-0.331
 **b**	69.262	35.64	3.8915	-0.244
 **c**	70.561	34.34	3.7796	-0.143
 **d**	70.865	34.04	3.8123	-0.088
 **e**	70.051	34.85	3.8216	-0.192
 **f**	68.114	36.79	3.8795	-0.377
 **g**	69.352	35.55	3.8038	-0.245

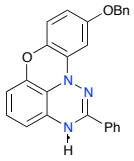
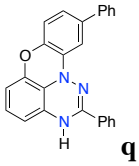
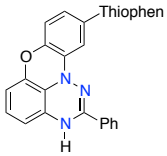
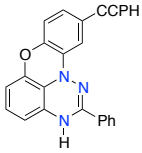
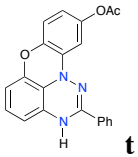
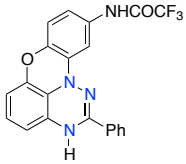
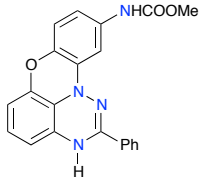
[a] Obtained at the (U)B3LYP/6-31G(2d,p) level of theory in vacuum. [b] Obtained at CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium. [c] Obtained at (U)B3LYP/6-31++G(2d,p) // (U)B3LYP/6-31G(2d,p) level of theory in CH_2Cl_2 dielectric medium using eq S3.

Table S7. Continues.

1-*leuco*	*BDE* in ***1-leuco*** [a] /kcal mol^{-1}	*RSE* in **1** [a] /kcal mol^{-1}	RDV^{-1} in **1** [b] /1	$E_{1/2}^{0/+1}$ in **1** [c] /V
 **h**	69.545	35.36	3.8051	-0.234
 **i**	69.502	35.40	3.8221	-0.246
 **j**	69.389	35.51	3.8906	-0.235
 **l**	67.913	36.99	3.8763	-0.447
 **m**	68.742	36.16	3.9221	-0.309
 **n**	69.494	35.41	3.8180	-0.253
 **o**	68.343	36.47	3.8590	–

[a] Obtained at the (U)B3LYP/6-31G(2d,p) level of theory in vacuum. [b] Obtained at CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium. [c] Obtained at (U)B3LYP/6-31++G(2d,p) // (U)B3LYP/6-31G(2d,p) level of theory in CH_2Cl_2 dielectric medium using eq S3.

Table S7. Continues.

1-*leuco*	*BDE* in ***1-leuco*** [a] /kcal mol^{-1}	*RSE* in **1** [a] /kcal mol^{-1}	RDV^{-1} in **1** [b] /1	$E_{1/2}^{0/+1}$ in **1** [c] /V
 **p**	68.156	36.74	3.9025	-0.418
 **q**	68.541	36.36	3.8948	-0.343
 **r**	68.686	36.21	3.8758	-0.331
 **s**	69.042	35.86	3.8346	-0.321
 **t**	69.412	35.49	3.8626	–
 **u**	69.696	35.20	3.8809	-0.193
 **v**	68.619	36.28	3.9102	-0.324

[a] Obtained at the (U)B3LYP/6-31G(2d,p) level of theory in vacuum. [b] Obtained at CAM-B3LYP/EPR-III // B3LYP/6-31G(2d,p) in benzene dielectric medium. [c] Obtained at (U)B3LYP/6-31++G(2d,p) // (U)B3LYP/6-31G(2d,p) level of theory in CH_2Cl_2 dielectric medium using eq S3.

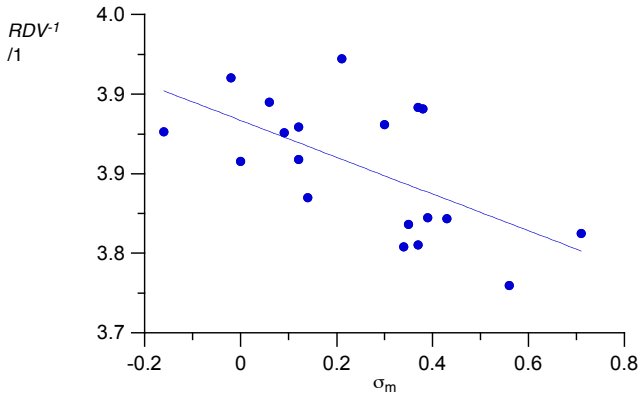


Figure S40. Inverse of Radical Delocalization Value $(RDV)^{-1}$ for series **1** *vs* Hammett substituent σ_m parameter. For data see Table S7.

f) electronic excitations

Electronic excitation energies in CH_2Cl_2 dielectric medium were obtained for selected derivatives **1** at the UCAM-B3LYP/6-31++G(2d,p) // UB3LYP/6-31G(2d,p) level of theory using the time-dependent TD-DFT method[24] supplied in the Gaussian 09 package. Solvation models in calculations were implemented with the PCM model[19] using the SCRF(solvent=CH2CL2) keyword. Three lowest excitation energies, classified as $\pi \rightarrow \pi^*$ transitions, and also energy of the $n \rightarrow \pi^*$ transition are listed in Table S8. Energies of MOs involved in low energy transitions are listed in Table S9 and their correlations with the σ_m substituent parameters are shown in Figures S41 and S42.

Table S8. Calculated electronic transition energies and oscillator strength values with the indicated main electronic transition.[a]

radical	π→π* β-HOMO→ β-LUMO /nm (*f*)	π →π* α-HOMO→ α-LUMO /nm (*f*)	π →π* α-HOMO→ α-LUMO+1 /nm (*f*)	n→π* β-HOMO–5→ β-LUMO /nm (*f*)
Blatter	445.0 (0.040)	515.9 (0.005)	381.0 (0.010)	387.7 (0.002)
1a, H	541.2 (0.044)	517.3 (0.032)	411.8 (0.017)	371.7 (0.001)
1b, CO_2Me	537.8 (0.035)	517.4 (0.038) [b]	442.1 (0.012)	376.5 (0.001)
1c, CN	538.2 (0.043)	514.5 (0.024)	446.1 (0.017)	381.8 (0.001)
1d, NO_2	534.1 (0.060)	563.6 (0.002)	481.0 (0.017)	383.8 (0.001)
1e, CF_3	538.5 (0.044)	510.2 (0.024)	422.3 (0.021)	378.9 (0.001)
1f, OMe	563.9 (0.073)	519.7 (0.012)	418.0 (0.019)	369.4 (0.001)
1g, F	550.0 (0.057)	510.9 (0.016)	412.9 (0.024)	376.2 (0.001)
1h, Cl	545.7 (0.056)	511.8 (0.018)	419.1 (0.022)	377.2 (0.001)
1i, Br	546.1 (0.056)	512.7 (0.019)	420.5 (0.022)	377.4 (0.001)
1j, COMe	538.9 (0.032)	521.7 (0.040) [b]	455.5 (0.013)	375.5 (0.001)
1l, NH_2	576.4 (0.080)	521.8 (0.10)	417.5 (0.014)	369.3 (0.001)
1m, NHAc	557.2 (0.073)	517.4 (0.016)	416.0 (0.013)	372.5 (0.001)
1n, I	545.3 (0.056)	513.8 (0.021)	421.0 (0.022)	377.1 (0.001)
1o, OH	563.4 (0.071)	516.9 (0.013)	413.8 (0.018)	371.5 (0.001)
1p, OBn	563.4 (0.075)	519.2 (0.012)	418.3 (0.021)	369.8 (0.001) [c]
1q, Ph	545.8 (0.063)	519.7 (0.025)	431.3 (0.016)	372.8 (0.001)
1r, Thioph	548.7 (0.070)	521.8 (0.017)	473.2 (0.009) [d]	373.8 (0.001)
1s CCPh	546.0 (0.076)	525.2 (0.015)	486.7 (0.014) [d]	375.2 (0.001)
1t, OAc	546.5 (0.058)	514.2 (0.020)	415.0 (0.020)	374.3 (0.001)
1u, $NHCOCF_3$	551.0 (0.067)	513.4 (0.015)	425.44 (0.013)	376.4 (0.001)
1v, NHCOOMe	558.3 (0.074)	516.8 (0.015)	414.9 (0.014)	372.7 (0.001)

[a] Obtained with the TD CAM-B3LYP/6-31++G(2d,p)//UB3LYP/6-31G(2d,p) method in CH_2Cl_2 dielectric medium. [b] Comparable contribution from β-HOMO→ β-LUMO transition. [c] Main contribution from β-HOMO–7→ β-LUMO transition. [d] Several weak transitions.

Table S9. Energies of MOs involved in low energy transitions.[a]

radical	α-HOMO, π /eV	α-LUMO, π* /eV	α-LUMO+1, π* /eV	β-HOMO–5, n /eV	β-HOMO, π* /eV	β-LUMO, π* /eV
Blatter	-6.243	-0.468	0.201	-9.026	-7.648	-1.694
1a, H	-6.209	-0.607	0.111	-9.076	-7.211	-1.834
1b, CO_2Me	-6.315	-0.779	-0.531	-9.147	-7.337	-1.927
1c, CN	-6.415	-0.850	-0.597	-9.263	-7.420	-2.031
1d, NO_2	-6.446	-1.801	-0.715	-9.362	-7.471	-2.077
1e, CF_3	-6.359	-0.702	-0.228	-9.238	-7.375	-1.974
1f, OMe	-6.176	-0.595	0.221	-9.073	-7.000	-1.838
1g, F	-6.298	-0.652	0.042	-9.137	-7.234	-1.937
1h, Cl	-6.316	-0.671	-0.057	-9.147	-7.267	-1.948
1i, Br	-6.317	-0.675	-0.076	-9.145	-7.266	-1.949
1j, COMe	-6.317	-0.912	-0.603	-9.119	-7.335	-1932
1l, NH_2	-6.130	-0.571	0.239	-9.041	-6.821	-1.806
1m, NHAc	-6.227	-0.630	0.069	-9.102	-7.050	-1.878
1n, I	-6.304	-0.671	-0.079	-9.043	-7.246	-1.938
1o, OH	-6.211	-0.613	0.157	-9.091	-7.042	-1.870
1p, OBn	-6.184	-0.601	0.127	-8.606	-7.015	-1.847
1q, Ph	-6.215	-0.630	-0.216	-8.820	-7.115	-1.854
1r, Thioph	-6.231	-0.666	-0.402	-8.872	-7.032	-1.877
1s, CCPh	-6.257	-0.794	-0.567	-8.921	-7.049	-1.899
1t, OAc	-6.266	-0.639	0.018	-9.118	-7.216	-1.898
1u, $NHCOCF_3$	-6.266	-0.696	-0.346	-9.158	-7.206	-1.956
1v, $NHCO_2Me$	-6.227	-0.626	0.102	-9.103	-7.045	-1.879

[a] Obtained with the TD CAM-B3LYP/6-31++G(2d,p)// UB3LYP/6-31G(2d,p) method in CH_2Cl_2 dielectric medium.

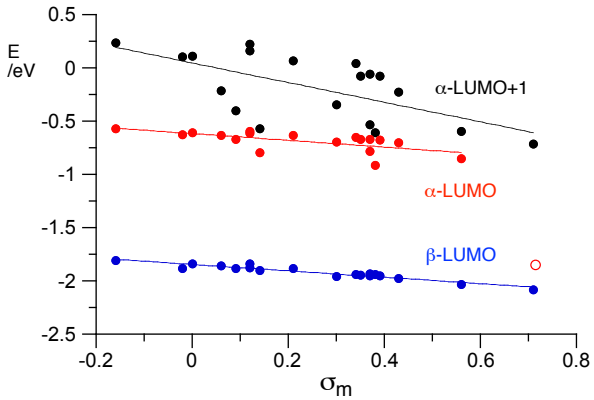


Figure S41. Correlation of TD-DFT calculated energies of the lowest unoccupied MOs for radicals **1**. Best fitting lines: $E_{\beta\text{-LUMO}} = -1.841(8) - 0.30(2) \times\sigma_m$, $r^2 = 0.907$ (blue); $E_{\alpha\text{-LUMO}} = -0.614(27) - 0.32(9)\times\sigma_m$, $r^2 = 0.43$ (red, data for NO_2 shown as an open circle is omitted); $E_{\alpha\text{-LUMO+1}} = -0.05(9) - 0.92(27)\times\sigma_m$, $r^2 = 0.40$ (black).

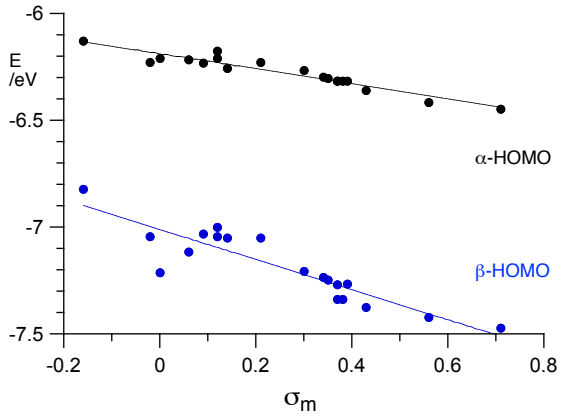


Figure S42. Correlation of TD-DFT calculated energies of the highest occupied MOs for radicals **1**. Best fitting lines: $E_{\beta\text{-HOMO}} = -7.009(27) - 0.70(8) \times\sigma_m$, $r^2 = 0.814$ (blue); $E_{\alpha\text{-HOMO}} = -6.187(9) - 0.352(27)\times\sigma_m$ $r^2 = 0.912$ (black).

g) partial output data for TD-DFT calculations

```
CAM-B3LYP/6-31++G(2d,p) TD(NStates=20) SCF=tight Geom(NoAngle, noDistance,
check)
#P guess=check SCRF(Solvent=CH2Cl2)

1a (X=H)
Excited State   1:  2.293-A'     2.2907 eV  541.24 nm  f=0.0437
<S**2>=1.064
     77A -> 79A       -0.15220
     77A -> 80A        0.10520
     78A -> 79A        0.43813
     77B -> 78B        0.80918
     77B -> 79B        0.10044
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -970.177418364
```

```
Excited State   2:  2.087-A'     2.3968 eV  517.29 nm  f=0.0316
<S**2>=0.839
     78A -> 79A        0.78218
     78A -> 80A        0.18315
     78A -> 88A        0.17780
     76B -> 78B        0.13152
     77B -> 78B       -0.46833

 Excited State   3:  2.690-A'     3.0111 eV  411.76 nm  f=0.0171
<S**2>=1.560
     73A -> 92A        0.16265
     74A -> 82A        0.17206
     76A -> 79A       -0.10891
     77A -> 80A        0.23405
     78A -> 79A       -0.20845
     78A -> 80A        0.74206
     73B -> 78B        0.19866
     73B -> 95B        0.10485
     74B -> 78B       -0.13790
     74B -> 84B        0.12343
     76B -> 79B        0.12583
     77B -> 80B       -0.25241

 Excited State   4:  3.361-A'     3.2326 eV  383.54 nm  f=0.0086
<S**2>=2.575
     75A -> 85A        0.28227
     76A -> 79A       -0.36730
     76A -> 88A        0.18967
     77A -> 79A       -0.33056
     78A -> 80A       -0.13435
     78A -> 88A        0.10495
     71B -> 89B       -0.11300
     75B -> 84B       -0.16462
     75B -> 85B       -0.22363
     76B -> 78B        0.19985
     76B -> 79B        0.36660
     76B -> 89B       -0.20091
     77B -> 78B       -0.15100
     77B -> 79B        0.38609

 Excited State   5:  2.096-A"     3.3352 eV  371.74 nm  f=0.0014
<S**2>=0.848
     72B -> 78B        0.96233
     72B -> 95B       -0.13389
```

1b (X=COOMe)

```
Excited State   1:  2.298-A'     2.3055 eV  537.77 nm  f=0.0346
<S**2>=1.070
     92A -> 95A       -0.16872
     93A -> 94A       -0.46926
     93A -> 95A        0.26414
     93A -> 96A        0.10604
     92B -> 93B        0.73414
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1197.99406228
```

```
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.144-A'     2.3964 eV  517.38 nm  f=0.0377
<S**2>=0.899
     93A -> 94A        0.69067
     93A -> 95A       -0.20700
     93A -> 96A       -0.16530
     93A ->103A       -0.16141
     91B -> 93B       -0.14570
     92B -> 93B        0.55989

 Excited State   3:  2.663-A'     2.8046 eV  442.07 nm  f=0.0123
<S**2>=1.523
     88A -> 94A       -0.12688
     89A -> 96A        0.13248
     91A -> 94A       -0.13440
     92A -> 94A        0.21690
     92A -> 95A        0.16807
     93A -> 94A        0.18879
     93A -> 95A        0.74999
     93A -> 96A       -0.17383
     87B -> 93B       -0.12780
     87B -> 95B        0.13037
     89B -> 97B       -0.11325
     91B -> 94B        0.12592
     92B -> 94B       -0.15755
     92B -> 95B       -0.18168

 Excited State   4:  3.353-A'     3.2223 eV  384.77 nm  f=0.0039
<S**2>=2.560
     90A ->100A       -0.27317
     90A ->105A        0.10843
     91A -> 94A       -0.24581
     91A -> 95A        0.26984
     91A ->103A       -0.21685
     92A -> 94A       -0.27290
     92A -> 95A        0.22912
     93A -> 94A       -0.10747
     93A -> 96A       -0.14161
     86B ->104B        0.11651
     90B ->100B       -0.28187
     91B -> 93B       -0.15493
     91B -> 94B        0.28428
     91B -> 95B       -0.23782
     91B ->104B        0.20729
     92B -> 93B        0.16770
     92B -> 94B        0.32908
     92B -> 95B       -0.22257

 Excited State   5:  2.094-A"     3.2935 eV  376.45 nm  f=0.0014
<S**2>=0.847
     88B -> 93B        0.96081
     88B ->107B        0.14261
```

1c (X=CN)

```
Excited State   1:  2.303-A'     2.3036 eV  538.21 nm  f=0.0431
<S**2>=1.076
     83A -> 86A        0.16703
     84A -> 85A       -0.36688
     84A -> 86A       -0.22716
     80B -> 84B        0.10880
     83B -> 84B        0.80432
     83B -> 86B       -0.10394
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1062.38566981

 Excited State   2:  2.173-A'     2.4098 eV  514.50 nm  f=0.0235
<S**2>=0.930
     83A -> 86A       -0.10153
     84A -> 85A        0.75546
     84A -> 86A        0.20519
     84A -> 87A       -0.19032
     84A -> 92A       -0.16260
     82B -> 84B       -0.15659
     83B -> 84B        0.44287

 Excited State   3:  2.671-A'     2.7795 eV  446.07 nm  f=0.0166
<S**2>=1.533
     78A -> 95A       -0.10508
     80A -> 85A       -0.10225
     80A -> 87A       -0.12611
     82A -> 85A        0.13615
     83A -> 85A       -0.22739
     83A -> 86A        0.15888
     84A -> 85A       -0.15160
     84A -> 86A        0.76040
     84A -> 87A        0.12303
     78B -> 84B        0.13658
     78B -> 86B        0.11049
     80B -> 87B        0.12068
     82B -> 85B       -0.13062
     83B -> 84B        0.10370
     83B -> 85B        0.16027
     83B -> 86B       -0.18368

 Excited State   4:  3.339-A'     3.2149 eV  385.65 nm  f=0.0029
<S**2>=2.538
     81A -> 91A       -0.25951
     81A -> 95A        0.11228
     82A -> 85A       -0.21469
     82A -> 86A       -0.25551
     82A -> 92A       -0.21779
     83A -> 85A       -0.27331
     83A -> 86A       -0.24475
     84A -> 85A       -0.11269
     84A -> 87A       -0.18415
     84A -> 92A       -0.10143
     77B -> 95B        0.11419
     81B -> 91B       -0.27689
     82B -> 84B       -0.14612
     82B -> 85B        0.26754
```

```
     82B -> 86B        0.23605
     82B -> 95B        0.20641
     83B -> 84B        0.16913
     83B -> 85B        0.33033
     83B -> 86B        0.23017

 Excited State   5:  2.095-A"     3.2477 eV  381.76 nm  f=0.0014
<S**2>=0.847
     79B -> 84B        0.95994
     79B -> 96B        0.14870
```

1d (X=NO_2)

```
Excited State   1:  2.374-A'     2.2001 eV  563.55 nm  f=0.0023
<S**2>=1.159
     83A -> 90A       -0.13524
     88A -> 90A        0.17488
     89A -> 90A        0.80011
     89A -> 91A       -0.36715
     89A -> 92A       -0.19590
     89A -> 94A       -0.13412
     88B -> 90B       -0.12815
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1174.64073138
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.301-A'     2.3212 eV  534.14 nm  f=0.0602
<S**2>=1.074
     88A -> 91A       -0.13566
     89A -> 90A        0.15794
     89A -> 91A        0.22745
     85B -> 89B        0.10112
     88B -> 89B        0.85155
     88B -> 90B       -0.21441
     88B -> 91B        0.11015

 Excited State   3:  2.230-A'     2.5774 eV  481.04 nm  f=0.0171
<S**2>=0.994
     83A -> 90A       -0.10597
     88A -> 90A        0.13764
     89A -> 90A        0.29466
     89A -> 91A        0.78688
     89A -> 98A        0.16106
     87B -> 89B        0.17138
     88B -> 89B       -0.29929

 Excited State   4:  3.452-A'     2.8752 eV  431.21 nm  f=0.0013
<S**2>=2.729
     80A -> 90A        0.65388
     80A -> 94A        0.17075
     80A ->104A       -0.13269
     84A -> 90A        0.15333
     89A -> 92A       -0.12073
     79B -> 89B       -0.19517
     79B -> 90B       -0.61443
     79B -> 92B       -0.10849
     79B -> 95B       -0.14096
```

```
     79B -> 97B        0.10111
     79B ->106B        0.10590
     85B -> 90B        0.12073
     80A <- 90A        0.16805
     79B <- 90B       -0.16290

 Excited State   5:  2.916-A'     3.0841 eV  402.01 nm  f=0.0276
<S**2>=1.875
     80A -> 90A        0.16199
     83A ->104A        0.10091
     84A -> 90A       -0.20852
     84A -> 92A       -0.13144
     84A -> 94A        0.12062
     86A -> 90A       -0.11482
     88A -> 90A       -0.17576
     88A -> 91A       -0.11794
     88A -> 92A        0.13988
     89A -> 90A        0.36293
     89A -> 92A        0.47643
     79B -> 90B       -0.14512
     82B -> 90B       -0.15630
     83B -> 89B        0.11210
     83B -> 90B       -0.13029
     85B -> 89B       -0.22348
     85B -> 92B       -0.13280
     85B -> 95B        0.11416
     87B -> 90B       -0.14023
     88B -> 90B        0.31023
     88B -> 92B       -0.16977

 Excited State   6:  3.331-A'     3.2101 eV  386.23 nm  f=0.0009
<S**2>=2.523
     86A -> 91A        0.23341
     86A -> 97A        0.24203
     87A -> 91A        0.23549
     87A -> 97A       -0.10764
     87A -> 98A       -0.21226
     88A -> 90A        0.13956
     88A -> 91A       -0.32806
     89A -> 91A       -0.10501
     89A -> 92A        0.18230
     86B -> 95B        0.14493
     86B -> 97B        0.22812
     87B -> 89B        0.13311
     87B -> 91B        0.33908
     87B ->100B       -0.18951
     88B -> 89B       -0.19529
     88B -> 90B       -0.23069
     88B -> 91B        0.35904

 Excited State   7:  2.094-A"     3.2309 eV  383.75 nm  f=0.0014
<S**2>=0.846
     84B -> 89B        0.93980
     84B -> 90B       -0.19636
     84B ->106B        0.12397
```

1e (X=CF_3)

```
Excited State   1:  2.301-A      2.3023 eV  538.52 nm  f=0.0435
<S**2>=1.073
     93A -> 95A        0.13852
     93A -> 96A       -0.11920
     94A -> 95A       -0.40869
     93B -> 94B        0.82269
     93B -> 95B       -0.10625
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1307.17331534

 Excited State   2:  2.103-A      2.4301 eV  510.20 nm  f=0.0237
<S**2>=0.856
     94A -> 95A        0.79822
     94A -> 96A        0.14928
     94A -> 97A        0.12899
     94A ->103A        0.17137
     92B -> 94B       -0.16478
     93B -> 94B        0.42938

 Excited State   3:  2.658-A      2.9361 eV  422.28 nm  f=0.0213
<S**2>=1.516
     88A ->106A        0.14181
     90A -> 97A       -0.17479
     92A -> 96A       -0.10021
     93A -> 96A        0.25381
     94A -> 95A       -0.18829
     94A -> 96A        0.76147
     94A -> 97A        0.14439
     88B -> 94B       -0.15832
     90B -> 94B        0.10790
     90B -> 97B       -0.13090
     92B -> 95B        0.10631
     93B -> 96B       -0.23991

 Excited State   4:  3.375-A      3.2272 eV  384.19 nm  f=0.0055
<S**2>=2.597
     91A -> 95A        0.11686
     91A ->101A        0.28281
     92A -> 95A       -0.32971
     92A -> 96A        0.10141
     92A ->103A        0.22441
     93A -> 95A       -0.35712
     94A ->103A        0.10337
     87B ->104B        0.10534
     91B ->101B        0.28914
     92B -> 94B       -0.17385
     92B -> 95B        0.35441
     92B ->104B       -0.21302
     93B -> 94B        0.15540
     93B -> 95B        0.39962

 Excited State   5:  2.095-A      3.2722 eV  378.91 nm  f=0.0014
<S**2>=0.847
     89B -> 94B        0.96052
     89B ->108B       -0.14555
```

1f (X=OMe)

```
Excited State   1:  2.233-A'     2.1987 eV  563.89 nm  f=0.0731
<S**2>=0.996
     86A -> 87A        0.15113
     83B -> 86B        0.14628
     85B -> 86B        0.92169
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1084.66955492
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.123-A'     2.3856 eV  519.71 nm  f=0.0121
<S**2>=0.877
     85A -> 87A       -0.19955
     86A -> 87A        0.86368
     86A -> 88A        0.22041
     86A -> 96A        0.17776
     84B -> 86B        0.10139
     85B -> 86B       -0.17760

 Excited State   3:  2.744-A'     2.9664 eV  417.96 nm  f=0.0193
<S**2>=1.632
     81A -> 92A       -0.12116
     84A -> 87A       -0.12281
     85A -> 88A        0.22582
     86A -> 87A       -0.25101
     86A -> 88A        0.69721
     81B -> 86B       -0.21668
     83B -> 86B        0.14070
     84B -> 86B        0.13204
     84B -> 87B        0.11672
     85B -> 87B        0.10875
     85B -> 88B       -0.28711

 Excited State   4:  3.278-A'     3.2087 eV  386.40 nm  f=0.0151
<S**2>=2.437
     82A -> 87A       -0.17355
     82A -> 96A        0.10387
     83A -> 92A       -0.12558
     83A -> 93A       -0.20988
     83A -> 96A       -0.10125
     84A -> 87A       -0.31931
     84A -> 93A       -0.11514
     84A -> 96A        0.11316
     85A -> 87A       -0.28636
     86A -> 88A       -0.24246
     79B -> 97B       -0.10234
     82B -> 92B        0.24233
     83B -> 87B       -0.16339
     83B -> 97B        0.12723
     84B -> 86B        0.25883
     84B -> 87B        0.32761
     84B -> 94B       -0.14035
     84B -> 97B       -0.12101
     85B -> 86B       -0.16658
     85B -> 87B        0.37811
```

```
 Excited State   5:  2.099-A"     3.3565 eV  369.38 nm  f=0.0013
<S**2>=0.852
     80B -> 86B        0.96178
```

1g (X=F)

```
Excited State   1:  2.271-A'     2.2541 eV  550.04 nm  f=0.0573
<S**2>=1.039
     81A -> 83A       -0.12718
     82A -> 83A        0.24177
     78B -> 82B       -0.13132
     81B -> 82B        0.89845
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1069.40437026

 Excited State   2:  2.101-A'     2.4269 eV  510.87 nm  f=0.0159
<S**2>=0.853
     81A -> 83A       -0.13445
     82A -> 83A        0.85201
     82A -> 84A        0.22407
     82A -> 92A        0.17906
     80B -> 82B        0.14151
     81B -> 82B       -0.26713

 Excited State   3:  2.709-A'     3.0029 eV  412.88 nm  f=0.0235
<S**2>=1.584
     77A -> 96A       -0.14470
     78A -> 86A        0.11538
     80A -> 83A       -0.11164
     81A -> 84A        0.21847
     81A -> 86A        0.10678
     82A -> 83A       -0.24247
     82A -> 84A        0.72582
     77B -> 82B       -0.25321
     78B -> 87B       -0.11814
     80B -> 83B        0.12328
     81B -> 84B       -0.25088

 Excited State   4:  3.354-A'     3.2237 eV  384.60 nm  f=0.0096
<S**2>=2.562
     79A -> 89A        0.27791
     80A -> 83A       -0.36300
     80A -> 86A        0.11382
     80A -> 92A        0.18945
     81A -> 83A       -0.32707
     82A -> 84A       -0.15254
     75B -> 92B       -0.11183
     79B -> 87B        0.11706
     79B -> 89B        0.25582
     80B -> 82B        0.20458
     80B -> 83B        0.36484
     80B -> 92B       -0.20015
     81B -> 82B       -0.15030
     81B -> 83B        0.38536

 Excited State   5:  2.096-A"     3.2954 eV  376.24 nm  f=0.0014
<S**2>=0.849
     76B -> 82B        0.96054
```

```
     76B -> 98B        0.12121
```

1h (X=Cl)

```
Excited State   1:  2.282-A'     2.2720 eV  545.70 nm  f=0.0557
<S**2>=1.052
     85A -> 87A       -0.13342
     86A -> 87A        0.28585
     82B -> 86B        0.14536
     85B -> 86B        0.87820
     85B -> 87B        0.10190
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1429.77511300

 Excited State   2:  2.103-A'     2.4228 eV  511.75 nm  f=0.0179
<S**2>=0.855
     85A -> 87A       -0.11649
     86A -> 87A        0.84046
     86A -> 88A        0.20666
     86A -> 95A        0.17892
     84B -> 86B        0.13696
     85B -> 86B       -0.31086

 Excited State   3:  2.723-A'     2.9585 eV  419.08 nm  f=0.0224
<S**2>=1.604
     81A -> 89A       -0.10724
     81A -> 99A       -0.14033
     82A -> 89A       -0.13526
     84A -> 87A       -0.10539
     85A -> 88A        0.25001
     86A -> 87A       -0.22629
     86A -> 88A        0.73150
     81B -> 86B       -0.23394
     82B -> 90B        0.14925
     84B -> 87B        0.11259
     85B -> 88B       -0.26899

 Excited State   4:  3.370-A'     3.2222 eV  384.78 nm  f=0.0072
<S**2>=2.590
     83A -> 93A        0.27770
     84A -> 87A       -0.36183
     84A -> 89A        0.10916
     84A -> 95A        0.19206
     85A -> 87A       -0.33488
     79B -> 96B       -0.11513
     83B -> 93B        0.27547
     84B -> 86B        0.19312
     84B -> 87B        0.36509
     84B -> 96B       -0.20192
     85B -> 86B       -0.15973
     85B -> 87B        0.39057

 Excited State   5:  2.096-A"     3.2870 eV  377.19 nm  f=0.0014
<S**2>=0.848
     80B -> 86B        0.96045
     80B -> 90B        0.10219
     80B ->101B       -0.13633
```

1i (X=Br)

```
Excited State   1:  2.288-A'     2.2706 eV  546.05 nm  f=0.0557
<S**2>=1.059
     80A -> 82A       -0.13577
     81A -> 82A        0.29952
     77B -> 81B        0.15272
     80B -> 81B        0.86979
     80B -> 82B        0.10268
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -982.703252787

 Excited State   2:  2.103-A'     2.4183 eV  512.69 nm  f=0.0190
<S**2>=0.855
     80A -> 82A       -0.11317
     81A -> 82A        0.83557
     81A -> 83A        0.20209
     81A -> 90A        0.17929
     79B -> 81B        0.12978
     80B -> 81B       -0.32568

 Excited State   3:  2.720-A'     2.9486 eV  420.49 nm  f=0.0223
<S**2>=1.599
     76A -> 84A       -0.12382
     76A -> 94A       -0.12917
     77A -> 84A       -0.11469
     79A -> 82A       -0.10664
     80A -> 83A        0.25192
     81A -> 82A       -0.22518
     81A -> 83A        0.73228
     76B -> 81B       -0.22903
     77B -> 85B        0.13298
     79B -> 82B        0.11231
     80B -> 83B       -0.26886

 Excited State   4:  3.371-A'     3.2134 eV  385.84 nm  f=0.0071
<S**2>=2.591
     77A -> 82A        0.11371
     78A -> 89A        0.27666
     79A -> 82A       -0.35784
     79A -> 84A        0.10649
     79A -> 90A        0.18546
     80A -> 82A       -0.33116
     74B -> 92B       -0.11304
     78B -> 89B       -0.27133
     79B -> 81B        0.18846
     79B -> 82B        0.36262
     79B -> 92B       -0.19944
     80B -> 81B       -0.16193
     80B -> 82B        0.38725

 Excited State   5:  2.096-A"     3.2854 eV  377.38 nm  f=0.0014
<S**2>=0.849
     75B -> 81B        0.96012
     75B -> 85B        0.10215
     75B -> 96B        0.12697
```

1j (X=COMe)

```
Excited State   1:  2.298-A'     2.3008 eV  538.88 nm  f=0.0315
<S**2>=1.070
     88A -> 91A        0.18479
     89A -> 90A       -0.39955
     89A -> 91A       -0.40924
     89A -> 92A        0.12172
     88B -> 89B        0.70455
     88B -> 91B        0.10909
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1122.77515629
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.187-A'     2.3764 eV  521.74 nm  f=0.0401
<S**2>=0.946
     89A -> 90A        0.60090
     89A -> 91A        0.33596
     89A -> 92A       -0.17342
     89A -> 98A       -0.13992
     85B -> 89B        0.10491
     87B -> 89B       -0.13616
     88B -> 89B        0.58852
     88B -> 90B       -0.10866

 Excited State   3:  2.655-A'     2.7220 eV  455.48 nm  f=0.0131
<S**2>=1.512
     83A -> 90A        0.17037
     84A -> 92A       -0.11607
     87A -> 90A        0.13912
     88A -> 90A       -0.26386
     89A -> 90A       -0.36003
     89A -> 91A        0.68374
     89A -> 92A        0.13737
     83B -> 89B        0.11301
     83B -> 90B       -0.13735
     87B -> 90B       -0.12731
     88B -> 89B        0.13725
     88B -> 90B        0.21202
     88B -> 91B        0.10588

 Excited State   4:  3.336-A'     3.2177 eV  385.32 nm  f=0.0037
<S**2>=2.532
     86A -> 96A        0.26157
     86A ->100A       -0.11219
     87A -> 90A        0.15421
     87A -> 91A        0.32792
     87A -> 98A        0.17457
     87A ->100A       -0.11939
     88A -> 90A        0.17999
     88A -> 91A        0.30647
     89A -> 90A        0.11376
     89A -> 92A        0.18235
     81B ->100B       -0.11182
     86B -> 96B        0.27532
     87B -> 89B        0.14314
     87B -> 90B       -0.18750
```

```
     87B -> 91B        0.31862
     87B ->100B       -0.19646
     88B -> 89B       -0.17186
     88B -> 90B       -0.22333
     88B -> 91B        0.32697

 Excited State   5:  2.096-A"     3.3023 eV  375.45 nm  f=0.0014
<S**2>=0.848
     82B -> 89B        0.83475
     82B ->101B        0.12579
     84B -> 89B        0.47678
```

11 (X=NH_2)

```
Excited State   1:  2.213-A      2.1509 eV  576.42 nm  f=0.0801
<S**2>=0.975
     82A -> 83A        0.10062
     79B -> 82B       -0.13882
     80B -> 82B        0.20319
     81B -> 82B        0.91942
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1025.52647378

 Excited State   2:  2.134-A      2.3760 eV  521.82 nm  f=0.0100
<S**2>=0.889
     81A -> 83A        0.23450
     82A -> 83A        0.86504
     82A -> 84A        0.20271
     82A -> 92A        0.17514
     81B -> 82B       -0.13286

 Excited State   3:  2.820-A      2.9700 eV  417.45 nm  f=0.0143
<S**2>=1.739
     80A -> 83A        0.14680
     81A -> 84A       -0.21727
     82A -> 83A       -0.25057
     82A -> 84A        0.60654
     77B -> 82B       -0.19326
     79B -> 82B       -0.13513
     79B -> 83B       -0.12044
     80B -> 82B        0.30337
     80B -> 83B       -0.12589
     81B -> 83B       -0.14537
     81B -> 84B       -0.30272

 Excited State   4:  2.926-A      3.1171 eV  397.76 nm  f=0.0117
<S**2>=1.891
     77A -> 88A        0.11223
     78A -> 83A        0.11405
     79A -> 89A       -0.10086
     80A -> 83A        0.13381
     80A -> 88A       -0.13414
     81A -> 83A        0.19869
     81A -> 88A        0.16731
     82A -> 84A       -0.33302
     77B -> 82B        0.21095
     77B -> 84B        0.11078
     78B -> 88B       -0.12143
```

```
     79B -> 83B       -0.14091
     80B -> 82B        0.50431
     80B -> 83B       -0.11369
     80B -> 90B        0.10297
     80B -> 91B       -0.12464
     81B -> 82B       -0.21745
     81B -> 83B       -0.31020
     81B -> 88B       -0.10851
     81B -> 90B       -0.12694
     81B -> 91B        0.15565

 Excited State   5:  3.164-A      3.3010 eV  375.59 nm  f=0.0021
<S**2>=2.253
     78A -> 83A       -0.22497
     78A -> 89A        0.14491
     78A -> 92A        0.10051
     79A -> 83A        0.10520
     79A -> 88A       -0.13923
     79A -> 89A        0.18421
     79A -> 92A       -0.12214
     80A -> 83A       -0.31364
     81A -> 83A       -0.12523
     81A -> 84A       -0.12301
     82A -> 92A       -0.11567
     78B -> 82B       -0.10502
     78B -> 88B        0.23857
     79B -> 82B       -0.25933
     79B -> 83B        0.21293
     79B -> 93B       -0.14850
     80B -> 82B        0.38920
     80B -> 83B        0.34504
     80B -> 93B       -0.10721
     81B -> 83B        0.12862
     81B -> 84B       -0.14558
     81B -> 91B        0.11652
```

1m (X=NHAc)

```
Excited State   1:  2.252-A      2.2253 eV  557.15 nm  f=0.0733
<S**2>=1.017
     92A -> 94A       -0.10989
     93A -> 94A        0.19164
     90B -> 93B        0.16242
     91B -> 93B        0.15820
     92B -> 93B        0.89732
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1178.13449543
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.112-A      2.3964 eV  517.38 nm  f=0.0161
<S**2>=0.865
     92A -> 94A       -0.17633
     93A -> 94A        0.86290
     93A -> 95A        0.17420
     93A ->103A        0.18201
     90B -> 93B       -0.10742
     92B -> 93B       -0.22533
```

```
 Excited State   3:  2.824-A      2.9806 eV  415.97 nm  f=0.0129
<S**2>=1.744
     88A -> 97A       -0.11882
     91A -> 94A       -0.11705
     91A -> 97A       -0.11320
     92A -> 95A        0.26322
     92A -> 97A        0.10491
     93A -> 94A       -0.20369
     93A -> 95A        0.67537
     93A -> 97A       -0.10869
     88B -> 93B       -0.24912
     90B -> 98B        0.11291
     91B -> 94B        0.11661
     91B -> 98B        0.10722
     92B -> 95B       -0.32016

 Excited State   4:  3.284-A      3.1888 eV  388.81 nm  f=0.0086
<S**2>=2.447
     89A -> 94A       -0.19678
     89A ->103A        0.11911
     90A ->100A       -0.22523
     90A ->103A       -0.10577
     91A -> 94A       -0.28856
     91A -> 97A        0.13943
     91A ->103A        0.10360
     92A -> 94A       -0.29276
     85B ->104B       -0.10458
     89B ->100B        0.23907
     90B -> 94B       -0.21676
     90B ->104B        0.13554
     91B -> 93B        0.32264
     91B -> 94B        0.27933
     91B -> 98B       -0.13690
     91B ->104B       -0.10340
     92B -> 93B       -0.21072
     92B -> 94B        0.38406

 Excited State   5:  2.097-A      3.3289 eV  372.45 nm  f=0.0013
<S**2>=0.849
     86B -> 93B        0.11734
     87B -> 93B        0.95463
     87B ->109B       -0.12108
```

1n (X=I)

```
Excited State   1:  2.290-A'     2.2738 eV  545.26 nm  f=0.0564
<S**2>=1.061
     80A -> 82A       -0.13678
     81A -> 82A        0.31527
     78B -> 81B        0.14933
     80B -> 81B        0.85694
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -980.916260976

 Excited State   2:  2.102-A'     2.4131 eV  513.79 nm  f=0.0208
<S**2>=0.854
     80A -> 82A       -0.11392
```

```
     81A -> 82A        0.83045
     81A -> 83A        0.19493
     81A -> 91A        0.17971
     78B -> 81B       -0.11335
     80B -> 81B       -0.34212

 Excited State   3:  2.720-A'     2.9451 eV  420.98 nm  f=0.0218
<S**2>=1.599
     75A -> 85A       -0.14612
     75A -> 94A       -0.10972
     79A -> 82A       -0.10287
     80A -> 83A        0.25211
     81A -> 82A       -0.22006
     81A -> 83A        0.73307
     76B -> 81B       -0.21588
     76B -> 86B        0.10456
     78B -> 86B        0.10152
     79B -> 82B        0.10717
     80B -> 84B       -0.27142

 Excited State   4:  3.370-A'     3.2133 eV  385.85 nm  f=0.0070
<S**2>=2.589
     77A -> 82A        0.19380
     77A -> 91A       -0.12166
     78A -> 89A       -0.26543
     78A -> 91A       -0.11735
     79A -> 82A       -0.32771
     79A -> 91A        0.14690
     80A -> 82A       -0.31903
     73B -> 93B       -0.10328
     77B -> 81B        0.10459
     77B -> 89B        0.26306
     78B -> 82B       -0.15427
     78B -> 89B        0.10499
     78B -> 93B        0.12713
     79B -> 81B        0.17784
     79B -> 82B        0.34327
     79B -> 93B       -0.17507
     80B -> 81B       -0.16701
     80B -> 82B        0.38084

 Excited State   5:  2.096-A"     3.2882 eV  377.05 nm  f=0.0013
<S**2>=0.848
     74B -> 81B        0.92803
     74B -> 96B        0.10721
     75B -> 81B       -0.24709
```

1o (X=OH)

```
Excited State   1:  2.237-A'     2.2007 eV  563.38 nm  f=0.0709
<S**2>=1.001
     81A -> 83A       -0.10099
     82A -> 83A        0.15665
     79B -> 82B       -0.14047
     81B -> 82B        0.92152
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1045.39331038
```

```
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.118-A'     2.3987 eV  516.87 nm  f=0.0128
<S**2>=0.872
     81A -> 83A       -0.18922
     82A -> 83A        0.86529
     82A -> 84A        0.21569
     82A -> 92A        0.18008
     80B -> 82B        0.10857
     81B -> 82B       -0.18504

 Excited State   3:  2.762-A'     2.9960 eV  413.83 nm  f=0.0183
<S**2>=1.658
     77A -> 88A       -0.12553
     77A -> 96A        0.11501
     80A -> 83A       -0.13151
     81A -> 84A        0.21802
     82A -> 83A       -0.24594
     82A -> 84A        0.69014
     77B -> 82B       -0.24783
     79B -> 82B       -0.10374
     80B -> 83B        0.13140
     81B -> 83B        0.10610
     81B -> 84B       -0.27920

 Excited State   4:  3.274-A'     3.2033 eV  387.06 nm  f=0.0132
<S**2>=2.429
     78A -> 83A       -0.16151
     79A -> 89A       -0.23062
     80A -> 83A       -0.31052
     80A -> 88A        0.12542
     80A -> 92A        0.12625
     81A -> 83A       -0.29298
     82A -> 84A       -0.21674
     75B -> 93B       -0.10740
     78B -> 88B        0.21988
     78B -> 90B       -0.10895
     79B -> 83B        0.15312
     79B -> 93B       -0.12271
     80B -> 82B        0.28552
     80B -> 83B        0.31379
     80B -> 90B       -0.14521
     80B -> 93B       -0.14026
     81B -> 82B       -0.16906
     81B -> 83B        0.38162

 Excited State   5:  2.098-A"     3.3374 eV  371.50 nm  f=0.0014
<S**2>=0.851
     76B -> 82B        0.96141
     76B -> 99B        0.11848
```

1p (X=OBn)

```
Excited State   1:  2.234-A      2.2008 eV  563.36 nm  f=0.0748
<S**2>=0.998
    106A ->107A        0.15335
    102B ->106B       -0.13053
    105B ->106B        0.92137
```

```
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1315.60545868
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.123-A      2.3879 eV  519.21 nm  f=0.0124
<S**2>=0.877
    105A ->107A       -0.19704
    106A ->107A        0.86301
    106A ->108A        0.22190
    106A ->119A       -0.17227
    104B ->106B       -0.10326
    105B ->106B       -0.17963

 Excited State   3:  2.738-A      2.9641 eV  418.29 nm  f=0.0208
<S**2>=1.625
    104A ->107A        0.11734
    105A ->108A        0.22337
    106A ->107A       -0.25256
    106A ->108A        0.69326
     99B ->106B       -0.21797
    102B ->106B       -0.11332
    104B ->106B       -0.12379
    104B ->107B        0.11494
    105B ->107B       -0.10570
    105B ->108B        0.27732

 Excited State   4:  3.287-A      3.2097 eV  386.29 nm  f=0.0145
<S**2>=2.452
    100A ->107A       -0.16678
    102A ->116A        0.21188
    104A ->107A       -0.31436
    104A ->116A        0.10209
    104A ->119A       -0.10762
    105A ->107A        0.28973
    106A ->108A        0.23104
    100B ->114B        0.22384
    102B ->107B        0.14099
    104B ->106B        0.25067
    104B ->107B       -0.33178
    104B ->117B        0.13695
    104B ->120B        0.10192
    105B ->106B        0.16531
    105B ->107B        0.37967

 Excited State   5:  2.099-A      3.3527 eV  369.81 nm  f=0.0013
<S**2>=0.852
     98B ->106B        0.96095
```

1q (X=Ph)

```
Excited State   1:  2.281-A      2.2718 eV  545.75 nm  f=0.0628
<S**2>=1.051
     97A -> 99A       -0.13240
     98A -> 99A       -0.31749
     95B -> 98B        0.14317
     96B -> 98B        0.19851
     97B -> 98B        0.84106
```

```
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1201.11749428

 Excited State   2:  2.107-A      2.3857 eV  519.70 nm  f=0.0251
<S**2>=0.860
     97A -> 99A        0.12312
     98A -> 99A        0.83282
     98A ->101A       -0.16566
     98A ->109A        0.13922
     98A ->110A       -0.11448
     95B -> 98B        0.14520
     97B -> 98B        0.34713

 Excited State   3:  2.937-A      2.8745 eV  431.33 nm  f=0.0115
<S**2>=1.907
     92A ->101A        0.12241
     92A ->109A        0.10292
     94A ->105A        0.10125
     96A -> 99A        0.10039
     96A ->100A        0.12166
     96A ->101A        0.11821
     97A ->100A       -0.31539
     98A -> 99A       -0.13730
     98A ->100A        0.59690
     98A ->101A       -0.24628
     92B -> 98B        0.18182
     96B -> 99B        0.10928
     96B ->100B       -0.17344
     96B ->102B        0.10461
     97B ->100B        0.32762

 Excited State   4:  3.339-A      3.2037 eV  387.00 nm  f=0.0041
<S**2>=2.538
     93A -> 99A        0.23379
     93A ->106A        0.12967
     93A ->109A       -0.13434
     95A -> 99A       -0.12569
     95A ->106A        0.21023
     95A ->110A       -0.13015
     96A -> 99A        0.25471
     96A ->100A       -0.16395
     97A -> 99A        0.29445
     98A -> 99A       -0.10505
     98A ->101A       -0.13439
     94B ->106B        0.25511
     95B -> 99B       -0.26502
     95B ->110B        0.13630
     96B -> 98B       -0.18262
     96B -> 99B        0.25228
     96B ->100B        0.15482
     97B -> 98B        0.19841
     97B -> 99B        0.36800

 Excited State   5:  2.097-A      3.3262 eV  372.76 nm  f=0.0013
<S**2>=0.849
     91B -> 98B        0.96060
     91B ->112B        0.12197
```

1r (X=thienyl)

```
Excited State   1:  2.275-A      2.2596 eV  548.70 nm  f=0.0703
<S**2>=1.044
     98A ->100A        0.11801
     99A ->100A        0.22705
     99A ->101A        0.11606
     96B -> 99B        0.13502
     97B -> 99B        0.34771
     98B -> 99B        0.81995
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1521.91246062

 Excited State   2:  2.202-A      2.3762 eV  521.78 nm  f=0.0167
<S**2>=0.962
     98A ->101A        0.17855
     99A ->100A        0.83602
     99A ->102A        0.19154
     99A ->110A        0.14386
     96B -> 99B       -0.13638
     98B -> 99B       -0.25188
     98B ->101B        0.14219

 Excited State   3:  3.210-A      2.6200 eV  473.23 nm  f=0.0094
<S**2>=2.327
     97A ->100A        0.11687
     97A ->101A       -0.17641
     97A ->102A       -0.11772
     98A ->100A        0.26124
     98A ->101A       -0.37879
     99A ->100A        0.11827
     99A ->101A        0.44891
     93B -> 99B       -0.11086
     97B ->100B       -0.15346
     97B ->101B        0.25297
     97B ->103B       -0.11444
     98B -> 99B       -0.15629
     98B ->100B        0.20802
     98B ->101B       -0.39897

 Excited State   4:  2.857-A      3.1056 eV  399.23 nm  f=0.0069
<S**2>=1.791
     94A ->100A       -0.13130
     96A ->100A        0.10787
     97A ->101A        0.26144
     98A ->100A       -0.15074
     98A ->102A        0.11069
     99A ->101A        0.47067
     99A ->102A       -0.41212
     99A ->108A       -0.10412
     91B -> 99B        0.10317
     96B ->100B        0.19594
     97B -> 99B       -0.19958
     97B ->101B       -0.22788
     98B -> 99B        0.17996
     98B ->100B       -0.20603
     98B ->103B       -0.14365
```

1s (X=CCPh)

```
Excited State   1:  2.284-A'     2.2709 eV  545.96 nm  f=0.0757
<S**2>=1.054
    102A ->106A       -0.10550
    104A ->105A       -0.12769
    104A ->106A        0.23774
    101B ->104B       -0.13132
    102B ->104B        0.39146
    103B ->104B        0.79017
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1277.23262934

 Excited State   2:  2.375-A'     2.3608 eV  525.18 nm  f=0.0150
<S**2>=1.160
    103A ->105A        0.10252
    103A ->106A        0.22946
    104A ->105A        0.69115
    104A ->106A       -0.40274
    104A ->107A       -0.22786
    104A ->117A       -0.14683
    101B ->104B       -0.12790
    103B ->104B        0.21449
    103B ->105B       -0.16084
    103B ->106B       -0.14852

 Excited State   3:  3.079-A'     2.5476 eV  486.67 nm  f=0.0144
<S**2>=2.120
     99A ->111A        0.10474
    102A ->105A       -0.16216
    103A ->105A        0.42449
    103A ->106A        0.13706
    104A ->106A        0.52008
    104A ->117A        0.10053
     99B ->111B       -0.11556
    102B ->105B        0.23578
    102B ->106B        0.13148
    102B ->108B        0.10974
    103B ->104B       -0.22538
    103B ->105B       -0.36144
    103B ->106B       -0.21686

 Excited State   4:  2.816-A'     3.0670 eV  404.25 nm  f=0.0040
<S**2>=1.732
     99A ->111A       -0.14039
    100A ->105A        0.11396
    102A ->105A        0.14743
    102A ->106A        0.21486
    103A ->105A       -0.15422
    103A ->107A       -0.10381
    104A ->105A        0.23240
    104A ->106A        0.45348
    104A ->107A       -0.43828
    104A ->112A       -0.12143
     96B ->104B       -0.10455
     99B ->111B        0.15761
    101B ->105B        0.15458
    102B ->104B       -0.15259
```

```
    102B ->105B       -0.13458
    102B ->106B       -0.19324
    103B ->104B        0.12961
    103B ->105B        0.17126
    103B ->108B        0.17082
```

1t (X=OAc)

```
Excited State   1:  2.280-A      2.2687 eV  546.51 nm  f=0.0580
<S**2>=1.050
     92A -> 94A        0.13369
     93A -> 94A       -0.29134
     89B -> 93B       -0.13590
     92B -> 93B        0.87906
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1197.99274023

 Excited State   2:  2.097-A      2.4110 eV  514.24 nm  f=0.0201
<S**2>=0.849
     92A -> 94A       -0.12263
     93A -> 94A        0.84127
     93A -> 95A        0.19011
     93A ->103A        0.18380
     91B -> 93B       -0.13090
     92B -> 93B        0.31898

 Excited State   3:  2.721-A      2.9873 eV  415.04 nm  f=0.0198
<S**2>=1.601
     89A -> 97A        0.13031
     91A -> 94A       -0.10981
     92A -> 95A        0.24532
     93A -> 94A       -0.21819
     93A -> 95A        0.72110
     88B -> 93B        0.24254
     91B -> 94B        0.12067
     92B -> 95B       -0.26609

 Excited State   4:  3.364-A      3.2247 eV  384.49 nm  f=0.0082
<S**2>=2.579
     90A ->100A       -0.27498
     91A -> 94A       -0.36331
     91A ->103A        0.18975
     92A -> 94A       -0.32948
     93A -> 95A       -0.12167
     86B ->105B        0.11432
     90B ->100B        0.26827
     91B -> 93B       -0.20131
     91B -> 94B        0.36566
     91B ->105B        0.19900
     92B -> 93B        0.15621
     92B -> 94B        0.38810

 Excited State   5:  2.096-A      3.3125 eV  374.29 nm  f=0.0014
<S**2>=0.849
     87B -> 93B        0.96087
```

1u (X=NHCOCF$_3$)

```
Excited State   1:  2.269-A      2.2504 eV  550.95 nm  f=0.0666
<S**2>=1.037
    104A ->106A       -0.11862
    105A ->106A        0.22317
    101B ->105B       -0.12958
    102B ->105B       -0.12030
    104B ->105B        0.89135
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1475.82048199
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.116-A      2.4148 eV  513.43 nm  f=0.0173
<S**2>=0.870
    104A ->106A       -0.12855
    105A ->106A        0.85748
    105A ->108A        0.19376
    105A ->113A        0.10791
    105A ->115A        0.16070
    103B ->105B        0.10917
    104B ->105B       -0.25740

 Excited State   3:  2.852-A      2.9143 eV  425.44 nm  f=0.0134
<S**2>=1.784
    100A ->108A       -0.11112
    100A ->113A        0.10242
    101A ->108A        0.13182
    103A ->106A        0.12352
    103A ->107A       -0.11587
    104A ->107A        0.28253
    105A ->106A        0.13274
    105A ->107A        0.60692
    105A ->108A       -0.31773
    105A ->123A       -0.10287
    100B ->105B        0.22110
    102B ->108B       -0.10164
    103B ->106B       -0.12822
    103B ->107B        0.12603
    104B ->107B       -0.29523

 Excited State   4:  3.357-A      3.2045 eV  386.90 nm  f=0.0055
<S**2>=2.567
    101A ->106A       -0.15212
    102A ->112A       -0.23283
    102A ->113A        0.10332
    102A ->115A       -0.11830
    103A ->106A       -0.31999
    103A ->107A       -0.14967
    103A ->113A        0.12078
    103A ->115A        0.13752
    104A ->106A       -0.32693
     98B ->117B       -0.10847
    101B ->112B        0.20690
    102B ->106B        0.12466
    102B ->112B       -0.16748
    102B ->117B       -0.11396
    103B ->105B        0.21536
    103B ->106B        0.32553
```

```
    103B ->107B        0.13722
    103B ->115B       -0.12648
    103B ->117B       -0.14014
    104B ->105B       -0.18543
    104B ->106B        0.39348

 Excited State   5:  2.097-A      3.2942 eV  376.37 nm  f=0.0014
<S**2>=0.849
     99B ->105B        0.96068
```

1v (NHCOOMe)

```
Excited State   1:  2.249-A      2.2206 eV  558.34 nm  f=0.0739
<S**2>=1.014
     96A -> 98A       -0.10743
     97A -> 98A        0.18227
     94B -> 97B        0.16281
     95B -> 97B        0.15373
     96B -> 97B        0.90096
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -1253.34591474
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:  2.113-A      2.3991 eV  516.80 nm  f=0.0154
<S**2>=0.866
     96A -> 98A       -0.18107
     97A -> 98A        0.86336
     97A -> 99A        0.19389
     97A ->107A        0.18274
     94B -> 97B       -0.10422
     96B -> 97B       -0.21560

 Excited State   3:  2.803-A      2.9884 eV  414.88 nm  f=0.0144
<S**2>=1.714
     92A ->101A       -0.12433
     92A ->111A        0.12700
     95A -> 98A       -0.12133
     96A -> 99A        0.24293
     96A ->101A        0.12107
     97A -> 98A       -0.21671
     97A -> 99A        0.69009
     92B -> 97B       -0.24805
     95B -> 98B        0.11892
     96B -> 99B       -0.30770

 Excited State   4:  3.273-A      3.1894 eV  388.73 nm  f=0.0095
<S**2>=2.429
     93A -> 98A       -0.19261
     93A ->107A        0.11781
     94A ->104A       -0.22392
     94A ->107A       -0.10470
     95A -> 98A       -0.28751
     95A ->101A        0.14744
     95A ->107A        0.10589
     96A -> 98A       -0.28951
     97A -> 99A       -0.11187
     90B ->108B       -0.10883
```

```
     93B ->103B        0.10744
     93B ->104B        0.22411
     94B -> 98B       -0.20983
     94B ->108B        0.14113
     95B -> 97B        0.32888
     95B -> 98B        0.27894
     95B ->103B       -0.13725
     95B ->108B       -0.11508
     96B -> 97B       -0.20737
     96B -> 98B        0.38161
     96B ->103B        0.10200

 Excited State   5:  2.097-A      3.3269 eV  372.67 nm  f=0.0014
<S**2>=0.849
     91B -> 97B        0.96162
```

8. Archive for (U)B3LYP/6-31G(2d,p) geometry optimization results

1a (X=H)

```
1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H12N3O1(2)\PIOTR\14-Apr-
 2016\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
 eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1) benzotrazinyl (p
 henazinoBT), Cs\\0,2\N,-0.2279945082,0.,-0.7068912291\N,1.6342308182,0
 .,1.3147774172\C,0.3141730381,0.,1.5107475896\N,-0.6511944713,0.,0.577
 2813358\C,2.8747587314,0.,-2.6901553245\C,1.525294733,0.,-2.3786764485
 \C,1.1192429656,0.,-1.0420625687\C,2.0563033272,0.,0.0130670541\C,3.42
 27100243,0.,-0.320281521\C,3.8144680324,0.,-1.6500459807\C,-1.17991954
 82,0.,-1.7366863092\C,-0.7265516782,0.,-3.0685289936\C,-1.6343949522,0
 .,-4.1176431627\C,-3.0025964506,0.,-3.8542738611\C,-3.4580568847,0.,-2
 .5364763795\C,-2.5535440658,0.,-1.48031653\C,-0.1674933344,0.,2.917057
 1338\C,-1.5355202766,0.,3.2213939115\C,-1.9627296157,0.,4.5448686804\C
 ,-1.0320885266,0.,5.5834203093\C,0.3304717827,0.,5.2886511585\C,0.7611
 634188,0.,3.9661225371\O,0.607802556,0.,-3.3994557106\H,4.1444354867,0
 .,0.4875266765\H,-1.2474203049,0.,-5.1300423865\H,-4.5217388028,0.,-2.
 3262246262\H,-2.8822307131,0.,-0.4505760941\H,-2.2557347868,0.,2.41322
 96866\H,-3.0252780726,0.,4.7664014926\H,1.0608349088,0.,6.0915258161\H
 ,1.8160583604,0.,3.7224448829\H,4.8703351187,0.,-1.898622529\H,3.17536
 91985,0.,-3.7308245809\H,-3.7063464888,0.,-4.6790512891\H,-1.367442019
 2,0.,6.615759843\\Version=ES64L-G09RevD.01\State=2-A"\HF=-970.7339788\
 S2=0.765494\S2-1=0.\S2A=0.750186\RMSD=4.138e-09\RMSF=1.718e-06\Dipole=
 -0.2970498,0.,-0.7847295\Quadrupole=5.3068963,-9.8608619,4.5539655,0.,
 -0.5464311,0.\PG=CS [SG(C19H12N3O1)]\\
No imaginary frequencies.
```

1b (X=COOMe)

```
1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H14N3O3(2)\PIOTR\05-May-
 2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
 eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-COOMe sec o
 rient benzotrazinyl, Cs\\0,2\N,-0.1596473134,0.8160516965,0.\N,-2.9064
 525107,0.8778039954,0.\C,-2.181847753,-0.243293261,0.\N,-0.8429312268,
 -0.3503453785,0.\C,-0.7194975137,4.455056265,0.\C,-0.0643532906,3.2360
 070125,0.\C,-0.7979516254,2.048171105,0.\C,-2.2088626573,2.0544645993,
 0.\C,-2.8608970603,3.3011702737,0.\C,-2.1217266261,4.4736162751,0.\C,1
 .2433265276,0.7821689285,0.\C,1.9426315505,2.004936735,0.\C,3.33199069
```

14,2.0185823276,0.\C,4.0369449018,0.8225606862,0.\C,3.3524572652,-0.39
71257489,0.\C,1.9560628523,-0.4154118111,0.\C,-2.918405793,-1.53391931
21,0.\C,-2.2414470352,-2.7611649563,0.\C,-2.9519148157,-3.9566523906,0
.\C,-4.3464038964,-3.9452031559,0.\C,-5.026614316,-2.7283272085,0.\C,-
4.3194785893,-1.5306801249,0.\O,1.3112996971,3.2194647631,0.\H,3.83634
9017,2.9776968783,0.\H,1.4106564375,-1.3468569734,0.\H,-1.1589257281,-
2.7670277305,0.\H,-2.4155560163,-4.9002262338,0.\H,-6.1118142075,-2.71
156792,0.\H,-4.834804867,-0.5785239475,0.\H,-2.6324631427,5.4304729372
,0.\H,-0.1366042534,5.3680135276,0.\H,5.1198370747,0.811693075,0.\H,-4
.8989816889,-4.8794361818,0.\H,-3.9441261548,3.3094273495,0.\C,4.16146
55494,-1.6454131672,0.\O,5.3714084956,-1.6734328415,0.\O,3.395474421,-
2.7551687923,0.\C,4.1193370326,-3.9921703298,0.\H,3.3627129565,-4.7762
866093,0.\H,4.7508133011,-4.0670060443,-0.8883829164\H,4.7508133011,-4
.0670060443,0.8883829164\\Version=ES64L-G09RevD.01\State=2-A"\HF=-1198
.624302\S2=0.765518\S2-1=0.\S2A=0.750183\RMSD=6.039e-09\RMSF=3.680e-06
\Dipole=-0.1206689,0.2533919,0.\Quadrupole=-8.943009,15.7362829,-6.793
2739,-0.1083726,0.,0.\PG=CS [SG(C21H12N3O3),X(H2)]\\
No imaginary frequencies.

1c (X=CN)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C20H11N4O1(2)\PIOTR\28-Jan-
2019\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CN benzotra
zinyl, Cs\\0,2\N,0.4918707959,-0.3073709472,0.\N,-1.9301161981,-1.5993
15204,0.\C,-1.791350529,-0.2716071392,0.\N,-0.6428526579,0.4270485217,
0.\C,1.6337807608,-3.8072972677,0.\C,1.6685437305,-2.4245914624,0.\C,0
.4785524447,-1.6951606949,0.\C,-0.7780780973,-2.3354815524,0.\C,-0.798
3291984,-3.7427877987,0.\C,0.3895854727,-4.4558136552,0.\C,1.726358092
2,0.3539464615,0.\C,2.9039315435,-0.4204555594,0.\C,4.1484220382,0.196
2930417,0.\C,4.2426785205,1.5821187079,0.\C,3.0759589325,2.3588732005,
0.\C,1.8188939779,1.7436946847,0.\C,-3.030333523,0.5470735543,0.\C,-2.
9807330234,1.9479003912,0.\C,-4.154452889,2.6935331395,0.\C,-5.3930969
442,2.053054602,0.\C,-5.4505263192,0.6600599721,0.\C,-4.278893543,-0.0
890666132,0.\O,2.8897323898,-1.7873119994,0.\H,5.0324681534,-0.4299667
16,0.\H,0.9097894185,2.3272096033,0.\H,-2.0188705865,2.4444569437,0.\H
,-4.1017954675,3.7774423221,0.\H,-6.4110840513,0.154960281,0.\H,-4.309
2831729,-1.1712698284,0.\H,0.3652342955,-5.5400747517,0.\H,2.565248926
7,-4.3600802229,0.\H,5.2125317008,2.0639104174,0.\H,-6.3080392627,2.63
68796308,0.\H,-1.7614255903,-4.238551869,0.\C,3.1673740475,3.787994881
7,0.\N,3.2484909322,4.9444164444,0.\\Version=ES64L-G09RevD.01\State=2-
A"\HF=-1062.9763189\S2=0.766177\S2-1=0.\S2A=0.750198\RMSD=4.826e-09\RM
SF=2.297e-06\Dipole=0.2829048,-1.8958087,0.\Quadrupole=10.8738161,-8.3
206835,-2.5531326,-13.3808711,0.,0.\PG=CS [SG(C20H11N4O1)]\\
No imaginary frequencies.

1d (X=NO_2)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H11N4O3(2)\PIOTR\21-Aug-
2019\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NO2 benzotr
azinyl, Cs\\0,2\N,0.1740075275,-0.5912901624,0.\N,-2.4796513212,-1.291
9222227,0.\C,-2.0394489326,-0.0312808682,0.\N,-0.7609224979,0.38435639
9,0.\C,0.4817664514,-4.2595262875,0.\C,0.8321536884,-2.9217720233,0.\C
,-0.1578145215,-1.9384733571,0.\C,-1.5278131968,-2.2730914555,0.\C,-1.
8705103077,-3.6383841063,0.\C,-0.8782093957,-4.6052405795,0.\C,1.52737
27934,-0.2308669305,0.\C,2.4967632923,-1.256339851,0.\C,3.8517047621,-
0.9450190871,0.\C,4.2648442238,0.3816429975,0.\C,3.2974400491,1.380915
9148,0.\C,1.9365843962,1.0999181989,0.\C,-3.0560553157,1.0508987352,0.

\C,-2.6835702086,2.4022875514,0.\C,-3.6534376223,3.3987756193,0.\C,-5.
0064804626,3.0615172225,0.\C,-5.3844716735,1.7195084307,0.\C,-4.417680
5699,0.7199304577,0.\O,2.1680530385,-2.5810062532,0.\H,4.5662248069,-1
.7592329262,0.\H,1.2073107099,1.8949660168,0.\H,-1.6329902242,2.663173
9537,0.\H,-3.3516826377,4.4411296207,0.\H,-6.4357849167,1.4501868296,0
.\H,-4.697401739,-0.3259222485,0.\H,-1.1508236683,-5.6549179771,0.\H,1
.2615781678,-5.011250259,0.\H,5.3116543172,0.6513036899,0.\H,-5.761872
5498,3.8408727586,0.\H,-2.9217795199,-3.8995169313,0.\N,3.7247375472,2
.7851065546,0.\O,2.8523215908,3.6453586969,0.\O,4.9299247591,3.0102355
39,0.\\Version=ES64L-G09RevD.01\State=2-A"\HF=-1175.2435108\S2=0.76595
2\S2-1=0.\S2A=0.750189\RMSD=4.184e-09\RMSF=4.229e-06\Dipole=-0.2091194
,-1.8865306,0.\Quadrupole=1.1105094,1.6616532,-2.7721626,-13.8781166,0
.,0.\PG=CS [SG(C19H11N4O3)]\\
No imaginary frequencies.

1e (X=CF_3)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C20H11F3N3O1(2)\PIOTR\29-Ja
n-2019\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CF3 benzo
trazinyl, C1\\0,2\N,-0.1511825702,-0.7509949659,0.0019305902\N,-2.8856
873624,-1.0031244808,-0.0095345499\C,-2.2420152411,0.1661806642,-0.011
2775541\N,-0.9130887467,0.3654554985,-0.0062244126\C,-0.4569389489,-4.
4201578281,0.0205375413\C,0.1126783642,-3.159064103,0.0168938474\C,-0.
7019592265,-2.025243303,0.0063016938\C,-2.1086733785,-2.1284797405,-0.
0002568146\C,-2.6733309861,-3.4173945873,0.0035257033\C,-1.8547846494,
-4.5354430062,0.0136968224\C,1.2435752303,-0.6202581221,0.0064562154\C
,2.0280314682,-1.7896441254,0.0165159904\C,3.4131286808,-1.7029265695,
0.0141324768\C,4.0344566611,-0.4582512982,0.0045368407\C,3.2597736991,
0.7011386528,-0.0021748332\C,1.8701329319,0.6257291727,-0.005327117\C,
-3.0667811749,1.4016640893,-0.0194401834\C,-2.4775806451,2.6734122756,
-0.0187821689\C,-3.2699748244,3.8161427111,-0.026028447\C,-4.660064984
7,3.706738791,-0.0341073286\C,-5.2534366959,2.4451069427,-0.0348664477
\C,-4.4642502715,1.3000039063,-0.0275423477\O,1.4838198837,-3.04680466
03,0.0238993996\H,3.9862300135,-2.6224234107,0.0155225003\H,1.25847733
75,1.5159060056,-0.0230902134\H,-1.3983254582,2.7568665547,-0.01232078
76\H,-2.8008421725,4.7947524333,-0.0253028393\H,-6.3347501874,2.352235
6631,-0.0411201678\H,-4.9117633427,0.3141790815,-0.027881938\H,-2.2977
873419,-5.5254437572,0.0165598427\H,0.1873570153,-5.2908484069,0.02862
41174\H,5.1149003146,-0.3890425686,-0.0054167574\H,-5.2768496875,4.599
8282391,-0.0397128231\H,-3.7533275269,-3.500698119,-0.0015250446\C,3.9
272068681,2.0488325485,0.0404255855\F,5.1328994739,2.0241667973,-0.556
6786147\F,3.1883115128,2.9932621553,-0.5679645904\F,4.1290667105,2.466
9267749,1.3070168136\\Version=ES64L-G09RevD.01\State=2-A\HF=-1307.7783
212\S2=0.765834\S2-1=0.\S2A=0.75019\RMSD=2.392e-09\RMSF=2.207e-06\Dipo
le=0.0503094,-1.1256041,-0.0323563\Quadrupole=-0.2079404,7.135302,-6.9
273616,-6.9090877,-0.2388503,-0.2194267\PG=C01 [X(C20H11F3N3O1)]\\
No imaginary frequencies.

1f (X=OMe)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C20H14N3O2(2)\PIOTR\05-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OMe 2nd orint
benzotrazinyl (phenazinoBT), Cs\\0,2\N,-0.3633656011,0.4985416597,0.\
N,-1.824449871,-1.8302987846,0.\C,-0.491581742,-1.7811693544,0.\N,0.28
7460985,-0.6872916609,0.\C,-3.7795730261,1.8789544623,0.\C,-2.39472214
58,1.8221901105,0.\C,-1.7504617182,0.5818851911,0.\C,-2.4780727487,-0.
6275457404,0.\C,-3.8819030796,-0.5513072773,0.\C,-4.5113188488,0.68433

68291,0.\C,0.3819200299,1.6845534658,0.\C,-0.3069404128,2.9060571541,0
.\C,0.4059715593,4.0985425137,0.\C,1.7929913799,4.0879469255,0.\C,2.48
52354255,2.8684575665,0.\C,1.7816192351,1.6661963162,0.\C,0.2384403204
,-3.0766140073,0.\C,1.6388727427,-3.1276582587,0.\C,2.2999146161,-4.35
12184369,0.\C,1.573922273,-5.5418190832,0.\C,0.1804682304,-5.499494600
8,0.\C,-0.4835359584,-4.2773179798,0.\O,-1.6823485163,2.9920047459,0.\
H,-4.4429035763,-1.4779540306,0.\H,-0.1480822485,5.0300482044,0.\H,2.2
705435771,0.7047829109,0.\H,2.1999194339,-2.2018367989,0.\H,3.38510135
92,-4.3760196505,0.\H,-0.3919265612,-6.4216770275,0.\H,-1.5651234287,-
4.2292052741,0.\H,-5.5949663365,0.7344505878,0.\H,-4.2664105303,2.8466
074595,0.\H,2.3602818571,5.0106922782,0.\H,2.091410231,-6.4959458246,0
.\O,3.8414510994,2.9605356566,0.\C,4.5918315069,1.7578130846,0.\H,4.38
67948655,1.1559409279,-0.8938912807\H,5.6404684445,2.0576946549,0.\H,4
.3867948655,1.1559409279,0.8938912807\\Version=ES64L-G09RevD.01\State=
2-A"\HF=-1085.2622773\S2=0.765743\S2-1=0.\S2A=0.750196\RMSD=9.070e-09\
RMSF=2.338e-06\Dipole=0.4425064,0.4888984,0.\Quadrupole=8.8378866,0.20
18879,-9.0397745,-3.6924413,0.,0.\PG=CS [SG(C20H12N3O2),X(H2)]\\
No imaginary frequencies.

1g (X=F)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H11F1N3O1(2)\PIOTR\06-Fe
b-2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-F benzotraz
inyl (phenazinoBT), Cs\\0,2\N,-0.2272885354,0.,-0.7084498124\N,1.63271
81068,0.,1.3126939453\C,0.3129552766,0.,1.5096657224\N,-0.652090512,0.
,0.5749367836\C,2.8766616423,0.,-2.6906542686\C,1.5267046931,0.,-2.381
09589\C,1.12046217,0.,-1.0444518059\C,2.0561061449,0.,0.0117056202\C,3
.4229905843,0.,-0.3200268849\C,3.815296485,0.,-1.6494472746\C,-1.17681
54404,0.,-1.7362626825\C,-0.7249725337,0.,-3.0692117177\C,-1.636786964
7,0.,-4.114363974\C,-3.0060913629,0.,-3.8565392632\C,-3.43260467,0.,-2
.5350751023\C,-2.5477552924,0.,-1.4697254298\C,-0.1691443289,0.,2.9153
109363\C,-1.5373913342,0.,3.2192185787\C,-1.9646184139,0.,4.5426199041
\C,-1.0339698995,0.,5.5810863262\C,0.3287728936,0.,5.2867088312\C,0.75
96016594,0.,3.9643626043\O,0.6101741294,0.,-3.4017738916\H,4.144014682
9,0.,0.4883322305\H,-1.2563936765,0.,-5.1289211151\H,-2.9001049147,0.,
-0.4489028388\H,-2.2583349296,0.,2.4117034177\H,-3.0271493958,0.,4.763
922495\H,1.058933596,0.,6.0897069795\H,1.8145747767,0.,3.721081174\H,4
.8712941411,0.,-1.8973991983\H,3.1788592321,0.,-3.7308535179\H,-3.7327
715305,0.,-4.6591665406\H,-1.3695056707,0.,6.6133405233\F,-4.747647368
7,0.,-2.2751050839\\Version=ES64L-G09RevD.01\State=2-A"\HF=-1069.96740
78\S2=0.765846\S2-1=0.\S2A=0.750194\RMSD=5.232e-09\RMSF=3.305e-06\Dipo
le=0.2754869,0.,-0.7770411\Quadrupole=-0.0585169,-7.8250385,7.8835554,
0.,-2.6157492,0.\PG=CS [SG(C19H11F1N3O1)]\\
No imaginary frequencies.

1h (X=Cl)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H11Cl1N3O1(2)\PIOTR\06-F
eb-2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #
P Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Cl benzotr
azinyl (phenazinoBT), Cs\\0,2\N,-0.2274057698,0.,-0.7077364119\N,1.632
8614611,0.,1.3128845684\C,0.3130364968,0.,1.5105061823\N,-0.6520237868
,0.,0.5756341802\C,2.875538267,0.,-2.6911206312\C,1.5265490452,0.,-2.3
801432009\C,1.1200653845,0.,-1.0438578913\C,2.0557791551,0.,0.01206529
84\C,3.4227157341,0.,-0.3206023561\C,3.8147395994,0.,-1.6499319095\C,-
1.1768841429,0.,-1.7365876745\C,-0.7243268632,0.,-3.0691275327\C,-1.63
63999988,0.,-4.1139544997\C,-3.0052770453,0.,-3.856115391\C,-3.4416062
047,0.,-2.5342816557\C,-2.5482520982,0.,-1.4712402659\C,-0.1688431383,

0.,2.9160701931\C,-1.5371364945,0.,3.2197879591\C,-1.9642914977,0.,4.5
432195822\C,-1.0337193286,0.,5.5817380548\C,0.3290226295,0.,5.28746982
3\C,0.7598800062,0.,3.9651176568\O,0.6078585143,0.,-3.4013940182\H,4.1
440148003,0.,0.4875338244\H,-1.2573778897,0.,-5.1291175956\H,-2.886150
3892,0.,-0.4457561007\H,-2.258426096,0.,2.4125777036\H,-3.0268214563,0
.,4.7643844918\H,1.0592488231,0.,6.0903905663\H,1.8148509331,0.,3.7219
93067\H,4.8706151079,0.,-1.898178345\H,3.177237728,0.,-3.731433379\H,-
3.720101942,0.,-4.6688725906\H,-1.3693497906,0.,6.613932495\Cl,-5.1631
54053,0.,-2.1973803969\\Version=ES64L-G09RevD.01\State=2-A"\HF=-1430.3
284514\S2=0.765997\S2-1=0.\S2A=0.750197\RMSD=7.175e-09\RMSF=2.619e-06\
Dipole=0.5277029,0.,-0.7415643\Quadrupole=-0.6680879,-7.7530668,8.4211
547,0.,-3.9883865,0.\PG=CS [SG(C19H11Cl1N3O1)]\\
No imaginary frequencies.

1i (X=Br)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\Gen\C19H11Br1N3O1(2)\PIOTR\12-Feb-2020\
0\\#P UB3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistan
ce,NoAngle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-Br benzotrazin
yl (phenazinoBT), Cs\\0,2\N,-0.2214531861,0.7673371436,0.\N,-2.9643933
868,0.9142058804,0.\C,-2.2758084713,-0.2293832557,0.\N,-0.9400701948,-
0.3773767152,0.\C,-0.6693780072,4.424788142,0.\C,-0.0491545013,3.18565
80399,0.\C,-0.8206969222,2.0202394086,0.\C,-2.2316269402,2.0690698837,
0.\C,-2.8467098299,3.3357864389,0.\C,-2.0712548737,4.4855306431,0.\C,1
.1766819576,0.6914193039,0.\C,1.9152657303,1.8903094487,0.\C,3.3028823
748,1.8524458646,0.\C,3.9769187558,0.6318460509,0.\C,3.2360885274,-0.5
47993683,0.\C,1.8466609895,-0.5362108252,0.\C,-3.0535207373,-1.4964855
419,0.\C,-2.4163033281,-2.7457960481,0.\C,-3.1656724712,-3.9183911624,
0.\C,-4.5598854556,-3.8612570242,0.\C,-5.2008565219,-2.622006871,0.\C,
-4.4547148723,-1.447241926,0.\O,1.3227465269,3.127243505,0.\H,-3.92972
64333,3.3769661227,0.\H,3.8450101121,2.7913625162,0.\H,1.2654506436,-1
.4466378364,0.\H,-1.3340553126,-2.7881977771,0.\H,-2.6599702587,-4.879
2534137,0.\H,-6.2854942244,-2.5699903908,0.\H,-4.9381995691,-0.4779531
026,0.\H,-2.552666784,5.458117878,0.\H,-0.0592545626,5.3205099748,0.\H
,5.0593543201,0.6046059431,0.\H,-5.1429872062,-4.7773725351,0.\Br,4.15
22744421,-2.2387305797,0.\\Version=ES64L-G09RevD.01\State=2-A"\HF=-983
.2804499\S2=0.766089\S2-1=0.\S2A=0.750199\RMSD=5.493e-09\RMSF=3.922e-0
6\Dipole=0.1937034,0.9024497,0.\Quadrupole=0.1139045,7.9726182,-8.0865
228,4.4618355,0.,0.\PG=CS [SG(C19H11Br1N3O1)]\\
No imaginary frequencies.

1j (X=COMe)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H14N3O2(2)\PIOTR\04-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-COMe benzot
razinyl, sec orient Ac, Cs\\0,2\N,-0.2088868957,0.6112797291,0.\N,2.41
77644144,1.4157062451,0.\C,2.0252013889,0.1401987089,0.\N,0.765282501,
-0.3265106365,0.\C,-0.6572816895,4.265593728,0.\C,-0.9572268129,2.9145
240794,0.\C,0.0711876671,1.9702931292,0.\C,1.4271645501,2.3592496588,0
.\C,1.7167666123,3.7359437001,0.\C,0.6872409415,4.6639636341,0.\C,-1.5
50109051,0.1990362901,0.\C,-2.5544413561,1.1851714903,0.\C,-3.89559095
76,0.81830653,0.\C,-4.246641382,-0.5235295628,0.\C,-3.2598971777,-1.51
87038841,0.\C,-1.9125065515,-1.1475551212,0.\C,3.0856594508,-0.9009273
685,0.\C,2.7701981106,-2.266455356,0.\C,3.7797207607,-3.2228788485,0.\
C,5.1179716456,-2.831009057,0.\C,5.4398935777,-1.4745840545,0.\C,4.432
6896416,-0.5154503349,0.\O,-2.2767762778,2.5251928921,0.\H,-4.64222983
9,1.603964904,0.\H,-1.1172623802,-1.8788973118,0.\H,1.7306000782,-2.56
82430679,0.\H,3.5214309615,-4.2770399351,0.\H,6.4792324803,-1.16207064

63,0.\H,4.6685397815,0.5411558587,0.\H,0.9191183838,5.7234876542,0.\H,
-1.4660814665,4.9860857244,0.\H,-5.2854407429,-0.8303091741,0.\H,5.904
6923768,-3.5787447138,0.\H,2.7571527294,4.0376525258,0.\C,-3.699921573
,-2.9498881529,0.\O,-4.8836726685,-3.2287851645,0.\C,-2.6435011955,-4.
0391805127,0.\H,-1.9989875934,-3.9596526238,-0.8820643565\H,-1.9989875
934,-3.9596526238,0.8820643565\H,-3.1418116504,-5.0085032952,0.\\Versi
on=ES64L-G09RevD.01\State=2-A"\HF=-1123.3887124\S2=0.765489\S2-1=0.\S2
A=0.750183\RMSD=4.125e-09\RMSF=1.132e-06\Dipole=0.4014171,0.6724903,0.
\Quadrupole=-7.0037245,10.2905007,-3.2867763,-10.69653,0.,0.\PG=CS [SG
(C21H12N3O2),X(H2)]\\@

No imaginary frequencies.

1l (X=NH_2)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H13N4O1(2)\PIOTR\21-Aug-
2019\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NH2 benzotr
azinyl, C1\\0,2\N,0.1857312541,-0.5836669205,-0.0147964334\N,-2.472508
2021,-1.2860319717,0.0058234125\C,-2.0287820219,-0.0282014217,-0.00447
08844\N,-0.7530581683,0.390215469,-0.0132237936\C,0.4864863447,-4.2565
09212,-0.0027934636\C,0.84543663,-2.9173266945,-0.0105308678\C,-0.1470
280621,-1.9326006403,-0.0073319714\C,-1.5182963977,-2.2677891451,0.003
9643006\C,-1.8636268369,-3.6303565153,0.0119862836\C,-0.8714220721,-4.
5994251566,0.008392021\C,1.5394701743,-0.2227976834,-0.020191918\C,2.5
018759932,-1.2469817436,-0.0225626619\C,3.8487379103,-0.9191067545,-0.
0237931522\C,4.2523764929,0.4112200026,-0.0234271115\C,3.3011450744,1.
4438277854,-0.0212575912\C,1.9428031847,1.1124788995,-0.017617143\C,-3
.0480440882,1.0545767961,-0.00572611\C,-2.679792783,2.4056005462,-0.05
9268379\C,-3.6506344493,3.4014927558,-0.060504178\C,-5.0027420823,3.06
45038378,-0.0076163729\C,-5.3771391708,1.7227006842,0.0455942838\C,-4.
4085652558,0.7243394232,0.0459235586\O,2.17313617,-2.5865642516,-0.021
2502073\H,4.5745991587,-1.7241459569,-0.0231079726\H,1.1790664485,1.87
84706412,-0.0167920469\H,-1.629399819,2.6639527103,-0.102364199\H,-3.3
512093395,4.4439526456,-0.1037903892\H,-6.4274852205,1.4520900403,0.08
66176864\H,-4.6847043315,-0.3217802647,0.0855097651\H,-1.1463565005,-5
.6488246306,0.0142812865\H,1.2654615104,-5.0092490436,-0.0057329952\H,
5.3104508191,0.6521045867,-0.0300791787\H,-5.7591822919,3.8429682034,-
0.0085830162\H,-2.915337369,-3.8897378437,0.0203475735\N,3.7028943413,
2.781204576,-0.0872044058\H,3.0243867085,3.4349645579,0.2792946566\H,4
.6172970871,2.9574633489,0.3062816149\\Version=ES64L-G09RevD.01\State=
2-A\HF=-1026.0933031\S2=0.765659\S2-1=0.\S2A=0.750193\RMSD=8.397e-09\R
MSF=1.530e-06\Dipole=1.170485,0.4215358,0.3996691\Quadrupole=5.0359232
,6.9301694,-11.9660926,3.7440516,3.1816031,2.7700216\PG=C01 [X(C19H13N
4O1)]\\

No imaginary frequencies.

1m (X=NHAc)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H15N4O2(2)\PIOTR\07-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck guess=check\\Parent flat C(8)-O-Ph(N1)
-NHAc benzotrazinyl, C1\\0,2\N,0.3436971215,0.7247270029,-0.0028464104
\N,3.0911126289,0.6933069417,0.0038505135\C,2.3293671128,-0.4015133934
,-0.0007680321\N,0.9876283758,-0.4648207236,-0.0040319818\C,1.02901205
42,4.3438376812,0.0062527886\C,0.3279026573,3.1485987344,0.0018470165\
C,1.0228954636,1.9359978634,0.0012550064\C,2.4335762306,1.8940609901,0
.004877964\C,3.128858235,3.1159498897,0.0093570891\C,2.4298234344,4.31
35683841,0.0100172232\C,-1.0570691623,0.7399683577,-0.0054864157\C,-1.
7151313475,1.9817313831,-0.0049872486\C,-3.1001660002,2.0221301594,-0.

0077529658\C,-3.8554918211,0.8527763553,-0.0107375265\C,-3.2022837311,
-0.3881235426,-0.010542739\C,-1.8049921064,-0.4350796793,-0.0082290393
\C,3.0243165776,-1.715970935,-0.0025946301\C,2.3100664933,-2.921600424
6,-0.0099245149\C,2.9817178032,-4.139366929,-0.0116269896\C,4.37576827
9,-4.1723352192,-0.0059931865\C,5.0936409869,-2.9773316634,0.001286388
6\C,4.4246785126,-1.7578432407,0.0029530199\O,-1.0421219937,3.18220732
97,-0.0019465319\H,-3.5850516407,2.991573949,-0.0076138996\H,-1.270766
3193,-1.376513858,-0.0081027339\H,1.2279227254,-2.892600672,-0.0144260
588\H,2.4158994897,-5.0656745567,-0.0174368817\H,6.1788469422,-2.99464
8923,0.0056617508\H,4.9693553038,-0.8222178566,0.0085190031\H,2.973498
7355,5.2522240591,0.0134952754\H,0.4783726287,5.2766589553,0.006698856
2\H,-4.9335716798,0.8875975439,-0.0131403407\H,4.8986200067,-5.1235108
167,-0.0073432931\H,4.2116904061,3.0866038926,0.0121644521\N,-3.883313
7677,-1.6193921397,-0.013132242\H,-3.287740324,-2.433617363,-0.0082239
285\C,-5.240729392,-1.8616112263,-0.0029229241\O,-6.0855531361,-0.9865
74109,-0.008644209\C,-5.5933059259,-3.3407202809,0.0349192091\H,-5.028
1471335,-3.9153149034,-0.7059343689\H,-5.374285828,-3.7579297995,1.023
9696723\H,-6.6597538956,-3.444466217,-0.1611581362\\Version=ES64L-G09R
evD.01\State=2-A\HF=-1178.7616394\S2=0.765494\S2-1=0.\S2A=0.750187\RMS
D=3.091e-09\RMSF=6.556e-07\Dipole=0.0297059,-0.6275593,0.0273388\Quadr
upole=-11.1414797,17.1288716,-5.9873919,7.7310182,-0.2453787,-0.110895
1\PG=C01 [X(C21H15N4O2)]\\@

No imaginary frequencies.

1n (X=I)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\Gen\C19H11I1N3O1(2)\PIOTR\11-Feb-2020\0
\\#P UB3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistanc
e,NoAngle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-I benzotrazinyl
(phenazinoBT), Cs\\0,2\N,-0.2224474548,0.768670183,0.\N,-2.9653629759
,0.9156925308,0.\C,-2.2768591397,-0.2279584603,0.\N,-0.9411874793,-0.3
758588676,0.\C,-0.6686589454,4.4257555226,0.\C,-0.0489027481,3.1864973
091,0.\C,-0.8212413554,2.0214641532,0.\C,-2.2322462367,2.0705014336,0.
\C,-2.8466697588,3.3374491012,0.\C,-2.0706212899,4.4868625016,0.\C,1.1
759208147,0.6922423794,0.\C,1.9150277943,1.8902754488,0.\C,3.302535517
,1.8504131178,0.\C,3.9754586186,0.6288277845,0.\C,3.2364810565,-0.5544
192777,0.\C,1.8454523736,-0.5356769989,0.\C,-3.0535229485,-1.495776811
5,0.\C,-2.4146013319,-2.7442376095,0.\C,-3.1623722642,-3.9178388411,0.
\C,-4.5567048264,-3.862559775,0.\C,-5.1993357712,-2.6242459664,0.\C,-4
.4547319248,-1.4484324569,0.\O,1.3233998242,3.1272412847,0.\H,-3.92967
91378,3.3792216681,0.\H,3.8458056302,2.7888389494,0.\H,1.2564462332,-1
.4410760044,0.\H,-1.332322523,-2.7850312793,0.\H,-2.6553119416,-4.8780
024938,0.\H,-6.2840355841,-2.5737481609,0.\H,-4.939762723,-0.479898361
6,0.\H,-2.5517834202,5.4595830302,0.\H,-0.0584451012,5.3214016158,0.\H
,5.0583595057,0.6087415101,0.\H,-5.1384629062,-4.7795374635,0.\I,4.237
0152299,-2.4149242056,0.\\Version=ES64L-G09RevD.01\State=2-A"\HF=-981.
4938655\S2=0.766052\S2-1=0.\S2A=0.750198\RMSD=9.723e-09\RMSF=1.863e-06
\Dipole=0.233742,0.8358537,0.\Quadrupole=-0.2698729,9.041333,-8.771460
1,3.0390022,0.,0.\PG=CS [SG(C19H11I1N3O1)]\\

No imaginary frequencies.

1o (X=OH)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C19H12N3O2(2)\PIOTR\06-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OH 2nd orint
benzotrazinyl (phenazinoBT), Cs\\0,2\N,-0.0797052931,0.5969250716,0.\N
,-1.6996514839,-1.622756539,0.\C,-0.3666456122,-1.6680362644,0.\N,0.48
72861285,-0.6312149831,0.\C,-3.3897221102,2.2141503632,0.\C,-2.0122498

294,2.060750726,0.\C,-1.4572149862,0.7779762824,0.\C,-2.2677467572,-0.
3773267205,0.\C,-3.6628092973,-0.2030522698,0.\C,-4.2036350167,1.07380
86023,0.\C,0.7468865165,1.7263184144,0.\C,0.1468519167,2.9963421012,0.
\C,0.9409715629,4.1343869652,0.\C,2.3270870233,4.0299168742,0.\C,2.925
0452984,2.7659866872,0.\C,2.1397448677,1.6163074347,0.\C,0.2702949969,
-3.011459415,0.\C,1.6636522649,-3.16146059,0.\C,2.236425175,-4.4287469
735,0.\C,1.4278693859,-5.5648498285,0.\C,0.0408806142,-5.424080462,0.\
C,-0.5349065907,-4.157992745,0.\O,-1.2195587715,3.1774257634,0.\H,-4.2
875360979,-1.087966434,0.\H,0.4524758583,5.1018734583,0.\H,2.578083172
3,0.6264117147,0.\H,2.2890481907,-2.2778522639,0.\H,3.3171088984,-4.53
03229085,0.\H,-0.5952144308,-6.3035014486,0.\H,-1.6103855872,-4.033555
8699,0.\H,-5.2810496103,1.2000710067,0.\H,-3.8077630938,3.2134607144,0
.\H,2.9548695258,4.9124813092,0.\H,1.8765857017,-6.5531803464,0.\O,4.2
867252397,2.7193017612,0.\H,4.5714938405,1.7985254519,0.\\Version=ES64
L-G09RevD.01\State=2-A"\HF=-1045.9580301\S2=0.765697\S2-1=0.\S2A=0.750
193\RMSD=2.875e-09\RMSF=4.789e-06\Dipole=0.2463683,0.3878941,0.\Quadru
pole=6.3996933,1.9819544,-8.3816477,-5.2024429,0.,0.\PG=CS [SG(C19H12N
3O2)]\\@

No imaginary frequencies.

1p (X=OBn)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C26H18N3O2(2)\PIOTR\07-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OBn 2nd orien
t benzotrazinyl (phenazinoBT), C1\\0,2\N,-1.7236151143,-0.6739409862,-
0.0149607907\N,-4.2247124752,0.4665901651,0.0089230512\C,-3.085218189,
1.1589512651,-0.0252763119\N,-1.8328291219,0.6741260023,-0.038130581\C
,-3.8155196518,-3.7057757966,0.0753142614\C,-2.6908647189,-2.896548849
5,0.0409213224\C,-2.8356612385,-1.5066232011,0.0192118513\C,-4.1085298
295,-0.8971463097,0.031487944\C,-5.2384877421,-1.7330616991,0.06658715
14\C,-5.0838477481,-3.1109152744,0.087855627\C,-0.4487633742,-1.254201
9452,-0.022789116\C,-0.351608547,-2.6529436652,-0.0000933683\C,0.89967
27394,-3.2565341927,-0.0052871861\C,2.0516200669,-2.4846709181,-0.0338
317005\C,1.9589808783,-1.0856628516,-0.0570077994\C,0.7098883551,-0.46
85221481,-0.0500854098\C,-3.1889663422,2.6420112885,-0.0524786534\C,-2
.0489231597,3.4548247251,-0.1127686924\C,-2.1709464396,4.8399578718,-0
.1379451688\C,-3.4317235065,5.4347001419,-0.102791381\C,-4.5707116985,
4.6330207621,-0.0428307305\C,-4.4519572754,3.2474400887,-0.0181680649\
O,-1.4522282825,-3.481344247,0.0285206404\H,-6.2167397078,-1.267912829
9,0.0759636314\H,0.9497524824,-4.3390262778,0.0131876605\H,0.587959104
7,0.6030166816,-0.0610358549\H,-1.0714516606,2.9904210962,-0.141002774
7\H,-1.2794410342,5.457327182,-0.1856685511\H,-5.555607662,5.088311042
9,-0.0152840567\H,-5.3277768412,2.6126433848,0.0276408698\H,-5.9608348
831,-3.7488352652,0.1147983838\H,-3.6893667675,-4.7814988506,0.0918065
872\H,3.0329111374,-2.9432941007,-0.0374799259\H,-3.5252153852,6.51591
83484,-0.1223800693\O,3.1439927545,-0.4190551059,-0.0793142967\C,3.121
5825615,1.0047898261,-0.1452251902\H,2.6234925976,1.4170079984,0.74218
48262\H,2.5413867736,1.3161963993,-1.0266880579\C,4.539267398,1.509788
8435,-0.2362357993\C,5.4826343669,0.8546781664,-1.033044039\C,4.912754
7751,2.669339717,0.4449648374\C,6.7770576093,1.3542263611,-1.144670280
1\C,6.2058520242,3.1759991429,0.3261019878\C,7.1415802697,2.518370692,
-0.4685894553\H,5.1991965906,-0.0539920571,-1.5522221143\H,4.189064662
3,3.1787955558,1.0751409828\H,7.5028840349,0.834225231,-1.7617574009\H
,6.482469797,4.0780591024,0.8622607606\H,8.1508082475,2.9071087894,-0.
5575086856\\Version=ES64L-G09RevD.01\State=2-A\HF=-1316.3237708\S2=0.7
65765\S2-1=0.\S2A=0.750196\RMSD=6.610e-09\RMSF=1.331e-06\Dipole=0.7036
28,-0.1956697,-0.0494546\Quadrupole=2.7653557,7.1419043,-9.9072599,6.1
137531,-1.7915708,1.7072673\PG=C01 [X(C26H18N3O2)]\\@

No imaginary frequencies.

1q (X=Ph)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C25H16N3O1(2)\PIOTR\09-Feb-
2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Ph benzotrazi
nyl (phenazinoBT), C1\\0,2\N,-0.2971786719,-1.2456028721,-1.0550575944
\N,1.4980172435,-2.4699340769,0.628016017\C,0.1791606269,-2.4425177462
,0.8299020214\N,-0.7544803062,-1.8653713235,0.0562727471\C,2.847773095
9,-0.5256495653,-2.8323353764\C,1.4961105589,-0.5547513093,-2.53158029
72\C,1.0527595978,-1.2045202316,-1.377019935\C,1.955010097,-1.83946246
73,-0.4972685671\C,3.3241525449,-1.8006068335,-0.8168339991\C,3.752731
5248,-1.1533090936,-1.9653754263\C,-1.2142211108,-0.6177599284,-1.9109
267005\C,-0.7228923836,0.0203217632,-3.0637497715\C,-1.6030446287,0.64
50700921,-3.9344444674\C,-2.9685680433,0.6409077799,-3.670457521\C,-3.
48200933,0.0086751954,-2.5278744474\C,-2.5855217917,-0.6194496567,-1.6
562351852\C,-0.3399578001,-3.1220133542,2.0457760117\C,-1.7117928763,-
3.1674988092,2.3289781813\C,-2.1742059841,-3.8095351975,3.4727405436\C
,-1.2753848362,-4.4149010769,4.3502913976\C,0.0907320782,-4.3741263655
,4.0752678535\C,0.556561567,-3.7333462421,2.932029204\O,0.6126060636,0
.061028913,-3.3826285735\H,4.0185750721,-2.2874725645,-0.1428784003\H,
-1.1972102652,1.1386721737,-4.8099158579\H,-2.9357777101,-1.142680029,
-0.7778981815\H,-2.4077399873,-2.6979281207,1.6455840647\H,-3.23939089
03,-3.8380158635,3.679203087\H,0.7964322739,-4.8432494365,4.7534868428
\H,1.6146044361,-3.6946740954,2.7057447703\H,4.810425373,-1.1280147378
,-2.2046173382\H,3.1766335118,-0.0182380358,-3.7310857983\H,-3.6395651
567,1.1588783695,-4.3459737223\H,-1.6380034556,-4.9155953791,5.2424794
674\C,-4.9375937059,0.0062939337,-2.2444743333\C,-5.4170748848,0.12023
00164,-0.9312042286\C,-5.8724925072,-0.1084465311,-3.2838709818\C,-6.7
833231527,0.1189794552,-0.6666542738\C,-7.2388820197,-0.1084601212,-3.
019857435\C,-7.7006023893,0.0050866426,-1.7097966843\H,-4.7118246277,0
.2365244628,-0.1148854964\H,-5.5234871414,-0.226409092,-4.3044892576\H
,-7.1315190893,0.2159170983,0.3567257881\H,-7.9437609702,-0.2066444576
,-3.8393188461\H,-8.7658441788,0.0046175381,-1.5035354503\\Version=ES6
4L-G09RevD.01\State=2-A\HF=-1201.8004269\S2=0.765616\S2-1=0.\S2A=0.750
19\RMSD=3.318e-09\RMSF=2.208e-06\Dipole=-0.3452567,0.4263615,-0.630949
1\Quadrupole=7.1726485,-9.0513744,1.878726,0.3010548,-3.0159191,-4.931
7652\PG=C01 [X(C25H16N3O1)]\\

No imaginary frequencies.

1r (X=thienyl)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C23H14N3O1S1(2)\PIOTR\10-Fe
b-2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Thio benzot
razinyl (phenazinoBT), C1\\0,2\N,-0.5100749881,-2.2146382221,-2.177187
2015\N,1.0764676153,-4.3784702938,-1.5823487388\C,-0.236448372,-4.3249
826045,-1.3500317509\N,-1.0719078925,-3.3063054149,-1.6110011507\C,2.7
528745816,-0.9596044368,-3.3366241669\C,1.3977516007,-1.005020143,-3.0
544049175\C,0.8454408024,-2.1472016808,-2.4697983587\C,1.6395889668,-3
.2703171237,-2.1542981975\C,3.0138723192,-3.2081705935,-2.4469455762\C
,3.5510163072,-2.0695927052,-3.0273593979\C,-1.3208689403,-1.110091016
5,-2.4769649018\C,-0.7218151374,0.0168994085,-3.0685434969\C,-1.496844
5007,1.1227196434,-3.3846668208\C,-2.860189399,1.1239986407,-3.1130305
473\C,-3.4796668491,0.0082851929,-2.5269309556\C,-2.6905034735,-1.1085
215502,-2.2205805022\C,-0.8695936971,-5.518498772,-0.7304915862\C,-2.2
46233018,-5.5637898694,-0.4719192783\C,-2.8174606713,-6.6911860607,0.1
081899868\C,-2.0239396537,-7.7891406302,0.4389818904\C,-0.6537216246,-

7.7517959557,0.1845977388\C,-0.0792624018,-6.626020712,-0.3960230537\O
,0.6184944334,0.0835910031,-3.358510602\H,3.6256922267,-4.0689793578,-
2.2059154643\H,-1.0107610069,1.980658896,-3.8343860752\H,-3.1278032733
,-2.0018428827,-1.7987844896\H,-2.8599449246,-4.7104454355,-0.73082673
85\H,-3.8851544432,-6.7133341667,0.302019734\H,-0.0297102667,-8.602615
6153,0.4390450021\H,0.983203994,-6.5835638658,-0.5998446998\H,4.611868
7764,-2.0297267387,-3.2500031649\H,3.1670626991,-0.0674098739,-3.79027
53845\H,-3.4436234939,2.0092099359,-3.3401232932\H,-2.4712874388,-8.66
83817253,0.8917223533\C,-4.9140201227,-0.0085638879,-2.2251302543\C,-5
.5761612808,-0.7189513669,-1.251496788\C,-6.9815959937,-0.5025951935,-
1.2418943487\C,-7.3887389431,0.3717181344,-2.2101014373\S,-6.054982468
4,0.9378270752,-3.1524125197\H,-5.0629464658,-1.3572392699,-0.54297358
09\H,-7.6571183877,-0.9731265834,-0.5382624749\H,-8.3876063241,0.71708
34882,-2.4306249799\\Version=ES64L-G09RevD.01\State=2-A\HF=-1522.55560
1\S2=0.76587\S2-1=0.\S2A=0.750197\RMSD=2.447e-09\RMSF=2.208e-06\Dipole
=-0.2130941,0.5711108,-0.0645579\Quadrupole=9.1781672,-1.5693477,-7.60
88195,1.983991,-5.4402635,-5.1294693\PG=C01 [X(C23H14N3O1S1)]\\
No imaginary frequencies.

1s (X=CCPh)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C27H16N3O1(2)\PIOTR\14-Feb-
2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-CCPh benzotra
zinyl (phenazinoBT), Cs\\0,2\N,0.7276841485,1.6986784905,0.\N,-0.78675
67277,3.9915911126,0.\C,-1.2950427192,2.7574130416,0.\N,-0.6204964611,
1.596085887,0.\C,3.3985999406,4.2340927276,0.\C,2.7715571274,2.9995586
808,0.\C,1.3768768789,2.9255783237,0.\C,0.5778128642,4.0885311606,0.\C
,1.2296876492,5.3350253376,0.\C,2.6145261269,5.3962025123,0.\C,1.49859
70175,0.5268385341,0.\C,2.9010504055,0.6493915094,0.\C,3.698783198,-0.
4869814404,0.\C,3.1195942932,-1.7489243521,0.\C,1.7199655557,-1.891173
679,0.\C,0.9181145215,-0.7392478526,0.\C,-2.7755575962,2.6281338923,0.
\C,-3.3995723792,1.3731849309,0.\C,-4.786927912,1.2770584848,0.\C,-5.5
711847509,2.4301047304,0.\C,-4.9576882652,3.6819763691,0.\C,-3.5704476
835,3.7818986557,0.\O,3.5418150763,1.8621794216,0.\H,0.6187672266,6.22
9550761,0.\H,4.7749468906,-0.3589910982,0.\H,-0.1592632645,-0.81648699
57,0.\H,-2.7888111177,0.4794011608,0.\H,-5.2575463398,0.2990238039,0.\
H,-5.5613603263,4.5839503708,0.\H,-3.0804145758,4.7473103717,0.\H,3.10
94788498,6.3613841942,0.\H,4.4809993763,4.2759180651,0.\H,3.7451172198
,-2.6332527051,0.\H,-6.6538617179,2.3527135553,0.\C,1.123006032,-3.182
5270184,0.\C,0.6179015402,-4.2856952506,0.\C,0.0201909143,-5.577843299
7,0.\C,-1.3795254302,-5.7172582548,0.\C,0.8182264325,-6.7361503589,0.\
C,-1.959692119,-6.9800784604,0.\C,0.2296917828,-7.995156418,0.\C,-1.15
93394022,-8.1225275223,0.\H,-1.9980934794,-4.8268496548,0.\H,1.8975517
113,-6.6328158168,0.\H,-3.0408582542,-7.0733537829,0.\H,0.857270616,-8
.8804484502,0.\H,-1.615758164,-9.1068448443,0.\\Version=ES64L-G09RevD.
01\State=2-A"\HF=-1277.9574937\S2=0.766056\S2-1=0.\S2A=0.750202\RMSD=2
.043e-09\RMSF=4.718e-07\Dipole=0.5946377,-0.48837,0.\Quadrupole=6.7679
82,8.208763,-14.976745,5.8086655,0.,0.\PG=CS [SG(C27H16N3O1)]\\
No imaginary frequencies.

1t (X=OAc)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H14N3O3(2)\PIOTR\27-Sep-
2020\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OAc benzotraz
inyl (phenazinoBT), C1\\0,2\N,0.0162894508,0.6301359637,-0.0385883945\
N,-2.5959053823,-0.2176247815,0.0298982997\C,-1.5421607761,-1.03617695
9,0.0304617753\N,-0.2430336138,-0.6962244007,-0.0014674561\C,-1.715730

634,3.8799171423,-0.088017912\C,-0.6916424333,2.9474491368,-0.08378503
96\C,-0.9930866872,1.5838251812,-0.0439782252\C,-2.3265090205,1.123498
2505,-0.0079106787\C,-3.3543281889,2.0834543556,-0.0127588009\C,-3.044
1524336,3.4340317539,-0.0520242534\C,1.3483191721,1.0613783854,-0.0720
402973\C,1.6072312009,2.4428669804,-0.1128819588\C,2.9149091904,2.9032
763276,-0.1514853522\C,3.9831850427,2.009988479,-0.1494319962\C,3.7168
672353,0.643355995,-0.1021590346\C,2.4154804665,0.1624283146,-0.063252
1339\C,-1.8117134249,-2.4973499583,0.0701505522\C,-0.768449689,-3.4331
42257,0.0745179858\C,-1.0445777711,-4.7956204286,0.1120558905\C,-2.364
5319639,-5.2441293483,0.1458074387\C,-3.4077355301,-4.3193284066,0.141
5730329\C,-3.1351431165,-2.9559529373,0.1041846511\O,0.607840462,3.387
0269105,-0.1200851432\H,-4.3790628088,1.7333860128,0.0149534854\H,3.08
23812017,3.9733521642,-0.1842611657\H,2.218865888,-0.8991778043,-0.033
3393159\H,0.2552986293,-3.0822555133,0.0483566788\H,-0.2270843555,-5.5
095931633,0.1149830552\H,-4.4376724238,-4.6607308234,0.1676127107\H,-3
.9352823641,-2.2266298728,0.1008371286\H,-3.842633771,4.1682184245,-0.
0551753174\H,-1.4683108716,4.9340364183,-0.1187889309\H,5.0006086691,2
.3724151491,-0.1746416649\H,-2.5781463838,-6.3079235543,0.1751229873\O
,4.7145362203,-0.3230393394,-0.1728066568\C,5.8227470089,-0.234220838,
0.6291390379\O,6.0207301649,0.6515434861,1.4140864813\C,6.7272121236,-
1.4096094707,0.3659678717\H,6.1978218241,-2.342965555,0.5773420939\H,7
.0146588128,-1.4310414123,-0.6890385767\H,7.6128850905,-1.3313235472,0
.994782018\\Version=ES64L-G09RevD.01\State=2-A\HF=-1198.6203984\S2=0.7
65645\S2-1=0.\S2A=0.750189\RMSD=1.932e-09\RMSF=6.925e-07\Dipole=0.4960
087,0.0654465,-0.4502107\Quadrupole=3.3201283,7.5366976,-10.8568259,-8
.1856253,-5.281074,-2.3547451\PG=C01 [X(C21H14N3O3)]\\
No imaginary frequencies.

1u (X=NHCOCF$_3$)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H12F3N4O2(2)\PIOTR\09-Ma
y-2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-NHCOCF
3 2nd orient benzotrazinyl, C1\\0,2\N,1.2710187132,-0.8598085029,0.000
0036279\N,3.6469137627,0.5168312149,-0.000014895\C,2.4461126557,1.0977
332315,-0.0000179467\N,1.2462108787,0.4924596514,-0.0000075953\C,3.644
777066,-3.6756326933,0.0000260833\C,2.4482733654,-2.9785478149,0.00002
33615\C,2.4574534068,-1.5813665306,0.0000087439\C,3.6647702138,-0.8514
218078,-0.0000021811\C,4.8710433444,-1.5744918415,0.0000006863\C,4.850
5458893,-2.9605665176,0.0000143565\C,0.0594820431,-1.5607992316,0.0000
020636\C,0.0953940349,-2.9669852818,0.0000179464\C,-1.0897254348,-3.68
54426698,0.0000151025\C,-2.3224618485,-3.0385759447,-0.0000070038\C,-2
.3578732078,-1.6389836329,-0.0000272438\C,-1.1693156334,-0.9052403708,
-0.0000199383\C,2.4059373727,2.5834111709,-0.0000130585\C,1.1919045436
,3.2835461932,0.0000120291\C,1.1800238163,4.6741869951,0.0000166388\C,
2.3787697802,5.3864875636,-0.0000037794\C,3.5906441813,4.6973883784,-0
.0000284484\C,3.6058950338,3.3066545659,-0.0000325435\O,1.268880731,-3
.6805877522,0.0000360122\H,-1.0336368818,-4.7677063698,0.0000290109\H,
-1.1700568289,0.1770943304,-0.0000367567\H,0.2623054466,2.7288522118,0
.0000287774\H,0.2325849365,5.2036774202,0.0000365468\H,4.5277846947,5.
2447801264,-0.0000443566\H,4.5397033478,2.7589097313,-0.0000511492\H,5
.7850773352,-3.5111294867,0.0000162566\H,3.6238300519,-4.7586106122,0.
000037081\H,-3.2431440626,-3.6011906199,-0.0000111834\H,2.3676755271,6
.4717849174,-0.0000001387\H,5.7998181939,-1.0170646353,-0.0000080291\N
,-3.5612553846,-0.9023936074,-0.0000640889\H,-3.4670153013,0.102833068
2,-0.0000606288\C,-4.835203126,-1.3748116216,-0.0001182399\O,-5.198691
1787,-2.5310815196,-0.0001073601\C,-5.9069047089,-0.2546737964,-0.0002
552451\F,-6.6782918089,-0.3599256872,1.0817571921\F,-5.3616635163,0.98
5480763,0.000022801\F,-6.6777299239,-0.3596740349,-1.0827024377\\Versi

on=ES64L-G09RevD.01\State=2-A\HF=-1476.4760905\S2=0.765777\S2-1=0.\S2A
=0.750192\RMSD=8.742e-09\RMSF=2.867e-06\Dipole=0.877358,0.0317089,0.00
00633\Quadrupole=-7.8664746,10.1530096,-2.286535,-10.9601059,-0.000745
8,-0.0001726\PG=C01 [X(C21H12F3N4O2)]\\@

No imaginary frequencies.

1v (X=NHCOOMe)

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(2d,p)\C21H15N4O3(2)\PIOTR\09-May-
2021\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-NHCOOMe
2nd orient benzotrazinyl, C1\\0,2\N,-0.7310286981,-0.8863007903,0.0000
025866\N,-3.1628247015,0.3927253433,0.0000052658\C,-1.9860712203,1.020
5785698,0.0000051157\N,-0.7627931118,0.4658527552,0.0000028761\C,-2.98
93505946,-3.7966272572,0.0000056396\C,-1.8207830884,-3.0518115116,0.00
00040444\C,-1.8874352404,-1.6556745088,0.0000042499\C,-3.1241760336,-0
.9755861487,0.00000558\C,-4.2996018984,-1.7469497906,0.0000068896\C,-4
.2225527808,-3.131479747,0.000007049\C,0.5090547814,-1.5373833488,-0.0
00000149\C,0.5293656322,-2.9423923207,-0.0000005909\C,1.7440715759,-3.
6091322193,-0.0000042829\C,2.9483762998,-2.9113063089,-0.0000083169\C,
2.9310632737,-1.5098282942,-0.0000081982\C,1.7097341845,-0.830629823,-
0.0000034199\C,-2.0059771575,2.5071899382,-0.0000000554\C,-0.820637049
1,3.2546869958,-0.0000023337\C,-0.8635614862,4.6447031643,-0.000006674
9\C,-2.0893555561,5.3095191055,-0.0000091812\C,-3.2730572981,4.5730649
956,-0.0000072299\C,-3.2334033878,3.1827226025,-0.0000027062\O,-0.6163
756449,-3.7054300308,0.0000016479\H,1.7344516696,-4.6930105639,-0.0000
047704\H,1.6645438711,0.2505990014,-0.0000035894\H,0.1295348709,2.7359
944863,-0.0000003174\H,0.0623576968,5.211142319,-0.0000081185\H,-4.231
1803074,5.0829800456,-0.0000092158\H,-4.14462637,2.5980285636,-0.00000
11127\H,-5.134108403,-3.7195167381,0.0000080005\H,-2.9241838433,-4.877
8807168,0.0000054224\H,3.891964102,-3.4350062461,-0.0000120241\H,-2.12
10892275,6.3944661259,-0.0000126688\H,-5.2504247611,-1.2280085208,0.00
00077281\N,4.0965367524,-0.7265210636,-0.0000144006\H,3.9720475771,0.2
743580726,-0.0000150091\C,5.4008813173,-1.1475908122,-0.0000252965\O,5
.7994550344,-2.2903785868,-0.0000282382\O,6.2043590248,-0.0552470808,-
0.0000317122\C,7.6058437773,-0.348522387,-0.0000438682\H,7.881159472,-
0.920494686,0.8890974185\H,7.8811517904,-0.9204563881,-0.8892124718\H,
8.1062596963,0.6196361757,-0.000025971\\Version=ES64L-G09RevD.01\State
=2-A\HF=-1253.9902246\S2=0.765535\S2-1=0.\S2A=0.750188\RMSD=4.290e-09\
RMSF=1.822e-06\Dipole=0.6466657,0.2122292,-0.0000049\Quadrupole=7.7046
37,1.5659275,-9.2705646,11.5967341,-0.0000526,-0.0000631\PG=C01 [X(C21
H15N4O3)]\\@

No imaginary frequencies.

1a-*leuco* (X=H)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H13N3O1\PIOTR\06-Apr-201
9\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1) benzotrazinyl-4H (ph
enazinoBT), C1\\0,1\N,0.0167277772,0.7451214957,0.3708922059\N,1.15486
23131,-1.7161458632,0.38724341\C,-0.2270204202,-1.5189771724,0.2070427
82\N,-0.7915675717,-0.3619473404,0.2038294813\C,3.5393804118,1.6655850
455,-0.3518977142\C,2.1697159592,1.7792579174,-0.1172916585\C,1.399999
2908,0.6471106849,0.1169281347\C,1.9968058361,-0.6117489938,0.11486982
38\C,3.3587537463,-0.7394560519,-0.1315097284\C,4.1262518644,0.4055593
009,-0.3609443181\C,-0.5804547593,2.0089483589,0.2603083741\C,0.239532
7719,3.1294250841,0.0391826494\C,-0.3047499695,4.4002592318,-0.0453814
167\C,-1.6819154183,4.5840038847,0.08716088\C,-2.501989242,3.481264681
8,0.3006540108\C,-1.9568473231,2.2008277216,0.3867527469\C,-1.06570399

38,-2.7232846194,0.0564529698\C,-2.329136759,-2.6303749526,-0.54657280
95\C,-3.1232880971,-3.7597415302,-0.6938195705\C,-2.6730277563,-5.0032
086685,-0.2454452161\C,-1.423660435,-5.1048711895,0.359785964\C,-0.624
0384014,-3.9741342687,0.5112414451\O,1.6151069955,3.0326801997,-0.1054
959669\H,3.816435608,-1.7233824153,-0.1320347781\H,0.3669148998,5.2329
813717,-0.2215270072\H,-3.5742999623,3.6085030655,0.404122909\H,-2.582
2242991,1.3336596503,0.5511865113\H,-2.6652766995,-1.6635665284,-0.900
8327962\H,-4.0957029009,-3.6727963027,-1.1676713577\H,-1.0698628825,-6
.0638450789,0.7240548013\H,0.3276278129,-4.0629926599,1.0246553126\H,5
.1910639475,0.3100480123,-0.5408698002\H,4.1156426437,2.5675354243,-0.
5194287141\H,-2.1006221952,5.5819369698,0.0217749758\H,-3.2939311296,-
5.8846798643,-0.366853654\H,1.4908343576,-2.5924113106,0.0106096488\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-971.3414708\RMSD=3.532e-09\RMSF=
7.946e-07\Dipole=0.2702364,-1.0986145,-0.3057615\Quadrupole=3.5557137,
6.1188852,-9.6745989,-0.882348,0.350537,-0.403506\PG=C01 [X(C19H13N3O1
)]\\
No imaginary frequencies.

1b-*leuco* (X=COOMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H15N3O3\PIOTR\06-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-COOMe benzotraz
inyl 4H, C1\\0,1\N,0.2737290629,0.739901808,-0.3005789197\N,2.98182799
79,0.7582669409,-0.4174393953\C,2.2407666574,-0.4126685411,-0.17551278
97\N,0.9551406783,-0.4497646061,-0.1231961903\C,0.9096221294,4.3491080
433,0.2815335991\C,0.2376625744,3.1403814573,0.1125726969\C,0.94185465
49,1.9654444728,-0.1103810027\C,2.3340035074,1.9894996144,-0.162024221
5\C,3.0180225438,3.185976112,0.0190623539\C,2.2991269597,4.3643275915,
0.2368620916\C,-1.1182089122,0.7202436751,-0.1374020544\C,-1.792968063
8,1.938357351,0.0714434849\C,-3.1733746958,1.9713401724,0.2064930744\C
,-3.9099894023,0.7941594734,0.1391734463\C,-3.2546444933,-0.4216135716
,-0.0612523479\C,-1.8612185956,-0.4550729493,-0.1988135156\C,2.9979450
117,-1.6688874751,-0.0143356262\C,2.4167315645,-2.7587779736,0.6507738
215\C,3.1227358856,-3.9439875213,0.808062512\C,4.4205154104,-4.0643758
913,0.307069412\C,5.0034276949,-2.9907331826,-0.3601919211\C,4.2986357
196,-1.7999085199,-0.5214380023\O,-1.1362878428,3.1484826825,0.1537225
307\H,-3.6493343087,2.9313787946,0.3701120665\H,-1.3448387172,-1.39079
28652,-0.352982835\H,1.4129227399,-2.6525763794,1.0435583914\H,2.66250
65855,-4.7765978581,1.3300739894\H,6.0062605262,-3.0789596649,-0.76508
55396\H,4.750262488,-0.9881091726,-1.0819926833\H,2.8305197586,5.30034
48894,0.3656354071\H,0.3309106568,5.250794348,0.4414164025\H,-4.987835
4969,0.7995161474,0.2413097278\H,4.9712528968,-4.9903228435,0.43575197
33\H,4.1023418407,3.1979879385,-0.0212178588\C,-4.0826776467,-1.652826
9405,-0.1249941848\O,-5.2884923566,-1.6782411711,-0.0153555881\O,-3.34
0928648,-2.7657301745,-0.3225168647\C,-4.0877217297,-3.9842355984,-0.3
975546808\H,-3.3523248597,-4.7721698192,-0.5603270569\H,-4.6369884357,
-4.1580365498,0.5310813102\H,-4.8010963519,-3.9491299328,-1.2246083504
\H,3.9340454014,0.7136306892,-0.0804037424\\Version=ES64L-G09RevD.01\S
tate=1-A\HF=-1199.2328528\RMSD=3.648e-09\RMSF=7.899e-07\Dipole=2.08856
68,-0.142675,0.2024914\Quadrupole=-2.75298,10.524139,-7.771159,-0.2527
713,0.2406442,0.313051\PG=C01 [X(C21H15N3O3)]\\
No imaginary frequencies.

1c-*leuco* (X=CN)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H12N4O1\PIOTR\08-Apr-201
9\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CN benzotraziny

l 4H, C1\\0,1\N,-0.0069506008,-0.5901947333,-0.3282416145\N,-2.3536649
97,0.7676054778,-0.3513826988\C,-1.1129182724,1.4030864685,-0.18243454
58\N,0.0168109879,0.7850834415,-0.1773298766\C,-2.361709455,-3.3828506
803,0.3180875232\C,-1.1779754774,-2.6795295534,0.1091219479\C,-1.19753
32168,-1.3083353084,-0.1007588971\C,-2.4099315167,-0.6224535034,-0.103
4559141\C,-3.5984497293,-1.3094039096,0.1163058757\C,-3.567829008,-2.6
90737421,0.323910268\C,1.2039599427,-1.2752558326,-0.2180385268\C,1.17
88924387,-2.6710492861,-0.0206138013\C,2.3566498693,-3.396912732,0.065
3894592\C,3.5884058472,-2.7579066241,-0.0387517193\C,3.6259299976,-1.3
73042554,-0.2263893317\C,2.4358488957,-0.6348069192,-0.3149221376\C,-1
.1227712886,2.8721954546,-0.042303557\C,-0.0442751564,3.5261445942,0.5
712859796\C,-0.0466121395,4.9080765152,0.7074858139\C,-1.1235825135,5.
6614357039,0.2365918006\C,-2.1957893318,5.0218059074,-0.3793294407\C,-
2.197464297,3.6358854411,-0.5193566088\O,0.0052030945,-3.382424044,0.0
980240078\H,2.2887631673,-4.4671398162,0.2216802987\H,2.4582456242,0.4
360620178,-0.4583532461\H,0.7824810407,2.9328021423,0.9421172681\H,0.7
919770902,5.4004250681,1.1887496113\H,-3.0307267978,5.600163076,-0.760
8888186\H,-3.0190676016,3.1561394425,-1.0409319728\H,-4.4949324343,-3.
2290584424,0.4839154368\H,-2.3144514535,-4.4545989606,0.4680465522\H,4
.508858131,-3.3240906592,0.0279044258\H,-1.1239458518,6.7406220884,0.3
483682412\H,-4.5402722602,-0.7706007858,0.1143155775\C,4.8846113292,-0
.6979699476,-0.328647149\N,5.9061032675,-0.1548878166,-0.4095103574\H,
-3.1372136143,1.2920057904,0.0130542464\\Version=ES64L-G09RevD.01\Stat
e=1-A\HF=-1063.5870263\RMSD=5.724e-09\RMSF=1.013e-06\Dipole=-2.9144592
,0.1518635,0.4542467\Quadrupole=-14.0838188,16.9772445,-2.8934257,-6.3
360503,2.4617314,0.0785809\PG=C01 [X(C20H12N4O1)]\\
No imaginary frequencies.

1d-*leuco* (X=NO_2)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H12N4O3\PIOTR\21-Aug-201
9\0\\#P B3LYP/6-31G(2d,p) Opt=(tight, ReadFC) freq(noraman, ReadIso) #
P Geom=(NoDistance,NoAngle) fcheck guess=check\\Parent flat C(8)-O-Ph(
N1)-NO2 benzotrazinyl 4H, C1\\0,1\N,0.2413745445,0.7487165884,-0.25457
36698\N,2.9529050818,0.7398707176,-0.3476853503\C,2.1970960549,-0.4261
851271,-0.1462641971\N,0.9101664431,-0.4528941879,-0.108661213\C,0.904
3833949,4.3618540908,0.2531981906\C,0.2260019902,3.1554207603,0.100904
766\C,0.9211830924,1.9698324461,-0.0854876642\C,2.3137672187,1.9792373
209,-0.1226739768\C,3.0051739175,3.1743561096,0.0399000075\C,2.2946877
639,4.3630937166,0.2255934458\C,-1.1463282945,0.7419693916,-0.11798567
59\C,-1.8169588275,1.9723976292,0.054109364\C,-3.1991485768,2.02201533
82,0.1645826402\C,-3.9532314054,0.8533783694,0.1118389867\C,-3.2833158
233,-0.3516443096,-0.0480379303\C,-1.8967405005,-0.4287715685,-0.16305
92008\C,2.940814255,-1.6937140183,-0.0117522214\C,2.3450248407,-2.7941
725725,0.6217908133\C,3.0388366347,-3.9901162881,0.7507314049\C,4.3377
289312,-4.1094132063,0.2528448648\C,4.9349663722,-3.0244617999,-0.3829
674538\C,4.2427430021,-1.8230708325,-0.5158898229\O,-1.1513068126,3.17
37595108,0.1232455172\H,-3.6682131693,2.9895272856,0.2987230086\H,-1.4
100563809,-1.3839185815,-0.2853821487\H,1.340044484,-2.6904193718,1.01
20923468\H,2.5672031112,-4.8319119901,1.2468412392\H,5.9386510999,-3.1
121640021,-0.7856581951\H,4.7045126168,-1.001317841,-1.0531457203\H,2.
8331832679,5.2965346686,0.3418744953\H,0.3320039503,5.2717386365,0.386
7182326\H,-5.0304575374,0.8642184653,0.1959928213\H,4.8783184185,-5.04
41361445,0.3586932701\H,4.0898073691,3.1768089266,0.0104233509\N,-4.05
94618363,-1.5939164712,-0.0972694671\O,-3.4453379958,-2.6478720873,-0.
2270085933\O,-5.2802715161,-1.5084424191,-0.0049272385\H,3.9000268209,
0.682848847,0.0005219736\\Version=ES64L-G09RevD.01\State=1-A\HF=-1175.
8545581\RMSD=3.831e-09\RMSF=1.545e-06\Dipole=2.6648671,1.3140726,0.343
4036\Quadrupole=-0.9097982,4.4973376,-3.5875394,-13.0414928,-1.1025844

,-0.9778252\PG=C01 [X(C19H12N4O3)]\\
No imaginary frequencies.

1e-*leuco* (X=CF_3)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H12F3N3O1\PIOTR\14-Feb-2
020\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geo
m=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CF3 benzotraz
inyl leuco, C1\\0,1\N,-0.1470126049,-0.7621206254,-0.3222368077\N,-2.8
478551662,-1.0114641851,-0.3600014225\C,-2.2024919312,0.2220509054,-0.
1688369228\N,-0.923577615,0.3698912548,-0.1558794148\C,-0.4582771846,-
4.4089935832,0.2863495713\C,0.1038314603,-3.1491533073,0.0920267424\C,
-0.7043787032,-2.0391360364,-0.1101808628\C,-2.0901291005,-2.180620718
1,-0.1196583755\C,-2.6646765135,-3.429777672,0.0853293335\C,-1.8423228
066,-4.541515893,0.2852687901\C,1.2377417167,-0.6225674583,-0.19495889
28\C,2.0219939911,-1.7770813717,-0.0047126796\C,3.3994123485,-1.686918
7609,0.1056100591\C,4.032484832,-0.4472686681,0.0275845737\C,3.2638758
032,0.696515057,-0.157003459\C,1.8742559469,0.6145090052,-0.2634087769
\C,-3.0602028517,1.4130451396,-0.0146424236\C,-2.5600705072,2.56297906
84,0.6138745054\C,-3.3623749544,3.6862937483,0.764648322\C,-4.67682945
39,3.6831839919,0.2938284811\C,-5.180015102,2.5489103636,-0.3371452944
\C,-4.3785831167,1.4200949014,-0.4919642723\O,1.473933174,-3.041142595
2,0.0872068841\H,3.9622884107,-2.5997303655,0.2624147478\H,1.272696639
6,1.5030420849,-0.3923517433\H,-1.5424416783,2.552894628,0.9846500665\
H,-2.9638504196,4.5668625152,1.2577661002\H,-6.1956493993,2.5415755423
,-0.7189109902\H,-4.7703616342,0.5601565968,-1.0250440847\H,-2.2883542
195,-5.5182701743,0.4337899064\H,0.1990749945,-5.2578253893,0.43074600
43\H,5.108608442,-0.3754458852,0.1181398267\H,-5.3022992839,4.56107931
81,0.4174167684\H,-3.7447398676,-3.5337004057,0.0773827047\C,3.9276344
113,2.0372722864,-0.2951417567\F,5.128934164,2.0690777435,0.3119520317
\F,4.1384433084,2.3656250926,-1.5881618685\F,3.1804439852,3.0260832002
,0.2332081482\H,-3.7896687644,-1.041140559,0.0061482704\\Version=ES64L
-G09RevD.01\State=1-A\HF=-1308.3879449\RMSD=9.273e-09\RMSF=1.002e-06\D
ipole=-1.9310798,-0.8247491,0.4135255\Quadrupole=6.1989651,2.2011622,-
8.4001273,-6.4984726,0.9657565,0.7515721\PG=C01 [X(C20H12F3N3O1)]\\
No imaginary frequencies.

1f-*leuco* (X=OMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H15N3O2\PIOTR\05-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-)-10-OMe 2nd orin
t benzotrazinyl (phenazinoBT) Leuco\\0,1\N,0.3072215837,0.4277042283,0
.3013737457\N,-2.2105811428,1.4325770503,0.4035332576\C,-1.9440776703,
0.0698914473,0.1759264613\N,-0.7586650237,-0.4317675881,0.1329498462\C
,1.0250086545,4.0208859962,-0.3030279882\C,1.2185334443,2.6511881681,-
0.1222942136\C,0.1320711163,1.8138175718,0.1014637189\C,-1.1564869514,
2.341337942,0.1443651974\C,-1.3622359795,3.7023967511,-0.0476570519\C,
-0.2643062587,4.5382718581,-0.2681876326\C,1.5990493619,-0.0941335962,
0.1520693295\C,2.6659805214,0.7904291551,-0.0551983645\C,3.9589525705,
0.3051045959,-0.1747148608\C,4.2155172013,-1.0587140584,-0.0927060086\
C,3.1557647432,-1.9464185282,0.1085692338\C,1.8493979043,-1.4670410073
,0.2302353145\C,-3.1048149848,-0.827395925,0.0242147295\C,-2.959717022
3,-2.0627925949,-0.6250519991\C,-4.0480342972,-2.9121199207,-0.7732805
352\C,-5.3020493128,-2.5459265402,-0.2799092037\C,-5.455417143,-1.3248
301271,0.3705083116\C,-4.3658480596,-0.4700919428,0.5230557431\O,2.497
4577994,2.1676697025,-0.1528827307\H,-2.3690559733,4.1057423675,-0.013
3391363\H,4.7611323822,1.0158042083,-0.339000759\H,1.0068100833,-2.123
4879603,0.3844184748\H,-1.9857452052,-2.3326702914,-1.0146971973\H,-3.

921578757,-3.8615584226,-1.2835257048\H,-6.4225683208,-1.0363307647,0.
7691070328\H,-4.4918984116,0.4578643648,1.0708294072\H,-0.4200316876,5
.6022845892,-0.4062998763\H,1.8912467883,4.6512736832,-0.4640726766\H,
5.221675417,-1.4489162312,-0.1833117122\H,-6.151628638,-3.2096305814,-
0.4022349763\O,3.4903140536,-3.2672024042,0.1748301798\C,2.4544149098,
-4.2075097151,0.3849591993\H,1.7172692411,-4.1871966632,-0.4279445064\
H,2.9353952199,-5.1867131688,0.4083441041\H,1.9381685154,-4.0361265554
,1.3381230558\H,-3.1090247818,1.7336682574,0.0502280611\\Version=ES64L
-G09RevD.01\State=1-A\HF=-1085.8691812\RMSD=2.338e-09\RMSF=1.102e-06\D
ipole=-1.4419098,-0.0403254,-0.1966803\Quadrupole=2.5626632,6.7739385,
-9.3366017,-0.1461916,-0.2655979,-0.1238628\PG=C01 [X(C20H15N3O2)]\\
No imaginary frequencies.

1g-*leuco* (X=F)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H12F1N3O1\PIOTR\07-Feb-2
020\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geo
m=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Cl benzotraziny
l (phenazinoBT) Leuco\\0,1\N,0.0073638744,0.6083329132,0.3158769204\N,
-1.8486057973,-1.3651318849,0.4713106896\C,-0.4881034877,-1.6185392406
,0.2261704155\N,0.4138061277,-0.7017342776,0.1590180266\C,-3.085015372
5,2.5997546273,-0.1762543453\C,-1.7363684375,2.2730636973,-0.039713334
6\C,-1.3512272541,0.9539764996,0.1627333673\C,-2.3136866401,-0.0507359
554,0.2319920636\C,-3.6602298702,0.2611414148,0.0849738328\C,-4.039288
3442,1.5908438705,-0.1168309111\C,0.9626457784,1.6125990972,0.14745763
32\C,0.5289253633,2.9387869602,-0.0386027057\C,1.4445894769,3.96640964
55,-0.180415709\C,2.8169873743,3.709130124,-0.1436200745\C,3.227118031
3,2.3991579069,0.0335405508\C,2.3317743438,1.3477792422,0.1788373966\C
,-0.0816664351,-3.0295533224,0.0819139073\C,1.1055005022,-3.35400715,-
0.5913372549\C,1.4944919234,-4.6795723837,-0.7315356932\C,0.7069307479
,-5.7055973193,-0.2054522864\C,-0.4700327765,-5.3934210481,0.469187923
\C,-0.863872352,-4.0649566769,0.6133645754\O,-0.8143144505,3.284953394
2,-0.0925282671\H,-4.4049552807,-0.5261223485,0.1395364143\H,1.0679206
081,4.9722024481,-0.3265888254\H,2.6850566571,0.3358321141,0.314993751
2\H,1.7046104748,-2.5516886799,-1.0042890365\H,2.4126094619,-4.9155972
354,-1.2596186227\H,-1.0820019774,-6.182803528,0.8931961473\H,-1.76061
24666,-3.8353281447,1.1792678591\H,-5.0895628878,1.8386378526,-0.22080
08369\H,-3.3572456747,3.638003151,-0.3229995702\H,3.547086304,4.500882
5857,-0.251891561\H,1.0114099004,-6.7406243168,-0.3205713624\F,4.54180
92651,2.1216775013,0.0692003071\H,-2.46582672,-2.0927896833,0.13706492
56\\Version=ES64L-G09RevD.01\State=1-A\HF=-1070.576054\RMSD=4.653e-09\
RMSF=8.146e-07\Dipole=-1.2267874,-0.9903159,-0.264507\Quadrupole=-1.05
30803,8.9475382,-7.8944579,0.2546711,-1.4473683,-0.524228\PG=C01 [X(C1
9H12F1N3O1)]\\
No imaginary frequencies.

1h-*leuco* (X=Cl)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H12Cl1N3O1\PIOTR\07-Feb-
2020\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Ge
om=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Cl benzotrazin
yl (phenazinoBT) Leuco\\0,1\N,-0.2324809419,-0.3394444773,-0.720182103
1\N,1.6015715396,-0.4712006933,1.2745196647\C,0.2371436029,-0.23401521
61,1.5124398714\N,-0.6548463207,-0.1764564544,0.5856286909\C,2.8773349
066,0.1838546887,-2.6768069894\C,1.5275264912,0.0337238594,-2.36391284
19\C,1.1283636283,-0.1719803524,-1.0500502109\C,2.0798948246,-0.229850
4312,-0.0342203431\C,3.4282808022,-0.0692762568,-0.3315118396\C,3.8207
389058,0.1349505348,-1.6568529155\C,-1.177087755,-0.1648898047,-1.7346
896182\C,-0.7288793338,0.0253014481,-3.0551837764\C,-1.6339144098,0.17

44463287,-4.0913903829\C,-3.0081995952,0.1406956078,-3.8479817067\C,-3
.4411133427,-0.0409279064,-2.5425586512\C,-2.5495156494,-0.1930400542,
-1.4844981247\C,-0.1851981457,-0.0856411761,2.9185519041\C,-1.38170714
13,0.5784157739,3.227227278\C,-1.7848871794,0.7220856641,4.5481851628\
C,-1.0026691529,0.2090749444,5.5847653904\C,0.1833939656,-0.4566647818
,5.2881553643\C,0.591277807,-0.6045884033,3.9644260533\O,0.6142763471,
0.0750385653,-3.3871806468\H,4.1646346149,-0.1147283164,0.4641692989\H
,-1.2480307492,0.324096805,-5.0932379547\H,-2.8988334388,-0.3321342988
,-0.4720109996\H,-1.9770218375,0.9816931468,2.4172043156\H,-2.71017655
36,1.2427708271,4.7722190702\H,0.7912663537,-0.8709335558,6.0857865003
\H,1.4948358958,-1.1644820075,3.7470830525\H,4.8726954893,0.2489847341
,-1.8925685403\H,3.1595308295,0.332232545,-3.7121105696\H,-3.718261440
6,0.2559067952,-4.6562580093\H,-1.318545877,0.3272308694,6.6160130096\
Cl,-5.1666410095,-0.0821711022,-2.2035884647\H,2.2088573095,-0.1347682
492,2.0094015616\\Version=ES64L-G09RevD.01\State=1-A\HF=-1430.9377286\
RMSD=4.577e-09\RMSF=1.627e-06\Dipole=1.5162444,0.2840572,1.0329265\Qua
drupole=-1.8032123,-8.2057642,10.0089764,-1.2602055,-0.2875415,-0.5572
144\PG=C01 [X(C19H12Cl1N3O1)]\\
No imaginary frequencies.

1i-*leuco* (X=Br)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\Gen\C19H12Br1N3O1\PIOTR\13-Feb-2020\0\\
#P B3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistance,N
oAngle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-Br benzotrazinyl (
phenazinoBT) Leuco\\0,1\N,-0.4258326291,0.3950283836,-0.2878367303\N,2
.0350104758,1.5360325796,-0.3766455675\C,1.8432548037,0.1595520373,-0.
1695877116\N,0.6875460414,-0.408085951,-0.1329669091\C,-1.3485316874,3
.9461529696,0.2806767801\C,-1.459938484,2.5664716675,0.1073918998\C,-0
.3270620287,1.7888841391,-0.098978709\C,0.9319285068,2.3866271718,-0.1
339336005\C,1.0575063838,3.7600458619,0.0495545219\C,-0.0883189315,4.5
347694465,0.2541357673\C,-1.6817241443,-0.1975999708,-0.140085344\C,-2
.8055485445,0.6293822778,0.0509306327\C,-4.0712431916,0.0803161237,0.1
732511706\C,-4.2582612077,-1.3032456408,0.1118039743\C,-3.143718908,-2
.1109985281,-0.0698343879\C,-1.8614232224,-1.581983822,-0.1958665051\C
,3.0525861342,-0.6760491678,-0.0275581444\C,2.9731924148,-1.9250112204
,0.6082880624\C,4.1069609798,-2.7160205965,0.7479206036\C,5.3396504453
,-2.2761350044,0.2587669848\C,5.4272256399,-1.0408803117,-0.3792296241
\C,4.292243806,-0.2444670137,-0.523251512\O,-2.7122630723,2.0070536973
,0.1276740596\H,2.0405366953,4.219995065,0.02190721\H,-4.9105172192,0.
7504852535,0.3240060227\H,-0.9975257195,-2.2155321774,-0.3358813861\H,
2.0148631232,-2.2532445394,0.9932324631\H,4.0317904218,-3.6773145451,1
.2468099521\H,6.3776657081,-0.6966232512,-0.7750568719\H,4.3676073458,
0.6953026562,-1.0613230867\H,0.0064872928,5.6070809832,0.3866532989\H,
-2.2505761705,4.5283971939,0.4292042557\H,-5.2485861266,-1.7298047986,
0.2063619253\H,6.2242756655,-2.8947418,0.3735145106\H,2.91723395,1.884
2953833,-0.0274068518\Br,-3.3648525967,-4.0246210218,-0.1518009336\\Ve
rsion=ES64L-G09RevD.01\State=1-A\HF=-983.8898511\RMSD=3.607e-09\RMSF=8
.899e-07\Dipole=1.4824514,1.1880863,0.3209342\Quadrupole=9.2589984,0.2
682671,-9.5272655,-2.1080097,-0.5576112,-0.6330079\PG=C01 [X(C19H12Br1
N3O1)]\\
No imaginary frequencies.

1j-*leuco* (X=COMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H15N3O2\PIOTR\05-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-Ac benzotraz
inyl-H, 2nd orient leuco C1\\0,1\N,-0.1575630648,0.6011764923,0.298622

3979\N,2.4652017691,1.271367821,0.4126788682\C,2.0289194731,-0.0436562
235,0.1718619509\N,0.7899190966,-0.3900118729,0.1203564123\C,-0.411702
6277,4.2565067827,-0.2874946495\C,-0.7723274108,2.921455106,-0.1176283
716\C,0.1948062786,1.951422048,0.1055850346\C,1.5398838504,2.310380721
4,0.1564621602\C,1.9152156436,3.6362029498,-0.0257900964\C,0.933163118
7,4.6062337263,-0.2437167268\C,-1.504500451,0.2475687734,0.1404238414\
C,-2.4529153067,1.2655059309,-0.0687823389\C,-3.8016447041,0.961898907
9,-0.196999007\C,-4.2300878502,-0.3572108642,-0.1229260395\C,-3.304296
6315,-1.3854845795,0.0779695629\C,-1.9439632471,-1.07205237,0.20822873
66\C,3.067630519,-1.0795493868,0.0130423925\C,2.7746001417,-2.27162042
52,-0.6657066445\C,3.7468639605,-3.2513005396,-0.818072605\C,5.0287116
909,-3.060204751,-0.2985976339\C,5.3276934794,-1.8828591797,0.38136386
82\C,4.3553029678,-0.8975567255,0.53736115\O,-2.1077890676,2.597593791
4,-0.1580113957\H,-4.4961891487,1.7781134678,-0.3608778063\H,-1.198878
9427,-1.8396782838,0.3628442012\H,1.780428415,-2.4063801116,-1.0739996
768\H,3.5075124384,-4.1657908739,-1.3509483582\H,6.3169919571,-1.73043
40374,0.8001676366\H,4.590793837,-0.0047123684,1.1070608284\H,1.223155
4942,5.642655291,-0.3732330236\H,-1.1908292871,4.9919704139,-0.4472949
401\H,-5.2774896874,-0.6142302719,-0.2204416175\H,5.7874313986,-3.8256
941665,-0.4232554681\H,2.9645860884,3.9096101096,0.013940938\C,-3.8108
263991,-2.789647387,0.1473722193\O,-4.9987667545,-3.0293633509,0.03211
7002\C,-2.8150687056,-3.9164508975,0.3650968101\H,-2.0674026937,-3.939
0787372,-0.4348910196\H,-2.275450002,-3.7856018167,1.3091942633\H,-3.3
574571604,-4.8618050685,0.3839323903\H,3.4008772249,1.4569365256,0.077
4249146\\Version=ES64L-G09RevD.01\State=1-A\HF=-1123.9974364\RMSD=2.93
5e-09\RMSF=6.932e-07\Dipole=2.4469887,0.7225207,-0.1950154\Quadrupole=
-3.0453229,6.9139044,-3.8685815,-8.6660597,0.1744619,0.0459584\PG=C01
[X(C21H15N3O2)]\\
No imaginary frequencies.

1l-*leuco* (X=NH_2)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H14N4O1\PIOTR\23-Aug-201
9\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NH2 benzotrazin
yl 4H, C1\\0,1\N,0.2358419812,0.7390880434,-0.2556608378\N,2.946429161
2,0.7383962307,-0.4092859893\C,2.1966040168,-0.4256073784,-0.157868587
5\N,0.9107453799,-0.4517723101,-0.0927815185\C,0.9093749059,4.35318506
26,0.2636509925\C,0.2189859618,3.1491426652,0.1188250813\C,0.915119088
1,1.9645635722,-0.0930134097\C,2.3067836203,1.977070391,-0.1610447653\
C,3.0046584496,3.1686713163,-0.0048434754\C,2.297565364,4.3558460833,0
.2048981242\C,-1.1549829155,0.7328295773,-0.0933595798\C,-1.8167065324
,1.9567401207,0.1017482888\C,-3.1931447604,1.9848637674,0.2325223074\C
,-3.9397181251,0.809203582,0.1741074108\C,-3.2951048339,-0.4175190576,
-0.0133114857\C,-1.9000527433,-0.4426609396,-0.1467304169\C,2.94342426
56,-1.6885825271,-0.0075729101\C,2.3615310722,-2.7746849432,0.66373905
72\C,3.0584020713,-3.9666015844,0.8105003455\C,4.3489901758,-4.0984273
569,0.2935174009\C,4.9331356348,-3.0285704497,-0.3786512951\C,4.237298
7201,-1.8310162751,-0.5295820843\O,-1.146137854,3.174514234,0.17405436
16\H,-3.6748999331,2.9444719047,0.3841301035\H,-1.3746988207,-1.378575
1693,-0.2885174724\H,1.3644647007,-2.6587318626,1.0708214163\H,2.59728
38328,-4.7955193042,1.3377935936\H,5.9304978329,-3.1248112747,-0.79530
06085\H,4.6891622623,-1.0215928518,-1.0932510659\H,2.8380912175,5.2891
564037,0.3157453108\H,0.3407998913,5.2625500606,0.4171532427\H,-5.0188
957883,0.8474936335,0.280797375\H,4.8929366298,-5.0294575823,0.4144583
972\H,4.088455167,3.1697210681,-0.0588308773\N,-4.0196466649,-1.619525
8842,-0.0062380008\H,3.8960676582,0.6896258953,-0.0649883212\H,-3.5744
77442,-2.3606170671,-0.5316452351\H,-4.9795764774,-1.5105590736,-0.306
2240627\\Version=ES64L-G09RevD.01\State=1-A\HF=-1026.7000702\RMSD=4.51

6e-09\RMSF=7.009e-07\Dipole=0.7137666,-0.5224288,-0.1773772\Quadrupole
=10.158486,1.6047048,-11.7631908,2.3917306,3.0949437,1.6471008\PG=C01
[X(C19H14N4O1)]\\
No imaginary frequencies.

1m-*leuco* (X=NHAc)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H16N4O2\PIOTR\07-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NHAc 2nd benzot
razinyl-H, leuco C1\\0,1\N,-0.1156168843,0.8929375091,-0.2732281545\N,
-2.8112680489,0.6495960079,-0.4322013213\C,-1.9645614879,-0.4416142185
,-0.167819861\N,-0.6815605213,-0.354069096,-0.0971006867\C,-1.10834244
28,4.4313480958,0.2532019033\C,-0.3147275905,3.2934207621,0.109130487\
C,-0.9013161687,2.0527579239,-0.1084086103\C,-2.28794316,1.9411003719,
-0.1816227873\C,-3.0893225548,3.0657312595,-0.0260693409\C,-2.49125613
45,4.3106010874,0.1882709267\C,1.2680178788,1.0125232037,-0.0947614597
\C,1.8196877047,2.289101595,0.1062507878\C,3.1865246633,2.4377778481,0
.2541494391\C,4.0464093539,1.3399173151,0.2098964337\C,3.5039002871,0.
0674266782,0.0164532081\C,2.1184270919,-0.0872248627,-0.1339463151\C,-
2.5994472916,-1.7636823029,-0.0080190939\C,-1.9346060821,-2.7842861148
,0.6880546164\C,-2.526043001,-4.0308537014,0.8438354718\C,-3.791759524
5,-4.2830528131,0.3107266344\C,-4.4575657791,-3.278570085,-0.386090389
3\C,-3.8675518669,-2.0266929352,-0.5458356771\O,1.0450738536,3.4389766
729,0.168902171\H,3.5779294408,3.4365251973,0.4123591555\H,1.678708616
3,-1.0660719983,-0.2825088887\H,-0.9583687383,-2.5747797132,1.10803875
7\H,-2.0025560546,-4.8083043523,1.390888118\H,-5.4360563384,-3.4683783
071,-0.8150224727\H,-4.380231988,-1.2680839908,-1.1278824152\H,-3.1129
683784,5.1919395364,0.2980585356\H,-0.623337186,5.3872486429,0.4102601
68\H,5.1119783682,1.4595543735,0.3234838371\H,-4.2536200165,-5.2564959
691,0.4384820396\H,-4.168781272,2.9710935762,-0.0835427502\N,4.2810671
247,-1.1078737542,-0.044144874\H,3.7548211216,-1.954815173,-0.19413284
84\C,5.6415506161,-1.2568289791,0.0920723224\O,6.4147469098,-0.3344681
209,0.2751833026\C,6.1125412647,-2.702852443,0.0235378587\H,6.09648075
04,-3.141139826,1.0274440745\H,5.495053691,-3.3253139287,-0.6308741101
\H,7.1430192293,-2.7116013319,-0.3324255849\H,-3.7580564854,0.51731809
01,-0.1025928271\\Version=ES64L-G09RevD.01\State=1-A\HF=-1179.3690777\
RMSD=1.952e-09\RMSF=9.368e-07\Dipole=-1.9845237,-1.2259717,0.0865709\Q
uadrupole=-3.9068964,11.1421413,-7.235245,-7.5160972,-0.856773,-0.1241
723\PG=C01 [X(C21H16N4O2)]\\@
No imaginary frequencies.

1n-*leuco* (X=I)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\Gen\C19H12I1N3O1\PIOTR\11-Feb-2020\0\\#
P B3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistance,No
Angle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-I benzotrazinyl (ph
enazinoBT) Leuco\\0,1\N,-0.4263884612,0.3916557444,-0.2796180577\N,2.0
331826912,1.5318348126,-0.3827289163\C,1.8425443588,0.1563098643,-0.16
7000776\N,0.6869758331,-0.4112879179,-0.1235249879\C,-1.3460313494,3.9
441581953,0.2867961396\C,-1.4582670077,2.5641262465,0.1173017501\C,-0.
326947301,1.7857534935,-0.0938506947\C,0.9317586096,2.3835192601,-0.13
67738079\C,1.0585973299,3.7572654417,0.043358781\C,-0.0859701121,4.532
6910987,0.2522110264\C,-1.683630227,-0.2000301751,-0.1363671321\C,-2.8
05413749,0.628372088,0.0595915716\C,-4.0723050181,0.0816107581,0.17665
14698\C,-4.2623434381,-1.3008278976,0.1042374745\C,-3.1513474076,-2.11
49627962,-0.0834495469\C,-1.8671770017,-1.5840614357,-0.2032699385\C,3
.0533270664,-0.6768907829,-0.0242592525\C,2.979618843,-1.9210930276,0.
6214470787\C,4.1157407302,-2.7089864613,0.7608554335\C,5.3449421535,-2

.2705977237,0.2617719742\C,5.4267856048,-1.040062686,-0.3860161655\C,4
.2896253762,-0.2467609696,-0.529641053\O,-2.7104373369,2.0047066483,0.
1471057936\H,2.0416044248,4.2168619804,0.0097392297\H,-4.9102128127,0.
7526522518,0.3318725339\H,-1.0001430823,-2.2130566085,-0.3469229138\H,
2.0238914931,-2.2480809655,1.0139494172\H,4.0450568184,-3.6665400072,1
.2675313991\H,6.3744638333,-0.6970030574,-0.7894324679\H,4.3607114367,
0.6890545133,-1.0751310494\H,0.009594892,5.6053002354,0.3816722862\H,-
2.247337586,4.5266729844,0.4387322695\H,-5.2567313183,-1.7184225364,0.
1960387479\H,6.2313552789,-2.8866178447,0.3766695749\H,2.9170720215,1.
8817038451,-0.03928481\I,-3.4076350965,-4.2138729082,-0.1934106012\\Ve
rsion=ES64L-G09RevD.01\State=1-A\HF=-982.1033435\RMSD=4.916e-09\RMSF=2
.149e-06\Dipole=1.4797592,1.1418725,0.3154124\Quadrupole=9.3485127,1.6
085691,-10.9570818,-0.1412885,-0.3737848,-0.3799882\PG=C01 [X(C19H12I1
N3O1)]\\
No imaginary frequencies.

1o-*leuco* (X=OH)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H13N3O2\PIOTR\06-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OH 2nd orint benz
otrazinyl lecuo\\0,1\N,-0.6063827115,0.0822259378,-0.2963519076\N,1.60
72353882,1.6477021358,-0.3882327605\C,1.666001892,0.2590991888,-0.1736
342084\N,0.6309934358,-0.5066635767,-0.1367988791\C,-2.147507862,3.405
5742021,0.3051455845\C,-2.0145203375,2.0288322476,0.122603543\C,-0.760
7103711,1.4701400268,-0.0951386337\C,0.3689087667,2.2844318625,-0.1321
387397\C,0.2495174285,3.6554518171,0.0615361913\C,-1.0148870039,4.2102
583401,0.2772863769\C,-1.7388056826,-0.7276133709,-0.1614110825\C,-2.9
881177771,-0.119089175,0.0407329903\C,-4.1311184348,-0.8928685387,0.14
73286464\C,-4.0654278395,-2.282133203,0.0581300541\C,-2.8271445372,-2.
889463082,-0.136503246\C,-1.668212715,-2.1181693068,-0.2451959127\C,3.
0045305508,-0.3437347781,-0.028972573\C,3.1547644967,-1.576958495,0.62
2819064\C,4.4115645671,-2.1503865052,0.7631914657\C,5.542354906,-1.504
7289227,0.2588066509\C,5.4032811301,-0.2830706188,-0.3938705395\C,4.14
42072016,0.2955790155,-0.5380056867\O,-3.1446192074,1.2592596038,0.146
4460715\H,1.1339242606,4.2834624568,0.0318618085\H,-5.0775806396,-0.38
8848917,0.3078378907\H,-0.6986331948,-2.5780829226,-0.3949579283\H,2.2
729345554,-2.0641081045,1.0207630741\H,4.5126881334,-3.1016751618,1.27
55841627\H,6.2741190394,0.2206219474,-0.8005878756\H,4.0468832101,1.22
66074439,-1.0864518782\H,-1.1133951963,5.2808371646,0.4172483924\H,-3.
1378144513,3.8157930014,0.4623516398\H,-4.955363035,-2.8937279417,0.13
89224555\H,6.5236707046,-1.9529443211,0.374410758\O,-2.7951172504,-4.2
531814452,-0.2165619409\H,-1.8843745665,-4.5340556746,-0.3577452431\H,
2.4103637565,2.1475014992,-0.0308411849\\Version=ES64L-G09RevD.01\Stat
e=1-A\HF=-1046.5653141\RMSD=3.533e-09\RMSF=1.023e-06\Dipole=1.502717,0
.49029,0.2056594\Quadrupole=3.5831837,4.7226814,-8.3058651,-2.8227687,
-0.4751933,-0.1365053\PG=C01 [X(C19H13N3O2)]\\@
No imaginary frequencies.

1p-*leuco* (X=OBn)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C26H19N3O2\PIOTR\08-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OBn 2nd orient be
nzotrazinyl leuco, C1\\0,1\N,-1.6848221201,-0.6839098644,0.2747081037\
N,-4.1551787527,0.4167731731,0.45934388\C,-3.0077156174,1.1720528701,0
.1553219661\N,-1.8229981178,0.6740312576,0.0716561465\C,-3.7730987143,
-3.7220353943,-0.1675915256\C,-2.6523744796,-2.8990865328,-0.055801144
9\C,-2.8048416739,-1.5322029721,0.143801707\C,-4.0800349908,-0.9782602

241,0.2301439923\C,-5.2038215734,-1.7866874429,0.1063893521\C,-5.04217
24198,-3.1608528857,-0.0894089151\C,-0.4153272907,-1.2472517993,0.0945
602314\C,-0.3088609979,-2.6328217184,-0.0857525937\C,0.9377421715,-3.2
211348946,-0.2319582648\C,2.0942745488,-2.4499249861,-0.2049144903\C,1
.9946477137,-1.0676085878,-0.0311165166\C,0.7432589516,-0.4653909336,0
.1190257314\C,-3.1867884889,2.6241401683,-0.0320594094\C,-2.2429418908
,3.3620801665,-0.7621220784\C,-2.406277607,4.7289421564,-0.9442069176\
C,-3.5138445801,5.3859070786,-0.4041622863\C,-4.4529553799,4.663715346
5,0.326753925\C,-4.2927044957,3.2924051392,0.5128993908\O,-1.4140112,-
3.4757555314,-0.1293702982\H,-6.1941139688,-1.3482158291,0.1738795511\
H,0.9856990083,-4.2949563724,-0.3738743214\H,0.627039836,0.5984603506,
0.2580199377\H,-1.3931411614,2.8416488244,-1.1867673737\H,-1.671110531
6,5.2849441923,-1.5170230669\H,-5.3103112513,5.166785537,0.7619107895\
H,-5.0102900258,2.7518848208,1.1211452332\H,-5.9163639092,-3.796477632
,-0.1743585073\H,-3.6249769762,-4.7856301971,-0.3108777301\H,3.0730195
691,-2.8998595568,-0.3163767677\H,-3.6412064369,6.4531254048,-0.552679
1054\O,3.1761263252,-0.3839728937,-0.0132813654\C,3.1385031982,1.02923
80354,0.1191174398\H,2.6742037512,1.3117160232,1.0739699987\H,2.519048
8582,1.456270217,-0.6846097409\C,4.5448315448,1.5713139617,0.041984025
6\C,5.5180837491,0.9497829597,-0.7442827301\C,4.8737468361,2.740758676
4,0.7309999046\C,6.7975199765,1.4921346071,-0.8388980452\C,6.150635874
3,3.2888215985,0.6298605268\C,7.1172474411,2.6644672891,-0.1557672364\
H,5.2688808813,0.0344309667,-1.2680482981\H,4.1267156987,3.224616637,1
.3545136282\H,7.5469010277,0.9967572852,-1.4482660314\H,6.3917482052,4
.1971644315,1.1728048151\H,8.1146970627,3.0854174562,-0.2306634498\H,-
5.0153152072,0.8407151579,0.1382069143\\Version=ES64L-G09RevD.01\State
=1-A\HF=-1316.9308291\RMSD=9.741e-09\RMSF=8.295e-07\Dipole=-1.0469766,
0.9725443,-0.2275291\Quadrupole=10.1234544,1.7219076,-11.845362,-0.031
0142,-1.8311539,2.005953\PG=C01 [X(C26H19N3O2)]\\
No imaginary frequencies.

1q-*leuco* (X=Ph)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C25H17N3O1\PIOTR\09-Feb-202
0\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Ph benzotrazinyl
leuco (phenazinoBT), C1\\0,1\N,-0.272352841,-0.9471521701,-0.884110085
1\N,1.5124062871,-2.0174623028,0.8590822147\C,0.1260586388,-2.23406807
59,0.9598910446\N,-0.7403713895,-1.7299188034,0.1520689334\C,2.8395566
383,-0.6357024819,-2.8827504765\C,1.4972167551,-0.5592241048,-2.514138
4755\C,1.0785718032,-1.0319239194,-1.2770298636\C,2.0044154013,-1.5867
670238,-0.3958361986\C,3.3432129343,-1.6810447801,-0.7571066719\C,3.75
54638072,-1.2002262207,-2.0028183239\C,-1.2018940672,-0.4867603461,-1.
8263669457\C,-0.7304429632,-0.0074673123,-3.0610024664\C,-1.6174687006
,0.4753727848,-4.0077204314\C,-2.9864908443,0.488355003,-3.748878405\C
,-3.4829079811,0.0101381407,-2.5314137704\C,-2.5728335855,-0.475777673
9,-1.5802148264\C,-0.3469139764,-3.0543183102,2.0912979745\C,-1.600485
4663,-3.6812619085,2.0297753369\C,-2.0528280475,-4.4544796253,3.090637
7696\C,-1.2639797254,-4.6193930781,4.2309879817\C,-0.0210017818,-3.996
9249613,4.3039180948\C,0.4365580626,-3.2189926498,3.2425900699\O,0.613
2915469,0.0086602268,-3.3954640781\H,4.0583327255,-2.1150228813,-0.065
8491547\H,-1.2168699313,0.842490523,-4.9459948507\H,-2.9215367559,-0.8
804460285,-0.6400036861\H,-2.2009879399,-3.5558572553,1.1371072782\H,-
3.0223415769,-4.9376852181,3.0261644329\H,0.5939459493,-4.1077786456,5
.1910765103\H,1.3876792481,-2.7048092905,3.3325546634\H,4.8012197501,-
1.2617074919,-2.2818780347\H,3.1370536248,-0.2487686352,-3.8499181745\
H,-3.6642372559,0.8998936813,-4.4877060316\H,-1.6184274678,-5.22819706
82,5.0562148112\C,-4.9376686069,0.0177788175,-2.2425736375\C,-5.418750
685,0.2992057069,-0.9550005391\C,-5.8739870627,-0.2549860209,-3.251277

3169\C,-6.7842632071,0.3075791406,-0.6859998751\C,-7.2397365022,-0.244
6516436,-2.9837672762\C,-7.7020243703,0.0364607879,-1.6993095377\H,-4.
7139808698,0.5377880766,-0.1653798771\H,-5.523671165,-0.5029555483,-4.
2478069565\H,-7.1318313314,0.5354448704,0.3168435828\H,-7.9440668084,-
0.4662098917,-3.7795653078\H,-8.7667790732,0.0435407033,-1.4899920586\
H,2.0690825871,-2.7394870757,1.2963674239\\Version=ES64L-G09RevD.01\St
ate=1-A\HF=-1202.4080488\RMSD=6.274e-09\RMSF=1.702e-06\Dipole=0.685372
7,-0.8014166,0.7051276\Quadrupole=6.3694194,-8.9334323,2.5640129,-2.38
53667,2.8898315,-6.3366172\PG=C01 [X(C25H17N3O1)]\\
No imaginary frequencies.

1r-*leuco* (X=thienyl)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C23H15N3O1S1\PIOTR\13-Feb-2
020\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geo
m=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Thio benzotrazi
nyl Leuco (phenazinoBT), C1\\0,1\N,-0.5730864355,-2.315085979,-2.44725
94243\N,0.9537744986,-4.517798067,-2.03875457\C,-0.3494010262,-4.39068
31929,-1.5243782646\N,-1.0976945341,-3.3598306306,-1.712046867\C,2.784
5319476,-0.9032115268,-3.1596756711\C,1.4042720807,-0.9968944653,-2.98
81084969\C,0.8219602345,-2.1996509186,-2.6098987259\C,1.6199096174,-3.
3216677815,-2.3965739994\C,2.9987116048,-3.2376488497,-2.5502954211\C,
3.5751269685,-2.024374691,-2.9360205314\C,-1.3474416896,-1.1557058116,
-2.5789832703\C,-0.717198805,0.035519345,-2.982326736\C,-1.4576609698,
1.191782517,-3.1586768033\C,-2.8316968646,1.1919087187,-2.9321638213\C
,-3.4826642442,0.0193258383,-2.5300595361\C,-2.7224032811,-1.150615622
1,-2.3636057044\C,-0.8871986692,-5.5343535022,-0.7631994129\C,-1.94004
16366,-5.3433073098,0.1440309564\C,-2.4507945318,-6.4149920984,0.86427
9711\C,-1.9209455295,-7.6958028607,0.6953377873\C,-0.8800395211,-7.896
6520542,-0.2068629031\C,-0.3649513901,-6.8246565165,-0.9323371227\O,0.
6434396912,0.1205192224,-3.219782385\H,3.6142898968,-4.1151861101,-2.3
815052601\H,-0.9369624744,2.0939479078,-3.4591649312\H,-3.196338656,-2
.0811884234,-2.0839632499\H,-2.3373489691,-4.344168224,0.274984096\H,-
3.2612531532,-6.2509768152,1.5670588465\H,-0.470344212,-8.8903945844,-
0.3552970857\H,0.4165685023,-7.0047473508,-1.6630734089\H,4.649108842,
-1.9594730271,-3.0686213191\H,3.2084508231,0.0451874047,-3.4669707848\
H,-3.3899275462,2.1143010436,-3.0452133028\H,-2.3192303198,-8.53010422
65,1.2632724223\C,-4.9264000026,-0.0124571886,-2.2755685528\C,-5.63268
17902,-0.8362224628,-1.4310731986\C,-7.0344651329,-0.5937591359,-1.432
7000463\C,-7.3963974476,0.4142508527,-2.2811547951\S,-6.0225025238,1.0
756772751,-3.0969961774\H,-5.1523630218,-1.5777408365,-0.8048970239\H,
-7.739851314,-1.14319681,-0.8212965866\H,-8.3818412424,0.8080321841,-2
.4798698357\H,1.5290840467,-5.1742530564,-1.5283545237\\Version=ES64L-
G09RevD.01\State=1-A\HF=-1523.1635224\RMSD=8.659e-09\RMSF=1.220e-06\Di
pole=0.7188296,-1.154,0.6979233\Quadrupole=6.6930246,2.9255512,-9.6185
759,-3.7697979,-3.6028197,-5.9690165\PG=C01 [X(C23H15N3O1S1)]\\
No imaginary frequencies.

1s-*leuco* (X=CCPh)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C27H17N3O1\PIOTR\14-Feb-202
0\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-CCPh benzotraziny
l leuco (phenazinoBT), C1\\0,1\N,0.7305289939,1.6819129669,0.319109693
\N,-0.7598708781,3.9367209378,0.5145312937\C,-1.318506663,2.682120721,
0.2094746088\N,-0.6343792989,1.5953824851,0.1196741497\C,3.3843366683,
4.2381509953,-0.1249707977\C,2.7524111083,3.000704535,-0.0158507725\C,
1.381253564,2.9249034341,0.1886877005\C,0.6267837498,4.0925654934,0.28
14271117\C,1.2423179301,5.3328296795,0.1596862819\C,2.6239300977,5.398

7753881,-0.0397861364\C,1.4901672156,0.5209459236,0.1262764563\C,2.879
3525878,0.6448730102,-0.0638217239\C,3.6708558161,-0.4809232122,-0.229
732757\C,3.1038113354,-1.7507927548,-0.2117266453\C,1.7208568988,-1.89
74825312,-0.0273806852\C,0.9242408342,-0.7496464401,0.1399727202\C,-2.
7810360168,2.6221365385,0.0242353946\C,-3.3544608866,1.5698557463,-0.7
050437332\C,-4.7298521428,1.5072350089,-0.8855102435\C,-5.5584903751,2
.4922101629,-0.3444054725\C,-4.999485412,3.5367892188,0.3864690163\C,-
3.6202498593,3.6033281816,0.5710488444\O,3.5229116489,1.8675019397,-0.
0974938243\H,0.6487981389,6.2383970159,0.2317653705\H,4.7355388651,-0.
3410440761,-0.3784516721\H,-0.1433766728,-0.8417682236,0.2809641663\H,
-2.7027159723,0.8157965788,-1.1291729619\H,-5.1584432678,0.6904833773,
-1.4571678554\H,-5.6358643785,4.2996359643,0.8229481163\H,-3.204443111
6,4.3992375263,1.1799281149\H,3.1079848974,6.3652524101,-0.1223052547\
H,4.4573226558,4.2650750825,-0.2717657274\H,3.7254225914,-2.6283880848
,-0.3399396359\H,-6.6323656509,2.4428922105,-0.4913841395\C,1.12494504
65,-3.1898544359,-0.0044246911\C,0.6189511403,-4.2927530126,0.01776008
04\C,0.0248156674,-5.5860420161,0.0470300152\C,-1.3519943694,-5.736724
0992,0.2944286232\C,0.8032253647,-6.7378448481,-0.1694086676\C,-1.9278
161937,-7.0013070845,0.3239783894\C,0.2194254032,-7.9987214283,-0.1383
745929\C,-1.1465727969,-8.1365891674,0.1081077555\H,-1.9562950089,-4.8
523294521,0.4626753605\H,1.864803792,-6.6273244135,-0.360458447\H,-2.9
911810383,-7.1015535246,0.5167461478\H,0.8331651649,-8.8777922708,-0.3
070751321\H,-1.5993458149,-9.1223483926,0.1321484992\H,-1.3216944079,4
.7178869162,0.2037674992\\Version=ES64L-G09RevD.01\State=1-A\HF=-1278.
5657506\RMSD=1.585e-09\RMSF=1.031e-06\Dipole=-0.7947286,1.1153647,-0.2
391737\Quadrupole=3.9867,12.564858,-16.5515579,-2.6427588,-1.0565746,1
.0717422\PG=C01 [X(C27H17N3O1)]\\
No imaginary frequencies.

1t-*leuco* (X=OAc)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H15N3O3\PIOTR\29-Sep-202
0\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-OAc benzotra
zinyl-H, leuco C1\\0,1\N,-0.2696257976,0.7514850191,0.3829818941\N,-2.
9809592154,0.7537779493,0.3261203522\C,-2.2194849171,-0.4197227428,0.1
829273941\N,-0.9327182157,-0.4490292632,0.2150399659\C,-0.8900834053,4
.3324116771,-0.3744444454\C,-0.2193440225,3.1378539213,-0.1157354474\C
,-0.9314191042,1.9657781922,0.1044468791\C,-2.3238465923,1.9795873761,
0.0657389779\C,-3.0036167084,3.1615952771,-0.2040191632\C,-2.279309929
2,4.3368052417,-0.4203944452\C,1.1272190437,0.7378274178,0.2979592155\
C,1.8084884861,1.9498735994,0.090461882\C,3.1913186197,1.9786625245,0.
0339600009\C,3.9381263722,0.8092293753,0.1802029109\C,3.2589391515,-0.
3855265048,0.374117795\C,1.8697810007,-0.4338088511,0.4334774823\C,-2.
9583548053,-1.687676954,0.029512138\C,-2.3337823764,-2.7990253647,-0.5
559731997\C,-3.0228947364,-3.9951880852,-0.7054498048\C,-4.3470625241,
-4.1052900071,-0.2762609673\C,-4.9737137077,-3.0098931926,0.3112622117
\C,-4.2859745711,-1.8080900231,0.4644526418\O,1.1502165283,3.160041679
,-0.0649897655\H,-4.0883352902,3.1650143335,-0.2332603682\H,3.67773264
63,2.9329007719,-0.1326019496\H,1.3614469873,-1.3744347261,0.590293729
2\H,-1.30989874,-2.7002995083,-0.8952928483\H,-2.5287093875,-4.8445276
9,-1.1658899017\H,-5.9981261076,-3.0893408657,0.660126277\H,-4.7736835
602,-0.9772533519,0.9634922721\H,-2.8070627478,5.2626634456,-0.6192614
075\H,-0.3085747417,5.2329027726,-0.5311684013\H,5.0172388542,0.833153
664,0.1302748268\H,-4.884377442,-5.0399066325,-0.3989169958\O,3.914781
0511,-1.5950407306,0.6059770095\C,4.9023536363,-2.0158171337,-0.239893
4881\O,5.2775897367,-1.4097116434,-1.2060314968\C,5.4341599399,-3.3456
329817,0.2321074991\H,5.8306998759,-3.2498619536,1.2469672282\H,4.6259
219913,-4.0814557781,0.2678136099\H,6.2177810223,-3.6822396969,-0.4452

530988\H,-3.9074402977,0.6881834435,-0.0734949984\\Version=ES64L-G09Re
vD.01\State=1-A\HF=-1199.2284708\RMSD=4.708e-09\RMSF=4.826e-07\Dipole=
-1.4587533,-0.4492958,0.1951928\Quadrupole=6.079383,6.7628533,-12.8422
363,-3.1060008,6.6319385,-1.2011255\PG=C01 [X(C21H15N3O3)]\\

No imaginary frequencies.

1u-*leuco* (X=NHCOCF$_3$)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H13F3N4O2\PIOTR\09-May-2
021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geo
m=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-NHCOCF3 2n
d benzotrazinyl-H, leuco C1\\0,1\N,-1.2416505455,-0.8782728321,0.27817
47278\N,-3.5936703539,0.4634047892,0.4039509135\C,-2.3675751342,1.1046
933932,0.1617712512\N,-1.235141001,0.493498894,0.1070795347\C,-3.60681
75977,-3.6886205423,-0.2537054573\C,-2.4156919451,-2.9804163093,-0.101
6593301\C,-2.4364418605,-1.60735813,0.1055006304\C,-3.6518622046,-0.92
94543808,0.1619349315\C,-4.8456887398,-1.6220453149,-0.0013924362\C,-4
.8156814356,-3.0040817819,-0.2062134348\C,-0.0326483598,-1.5594632622,
0.1172032072\C,-0.0566421801,-2.9529916712,-0.0754666743\C,1.125669127
3,-3.6578153426,-0.2094939166\C,2.3633074183,-3.0149922137,-0.15948277
45\C,2.389714212,-1.6326550212,0.0250144175\C,1.1969604181,-0.91091742
26,0.1614511797\C,-2.3944744797,2.5716528918,0.004320984\C,-1.36329693
84,3.2238683411,-0.6874575931\C,-1.3819124022,4.6040167941,-0.83982739
95\C,-2.42920267,5.3584180803,-0.3074256185\C,-3.4547354561,4.72073209
81,0.3852089347\C,-3.4397775383,3.336538737,0.541282748\O,-1.235204998
1,-3.6768347181,-0.1430674837\H,1.0677771862,-4.7296045245,-0.36152834
32\H,1.2045662404,0.1630365997,0.3013423407\H,-0.5613219871,2.62879581
16,-1.1069240867\H,-0.5807885319,5.0943859833,-1.3832165397\H,-4.26628
96978,5.2995818734,0.8137243451\H,-4.2229134146,2.8583005609,1.1201416
098\H,-5.7458123739,-3.5486564221,-0.3222029791\H,-3.5606080779,-4.760
5876946,-0.4029237646\H,3.2829606481,-3.5690431761,-0.2636840921\H,-2.
4433370894,6.4360819612,-0.4322391472\H,-5.7893322646,-1.0881594712,0.
0424640197\N,3.5873383365,-0.8848859549,0.0867836291\H,3.4811471161,0.
1065654429,0.243566461\C,4.8635669492,-1.3260367241,-0.0400113624\O,5.
2464697108,-2.4618062997,-0.2263747337\C,5.9175440355,-0.1944655031,0.
0666054482\H,-4.3968696449,0.9782667737,0.0692994721\F,5.3625793715,1.
0138146333,0.329939154\F,6.5923739895,-0.086714789,-1.0801239117\F,6.7
853383331,-0.4633338166,1.0419838991\\Version=ES64L-G09RevD.01\State=1
-A\HF=-1477.0851582\RMSD=3.855e-09\RMSF=5.730e-07\Dipole=-2.4544922,1.
4042853,-0.1131452\Quadrupole=-2.7889618,7.6519615,-4.8629996,3.270043
,0.8389889,-0.4204144\PG=C01 [X(C21H13F3N4O2)]\\@

No imaginary frequencies.

1v-*leuco* (X=NHCOOMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H16N4O3\PIOTR\11-May-202
1\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=
(NoDistance,NoAngle) fcheck guess=check\\Parent flat C(8)-O-Ph(N1)-10-
NHCOOMe 2nd benzotrazinyl-H, leuco C1\\0,1\N,-0.6956190499,-0.90062781
56,-0.2755873936\N,-3.1050591626,0.3336128723,-0.4255670157\C,-1.91050
7185,1.0287509564,-0.1654290499\N,-0.7532514436,0.467532597,-0.0992748
317\C,-2.9387034991,-3.8111553384,0.2552250028\C,-1.7772594823,-3.0528
14139,0.1084293134\C,-1.8576769882,-1.6825624768,-0.1080864027\C,-3.10
1975855,-1.0601042834,-0.1769017275\C,-4.2655488173,-1.8033019418,-0.0
186022549\C,-4.1761561014,-3.1816804292,0.1942877271\C,0.5432655327,-1
.5291627515,-0.1038056489\C,0.5777483794,-2.9193212038,0.0974840381\C,
1.7901927318,-3.5683462,0.2406629506\C,2.9976641464,-2.8713575495,0.19
0439135\C,2.969207563,-1.4892650533,-0.0045589673\C,1.7430378259,-0.82
64214493,-0.149500986\C,-2.0044789797,2.4922670282,-0.0050382639\C,-1.
0024231388,3.1912690521,0.6845266708\C,-1.0850939155,4.5686865613,0.83

97752557\C,-2.1685940715,5.2748215448,0.3132283967\C,-3.165462817,4.59
10671224,-0.3770526304\C,-3.0861258288,3.2093518778,-0.5363682677\O,-0
.5706976039,-3.6964455854,0.1651966832\H,1.780534983,-4.640850344,0.39
98023998\H,1.7024392541,0.2455426782,-0.2983416826\H,-0.1720297943,2.6
330341917,1.0994271929\H,-0.3056159681,5.0948409891,1.3813474833\H,-4.
0050751795,5.1320168947,-0.8011440756\H,-3.8482716691,2.6968212454,-1.
1138962686\H,-5.0822091958,-3.7664190654,0.3061150348\H,-2.8461809644,
-4.8792178292,0.4112074679\H,3.9406098377,-3.3835172496,0.3019732928\H
,-2.2327708221,6.3503657086,0.4409975848\H,-5.23126279,-1.3113846054,-
0.0727176959\N,4.1282392201,-0.693138506,-0.0701968574\H,3.9919600562,
0.2931950674,-0.2293469256\C,5.432956389,-1.0829774385,0.0539417737\O,
5.8502658704,-2.2029604832,0.2473433261\O,6.2251638334,0.0145902355,-0
.0766496886\C,7.6261145993,-0.2520412366,0.0307456705\H,7.867168912,-0
.6748219757,1.009142553\H,7.9489447188,-0.9508930435,-0.7447324472\H,8
.1182813581,0.7121178018,-0.0979904084\H,-3.9320547584,0.8100075292,-0
.0914357131\\Version=ES64L-G09RevD.01\State=1-A\HF=-1254.5978043\RMSD=
3.614e-09\RMSF=1.834e-06\Dipole=-1.008754,1.5254916,0.1188601\Quadrupo
le=11.1696735,-0.1269464,-11.0427271,5.5502957,-0.5053337,0.457126\PG=
C01 [X(C21H16N4O3)]\\@

No imaginary frequencies.

1a^{+} (X=H)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H12N3O1(1+)\PIOTR\04-May
-2016\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman, ReadIso) SCF=Di
rect #P Geom=(NoDistance,NoAngle) fcheck\\Oxo benzotrazinyl cat (phena
zinoBT), start at the radical Cs geom\\1,1\N,-0.1988756319,0.,-0.69250
91965\N,1.649128296,0.,1.2964759969\C,0.3412030135,0.,1.5256934831\N,-
0.6134412803,0.,0.5410135783\C,2.8625278201,0.,-2.6962208256\C,1.51966
04648,0.,-2.3978540063\C,1.118153928,0.,-1.0434203374\C,2.0740464367,0
.,0.0203671905\C,3.4412905429,0.,-0.3178600457\C,3.8089626238,0.,-1.64
80047498\C,-1.1732753446,0.,-1.7287606829\C,-0.7240976806,0.,-3.060539
4953\C,-1.6438131199,0.,-4.1041960641\C,-3.0001260818,0.,-3.8129766803
\C,-3.4508090052,0.,-2.4846954744\C,-2.5429470151,0.,-1.4412025678\C,-
0.1569013212,0.,2.9039115534\C,-1.5346643329,0.,3.1818566201\C,-1.9792
283511,0.,4.4972434193\C,-1.059841532,0.,5.546625932\C,0.3101547508,0.
,5.2781598268\C,0.7630283998,0.,3.9664806456\O,0.5966566135,0.,-3.3938
721534\H,4.1706632214,0.,0.4818754068\H,-1.2738937171,0.,-5.1222885159
\H,-4.5128356526,0.,-2.2714798608\H,-2.8645748475,0.,-0.4094441052\H,-
2.2500106585,0.,2.3697819535\H,-3.0432015111,0.,4.7057863922\H,1.02439
10228,0.,6.0938504792\H,1.8235924053,0.,3.749516488\H,4.8613610169,0.,
-1.9094092749\H,3.1747001851,0.,-3.7333910196\H,-3.7170824135,0.,-4.62
61666533\H,-1.4105242441,0.,6.5730927436\\Version=ES64L-G09RevD.01\Sta
te=1-A'\HF=-970.5216544\RMSD=3.632e-09\RMSF=3.145e-06\Dipole=-0.082706
1,0.,-1.4724509\Quadrupole=8.4409884,-28.9286831,20.4876947,0.,0.32620
55,0.\PG=CS [SG(C19H12N3O1)]\\

No imaginary frequencies.

1b^{+} (X=COOMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H14N3O3(1+)\PIOTR\09-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-COOMe sec o
rient cat benzotrazinyl, Cs\\1,1\N,-0.1838497452,0.8332110225,0.\N,-2.
8978479055,0.8992782189,0.\C,-2.2026127901,-0.2324852157,0.\N,-0.83263
55385,-0.2945320811,0.\C,-0.7120374364,4.4535623663,0.\C,-0.0464956414
,3.2503165179,0.\C,-0.7940304287,2.0519926514,0.\C,-2.2239846733,2.062
7316244,0.\C,-2.8769482445,3.311275201,0.\C,-2.1248129902,4.4678731717
,0.\C,1.2389450058,0.7910340847,0.\C,1.9380552823,2.0117919295,0.\C,3.

3300549581,2.0159123926,0.\C,4.0094584259,0.8102952149,0.\C,3.3158446448,-0.4127748076,0.\C,1.9293096863,-0.4236460355,0.\C,-2.9043325972,-1.5187406257,0.\C,-2.1985850975,-2.7343221766,0.\C,-2.8889710742,-3.9389964515,0.\C,-4.2841410544,-3.9463864144,0.\C,-4.9915499936,-2.7428199525,0.\C,-4.3097433031,-1.5342622934,0.\O,1.3124248803,3.2189803856,0.\H,3.8481457247,2.9671994533,0.\H,1.3821506798,-1.3545738941,0.\H,-1.1163380548,-2.7309897577,0.\H,-2.339980041,-4.8739550902,0.\H,-6.0757200251,-2.7489398907,0.\H,-4.8505359653,-0.596493602,0.\H,-2.6263168204,5.4293036609,0.\H,-0.1421080712,5.3746376608,0.\H,5.0929606374,0.7820437863,0.\H,-4.8201321337,-4.8894281291,0.\H,-3.9592412858,3.327222131,0.\C,4.1306650906,-1.6706426891,0.\O,5.3368187035,-1.6670380192,0.\O,3.364764001,-2.7670088992,0.\C,4.0840319767,-4.0193608974,0.\H,3.3193854627,-4.7940048089,0.\H,4.7109043691,-4.0910737376,-0.8904501794\H,4.7109043691,-4.0910737376,0.8904501794\\Version=ES64L-G09RevD.01\State=1-A'\HF=-1198.4086879\RMSD=5.732e-09\RMSF=2.561e-06\Dipole=-0.9660029,1.395755,0.\Quadrupole=3.6598874,25.1296873,-28.7895747,0.0917096,0.,0.\PG=CS [SG(C21H12N3O3),X(H2)]\\@

No imaginary frequencies.

1c^{+} (X=CN)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H11N4O1(1+)\PIOTR\10-May-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CN benzotrazinyl cat, Cs\\1,1\N,0.4714064961,-0.3340878567,0.\N,-1.9155619688,-1.6188126063,0.\C,-1.8104472302,-0.2928126554,0.\N,-0.6151023891,0.3801789754,0.\C,1.6410209183,-3.7989353221,0.\C,1.6901105128,-2.4258991558,0.\C,0.4813813637,-1.6954077116,0.\C,-0.7902707006,-2.3516884198,0.\C,-0.8073917089,-3.7616052864,0.\C,0.3863071396,-4.4517800603,0.\C,1.7237655933,0.3475893317,0.\C,2.8986143413,-0.4232724992,0.\C,4.1411101674,0.2069589796,0.\C,4.2066555853,1.5887673905,0.\C,3.0289497239,2.3646009964,0.\C,1.7851159259,1.7402443157,0.\C,-3.0166776825,0.5352572817,0.\C,-2.9380566379,1.939310656,0.\C,-4.0986785031,2.7008009981,0.\C,-5.3457760799,2.0749225609,0.\C,-5.4318255106,0.6812094673,0.\C,-4.2771466395,-0.0878714646,0.\O,2.8894508558,-1.7808969004,0.\H,5.0351778861,-0.404481426,0.\H,0.8713271615,2.3167662481,0.\H,-1.9727798984,2.4285690886,0.\H,-4.0322692964,3.7828760749,0.\H,-6.4013626497,0.196050965,0.\H,-4.3352679849,-1.1688255504,0.\H,0.375101915,-5.5360586378,0.\H,2.5655778275,-4.3633414954,0.\H,5.1702251399,2.0843139765,0.\H,-6.2507456727,2.6729014071,0.\H,-1.7652154862,-4.2657971571,0.\C,3.1065883118,3.7942267006,0.\N,3.1668742944,4.9506923109,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-1062.7511038\RMSD=4.922e-09\RMSF=1.844e-06\Dipole=0.5017247,-2.5609908,0.\Quadrupole=24.8661209,-1.6884381,-23.1776828,-13.1602527,0.,0.\PG=CS [SG(C20H11N4O1)]\\

No imaginary frequencies.

1d^{+} (X=NO$_2$)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H11N4O3(1+)\PIOTR\11-May-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NO2 benzotrazinyl cat, Cs\\1,1\N,0.1488758498,-0.6143173056,0.\N,-2.469022437,-1.3147092577,0.\C,-2.0613379997,-0.047892488,0.\N,-0.7430169924,0.3309866746,0.\C,0.4909211474,-4.2540562242,0.\C,0.8544141609,-2.9295258324,0.\C,-0.1543855407,-1.9412118807,0.\C,-1.5430452417,-2.286686041,0.\C,-1.8839727805,-3.6554143356,0.\C,-0.8808885078,-4.6010249233,0.\C,1.524655176,-0.23941782,0.\C,2.4934988919,-1.2594194578,0.\C,3.8489447515,-0.9344943438,0.\C,4.2327189478,0.3966005258,0.\C,3.2528284341,1.3921949399,0.\C,1.9039188664,1.1015838271,0.\C,-3.0428127981,1.0365722365,0.

\C,-2.639799022,2.3840987253,0.\C,-3.5922378544,3.3939117581,0.\C,-4.9
504962234,3.0742683938,0.\C,-5.3580236248,1.7385728218,0.\C,-4.4134255
964,0.7225592171,0.\O,2.1709216872,-2.5777788155,0.\H,4.5769009503,-1.
7365013315,0.\H,1.1720237937,1.8956803287,0.\H,-1.5873147049,2.6360421
873,0.\H,-3.2764632632,4.4309969077,0.\H,-6.4137297733,1.4919113289,0.
\H,-4.7207297617,-0.3154032044,0.\H,-1.1407897292,-5.6537517573,0.\H,1
.2605853896,-5.0162948039,0.\H,5.2762973068,0.6842222898,0.\H,-5.69200
24399,3.865947964,0.\H,-2.9320751865,-3.9258696481,0.\N,3.6655550896,2
.8121053411,0.\O,2.7739682548,3.6469465286,0.\O,4.8645816197,3.0355991
349,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-1175.0175948\RMSD=3.14
0e-09\RMSF=1.374e-06\Dipole=-0.5630317,-2.8929906,0.\Quadrupole=15.074
8608,8.6000356,-23.6748964,-14.9554046,0.,0.\PG=CS [SG(C19H11N4O3)]\\
No imaginary frequencies.

1e$^+$ (X=CF$_3$)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H11F3N3O1(1+)\PIOTR\11-M
ay-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-CF3 benzo
trazinyl, C1\\1,1\N,-0.1803658991,-0.7663288318,0.0052429049\N,-2.8801
636159,-1.0265969822,-0.0156797013\C,-2.2690176848,0.1537493946,-0.017
3470721\N,-0.9064690161,0.3124095095,-0.0068140236\C,-0.4449212954,-4.
414386978,0.0232431896\C,0.1324017736,-3.1669890424,0.0210163287\C,-0.
6996731149,-2.0256962259,0.0078531294\C,-2.1255607309,-2.1384490088,-0
.003233344\C,-2.6871743956,-3.43122032,-0.0005905092\C,-1.8536993184,-
4.5301385091,0.0123844388\C,1.2364259417,-0.6228428597,0.0170741723\C,
2.0209361637,-1.787087864,0.0291767795\C,3.4105572506,-1.6878389143,0.
0375408911\C,4.001747068,-0.4363959442,0.0348857123\C,3.2146768183,0.7
266561172,0.0257572825\C,1.8361663361,0.6398570822,0.0145869368\C,-3.0
602498142,1.3853762485,-0.0308469522\C,-2.4430851584,2.6486729982,-0.0
337620415\C,-3.2175348979,3.8007948264,-0.0465620991\C,-4.6096376285,3
.7080895535,-0.0565174124\C,-5.2295262111,2.4569296624,-0.0537165807\C
,-4.4634399173,1.300225284,-0.0409925936\O,1.4867169025,-3.0369970354,
0.0311815626\H,3.9976601737,-2.5980238115,0.043684656\H,1.2201763246,1
.5269320911,0.0022693805\H,-1.3635534992,2.7244330231,-0.0260857127\H,
-2.7364819839,4.7723688093,-0.0487878364\H,-6.3113239563,2.3856279685,
-0.0614657584\H,-4.9360641355,0.3263236975,-0.038701511\H,-2.284249760
4,-5.5253463691,0.0144119392\H,0.1891597636,-5.2925319722,0.0332788691
\H,5.0825514747,-0.3525864724,0.0359123783\H,-5.2116716258,4.610328093
9,-0.0664656024\H,-3.765455028,-3.5253056789,-0.0089061748\C,3.8993042
5,2.0760116528,0.0451180172\F,4.8324258379,2.1431251593,-0.9134446313\
F,3.0245179346,3.0719503707,-0.1455085116\F,4.5105454159,2.2771871816,
1.2208094992\\Version=ES64L-G09RevD.01\State=1-A\HF=-1307.5581919\RMSD
=2.565e-09\RMSF=2.351e-06\Dipole=-0.9638605,-2.4253393,-0.0169639\Quad
rupole=12.6985269,15.0709282,-27.7694551,-8.9768706,0.2815242,-0.33189
76\PG=C01 [X(C20H11F3N3O1)]\\
No imaginary frequencies.

1f$^+$ (X=OMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C20H14N3O2(1+)\PIOTR\10-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OMe 2nd orint
benzotrazinyl (phenazinoBT), Cs\\1,1\N,-0.3903760638,0.4808437228,0.\
N,-1.8422802643,-1.8161876787,0.\C,-0.5167406261,-1.7997234229,0.\N,0.
2443160198,-0.6582287346,0.\C,-3.7717836398,1.8881443558,0.\C,-2.39502
2643,1.8397634048,0.\C,-1.7508822631,0.5829199394,0.\C,-2.4956058109,-
0.637316401,0.\C,-3.8994629219,-0.5554428771,0.\C,-4.507287188,0.68584
04873,0.\C,0.378190382,1.6742077874,0.\C,-0.3106638007,2.8953703794,0.

\C,0.4110155722,4.0902425027,0.\C,1.7881499899,4.0535545826,0.\C,2.487
7870732,2.8226471699,0.\C,1.7780963931,1.6270907336,0.\C,0.2252320781,
-3.0657475777,0.\C,1.6299795056,-3.0892560641,0.\C,2.3066443998,-4.301
923165,0.\C,1.5939774324,-5.5011468478,0.\C,0.1982002305,-5.4857197105
,0.\C,-0.4853461858,-4.2778328218,0.\O,-1.6689573131,2.9850127344,0.\H
,-4.4698249222,-1.4753625579,0.\H,-0.1322205697,5.0273676609,0.\H,2.26
49982927,0.6650102887,0.\H,2.184965191,-2.1601483143,0.\H,3.3909000225
,-4.3138246177,0.\H,-0.3563294846,-6.4174097333,0.\H,-1.5676250208,-4.
2564780524,0.\H,-5.5899006226,0.7476488214,0.\H,-4.2678482977,2.850903
9757,0.\H,2.3683269364,4.9688984934,0.\H,2.1255334682,-6.4466851897,0.
\O,3.823197456,2.9266505433,0.\C,4.6088334812,1.7345823954,0.\H,4.4136
795032,1.1379395405,-0.8978194327\H,5.6461823938,2.0656545477,0.\H,4.4
136795032,1.1379395405,0.8978194327\\Version=ES64L-G09RevD.01\State=1-
A'\HF=-1085.0535646\RMSD=6.671e-09\RMSF=1.713e-06\Dipole=-0.30248,0.89
26329,0.\Quadrupole=15.6751945,13.8309531,-29.5061477,-3.5778632,0.,0.
\PG=CS [SG(C20H12N3O2),X(H2)]\\
No imaginary frequencies.

1g^{+} (X=F)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H11F1N3O1(1+)\PIOTR\11-M
ay-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-F benzotraz
inyl (phenazinoBT), Cs\\1,1\N,-0.1976912344,0.,-0.6928742098\N,1.64726
67009,0.,1.2954604074\C,0.33916695,0.,1.5255647658\N,-0.6151190625,0.,
0.539786225\C,2.8635589966,0.,-2.6967623607\C,1.5202160319,0.,-2.39942
29547\C,1.1183326378,0.,-1.0449204285\C,2.0737970902,0.,0.0199921746\C
,3.4407623252,0.,-0.3175054372\C,3.8089725181,0.,-1.647888882\C,-1.172
1475631,0.,-1.7293422404\C,-0.7232417067,0.,-3.0597317809\C,-1.6476189
09,0.,-4.1023283392\C,-3.0026313882,0.,-3.8181022098\C,-3.4294589247,0
.,-2.4851231247\C,-2.5372889753,0.,-1.4317235341\C,-0.158694043,0.,2.9
031158687\C,-1.5366450875,0.,3.1812609324\C,-1.9805090662,0.,4.4967995
369\C,-1.0605821813,0.,5.5457440519\C,0.3095162735,0.,5.277134818\C,0.
7618178516,0.,3.9653978639\O,0.5969196886,0.,-3.3951044486\H,4.1699694
516,0.,0.4823533614\H,-1.282245549,0.,-5.1219599822\H,-2.8827487458,0.
,-0.4084030957\H,-2.2529296506,0.,2.3699911285\H,-3.0443508742,0.,4.70
58537151\H,1.0239554381,0.,6.0926163296\H,1.8222762019,0.,3.7479935952
\H,4.8614965942,0.,-1.9087865674\H,3.1767619944,0.,-3.7336354122\H,-3.
7415875048,0.,-4.6105093652\H,-1.4110008118,0.,6.572299281\F,-4.729612
0266,0.,-2.228269902\\Version=ES64L-G09RevD.01\State=1-A'\HF=-1069.750
8946\RMSD=5.307e-09\RMSF=1.406e-06\Dipole=0.8405885,0.,-1.2952468\Quad
rupole=3.8652904,-27.1898766,23.3245862,0.,-1.5305675,0.\PG=CS [SG(C19
H11F1N3O1)]\\
No imaginary frequencies.

1h^{+} (X=Cl)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H11Cl1N3O1(1+)\PIOTR\11-
May-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #
P Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Cl benzotr
azinyl (phenazinoBT), Cs\\1,1\N,-0.1976569996,0.,-0.6925854007\N,1.648
1923376,0.,1.2952993551\C,0.339836367,0.,1.5257476734\N,-0.6141744531,
0.,0.5401004146\C,2.8634598695,0.,-2.6969372637\C,1.5207159623,0.,-2.3
989607285\C,1.1184222545,0.,-1.0447536264\C,2.0740182623,0.,0.01981465
46\C,3.4414318542,0.,-0.3181043328\C,3.8095876111,0.,-1.6481269237\C,-
1.1721091102,0.,-1.7301182732\C,-0.7221026948,0.,-3.0600643046\C,-1.64
72058961,0.,-4.1006930875\C,-3.0022391458,0.,-3.8147168256\C,-3.442990
6273,0.,-2.4816074047\C,-2.5379708063,0.,-1.4343509514\C,-0.1584654304
,0.,2.903081771\C,-1.5365862046,0.,3.1807838536\C,-1.9811013727,0.,4.4

961315179\C,-1.0616545141,0.,5.5454451291\C,0.3085434322,0.,5.27725039
42\C,0.7615528223,0.,3.9657177177\O,0.5965871071,0.,-3.3952777618\H,4.
1704489055,0.,0.4819863773\H,-1.2844097055,0.,-5.1213667821\H,-2.86688
44559,0.,-0.4057267103\H,-2.2526334151,0.,2.3693214861\H,-3.0450832732
,0.,4.7044465049\H,1.0226030937,0.,6.0930720451\H,1.8221182244,0.,3.74
89541295\H,4.8620367027,0.,-1.9092296573\H,3.1763173158,0.,-3.73391789
37\H,-3.7284009267,0.,-4.6184587635\H,-1.4124652893,0.,6.5718556549\Cl
,-5.1452721016,0.,-2.1455381874\\Version=ES64L-G09RevD.01\State=1-A'\H
F=-1430.1106646\RMSD=3.647e-09\RMSF=4.486e-06\Dipole=1.310372,0.,-1.08
32957\Quadrupole=6.0304869,-28.0843397,22.0538528,0.,-2.2180346,0.\PG=
CS [SG(C19H11Cl1N3O1)]\\
No imaginary frequencies.

1i^{+} (X=Br)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\Gen\C19H11Br1N3O1(1+)\PIOTR\11-May-2021
\0\\#P B3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistan
ce,NoAngle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-Br benzotrazin
yl (phenazinoBT) cat, Cs\\1,1\N,-0.2524646909,0.7810753508,0.\N,-2.961
3848462,0.9378392923,0.\C,-2.3050215792,-0.217700441,0.\N,-0.937516027
4,-0.3250755705,0.\C,-0.6570303823,4.4193379064,0.\C,-0.0307741642,3.1
93205539,0.\C,-0.8194241506,2.0200141918,0.\C,-2.2498621997,2.07879521
91,0.\C,-2.8609222822,3.3493964782,0.\C,-2.0691501418,4.480843581,0.\C
,1.1683190664,0.6909694359,0.\C,1.9068305272,1.8860852926,0.\C,3.29923
71205,1.8352668508,0.\C,3.942234353,0.6069643853,0.\C,3.1967528784,-0.
584489338,0.\C,1.8119216431,-0.551520239,0.\C,-3.0503659359,-1.4799227
382,0.\C,-2.3861446903,-2.719883894,0.\C,-3.1176696327,-3.9010464194,0
.\C,-4.5131955151,-3.860188958,0.\C,-5.1796765944,-2.6321644494,0.\C,-
4.4565142592,-1.4468493351,0.\O,1.3250298169,3.1148162185,0.\H,-3.9426
253898,3.4020458982,0.\H,3.8559939295,2.7651716795,0.\H,1.2221063261,-
1.4567464048,0.\H,-1.3039228495,-2.7548467573,0.\H,-2.6006883357,-4.85
46341753,0.\H,-6.2639815514,-2.6012800254,0.\H,-4.9641976998,-0.490178
4516,0.\H,-2.5381584668,5.4591397964,0.\H,-0.0564827969,5.3214669458,0
.\H,5.025049242,0.5656059773,0.\H,-5.0816059385,-4.7846841898,0.\Br,4.
1007855471,-2.2596651521,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-9
83.0625834\RMSD=9.662e-09\RMSF=3.782e-06\Dipole=-0.796885,2.1112732,0.
\Quadrupole=13.3238502,16.1030864,-29.4269366,5.5570998,0.,0.\PG=CS [S
G(C19H11Br1N3O1)]\\
No imaginary frequencies.

1j^{+} (X=Ac)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H14N3O2(1+)\PIOTR\11-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-COMe benzot
razinyl cat, sec orient Ac, Cs\\1,1\N,-0.1862105169,0.6345618623,0.\N,
2.4072596737,1.4383193651,0.\C,2.0473013947,0.1598471568,0.\N,0.746169
3216,-0.2738399465,0.\C,-0.6649268544,4.2617667307,0.\C,-0.9768073341,
2.9226101343,0.\C,0.0688676738,1.973434392,0.\C,1.441663463,2.37397989
09,0.\C,1.7293940937,3.7531966317,0.\C,0.6903326718,4.6609592043,0.\C,
-1.5432410367,0.2065338851,0.\C,-2.5478616984,1.189911611,0.\C,-3.8887
682633,0.8125574944,0.\C,-4.211636857,-0.5315034945,0.\C,-3.214127962,
-1.5273075974,0.\C,-1.8787454625,-1.151534814,0.\C,3.0747864874,-0.884
99783,0.\C,2.7305494558,-2.2477021545,0.\C,3.7246697682,-3.2169045442,
0.\C,5.0682504896,-2.8408992405,0.\C,5.4179071228,-1.4893695134,0.\C,4
.4305172434,-0.5143218669,0.\O,-2.2757243581,2.5212690721,0.\H,-4.6469
628393,1.5864741325,0.\H,-1.0811305886,-1.8805534518,0.\H,1.6890641547
,-2.5418301989,0.\H,3.4535791683,-4.2666876549,0.\H,6.4620679023,-1.19
75265757,0.\H,4.693136239,0.5358123305,0.\H,0.9105321768,5.7227195505,

0.\H,-1.4645934208,4.9923690671,0.\H,-5.2460340707,-0.8559978296,0.\H,
5.8425625474,-3.6005082847,0.\H,2.766335215,4.063625949,0.\C,-3.667276
9776,-2.9703687114,0.\O,-4.8548270276,-3.2059864424,0.\C,-2.6260828861
,-4.0654931646,0.\H,-1.9834990677,-3.9941771626,-0.8846941032\H,-1.983
4990677,-3.9941771626,0.8846941032\H,-3.1327367821,-5.0300257815,0.\\V
ersion=ES64L-G09RevD.01\State=1-A'\HF=-1123.1708162\RMSD=7.177e-09\RMS
F=1.011e-06\Dipole=0.6182815,1.6510001,0.\Quadrupole=6.422527,18.16469
68,-24.5872238,-10.7332652,0.,0.\PG=CS [SG(C21H12N3O2),X(H2)]\\
No imaginary frequencies.

1l^{+} (X=NH$_2$)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C19H13N4O1(1+)\PIOTR\10-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NH2 benzotr
azinyl cat, C1\\1,1\N,0.1611049368,-0.6043423051,-0.0018467601\N,-2.46
40139392,-1.3060774791,0.0035097137\C,-2.0533233391,-0.0461413767,0.00
07173834\N,-0.7375392117,0.341454392,-0.0010349326\C,0.4970858171,-4.2
525938283,-0.0039097414\C,0.8618605352,-2.9231385182,-0.0045008809\C,-
0.1459202424,-1.9332672518,-0.001362595\C,-1.5327347919,-2.2814979331,
0.0022179664\C,-1.8727220876,-3.6450923696,0.0032930144\C,-0.868740097
6,-4.5960679514,0.0001163372\C,1.5291910269,-0.2231731404,-0.003301495
3\C,2.4893887103,-1.2477553217,-0.0071833727\C,3.8417238544,-0.9093990
026,-0.0088636503\C,4.2176568391,0.4171789231,-0.0083991145\C,3.257081
8002,1.4632665428,-0.0042268863\C,1.9019319332,1.1204415969,0.00167658
72\C,-3.0412494093,1.0395332849,-0.0004986949\C,-2.6448161539,2.386936
0889,-0.0262025252\C,-3.6004678241,3.3946841461,-0.0285135068\C,-4.957
4204223,3.0724002934,-0.0044545368\C,-5.3588384347,1.735797727,0.02130
99204\C,-4.4098105179,0.7229742217,0.0228566665\O,2.170080395,-2.57183
75199,-0.0084228365\H,4.5774747614,-1.7044790446,-0.0105682497\H,1.131
6773204,1.8785052649,0.004896223\H,-1.5925275524,2.6389232587,-0.04648
95841\H,-3.2883487257,4.4328985852,-0.0495866983\H,-6.4134440013,1.484
6185006,0.039966406\H,-4.7121455798,-0.3162943146,0.0422470581\H,-1.13
28914732,-5.6477706576,0.0005338192\H,1.2686276151,-5.0126398092,-0.00
67021222\H,5.2730844596,0.668910778,-0.0150016948\H,-5.7014947481,3.86
16966142,-0.0061001753\H,-2.920806056,-3.9153873983,0.0059734138\N,3.6
651581001,2.768079245,-0.055232277\H,3.0017995874,3.4927509633,0.16922
87764\H,4.6203677558,2.982936455,0.1838590451\\Version=ES64L-G09RevD.0
1\State=1-A\HF=-1025.887688\RMSD=5.102e-09\RMSF=1.536e-06\Dipole=1.804
312,0.0318124,0.2543333\Quadrupole=19.8179719,13.1744402,-32.9924121,3
.059585,1.997198,1.7925956\PG=C01 [X(C19H13N4O1)]\\
No imaginary frequencies.

1m^{+} (X=NHAc)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H15N4O2(1+)\PIOTR\10-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-NHAc benzot
razinyl cat, C1\\1,1\N,0.3718112963,0.7311935285,0.0010054678\N,3.0884
265842,0.715552541,0.0010727131\C,2.359952321,-0.3922553639,0.00231906
01\N,0.9886318984,-0.4178097556,0.0023235754\C,1.0104873642,4.33730507
68,-0.0030864325\C,0.3076138315,3.1524987368,-0.0017508833\C,1.0187014
5,1.9318105868,-0.0003492015\C,2.4483871299,1.9012669189,-0.0002883371
\C,3.1371542059,3.1273044678,-0.0016704452\C,2.4197991127,4.3085084187
,-0.0030277976\C,-1.0477884302,0.7292687809,0.0009856347\C,-1.70669842
72,1.9691213604,-0.00043761\C,-3.0976321645,1.9975963509,-0.0004926433
\C,-3.8224871751,0.8206520732,0.000837675\C,-3.1631094815,-0.435362774
8,0.0022813362\C,-1.768932088,-0.464932678,0.002335937\C,3.0272978419,
-1.699267766,0.0038184729\C,2.2909727081,-2.8956754346,0.0051515744\C,

2.9484269214,-4.1188887915,0.0065559404\C,4.3426863251,-4.163813548,0.
0066484599\C,5.0810651413,-2.9793045001,0.0053289471\C,4.4312512938,-1
.7528826351,0.0039204411\O,-1.0478087929,3.1607108717,-0.0017843475\H,
-3.5975347335,2.958810147,-0.0015964657\H,-1.2243368929,-1.3994319068,
0.0034098542\H,1.2092273167,-2.8626800136,0.0050815794\H,2.3747835288,
-5.039036569,0.0075804696\H,6.1647512098,-3.013712458,0.0054004357\H,4
.9961982787,-0.8295215732,0.0028915823\H,2.9514453509,5.253607707,-0.0
040933995\H,0.4673430748,5.2743512551,-0.0041625772\H,-4.9021931054,0.
8385739463,0.0007997971\H,4.8535039182,-5.1207183207,0.0077474179\H,4.
2194048576,3.1109567527,-0.0016318828\N,-3.8509460088,-1.6439626501,0.
0036502751\H,-3.2769613986,-2.4746596968,0.0046109997\C,-5.2339423516,
-1.8576721798,0.0038834322\O,-6.0346961463,-0.9496498349,0.0028358593\
C,-5.6175979547,-3.3214071555,0.0055573472\H,-5.2219084878,-3.83040234
9,-0.8797197612\H,-5.2219406309,-3.828367173,0.8920158938\H,-6.7040156
913,-3.3929333928,0.0056196061\\Version=ES64L-G09RevD.01\State=1-A\HF=
-1178.5512413\RMSD=3.733e-09\RMSF=5.279e-07\Dipole=0.7344484,0.3250275
,-0.0003527\Quadrupole=5.8429963,23.5231153,-29.3661116,8.6998052,-0.0
093032,-0.0601303\PG=C01 [X(C21H15N4O2)]\\

No imaginary frequencies.

1n^{+} (X=I)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\Gen\C19H11I1N3O1(1+)\PIOTR\11-May-2021\
0\\#P B3LYP/gen FOpt=tight freq(noraman) SCF=Direct #P Geom=(NoDistanc
e,NoAngle) fcheck Pseudo=Read\\Parent C(8)-O-Ph(N1)-10-I benzotrazinyl
(phenazinoBT) cat, Cs\\1,1\N,-0.2528327453,0.7824188907,0.\N,-2.96208
1681,0.9389644068,0.\C,-2.3056266899,-0.2162243583,0.\N,-0.9382157782,
-0.3236520661,0.\C,-0.6569488338,4.4206167752,0.\C,-0.0307659555,3.194
3618869,0.\C,-0.8199372927,2.0213494066,0.\C,-2.2502051454,2.079991038
1,0.\C,-2.8609479752,3.3505479926,0.\C,-2.0690001106,4.4820134289,0.\C
,1.1676927251,0.6920596058,0.\C,1.9066095835,1.886716975,0.\C,3.298646
2688,1.8337823414,0.\C,3.9400393188,0.6040248858,0.\C,3.1975463111,-0.
5918684739,0.\C,1.8113835753,-0.5505974927,0.\C,-3.0501482418,-1.47922
00632,0.\C,-2.3844365203,-2.7183246767,0.\C,-3.1145162237,-3.900410739
4,0.\C,-4.5100960427,-3.8612884782,0.\C,-5.178027541,-2.6341427371,0.\
C,-4.456255653,-1.4478987936,0.\O,1.3251681301,3.1155708993,0.\H,-3.94
26539406,3.4034931488,0.\H,3.8566551372,2.7630630565,0.\H,1.2133552526
,-1.4503921344,0.\H,-1.3021872837,-2.751755824,0.\H,-2.596300278,-4.85
335217,0.\H,-6.262365167,-2.6045984201,0.\H,-4.9653241252,-0.491929135
,0.\H,-2.5381828668,5.4602350422,0.\H,-0.0564393045,5.3227475928,0.\H,
5.0234662987,0.5701389183,0.\H,-5.0772850347,-4.7865424504,0.\I,4.1868
506389,-2.4394417885,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-981.2
768486\RMSD=5.504e-09\RMSF=1.650e-06\Dipole=-1.3726553,2.3943704,0.\Qu
adrupole=14.0620568,17.4813742,-31.5434311,1.5647732,0.,0.\PG=CS [SG(C
19H11I1N3O1)]\\

No imaginary frequencies.

1p^{+} (X=OBn)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C26H18N3O2(1+)\PIOTR\13-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-OBn 2nd orien
t benzotrazinyl (phenazinoBT) cat, C1\\1,1\N,-1.7540889369,-0.66090886
11,0.0241652988\N,-4.2417210836,0.4343179902,-0.0121878494\C,-3.133153
3696,1.1565872627,-0.0880080755\N,-1.8643303708,0.6351896592,-0.072297
6803\C,-3.773658588,-3.7051898883,0.2937176052\C,-2.6587207074,-2.8995
317932,0.2114342559\C,-2.8261620626,-1.501220959,0.1082759552\C,-4.125
0030281,-0.9052503515,0.0874592124\C,-5.2433611851,-1.7530579228,0.173
0109712\C,-5.0545991999,-3.1188030579,0.2732913302\C,-0.4505199736,-1.

2210533176,0.0421633479\C,-0.3406274041,-2.6152179292,0.1460936907\C,0
.9250035659,-3.2034499739,0.1669443385\C,2.0462078701,-2.4076855717,0.
0852872142\C,1.9426776897,-0.9978242177,-0.0199587679\C,0.6840994877,-
0.4037929621,-0.0413812267\C,-3.2244920744,2.6174330356,-0.1973508951\
C,-2.0724410069,3.4172527414,-0.2798586635\C,-2.1879981514,4.797381964
6,-0.3826063499\C,-3.4485287631,5.3943965116,-0.4042509426\C,-4.597672
7879,4.6061504053,-0.3226783703\C,-4.4904784076,3.2262580261,-0.219789
8527\O,-1.417409274,-3.4440245384,0.2294227173\H,-6.2300469374,-1.3083
157195,0.1578050772\H,0.9977791253,-4.2812192274,0.2475188875\H,0.5491
780086,0.6628790029,-0.1199396002\H,-1.0935476744,2.9560219302,-0.2632
308912\H,-1.2950738434,5.4092806897,-0.445944847\H,-5.5777093902,5.069
6943788,-0.339459556\H,-5.3763754811,2.6074141273,-0.1560544092\H,-5.9
181120786,-3.77139232,0.3391944771\H,-3.6469528511,-4.7778687958,0.372
8861521\H,3.0385313758,-2.8431362737,0.0996760759\H,-3.5355981331,6.47
26392215,-0.4845847936\O,3.1078997409,-0.3473831084,-0.0913996338\C,3.
1060216478,1.1006519257,-0.2014719108\H,2.5877409215,1.512206885,0.672
7019911\H,2.5541322272,1.3768227657,-1.1077390092\C,4.5295029822,1.567
584443,-0.2638486865\C,5.1782857004,1.6875206145,-1.4956576912\C,5.223
6986666,1.8705111345,0.9104533767\C,6.5064844972,2.1009454827,-1.55308
30249\C,6.5519320538,2.284074759,0.854846391\C,7.1939900708,2.39883307
58,-0.3773569665\H,4.6418823613,1.4575688792,-2.4117657407\H,4.7227015
776,1.7832275701,1.870268011\H,7.0026768434,2.1946373288,-2.5130191906
\H,7.083520601,2.5203936195,1.7702860387\H,8.2276965802,2.724790659,-0
.4216569205\\Version=ES64L-G09RevD.01\State=1-A\HF=-1316.1169621\RMSD=
2.064e-09\RMSF=1.078e-06\Dipole=-1.7021816,-1.4117713,0.1394586\Quadru
pole=24.4445931,9.5223489,-33.966942,11.4892162,-1.9812561,-3.5465444\
PG=C01 [X(C26H18N3O2)]\\@

No imaginary frequencies.

1q^{+} (X=Ph)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C25H16N3O1(1+)\PIOTR\12-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Ph benzotrazi
nyl (phenazinoBT) cat, C1\\1,1\N,-0.2707841031,-1.2482511569,-1.049940
6531\N,1.5069703121,-2.4552131415,0.6129618688\C,0.1992494456,-2.44562
40221,0.8366936912\N,-0.7209548808,-1.8431192902,0.0179576681\C,2.8410
218924,-0.5195622777,-2.8364295974\C,1.4944892391,-0.5426658154,-2.550
582065\C,1.0513808461,-1.1991662835,-1.3809519965\C,1.9695622921,-1.83
85712032,-0.4910905633\C,3.3396918355,-1.7973984196,-0.8104116608\C,3.
7487655246,-1.1493154858,-1.9592329573\C,-1.2077319478,-0.616436652,-1
.9123081725\C,-0.7158846709,0.0143642634,-3.0675773743\C,-1.6059738591
,0.6315962666,-3.939898976\C,-2.9600746101,0.6157886716,-3.6544985684\
C,-3.4780272762,-0.0136077738,-2.4984012652\C,-2.5765999911,-0.6320995
439,-1.6345670555\C,-0.3398166794,-3.1107427633,2.0276654033\C,-1.7211
702023,-3.1431311802,2.2833793997\C,-2.2042476228,-3.7817884861,3.4180
102322\C,-1.3200838465,-4.3921558477,4.307744681\C,0.0534479395,-4.363
8606124,4.0600955986\C,0.5443546325,-3.7286878371,2.9280258092\O,0.607
600302,0.0570931791,-3.3840321216\H,4.0398524865,-2.2797701654,-0.1405
767938\H,-1.2143058864,1.1234503046,-4.822088582\H,-2.9214501515,-1.15
04346871,-0.7516831733\H,-2.4094134414,-2.6719092207,1.5937867616\H,-3
.2712705401,-3.8048613379,3.6092928756\H,0.7408769404,-4.8382434125,4.
7514555845\H,1.6078903648,-3.702370941,2.727966782\H,4.8043416831,-1.1
178562357,-2.2054288206\H,3.1831204226,-0.0170348405,-3.7328163049\H,-
3.6415708061,1.1222508093,-4.328106045\H,-1.7007762432,-4.889913172,5.
1931585158\C,-4.9296795675,-0.0093123128,-2.2160754204\C,-5.4032606154
,0.1043390274,-0.9003450007\C,-5.8596507843,-0.1190938031,-3.260852073
2\C,-6.7688479406,0.1078595448,-0.6376369551\C,-7.2248883818,-0.121690
1219,-2.9952168875\C,-7.6832308058,-0.0069789575,-1.6838207181\H,-4.70

03472988,0.2286343572,-0.0827934235\H,-5.5151638425,-0.2374836769,-4.2
829940052\H,-7.1196958534,0.2108253983,0.3834637287\H,-7.9307235649,-0
.2189063489,-3.812830826\H,-8.748054975,-0.0039259761,-1.4782166943\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-1201.591051\RMSD=2.549e-09\RMSF=
2.954e-06\Dipole=1.3113743,0.27872,-0.7450005\Quadrupole=22.7100265,-2
4.5055985,1.795572,-4.7733948,-1.6203061,-19.4094576\PG=C01 [X(C25H16N
3O1)]\\
No imaginary frequencies.

1r^{+} (X=2-thienyl)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C23H14N3O1S1(1+)\PIOTR\12-M
ay-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-Thio benzot
razinyl (phenazinoBT), C1\\1,1\N,-0.4842604176,-2.2243639445,-2.174869
0501\N,1.0895375958,-4.3586947875,-1.5834592201\C,-0.2145549554,-4.333
3450528,-1.3422765422\N,-1.0339441629,-3.2712358188,-1.6264309851\C,2.
7456767678,-0.953382077,-3.3415890495\C,1.39685324,-0.9866903394,-3.06
62460421\C,0.8443885248,-2.142011201,-2.4708322783\C,1.6549944207,-3.2
750781523,-2.1494089572\C,3.0296620207,-3.210883672,-2.4423428034\C,3.
5467785263,-2.0698595569,-3.0245813473\C,-1.3159752999,-1.1113554492,-
2.4772675668\C,-0.7169412877,0.0093838938,-3.0772450333\C,-1.504211935
4,1.1106703023,-3.3997641847\C,-2.8569683575,1.0886999617,-3.117652409
3\C,-3.4830041907,-0.0299698153,-2.5124436564\C,-2.684019135,-1.134368
4555,-2.2068114835\C,-0.8627598682,-5.4984723525,-0.7304892634\C,-2.24
57585545,-5.5179892234,-0.4835798379\C,-2.8344032026,-6.6347304733,0.0
95019144\C,-2.0542161011,-7.7403758667,0.4338958189\C,-0.679535852,-7.
7281265936,0.1915897655\C,-0.0837426354,-6.6163902417,-0.3873306102\O,
0.6105443551,0.0781655337,-3.3653000959\H,3.6486402227,-4.0655267329,-
2.2015013135\H,-1.0335736387,1.9716990379,-3.8586621438\H,-3.109833867
1,-2.0280983077,-1.7754445931\H,-2.852836689,-4.6617361349,-0.74725691
05\H,-3.9024132252,-6.6446692559,0.2818218399\H,-0.0730538183,-8.58747
74072,0.454832255\H,0.981501301,-6.598685659,-0.5791847476\H,4.6061972
088,-2.0208572537,-3.2505027831\H,3.1708720829,-0.0682142059,-3.798513
3728\H,-3.4497921959,1.9651119978,-3.3547796502\H,-2.5167066635,-8.611
2155769,0.885992914\C,-4.9093559709,-0.0340200597,-2.2105603977\C,-5.5
86038495,-0.8125937249,-1.2948355161\C,-6.9799160939,-0.5613046762,-1.
2592224983\C,-7.3630033482,0.4059904752,-2.1501330404\S,-6.0257134481,
1.0231130567,-3.0418361507\H,-5.0935690661,-1.5218570522,-0.6409489539
\H,-7.6685665371,-1.0697055578,-0.5969845813\H,-8.3536283835,0.7923180
892,-2.3390248571\\Version=ES64L-G09RevD.01\State=1-A\HF=-1522.3453716
\RMSD=6.910e-09\RMSF=1.830e-06\Dipole=1.2747426,0.2978556,-0.2465756\Q
uadrupole=23.2423822,3.620537,-26.8629193,-5.6975095,-9.4290689,-16.70
52568\PG=C01 [X(C23H14N3O1S1)]\\
No imaginary frequencies.

1s^{+} (X=CCPh)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C27H16N3O1(1+)\PIOTR\12-May
-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent C(8)-O-Ph(N1)-10-CCPh benzotra
zinyl (phenazinoBT), Cs\\1,1\N,0.7111553334,1.7308806367,0.\N,-0.76089
46222,4.0145067312,0.\C,-1.3039269955,2.8040812548,0.\N,-0.58873193,1.
6343586956,0.\C,3.4101802017,4.2053911245,0.\C,2.786702182,2.977591653
7,0.\C,1.3760153315,2.9216345242,0.\C,0.5828209529,4.1107947248,0.\C,1
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\C,-3.3749375249,1.3973938808,0.\C,-4.7597480753,1.2928554286,0.\C,-5.
5486613279,2.4432774645,0.\C,-4.948590902,3.7036976416,0.\C,-3.5654411
745,3.8169780818,0.\O,3.5218192339,1.8364667358,0.\H,0.6535313171,6.25
50072594,0.\H,4.734228042,-0.4078875334,0.\H,-0.2255815773,-0.77918142
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H,-5.5615178231,4.5980913763,0.\H,-3.0916789712,4.7903210507,0.\H,3.14
16504041,6.3354583216,0.\H,4.4923366755,4.2498111951,0.\H,3.6517158339
,-2.6468095334,0.\H,-6.6300662135,2.35822805,0.\C,1.0386976263,-3.1662
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,0.\C,-1.3952810352,-5.7668873263,0.\C,0.842285055,-6.7165090302,0.\C,
-1.9325025687,-7.047192415,0.\C,0.2944637542,-7.9922933797,0.\C,-1.090
9367613,-8.1605196321,0.\H,-2.0421976468,-4.8970171307,0.\H,1.91737105
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9546,0.,0.\PG=CS [SG(C27H16N3O1)]\\

No imaginary frequencies.

1u^{+} (X=NHCOCF$_3$)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H12F3N4O2(1+)\PIOTR\13-M
ay-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P
Geom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-NHCOCF
3 2nd orient benzotrazinyl, C1\\1,1\N,-1.3378654687,-0.7927629844,-0.0
038992592\N,-3.9151048507,0.0579534443,0.0078002655\C,-2.8810488094,0.
889951279,-0.0015078129\N,-1.5690746051,0.489435871,-0.0071467036\C,-3
.0533976022,-4.0263677262,0.0160353476\C,-2.0203679856,-3.1167908166,0
.006866324\C,-2.321280396,-1.7362687374,0.0044072138\C,-3.6722379333,-
1.2657853805,0.0109444587\C,-4.7059371082,-2.220806786,0.0204336896\C,
-4.3867807097,-3.5644244888,0.0228142992\C,0.0146507837,-1.2301191499,
-0.008742816\C,0.2610715318,-2.6119604723,-0.0066281994\C,1.5752941786
,-3.069140604,-0.0114479436\C,2.6277401315,-2.171958096,-0.0173276506\
C,2.3810265153,-0.7788800409,-0.0181682135\C,1.0680343221,-0.315959727
4,-0.0144778356\C,-3.1129138927,2.3375788204,-0.0061784592\C,-2.043539
9822,3.2492636058,-0.0201468938\C,-2.2926017836,4.6152437049,-0.024635
9332\C,-3.6054592534,5.0871526574,-0.0151157744\C,-4.6729237251,4.1877
07094,-0.0011999736\C,-4.4324214548,2.8209297231,0.0031932695\O,-0.731
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45881\H,0.8410457248,0.7415890179,-0.0149196696\H,-1.0240938296,2.8860
53767,-0.0278220443\H,-1.4635746535,5.3139610613,-0.0356077519\H,-5.69
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68072\H,-5.1830858108,-4.3004189229,0.0301175286\H,-2.8263670629,-5.08
54276411,0.0179714497\H,3.6487627558,-2.5246239789,-0.021056811\H,-3.7
965915212,6.1548617042,-0.0185998329\H,-5.7305800477,-1.87200915,0.025
5407586\N,3.4103093384,0.165367772,-0.0208258169\H,3.1407748312,1.1394
04465,-0.0242662275\C,4.7642071911,-0.0701559419,-0.0201789472\O,5.308
6872875,-1.1466181358,-0.0270151718\C,5.612997584,1.2293128528,0.00403
08846\F,6.4503679496,1.2398229331,-1.0239328349\F,4.8322615575,2.33363
97113,-0.0707827105\F,6.3053391305,1.2883929592,1.1364797335\\Version=
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5271,-27.7142401,6.4252451,-0.231846,-0.1976576\PG=C01 [X(C21H12F3N4O2
)]\\

No imaginary frequencies.

1v^{+} (X=NHCOOMe)

1\1\GINC-LOCALHOST\FOpt\RB3LYP\6-31G(2d,p)\C21H15N4O3(1+)\PIOTR\13-May

-2021\0\\#P B3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P G
eom=(NoDistance,NoAngle) fcheck\\Parent flat C(8)-O-Ph(N1)-10-NHCOOMe
2nd orient benzotrazinyl cat, C1\\1,1\N,-0.7580464186,-0.8795713628,-0
.0000012084\N,-3.1696559097,0.3709699279,0.0000111706\C,-2.0168142884,
1.0256731194,0.0000049415\N,-0.7841502932,0.424048557,-0.0000011721\C,
-2.9672772713,-3.8004804121,0.0000068447\C,-1.8022000648,-3.0650969421
,0.0000017701\C,-1.8804317762,-1.6544741908,0.0000037169\C,-3.13939231
92,-0.9763024072,0.0000107577\C,-4.3103494322,-1.7549038895,0.00001620
32\C,-4.2088221318,-3.1332629139,0.0000141644\C,0.5070984055,-1.523163
8749,-0.0000074007\C,0.5299272266,-2.9267433024,-0.0000094315\C,1.7562
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\O,5.7392496228,-2.2963999861,-0.0000277292\O,6.2007429006,-0.07430836
92,-0.0000237356\C,7.6110884961,-0.3774195356,-0.0000293538\H,7.873846
5181,-0.9492646851,0.8915281121\H,7.8738428151,-0.9492483161,-0.891598
5504\H,8.1115060083,0.5892009274,-0.0000217607\\Version=ES64L-G09RevD.
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,8.2512311,-0.0002042,-0.000098\PG=C01 [X(C21H15N4O3)]\\@

No imaginary frequencies.

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