Supporting Information for

Sensitive Hydrazine Detection and Quantification with a Fluorescent Benzothiadiazole Sensor: Selective Lipid Droplets and In Vivo Imaging

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Summary

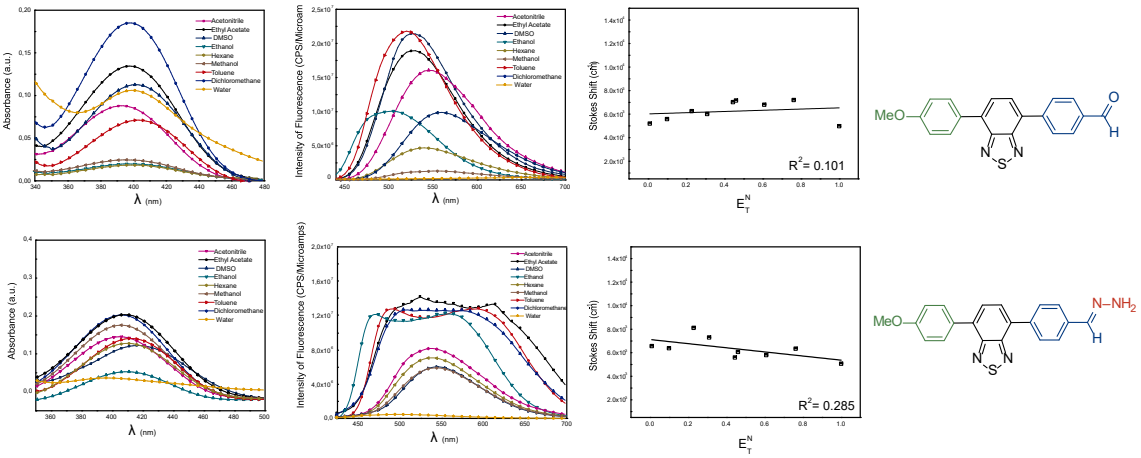

Figure S1. UV-Vis (left), fluorescence (center) and solvatochromic effect (Reichardt, right) of the synthesized BTDs (**BTD-CHO** and **BTD-HZN**). 10 μM for all analyses.

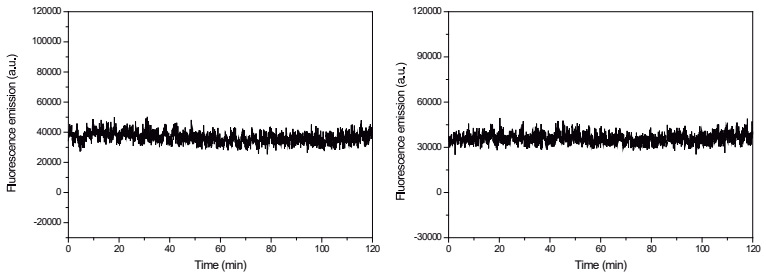

Figure S2. Photostability of the synthesized dyes (10 μM) acquired at room temperature upon excitation at 254 nm while monitoring the emission at the emission maxima of each molecule in aqueous solutions. Time-dependence of photoluminescence intensity was carried out with a Xe lamp (400 W). (Right) **BTD-CHO** and (Left) **BTD-HZN**.

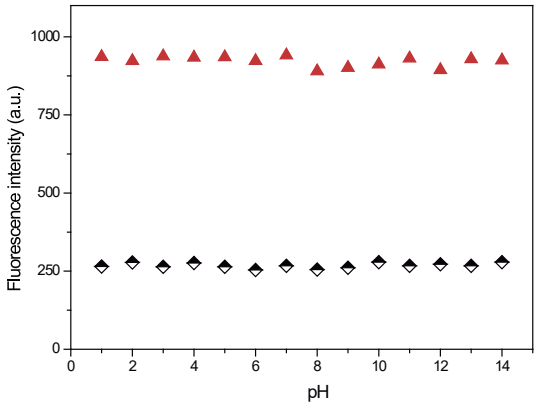

Figure S3. pH effect over the fluorescence emission of the dyes **BTD-CHO** (black) and **BTD-HZN** (red). Concentration: 10 μM.

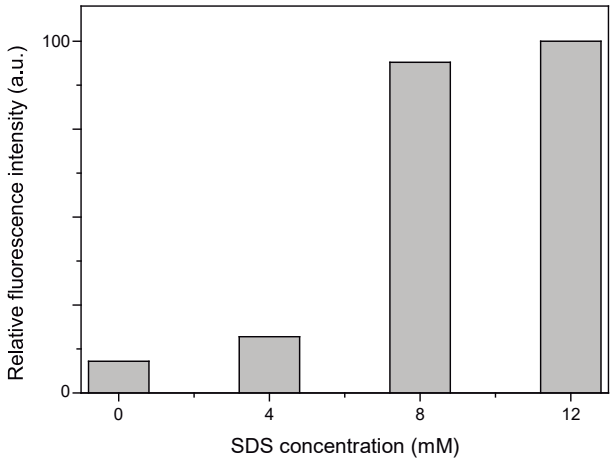

Figure S4. BTD-CHO (10 μM) before and after addition of SDS (CMC = 8 mM). The light-up in the emission intensity of the dye is 11-fold when compared with the emission in the absence of SDS.

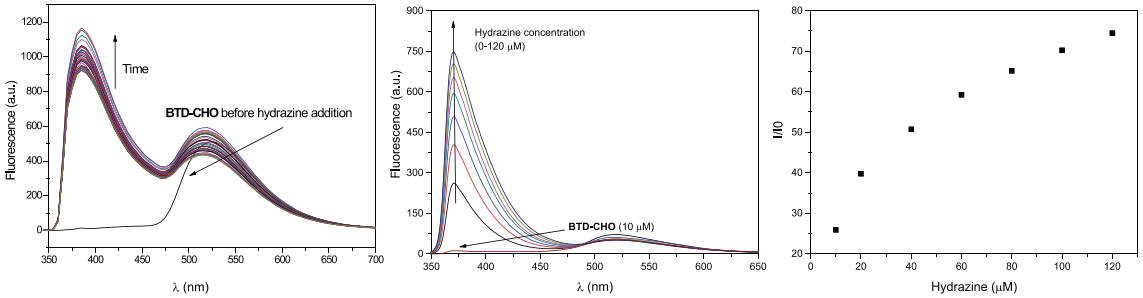

Figure S5. BTD-CHO (10 μM) in phosphate buffer solutions (pH = 7.0) before and after addition of hydrazine (0-120 μM). The reaction was fast, as expected, and in a few minutes, it was noted the dye total consume affording **BTD-HZN**. (Left) Hydrazine addition (10 μM) and fast **BTD-CHO** consumption monitoring for a period of ten minutes. (Center) Fluorescence increase after analyte (hydrazine) addition. (Right) Fluorescence intensity as a function of the analyte concentration. Excitation wavelength at 340 nm.

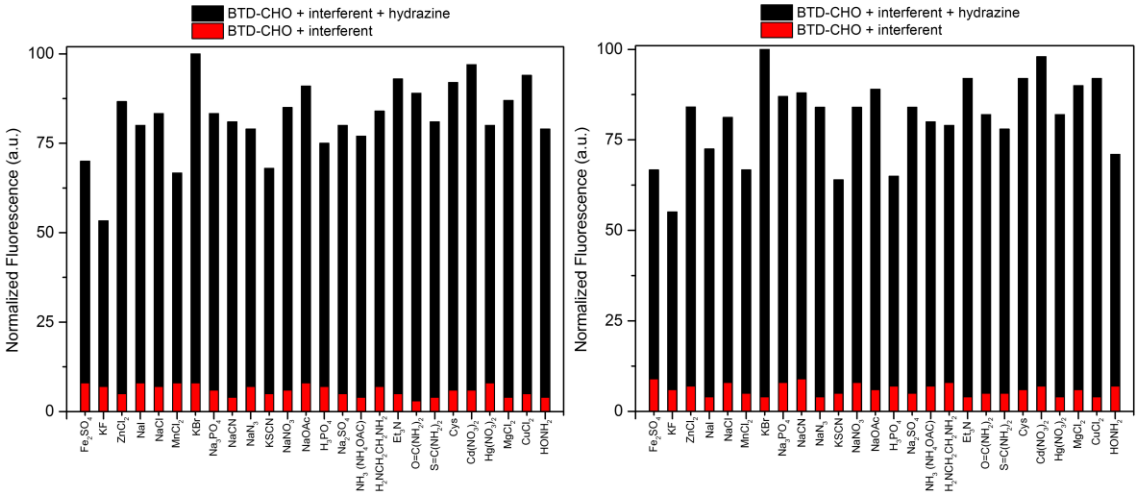

Figure S6. BTD-CHO (10 μM) in phosphate buffer solutions (pH = 7.0) in the presence of both interfering species (1 and 10 equivalents, respectively) and hydrazine (10 μM). Note that independent of the presence of other analytes, the formation of **BTD-HZN** is always favored and fast. Excitation wavelength at 340 nm and monitoring at 375 nm.

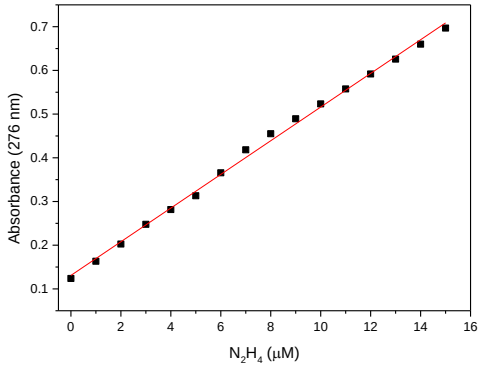

Figure S7. Calibration curve (UV-Vis) from three independent experiments monitored at 375 nm during the titration with aqueous hydrazine (50%) and a DMSO solution with the sensor **BTD-CHO** (1.0 μM). H_4N_2 concentration in the range of 1 to 15 μM. $R^2 = 0.997$.

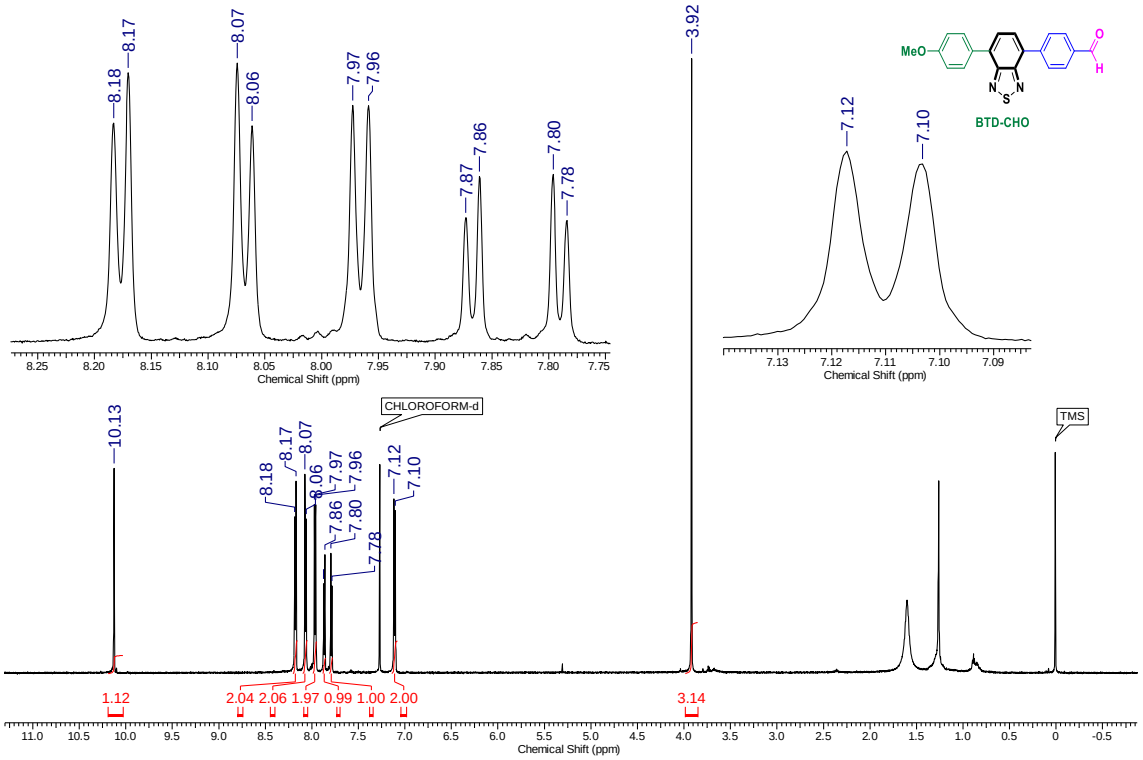

Figure S8. ^{1}H NMR (600 MHz, $CDCl_3$) of the sensor named **BTD-CHO**.

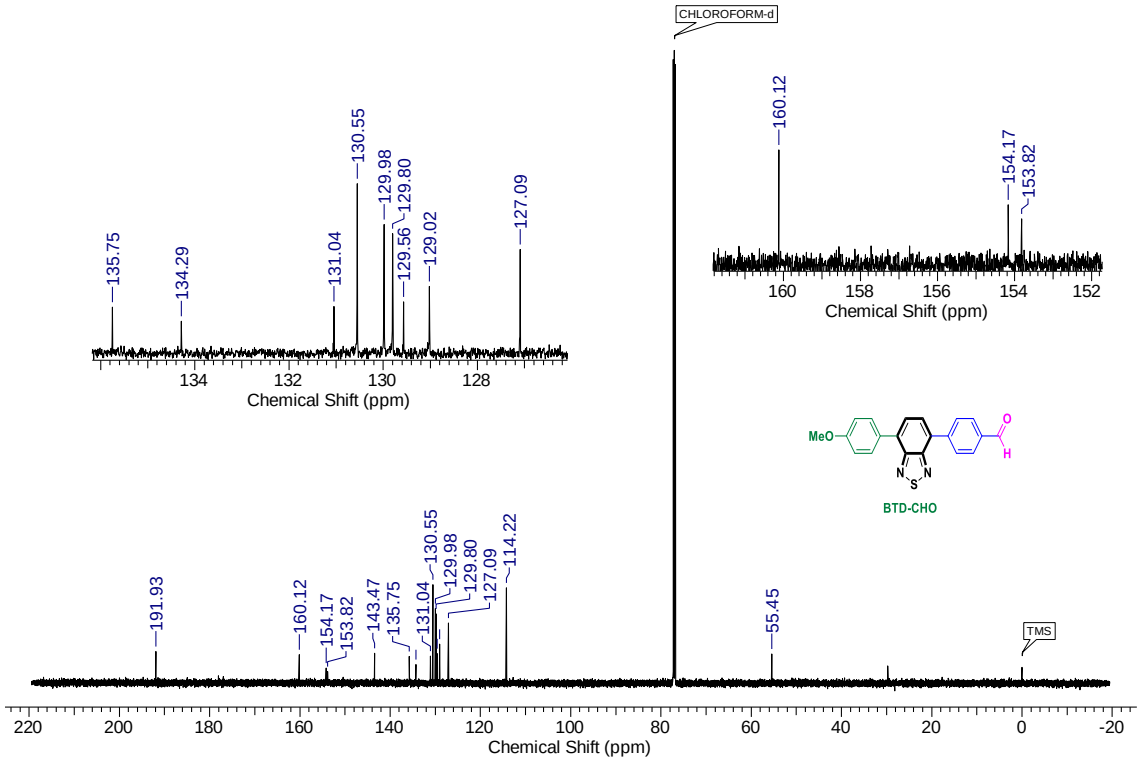

Figure S9. ^{13}C NMR (150 MHz, $CDCl_3$) of the sensor named **BTD-CHO**.

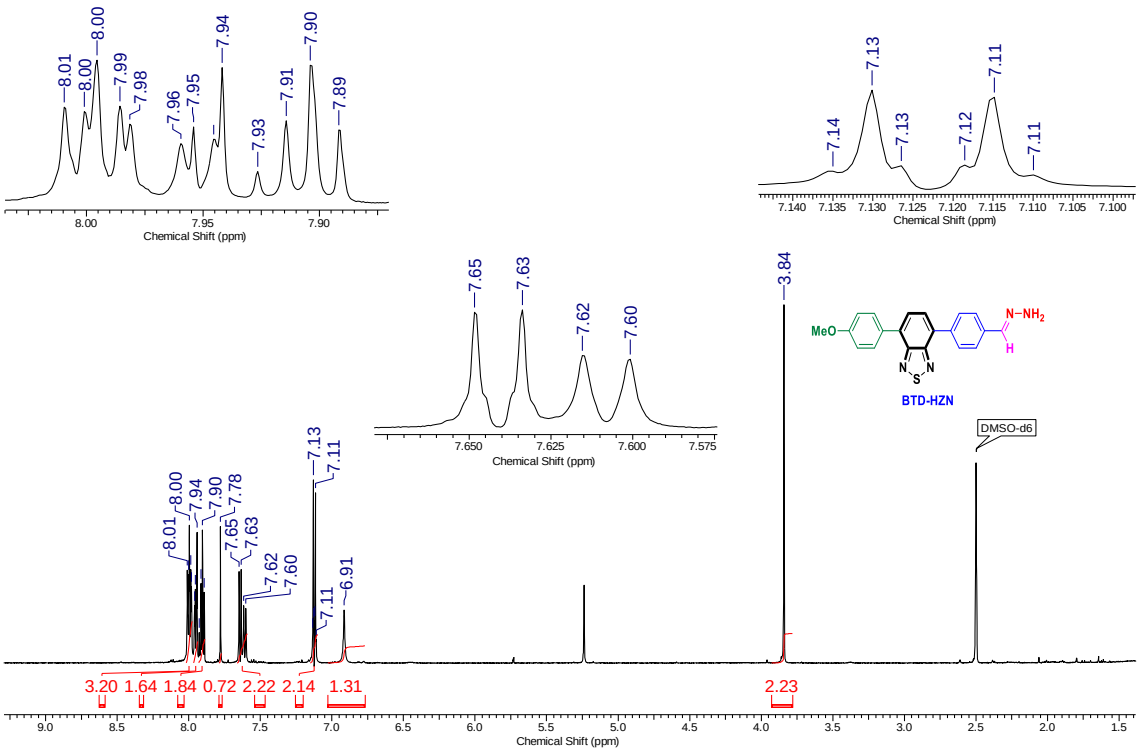

Figure S10. [1]H NMR (600 MHz, DMSO-d_6) of the dye named **BTD-HZN**.

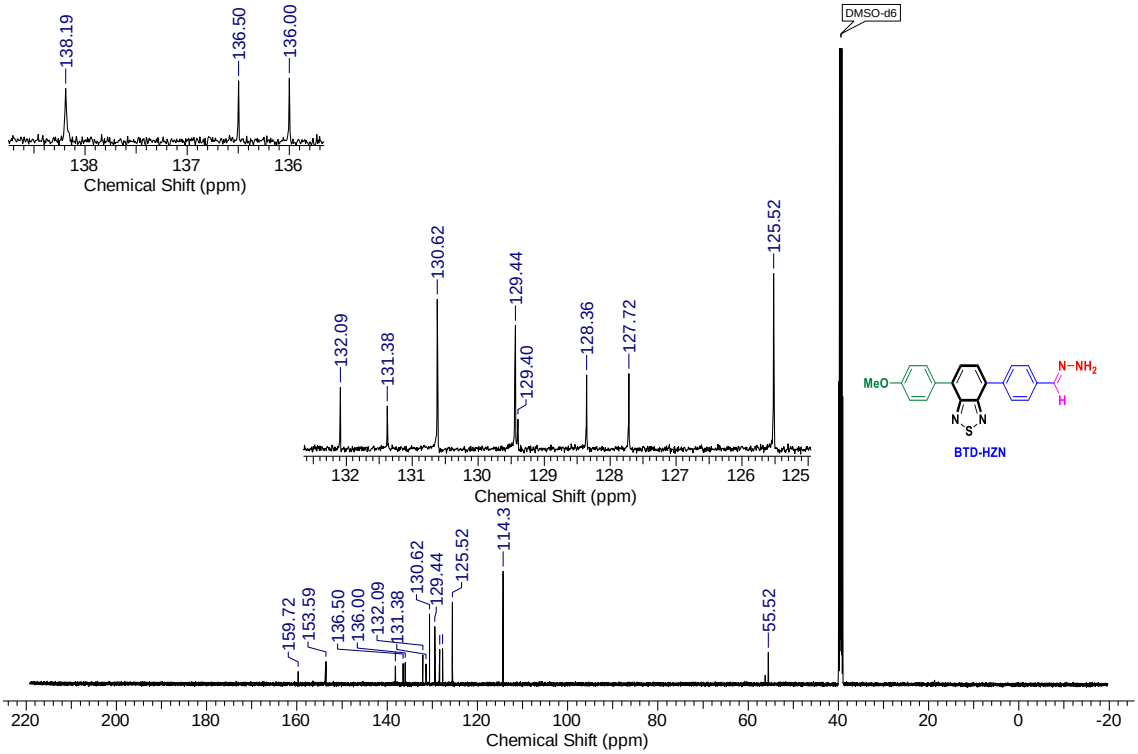

Figure S11. [13]C NMR (150 MHz, DMSO-d_6) of the dye named **BTD-HZN**.

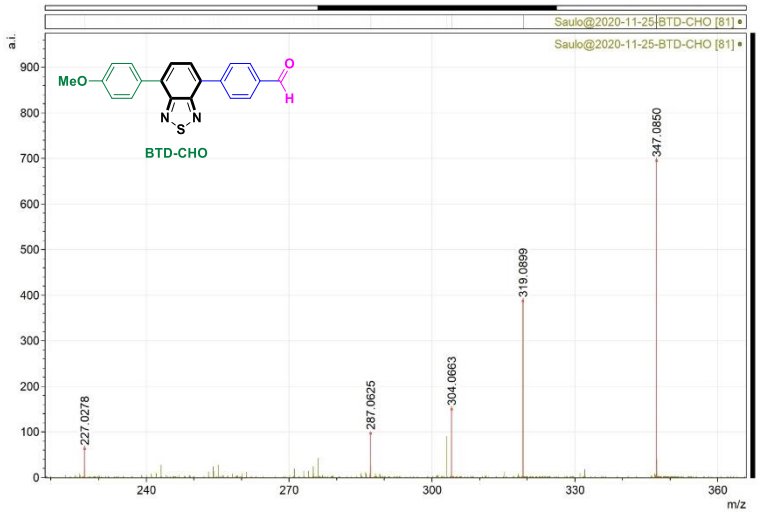

Figure S12. ESI(+)-MS/MS of the protonated **BTD-CHO** (*m/z* 347). Calculated for $[C_{20}H_{14}N_2O_2S+H]^+$, 347.0854. Found, 347.0846. Error = -2.3 ppm.

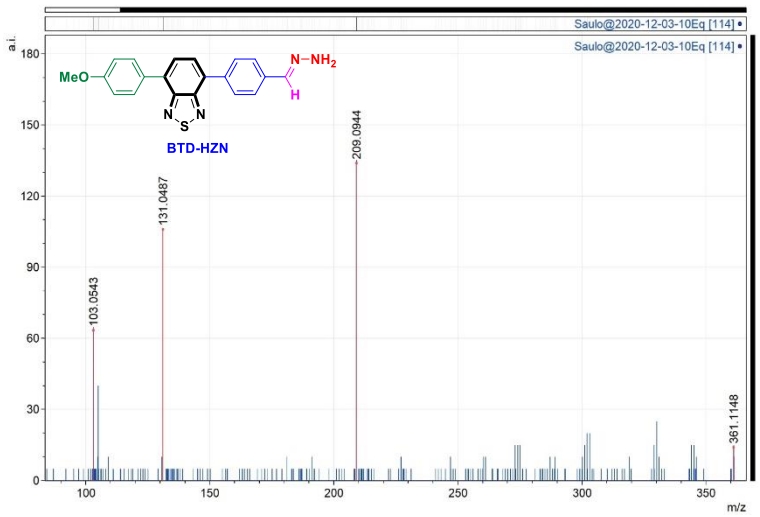

Figure S13. ESI(+)-MS/MS of the protonated **BTD-HZN** (*m/z* 361). Calculated for $[C_{20}H_{16}N_4OS+H]^+$, 361.1123. Found, 361.1153. Error = 6.9 ppm.

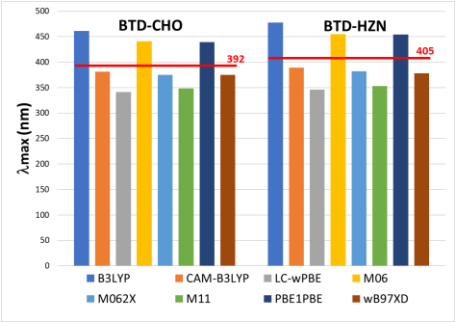

Figure S14. CAM-B3LYP/6-311+G(d,p) vertical absorption wavelengths of the BTD dyes in acetonitrile (IEF-PCM) associated with the lowest energy $S_0 \rightarrow S_1$ electronic transitions. Horizontal red lines stand for the experimentally determined λ_{max} in acetonitrile.

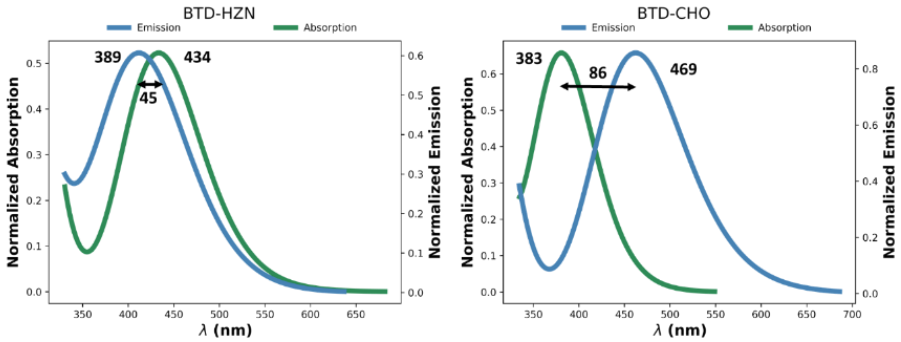

Figure S15. CAM-B3LYP/6-311+G(d,p) absorption and emission spectra of the BTD dyes in acetonitrile (IEF-PCM) associated with the lowest energy $S_0 \rightarrow S_1$ electronic transitions.

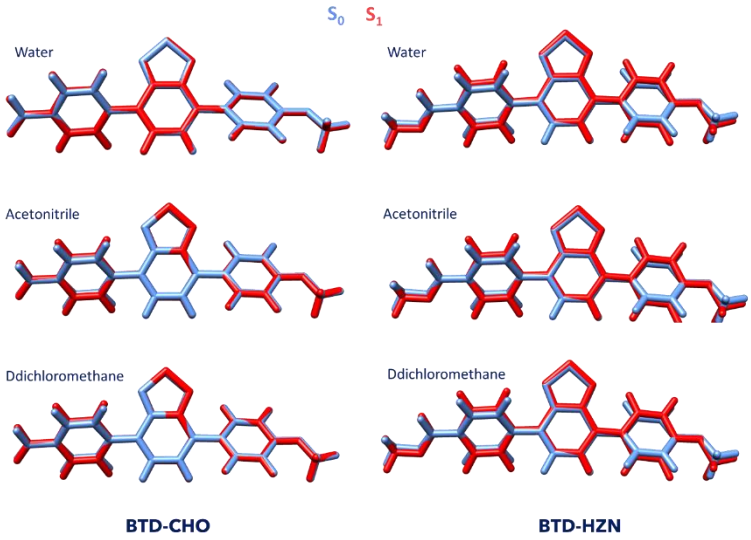

Figure S16. Overlay of the ground (S_0) and first excited (S_1) state geometries in different solvents for **BTD-CHO** and **BTD-HZN**.

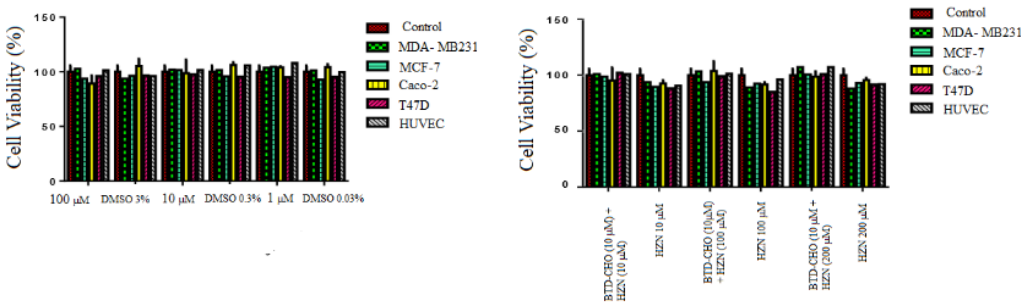

Figure S17. Cellular viability assays (MTT) after 24 h for the **BTD-CHO** (left) and *in situ* formed **BTD-HZN** (right). The graphic bar shows no statistically significant cytotoxic effect after 24 h of incubation for the tested compounds in solutions at different concentrations (1-100 µM).

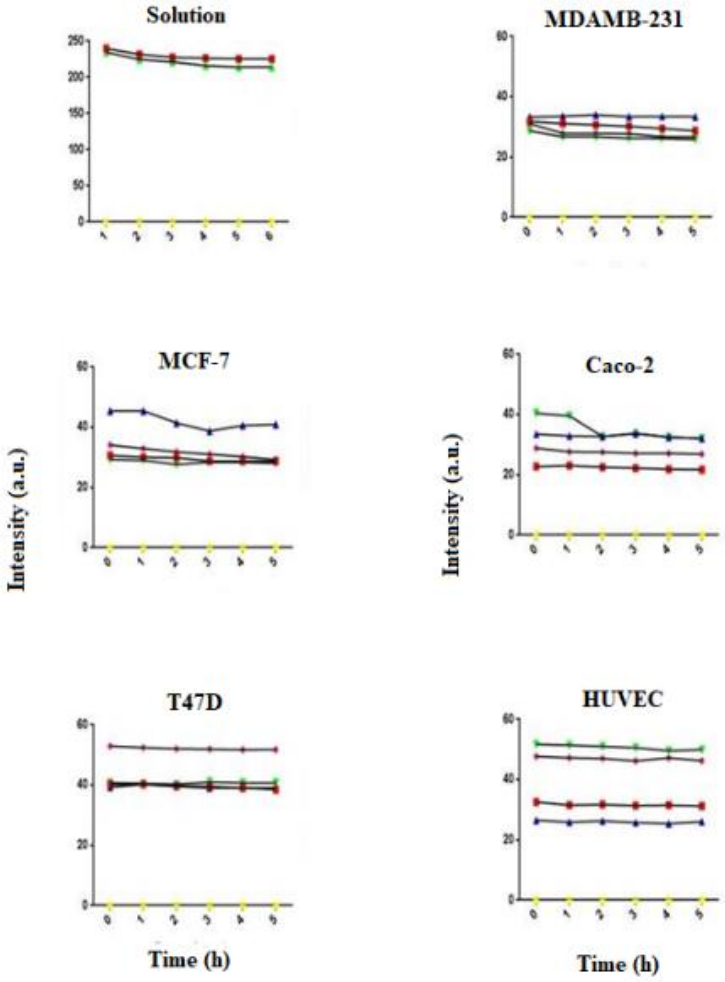

Figure S18. Fluorescence emissions (photostabilities) inside the different cells' lineages. Yellow is the PBS solution without no fluorescent dye, red and green (**BTD-CHO** and **BTD-HZN**, respectively) are referred to live cells (except for the solution measurement which is a dye-containing PBS solution), blue and purple (**BTD-CHO** and **BTD-HZN**, respectively) is referred to fixed cells.

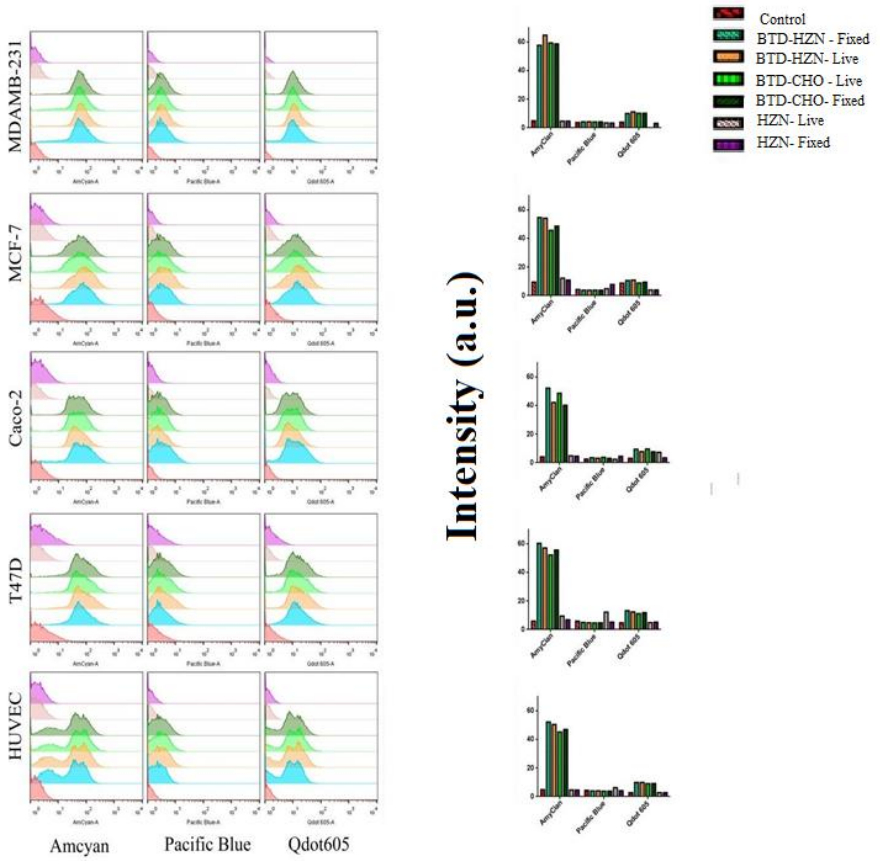

Figure S19. Flow cytometry analyses of **BTD-CHO** and **BTD-HZN** to depict the fluorescence intensity of both dyes (10 μM each) inside the different cells' lineages in comparison with commercial standards. Blue and dark green (live cells), orange and green (fixed cells) and red, purple and pink (controls). Analyses refer to 10 thousand events per channel using the following standards: Amycian (green channel), Pacific Blue (blue channel) and Qdot605 (red channel).

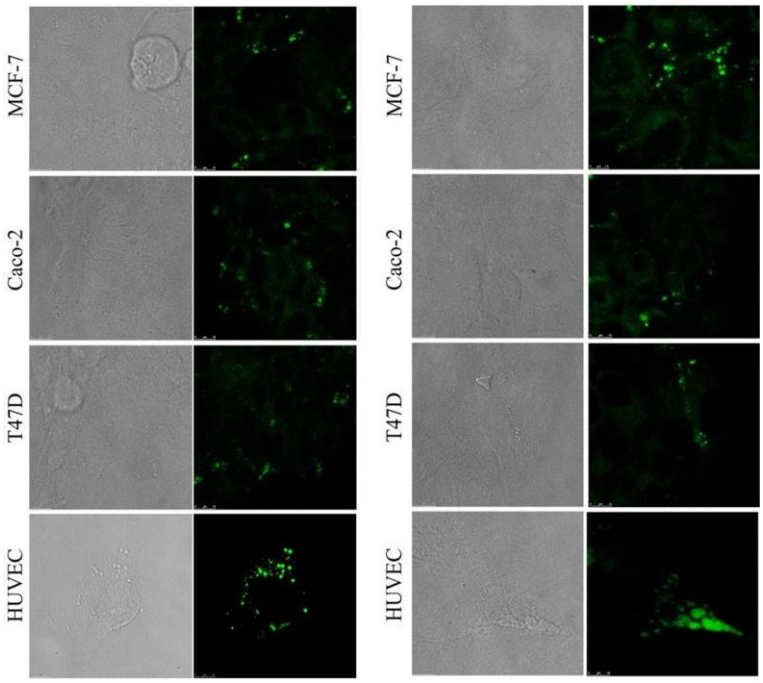

Figure S20. Live (left) and fixed (right) cells lineages stained with **BTD-CHO** (10 μM) indicating their lipid droplets selectivity. Scale bar of 10 μm.

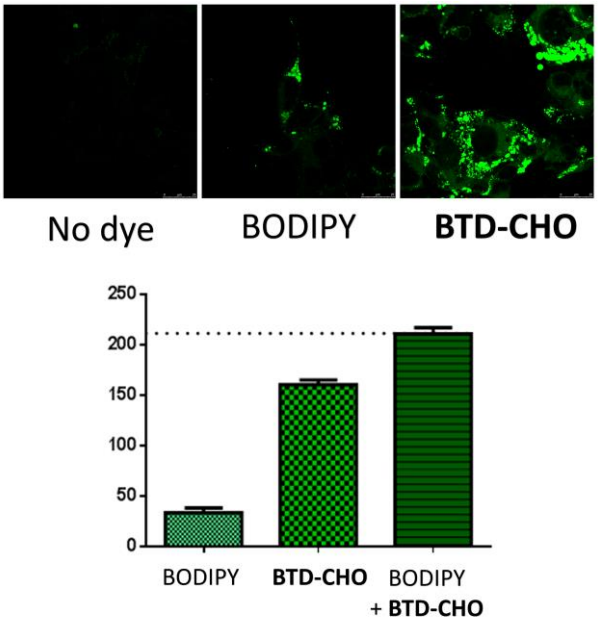

Figure S21. Experiments using BODIPY (12 μM) and **BTD-CHO** (10 μM) showing the relative intensity of the dyes (bottom) and their lipid droplets staining (top). Note the developed dye is far more intense with a lower concentration.

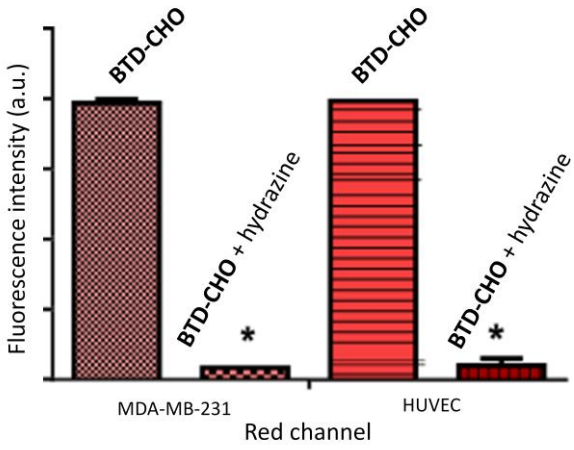

Figure S22. Red channel fluorescence intensity before and after hydrazine addition in two different cellular models i.e. MDA-MB-231 and HUVEC cells lineages.

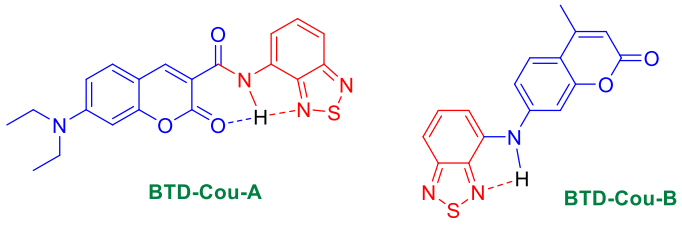

Figure S23. Structures of lipophilic fluorescent BTD derivatives previously published[1] also tested in this work for microalgae and for *C. elegans* staining.

Table S1. Limit of detection of some available hydrazine selective sensors and of this work.

Sensor	LOD	Reference
AIE coumarin-based sensor	0.101 µM	2
Naphthalimide-based probe	0.31 µM (10 ppb)	3
4*H*-chromene derivative	6.1 ppb	4
1,8-naphthalene imide derivative	9.40 nM	5
Phthalimide-based UiO-66 MOF	0.87 µM	6
Benzimidazole-based probe	1.22 ppb	7
Coumarin-based probe	69 nM	8
Carbon dots derivative	0.504 µM	9
2,3-Dihydro-1*H*-xanthene-based sensor	5.4 ppb	10
Benzothiadiazole-based sensor	7.3 ppb	This work

Table S2. Comparison of TD-DFT results employing different Exchange-Correlation (XC) functionals associated with the lowest absorption energy. Horizontal red line stands for the experimentally determined λ_{max} in acetonitrile.

BTD-CHO

XC-Functional	$S_0 \rightarrow S_1$ excitation energy (eV)	λ_{max} absorption wavelength (nm)	Oscillator Strength f
B3LYP	2.69	461	0.54
CAM-B3LYP	3.25	381	0.75
LC-ωPBE	3.63	341	0.90
M06	2.81	441	0.60
M062X	3.31	375	0.79
M11	3.56	348	0.89
PBE1PBE	2.82	439	0.59
ωB97XD	3.30	375	0.77

BTD-HZN

XC-Functional	$S_0 \rightarrow S_1$ excitation energy (eV)	λ_{max} absorption wavelength (nm)	Oscillator Strength f
B3LYP	2.59	478	0.52
CAM-B3LYP	3.19	389	0.78
LC-ωPBE	3.59	346	0.98
M06	2.73	455	0.60
M062X	3.24	382	0.84
M11	3.51	353	1.00
PBE1PBE	2.73	454	0.59
ωB97XD	3.28	378	0.82

Cartesian coordinates of the optimized BTD-CHO and BTD-HZN structures obtained at the CAM-B3LYP/6-311+G(d) level of theory.

BTD-CHO (S_0)

Solvent: Acetonitrile Energy: -1428.414710 Eh	Solvent: Water Energy: -1428.294515 Eh	Solvent: Dichloromethane Energy: -1428.291604 Eh
S -0.10509800 3.18634100 0.01255000	S -0.10518800 3.18604300 0.01270500	S -0.10564700 3.18862100 0.01163700
O 7.01936000 -0.43565200 -0.25382600	O 7.01925200 -0.43518700 -0.25452300	O 7.01933400 -0.43869700 -0.25357600
N -1.33454200 2.12764300 0.02460400	N -1.33464600 2.12704200 0.02468100	N -1.33515600 2.12967700 0.02799500
N 1.13870100 2.14649600 -0.01875700	N 1.13872600 2.14594800 -0.01864300	N 1.13852900 2.14912400 -0.02198400
C 2.86121300 -0.32669200 -0.07253900	C 2.86110200 -0.32710300 -0.07290200	C 2.86174900 -0.32454900 -0.07095100
C -3.01410800 -0.38028500 0.04407400	C -3.01397600 -0.38075400 0.04428700	C -3.01426800 -0.37890900 0.04525200
C 5.66665000 -0.45200800 -0.14858000	C 5.66647300 -0.45187900 -0.14917800	C 5.66675700 -0.45357000 -0.14760500
C -0.81003300 0.90614000 0.00936000	C -0.80995500 0.90549400 0.00914500	C -0.81012000 0.90847600 0.01170400
C 3.59994500 0.54242800 -0.88537400	C 3.59938900 0.54014500 -0.88817000	C 3.60211500 0.54959900 -0.87681000
H 3.08685100 1.27010200 -1.50053300	H 3.08590800 1.26578900 -1.50538900	H 3.09021000 1.28373300 -1.48496100
C 0.63338300 0.91665300 -0.02655800	C 0.63326600 0.91603200 -0.02640500	C 0.63337500 0.91932000 -0.02671700
C 1.38366200 -0.30610800 -0.05250700	C 1.38349900 -0.30656600 -0.05243700	C 1.38433700 -0.30313600 -0.05153200
C -1.53647000 -0.32946200 0.01291400	C -1.53632100 -0.32996800 0.01279800	C -1.53662900 -0.32706600 0.01579700
O -7.95716100 -1.40009700 -0.44871000	O -7.95736800 -1.39778600 -0.44998400	O -7.95443800 -1.40994700 -0.44839900
C -3.75233600 0.46454300 0.87583500	C -3.75184500 0.46275400 0.87780200	C -3.75481000 0.46989800 0.87064200
H -3.24284300 1.18903100 1.49647700	H -3.24196200 1.18559000 1.50002800	H -3.24692700 1.19990000 1.48595600
C -3.69731400 -1.31066200 -0.75046700	C -3.69752300 -1.30959200 -0.75168200	C -3.69560200 -1.31388800 -0.74520900
H -3.13883200 -1.95510600 -1.41900300	H -3.13930600 -1.95324800 -1.42115000	H -3.13539600 -1.95997000 -1.41082400
C -5.80499600 -0.55837300 0.12985700	C -5.80485800 -0.55806300 0.13018100	C -5.80510100 -0.56004600 0.12795000
C 4.97807500 0.47878000 -0.92850500	C 4.97752800 0.47675100 -0.93139900	C 4.97973300 0.48387400 -0.92046100
H 5.54459800 1.14614500 -1.56762900	H 5.54377400 1.14247100 -1.57248700	H 5.54827500 1.15499000 -1.55366700
C 3.56401000 -1.24751300 0.70000600	C 3.56430600 -1.24597800 0.70156100	C 3.56309000 -1.25106800 0.69561200
H 3.02391500 -1.91956900 1.35739200	H 3.02448900 -1.91682000 1.36037100	H 3.02175100 -1.92539700 1.34971900
C -0.77928400 -1.46617900 -0.01459400	C -0.77918300 -1.46679400 -0.01461800	C -0.77866900 -1.46333500 -0.01133900
H -1.27266900 -2.43108400 0.00156300	H -1.27263800 -2.43163300 0.00142500	H -1.27254800 -2.42803300 0.00625200
C -5.07489800 -1.40046400 -0.70956600	C -5.07513900 -1.39894600 -0.71074900	C -5.07304600 -1.40547100 -0.70575700
H -5.59832700 -2.11721700 -1.33113300	H -5.59878900 -2.11454700 -1.33344900	H -5.59630900 -2.12520900 -1.32399800
C 4.95225500 -1.31837200 0.67260000	C 4.95256700 -1.31653700 0.67409000	C 4.95108100 -1.32398500 0.66776000
H 5.45548500 -2.04334600 1.29774200	H 5.45614800 -2.03997600 1.30070400	H 5.45342100 -2.05327000 1.28865200
C -7.27331300 -0.63304000 0.19411600	C -7.27307800 -0.63218100 0.19440300	C -7.27398000 -0.63726500 0.18928000
H -7.75083000 0.07875800 0.89170200	H -7.75036400 0.07825200 0.89334600	H -7.75426100 0.07864900 0.88170700
C -5.13362100 0.37175400 0.92029400	C -5.13307900 0.37037600 0.92233800	C -5.13586100 0.37539300 0.91343900
H -5.69635800 1.02654600 1.57771700	H -5.69553900 1.02393000 1.58118800	H -5.70071400 1.03383600 1.56558800
C 0.64352800 -1.45502400 -0.04812600	C 0.64345400 -1.45560300 -0.04787600	C 0.64382900 -1.45193000 -0.04607300
H 1.15210500 -2.41125300 -0.08511300	H 1.15217100 -2.41175300 -0.08445200	H 1.15320500 -2.40772000 -0.08411400
C 7.76934900 -1.37005300 0.50740200	C 7.76959300 -1.36773000 0.50915300	C 7.76771900 -1.37857600 0.50031400
H 8.81259300 -1.18540800 0.26537500	H 8.81275600 -1.18313300 0.26687700	H 8.81106900 -1.19431600 0.25829100
H 7.51061900 -2.39652000 0.23764100	H 7.51122700 -2.39481100 0.24163300	H 7.50706800 -2.40316500 0.22437000
H 7.61436800 -1.22187100 1.57849900	H 7.61417700 -1.21709400 1.57979000	H 7.61452700 -1.23701800 1.57278300

BTD-CHO (S_1)

Solvent: Acetonitrile Energy: -1428.260356 Eh	Solvent: Water Energy: -1428.275526Eh	Solvent: Dichloromethane Energy: -1428.257879Eh
C 0.61892900 -1.49799000 -0.11410700	C 0.64192300 -1.45091100 -0.04681200	C 0.62047800 -1.49288100 -0.10529600
C -0.76374800 -1.49513900 -0.10980700	C -0.78014000 -1.46078800 -0.00704200	C -0.76244500 -1.49151400 -0.10297300
C -1.53749100 -0.31525200 -0.04867400	C -1.54078600 -0.32402600 0.01963900	C -1.53775100 -0.31249700 -0.04547800
C -0.79749000 0.91184500 -0.01013200	C -0.80736500 0.90988100 0.01207800	C -0.79771400 0.91496200 -0.00794600
C 0.63510200 0.90809400 -0.01109900	C 0.63714300 0.91870100 -0.02384100	C 0.63392600 0.91314300 -0.00781600
C 1.36623300 -0.31134800 -0.07318100	C 1.38583100 -0.30420100 -0.05141400	C 1.36741500 -0.30635400 -0.06587800
N -1.32178200 2.14335900 -0.02060300	N -1.32869200 2.13297100 0.02281600	N -1.32420400 2.14599100 -0.01935300
S -0.05368600 3.21985300 0.06673500	S -0.09805500 3.19062800 0.00910400	S -0.05891600 3.22274500 0.06579800
N 1.18761700 2.12854800 0.02343200	N 1.14471900 2.14779800 -0.01882400	N 1.18467800 2.13428000 0.02439400
H 1.13810300 -2.44703000 -0.16520200	H 1.14900800 -2.40820200 -0.08383600	H 1.13999600 -2.44181900 -0.15585800
H -1.26984700 -2.45174900 -0.11997400	H -1.27286900 -2.42582500 0.01559300	H -1.26795000 -2.44845100 -0.11183300
C -2.97958300 -0.37330000 0.00290300	C -3.01495100 -0.37099200 0.04592800	C -2.97936900 -0.37200100 0.00266500
C -3.74331200 0.63104600 0.65175900	C -3.76854300 0.50675900 0.84301400	C -3.74638400 0.63522400 0.64380000
C -3.68482300 -1.46136500 -0.57571900	C -3.70439700 -1.32783200 -0.70509200	C -3.68200400 -1.46449300 -0.57141500
C -5.11638800 0.54868800 0.70701100	C -5.14128200 0.42600700 0.89857600	C -5.11925100 0.55029900 0.69661300
H -3.23415900 1.45570800 1.12793000	H -3.26284600 1.25622700 1.43735900	H -3.23941300 1.46444700 1.11427000
C -5.05266900 -1.53309300 -0.52531100	C -5.08244400 -1.42226700 -0.67093500	C -5.04950800 -1.53864200 -0.52295000
H -3.14026700 -2.23298800 -1.10529400	H -3.15130700 -2.00294500 -1.34855100	H -3.13519700 -2.23719600 -1.09722700
C -5.79940700 -0.52701500 0.12180500	C -5.83051800 -0.54273300 0.13863000	C -5.79911700 -0.53030700 0.11735400
H -5.67908200 1.32219400 1.22004200	H -5.69698500 1.10823100 1.53180200	H -5.68459100 1.32626200 1.20313900
H -5.57568100 -2.36047700 -0.98960100	H -5.58958600 -2.16690900 -1.27301700	H -5.57181800 -2.36851900 -0.98352200
C 2.83022800 -0.33307800 -0.08229000	C 2.86370500 -0.32812300 -0.07308000	C 2.83107300 -0.32942500 -0.07617600
C 3.57894000 0.53532700 -0.90669900	C 3.60396600 0.53681400 -0.88906000	C 3.58114400 0.55389800 -0.88346200
C 3.53011800 -1.25773300 0.71571600	C 3.56616300 -1.24766900 0.70129800	C 3.53074900 -1.26971200 0.70341400
C 4.94725500 0.47091100 -0.93478300	C 4.98219100 0.47100200 -0.93282200	C 4.94941600 0.48764000 -0.91392900
H 3.06242700 1.25326700 -1.52823700	H 3.09164400 1.26346400 -1.50614000	H 3.06534800 1.28582200 -1.48878700
C 4.90591800 -1.33332200 0.69615500	C 4.95448100 -1.32168400 0.67254800	C 4.90660600 -1.34673000 0.68160700
H 2.97764900 -1.91982200 1.37125100	H 3.02545800 -1.91709900 1.36088300	H 2.97817600 -1.94209400 1.34835100
C 5.63046700 -0.46463800 -0.13424800	C 5.66982700 -0.45878000 -0.15105100	C 5.63184200 -0.46398800 -0.13278800
H 5.52767700 1.12902000 -1.56950400	H 5.54929800 1.13574900 -1.57424400	H 5.53060200 1.15735500 -1.53567200
H 5.40975800 -2.05516700 1.32338900	H 5.45679900 -2.04626300 1.29893500	H 5.40991100 -2.08019200 1.29577500
O 6.96112000 -0.45077500 -0.23069600	O 7.02316000 -0.44483200 -0.25713100	O 6.96306500 -0.45109700 -0.23105200
C 7.73602600 -1.37095600 0.53745200	C 7.77143800 -1.37815200 0.50725600	C 7.73611800 -1.38792200 0.51641900
H 7.48593500 -2.39908500 0.27264500	H 7.51105800 -2.40501500 0.24070400	H 7.48239500 -2.41029500 0.23241200
H 8.77104600 -1.16711300 0.28167600	H 8.81506600 -1.19600200 0.26501100	H 8.77139800 -1.18282900 0.26235500
H 7.58101900 -1.20811200 1.60460700	H 7.61628400 -1.22645000 1.57782100	H 7.58491900 -1.24601200 1.58733700
C -7.25154200 -0.58963300 0.19359500	C -7.25219100 -0.62247500 0.18986800	C -7.25186300 -0.59755000 0.18669800
H -7.73418500 0.24773400 0.72851100	H -7.84078800 0.06179200 0.81788100	H -7.73835800 0.24315300 0.71389800
O -7.94097400 -1.47918400 -0.28703800	O -7.95664200 -1.46734100 -0.46786100	O -7.93634500 -1.49294800 -0.28738200
BTD-HZN (S_0)		
Solvent: Acetonitrile Energy: -1463.848083 Eh	Solvent: Water Energy: -1463.730077Eh	Solvent: Dichloromethane Energy: -1463.726842 Eh
C 0.61892900 -1.49799000 -0.11410700	C 1.01287300 -1.42277500 -0.02651100	C 1.01090200 -1.41769100 -0.02633200
C -0.76374800 -1.49513900 -0.10980700	C -0.40964300 -1.39126400 0.01790800	C -0.41139400 -1.38438500 0.01841200
C -1.53749100 -0.31525200 -0.04867400	C -1.13438100 -0.23303800 0.03776600	C -1.13573600 -0.22581900 0.03746000
C -0.79749000 0.91184500 -0.01013200	C -0.36901200 0.97938100 0.01599500	C -0.36834400 0.98577300 0.01671400
C 0.63510200 0.90809400 -0.01109900	C 1.07436400 0.94695800 -0.02713600	C 1.07546600 0.95149200 -0.02756400
C 1.36623300 -0.31134800 -0.07318100	C 1.78764300 -0.29727800 -0.04632600	C 1.78771400 -0.29362700 -0.04610200
N -1.32178200 2.14335900 -0.02060300	N -0.85637900 2.21658100 0.02128400	N -0.85398100 2.22333800 0.02376700
S -0.05368600 3.21985300 0.06673500	S 0.40380100 3.23850200 -0.00802300	S 0.40785700 3.24307800 -0.00699300
N 1.18761700 2.12854800 0.02343200	N 1.61664200 2.16114300 -0.03478000	N 1.61945600 2.16455400 -0.03644600
H 1.13810300 -2.44703000 -0.16520200	H 1.49275100 -2.39414400 -0.05680300	H 1.48980500 -2.38955100 -0.05803200
H -1.26984700 -2.45174900 -0.11997400	H -0.93143000 -2.34086100 0.04768800	H -0.93437500 -2.33330000 0.04943300
C -2.97958300 -0.37330000 0.00290300	C -2.61271900 -0.23778800 0.07399100	C -2.61402500 -0.23066500 0.07123800
C -3.74331200 0.63104600 0.65175900	C -3.32863700 0.63099700 0.89796600	C -3.33272000 0.64901300 0.88097200
C -3.68482300 -1.46136500 -0.57571900	C -3.33302300 -1.15052900 -0.70557200	C -3.33214700 -1.15476500 -0.69706500
C -5.11638800 0.54868800 0.70701100	C -4.71325300 0.57884800 0.94851100	C -4.71711200 0.59463200 0.93039500
H -3.23415900 1.45570800 1.12793000	H -2.80066200 1.34754900 1.51336600	H -2.80681100 1.37686000 1.48448800
C -5.05266900 -1.53309300 -0.52531100	C -4.71393200 -1.19909300 -0.65973600	C -4.71266100 -1.20595400 -0.65203200
H -3.14026700 -2.23298800 -1.10529400	H -2.80135500 -1.82016500 -1.37217100	H -2.79860000 -1.83058800 -1.35592300
C -5.79940700 -0.52701500 0.12180500	C -5.42823400 -0.33381200 0.17300000	C -5.42926900 -0.33092300 0.16826800
H -5.67908200 1.32219400 1.22004200	H -5.24699900 1.25863600 1.60475000	H -5.25325700 1.28373400 1.57507100
H -5.57568100 -2.36047700 -0.98960100	H -5.25127700 -1.90729900 -1.27852800	H -5.24960700 -1.92218300 -1.26181900
C 2.83022800 -0.33307800 -0.08229000	C 3.26419600 -0.36175600 -0.07533400	C 3.26398500 -0.36076800 -0.07405500
C 3.57894000 0.53532700 -0.90669900	C 4.02224700 0.47287100 -0.90624200	C 4.02535200 0.47911700 -0.89665700
C 3.53011800 -1.25773300 0.71571600	C 3.94581900 -1.28976800 0.70726800	C 3.94248300 -1.29620300 0.70213800
C 4.94725500 0.47091100 -0.93478300	C 5.39798300 0.37013100 -0.95607500	C 5.40043100 0.37276600 -0.94617600
H 3.06242700 1.25326700 -1.52823700	H 3.52584400 1.20476100 -1.53011900	H 3.53147800 1.21884300 -1.51303300
C 4.90591800 -1.33332200 0.69615500	C 5.33159400 -1.40035200 0.67289700	C 5.32786100 -1.41042800 0.66809100
H 2.97764900 -1.91982200 1.37125100	H 3.39096800 -1.93640500 1.37776100	H 3.38520500 -1.94511400 1.36849300
C 5.63046700 -0.46463800 -0.13424800	C 6.06490000 -0.56704300 -0.16527600	C 6.06412900 -0.57286000 -0.16298500
H 5.52767700 1.12902000 -1.56950400	H 5.97873400 1.01144100 -1.60898900	H 5.98473800 1.01789600 -1.59203200
H 5.40975800 -2.05516700 1.32338900	H 5.81791400 -2.12975800 1.30621800	H 5.81197000 -2.14533300 1.29685300
O 6.96112000 -0.45077500 -0.23069600	C -6.89248700 -0.35230100 0.25679900	C -6.89338500 -0.35339400 0.25075200
C 7.73602600 -1.37095600 0.53745200	H -7.35914300 0.38461300 0.91924000	H -7.36382200 0.39559600 0.89741000
H 7.48593500 -2.39908500 0.27264500	O 7.41758500 -0.58967600 -0.27782500	O 7.41663500 -0.59836000 -0.27524000
H 8.77104600 -1.16711300 0.28167600	C 8.14571100 -1.52998500 0.49752500	C 8.14147700 -1.54473900 0.49307000
H 7.58101900 -1.20811200 1.60460700	H 7.85894500 -2.55388700 0.24727800	H 7.85228300 -2.56672600 0.23659700
C -7.25154200 -0.58963300 0.19359500	H 9.19250100 -1.37739700 0.24856200	H 9.18881600 -1.39372600 0.24511500
H -7.73418500 0.24773400 0.72851100	H 7.99888400 -1.35855200 1.56627300	H 7.99577000 -1.38019700 1.56334200
O -7.94097400 -1.47918400 -0.28703800	N -7.60164400 -1.17648200 -0.40289200	N -7.59843700 -1.19359300 -0.39226700
	N -8.96388800 -1.07585200 -0.31049300	N -8.96048300 -1.09723500 -0.30312100
	H -9.39749200 -1.96925200 -0.49143900	H -9.39078500 -1.99406000 -0.47341100
	H -9.30482900 -0.67004900 0.55755900	H -9.30553300 -0.67740400 0.55647400
BTD-HZN (S_1)		
Solvent: Acetonitrile Energy: -1463.749434 Eh	Solvent: Water Energy: -1463.750069 Eh	Solvent: Dichloromethane Energy: -1463.746255 Eh
C 0.97618600 -1.37712000 0.00988000	C 0.97630600 -1.37691000 0.01177800	C 0.97565800 -1.37820300 0.00046600
C -0.38601300 -1.34337600 -0.00364700	C -0.38575700 -1.34328400 -0.00177400	C -0.38722200 -1.34394500 -0.01282000
C -1.14654400 -0.13181300 0.00687200	C -1.14670500 -0.13174500 0.00802100	C -1.14561400 -0.13225800 0.00141600
C -0.37140000 1.08040300 0.01235900	C -0.37152800 1.08053200 0.01274900	C -0.37078700 1.07967200 0.01028700
C 1.08694500 1.04173700 -0.00652200	C 1.08703200 1.04199900 -0.00583000	C 1.08641700 1.04046400 -0.01043800
C 1.79656300 -0.20573000 -0.00289000	C 1.79695900 -0.20545100 -0.00178700	C 1.79456900 -0.20707400 -0.00856200
N -0.85828400 2.31184900 0.01210500	N -0.85833100 2.31193600 0.01143100	N -0.85824400 2.31129500 0.01502800
S 0.41960300 3.37296900 0.00539500	S 0.41932000 3.37330300 0.00466300	S 0.42072900 3.37131400 0.00791300
N 1.63985100 2.24708100 -0.00264200	N 1.63957600 2.24740600 -0.00227600	N 1.64104200 2.24555800 -0.00557000
H 1.44779500 -2.34924700 -0.00584000	H 1.44779100 -2.34908500 -0.00315400	H 1.44795100 -2.35004500 -0.01900900
H -0.90471500 -2.29083500 0.01262800	H -0.90422600 -2.29086100 0.01506300	H -0.90712700 -2.29081300 0.00094700
C -2.58330100 -0.17320300 0.01901900	C -2.58329100 -0.17330400 0.02014400	C -2.58328000 -0.17286600 0.01410600
C -3.38250500 0.94104100 0.37781400	C -3.38296400 0.94099900 0.37814200	C -3.38001000 0.94050400 0.37878600
C -3.28229900 -1.36563100 -0.32188100	C -3.28207900 -1.36614700 -0.32008400	C -3.28330100 -1.36274500 -0.33164800
C -4.75698600 0.85755400 0.40856800	C -4.75745000 0.85739600 0.40838000	C -4.75447700 0.85751800 0.41233100
H -2.90132300 1.86800600 0.64490500	H -2.90221400 1.86812800 0.64545100	H -2.89660700 1.86620700 0.64626000
C -4.65143000 -1.43569600 -0.30526300	C -4.65122700 -1.43628600 -0.30403000	C -4.65237100 -1.43246500 -0.31213600
H -2.73656500 -2.24234900 -0.64194700	H -2.73619600 -2.24314600 -0.63909400	H -2.73827000 -2.23754900 -0.65827000
C -5.42729300 -0.32417700 0.06766800	C -5.42751800 -0.32459800 0.06769700	C -5.42599100 -0.32233800 0.06852200
H -5.33291600 1.72824500 0.70497400	H -5.33362100 1.72807400 0.70432300	H -5.32914600 1.72773900 0.71271000
H -5.14790400 -2.35512400 -0.58951600	H -5.14720300 -2.35614500 -0.58777500	H -5.15137200 -2.34933300 -0.60011900
C 3.23067300 -0.32091000 -0.01968500	C 3.23082400 -0.32062600 -0.01908000	C 3.22989000 -0.32225300 -0.02276900
C 4.08566200 0.74563000 -0.40676200	C 4.08595700 0.74612200 -0.40570800	C 4.08424400 0.74334500 -0.41170900

C	3.86840000	-1.53398900	0.34009700	C	3.86871000	-1.53415300	0.33958800	C	3.86678300	-1.53318600	0.34234600
C	5.44895800	0.59854300	-0.44300300	C	5.44921200	0.59896400	-0.44235100	C	5.44773400	0.59658300	-0.44581300
H	3.64926600	1.68976200	-0.69106300	H	3.64973900	1.69037800	-0.68983900	H	3.64700000	1.68688000	-0.69685800
C	5.23780100	-1.68388400	0.32155100	C	5.23802300	-1.68412200	0.32055400	C	5.23660400	-1.68274200	0.32634400
H	3.28244500	-2.37681300	0.67958500	H	3.28294300	-2.37734300	0.67841900	H	3.27985000	-2.37427000	0.68480100
C	6.04752100	-0.61497400	-0.07808200	C	6.04780900	-0.61492900	-0.07842900	C	6.04605900	-0.61515400	-0.07614900
H	6.08631200	1.41688400	-0.75686900	H	6.08646300	1.41746500	-0.75603600	H	6.08566500	1.41416500	-0.76036600
H	5.66887100	-2.62809800	0.62460100	H	5.66902600	-2.62864900	0.62265100	H	5.66788300	-2.62551500	0.63388000
C	-6.87860700	-0.36224200	0.10780800	C	-6.87887500	-0.36246400	0.10691900	C	-6.87714800	-0.36133200	0.11309300
H	-7.39722600	0.55868300	0.39155100	H	-7.39751100	0.55848800	0.39027700	H	-7.39551700	0.55902800	0.40039200
O	7.38708400	-0.65846000	-0.13923600	O	7.38721200	-0.65848100	-0.13999400	O	7.38641800	-0.65825000	-0.13517000
C	8.06129300	-1.86233100	0.21543600	C	8.06164400	-1.86298600	0.21314100	C	8.05961300	-1.85888000	0.22709100
H	7.76255400	-2.68294000	-0.43896400	H	7.76225600	-2.68281500	-0.44185200	H	7.76382100	-2.68352300	-0.42400600
H	9.11970200	-1.65797500	0.08343700	H	9.11994700	-1.65855100	0.08055700	H	9.11849100	-1.65493700	0.09746900
H	7.86655500	-2.12495100	1.25659800	H	7.86753200	-2.12643400	1.25415900	H	7.86224500	-2.11712400	1.26911400
N	-7.53633800	-1.42195000	-0.17663600	N	-7.53656500	-1.42214000	-0.17796900	N	-7.53517400	-1.42053000	-0.17124900
N	-8.88793100	-1.35694100	-0.17638400	N	-8.88826800	-1.35678100	-0.17890000	N	-8.88627300	-1.35708100	-0.16534800
H	-9.30976100	-2.26217800	-0.03555900	H	-9.31028600	-2.26181300	-0.03704600	H	-9.30719400	-2.26352000	-0.03105600
H	-9.30625600	-0.63016900	0.39794300	H	-9.30663600	-0.62967600	0.39500600	H	-9.30435900	-0.63298900	0.41237700

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