Supporting Information

Stimuli-Responsive Benzothiazole-Phenothiazine derivatives: Mechanochromism, AIE, Acid Sensing, and Anticancer Efficacy in Benzo[a]pyrene-Induced Cancer Models

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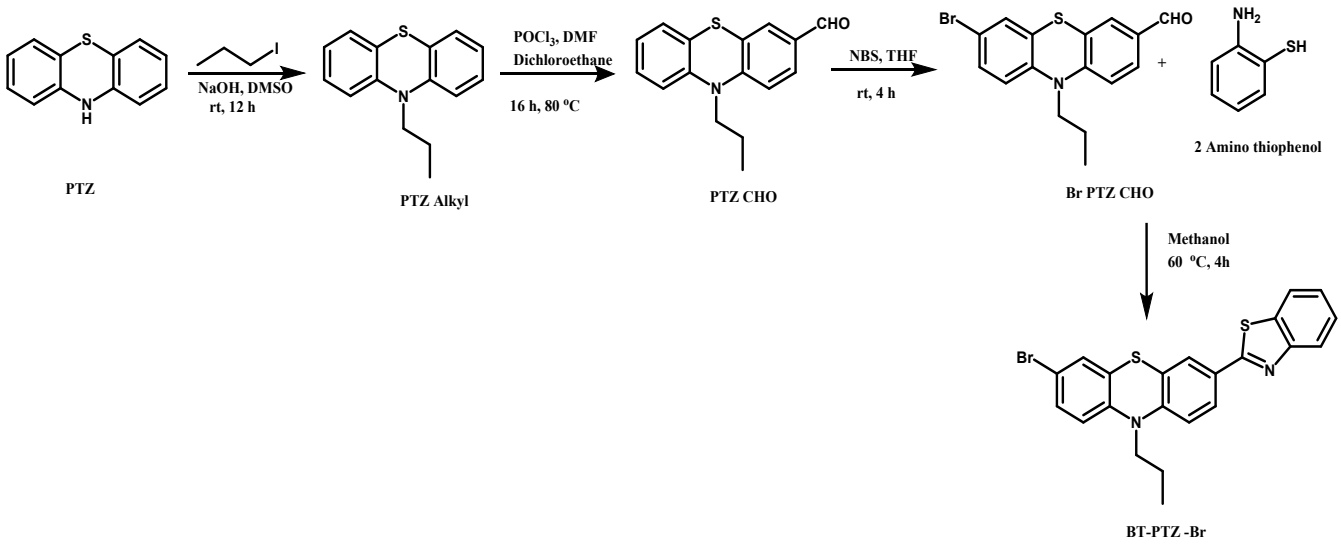
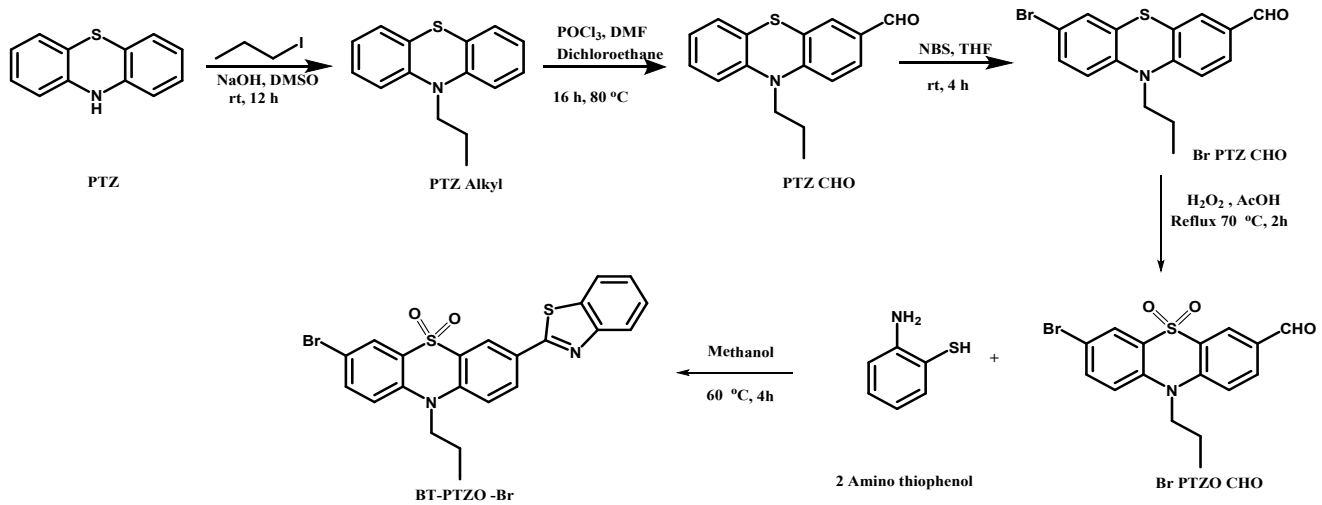
Experimental Section





Scheme S1 Synthetic scheme for Intermediate **BT-PTZ-Br** and **BT-PTZO-Br.**

Solvatochromism:

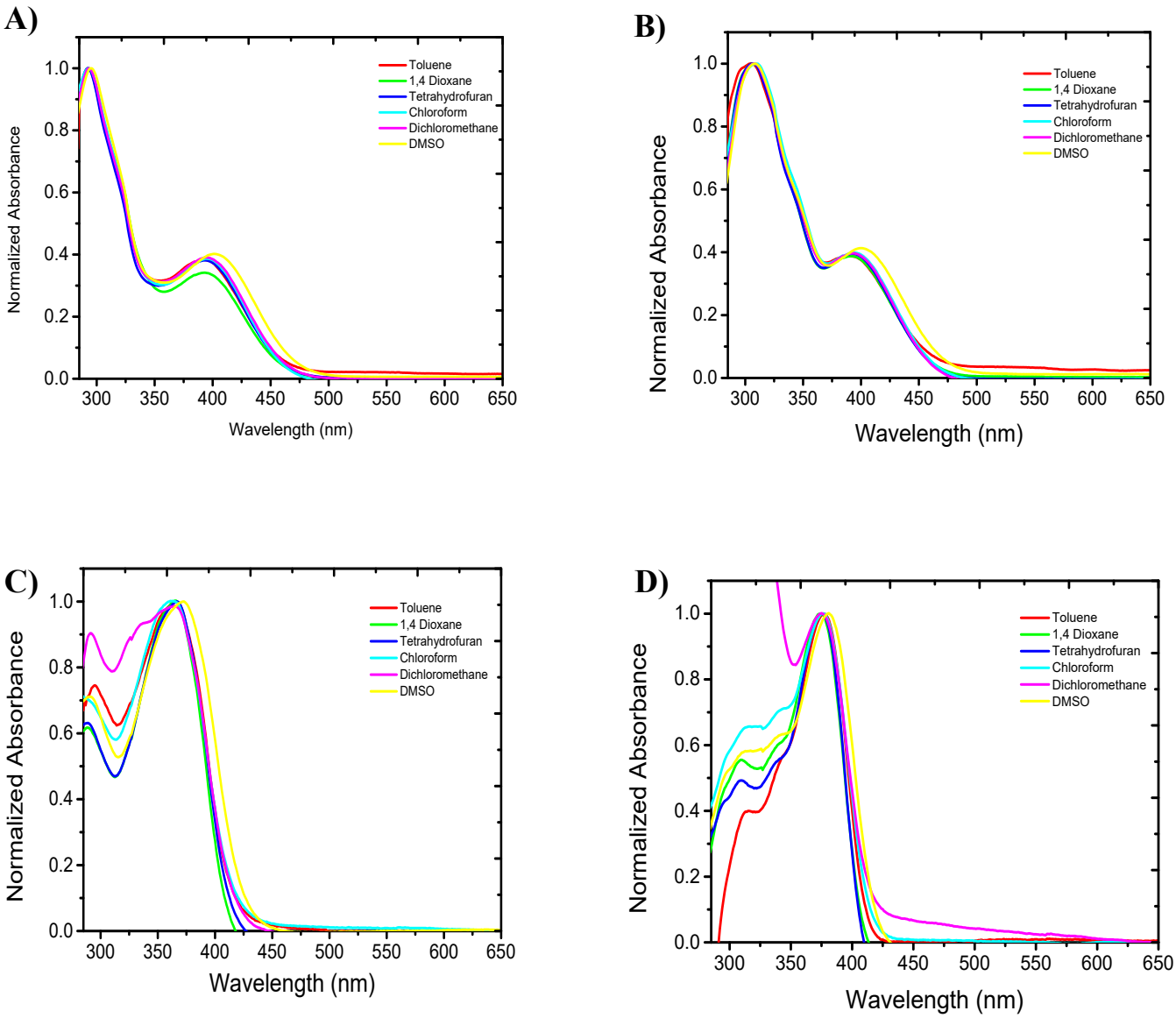


Fig. S1 UV- vis absorption Spectra of (A) **BT-PTZ-1**, (B) **BT-PTZ-2**, (C) **BT-PTZO1** and (D) **BT-PTZO-2** in different polarity of solvents respectively.

Table S1 Photophysical properties of the compounds **BT-PTZ-1**, **BT-PTZ-2**, **BT-PTZO1** and **BT-PTZO-2**

Compound	Solvent	λ_{abs} (nm)[a]	λ_{em} (nm) [a]	Stokes shift (cm^{-1})	$Ø_f$ [b]
BT-PTZ-1	Toluene	393	515	6028	0.55
	1,4 Dioxane	393	539	6893	0.60
	Tetrahydrofuran	394	546	7065	0.56
	Chloroform	395	550	7135	0.58
	Dichloromethane	395	550	7135	0.61
	DMSO	402	567	7239	0.31
BT-PTZ-2	Toluene	392	529	6607	0.58
	1,4 Dioxane	393	537	6824	0.62
	Tetrahydrofuran	393	543	7029	0.60
	Chloroform	394	548	7132	0.64
	Dichloromethane	394	558	7459	0.62
	DMSO	401	572	7455	0.66
BT-PTZO-1	Toluene	364	493	7189	0.35
	1,4 Dioxane	366	482	6576	0.40
	Tetrahydrofuran	367	522	8090	0.31
	Chloroform	364	508	7787	0.34
	Dichloromethane	365	405	2706	0.11
	DMSO	373	415	2713	0.06
BT-PTZO-2	Toluene	377	429	3215	0.22
	1,4 Dioxane	374	441	4062	0.31
	Tetrahydrofuran	376	490	6187	0.57
	Chloroform	377	489	6076	0.53
	Dichloromethane	376	529	7692	0.55

	DMSO	381	599	9552	0.10

([a] absorption and emission maxima values recorded in different polarity solvents, [b] the fluorescence quantum yields were measured using quinine sulphate as a standard in 0.5 M H_2SO_4).

Aggregation Induced Emission (AIE)

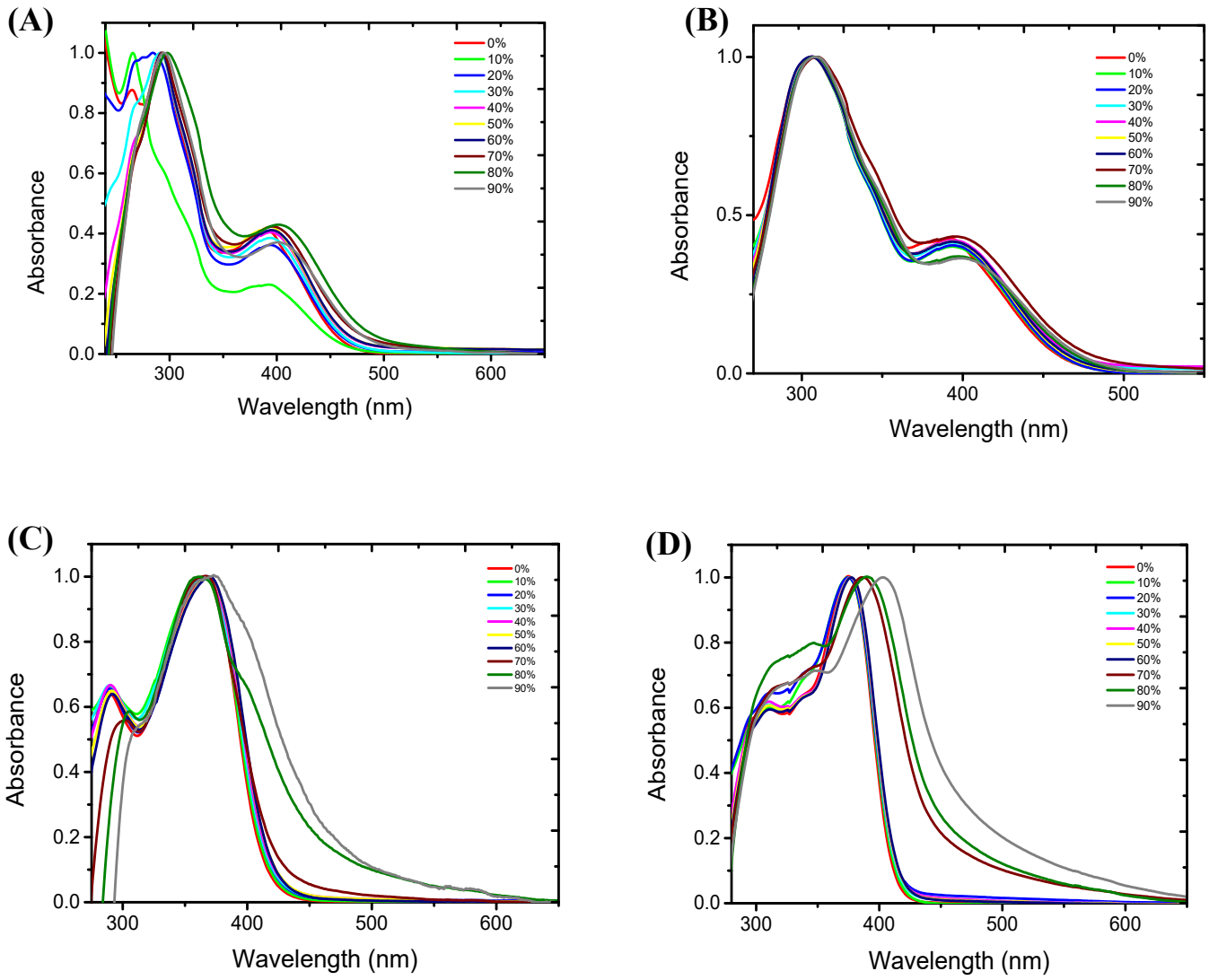


Fig. S2 Absorption spectra of (A) **BT-PTZ-1**, (B) **BT-PTZ-2**, (C) **BT-PTZO-1**, and (D) **BT-PTZO-2** in different THF- Water Mixture with increasing water percentage.

Aggregation Induced Emission (AIE)

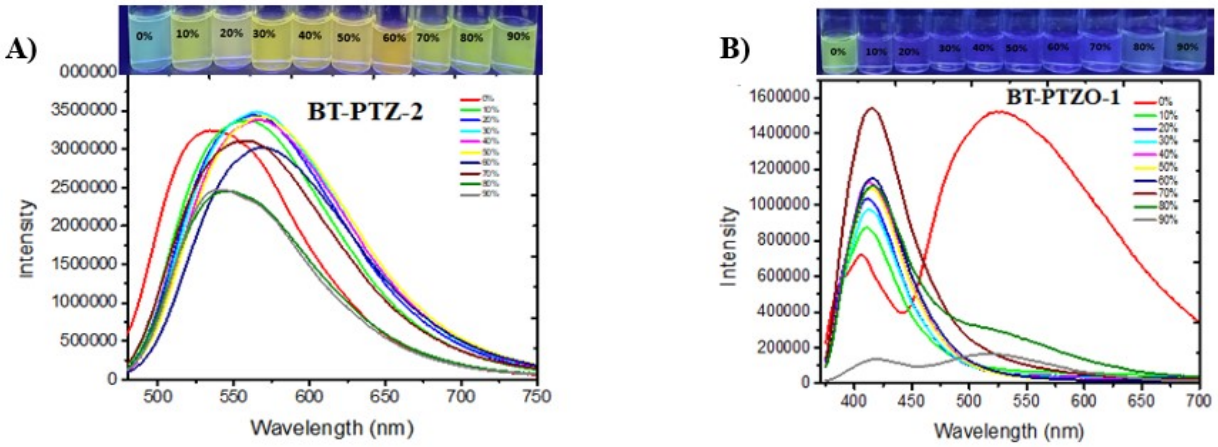


Fig. S3 Emission spectra of A) **BT-PTZ-2** and D) **BT-PTZO-1** in different THF-Water Mixture with increasing water percentage (Inset: Photographs under 365 nm UV illuminations.)

Table S2. Fluorescence quantum yields of **BT-PTZ-1**, **BT-PTZ-2**, **BT-PTZO-1**, and **BT-PTZO-2** in different THF-water mixtures with increasing water percentage.

Water Vol %	$\phi_f{}^a$			
	BT-PTZ-1	**BT-PTZ-2**	**BT-PTZO-1**	**BT-PTZO-2**
0%	0.45	0.44	0.22	0.39
10%	0.41	0.45	0.02	0.11
20%	0.42	0.43	0.02	0.09
30%	0.40	0.43	0.02	0.09
40%	0.39	0.42	0.02	0.06
50%	0.33	0.40	0.02	0.05
60%	0.25	0.45	0.03	0.05
70%	0.28	0.46	0.06	0.35
80%	0.43	0.39	0.08	0.32
90%	0.25	0.40	0.06	0.30

([a] Fluorescence quantum yields recorded using quinine sulphate as a standard in 0.5 M H2SO4 solution.)

PXRD Studies

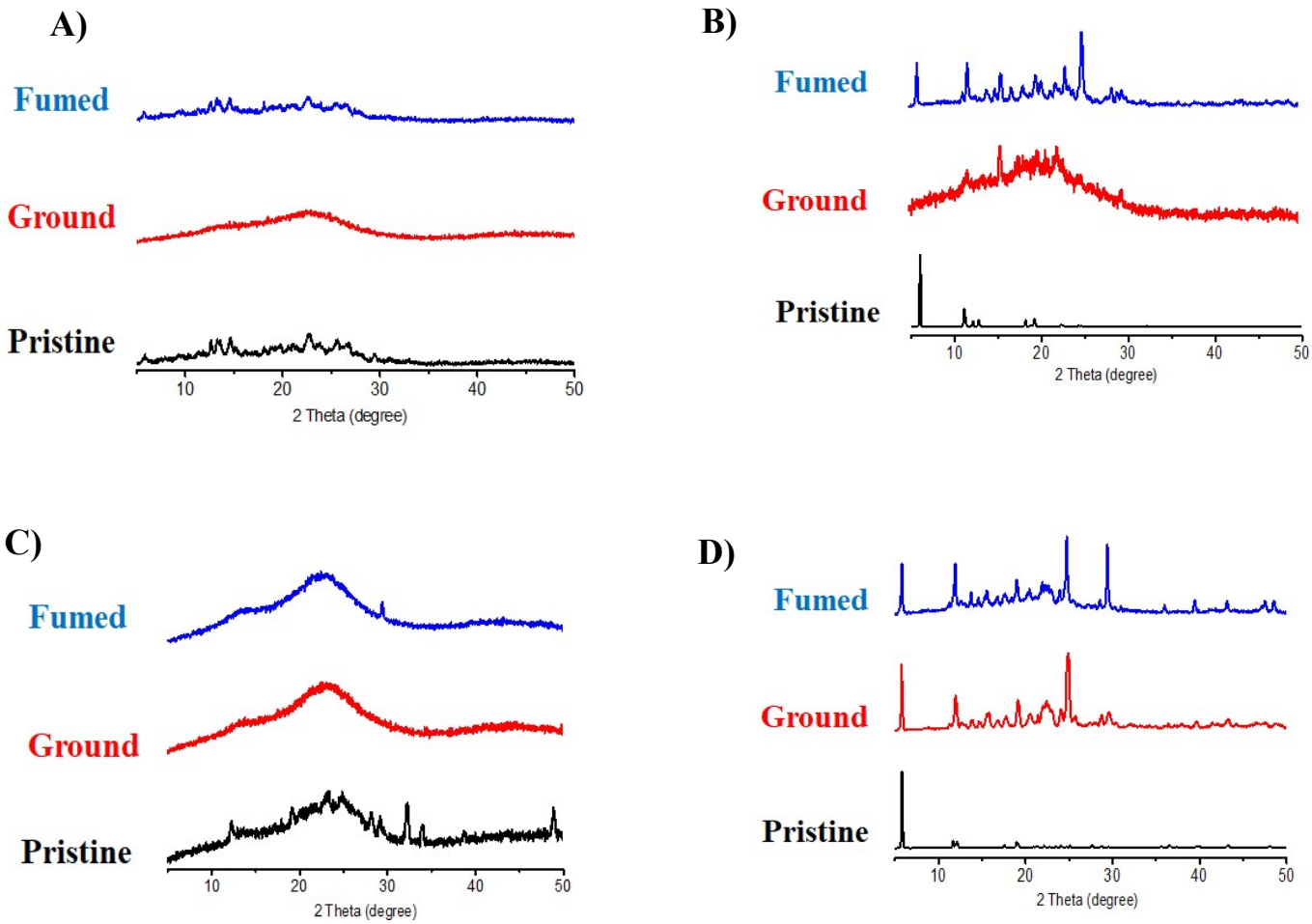


Fig. S4 PXRD curves of (A) **BT-PTZ-1**, (B) **BT-PTZ-2**, (C) **BT-PTZO-1** and (D) **BT-PTZO-2** in pristine, ground, and fumed form

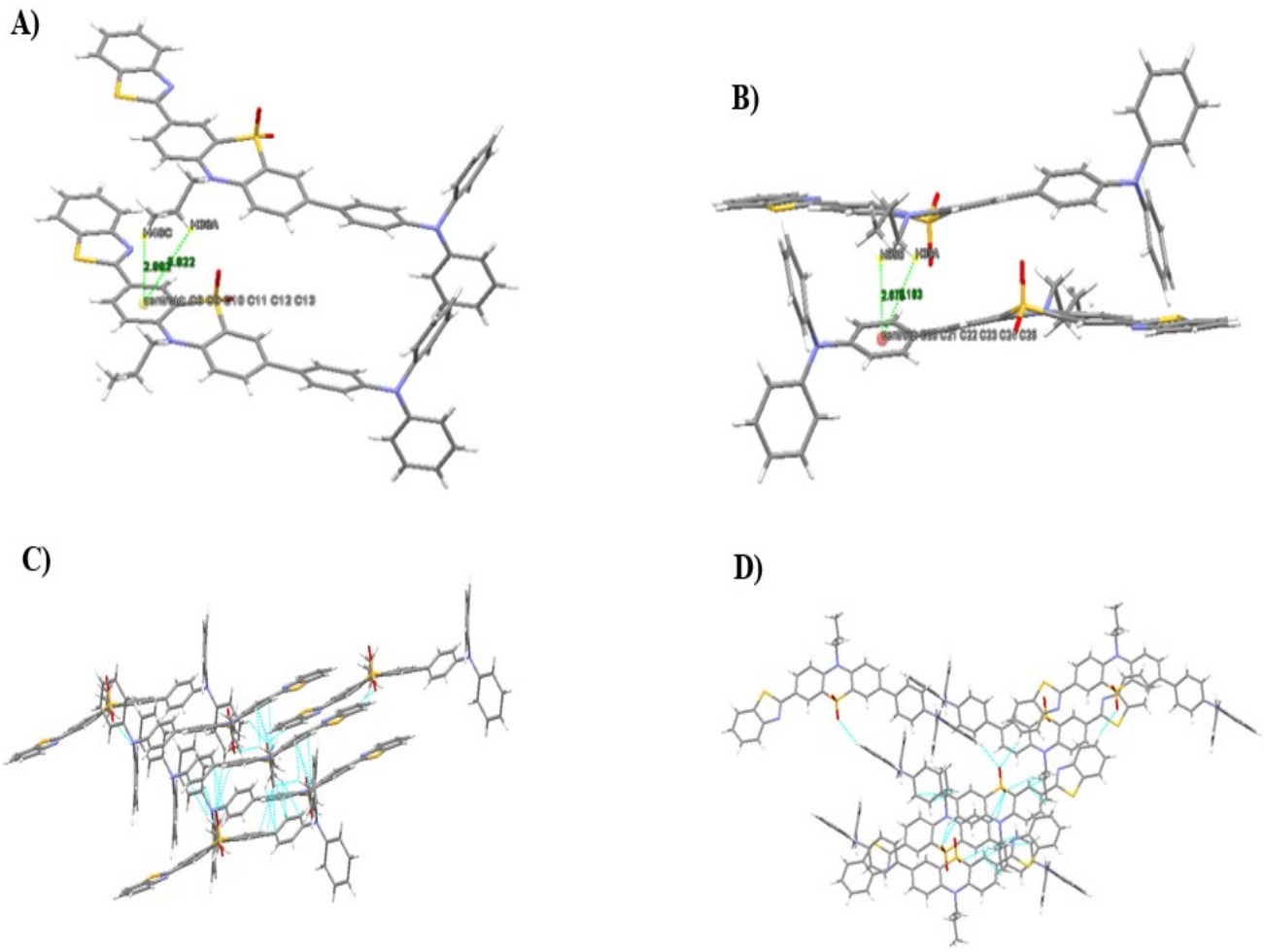


Fig. S5 A) and B) crystal packing diagram of **BT-PTZO-2** depicting intermolecular interactions, C) and D) Crystal packing of **BT-PTZO-2** and different dimeric interactions.

Crystallographic data

The crystal and refinement data are summarized in Table S2. The CCDC number **2252673** contains the supplementary crystallographic data for BT-PTZO-2. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223- 336-033; or deposit@ccdc.cam.ac.uk)

Table S3 Crystal data and structure refinement for **BT-PTZO-2.**

Identification code	**shelx**
Empirical formula	C40 H31 N3 O2 S2
Formula weight	649.80
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
a/(A°)	8.0182
b/(A°)	14.2098
c/(A°)	15.2021
Alpha/(°)	85.714
Beta/(°)	83.289
Gamma/(°)	80.170
Volume	1692.30(18) A^3
Z, Calculated density	2, 1.275 Mg/m^3
Absorption coefficient	0.197 mm^{-1}
F(000)	680
Crystal size	0.400 x 0.350 x 0.320 mm
Theta range for data collection	3.048 to 29.840 deg.
Reflections collected / unique	16587 / 8026 [R(int) = 0.0844]
Completeness to theta	25.242 99.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8026 / 35 / 491
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0784, wR2 = 0.2177
R indices (all data)	R1 = 0.1409, wR2 = 0.2903
Extinction coefficient	n/a
Largest diff. peak and hole	0.333 and -0.506 $e.A^{-3}$

Table S4 The computed vertical transitions; oscillator strengths and configurations of **BT-PTZ-1**, **BT-PTZ-2**, **BT-PTZO-1** and **BT-PTZO-2**.

Compound	Wavelength (nm)	*f*[a]	Configuration	Assignment
BT-PTZ-1	301	0.7478	(HOMO-2)→LUMO(0.4689)	π–π*
	377	0.1440	HOMO→(LUMO+2)(0.6167)	ICT
BT-PTZ-2	319	0.7456	(HOMO-2)→LUMO(0.6157)	π–π*
	374	0.4870	HOMO→(LUMO+1)(0.6496)	ICT
BT-PTZO-1	295	0.2347	(HOMO-3)→LUMO(0.1516)	π–π*
	356	0.6204	HOMO→(LUMO+2)(0.5145)	ICT
BT-PTZO-2	294	0.2175	(HOMO-2)→LUMO(0.5898)	π–π*
	370	0.7139	HOMO→(LUMO+2)(0.6535)	ICT

[a]Oscillator strength.

Thermal Properties

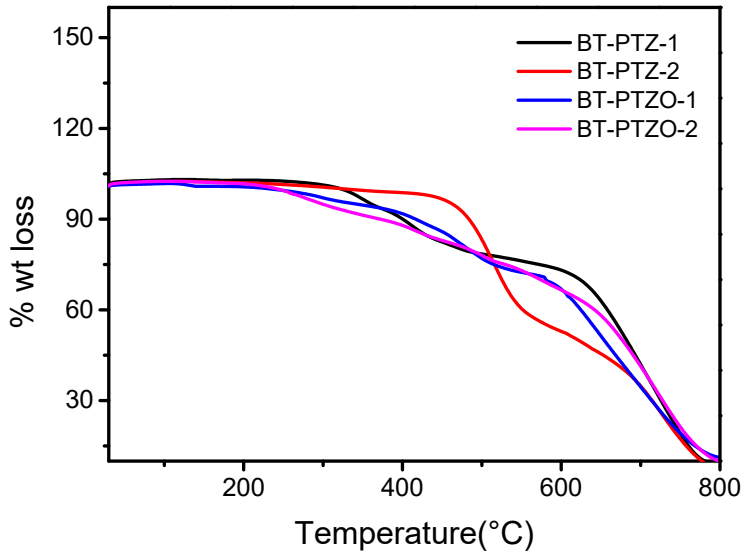


Fig. S6 Thermogravimetric analysis (TGA) of **BT-PTZ-1**, **BT-PTZ-2**, **BT-PTZO-1** and **BT-PTZO-2** measured at a heating rate of 10 °C min^{-1} under a nitrogen atmosphere.

Acidochromism

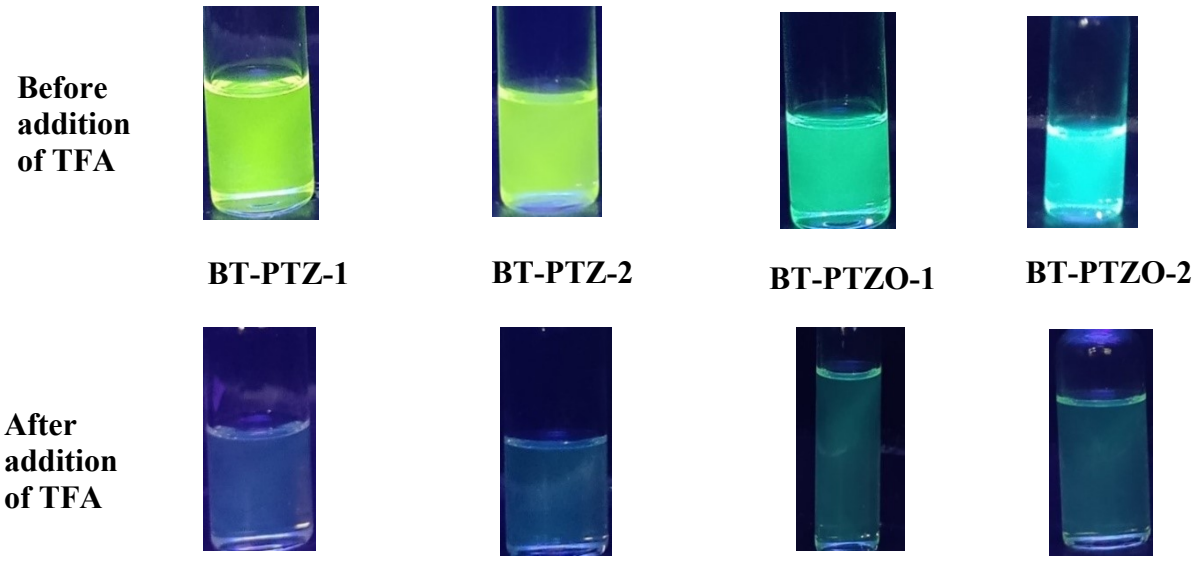


Fig. S7 Emission photographs of **BT-PTZ-1**, **BT-PTZ-2**, **BT-PTZO-1** and **BT-PTZO-2** in response to TFA.

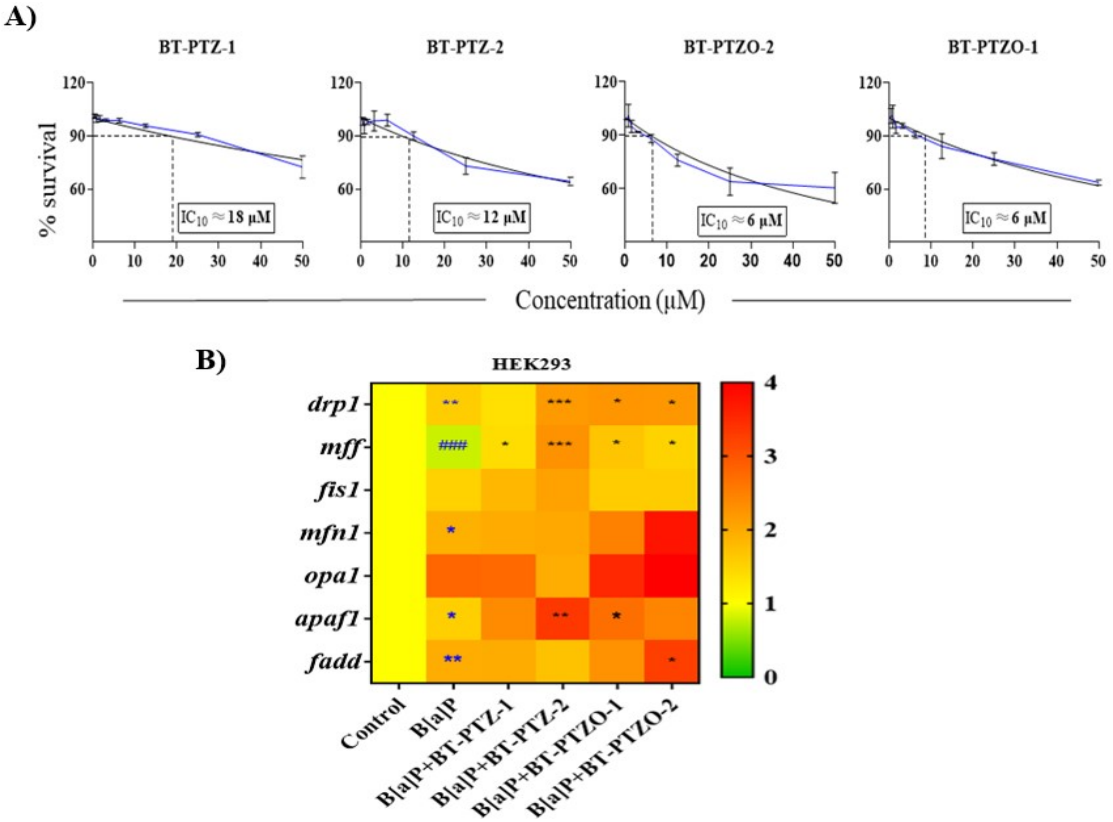


Fig. S8 Cytotoxicity and transcript expression analysis in HEK293 cells. (A) Cytotoxicity assessment via MTT assay of HEK293 cells after 24-hour exposure to the compounds. **(B)** Heat map depicting relative transcript expression of mitochondrial-associated markers (*drp1, fis1, mff, mfn1, opa1*) and cell death-associated markers (*fadd, apaf1*) in HEK293 cells. Cells were pre-exposed to B[a]P for 24 hours, followed by compound treatment for an additional 24 hours. Experiments were conducted with three biological replicates and two technical replicates. Results are presented as the mean ± standard deviation (SD). Statistical analysis was performed using an unpaired t-test, with p-values calculated using GraphPad Prism version 9.5.1. Statistically significant p-values were denoted as follows: * or # ($p < 0.05$), ** or ## ($p < 0.01$), and *** or ### ($p < 0.001$), indicating upregulation or downregulation, respectively.

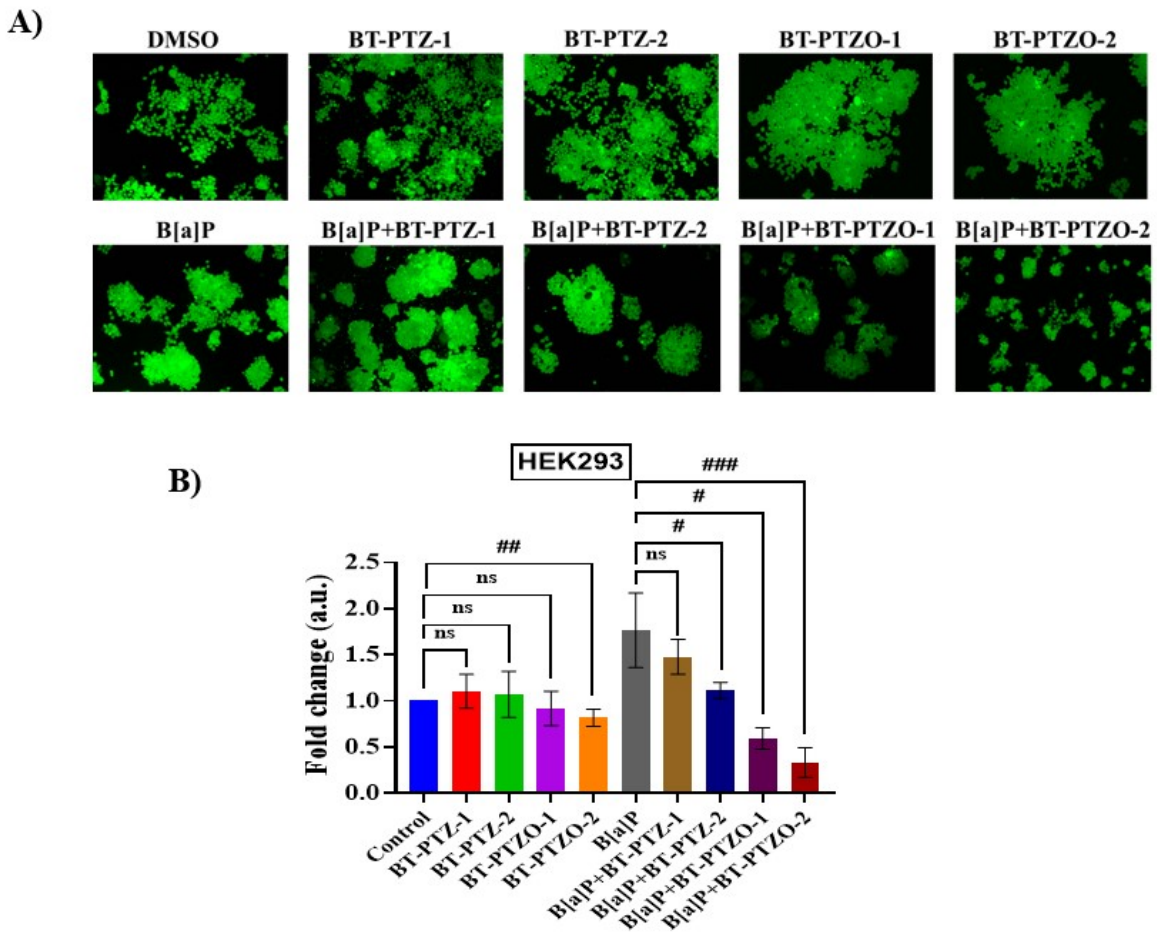


Fig. S9 Effect of compounds on oxidative stress in HEK293 cells. **(A)** Fluorescence microscopy image of HEK293 cells stained with H2DCFDA dye, following 24-hour pre-exposure to B[a]P and subsequent 24-hour treatment with compounds. **(B)** Quantification of fluorescence intensities of the green signal in HEK293 cells. Experiments were conducted with three biological replicates and two technical replicates. Results are presented as the mean ± standard deviation (SD). Statistical analysis was performed using an unpaired t-test, with p-values calculated using GraphPad Prism version 9.5.1. Statistically significant p-values were denoted as follows: * or # ($p < 0.05$), ** or ## ($p < 0.01$), and *** or ### ($p < 0.001$), indicating upregulation or downregulation, respectively.

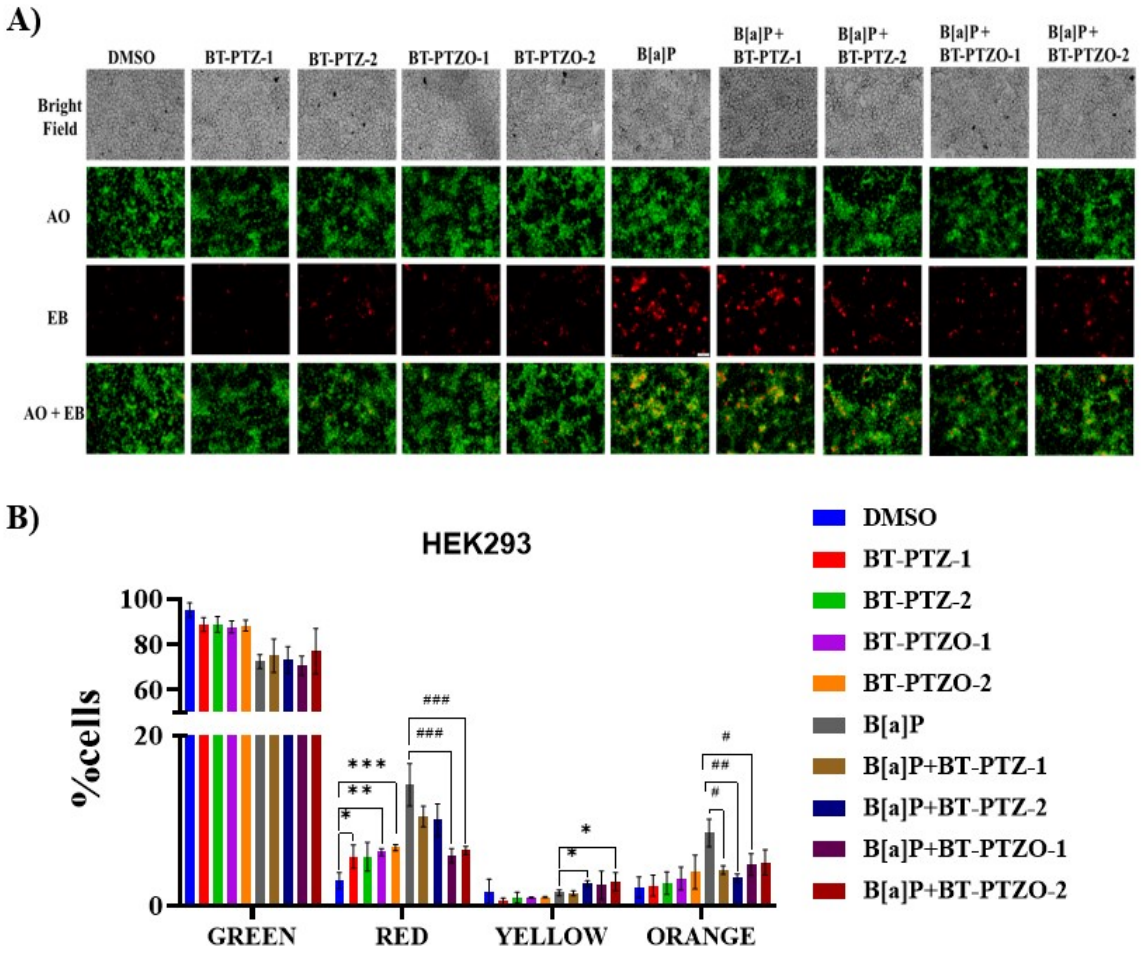


Fig. S10 Effect of compounds on apoptosis in HEK293 cells. **(A)** Representative image displaying live (green), necrotic (red), and early/late apoptotic (orange/yellow) cells as detected by AO/EB staining under fluorescence microscopy. **(B)** Bar graph quantifying live, necrotic, early, and late apoptotic cells in HEK293 cells following 24-hour pre-exposure to B[a]P and subsequent 24-hour compound treatment. Experiments were conducted with three biological replicates. Results are presented as mean ± standard deviation (SD). Statistical analysis was performed using an unpaired t-test, with p-values calculated using GraphPad Prism version 9.5.1. Statistically significant p-values are denoted as follows: * or # ($p < 0.05$), ** or ## ($p < 0.01$), and *** or ### ($p < 0.001$), indicating upregulation or downregulation, respectively.

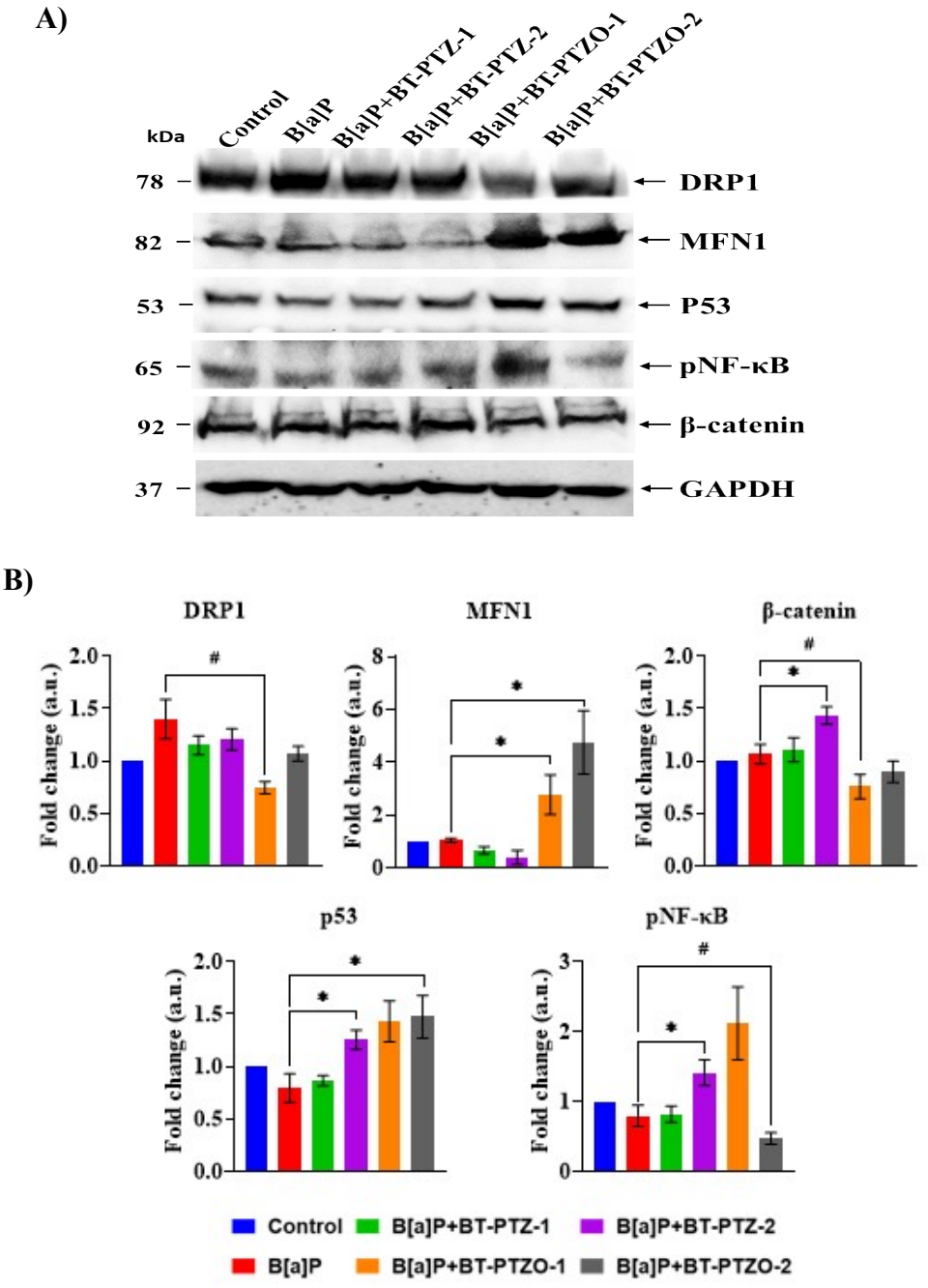
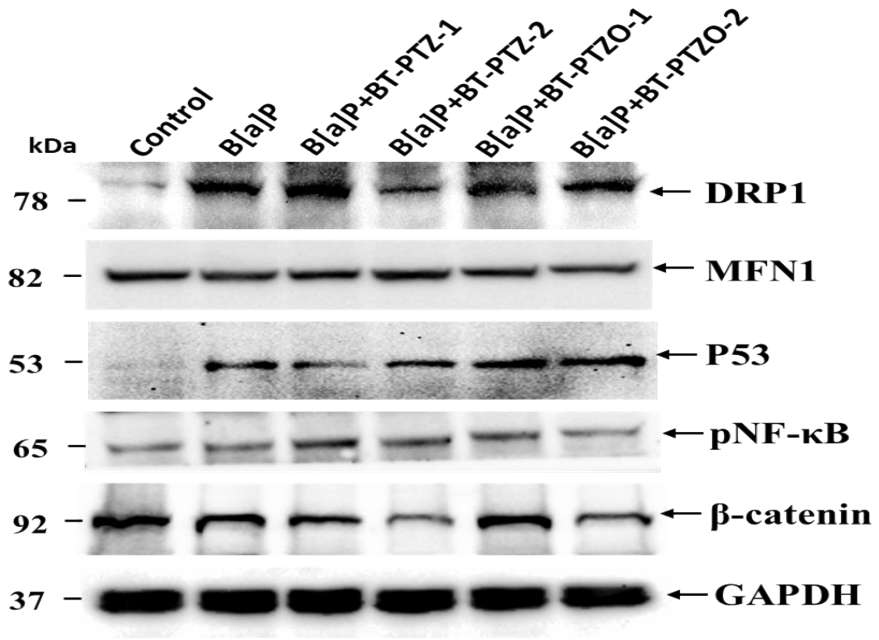
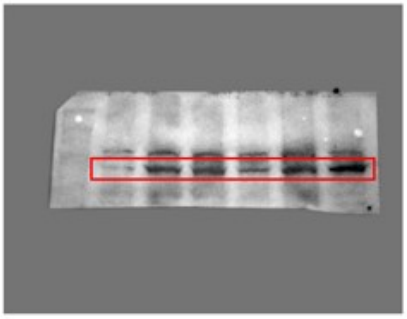


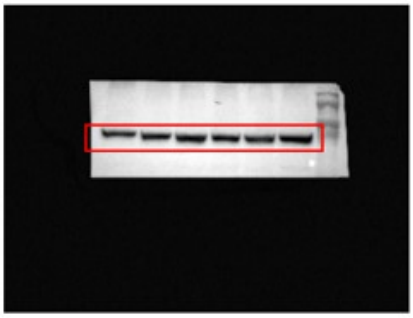
Fig. S11 Effects of co-exposure to B[a]P and compounds on DRP1, MFN1, p53, β-Catenin, and pNF-κB expression in HEK293 cells. (A) Representative Western blot image displaying the expression levels of DRP1, MFN1, p53, β-catenin, and pNF-κB following 24-hour pre-exposure to B[a]P and subsequent 24-hour treatment with compounds. (B) Bar graph quantifying the Western blot results. Experiments were conducted with three biological replicates and two technical replicates. Results are presented as mean ± standard deviation (SD). Statistical analysis was performed using an unpaired t-test, with p-values calculated using GraphPad Prism version 9.5.1. Statistically significant p-values are denoted as follows: * or # ($p < 0.05$), ** or ## ($p < 0.01$), and *** or ### ($p < 0.001$), indicating upregulation or downregulation, respectively.



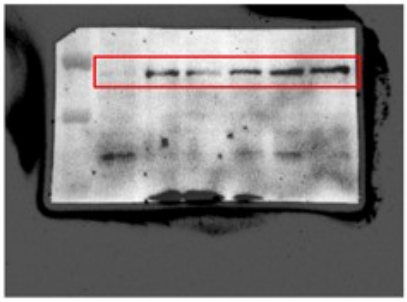
1] DRP1



2] MFN1



3] P53



4] pNF-κβ

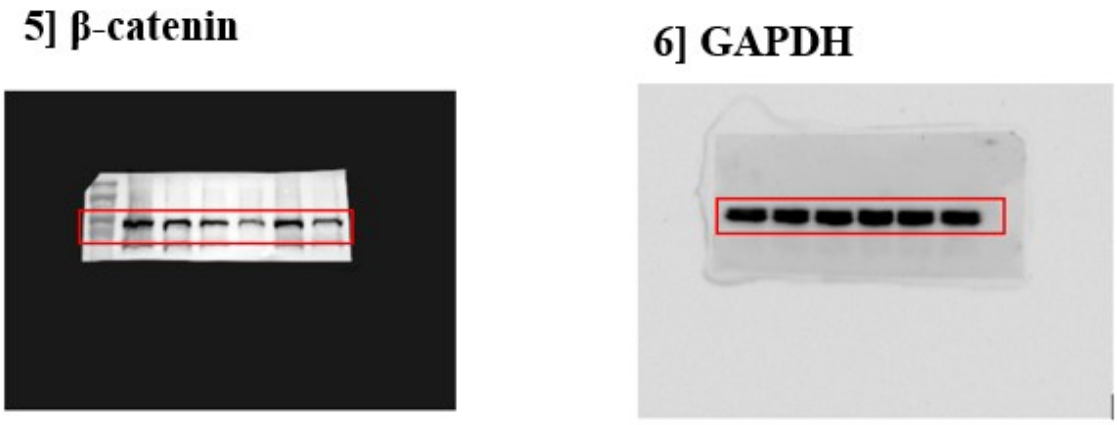


Fig. S12 The raw images for the western blot data shown in fig.12 .

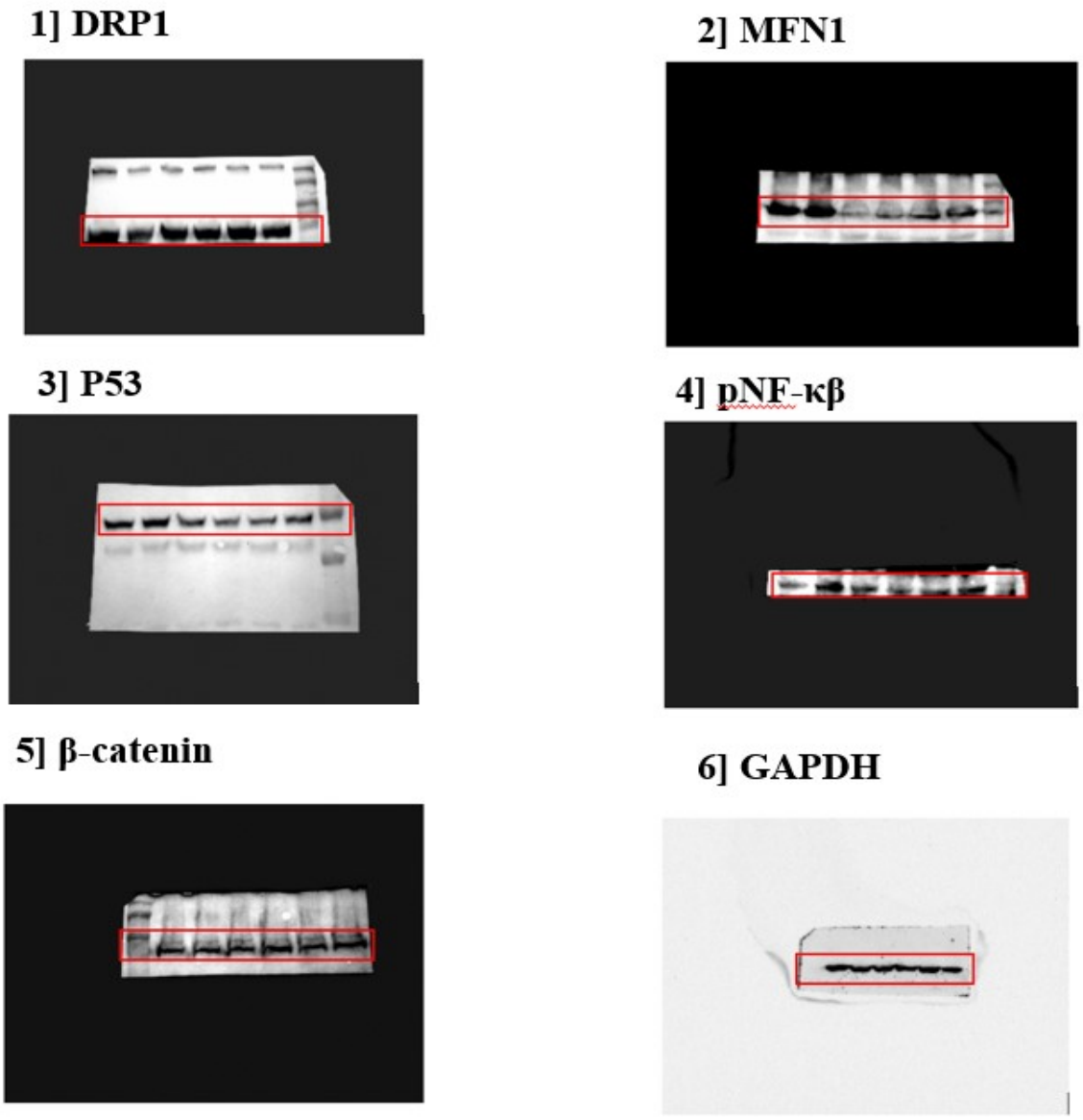


Fig. S13 The raw images for the western blot data shown in fig. S10.

Table S5 ADMET properties prediction using admetSAR 3.0

Name	BT-PTZ-1	BT-PTZ-2	BT-PTZO-1	BT-PTZO-2
MW	613.17	617.2	645.16	649.19
Vol	626.3902527	651.8598071	643.9707066	669.440261
Dense	0.978894543	0.946829354	1.001846813	0.969750458
nHA	3	3	5	5
nHD	0	0	0	0
TPSA	19.37	19.37	53.51	53.51
nRot	6	7	6	7
nRing	4	4	4	4
MaxRing	14	14	14	14
nHet	6	5	8	7
fChar	0	0	0	0
nRig	42	44	44	46
Flex	0.142857143	0.159090909	0.136363636	0.152173913
nStereo	0	0	0	0
gasa	1	0	0	0
QED	0.186	0.177	0.18	0.172
Synth	2.882	2.71	3.039	2.87
Fsp3	0.162	0.075	0.162	0.075
MCE-18	80	78	86	84
Natural Product-likeness	-1.07	-1.157	-1.232	-1.194
Chelating	['-']	['-']	['-']	['-']
PAINS	['-']	['-']	['-']	['-']
Lipinski	1	1	1	1
Pfizer	1	1	1	1
GSK	1	1	1	1
GoldenTriangle	1	1	1	1
logS	-11.70470785	-12.49938122	-9.33835679	-9.982755029
logD	5.019515919	5.860358902	4.086822113	4.738757919
logP	10.88641515	11.69051075	8.19915726	9.070230435
mp	267.8534865	298.4897542	219.1994953	255.2865362
bp	610.8250513	653.9644682	557.2079704	590.1259137
pka_acidic	14.94742829	14.59363633	12.44511574	12.39267053
pka_basic	0.866336438	-0.198443628	1.512711917	0.671159463
caco2	-4.662304949	-4.998146451	-4.748760471	-5.167901826
MDCK	-4.810895703	-4.577096363	-4.829729335	-4.761904682
PAMPA	0.002405705	0.007756432	0.019457929	0.054873306
pgp_inh	0.960912108	0.913223684	0.962376952	0.925488174
pgp_sub	0.878201783	0.504688263	0.238809392	0.053119496
hia	1.19E-06	9.54E-07	1.43E-06	1.19E-06
f20	0.908893771	0.054148018	0.949379977	0.09885639
f30	0.847859979	0.037126482	0.955377143	0.153490484
f50	0.99987648	0.791023985	0.999018654	0.331597924
OATP1B1	0.906186938	0.987992525	0.488739312	0.884528637

Name	BT-PTZ-1	BT-PTZ-2	BT-PTZO-1	BT-PTZO-2
OATP1B3	0.968854427	0.984597564	0.12046627	0.216627389
BCRP	0.685575366	0.800441444	0.008124067	0.015747594
BSEP	1	1	1	1
BBB	0.865089655	0.020429241	0.02347986	7.95E-05
MRP1	0.984040618	0.974593639	0.985419691	0.972355604
PPB	100.2261662	100.4139467	99.76397466	99.83210228
logVDss	1.103490089	1.158085668	0.023477166	-0.034064217
Fu	0.22889294	0.110121911	0.237394354	0.146803202
CYP1A2-inh	0.999164701	0.994454324	0.999860764	0.996490777
CYP1A2-sub	1	0.999267757	1	0.993070304
CYP2C19-inh	0.999999762	0.999999642	0.999843955	0.999188364
CYP2C19-sub	0.709028244	2.30E-05	0.996316791	0.002842188
CYP2C9-inh	0.147088066	0.959410667	0.06779772	0.934987187
CYP2C9-sub	0.990382016	7.91E-05	0.968025744	3.43E-05
CYP2D6-inh	0.999931455	0.951596081	0.99946636	0.577515483
CYP2D6-sub	0.999994993	0.98550421	0.983913004	0.006810627
CYP3A4-inh	0.995847583	0.999016643	0.991821826	0.996976256
CYP3A4-sub	0.993088663	0.79436779	0.60070926	0.023552533
CYP2B6-inh	0.999995232	1	0.99998498	1
CYP2B6-sub	0.963571727	0.000167654	0.723377585	2.67E-05
CYP2C8-inh	0.999999881	1	0.999965787	1
LM-human	0.999774635	0.998904943	0.999896288	0.999489903
cl-plasma	6.530465614	4.17422271	5.129742703	3.154428946
t0.5	0.249020897	0.427587069	0.258036386	0.412301049
BCF	2.178975535	2.432112095	1.715559827	2.082505506
IGC50	5.825891509	5.679155321	5.229168985	5.090145472
LC50DM	8.038096167	7.389901092	7.044876433	6.530842341
LC50FM	8.608012446	7.692378945	7.06376808	6.382762877
hERG	0.968768179	0.859173656	0.910451889	0.667252421
hERG-10um	0.970196962	0.97993958	0.938197732	0.958041131
DILI	0.999999762	0.999966621	0.999998569	0.999805868
Ames	0.845941484	0.606791556	0.895098686	0.703343034
ROA	0.768248916	0.188905492	0.611992657	0.100664765
FDAMDD	0.878722727	0.92618525	0.959279895	0.976564288
SkinSen	0.999423027	0.997296751	0.971316516	0.885920644
Carcinogenicity	0.759638608	0.927610993	0.839057922	0.954525828
EC	2.18E-11	3.22E-09	1.52E-09	2.19E-07
EI	0.003794322	0.242738515	0.00649927	0.353414029
Respiratory	0.999424815	0.997999966	0.981661201	0.940068185
H-HT	0.730246782	0.957393587	0.792500019	0.968467832
Neurotoxicity-DI	0.996783972	0.999698281	0.992272019	0.999281108
Ototoxicity	0.618860006	0.977191687	0.510903001	0.964516878
Hematotoxicity	0.771644533	0.944673061	0.571428835	0.870358348
Nephrotoxicity-DI	0.919334769	0.997553289	0.847280383	0.994819582
Genotoxicity	0.996340156	1	0.99987042	1
RPMI-8226	0.258406132	0.174673721	0.238864124	0.157971382
A549	0.979188859	0.801273227	0.642495215	0.135120347

Name	BT-PTZ-1	BT-PTZ-2	BT-PTZO-1	BT-PTZO-2
HEK293	0.998480499	0.999415994	0.984270394	0.993897736
NR-AhR	0.999437988	0.999715149	0.999381423	0.999614477
NR-AR	0.633356512	0.034468368	0.809978366	0.084733702
NR-AR-LBD	0.736457109	0.602147996	0.924707174	0.843703151
NR-Aromatase	0.88047272	0.949086547	0.67497015	0.818391204
NR-ER	0.874230206	0.989339411	0.815588236	0.982480943
NR-ER-LBD	0.008729187	0.424299031	0.002148574	0.126872644
NR-PPAR-gamma	0.820520997	0.273231506	0.78676033	0.241994783
SR-ARE	0.991290092	0.999235868	0.988200784	0.99896121
SR-ATAD5	0.540379882	0.678446531	0.386974961	0.523831546
SR-HSE	0.836855471	0.955584586	0.38260895	0.720810235
SR-MMP	0.99975425	0.999985933	0.999475896	0.999961376
SR-p53	0.959701538	0.969572246	0.780841172	0.795073628
NonBiodegradable	['-']	[(12,)]	['-']	[(12,)]
NonGenotoxic_Carcinogenicity	['-']	['-']	['-']	['-']
SureChEMBL	['-']	['-']	['-']	['-']
LD50_oral	[(2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 40, 41, 42)]	[(2, 3, 4, 5, 6, 7, 27, 28, 29, 30, 31, 32, 42, 43, 44)]	[(2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 42, 43, 44)]	[(2, 3, 4, 5, 6, 7, 27, 28, 29, 32, 33, 34, 44, 45, 46)]
Skin_Sensitization	[(23, 24, 25, 26, 27, 28, 29, 30, 31, 32)]	[(32, 33, 34, 35, 36, 37, 38, 39, 40, 41)]	[(25, 26, 27, 28, 29, 30, 31, 32, 33, 34)]	[(34, 35, 36, 37, 38, 39, 40, 41, 42, 43)]
Acute_Aquatic_Toxicity	['-']	['-']	['-']	['-']
Toxicophores	[(3, 4, 5, 6, 7, 8, 9), (32, 31, 26, 25, 24)]	[(3, 4, 5, 6, 7, 27, 28), (41, 40, 35, 34, 33)]	[(3, 4, 5, 6, 7, 8, 9), (34, 33, 28, 27, 26)]	[(3, 4, 5, 6, 7, 27, 28), (43, 42, 37, 36, 35)]
Carcinogenicity_Mutagenicity	[(4, 3)]	[(4, 3)]	[(4, 3)]	[(4, 3)]
Aggregators	1	1	1	1
Fluc	0.969	0.902	0.87	0.796
Blue_fluorescence	0.98	0.966	0.904	0.934
Green_fluorescence	0.999	1	0.999	1
Reactive	0.541	0.228	0.195	0.049
Other_assay_interference	0.906	0.697	0.88	0.677
Promiscuous	0.453	0.097	0.053	0.004

Table S6: Toxicity of the compounds predicted using the ProTox-III

Parameters		BT-PTZ-1		BT-PTZ-2		BT-PTZO-1		BT-PTZO-2	
Classification	**Target**	**Prediction**	**Probability**	**Prediction**	**Probability**	**Prediction**	**Probability**	**Prediction**	**Probability**
Organ toxicity	Hepatotoxicity	Inactive	0.56	Inactive	0.56	Inactive	0.62	Inactive	0.58
Organ toxicity	Neurotoxicity	Active	0.81	Active	0.78	Active	0.62	Active	0.57
Organ toxicity	Nephrotoxicity	Inactive	0.82	Inactive	0.83	Inactive	0.62	Inactive	0.62
Organ toxicity	Respiratory toxicity	Active	0.84	Active	0.84	Active	0.79	Active	0.8
Organ toxicity	Cardiotoxicity	Inactive	0.93	Inactive	0.92	Inactive	0.82	Inactive	0.81
Toxicity end points	Carcinogenicity	Inactive	0.76	Inactive	0.69	Inactive	0.65	Inactive	0.61
Toxicity end points	Immunotoxicity	Inactive	0.86	Inactive	0.88	Inactive	0.97	Inactive	0.99
Toxicity end points	Mutagenicity	Inactive	0.57	Active	0.51	Inactive	0.56	Inactive	0.53
Toxicity end points	Cytotoxicity	Inactive	0.62	Inactive	0.65	Inactive	0.56	Inactive	0.57
Toxicity end points	BBB-barrier	Active	0.92	Active	0.91	Active	0.92	Active	0.9
Toxicity end points	Ecotoxicity	Active	0.77	Active	0.76	Inactive	0.56	Inactive	0.58
Toxicity end points	Clinical toxicity	Inactive	0.52	Active	0.55	Active	0.54	Active	0.61
Toxicity end points	Nutritional toxicity	Inactive	0.73	Inactive	0.71	Inactive	0.67	Inactive	0.66
Tox21-Nuclear receptor signalling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.75	Inactive	0.6	Inactive	0.83	Inactive	0.82
Tox21-Nuclear receptor signalling pathways	Androgen Receptor (AR)	Inactive	0.9	Inactive	0.9	Inactive	0.95	Inactive	0.95
Tox21-Nuclear receptor signalling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.93	Inactive	0.92	Inactive	0.95	Inactive	0.94
Tox21-Nuclear receptor signalling pathways	Aromatase	Inactive	0.85	Inactive	0.85	Inactive	0.93	Inactive	0.91
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.88	Inactive	0.83	Inactive	0.87	Inactive	0.86
Tox21-Nuclear receptor signalling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.96	Inactive	0.95	Inactive	0.93	Inactive	0.92
Tox21-Nuclear receptor signalling pathways	Peroxisome Proliferator Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.92	Inactive	0.91	Inactive	0.94	Inactive	0.93
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	Inactive	0.93	Inactive	0.93	Inactive	0.93	Inactive	0.93
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.93	Inactive	0.93	Inactive	0.93	Inactive	0.93
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.69	Inactive	0.66	Inactive	0.77	Inactive	0.76
Tox21-Stress response pathways	Phosphoprotein (Tumor Supressor) p53	Inactive	0.77	Inactive	0.75	Inactive	0.9	Inactive	0.89
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5	Inactive	0.9	Inactive	0.83	Inactive	0.92	Inactive	0.86

Parameters		BT-PTZ-1		BT-PTZ-2		BT-PTZO-1		BT-PTZO-2	
Classification	**Target**	**Prediction**	**Probability**	**Prediction**	**Probability**	**Prediction**	**Probability**	**Prediction**	**Probability**
	(ATAD5)								
Molecular Initiating Events	Thyroid hormone receptor alpha (THRÎ±)	Inactive	0.9	Inactive	0.9	Inactive	0.9	Inactive	0.9
Molecular Initiating Events	Thyroid hormone receptor beta (THRÎ²)	Inactive	0.78	Inactive	0.78	Inactive	0.78	Inactive	0.78
Molecular Initiating Events	Transtyretrin (TTR)	Inactive	0.97	Inactive	0.97	Inactive	0.97	Inactive	0.97
Molecular Initiating Events	Ryanodine receptor (RYR)	Inactive	0.98	Inactive	0.98	Inactive	0.98	Inactive	0.98
Molecular Initiating Events	GABA receptor (GABAR)	Inactive	0.96	Inactive	0.96	Inactive	0.96	Inactive	0.96
Molecular Initiating Events	Glutamate N-methyl-D-aspartate receptor (NMDAR)	Inactive	0.92	Inactive	0.92	Inactive	0.92	Inactive	0.92
Molecular Initiating Events	alpha-amino-3-hydroxy-5-methyl-4-isoxazolepropionate receptor (AMPAR)	Inactive	0.97	Inactive	0.97	Inactive	0.97	Inactive	0.97
Molecular Initiating Events	Kainate receptor (KAR)	Inactive	0.99	Inactive	0.99	Inactive	0.99	Inactive	0.99
Molecular Initiating Events	Achetylcholinesterase (AChE)	Inactive	0.56	Inactive	0.56	Inactive	0.62	Inactive	0.58
Molecular Initiating Events	Constitutive androstane receptor (CAR)	Inactive	0.98	Inactive	0.98	Inactive	0.98	Inactive	0.98
Molecular Initiating Events	Pregnane X receptor (PXR)	Inactive	0.92	Inactive	0.92	Inactive	0.92	Inactive	0.92
Molecular Initiating Events	NADH-quinone oxidoreductase (NADHOX)	Inactive	0.97	Inactive	0.97	Inactive	0.97	Inactive	0.97
Molecular Initiating Events	Voltage gated sodium channel (VGSC)	Inactive	0.95	Inactive	0.95	Inactive	0.95	Inactive	0.95
Molecular Initiating Events	Na+/I- symporter (NIS)	Inactive	0.98	Inactive	0.98	Inactive	0.98	Inactive	0.98
Metabolism	Cytochrome CYP1A2	Active	0.52	Active	0.53	Inactive	0.67	Inactive	0.65
Metabolism	Cytochrome CYP2C19	Inactive	0.58	Active	0.51	Inactive	0.54	Active	0.5
Metabolism	Cytochrome CYP2C9	Inactive	0.5	Inactive	0.5	Active	0.57	Active	0.61
Metabolism	Cytochrome CYP2D6	Active	0.85	Active	0.83	Active	0.61	Active	0.57
Metabolism	Cytochrome CYP3A4	Inactive	0.72	Inactive	0.65	Inactive	0.6	Inactive	0.54
Metabolism	Cytochrome CYP2E1	Inactive	0.95	Inactive	0.96	Inactive	0.99	Inactive	0.99

Table S7 SuperPRED target prediction of probable macromolecular targets for compounds

A) BT-PTZ-1

BT-PTZ-1						
Target Name	**ChEMBL-ID**	**UniProt ID**	**PDB Visualization**	**TTD ID**	**Probability**	**Model accuracy**
Cathepsin D	CHEMBL2581	P07339	4OD9	T67102	0.9905	0.9895
Kruppel-like factor 5	CHEMBL1293249	Q13887	Not Available	Not Available	0.9793	0.8633
Nuclear factor NF-kappa-B p105 subunit	CHEMBL3251	P19838	1SVC	Not Available	0.9689	0.9609
Tyrosyl-DNA phosphodiesterase 1	CHEMBL1075138	Q9NUW8	6N0D	Not Available	0.9655	0.7122
Cyclooxygenase-2	CHEMBL230	P35354	5F19	Not Available	0.9496	0.8963
Cyclooxygenase-1	CHEMBL221	P23219	6Y3C	Not Available	0.9354	0.9017
Beta amyloid A4 protein	CHEMBL2487	P05067	5BUO	T87024	0.9299	0.9674
G-protein coupled bile acid receptor 1	CHEMBL5409	Q8TDU6	7CFM	T86273	0.9134	0.9365
Hypoxia-inducible factor 1 alpha	CHEMBL4261	Q16665	4H6J	Not Available	0.8982	0.8514
Dual specificty protein kinase CLK1	CHEMBL4224	P49759	6KHD	Not Available	0.8979	0.853
Geranylgeranyl pyrophosphate synthetase	CHEMBL4769	O95749	6R4V	Not Available	0.8745	0.9208
DCN1-like protein 1	CHEMBL4105838	Q96GG9	6BG3	Not Available	0.8621	0.95
Dual specificity protein phosphatase 3	CHEMBL2635	P51452	3F81	Not Available	0.8571	0.94
Transmembrane protease serine 6	CHEMBL1795139	Q8IU80	Not Available	Not Available	0.8473	0.9833
Casein kinase I delta	CHEMBL2828	P48730	6PXN	Not Available	0.8437	0.9308
Anandamide amidohydrolase	CHEMBL2243	O00519	Not Available	T11754	0.8424	0.9753
Nuclear receptor ROR-beta	CHEMBL3091268	Q92753	Not Available	Not Available	0.8393	0.955
Dual-specificity tyrosine-phosphorylation regulated kinase 1A	CHEMBL2292	Q13627	6S14	T92803	0.8318	0.9324
Aminopeptidase N	CHEMBL1907	P15144	4FYT	T67272	0.8305	0.9331
Signal transducer and activator of transcription 1-alpha/beta	CHEMBL6101	P42224	1YVL	T64205	0.8263	0.7262
Aldose reductase	CHEMBL1900	P15121	1US0	T26623	0.8196	0.9238
DNA topoisomerase I	CHEMBL1781	P11387	1K4T	T09826	0.8157	0.97
Ras-related protein Rab-9A	CHEMBL1293294	P51151	1WMS	T66350	0.8123	0.8767
Cytochrome P450 2A6	CHEMBL5282	P11509	2FDV	T06455	0.8123	0.7178
Nuclear factor erythroid 2-related factor 2	CHEMBL1075094	Q16236	2FLU	Not Available	0.8083	0.96
GABA-A receptor; alpha-1/beta-3/gamma-2	CHEMBL2094121	P14867	6HUJ	T51487	0.8003	0.955

B) BT-PTZ-2

BT-PTZ-2						
Target Name	**ChEMBL-ID**	**UniProt ID**	**PDB Visualization**	**TTD ID**	**Probability**	**Model accuracy**
Cathepsin D	CHEMBL2581	P07339	4OD9	T67102	0.9948	0.9895
Kruppel-like factor 5	CHEMBL1293249	Q13887	Not Available	Not Available	0.9825	0.8633
Nuclear factor NF-kappa-B p105 subunit	CHEMBL3251	P19838	1SVC	Not Available	0.9743	0.9609
Beta amyloid A4 protein	CHEMBL2487	P05067	5BUO	T87024	0.9718	0.9674
Tyrosyl-DNA phosphodiesterase 1	CHEMBL1075138	Q9NUW8	6N0D	Not Available	0.9669	0.7122
Protein-tyrosine phosphatase 1B	CHEMBL335	P18031	5QGF	Not Available	0.9575	0.9517
Cyclooxygenase-1	CHEMBL221	P23219	6Y3C	Not Available	0.9361	0.9017
Ras-related protein Rab-9A	CHEMBL1293294	P51151	1WMS	T66350	0.9284	0.8767
HERG	CHEMBL240	Q12809	5VA1	T20251	0.9183	0.8976
Geranylgeranyl pyrophosphate synthetase	CHEMBL4769	O95749	6R4V	Not Available	0.8905	0.9208
15-hydroxyprostaglandin dehydrogenase [NAD+]	CHEMBL1293255	P15428	2GDZ	Not Available	0.8866	0.8357
Choline kinase alpha	CHEMBL3117	P35790	4DA5	T55709	0.8728	0.78
Glyoxalase I	CHEMBL2424	Q04760	3W0T	Not Available	0.8722	0.9167
Muscarinic acetylcholine receptor M5	CHEMBL2035	P08912	6OL9	T79961	0.8688	0.9462
DCN1-like protein 1	CHEMBL4105838	Q96GG9	6BG3	Not Available	0.8589	0.95
DNA topoisomerase I	CHEMBL1781	P11387	1K4T	T09826	0.8482	0.97
Monoamine oxidase A	CHEMBL1951	P21397	2Z5Y	Not Available	0.8436	0.9149
Calpain 1	CHEMBL3891	P07384	1ZCM	Not Available	0.8416	0.9304
Nuclear receptor ROR-beta	CHEMBL3091268	Q92753	Not Available	Not Available	0.8411	0.955
Pregnane X receptor	CHEMBL3401	O75469	6TFI	T82702	0.8366	0.9473
Aminopeptidase N	CHEMBL1907	P15144	4FYT	T67272	0.8336	0.9331
G-protein coupled bile acid receptor 1	CHEMBL5409	Q8TDU6	7CFM	T86273	0.8294	0.9365
Aldose reductase	CHEMBL1900	P15121	1US0	T26623	0.8291	0.9238
Nuclear factor erythroid 2-related factor 2	CHEMBL1075094	Q16236	2FLU	Not Available	0.8242	0.96
Signal transducer and activator of transcription 1-alpha/beta	CHEMBL6101	P42224	1YVL	T64205	0.822	0.7262
Transmembrane protease serine 6	CHEMBL1795139	Q8IU80	Not Available	Not Available	0.8169	0.9833
Dual specificity protein phosphatase 3	CHEMBL2635	P51452	3F81	Not Available	0.8118	0.94

C) BT-PTZO-1

BT-PTZO-1						
Target Name	**ChEMBL-ID**	**UniProt ID**	**PDB Visualization**	**TTD ID**	**Probability**	**Model accuracy**
Cathepsin D	CHEMBL2581	P07339	4OD9	T67102	0.9934	0.9895
Nuclear factor NF-kappa-B p105 subunit	CHEMBL3251	P19838	1SVC	Not Available	0.9691	0.9609
Kruppel-like factor 5	CHEMBL1293249	Q13887	Not Available	Not Available	0.9595	0.8633
Tyrosyl-DNA phosphodiesterase 1	CHEMBL1075138	Q9NUW8	6N0D	Not Available	0.9213	0.7122
G-protein coupled bile acid receptor 1	CHEMBL5409	Q8TDU6	7CFM	T86273	0.9186	0.9365
Hypoxia-inducible factor 1 alpha	CHEMBL4261	Q16665	4H6J	Not Available	0.9182	0.8514
Nuclear factor erythroid 2-related factor 2	CHEMBL1075094	Q16236	2FLU	Not Available	0.8876	0.96
Cyclooxygenase-2	CHEMBL230	P35354	5F19	Not Available	0.8814	0.8963
Dual specificity protein phosphatase 3	CHEMBL2635	P51452	3F81	Not Available	0.8732	0.94
Cyclooxygenase-1	CHEMBL221	P23219	6Y3C	Not Available	0.8681	0.9017
15-hydroxyprostaglandin dehydrogenase [NAD+]	CHEMBL1293255	P15428	2GDZ	Not Available	0.8638	0.8357
Cytochrome P450 2A6	CHEMBL5282	P11509	2FDV	T06455	0.8597	0.7178
Beta amyloid A4 protein	CHEMBL2487	P05067	5BUO	T87024	0.8515	0.9674
Signal transducer and activator of transcription 1-alpha/beta	CHEMBL6101	P42224	1YVL	T64205	0.8498	0.7262
DCN1-like protein 1	CHEMBL4105838	Q96GG9	6BG3	Not Available	0.8471	0.95
Anandamide amidohydrolase	CHEMBL2243	O00519	Not Available	T11754	0.8435	0.9753
Butyrylcholinesterase	CHEMBL1914	P06276	5LKR	T99799	0.8399	0.95
Dual specificty protein kinase CLK1	CHEMBL4224	P49759	6KHD	Not Available	0.8388	0.853
Transmembrane protease serine 6	CHEMBL1795139	Q8IU80	Not Available	Not Available	0.8351	0.9833
Aminopeptidase N	CHEMBL1907	P15144	4FYT	T67272	0.8341	0.9331
Ras-related protein Rab-9A	CHEMBL1293294	P51151	1WMS	T66350	0.828	0.8767
Aldose reductase	CHEMBL1900	P15121	1US0	T26623	0.8278	0.9238
DNA topoisomerase I	CHEMBL1781	P11387	1K4T	T09826	0.8267	0.97
Geranylgeranyl pyrophosphate synthetase	CHEMBL4769	O95749	6R4V	Not Available	0.8195	0.9208
Proteasome component C5	CHEMBL4208	P20618	6KWY	Not Available	0.8147	0.9
Calpain 1	CHEMBL3891	P07384	1ZCM	Not Available	0.8068	0.9304

D) BT-PTZO-2

BT-PTZO-2						
Target Name	**ChEMBL-ID**	**UniProt ID**	**PDB Visualization**	**TTD ID**	**Probability**	**Model accuracy**
Cathepsin D	CHEMBL2581	P07339	4OD9	T67102	0.996	0.9895
Nuclear factor NF-kappa-B p105 subunit	CHEMBL3251	P19838	1SVC	Not Available	0.9746	0.9609
Ras-related protein Rab-9A	CHEMBL1293294	P51151	1WMS	T66350	0.9718	0.8767
Kruppel-like factor 5	CHEMBL1293249	Q13887	Not Available	Not Available	0.9637	0.8633
Beta amyloid A4 protein	CHEMBL2487	P05067	5BUO	T87024	0.9539	0.9674
HERG	CHEMBL240	Q12809	5VA1	T20251	0.9057	0.8976
Nuclear factor erythroid 2-related factor 2	CHEMBL1075094	Q16236	2FLU	Not Available	0.9018	0.96
Niemann-Pick C1 protein	CHEMBL1293277	O15118	6W5S	Not Available	0.8952	0.8111
Tyrosyl-DNA phosphodiesterase 1	CHEMBL1075138	Q9NUW8	6N0D	Not Available	0.8949	0.7122
Calpain 1	CHEMBL3891	P07384	1ZCM	Not Available	0.8788	0.9304
15-hydroxyprostaglandin dehydrogenase [NAD+]	CHEMBL1293255	P15428	2GDZ	Not Available	0.8712	0.8357
Choline kinase alpha	CHEMBL3117	P35790	4DA5	T55709	0.8689	0.78
Monoamine oxidase A	CHEMBL1951	P21397	2Z5Y	Not Available	0.8667	0.9149
DNA topoisomerase I	CHEMBL1781	P11387	1K4T	T09826	0.8621	0.97
Dual specificity protein phosphatase 3	CHEMBL2635	P51452	3F81	Not Available	0.8522	0.94
T-cell protein-tyrosine phosphatase	CHEMBL3807	P17706	1L8K	Not Available	0.8511	0.93
Signal transducer and activator of transcription 1-alpha/beta	CHEMBL6101	P42224	1YVL	T64205	0.8435	0.7262
Geranylgeranyl pyrophosphate synthetase	CHEMBL4769	O95749	6R4V	Not Available	0.8412	0.9208
G-protein coupled bile acid receptor 1	CHEMBL5409	Q8TDU6	7CFM	T86273	0.838	0.9365
DCN1-like protein 1	CHEMBL4105838	Q96GG9	6BG3	Not Available	0.8364	0.95
Aminopeptidase N	CHEMBL1907	P15144	4FYT	T67272	0.8269	0.9331
Pregnane X receptor	CHEMBL3401	O75469	6TFI	T82702	0.8242	0.9473
Glycine transporter 2	CHEMBL3060	Q9Y345	Not Available	Not Available	0.8242	0.9917
Protein-tyrosine phosphatase 1B	CHEMBL335	P18031	5QGF	Not Available	0.8202	0.9517
Transcription intermediary factor 1-alpha	CHEMBL3108638	O15164	4YBM	Not Available	0.81	0.9556
Cytochrome P450 2A6	CHEMBL5282	P11509	2FDV	T06455	0.8036	0.7178
Transmembrane protease serine 6	CHEMBL1795139	Q8IU80	Not Available	Not Available	0.803	0.9833

Table S8 Primer sequence for qRT-PCR

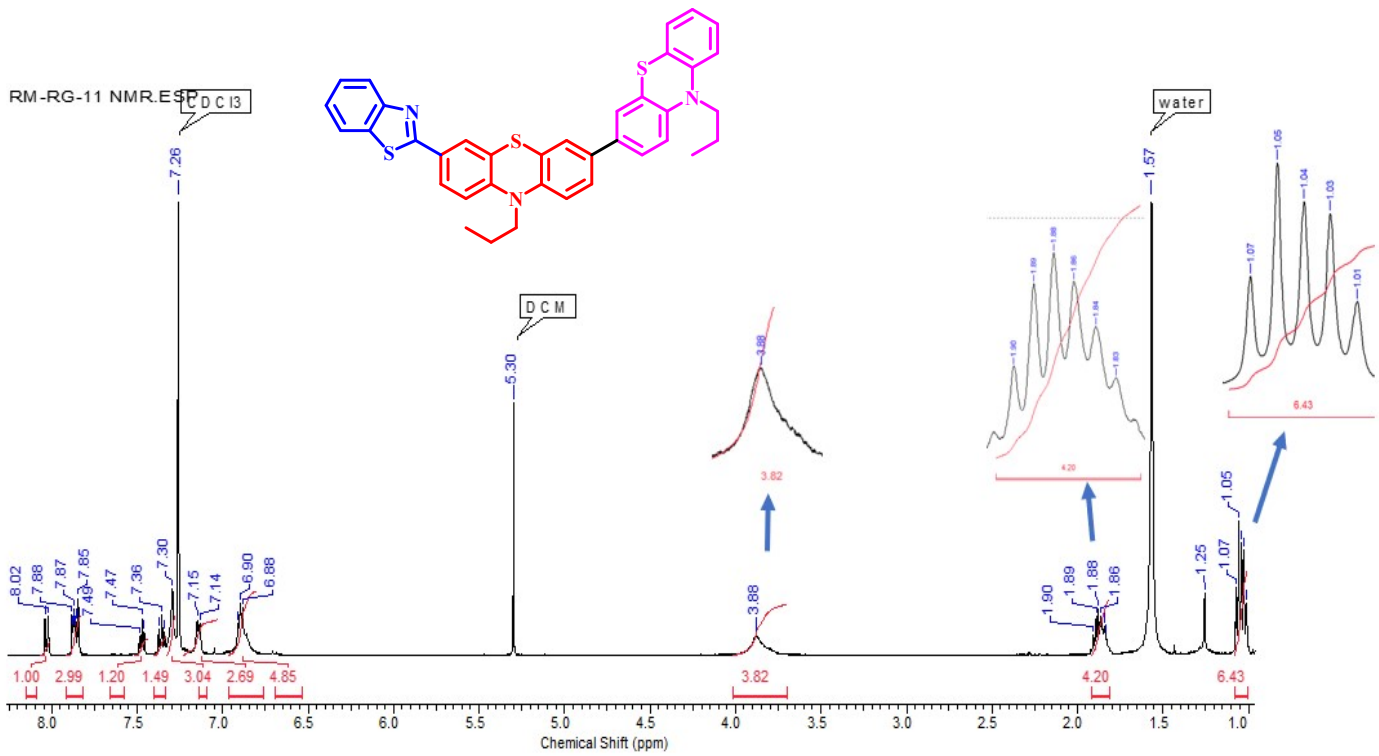
Gene	Primers
drp1	F- TGGGCGCCGACATCA
	R- GCTCTGCGTTCCCACTACGA
fis1	F- TACGTCCGCGGGTTGCT
	R- CCAGTTCCTTGGCCTGGTT
mff	F- CCAAACGCTGACCTGGAAC
	R- TTTCCTGCTACAACAATCCTCTCC
mfn1	F- GGCATCTGTGGCCGAGTT
	R- ATTATGCTAAGTCTCCGCTCCAA
opa1	F- GTGCTGCCCGCCTAGAAA
	R- TGACAGGCACCCGTACTCAGT
apaf1	F- CTTGCTGCCCTTCTCCATGA
	R- TTGCGAAGCATCAGAATGCG
fadd	F- CACCAAGATCGACAGCATCG
	R- AGATTCTCAGTGACTCCCGC
gapdh	F- TGCACCACCAACTGCTTAG
	R- GATGCAGGGATGATGTTC

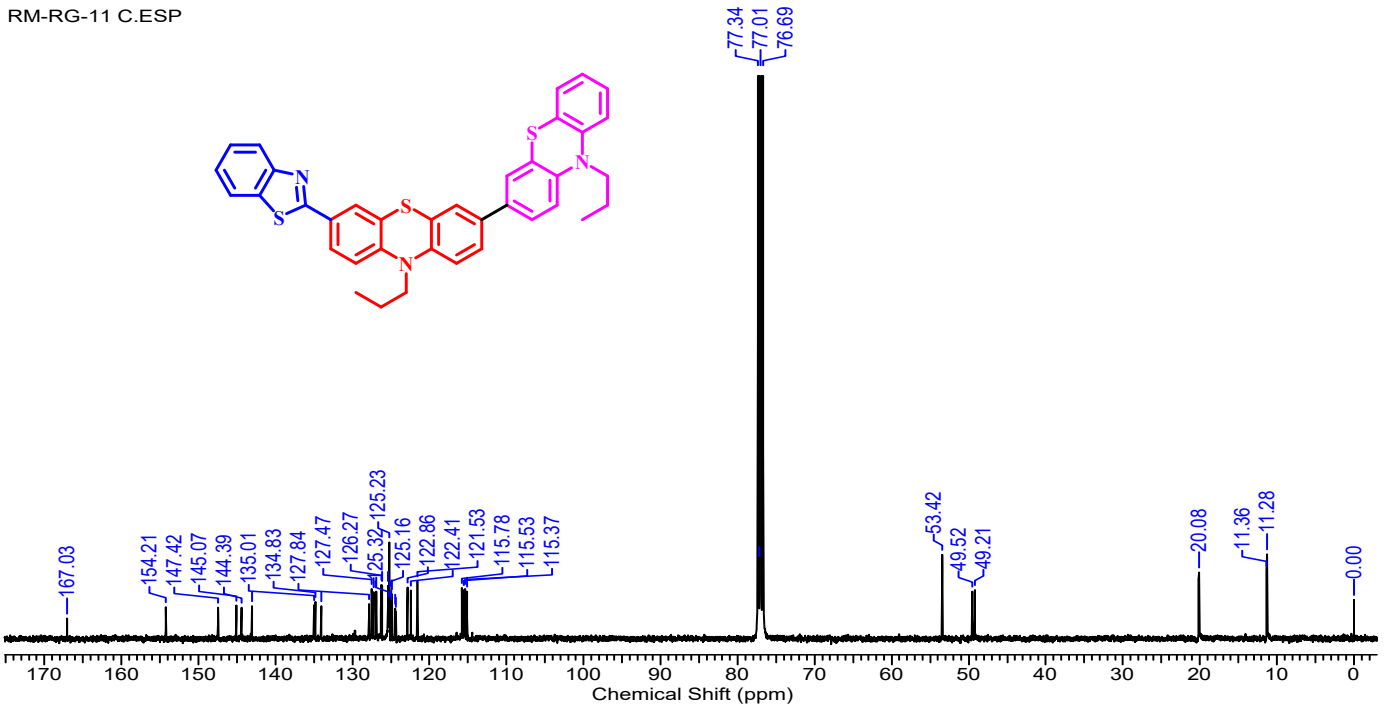
Table S9 The drug vs. normalized response data were fitted using a four-parameter logistic (4PL) nonlinear regression model to estimate the IC_{50} value.

Cell Line	Compound	Conc. (μM)
A549	**BT-PTZ-1**	166.8 μM
A549	**BT-PTZ-2**	136.6 μM
A549	**BT-PTZO-1**	157.8 μM
A549	**BT-PTZO-2**	115.9 μM
HEK	**BT-PTZ-1**	163.2 μM
HEK	**BT-PTZ-2**	87.14 μM
HEK	**BT-PTZO-1**	88.5 μM
HEK	**BT-PTZO-2**	54.45 μM

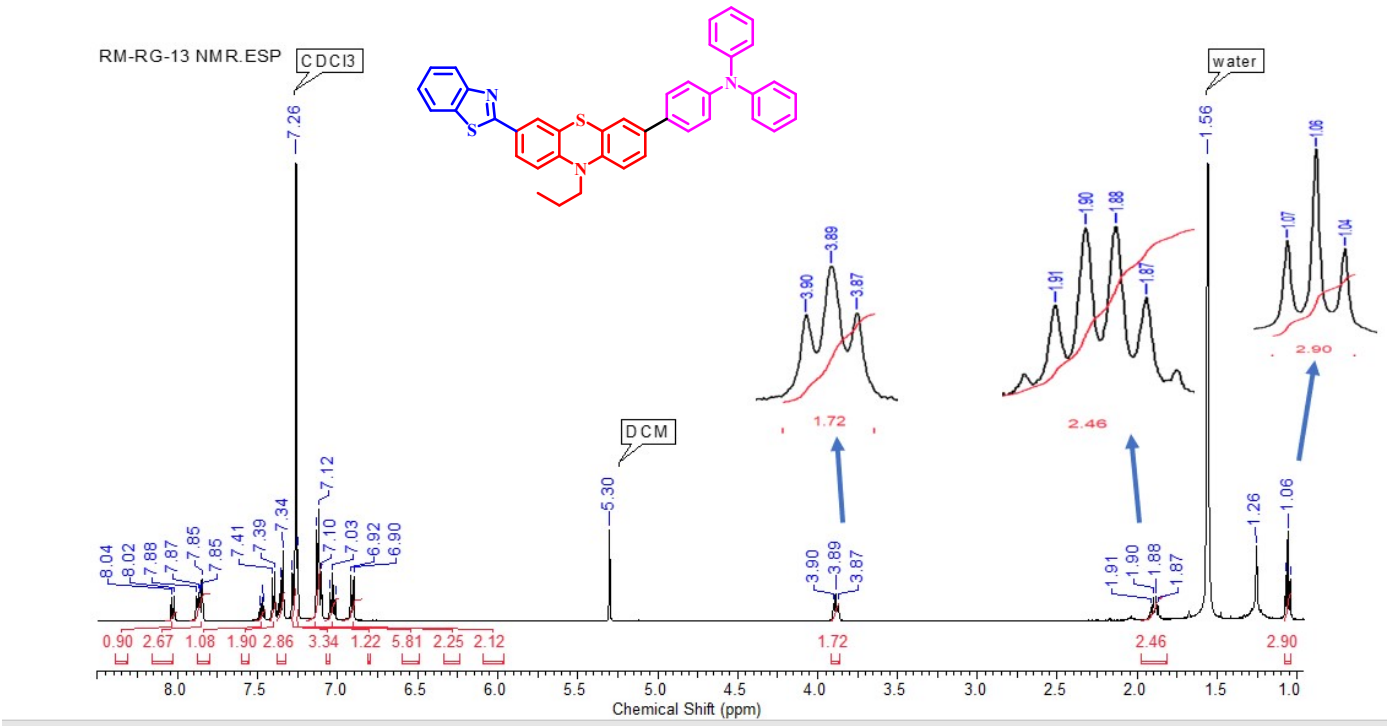
Copies of NMR and HRMS spectra of new compounds

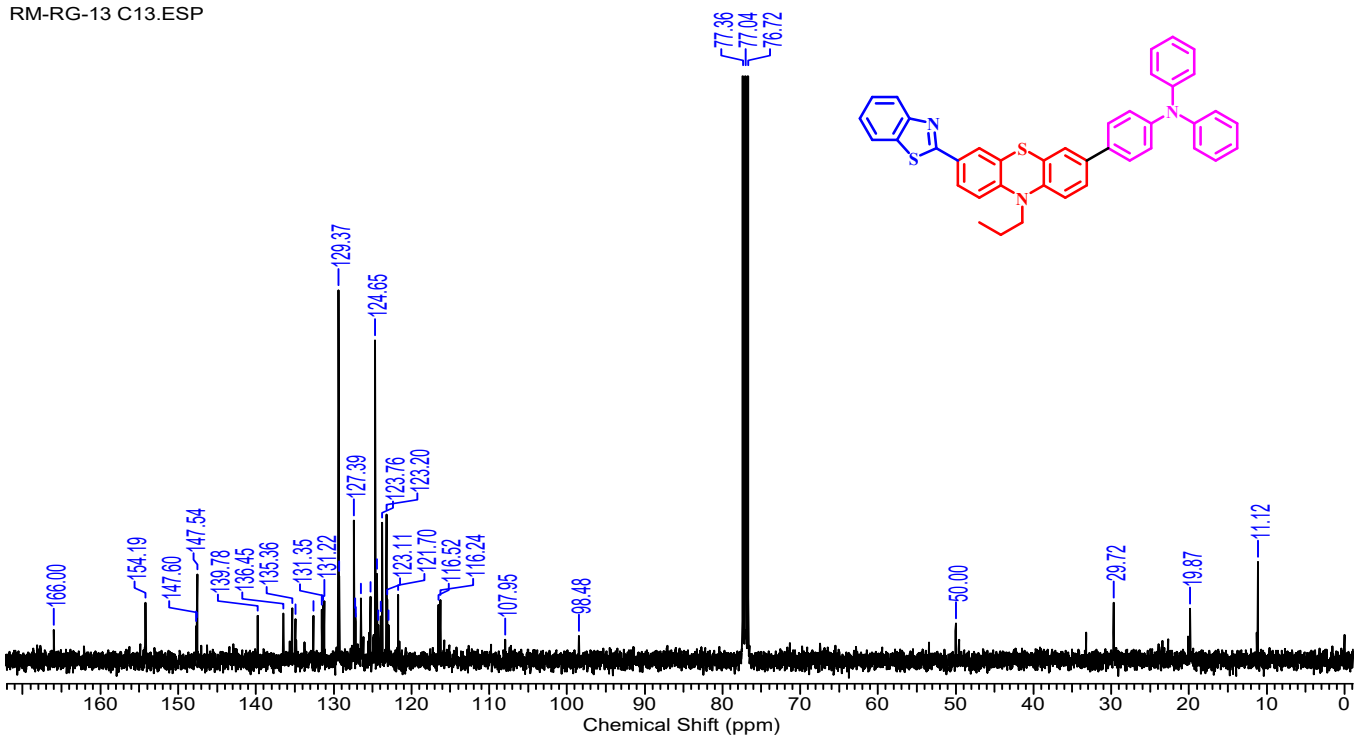
^{1}H NMR and ^{13}C NMR of **BT-PTZ-1**



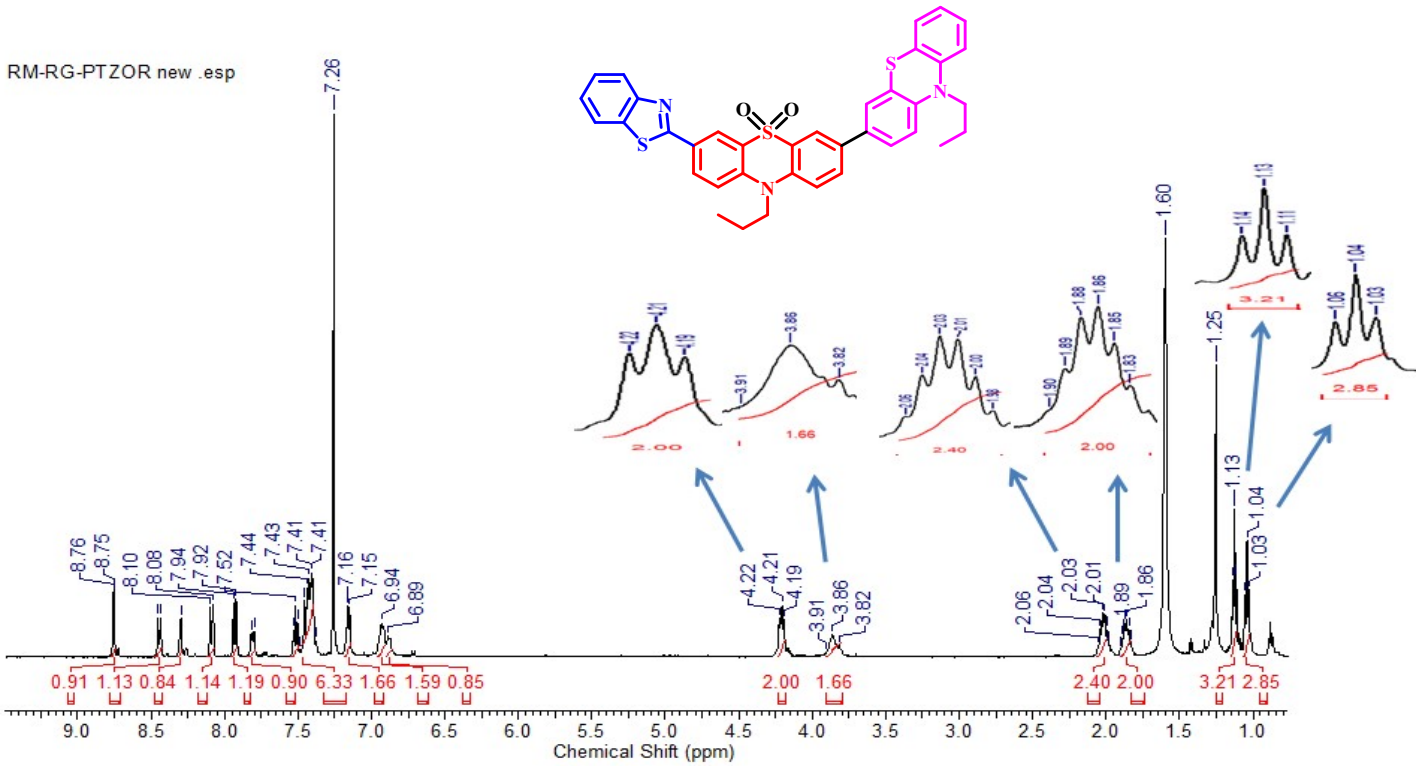


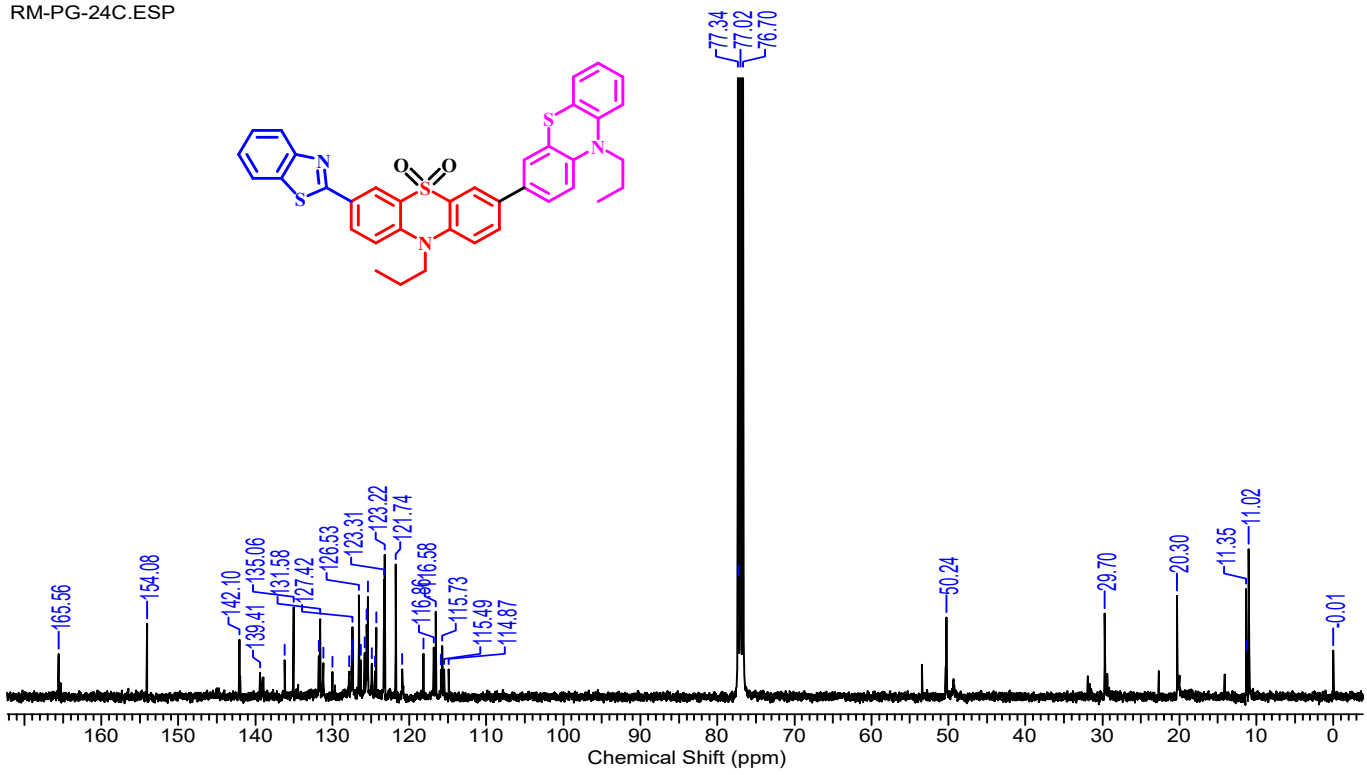
^{1}H NMR and ^{13}C NMR of **BT-PTZ-2**



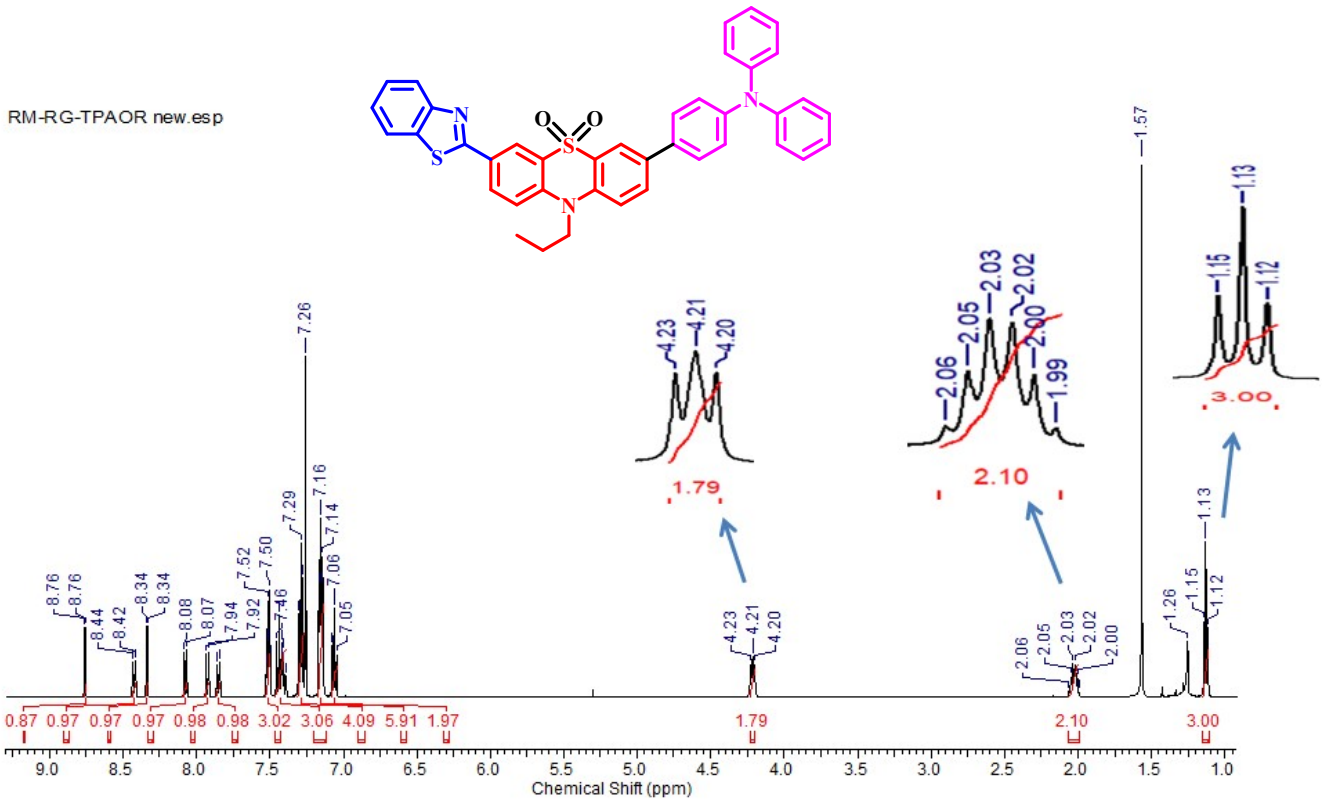


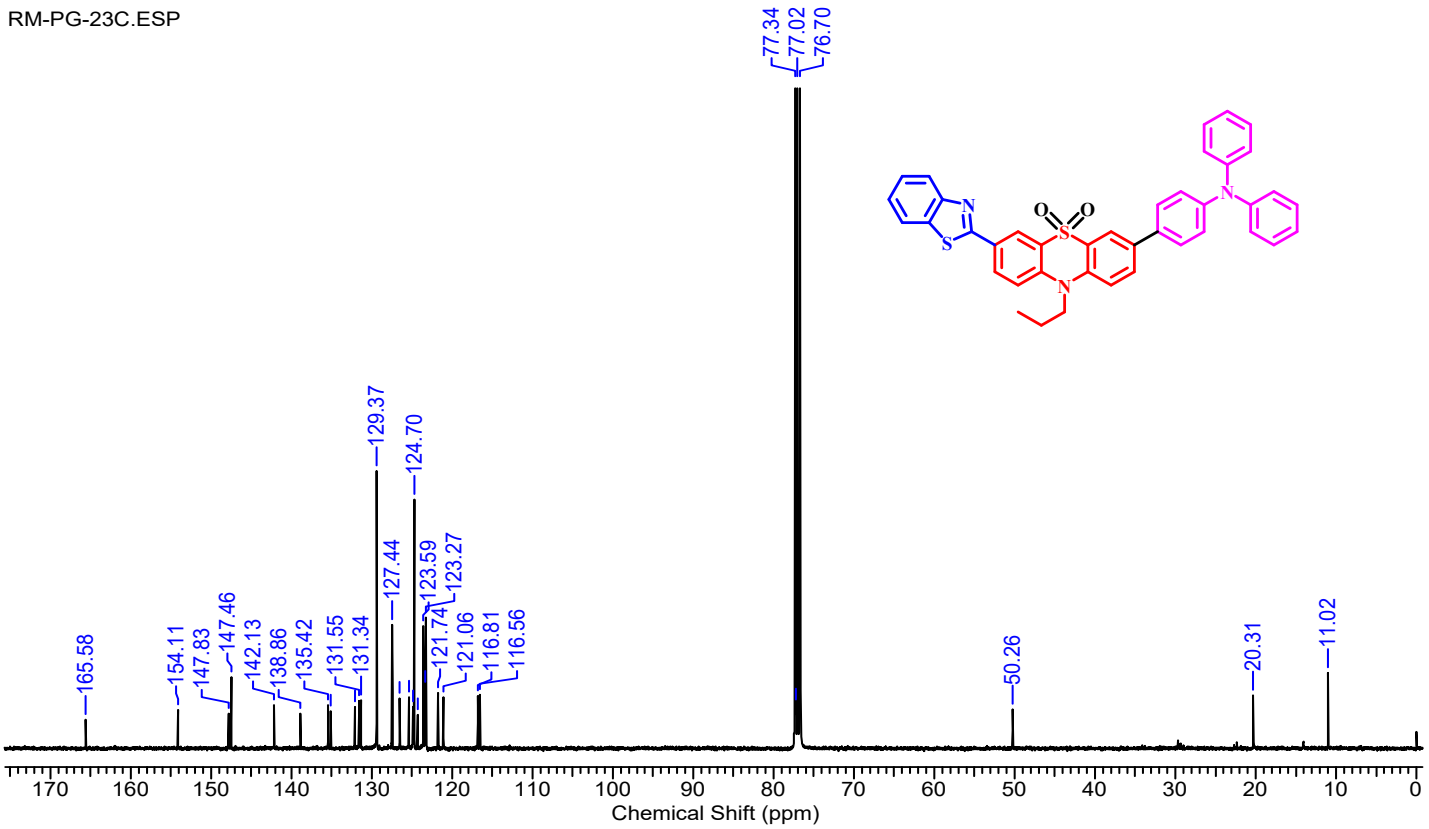
^{1}H NMR and ^{13}C NMR of **BT-PTZO-1**



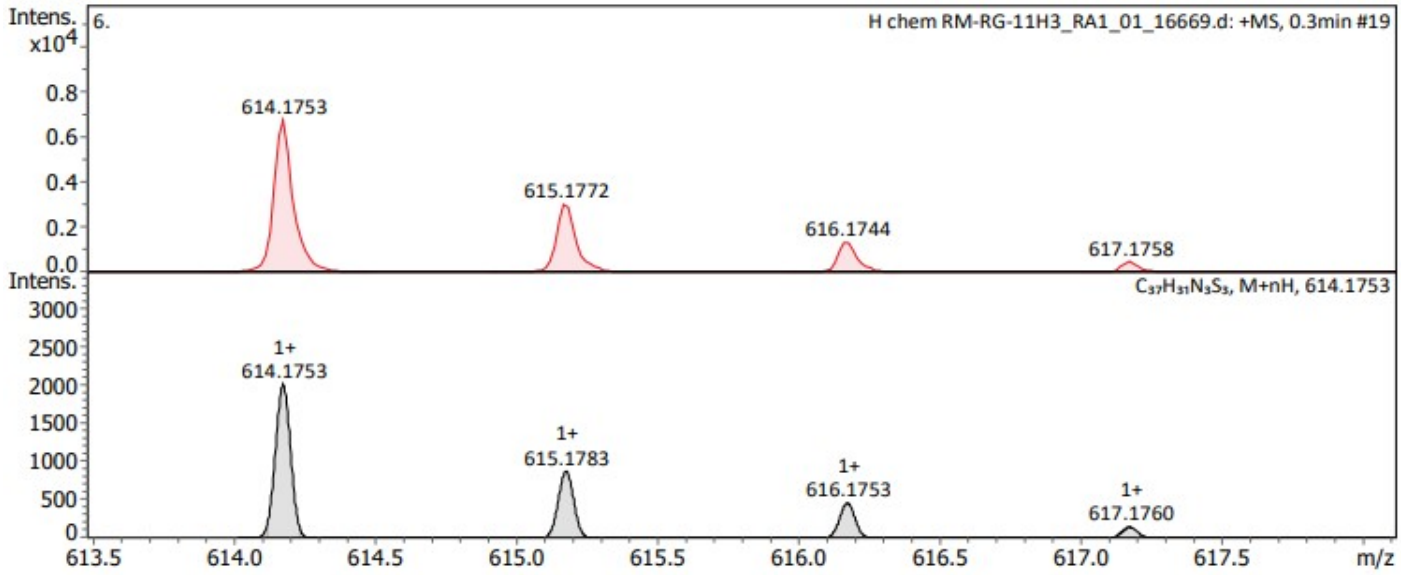


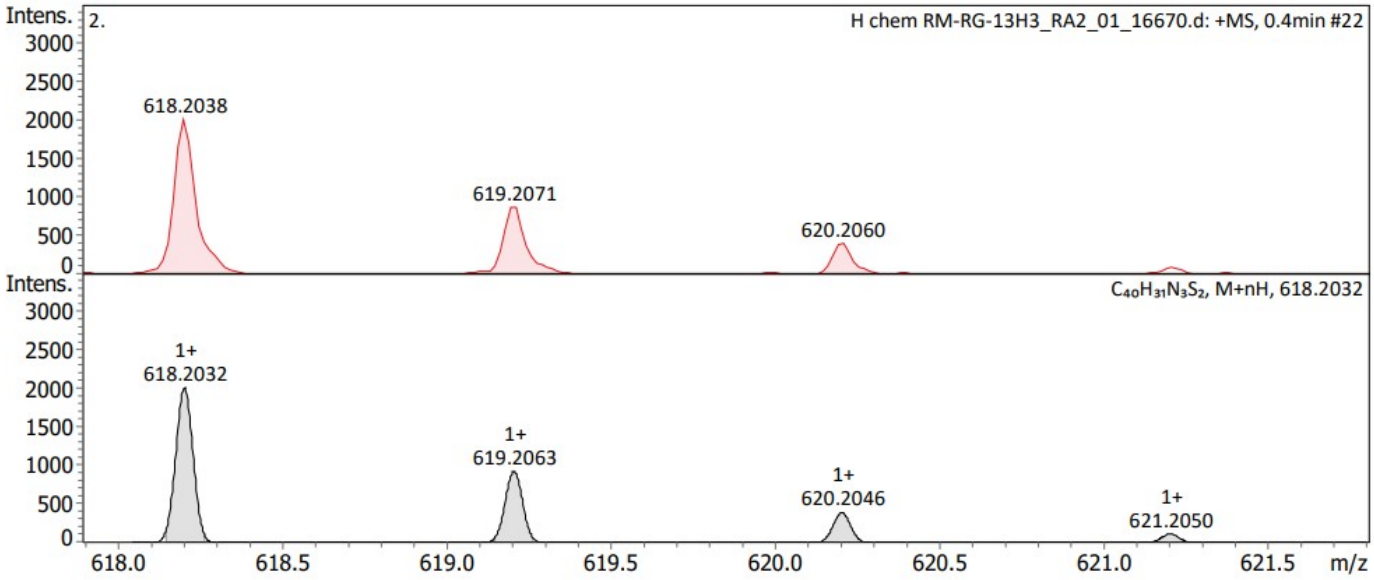
^{1}H NMR and ^{13}C NMR of **BT-PTZO-2**



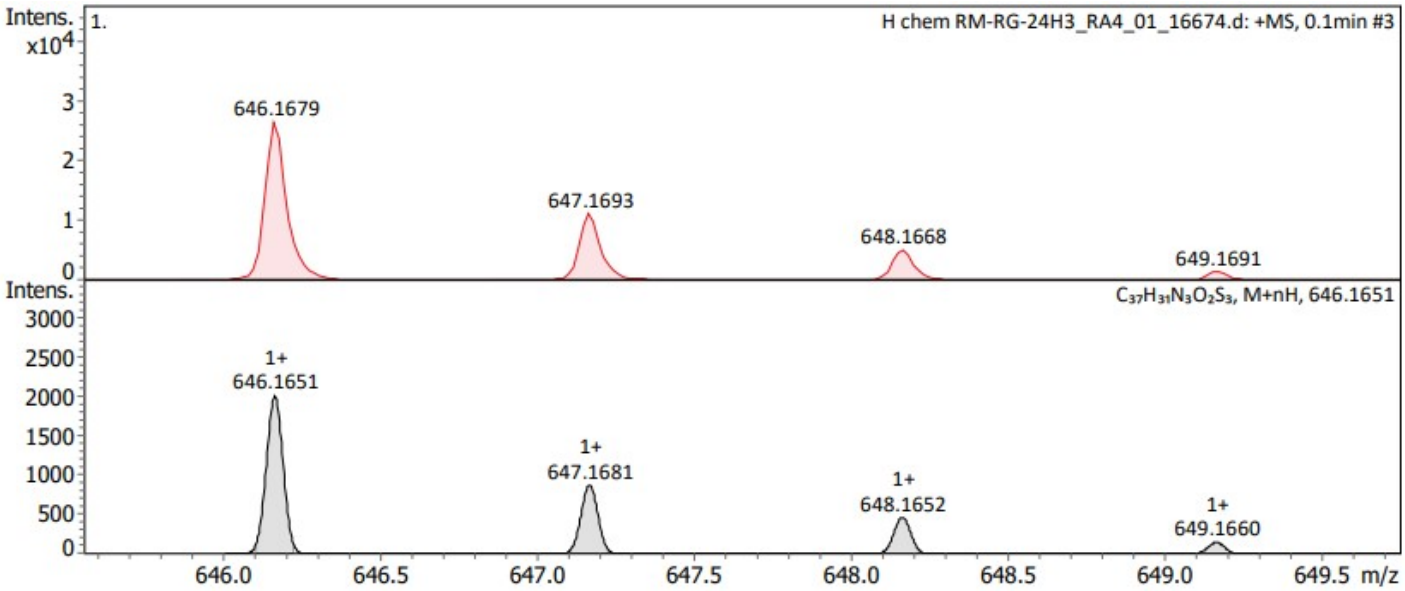


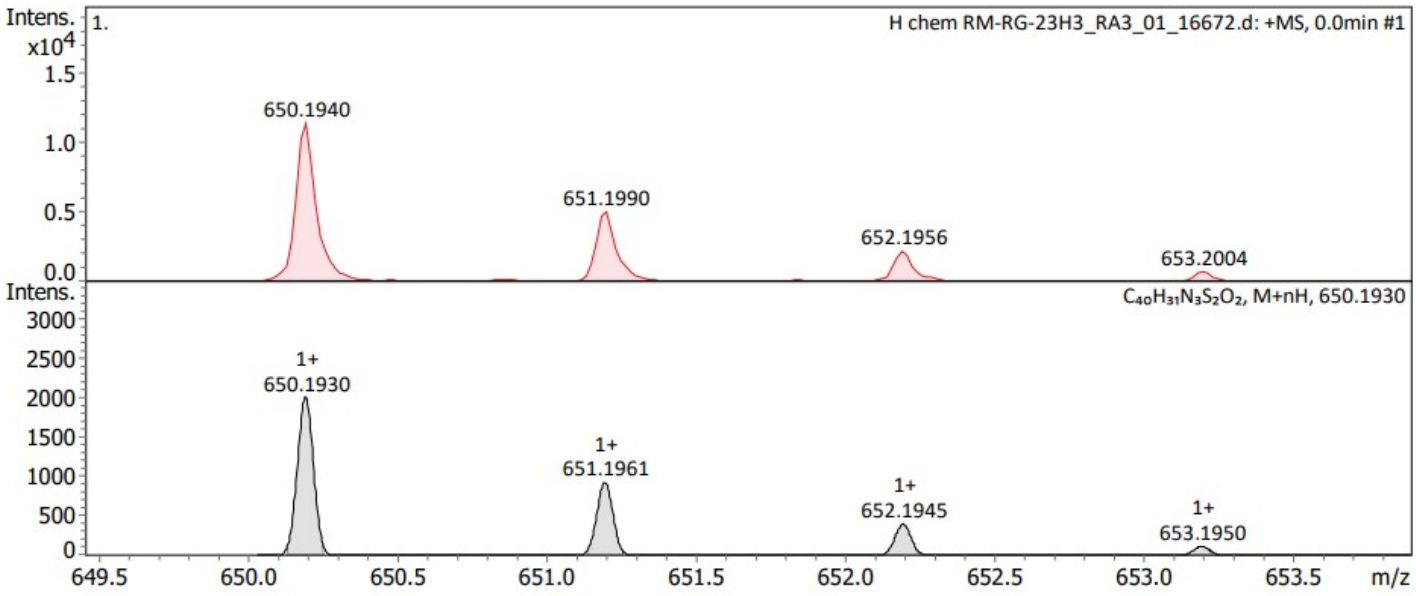
HRMS of **BT-PTZ-1** and **BT-PTZ-2**





HRMS of **BT-PTZO-1** and **BT-PTZO-2**





DFT Calculation data of BT-PTZ-1, BT-PTZ-2, BT-PTZO-1 and BT-PTZO-2

Calculation method: B3LYP/6-31G (d,p) with Gaussian 09

BT-PTZ-1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.522681	-2.744439	-0.024962
2	6	0	8.557244	-2.068187	0.669570
3	6	0	9.776851	-2.690636	0.949498
4	6	0	9.954993	-4.007205	0.525153
5	6	0	8.935916	-4.689804	-0.164860
6	6	0	7.722086	-4.069868	-0.443267
7	6	0	6.461590	-0.810387	0.262580
8	1	0	10.565455	-2.168199	1.481700
9	1	0	10.894750	-4.510442	0.731738
10	1	0	9.100979	-5.714590	-0.483496
11	1	0	6.927990	-4.584777	-0.974044
12	7	0	6.371091	-2.009537	-0.232625
13	16	0	8.023905	-0.446323	1.058764
14	6	0	-1.376047	2.682057	0.924883
15	6	0	-0.076654	3.177507	0.815307
16	6	0	0.892210	2.503977	0.054967
17	6	0	0.521289	1.285589	-0.545678
18	6	0	-0.766982	0.773982	-0.397015
19	6	0	-1.752924	1.472305	0.321190

20	6	0	3.166611	0.796974	-0.577935
21	6	0	3.279814	2.079347	0.005167
22	6	0	4.469834	2.386412	0.687200
23	1	0	4.591531	3.352307	1.162414
24	6	0	5.509744	1.463656	0.766100
25	6	0	5.391591	0.189185	0.192645
26	6	0	4.191486	-0.134835	-0.467427
27	1	0	-2.107580	3.254742	1.486405
28	1	0	0.174975	4.100262	1.325615
29	1	0	-0.998836	-0.190664	-0.837711
30	1	0	6.414196	1.745743	1.296855
31	1	0	4.083046	-1.119918	-0.907505
32	7	0	2.213804	2.994574	-0.107862
33	16	0	1.716447	0.417515	-1.543782
34	6	0	-8.310040	-4.125001	0.295056
35	6	0	-8.075086	-2.882339	0.889277
36	6	0	-7.324117	-1.898589	0.224382
37	6	0	-6.773917	-2.218280	-1.033775
38	6	0	-6.979205	-3.475241	-1.605910
39	6	0	-7.767113	-4.427246	-0.954256
40	6	0	-5.051879	-0.224030	-0.506103
41	6	0	-5.779500	-0.090184	0.692930
42	6	0	-5.151022	0.558345	1.767851
43	1	0	-5.664290	0.658907	2.717223
44	6	0	-3.860791	1.071689	1.641808
45	6	0	-3.130749	0.937041	0.450052
46	6	0	-3.750594	0.262301	-0.615874
47	1	0	-8.905804	-4.862070	0.825320

48	1	0	-8.473463	-2.686181	1.878239
49	1	0	-6.530416	-3.698349	-2.569310
50	1	0	-7.940537	-5.395461	-1.413213
51	1	0	-3.403267	1.550858	2.501976
52	1	0	-3.227836	0.144036	-1.560139
53	7	0	-7.091772	-0.613433	0.775404
54	16	0	-5.859753	-0.964522	-1.914163
55	6	0	-8.015339	-0.078441	1.781661
56	6	0	-8.343833	1.409316	1.572349
57	6	0	-9.063211	1.691830	0.248910
58	6	0	2.477778	4.431079	0.043356
59	6	0	3.409062	4.993847	-1.043409
60	6	0	2.826116	4.891596	-2.457086
61	1	0	1.880306	5.440611	-2.537074
62	1	0	3.518726	5.310660	-3.194150
63	1	0	2.632220	3.850029	-2.730430
64	1	0	4.381647	4.491878	-1.007674
65	1	0	3.595640	6.045698	-0.789785
66	1	0	2.869075	4.664613	1.045276
67	1	0	1.515976	4.939373	-0.043292
68	1	0	-8.945318	-0.642538	1.687831
69	1	0	-7.644036	-0.249712	2.804180
70	1	0	-7.431349	2.011731	1.633305
71	1	0	-8.974984	1.718919	2.415830
72	1	0	-9.283878	2.759320	0.145628
73	1	0	-8.450768	1.388584	-0.605555
74	1	0	-10.012941	1.146739	0.190309

Total Energy (HF) = -2787. 5667306 Hartree

BT-PTZ-2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.879419	-2.567097	-0.792300
2	6	0	8.868624	-2.118263	0.118824
3	6	0	10.091637	-2.780824	0.253916
4	6	0	10.319760	-3.906504	-0.537310
5	6	0	9.346322	-4.362418	-1.445678
6	6	0	8.128893	-3.702762	-1.579559
7	6	0	6.760345	-0.821126	0.013062
8	1	0	10.845315	-2.432799	0.953136
9	1	0	11.263104	-4.436938	-0.448989
10	1	0	9.549856	-5.241536	-2.049579
11	1	0	7.369704	-4.043988	-2.275730
12	7	0	6.718870	-1.817511	-0.821858
13	16	0	8.280089	-0.694772	0.951604
14	6	0	-1.174580	2.262122	1.348094
15	6	0	0.118399	2.775915	1.441954
16	6	0	1.130186	2.352379	0.565711
17	6	0	0.806461	1.353637	-0.372865
18	6	0	-0.479579	0.820544	-0.439822

19	6	0	-1.507123	1.278304	0.403222
20	6	0	3.460402	0.925050	-0.447156
21	6	0	3.526903	1.982025	0.488840
22	6	0	4.686842	2.089621	1.274993
23	1	0	4.771656	2.877059	2.014042
24	6	0	5.742482	1.194724	1.121438
25	6	0	5.670867	0.142178	0.197158
26	6	0	4.500554	0.012399	-0.574077
27	1	0	-1.925129	2.606113	2.053023
28	1	0	0.338158	3.498623	2.219596
29	1	0	-0.690496	0.062900	-1.188304
30	1	0	6.622720	1.319607	1.745013
31	1	0	4.428177	-0.801727	-1.286630
32	7	0	2.446485	2.878957	0.607869
33	16	0	2.052118	0.831655	-1.537587
34	6	0	-4.407121	-1.135653	-0.093630
35	6	0	-5.523968	-0.308264	0.111718
36	6	0	-5.303196	1.045163	0.417426
37	1	0	-6.150891	1.703645	0.576121
38	6	0	-4.008755	1.551342	0.500889
39	6	0	-2.882593	0.731698	0.304643
40	6	0	-3.116223	-0.623903	0.010867
41	1	0	-3.872823	2.608082	0.711588
42	1	0	-2.274934	-1.296355	-0.129007
43	6	0	2.675359	4.212724	1.178144
44	6	0	3.633437	5.075438	0.339618

45	6	0	3.104788	5.381239	-1.065896
46	1	0	2.150628	5.919933	-1.022649
47	1	0	3.814390	6.003279	-1.620987U
48	1	0	2.943717	4.461819	-1.636842
49	1	0	4.615086	4.595224	0.268966
50	1	0	3.787422	6.010621	0.893946
51	1	0	3.024375	4.149716	2.220124
52	1	0	1.706996	4.715161	1.202297
53	7	0	-6.842964	-0.824065	0.011693
54	6	0	-7.963682	-2.997905	-0.192608
55	6	0	-7.149412	-2.111807	0.532723
56	6	0	-6.645080	-2.517136	1.780034
57	6	0	-6.943414	-3.784087	2.282529
58	6	0	-7.760713	-4.660703	1.562401
59	6	0	-8.271150	-4.256389	0.325156
60	1	0	-8.353689	-2.694972	-1.158808
61	1	0	-6.020163	-1.837044	2.349713
62	1	0	-6.544684	-4.080316	3.248705
63	1	0	-7.996210	-5.643414	1.959301
64	1	0	-8.902162	-4.928363	-0.249773
65	6	0	-9.875239	1.456523	-1.878494
66	6	0	-8.595524	1.381268	-2.436734
67	6	0	-7.596546	0.625618	-1.822146
68	6	0	-7.860185	-0.057443	-0.622941
69	6	0	-9.144672	0.026167	-0.060022
70	6	0	-10.142667	0.770553	-0.689804

71	1	0	-10.652152	2.040408	-2.362477
72	1	0	-8.373769	1.902540	-3.363746
73	1	0	-6.608834	0.561501	-2.267040
74	1	0	-9.355537	-0.495289	0.868002
75	1	0	-11.130163	0.824222	-0.240095
76	1	0	-4.553263	-2.185590	-0.325003

Total Energy (HF) = -2503.6975827 Hartree

BT-PTZO-1:

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.371624	2.809143	-0.103889
2	6	0	8.441712	2.139007	-0.748890
3	6	0	9.653567	2.783188	-1.013135
4	6	0	9.786235	4.115289	-0.622792
5	6	0	8.731498	4.791941	0.018359
6	6	0	7.525713	4.150673	0.281072
7	6	0	6.368277	0.842964	-0.364405
8	1	0	10.469869	2.265937	-1.507123
9	1	0	10.718842	4.636154	-0.817618
10	1	0	8.862949	5.829092	0.311288
11	1	0	6.704223	4.659650	0.774353
12	7	0	6.232818	2.051827	0.092183

13	16	0	7.959610	0.493338	-1.103989
14	6	0	-1.471264	-2.714090	-1.011332
15	6	0	-0.181819	-3.229477	-0.936314
16	6	0	0.828287	-2.554579	-0.223462
17	6	0	0.456102	-1.343692	0.392385
18	6	0	-0.826096	-0.808283	0.286985
19	6	0	-1.828784	-1.489572	-0.413800
20	6	0	3.104444	-0.838684	0.418490
21	6	0	3.225661	-2.116510	-0.172748
22	6	0	4.457166	-2.409715	-0.794098
23	1	0	4.616357	-3.370645	-1.266827
24	6	0	5.471594	-1.462821	-0.847363
25	6	0	5.317280	-0.177774	-0.295407
26	6	0	4.106608	0.120435	0.346016
27	1	0	-2.220807	-3.279672	-1.556128
28	1	0	0.040075	-4.150245	-1.462405
29	1	0	-1.019866	0.155119	0.747408
30	1	0	6.394782	-1.729224	-1.353573
31	1	0	3.955349	1.094675	0.797871
32	7	0	2.157751	-3.023472	-0.178714
33	6	0	-8.339549	4.161249	-0.380303
34	6	0	-8.123768	2.905664	-0.954322
35	6	0	-7.368058	1.930064	-0.283310
36	6	0	-6.793387	2.269653	0.958067
37	6	0	-6.979518	3.538885	1.509309
38	6	0	-7.772367	4.483502	0.853060

39	6	0	-5.093555	0.256008	0.437466
40	6	0	-5.844577	0.102412	-0.745693
41	6	0	-5.242124	-0.575299	-1.817697
42	1	0	-5.773781	-0.691807	-2.754918
43	6	0	-3.955003	-1.098490	-1.703808
44	6	0	-3.202764	-0.943392	-0.528745
45	6	0	-3.794777	-0.238999	0.533846
46	1	0	-8.939473	4.892242	-0.914211
47	1	0	-8.540833	2.693525	-1.932203
48	1	0	-6.511115	3.777779	2.459418
49	1	0	-7.930462	5.461788	1.295832
50	1	0	-3.519141	-1.600242	-2.562421
51	1	0	-3.253553	-0.103773	1.465338
52	7	0	-7.152916	0.632758	-0.815154
53	16	0	-5.869900	1.027843	1.845460
54	6	0	-8.098077	0.085946	-1.795201
55	6	0	-8.433526	-1.395367	-1.553691
56	6	0	-9.134102	-1.649652	-0.214518
57	6	0	2.439285	-4.465406	-0.313923
58	6	0	3.271035	-5.034211	0.847553
59	6	0	2.567362	-4.942220	2.206322
60	1	0	1.613898	-5.484083	2.195306
61	1	0	3.190132	-5.383253	2.991168
62	1	0	2.362732	-3.904372	2.485237
63	1	0	4.242971	-4.531527	0.897898
64	1	0	3.480287	-6.083383	0.599789

65	1	0	2.918920	-4.673996	-1.279285
66	1	0	1.478488	-4.979114	-0.322936
67	1	0	-9.022099	0.658454	-1.695039
68	1	0	-7.743703	0.236655	-2.826881
69	1	0	-7.526549	-2.005741	-1.618449
70	1	0	-9.080138	-1.715088	-2.381525
71	1	0	-9.362360	-2.713290	-0.090333
72	1	0	-8.505863	-1.338345	0.625405
73	1	0	-10.078029	-1.095328	-0.149982
74	16	0	1.661479	-0.528760	1.413675
75	8	0	1.381821	0.915210	1.477385
76	8	0	1.799840	-1.292858	2.669427

Total Energy (HF) = -2937.9517787 Hartree

BT-PTZO-2:

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.702382	2.682725	0.660466
2	6	0	8.732142	2.219613	-0.197070
3	6	0	9.947306	2.900148	-0.313210
4	6	0	10.124785	4.058141	0.443150
5	6	0	9.110622	4.528353	1.298561
6	6	0	7.901376	3.851117	1.413568
7	6	0	6.646646	0.888855	-0.119207

8	1	0	10.732499	2.541551	-0.971079
9	1	0	11.060894	4.603332	0.369228
10	1	0	9.276468	5.432596	1.876146
11	1	0	7.110906	4.202015	2.068756
12	7	0	6.555178	1.912878	0.675390
13	16	0	8.200431	0.754865	-0.996050
14	6	0	-1.281620	-2.291568	-1.432201
15	6	0	0.000531	-2.813306	-1.562229
16	6	0	1.051575	-2.369581	-0.735529
17	6	0	0.725504	-1.378915	0.211475
18	6	0	-0.553596	-0.838376	0.325915
19	6	0	-1.596121	-1.289310	-0.492989
20	6	0	3.380350	-0.920649	0.275155
21	6	0	3.456852	-1.974932	-0.662708
22	6	0	4.659993	-2.086258	-1.389869
23	1	0	4.784033	-2.871966	-2.124226
24	6	0	5.688728	-1.171391	-1.209567
25	6	0	5.578305	-0.098605	-0.305599
26	6	0	4.397129	0.011232	0.441817
27	1	0	-2.050248	-2.639200	-2.115710
28	1	0	0.190083	-3.532088	-2.350549
29	1	0	-0.725899	-0.082325	1.084959
30	1	0	6.588080	-1.288022	-1.807073
31	1	0	4.280696	0.814779	1.160819
32	7	0	2.373868	-2.834817	-0.887625
33	6	0	2.627793	-4.179831	-1.438874
34	6	0	3.483153	-5.063233	-0.515748
35	6	0	2.819262	-5.359774	0.833812

36	1	0	1.858274	-5.870509	0.698072
37	1	0	3.457515	-6.010158	1.440428
38	1	0	2.637660	-4.443668	1.403657
39	1	0	4.463508	-4.602025	-0.353841
40	1	0	3.669637	-5.998767	-1.059792
41	1	0	3.077357	-4.105283	-2.437649
42	1	0	1.659436	-4.662509	-1.565624
43	16	0	1.981034	-0.900899	1.375244
44	8	0	1.729288	0.466523	1.860307
45	8	0	2.154794	-1.992380	2.354236
46	6	0	-2.965417	-0.732921	-0.381836
47	6	0	-3.181274	0.626093	-0.090623
48	6	0	-4.465622	1.150953	0.020985
49	1	0	-2.332240	1.289965	0.043404
50	6	0	-5.388494	-1.024602	-0.469299
51	6	0	-5.593080	0.333588	-0.170742
52	1	0	-4.598708	2.202959	0.250004
53	1	0	-6.243750	-1.675926	-0.615514
54	7	0	-6.903843	0.863080	-0.063966
55	6	0	-7.931088	0.102800	0.564216
56	6	0	-7.198102	2.159156	-0.573456
57	6	0	-9.212334	0.030246	-0.006682
58	6	0	-7.679710	-0.580795	1.765445
59	6	0	-6.702383	2.565227	-1.823732
60	6	0	-7.994249	3.049636	0.165856
61	6	0	-10.220364	-0.705350	0.617632
62	1	0	-9.413059	0.553888	-0.935742
63	6	0	-8.688566	-1.327728	2.374586

64	1	0	-6.694531	-0.523174	2.216922
65	6	0	-6.990708	3.838682	-2.315586
66	1	0	-6.092446	1.880753	-2.404367
67	6	0	-8.292090	4.314844	-0.341143
68	1	0	-8.377773	2.744986	1.134115
69	6	0	-9.965325	-1.392536	1.808292
70	1	0	-11.205837	-0.750653	0.162686
71	1	0	-8.477105	-1.849535	3.303631
72	6	0	-7.789763	4.720294	-1.581288
73	1	0	-6.598958	4.136154	-3.284204
74	1	0	-8.908981	4.990844	0.244194
75	1	0	-10.750074	-1.969144	2.288323
76	1	0	-8.017631	5.708133	-1.969780
77	6	0	-4.100219	-1.543467	-0.563592
78	1	0	-3.978149	-2.603043	-0.769129

Total Energy (HF) = -2654.0831653 Hartree

TDDFT calculation data of BT-PTZ-1, BT-PTZ-2, BT-PTZO-1 and **BT-PTZO-2**

BT-PTZ-1:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8344 eV 437.43 nm f=0.2332 <S**2>=0.000

160 -> 162 -0.44791

161 -> 162 0.49221

161 -> 163 0.20311

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2787.00321690

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

Excited State 2: Singlet-A 2.9984 eV 413.50 nm f=0.0231 <S**2>=0.000

160 -> 162 0.40767

160 -> 163 0.17702

161 -> 162 0.18845

161 -> 163 0.48530

161 -> 165 0.11892

Excited State 3: Singlet-A 3.1210 eV 397.26 nm f=0.0264 <S**2>=0.000

160 -> 162 -0.23386

160 -> 163 -0.23099

161 -> 162 -0.43188

161 -> 163 0.43966

Excited State 4: Singlet-A 3.2296 eV 383.90 nm f=0.0365 <S**2>=0.000

160 -> 162 -0.25892

160 -> 163 0.59572

160 -> 164 0.11669

161 -> 162 -0.17139

161 -> 165 0.10975

Excited State 5: Singlet-A 3.2832 eV 377.63 nm f=0.1440 <S**2>=0.000

160 -> 164 -0.10244

160 -> 165 0.16382

161 -> 164 0.61675

161 -> 165 0.23262

Excited State 6: Singlet-A 3.4160 eV 362.96 nm f=0.0525 <S**2>=0.000

160 -> 163 -0.19078

160 -> 164 0.54944

161 -> 165 0.35332

Excited State 7: Singlet-A 3.6848 eV 336.48 nm f=0.0562 <S**2>=0.000

160 -> 164 -0.33383

161 -> 164 -0.28905

161 -> 165 0.45933

161 -> 166 -0.20453

161 -> 168 0.13518

Excited State 8: Singlet-A 3.7195 eV 333.33 nm f=0.0537 <S**2>=0.000

160 -> 164 -0.12054

160 -> 166 0.19754

161 -> 165 0.15556

161 -> 166 0.62891

Excited State 9: Singlet-A 3.8412 eV 322.78 nm f=0.0462 <S**2>=0.000

160 -> 164 0.16204

160 -> 165 0.63024

161 -> 164 -0.11484

161 -> 165 -0.12751

161 -> 168 0.13937

Excited State 10: Singlet-A 4.0223 eV 308.24 nm f=0.0322 <S**2>=0.000

160 -> 165 -0.16324

160 -> 167 -0.14749

160 -> 168 -0.27494

161 -> 167 0.23559

161 -> 168 0.51450

161 -> 169 0.12266

Excited State 11: Singlet-A 4.1065 eV 301.92 nm f=0.7478 <S**2>=0.000

158 -> 162 0.33922

159 -> 162 0.46897

159 -> 163 0.10847

160 -> 167 -0.20563

161 -> 167 0.15838

161 -> 168 -0.18313

Excited State 12: Singlet-A 4.1421 eV 299.33 nm f=0.1756 <S**2>=0.000

158 -> 162 -0.10144

159 -> 162 -0.30892

160 -> 167 -0.29500

161 -> 167 0.45567

161 -> 168 -0.25322

161 -> 169 -0.11781

Excited State 13: Singlet-A 4.1615 eV 297.93 nm f=0.0133 <S**2>=0.000

159 -> 162 0.12211

160 -> 168 0.53456

161 -> 167 0.29730

161 -> 168 0.12591

161 -> 169 0.18903

Excited State 14: Singlet-A 4.2091 eV 294.56 nm f=0.0714 <S**2>=0.000

156 -> 162 -0.21103

157 -> 162 0.12746

158 -> 162 0.52174

159 -> 162 -0.31768

160 -> 168 0.10083

161 -> 169 0.14290

Excited State 15: Singlet-A 4.2409 eV 292.36 nm f=0.0082 <S**2>=0.000

158 -> 162 -0.12476

160 -> 166 -0.35108

160 -> 167 -0.11135

161 -> 166 0.14530

161 -> 168 -0.17817

161 -> 169 0.45171

161 -> 170 0.12832

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

BT-PTZ-2:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7397 eV 452.54 nm f=0.5356 <S**2>=0.000

161 -> 163 -0.17877

162 -> 163 0.67065

162 -> 164 0.10012

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2503.56752342

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

Excited State 2: Singlet-A 3.2290 eV 383.98 nm f=0.0105 <S**2>=0.000

161 -> 163 0.63460

161 -> 164 0.10802

162 -> 163 0.20373

162 -> 164 -0.17514

Excited State 3: Singlet-A 3.3078 eV 374.83 nm f=0.4870 <S**2>=0.000

160 -> 163 0.10722

161 -> 163 0.17699

162 -> 164 0.64961

162 -> 165 0.10609

Excited State 4: Singlet-A 3.4750 eV 356.79 nm f=0.0101 <S**2>=0.000

161 -> 165 0.13766

162 -> 165 0.65438

Excited State 5: Singlet-A 3.6131 eV 343.16 nm f=0.1064 <S**2>=0.000

161 -> 164 0.49665

161 -> 167 0.14038

162 -> 166 0.33504

162 -> 167 -0.26998

Excited State 6: Singlet-A 3.6874 eV 336.23 nm f=0.1455 <S**2>=0.000

160 -> 163 0.13122

161 -> 165 0.20550

161 -> 166 0.15201

162 -> 166 0.39373

162 -> 167 0.31589

162 -> 168 0.34975

Excited State 7: Singlet-A 3.7199 eV 333.30 nm f=0.1526 <S**2>=0.000

160 -> 163 -0.14693

161 -> 164 -0.36900

161 -> 165 -0.13885

161 -> 166 0.14951

162 -> 166 0.40637

162 -> 168 -0.31943

Excited State 8: Singlet-A 3.7918 eV 326.98 nm f=0.0624 <S**2>=0.000

160 -> 163 0.10851

161 -> 164 0.27310

161 -> 165 -0.17895

161 -> 167 -0.10046

162 -> 167 0.44475

162 -> 168 -0.36351

Excited State 9: Singlet-A 3.8830 eV 319.30 nm f=0.7456 <S**2>=0.000

160 -> 163 0.61571

162 -> 167 -0.22999

Excited State 10: Singlet-A 4.0107 eV 309.14 nm f=0.0222 <S**2>=0.000

161 -> 165 0.56051

161 -> 168 -0.19216

162 -> 165 -0.11700

162 -> 168 -0.31152

Excited State 11: Singlet-A 4.1013 eV 302.30 nm f=0.0045 <S**2>=0.000

158 -> 163 0.54543

159 -> 163 0.14339

160 -> 169 -0.10130

161 -> 169 0.13115

162 -> 169 -0.34823

Excited State 12: Singlet-A 4.1376 eV 299.66 nm f=0.0082 <S**2>=0.000

161 -> 170 -0.14196

162 -> 169 -0.11196

162 -> 170 0.64951

Excited State 13: Singlet-A 4.1741 eV 297.03 nm f=0.0449 <S**2>=0.000

159 -> 163 -0.12666

161 -> 165 0.20982

161 -> 166 0.21812

161 -> 168 0.37286

162 -> 165 -0.10732

162 -> 171 0.19993

162 -> 173 -0.13441

162 -> 175 0.31142

162 -> 176 -0.11787

Excited State 14: Singlet-A 4.2029 eV 295.00 nm f=0.0225 <S**2>=0.000

159 -> 163 0.39077

161 -> 167 -0.20016

162 -> 167 -0.14850

162 -> 169 0.32572

162 -> 170 0.10389

162 -> 171 0.16321

162 -> 173 -0.26236

Excited State 15: Singlet-A 4.2178 eV 293.96 nm f=0.0446 <S**2>=0.000

161 -> 166 0.51678

162 -> 166 -0.15225

162 -> 167 -0.12464

162 -> 171 -0.27911

162 -> 172 -0.22566

162 -> 174 0.10556

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

BT-PTZO-1:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.0449 eV 407.18 nm f=0.1370 <S**2>=0.000

169 -> 170 0.68681

169 -> 171 0.11457

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2937.79909426

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

Excited State 2: Singlet-A 3.0941 eV 400.71 nm f=0.0069 <S**2>=0.000

169 -> 170 -0.12018

169 -> 171 0.68682

Excited State 3: Singlet-A 3.4786 eV 356.42 nm f=0.6204 <S**2>=0.000

168 -> 170 0.43343

169 -> 170 0.11108

169 -> 172 0.51450

Excited State 4: Singlet-A 3.5107 eV 353.17 nm f=0.1162 <S**2>=0.000

168 -> 170 0.32759

168 -> 171 0.49351

169 -> 172 -0.33736

Excited State 5: Singlet-A 3.5497 eV 349.28 nm f=0.1595 <S**2>=0.000

168 -> 170 -0.41848

168 -> 171 0.46629

169 -> 172 0.25354

Excited State 6: Singlet-A 3.8620 eV 321.04 nm f=0.0396 <S**2>=0.000

167 -> 170 0.10437

167 -> 172 -0.10173

169 -> 173 -0.23182

169 -> 174 0.59876

169 -> 175 0.11922

169 -> 177 -0.13796

Excited State 7: Singlet-A 4.0107 eV 309.14 nm f=0.1108 <S**2>=0.000

165 -> 170 0.16771

167 -> 170 0.52355

168 -> 172 0.12218

169 -> 173 0.26564

169 -> 175 0.17202

169 -> 177 -0.20864

Excited State 8: Singlet-A 4.0263 eV 307.94 nm f=0.0335 <S**2>=0.000

165 -> 170 -0.28054

167 -> 170 -0.24467

167 -> 171 -0.28015

168 -> 173 -0.15420

169 -> 172 -0.10549

169 -> 173 0.39719

169 -> 174 0.17424

169 -> 175 0.10015

Excited State 9: Singlet-A 4.0487 eV 306.23 nm f=0.0475 <S**2>=0.000

167 -> 170 -0.22210

167 -> 171 0.40986

169 -> 174 -0.13912

169 -> 175 0.26564

169 -> 176 0.16375

169 -> 177 -0.34553

Excited State 10: Singlet-A 4.0668 eV 304.87 nm f=0.0165 <S**2>=0.000

165 -> 170 0.18242

167 -> 171 0.37962

169 -> 173 0.40121

169 -> 174 0.21139

169 -> 175 -0.14955

169 -> 176 -0.13239

169 -> 177 0.20423

Excited State 11: Singlet-A 4.0819 eV 303.74 nm f=0.0773 <S**2>=0.000

165 -> 170 0.46191

166 -> 170 -0.31216

167 -> 170 -0.25455

167 -> 171 -0.25180

169 -> 177 -0.10938

Excited State 12: Singlet-A 4.1947 eV 295.57 nm f=0.2347 <S**2>=0.000

165 -> 170 0.13699

166 -> 170 0.15160

167 -> 170 -0.13784

167 -> 172 0.11255

168 -> 172 0.58316

169 -> 173 -0.12894

169 -> 178 0.11517

169 -> 180 -0.10170

Excited State 13: Singlet-A 4.2667 eV 290.59 nm f=0.1260 <S**2>=0.000

164 -> 170 0.11362

165 -> 170 0.27150

166 -> 170 0.55974

168 -> 172 -0.22703

Excited State 14: Singlet-A 4.2894 eV 289.05 nm f=0.0359 <S**2>=0.000

166 -> 171 0.13613

167 -> 172 0.11672

168 -> 172 -0.16222

168 -> 173 0.14483

169 -> 175 0.26182

169 -> 177 0.16838

169 -> 178 0.46355

169 -> 180 -0.18467

Excited State 15: Singlet-A 4.3162 eV 287.25 nm f=0.0210 <S**2>=0.000

162 -> 170 -0.12372

165 -> 171 0.26057

166 -> 171 0.48472

167 -> 171 -0.12329

168 -> 173 0.21636

169 -> 175 -0.13020

169 -> 178 -0.18273

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.

BT-PTZO-2:

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8772 eV 430.92 nm f=0.3916 <S**2>=0.000

170 -> 171 0.69357

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2653.96254158

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

Excited State 2: Singlet-A 3.2175 eV 385.35 nm f=0.0372 <S**2>=0.000

170 -> 172 0.68341

170 -> 174 0.12749

Excited State 3: Singlet-A 3.3459 eV 370.55 nm f=0.7139 <S**2>=0.000

169 -> 171 -0.21104

170 -> 171 0.11905

170 -> 173 0.65354

Excited State 4: Singlet-A 3.5384 eV 350.40 nm f=0.4770 <S**2>=0.000

169 -> 171 0.65554

170 -> 173 0.20904

Excited State 5: Singlet-A 3.6144 eV 343.03 nm f=0.0161 <S**2>=0.000

169 -> 172 -0.12690

170 -> 174 0.59447

170 -> 175 -0.30951

Excited State 6: Singlet-A 3.8244 eV 324.19 nm f=0.0202 <S**2>=0.000

169 -> 172 0.63364

169 -> 173 0.11014

170 -> 175 -0.20095

Excited State 7: Singlet-A 3.8725 eV 320.17 nm f=0.1820 <S**2>=0.000

170 -> 176 0.68748

Excited State 8: Singlet-A 3.9280 eV 315.64 nm f=0.0149 <S**2>=0.000

169 -> 172 0.16428

169 -> 174 0.10287

170 -> 174 0.31968

170 -> 175 0.57639

Excited State 9: Singlet-A 4.0462 eV 306.42 nm f=0.0070 <S**2>=0.000

167 -> 171 0.67192

169 -> 177 -0.11020

Excited State 10: Singlet-A 4.1296 eV 300.24 nm f=0.0378 <S**2>=0.000

168 -> 171 0.34700

169 -> 173 0.59630

Excited State 11: Singlet-A 4.2060 eV 294.78 nm f=0.2175 <S**2>=0.000

168 -> 171 0.58980

169 -> 173 -0.32417

Excited State 12: Singlet-A 4.2766 eV 289.91 nm f=0.0029 <S**2>=0.000

170 -> 178 0.25874

170 -> 180 -0.23348

170 -> 181 0.57222

170 -> 182 0.11827

Excited State 13: Singlet-A 4.3090 eV 287.73 nm f=0.0098 <S**2>=0.000

170 -> 178 0.54357

170 -> 180 -0.12042

170 -> 181 -0.32761

170 -> 182 0.17220

170 -> 184 -0.15846

Excited State 14: Singlet-A 4.3269 eV 286.54 nm f=0.0251 <S**2>=0.000

169 -> 174 -0.26044

169 -> 175 -0.13732

170 -> 178 0.13853

170 -> 183 0.45783

170 -> 184 0.33211

Excited State 15: Singlet-A 4.3882 eV 282.54 nm f=0.0030 <S**2>=0.000

160 -> 171 -0.13836

168 -> 172 0.23289

169 -> 174 0.47272

169 -> 175 0.14410

170 -> 175 -0.12810

170 -> 177 -0.20176

170 -> 183 0.18177

170 -> 184 0.16528

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 15 LETran= 280.