

Supporting Information

Photophysical origin of the reduced photodynamic therapy activity of temocene compared to

Foscan®: Insights from theory

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Cartesian coordinates (Angstrom) for the ground (S_0) and second electronic excited state (S_2) optimized structures of *m*-THPPo calculated at PBE0/6-31G(d) level of theory.

m-THPPo (S_0)

C	-5.78501400	5.27853600	-0.69112800
C	-4.57095500	4.59496900	-0.70813000
C	-4.38642800	3.45662100	0.08107000
C	-5.43826200	3.01197700	0.89740900
C	-6.64683600	3.69719300	0.90510200
C	-6.83129000	4.82733800	0.11505000
H	-3.77999900	4.94843200	-1.36243800
H	-5.29156400	2.15520500	1.54740200
H	-7.78153000	5.35851800	0.12628100
C	-2.85318400	1.34977400	0.01528500
C	-1.84605500	3.37913600	0.10733900
C	-0.85675500	2.35987100	0.09877400
H	-1.65263700	4.44159700	0.17438500
C	-3.08719600	2.77368800	0.06787600
N	-1.50587100	1.17004400	0.04601700
C	1.35104900	3.63543300	0.23619000
C	2.60934000	1.75995100	0.19505600
H	1.18610300	-0.33811200	0.01694700
C	2.65544700	3.22172500	0.29027900
H	0.98892300	4.65390500	0.30126600
C	0.54990200	2.44687700	0.14350500
N	1.32328800	1.34431600	0.11749100
C	3.83762400	4.08307800	0.41452400
C	3.93257700	5.23498700	-0.37155100

C	4.85988800	3.79952600	1.33475300
C	5.02592200	6.08963600	-0.24810400
H	3.16509400	5.46757500	-1.10326200
C	5.94857200	4.65521600	1.44907200
H	4.77712000	2.93118000	1.98099100
C	6.04281100	5.79915800	0.66270700
H	6.73343300	4.43700700	2.16838500
H	6.89939600	6.46458700	0.75732900
O	5.05092200	7.18784400	-1.04769300
H	5.85982800	7.68486900	-0.86768400
O	-5.89285500	6.37316000	-1.48756100
H	-6.77997100	6.74384000	-1.39020000
H	-7.45709400	3.35496200	1.54318100
C	3.74690500	0.93262000	0.12828500
H	4.68603600	1.47817700	0.17181400
C	3.89280400	-0.44524200	0.00266400
H	4.91950000	-0.80030500	-0.01248800
C	3.17747800	-2.89239900	-0.22008600
C	0.94687400	-2.48819600	-0.12749500
C	1.93766900	-3.50204500	-0.21858600
H	1.74440200	-4.56210200	-0.31712500
C	2.94237400	-1.47253700	-0.10290600
N	1.59464000	-1.29858600	-0.05786900
C	-1.26297200	-3.76782000	-0.18833600
C	-2.52162400	-1.89391300	-0.10331300
H	-1.09768100	0.20776500	-0.00024000
C	-2.56957700	-3.35762700	-0.15812800

H	-0.90170200	-4.78853900	-0.20620500
C	-0.46064800	-2.57798400	-0.12905600
N	-1.23414600	-1.47637400	-0.07726200
C	-3.75523800	-4.22215200	-0.17618600
C	-4.81914900	-4.00619300	0.70546200
C	-3.81724400	-5.30671900	-1.06540200
C	-5.92845200	-4.85082500	0.69540600
H	-4.78442800	-3.20330200	1.43512000
C	-4.92351600	-6.14513300	-1.06610500
H	-3.00265900	-5.46826500	-1.76488900
C	-5.98513100	-5.92482700	-0.19275500
H	-4.96949100	-6.97985200	-1.76050700
H	-6.85151800	-6.58418400	-0.19989200
C	4.47630400	-3.56798900	-0.32855400
C	4.71195400	-4.72921000	0.41212300
C	5.47522400	-3.09315200	-1.19304500
C	5.92498400	-5.40582300	0.29995100
H	3.96282000	-5.10709100	1.10113100
C	6.68310500	-3.77160800	-1.29568200
H	5.28614000	-2.21804900	-1.80672900
C	6.91880400	-4.92480600	-0.55392000
H	7.45179000	-3.40612000	-1.97122900
H	7.86803800	-5.45091900	-0.63975900
C	-3.65583100	-1.06048100	-0.15489500
H	-4.59132400	-1.60354500	-0.26186200
C	-3.80117100	0.32224300	-0.10843600
H	-4.82348700	0.68133000	-0.18809100

O	-6.92117900	-4.58136100	1.58364300
H	-7.61424200	-5.24757300	1.48580100
O	6.08438500	-6.52416100	1.05374000
H	6.96465700	-6.88787600	0.89038600

m-THPPo (S_2)

C	-5.8820179	5.2012428	-0.6726919
C	-4.6555499	4.5410644	-0.6985638
C	-4.4567159	3.3782183	0.0533724
C	-5.5108756	2.8903279	0.8447152
C	-6.7323104	3.5520027	0.8604615
C	-6.9296690	4.7043330	0.1055389
H	-3.8648301	4.9307342	-1.3321840
H	-5.3539848	2.0210834	1.4752753
H	-7.8891216	5.2185145	0.1242670
C	-2.8856433	1.3098843	-0.0062553
C	-1.9087972	3.3552942	0.0540399
C	-0.9084992	2.3579842	0.0546212
H	-1.7351020	4.4214016	0.1129559
C	-3.1483988	2.7204189	0.0316558
N	-1.5286471	1.1536259	0.0195369
C	1.2866933	3.6669742	0.1848309
C	2.5834705	1.8123037	0.1871728
H	1.1940568	-0.3259224	0.0086653
C	2.6040445	3.2761344	0.2694768

H	0.9030288	4.6780195	0.2387805
C	0.5143624	2.4673492	0.1018024
N	1.3011614	1.3736114	0.0999607
C	3.7664620	4.1519294	0.4051703
C	3.8259910	5.3429677	-0.3292120
C	4.8156123	3.8495214	1.2940442
C	4.9080613	6.2085507	-0.1919834
H	3.0408913	5.5933046	-1.0357362
C	5.8913664	4.7181057	1.4239305
H	4.7582530	2.9576951	1.9097307
C	5.9505088	5.8959497	0.6844833
H	6.6933490	4.4841257	2.1188402
H	6.7983556	6.5708822	0.7892214
O	4.9019731	7.3391478	-0.9436581
H	5.7082292	7.8402367	-0.7608001
O	-6.0031509	6.3197980	-1.4329601
H	-6.8994811	6.6683144	-1.3342687
H	-7.5420685	3.1754103	1.4795622
C	3.7360938	1.0023363	0.1174965
H	4.6674042	1.5607127	0.1519265
C	3.9046388	-0.3760548	-0.0006714
H	4.9385241	-0.7108811	-0.0019712
C	3.2401416	-2.8391918	-0.2051679
C	1.0018186	-2.4830488	-0.0999103
C	2.0022835	-3.4771857	-0.1794091

H	1.8274803	-4.5414738	-0.2629286
C	2.9776329	-1.4315933	-0.1087728
N	1.6208663	-1.2788859	-0.0571007
C	-1.1918833	-3.7965455	-0.1499450
C	-2.4950856	-1.9476705	-0.0741753
H	-1.1021339	0.1992633	-0.0122973
C	-2.5144208	-3.4136711	-0.1134873
H	-0.8065598	-4.8083525	-0.1544989
C	-0.4217356	-2.5950654	-0.0988378
N	-1.2115503	-1.5043288	-0.0526479
C	-3.6721099	-4.3043115	-0.1261879
C	-4.7920256	-4.0634575	0.6802957
C	-3.6568386	-5.4535735	-0.9390079
C	-5.8757789	-4.9393198	0.6668200
H	-4.8179559	-3.2177339	1.3599156
C	-4.7385465	-6.3214921	-0.9435322
H	-2.8018427	-5.6368791	-1.5824810
C	-5.8544968	-6.0728681	-0.1477771
H	-4.7238994	-7.2020101	-1.5803044
H	-6.7022165	-6.7558954	-0.1570415
C	4.5468740	-3.4907781	-0.3182123
C	4.7971681	-4.6655506	0.3985407
C	5.5467358	-2.9834666	-1.1658688
C	6.0222749	-5.3188594	0.2829554
H	4.0493032	-5.0702606	1.0735672

C	6.7670539	-3.6386180	-1.2714263
H	5.3461824	-2.1038068	-1.7692945
C	7.0162829	-4.8030348	-0.5512442
H	7.5341070	-3.2476311	-1.9344495
H	7.9743627	-5.3123425	-0.6402852
C	-3.6425468	-1.1310408	-0.1593363
H	-4.5686146	-1.6858803	-0.2812345
C	-3.8087898	0.2524520	-0.1344324
H	-4.8364394	0.5902729	-0.2385406
O	-6.9235690	-4.6437808	1.4785018
H	-7.5905913	-5.3381262	1.3918876
O	6.1961694	-6.4501687	1.0134349
H	7.0855528	-6.7925079	0.8510336

Cartesian coordinates (Angstrom) for the optimized ground (S_0) structures of *m*-THPC calculated at PBE0/6-31G(d) level of theory.

m-THPC (S_0)

C	-4.17650400	-1.17368200	-0.16381500
C	-4.32384900	0.17387000	-0.16224600
C	-2.98557000	0.72606000	-0.18870800
C	-2.75061000	-1.42329500	-0.17170100
H	-4.95170500	-1.92716400	-0.15906200
H	-5.24348300	0.74187600	-0.14131800
N	-2.04596900	-0.25865300	-0.18862500

C	-2.72686100	2.11511300	-0.19933500
C	-1.46250400	2.70380200	-0.19583400
C	-1.15613300	4.09638000	-0.26763100
C	0.78002200	2.92478200	-0.20917200
C	0.20442200	4.23167100	-0.26976800
H	-1.89537000	4.88251100	-0.32040700
H	0.77679300	5.14670100	-0.32088600
N	-0.25634600	2.04152900	-0.16267100
H	-0.17330200	1.03231300	-0.12964600
C	-3.89220900	3.04502300	-0.23475200
C	-4.15306500	3.88739600	0.84651200
C	-4.73162900	3.08658100	-1.35630200
C	-5.24015400	4.76179600	0.81382800
H	-3.52356000	3.86470600	1.73074800
C	-5.81138200	3.96072700	-1.38255700
H	-4.52645600	2.43648900	-2.20115500
C	-6.07342300	4.80073500	-0.30394400
H	-6.45857000	3.99549200	-2.25489000
H	-6.92157400	5.48305400	-0.32996500
O	-5.43701200	5.54911400	1.90374000
H	-6.22431900	6.09013200	1.75804500
C	2.15651000	2.63226500	-0.21778500
C	3.07619500	3.81297100	-0.24564500
C	3.43886700	4.44570800	0.94284400
C	3.58140800	4.29258600	-1.46057500
C	4.30164300	5.54305800	0.92473400
H	3.05316200	4.09605800	1.89592500

C	4.43979200	5.38643000	-1.47342400
H	3.29076400	3.80823000	-2.38842400
C	4.80571900	6.01564000	-0.28724600
H	4.82912200	5.76008400	-2.41684000
H	5.47799000	6.87205900	-0.30271500
O	4.61323500	6.10916200	2.11957100
H	5.20766700	6.85536600	1.96543300
C	2.73708700	1.36559200	-0.21133100
C	4.24433400	1.19346700	-0.21555500
C	4.41021400	-0.32054800	-0.17785800
H	4.69818900	1.69991700	0.64296000
H	4.68655300	1.64978000	-1.10771900
C	2.97602500	-0.81496700	-0.19468500
H	4.97182800	-0.71610700	-1.03087900
H	4.93155300	-0.67061800	0.71960800
N	2.07655800	0.18998200	-0.20350200
C	2.68283900	-2.17674800	-0.20157900
C	3.83456500	-3.13280200	-0.19606400
C	4.41893000	-3.52036300	1.00922400
C	4.33468500	-3.64781500	-1.39848000
C	5.49541100	-4.40885900	1.01951300
H	4.04045200	-3.14248500	1.95452100
C	5.40638500	-4.53396200	-1.38288500
H	3.87602100	-3.35237600	-2.33765200
C	5.99257800	-4.91797100	-0.18060800
H	5.79325700	-4.93458600	-2.31619200
H	6.83151100	-5.61208700	-0.17380100

O	6.01506800	-4.74284600	2.22936500
H	6.74176900	-5.36564000	2.09535900
C	1.40144800	-2.75865600	-0.21043300
C	1.12092800	-4.15930500	-0.16849100
C	-0.83588900	-3.02440500	-0.20663400
C	-0.23708900	-4.31954200	-0.16050100
H	1.87718400	-4.93020100	-0.13242600
H	-0.79032900	-5.24647000	-0.11368500
N	0.19942100	-2.11808300	-0.23809100
H	0.06423400	-1.11412700	-0.25626300
C	-2.19720600	-2.72282100	-0.18220700
C	-3.12938800	-3.88730800	-0.16482200
C	-3.22751600	-4.73226600	-1.27818600
C	-3.90739000	-4.14852600	0.96351500
C	-4.09617600	-5.81716400	-1.25208200
H	-2.62922000	-4.52536300	-2.16024900
C	-4.77608800	-5.23998800	0.98339600
H	-3.84219200	-3.51181900	1.84034500
C	-4.87267400	-6.07879100	-0.12740800
H	-4.17618600	-6.46792000	-2.11877900
H	-5.55137100	-6.93009300	-0.11197600
O	-5.49958600	-5.43777000	2.11627400
H	-6.04989500	-6.22362900	2.00070000