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Computational and experimental studies supporting the anti-breast cancer potential of N-hydroxyphthalimide

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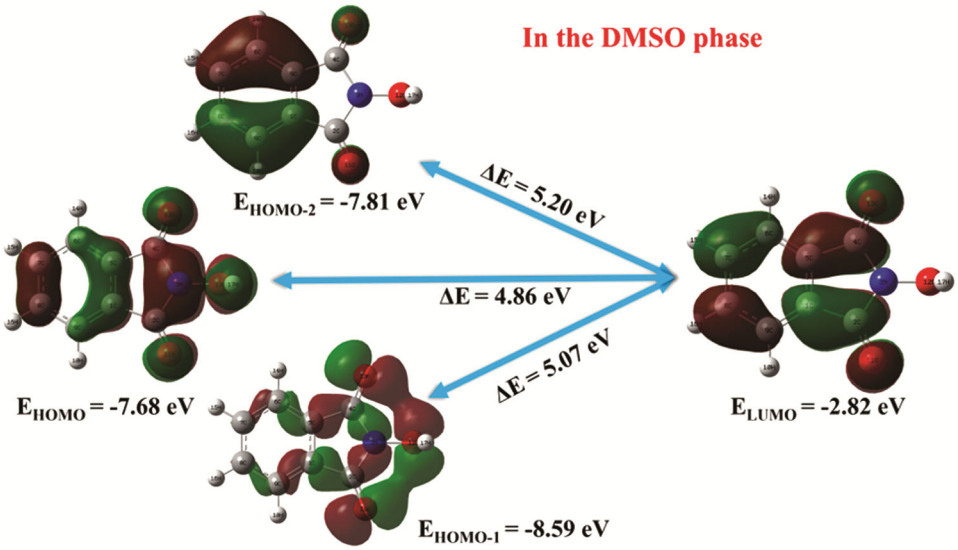
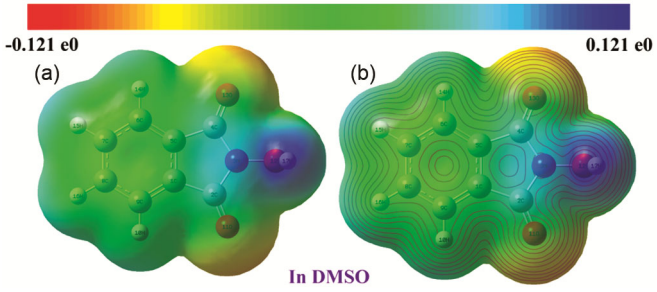
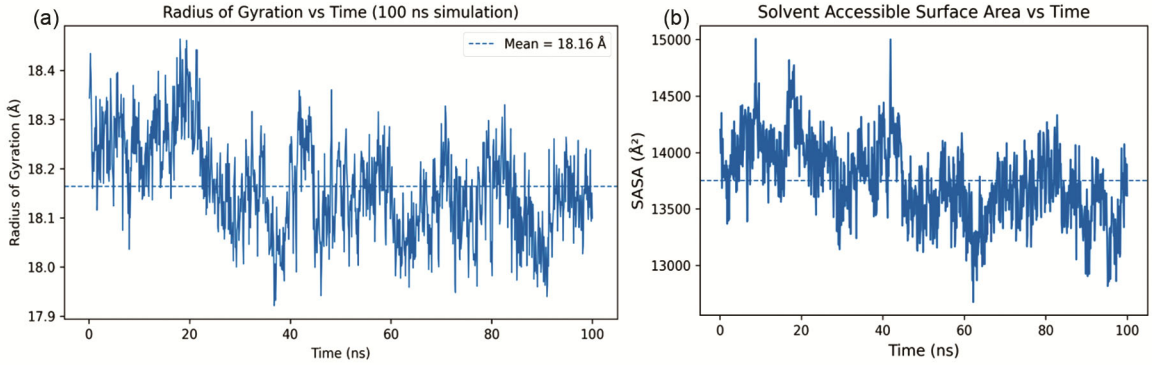
Supplementary data



Suppl. Fig. S1 — Molecular orbital energies for N-Hydroxyphthalimide in the DMSO phase



Suppl. Fig. S2 — (a) Molecular Electrostatic potential and (b) Contours with electrostatic potential surface in the DMSO phase for N-Hydroxyphthalimide



Suppl. Fig. S3 — Molecular Dynamics Simulations of 7KBS-NHP: (a) Radius of Gyration (R_g), and (b) Solvent Accessible Surface Area

Suppl. Table S1 — The vibrational assignments based on PED calculations for N-Hydroxyphthalimide

S.No	Observed wavenumber (cm^{-1})		Wavenumber (cm^{-1})		IR Intensity (Km mol^{-1})	Raman activity (Å^4 amu^{-1})	Assignment with PED (%)
	FT-IR	FT- Raman	Calculated	Scaled			
1	3490 (vw)	-	3760	3615	82	156	υOH(100)
2	3100 (ms)	3088 (ms)	3202	3078	7	273	υCH (99)
3	-	3070 (ms)	3199	3075	2	25	υCH (98)
4	-	3068 (ms)	3187	3064	5	117	υCH (96)
5	-	3047 (vw)	3175	3052	1	59	υCH (97)
6	1783 (w)	1779 (vs)	1844	1773	97	151	υC=O(95)
7	1715 (vs)	1720 (ms)	1799	1729	756	26	υC=O(96)
8	-	1598 (ms)	1647	1583	13	35	υCC(94)
9	1581 (w)	-	1641	1577	2	6	υCC(93)
10	-	1460 (vw)	1496	1438	7	3	υNO(92)
11	1450 (s)	-	1492	1434	1	1	υCC(91)
12	1375 (ms)	1390 (ms)	1450	1394	117	2	υCC(90)
13	-	1355 (vw)	1386	1332	26	14	υCC(89)
14	1272 (ms)	-	1330	1278	7	26	υCC(88)
15	1218 (vw)	-	1310	1260	1	0	υCC(87)
16	1170 (ms)	1186 (ms)	1210	1163	78	58	υCN(85)
17	-	1155 (vw)	1188	1142	1	3	υCN(86)
18	1130 (ms)	1139 (vw)	1181	1136	18	11	bOH (84)
19	1074 (ms)	1083 (vw)	1131	1088	74	4	bNO(83)
20	-	1030 (ms)	1090	1048	47	4	bCH(82)
21	-	980 (ms)	1036	996	4	27	bCH (81)
22	971 (ms)	-	1010	971	0	0	bCH (80)
23	-	-	984	946	3	0	bCH (79)
24	-	910 (vw)	979	941	110	8	Rasymd(77)
25	878 (ms)	-	909	874	0	0	Rsymd(76)
26	-	820 (vw)	887	853	36	3	Rtrigd(78)
27	780 (ms)	-	798	767	1	0	Rasymd(75)
28	-	760 (vw)	798	767	14	1	Rsymd(74)
29	-	700 (ms)	718	690	82	2	Rtrigd(72)
30	692 (vs)	-	718	690	4	0	bC=O(71)
31	-	-	715	687	15	18	bC=O(69)

32	520 (ms)	-	680	654	0	0	ωCH(68)
33	-	600 (ms)	604	581	1	10	ωCH(66)
34	510 (ms)	-	526	505	10	1	ωCH(64)
35	-	466 (ms)	473	454	1	9	ωCH(65)
36	446 (vw)	-	464	446	0	0	ωC=O(63)
37	-	-	413	397	0	0	ωC=O(62)
38	-	-	342	328	11	1	ωNO (60)
39	-	-	303	292	7	1	ωOH(61)
40	-	-	243	233	0	1	tRsymd(58)
41	-	-	240	231	1	3	tRasymd(59)
42	-	-	214	206	86	4	tRtrigd(57)
43	-	-	145	140	2	1	tRsymd(55)
44	-	-	137	132	0	1	tRasymd(54)
45	-	-	115	110	6	1	Butterfly(53)

Suppl. Table S2 — Global reactivity descriptors for N-Hydroxyphthalimide.

Molecular Properties	B3LYP/*6-311++G(d,p)*					
	In the gas phase			In DMSO		
	H-1→L	H→L	H-4→L	H-2→L	H→L	H-1→L
HOMO (eV)	-	-7.81	-	-	-7.68	-
LUMO (eV)	-2.79	-2.79	-2.79	-2.82	-2.82	-2.82
HOMO-1	-7.81	-	-	-	-	-7.89
HOMO-2	-	-	-	-8.02	-	-
HOMO-4	-	-	-8.59	-	-	-
ΔE (eV)	5.03	5.02	5.81	5.20	4.86	5.07
Ionization potential (I) (eV)	7.81	7.81	8.59	8.02	7.68	7.89
Electron affinity (A) (eV)	2.79	2.79	2.79	2.82	2.82	2.82
Global hardness (η) (eV)	2.51	2.51	2.90	2.60	2.43	2.54
Global softness (S) (eV^{-1})	0.20	0.20	0.17	0.19	0.21	0.20
Electronegativity (χ) (eV)	5.30	5.30	5.69	5.42	5.25	5.35
Chemical potential (μ) (eV)	-5.30	-5.30	-5.69	-5.42	-5.25	-5.35
Global electrophilicity (ω) (eV)	5.59	5.59	5.58	5.65	5.67	5.65

Suppl. Table S3 — Pharmacokinetic prediction of N-Hydroxyphthalimide

ADMET properties		NHP	ADMET properties		NHP
Absorption	Caco-2 permeability (log Papp in 10^{-6} cm/s)	1.167	Excretion	Total Clearance (log mL/min/kg)	-0.098
	Human Intestinal absorption (%)	87.2		Renal OCT2 substrate	No
	Skin Permeability (log Kp)	-3.2			
Distribution	VDss (human) (log L/kg)	-0.133	Toxicity	AMES toxicity test	No
	Fraction unbound (human)	0.522		hERG I inhibitor	No
	BBB permeability (log BB)	-0.268		hERG II inhibitor	No
				Oral Rat Acute Toxicity (LD_{50}) (mol/kg)	2.176
	CNS permeability (log PS)	-2.846		Oral Rat Chronic Toxicity (log mg/kg_bw/day)	2.554
Metabolism	CYP2D6 substrate	No		Skin Sensitisation	No
	CYP3A4 substrate	No		T.Pyriformis toxicity (log ug/L)	0.37
	CYP1A2 inhibitor	No		Minnow toxicity (log mM)	2.048
	CYP2C19 inhibitor	No		Hepatotoxicity	No
	CYP2C9 inhibitor	No			
	CYP2D6 inhibitor	No			
	CYP3A4 inhibitor	No			