Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Studies on the interaction of 2-amino-3-hydroxy-anthraquinone with surfactant micelles reveal its nucleation in human MDA-MB-231 breast adinocarcinoma cells

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Table S1: Some important bond lengths, bond angles of AQ

(a) Bond length (Å)

Types of bond	Bond length (Å)	Types of bond	Bond length (Å)	Types of bond	Bond length (Å)
N23-H24	1.015	O26-H27	0.970	C2-H17	1.084
N23-H25	1.013	C11-H12	1.084	C1-H16	1.085
N23-C14	1.394	C15-H20	1.085	C6-H19	1.085
C14-C13	1.419	C8-O21	1.234	C5-H18	1.084
O26-C13	1.365	C7-O22	1.235	C1-C6	1.399

(b) Bond angle (degree)

Types of Bond	BA (°)	Types of Bond	BA (°)	Types of Bond	BA (°)
H25-N23-H24	110.22	H27-O26-C13	110.01	C3-C7-O22	120.79
H25-N23-C14	114.46	C13-C11-H12	119.49	C4-C8-O21	120.85
H24-N23-C14	115.58	C14-C15-H20	119.79	C4-C5-H18	118.83
N23-C14-C13	113.08	C9-C8-O21	121.43	C6-C1-H16	120.08
C14-C13-O26	120.68	C10-C7-O22	121.52	C1-C2-H17	120.81

Table S2. TDDFT results for low lying excited state of AQ.

Excited state	ΔE (eV)	Oscillator strength (f)	Contribution	Coefficient	Eigen values
1	2.846	0.0263	(HOMO-4) → LUMO (HOMO -2) → LUMO HOMO → LUMO	0.1089 -0.10805 0.68707	0.9970
2	3.075	0.0012	(HOMO -5) → (LUMO+1) (HOMO -2) → LUMO (HOMO -1) → LUMO HOMO → LUMO	-0.10653 0.67464 0.12443 0.11057	0.9705
3	3.336	0.002	(HOMO -5) → LUMO (HOMO -4) → LUMO (HOMO -2) → LUMO	0.67145 0.11391 -0.15454	0.9403

Table S3. Comparison of theoretical and experimental IR stretching frequency of AQ.

υ_{cal} (cm^{-1})	υ_{scaled} (cm^{-1})	Intensity	PED (%)	Interpretation	υ_{expt} (cm^{-1})
3758	3612	174	S_1(100)	υ_{sym} (O_{236}-H_{27})	3730
3643	3502	50	S_2(96)	υ_{sym} (N_{23}-H_{24}), υ_{sym} (N_{23}-H_{25})	3486
3541	3403	86	S_3(96)	υ_{sym} (N_{23}-H_{24}), υ_{sym} (N_{23}-H_{25})	3356
3225	3100	22	S_7(81)	υ_{asym} (C_1-H_{16})	3073
3210	3085	17	S_9 (94)	υ_{sym} (C_{15}-H_{20})	2804
1701	1635	480	S_{10}(-64)	υ_{asym} (O_{21}-C_8)	1656
1688	1622	26	S_{11}(72)	υ_{asym} (O_{22}-C_7)	1613
1665	1600	32	S_{32}(72), S_{53}(10)	β (H_{25}-N_{23} –H_{24}), τ (H_{24}-N_{23}-C_{14}-C_{13}),	1588
1621	1558	306	S_{20}(-34), S_{27}(14)	υ_{sym} (C_1-C_2), β (C_{13}-C_{11} –C_{10})	1543
1613	1550	336	S_{17}(43), S_{48}(-14)	υ_{sym} (C_1-C_6), υ_{sym} (C_5-C_6), β(C_{15}-C_{14} –N_{23})	-
1599	1537	392	S_{20}(41), S_{41}(-12)	υ_{sym} (C_1-C_6), υ_{sym} (C_1-C_2), β (C_1-C_2 –C_3), β (C_4-C_5 –C_6), β (C_{10}-C_{11} –C_{13}), β (C_9-C_{15} –C_{14})	-
1541	1481	135	S_{22}(-14), S_{35}(-14)	υ_{sym} (N_{23}-C_{14}), β (H_{17}-C_2 –C_1)	1466
1488	1430	4	S_{18}(-25)	υ_{sym} (C_4-C_5)	1448
1472	1415	61	S_{15}(27)	υ_{sym} (C_{10}-C_{11})	1362
1415	1360	11	S_{12}(53)	υ_{sym} (C_9-C_{10})	1287

1371	1317	120	$S_{13}(70)$	$\upsilon_{sym}(C_4\text{-}C_5)$, $\upsilon_{sym}(C_1\text{-}C_2)$, $\upsilon_{sym}(C_3\text{-}C_4)$, $\upsilon_{sym}(C_5\text{-}C_6)$	1269
1352	1299	1344	$S_{21}(-59)$	$\upsilon_{sym}(C_8\text{-}C_9)$, $\upsilon_{sym}(C_9\text{-}C_{15})$, $\upsilon_{sym}(N_{23}\text{-}C_{14})$	-
1314	1263	365	$S_{25}(16)$	$\upsilon_{sym}(C_7\text{-}C_{10})$, $\upsilon_{sym}(C_9\text{-}C_8)$	-
1289	1239	709	$S_{24}(-24)$	$\upsilon_{sym}(N_{23}\text{-}C_{14})$, $\upsilon_{sym}(C_4\text{-}C_8)$	-
1283	1233	69	$S_{23}(13)$, $S_{24}(-14)$	$\upsilon_{sym}(O_{26}\text{-}C_{13})$, $\upsilon_{sym}(N_{23}\text{-}C_{14})$, $\upsilon_{sym}(C_4\text{-}C_8)$,	1197
1236	1188	93	$S_{23}(13)$	$\upsilon_{sym}(O_{26}\text{-}C_{13})$	-
1193	1146	100	$S_{30}(11)$	$\beta(H_{27}\text{-}O_{26}\text{–}C_{13})$	1115
1130	1086	97	$S_{34}(15)$	$\beta(H_{16}\text{-}C_1\text{–}C_2)$, $\beta(H_{19}\text{-}C_6\text{–}C_1)$	1085
1104	1061	36	$S_{37}(-11)$	$\beta(H_{20}\text{-}C_{15}\text{–}C_{14})$, $\beta(H_{12}\text{-}C_{11}\text{–}C_{13})$	968
979	941	80	$S_{19}(25)$	$\upsilon_{sym}(C_1\text{-}C_6)$, $\upsilon_{sym}(C_5\text{-}C_6)$	891
925	889	56	$S_{59}(82)$	$\tau(H_{12}\text{-}C_{11}\text{-}C_{13}\text{-}C_{14})$, $\tau(H_{20}\text{-}C_{15}\text{-}C_{14}\text{-}N_{23})$	879
797	766	96	$S_{22}(-18)$, $S_{23}(-10)$	$\upsilon_{sym}(N_{23}\text{-}C_{14})$, $\upsilon_{sym}(C_9\text{-}C_{15})$, $\upsilon_{sym}(O_{26}\text{-}C_{13})$	812
750	720	46	$S_{43}(10)$, $S_{44}(24)$	$\beta(C_1\text{-}C_6\text{–}C_5)$, $\beta(C_{13}\text{-}C_{11}\text{–}C_{10})$	793
731	702	175	$S_{55}(-39)$, $S_{70}(-41)$	$\tau(H_{16}\text{-}C_1\text{-}C_6\text{-}C_5)$, $\tau(H_{19}\text{-}C_6\text{-}C_1\text{-}C_2)$, $\tau(O_{21}\text{-}C_4\text{-}C_9\text{-}C_8)$, $\tau(O_{22}\text{-}C_3\text{-}C_{10}\text{-}C_7)$	740
723	695	108	$S_{53}(-10)$, $S_{72}(54)$	$\tau(H_{24}\text{-}N_{23}\text{-}C_{14}\text{-}C_{13})$, $\tau(H_{25}\text{-}N_{23}\text{-}C_{14}\text{-}C_{13})$, $\tau(N_{23}\text{-}C_{13}\text{-}C_{15}\text{-}C_{14})$, $\tau(O_{26}\text{-}C_{11}\text{-}C_{14}\text{-}C_{13})$,	714
678	651	77	$S_{29}(10)$, $S_{43}(12)$, $S_{45}(30)$	$\beta(C_{15}\text{-}C_{14}\text{–}N_{23})$, $\beta(C_{10}\text{-}C_9\text{–}C_{15})$, $\beta(C_{11}\text{-}C_{13}\text{–}O_{26})$, $\beta(C_1\text{-}C_6\text{–}C_5)$, $\beta(C_9\text{-}C_8\text{–}O_{21})$, β	676

				(H_9-C_{15}–C_{14}),	
673	646	360	S_{53}(-42), S_{72}(-13)	τ (H_{24}-N_{23}-C_{14}-C_{13}), τ (H_{25}-N_{23}-C_{14}-C_{13}), τ (N_{23}-C_{13}-C_{15}-C_{14}), τ (O_{26}-C_{11}-C_{14}-C_{13}),	615
624	599	95	S_{41}(62)	β (C_1-C_2–C_3), β (C_4-C_5–C_6), β (C_{10}-C_{11}–C_{13}), β (C_9-C_{15}–C_{14})	-
606	582	50	S_{45}(-21), S_{48}(12)	β (C_9-C_8–O_{21}), β (C_{10}-C_7–O_{22})	-
512	492	155	S_{30}(11)	β (H_{27}-O_{26}–C_{13}),	-