Appendix A

Supplementary Information

Design, synthesis and photophysical properties of 8-hydroxyquinoline-functionalized tripodal molecular switch as a highly selective sequential pH sensor in aqueous solution

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Experimental

Synthesis of 1,1,1 Tris (aminomethyl)ethane (TAME)

The synthesis of 1,1,1 Tris (aminomethyl)ethane (TAME) **1c** was carried out under multistep reactions as detailed below:

1.1 1,1,1–tris[(4-tolylsulfonyl)methyl]ethane (**1a**)

1,1,1–Tris(hydroxymethyl)ethane (10 g, 0.083 mol) was dissolved in THF (45 mL) and added to 70 ml of aqueous solution of NaOH (16.66 g, 0.41 mol). The solution was cooled in an ice–water bath and THF solution of tosyl chloride (47.66 g, 0.25 mol) was added dropwise with stirring for about 2 hours. During addition, the solution became pale yellow while an off–white slurry appeared progressively; the mixture was stirred for 4 hrs further at 0°C. The reaction mixture was poured into ice water (250 mL) and extracted with toluene (3×100 mL). The combined organic phases were washed with water (2×100 mL), dried over anhydrous $MgSO_4$, and concentrated on rotary evaporator. The thick jelly residue was poured into methanol (500 mL) with stirring. The resulting suspension was filtered on a Buchner funnel and the precipitate was washed with water followed by methanol and diethyl ether, and dried under vacuum. The pure product was isolated as a white solid after recrystallization from

n–propanol. Yield: 87%, mp: 105ºC. FTIR (KBr): 3023, 2954, 1889, 1686, 1605, 1478, 1458, 1367, 1302, 1290, 1153, 1099, 1012, 991, 941, 882, 805, 797, 701, 677, 532, 498 cm^{-1}.

1.2 1,1,1–tris(azidomethyl)ethane (**1b**)

Solution of 1,1,1–tris[(4-tolylsulfonyl)methyl]ethane (**1a**) (25.0 g, 42.76 mmol) and sodium azide (29.58 g, 357.17 mmol) in dry DMSO (250 mL) was stirred under N_2 atmosphere at 125ºC for 8 hrs. The reaction mixture was poured into cold water (1.5 L), after cooling to room temperature. The aqueous solution was extracted with ethyl acetate (3×250 mL). The organic phases were washed with water (2×100 mL), dried over anhydrous $NaSO_4$ and reduced on a rotary evaporator. The residual oil shows strong absorption band at 2123 cm^{-1} in the infrared spectrum which confirms the presence of an azide and the product was used readily for the next step.

1.3 1,1,1–tris(aminomethyl)ethane **(1c)**

1,1,1–tris(azidomethyl)ethane (**1b**) (21g, 107.69 mmol) in freshly distilled THF(60 mL) was added to a vigrously stirred mixture of $LiAlH_4$ (18.63g 374.39mmol) in dry THF(300 mL) over a period of 3h under dry nitrogen. After complete addition, the mixture was refluxed for 12h, cooled, followed by addition of water (22 mL), then by NaOH (34mL of 15% aqueous solution) and again with water (50mL). The resulting slurry was stirred for 25 min and filtered through sintered glass G4 funnel under vaccum. The white residue was further refluxed over night with THF to extract remaining product. The solvent was removed from all combined filtrates to give pale yellow oil. The crude product was taken up in super dry EtOH (300mL) and concentrated HCl (12mL) was added dropwise to precipitate the compound as the trihydrochloride salt. The pure product was reprecipitated from an ethanol solution to yield a fine white powder. Yield:9.1g, 77.77mmol (72.22%), decomposes at ≥ 250˚C. ^{1}HNMR (D_2O) (δ): 3.24(s, 6H, $3CH_2$) 1.20 (s, 3H ,CH_3).

2. 8-hydroxyquinoline-5-methylchloride hydrochloride **(2a)**

Dry hydrogen chloride gas was passed through a solution of 8–hydroxyquinoline **2** (14.51g, 0.1 mol) and formaldehyde (20 mL, 40%) in 37% hydrochloric acid (50 mL) for 5 hours at 60°C. After filtration, the yellow solid product was washed several times with acetone and dried in vaccuo to afford **2a** (14.01g) in 96.5% yield. m.p. 281°C; ^{1}HNMR (300 MHz, D_2O, 25°C, TMS): δ = 8.81 (d, $^{3}J_{H,H}$ = 4.1 Hz, 1H, Ar–H), 8.51 (d, $^{3}J_{H,H}$ = 8.5 Hz, 1H, Ar–H), 7.59 (dd, $^{3}J_{H,H}$ = 8.2 Hz, $^{3}J_{H,H}$ = 4.1 Hz, 1H, Ar–H), 7.40 (d, $^{3}J_{H,H}$ = 7.8 Hz, 1H, Ar–H), 7.01 (d, $^{3}J_{H,H}$ = 7.8 Hz, 1H, Ar–H), 4.82 (s, 2H, ArCH2Cl) ppm. IR (ATR) ν(cm^{-1}) = 3032, 2731, 1564, 1510, 1439, 1330, 1006. Elemental Analysis calcd (%) for $C_{10}H_9NOCl_2$: 52.20 C, 3.94 H, 6.09 N; found: 52.29 C, 3.89 H, 6.13 N; MS (ES^{+}), m/Z (I,%) = 320.07$[M+1]^{+}$(90).

Table S1: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_9)^{+6}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis - (methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_9: coordinates in Angstrom

C	0.8875000000	-2.3305760000	-0.7017980000
C	1.9506970000	-2.4082620000	0.4304770000
C	-0.4764800000	-2.6676250000	-0.0261170000
C	0.8287260000	-0.9141280000	-1.3547580000
C	1.2246570000	-3.3667650000	-1.8011370000
N	-1.5117650000	-3.1109100000	-0.9711310000
N	3.2522170000	-1.8195860000	0.0699120000
N	1.1532650000	0.1636230000	-0.4062600000
C	0.9924430000	1.5369250000	-0.9224280000
C	4.3238190000	-2.0347720000	1.0650250000
C	-2.8590890000	-3.3003290000	-0.4028760000
C	5.6232300000	-1.3843060000	0.6440860000
C	-0.4354900000	2.0498150000	-0.9387440000
C	-3.7618250000	-2.0797020000	-0.5316520000
C	-3.4810870000	-1.0989190000	-1.4629850000
C	-4.2996610000	0.0406100000	-1.6183020000
C	-5.4140560000	0.2316760000	-0.8213580000
C	-4.9451580000	-1.9416540000	0.2666730000
C	-5.7798860000	-0.7751480000	0.1284500000
N	-6.9113040000	-0.5897080000	0.8797940000
C	-7.2603840000	-1.5262500000	1.7563850000
C	-6.5170620000	-2.7141860000	1.9570910000
C	-5.3696940000	-2.9154860000	1.2167690000
C	6.6771000000	-2.1627680000	0.1982040000
C	7.9012990000	-1.5972320000	-0.2279810000
C	8.0837080000	-0.2275340000	-0.2112320000
C	5.7932790000	0.0403350000	0.6716860000
C	7.0308930000	0.6286970000	0.2436860000
N	7.2469080000	1.9821880000	0.2564950000
C	6.2737980000	2.7785640000	0.6875990000
C	5.0205340000	2.2961350000	1.1390970000
C	4.7845580000	0.9366210000	1.1273650000
C	-3.0670660000	3.1214680000	-1.0447330000
C	-2.3179780000	3.0327250000	-2.1949630000
C	-1.0049570000	2.4986610000	-2.1216740000
C	-2.5163560000	2.7127150000	0.2039500000
C	-1.2068270000	2.1536390000	0.2675280000
C	-0.7659610000	1.7423580000	1.5579770000
C	-1.5908690000	1.9140960000	2.6551120000
C	-2.8727070000	2.4933550000	2.4864960000
N	-3.3262650000	2.8780420000	1.2963340000
O	-4.3850420000	3.5542450000	-1.0435370000
O	9.2552930000	0.3799380000	-0.6155950000
O	-6.2014930000	1.3589920000	-0.9055540000
H	1.5755990000	-1.8600500000	1.3038410000

H	2.0477190000	-3.4689820000	0.7342430000
H	-0.3041910000	-3.4280680000	0.7638830000
H	-0.8355750000	-1.7621390000	0.4761120000
H	1.5091420000	-0.8892570000	-2.2298650000
H	-0.1840160000	-0.7603950000	-1.7424020000
H	2.2347110000	-3.2118510000	-2.1991480000
H	1.1756380000	-4.3920470000	-1.4116680000
H	0.5314440000	-3.2781260000	-2.6443410000
H	1.6015140000	2.1845470000	-0.2761870000
H	1.4056950000	1.6458930000	-1.9433600000
H	3.9704370000	-1.6210530000	2.0190870000
H	4.5051610000	-3.1101610000	1.2478560000
H	-3.3226920000	-4.1501440000	-0.9255830000
H	-2.7886380000	-3.6014350000	0.6573210000
H	-2.5967880000	-1.2179870000	-2.0775130000
H	-4.0368070000	0.7857390000	-2.3605140000
H	-8.1651550000	-1.3401810000	2.3281390000
H	-6.8524730000	-3.4484850000	2.6819020000
H	-4.7919360000	-3.8224180000	1.3540310000
H	6.5691910000	-3.2435170000	0.1770980000
H	8.7016900000	-2.2484450000	-0.5686610000
H	6.4836360000	3.8439430000	0.6820260000
H	4.2664050000	2.9935180000	1.4875310000
H	3.8327880000	0.5410830000	1.4599870000
H	-2.7362760000	3.3544540000	-3.1412640000
H	-0.4239140000	2.4373860000	-3.0373580000
H	0.1983350000	1.2602710000	1.6518710000
H	-1.2725620000	1.6026700000	3.6437660000
H	-3.5359180000	2.6364500000	3.3330500000
H	-4.6635650000	3.5915350000	-0.0895680000
H	9.9140440000	-0.2819630000	-0.9039460000
H	-5.7244100000	2.0911280000	-1.3603120000
H	3.5639070000	-2.0811430000	-0.8635820000
H	-1.2189880000	-3.9241700000	-1.5018910000
H	2.1072620000	0.0075680000	-0.0734180000
H	8.5775950000	2.5620840000	-0.2109090000
H	-7.7597630000	0.6654810000	0.7063440000
H	-4.7182630000	3.4837600000	1.1515960000
H	3.1068930000	-0.8219350000	0.0117420000
H	-1.5934320000	-2.3918180000	-1.6731090000
H	0.5511200000	0.0677800000	0.3984250000

Table S2: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_8)^{+5}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis - (methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_8: coordinates in Angstrom

C	0.8924890000	-2.3263530000	-0.6968260000
C	1.9556860000	-2.4040390000	0.4354490000
C	-0.4714910000	-2.6634020000	-0.0211450000
C	0.8337150000	-0.9099050000	-1.3497860000
C	1.2296460000	-3.3625420000	-1.7961650000
N	-1.5067760000	-3.1066870000	-0.9661590000
N	3.2572060000	-1.8153630000	0.0748840000
N	1.1582540000	0.1678460000	-0.4012880000
C	0.9974320000	1.5411480000	-0.9174560000
C	4.3288080000	-2.0305490000	1.0699970000
C	-2.8541000000	-3.2961060000	-0.3979040000
C	5.6282190000	-1.3800830000	0.6490580000
C	-0.4305010000	2.0540380000	-0.9337720000
C	-3.7568360000	-2.0754790000	-0.5266800000
C	-3.4760980000	-1.0946960000	-1.4580130000
C	-4.2946720000	0.0448330000	-1.6133300000
C	-5.4090670000	0.2358990000	-0.8163860000
C	-4.9401690000	-1.9374310000	0.2716450000
C	-5.7748970000	-0.7709250000	0.1334220000
N	-6.9063150000	-0.5854850000	0.8847660000
C	-7.2553950000	-1.5220270000	1.7613570000
C	-6.5120730000	-2.7099630000	1.9620630000
C	-5.3647050000	-2.9112630000	1.2217410000
C	6.6820890000	-2.1585450000	0.2031760000
C	7.9062880000	-1.5930090000	-0.2230090000
C	8.0886970000	-0.2233110000	-0.2062600000
C	5.7982680000	0.0445580000	0.6766580000
C	7.0358820000	0.6329200000	0.2486580000
N	7.2518970000	1.9864110000	0.2614670000
C	6.2787870000	2.7827870000	0.6925710000
C	5.0255230000	2.3003580000	1.1440690000
C	4.7895470000	0.9408440000	1.1323370000
C	-3.0620770000	3.1256910000	-1.0397610000
C	-2.3129890000	3.0369480000	-2.1899910000
C	-0.9999680000	2.5028840000	-2.1167020000
C	-2.5113670000	2.7169380000	0.2089220000
C	-1.2018380000	2.1578620000	0.2725000000
C	-0.7609720000	1.7465810000	1.5629490000
C	-1.5858800000	1.9183190000	2.6600840000
C	-2.8677180000	2.4975780000	2.4914680000
N	-3.3212760000	2.8822650000	1.3013060000
O	-4.3800530000	3.5584680000	-1.0385650000
O	9.2602820000	0.3841610000	-0.6106230000
O	-6.1965040000	1.3632150000	-0.9005820000

H	1.5805880000	-1.8558270000	1.3088130000
H	2.0527080000	-3.4647590000	0.7392150000
H	-0.2992020000	-3.4238450000	0.7688550000
H	-0.8305860000	-1.7579160000	0.4810840000
H	1.5141310000	-0.8850340000	-2.2248930000
H	-0.1790270000	-0.7561720000	-1.7374300000
H	2.2397000000	-3.2076280000	-2.1941760000
H	1.1806270000	-4.3878240000	-1.4066960000
H	0.5364330000	-3.2739030000	-2.6393690000
H	1.6065030000	2.1887700000	-0.2712150000
H	1.4106840000	1.6501160000	-1.9383880000
H	3.9754260000	-1.6168300000	2.0240590000
H	4.5101500000	-3.1059380000	1.2528280000
H	-3.3177030000	-4.1459210000	-0.9206110000
H	-2.7836490000	-3.5972120000	0.6622930000
H	-2.5917990000	-1.2137640000	-2.0725410000
H	-4.0318180000	0.7899620000	-2.3555420000
H	-8.1601660000	-1.3359580000	2.3331110000
H	-6.8474840000	-3.4442620000	2.6868740000
H	-4.7869470000	-3.8181950000	1.3590030000
H	6.5741800000	-3.2392940000	0.1820700000
H	8.7066790000	-2.2442220000	-0.5636890000
H	6.4886250000	3.8481660000	0.6869980000
H	4.2713940000	2.9977410000	1.4925030000
H	3.8377770000	0.5453060000	1.4649590000
H	-2.7312870000	3.3586770000	-3.1362920000
H	-0.4189250000	2.4416090000	-3.0323860000
H	0.2033240000	1.2644940000	1.6568430000
H	-1.2675730000	1.6068930000	3.6487380000
H	-3.5309290000	2.6406730000	3.3380220000
H	-4.6585760000	3.5957580000	-0.0845960000
H	9.9190330000	-0.2777400000	-0.8989740000
H	-5.7194210000	2.0953510000	-1.3553400000
H	3.5688960000	-2.0769200000	-0.8586100000
H	-1.2139990000	-3.9199470000	-1.4969190000
H	2.1122510000	0.0117910000	-0.0684460000
H	8.5825830000	2.5663070000	-0.2059370000
H	-7.7547750000	0.6697040000	0.7113160000
H	-4.7132740000	3.4879830000	1.1565680000
H	3.1118840000	-0.8177120000	0.0167130000
H	-1.5884440000	-2.3875950000	-1.6681370000

Table S3: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_7)^{+4}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis - (methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_7: coordinates in Angstrom

C	0.8720660000	-2.3513100000	-0.7163960000
C	1.9352630000	-2.4289960000	0.4158790000
C	-0.4919140000	-2.6883590000	-0.0407150000
C	0.8132920000	-0.9348620000	-1.3693560000
C	1.2092230000	-3.3874990000	-1.8157350000
N	-1.5271990000	-3.1316440000	-0.9857290000
N	3.2367830000	-1.8403200000	0.0553140000
N	1.1378310000	0.1428890000	-0.4208580000
C	0.9770090000	1.5161910000	-0.9370260000
C	4.3083850000	-2.0555060000	1.0504270000
C	-2.8745230000	-3.3210630000	-0.4174740000
C	5.6077960000	-1.4050400000	0.6294880000
C	-0.4509240000	2.0290810000	-0.9533420000
C	-3.7772590000	-2.1004360000	-0.5462500000
C	-3.4965210000	-1.1196530000	-1.4775830000
C	-4.3150950000	0.0198760000	-1.6329000000
C	-5.4294900000	0.2109420000	-0.8359560000
C	-4.9605920000	-1.9623880000	0.2520750000
C	-5.7953200000	-0.7958820000	0.1138520000
N	-6.9267380000	-0.6104420000	0.8651960000
C	-7.2758180000	-1.5469840000	1.7417870000
C	-6.5324960000	-2.7349200000	1.9424930000
C	-5.3851280000	-2.9362200000	1.2021710000
C	6.6616660000	-2.1835020000	0.1836060000
C	7.8858650000	-1.6179660000	-0.2425790000
C	8.0682740000	-0.2482680000	-0.2258300000
C	5.7778450000	0.0196010000	0.6570880000
C	7.0154590000	0.6079630000	0.2290880000
N	7.2314740000	1.9614540000	0.2418970000
C	6.2583640000	2.7578300000	0.6730010000
C	5.0051000000	2.2754010000	1.1244990000
C	4.7691240000	0.9158870000	1.1127670000
C	-3.0825000000	3.1007340000	-1.0593310000
C	-2.3334120000	3.0119910000	-2.2095610000
C	-1.0203910000	2.4779270000	-2.1362720000
C	-2.5317900000	2.6919810000	0.1893520000
C	-1.2222610000	2.1329050000	0.2529300000
C	-0.7813950000	1.7216240000	1.5433790000
C	-1.6063030000	1.8933620000	2.6405140000
C	-2.8881410000	2.4726210000	2.4718980000
N	-3.3416990000	2.8573080000	1.2817360000
O	-4.4004760000	3.5335110000	-1.0581350000

O	9.2398590000	0.3592040000	-0.6301930000
O	-6.2169270000	1.3382580000	-0.9201520000
H	1.5601650000	-1.8807840000	1.2892430000
H	2.0322850000	-3.4897160000	0.7196450000
H	-0.3196250000	-3.4488020000	0.7492850000
H	-0.8510090000	-1.7828730000	0.4615140000
H	1.4937080000	-0.9099910000	-2.2444630000
H	-0.1994500000	-0.7811290000	-1.7570000000
H	2.2192770000	-3.2325850000	-2.2137460000
H	1.1602040000	-4.4127810000	-1.4262660000
H	0.5160100000	-3.2988600000	-2.6589390000
H	1.5860800000	2.1638130000	-0.2907850000
H	1.3902610000	1.6251590000	-1.9579580000
H	3.9550030000	-1.6417870000	2.0044890000
H	4.4897270000	-3.1308950000	1.2332580000
H	-3.3381260000	-4.1708780000	-0.9401810000
H	-2.8040720000	-3.6221690000	0.6427230000
H	-2.6122220000	-1.2387210000	-2.0921110000
H	-4.0522410000	0.7650050000	-2.3751120000
H	-8.1805890000	-1.3609150000	2.3135410000
H	-6.8679070000	-3.4692190000	2.6673040000
H	-4.8073700000	-3.8431520000	1.3394330000
H	6.5537570000	-3.2642510000	0.1625000000
H	8.6862560000	-2.2691790000	-0.5832590000
H	6.4682020000	3.8232090000	0.6674280000
H	4.2509710000	2.9727840000	1.4729330000
H	3.8173540000	0.5203490000	1.4453890000
H	-2.7517100000	3.3337200000	-3.1558620000
H	-0.4393480000	2.4166520000	-3.0519560000
H	0.1829010000	1.2395370000	1.6372730000
H	-1.2879960000	1.5819360000	3.6291680000
H	-3.5513520000	2.6157160000	3.3184520000
H	-4.6789990000	3.5708010000	-0.1041660000
H	9.8986100000	-0.3026970000	-0.9185440000
H	-5.7398440000	2.0703940000	-1.3749100000
H	3.5484730000	-2.1018770000	-0.8781800000
H	-1.2344220000	-3.9449040000	-1.5164890000
H	2.0918280000	-0.0131660000	-0.0880160000
H	8.5621600000	2.5413490000	-0.2255070000
H	-7.7751980000	0.6447460000	0.6917460000
H	-4.7336960000	3.4630270000	1.1369980000
H	3.0914600000	-0.8426690000	-0.0028570000

Table S4: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_6)^{+3}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis - (methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_6: coordinates in Angstrom

C	0.9077810000	-2.3579550000	-0.7161390000
C	1.9709780000	-2.4356410000	0.4161360000
C	-0.4561990000	-2.6950040000	-0.0404580000
C	0.8490070000	-0.9415070000	-1.3690990000
C	1.2449380000	-3.3941440000	-1.8154780000
N	-1.4914840000	-3.1382890000	-0.9854720000
N	3.2724980000	-1.8469650000	0.0555710000
N	1.1735460000	0.1362440000	-0.4206010000
C	1.0127240000	1.5095460000	-0.9367690000
C	4.3441000000	-2.0621510000	1.0506840000
C	-2.8388080000	-3.3277080000	-0.4172170000
C	5.6435110000	-1.4116850000	0.6297450000
C	-0.4152090000	2.0224360000	-0.9530850000
C	-3.7415440000	-2.1070810000	-0.5459930000
C	-3.4608060000	-1.1262980000	-1.4773260000
C	-4.2793800000	0.0132310000	-1.6326430000
C	-5.3937750000	0.2042970000	-0.8356990000
C	-4.9248770000	-1.9690330000	0.2523320000
C	-5.7596050000	-0.8025270000	0.1141090000
N	-6.8910230000	-0.6170870000	0.8654530000
C	-7.2401030000	-1.5536290000	1.7420440000
C	-6.4967810000	-2.7415650000	1.9427500000
C	-5.3494130000	-2.9428650000	1.2024280000
C	6.6973810000	-2.1901470000	0.1838630000
C	7.9215800000	-1.6246110000	-0.2423220000
C	8.1039890000	-0.2549130000	-0.2255730000
C	5.8135600000	0.0129560000	0.6573450000
C	7.0511740000	0.6013180000	0.2293450000
N	7.2671890000	1.9548090000	0.2421540000
C	6.2940790000	2.7511850000	0.6732580000
C	5.0408150000	2.2687560000	1.1247560000
C	4.8048390000	0.9092420000	1.1130240000
C	-3.0467850000	3.0940890000	-1.0590740000
C	-2.2976970000	3.0053460000	-2.2093040000
C	-0.9846760000	2.4712820000	-2.1360150000
C	-2.4960750000	2.6853360000	0.1896090000
C	-1.1865460000	2.1262600000	0.2531870000
C	-0.7456800000	1.7149790000	1.5436360000
C	-1.5705880000	1.8867170000	2.6407710000
C	-2.8524260000	2.4659760000	2.4721550000
N	-3.3059840000	2.8506630000	1.2819930000
O	-4.3647610000	3.5268660000	-1.0578780000

O	9.2755740000	0.3525590000	-0.6299360000
O	-6.1812120000	1.3316130000	-0.9198950000
H	1.5958800000	-1.8874290000	1.2895000000
H	2.0680000000	-3.4963610000	0.7199020000
H	-0.2839100000	-3.4554470000	0.7495420000
H	-0.8152940000	-1.7895180000	0.4617710000
H	1.5294230000	-0.9166360000	-2.2442060000
H	-0.1637350000	-0.7877740000	-1.7567430000
H	2.2549920000	-3.2392300000	-2.2134890000
H	1.1959190000	-4.4194260000	-1.4260090000
H	0.5517250000	-3.3055050000	-2.6586820000
H	1.6217950000	2.1571680000	-0.2905280000
H	1.4259760000	1.6185140000	-1.9577010000
H	3.9907180000	-1.6484320000	2.0047460000
H	4.5254420000	-3.1375400000	1.2335150000
H	-3.3024110000	-4.1775230000	-0.9399240000
H	-2.7683570000	-3.6288140000	0.6429800000
H	-2.5765070000	-1.2453660000	-2.0918540000
H	-4.0165260000	0.7583600000	-2.3748550000
H	-8.1448740000	-1.3675600000	2.3137980000
H	-6.8321920000	-3.4758640000	2.6675610000
H	-4.7716550000	-3.8497970000	1.3396900000
H	6.5894720000	-3.2708960000	0.1627570000
H	8.7219710000	-2.2758240000	-0.5830020000
H	6.5039170000	3.8165640000	0.6676850000
H	4.2866860000	2.9661390000	1.4731900000
H	3.8530690000	0.5137040000	1.4456460000
H	-2.7159950000	3.3270750000	-3.1556050000
H	-0.4036330000	2.4100070000	-3.0516990000
H	0.2186160000	1.2328920000	1.6375300000
H	-1.2522810000	1.5752910000	3.6294250000
H	-3.5156370000	2.6090710000	3.3187090000
H	-4.6432840000	3.5641560000	-0.1039090000
H	9.9343250000	-0.3093420000	-0.9182870000
H	-5.7041290000	2.0637490000	-1.3746530000
H	3.5841880000	-2.1085220000	-0.8779230000
H	-1.1987070000	-3.9515490000	-1.5162320000
H	2.1275430000	-0.0198110000	-0.0877590000
H	8.5978760000	2.5347050000	-0.2252500000
H	-7.7394830000	0.6381020000	0.6920030000
H	-4.6979790000	3.4563900000	1.1372600000

Table S5: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_5)^{+2}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_5: coordinates in Angstrom

C	0.8489380000	-2.3122530000	-0.7019740000
C	1.9121350000	-2.3899390000	0.4303010000
C	-0.5150420000	-2.6493020000	-0.0262930000
C	0.7901640000	-0.8958050000	-1.3549340000
C	1.1860950000	-3.3484420000	-1.8013130000
N	-1.5503270000	-3.0925870000	-0.9713070000
N	3.2136550000	-1.8012630000	0.0697360000
N	1.1147030000	0.1819460000	-0.4064360000
C	0.9538810000	1.5552480000	-0.9226040000
C	4.2852570000	-2.0164490000	1.0648490000
C	-2.8976510000	-3.2820060000	-0.4030520000
C	5.5846680000	-1.3659830000	0.6439100000
C	-0.4740520000	2.0681380000	-0.9389200000
C	-3.8003870000	-2.0613790000	-0.5318280000
C	-3.5196490000	-1.0805960000	-1.4631610000
C	-4.3382230000	0.0589330000	-1.6184780000
C	-5.4526180000	0.2499990000	-0.8215340000
C	-4.9837200000	-1.9233310000	0.2664970000
C	-5.8184480000	-0.7568250000	0.1282740000
N	-6.9498660000	-0.5713850000	0.8796180000
C	-7.2989460000	-1.5079270000	1.7562090000
C	-6.5556240000	-2.6958630000	1.9569150000
C	-5.4082560000	-2.8971630000	1.2165930000
C	6.6385380000	-2.1444450000	0.1980280000
C	7.8627370000	-1.5789090000	-0.2281570000
C	8.0451460000	-0.2092110000	-0.2114080000
C	5.7547170000	0.0586580000	0.6715100000
C	6.9923310000	0.6470200000	0.2435100000
N	7.2083460000	2.0005110000	0.2563190000
C	6.2352360000	2.7968870000	0.6874230000
C	4.9819720000	2.3144580000	1.1389210000
C	4.7459960000	0.9549440000	1.1271890000
C	-3.1056280000	3.1397910000	-1.0449090000
C	-2.3565400000	3.0510480000	-2.1951390000
C	-1.0435190000	2.5169840000	-2.1218500000
C	-2.5549180000	2.7310380000	0.2037740000
C	-1.2453890000	2.1719620000	0.2673520000
C	-0.8045230000	1.7606810000	1.5578010000
C	-1.6294310000	1.9324190000	2.6549360000
C	-2.9112690000	2.5116780000	2.4863200000
N	-3.3648270000	2.8963650000	1.2961580000
O	-4.4236040000	3.5725680000	-1.0437130000
O	9.2167310000	0.3982610000	-0.6157710000
O	-6.2400550000	1.3773150000	-0.9057300000

H	1.5370370000	-1.8417270000	1.3036650000
H	2.0091570000	-3.4506590000	0.7340670000
H	-0.3427530000	-3.4097450000	0.7637070000
H	-0.8741370000	-1.7438160000	0.4759360000
H	1.4705800000	-0.8709340000	-2.2300410000
H	-0.2225780000	-0.7420720000	-1.7425780000
H	2.1961490000	-3.1935280000	-2.1993240000
H	1.1370760000	-4.3737240000	-1.4118440000
H	0.4928820000	-3.2598030000	-2.6445170000
H	1.5629520000	2.2028700000	-0.2763630000
H	1.3671330000	1.6642160000	-1.9435360000
H	3.9318750000	-1.6027300000	2.0189110000
H	4.4665990000	-3.0918380000	1.2476800000
H	-3.3612540000	-4.1318210000	-0.9257590000
H	-2.8272000000	-3.5831120000	0.6571450000
H	-2.6353500000	-1.1996640000	-2.0776890000
H	-4.0753690000	0.8040620000	-2.3606900000
H	-8.2037170000	-1.3218580000	2.3279630000
H	-6.8910350000	-3.4301620000	2.6817260000
H	-4.8304980000	-3.8040950000	1.3538550000
H	6.5306290000	-3.2251940000	0.1769220000
H	8.6631280000	-2.2301220000	-0.5688370000
H	6.4450740000	3.8622660000	0.6818500000
H	4.2278430000	3.0118410000	1.4873550000
H	3.7942260000	0.5594060000	1.4598110000
H	-2.7748380000	3.3727770000	-3.1414400000
H	-0.4624760000	2.4557090000	-3.0375340000
H	0.1597730000	1.2785940000	1.6516950000
H	-1.3111240000	1.6209930000	3.6435900000
H	-3.5744800000	2.6547730000	3.3328740000
H	-4.7021270000	3.6098580000	-0.0897440000
H	9.8754820000	-0.2636400000	-0.9041220000
H	-5.7629720000	2.1094510000	-1.3604880000
H	3.5253450000	-2.0628200000	-0.8637580000
H	-1.2575500000	-3.9058470000	-1.5020670000
H	2.0687000000	0.0258910000	-0.0735940000
H	8.5390330000	2.5804070000	-0.2110850000
H	-7.7983240000	0.6838040000	0.7061670000

Table S6: Cartesian (X, Y, Z) coordinates of minimized structure of $[(LH_4)^+$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_4: coordinates in Angstrom

C	0.7510940000	-2.3002160000	-0.6929570000
C	1.8142910000	-2.3779020000	0.4393180000
C	-0.6128860000	-2.6372650000	-0.0172760000
C	0.6923200000	-0.8837680000	-1.3459170000
C	1.0882510000	-3.3364050000	-1.7922960000
N	-1.6481710000	-3.0805500000	-0.9622900000
N	3.1158110000	-1.7892260000	0.0787530000
N	1.0168590000	0.1939830000	-0.3974190000
C	0.8560370000	1.5672850000	-0.9135870000
C	4.1874130000	-2.0044120000	1.0738660000
C	-2.9954950000	-3.2699690000	-0.3940350000
C	5.4868240000	-1.3539460000	0.6529270000
C	-0.5718960000	2.0801750000	-0.9299030000
C	-3.8982310000	-2.0493420000	-0.5228110000
C	-3.6174930000	-1.0685590000	-1.4541440000
C	-4.4360670000	0.0709700000	-1.6094610000
C	-5.5504620000	0.2620360000	-0.8125170000
C	-5.0815640000	-1.9112940000	0.2755140000
C	-5.9162920000	-0.7447880000	0.1372910000
N	-7.0477100000	-0.5593480000	0.8886350000
C	-7.3967900000	-1.4958900000	1.7652260000
C	-6.6534680000	-2.6838260000	1.9659320000
C	-5.5061000000	-2.8851260000	1.2256100000
C	6.5406940000	-2.1324080000	0.2070450000
C	7.7648930000	-1.5668720000	-0.2191400000
C	7.9473020000	-0.1971740000	-0.2023910000
C	5.6568730000	0.0706950000	0.6805270000
C	6.8944870000	0.6590570000	0.2525270000
N	7.1105020000	2.0125480000	0.2653360000
C	6.1373920000	2.8089240000	0.6964400000
C	4.8841280000	2.3264950000	1.1479380000
C	4.6481520000	0.9669810000	1.1362060000
C	-3.2034720000	3.1518280000	-1.0358920000
C	-2.4543840000	3.0630850000	-2.1861220000
C	-1.1413630000	2.5290210000	-2.1128330000
C	-2.6527620000	2.7430750000	0.2127910000
C	-1.3432330000	2.1839990000	0.2763690000
C	-0.9023670000	1.7727180000	1.5668180000
C	-1.7272750000	1.9444560000	2.6639530000
C	-3.0091130000	2.5237150000	2.4953370000
N	-3.4626710000	2.9084020000	1.3051750000
O	-4.5214480000	3.5846050000	-1.0346960000
O	9.1188870000	0.4102980000	-0.6067540000
O	-6.3378990000	1.3893520000	-0.8967130000

H	1.4391930000	-1.8296900000	1.3126820000
H	1.9113130000	-3.4386220000	0.7430840000
H	-0.4405970000	-3.3977080000	0.7727240000
H	-0.9719810000	-1.7317790000	0.4849530000
H	1.3727360000	-0.8588970000	-2.2210240000
H	-0.3204220000	-0.7300350000	-1.7335610000
H	2.0983050000	-3.1814910000	-2.1903070000
H	1.0392320000	-4.3616870000	-1.4028270000
H	0.3950380000	-3.2477660000	-2.6355000000
H	1.4651080000	2.2149070000	-0.2673460000
H	1.2692890000	1.6762530000	-1.9345190000
H	3.8340310000	-1.5906930000	2.0279280000
H	4.3687550000	-3.0798010000	1.2566970000
H	-3.4590980000	-4.1197840000	-0.9167420000
H	-2.9250440000	-3.5710750000	0.6661620000
H	-2.7331940000	-1.1876270000	-2.0686720000
H	-4.1732130000	0.8160990000	-2.3516730000
H	-8.3015610000	-1.3098210000	2.3369800000
H	-6.9888790000	-3.4181250000	2.6907430000
H	-4.9283420000	-3.7920580000	1.3628720000
H	6.4327850000	-3.2131570000	0.1859390000
H	8.5652840000	-2.2180850000	-0.5598200000
H	6.3472300000	3.8743030000	0.6908670000
H	4.1299990000	3.0238780000	1.4963720000
H	3.6963820000	0.5714430000	1.4688280000
H	-2.8726820000	3.3848140000	-3.1324230000
H	-0.5603200000	2.4677460000	-3.0285170000
H	0.0619290000	1.2906310000	1.6607120000
H	-1.4089680000	1.6330300000	3.6526070000
H	-3.6723240000	2.6668100000	3.3418910000
H	-4.7999710000	3.6218950000	-0.0807270000
H	9.7776380000	-0.2516030000	-0.8951050000
H	-5.8608160000	2.1214880000	-1.3514710000
H	3.4275010000	-2.0507830000	-0.8547410000
H	-1.3553940000	-3.8938100000	-1.4930500000
H	1.9708560000	0.0379280000	-0.0645770000
H	8.4411930000	2.5924400000	-0.2020630000

Table S7: Cartesian (X, Y, Z) coordinates of minimized structure of [(LH_3) species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_3: coordinates in Angstrom

C	0.8550200000	-2.2641710000	-0.6951800000
C	1.9182170000	-2.3418570000	0.4370950000
C	-0.5089600000	-2.6012200000	-0.0194990000
C	0.7962460000	-0.8477230000	-1.3481400000
C	1.1921770000	-3.3003590000	-1.7945190000
N	-1.5442450000	-3.0445050000	-0.9645140000
N	3.2197370000	-1.7531810000	0.0765300000
N	1.1207850000	0.2300280000	-0.3996410000
C	0.9599630000	1.6033300000	-0.9158090000
C	4.2913390000	-1.9683670000	1.0716440000
C	-2.8915690000	-3.2339240000	-0.3962590000
C	5.5907500000	-1.3179010000	0.6507050000
C	-0.4679700000	2.1162200000	-0.9321250000
C	-3.7943050000	-2.0132970000	-0.5250350000
C	-3.5135670000	-1.0325140000	-1.4563670000
C	-4.3321410000	0.1070160000	-1.6116840000
C	-5.4465360000	0.2980810000	-0.8147400000
C	-4.9776380000	-1.8752490000	0.2732900000
C	-5.8123660000	-0.7087430000	0.1350670000
N	-6.9437840000	-0.5233030000	0.8864110000
C	-7.2928640000	-1.4598450000	1.7630020000
C	-6.5495420000	-2.6477810000	1.9637080000
C	-5.4021740000	-2.8490810000	1.2233860000
C	6.6446200000	-2.0963630000	0.2048230000
C	7.8688190000	-1.5308270000	-0.2213620000
C	8.0512280000	-0.1611290000	-0.2046140000
C	5.7607990000	0.1067400000	0.6783050000
C	6.9984120000	0.6951020000	0.2503030000
N	7.2144270000	2.0485930000	0.2631120000
C	6.2413160000	2.8449690000	0.6942140000
C	4.9880520000	2.3625400000	1.1457120000
C	4.7520770000	1.0030260000	1.1339810000
C	-3.0995460000	3.1878730000	-1.0381140000
C	-2.3504570000	3.0991310000	-2.1883440000
C	-1.0374360000	2.5650670000	-2.1150550000
C	-2.5488360000	2.7791200000	0.2105690000
C	-1.2393070000	2.2200440000	0.2741470000
C	-0.7984410000	1.8087630000	1.5645960000
C	-1.6233490000	1.9805000000	2.6617310000
C	-2.9051870000	2.5597590000	2.4931150000
N	-3.3587450000	2.9444470000	1.3029530000
O	-4.4175220000	3.6206500000	-1.0369180000
O	9.2228130000	0.4463430000	-0.6089760000
O	-6.2339730000	1.4253970000	-0.8989360000

H	1.5431190000	-1.7936450000	1.3104590000
H	2.0152390000	-3.4025770000	0.7408610000
H	-0.3366710000	-3.3616630000	0.7705000000
H	-0.8680550000	-1.6957340000	0.4827300000
H	1.4766630000	-0.8228510000	-2.2232470000
H	-0.2164960000	-0.6939900000	-1.7357840000
H	2.2022320000	-3.1454450000	-2.1925300000
H	1.1431580000	-4.3256420000	-1.4050510000
H	0.4989650000	-3.2117200000	-2.6377230000
H	1.5690340000	2.2509520000	-0.2695680000
H	1.3732160000	1.7122990000	-1.9367410000
H	3.9379570000	-1.5546490000	2.0257060000
H	4.4726810000	-3.0437560000	1.2544740000
H	-3.3551720000	-4.0837390000	-0.9189660000
H	-2.8211180000	-3.5350300000	0.6639380000
H	-2.6292670000	-1.1515810000	-2.0708950000
H	-4.0692860000	0.8521450000	-2.3538960000
H	-8.1976350000	-1.2737770000	2.3347560000
H	-6.8849530000	-3.3820810000	2.6885180000
H	-4.8244160000	-3.7560130000	1.3606480000
H	6.5367110000	-3.1771120000	0.1837170000
H	8.6692100000	-2.1820400000	-0.5620420000
H	6.4511540000	3.9103480000	0.6886410000
H	4.2339230000	3.0599230000	1.4941450000
H	3.8003070000	0.6074880000	1.4666020000
H	-2.7687550000	3.4208600000	-3.1346450000
H	-0.4563930000	2.5037920000	-3.0307390000
H	0.1658550000	1.3266760000	1.6584900000
H	-1.3050420000	1.6690740000	3.6503850000
H	-3.5683980000	2.7028540000	3.3396690000
H	-4.6960450000	3.6579400000	-0.0829490000
H	9.8815640000	-0.2155580000	-0.8973260000
H	-5.7568900000	2.1575330000	-1.3536940000
H	3.5314270000	-2.0147380000	-0.8569640000
H	-1.2514680000	-3.8577650000	-1.4952740000
H	2.0747820000	0.0739730000	-0.0667990000

Table S8: Cartesian (X, Y, Z) coordinates of minimized structure of [$(LH_2)^-$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH_2: coordinates in Angstrom

C	0.8875000000	-2.3305760000	-0.7017980000
C	1.9506970000	-2.4082620000	0.4304770000
C	-0.4764800000	-2.6676250000	-0.0261170000
C	0.8287260000	-0.9141280000	-1.3547580000
C	1.2246570000	-3.3667650000	-1.8011370000
N	-1.5117650000	-3.1109100000	-0.9711310000
N	3.2522170000	-1.8195860000	0.0699120000
N	1.1532650000	0.1636230000	-0.4062600000
C	0.9924430000	1.5369250000	-0.9224280000
C	4.3238190000	-2.0347720000	1.0650250000
C	-2.8590890000	-3.3003290000	-0.4028760000
C	5.6232300000	-1.3843060000	0.6440860000
C	-0.4354900000	2.0498150000	-0.9387440000
C	-3.7618250000	-2.0797020000	-0.5316520000
C	-3.4810870000	-1.0989190000	-1.4629850000
C	-4.2996610000	0.0406100000	-1.6183020000
C	-5.4140560000	0.2316760000	-0.8213580000
C	-4.9451580000	-1.9416540000	0.2666730000
C	-5.7798860000	-0.7751480000	0.1284500000
N	-6.9113040000	-0.5897080000	0.8797940000
C	-7.2603840000	-1.5262500000	1.7563850000
C	-6.5170620000	-2.7141860000	1.9570910000
C	-5.3696940000	-2.9154860000	1.2167690000
C	6.6771000000	-2.1627680000	0.1982040000
C	7.9012990000	-1.5972320000	-0.2279810000
C	8.0837080000	-0.2275340000	-0.2112320000
C	5.7932790000	0.0403350000	0.6716860000
C	7.0308930000	0.6286970000	0.2436860000
N	7.2469080000	1.9821880000	0.2564950000
C	6.2737980000	2.7785640000	0.6875990000
C	5.0205340000	2.2961350000	1.1390970000
C	4.7845580000	0.9366210000	1.1273650000
C	-3.0670660000	3.1214680000	-1.0447330000
C	-2.3179780000	3.0327250000	-2.1949630000
C	-1.0049570000	2.4986610000	-2.1216740000
C	-2.5163560000	2.7127150000	0.2039500000
C	-1.2068270000	2.1536390000	0.2675280000
C	-0.7659610000	1.7423580000	1.5579770000
C	-1.5908690000	1.9140960000	2.6551120000
C	-2.8727070000	2.4933550000	2.4864960000
N	-3.3262650000	2.8780420000	1.2963340000
O	-4.3850420000	3.5542450000	-1.0435370000
O	9.2552930000	0.3799380000	-0.6155950000
O	-6.2014930000	1.3589920000	-0.9055540000

H	1.5755990000	-1.8600500000	1.3038410000
H	2.0477190000	-3.4689820000	0.7342430000
H	-0.3041910000	-3.4280680000	0.7638830000
H	-0.8355750000	-1.7621390000	0.4761120000
H	1.5091420000	-0.8892570000	-2.2298650000
H	-0.1840160000	-0.7603950000	-1.7424020000
H	2.2347110000	-3.2118510000	-2.1991480000
H	1.1756380000	-4.3920470000	-1.4116680000
H	0.5314440000	-3.2781260000	-2.6443410000
H	1.6015140000	2.1845470000	-0.2761870000
H	1.4056950000	1.6458930000	-1.9433600000
H	3.9704370000	-1.6210530000	2.0190870000
H	4.5051610000	-3.1101610000	1.2478560000
H	-3.3226920000	-4.1501440000	-0.9255830000
H	-2.7886380000	-3.6014350000	0.6573210000
H	-2.5967880000	-1.2179870000	-2.0775130000
H	-4.0368070000	0.7857390000	-2.3605140000
H	-8.1651550000	-1.3401810000	2.3281390000
H	-6.8524730000	-3.4484850000	2.6819020000
H	-4.7919360000	-3.8224180000	1.3540310000
H	6.5691910000	-3.2435170000	0.1770980000
H	8.7016900000	-2.2484450000	-0.5686610000
H	6.4836360000	3.8439430000	0.6820260000
H	4.2664050000	2.9935180000	1.4875310000
H	3.8327880000	0.5410830000	1.4599870000
H	-2.7362760000	3.3544540000	-3.1412640000
H	-0.4239140000	2.4373860000	-3.0373580000
H	0.1983350000	1.2602710000	1.6518710000
H	-1.2725620000	1.6026700000	3.6437660000
H	-3.5359180000	2.6364500000	3.3330500000
H	-4.6635650000	3.5915350000	-0.0895680000
H	-5.7244100000	2.0911280000	-1.3603120000
H	3.5639070000	-2.0811430000	-0.8635820000
H	-1.2189880000	-3.9241700000	-1.5018910000
H	2.1072620000	0.0075680000	-0.0734180000

Table S9: Cartesian (X, Y, Z) coordinates of minimized structure of [$(LH)^{2-}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of LH: coordinates in Angstrom

C	0.8486750000	-2.2618400000	-0.6925920000
C	1.9118720000	-2.3395260000	0.4396830000
C	-0.5153050000	-2.5988890000	-0.0169110000
C	0.7899010000	-0.8453920000	-1.3455520000
C	1.1858320000	-3.2980290000	-1.7919310000
N	-1.5505900000	-3.0421740000	-0.9619250000
N	3.2133920000	-1.7508500000	0.0791180000
N	1.1144400000	0.2323590000	-0.3970540000
C	0.9536180000	1.6056610000	-0.9132220000
C	4.2849940000	-1.9660360000	1.0742310000
C	-2.8979140000	-3.2315930000	-0.3936700000
C	5.5844050000	-1.3155700000	0.6532920000
C	-0.4743150000	2.1185510000	-0.9295380000
C	-3.8006500000	-2.0109660000	-0.5224460000
C	-3.5199120000	-1.0301830000	-1.4537790000
C	-4.3384860000	0.1093460000	-1.6090960000
C	-5.4528810000	0.3004120000	-0.8121520000
C	-4.9839830000	-1.8729180000	0.2758790000
C	-5.8187110000	-0.7064120000	0.1376560000
N	-6.9501290000	-0.5209720000	0.8890000000
C	-7.2992090000	-1.4575140000	1.7655910000
C	-6.5558870000	-2.6454500000	1.9662970000
C	-5.4085190000	-2.8467500000	1.2259750000
C	6.6382750000	-2.0940320000	0.2074100000
C	7.8624740000	-1.5284960000	-0.2187750000
C	8.0448830000	-0.1587980000	-0.2020260000
C	5.7544540000	0.1090710000	0.6808920000
C	6.9920680000	0.6974330000	0.2528920000
N	7.2080830000	2.0509240000	0.2657010000
C	6.2349730000	2.8473000000	0.6968050000
C	4.9817090000	2.3648710000	1.1483030000
C	4.7457330000	1.0053570000	1.1365710000
C	-3.1058910000	3.1902040000	-1.0355270000
C	-2.3568030000	3.1014610000	-2.1857570000
C	-1.0437820000	2.5673970000	-2.1124680000
C	-2.5551810000	2.7814510000	0.2131560000
C	-1.2456520000	2.2223750000	0.2767340000
C	-0.8047860000	1.8110940000	1.5671830000
C	-1.6296940000	1.9828320000	2.6643180000
C	-2.9115320000	2.5620910000	2.4957020000
N	-3.3650900000	2.9467780000	1.3055400000
O	-4.4238670000	3.6229810000	-1.0343310000
O	9.2164680000	0.4486740000	-0.6063890000
O	-6.2403180000	1.4277280000	-0.8963480000

H	1.5367740000	-1.7913140000	1.3130470000
H	2.0088940000	-3.4002460000	0.7434490000
H	-0.3430160000	-3.3593320000	0.7730890000
H	-0.8744000000	-1.6934030000	0.4853180000
H	1.4703170000	-0.8205210000	-2.2206590000
H	-0.2228410000	-0.6916590000	-1.7331960000
H	2.1958860000	-3.1431150000	-2.1899420000
H	1.1368130000	-4.3233110000	-1.4024620000
H	0.4926190000	-3.2093900000	-2.6351350000
H	1.5626890000	2.2532830000	-0.2669810000
H	1.3668700000	1.7146290000	-1.9341540000
H	3.9316120000	-1.5523170000	2.0282930000
H	4.4663360000	-3.0414250000	1.2570620000
H	-3.3615170000	-4.0814080000	-0.9163770000
H	-2.8274630000	-3.5326990000	0.6665270000
H	-2.6356130000	-1.1492510000	-2.0683070000
H	-4.0756320000	0.8544750000	-2.3513080000
H	-8.2039800000	-1.2714450000	2.3373450000
H	-6.8912980000	-3.3797490000	2.6911080000
H	-4.8307610000	-3.7536820000	1.3632370000
H	6.5303660000	-3.1747810000	0.1863040000
H	8.6628650000	-2.1797090000	-0.5594550000
H	6.4448110000	3.9126790000	0.6912320000
H	4.2275800000	3.0622540000	1.4967370000
H	3.7939630000	0.6098190000	1.4691930000
H	-2.7751010000	3.4231900000	-3.1320580000
H	-0.4627390000	2.5061220000	-3.0281520000
H	0.1595100000	1.3290070000	1.6610770000
H	-1.3113870000	1.6714060000	3.6529720000
H	-3.5747430000	2.7051860000	3.3422560000
H	-5.7632350000	2.1598640000	-1.3511060000
H	3.5250820000	-2.0124070000	-0.8543760000
H	-1.2578130000	-3.8554340000	-1.4926850000
H	2.0684370000	0.0763040000	-0.0642120000

Table S10: Cartesian (X, Y, Z) coordinates of minimized structure of $[(L)^{3-}$ species of 5,5'-(2(((8-hydroxyquinolin-5-yl)methylamino)methyl)2-methylpropane-1,3-diyl)bis(azanediyl)-bis-(methylene)diquinolin-8-ol, (TAME5OX)].

XYZ file of L: coordinates in Angstrom

C	0.8486750000	-2.2618400000	-0.6925920000
C	1.9118720000	-2.3395260000	0.4396830000
C	-0.5153050000	-2.5988890000	-0.0169110000
C	0.7899010000	-0.8453920000	-1.3455520000
C	1.1858320000	-3.2980290000	-1.7919310000
N	-1.5505900000	-3.0421740000	-0.9619250000
N	3.2133920000	-1.7508500000	0.0791180000
N	1.1144400000	0.2323590000	-0.3970540000
C	0.9536180000	1.6056610000	-0.9132220000
C	4.2849940000	-1.9660360000	1.0742310000
C	-2.8979140000	-3.2315930000	-0.3936700000
C	5.5844050000	-1.3155700000	0.6532920000
C	-0.4743150000	2.1185510000	-0.9295380000
C	-3.8006500000	-2.0109660000	-0.5224460000
C	-3.5199120000	-1.0301830000	-1.4537790000
C	-4.3384860000	0.1093460000	-1.6090960000
C	-5.4528810000	0.3004120000	-0.8121520000
C	-4.9839830000	-1.8729180000	0.2758790000
C	-5.8187110000	-0.7064120000	0.1376560000
N	-6.9501290000	-0.5209720000	0.8890000000
C	-7.2992090000	-1.4575140000	1.7655910000
C	-6.5558870000	-2.6454500000	1.9662970000
C	-5.4085190000	-2.8467500000	1.2259750000
C	6.6382750000	-2.0940320000	0.2074100000
C	7.8624740000	-1.5284960000	-0.2187750000
C	8.0448830000	-0.1587980000	-0.2020260000
C	5.7544540000	0.1090710000	0.6808920000
C	6.9920680000	0.6974330000	0.2528920000
N	7.2080830000	2.0509240000	0.2657010000
C	6.2349730000	2.8473000000	0.6968050000
C	4.9817090000	2.3648710000	1.1483030000
C	4.7457330000	1.0053570000	1.1365710000
C	-3.1058910000	3.1902040000	-1.0355270000
C	-2.3568030000	3.1014610000	-2.1857570000
C	-1.0437820000	2.5673970000	-2.1124680000
C	-2.5551810000	2.7814510000	0.2131560000
C	-1.2456520000	2.2223750000	0.2767340000
C	-0.8047860000	1.8110940000	1.5671830000
C	-1.6296940000	1.9828320000	2.6643180000
C	-2.9115320000	2.5620910000	2.4957020000
N	-3.3650900000	2.9467780000	1.3055400000
O	-4.4238670000	3.6229810000	-1.0343310000
O	9.2164680000	0.4486740000	-0.6063890000
O	-6.2403180000	1.4277280000	-0.8963480000

H	1.5367740000	-1.7913140000	1.3130470000
H	2.0088940000	-3.4002460000	0.7434490000
H	-0.3430160000	-3.3593320000	0.7730890000
H	-0.8744000000	-1.6934030000	0.4853180000
H	1.4703170000	-0.8205210000	-2.2206590000
H	-0.2228410000	-0.6916590000	-1.7331960000
H	2.1958860000	-3.1431150000	-2.1899420000
H	1.1368130000	-4.3233110000	-1.4024620000
H	0.4926190000	-3.2093900000	-2.6351350000
H	1.5626890000	2.2532830000	-0.2669810000
H	1.3668700000	1.7146290000	-1.9341540000
H	3.9316120000	-1.5523170000	2.0282930000
H	4.4663360000	-3.0414250000	1.2570620000
H	-3.3615170000	-4.0814080000	-0.9163770000
H	-2.8274630000	-3.5326990000	0.6665270000
H	-2.6356130000	-1.1492510000	-2.0683070000
H	-4.0756320000	0.8544750000	-2.3513080000
H	-8.2039800000	-1.2714450000	2.3373450000
H	-6.8912980000	-3.3797490000	2.6911080000
H	-4.8307610000	-3.7536820000	1.3632370000
H	6.5303660000	-3.1747810000	0.1863040000
H	8.6628650000	-2.1797090000	-0.5594550000
H	6.4448110000	3.9126790000	0.6912320000
H	4.2275800000	3.0622540000	1.4967370000
H	3.7939630000	0.6098190000	1.4691930000
H	-2.7751010000	3.4231900000	-3.1320580000
H	-0.4627390000	2.5061220000	-3.0281520000
H	0.1595100000	1.3290070000	1.6610770000
H	-1.3113870000	1.6714060000	3.6529720000
H	-3.5747430000	2.7051860000	3.3422560000
H	3.5250820000	-2.0124070000	-0.8543760000
H	-1.2578130000	-3.8554340000	-1.4926850000
H	2.0684370000	0.0763040000	-0.0642120000

Table S11: Theoretically calculated energies (Hartrees) of $(LH_9)^{+6}$, $(LH_8)^{+5}$, $(LH_7)^{+4}$, $(LH_6)^{+3}$, $(LH_5)^{+2}$, $(LH_4)^{+1}$, (LH_3), $(LH_2)^{-1}$, $(LH)^{-2}$ and $(L)^{-3}$ of TAME5OX.

Species	Total energy	Dispersion energy	Dispersion corrected energy
$\mathbf{(H_9L)^{6+}}$	-1969.02992149	-0.11561753	-1969.14553902
$\mathbf{(H_8L)^{5+}}$	-1968.43339077	-0.11206523	-1968.54545600
$\mathbf{(H_7L)^{4+}}$	-1968.14844068	-0.10944861	-1968.25788929
$\mathbf{(H_6L)^{3+}}$	-1968.14844066	-0.10626730	-1968.25470896
$\mathbf{(H_5L)^{2+}}$	-1968.14797797	-0.10343338	-1968.25141195
$\mathbf{(H_4L)^{+}}$	-1968.14797795	-0.10096540	-1968.24894335
$\mathbf{(H_3L)}$	-1968.14352995	-0.09862247	-1968.24215242
$\mathbf{(H_2L)^{-}}$	-1968.14352992	-0.09798300	-1968.24151302
$\mathbf{(HL)^{2-}}$	-1967.91875902	-0.09673875	-1968.01549887
$\mathbf{(L)^{3-}}$	-1967.70686613	-0.09531566	-1967.80218279

Dispersion correction for the B3LYP functional was carried out with zero-damping, using DFTD3 V2.1 Rev 6 S. Grimme, University Muenster and coordinates from the B3LYP/ 6-31 G optimised structures.