

Supporting Information

Aggregation-Induced Emission Luminogen with Near-Infrared-II Excitation and Near-Infrared-I Emission for Ultradeep Intravital Two-Photon Microscopy

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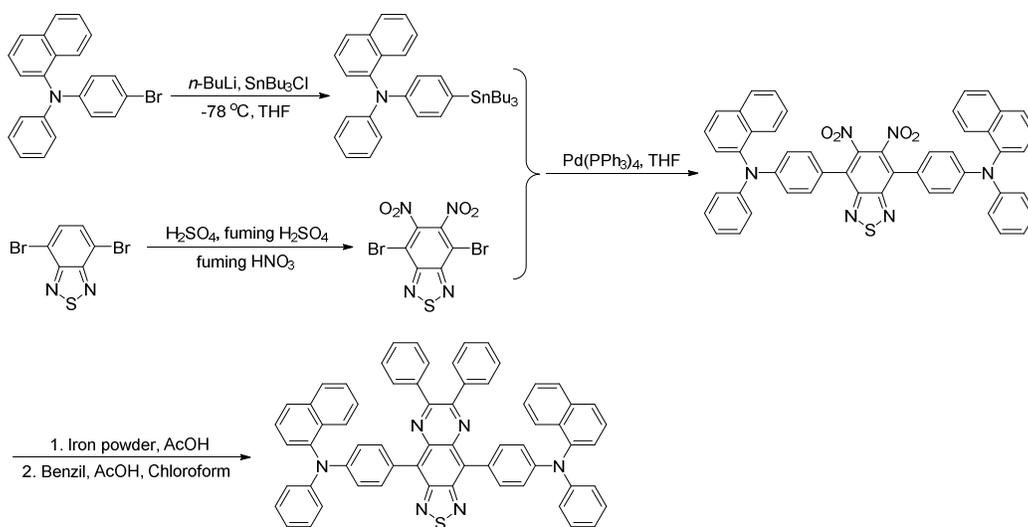
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Scheme S1. Synthetic route to TQ-BPN.

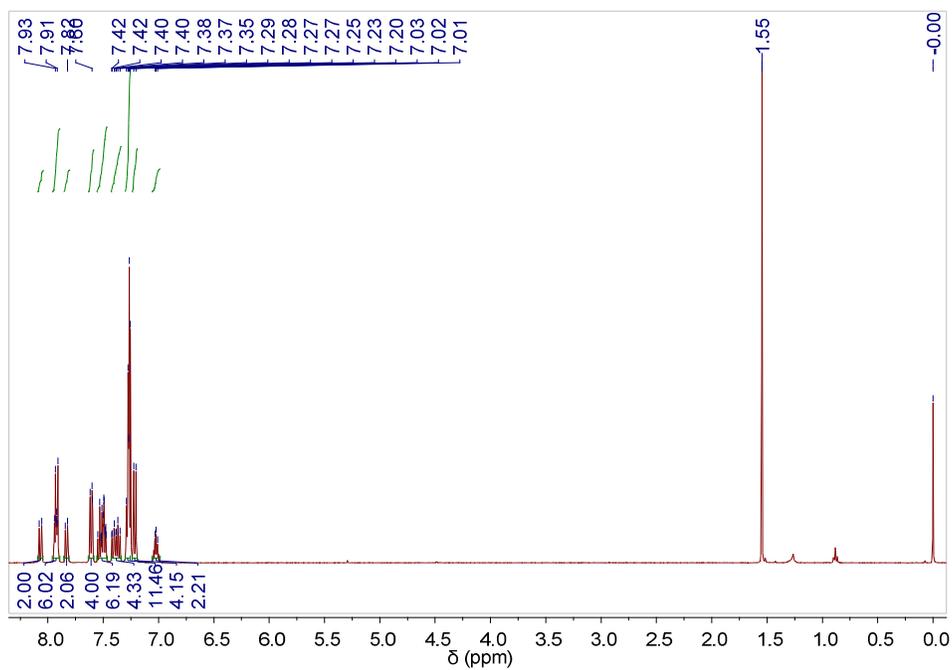


Figure S1. ^1H NMR spectrum of TQ-BPN in CDCl_3 at 298 K.

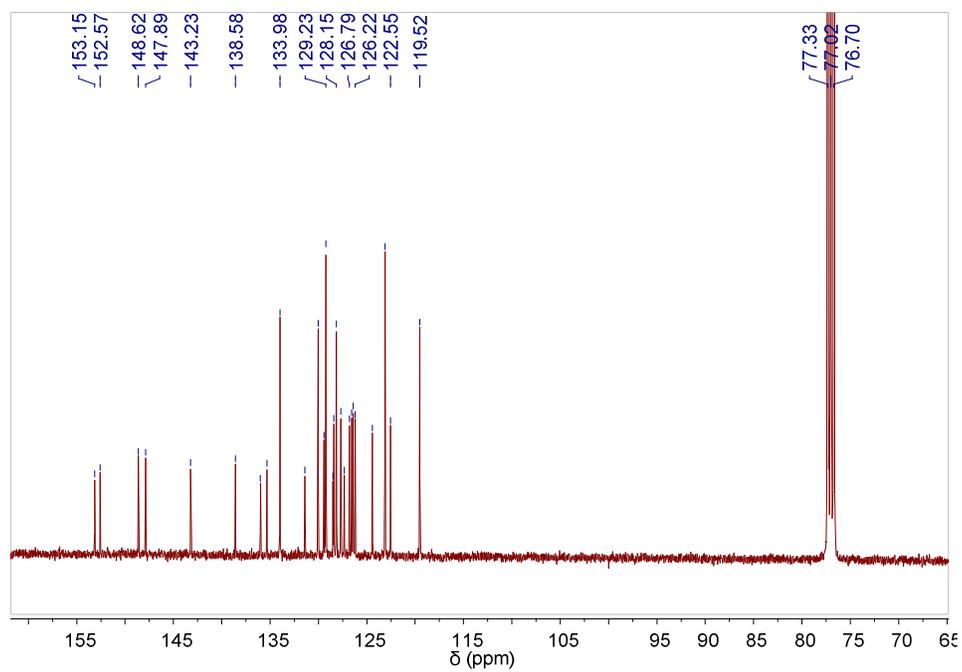


Figure S2. ^{13}C NMR spectrum of TQ-BPN in CDCl_3 at 298 K.



Figure S3. HRMS of TQ-BPN.

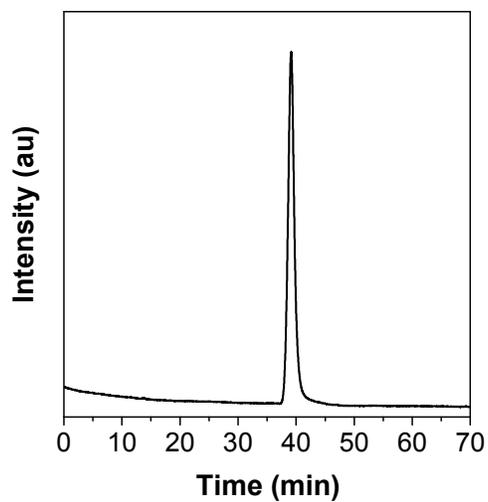


Figure S4. HPLC spectrum of TQ-BPN.

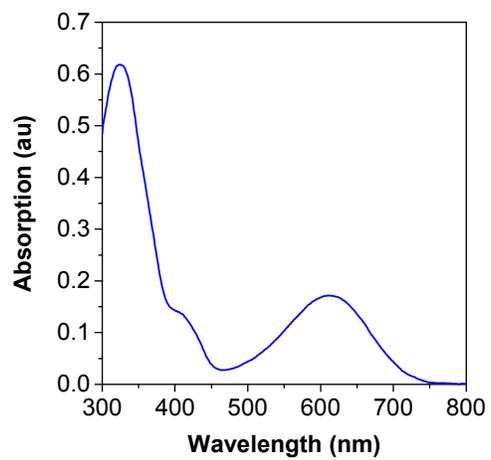


Figure S5. Absorption spectrum of TQ-BPN in THF.

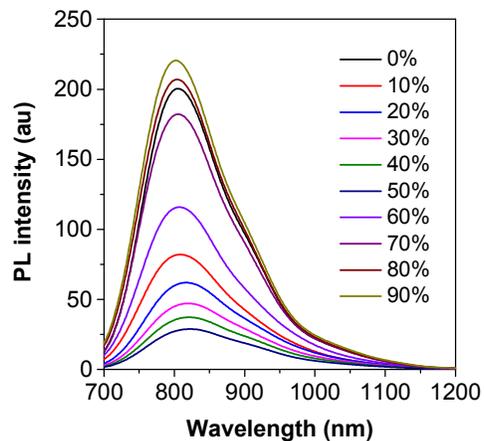


Figure S6. Photoluminescence (PL) spectra of TQ-BPN in THF/H₂O mixtures with different water fractions as indicated in the figure.

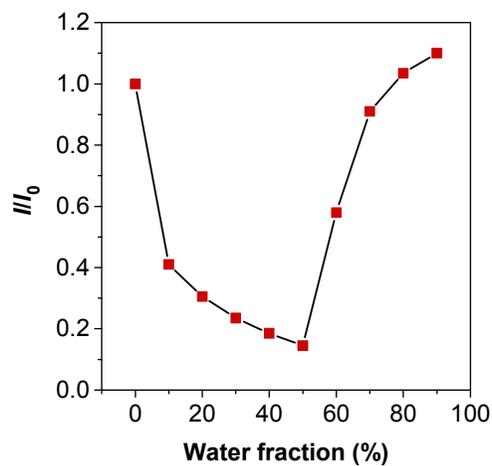


Figure S7. Plot of maximal PL intensity of TQ-BPN versus water fraction (f_w) of THF/water mixture. I_0 and I are the maximal PL intensities of TQ-BPN in pure THF ($f_w = 0$) and THF/water mixtures with different f_w s.

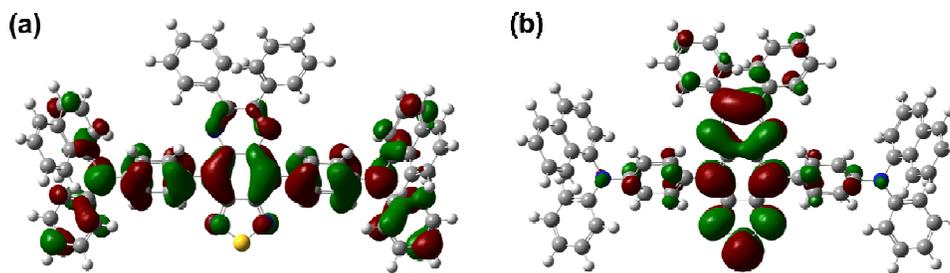


Figure S8. (a) The highest occupied molecular orbital (HOMO) and (b) lowest unoccupied molecular orbital (LUMO) energy levels of TQ-BPN.

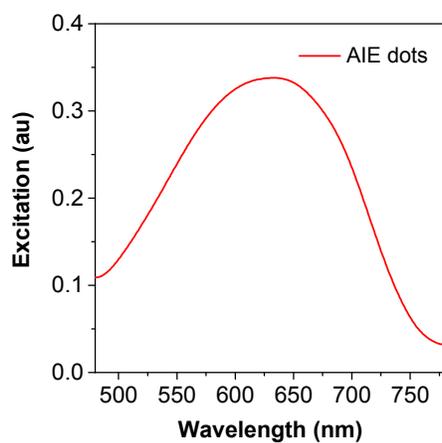


Figure S9. Excitation spectrum of the AIE dots in aqueous dispersion.

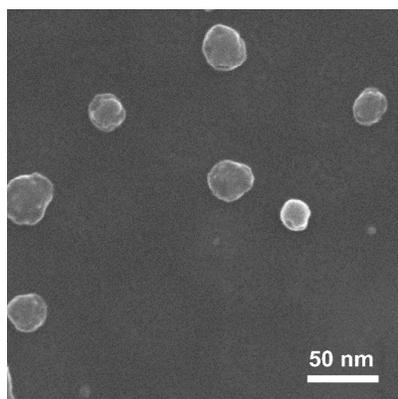


Figure S10. Representative scanning electron microscopy (SEM) image of the AIE dots.

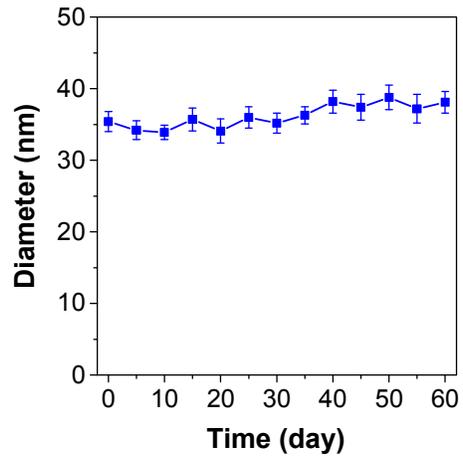


Figure S11. Average diameters of the AIE dots in PBS after storing in ambient condition for different time.

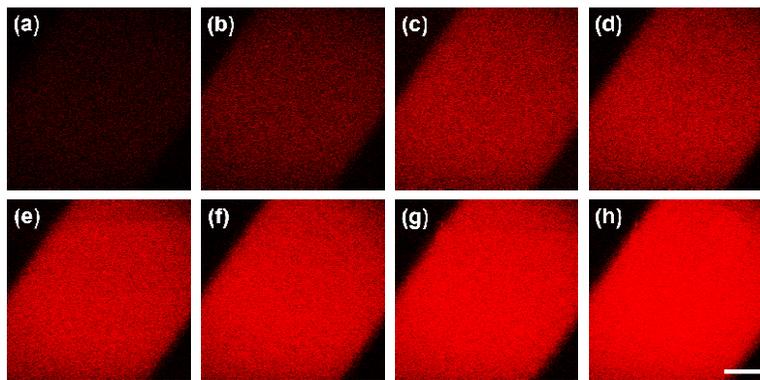


Figure S12. Two-photon fluorescence imaging of the AIE dots in capillary glass tube with various 1300-nm excitation powers. The excitation power gradually increases from (a) to (h).

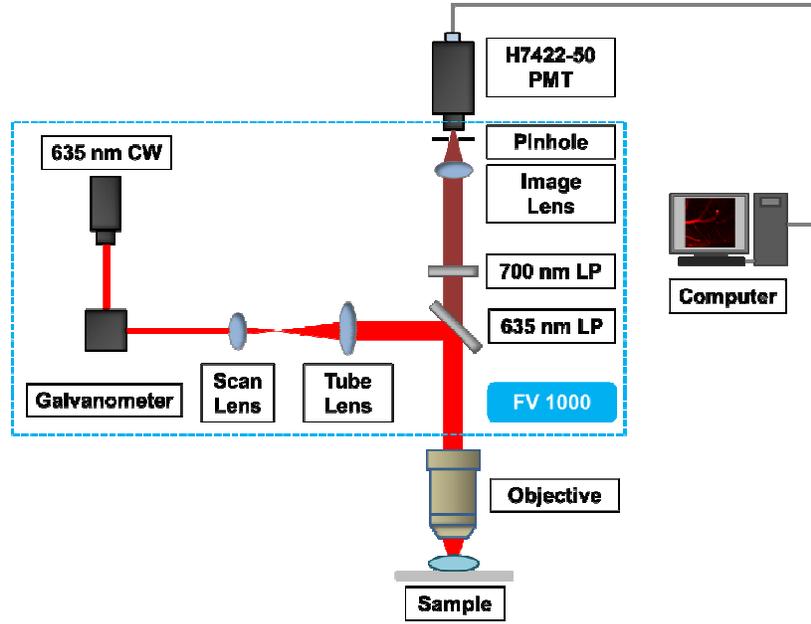


Figure S13. Schematic illustration of the setup for one-photon fluorescence confocal microscopic imaging.

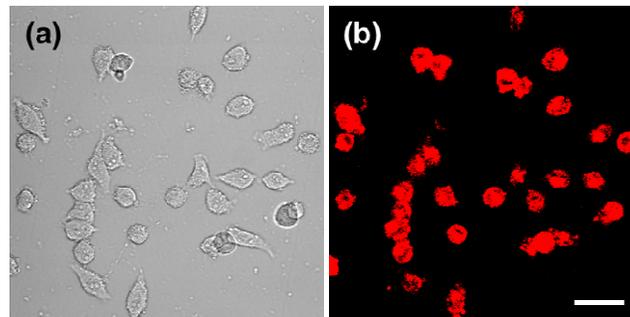


Figure S14. One-photon fluorescence confocal images of the AIE dots treated HeLa cells. The scale bar indicates 50 μm .

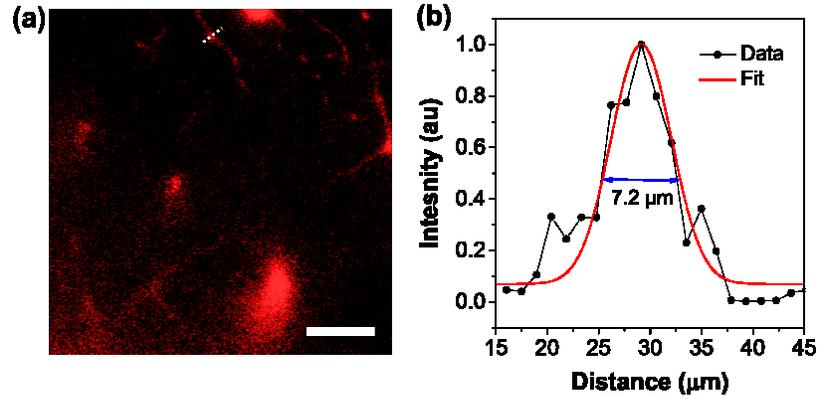


Figure S15. The full width at half-maximum (FWHM) of a blood vessel from one-photon fluorescence confocal image of mouse brain at 600 μm as indicated with the dotted white line in (a). The scale bar indicates 100 μm.

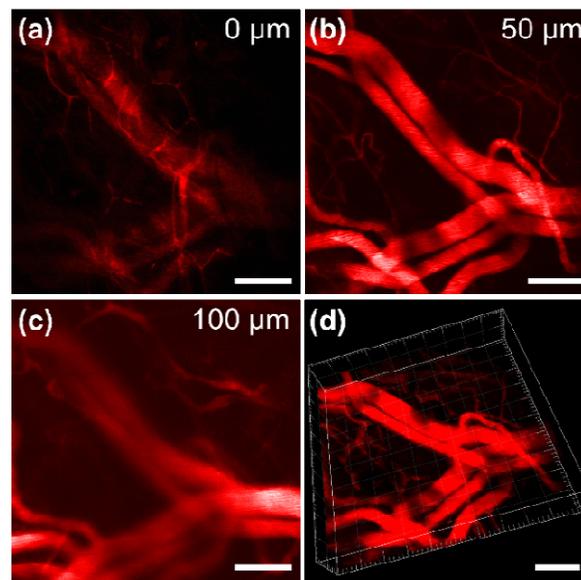


Figure S16. (a-c) *In vivo* one-photon fluorescence confocal images at different vertical depths and (d) 3D reconstruction of the AIE dots-stained mouse ear. The scale bars indicate 100 μm.

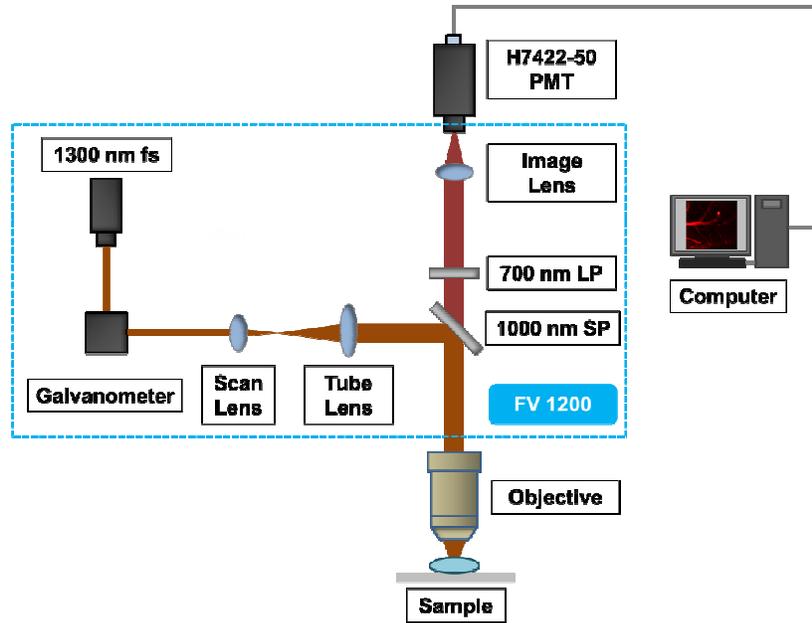


Figure S17. Schematic illustration of the setup for TPFM imaging system for cell and mice ear imaging.

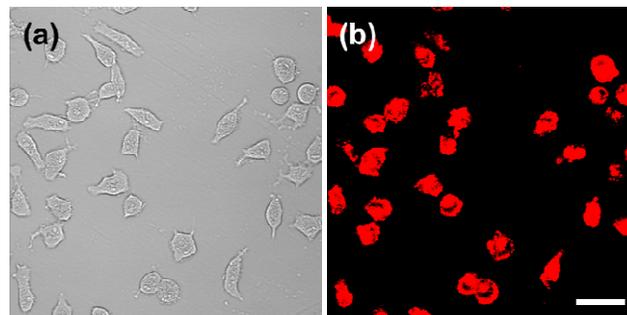


Figure S18. TPFM images of the AIE dots treated HeLa cells. The scale bar indicates 50 μm .

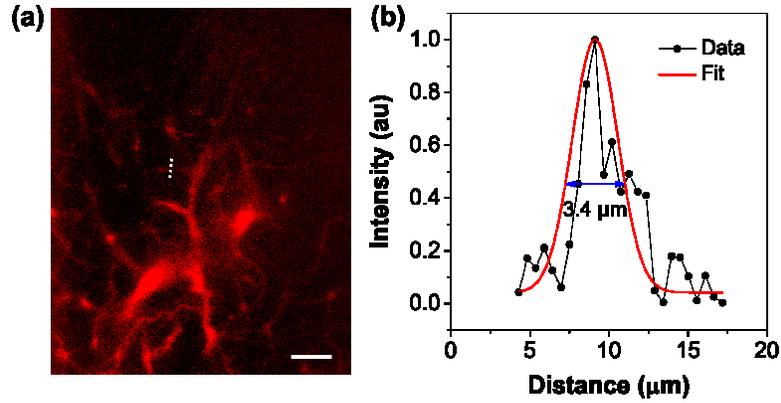


Figure S19. The full width at half-maximum (FWHM) of a blood vessel from TPFM image of mouse brain at 600 μm as indicated with the dotted white line in (a). The scale bar indicates 100 μm.

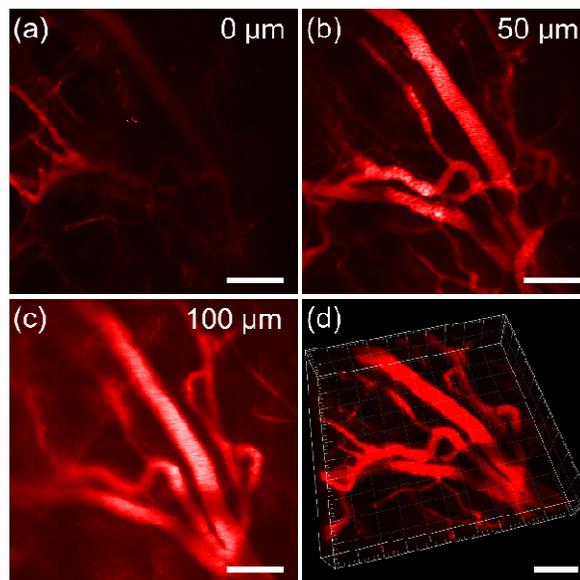


Figure S20. (a-c) *In vivo* TPFM images at different vertical depths and (d) 3D reconstruction of the AIE dots-stained mouse ear. The scale bars indicate 100 μm.

Video S1.

In vivo confocal fluorescence imaging of blood vessels in the brain of mouse treated with the AIE dots at various vertical depths (0-700 μm).

Video S2.

In vivo confocal fluorescence imaging of blood vessels in the ear of mouse treated with the AIE dots at various vertical depths (0-100 μm).

Video S3.

In vivo TPFM imaging of blood vessels in the ear of mouse treated with the AIE dots at various vertical depths (0-100 μm).

Table S1. Cartesian coordinates of optimized TQ-BPN calculated by the DFT, B3LYP/6-31G(d), Gaussian 09 program.

Atom	X	Y	Z
C	-0.70693	-2.33829	-0.28535
C	0.75531	-2.31564	-0.31614
C	1.49675	-1.09737	-0.31789
C	0.71501	0.07581	-0.33236
C	-0.7387	0.05126	-0.37802
C	-1.48233	-1.14422	-0.30285
C	2.97445	-1.10279	-0.28461
C	-2.95463	-1.17068	-0.24461
C	-3.70582	-2.09557	-0.99248
C	-5.09389	-2.11559	-0.9401
C	-5.79208	-1.22518	-0.10667
C	-5.05031	-0.30776	0.65842
C	-3.66557	-0.27792	0.57995
C	3.70592	-0.24713	0.56179
C	5.09252	-0.28767	0.6077

C	5.81494	-1.17355	-0.21015
C	5.09679	-2.01936	-1.07109
C	3.70776	-1.99144	-1.09249
N	7.23168	-1.18748	-0.15959
C	7.97074	-2.37804	-0.38949
C	7.92221	0.06479	-0.0932
N	-7.20627	-1.22614	-0.03044
C	-7.88536	0.03394	0.01422
C	-7.96064	-2.41615	-0.21165
C	-9.1803	-2.38993	-0.90598
C	-9.93579	-3.55331	-1.04529
C	-9.48783	-4.76233	-0.51314
C	-8.27209	-4.7926	0.17432
C	-7.51736	-3.63384	0.33532
C	-7.68408	0.95381	-0.99819
C	-8.3333	2.20787	-0.98087
C	-9.19458	2.52979	0.04244
C	-9.42547	1.61758	1.10632
C	-8.75405	0.34914	1.11062
C	9.18228	-2.34225	-1.09784
C	9.92342	-3.50821	-1.28443
C	9.46891	-4.7294	-0.78679
C	8.26097	-4.76926	-0.08608
C	7.52082	-3.60873	0.12222
C	8.81813	0.34069	0.992
C	9.50246	1.60205	1.0086
C	9.25779	2.54654	-0.0235
C	8.37019	2.26255	-1.03539
C	7.70781	1.01589	-1.07363
C	9.03959	-0.56838	2.0613
C	9.90779	-0.25716	3.08364
C	10.59994	0.97702	3.08971
C	10.39735	1.88439	2.07602
C	-10.29358	1.93912	2.18471
C	-10.48283	1.06256	3.22768
C	-9.80336	-0.1786	3.24136
C	-8.96087	-0.52737	2.20968
N	-1.21368	-3.58437	-0.21926
S	0.0594	-4.60859	-0.20813
N	1.29936	-3.54717	-0.27531
N	1.34428	1.29028	-0.27052
C	0.66643	2.40783	-0.35642
C	-0.76592	2.36602	-0.65806
N	-1.40792	1.22507	-0.6014

C	-1.56091	3.53783	-1.1172
C	1.43259	3.65396	-0.08449
C	-2.9222	3.61857	-0.77935
C	-3.70659	4.67193	-1.24163
C	-3.15091	5.65153	-2.06793
C	-1.8055	5.56782	-2.42963
C	-1.01384	4.52324	-1.95551
C	0.86822	4.73022	0.61998
C	1.63532	5.85164	0.93054
C	2.97224	5.92093	0.53531
C	3.54414	4.85336	-0.16067
C	2.78463	3.72539	-0.4603
H	-3.19512	-2.79404	-1.64449
H	-5.64351	-2.82188	-1.55206
H	-5.56926	0.37308	1.3246
H	-3.11786	0.42627	1.19526
H	3.17688	0.44458	1.20425
H	5.62732	0.36468	1.28981
H	5.62984	-2.69935	-1.72619
H	3.18195	-2.65807	-1.76559
H	-9.53206	-1.45758	-1.33344
H	-10.87756	-3.5115	-1.58512
H	-10.07656	-5.66686	-0.6294
H	-7.91165	-5.72332	0.60318
H	-6.58271	-3.6646	0.88471
H	-7.01647	0.69792	-1.81461
H	-8.15818	2.90806	-1.7922
H	-9.70569	3.4886	0.05486
H	9.53894	-1.40022	-1.49924
H	10.85904	-3.45831	-1.83424
H	10.04634	-5.63577	-0.93974
H	7.8954	-5.70976	0.31639
H	6.59245	-3.64785	0.68154
H	9.77904	3.49953	0.00452
H	8.18454	2.98768	-1.82218
H	7.02061	0.78924	-1.88246
H	8.51206	-1.51471	2.06459
H	10.06169	-0.96339	3.89414
H	11.28552	1.20717	3.89993
H	10.91708	2.83895	2.07853
H	-10.80386	2.89869	2.17154
H	-11.14824	1.32239	4.04568
H	-9.94678	-0.8604	4.07437
H	-8.44306	-1.47889	2.22788

H	-3.35477	2.83852	-0.16298
H	-4.75465	4.72453	-0.96137
H	-3.76365	6.47087	-2.43254
H	-1.36963	6.31559	-3.08557
H	0.02802	4.46585	-2.25024
H	-0.16769	4.68525	0.93769
H	1.18744	6.67093	1.48506
H	3.566	6.79895	0.77233
H	4.58559	4.89707	-0.46574
H	3.226	2.88212	-0.97988
