

Electronic Supplementary Information:

Using C₆₀-bodipy dyads that show strong absorption of visible light and long-lived triplet excited states as organic triplet photosensitizers for triplet-triplet annihilation upconversion

Pei Yang, Wanhua Wu, Jianzhang Zhao,* Dandan Huang and Xiuyu Yi

State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology,

E-208 West Campus, 2 Ling-Gong Road, Dalian 116024, P. R. China

E-mail: zhaojzh@dlut.edu.cn

Group homepage: <http://finechem.dlut.edu.cn/photochem>

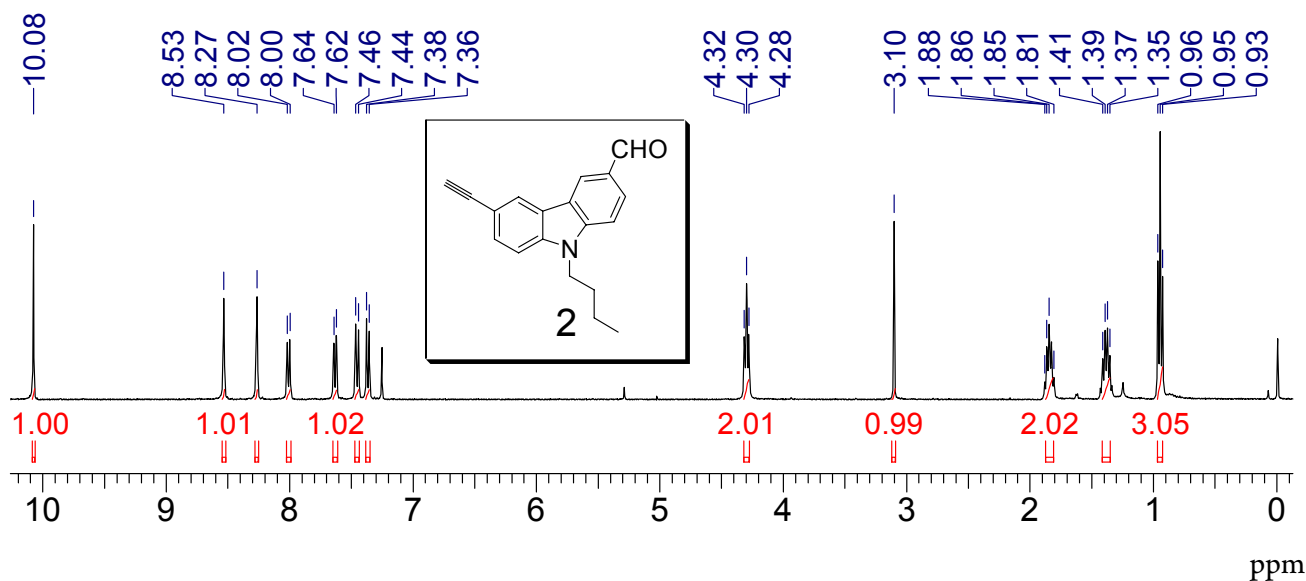


Fig. S1 ^1H NMR of compound **2** (CDCl_3 , 400 MHz).

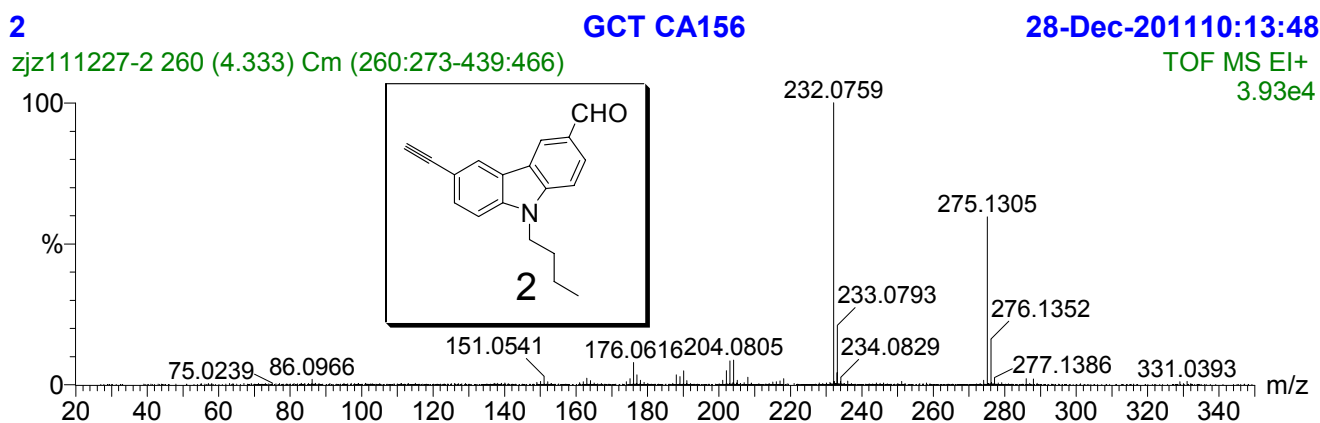


Fig. S2 TOF MS EI+ of compound **2**.

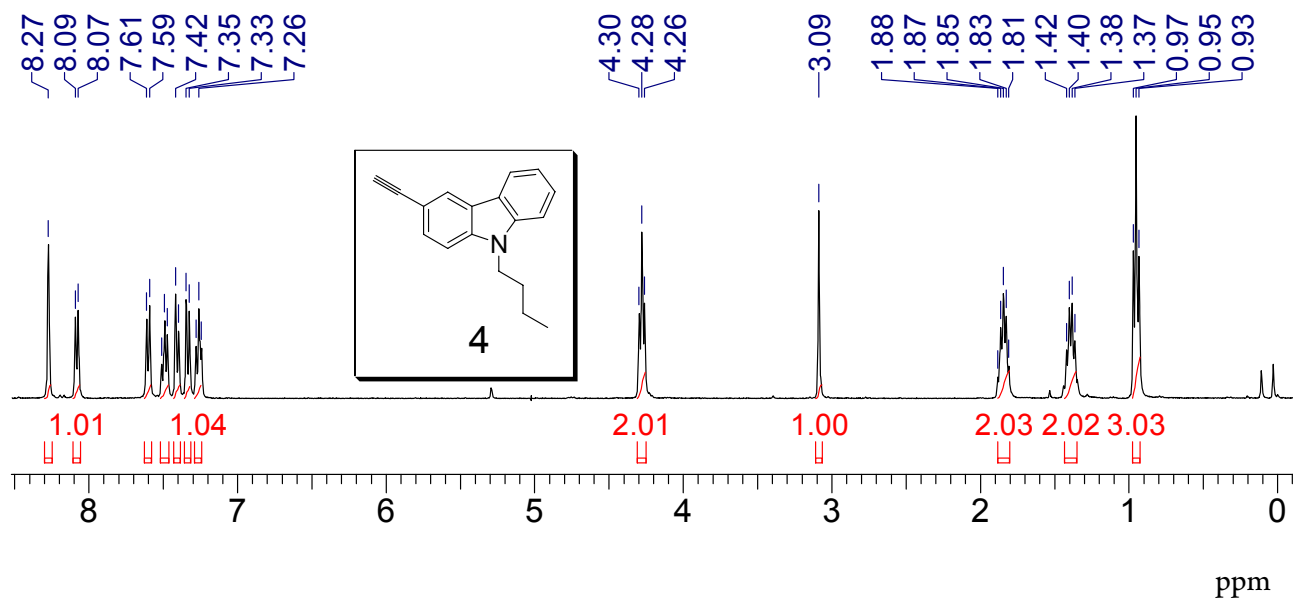


Fig. S3 ^1H NMR of compound 4 (CDCl_3 , 400 MHz).

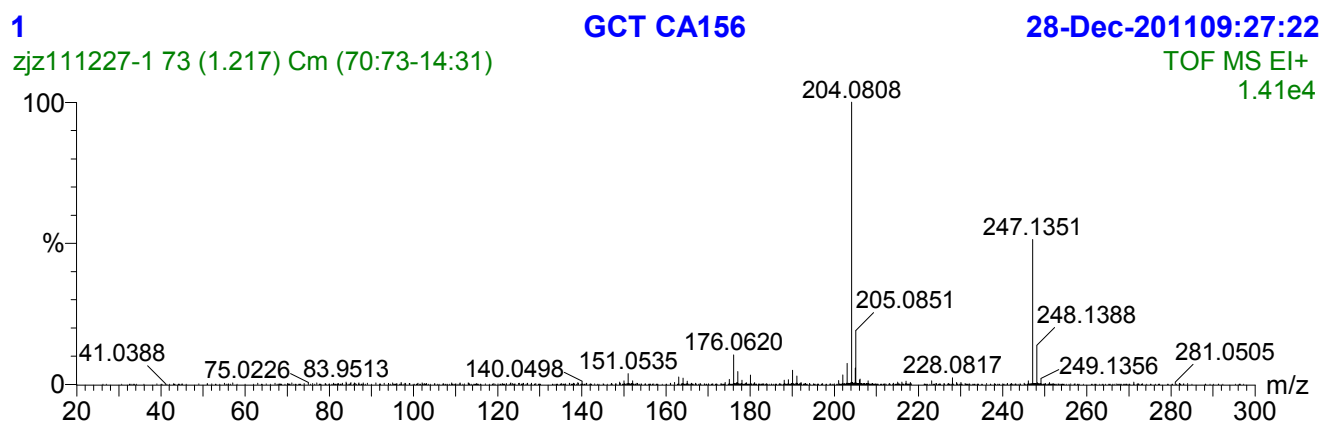
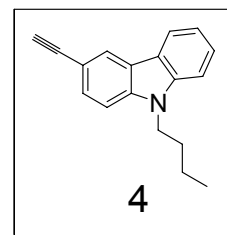


Fig. S4 TOF MS EI+ of compound 4.



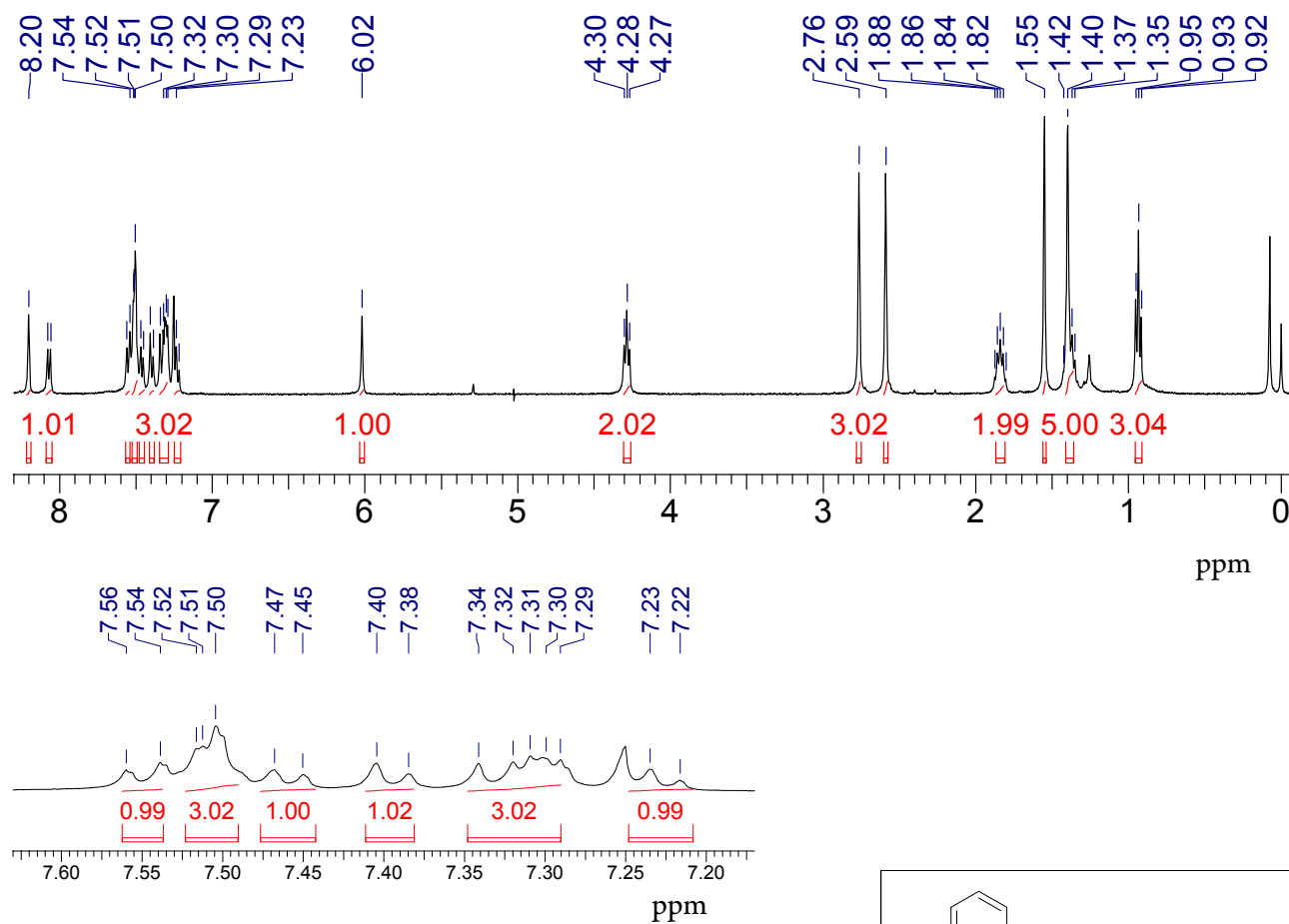
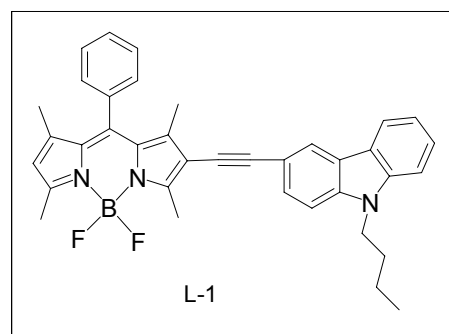


Fig. S5 ¹H NMR of compound L-1 (CDCl₃, 400 MHz).



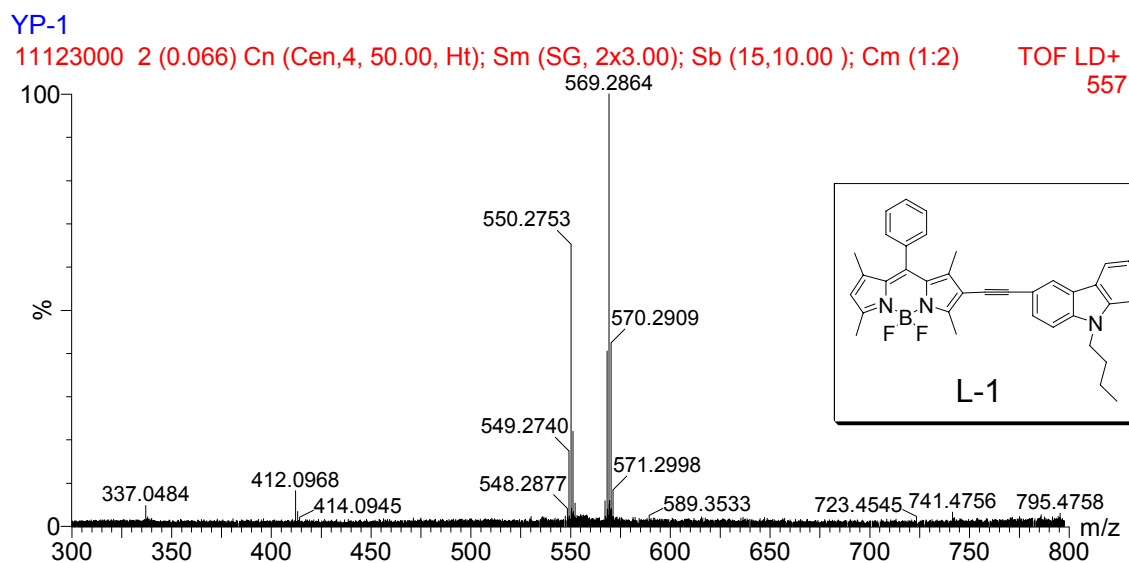


Fig. S6 TOF MS LD+ of compound L-1.

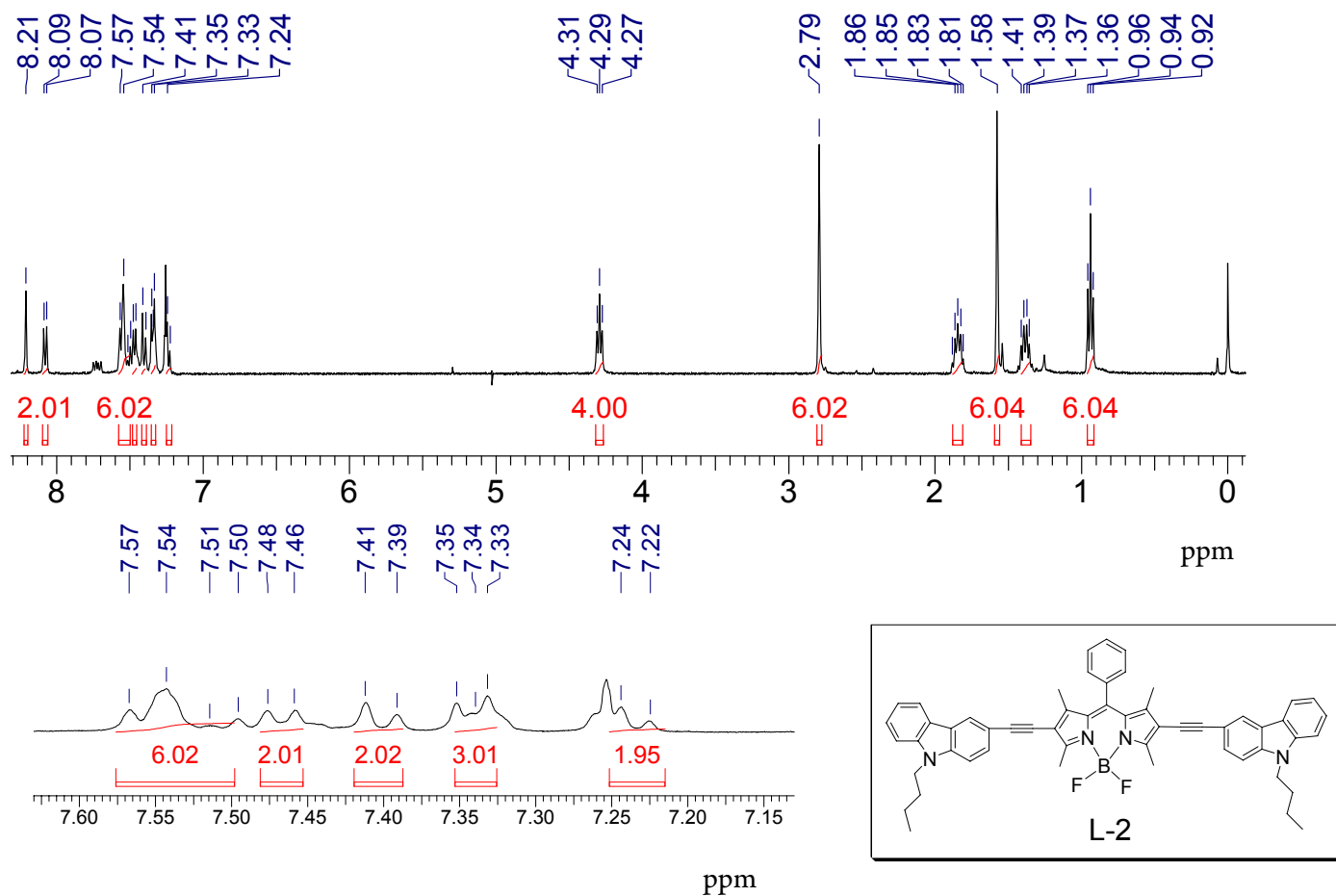


Fig. S7 ^1H NMR of compound L-2 (CDCl_3 , 400 MHz).

YP-1

12010703 1 (0.034) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (1:4) TOF LD+ 3.52e3

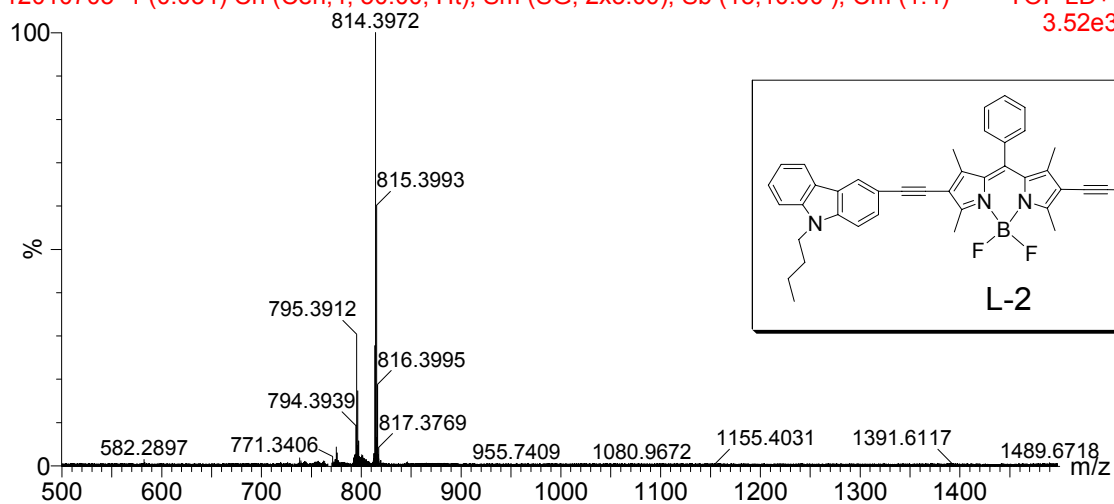


Fig. S8 TOF MS LD+ of compound L-2.

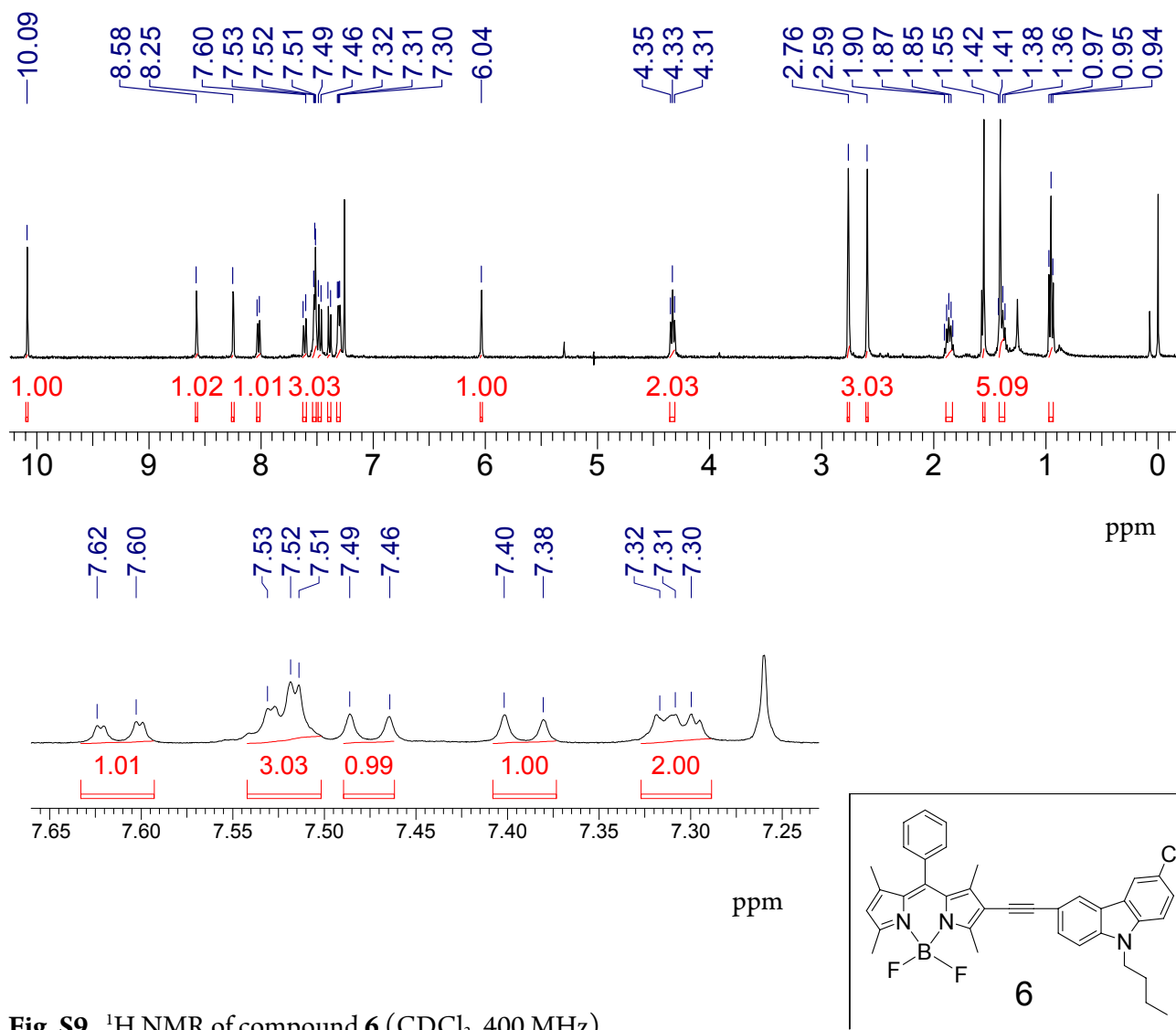
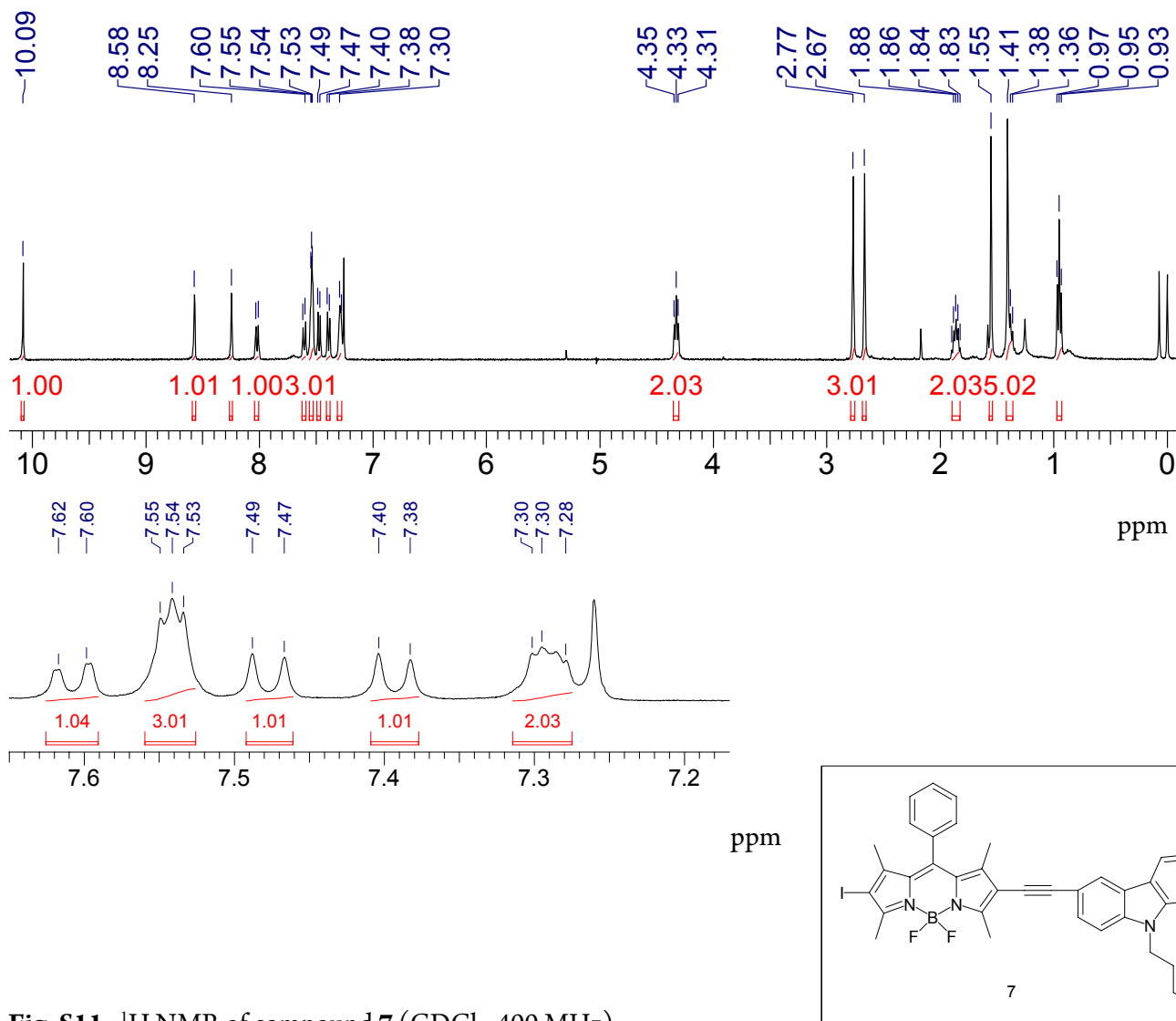
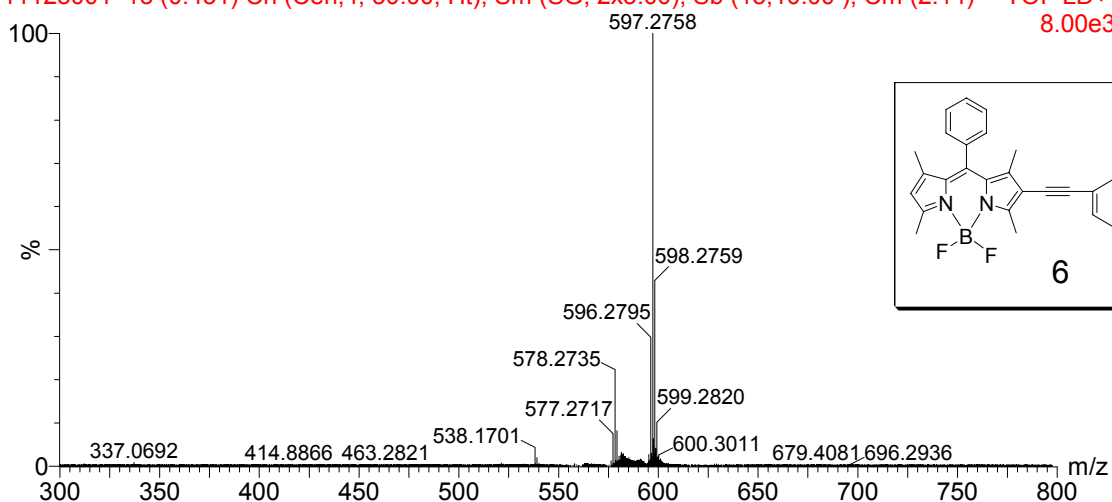


Fig. S9 ^1H NMR of compound 6 (CDCl_3 , 400 MHz).

YP-2

11123001 13 (0.431) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (2:14) TOF LD+
8.00e3



YP

12021608 1 (0.031) Cn (Cen,4, 50.00, Ht); Sm (SG, 3x5.00); Sb (15,10.00); Cm (1:8) TOF LD+
2.65e3

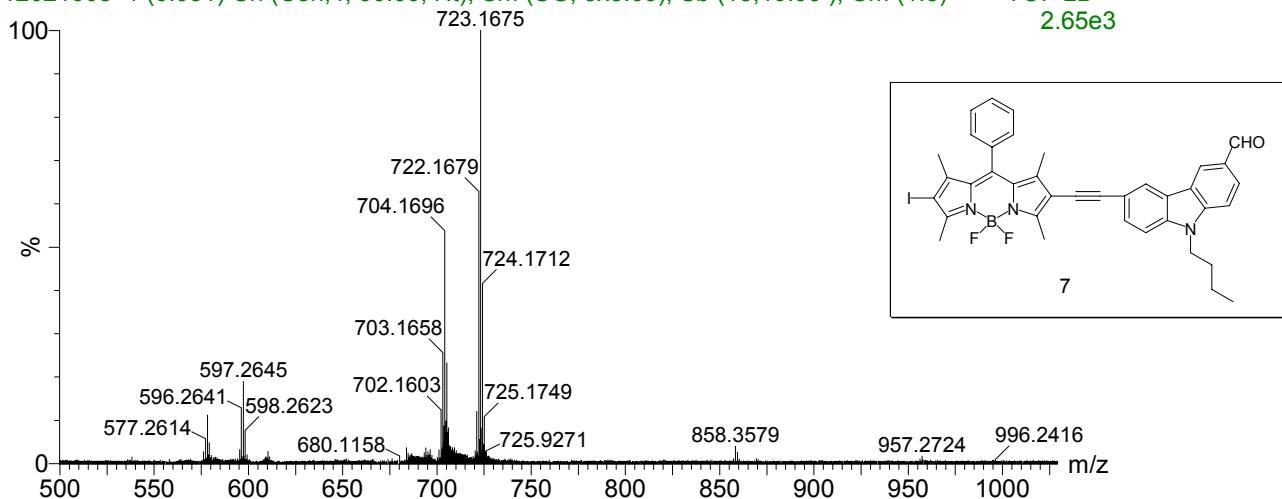


Fig. S12 TOF MS LD+ of compound 7.

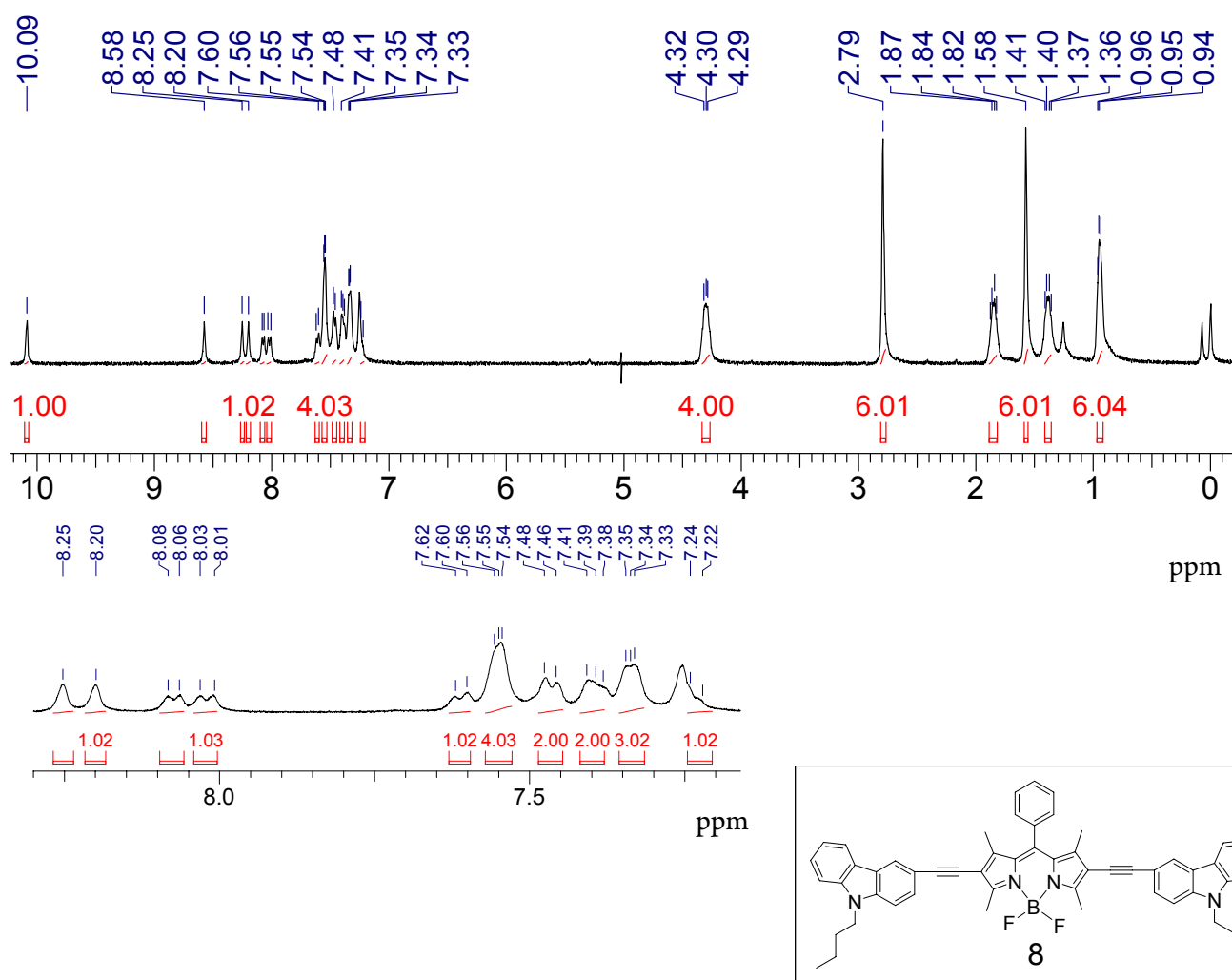


Fig. S13 ^1H NMR of compound 8 (CDCl_3 , 400 MHz).

YP-2

12010704 13 (0.431) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (12:13) TOF LD+
1.12e3

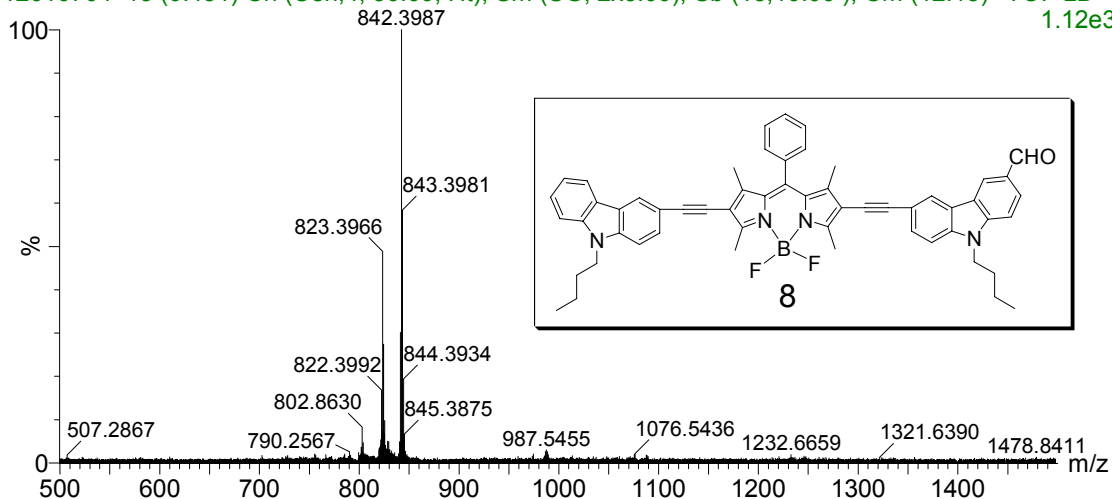


Fig. S14 TOF MS LD+ of compound 8.

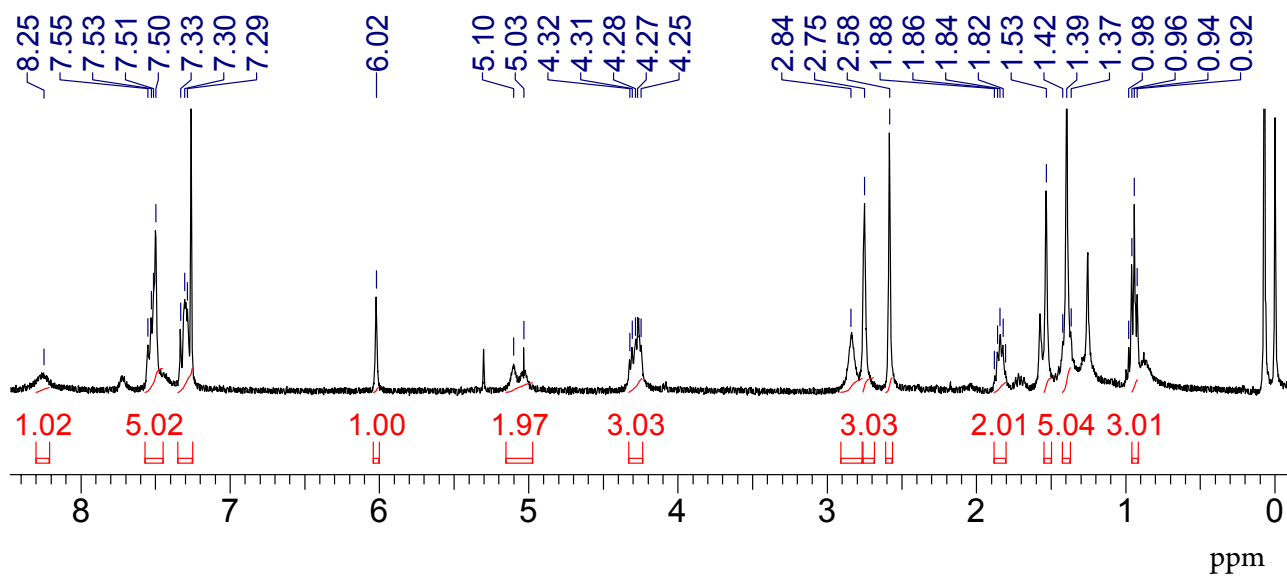
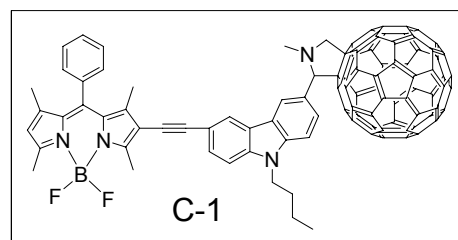


Fig. S15 ^1H NMR of compound C-1 (CDCl_3 , 400 MHz).



YP(CHCA)

11112310 25 (0.833) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (25:27) TOF LD+
263

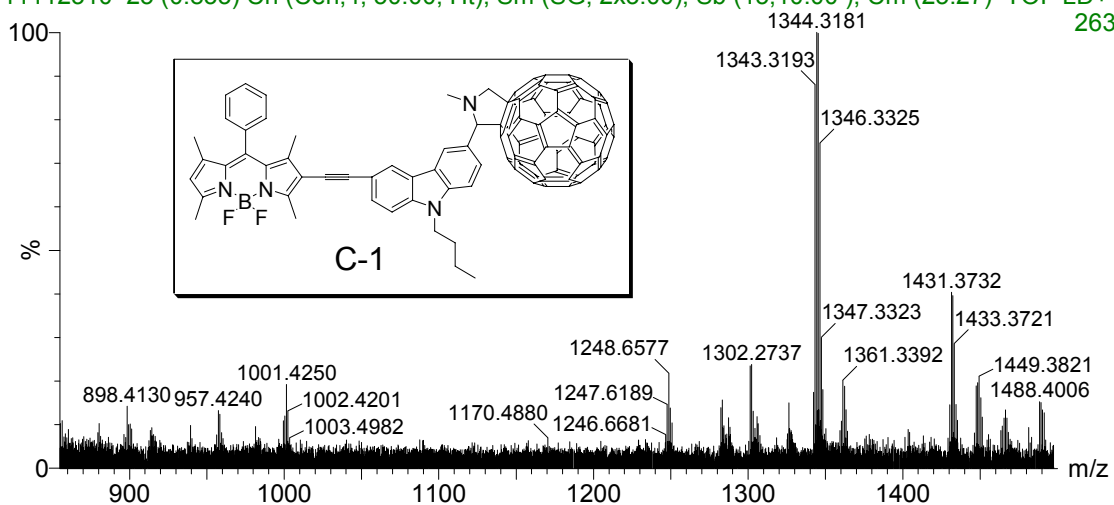


Fig. S16 TOF MS LD+ of compound C-1.

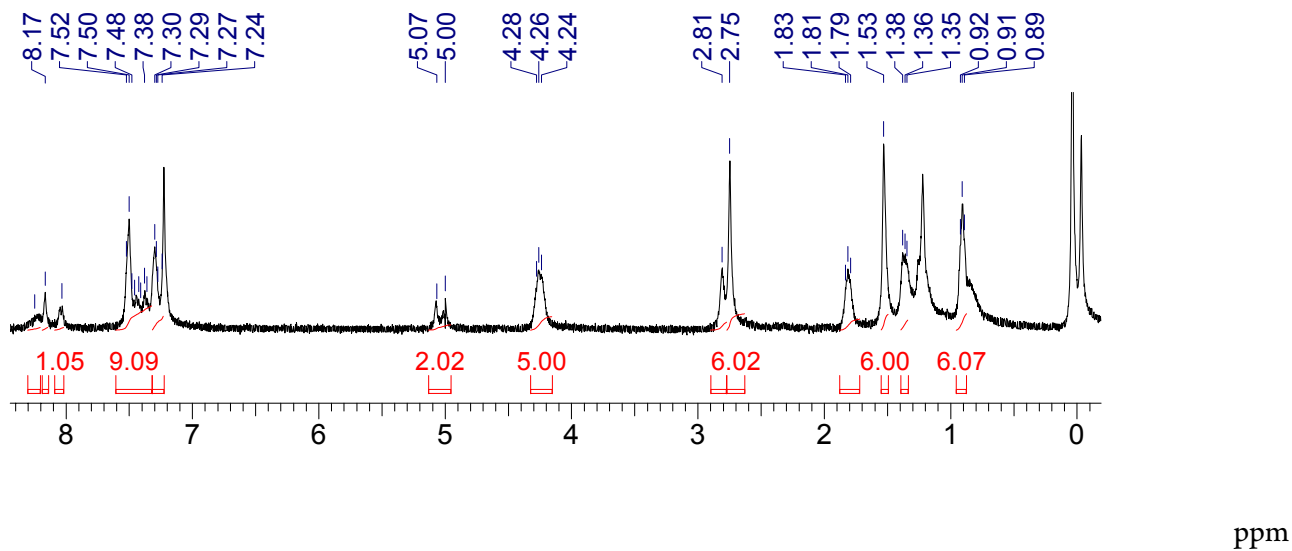
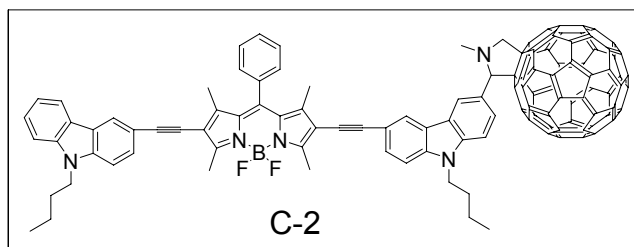


Fig. S17 ¹H NMR of compound C-2 (CDCl₃, 400 MHz).



YP-3(CHCA)

12010705 8 (0.264) Cn (Cen,4, 50.00, Ht); Sm (SG, 2x3.00); Sb (15,10.00); Cm (8:14)

TOF LD-
1.07e3

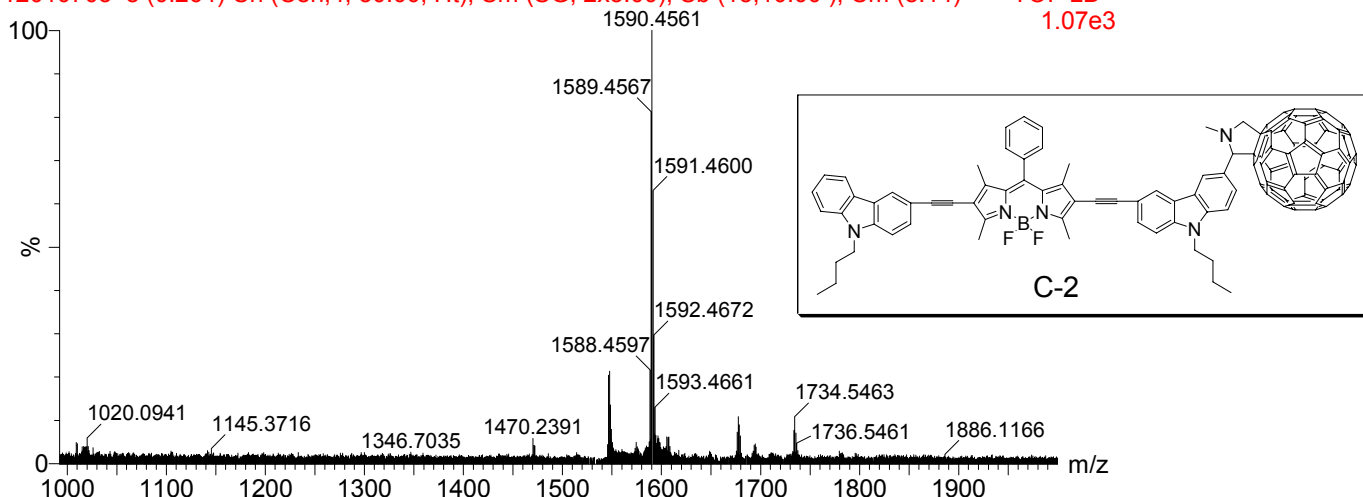


Fig. S18 TOF MS LD- of compound C-2.

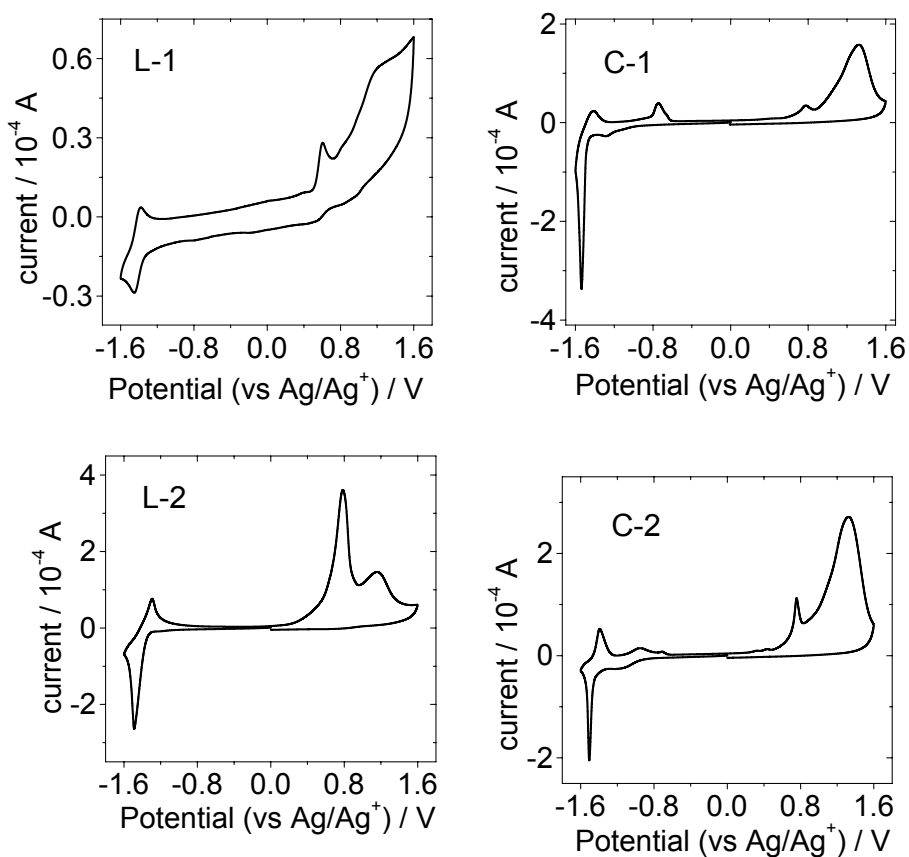


Fig. S19 Cyclic voltammograms of L-1, L-2, C-1 and C-2 in deaerated CH₃CN with 0.1M [NBu₄][PF₆] at a scan rate of 100 mV s⁻¹ [all versus Ag/Ag⁺ electrode] at room temperature. 20 °C.

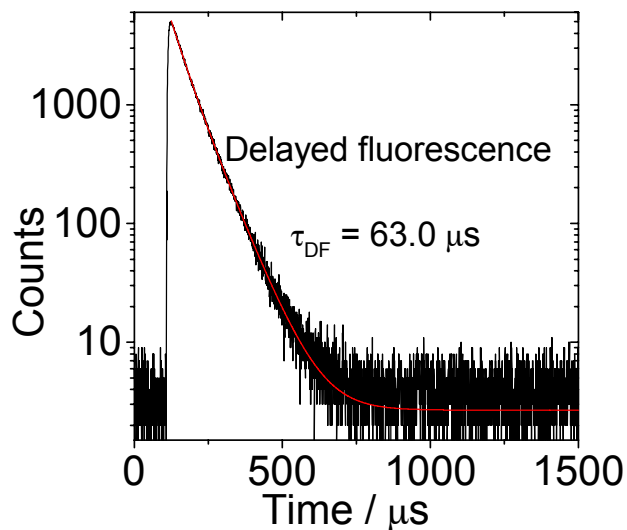


Fig. S20 Delayed fluorescence observed in the TTA upconversion with **C-2** as triplet photosensitizer and perylene as the triplet acceptor. Excited at 589 nm (nanosecond pulsed OPO laser, synchronized with spectrofluorometer), the decay trace was monitored at 470 nm. Under this circumstance **C-2** was selectively excited and the emission is due to the upconverted emission of perylene. In deaerated toluene. c [Sensitizer] = 5.0×10^{-6} M; c [Perylene] = 3.0×10^{-4} M, 20 °C.

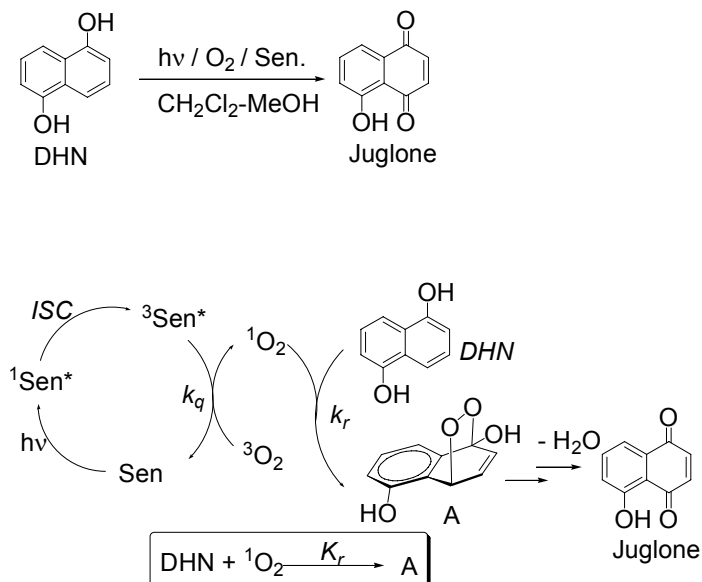


Fig. S21 Mechanism for the photooxidation of DHN with a sensitizer.

Please refer to Takizawa, S.; Aboshi, R.; Murata, S. *Photochem. Photobiol. Sci.* **2011**, *10*, 895–903.

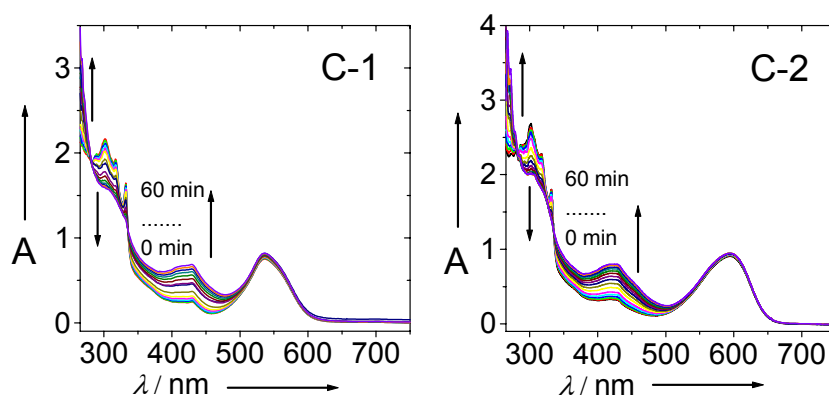
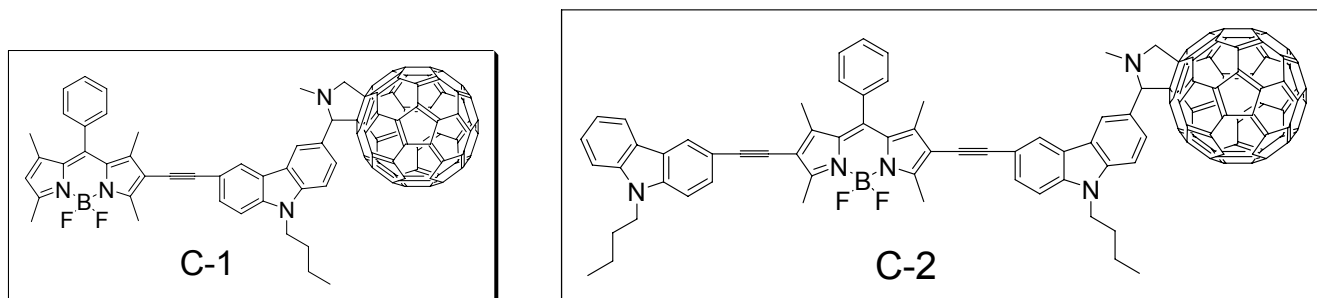


Fig. S22 Absorption spectral change for the photooxidation of DHN using compounds **C-1** and **C-2**, and the components as sensitizers. A CH₂Cl₂-MeOH (9:1) solution containing DHN (1.5×10^{-4} M) and sensitizers (10 mol% vs. DHN) was irradiated using a xenon arc lamp through a cut-off filter (>385 nm)(sodium nitrite aqueous solution 50 g/L: it can filtrate UV-light under 385nm) for 60 min.



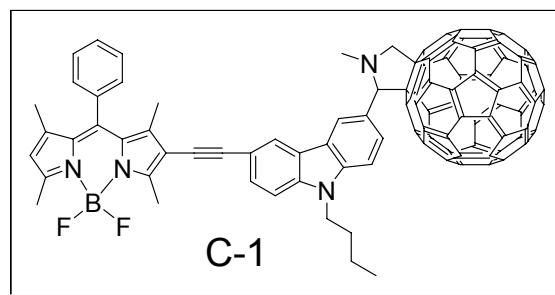
The coordinates of the compounds (optimized geometry).

Compound C-1 (DFT//B3LYP/6-31G(d))

Ground state

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



| | | | |
|---|--------------|-------------|-------------|
| C | -11.86390300 | -4.29877500 | 0.73321200 |
| C | -13.39662200 | -2.77751400 | 0.02231400 |
| C | -13.22643200 | -4.09344100 | 0.43609200 |
| C | -12.09302600 | -2.17561900 | 0.07245200 |
| C | -11.65005900 | -0.87852700 | -0.22818600 |
| C | -10.29433400 | -0.52377300 | -0.09506400 |
| C | -9.60284000 | 0.69948000 | -0.34021300 |
| C | -8.25160700 | 0.45347800 | -0.03213200 |
| C | -8.14469600 | -0.90254100 | 0.39098100 |
| N | -11.18922600 | -3.15193700 | 0.51478700 |
| N | -9.35892100 | -1.47105500 | 0.34968400 |
| B | -9.66577400 | -2.94986600 | 0.73197500 |
| F | -9.33478700 | -3.17285900 | 2.07033800 |
| F | -8.94187100 | -3.81319600 | -0.09223900 |
| C | -14.71170500 | -2.17878400 | -0.38147600 |
| H | -14.97654300 | -1.31156700 | 0.23237800 |
| H | -14.70658800 | -1.83722300 | -1.42212300 |
| H | -15.50416100 | -2.92575800 | -0.27448100 |
| C | -6.91310600 | -1.62909000 | 0.81526100 |
| H | -6.05754800 | -0.95068100 | 0.81615100 |
| H | -7.04401400 | -2.05369400 | 1.81570700 |
| H | -6.70885100 | -2.46604400 | 0.13871600 |
| C | -10.12476700 | 2.01695100 | -0.82657300 |
| H | -10.86602700 | 2.44324700 | -0.14217300 |
| H | -9.29668100 | 2.72558300 | -0.91687200 |
| H | -10.61086100 | 1.93048500 | -1.80390500 |
| C | -11.20520300 | -5.54870600 | 1.21835300 |
| H | -10.73183800 | -5.38295100 | 2.19220300 |
| H | -11.93742200 | -6.35436400 | 1.31033900 |
| H | -10.41248300 | -5.86138700 | 0.53044500 |
| C | -12.63459600 | 0.14503100 | -0.69599500 |
| C | -12.91687900 | 0.28587000 | -2.06148500 |
| C | -13.28606700 | 0.97319600 | 0.22805900 |
| C | -13.83740800 | 1.24174100 | -2.49554300 |
| C | -14.20698900 | 1.92757000 | -0.20822000 |

| | | | |
|---|--------------|-------------|-------------|
| H | -13.07051300 | 0.86727600 | 1.28771300 |
| H | -14.04821200 | 1.34275600 | -3.55659500 |
| H | -14.70678000 | 2.56386800 | 0.51692200 |
| C | -14.48423200 | 2.06391300 | -1.57024700 |
| H | -15.20055000 | 2.80724400 | -1.90885100 |
| H | -12.41401100 | -0.35391900 | -2.78148500 |
| C | -5.11024500 | 3.00851100 | -0.28568600 |
| C | -5.25590300 | 4.28913100 | -0.88204900 |
| C | -3.85372500 | 2.61676600 | 0.21028700 |
| C | -4.18778300 | 5.16895600 | -0.99771700 |
| H | -6.23246300 | 4.58135200 | -1.25504800 |
| C | -2.77039500 | 3.48775200 | 0.10326600 |
| H | -3.73938700 | 1.64003700 | 0.67064600 |
| C | -2.94079500 | 4.75942500 | -0.51062300 |
| H | -4.32963400 | 6.14444200 | -1.45201300 |
| C | -1.37868800 | 3.40602000 | 0.49631400 |
| C | -0.77443500 | 4.62613600 | 0.09840300 |
| C | -0.60930800 | 2.43164100 | 1.13851300 |
| C | 0.58184400 | 4.86761800 | 0.33770500 |
| C | 0.75011000 | 2.64805100 | 1.38429800 |
| H | -1.07117400 | 1.49808400 | 1.45242200 |
| C | 1.32372800 | 3.87382500 | 0.97042500 |
| H | 1.05653900 | 5.79801200 | 0.04201100 |
| H | 2.37996700 | 4.05807400 | 1.13005500 |
| C | -7.16922400 | 1.35925700 | -0.12014000 |
| C | -6.22603800 | 2.12729900 | -0.19566300 |
| N | -1.72541800 | 5.42780200 | -0.52088200 |
| C | -1.50354600 | 6.76942200 | -1.02464400 |
| H | -1.68972900 | 7.53101000 | -0.25714300 |
| H | -0.47233300 | 6.86249700 | -1.37294500 |
| H | -2.16435900 | 6.95489500 | -1.87486100 |
| C | 4.23440300 | 1.84085600 | -2.04448200 |
| C | 5.62572000 | 2.24485700 | -2.13057900 |
| C | 6.51972400 | 1.52074100 | -2.91962900 |
| C | 6.05834400 | 0.34903200 | -3.64729100 |
| C | 4.71914900 | -0.03918300 | -3.56955800 |
| C | 3.78740000 | 0.72570100 | -2.76120700 |
| C | 3.77034300 | 2.08409700 | -0.69672600 |
| C | 4.90296100 | 2.65389300 | 0.06828600 |
| C | 6.03464500 | 2.74250000 | -0.82966400 |
| C | 7.33150600 | 2.49427800 | -0.36719000 |
| C | 7.86140700 | 1.24865400 | -2.42926800 |
| C | 7.10837000 | -0.64904000 | -3.59550300 |
| C | 6.78291800 | -2.00074200 | -3.46462800 |
| C | 5.39123800 | -2.40744200 | -3.38160700 |

| | | | |
|---|------------|-------------|-------------|
| C | 4.37922000 | -1.44672200 | -3.43406000 |
| C | 3.23851600 | -1.54565600 | -2.54020100 |
| C | 2.87901400 | -0.19829200 | -2.12749400 |
| C | 2.46337400 | 0.04361800 | -0.81298200 |
| C | 2.88099800 | 1.21893200 | -0.09637900 |
| C | 5.09004500 | 2.31932800 | 1.39245700 |
| C | 4.04765400 | 1.58865200 | 2.24615200 |
| C | 2.80846800 | 0.97499500 | 1.41604100 |
| C | 2.75255500 | -0.55935100 | 1.42812600 |
| C | 2.37835400 | -1.05423600 | 0.13158000 |
| C | 2.70456200 | -2.35384400 | -0.27147500 |
| C | 3.15177400 | -2.60049400 | -1.63280100 |
| C | 4.20191000 | -3.60285900 | -1.57890100 |
| C | 5.30071900 | -3.50772100 | -2.43513100 |
| C | 8.22338000 | -0.09288600 | -2.84297400 |
| C | 7.93679800 | -3.57864900 | 0.15612700 |
| C | 8.82097500 | -2.68989700 | -0.45933600 |
| C | 9.28898200 | -1.51783000 | 0.25902400 |
| C | 8.85664700 | -1.28077900 | 1.56545400 |
| C | 7.93554500 | -2.20661100 | 2.20555200 |
| C | 6.08826800 | -3.72799000 | 1.59603400 |
| C | 5.68182000 | -4.23130900 | 0.29356500 |
| C | 6.82194000 | -4.13492800 | -0.59688300 |
| C | 6.63663000 | -3.77921700 | -1.93448000 |
| C | 7.55355300 | -2.84916300 | -2.57140900 |
| C | 8.62279300 | -2.31622400 | -1.84950800 |
| C | 9.37895600 | -0.41775900 | -0.68771600 |
| C | 9.03243400 | 0.87492600 | -0.28999400 |
| C | 8.58110600 | 1.11964900 | 1.06867700 |
| C | 8.49357600 | 0.06465400 | 1.97591000 |
| C | 7.34911400 | -0.03660400 | 2.86723300 |
| C | 7.00908200 | -1.43127900 | 3.00999000 |
| C | 5.66147000 | -1.80110300 | 3.07896800 |
| C | 5.19652800 | -2.97275800 | 2.35852400 |
| C | 4.39598200 | -3.97178100 | -0.18539000 |
| C | 3.46548200 | -3.19890700 | 0.61611200 |
| C | 3.86007100 | -2.69944500 | 1.86200000 |
| C | 3.48730900 | -1.36243000 | 2.27058900 |
| C | 4.62022300 | -0.79771500 | 3.03552000 |
| C | 4.94281500 | 0.53440700 | 2.91241800 |
| C | 6.32468100 | 0.91485100 | 2.79869700 |
| C | 6.41707500 | 2.01566600 | 1.85755500 |
| C | 7.52785500 | 2.12088800 | 1.01250900 |
| C | 8.96669300 | -0.91131900 | -1.98962500 |
| C | 8.25842300 | 1.72671100 | -1.17876800 |

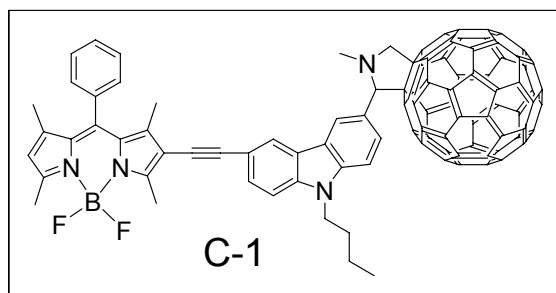
| | | | |
|---|--------------|-------------|------------|
| C | 7.48483000 | -3.33154400 | 1.51127700 |
| C | 3.35500900 | 2.50042400 | 3.30271000 |
| C | 1.51972500 | 1.56136600 | 2.13588900 |
| H | 3.89492700 | 2.49261500 | 4.25611200 |
| H | 3.33375300 | 3.54805200 | 2.95361800 |
| H | 0.80954400 | 0.73765300 | 2.27238500 |
| N | 2.04299500 | 1.90738200 | 3.46287800 |
| C | 1.14221000 | 2.60186500 | 4.36731700 |
| H | 0.89670200 | 3.62861500 | 4.04662700 |
| H | 0.20645800 | 2.03970600 | 4.45434500 |
| H | 1.60237500 | 2.65219300 | 5.36026800 |
| H | -14.00169600 | -4.84422500 | 0.52098700 |

Compound C-1 (DFT//B3LYP/6-31G(d))

Symbolic Z-matrix:

Triplet state

Charge = 0 Multiplicity = 3



| | | | |
|---|--------------|-------------|-------------|
| C | -11.87662600 | -4.30767200 | 0.71792400 |
| C | -13.40926700 | -2.78675900 | 0.00611200 |
| C | -13.23859400 | -4.10337100 | 0.41733500 |
| C | -12.10650800 | -2.18334000 | 0.06126500 |
| C | -11.66430300 | -0.88521100 | -0.23560300 |
| C | -10.30928000 | -0.52910300 | -0.09805800 |
| C | -9.61856400 | 0.69526700 | -0.33932700 |
| C | -8.26783500 | 0.45022000 | -0.02797200 |
| C | -8.16054600 | -0.90633800 | 0.39318700 |
| N | -11.20275400 | -3.15953800 | 0.50405100 |
| N | -9.37403700 | -1.47609600 | 0.34764200 |
| B | -9.68032800 | -2.95578600 | 0.72695000 |
| F | -9.35390900 | -3.17999100 | 2.06628500 |
| F | -8.95232600 | -3.81708100 | -0.09565800 |
| C | -14.72393100 | -2.18864000 | -0.39988300 |
| H | -14.99111900 | -1.32278800 | 0.21487000 |
| H | -14.71653500 | -1.84519500 | -1.43989600 |
| H | -15.51589900 | -2.93659500 | -0.29622400 |
| C | -6.92929900 | -1.63224400 | 0.81956600 |
| H | -6.07523100 | -0.95199100 | 0.82743300 |
| H | -7.06379500 | -2.06186400 | 1.81736200 |
| H | -6.72004300 | -2.46549800 | 0.13995000 |

| | | | |
|---|--------------|-------------|-------------|
| C | -10.14060300 | 2.01299000 | -0.82490000 |
| H | -10.88338300 | 2.43783900 | -0.14124300 |
| H | -9.31290900 | 2.72238300 | -0.91278900 |
| H | -10.62490600 | 1.92746700 | -1.80319300 |
| C | -11.21772600 | -5.55802300 | 1.20168500 |
| H | -10.74262000 | -5.39265600 | 2.17471200 |
| H | -11.95014600 | -6.36338700 | 1.29459400 |
| H | -10.42633000 | -5.87097700 | 0.51232600 |
| C | -12.64867100 | 0.13809500 | -0.70428800 |
| C | -12.92762800 | 0.28085400 | -2.07025600 |
| C | -13.30330200 | 0.96410700 | 0.21946500 |
| C | -13.84800300 | 1.23651800 | -2.50510400 |
| C | -14.22408100 | 1.91825100 | -0.21761100 |
| H | -13.09034000 | 0.85667900 | 1.27949100 |
| H | -14.05621300 | 1.33903400 | -3.56652200 |
| H | -14.72636700 | 2.55286600 | 0.50728100 |
| C | -14.49800400 | 2.05652700 | -1.58011900 |
| H | -15.21421700 | 2.79967800 | -1.91933400 |
| H | -12.42231100 | -0.35727800 | -2.79001400 |
| C | -5.12900500 | 3.00973000 | -0.26586200 |
| C | -5.27743300 | 4.29691800 | -0.84735200 |
| C | -3.87074300 | 2.61339200 | 0.22188200 |
| C | -4.21048600 | 5.17900100 | -0.95593900 |
| H | -6.25531000 | 4.59244900 | -1.21421600 |
| C | -2.78852000 | 3.48659100 | 0.12174100 |
| H | -3.75427300 | 1.63155000 | 0.67066600 |
| C | -2.96185800 | 4.76511800 | -0.47675900 |
| H | -4.35437400 | 6.15947200 | -1.39869600 |
| C | -1.39570000 | 3.40184800 | 0.50994300 |
| C | -0.79392000 | 4.62744400 | 0.12511600 |
| C | -0.62326200 | 2.42036900 | 1.13739500 |
| C | 0.56272900 | 4.86777300 | 0.36396900 |
| C | 0.73660800 | 2.63560200 | 1.38197200 |
| H | -1.08297000 | 1.48210800 | 1.44016800 |
| C | 1.30759500 | 3.86738100 | 0.98242500 |
| H | 1.03549100 | 5.80236900 | 0.07874600 |
| H | 2.36404700 | 4.05132500 | 1.14096300 |
| C | -7.18635000 | 1.35746100 | -0.11108600 |
| C | -6.24395300 | 2.12693400 | -0.18186200 |
| N | -1.74728800 | 5.43510500 | -0.48209900 |
| C | -1.52849600 | 6.78253700 | -0.97177700 |
| H | -1.71810600 | 7.53550700 | -0.19669900 |
| H | -0.49706200 | 6.88205000 | -1.31747300 |
| H | -2.18854300 | 6.97483000 | -1.82109200 |
| C | 4.25755000 | 1.89437200 | -2.04723800 |

| | | | |
|---|------------|-------------|-------------|
| C | 5.64444300 | 2.30016300 | -2.11579300 |
| C | 6.55104300 | 1.56982000 | -2.89988400 |
| C | 6.09876300 | 0.39830400 | -3.62416600 |
| C | 4.76323800 | 0.00812100 | -3.56633200 |
| C | 3.81934200 | 0.77593600 | -2.77064800 |
| C | 3.77781900 | 2.12397900 | -0.70106600 |
| C | 4.90117000 | 2.68667100 | 0.07858100 |
| C | 6.04057400 | 2.78361800 | -0.81078400 |
| C | 7.33238400 | 2.52089200 | -0.33205400 |
| C | 7.87701900 | 1.28142500 | -2.38983800 |
| C | 7.15624100 | -0.60817400 | -3.56999200 |
| C | 6.82074900 | -1.97390100 | -3.45686600 |
| C | 5.44629600 | -2.37507600 | -3.39240800 |
| C | 4.41924300 | -1.40267200 | -3.44670500 |
| C | 3.29473900 | -1.50112300 | -2.56732900 |
| C | 2.91435600 | -0.15339200 | -2.15144500 |
| C | 2.48772100 | 0.07501800 | -0.84039600 |
| C | 2.88726800 | 1.24755900 | -0.11530900 |
| C | 5.07696900 | 2.33365400 | 1.40120300 |
| C | 4.03343600 | 1.58293300 | 2.23483400 |
| C | 2.80902000 | 0.97870900 | 1.39203000 |
| C | 2.75847600 | -0.55607300 | 1.37866700 |
| C | 2.39814900 | -1.03100800 | 0.10200300 |
| C | 2.73820900 | -2.34725100 | -0.32042400 |
| C | 3.19714000 | -2.57257500 | -1.65083600 |
| C | 4.24607100 | -3.59199600 | -1.60706900 |
| C | 5.34549400 | -3.48623200 | -2.45461700 |
| C | 8.24646300 | -0.06684000 | -2.81401700 |
| C | 7.95985000 | -3.60383400 | 0.15124700 |
| C | 8.84202900 | -2.70161100 | -0.44776400 |
| C | 9.28914700 | -1.52762200 | 0.28257000 |
| C | 8.84208500 | -1.30935400 | 1.58310100 |
| C | 7.93223800 | -2.24683700 | 2.20908900 |
| C | 6.10214900 | -3.77825900 | 1.57479100 |
| C | 5.70769600 | -4.26229400 | 0.26662100 |
| C | 6.85306000 | -4.15355000 | -0.61693100 |
| C | 6.67697800 | -3.77632300 | -1.95004500 |
| C | 7.59130700 | -2.83249200 | -2.56700700 |
| C | 8.65129200 | -2.30653900 | -1.83171300 |
| C | 9.38771700 | -0.41769600 | -0.65690700 |
| C | 9.03263900 | 0.88842800 | -0.24387100 |
| C | 8.56109500 | 1.11393400 | 1.08793300 |
| C | 8.45587900 | 0.03909500 | 1.99951000 |
| C | 7.33047100 | -0.06644200 | 2.86820700 |
| C | 6.98879700 | -1.47260400 | 2.99521700 |

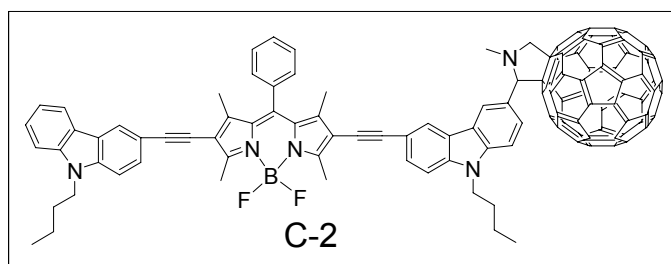
| | | | |
|---|--------------|-------------|-------------|
| C | 5.65082900 | -1.84965100 | 3.05289700 |
| C | 5.19714500 | -3.02408700 | 2.33922000 |
| C | 4.42530700 | -3.98790500 | -0.22521100 |
| C | 3.49754700 | -3.20619600 | 0.57162800 |
| C | 3.87810500 | -2.72991600 | 1.82207800 |
| C | 3.50557800 | -1.37852000 | 2.23983200 |
| C | 4.59728300 | -0.83659600 | 2.99805400 |
| C | 4.93146100 | 0.52420300 | 2.89187200 |
| C | 6.28679500 | 0.90068800 | 2.80253200 |
| C | 6.39518900 | 2.01506200 | 1.87165200 |
| C | 7.51205600 | 2.12988600 | 1.03953600 |
| C | 8.99314700 | -0.89516100 | -1.94928400 |
| C | 8.26431200 | 1.74682100 | -1.13599100 |
| C | 7.49260700 | -3.37554300 | 1.50535600 |
| C | 3.33113900 | 2.47145800 | 3.30702000 |
| C | 1.50902900 | 1.53983000 | 2.11637200 |
| H | 3.86918400 | 2.45310000 | 4.26099900 |
| H | 3.29973700 | 3.52379300 | 2.97441300 |
| H | 0.80408400 | 0.70887400 | 2.23264300 |
| N | 2.02460700 | 1.86175500 | 3.45324900 |
| C | 1.11449700 | 2.53397000 | 4.36578400 |
| H | 0.86226300 | 3.56380800 | 4.06110200 |
| H | 0.18311200 | 1.96281800 | 4.43954300 |
| H | 1.57062800 | 2.57096600 | 5.36111700 |
| H | -14.01314300 | -4.85531600 | 0.49836700 |

Compound C-2 (DFT//B3LYP/6-31G(d))

Symbolic Z-matrix:

Ground state

Charge = 0 Multiplicity = 1



| | | | |
|---|--------------|-------------|-------------|
| C | -10.05086300 | -0.43206100 | 0.20111600 |
| C | -11.06318900 | 1.51145900 | -0.45083100 |
| C | -11.30281200 | 0.16274300 | -0.13175500 |
| C | -9.65687700 | 1.71062800 | -0.30503500 |
| C | -8.84975600 | 2.84710600 | -0.48533000 |
| C | -7.46063200 | 2.79536000 | -0.27210800 |

| | | | |
|---|--------------|-------------|-------------|
| C | -6.44408300 | 3.79010200 | -0.39048300 |
| C | -5.23518900 | 3.15707600 | -0.04761400 |
| C | -5.53226500 | 1.80023200 | 0.27044000 |
| N | -9.08478800 | 0.49210800 | 0.09509800 |
| N | -6.85102600 | 1.59699700 | 0.13299600 |
| B | -7.57509400 | 0.24125400 | 0.37804300 |
| F | -7.39856500 | -0.16265500 | 1.70084500 |
| F | -7.08129000 | -0.72771400 | -0.49545200 |
| C | -12.13310600 | 2.47883700 | -0.85479500 |
| H | -12.18114600 | 3.34305600 | -0.18403200 |
| H | -11.97133000 | 2.87127200 | -1.86444200 |
| H | -13.10388900 | 1.97572800 | -0.83560900 |
| C | -4.57652800 | 0.73651900 | 0.69438300 |
| H | -3.55795800 | 1.12971900 | 0.70540100 |
| H | -4.83151400 | 0.36634300 | 1.69327500 |
| H | -4.62816500 | -0.12014400 | 0.01451800 |
| C | -6.55036000 | 5.22993200 | -0.79063000 |
| H | -7.17396100 | 5.80367200 | -0.09662200 |
| H | -5.55308000 | 5.67854700 | -0.80280800 |
| H | -6.99273800 | 5.34915300 | -1.78498500 |
| C | -9.79731200 | -1.84327200 | 0.61181900 |
| H | -9.36807500 | -1.87924800 | 1.61892700 |
| H | -10.72958000 | -2.41142300 | 0.59710100 |
| H | -9.07284000 | -2.31522100 | -0.05992000 |
| C | -9.47996300 | 4.13610100 | -0.90591600 |
| C | -9.64208300 | 4.43685000 | -2.26503800 |
| C | -9.91455700 | 5.05658200 | 0.05731800 |
| C | -10.22974800 | 5.64210000 | -2.65404000 |
| C | -10.50331200 | 6.26044100 | -0.33418800 |
| H | -9.79100600 | 4.82699000 | 1.11207400 |
| H | -10.34984300 | 5.86566100 | -3.71047600 |
| H | -10.83751300 | 6.96651500 | 0.42094100 |
| C | -10.66154500 | 6.55572700 | -1.69000900 |
| H | -11.11919900 | 7.49300500 | -1.99389200 |
| H | -9.30680500 | 3.72589000 | -3.01517000 |
| C | -1.52156900 | 4.78921600 | 0.02459400 |
| C | -1.31745600 | 6.12417800 | -0.41516800 |
| C | -0.42382200 | 4.03539800 | 0.47723100 |
| C | -0.05860300 | 6.70984200 | -0.41749300 |
| H | -2.17448700 | 6.69636400 | -0.75610400 |
| C | 0.84760000 | 4.60769900 | 0.48252000 |
| H | -0.57727500 | 3.01588100 | 0.81788700 |
| C | 1.02561500 | 5.94319000 | 0.02589500 |
| H | 0.06730300 | 7.73462300 | -0.75219200 |
| C | 2.15847800 | 4.13033600 | 0.87276900 |

| | | | |
|---|-------------|-------------|-------------|
| C | 3.06395000 | 5.19522500 | 0.63115600 |
| C | 2.63484700 | 2.92458600 | 1.39577100 |
| C | 4.42718400 | 5.05644500 | 0.90887000 |
| C | 3.99501700 | 2.75967300 | 1.67554900 |
| H | 1.94274700 | 2.10788800 | 1.58902900 |
| C | 4.87209600 | 3.84061900 | 1.42041100 |
| H | 5.13047400 | 5.86434200 | 0.73299400 |
| H | 5.93403300 | 3.73222500 | 1.60875400 |
| C | -3.94363300 | 3.73177900 | -0.01906900 |
| C | -2.82839800 | 4.22260900 | 0.00351000 |
| N | 2.36909400 | 6.27787000 | 0.10652800 |
| C | 2.94107200 | 7.56743400 | -0.22949900 |
| H | 2.93287100 | 8.25442300 | 0.62590700 |
| H | 3.97187500 | 7.43344900 | -0.56572800 |
| H | 2.37516500 | 8.01615700 | -1.04936500 |
| C | 7.30723400 | 1.53255400 | -1.79388500 |
| C | 8.75721200 | 1.59091500 | -1.81470600 |
| C | 9.48059200 | 0.76958300 | -2.67974900 |
| C | 8.77931500 | -0.15800600 | -3.55286700 |
| C | 7.38386500 | -0.21289900 | -3.53760400 |
| C | 6.63294900 | 0.65459700 | -2.64895200 |
| C | 6.86200900 | 1.71926100 | -0.43094300 |
| C | 8.06692700 | 1.89910400 | 0.41090000 |
| C | 9.22165300 | 1.81498200 | -0.45772000 |
| C | 10.40067200 | 1.20371400 | -0.01739600 |
| C | 10.69629600 | 0.12139100 | -2.21430100 |
| C | 9.55434900 | -1.38132400 | -3.61724000 |
| C | 8.90637500 | -2.61778700 | -3.65958900 |
| C | 7.45577200 | -2.67814600 | -3.64131500 |
| C | 6.70872500 | -1.49999800 | -3.58281100 |
| C | 5.54266800 | -1.42283000 | -2.72013300 |
| C | 5.50315200 | -0.08757800 | -2.14532000 |
| C | 5.10630800 | 0.08965000 | -0.81479000 |
| C | 5.76739600 | 1.03237000 | 0.04756400 |
| C | 8.11414300 | 1.37419400 | 1.68485600 |
| C | 6.89262000 | 0.82345600 | 2.42968000 |
| C | 5.57676000 | 0.63600800 | 1.51647100 |
| C | 5.15058400 | -0.82816100 | 1.33570500 |
| C | 4.72052700 | -1.05849000 | -0.01637000 |
| C | 4.73824200 | -2.34097700 | -0.57612600 |
| C | 5.16811000 | -2.52481200 | -1.95274500 |
| C | 5.94146500 | -3.75292600 | -2.01505300 |
| C | 7.06418900 | -3.82797800 | -2.84176600 |
| C | 10.73933400 | -1.20880700 | -2.78930100 |
| C | 9.49863800 | -4.85055600 | -0.25433800 |

| | | | |
|---|--------------|-------------|-------------|
| C | 10.59477200 | -4.13803300 | -0.74487200 |
| C | 11.30343200 | -3.21071300 | 0.11945100 |
| C | 10.88960900 | -3.03306000 | 1.44120300 |
| C | 9.74672000 | -3.77467700 | 1.95088000 |
| C | 7.61250900 | -4.71318900 | 1.13701400 |
| C | 7.14916400 | -4.94330500 | -0.22209200 |
| C | 8.31363800 | -5.02324000 | -1.08219700 |
| C | 8.27360700 | -4.47647600 | -2.36662900 |
| C | 9.41264700 | -3.72951800 | -2.87262700 |
| C | 10.54910400 | -3.56443300 | -2.07914800 |
| C | 11.69440000 | -2.06121400 | -0.68064900 |
| C | 11.65605000 | -0.77972800 | -0.12733300 |
| C | 11.22179600 | -0.59646100 | 1.24644100 |
| C | 10.84630400 | -1.69850500 | 2.01351800 |
| C | 9.67610300 | -1.62244300 | 2.87332100 |
| C | 9.00354000 | -2.89799200 | 2.83697400 |
| C | 7.60462800 | -2.93213000 | 2.84598900 |
| C | 6.89976500 | -3.85956200 | 1.97971300 |
| C | 5.98416300 | -4.32195900 | -0.67720600 |
| C | 5.23613300 | -3.44634700 | 0.20586700 |
| C | 5.68959100 | -3.21061800 | 1.50841900 |
| C | 5.63508400 | -1.88145200 | 2.07761500 |
| C | 6.83891100 | -1.70681000 | 2.91929500 |
| C | 7.47931400 | -0.48954500 | 2.96644800 |
| C | 8.91524400 | -0.44838200 | 2.91417700 |
| C | 9.30862200 | 0.70105400 | 2.12039000 |
| C | 10.44503600 | 0.63149100 | 1.30622500 |
| C | 11.22734200 | -2.27986100 | -2.03787800 |
| C | 11.14700100 | 0.33544200 | -0.90987800 |
| C | 9.06564600 | -4.66366500 | 1.11664200 |
| C | 6.39865400 | 1.74133100 | 3.58780100 |
| C | 4.44127100 | 1.43242300 | 2.29022600 |
| H | 6.88027100 | 1.48394800 | 4.53771400 |
| H | 6.64734800 | 2.79663900 | 3.37754900 |
| H | 3.54514100 | 0.80143500 | 2.31242100 |
| N | 4.97627700 | 1.47423800 | 3.65629400 |
| C | 4.23409000 | 2.25307100 | 4.63323600 |
| H | 4.25541600 | 3.33975100 | 4.44328700 |
| H | 3.18791100 | 1.92939500 | 4.64031200 |
| H | 4.65342100 | 2.06963800 | 5.62861000 |
| C | -14.87131900 | -1.76743600 | -0.11928700 |
| C | -16.05893800 | -1.06522700 | -0.45593500 |
| C | -14.94684600 | -3.13166100 | 0.21549800 |
| C | -17.30015600 | -1.68716200 | -0.46222300 |
| H | -15.98568300 | -0.01435200 | -0.71778600 |

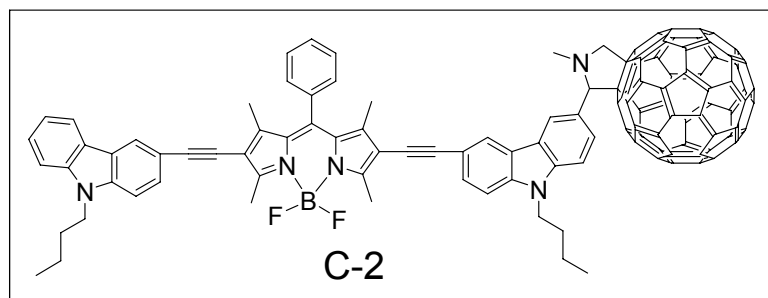
| | | | |
|---|--------------|-------------|-------------|
| C | -16.18489500 | -3.77265100 | 0.21436200 |
| H | -14.04046700 | -3.67297500 | 0.46949100 |
| C | -17.36030800 | -3.04342800 | -0.11928500 |
| H | -18.19019700 | -1.12788600 | -0.73274100 |
| C | -16.60826500 | -5.12930800 | 0.49629200 |
| C | -18.01778100 | -5.15667900 | 0.32019900 |
| C | -15.93584800 | -6.29760700 | 0.87303700 |
| C | -18.75513700 | -6.33090400 | 0.50265300 |
| C | -16.66680200 | -7.46803600 | 1.06250000 |
| H | -14.85809800 | -6.29186600 | 1.01333200 |
| C | -18.06077800 | -7.48023700 | 0.87719200 |
| H | -19.83031900 | -6.35693600 | 0.35480900 |
| H | -18.61117600 | -8.40536400 | 1.02522300 |
| C | -12.54646300 | -0.50991900 | -0.12917600 |
| C | -13.61799400 | -1.09055700 | -0.12527300 |
| N | -18.45783800 | -3.88508300 | -0.03475200 |
| C | -19.82736300 | -3.52508800 | -0.34533600 |
| H | -20.06973000 | -3.70514300 | -1.40031300 |
| H | -20.50959500 | -4.10804700 | 0.27840600 |
| H | -19.98691500 | -2.46783200 | -0.12150400 |
| H | -16.15689300 | -8.38187000 | 1.35343800 |

Compound C-2 (DFT//B3LYP/6-31G(d))

Symbolic Z-matrix:

Triplet state

Charge = 0 Multiplicity = 3



| | | | |
|---|--------------|-------------|-------------|
| C | -10.04713300 | -0.43161000 | 0.20485000 |
| C | -11.06094000 | 1.50837700 | -0.45527900 |
| C | -11.29918900 | 0.16019400 | -0.13316000 |
| C | -9.65532600 | 1.71034300 | -0.30605400 |
| C | -8.84970100 | 2.84766800 | -0.48700000 |
| C | -7.46100200 | 2.79882900 | -0.26978900 |
| C | -6.44587500 | 3.79490300 | -0.38818000 |
| C | -5.23680600 | 3.16476800 | -0.04034300 |
| C | -5.53245800 | 1.80834400 | 0.28061700 |
| N | -9.08231400 | 0.49383800 | 0.09897100 |
| N | -6.85052100 | 1.60258800 | 0.14022400 |

| | | | |
|---|--------------|-------------|-------------|
| B | -7.57315500 | 0.24655900 | 0.38792600 |
| F | -7.40061200 | -0.15202800 | 1.71290400 |
| F | -7.07465200 | -0.72481900 | -0.48011700 |
| C | -12.13129100 | 2.47284100 | -0.86498100 |
| H | -12.18311500 | 3.33849700 | -0.19634400 |
| H | -11.96689100 | 2.86325800 | -1.87497700 |
| H | -13.10120400 | 1.96799400 | -0.84780600 |
| C | -4.57604700 | 0.74727300 | 0.70967100 |
| H | -3.55885200 | 1.14376700 | 0.72772100 |
| H | -4.83650900 | 0.37503500 | 1.70633900 |
| H | -4.62022600 | -0.10876300 | 0.02842700 |
| C | -6.55343800 | 5.23340300 | -0.79274100 |
| H | -7.17986100 | 5.80810400 | -0.10207700 |
| H | -5.55688200 | 5.68365600 | -0.80356400 |
| H | -6.99335100 | 5.34897900 | -1.78860900 |
| C | -9.79244700 | -1.84121600 | 0.62028400 |
| H | -9.36644700 | -1.87360600 | 1.62889600 |
| H | -10.72366100 | -2.41104800 | 0.60414200 |
| H | -9.06493800 | -2.31372200 | -0.04775600 |
| C | -9.48091500 | 4.13458900 | -0.91242400 |
| C | -9.63991900 | 4.43187100 | -2.27267700 |
| C | -9.91957200 | 5.05659800 | 0.04749500 |
| C | -10.22857700 | 5.63522000 | -2.66603900 |
| C | -10.50932600 | 6.25854000 | -0.34837500 |
| H | -9.79839200 | 4.82967000 | 1.10310000 |
| H | -10.34625900 | 5.85610600 | -3.72330700 |
| H | -10.84670600 | 6.96581300 | 0.40421300 |
| C | -10.66447900 | 6.55036800 | -1.70530100 |
| H | -11.12292400 | 7.48614300 | -2.01260500 |
| H | -9.30146100 | 3.71973400 | -3.02026200 |
| C | -1.52616900 | 4.80329600 | 0.03604600 |
| C | -1.32490800 | 6.14015500 | -0.39947400 |
| C | -0.42666800 | 4.04994600 | 0.48508200 |
| C | -0.06716000 | 6.72806700 | -0.40129700 |
| H | -2.18334300 | 6.71187400 | -0.73761800 |
| C | 0.84374900 | 4.62453700 | 0.49079600 |
| H | -0.57796100 | 3.02900600 | 0.82240700 |
| C | 1.01885300 | 5.96176200 | 0.03829800 |
| H | 0.05667300 | 7.75411200 | -0.73284400 |
| C | 2.15603600 | 4.14824500 | 0.87740000 |
| C | 3.05936200 | 5.21547200 | 0.63769900 |
| C | 2.63545000 | 2.94132100 | 1.39480900 |
| C | 4.42350600 | 5.07780700 | 0.91188400 |
| C | 3.99658700 | 2.77772400 | 1.67078500 |
| H | 1.94515300 | 2.12263900 | 1.58596200 |

| | | | |
|---|-------------|-------------|-------------|
| C | 4.87156600 | 3.86088600 | 1.41773500 |
| H | 5.12517000 | 5.88739900 | 0.73749400 |
| H | 5.93425600 | 3.75363200 | 1.60237800 |
| C | -3.94632500 | 3.74169700 | -0.01003700 |
| C | -2.83195500 | 4.23443400 | 0.01393300 |
| N | 2.36186400 | 6.29856800 | 0.11810700 |
| C | 2.93067700 | 7.59018500 | -0.21583300 |
| H | 2.91706800 | 8.27689700 | 0.63968100 |
| H | 3.96303100 | 7.45966400 | -0.54843700 |
| H | 2.36611800 | 8.03708800 | -1.03765500 |
| C | 7.32371100 | 1.56164100 | -1.80920400 |
| C | 8.76927800 | 1.61477800 | -1.82671900 |
| C | 9.49179000 | 0.77341600 | -2.68685000 |
| C | 8.78737600 | -0.16183100 | -3.54131100 |
| C | 7.39558800 | -0.21186600 | -3.53205700 |
| C | 6.64589500 | 0.67387600 | -2.65665100 |
| C | 6.87381000 | 1.75356400 | -0.44701800 |
| C | 8.07629700 | 1.93016200 | 0.39519500 |
| C | 9.23155100 | 1.83860800 | -0.47403300 |
| C | 10.40355200 | 1.21249700 | -0.02496300 |
| C | 10.68980500 | 0.11077400 | -2.20961400 |
| C | 9.56217800 | -1.39885200 | -3.60052800 |
| C | 8.89634000 | -2.64218500 | -3.64437000 |
| C | 7.46438500 | -2.69364200 | -3.62931100 |
| C | 6.71082800 | -1.49700600 | -3.57520300 |
| C | 5.56955100 | -1.40935200 | -2.71654200 |
| C | 5.52053600 | -0.06360500 | -2.15046700 |
| C | 5.12345700 | 0.11745500 | -0.82286300 |
| C | 5.77783500 | 1.06631500 | 0.03247700 |
| C | 8.11830700 | 1.40167900 | 1.66958800 |
| C | 6.89658500 | 0.84606000 | 2.40911000 |
| C | 5.58835400 | 0.66213900 | 1.49884000 |
| C | 5.16062700 | -0.80082800 | 1.31038000 |
| C | 4.73459400 | -1.02827100 | -0.01330400 |
| C | 4.75173900 | -2.33310800 | -0.58254500 |
| C | 5.18307600 | -2.51714300 | -1.92838700 |
| C | 5.94608200 | -3.76374500 | -1.99878800 |
| C | 7.06359800 | -3.84161300 | -2.82551300 |
| C | 10.72805800 | -1.23198100 | -2.78405200 |
| C | 9.48577800 | -4.89102200 | -0.24315800 |
| C | 10.58075100 | -4.17571000 | -0.73276600 |
| C | 11.28097500 | -3.23756900 | 0.12822200 |
| C | 10.86208600 | -3.05998200 | 1.44417600 |
| C | 9.72968900 | -3.80483400 | 1.95613800 |
| C | 7.59911700 | -4.75342700 | 1.14560800 |

| | | | |
|---|--------------|-------------|-------------|
| C | 7.13842900 | -4.97805900 | -0.21021600 |
| C | 8.30215500 | -5.06073200 | -1.07235400 |
| C | 8.26604800 | -4.50780600 | -2.35448400 |
| C | 9.40332400 | -3.75808200 | -2.85665300 |
| C | 10.53680800 | -3.59612600 | -2.06311800 |
| C | 11.67925800 | -2.09048300 | -0.67782800 |
| C | 11.64573400 | -0.79055100 | -0.11923300 |
| C | 11.20228500 | -0.60336800 | 1.22803000 |
| C | 10.80760100 | -1.71209800 | 2.01081900 |
| C | 9.66402700 | -1.62995200 | 2.85803600 |
| C | 8.98229600 | -2.91198200 | 2.82275700 |
| C | 7.59130900 | -2.94871600 | 2.83342200 |
| C | 6.88456200 | -3.88751800 | 1.98895800 |
| C | 5.97876500 | -4.34169900 | -0.67086500 |
| C | 5.24760100 | -3.44674700 | 0.20764800 |
| C | 5.69476000 | -3.22020000 | 1.50551700 |
| C | 5.65442200 | -1.87292300 | 2.07395600 |
| C | 6.82182500 | -1.70628200 | 2.89283900 |
| C | 7.48517000 | -0.46822100 | 2.94283500 |
| C | 8.89327400 | -0.43312100 | 2.89984500 |
| C | 9.30198700 | 0.71536200 | 2.10352500 |
| C | 10.43819100 | 0.64027800 | 1.29329100 |
| C | 11.21933700 | -2.30966700 | -2.01710300 |
| C | 11.14092000 | 0.32476800 | -0.90964700 |
| C | 9.04733800 | -4.70409600 | 1.12686500 |
| C | 6.40206400 | 1.75572900 | 3.57556800 |
| C | 4.44596400 | 1.44833800 | 2.27740300 |
| H | 6.88712000 | 1.49568500 | 4.52267400 |
| H | 6.64456100 | 2.81288400 | 3.36938600 |
| H | 3.55210200 | 0.81439100 | 2.29414000 |
| N | 4.98084600 | 1.48019100 | 3.64440600 |
| C | 4.23641800 | 2.25141900 | 4.62621000 |
| H | 4.25387400 | 3.33900100 | 4.44185100 |
| H | 3.19151800 | 1.92375100 | 4.63226000 |
| H | 4.65722800 | 2.06388400 | 5.62013800 |
| C | -14.86478700 | -1.77534100 | -0.12418500 |
| C | -16.05251700 | -1.07579000 | -0.46595100 |
| C | -14.93928400 | -3.13860000 | 0.21475600 |
| C | -17.29287700 | -1.69940700 | -0.47325100 |
| H | -15.98002700 | -0.02566000 | -0.73097800 |
| C | -16.17646500 | -3.78124400 | 0.21269600 |
| H | -14.03279800 | -3.67787900 | 0.47266500 |
| C | -17.35204300 | -3.05465000 | -0.12610300 |
| H | -18.18301600 | -1.14220700 | -0.74770100 |
| C | -16.59873100 | -5.13754000 | 0.49799100 |

| | | | |
|---|--------------|-------------|-------------|
| C | -18.00778000 | -5.16733200 | 0.31863500 |
| C | -15.92569300 | -6.30372900 | 0.88013200 |
| C | -18.74403500 | -6.34192400 | 0.50317400 |
| C | -16.65556500 | -7.47449100 | 1.07167600 |
| H | -14.84828700 | -6.29612200 | 1.02297000 |
| C | -18.04908200 | -7.48911600 | 0.88310700 |
| H | -19.81882700 | -6.36985100 | 0.35286900 |
| H | -18.59863100 | -8.41447100 | 1.03285900 |
| C | -12.54173400 | -0.51450200 | -0.13202300 |
| C | -13.61239300 | -1.09674800 | -0.12916500 |
| N | -18.44865100 | -3.89745800 | -0.04148600 |
| C | -19.81788000 | -3.54019400 | -0.35652700 |
| H | -20.05714800 | -3.72293000 | -1.41174800 |
| H | -20.50087900 | -4.12282200 | 0.26666900 |
| H | -19.97963600 | -2.48268300 | -0.13545000 |
| H | -16.14515000 | -8.38669700 | 1.36680600 |