Electronic Supplementary Information for:

Preparation of ketocoumarins as heavy atom-free triplet photosensitizers for triplet-triplet annihilation upconversion

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1.0 NMR and HR-MS spectra.

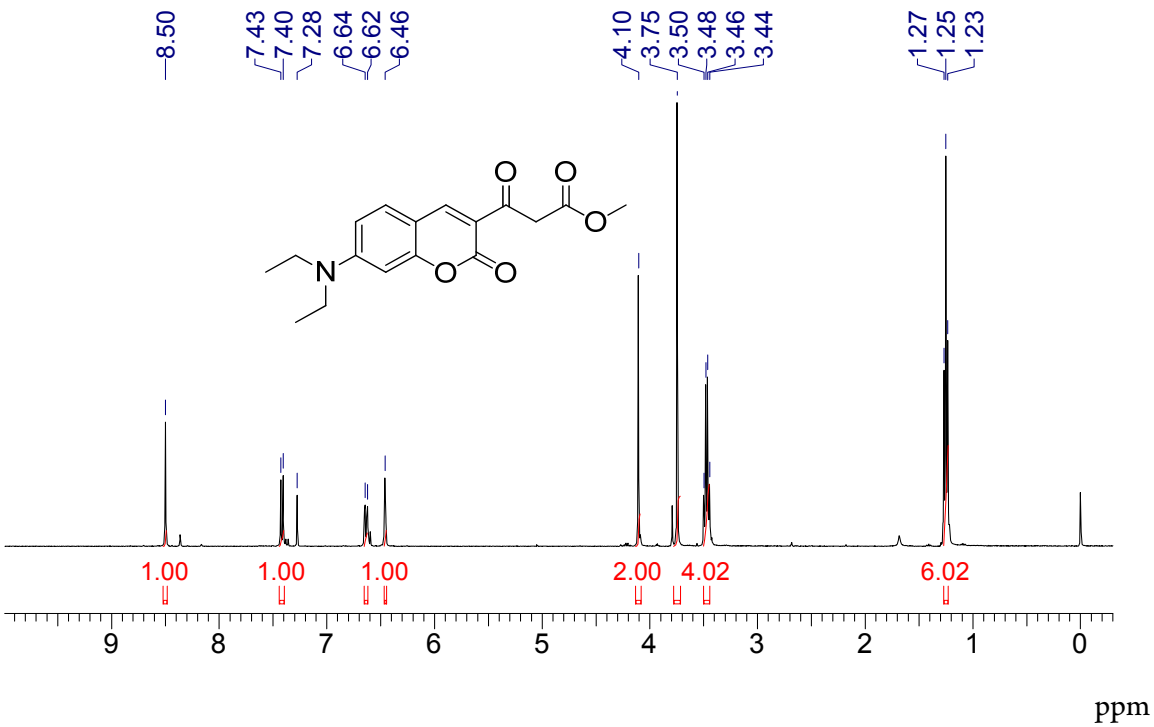

Fig. S1 ^{1}H NMR of **K0** ($CDCl_3$, 400 MHz).

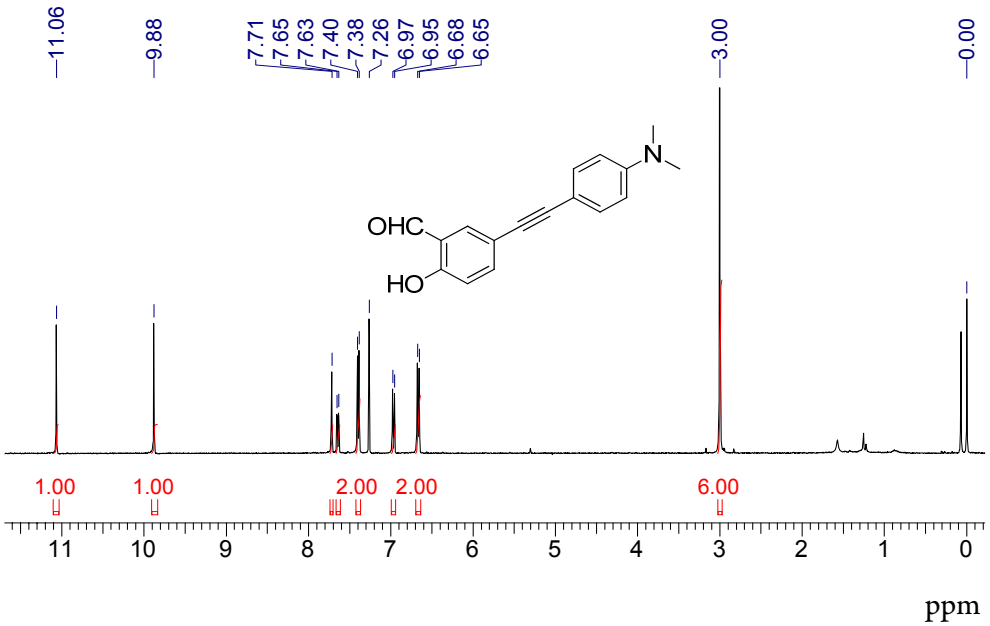

Fig. S2 ^{1}H NMR of **K1** ($CDCl_3$, 400 MHz).

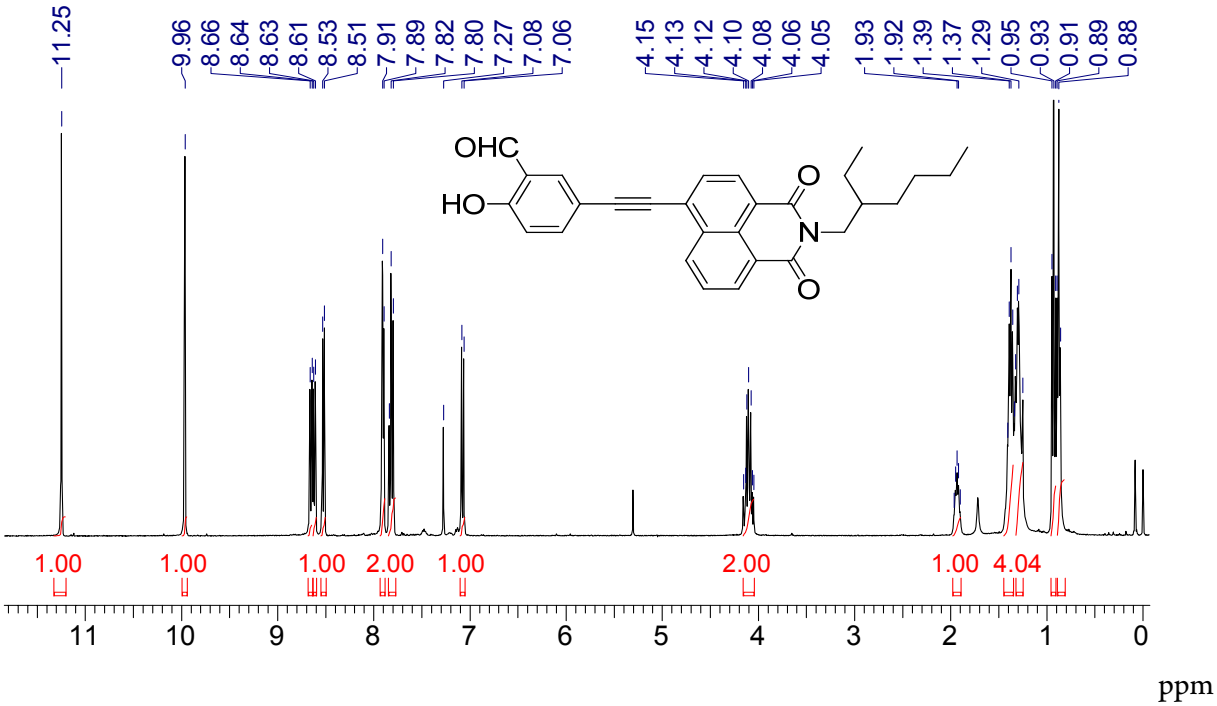

Fig. S3 ^{1}H NMR of K2 ($CDCl_3$, 400 MHz).

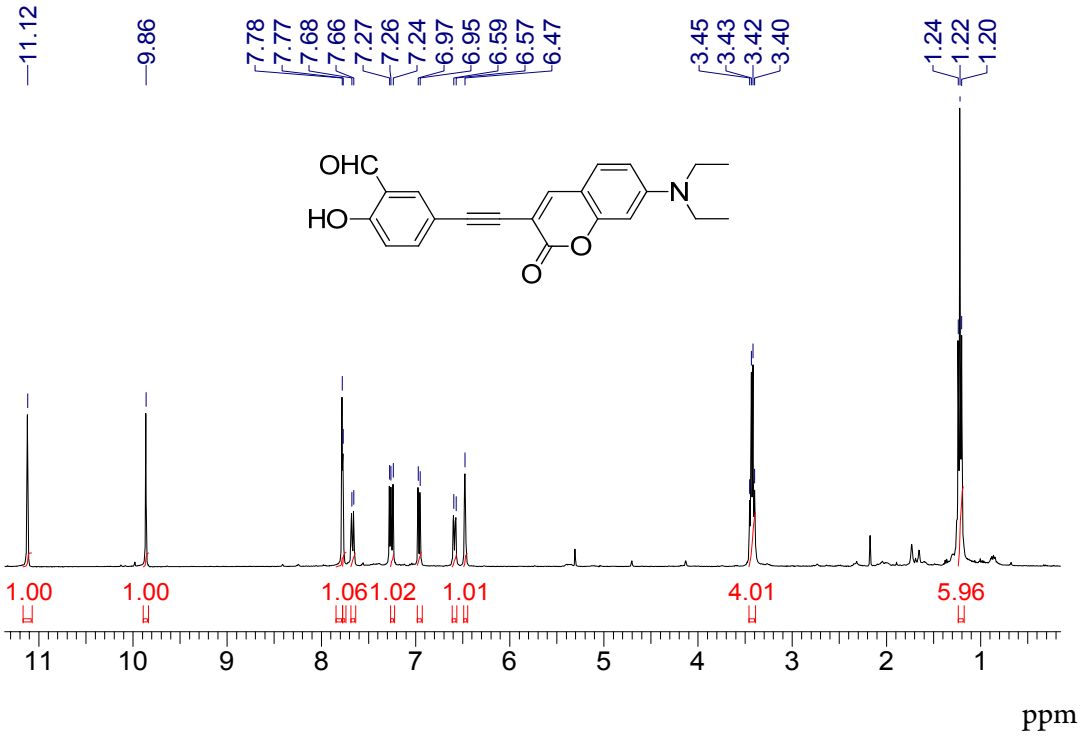

Fig. S4 ^{1}H NMR of **K3** ($CDCl_3$, 400 MHz).

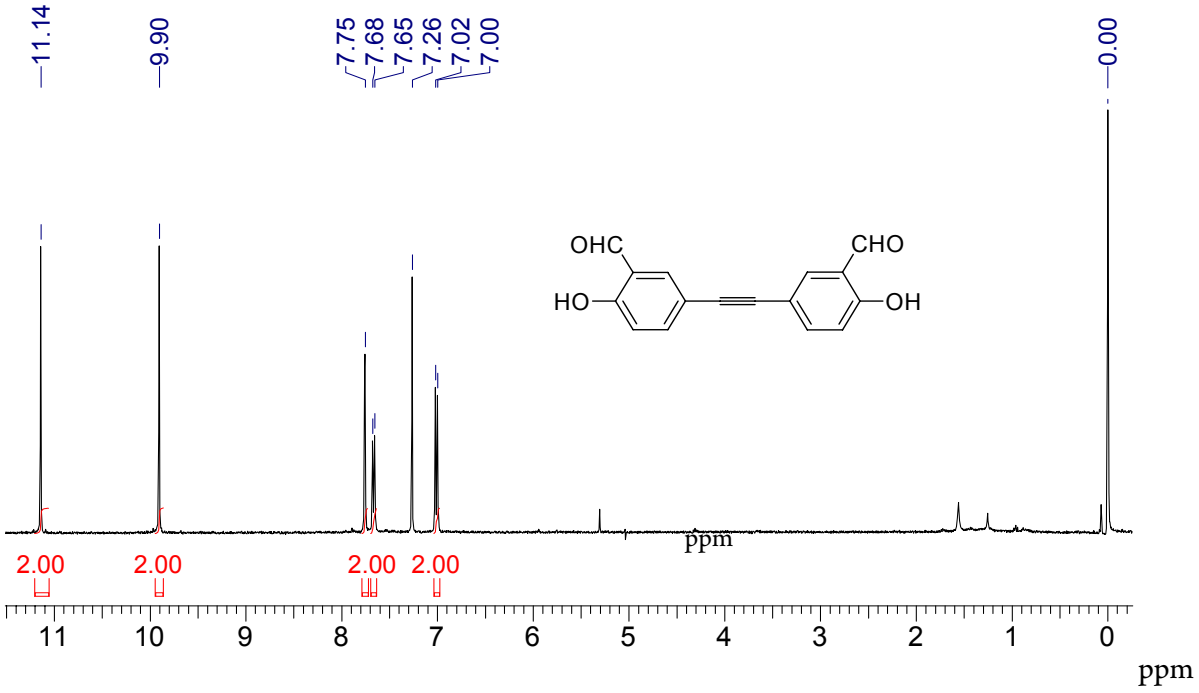

Fig. S5 ^{1}H NMR of **K4** ($CDCl_3$, 400 MHz).

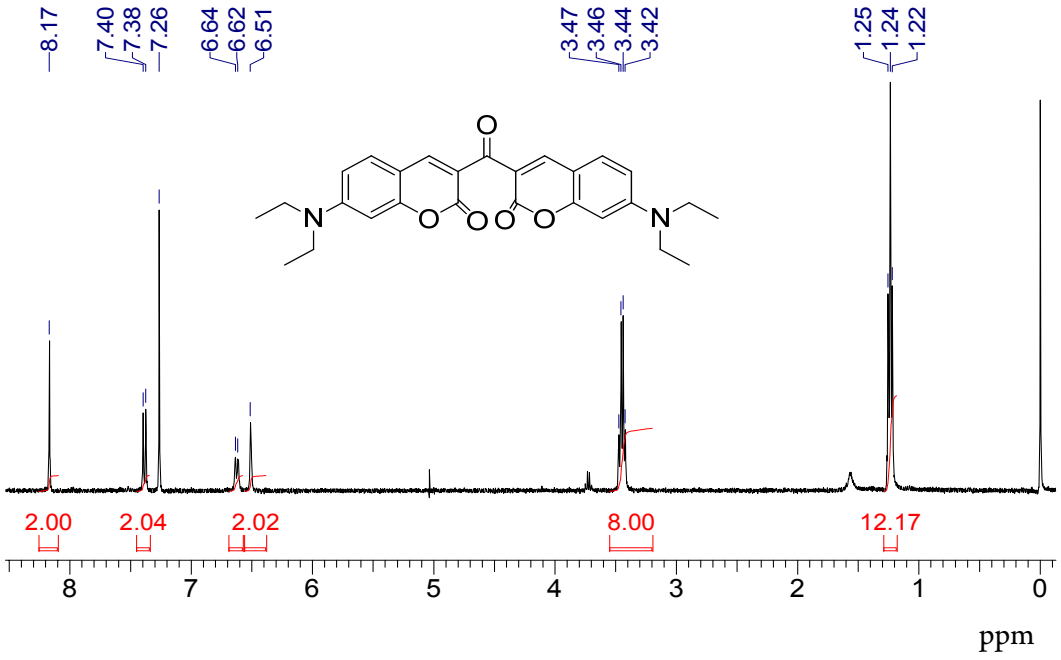

Fig. S6 ^{1}H NMR of **1** ($CDCl_3$, 400 MHz).

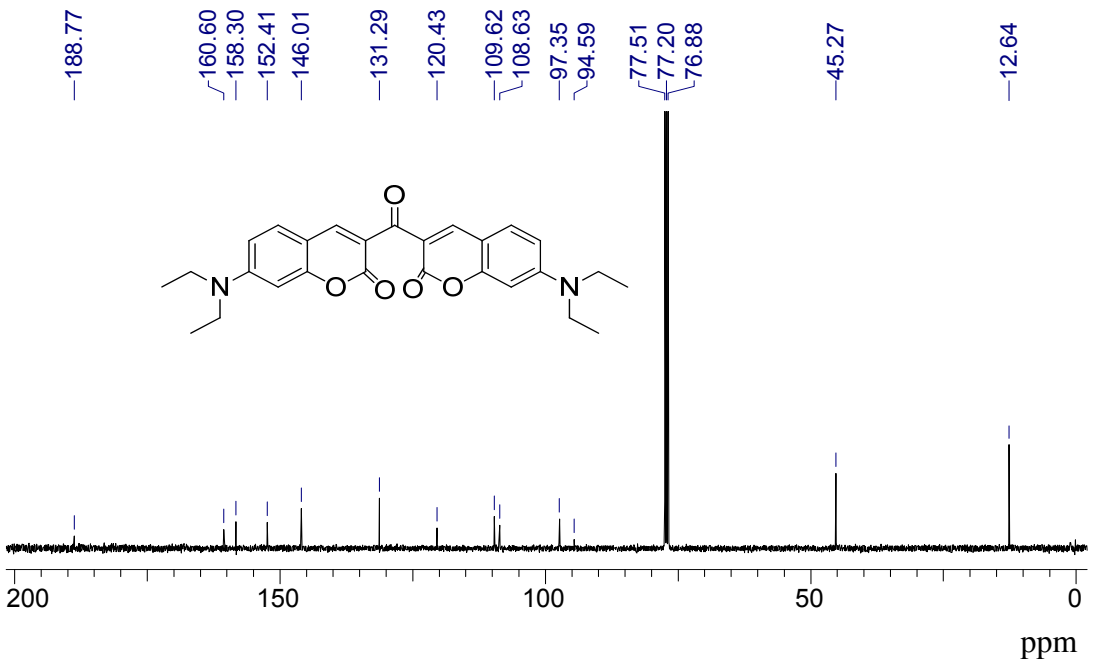

Fig. S7 ^{13}C NMR of **1** ($CDCl_3$, 100 MHz).

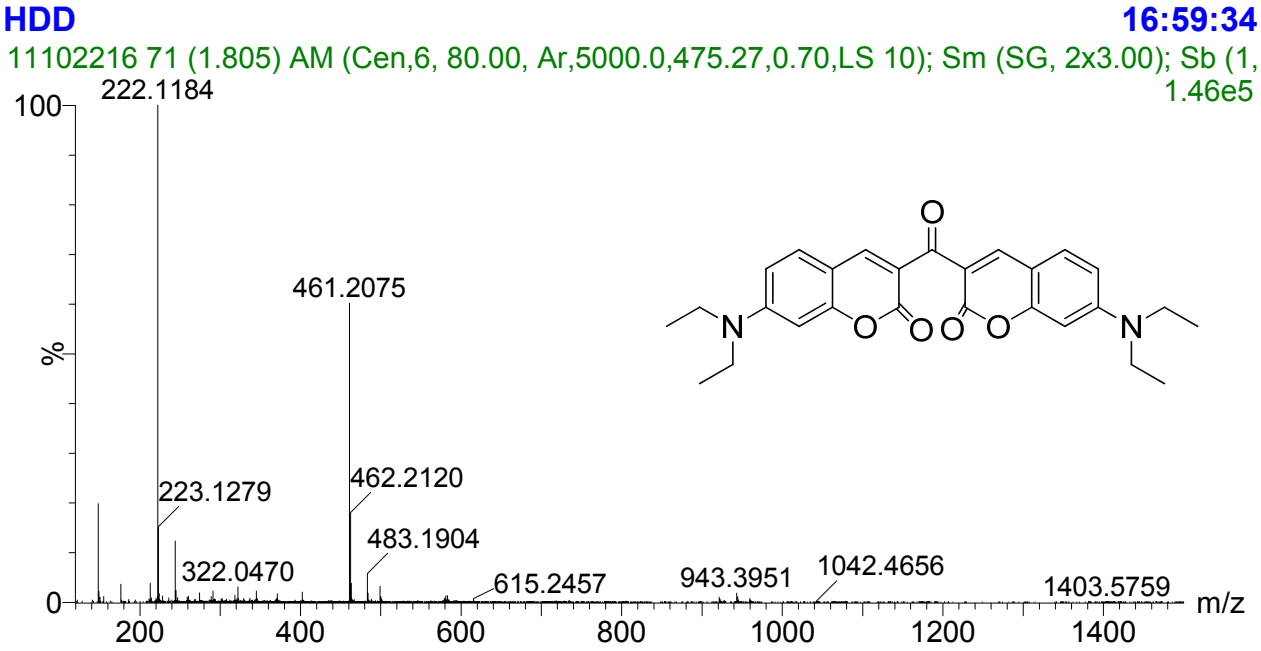

Fig. S8 TOF MS EI of **1**.

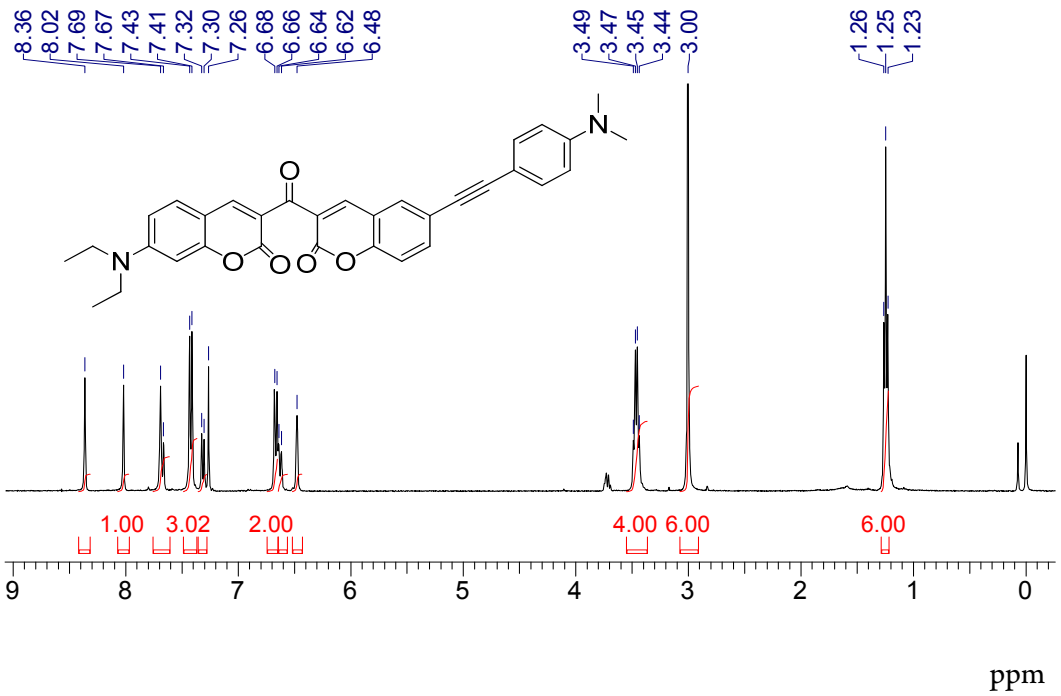

Fig. S9 ^{1}H NMR of **2** ($CDCl_3$, 400 MHz).

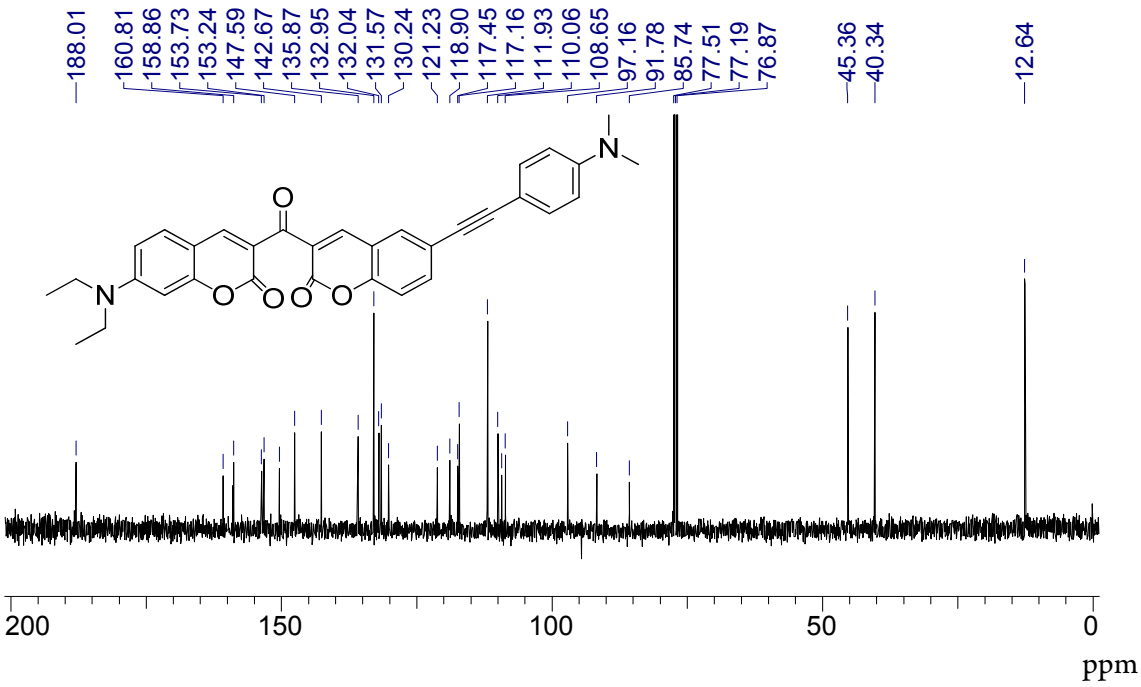

Fig. S10 ^{13}C NMR of **2** ($CDCl_3$, 100 MHz).

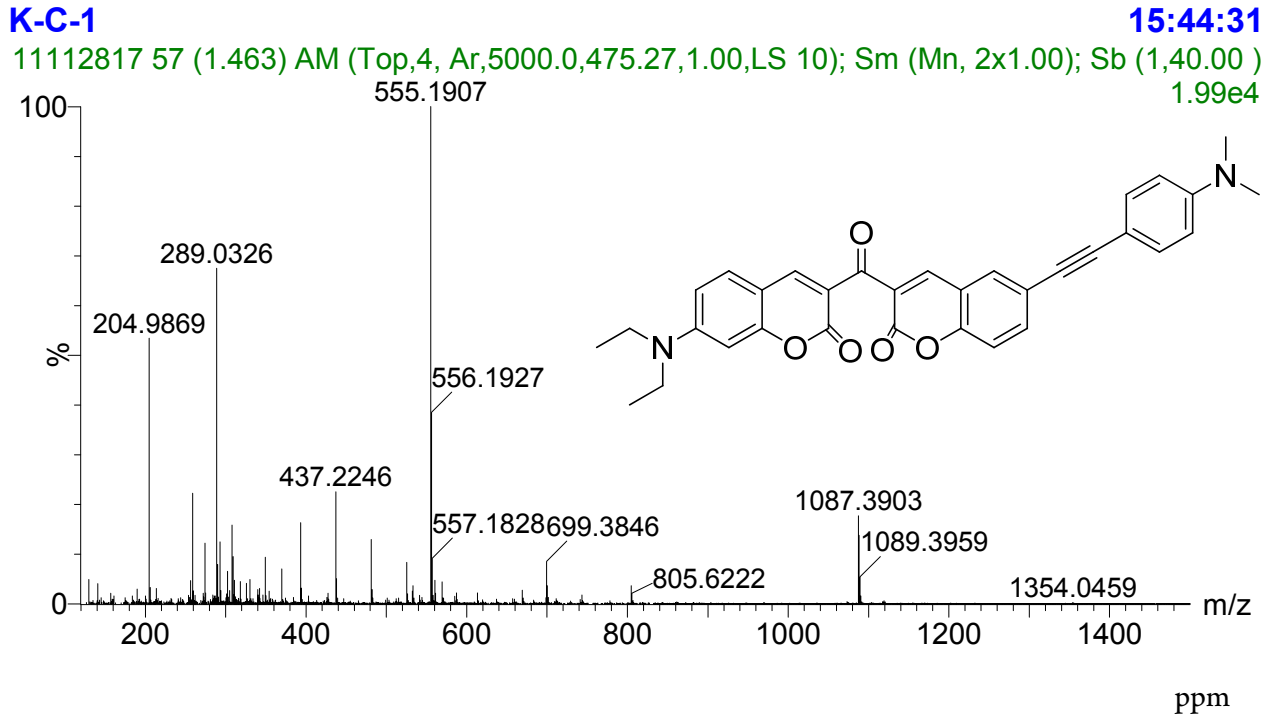

Fig. S11 TOF MS EI of **2**.

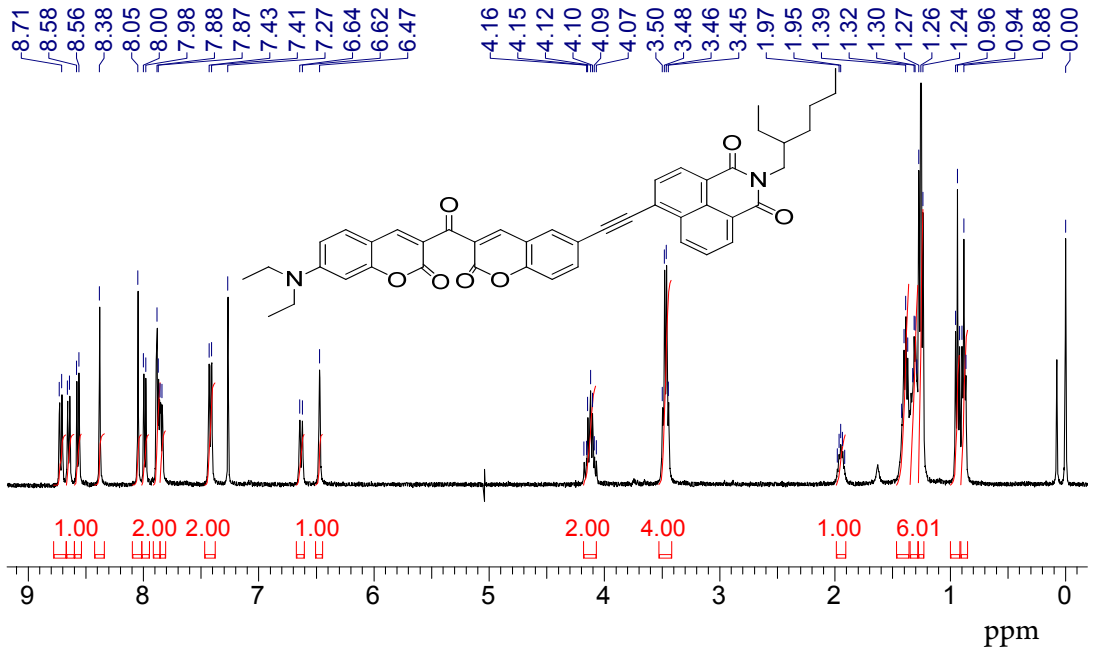

Fig. S12 ^{1}H NMR of **3** ($CDCl_3$, 400 MHz).

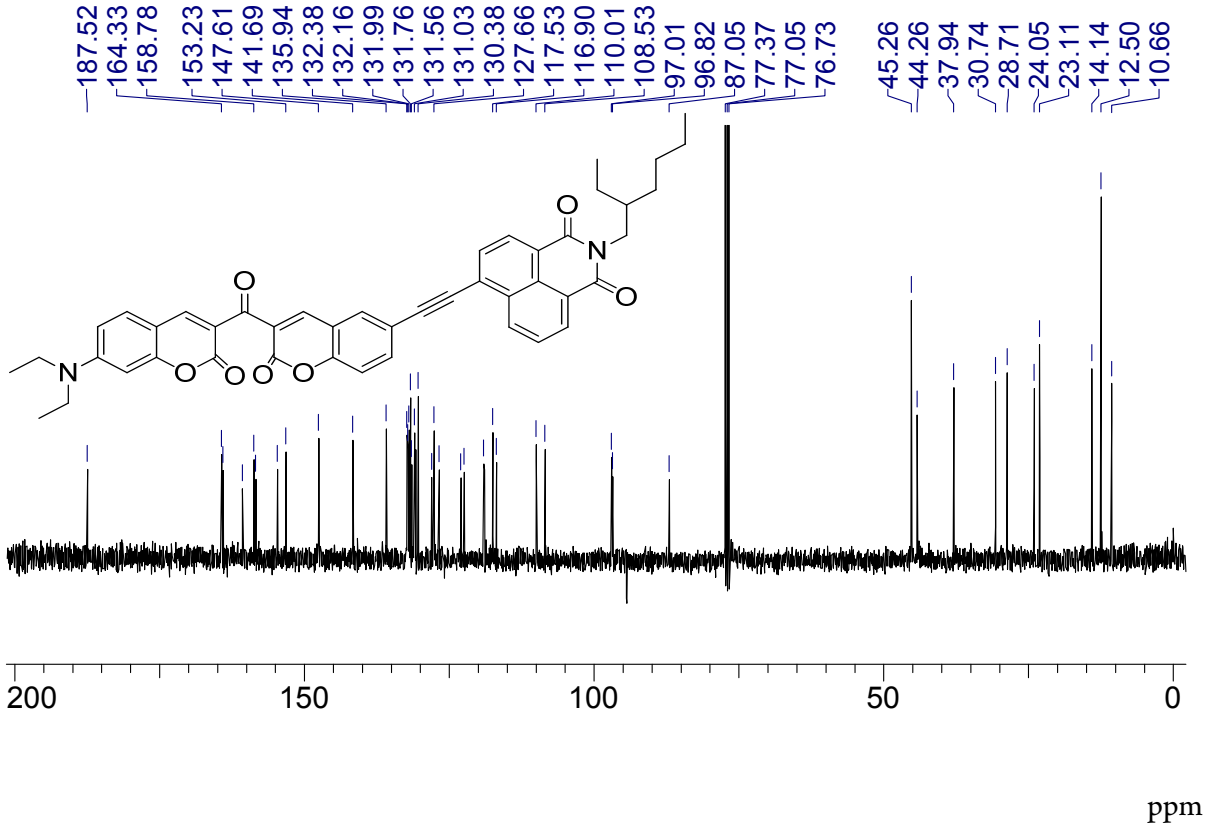

Fig. S13 ^{13}C NMR of **3** ($CDCl_3$, 100 MHz).

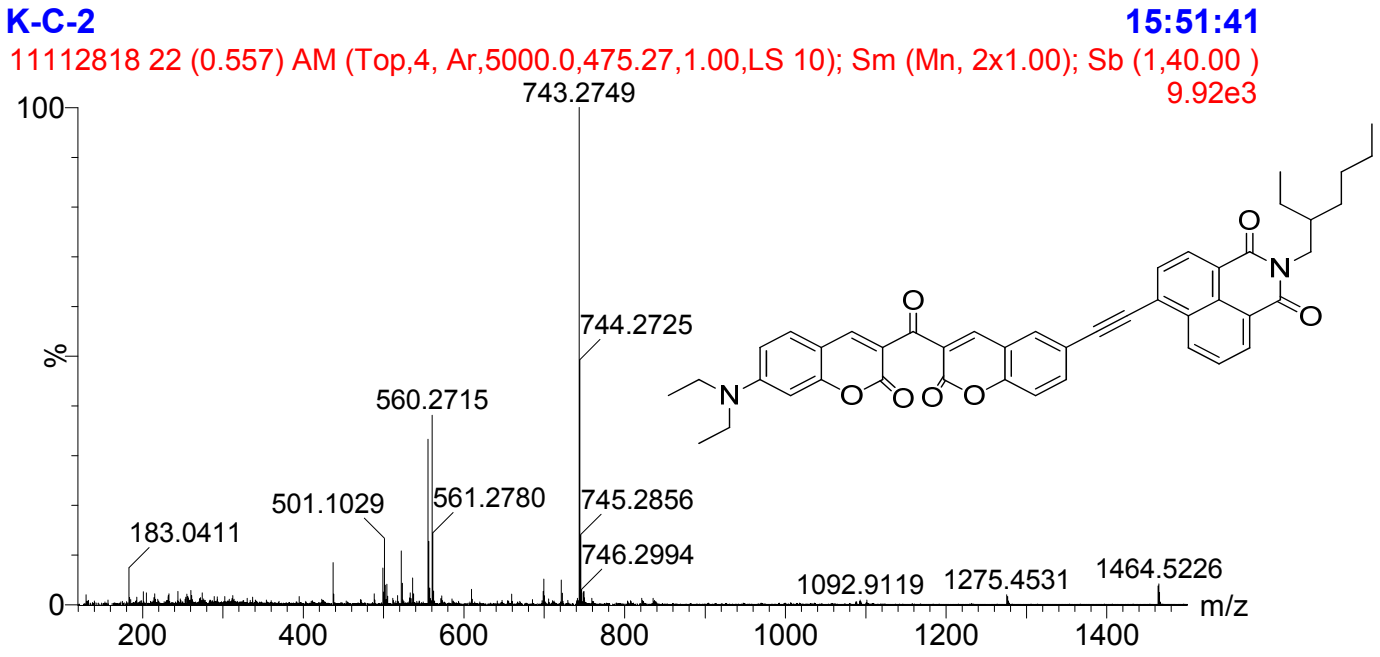

Fig. S14 TOF MS EI of **3**.

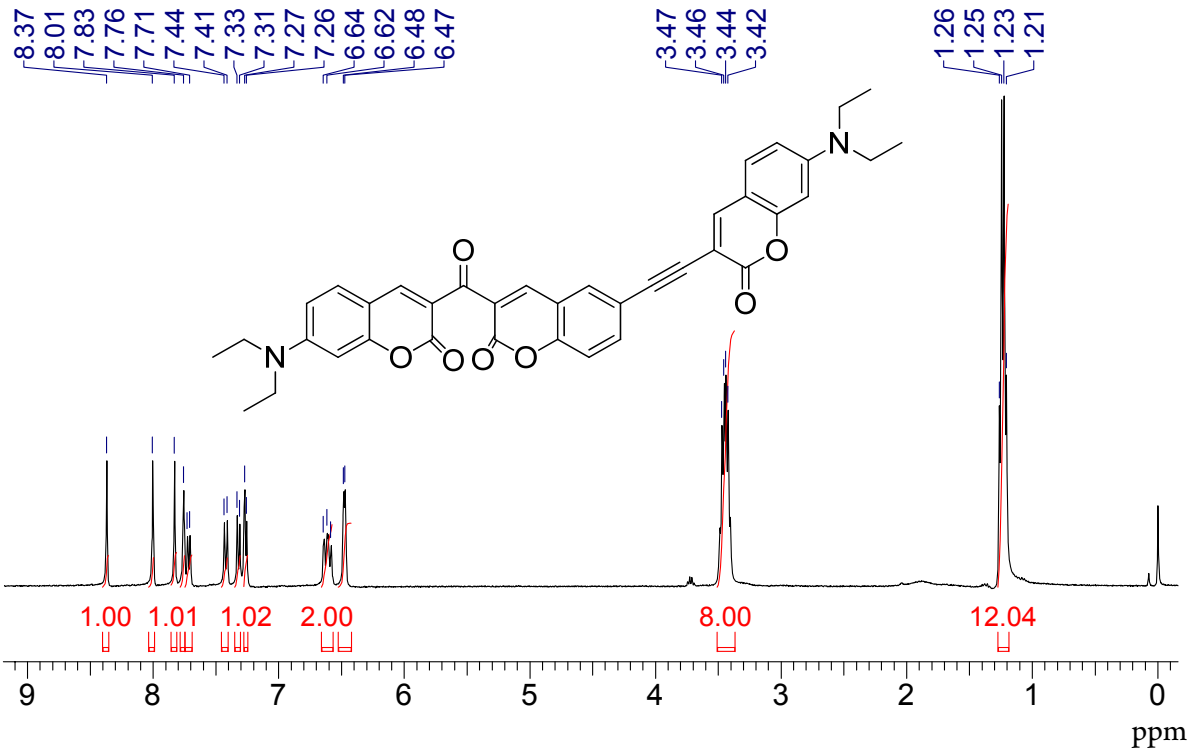

Fig. S15 ^{1}H NMR of **4** ($CDCl_3$, 400 MHz).

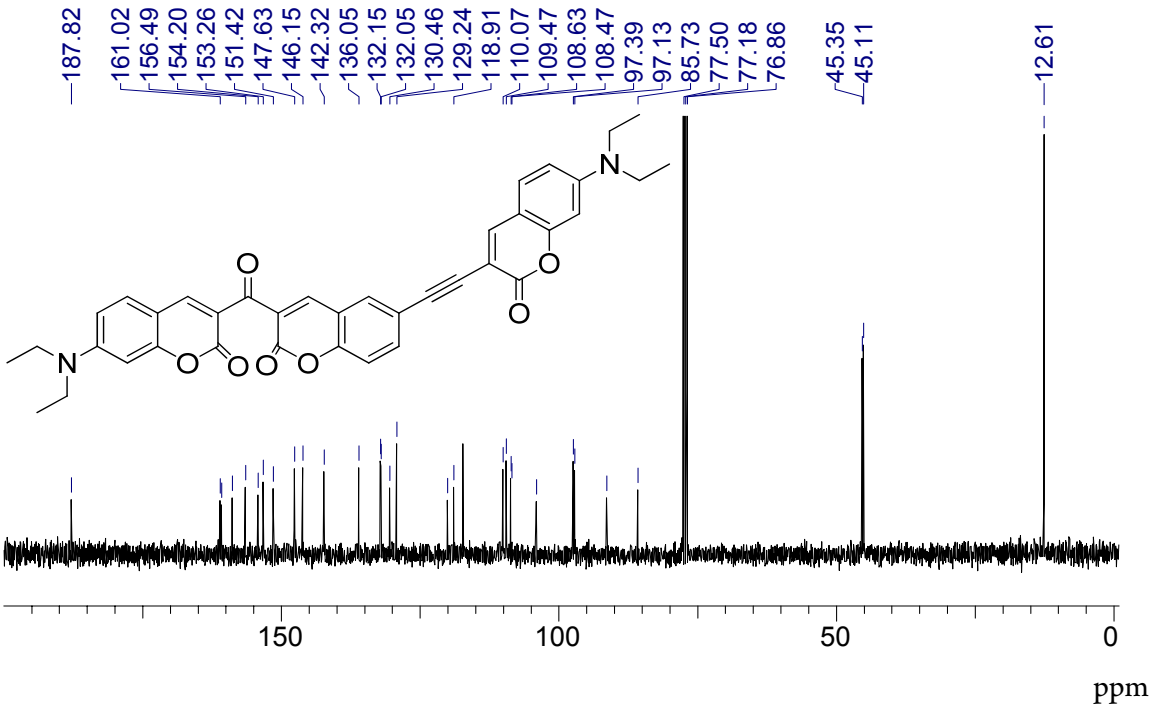

Fig. S16 ^{13}C NMR of **4** ($CDCl_3$, 100 MHz).

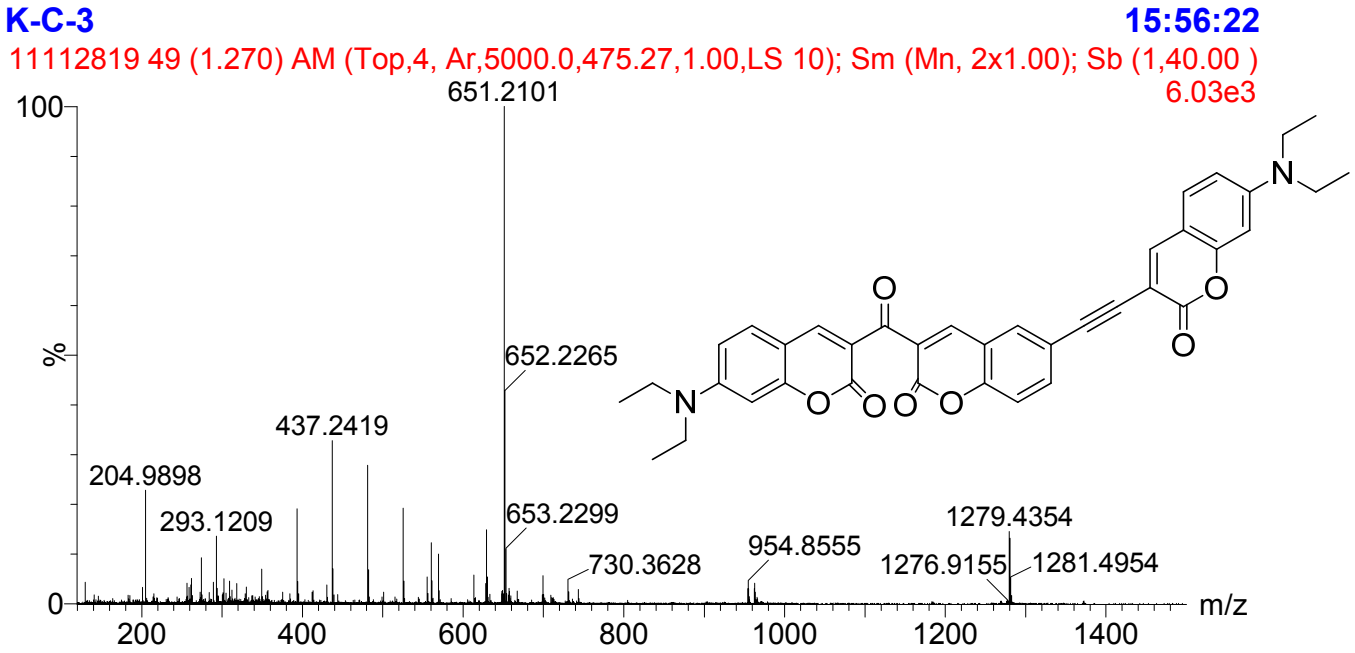

Fig. S17 TOF MS EI of **4**.

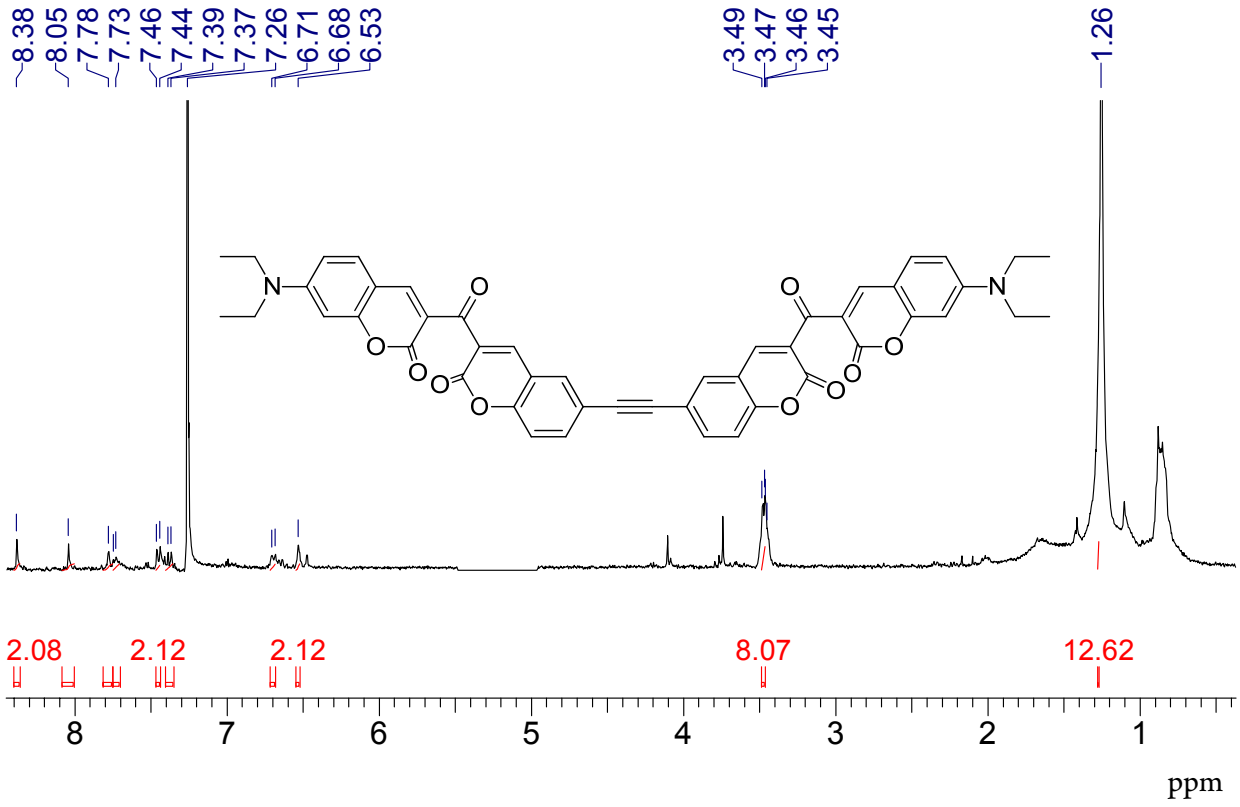

Fig. S18 ^{1}H NMR of **5** ($CDCl_3$, 400 MHz).

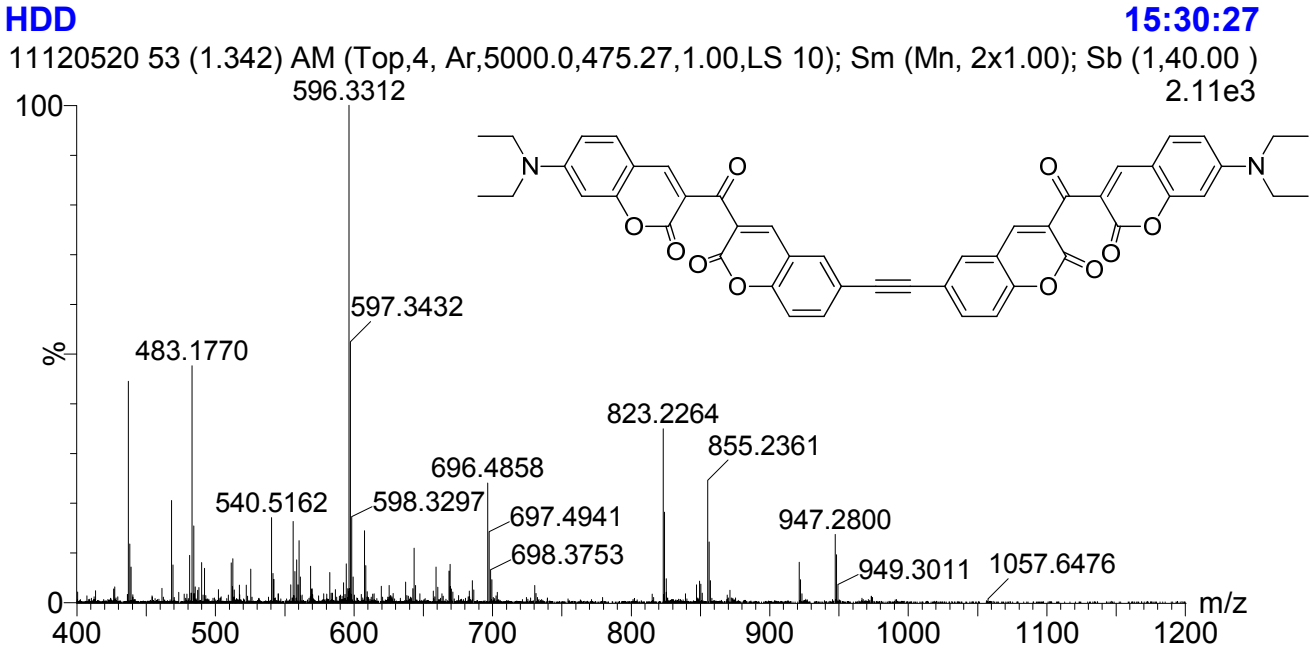

Fig. S19 TOF MS EI of **5**.

2.0 Photophysical properties of the ketocoumarin compounds.

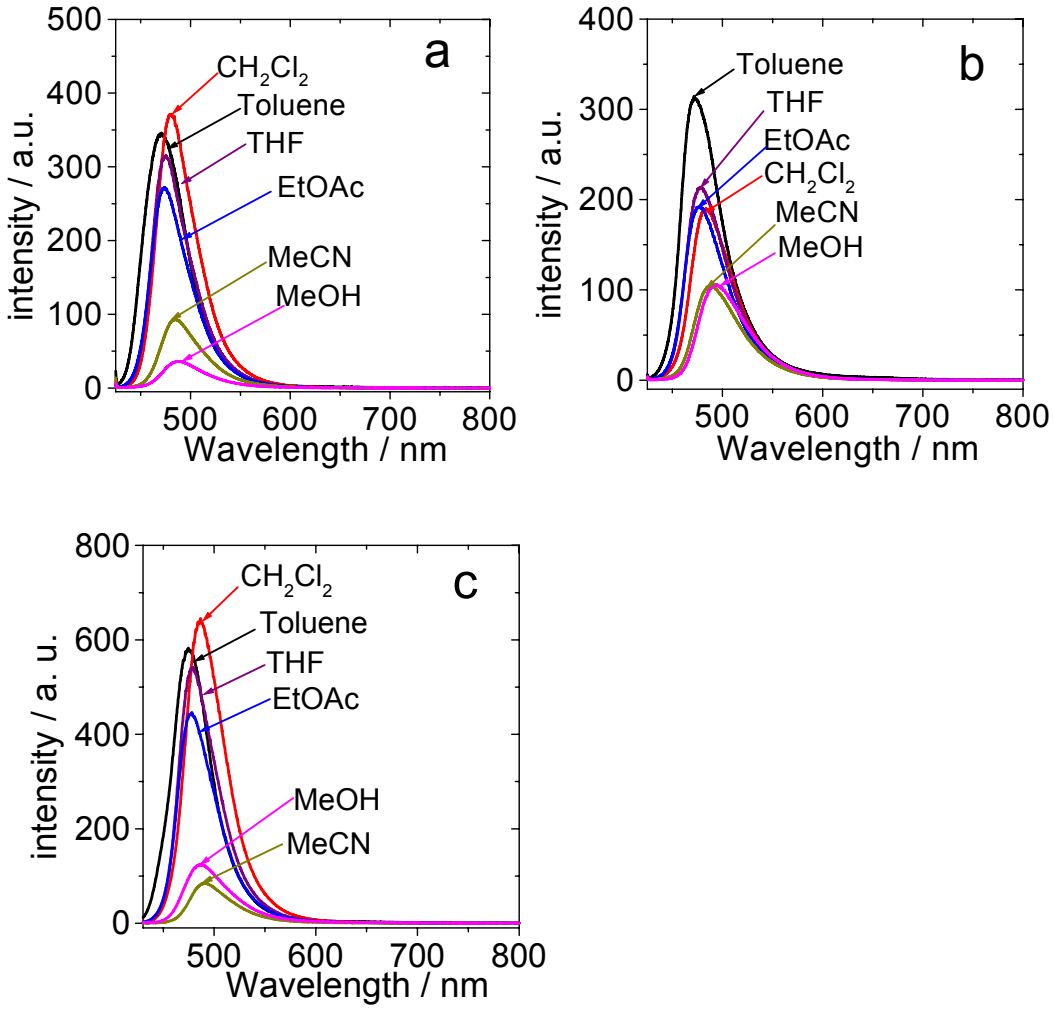

Fig. S20 Emission spectra of (a) **3**, (b) **4** and (c) **5** in different solutions at the same condition, $c = 1.0\times10^{-5}$ M, 25 °C.

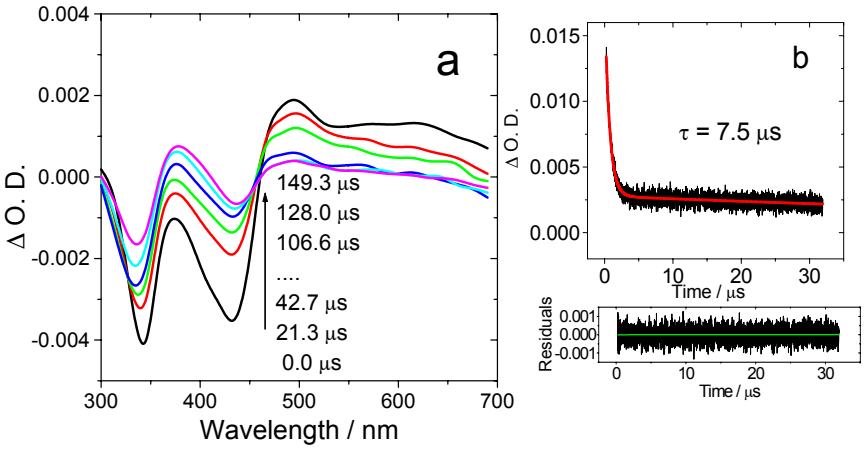

Fig. S21 (a) Nanosecond time-resolved transient absorption difference spectra of **2** after pulsed laser excitation (λ_{ex} = 355 nm). (b) Decay trace of **2** at 445 nm. c = 1.0×10^{-5} M, in deaerated toluene, 25 °C.

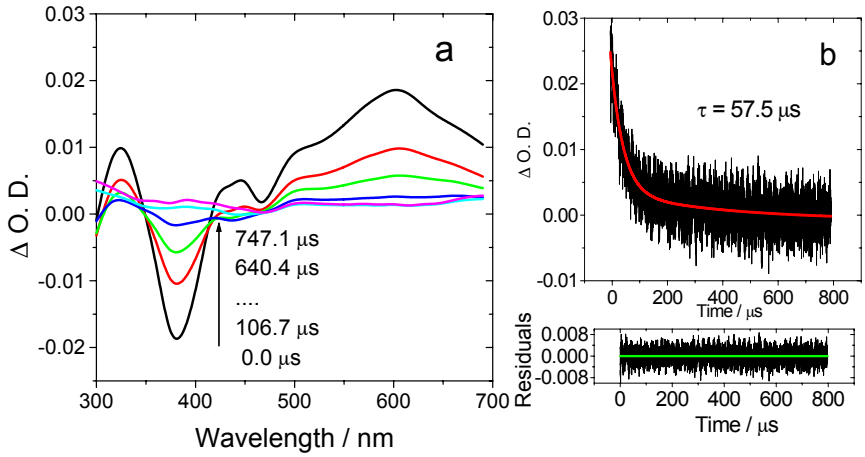

Fig. S22 (a) Nanosecond time-resolved transient absorption difference spectra of **3** after pulsed laser excitation (λ_{ex} = 355 nm). (b) Decay trace of **3** at 445 nm. c = 1.0×10^{-5} M, in deaerated toluene, 25 °C.

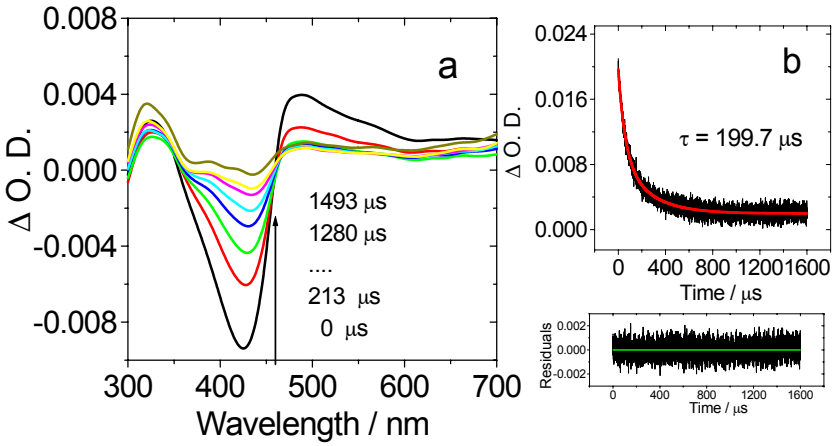

Fig. S23 (a) Nanosecond time-resolved transient absorption difference spectra of **4** after pulsed laser excitation (λ_{ex} = 355 nm). (b) Decay trace of **4** at 445nm. c = 1.0×10^{-5} M, in deaerated toluene, 25 °C.

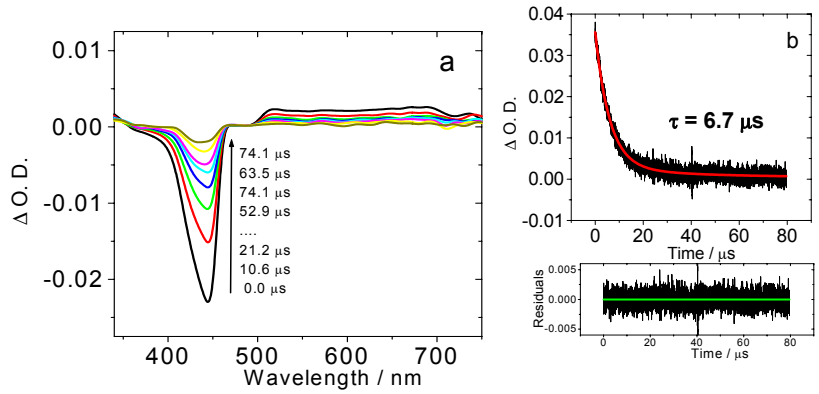

Fig. S24 (a) Nanosecond time-resolved transient absorption difference spectra of **5** after pulsed laser excitation (λ_{ex} = 355 nm). (b) Decay trace of **5** at 445 nm. c = 1.0×10^{-5} M, in deaerated toluene, 25 °C.

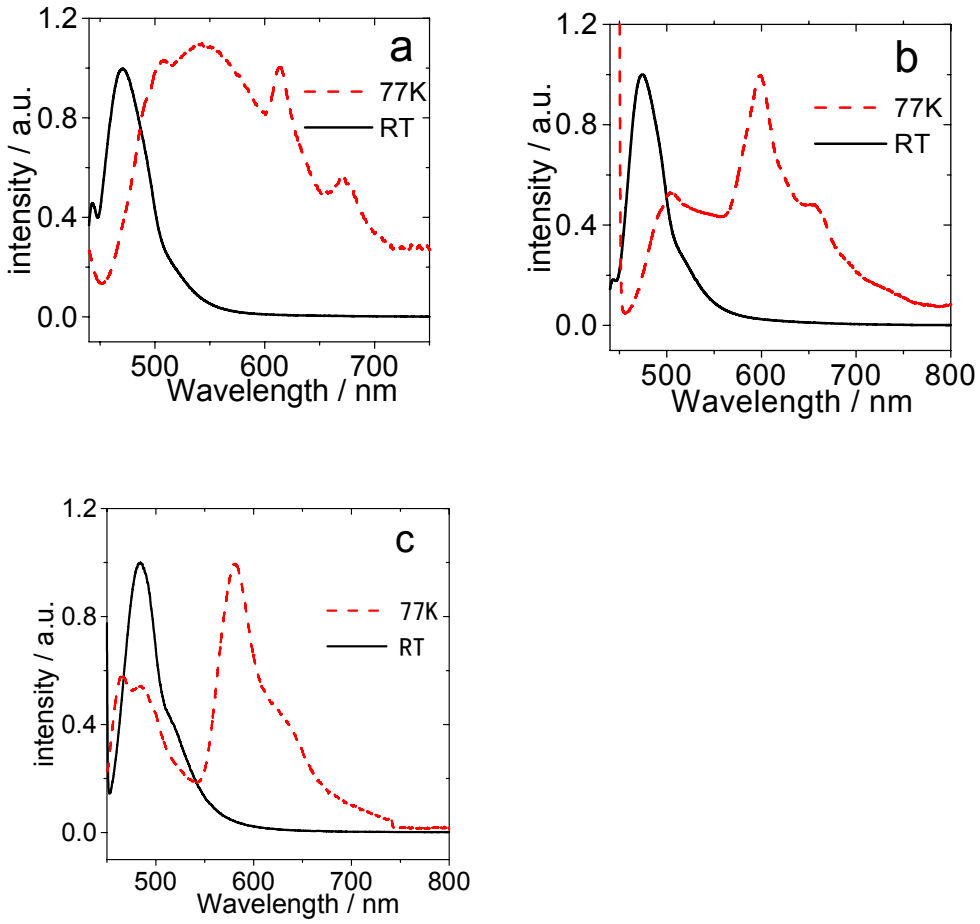

Fig. S25 Luminescence spectra of (a) **3**, (b) **4** and (c) **5** at RT and 77 K. For **3**, **4** in methyl cyclohexane : methyltetrahydrofuran : iodoethane = 2:1:1 (v/v). For **5**, the measurements were carried out in methanol : ethanol = 1:4 (v/v). $c = 1.0\times10^{-5}$ M.

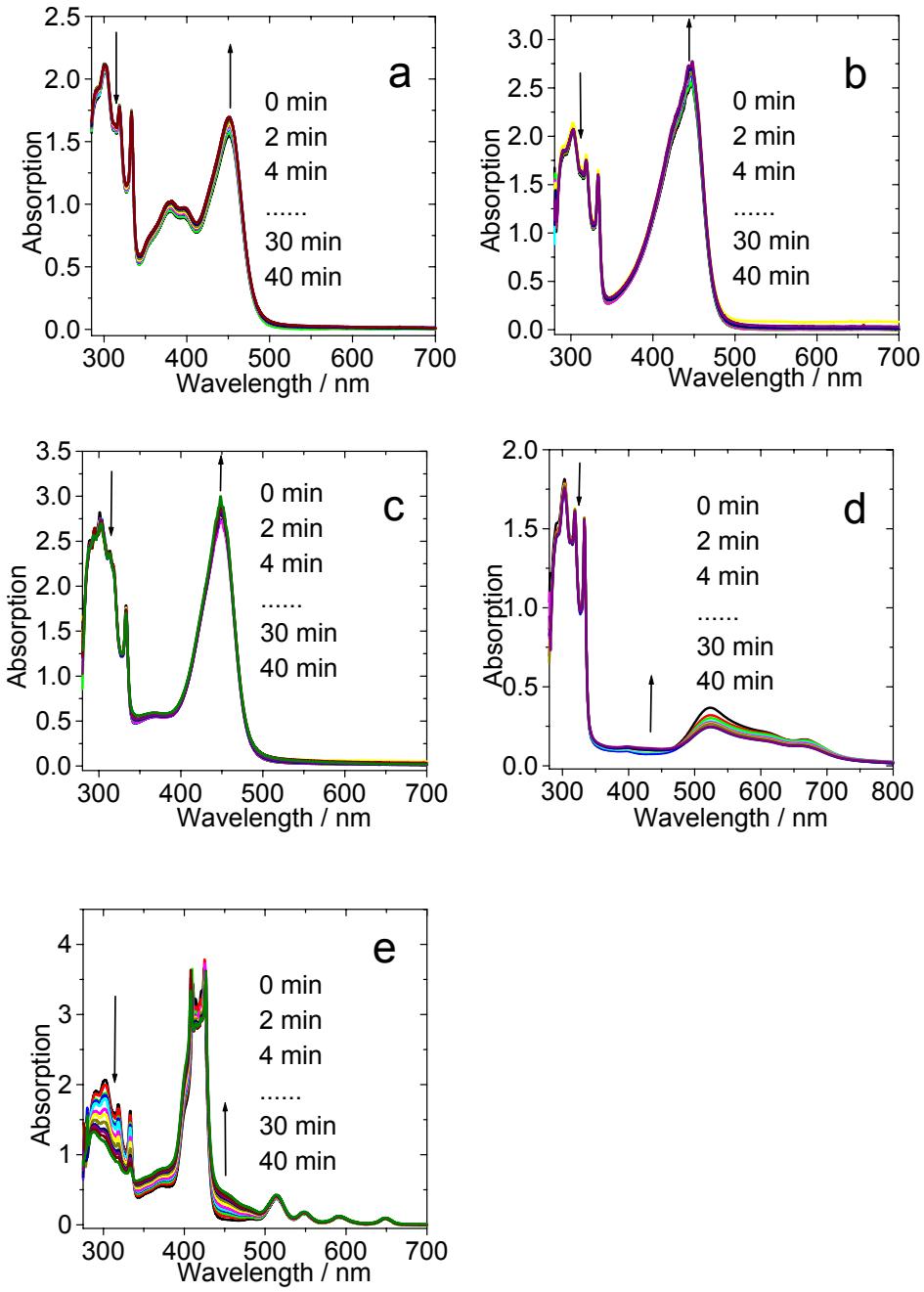

Fig. S26 Absorption spectral change for the photooxidation of DHN using (a) **3**, (b) **4**, (c) **5**, (d) MB and (e) TPP as photosensitizer. c [sensitizer] = 2.0×10^{-5} M, c [DHN] = 2.0×10^{-4} M. In toluene, 20 mW cm^{-2}, 25 °C.

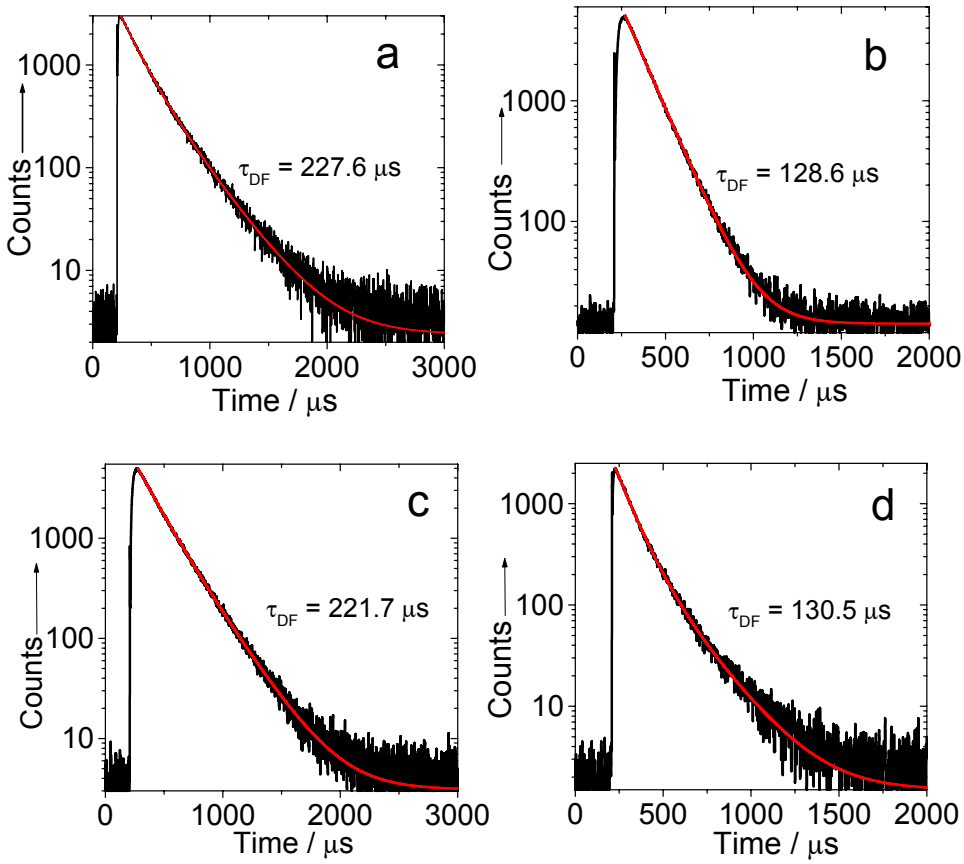

Fig. S27 Delayed fluorescence decay-profile observed in the TTA upconversion with (a) **2**, (b) **3**, (c) **4**, and (d) **5** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 445 nm and monitored at 410 nm. Under this circumstance the ketocoumarins are selectively excited and the emission is due to the upconverted emission of DPA. In deaerated toluene. *c* [sensitizers] = 1.0×10^{-5} M; *c* [DPA] = 1.3×10^{-5} M, 25 °C.

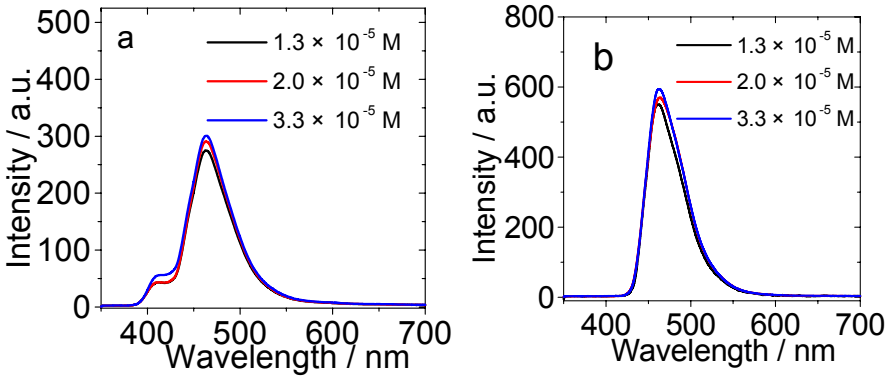

Fig. S28 Upconversion with the (a) compound **2** and (b) compound **5** as triplet sensitizers. *c*[photosensitizers] = 1.0 ×10^{-5} M. Different concentration of DPA (triplet acceptor) was used. Excited with 445 nm laser (5 mW). In deaerated toluene, 25 °C.

Optimized geometries of 1 (DFT//B3LYP/ rb3lyp/6-31g(d))

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-6.11256805	-1.14450179	0.38296137
C	-4.93826237	-1.84803672	0.53610493
C	-3.70228277	-1.33555459	0.08563246
C	-3.72507248	-0.06513882	-0.52870297
C	-4.89178301	0.66487271	-0.69134400
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H	-7.02819556	-1.58177834	0.75739290
H	-4.95642256	-2.82072800	1.02054961
C	-2.44694069	-1.98128879	0.22830369
H	-4.81167316	1.63510406	-1.16149776
C	-1.32153709	-0.11788081	-0.89605486
C	-1.28144424	-1.39317895	-0.18654739
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C	-8.85085198	0.52128443	1.54381123
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H	-9.81228025	0.07477000	1.82270982
H	-8.07149126	0.06616382	2.16320782
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C	0.00005073	-2.12934868	-0.00040846
C	6.13004767	0.13946493	0.24962817
C	4.89158642	0.66501032	0.69156550
C	3.72496148	-0.06506169	0.52871548
C	3.70227130	-1.33542608	-0.08575093
C	4.93833555	-1.84783579	-0.53610477
C	6.11257265	-1.14423865	-0.38277208
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O	2.57225649	0.49636922	0.99732870
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C	6.93539380	3.30902608	0.11482081
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H	7.65019764	3.39710528	-0.70968182
H	5.93860479	3.16787245	-0.31425128
C	8.58489056	0.29552208	-0.04787783
C	8.85249137	0.52088267	-1.54190280
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Optimized geometries of 2 (DFT//B3LYP/ rb3lyp/6-31g(d))

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-3.96882700	1.10605300	-0.44825100
C	-2.96249600	0.14007600	-0.57934300
C	-1.62523100	0.51431800	-0.79198800
C	-1.30644400	1.88300000	-0.87553800
C	-2.29181400	2.86302900	-0.74219000
C	-3.60623100	2.47545200	-0.53149000
H	-0.75034400	-1.48676800	-0.84480200
H	-3.21391900	-0.91399600	-0.51393000
C	-0.54346500	-0.42194300	-0.91008200
H	-2.01377500	3.90942500	-0.80868000
C	1.04117400	1.41891600	-1.24959700
C	0.74054200	-0.00476200	-1.06824300
O	-0.02642500	2.29700800	-1.10202400
O	2.11039800	1.89636300	-1.55771900
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C	1.83296700	-1.02691700	-1.17696300
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C	6.94384100	-0.05695000	1.07364500
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C	5.55264800	-1.26532400	-0.54710900
C	6.72315800	-1.89869200	-1.02232300
C	7.95940300	-1.63403800	-0.47871900
H	6.97089600	0.67112800	1.87218900
C	4.25049200	-1.46098600	-1.06602900
H	6.63865400	-2.60728000	-1.84188500
H	8.82232800	-2.13965200	-0.89041800
C	3.16711000	-0.77200400	-0.57979000
C	3.32515700	0.11875500	0.56479200
H	4.09381000	-2.15871700	-1.88465500
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O	4.62762600	0.30313000	1.03208900
N	9.33969900	-0.46405400	1.16537400
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C	9.55707900	1.98218500	1.76775100
H	10.41838500	0.27284700	2.77245100
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H	9.64546800	2.64875800	2.63315200
H	10.42204100	2.15125800	1.11876500
H	8.65663000	2.26341100	1.21310800
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H	10.33432700	-2.17615100	0.47407300
H	11.28204400	-1.10776500	1.48018200
H	12.04889500	-1.03891300	-0.90147300
H	10.45686300	-0.44823800	-1.41436100

H	11.48233800	0.55738300	-0.37801900
C	-6.48866300	0.42063200	-0.05173300
C	-7.84635100	0.05730000	0.15945900
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C	-8.24654500	-1.29431700	0.19655100
C	-10.17182200	0.68676900	0.54852400
H	-8.56925500	2.08504600	0.32415300
C	-9.56962100	-1.65347400	0.40136500
H	-7.49959500	-2.07156500	0.06375800
C	-10.57770400	-0.67173500	0.57817600
H	-10.89876200	1.47766100	0.68779700
H	-9.82179000	-2.70667400	0.42574200
N	-11.89759300	-1.02318300	0.76738500
C	-12.26693400	-2.42504300	0.88599100
H	-11.78914600	-2.91112100	1.74951000
H	-13.34819500	-2.50061200	1.00848800
H	-11.99197600	-2.98822200	-0.01493000
C	-12.88943100	0.00200500	1.05245600
H	-12.95905000	0.73028600	0.23427100
H	-13.86734600	-0.46808100	1.16418800
H	-12.66571400	0.55171700	1.97857300
H	-4.37942700	3.22981900	-0.42844500
C	-5.32509700	0.73166300	-0.23436000

1 2 1.5 6 1.5 68 1.5
2 3 1.5 8 1.0
3 4 1.5 9 1.5
4 5 1.5 13 1.0
5 6 1.5 10 1.0
6 67 1.0
7 9 1.0
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9 12 2.0
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11 12 1.0 13 1.0 14 2.0
12 16 1.0
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15 16 2.0
16 27 1.0
17 18 1.5 22 1.5 32 1.5
18 19 2.0 23 1.0
19 20 1.5 31 1.0
20 21 1.5 24 1.5
21 22 2.0 25 1.0
22 26 1.0
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24 27 2.0 29 1.0
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27 28 1.0

28 30 2.0 31 1.0
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32 33 1.0 40 1.0
33 34 1.0 35 1.0 36 1.0
34 37 1.0 38 1.0 39 1.0
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40 41 1.0 42 1.0 43 1.0
41 44 1.0 45 1.0 46 1.0
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47 48 1.5 68 3.0
48 49 1.5 50 1.5
49 51 1.5 52 1.0
50 53 1.5 54 1.0
51 55 1.5 56 1.0
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53 55 1.5 57 1.0
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55 58 1.5
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58 59 1.0 63 1.0
59 60 1.0 61 1.0 62 1.0
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63 64 1.0 65 1.0 66 1.0
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Optimized geometries of 3 (DFT//B3LYP/ rb3lyp/6-31g(d))

Symbolic Z-matrix:
Charge = 0 Multiplicity = 3

C	-2.44465000	1.86302000	-0.31719200
C	-1.50655200	0.86446900	-0.60894200
C	-0.14657700	1.17728400	-0.75613400

C	0.26140900	2.51711800	-0.60669400
C	-0.65801000	3.52690000	-0.31120700
C	-1.99728400	3.20047600	-0.16932200
H	0.59169100	-0.84035900	-1.15631800
H	-1.82981900	-0.16558300	-0.72228600
C	0.87127800	0.20264400	-1.03551400
H	-0.30866200	4.54771800	-0.20099000
C	2.57753600	1.96358000	-1.05319800
C	2.18018900	0.55356300	-1.12117300
O	1.56549100	2.87568200	-0.75744600
O	3.67761700	2.41484000	-1.27231600
O	2.91513900	-1.40284600	-2.20567300
C	3.20426200	-0.50484600	-1.41637400
C	9.41333800	-1.07770000	0.52462400
C	8.28738100	-0.42318100	1.08401800
C	7.05914900	-0.48447000	0.44863200
C	6.86532300	-1.17260100	-0.77056400
C	7.99593000	-1.81013400	-1.33093100
C	9.22654400	-1.76661600	-0.71801800
H	8.34559400	0.13636300	2.00705000
C	5.57310400	-1.15406600	-1.34377200
H	7.88389400	-2.34197000	-2.27191500
H	10.05932500	-2.26288700	-1.19710600
C	4.53200900	-0.47308100	-0.76023800
C	4.72295900	0.18337300	0.52797000
H	5.38913200	-1.67487100	-2.27991800
O	3.87584500	0.72016900	1.21141400
O	6.01540100	0.15465800	1.05346700
N	10.63124200	-1.06719200	1.15503100
C	10.82587700	-0.33814300	2.41485700
C	11.05265100	1.17090700	2.25534500
H	11.68901400	-0.78750700	2.91390800
H	9.96742600	-0.52640300	3.06824900
H	11.15755400	1.63580700	3.24220500
H	11.96430100	1.37556100	1.68510300
H	10.21513100	1.65203300	1.74075400
C	11.80565200	-1.71825300	0.56072700
C	12.51726800	-0.89544700	-0.52113900
H	11.50959400	-2.69467400	0.16327300
H	12.50179800	-1.92552700	1.37818200
H	13.37074600	-1.45929100	-0.91459200
H	11.84847800	-0.66357100	-1.35607600
H	12.89184300	0.04945300	-0.11521200
H	-2.72069800	3.97625700	0.05848700
C	-6.53709800	-2.73896700	-0.22664000
C	-6.02662400	-1.45678600	-0.17051100
C	-6.87661200	-0.34505100	0.05092200
C	-8.27526100	-0.57766400	0.21536600
C	-8.77812100	-1.90315000	0.15409000
C	-7.91765700	-2.96548400	-0.06411500
H	-5.87217800	-3.58010000	-0.39696000

H	-4.96247800	-1.28392500	-0.29551200
C	-6.39044900	1.00847900	0.11852100
C	-9.15755000	0.50904400	0.43908500
H	-8.32717300	-3.96898400	-0.10684100
C	-8.66296900	1.80186200	0.49904500
C	-7.29218000	2.05088400	0.34086900
H	-9.35531800	2.61899800	0.67100000
H	-6.92025900	3.06872800	0.39091000
C	-10.22808500	-2.16906700	0.32246800
C	-10.60838300	0.27301600	0.61002100
N	-11.05156800	-1.05389800	0.54291700
C	-12.49295700	-1.26606500	0.71771400
H	-12.68025000	-2.33562500	0.66569300
H	-12.80952200	-0.86845900	1.68458800
H	-13.04304400	-0.74414600	-0.06908000
O	-11.41242900	1.17855400	0.80398100
O	-10.69616700	-3.30090200	0.27435300
C	-5.00748100	1.29182700	-0.03707900
C	-3.82419700	1.54721600	-0.16793000

1 2 1.5 6 1.5 73 1.5
2 3 1.5 8 1.0
3 4 1.5 9 1.5
4 5 1.5 13 1.0
5 6 2.0 10 1.0
6 47 1.0
7 9 1.0
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9 12 2.0
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11 12 1.0 13 1.0 14 2.0
12 16 1.0
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15 16 2.0
16 27 1.0
17 18 1.5 22 1.5 32 1.5
18 19 2.0 23 1.0
19 20 1.5 31 1.0
20 21 1.5 24 1.5
21 22 2.0 25 1.0
22 26 1.0
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24 27 2.0 29 1.0
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27 28 1.0
28 30 2.0 31 1.0
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32 33 1.0 40 1.0
33 34 1.0 35 1.0 36 1.0
34 37 1.0 38 1.0 39 1.0
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40 41 1.0 42 1.0 43 1.0
41 44 1.0 45 1.0 46 1.0
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48 49 2.0 53 1.5 54 1.0
49 50 1.5 55 1.0
50 51 1.5 56 1.5
51 52 1.5 57 1.5
52 53 2.0 63 1.0
53 58 1.0
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56 60 1.5 72 1.5
57 59 2.0 64 1.0
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59 60 1.5 61 1.0
60 62 1.0
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63 65 1.0 71 2.0
64 65 1.0 70 2.0
65 66 1.0
66 67 1.0 68 1.0 69 1.0
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72 73 3.0
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Optimized geometries of 4 (DFT//B3LYP/ rb3lyp/6-31g(d))

Symbolic Z-matrix:
Charge = 0 Multiplicity = 3

C	1.94055200	1.53977000	-0.28336200
C	0.97303500	0.56480300	-0.55633600

C	-0.38252300	0.91036800	-0.67953800
C	-0.75664800	2.25925100	-0.52653800
C	0.19162600	3.24618900	-0.24834200
C	1.52531200	2.88752200	-0.12890600
H	-1.17627500	-1.08922500	-1.05886200
H	1.26896400	-0.47305000	-0.67363800
C	-1.42770800	-0.03908000	-0.93752600
H	-0.13016200	4.27564100	-0.13362700
C	-3.09261500	1.76142500	-0.93252100
C	-2.73047500	0.34225200	-1.00311700
O	-2.05651900	2.64838600	-0.65678100
O	-4.18692400	2.23752100	-1.13417300
O	-3.51932500	-1.62149700	-2.03773400
C	-3.78151300	-0.69337900	-1.27413200
C	-10.02436900	-0.97331700	0.60099200
C	-8.88096200	-0.37177600	1.17938000
C	-7.64932200	-0.49353000	0.55805100
C	-7.47620300	-1.20012100	-0.65381000
C	-8.62522700	-1.79652100	-1.22206700
C	-9.86046300	-1.69405100	-0.62383700
H	-8.93259900	0.18627700	2.10443200
C	-6.17689900	-1.24349800	-1.21447500
H	-8.52242400	-2.34560800	-2.15418000
H	-10.71324700	-2.16570200	-1.09450800
C	-5.11335300	-0.60527500	-0.62654700
C	-5.28476900	0.06133100	0.65990500
H	-6.00847300	-1.77747100	-2.14614200
O	-4.41900500	0.55379500	1.35242000
O	-6.58278700	0.09763100	1.17122000
N	-11.25140300	-0.86978100	1.19655100
C	-11.40047800	-0.11803100	2.43691900
H	-12.44431200	-0.14775300	2.74925800
H	-11.11111100	0.93284200	2.30782000
C	-12.42379600	-1.49013600	0.59032100
H	-12.63135900	-1.07827400	-0.40571000
H	-13.29156400	-1.30117800	1.22233900
H	2.27179100	3.64523800	0.08507800
C	5.86824700	0.58935400	0.06348900
C	6.34291300	-0.69212000	-0.09210800
C	7.72602200	-0.99238100	0.03029700
C	8.61458200	0.06520300	0.31869100
C	6.80213000	1.68485800	0.36527200
H	7.63273500	-3.11547200	-0.34094800
H	5.64523100	-1.49512700	-0.31475300
C	8.28980500	-2.27903500	-0.11764200
C	10.53383700	-1.41552700	0.30664400
C	9.64481000	-2.49448100	0.01339700
C	4.49584500	0.91834600	-0.05581300
C	3.31556000	1.19547500	-0.16103100
C	9.98062500	-0.12195400	0.45611300
H	10.59302700	0.74203500	0.67693600

H	10.03071800	-3.49820900	-0.10945600
O	6.51444500	2.85015300	0.52606800
O	8.14521100	1.34080000	0.47518900
C	12.43981400	-2.96219400	0.26892000
H	12.24985800	-3.35690400	-0.73784800
H	12.02696400	-3.66984100	0.99946900
H	13.51906300	-2.91713900	0.41616400
H	-10.78983700	-0.54646400	3.24200500
H	-12.30185800	-2.57657700	0.49650000
C	12.76995400	-0.50903600	0.72816900
H	13.79430300	-0.87533200	0.79860100
H	12.51337300	-0.02699700	1.68053600
H	12.73214300	0.25232000	-0.06219200
N	11.88143100	-1.62687200	0.43910300

1 2 1.5 6 1.5 51 1.5
2 3 1.5 8 1.0
3 4 1.5 9 1.5
4 5 1.5 13 1.0
5 6 1.5 10 1.0
6 39 1.0
7 9 1.0
8
9 12 2.0
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11 12 1.0 13 1.0 14 2.0
12 16 1.0
13
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15 16 2.0
16 27 1.0
17 18 1.5 22 1.5 32 1.5
18 19 2.0 23 1.0
19 20 1.5 31 1.0
20 21 1.5 24 1.5
21 22 2.0 25 1.0
22 26 1.0
23
24 27 2.0 29 1.0
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27 28 1.0
28 30 2.0 31 1.0
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32 33 1.0 36 1.0
33 34 1.0 35 1.0 61 1.0
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36 37 1.0 38 1.0 62 1.0

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40 41 2.0 44 1.0 50 1.5
41 42 1.5 46 1.0
42 43 1.5 47 1.5
43 52 2.0 56 1.0
44 55 2.0 56 1.0
45 47 1.0
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47 49 2.0
48 49 1.5 52 1.5 67 1.5
49 54 1.0
50 51 3.0
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52 53 1.0
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57 58 1.0 59 1.0 60 1.0 67 1.0
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63 64 1.0 65 1.0 66 1.0 67 1.0
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Optimized geometries of 5 (DFT//B3LYP/ rb3lyp/6-31g(d))

Symbolic Z-matrix:
Charge = 0 Multiplicity = 3

C	-2.03204700	3.27986400	0.25958000
C	-2.75659200	2.24532600	-0.34508800
C	-4.16027800	2.26834300	-0.36850700
C	-4.83165400	3.35446200	0.22525300
C	-4.12787300	4.39300800	0.83895500
C	-2.74226800	4.35328600	0.85407900
H	-4.48211700	0.37508500	-1.41111000
H	-2.23151100	1.41191900	-0.80126500
C	-4.96634700	1.23116700	-0.94920300
H	-4.67626200	5.21316100	1.28949400
C	-7.00478300	2.46518900	-0.37019600
C	-6.32312400	1.28147000	-0.90394900
O	-6.19151900	3.43503000	0.20977200
O	-8.19014800	2.70093200	-0.42432600
O	-6.70412600	-0.35615200	-2.55390600

C	-7.11811700	0.16739400	-1.52069500
C	-12.96059300	-2.25052900	0.11827400
C	-11.94170400	-1.60781500	0.86483100
C	-10.76807300	-1.21232200	0.24623800
C	-10.52064000	-1.42930000	-1.12789500
C	-11.53284000	-2.08788400	-1.86250500
C	-12.70734100	-2.49269500	-1.27106100
H	-12.03890000	-1.41129800	1.92335400
C	-9.29603500	-0.96466200	-1.66235300
H	-11.37222200	-2.27741700	-2.92040400
H	-13.44315500	-3.00025400	-1.87979200
C	-8.37606400	-0.29899300	-0.88965400
C	-8.60486000	-0.14431900	0.54265700
H	-9.07479600	-1.11320700	-2.71615400
O	-7.83323300	0.30370200	1.36500700
O	-9.83048200	-0.60181000	1.02841000
N	-14.14975100	-2.61333600	0.69863700
C	-14.40085100	-2.36998700	2.12450000
C	-13.80223000	-3.41998900	3.06936300
H	-15.48591600	-2.33349100	2.25689000
H	-14.03137300	-1.37193000	2.38172800
H	-14.00764200	-3.14345700	4.10973000
H	-14.23746200	-4.40791400	2.88831500
H	-12.71761500	-3.49927400	2.94629700
C	-15.18687800	-3.32181400	-0.06177700
C	-14.95089100	-4.82958000	-0.21881900
H	-15.29506800	-2.84976100	-1.04388600
H	-16.13383500	-3.15263200	0.45836100
H	-15.75571300	-5.27094100	-0.81777300
H	-14.00032500	-5.03780400	-0.72007900
H	-14.93754900	-5.33103200	0.75402800
H	-2.18519300	5.15577800	1.32625600
C	2.03240800	3.23265500	0.32006600
C	2.75125300	2.21913700	-0.32559400
C	4.15508100	2.20847500	-0.30602500
C	4.83276500	3.23830600	0.37449500
C	4.13445900	4.25548300	1.02895000
C	2.74847900	4.25027000	0.99957100
H	4.46470200	0.37999000	-1.46140200
H	2.22143400	1.42880800	-0.84815400
C	4.95440300	1.19090300	-0.92913100
H	4.68740900	5.03249100	1.54555700
C	7.00231600	2.33049800	-0.20681900
C	6.30977500	1.20349200	-0.83976800
O	6.19404800	3.28383500	0.40673500
O	8.19452100	2.53587600	-0.20586200
O	6.70927800	-0.31950900	-2.59125400
C	7.09726200	0.11383200	-1.50738700
C	12.75882600	-2.68002900	0.16874600
C	11.74901200	-2.02760100	0.91916500
C	10.61932100	-1.53580900	0.28797000

C	10.42011400	-1.63971200	-1.10708300
C	11.43883200	-2.27656000	-1.85191100
C	12.56978200	-2.77618200	-1.24840400
H	11.82188700	-1.89310400	1.98922900
C	9.23869800	-1.08390900	-1.65100200
H	11.32176000	-2.36551800	-2.92858200
H	13.32254200	-3.24263000	-1.86924500
C	8.31432200	-0.43868500	-0.86604700
C	8.49477500	-0.39078300	0.58063700
H	9.05339500	-1.14756700	-2.72016500
O	7.71314900	0.03614700	1.40470600
O	9.68041600	-0.93564700	1.07641400
N	13.86682500	-3.21382200	0.77677900
C	14.06859700	-3.08697000	2.22560100
C	14.63066100	-1.73368900	2.68017600
H	14.75285100	-3.88601500	2.52405200
H	13.12100200	-3.29510200	2.73392200
H	14.71992900	-1.71786200	3.77234000
H	15.62374800	-1.55595200	2.25568500
H	13.98052200	-0.90586600	2.38069500
C	14.92369500	-3.87191800	-0.00135100
C	15.93088600	-2.91503400	-0.65212000
H	14.46108000	-4.51125300	-0.76031800
H	15.44840900	-4.54689400	0.68064400
H	16.66228400	-3.48542600	-1.23605700
H	15.43519500	-2.20764700	-1.32435300
H	16.47464700	-2.33928900	0.10350400
H	2.19571200	5.03648800	1.50314200
C	0.60815300	3.24502300	0.29840600
C	-0.60789000	3.25880200	0.28050700

1 2 1.5 6 1.5 96 1.5
2 3 1.5 8 1.0
3 4 1.5 9 1.5
4 5 1.5 13 1.0
5 6 1.5 10 1.0
6 47 1.0
7 9 1.0
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9 12 2.0
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11 12 1.0 13 1.0 14 2.0
12 16 1.0
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15 16 2.0
16 27 1.0
17 18 1.5 22 1.5 32 1.5
18 19 2.0 23 1.0
19 20 1.5 31 1.0
20 21 1.5 24 1.5

21 22 2.0 25 1.0
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28 30 2.0 31 1.0
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32 33 1.0 40 1.0
33 34 1.0 35 1.0 36 1.0
34 37 1.0 38 1.0 39 1.0
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40 41 1.0 42 1.0 43 1.0
41 44 1.0 45 1.0 46 1.0
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48 49 1.5 53 1.5 95 1.5
49 50 1.5 55 1.0
50 51 1.5 56 1.5
51 52 1.5 60 1.0
52 53 1.5 57 1.0
53 94 1.0
54 56 1.0
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56 59 2.0
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58 59 1.0 60 1.0 61 2.0
59 63 1.0
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62 63 2.0
63 74 1.0
64 65 1.5 69 1.5 79 1.5
65 66 2.0 70 1.0
66 67 1.5 78 1.0
67 68 1.5 71 1.5
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