Supporting Information

Diketopyrrolopyrrole–fullerene C_{60} architectures as highly efficient heavy atom-free photosensitizers: synthesis, photophysical properties and photodynamic activity

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Figure S5. Absorption spectra changes for the photooxidation of DMA photosensitized by (A) **DPP-C_{60}** and (B) **C_{60}-DPP-C_{60}** after different irradiation times (Δt = 3 min) in toluene and (C) **DPP-C_{60}** and (D) **C_{60}-DPP-C_{60}** after different irradiation times (Δt = 5 min) in DMF.

Figure S6. NMR and MS spectroscopic data.

Scheme S1. Molecular structure of **MC_{60}**.

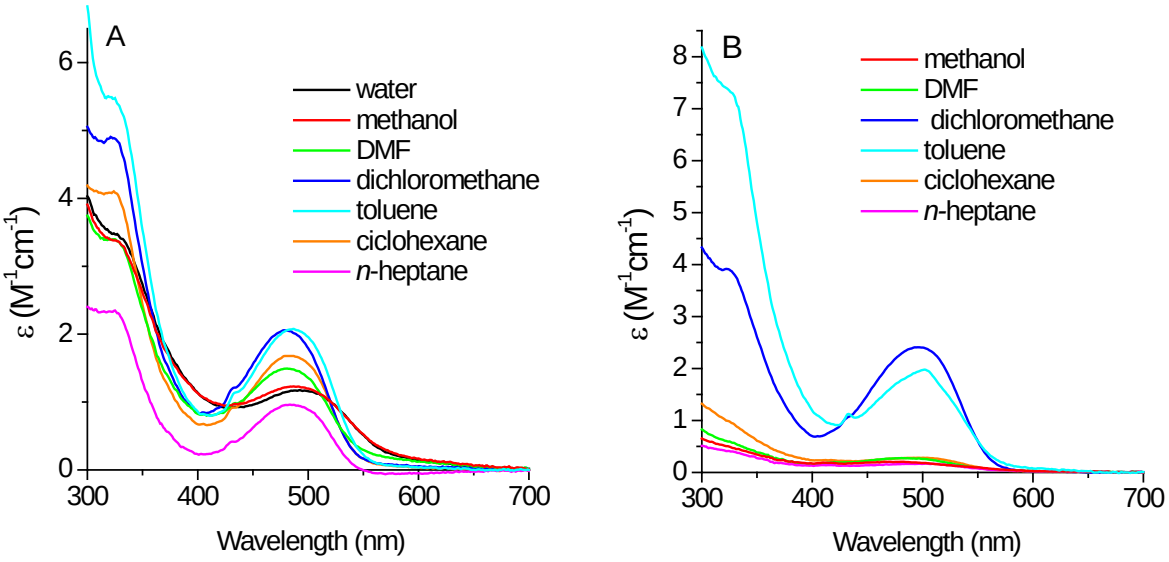


Figure S1. Absorption spectra of (A) **DPP-C_{60}** and (B) **C_{60}-DPP-C_{60}** in different solvents.

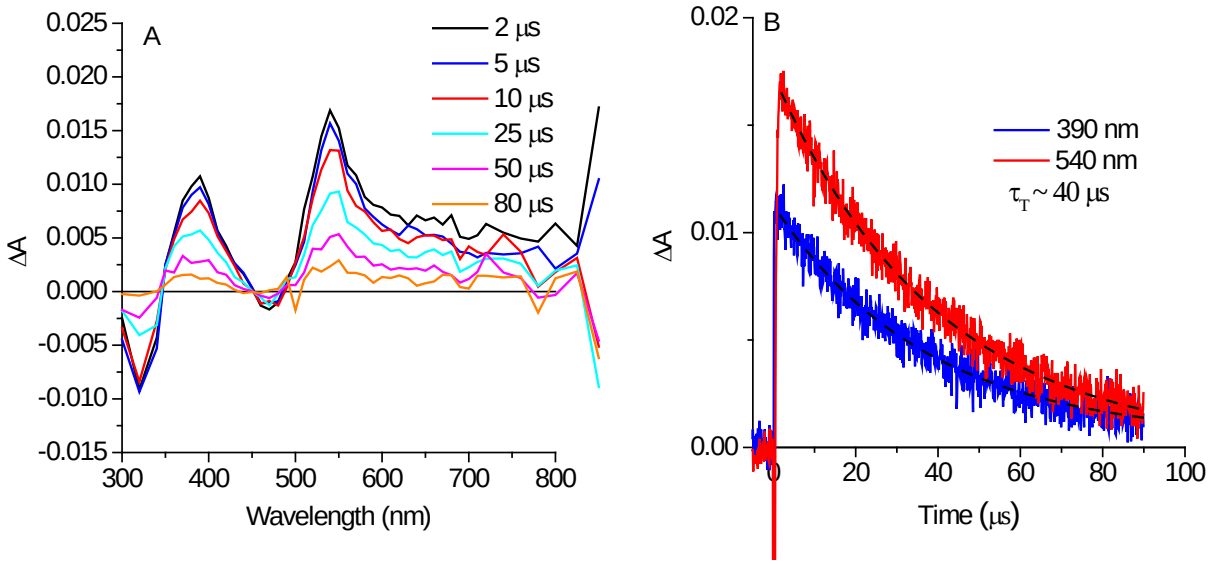


Figure S2. (A) Transient absorption spectrum of **DPP4** determined at different times after laser flash excitation at 532 nm in argon-saturated solution and (B) absorption decay monitored at 390 nm and 540 nm in toluene.

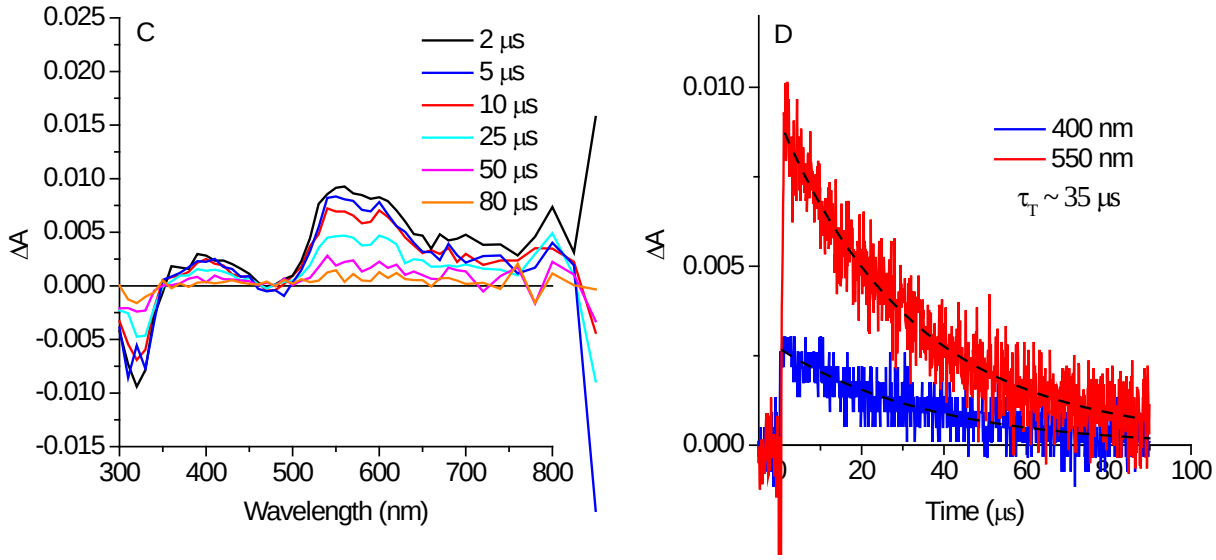


Figure S3. (A) Transient absorption spectrum of **DPP5** determined at different times after laser flash excitation at 532 nm in argon-saturated solution and (B) absorption decay monitored at 400 nm and 550 nm in toluene.

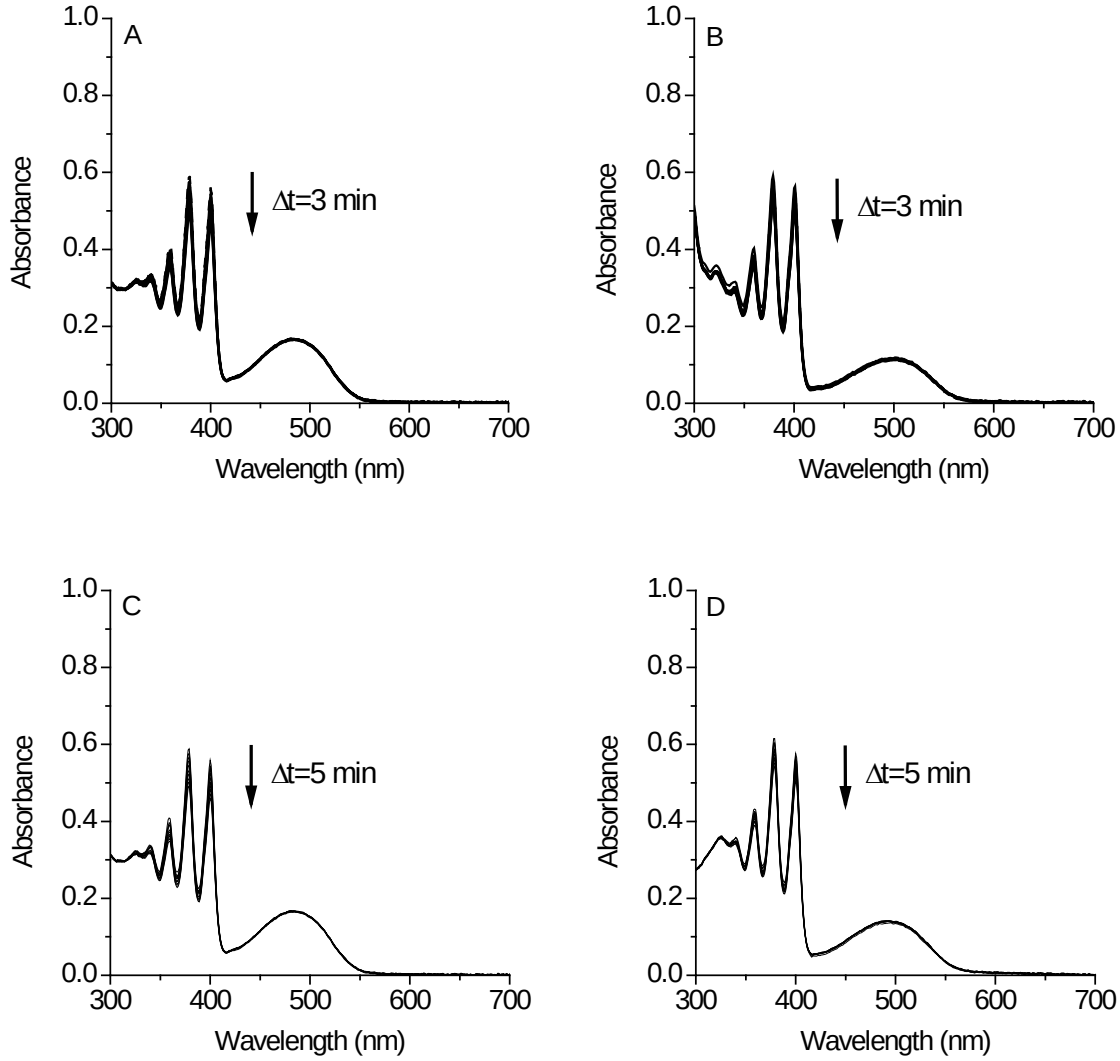


Figure S4. Absorption spectra changes for the photooxidation of DMA photosensitized by (A) **DPP4** and (B) **DPP5** after different irradiation times (Δt = 3 min) in toluene and (C) **DPP4** and (D) **DPP5** after different irradiation times (Δt = 5 min) in DMF.

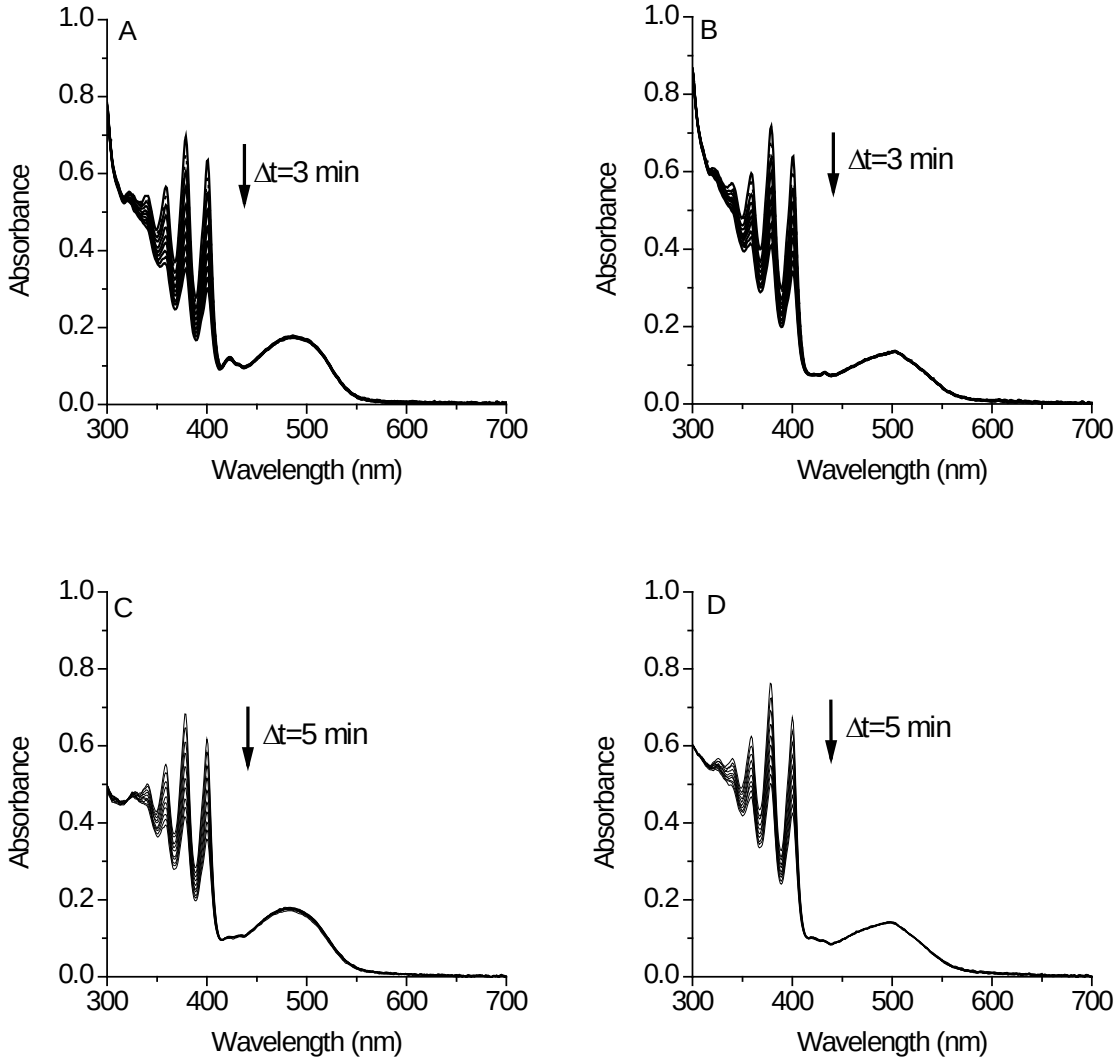
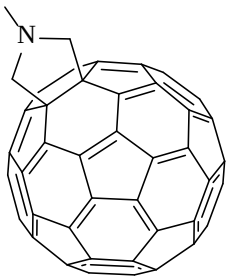


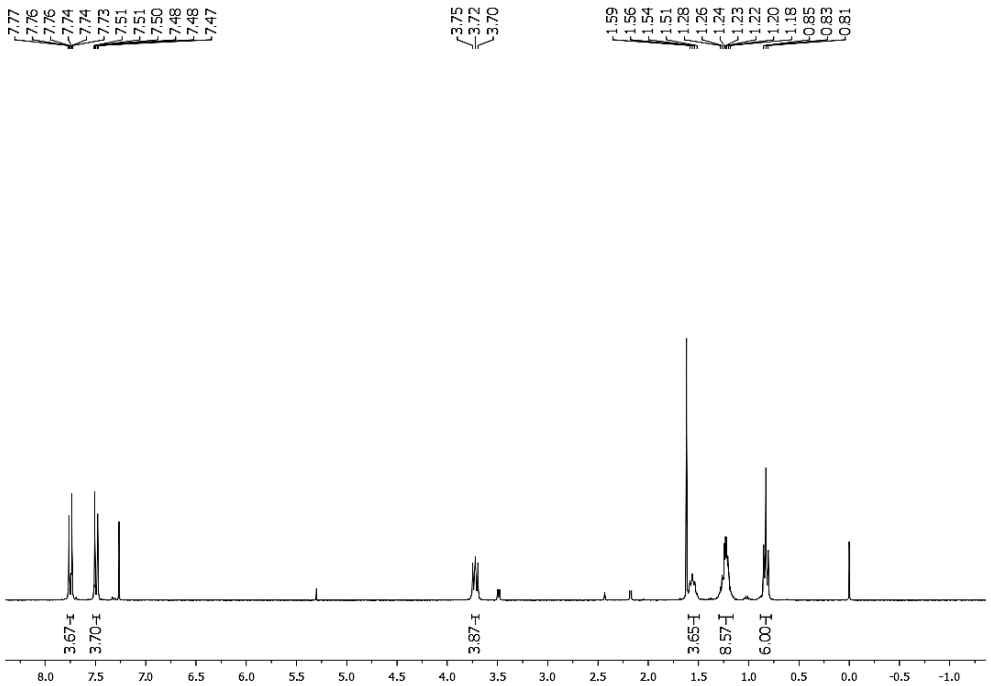
Figure S5. Absorption spectra changes for the photooxidation of DMA photosensitized by (A) **DPP-C_{60}** and (B) **C_{60}-DPP-C_{60}** after different irradiation times (Δt = 3 min) in toluene and (C) **DPP-C_{60}** and (D) **C_{60}-DPP-C_{60}** after different irradiation times (Δt = 5 min) in DMF.

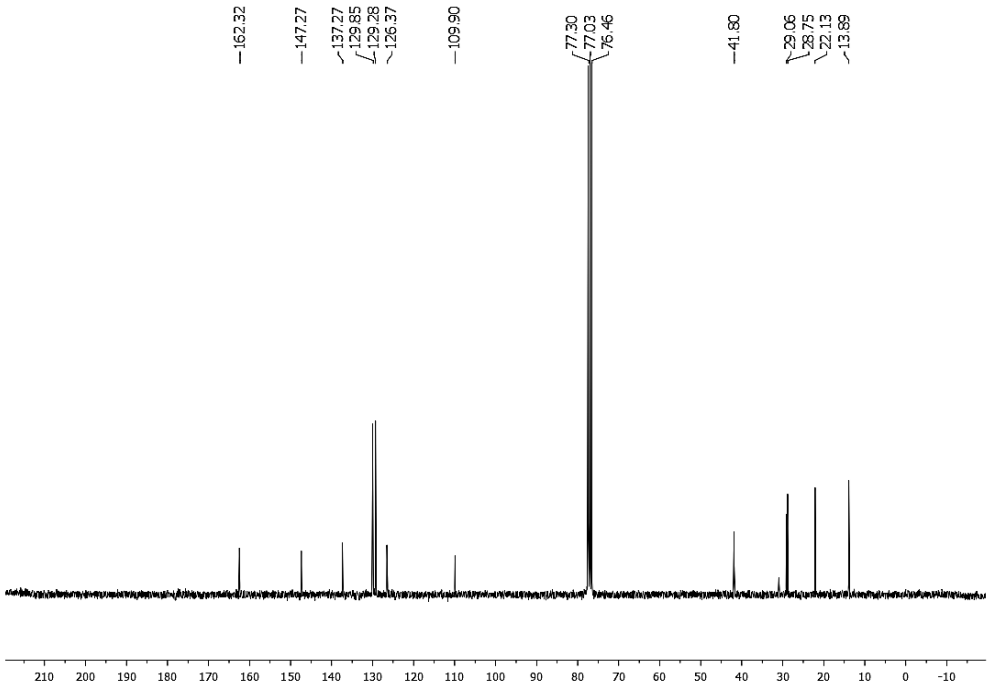


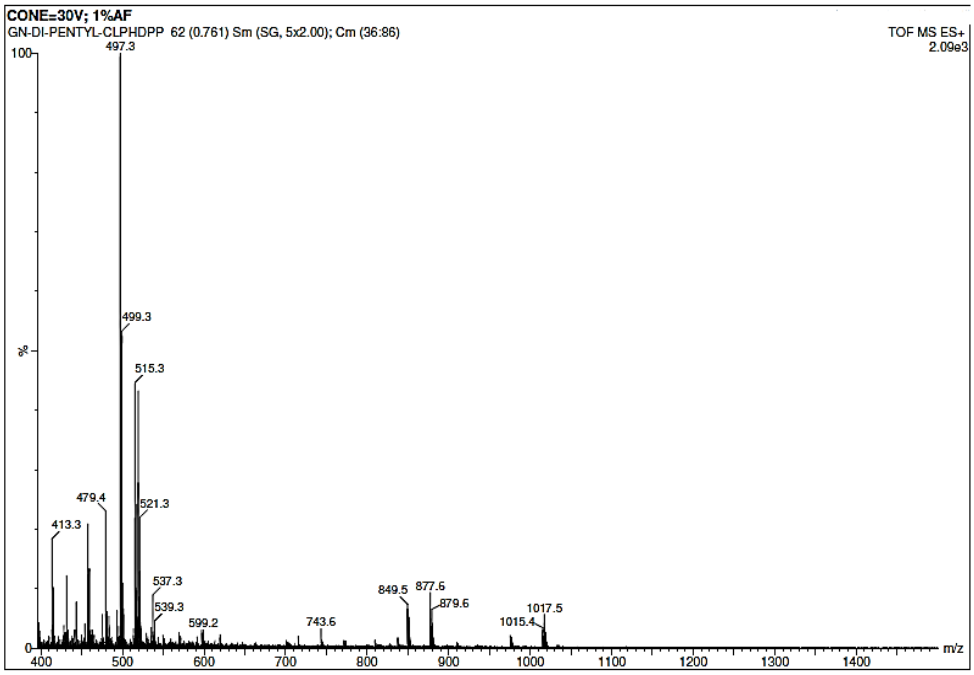
MC_{60}

Scheme S1. Molecular structure of **MC_{60}**.

DPP1


7.77
7.76
7.76
7.74
7.74
7.73
7.51
7.51
7.50
7.48
7.48
7.47
3.75
3.72
3.70
1.59
1.56
1.54
1.51
1.28
1.26
1.24
1.23
1.22
1.20
1.18
0.85
0.83
0.81
3.67
3.70
3.87
3.65
8.57
6.00


162.32
147.27
137.27
129.85
129.28
126.37
109.90
77.30
77.03
76.46
41.80
29.06
28.75
22.13
13.89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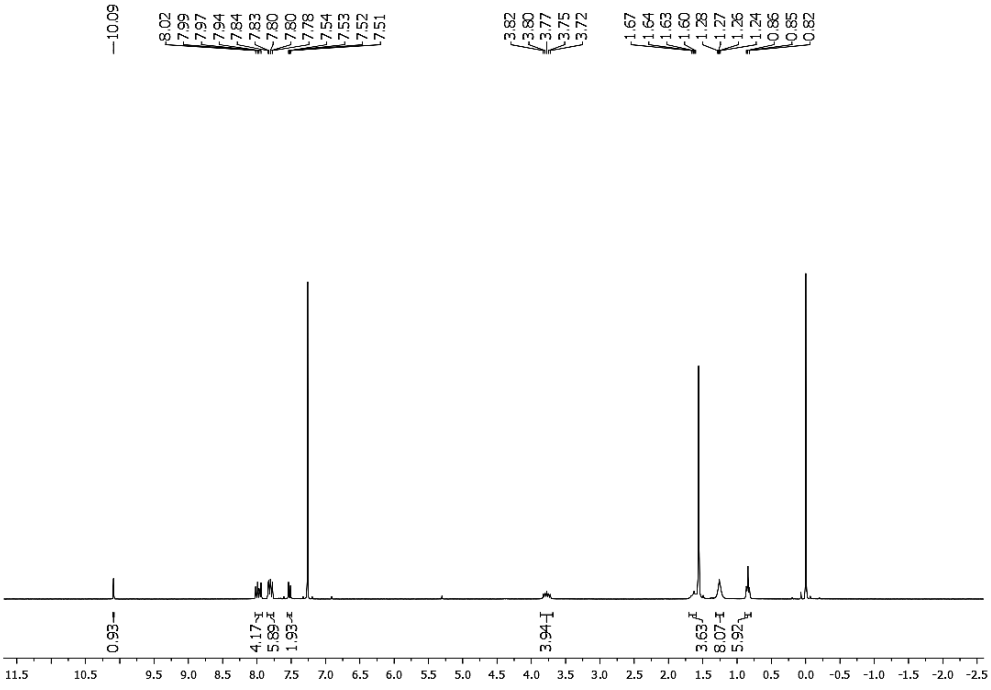
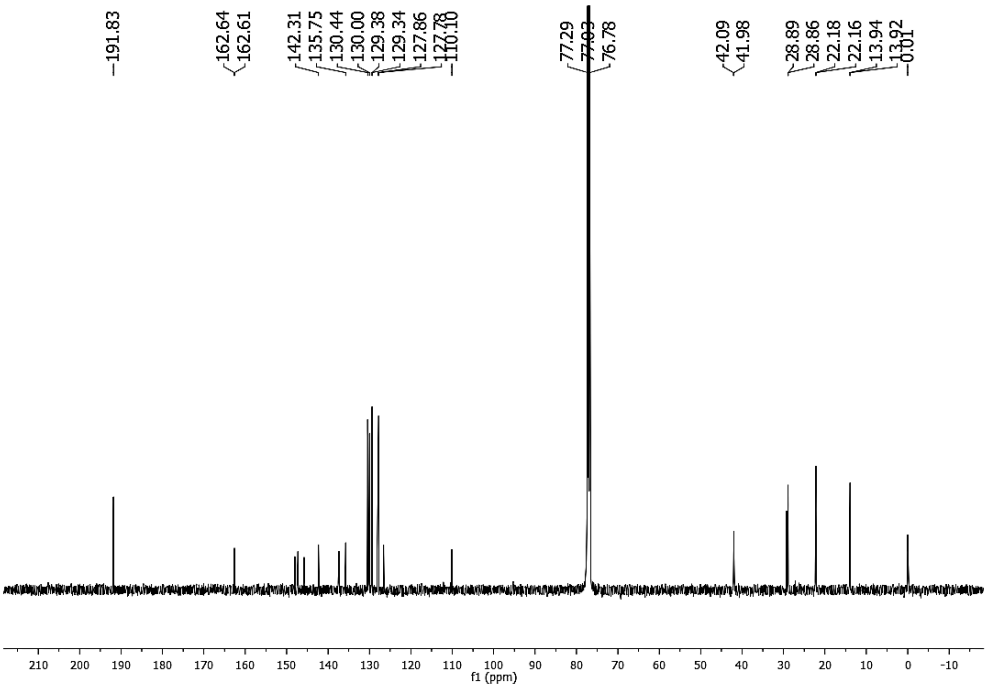
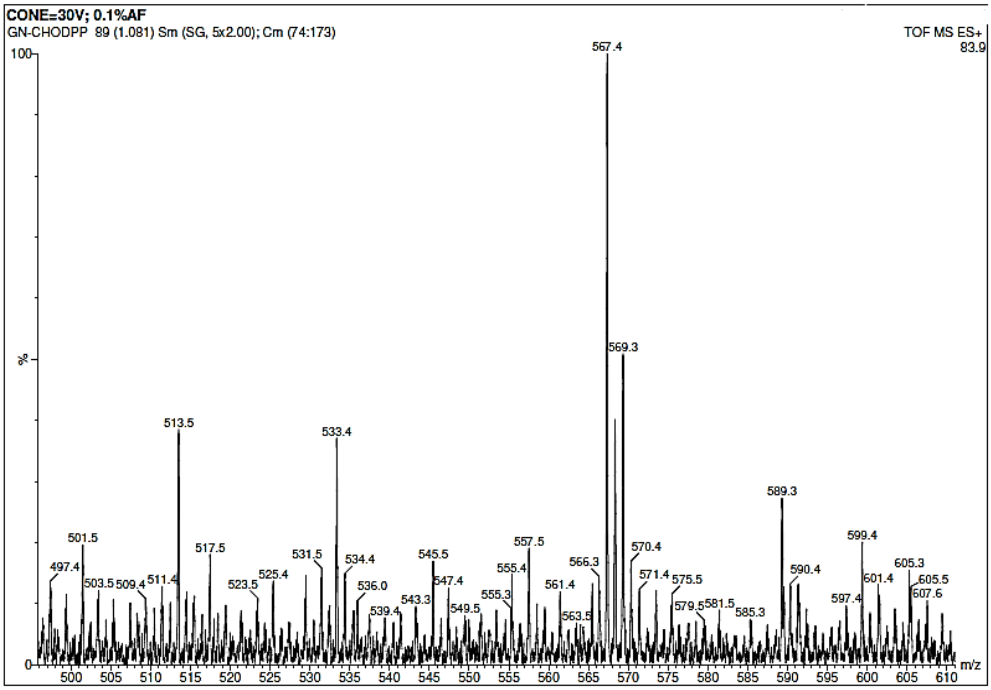
TOF MS ES+
2.09e3
100
%
0
497.3
499.3
515.3
479.4
521.3
413.3
537.3
539.3
599.2
743.6
849.5
877.5
879.5
1015.4
1017.5
m/z
400
500
600
700
800
900
1000
1100
1200
1300
1400

DPP4


10.09
8.02
7.99
7.97
7.94
7.84
7.83
7.80
7.80
7.78
7.54
7.53
7.52
7.51
3.82
3.80
3.77
3.75
3.72
1.67
1.64
1.63
1.60
1.28
1.27
1.26
1.24
0.86
0.85
0.82
0.93
4.17
5.89
1.93
3.94
3.63
8.07
5.92
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5


191.83
162.64
162.61
142.31
135.75
130.44
130.00
129.38
129.34
127.86
127.78
110.10
77.29
77.03
76.78
42.09
41.98
28.89
28.86
22.18
22.16
13.94
13.92
0.01
f1 (ppm)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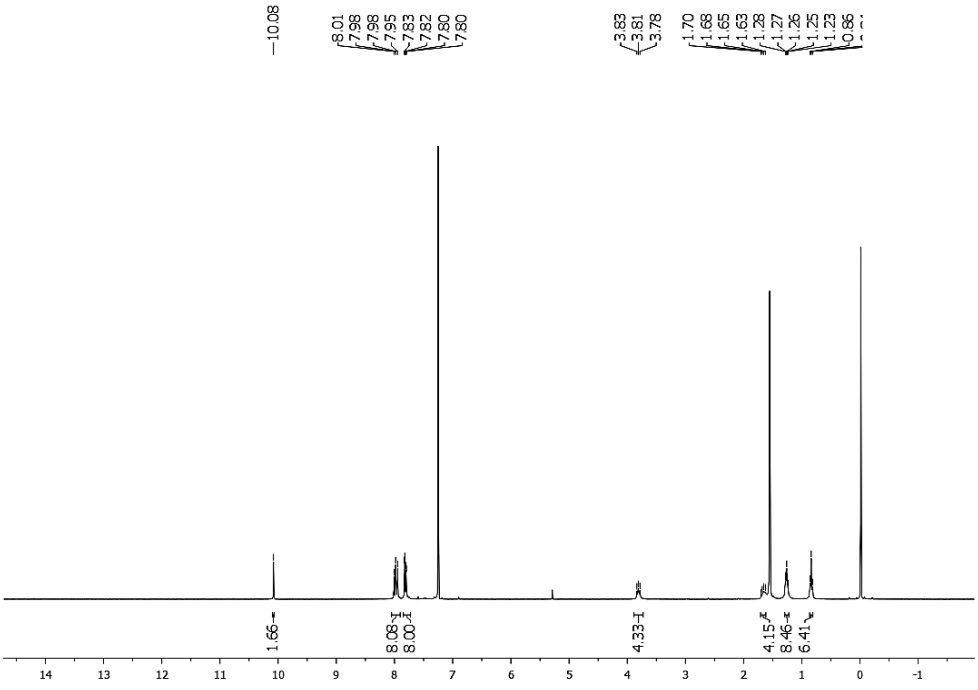
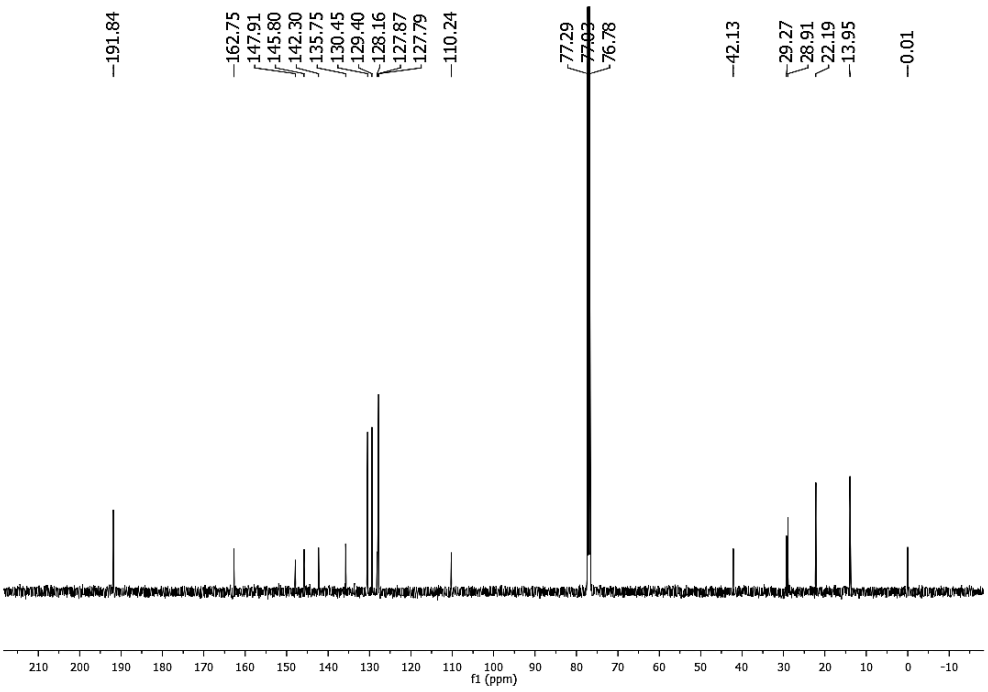
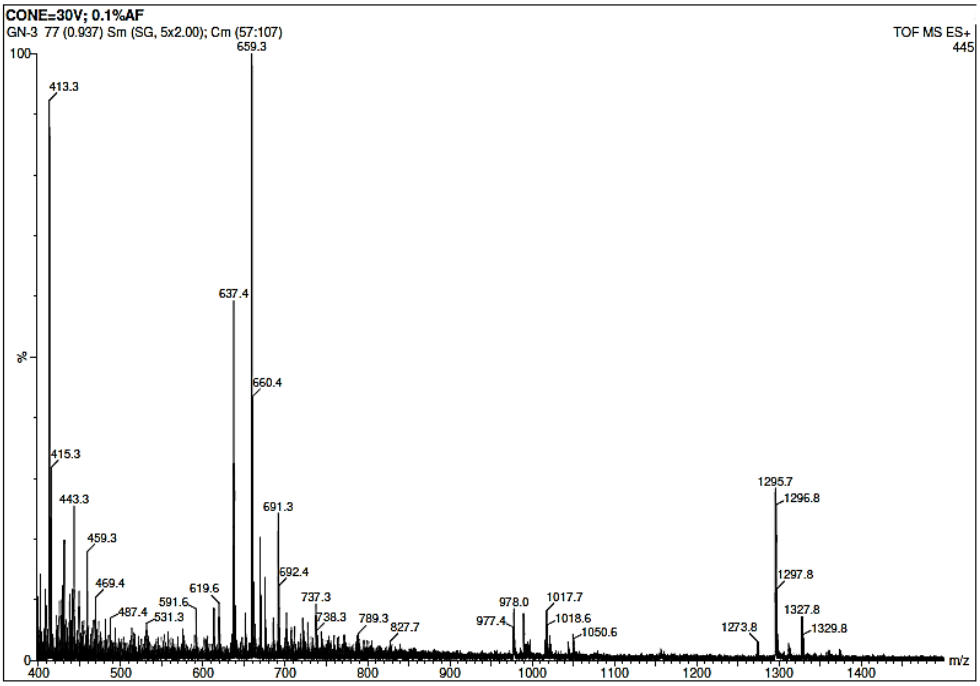
GN-CHODPP 89 (1.081) Sm (SG, 5x2.00); Cm (74:173)
TOF MS ES+
83.9
100
%
0
m/z
567.4
569.3
513.5
533.4
589.3
501.5
517.5
531.5
534.4
545.5
570.4
599.4
497.4
503.5
509.4
511.4
523.5
525.4
536.0
539.4
543.3
547.4
549.5
555.4
555.3
557.5
561.4
563.5
566.3
571.4
575.5
579.5
581.5
585.3
590.4
597.4
601.4
605.3
605.5
607.6

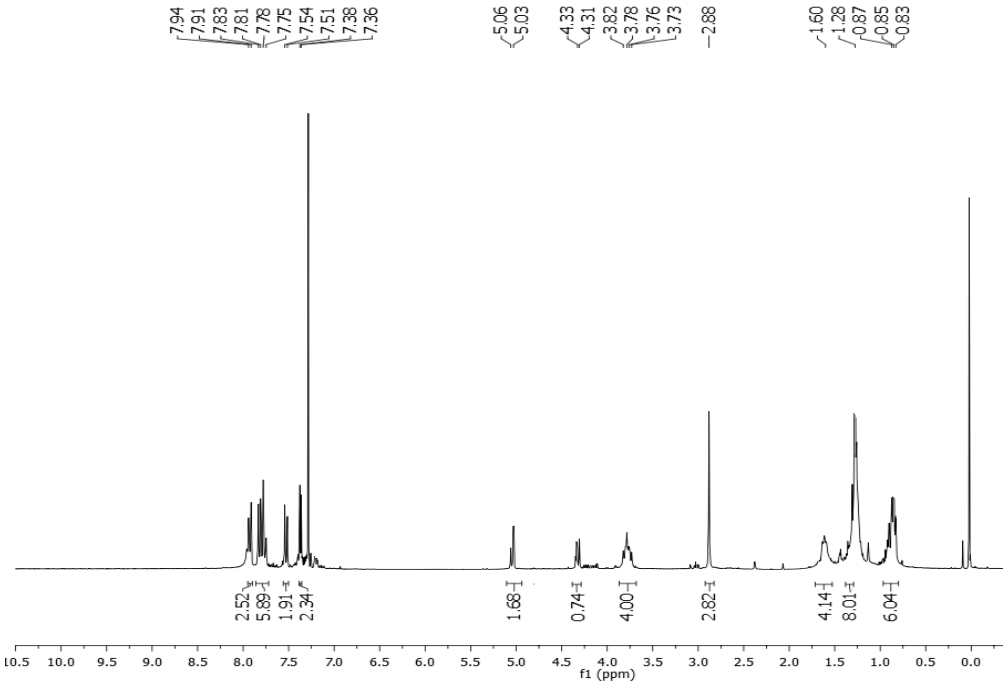
DPP5

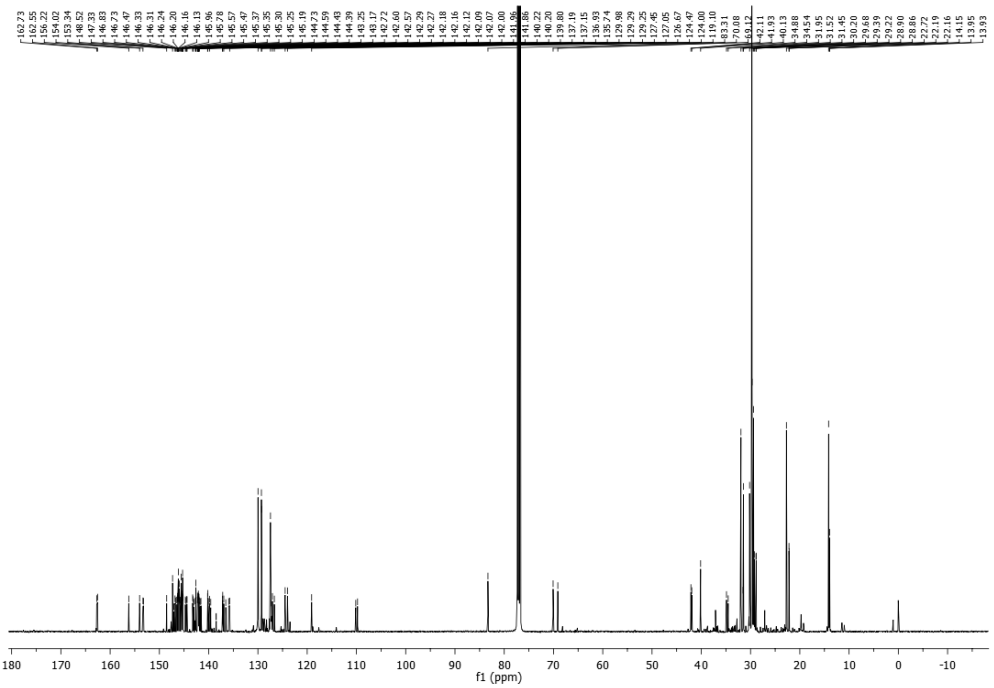

10.08
8.01
7.98
7.98
7.95
7.83
7.82
7.80
7.80
3.83
3.81
3.78
1.70
1.68
1.65
1.63
1.28
1.27
1.26
1.25
1.23
0.86
1.66
8.03
8.00
4.33
4.15
8.46
6.41

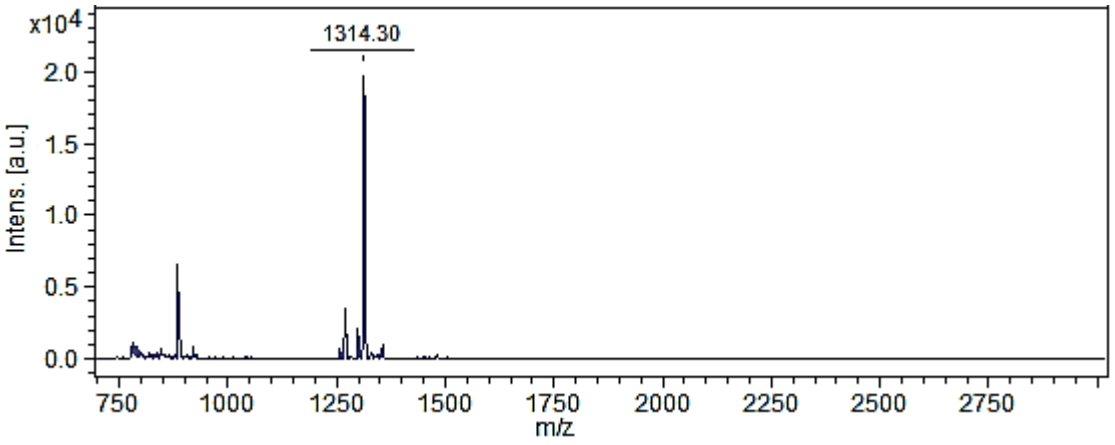

191.84
162.75
147.91
145.80
142.30
135.75
130.45
129.40
128.16
127.87
127.79
110.24
77.29
77.03
76.78
42.13
29.27
28.91
22.19
13.95
0.01
f1 (ppm)


CONE=30V; 0.1%AF
GN-3 77 (0.937) Sm (SG, 5x2.00); Cm (57:107)
TOF MS ES+
445
659.3
413.3
637.4
660.4
415.3
443.3
691.3
459.3
592.4
469.4
619.6
737.3
591.6
487.4
531.3
738.3
789.3
827.7
978.0
977.4
1017.7
1018.6
1050.6
1273.8
1295.7
1296.8
1297.8
1327.8
1329.8
%
m/z

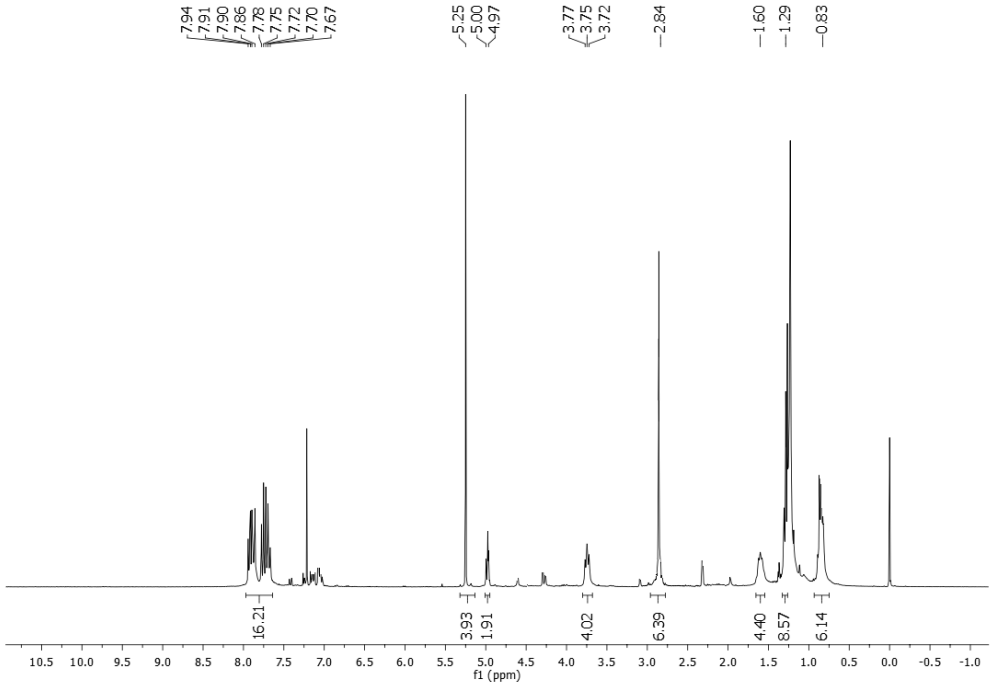
DPP-C$_{60}$

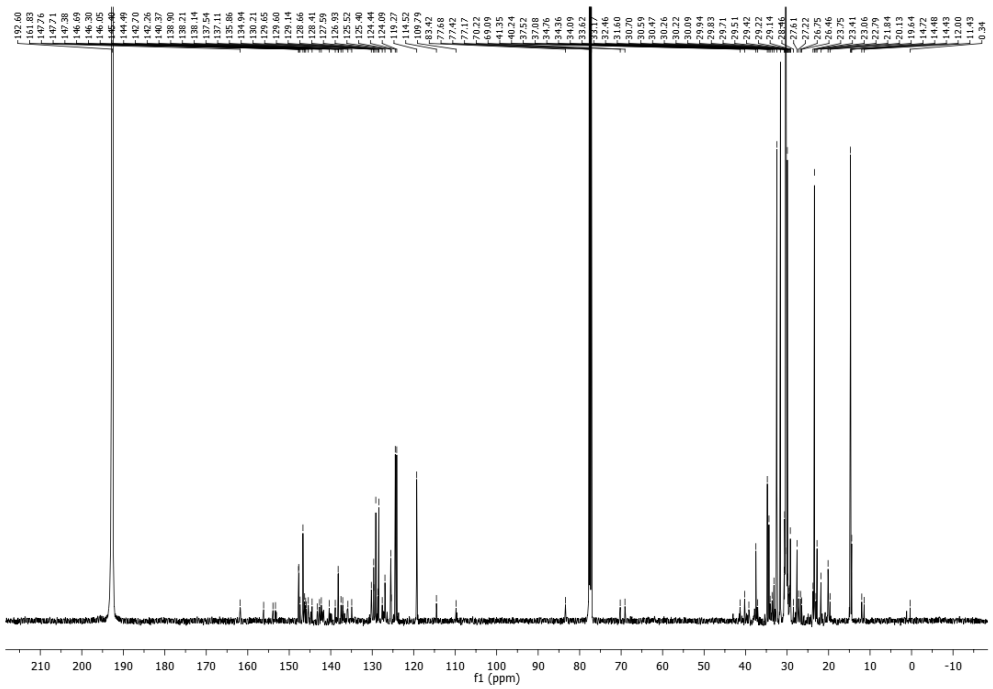

7.94
7.91
7.83
7.81
7.78
7.75
7.54
7.51
7.38
7.36
5.06
5.03
4.33
4.31
3.82
3.78
3.76
3.73
2.88
1.60
1.28
0.87
0.85
0.83
2.52
5.89
1.91
2.34
1.68
0.74
4.00
2.82
4.14
8.01
6.04
f1 (ppm)





C_{60}-DPP-C_{60}


7.94
7.91
7.90
7.86
7.78
7.75
7.72
7.70
7.67
5.25
5.00
4.97
3.77
3.75
3.72
2.84
1.60
1.29
0.83
16.21
3.93
1.91
4.02
6.39
4.40
8.57
6.14
f1 (ppm)


f1 (ppm)

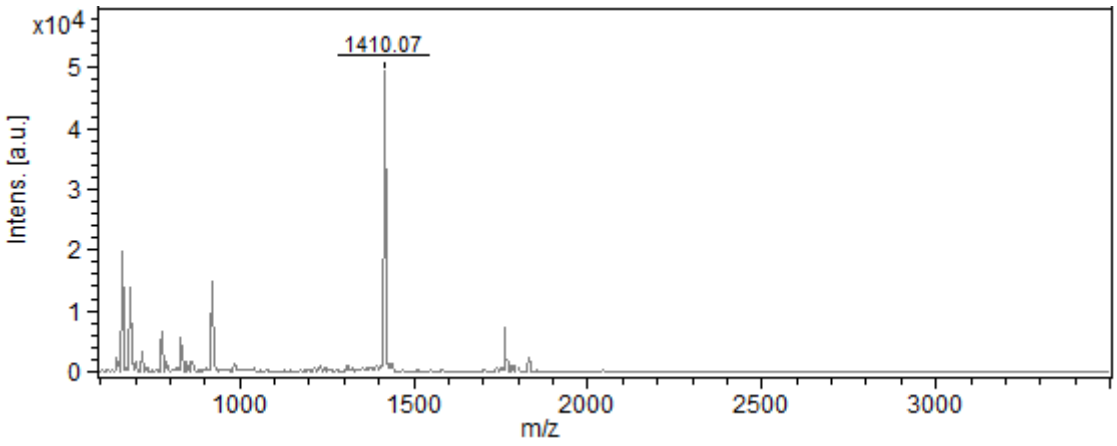


Figure S6. NMR and MS spectroscopic data.