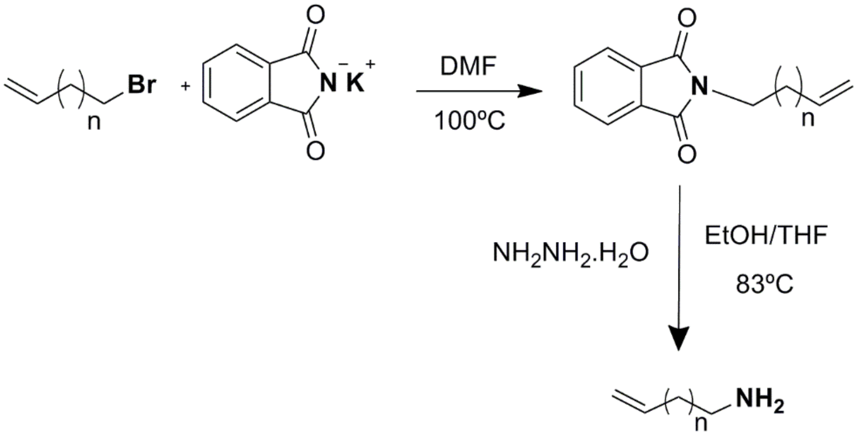
General. All solvents were dried according to standard procedures. Reagents used as purchased. Flash chromatography was performed using silica gel (Scharlau 60, 230-240 mesh). Analytical thin layer chromatography (TLC) were performed using aluminiun-coated Merck Kieselgel 60 F254 plates. NMR spectra were recorded on a Bruker Avance 300 (^{1} H: 300MHz, ^{13}C: 75 MHz) spectrometers at 298K, unless otherwise stated using partially deuterated solvents as internal standards. Coupling constants (J) are denoted in Hz and chemical shifts (δ) in ppm. Multiplicities are denoted as follows: s= singlet, d= doublet, t= triplet, m= multiplet. Electrospray ionization mass spectrometry (ESI-HR-MS) and Matrix-assisted Laser desorption ionization (coupled to a Time-Of-Flight analyzer) experiments (MALDI-TOF HR-MS) were recorded on an HP1100MSDspectrometer and a Bruker REFLEX spectrometer, respectively. Thermogravimetric analyses (TGA) were performed using a TA Instruments TGAQ500 with a ramp of 10 °C/min under air from 100 to 1000 °C.

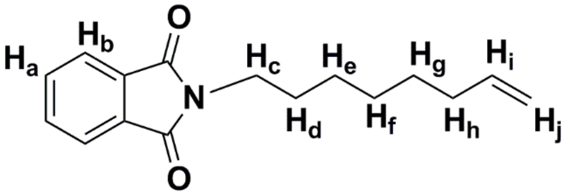
UV-vis-NIR spectrums were performed using a Shimadzu UV-VIS-NIR Spectrophotometer UV-3600.Photoluminescence excitation intensity maps (PLE) were obtained with NanoLog 4 HORIBA. Raman spectra were acquired with a Bruker Senterra confocal Raman microscopy instrument, equipped with 532, 633 and 785 nm lasers. Transmission electron microscopy (TEM) images were obtained with JEOL-JEM 2100F (2.5 Å resolution) instrument.

XPS (X ray Photoelectron Spectroscopy) measurements were performed under Ultra High Vacuum conditions (UHV, with a base pressure of 7×10^{-10} mbar), using a monochromatic Al Kα line as exciting photon source for core level analysis (hν = 1486.7 eV) and He I line for the Ultraviolet Photoelectron Spectroscopy valence band measurements (UPS, hν = 21.2 eV). The emitted photoelectrons were collected in a hemispherical energy analyzer (SPHERA-U7, pass energy set to 20 eV for the XPS measurements to have a resolution of 0.6 eV and 5 eV to have a resolution of 0.1 eV for UPS) and to compensate the built up charge on the sample surface it was necessary (for the XPS measurements) the use of a Flood Gun (FG-500, Specs), with low energy electrons of 3 eV and 40 μA.

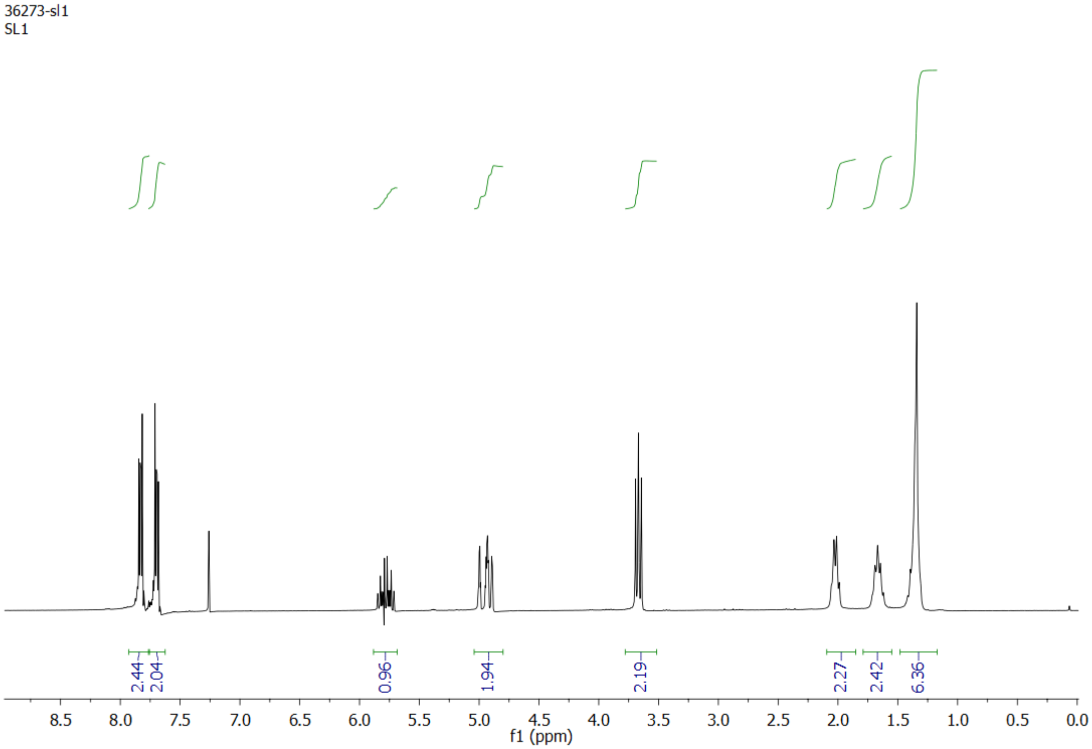
General procedure synthesis lineal amines.

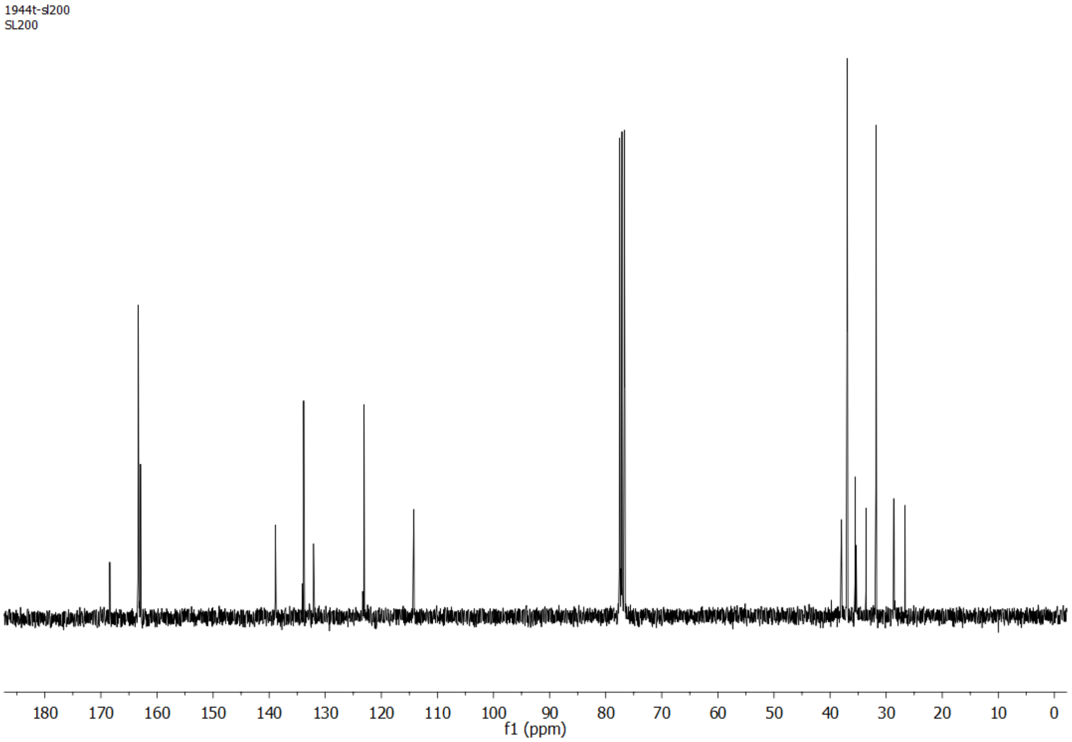


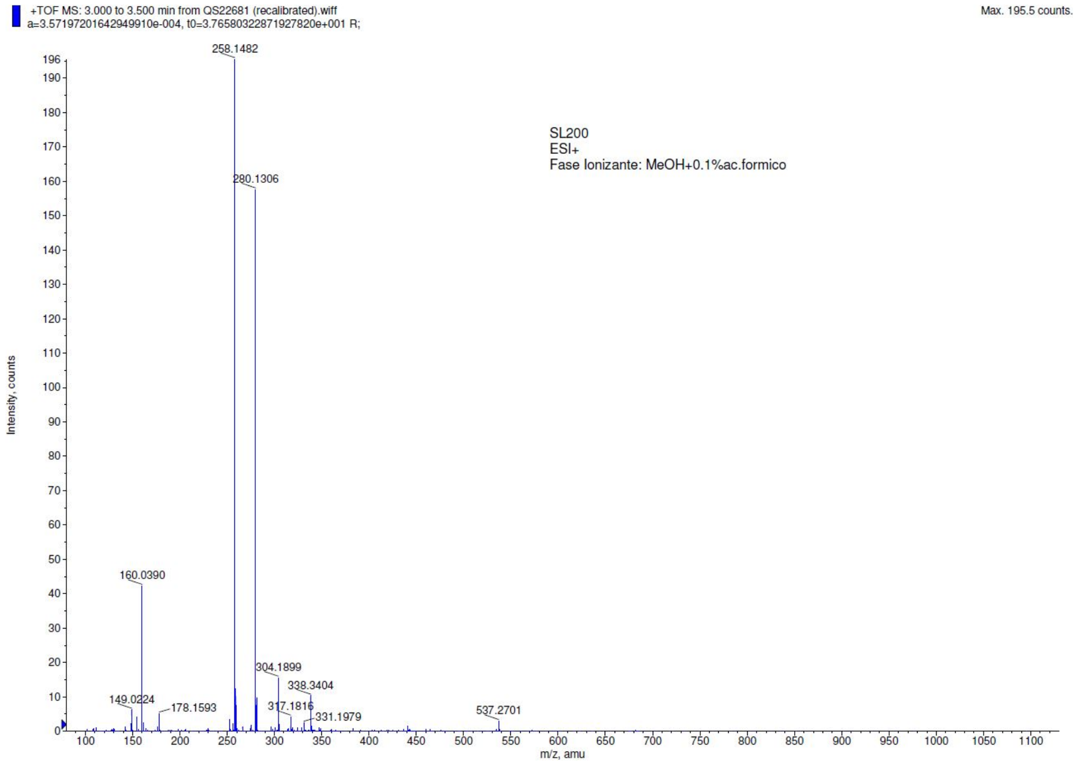
Compound 7 a-c: the alkene was charged in a flask, N, N-dimethylformamide was added and the reaction was heated at 100^{0}C during 2h. The solution was then allowed to come back to room temperature and filtered over celite and the filtrate concentrate in vacuo to give a pale yellow solid in 90-92% yield.

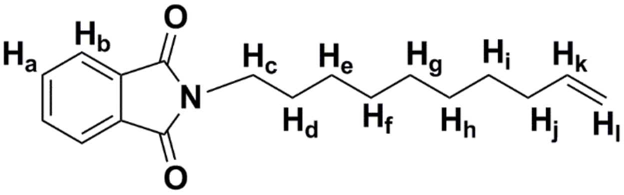


Compound 7a: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.99 (m, 2H$_b$), 7.76 (m, 2H$_a$), 5.78 (m, 1H$_i$), 5.10 (m, 2H$_j$), 3.78 (m, 2H$_c$), 2.01 (m, 2H$_h$), 1.53 (m, 2H$_d$), 1.49 (m, 6H$_{e,f,g}$),^{13}C NMR (75 MHz, CDCl$_3$) δ 168.42, 138.89 , 133.97, 132.09, 123.21, 114.20, 28.65, 28.58, 28.48, 26.64. HR-MS m/z calculated for $C_{16}H_{19}NO_2$ [M-H$^+$] 257.1416 found HR-MS 257.1432.

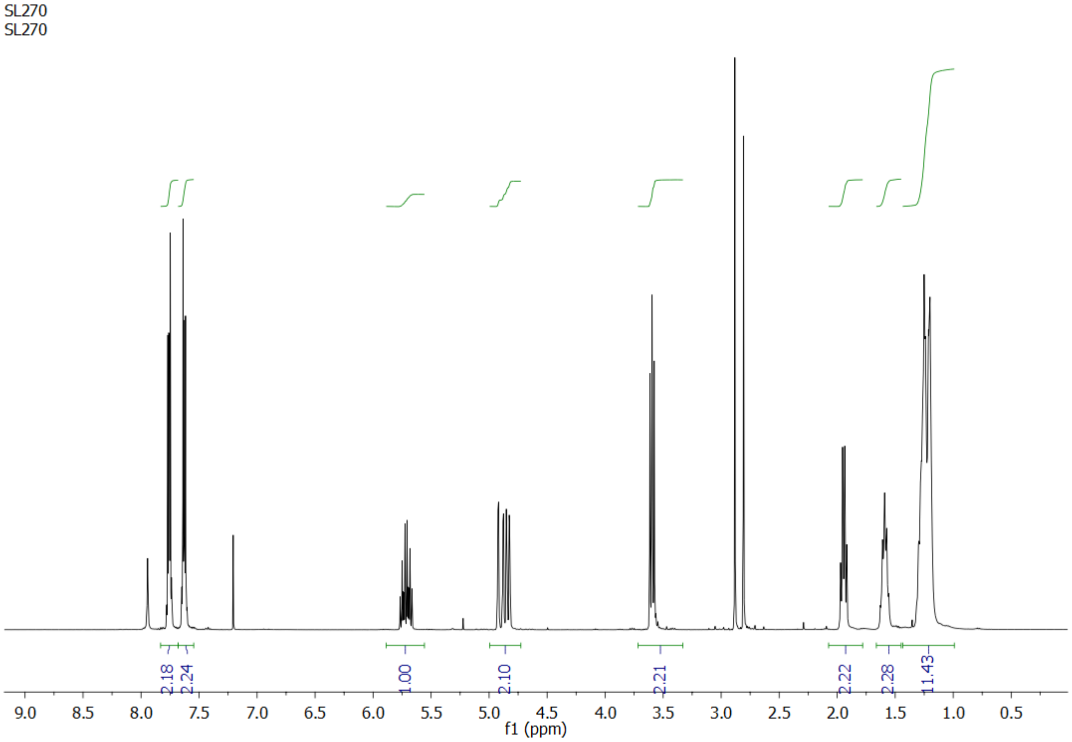

36273-sl1
SL1
2.44
2.04
0.96
1.94
2.19
2.27
2.42
6.36
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

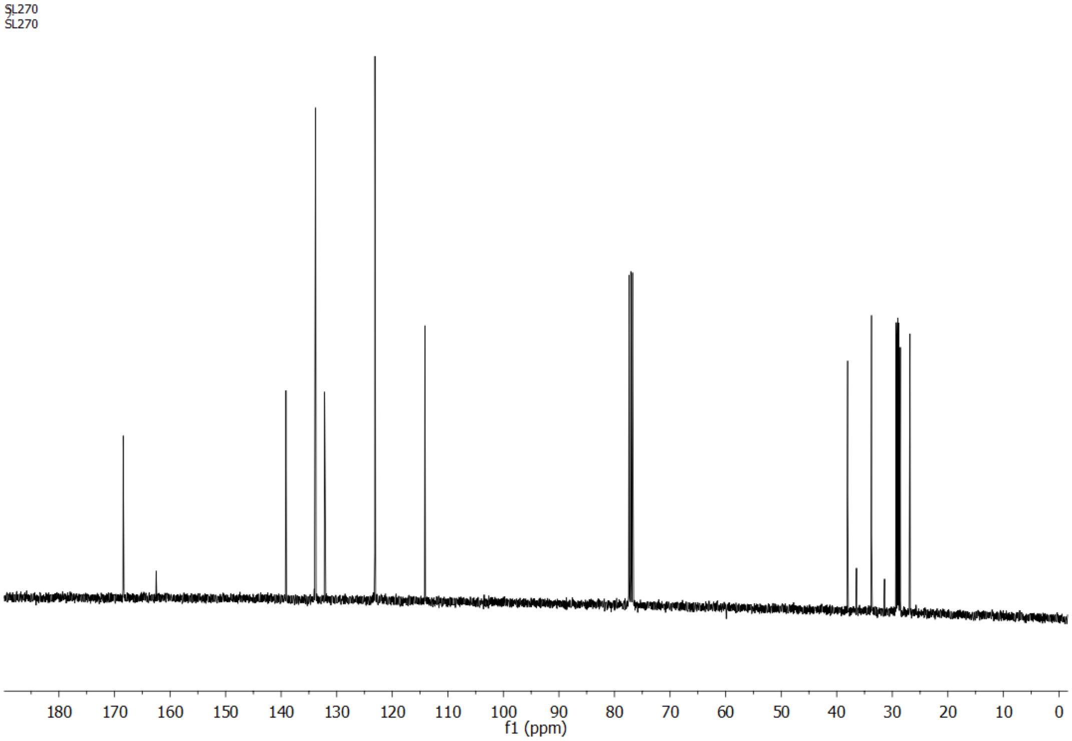

1944t-sl200
SL200
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

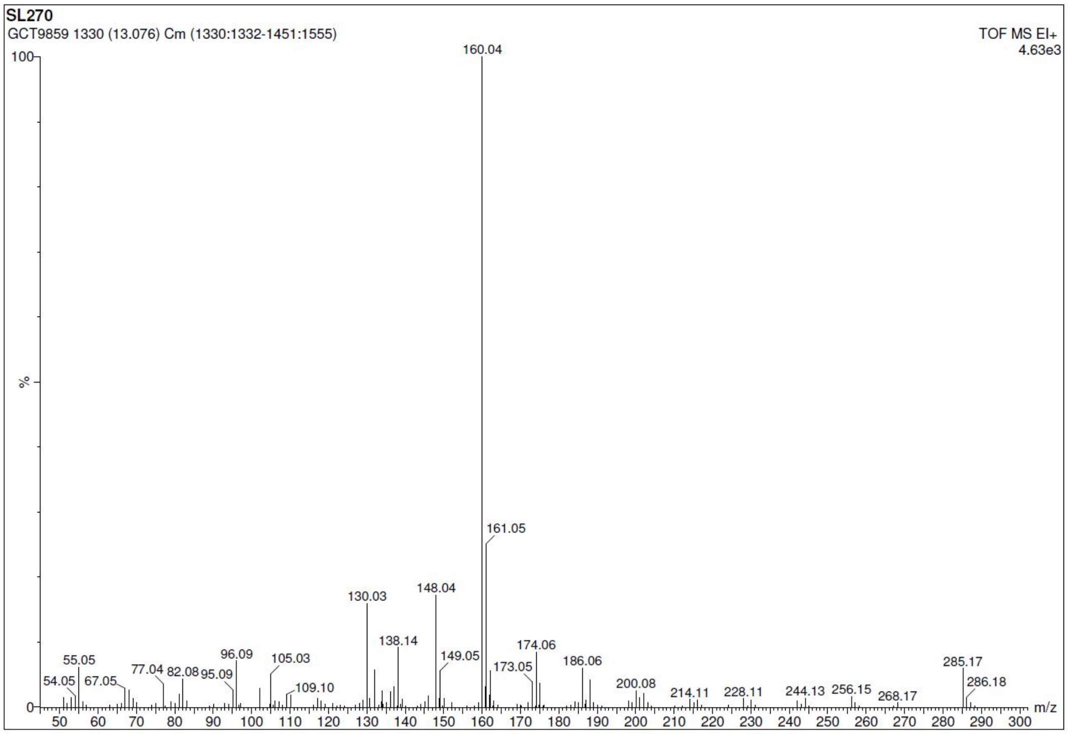


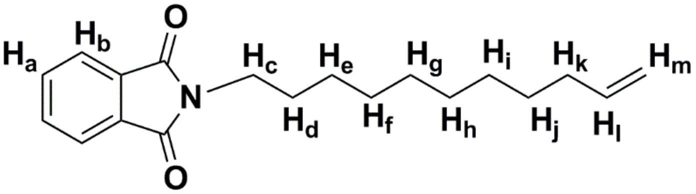


Compound 7b: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.89 (m, 2H$_b$), 7.70 (m, 2H$_a$), 5.72 (m, 1H$_k$), 5.04 (m, 2H$_l$), 3.70 (m, 2H$_c$), 2.03 (m, 2H$_j$),1,53 (m, 2H$_d$), 1.45 (m, 10H$_{e,f,g,h,i}$), ^{13}C NMR (75 MHz, CDCl$_3$) δ 168.43, 139.14, 133.81, 132.18, 123.12, 114.12, 38.04, 33.74, 29.28, 29.10, 29.00, 28.84, 28.57, 26.82. MS m/z calculated for $C_{18}H_{23}NO_2$ 285.17 found MALDI TOF 285.17.

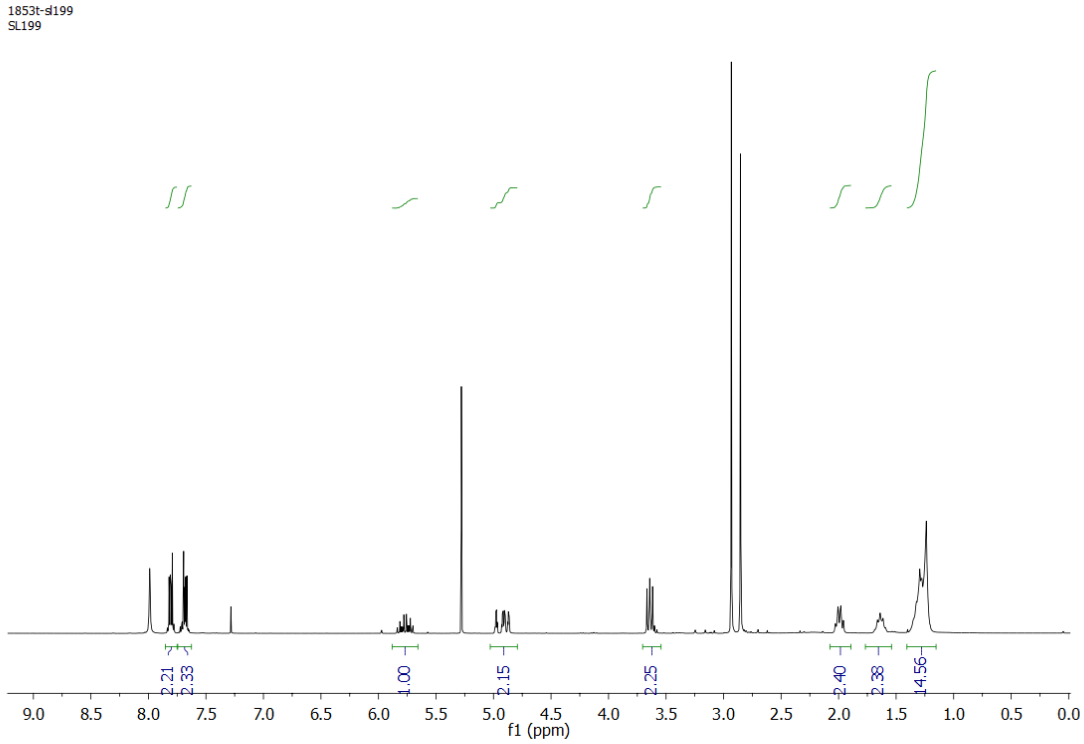

SL270
SL270
2.18
2.24
1.00
2.10
2.21
2.22
2.28
11.43
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

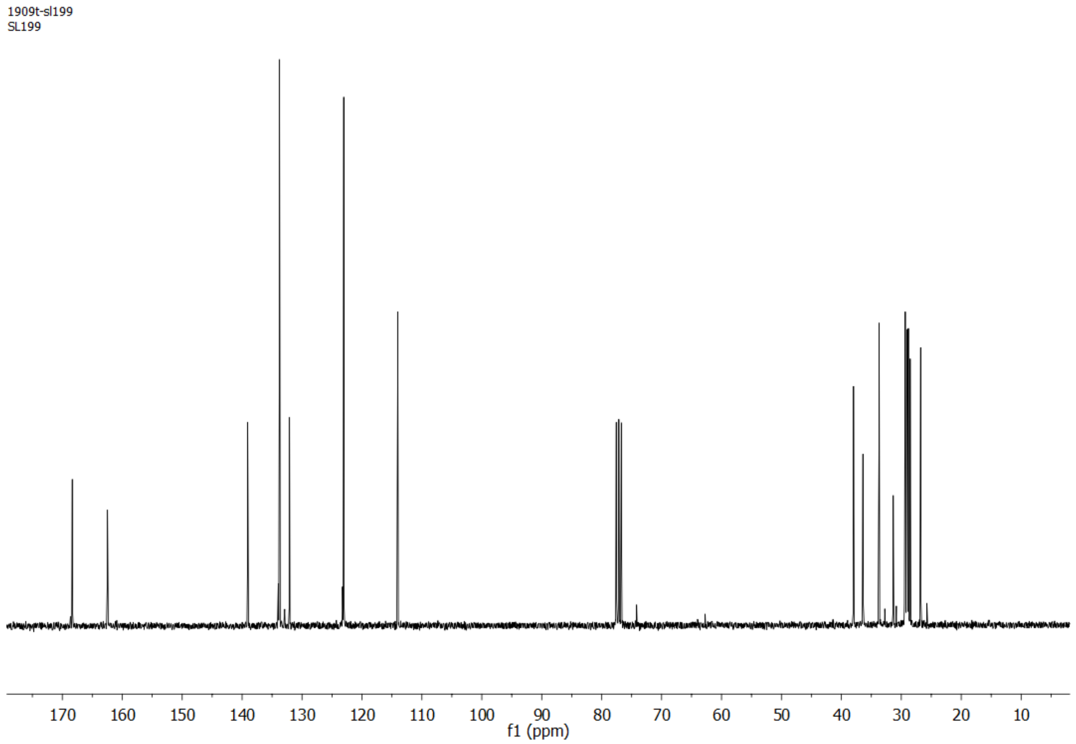

SL270
SL270
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

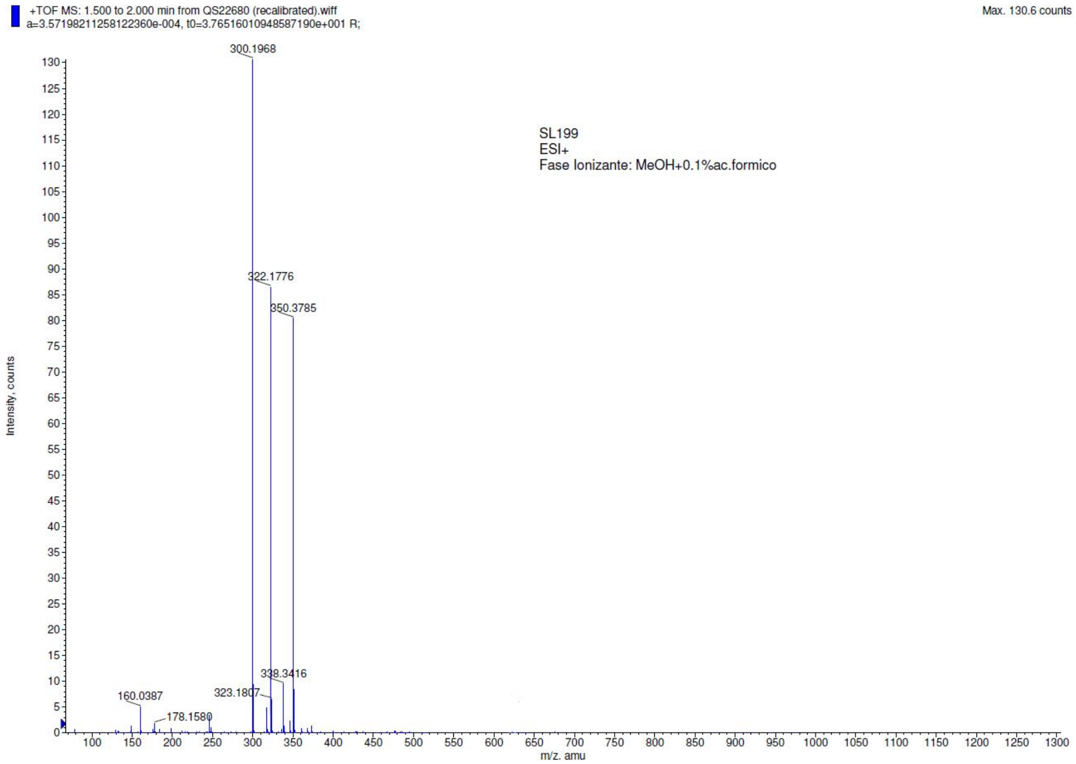




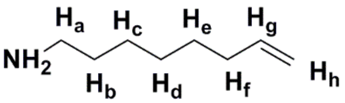
Compound 7c: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.89 (m, 2H$_b$), 7.69 (m, 2H$_a$), 5.93 (m, 1H$_l$), 5.06 (m, 2H$_m$), 3.75 (m, 2H$_c$), 2.10 (m, 2H$_k$),1.53 (m, 2H$_d$), 1.46 (m, 12H$_{e,f,g,h,i,j}$) ^{13}C NMR (75 MHz, CDCl$_3$) δ 168.34, 139.08, 133.86, 132.10, 123.14, 114.03, 37.97, 33.70, 29.37, 29.03, 28.81, 28.51, 26.77. HR-MS m/z calculated for $C_{19}H_{25}NO_2$ 299.1885 found HR-MS 299.1968.


1853t-sl199
SL199
2.21
2.33
1.00
2.15
2.25
2.40
2.38
14.56
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
f1 (ppm)

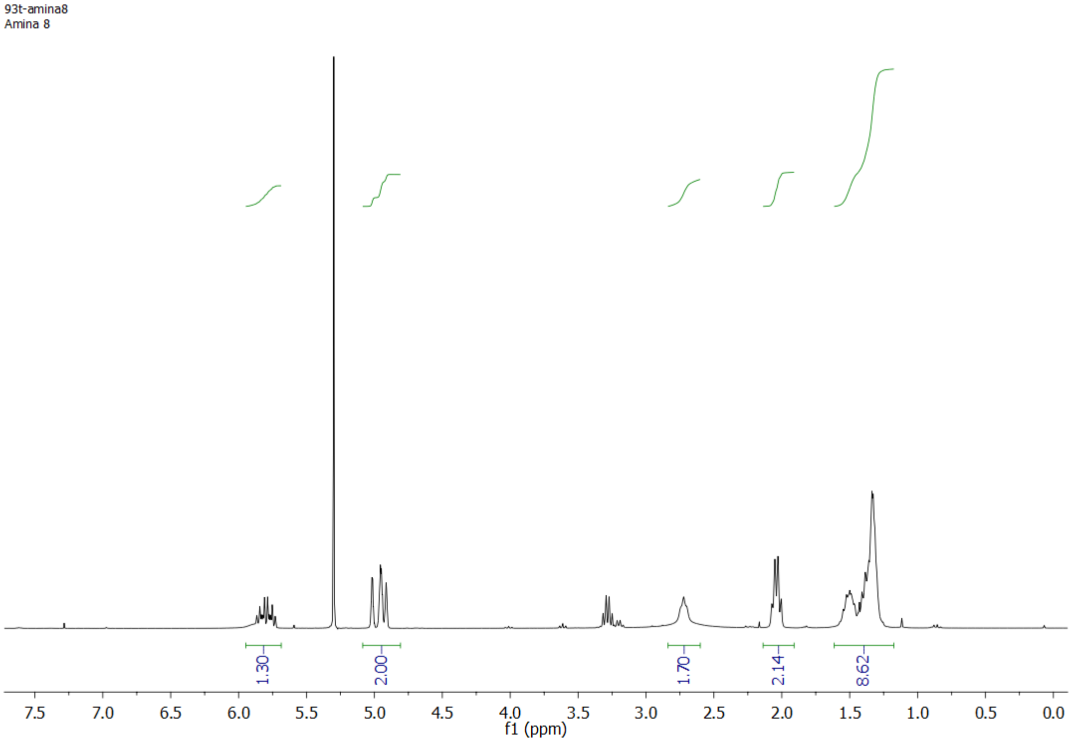

1909t-sl199
SL199
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

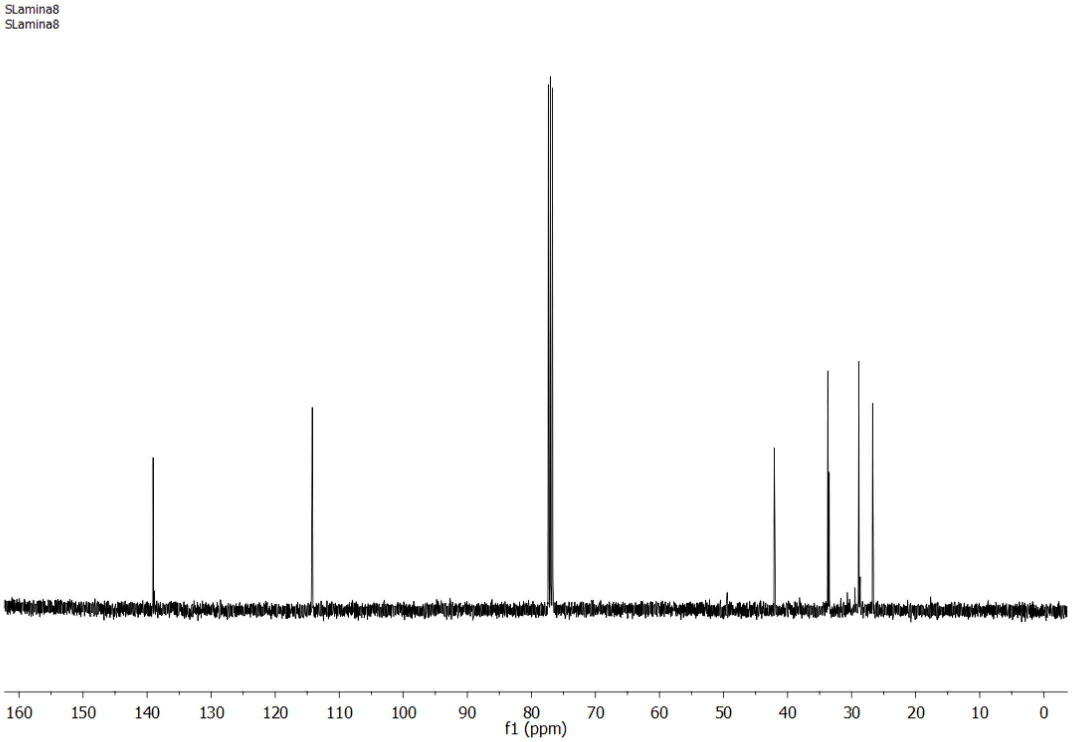


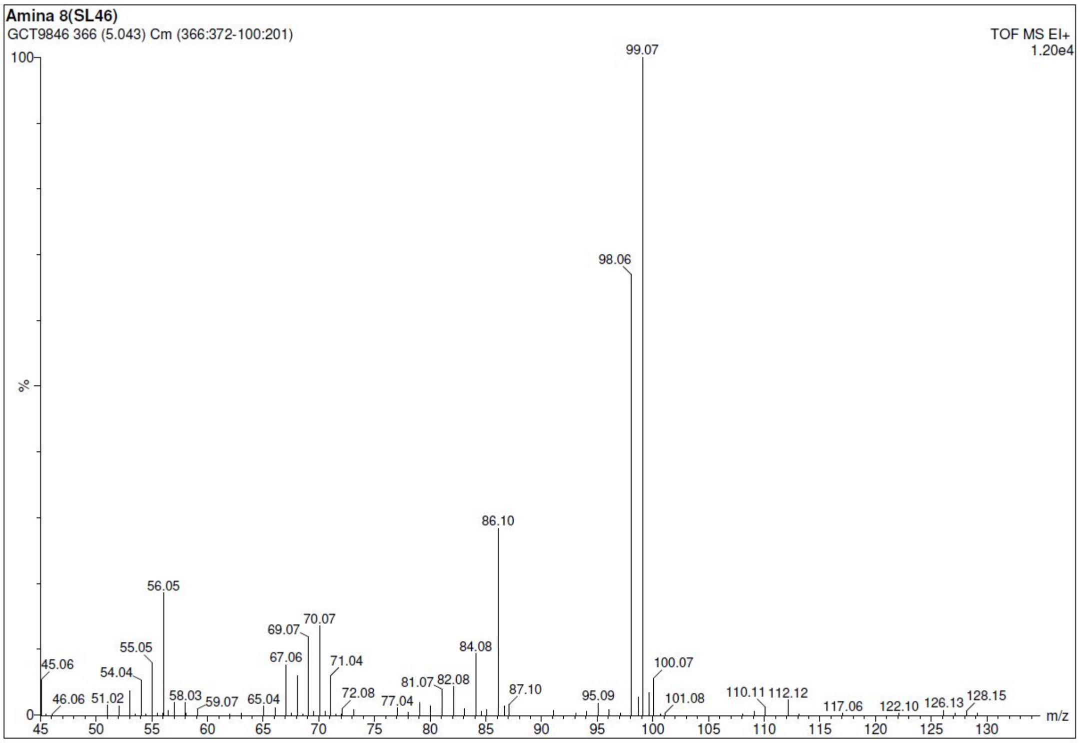
Compound 8 a-c: The previously obtained solid (5 g, 16. 7 mmol) was dissolved in a mixture of THF/Ethanol (120 ml/120 ml), the hydrazine monohydrate (3,2 g, 100. 2 mmol) was added and the reaction was heated at 83ºC during 2h. The solvent was removed in vacuo and the residue was poured onto NaOH 1M (30ml). The mixture was extracted with DCM. The organic layer was dried with sodium sulfate and the solvent was removed in vacuo afforded a yellow oil 83-87% yield.

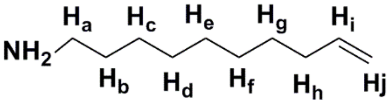


Compound 8a: ^{1}H NMR (300 MHz, CDCl$_3$) δ 5.76 (m, 1H$_g$), 5.17 (m, 2H$_h$), 2.71 (t, *J* = 6.9 Hz, 2H$_a$), 2.11 (m, 2H$_f$), 1.58 (m, 8H$_{b,\ c,\ d,\ e}$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 138.98, 114.21, 42.08, 33.71, 33.51, 28.93, 28.86, 26.71. MS m/z calculated for $C_8H_{17}N$ [M-H$^+$] 128.14 found MALDI TOF 128.15.


93t-amina8
Amina 8
1.30
2.00
1.70
2.14
8.62
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
f1 (ppm)

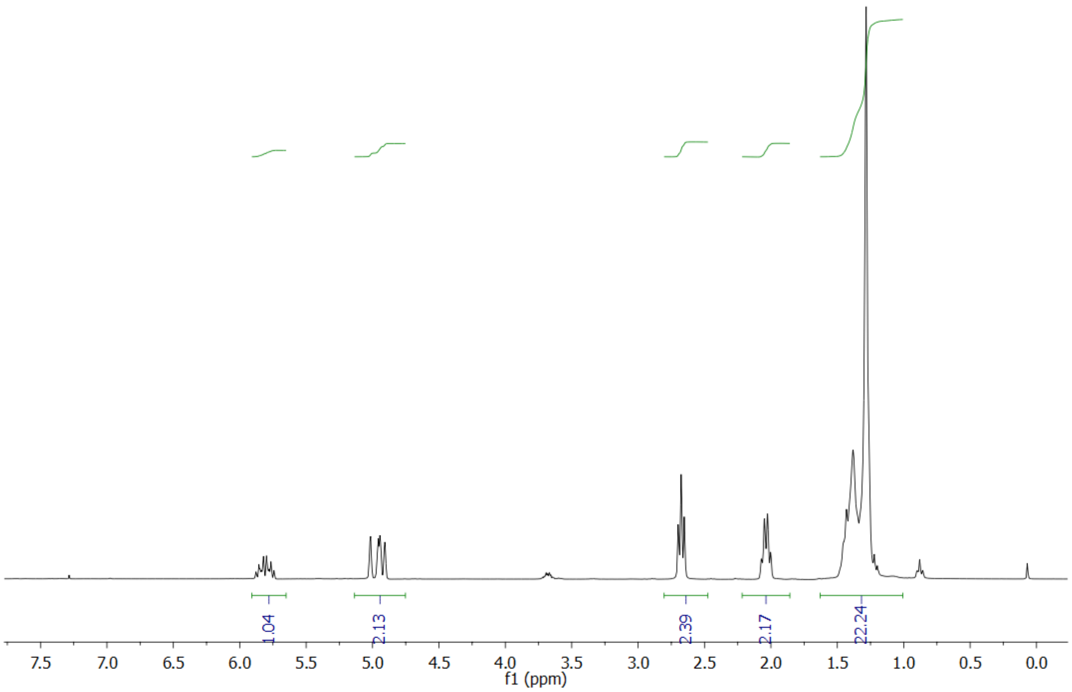

SLamina8
SLamina8
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



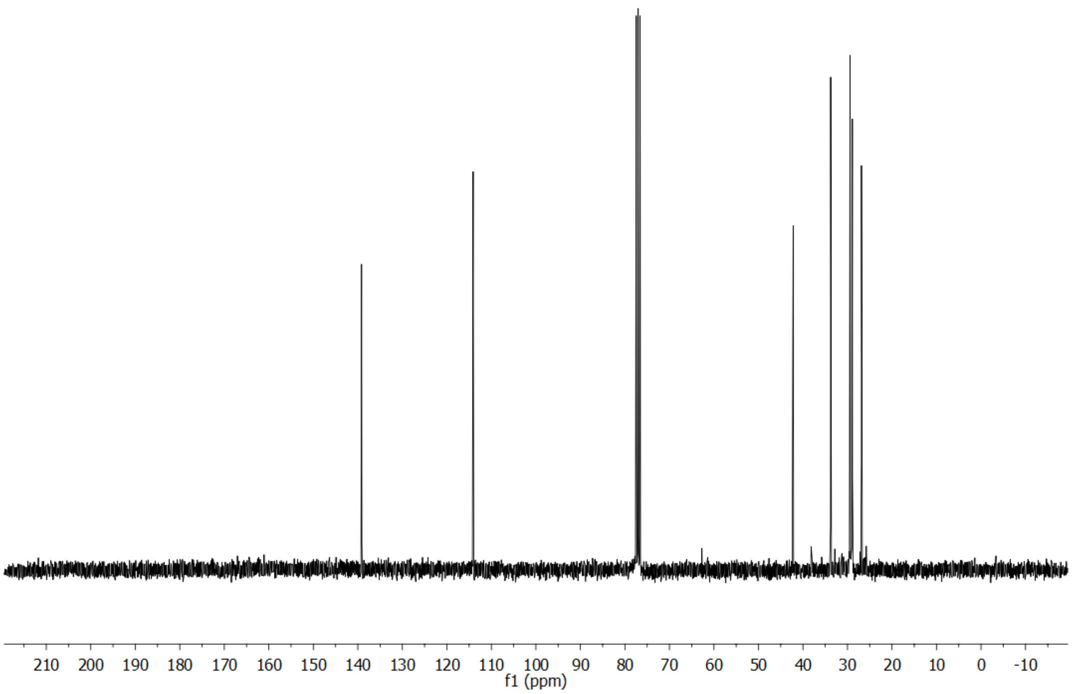


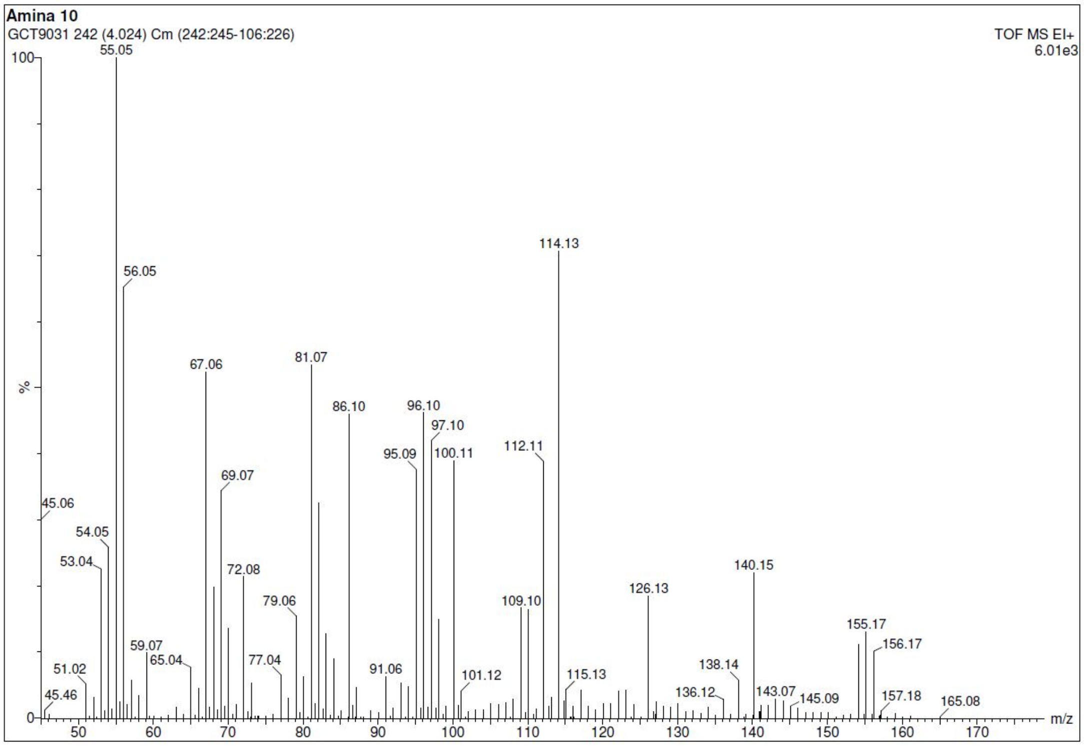
Compound 8b: ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.06 (m, 1H_i), 5.13 (m, 2H_j), 2.68 (t, *J*= 6.9 Hz, 2H_a), 2.04 (m, 2H_h), 1.58 (m, 12$H_{c,\ d,\ e,\ f,\ g}$).^{13}C NMR (75 MHz, $CDCl_3$) δ 139.17, 114.09, 42.19, 33.77, 33.75, 29.44, 29.43, 29.06, 28.90, 26.86. MS m/z calculated for $C_{10}H_{21}N$ [M-H$^+$] 156.17 found MALDI TOF 156.17.

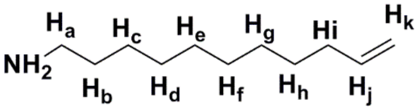
289t-amina10
AMINA 10



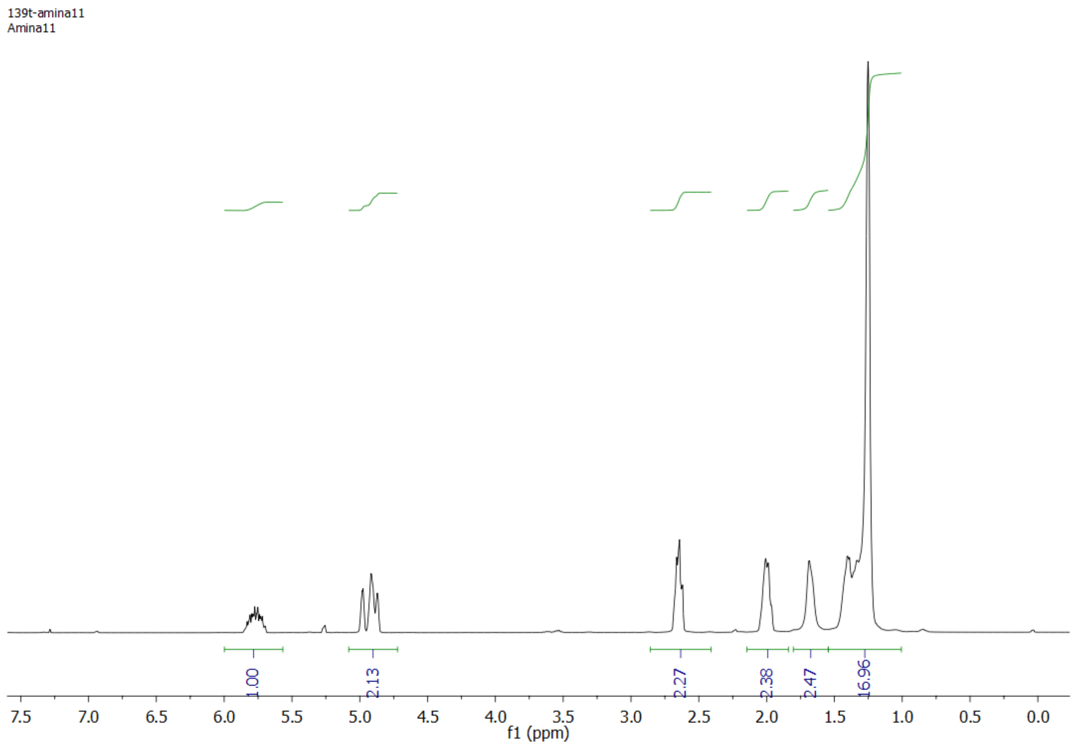
1618t-amina10
Amina 10

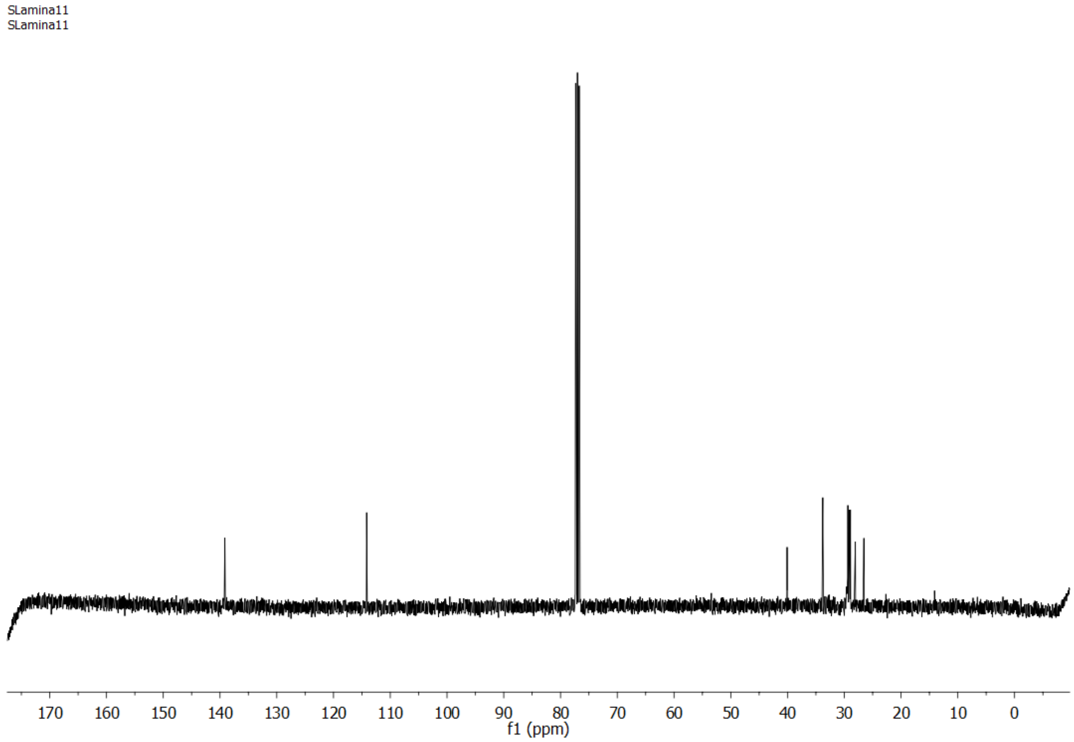


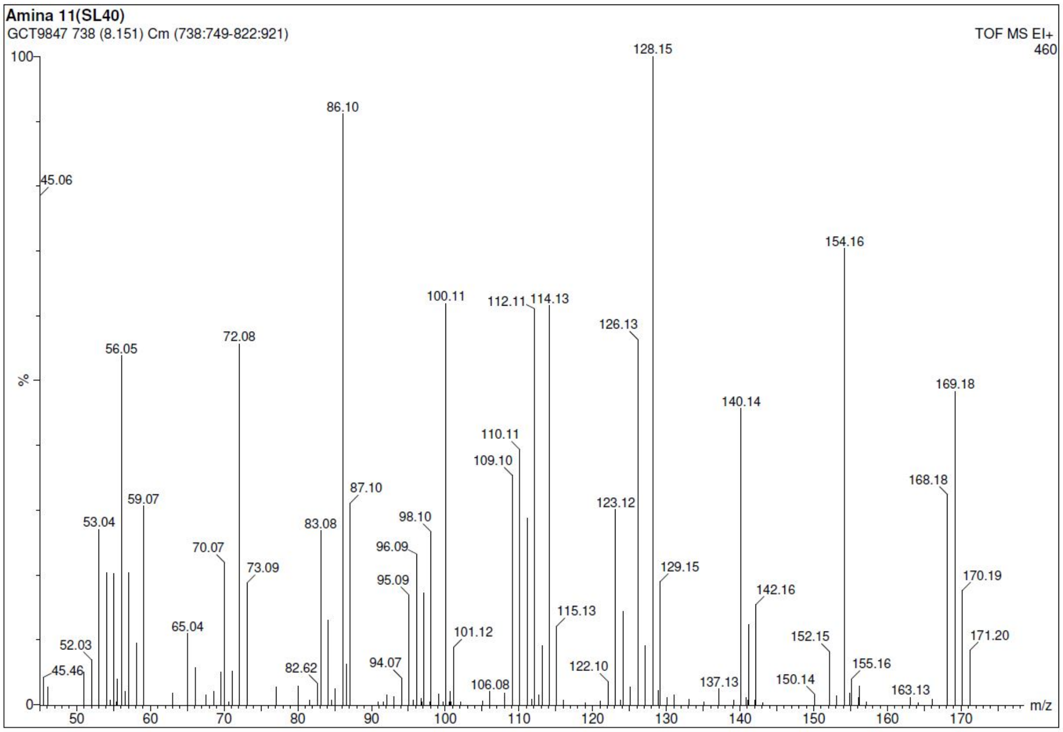




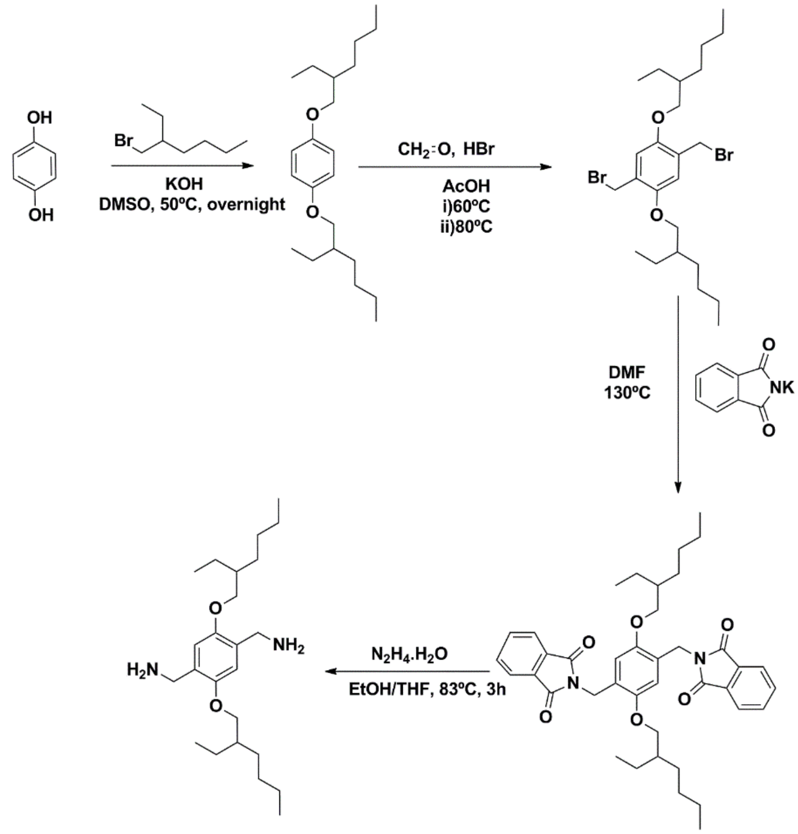
Compound 8c: ^{1}H NMR (300 MHz, CDCl$_3$) δ 5.91 (m, 1H$_j$), 5.06 (m, 2H$_k$), 2.64 (t, *J* = 6,9 Hz, 2H$_b$), 2.05 (m, 2H$_i$), 1.55 (m, 14H$_{c, d, e, f, g, h}$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 139.14, 114.16, 40.07, 33.78, 29.37, 29.35, 29.06, 29.01, 28.91, 28.05, 26.55. MS m/z calculated for $C_{11}H_{23}N$ [M-H$^+$] 169.18 found MALDI TOF 169.18.


139t-amina11
Amina11
1.00
2.13
2.27
2.38
2.47
16.96
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
f1 (ppm)

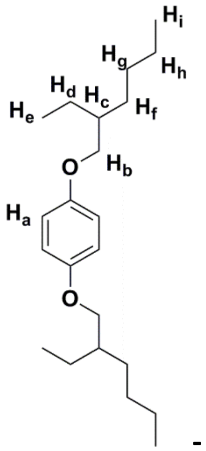

SLamina11
SLamina11
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



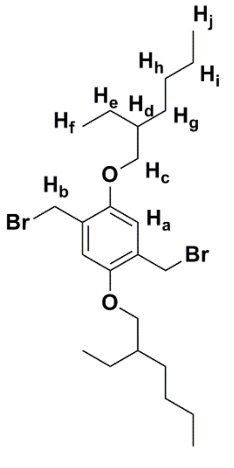
General procedure synthesis aromatic spacer



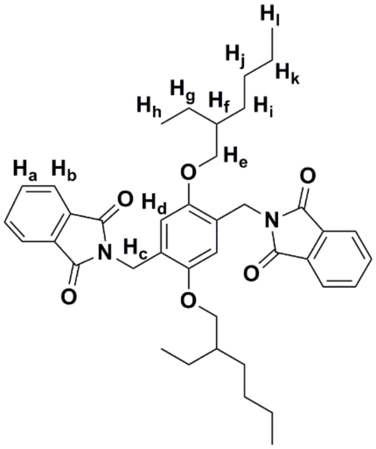
The compound 1, 4- Bis (2-ethyl-hexyloxy)-benzene and the 1, 4-Dibromo-2, 5-bis-(2-ethyl-hexyloxy)-benzene (II) were synthetized as described in Macromolecules **2012**, 45, 5051-5057.



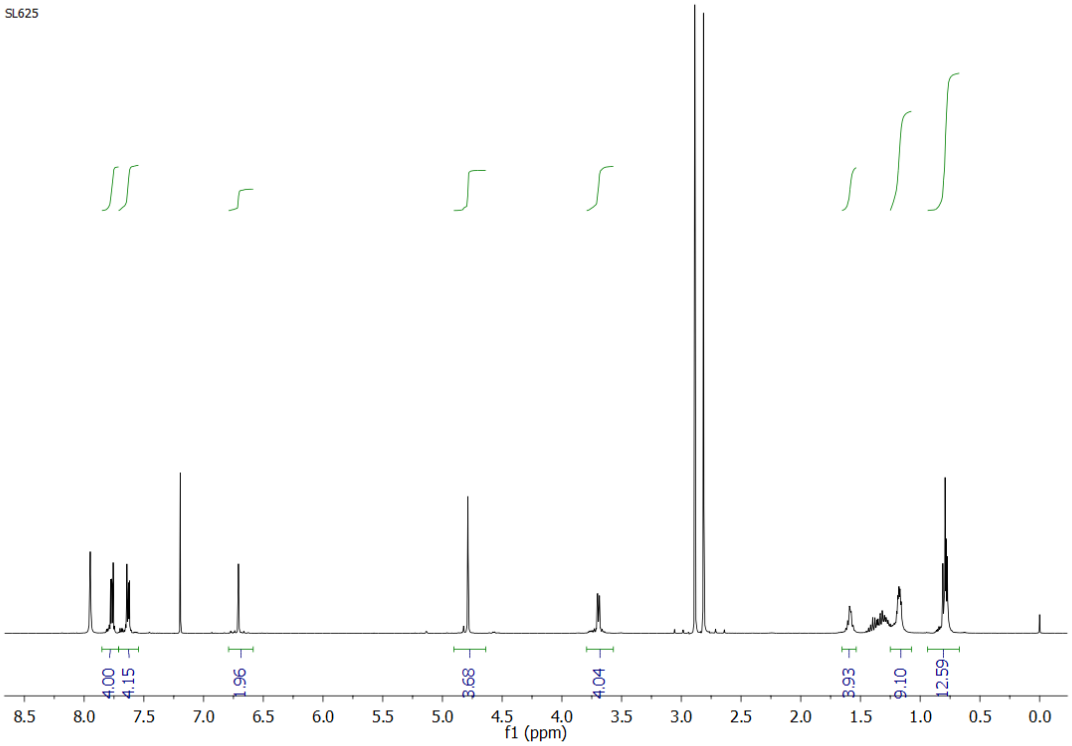
Compound 9. ^{1}H NMR (300 MHz, CDCl3) δ 6.82 (s, $4H_a$), 3.78 (dd, *J* = 5.8, 1.2 Hz, $4H_b$), 1.69 (sep, *J* = 6.1 Hz, $2H_c$), 1.28-1.54 (m, $16H_{d,\ e,\ f,\ g}$) 0.92 (m, $4H_h$). ^{13}C NMR (75 MHz, CDCl3) δ 153.43, 115.35, 71.20, 39.47, 30.53, 29.09, 23.86, 23.06, 14.08, 11.09. HR-MS m/z calculated for $C_{22}H_{38}O_2$ 334.2812 found HR-MS 334.2873.

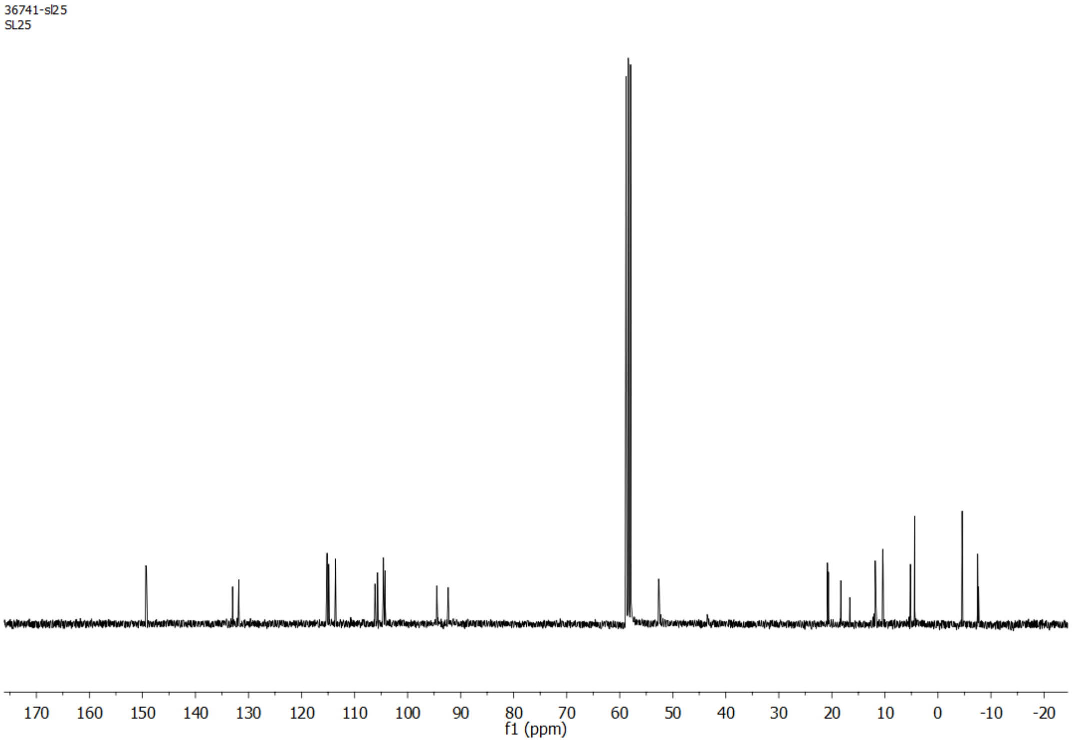


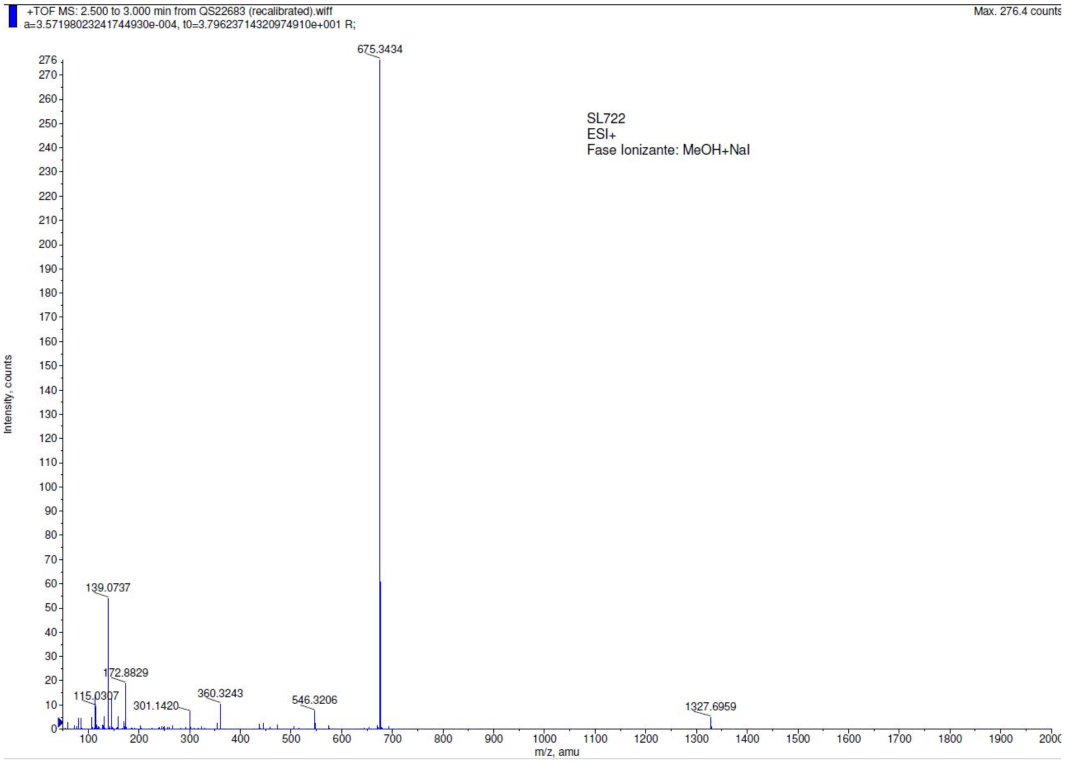
Compound 10. ^{1}H NMR (300 MHz, CDCl3, ppm) δ 6.85 (s, 2H$_a$), 4.52 (s, 4H$_b$), 3.87 (d, *J* = 5.4 Hz, 4H$_c$), 1.75 (sep, J = 6.2 Hz, 2H$_d$), 1.61 – 1.29 (m, 16H $_{e, g, h, i}$), 0.97 – 0.89 (m, 12H$_{f, j}$). ^{13}C NMR (75 MHz, CDCl3) δ 150.69, 127.36, 114.21, 70.91, 39.59, 30.62, 29.10, 28.73, 24.01, 23.04, 14.08, 11.23.MS m/z calculated for $C_{24}H_{40}Br_2O_2$ 518.139 found MALDI TOF 518.139.

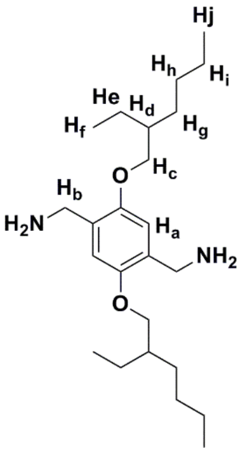


Compound 11 : the previously product (5g, 9.6 mmol) and the potassium phthalamide (7g, 38.4mmol) were charged in a flask N,N-dimethylformamide (80 ml) was added and the reaction was heated at 100ºC during 2h. The solution was then allowed to come back to room temperature and filtered over celite and the filtrate concentrate in vacuo to give a pale white solid (80%). ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.82 – 7.68 (m, 8H$_{a,b}$), 6.77 (s, 2H$_d$), 4.85 (s, 4H$_c$), 3,77 (m, 4H$_e$), 1.75 (sep, J = 6.2 Hz, 2H$_f$), 1.61 (m, 16H$_{g,i,j,k}$), 0.97 (m, 12H$_{h,l}$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 168.09, 151.79 , 150.59, 133.97, 133.66, 124.95, 124.46, 123.35, 123.02, 113.29, 111.12, 71.41, 39.52, 37.17, 35.40, 30.54, 29.16, 23.94, 23.17, 14.22, 11.22. MS m/z calculated for $C_{40}H_{48}N_2O_6$ [M + Na+] 675.3410 found HR-MS 675.3434.


SL625
4.00
4.15
1.96
3.68
4.04
3.93
9.10
12.59
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
f1 (ppm)

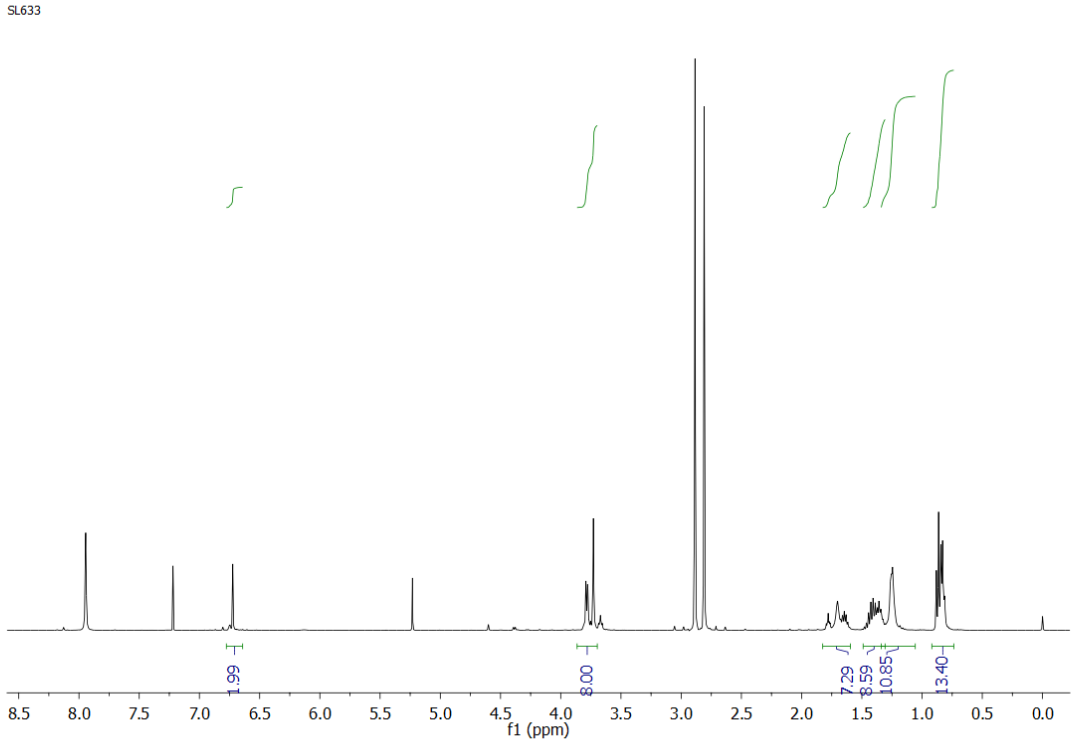

36741-sl25
SL25
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

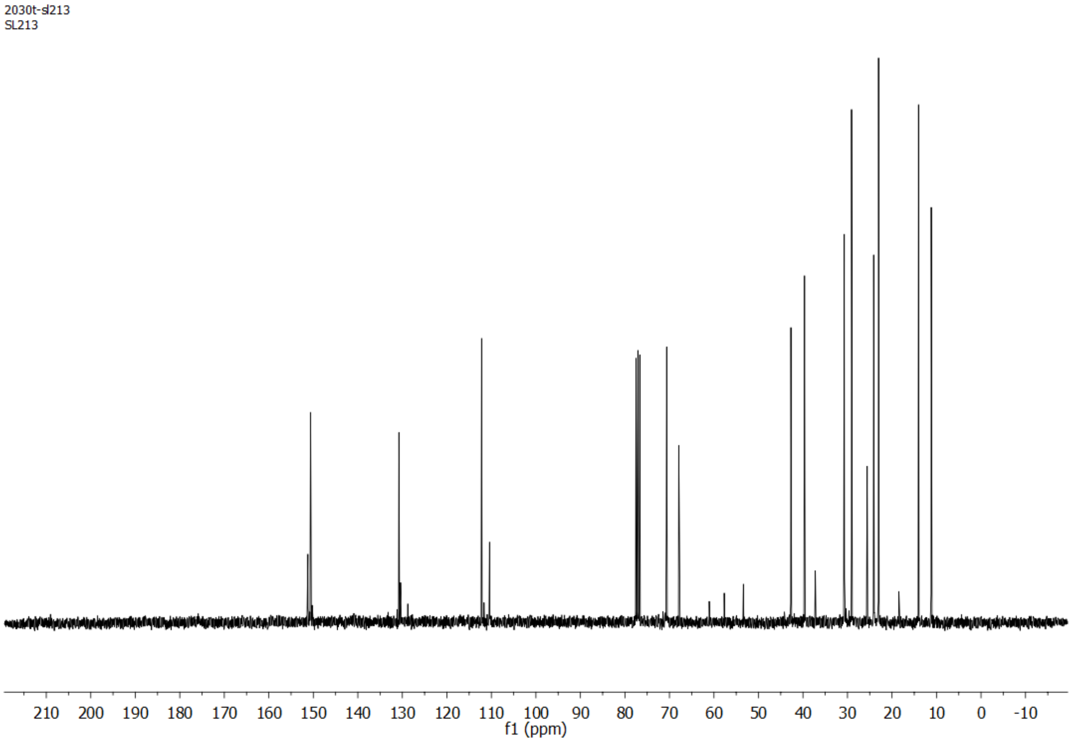




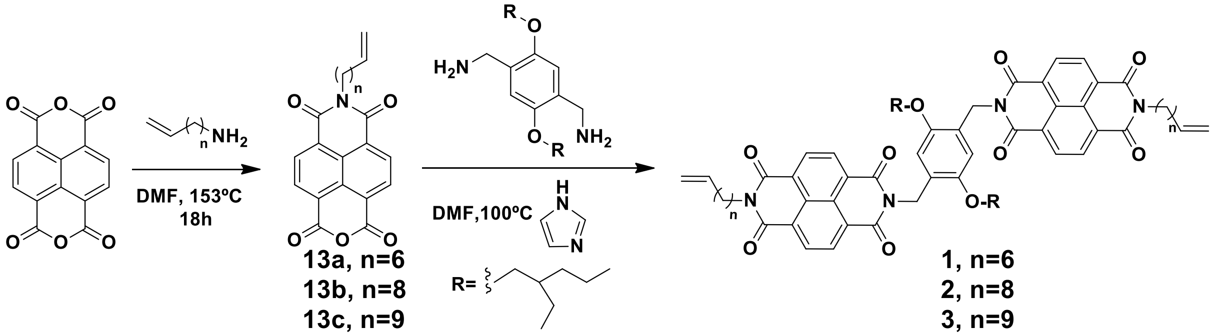
Compound 12: The previously obtained solid (4g, 6.1mmol) was dissolved in a mixture of THF/Ethanol (15ml/15ml), the hydrazine monohydrate (2,5g, 79. 3 mmol) was added and the reaction was heated at 83ºC during 2h. The solvent was removed in vacuo and the residue was poured onto NaOH 1M (30ml). The mixture was extracted with DCM. The organic layer was dried with sodium sulfate and the solvent was removed in vacuo afforded 3,4 mg of a brown oil (92%)..

^{1}H NMR (300 MHz, CDCl$_3$) δ 6.68 (s, 2H$_1$), 3.87 (m, 4H$_c$), 3.74 (s, 4H$_b$), 1.75 (sep, J = 6.2 Hz, 2H$_d$), 1.61 – 1.29 (m, 16H$_{e,g,h,i,}$), 0.97 – 0.89 (m, 12H$_{f,j}$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 151.25, 150.14, 130.77, 12.20, 110.41, 70.66, 67.91, 42.71, 39.61, 30.72, 29.09, 25.58 , 24.12, 23.02 , 14.04, 11.17. MS m/z calculated for $C_{24}H_{44}N_2O_2$ 392.34 found MALDI TOF 392.4.



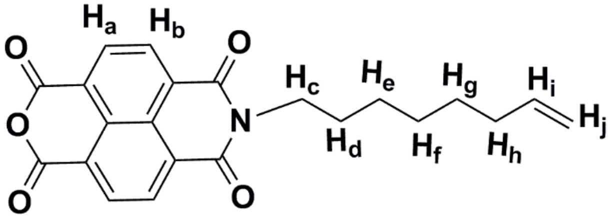


General procedure Synthesis linear receptor

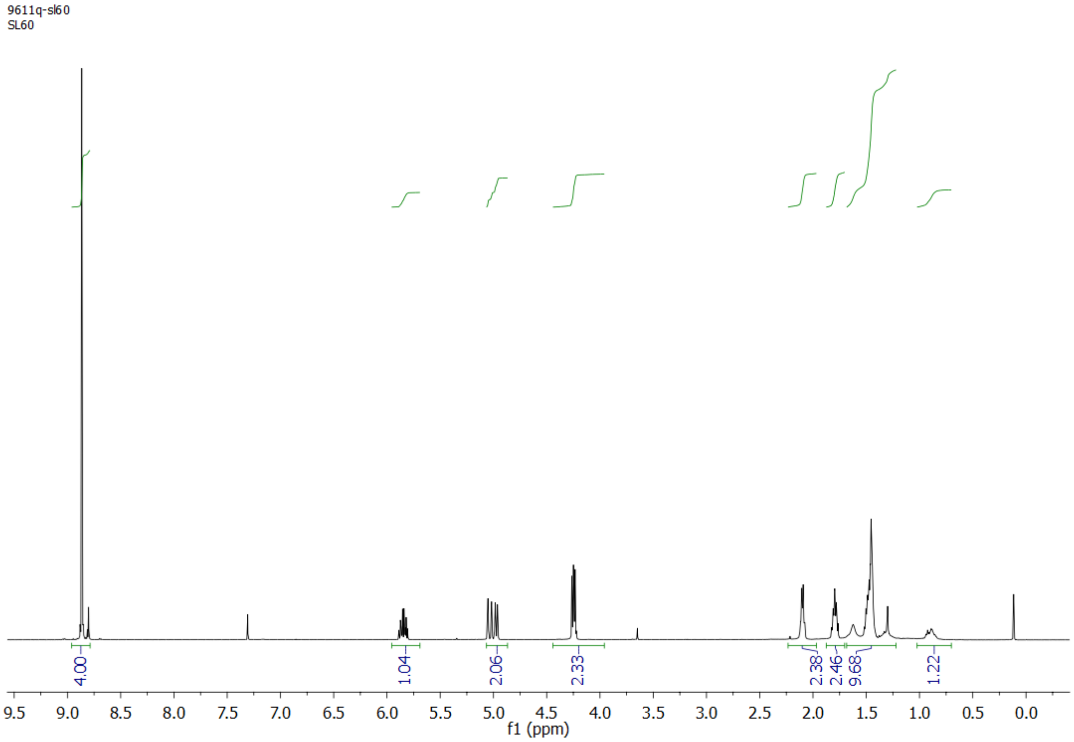


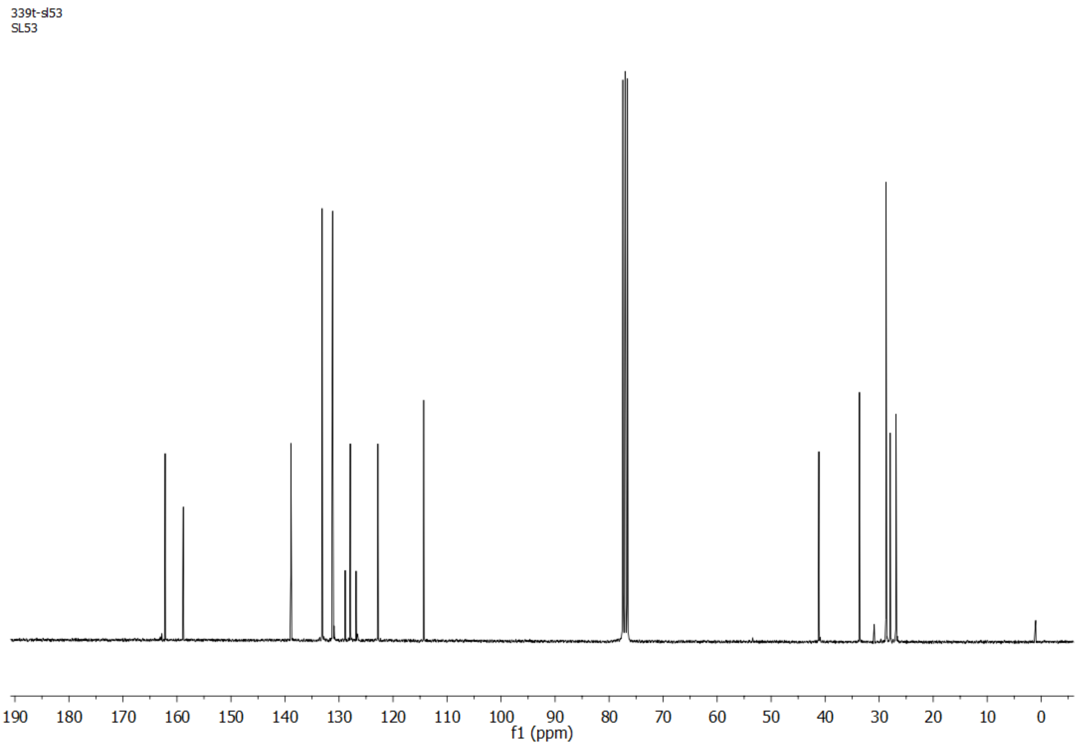
The compounds **13 a-c** were synthetized as described in J. Phys. Chem. **2001**, 105, 7216-7219.

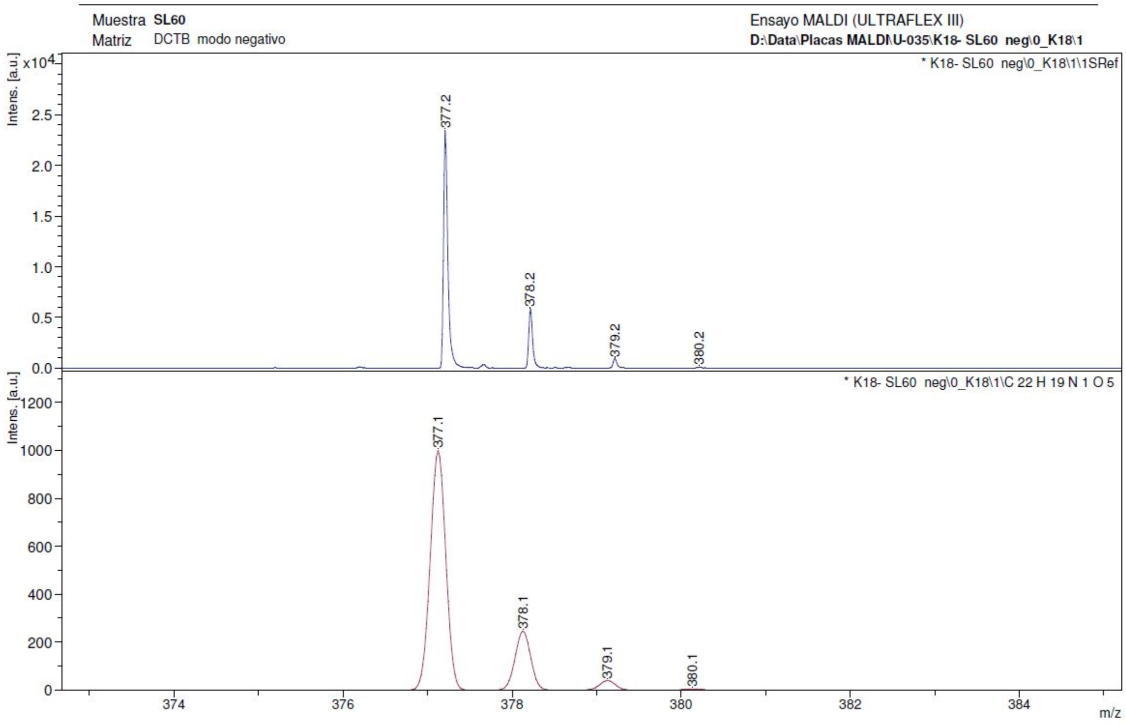
Compound 13 a-c:

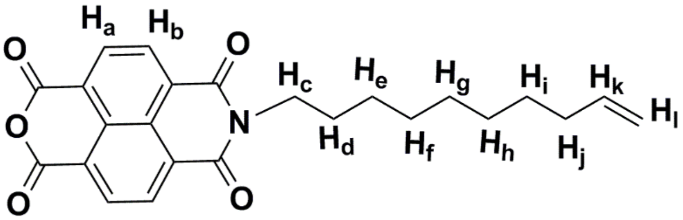


Compound 13a: 1H NMR (300MHz, CDCl3) 1H NMR δ 8.83 (s, 4H, $H_{a,\ b}$), 5.65 (m,1H,H_j), 4.97 (m, 2H,H_i), 4.17 (m, 2H,H_c), 2.08 (m, 2H,H_h), 1.76 (m, 2H,H_d),1,33 (m,6H,$H_{e,\ f,\ g}$)**,** ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.04 (C=O), 158.51 (C=O), 139.11, 133.13, 130.80, 128.77 , 127.91, 126.84 , 122.81, 114.01, 41.15, 33.64, 28.50, 27.95, 26.88. MS m/z calculated for $C_{22}H_{19}NO_5$ 377.1 found MALDI TOF 377.2.

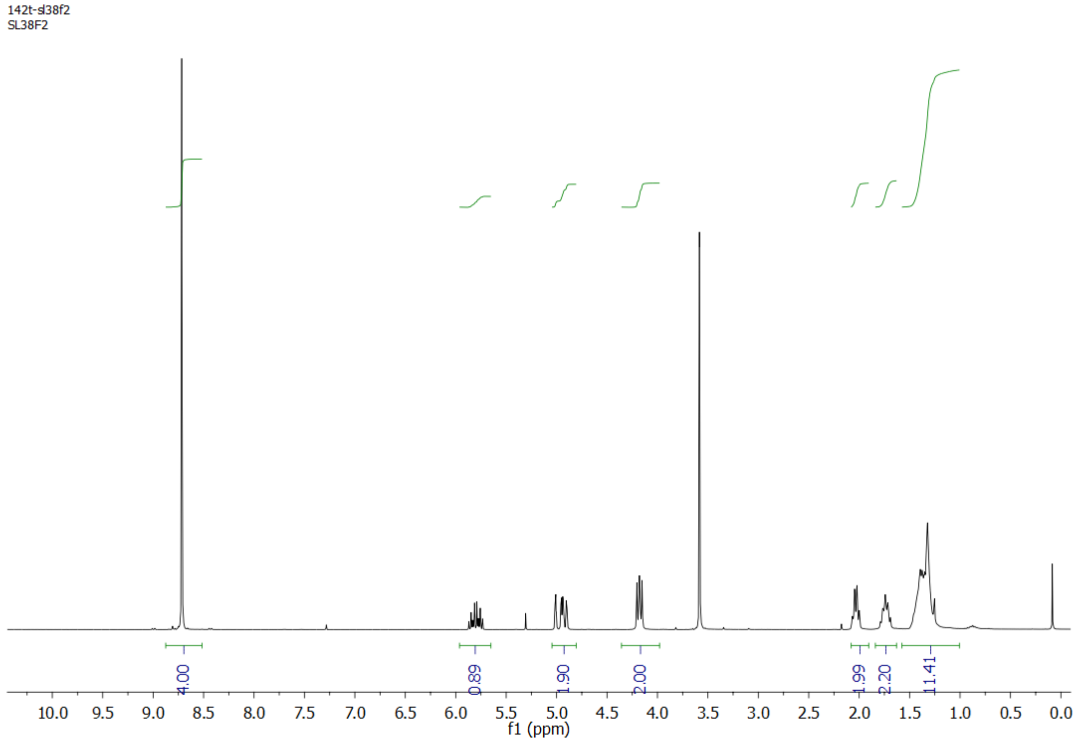


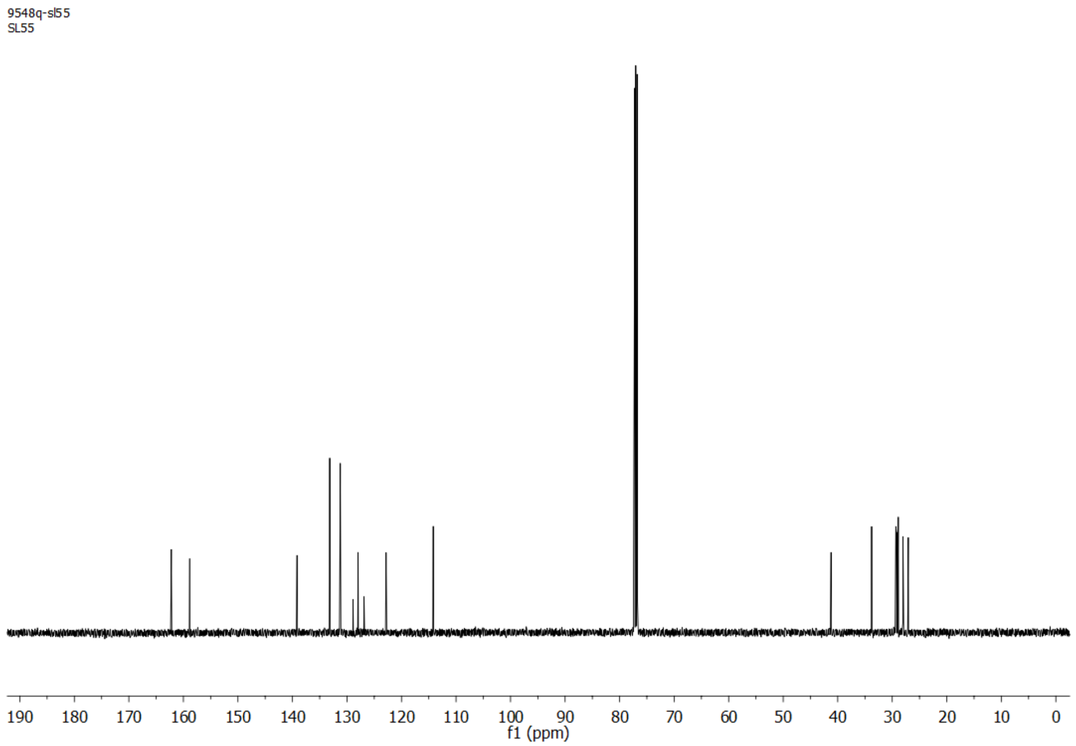

339t-sl53
SL53
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

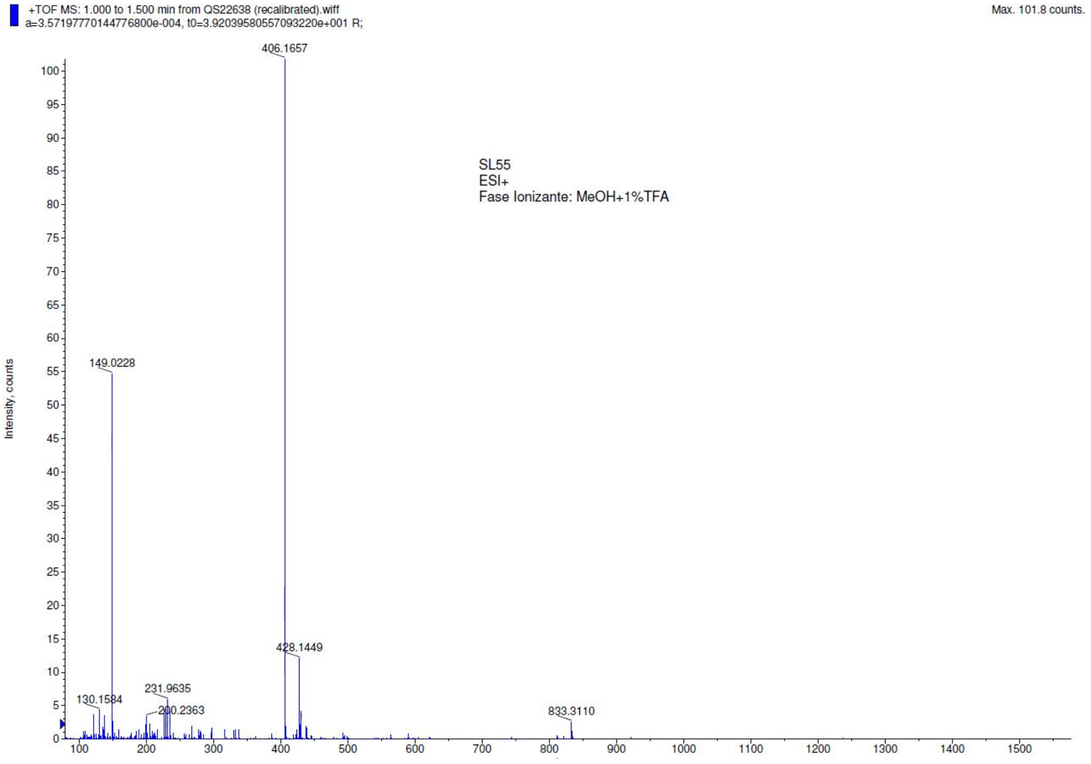

Muestra SL60
Matriz DCTB modo negativo
Ensayo MALDI (ULTRAFLEX III)
D:\Data\Placas MALDI\U-035\K18- SL60 neg\0_K18\1
* K18- SL60 neg\0_K18\1\1SRef
Intens. [a.u.]
x10^4
2.5
2.0
1.5
1.0
0.5
0.0
377.2
378.2
379.2
380.2
* K18- SL60 neg\0_K18\1\C 22 H 19 N 1 O 5
Intens. [a.u.]
1200
1000
800
600
400
200
0
377.1
378.1
379.1
380.1
374
376
378
380
382
384
m/z

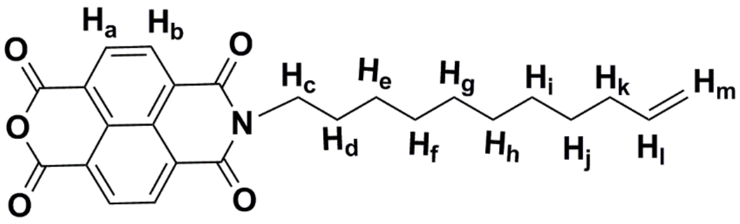


Compound 13b: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.84 (s, 4H$_{a,b}$), 5.83 (m, 1H$_k$), 4.83 (m, 2H$_l$), 4.22 (m, 2H$_c$), 2.06 (m, 2H$_j$), 1.77 (m, 2H$_d$), 1.36 (m, 10H$_{e,f,g,h,i}$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 162.18 (C=O), 158.82 (C=O), 139.13, 133.13, 131.18, 128.86, 127.93, 126.84, 122.80, 114.15, 53.42, 41.19, 33.75, 28.00, 27.02. HR-MS m/z calculated for $C_{24}H_{23}NO_5$ 405.1576 found HR-MS 406.1657.

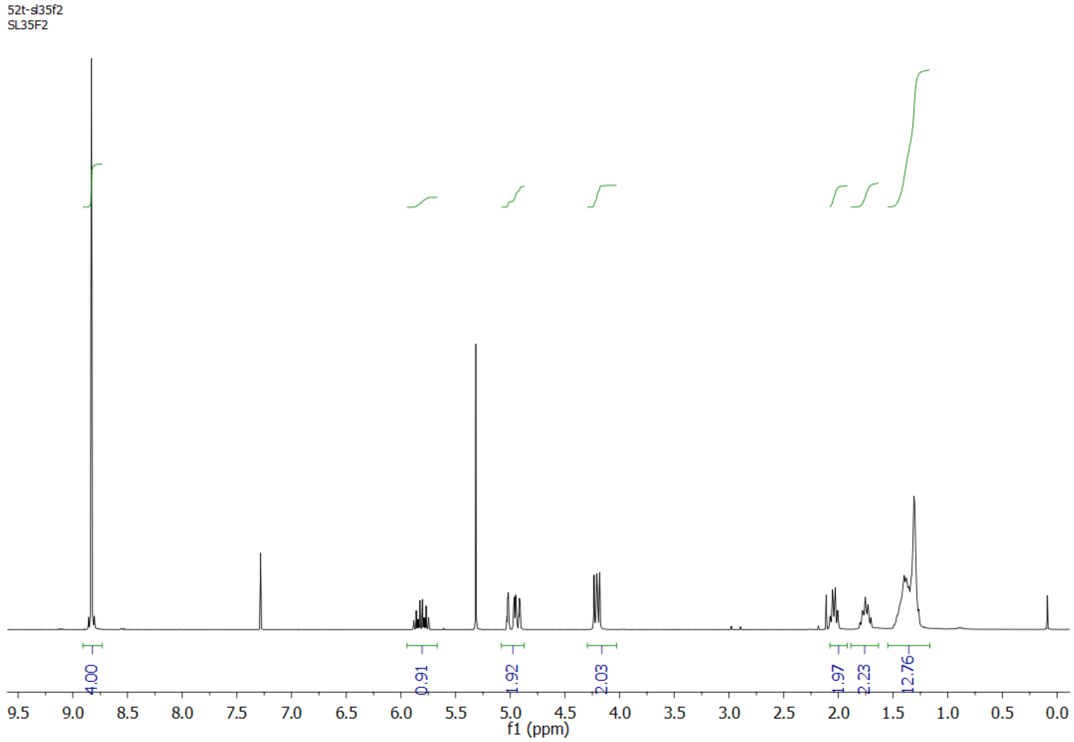


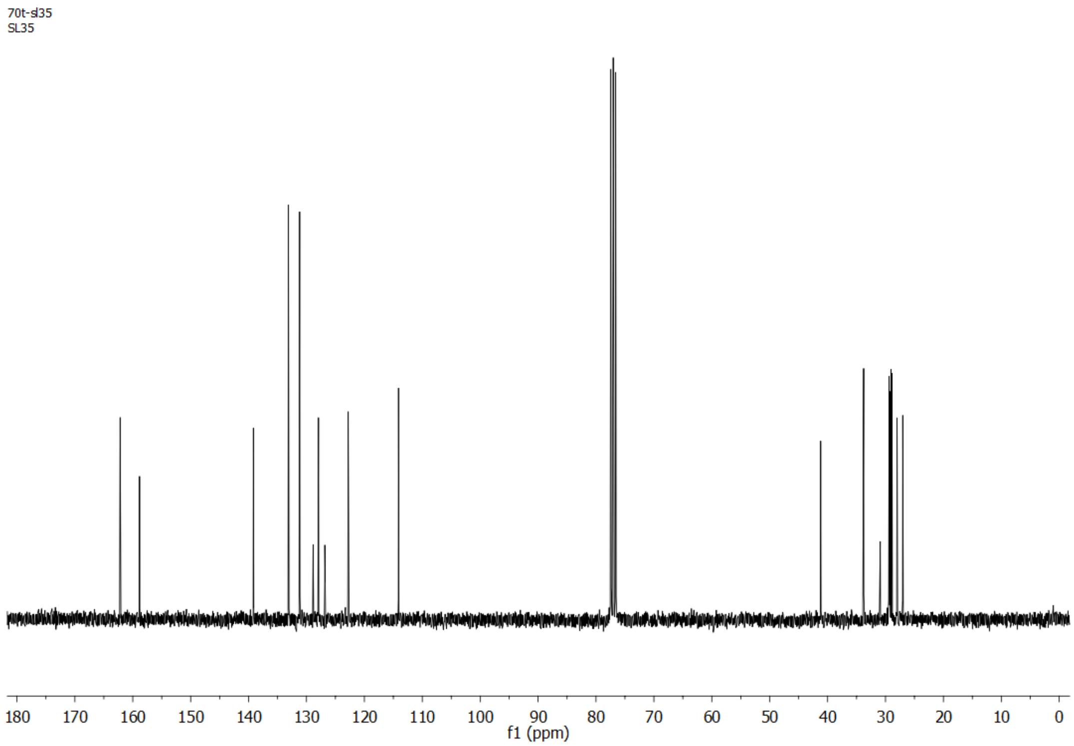

9548q-sl55
SL55
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

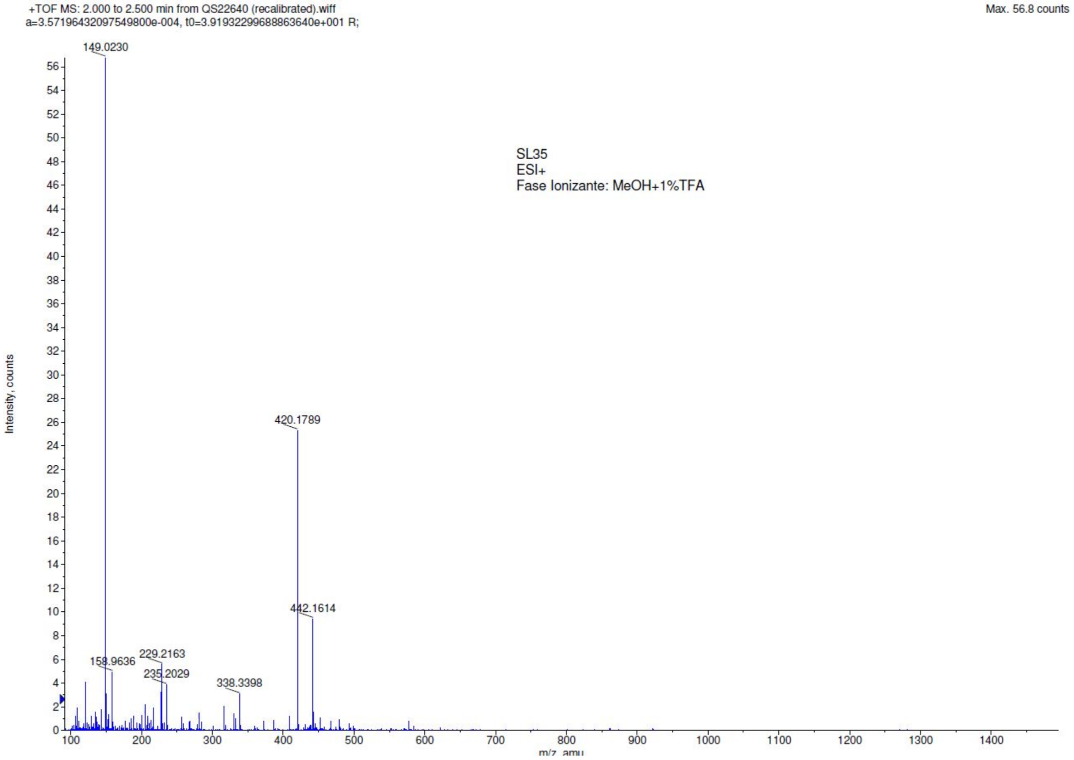

+TOF MS: 1.000 to 1.500 min from QS22638 (recalibrated).wiff
a=3.57197770144776800e-004, t0=3.92039580557093220e+001 R;
Max. 101.8 counts.
SL55
ESI+
Fase Ionizante: MeOH+1%TFA
406.1657
149.0228
428.1449
231.9635
200.2363
130.1584
833.3110
Intensity, counts
0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100
100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500



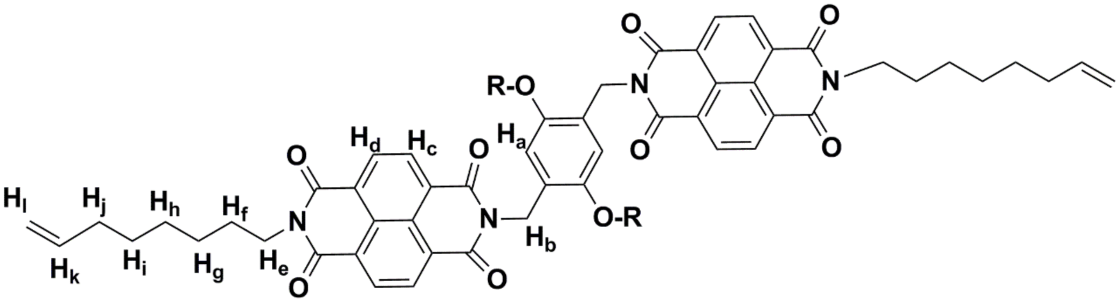
Compound 13c: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.98 (s, 8H$_{a,b}$), 5.81 (m, 1H$_l$),4.84 (m, 2H$_m$), 4.21 (m, 2H$_c$), 2.09 (m, 2H$_k$), 1.75 (m, 2H$_d$), 1.53 (m, 12H $_{e,\ f,\ g,\ h,\ i,\ j}$),^{13}C NMR (75 MHz, CDCl$_3$) δ 162.35 (C=O), 158.83 (C=O), 139.09, 133.12, 131.18, 128.79, 127.92, 126.83, 122.80, 114.01, 41.19, 33.77, 30.90, 29.39, 29.24, 29.06 (s), 28.88 (s), 28.00, 27.02. HR-MS m/z calculated for $C_{25}H_{25}NO_5$ 419.1733 found HR-MS 420.1789.



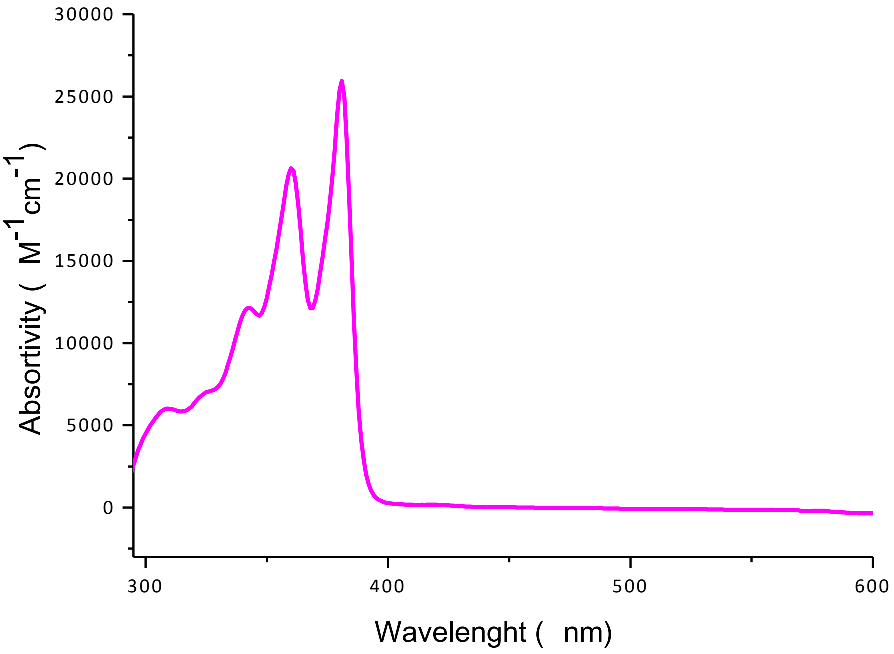

70t-sl35
SL35
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

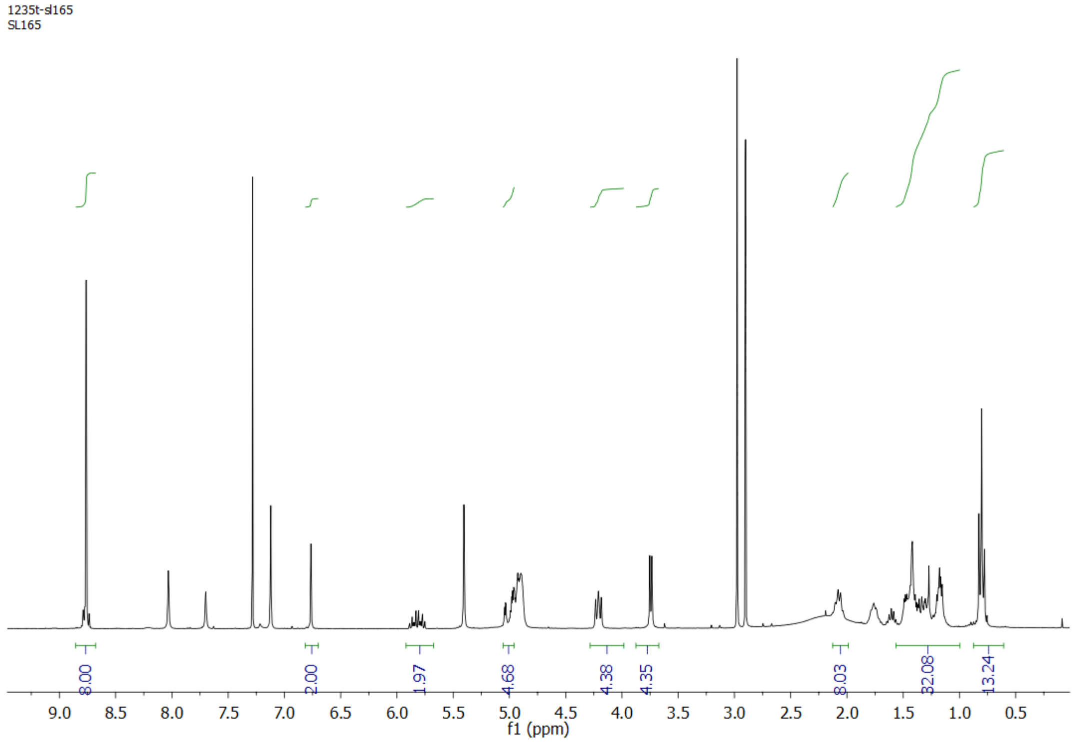

+TOF MS: 2.000 to 2.500 min from QS22640 (recalibrated).wiff
a=3.57196432097549800e-004, t0=3.91932299688863640e+001 R;
Max. 56.8 counts
SL35
ESI+
Fase Ionizante: MeOH+1%TFA
149.0230
420.1789
442.1614
158.9636
229.2163
235.2029
338.3398
Intensity, counts
m/z, amu

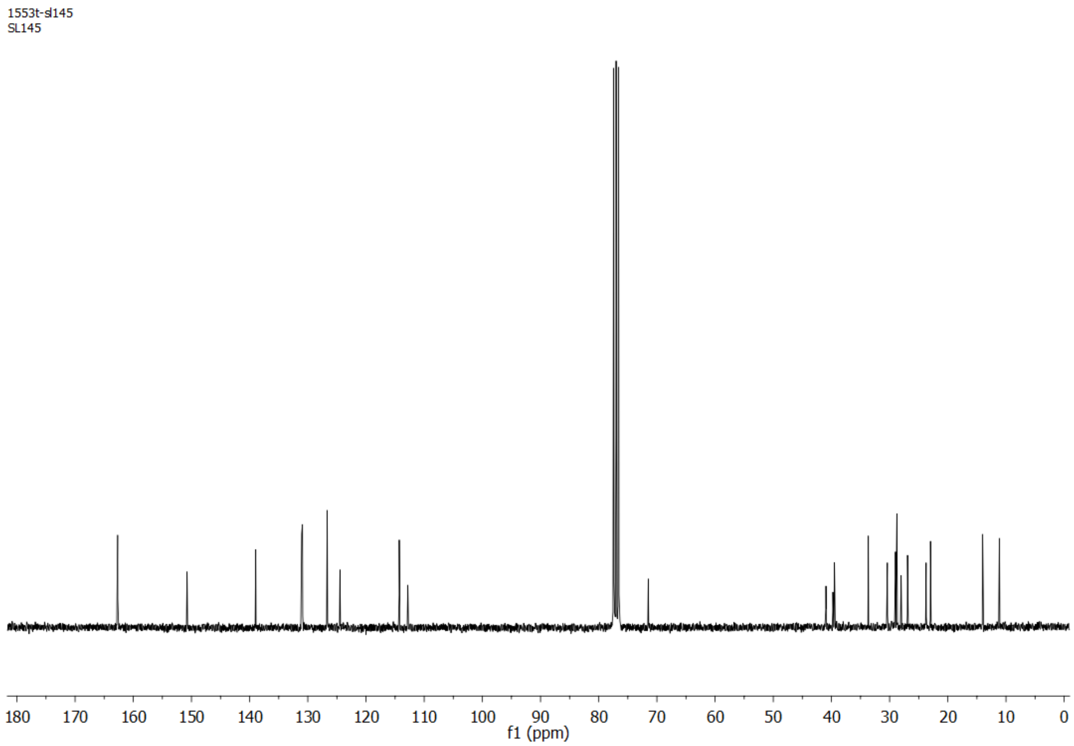
Compound 1-3: The previously obtained solid (200 mg, 0.47 mmol) was dissolved N, N-dimethylformamide (8ml), the imidazole (630 mg, 9.4 mmol) and the compound **12** (92mg, 0.23mmol) were added and the mixture was stirred at 130^0C during 5 h. The reaction was cooled to room temperature and it was poured onto HCl 1M. The solid was filtered and the crude was purified by Flash chromatography on silica (eluent: DCM) afforded a pink solid (76-80 %).

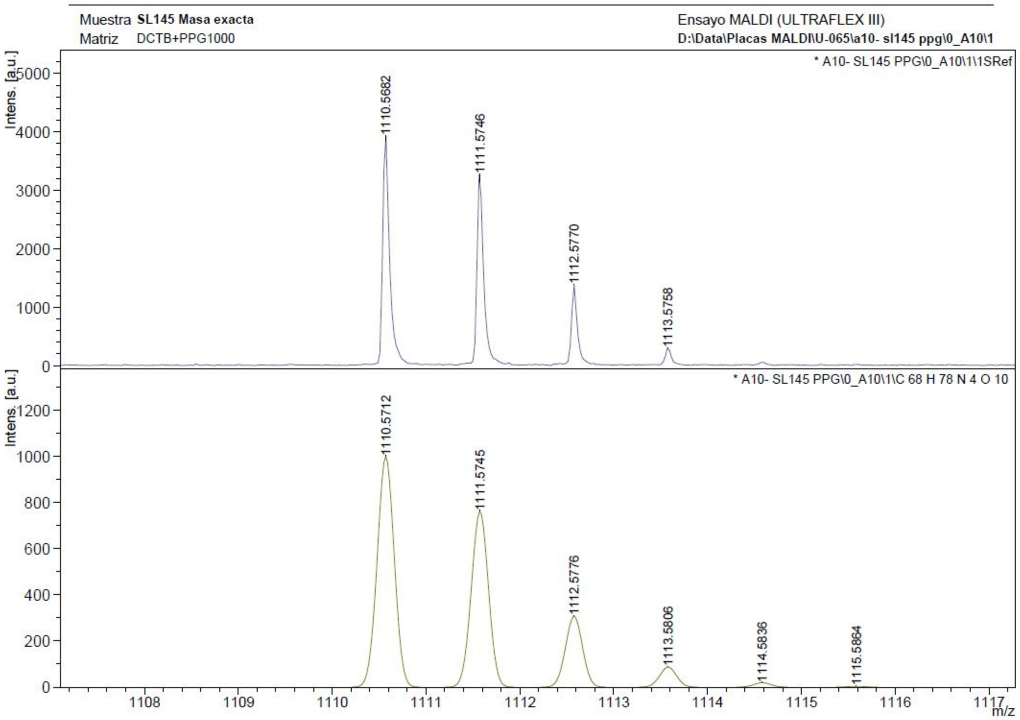


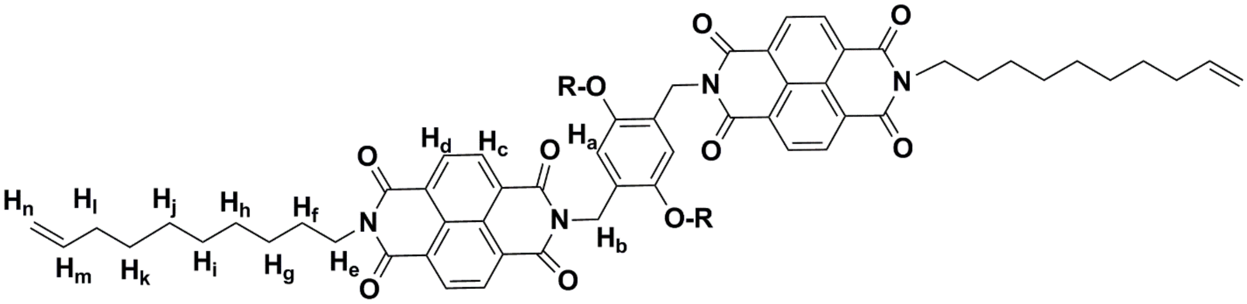
Compound 1: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.54 (m, 8H, H$_{c,d}$), 6.77 (s, 2H,H$_a$), 5.82 (m,2H,H$_k$),5,40 (s, 4H,H$_b$) 4.97 (m, 4H,H$_l$), 4.42 (t, J = 5.6 Hz, 4H,H$_e$), 3.73 (m, 4H, H$_R$), 2.04 (m, 2H,H$_j$), 1.71 (m, 2H,H$_f$), 1.58 (m,16H,H$_R$),1.26 (m, 24H,H$_{g,h,i}$), 0.81 (12H,H$_R$) ^{13}C NMR (75 MHz, CDCl$_3$) δ 162.80 (C=O), 162.68 (C=O), 150.76, 138.95, 131.04, 130.92, 126.71, 126.66, 124.47, 114.28, 112.81, 77.43, 77.21, 77.01, 76.59, 71.48, 40.94, 39.75, 39.48, 33.66, 30.39, 28.99, 28.75, 28.02, 26.92, 23.73, 22.98, 14.02, 11.13. HR-MS m/z calculated for C$_{68}$H$_{23}$N$_4$O$_{10}$ 1110.5718 found HR-MS 1110.5882. ε (λ$_{max}$=380) = 25555 M^{-1}cm^{-1}.


30000
25000
20000
15000
10000
5000
0
Absortivity ($M^{-1}cm^{-1}$)
300
400
500
600
Wavelenght (nm)

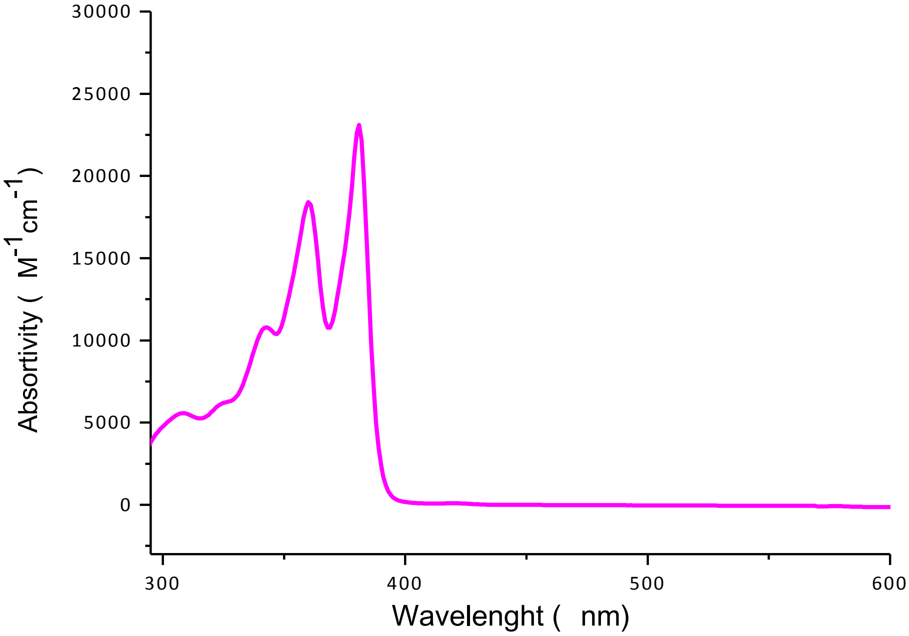

1235t-sl165
SL165
8.00
2.00
1.97
4.68
4.38
4.35
8.03
32.08
13.24
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

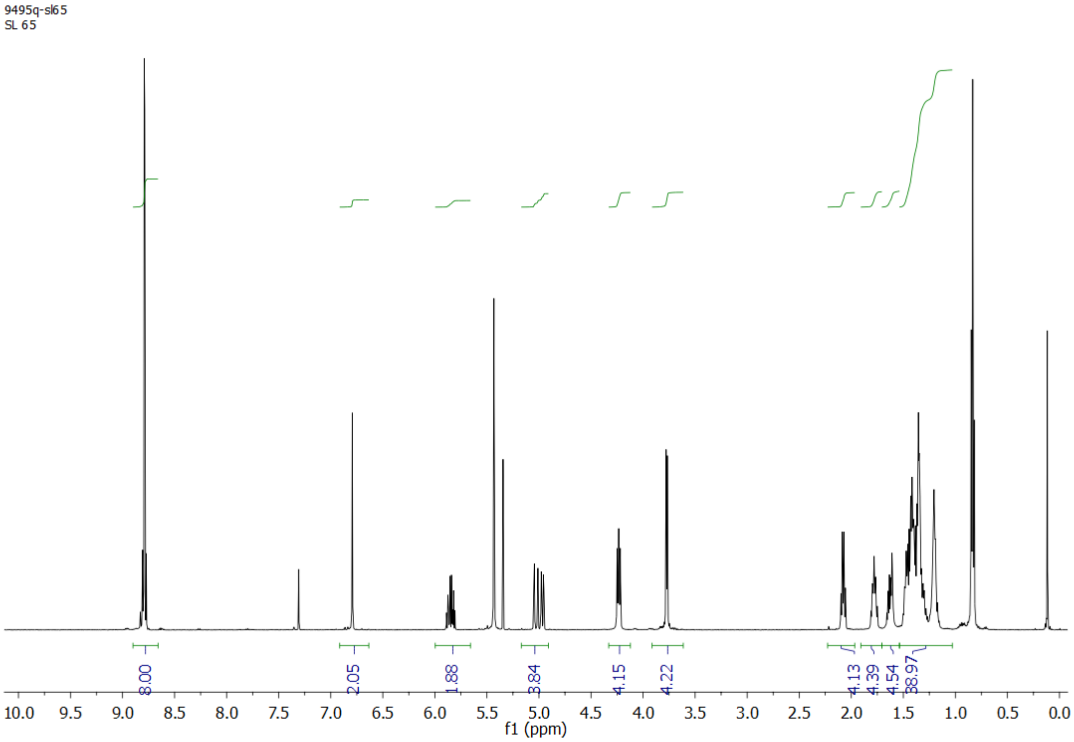

1553t-sl145
SL145
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

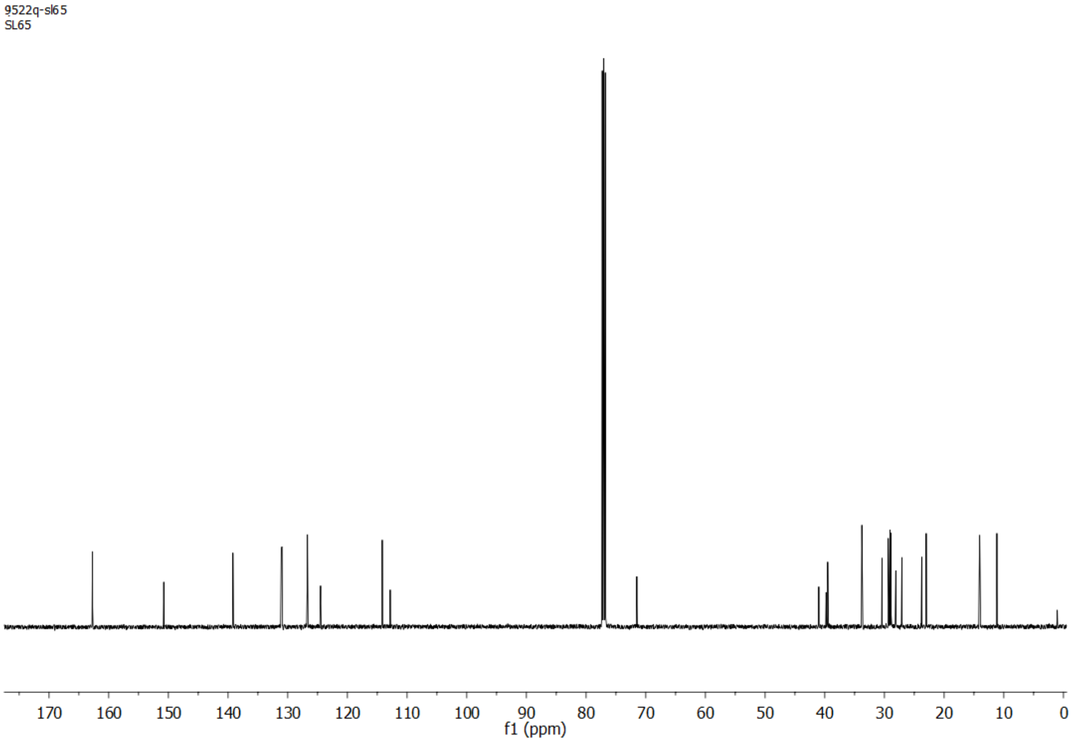

Muestra SL145 Masa exacta
Matriz DCTB+PPG1000
Ensayo MALDI (ULTRAFLEX III)
D:\Data\Placas MALDI\U-065\a10- sl145 ppg\0_A10\1
* A10- SL145 PPG\0_A10\1\1SRef
Intens. [a.u.]
5000
4000
3000
2000
1000
0
1110.5682
1111.5746
1112.5770
1113.5758
* A10- SL145 PPG\0_A10\1\C 68 H 78 N 4 O 10
Intens. [a.u.]
1200
1000
800
600
400
200
0
1110.5712
1111.5745
1112.5776
1113.5806
1114.5836
1115.5864
1108 1109 1110 1111 1112 1113 1114 1115 1116 1117
m/z

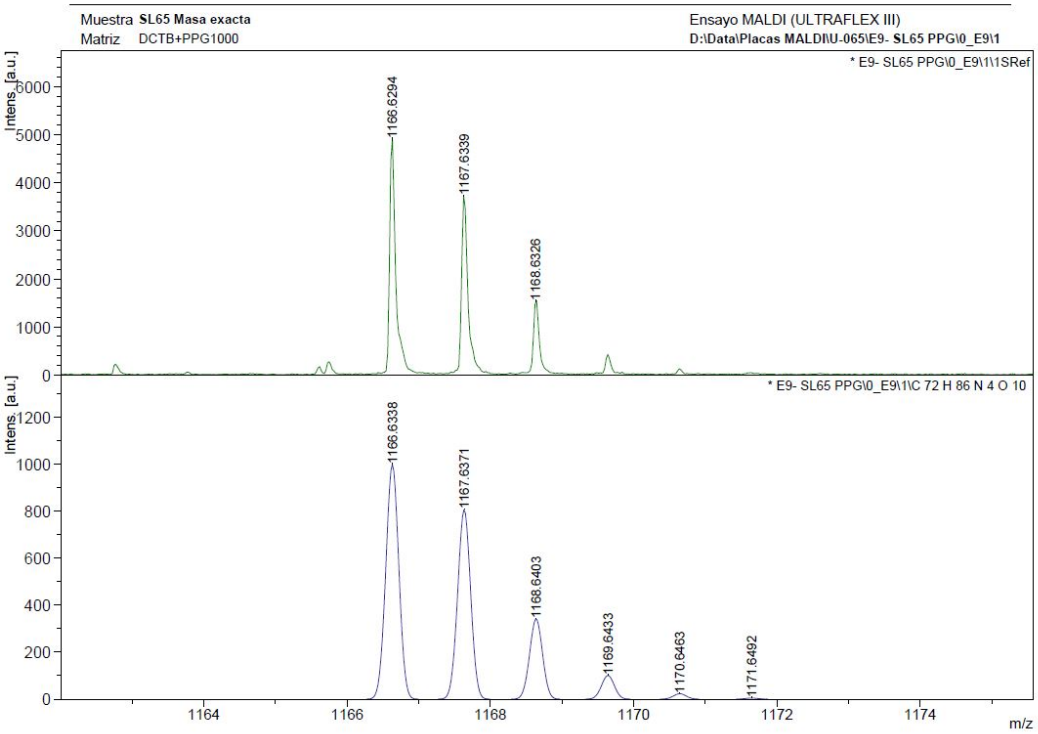


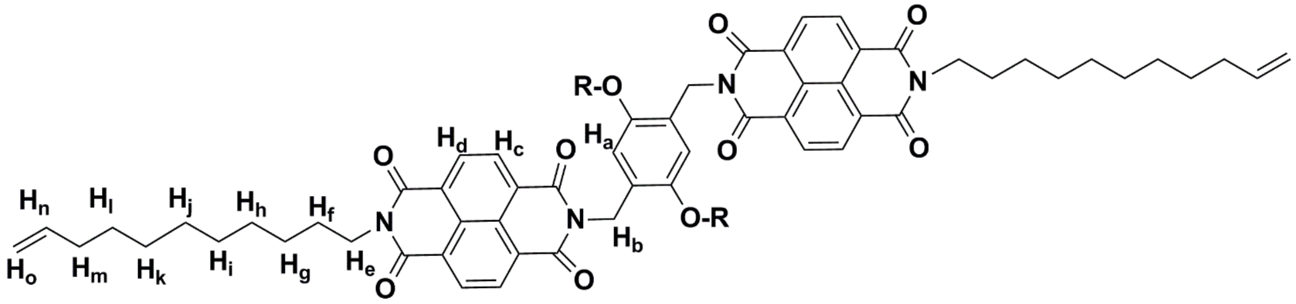
Compound 2: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79 (m, 8H,$H_{c,d}$), 6.79 (s, 2H,H_a), 5.85 (m,2H,H_m), 5.43 (s, 4H,H_b), 4.84 (m, 4H,H_n), 4.29 (d, J = 5.6 Hz, 4H,H_e), 3.65 (m, 4H, H_R), 2.08 (m, 2H,H_l), 1.78 (m, 2H,H_f), 1.57 (m,16H,H_R), 1.28 (m, 24H,$H_{g,h,i,j,k}$), 0.84 (12H,H_R). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.83 (C=O), 162.71 (C=O), 150.78, 139.18, 131.01, 127.57, 125.83, 124.49, 114.16, 112.82, 71.50, 41.00, 39.77, 39.50, 33.79, 30.41, 29.36, 29.27, 29.06, 29.01, 28.89, 28.09, 27.08, 23.75, 23.00, 14.05, 11.15. HR-MS m/z calculated for $C_{72}H_{86}N_4O_{10}$ 1166. 6344 found HR-MS 1166.6338. ε (λ_{max}=380nm) = 22399 $M^{-1}cm^{-1}$.



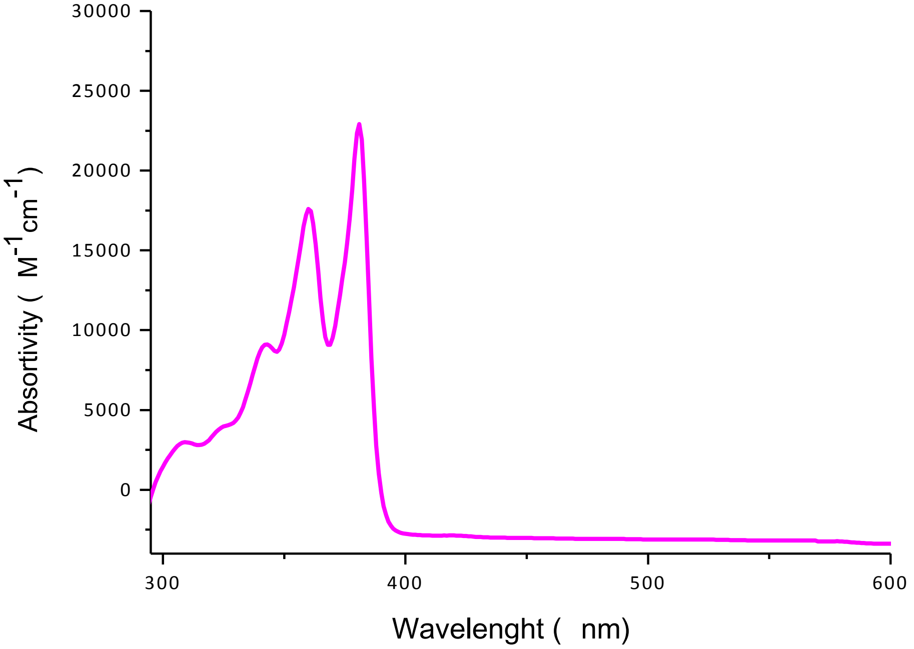

9495q-sl65
SL 65
8.00
2.05
1.88
3.84
4.15
4.22
4.13
4.39
4.54
38.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

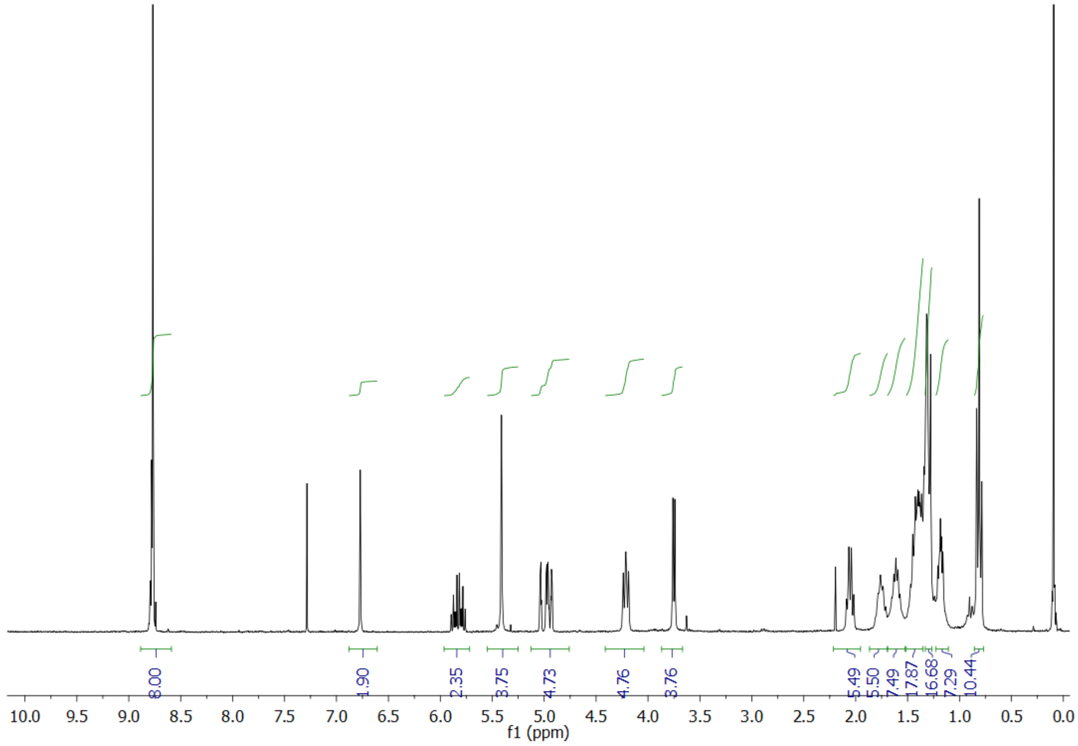

9522q-sl65
SL65
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

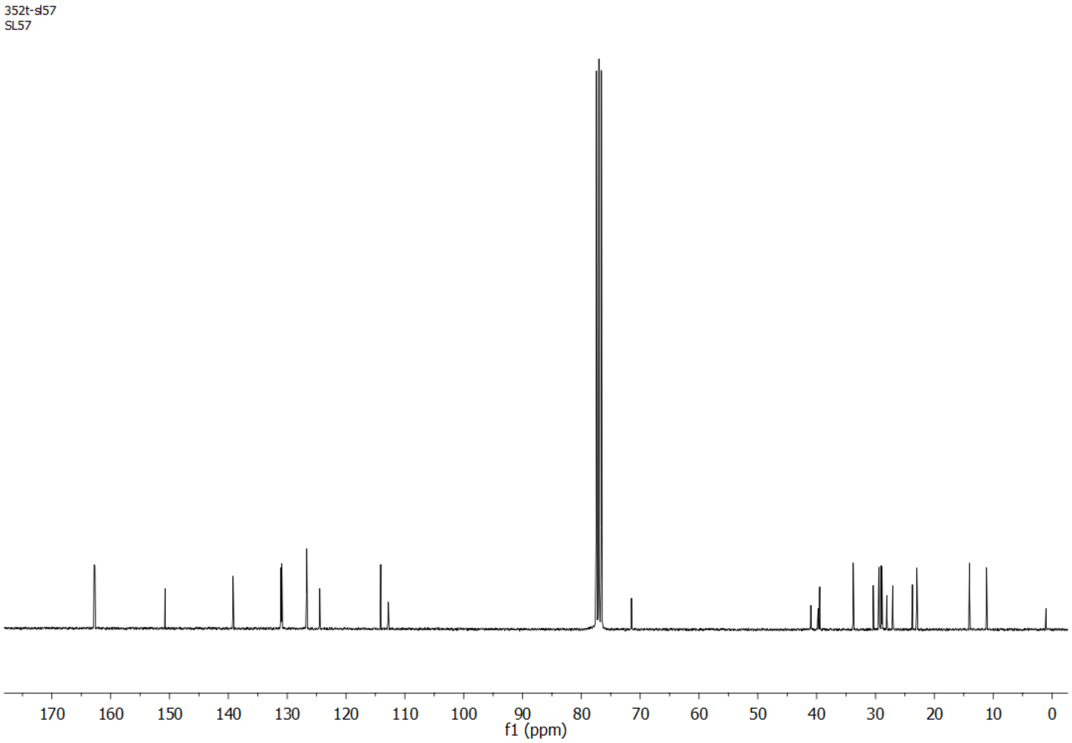


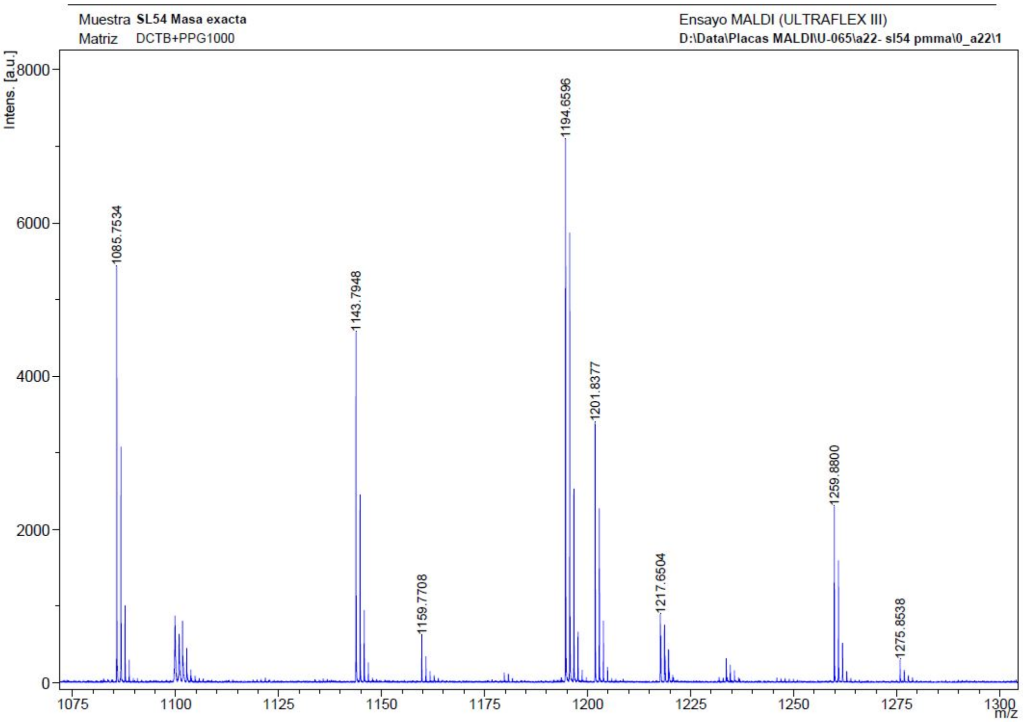


Compound 3: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.79 (s, 8H,H$_{c,d}$), 6.77 (s, 2H,H$_a$), 5.83 (m,2H,H$_n$), 5.42 (s, 4H,H$_b$), 4.41 (m, 4H,H$_o$), 4.21(d, J = 5.6 Hz, 4H,H$_e$), 3.76 (m, 4H, H$_R$), 2.04(m, 2H,H$_m$),1.76 (m, 2H,H$_f$) 1.38 (m,16H,H$_R$),1.17(m, 24H,H$_{g,h,i,j,k,l}$) 0.81 (12H,H$_R$). ^{13}C NMR (75 MHz, CDCl$_3$) δ 162.75 (C=O), 150.75, 139.20, 130.99, 126.70, 124.47, 114.10, 112.80, 71.48, 40.99, 39.75, 39.48, 33.79, 30.39, 28.08, 27.06, 23.73, 22.97, 14.02, 11.13. HR-MS m/z calculated for $C_{74}H_{90}N_4O_{10}$ 1194.6657 found HR-MS 1194.6598. ε (λ_{max}=380nm) = 22355 M^{-1}cm^{-1}.

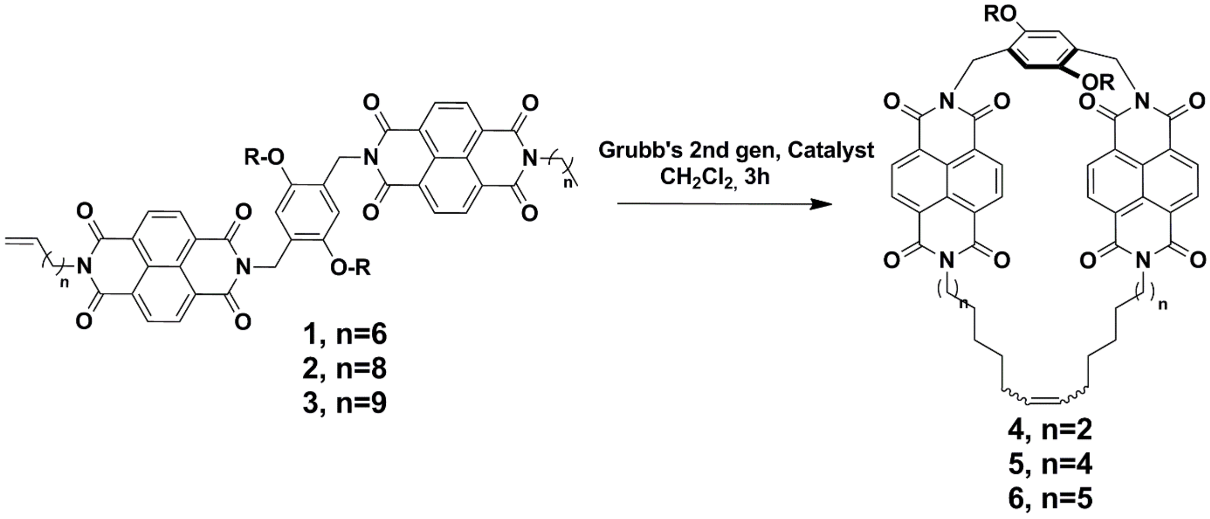

30000
25000
20000
15000
10000
5000
0
Absortivity ($M^{-1}cm^{-1}$)
300
400
500
600
Wavelenght (nm)


8.00
1.90
2.35
3.75
4.73
4.76
3.76
5.49
5.50
7.49
17.87
16.68
7.29
10.44
10.0
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
f1 (ppm)


352t-sl57
SL57
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Muestra SL54 Masa exacta
Matriz DCTB+PPG1000
Ensayo MALDI (ULTRAFLEX III)
D:\Data\Placas MALDI\U-065\a22- sl54 pmma\0_a22\1
Intens. [a.u.]
8000
6000
4000
2000
0
1085.7534
1143.7948
1159.7708
1194.6596
1201.8377
1217.6504
1259.8800
1275.8538
1075
1100
1125
1150
1175
1200
1225
1250
1275
1300
m/z

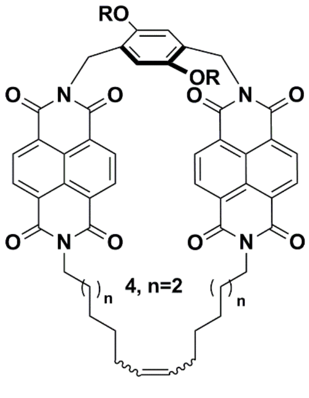
General procedure for the metathesis reaction.



1, n=6
2, n=8
3, n=9

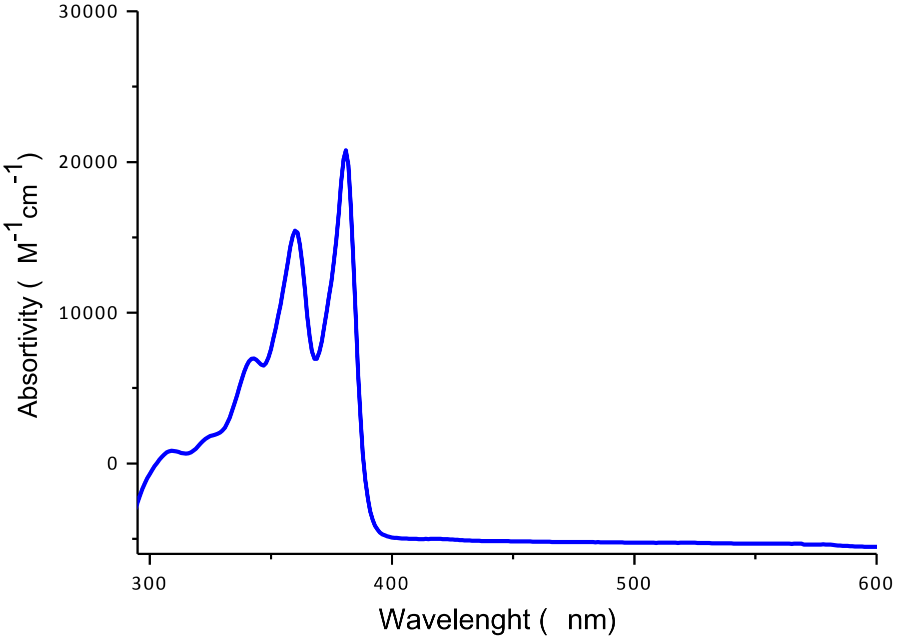
4, n=2
5, n=4
6, n=5

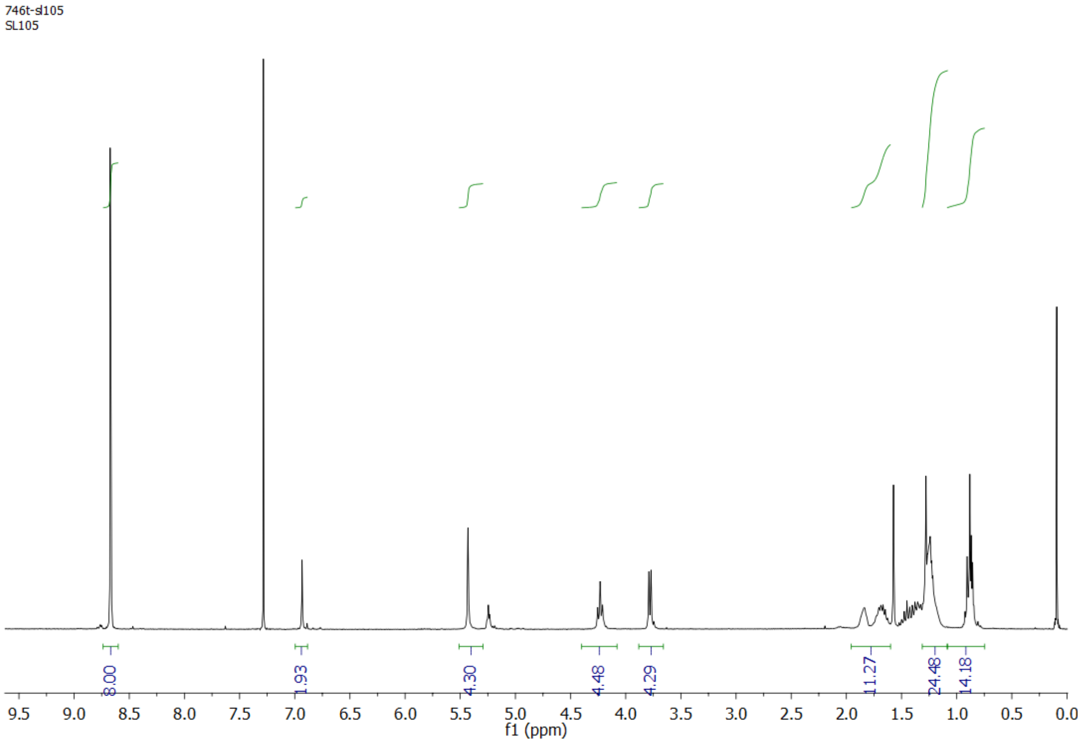
A 10^{-4} M solution of linear receptor **4-6** was prepared in dichloromethane and was degassed by nitrogen bubbling during 30 minutes. Then, a catalytic amount of Grubb's 2nd generation catalyst was introduced and the mixture was stirred for three hours at room temperature. The mixture was filtered on celite and concentrated in vacuo. The desired macrocycles were finally isolated by silica gel chromatography (eluent: CH_2Cl_2) afforded a pink solid in 82-85% yield.

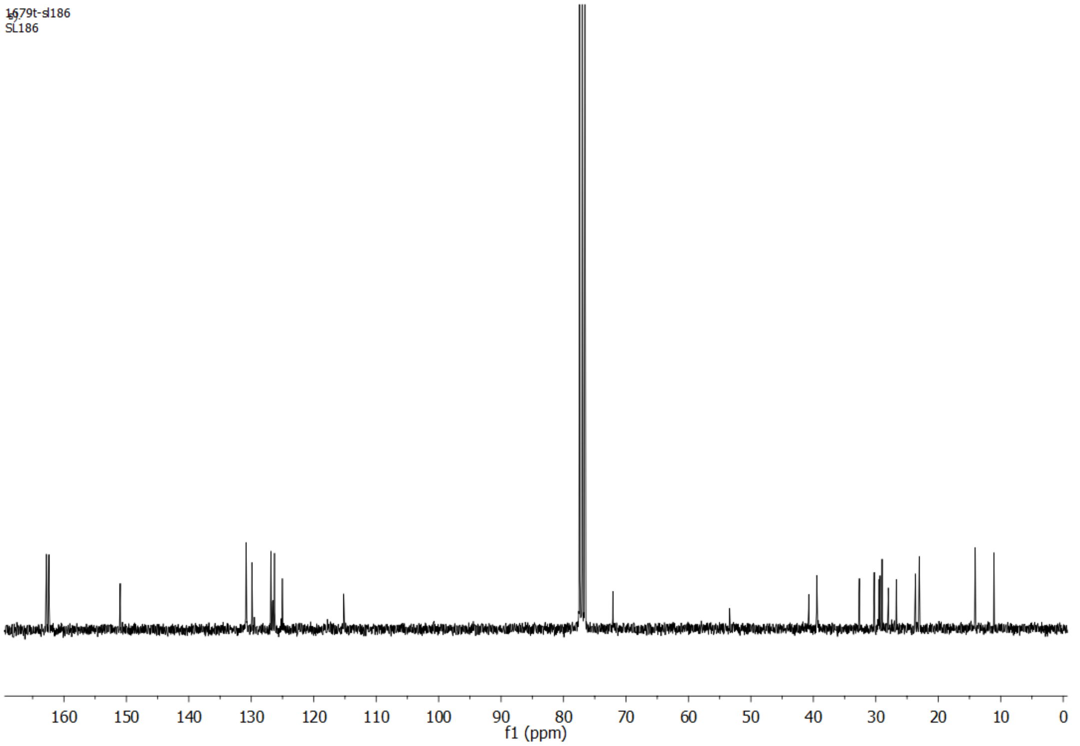


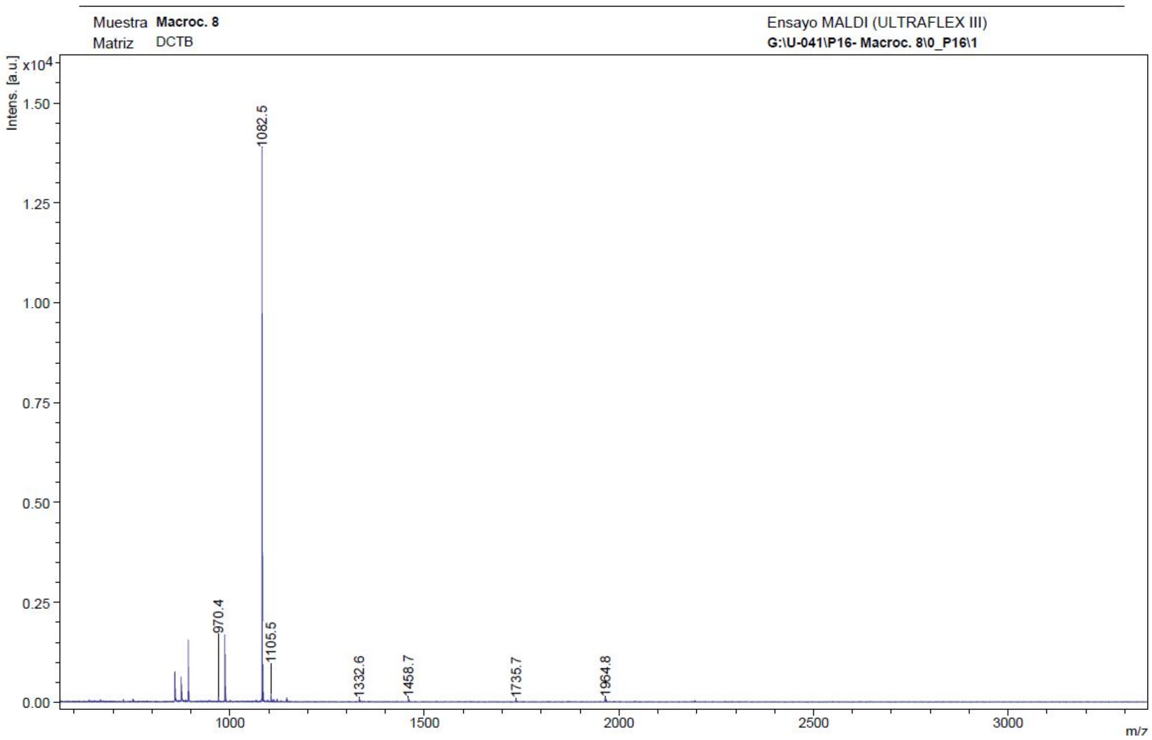
4, n=2

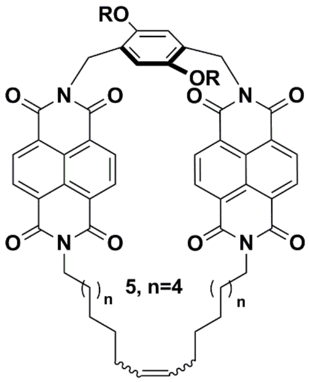
Compound 4: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.72 (m, 8H), 6.91 (s, 2H), 5.43 (s, 4H), 5.31 (m, 2H), 4.23 (m, 4H), 3.73 (m, 4H), 1.84 (m, 4H), 1.68 (m, 2H), 1.41 (m, 38H), 1.08 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.80 (C=O), 162.41 (C=O), 150.98, 130.83, 130.79, 130.74, 129.90, 126.85, 126.58, 126.52, 126.28, 125.03, 115.20, 72.09, 53.41, 40.73, 39.45, 39.35, 32.63, 30.25, 29.48, 29.32, 28.99, 28.00, 26.71, 23.64, 23.00, 22.35, 14.09, 11.08. HR-MS m/z calculated for $C_{66}H_{74}N_4O_{10}$ 1082.5405 found HR-MS 1082.5359. ε (λ_{max}=380nm) = 20210 $M^{-1}cm^{-1}$.




746t-sl105
SL105
8.00
1.93
4.30
4.48
4.29
11.27
24.48
14.18
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
f1 (ppm)

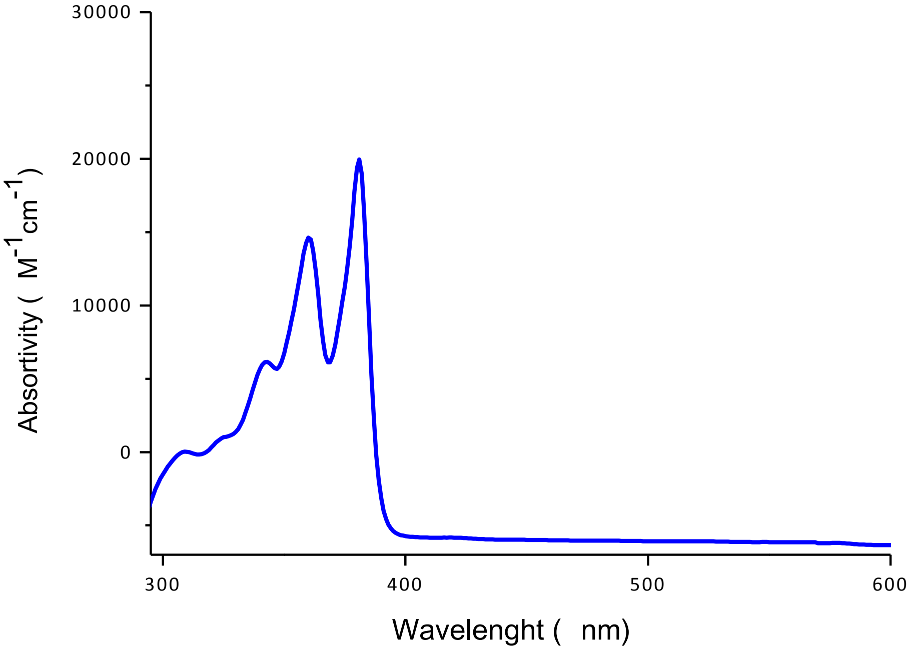

1679t-sl186
SL186
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

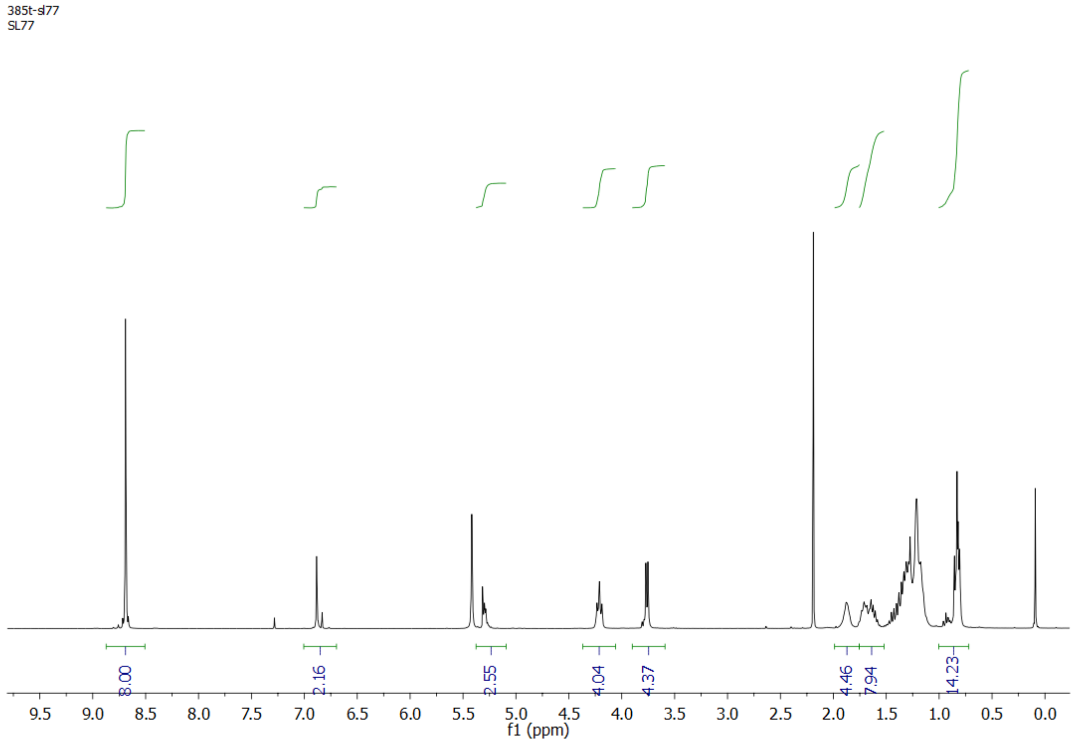




5, n=4

Compound 5: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.87 (s, 8H), 6.86 (s, 2H), 5, 42 (s, 4H) 5.32 (m, 2H), 4.21 (m, 4H), 3.78 (m, 4H), 1.88 (m, 4H), 1.57 (m, 2H), 1.55 (m, 44H), 1.00 (m, 12H), ^{13}C NMR (75 MHz, CDCl$_3$) δ 162.79 (C=O), 162.48 (C=O), 150.88, 130.85, 130.08, 126.79, 126.4, 124.61, 71.77, 40.83, 39.86, 39.43, 32.50, 30.91, 30.27, 29.64, 29.40, 29.30, 29.11, 28.96, 28.02, 26.88, 23.63, 22.99, 14.05, 11.08. MS m/z calculated for $C_{70}H_{82}N_4O_{10}$ 1138.6031 found HR-MS 1138.5971. ε (λ_{max}=380nm) = 19955 $M^{-1}cm^{-1}$.

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SL77
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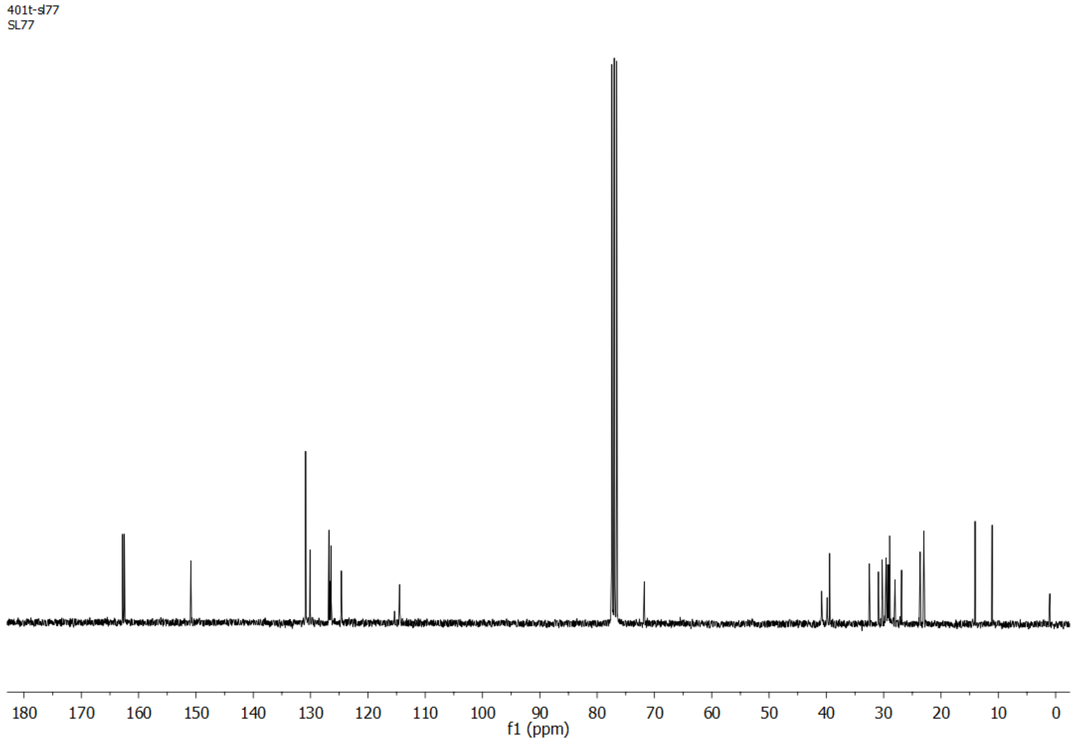
2.16
2.55
4.04
4.37
4.46
7.94
14.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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SL77
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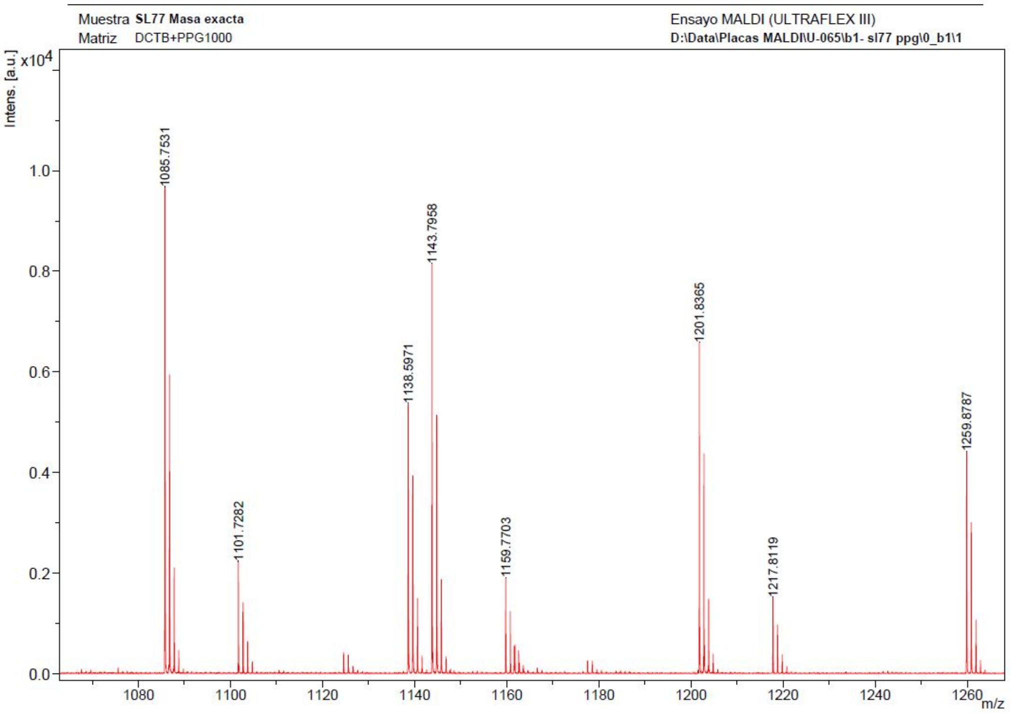
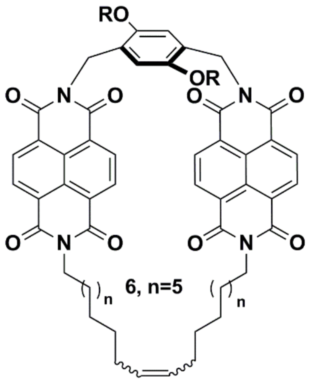
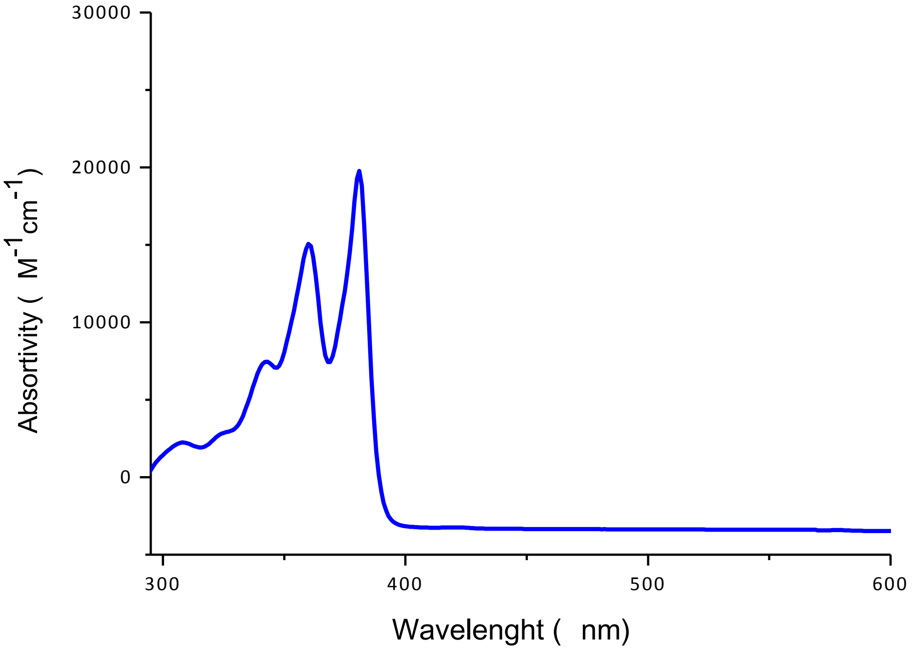




Compound 6: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.78 (m, 8H), 6.90 (s, 2H), 5.46 (s, 4H), 5.36 (m, 2H), 4.24 (m, 4H), 3.78 (m, 4H), 1.90 (m, 4H), 1.77 (m, 2H), 1.53 (m, 48H), 1.04 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.84 (C=O), 162.55 (C=O), 130.89, 130.27, 126.79, 126.51, 77.32, 77.21, 77.00, 76.69, 39.43, 32.55, 30.28, 29.43, 29.29, 29.14, 28.96, 28.90, 26.82, 23.63, 22.98, 14.04, 11.08. MS m/z calculated for $C_{72}H_{86}N_4O_{10}$ 1166.6344 found HR-MS 1166.6295. ε (λ_{max}=380nm)= 19066 $M^{-1}cm^{-1}$.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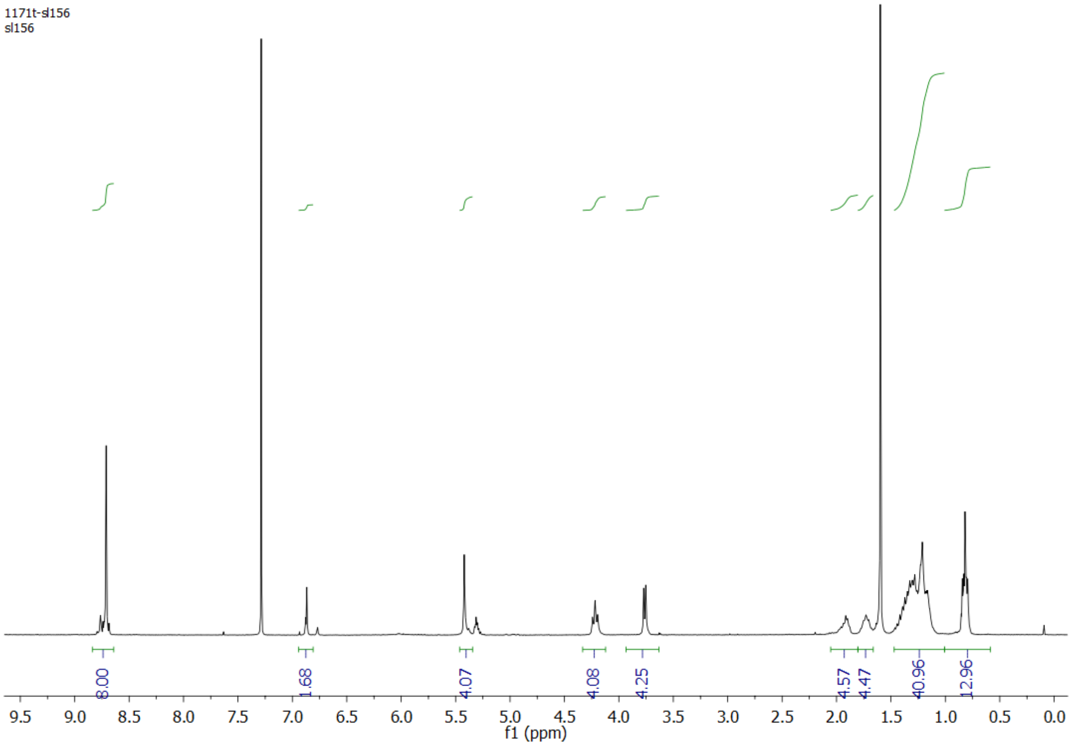
20000
10000
0
Absortivity (M-1cm-1)
300
400
500
600
Wavelenght (nm)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8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
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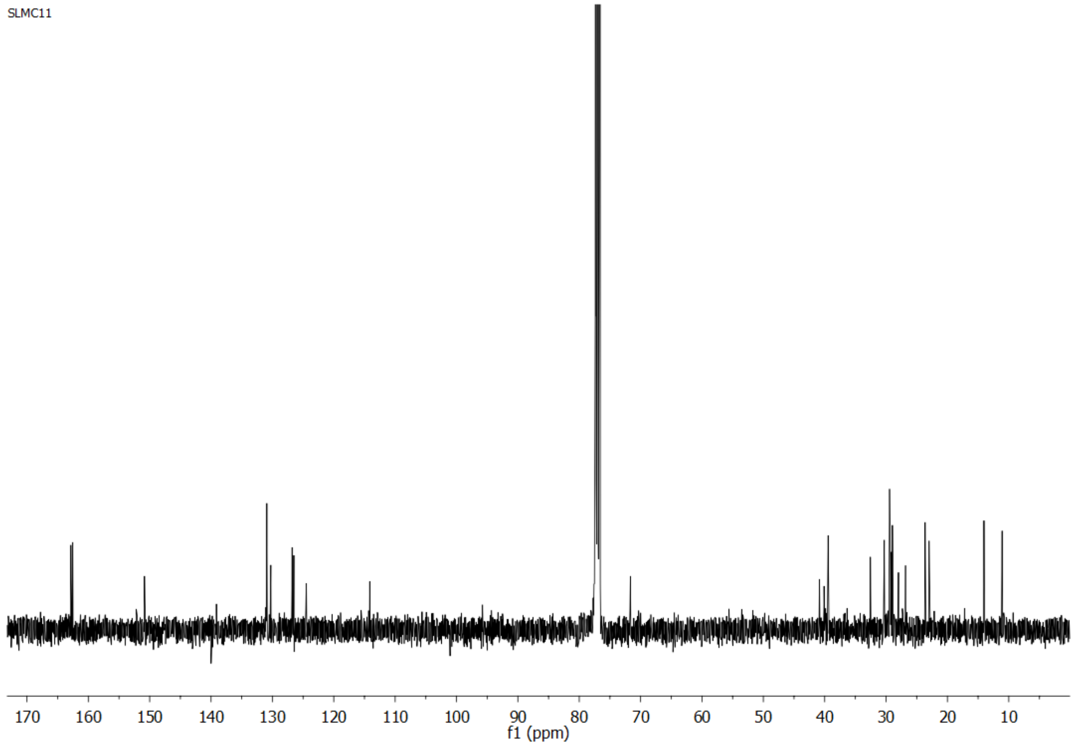
0.0
f1 (ppm)


SLMC11
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100
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80
70
60
50
40
30
20
10
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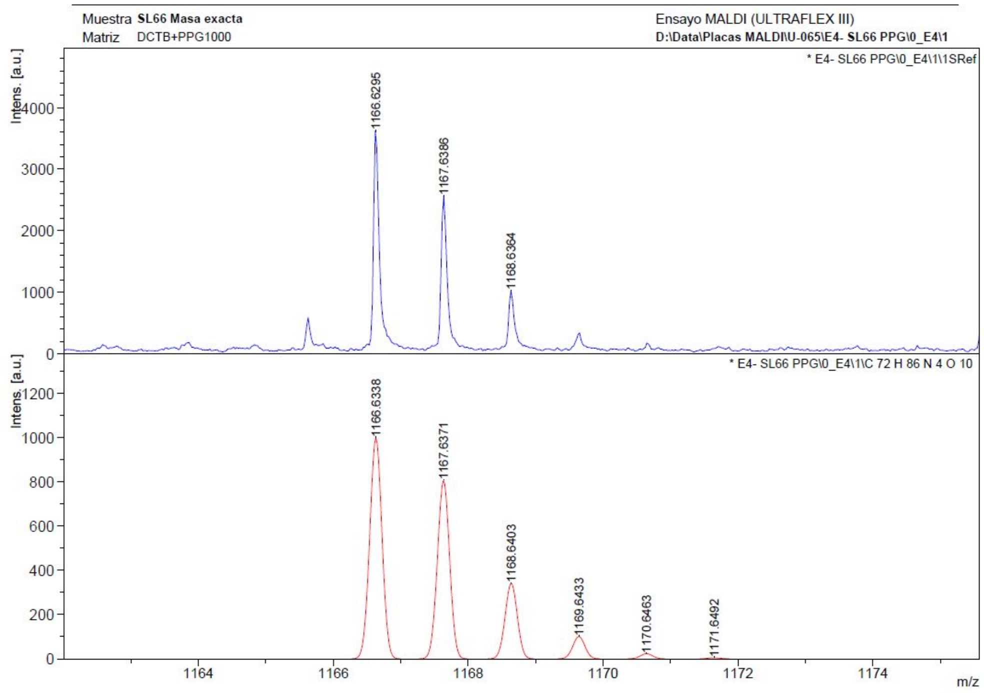
Muestra **SL66 Masa exacta**
Matriz DCTB+PPG1000
Ensayo MALDI (ULTRAFLEX III)
D:\Data\Placas MALDI\U-065\E4- SL66 PPG\0_E4\1
* E4- SL66 PPG\0_E4\1\1SRef
Intens. [a.u.]
4000
3000
2000
1000
0
1166.6295
1167.6386
1168.6364
* E4- SL66 PPG\0_E4\1\C 72 H 86 N 4 O 10
Intens. [a.u.]
1200
1000
800
600
400
200
0
1166.6338
1167.6371
1168.6403
1169.6433
1170.6463
1171.6492
1164
1166
1168
1170
1172
1174
m/z

General procedure for SWNTs functionalization.

The nanotubes (5mg) were suspended in 5 ml of either tetrachloroethane (TCE) or N, N-dimethylformamide (DMF) through sonication during 10 min. After sonication the linear precursor **4-6** was added and the mixture was degasified during 20 min, the Grubb's 2nd generation catalyst was added and the mixture was stirred at room temperature for 72 h. The suspension was filtered through a PTFE membrane of 0.2 µm pore size and the solid washed with dichloromethane (DMC). The solid was re-suspended in 20 ml of DMC through sonication during 10 min and filtered through PTFE membrane again. This washing was repeated three times.

General Procedure for SWNTs Functionalization varying the relative c concentration of 5 with respect to SWNTs.

The nanotube (1mg /1ml) were suspended in TCE and DMF through sonication (10 min) and mixed with the linear precursor 5 (0.044 mM, 2.3 mM, 4.5 mM) and Grubb's 2nd generation catalyst at room temperature for 72h. The suspension was filtered and washed using the same procedure described above.

General Procedure for SWNTs Functionalization (control experiment).

The nanotubes (5mg) were suspended in 5 ml of tetrachloroethane (TCE) and N, N-dimethylformamide (DMF) through sonication during 10 min. After sonication the solvent was the linear precursor **1-3** or macrocycle **4-6** was added and the mixture was degasified during 20 min, the Grubb's 2nd generation catalyst was added and the mixture was stirred at room temperature for 72 h. The suspension as filtered through a PTFE membrane of 0.2 µm pore size and the solid washed with dichloromethane (DMC). The solid was re-suspended in 20 ml of DMC through sonication during 10 min and filtered through PTFE membrane again. This washing was repeated three times.

General Procedure for de-threading Functionalized SWNTs.

The functionalized nanotubes (2mg) were suspended in 5 ml of TCE by sonication for 5 min and then heated to reflux (bp = 146^0C) for 30 min. The suspension was filtered through a PTFE of 0.2 µm pore size and the solid washed profusely with DCM. De-threading was observed by TGA.

Chirality	Diameter	CNT (kJ/mol)	SYS (kJ/mol)	CMB (kJ/mol)	Eb (kJ/mol)	Eb (kcal/mol)	atoms
(6,5)	7.4700E-01	2.2188E+04	6.8350E+02	2.2870E+04	-8.9600E-01	-2.1410E-01	476
(7,5)	8.1800E-01	2.5372E+04	1.1134E+03	2.6601E+04	1.1613E+02	2.7749E+01	548
(7,6)	8.8200E-01	2.8622E+04	1.4844E+03	3.0707E+04	6.0060E+02	1.4351E+02	620
(8,3)	7.7100E-01	2.3386E+04	8.1166E+02	2.4234E+04	3.6141E+01	8.6358E+00	500
(8,4)	8.2900E-01	2.5733E+04	1.1975E+03	2.7066E+04	1.3618E+02	3.2540E+01	560
(9,5)	9.6220E-01	3.2656E+04	2.3079E+03	3.5807E+04	8.4292E+02	2.0141E+02	716
(8,6)	9.5300E-01	3.2153E+04	2.2418E+03	3.5205E+04	8.0949E+02	1.9343E+02	704
(9,3)	8.4700E-01	2.6900E+04	1.3427E+03	2.8410E+04	1.6697E+02	3.9897E+01	580
(11,0)	8.6100E-01	1.6413E+04	1.4627E+03	1.8065E+04	1.8949E+02	4.5278E+01	420
(10,2)	8.7200E-01	2.8180E+04	1.5678E+03	2.9959E+04	2.1138E+02	5.0509E+01	608

Figure S1: Dataset interaction energies of a series of SWNTs with macrocycle 6.

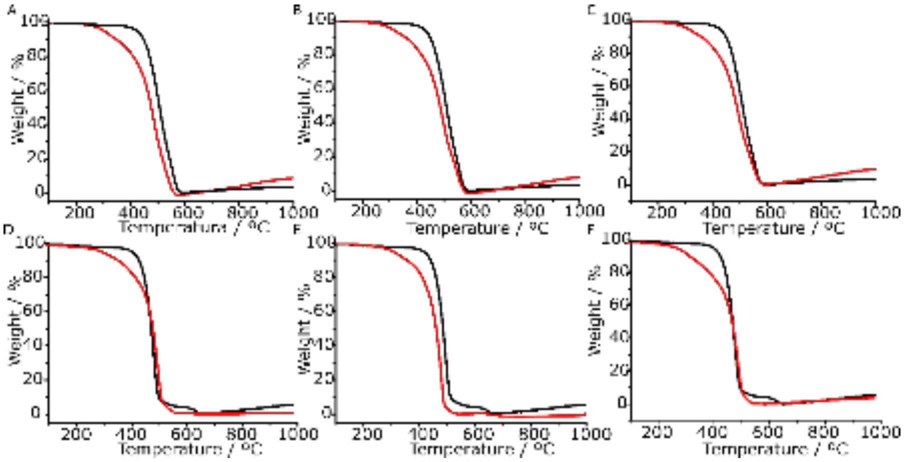

Figure S2:A-F: TGA (air, 10 min^{-1}) of: a) (6,5) SWNTs (Black line), **1**-(6,5)-TCE (red line), b) (6,5) SWNTs (Black line), ***2**-(6,5)-TCE (red line), c) (6,5) SWNTs (Black line), **3**-(6,5)-TCE (red line), d) (7,6) SWNTs (Black line), **1**-(7,6)-TCE* (red line), e) (7,6) SWNTs (Black line), **2**-(7,6)-TCE (red line), f) (7,6) SWNTs (Black line), **3**-(7,6)-TCE (red line).

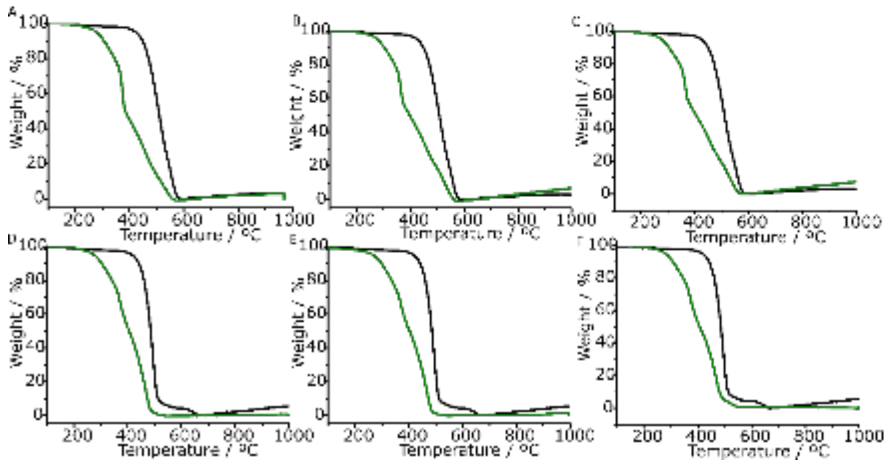

Figure S3: A-F: TGA (air, 10 min^{-1}) of: a) (6,5) SWNTs (Black line), **1**-(6,5)-DMF (green line),b) (6,5) SWNTs (Black line), **2**-(6,5)-DMF (green line), c) (6,5) SWNTs (Black line), **3**-(6,5)-DMF (green line), d) (7,6) SWNTs (Black line), **1**-(7,6)-DMF (green line), e) (7,6) SWNTs (Black line), **2**-(7,6)-DMF (green line), f) (7,6) SWNTs (Black line), **3**-(7,6)- TCE (green line).

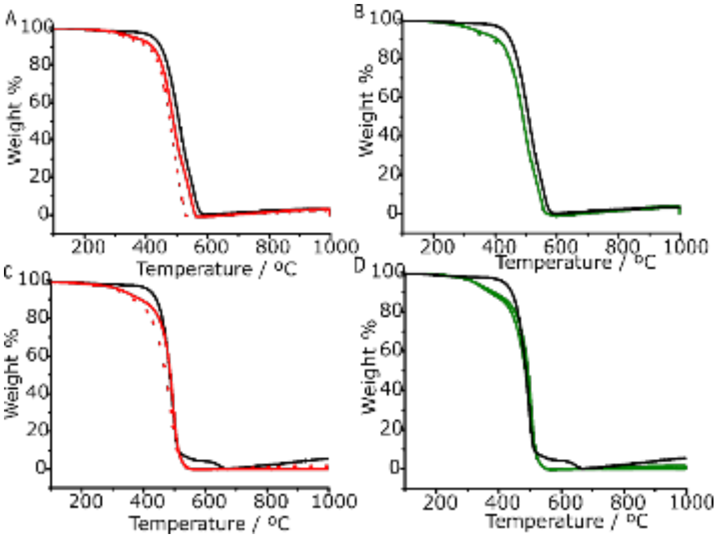

Figure S4: A-D: TGA (air, 10 min^{-1}) of: a) **2**-(6,5)-TCE reaction with catalyst (Black line), **2**-(6,5)-TCE without catalyst (solid red line), **2**-(6,5)-TCE (dashed red line) b) **2**-(6,5)-DMF reaction with catalyst (Black line), **2**-(6,5)-DMF without catalyst (solid green line), **2**-(6,5)-DMF (dashed green line), c) **3**-(7,6)-TCE reaction with catalyst (Black line), **3**-(7,6)-TCE without catalyst (solid red line), **3**-(7,6)-TCE (dashed red line), d) **3**-(7,6)-DMF reaction with catalyst (Black line), **3**-(7,6)-DMF without catalyst (solid green line), **3**-(7,6)-DMF (dashed green line).

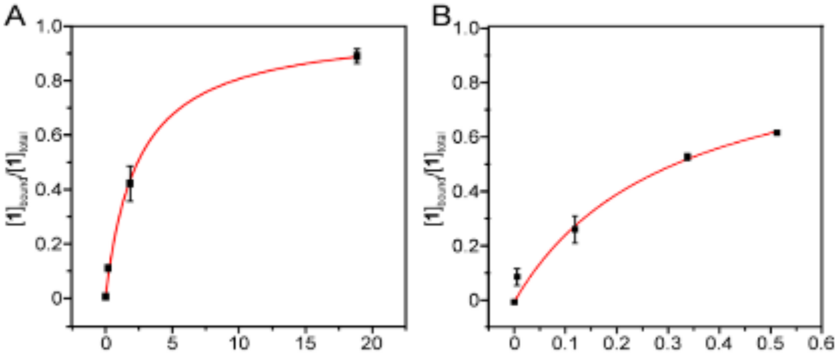

Figure S5: Titration of **3** *vs* (6,5)-SWNTs in a) TCE (K_a= 2.6 ± 0.1 M^{-1}, r^2= 0.9967) and b) DMF K_a = 3.5 ± 0.2 M^{-1}, r^2 = 0.8713).

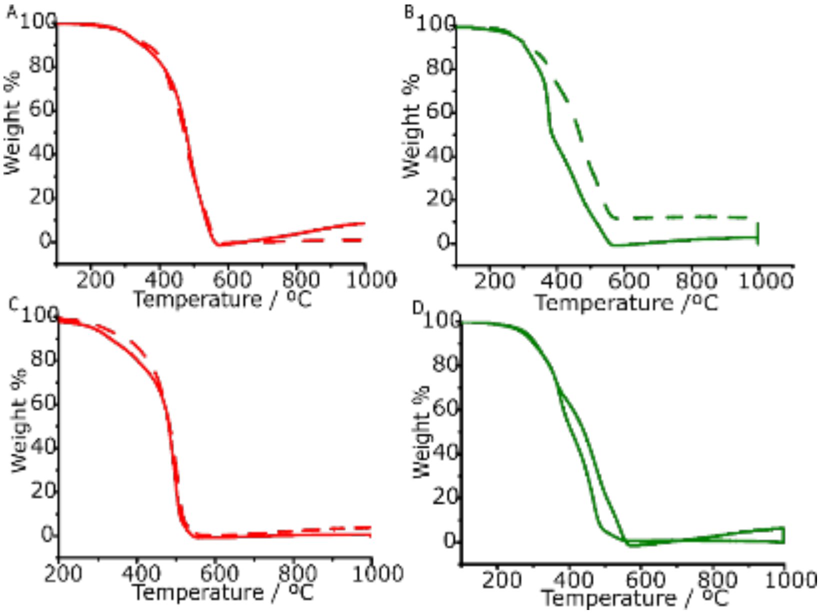

Figure S6: A-D: TGA (air, 10 min^{-1}) of: a) **1**-(6,5)-TCE (solid red line), **1**-(6,5)-TCE after heating at reflux in TCE for 30 min (dashed red line),b) **1**-(6,5)-DMF (solid green line), **1**-(6,5)-DMF after heating at reflux in TCE for 30 min (dashed green line), c) **3**-(7,6)-TCE (solid red line), **3**-(7,6)-TCE after heating at reflux in TCE for 30 min (dashed red line),d) **3**-(7,6)-DMF (solid green line), **3**-(7,6)-DMF after heating at reflux in TCE for 30 min (dashed green line).

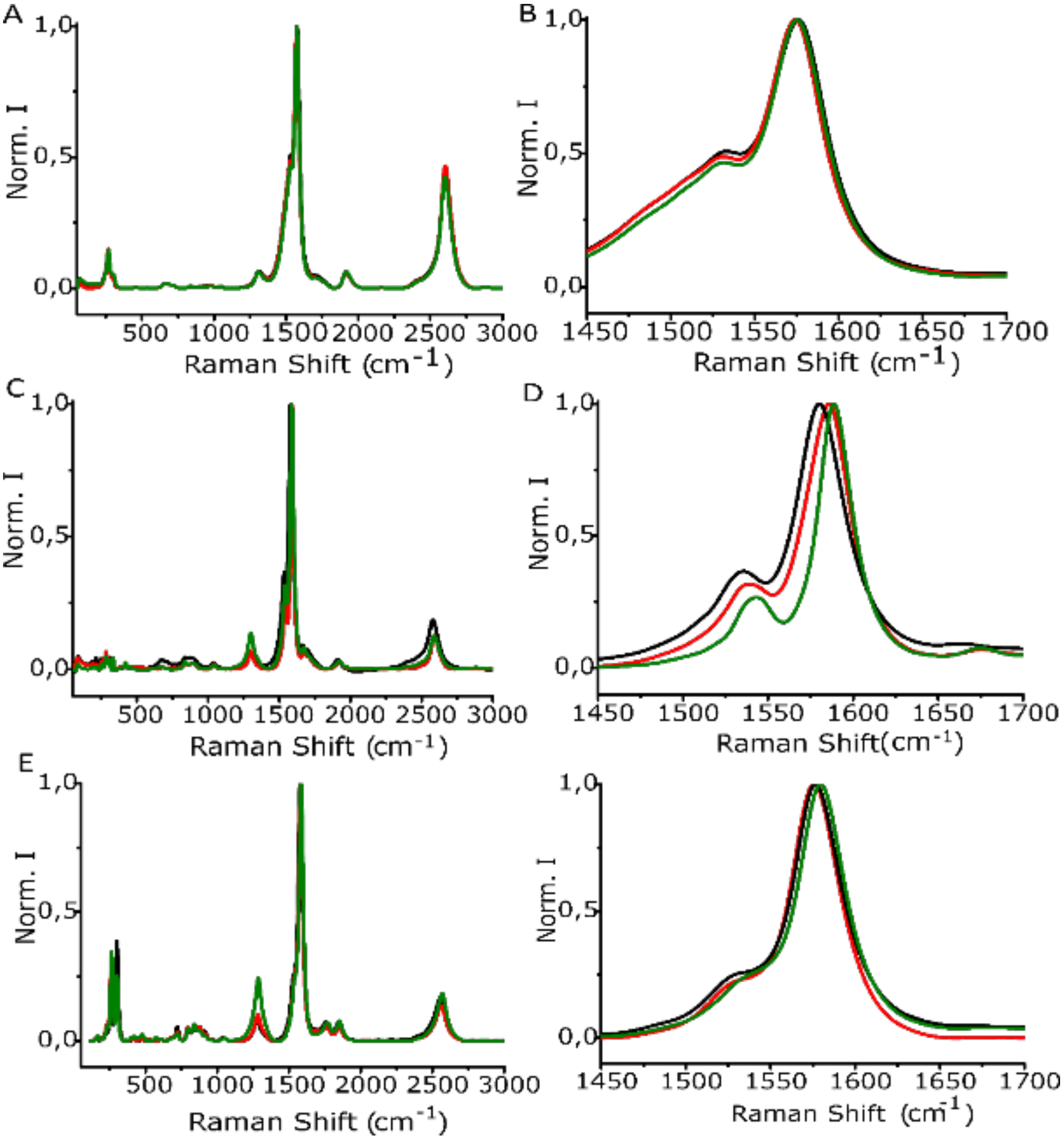

Figure S7 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (6,5) SWNTs (black line), **1**-(6,5)-TCE (red line) and **1**-(6,5)-DMF (green line), b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (6,5) SWNTs (black line), **1**-(6,5)-TCE (solid red line) and **1**-(6,5)-DMF (green line), d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (6,5) SWNTs (black line), **1**-(6,5)-TCE (solid red line) and **1**-(6,5)-DMF (green line), f) Zoom in of the G band of the spectra.

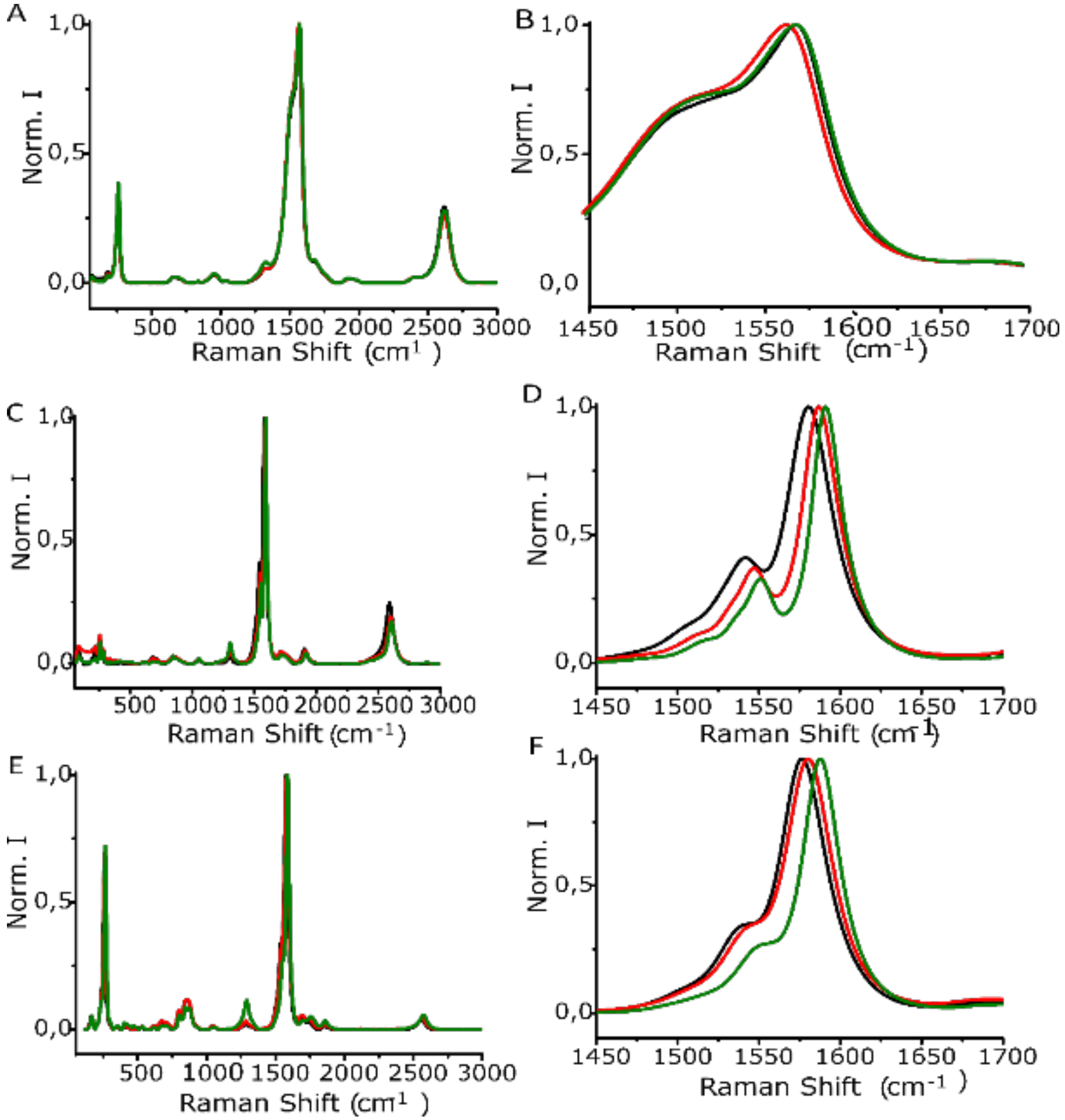

Figure S8 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (7,6) SWNTs (black line), **1**-(7,6)-TCE (red line) and **1**-(7,6)-DMF (green line), b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (7,6) SWNTs (black line) and **1**-(7,6)-TCE (solid red line), **1**-(7,6)-DMF (green line), d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (7,6) SWNTs (black line), **1**-(7,6)-TCE (solid red line) and **1**-(7,6)-DMF (green line), f) Zoom in of the G band of the spectra.

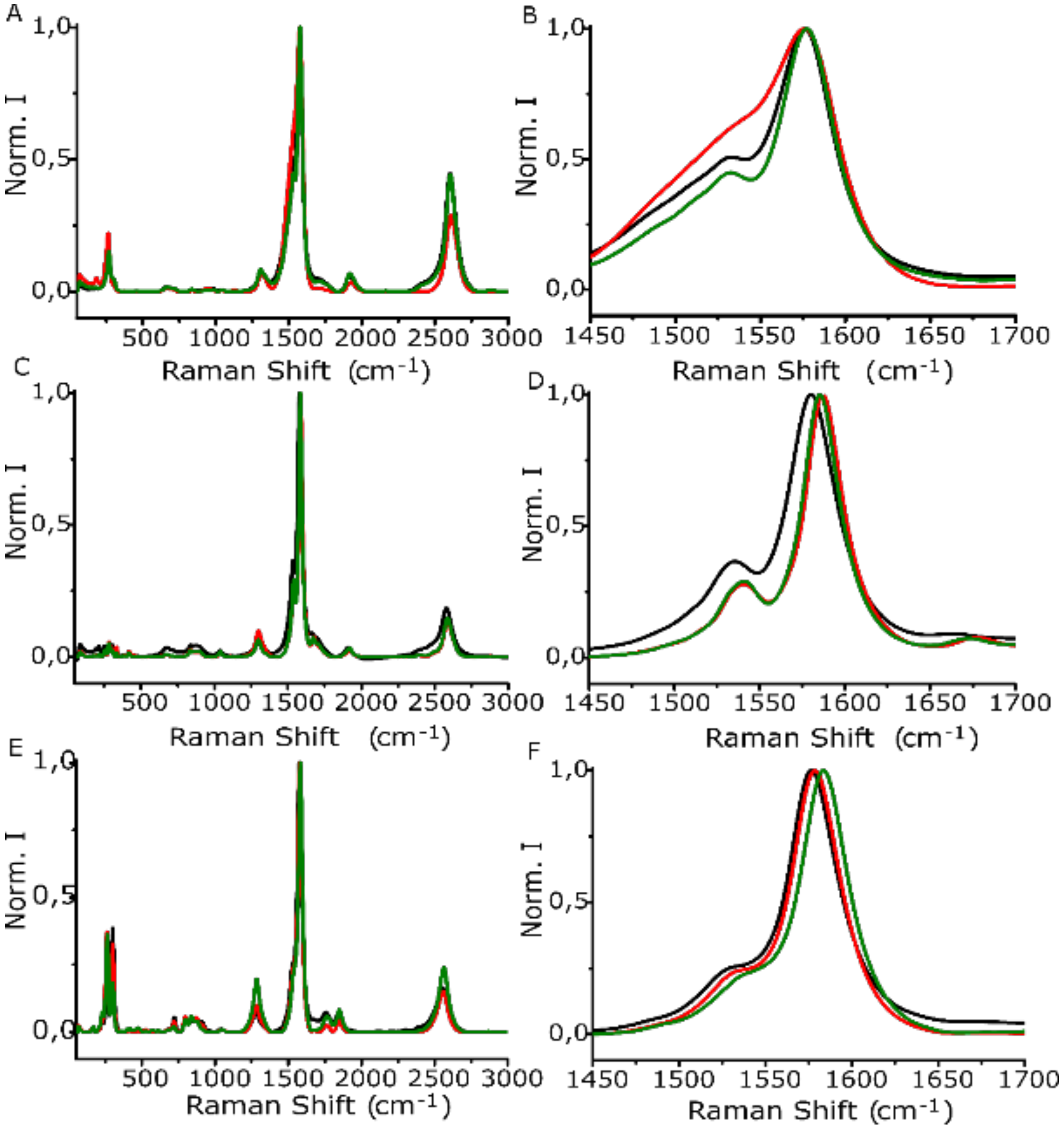

Figure S9 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (6,5) SWNTs (black line), **2**-(6,5)-TCE (red line) and **2**-(6,5)-DMF (green line), b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (6,5) SWNTs (black line), **2**-(6,5)-TCE (solid red line) and **2**-(6,5)-DMF (green line), d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (6,5) SWNTs (black line), **2**-(6,5)-TCE (solid red line) and **2**-(6,5)-DMF (green line), f) Zoom in of the G band of the spectra.

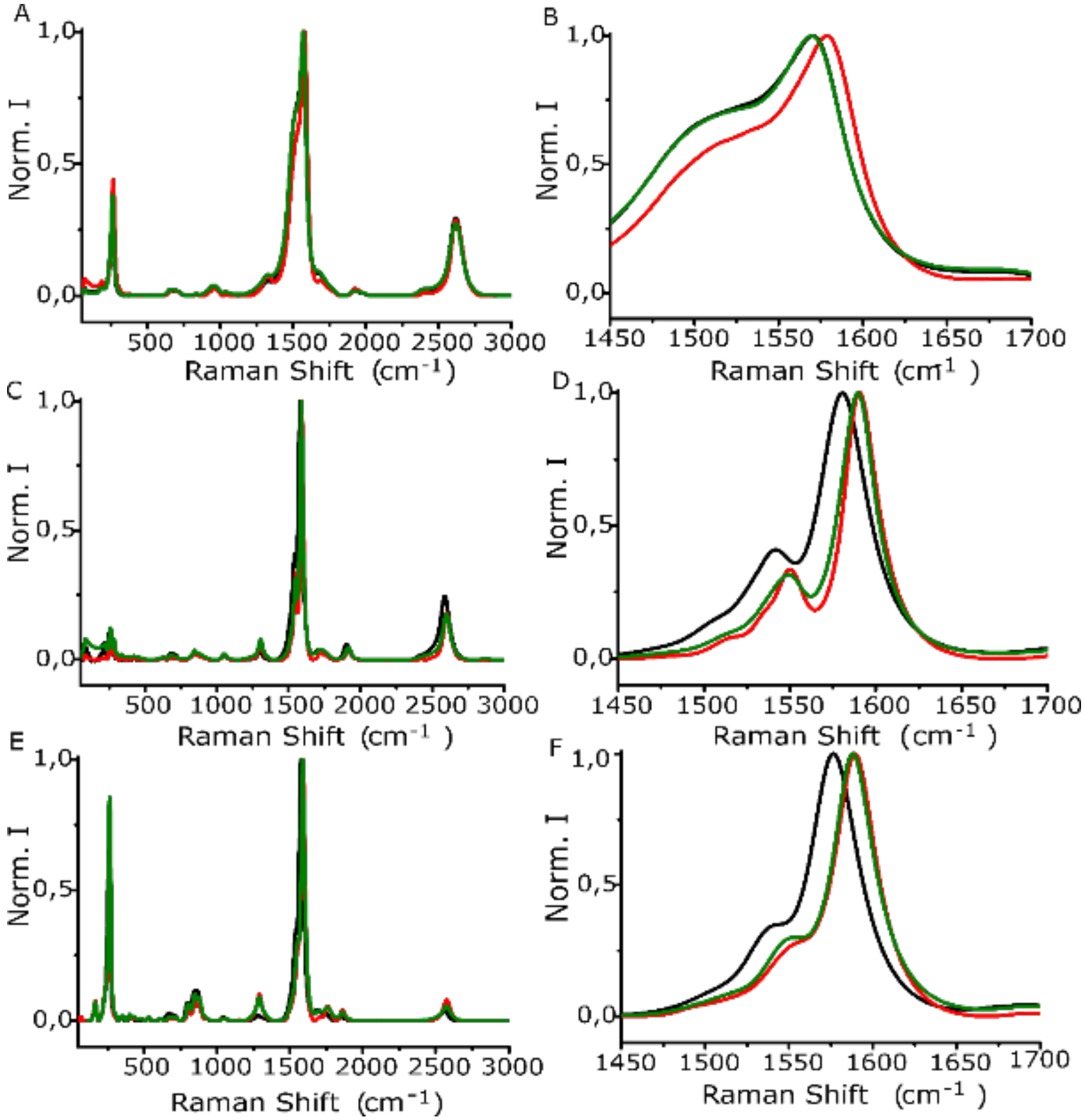

Figure S10 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (7,6) SWNTs (black line), **2**-(7,6)-TCE (red line) and **2**-(7,6)-DMF (green line), b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (7,6) SWNTs (black line), **2**-(7,6)-TCE (solid red line) and **2**-(7,6)-DMF (green line). d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (7,6) SWNTs (black line), **2**-(7,6)-TCE (solid red line) and **2**-(7,6)-DMF (green line), f) Zoom in of the G band of the spectra.

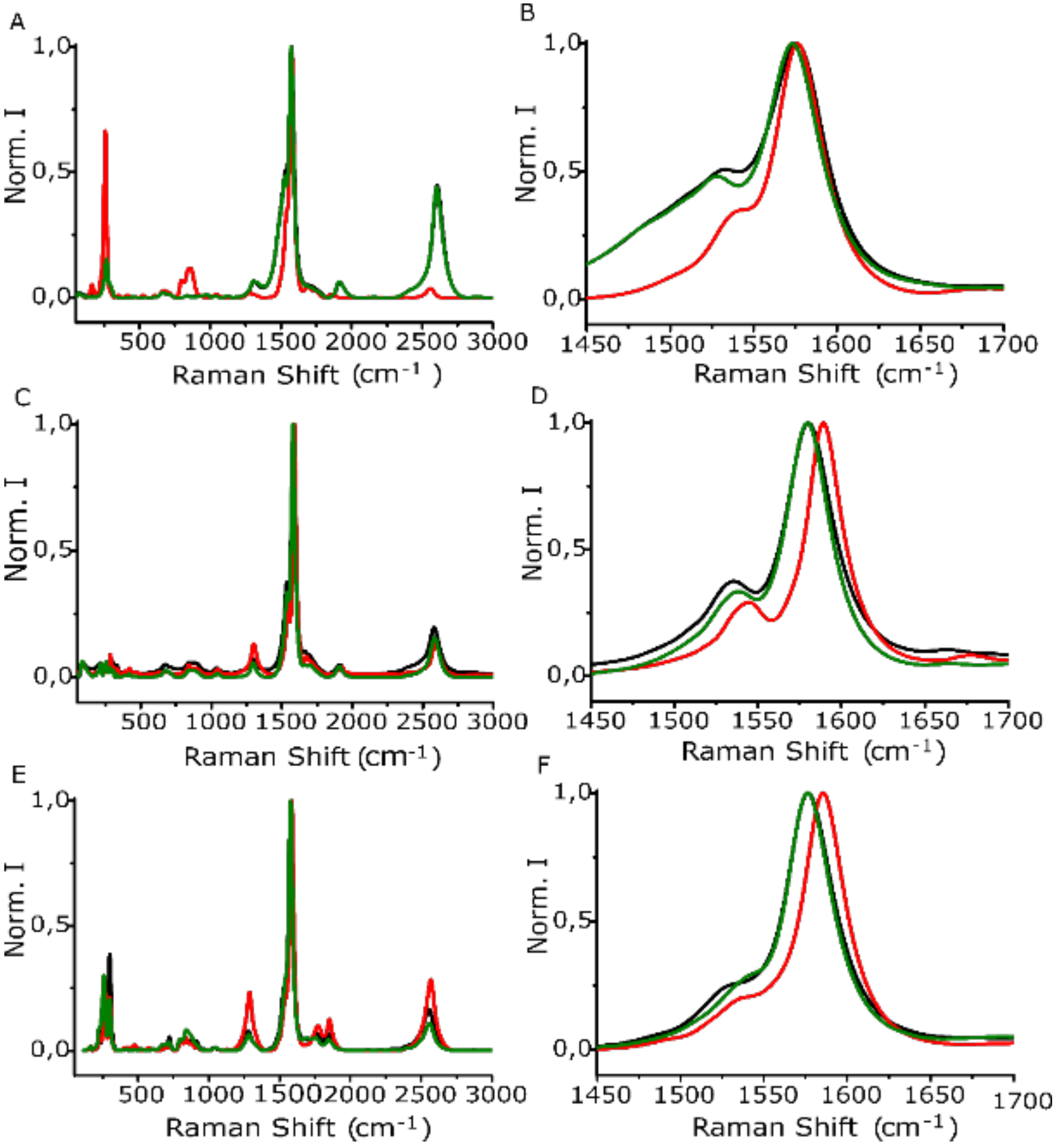

Figure S11 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (6,5) SWNTs (black line), **3**-(6,5)-TCE (red line), **3**-(6,5)-DMF (green line). b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (6,5) SWNTs (black line) and **3**-(6,5)-TCE (solid red line), **3**-(6, 5)-DMF (green line). d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (6,5) SWNTs (black line) and **3**-(6,5)-TCE (solid red line), **3**-(6,5)-DMF (green line), f) Zoom in of the G band of the spectra.

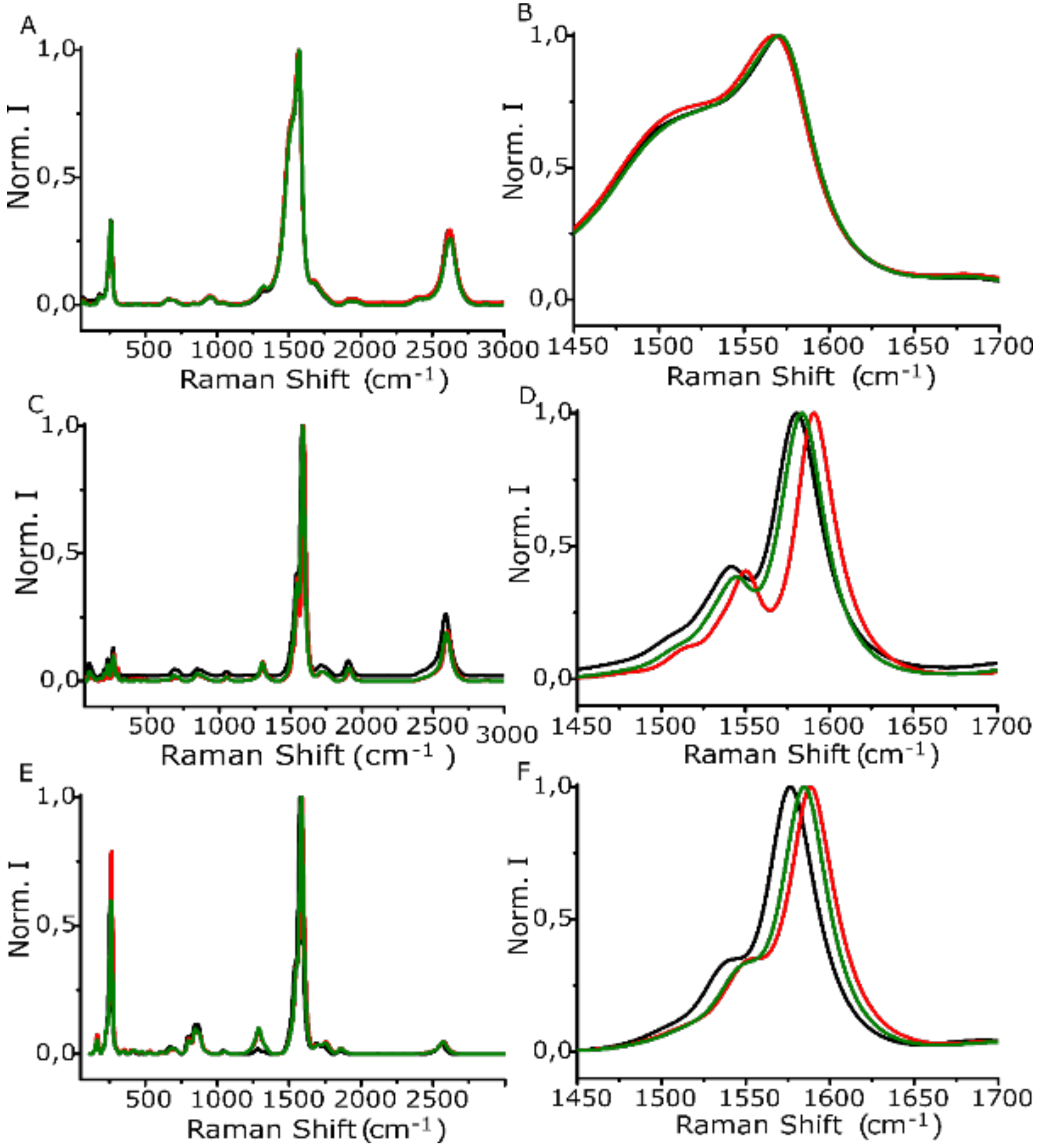

Figure S12 A-F: Raman spectra (λ_{exc} = 532 nm) of a) (7,6) SWNTs (black line), **3**-(7,6)-TCE (red line) and **3**-(7,6)-DMF (green line), b) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 633 nm) of c) (7,6) SWNTs (black line), **3**-(7,6)-TCE (solid red line) and **3**-(7,6)-DMF (green line), d) Zoom in of the G band of the spectra, Raman spectra (λ_{exc} = 785 nm) of e) (7,6) SWNTs (black line), **3**-(7,6)-TCE (solid red line) and **3**-(7,6)-DMF (green line), f) Zoom in of the G band of the spectra.

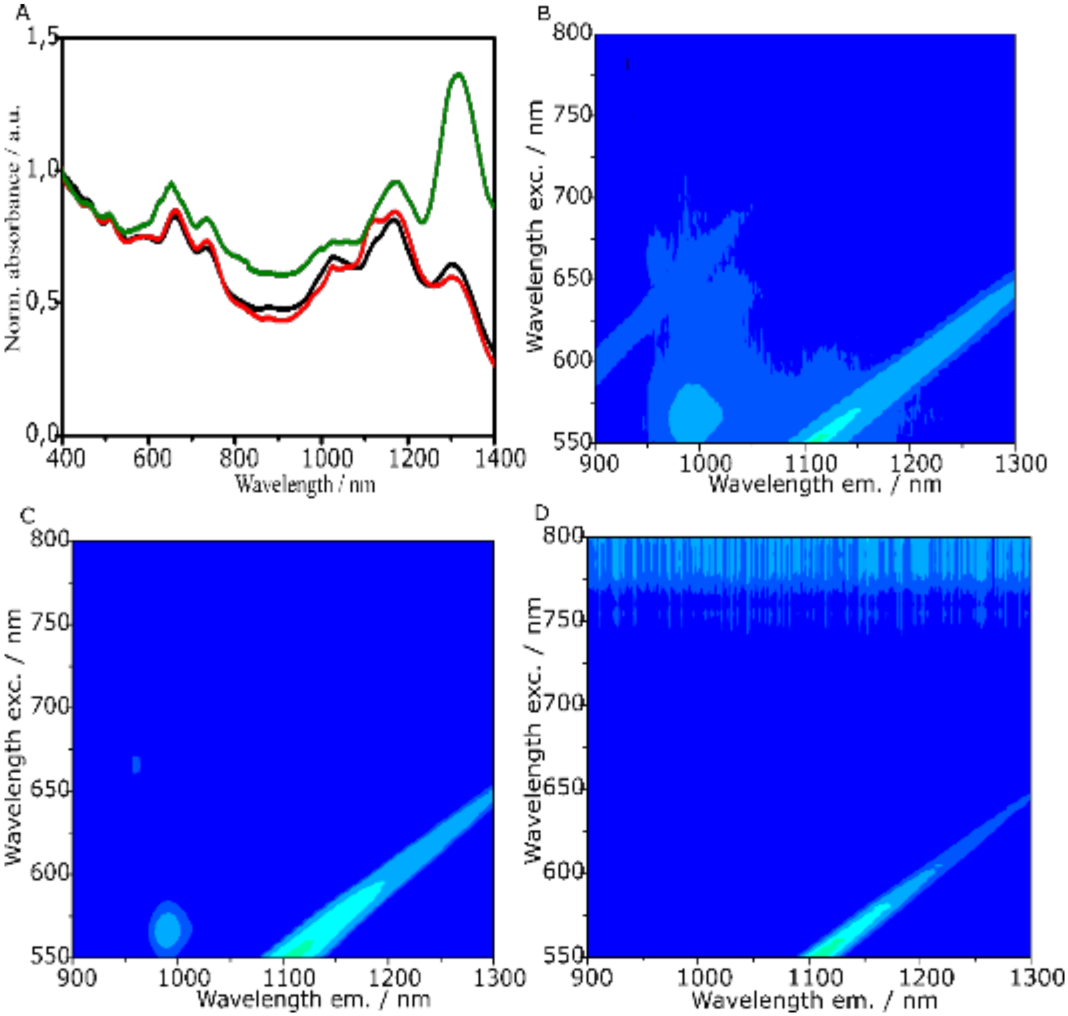

Figure S13 A-D: a) UV-vis-NIR absorption spectra (D_2O, 1% SDS, room temperature) of pristine (6,5)-enriched SWNTs (black), and the products of their reactions with **3** in TCE (red) and DMF (green). PLE intensity maps (D_2O, 1% SDS, room temperature) of b) pristine (6,5) enriched SWNTs, c) **3**-(6,5)-TCE and d) **3**-(6,5)-DMF.