

Electronic Supplementary Information (ESI) for pH-sensitive perylene tetra-(alkoxycarbonyl) probes for live cell imaging

Yongshan Ma ^{a, b, c}, Jiaofu Li ^a, Shuguo Hou ^{b, c}, Jinfeng Zhang ^b, Zhiqiang Shi ^{*a}, Tianyi Jiang ^{b, c}
and Xiaofeng Wei ^b

^aDepartment of Chemistry, Shandong Normal University, 88 Wenhua Donglu Road, Jinan 250014,
P. R. China. E-mail address: zshi@sdsu.edu.cn. Tel.: +86 531 86182540; fax: +86 531 82615258.

^bSchool of Municipal and Environmental Engineering, Shandong Jianzhu University, Jinan
250101, P. R. China.

^cCo-Innovation Center of Green Building, Jinan 250101, P. R. China.

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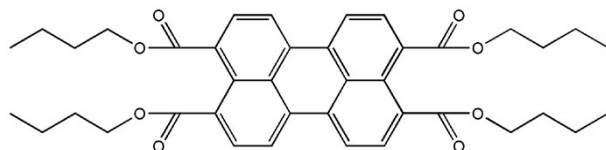
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General Experimental Section

All chemicals and solvents were of analytical grade, obtained from commercial sources and used without further purification. ^1H NMR and ^{13}C NMR were recorded on a Bruker 300 MHz spectrometer (Bruker, Germany) in the solvent CDCl_3 with tetramethylsilane (TMS) as an internal standard. Infrared spectra were obtained through TENSOR27 Fourier transform FT-IR spectrophotometer (Bruker, Germany). Mass spectra data were taken on a Finnigan ESI instrument (Thermo, America). Absorption spectra were measured on a CARY50 UV-vis spectrophotometer (Varian, America). Fluorescence spectra measurements were performed on an FL4500 PC fluorescence spectrophotometer (Hitachi, Japan). Fluorescent images were taken on a BH2 fluorescence microscope (Olympus, Japan). The pH values were measured with a PB-10 pH meter (Beijing Sartorius Device Works, Beijing, China).

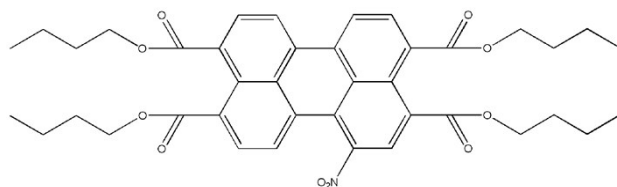
Characteristic Data

3,4,9,10-Tetra (n-butoxyloxycarbonyl) perylene (PTBAC).



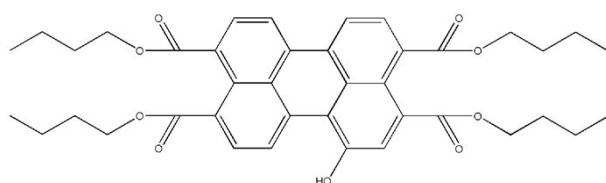
Yield: 4.58g (70%). Yellow solid. ^1H NMR (300 MHz, CDCl_3) δ : 8.08 (d, $J=7.9\text{Hz}$, 4H), 7.93 (d, $J=7.9\text{Hz}$, 4H), 4.39 (d, 8H), 1.87 (m, 8H), 1.59 (m, 8H), 1.02 (m, 12H). ^{13}C NMR (75 MHz, CDCl_3 , ppm) δ : 168.51, 132.78, 130.35, 130.26, 128.81, 126.62, 121.26, 65.29, 53.39, 30.68, 19.28, 13.78. FT-IR (KBr, cm^{-1}): ν = 2952, 2868, 2109, 1893, 1714, 1584, 1511, 1469, 1405, 1266, 1164, 1128, 1097, 1032, 939, 890, 841, 803, 743, 588, 507, 436. MALDI-TOF MS: calcd 652.3; found, 652.3046 ($\text{M} + \text{Na}^+$). Elemental analysis: Calculated for $\text{C}_{40}\text{H}_{44}\text{O}_8$ C 73.60, H 6.79, O 19.61%; found C 73.48, H 6.43, O 19.82%.

1-nitro-perylene-3,4,9,10-tetra (n-butoxyloxycarbonyl) perylene (NPTBAC).



Yield: 0.9g (86%). Red solid. ^1H -NMR(300 MHz, CDCl_3 , ppm): δ =8.40 (s, 1H), 8.37 (m, 2H), 8.26 (d, 1H), 8.14 (d, 1H, $J=6$ Hz), 7.97 (d, 1H, $J=6$ Hz), 7.93 (d, 1H, $J=9$ Hz), 4.37 (m, 8H), 1.82 (m, 8H), 1.55 (m, 8H), 1.03 (m, 12H). ^{13}C NMR (75 MHz, CDCl_3 , ppm) δ : 168.06, 167.86, 167.79, 166.60, 146.32, 133.91, 132.53, 131.96, 131.61, 130.83, 130.51, 130.38, 130.00, 129.15, 128.73, 128.48, 127.92, 127.40, 126.63, 125.62, 123.13, 122.61, 66.02, 65.64, 65.58, 30.60, 19.23, 13.74. FT-IR (KBr, cm^{-1}): ν = 2959, 2871, 1711, 1589, 1529, 1460, 1394, 1353, 1274, 1249, 1163, 1108, 1062, 1021, 959, 899, 846, 801, 736, 702, 604, 506, 434. MALDI-TOF MS: calcd 697.29; found, 697.2913 ($\text{M} + \text{Na}^+$). Elemental analysis: Calculated for $\text{C}_{40}\text{H}_{43}\text{NO}_{10}$ C 68.85, H 6.21, N 2.01, O 22.93%; found C 68.75, H 6.33, O 22.87%.

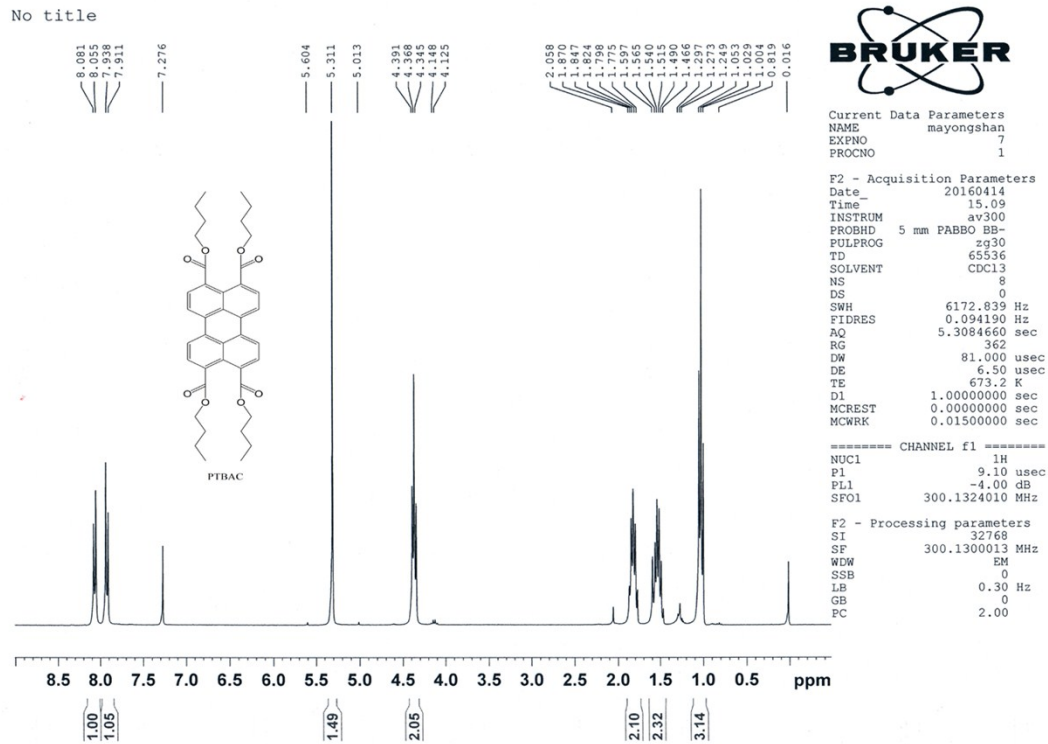
1- hydroxyl-3,4,9,10-tetra(n-butoxyloxycarbonyl) perylene (HPTBAC).



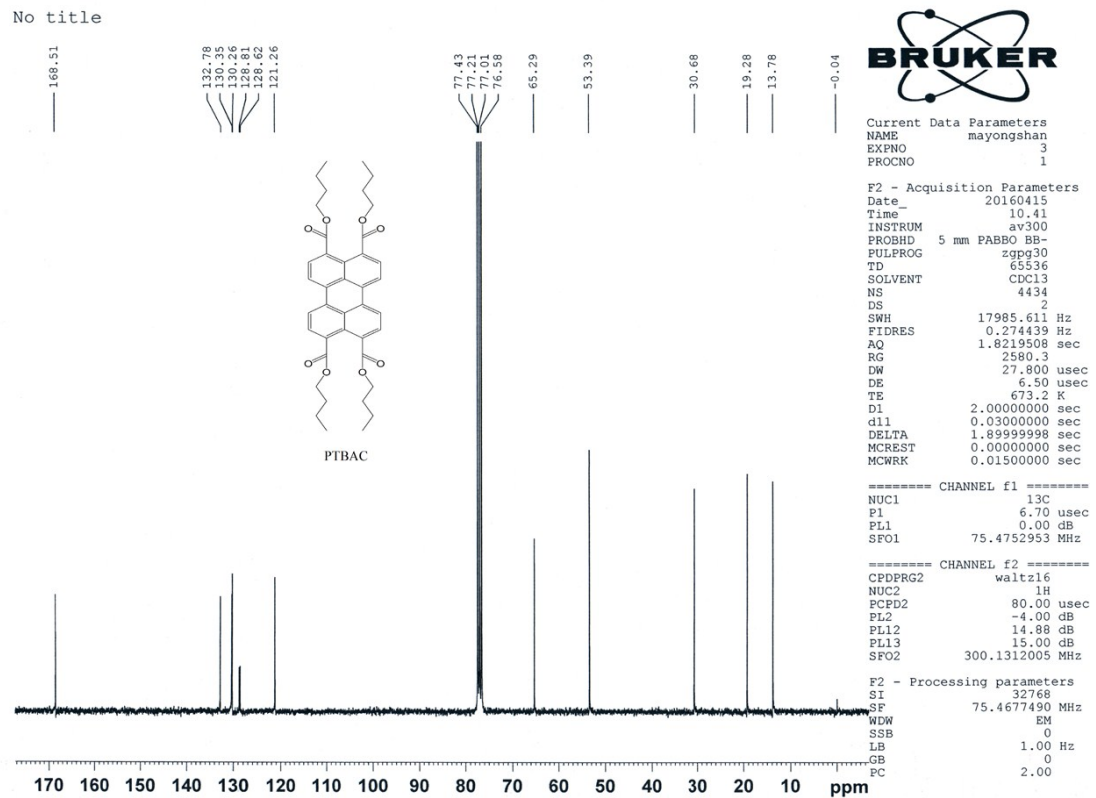
Yield: 52 mg (79%). Red solid. ^1H -NMR (CHCl_3 , TMS, ppm): δ = 10.67 (s, 1H), 9.34 (d, 1H), 8.25 (d, 1H), 7.99-7.95 (m, 3H), 7.84 (d, 1H), 7.82 (s, 1H), 4.23-4.17(m, 8H), 2.62-2.39(m, 8H), 1.71-1.64(m, 8H), 1.44-1.34(m, 12H). ^{13}C NMR (75 MHz, CDCl_3 , ppm): δ = 168.78, 167.80, 167.71, 157.31, 144.10, 133.47, 132.33, 131.95, 131.82, 129.85,

129.30, 128.61, 127.65, 127.40, 126.34, 125.87, 125.64, 122.24, 120.78, 113.56, 80.00, 65.35, 65.27, 65.21, 30.66, 30.58, 19.25, 13.77. FT-IR (KBr, cm^{-1}): $\nu = 2957, 2928, 2870, 1708, 1588, 1514, 1460, 1406, 1344, 1271, 1196, 1160, 1063, 1024, 961, 939, 896, 837, 801, 750, 707, 580, 507, 438$. MALDI-TOF MS: calcd 667.3; found, 667.29 ($M + \text{Na}^+$). Elemental analysis: Calculated for $\text{C}_{40}\text{H}_{44}\text{O}_9$ C 71.84, H 6.63, O 21.53%; found C 71.76, H 6.25, O 21.61%.

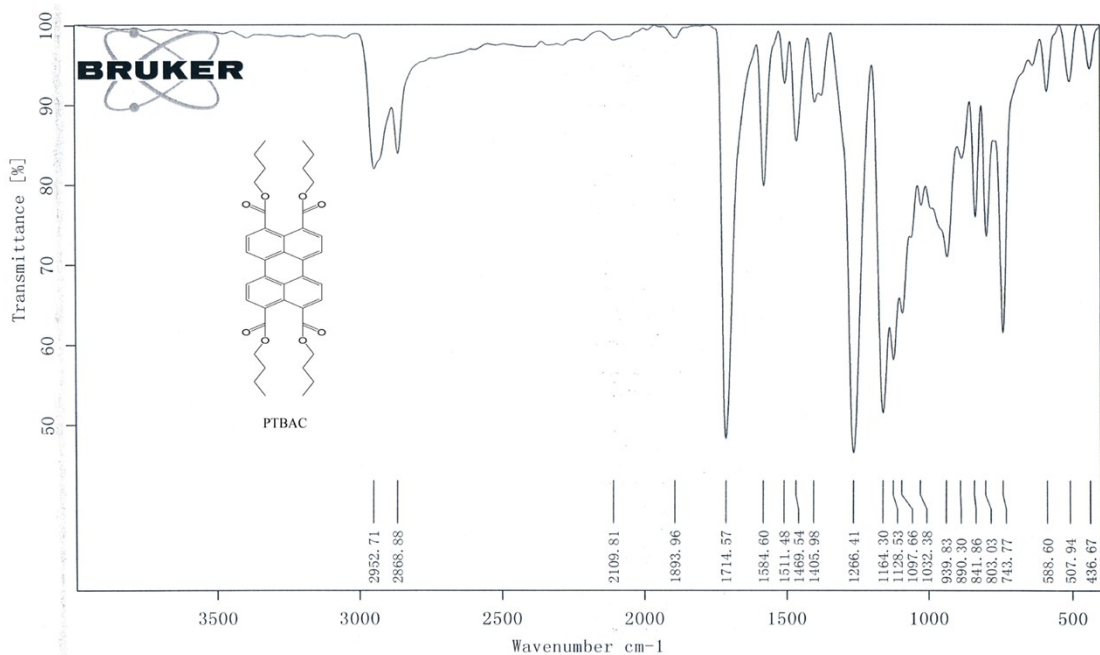
Copies of (1H & 13C) NMR, FTIR and MS Spectra



¹H-NMR spectrum of PTBAC.

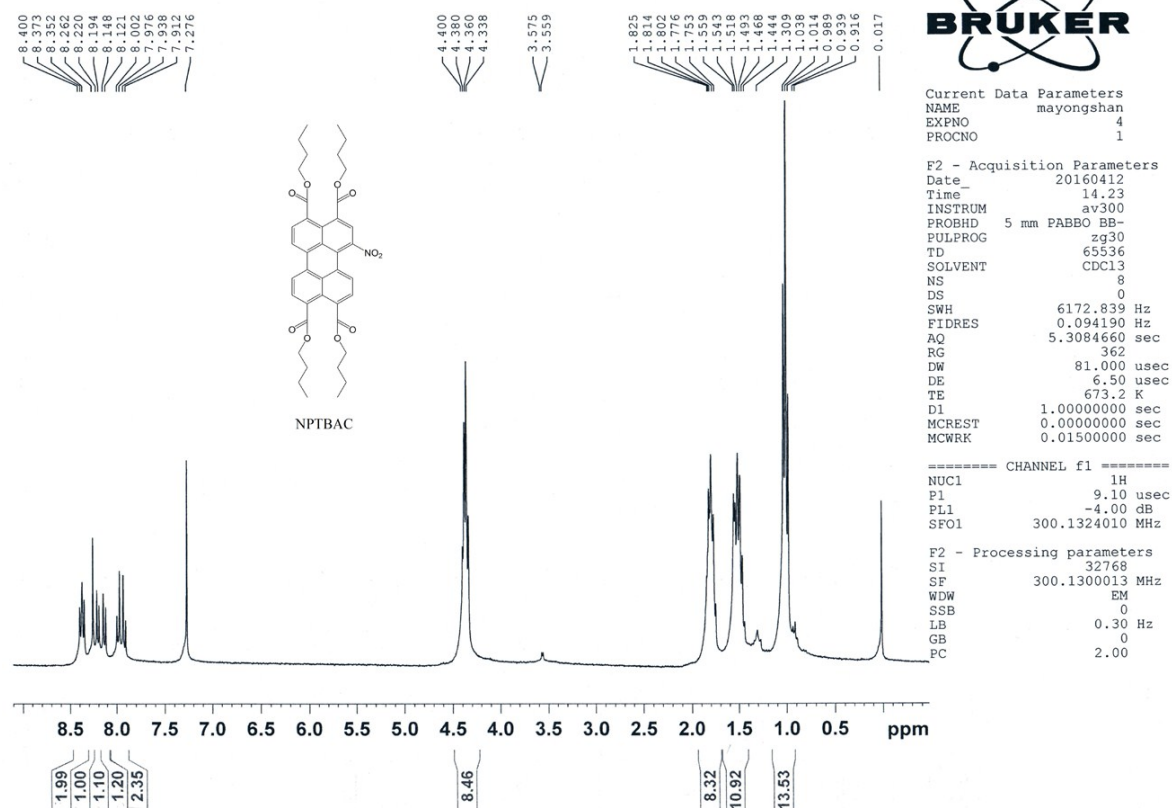


¹³C-NMR spectrum of PTBAC.



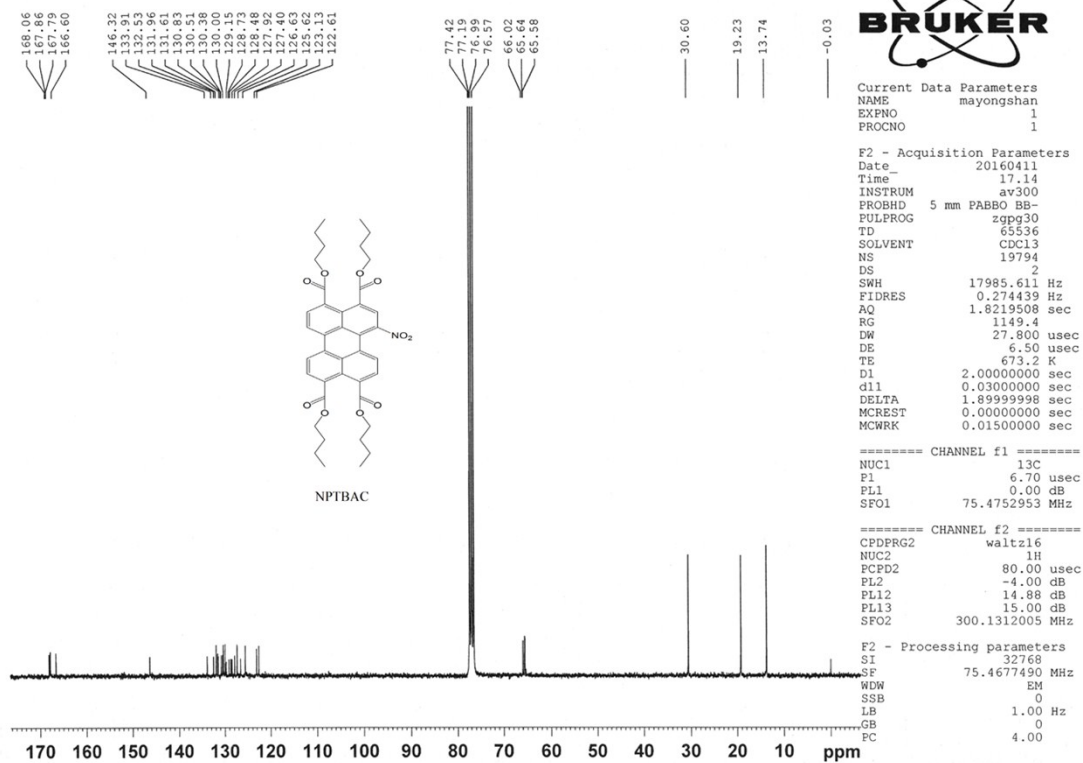
FTIR spectrum of PTBAC.

No title

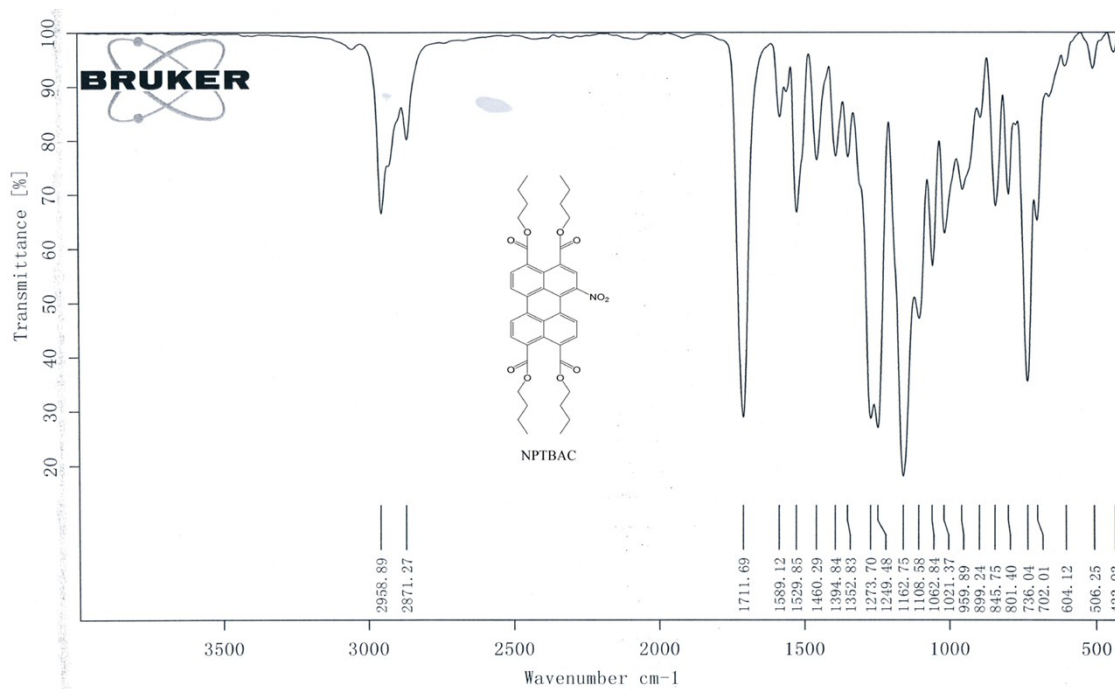


¹H-NMR spectrum of NPTBAC.

No title

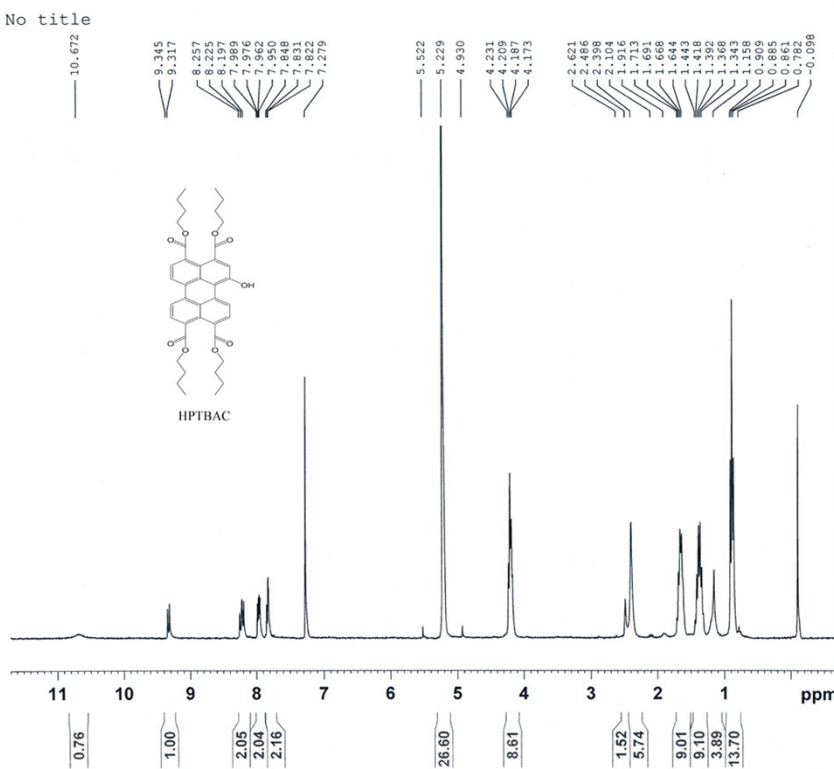


¹³C-NMR spectrum of NPTBAC.



FTIR spectrum of NPTBAC.

No title



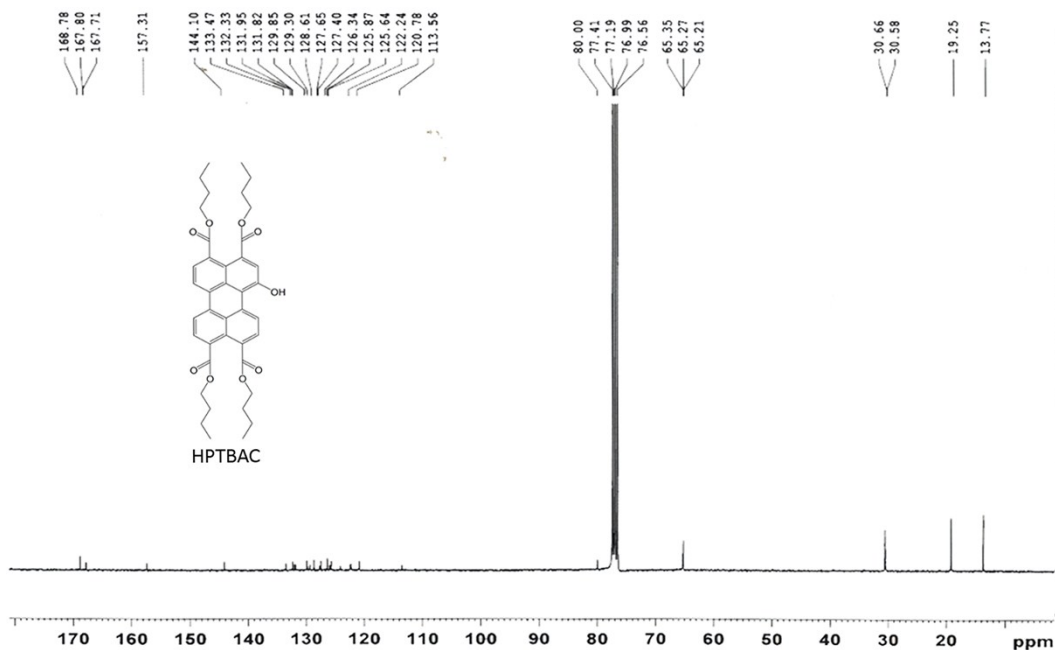
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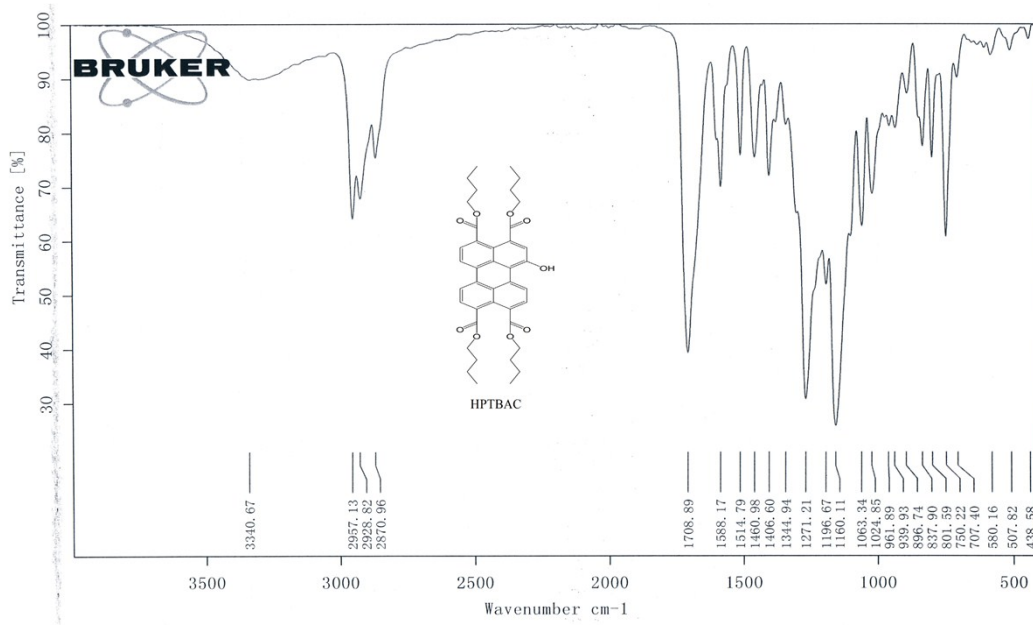
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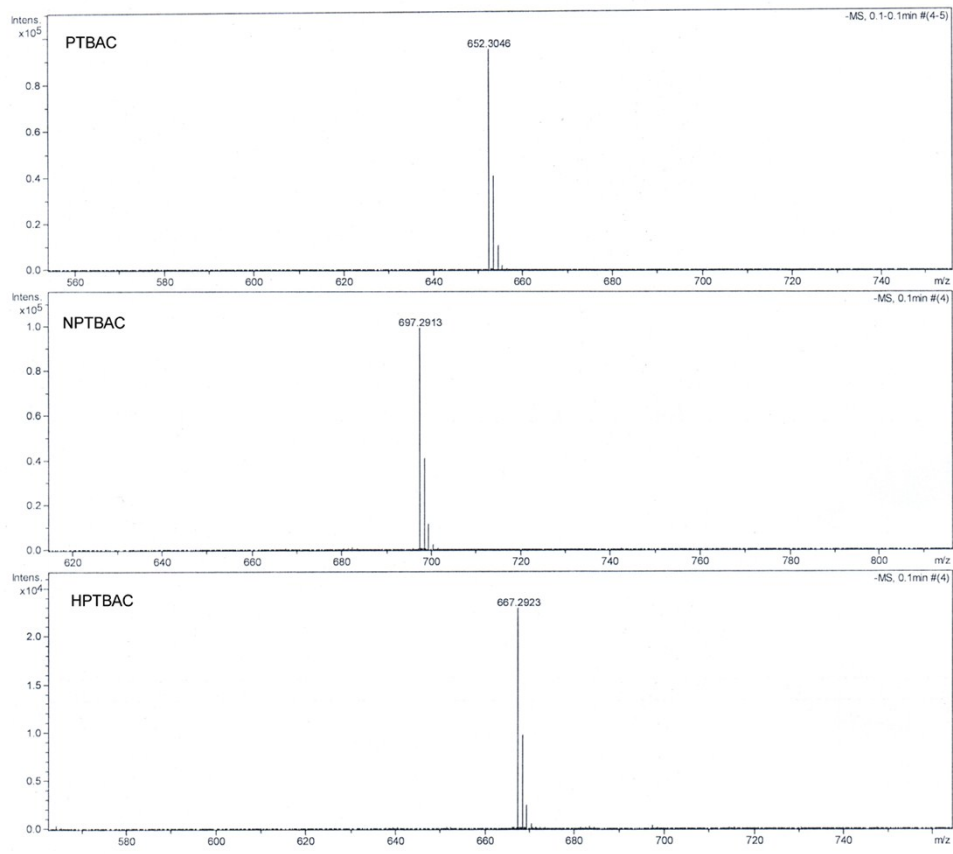
¹H-NMR spectrum of HPTBAC.



¹³C-NMR spectrum of HPTBAC.

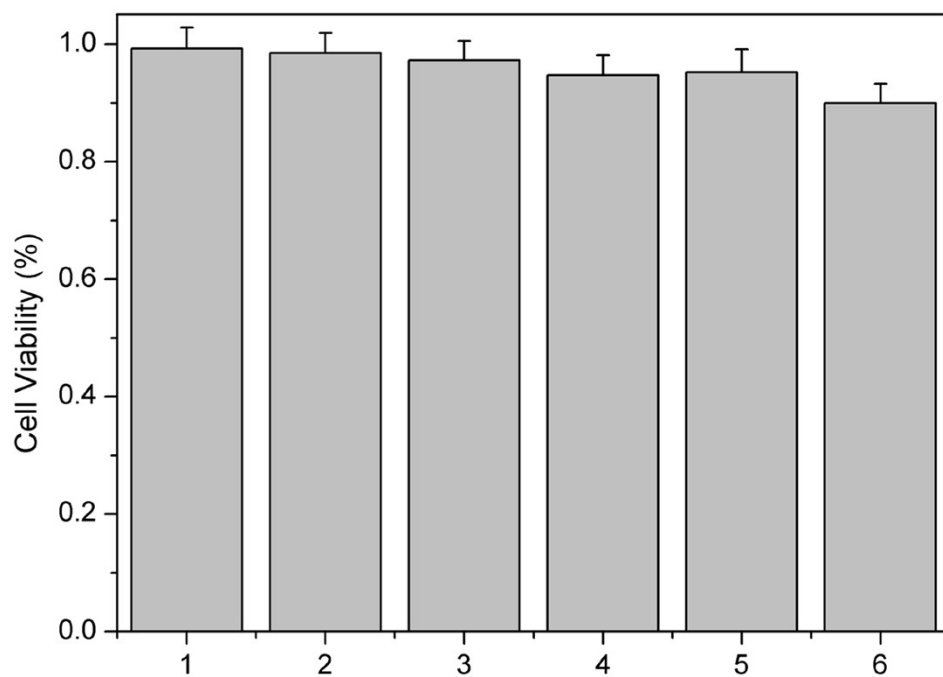


FTIR spectrum of HPTBAC.



MS Spectra of PTBAC, NPTBAC and HPTBAC.

Cell cytotoxic effect of HPTBAC on Human Lung Cancer A549 Cells.



Cell cytotoxic effect of HPTBAC on Human Lung Cancer A549 Cells. 1, control; 2, 0.01 μM; 3, 0.1 μM; 4, 1 μM; 5, 10 μM; 6, 50 μM. Data are expressed as mean values standard error of the mean of five independent experiments.