Supporting Information

Fine tuning of pyridinium-functionalized dibenzo[a,c]phenazine near-infrared AIE fluorescence biosensor for detection of lipopolysaccharide, bacterial imaging and photodynamic antibacterial therapy

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[b]*Department of Oncology, Shanghai Medical College, Fudan University, Shanghai 200032, P. R. China. E-mail: neck130@hotmail.com*

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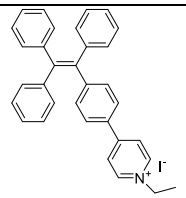
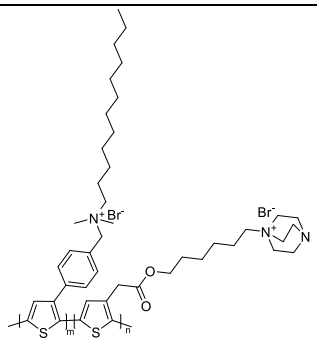
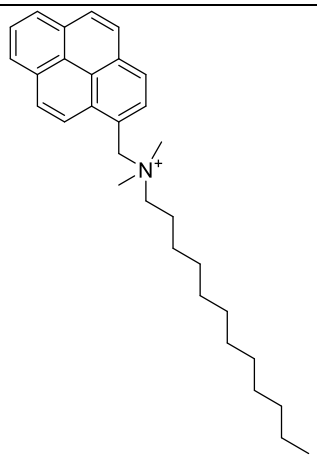
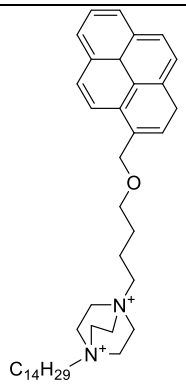
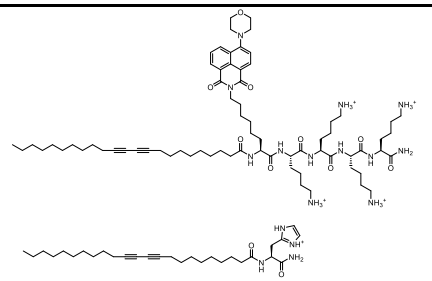
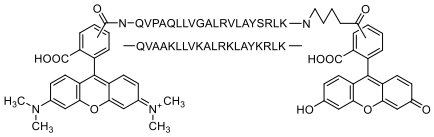
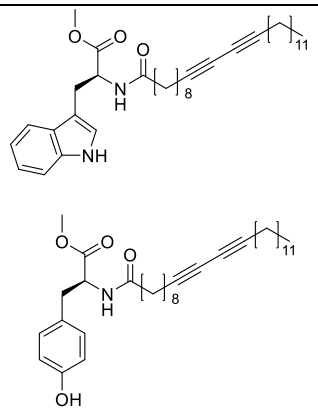
Table S1 The reported work previously

Probe structure	Fluorescence change	Range of linear correlation	LOD	Time	Ref.
	Turn-on 515 nm	0-0.5 μM	4 nM	immediately	1
	Ratiometric 566 nm to 600 nm	0.3-30 μM	270 pM	Not mentioned	2
	Turn-on 486 nm	0.1-1.5 μM	100 nM	Upon addition	3
Magnetic-nano-particals	Turn-On 539 nm	2–20 μM	280 ng mL^{-1}	15 min	4
gold nanoparticles	Turn-on 519 nm			10 min	5
	Ratiometric 395 nm to 489 nm	1.3–68 μM	0.068 μM		6

	Turn-on 515 nm				7
	Turn-on 588 and 520 nm of sensors 1 and 2	0.5-1.5 μM	about 0.5 μM		8
					9

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2. M. Lan, J. Wu, W. Liu, W. Zhang, J. Ge, H. Zhang, J. Sun, W. Zhao and P. Wang, *J Am Chem Soc*, 2012, **134**, 6685-6694.

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7. J. Wu, A. Zawistowski, M. Ehrmann, T. Yi and C. Schmuck, *J. Am. Chem. Soc.*, 2011, **133**, 9720-9723.

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UV-Vis absorption spectra of ABDA/RB mixture under light irradiation

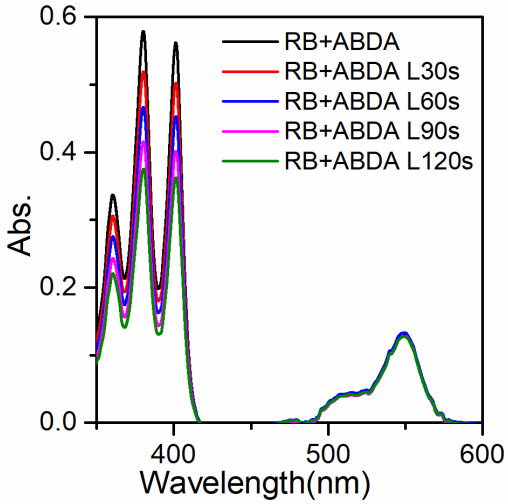


Fig. S1 UV-Vis absorption spectra of ABDA/RB mixture in DMSO and PBS mixtures (99.8% PBS in volume) under 530nm light irradiation.

Agar plates containing 0-50 μM BD2C plated with bacteria

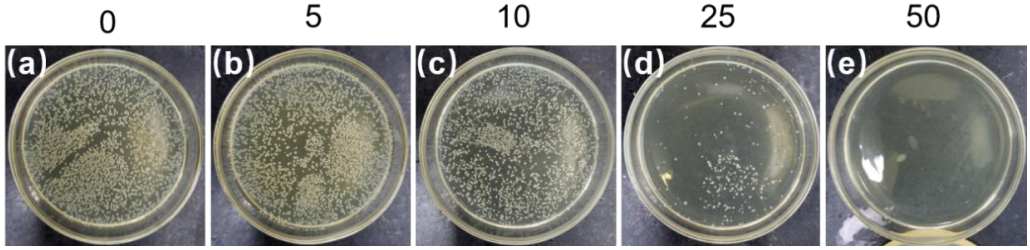


Fig. S2 Agar plates containing 0-50 μM **BD2C** plated with bacteria.

Cell viability of RAW264.7 incubated with 0-20 μM of BD2C\BD8C\BD16C for 24h

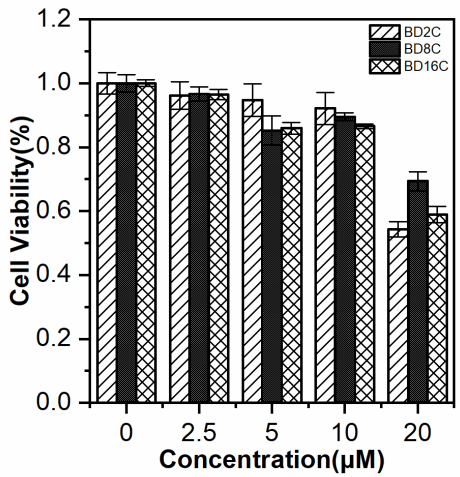
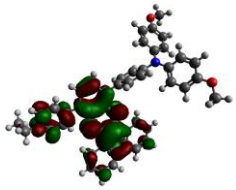
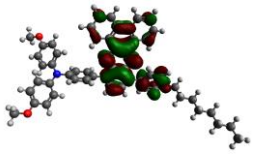
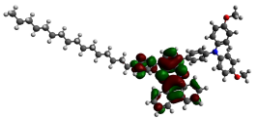
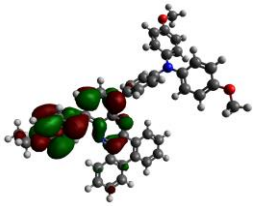
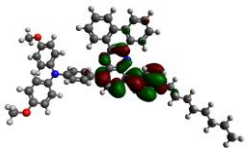
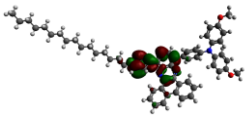
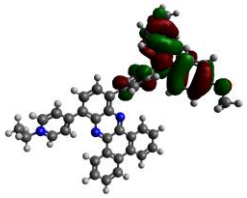
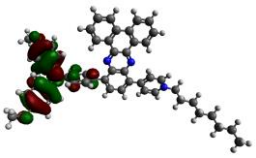
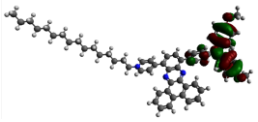
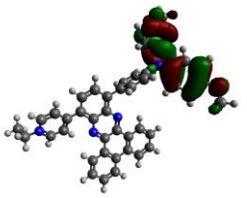
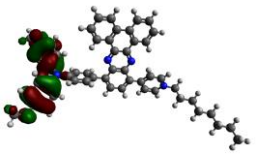
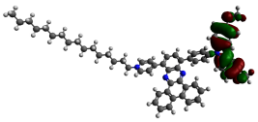


Fig. S3 The cell viability of RAW264.7 incubated with 0-20 μM of **BD2C\BD8C\BD16**C for 24h.

Original molecular orbital distributions and energy optimized of BD2C/BD8C/BD16C in vacuum

Table S2. Molecular orbital distributions and energy optimized in vacuum (isodensity=0.020 a.u.).

	BD2C	BD8C	BD16C
LUMO+1	 -3.44 eV	 -3.36 eV	 -3.36 eV
LUMO	 -4.79eV	 -4.69eV	 -4.69eV
HOMO	 -6.98eV	 -6.96eV	 -6.96eV
HOMO-1	 -8.52eV	 -8.54eV	 -8.52eV

BD2C $S_1 = 1.1724$ $T_1 = 1.1128$ $T_2 = 1.6835$

BD8C $S_1 = 1.2464$ $T_1 = 1.1541$ $T_2 = 1.7387$

BD16C $S_1 = 1.2495$ $T_1 = 1.1560$ $T_2 = 1.7410$

Calculation Methodology

Geometry optimizations were carried out on the molecules 2C in the gas phase, using the software Avogadro [1] to enter the starting geometry. The molecules were distorted to form a variety of conformers which were then allowed to optimize, in order to find the global minimum on the potential energy surface. Frequency calculations were performed on all the optimized geometries to distinguish whether they were minima or transition states on the potential energy surfaces. Where transition state geometries were found, the bond lengths and angles were distorted in the direction of the vibration and the structure was reoptimised until only positive frequencies were obtained. All calculations were carried out using the Gaussian 09 program [2] with the CAM-B3LYP functional [3] and the standard 6-31G(d) basis set.

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2. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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Original spectral date.

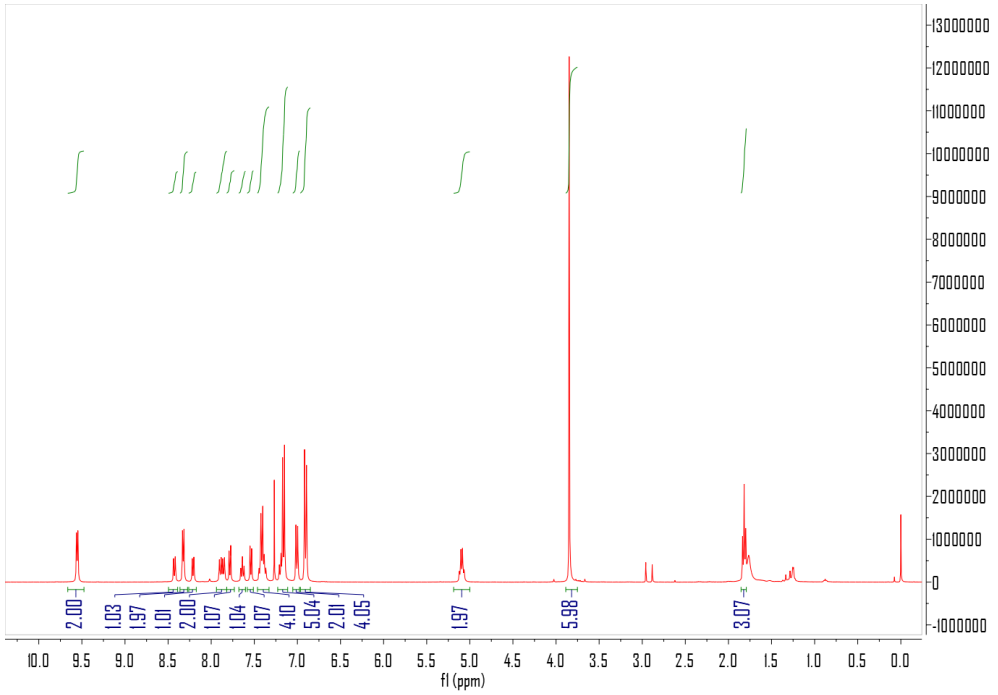


Fig. S3 ^{1}H NMR spectrum of **BD2C** in $CDCl_3$

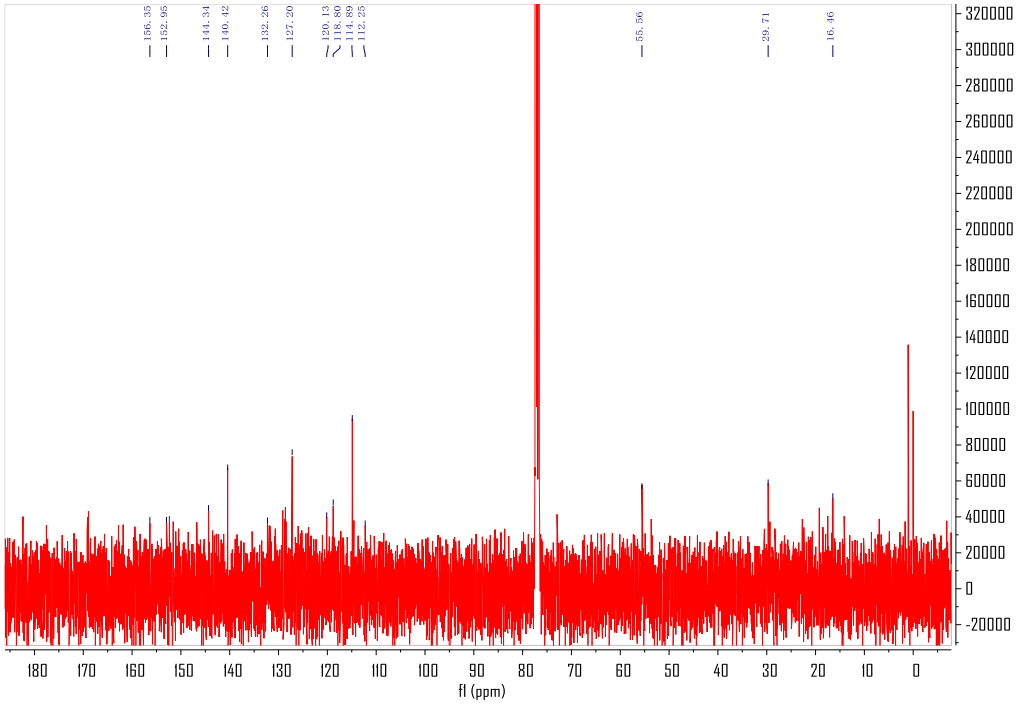
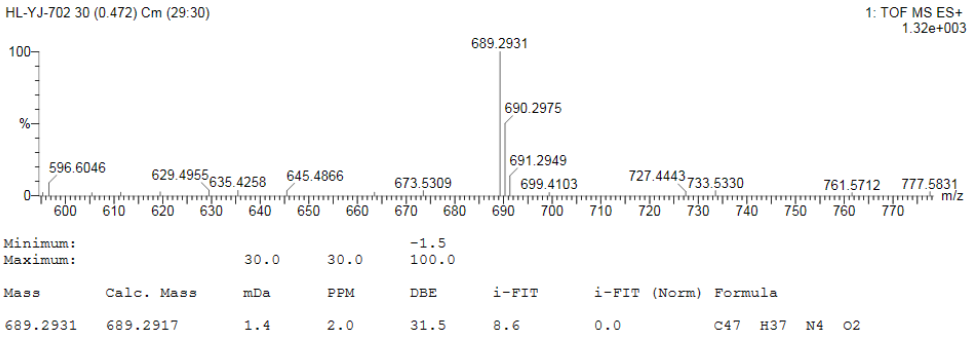


Fig. S4 ^{13}C NMR spectrum of **BD2C** in $CDCl_3$



Minimum:				-1.5			
Maximum:		30.0	30.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
689.2931	689.2917	1.4	2.0	31.5	8.6	0.0	C47 H37 N4 O2

Fig. S5 HR mass spectrum of **BD2C**

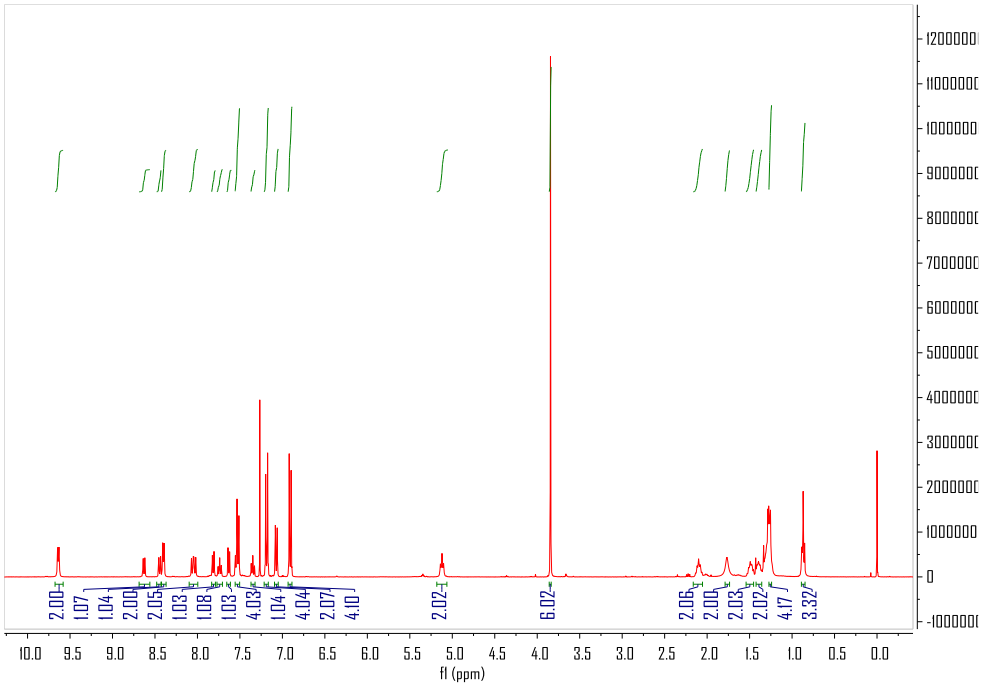


Fig. S6 ^{1}H NMR spectrum of **BD8C** in $CDCl_3$

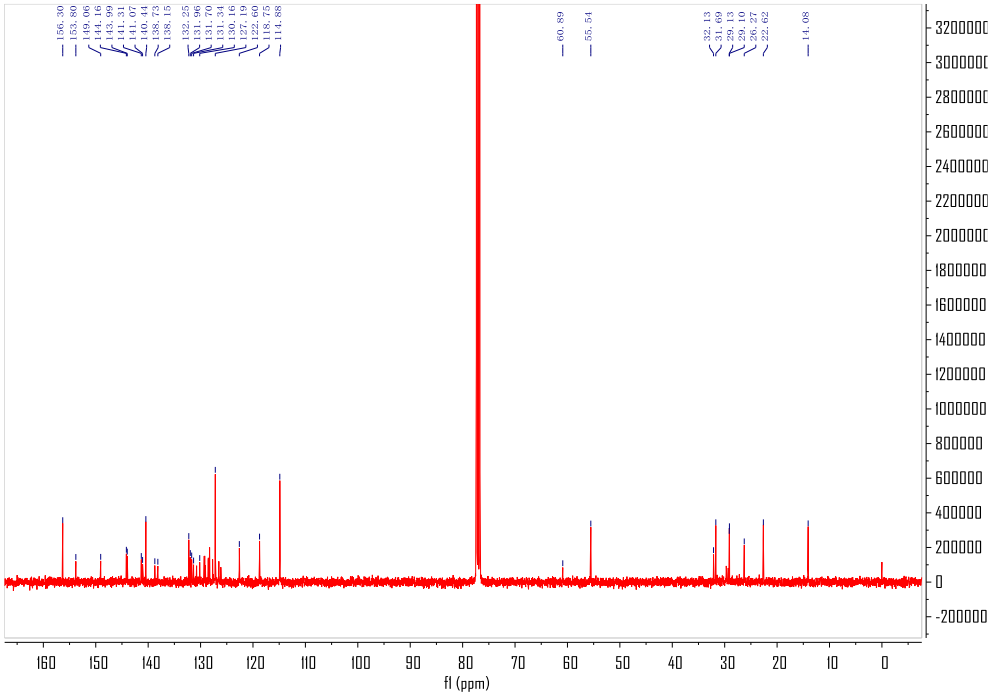


Fig. S7 ^{13}C NMR spectrum of **BD8C** in $CDCl_3$

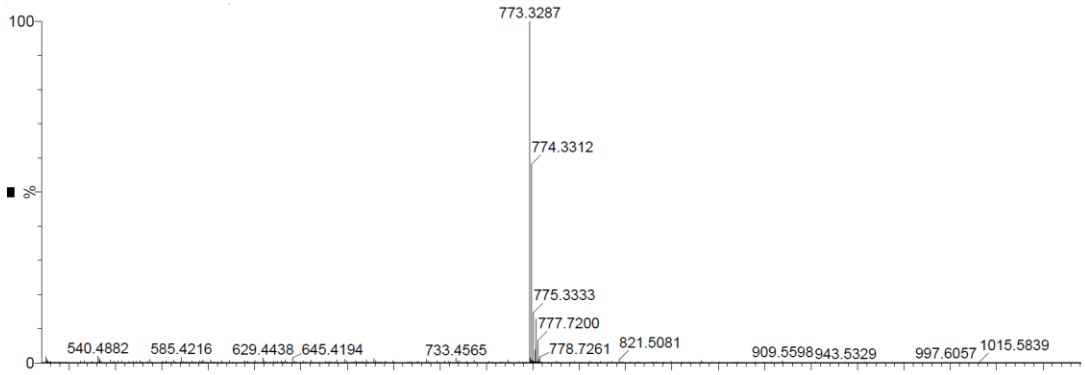


Fig. S8 HR mass spectrum of **BD8C**

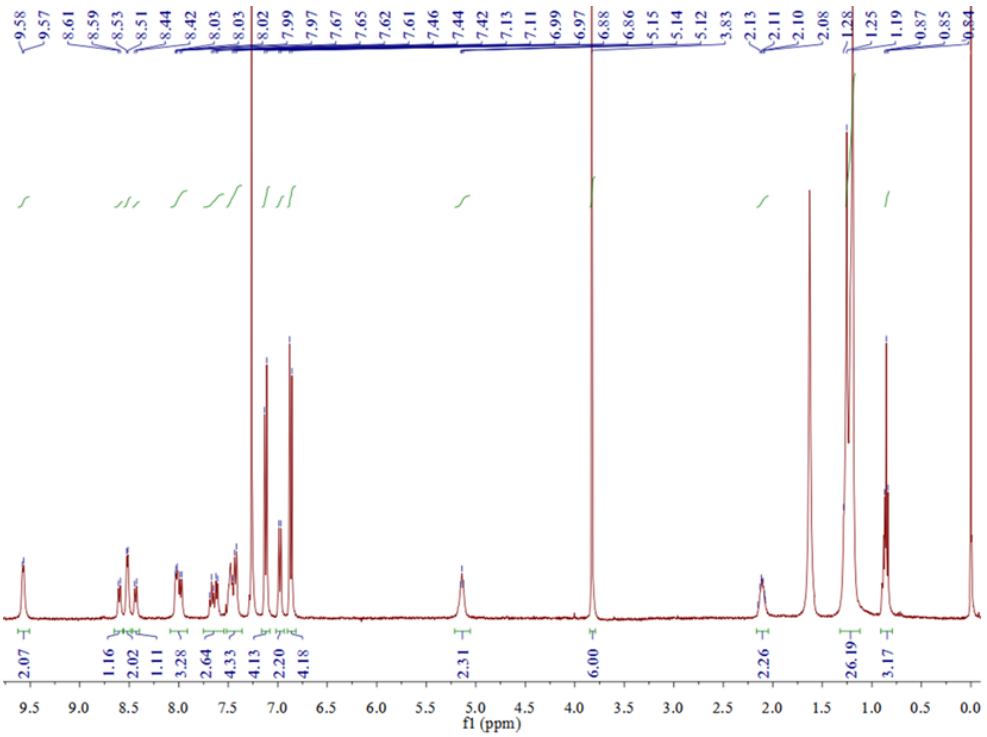


Fig. S9 ^{1}H NMR spectrum of **BD16C** in $CDCl_3$

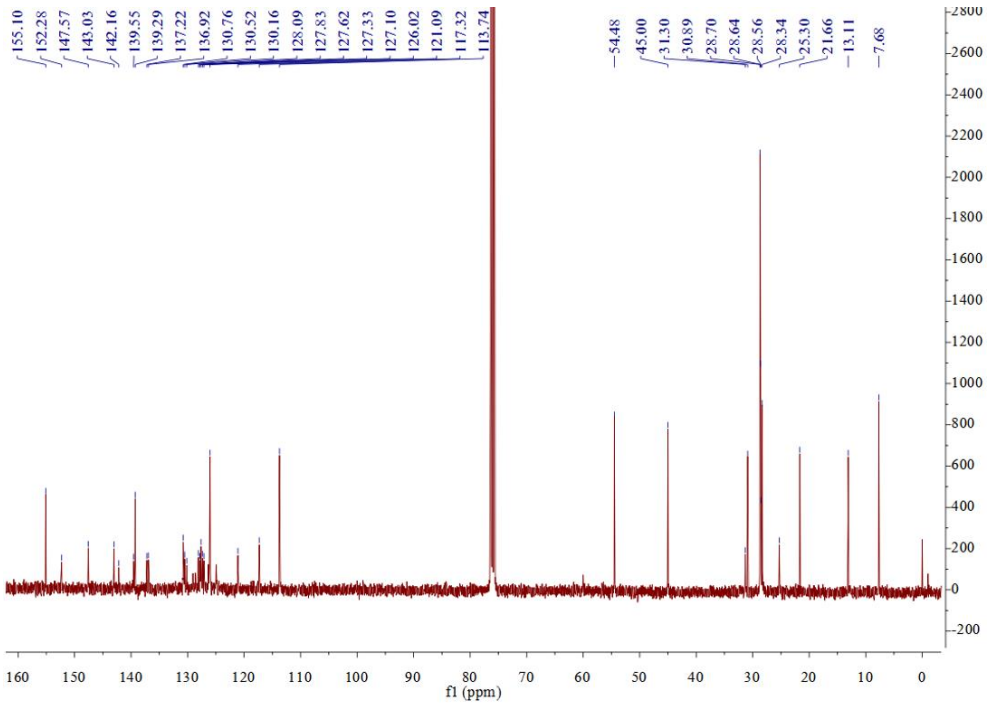


Fig. S10 ^{13}C NMR spectrum of **BD16C** in $CDCl_3$

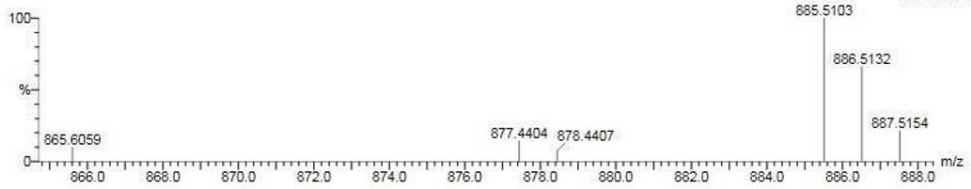
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-61 H: 0-66 N: 0-4 O: 0-2

JL-HUA ECUST institute of Fine Chem 23-Jun-2015 13:15:12

HL-JT-303 220 (1.464) Cm (220:225) 1: TOF MS ES+ 2.11e+003



Minimum:				-1.5			
Maximum:		300.0	50.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
885.5103	885.5102	-0.5	-0.6	31.5	9.3	0.0	C61 H65 N4 O2

Fig. S11 HR mass spectrum of **BD16C**