Supporting Information for:

Simple Biphenyl or Carbazole Derivatives with Four Di(anisyl)amino Substituents as Efficient Hole-Transporting Materials for Perovskite Solar Cells

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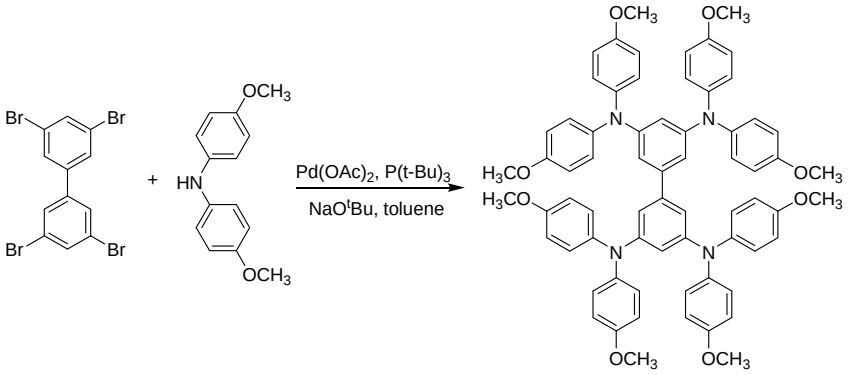
Note added after first publication: This version of the ESI replaces that published on 26 September, 2016. In the original version of the ESI, an incorrect CCDC number was given.

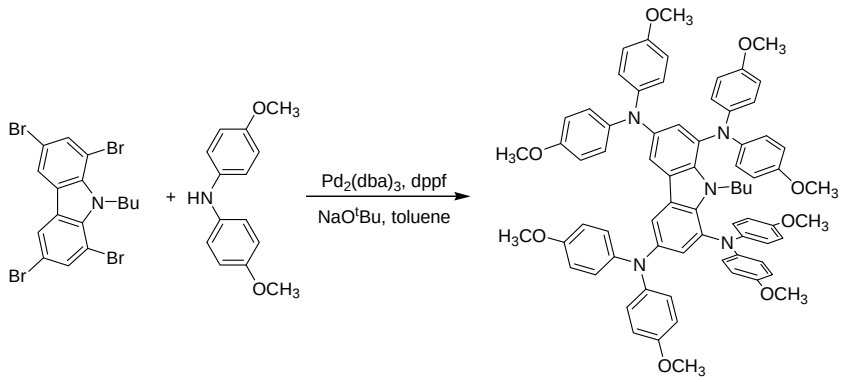
Synthesis

NMR spectra were recorded in the designated solvent on Bruker Avance 400 MHz spectrometer. Spectra are reported in ppm values from residual protons of deuterated solvent. Mass data were obtained with a Bruker Daltonics Inc. Apex II FT-ICR or Autoflex III MALDI-TOF mass spectrometer. The matrix for MALDI-TOF measurement is α-cyano-4-hydroxycinnamic acid. Microanalysis was carried out using Flash EA 1112 or Carlo Erba 1106 analyzer at the Institute of Chemistry, Chinese Academy of Sciences.



TDAB

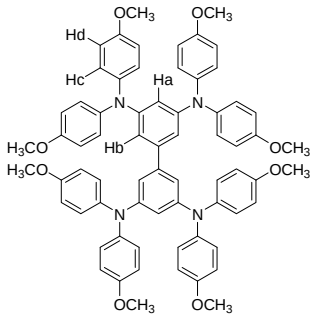
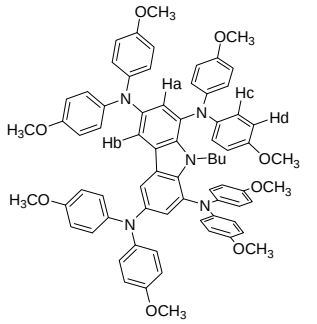
A suspension of 3,3',5,5'-tetrabromo-1,1'-biphenyl (186 mg, 0.40 mmol), di-p-anisylamine (458 mg, 2.0 mmol), [$Pd(OAc)_2$] (18 mg, 0.080 mmol), $P(t\text{-}Bu)_3$ (16 mg, 0.080 mmol), and NaO^tBu (192 mg, 2.0 mmol) in toluene (10 mL) was heated at 140 ^oC for 18 h under a N_2 atmosphere. The system was then cooled to room temperature and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography (eluent: ether/ethyl acetate, 2/1) to yield 292 mg of 3,3',5,5'-tetrakis(di-p-anisylamino)-1,1'-biphenyl (**TDAB**) in 69% yield. ^1H NMR (400 MHz, CD_2Cl_2): δ 3.78 (s, 24H), 6.33 (s, 4H), 6.36 (s, 2H), 6.75 (d, J = 8.0 Hz, 16 H), 6.95 (d, J = 8.0 Hz, 16 H) (Table S1). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 56.03, 112.3, 112.6, 115.1, 126.9, 141.4, 143.6, 149.9, 156.4. MALDI-TOF-MS: m/z 1062.6 for $[M]^+$. HRMS-MALDI-TOF calcd for $C_{68}H_{62}N_4O_8$: 1062.4562. Found: 1062.4543. HPLC analysis shows a purity of 98.2% of the obtained **TDAB** sample (Fig. S1).



TDAC

A suspension of 1,3,6,8-tetrabromo-9-butyl-carbazole (100 mg, 0.19 mmol), di-p-anisylamine (266 mg, 1.16 mmol), [$Pd_2(dba)_3$] (27 mg, 0.029 mmol), dppf (16 mg, 0.029 mmol), and NaO^tBu (111 mg, 1.16 mmol) in toluene (10 mL) was heated at 140 ^oC for 48 h under a N_2 atmosphere in a sealed pressure tube. The system was then cooled to room temperature and the solvent was removed under vacuum. The crude product was purified by silica gel chromatography (eluent: ether/ethyl acetate, 2/1) to yield 109 mg of 1,3,6,8-tetrakis(di-p-anisylamino)-9-butyl-9H-carbazole (**TDAC**) in 51% yield. ^1H NMR (400 MHz, CD_2Cl_2): δ 0.64 (t, J = 6.8 Hz, 3H), 0.92 (m, 4H), 3.76 (s, 24 H), 4.16 (t, J = 8.2 Hz, 2H), 6.73 (m, 16H), 6.84 (d, J = 7.6 Hz, 10H), 6.93 (d, J = 7.6 Hz, 8H), 7.34 (s, 2H) (Table S1). MALDI-TOF-MS: m/z 1131.7 for $[M]^+$. HRMS-MALDI-TOF calcd for $C_{72}H_{69}N_5O_8$: 1131.5141. Found: 1131.5143. No satisfactory ^{13}C NMR spectrum was obtained for **TDAC** because this compound was readily oxidized in deuterated solvents such as $CDCl_3$, CD_2Cl_2, D_6-acetone, and D_6-DMSO. HPLC analysis shows a purity of 97.7% of the obtained **TDAC** sample (Fig. S1).

Table S1. ^{1}H NMR spectra assignment.

	H_{CH3}	3.78 (s, 24H)
	H_a	6.36 (s, 2H)
	H_b	6.33 (s, 4H)
	H_c and H_d	6.75 (d, J = 8.0 Hz, 16 H); 6.95 (d, J = 8.0 Hz, 16 H)
	H_{Bu}	0.64 (t, J = 6.8 Hz, 3H), 0.92 (m, 4H), 4.16 (t, J = 8.2 Hz, 2H)
	H_{OCH3}	3.76 (s, 24 H)
	H_a	7.34 (s, 2H)
	H_b, H_c, H_d	6.73 (m, 16H), 6.84 (d, J = 7.6 Hz, 10H), 6.93 (d, J = 7.6 Hz, 8H)

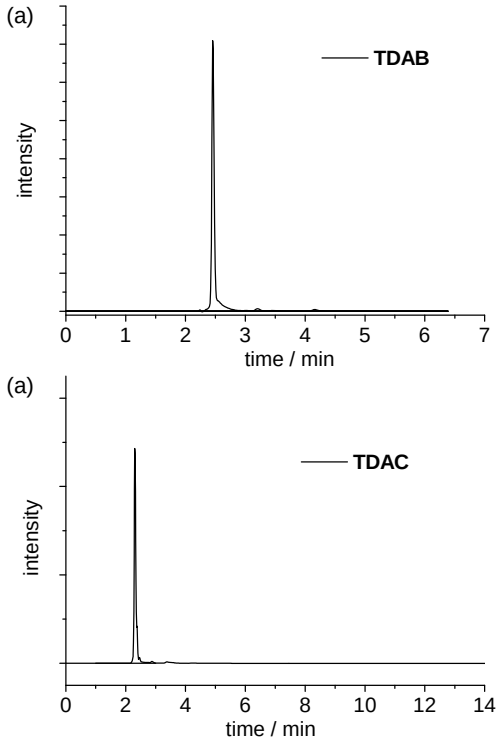


Fig. S1. HPLC spectra of (a) TBAB (98.2%) and (b) TBAC (97.7%).

Computational Methods.

DFT calculations are carried out using the B3LYP exchange correlation functional[1] and implemented in the *Gaussian* 09 package.[2] The electronic structures of complexes were determined using 6-31G* all atoms. No symmetry constraints were used in the optimization (nosymm keyword). Solvation effects in CH_2Cl_2 were included for all calculations using the conductor-like polarizable continuum model (CPCM).[3] Frequency calculations have been performed with the same level of theory to ensure the optimized geometries to be local minima. All orbitals have been computed at an isovalue of 0.02 e/bohr^3. TDDFT calculations were performed on the same level of theory.

[1] Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[2] Gaussian 09, Revision A.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[3] Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669.

Table S2. TDDFT results.[a]

	S_n	E/eV	E/nm	f	dominant transitions (percent contribution[b])
TDAB	2	4.00	309	0.181	HOMO-1 → LUMO (40%); HOMO → LUMO (32%)
	5	4.40	282	0.2572	HOMO → LUMO+1 (31%)
	6	4.46	278	0.2399	HOMO-2 → LUMO+1 (33%)
	7	4.51	275	0.3549	HOMO-1 → LUMO+3 (18%); HOMO-1 → LUMO+1 (12%)
	8	4.56	271	0.2335	HOMO-3 → LUMO+3 (15%); HOMO-2 → LUMO+3 (10%)
	9	4.59	269	0.2125	HOMO-2 → LUMO+4 (19%); HOMO → LUMO+7 (12%)
	10	4.61	268	0.3011	HOMO-1 → LUMO+7 (15%); HOMO-1 → LUMO+10 (10%)
TDAC	1	3.47	357	0.1519	HOMO → LUMO (87%)
	2	3.87	320	0.2022	HOMO-1 → LUMO (70%)
	3	4.13	300	0.1983	HOMO-2 → LUMO (38%)
	4	4.17	298	0.4816	HOMO-2 → LUMO (25%); HOMO → LUMO+1 (24%)
	5	4.27	290	0.2403	HOMO-3 → LUMO (41%)
	7	4.40	282	0.1274	HOMO-1 → LUMO+4 (20%); HOMO → LUMO+2 (27%)
	8	4.42	281	0.1187	HOMO-3 → LUMO+1 (21%)
	9	4.44	279	0.1979	HOMO-3 → LUMO (16%); HOMO-2 → LUMO+3 (15%)
	10	4.50	275	0.2546	HOMO-1 → LUMO+7 (30%); HOMO → LUMO+7 (34%)

[a] The involved molecular orbitals are shown in Fig. S2 and S3.

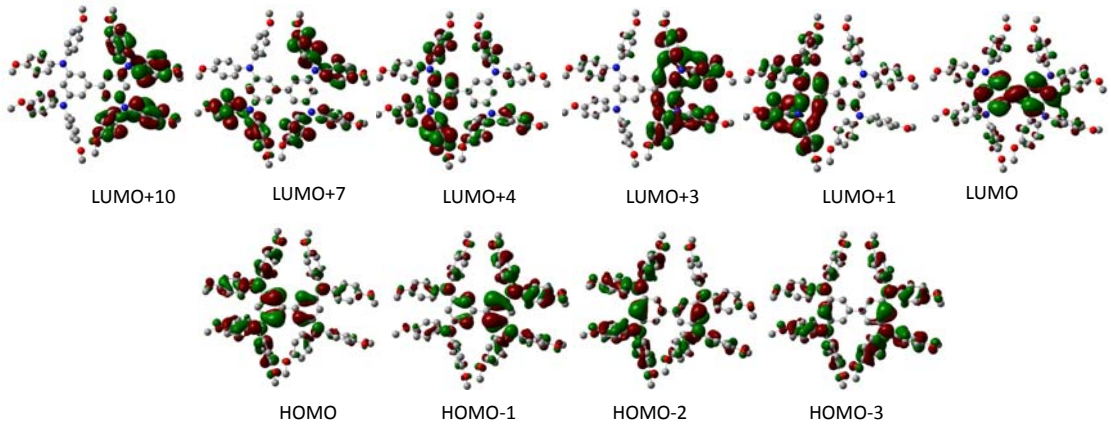


Fig. S2 Isodensity plots of selected frontier orbitals of **TDAB**.

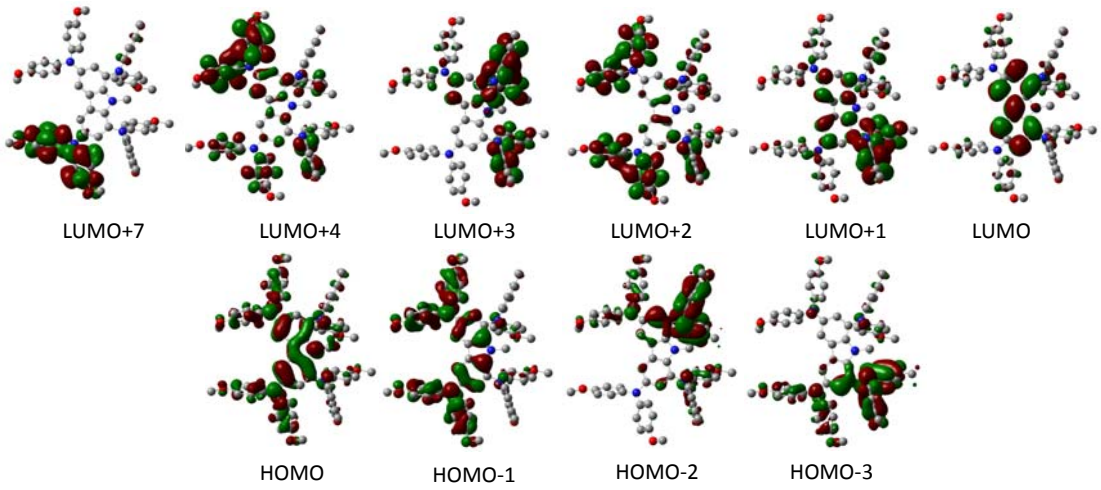


Fig. S3 Isodensity plots of selected frontier orbitals of **TDAC**.

Electrochemical Measurement

All cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were taken using a CHI 660D potentiostat with one-compartment electrochemical cell under an atmosphere of nitrogen. All measurements were carried out in 0.1 M of Bu_4NClO_4 in dichloromethane. The scan rate for CV measurement is 100 mV/s. The working electrode was a glassy carbon with a diameter of 3 mm. The electrode was polished prior to use with 0.05 μm alumina and rinsed thoroughly with water and acetone. A large area platinum wire coil was used as the counter electrode. All potentials are referenced to a Ag/AgCl electrode in saturated aqueous NaCl without regard for the liquid junction potential.

Spectroscopic Measurements

UV-Vis and NIR spectra were recorded on a TU-1810DSPC spectrophotometer at room temperature in dichloromethane, with a conventional 1 cm quartz cell. Emission spectra were recorded using an F-380 spectrofluorimeter of Tianjin Gangdong Sic. & Tech Development Co. Ltd., with a red-sensitive photomultiplier tube R928F.

Fabrication of the perovskite solar cells

Substrates are fluorine-doped tin oxide conducting glass (FTO, Pilkington, thickness: 2.2 mm, sheet resistance 14 Ω/square). Patterned FTO glass was first rinsed with mild detergent, then distilled water for several times and subsequently with ethanol in an ultrasonic bath, finally dried under air stream. For fabricating the device, 30 nm-thickness TiO_2 compact layer and 150 nm-thickness mesoporous TiO_2 anatase compact layer were deposited on FTO glass by spinning coating method in sequence by following the previous work.[4] The perovskite layer was prepared by spin-coating the mixed-cation precursor consisting of PbI_2, $PbBr_2$, formamidinium iodide (FAI) and methylammonium bromide (MABr) according to the literature.[5] Total concentration of PbI_2 and $PbBr_2$ is 1.35 M. Molar ratio of PbI_2 to $PbBr_2$ is 85:15. The concentration of MABr equals to $PbBr_2$ and the concentration of FAI is 95% of PbI_2. The mixture is dissolved in the mixed solvent of DMF and DMSO with the volume ratio of 4:1. The precursor is continuously spin-coated on

[4] Zhu, L.; Shi, J.; Lv, S.; Yang, Y.; Xu, X.; Xu, Y.; Xiao, J.; Wu, H.; Luo, Y.; Li, D. *Nano Energy* **2015**, *15*, 540.

[5] Bi, D.; Tress, W.; Dar, M. I.; Gao, P.; Luo, J.; Renevier, C.; Schenk, K.; Abate, A.; Giordano, F.; Baena, J.-P. C.; Decoppet, J.-D.; Zakeeruddin, S. M.; Nazeeruddin, M. K.; Grätzel, M.; Hagfeldt, A. *Sci. Adv.* **2016**, *2*, e1501170.

mesoporous TiO_2 films at 1000 and 5000 rpm for 10 and 30 s. In the second spin coating step, 110 μL of chlorobenzene is dropped on the substrate to give the perovskite film after 15 s. The obtained-perovskite layer is heated at 150 °C for 10 min and 100 °C for 40 min. After that, the HTM solution in chlorobenzene consisting of 60 mg/mL of TDAB, TDAC, or spiro-OMeTAD, 30 mM of lithium bis(trifluomethanesulfonyl)imide (LiTFSI), 35 μL of *tert*-butylpyridine, and 55 mM of tris(2-(1H-pyrazol-1-yl)-4-tert-butylpyrine)-cobalt(III) tris(trifluomethyl-sulfonyl)imide (FK209) was spin-coated (3000 rpm for 20 s; about 150 nm thick) on the top of the perovskite layer. All the precursor preparation and spin-coating processes are carried out in the glove box filled with nitrogen. Finally, 80 nm-thickness Au photocathode was deposited by thermal evaporation under the vacuum of 10^{-7} Torr.

Device measurements

The cells were illuminated under 100 $mW \cdot cm^{-2}$ (AM 1.5G) by an Oriel solar simulator 91192, and the JV characteristics of the cells were recorded on Princeton Applied Research, Model 263A. For J-V characteristics, a mask with a window of 0.10 cm^2 was clipped on the TiO_2 side to define the active area of the cell. Photoluminescence spectra were obtained on a PL Spectrometer (Edinburgh Instruments, FLS 900), excited with a picosecond pulsed diode laser (EPL-445). Electrochemical impedance spectra (EIS) of the perovskite solar cells were performed on a ZAHNER IM6e electrochemical workstation in the dark in the frequency ranging from 5 to 10^6 Hz with a perturbation amplitude of 10 mV. The obtained impedance spectra were fitted with *Zview* software based on appropriate equivalent circuit.

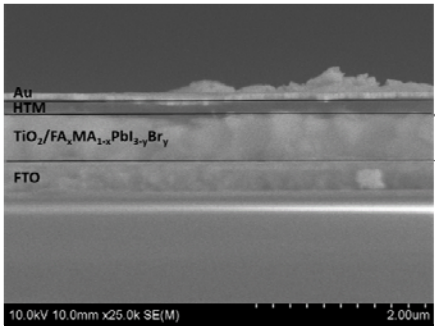


Fig. S4 Cross sectional SEM image of the perovskite solar cell.

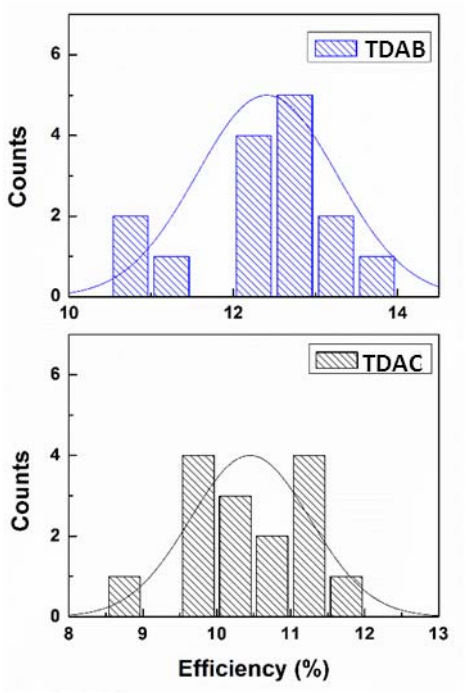
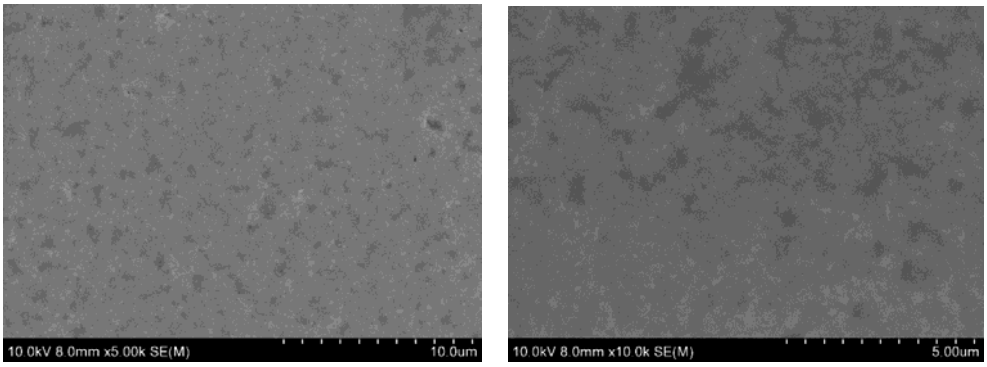


Fig. S5 Histograms of PCEs measured for total 15 devices for each HTM.



(a) (b)

Fig. S6 Top-view of the SEM images of (a) **TDAB** film and (b) **TDAC** film.

Table S3. PL lifetimes of $Al_2O_3/FA_xMA_{1-x}PbI_{3-y}Br_y$/HTM films.[a]

HTM	τ_1 (ns)	A_1	τ_2 (ns)	A_2	$\tau_{Average}$ (ns)
TDAB	3.35	0.55	29.54	0.46	26.41
TDAC	4.80	0.49	36.98	0.35	32.03
Spiro-OMeTAD	4.14	0.50	25.39	0.44	22.1

[a]The time-resolved PL spectra are well fitted with a bi-exponential model:

$$\tau = \frac{A_1\tau_1^2 + A_2\tau_2^2}{A_1\tau_1 + A_2\tau_2}$$

X-ray Crystallography

The X-ray diffraction data were collected using a Rigaku Saturn 724 diffractometer on a rotating anode (Mo-K radiation, 0.71073 Å) at 173 K. The structure was solved by the direct method using SHELXS-97[6] and refined with Olex2.[7] The structure graphics were generated using Olex2.

Crystallographic data for **TDAB** (CCDC No. 1507223):

$C_{68}H_{62}N_4O_8$, M = 1063.22, monoclinic, space group C 1 2/c 1, a = 31.847(6), b = 18.611(3), c = 9.5547(18) Å, α = 90º, β = 101.296(3)º, γ = 90º, U = 5553.5(18) Å^3, T = 173 K, Z = 4, 13102 reflections measured, radiation type MoK-a, radiation wavelength 0.71073 Å, final R indices R1 = 0.0978, wR2 = 0.2188, R indices (all data) R1 = 0.1241, wR2 = 0.2384.

[6] Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.

[7] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339.

Cartesian coordinates of DFT-optimized structure of **TDAB**:

Charge = 0; multiplicity = 1

C	-3.49928534	-2.00949522	0.27268156
C	-2.12008792	-2.01976727	0.04473778
C	-1.38005031	-0.84059954	0.12024474
C	-2.02769980	0.36331005	0.39571392
C	-3.41190968	0.39304651	0.59301771
C	-4.14070442	-0.79775450	0.53798126
H	-1.63024251	-2.95155618	-0.20726489
H	-1.45493721	1.27745715	0.49173224
H	-5.20945485	-0.78064252	0.70697890
C	0.09595812	-0.87266972	-0.06404768
C	0.75631767	0.18834186	-0.68146288
C	0.82047816	-1.98172319	0.37250929
C	2.14633866	0.15649465	-0.83284589
H	0.19331806	1.02841683	-1.06909742
C	2.21013947	-2.02878294	0.22214703
H	0.30494572	-2.80291698	0.85220882
C	2.86715373	-0.94309104	-0.36340976
H	3.94528830	-0.95200063	-0.45443365
N	2.94259349	-3.13711066	0.68551566
N	2.82122469	1.22850045	-1.44977022
N	-4.23249318	-3.21147536	0.22209677
C	4.16618038	-3.52471823	0.07359744
C	5.26079536	-3.88230638	0.86847613
C	4.30364281	-3.58515789	-1.31075267
C	6.44937889	-4.29298697	0.29273735
H	5.16929468	-3.84064674	1.94885269
C	5.50420429	-3.97353193	-1.89999576
H	3.46389974	-3.31791873	-1.94332124
C	6.58350008	-4.33699052	-1.09753491
H	7.29826641	-4.57434481	0.90690961
H	5.57523533	-4.00087233	-2.98024960
C	2.38463052	-4.00013410	1.67269317
C	2.21104038	-5.35646584	1.41821831
C	1.99476734	-3.49588946	2.91798845
C	1.65541423	-6.20384070	2.37373945
H	2.51111940	-5.76002921	0.45655598
C	1.42102020	-4.32376893	3.86541682
H	2.13340307	-2.44117006	3.13194941
C	1.24416611	-5.68506660	3.59961963
H	1.52655693	-7.25320670	2.14005720
H	1.10874059	-3.93681746	4.82961176
C	2.33225828	2.55804449	-1.33310943

C	2.22008267	3.37248563	-2.45591616
C	1.97821670	3.08775878	-0.08637329
C	1.78700351	4.69177609	-2.35095045
H	2.48481634	2.97466291	-3.43002913
C	1.52532747	4.38994701	0.02471825
H	2.06162220	2.46809017	0.80021009
C	1.43817183	5.20843887	-1.10522334
H	1.71937304	5.29625092	-3.24666929
H	1.25248438	4.80394458	0.98970868
C	4.00278656	1.00219052	-2.20709848
C	4.05600633	0.00247572	-3.17495348
C	5.13846038	1.79346986	-2.00204335
C	5.21373021	-0.22507151	-3.91435450
H	3.18149234	-0.61489041	-3.35156229
C	6.28522536	1.59095065	-2.74859370
H	5.11373871	2.57635043	-1.25128468
C	6.33506830	0.57579996	-3.70742610
H	5.21916905	-1.01515117	-4.65499720
H	7.16640634	2.20465406	-2.59404411
N	-4.06421340	1.60949941	0.87418961
C	-5.20238790	1.64437460	1.72630627
C	-6.35756875	2.33092012	1.33689384
C	-5.19023376	1.01454240	2.96780875
C	-7.46018681	2.38823963	2.17025387
H	-6.38257704	2.82626375	0.37185978
C	-6.30337836	1.04618914	3.80346757
H	-4.29974895	0.48317256	3.28696726
C	-7.44485189	1.74111154	3.40882584
H	-8.35672087	2.92185733	1.87282156
H	-6.25907876	0.53986464	4.75961617
C	-3.57384855	2.83528511	0.34788248
C	-3.42065927	3.94891180	1.16825333
C	-3.26211436	2.96042336	-1.01147669
C	-2.98861194	5.16968921	0.65602206
H	-3.65246477	3.86719184	2.22500601
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H	-3.37840316	2.10381075	-1.66700714
C	-2.68261204	5.28286699	-0.69813252
H	-2.88909361	6.01517716	1.32495758
H	-2.57263704	4.26347326	-2.57855396
C	-5.58952328	-3.22288470	-0.20103781
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C	-7.88431931	-3.94377581	0.11693609

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C	-2.90357472	-4.55141858	1.79191215
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O	7.51088284	0.44976470	-4.38130924
O	1.01941889	6.48511698	-0.88851956
O	0.65881575	-6.41241231	4.58883679
O	-1.82165498	-8.00637007	1.77500546
O	-8.58105450	1.84569170	4.15012754
O	-2.27026199	6.43003953	-1.30326550
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C	-10.54194900	-3.93127181	-0.82447198
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H	-11.46512454	-3.78015708	-1.38387727
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H	0.63937342	8.32242589	-1.61519392
H	1.89579162	7.44094117	-2.51805011
H	0.17083252	7.00099347	-2.71519291

C	0.52402336	-7.81274253	4.39557799
H	0.08351368	-8.19977864	5.31465602
H	-0.13704014	-8.03425639	3.55188438
H	1.50011938	-8.28463645	4.23624263
C	7.97227285	-4.82009749	-2.96865887
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H	8.99272683	-5.16918168	-3.12624361
H	7.27212680	-5.52974366	-3.42365917
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H	8.61392408	-0.49224102	-5.77593639
H	7.46177911	-1.55843313	-4.93061533
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Cartesian coordinates of DFT-optimized structure of **TDAC**:

Charge = 0; multiplicity = 1

C	-2.36158768	-5.23448215	-0.17305645
C	-0.96284075	-5.17943297	-0.06030403
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C	-0.98771575	-2.79347400	0.09591817
C	-2.38565343	-2.84032931	-0.08679357
C	-3.07953348	-4.04461570	-0.19444679
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C	-3.09638343	1.27324664	-0.06722608
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C	-2.84670092	-1.46932903	-0.08872303
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H	0.13848129	5.96992541	1.18253199
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C	1.24927316	-5.03304343	2.53529161
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H	-9.82465580	-0.19796155	-1.20625308
H	-6.86039255	-0.50518516	-4.29148687
C	-5.82478109	2.18783802	0.63857002
C	-5.39670860	2.20920010	1.96469086
C	-6.55456742	3.28389231	0.16035855
C	-5.66605951	3.29441880	2.79471467
H	-4.83565115	1.36824938	2.35784523

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H	-6.89387439	3.29108628	-0.86990798
C	-6.40015922	4.37362219	2.30938726
H	-5.30827695	3.27506842	3.81671248
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C	-0.41954886	1.24780284	-2.39956181
C	2.29596345	1.81258748	-2.22239702
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C	0.37540801	1.19531375	-3.53173006
H	-1.47878802	1.03248705	-2.48114170
C	1.73905496	1.48043913	-3.45685837
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O	2.42937075	1.41287165	-4.62795197
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O	-9.48305416	-0.88428729	-3.61705668
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C	6.01940364	-1.41547947	-2.96148190

H	6.47703189	-0.92979824	-3.82345247
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H	6.49038531	-2.39220551	-2.80286293
C	-8.68200977	-7.79682276	-3.00904396
H	-9.40980423	-7.76216906	-3.81972602
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C	3.83109210	1.61523043	-4.58360075
H	4.18234297	1.51384907	-5.61080552
H	4.08031717	2.61732563	-4.21643034
H	4.31512781	0.85901210	-3.95746996
C	0.63721061	-1.02489192	0.88673887
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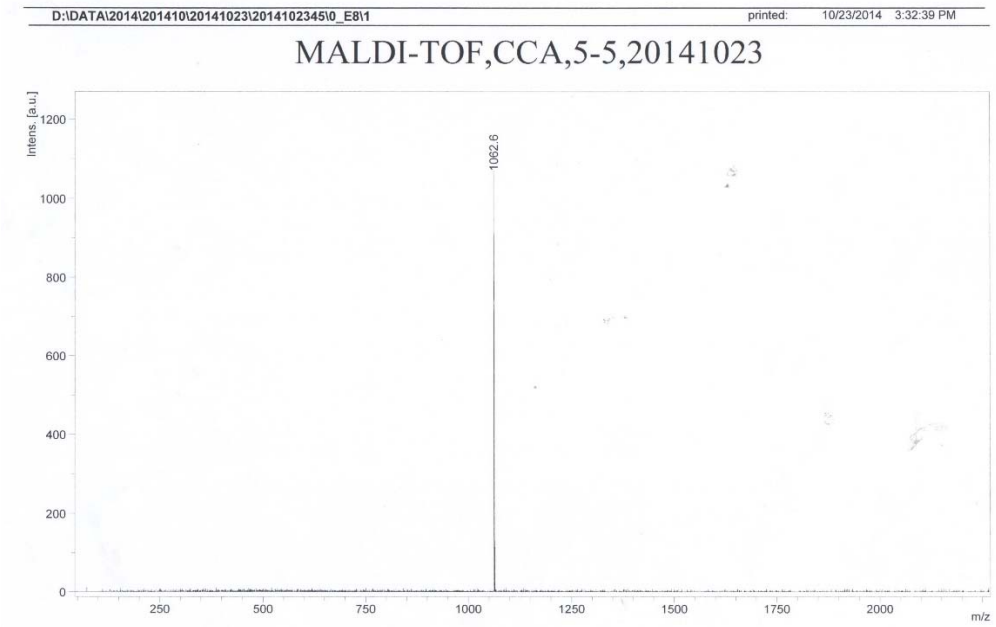
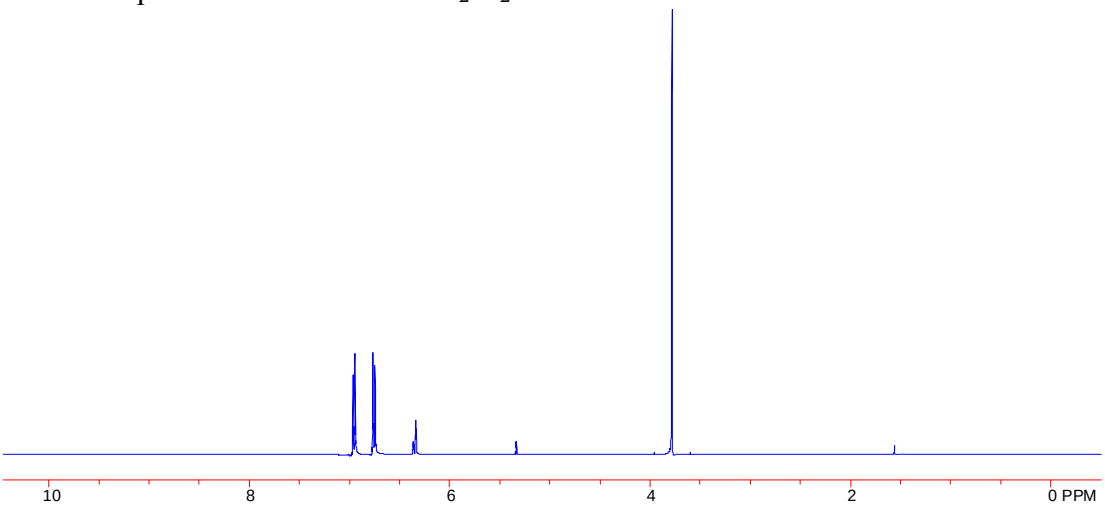
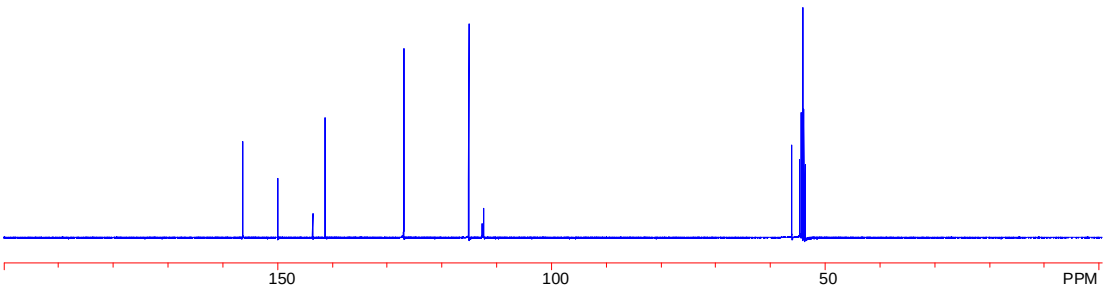
MALDI-TOF mass spectrum of **TDAB**:



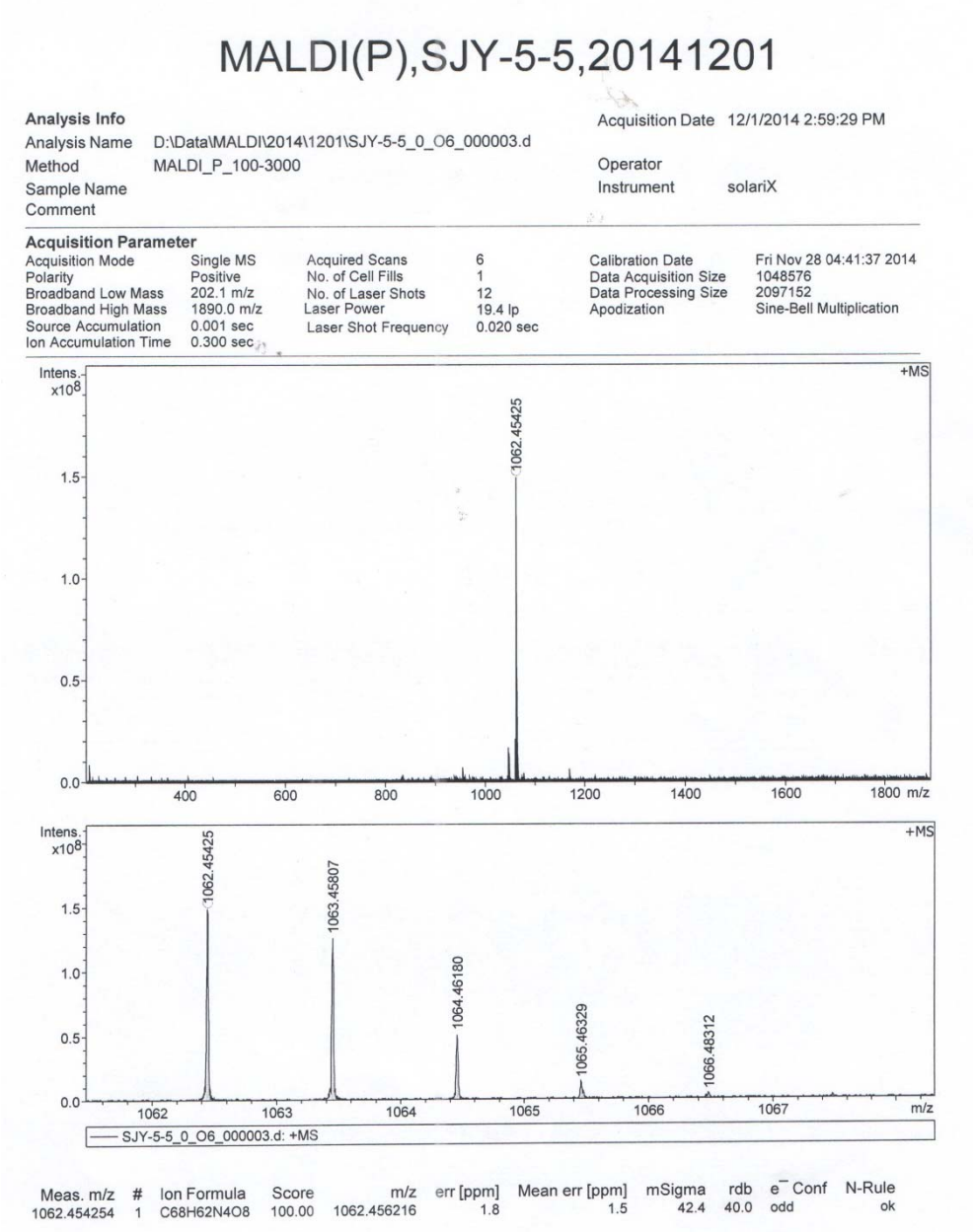
^{1}H NMR spectrum of **TDAB** in CD_2Cl_2:



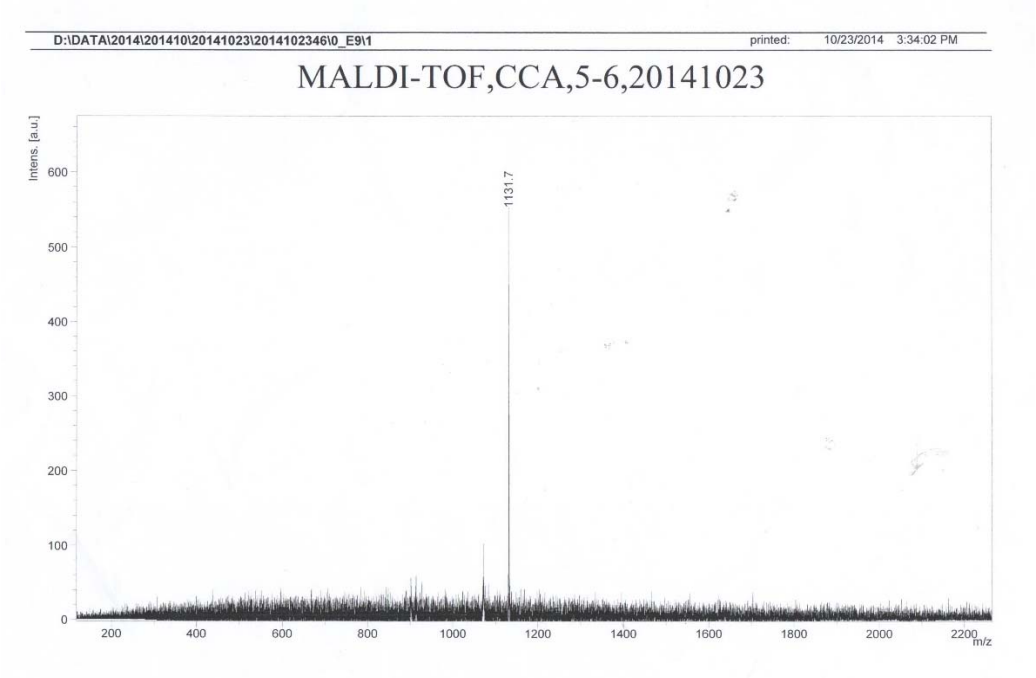
^{13}C NMR spectrum of **TDAB** in CD_2Cl_2:



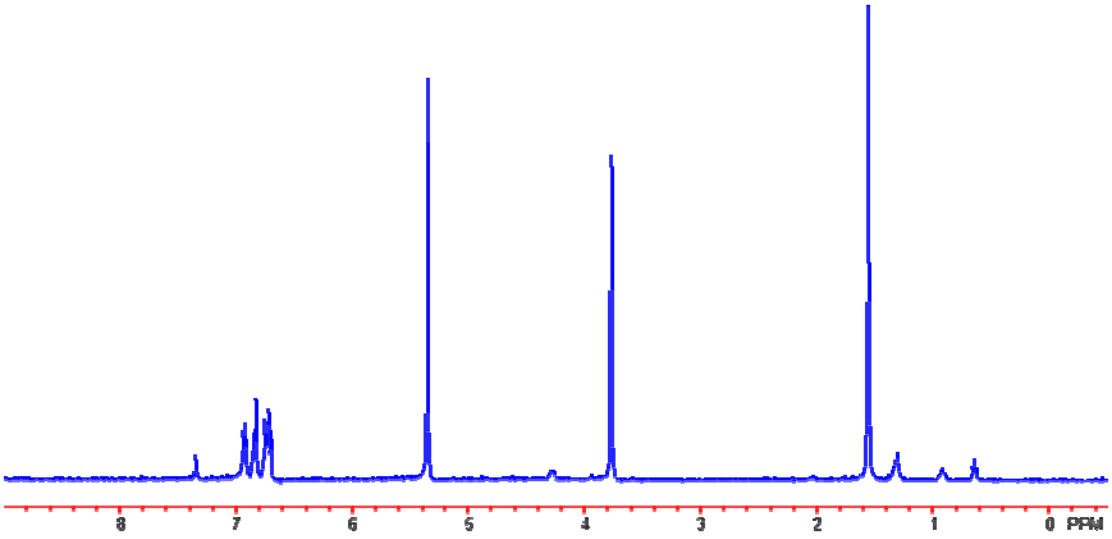
HR-MALDI-TOF mass spectrum of **TDAB**:



MALDI-TOF mass spectrum of **TDAC**:



^{1}H NMR spectrum of **TDAC** in CD_2Cl_2:



HR-MALDI-TOF mass spectrum of **TDAC**: