

The Enhanced Two-Photon Absorption Behavior of Twistfuranacenes to Phenylacetylene-Functionalized Twistacenes

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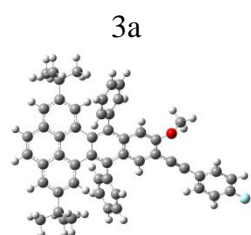
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Table S1. Crystallographic Data for the Resulting Derivatives.

	2	3b	5a	5b
formula	C ₄₅ H ₃₉ BrO	C ₅₄ H ₄₆ O ₂	C ₅₂ H ₄₁ FO	C ₅₃ H ₄₄ O ₂
Formula weight	675.7	726.9	700.9	712.9
Crystal system	monoclinic	triclinic	monoclinic	orthorhombic
Space group	P2(1)/n	P-1	P2/c	Fdd2
<i>a</i> [Å]	14.7129(12)	14.8148(13)	19.0001(19)	17.9559(15)
<i>b</i> [Å]	27.748(3)	15.4447(14)	7.8680(7)	69.780(4)
<i>c</i> [Å]	18.5982(16)	23.368(2)	27.690(3)	13.5926(12)
<i>α</i> (deg)	90.00	75.758(2)	90.00	90.00
<i>β</i> (deg)	92.2830(10)	88.856(3)	105.364(3)	90.00
<i>γ</i> (deg)	90.00	66.3290(10)	90.00	90.00
Volume [Å ³]	7586.7(11)	4727.7(7)	3991.5(6)	17031(2)
Temperature [K]	298	298	298	298
<i>Z</i>	4	4	4	8
Absorption				
Coefficient (mm ⁻¹)	1.223	0.234	0.071	0.162
<i>F</i> (000)	3048	1776	1480	6512
crystal size	0.41×0.20 ×0.13	0.38×0.30 ×0.18	0.37×0.30 ×0.06	0.40×0.30 ×0.10

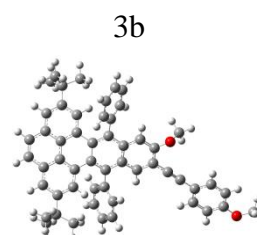
Table S2 Optimized structures, Z-matrices (in Å) of the ground states and their corresponding total SCF (ESCF) and zero-point (EZP) energies (in Hartree). There are no imaginary frequencies for six compounds.

	3a	3b	3c	5a	5b	D5c
HOMO	-1.8 eV	-1.7 eV	-1.72 eV	-5.16 eV	-5.01 eV	-4.84 eV
LUMO	-5.16 eV	-5.01 eV	-4.84 eV	-1.81 eV	-1.67 eV	-1.68 eV



optimized structure

C	-5.82213	-1.13347	0.95082
C	-5.37384	0.14098	0.57059
C	-3.99395	0.34164	0.27783
C	-3.11187	-0.7697	0.26654
C	-3.60317	-2.00405	0.71606
C	-4.94627	-2.20994	1.07481
C	-6.27598	1.25348	0.46842
C	-5.8307	2.48569	0.10573
C	-4.43683	2.73101	-0.13887
C	-3.51146	1.65852	-0.01013
C	-3.97746	4.01087	-0.49897
C	-2.63055	4.25575	-0.73385
C	-1.72473	3.193	-0.53969
C	-2.11666	1.90716	-0.15132
C	-1.16124	0.77941	-0.00565
C	-1.69623	-0.56396	-0.1153
C	0.22436	0.94341	0.1553
C	1.0997	-0.16832	-0.0658
C	0.56061	-1.40658	-0.55121
C	-0.85187	-1.61132	-0.52459
C	2.50462	-0.07506	0.1204
C	3.37759	-1.08647	-0.25652
C	2.83081	-2.26546	-0.86002
C	1.47301	-2.40874	-0.99233
C	-5.47181	-3.57823	1.55304



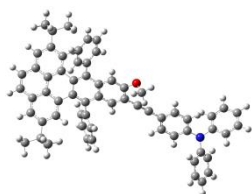
optimized structure

C	-6.03277	-1.23876	1.02155
C	-5.60963	0.04597	0.65164
C	-4.24299	0.26577	0.31449
C	-3.34712	-0.8343	0.25811
C	-3.81559	-2.08464	0.6919
C	-5.14431	-2.31068	1.08725
C	-6.52769	1.15081	0.60197
C	-6.11362	2.39257	0.23795
C	-4.73367	2.65691	-0.06508
C	-3.79032	1.59277	0.0206
C	-4.30062	3.93687	-0.44062
C	-2.96733	4.19412	-0.75495
C	-2.04499	3.14522	-0.60289
C	-2.41002	1.85963	-0.17453
C	-1.43302	0.75368	-0.0338
C	-1.93928	-0.60037	-0.13963
C	-0.05251	0.9539	0.13227
C	0.84979	-0.13567	-0.08635
C	0.33918	-1.38481	-0.57628
C	-1.06799	-1.62573	-0.54979
C	2.25144	-0.01198	0.10668
C	3.14971	-1.00075	-0.2715
C	2.63032	-2.1887	-0.88268
C	1.2766	-2.36309	-1.019
C	-5.64513	-3.68887	1.56299

C	-6.28252	-3.40833	2.85928	C	-6.30874	-3.55149	2.95377
C	-4.33656	-4.58179	1.83104	C	-4.50986	-4.72267	1.6797
C	-6.38681	-4.16992	0.45417	C	-6.68461	-4.22378	0.54909
C	-2.1022	5.63405	-1.17609	C	-2.54947	5.60157	-1.22578
C	-1.25814	5.48492	-2.46401	C	-1.078	5.66164	-1.67613
C	-1.22083	6.22806	-0.05249	C	-2.74029	6.59796	-0.05719
C	-3.24252	6.62767	-1.46969	C	-3.42922	6.0381	-2.42089
C	4.78131	-0.93034	-0.08999	C	4.54868	-0.8142	-0.09935
C	5.979	-0.77514	0.05979	C	5.74284	-0.63374	0.0544
C	7.38132	-0.59453	0.2266	C	7.13913	-0.4222	0.22798
C	7.88249	0.47656	0.99497	C	7.61946	0.65733	1.00277
C	9.25187	0.6559	1.16005	C	8.97831	0.8626	1.17149
C	10.12362	-0.24178	0.55248	C	9.9059	-0.00402	0.57101
C	9.66792	-1.30993	-0.21329	C	9.44958	-1.07982	-0.20171
C	8.29727	-1.48307	-0.37401	C	8.08081	-1.28048	-0.36685
F	11.45212	-0.07091	0.71044	C	-1.5659	-2.94477	-1.05436
C	-1.38616	-2.91653	-1.02873	C	-1.18943	-4.16297	-0.46416
C	-1.04468	-4.14463	-0.43783	C	-1.63203	-5.37896	-0.98603
C	-1.5272	-5.34748	-0.95513	C	-2.45796	-5.4013	-2.11147
C	-2.35848	-5.34649	-2.07682	C	-2.83609	-4.19812	-2.71061
C	-2.70038	-4.13344	-2.6778	C	-2.39284	-2.98375	-2.18845
C	-2.217	-2.9324	-2.16045	C	0.51439	2.25199	0.61695
C	0.83889	2.22258	0.63347	C	0.13427	2.74674	1.87486
C	0.53203	2.70146	1.91649	C	0.6753	3.93185	2.37145
C	1.13777	3.85556	2.41287	C	1.61237	4.64588	1.62195
C	2.0628	4.5548	1.63542	C	2.00473	4.16345	0.3719
C	2.37706	4.09092	0.35623	C	1.46229	2.97745	-0.12458
C	1.77412	2.93384	-0.13794	O	3.48389	-3.14817	-1.3756
O	3.66302	-3.24543	-1.34838	C	4.04953	-4.01833	-0.39322
C	4.1953	-4.13358	-0.36325	O	11.21784	0.28591	0.79929
H	-6.87928	-1.25593	1.16847	C	12.205	-0.55217	0.21692
H	-2.91547	-2.82913	0.80142	H	-7.07976	-1.37596	1.27698
H	-7.32916	1.08439	0.67669	H	-3.11948	-2.9056	0.73882
H	-6.52322	3.31806	0.01186	H	-7.56964	0.96526	0.84925
H	-4.7132	4.80056	-0.60229	H	-6.81967	3.21697	0.18224
H	-0.67866	3.38352	-0.71965	H	-5.04279	4.7279	-0.49975
H	2.92571	0.82294	0.55132	H	-1.01111	3.33144	-0.84147
H	1.10598	-3.32027	-1.4448	H	2.65015	0.89315	0.54401
H	-7.15345	-2.76086	2.72553	H	0.93291	-3.28134	-1.47614
H	-6.64751	-4.38142	3.20637	H	-7.1631	-2.86871	2.93812

H	-5.66329	-2.9762	3.6521	H	-6.67056	-4.5266	3.29868
H	-3.64175	-4.20696	2.59038	H	-5.59403	-3.1743	3.6925
H	-4.76167	-5.51909	2.20479	H	-3.73909	-4.39916	2.38725
H	-3.76399	-4.81732	0.92976	H	-4.91563	-5.67201	2.04494
H	-5.8295	-4.31699	-0.47655	H	-4.02972	-4.91693	0.71662
H	-6.7881	-5.14015	0.76923	H	-6.23578	-4.34093	-0.44255
H	-7.23307	-3.51037	0.23807	H	-7.06454	-5.20078	0.8693
H	-1.85278	5.05437	-3.27634	H	-7.53991	-3.54837	0.45135
H	-0.89412	6.46502	-2.79223	H	-0.87872	4.96978	-2.50139
H	-0.38476	4.84512	-2.31125	H	-0.84442	6.67197	-2.02804
H	-1.80091	6.36343	0.86642	H	-0.38736	5.42932	-0.86093
H	-0.37028	5.58294	0.18135	H	-3.77962	6.62621	0.28422
H	-0.82908	7.20684	-0.35327	H	-2.11433	6.31926	0.79665
H	-3.90864	6.26374	-2.25903	H	-2.46144	7.61136	-0.36835
H	-3.84612	6.83245	-0.57959	H	-4.49034	6.08124	-2.15962
H	-2.82087	7.58094	-1.80402	H	-3.13342	7.03583	-2.76404
H	7.18555	1.16494	1.46077	H	-3.32015	5.3447	-3.26121
H	9.65063	1.47497	1.74832	H	6.90795	1.33036	1.46975
H	10.38323	-1.98465	-0.67049	H	9.3528	1.68953	1.76552
H	7.92075	-2.30715	-0.97035	H	10.14567	-1.76073	-0.67637
H	-0.40544	-4.15306	0.44006	H	7.73023	-2.11235	-0.96896
H	-1.25394	-6.28534	-0.47996	H	-0.55255	-4.15307	0.41535
H	-2.7322	-6.28247	-2.48136	H	-1.33186	-6.30895	-0.51162
H	-3.34006	-4.1217	-3.55557	H	-2.80023	-6.3476	-2.51989
H	-2.48319	-1.99172	-2.63217	H	-3.4728	-4.20441	-3.59063
H	-0.18386	2.15837	2.52559	H	-2.68586	-2.05062	-2.65933
H	0.88961	4.2061	3.41052	H	-0.59161	2.1931	2.46209
H	2.53566	5.45242	2.02274	H	0.36883	4.29464	3.34838
H	3.09448	4.62758	-0.25789	H	2.03603	5.56753	2.00996
H	2.02474	2.57589	-1.1322	H	2.73345	4.70995	-0.21986
H	4.82557	-4.84524	-0.9002	H	1.76717	2.61173	-1.10051
H	4.80164	-3.59942	0.37656	H	4.69533	-4.71292	-0.93424
H	3.39129	-4.67683	0.15015	H	4.64652	-3.46571	0.34033
E(SCF)=	-2220.67398488	a.u.		H	3.26549	-4.58355	0.12755
E(ZP)=	-2219.872444	a.u.		H	13.16734	-0.1422	0.526
				H	12.12092	-1.58574	0.5758
				H	12.14525	-0.54633	-0.87871
				E(SCF)=	-2235.96773421	a.u.	
				E(ZP)=	-2235.125339	a.u.	

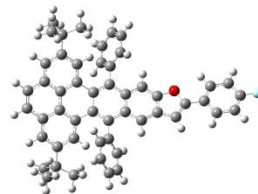
3c



optimized structure

C	-7.9596	-1.29374	1.32269
C	-7.57412	0.00418	0.95339
C	-6.23397	0.2461	0.53451
C	-5.33757	-0.84438	0.38902
C	-5.7605	-2.10681	0.83041
C	-7.05697	-2.35518	1.31246
C	-8.50138	1.10023	0.98644
C	-8.11698	2.35494	0.63101
C	-6.75914	2.63997	0.25953
C	-5.80661	1.58367	0.25473
C	-6.36055	3.94133	-0.09627
C	-5.04827	4.2226	-0.45518
C	-4.10845	3.17387	-0.38976
C	-4.43736	1.86761	-0.01161
C	-3.45214	0.75719	-0.00111
C	-3.96962	-0.59179	-0.11793
C	-2.06111	0.9468	0.04013
C	-1.18914	-0.13378	-0.30854
C	-1.74756	-1.3619	-0.79753
C	-3.14676	-1.60133	-0.64875
C	0.22484	-0.02596	-0.22771
C	1.07983	-1.00226	-0.72177
C	0.50031	-2.14998	-1.35777
C	-0.86127	-2.31397	-1.3806
C	-7.50727	-3.75128	1.78633
C	-8.16457	-3.64921	3.18273
C	-6.33484	-4.74499	1.8905
C	-8.53525	-4.3131	0.77513
C	-4.59312	5.62383	-0.90593
C	-3.58707	6.1938	0.12124
C	-5.77272	6.60816	-1.02229
C	-3.91317	5.53094	-2.2925
C	2.48749	-0.87273	-0.57504

5a



optimized structure

C	-4.71891	3.09026	0.6268
C	-4.84489	1.73442	0.28975
C	-3.67424	0.94328	0.10904
C	-2.39503	1.55568	0.17174
C	-2.33124	2.90136	0.56513
C	-3.47182	3.68459	0.8096
C	-6.13428	1.12289	0.11881
C	-6.25118	-0.18916	-0.21433
C	-5.09104	-1.02481	-0.36163
C	-3.80037	-0.46052	-0.15041
C	-5.20576	-2.3795	-0.70667
C	-4.08326	-3.189	-0.86989
C	-2.82517	-2.62782	-0.5928
C	-2.65332	-1.29576	-0.18665
C	-1.32126	-0.70625	0.09212
C	-1.18571	0.73057	-0.06069
C	-0.19177	-1.46351	0.43029
C	1.1164	-0.87649	0.34872
C	1.24851	0.4547	-0.20356
C	0.07774	1.26751	-0.34905
C	2.28139	-1.59111	0.73822
C	3.53436	-1.06507	0.47786
C	3.62648	0.18597	-0.18518
C	2.54516	0.94915	-0.52742
C	-3.38435	5.1619	1.24168
C	-1.94112	5.60484	1.54644
C	-4.22764	5.38668	2.51893
C	-3.93422	6.05062	0.10052
C	-4.2568	-4.65412	-1.31739
C	-2.91177	-5.35664	-1.58029
C	-5.08264	-4.70794	-2.6243
C	-5.00241	-5.43274	-0.20736
C	4.89487	-1.48657	0.68395

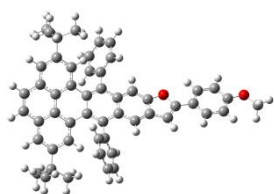
C	3.68979	-0.74162	-0.43159	C	5.69624	-0.51819	0.15034
C	5.09237	-0.5951	-0.25342	O	4.94362	0.51259	-0.38967
C	5.63603	0.58673	0.29097	C	7.14259	-0.376	0.04542
C	7.00367	0.72695	0.4772	C	7.70846	0.72478	-0.62294
C	7.8881	-0.30498	0.11285	C	9.08949	0.86367	-0.72771
C	7.35296	-1.48343	-0.43956	C	9.90647	-0.10607	-0.15912
C	5.98382	-1.62753	-0.61156	C	9.38251	-1.20791	0.51072
N	9.28289	-0.16119	0.29863	C	8.0022	-1.33667	0.61025
C	10.07484	-1.2763	0.69455	C	-0.3014	-2.8588	0.96324
C	9.90708	1.10308	0.09937	C	0.31867	-3.95195	0.33426
C	11.31711	-1.51484	0.0864	C	0.23002	-5.23502	0.87534
C	12.09663	-2.59899	0.48461	C	-0.47745	-5.45077	2.05982
C	11.64631	-3.47009	1.47844	C	-1.09278	-4.37255	2.69858
C	10.40746	-3.23893	2.07968	C	-1.00296	-3.09074	2.15706
C	9.62894	-2.14706	1.70139	C	0.24795	2.65134	-0.89612
C	10.85766	1.57776	1.01633	C	1.02746	3.62529	-0.24896
C	11.4769	2.8091	0.81114	C	1.20009	4.89239	-0.80748
C	11.14839	3.59299	-0.29658	C	0.59907	5.21044	-2.027
C	10.19726	3.12628	-1.20606	C	-0.17405	4.25074	-2.68309
C	9.58607	1.88815	-1.01923	C	-0.34497	2.98467	-2.12451
C	-3.6996	-2.89806	-1.15337	F	11.24504	0.02264	-0.25687
C	-3.26339	-4.13933	-0.66011	H	-5.62909	3.66805	0.76129
C	-3.76775	-5.33317	-1.17773	H	-1.36148	3.35053	0.70142
C	-4.71688	-5.3096	-2.20136	H	-7.01832	1.74177	0.24803
C	-5.1543	-4.08288	-2.70502	H	-7.2302	-0.63714	-0.36314
C	-4.6486	-2.89095	-2.18839	H	-6.20243	-2.78168	-0.86576
C	-1.43172	2.2181	0.51883	H	-1.9501	-3.24505	-0.71292
C	-1.64511	2.64296	1.83955	H	2.18565	-2.55496	1.21989
C	-1.01973	3.78769	2.33281	H	2.67617	1.91033	-1.00407
C	-0.1684	4.53244	1.51447	H	-1.49285	5.00239	2.34373
C	0.05121	4.12371	0.19736	H	-1.94199	6.64761	1.88079
C	-0.57115	2.97579	-0.294	H	-1.29509	5.54135	0.66653
O	1.29727	-3.13733	-1.88624	H	-4.16594	6.43461	2.83327
C	1.94603	-2.80439	-3.11604	H	-3.86399	4.76378	3.34269
H	-8.98688	-1.44821	1.6405	H	-5.28442	5.15138	2.3644
H	-5.05392	-2.92037	0.81105	H	-3.34437	5.91924	-0.81233
H	-9.52538	0.90034	1.29092	H	-3.89302	7.10868	0.38405
H	-8.83054	3.17472	0.63948	H	-4.9747	5.80688	-0.13491
H	-7.1164	4.71891	-0.09752	H	-3.09502	-6.38061	-1.92251
H	-3.08843	3.3915	-0.66547	H	-2.29379	-5.41604	-0.68005

H	0.66564	0.84604	0.23605	H	-2.33446	-4.84691	-2.35902
H	-1.24904	-3.21304	-1.84063	H	-6.07855	-4.27292	-2.50149
H	-9.04854	-3.00518	3.17982	H	-5.21356	-5.74678	-2.94741
H	-8.48157	-4.64107	3.52349	H	-4.57767	-4.1637	-3.42906
H	-7.46058	-3.24703	3.91856	H	-4.42971	-5.42273	0.72562
H	-5.56411	-4.38788	2.58186	H	-5.15133	-6.47702	-0.50528
H	-6.70071	-5.70494	2.26982	H	-5.986	-4.99962	-0.00105
H	-5.86446	-4.93253	0.92134	H	5.22498	-2.39839	1.1593
H	-8.08902	-4.40757	-0.22011	H	7.0566	1.4712	-1.06111
H	-8.88142	-5.3044	1.08989	H	9.53668	1.7077	-1.24105
H	-9.41163	-3.66313	0.68915	H	10.05393	-1.94159	0.94277
H	-4.04845	6.28224	1.11043	H	7.58864	-2.19148	1.13528
H	-2.70297	5.5595	0.22153	H	0.86473	-3.79304	-0.59088
H	-3.25253	7.19122	-0.18725	H	0.71245	-6.06647	0.36923
H	-6.26672	6.76981	-0.05868	H	-0.54513	-6.44892	2.48241
H	-5.40824	7.58036	-1.36954	H	-1.63971	-4.52771	3.62417
H	-6.52413	6.25995	-1.73863	H	-1.48062	-2.25453	2.65796
H	-4.60261	5.12713	-3.04117	H	1.49132	3.38842	0.70398
H	-3.59573	6.52578	-2.62453	H	1.80322	5.63131	-0.28762
H	-3.02619	4.89149	-2.27377	H	0.73505	6.19571	-2.46312
H	4.96747	1.39001	0.58315	H	-0.64046	4.48553	-3.63558
H	7.39801	1.63861	0.91216	H	-0.94373	2.24004	-2.63957
H	8.02075	-2.28561	-0.73343				$E_{(\text{SCF})}=-2181.42744271$ a.u.
H	5.58751	-2.5432	-1.03819				$E_{(\text{ZP})}=-2195.904836$ a.u.
H	11.66417	-0.8475	-0.69534				
H	13.05566	-2.76986	0.00404				
H	12.2531	-4.31788	1.78101				
H	10.04805	-3.90359	2.85998				
H	8.67353	-1.96281	2.18115				
H	11.10559	0.97685	1.88489				
H	12.21042	3.16224	1.53025				
H	11.62778	4.55492	-0.44946				
H	9.93808	3.72169	-2.07682				
H	8.85855	1.52253	-1.73622				
H	-2.53047	-4.1659	0.14056				
H	-3.41822	-6.28138	-0.77945				
H	-5.10812	-6.23842	-2.60595				
H	-5.88632	-4.05326	-3.50703				
H	-4.9894	-1.93963	-2.58488				
H	-2.30282	2.0638	2.48016				

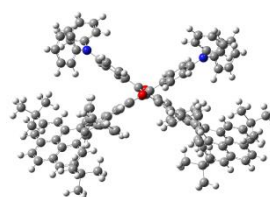
H	-1.1941	4.09499	3.35991
H	0.32036	5.4226	1.8993
H	0.71044	4.69641	-0.44871
H	-0.39345	2.66106	-1.31811
H	2.53463	-3.67973	-3.3977
H	1.20887	-2.59484	-3.90181
H	2.61187	-1.94247	-3.00202

$E(\text{SCF}) = -2638.90688740 \text{ a.u.}$
 $E(\text{ZP}) = -2637.919371 \text{ a.u.}$

5b



D5c



optimized structure

C	-5.03052	3.02655	0.64462
C	-5.13597	1.6686	0.30898
C	-3.95354	0.89693	0.12062
C	-2.684	1.53021	0.17493
C	-2.64035	2.87704	0.56736
C	-3.79219	3.64139	0.81881
C	-6.41604	1.03543	0.1468
C	-6.5134	-0.27841	-0.18572
C	-5.34058	-1.09458	-0.34153
C	-4.05822	-0.50869	-0.13843
C	-5.43488	-2.45068	-0.68748
C	-4.29983	-3.24035	-0.86083
C	-3.04966	-2.65822	-0.59135
C	-2.89754	-1.32445	-0.18314
C	-1.5739	-0.71357	0.08918
C	-1.46262	0.72493	-0.06398
C	-0.43061	-1.45309	0.42072
C	0.86757	-0.84538	0.33494
C	0.97555	0.48828	-0.21639
C	-0.20867	1.28193	-0.35671
C	2.04582	-1.54142	0.71917

optimized structure

C	8.57396	-3.46471	5.03863
C	8.84378	-2.23529	4.41923
C	7.92687	-1.71346	3.4624
C	6.80367	-2.48819	3.07056
C	6.5544	-3.68005	3.76813
C	7.41296	-4.18337	4.76026
C	10.03117	-1.48704	4.72879
C	10.28842	-0.29669	4.12632
C	9.3607	0.2796	3.19195
C	8.15387	-0.41699	2.89546
C	9.61861	1.51178	2.57353
C	8.73104	2.067	1.65383
C	7.52166	1.39071	1.42003
C	7.1815	0.18601	2.05508
C	5.90758	-0.52782	1.79427
C	5.88643	-1.95871	2.03354
C	4.76242	0.09196	1.27402
C	3.70784	-0.70588	0.7135
C	3.89731	-2.137	0.6073
C	4.96889	-2.75362	1.33098
C	2.51853	-0.11894	0.20127

C	3.28946	-0.99486	0.45618	C	1.61624	-0.89331	-0.50254
C	3.35827	0.25887	-0.20563	C	1.8858	-2.26951	-0.68394
C	2.26337	1.00407	-0.54362	C	2.97637	-2.90722	-0.16089
C	-3.72589	5.12049	1.24887	C	7.13009	-5.50304	5.50538
C	-2.28854	5.58545	1.54846	C	5.71284	-6.04259	5.23446
C	-4.56825	5.33452	2.52853	C	7.27027	-5.2927	7.03137
C	-4.29262	5.99937	0.10834	C	8.15383	-6.56557	5.03868
C	-4.45043	-4.70798	-1.30863	C	9.08315	3.39884	0.96155
C	-3.09571	-5.38099	-1.59853	C	8.07096	3.78483	-0.13317
C	-5.29895	-4.77821	-2.60007	C	10.47845	3.29749	0.30171
C	-5.15824	-5.50391	-0.18619	C	9.09861	4.52436	2.02371
C	4.65716	-1.39288	0.65779	C	-0.02825	-1.84846	-1.72265
C	5.44173	-0.40983	0.12375	O	0.88809	-2.84696	-1.42425
O	4.66844	0.60832	-0.41311	C	-1.15916	-2.28124	-2.53144
C	6.88329	-0.24073	0.01646	C	-1.4271	-3.65361	-2.70177
C	7.43544	0.86717	-0.65738	C	-2.50374	-4.08984	-3.46129
C	8.8079	1.0265	-0.7608	C	-3.35376	-3.16849	-4.10252
C	9.6765	0.08234	-0.19273	C	-3.07961	-1.79589	-3.94946
C	9.14495	-1.02524	0.48236	C	-2.01052	-1.36417	-3.17768
C	7.7644	-1.1756	0.58117	C	4.55735	1.57262	1.36119
C	-0.51587	-2.85098	0.95147	C	4.32076	2.36915	0.22772
C	0.11785	-3.93303	0.31694	C	4.0934	3.74075	0.34905
C	0.0519	-5.21855	0.8554	C	4.09829	4.34422	1.60807
C	-0.6459	-5.44804	2.04307	C	4.32668	3.56427	2.74355
C	-1.27436	-4.38089	2.68755	C	4.5499	2.19365	2.62094
C	-1.20726	-3.09661	2.14852	C	5.11848	-4.24058	1.2286
O	11.00707	0.32966	-0.34899	C	6.26914	-4.78064	0.63228
C	11.93446	-0.59332	0.20284	C	6.42062	-6.15893	0.48435
C	-0.06266	2.66862	-0.90373	C	5.42067	-7.02784	0.92534
C	-0.66418	2.99263	-2.13045	C	4.26758	-6.50578	1.51493
C	-0.51474	4.26126	-2.68944	C	4.11795	-5.12636	1.66341
C	0.24495	5.23303	-2.03546	N	-4.44555	-3.60766	-4.88148
C	0.8541	4.9245	-0.81751	C	-5.64187	-2.83497	-4.95346
C	0.70292	3.65487	-0.25862	C	-4.3646	-4.82287	-5.6218
H	-5.9494	3.58907	0.78472	C	-3.22552	-5.12058	-6.38568
H	-1.67725	3.3422	0.69713	C	-3.15589	-6.31182	-7.10532
H	-7.30944	1.63947	0.28201	C	-4.22304	-7.21221	-7.09156
H	-7.48589	-0.74255	-0.32793	C	-5.36193	-6.91211	-6.34171
H	-6.42579	-2.86948	-0.83954	C	-5.43326	-5.73185	-5.60437

H	-2.16481	-3.25962	-0.71933	C	-6.26221	-2.60797	-6.19116
H	1.96734	-2.50753	1.19946	C	-7.43921	-1.86491	-6.25971
H	2.37756	1.96786	-1.01938	C	-8.00416	-1.3227	-5.10394
H	-1.82853	4.99022	2.34446	C	-7.3846	-1.54142	-3.87178
H	-2.30397	6.62837	1.88208	C	-6.21883	-2.30067	-3.79111
H	-1.64479	5.53104	0.66635	H	9.29236	-3.83665	5.76374
H	-4.52123	6.38375	2.84123	H	5.65375	-4.22687	3.5427
H	-4.19254	4.71834	3.35195	H	10.72899	-1.90426	5.45012
H	-5.62189	5.08315	2.37794	H	11.19877	0.25234	4.35239
H	-3.70287	5.87659	-0.80576	H	10.54638	2.02042	2.82009
H	-4.26774	7.05826	0.39083	H	6.82673	1.81178	0.71225
H	-5.32958	5.73869	-0.12446	H	2.32889	0.93655	0.33876
H	-3.26373	-6.40681	-1.94319	H	3.11816	-3.9684	-0.30895
H	-2.46088	-5.43255	-0.70965	H	4.94317	-5.31865	5.5227
H	-2.54281	-4.85511	-2.38423	H	5.54917	-6.95172	5.82271
H	-5.41258	-5.81926	-2.92263	H	5.563	-6.30117	4.18282
H	-4.8211	-4.22172	-3.41299	H	7.06709	-6.22999	7.56117
H	-6.30192	-4.3659	-2.4583	H	6.56103	-4.53971	7.39025
H	-4.56862	-5.48204	0.73597	H	8.27482	-4.9671	7.31505
H	-5.29011	-6.551	-0.48249	H	8.06129	-6.74717	3.96302
H	-6.14694	-5.09207	0.03881	H	7.98786	-7.51496	5.56108
H	5.00464	-2.29972	1.13021	H	9.18193	-6.24735	5.23768
H	6.77299	1.60183	-1.10024	H	8.38199	4.72348	-0.60363
H	9.23642	1.87763	-1.27928	H	7.06525	3.93544	0.26854
H	9.79209	-1.76815	0.93251	H	8.01597	3.02617	-0.92129
H	7.37067	-2.03677	1.11204	H	10.73461	4.24305	-0.18917
H	0.65714	-3.76331	-0.61022	H	10.49642	2.50692	-0.4557
H	0.54476	-6.0412	0.34491	H	11.26575	3.07993	1.02895
H	-0.69588	-6.44811	2.46367	H	8.1151	4.62845	2.49317
H	-1.81387	-4.54656	3.61571	H	9.35975	5.48373	1.56207
H	-1.69501	-2.26899	2.65396	H	9.82764	4.32355	2.81488
H	11.82133	-1.59196	-0.23755	H	-0.788	-4.38174	-2.21588
H	11.83146	-0.66732	1.29277	H	-2.6931	-5.15261	-3.56282
H	12.92459	-0.20468	-0.03841	H	-3.7058	-1.0667	-4.45082
H	-1.25232	2.23851	-2.64393	H	-1.81632	-0.30149	-3.09767
H	-0.98732	4.48867	-3.64072	H	4.31078	1.90876	-0.75554
H	0.36438	6.22027	-2.47204	H	3.9045	4.33133	-0.54236
H	1.44719	5.67272	-0.29937	H	3.91838	5.41102	1.704
H	1.17347	3.42499	0.69273	H	4.32246	4.02191	3.72873

$E_{\text{(SCF)}} = -2181.42744271$ a.u.

$E_{\text{(ZP)}} = -2195.904836$ a.u.

H	4.72201	1.59037	3.50674
H	7.04761	-4.108	0.2861
H	7.31859	-6.55406	0.01798
H	5.53667	-8.10121	0.8073
H	3.48278	-7.17207	1.86168
H	3.22118	-4.72803	2.12874
H	-2.40092	-4.41601	-6.40999
H	-2.26761	-6.52846	-7.69167
H	-4.16818	-8.13583	-7.65937
H	-6.19723	-7.60603	-6.31843
H	-6.31426	-5.50574	-5.01304
H	-5.81767	-3.01662	-7.09246
H	-7.90796	-1.69798	-7.22522
H	-8.91609	-0.73669	-5.16221
H	-7.81533	-1.12955	-2.9637
H	-5.75301	-2.48566	-2.82908
C	-0.36178	0.63899	-1.1868
C	-1.61656	0.89285	-0.50355
C	0.02802	1.84684	-1.72444
C	-2.51888	0.11915	0.20095
C	-1.88614	2.26886	-0.6863
O	-0.88837	2.84561	-1.42709
C	1.15903	2.27885	-2.5335
C	-3.70821	0.70658	0.71258
H	-2.32927	-0.93622	0.33945
C	-2.97676	2.90706	-0.16396
C	1.42714	3.65105	-2.7049
C	2.01035	1.36116	-3.1789
C	-4.76276	-0.09074	1.27389
C	-3.89771	2.1376	0.60497
H	-3.11857	3.96808	-0.31312
C	2.50394	4.08654	-3.46462
H	0.78806	4.37965	-2.21968
C	3.07959	1.79213	-3.95089
H	1.81597	0.29857	-3.09806
C	-5.90784	0.52953	1.79372
C	-4.55773	-1.57134	1.36226
C	-4.96929	2.7549	1.32807
C	3.35395	3.16457	-4.10497

H	2.69345	5.14921	-3.56696
H	3.70575	1.06246	-4.45158
C	-7.18169	-0.18406	2.05549
C	-5.88668	1.96065	2.03158
C	-4.32136	-2.36876	0.22936
C	-4.55007	-2.19137	2.62249
C	-5.11915	4.24172	1.22406
N	4.44596	3.60297	-4.88406
C	-8.1538	0.41965	2.89566
C	-7.52203	-1.38929	1.42157
C	-6.8037	2.49112	3.0683
C	-4.09402	-3.74028	0.35173
H	-4.31151	-1.90914	-0.75425
C	-4.32687	-3.5619	2.74613
H	-4.722	-1.58739	3.50785
C	-6.27008	4.78087	0.62745
C	-4.11866	5.1282	1.65756
C	5.64217	2.83003	-4.95525
C	4.36544	4.81772	-5.62518
C	-7.92668	1.71667	3.4613
C	-9.36049	-0.27674	3.19319
C	-8.73132	-2.06541	1.65635
H	-6.82733	-1.81093	0.71389
C	-6.55435	3.68373	3.76455
C	-4.09871	-4.34275	1.61122
H	-3.90527	-4.33156	-0.53924
H	-4.32248	-4.01877	3.73168
C	-6.42186	6.15896	0.47794
H	-7.04852	4.10768	0.28227
C	-4.26859	6.50741	1.50748
H	-3.2217	4.73059	2.12313
C	6.26271	2.60207	-6.19266
C	6.21881	2.29645	-3.79241
C	3.22663	5.11516	-6.38957
C	5.43427	5.72651	-5.60804
C	-8.8433	2.23934	4.41796
C	-10.28789	0.30034	4.12738
C	-9.61857	-1.50946	2.57592
C	-9.08356	-3.39787	0.96531

C	-7.41261	4.18796	4.75648
H	-5.65387	4.23045	3.53819
H	-3.91881	-5.40948	1.70796
C	-5.42193	7.02857	0.91759
H	-7.32004	6.55337	0.01136
H	-3.48381	7.17426	1.85322
C	7.43962	1.8588	-6.26046
H	5.81842	3.01017	-7.09433
C	7.38449	1.53697	-3.87232
H	5.75283	2.48217	-2.8306
C	3.15743	6.30595	-7.11
H	2.40191	4.41073	-6.41366
C	5.36337	6.90631	-6.34616
H	6.31506	5.50062	-5.01631
C	-8.57339	3.46941	5.03604
C	-10.0305	1.49126	4.72866
H	-11.19812	-0.24854	4.3543
H	-10.54622	-2.01794	2.82326
C	-8.07213	-3.78433	-0.12994
C	-10.47941	-3.2975	0.3065
C	-9.09779	-4.52258	2.02836
C	-7.1296	5.50845	5.50008
H	-5.53816	8.10178	0.79831
C	8.00426	1.3173	-5.1042
H	7.90854	1.69113	-7.22576
H	7.81497	1.12566	-2.96386
C	4.22476	7.20614	-7.09653
H	2.26936	6.52237	-7.69675
H	6.1988	7.60008	-6.32309
H	-9.29158	3.84197	5.76105
H	-10.7281	1.90909	5.44986
H	-8.38329	-4.72335	-0.59955
H	-7.06606	-3.93442	0.27106
H	-8.01797	-3.02615	-0.91858
H	-10.73558	-4.2435	-0.18354
H	-10.49827	-2.50746	-0.45144
H	-11.26625	-3.07976	1.03417
H	-8.11389	-4.6259	2.49716
H	-9.35889	-5.48242	1.56768

H	-9.8263	-4.3214	2.81991
C	-5.71249	6.04782	5.2281
C	-7.26926	5.29974	7.02634
C	-8.15359	6.57039	5.03257
H	8.91611	0.73112	-5.16188
H	4.17023	8.1294	-7.66495
H	-4.94267	5.32429	5.51697
H	-5.54872	6.95766	5.81522
H	-5.56299	6.30516	4.1761
H	-7.0659	6.2376	7.55508
H	-6.5599	4.54714	7.38578
H	-8.27372	4.97444	7.3107
H	-8.06141	6.75086	3.95669
H	-7.98754	7.52035	5.5539
H	-9.18159	6.25228	5.23223
C	0.36152	-0.64009	-1.18614

$E_{(\text{SCF})} = -5198.12385334$ a.u.

$E_{(\text{ZP})} = -5196.219761$ a.u.

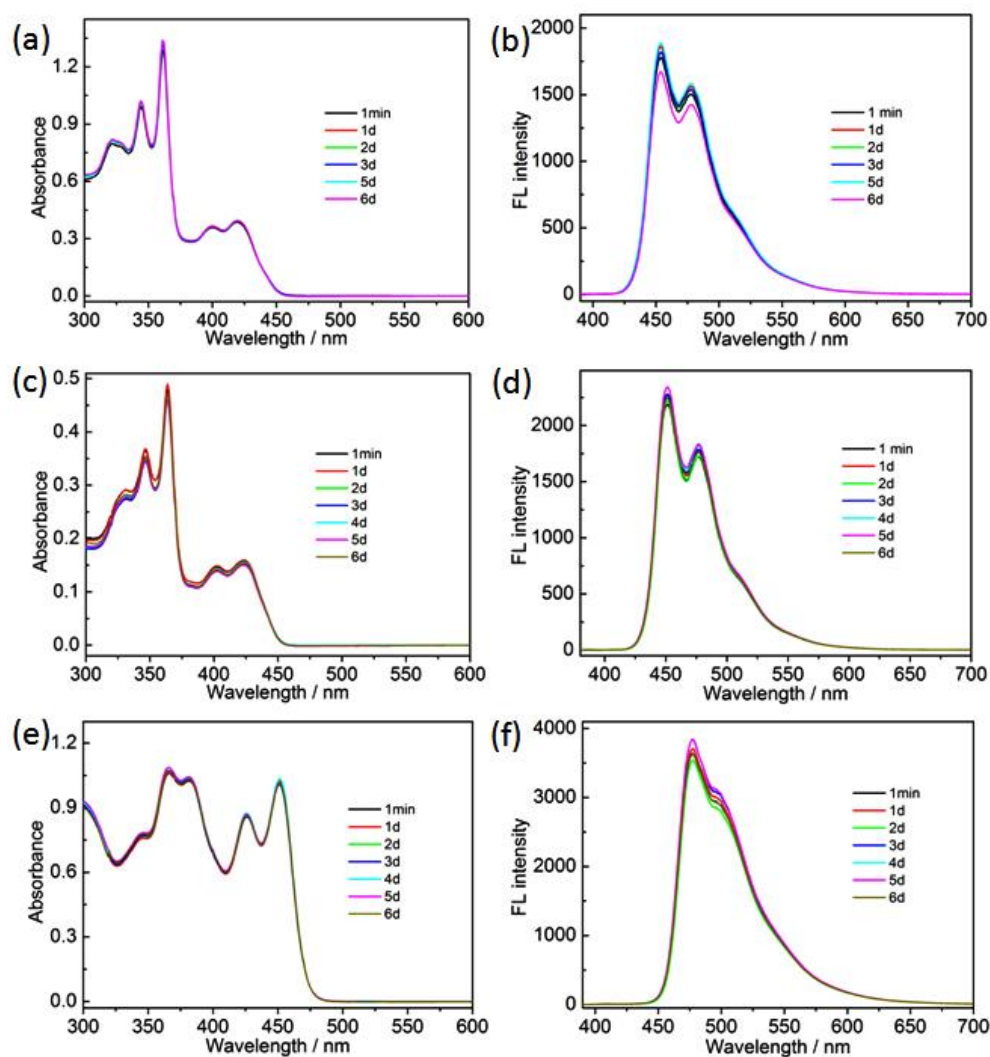


Figure S1 UV-Vis absorption and emission spectra of **5a** (a)/(b), **5b** (c)/(d) and **D5c** (e)/(f) in toluene ($[c] = 1 \times 10^{-5} \text{M}$) in different monitored time.

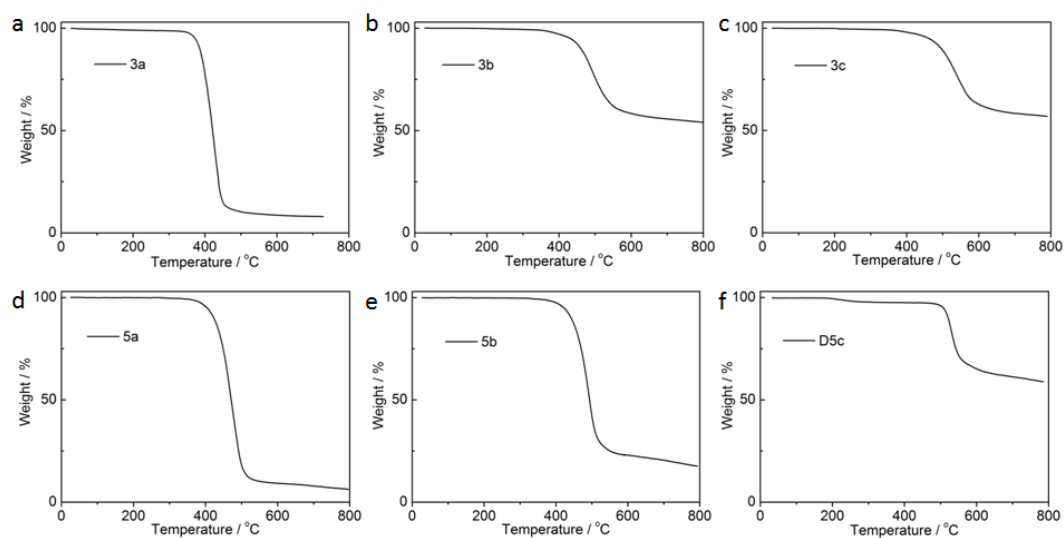


Figure S2 TGA data of compounds **3** and **5/D5c**.

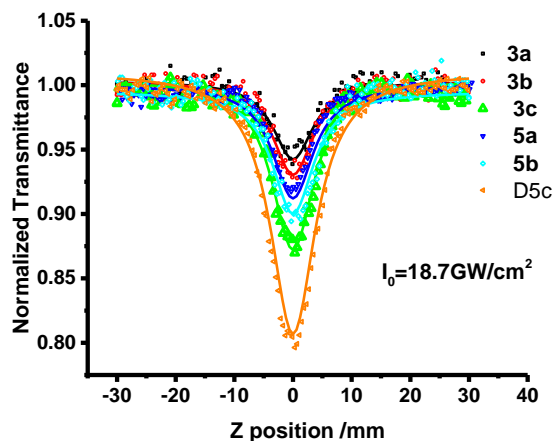


Figure S3 Open-aperture Z-scan of **3a**, **3b**, **3c**, **5a**, **5b**, **D5c** with a 190 fs pulse at 515 nm. The dots represent the experimental data whereas the solid lines represent the numerical fitting.

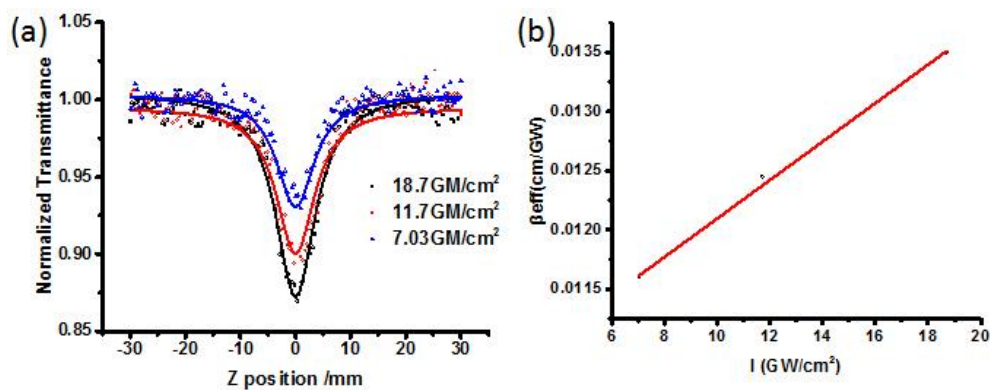


Figure S4 Open-aperture Z-scan of **3c** at 515 nm under 190 fs. The dots was experimental data, and solid lines represent theoretical fitting. (b) Example of the intensity dependence of the nonlinear absorption coefficient for **3c**.

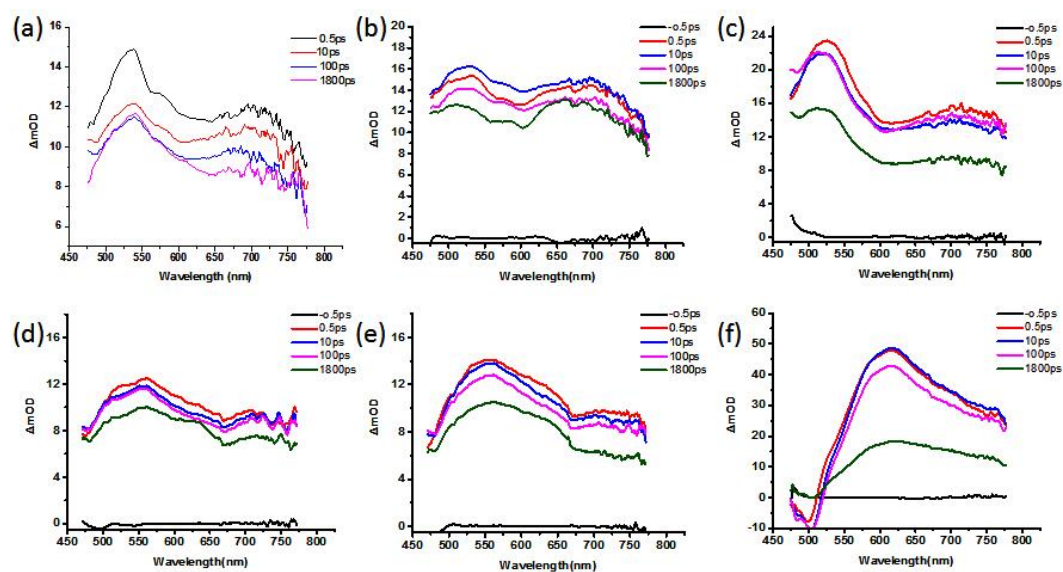


Figure S5 The transient absorption spectra of the samples (a) **3a**, (b) **3b**, (c) **3c**, (d) **5a**, (e) **5b**, (f) **D5c**.

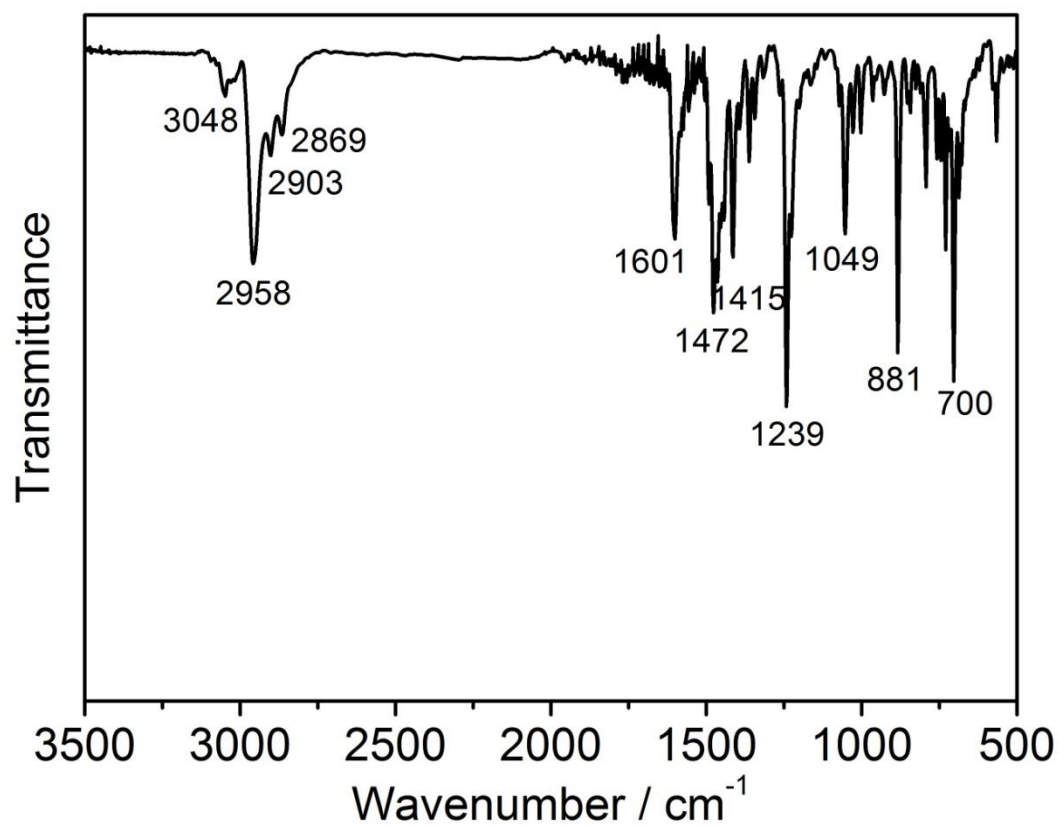


Figure S6 FT-IR spectrum of **2**.

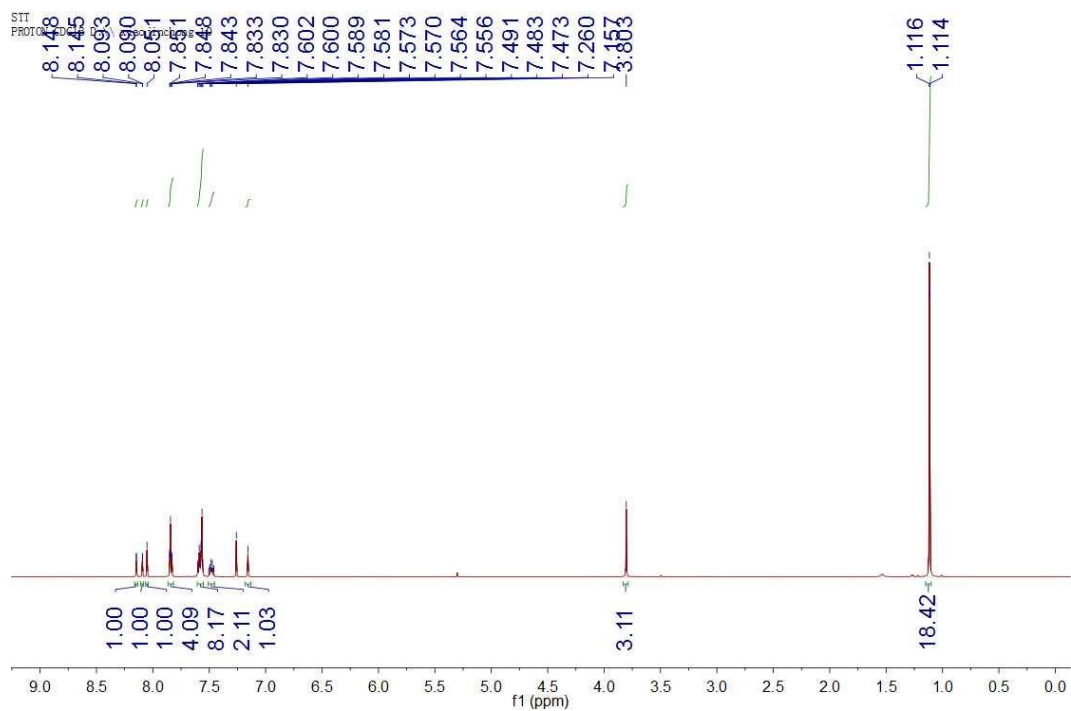


Figure S7 ^1H NMR spectrum of **2**.

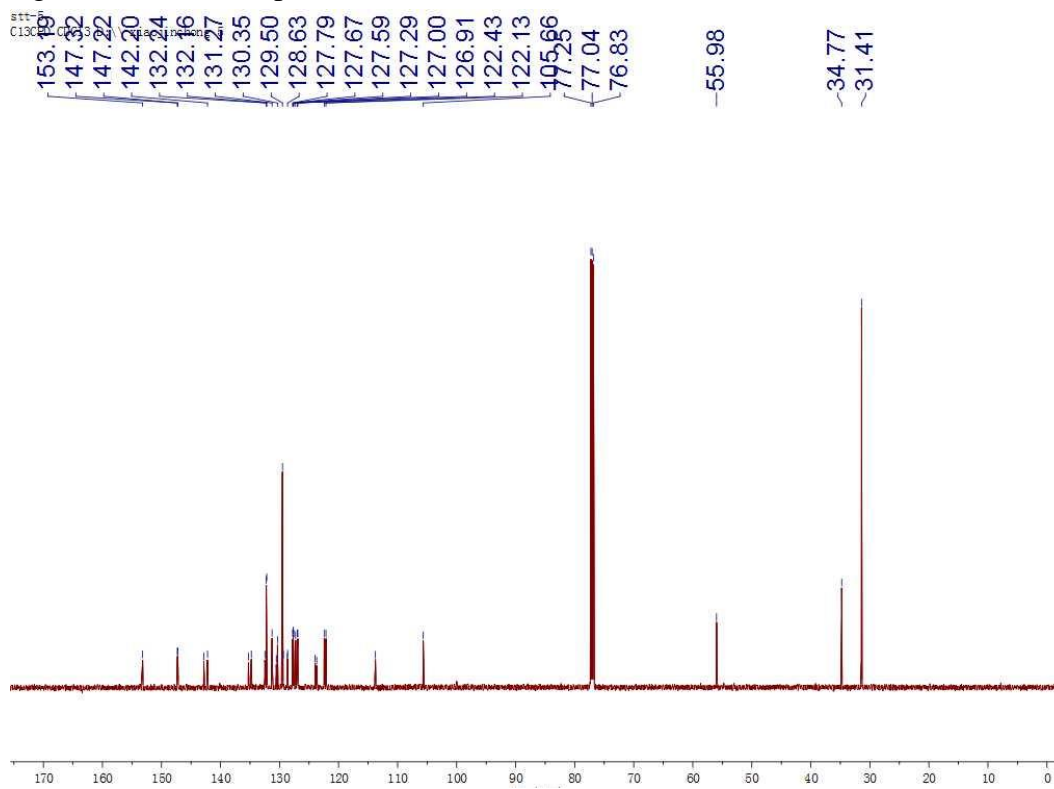


Figure S8 ^{13}C NMR spectrum of **2**.

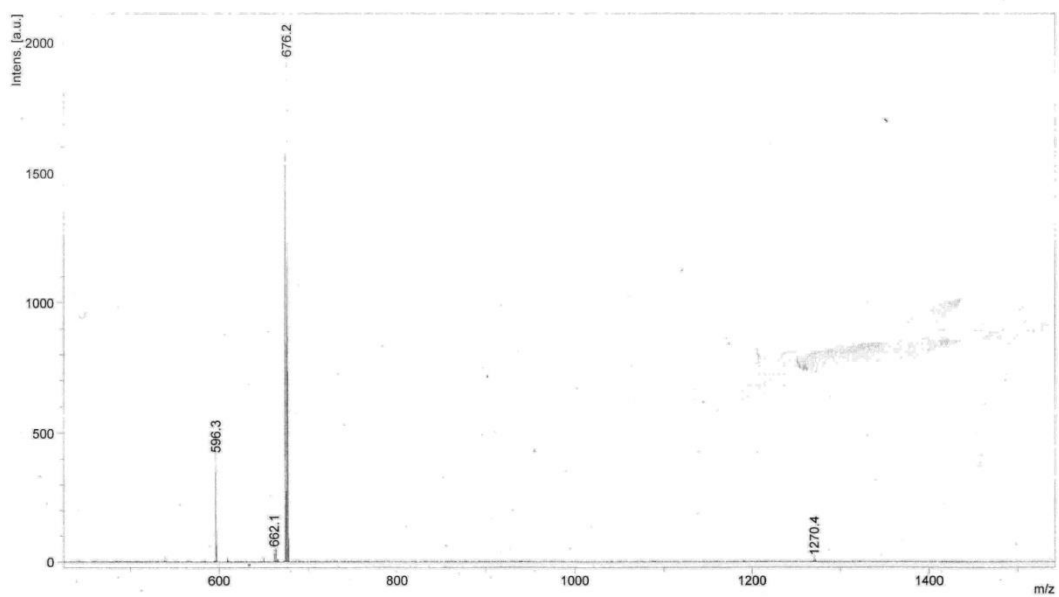


Figure S9 MALDI-TOF spectrum of **2**.

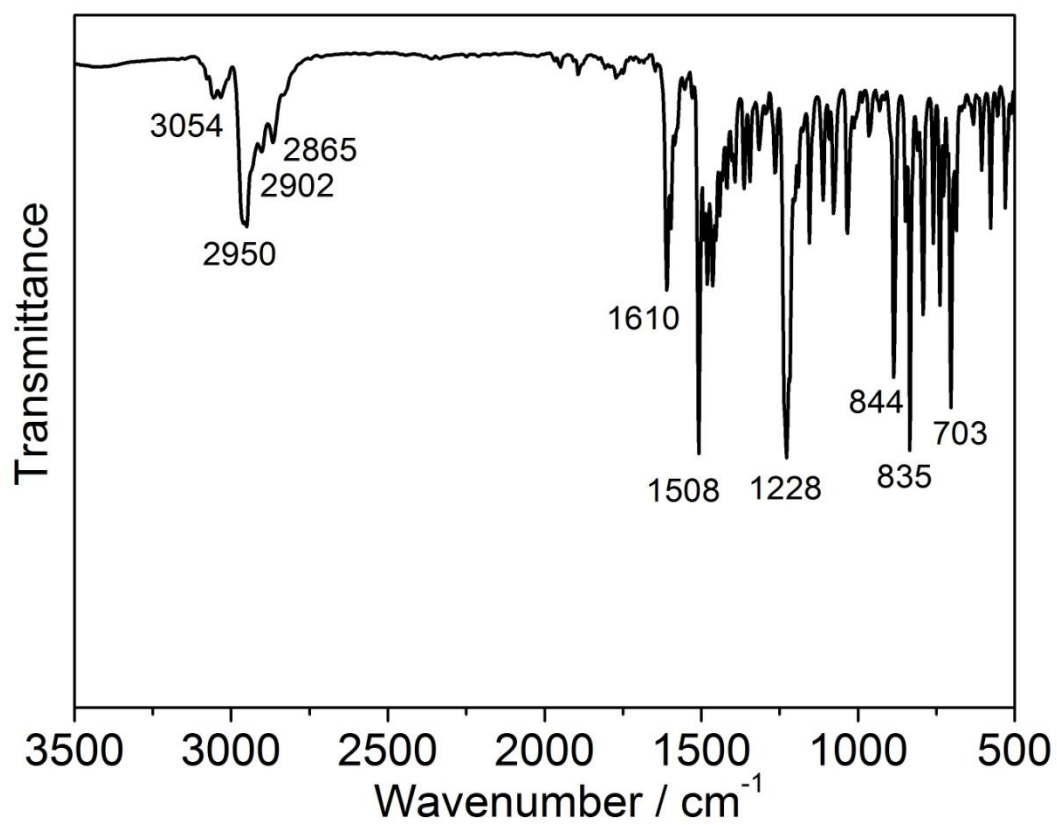


Figure S10 FT-IR spectrum of **3a**.

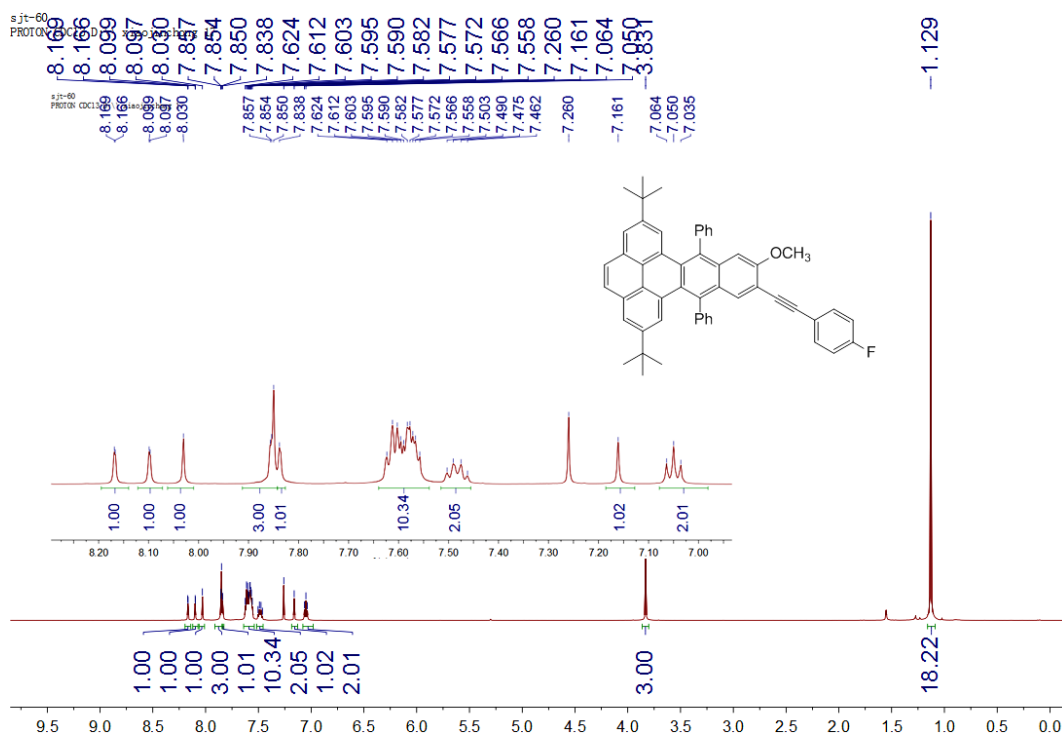


Figure S11 ¹H NMR spectrum of **3a** (600 MHz).

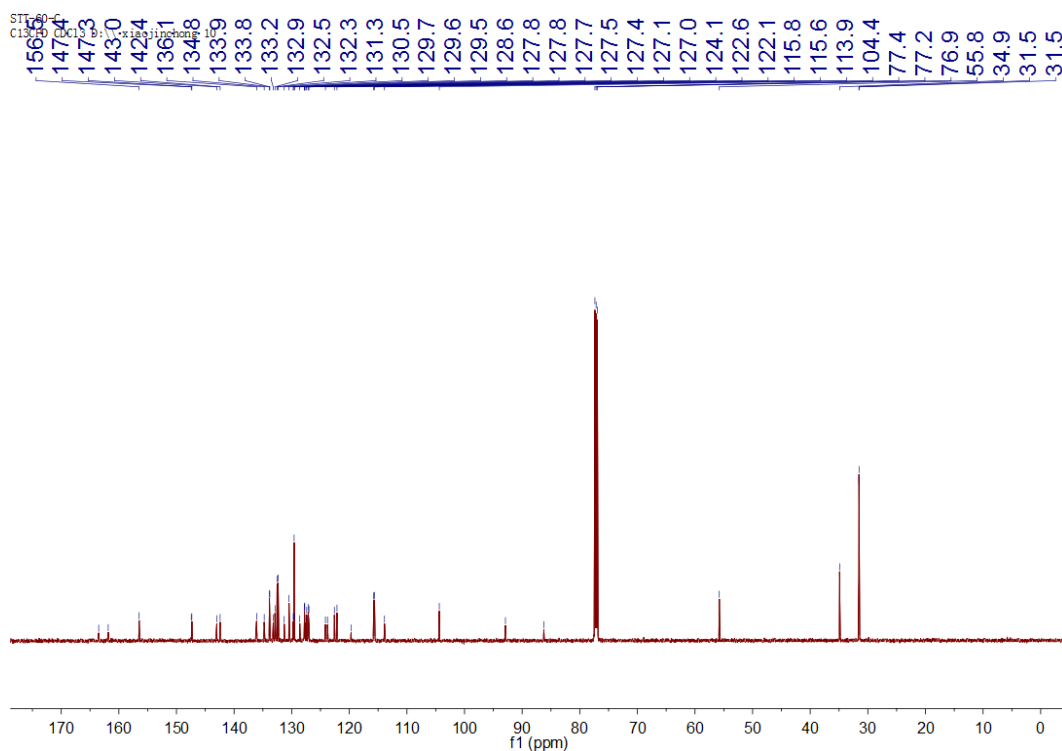


Figure S12 ¹³C NMR spectrum of **3a** (150 MHz).

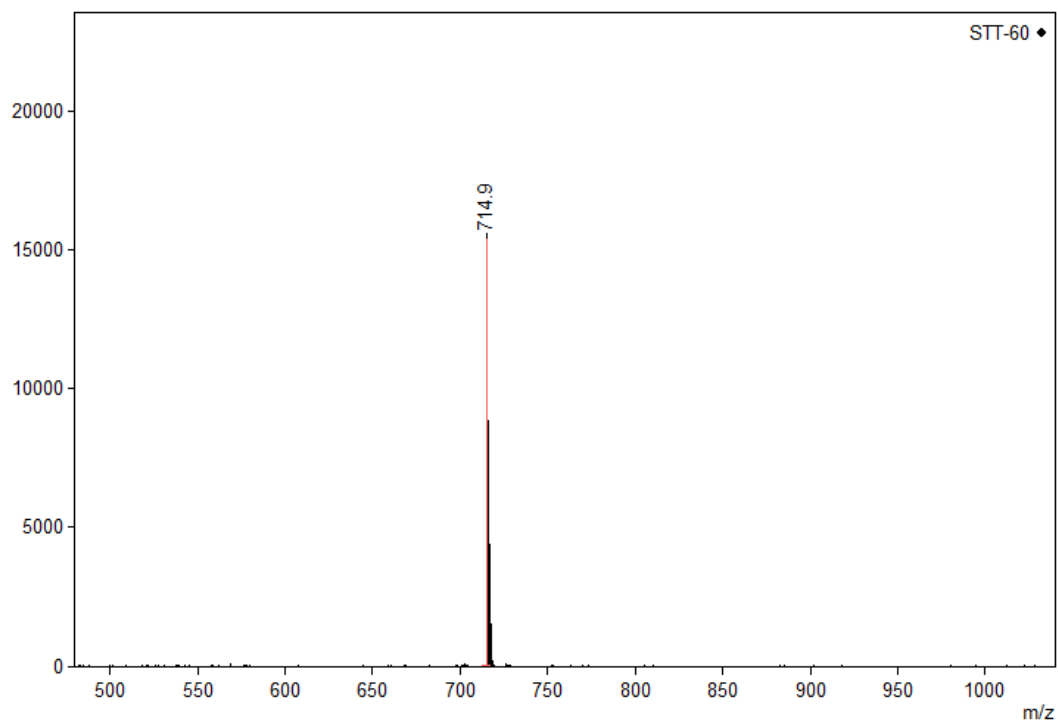
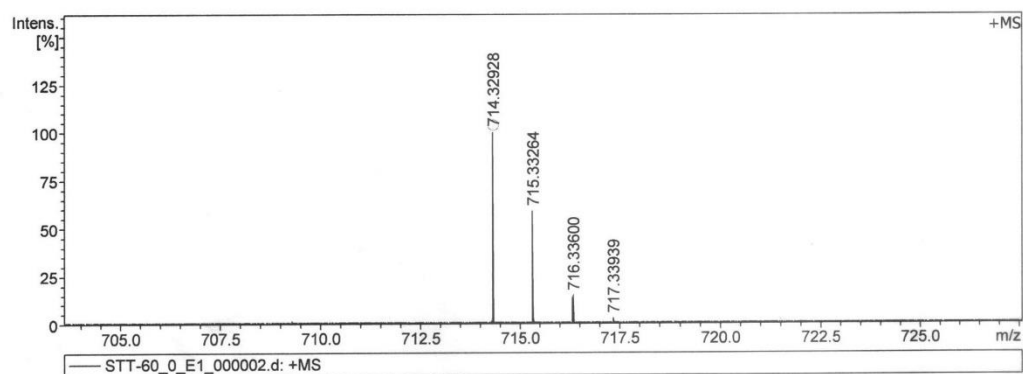


Figure S13 MALDI-TOF spectrum of **3a**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
714.329281	1	C ₅₃ H ₄₃ FO	100.00	714.329246	0.0	-0.0	10.0	32.0	odd	ok

Figure S14 HR-MS spectrum of **3a**.

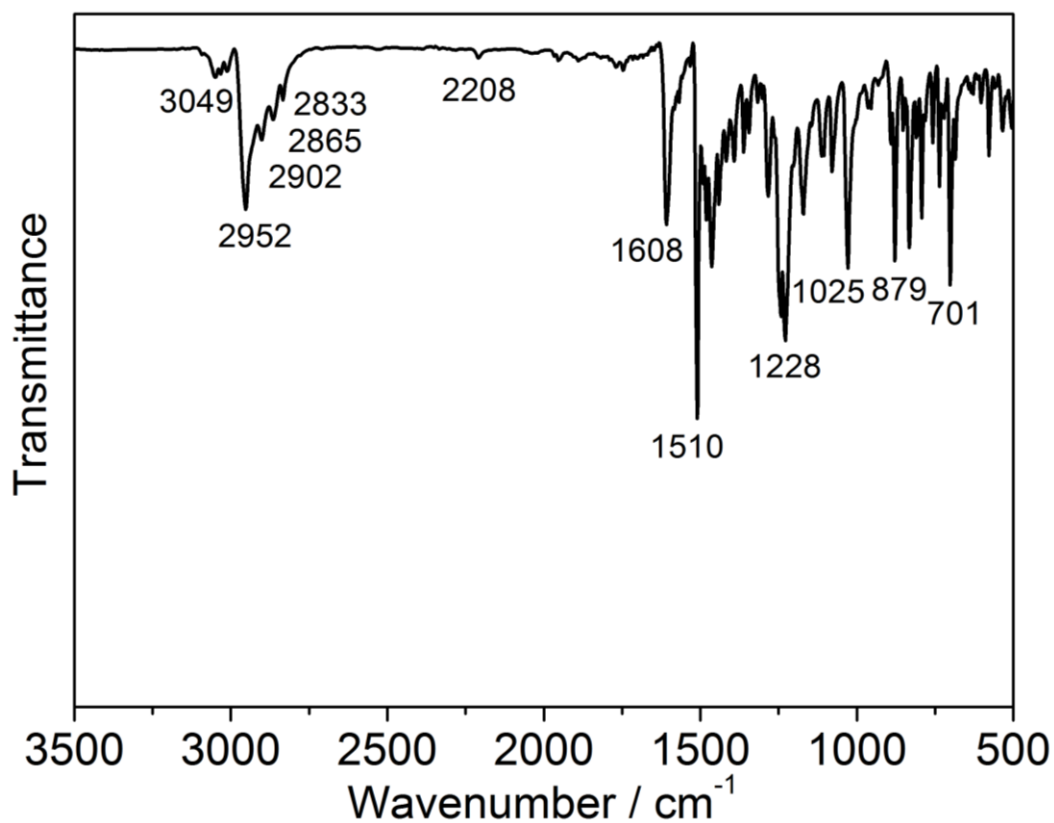


Figure S15 FT-IR spectrum of **3b**.

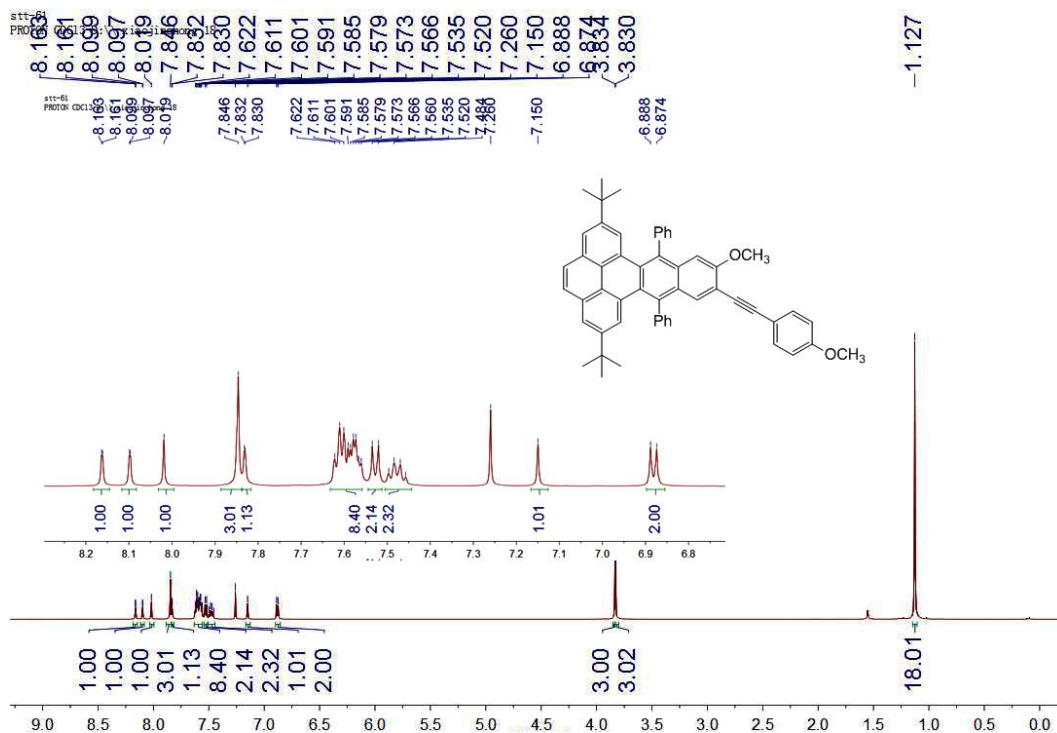


Figure S16 ^1H NMR spectrum of **3b**.

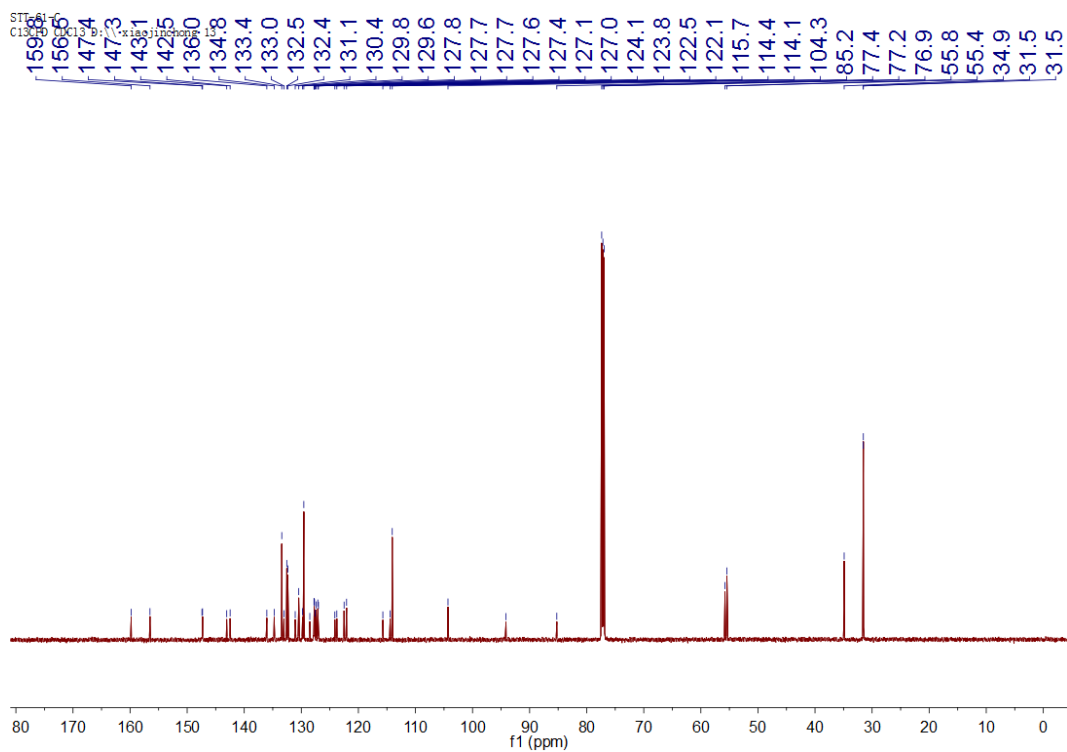


Figure S17 ^{13}C NMR spectrum of **3b**.

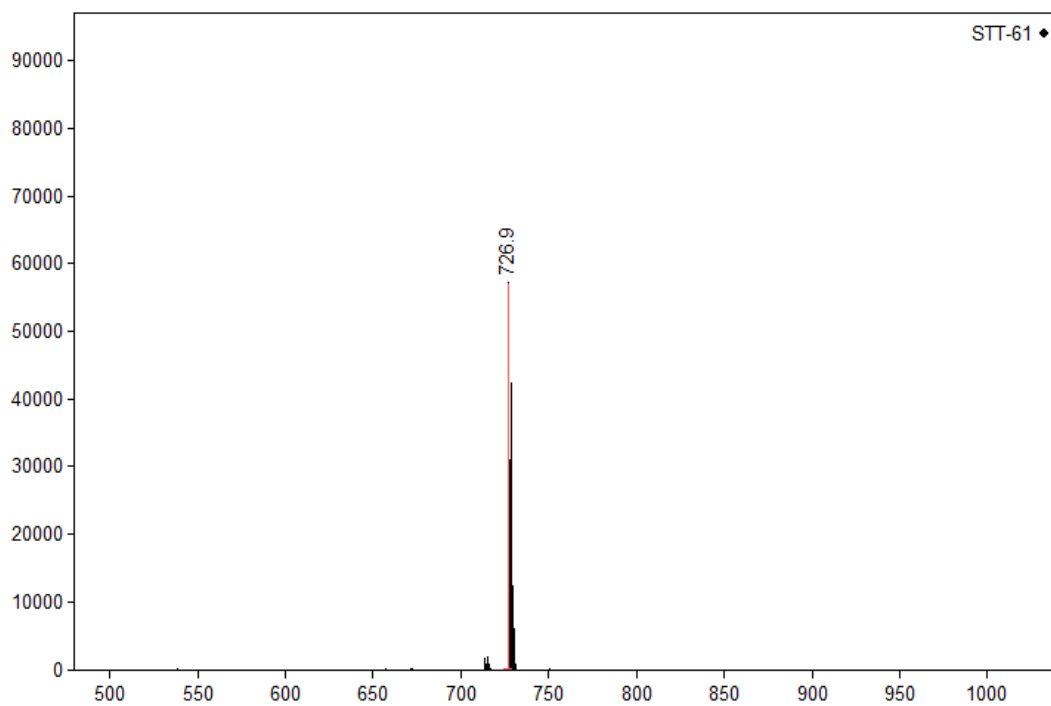
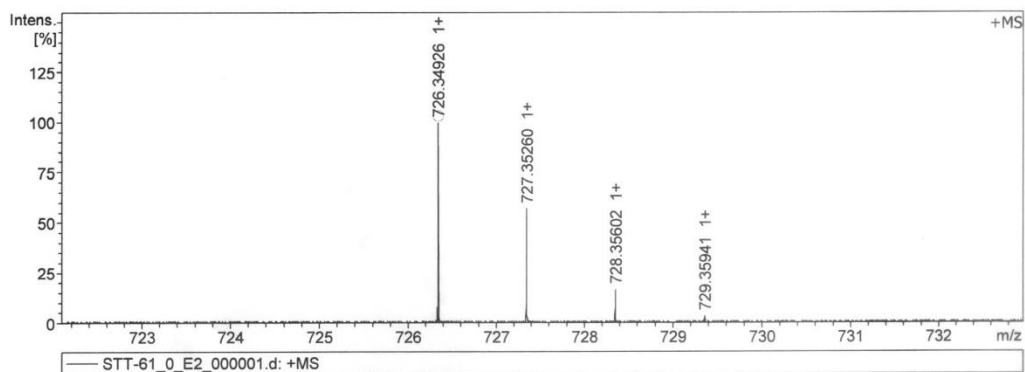


Figure S18 MALDI-TOF spectrum of **3b**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
726.349263	1	C54H46O2	100.00	726.349232	0.0	-0.0	8.4	32.0	odd	ok

Figure S19 HR-MS spectrum of **3b**.

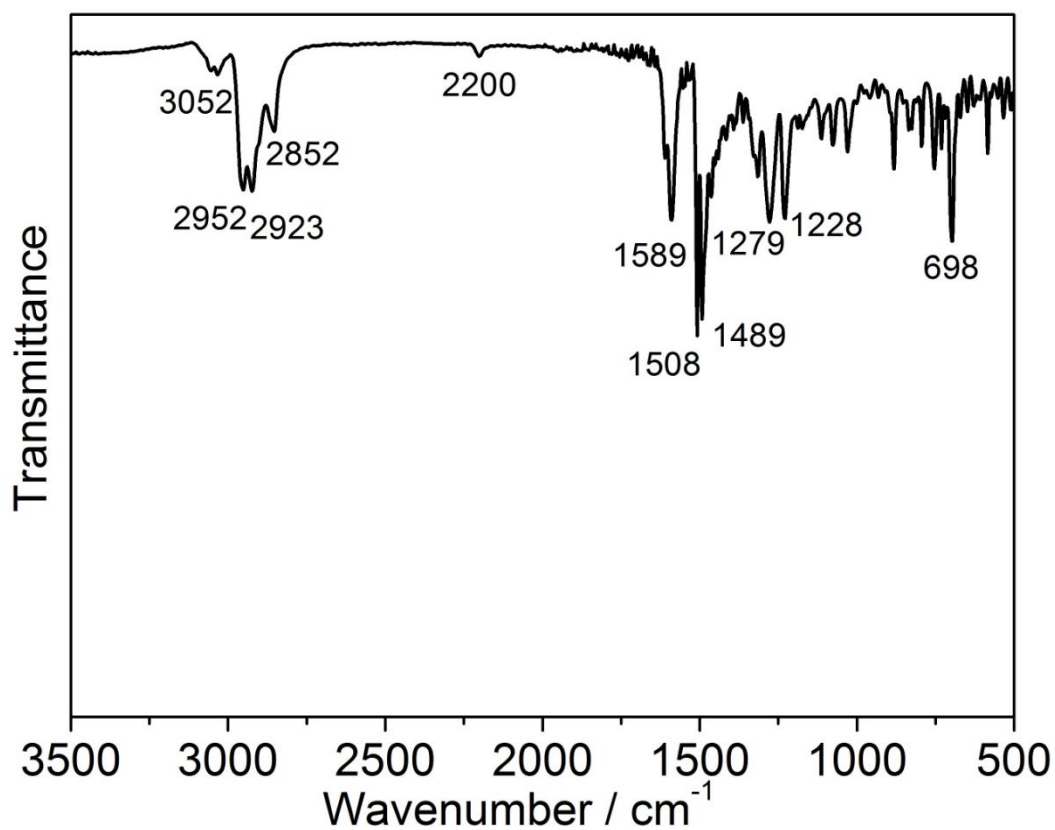


Figure S20 FT-IR spectrum of **3c**.

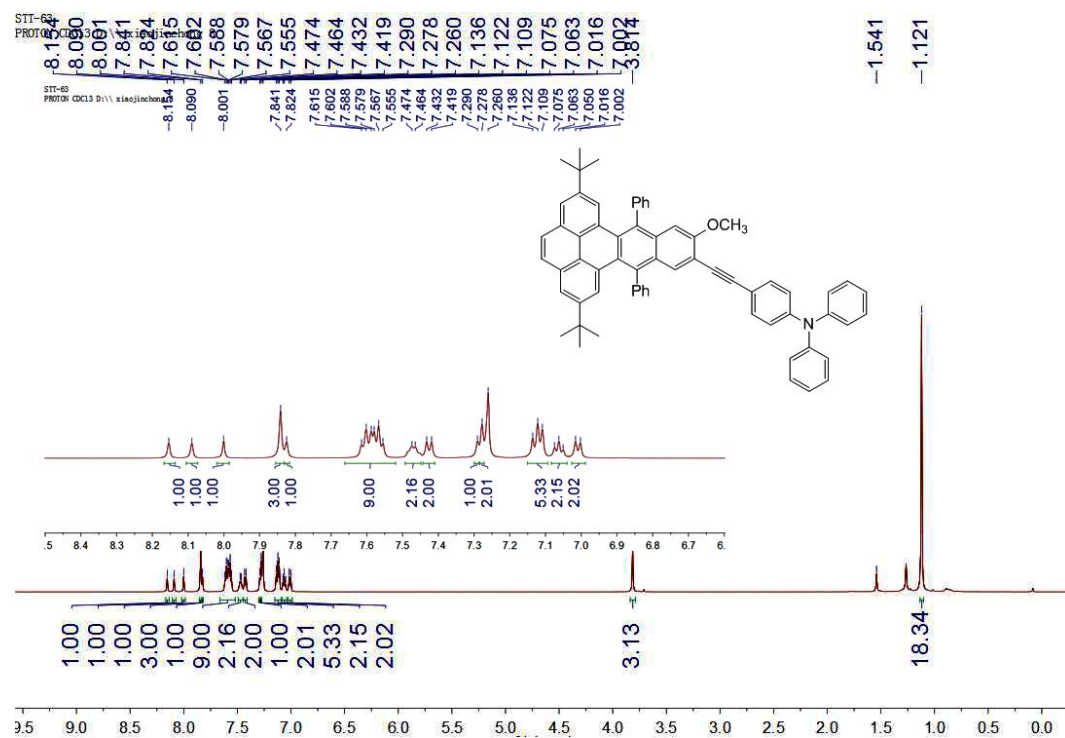


Figure S21 ¹H NMR spectrum of **3c**.

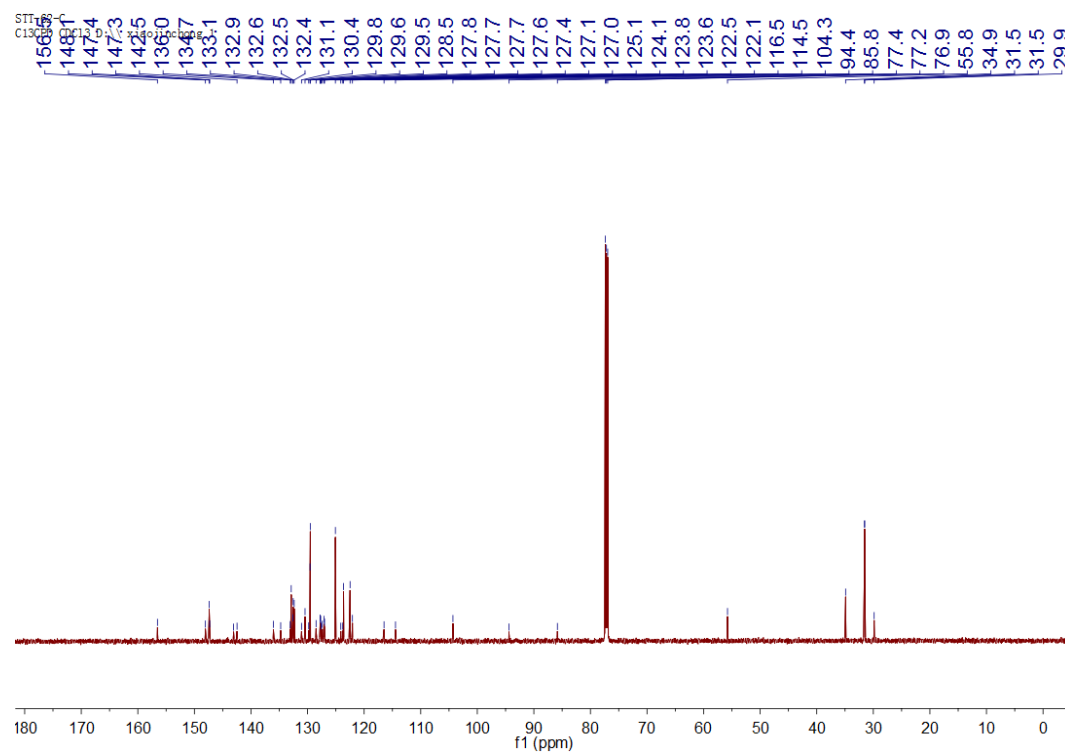


Figure S22 ¹³C NMR spectrum of **3c**.

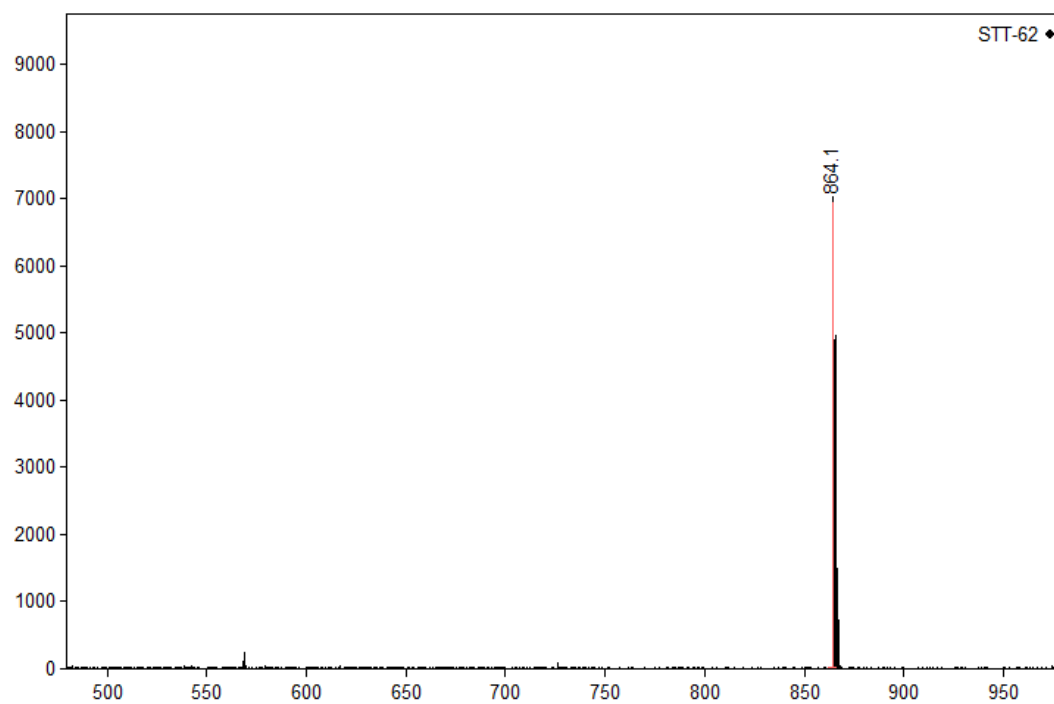
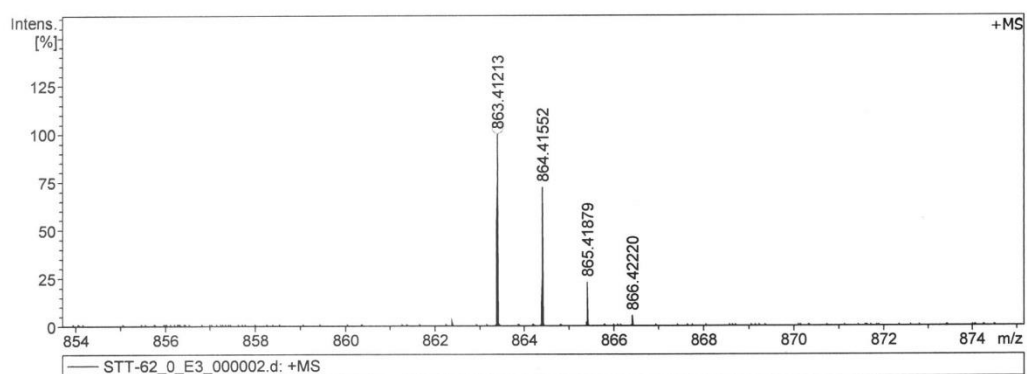


Figure S23 MALDI-TOF spectrum of **3c**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
863.412134	1	C ₆ H ₅ N ₃ O	100.00	863.412167	-0.0	0.0	12.1	40.0	odd	ok

Figure S24 HR-MS spectrum of **3c**.

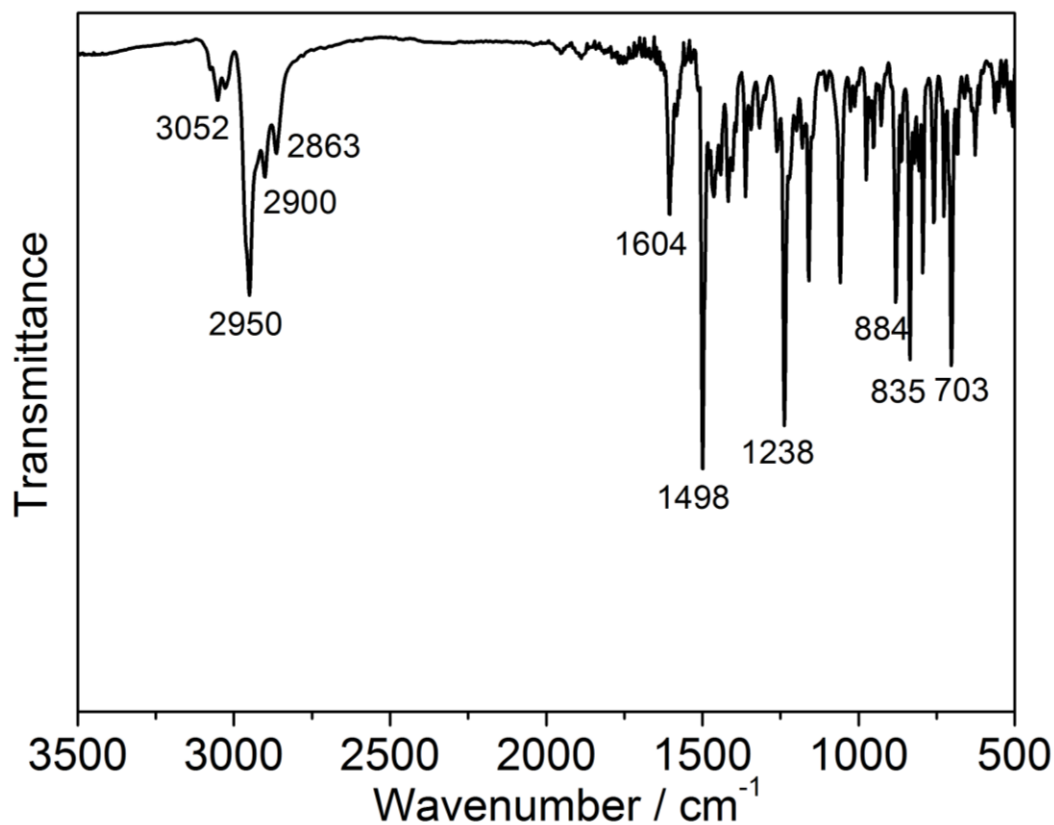


Figure S25 FT-IR spectrum of **4a**.

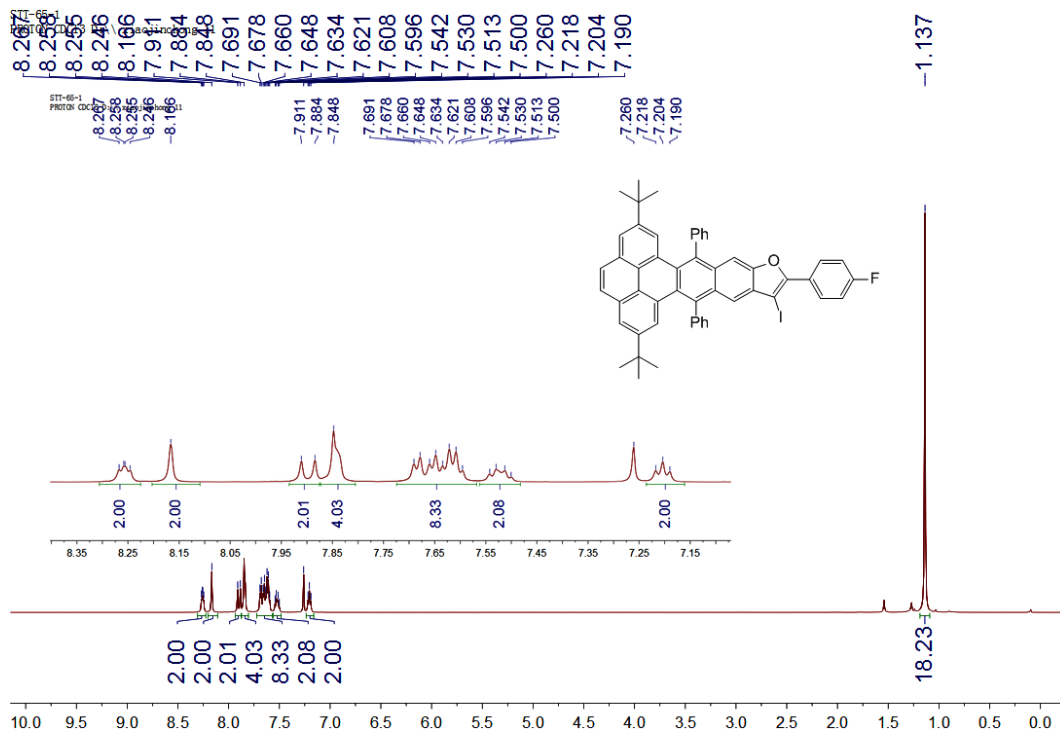


Figure S26 ^1H NMR spectrum of **4a**.

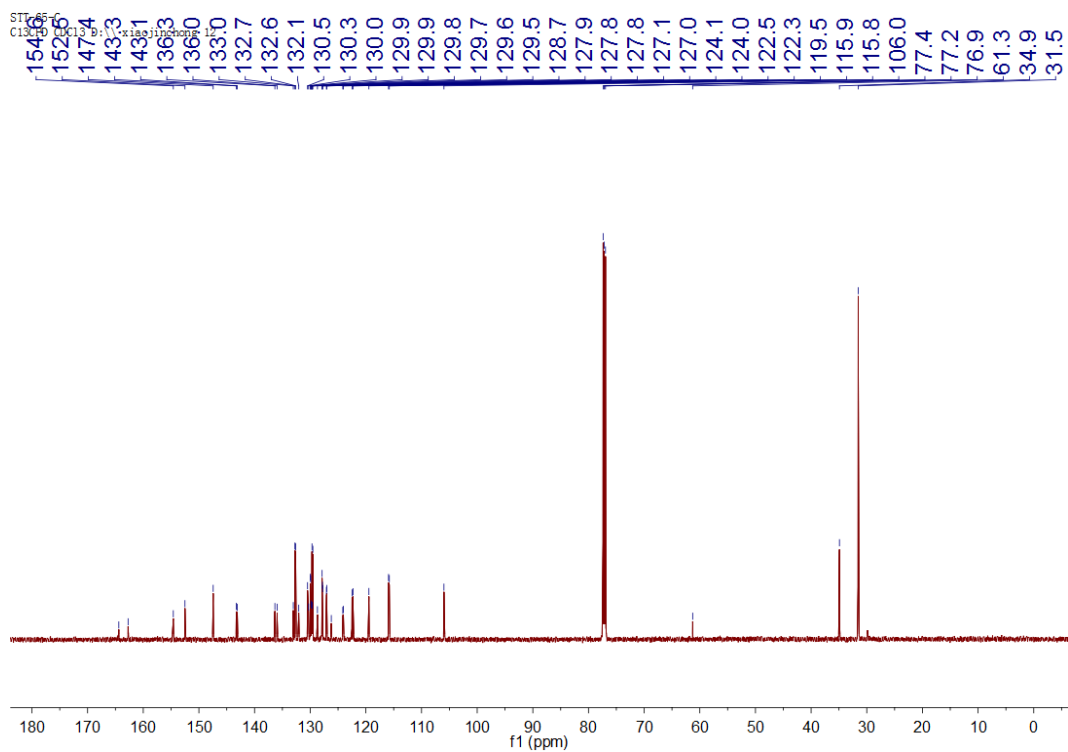


Figure S27 ^{13}C NMR spectrum of **4a**.

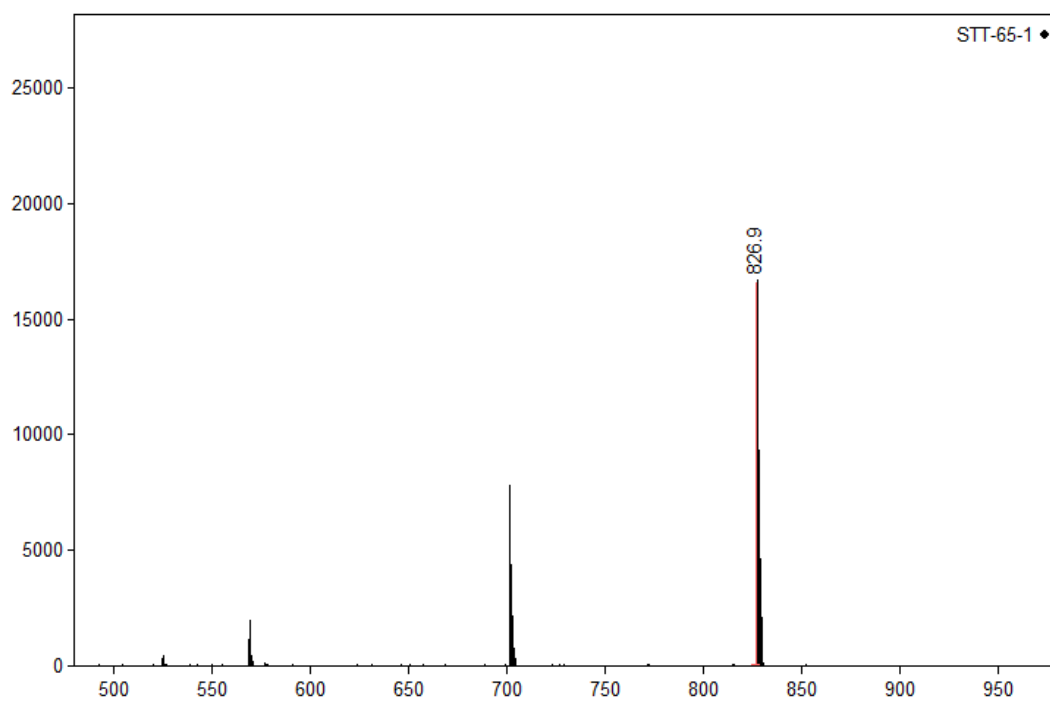


Figure S28 MALDI-TOF spectrum of **4a**.

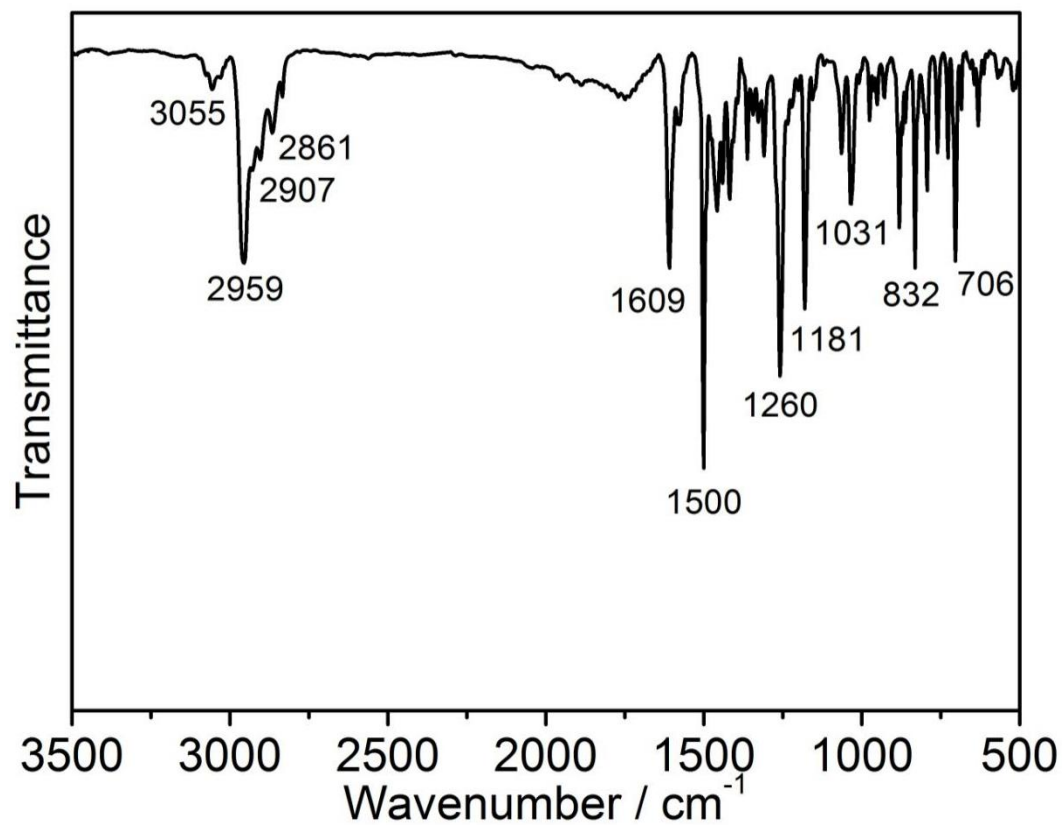


Figure S29 FT-IR spectrum of **4b**.

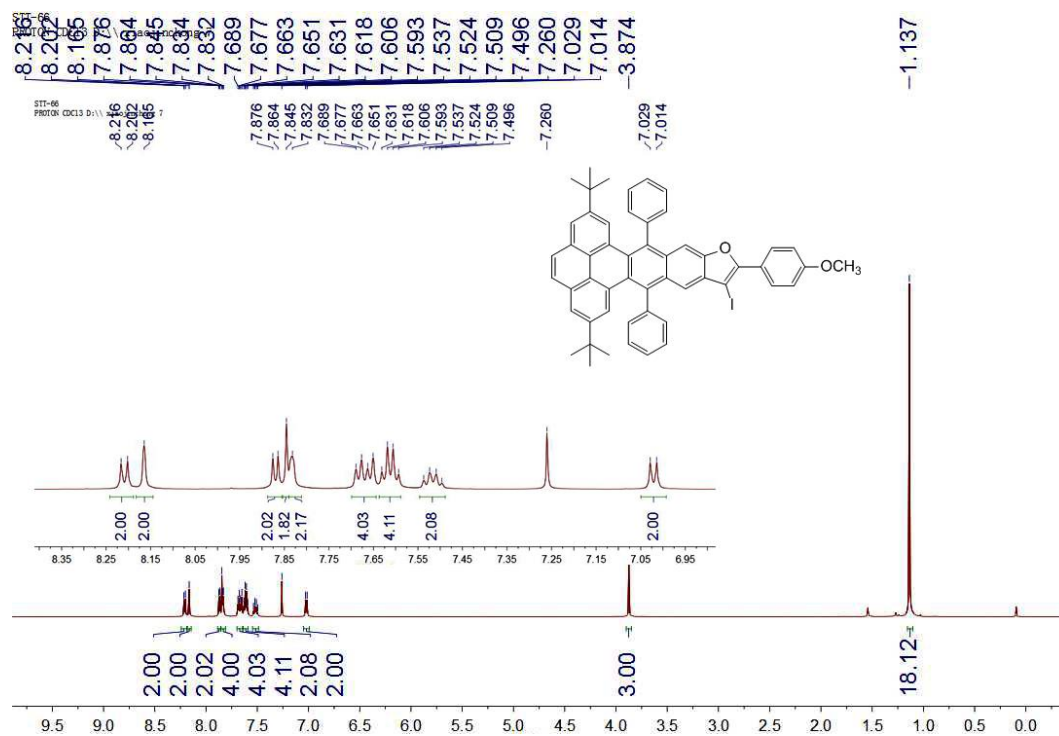


Figure S30 ^1H NMR spectrum of **4b**.

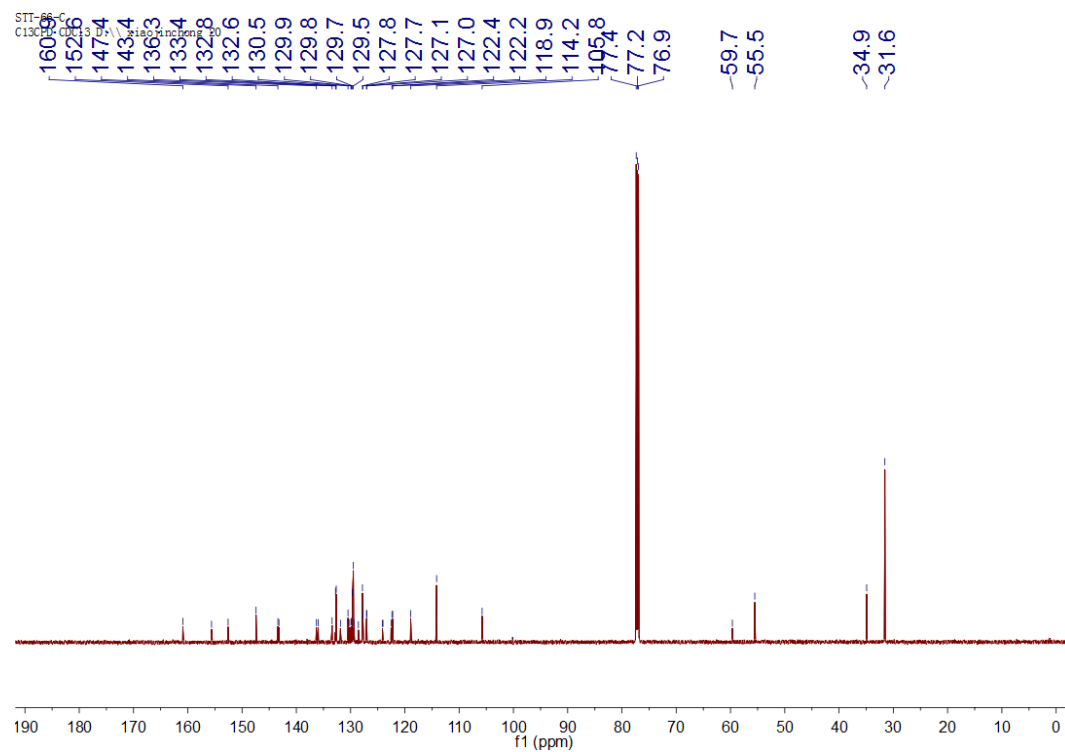


Figure S31 ^{13}C NMR spectrum of **4b**.

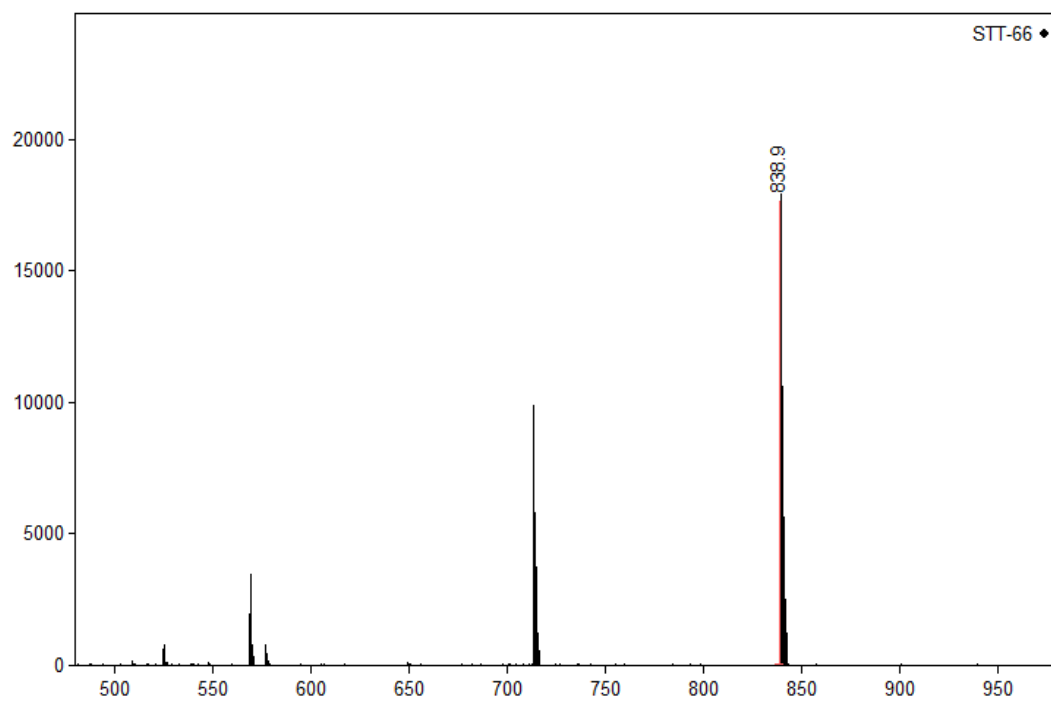


Figure S32 MALDI-TOF spectrum of **4b**.

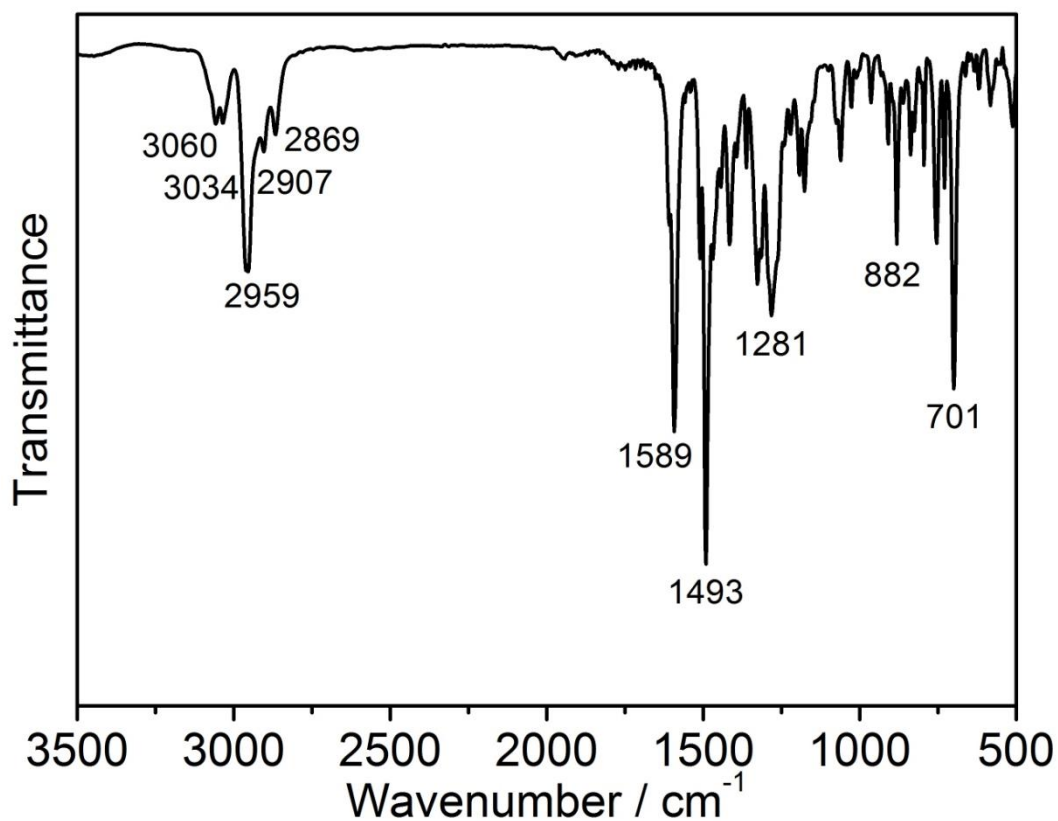


Figure S33 FT-IR spectrum of **D5c**.

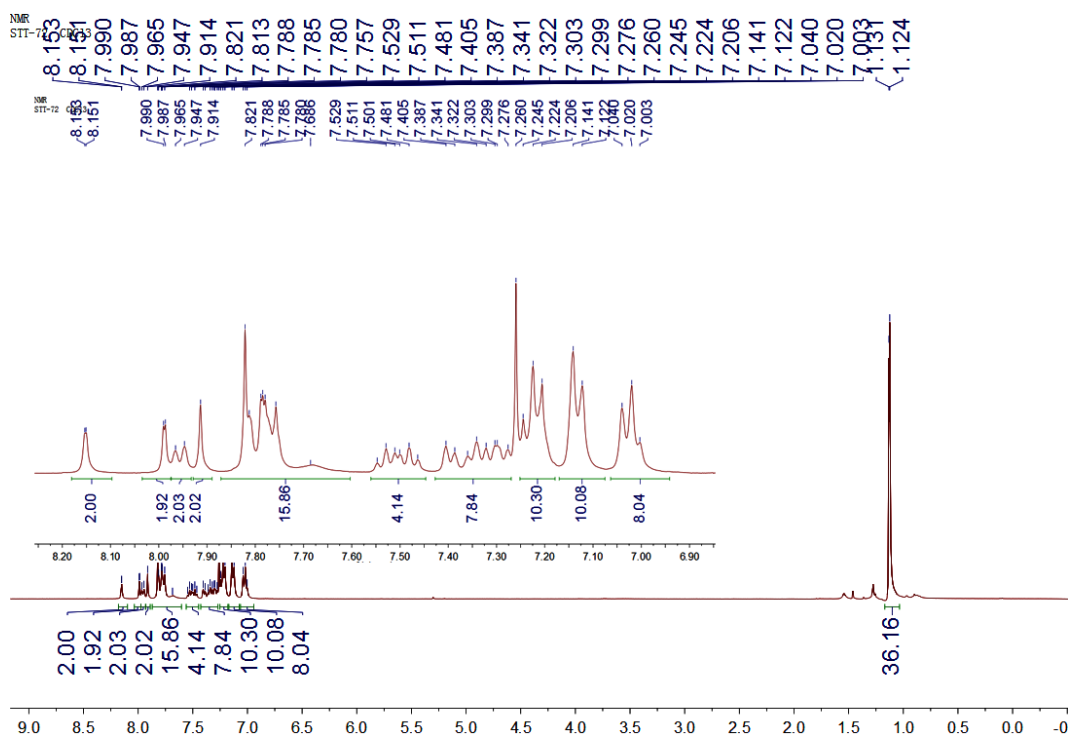


Figure S34 ^1H NMR spectrum of **D5c** (400 MHz).

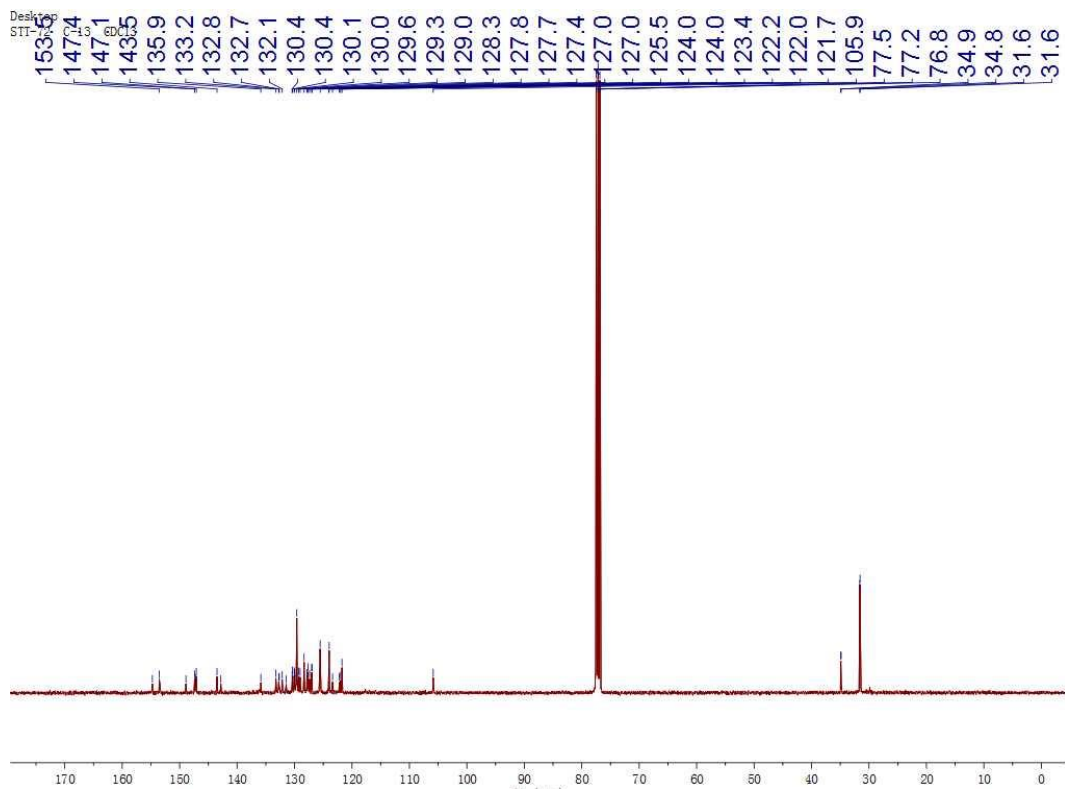


Figure S35 ^{13}C NMR spectrum of **D5c** (100MHz).

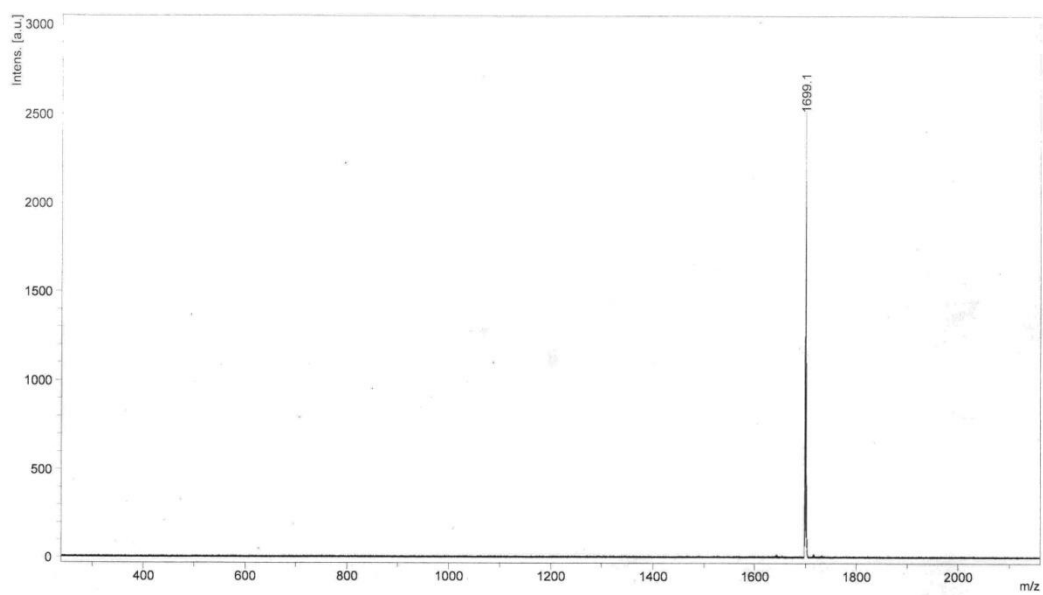


Figure S36 MALDI-TOF spectrum of **D5c**.

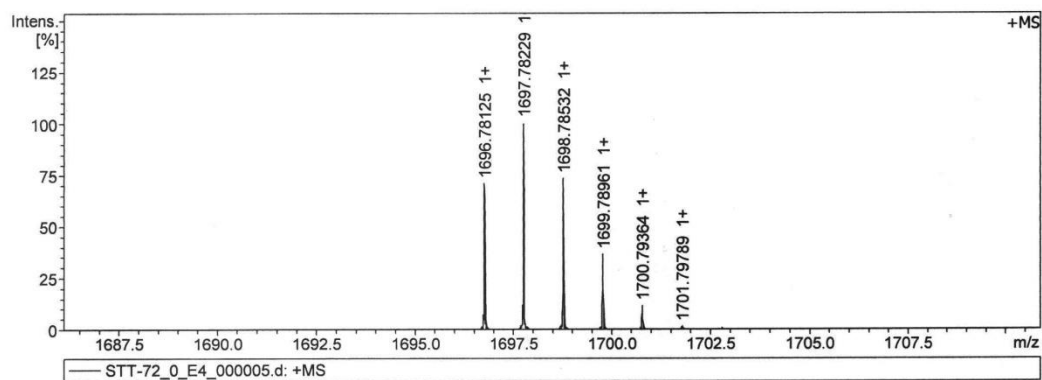


Figure S37 HR-MS spectrum of **D5c**.

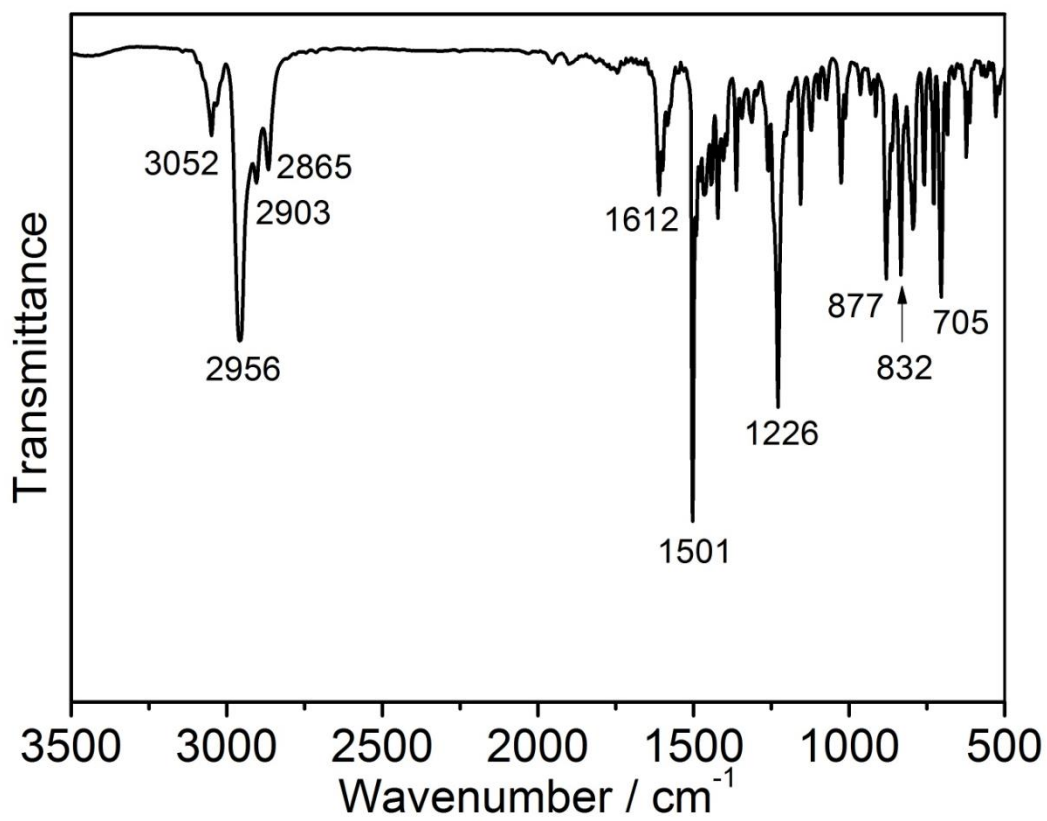


Figure S38 FT-IR spectrum of **5a**.

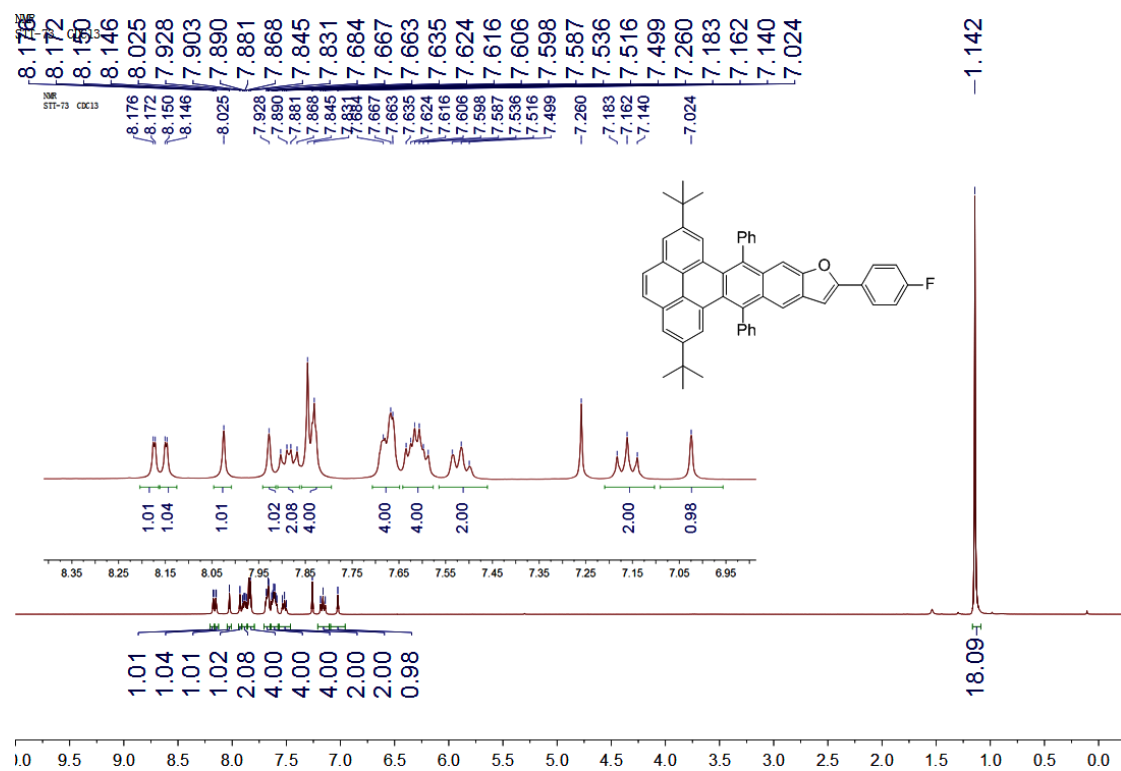


Figure S39 ¹H NMR spectrum of 5a (400 MHz).

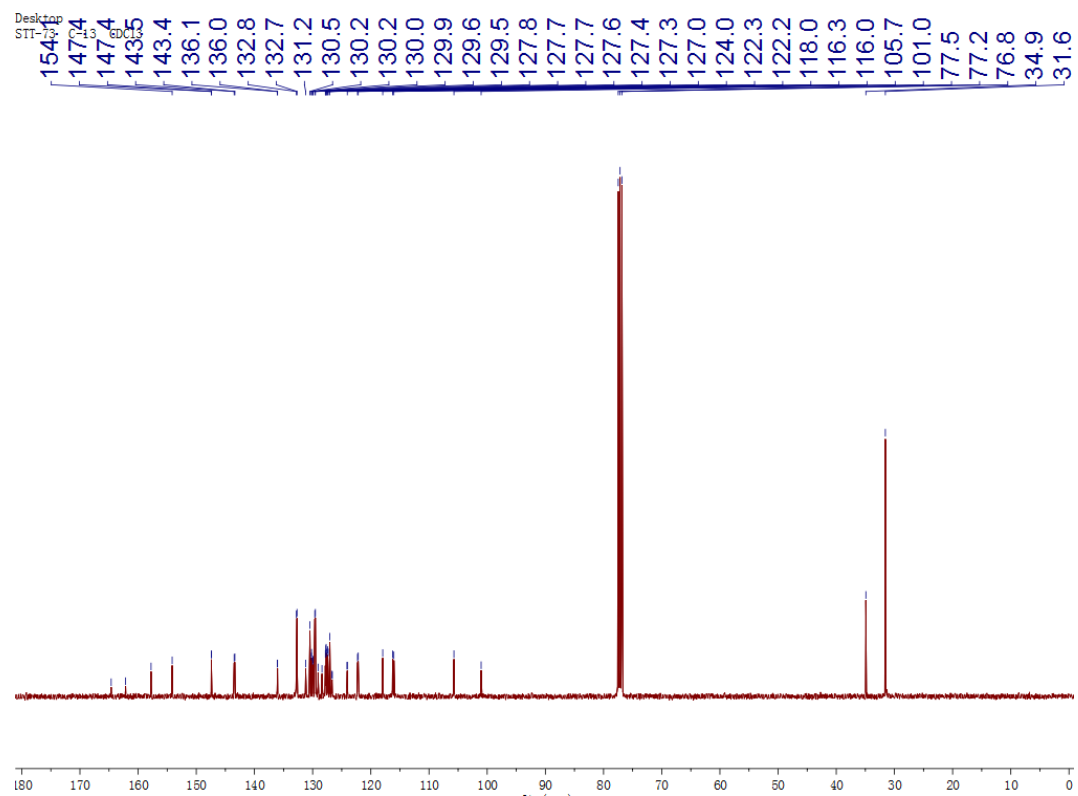
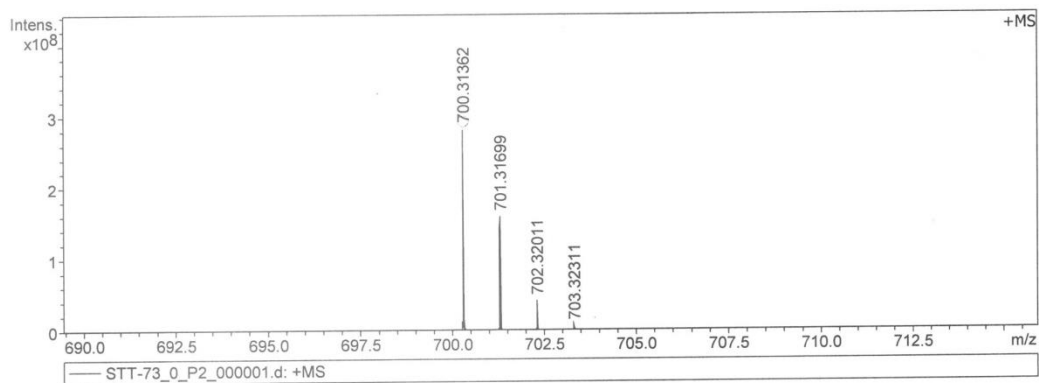


Figure S40 ¹³C NMR spectrum of 5a (100 MHz).



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
700.313617	1	C52H41FO	100.00	700.313596	-0.0	0.0	5.9	32.0	odd	ok

Figure S41 HR-MS spectrum of **5a**.

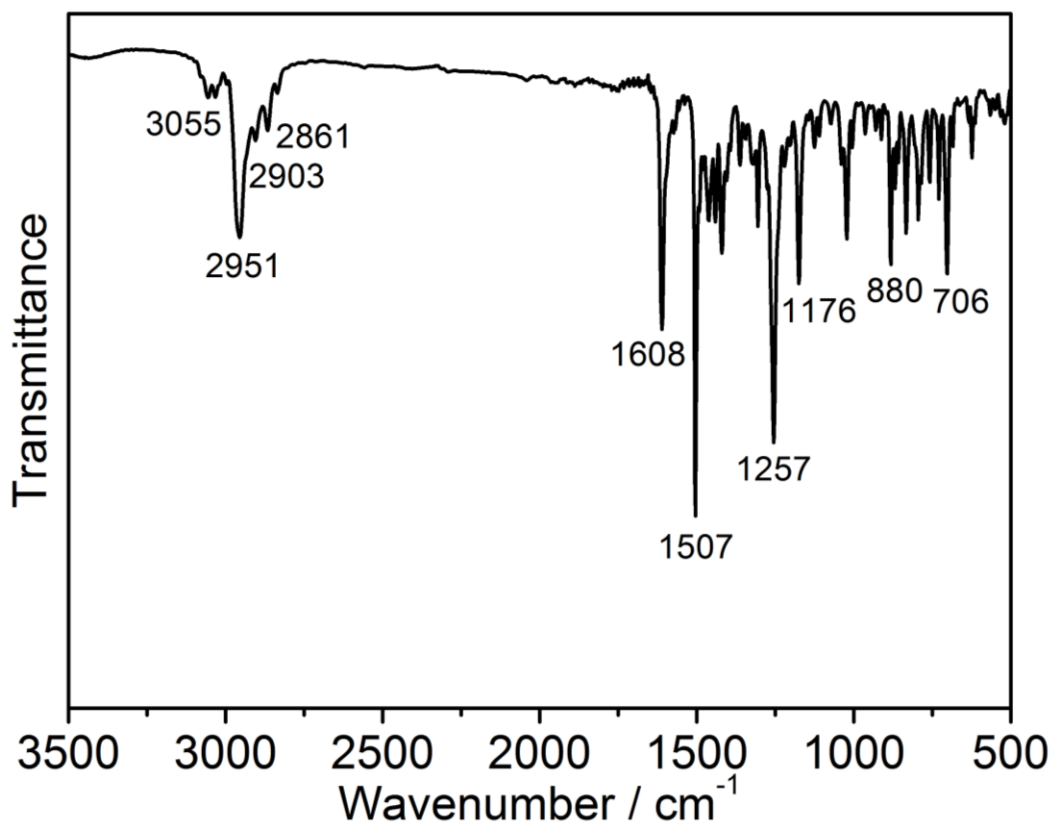


Figure S42 FT-IR spectrum of **5b**.

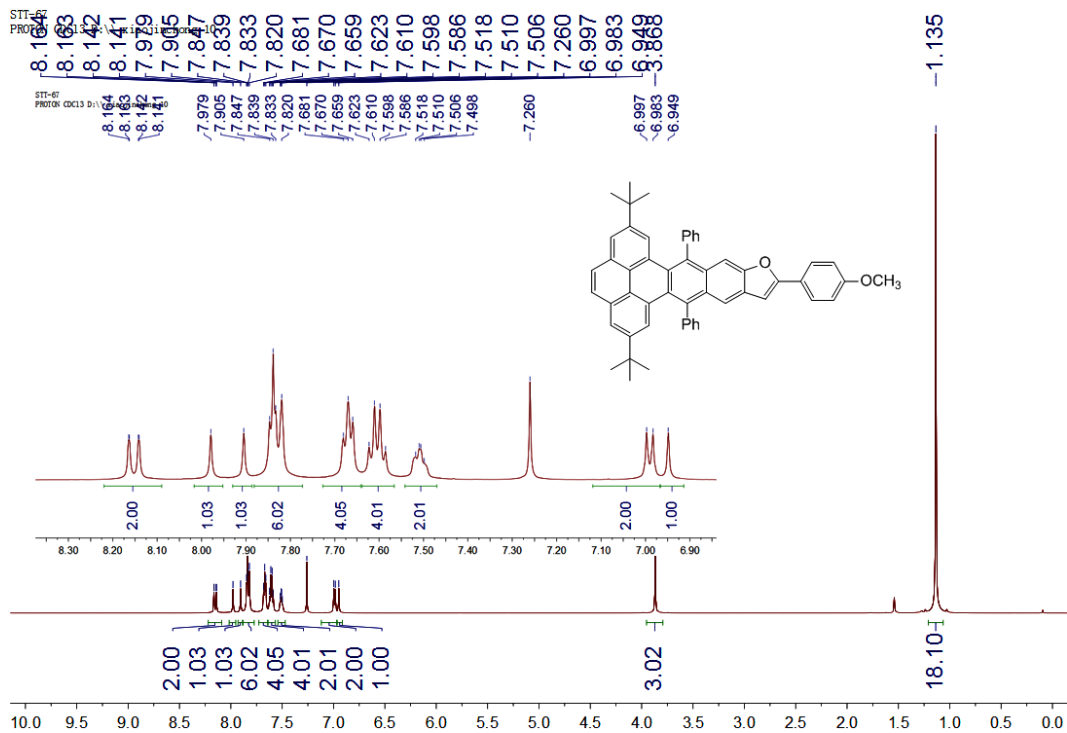


Figure S43 ¹H NMR spectrum of **5b** (600 MHz).

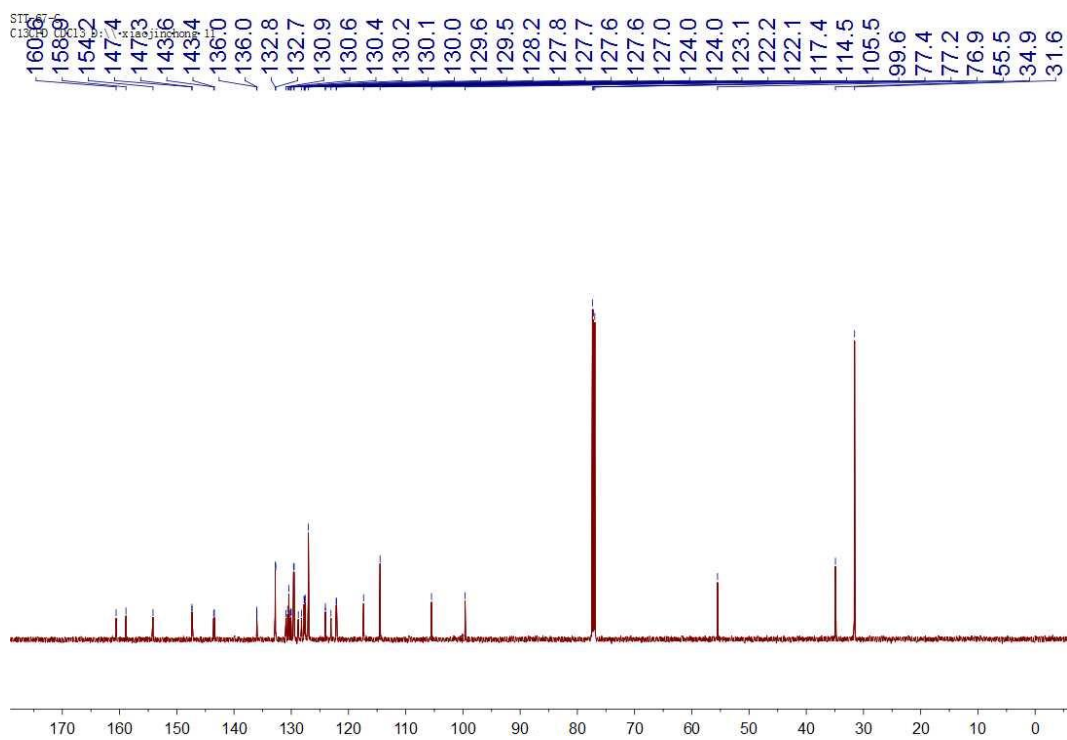


Figure S44 ¹³C NMR spectrum of **5b**.

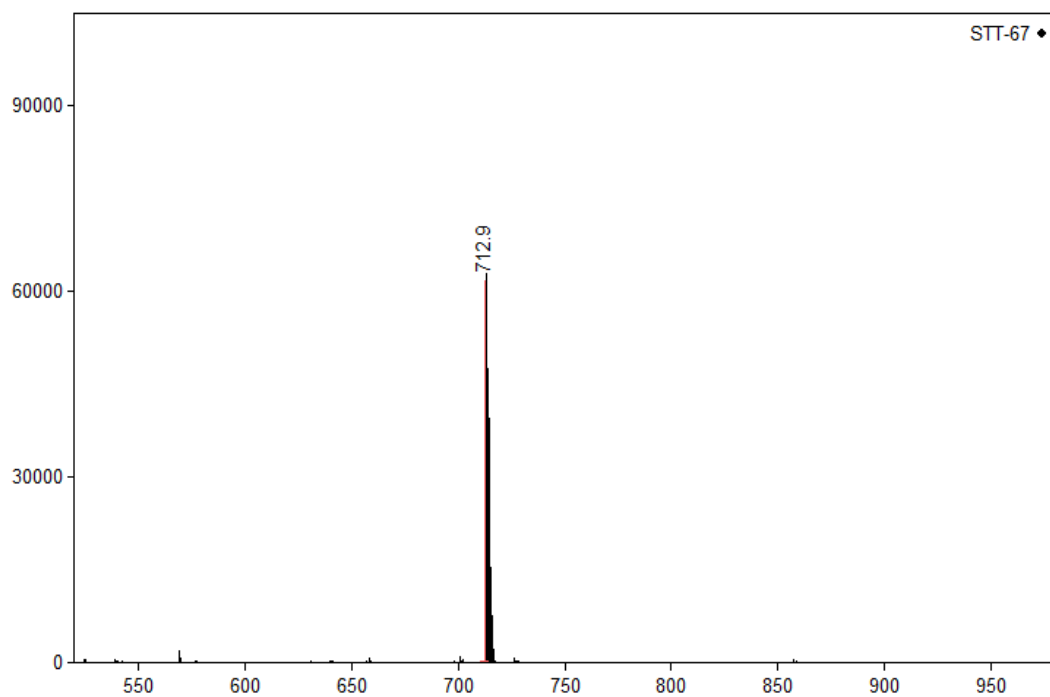
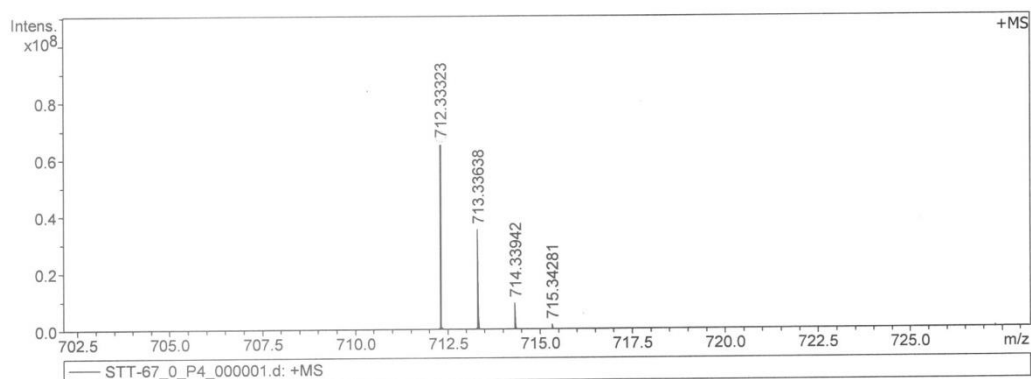


Figure S45 MALDI-TOF spectrum of **5b**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
712.333230	1	C ₅₃ H ₄₄ O ₂	100.00	712.333582	-0.5	0.7	22.4	32.0	odd	ok

Figure S46 HR-MS spectrum of **5b**.