Supplementary Information (SI) for Chemical Science.
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Supporting Information

Palladium/Norbornenes-Catalyzed C−H Bond Activation and Annulation to Construct Polycyclic Aromatic Hydrocarbons-based Fluorescent Materials

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1. General Information

Unless otherwise noted, commercial available reagents were purchased from commercial suppliers (such as Energy Chemical, Bide Pharmatech Ltd. and Adamas) and used as received. Solvents were generally dried over 4Å molecular sieves. Purification of products was performed by flash column chromatography using silica gel. ^{1}H and ^{13}C NMR spectra were recorded on a Agilent 400MR DD2 spectrometer (400 MHz and 101 MHz, respectively). Chemical shifts are reported parts per million (ppm) referenced to $CDCl_3$ (δ 7.26 ppm), tetramethylsilane (TMS, δ 0.00 ppm) for ^{1}H NMR; $CDCl_3$ (δ 77.16 ppm) for ^{13}C NMR. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet and m = multiplet. To distinguish, some ^{13}C NMR chemical shifts retain two decimal places. High-resolution mass spectra (HRMS) were obtained on an Agilent 6546 Q-TOF LC/MS system with an ESI source at the School of Pharmaceutical Sciences of Chongqing University. UV−vis spectra were recorded on Agilent Cary60 spectrometer. Fluorescence spectra were collected on HITACHI F-700003040428 Fluorescence Spectrometer or Agilent Technologies Cary Eclipse Fluorescence Spectrometer. The absolute quantum yields were taken using Edinburgh Instruments FLS1000 fluorescence spectrometer with a calibrated integrating sphere system. The excited-state lifetimes were performed using Edinburgh Instruments FLS1000.

2. DFT Calculation

All calculations were performed using the Gaussian 16, Revision A.03.[S1] Geometries were optimized in toluene with the SMD solvation model by the B3-LYP-D3 functional and a basis set of 6-31G(d). Vibrational frequencies were calculated at the same level and check the optimized structure. Solvation energies were computed through a self-consistent reaction field using the SMD model. Calculations were performed at the M06/SDD-6-31+G(d,p)-SMD(toluene) level of theory.

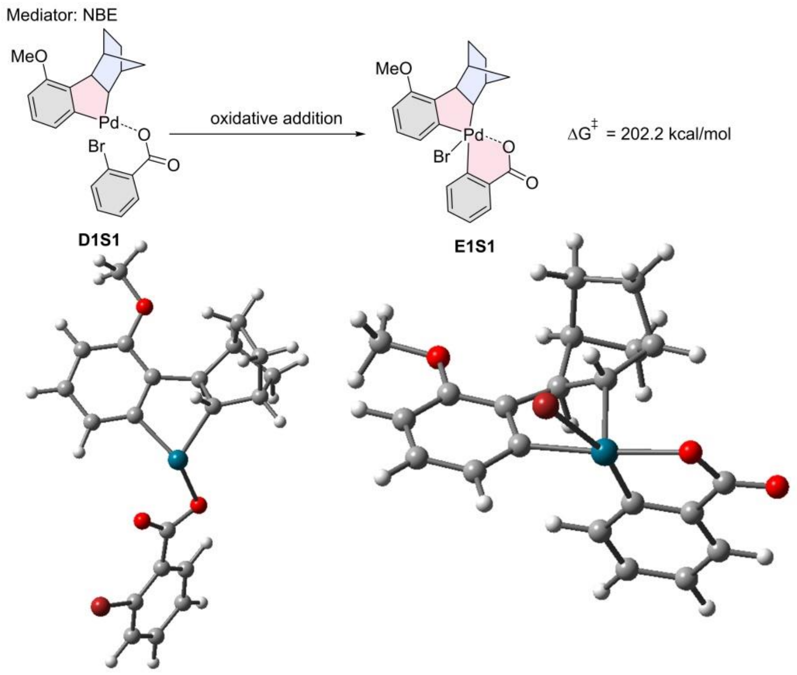


Fig. S1. DFT calculates the free-energy barrier of the reaction of the rate-determining step using norbornene (NBE) as a mediator.

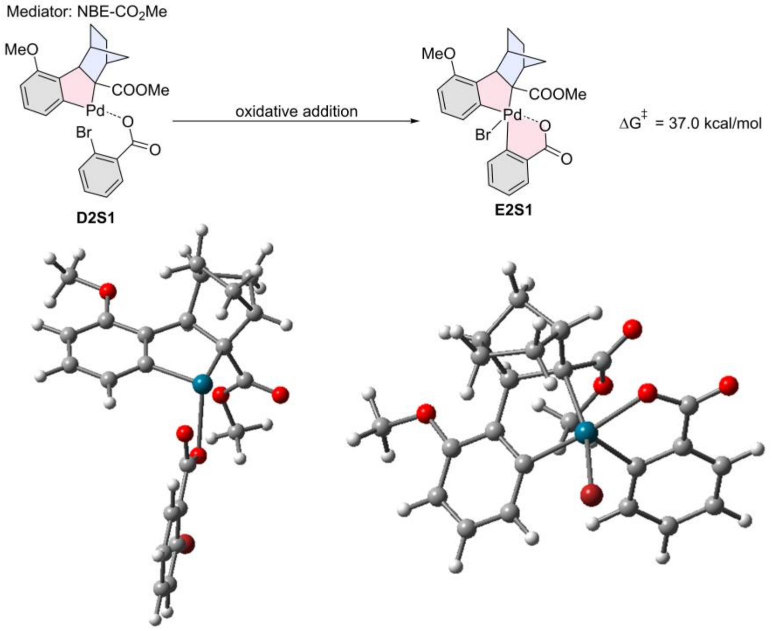


Fig. S2. DFT calculates the free-energy barrier of the reaction of the rate-determining step using methyl bicyclo[2.2.1]hept-2-ene-2-carboxylate (NBE-CO_2Me) as a mediator.

Cartesian coordinates of the structures

D1S1

C	-2.00716	-1.35636	-0.32571
C	-2.62379	3.31508	1.17352
C	-1.44274	3.57769	0.45362
C	-0.78516	2.55658	-0.25536
C	-1.3515	1.27305	-0.23643
C	-2.52727	0.97071	0.46851
C	-3.16388	2.01622	1.18084
C	-4.26955	-0.09583	-1.79398
C	-4.36042	-0.71481	-0.37102
C	-3.0324	-0.44225	0.42772
C	-3.22945	-1.01968	-2.52092
C	-2.83758	-2.05852	-1.42299
C	-4.20128	-2.2309	-0.67786
Pd	-0.46398	-0.24275	-1.22047
C	5.80371	0.58778	0.25377
C	6.3287	1.33408	-0.81154
C	5.49278	1.7191	-1.87301
C	4.1441	1.35166	-1.85307
C	3.58989	0.59818	-0.78825
C	4.44786	0.22077	0.26925
Br	3.88601	-0.8049	1.81801
C	2.13653	0.27648	-0.89713
O	1.5118	-0.42133	0.00047
O	1.46732	0.71723	-1.92283
O	-4.32008	1.658	1.86568
C	-5.02381	2.64445	2.66166
C	-1.14855	-2.26722	0.47886
O	-0.59014	-3.28981	0.03156
O	-0.98005	-1.85739	1.77622
C	-0.00882	-2.58372	2.59904
H	-3.10802	4.12514	1.72141
H	-1.03041	4.59153	0.44866
H	0.13457	2.76111	-0.80917
H	-3.95512	0.96144	-1.7699
H	-5.25475	-0.13325	-2.29298
H	-5.25731	-0.41761	0.19181
H	-3.18025	-0.80996	1.45888
H	-3.67358	-1.53589	-3.39151
H	-2.35469	-0.45733	-2.90028
H	-2.36452	-2.97384	-1.80549
H	-4.99541	-2.63423	-1.3326
H	-4.12848	-2.86048	0.22702
H	6.44959	0.28661	1.08199
H	7.38694	1.61061	-0.80635
H	5.88987	2.30095	-2.70906
H	3.47111	1.63703	-2.66385

H	-5.87751	2.11178	3.10652
H	-4.37785	3.04563	3.4655
H	-5.39403	3.47696	2.03365
H	-0.07017	-2.11984	3.59367
H	-0.26983	-3.65424	2.64583
H	1.00048	-2.46321	2.17172

E1S1

C	0.60361	1.62205	-0.00889
C	3.48631	-2.36522	0.80719
C	2.38377	-3.16964	0.46346
C	1.17873	-2.59879	0.02566
C	1.0719	-1.19731	-0.07192
C	2.17037	-0.37298	0.25384
C	3.37544	-0.97004	0.70856
C	2.38703	1.13015	-2.39376
C	2.79602	1.81789	-1.06553
C	2.06851	1.12735	0.1535
C	0.88558	1.53913	-2.54396
C	0.60569	2.45328	-1.29897
C	2.00396	3.15085	-1.14219
Pd	-0.59934	-0.13198	-0.63962
C	-1.60308	-1.48091	1.92641
C	-2.57248	-1.60902	2.94384
C	-3.72629	-0.80482	2.94145
C	-3.93008	0.13051	1.9148
C	-2.97841	0.27221	0.89065
C	-1.81784	-0.51882	0.93768
Br	-1.4884	-2.0978	-2.03715
C	-3.17227	1.21657	-0.26042
O	-2.1743	1.18151	-1.14107
O	-4.18487	1.93994	-0.37743
O	4.38637	-0.08247	1.04782
C	5.65905	-0.58078	1.53792
C	-0.12069	2.27689	1.15194
O	-0.82756	3.27517	0.95114
O	-0.00058	1.85672	2.44496
C	0.81624	0.78412	3.00694
H	4.41278	-2.83284	1.14485
H	2.46791	-4.25817	0.54055
H	0.33888	-3.24361	-0.23699
H	2.99597	1.51954	-3.22872
H	2.53184	0.03692	-2.36651
H	3.8807	1.89145	-0.90506
H	2.5145	1.56997	1.06391
H	0.2063	0.66473	-2.63031
H	0.69442	2.12375	-3.46051
H	-0.27463	3.09478	-1.39812
H	2.25141	3.76804	-2.02447
H	2.08253	3.77537	-0.23482

H	-0.71996	-2.12124	1.93069
H	-2.41787	-2.35063	3.73362
H	-4.47239	-0.91882	3.73301
H	-4.82445	0.7597	1.87173
H	6.26806	0.31355	1.74015
H	5.53091	-1.15817	2.47345
H	6.16455	-1.20602	0.77785
H	0.35185	0.55982	3.97921
H	0.81245	-0.11562	2.3773
H	1.8489	1.13891	3.16932

D2S2

C	2.48081	-1.28104	0.65082
C	2.142	3.34026	-0.2073
C	0.94322	3.27496	0.49893
C	0.38519	2.04918	0.86589
C	1.08443	0.91196	0.50708
C	2.26263	0.94621	-0.22676
C	2.80714	2.17248	-0.58641
C	5.13023	-0.79989	0.10779
C	4.11563	-0.91813	-1.06012
C	2.72982	-0.42708	-0.598
C	4.75448	-1.99407	1.05818
C	3.41186	-2.50478	0.45114
C	3.78835	-2.44234	-1.05736
Pd	0.47828	-0.95681	1.01287
C	-5.36954	0.04562	-1.22582
C	-5.38847	-0.58213	-2.46163
C	-4.25903	-1.25886	-2.90984
C	-3.13227	-1.29576	-2.10991
C	-3.10488	-0.6712	-0.85892
C	-4.23824	0.00658	-0.42251
Br	-4.36262	0.93044	1.24632
C	-1.83234	-0.79909	-0.10721
O	-0.83895	-1.40762	-0.69211
O	-1.66822	-0.35285	1.07866
O	3.98831	2.12572	-1.30167
C	4.59442	3.38028	-1.69928
H	2.80343	-0.73151	1.54812
H	2.54416	4.30833	-0.47033
H	0.43302	4.19363	0.76139
H	-0.56393	1.97988	1.37985
H	5.03555	0.17277	0.59551
H	6.15519	-0.9028	-0.25684
H	4.45105	-0.48471	-1.99898
H	2.02567	-0.76711	-1.37403
H	5.51064	-2.78367	1.00429
H	4.64559	-1.68334	2.10008
H	3.07436	-3.46627	0.83579
H	2.96172	-2.69515	-1.72566

H	4.65552	-3.06859	-1.28172
H	-6.2388	0.57867	-0.868
H	-6.28247	-0.53917	-3.07052
H	-4.25994	-1.75025	-3.87373
H	-2.23337	-1.80702	-2.42236
H	5.49738	3.10349	-2.24138
H	3.93369	3.95685	-2.35554
H	4.86043	3.99253	-0.83079

E2S2

C	0.06398	0.40018	1.20071
C	-3.74184	0.00752	-1.68353
C	-3.14362	-1.12643	-2.21022
C	-1.85103	-1.48933	-1.83168
C	-1.14377	-0.68022	-0.91686
C	-1.76417	0.47488	-0.39466
C	-3.04449	0.82885	-0.77884
C	-1.58029	1.87853	2.76817
C	-1.05833	2.46479	1.43001
C	-0.82109	1.32984	0.39648
C	-0.30759	1.21225	3.40637
C	0.74143	1.29098	2.24932
C	0.44619	2.73358	1.75276
Pd	0.78811	-0.99752	-0.14916
C	1.35702	1.21011	-2.17676
C	2.25308	2.1125	-2.75451
C	3.56002	2.22059	-2.28181
C	3.98704	1.41407	-1.23414
C	3.10443	0.50994	-0.66463
C	1.79958	0.42194	-1.12559
Br	-0.93973	-2.93402	0.62152
C	3.5287	-0.39743	0.44622
O	2.55794	-1.25744	0.80134
O	4.64384	-0.3582	0.9534
O	-3.54174	1.99852	-0.25507
C	-4.87827	2.42454	-0.63205
H	-0.48836	-0.40932	1.68043
H	-4.74873	0.26186	-1.98295
H	-3.69209	-1.74117	-2.91259
H	-1.39402	-2.3778	-2.24597
H	-2.38159	1.15733	2.59044
H	-1.96779	2.671	3.4125
H	-1.64015	3.29099	1.03111
H	-0.18857	1.80855	-0.36042
H	0.05337	1.79763	4.25649
H	-0.48563	0.18667	3.73691
H	1.75861	1.03355	2.53179
H	1.02514	3.01807	0.87124
H	0.5903	3.46844	2.54774
H	0.34225	1.13239	-2.54714

H	1.92453	2.73197	-3.58032
H	4.24018	2.92947	-2.73657
H	4.9945	1.45324	-0.83633
H	-5.03838	3.35965	-0.09848
H	-4.9554	2.59799	-1.71019
H	-5.63277	1.69316	-0.32564

The time-dependent density functional theory (TDDFT) calculations of the excitation energies were calculated at the optimized geometries of the ground states. Calculations were performed at the B3LYP-6-31+G(d) (**6u**) and MPWLPW91-6-31+G(d) (**6w**) level of theory.

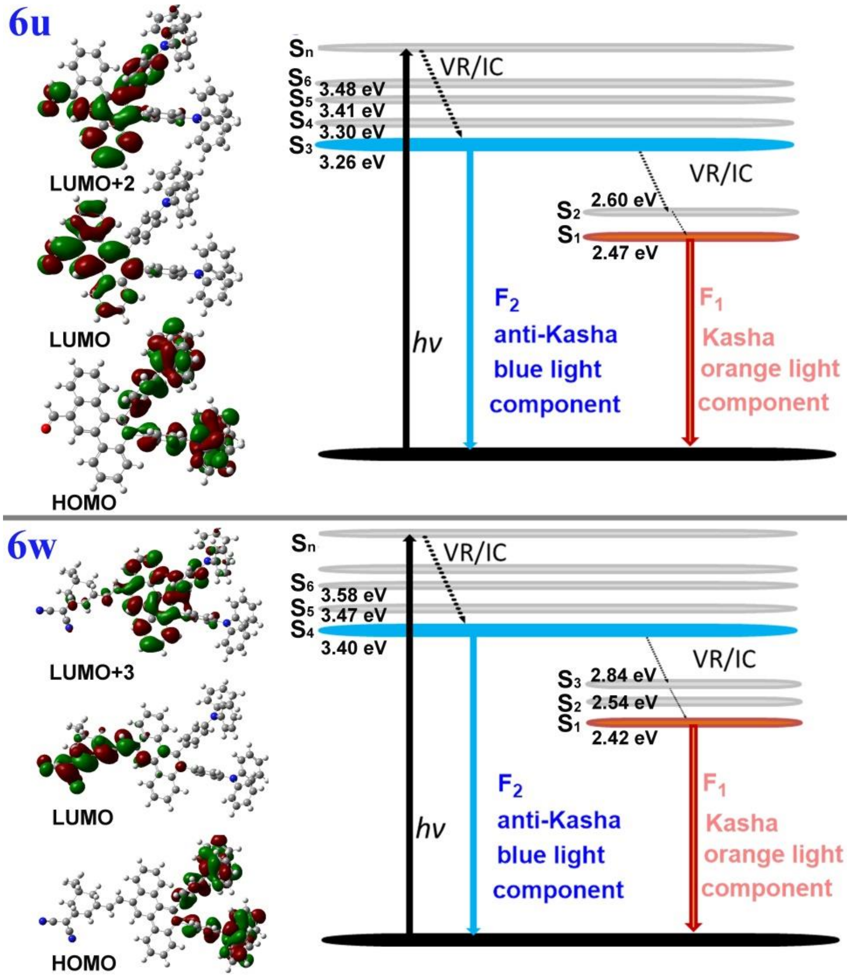


Fig. S3. Molecular orbitals of the S_0, S_1, S_3, or S_4 states of **6u** and **6w**; Jablonski diagram illustrating the anti-Kasha dual-emission mechanism of **6u** and **6w**.

Cartesian coordinates of the structures

6u

C	-6.74854	-0.45937	0.38766
C	-6.06282	0.74942	-0.00307
C	-6.09785	-1.66765	0.29141
C	-4.72465	-1.78524	-0.0533
C	-3.95104	-0.60275	-0.23434
C	-4.66898	0.67204	-0.35517
C	-2.50155	-0.72984	-0.28322
C	-4.11452	-3.09744	-0.16862
C	-4.87573	-4.29631	-0.13281
C	-4.27338	-5.53575	-0.25993
C	-2.87512	-5.63039	-0.42192
C	-2.10752	-4.4812	-0.4634
C	-2.70239	-3.19379	-0.35011
C	-1.90697	-1.98796	-0.34839
C	-1.59638	0.45695	-0.11741
C	-0.41248	-2.13113	-0.35468
C	-4.07113	1.84667	-0.89147
C	-4.76469	3.03921	-1.00534
C	-6.10599	3.12397	-0.58704
C	-6.74103	1.9932	-0.10847
C	-1.57773	1.16175	1.10019
C	-0.70918	2.2337	1.30415
C	0.18438	2.63185	0.29221
C	0.17122	1.93359	-0.93
C	-0.70677	0.8674	-1.12682
C	0.28551	-2.42114	-1.54085
C	1.67444	-2.55842	-1.54864
C	2.41345	-2.39877	-0.36175
C	1.7207	-2.11991	0.83133
C	0.33091	-1.99833	0.83123
N	1.08884	3.71395	0.50534
C	1.35171	4.64878	-0.54328
C	2.66226	5.10345	-0.78253
C	2.91249	6.02465	-1.80268
C	1.8692	6.49454	-2.60992
C	0.56572	6.0379	-2.37877
C	0.30327	5.12975	-1.35014
C	1.75306	3.84969	1.76527
C	2.27722	2.71959	2.42028
C	2.91889	2.85701	3.65378
C	3.06335	4.11846	4.24444
C	2.55005	5.24497	3.58988
C	1.89219	5.11545	2.36412
N	3.83531	-2.51319	-0.37077
C	4.50961	-3.17672	0.70101
C	5.69958	-2.64577	1.2333
C	6.35957	-3.30311	2.27458

C	5.83932	-4.48645	2.81305
C	4.65128	-5.01223	2.29052
C	3.99338	-4.37113	1.23793
C	4.58914	-1.94198	-1.444
C	5.67474	-2.64136	-2.00323
C	6.41452	-2.07563	-3.04473
C	6.07646	-0.81638	-3.55556
C	4.9916	-0.12227	-3.00571
C	4.25615	-0.67258	-1.95291
C	-8.14139	-0.4775	0.87018
O	-8.77053	-1.52159	1.1327
H	-6.67609	-2.54595	0.54836
H	-5.95193	-4.25237	-0.02595
H	-4.87992	-6.43528	-0.23738
H	-2.40339	-6.60323	-0.51489
H	-1.03428	-4.55382	-0.58313
H	-3.05527	1.81147	-1.24815
H	-4.27188	3.90711	-1.43147
H	-6.64741	4.06103	-0.66699
H	-7.78837	2.05811	0.15863
H	-2.26106	0.87344	1.89276
H	-0.71682	2.76496	2.24895
H	0.85308	2.22633	-1.72029
H	-0.69342	0.33886	-2.07372
H	-0.26647	-2.54626	-2.46775
H	2.19204	-2.78553	-2.47359
H	2.27506	-1.99736	1.75478
H	-0.18351	-1.7747	1.75997
H	3.47544	4.73291	-0.16885
H	3.92873	6.3658	-1.97428
H	2.06833	7.20523	-3.40513
H	-0.25384	6.40009	-2.99178
H	-0.70983	4.79142	-1.16424
H	2.17981	1.74277	1.95981
H	3.31887	1.97659	4.14711
H	3.56775	4.22191	5.19943
H	2.64927	6.22783	4.04002
H	1.48406	5.98814	1.86691
H	6.09938	-1.72278	0.82901
H	7.27642	-2.88089	2.67416
H	6.35127	-4.99068	3.62591
H	4.24044	-5.93278	2.69342
H	3.08194	-4.79034	0.82697
H	5.93147	-3.62224	-1.61942
H	7.2491	-2.62736	-3.46613
H	6.64921	-0.38292	-4.36871
H	4.72373	0.85824	-3.38701
H	3.42564	-0.1253	-1.52103
H	-8.63759	0.49209	1.02219

6w

C	-11.32954	-1.65787	-0.19484
C	-9.02175	-0.83752	-0.10565
C	-10.4112	-0.79448	0.30746
C	-10.77766	0.22029	1.36132
C	-9.98681	1.53624	1.21941
C	-8.47945	1.20879	1.21012
C	-8.10616	0.06015	0.30123
C	-6.71677	-0.1045	-0.13436
C	-5.68308	0.6538	0.23614
C	2.47195	-2.03257	0.80061
C	3.82193	-2.33078	0.89196
C	4.55434	-2.64839	-0.24852
C	3.9013	-2.66531	-1.47802
C	2.55545	-2.34851	-1.56235
C	1.91514	1.0101	-1.27217
C	2.88645	1.9653	-1.02236
C	2.91794	2.63966	0.19537
C	1.95319	2.33577	1.1511
C	0.99244	1.37117	0.89706
C	-3.95334	2.80042	-0.72385
C	-3.17899	3.82985	-1.17855
C	-1.8347	3.58787	-1.48482
C	-1.29294	2.34588	-1.29231
C	1.8195	-2.02013	-0.42763
C	0.95382	0.69264	-0.31749
C	0.35899	-1.6842	-0.52342
C	-0.57947	-2.77976	-0.54842
C	-0.14575	-4.12753	-0.59583
C	-1.04018	-5.1599	-0.59176
C	-2.41655	-4.89011	-0.53968
C	-2.85902	-3.59855	-0.47976
C	-1.95522	-2.50773	-0.47262
C	-0.07115	-0.38527	-0.53301
C	-2.04822	1.265	-0.7745
C	-1.49726	-0.0817	-0.58539
C	-2.40186	-1.13175	-0.42901
C	-3.77841	-0.84363	-0.16936
C	-3.4208	1.50601	-0.53004
C	-4.28083	0.4112	-0.15648
C	-10.30282	2.44042	2.42148
C	-10.39023	2.26625	-0.07579
C	-10.98352	-2.65168	-1.16343
N	-10.68715	-3.44359	-1.9402
C	-12.69679	-1.63551	0.22104
N	-13.79236	-1.60664	0.56404
N	5.94024	-2.94567	-0.16277
C	6.84977	-2.361	-1.08698
C	7.83728	-3.13647	-1.68995

C	8.72919	-2.56295	-2.58291
C	8.63908	-1.21503	-2.89979
C	7.65063	-0.4424	-2.30701
C	6.76601	-1.00623	-1.40061
C	6.4233	-3.80248	0.86431
C	7.54138	-3.446	1.61465
C	8.01375	-4.28811	2.60954
C	7.36979	-5.48671	2.88158
C	6.25095	-5.84033	2.14086
C	5.78411	-5.01047	1.13333
N	3.91824	3.61284	0.46028
C	4.62244	3.58859	1.69538
C	4.85204	4.76859	2.39928
C	5.54737	4.74407	3.59825
C	6.00809	3.54392	4.12053
C	5.77255	2.36621	3.42573
C	5.09224	2.38553	2.21793
C	4.23342	4.59189	-0.52135
C	3.21822	5.29055	-1.17056
C	3.52612	6.23734	-2.13522
C	4.84827	6.51299	-2.45365
C	5.86175	5.82504	-1.80171
C	5.55967	4.865	-0.84825
H	-8.72435	-1.6296	-0.76429
H	-10.55589	-0.22291	2.3307
H	-11.83962	0.42402	1.3474
H	-8.15465	0.96466	2.21997
H	-7.93191	2.09791	0.91975
H	-6.54418	-0.92156	-0.81135
H	-5.8449	1.49559	0.88307
H	1.92737	-1.78654	1.69155
H	4.30895	-2.31742	1.84678
H	4.44892	-2.91912	-2.36387
H	2.07164	-2.36357	-2.52092
H	1.91329	0.50178	-2.21613
H	3.62268	2.18729	-1.7693
H	1.96097	2.84989	2.09165
H	0.25817	1.15198	1.64851
H	-4.99658	2.96868	-0.54857
H	-3.60285	4.80375	-1.32954
H	-1.22643	4.37346	-1.88963
H	-0.27755	2.19759	-1.56976
H	0.90195	-4.33724	-0.63635
H	-0.69337	-6.17417	-0.63327
H	-3.12235	-5.69797	-0.55292
H	-3.91392	-3.42544	-0.46382
H	-4.4242	-1.64714	0.10978
H	-10.05759	1.95208	3.35858
H	-9.73605	3.36371	2.36613
H	-11.35572	2.69883	2.44328

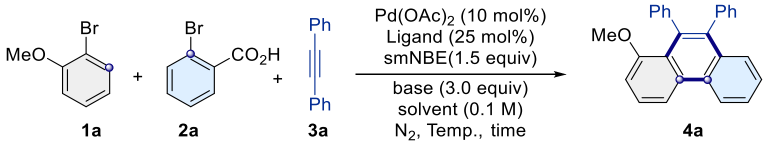
H	-9.86896	3.21419	-0.15323
H	-10.15971	1.68761	-0.96151
H	-11.45483	2.47257	-0.07943
H	7.90331	-4.18069	-1.45671
H	9.48584	-3.17286	-3.03806
H	9.32633	-0.77492	-3.59596
H	7.57284	0.6024	-2.53962
H	6.01007	-0.40231	-0.93873
H	8.03596	-2.51613	1.41485
H	8.87786	-4.00114	3.17758
H	7.73346	-6.13364	3.65609
H	5.74691	-6.76712	2.33758
H	4.92715	-5.29339	0.55471
H	4.48784	5.69685	2.00587
H	5.71805	5.66171	4.1279
H	6.54043	3.52675	5.05164
H	6.12729	1.43157	3.81601
H	4.92127	1.47301	1.6817
H	2.19606	5.08995	-0.91665
H	2.73328	6.7669	-2.62794
H	5.08445	7.25083	-3.19555
H	6.88831	6.02636	-2.0412
H	6.3456	4.32889	-0.35412

3. Experimental Section

3.1 Optimization of the reaction conditions

The oven-dried Schlenk tube (10 mL) equipped with a stirring bar was charged with substrates **1a** (0.1 mmol, 1.0 equiv), **2a** (0.2 mmol, 2.0 equiv), **3a** (0.15 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mol%), ligand (25 mol%) and base (2.5-4.5 equiv) in the air. Followed by the mediator smNBE (1.5 equiv) and the anhydrous solvent (0.1 M) was added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N_2 for three times. Finally, the reaction mixture was stirred at 130 ℃ for 24-72 h and then cooled to room temperature. Upon completion of the reaction, the mixture was diluted with 5 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (10 mL × 5). The filtrate was concentrated *in vacuo* to give the crude product. The crude ^1H NMR spectrum was taken using CH_2Br_2 (0.1 mmol) as internal standard.

Table S1. Screening of the reaction conditions.

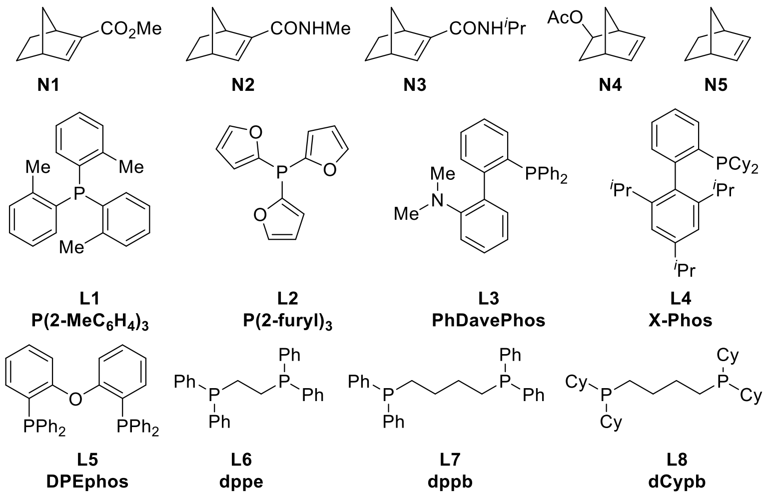


NO.	Ligand (25 mol%)	smNBE (1.5 eq.)	Base (3.0 eq.)	Solvent (0.1M)	Temp.	time	Yield^a (%)
1	L1	N5	K_2CO_3	DMF	130 °C	24 h	n.d.
2	L1	N1	K_2CO_3	toluene	130 °C	24 h	33
3	L2	N1	K_2CO_3	toluene	130 °C	24 h	7
4	L3	N1	K_2CO_3	toluene	130 °C	24 h	trace
5	L4	N1	K_2CO_3	toluene	130 °C	24 h	4
^{c}6	L5	N1	K_2CO_3	toluene	130 °C	24 h	11
^{c}7	L6	N1	K_2CO_3	toluene	130 °C	24 h	4
^{c}8	L7	N1	K_2CO_3	toluene	130 °C	24 h	2
^{c}9	L8	N1	K_2CO_3	toluene	130 °C	24 h	2
10	L1	N1	Na_2CO_3	toluene	130 °C	24 h	13
11	L1	N1	Cs_2CO_3	toluene	130 °C	24 h	8
12	L1	N1	^{t}BuONa	toluene	130 °C	24 h	n.d.
13	L1	N1	KOAc	toluene	130 °C	24 h	trace
14	L1	N1	CsOAc	toluene	130 °C	24 h	5
15	L1	N1	K_3PO_4	toluene	130 °C	24 h	36
16	L1	N2	K_3PO_4	toluene	130 °C	24 h	21
17	L1	N3	K_3PO_4	toluene	130 °C	24 h	35
18	L1	N4	K_3PO_4	toluene	130 °C	24 h	trace
19	L1	N5	K_3PO_4	toluene	130 °C	24 h	n.d.
20	L1	-	K_3PO_4	toluene	130 °C	24 h	n.d.
21	L1 (20 mol%)	N1	K_3PO_4	toluene	130 °C	24 h	30
22	L1 (15 mol%)	N1	K_3PO_4	toluene	130 °C	24 h	29
23	L1	N1	K_3PO_4	xylene	130 °C	24 h	34
24	L1	N1	K_3PO_4	DMF	130 °C	24 h	n.d.
25	L1	N1	K_3PO_4 (2.5 eq.)	toluene	130 °C	24 h	16
26	L1	N1	K_3PO_4 (3.5 eq.)	toluene	130 °C	24 h	50
27	L1	N1	K_3PO_4 (4.0 eq.)	toluene	130 °C	24 h	40
28	L1	N1	K_2CO_3 (3.5 eq.)	toluene	130 °C	24 h	38
29	L1	N1	K_2CO_3 (4.0 eq.)	toluene	130 °C	24 h	42
30	L1	N1	K_2CO_3 (4.5 eq.)	toluene	130 °C	24 h	51
31	L1	N1	K_2CO_3 (5.0 eq.)	toluene	130 °C	24 h	29
32	L1	N1	K_2CO_3 (4.5 eq.)	toluene	90 °C	24 h	5

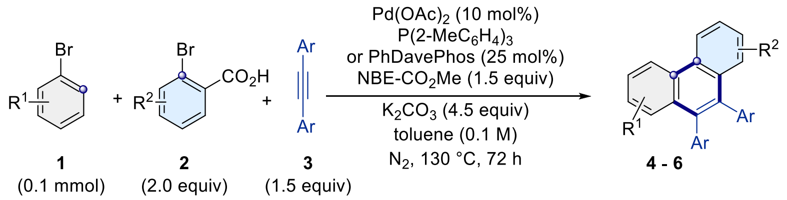
33	**L1**	**N1**	K_2CO_3 (4.5 eq.)	toluene	110 °C	24 h	13
34	**L1**	**N1**	K_2CO_3 (4.5 eq.)	toluene	120 °C	24 h	26
35	**L1**	**N1**	K_2CO_3 (4.5 eq.)	toluene	140 °C	24 h	40
36	**L1**	**N1**	K_2CO_3 (4.5 eq.)	dioxane	130 °C	24 h	7
37	**L1**	**N1**	K_2CO_3 (4.5 eq.)	*t*-Amyl OH	130 °C	24 h	4
38	**L1**	**N1**	K_2CO_3 (4.5 eq.)	toluene	130 °C	48 h	63
39	**L1**	**N1**	K_2CO_3 (4.5 eq.)	toluene	130 °C	72 h	71[b]

[a] Yield was determined by ^1H NMR with CH_2Br_2 (0.1mmol) as internal standard. [b] Isolated yield. [c] 12 mol% ligand was used. n.d. = not detected.

NBE mediators and ligands:



3.2 General procedures for synthesis of products



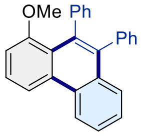
General procedure A:

The oven-dried Schlenk tube (10 mL) equipped with a stirring bar was charged with substrates **1** (0.1 mmol, 1.0 equiv), **2** (0.2 mmol, 2.0 equiv), **3** (0.15 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mol%), $P(2\text{-}MeC_6H_4)_3$ (25 mol%) and K_2CO_3 (4.5 equiv) in the air. Followed by the mediator NBE-CO_2Me (1.5 equiv) and the anhydrous toluene (1.0 mL) were added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N_2 for three times. Finally, the reaction mixture was stirred at 130 ℃ for 72 h and then cooled to room temperature. Upon completion of the reaction, the mixture was diluted with 5 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (10 mL × 5). The filtrate was concentrated *in vacuo* to give the crude product. The crude ^{1}H NMR spectrum was taken using CH_2Br_2 (0.1 mmol) as internal standard. Finally, the crude product was purified via silica gel column chromatography using PE/EtOAc as the eluent.

General procedure B:

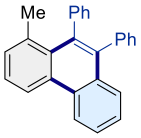
The oven-dried Schlenk tube (10 mL) equipped with a stirring bar was charged with substrates **1** (0.1 mmol, 1.0 equiv), **2** (0.2 mmol, 2.0 equiv), **3** (0.15 mmol, 1.5 equiv), $Pd(OAc)_2$ (10 mol%), PhDavePhos (25 mol%) and K_2CO_3 (4.5 equiv) in the air. Followed by the mediator NBE-CO_2Me (1.5 equiv) and the anhydrous toluene (1.0 mL) were added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N_2 for three times. Finally, the reaction mixture was stirred at 130 ℃ for 72 h and then cooled to room temperature. Upon completion of the reaction, the mixture was diluted with 5 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (10 mL × 5). The filtrate was concentrated *in vacuo* to give the crude product. The crude ^{1}H NMR spectrum was taken using CH_2Br_2 (0.1 mmol) as internal standard. Finally, the crude product was purified via silica gel column chromatography using PE/EtOAc as the eluent.

3.3 Characterization of products



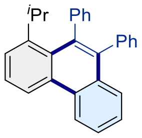
1-methoxy-9,10-diphenylphenanthrene (4a)

The general procedure A was followed. Yield: 71%, 25.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 (d, *J* = 8.4 Hz, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 7.66 – 7.55 (m, 2H), 7.48 – 7.39 (m, 2H), 7.26 – 7.11 (m, 3H), 7.12 – 6.99 (m, 7H), 6.96 (d, *J* = 8.0 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.9, 144.2, 139.9, 138.2, 135.2, 132.3, 132.1, 131.3, 129.7, 129.6, 127.9, 127.4, 127.0, 126.8, 126.4, 126.3, 126.2, 124.8, 123.1, 122.6, 115.6, 109.3, 56.0. HRMS (m/z, ESI): calcd for $C_{27}H_{21}O^+$ $(M+H)^+$ 361.1587, found 361.1551.



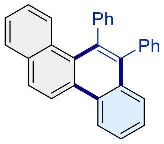
1-methyl-9,10-diphenylphenanthrene (4b)

The general procedure A was followed. Yield: 75%, 26.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.79 (d, *J* = 8.8 Hz, 1H), 8.75 (d, *J* = 8.8 Hz, 1H), 7.61 (t, *J* = 6.8 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.33 (d, *J* = 6.8 Hz, 1H), 7.22 – 7.13 (m, 3H), 7.12 – 6.99 (m, 7H), 1.91 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.2, 140.1, 139.0, 137.0, 136.96, 131.6, 131.59, 131.5, 131.3, 130.6, 130.5, 127.8, 127.5, 127.1, 126.6, 126.5, 126.3, 126.2, 123.0, 121.4, 25.5. HRMS (m/z, ESI): calcd for $C_{27}H_{21}^+$ $(M+H)^+$ 345.1565, found 345.1574.



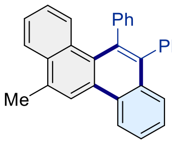
1-isopropyl-9,10-diphenylphenanthrene (4c)

The general procedure A was followed. Yield: 79%, 29.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (d, *J* = 8.4 Hz, 1H), 8.71 (d, *J* = 7.6 Hz, 1H), 7.69 – 7.56 (m, 3H), 7.45 – 7.36 (m, 2H), 7.24 – 7.12 (m, 3H), 7.12 – 6.98 (m, 7H), 2.88 (p, *J* = 6.8 Hz, 1H), 0.89 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.7, 143.6, 140.3, 138.9, 136.1, 131.7, 131.5, 131.3, 130.7, 130.6, 129.8, 127.8, 127.5, 127.3, 126.6, 126.5, 126.4, 126.3, 126.2, 126.0, 123.0, 120.7, 29.4, 24.8. HRMS (m/z, ESI): calcd for $C_{29}H_{25}^+$ $(M+H)^+$ 373.1878, found 373.1888.



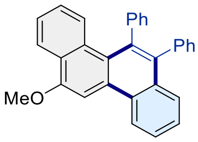
5,6-diphenylchrysene (4d)

The general procedure A was followed. Yield: 95%, 36.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.86 (d, *J* = 8.4 Hz, 1H), 8.82 (d, *J* = 9.2 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 6.8 Hz, 1H), 7.61 – 7.52 (m, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.28 – 7.19 (m, 3H), 7.19 – 7.12 (m, 3H), 7.12 – 7.05 (m, 4H), 7.01 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.7, 140.2, 139.5, 136.9, 133.9, 131.9, 131.4, 131.2, 130.2, 129.7, 128.8, 128.4, 128.2, 127.92, 127.9, 127.6, 126.7, 126.6, 126.4, 126.35, 125.7, 124.8, 123.3, 121.2. HRMS (m/z, ESI): calcd for $C_{30}H_{21}^+$ $(M+H)^+$ 381.1565, found 381.1578.



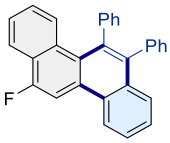
12-methyl-5,6-diphenylchrysene (4e)

The general procedure A was followed. Yield: 99%, 39.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.85 (d, *J* = 8.4 Hz, 1H), 8.66 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.73 – 7.62 (m, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.45 (dt, *J* = 12.5, 7.4 Hz, 2H), 7.22 (m, 3H), 7.16 – 7.11 (m, 3H), 7.10 – 6.97 (m, 5H), 2.89 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.7, 140.2, 138.6, 136.6, 133.7, 133.3, 131.9, 131.4, 131.37, 131.2, 129.7, 129.4, 129.3, 128.1, 127.8, 127.6, 127.0, 126.5, 126.4, 126.3, 126.2, 125.6, 124.3, 124.1, 123.2, 121.7, 20.8. HRMS (m/z, ESI): calcd for $C_{31}H_{23}^+$ $(M+H)^+$ 395.1722, found 395.1717.



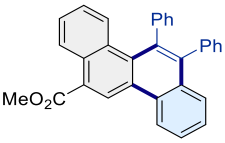
12-methoxy-5,6-diphenylchrysene (4f)

The general procedure A was followed. Yield: 93%, 38.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (d, *J* = 8.4 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.04 (s, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 9.6 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.17 (m, 3H), 7.17 – 6.96 (m, 8H), 4.24 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.5, 143.7, 140.3, 137.1, 136.7, 132.4, 132.1, 131.6, 131.2, 130.5, 129.6, 128.8, 128.1, 127.9, 127.5, 127.3, 126.6, 126.3, 126.2, 126.1, 125.4, 125.3, 123.2, 123.18, 121.9, 97.9, 55.7. HRMS (m/z, ESI): calcd for $C_{31}H_{23}O^+$ $(M+H)^+$ 411.1671, found 411.1692.



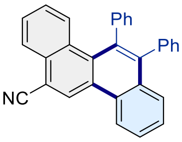
12-fluoro-5,6-diphenylchrysene (4g)

The general procedure A was followed. Yield: 91%, 36.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 (d, *J* = 8.4 Hz, 1H), 8.45 (d, *J* = 12.8 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.52 – 7.43 (m, 2H), 7.26 – 7.19 (m, 3H), 7.18 – 7.12 (m, 3H), 7.10 – 7.02 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.1 (d, $J_{C\text{-}F}$ = 250.8 Hz), 143.3, 139.9, 138.8 (d, $J_{C\text{-}F}$ = 2.1 Hz), 136.6, 132.9 (d, $J_{C\text{-}F}$ = 4.9 Hz), 131.9, 131.3, 131.1, 130.0 (d, $J_{C\text{-}F}$ = 8.8 Hz), 129.6 (d, $J_{C\text{-}F}$ = 4.4 Hz), 128.8 (d, $J_{C\text{-}F}$ = 2.7 Hz), 128.3, 127.9, 127.6, 127.0, 126.6, 126.5, 126.4, 126.0 (d, $J_{C\text{-}F}$ = 1.6 Hz), 125.9, 125.1 (d, $J_{C\text{-}F}$ = 2.3 Hz), 124.9 (d, $J_{C\text{-}F}$ = 16.8 Hz), 123.3, 120.6 (d, $J_{C\text{-}F}$ = 6.9 Hz), 103.9 (d, $J_{C\text{-}F}$ = 21.8 Hz). HRMS (m/z, ESI): calcd for $C_{30}H_{20}F^+$ $(M+H)^+$ 399.1471, found 399.1473.



methyl 11,12-diphenylchrysene-6-carboxylate (4h)

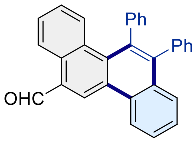
The general procedure A was followed. Yield: 83%, 36.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.48 (s, 1H), 8.86 (t, *J* = 10.0 Hz, 2H), 7.79 – 7.67 (m, 2H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.28 – 7.18 (m, 3H), 7.17 – 7.05 (m, 5H), 7.05 – 6.95 (m, 3H), 4.12 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.5, 143.1, 141.9, 139.7, 136.4, 132.0, 131.8, 131.3, 131.1, 130.8, 130.75, 130.3, 129.3, 128.2, 128.0, 127.9, 127.7, 127.2, 127.1, 126.8, 126.7, 126.6, 126.4, 126.1, 125.8, 124.8, 123.2, 52.6. HRMS (m/z, ESI): calcd for $C_{32}H_{23}O_2^+$ $(M+H)^+$ 439.1693, found 439.1661.



11,12-diphenylchrysene-6-carbonitrile (4i)

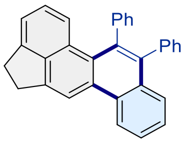
The general procedure A was followed. Yield: 61%, 25.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.30 (s, 1H), 8.79 (d, *J* = 8.4 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 7.77

(t, J = 6.8 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.64 – 7.51 (m, 3H), 7.32 – 7.21 (m, 3H), 7.21 – 7.14 (m, 3H), 7.15 – 7.11 (m, 1H), 7.11 – 7.06 (m, 2H), 7.06 – 6.99 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.0, 142.6, 139.3, 136.5, 132.0, 131.1, 131.0, 130.9, 130.7, 129.6, 129.5, 129.3, 128.4, 128.2, 127.9, 127.8, 127.76, 127.6, 127.4, 126.8, 126.79, 126.2, 125.6, 122.9, 118.7, 110.0. HRMS (m/z, ESI): calcd for $C_{31}H_{20}N^+$ $(M+H)^+$ 406.1517, found 406.1558.



11,12-diphenylchrysene-6-carbaldehyde (4j)

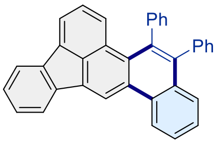
The general procedure A was followed. Yield: 54%, 22.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.58 (s, 1H), 9.32 (d, J = 8.4 Hz, 1H), 9.25 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.77 (t, J = 7.6 Hz, 1H), 7.72 (d, J = 8.8 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.54 (q, J = 7.6 Hz, 2H), 7.31 – 7.21 (m, 3H), 7.19 – 7.11 (m, 3H), 7.11 – 7.04 (m, 3H), 7.04 – 6.96 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.6, 143.3, 142.8, 139.4, 136.5, 134.3, 132.0, 131.9, 131.8, 131.1, 130.9, 130.3, 130.2, 130.0, 129.2, 128.3, 128.2, 128.0, 127.7, 127.64, 127.6, 127.3, 126.8, 126.6, 125.4, 124.8, 122.9. HRMS (m/z, ESI): calcd for $C_{31}H_{21}O^+$ $(M+H)^+$ 409.1514, found 409.1559.



11,12-diphenyl-4,5-dihydrocyclopenta[*hi*]chrysene (4k)

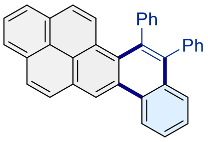
The general procedure A was followed. Yield: 86%, 35.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.89 (d, J = 8.4 Hz, 1H), 8.70 (s, 1H), 7.65 (t, J = 7.6 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.27 (d, J = 6.8 Hz, 1H), 7.26 – 7.15 (m, 6H), 7.15 – 7.07 (m, 4H), 7.03 (t, J = 8.0 Hz, 1H), 6.80 (d, J = 8.8 Hz, 1H), 3.54 (dd, J = 9.6, 5.6 Hz, 2H), 3.45 (dd, J = 8.8, 4.4 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.6, 145.5, 143.4, 140.2, 139.2, 137.9, 137.5, 132.0, 131.7, 131.5, 131.1, 130.4, 130.0, 128.2, 127.8, 127.5, 127.0, 126.6, 126.4, 126.3, 126.2, 125.5, 124.5, 123.6, 120.4, 114.5, 30.6, 29.9. HRMS (m/z, ESI): calcd for $C_{32}H_{23}^+$ $(M+H)^+$

407.1722, found 407.1722.



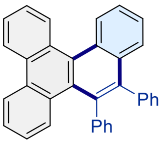
4,5-diphenylindeno[1,2,3-*hi*]chrysene (4l)

The general procedure A was followed. Yield: 98%, 45.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.36 (s, 1H), 9.02 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 6.4 Hz, 1H), 7.87 (d, *J* = 6.8 Hz, 1H), 7.79 (d, *J* = 6.8 Hz, 1H), 7.73 (t, *J* = 7.2 Hz, 1H), 7.63 – 7.48 (m, 2H), 7.47 – 7.36 (m, 2H), 7.32 – 7.02 (m, 11H), 6.92 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.0, 140.7, 139.9, 139.8, 138.5, 137.7, 136.9, 135.8, 133.0, 132.0, 131.23, 131.2, 131.19, 131.1, 129.0, 128.5, 128.4, 128.2, 128.0, 127.8, 127.6, 127.5, 127.1, 126.9, 126.74, 126.7, 126.5, 123.5, 121.7, 121.3, 119.4, 116.0. HRMS (m/z, ESI): calcd for $C_{36}H_{23}^+$ $(M+H)^+$ 455.1722, found 455.1714.



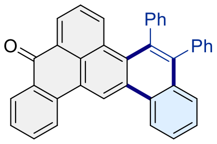
11,12-diphenylbenzo[*pqr*]picene (4m)

The general procedure A was followed. Yield: 75%, 34.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.48 (s, 1H), 9.10 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 9.2 Hz, 1H), 8.08 (d, *J* = 7.6 Hz, 1H), 8.01 (t, *J* = 6.4 Hz, 2H), 7.90 (dd, *J* = 14.4, 7.2 Hz, 2H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.65 – 7.51 (m, 3H), 7.30 – 7.21 (m, 3H), 7.19 – 7.09 (m, 5H), 7.09 – 7.02 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.9, 140.2, 139.1, 136.7, 131.8, 131.6, 131.4, 131.3, 130.5, 130.2, 130.1, 129.2, 128.7, 128.3, 128.2, 128.1, 128.0, 127.64, 127.6, 127.0, 126.8, 126.4, 126.3, 126.2, 126.18, 125.2, 125.1, 125.0, 124.9, 124.8, 123.5, 119.9. HRMS (m/z, ESI): calcd for $C_{36}H_{23}^+$ $(M+H)^+$ 455.1722, found 455.1718.



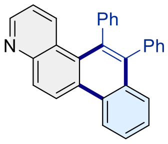
5,6-diphenylbenzo[*g*]chrysene (4n)

The general procedure A was followed. Yield: 61%, 26.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.80 (t, *J* = 8.8 Hz, 2H), 8.65 (d, *J* = 7.6 Hz, 1H), 8.55 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.66 (p, *J* = 6.4 Hz, 2H), 7.62 – 7.50 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.37 – 7.21 (m, 3H), 7.17 (d, *J* = 7.2 Hz, 2H), 7.12 – 7.01 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 139.5, 138.4, 135.9, 132.4, 132.0, 131.7, 131.5, 131.2, 130.8, 130.7, 129.94, 129.9, 129.6, 129.4, 128.9, 128.6, 128.5, 128.4, 127.9, 127.7, 127.0, 126.9, 126.6, 126.3, 126.2, 125.7, 125.6, 123.7, 123.2. HRMS (m/z, ESI): calcd for $C_{34}H_{23}^+$ (M+H)$^+$ 431.1722, found 431.1724.



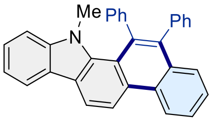
5,6-diphenyl-10H-dibenzo[*gh,m*]tetraphen-10-one (4o)

The general procedure A was followed. Yield: 84%, 40.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 8.95 (d, *J* = 8.4 Hz, 1H), 8.60 (dd, *J* = 7.2, 4.8 Hz, 2H), 8.52 (d, *J* = 7.6 Hz, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.82 (t, *J* = 7.2 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.66 – 7.51 (m, 3H), 7.33 – 7.19 (m, 4H), 7.19 – 7.14 (m, 3H), 7.10 (d, *J* = 7.6 Hz, 2H), 7.07 – 6.99 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 184.2, 143.0, 141.5, 139.6, 136.5, 136.4, 135.2, 133.5, 132.2, 131.2, 131.16, 131.1, 131.0, 130.2, 129.4, 129.3, 129.0, 128.6, 128.54, 128.5, 128.4, 128.3, 128.2, 127.8, 127.3, 127.28, 126.72, 126.7, 125.3, 125.1, 123.3, 122.9, 120.5. HRMS (m/z, ESI): calcd for $C_{37}H_{23}O^+$ (M+H)$^+$ 483.1743, found 483.1706.



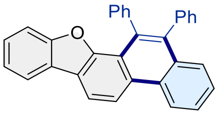
5,6-diphenylnaphtho[2,1-*f*]quinolone (4p)

The general procedure A was followed. Yield: 44%, 17.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.08 (d, *J* = 9.2 Hz, 1H), 8.89 (d, *J* = 8.8 Hz, 1H), 8.77 (s, 1H), 8.28 (d, *J* = 9.6 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.73 (t, *J* = 7.2 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.30 – 7.16 (m, 6H), 7.15 – 7.03 (m, 4H), 6.92 (dd, *J* = 9.2, 4.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.2, 149.0, 142.9, 140.2, 139.7, 136.6, 136.1, 132.1, 131.2, 131.0, 130.0, 129.5, 129.4, 128.6, 128.0, 127.7, 127.6, 127.1, 127.0, 126.8, 126.6, 125.1, 123.3, 119.3. HRMS (m/z, ESI): calcd for $C_{29}H_{20}N^+$ $(M+H)^+$ 382.1590, found 382.1567.



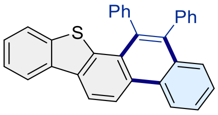
13-methyl-1,2-diphenyl-13*H*-naphtho[2,1-*a*]carbazole (4q)

The general procedure A was followed. Yield: 55%, 23.8 mg. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.84 (d, *J* = 8.4 Hz, 1H), 8.66 (d, *J* = 8.8 Hz, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.73 – 7.61 (m, 2H), 7.44 (dt, *J* = 16.8, 7.2 Hz, 2H), 7.38 – 7.27 (m, 4H), 7.21 – 7.05 (m, 4H), 7.05 – 6.91 (m, 4H), 2.89 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.5, 141.4, 140.4, 139.6, 137.5, 133.9, 132.8, 131.7, 131.6, 131.4, 130.8, 127.92, 127.87, 127.0, 126.7, 126.6, 126.3, 126.2, 125.6, 123.7, 123.6, 123.0, 120.0, 119.8, 119.6, 118.3, 115.6, 110.3, 36.6. HRMS (m/z, ESI): calcd for $C_{33}H_{24}N^+$ $(M+H)^+$ 434.1830, found 434.1866.



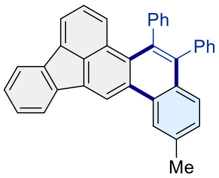
1,2-diphenylphenanthro[1,2-*b*]benzofuran (4r)

The general procedure B was followed. Yield: 50%, 21.1 mg. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.89 (d, *J* = 8.4 Hz, 1H), 8.83 (d, *J* = 8.8 Hz, 1H), 8.22 (d, *J* = 8.8 Hz, 1H), 8.03 – 7.95 (m, 1H), 7.70 (t, *J* = 7.2 Hz, 1H), 7.63 (q, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.35 – 7.14 (m, 11H), 7.07 – 7.01 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.7, 153.3, 141.5, 139.4, 138.8, 134.2, 132.4, 132.3, 132.0, 131.3, 130.9, 130.2, 129.9, 128.3, 127.6, 127.1, 126.9, 126.8, 126.6, 126.5, 126.3, 124.0, 123.2, 122.7, 122.3, 120.2, 119.2, 119.1, 118.2, 111.7. HRMS (m/z, ESI): calcd for $C_{32}H_{21}O^+$ $(M+H)^+$ 421.1587, found 421.1635.



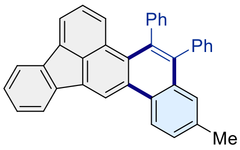
1,2-diphenylbenzo[*b*]phenanthro[2,1-*d*]thiophene (4s)

The general procedure A was followed. Yield: 67%, 29.5 mg. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.95 (d, *J* = 8.8 Hz, 1H), 8.90 (d, *J* = 8.4 Hz, 1H), 8.42 (d, *J* = 8.8 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 7.77 – 7.61 (m, 2H), 7.57 – 7.47 (m, 2H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.31 – 7.16 (m, 7H), 7.13 (d, *J* = 6.8 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.9, 139.7, 139.3, 139.2, 138.6, 136.0, 135.2, 134.6, 132.8, 131.7, 131.1, 130.6, 129.6, 128.14, 128.1, 128.07, 127.6, 127.0, 126.9, 126.8, 126.6, 126.3, 124.1, 123.3, 122.1, 121.3, 120.4, 120.2. HRMS (m/z, ESI): calcd for $C_{32}H_{21}S^+$ $(M+H)^+$ 437.1286, found 437.1288.



8-methyl-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5a)

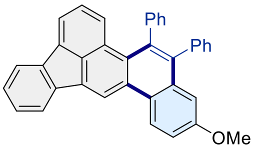
The general procedure A was followed. Yield: 97%, 45.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.33 (s, 1H), 8.77 (s, 1H), 8.13 (d, *J* = 6.8 Hz, 1H), 7.86 (d, *J* = 6.4 Hz, 1H), 7.77 (d, *J* = 6.4 Hz, 1H), 7.49 – 7.37 (m, 3H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.28 – 7.04 (m, 11H), 6.92 (d, *J* = 8.8 Hz, 1H), 2.69 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.1, 140.7, 140.0, 139.8, 138.6, 136.9, 136.8, 136.4, 135.6, 133.0, 131.4, 131.24, 131.2, 130.8, 130.1, 129.0, 128.7, 128.6, 128.3, 128.1, 128.0, 127.8, 127.6, 127.4, 127.0, 126.8, 126.4, 123.0, 121.7, 121.3, 119.3, 116.1, 22.4. HRMS (m/z, ESI): calcd for $C_{37}H_{25}^+$ $(M+H)^+$ 469.1878, found 469.1871.



7-methyl-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5b)

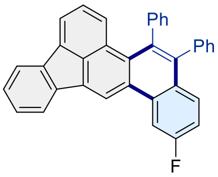
The general procedure A was followed. Yield: 94%, 44.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.35 (s, 1H), 8.91 (d, *J* = 8.8 Hz, 1H), 8.12 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 6.4 Hz, 1H), 7.80 (d, *J* = 6.8 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.48 – 7.38 (m, 2H), 7.32 (s, 1H), 7.28 – 7.19 (m, 6H), 7.19 – 7.13 (m, 3H), 7.10 (d, *J* = 7.6 Hz, 2H), 6.91 (d, *J* = 8.4 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.2, 140.8, 139.9, 139.6, 138.6, 137.8, 136.9, 136.5, 135.8, 132.9, 132.1, 131.3, 131.2, 129.3, 129.1, 128.8, 128.3, 128.1, 128.0, 127.8, 127.6, 127.5, 127.3, 127.1, 126.8, 126.4, 123.5, 121.7, 121.3, 119.2, 116.1, 21.9. HRMS (m/z, ESI): calcd for $C_{37}H_{25}^+$

(M+H)$^+$ 469.1878, found 469.1882.



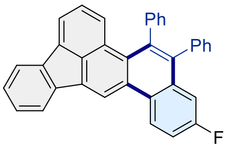
7-methoxy-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5c)

The general procedure A was followed. Yield: 98%, 47.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.26 (s, 1H), 8.90 (d, *J* = 9.2 Hz, 1H), 8.09 (dd, *J* = 6.0, 2.4 Hz, 1H), 7.91 – 7.83 (m, 1H), 7.77 (d, *J* = 6.8 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.36 (dd, *J* = 9.6, 2.8 Hz, 1H), 7.25 – 7.20 (m, 5H), 7.20 – 7.12 (m, 4H), 7.11 – 7.06 (m, 2H), 6.91 – 6.83 (m, 2H), 3.69 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.2, 143.1, 140.8, 139.9, 139.3, 138.6, 138.3, 136.9, 135.9, 133.5, 132.6, 131.4, 131.2, 131.1, 129.1, 128.3, 128.1, 127.7, 127.6, 127.4, 127.1, 127.06, 126.8, 126.5, 126.1, 125.3, 121.7, 121.2, 119.0, 117.7, 115.9, 107.7, 55.2. HRMS (m/z, ESI): calcd for $C_{37}H_{25}O^+$ (M+H)$^+$ 485.1827, found 485.1837.



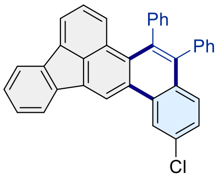
8-fluoro-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5d)

The general procedure A was followed. Yield: 71%, 34.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.07 (s, 1H), 8.53 (d, *J* = 11.6 Hz, 1H), 8.06 (d, *J* = 6.0 Hz, 1H), 7.84 (d, *J* = 6.8 Hz, 1H), 7.76 (d, *J* = 6.8 Hz, 1H), 7.57 – 7.47 (m, 1H), 7.42 (q, *J* = 8.0, 4.0 Hz, 2H), 7.29 – 7.16 (m, 7H), 7.16 – 7.00 (m, 5H), 6.88 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.6 (d, $J_{C\text{-}F}$ = 246.1 Hz), 142.8, 140.7, 139.6, 138.3, 136.9, 136.0, 133.2, 132.7 (d, $J_{C\text{-}F}$ = 8.3 Hz), 131.1, 130.6, 130.52, 130.5, 129.2, 128.9, 128.4, 128.3, 127.8, 127.7, 127.6, 127.2, 126.9, 126.6, 121.8, 121.3, 119.6, 116.0 (d, $J_{C\text{-}F}$ = 23.8 Hz), 115.8, 108.1 (d, $J_{C\text{-}F}$ = 22.5 Hz). HRMS (m/z, ESI): calcd for $C_{36}H_{22}F^+$ (M+H)$^+$ 473.1627, found 473.1615.



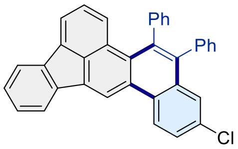
7-fluoro-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5e)

The general procedure A was followed. Yield: 95%, 44.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.13 (s, 1H), 8.86 (dd, *J* = 9.2, 5.6 Hz, 1H), 8.07 – 7.97 (m, 1H), 7.82 (m, 1H), 7.73 (d, *J* = 6.8 Hz, 1H), 7.45 – 7.34 (m, 3H), 7.25 – 7.15 (m, 6H), 7.15 – 7.05 (m, 4H), 7.04 – 6.98 (m, 2H), 6.83 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.3 (d, $J_{C\text{-}F}$ = 246.3 Hz), 142.7, 140.7, 139.3, 139.2 (d, $J_{C\text{-}F}$ = 4.3 Hz), 138.8, 138.4, 136.9, 136.2, 133.5 (d, $J_{C\text{-}F}$ = 8.7 Hz), 132.8, 131.13, 131.1, 131.0, 128.9, 128.4, 128.3, 127.94, 127.9, 127.8, 127.7, 127.5, 127.2, 127.0, 126.7, 126.0 (d, $J_{C\text{-}F}$ = 8.6 Hz), 121.7, 121.3, 119.4, 116.0 (d, $J_{C\text{-}F}$ = 24.1 Hz), 115.7, 111.8 (d, $J_{C\text{-}F}$ = 22.0 Hz). HRMS (m/z, ESI): calcd for $C_{36}H_{22}F^+$ $(M+H)^+$ 473.1627, found 473.1623.



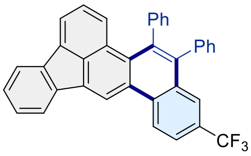
8-chloro-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5f)

The general procedure A was followed. Yield: 96%, 47.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.06 (s, 1H), 8.87 (s, 1H), 8.06 (d, *J* = 6.4 Hz, 1H), 7.82 (d, *J* = 6.4 Hz, 1H), 7.72 (d, *J* = 6.8 Hz, 1H), 7.49 – 7.35 (m, 4H), 7.29 – 7.16 (m, 6H), 7.15 – 6.96 (m, 5H), 6.84 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.7, 140.6, 139.44, 139.36, 138.3, 137.9, 136.9, 136.1, 133.1, 132.9, 132.2, 131.1, 131.0, 130.3, 130.2, 129.7, 129.1, 128.7, 128.4, 128.3, 127.8, 127.7, 127.6, 127.23, 127.2, 127.0, 126.7, 123.0, 121.9, 121.3, 119.6, 115.6. HRMS (m/z, ESI): calcd for $C_{36}H_{22}Cl^+$ $(M+H)^+$ 489.1332, found 489.1330.



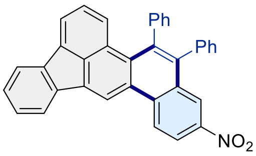
7-chloro-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5g)

The general procedure A was followed. Yield: 98%, 48.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.29 (s, 1H), 8.95 (d, *J* = 9.2 Hz, 1H), 8.17 – 8.09 (m, 1H), 7.92 – 7.85 (m, 1H), 7.82 (d, *J* = 7.2 Hz, 1H), 7.67 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.53 (s, 1H), 7.49 – 7.40 (m, 2H), 7.30 – 7.21 (m, 6H), 7.19 – 7.13 (m, 3H), 7.13 – 7.06 (m, 2H), 6.91 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.2, 147.4, 142.7, 140.8, 139.1, 139.0, 138.4, 137.0, 136.4, 133.1, 132.8, 131.2, 131.1, 131.0, 129.6, 128.9, 128.6, 128.4, 127.9, 127.8, 127.6, 127.4, 127.3, 127.1, 126.9, 126.8, 125.3, 121.8, 121.4, 119.6, 115.7. HRMS (m/z, ESI): calcd for $C_{36}H_{22}Cl^+$ $(M+H)^+$ 489.1332, found 489.1319.



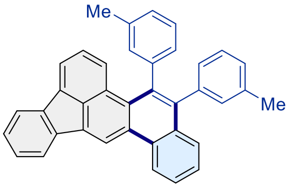
4,5-diphenyl-7-(trifluoromethyl)indeno[1,2,3-*hi*]chrysene (5h)

The general procedure A was followed (note: 20 mol% of $Pd(OAc)_2$ and 40 mol% of $P(2\text{-}MeC_6H_4)_3$ were used). Yield: 55%, 28.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.30 (s, 1H), 9.08 (d, *J* = 8.8 Hz, 1H), 8.18 – 8.08 (m, 1H), 7.94 – 7.86 (m, 2H), 7.84 (s, 1H), 7.81 (d, *J* = 7.2 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.31 – 7.20 (m, 6H), 7.20 – 7.11 (m, 3H), 7.11 – 7.03 (m, 2H), 6.91 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.5, 140.7, 140.1, 139.1, 138.7, 138.3, 137.0, 136.5, 133.3, 132.9, 131.3, 131.1, 131.0, 130.8, 129.8, 128.8, 128.54, 128.48, 128.36 (q, $J_{C\text{-}F}$ = 31.9 Hz), 127.93, 127.9, 127.7, 127.5, 127.2, 127.0, 125.4 (q, $J_{C\text{-}F}$ = 4.8 Hz), 124.5 (q, $J_{C\text{-}F}$ = 262.2 Hz), 124.6, 122.3 (q, $J_{C\text{-}F}$ = 4.8 Hz), 121.9, 121.4, 119.9, 115.8. HRMS (m/z, ESI): calcd for $C_{37}H_{22}F_3^+$ $(M+H)^+$ 523.1668, found 523.1793.



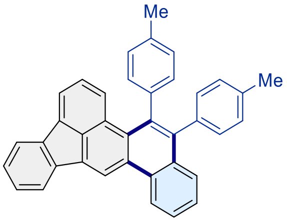
7-nitro-4,5-diphenylindeno[1,2,3-*hi*]chrysene (5i)

The general procedure A was followed. Yield: 50%, 24.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.89 (s, 1H), 9.26 (s, 1H), 8.23 (dd, *J* = 9.2, 2.0 Hz, 1H), 8.17 (d, *J* = 6.8 Hz, 1H), 7.85 (d, *J* = 6.4 Hz, 1H), 7.81 (d, *J* = 6.8 Hz, 1H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.46 (p, *J* = 7.2 Hz, 2H), 7.32 – 7.23 (m, 6H), 7.20 – 7.11 (m, 3H), 7.11 – 7.05 (m, 2H), 6.88 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.9, 142.2, 141.7, 140.7, 139.3, 138.7, 138.0, 137.4, 137.2, 135.1, 134.2, 133.3, 132.0, 131.1, 130.7, 130.5, 129.6, 128.8, 128.7, 128.5, 128.0, 127.94, 127.9, 127.7, 127.4, 127.1, 122.2, 121.4, 120.2, 120.1, 120.0, 115.3. HRMS (m/z, ESI): calcd for $C_{36}H_{22}NO_2^+$ $(M+H)^+$ 500.1572, found 500.1548.



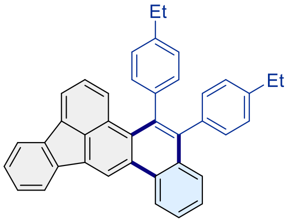
4,5-di-*m*-tolylindeno[1,2,3-*hi*]chrysene (6a)

The general procedure A was followed (note: the products were isolated as an inseparable mixture of diastereoisomers, *d.r.* = 1:1). Yield: 90%, 43.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.37 (s, 1H), 9.01 (d, *J* = 8.8 Hz, 1H), 8.16 – 8.07 (m, 1H), 7.91 – 7.84 (m, 1H), 7.81 (d, *J* = 6.8 Hz, 1H), 7.72 (t, *J* = 7.2 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.21 – 7.08 (m, 3H), 7.07 – 6.84 (m, 7H), 2.26 (s, 1.50H), 2.25 (s, 1.44H), 2.23 (s, 1.47H), 2.21 (s, 1.53H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 140.7, 140.1, 140.06, 139.7, 138.6, 137.8, 137.76, 137.7, 137.0, 136.9, 136.8, 135.7, 133.0, 132.1, 132.0, 131.9, 131.8, 131.2, 131.1, 129.1, 128.7, 128.6, 128.3, 128.24, 128.2, 128.16, 128.1, 128.05, 127.5, 127.4, 127.39, 127.3, 127.1, 127.08, 127.06, 126.6, 123.4, 121.7, 121.3, 119.4, 116.1, 21.5. HRMS (m/z, ESI): calcd for $C_{38}H_{27}^+$ $(M+H)^+$ 483.2035, found 483.2025.



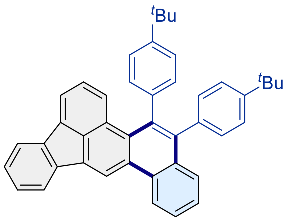
4,5-di-*p*-tolylindeno[1,2,3-*hi*]chrysene (6b)

The general procedure A was followed. Yield: 97%, 47.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.33 (s, 1H), 8.98 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 6.4 Hz, 1H), 7.85 (d, *J* = 6.4 Hz, 1H), 7.78 (d, *J* = 6.8 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 6.8 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.10 – 6.91 (m, 9H), 2.34 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.7, 140.1, 140.05, 138.6, 137.8, 136.9, 136.8, 136.2, 135.8, 135.7, 133.0, 132.3, 131.2, 131.17, 131.0, 130.9, 129.1, 128.9, 128.4, 128.1, 128.0, 127.4, 127.0, 126.6, 123.4, 121.7, 121.2, 119.3, 116.0, 21.5, 21.4. HRMS (m/z, ESI): calcd for $C_{38}H_{27}^{+}$ $(M+H)^{+}$ 483.2035, found 483.2026.



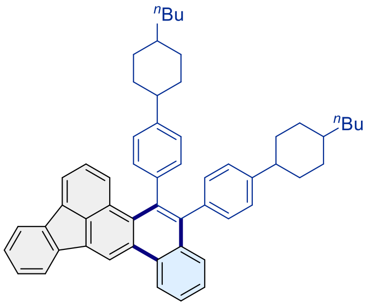
4,5-bis(4-ethylphenyl)indeno[1,2,3-*hi*]chrysene (6c)

The general procedure A was followed. Yield: 94%, 48.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.34 (s, 1H), 8.98 (d, *J* = 8.8 Hz, 1H), 8.13 – 8.05 (m, 1H), 7.85 (dd, *J* = 6.0, 2.0 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.69 (t, *J* = 7.2 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.14 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.08 – 6.94 (m, 9H), 2.61 (p, *J* = 7.4 Hz, 4H), 1.21 (t, *J* = 7.6 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 142.2, 140.7, 140.3, 140.2, 138.6, 137.9, 137.1, 136.8, 135.7, 133.0, 132.2, 131.2, 131.14, 131.1, 131.0, 129.1, 128.9, 128.14, 128.1, 128.0, 127.8, 127.4, 127.0, 126.6, 123.4, 121.7, 121.2, 119.3, 116.1, 28.8, 28.7, 16.1, 15.7. HRMS (m/z, ESI): calcd for $C_{40}H_{31}^{+}$ $(M+H)^{+}$ 511.2348, found 511.2340.



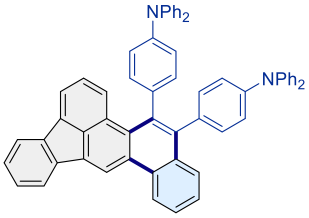
4,5-bis(4-(*tert*-butyl)phenyl)indeno[1,2,3-*hi*]chrysene (6d)

The general procedure A was followed. Yield: 89%, 50.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.38 (s, 1H), 9.02 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 6.4 Hz, 1H), 7.87 (d, *J* = 6.8 Hz, 1H), 7.80 (d, *J* = 6.0 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.41 (p, *J* = 7.2 Hz, 2H), 7.21 – 7.08 (m, 6H), 7.01 (d, *J* = 7.6 Hz, 2H), 6.97 (d, *J* = 7.6 Hz, 2H), 1.29 (s, 9H), 1.28 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.6, 149.0, 140.8, 140.4, 140.1, 138.6, 138.1, 136.8, 136.7, 135.7, 133.0, 132.1, 131.2, 131.1, 130.9, 130.7, 129.1, 128.8, 128.2, 128.1, 128.07, 127.4, 127.0, 126.6, 124.9, 124.2, 123.4, 121.7, 121.2, 119.3, 116.1, 34.6, 34.5, 31.53, 31.49. HRMS (m/z, ESI): calcd for $C_{44}H_{39}^{+}$ $(M+H)^{+}$ 567.2974, found 567.2960.



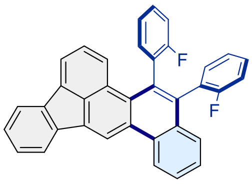
4,5-bis(4-(4-butylcyclohexyl)phenyl)indeno[1,2,3-*hi*]chrysene (6e)

The general procedure A was followed. Yield: 69%, 50.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.39 (s, 1H), 9.03 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 6.4 Hz, 1H), 7.88 (d, *J* = 6.8 Hz, 1H), 7.80 (d, *J* = 6.8 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.14 (t, *J* = 8.0 Hz, 1H), 7.06 – 6.91 (m, 9H), 2.41 (q, *J* = 11.6 Hz, 2H), 1.86 (d, *J* = 11.2 Hz, 8H), 1.47 – 1.35 (m, 4H), 1.35 – 1.19 (m, 14H), 1.06 (t, *J* = 11.6 Hz, 4H), 0.92 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.4, 145.8, 140.8, 140.4, 140.36, 138.6, 138.1, 137.1, 136.8, 135.7, 133.0, 132.2, 131.2, 131.1, 131.05, 130.9, 129.2, 128.9, 128.2, 128.1, 128.09, 127.4, 127.0, 126.6, 126.56, 125.8, 123.4, 121.7, 121.2, 119.3, 116.1, 44.5, 44.46, 37.5, 37.3, 34.7, 34.5, 33.8, 29.4, 23.2, 14.3. HRMS (m/z, ESI): calcd for $C_{56}H_{59}^{+}$ $(M+H)^{+}$ 731.4539, found 731.4511.



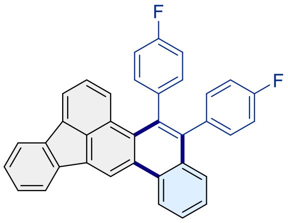
4,4'-(indeno[1,2,3-*hi*]chrysene-4,5-diyl)bis(*N*,*N*-diphenylaniline) (6f)

The general procedure A was followed. Yield: 73%, 57.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.39 (s, 1H), 9.04 (d, *J* = 8.8 Hz, 1H), 8.21 – 8.12 (m, 1H), 7.94 – 7.91 (m, 1H), 7.89 (d, *J* = 6.4 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.48 – 7.41 (m, 2H), 7.40 – 7.32 (m, 2H), 7.31 – 7.23 (m, 8H), 7.15 (t, *J* = 8.4 Hz, 8H), 7.07 – 6.99 (m, 12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.04, 148.0, 146.5, 146.3, 140.8, 140.0, 138.6, 137.85, 137.8, 137.0, 135.9, 134.1, 133.1, 132.22, 132.2, 132.1, 131.3, 131.29, 129.5, 129.0, 128.8, 128.2, 128.1, 127.6, 126.9, 126.8, 126.77, 124.4, 124.3, 124.2, 123.6, 123.1, 122.9, 122.8, 121.7, 121.3, 119.4, 116.1. HRMS (m/z, ESI): calcd for $C_{60}H_{41}N_2^+$ $(M+H)^+$ 789.3191, found 789.3170.



4,5-bis(2-fluorophenyl)indeno[1,2,3-*hi*]chrysene (6g)

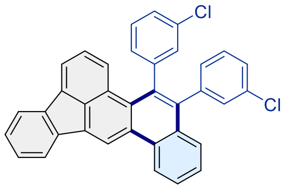
The general procedure A was followed. Yield: 45%, 22.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.32 (s, 1H), 8.98 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 6.4 Hz, 1H), 7.84 – 7.79 (m, 1H), 7.77 (d, J = 6.8 Hz, 1H), 7.73 – 7.65 (m, 1H), 7.53 – 7.41 (m, 2H), 7.40 – 7.31 (m, 2H), 7.31 – 7.13 (m, 5H), 7.06 – 6.96 (m, 3H), 6.95 – 6.86 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.9 (d, $J_{C\text{-}F}$ = 245.5 Hz), 159.8 (d, $J_{C\text{-}F}$ = 245.4 Hz), 140.7, 138.5, 137.2, 136.3, 134.9, 132.9, 132.2, 131.9, 131.6, 131.5, 131.0, 130.81, 129.8 (d, $J_{C\text{-}F}$ = 34.7 Hz), 129.7 (d, $J_{C\text{-}F}$ = 34.8 Hz), 128.5 (d, $J_{C\text{-}F}$ = 56.6 Hz), 128.3, 127.9, 127.6, 127.4 (d, $J_{C\text{-}F}$ = 17.9 Hz), 127.24, 127.22, 127.1, 126.2, 124.6 (d, $J_{C\text{-}F}$ = 3.4 Hz), 123.9 (d, $J_{C\text{-}F}$ = 3.7 Hz), 123.8, 121.8, 121.3, 119.6, 116.1, 115.6 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.1 (d, $J_{C\text{-}F}$ = 22.1 Hz). HRMS (m/z, ESI): calcd for $C_{36}H_{21}F_2^+$ $(M+H)^+$ 491.1533, found 491.1545.



4,5-bis(4-fluorophenyl)indeno[1,2,3-*hi*]chrysene (6h)

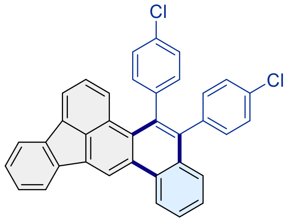
The general procedure A was followed. Yield: 90%, 44.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.36 (s, 1H), 9.02 (d, J = 8.4 Hz, 1H), 8.12 (d, J = 6.0 Hz, 1H), 7.89 (d, J = 6.8 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 7.76 (t, J = 6.4 Hz, 1H), 7.59 – 7.50 (m, 2H), 7.48 – 7.39 (m, 2H), 7.22 (t, J = 7.6 Hz, 1H), 7.13 – 7.01 (m, 4H), 7.00 – 6.88 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.9 (d, $J_{C\text{-}F}$ = 247.8 Hz), 161.6 (d, $J_{C\text{-}F}$ = 246.9 Hz), 140.7, 139.2, 138.9 (d, $J_{C\text{-}F}$ = 3.7 Hz), 138.5, 137.1, 137.0, 136.2, 135.6

(d, $J_{C\text{-}F}$ = 3.4 Hz), 133.0, 132.7, 132.64, 132.56, 132.0, 131.5, 131.3, 128.6 (d, $J_{C\text{-}F}$ = 39.9 Hz), 128.1 (d, $J_{C\text{-}F}$ = 54.3 Hz), 127.6, 127.5, 127.4, 127.0, 126.9, 123.6, 121.8, 121.4, 119.5, 116.0, 115.6 (d, $J_{C\text{-}F}$ = 21.1 Hz), 114.9 (d, $J_{C\text{-}F}$ = 21.4 Hz). HRMS (m/z, ESI): calcd for $C_{36}H_{21}F_2^+$ $(M+H)^+$ 491.1533, found 491.1520.



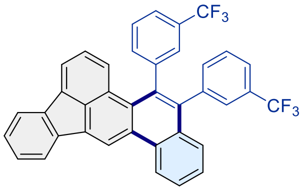
4,5-bis(3-chlorophenyl)indeno[1,2,3-*hi*]chrysene (6i)

The general procedure A was followed(note: the products were isolated as an inseparable mixture of diastereoisomers). Yield: 97%, 51.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.25 (s, 1H), 8.93 (d, *J* = 8.4 Hz, 1H), 8.09 – 7.97 (m, 1H), 7.87 – 7.78 (m, 1H), 7.75 (d, *J* = 6.8 Hz, 1H), 7.68 (t, *J* = 6.8 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.40 – 7.31 (m, 2H), 7.19 – 7.01 (m, 7H), 7.00 – 6.84 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 144.5, 141.3, 140.7, 138.5, 138.4, 137.1, 136.3, 136.2, 134.5, 134.4, 133.9, 133.7, 133.0, 131.6, 131.4, 131.34, 131.26, 131.2, 131.1, 129.8, 129.7, 129.5, 129.4, 129.3, 129.25, 129.1, 129.0, 128.6, 128.4, 127.8, 127.6, 127.5, 127.4, 127.35, 127.2, 127.1, 127.0, 123.6, 121.8, 121.4, 119.6, 115.9. HRMS (m/z, ESI): calcd for $C_{36}H_{21}Cl_2^+$ $(M+H)^+$ 523.0942, found 523.0927.



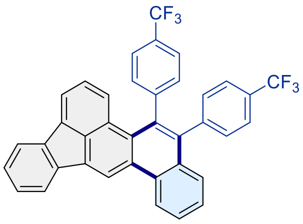
4,5-bis(4-chlorophenyl)indeno[1,2,3-*hi*]chrysene (6j)

The general procedure A was followed. Yield: 99%, 52.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.25 (s, 1H), 8.94 (d, *J* = 8.4 Hz, 1H), 8.05 (dd, *J* = 4.8, 2.0 Hz, 1H), 7.90 – 7.81 (m, 1H), 7.78 (d, *J* = 6.8 Hz, 1H), 7.72 (t, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.48 – 7.36 (m, 3H), 7.29 – 7.13 (m, 5H), 7.05 – 6.92 (m, 4H), 6.89 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.3, 140.6, 138.6, 138.4, 138.0, 137.1, 136.4, 136.2, 133.1, 132.9, 132.7, 132.4, 132.36, 131.6, 131.5, 131.3, 128.8, 128.6, 128.4, 128.1, 128.0, 127.7, 127.6, 127.4, 127.0, 126.9, 123.6, 121.8, 121.3, 119.5, 115.8. HRMS (m/z, ESI): calcd for $C_{36}H_{21}Cl_2^+$ $(M+H)^+$ 523.0942, found 523.0931.



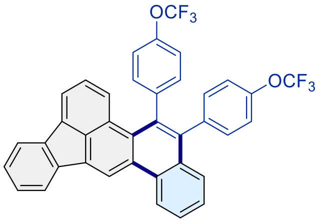
4,5-bis(3-(trifluoromethyl)phenyl)indeno[1,2,3-*hi*]chrysene (6k)

The general procedure A was followed (note: the products were isolated as an inseparable mixture of diastereoisomers, *d.r.* = 1:1). Yield: 91%, 53.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.21 (d, *J* = 3.2 Hz, 1H), 8.92 (d, *J* = 8.4 Hz, 1H), 8.05 – 7.95 (m, 1H), 7.84 – 7.75 (m, 1H), 7.75 – 7.65 (m, 2H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.45 – 7.19 (m, 9H), 7.18 – 7.01 (m, 3H), 6.81 (d, *J* = 4.0 Hz, 0.52H), 6.78 (d, *J* = 4.4 Hz, 0.49H). ^{13}C NMR (101 MHz, Chloroform-d) δ 143.5, 143.46, 140.6, 140.3, 140.2, 138.4, 138.3, 137.1, 136.3, 134.6, 134.5, 134.2, 132.9, 131.6, 131.56, 131.33, 131.3, 131.2, 131.17, 128.9, 128.4, 128.31, 128.28, 128.1 (q, $J_{C\text{-}F}$ = 3.6 Hz), 127.9 (q, $J_{C\text{-}F}$ = 3.6 Hz), 127.6, 127.5, 127.44, 127.4, 127.2, 127.1, 127.06, 127.0, 125.5, 125.4, 124.1 (q, $J_{C\text{-}F}$ = 273.4 Hz), 124.0 (q, $J_{C\text{-}F}$ = 273.7 Hz), 123.8, 123.7, 123.63, 123.6, 121.8, 121.3, 119.5, 115.7. HRMS (m/z, ESI): calcd for $C_{38}H_{21}F_6^+$ $(M+H)^+$ 591.1469, found 591.1501.



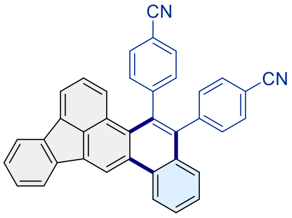
4,5-bis(4-(trifluoromethyl)phenyl)indeno[1,2,3-*hi*]chrysene (6l)

The general procedure A was followed. Yield: 93%, 55.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.29 (s, 1H), 8.99 (d, *J* = 8.4 Hz, 1H), 8.12 – 8.04 (m, 1H), 7.92 – 7.83 (m, 1H), 7.83 – 7.72 (m, 2H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 4H), 7.45 – 7.37 (m, 3H), 7.22 – 7.09 (m, 5H), 6.79 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.5, 143.3, 140.7, 138.3, 137.2, 136.5, 136.1, 133.0, 131.7, 131.5, 131.46, 131.4, 131.2, 129.5 (q, $J_{C\text{-}F}$ = 32.7 Hz), 129.2 (q, $J_{C\text{-}F}$ = 32.6 Hz), 128.5, 128.4, 127.7, 127.6, 127.58, 127.5, 127.3, 127.2, 127.1, 125.44 (q, $J_{C\text{-}F}$ = 3.6 Hz), 124.82 (q, $J_{C\text{-}F}$ = 3.6 Hz), 124.23 (q, $J_{C\text{-}F}$ = 273.3 Hz), 124.2 (q, $J_{C\text{-}F}$ = 273.2 Hz), 123.7, 121.9, 121.4, 119.7, 115.8. HRMS (m/z, ESI): calcd for $C_{38}H_{21}F_6^+$ $(M+H)^+$ 591.1469, found 591.1454.



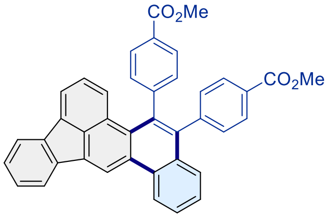
4,5-bis(4-(trifluoromethoxy)phenyl)indeno[1,2,3-*hi*]chrysene (6m)

The general procedure A was followed. Yield: 81%, 50.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.34 (s, 1H), 9.03 (d, *J* = 8.4 Hz, 1H), 8.18 – 8.05 (m, 1H), 7.94 – 7.86 (m, 1H), 7.82 (d, *J* = 6.8 Hz, 1H), 7.77 (t, *J* = 7.2 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.48 – 7.39 (m, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.15 – 7.03 (m, 8H), 6.93 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.3, 148.1, 141.7, 140.7, 138.7, 138.4, 138.2, 137.2, 136.5, 136.4, 133.0, 132.5, 132.4, 131.6, 131.5, 131.4, 128.6, 128.5, 128.0, 127.74, 127.7, 127.4, 127.3, 127.2, 127.1, 123.7, 121.8, 121.4, 121.2, 120.6 (q, $J_{C\text{-}F}$ = 258.1 Hz), 120.4, 119.6, 115.9. HRMS (m/z, ESI): calcd for $C_{38}H_{21}F_6O_2^+$ $(M+H)^+$ 623.1367, found 623.1337.



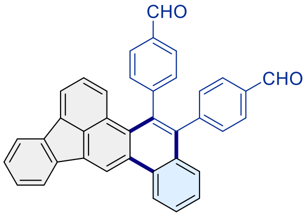
4,4'-(indeno[1,2,3-*hi*]chrysene-4,5-diyl)dibenzonitrile (6n)

The general procedure A was followed. Yield: 97%, 49.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.26 (s, 1H), 9.00 (d, *J* = 8.4 Hz, 1H), 8.13 – 8.04 (m, 1H), 7.94 – 7.85 (m, 1H), 7.84 – 7.76 (m, 2H), 7.60 – 7.48 (m, 5H), 7.48 – 7.41 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.21 – 7.07 (m, 5H), 6.71 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.5, 144.3, 140.6, 138.2, 137.6, 137.4, 136.8, 135.5, 132.9, 132.3, 132.26, 131.9, 131.85, 131.8, 131.4, 130.8, 128.7, 128.1, 127.9, 127.7, 127.6, 127.4, 127.3, 127.0, 126.8, 123.8, 121.9, 121.5, 119.8, 118.7, 118.6, 115.7, 111.4, 111.2. HRMS (m/z, ESI): calcd for $C_{38}H_{21}N_2^+$ $(M+H)^+$ 505.1699, found 505.1673.



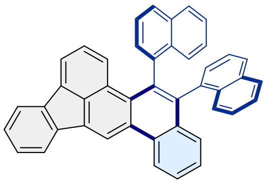
dimethyl 4,4'-(indeno[1,2,3-*hi*]chrysene-4,5-diyl)dibenzoate (6o)

The general procedure A was followed. Yield: 70%, 40.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.43 (s, 1H), 9.09 (d, *J* = 8.4 Hz, 1H), 8.21 – 8.14 (m, 1H), 8.00 – 7.90 (m, 5H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.80 (t, *J* = 7.2 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 3.95 (s, 3H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.1, 147.8, 144.6, 140.8, 137.2, 136.5, 131.7, 131.4, 131.3, 131.28, 129.8, 129.2, 129.1, 128.9, 128.7, 128.6, 128.5, 127.8, 127.7, 127.6, 127.4, 127.3, 127.1, 123.7, 121.9, 121.4, 119.7, 118.6, 118.0, 115.9, 52.3, 52.3. HRMS (m/z, ESI): calcd for $C_{40}H_{27}O_4^+$ $(M+H)^+$ 571.1831, found 571.1847.



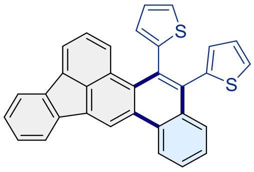
4,4'-(indeno[1,2,3-*hi*]chrysene-4,5-diyl)dibenzaldehyde (6p)

The general procedure A was followed. Yield: 89%, 45.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.99 (s, 1H), 9.97 (s, 1H), 9.31 (s, 1H), 9.01 (d, *J* = 8.4 Hz, 1H), 8.13 – 8.07 (m, 1H), 7.90 – 7.85 (m, 1H), 7.82 – 7.77 (m, 2H), 7.74 (dd, *J* = 8.0, 5.2 Hz, 4H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.13 (dd, *J* = 8.4, 7.2 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.04, 191.99, 149.3, 146.1, 140.6, 138.3, 138.2, 137.2, 136.6, 136.1, 135.0, 134.9, 133.0, 131.9, 131.87, 131.7, 131.4, 131.0, 129.8, 129.2, 128.6, 128.4, 127.8, 127.5, 127.4, 127.2, 127.1, 123.8, 121.9, 121.4, 119.7, 115.8. HRMS (m/z, ESI): calcd for $C_{38}H_{23}O_2^+$ $(M+H)^+$ 511.1620, found 511.1632.



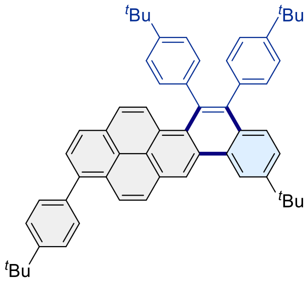
4,5-di(naphthalen-1-yl)indeno[1,2,3-*hi*]chrysene (6q)

The general procedure A was followed. Yield: 69%, 38.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.57 (s, 1H), 9.19 (d, *J* = 8.8 Hz, 1H), 8.20 (d, *J* = 7.2 Hz, 1H), 7.87 (d, *J* = 6.8 Hz, 1H), 7.83 – 7.70 (m, 4H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.51 (d, *J* = 9.2 Hz, 1H), 7.49 – 7.38 (m, 5H), 7.37 – 7.26 (m, 3H), 7.15 (d, *J* = 7.2 Hz, 1H), 7.01 – 6.85 (m, 4H), 6.74 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 140.8, 140.5, 139.1, 138.6, 137.3, 136.9, 136.8, 136.2, 133.4, 133.2, 133.1, 132.9, 132.5, 131.6, 130.1, 129.6, 129.2, 128.4, 128.3, 128.2, 128.1, 127.7, 127.66, 127.6, 127.3, 127.1, 127.05, 126.95, 126.7, 126.5, 126.1, 126.0, 125.8, 125.6, 125.4, 125.3, 124.8, 124.5, 123.7, 121.8, 121.3, 119.5, 116.3, 116.2. HRMS (m/z, ESI): calcd for $C_{44}H_{27}^+$ $(M+H)^+$ 555.2035, found 555.2013.



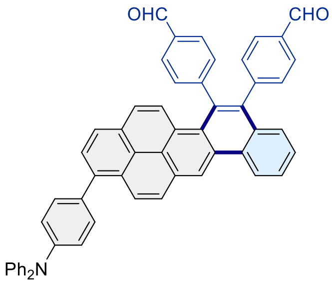
2,2'-(indeno[1,2,3-hi]chrysene-4,5-diyl)dithiophene (6r)

The general procedure A was followed. Yield: 85%, 39.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.33 (s, 1H), 9.00 (d, *J* = 8.4 Hz, 1H), 8.17 – 8.07 (m, 1H), 7.93 – 7.87 (m, 1H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.83 – 7.72 (m, 2H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.38 (dd, *J* = 10.4, 5.2 Hz, 2H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.11 (d, *J* = 8.8 Hz, 1H), 7.04 (q, *J* = 4.0 Hz, 2H), 6.94 (dd, *J* = 7.2, 3.2 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.9, 140.9, 139.9, 138.4, 137.0, 136.7, 134.7, 133.0, 132.7, 132.3, 131.9, 131.6, 129.7, 129.23, 129.2, 128.8, 128.5, 128.1, 127.64, 127.6, 127.4, 127.3, 127.2, 127.1, 126.9, 126.4, 126.3, 123.5, 121.8, 121.3, 119.7, 115.7. HRMS (m/z, ESI): calcd for $C_{32}H_{19}S_2^+$ $(M+H)^+$ 467.0850, found 467.0842.



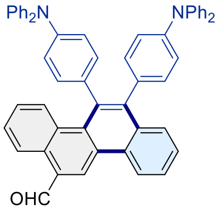
8-(*tert*-butyl)-3,11,12-tris(4-(*tert*-butyl)phenyl)benzo[*pqr*]picene (6s)

The general procedure A was followed. Yield: 46%, 34.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.56 (s, 1H), 9.16 (s, 1H), 8.29 – 8.21 (m, 2H), 8.17 (d, *J* = 9.6 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.67 – 7.56 (m, 5H), 7.31 – 7.21 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 1.61 (s, 9H), 1.49 (s, 9H), 1.35 (s, 9H), 1.33 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.2, 149.4, 148.94, 148.9, 141.2, 139.4, 138.6, 137.5, 137.3, 136.5, 131.0, 130.9, 130.5, 129.95, 129.9, 129.8, 129.5, 129.3, 128.9, 128.3, 128.2, 128.0, 127.9, 126.7, 126.0, 125.5, 125.4, 125.3, 125.2, 124.7, 124.2, 119.5, 119.2, 35.5, 34.8, 34.6, 34.5, 31.8, 31.7, 31.6, 31.5. HRMS (m/z, ESI): calcd for $C_{58}H_{59}^+$ (M+H)$^+$ 755.4539, found 755.4521.



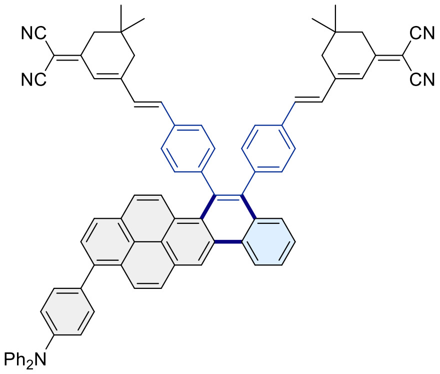
4,4'-(3-(4-(diphenylamino)phenyl)benzo[*pqr*]picene-11,12-diyl)dibenzaldehyde (6t)

The general procedure A was followed. Yield: 72%, 54.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.93 (s, 1H), 9.89 (s, 1H), 9.40 (s, 1H), 9.06 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 9.2 Hz, 1H), 8.10 (d, *J* = 9.6 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.77 – 7.65 (m, 4H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 9.6 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 3H), 7.25 (t, *J* = 8.0 Hz, 4H), 7.22 – 7.11 (m, 10H), 7.00 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.1, 192.0, 150.3, 147.9, 147.4, 146.7, 138.0, 137.6, 135.4, 135.0, 134.9, 134.5, 132.1, 132.0, 131.5, 130.8, 130.6, 130.4, 129.7, 129.6, 129.5, 129.3, 128.72, 128.69, 128.6, 128.0, 127.6, 127.55, 127.5, 127.1, 126.7, 125.6, 125.3, 125.1, 125.0, 124.8, 123.8, 123.3, 119.5. HRMS (m/z, ESI): calcd for $C_{56}H_{36}NO_2^+$ $(M+H)^+$ 754.2668, found 754.2647.



11,12-bis(4-(diphenylamino)phenyl)chrysene-6-carbaldehyde (6u)

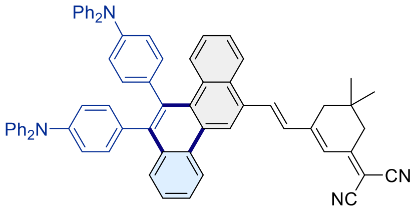
The general procedure A was followed. Yield: 64%, 47.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.47 (s, 1H), 9.24 (d, *J* = 8.0 Hz, 1H), 9.12 (s, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.50 (q, *J* = 7.6 Hz, 2H), 7.22 – 7.10 (m, 9H), 7.08 – 6.98 (m, 8H), 6.92 (t, *J* = 8.0 Hz, 6H), 6.88 – 6.80 (m, 4H), 6.75 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 193.4, 147.9, 147.8, 146.5, 146.3, 143.4, 137.5, 136.7, 134.3, 133.6, 132.1, 132.0, 131.9, 131.8, 130.32, 130.3, 130.1, 129.5, 129.4, 129.3, 128.2, 127.9, 127.6, 127.3, 125.2, 124.9, 124.5, 124.2, 124.0, 123.0, 122.94, 122.87. HRMS (m/z, ESI): calcd for $C_{55}H_{39}N_2O^+$ $(M+H)^+$ 743.2984, found 743.2968.



2,2'-(((1*E*,1'*E*)-((3-(4-(diphenylamino)phenyl)benzo[*pqr*]picene-11,12-diyl)bis(4,1-phenylene))bis(ethene-2,1-diyl))bis(5,5-dimethylcyclohex-2-en-3-yl-1-ylidene))di malononitrile (6v)

The general procedure A was followed (note: 0.05 mmol scale reaction was carried out). Yield: 42%, 22.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.38 (s, 1H), 9.04 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 9.2 Hz, 1H), 8.08 (d, *J* = 9.6 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 9.6 Hz, 1H), 7.76 – 7.68 (m, 1H), 7.56 –

7.48 (m, 3H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.20 (m, 5H), 7.21 – 7.11 (m, 7H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.99 (t, *J* = 7.2 Hz, 2H), 6.86 (d, *J* = 14.8 Hz, 2H), 6.82 (d, *J* = 13.6 Hz, 2H), 6.61 (s, 1H), 6.56 (s, 1H), 2.37 (s, 2H), 2.29 (s, 2H), 2.21 (s, 2H), 2.16 (s, 2H), 0.91 (s, 6H), 0.86 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.2, 169.1, 153.7, 153.6, 147.8, 147.3, 145.7, 141.9, 138.3, 137.8, 136.7, 135.9, 134.9, 134.1, 133.8, 132.1, 132.0, 131.5, 131.4, 130.3, 129.6, 129.55, 129.5, 129.45, 129.2, 129.1, 128.9, 128.7, 128.5, 128.2, 127.6, 127.32, 127.3, 127.1, 126.5, 125.6, 125.5, 125.4, 125.1, 125.0, 124.8, 123.7, 123.6, 123.5, 123.48, 123.3, 123.2, 119.6, 113.51, 113.49, 112.8, 112.7, 78.8, 78.7, 42.9, 42.8, 39.2, 39.1, 32.0, 31.9, 28.1, 28.0. HRMS (m/z, ESI): calcd for $C_{80}H_{60}N_5^+$ $(M+H)^+$ 1090.4770, found 1090.4719.



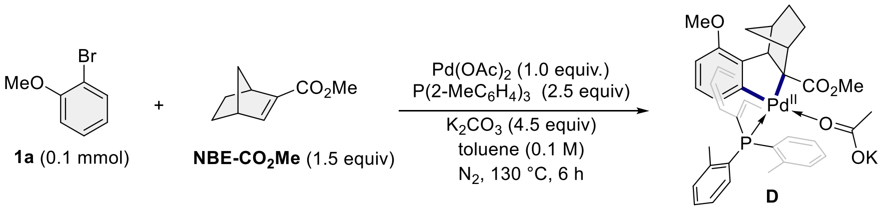
(*E*)-2-(3-(2-(11,12-bis(4-(diphenylamino)phenyl)chrysen-6-yl)vinyl)-5,5-dimethylcyclohex-2-en-1-ylidene)malononitrile (**6w**)

The general procedure A was followed (note: 0.05 mmol scale reaction was carried out). Yield: 40%, 18.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.98 (s, 1H), 8.84 (d, *J* = 8.4 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 15.6 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.70 (t, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.24 – 7.13 (m, 10H), 7.04 (t, *J* = 8.4 Hz, 8H), 6.97 – 6.91 (m, 7H), 6.90 – 6.85 (m, 4H), 6.82 (d, *J* = 8.4 Hz, 2H), 2.56 (s, 2H), 2.55 (s, 2H), 1.08 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.4, 153.9, 148.0, 147.9, 146.4, 146.1, 140.8, 138.1, 136.6, 134.6, 134.0, 132.3, 132.2, 132.0, 131.7, 131.5, 130.1, 129.9, 129.45, 129.43, 129.2, 129.0, 128.1, 127.2, 126.2, 124.7, 124.4, 124.3, 124.2, 124.1, 123.4, 123.2, 123.1, 122.9, 122.8, 120.8, 113.6, 112.9, 79.2, 43.2, 39.5, 32.3, 28.3. HRMS (m/z, ESI): calcd for $C_{67}H_{51}N_4^+$ $(M+H)^+$ 911.4035, found 911.4030.

3.4 Mechanistic Studies

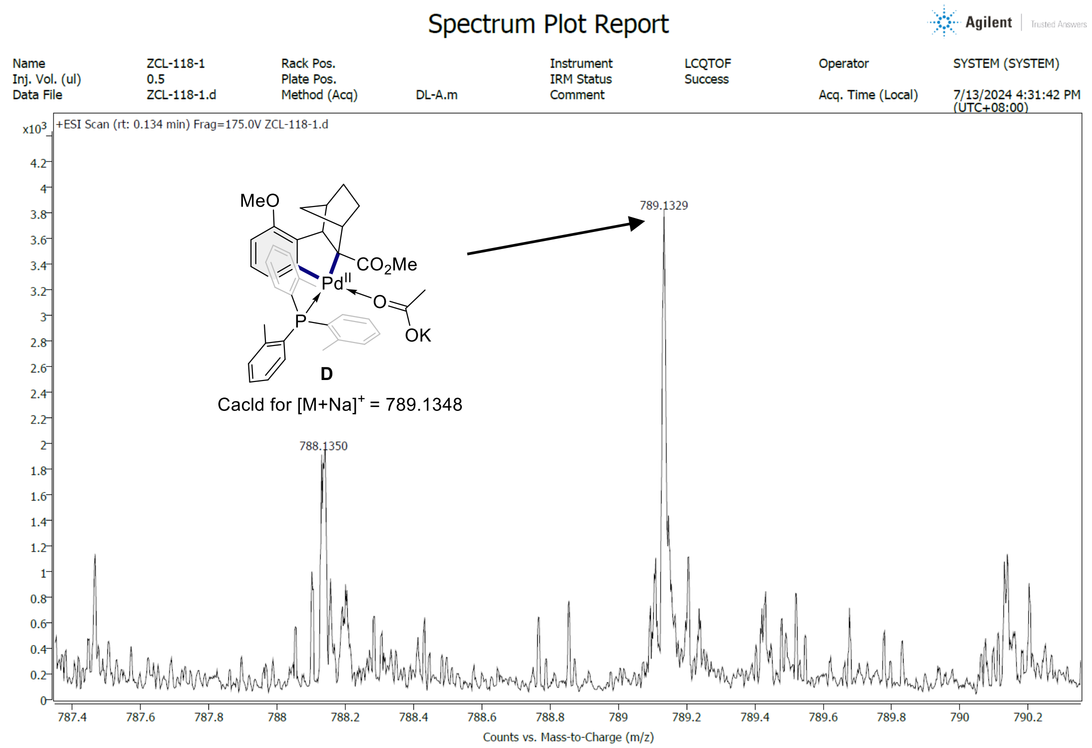
Control experiments:

(a) Reaction of **1a** with **NBE-CO_2Me** in the condition of quantitative $Pd(OAc)_2$:



(Detected by Q-TOF LC/MS)

The oven-dried Schlenk tube (10 mL) equipped with a stirring bar was charged with substrates **1a** (0.1 mmol, 1.0 equiv), $Pd(OAc)_2$ (1.0 equiv), $P(2-MeC_6H_4)_3$ (2.5 equiv) and K_2CO_3 (4.5 equiv) in the air. Followed by the mediator NBE-CO_2Me (1.5 equiv) and the anhydrous toluene (1.0 mL) were added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N_2 for three times. Finally, the reaction mixture was stirred at 130 ℃ for 6 h and then cooled to room temperature. Upon completion of the reaction, the mixture was analyzed by the Agilent 6546 Q-TOF LC/MS system detection and intermediate **D** were detected.



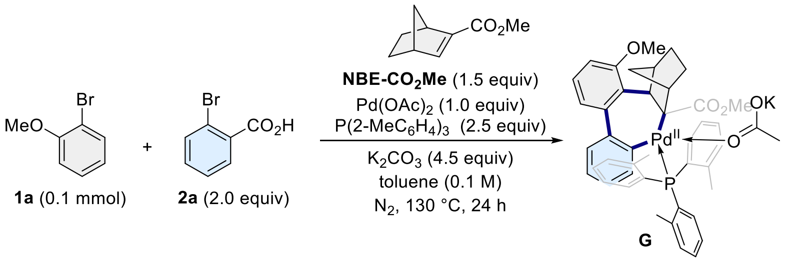
Spectrum Plot Report

Name	ZCL-118-1	Rack Pos.		Instrument	LCQTOF	Operator	SYSTEM (SYSTEM)
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	ZCL-118-1.d	Method (Acq)	DL-A.m	Comment		Acq. Time (Local)	7/13/2024 4:31:42 PM (UTC+08:00)

+ESI Scan (rt: 0.134 min) Frag=175.0V ZCL-118-1.d

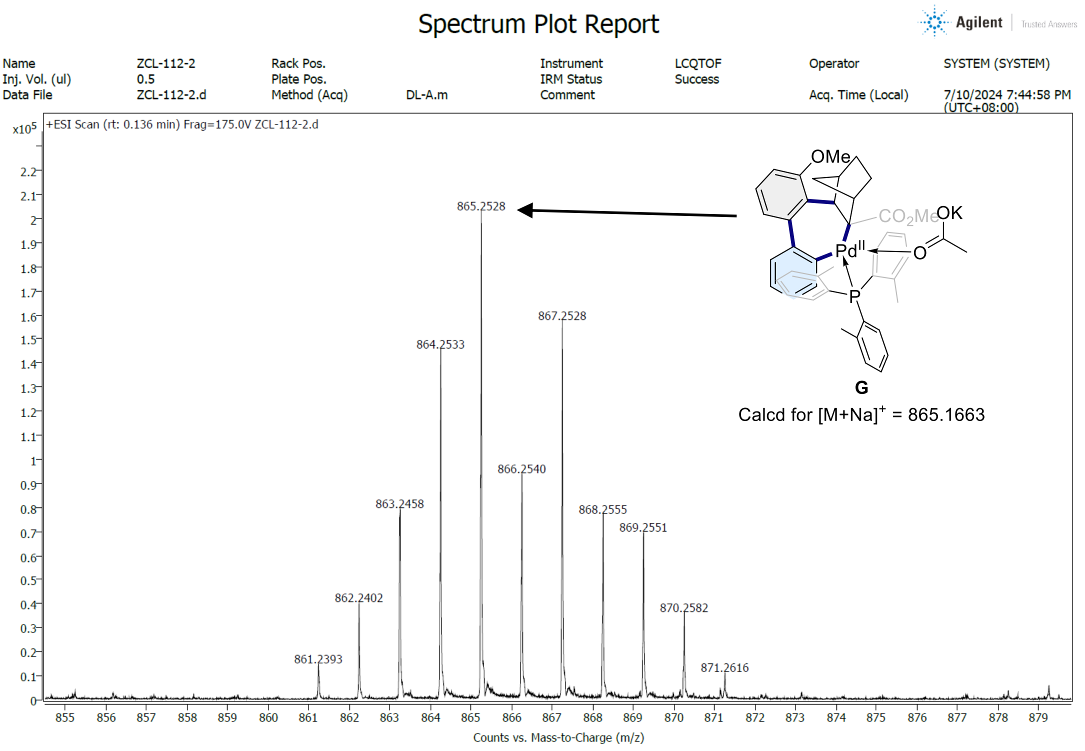
Fig. S4. MS spectrum of intermediate **D**.

(b) Reaction of **1a** with **NBE-CO$_2$Me** and **2a** in the condition of quantitative Pd(OAc)$_2$:



(Detected by Q-TOF LC/MS)

The oven-dried Schlenk tube (10 mL) equipped with a stirring bar was charged with substrates **1a** (0.1 mmol, 1.0 equiv), **2a** (2.0 equiv), Pd(OAc)$_2$ (1.0 equiv), P(2-MeC$_6$H$_4$)$_3$ (2.5 equiv) and K$_2$CO$_3$ (4.5 equiv) in the air. Followed by the mediator NBE-CO$_2$Me (1.5 equiv) and the anhydrous toluene (1.0 mL) were added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N$_2$ for three times. Finally, the reaction mixture was stirred at 130 ℃ for 24 h and then cooled to room temperature. Upon completion of the reaction, the mixture was analyzed by the Agilent 6546 Q-TOF LC/MS system detection and intermediate **G** were detected.


Spectrum Plot Report

Name	ZCL-112-2	Rack Pos.		Instrument	LCQTOF	Operator	SYSTEM (SYSTEM)
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	ZCL-112-2.d	Method (Acq)	DL-A.m	Comment		Acq. Time (Local)	7/10/2024 7:44:58 PM (UTC+08:00)

Fig. S5. MS spectrum of intermediate **G**.

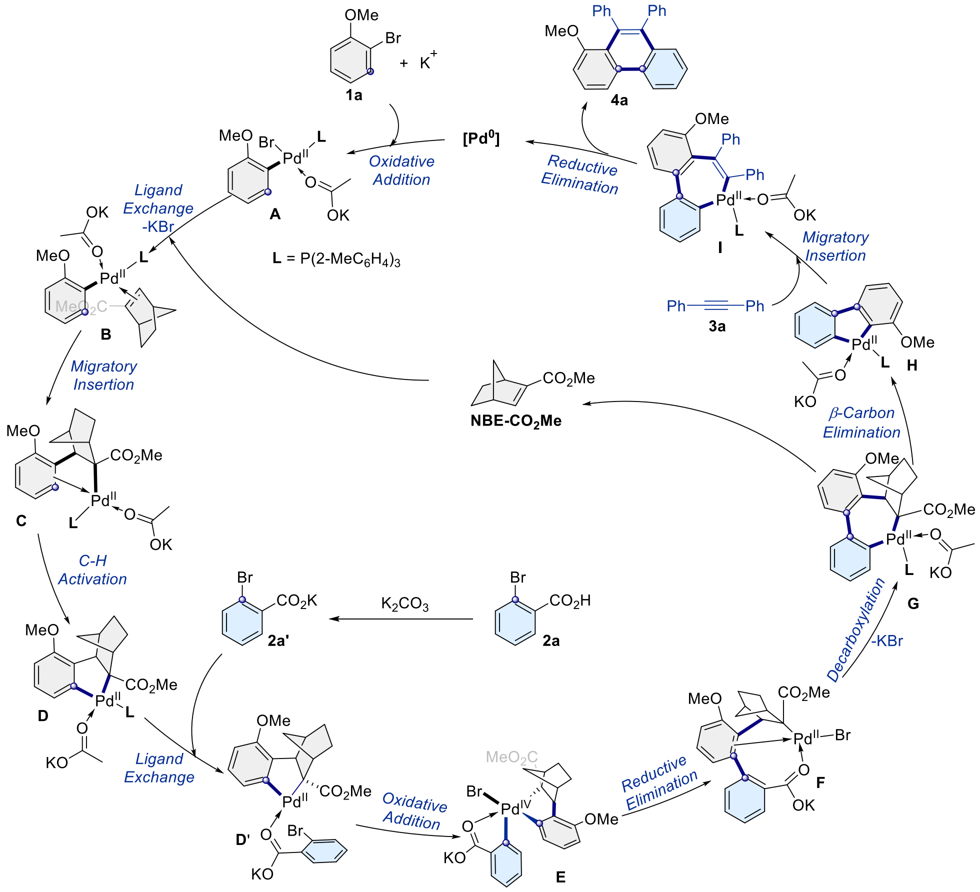
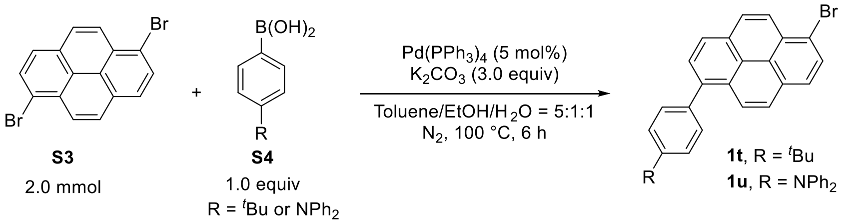


Fig. S6. Proposed reaction mechanism.

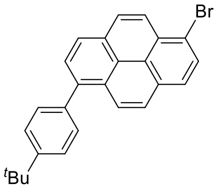
3.5 General procedures for the synthesis of substrates

(a)The synthesis of substrates 1t and 1u:

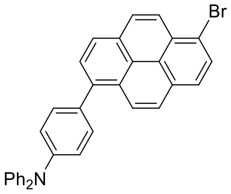


The oven-dried Schlenk tube (100 mL) equipped with a stirring bar was charged with 1,6-dibromopyrene (**S3**, 2.0 mmol, 1.0 equiv), 4-tert-butylphenylboronic acid or 4-(diphenylamino)phenyl boronic acid (**S4** 1.0 equiv), $Pd(PPh_3)_4$ (5 mol%), and K_2CO_3 (4.5 equiv) in the air. Followed by the toluene/EtOH/H_2O (5/1/1, 10 mL) were added via syringe under nitrogen flow. Then the tube was evacuated and back-filled with N_2 for three times. Finally, the reaction mixture was stirred at 100 ℃ for 6 h and then cooled to room temperature. Upon completion of the reaction, the mixture was quenched by 2N HCl aqueous solution and ethyl acetate (EA). The organic phases were separated and the aqueous phase was extracted with EA three times. The combined organic phases were washed with brine, dried with anhydrous Na_2SO_4 and concentrated *in vacuo*. The resulting residue was purified via silica gel column chromatography using PE/EA (200/1 – 20/1) as the eluent.

Characterization of substrates 1t and 1u:



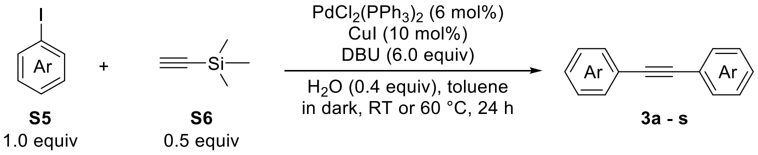
1-bromo-6-(4-(*tert*-butyl)phenyl)pyrene (1t): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 9.2 Hz, 1H), 8.30 – 8.21 (m, 3H), 8.19 (d, *J* = 9.2 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 8.00 – 7.92 (m, 2H), 7.64 – 7.52 (m, 4H), 1.46 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.5, 138.7, 138.0, 130.6, 130.4, 130.35, 130.3, 130.1, 129.2, 128.7, 128.5, 127.1, 126.3, 126.0, 125.9, 125.5, 125.4, 125.3, 124.5, 120.0, 34.8, 31.6. HRMS (m/z, ESI): calcd for $C_{26}H_{24}Br^+$ $(M+H)^+$ 415.0983, found 415.0795.



4-(6-bromopyren-1-yl)-*N,N*-diphenylaniline (1u): ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (d, *J* = 9.2 Hz, 1H), 8.31 (d, *J* = 9.2 Hz, 1H), 8.24 (dd, *J* = 7.6, 6.0 Hz, 2H), 8.18 (d, *J* = 9.2 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 4H), 7.30 – 7.18 (m, 6H), 7.09 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.8, 147.4, 138.4, 134.7, 131.5, 130.6, 130.31, 130.29, 130.1, 129.5, 129.2, 128.6, 128.4, 127.1, 126.3, 125.9, 125.4, 125.36, 124.8, 124.6, 123.3, 120.0. HRMS (m/z, ESI): calcd for $C_{34}H_{25}BrN^+$ $(M+H)^+$ 526.1092, found 526.0902.

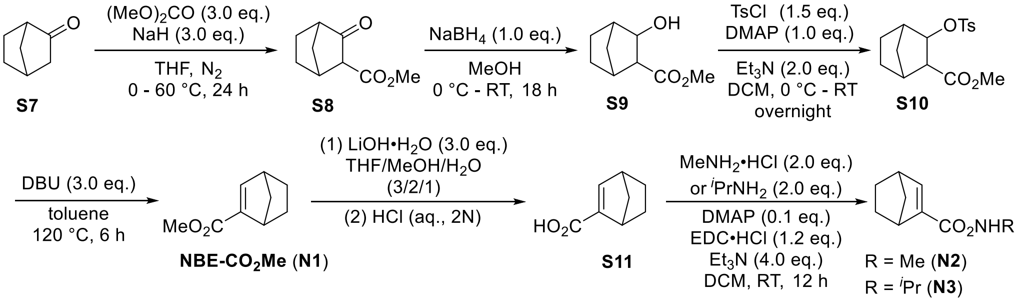
(b) The synthesis of symmetrical 1,2-diarylalkynes:

All the symmetrical 1,2-diarylalkynes were prepared according to the reported literatures[S2].



(c) The synthesis of norbornene mediators:

The structurally modified norbornenes were synthesized following the procedure as described in literatures[S3, S4].



4. Photophysical properties and applications of products.

4.1. The absorption and fluorescence properties of products

Fluorescence spectra were collected on HITACHI F-700003040428 Fluorescence Spectrometer. UV−vis spectra were recorded on Agilent Cary60 spectrometer. Samples for the experiments were prepared in a 4.0 mL glass cuvette with a septum screw cap. In a typical experiment, a 5.0×10^{-5} M and 1.0×10^{-6} M solution of product in DCM for the collection of emission spectrum and UV-vis spectrum were prepared respectively.

Table S2. Absorption maxima and emission maxima of products.

Compunds	Absorb.(λ_{abs}, nm) [a]	Emission (λ_{em}, nm) [b]	CIE_{1931}
4a	258, 303, 345, 362	370, 388	(0.16, 0.02)
4b	264, 298, 310	366, 381	(0.16, 0.03)
4c	265, 299, 310	369, 386	(0.16, 0.04)
4d	277, 319, 333	382, 399	(0.16, 0.02)
4e	277, 322, 335	386, 404	(0.16, 0.02)
4f	279, 327, 341, 378	393, 409	(0.16, 0.02)
4g	273, 317, 332, 373	384, 402	(0.16, 0.02)
4h	281, 345	415	(0.16, 0.03)
4i	282, 341, 356	409	(0.16, 0.02)
4j	255, 288, 360	435	(0.15, 0.06)
4k	279, 326, 341, 376	385, 403	(0.16, 0.01)
4l	267, 282, 292, 320, 371, 392	445	(0.15, 0.08)
4m	251, 290, 306, 319, 377, 398	428, 452	(0.15, 0.04)
4n	298, 333	404	(0.16, 0.02)
4o	252, 275, 327, 433	496	(0.15, 0.49)
4p	272, 332, 370	388, 401	(0.16, 0.02)
4q	310, 376, 395	428	(0.16, 0.03)
4r	290, 352, 370	379, 395, 415	(0.17, 0.01)
4s	265, 296, 359, 377	383, 403, 425	(0.17, 0.01)
5a	268, 284, 320, 375, 395	446	(0.15, 0.07)
5b	261, 284, 296, 320, 372, 391	445	(0.15, 0.08)
5c	264, 302, 322, 370, 388	446	(0.15, 0.08)
5d	283, 319, 373, 395	444	(0.15, 0.08)
5e	262, 281, 292, 320, 367, 385	450	(0.15, 0.13)
5f	271, 283, 322, 373, 395	445	(0.15, 0.10)
5g	285, 296, 321, 369, 388	451	(0.15, 0.13)
5h	286, 320, 370, 392	454	(0.15, 0.14)
5i	290, 356, 388	551	(0.37, 0.58)
6a	264, 282, 318, 372, 390	444	(0.15, 0.08)
6b	262, 284, 318, 372, 392	443	(0.15, 0.07)
6c	264, 282, 318, 372, 392	440	(0.15, 0.07)
6d	266, 282, 320, 373, 393	442	(0.15, 0.07)

6e	265, 282, 319, 373, 394	442	(0.15, 0.07)
6f	293, 376	527	(0.26, 0.60)
6g	264, 288, 318, 368, 386	449	(0.15, 0.13)
6h	264, 282, 318, 370, 390	446	(0.15, 0.10)
6i	264, 288, 318, 368, 388	449	(0.15, 0.12)
6j	264, 286, 318, 370, 388	446	(0.15, 0.10)
6k	288, 318, 377, 388	451	(0.15, 0.13)
6l	264, 288, 318, 368, 388	451	(0.15, 0.13)
6m	266, 288, 318, 370, 388	447	(0.15, 0.11)
6n	288, 320, 368, 388	456	(0.15, 0.15)
6o	260, 288, 320, 368, 388	448	(0.15, 0.12)
6p	260, 288, 318, 370, 388	449	(0.15, 0.12)
6q	288, 316, 370, 390	446	(0.15, 0.10)
6r	264, 282, 320, 372, 388	454	(0.15, 0.13)
6s	256, 292, 326, 392, 412	448, 463	(0.14, 0.09)
6t	288, 416	523	(0.24, 0.61)
6u [c]	290, 352	412, 436, 561	(0.31, 0.34)
6v	290, 414	535	(0.32, 0.62)
6w [d]	278, 306, 450	394, 418, 571	(0.33, 0.33)
6w NPs [e]	281, 305, 459	426, 465, 610	(0.33, 0.28)

[a] Absorption maximum in CH_2Cl_2 (1×10^{-6} M). [b] Emission maximum in CH_2Cl_2 (5.0×10^{-5} M). [c] CH_2Cl_2 used as solvent (2.5×10^{-7} M). [d] Toluene used as solvent (2.4×10^{-6} M). [e] H_2O used as solvent (2.0×10^{-5} M).

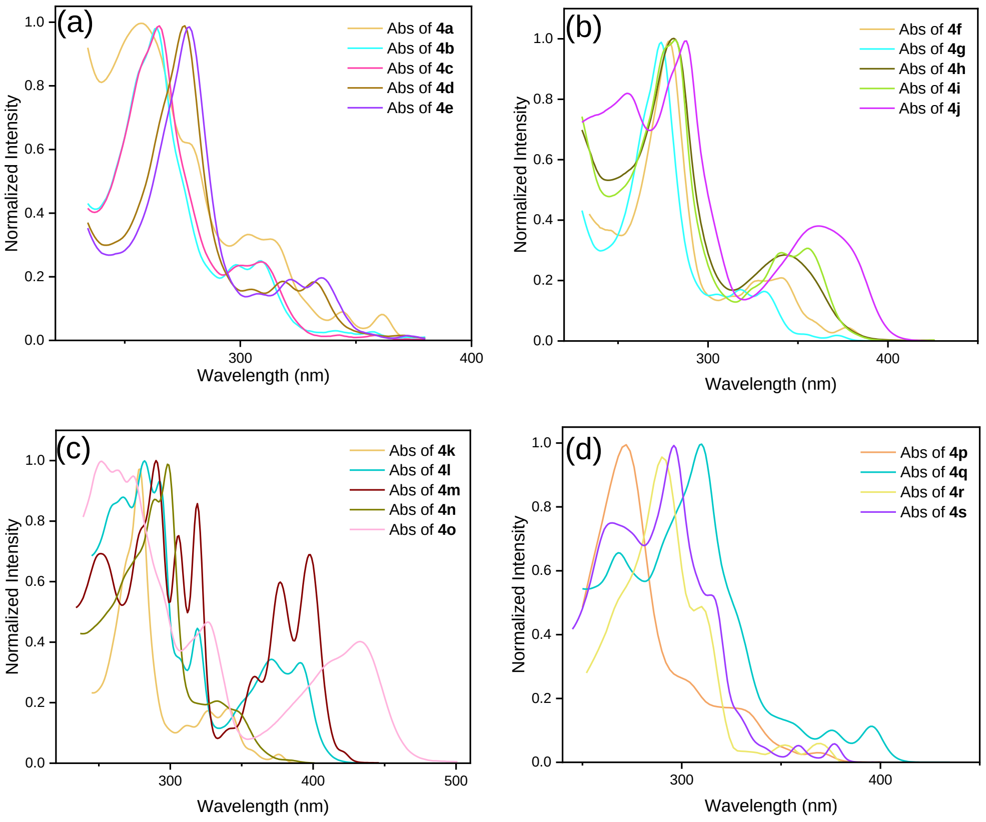


Fig. S7. Normalized UV-Vis absorption spectra of **4a-4s** in DCM (1×10^{-6} M).

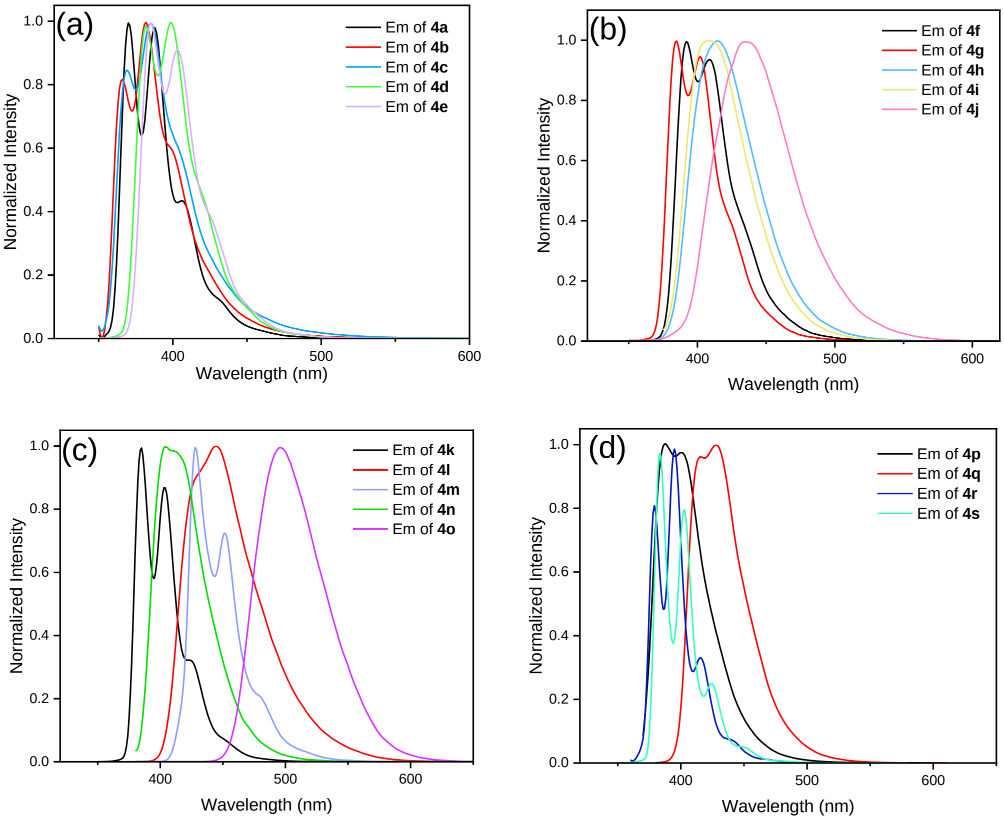


Fig. S8. Normalized fluorescence emission spectra of **4a-4s** in DCM (5.0×10^{-5} M).

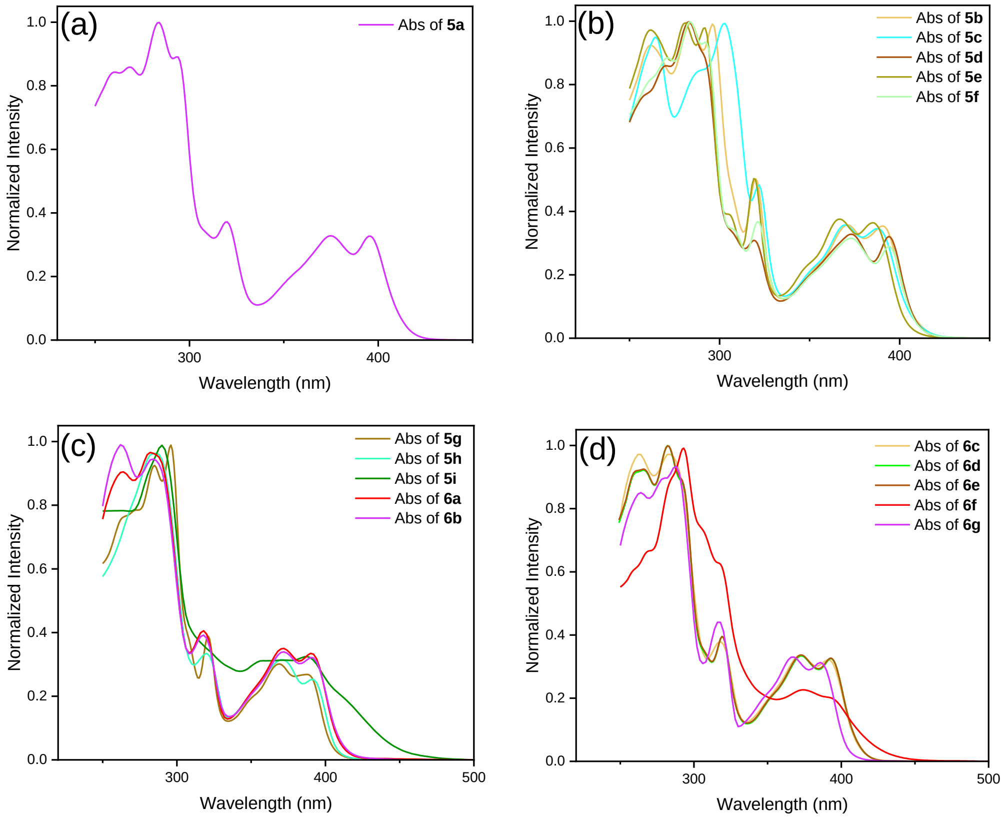


Fig. S9. Normalized UV-Vis absorption spectra of **5a-6g** in DCM (1×10^{-6} M).

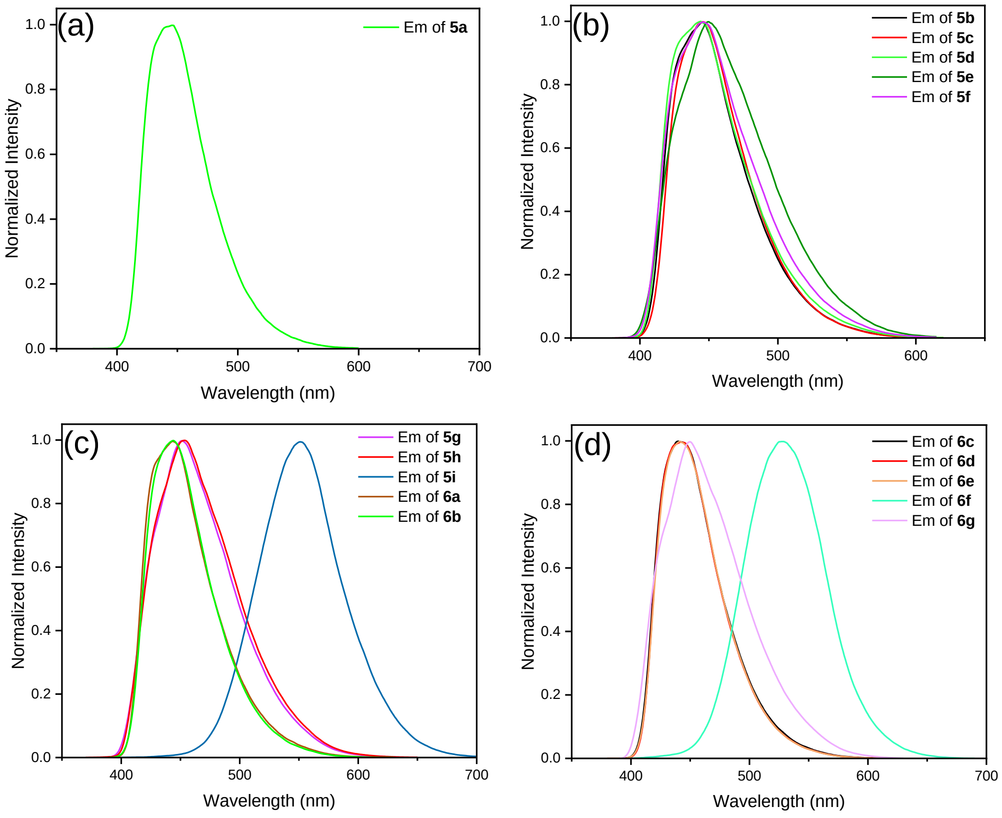


Fig. S10. Normalized fluorescence emission spectra of **5a-6g** in DCM (5.0×10^{-5} M).

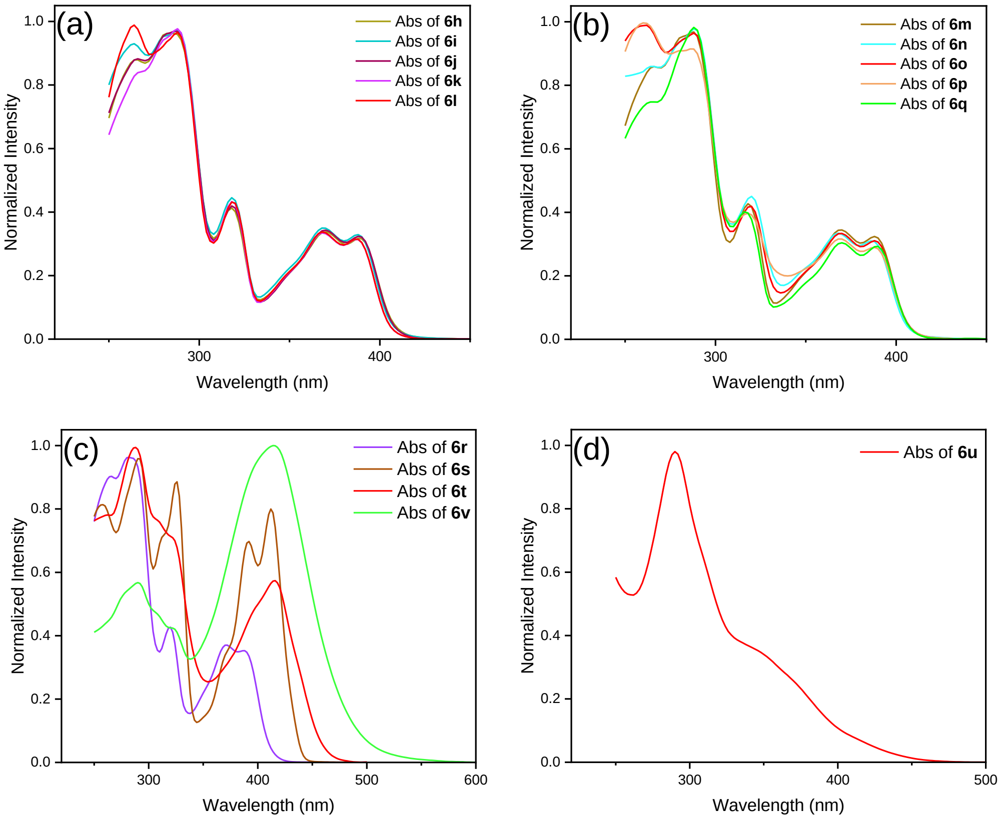


Fig. S11. Normalized UV-Vis absorption spectra of **6h-6v** in DCM (1×10^{-6} M).

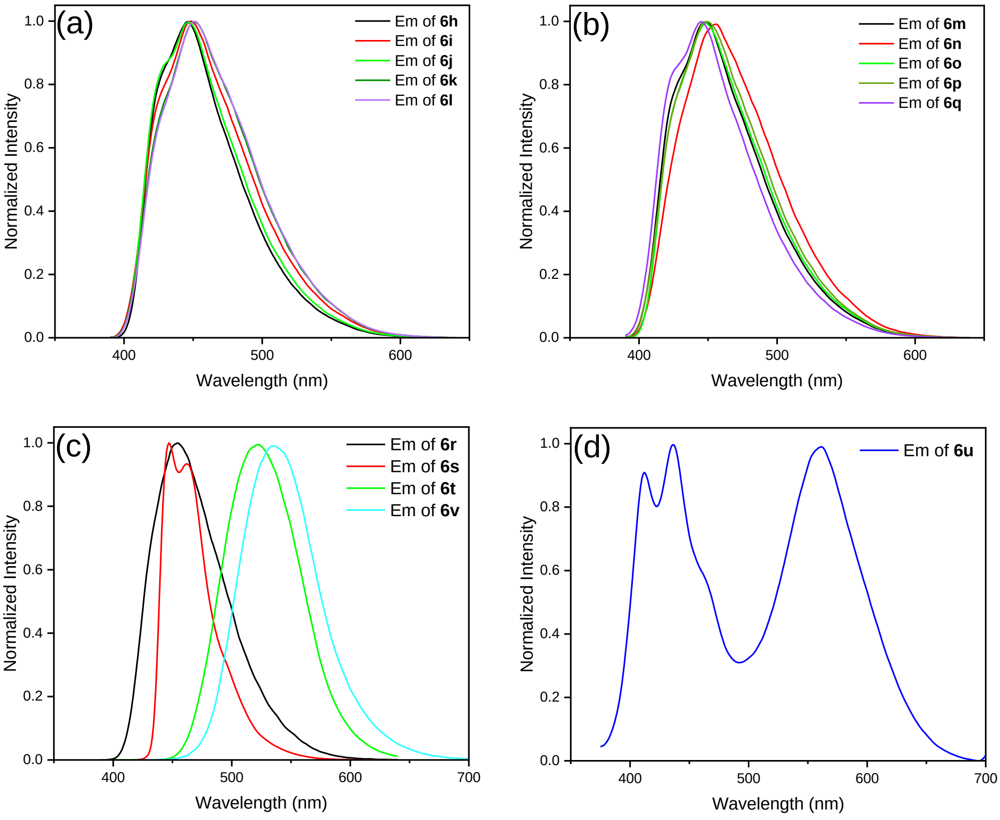


Fig. S12. (a - c) Normalized fluorescence emission spectra of **6h-6t** and **6v** in DCM

(5.0×10^{-5} M). (d) Normalized fluorescence emission spectra of **6u** in DCM (2.5×10^{-7} M).

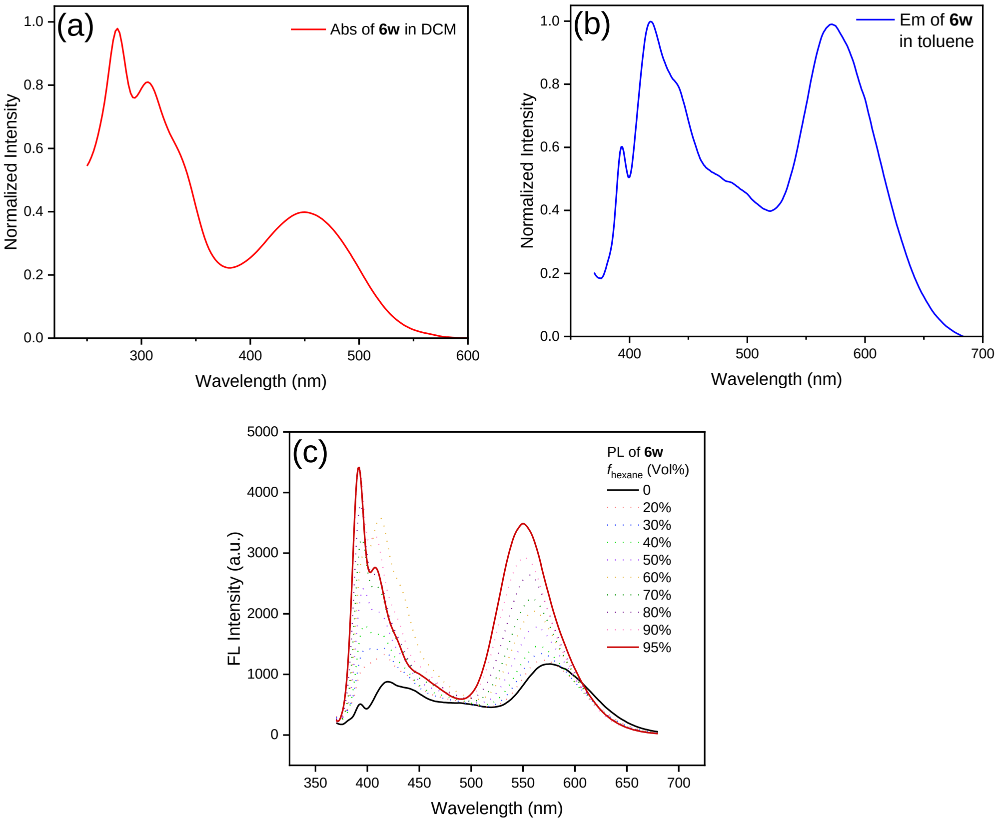


Fig. S13. (a) Normalized UV-Vis absorption spectra of **6w** in DCM (1×10^{-6} M); (b) Normalized fluorescence emission spectra of **6w** in toluene (2.4×10^{-6} M); (c) Fluorescence spectra of **6w** in toluene–hexane mixtures (2.4×10^{-6} M) with different fractions (f_{hexane}).

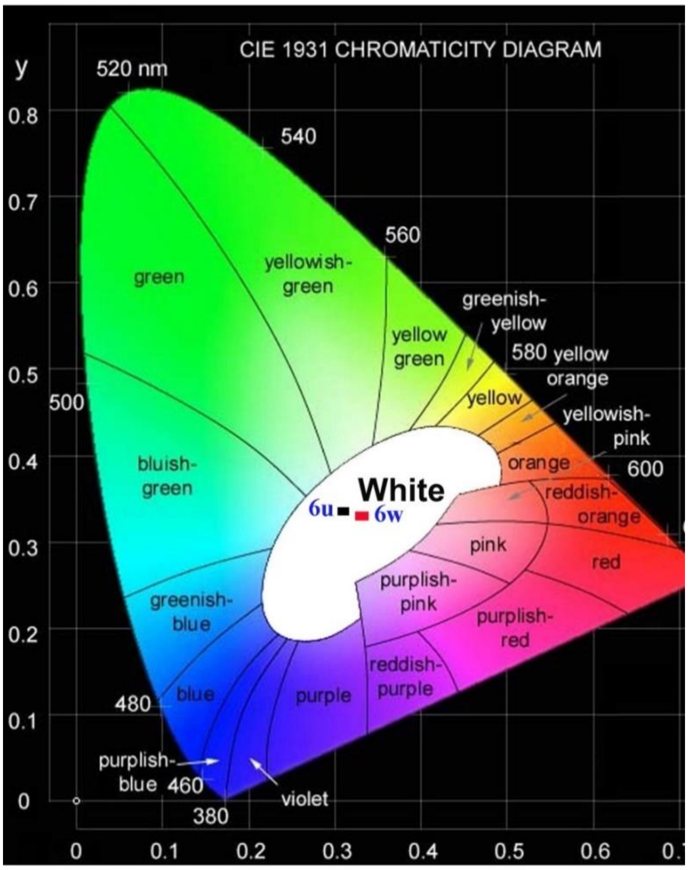


Fig. S14. The white-light emissions of **6u** and **6w**. CIE$_{1931}$ chromaticity diagrams **6u** (0.31, 0.34) and **6w** (0.33, 0.33) in CH_2Cl_2 (Concentration: **6u**: 2.5×10^{-7} M; **6w**: 2.4×10^{-6} M).

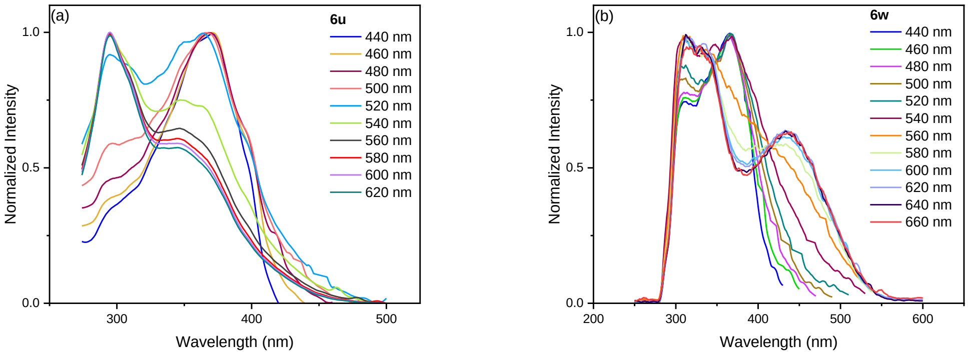


Fig. S15. (a) Emission-wavelength-dependent excitation spectra of **6u** (1.0×10^{-8} M in DCM). (b) Emission-wavelength-dependent excitation spectra of **6w** (1.3×10^{-7} M in toluene). Excitation spectra were collected by Edinburgh Instruments FLS1000.

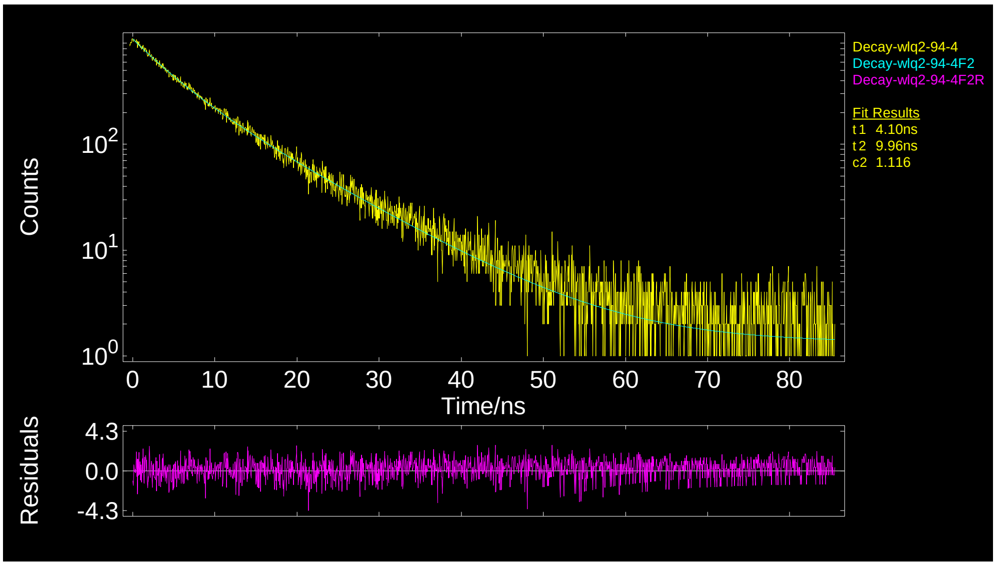
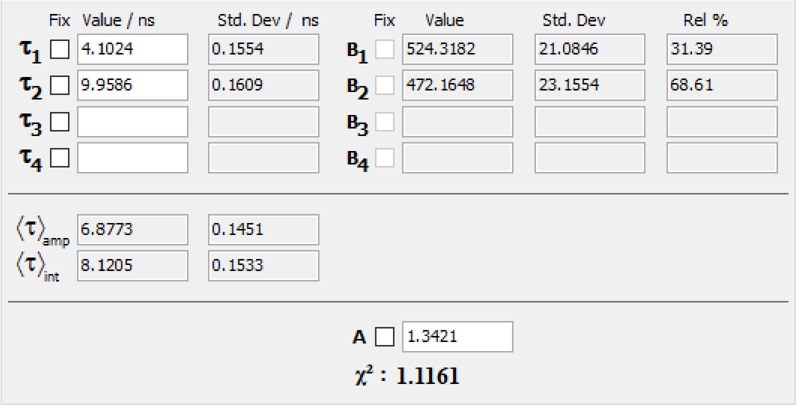


Fig. S16. Fluorescence lifetime decay curves of **6u** in TBCPF film (3 wt%).



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	4.1024	0.1554	B_1	☐	524.3182	21.0846	31.39
τ_2	☐	9.9586	0.1609	B_2	☐	472.1648	23.1554	68.61
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			

$\langle\tau\rangle_{amp}$	6.8773	0.1451
$\langle\tau\rangle_{int}$	8.1205	0.1533

A ☐ 1.3421

χ^2 : 1.1161

Fig. S17. The excited state lifetimes of **6u** in TBCPF film.

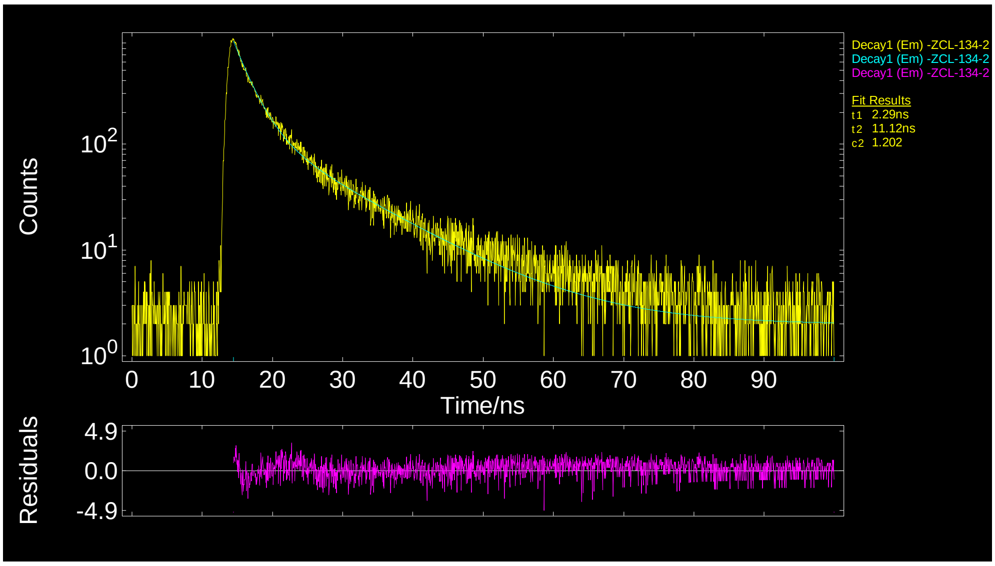
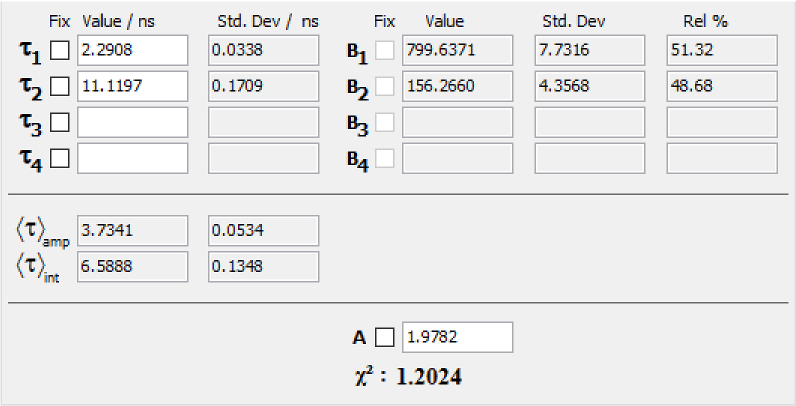


Fig. S18. Fluorescence lifetime decay curves of **6w** in TBCPF film (10 wt%).



	Fix	Value / ns	Std. Dev / ns		Fix	Value	Std. Dev	Rel %
τ_1	☐	2.2908	0.0338	B_1	☐	799.6371	7.7316	51.32
τ_2	☐	11.1197	0.1709	B_2	☐	156.2660	4.3568	48.68
τ_3	☐			B_3	☐			
τ_4	☐			B_4	☐			
$\langle\tau\rangle_{amp}$		3.7341	0.0534					
$\langle\tau\rangle_{int}$		6.5888	0.1348					

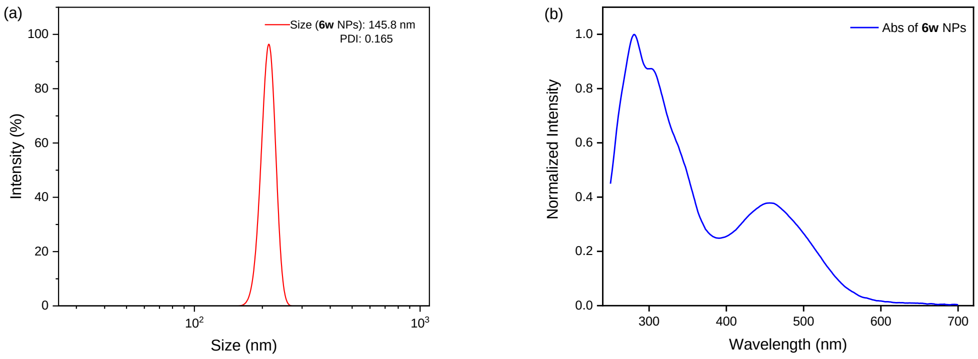
A ☐ 1.9782

χ^2 : 1.2024

Fig. S19. The excited state lifetimes of **6w** in TBCPF film.

4.2. Preparation and characterization of 6w NPs.

The compound **6w** (2.0 mg) was dissolved in THF (2 mL) followed by ultrasound for 10 min. Poloxamer 188 (60 mg) was added to the solution of **6w** in THF and the mixture was treated by ultrasound for 10 min. The resulted mixture was stirred three hours at RT. Then the solvent was removed by reduced pressure. The residue was dissolved in deionized water (2 mL) and stirred overnight at RT to drive the formation of NPs. To remove the residual THF, the nanoparticle suspensions were dialyzed by three times. The concentrations of nanoparticles were calibrated via the UV-vis spectra. Finally, the NPs solution was collected and stored at 4 °C.



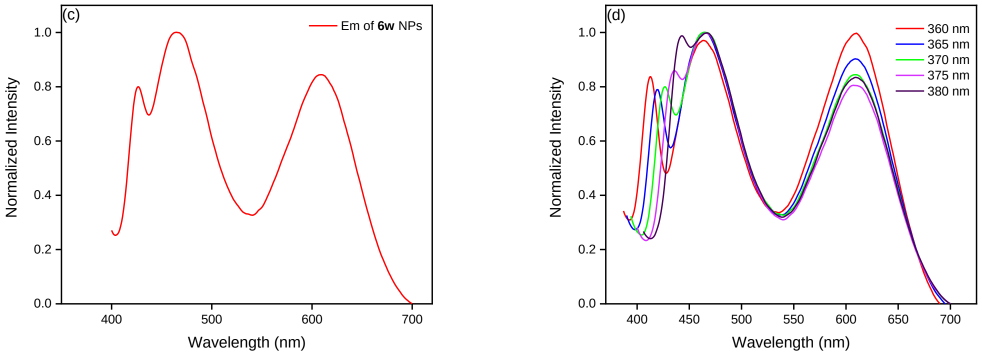


Fig. S20. (a) Hydrodynamic size distribution of **6w** NPs in aqueous solution. (b) Normalized UV-Vis absorption spectra emission spectra of **6w** NPs. in H_2O (1.0×10^{-6} M). (b) Normalized fluorescence emission spectra of **6w** NPs. in H_2O (2.0×10^{-5} M). (d) Excitation-wavelength-dependent fluorescence spectra of **6w** NPs in H_2O (2.0×10^{-5} M).

4.3. Cell imaging experiments

Cellular Experiments: The Hela cells were cultured in 10% FBS and 1% penicillin-streptomycin-containing DMEM medium at 37 ℃ with 5% CO_2.

Methyl thiazolyl tetrazolium (MTT) assay: To assess the safe usability of **6w** nanoparticles for biomedical applications, the cytotoxicity experiments in Hela cells were carried out using the standard methyl thiazolyl tetrazolium (MTT) assay.

Cell viability assay: The Hela cells were seeded into 96-well plates and incubated with a standard medium overnight. The cell suspensions were treated with different concentrations of **6w** NPs in a deionized water solution (0, 1, 5, 10, 20, 40 μM) and incubated for another 24 h. Live/dead cell staining was carried out after 20 min white light irradiation and without light irradiation, respectively.

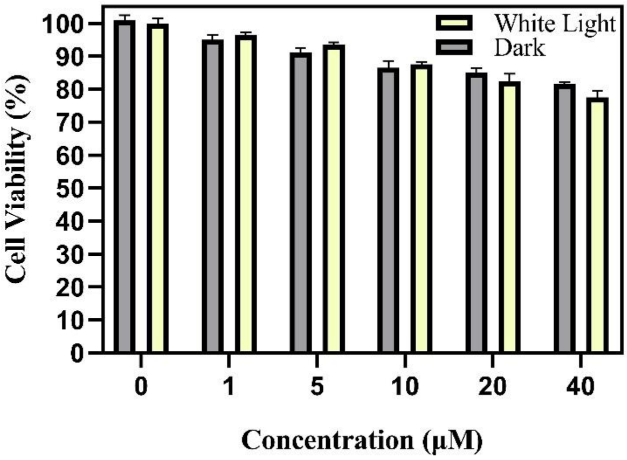


Fig. S21. In vitro cytotoxicity of the **6w** NPs. Cell viabilities of Hela cells incubated with **6w** NPs for 24 h.

Confocal imaging experiments: The confocal imaging experiments were performed on Leica TCS SP8. The nanoparticles of product **6w** (**6w** NPs) was used as fluorescent probe.

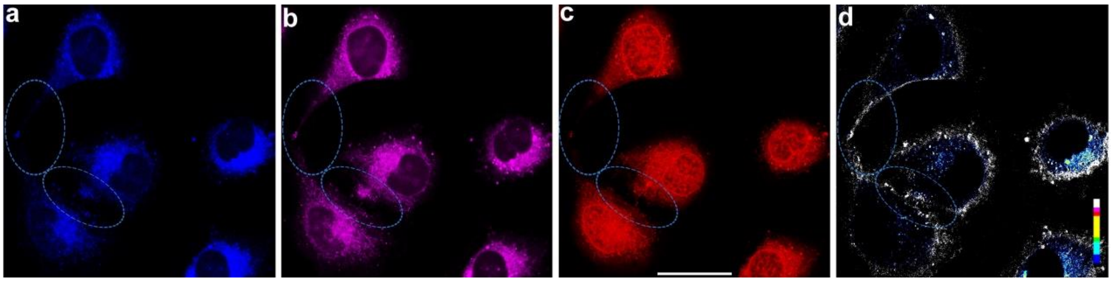


Fig. S22. Fluorescence microscopy images of HeLa cells incubated with **6w** NPs (10 μM) for 2 h at 37 ^{o}C. (a) Fluorescence microscope image from channel 1 at 425–500 nm (Excitation 405 nm). (b) Fluorescence microscope image from channel 1 at 500–700 nm (Excitation 405 nm). (c) Fluorescence microscope image from channel 2 at 500–700 nm (Excitation 488 nm). (d) The emission intensity ratio of (a) and (c) of HeLa cells (Image generation by Image J software). Elliptic: mark out the intercellular structure and cellular local imaging information. The scale bar is 25.0 μm.

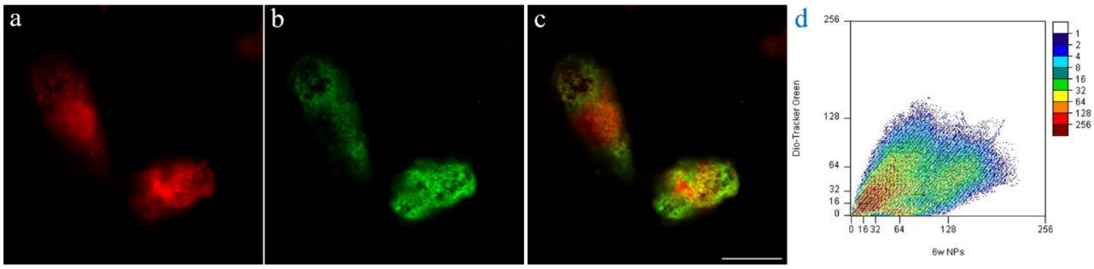


Fig. S23. The co-staining experiments. (a) Fluorescent image of HeLa cells cultured with **6w** NPs (10 μM) (λ_{ex} = 552 nm, λ_{em} = 575–750 nm). (b) Fluorescent image of HeLa cells with Dio-Tracker Green (λ_{ex} = 488 nm, λ_{em} = 508–540 nm). (c) Merged image of (a) and (b). (d) The Pearson correlation coefficient r = 0.57; The scale bar is 25.0 μm.

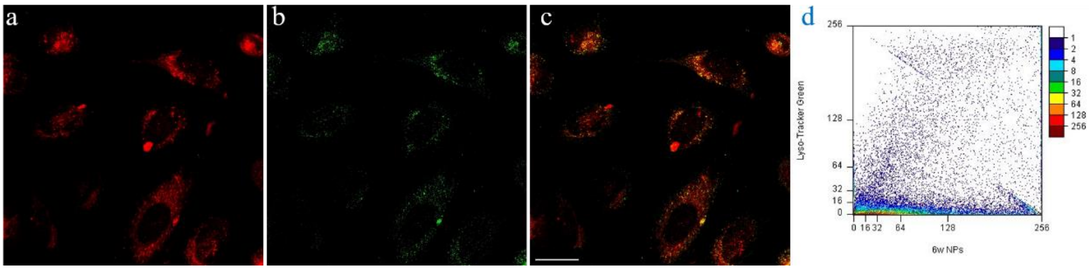


Fig. S24. The co-staining experiments. (a) Fluorescent image of HeLa cells cultured with **6w** NPs (10 μM) (λ_{ex} = 552 nm, λ_{em} = 575–750 nm). (b) Fluorescent image of HeLa cells with Lyso-Tracker Green (λ_{ex} = 488 nm, λ_{em} = 508–540 nm). (c) Merged image of (a) and (b). (d) The Pearson correlation coefficient r = 0.44; The scale bar is 25.0 μm.

5. References

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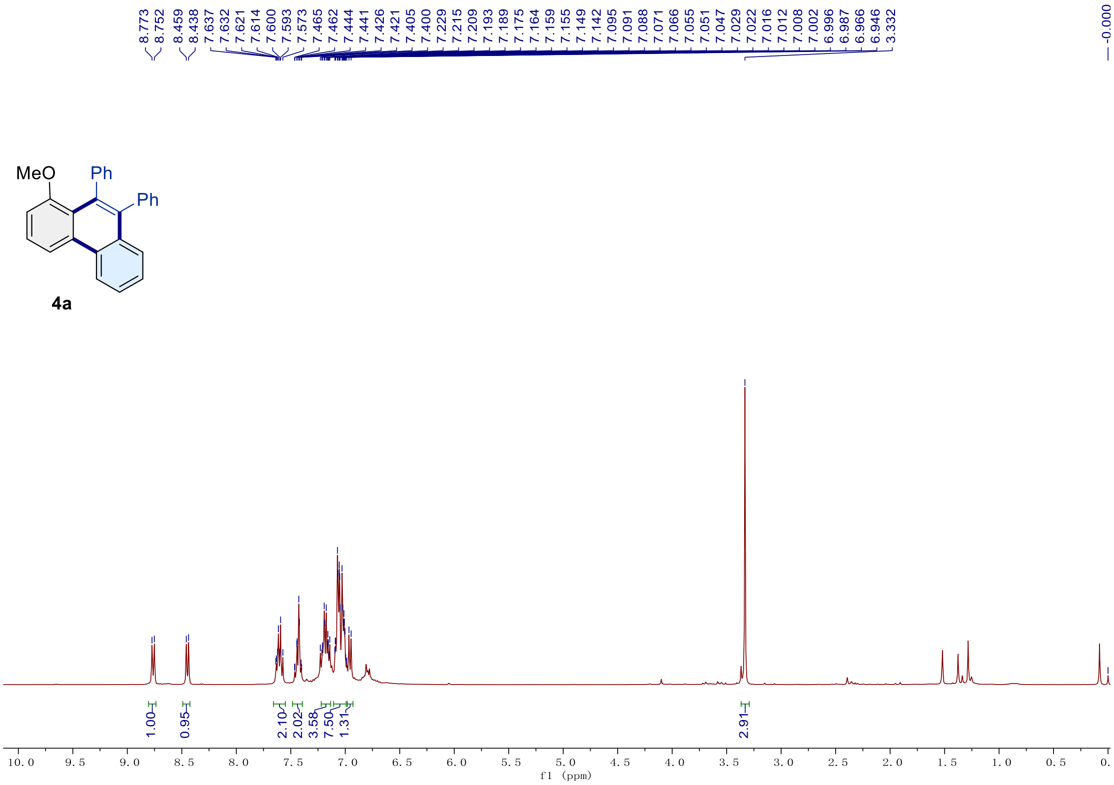
[S2] J. Bai, N. Xu, H. Wang and X. Luan. *Org. Lett.* **2022**, *24*, 5099–5104.

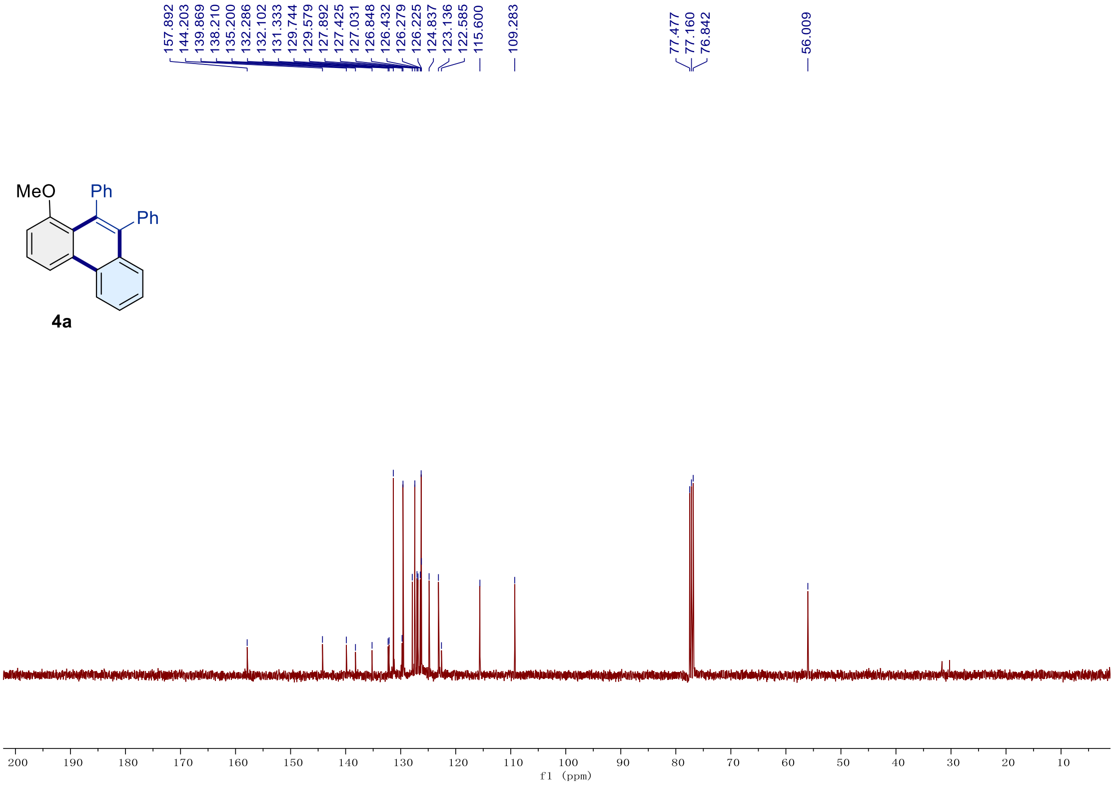
[S3] J. Wang, Z. Dong, C. Yang and G. Dong. *Nat. Chem.* **2019**, *11*, 1106–1112.

[S4] V. Sukowski, M. Borselen, S. Mathew and M. Á. Fernández-Ibáñez. *Angew. Chem. Int. Ed.* **2022**, *61*, e202201750.

6. NMR spectrum of compounds

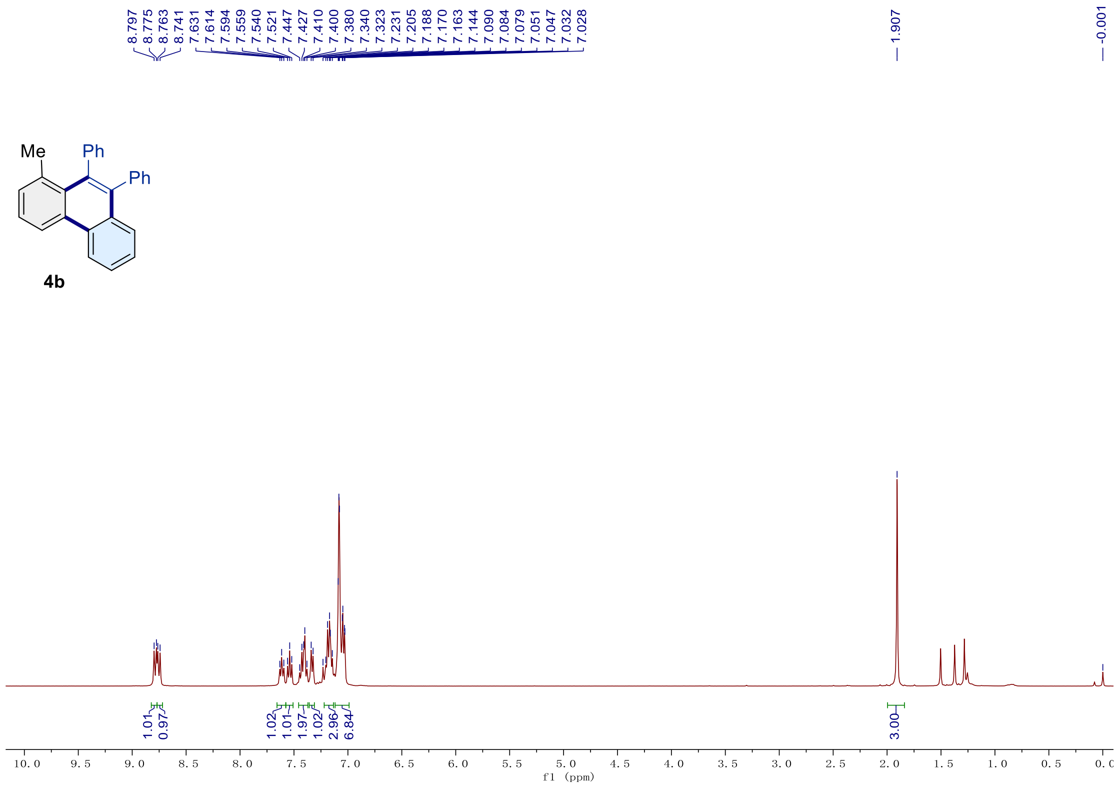
NMR spectrum of products 4a – 6w:





Me
Ph
Ph

4b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7.400
7.380
7.340
7.323
7.231
7.205
7.188
7.170
7.163
7.144
7.090
7.084
7.079
7.051
7.047
7.032
7.028
1.907
-0.001
1.01
0.97
1.02
1.01
1.97
1.02
2.96
6.84
3.00
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
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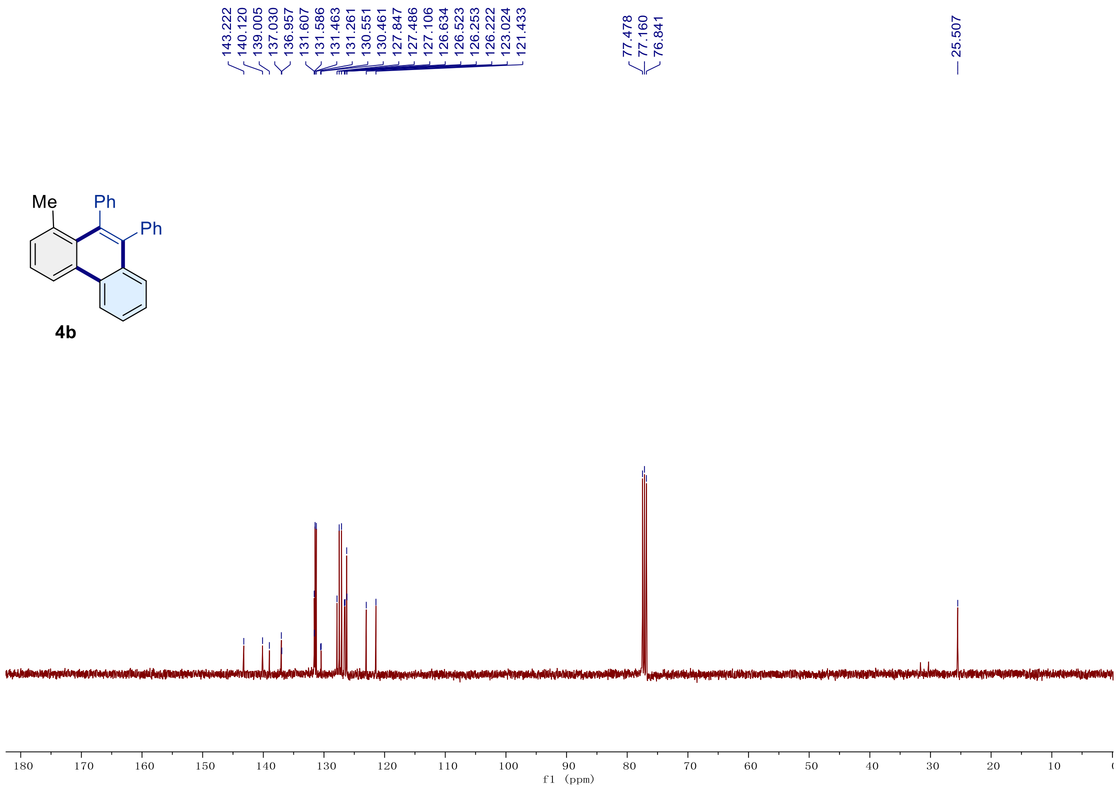
0.0
f1 (ppm)

Me
Ph
Ph

4b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127.106
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126.523
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126.222
123.024
121.433
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77.160
76.841
25.507
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160
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140
130
120
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100
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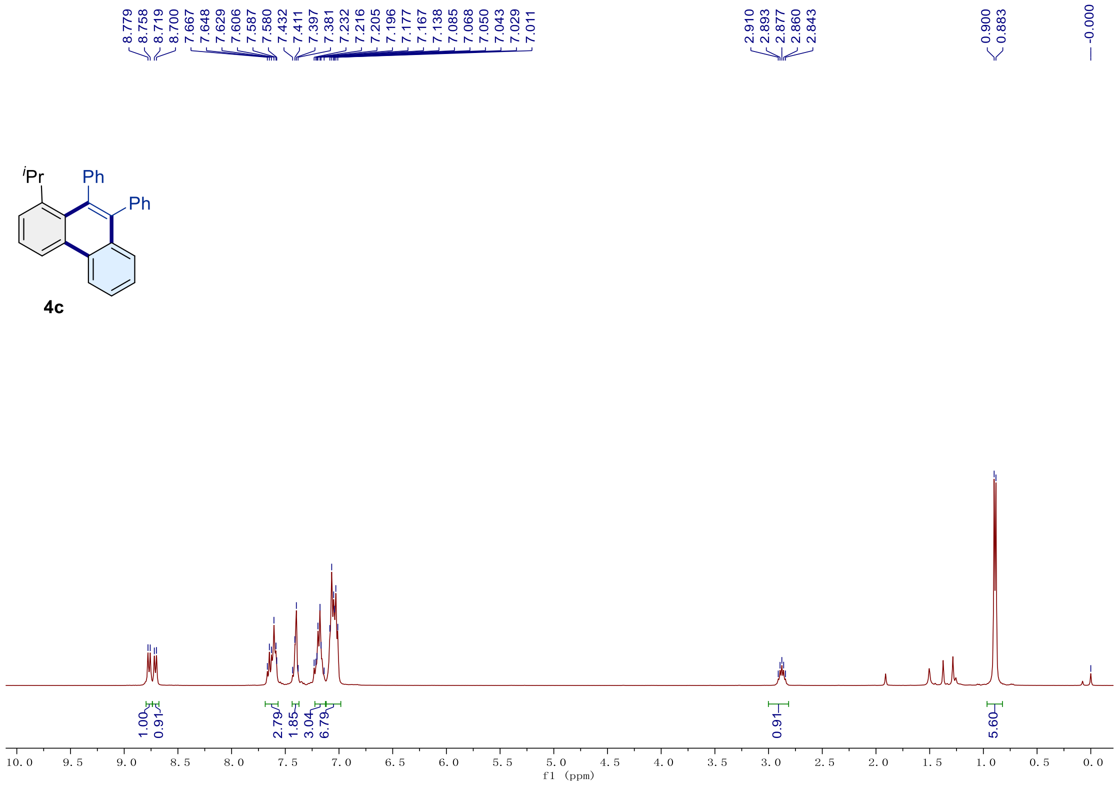
80
70
60
50
40
30
20
10
f1 (ppm)



iPr
Ph
Ph

4c

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7.580
7.432
7.411
7.397
7.381
7.232
7.216
7.205
7.196
7.177
7.167
7.138
7.085
7.068
7.050
7.043
7.029
7.011
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2.877
2.860
2.843
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0.883
-0.000
1.00
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2.79
1.85
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6.79
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6.0
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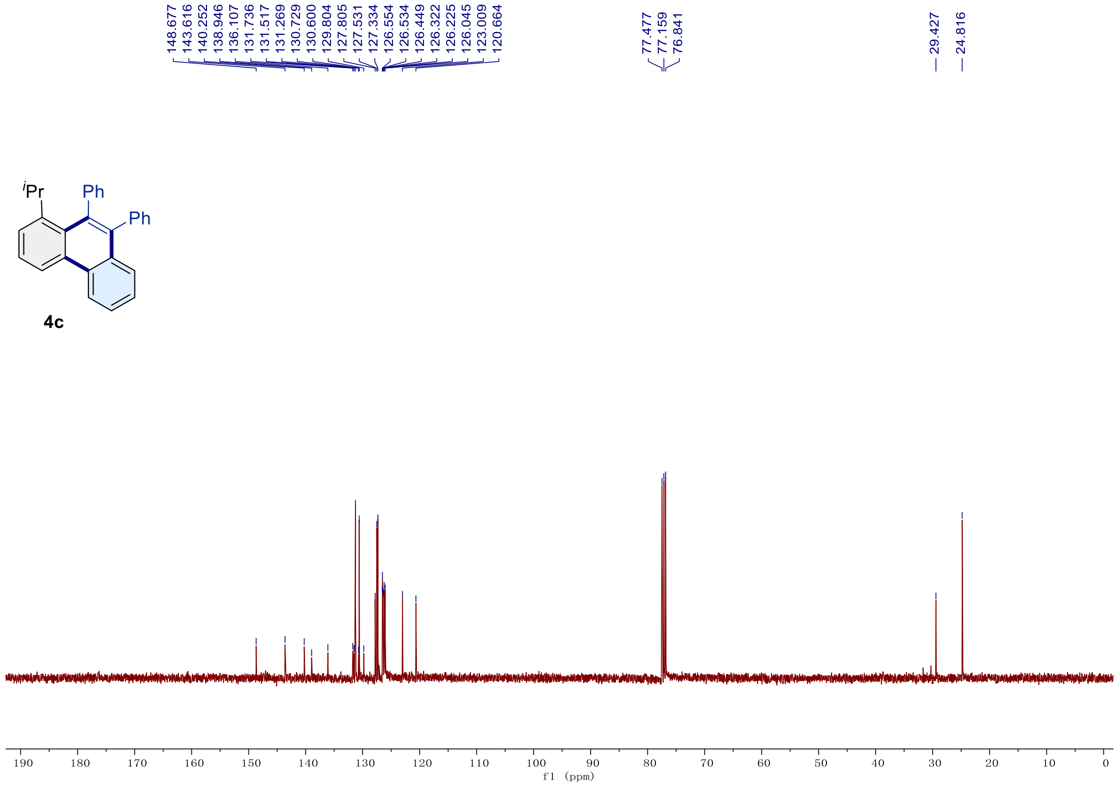
f1 (ppm)



iPr
Ph
Ph

4c

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127.805
127.531
127.334
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126.449
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126.045
123.009
120.664
77.477
77.159
76.841
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190
180
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50
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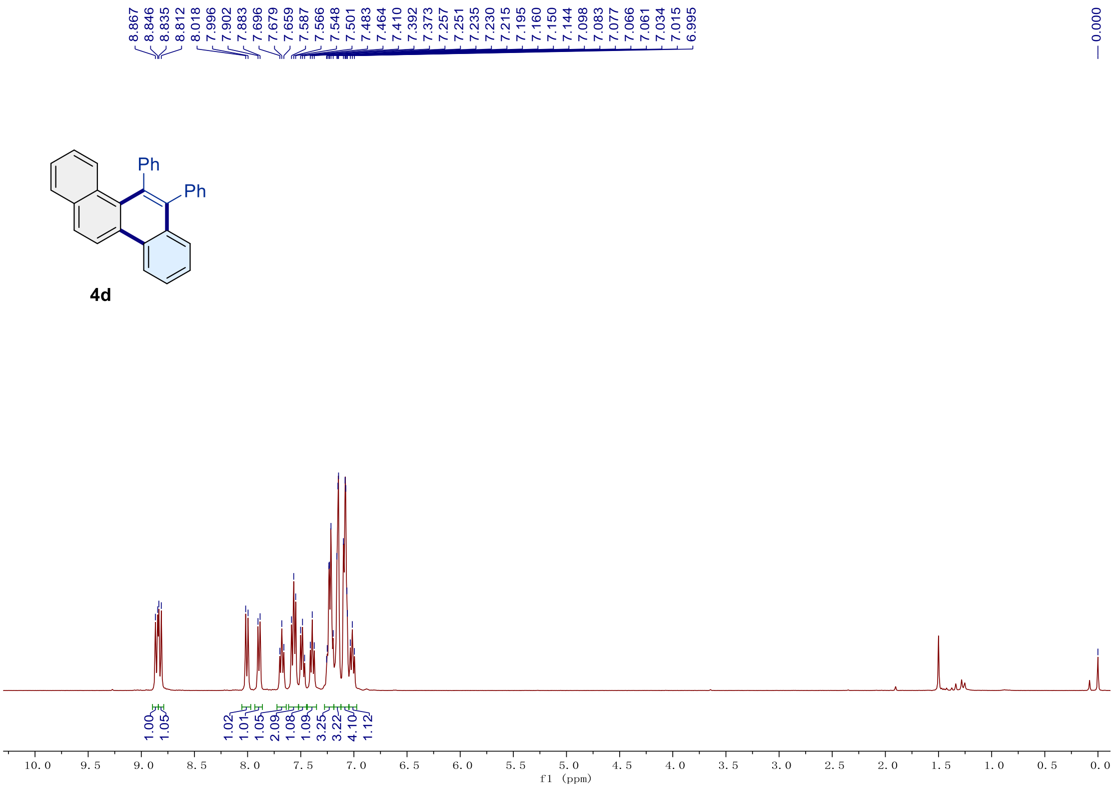
f1 (ppm)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7.464
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7.392
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7.230
7.215
7.195
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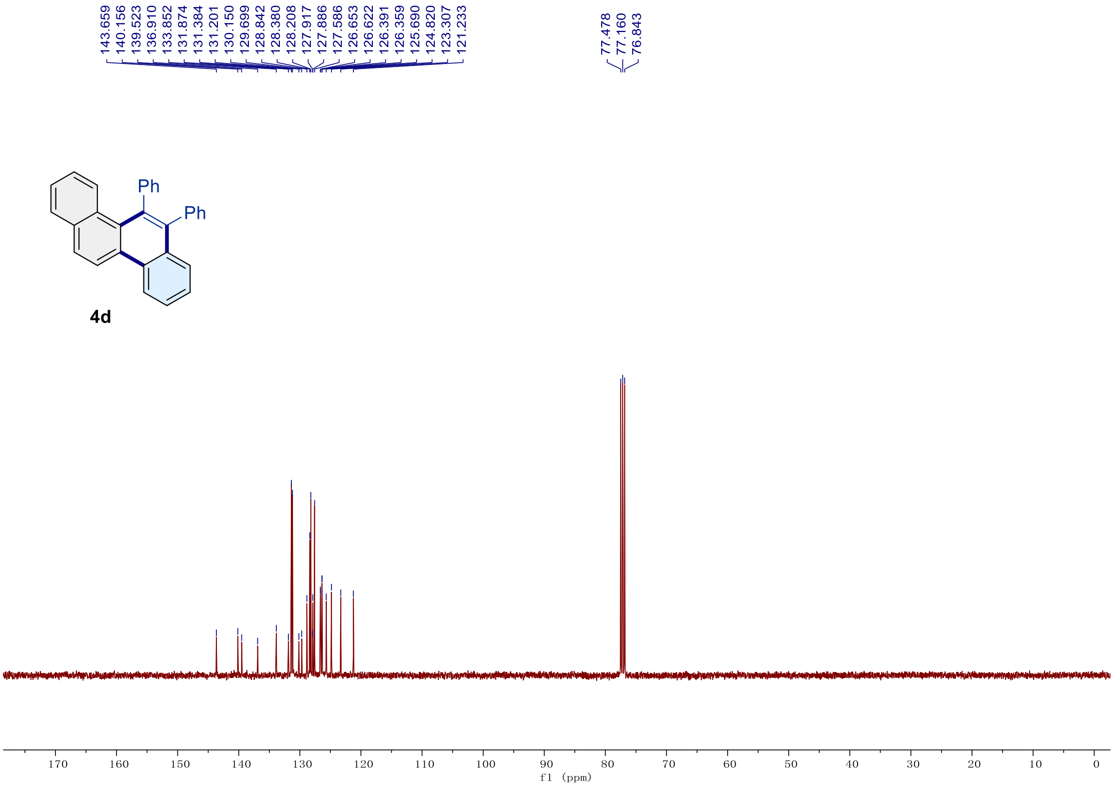
7.077
7.066
7.061
7.034
7.015
6.995
0.000
Ph
Ph
4d
1.00
1.05
1.02
1.01
1.05
2.09
1.08
1.09
3.25
3.22
4.10
1.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.586
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126.622
126.391
126.359
125.690
124.820
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121.233
77.478
77.160
76.843
Ph
Ph
4d
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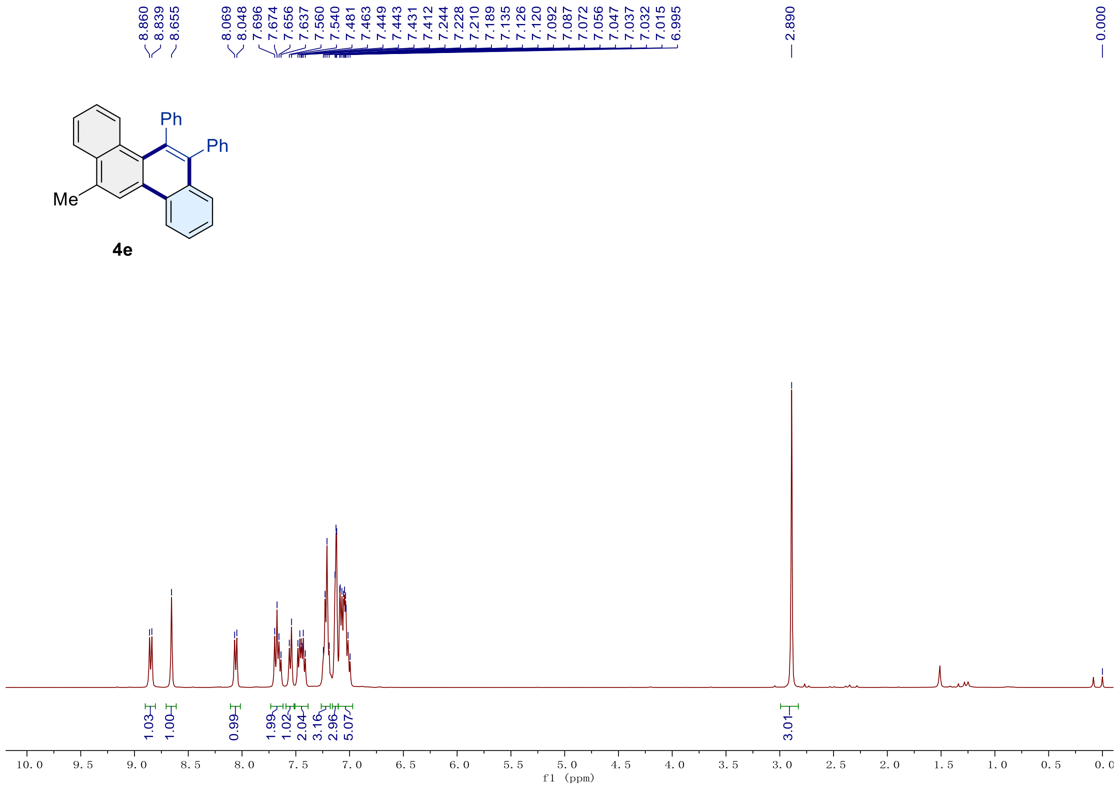
f1 (ppm)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7.431
7.412
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7.210
7.189
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7.126
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2.890
0.000
Ph
Ph
Me
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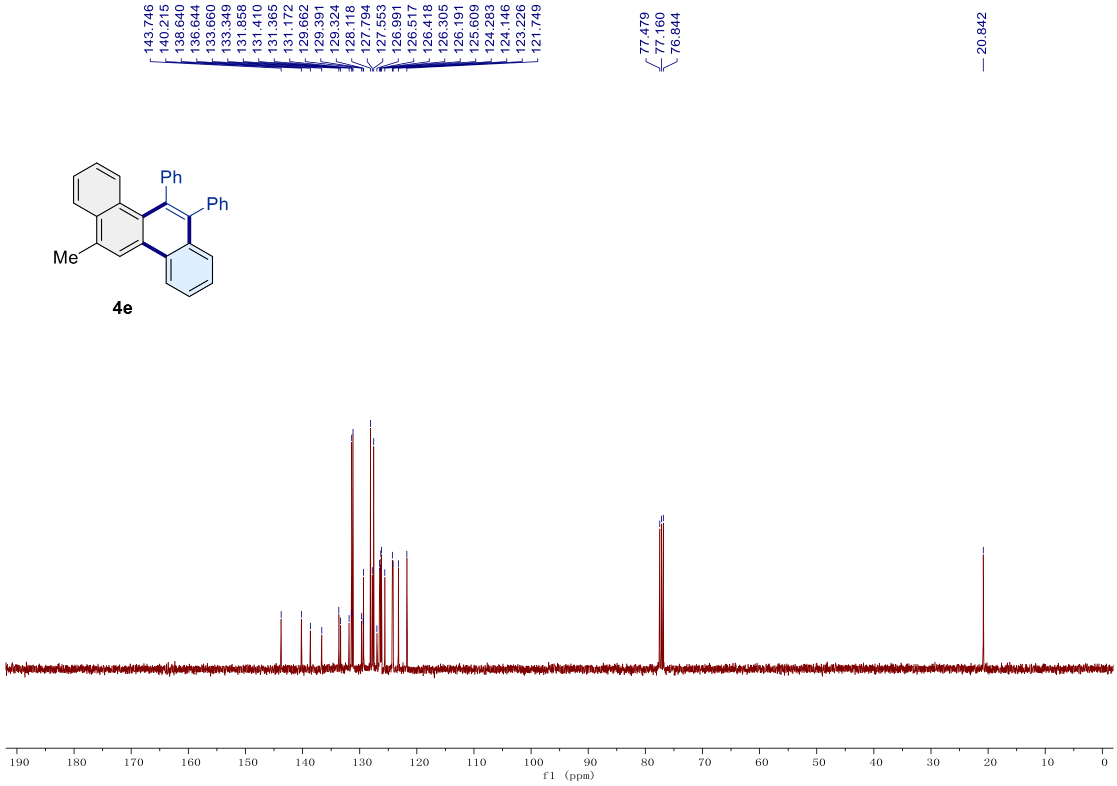
1.00
0.99
1.99
1.02
2.04
3.16
2.96
5.07
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

4e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127.553
126.991
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126.418
126.305
126.191
125.609
124.283
124.146
123.226
121.749
77.479
77.160
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20.842
Ph
Ph
Me
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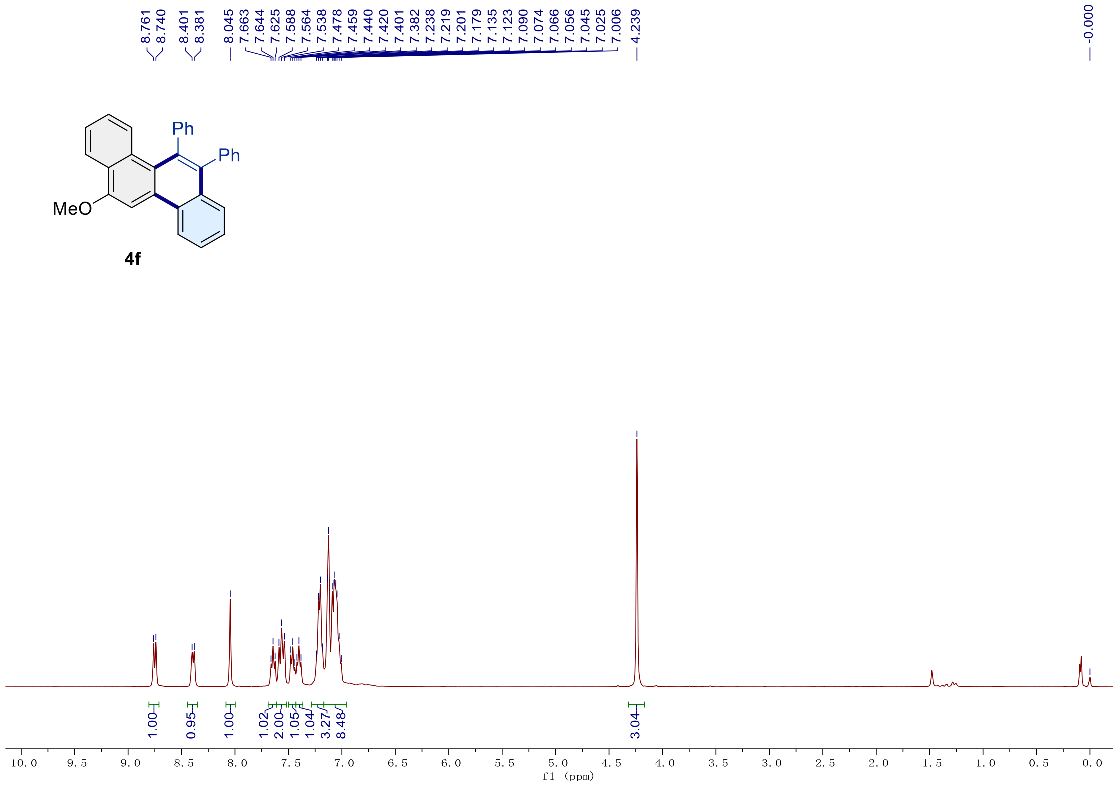
f1 (ppm)

4e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4f
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6.5
6.0
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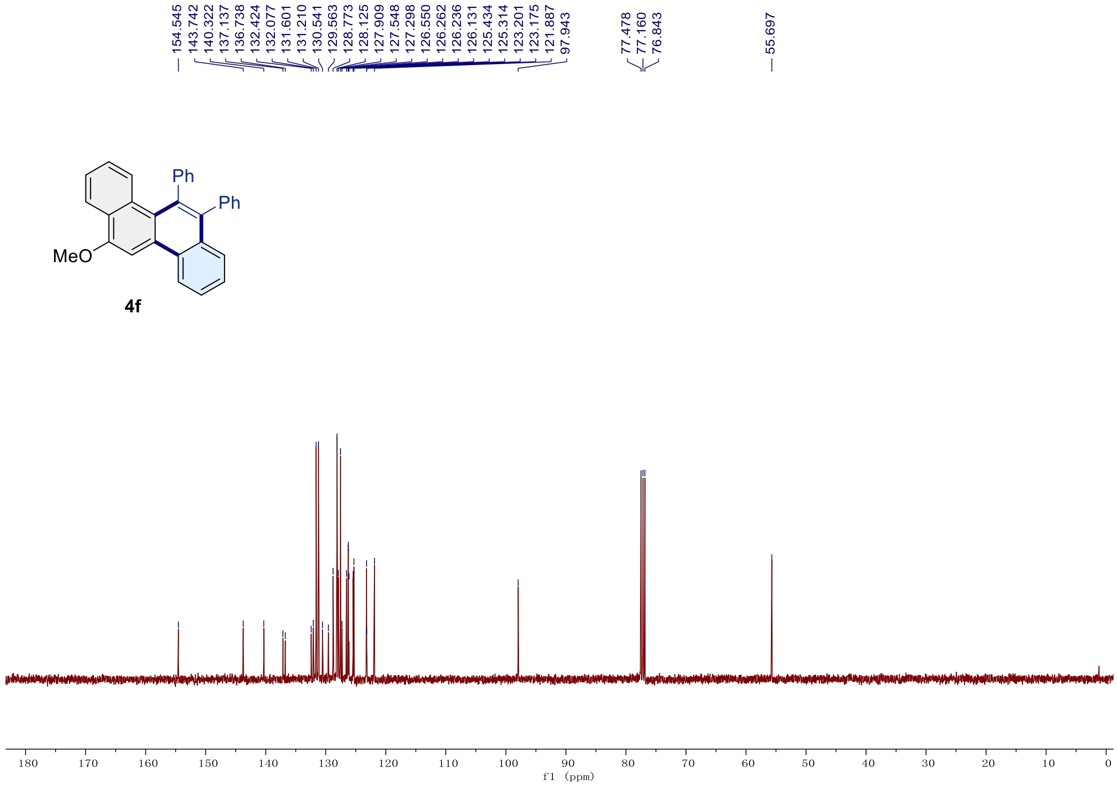
0.0
f1 (ppm)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127.909
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126.236
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76.843
55.697
Ph
Ph
MeO
4f
180
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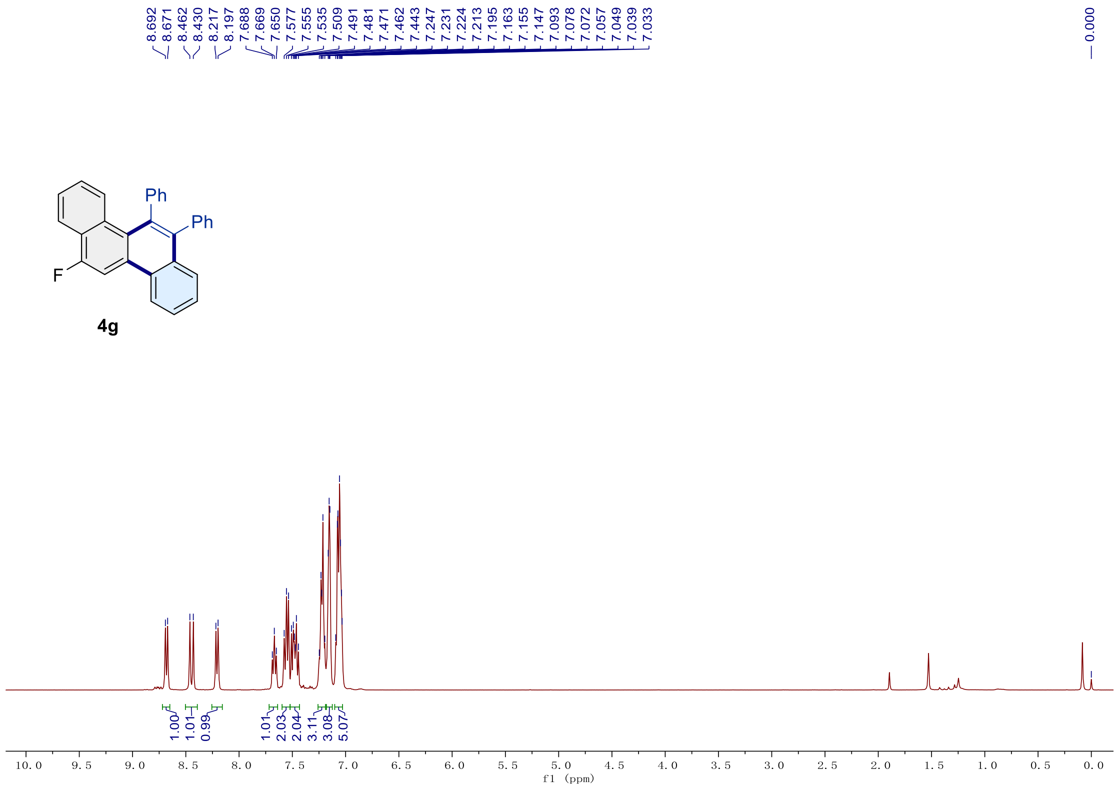
f1 (ppm)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Ph
F
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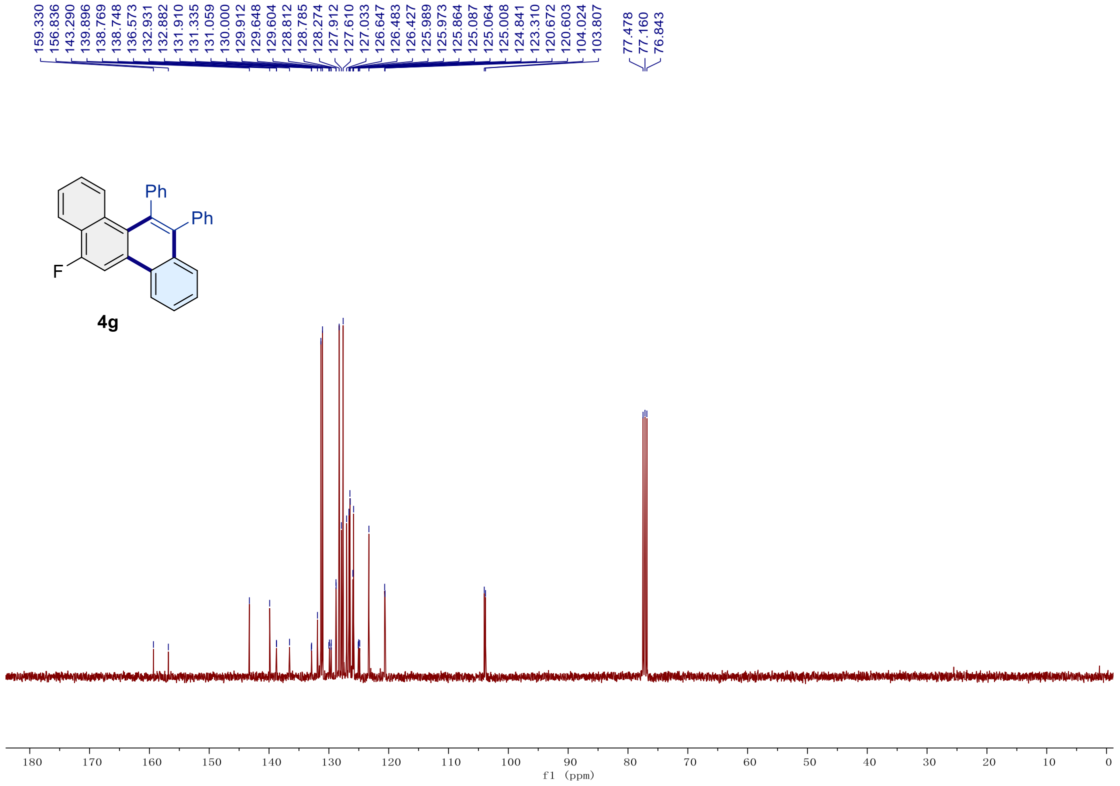
1.01
0.99
1.01
2.03
2.04
3.11
3.08
5.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

4g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104.024
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Ph
Ph
F
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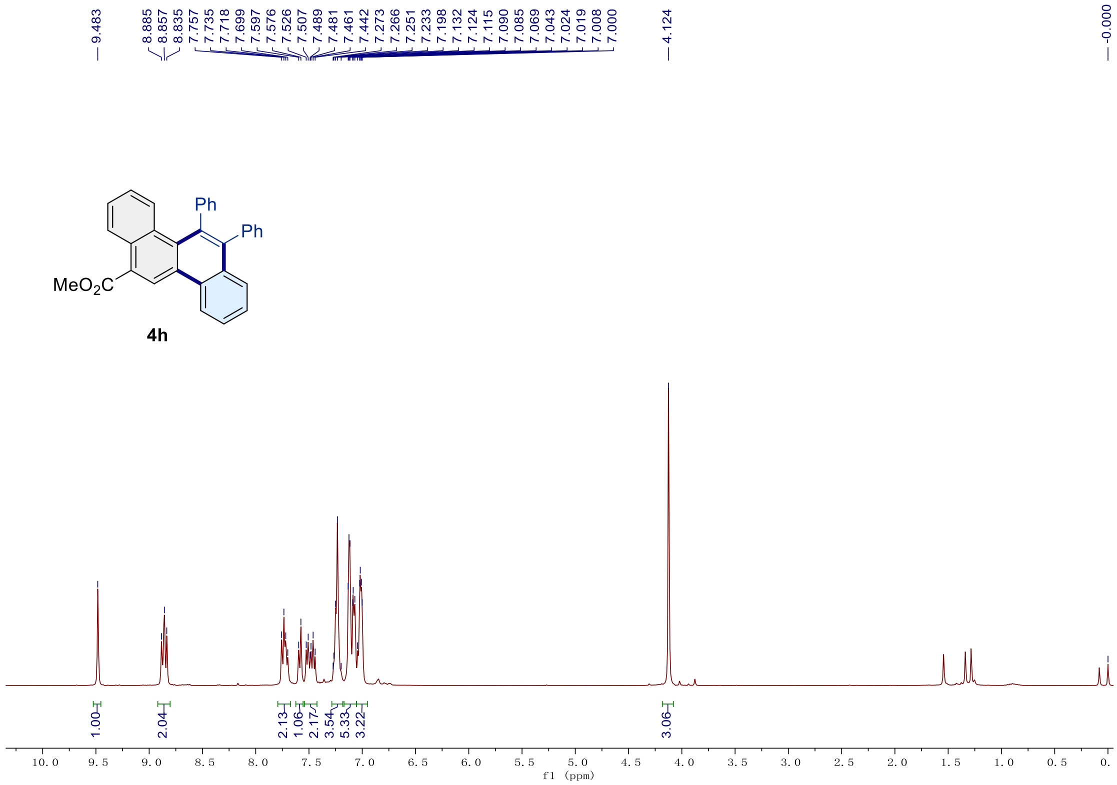
f1 (ppm)

4g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4h
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1.06
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5.33
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3.06
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9.0
8.5
8.0
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6.0
5.5
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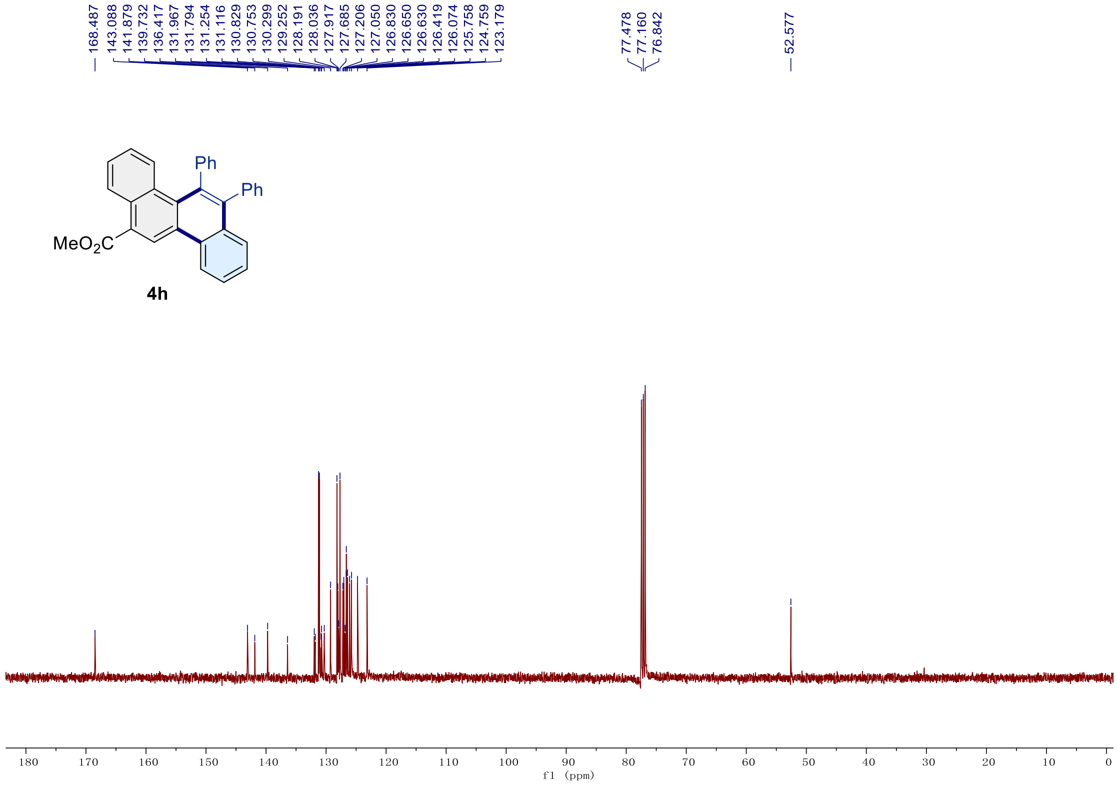
0.5
0.
f1 (ppm)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Ph
Ph
MeO2C
4h
180
170
160
150
140
130
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110
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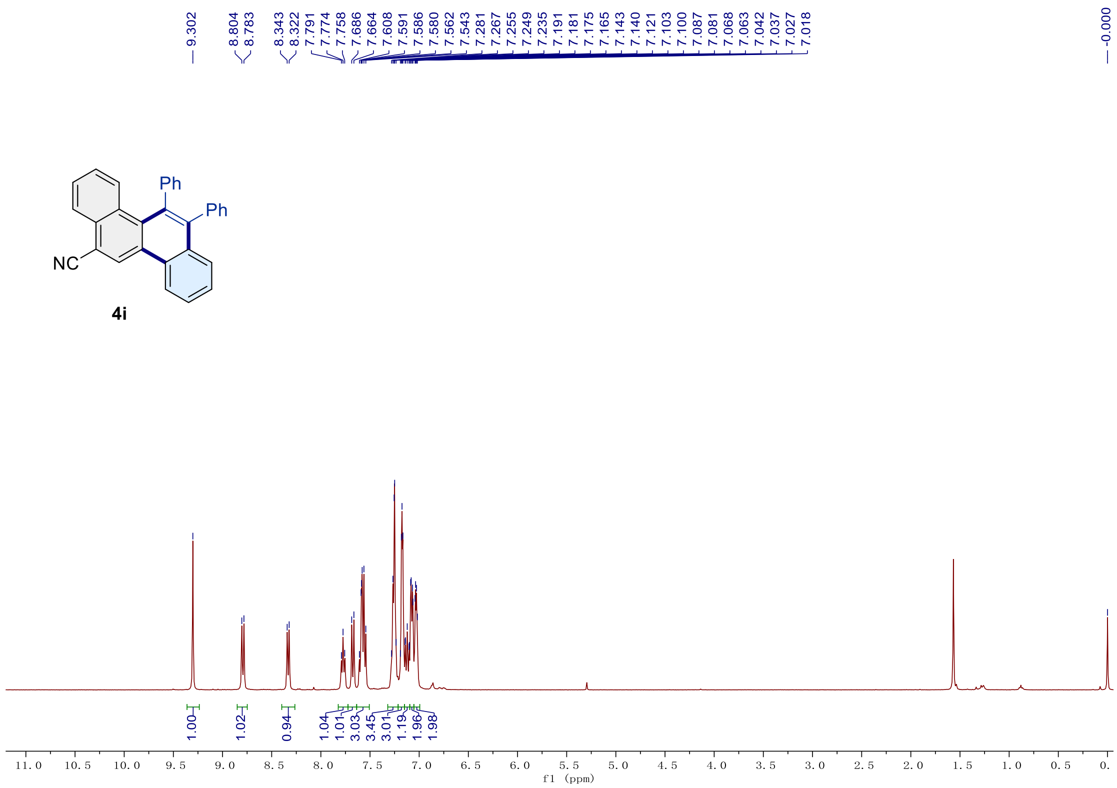
f1 (ppm)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7.580
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7.543
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7.191
7.181
7.175
7.165
7.143
7.140
7.121
7.103
7.100
7.087
7.081
7.068
7.063
7.042
7.037
7.027
7.018
-0.000
Ph
Ph
NC
1.00
1.02
0.94
1.04
1.01
3.03
3.45
3.01
1.19
1.96
1.98
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10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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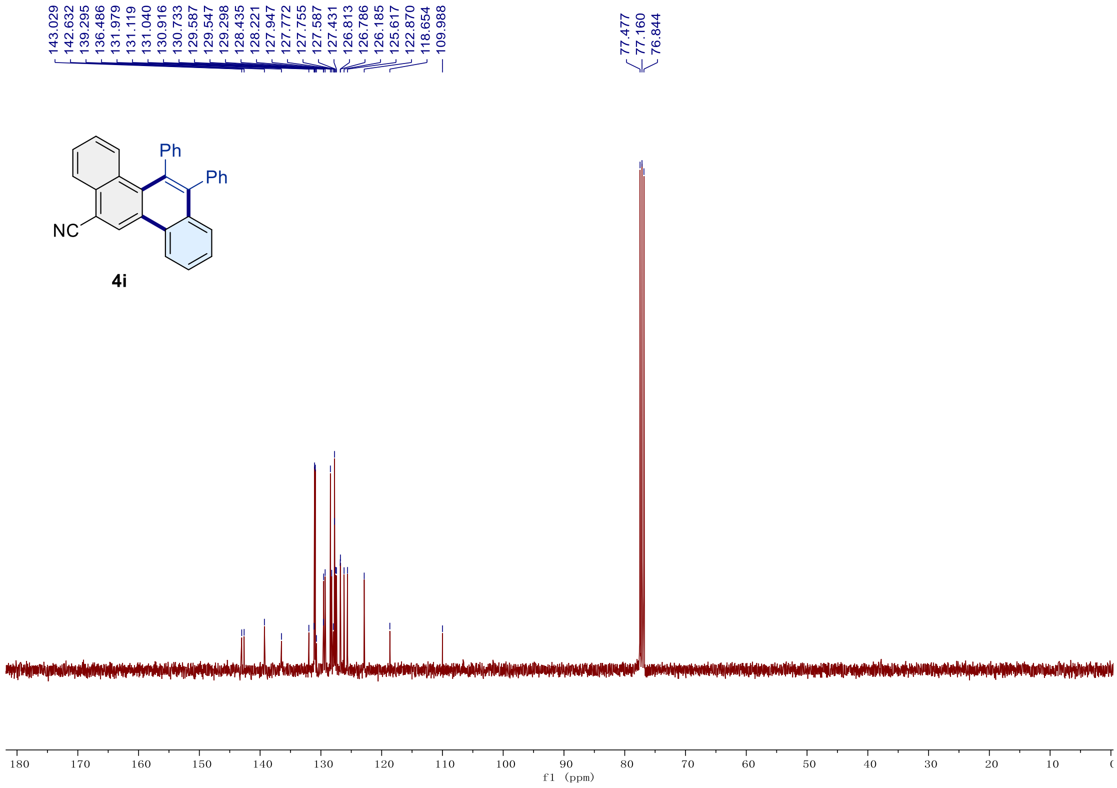
f1 (ppm)

4i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128.221
127.947
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127.587
127.431
126.813
126.786
126.185
125.617
122.870
118.654
109.988
77.477
77.160
76.844
Ph
Ph
NC
180
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80
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40
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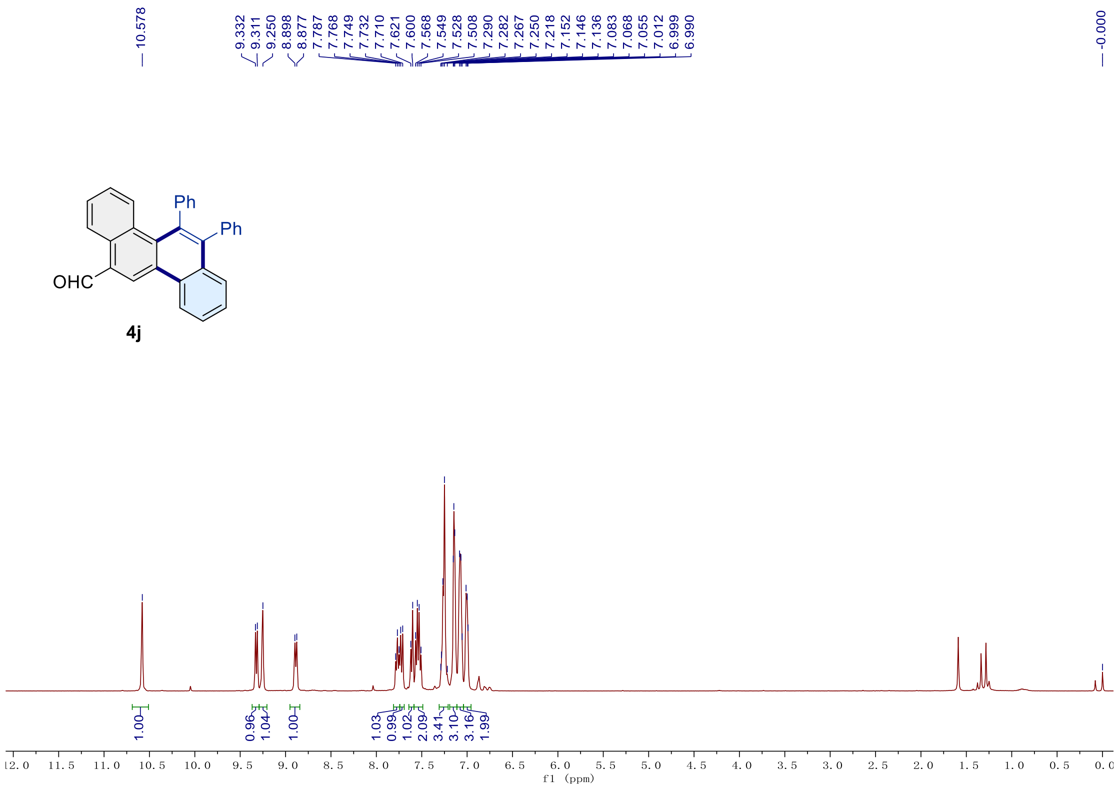
10
f1 (ppm)

4i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7.621
7.600
7.568
7.549
7.528
7.508
7.290
7.282
7.267
7.250
7.218
7.152
7.146
7.136
7.083
7.068
7.055
7.012
6.999
6.990
-0.000
Ph
Ph
OHC
4j
1.00
0.96
1.04
1.00
1.03
0.99
1.02
2.09
3.41
3.10
3.16
1.99
12.0
11.5
11.0
10.5
10.0
9.5
9.0
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6.5
6.0
5.5
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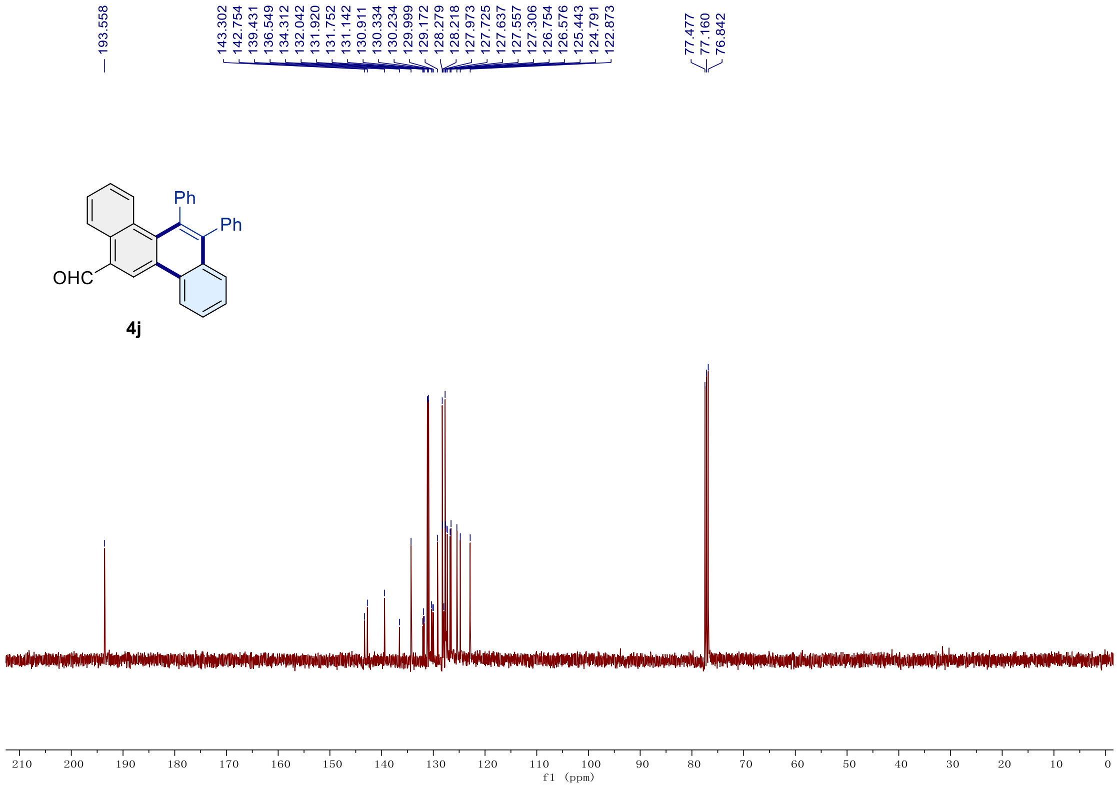
f1 (ppm)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128.279
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127.973
127.725
127.637
127.557
127.306
126.754
126.576
125.443
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122.873
77.477
77.160
76.842
Ph
Ph
OHC
4j
210
200
190
180
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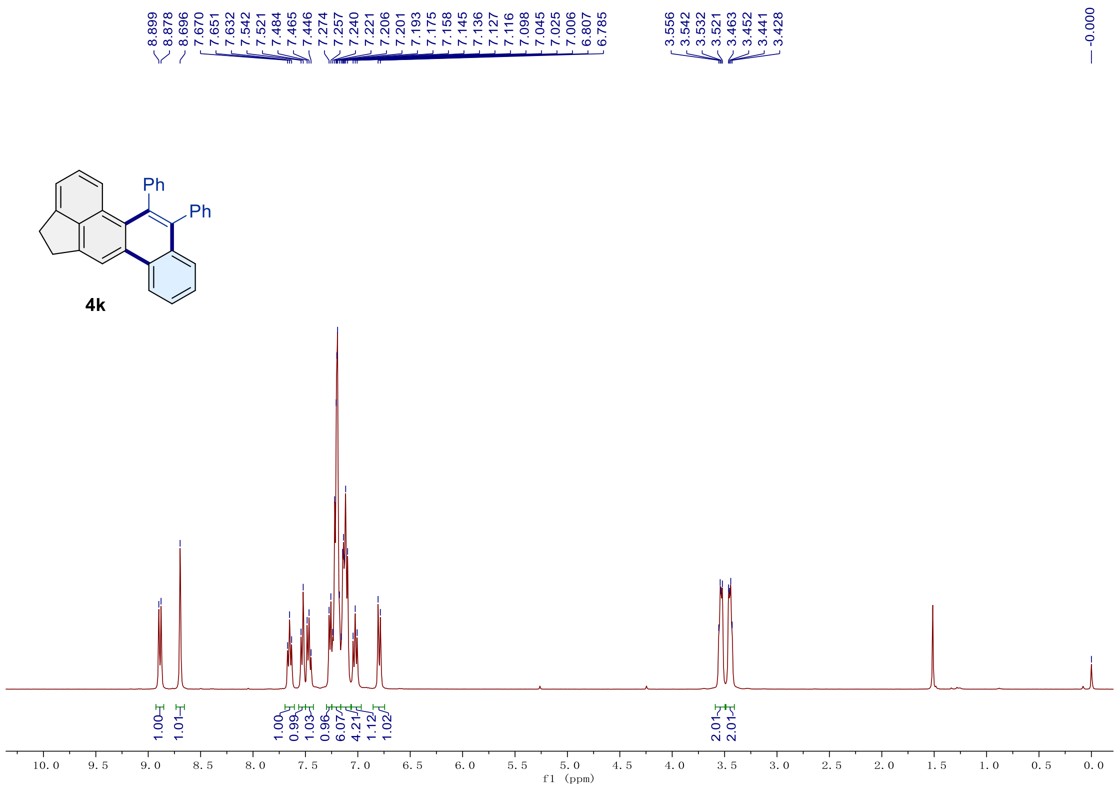
f1 (ppm)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7.257
7.240
7.221
7.206
7.201
7.193
7.175
7.158
7.145
7.136
7.127
7.116
7.098
7.045
7.025
7.006
6.807
6.785
3.556
3.542
3.532
3.521
3.463
3.452
3.441
3.428
-0.000
Ph
Ph
4k
1.00
1.01
1.00
0.99
1.03
0.96
6.07
4.21
1.12
1.02
2.01
2.01
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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2.5
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1.0
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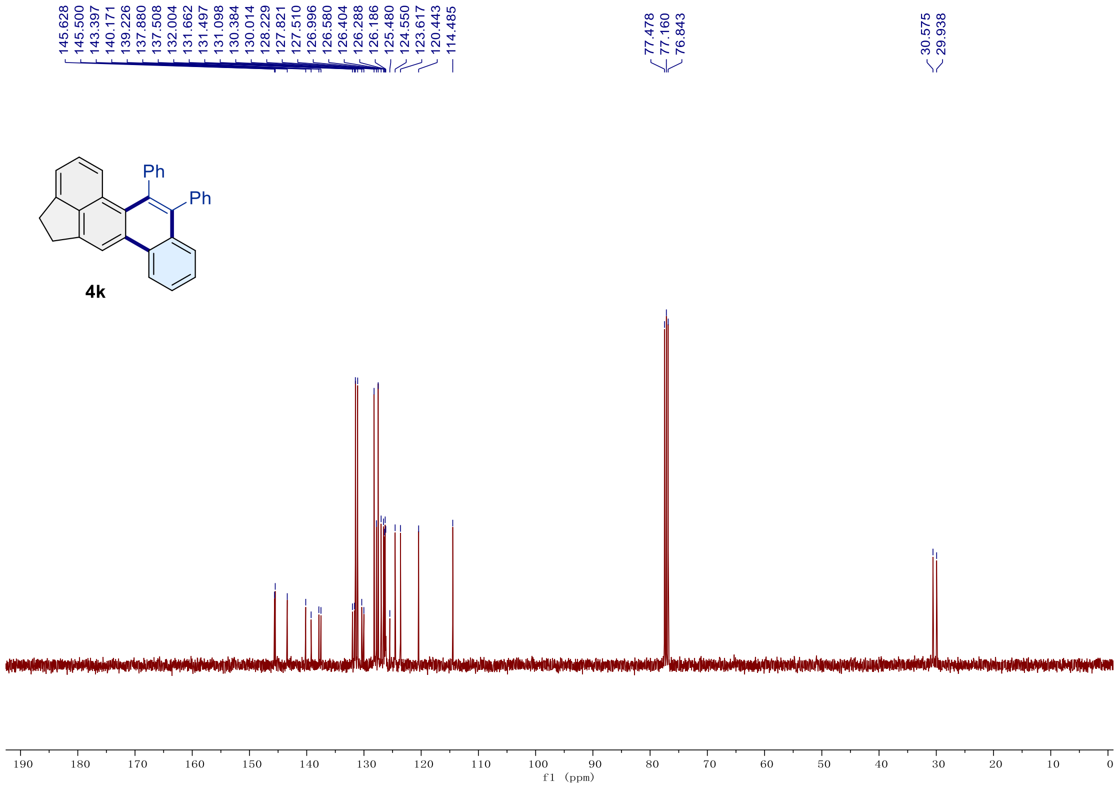
f1 (ppm)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137.508
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131.497
131.098
130.384
130.014
128.229
127.821
127.510
126.996
126.580
126.404
126.288
126.186
125.480
124.550
123.617
120.443
114.485
77.478
77.160
76.843
30.575
29.938
Ph
Ph
4k
190
180
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120
110
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90
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10
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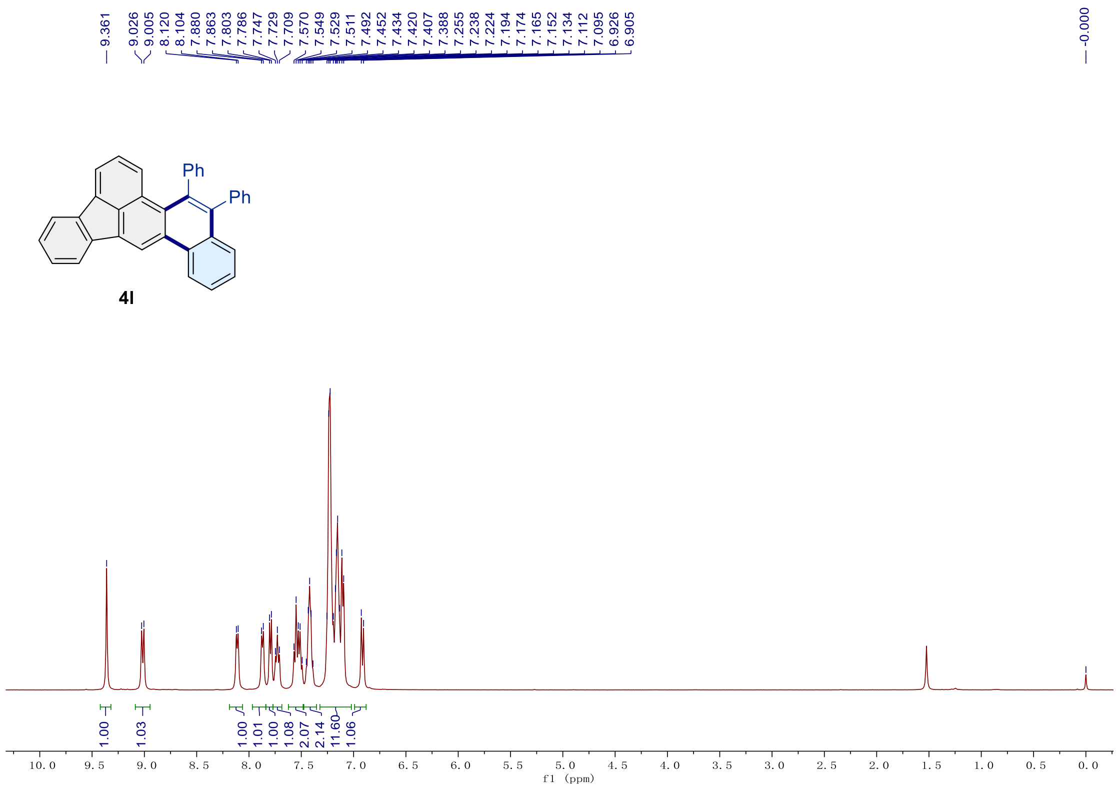
f1 (ppm)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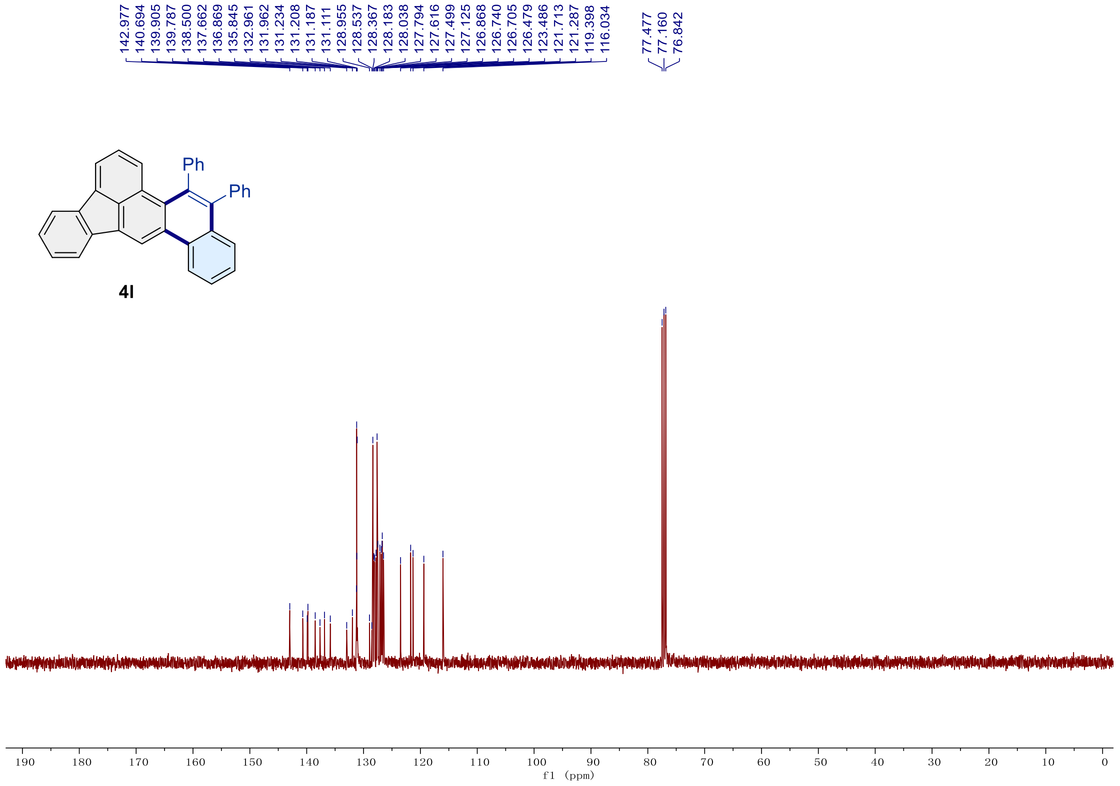
7.709
7.570
7.549
7.529
7.511
7.492
7.452
7.434
7.420
7.407
7.388
7.255
7.238
7.224
7.194
7.174
7.165
7.152
7.134
7.112
7.095
6.926
6.905
-0.000
Ph
Ph
4l
1.00
1.03
1.00
1.01
1.00
1.08
2.07
2.14
11.60
1.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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135.845
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131.962
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131.187
131.111
128.955
128.537
128.367
128.183
128.038
127.794
127.616
127.499
127.125
126.868
126.740
126.705
126.479
123.486
121.713
121.287
119.398
116.034
77.477
77.160
76.842
Ph
Ph
4l
190
180
170
160
150
140
130
120
110
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90
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20
10
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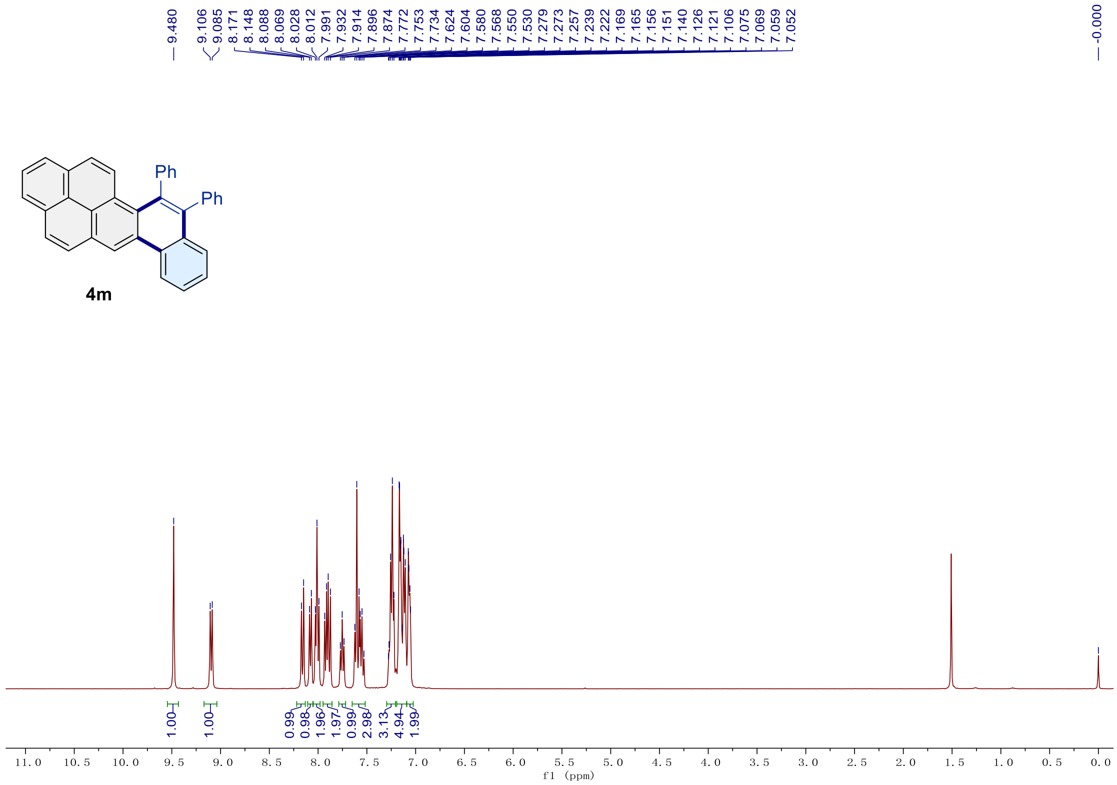
f1 (ppm)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8.028
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7.896
7.874
7.772
7.753
7.734
7.624
7.604
7.580
7.568
7.550
7.530
7.279
7.273
7.257
7.239
7.222
7.169
7.165
7.156
7.151
7.140
7.126
7.121
7.106
7.075
7.069
7.059
7.052
-0.000
Ph
Ph
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1.00
0.99
0.98
1.96
1.97
0.99
2.98
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4.94
1.99
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10.5
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9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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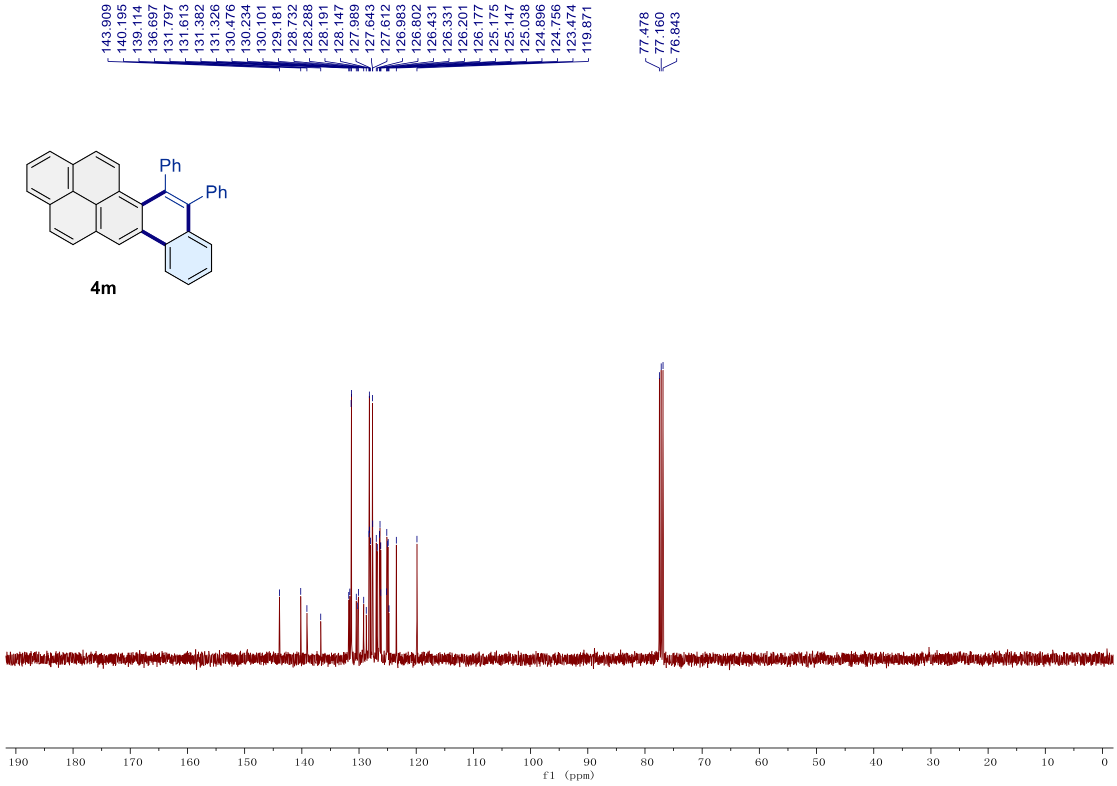
1.0
0.5
0.0
f1 (ppm)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130.234
130.101
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128.288
128.191
128.147
127.989
127.643
127.612
126.983
126.802
126.431
126.331
126.201
126.177
125.175
125.147
125.038
124.896
124.756
123.474
119.871
77.478
77.160
76.843
Ph
Ph
4m
190
180
170
160
150
140
130
120
110
100
90
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70
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10
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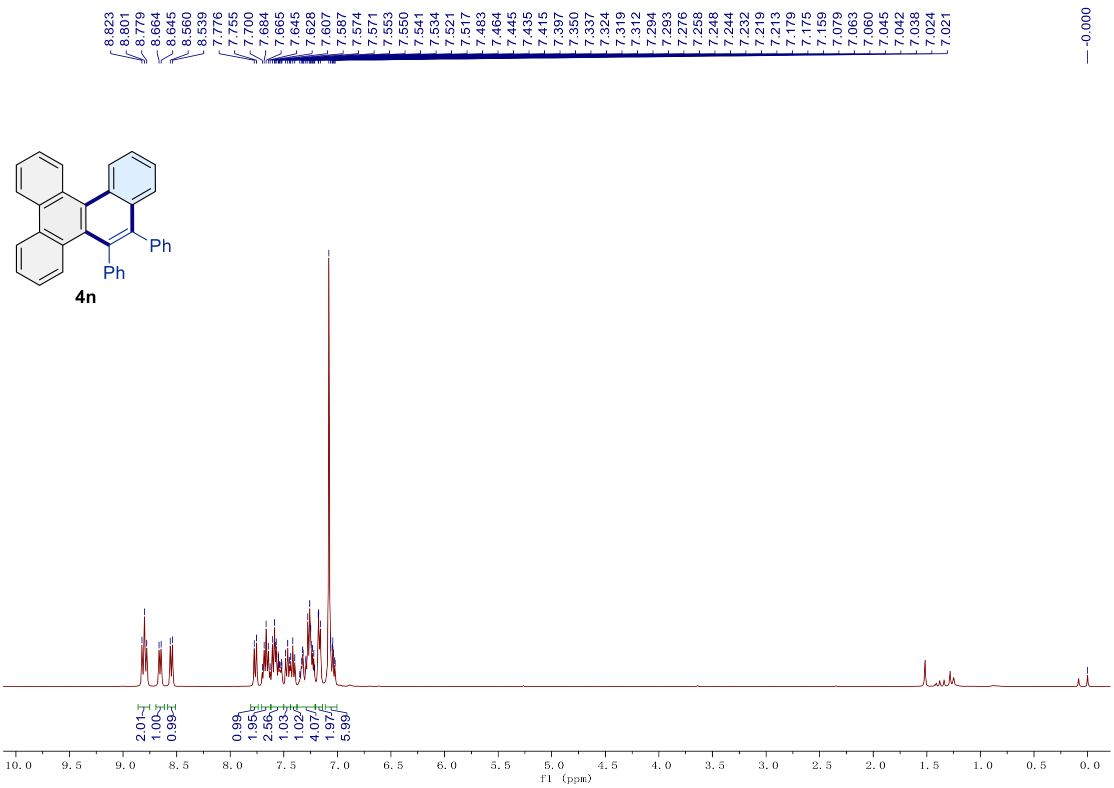
f1 (ppm)



4n

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7.665
7.645
7.628
7.607
7.587
7.574
7.571
7.553
7.550
7.541
7.534
7.521
7.517
7.483
7.464
7.445
7.435
7.415
7.397
7.350
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7.324
7.319
7.312
7.294
7.293
7.276
7.258
7.248
7.244
7.232
7.219
7.213
7.179
7.175
7.159
7.079
7.063
7.060
7.045
7.042
7.038
7.024
7.021
-0.000
Ph
Ph
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1.00
0.99
0.99
1.95
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1.02
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9.0
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6.0
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1.0
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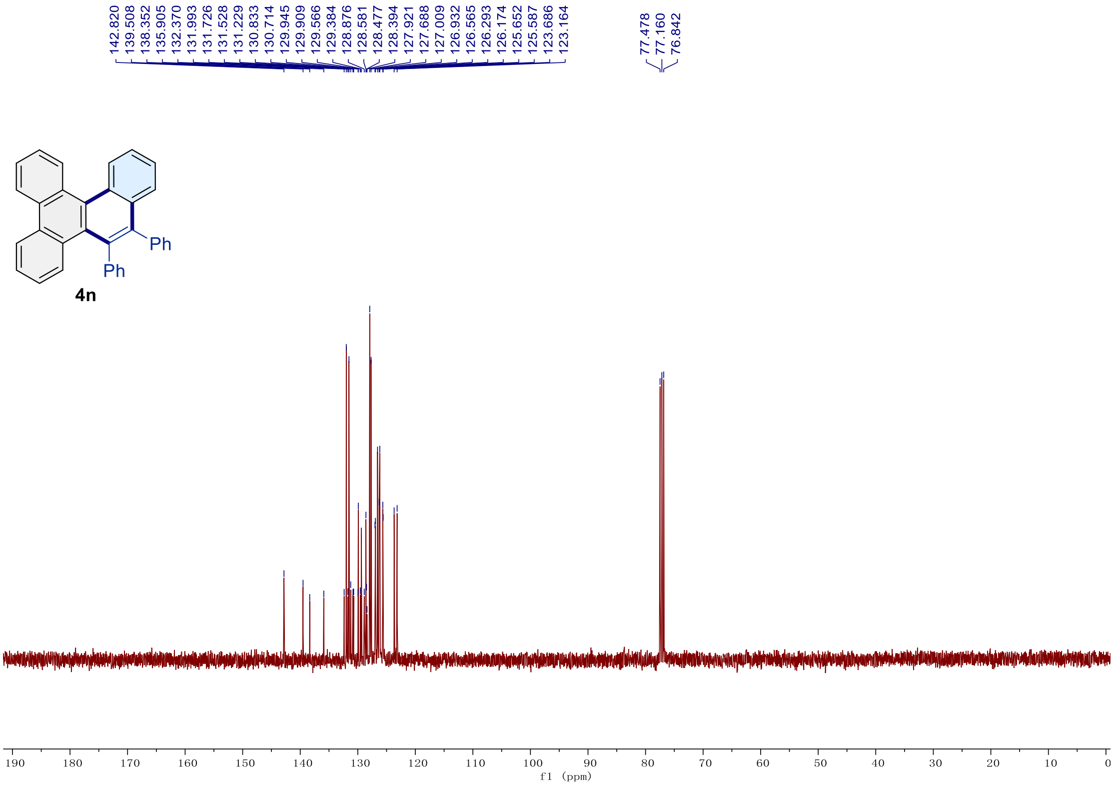
f1 (ppm)



4n

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128.581
128.477
128.394
127.921
127.688
127.009
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126.565
126.293
126.174
125.652
125.587
123.686
123.164
77.478
77.160
76.842
Ph
Ph
190
180
170
160
150
140
130
120
110
100
90
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70
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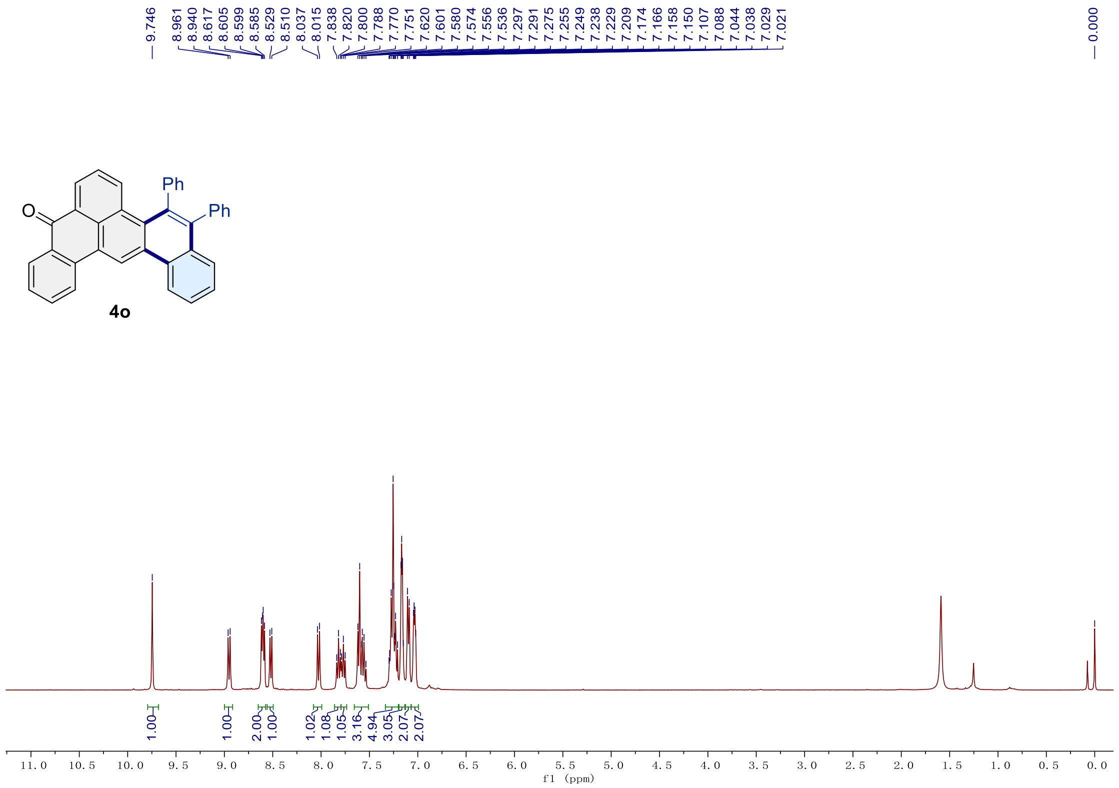
50
40
30
20
10
0
f1 (ppm)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7.770
7.751
7.620
7.601
7.580
7.574
7.556
7.536
7.297
7.291
7.275
7.255
7.249
7.238
7.229
7.209
7.174
7.166
7.158
7.150
7.107
7.088
7.044
7.038
7.029
7.021
0.000
O
Ph
Ph
4o
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1.00
2.00
1.00
1.02
1.08
1.05
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3.05
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2.07
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10.0
9.5
9.0
8.5
8.0
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7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
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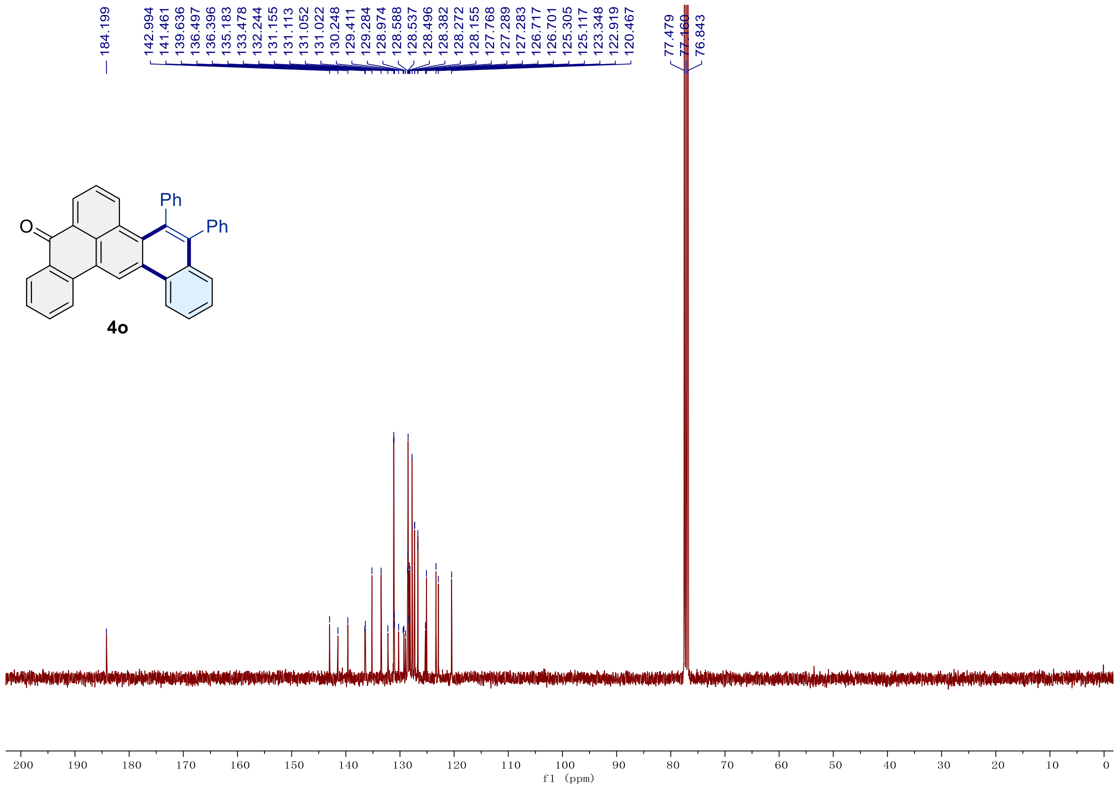
1.0
0.5
0.0
f1 (ppm)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131.113
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130.248
129.411
129.284
128.974
128.588
128.537
128.496
128.382
128.272
128.155
127.768
127.289
127.283
126.717
126.701
125.305
125.117
123.348
122.919
120.467
77.479
77.160
76.843
O
Ph
Ph
4o
200
190
180
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110
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90
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20
10
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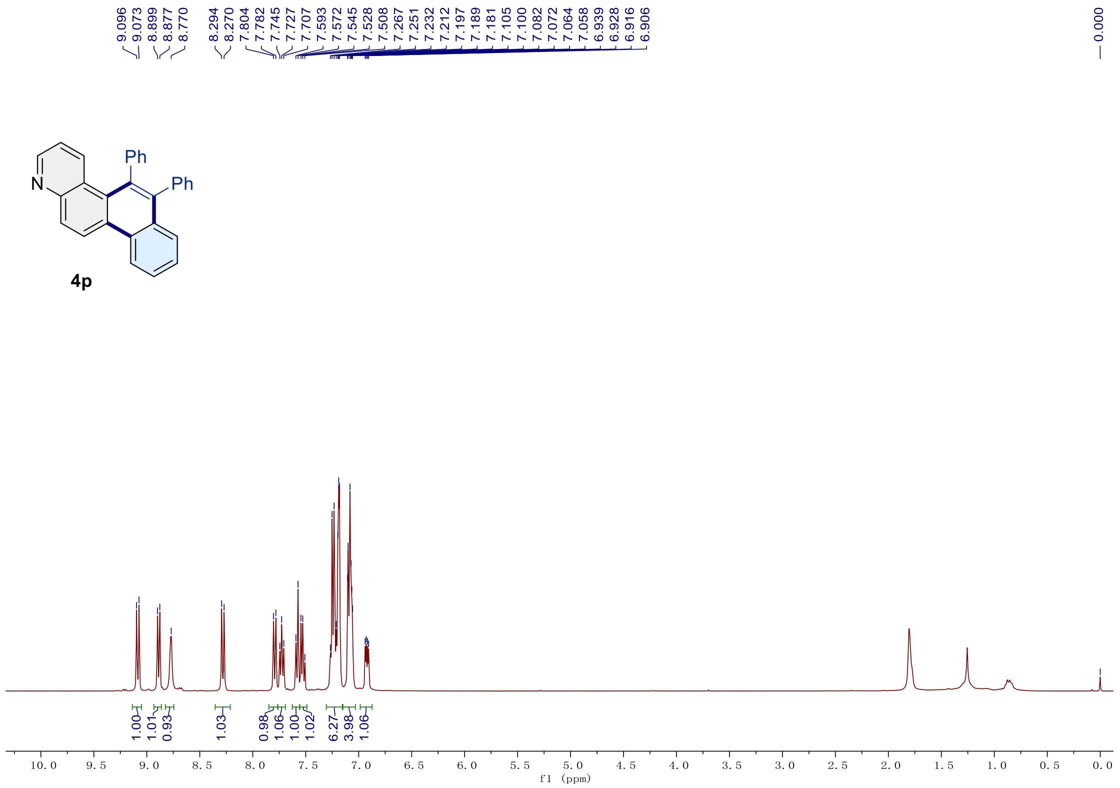
f1 (ppm)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7.707
7.593
7.572
7.545
7.528
7.508
7.267
7.251
7.232
7.212
7.197
7.189
7.181
7.105
7.100
7.082
7.072
7.064
7.058
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6.928
6.916
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N
Ph
Ph
4p
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1.03
0.98
1.06
1.00
1.02
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1.06
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8.0
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6.0
5.5
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3.0
2.5
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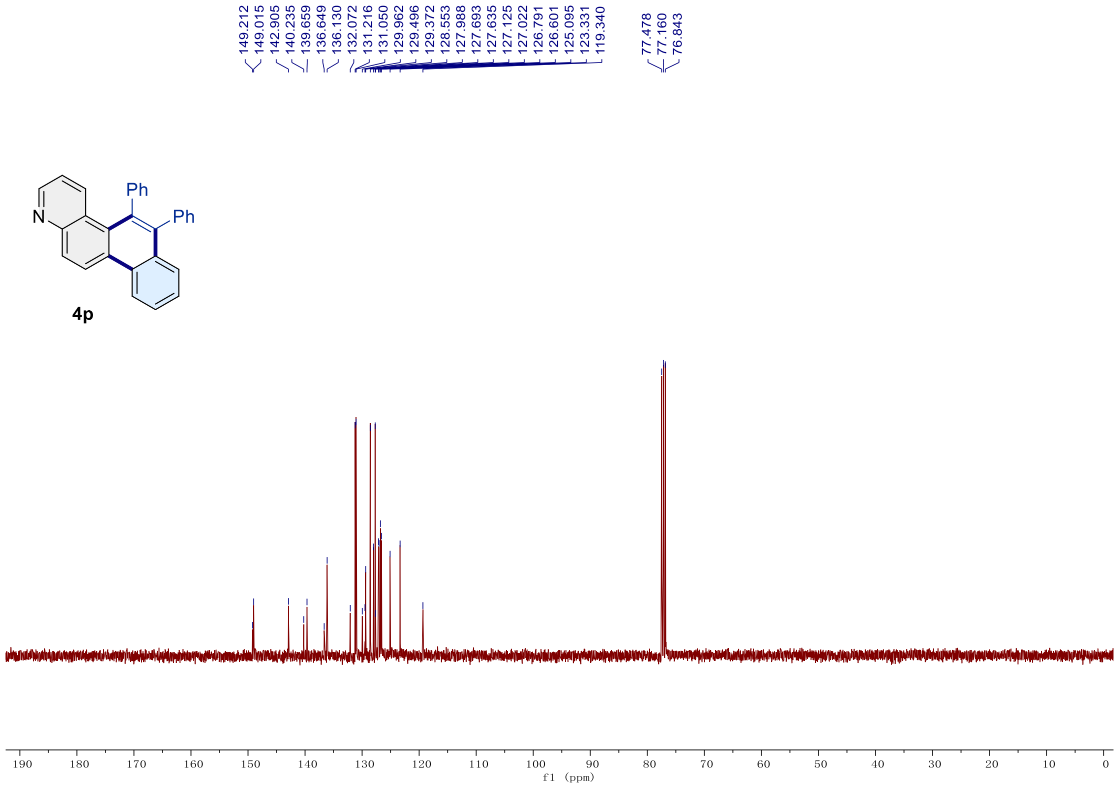
f1 (ppm)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131.050
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129.372
128.553
127.988
127.693
127.635
127.125
127.022
126.791
126.601
125.095
123.331
119.340
77.478
77.160
76.843
N
Ph
Ph
4p
190
180
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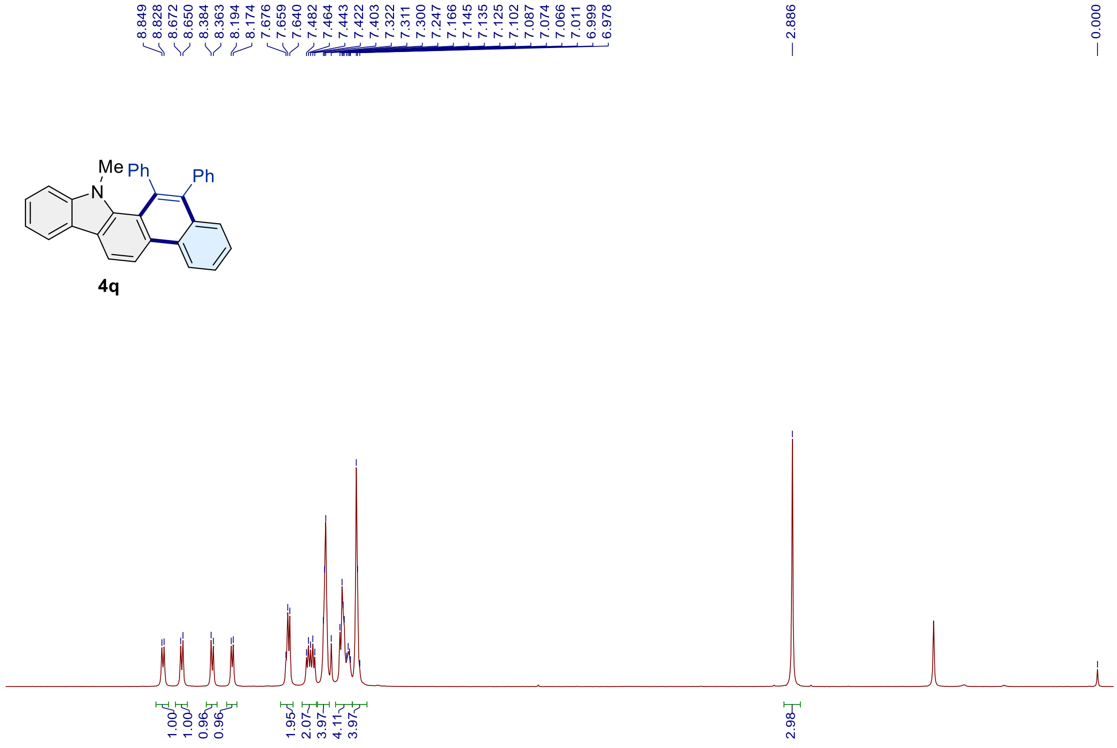
f1 (ppm)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7.422
7.403
7.322
7.311
7.300
7.247
7.166
7.145
7.135
7.125
7.102
7.087
7.074
7.066
7.011
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Me
N
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Ph
4q
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1.00
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1.95
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3.97
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1.0
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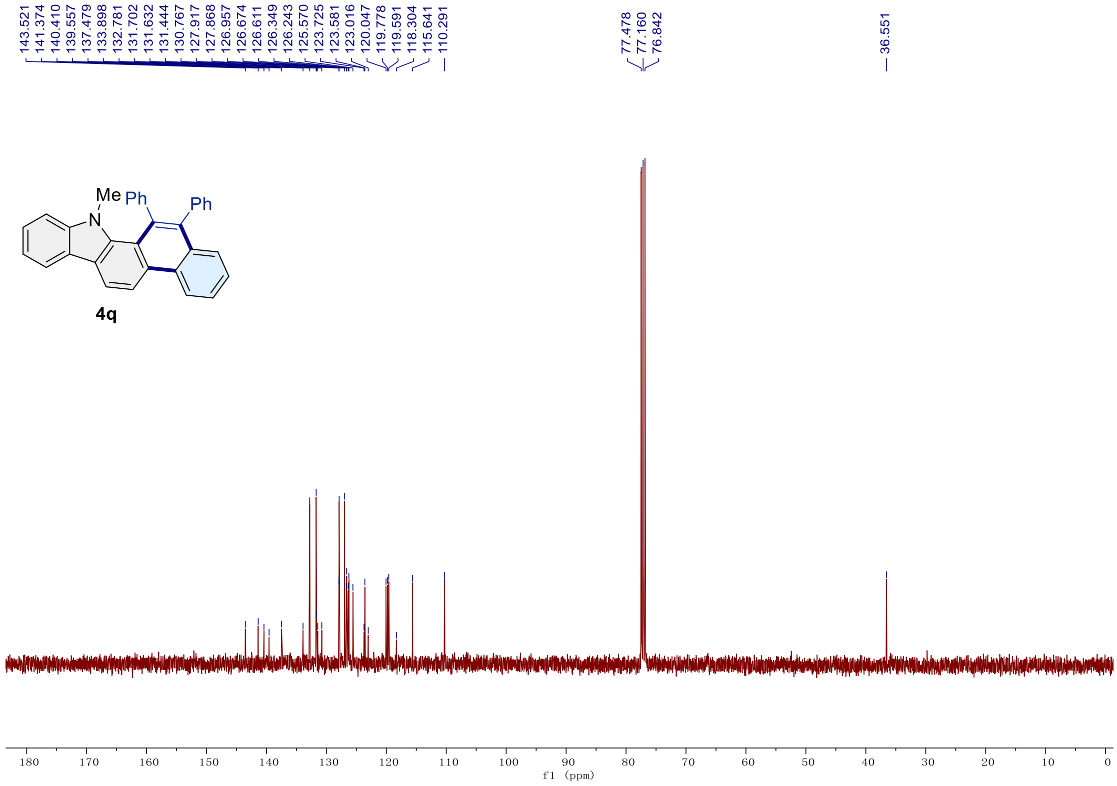
f1 (ppm)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125.570
123.725
123.581
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119.778
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118.304
115.641
110.291
77.478
77.160
76.842
36.551
Me
N
Ph
Ph
4q
180
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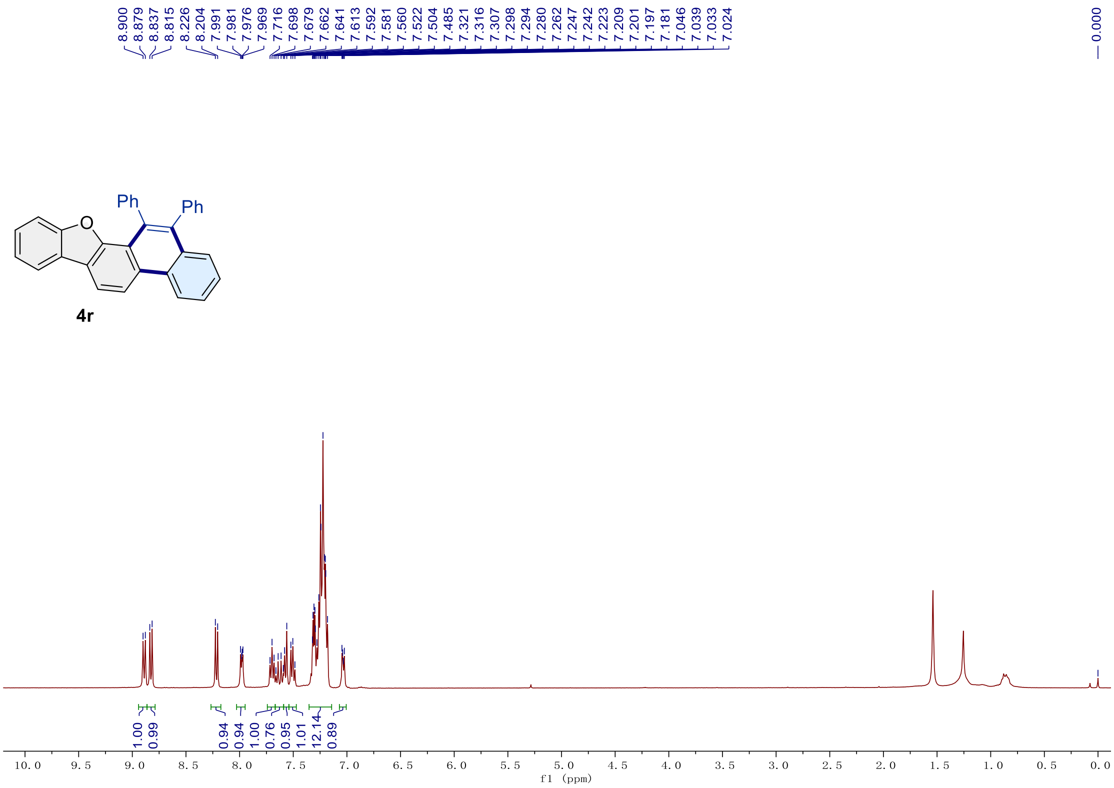
f1 (ppm)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7.662
7.641
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7.592
7.581
7.560
7.522
7.504
7.485
7.321
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7.307
7.298
7.294
7.280
7.262
7.247
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7.223
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7.201
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Ph
O
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1.00
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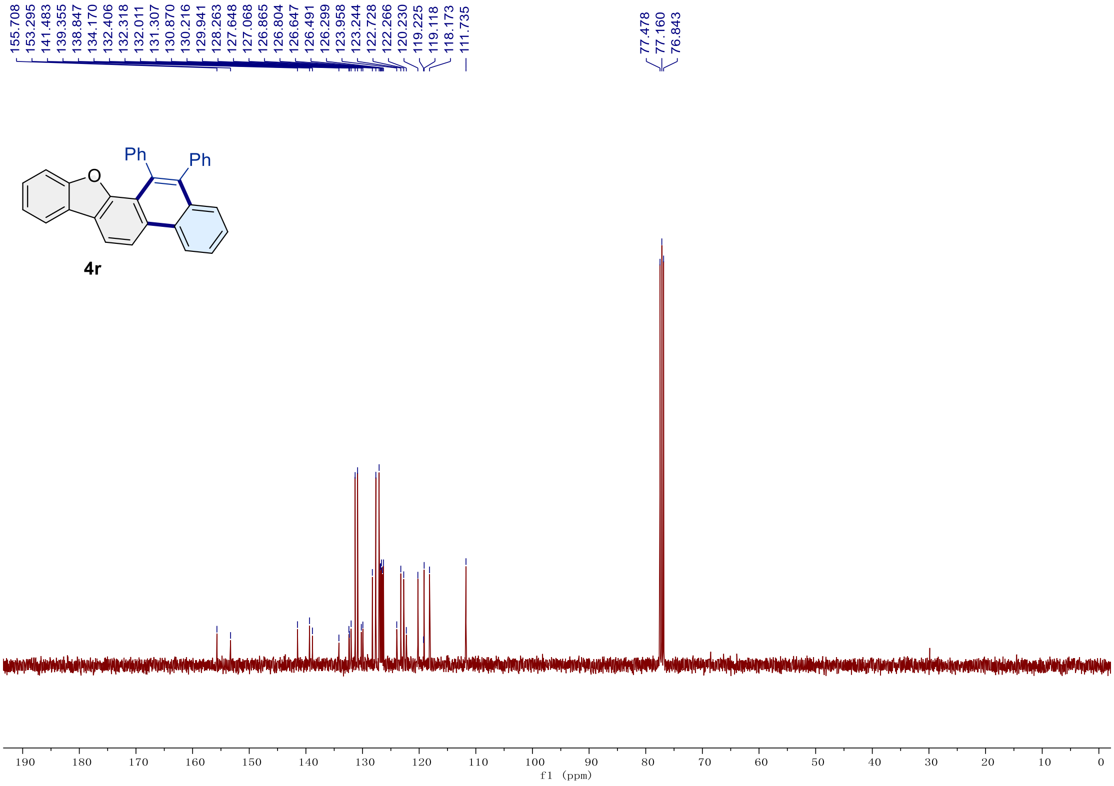
f1 (ppm)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77.160
76.843
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Ph
O
4r
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180
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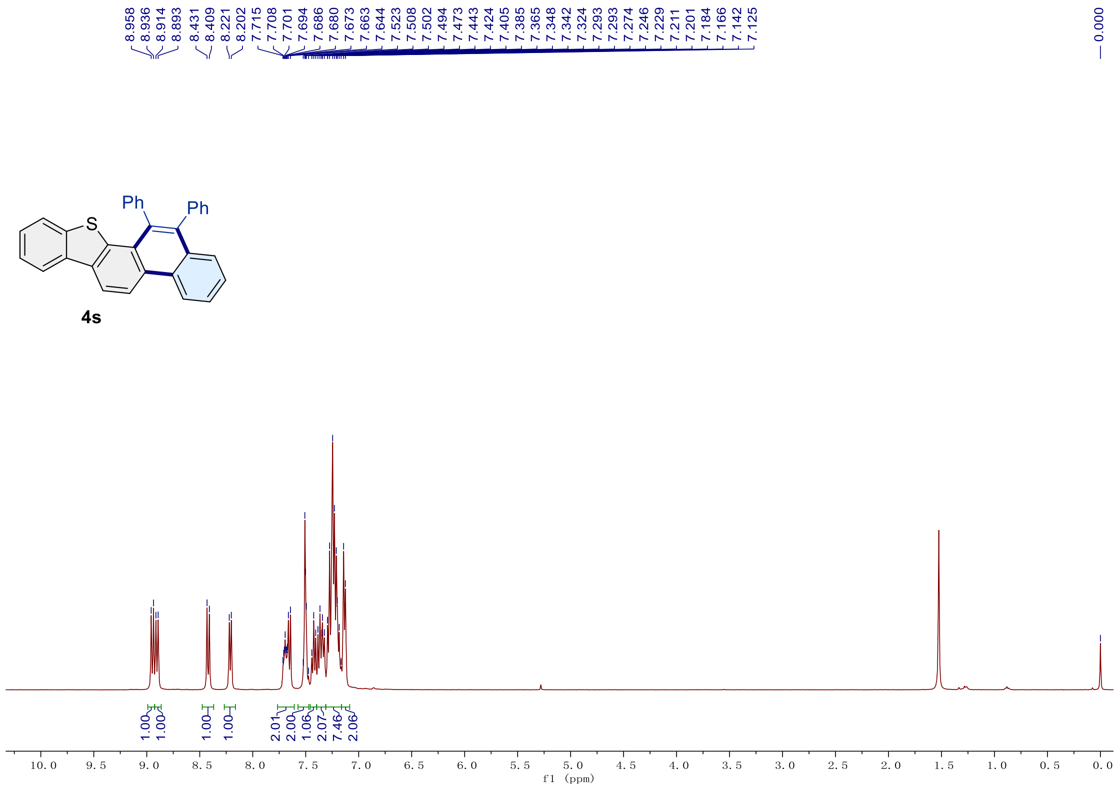
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Ph
Ph
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2.00
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2.07
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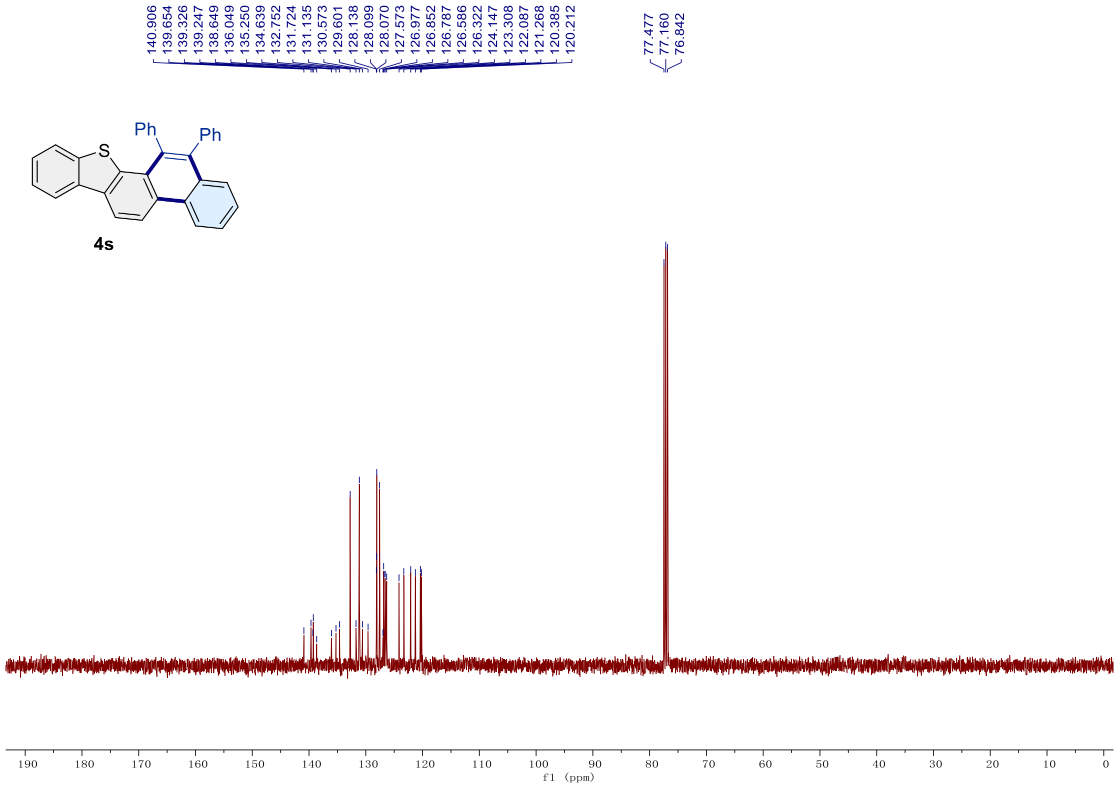
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124.147
123.308
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76.842
S
Ph
Ph
4s
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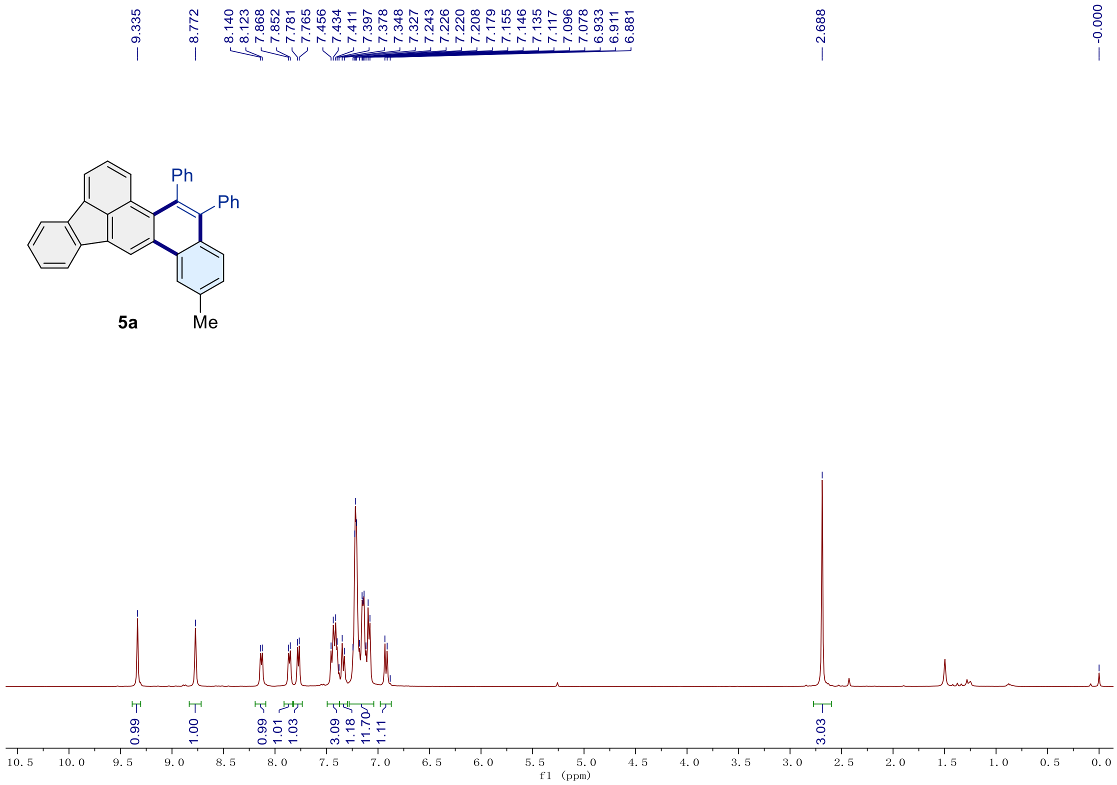
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7.243
7.226
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7.135
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7.078
6.933
6.911
6.881
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Ph
5a
Me
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0.99
1.01
1.03
3.09
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3.03
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8.0
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6.0
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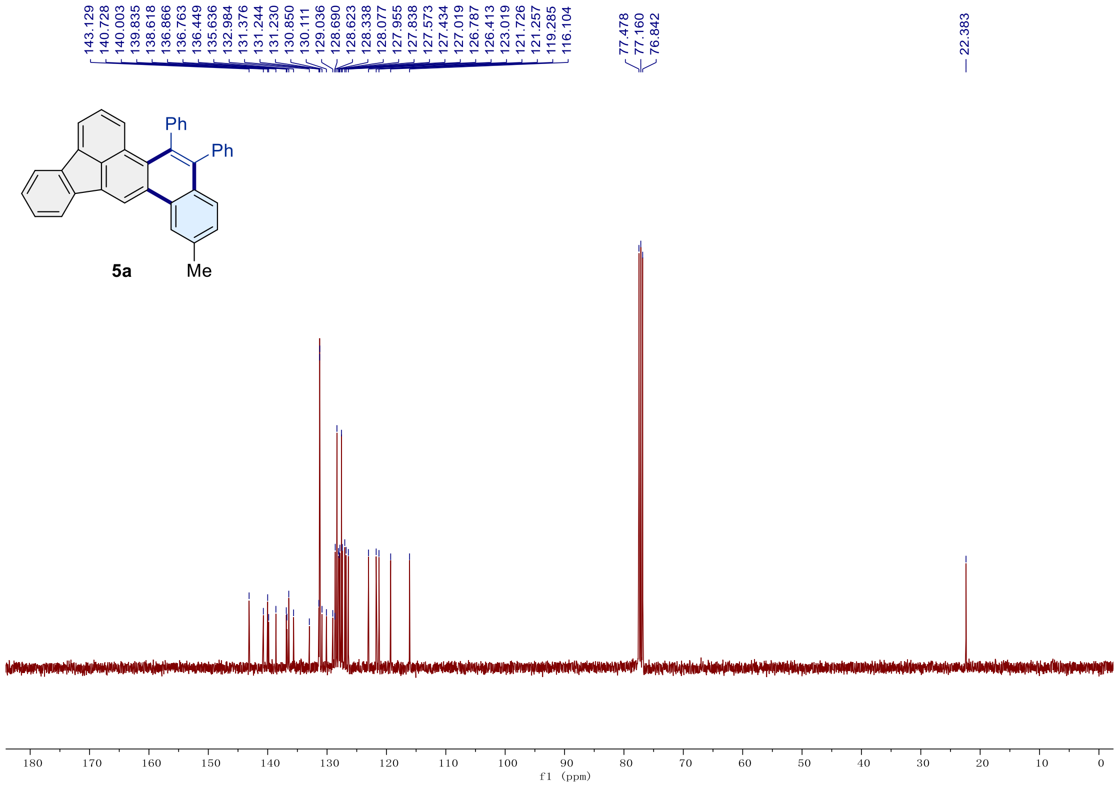
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77.160
76.842
22.383
Ph
Ph
5a
Me
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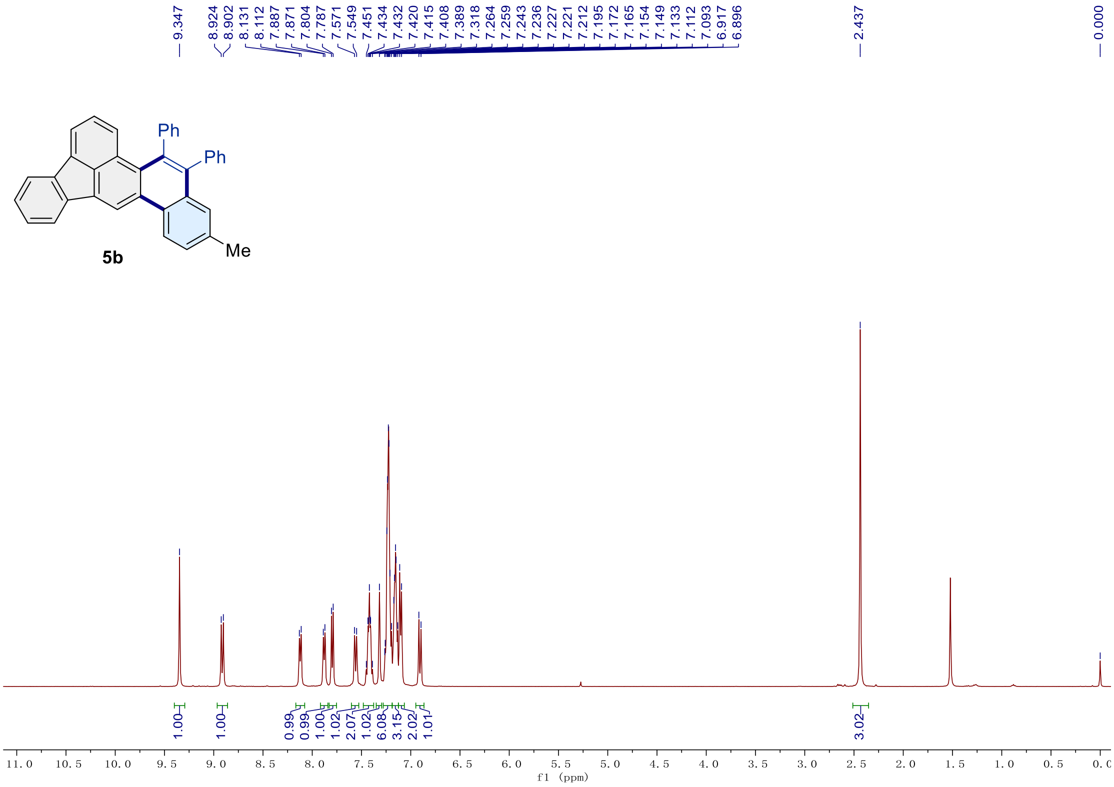
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7.434
7.432
7.420
7.415
7.408
7.389
7.318
7.264
7.259
7.243
7.236
7.227
7.221
7.212
7.195
7.172
7.165
7.154
7.149
7.133
7.112
7.093
6.917
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Ph
Me
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1.00
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1.00
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2.07
1.02
6.08
3.15
2.02
1.01
3.02
11.0
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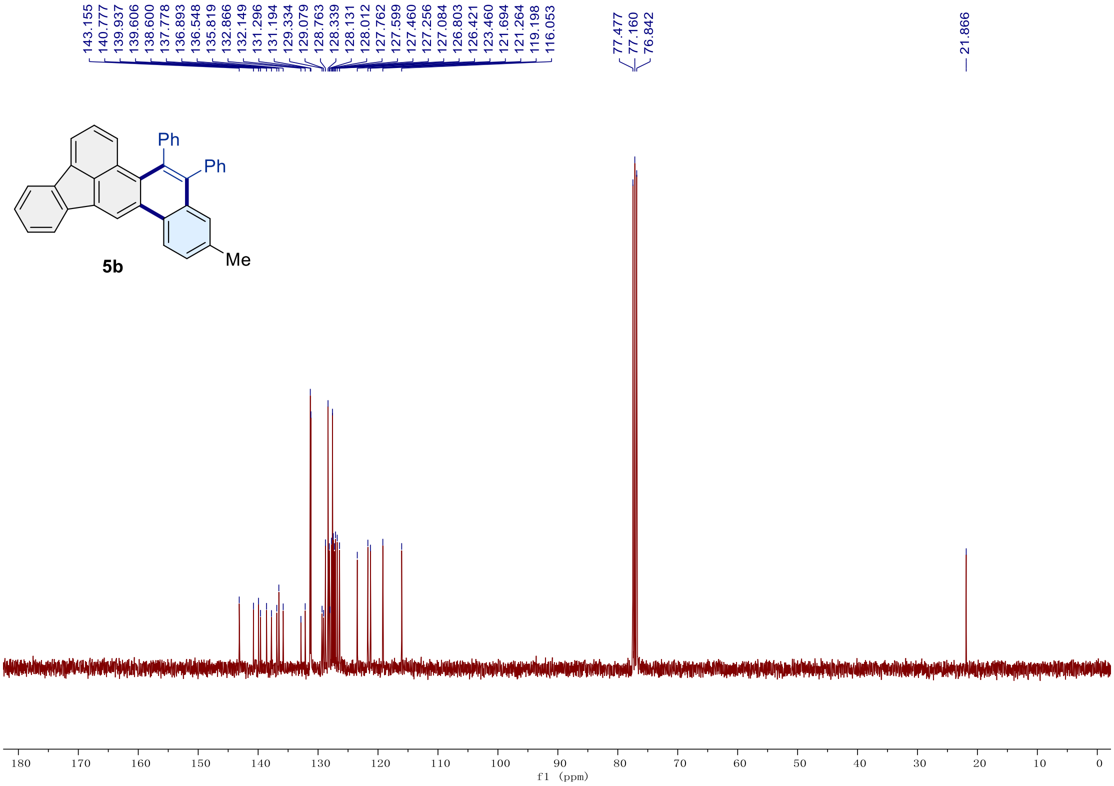
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128.339
128.131
128.012
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126.803
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123.460
121.694
121.264
119.198
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77.477
77.160
76.842
21.866
Ph
Ph
Me
5b
180
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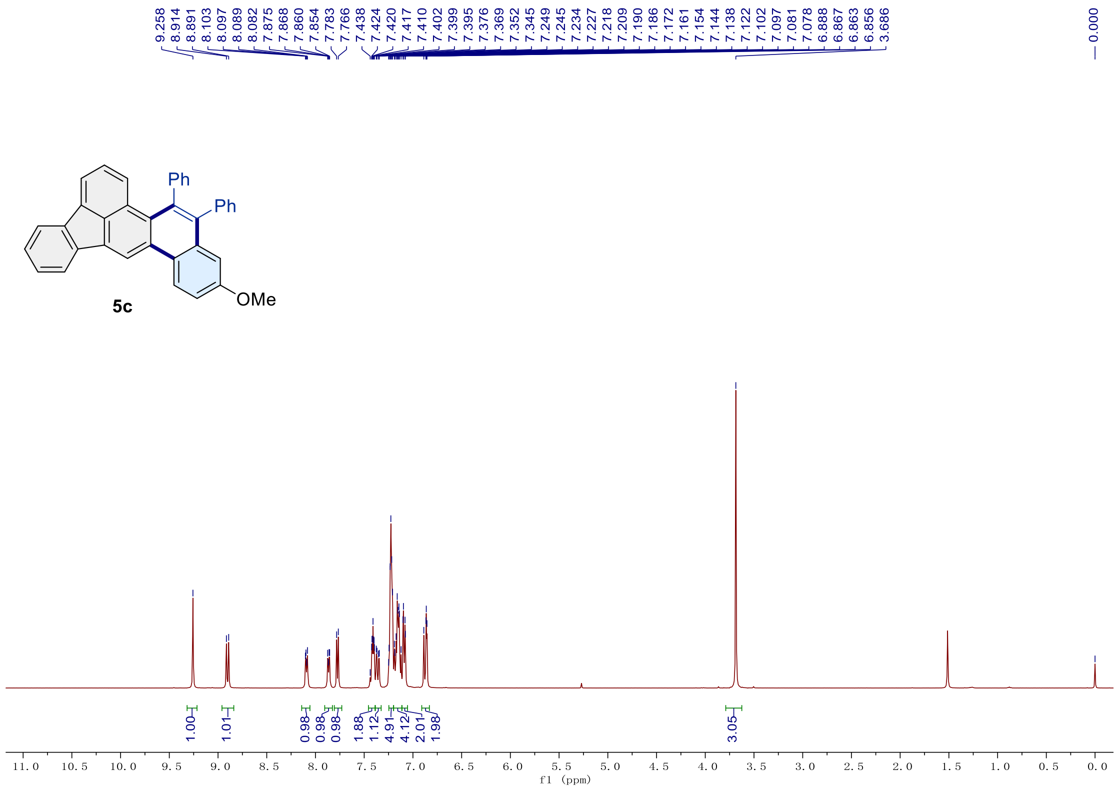
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7.410
7.402
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7.395
7.376
7.369
7.352
7.345
7.249
7.245
7.234
7.227
7.218
7.209
7.190
7.186
7.172
7.161
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7.144
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Ph
OMe
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0.98
0.98
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4.12
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6.0
5.5
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3.0
2.5
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1.0
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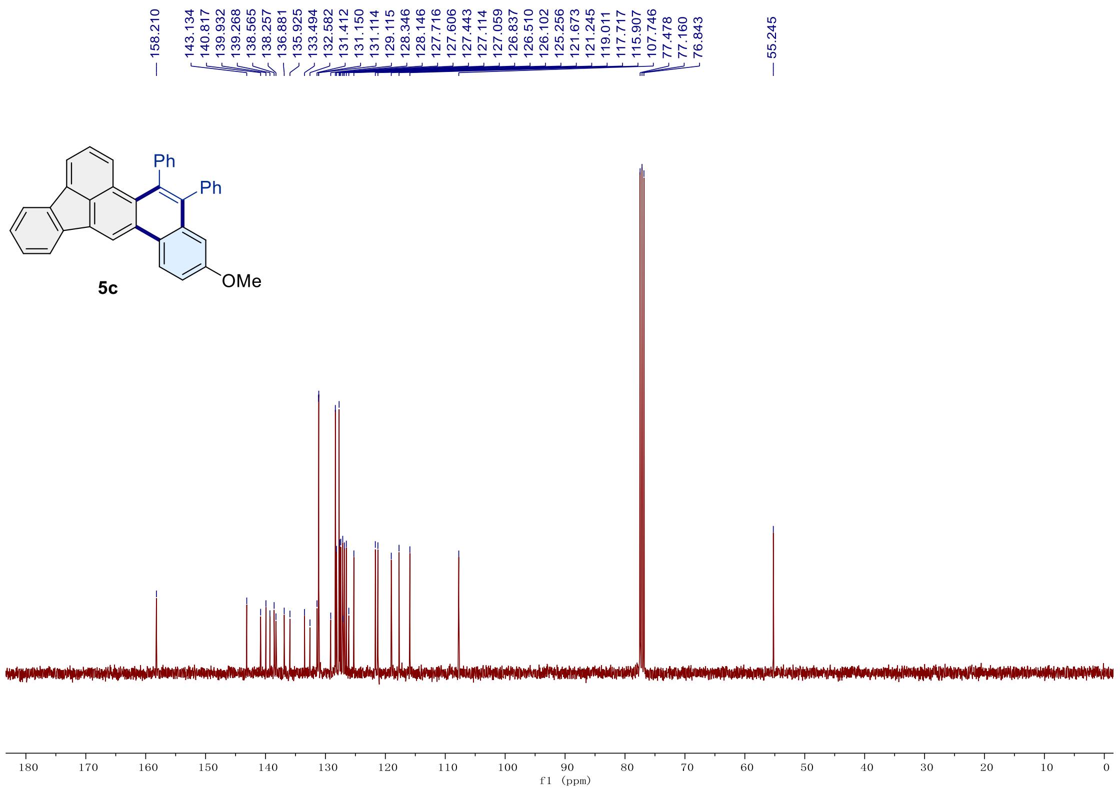
f1 (ppm)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127.114
127.059
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126.510
126.102
125.256
121.673
121.245
119.011
117.717
115.907
107.746
77.478
77.160
76.843
55.245
Ph
Ph
OMe
5c
180
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130
120
110
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90
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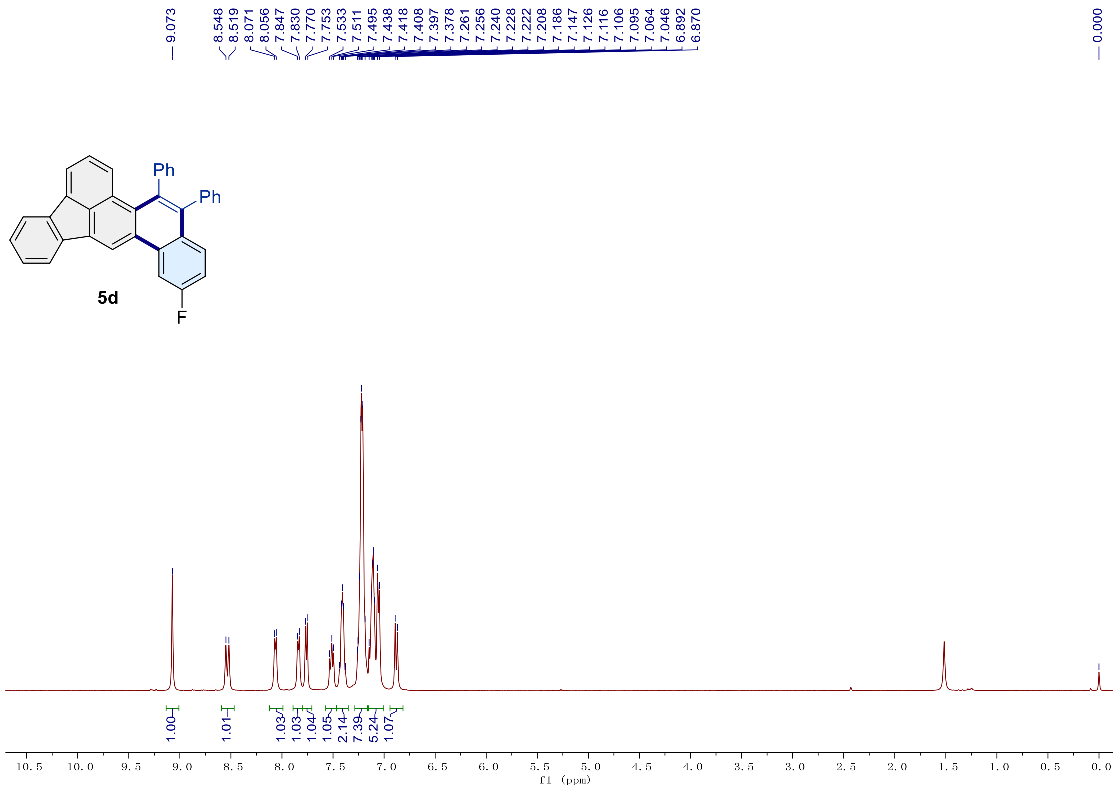
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7.438
7.418
7.408
7.397
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7.256
7.240
7.228
7.222
7.208
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7.147
7.126
7.116
7.106
7.095
7.064
7.046
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6.870
0.000
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Ph
F
5d
1.00
1.01
1.03
1.03
1.04
1.05
2.14
7.39
5.24
1.07
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10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
2.0
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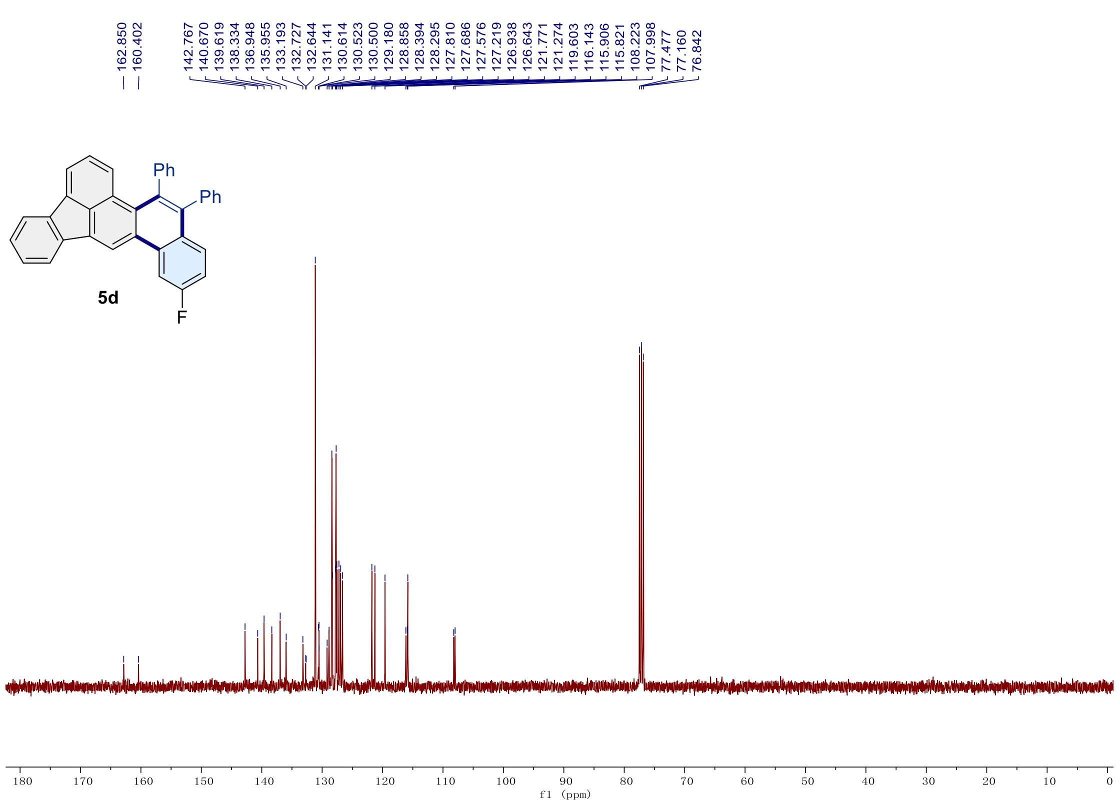
f1 (ppm)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131.141
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130.523
130.500
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128.394
128.295
127.810
127.686
127.576
127.219
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126.643
121.771
121.274
119.603
116.143
115.906
115.821
108.223
107.998
77.477
77.160
76.842
Ph
Ph
F
5d
180
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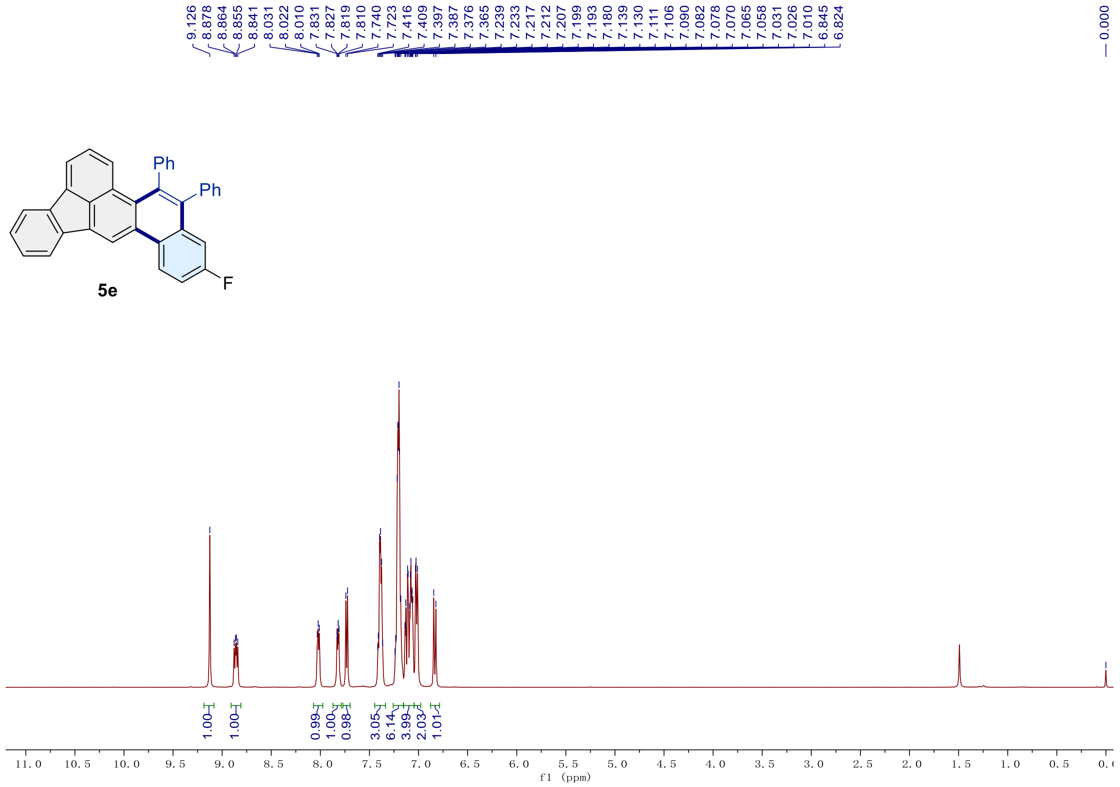
f1 (ppm)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7.409
7.397
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7.376
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7.233
7.217
7.212
7.207
7.199
7.193
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7.139
7.130
7.111
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Ph
F
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1.00
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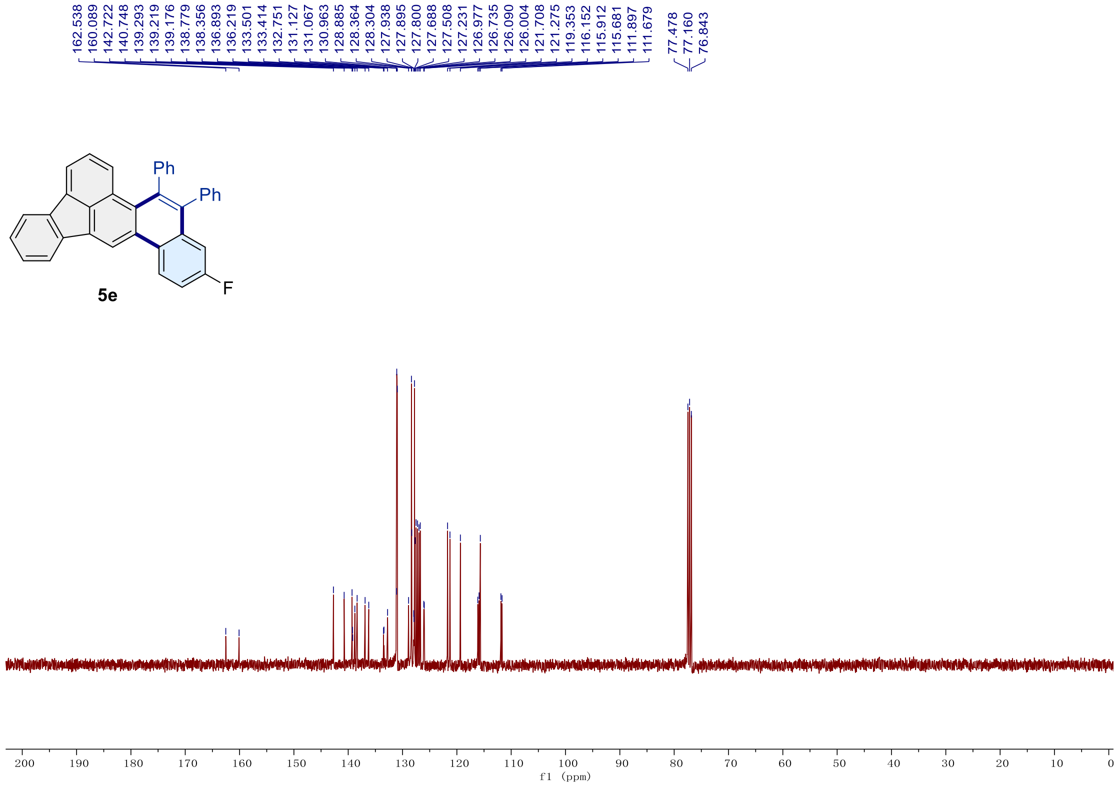
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127.231
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126.735
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119.353
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111.679
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77.160
76.843
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Ph
F
5e
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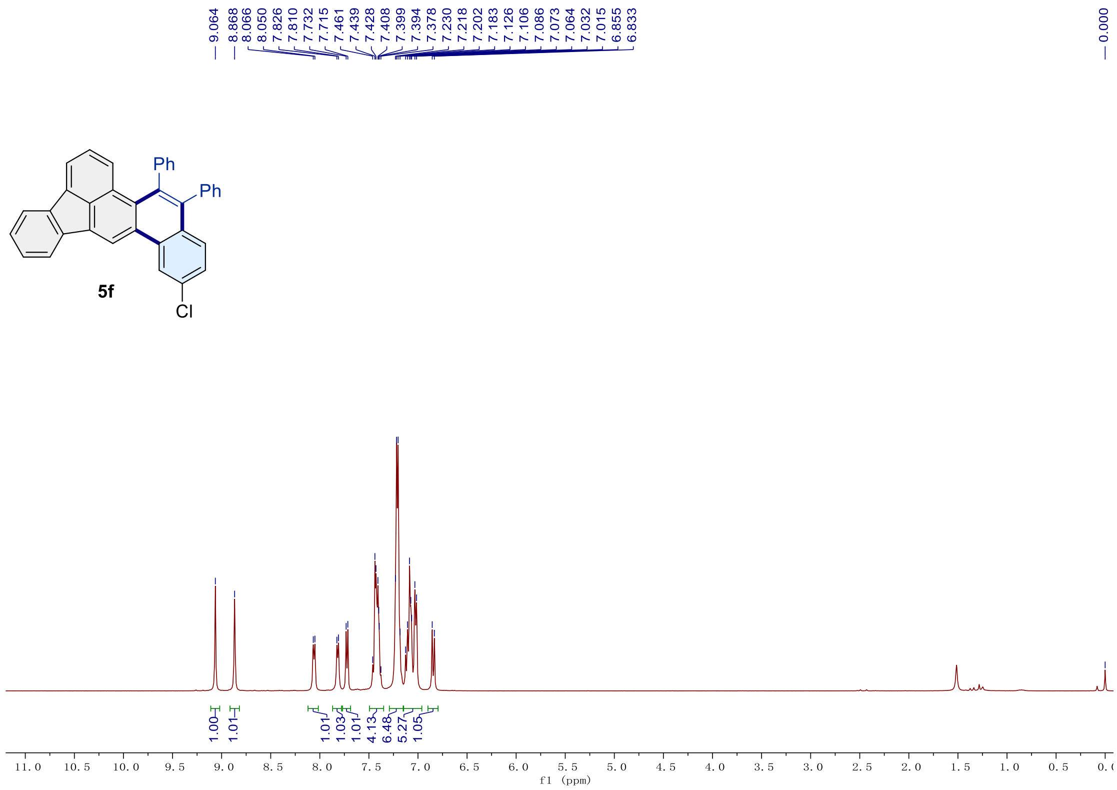
f1 (ppm)

Ph
Ph
Cl

5f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7.408
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7.378
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1.01
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6.0
5.5
5.0
4.5
4.0
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2.0
1.5
1.0
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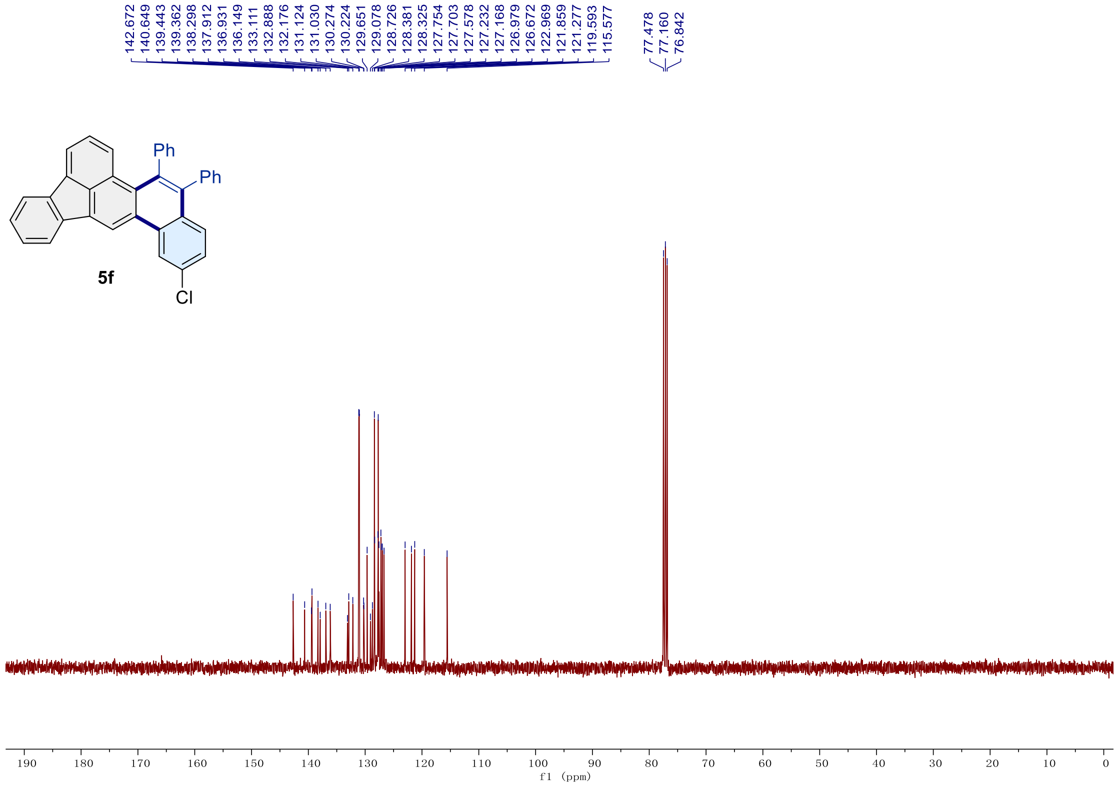
0.0
f1 (ppm)

Ph
Ph
Cl

5f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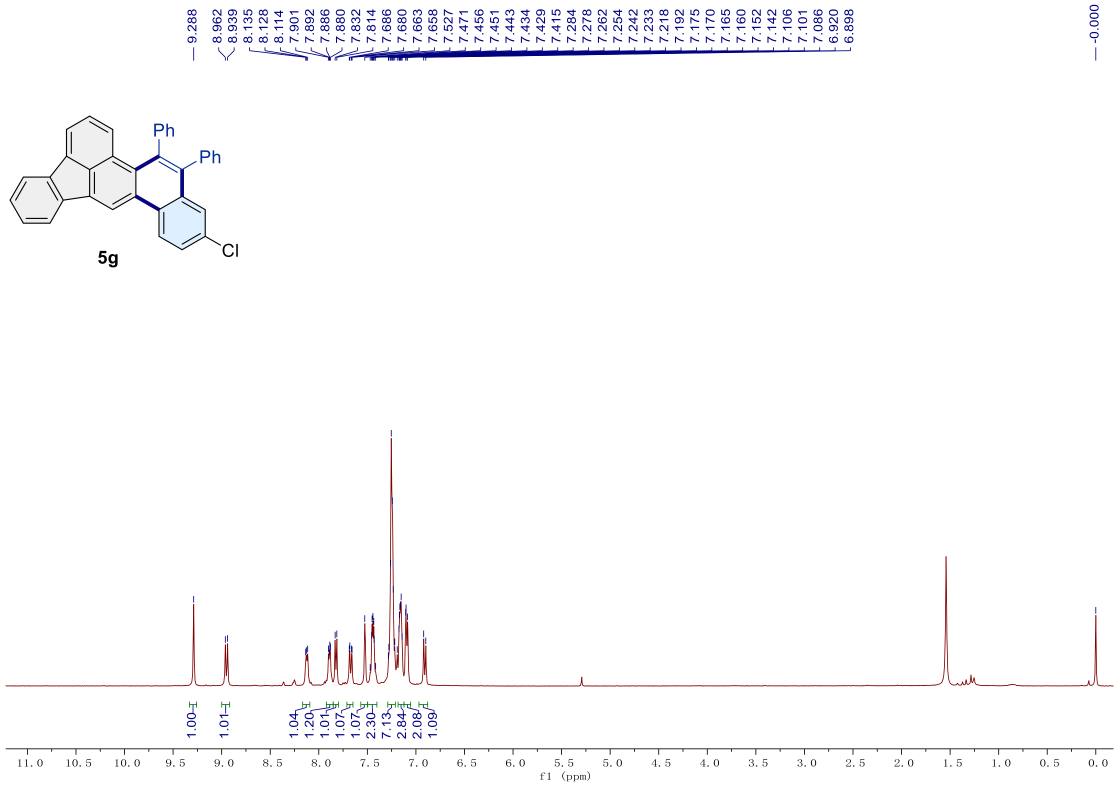
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7.233
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Ph
Cl
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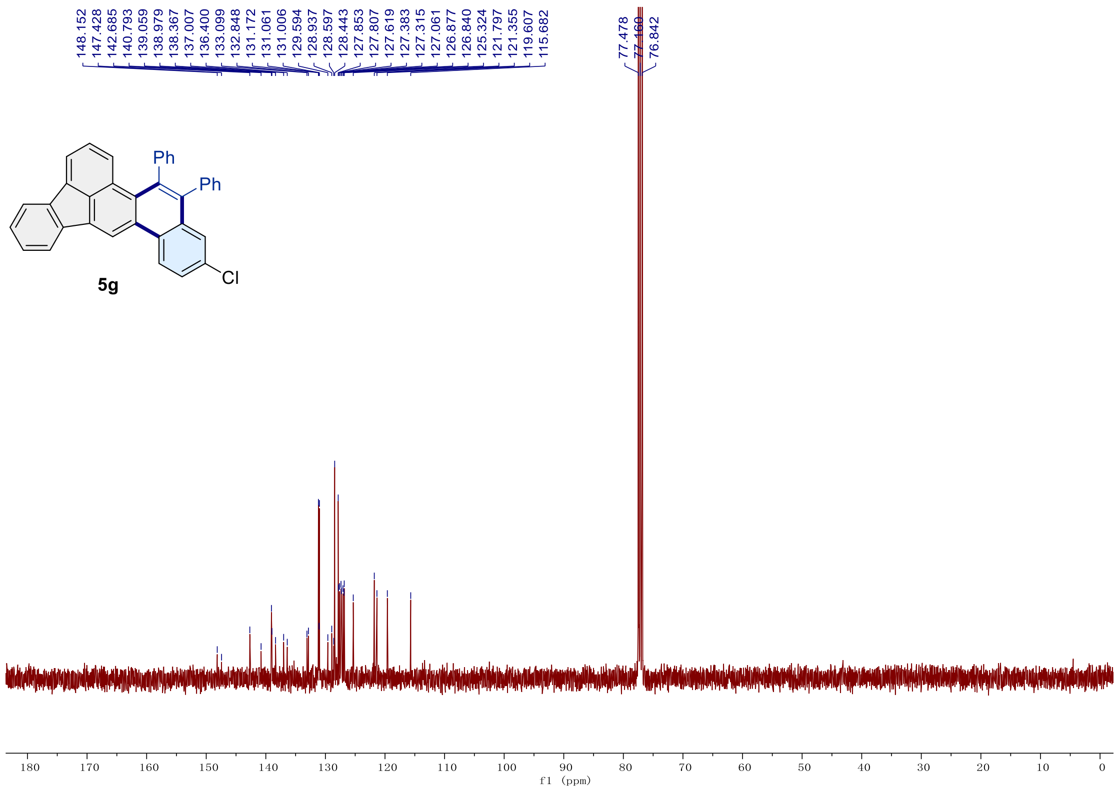
f1 (ppm)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77.160
76.842
Ph
Ph
Cl
5g
180
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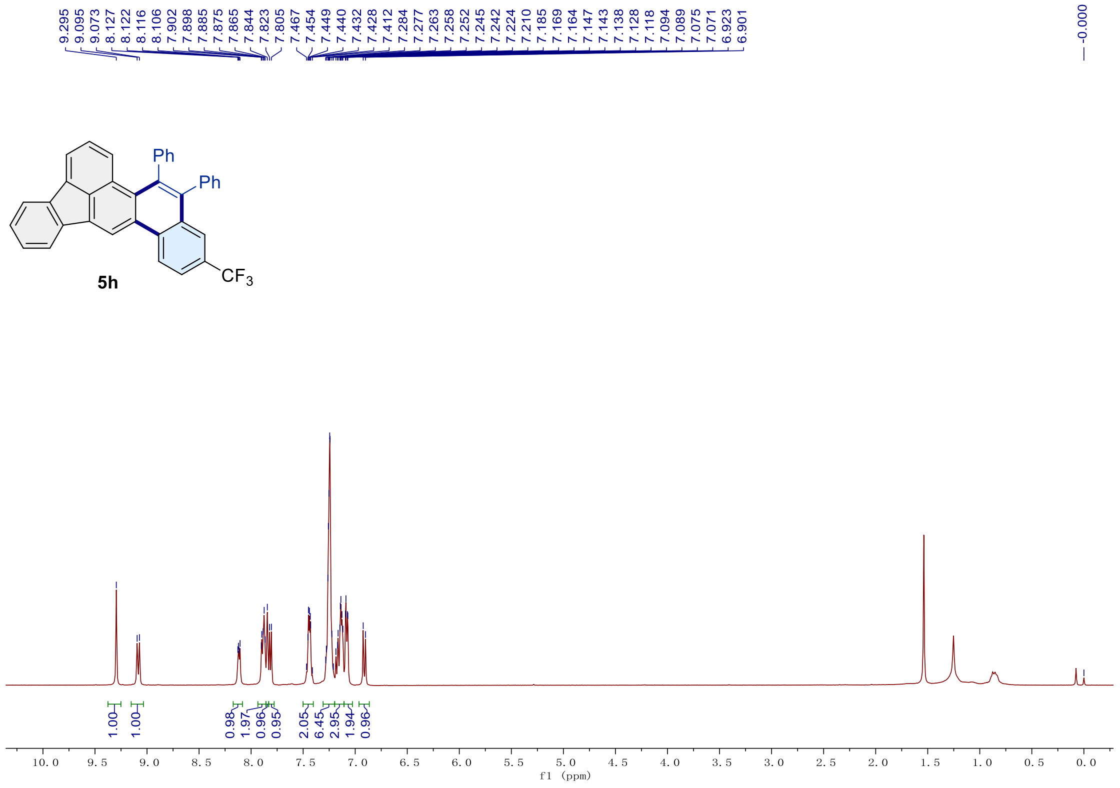
f1 (ppm)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Ph
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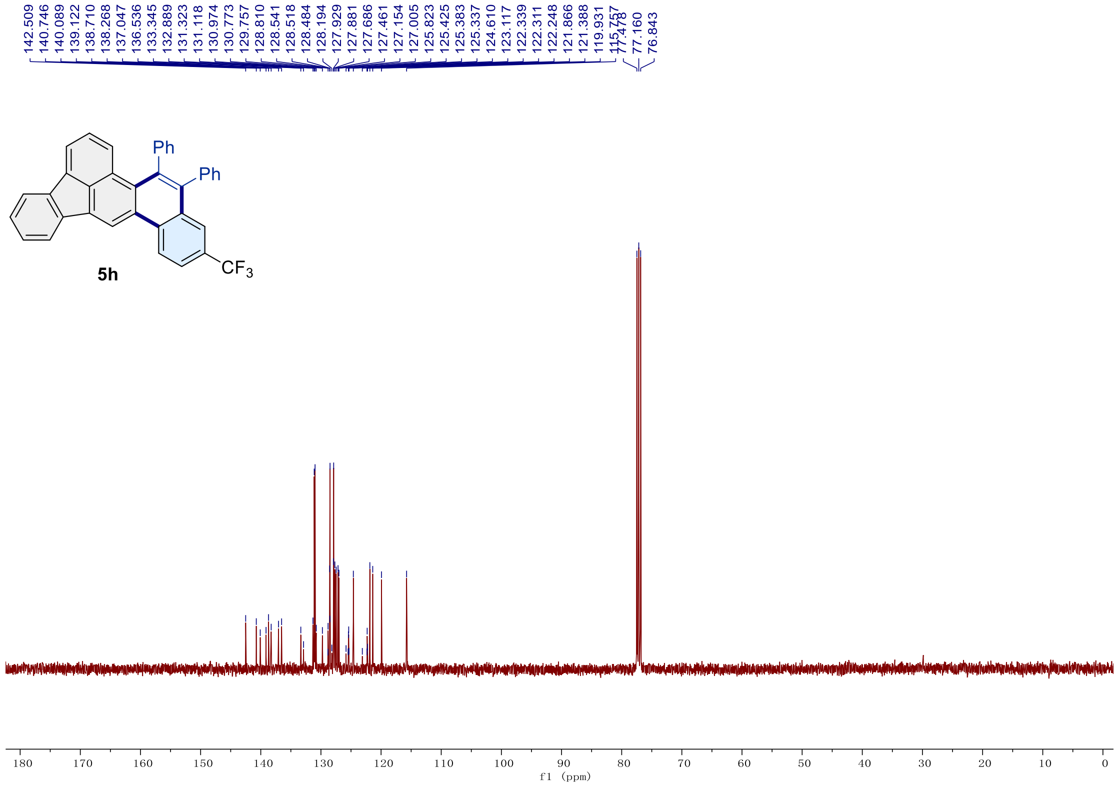
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123.117
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122.311
122.248
121.866
121.388
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115.757
77.478
77.160
76.843
Ph
Ph
CF3
5h
180
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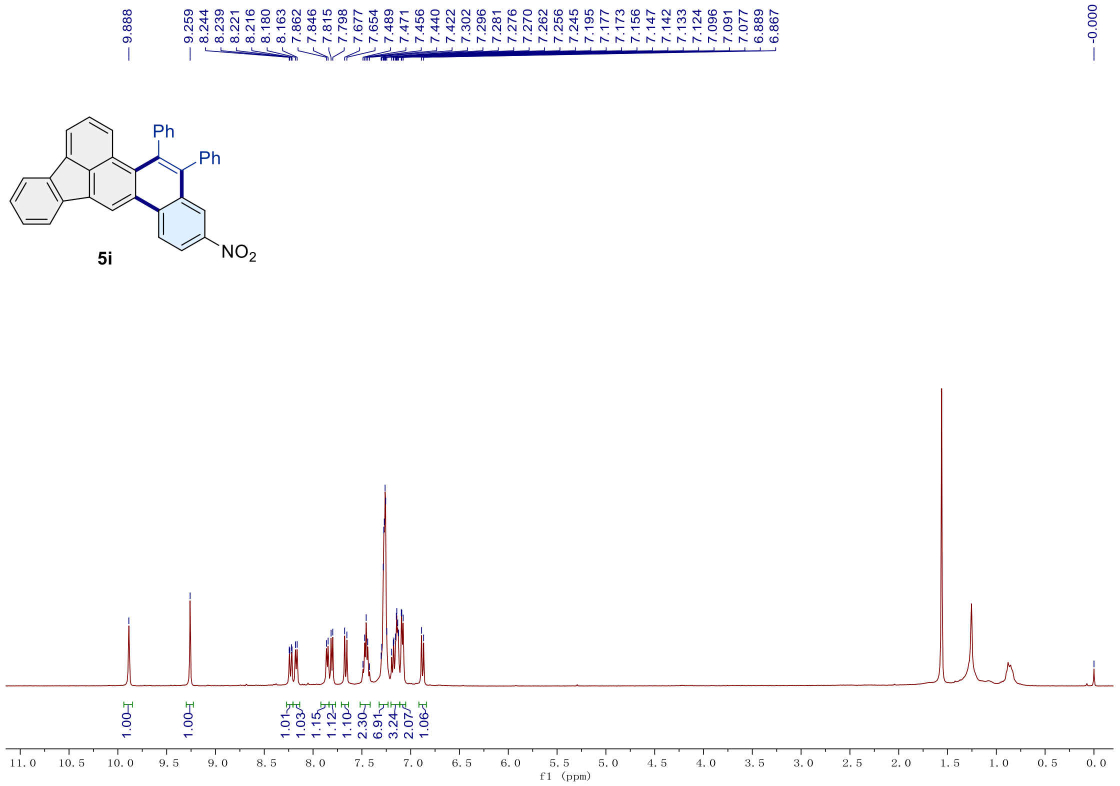
f1 (ppm)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7.245
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7.156
7.147
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7.091
7.077
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Ph
Ph
NO2
5i
1.00
1.00
1.01
1.03
1.15
1.12
1.10
2.30
6.91
3.24
2.07
1.06
11.0
10.5
10.0
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9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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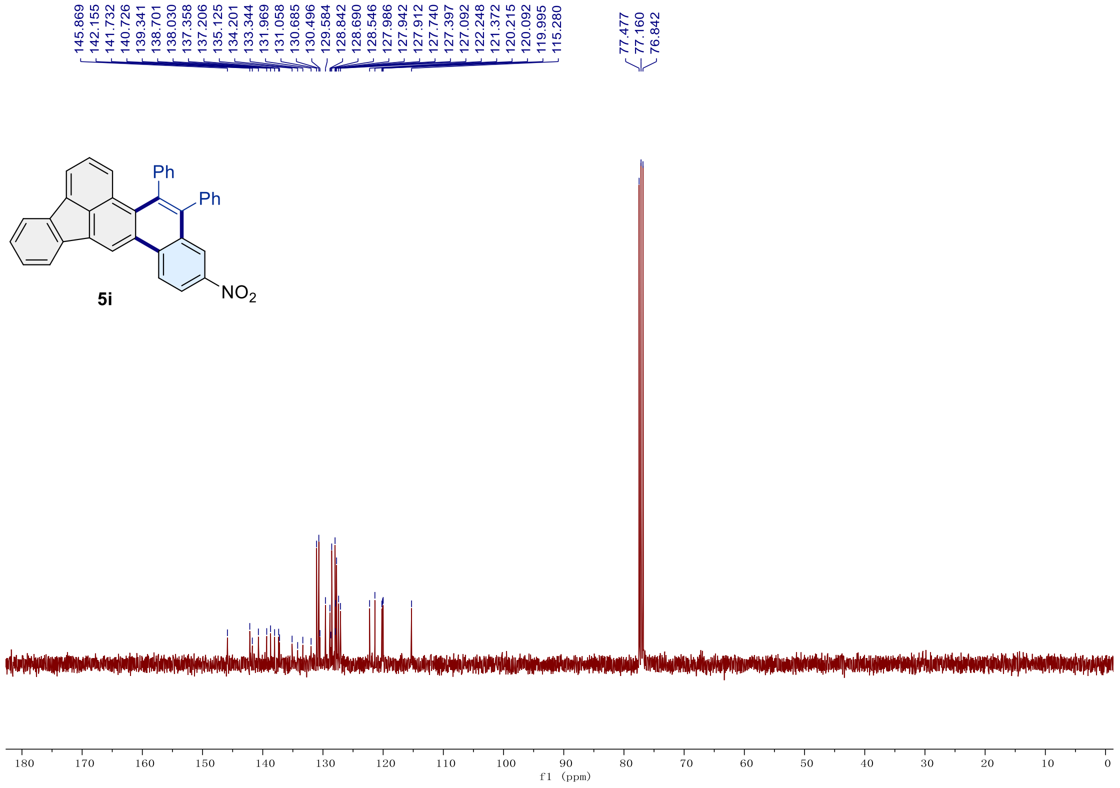
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130.685
130.496
129.584
128.842
128.690
128.546
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127.942
127.912
127.740
127.397
127.092
122.248
121.372
120.215
120.092
119.995
115.280
77.477
77.160
76.842
Ph
Ph
NO2
5i
180
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140
130
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110
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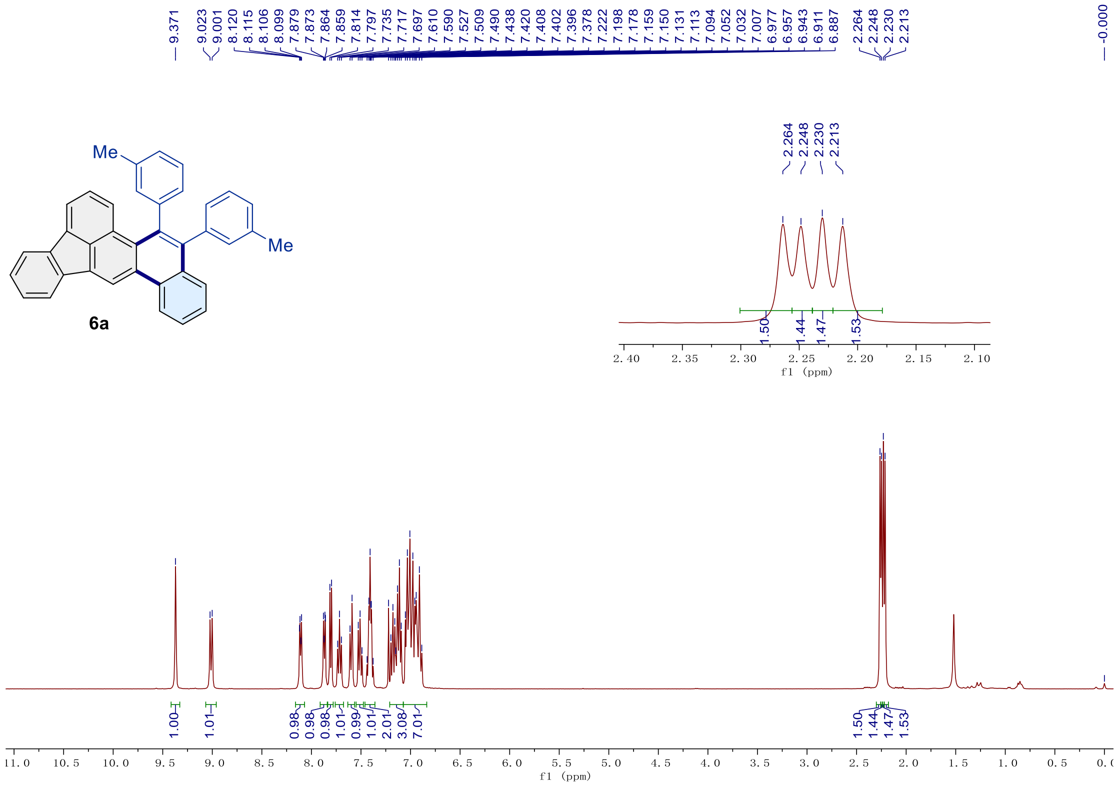
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7.735
7.717
7.697
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7.590
7.527
7.509
7.490
7.438
7.420
7.408
7.402
7.396
7.378
7.222
7.198
7.178
7.159
7.150
7.131
7.113
7.094
7.052
7.032
7.007
6.977
6.957
6.943
6.911
6.887
2.264
2.248
2.230
2.213
-0.000
Me
Me
6a
1.50
1.44
1.47
1.53
2.40
2.35
2.30
2.25
2.20
2.15
2.10
f1 (ppm)
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0.98
0.98
0.98
1.01
0.99
1.01
2.01
3.08
7.01
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10.5
10.0
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9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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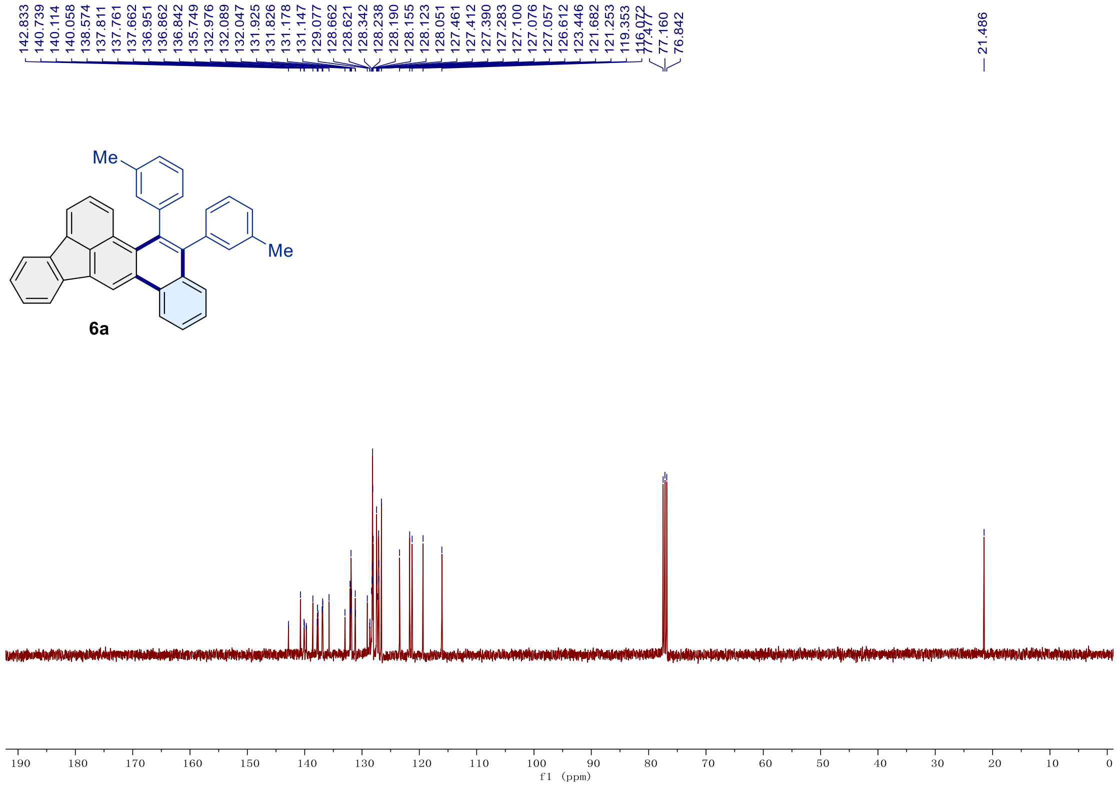
f1 (ppm)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127.412
127.390
127.283
127.100
127.076
127.057
126.612
123.446
121.682
121.253
119.353
116.072
77.477
77.160
76.842
21.486
Me
Me
6a
190
180
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120
110
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70
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50
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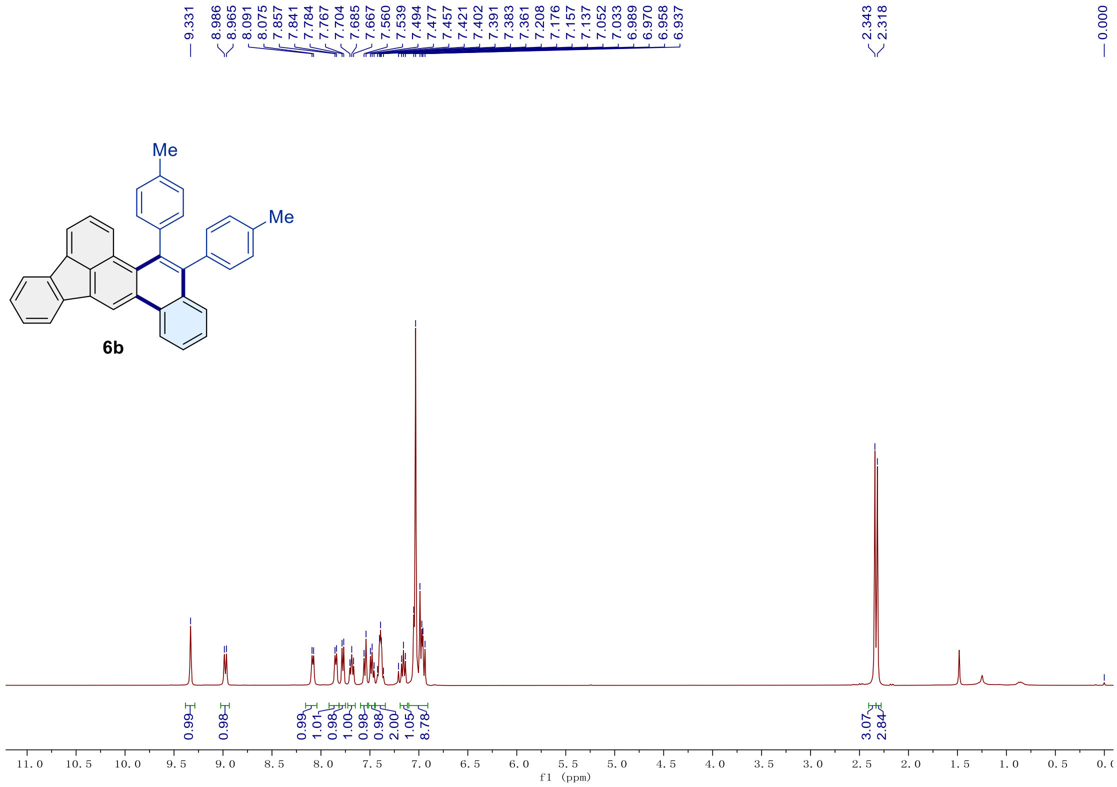
f1 (ppm)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7.685
7.667
7.560
7.539
7.494
7.477
7.457
7.421
7.402
7.391
7.383
7.361
7.208
7.176
7.157
7.137
7.052
7.033
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6.970
6.958
6.937
2.343
2.318
0.000
Me
Me
6b
0.99
0.98
0.99
1.01
0.98
1.00
0.98
0.98
2.00
1.05
8.78
3.07
2.84
11.0
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10.0
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9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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3.0
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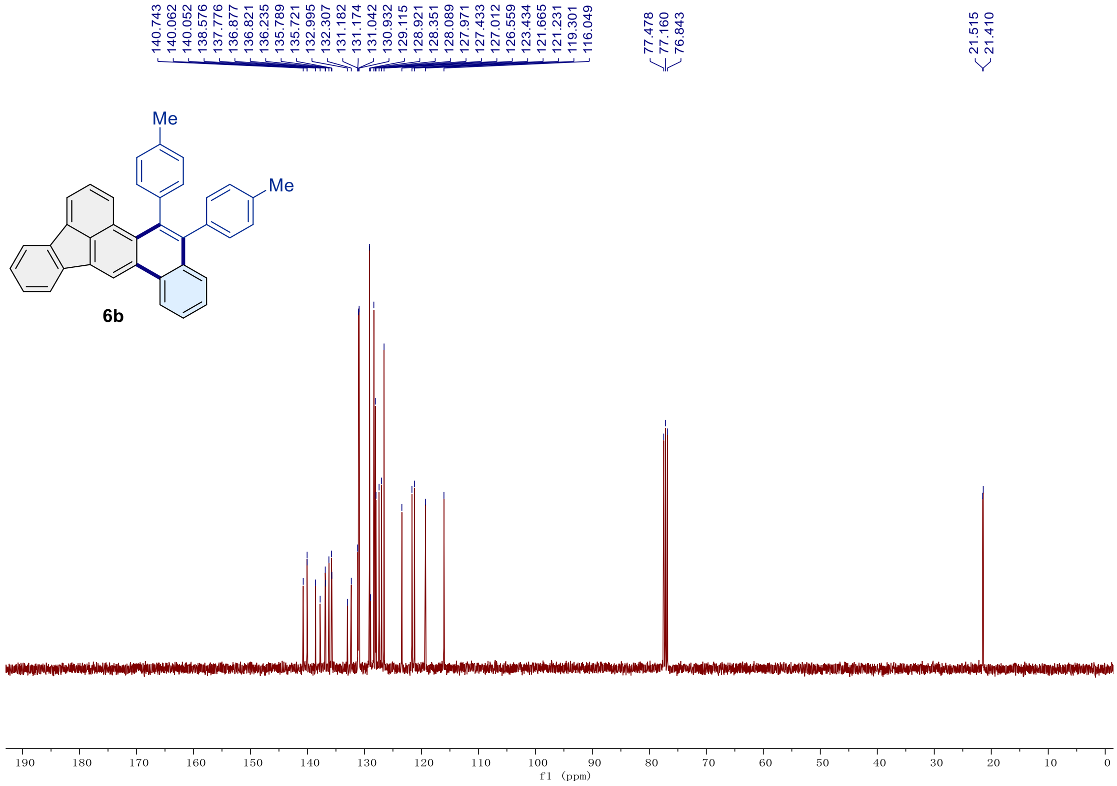
0.0
f1 (ppm)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131.174
131.042
130.932
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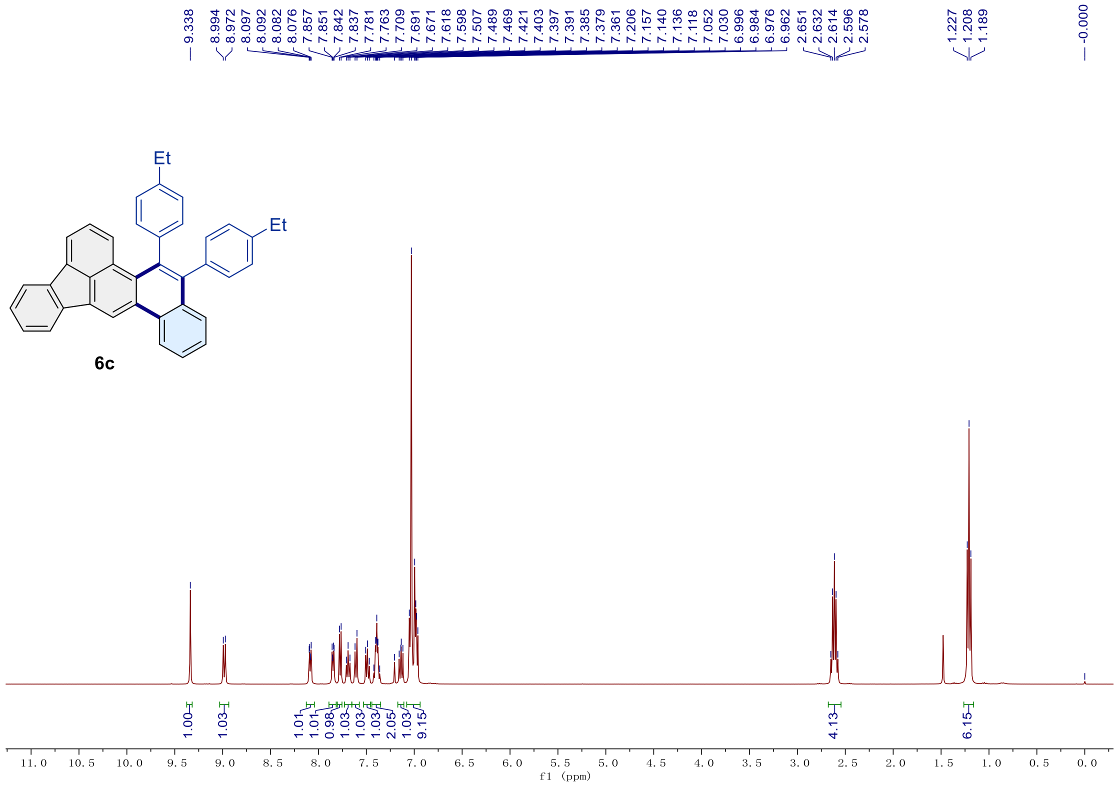
128.921
128.351
128.089
127.971
127.433
127.012
126.559
123.434
121.665
121.231
119.301
116.049
77.478
77.160
76.843
21.515
21.410
Me
Me
6b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.851
7.842
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7.781
7.763
7.709
7.691
7.671
7.618
7.598
7.507
7.489
7.469
7.421
7.403
7.397
7.391
7.385
7.379
7.361
7.206
7.157
7.140
7.136
7.118
7.052
7.030
6.996
6.984
6.976
6.962
2.651
2.632
2.614
2.596
2.578
1.227
1.208
1.189
-0.000
Et
Et
1.00
1.03
1.01
1.01
0.98
1.03
1.03
1.03
2.05
1.03
9.15
4.13
6.15
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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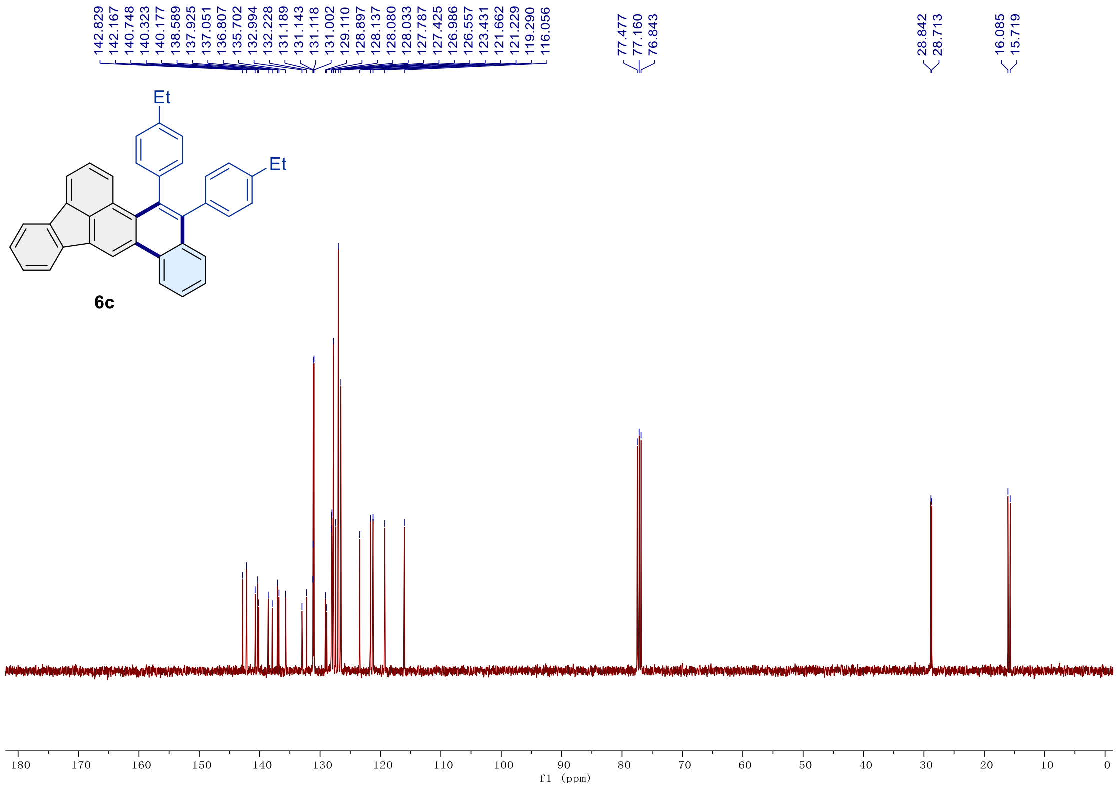
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.189
131.143
131.118
131.002
129.110
128.897
128.137
128.080
128.033
127.787
127.425
126.986
126.557
123.431
121.662
121.229
119.290
116.056
77.477
77.160
76.843
28.842
28.713
16.085
15.719
Et
Et
180
170
160
150
140
130
120
110
100
90
80
70
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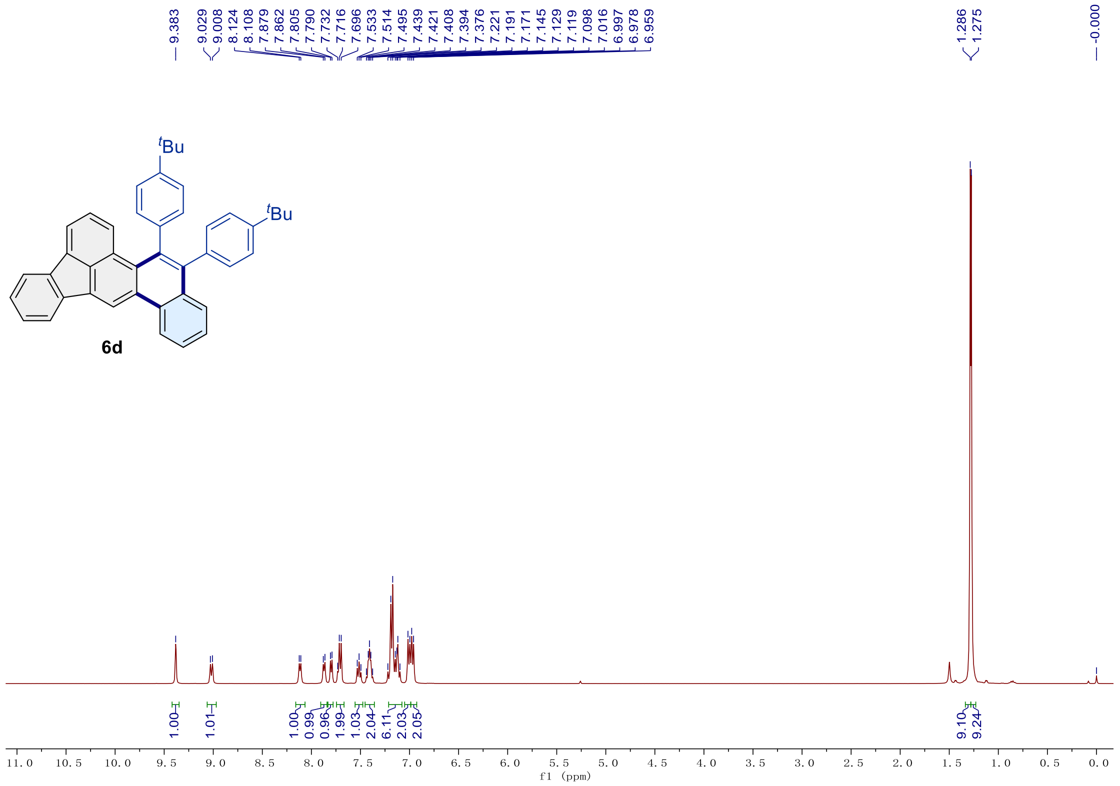
50
40
30
20
10
0
f1 (ppm)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7.533
7.514
7.495
7.439
7.421
7.408
7.394
7.376
7.221
7.191
7.171
7.145
7.129
7.119
7.098
7.016
6.997
6.978
6.959
1.286
1.275
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tBu
tBu
6d
1.00
1.01
1.00
0.99
0.96
1.99
1.03
2.04
6.11
2.03
2.05
9.10
9.24
11.0
10.5
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
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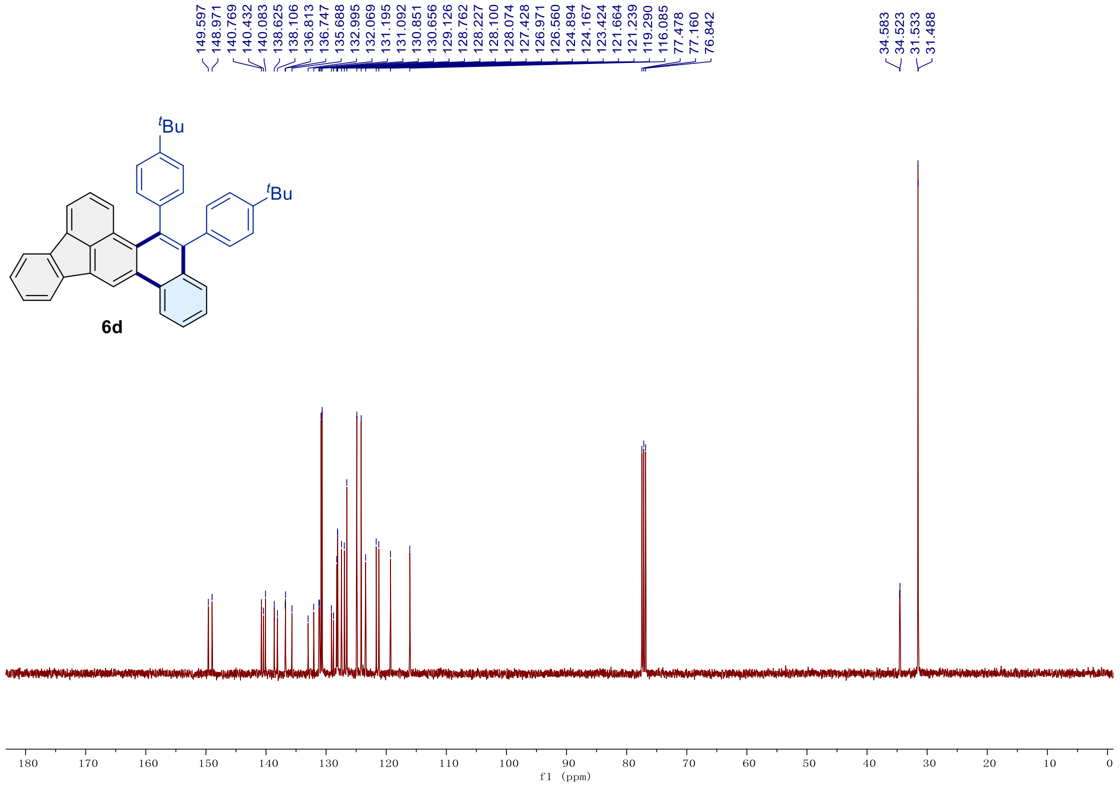
1.0
0.5
0.0
f1 (ppm)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131.092
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129.126
128.762
128.227
128.100
128.074
127.428
126.971
126.560
124.894
124.167
123.424
121.664
121.239
119.290
116.085
77.478
77.160
76.842
34.583
34.523
31.533
31.488
tBu
tBu
6d
180
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140
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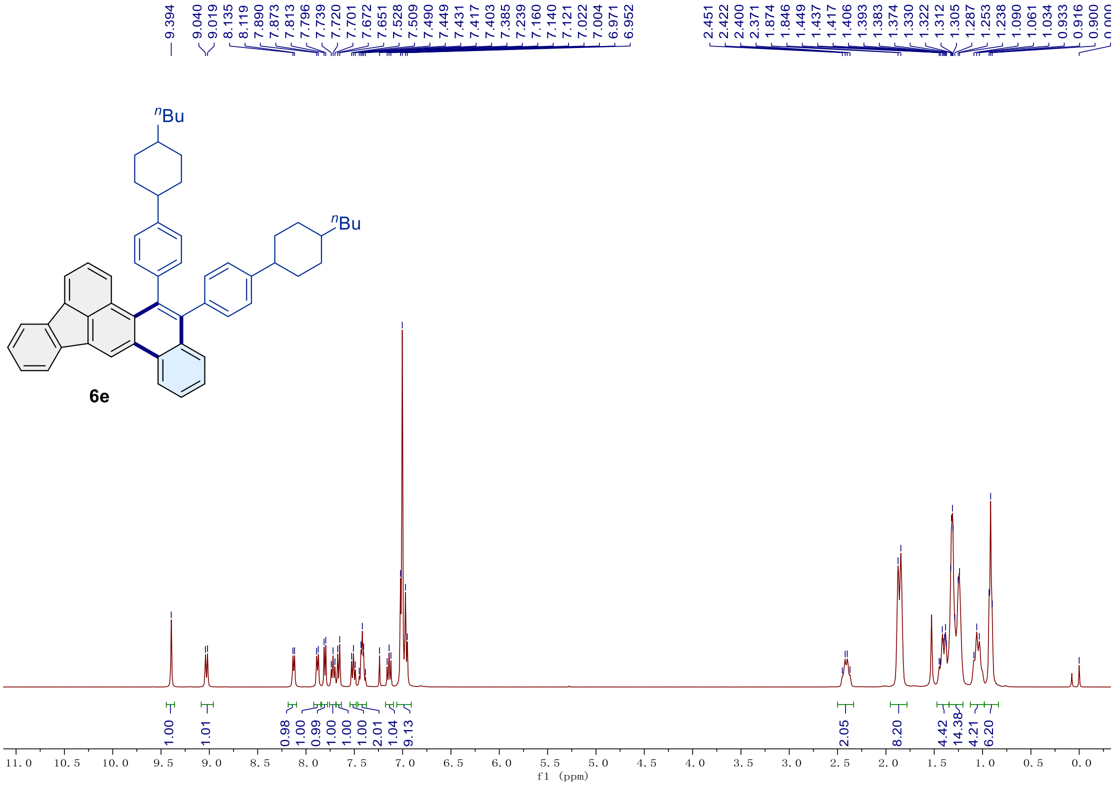
f1 (ppm)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7.672
7.651
7.528
7.509
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7.449
7.431
7.417
7.403
7.385
7.239
7.160
7.140
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7.022
7.004
6.971
6.952
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2.422
2.400
2.371
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1.846
1.449
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1.406
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1.383
1.374
1.330
1.322
1.312
1.305
1.287
1.253
1.238
1.090
1.061
1.034
0.933
0.916
0.900
0.000
^{n}Bu
^{n}Bu
6e
1.00
1.01
0.98
1.00
0.99
1.00
1.00
1.00
2.01
1.04
9.13
2.05
8.20
4.42
14.38
4.21
6.20
11.0
10.5
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
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3.0
2.5
2.0
1.5
1.0
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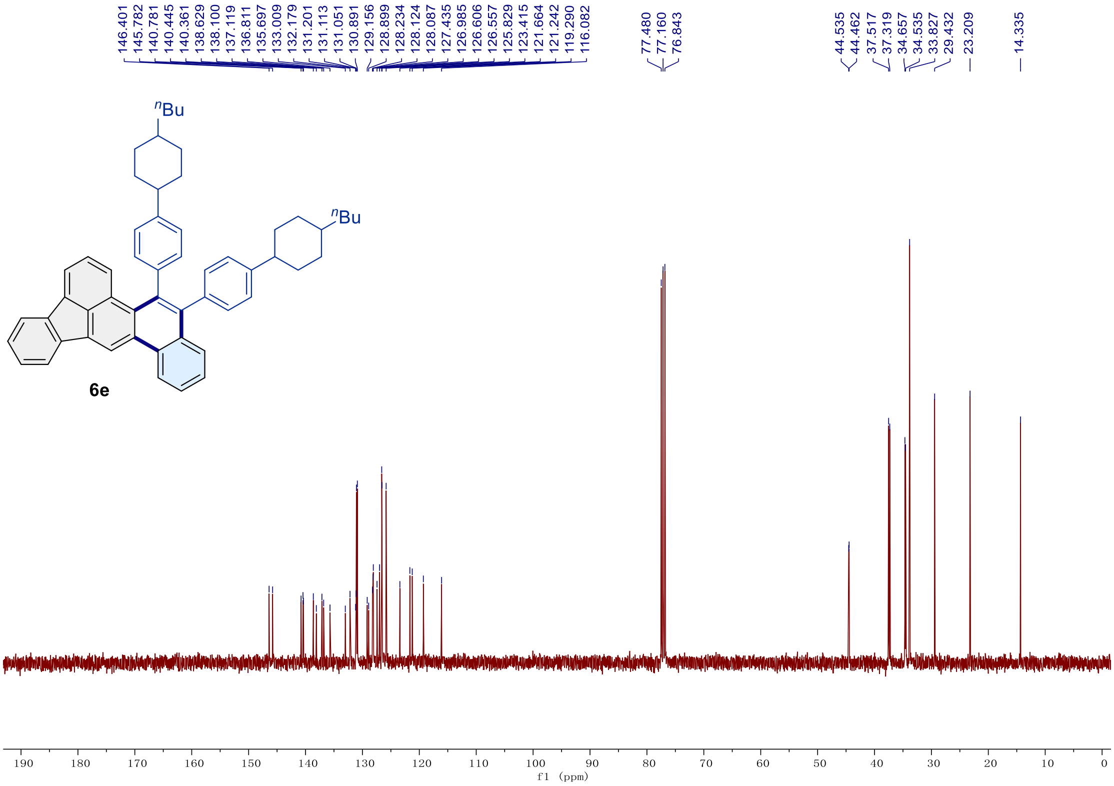
0.0
f1 (ppm)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131.051
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128.087
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126.606
126.557
125.829
123.415
121.664
121.242
119.290
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76.843
44.535
44.462
37.517
37.319
34.657
34.535
33.827
29.432
23.209
14.335
^{n}Bu
^{n}Bu
6e
190
180
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120
110
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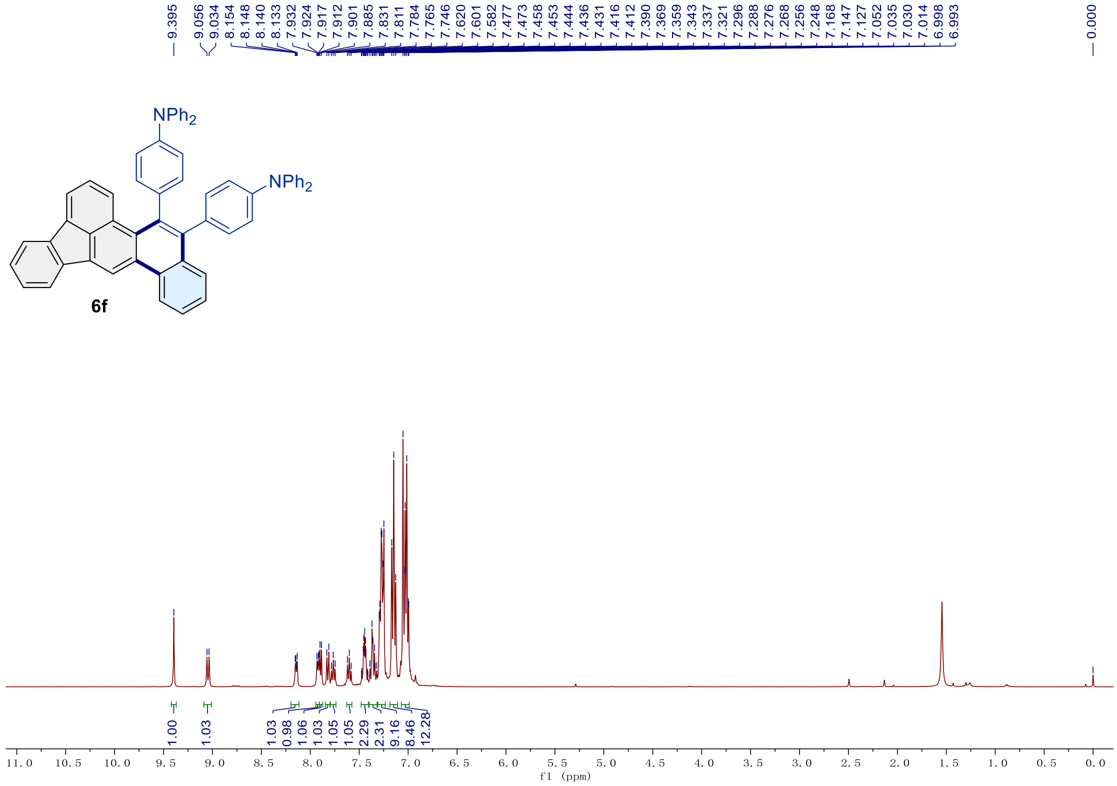
f1 (ppm)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7.831
7.811
7.784
7.765
7.746
7.620
7.601
7.582
7.477
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7.035
7.030
7.014
6.998
6.993
0.000
NPh2
NPh2
6f
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1.03
1.03
0.98
1.06
1.03
1.05
1.05
2.29
2.31
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8.46
12.28
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10.5
10.0
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
2.0
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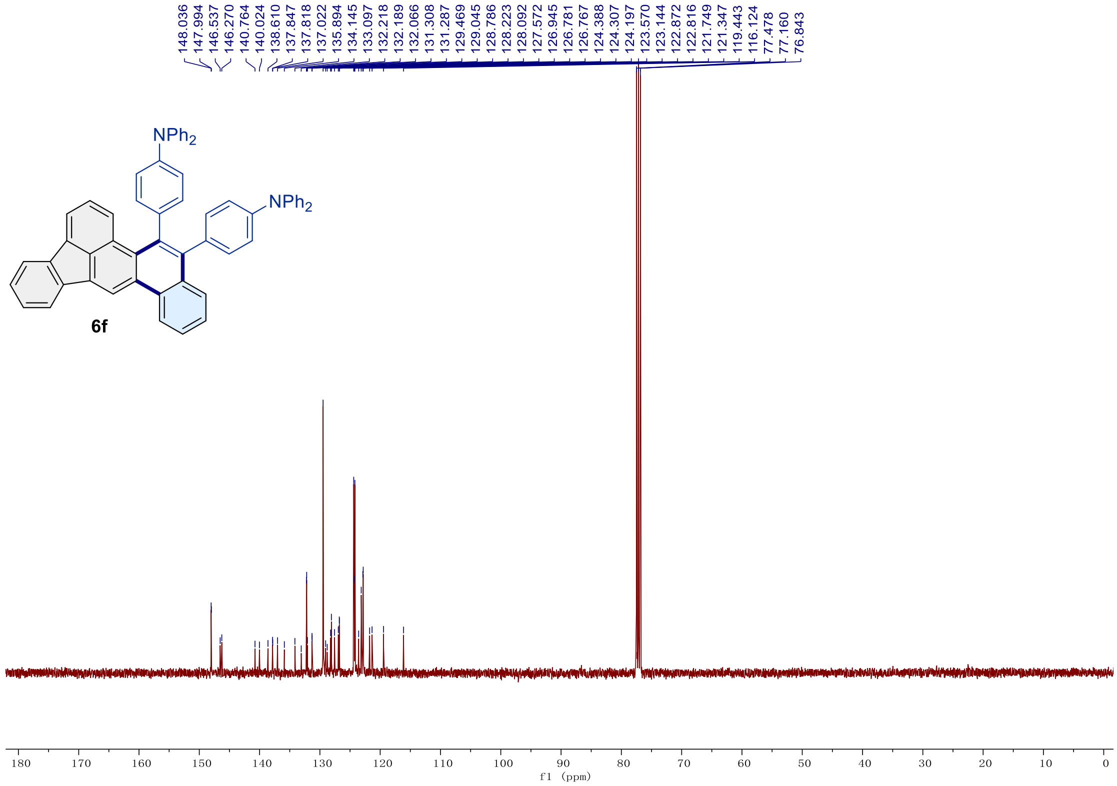
f1 (ppm)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128.786
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128.092
127.572
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126.781
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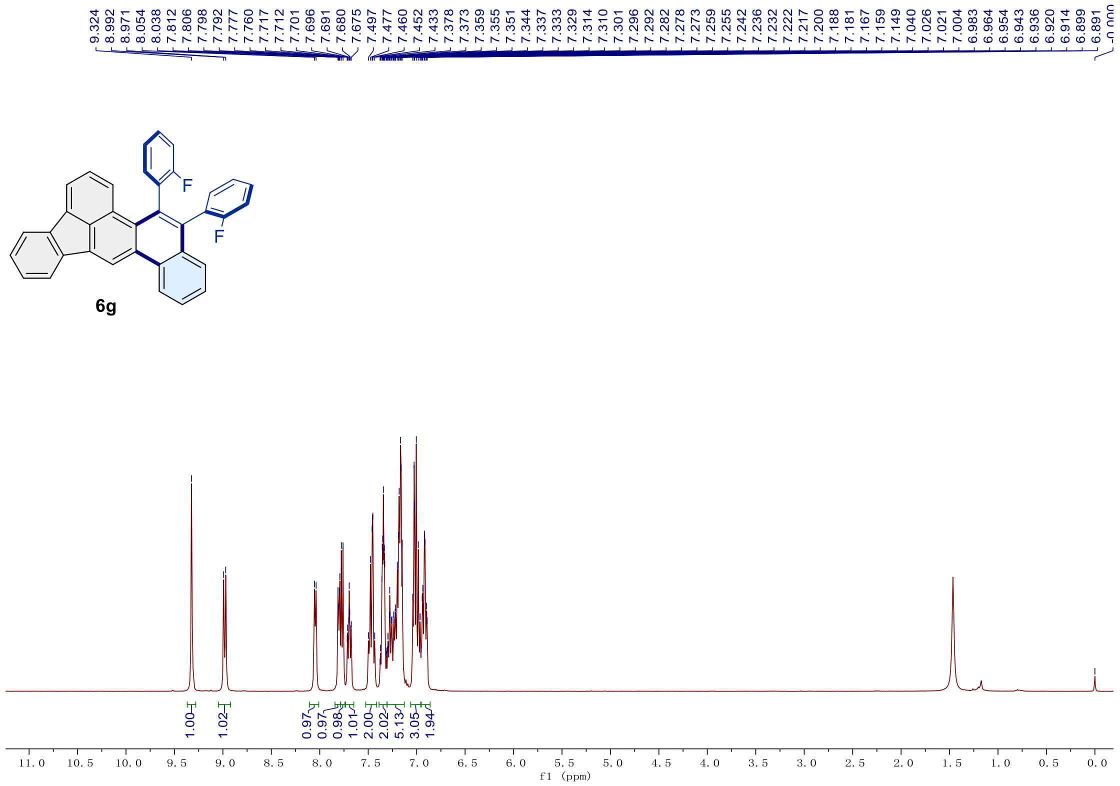
122.816
121.749
121.347
119.443
116.124
77.478
77.160
76.843
NPh2
NPh2
6f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.712
7.701
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7.691
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7.373
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7.310
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7.232
7.222
7.217
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7.188
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7.167
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7.149
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7.026
7.021
7.004
6.983
6.964
6.954
6.943
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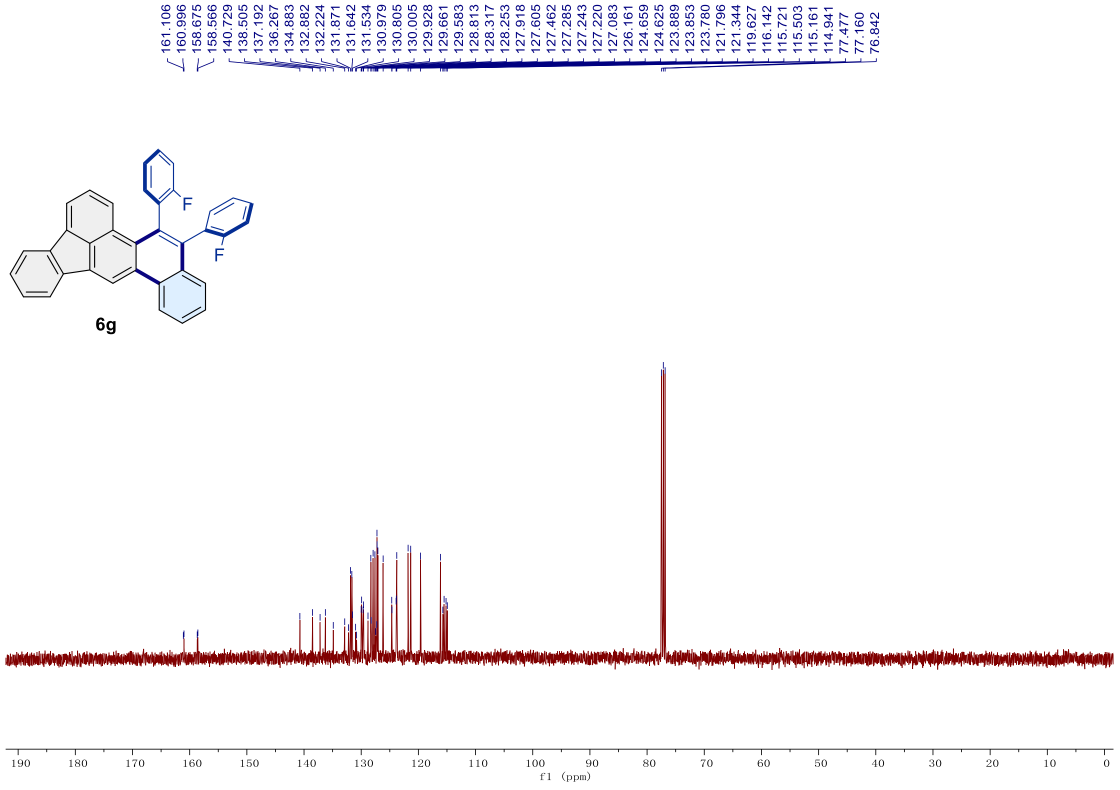
6.920
6.914
6.899
6.891
-0.000
F
F
6g
1.00
1.02
0.97
0.97
0.98
1.01
2.00
2.02
5.13
3.05
1.94
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.805
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129.661
129.583
128.813
128.317
128.253
127.918
127.605
127.462
127.285
127.243
127.220
127.083
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124.659
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123.889
123.853
123.780
121.796
121.344
119.627
116.142
115.721
115.503
115.161
114.941
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77.160
76.842
F
F
6g
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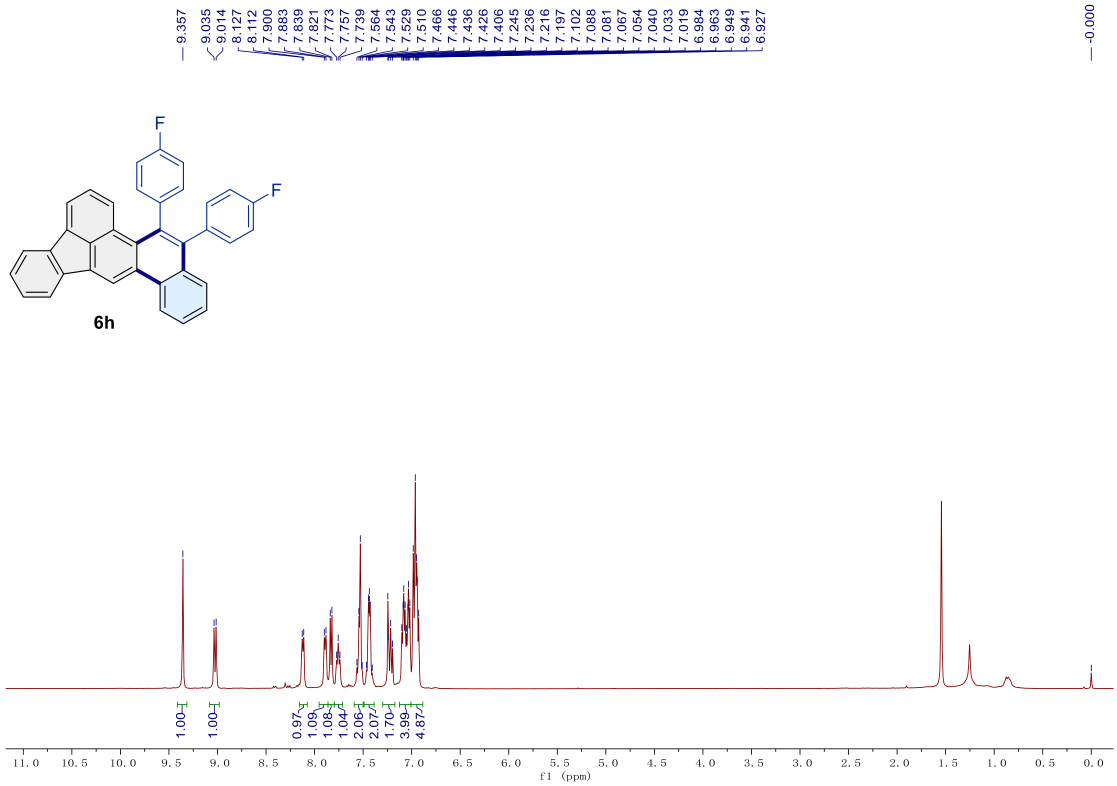
f1 (ppm)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7.529
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7.466
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7.436
7.426
7.406
7.245
7.236
7.216
7.197
7.102
7.088
7.081
7.067
7.054
7.040
7.033
7.019
6.984
6.963
6.949
6.941
6.927
-0.000
F
F
6h
1.00
1.00
0.97
1.09
1.08
1.04
2.06
2.07
1.70
3.99
4.87
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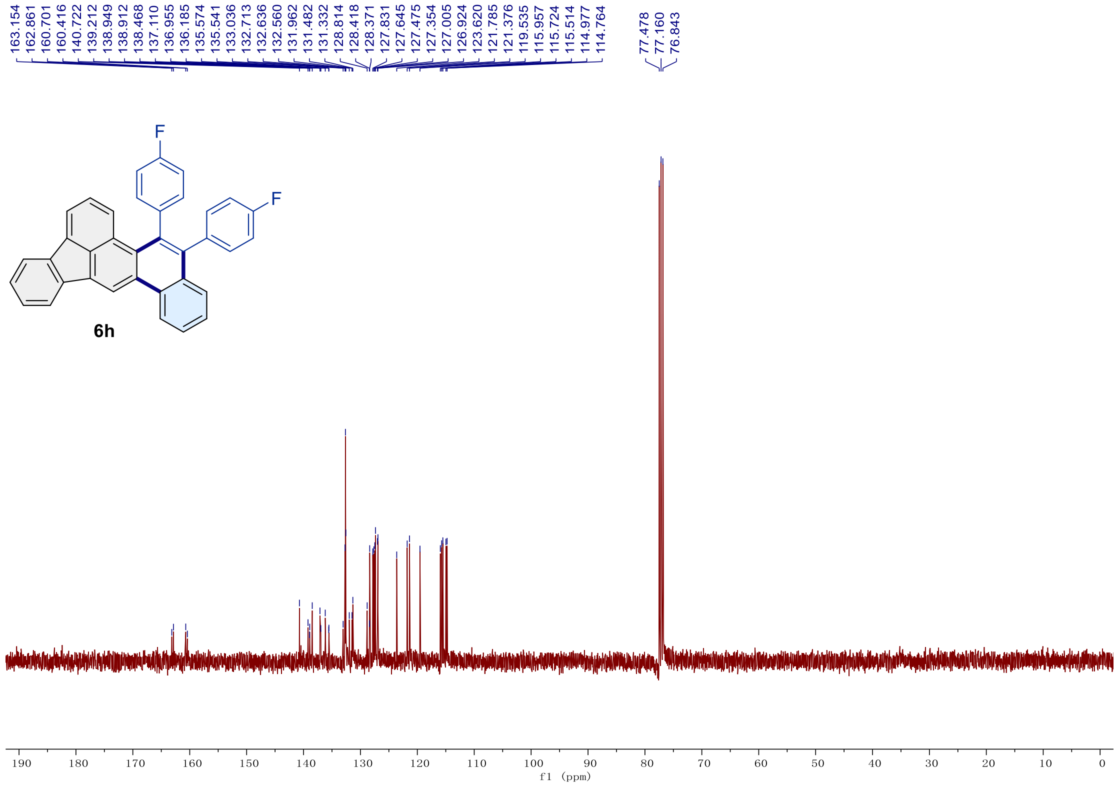
f1 (ppm)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135.574
135.541
133.036
132.713
132.636
132.560
131.962
131.482
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128.814
128.418
128.371
127.831
127.645
127.475
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127.005
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119.535
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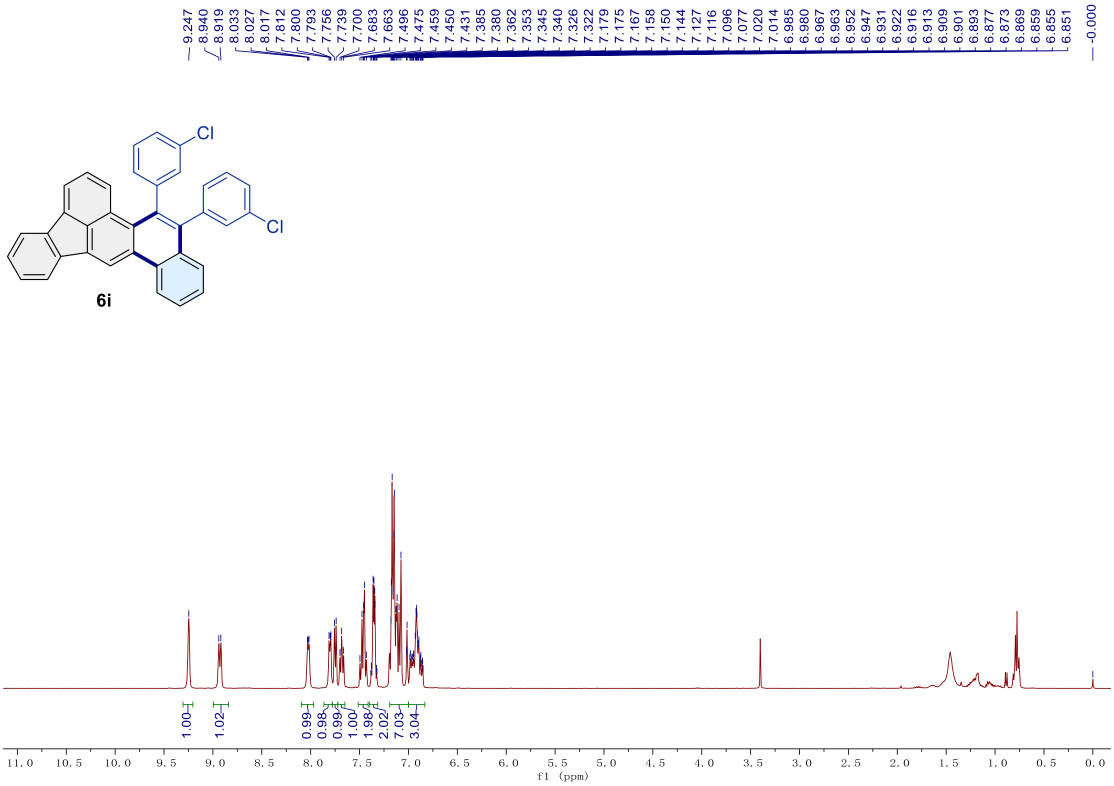
115.724
115.514
114.977
114.764
77.478
77.160
76.843
F
F
6h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.700
7.683
7.663
7.496
7.475
7.459
7.450
7.431
7.385
7.380
7.362
7.353
7.345
7.340
7.326
7.322
7.179
7.175
7.167
7.158
7.150
7.144
7.127
7.116
7.096
7.077
7.020
7.014
6.985
6.980
6.967
6.963
6.952
6.947
6.931
6.922
6.916
6.913
6.909
6.901
6.893
6.877
6.873
6.869
6.859
6.855
6.851
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Cl
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1.02
0.99
0.98
0.99
1.00
1.98
2.02
7.03
3.04
11.0
10.5
10.0
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9.0
8.5
8.0
7.5
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6.0
5.5
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3.0
2.5
2.0
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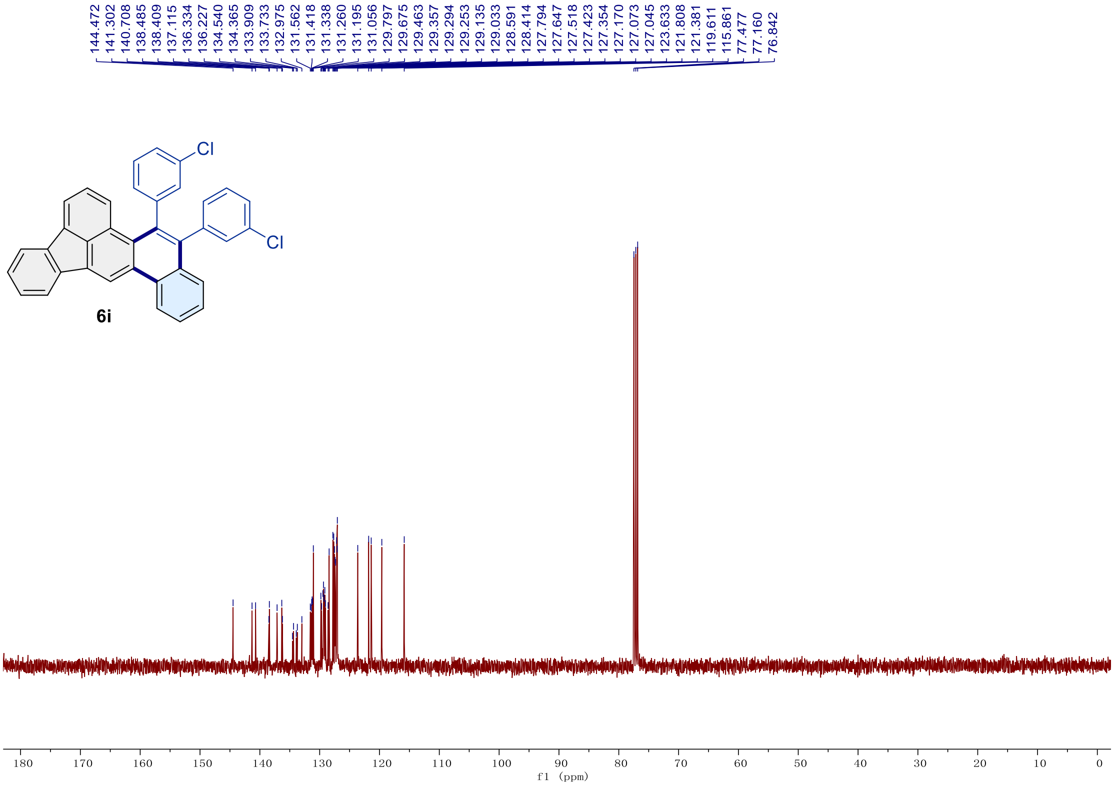
1.0
0.5
0.0
f1 (ppm)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132.975
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129.294
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127.794
127.647
127.518
127.423
127.354
127.170
127.073
127.045
123.633
121.808
121.381
119.611
115.861
77.477
77.160
76.842
Cl
Cl
180
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140
130
120
110
100
90
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70
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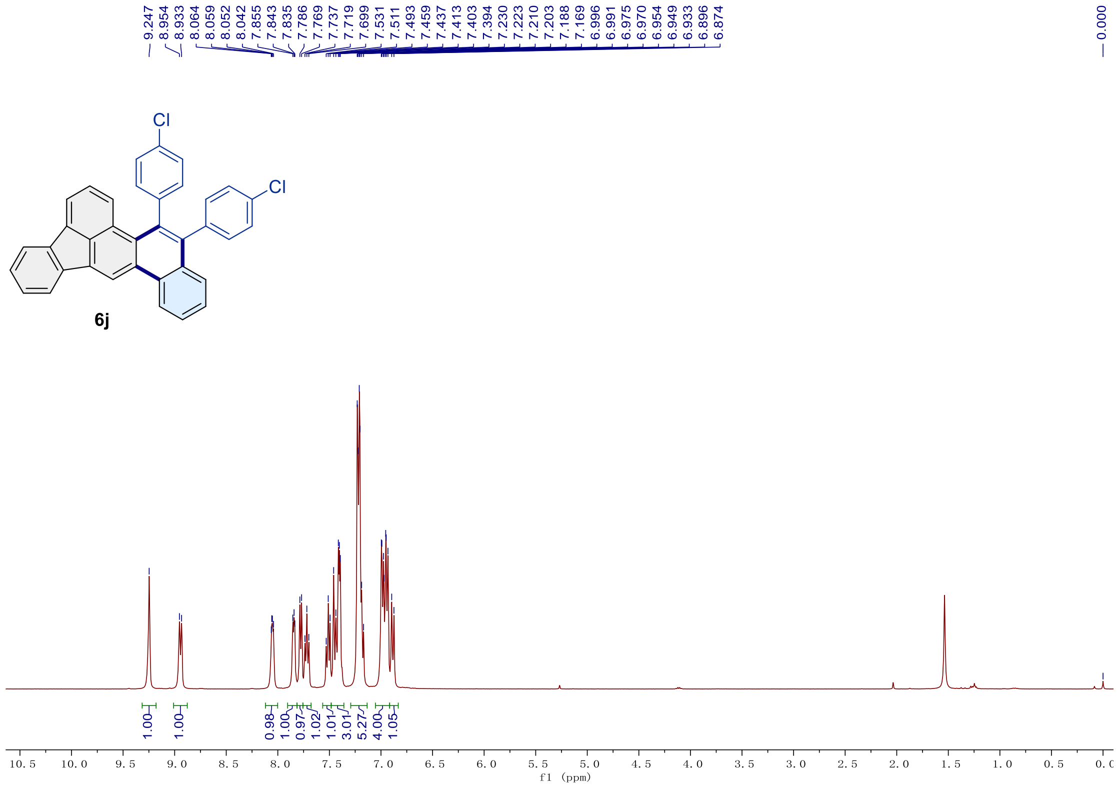
50
40
30
20
10
0
f1 (ppm)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7.737
7.719
7.699
7.531
7.511
7.493
7.459
7.437
7.413
7.403
7.394
7.230
7.223
7.210
7.203
7.188
7.169
6.996
6.991
6.975
6.970
6.954
6.949
6.933
6.896
6.874
0.000
Cl
Cl
6j
1.00
1.00
0.98
1.00
0.97
1.02
1.01
3.01
5.27
4.00
1.05
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
5.5
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2.5
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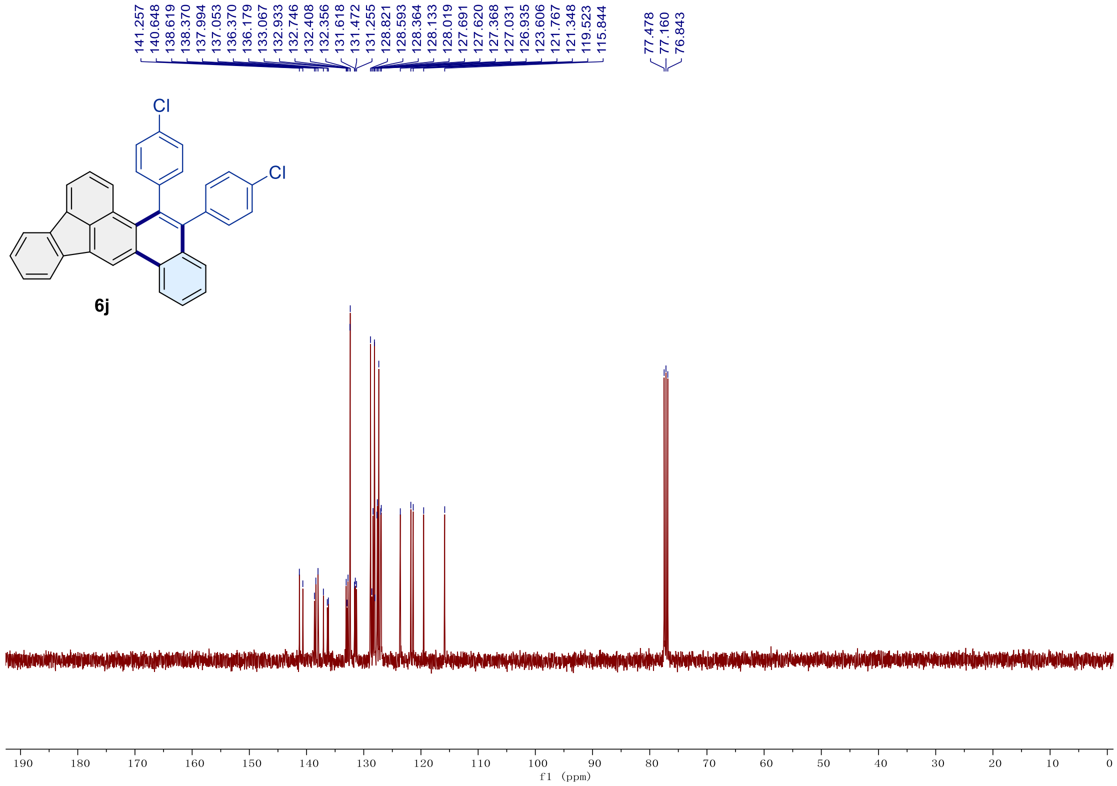
f1 (ppm)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132.356
131.618
131.472
131.255
128.821
128.593
128.364
128.133
128.019
127.691
127.620
127.368
127.031
126.935
123.606
121.767
121.348
119.523
115.844
77.478
77.160
76.843
Cl
Cl
6j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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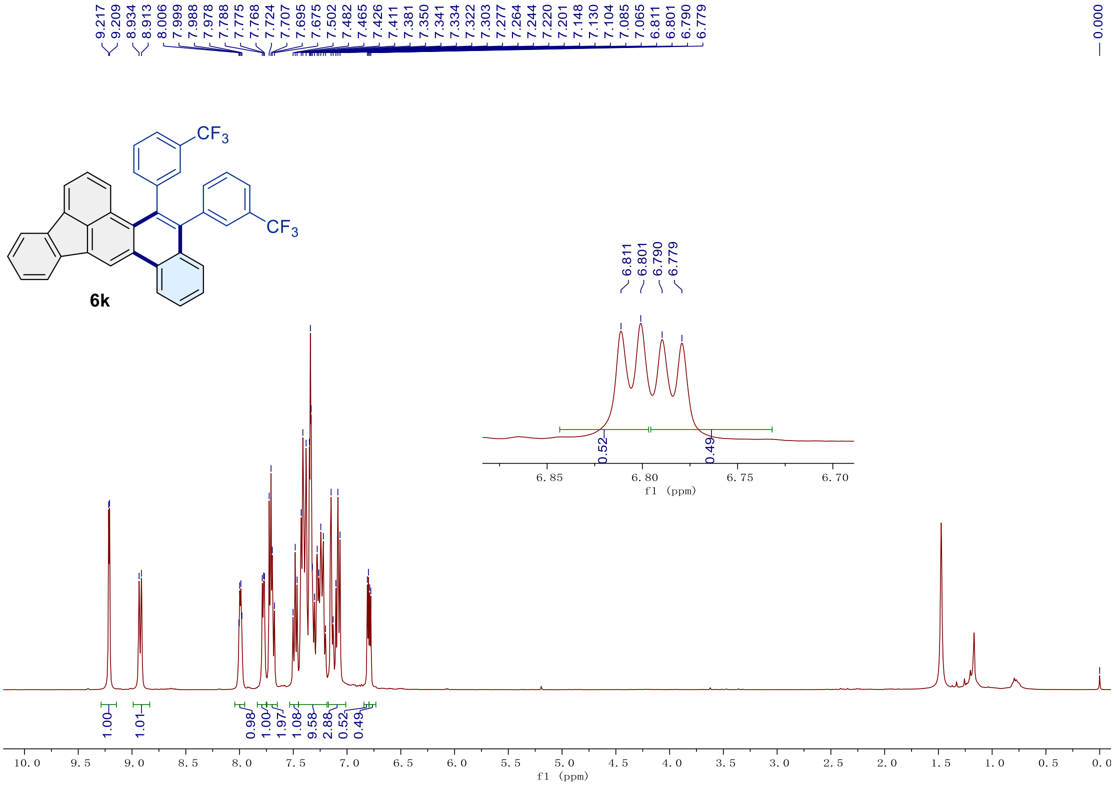
30
20
10
0
f1 (ppm)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7.724
7.707
7.695
7.675
7.502
7.482
7.465
7.426
7.411
7.381
7.350
7.341
7.334
7.322
7.303
7.277
7.264
7.244
7.220
7.201
7.148
7.130
7.104
7.085
7.065
6.811
6.801
6.790
6.779
0.000
CF3
CF3
6k
6.811
6.801
6.790
6.779
0.52
0.49
6.85
6.80
6.75
6.70
f1 (ppm)
1.00
1.01
0.98
1.00
1.97
1.08
9.58
2.88
0.52
0.49
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
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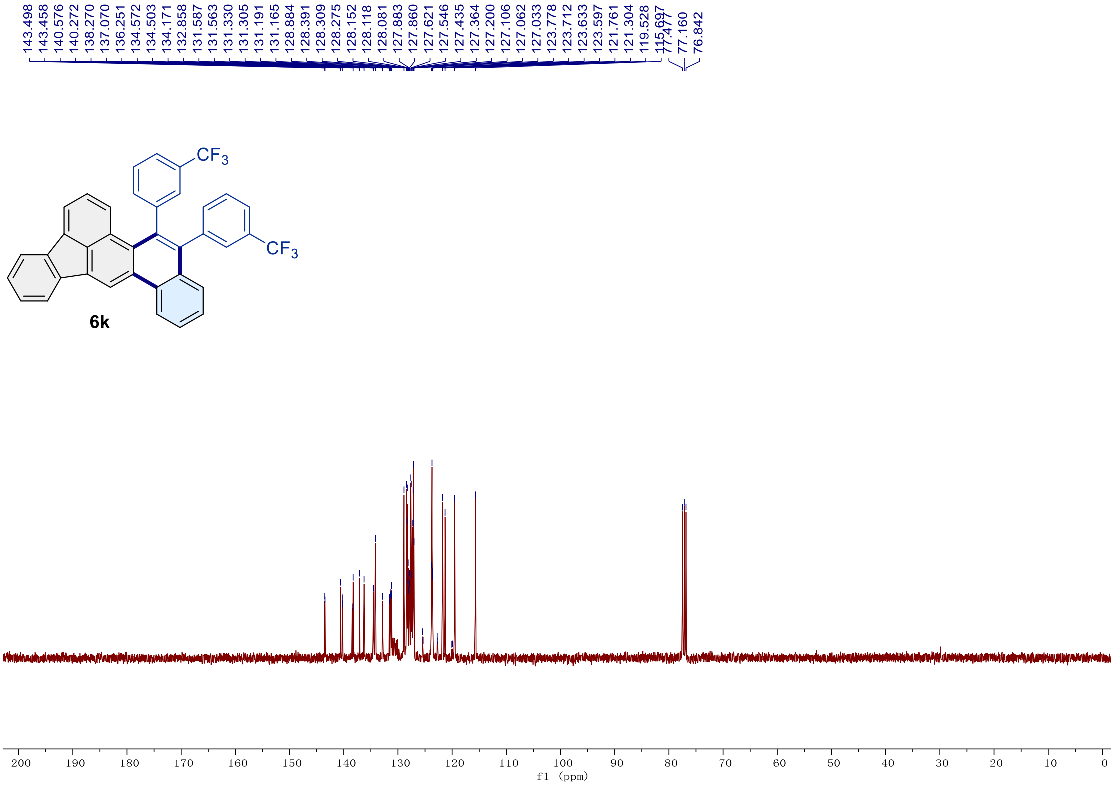
f1 (ppm)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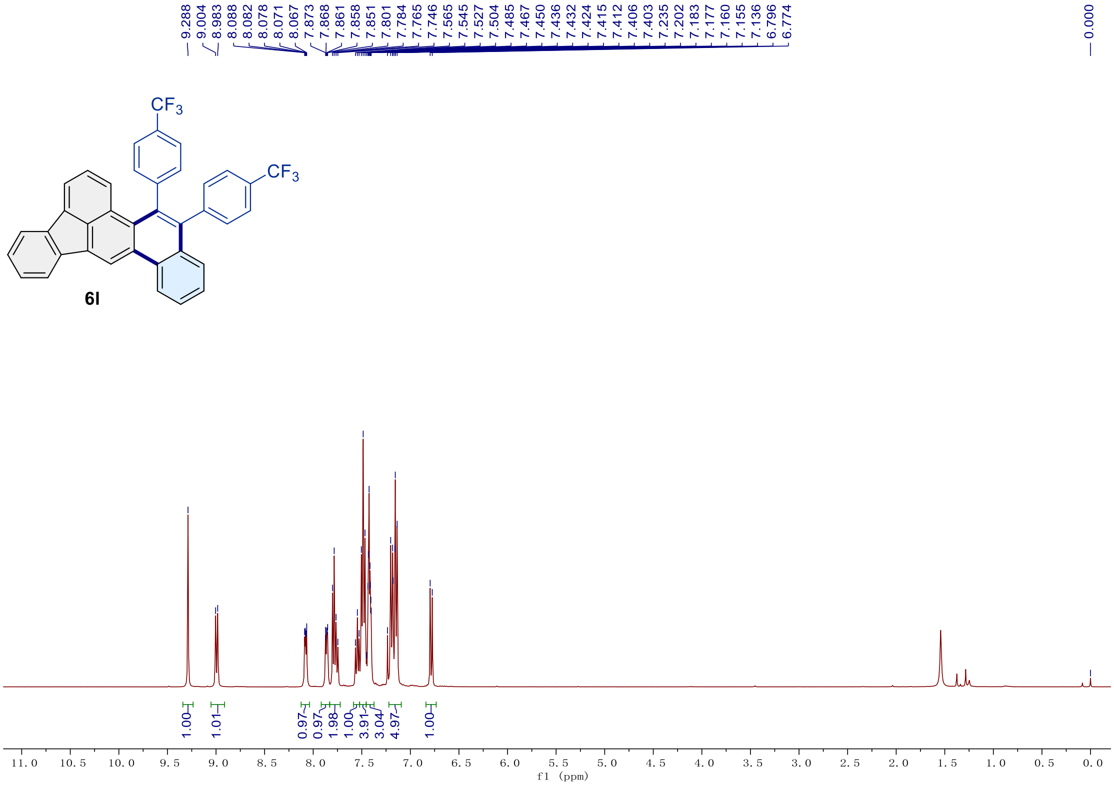
131.330
131.305
131.191
131.165
128.884
128.391
128.309
128.275
128.152
128.118
128.081
127.883
127.860
127.621
127.546
127.435
127.364
127.200
127.106
127.062
127.033
123.778
123.712
123.633
123.597
121.761
121.304
119.528
115.697
77.477
77.160
76.842
CF3
CF3
6k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.858
7.851
7.801
7.784
7.765
7.746
7.565
7.545
7.527
7.504
7.485
7.467
7.450
7.436
7.432
7.424
7.415
7.412
7.406
7.403
7.235
7.202
7.183
7.177
7.160
7.155
7.136
6.796
6.774
0.000
CF3
CF3
6l
1.00
1.01
0.97
0.97
1.98
1.00
3.91
3.04
4.97
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
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1.0
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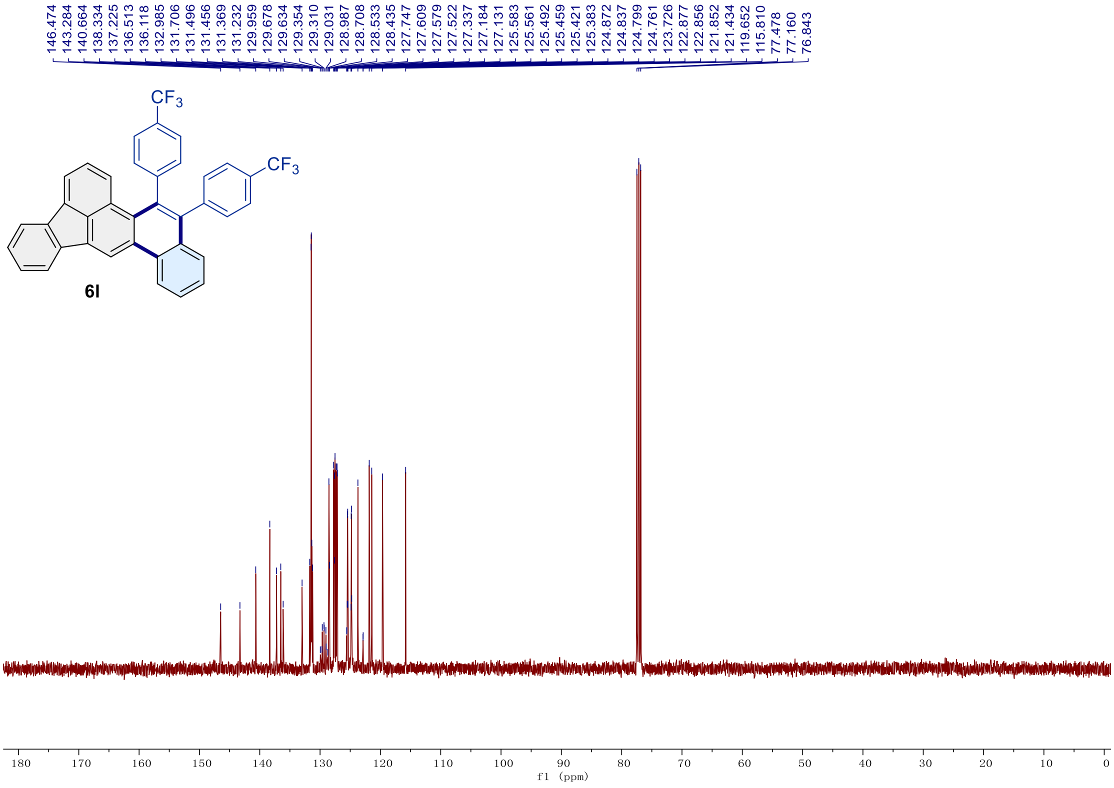
f1 (ppm)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131.369
131.232
129.959
129.678
129.634
129.354
129.310
129.031
128.987
128.708
128.533
128.435
127.747
127.609
127.579
127.522
127.337
127.184
127.131
125.583
125.561
125.492
125.459
125.421
125.383
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124.837
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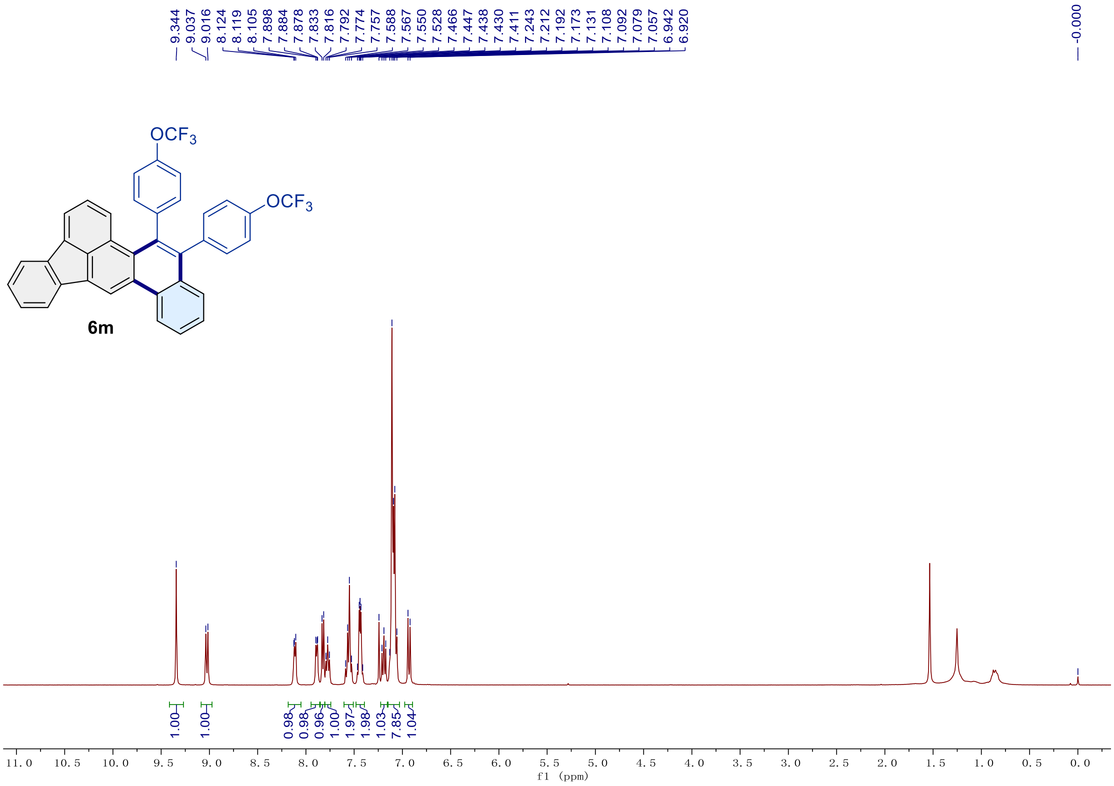
124.761
123.726
122.877
122.856
121.852
121.434
119.652
115.810
77.478
77.160
76.843
CF3
CF3
6l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.774
7.757
7.588
7.567
7.550
7.528
7.466
7.447
7.438
7.430
7.411
7.243
7.212
7.192
7.173
7.131
7.108
7.092
7.079
7.057
6.942
6.920
-0.000
OCF3
OCF3
1.00
1.00
0.98
0.98
0.96
1.00
1.97
1.98
1.03
7.85
1.04
11.0
10.5
10.0
9.5
9.0
8.5
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6.5
6.0
5.5
5.0
4.5
4.0
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2.0
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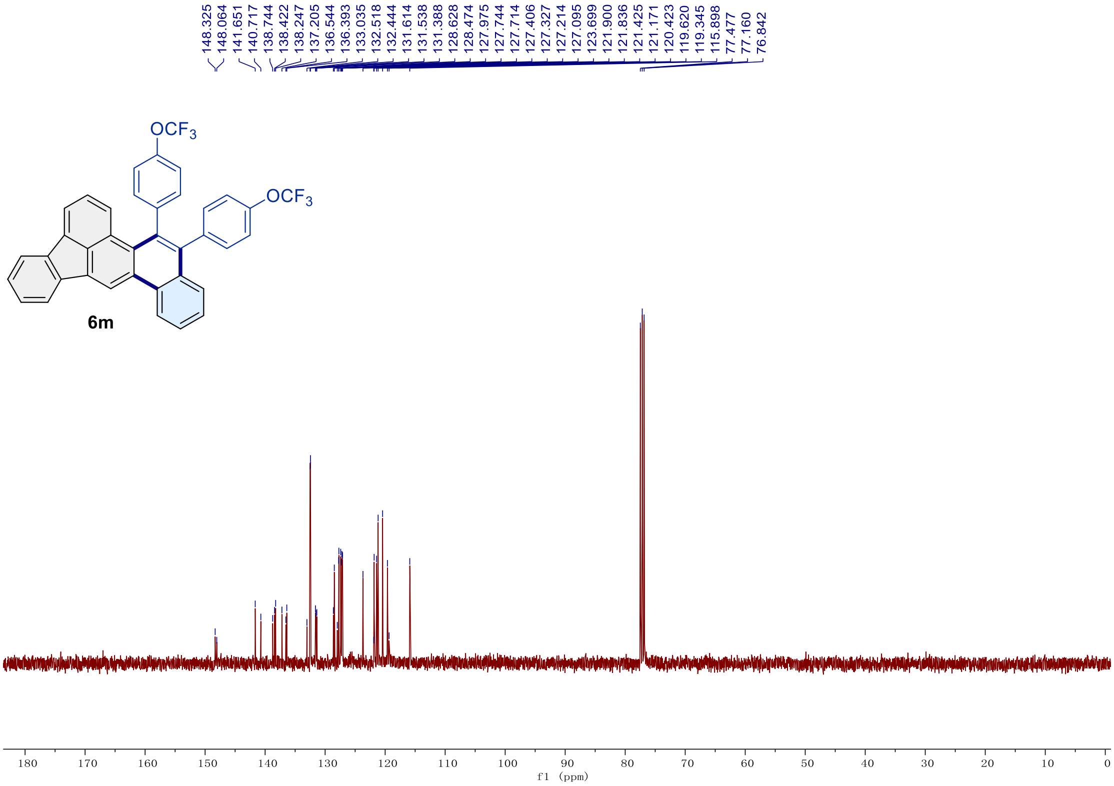
f1 (ppm)

6m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131.614
131.538
131.388
128.628
128.474
127.975
127.744
127.714
127.406
127.327
127.214
127.095
123.699
121.900
121.836
121.425
121.171
120.423
119.620
119.345
115.898
77.477
77.160
76.842
OCF3
OCF3
180
170
160
150
140
130
120
110
100
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70
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50
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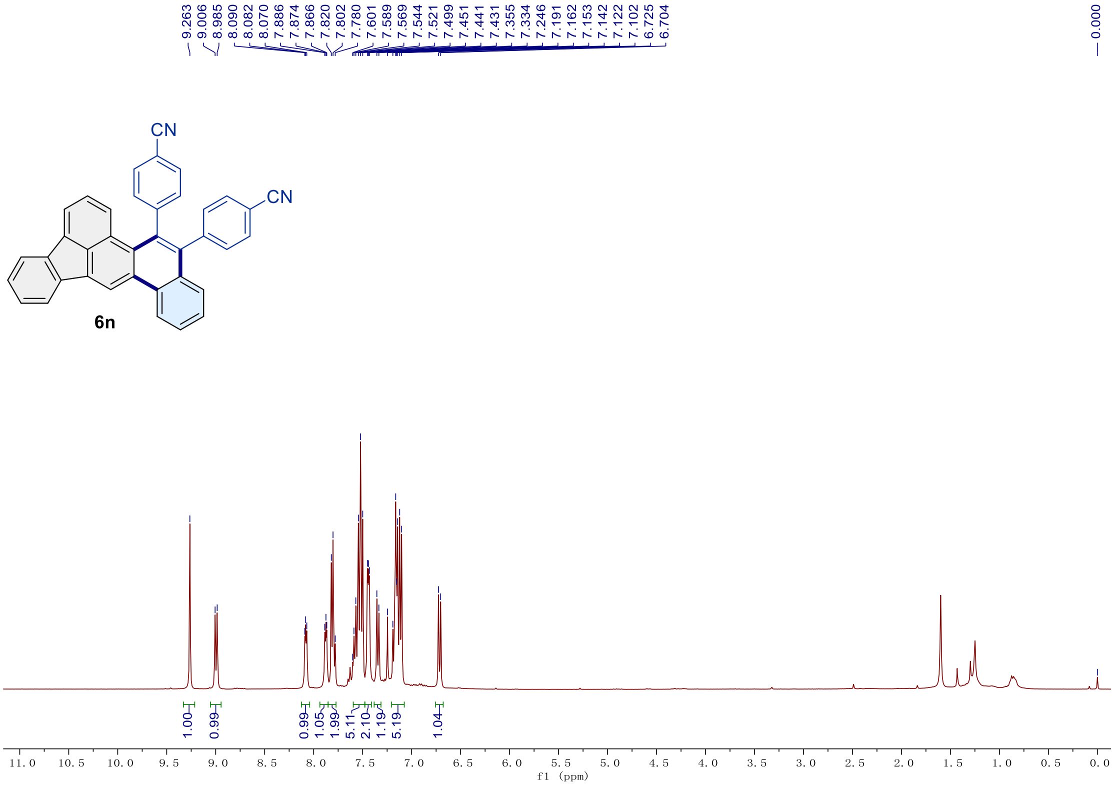
30
20
10
0
f1 (ppm)

6m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7.569
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7.441
7.431
7.355
7.334
7.246
7.191
7.162
7.153
7.142
7.122
7.102
6.725
6.704
0.000
CN
CN
6n
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0.99
1.05
1.99
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2.10
1.19
5.19
1.04
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10.0
9.5
9.0
8.5
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6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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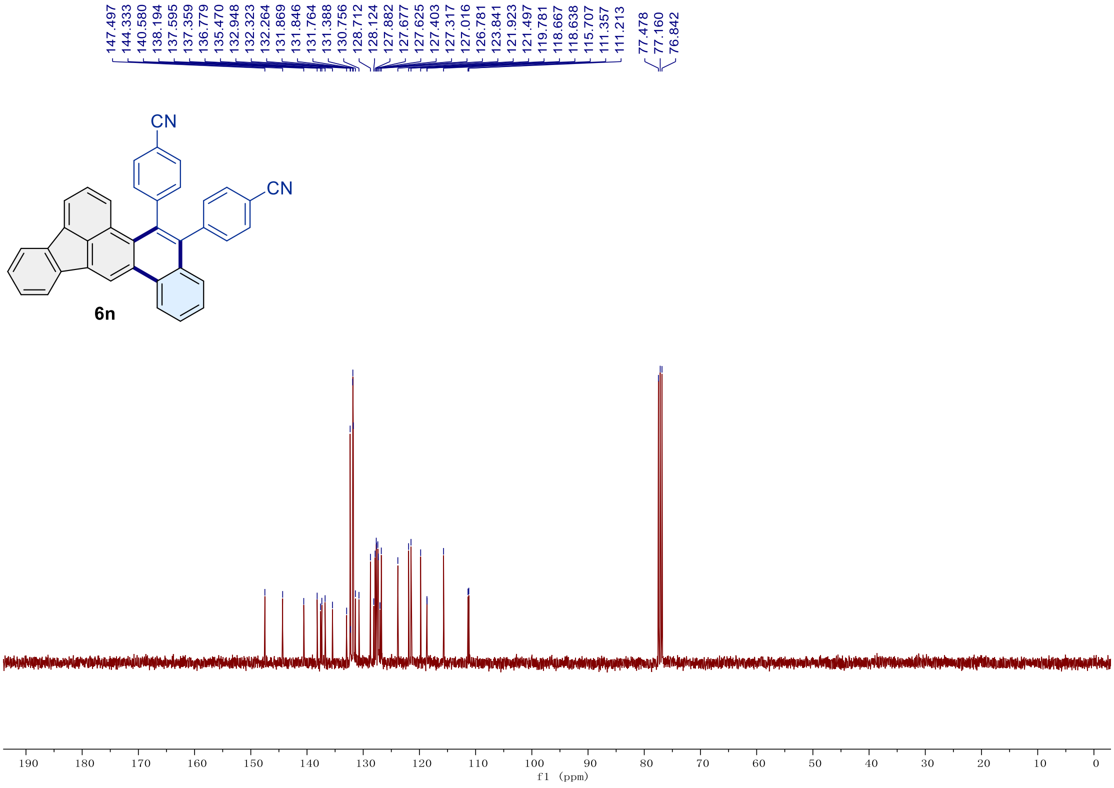
0.0
f1 (ppm)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131.764
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130.756
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128.124
127.882
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127.625
127.403
127.317
127.016
126.781
123.841
121.923
121.497
119.781
118.667
118.638
115.707
111.357
111.213
77.478
77.160
76.842
CN
CN
6n
190
180
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110
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10
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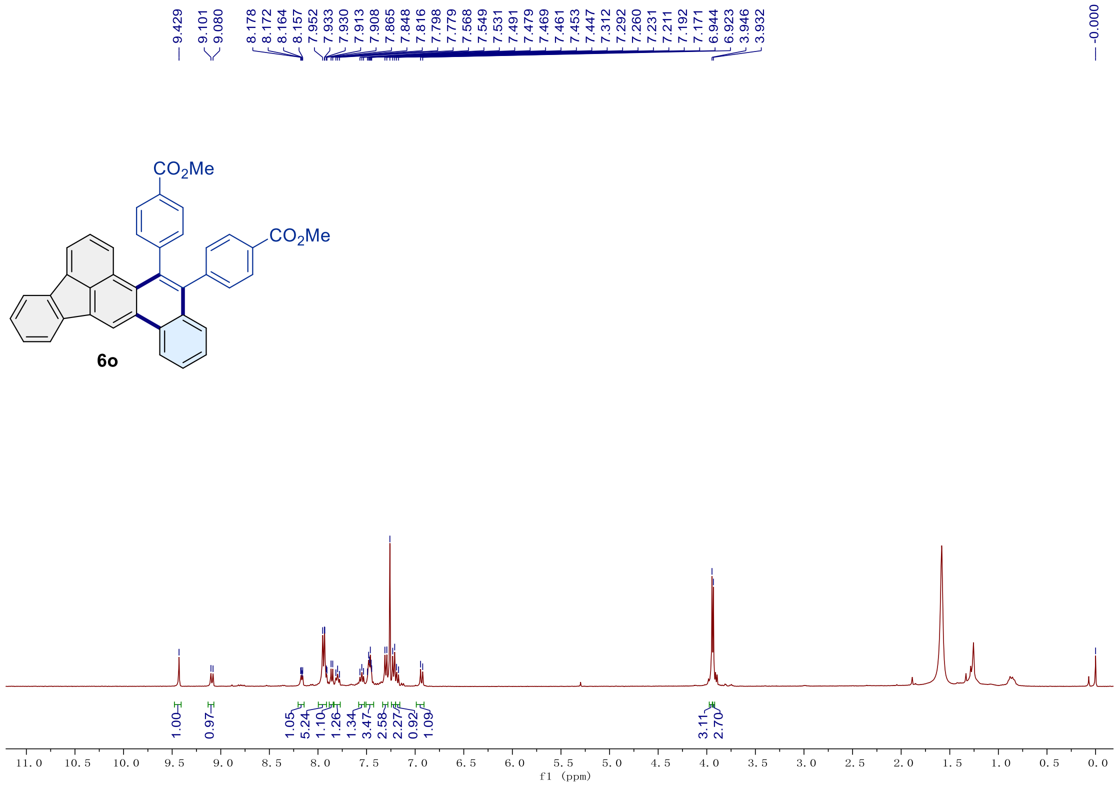
f1 (ppm)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7.865
7.848
7.816
7.798
7.779
7.568
7.549
7.531
7.491
7.479
7.469
7.461
7.453
7.447
7.312
7.292
7.260
7.231
7.211
7.192
7.171
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6.923
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3.932
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CO2Me
CO2Me
6o
1.00
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1.05
5.24
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1.26
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9.0
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7.0
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6.0
5.5
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2.5
2.0
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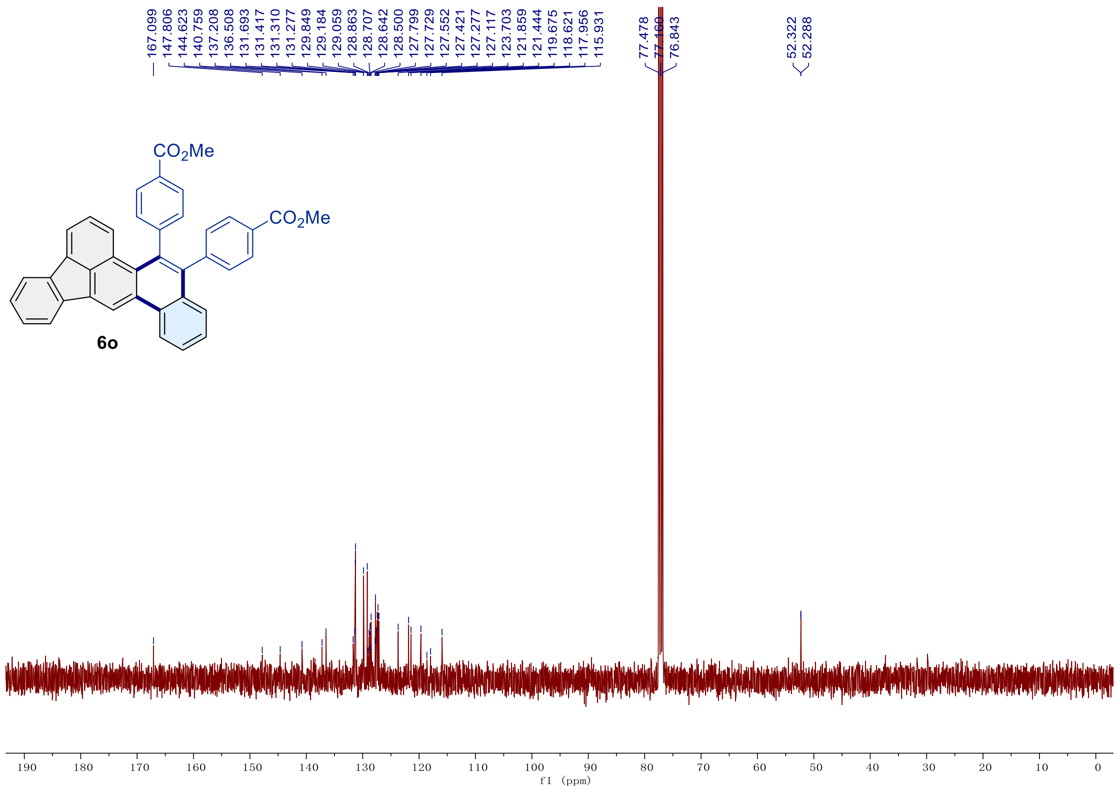
1.0
0.5
0.0
f1 (ppm)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128.863
128.707
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128.500
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123.703
121.859
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117.956
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77.478
77.160
76.843
52.322
52.288
CO2Me
CO2Me
6o
190
180
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110
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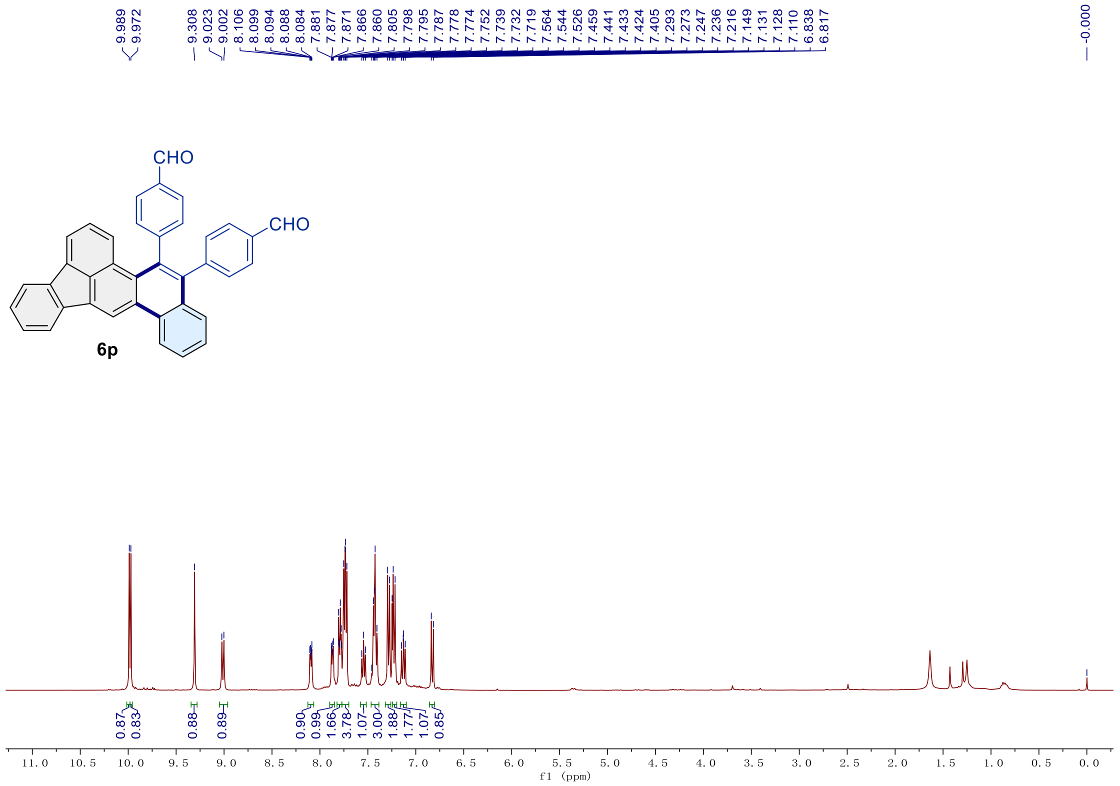
f1 (ppm)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CHO
CHO
6p
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1.77
1.07
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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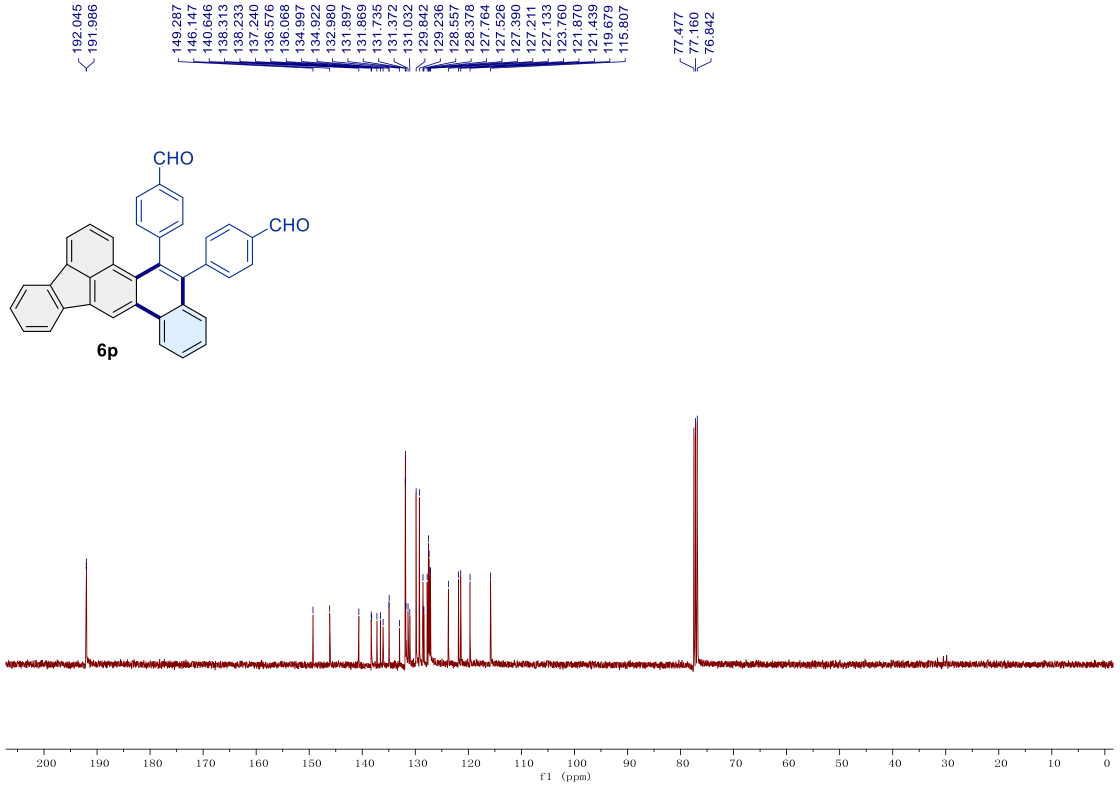
1.0
0.5
0.0
f1 (ppm)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132.980
131.897
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127.526
127.390
127.211
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123.760
121.870
121.439
119.679
115.807
77.477
77.160
76.842
CHO
CHO
6p
200
190
180
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50
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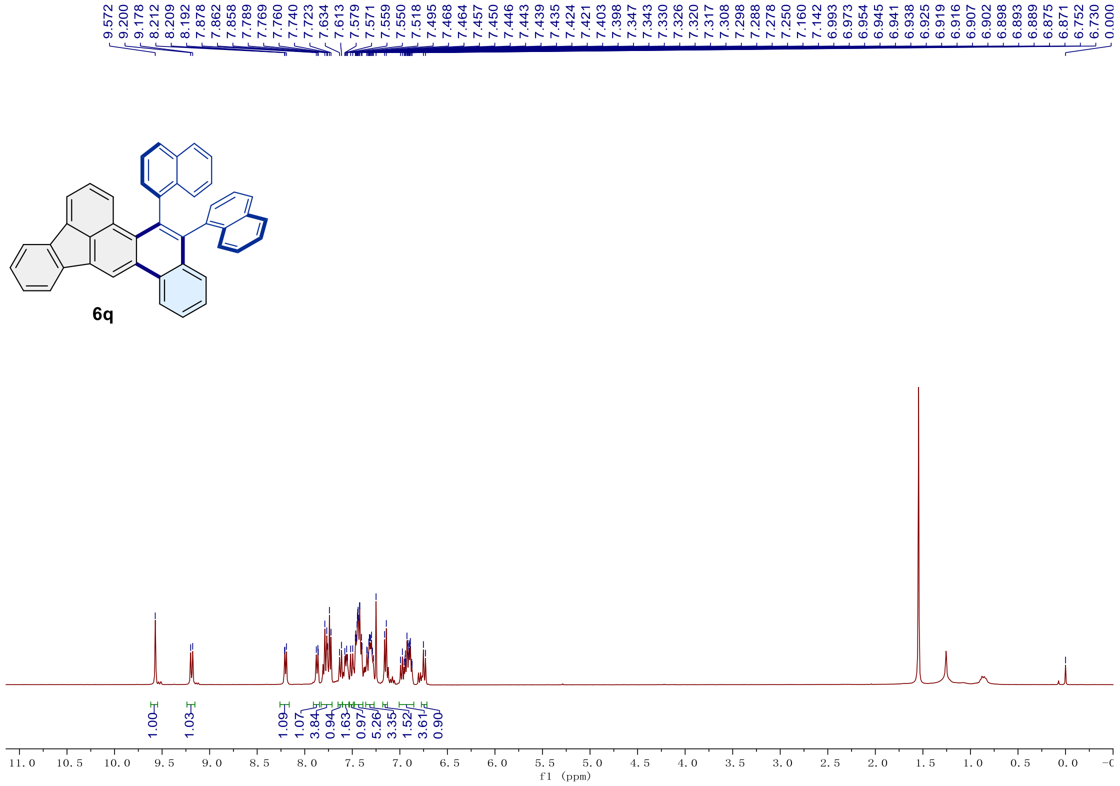
f1 (ppm)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7.740
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10.0
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5.0
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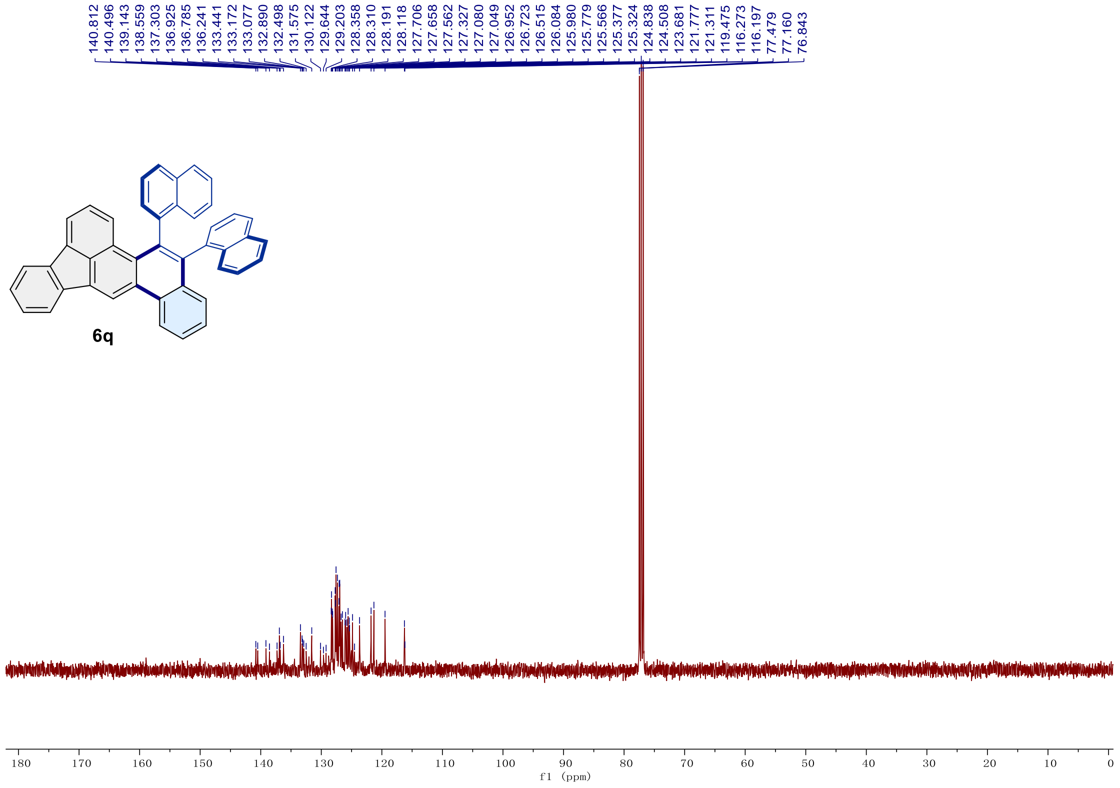
f1 (ppm)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123.681
121.777
121.311
119.475
116.273
116.197
77.479
77.160
76.843
6q
180
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140
130
120
110
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90
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50
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30
20
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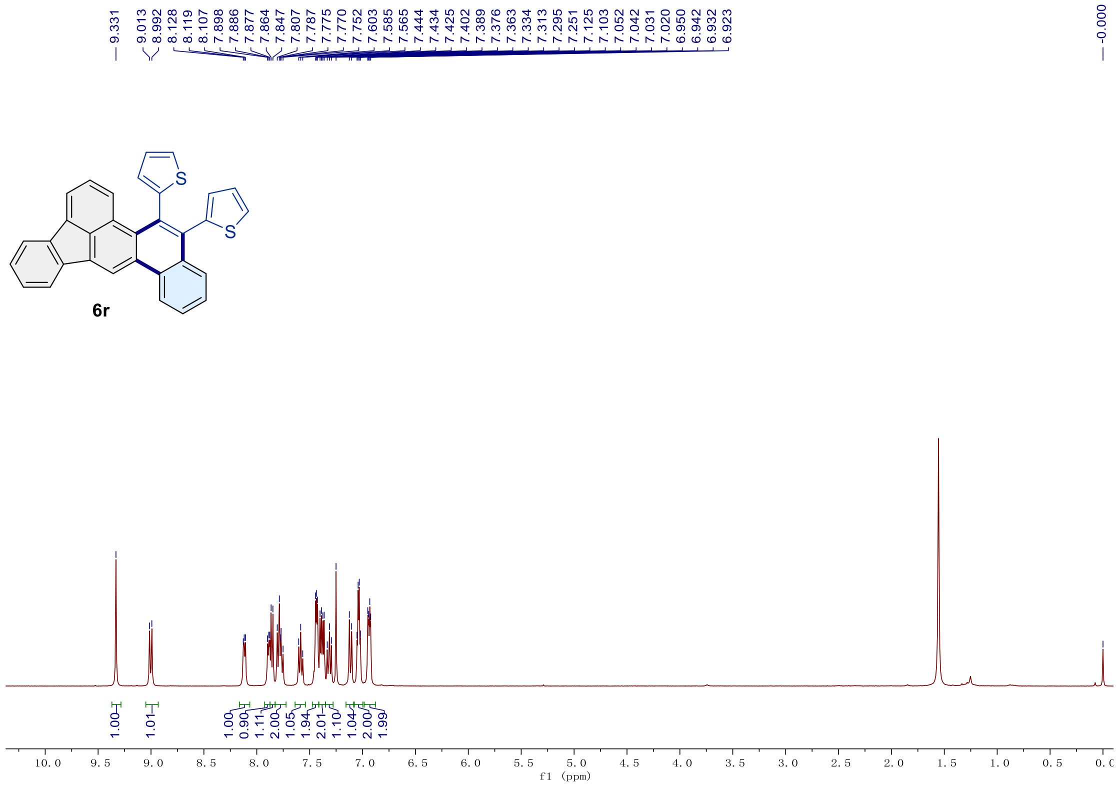
f1 (ppm)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7.898
7.886
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7.847
7.807
7.787
7.775
7.770
7.752
7.603
7.585
7.565
7.444
7.434
7.425
7.402
7.389
7.376
7.363
7.334
7.313
7.295
7.251
7.125
7.103
7.052
7.042
7.031
7.020
6.950
6.942
6.932
6.923
-0.000
S
S
1.00
1.01
1.00
0.90
1.11
2.00
1.05
1.94
2.01
1.10
1.04
2.00
1.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
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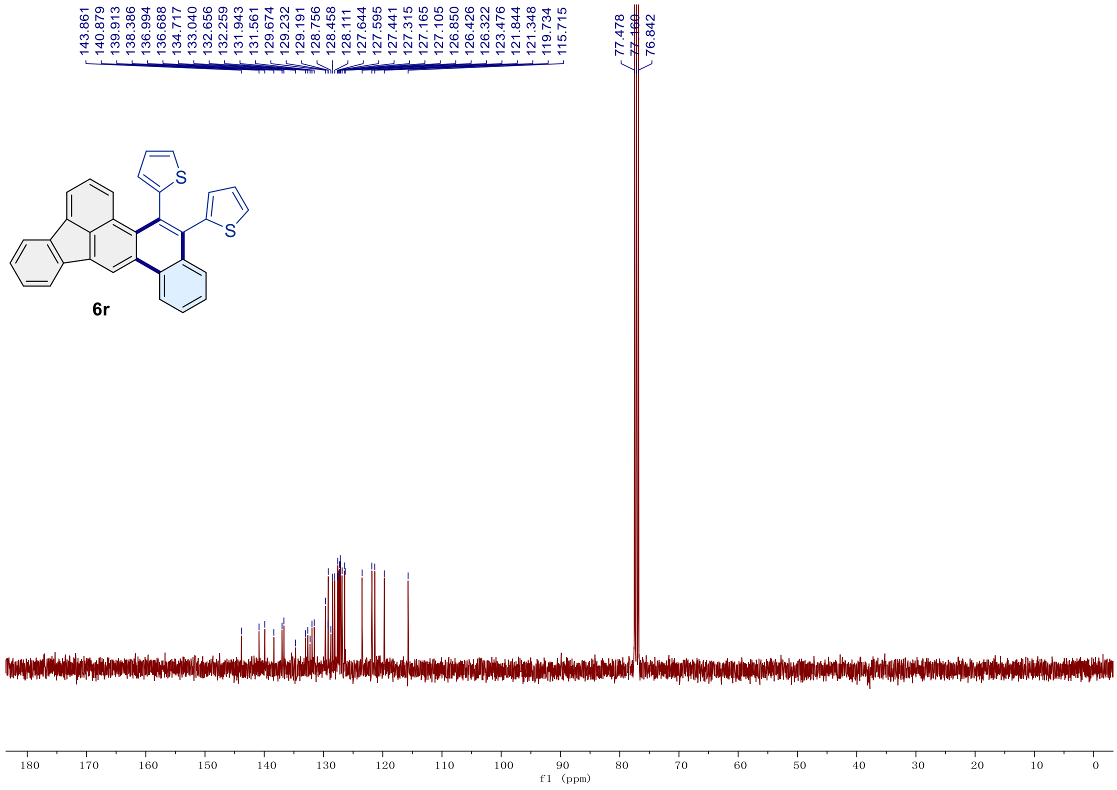
0.0
f1 (ppm)

6r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136.688
134.717
133.040
132.656
132.259
131.943
131.561
129.674
129.232
129.191
128.756
128.458
128.111
127.644
127.595
127.441
127.315
127.165
127.105
126.850
126.426
126.322
123.476
121.844
121.348
119.734
115.715
77.478
77.160
76.842
S
S
180
170
160
150
140
130
120
110
100
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80
70
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50
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30
20
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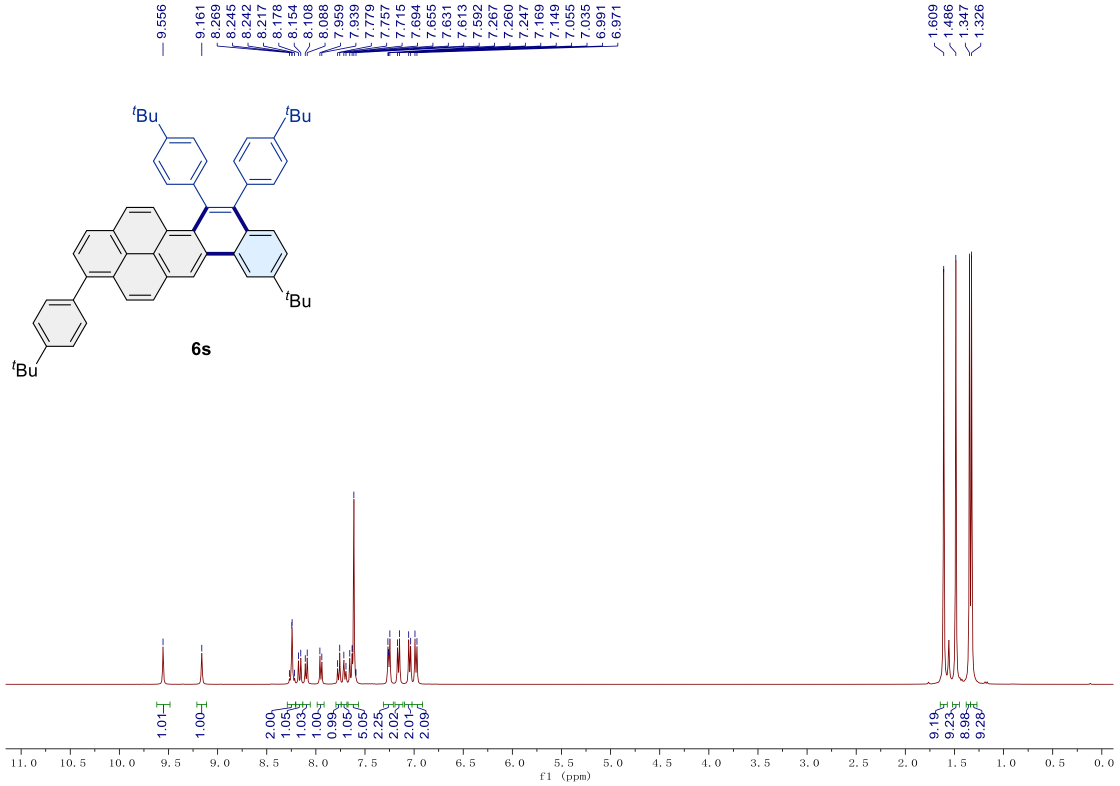
0
f1 (ppm)

6r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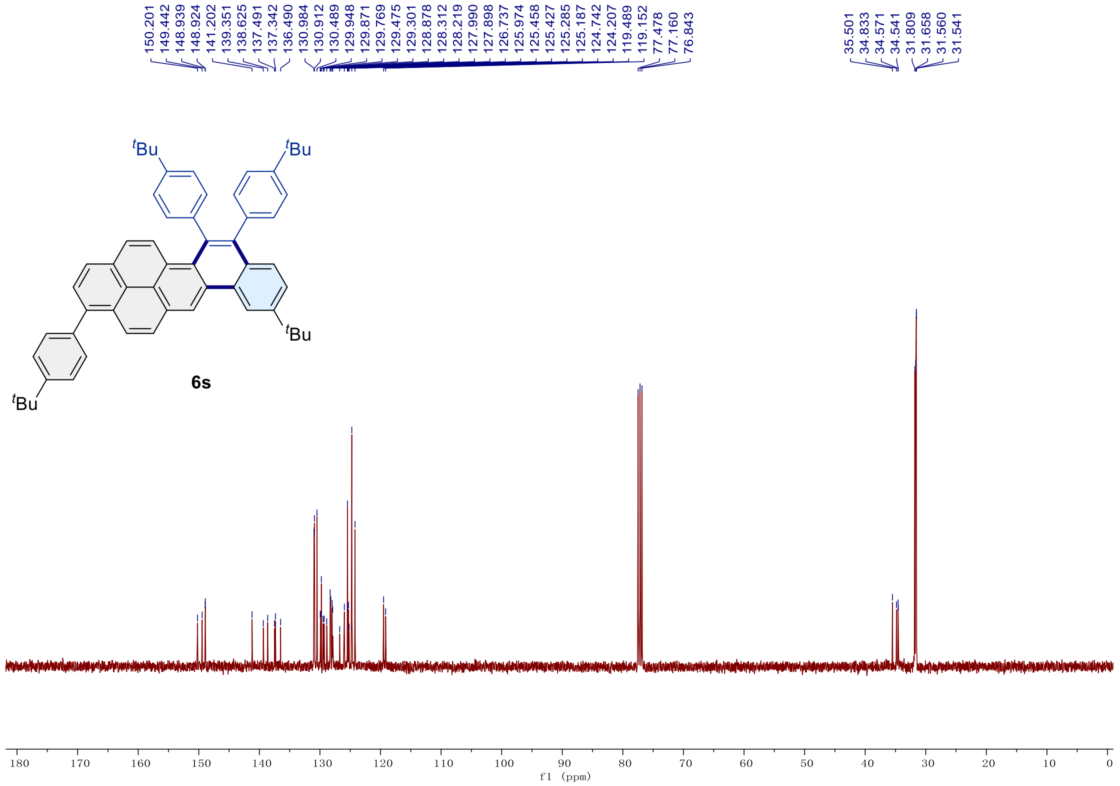
8.217
8.178
8.154
8.108
8.088
7.959
7.939
7.779
7.757
7.715
7.694
7.655
7.631
7.613
7.592
7.267
7.260
7.247
7.169
7.149
7.055
7.035
6.991
6.971
1.609
1.486
1.347
1.326
tBu
tBu
tBu
tBu
6s
1.01
1.00
2.00
1.05
1.03
1.00
0.99
1.05
5.05
2.25
2.02
2.01
2.09
9.19
9.23
8.98
9.28
11.0
10.5
10.0
9.5
9.0
8.5
8.0
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)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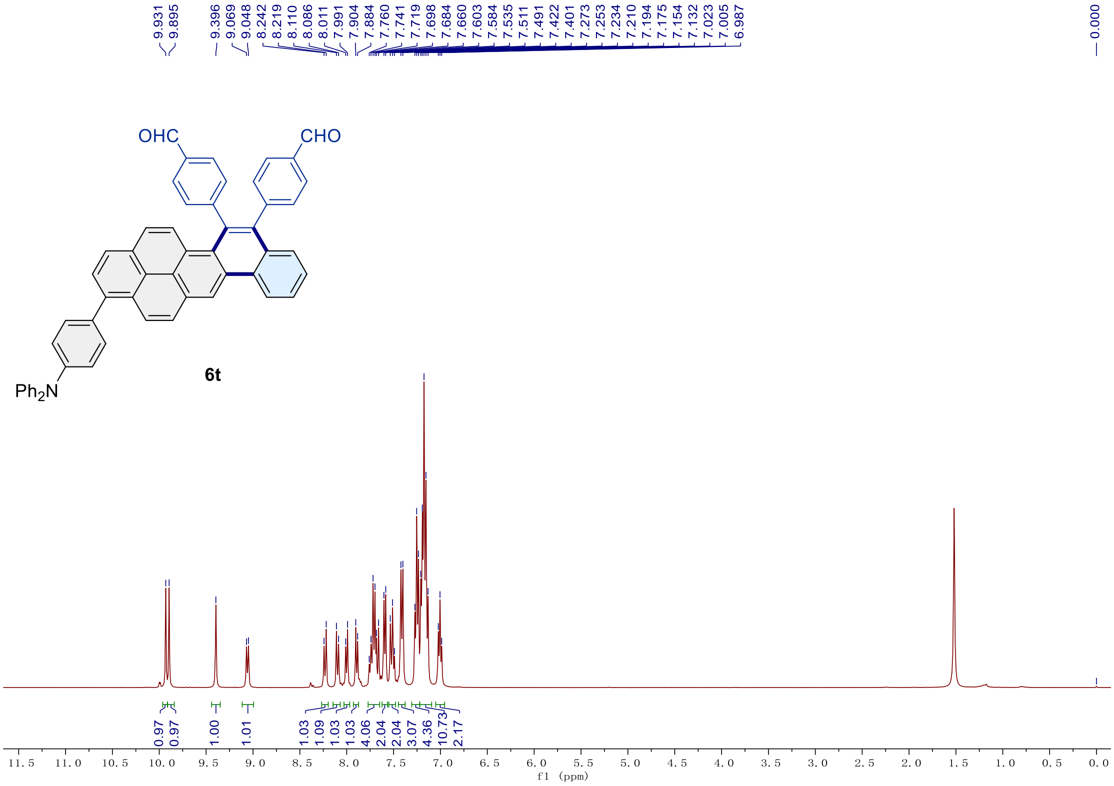
149.442
148.939
148.924
141.202
139.351
138.625
137.491
137.342
136.490
130.984
130.912
130.489
129.948
129.871
129.769
129.475
129.301
128.878
128.312
128.219
127.990
127.898
126.737
125.974
125.458
125.427
125.285
125.187
124.742
124.207
119.489
119.152
77.478
77.160
76.843
35.501
34.833
34.571
34.541
31.809
31.658
31.560
31.541
tBu
tBu
tBu
tBu
6s
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.895
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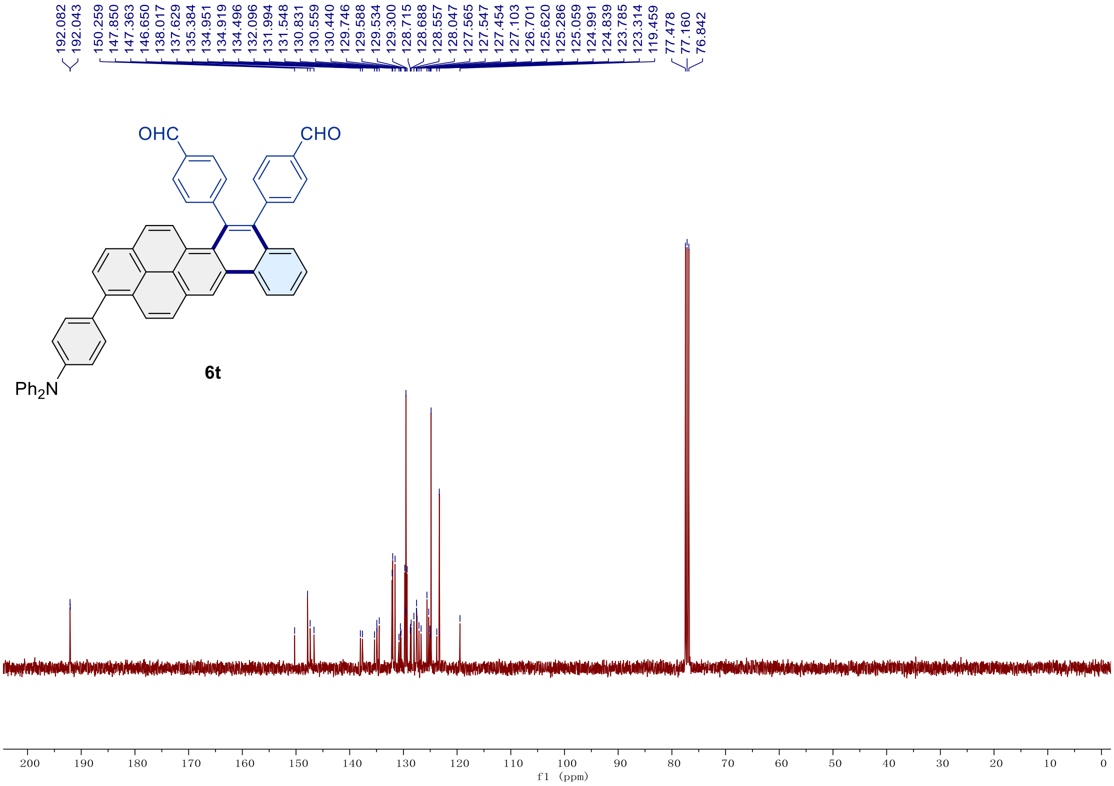
8.242
8.219
8.110
8.086
8.011
7.991
7.904
7.884
7.760
7.741
7.719
7.698
7.684
7.660
7.603
7.584
7.535
7.511
7.491
7.422
7.401
7.273
7.253
7.234
7.210
7.194
7.175
7.154
7.132
7.023
7.005
6.987
0.000
OHC
CHO
Ph$_2$N
6t
0.97
0.97
1.00
1.01
1.03
1.09
1.03
1.03
4.06
2.04
2.04
3.07
4.36
10.73
2.17
11.5 11.0 10.5 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)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138.017
137.629
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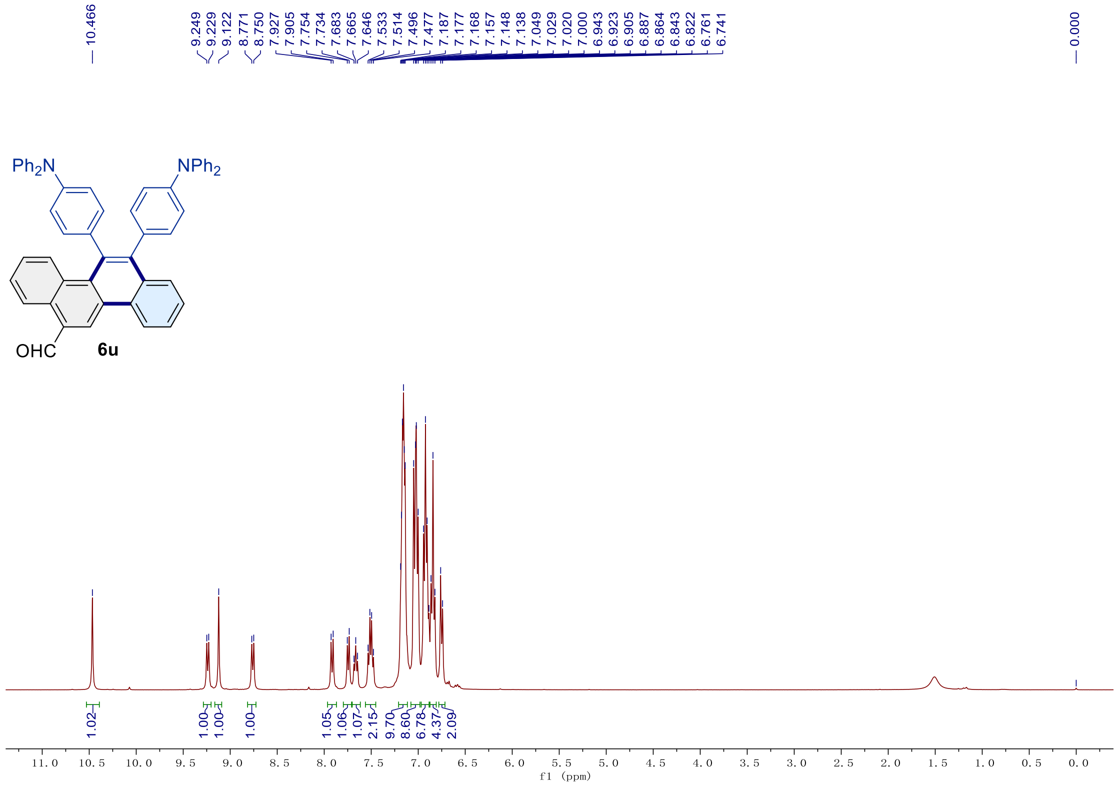
134.951
134.919
134.496
132.096
131.994
131.548
130.831
130.559
130.440
129.746
129.588
129.534
129.300
128.715
128.688
128.557
128.047
127.565
127.547
127.454
127.103
126.701
125.620
125.286
125.059
124.991
124.839
123.785
123.314
119.459
77.478
77.160
76.842
OHC
CHO
Ph$_2$N
6t
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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9.229
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8.771
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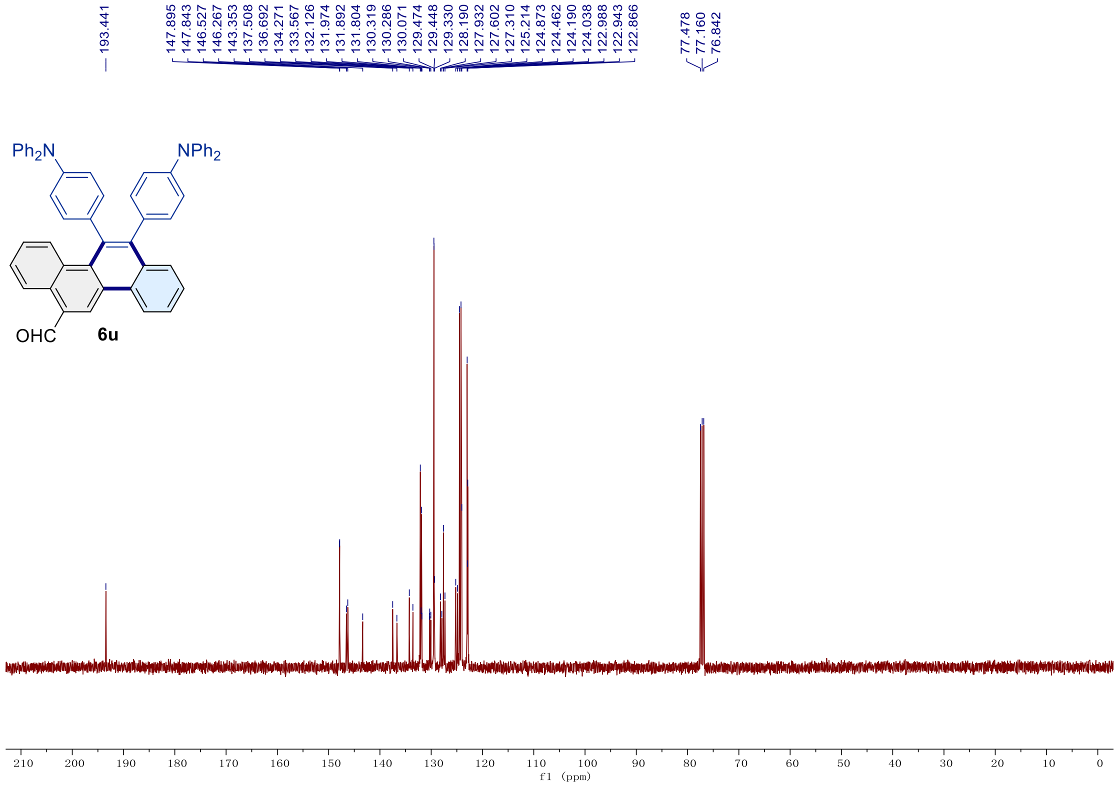
7.905
7.754
7.734
7.683
7.665
7.646
7.533
7.514
7.496
7.477
7.187
7.177
7.168
7.157
7.148
7.138
7.049
7.029
7.020
7.000
6.943
6.923
6.905
6.887
6.864
6.843
6.822
6.761
6.741
0.000
Ph2N
NPh2
OHC
6u
1.02
1.00
1.00
1.00
1.05
1.06
1.07
2.15
9.70
8.60
6.78
4.37
2.09
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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)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147.843
146.527
146.267
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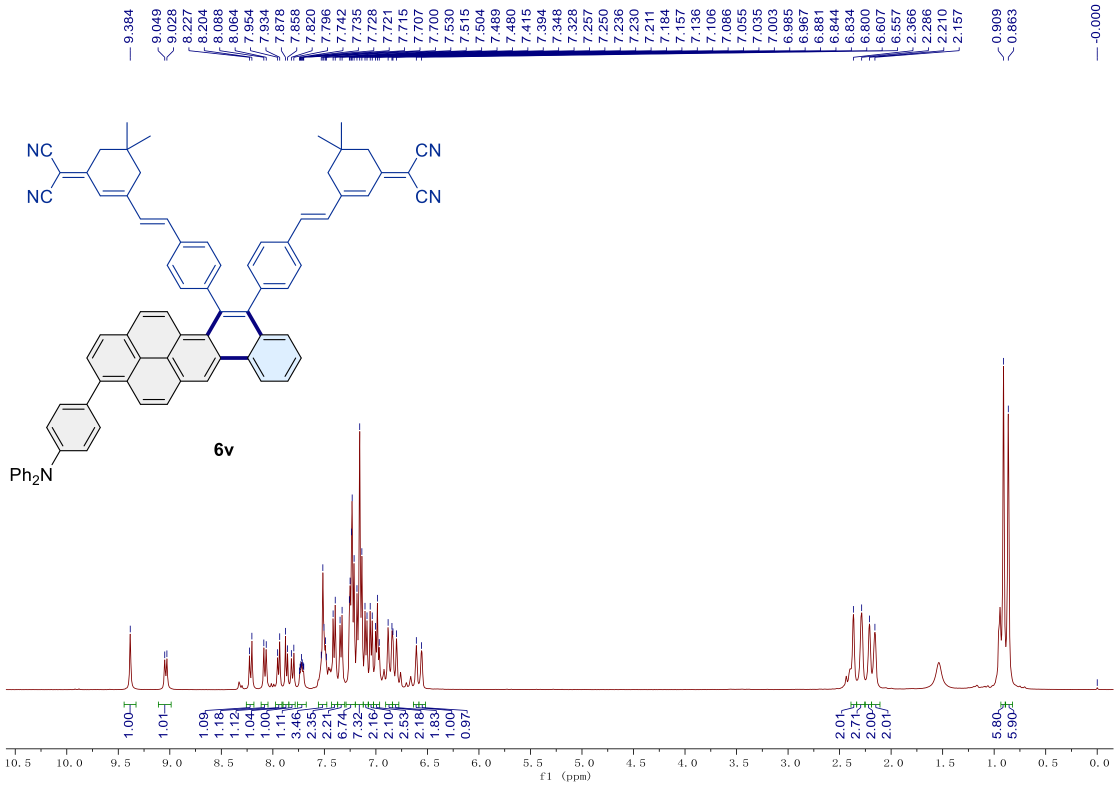
136.692
134.271
133.567
132.126
131.974
131.892
131.804
130.319
130.286
130.071
129.474
129.448
129.330
128.190
127.932
127.602
127.310
125.214
124.873
124.462
124.190
124.038
122.988
122.943
122.866
77.478
77.160
76.842
Ph2N
NPh2
OHC
6u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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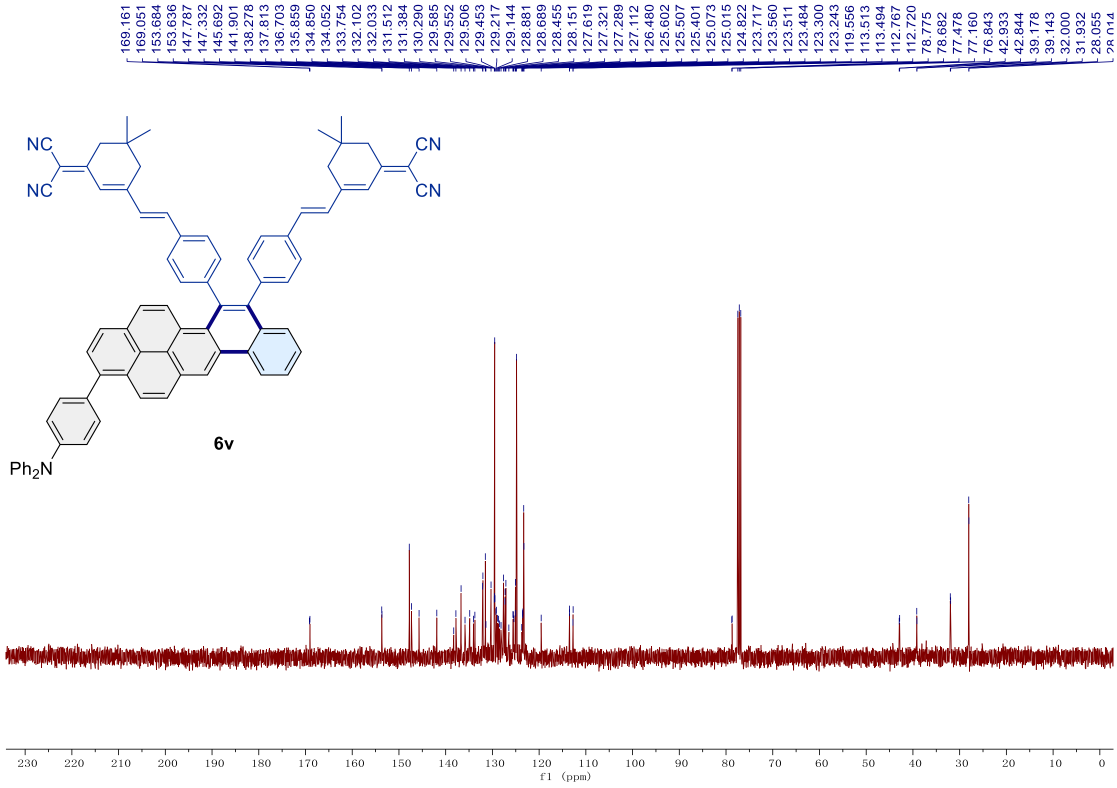
8.204
8.088
8.064
7.954
7.934
7.878
7.858
7.820
7.796
7.742
7.735
7.728
7.721
7.715
7.707
7.700
7.530
7.515
7.504
7.489
7.480
7.415
7.394
7.348
7.328
7.257
7.250
7.236
7.230
7.211
7.184
7.157
7.136
7.106
7.086
7.055
7.035
7.003
6.985
6.967
6.881
6.844
6.834
6.800
6.607
6.557
2.366
2.286
2.210
2.157
0.909
0.863
-0.000
NC
NC
CN
CN
Ph$_2$N
1.00
1.01
1.09
1.18
1.12
1.04
1.00
1.11
3.46
2.35
2.21
6.74
7.32
2.16
2.10
2.53
2.18
1.83
1.00
0.97
2.01
2.71
2.00
2.01
5.80
5.90
10.5
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)

6v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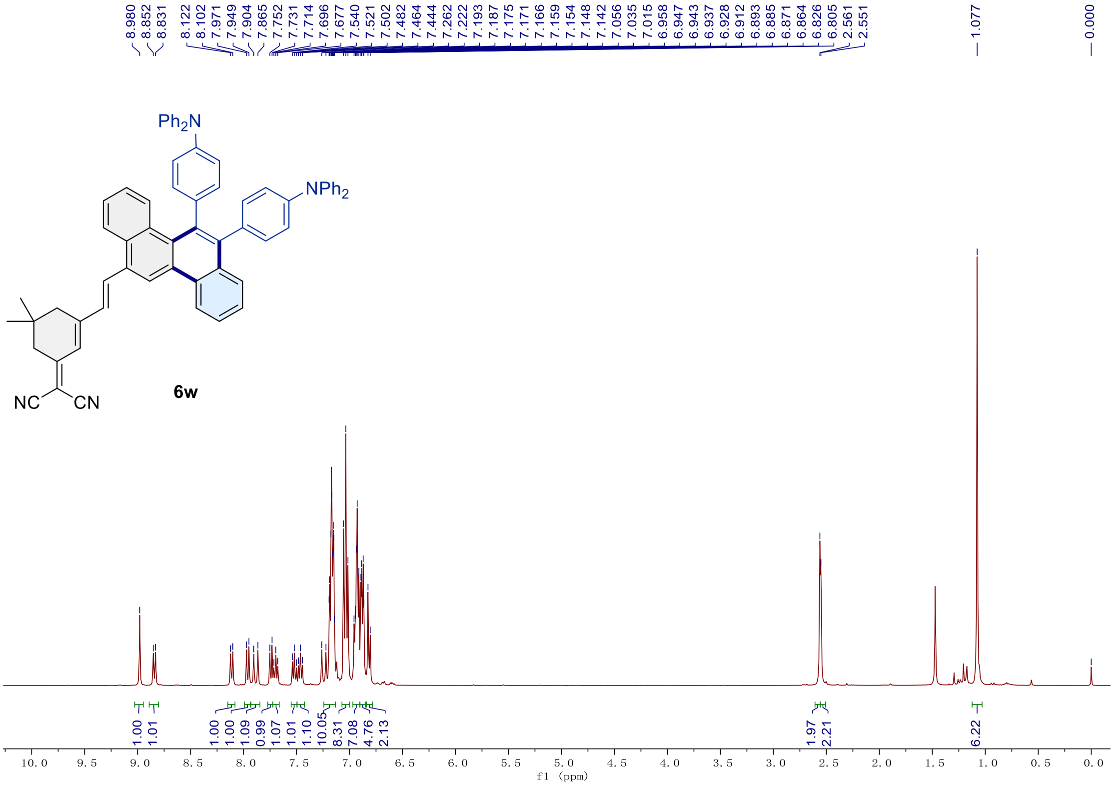
141.901
138.278
137.813
136.703
135.859
134.850
134.052
133.754
132.102
132.033
131.512
131.384
130.290
129.585
129.552
129.506
129.453
129.217
129.144
128.881
128.689
128.455
128.151
127.619
127.321
127.289
127.112
126.480
125.602
125.507
125.401
125.073
125.015
124.822
123.717
123.560
123.511
123.484
123.300
123.243
119.556
113.513
113.494
112.767
112.720
78.775
78.682
77.478
77.160
76.843
42.933
42.844
39.178
39.143
32.000
31.932
28.055
28.014
NC
NC
CN
CN
Ph$_2$N
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

6v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7.904
7.865
7.752
7.731
7.714
7.696
7.677
7.540
7.521
7.502
7.482
7.464
7.444
7.262
7.222
7.193
7.187
7.175
7.171
7.166
7.159
7.154
7.148
7.142
7.056
7.035
7.015
6.958
6.947
6.943
6.937
6.928
6.912
6.893
6.885
6.871
6.864
6.826
6.805
2.561
2.551
1.077
0.000
Ph2N
NPh2
NC
CN
6w
1.00
1.01
1.00
1.00
1.09
0.99
1.07
1.01
1.10
10.05
8.31
7.08
4.76
2.13
1.97
2.21
6.22
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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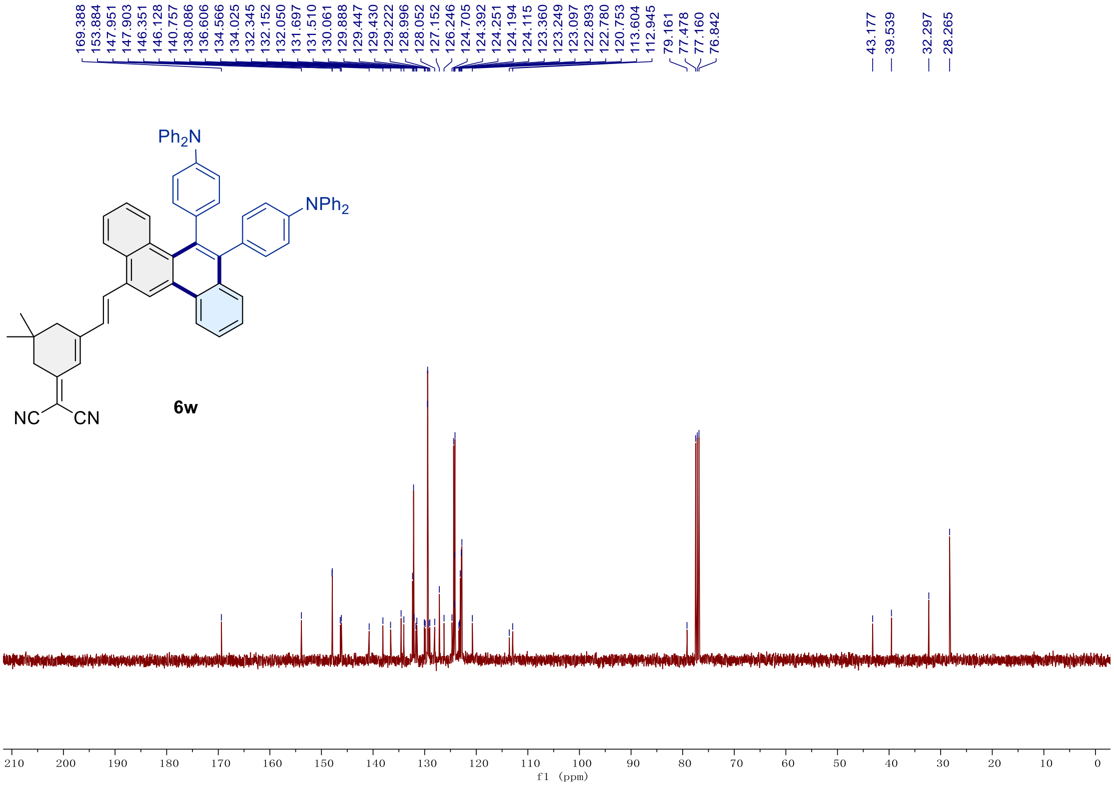
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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138.086
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134.566
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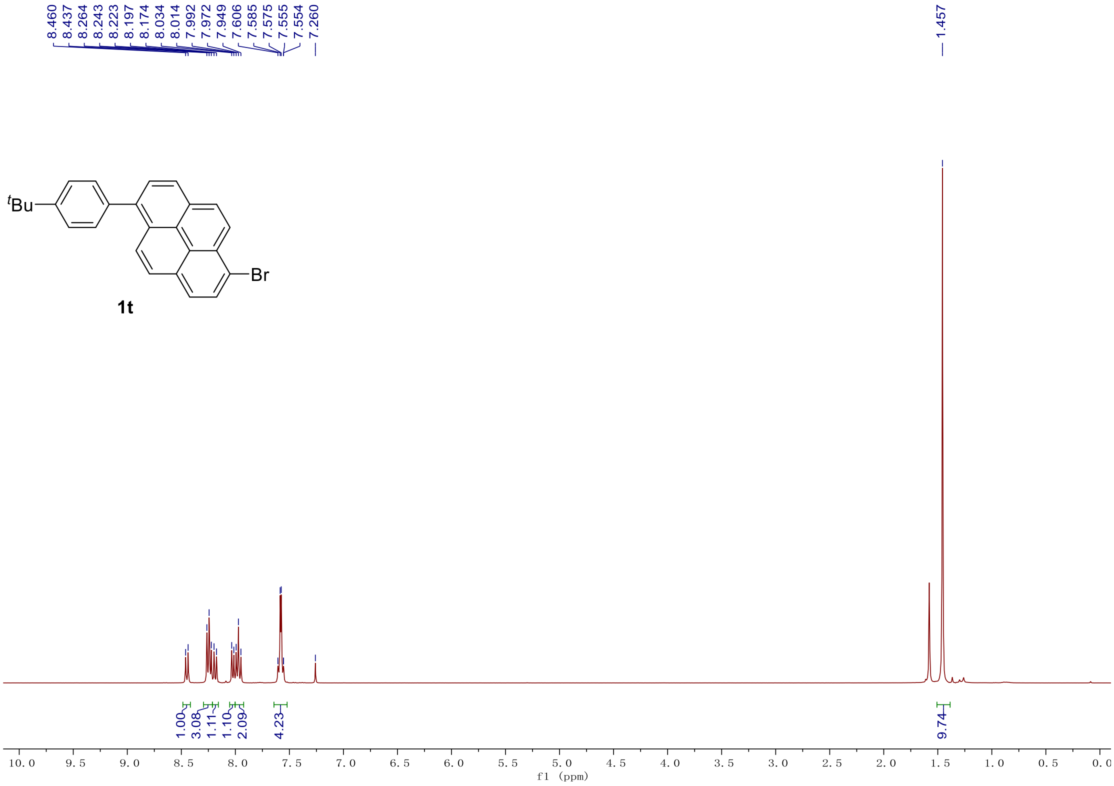
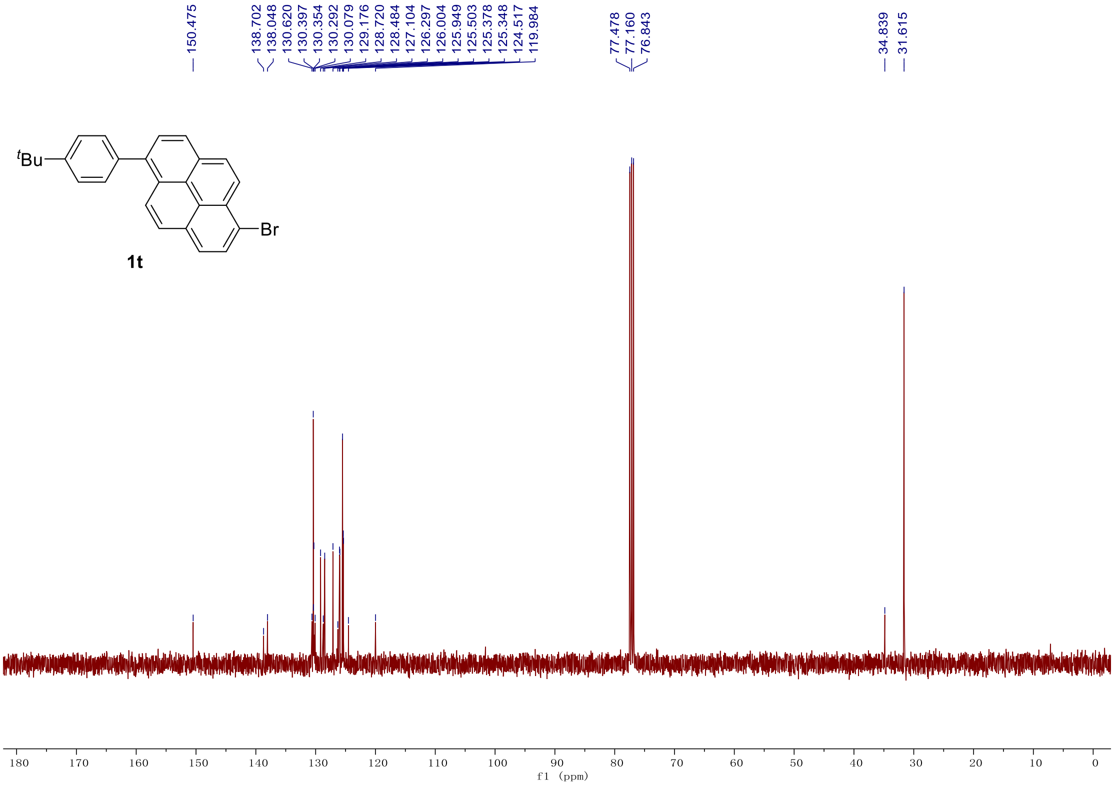
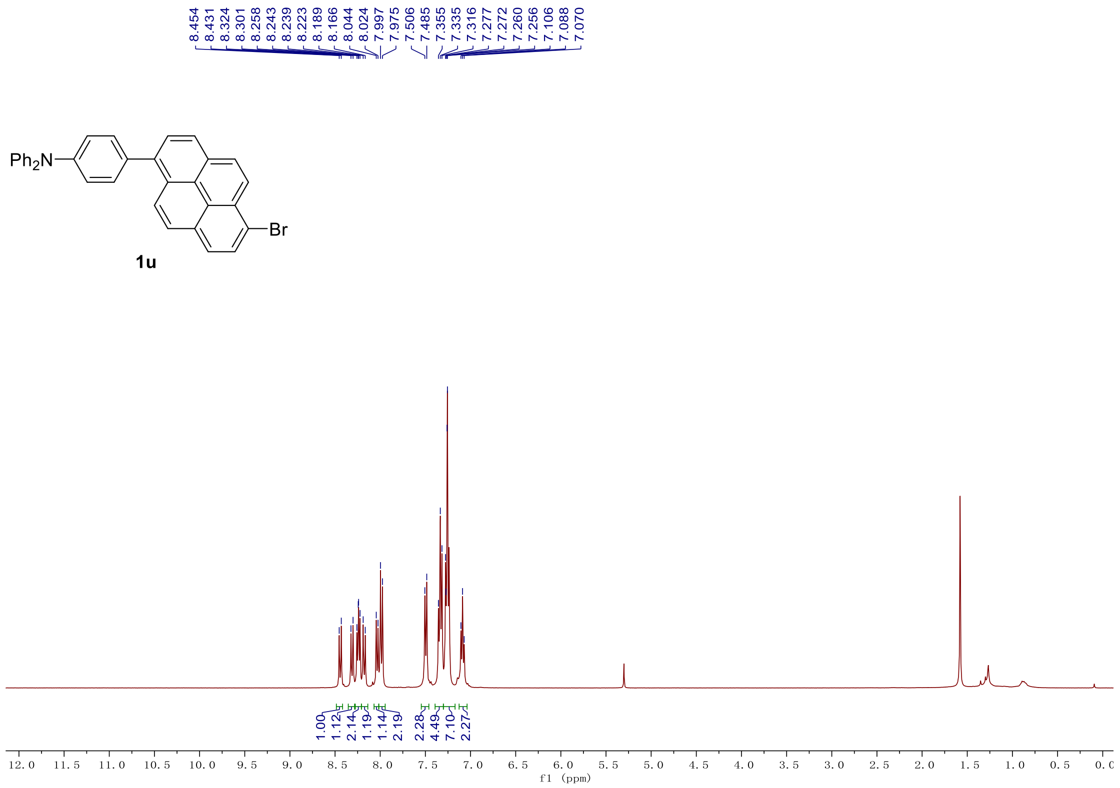
132.345
132.152
132.050
131.697
131.510
130.061
129.888
129.447
129.430
129.222
128.996
128.052
127.152
126.246
124.705
124.392
124.251
124.194
124.115
123.360
123.249
123.097
122.893
122.780
120.753
113.604
112.945
79.161
77.478
77.160
76.842
43.177
39.539
32.297
28.265
Ph2N
NPh2
NC
CN
6w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

NMR spectrum of substrates 1t – u:



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8.301
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8.243
8.239
8.223
8.189
8.166
8.044
8.024
7.997
7.975
7.506
7.485
7.355
7.335
7.316
7.277
7.272
7.260
7.256
7.106
7.088
7.070
Ph$_2$N
Br
1u
1.00
1.12
2.14
1.19
1.14
2.19
2.28
4.49
7.10
2.27
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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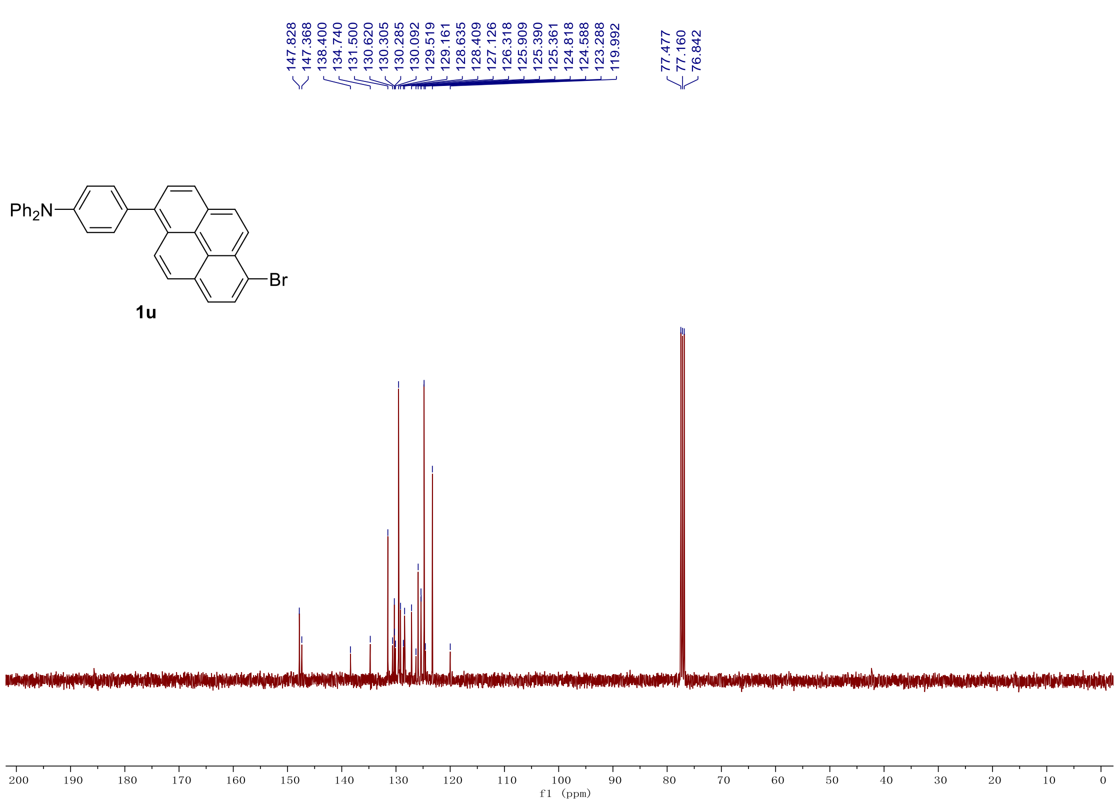
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.305
130.285
130.092
129.519
129.161
128.635
128.409
127.126
126.318
125.909
125.390
125.361
124.818
124.588
123.288
119.992
77.477
77.160
76.842
Ph$_2$N
Br
1u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)