

Supporting information

Synthesis of Highly Emissive 1,8-diaryl Anthracene Derivatives and Fabrication of their Micro/nanostructures

Neeraj Agarwal*, Manish Patil and Mahendra Patil

UM-DAE, Centre for Excellence in Basic Sciences, University of Mumbai, Kalina
campus, Santacruz (E), Mumbai 400098, India

Email: na@cbs.ac.in

Figure SI 1: $^1\text{H-NMR}$ of **7** in CDCl_3 .

Figure SI 2: $^1\text{H-NMR}$ (top) and $^{13}\text{C-NMR}$ (bottom) of **1** in CDCl_3 .

Figure SI 3: $^1\text{H-NMR}$ (top) and $^{13}\text{C-NMR}$ (bottom) of **2** in CDCl_3 .

Figure SI 4: $^1\text{H-NMR}$ of **3** in CDCl_3 .

Figure SI 5: $^1\text{H-NMR}$ of **4** in CDCl_3 .

Figure SI 6: $^1\text{H-NMR}$ (top) and $^{13}\text{C-NMR}$ (bottom) of **5** in CDCl_3 .

Figure SI 7: $^1\text{H-NMR}$ (top) and $^{13}\text{C-NMR}$ (bottom) of **6** in CDCl_3 .

Figure SI 8: Absorption spectra of drop casted thin films of **1-6**

Figure SI 9: Cyclic voltammograms and Differential pulse voltammograms of **1-6** (except **3**) in acetonitrile.

Figure SI 10: MALDI-TOF mass spectrum of compound **1**

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Figure SI 13: MALDI-TOF mass spectrum of compound **4**

Figure SI 14: MALDI-TOF mass spectrum of compound **5**

Figure SI 15: MALDI-TOF mass spectrum of compound **6**

Figure SI 16: Fluorescence decay spectra of **1-6**.

Table SI 1. The optimized geometries (Cartesian coordinates in Å) and energies (a.u.) of dimers of **1** and **5** computed at the B3LYP/6-311G** level of theory. (Eg = Total electronic energy, THc = Thermal correction to Gibbs Free energy computed at the B3LYP level).

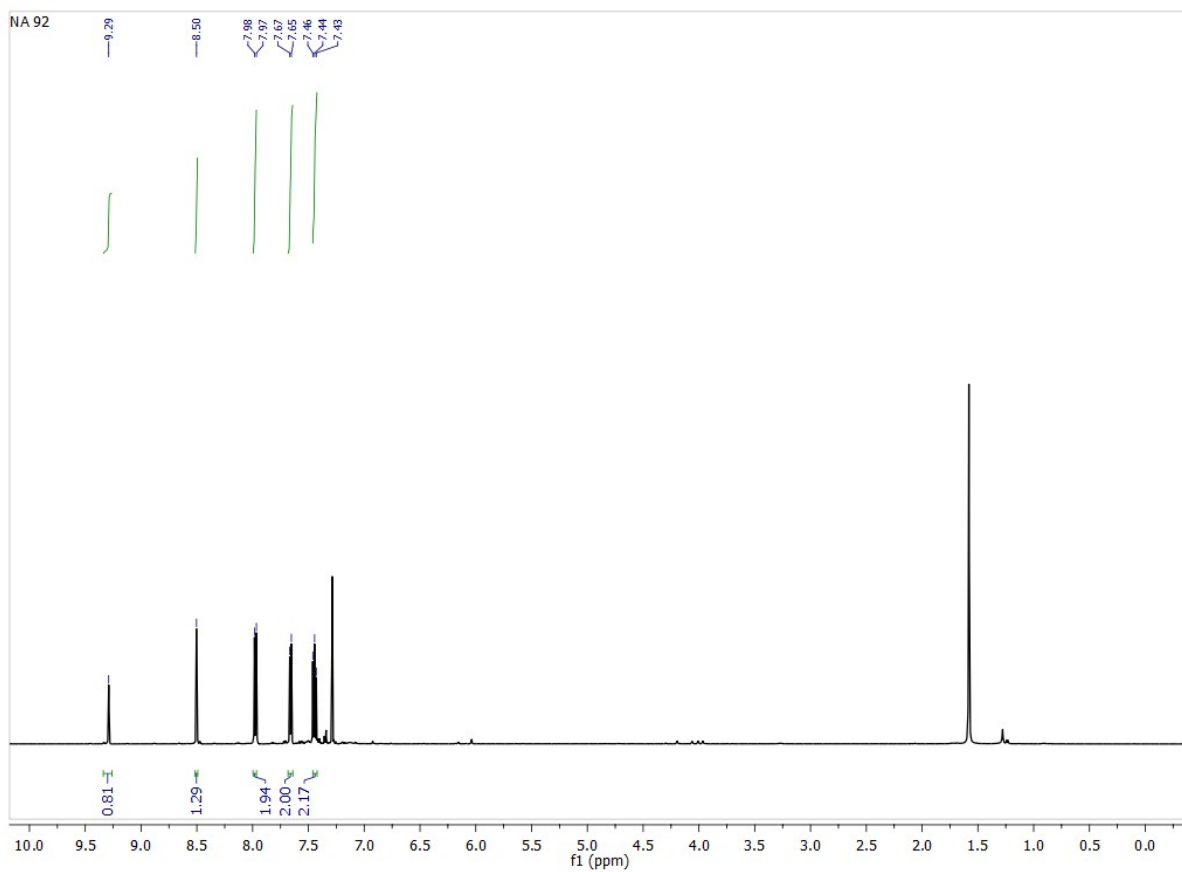


Figure S1: $^1\text{H-NMR}$ of **7** in CDCl_3 .

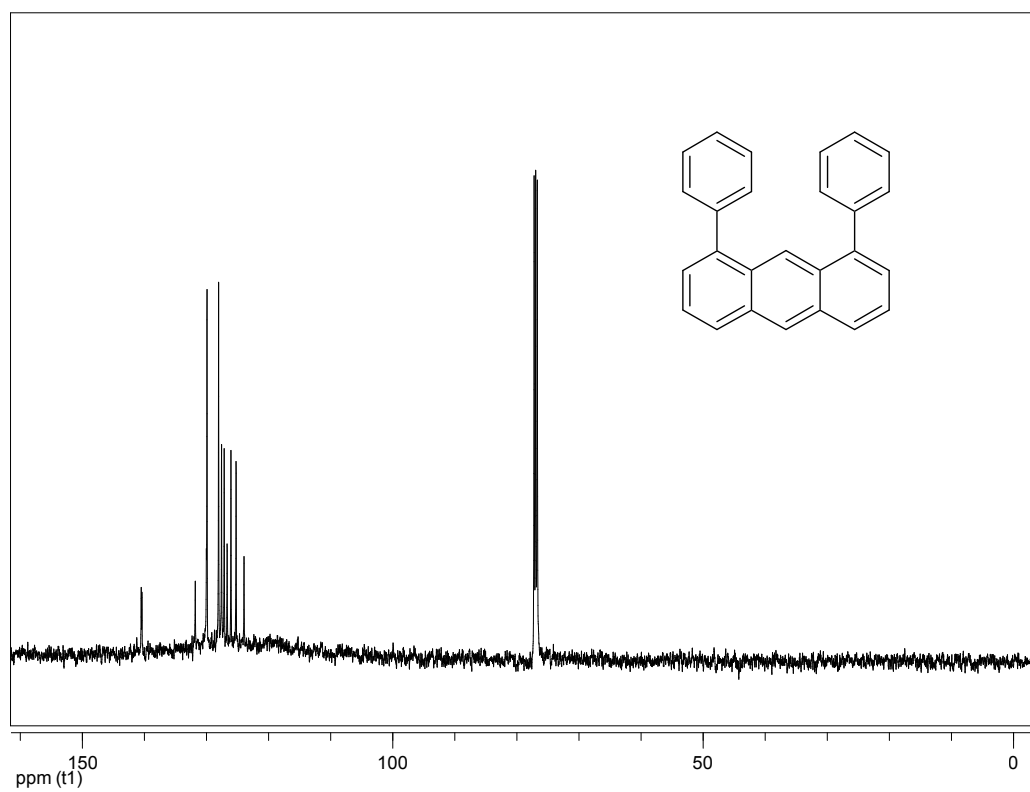
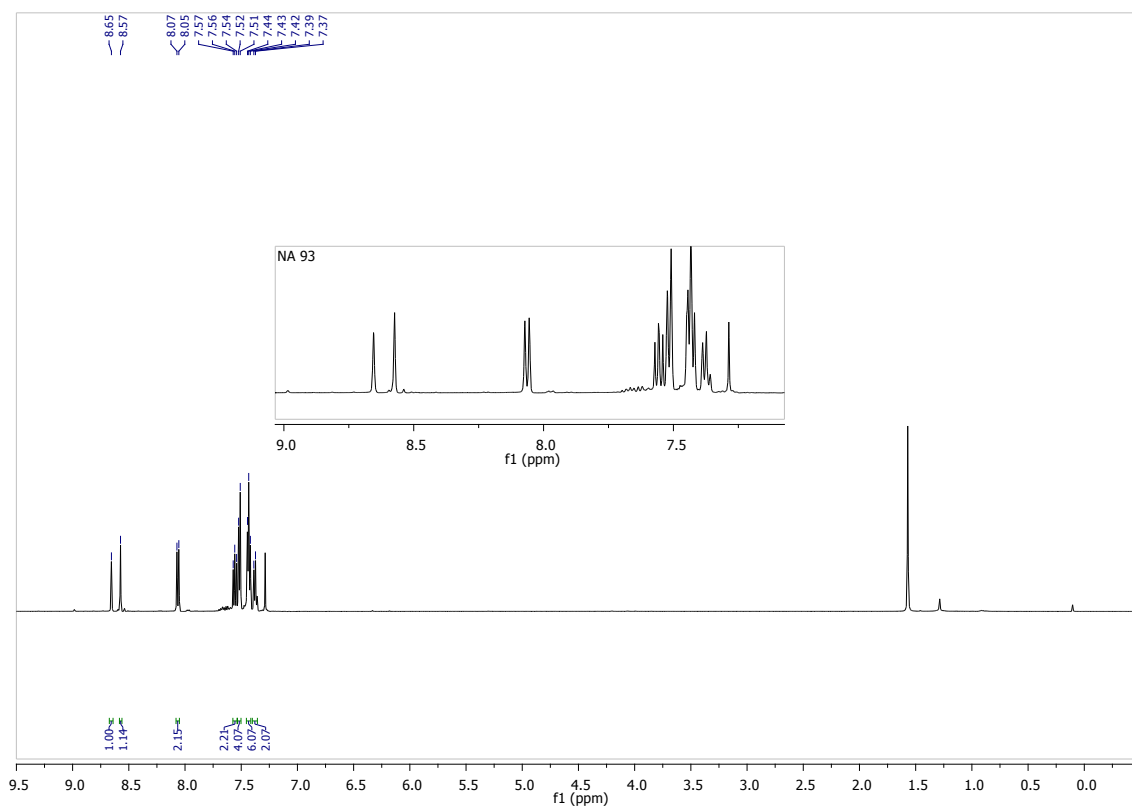


Figure S2: ^1H -NMR (top) and ^{13}C -NMR (bottom) of **1** in CDCl_3 .

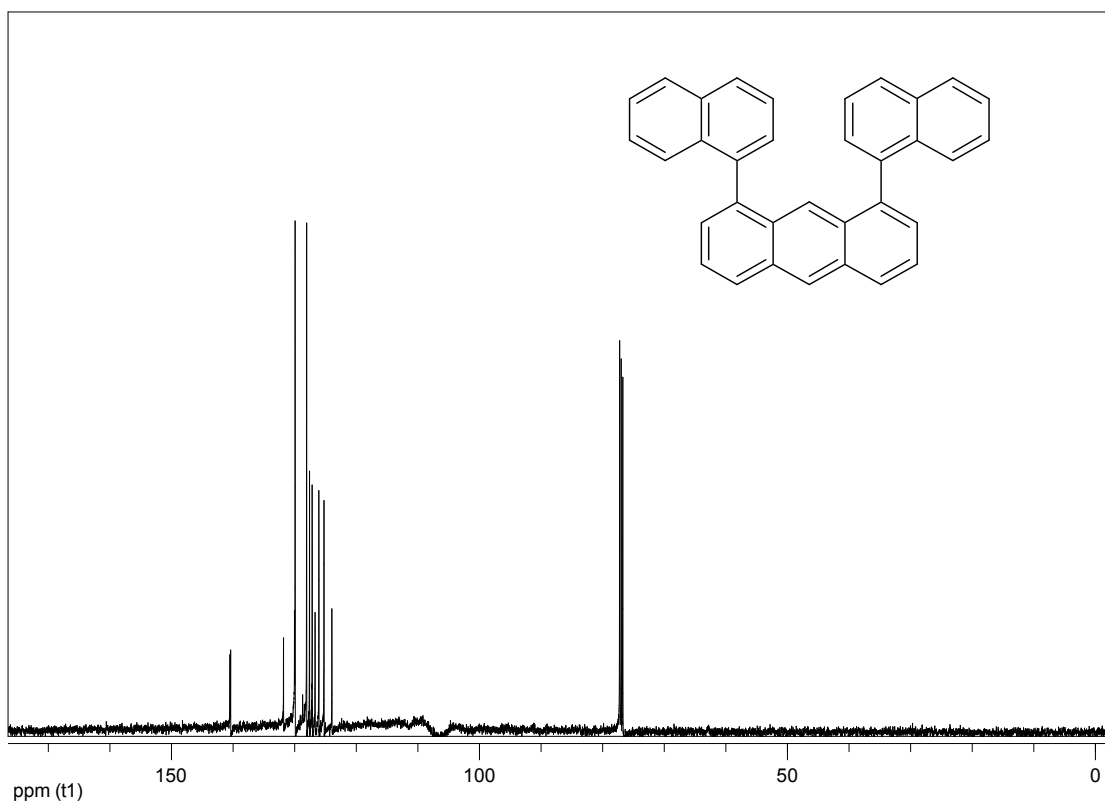
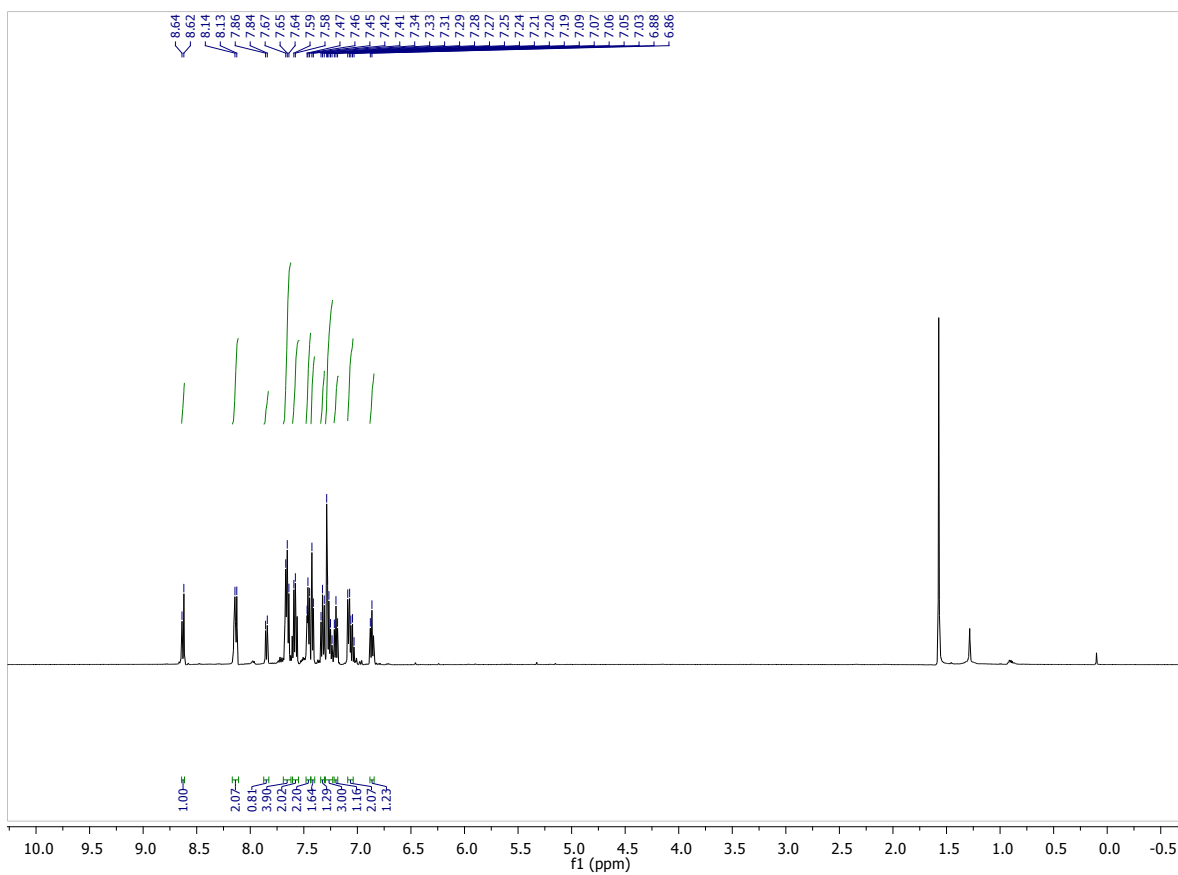


Figure S3: ^1H -NMR (top) and ^{13}C -NMR (bottom) of **2** in CDCl_3 .

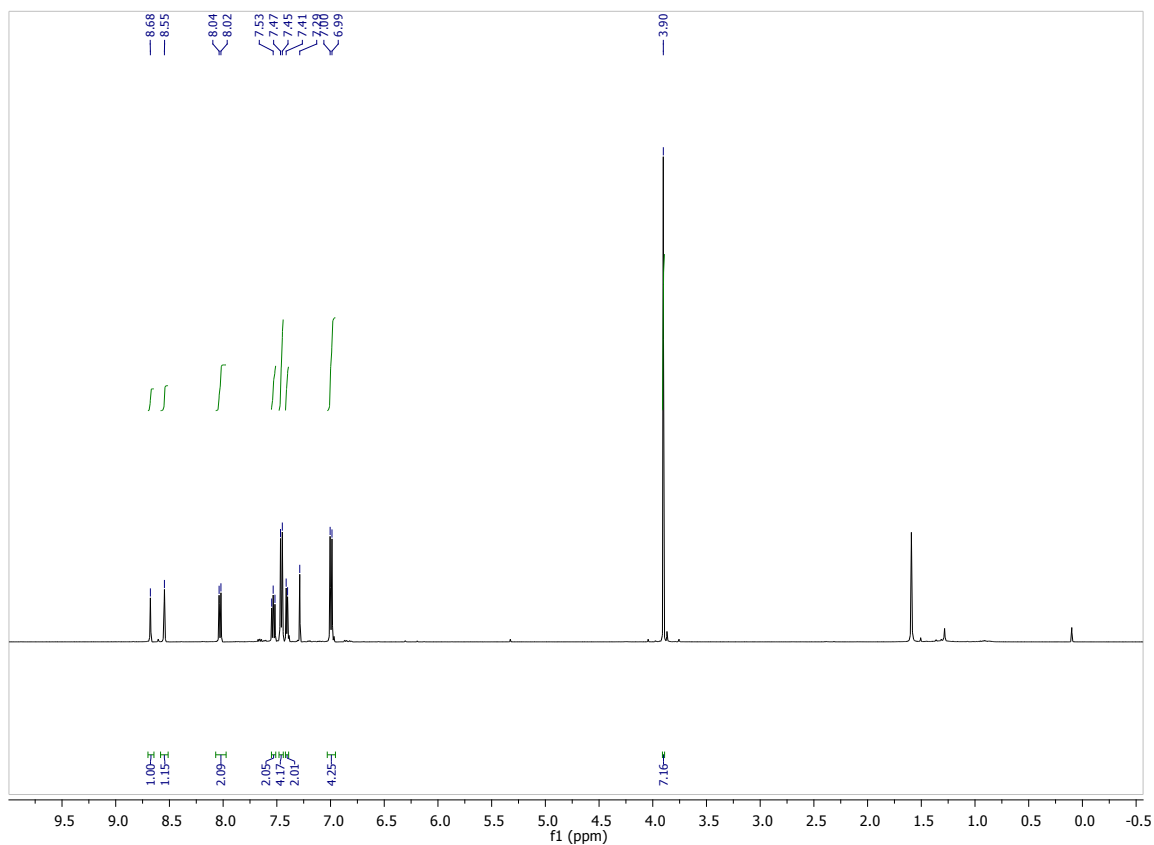


Figure S4: $^1\text{H-NMR}$ of **3** in CDCl_3 .

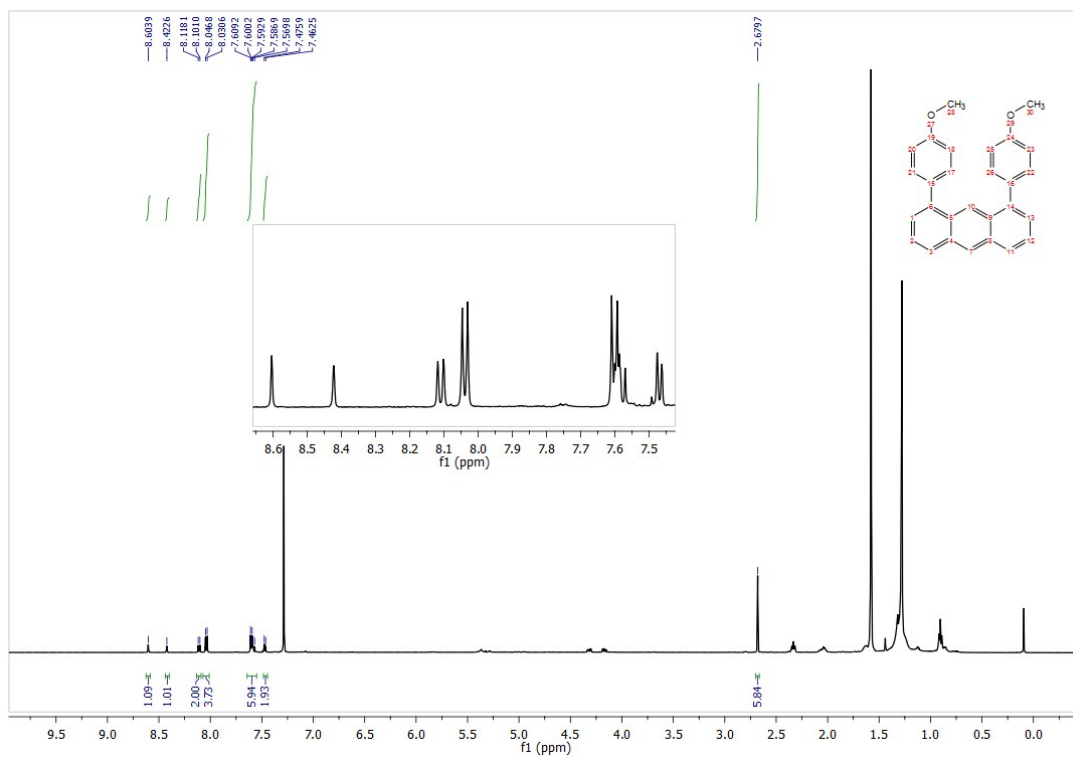


Figure S5: $^1\text{H-NMR}$ of **4** in CDCl_3 .

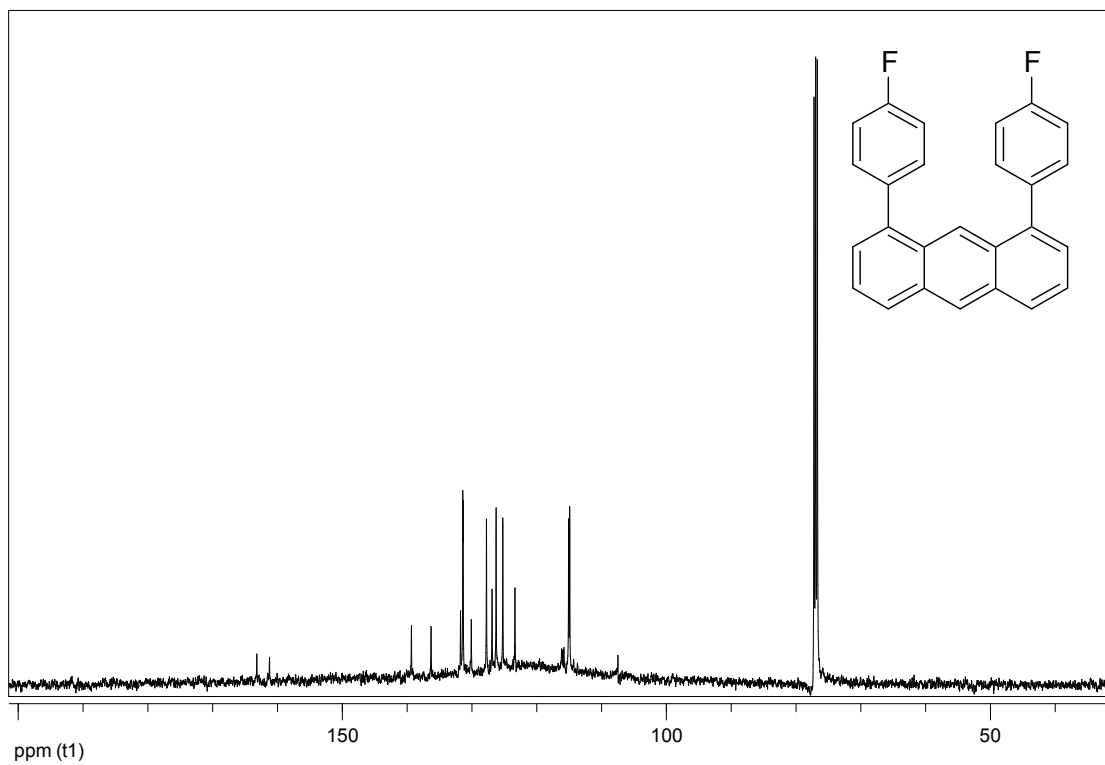
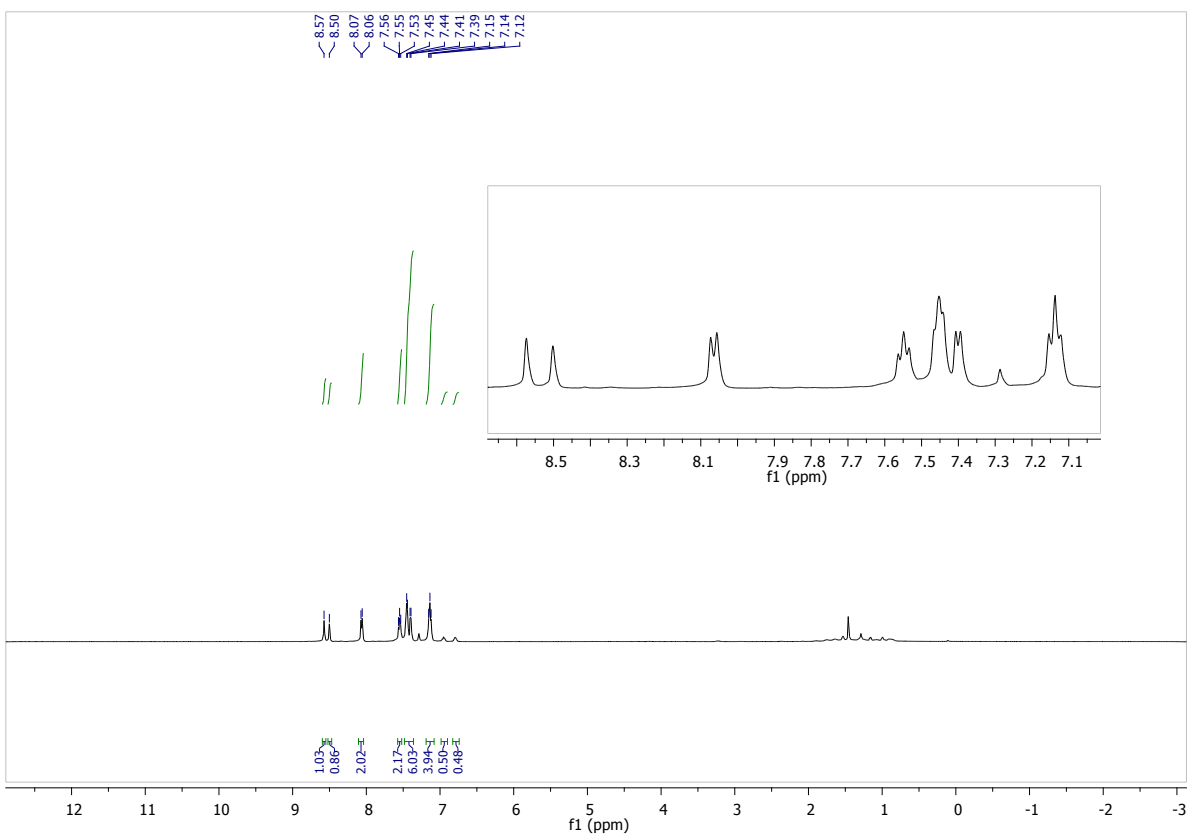


Figure S6: ^1H -NMR (top) and ^{13}C -NMR (bottom) of **5** in CDCl_3 .

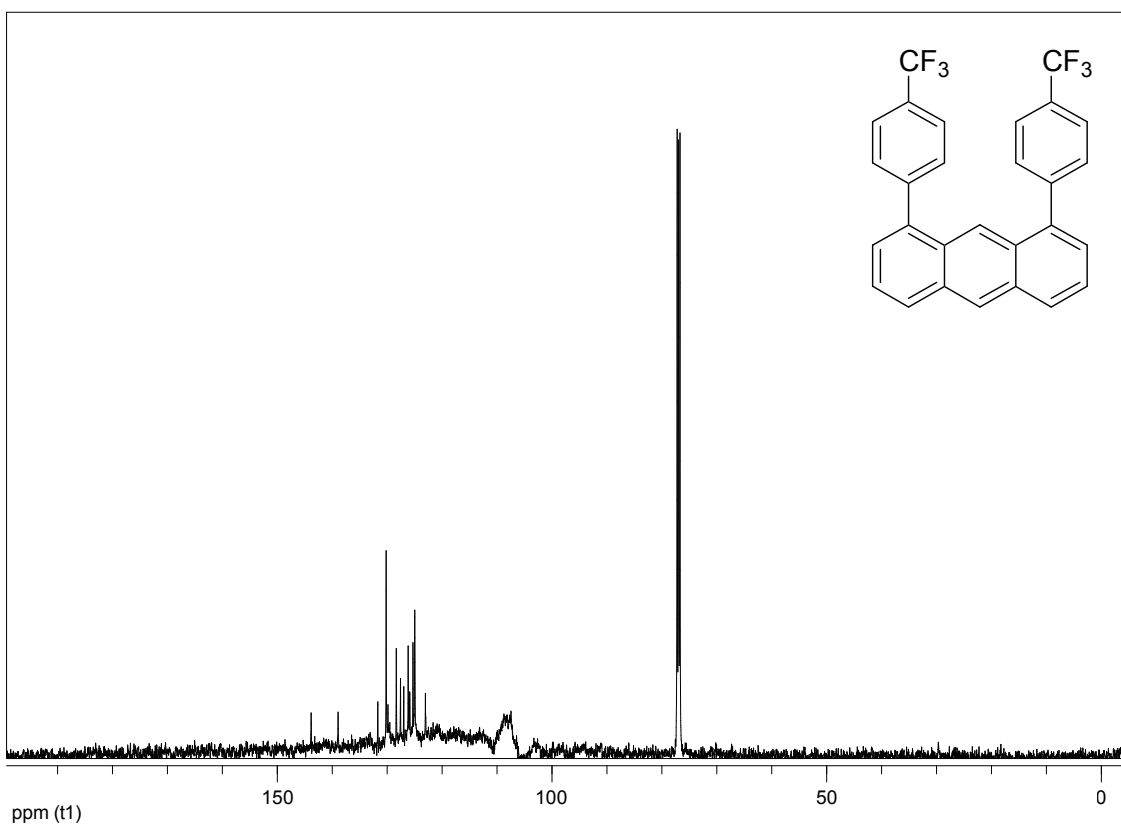
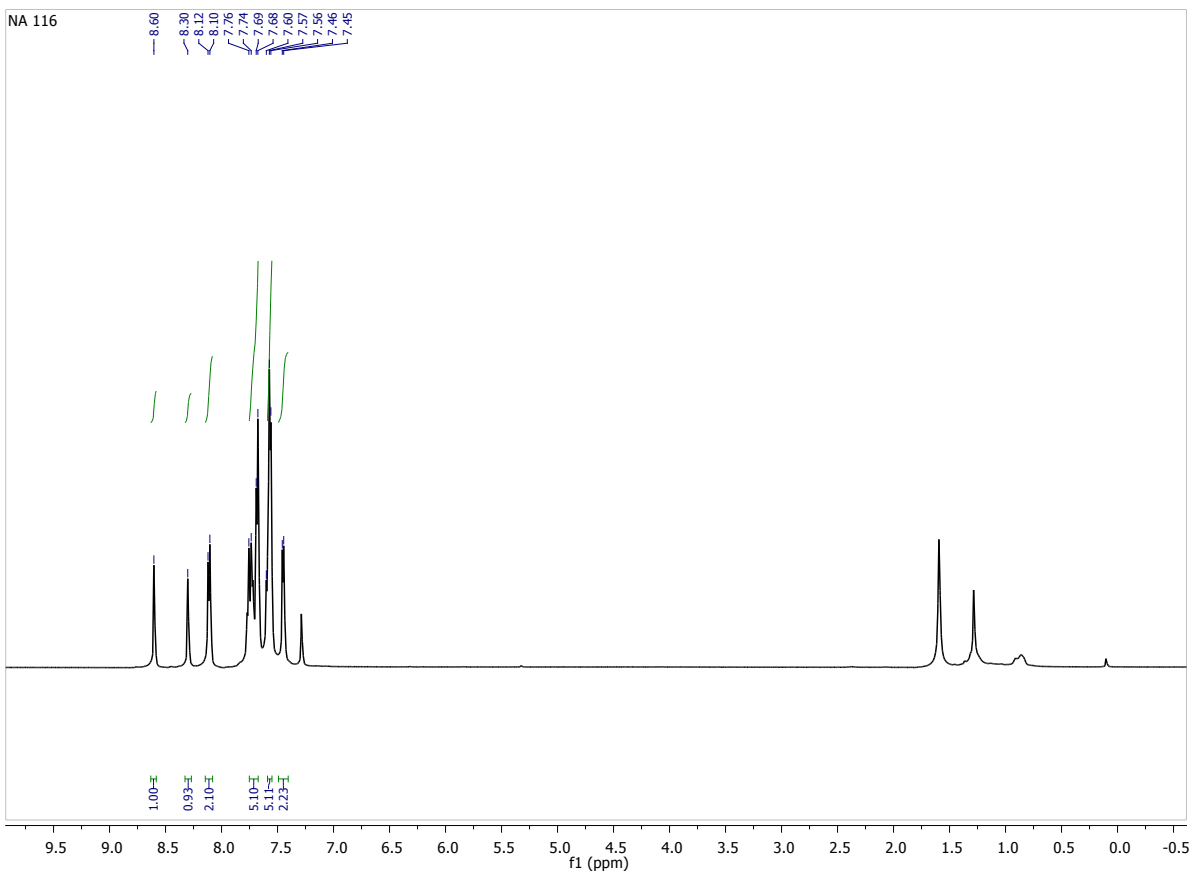


Figure S7: $^1\text{H-NMR}$ (top) and $^{13}\text{C-NMR}$ (bottom) of **6** in CDCl_3 .

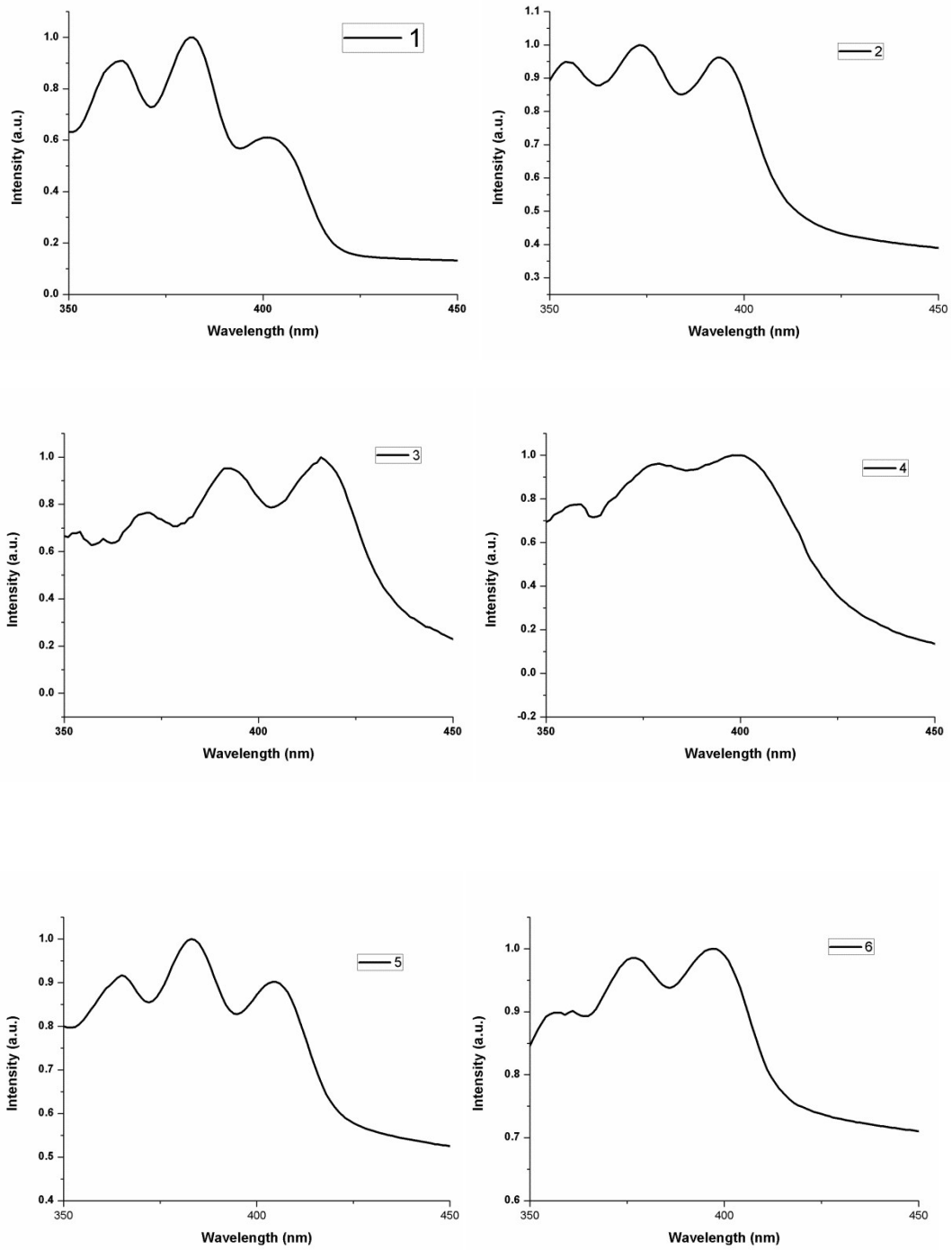


Figure SI 8: Absorption spectra of drop casted thin films of 1-6

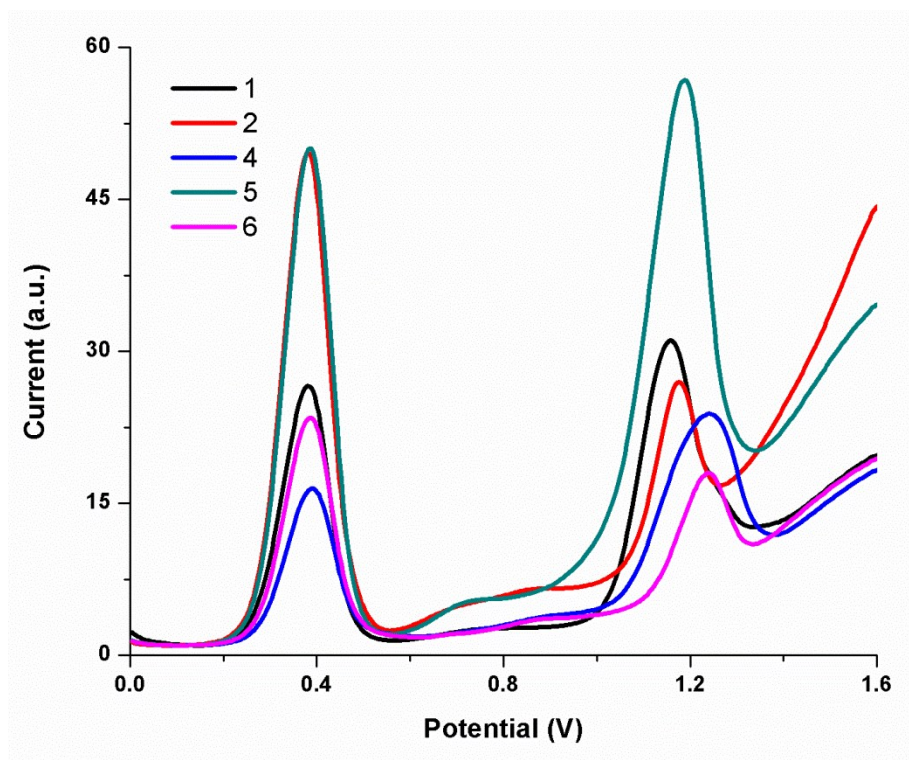
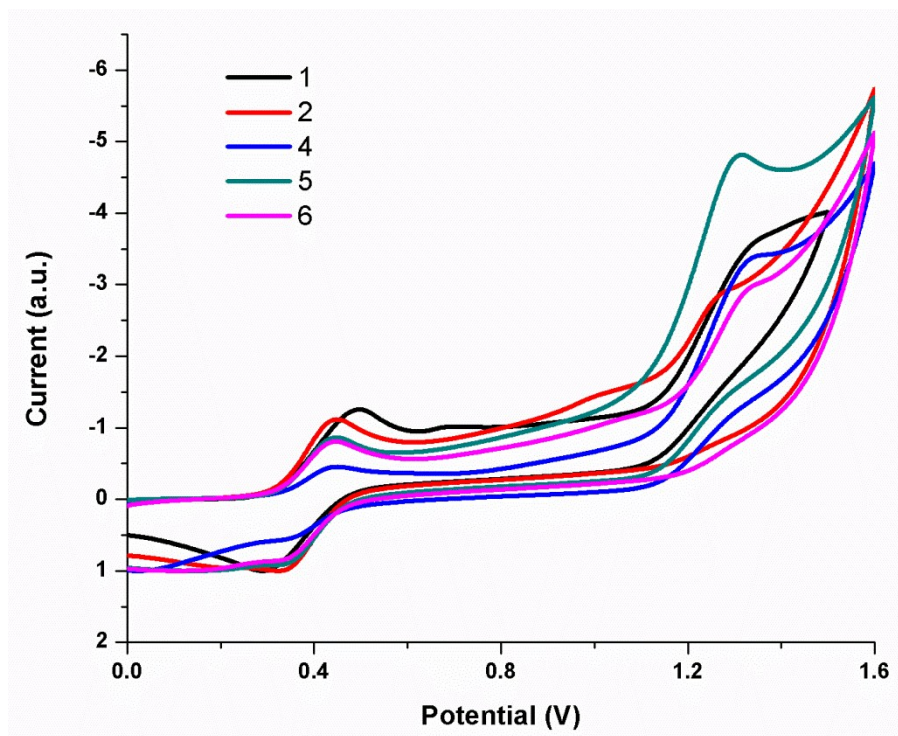


Figure SI 9: Cyclic voltammograms and Differential pulse voltammograms of 1-6 (except 3) in acetonitrile.

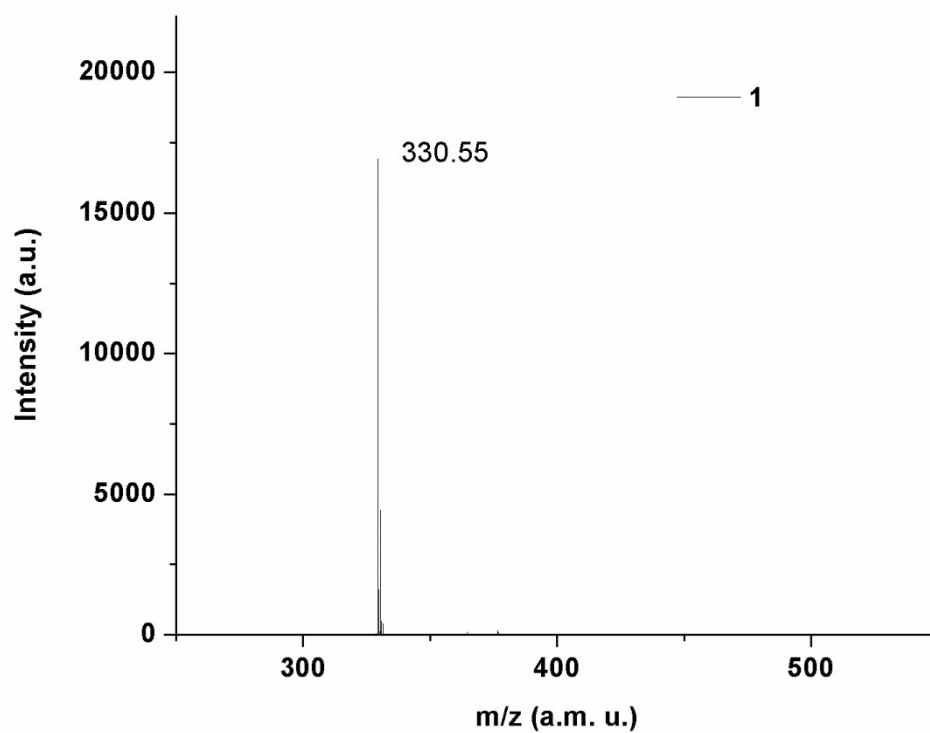


Figure S 10: MALDI-TOF mass spectrum of compound 1

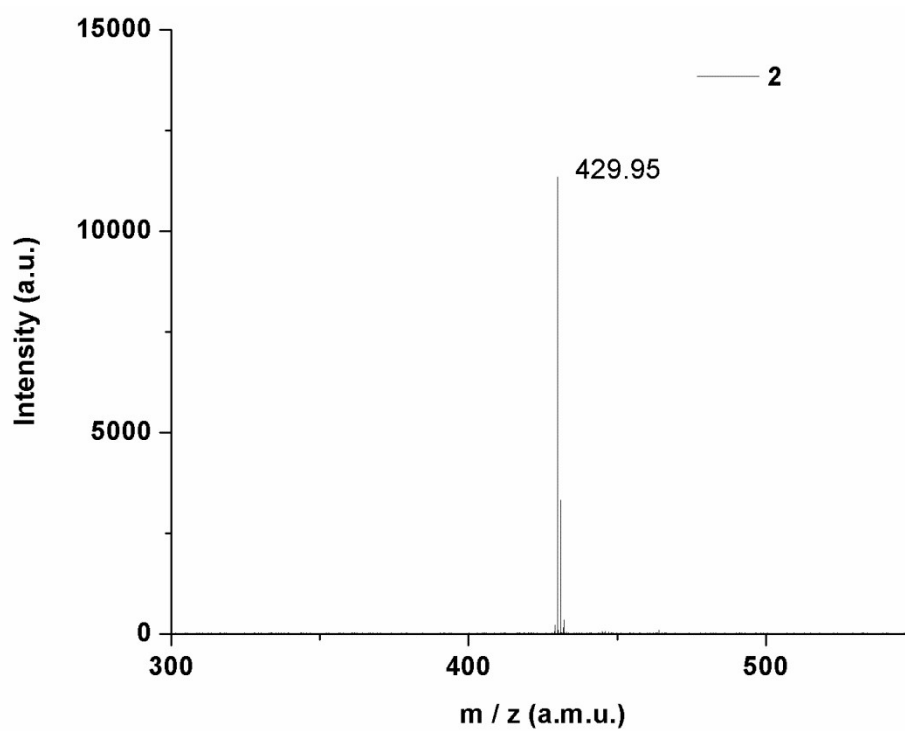


Figure SI 11: MALDI-TOF mass spectrum of compound 2

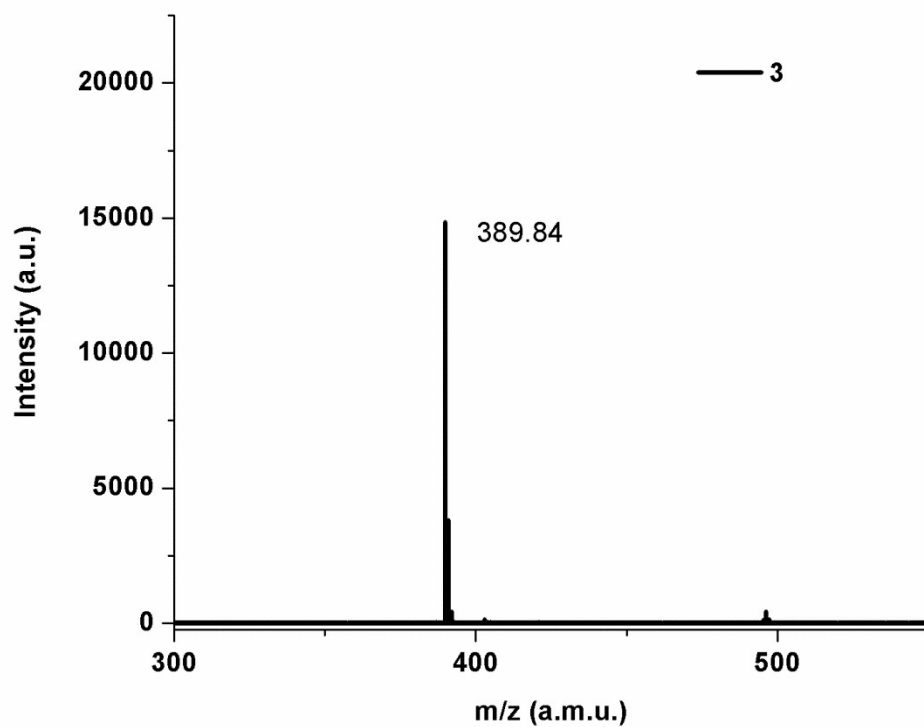


Figure SI 12: MALDI-TOF mass spectrum of compound 3

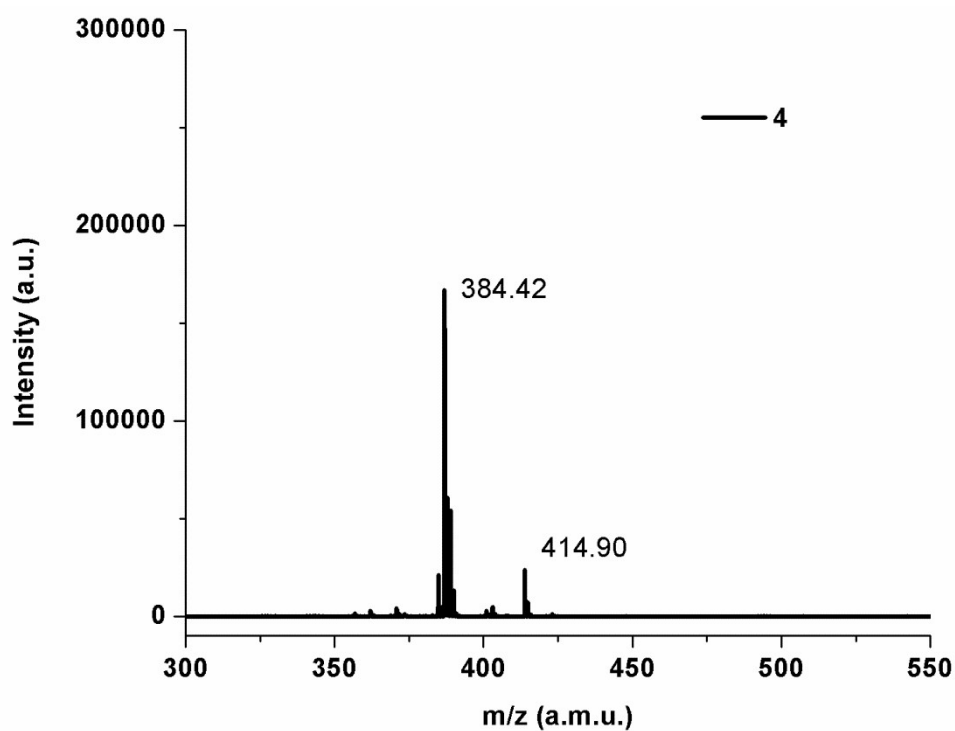


Figure SI 13: MALDI-TOF mass spectrum of compound 4

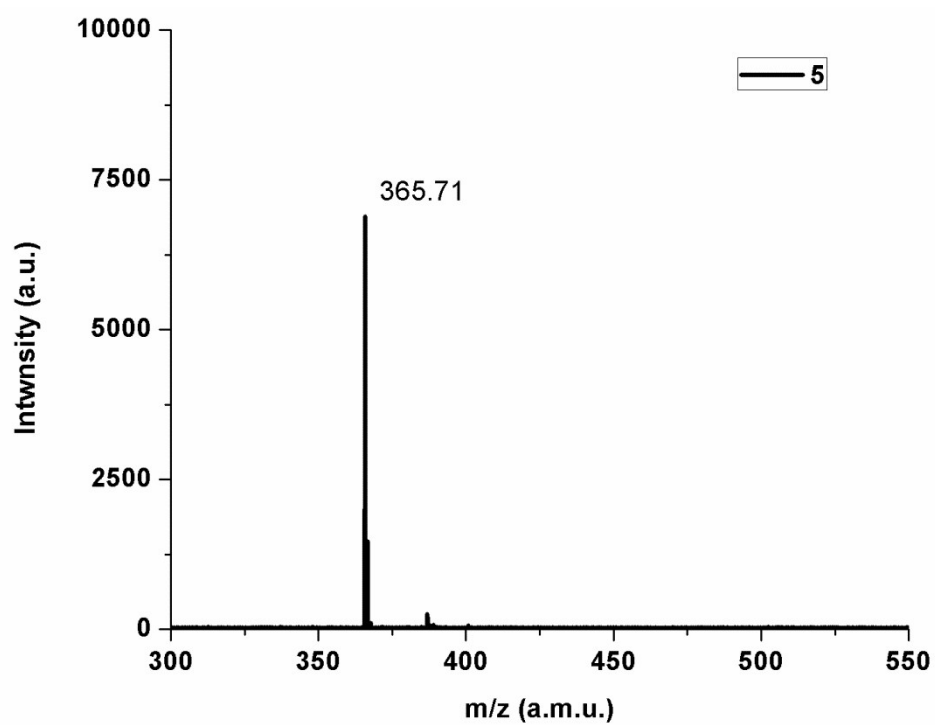


Figure SI 14: MALDI-TOF mass spectrum of compound 5

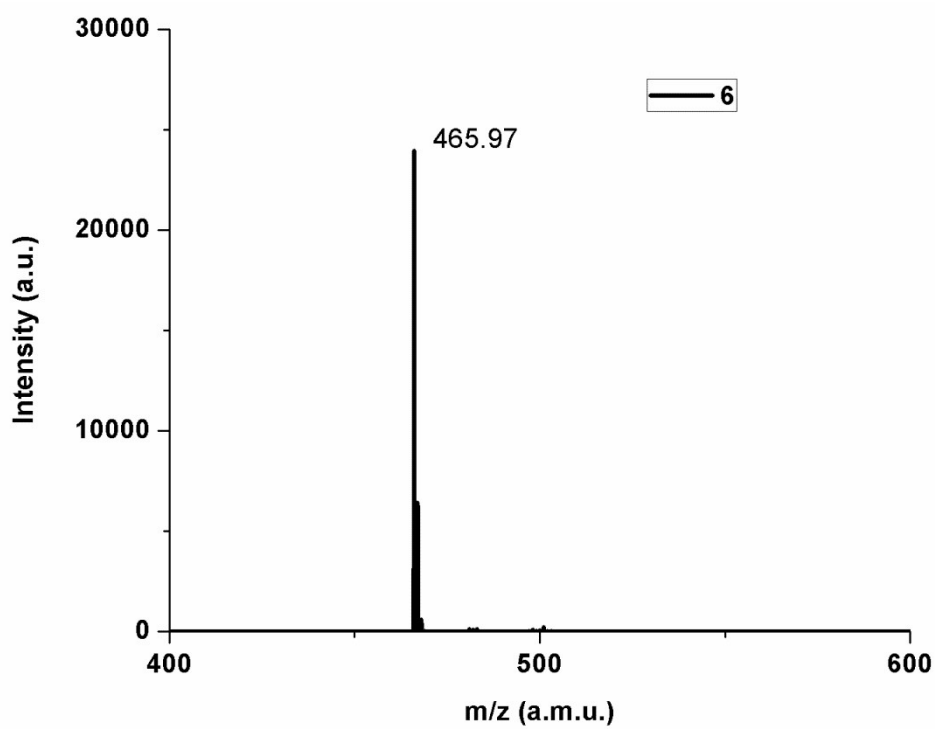


Figure SI 15: MALDI-TOF mass spectrum of compound 6

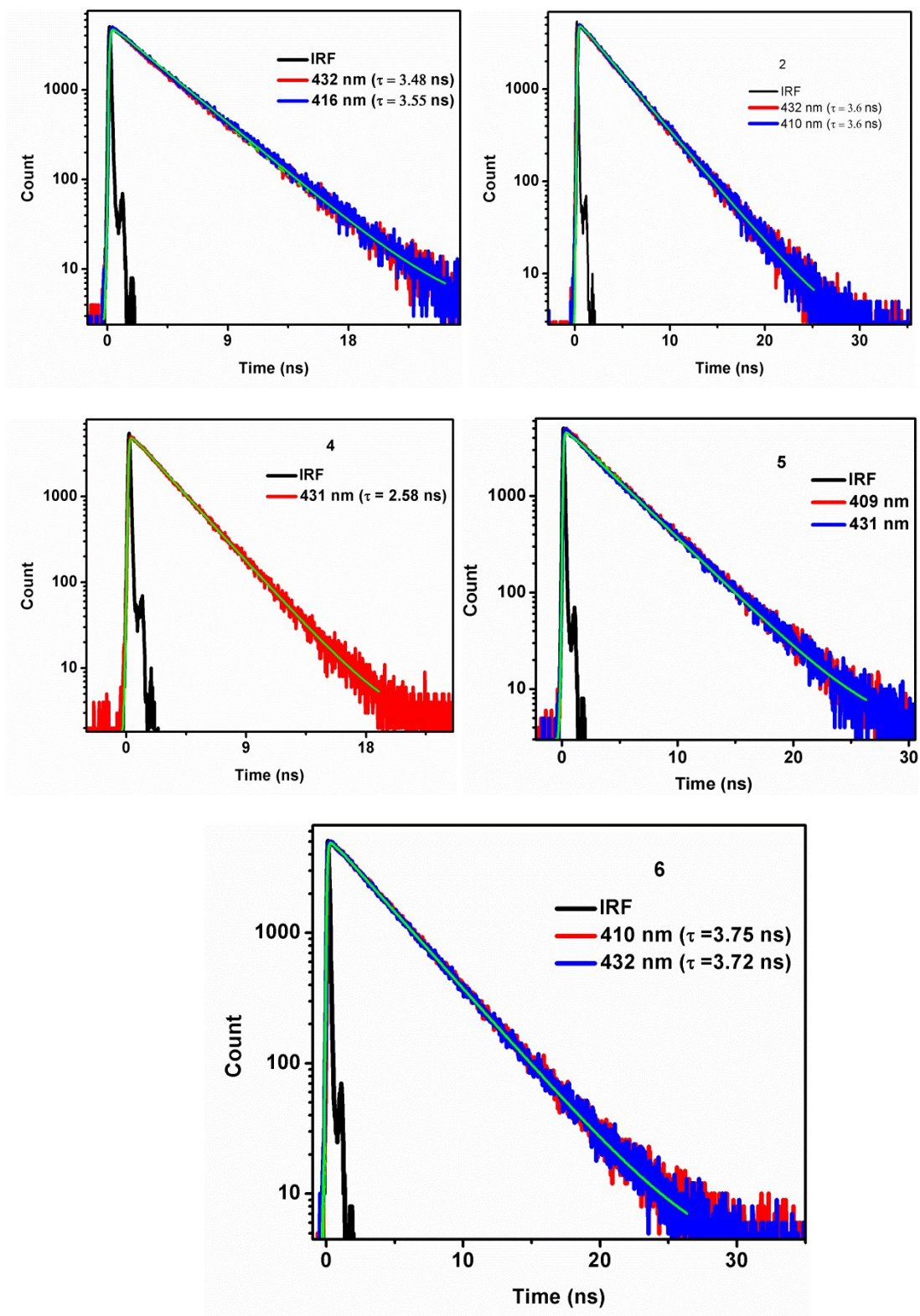


Figure SI 16: Fluorescence decay spectra of 1-6 (except for 3).

Table SI 1. The optimized geometries (Cartesian coordinates in Å) and energies (a.u.) of dimers of **1** and **5** computed at the B3LYP/6-311G** level of theory. (Eg = Total electronic energy, THc = Thermal correction to Gibbs Free energy computed at the B3LYP level).

1				5			
Eg = -2003.7349977 NIMAG = 0				Eg = -2400.7984208 NIMAG = 0			
THc = 0.623704				THc = 0.590949			
C	9.02169600	-2.69098900	0.16454000	C	8.74021100	-2.97641300	-0.62642700
C	9.34829000	-1.36593500	0.16344800	C	9.15753700	-1.68432500	-0.76375200
C	8.33035200	-0.36910500	0.08365500	C	8.25265600	-0.60330900	-0.54279700
C	6.94695000	-0.77226000	-0.00461200	C	6.88469000	-0.88624100	-0.17851200
C	6.63905000	-2.18389700	-0.03727700	C	6.46827400	-2.26591300	-0.07220100
C	7.66397400	-3.09539800	0.06181800	C	7.39220300	-3.26246300	-0.28168000
C	8.64006600	0.99310200	0.09426300	C	8.66066500	0.72735900	-0.66535500
C	5.95931900	0.22145300	-0.02241000	C	6.02656500	0.18877100	0.08717000
C	6.26538000	1.58821900	0.01922800	C	6.44043400	1.52378500	-0.00794600
C	7.65419300	1.98210800	0.05087400	C	7.79580700	1.79758500	-0.42286900
C	7.99087300	3.36862400	0.03332200	C	8.22032400	3.15065800	-0.58160900
H	9.03828700	3.65008000	0.05851300	H	9.24158900	3.34250900	-0.89315200
C	7.01246300	4.31859700	-0.01819100	C	7.35469000	4.18002700	-0.35010800
C	5.64390900	3.93919600	-0.03204200	C	6.02453700	3.91829900	0.07433500
C	5.25384400	2.62061800	-0.00012000	C	5.56004300	2.63764800	0.26120500
H	9.68246900	1.29374100	0.13910000	H	9.68482600	0.93695200	-0.95879000
H	9.79581600	-3.44737700	0.22881400	H	9.42943600	-3.79669600	-0.79231800
H	10.38357700	-1.04823800	0.22777900	H	10.18209500	-1.45720400	-1.03861400
H	7.43091600	-4.15378000	0.03179100	H	7.07629500	-4.29700600	-0.20743800
H	4.92275100	-0.07905000	-0.07009300	H	5.00643100	-0.01937900	0.37495900
H	7.26990600	5.37170100	-0.03390400	H	7.67780100	5.20747800	-0.47408700
H	4.88378300	4.71221700	-0.03929700	H	5.36475800	4.75312100	0.28235800
C	3.79850600	2.29978700	0.01589900	C	4.16061800	2.43519800	0.73281200
C	2.96038600	2.77145400	-1.00357900	C	3.08423400	2.94423800	-0.00581000
C	3.22272700	1.57058100	1.06644400	C	3.88572700	1.77912100	1.94143400
C	1.59039500	2.52117200	-0.97616400	C	1.77053300	2.80671800	0.43634100
H	3.39252100	3.32738400	-1.82822300	H	3.27692200	3.44571300	-0.94711900
C	1.85356000	1.32177300	1.09435800	C	2.58018900	1.63380300	2.40008900
H	3.85133800	1.21212700	1.87350200	H	4.70298000	1.39050400	2.53746900
C	1.03097600	1.79435500	0.07255900	C	1.54658800	2.15155300	1.63549600
H	0.95990000	2.89023400	-1.77770800	H	0.93555500	3.19249500	-0.13473400
H	1.42641800	0.76142700	1.91855200	H	2.35811900	1.13517300	3.33525800
C	5.24157100	-2.68296100	-0.17937800	C	5.06468700	-2.63813300	0.26419100
C	4.69002000	-3.52723700	0.79359400	C	4.79300800	-3.41630800	1.39718100
C	4.46809200	-2.37098800	-1.30659600	C	3.99204800	-2.26665100	-0.55940700
C	3.40521600	-4.04452000	0.64580300	C	3.49421500	-3.81270800	1.70591800
H	5.27271000	-3.76873100	1.67559200	H	5.60755700	-3.70562500	2.05099400
C	3.18538900	-2.89042300	-1.45588700	C	2.68769600	-2.65551000	-0.26850600
H	4.88340800	-1.73212700	-2.07762700	H	4.18056700	-1.67766700	-1.44922600
C	2.64807400	-3.72859400	-0.47995200	C	2.46613700	-3.42300600	0.86402100
H	2.99590100	-4.69389700	1.41191400	H	3.27417700	-4.40954400	2.58231500
H	2.60646800	-2.64566800	-2.33946700	H	1.85764600	-2.37862100	-0.90617100
C	-7.01246000	-4.31862000	0.01853400	F	0.27243400	2.00820800	2.08243100
C	-7.99087100	-3.36865200	-0.03306100	F	1.19890300	-3.80958100	1.16258800
C	-7.65419100	-1.98213600	-0.05071700	C	-7.35473300	-4.18002800	0.34998800
C	-6.26538000	-1.58824500	-0.01907600	C	-8.22037700	-3.15065700	0.58144300
C	-5.25384600	-2.62063700	0.00038400	C	-7.79585100	-1.79758500	0.42271800
C	-5.64390800	-3.93921500	0.03238000	C	-6.44046200	-1.52378900	0.00784300
C	-8.64006000	-0.99313200	-0.09420900	C	-5.56006300	-2.63765700	-0.26127400
C	-5.95931000	-0.22147800	0.02241300	C	-6.02456200	-3.91830600	-0.07440100
C	-6.94693900	0.77223700	0.00450400	C	-8.66071600	-0.72735700	0.66517000
C	-8.33034300	0.36907500	-0.08372600	C	-6.02658300	-0.18877400	-0.08723200
C	-9.34828000	1.36589700	-0.16362300	C	-6.88470900	0.88624200	0.17843600
H	-10.38356600	1.04819300	-0.22792800	C	-8.25269700	0.60331100	0.54264100
C	-9.02168700	2.69095000	-0.16484000	C	-9.15758700	1.68432800	0.76355500
C	-7.66396400	3.09537000	-0.06215800	H	-10.18216100	1.45720600	1.03835800

C	-6.63904000	2.18387900	0.03702500	C	-8.74025400	2.97641600	0.62625500
H	-9.68246400	-1.29377400	-0.13903300	C	-7.39222600	3.26246700	0.28158900
H	-7.26990100	-5.37172300	0.03431800	C	-6.46828100	2.26591900	0.07217000
H	-9.03828500	-3.65010900	-0.05825300	H	-9.68489100	-0.93694800	0.95855700
H	-4.88377900	-4.71223200	0.03970900	H	-7.67785000	-5.20747800	0.47396300
H	-4.92273800	0.07902200	0.07005900	H	-9.24165300	-3.34250500	0.89294800
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H	-7.43090600	4.15375400	-0.03223500	H	-5.00643800	0.01937400	-0.37497100
C	-3.79851200	-2.29979000	-0.01562100	H	-9.42948700	3.79669900	0.79210700
C	-3.22274100	-1.57055700	-1.06615100	H	-7.07631400	4.29701100	0.20737200
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H	-1.42643700	-0.76136900	-1.91823900	H	-3.27699000	-3.44561800	0.94721200
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C	-3.18541300	2.89062900	1.45560900	C	-3.99208000	2.26666400	0.55951500
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C	-3.40519700	4.04440800	-0.64626100	C	-2.68771200	2.65551900	0.26868100
H	-5.27266800	3.76845900	-1.67604900	H	-4.18064100	1.67766200	1.44931300
C	-2.64808100	3.72865700	0.47955900	C	-3.49413300	3.81276900	-1.70575100
H	-2.60651000	2.64601300	2.33923900	H	-5.60745600	3.70569300	-2.05093700
H	-2.99586900	4.69367400	-1.41245900	C	-2.46609500	3.42303800	-0.86381900
H	-1.64843300	4.13112000	0.59733400	H	-1.85769200	2.37860600	0.90637400
H	-0.03457500	1.59733600	0.09426000	H	-3.27405000	4.40962100	-2.58212700
H	0.03455800	-1.59728600	-0.09394800	F	-1.19884400	3.80960600	-1.16231900
H	1.64842200	-4.13103700	-0.59776300	F	-0.27236700	-2.00823200	-2.08226100