

Supplementary data

Asymmetric Anthracene-Based Blue Host Materials: Synthesis and Electroluminescence Properties of 9-(2-naphthyl)-10-arylanthracenes

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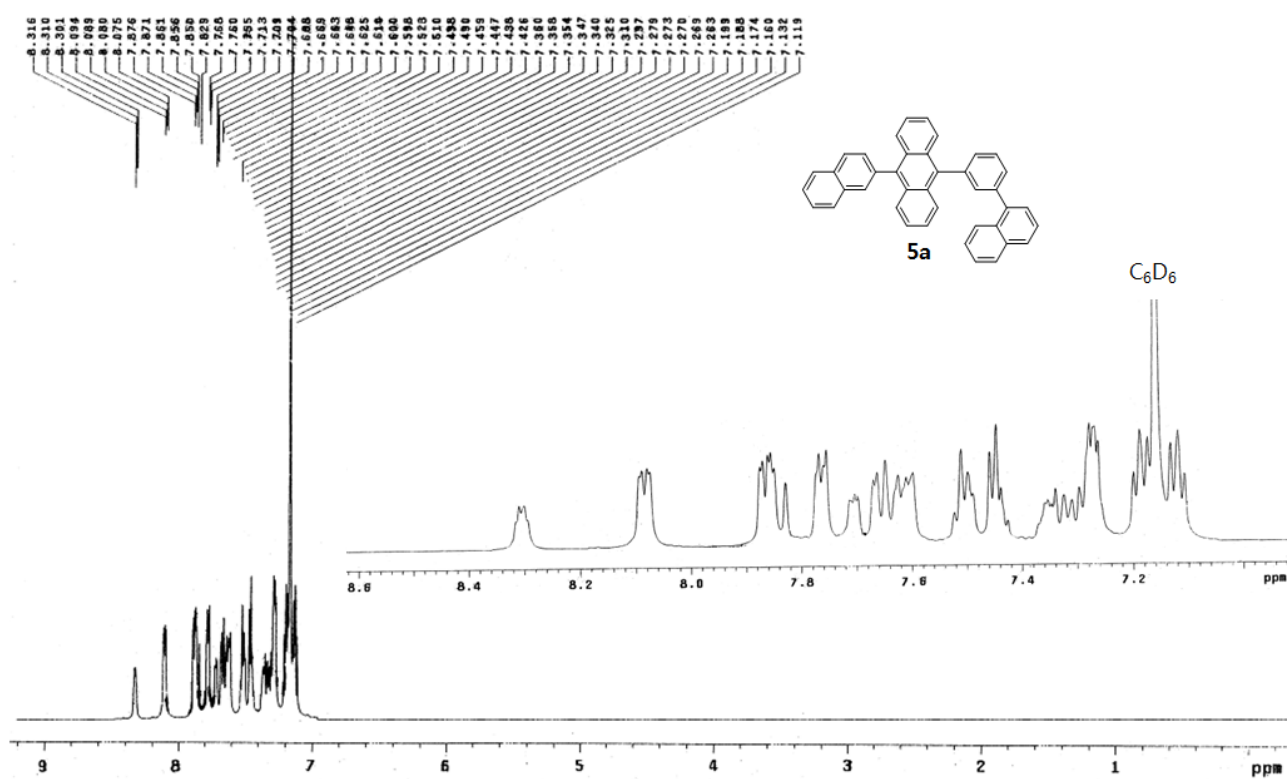
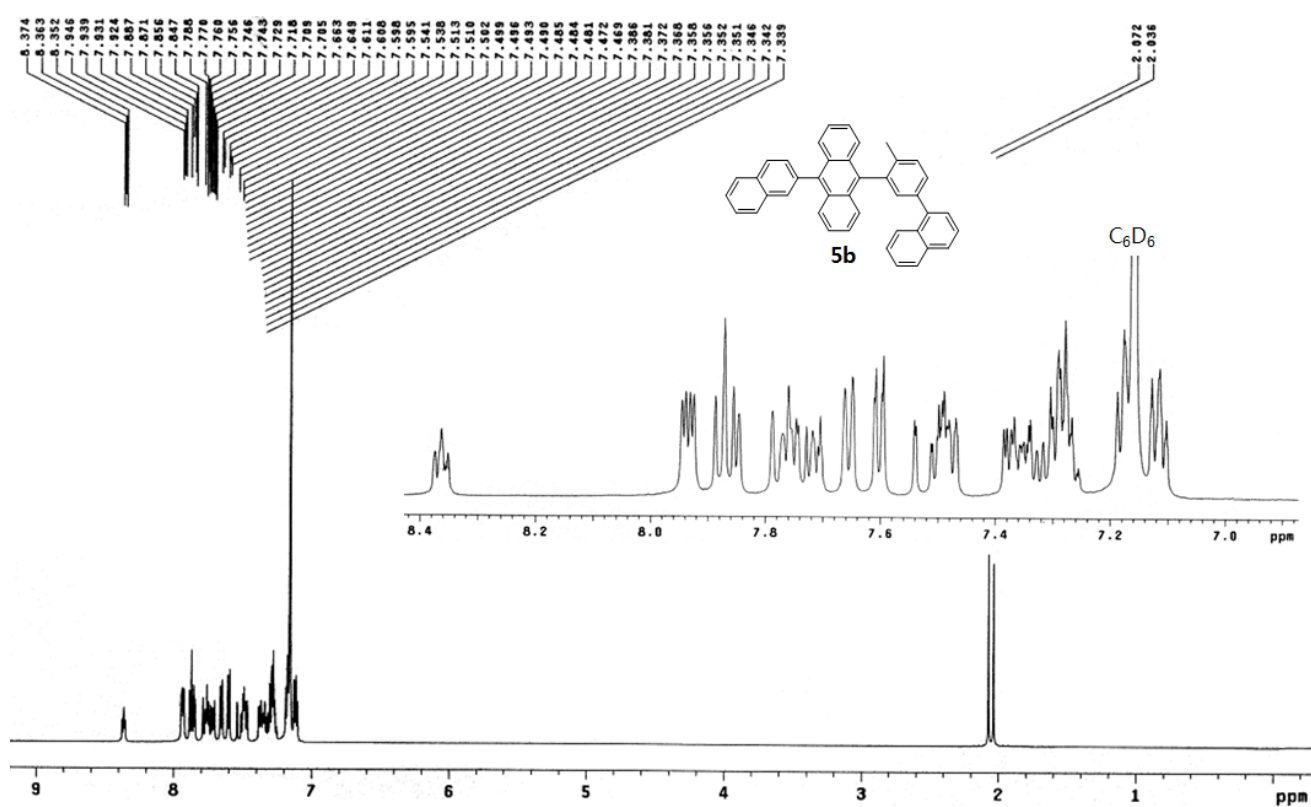
Figure S1 (a). 1H -NMR spectrum of **5a** in C_6D_6 .

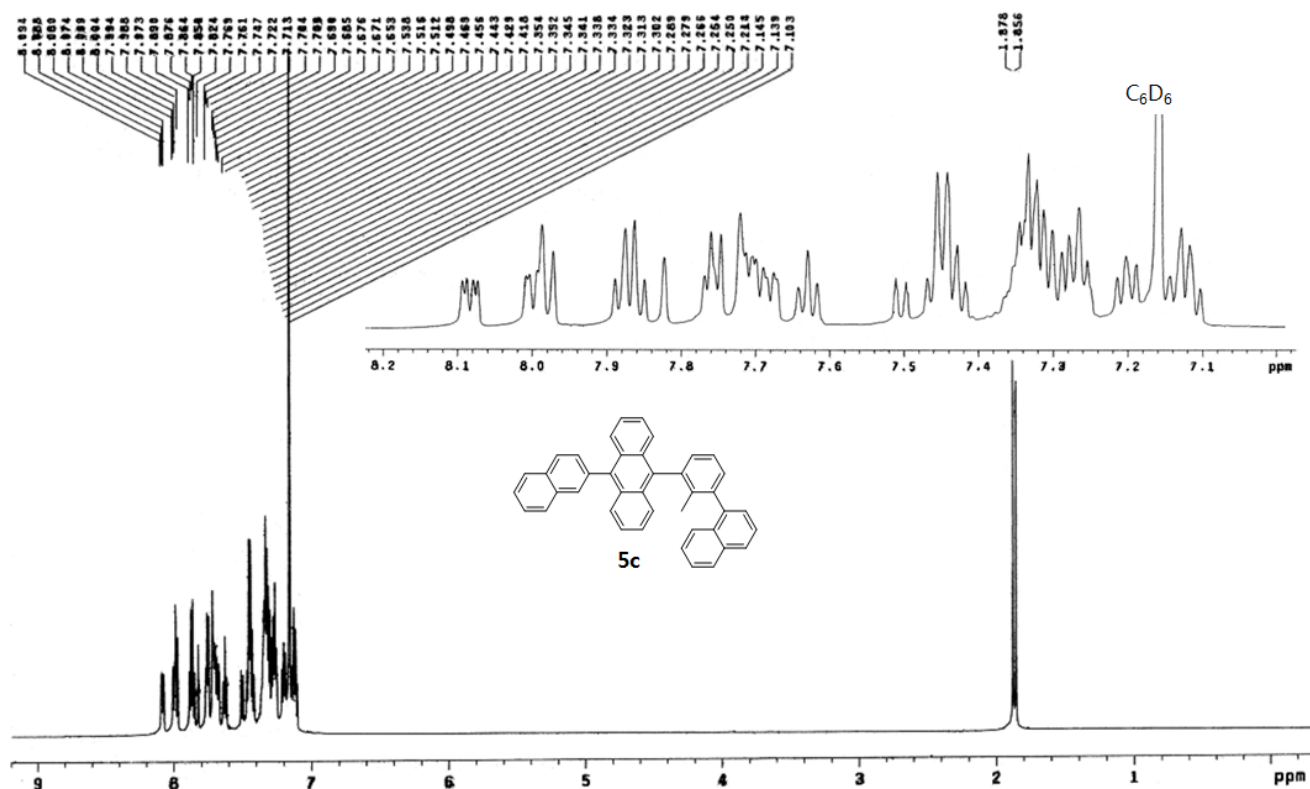
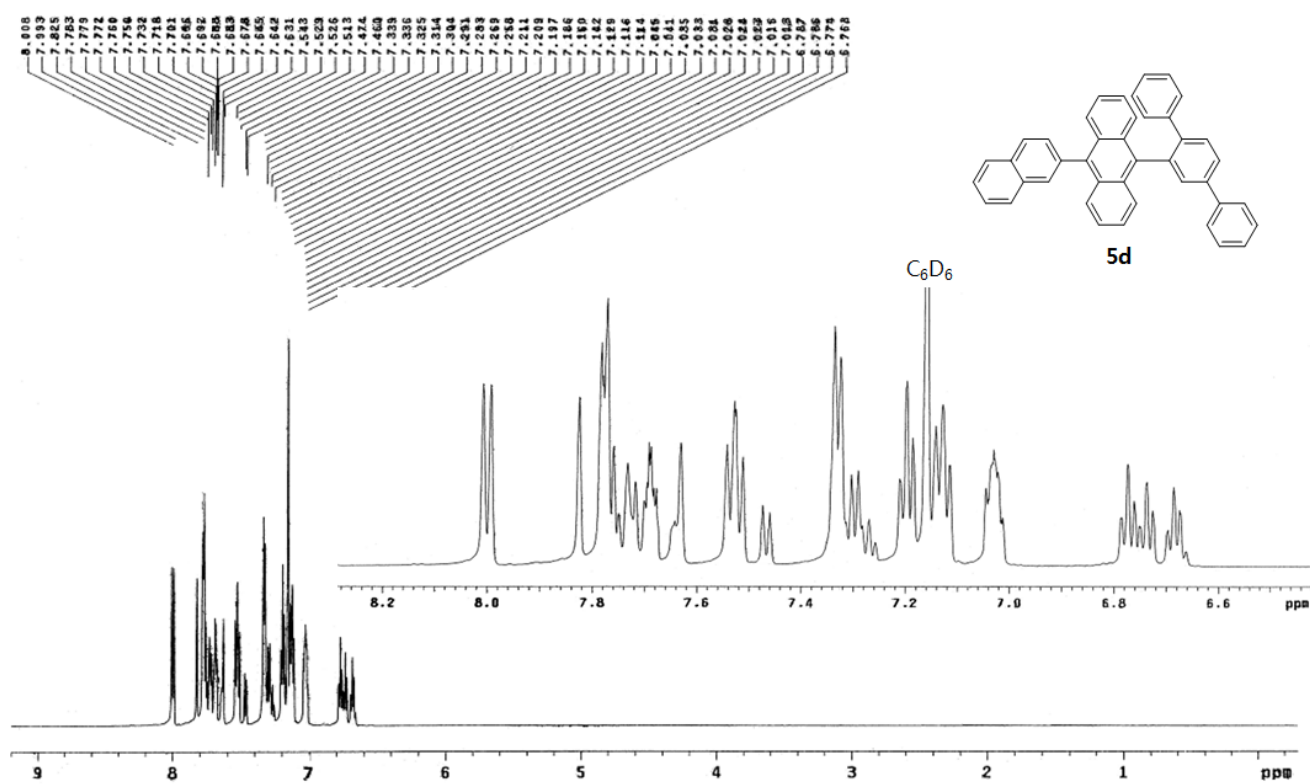
Figure S1 (b). $^1\text{H-NMR}$ spectrum of **5b** in C_6D_6 .**Figure S1 (c).** $^1\text{H-NMR}$ spectrum of **5c** in C_6D_6 .

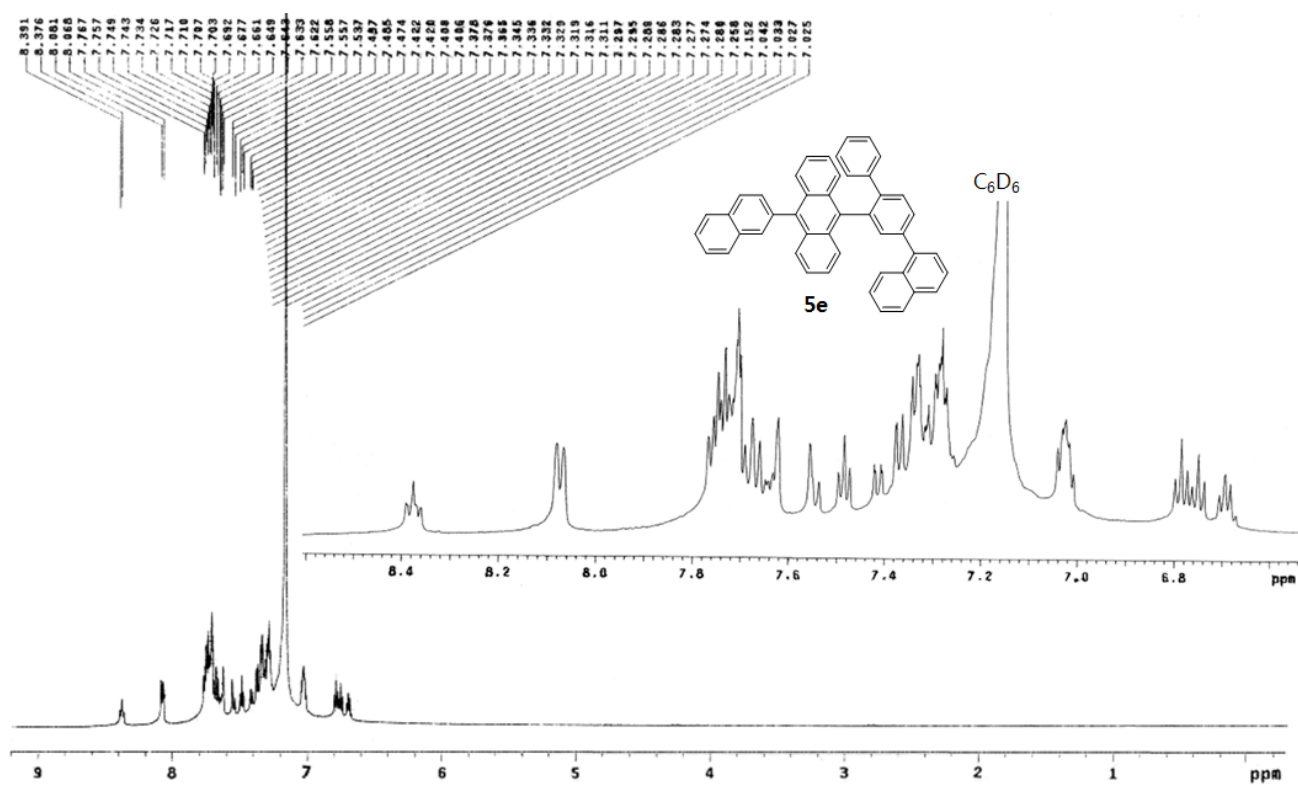
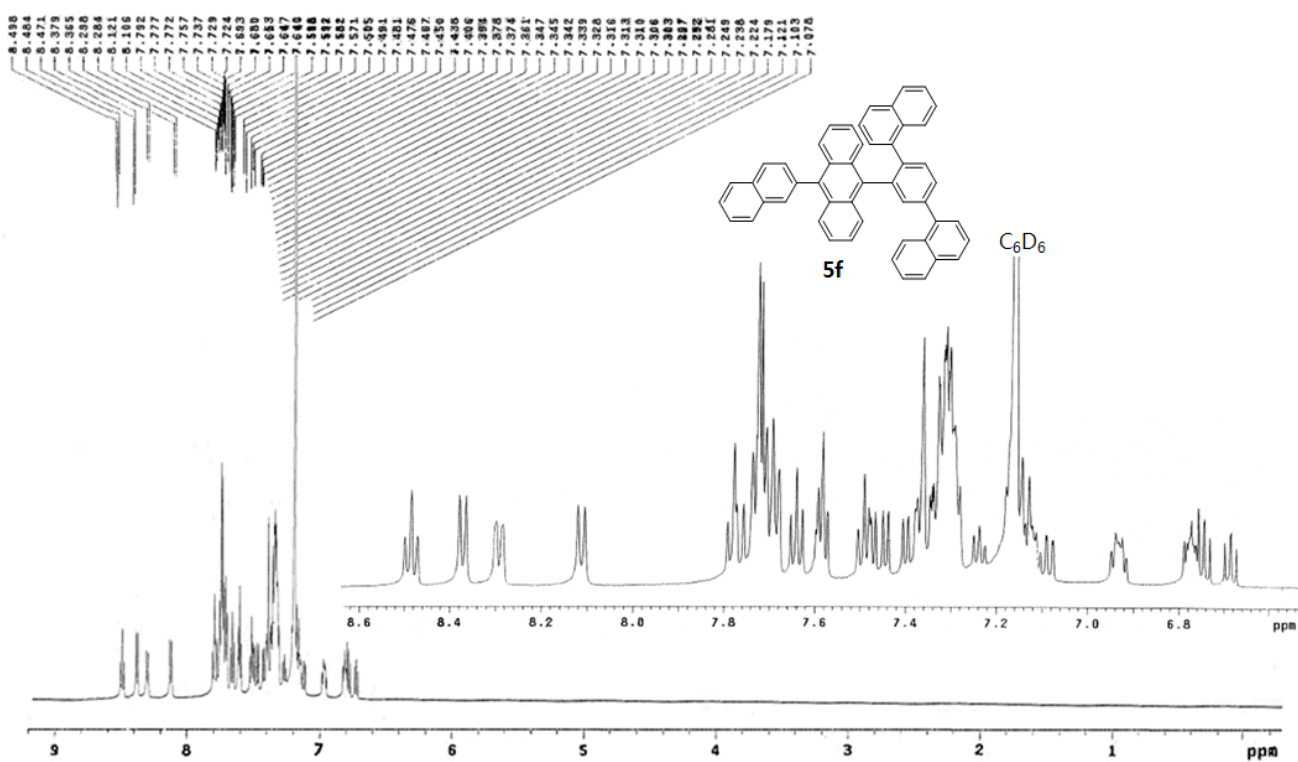
Figure S1 (d). $^1\text{H-NMR}$ spectrum of **5d** in C_6D_6 .Figure S1 (e). $^1\text{H-NMR}$ spectrum of **5e** in C_6D_6 .

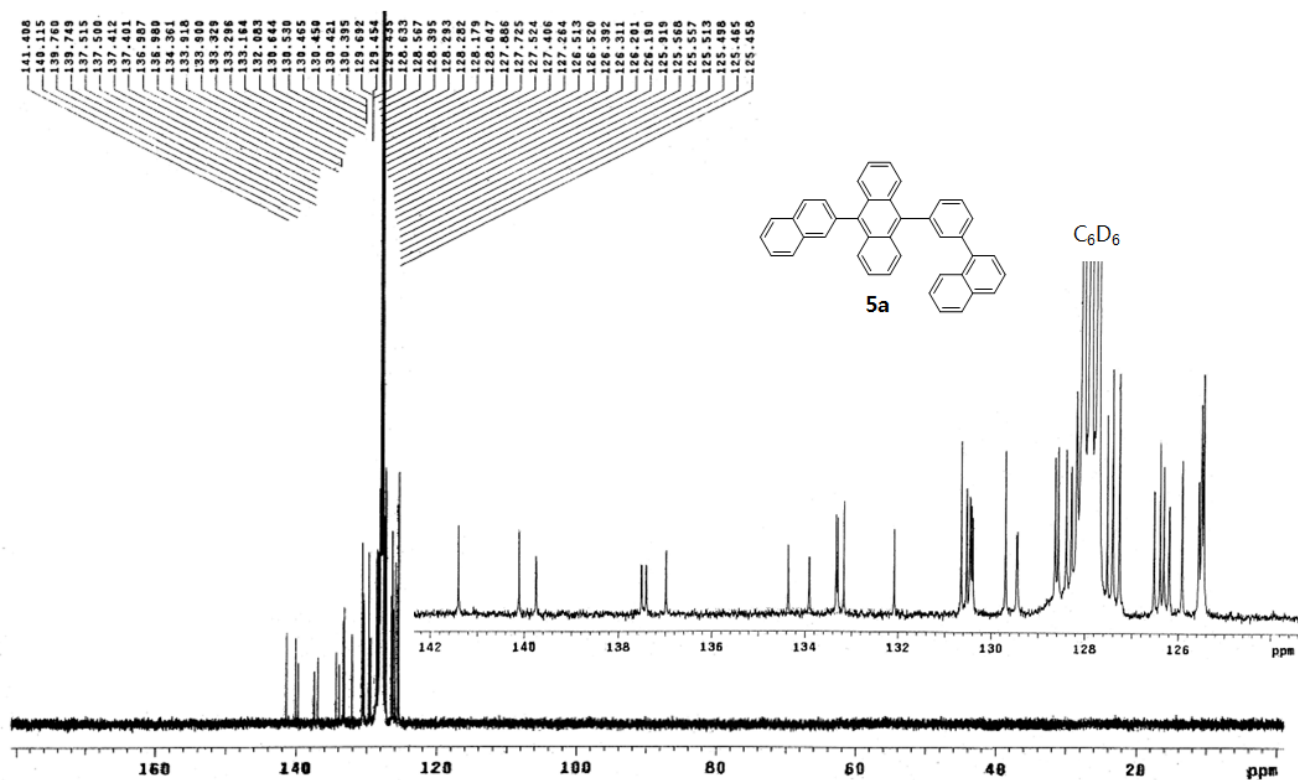
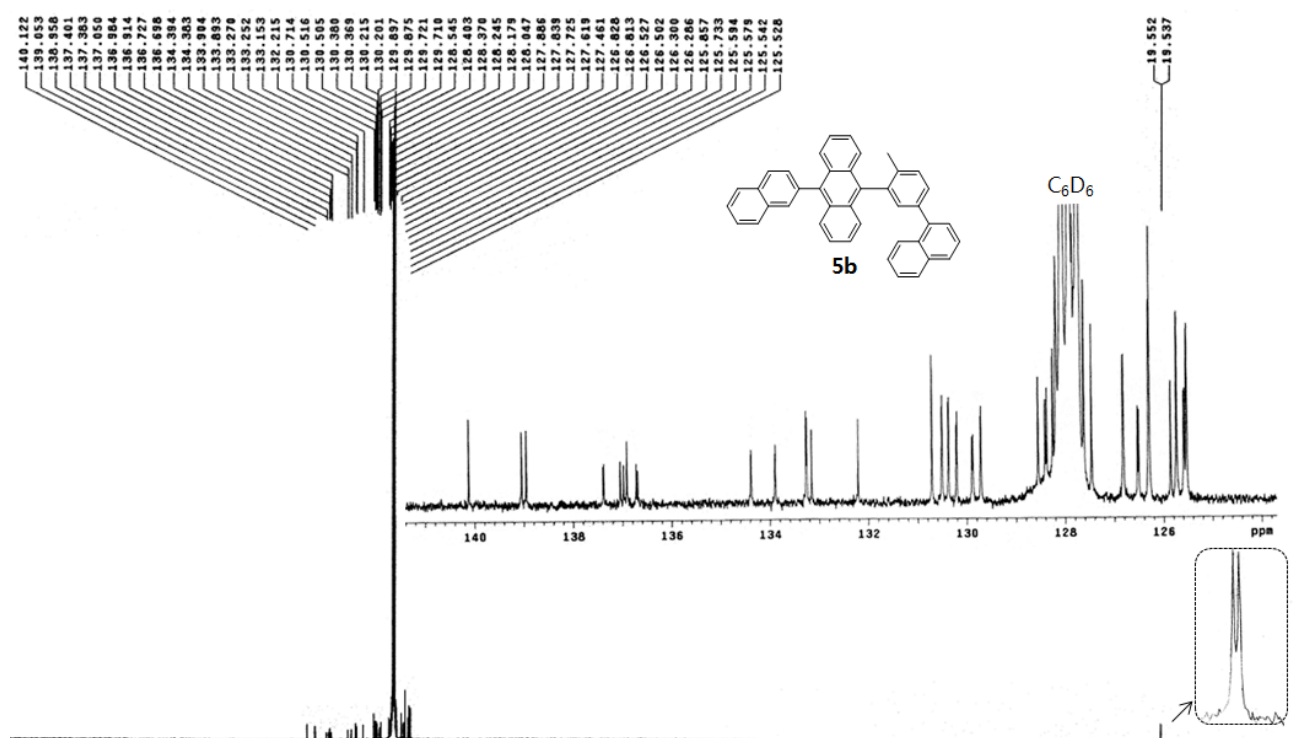
Figure S1 (f). $^1\text{H-NMR}$ spectrum of **5f** in C_6D_6 .Figure S2 (a). $^{13}\text{C-NMR}$ spectrum of **5a** in C_6D_6 .

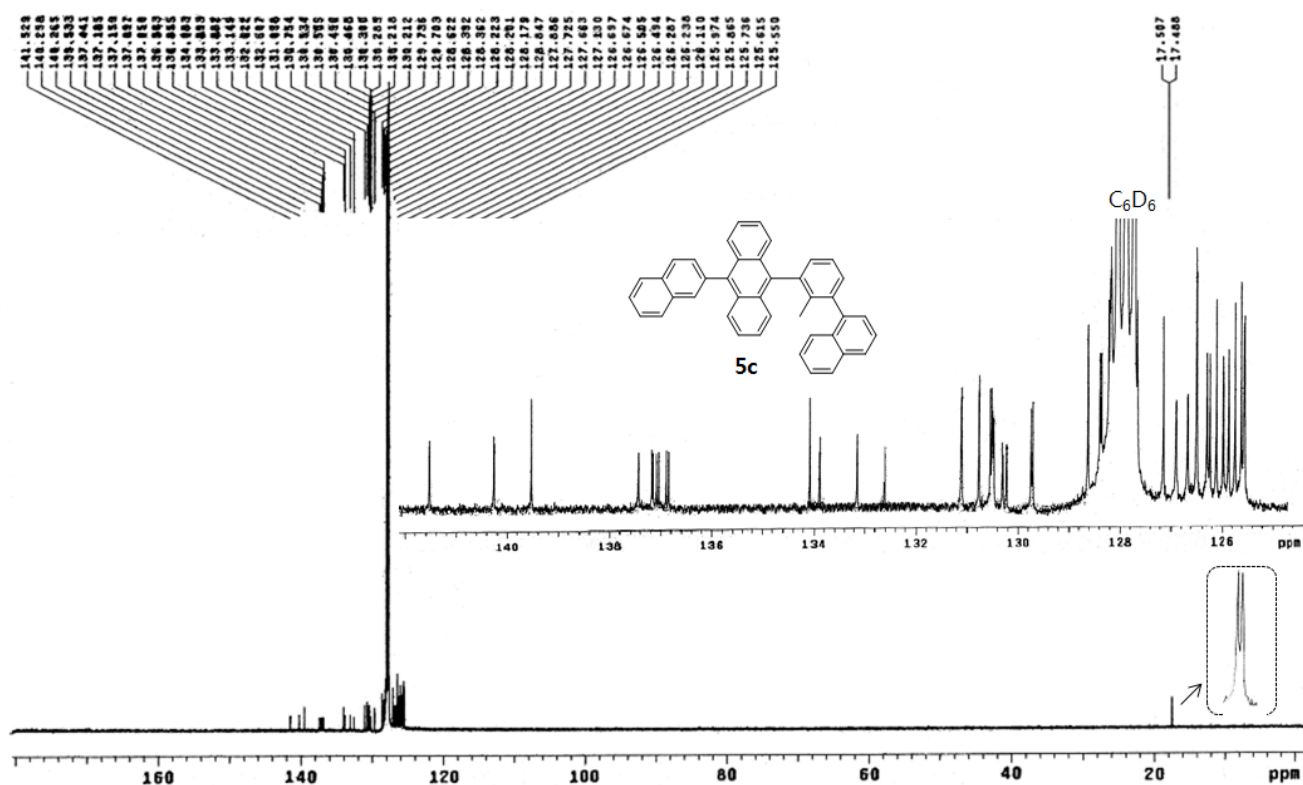
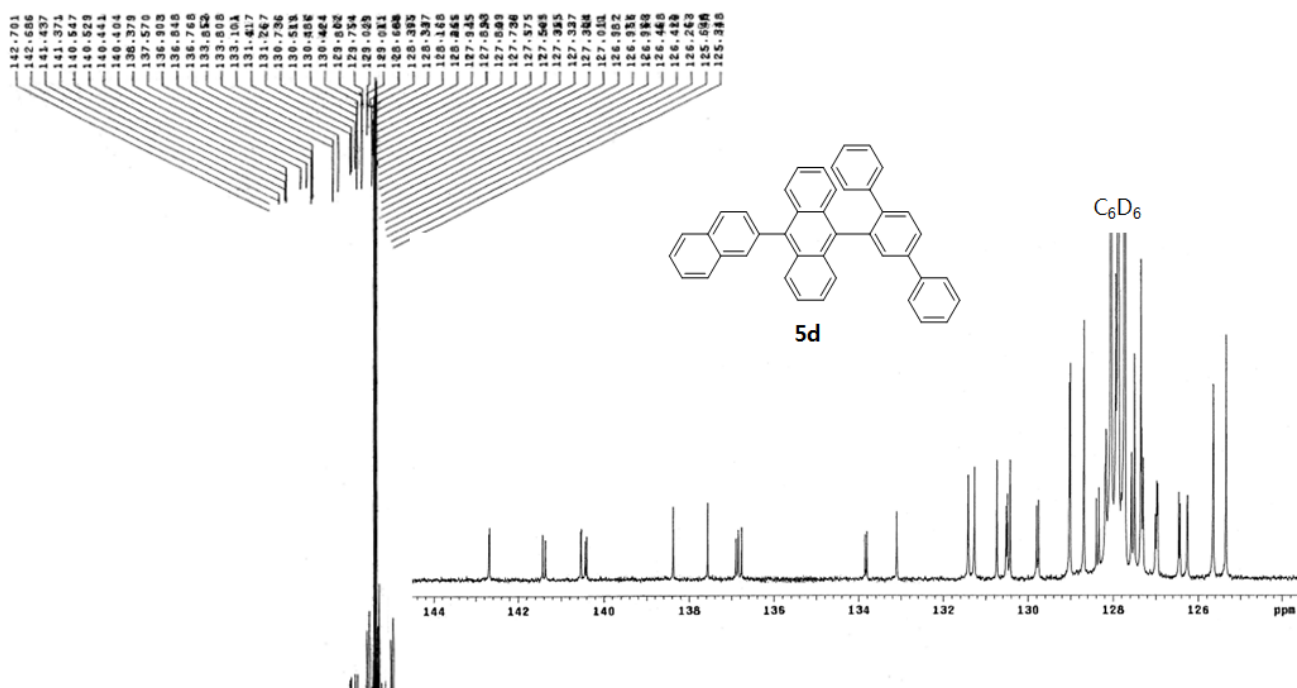
Figure S2 (b). ^{13}C -NMR spectrum of **5b** in C_6D_6 .Figure S2 (c). ^{13}C -NMR spectrum of **5c** in C_6D_6 .

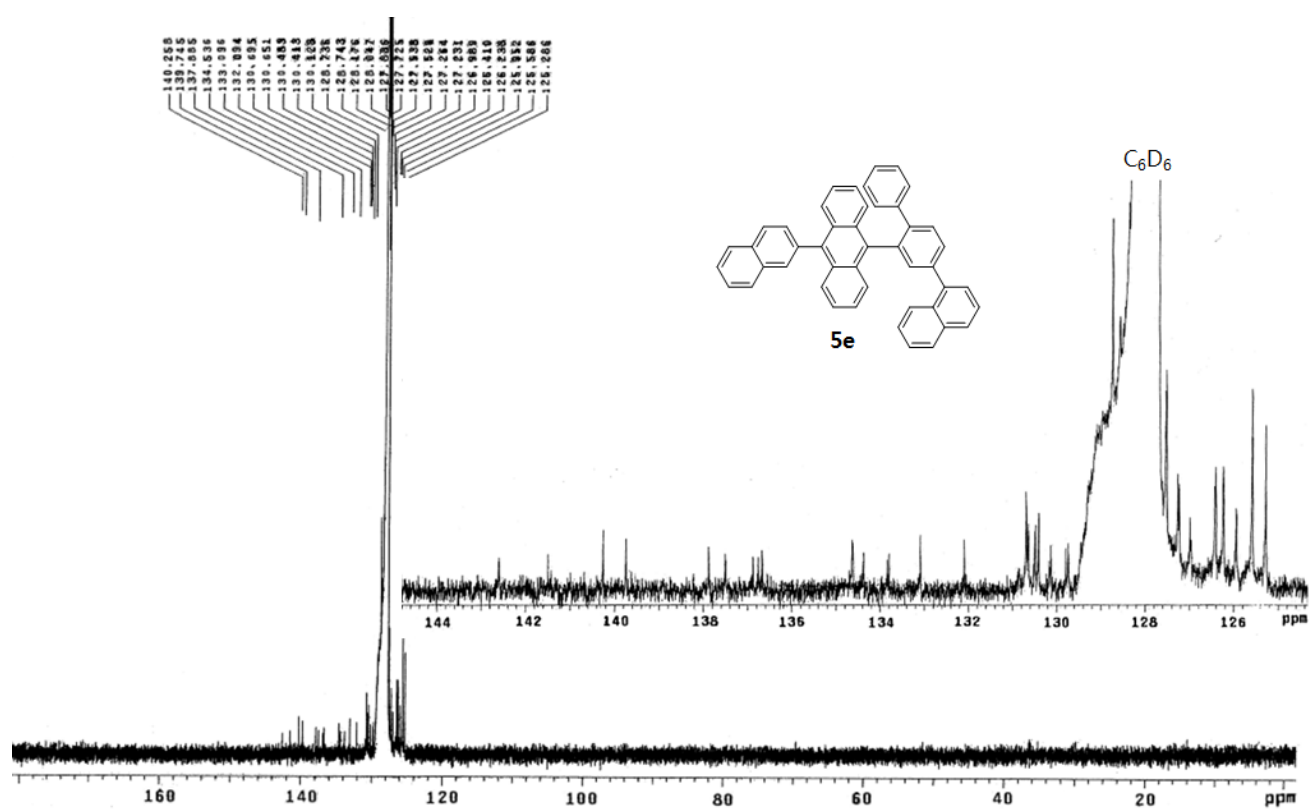
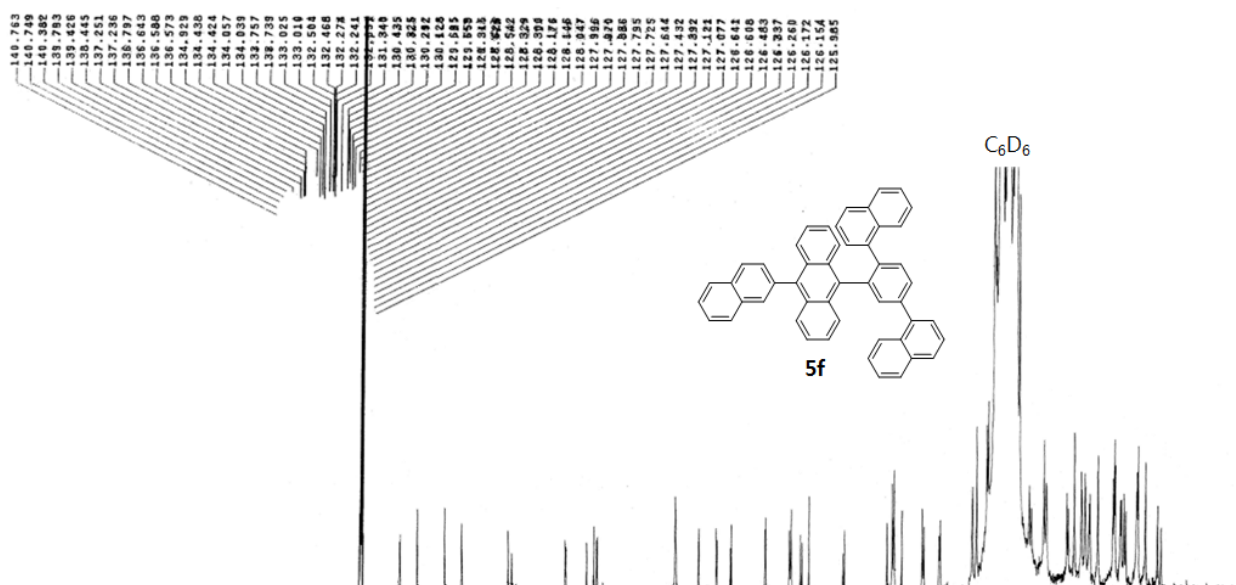
Figure S2 (d). ^{13}C -NMR spectrum of **5d** in C_6D_6 .Figure S2 (e). ^{13}C -NMR spectrum of **5e** in C_6D_6 .

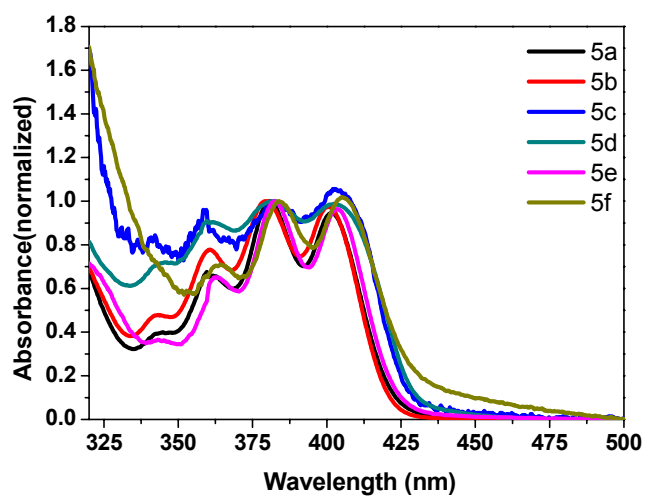
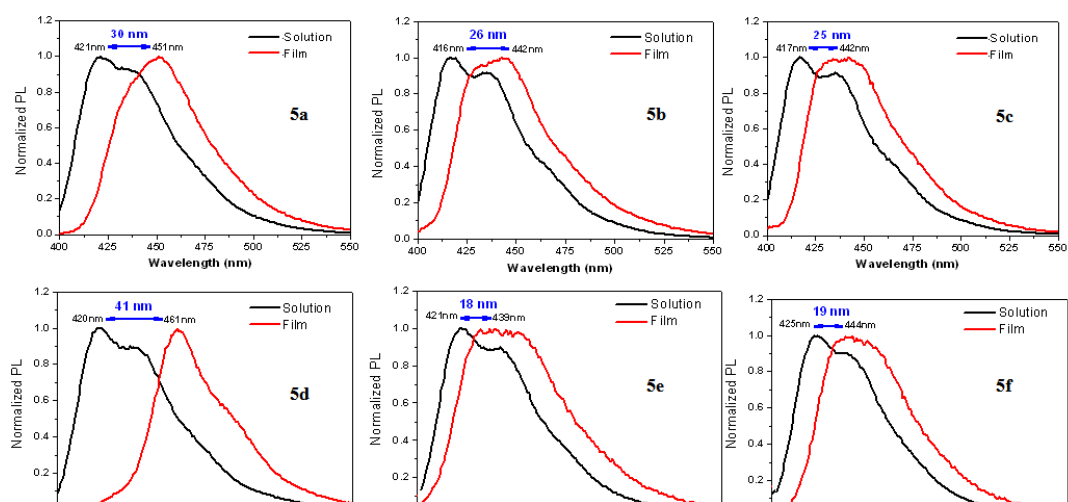
Figure S2 (f). ^{13}C -NMR spectrum of **5f** in C_6D_6 .**Figure S3.** UV/vis absorbance spectra of **5a-5f** in film state.

Figure S4. Photoluminescence spectra of **5a–5f** in solution (black line) and a film state (red line).

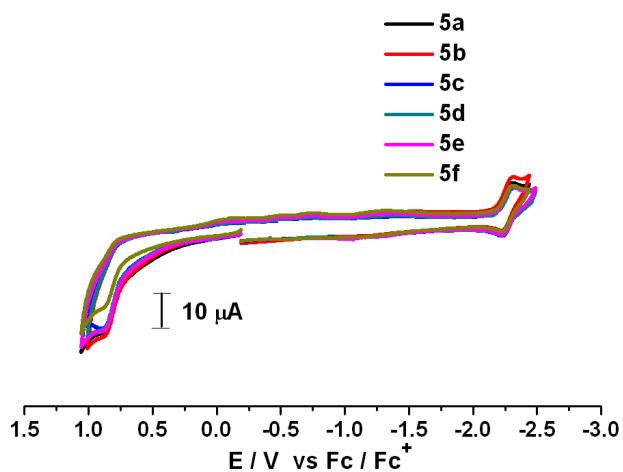


Figure S5. Cyclic voltammetry of **5a–5f** in DMF solution containing 0.1 M TBAP.

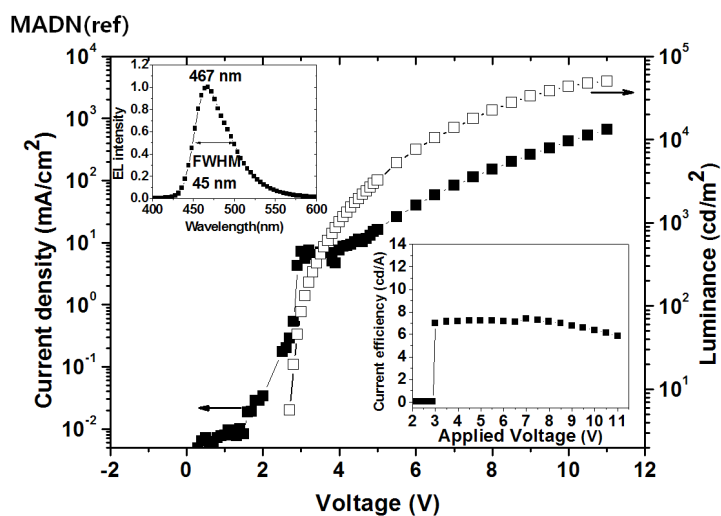


Figure S6. The I - V - L curve of the MADN(ref) based device. (The insets denote the current efficiency and EL spectrum.)

Theoretical Calculation

Task parameters

Calculate energy

Symmetry on

Electronic parameters

Spin_polarization: restricted

Charge: 0

Basis: dnd

Pseudopotential: none

Functional: pwc

Harris: off

Aux_density: octupole

Integration_grid: medium

Occupation: fermi

Cutoff_Global: 3.3000 angstrom

Scf_density_convergence: 1.0000e-005

Scf_charge_mixing: 0.2000

Scf_iterations: 50

Scf_diis: 6 pulay

Table S1 (a). Optimized Modeling Coordinates for **5a**.

ATOM	X	Y	Z
C	44.05717341975907	-44.13728205848126	-1.19885865840842
C	43.46360301349545	-46.25771420502752	0.33056931483415
C	45.23570438116833	-47.14139110844718	2.13325499277151
C	47.60725132685552	-45.80591048196364	2.50153322173261
C	48.15588323706400	-43.62982233323341	1.04345000829730
C	46.44112957707891	-42.81995338904341	-0.84784413962522
C	44.75619147165284	-49.33952879514289	3.64090418989751
C	46.47074980198674	-50.17578509259567	5.40638003604671
C	48.78117973934489	-48.85547748724027	5.78200991757448
C	49.32233744635777	-46.73567977466652	4.37838229181732
C	46.97773233359353	-40.69044415281536	-2.43536811241683
C	45.29225970023575	-39.88341008505122	-4.24066629892747
C	42.94021187656178	-41.14324233480389	-4.55397156721247
C	42.34223825724884	-43.19143551636861	-3.07015792411747
C	40.92230192842613	-47.49128127609081	0.10651586812438
C	40.30052929293682	-49.04767189381013	-1.91102001817347
C	37.84802173684233	-50.12205404103165	-2.16983339714145
C	35.97020821101466	-49.59058907757484	-0.27595647170677
C	36.65102131038331	-48.01899358361409	1.79523250361408
C	39.04691985840143	-47.00632868409986	1.98567129792204
H	42.99386653216775	-50.36227195557077	3.35228544388405
H	46.06379910266536	-51.86185494554937	6.52283086564090
H	50.12768809317743	-49.53282036158311	7.18958587284651
H	51.09739223675578	-45.73531197311341	4.66991558322035
H	48.77314550258406	-39.71429386051710	-2.19628957611944
H	45.75262026571005	-38.26455109317417	-5.43237899200931
H	41.60278380604821	-40.47499789459943	-5.97435962561674
H	40.53450353157196	-44.14084257462132	-3.31644136251984
H	41.71622189214653	-49.44576213787323	-3.35846901326916
H	35.23479403962269	-47.60683701763070	3.23903419689743
H	39.53282469283539	-S1145.78916081319653	3.57620522648554

C	37.17850623661059	-51.69251687850651	-4.24825969848813
C	34.76873757126656	-52.67661263201170	-4.46318157093246
C	32.91633625277803	-52.14600136178048	-2.59885041897575
C	33.50889554596065	-50.63537423407123	-0.55249473339565
H	38.60568355563811	-52.10122929012574	-5.68196437343632
H	34.28065447598448	-53.87169619398885	-6.07086151942052
H	31.02013001879634	-52.93369339857445	-2.79204226645809
H	32.08704352995543	-50.21816565158856	0.88425970440524
C	50.46384503714535	-42.06318377231221	1.58046098722889
C	50.22976186335800	-39.92472105905737	3.14291782423069
C	52.30641541640629	-38.35389048087858	3.57674261735233
C	54.64116884830899	-38.89851154376279	2.47384048912637
C	54.95283392691407	-41.05175201358085	0.94062086734140
C	52.83276818692510	-42.60985903552444	0.51449226921244
C	57.42391610753771	-41.59782774795184	-0.30802003690519
C	57.47400218921143	-42.01981295903531	-2.90430460653541
C	59.76380045578485	-42.41777719238094	-4.22385911256630
C	62.03614239239646	-42.38948153131616	-2.94477833738187
C	62.10225261272722	-42.00199623373501	-0.28801964614006
C	59.76918032275928	-41.63350721527330	1.07510134296962
C	59.90997552610404	-41.36532889220179	3.75093032823401
C	62.20388053793340	-41.35517339062251	5.00190762183140
C	64.49169344312209	-41.63958306271038	3.64536786284448
C	64.42843949469639	-41.97995473844392	1.05915161983767
H	48.40166433335001	-39.49511644767149	3.99313471909626
H	52.09621109594465	-36.67784944037503	4.75967680125956
H	56.23299894191135	-37.62452298900094	2.76695142405403
H	53.04261722564716	-44.28636421166155	-0.66738109992699
H	55.70276645594353	-41.96611307661399	-3.95792237317564
H	59.72005370039264	-42.70964731045821	-6.26453516202705
H	63.81670438707411	-42.65847852531898	-3.95231129254064
H	58.17005623402405	-41.18215803181371	4.83191904680563
H	62.24776850500002	-41.13773386062830	7.05226734794226
H	66.29474174438504	-41.61591432803251	4.64488667092086
H	66.18031000438539	-42.23773489264553	-0.00101683895115

Table S1 (b). Optimized Modeling Coordinates for **5b**.

ATOM	X	Y	Z
C	44.62210335230105	-43.54799413633403	-0.81770021869581
C	44.09200023509402	-45.77654802514787	0.57744814357754
C	45.86007162574507	-46.66945668855323	2.38725095906946
C	48.14536182403567	-45.23708378108410	2.90113025970846
C	48.66494667460838	-43.00315538644885	1.52086209605155
C	46.96198484328229	-42.18060826968627	-0.37365209794480
C	45.48105352385669	-48.98712351163100	3.73531723902423
C	47.17126633488805	-49.81151055078655	5.53021585826764
C	49.36142165591534	-48.36141357884794	6.09798227917187
C	49.82982950104019	-46.14998139863206	4.81581660167744
C	47.46733014829973	-39.97697259679498	-1.86712110014394
C	45.77321792142452	-39.11608472274747	-3.63946222114975
C	43.44221212634276	-40.39930401326345	-4.00963421080113
C	42.88943788355596	-42.53995493110529	-2.64299679475162
C	41.64347060162554	-47.15117700605258	0.21448798943630
C		41.06229266213140	48.38690697071114
			-2.02718588235924

C	38.73008289229979	-49.67708125839042	-2.37356472910303
C	36.92686815151867	-49.70617236754217	-0.33953317779572
C	37.55278021129779	-48.43442738823249	1.94229541639967
C	39.83306227064001	-47.19860282766356	2.21538989033123
H	43.81796982327645	-50.11831182772469	3.30704529462704
H	46.83785806181962	-51.59135013718168	6.51771494616298
H	50.68032044398840	-49.01910309362098	7.54069315450574
H	51.52408185110756	-45.05959168565163	5.23084587073454
H	49.24635886266325	-38.98375620108998	-1.57671583539780
H	46.20859640012298	-37.43827535968410	-4.75759944989679
H	42.08506837498150	-39.67960354387959	-5.38603448113567
H	41.09285393663441	-43.49674405328719	-2.93578065966101
H	42.42823154280853	-48.37927822949249	-3.57298880490641
H	36.18766201222058	-48.43641738700513	3.49050630923353
H	40.27575796353624	-46.21876230842403	3.97333073323648
C	38.11558902453023	-50.94174821180716	-4.66460586476941
C	35.83025085365222	-52.17576484871559	-4.94538231539430
C	34.05316871215498	-52.19968208426862	-2.93960781804703
C	34.59445677625541	-50.99226155488856	-0.68731968530947
H	39.48535601790507	-50.92188719212320	-6.20817951709118
H	35.38546564522616	-53.13731390187825	-6.71486365905310
H	32.25325537393682	-53.17573719673115	-3.18381713651831
H	33.22847094155325	-51.00646313773571	0.85978177010339
C	50.99338217003958	-41.48131985278607	2.09501327036361
C	50.86161262370069	-39.31246997872419	3.65776853291506
C	53.09821099159095	-37.95757278669264	4.10646850932002
C	55.41040758099101	-38.69960431599146	3.07478320077347
C	55.57487219742532	-40.86490767111469	1.54074841916832
C	53.33144809152843	-42.21759005688459	1.07774105604020
C	57.99704076939059	-41.65101519145011	0.33231423880508
C	58.04458875801610	-42.04170535115568	-2.26822505675447
C	60.29010542568135	-42.70229217701603	-3.55402545237498
C	62.52383461861657	-42.97557395682165	-2.23660757085649
C	62.58438942775424	-42.63864715354821	0.42727423892306
C	60.29069306814525	-41.99869626547417	1.75508866414699
C	60.40056765611570	-41.81536512985453	4.43964631139025
C	62.64631144051527	-42.14651567909129	5.73366246330425
C	64.90716051447922	-42.69796407113154	4.41450045716897
C	64.86364149754122	-42.95338614192643	1.81817490693800
H	53.02453767156823	-36.26662239854717	5.28817878564622
H	57.09621508137704	-37.56914591795191	3.42609824081260
H	53.40928826143622	-43.91529291835483	-0.08872916490303
H	56.31177549001133	-41.76017838446190	-3.34888208681718
H	60.24797454675272	-42.96531691269877	-5.59883189890384
H	64.27495153009336	-43.45403699875278	-3.21790293543760
H	58.67089767917874	-41.43843324403417	5.48754090829038
H	62.67286780710323	-42.00282629026623	7.79109903800869
H	66.67037071695454	-42.94713317990828	5.45456365106190
H	66.58975497211642	-43.41662434643907	0.78590974348890
C	48.38902014183261	-38.45118349907596	4.81095260536870
H	47.46969744601103	-39.98762992837484	5.87093054952849
H	47.04452841868299	-37.84063091970173	3.34454782420498
H	48.69466367239109	-36.85621584972457	6.10539290631145

Table S1 (c). Optimized Modeling Coordinates for **5c**.

ATOM	X	Y	Z
C	45.02799229577102	-43.70221297708235	-0.76731538454981
C	44.32536632206762	-45.78747030577909	0.76494524846987
C	45.98058582722323	-46.64916970381371	2.68772239048205
C	48.36870849616716	-45.36529903604080	3.12172901494117
C	49.05859822223471	-43.26570441948442	1.60963366262937
C	47.43155442210892	-42.44172532117666	-0.34906999815949
C	45.39097041931799	-48.80047189477344	4.22650166589525
C	47.00391582887114	-49.62155773923588	6.09251525046966
C	49.32954172863258	-48.34810786035460	6.53169991348388
C	49.98753945395715	-46.29260987442356	5.08390048379612
C	48.07462442409472	-40.34301794048460	-1.93581459498482
C	46.47872471268560	-39.51697546911821	-3.81287057307268
C	44.10982935699770	-40.72705140385460	-4.19906781631950
C	43.40914742392757	-42.74152596217584	-2.71366036309287
C	41.82669463134787	-47.06609691930444	0.37682373301477
C	41.38265009162787	-48.58686463676413	-1.71387055128263
C	39.02380659171047	-49.81485728976899	-2.10022539957800
C	37.04534582349781	-49.47346314181071	-0.26692096544835
C	37.53305136661792	-47.90593098987626	1.86077529966073
C	39.84368354246596	-46.73635228851015	2.17607020767040
H	43.62649736011647	-49.80201717144694	3.88708472326375
H	46.50819005752997	-51.26832938059698	7.23062013614589
H	50.60112525919077	-49.01978547939389	8.00999967967630
H	51.77946825332184	-45.33400969541525	5.40956841597987
H	49.87463268892531	-39.39593234652576	-1.62273539463616
H	47.01925747404087	-37.91946637056503	-4.99919698733935
H	42.83752556866533	-40.04130314676053	-5.67014818620757
H	41.58601213708956	-43.64627940814567	-3.01073902746380
H	42.88369466949086	-48.86530366246830	-3.10144818503964
H	36.03658807636619	-47.62999951546666	3.25563349637732
H	40.18530585028738	-45.53498516606944	3.81568766150653
C	38.55257414460070	-51.37777731754127	-4.23628494434024
C	36.24532066111416	-52.55789394247285	-4.55355113527500
C	34.29462873989659	-52.21847531987483	-2.74559836354918
C	34.69001500697279	-50.70867377571506	-0.65159470582402
H	40.05494492469931	-51.63431349338070	-5.62789811091389
H	35.91035432208374	-53.75375624357859	-6.19975446040126
H	32.47807090372910	-53.15583961273640	-3.01700451647643
H	33.19040058895900	-50.44227844136783	0.74115781253519
C	51.45761379790696	-41.83522295023216	2.15588249213396
C	51.34214491384896	-39.87389300287683	3.94345518932162
C	53.47917904895537	-38.44065930437078	4.52090471995813
C	55.75504456512019	-38.96446128288184	3.29999930148163
C	55.93429926858067	-40.91556120163896	1.50210656804044
C	53.76813427582320	-42.38912419355455	0.91969190673243
C	58.42304772584890	-41.30584521762629	0.20497736256635
C	58.63418262493325	-40.81155325519547	-2.36608502680441
C	60.96943172443964	-41.01383841943785	-3.64889765203774
C	63.12610772769128	-41.69774387797578	-2.35081947523655
C	63.02381313923355	-42.23707793313763	0.27807348275173
C	60.63852217764477	-42.06353970600730	1.58894668145070
C	60.58526160930435	-42.67441531516534	4.21329745970988
C	62.75975860674762	-43.35773849995129	5.48788286368132
C	65.10589442601901	-43.48088498031745	4.20464095125390

C	65.22503527281526	-42.94540309973605	1.65375949141308
H	53.36801000236876	-36.91620529626935	5.90561497777939
H	57.43529278037458	-37.84356788858149	3.71301331179699
H	56.95849086439910	-40.21286344290924	-3.40842201287025
H	61.05906792386759	-40.59238606387847	-5.66589341114536
H	64.94001310836495	-41.83242681508158	-3.32575873843734
H	58.78692865849317	-42.59454200592721	5.21026648867170
H	62.67338356627507	-43.81290570119162	7.49786463593492
H	66.81027018822633	-44.01920731012704	5.23589002219368
H	67.02484209851011	-43.06056680436323	0.65032389713030
C	53.91675264485898	-44.53769587199313	-0.97884656109231
H	49.54457142507014	-39.48583440207361	4.87654121026634
H	55.74076518980738	-45.52247625626587	-0.85422089571209
H	53.73460422646001	-43.84458305550297	-2.93671150284539
H	52.39146909045237	-45.90856683203184	-0.66748848739349

Table S1 (d). Optimized Modeling Coordinates for **5d**.

ATOM	X	Y	Z
C	44.67951869139713	-43.47131203027990	-0.71477784999127
C	44.22356762420125	-45.77739821860069	0.57277197470727
C	46.07031538101149	-46.76014505725196	2.24808760415349
C	48.37621216397250	-45.35185911675696	2.73326076686748
C	48.80540877025991	-43.01912078107956	1.49133433544300
C	47.02008233571497	-42.10301263789797	-0.28399226182247
C	45.73809369343311	-49.13596379498510	3.50670783459218
C	47.50456688411874	-50.05350972495054	5.17828238834657
C	49.72846425532428	-48.64162646023002	5.70825908098611
C	50.14683974368913	-46.36910311557959	4.51681603103533
C	47.44109802281001	-39.81547850510724	-1.66906755803929
C	45.66931870037364	-38.88043930292397	-3.32359324646866
C	43.34485642404010	-40.17569983382209	-3.68638799477190
C	42.87071013640862	-42.39656588968135	-2.42242161007286
C	41.76283279582228	-47.13913001523383	0.23062039806193
C	41.15707234080308	-48.36296248719712	-2.00962069850344
C	38.81069406966986	-49.63187687031060	-2.34167819911719
C	37.02262096733512	-49.64804246630645	-0.29419088128275
C	37.67521041932216	-48.38684008763440	1.98605392777810
C	39.96887544727200	-47.17200695068178	2.24480255528041
H	44.04582214673104	-50.23447061110667	3.10735026082117
H	47.20131570148107	-51.87175523772574	6.10345078563992
H	51.11197117712311	-49.37282052736501	7.05142834355784
H	51.86418248909218	-45.30806718746173	4.91491640780990
H	49.21568717902165	-38.81278244380512	-1.39365583957230
H	46.04283333019147	-37.13553077104658	-4.35794442756453
H	41.93238570015910	-39.40409547583639	-4.97641433012368
H	41.08351748960086	-43.37181569913516	-2.71050976634385
H	42.51115082977795	-48.35978762636465	-3.56629431404834
H	36.32128130185912	-48.38235451087192	3.54409379452438
H	40.43763881791109	-46.20154851347200	4.00121948335421
C	38.16859818559669	-50.88718628546050	-4.63006896365765
C	35.87196872537731	-52.10350442589392	-4.89543638903809
C	34.10974481632005	-52.11580548472099	-2.87654780843408
C	34.67677828049053	-50.91432718402317	-0.62758344316818
H	39.52727335022266	-50.87525348512231	-6.18352663383440

H	35.40560402568266	-53.05815621302640	-6.66316138533152
H	32.30060971854686	-53.07751153633013	-3.10834815337819
H	33.32177295644040	-50.91992760660282	0.92925067437541
C	51.13465390184184	-41.49453474348295	2.06747828642510
C	51.04282556152738	-39.30334821969623	3.61727851451913
C	53.29230290995744	-37.93170421427376	3.98262675713850
C	55.57302687230536	-38.68034501156186	2.90149460646426
C	55.70730436300187	-40.86515165554442	1.38958383693117
C	53.45295249815773	-42.22207512720047	0.99778767343698
C	58.13772749300715	-41.70225553106906	0.26136816396705
C	58.22602825321819	-42.82927209910756	-2.14904027382579
C	60.51935600662869	-43.59314756038999	-3.21069440694818
C	62.78349741247020	-43.25187562479968	-1.88827779731742
C	62.72936808789725	-42.14118109184455	0.51016593589105
C	60.43454364871905	-41.38164746152746	1.57132193342745
H	53.24023145934009	-36.25017789220337	5.17493648084363
H	57.26222654635905	-37.54092568719514	3.21012853790868
H	53.49298958699602	-43.92861880778484	-0.15709937484708
H	56.48351703168242	-43.05856012686781	-3.22527225127436
H	60.53855381937018	-44.44585524089995	-5.08874963819587
H	64.57436593185959	-43.84992487095213	-2.71686585449609
C	48.67751169793950	-38.38386449464237	4.84571158520495
C	47.20240605833739	-39.96722080685641	6.39462816791429
C	45.02742736592540	-39.04979582125270	7.57866366908936
C	44.27778905969470	-36.53717829188120	7.23831686404134
C	45.72862256750834	-34.94026999017547	5.70987675835870
C	47.90933908070706	-35.85642285750526	4.53321916749481
H	47.78370869707906	-41.91698213244371	6.70040580288723
H	43.91974909853771	-40.30431024940880	8.78496349639099
H	42.57147763401001	-35.82793150396189	8.15355211060045
H	45.15461209842410	-32.98091599714823	5.41794440782067
H	49.01974511484386	-34.61106039564922	3.32150364968060
H	64.47959720981999	-41.88181947687154	1.56997474389349
H	60.41455947180407	-40.56579242811188	3.46433363074826

Table S1 (e). Optimized Modeling Coordinates for 5e.

ATOM	X	Y	Z
C	44.60766574077117	-43.53893238177974	-0.70059799899456
C	44.13148624577920	-45.83331277311309	0.60121851339559
C	45.95423102449294	-46.80059035527915	2.31280604875209
C	48.24452695044138	-45.37920179649581	2.83201482870811
C	48.69249149268164	-43.05723874343381	1.57599326648856
C	46.94038164350973	-42.16447612751203	-0.24335854676227
C	45.61106460066780	-49.17233224700311	3.57557582296399
C	47.34441753665934	-50.06632895423999	5.29387293675195
C	49.54637096401582	-48.63605106896262	5.86465872237444
C	49.97902457102561	-46.37127796169260	4.66328621232455
C	47.39267279875084	-39.89970851556557	-1.65673561541815
C	45.65759118854330	-38.99213306976371	-3.36445874966617
C	43.33151155609061	-40.28137461319413	-3.73995435481440
C	42.82627927181326	-42.47847914126388	-2.44654801941067
C	41.67482243549404	-47.19714219220114	0.24919220500945
C		41.06856799850686	48.41747675654062
			-1.99332771229006

C	38.72350204579142	-49.68847885994413	-2.32516100823743
C	36.93580427896991	-49.70871838421202	-0.27693065198037
C	37.58841855250959	-48.45083000501729	2.00463046659983
C	39.88205764207864	-47.23645128672650	2.26412841586412
H	43.93576405879495	-50.28512983537575	3.14539430275859
H	47.03310791931783	-51.88150414205252	6.22232026020573
H	50.90177311543439	-49.34695491236752	7.24669403885070
H	51.68032823381743	-45.29615905371865	5.09080010253533
H	49.16583195007082	-38.89851320672179	-1.36690421325302
H	46.05721661398499	-37.26922253924091	-4.42562374985782
H	41.94220598511080	-39.52339950804246	-5.06276988185070
H	41.03615076161552	-43.44613302837265	-2.74162024817113
H	42.42262766958898	-48.41247398063499	-3.54977978768242
H	36.23496252042304	-48.44778390823326	3.56308648694363
H	40.35106278616789	-46.26739337468083	4.02117096800723
C	38.08172232234759	-50.94372676828811	-4.61384296634567
C	35.78647372469200	-52.16253588522826	-4.87890329233354
C	34.02385777494256	-52.17630939786494	-2.86025303453979
C	34.59026283147717	-50.97535403729823	-0.61102147522790
H	39.44046159782208	-50.93119251347775	-6.16718636478364
H	35.32088274690305	-53.11805402486164	-6.64635551044028
H	32.21532596278615	-53.13906903981890	-3.09243617752558
H	33.23511444571075	-50.98110682282616	0.94568030290544
C	51.00962621423606	-41.52430181522851	2.17427230333782
C	50.88979958960848	-39.30166093237210	3.67515720690215
C	53.13159784884675	-37.91845131929480	4.05205734343388
C	55.43627349456523	-38.68944911865808	3.03710238687399
C	55.59540567993031	-40.90833801832345	1.57845703093910
C	53.35114438378608	-42.27359612138459	1.16823412910282
C	58.01824664857619	-41.73403271772186	0.40081112842964
C	58.07521828564731	-42.18971770769990	-2.18882618593673
C	60.32789185070477	-42.87261535450838	-3.4499291870488
C	62.55679709062785	-43.10538005126051	-2.11652979973717
C	62.60699644815468	-42.70668132672353	0.53910736172617
C	60.30785106515399	-42.03576101542882	1.84200570074890
C	60.40940901380177	-41.77603650123022	4.52071451713393
C	62.64989745095047	-42.08080263383859	5.83079047817529
C	64.91402437015151	-42.67112520749542	4.53555770357449
C	64.88022336807705	-42.98965969000871	1.94602125900921
H	53.04979075829846	-36.20789663264917	5.20095308873796
H	57.12390625306951	-37.55104976451869	3.35310965927182
H	53.42498649225655	-43.99321822609372	0.03371550708510
H	56.34517873875154	-41.94058205652419	-3.28150453488879
H	60.29573983876480	-43.18508309995423	-5.48770941516894
H	64.31288582807579	-43.60266726172480	-3.07921919679161
H	58.67892692706260	-41.36306901219261	5.55369263456574
H	62.66977039669600	-41.88007014039010	7.88345703076146
H	66.67200176980863	-42.89778000394570	5.58927445595887
H	66.61011827722494	-43.47909469725033	0.93251473217070
C	48.50722913066157	-38.36235816790015	4.85267901298670
C	47.01427536606986	-39.92314993130842	6.40847157396144
C	44.83034750331694	-38.98867422655836	7.56177770760494
C	44.08931330910594	-36.47805989380674	7.18489753036054
C	45.55796388426030	-34.90275090848640	5.65087815191304
C	47.74699111060056	-35.83660178474186	4.50370328948414
H	47.58990800440569	-41.86998482701856	6.74198786188545
H	43.70819482387279	-40.22760756612688	8.77096067493767
H		42.37762023065563	35.75346534934342
			8.07816048717871

H	44.99129957241915	-32.94532543955122	5.33188487035277
H	48.87209346922239	-34.60705405532176	3.28934384262037

Table S1 (f). Optimized Modeling Coordinates for **5f**.

ATOM	X	Y	Z
C	44.68608281004984	-43.56160360940471	-0.73019678306978
C	44.19459278422880	-45.79171645235180	0.67479129242956
C	46.01353238207135	-46.69252804867764	2.42701302283670
C	48.30920381161660	-45.25928933294873	2.88691137074945
C	48.76937152487066	-42.99854813778008	1.52867920328061
C	47.02873336207546	-42.18630783296763	-0.33666140446727
C	45.66770752554864	-49.01446721938087	3.77715395751506
C	47.40214218612757	-49.85008510498767	5.52331576142772
C	49.60920398350608	-48.40626143796894	6.03596465382783
C	50.04211299267085	-46.18622737372046	4.75366313148117
C	47.51026650598159	-40.00877467303057	-1.87188633558594
C	45.79049452331405	-39.17403109189221	-3.63044273032024
C	43.45140933268625	-40.45607019364108	-3.94238285478336
C	42.91962257721624	-42.57428108995959	-2.53402629711279
C	41.73942094484467	-47.16771399559295	0.36005801102423
C	41.13163894774435	-48.42502839315393	-1.86161177559160
C	38.78703268224717	-49.70002649252408	-2.17417595187189
C	37.00063518117020	-49.69002182321491	-0.12505485619828
C	37.65438375903696	-48.39603019238712	2.13672545212334
C	39.94674417109271	-47.17459857400193	2.37629443849059
H	43.98990436834586	-50.13879477139419	3.38969881996286
H	47.08911638565974	-51.63084630514478	6.51583172447531
H	50.96716972037829	-49.07106406329015	7.43844863623141
H	51.74892038642568	-45.10221567160503	5.13388843199217
H	49.29223698912924	-39.01259933093097	-1.63099854904031
H	46.20955190045383	-37.51279740484244	-4.77829724597808
H	42.07301460760487	-39.75429912825717	-5.30665490442167
H	41.11990265246698	-43.53562317086841	-2.78590426025958
H	42.48410070798914	-48.43912510753950	-3.41889513205772
H	36.30110011910588	-48.37022904350665	3.69519382749655
H	40.41358116058916	-46.17315457342065	4.11585294972797
C	38.14327311919835	-50.98284601336804	-4.44712670532863
C	35.84521144499747	-52.19899958700186	-4.69736988908140
C	34.08505845467523	-52.18724363290362	-2.67643167939688
C	34.65509958993873	-50.96123609750883	-0.44159302258449
H	39.50094646819587	-50.98868433734901	-6.00155104033819
H	35.37629831167325	-53.17265918436259	-6.45409481605741
H	32.27523099715465	-53.15069201388972	-2.89540217668043
H	33.30166900679390	-50.95059506292708	1.11672394415213
C	51.09944425256039	-41.45855159528347	2.05378413850622
C	50.99228338500475	-39.17125036556846	3.45045723386242
C	53.25133988744324	-37.81366039128758	3.81739811309350
C	55.55700511659298	-38.65994527253364	2.86112907944599
C	55.69620630004651	-40.92833881537969	1.47626571979354
C	53.44150720936526	-42.28450324074311	1.10643938750659
C	58.10827594316350	-41.80631973087984	0.31383832789951
C	58.14989987282348	-42.31752512007458	-2.26599556732083
C	60.39264095610974	-	43.03811222816929
			-3.52399541201104

C	62.62617141032786	-43.25726702666236	-2.19621687457596
C	62.69083088602273	-42.80500306080074	0.45039995701946
C	60.40285332332758	-42.08963259269668	1.74981635282469
C	60.51879073663238	-41.76590447382887	4.42013176354268
C	62.76270669288618	-42.06041290279993	5.72685924138440
C	65.01598332813163	-42.69735235166707	4.43453439624199
C	64.96840793091840	-43.07260425395476	1.85291545627535
H	53.18157402026958	-36.05447796619287	4.89047643999563
H	57.25918547246706	-37.53641985823778	3.15216455273701
H	53.50289694485838	-44.05155671907858	0.04663044911306
H	56.41515064276460	-42.08375308024508	-3.35436647076413
H	60.34894246243304	-43.39169503026528	-5.55459401125064
H	64.37394808159036	-43.78709186091050	-3.15701225393737
H	58.79650590765765	-41.30969652104300	5.44924419674197
H	62.79441656749440	-41.80966534169578	7.77376760949510
H	66.77708865727291	-42.91527331584778	5.48454408044588
H	66.69034668489923	-43.59613998139316	0.84272598271157
C	48.58590971468948	-38.21764232708715	4.59344835981361
C	47.38131365501350	-39.65451742390113	6.43323436746910
C	45.13132348026654	-38.82644822882460	7.61074966344715
C	44.06493591012367	-36.54189454562203	6.94431171827024
C	45.20799690680860	-34.99844056776603	5.06819716205360
C	47.50691606691540	-35.83214422883836	3.86091877598294
C	48.56992304363232	-34.25698583012373	1.95337134877238
C	47.46458488646616	-31.98291811057711	1.29480208334021
C	45.22024285366297	-31.16353967146312	2.49937591605749
C	44.12133487136177	-32.64902544249927	4.34141954360972
H	48.20469473815065	-41.45501279398633	6.99826168515721
H	44.25492616848722	-40.00338197670548	9.05964973766024
H	42.32420034895426	-35.89123418464490	7.84124119352571
H	50.28832376732426	-34.86713506635384	1.00107625042873
H	48.32184831304908	-30.81423433626065	-0.17292770386249
H	44.35968071359735	-29.36894713871907	1.95775950826339
H	42.37965264055170	-32.04212619883290	5.26838309568414
