

Supplementary material

Stable Negative Differential Resistance in Porphyrin Based σ - π - σ Monolayers

Grafted on Silicon

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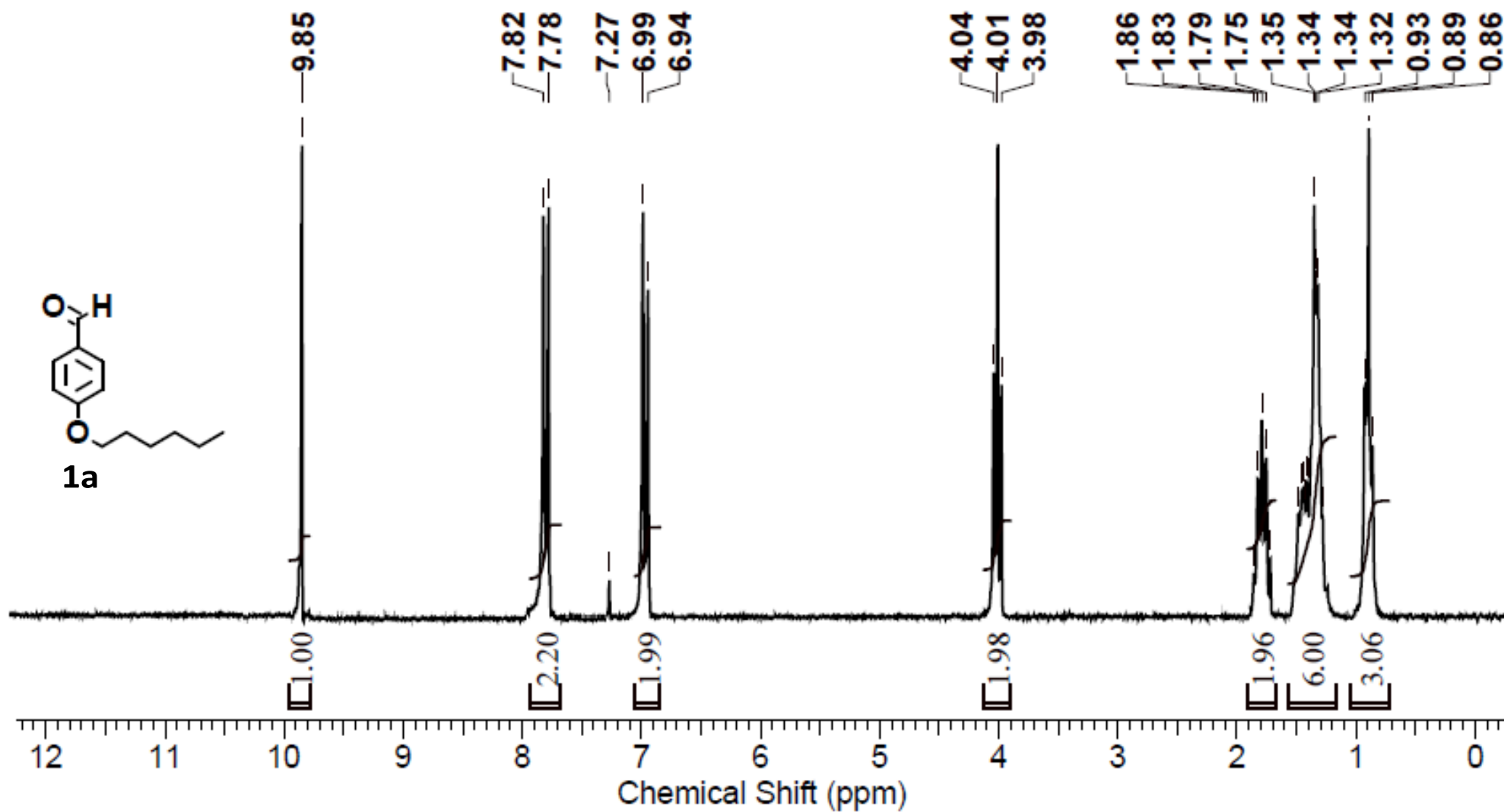
E-mail: schatt@barc.gov.in

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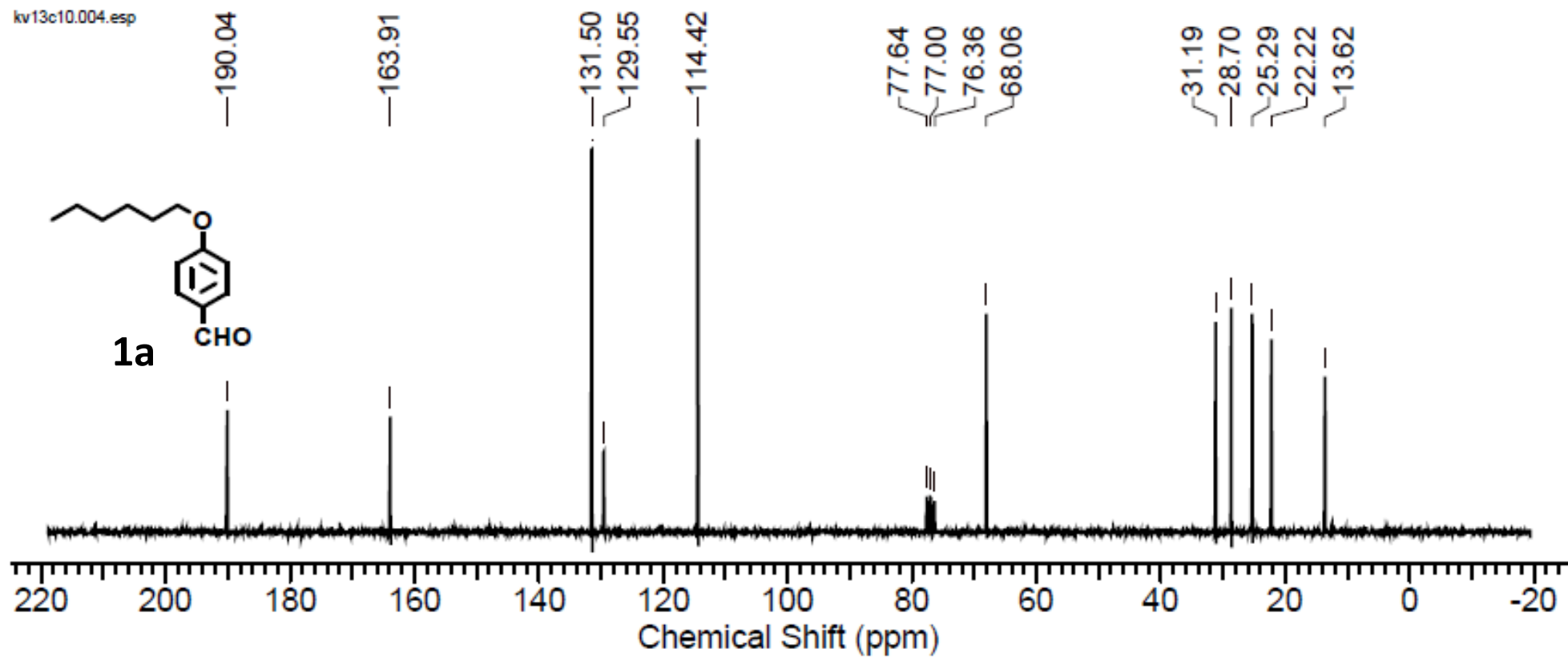
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CHLOROFORM-d

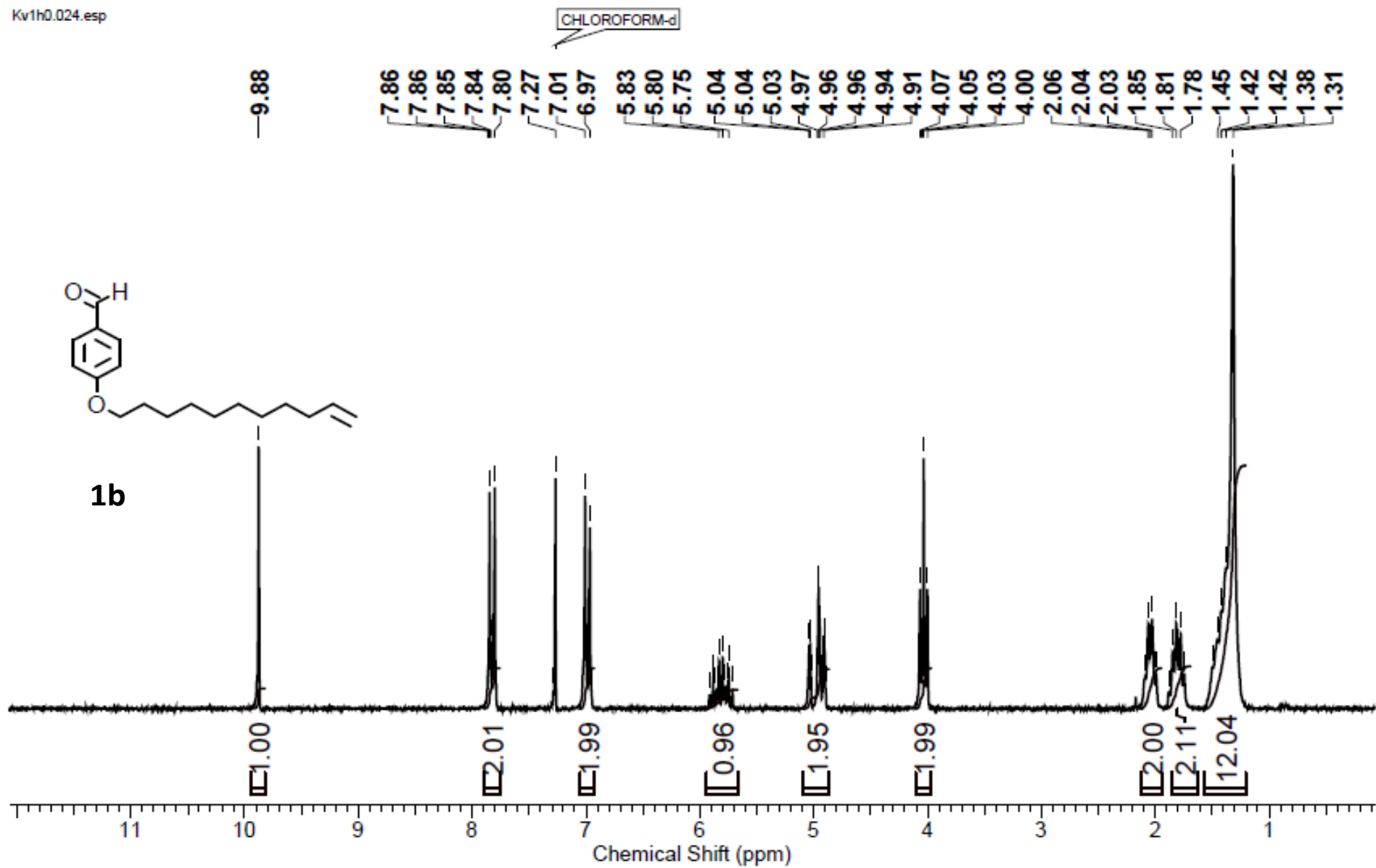


^1H NMR of *p*-hexyloxybenzaldehyde (1a)

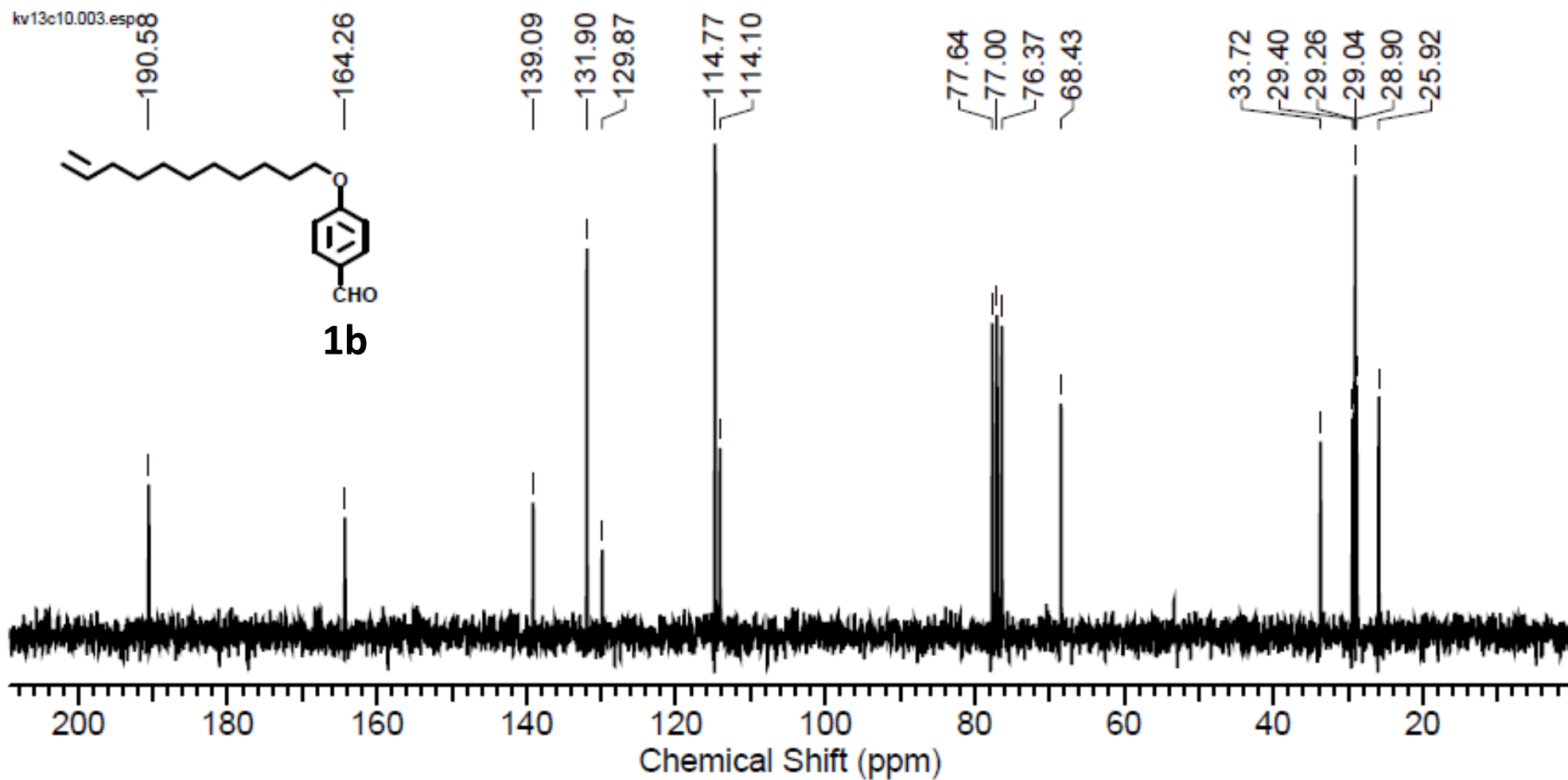
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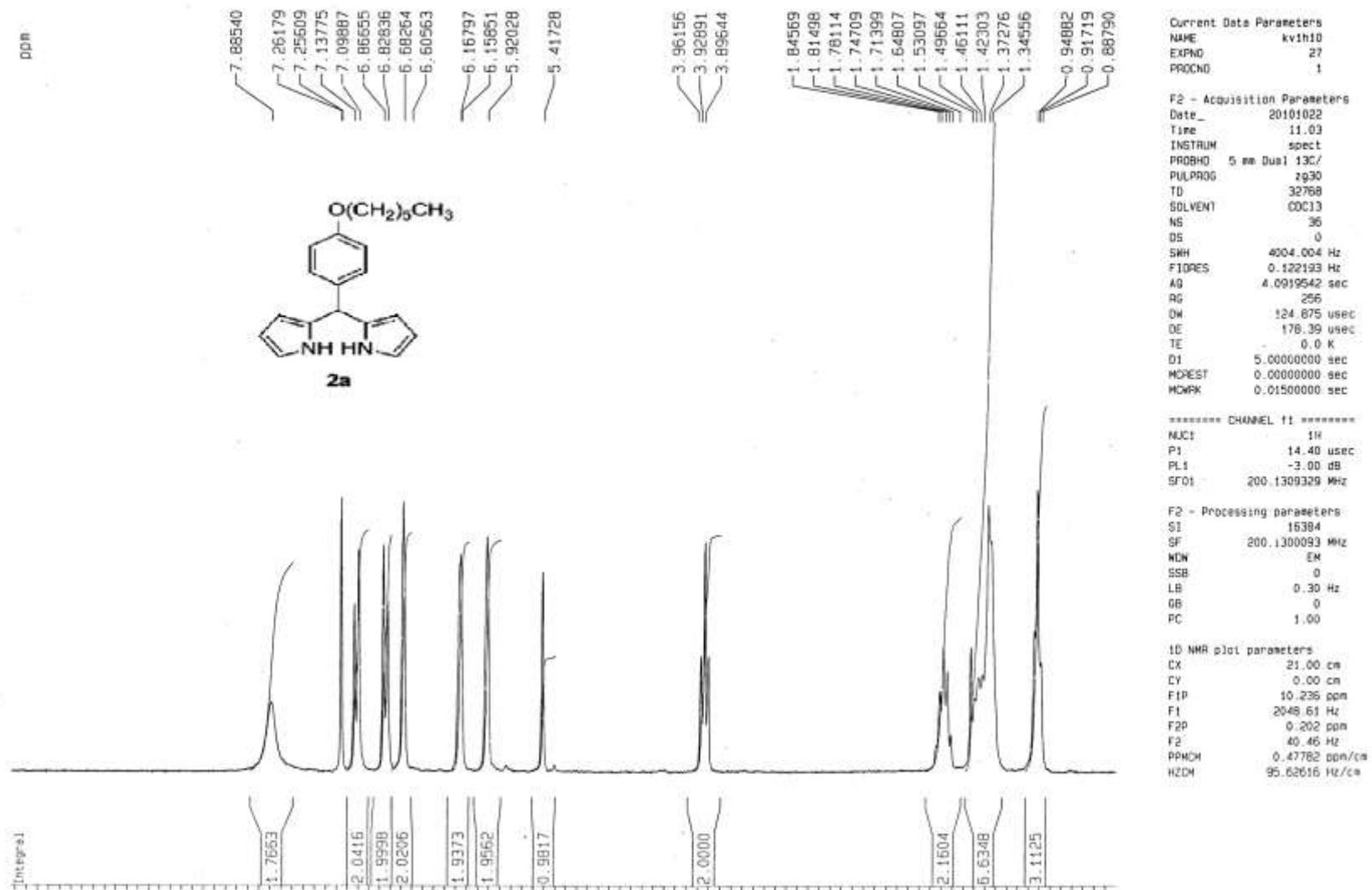
^{13}C NMR of *p*-hexyloxybenzaldehyde (1a)



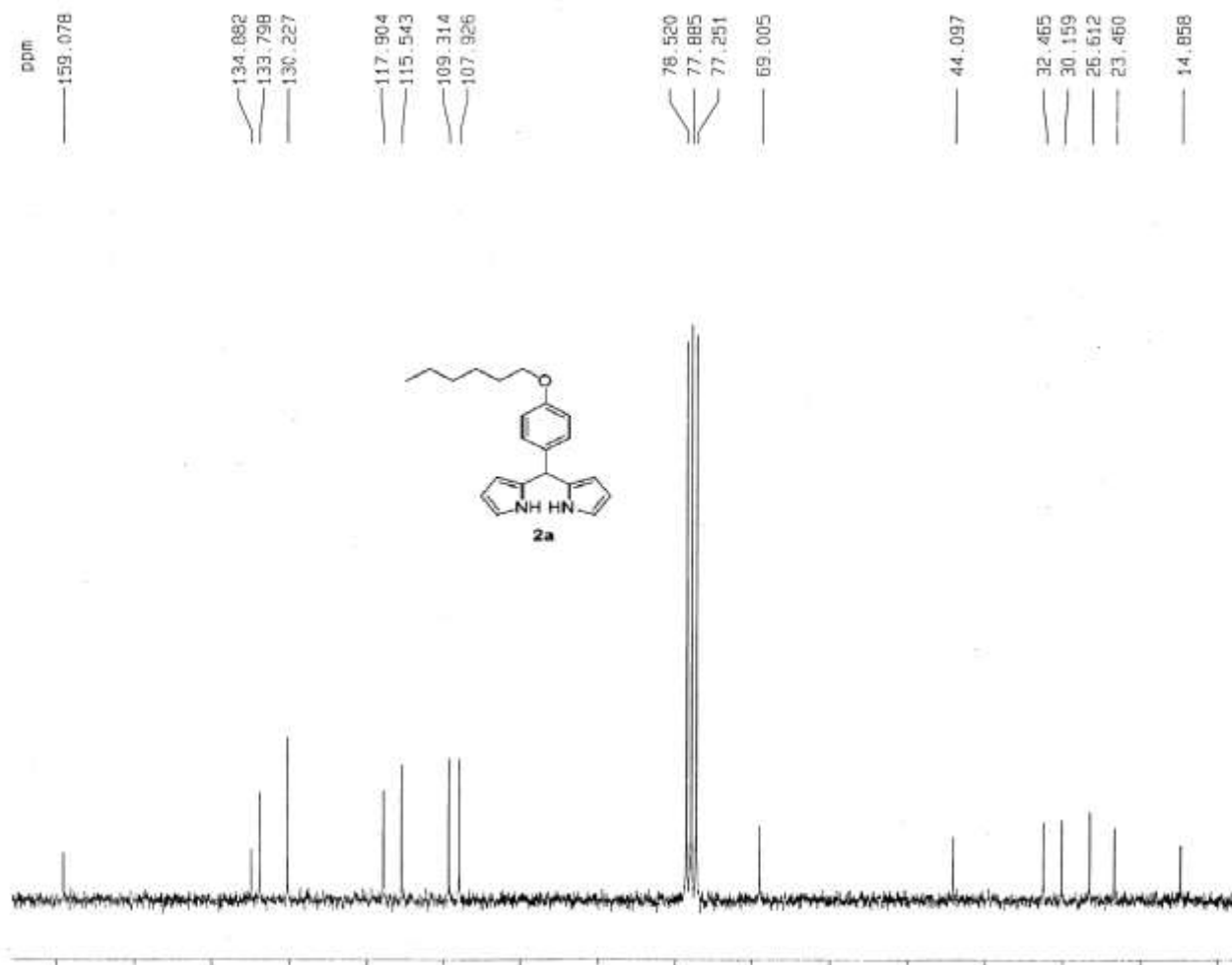
^1H NMR of *p*-undecenyloxybenzaldehyde (1b)



^{13}C NMR of *p*-undecenyoxybenzaldehyde (1b)



¹H NMR of dipyrromethane (2a)



```

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PROCNO       1

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DE           6.00 usec
TE           0.2 K
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d11          0.0300000 sec
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MRES1        0.0000000 sec
MRES2        0.0100000 sec

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PL1           -3.00 dB
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***** CHANNEL f2 *****
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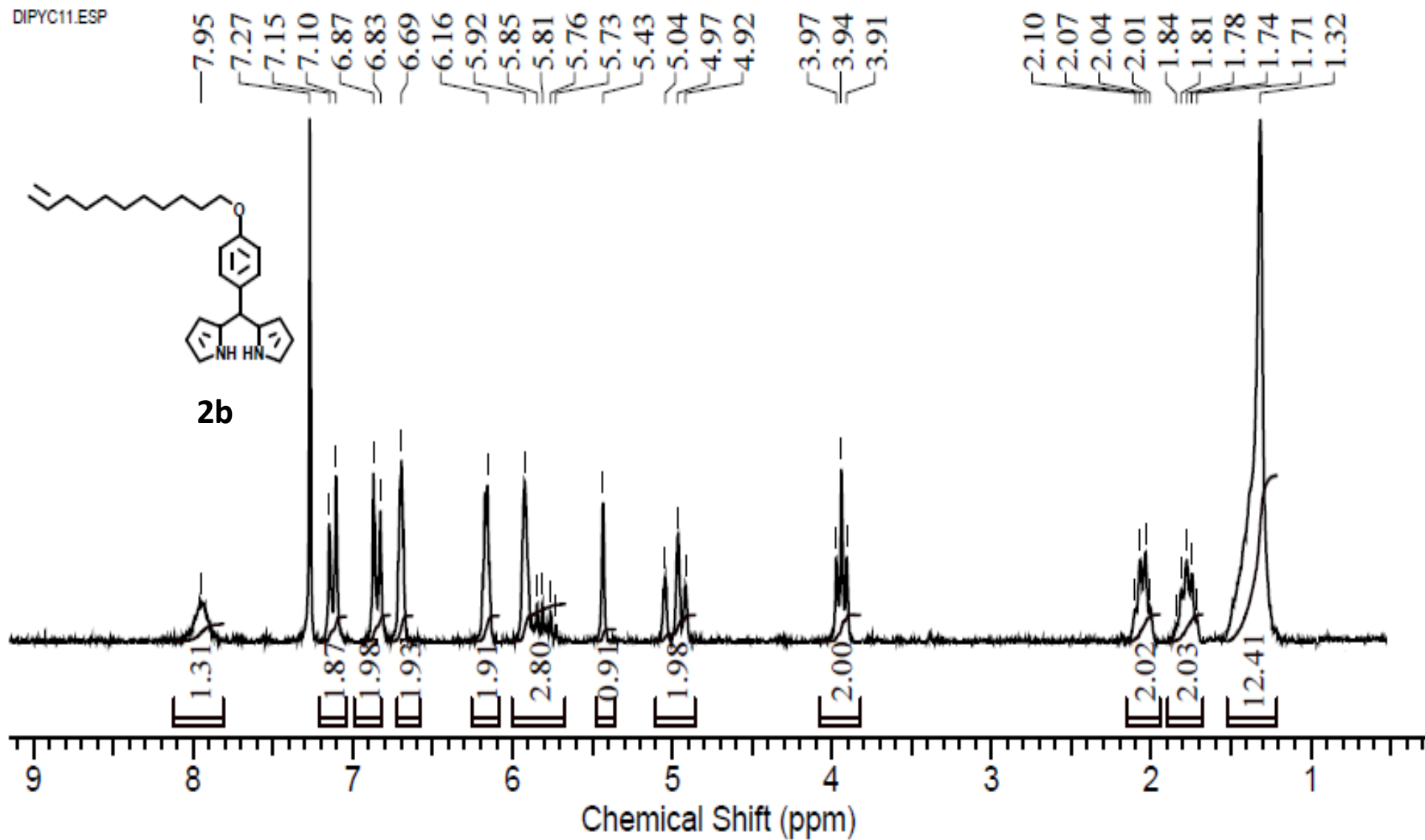
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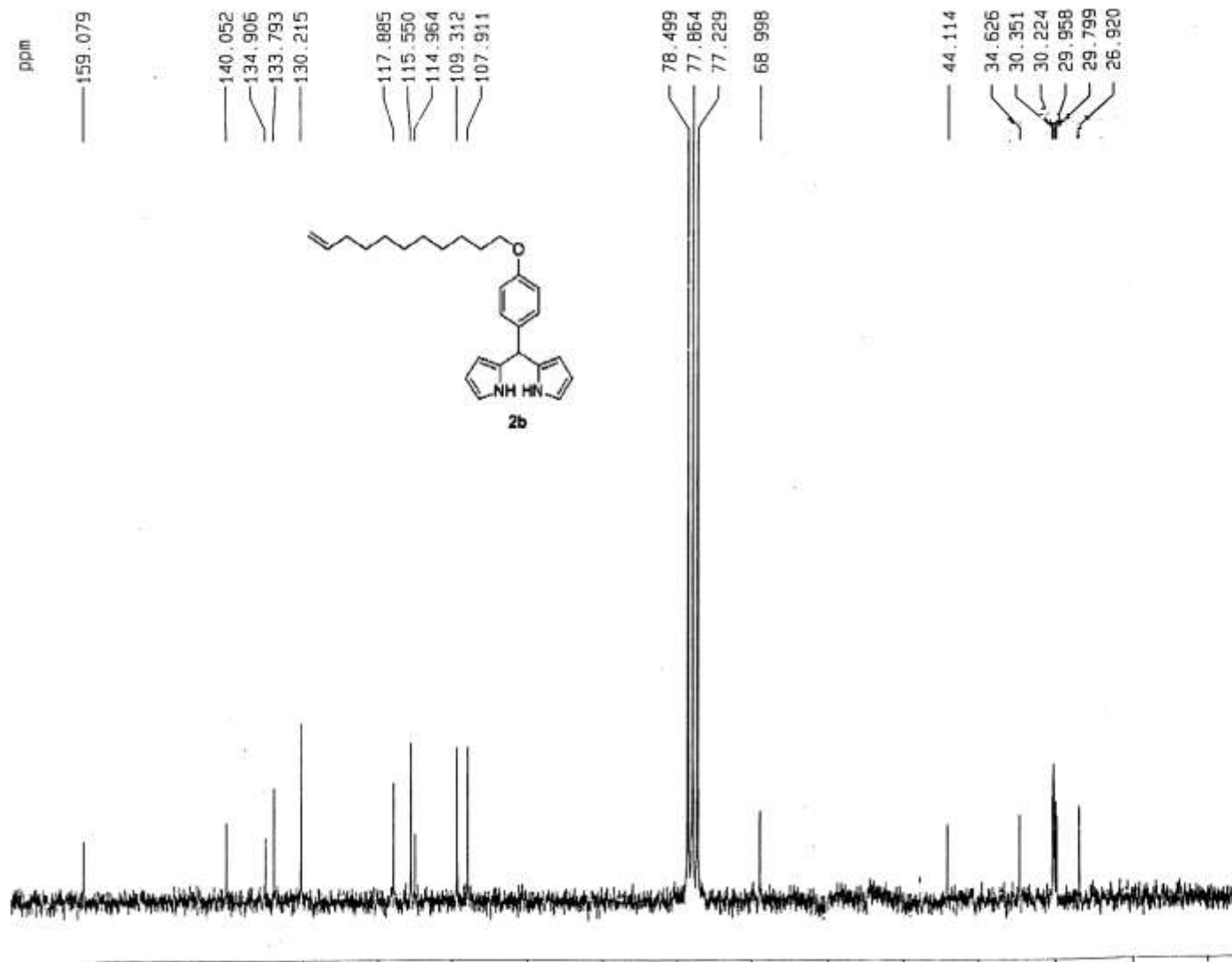
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¹³C NMR of dipyrromethane (2a)

DIPYC11.ESP



¹H NMR of dipyrromethane (2b)



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----- CHANNEL F1 -----
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----- CHANNEL F2 -----
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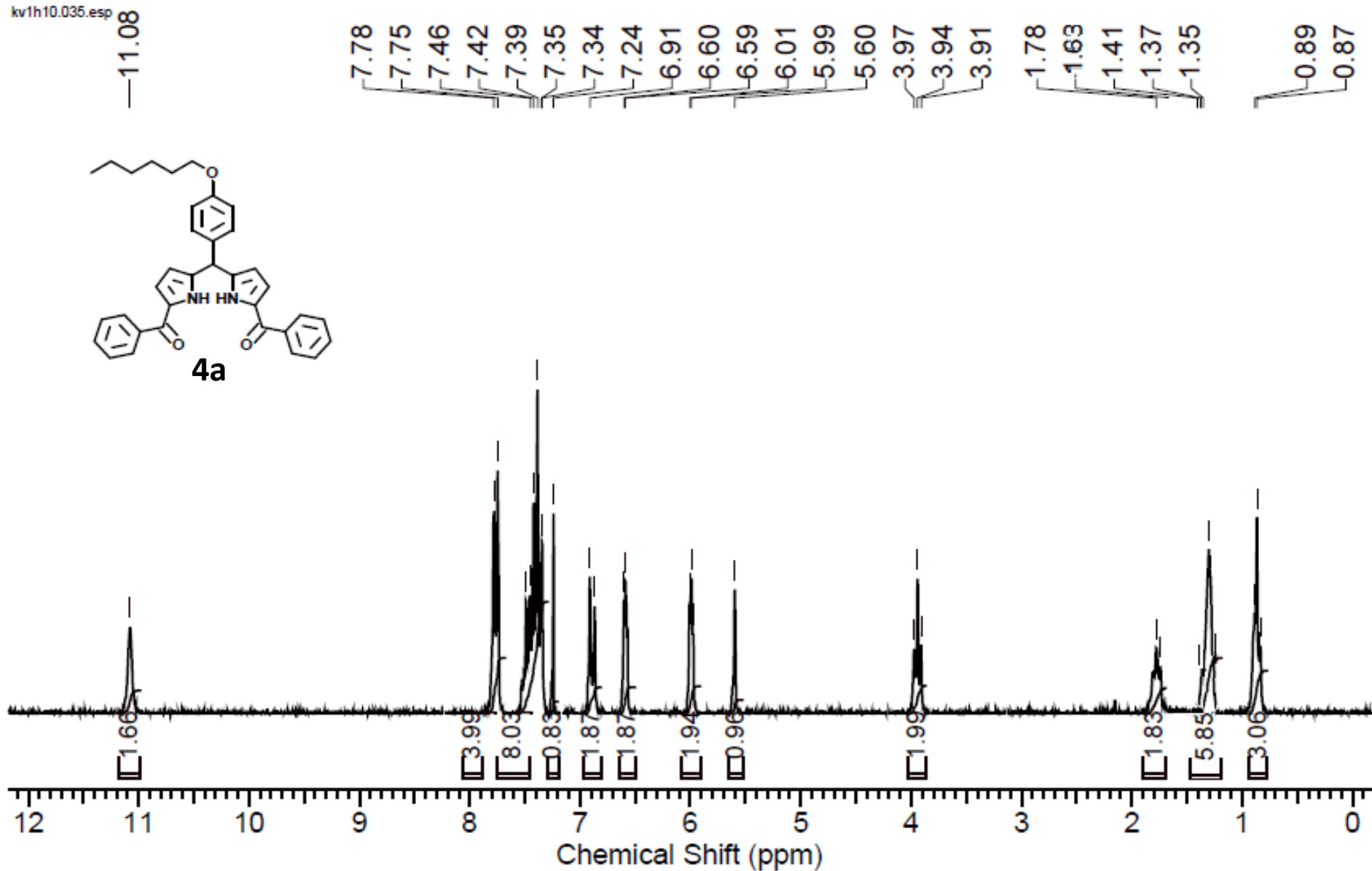
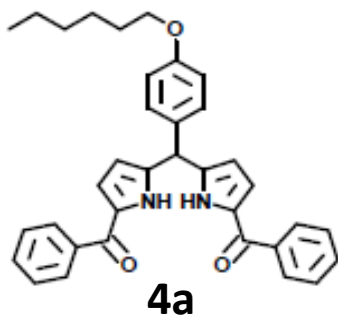
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1D NMR plot parameters
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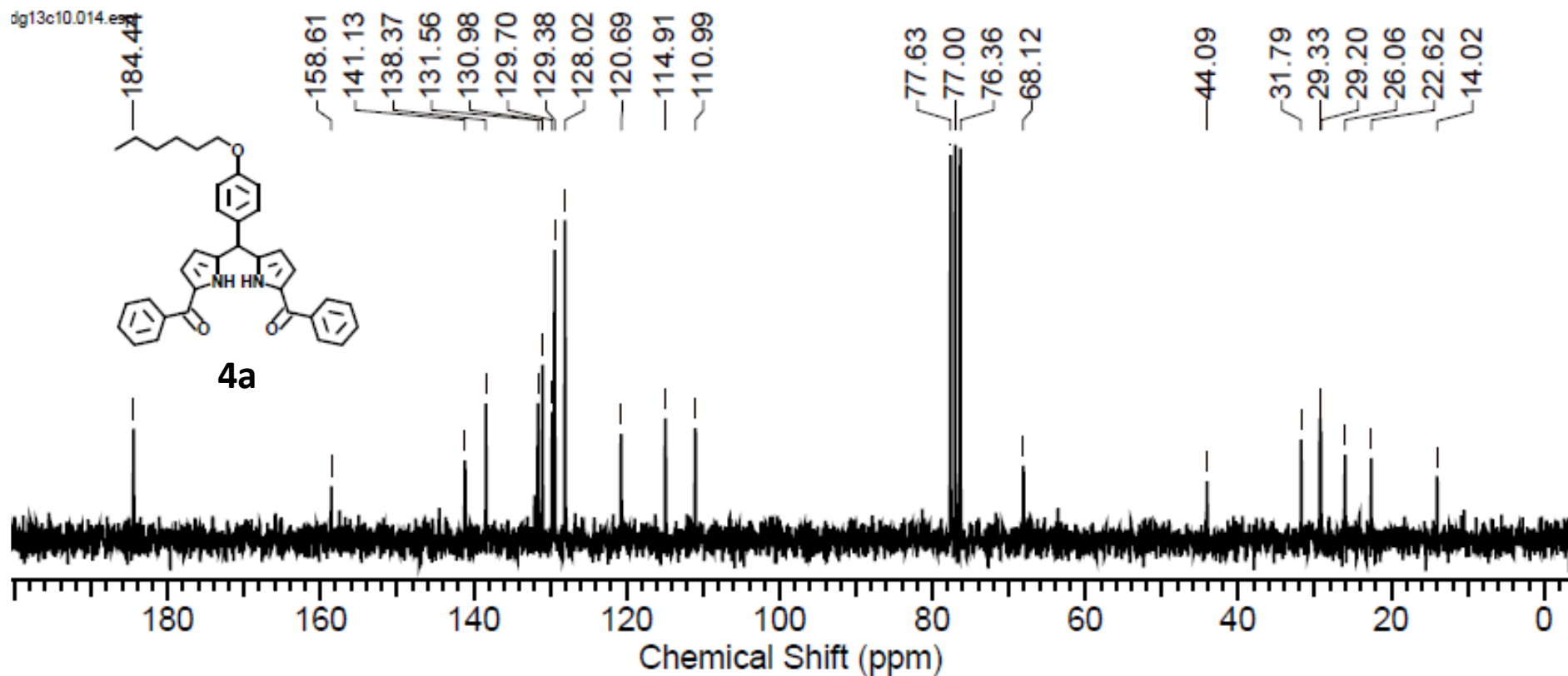
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¹³C NMR of dipyrromethane (2b)

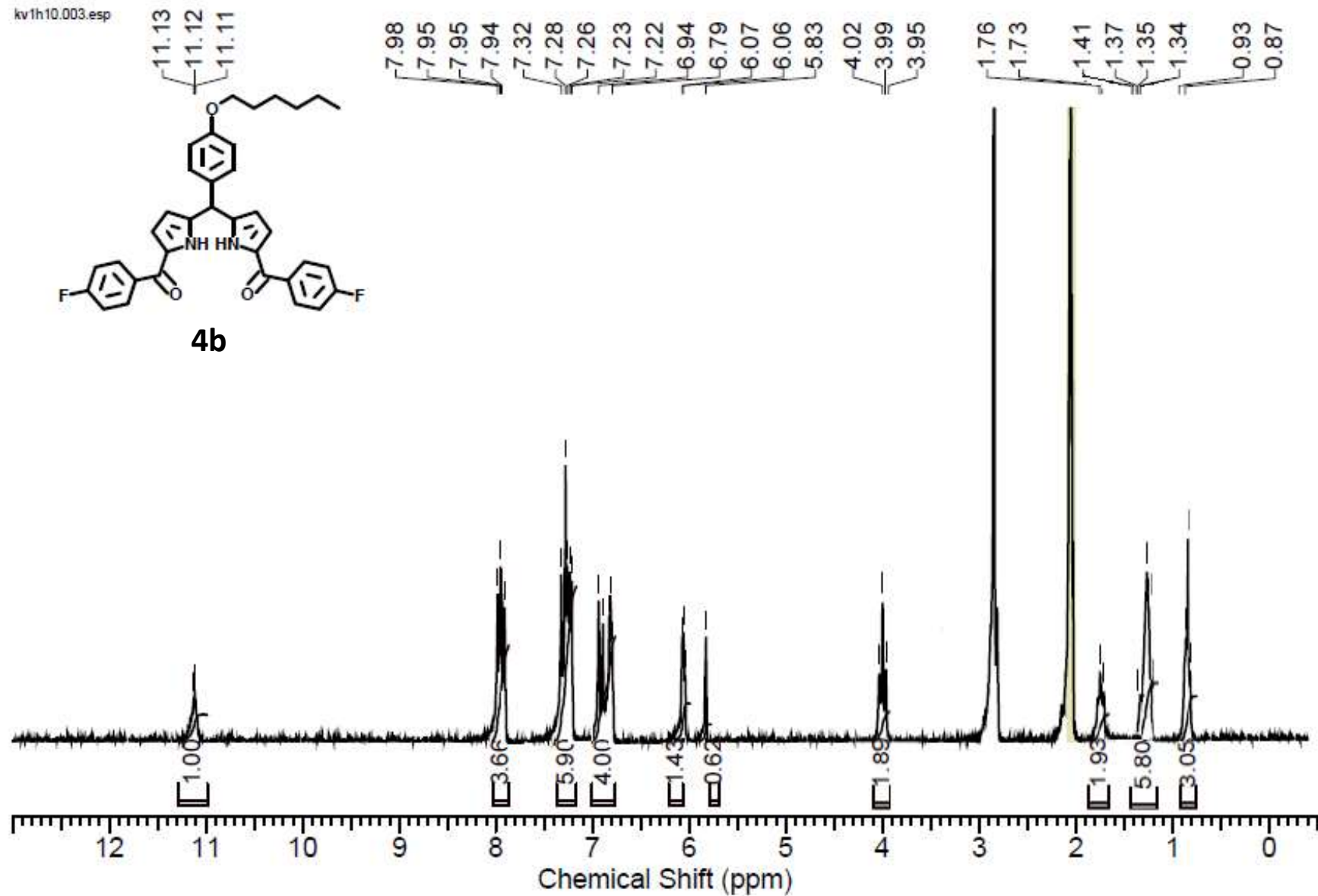
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^1H NMR of diacyldipyrromethane (4a)

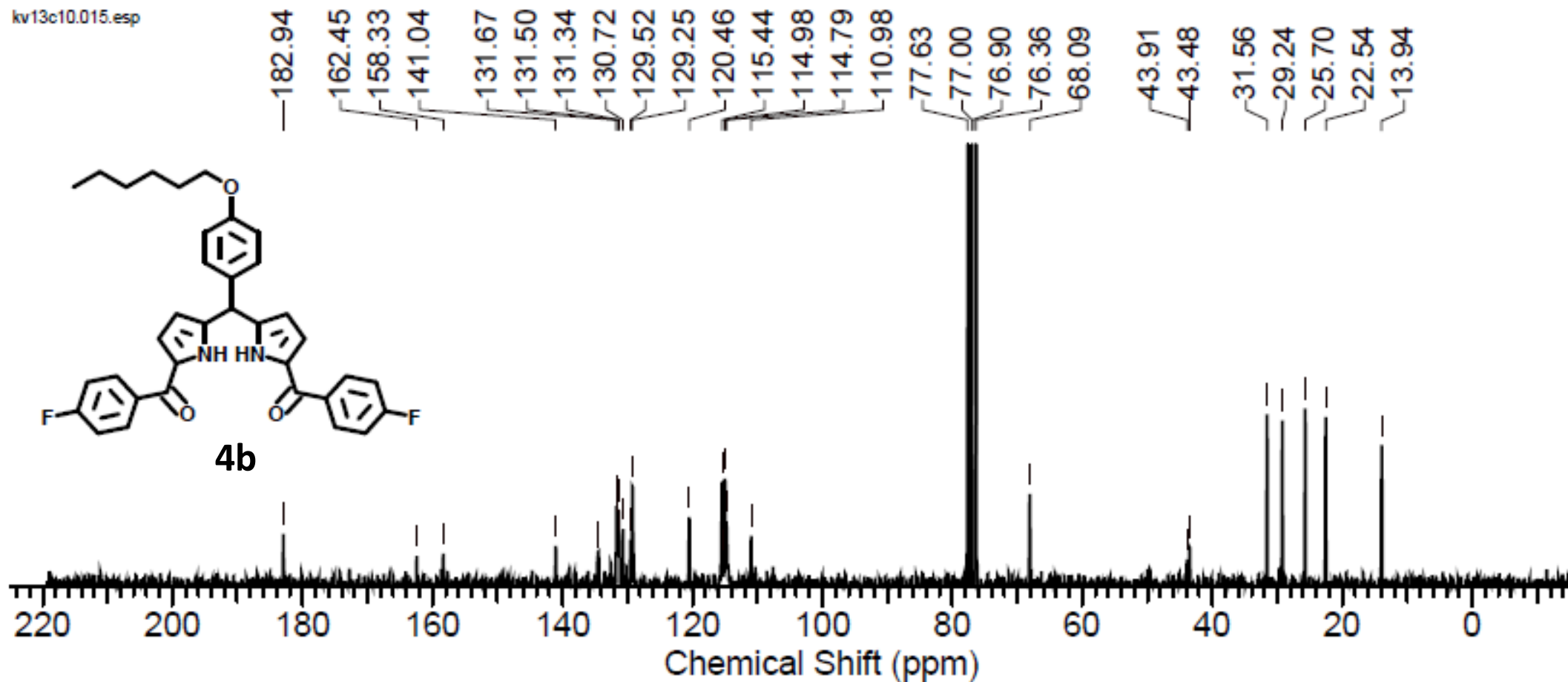


¹³C NMR of diacyldipyrromethane (4a)

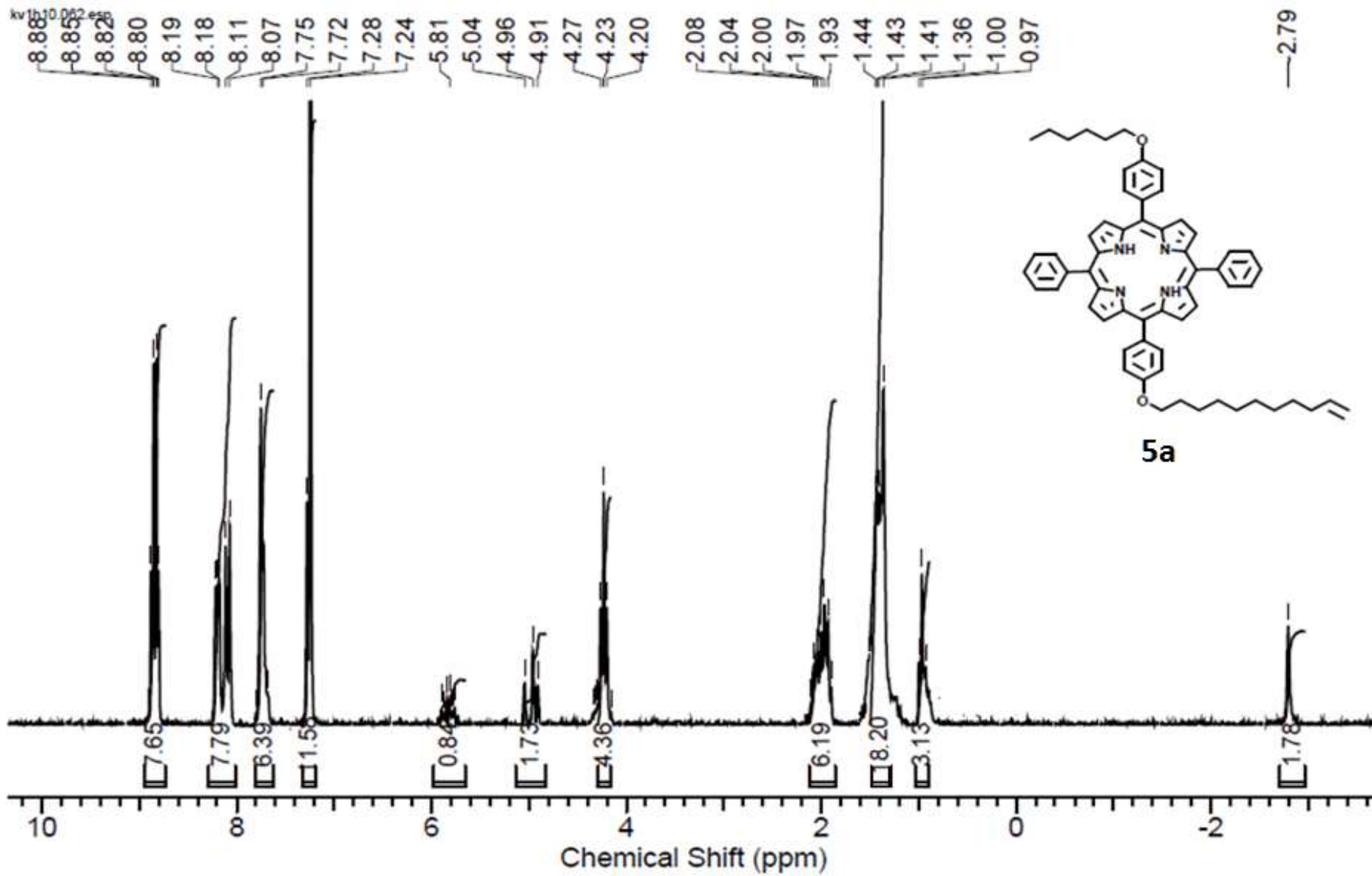


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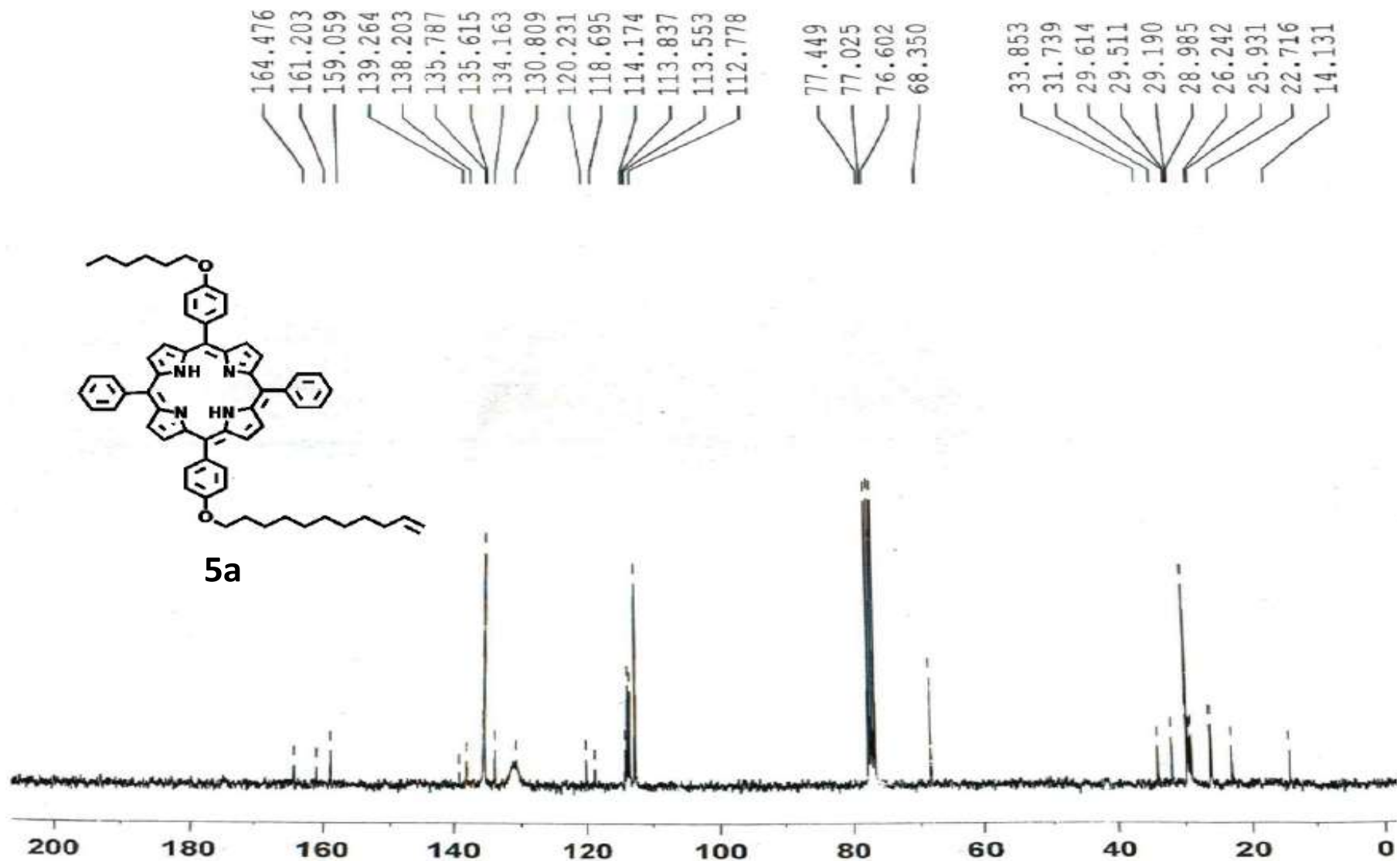
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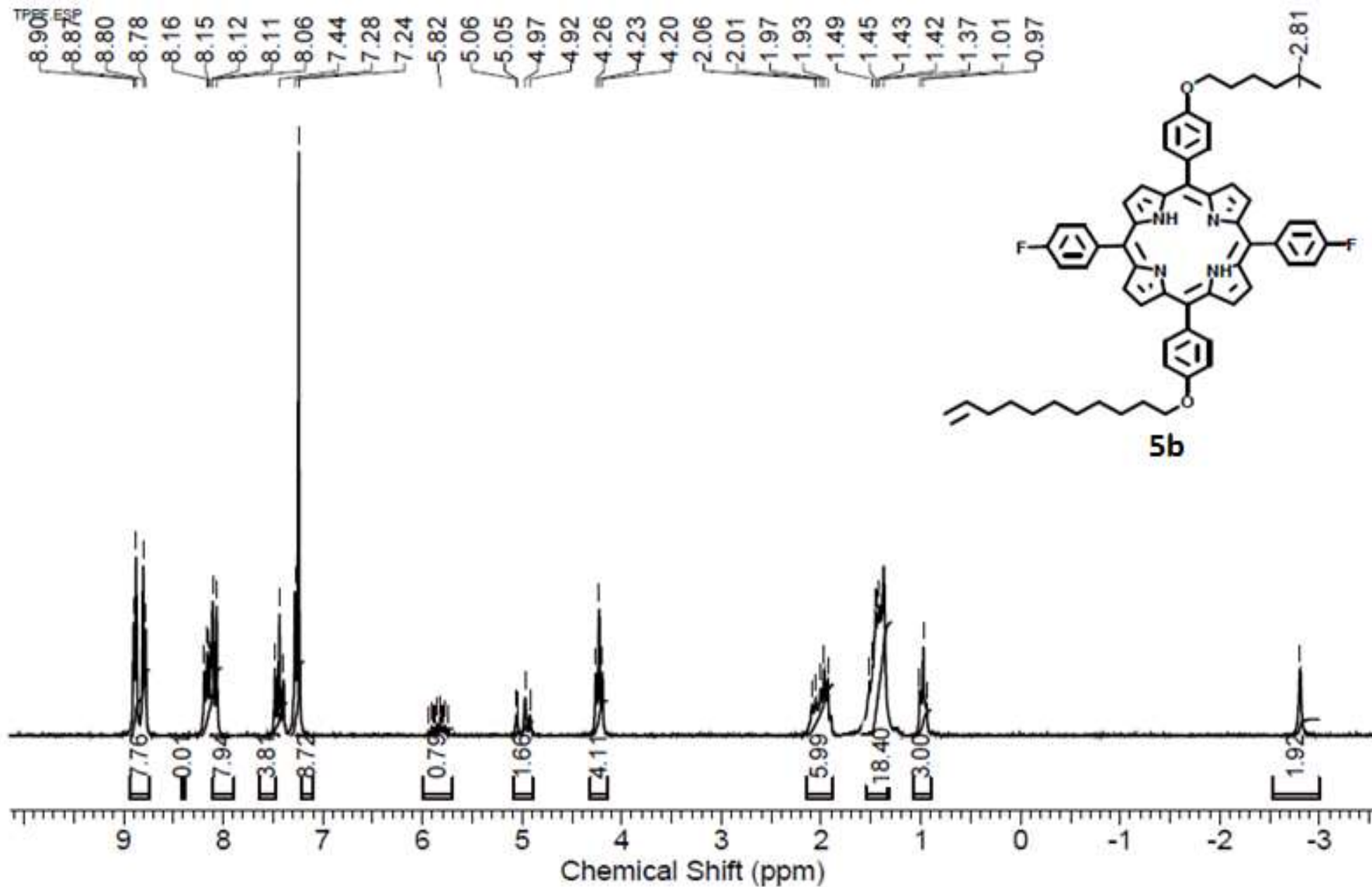
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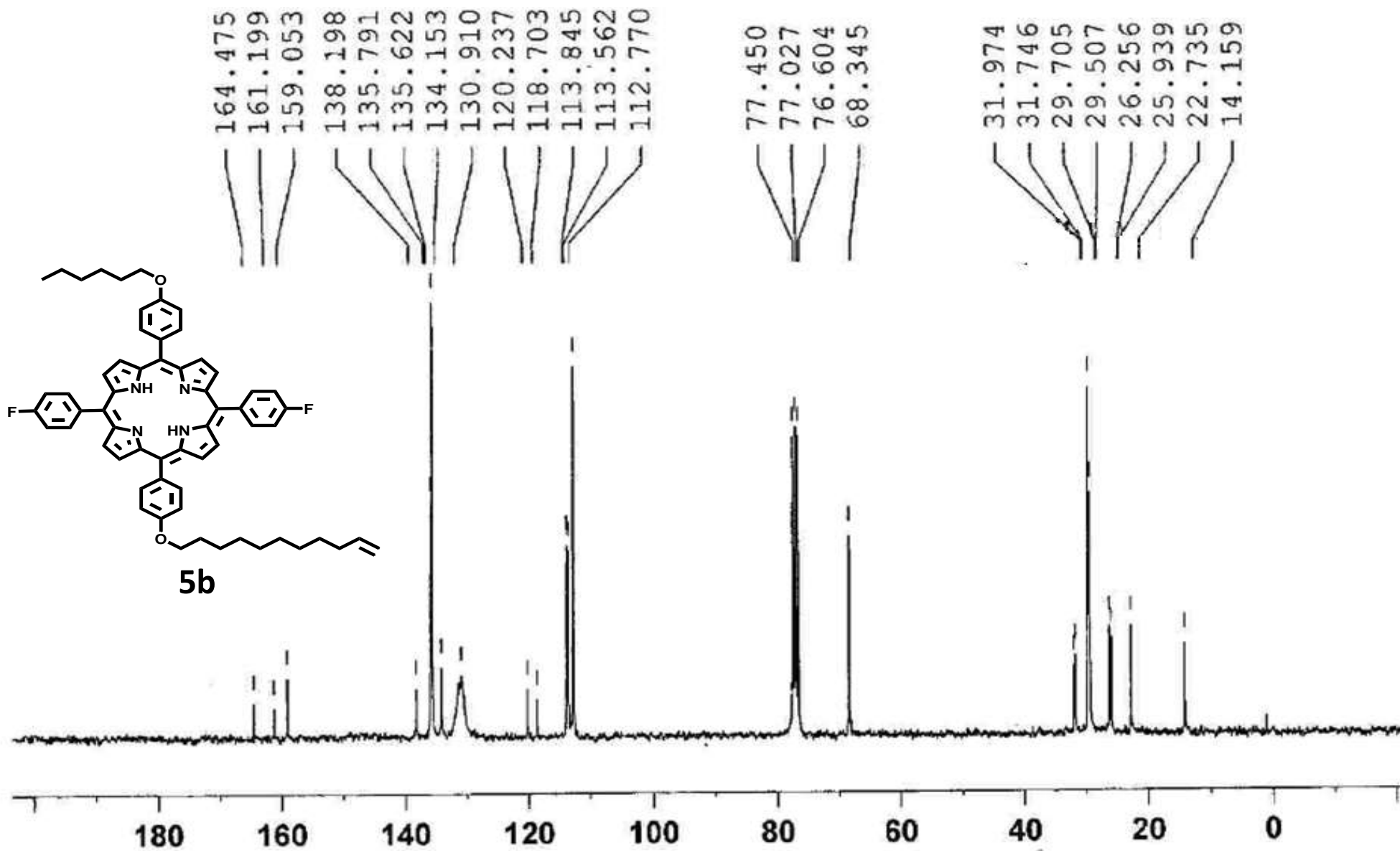


^1H NMR of porphyrin (5a)



¹³C NMR of porphyrin (5a)





^{13}C NMR of porphyrin (5b)

Fig. SL1. Mechanism of monolayer deposition

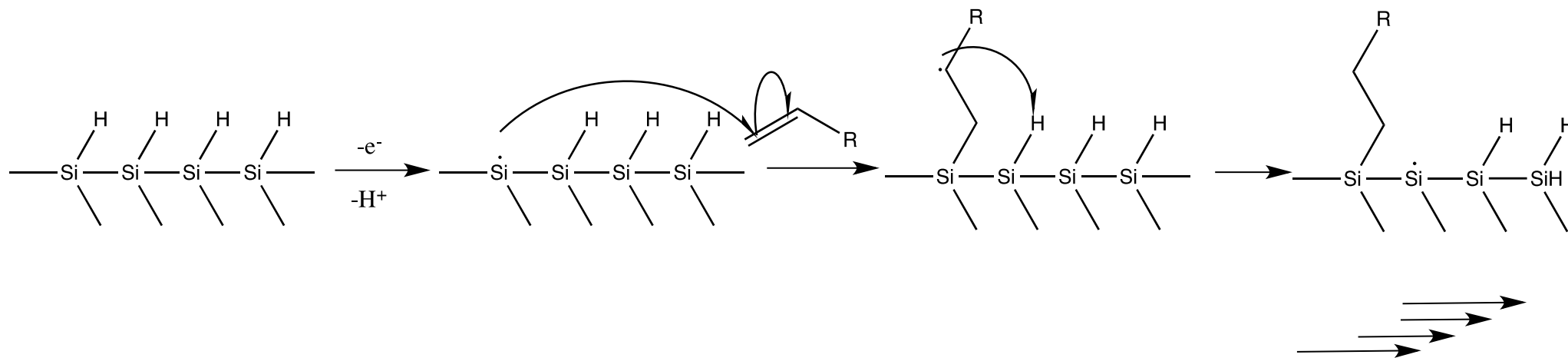
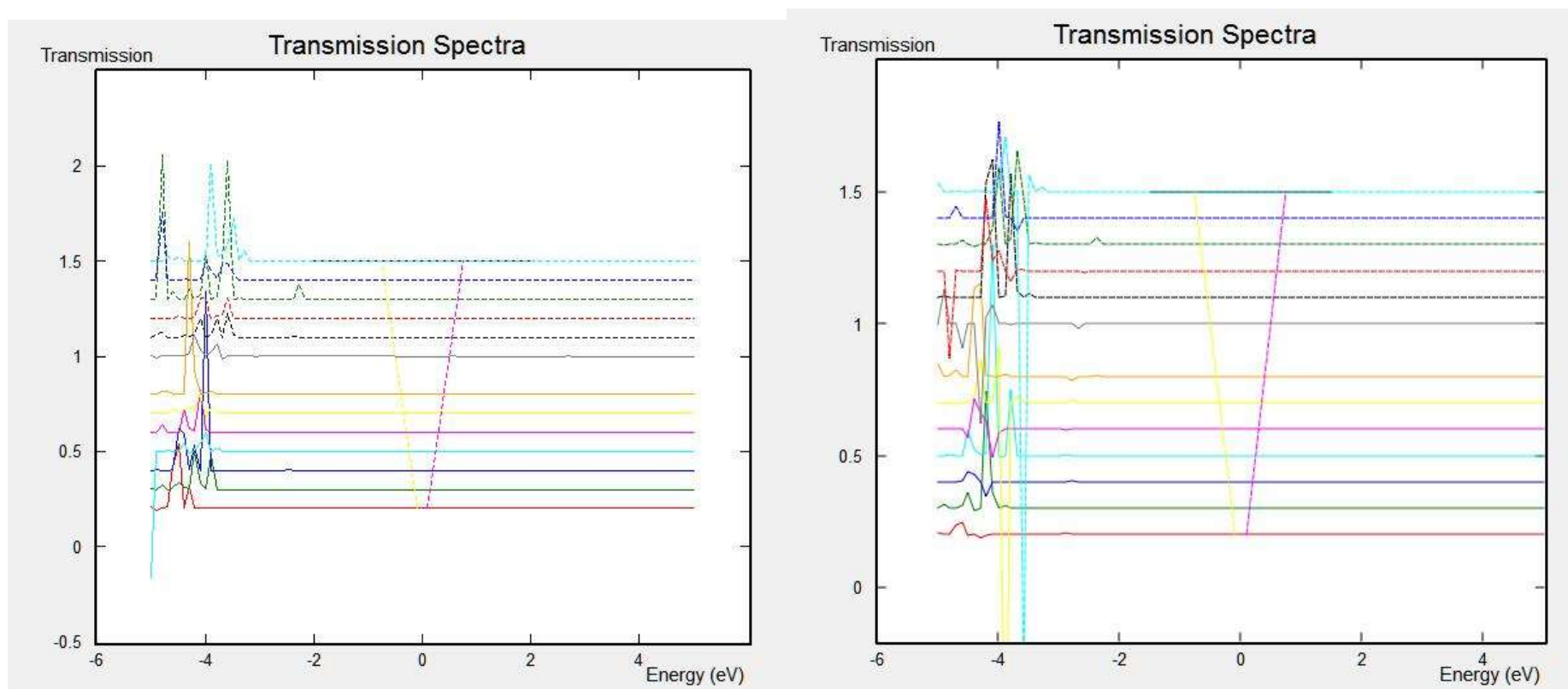


Fig. SL2. Transmission spectra for I-V measurement using ATK-Toolkit



5a

5b

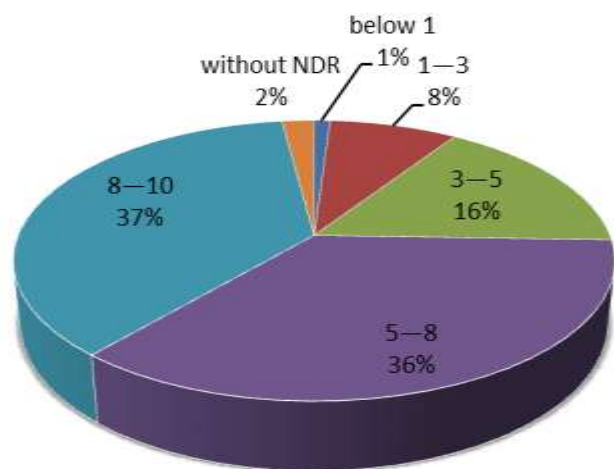
Table S11. *J-V curve details*

Voltages	5a (V)	5b (V)
V_{onset}	0.38±0.047	0.30±0.033
V_p	1.18±0.138	1.03 ±0.115
V_{onset-rev}	0.98 ±0.082	1.03±0.063
V_{p-rev}	0.85±0.091	0.73±0.072

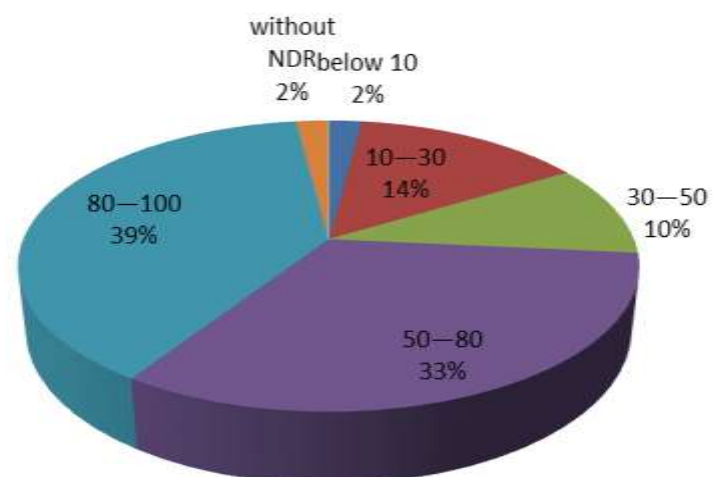
	RMS roughness in nm	Average roughness nm	Maximum counts nm
TPP(5a)	1.45	1.16	2.3
TPP-f(5b)	0.890	0.725	2.97

Table SI2. Statistics of NDR devices

Molecules	No. of samples	No. of devices in each sample	Total no. of devices	No. of devices with reversible NDR	No. of devices with stable NDR(8h)
5a	12	8	96	94	80
5b	6	8	48	46	43



Statistics for NDR of 5a



Statistics for NDR of 5b

Table SI3. HOMO and LUMO values for Fig. 9

Energy Levels	5a	5a⁺	5b	5b⁺
HOMO	-4.67 eV	-7.46 eV	-4.77 eV	-7.36 eV
LUMO	-2.02 eV	-5.24 eV	-2.12 eV	-5.33 eV

Optimized coordinates of **5a**

C	6.0	4.1736897300	-1.3053972331	-0.5957440463
C	6.0	4.6031571846	-2.6675024087	-0.7290394950
C	6.0	3.4902800019	-3.4645446270	-0.7675026394
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C	6.0	-0.1117213819	-2.1764529379	-0.3563003606
C	6.0	-1.4601418751	-2.6691960593	-0.0962005278
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C	6.0	-1.3703786503	-0.4164296738	-0.1196106685
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C	6.0	0.8141710635	3.3863125808	-0.2507447643
N	7.0	0.3553244920	2.0914598286	-0.1670056605
C	6.0	2.1589077070	3.7973873278	-0.2947525680
C	6.0	3.2744996175	2.9315674740	-0.3184643754
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H	1.0	-16.9111389118	-1.2875834389	1.9873170756
H	1.0	-17.6691022092	-3.1954746199	0.5402772910
H	1.0	-18.2572863720	-2.0575254243	-0.6688040196
H	1.0	-19.3586037554	-2.2555119416	2.2163923253
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H	1.0	10.8764896945	-1.9775519824	1.4555740046
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H	1.0	17.9865359529	-2.9803380321	3.1635976788
H	1.0	17.8885277626	-2.1507759366	1.6041630440
H	1.0	17.3949629053	-3.8431601228	1.7368345482

Total Energy: -2729.6278477456 Hartree

Optimized coordinates of 5b

C	6.0	4.1592043426	-1.4221718604	-0.6404105945
C	6.0	4.6085167832	-2.7758171010	-0.7945966555
C	6.0	3.5073893005	-3.5878462846	-0.8550678881
C	6.0	2.3383351025	-2.7683046389	-0.7074972062
N	7.0	2.7840017678	-1.4699878915	-0.6062182638
C	6.0	4.9636254940	-0.2768570606	-0.5220130647
C	6.0	1.0040899020	-3.2000507914	-0.6234094855
C	6.0	-0.1143156747	-2.3590460074	-0.4233365644
C	6.0	-1.4535703330	-2.8747390076	-0.1581639186
C	6.0	-2.2487491419	-1.7938040549	0.0246207087
C	6.0	-1.3960033165	-0.6208528084	-0.1490540825
N	7.0	-0.1033411949	-0.9926362152	-0.3983362349
C	6.0	-1.8799625484	0.7055946363	-0.0677538363
C	6.0	-1.0805725166	1.8619413426	-0.1516418981
C	6.0	-1.5381802321	3.2188818659	-0.2272997274
C	6.0	-0.4425200690	4.0375817056	-0.3100621618
C	6.0	0.7323240761	3.2162185511	-0.2804091238
N	7.0	0.2945162056	1.9137460636	-0.1961115950
C	6.0	2.0703684446	3.6482441341	-0.3281080018
C	6.0	3.1989029505	2.7996665093	-0.3499692421
C	6.0	4.5726731052	3.2952737572	-0.3038268115
C	6.0	5.3731492630	2.2038135842	-0.3459798502
C	6.0	4.4857376626	1.0464412939	-0.4147913747
N	7.0	3.1747018460	1.4342254978	-0.4053634844
C	6.0	0.7648952274	-4.6762515664	-0.7194350681
C	6.0	2.2959684847	5.1289262274	-0.3576057584
C	6.0	1.9558644628	5.9356510009	0.7410630379
C	6.0	2.1628635372	7.3150235943	0.7181070104
C	6.0	2.7164418155	7.8875813580	-0.4212460076
C	6.0	3.0667357130	7.1251395502	-1.5297487678
C	6.0	2.8530129025	5.7473667629	-1.4894746451
C	6.0	1.2265141796	-5.5523755242	0.2769683734
C	6.0	1.0018422595	-6.9267266000	0.1933811761
C	6.0	0.3052602384	-7.4231406700	-0.9023256700
C	6.0	-0.1707687308	-6.5899248195	-1.9083143568
C	6.0	0.0630164991	-5.2182959639	-1.8088000766
C	6.0	6.4462694496	-0.5050308743	-0.4866599049
C	6.0	-3.3470116176	0.9169550999	0.1265092068
C	6.0	-4.2865877722	0.4372504462	-0.7964908855
C	6.0	-5.6604472502	0.5961109494	-0.5987116229
C	6.0	-6.1252689856	1.2546043671	0.5466771550
C	6.0	-5.1989331526	1.7608099389	1.4716649589
C	6.0	-3.8368865693	1.5920614568	1.2615837352
C	6.0	7.1477186446	-0.4207993053	0.7214203358
C	6.0	8.5240933026	-0.6534650229	0.7895246222
C	6.0	9.2297206914	-0.9779341724	-0.3758461095
C	6.0	8.5424722199	-1.0577770072	-1.5968700576
C	6.0	7.1730622719	-0.8250852064	-1.6470527169
O	8.0	-7.4389584113	1.4525019372	0.8523258740
O	8.0	10.5690468900	-1.2309849713	-0.4297605777
C	6.0	-8.4368709567	0.8084098094	0.0588172276
C	6.0	-9.7861130044	1.0631519964	0.7181599614
C	6.0	-10.9363878516	0.3238432789	0.0220053514
C	6.0	-12.2906643466	0.5429889055	0.7102114003
C	6.0	-13.4394186404	-0.2503494638	0.0731936475

C	6.0	-14.7806463001	-0.0620104893	0.7951043744
C	6.0	-15.9273682403	-0.8799568019	0.1861740807
C	6.0	-17.2577885410	-0.7090135415	0.9313078112
C	6.0	-18.4053285586	-1.5425705011	0.3281963751
C	6.0	-19.6879902901	-1.4243250565	1.1063578452
C	6.0	-20.8422204543	-0.9565815018	0.6291742555
C	6.0	11.3135034483	-1.2598327418	0.7880781808
C	6.0	12.7515539094	-1.6287512608	0.4486631147
C	6.0	13.6316151123	-1.7625397175	1.6987553877
C	6.0	15.0888870837	-2.1208828518	1.3761709869
C	6.0	15.9668651825	-2.2854009161	2.6237944053
C	6.0	17.4222859018	-2.6368829182	2.2961627209
F	9.0	2.9200866458	9.2221471505	-0.4516024180
F	9.0	0.0835006882	-8.7520830771	-0.9921093155
H	1.0	5.6457328311	-3.0705533650	-0.8548346705
H	1.0	3.4928161822	-4.6605882246	-0.9781281847
H	1.0	2.1775501471	-0.6607644083	-0.5151003272
H	1.0	-1.7289273675	-3.9176878353	-0.0899568401
H	1.0	-3.2997853034	-1.7818394310	0.2738182622
H	1.0	-2.5771959128	3.5124324894	-0.2408264459
H	1.0	-0.4368084546	5.1139011195	-0.3985478354
H	1.0	0.9067295091	1.1040376911	-0.2080995470
H	1.0	4.8688087573	4.3326401021	-0.2390786220
H	1.0	6.4534903312	2.1700581716	-0.3379356107
H	1.0	1.5329738181	5.4733302377	1.6284732898
H	1.0	1.9092617276	7.9430964663	1.5663256871
H	1.0	3.4915522962	7.6099542187	-2.4030575860
H	1.0	3.1166000334	5.1392763595	-2.3500576850
H	1.0	1.7586827364	-5.1490954007	1.1337837619
H	1.0	1.3504158783	-7.6082157111	0.9630117865
H	1.0	-0.7074309895	-7.0163395650	-2.7499796735
H	1.0	-0.2989835834	-4.5554496827	-2.5895145033
H	1.0	-3.9391484310	-0.0700112353	-1.6923952828
H	1.0	-6.3512517298	0.2107155193	-1.3405350370
H	1.0	-5.5737551527	2.2653871460	2.3571704188
H	1.0	-3.1342191747	1.9695342639	1.9995610885
H	1.0	6.6076035883	-0.1759560464	1.6323460973
H	1.0	9.0271929142	-0.5830051449	1.7473443382
H	1.0	9.1045086246	-1.3040081403	-2.4928854512
H	1.0	6.6545605388	-0.8900454733	-2.6001116006
H	1.0	-8.2271038415	-0.2705573961	0.0068628292
H	1.0	-8.4168466517	1.2045056733	-0.9675191430
H	1.0	-9.9783380142	2.1440576339	0.7303428988
H	1.0	-9.7201260288	0.7447760217	1.7668725041
H	1.0	-10.7145437874	-0.7539080006	0.0006146297
H	1.0	-11.0036387487	0.6420930428	-1.0290773570
H	1.0	-12.5361403590	1.6154266578	0.7001393567
H	1.0	-12.2037311364	0.2620593136	1.7705224183
H	1.0	-13.1796296957	-1.3198668372	0.0670419212
H	1.0	-13.5470507442	0.0420335991	-0.9820873202
H	1.0	-15.0509486139	1.0045334556	0.7898313098
H	1.0	-14.6623625416	-0.3390527144	1.8534609174
H	1.0	-15.6503464032	-1.9450468091	0.1809540881
H	1.0	-16.0598130820	-0.5956808497	-0.8684417289
H	1.0	-17.5480344365	0.3509244132	0.9339614360
H	1.0	-17.1217710634	-0.9907088586	1.9861330748
H	1.0	-18.0923276500	-2.5984597383	0.3012266876
H	1.0	-18.5752965951	-1.2406955174	-0.7141264354
H	1.0	-19.6384159180	-1.7439394875	2.1496811158

H	1.0	-21.7340250372	-0.8904068738	1.2475301813
H	1.0	-20.9418217955	-0.6241437794	-0.4028391415
H	1.0	10.8749395847	-1.9991572771	1.4754110210
H	1.0	11.2684281428	-0.2763599858	1.2796769334
H	1.0	13.1630670385	-0.8663289249	-0.2258030434
H	1.0	12.7453631664	-2.5735700041	-0.1102939476
H	1.0	13.2090509931	-2.5322849644	2.3618093176
H	1.0	13.6092098805	-0.8223743896	2.2698790279
H	1.0	15.5188920169	-1.3424071329	0.7283276769
H	1.0	15.1123813133	-3.0512911299	0.7896131428
H	1.0	15.5380663606	-3.0673436115	3.2672768050
H	1.0	15.9376814623	-1.3573698462	3.2127748940
H	1.0	18.0211825187	-2.7491551629	3.2073208493
H	1.0	17.8904814247	-1.8565101035	1.6831552259
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Total energy: -2927.9402974Hartree

Input file for 5a

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$STATPT NSTEP=400 OPTTOL=0.0001 $END
$SCF DIRSCF=.T. SHIFT=.T. DAMP=.T. DIIS=.T. CONV=1.0d-04 $END
# $DFT DFTTYP=B3LYP METHOD=GRID $END
$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.F. DIFFS=.F. $END
$DATA
DMS:/B3LYP/6-31++G(d,p)/acn
CN 1

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C      6.0    4.2950557950   -2.7648525514   -0.8814580116
C      6.0    3.1253066840   -3.4775373352   -0.8551191076
C      6.0    2.0481370341   -2.5632034316   -0.6000580286
N      7.0    2.6106403007   -1.3080287441   -0.5433727764
C      6.0    4.8849135855   -0.3131685189   -0.5737803717
C      6.0    0.6959936251   -2.8708980193   -0.3699326928
C      6.0   -0.3148349862   -1.9131591969   -0.1166572483
C      6.0   -1.6541215977   -2.2722398176    0.3337499279
C      6.0   -2.3473935331   -1.1116659741    0.4287842590
C      6.0   -1.4310675395   -0.0495707922    0.0233909187
N      7.0   -0.1929325760   -0.5586875913   -0.2551095857
C      6.0   -1.8196237793    1.3087855557   -0.0913353540
C      6.0   -0.9271353681    2.3823659061   -0.2802461478
C      6.0   -1.2551262384    3.7579608151   -0.5130985846
C      6.0   -0.0864878805    4.4719077815   -0.5757863921
C      6.0    1.0052250031    3.5604704240   -0.3956950381
N      7.0    0.4477184701    2.3126037622   -0.2417978327
C      6.0    2.3797706811    3.8701377196   -0.3811828290
C      6.0    3.4216762603    2.9155627965   -0.3543327439
C      6.0    4.8348848341    3.2731254820   -0.2486235961
C      6.0    5.5268417581    2.1101852771   -0.3061826750
C      6.0    4.5344495758    1.0476172679   -0.4325902487
N      7.0    3.2671204715    1.5594416501   -0.4395681001
C      6.0    0.3048048248   -4.3150252265   -0.3852384742
C      6.0    2.7371849952    5.3233165653   -0.3857212804
C      6.0    2.3044178615    6.1671907851    0.6527438265
C      6.0    2.6433174767    7.5208162475    0.6658833053
C      6.0    3.4239442043    8.0584572518   -0.3607176589
C      6.0    3.8555834600    7.2338069935   -1.4026623674
C      6.0    3.5152054322    5.8803306090   -1.4152912198
C      6.0    0.8751186420   -5.2404300986    0.5079424813
C      6.0    0.4954617895   -6.5831636948    0.4852254658
C      6.0   -0.4632361108   -7.0269008747   -0.4293417531
C      6.0   -1.0406003134   -6.1190280279   -1.3187341950
C      6.0   -0.6605113843   -4.7777290933   -1.2987812593
C      6.0    6.3397020696   -0.6822202456   -0.5589212608
C      6.0   -3.2771866607    1.6173558378   -0.0211948825
C      6.0   -4.1861538483    0.9315038789   -0.8429395537
C      6.0   -5.5625756303    1.1285484391   -0.7453519018
C      6.0   -6.0699458808    2.0455885863    0.1849002070
C      6.0   -5.1772628641    2.7764986434    0.9836946206
C      6.0   -3.8083038409    2.5586328600    0.8842272044
C      6.0    7.0295435030   -0.7650968950    0.6559393264
C      6.0    8.3803633187   -1.1164053854    0.7119885905
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C	6.0	9.0699451582	-1.4020940527	-0.4735229167
C	6.0	8.3911163815	-1.3295031066	-1.6983984378
C	6.0	7.0480046732	-0.9715437568	-1.7369647445
O	8.0	-7.4008155927	2.2794126734	0.3797508614
O	8.0	10.3867695452	-1.7567491517	-0.5379350401
C	6.0	-8.3209061132	1.3069581196	-0.1244242644
C	6.0	-9.7149402622	1.6063592983	0.4114921533
C	6.0	-10.6624445622	0.4270435139	0.1496461606
C	6.0	-12.1310994254	0.6935130844	0.5069797083
C	6.0	-12.9946720583	-0.5699157489	0.3917080246
C	6.0	-14.4927639144	-0.3370887357	0.6247989742
C	6.0	-15.3089518686	-1.6376072608	0.6044971815
C	6.0	-16.8203446017	-1.4228425522	0.7485443817
C	6.0	-17.6159843144	-2.7423482277	0.7896862688
C	6.0	-19.0991453439	-2.5328209136	0.9302958696
C	6.0	-20.0219009513	-2.9438935826	0.0599728508
C	6.0	11.1402619008	-1.7664051158	0.6719927407
C	6.0	12.5833177396	-2.1260509604	0.3450616042
C	6.0	13.4915956852	-1.9742615372	1.5743212961
C	6.0	14.9350500966	-2.4351190217	1.3399911859
C	6.0	15.8602659918	-2.1484603058	2.5303427315
C	6.0	17.2934253788	-2.6488443307	2.3242885499
H	1.0	5.2942653664	-3.1451874425	-1.0339457640
H	1.0	3.0046156664	-4.5398947412	-0.9912269845
H	1.0	2.0863016196	-0.4469850772	-0.4230949740
H	1.0	-1.9931821434	-3.2694186047	0.5710372985
H	1.0	-3.3641246624	-0.9762837280	0.7659078012
H	1.0	-2.2583785764	4.1369784583	-0.6344189929
H	1.0	0.0247277583	5.5296652548	-0.7550551504
H	1.0	0.9812355326	1.4538143213	-0.1634515013
H	1.0	5.2285170538	4.2727097468	-0.1354118123
H	1.0	6.5975156055	1.9691001472	-0.2660203370
H	1.0	1.7081888807	5.7479822148	1.4591154194
H	1.0	2.3040649040	8.1538993925	1.4819450470
H	1.0	3.6908587787	9.1120386287	-0.3495189762
H	1.0	4.4548538275	7.6469179514	-2.2100417375
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H	1.0	0.9444918901	-7.2807299296	1.1866161616
H	1.0	-0.7585914758	-8.0719339664	-0.4447561268
H	1.0	-1.7865467228	-6.4554984471	-2.0346107922
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H	1.0	-6.2254445749	0.5693416452	-1.3967440201
H	1.0	-5.5811460345	3.4836223884	1.7014968034
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H	1.0	8.8753088551	-1.1681167039	1.6743273921
H	1.0	8.9404527801	-1.5481489482	-2.6087888185
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H	1.0	-8.3266152559	1.3196079112	-1.2244582267
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H	1.0	-12.5309590766	1.4793602217	-0.1508915415
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H	1.0	-12.6277405600	-1.3178855398	1.1107345030

H	1.0	-12.8514190660	-1.0160784841	-0.6038895275
H	1.0	-14.8785313266	0.3499359242	-0.1433107174
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H	1.0	-14.9558708885	-2.2946688991	1.4134889335
H	1.0	-15.1080375584	-2.1775271639	-0.3325468701
H	1.0	-17.1871142997	-0.8081090536	-0.0847940596
H	1.0	-17.0248924197	-0.8480595302	1.6634354817
H	1.0	-17.2503718614	-3.3412189658	1.6381418610
H	1.0	-17.4108279441	-3.3260380901	-0.1173436957
H	1.0	-19.4186266043	-1.9856063461	1.8193232464
H	1.0	-21.0808817348	-2.7550427376	0.2137843239
H	1.0	-19.7510238450	-3.4930499658	-0.8398314810
H	1.0	10.7135210745	-2.4978244401	1.3752739960
H	1.0	11.0871986460	-0.7767499642	1.1502996793
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H	1.0	12.6222706282	-3.1546164821	-0.0367787005
H	1.0	13.0687050596	-2.5381730182	2.4194190364
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H	1.0	15.3367729163	-1.9392404675	0.4440610490
H	1.0	14.9434810466	-3.5123453878	1.1189799209
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H	1.0	15.8726710367	-1.0660769162	2.7216180582
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H	1.0	17.7451394423	-2.1986103816	1.4325676280
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\$END

Input file for 5a⁺¹

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DMS:/B3LYP/6-31++G(d,p)/acn
CN 1
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N	7.0	2.7987053250	-1.3319367093	-0.5534891669
C	6.0	4.9947621584	-0.1700365247	-0.4952691762
C	6.0	0.9946287983	-3.0364744411	-0.5381040961
C	6.0	-0.1117213819	-2.1764529379	-0.3563003606
C	6.0	-1.4601418751	-2.6691960593	-0.0962005278
C	6.0	-2.2415523924	-1.5746087289	0.0617778404
C	6.0	-1.3703786503	-0.4164296738	-0.1196106685
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C	6.0	-1.0205364052	2.0621154923	-0.1397904603
C	6.0	-1.4560466215	3.4254435158	-0.2262765575
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N	7.0	0.3553244920	2.0914598286	-0.1670056605
C	6.0	2.1589077070	3.7973873278	-0.2947525680
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C	6.0	4.6553094287	3.4077055484	-0.2808342369
C	6.0	5.4399972296	2.3052089514	-0.3286854028
C	6.0	4.5362722682	1.1603402909	-0.3894060922
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C	6.0	0.7356550841	-4.5111695888	-0.6089753582
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C	6.0	2.2936325514	7.4625273774	0.7384311480
C	6.0	2.8676614546	8.0531066499	-0.3888292931
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C	6.0	2.9828470596	5.8821354760	-1.4518663324
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C	6.0	0.9383440314	-6.7448616953	0.3372939693
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C	6.0	-0.2126259432	-6.4340599708	-1.7607810167
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C	6.0	6.4739557071	-0.4207519249	-0.4762462024
C	6.0	-3.3058864063	1.1465485545	0.0961277324
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C	6.0	-5.6011509840	0.8165485348	-0.6792035739
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C	6.0	-5.1878750101	2.0148851449	1.3819357307
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C	6.0	15.9545603108	-2.4349731910	2.5759904125
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H	1.0	4.9645769594	4.4406405829	-0.2197123667
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H	1.0	-16.9111389118	-1.2875834389	1.9873170756
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Input file for 5b

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DMS:/B3LYP/6-31++G(d,p)/acn
CN 1
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C	6.0	0.6251568737	-2.9422863759	-0.3380823270
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C	6.0	-1.3631171733	3.6820934832	-0.3649134025
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C	6.0	0.8990870502	3.4799990174	-0.3048124009
N	7.0	0.3432273291	2.2256708878	-0.1933868115
C	6.0	2.2711686007	3.7939204979	-0.3154004333
C	6.0	3.3227676420	2.8511017641	-0.3002367133
C	6.0	4.7333269409	3.2282282616	-0.2413043596
C	6.0	5.4384237669	2.0726546347	-0.2734775436
C	6.0	4.4569399910	0.9942291728	-0.3377061189
N	7.0	3.1835183029	1.4919568994	-0.3414815547
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C	6.0	2.6200139033	7.4470935254	0.7178594123
C	6.0	3.2879516727	7.9606020612	-0.3877807767
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C	6.0	3.2933377596	5.8099299003	-1.4440126492
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C	6.0	0.3126629891	-6.5997672147	0.6979829594
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C	6.0	-12.2629673006	0.8899423311	0.5074292827
C	6.0	-13.1950000247	-0.3018692137	0.2456709446
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C	6.0	-15.5237042499	-1.3251719410	0.4931248195
C	6.0	-17.0074278680	-1.1028319961	0.8136756231
C	6.0	-17.8450547339	-2.3900951218	0.6814572789
C	6.0	-19.3061004658	-2.1811968940	0.9741158352
C	6.0	-20.3045792799	-2.4288082344	0.1262182418
C	6.0	11.1292852344	-1.7323266068	0.7246775202
C	6.0	12.5396196299	-2.1737808576	0.3560921313
C	6.0	13.4767600841	-2.1888415740	1.5710456665
C	6.0	14.9070956984	-2.6301523395	1.2320590099
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C	6.0	17.2697177201	-3.0873784246	2.1105259981
F	9.0	3.6128631725	9.2712497424	-0.4065526111
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H	1.0	15.8808246581	-1.6115022137	2.8713643865
H	1.0	17.9148771586	-3.0590150020	2.9962351487
H	1.0	17.7257050189	-2.4502824506	1.3438985426
H	1.0	17.2747469522	-4.1161280456	1.7295506101

\$END

Input file for 5b⁺¹

```
$SYSTEM TIMLIM=600000.0 MEMORY=51200000 $END
$CONTRL SCFTYP=ROHF MPLEVL=0 MAXIT=200 ICHARG=+1 MULT=2 COORD=CART
RUNTYP=ENERGY DFTTYP=B3LYP QMTTOL=1.0E-06 MPLEVL=0 $END
$STATPT NSTEP=400 OPTTOL=0.0001 $END
$SCF DIRSCF=.T. SHIFT=.T. DAMP=.T. DIIS=.T. CONV=1.0d-04 $END
# $DFT DFTTYP=B3LYP METHOD=GRID $END
$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=0 DIFFSP=.F. DIFFS=.F. $END
$DATA
DMS:/B3LYP/6-31++G(d,p)/acn
CN 1
```

C	6.0	4.1592043426	-1.4221718604	-0.6404105945
C	6.0	4.6085167832	-2.7758171010	-0.7945966555
C	6.0	3.5073893005	-3.5878462846	-0.8550678881
C	6.0	2.3383351025	-2.7683046389	-0.7074972062
N	7.0	2.7840017678	-1.4699878915	-0.6062182638
C	6.0	4.9636254940	-0.2768570606	-0.5220130647
C	6.0	1.0040899020	-3.2000507914	-0.6234094855
C	6.0	-0.1143156747	-2.3590460074	-0.4233365644
C	6.0	-1.4535703330	-2.8747390076	-0.1581639186
C	6.0	-2.2487491419	-1.7938040549	0.0246207087
C	6.0	-1.3960033165	-0.6208528084	-0.1490540825
N	7.0	-0.1033411949	-0.9926362152	-0.3983362349
C	6.0	-1.8799625484	0.7055946363	-0.0677538363
C	6.0	-1.0805725166	1.8619413426	-0.1516418981
C	6.0	-1.5381802321	3.2188818659	-0.2272997274
C	6.0	-0.4425200690	4.0375817056	-0.3100621618
C	6.0	0.7323240761	3.2162185511	-0.2804091238
N	7.0	0.2945162056	1.9137460636	-0.1961115950
C	6.0	2.0703684446	3.6482441341	-0.3281080018
C	6.0	3.1989029505	2.7996665093	-0.3499692421
C	6.0	4.5726731052	3.2952737572	-0.3038268115
C	6.0	5.3731492630	2.2038135842	-0.3459798502
C	6.0	4.4857376626	1.0464412939	-0.4147913747
N	7.0	3.1747018460	1.4342254978	-0.4053634844
C	6.0	0.7648952274	-4.6762515664	-0.7194350681
C	6.0	2.2959684847	5.1289262274	-0.3576057584
C	6.0	1.9558644628	5.9356510009	0.7410630379
C	6.0	2.1628635372	7.3150235943	0.7181070104
C	6.0	2.7164418155	7.8875813580	-0.4212460076
C	6.0	3.0667357130	7.1251395502	-1.5297487678
C	6.0	2.8530129025	5.7473667629	-1.4894746451
C	6.0	1.2265141796	-5.5523755242	0.2769683734
C	6.0	1.0018422595	-6.9267266000	0.1933811761
C	6.0	0.3052602384	-7.4231406700	-0.9023256700
C	6.0	-0.1707687308	-6.5899248195	-1.9083143568
C	6.0	0.0630164991	-5.2182959639	-1.8088000766
C	6.0	6.4462694496	-0.5050308743	-0.4866599049
C	6.0	-3.3470116176	0.9169550999	0.1265092068
C	6.0	-4.2865877722	0.4372504462	-0.7964908855
C	6.0	-5.6604472502	0.5961109494	-0.5987116229
C	6.0	-6.1252689856	1.2546043671	0.5466771550
C	6.0	-5.1989331526	1.7608099389	1.4716649589
C	6.0	-3.8368865693	1.5920614568	1.2615837352
C	6.0	7.1477186446	-0.4207993053	0.7214203358
C	6.0	8.5240933026	-0.6534650229	0.7895246222

C	6.0	9.2297206914	-0.9779341724	-0.3758461095
C	6.0	8.5424722199	-1.0577770072	-1.5968700576
C	6.0	7.1730622719	-0.8250852064	-1.6470527169
O	8.0	-7.4389584113	1.4525019372	0.8523258740
O	8.0	10.5690468900	-1.2309849713	-0.4297605777
C	6.0	-8.4368709567	0.8084098094	0.0588172276
C	6.0	-9.7861130044	1.0631519964	0.7181599614
C	6.0	-10.9363878516	0.3238432789	0.0220053514
C	6.0	-12.2906643466	0.5429889055	0.7102114003
C	6.0	-13.4394186404	-0.2503494638	0.0731936475
C	6.0	-14.7806463001	-0.0620104893	0.7951043744
C	6.0	-15.9273682403	-0.8799568019	0.1861740807
C	6.0	-17.2577885410	-0.7090135415	0.9313078112
C	6.0	-18.4053285586	-1.5425705011	0.3281963751
C	6.0	-19.6879902901	-1.4243250565	1.1063578452
C	6.0	-20.8422204543	-0.9565815018	0.6291742555
C	6.0	11.3135034483	-1.2598327418	0.7880781808
C	6.0	12.7515539094	-1.6287512608	0.4486631147
C	6.0	13.6316151123	-1.7625397175	1.6987553877
C	6.0	15.0888870837	-2.1208828518	1.3761709869
C	6.0	15.9668651825	-2.2854009161	2.6237944053
C	6.0	17.4222859018	-2.6368829182	2.2961627209
F	9.0	2.9200866458	9.2221471505	-0.4516024180
F	9.0	0.0835006882	-8.7520830771	-0.9921093155
H	1.0	5.6457328311	-3.0705533650	-0.8548346705
H	1.0	3.4928161822	-4.6605882246	-0.9781281847
H	1.0	2.1775501471	-0.6607644083	-0.5151003272
H	1.0	-1.7289273675	-3.9176878353	-0.0899568401
H	1.0	-3.2997853034	-1.7818394310	0.2738182622
H	1.0	-2.5771959128	3.5124324894	-0.2408264459
H	1.0	-0.4368084546	5.1139011195	-0.3985478354
H	1.0	0.9067295091	1.1040376911	-0.2080995470
H	1.0	4.8688087573	4.3326401021	-0.2390786220
H	1.0	6.4534903312	2.1700581716	-0.3379356107
H	1.0	1.5329738181	5.4733302377	1.6284732898
H	1.0	1.9092617276	7.9430964663	1.5663256871
H	1.0	3.4915522962	7.6099542187	-2.4030575860
H	1.0	3.1166000334	5.1392763595	-2.3500576850
H	1.0	1.7586827364	-5.1490954007	1.1337837619
H	1.0	1.3504158783	-7.6082157111	0.9630117865
H	1.0	-0.7074309895	-7.0163395650	-2.7499796735
H	1.0	-0.2989835834	-4.5554496827	-2.5895145033
H	1.0	-3.9391484310	-0.0700112353	-1.6923952828
H	1.0	-6.3512517298	0.2107155193	-1.3405350370
H	1.0	-5.5737551527	2.2653871460	2.3571704188
H	1.0	-3.1342191747	1.9695342639	1.9995610885
H	1.0	6.6076035883	-0.1759560464	1.6323460973
H	1.0	9.0271929142	-0.5830051449	1.7473443382
H	1.0	9.1045086246	-1.3040081403	-2.4928854512
H	1.0	6.6545605388	-0.8900454733	-2.6001116006
H	1.0	-8.2271038415	-0.2705573961	0.0068628292
H	1.0	-8.4168466517	1.2045056733	-0.9675191430
H	1.0	-9.9783380142	2.1440576339	0.7303428988
H	1.0	-9.7201260288	0.7447760217	1.7668725041
H	1.0	-10.7145437874	-0.7539080006	0.0006146297
H	1.0	-11.0036387487	0.6420930428	-1.0290773570
H	1.0	-12.5361403590	1.6154266578	0.7001393567
H	1.0	-12.2037311364	0.2620593136	1.7705224183
H	1.0	-13.1796296957	-1.3198668372	0.0670419212

H	1.0	-13.5470507442	0.0420335991	-0.9820873202
H	1.0	-15.0509486139	1.0045334556	0.7898313098
H	1.0	-14.6623625416	-0.3390527144	1.8534609174
H	1.0	-15.6503464032	-1.9450468091	0.1809540881
H	1.0	-16.0598130820	-0.5956808497	-0.8684417289
H	1.0	-17.5480344365	0.3509244132	0.9339614360
H	1.0	-17.1217710634	-0.9907088586	1.9861330748
H	1.0	-18.0923276500	-2.5984597383	0.3012266876
H	1.0	-18.5752965951	-1.2406955174	-0.7141264354
H	1.0	-19.6384159180	-1.7439394875	2.1496811158
H	1.0	-21.7340250372	-0.8904068738	1.2475301813
H	1.0	-20.9418217955	-0.6241437794	-0.4028391415
H	1.0	10.8749395847	-1.9991572771	1.4754110210
H	1.0	11.2684281428	-0.2763599858	1.2796769334
H	1.0	13.1630670385	-0.8663289249	-0.2258030434
H	1.0	12.7453631664	-2.5735700041	-0.1102939476
H	1.0	13.2090509931	-2.5322849644	2.3618093176
H	1.0	13.6092098805	-0.8223743896	2.2698790279
H	1.0	15.5188920169	-1.3424071329	0.7283276769
H	1.0	15.1123813133	-3.0512911299	0.7896131428
H	1.0	15.5380663606	-3.0673436115	3.2672768050
H	1.0	15.9376814623	-1.3573698462	3.2127748940
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H	1.0	17.4860055474	-3.5787880715	1.7368762076

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