Supporting Information for

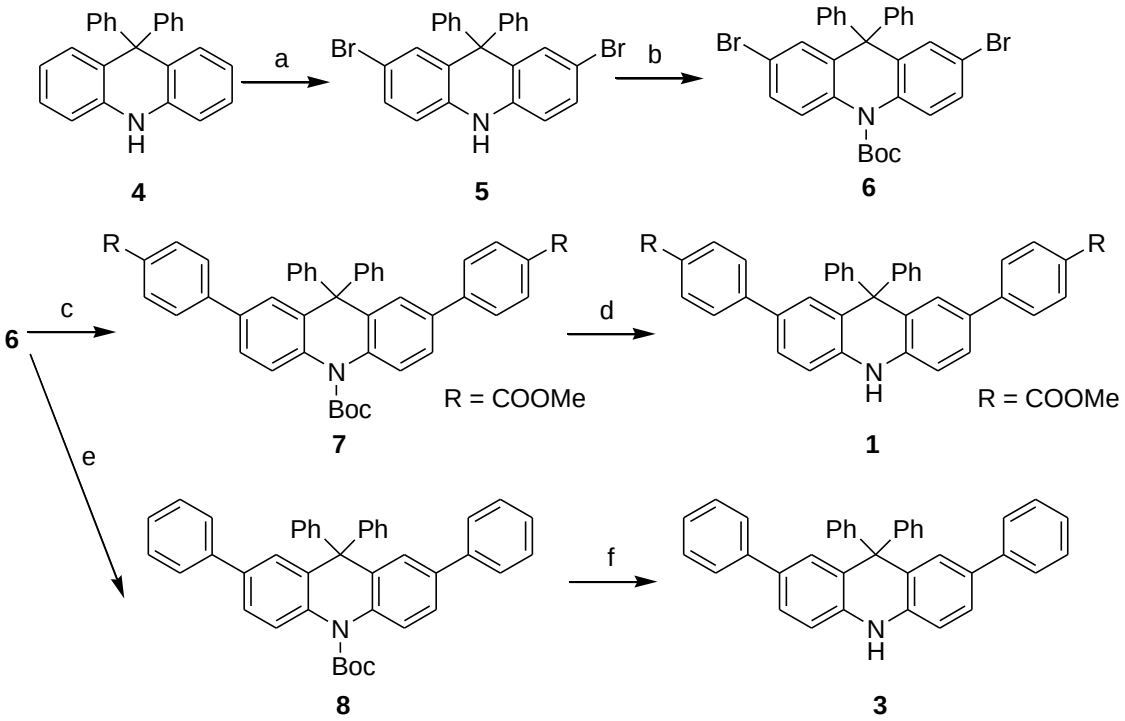
Synthesis of ester-substituted dihydroacridine derivatives and their spectroscopic properties

Ryota Suzuki, Reiki Tada, Takumi Hosoda, Youhei Miura, and Naoki Yoshioka*

Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Yokohama, 223-8522, Japan

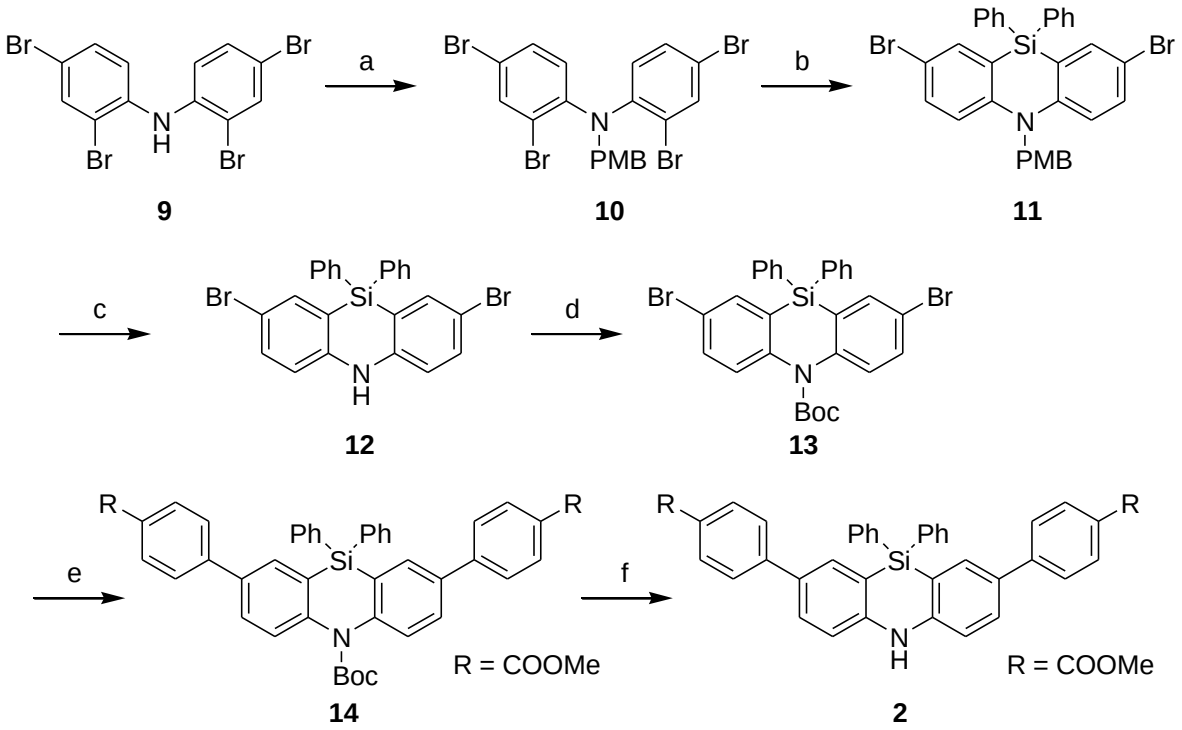
Contents:

1. The synthetic routes



(a) NBS, DMF (95%); (b) $(Boc)_2O$, DMAP, THF (92%); (c) 2-(4-methoxycarbonylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, $Pd(PPh_3)_4$, K_2CO_3, THF (75%); (d) HCl, AcOEt (56%); (e) $PhB(OH)_2$, $Pd(PPh_3)_4$, K_2CO_3, THF (90%); (f) HCl, AcOEt (95%).

Scheme S1. The synthetic routes of **1** and **3**.



(a) PMBCl, NaH, DMF (90%); (b) *n*-BuLi, $SiPh_2Cl_2$, Et_2O (77%); (c) Pd black, H_2, CH_2Cl_2 (63%); (d)$(Boc)_2O$, DMAP, THF (89%); (e) 2-(4-methoxycarbonylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, $Pd(PPh_3)_4$, K_2CO_3, THF (51%); (d) H_2SO_4, MeOH (65%).

Scheme S2. The synthetic route of **2**.

2. UV-vis measurements

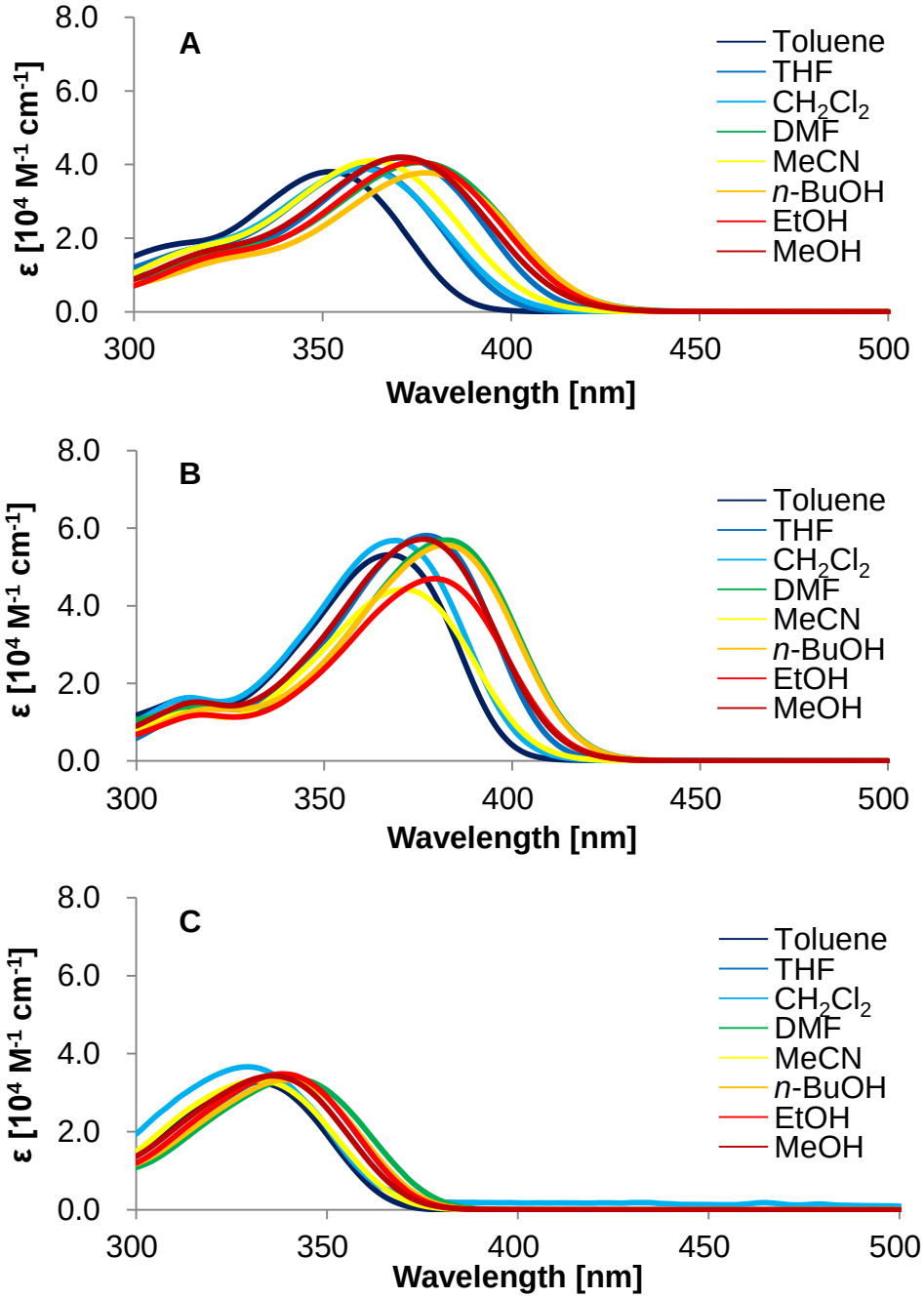


Figure S1 UV-vis spectra of **1** (A)**, 2** (B) and **3** (C) in various solvents.

3. Electrochemical measurements

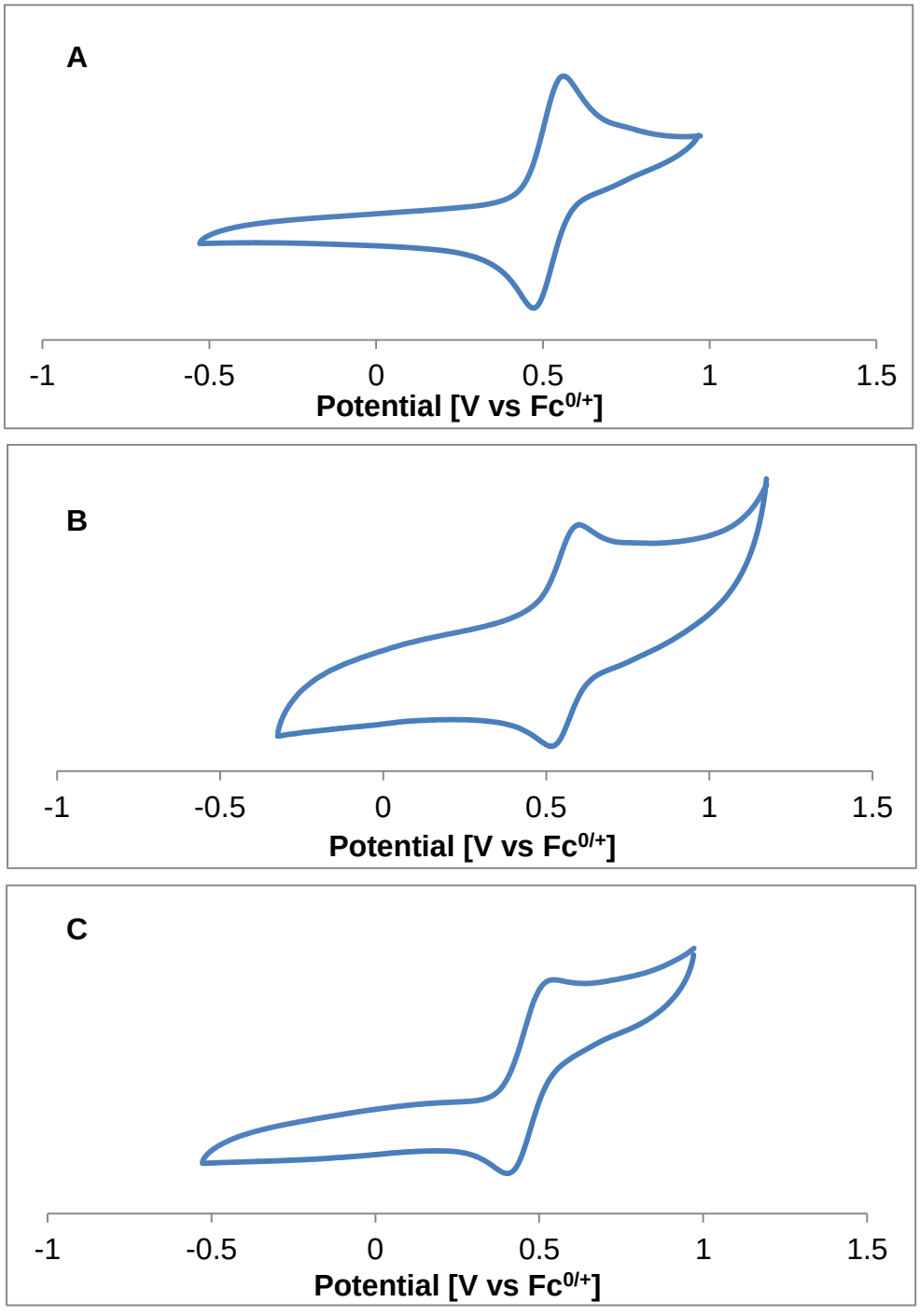


Figure S2 Cyclic voltammograms of **1**, **2** and **3** in dichloromethane containing 0.1 M tetrabutylammonium hexafluorophosphate at room temperature.

4. Geometry Optimization at Excited States

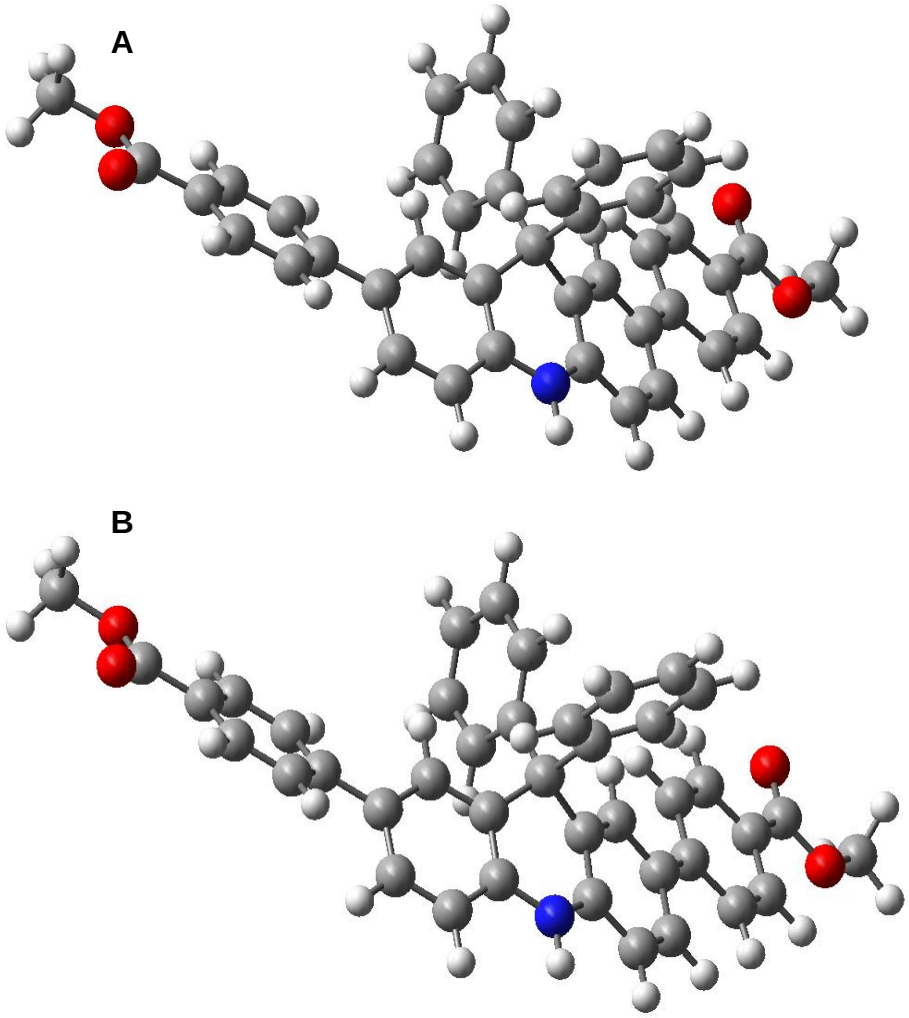
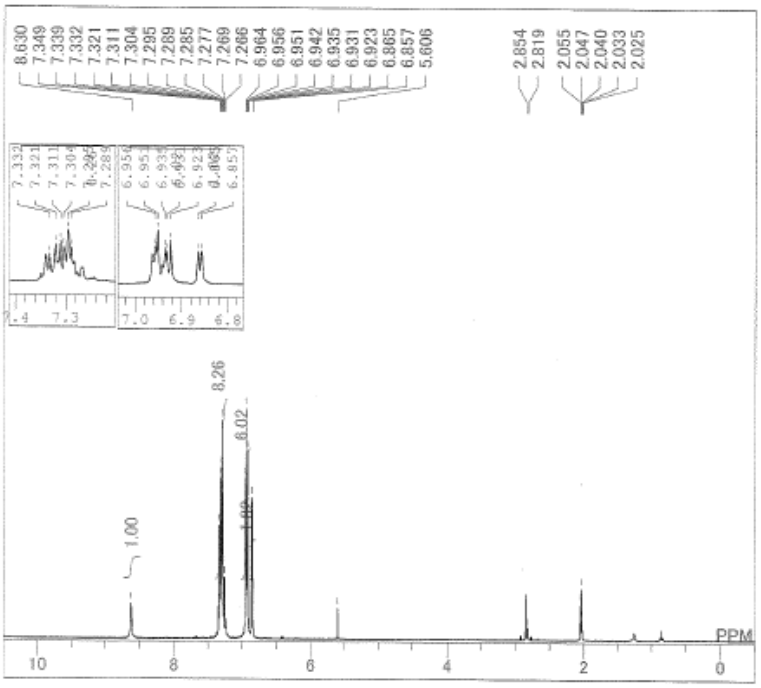


Figure S3 The geometry optimization at the excited states in toluene (A) and MeOH (B) by using TD-DFT (B3LYP/6-31G*)

5. ^{1}H and ^{13}C NMR spectra



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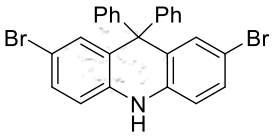

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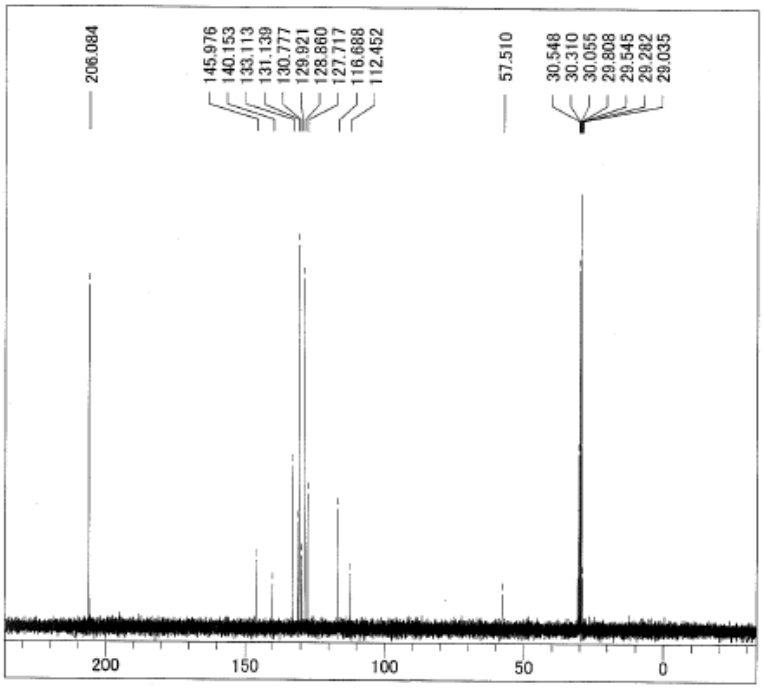

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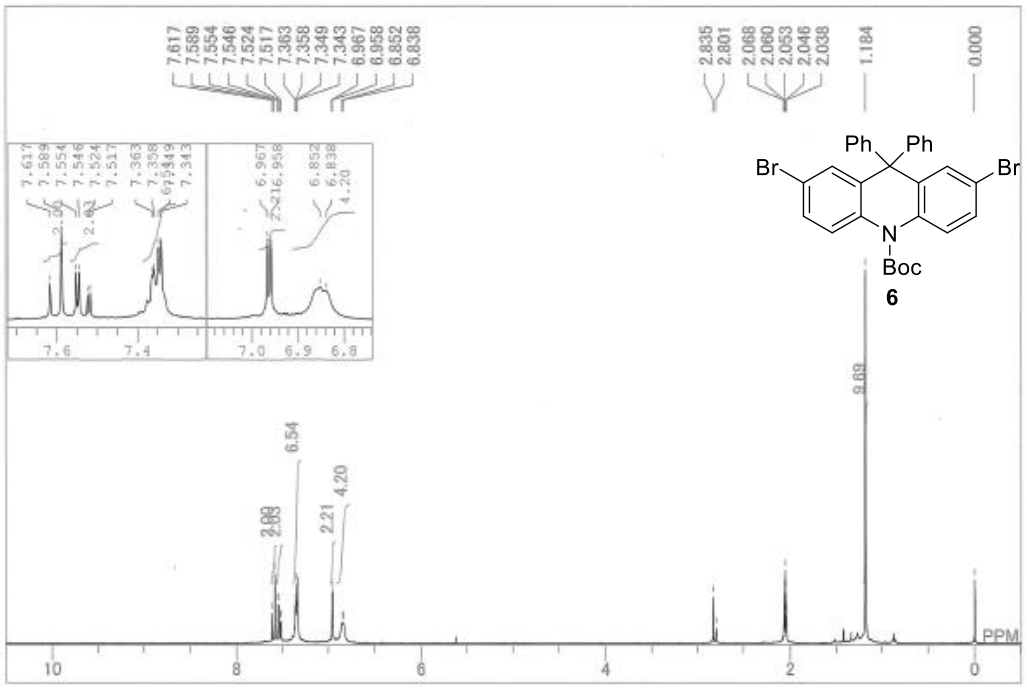
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2.801
2.068
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2.046
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0.000
Ph
Ph
Br
Br
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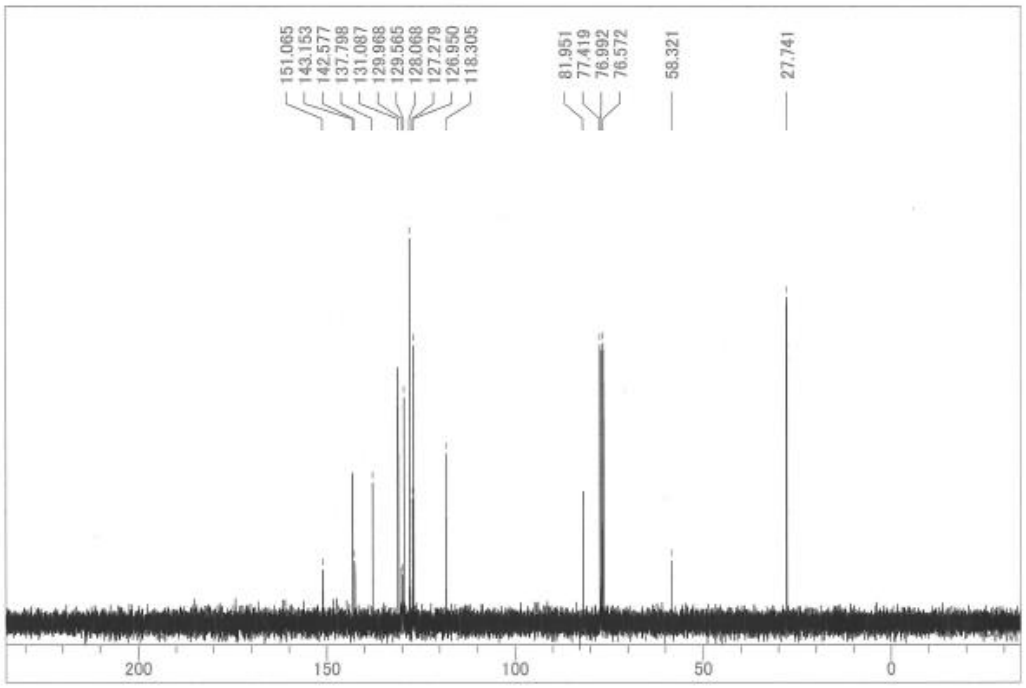
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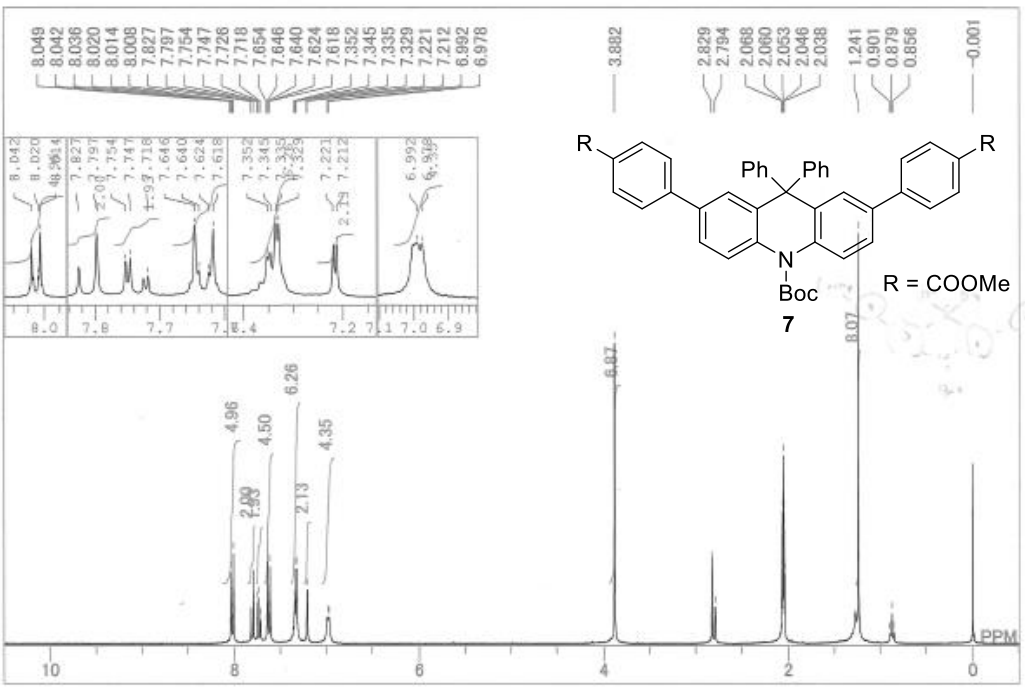
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Boc
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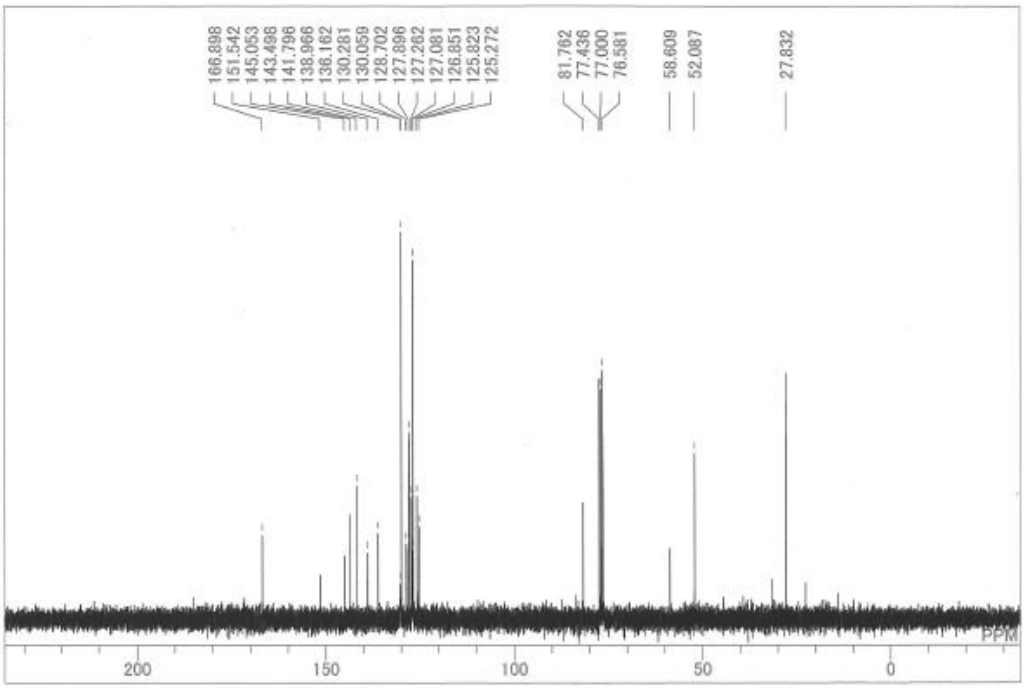
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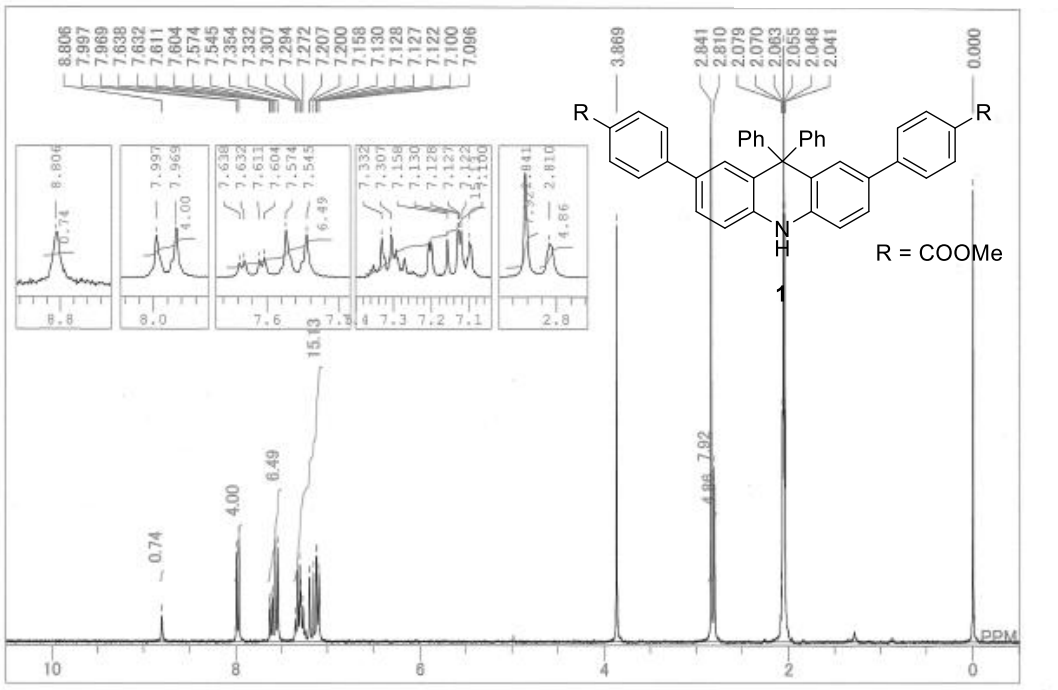

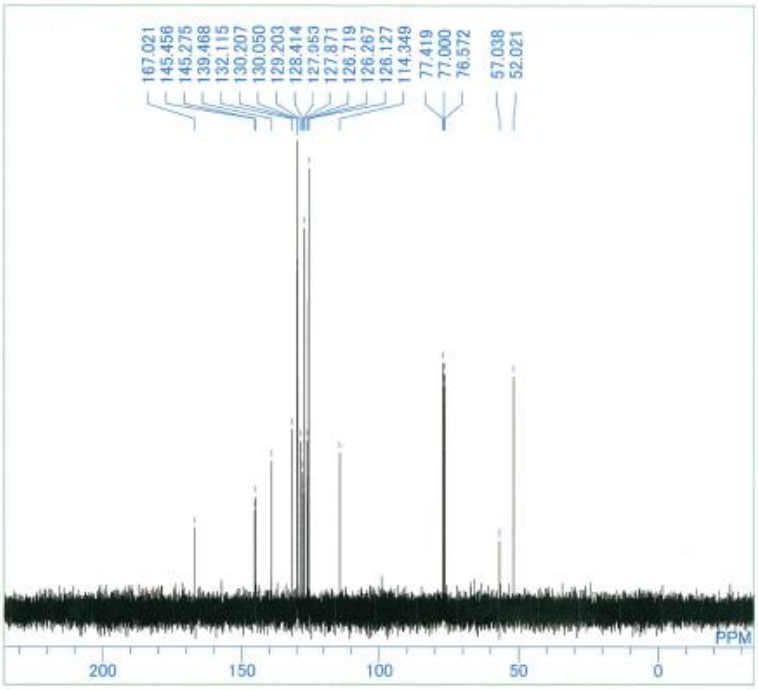

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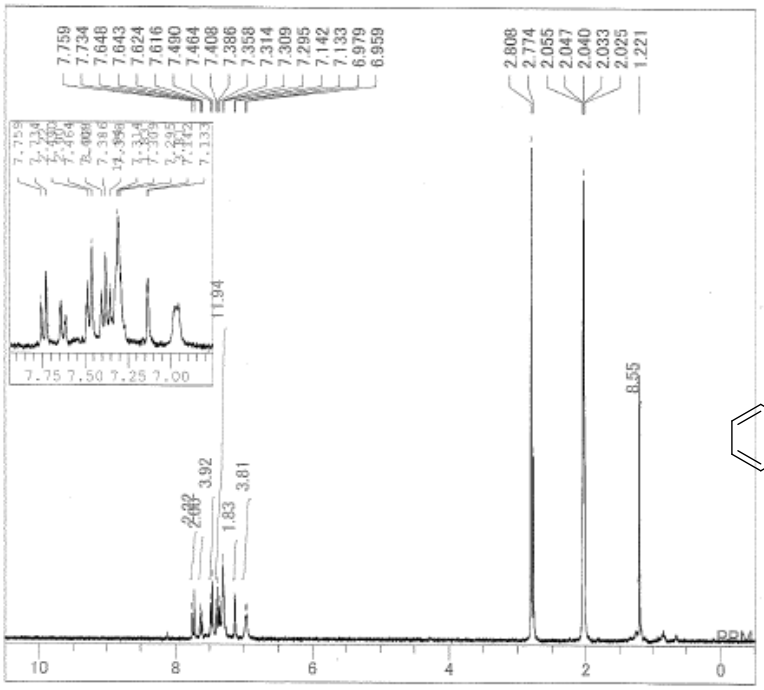

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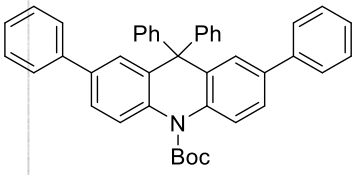

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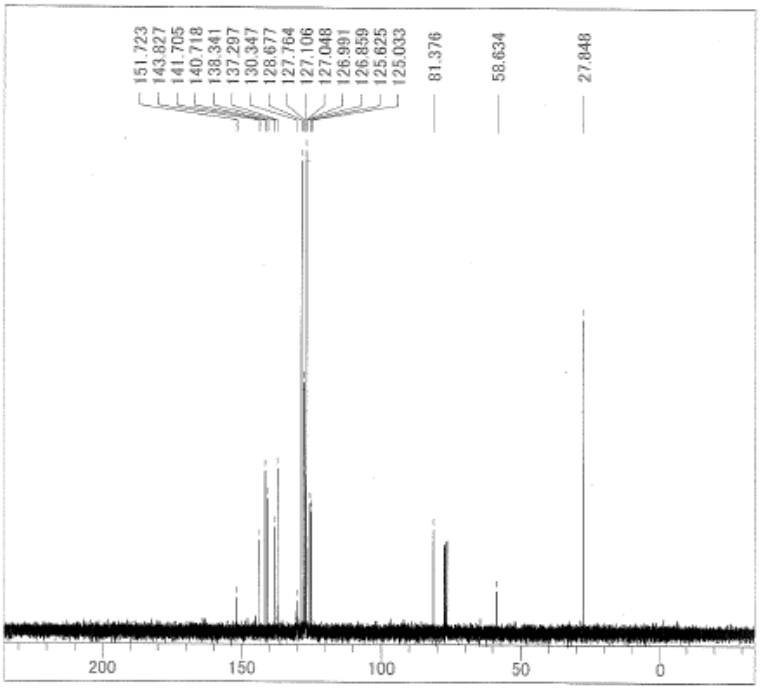

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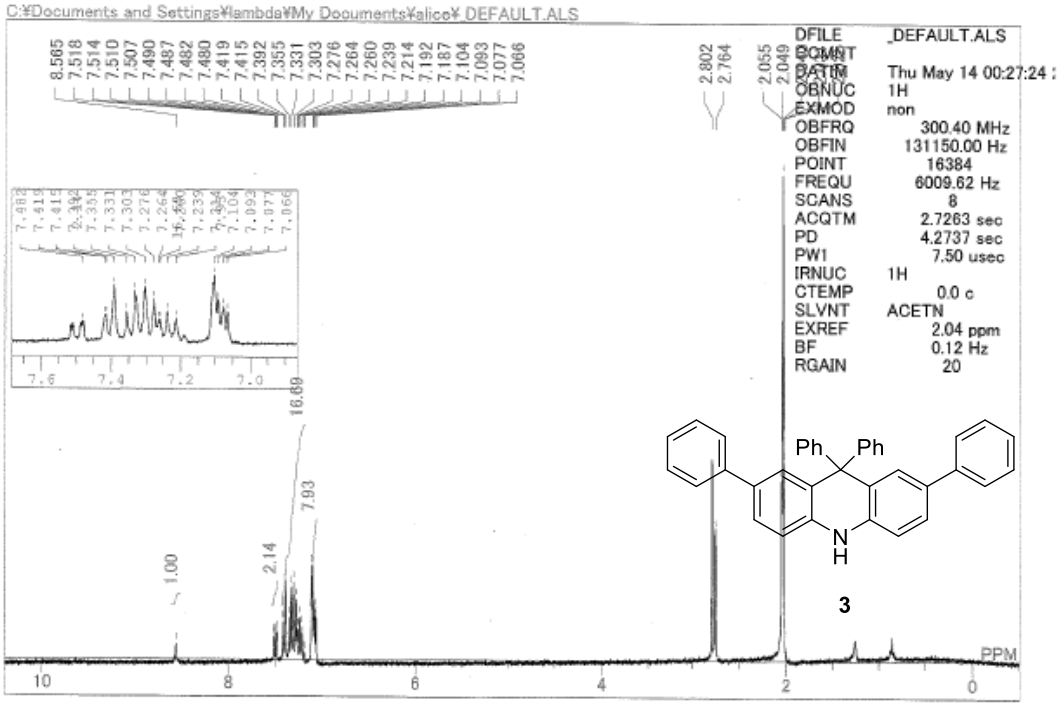
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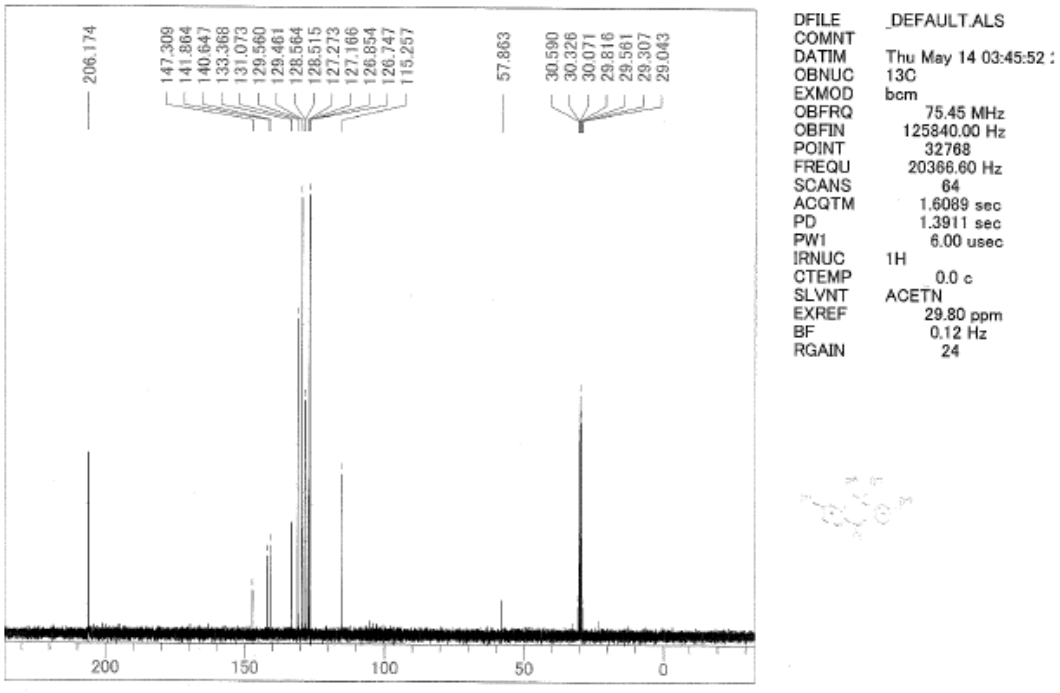
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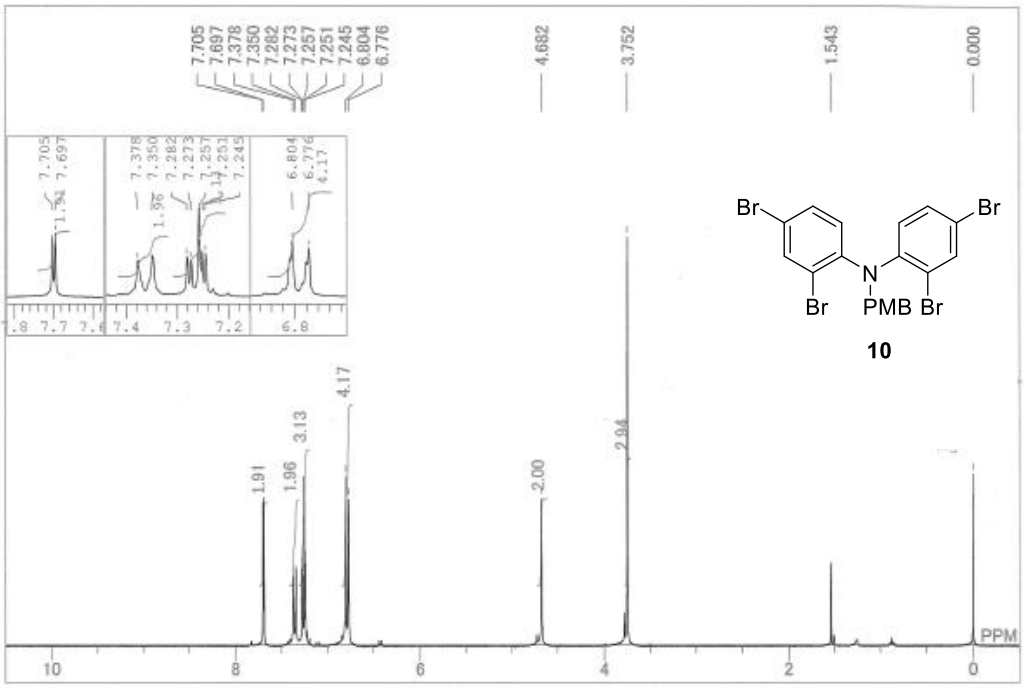
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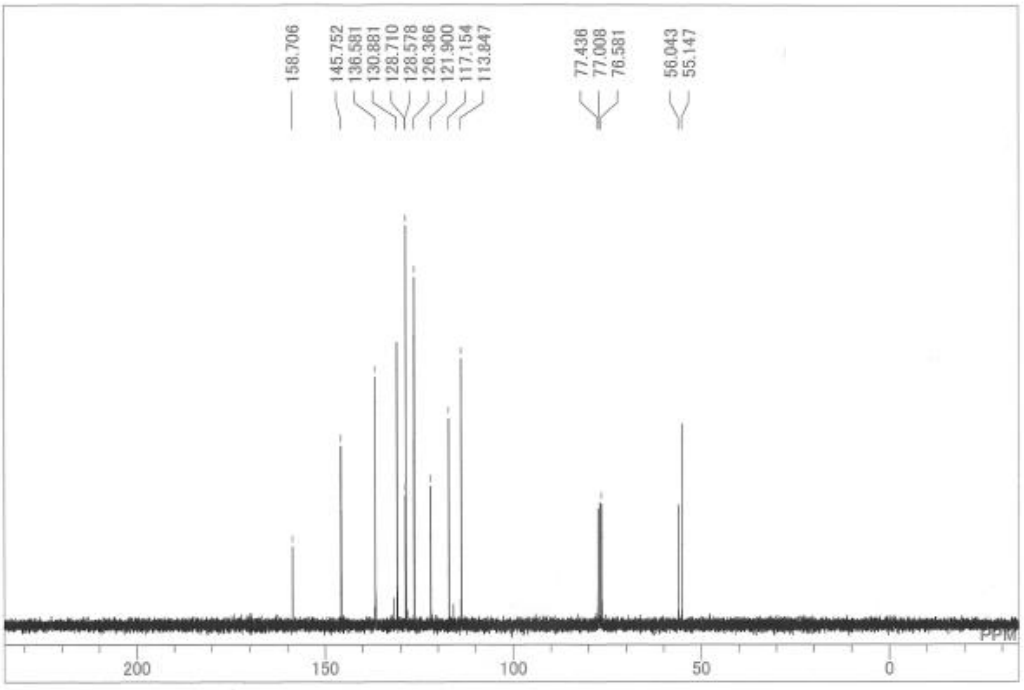
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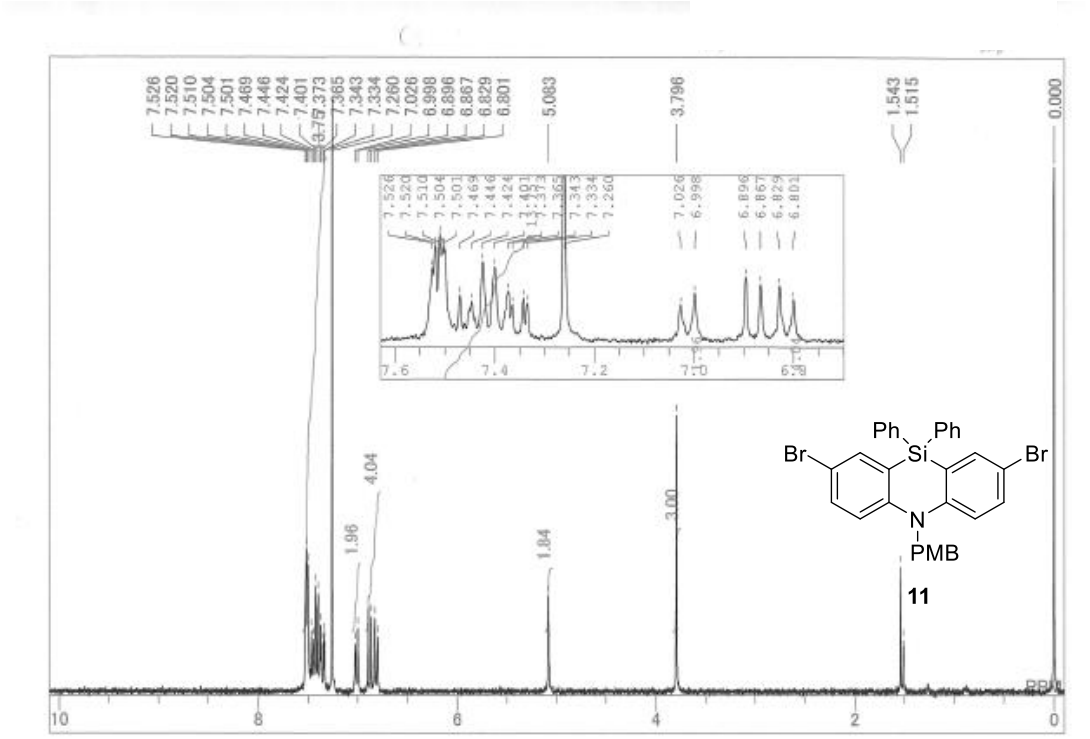
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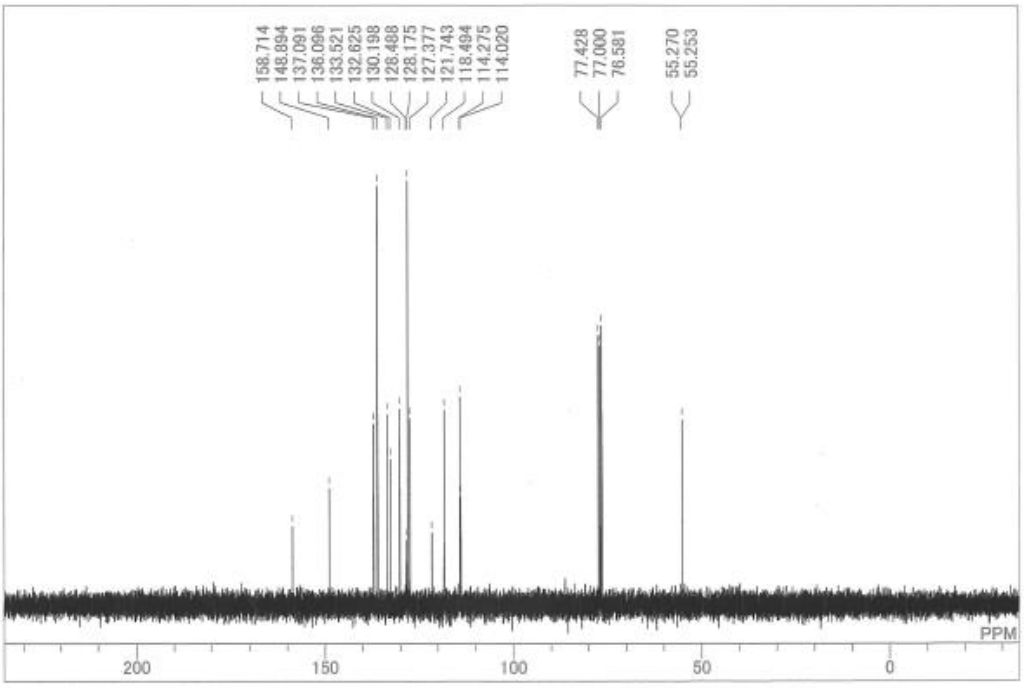
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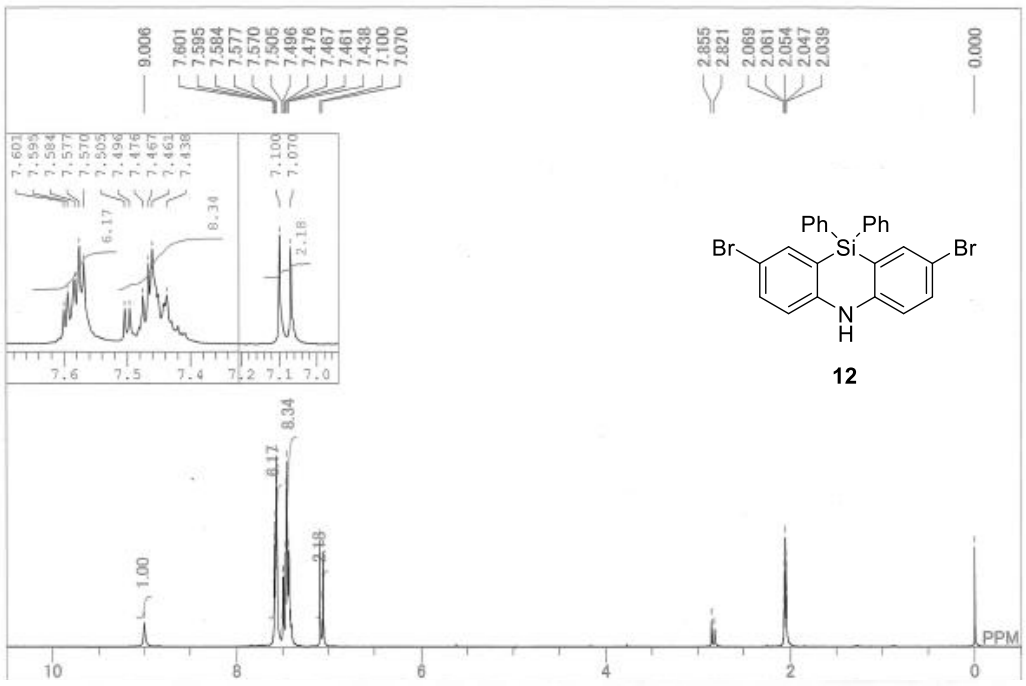
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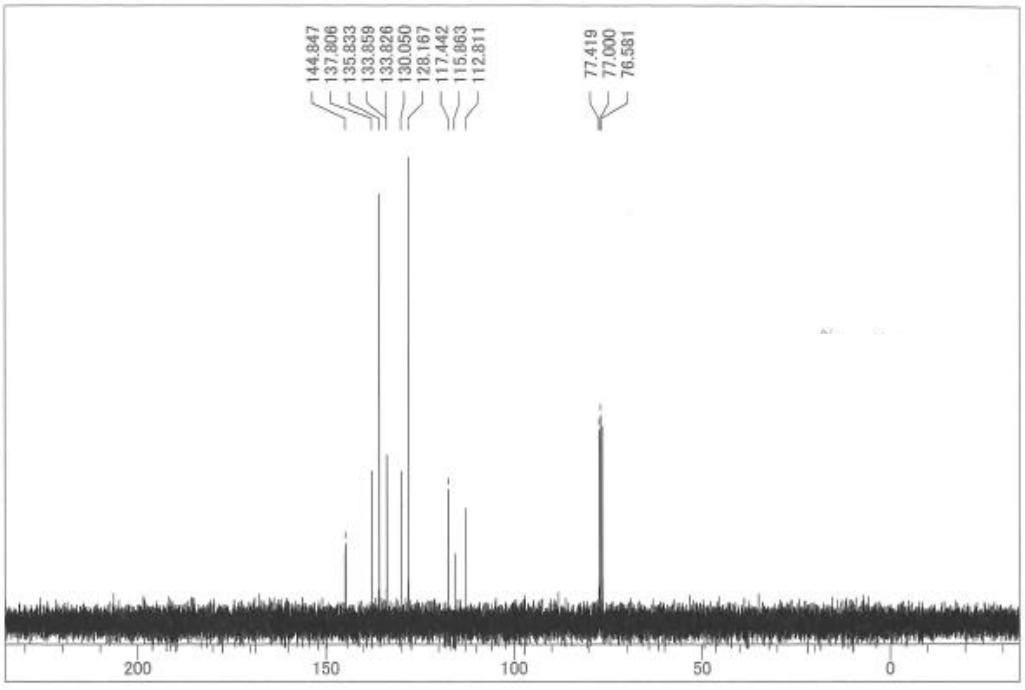
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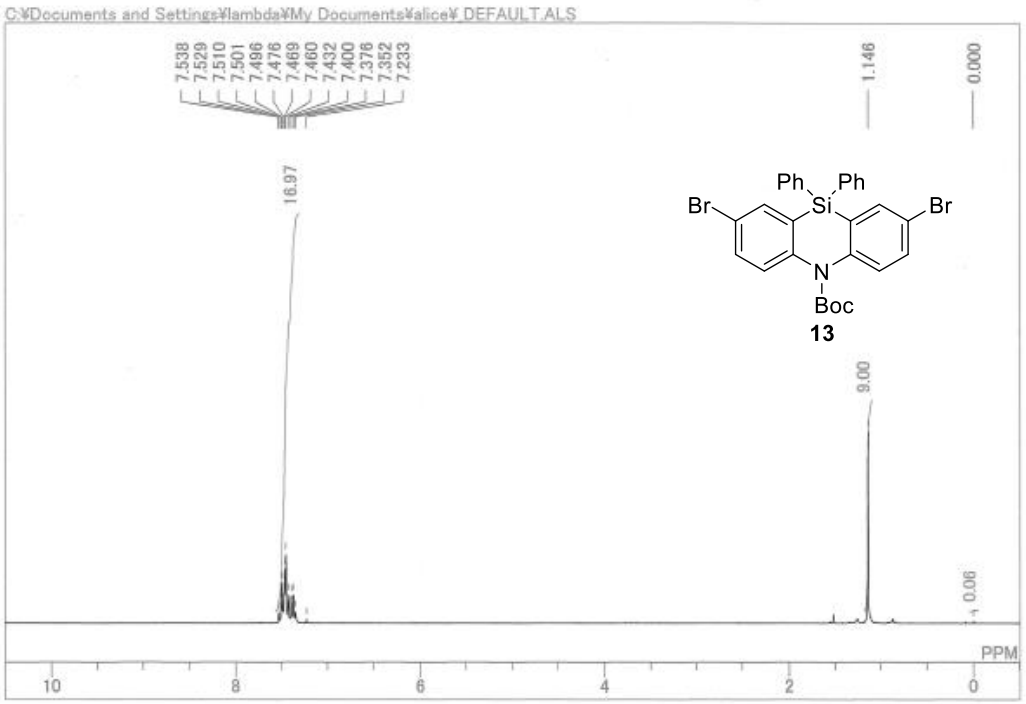
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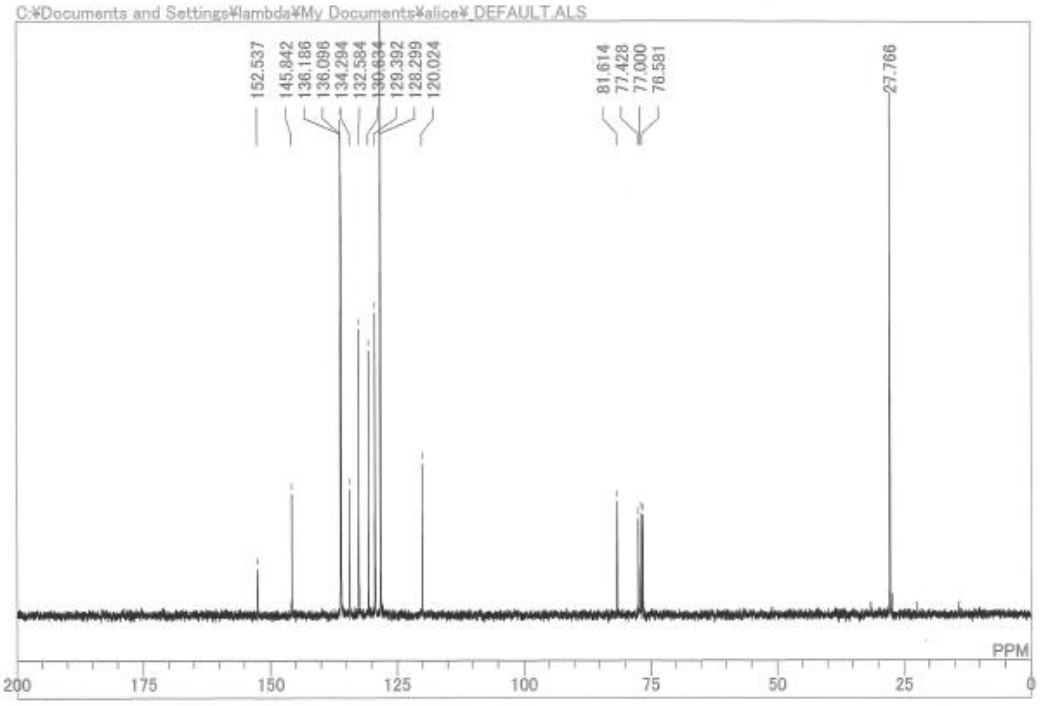
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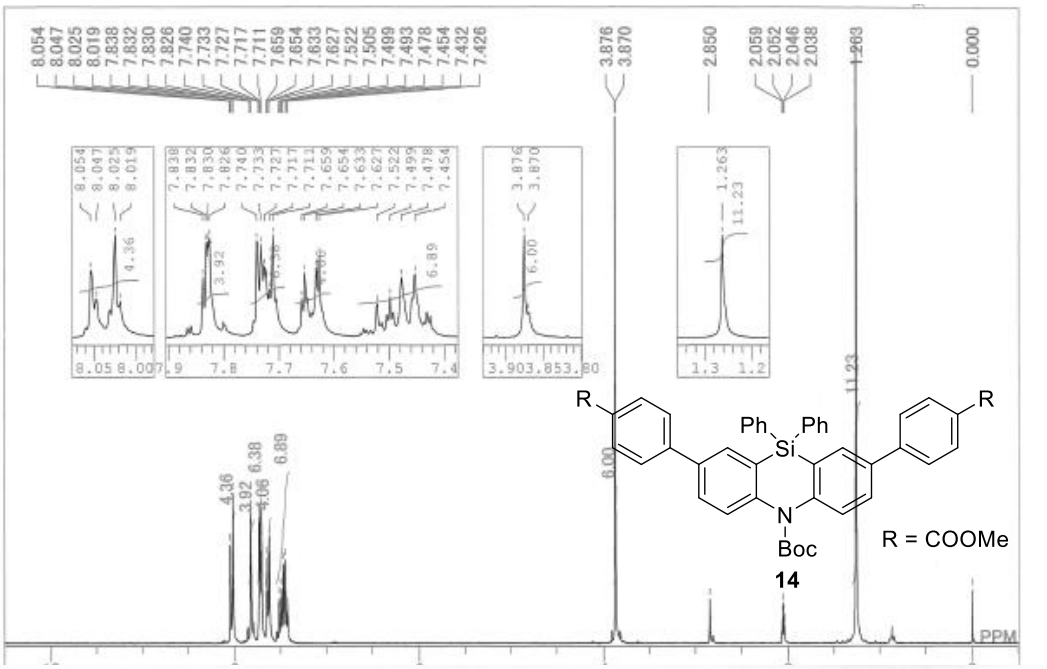
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Ph
Si
N
Boc
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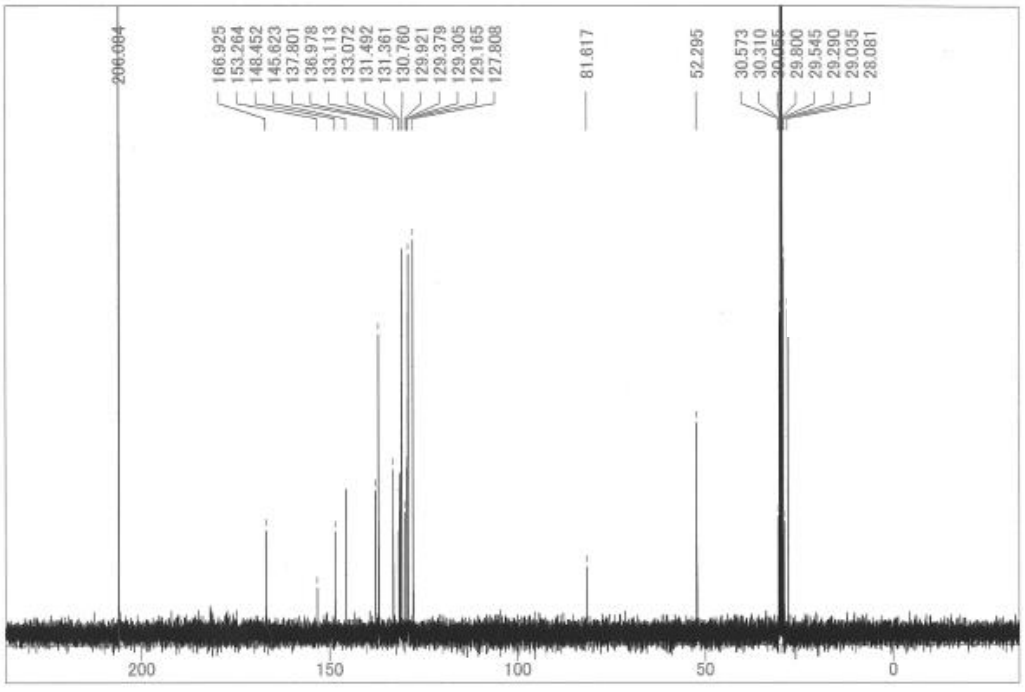
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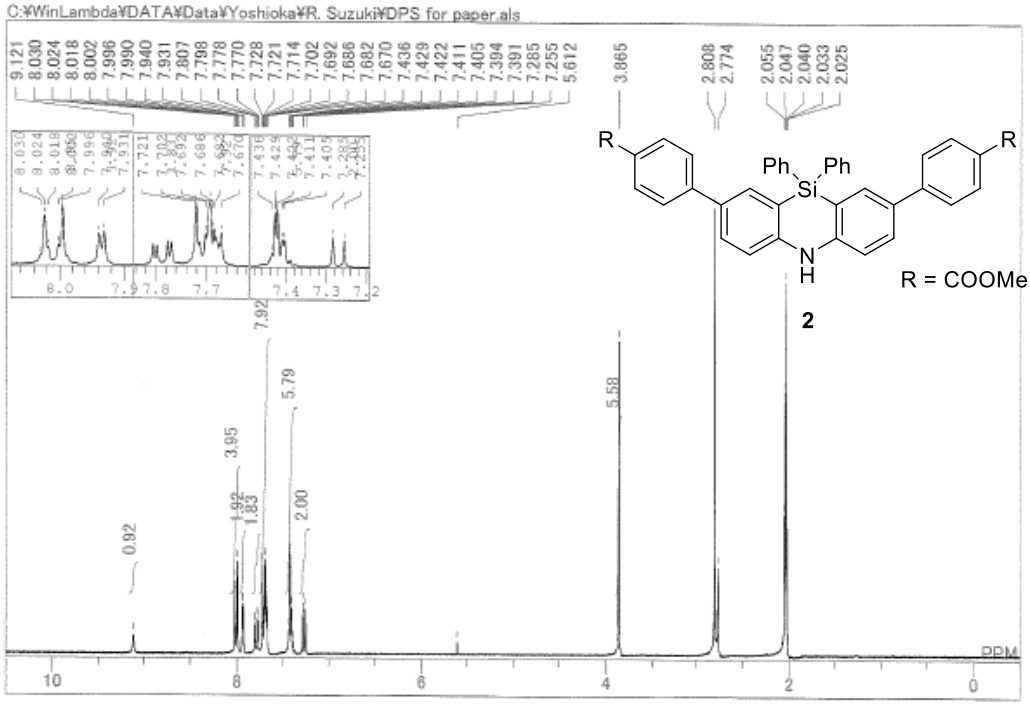

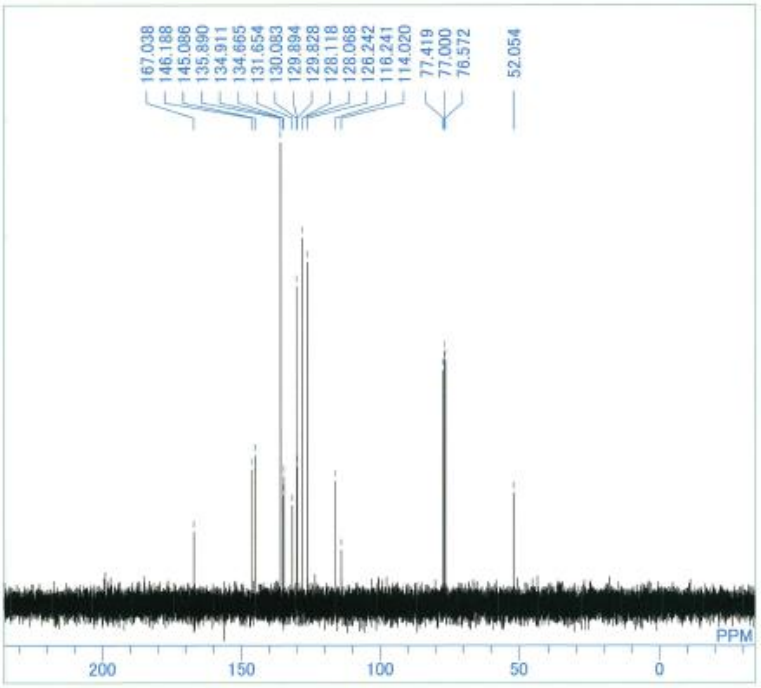

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PD 1.3911 sec
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EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 26

6. Crystal data and the parameter

TableS1. Crystal data and the parameter for refinement of **1** and **2**·CH_3CN..

Compounds	**1**	**2**·CH_3CN
Formula	$C_{41}H_{31}NO_4$	$C_{40}H_{31}NO_4Si$ · CH_3CN
T (K)	296.(2)	296.(2)
λ(Å)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	*P* 2_1/n	*P* 2_1/c
Z	4	8
a (Å)	12.2394(7)	35.973(9)
b (Å)	18.8894(11)	9.0438(19)
c (Å)	13.5842(8)	21.966(6)
α (°)	90	90
β (°)	92.6687(18)	99.707(8)
γ (°)	90	90
V ($Å^3$)	3137.2(3)	7044.(3)
D_{calc} (g cm^{-3})	1.274	1.165
μ(Mo Kα) (mm^{-1})	0.082	0.112
Unique data	5890	10183
no. of parameters	417	889
Goodness of fit on F^2	1.035	0.955
wR^2	0.1350	0.1541
R	0.0458	0.0745

7. Gaussian 03 archive files[1]

Geometry optimization of 1

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d)|C41H31N1O4|PCUSER|30-Oct-2014|0||#OPTB3LYP/6-31G*||PMPDA_opt_631g_s||0,1|N,-2.1763470815,0.6175987095,-2.54989443|C,-2.1945937736,0.4971096123,1.1258068646|H,-1.483399023,0.5196972519,1.9442016482|C,-0.2403995616,0.952964959,-0.5044389465|C,1.3865056757,-0.1983414028,-2.1509977637|H,2.1532265761,-0.1455116292,-1.3859957931|C,-0.093972657,2.4991934981,-0.6816160337|C,-2.6391090803,0.5520574244,-1.2371977998|C,-1.7135663087,0.6266065938,-0.1779857584|C,0.1087686905,0.2713596833,-1.8449372034|C,0.682904753,0.4275906273,0.6196387155|C,-0.8760999794,0.2177634022,-2.8507548837|C,-0.9315637063,3.3945551293,-0.0011775435|H,-1.7283015466,3.0169186761,0.6297007898|C,0.9170348843,3.0377246182,-1.4919551499|H,1.581648492,2.3769315258,-2.0374391834|C,1.0845545732,4.4173143045,-1.6176958473|H,1.8758992842,4.8030997305,-2.2552966454|C,-4.0056694267,0.3902698692,-0.9698663151|H,-4.7115927527,0.343874233,-1.7964733234|C,1.4998046649,1.2620328552,1.3889996887|H,1.5064085707,2.3302788609,1.2055601189|C,1.7303319121,-0.6902178465,-3.4217981097|C,0.7028583047,-0.9520110248,0.893323111|H,0.0721855435,-1.6185961371,0.3119451187|C,-3.5584482321,0.3223100035,1.4168183351|C,2.3157429245,0.7373531258,2.3979978672|H,2.9412729145,1.4089467808,2.9801900886|C,-0.5529971505,-0.2575950805,-4.1292963363|H,-1.3251891601,-0.3053795993,-4.8942565069|C,-0.7669871345,4.7754771246,-0.1261098255|H,-1.4356731086,5.4432942168,0.4110439152|C,0.2414150586,5.2954313978,-0.9364939496|H,0.3675601718,6.3700633944,-1.0378450247|C,-4.4576479698,0.28254297,0.3376206168|H,-5.522466181,0.1789843694,0.5240424693|C,1.5137279402,-1.4763988051,1.8962287347|H,1.507983456,-2.5463805439,2.0875522118|C,0.7326918212,-0.697121473,-4.4115458865|H,0.9518891642,-1.092644798,-5.3988831086|C,2.3279647592,-0.6307594091,2.6558448578|H,2.9611287576,-1.0376548074,3.4396717795|C,-4.0304032701,0.1901787073,2.815337758|C,-5.103990222,-0.6606064513,3.1388413968|C,-3.4213990669,0.9075655504,3.8624860591|C,-5.5532975449,-0.7902375589,4.4482908621|H,-5.573291751,-1.2491070959,2.3557834946|C,-3.8644836425,0.7792052672,5.1727874927|H,-2.6075248777,1.5914558051,3.6404327949|C,-4.9360546387,-0.0700466953,5.4804633288|H,-6.3763085794,-1.4576358932,4.6784003891|H,-3.3977027354,1.3393878682,5.9764229247|C,3.0994298537,-1.1816844298,-3.702676374|C,3.8484385899,-1.8434712638,-2.7114951272|C,

3.6912108458,-1.006694342,-4.9680955782|C,5.1326714257,-2.309705772,-2 .969728
4089|H,3.4069007849,-2.0153708724,-1.7342471608|C,4.9719360105,
-1.4753941337,-5.2323308429|H,3.1489194322,-0.4728736228,-5.7430761224
|C,5.7071845578,-2.131842971,-4.2360861387|H,5.6915632515,-2.822985919
9,-2.195246743|H,5.428336497,-1.3330748352,-6.2065089833|C,-5.36956417
91,-0.1657129696,6.8995327124|O,-4.8622728532,0.4456309374,7.820649497
|O,-6.4081690868,-1.0201671498,7.0681423801|C,7.0732771896,-2.61126922
08,-4.574792642|O,7.6040908679,-2.4769663695,-5.6610642488|O,7.6808199
199,-3.2259615874,-3.5308344614|C,-6.8720703911,-1.1568435471,8.418588
2185|H,-7.2242950414,-0.1961230081,8.8041811037|H,-7.6909566065,-1.875
8964904,8.3752680442|H,-6.0711617735,-1.5243981073,9.065877838|C,9.004
2505531,-3.711899482,-3.7949884808|H,9.3390363452,-4.1698619735,-2.863
5068665|H,8.9903745041,-4.4491698326,-4.6024500802|H,9.6669267518,-2.8
899167693,-4.0792707397|H,-2.86704089,0.4636543555,-3.2729368167||Vers
ion=x86-Win32-G03RevB.04|State=1-A|HF=-1936.7398337|RMSD=7.352e-009|RM
SF=3.330e-005|Dipole=-1.0112381,-0.4346685,-0.2792111|PG=C01 [X(C41H31
N1O4)]||@

Energy calculation of 1

1|1|UNPC-UNK|SP|RB3LYP|6-31G(d)|C41H31N1O4|PCUSER|08-Nov-2014|0||# B3L
Y P / 6 - 3 1 G * F O R M C H E C K = A L L P O P = R E G
S C F = (M A X C Y C L E = 2 0 0) | | P M P D A _ o p t _ 6 3 1 g _ s | |
0,1|N|C,1,3.67772065|H,2,1.08447192,1,138.61619141|C,2,2.58541734,1,50 .22797781
,3,7.72740618,0|C,4,2.5852434,2,143.01040292,1,-75.71506453,0
|H,5,1.08437985,4,88.50656252,2,-101.41128065,0|C,4,1.56322005,2,108.4
6165416,1,94.43969913,0|C,1,1.39341861,4,63.43853006,2,3.23387473,0|C,
2,1.39571944,1,20.21985594,8,-172.46782946,0|C,5,1.39531504,4,30.01517
671,2,74.68582863,0|C,4,1.54662815,2,86.16131964,1,-154.42457217,0|C,1 ,1.393207
87,8,119.99236703,9,26.02389588,0|C,7,1.40222266,4,121.375052
47,2,0.78903362,0|H,13,1.08416204,7,119.92931553,4,-2.71533271,0|C,7,1 .40313963,
4,120.83592596,2,178.38374452,0|H,15,1.08439439,7,119.883574
6,4,2.60057703,0|C,15,1.39539993,7,121.19798268,4,-177.68779214,0|H,17 ,1.087009
82,15,119.41536811,7,-179.85438275,0|C,8,1.4018307,1,120.5861
0065,12,-152.86023193,0|H,19,1.08800654,8,119.50732117,1,-1.72450844,0
|C,11,1.39840396,4,123.08603994,2,-106.42564541,0|H,21,1.08390201,11,1
19.90341703,4,-0.22974653,0|C,5,1.40538021,4,152.34294041,2,87.1059848

2,0|C,11,1.40662762,4,118.88427256,2,73.19677722,0|H,24,1.086317,11,11
9.30541873,4,0.0189603,0|C,2,1.40546814,1,102.46433163,12,-155.5886003
8,0|C,21,1.3996862,11,120.8945826,4,179.83688385,0|H,27,1.0868643,21,1
19.34193639,11,179.95382124,0|C,12,1.40179547,1,120.62341454,8,153.191
60672,0|H,29,1.08799282,12,119.51014495,1,0.53576785,0|C,13,1.39629465 ,7,121.17
651799,4,177.73329231,0|H,31,1.08703944,13,119.3973162,7,179.
72653503,0|C,31,1.3942562,13,120.40262393,7,0.0066141,0|H,33,1.0867468
4,31,120.45937095,13,179.72937813,0|C,19,1.38759241,8,120.4101138,1,17
7.93147971,0|H,35,1.08596216,19,119.24496285,8,178.70690786,0|C,24,1.3
9223266,11,121.18722894,4,-179.86507695,0|H,37,1.08696703,24,119.63568
668,11,179.88736508,0|C,29,1.38774766,12,120.42741877,1,-177.81760124,
0|H,39,1.08596546,29,119.16128522,12,177.94233225,0|C,27,1.39225167,21 ,120.462
86599,11,-0.05722358,0|H,41,1.08666706,27,120.44125561,21,-179 .96387477,0|C,26,
1.48191045,2,121.03366736,1,178.66204595,0|C,43,1.407
50818,26,120.91217937,2,-144.44585747,0|C,43,1.40785284,26,121.2475596
8,2,35.47622354,0|C,44,1.39044622,43,121.28413067,26,-179.98587195,0|H ,44,1.086
16513,43,119.43075182,26,1.76242707,0|C,45,1.38913229,43,121.
0991123,26,-179.86189888,0|H,45,1.0860045,43,119.53704763,26,1.6530442 ,0|C,48,1
.40148359,45,120.46092462,43,-0.16526676,0|H,46,1.08430549,44 ,120.16612016,43,-
179.45938677,0|H,48,1.0851359,45,120.90732084,43,-179.530049,0|C,23,1.48150669,5,120.90569704,4,172.76489308,0|C,53,1.4076
2788,23,120.94381796,5,34.55105702,0|C,53,1.40787468,23,121.17251246,5 ,-145.66
599,0|C,54,1.39043567,53,121.22062147,23,179.8549406,0|H,54,1.
0860571,53,119.45159591,23,1.38541582,0|C,55,1.38915718,53,121.1015121
4,23,-179.60006642,0|H,55,1.0861122,53,119.50867225,23,2.07679261,0|C,
58,1.40143387,55,120.43182682,53,-0.23907089,0|H,56,1.08426869,54,120.
14299861,53,-179.59529892,0|H,58,1.08516312,55,120.94811148,53,-179.57
142744,0|C,50,1.48688916,48,118.12729666,45,-179.86449857,0|O,63,1.216
36456,50,124.66650227,48,0.2170944,0|O,63,1.35544116,50,112.50001228,4
8,-179.77515422,0|C,60,1.48686993,58,118.10719451,55,-179.94923496,0|O ,66,1.216
46469,60,124.66184616,58,-0.10733555,0|O,66,1.35528663,60,112.49707913,58,179.9
05196 35,0|C,65,1.43442973,63,115.14976974,50,179.941
09394,0|H,69,1.09349333,65,110.63643766,63,60.82548239,0|H,69,1.090636
77,65,105.56008178,63,-179.52817656,0|H,69,1.09340563,65,110.63863725,
63,-59.84656035,0|C,68,1.43435793,66,115.17644197,60,-180.,0|H,73,1.09
062742,68,105.55698668,66,179.97709545,0|H,73,1.09350553,68,110.652373

76,66,-60.36641329,0|H,73,1.09344031,68,110.63297833,66,60.31425647,0|H,1,1.01170499,12,116.0494823,29,5.32517867,0||Version=x86-Win32-G03RevB.04|State=1-A|HF=-1936.7395955|RMSD=4.776e-006|Dipole=-1.0409532,-0.3732697,-0.2602341|PG=C01 [X(C41H31N1O4)]||@

Geometry optimization of 2

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d)|C40H31N1O4Si1|PCUSER|06-Nov-2014|0|| #OPT B3LYP/6-31G*||PMPDS_opt_631g_s||0,1|N,-2.1511840384,-0.2647326162,-2.2666127388|C,-2.4015921465,0.539997916,1.3525792|H,-1.7565359918,0.766610598,2.198498154|C,1.5418915738,-0.6688624516,-2.2894506627|H,2.4037289775,-0.4710771655,-1.6562087671|C,0.3902909278,2.4808362232,-0.4264952507|C,-2.6427005887,-0.0097686709,-0.986722912|C,-1.8071563081,0.3577803991,0.0944702312|C,0.2747881014,-0.2828468839,-1.8271692321|C,1.0887798588,-0.0715786358,1.1706075125|C,-0.8424965275,-0.5528699908,-2.6525368523|C,-0.3641956906,3.4606710183,0.2444184753|H,-1.2022471019,3.1618786914,0.8699337825|C,1.4460280956,2.9190005219,-1.2478547347|H,2.0386741082,2.193550321,-1.8005291154|C,1.744583849,4.275485857,-1.3834703054|H,2.5643243245,4.5879995926,-2.0255044716|C,-4.0308141859,-0.1327210336,-0.7812315083|H,-4.6767073162,-0.3988195374,-1.6161411263|C,1.9858583022,0.723476417,1.9057453073|H,2.0772767007,1.7823207077,1.6779462549|C,1.7554694366,-1.2672761009,-3.5392369488|C,1.0025177226,-1.4392346255,1.498792015|H,0.318449216,-2.0843198674,0.9511677824|C,-3.7795356562,0.4106242801,1.5786213727|C,2.7661739608,0.177126998,2.9276029103|H,3.4526498329,0.8115190711,3.4826764796|C,-0.6463492504,-1.1431338437,-3.9163297416|H,-1.505510523,-1.3550914463,-4.5503307133|C,-0.0706569205,4.8190320542,0.1125121714|H,-0.6704032416,5.5565745069,0.6400018163|C,0.9868989092,5.2290488785,-0.7009537813|H,1.2155760802,6.2864016483,-0.8076361134|C,-4.5830019408,0.0781362662,0.4710703332|H,-5.6595748343,-0.0021233911,0.5918157482|C,1.7791594907,-1.9892133921,2.5176906875|H,1.6949107525,-3.0469857116,2.7539127651|C,0.6242427615,-1.4837186151,-4.3494245547|H,0.739321496,-1.964423695 6,-5.316788068 2|C,2.6639568795,-1.1796934661,3.2349286875|H,3.2699148655,-1.6062819792,4.0302850833|C,-4.3669644704,0.6123954778,2.9231372538|C,-5.4664945085,-0.1522703024,3.3565007474|C,-3.8442492009,1.5726007712,3.8102359193|C,-6.0222544109,0.0320357457,4.6177120288|H,-5.8723499426,-0.9213987168,2.7056841382|C,-4.3930124163,1.7578242225,5.0727300777|H,-3.0139540

116,2.1971142326,3.4940063084|C,-5.4890129789,0.990684282,5.4904383736|H,-6.8638896386,-0.5731333825,4.9357762853|H,-3.991883354,2.5037537503,5.7511332518|C,3.1117821133,-1.6525312156,-3.992477719|C,4.0718703479,-2.1344941181,-3.0830571314|C,3.481413209,-1.5498310909,-5.3471147715|C,5.3466870826,-2.4960456015,-3.5047154079|H,3.8052034615,-2.2515366895,-2.0367751466|C,4.7519607777,-1.9146770896,-5.7739305075|H,2.7711615158,-1.1532932589,-6.0669412297|C,5.6992095704,-2.3911378464,-4.857556747|H,6.0702806916,-2.8717366606,-2.7898803495|H,5.0363803534,-1.827913219,-6.8175612948|C,-6.0366882825,1.2344053865,6.8511948375|O,-5.6048748665,2.0605414193,7.6324797962|O,-7.0859335652,0.4267612394,7.1406713658|C,7.0435653329,-2.7653630523,-5.3711249125|O,7.3834519865,-2.6918096227,-6.5367429332|O,7.8691601119,-3.2060266702,-4.3909433086|C,-7 .657086238,0.6127523611,8.4434709532|H,-8.0365091675,1.6320736506,8.5558725323|H,-8.4716150016,-0.1092981929,8.5115145326|H,-6.91147313,0.4260293883,9.2210734274|C,9.1833955904,-3.5842055017,-4.824313787|H,9.7094515545,-3.8989744684,-3.9223123963|H,9.1302146692,-4.4053240245,-5.5444680443|H,9.6935884327,-2.7375875685,-5.2916326836|H,-2.8559227061,-0.528361184,-2.9422688035|Si,0.0202682022,0.6360430073,-0.2142500012||Version=x86-Win32-G03RevB.04|State=1-A|HF=-2188.1645478|RMSD=6.290e-009|RMSF=3.932e-005|Dipole=-0.7809172,-0.623071,-0.0648634|PG=C01 [X(C40H31N1O4Si1)]||@

Energy calculation of 2

1|1|UNPC-UNK|SP|RB3LYP|6-31G(d)|C40H31N1O4Si1|PCUSER|08-Nov-2014|0||#B3LYP/6-31G* FORMCHECK=ALL POP=REG SCF=(MAXCYCLE=200)||PMPDS_eng_631g_s||0,1|N|C,1,3.71602531|H,2,1.08767186,1,139.69591669|C,1,3.71519138,2 ,95.53929504,3,9.11068386,0|H,4,1.08760264,1,139.84848115,2,-12.39963157,0|C,4,3.83632404,1,67.00256052,2,-46.27705007,0|C,1,1.39452962,4,112.07946575,6,-49.43334164,0|C,2,1.40335129,1,21.59572298,7,-173.48803518,0|C,4,1.40294802,1,21.60401509,7,-19.52324527,0|C,6,3.09086461,4,60 .33641702,1,98.47869769,0|C,1,1.39449764,7,128.50232994,8,18.14626194,0|C,6,1.40693038,4,164.65152711,1,15.31062438,0|H,12,1.08760066,6,119.74562078,4,32.68902072,0|C,6,1.40755159,4,75.3481772,1,-133.80672224,0|H,14,1.08763781,6,119.84033586,4,-7.47186054,0|C,14,1.39555648,6,121.

31530957,4,171.80200502,0|H,16,1.08712834,14,119.87591682,6,-179.90067
775,0|C,7,1.4086175,1,117.72710906,11,-161.64939046,0|H,18,1.0886044,7 ,119.6128
3131,1,-1.23774851,0|C,10,1.406161,6,86.98476428,4,125.228538
44,0|H,20,1.08692326,10,119.66252756,6,0.5257709,0|C,4,1.40202743,1,10
1.73212983,11,-3.73113429,0|C,10,1.40912386,6,155.23051434,4,-53.60630
582,0|H,23,1.08810749,10,119.7803358,6,-1.35384939,0|C,2,1.40234088,1,
101.72555601,11,-163.8650365,0|C,20,1.39699074,10,121.17352267,6,-179.
44791345,0|H,26,1.08711066,20,119.86646218,10,-179.97802104,0|C,11,1.4
0856637,1,117.74738357,7,162.16750054,0|H,28,1.0885957,11,119.61908367 ,1,0.078
56166,0|C,12,1.39596235,6,121.32232179,4,-146.51602087,0|H,30,
1.08715693,12,119.88694096,6,179.86890738,0|C,30,1.39580239,12,120.015
02994,6,0.20126707,0|H,32,1.08704662,30,120.15286177,12,179.81651929,0
|C,18,1.38478593,7,120.76937781,1,178.62218132,0|H,34,1.08629169,18,11
8.97681271,7,178.6162896,0|C,23,1.39420337,10,121.26324205,6,178.68249
806,0|H,36,1.08709817,23,119.96463091,10,179.93725296,0|C,28,1.3849092
5,11,120.75689715,1,-178.49895133,0|H,38,1.08632988,28,118.97901932,11 ,178.1990
8392,0|C,26,1.39494032,20,120.04143875,10,0.,0|H,40,1.0870853
5,26,120.13490253,20,-179.95518111,0|C,25,1.48104978,2,121.56668523,1,
178.59628886,0|C,42,1.40765265,25,121.01664306,2,-144.91269202,0|C,42,
1.40789462,25,121.17534206,2,34.99882144,0|C,43,1.39050018,42,121.2941
2581,25,179.97840591,0|H,43,1.08620402,42,119.47509708,25,1.7555112,0|
C,44,1.38900672,42,121.12886114,25,-179.77488727,0|H,44,1.0860058,42,1
19.51015127,25,1.79315648,0|C,47,1.40149968,44,120.45509108,42,-0.2351
0931,0|H,45,1.08431752,43,120.15301636,42,-179.48181134,0|H,47,1.08514
832,44,120.92084944,42,-179.56359694,0|C,22,1.48102422,4,121.55632063,
1,-178.68911854,0|C,52,1.40751698,22,121.06545003,4,35.26785472,0|C,52 ,1.407911
77,22,121.05819234,4,-144.8079314,0|C,53,1.3905656,52,121.228
10408,22,-179.94171546,0|H,53,1.08605574,52,119.46374035,22,1.6980288,
0|C,54,1.38909179,52,121.10516389,22,-179.80501847,0|H,54,1.08620925,5
2,119.51034482,22,1.88804921,0|C,57,1.40144011,54,120.43840867,52,-0.2
2534951,0|H,55,1.08430652,53,120.13019116,52,-179.57634515,0|H,57,1.08
516657,54,120.94609052,52,-179.56763181,0|C,49,1.48694557,47,118.10366
41,44,-179.86769125,0|O,62,1.21629315,49,124.63889604,47,0.35574014,0|
O,62,1.35535999,49,112.51456582,47,-179.58723683,0|C,59,1.4869731,57,1
18.08683817,54,-179.93651138,0|O,65,1.21638711,59,124.63653112,57,-0.2
2734796,0|O,65,1.35519288,59,112.50775917,57,179.79391771,0|C,64,1.434

60646,62,115.14485032,49,179.87303472,0|H,68,1.0934403,64,110.63165889 ,62,60.6
9688946,0|H,68,1.09061622,64,105.55514826,62,-179.64690565,0|H ,68,1.0933753,64,
110.62286998,62,-59.97631739,0|C,67,1.43458822,65,115 .17128271,59,179.9521266,
0|H,72,1.09060586,67,105.55269624,65,179.43857904,0|H,72,1.09347487,67,110.63132153,65,-60.92026449,0|H,72,1.09336426,67,110.63862651,65,59.75851995,0|H,1,1.01127074,11,114.53408244,28,1.01804986,0|Si,9,1.8736717,4,122.77052082,1,-179.5554402,0||Version=x86-Win32-G03RevB.04|State=1-A|HF=-2188.1644241|RMSD=6.467e-006|Dipole=-0.8248433,-0.5498417,-0.1467015|PG=C01 [X(C40H31N1O4Si1)]||@

Geometry optimization of 3

1|1|UNPC-UNK|FOpt|RB3LYP|6-31G(d)|C37H27N1|PCUSER|21-Aug-2015|0||# OPT B3LYP/6-31G*||3_opt_631g_s||0,1|N,-1.9368904571,0.2577109985,-2.1580581234|C,-1.939950314,0.2553701958,1.5214570348|H,-1.2239068815,0.2529448253,2.3360320734|C,0.0306305049,0.5215825008,-0.1332098922|C,1.5648571929,-0.7919406068,-1.7473767351|H,2.3395186337,-0.7659747078,-0.9887483193|C,0.2809611679,2.0481877784,-0.3590401157|C,-2.3944988733,0.2661721001,-0.8408032201|C,-1.4594480957,0.3093993732,0.2112903739|C,0.3231543483,-0.2265569901,-1.4514445367|C,0.9252571884,-0.0295688593,1.0015921461|C,-0.6698501902,-0.2456351962,-2.4498140643|C,-0.4621257395,3.0170748357,0.330845093|H,-1.2563978166,2.7110835478,1.0024817521|C,1.2914256565,2.4941528382,-1.2241467178|H,1.8834121223,1.7748146023,-1.7790044214|C,1.5497576902,3.8552520353,-1.3930597843|H,2.3378889715,4.1685590263,-2.0731146341|C,-3.7666797683,0.2103664221,-0.5612405289|H,-4.4800464974,0.1867050818,-1.38262781|C,1.8221763883,0.765436326,1.7220002982|H,1.9131675795,1.8208870189,1.4925636161|C,1.8656433696,-1.3507883756,-3.0006739649|C,0.8393712241,-1.3939912957,1.3323013724|H,0.1472582366,-2.0298438011,0.7876712274|C,-3.3100429715,0.1894410147,1.8252849953|C,2.6111277831,0.2176157694,2.7401209456|H,3.3005375614,0.8589291061,3.2832088704|C,-0.3887949834,-0.7874542809,-3.7114018501|H,-1.1679281141,-0.8086293208,-4.4707422926|C,-0.2064737097,4.3792718484,0.1631445376|H,-0.8034617803,5.1055817611,0.7089769993|C,0.8006352466,4.8070139293,-0.7013204326|H,0.9973024262,5.8673530402,-0.8363441815|C,-4.2161563676,0.1801820926,0.7518302311|H,-5.2843903151,0.1596854375,0.9471507583|C,1.6227190044,-1.9414131896,2.3446687399|H,1.5339322184,-2.9987997867,2.5806176784|C,0.8619825297,-1.3253037962,-3.9832707355|H,1

.0475884132,-1.7698014324,-4.9568000714|C,2.5164187804,-1.1349804878,3.0560569068|H,3.1287699629,-1.5600143208,3.8469028007|C,-3.7816621237,0.1371412606,3.231724332|C,-4.8979184514,-0.6389253742,3.5906074076|C,-3.1283100699,0.8583068097,4.2464889931|C,-5.3444343463,-0.6904911069,4.9100991743|H,-5.4036039267,-1.2285975035,2.8307825934|C,-3.5712067848,0.803579079,5.5670762266|H,-2.2784647918,1.4860372114,3.9932377361|C,-4.6827157173,0.0299280797,5.9061478967|H,-6.20560608,-1.3041884713,5.1621035834|H,-3.0514057726,1.3754136788,6.3315717927|C,3.1993187808,-1.9422604779,-3.2715976881|C,3.8962610216,-2.6420467561,-2.2706267089|C,3.8038697182,-1.8234769288,-4.5352958407|C,5.148982071,-3.1986679591,-2.5230694282|H,3.4399531587,-2.7693424916,-1.2928359858|C,5.0544002169,-2.3845927037,-4.7898239993|H,3.2990383992,-1.263065374,-5.3175141219|C,5.7343061612,-3.0745703586,-3.7845266766|H,5.6647707937,-3.7397040605,-1.7338350449|H,5.5032394327,-2.2728418445,-5.7735982417|H,-2.6418365112,0.123710813,-2.8711597631|H,6.7101012335,-3.5102235551,-3.9818242447|H,-5.029122685,-0.0115127428,6.9352918058||Version=x86-Win32-G03RevB.04|State=1-A|HF=-1480.9781614|RMSD=6.948e-009|RMSF=2.135e-006|Dipole=-0.3221695,-0.0752995,-0.3085221|PG=C01 [X(C37H27N1)]||@

Energy calculation of 3

1|1|UNPC-UNK|SP|RB3LYP|6-31G(d)|C37H27N1|PCUSER|21-Aug-2015|0||# B3LYP/6-31G* FORMCHECK=ALL POP=REG SCF=(MAXCYCLE=200)||3_eng_631g_s||0,1|N|C,1,3.67945965|H,2,1.0845251,1,138.6388452|C,2,2.58679957,1,50.18337912,3,7.81504673,0|C,4,2.5855196,2,143.04529499,1,-75.8631056,0|H,5,1.0844566,4,88.5661365,2,-101.43262763,0|C,4,1.56343577,2,108.35243758,1,94.43796391,0|C,1,1.39444656,4,63.42457134,2,3.22271387,0|C,2,1.39654246,1,20.20689894,8,-172.50821265,0|C,5,1.39609842,4,30.02034049,2,74.67271613,0|C,4,1.5465661,2,86.25586743,1,-154.47546165,0|C,1,1.39426149,8,119.87438339,9,26.2075358,0|C,7,1.40248283,4,121.24333073,2,2.82325247,0|H,13,1.08421939,7,119.86300715,4,-2.72731051,0|C,7,1.40299738,4,120.98497762,2,-179.50781448,0|H,15,1.08432872,7,119.85744798,4,2.59221995,0|C,15,1.39567331,7,121.1952072,4,-177.71809371,0|H,17,1.08703154,15,119.40509087,7,-179.82193348,0|C,8,1.40145254,1,120.63170044,12,-152.75687559,0|H,19,1.08817201,8,119.4797718,1,-1.60979447,0|C,11,1.39836974,4,123.12072061,2,-107.63508422,0|H,21,1.08388041,11,119.89602635,

4,-0.04085141,0|C,5,1.40485371,4,152.38667739,2,86.85076905,0|C,11,1.40657295,4,118.87194578,2,72.33139028,0|H,24,1.08623072,11,119.26601721,4,-0.14540261,0|C,2,1.40496818,1,102.53806631,12,-155.57297307,0|C,21,1.39970971,11,120.91163479,4,-179.94457146,0|H,27,1.08696026,21,119.34489461,11,179.94221856,0|C,12,1.40148888,1,120.67733345,8,152.97544816,0|H,29,1.08819036,12,119.4760085,1,0.35681084,0|C,13,1.39610227,7,121.19279227,4,177.75965051,0|H,31,1.08714307,13,119.40220647,7,179.71599978,0|C,31,1.39446545,13,120.40163612,7,0.03472258,0|H,33,1.08682419,31,120.46187654,13,179.70494975,0|C,19,1.38818694,8,120.43711442,1,178.14260529,0|H,35,1.08615151,19,119.27274353,8,178.63411674,0|C,24,1.3922294,11,121.19701912,4,179.95900085,0|H,37,1.08702361,24,119.62496782,11,179.85757178,0|C,29,1.38832958,12,120.44638695,1,-177.97941661,0|H,39,1.08619771,29,119.21063509,12,177.97092795,0|C,27,1.39229166,21,120.46360801,11,-0.03806813,0|H,41,1.08668272,27,120.44883765,21,-179.96825603,0|C,26,1.48434127,2,121.09348003,1,178.70487962,0|C,43,1.40609121,26,120.90077249,2,-143.42393317,0|C,43,1.40594405,26,121.2071764,2,36.49292769,0|C,44,1.39388898,43,121.08489304,26,-179.98150358,0|H,44,1.08661141,43,119.36720721,26,1.67950945,0|C,45,1.39395826,43,121.06144155,26,-179.78969115,0|H,45,1.08650748,43,119.44975604,26,1.62302831,0|C,46,1.39601108,44,120.29738885,43,-0.21431388,0|H,46,1.08714884,44,119.60752096,43,-179.5521797,0|H,48,1.08701322,45,119.58311583,43,-179.65189233,0|C,23,1.483921,5,120.91849904,4,172.83238116,0|C,53,1.40614832,23,120.92251222,5,36.04797425,0|C,53,1.40589521,23,121.12420086,5,-144.08021515,0|C,54,1.39382728,53,121.01765364,23,179.98461688,0|H,54,1.08650131,53,119.39054088,23,1.39069002,0|C,55,1.39405063,53,121.05293256,23,-179.72449611,0|H,55,1.0866238,53,119.3953193,23,1.87852256,0|C,58,1.39607066,55,120.28676188,53,-0.25623831,0|H,56,1.08696672,54,119.59175786,53,-179.66387618,0|H,58,1.08710313,55,119.61820766,53,-179.59155978,0|H,1,1.01170275,12,115.96868288,29,5.6642064,0|H,60,1.08665997,58,120.31274932,55,-179.86287722,0|H,50,1.0866515,46,120.32786006,44,-179.87759434,0||Version=x86-Win32-G03RevB.04|State=1-A|HF=-1480.977996|RMSD=3.385e-006|Dipole=-0.3224312,-0.076857,-0.3086617|PG=C01 [X(C37H27N1)]||@

8. Gaussian 09 archive files[2]

Geometry optimization of 1 in toluene at excited state

1¥1¥GINC-YAMATO¥FOpt¥RTD-FC¥6-31G(d)¥C41H31N1O4¥GUSER01¥16-Dec-2
015¥0¥ ¥#optTD=(root=1)/6-31g*scrf=(solvent=toluene)¥¥PMPDA_opt_ex_TD_Toluene_6-31Gd_s_mem32¥¥0,1¥N,0.0492787923,-0.1398726851,0.0187426685¥C,0.09587
82773,-0.1446196205,3.6407796532¥H,0.8056703969,-0.0844341873,4.4372508679¥
C,2.0175492226,0.3017035162,2.0112265949¥C,3.6195308984,-0.7939144304,0.3231
680023¥H,4.3980072096,-0.7197065609,1.0568277473¥C,2.1361870817,1.850945877
3,1.8372349965¥C,-0.3892995419,-0.0716747669,1.2993822695¥C,0.5521827515,-0.0
210154553,2.366089904¥C,2.3460298122,-0.3734177373,0.6650113572¥C,2.9687062
95,-0.2223978746,3.1092117051¥C,1.3464595892,-0.4581818884,-0.3123413406¥C,1.
4330292187,2.7218532846,2.6691656266¥H,0.7727253914,2.3357799062,3.41980631
9¥C,2.9782531383,2.4162159836,0.883463516¥H,3.5416467685,1.7929079048,0.2187
975624¥C,3.1127406174,3.7919564125,0.7643964621¥H,3.771595064,4.1933858844,
0.0150477389¥C ,-1.7777111499,-0.1091226016,1.5860278937¥H,-2.4776261735,-0.0
911334704,0.768742966¥C,3.8481184165,0.5914559776,3.8049557268¥H,3.89002096
08,1.643215606,3.6027309651¥C,3.9432640633,-1.2617506388,-0.9505158974¥C,2.9
602840131,-1.5883207237,3.4110975729¥H,2.2899695287,-2.2431074666,2 .8849122
128¥C,-1.3055136817,-0.286938511,3.9741465091¥C,4.6940606704,0 .0637681152,4.
7778216026¥H,5.3657216387,0.7193675091,5.3026521234¥C,1.6505086631,-0.90121
75422,-1.6014948105¥H,0.8709773213,-0.9623831186,-2 .3404313699¥C,1.56588164
29,4.0953407283,2.5531803232¥H,1.0073943357,4.7364950911,3.2117173652¥C,2.40
66696052,4.6405424986,1.5970470725¥H,2.5077368454,5.7069746483,1.5033123294
¥C,-2.2237186816,-0.2032622984,2.8598009807¥H,-3.2800671312,-0.2538672806,3.0
25955704¥C,3.796344715,-2.1135189329,4.3747724147¥H,3.7665272108,-3.1669478
113,4.5891113478¥C,2.9298007383,-1.2914362855,-1.9136881861¥H,3.1359485808,-
1.6594791409,-2.9016615695¥C,4.6721311067,-1.2842717924,5.0673687253¥H,5.323
7322912,-1.6911433456,5.8197225259¥C,-1.7393406734,-0.4766513396,5.302586193
1¥C,-3.1342903963,-0.4621153103,5.6658253431¥C,-0.8167817977,-0.6988770228,6.
3883300263¥C,-3.5461689437,-0.6267511655,6.9534411825¥H,-3.8816182133,-0.296
3442397,4.9158847628¥C,-1.2452555766,-0.870355041,7.6689251136¥H,0.23511555
82,-0.7629660206,6.1940223708¥C,-2.6169265554,-0.8342673333,7.9948929897¥H,-
4.5940985869,-0.5967258834,7.1810531565¥H,-0.5347588312,-1.0430945825,8.4544
821483¥C,5.3217514026,-1.7078356566,-1.2694316419¥C,6.0866716306,-2.40012389
11,-0.3283619116¥C,5.8896838865,-1.4510642612,-2.5198714243¥C,7.3693327521,-2
.8198300995,-0.6233046605¥H,5.6683375292,-2.6324003948,0.6334573273¥C,7.1698

283199,-1.8722211116,-2.8170030194¥H,5.3358814335,-0.8978119645,-3.2556580783¥C,7.922501905,-2.5609691206,-1.8722964108¥H,7.9357321789,-3.3563358103,0.1127488722¥H,7.5989977347,-1.6632806435,-3.7782645152¥C,-3.0159212745,-1.0183366157,9 .3923174648¥O,-2.2504458363,-1.1964587087,10.300478727¥O,-4.3332300644 ,-0.9701999613,9.5748831447¥C,9.2964963123,-2.9952985289,-2.2397033387¥O,9.7985199807,-2.7893893223,-3.3035400359¥O,9.9151496288,-3.6389881451,-1.2649980548¥C,-4.8059678175,-1.1381008072,10.8979705663¥H,-4.4159129701,-0.3643591787,11.5434160922¥H,-5.880949231,-1.0657691554,10.8382862612¥H,-4.5188820665,-2.1048536141,11.2858191063¥C,11.233499739,-4.095192542,-1.5229470861¥H,11.5552749796,-4.5870787616,-0.6189471482¥H,11.2371825734,-4.790024626,-2.3496945599¥H,11.8834114297,-3.2627602809 ,-1.7486595297¥H,-0.6360134887,-0.2003631922,-0.7027798818¥¥Version=ES64L-G09RevD.01¥State=1-A¥HF=-1924.6210309¥RMSD=4.477e-09¥RMSF=1.400e-06¥Dipole=-0.5624894,0.2474498,-2.1679879¥PG=C01 [X(C41H31N1O4)]¥¥@

Geometry optimization of 1 in MeOH at excited state

1¥1¥GINC-YAMATO¥FOpt¥RTD-FC¥6-31G(d)¥C41H31N1O4¥GUSER01¥15-Dec-2015¥0¥ ¥#optTD=(root=1)/6-31g*scrf=(solvent=methanol)¥¥PMPDA_opt_ex_TD_MeOH_6-31Gd_s_mem32¥¥0,1¥N,0.0215948235,0.0473212495,0.002158779¥C,-0.0094528278,0.0378663418,3.6211280263¥H,0.6849526189,0.0565781242,4.432825063¥C,1.9678222988,0.4034499444,2.0398062113¥C,3.5662622774,-0.7184804195,0.369320812¥H,4.3338477942,-0.6690599985,1.1162805917¥C,2.1492186388,1.9498284611,1.8972652696¥C,-0.4381184719,0.1352560737,1.2688351117¥C,0.480768598,0.144330474,2.3594532802¥C,2.2971532743,-0.267258632,0.69191841¥C,2.8760035026,-0.1805930313,3.1447101409¥C,1.3152881281,-0.3158463971,-0.3031665631¥C,1.5615503016,2.8204340973,2.8173195941¥H,0.9607232527,2.4342408976,3.6167334437¥C,2.9193362561,2.5132367954,0.8849992446¥H,3.3950587468,1.8925402099,0.1530338702¥C,3.0940507597,3.8884740511,0.7910436711¥H,3.693690932,4.2888522314,-0.0068701839¥C,-1.8357510918,0.1624453398,1.524341767¥H,-2.5133637956,0.216378308,0.6908884506¥C,3.8153781304,0.570716409,3.8331604536¥H,3.9311939134,1.6163863216,3.6283325237¥C,3.897678951,-1.1864644718,-0.9012654441¥C,2.7780245329,-1.5432245823,3.4458430488¥H,2.0644276162,-2.1526047428,2.9220827976¥C ,-1.4263246912,-0.0419249398,3.9244282991¥C,4.6299931493,-0.0131708098 ,4.8009323379¥H,5.3496563957,0.5947490325,5.3194462834¥C,1.6266693834,-0.7622797734,-1.5888699035¥H,0.8587033435,-0.7957261943,-2.3408658316¥C,1.7359848012,4.1901511484,2.728531137¥H,1.2685755521,4.8303519162,3 .4552697619¥C,2.503457200

9,4.7350843827,1.7097901453¥H,2.6357290219,5.7995745233,1.6362994212¥C,-2.31
40983863,0.0866389135,2.7849603868¥H,-3 .3752423876,0.0906819357,2.924688489
1¥C,3.5825707115,-2.1244854026,4.4047765356¥H,3.4840630755,-3.1739220913,4.6
176406338¥C,2.9009417224,-1.1858993305,-1.8813933883¥H,3.113550303,-1.551565
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