

Supporting Information

Some Cyclization Reactions of 1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one: Preparation and Computational Analysis of Non Symmetrical Zwitterionic Biscyanines

**Theodosia A. Ioannou, Panayiotis A. Koutentis*, Harry Krassos, Georgia Loizou and
Daniele Lo Re**

Department of Chemistry, University of Cyprus, P.O. Box 20537, 1678 Nicosia, Cyprus,
koutenti@ucy.ac.cy

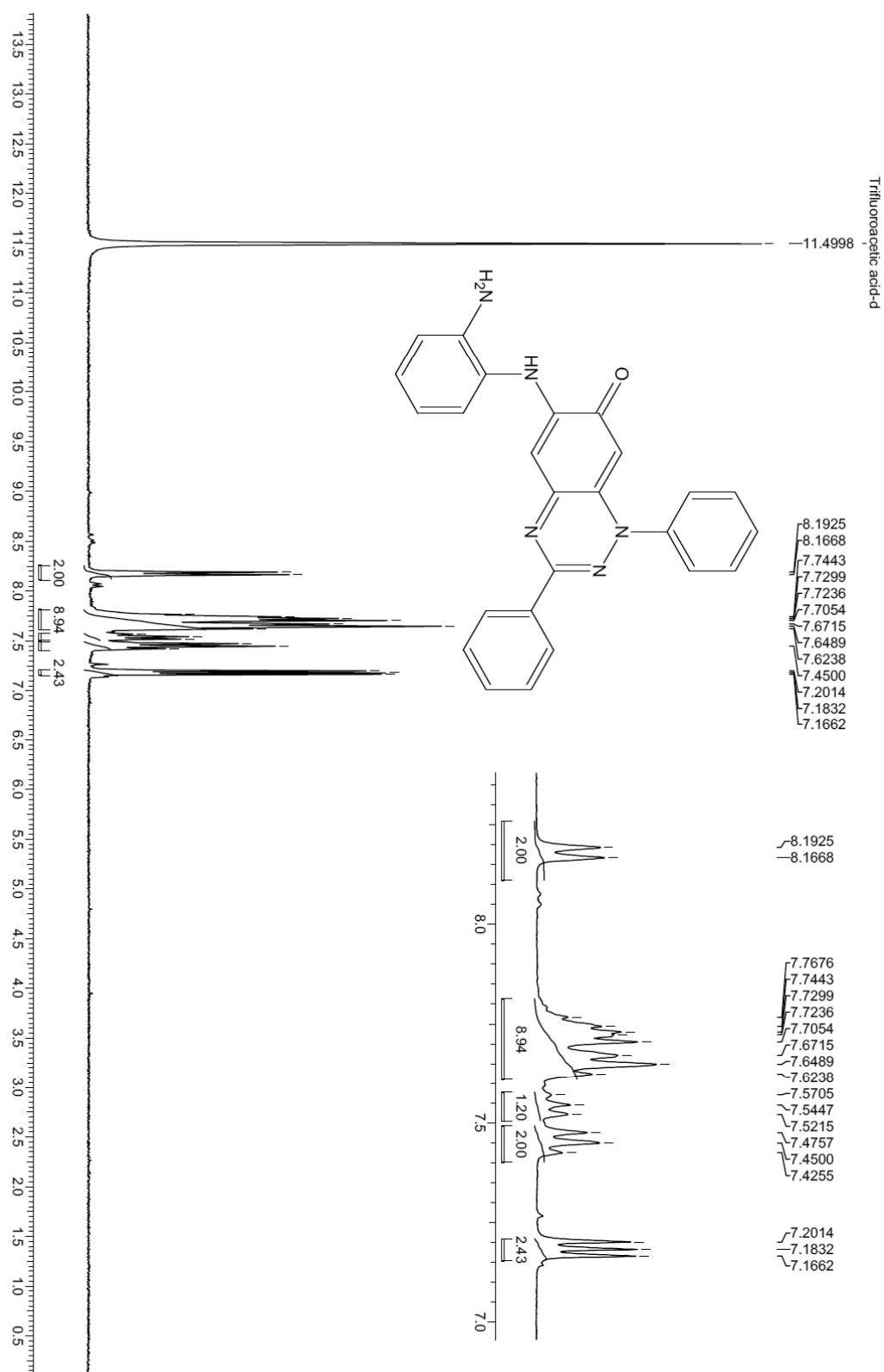
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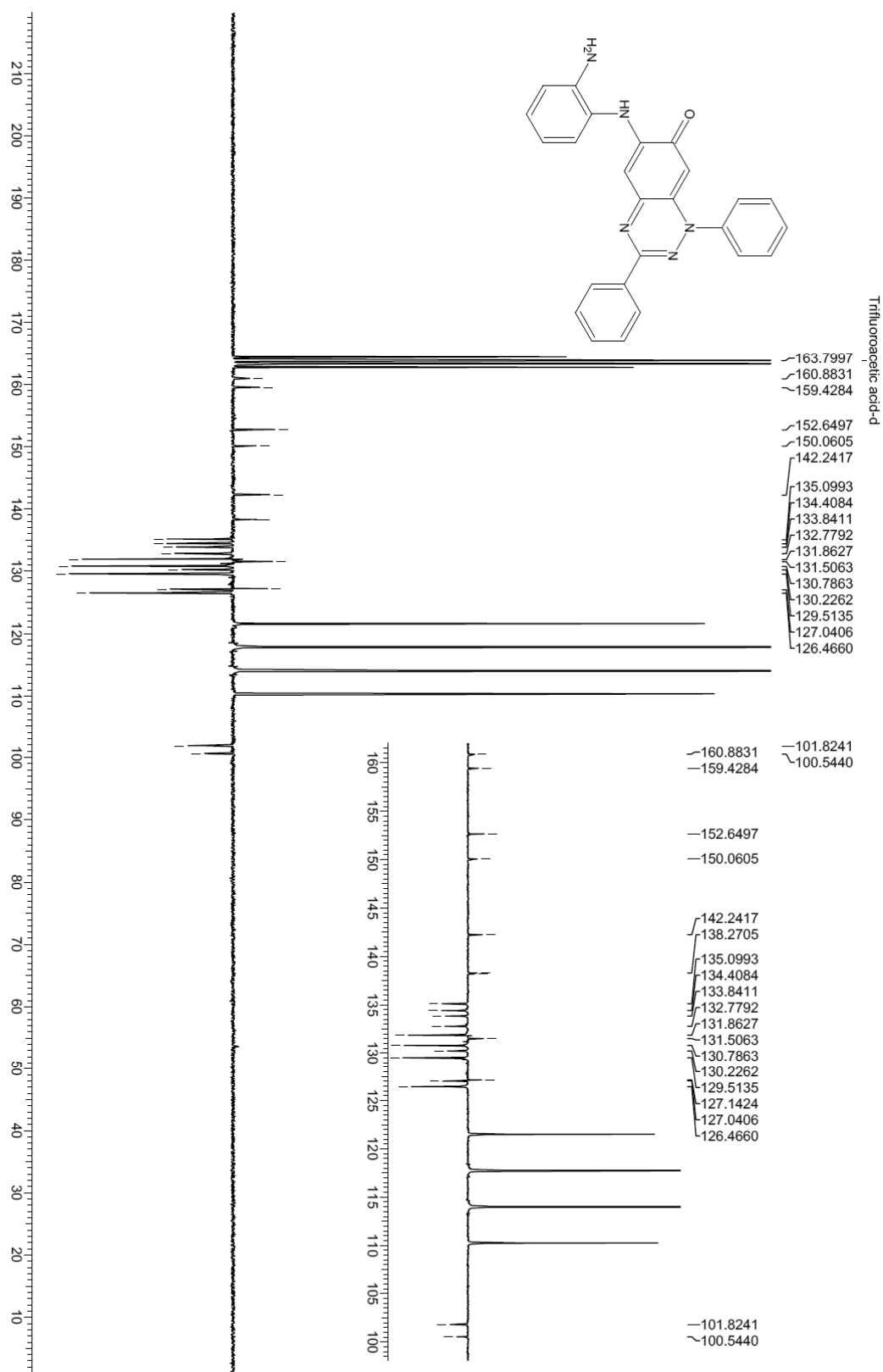
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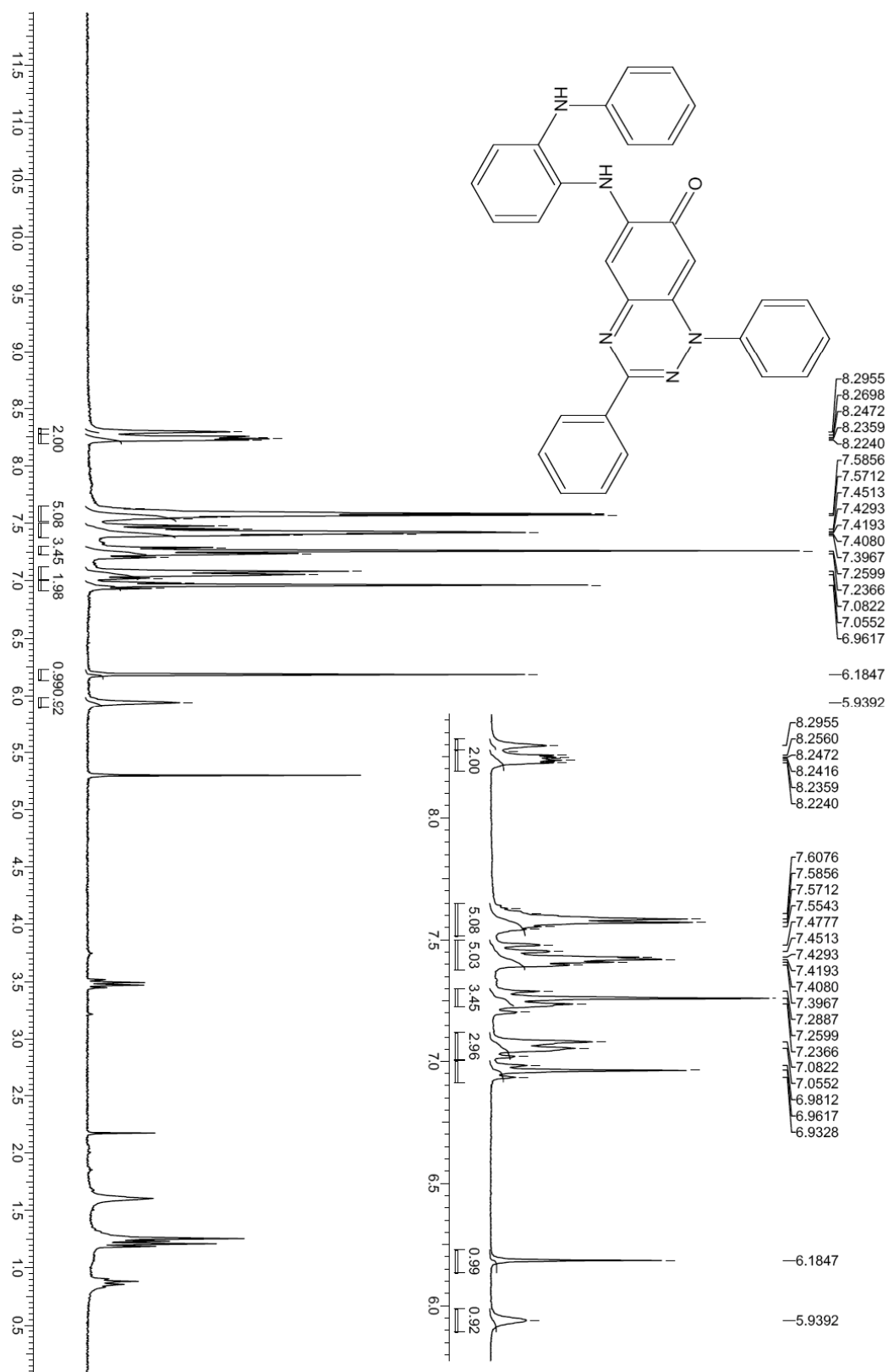
¹H-NMR of 6-(2-Aminophenylamino)-1,3-diphenylbenzo[e][1,2,4]triazin-7(1*H*)-one (9).



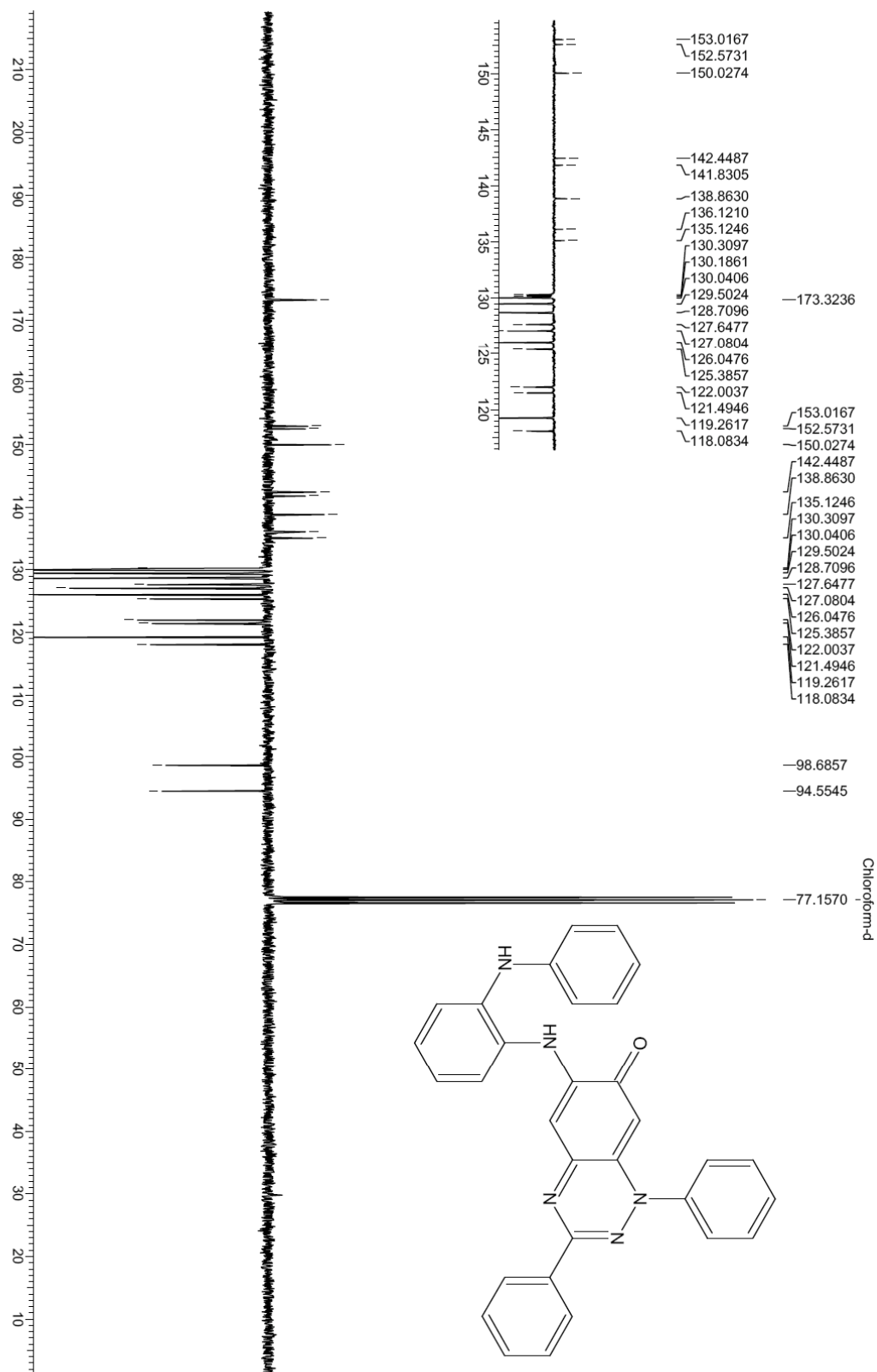
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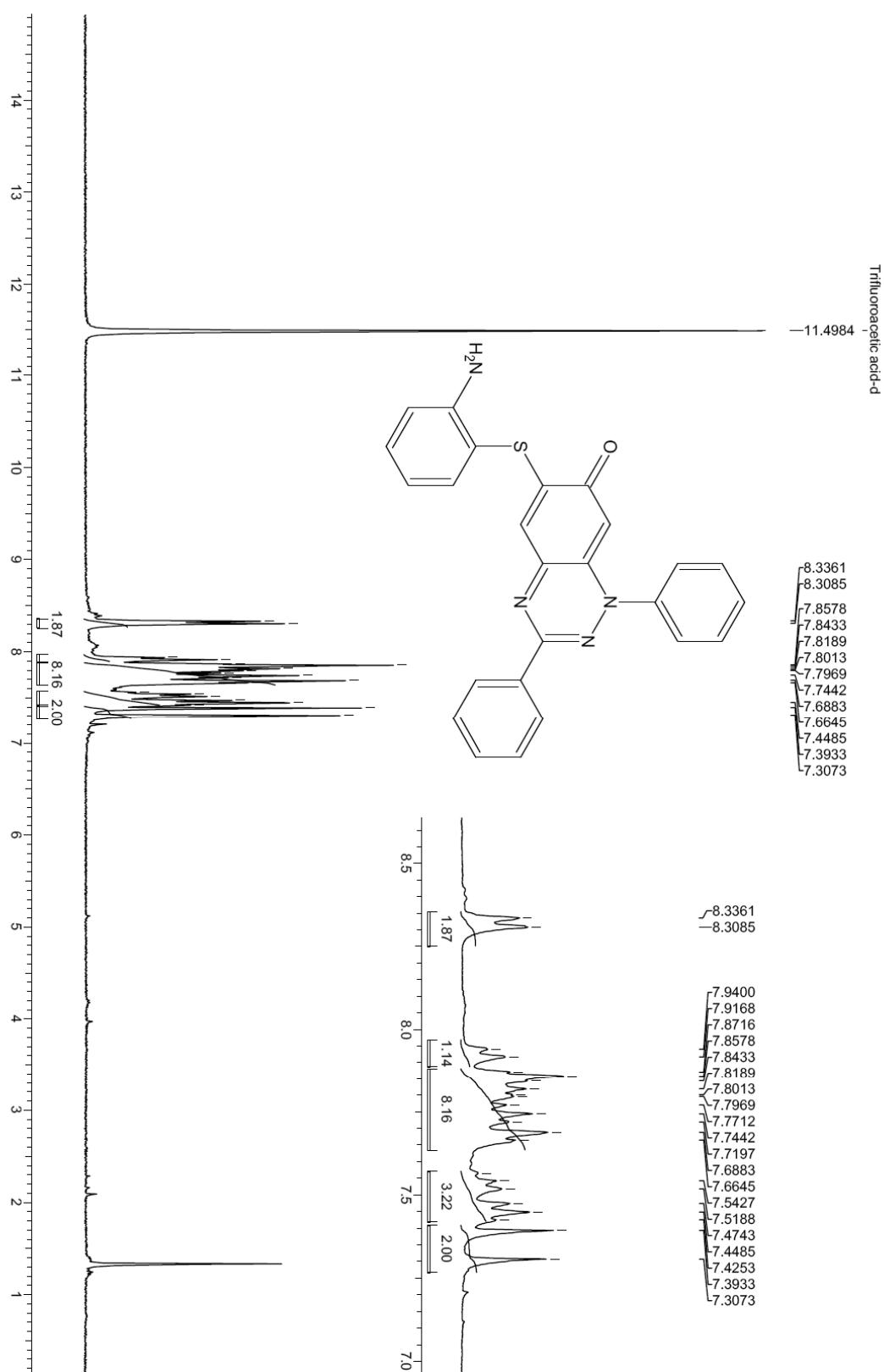
¹H-NMR of 1,3-Diphenyl-6-[2-(phenylamino)phenylamino]benzo[*e*][1,2,4]triazin-7(1*H*)-one (10)



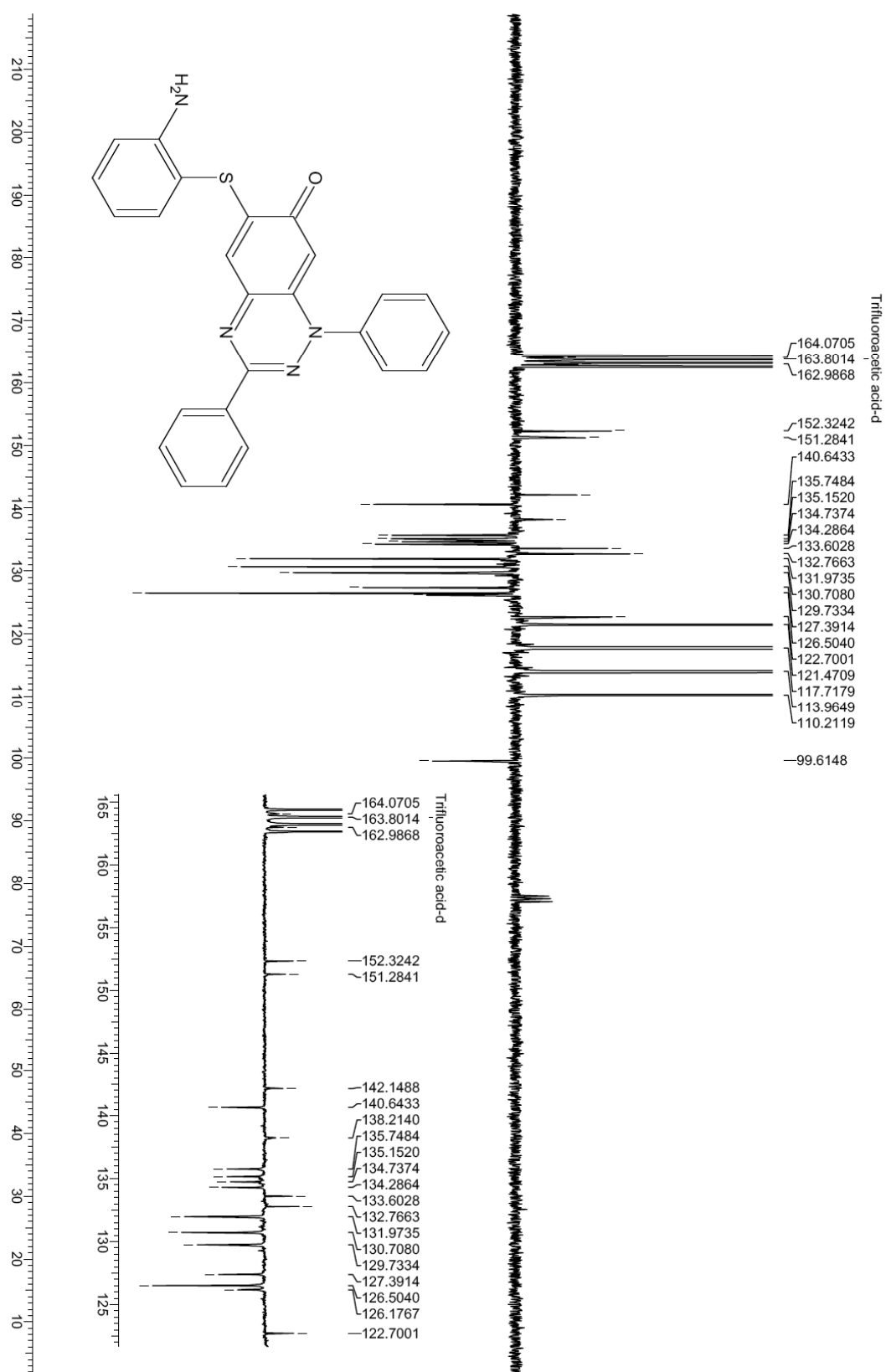
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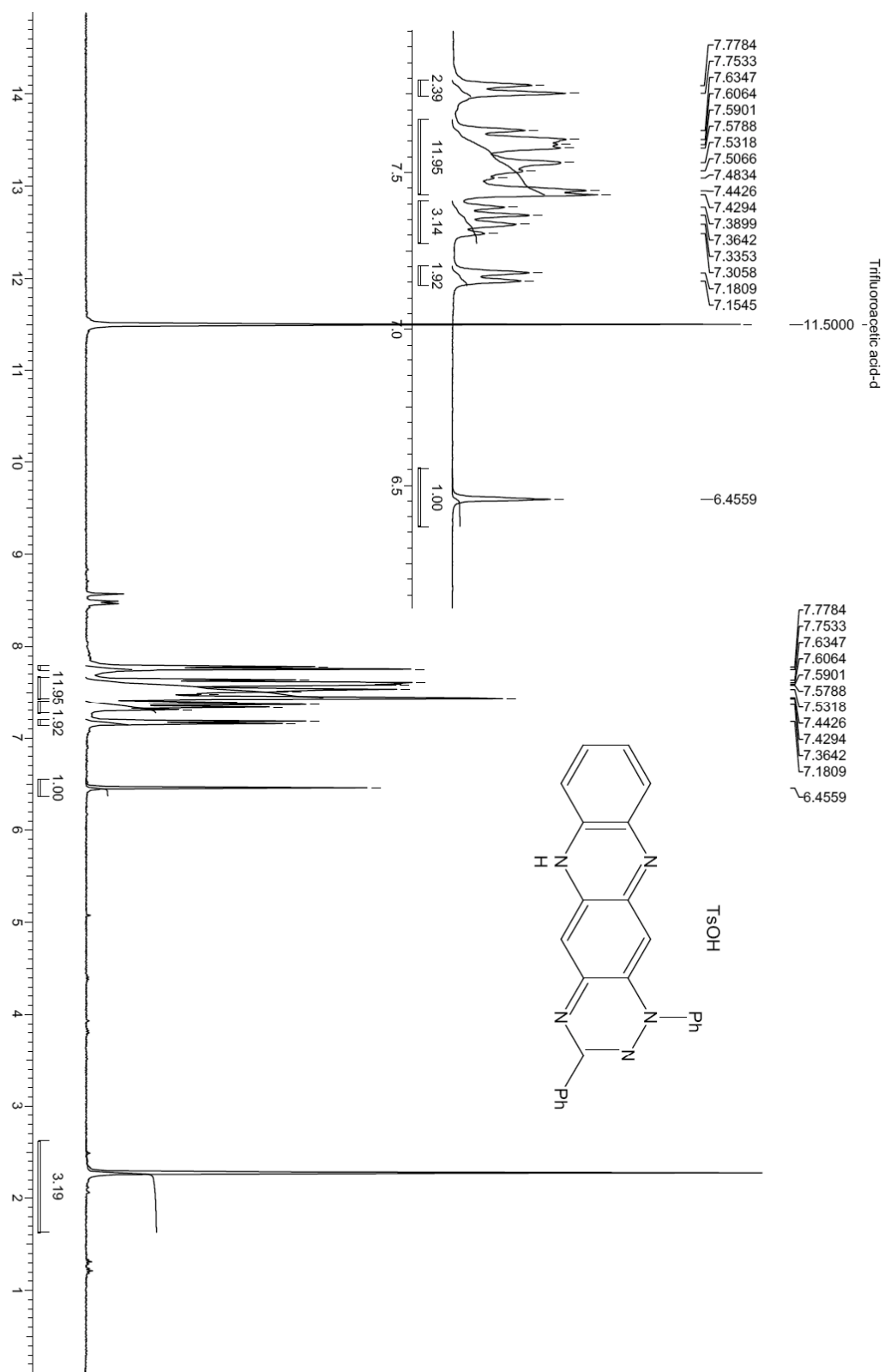
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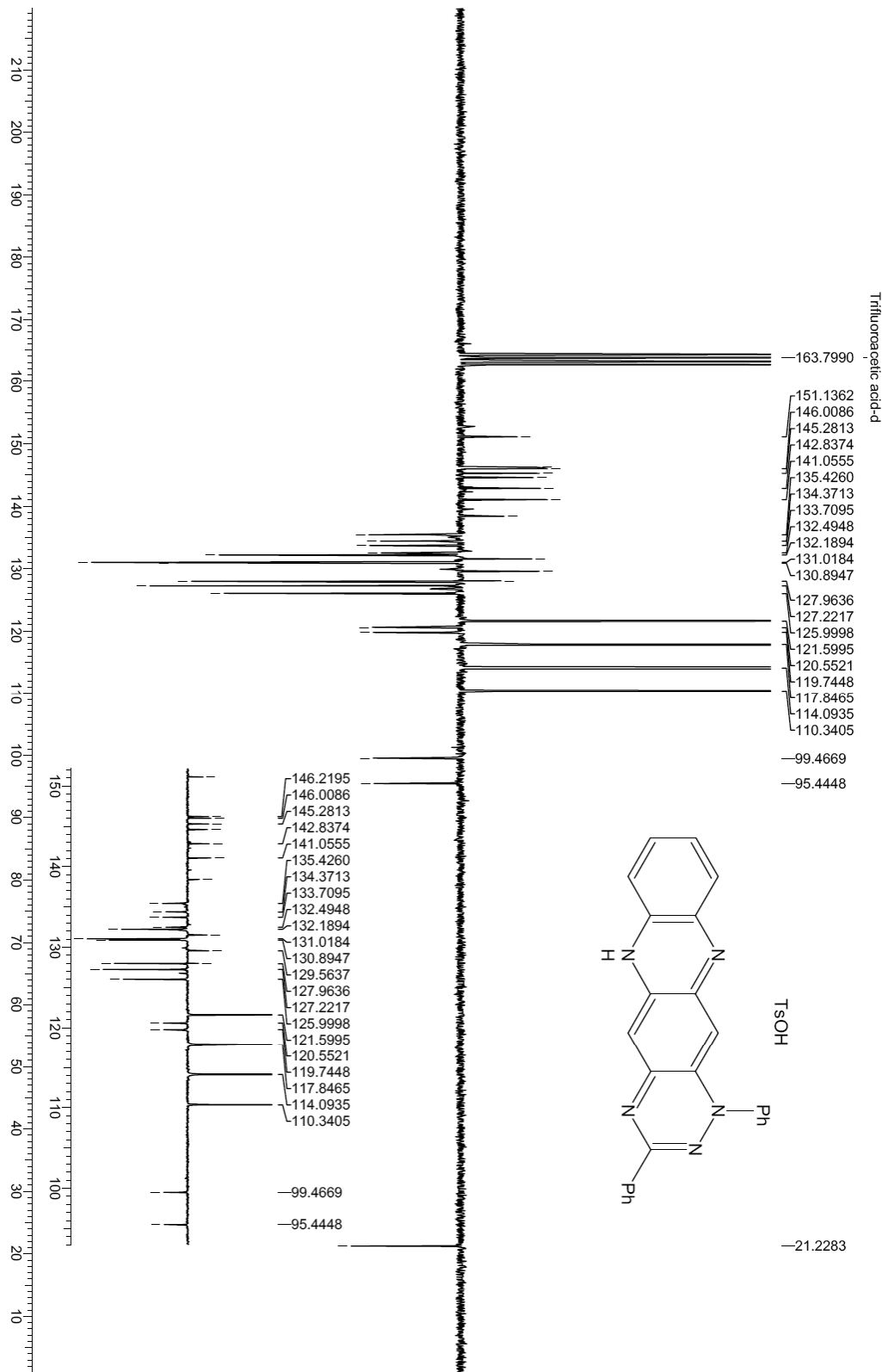
^{13}C -NMR of 6-(2-Aminothiophenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (11)



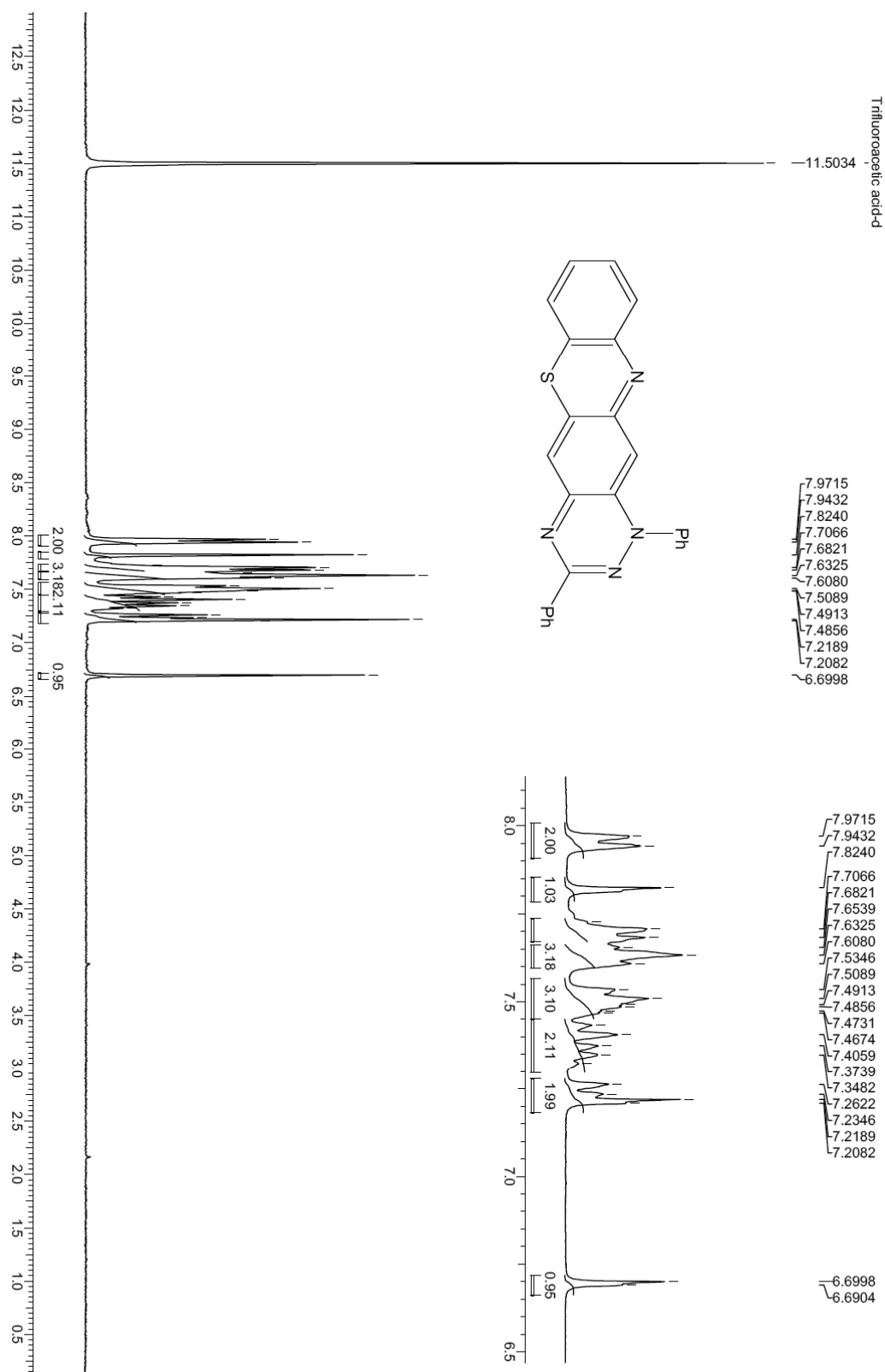
¹H-NMR of 1,3-Diphenyl-1,6-dihydro-[1,2,4]triazino[5,6-*b*]phenazin-4-ium 4-methylbenzene-sulfonate (12)



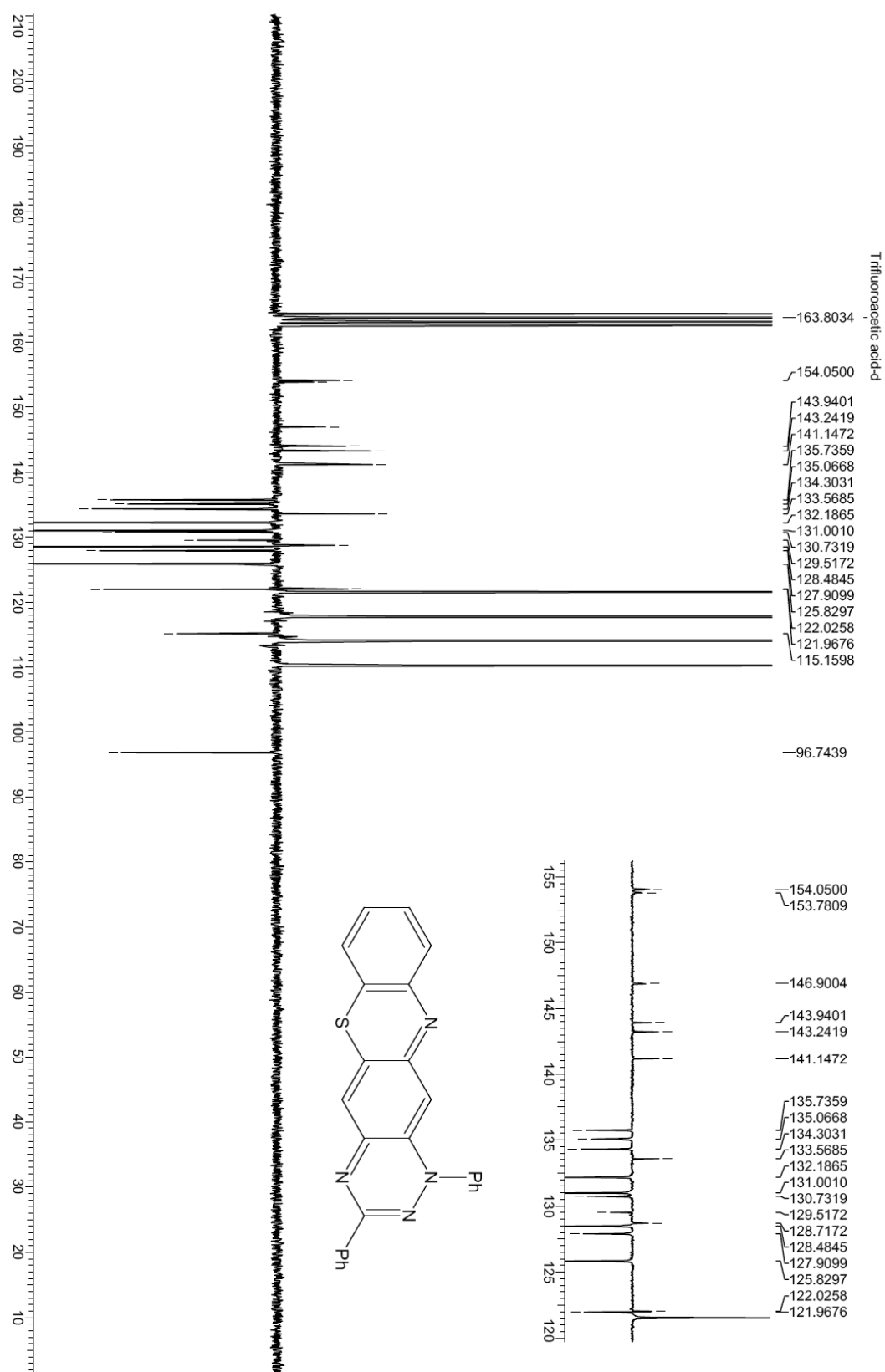
¹³C-NMR of 1,3-Diphenyl-1,6-dihydro-[1,2,4]triazino[5,6-*b*]phenazin-4-ium 4-methylbenzene-sulfonate (12)



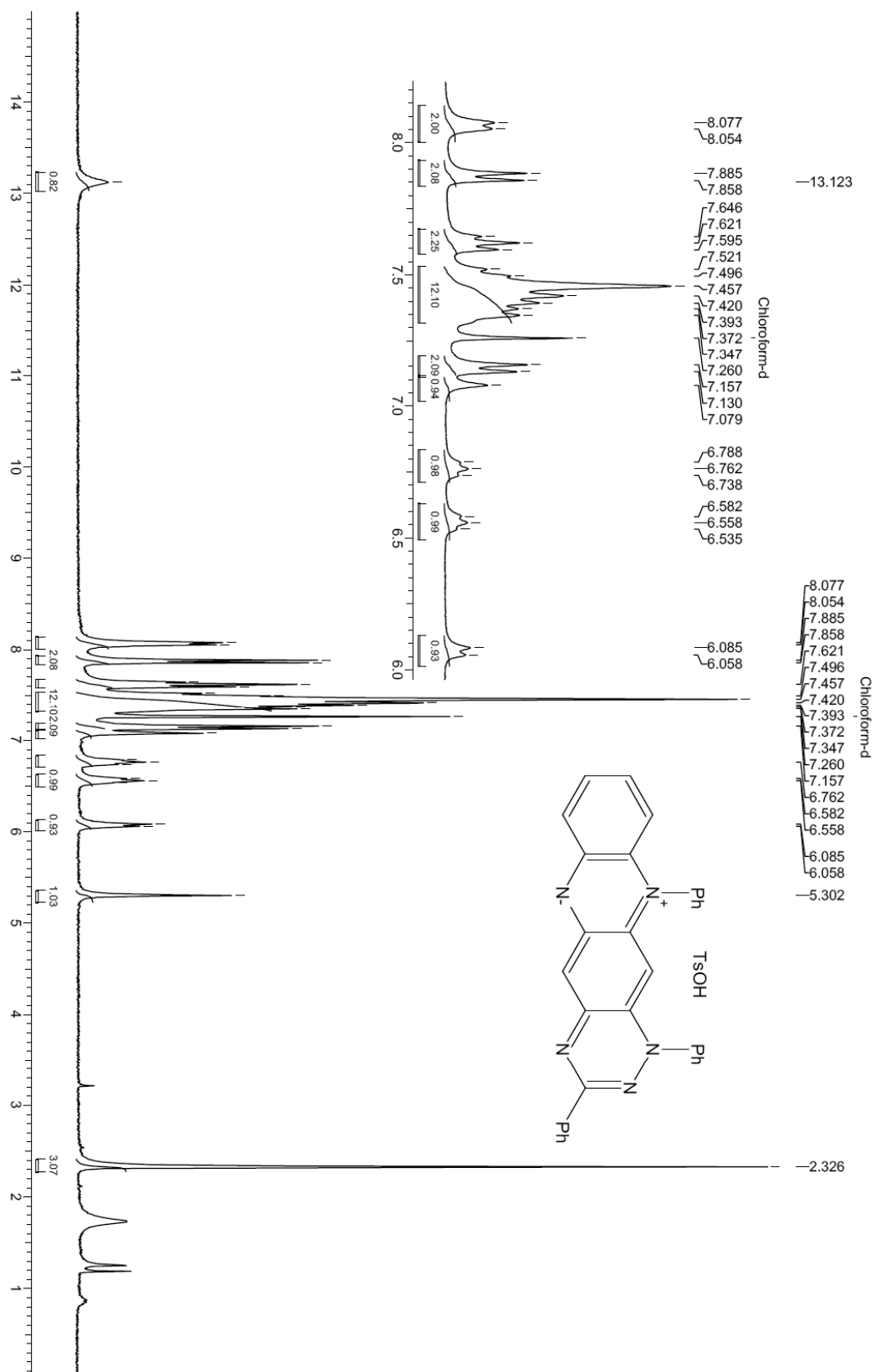
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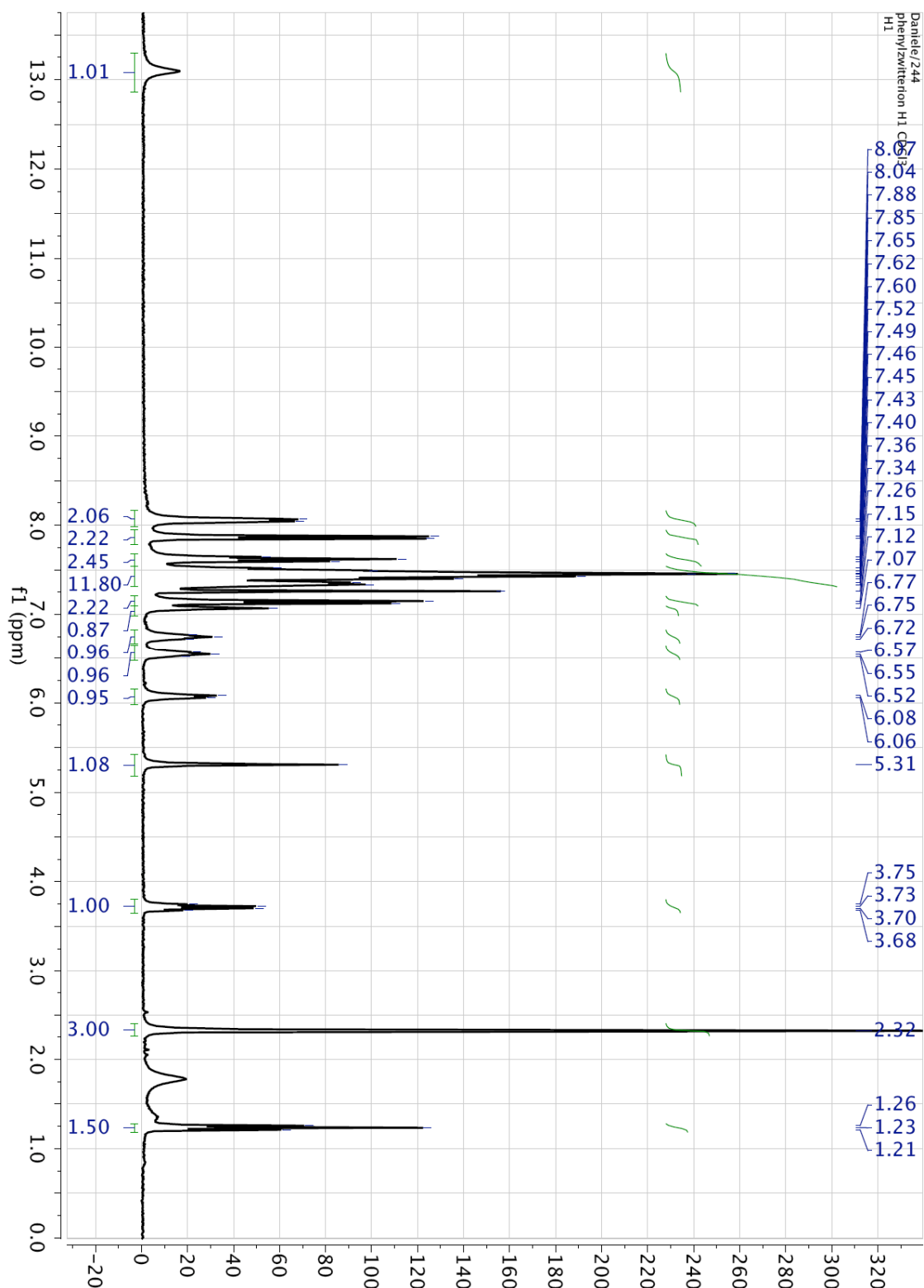
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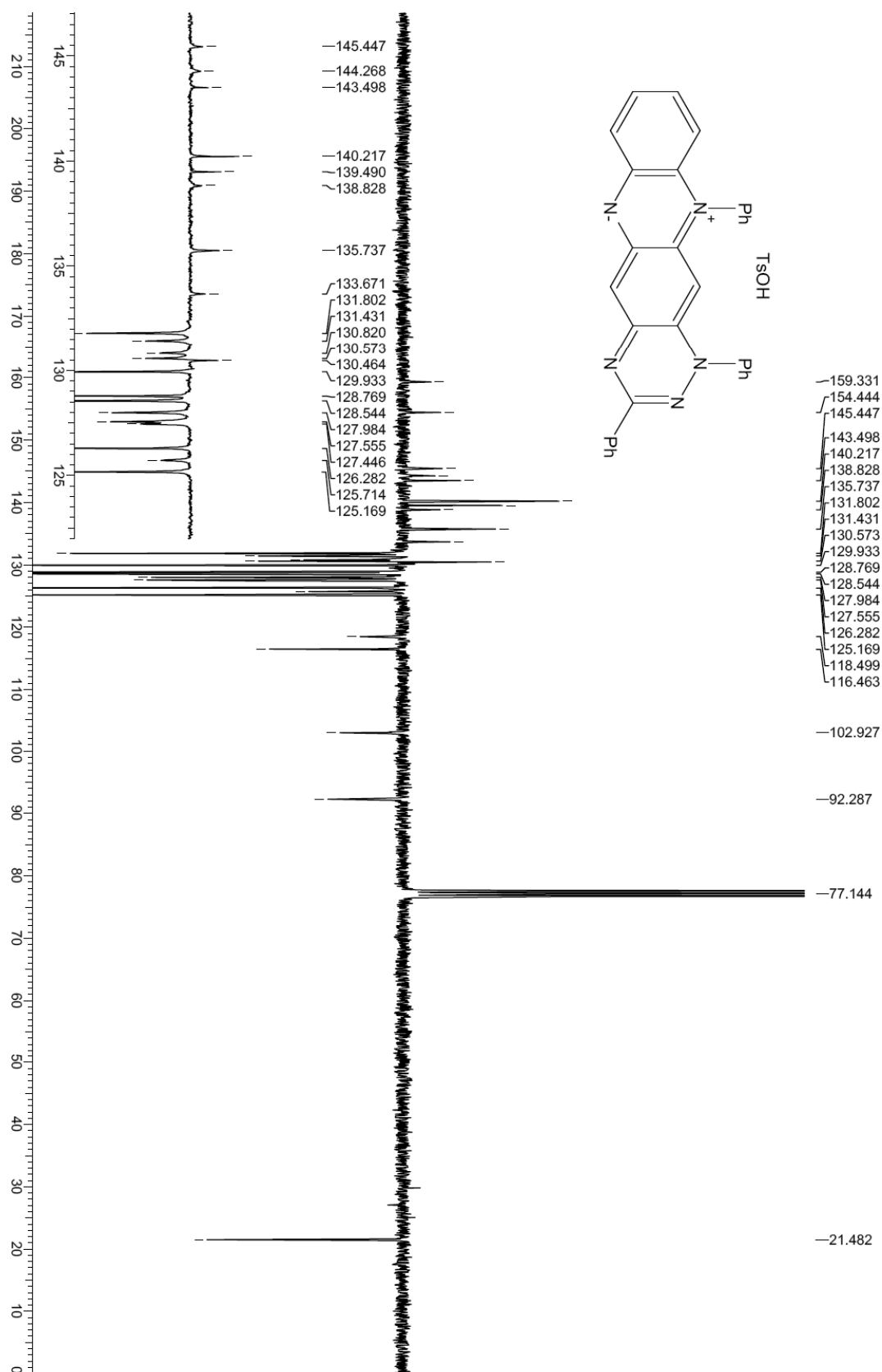
¹H-NMR of 1,3,11-Triphenyl-1,6-dihydro-[1,2,4]triazino[5,6-*b*]phenazin-11-ium 4-methylbenzene-sulfonate (15)



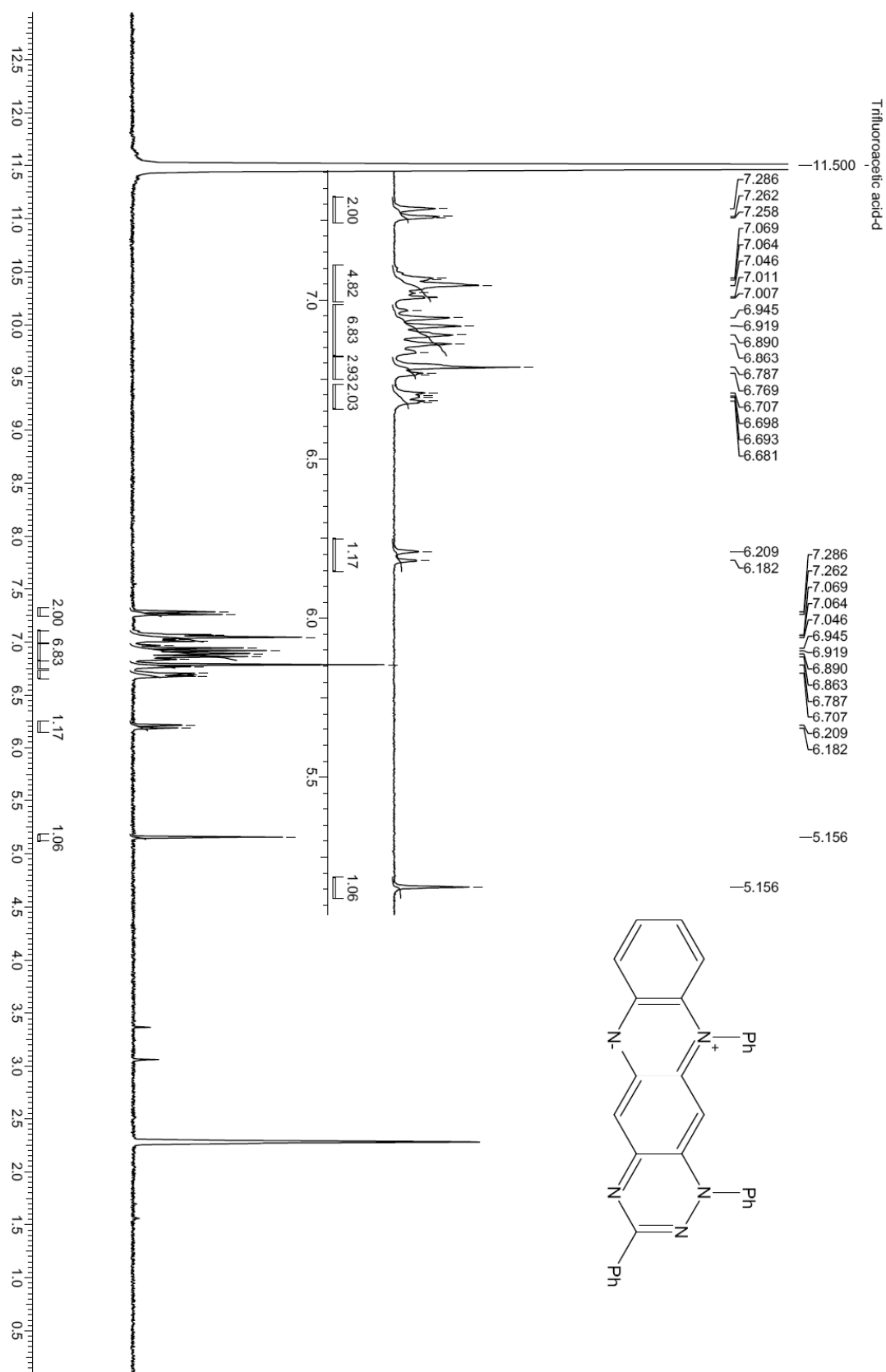
¹H-NMR of 1,3,11-Triphenyl-1,6-dihydro-[1,2,4]triazino[5,6-*b*]phenazin-11-ium 4-methylbenzene-sulfonate (15) crystallised with ½ EtOH



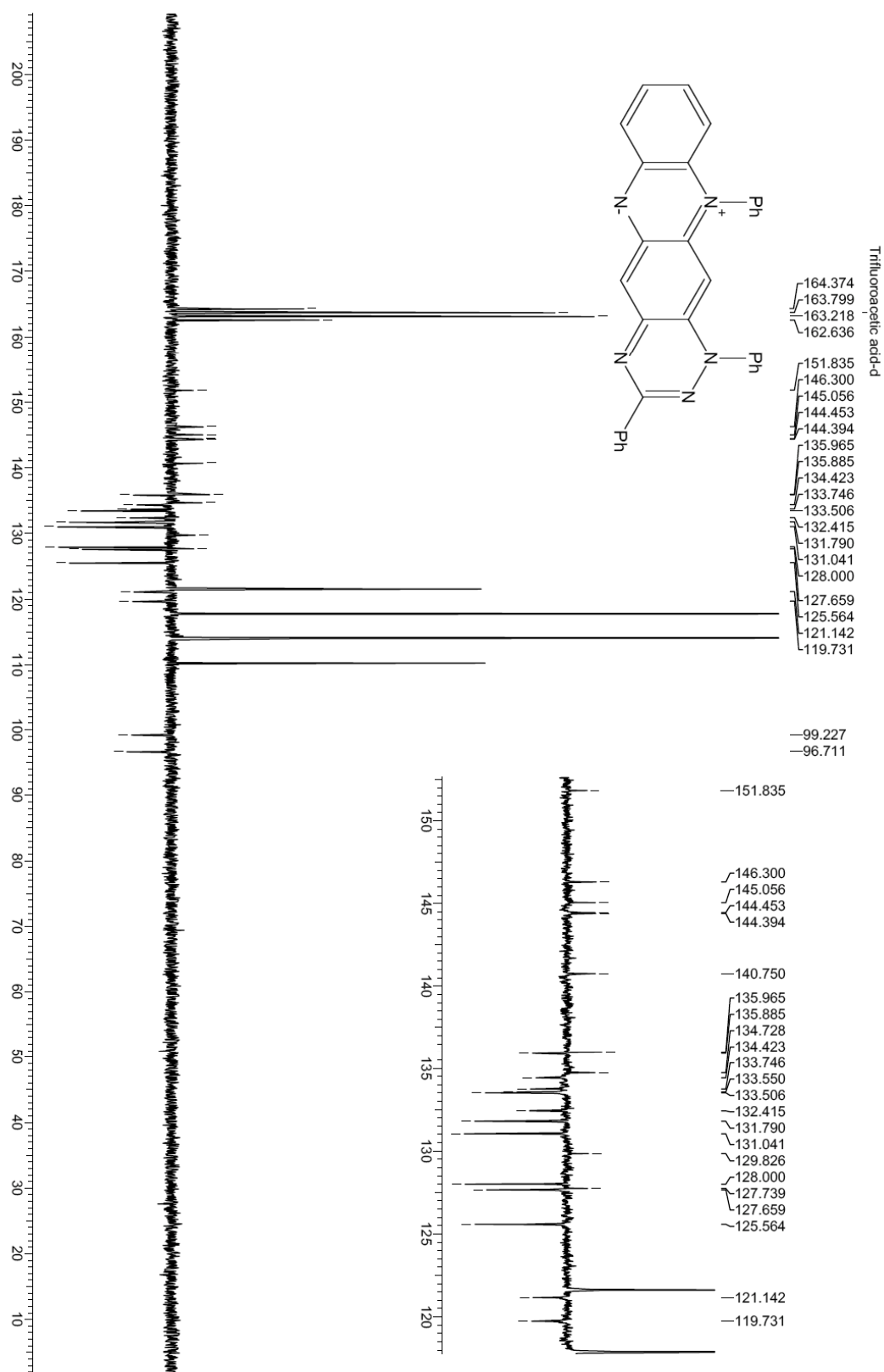
^{13}C -NMR of 1,3,11-Triphenyl-1,6-dihydro-[1,2,4]triazino[5,6-*b*]phenazin-11-ium 4-methylbenzene-sulfonate (15)



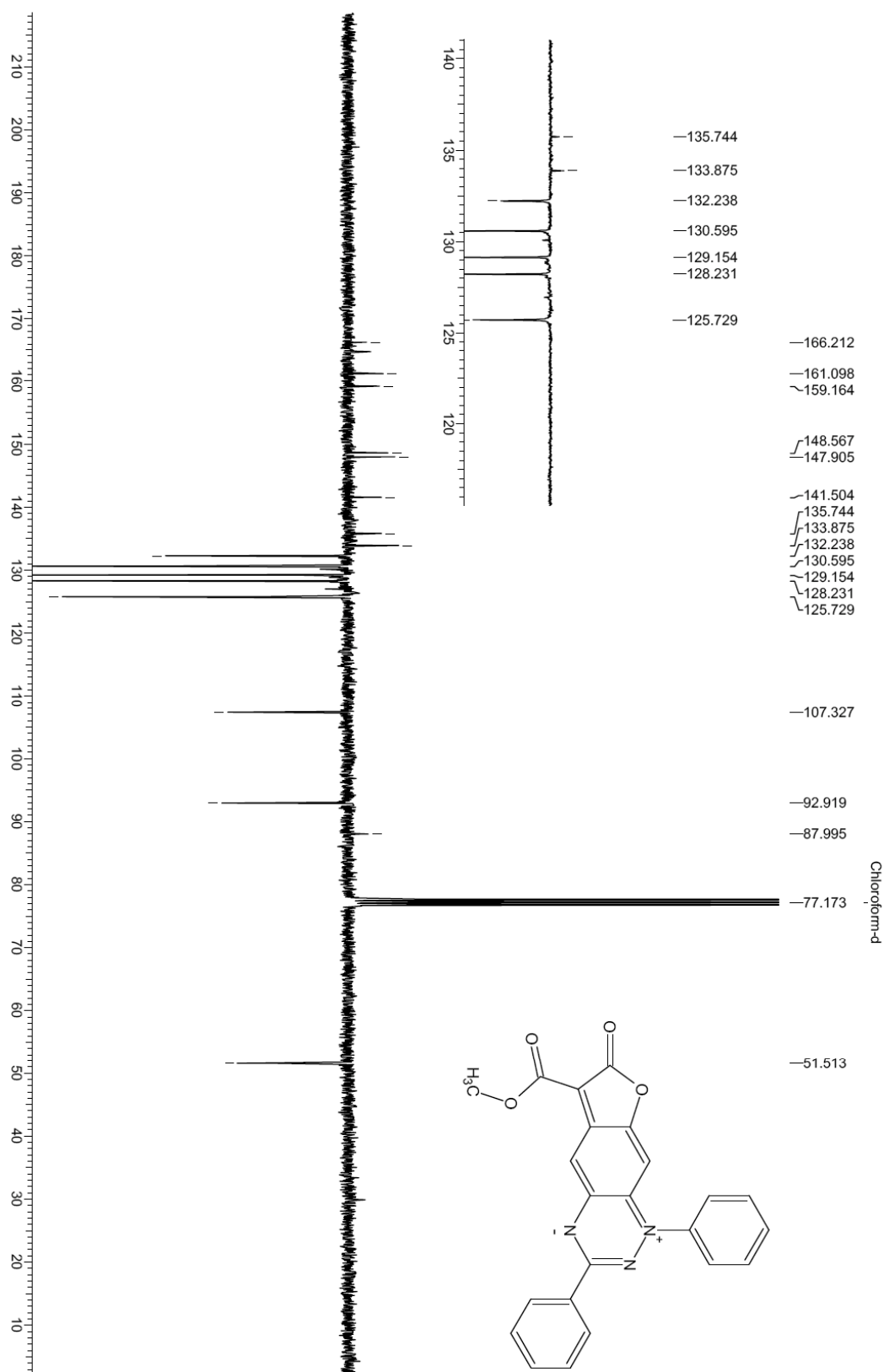
¹H-NMR of 1,3,11-Triphenyl-1H-[1,2,4]triazino[5,6-*b*]phenazin-11-ium-6-ide (16)



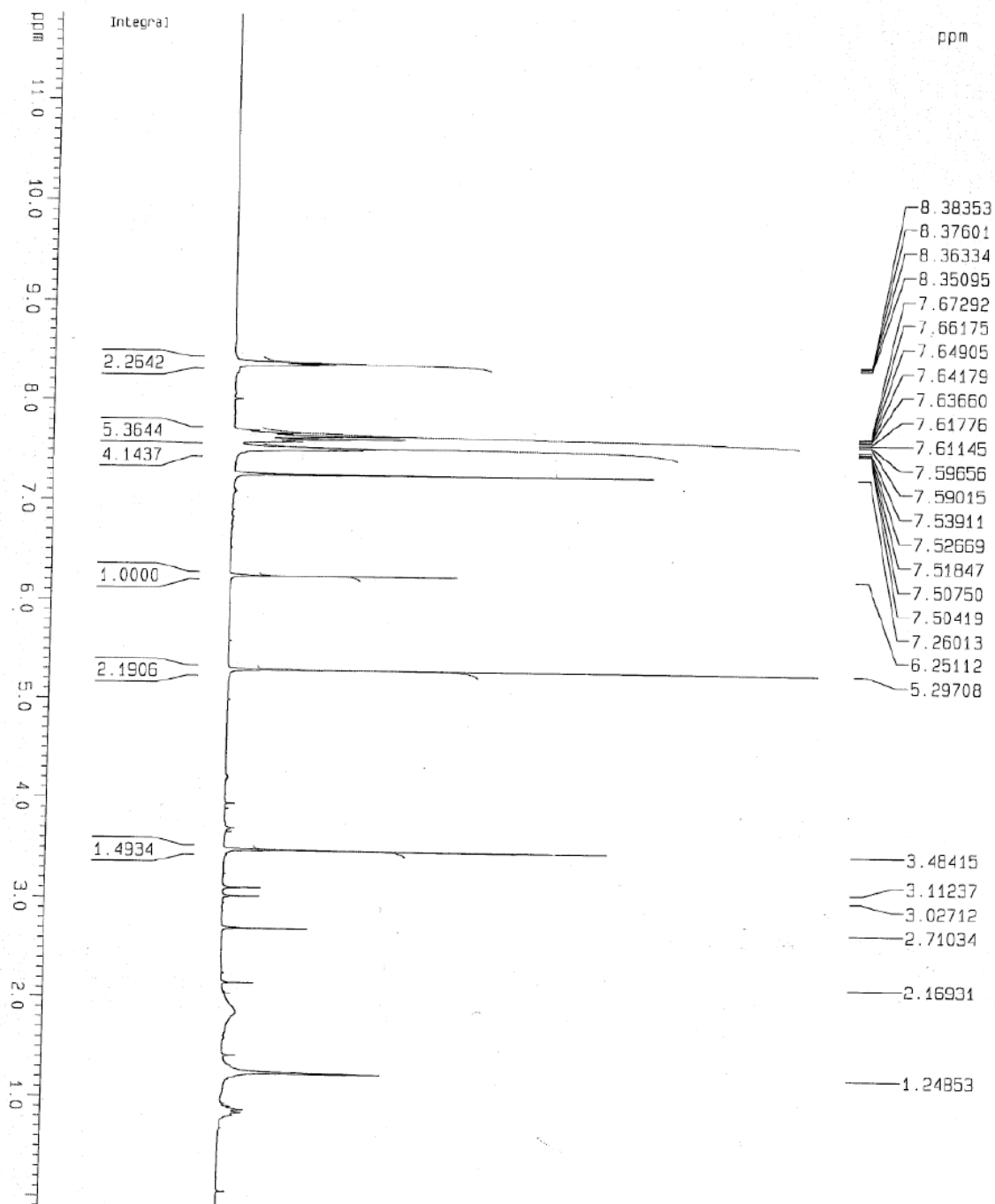
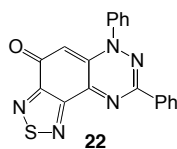
^{13}C -NMR of 1,3,11-Triphenyl-1H-[1,2,4]triazino[5,6-*b*]phenazin-11-ium-6-ide (16)

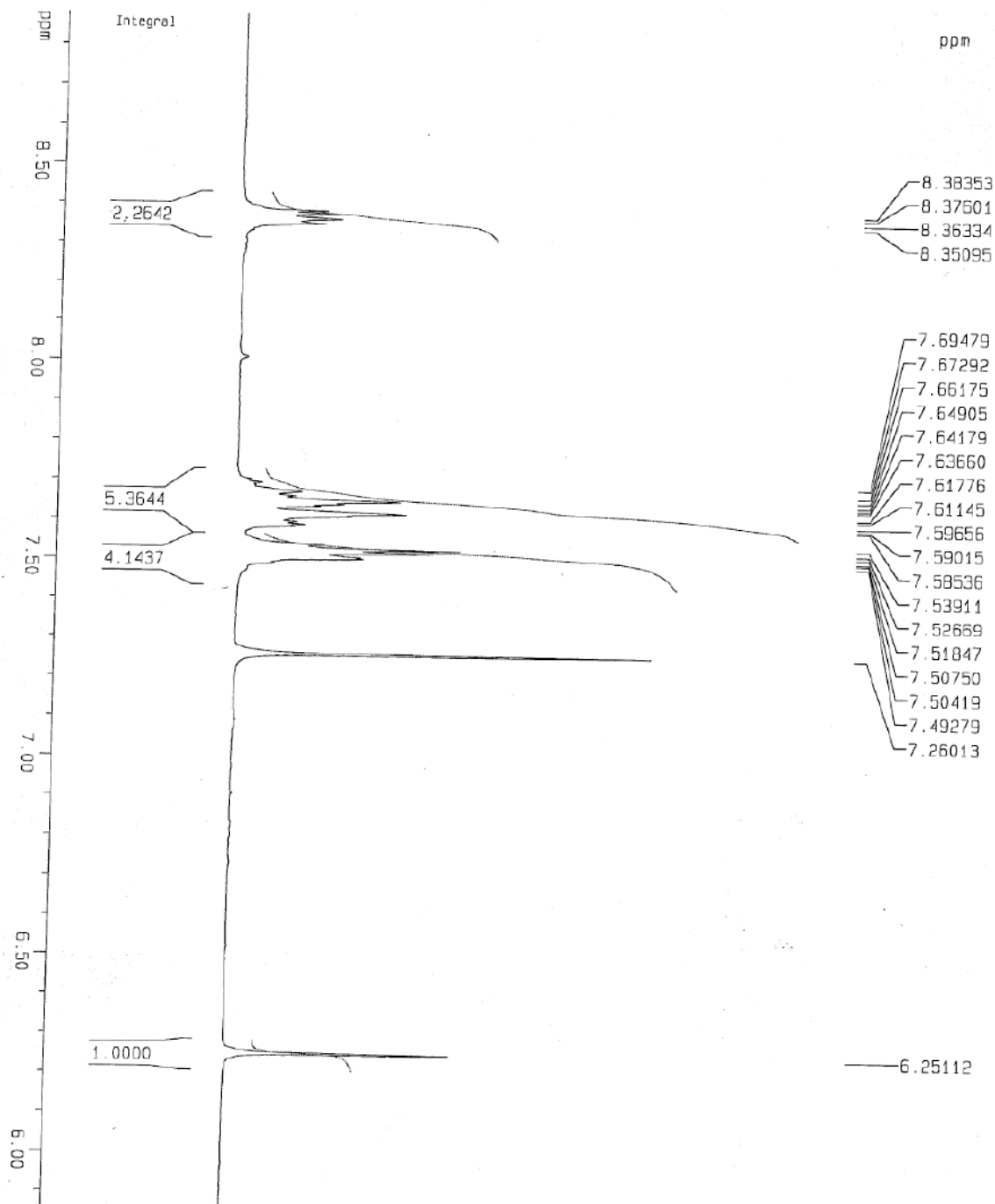
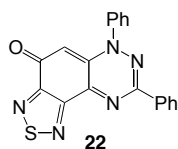


^{13}C -NMR of 6-(Methoxycarbonyl)-7-oxo-1,3-diphenyl-7H-benzofuro[5,6-*e*][1,2,4]triazin-1-ium-4-ide (17)

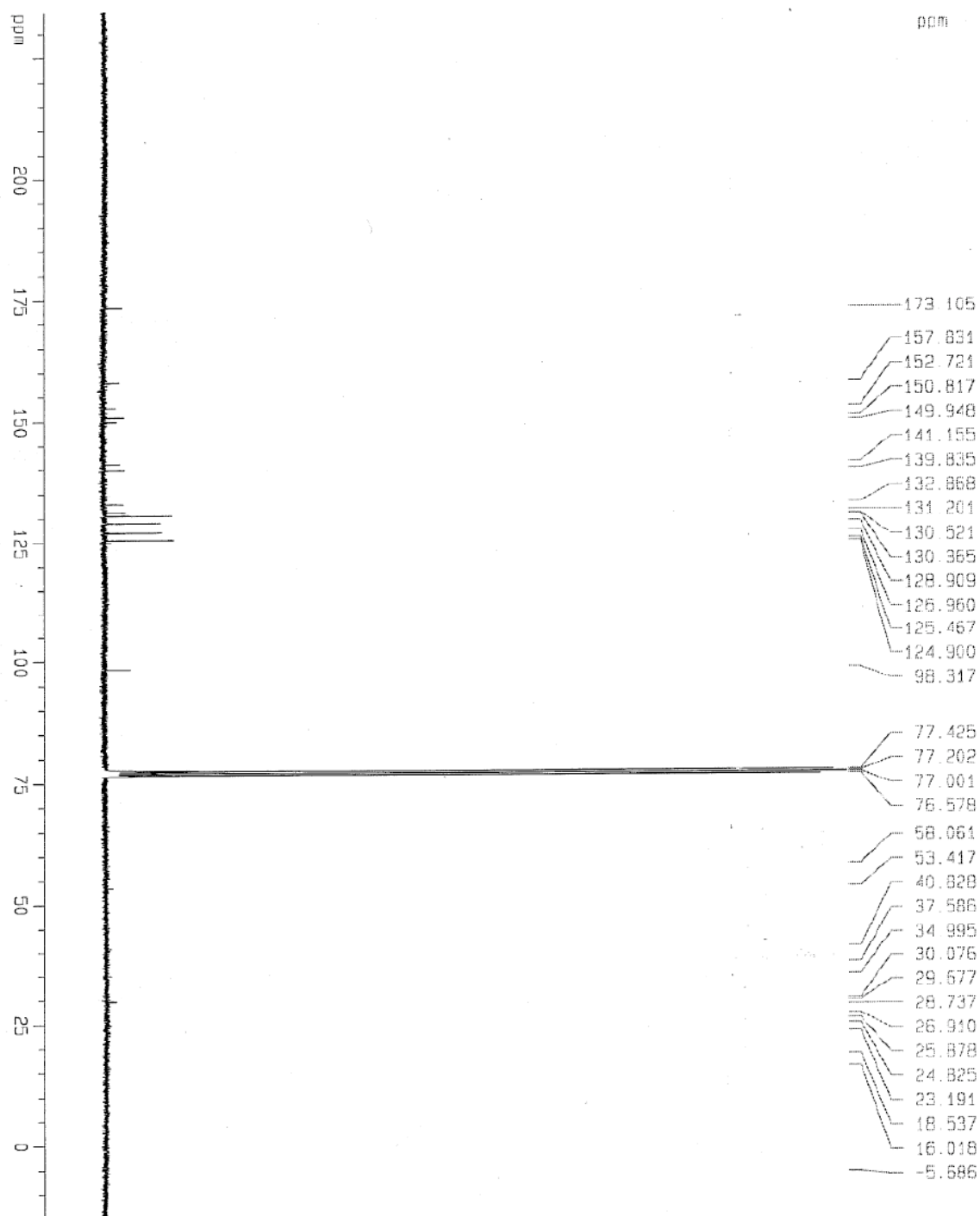
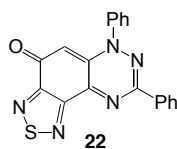


¹H-NMR of [5,6-*c*]-Thiadiazolo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (22)





¹³C-NMR of [5,6-*c*]-Thiadiazolo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (22)



Computational Parameters

Table 1. Computational output parameters for singlet 16.

```
1\1\GINC-N12\FOpt\UB3LYP\6-31G(d)\C31H21N5\KH800\30-May-2011\0\#\UB3LYP/6-31G* OPT FREQ\singlet 1 B3LYP\0,1\C,-1.1276240298,-2.1921909847,-0.085247\C,-1.5182180106,-0.7805029794,-0.017318\C,-0.5574329969,0.2267300076,-0.009312\C,0.8083379986,-0.102780011,-0.069636\C,1.2340869796,-1.4982430168,-0.092778\C,0.2573819663,-2.4806820035,-0.114602\N,2.5562809755,-1.8050100347,-0.083877\C,3.4262499893,-0.7901250466,-0.03392\N,3.140591007,0.5130019573,-0.035508\N,1.8028900111,0.8179279755,-0.087704\N,-2.8631920068,-0.5012719611,0.04153\C,-3.8261880208,-1.529783948,0.027954\C,-3.346185039,-2.8662709545,-0.051377\N,-2.0183060432,-3.1791659726,-0.105258\C,-5.2015400172,-1.2667369293,0.088082\C,-6.1090820315,-2.321017917,0.067298\C,-5.6554050496,-3.6466169231,-0.012817\C,-4.2973550532,-3.9112619416,-0.070455\C,-3.3060609882,0.8703450449,0.116218\C,-3.5775459786,1.5731380486,-1.059668\C,-4.0149899606,2.8961790546,-0.9837\C,-4.1785499523,3.5104370568,0.259812\C,-3.9047469619,2.8014730531,1.431326\C,-3.4676809799,1.4777800471,1.363075\C,4.8756549847,-1.1269720663,0.019046\C,5.8557319983,-0.1224160796,0.040982\C,7.2068279938,-0.4581660979,0.092115\C,7.5984849756,-1.7989731033,0.121486\C,6.6279309619,-2.8027040901,0.098965\C,5.2752079664,-2.4709970717,0.048126\C,1.5642440304,2.2370949787,-0.120661\C,0.8355250382,2.8079279886,-1.166365\C,0.6471890569,4.1900599912,-1.195259\C,1.1912910679,4.9956119838,-0.193628\C,1.93261906,4.4160509737,0.838926\C,2.1251030413,3.0363129711,0.877837\H,-0.8597799829,1.2616860117,0.053051\H,0.5596809522,-3.5207700076,-0.140197\H,-5.5591940033,-0.2454739245,0.150122\H,-7.1730790286,-2.1081339025,0.113694\H,-6.3695830607,-4.4651309134,-0.028662\H,-3.9133300669,-4.9246119468,-0.130998\H,-3.4503229853,1.0801060469,-2.018734\H,-4.2303209532,3.4447370575,-1.896253\H,-4.5199419383,4.5401910614,0.315744\H,-4.0317129555,3.2764810548,2.399817\H,-3.2528669876,0.9125550442,2.264861\H,5.5465940125,0.9165519246,0.014466\H,7.9566450045,0.3287358919,0.107547\H,8.653254972,-2.0590571176,0.160852\H,6.9248919477,-3.8481170941,0.121059\H,4.510751956,-3.2394690613,0.029389\H,0.4334910296,2.1777049941,-1.952993\H,0.084679063,4.6361189988,-2.010497\H,1.0457030825,6.0717889858,-0.221689\H,2.3651760685,5.0392499679,1.616465\H,2.7118280349,2.5702999631,1.661644\Version=AM64L-G03RevC.02\State=1-A\HF=-1467.6848303\S2=0.\S2-1=0.\S2A=0.\RMSD=3.822e-09\RMSEF=1.772e-06\Dipole=-1.6954427,2.8508683,0.1443935\PG=C01 [X(C31H21N5)]\@
```

Table 2. Computational output parameters for triplet 16.

```
1\1\GINC-N14\FOpt\UB3LYP\6-31G(d)\C31H21N5(3)\KH800\05-Jun-2011\0\#\UB3LYP/6-31G(D) OPT=FCCARDS FREQ\triplet 1 B3LYP\0,3\C,-1.7356391064,-1.7150802164,-0.0179824626\C,-1.6813414715,-0.2952962757,0.1526852801\C,-0.4651233232,0.3866065064,0.0494851083\C,0.7106223546,-0.3158163116,-0.2310498185\C,0.6986919517,-1.7330482036,-0.3575460454\C,-0.5326573052,-2.3976555951,-0.2641707276\N,1.8460992814,-2.464519023,-0.5235183524\C,2.9901380476,-1.7717914206,-0.4843985887\N,3.1180842951,-0.4409176679,-0.4018575355\N,1.9733777985,0.2959486878,-0.363389124\N,-2.8848434049,0.3761998777,0.4249539743\C,-4.0831696707,-0.3405392302,0.51239
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Table 3. Computational output parameters for singlet 17.

1\1\GINC-N13\FOpt\UB3LYP\6-31G(d)\C23H15N3O4\KH800\30-May-2011\0\#\UB3
LYP/6-31G* OPT FREQ\singlet 2 B3LYP\0,1\N, 2.17727003, 1.0454039375, -0
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30394, -0.174179\N, 0.0694719779, -0.769654002, -0.113365\N, -0.1604679805,
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17165\O, 3.3043530504, 1.7542439051, -0.009266\N, 4.427767023, 0.8021788728
, -0.096637\N, 3.8448559851, -0.5194301104, -0.113901\O, 5.5365210363, 1.262
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Table 4. Computational output parameters for triplet 17.

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UB3LYP/6-31G(D) OPT=FCCARDS FREQ\\triplet 2 B3LYP\\0,3\C,-2.2753451952
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044\C,-5.9833625083,-2.4877341474,-0.1960892871\C,1.3532587824,2.79568
11259,0.1600882734\C,0.9954760225,3.3703566631,1.3850092923\C,1.163687
7974,4.74141592,1.576879885\C,1.6995133008,5.5354442771,0.5613944758\C
,2.0726343173,4.9509069881,-0.6512439759\C,1.9015984336,3.5836749976,-
0.8574999794\C,3.5229789844,-1.1672169292,-1.2554550495\C,4.6555540634
, -0.3961724238,-1.5623295602\C,5.7986494497,-1.0018882728,-2.077718367
5\C,5.8282195508,-2.3822948322,-2.2925767833\C,4.7056475108,-3.1543314
316,-1.9874360167\C,3.559018748,-2.5528856418,-1.4721636127\H,-0.92829
45536,-2.6161355192,0.1882402424\H,-1.2782624143,2.3869266914,0.594865
1043\H,-6.6315970251,-3.2115835024,-0.6920981298\H,-6.5683171464,-1.80
42572082,0.4191755595\H,-5.4249338387,-1.9241420441,-0.9508419646\H,0.
6083762665,2.7475297805,2.1850384279\H,0.888254622,5.1842729499,2.5297
035074\H,1.8318596497,6.6022715313,0.7163399419\H,2.4952260058,5.56180
74515,-1.4438776889\H,2.1925883397,3.1162092461,-1.7915177637\H,4.6304
772116,0.6738462049,-1.3891580374\H,6.670170516,-0.3956768233,-2.31004
96948\H,6.7219375649,-2.8527658748,-2.693953945\H,4.7219455104,-4.2285
250118,-2.1508629269\H,2.6825135288,-3.143268354,-1.2307672182\\Versio
n=AM64L-G03RevC.02\State=3-A\HF=-1350.5713914\S2=2.046\S2-1=0.\S2A=2.0
01217\RMSD=5.645e-09\RMSF=1.099e-06\Dipole=0.9334352,1.6919687,-1.0955
446\PG=C01 [X(C23H15N3O4)]\\@

Table 5. Computational output parameters for singlet 18.

1\1\GINC-CHEM54\FOpt\UB3LYP\6-31G(d)\C30H20N4\GAUSSIAN\29-Aug-2011\0\\#
opt ub3lyp/6-31g(d) geom=connectivity pop=(mk,dipole)\\OPT and ESP\\
0,1\C,0.0343071722,-0.0000428746,-0.0193194914\C,0.0392507726,-0.00004
20867,1.3821592264\C,1.2074308648,-0.0000343465,2.1564462432\C,2.48464

65129,-0.00002373,1.4426925075\C,2.5202597144,-0.000026789,0.044455187
9\C,1.3325005215,-0.0000371362,-0.6941668967\N,1.3393857799,-0.0000410
505,-2.0635363579\N,-1.1216486807,-0.0000479604,-0.7029248796\C,-1.076
3401203,-0.0000520751,-2.057874907\C,0.1396052652,-0.000050068,-2.8034
068617\H,3.4711508191,-0.0000209665,-0.4682436504\C,-2.2909501008,-0.0
000594985,-2.7902944106\C,0.1262321046,-0.0000574468,-4.2053361252\C,-
2.2970897214,-0.0000658355,-4.1726048557\C,-1.0856969456,-0.0000651751
, -4.8861665647\H,-3.2101966958,-0.0000603682,-2.2132161901\H,-3.241556
0576,-0.0000719085,-4.7101069819\H,-1.0884173522,-0.0000706564,-5.9721
272068\H,1.0578594828,-0.000057048,-4.7595373495\N,3.6325004453,-0.000
0120197,2.1894521851\N,1.1433298161,-0.0000372973,3.4978796944\C,3.591
3243742,-0.0000113201,3.5984185112\C,2.3002514262,-0.0000257817,4.2046
134589\C,4.755249067,0.000003779,4.3799965651\C,2.2447011787,-0.000027
2349,5.6218754648\C,4.6580704569,0.0000027052,5.7666679939\H,5.5638655
912,0.000014732,6.3657114359\C,3.396209582,-0.0000134027,6.386628467\H
,3.3262637732,-0.0000146558,7.4710789302\H,1.2574125555,-0.0000388692,
6.0727576888\H,5.7302279736,0.0000163468,3.9061984168\H,-0.9144137534,
-0.0000481308,1.8963534454\C,2.5951619032,-0.000029109,-2.7765597437\C
,3.1917950492,1.2135554734,-3.1239161638\C,3.1918289282,-1.2135910936,
-3.1239106095\C,4.3988861494,1.2096135822,-3.8243123399\H,2.7078381842
,2.1455394454,-2.8481624703\C,4.3989244516,-1.2096156242,-3.8243109104
\H,2.7079077334,-2.1455939661,-2.8481580739\C,5.0025995758,0.000004937
, -4.174270011\H,4.8648594293,2.1519625275,-4.0978123478\H,4.8649190237
, -2.1519561092,-4.0978034648\H,5.9413629935,0.0000223175,-4.721018927\
C,4.9183012884,-0.0000068846,1.5321145441\C,5.5363899529,-1.2135832695
,1.2245210631\C,5.5363778643,1.2135633776,1.2245023194\C,6.7848869956,
-1.2096246932,0.6009196185\H,5.0400654869,-2.145573865,1.4773134757\C,
6.7848808813,1.2096045345,0.60089943\H,5.0400539186,2.1455595745,1.477
2752233\C,7.4090139268,-0.0000077108,0.2888528394\H,7.2694661408,-2.15
19671773,0.3619037712\H,7.2694452695,2.1519514524,0.3618715188\H,8.381
6882565,-0.0000121353,-0.19500228\\Version=AM64L-G03RevD.02\State=1-A\
HF=-1374.2434712\S2=0.\S2-1=0.\S2A=0.\RMSD=8.908e-09\RMSF=6.720e-06\Th
ermal=0.\Dipole=3.4059224,0.0000225,-1.8364281\PG=C01 [X(C30H20N4)]\@