A One-Pot Synthesis of Benzo[1,4]thiazin-3(4*H*)-ones and Theoretical Study on S-N Type Smiles Rearrangement Mechanism

Yongmei Zhao, Yanmiao Wu, Jiong Jia, Dongju Zhang and Chen Ma**

Supporting Information

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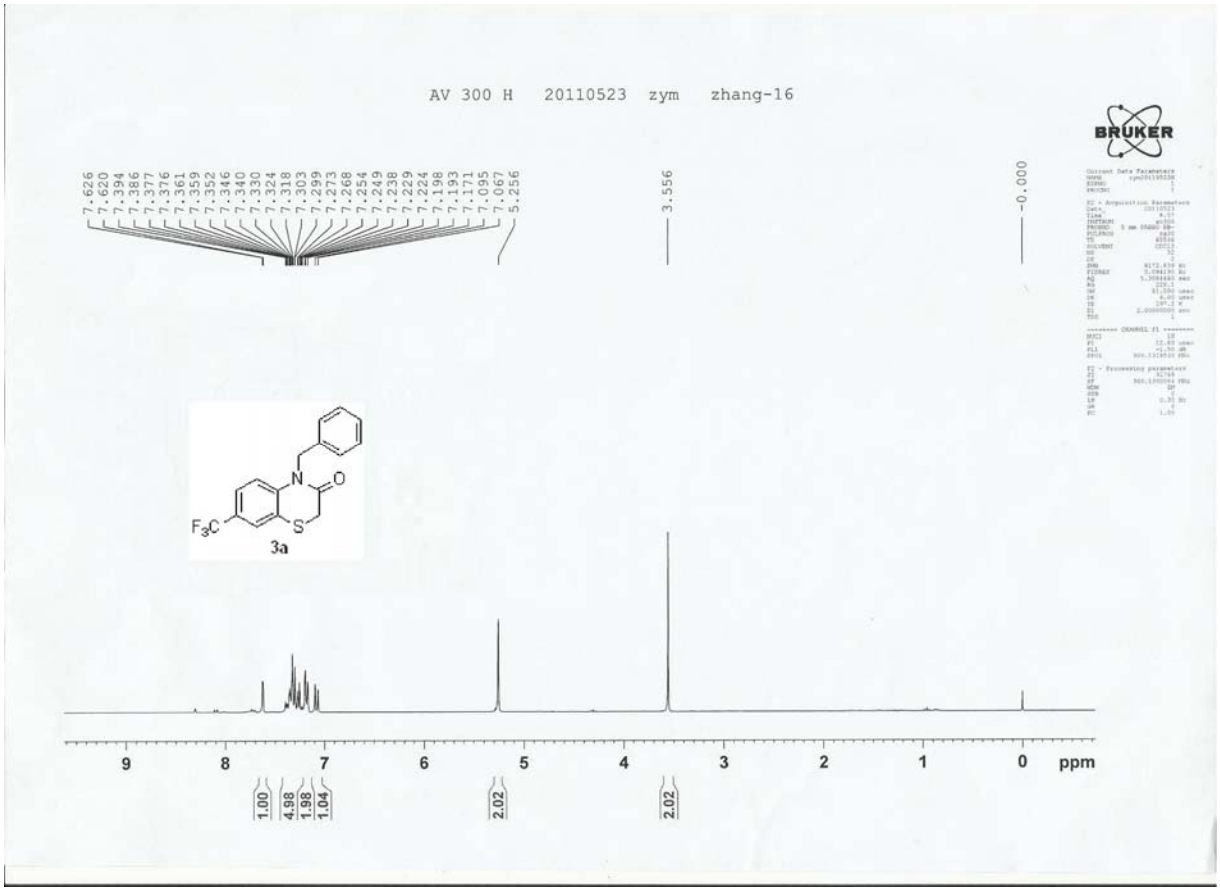
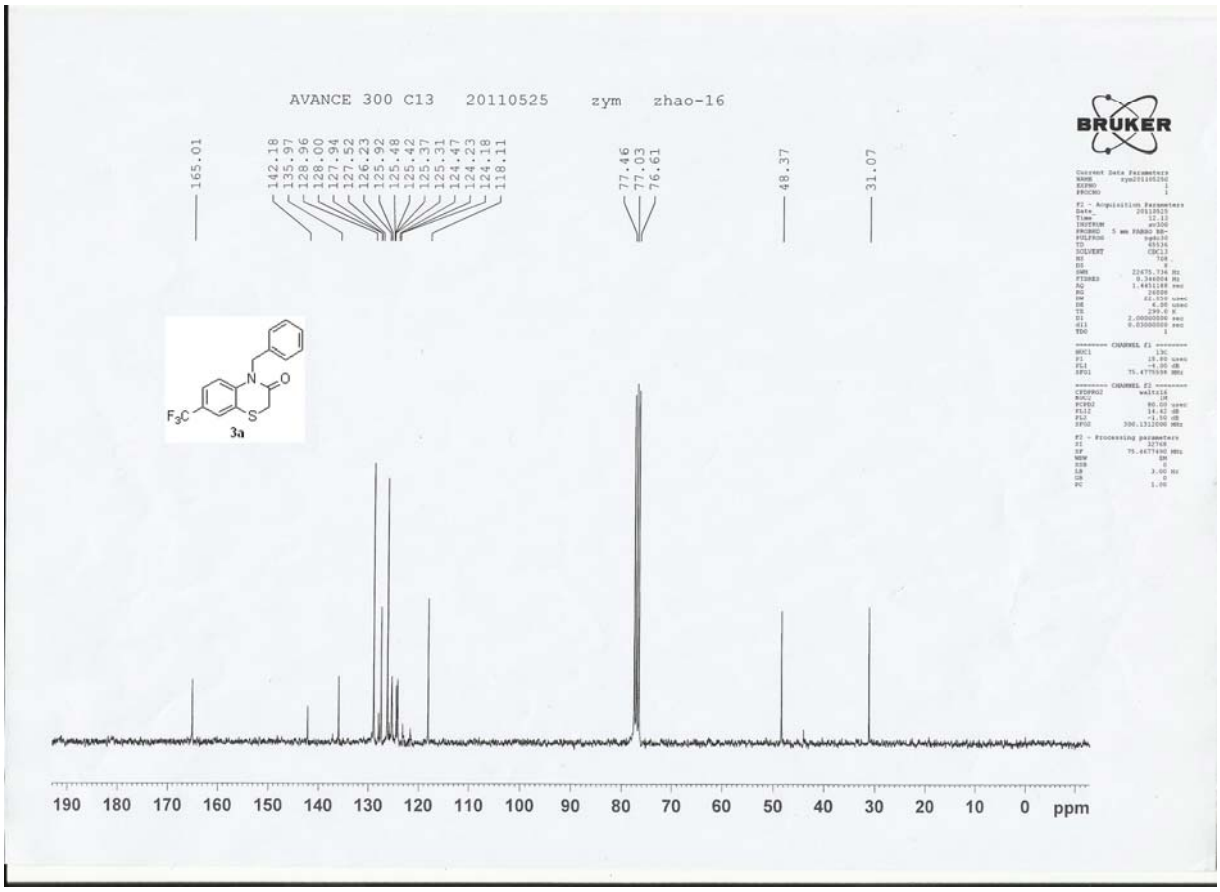
1. Copies of ^{1}H NMR and ^{13}C NMR spectrum of 3a-3d, 5a-5k

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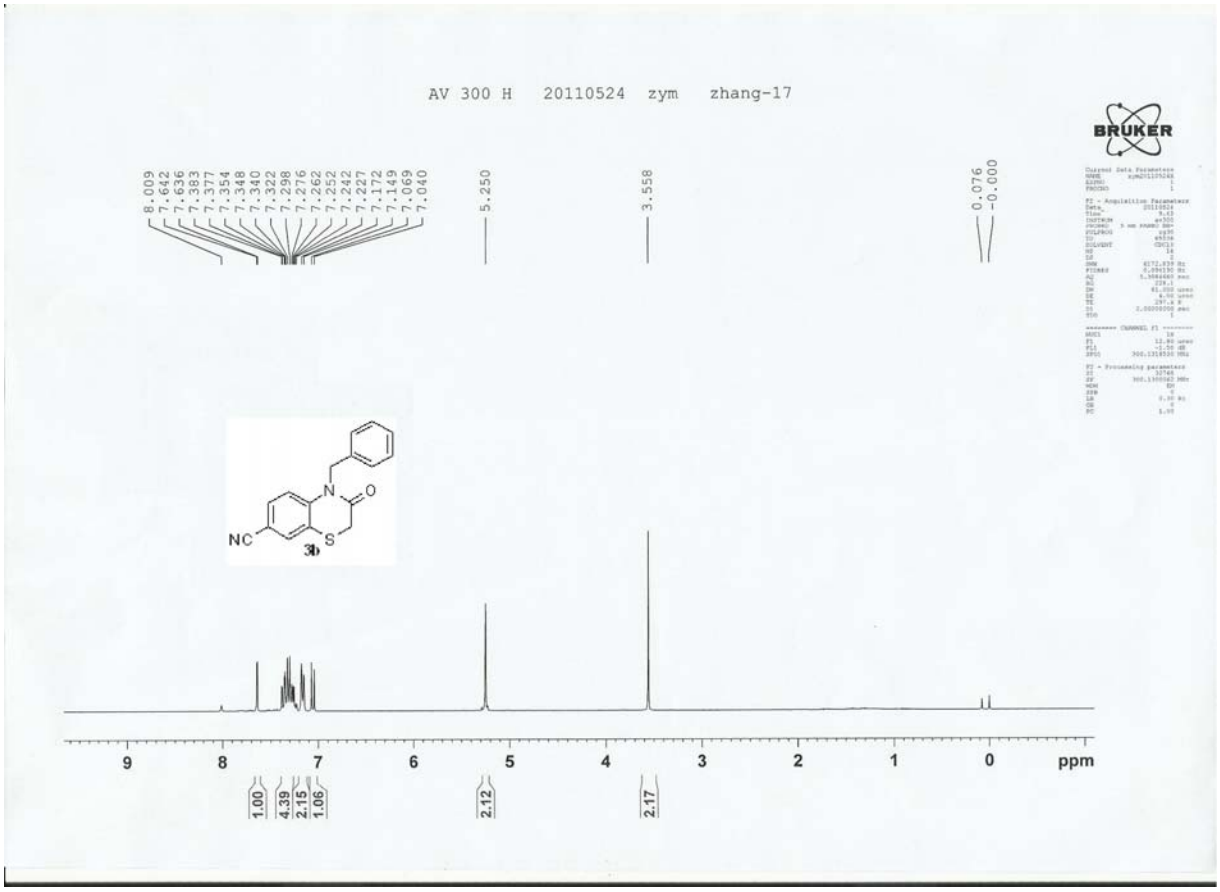
BRUKER
165.01
142.18
135.97
128.96
128.00
127.94
127.52
126.23
125.92
125.48
125.42
125.37
125.31
124.47
124.23
124.18
118.11
77.46
77.03
76.61
48.37
31.07
F3C
O
N
S
3a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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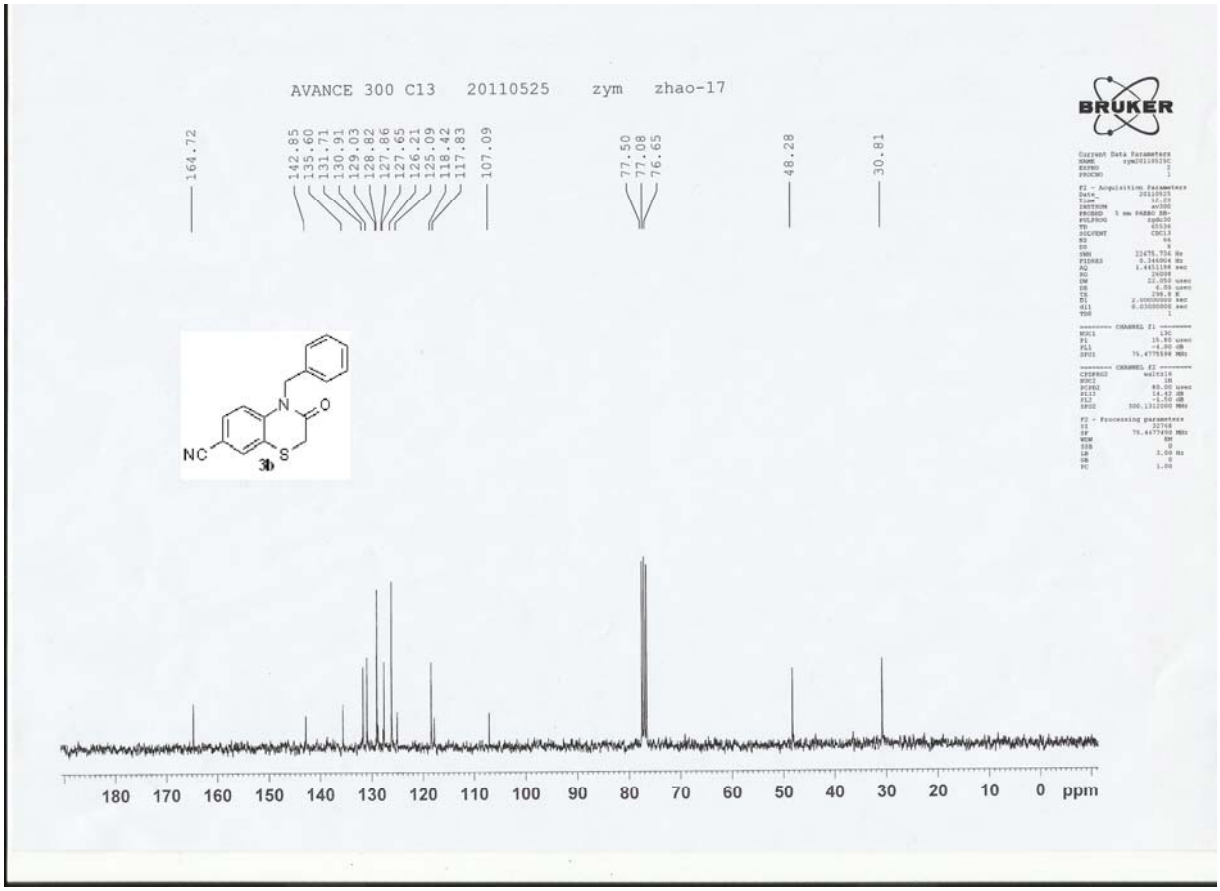
BRUKER
8.009
7.642
7.636
7.383
7.377
7.354
7.348
7.340
7.322
7.298
7.276
7.262
7.252
7.242
7.227
7.172
7.149
7.069
7.040
5.250
3.558
0.076
0.000
NC
O
N
S
3b
9 8 7 6 5 4 3 2 1 0 ppm
1.00
4.39
2.15
1.06
2.12
2.17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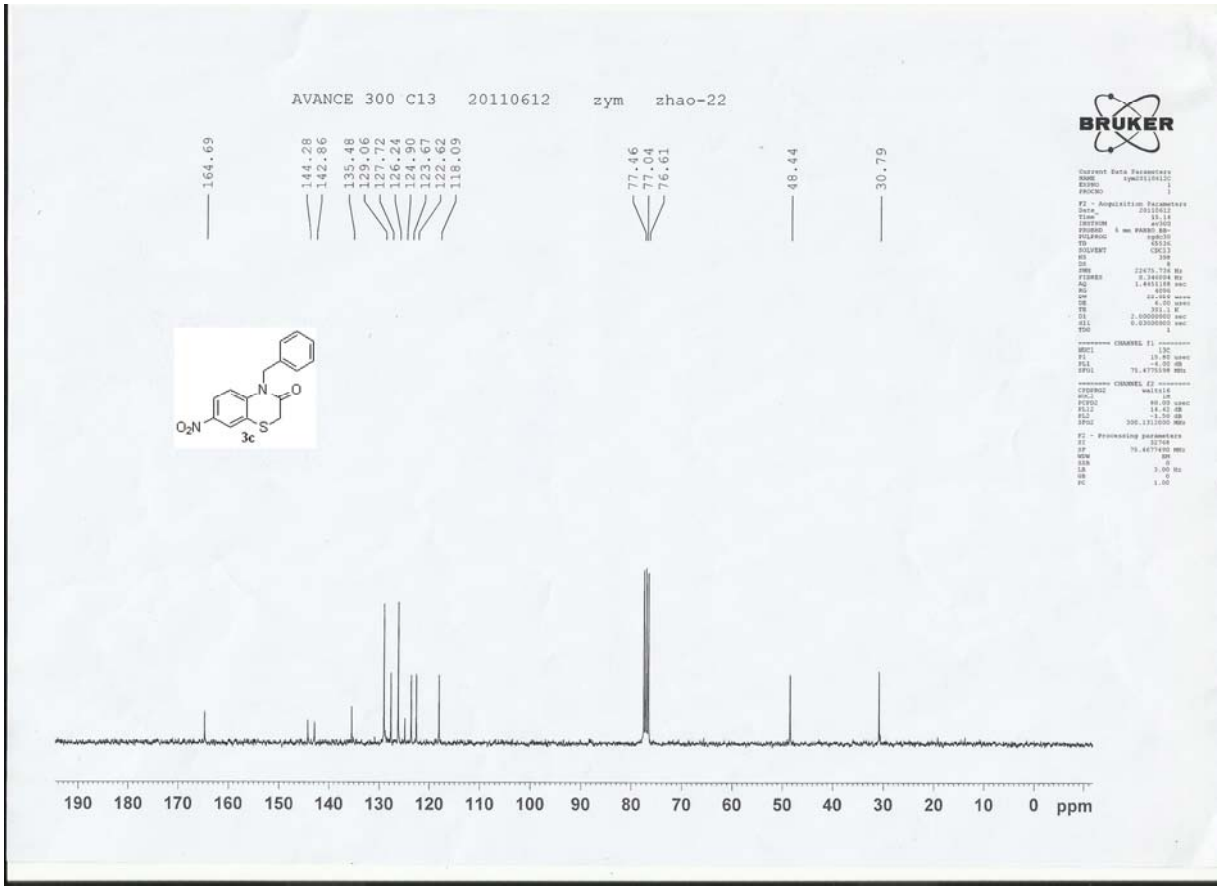
164.72
142.85
135.60
133.71
130.91
129.03
128.82
127.86
127.65
126.21
125.09
118.42
117.83
107.09
77.50
77.08
76.65
48.28
30.81
NC
3b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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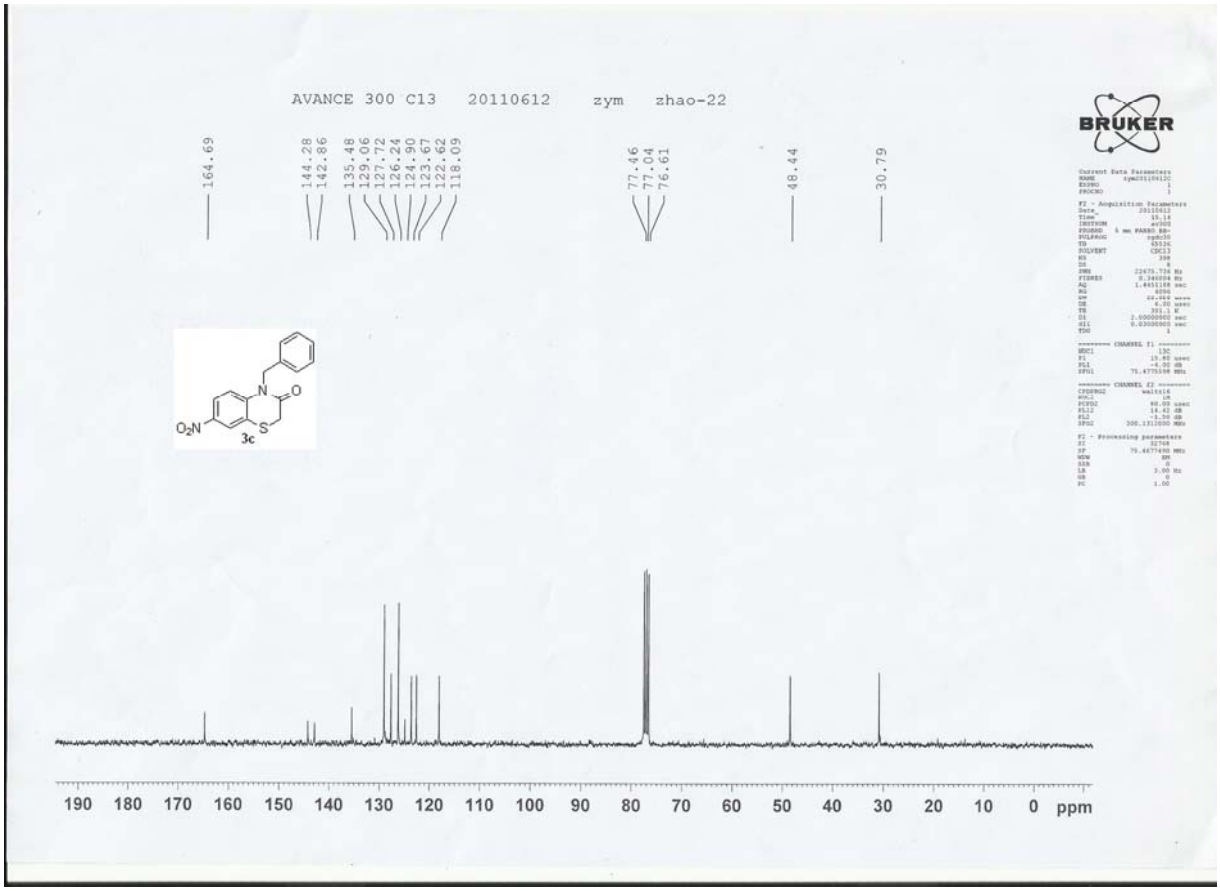
144.28
142.86
135.48
129.06
127.72
126.24
124.90
123.67
122.62
118.09
77.46
77.04
76.61
48.44
30.79
O2N
3c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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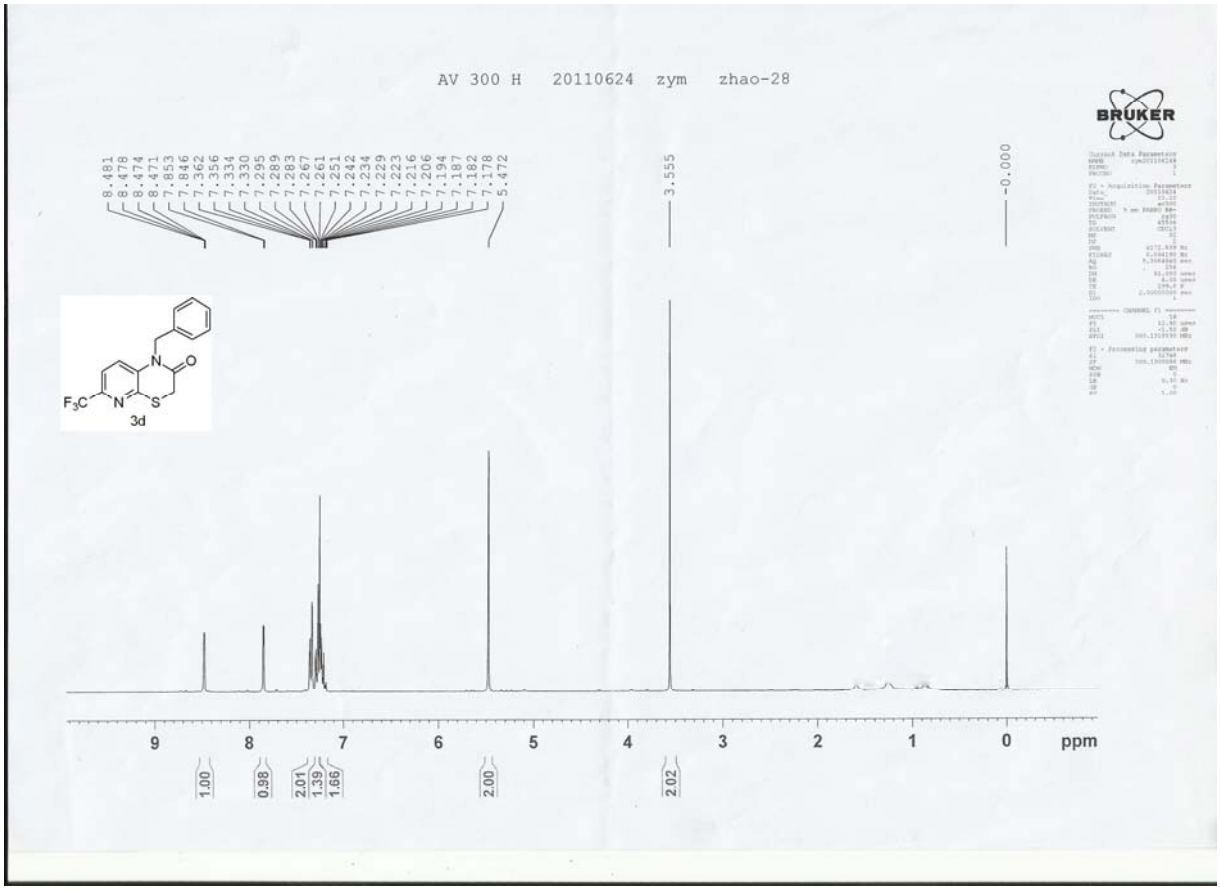
144.28
142.86
135.48
129.06
127.72
126.24
124.90
123.67
122.62
118.09
77.46
77.04
76.61
48.44
30.79
BRUKER
3c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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8.481
8.478
8.474
8.471
7.853
7.846
7.362
7.356
7.334
7.330
7.295
7.289
7.283
7.267
7.261
7.251
7.242
7.234
7.229
7.223
7.216
7.206
7.194
7.187
7.182
7.178
5.472
3.555
0.000
BRUKER
3d
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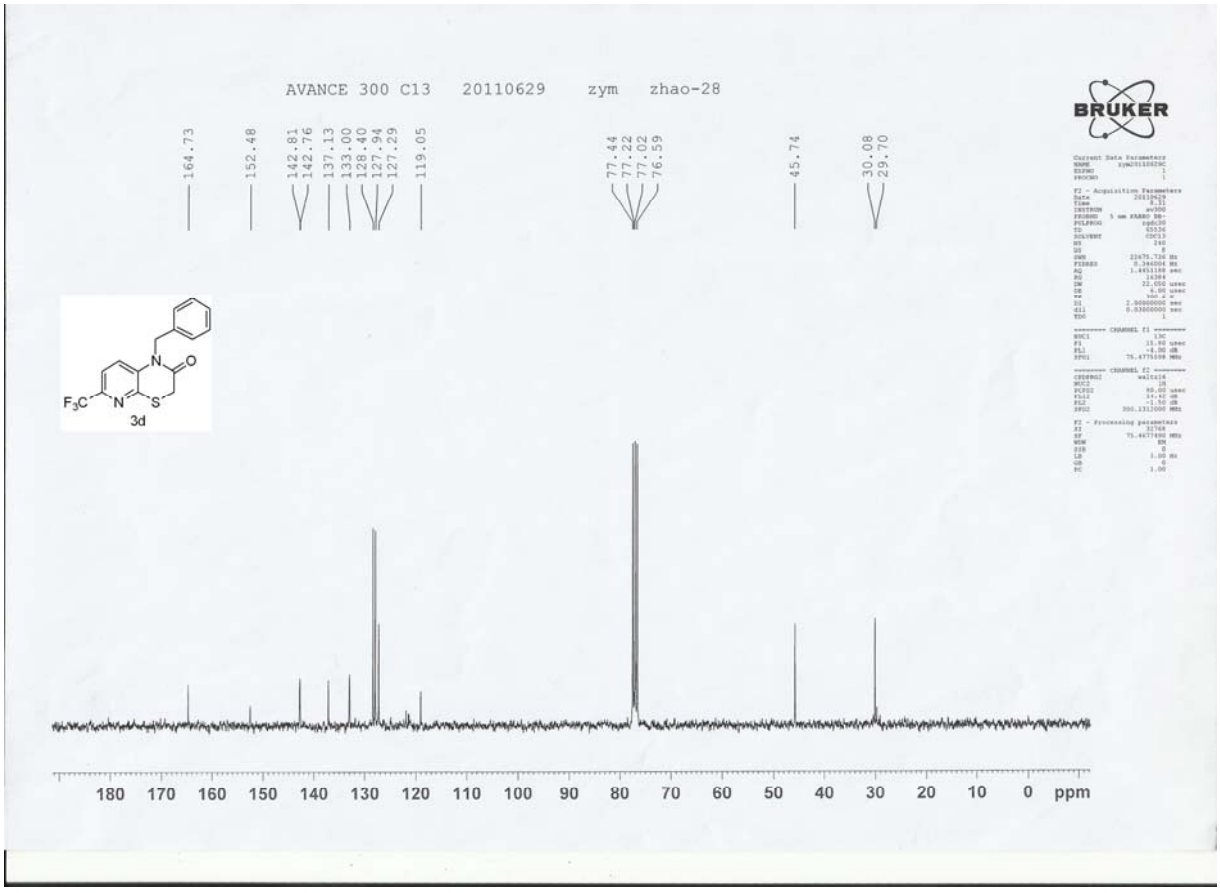
1.00
0.98
2.01
1.39
1.66
2.00
2.02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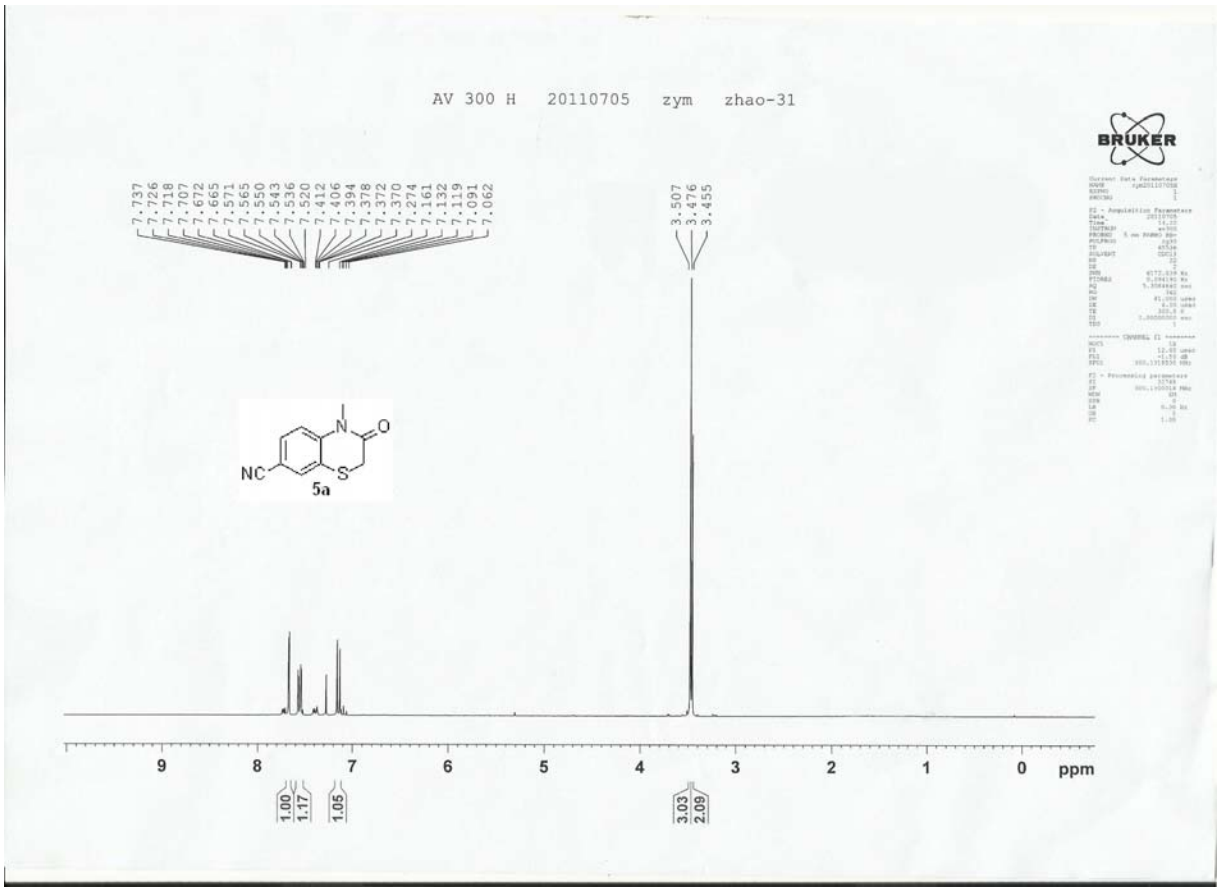
152.48
142.81
142.76
137.13
133.00
128.40
127.94
127.29
119.05
77.44
77.22
77.02
76.59
45.74
30.08
29.70
3d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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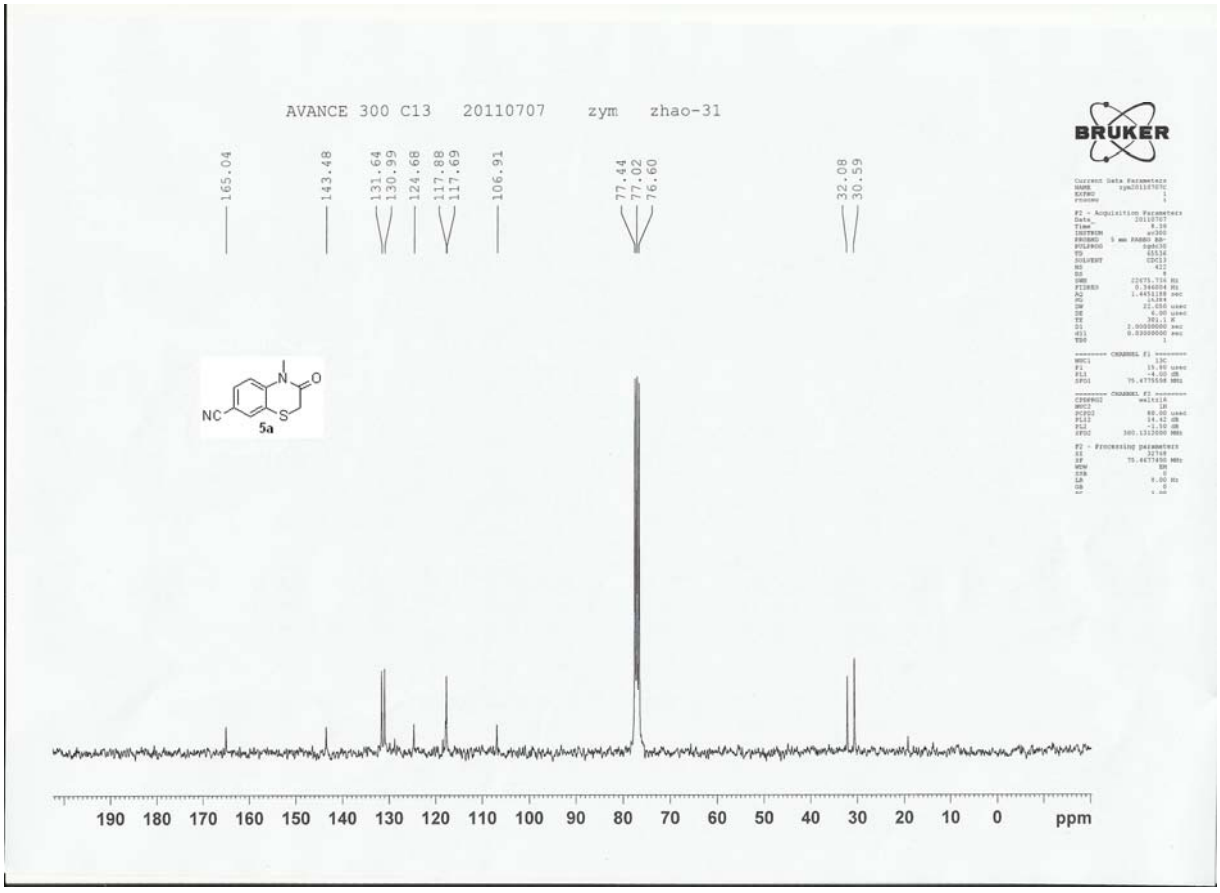
BRUKER
7.737
7.726
7.718
7.707
7.672
7.665
7.571
7.565
7.550
7.543
7.536
7.520
7.412
7.406
7.394
7.378
7.372
7.370
7.274
7.161
7.132
7.119
7.091
7.062
3.507
3.476
3.455
5a
9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.17
1.05
3.03
2.09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165.04
143.48
131.64
130.99
124.68
117.88
117.69
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77.44
77.02
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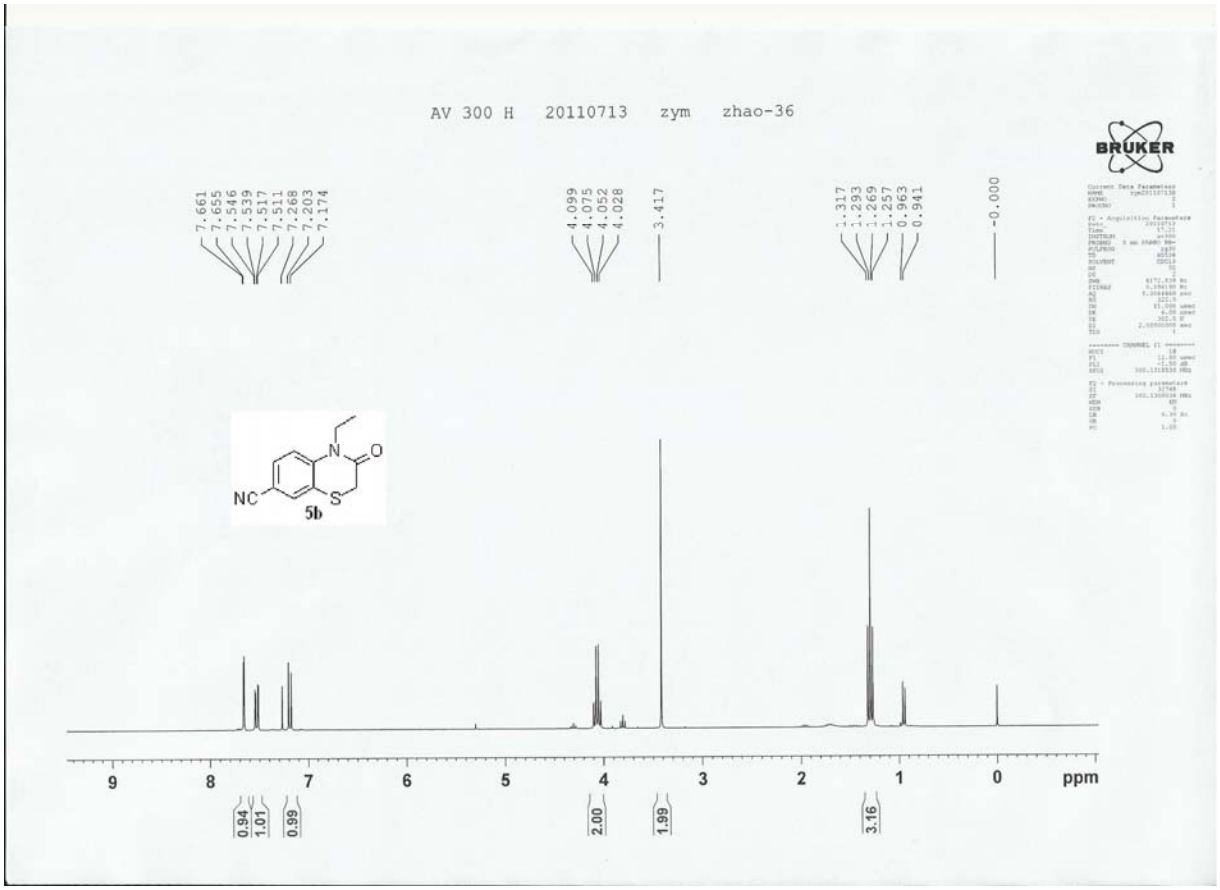
NC
O
N
S
5a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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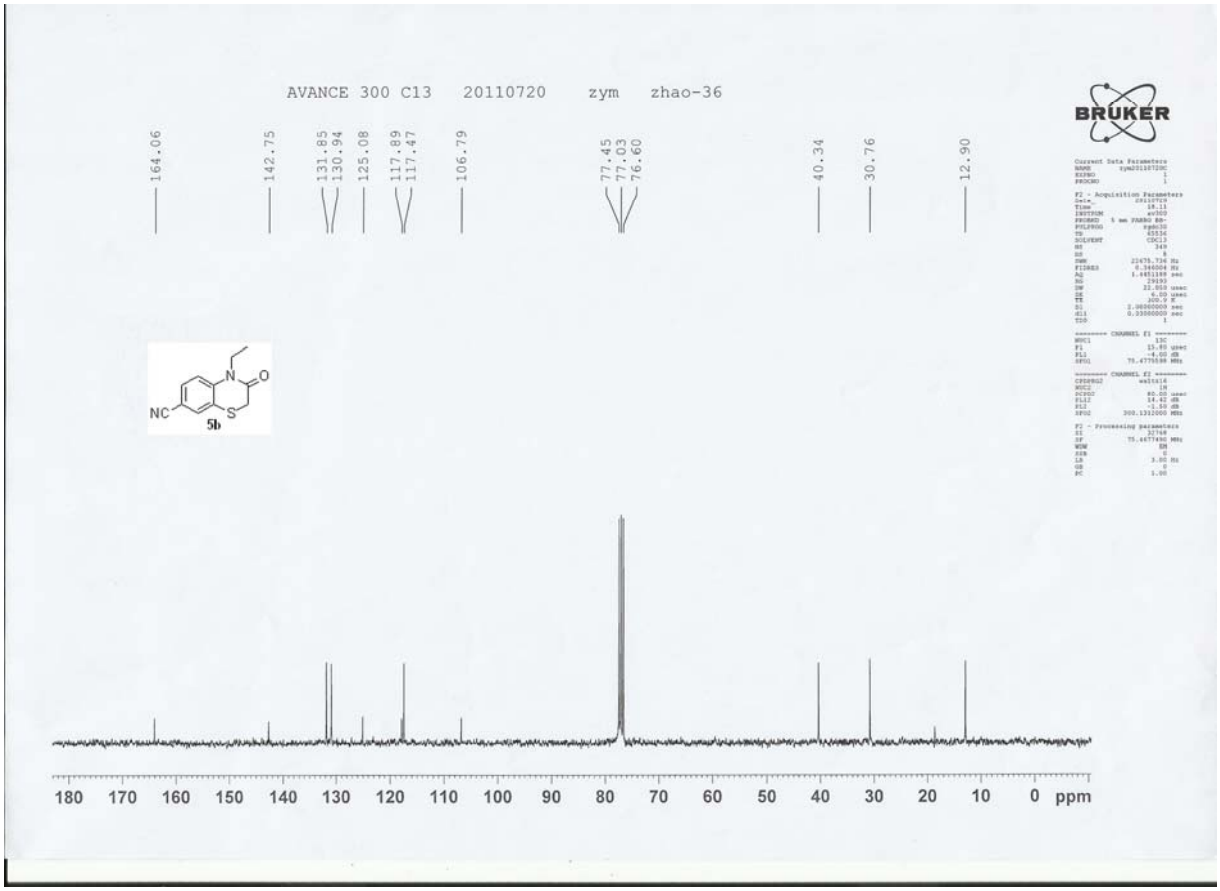
BRUKER
7.661
7.655
7.546
7.539
7.517
7.511
7.268
7.203
7.174
4.099
4.075
4.052
4.028
3.417
1.317
1.293
1.269
1.257
0.963
0.941
-0.000
NC
O
N
S
5b
9 8 7 6 5 4 3 2 1 0 ppm
0.94
1.01
0.99
2.00
1.99
3.16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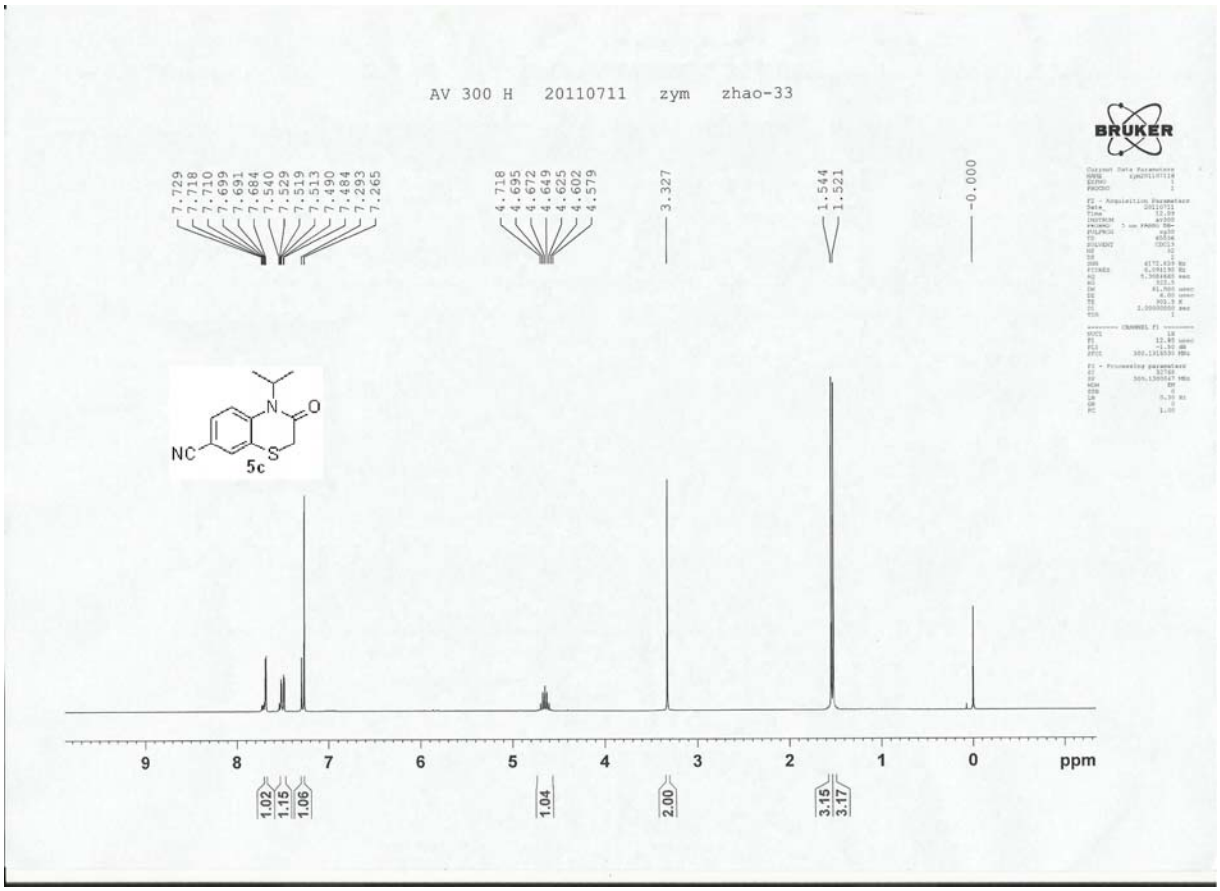
BRUKER
164.06
142.75
131.85
130.94
125.08
117.89
117.47
106.79
77.45
77.03
76.60
40.34
30.76
12.90
NC
O
N
S
5b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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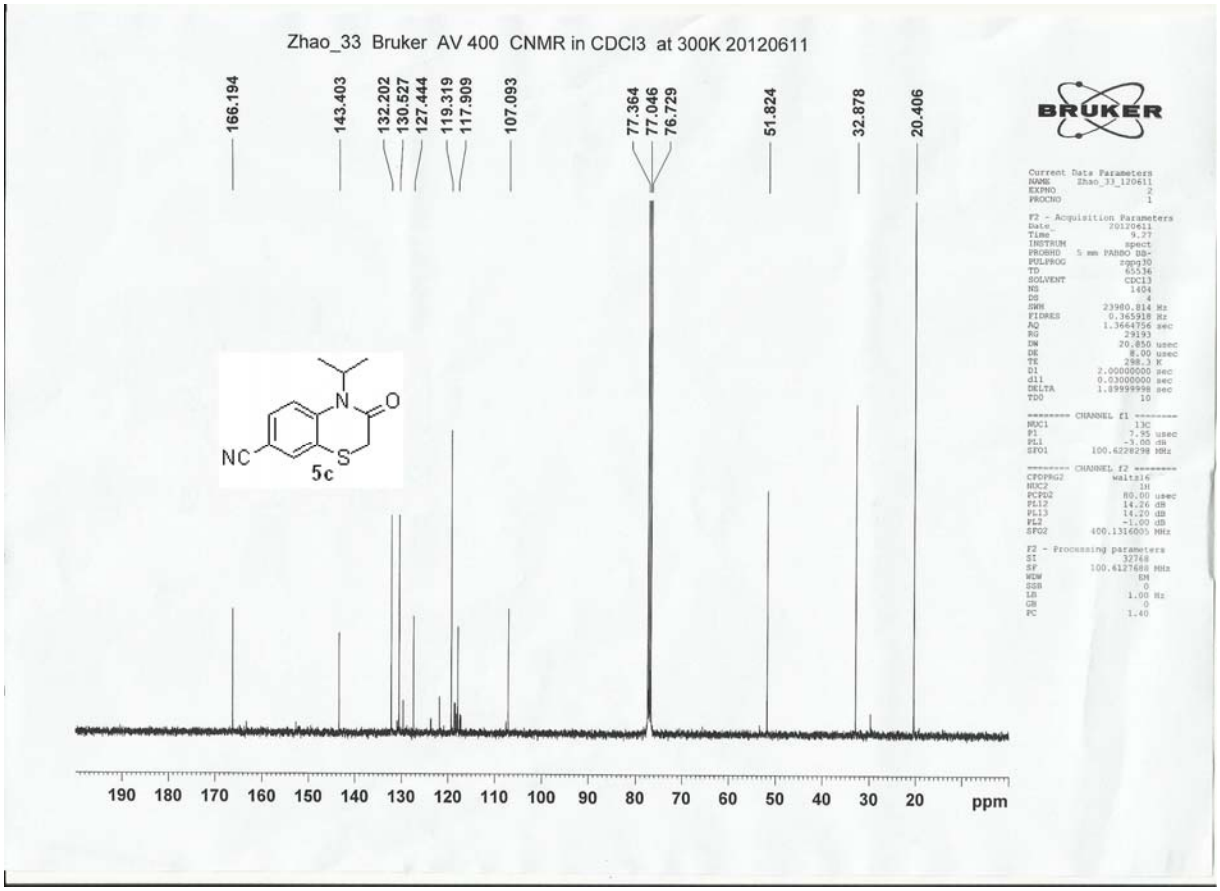
BRUKER
7.729
7.718
7.710
7.699
7.691
7.684
7.540
7.529
7.519
7.513
7.490
7.484
7.293
7.265
4.718
4.695
4.672
4.649
4.625
4.602
4.579
3.327
1.544
1.521
0.000
NC
O
N
S
5c
9 8 7 6 5 4 3 2 1 0 ppm
1.02
1.15
1.06
1.04
2.00
3.15
3.17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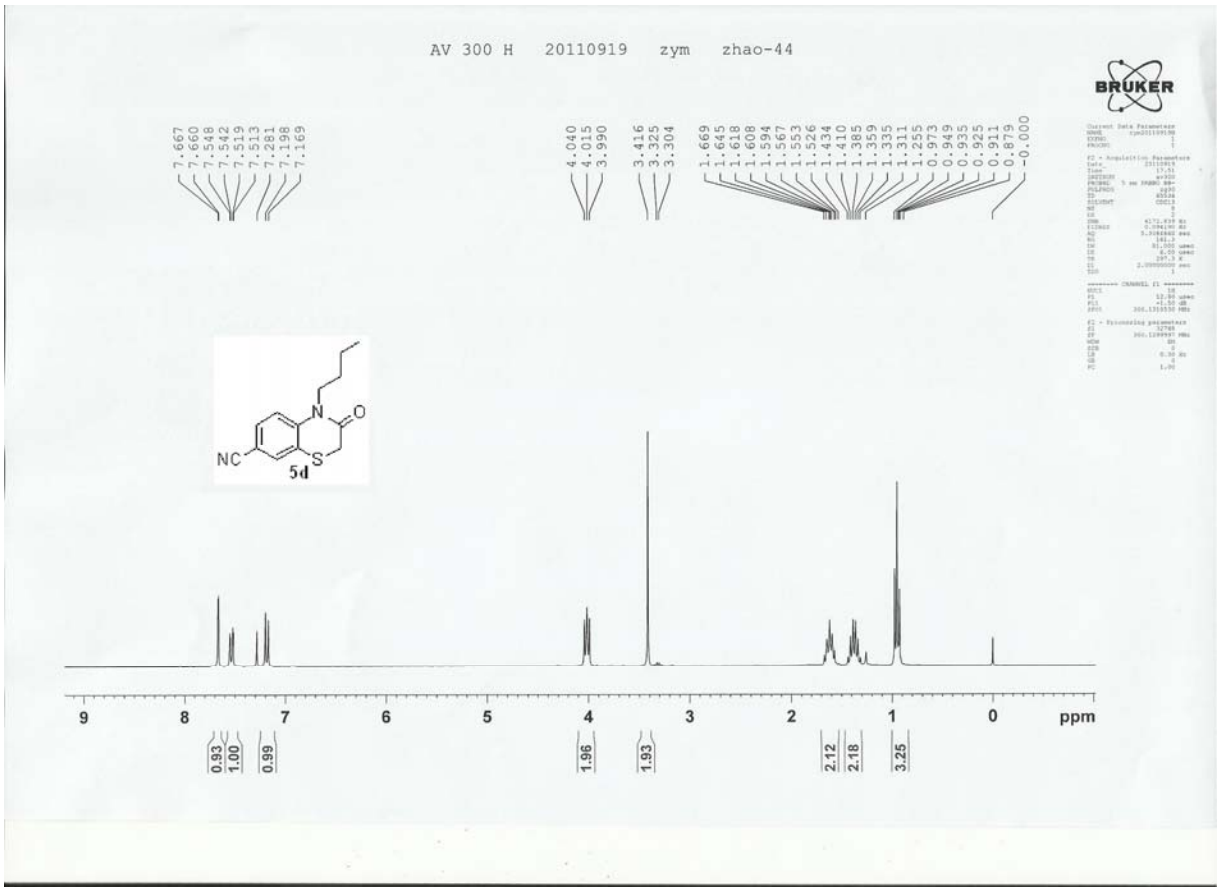
143.403
132.202
130.527
127.444
119.319
117.909
107.093
77.364
77.046
76.729
51.824
32.878
20.406
BRUKER
NC
O
N
S
5c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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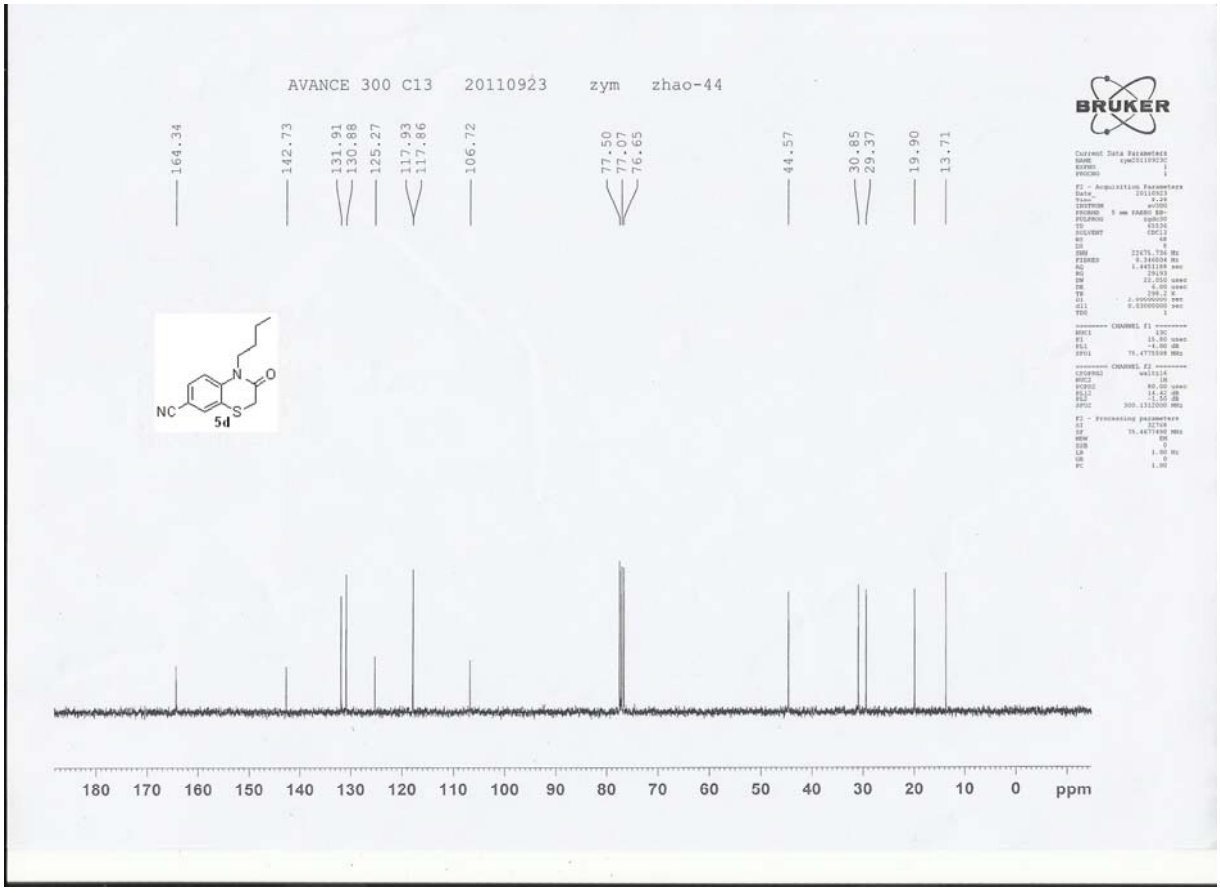
BRUKER
7.667
7.660
7.548
7.542
7.519
7.513
7.281
7.198
7.169
4.040
4.015
3.990
3.416
3.325
3.304
1.669
1.645
1.618
1.608
1.594
1.567
1.553
1.526
1.434
1.410
1.385
1.359
1.335
1.311
1.255
0.973
0.949
0.935
0.925
0.911
0.879
0.000
NC
O
N
S
5d
9 8 7 6 5 4 3 2 1 0 ppm
0.93
1.00
0.99
1.96
1.93
2.12
2.18
3.25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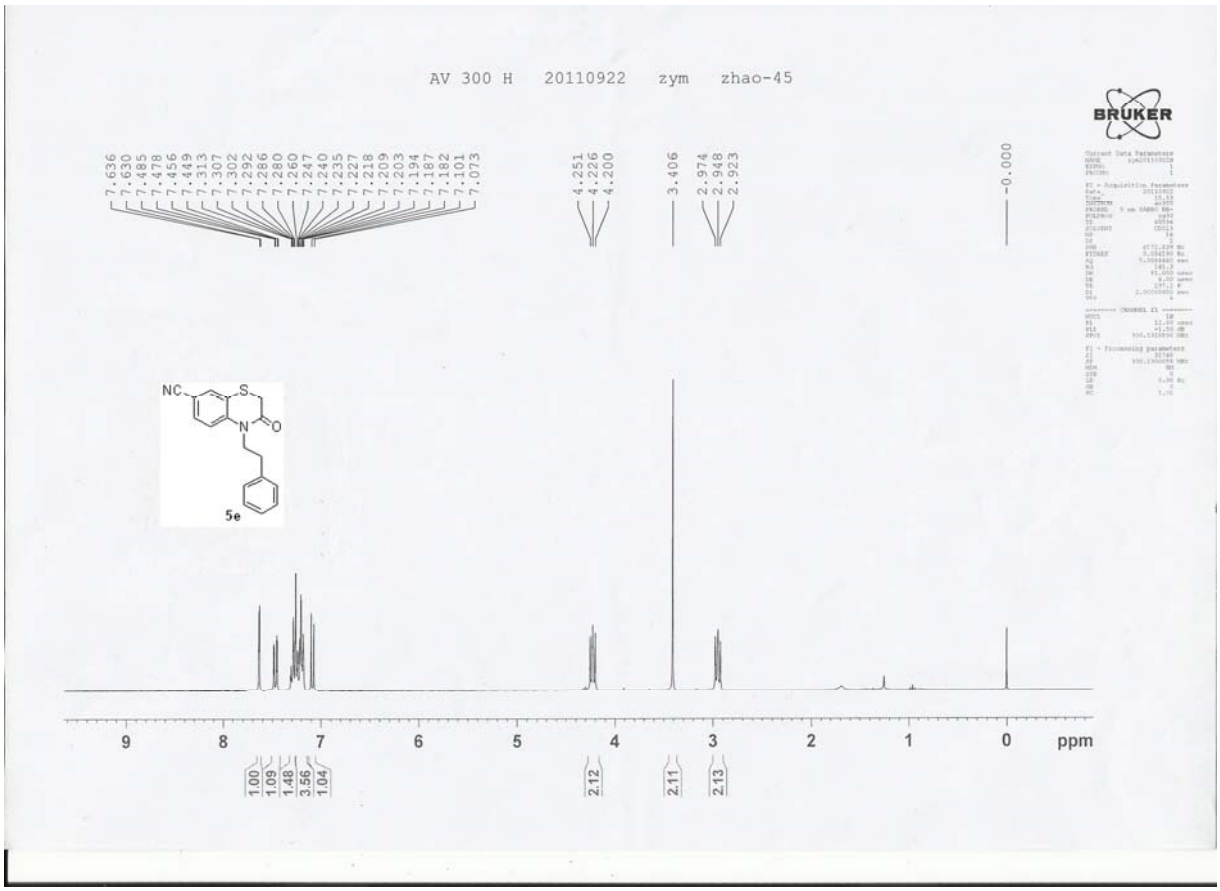
BRUKER
164.34
142.73
131.91
130.88
125.27
117.93
117.86
106.72
77.50
77.07
76.65
44.57
30.85
29.37
19.90
13.71
NC
O
N
S
5d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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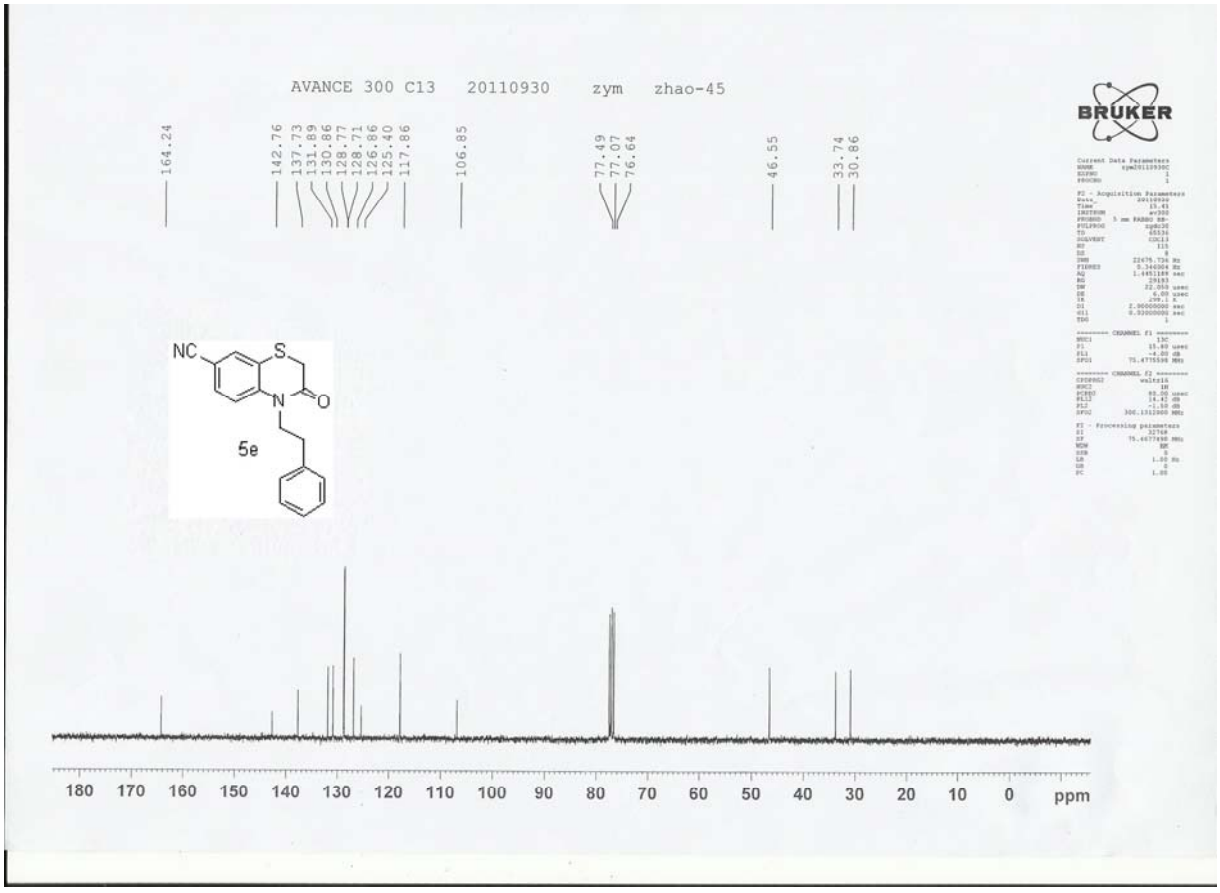
BRUKER
7.636
7.630
7.485
7.478
7.456
7.449
7.313
7.307
7.302
7.292
7.286
7.280
7.260
7.247
7.240
7.235
7.227
7.218
7.209
7.203
7.194
7.187
7.182
7.101
7.073
4.251
4.226
4.200
3.406
2.974
2.948
2.923
-0.000
NC
S
N
O
5e
9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.09
1.48
3.56
1.04
2.12
2.11
2.13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164.24
142.76
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128.77
128.71
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125.40
117.86
106.85
77.49
77.07
76.64
46.55
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30.86
NC
S
N
O
5e
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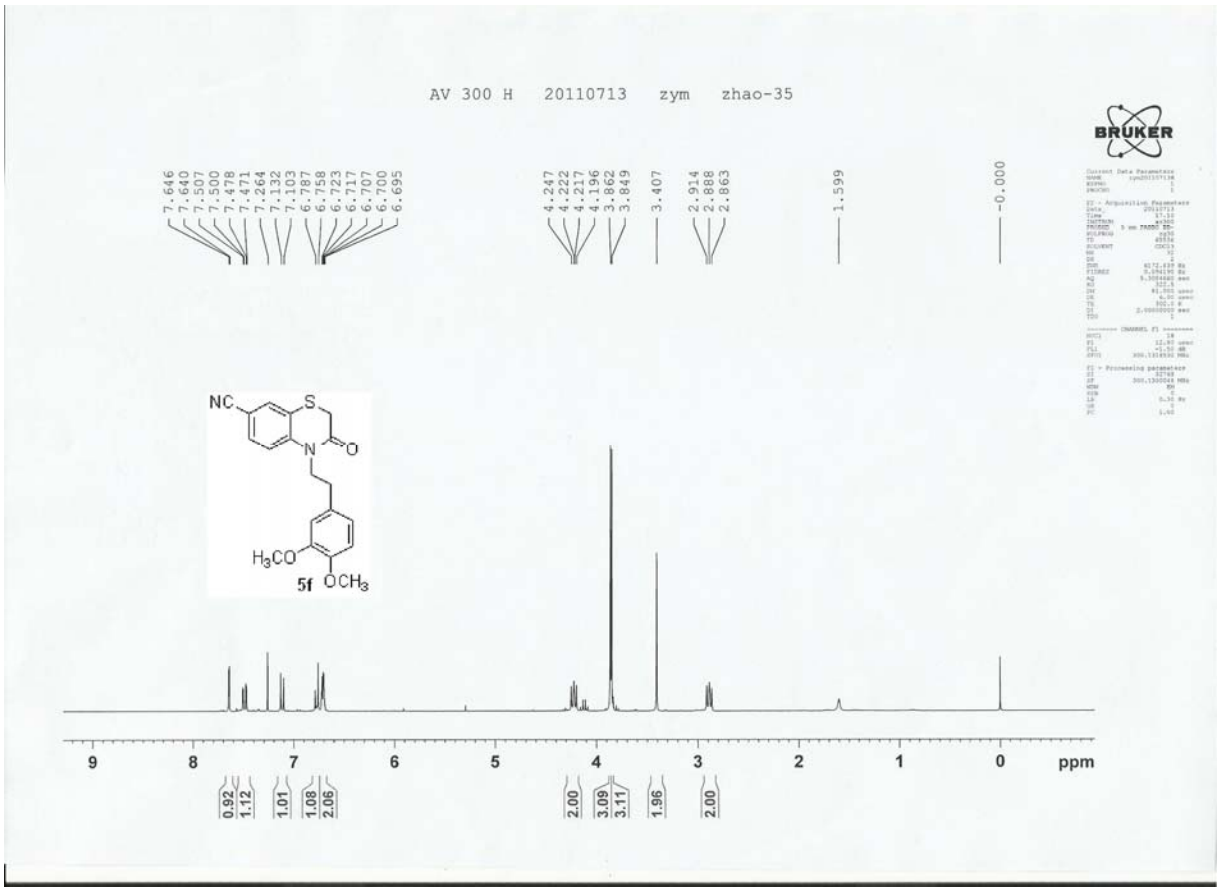
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BRUKER
7.646
7.640
7.507
7.500
7.478
7.471
7.264
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7.103
6.787
6.758
6.723
6.717
6.707
6.700
6.695
4.247
4.222
4.217
4.196
3.862
3.849
3.407
2.914
2.888
2.863
1.599
0.000
NC
S
N
O
H3CO
OCH3
5f
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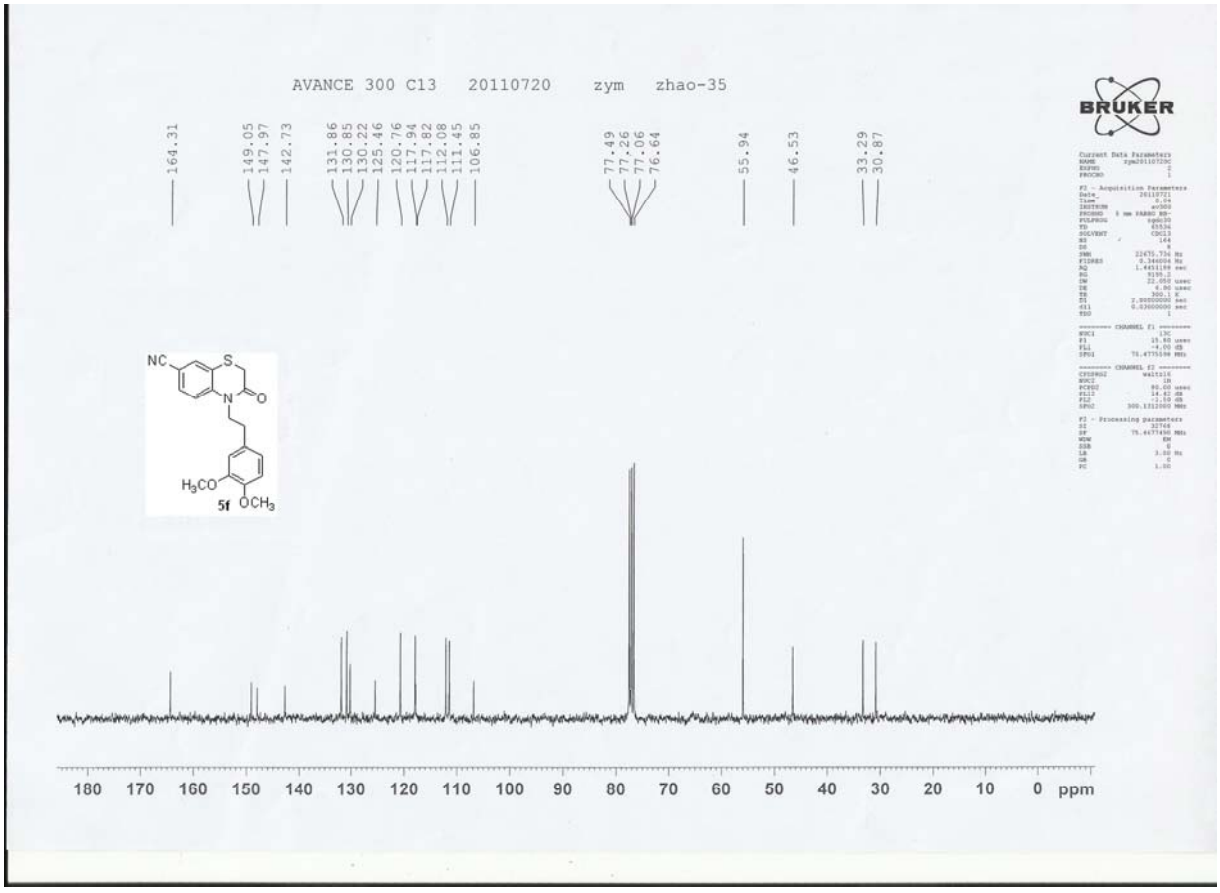
1.01
1.08
2.06
2.00
3.09
3.11
1.96
2.00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BRUKER
164.31
149.05
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142.73
131.86
130.85
130.22
125.46
120.76
117.94
117.82
112.08
111.45
106.85
77.49
77.26
77.06
76.64
55.94
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H3CO
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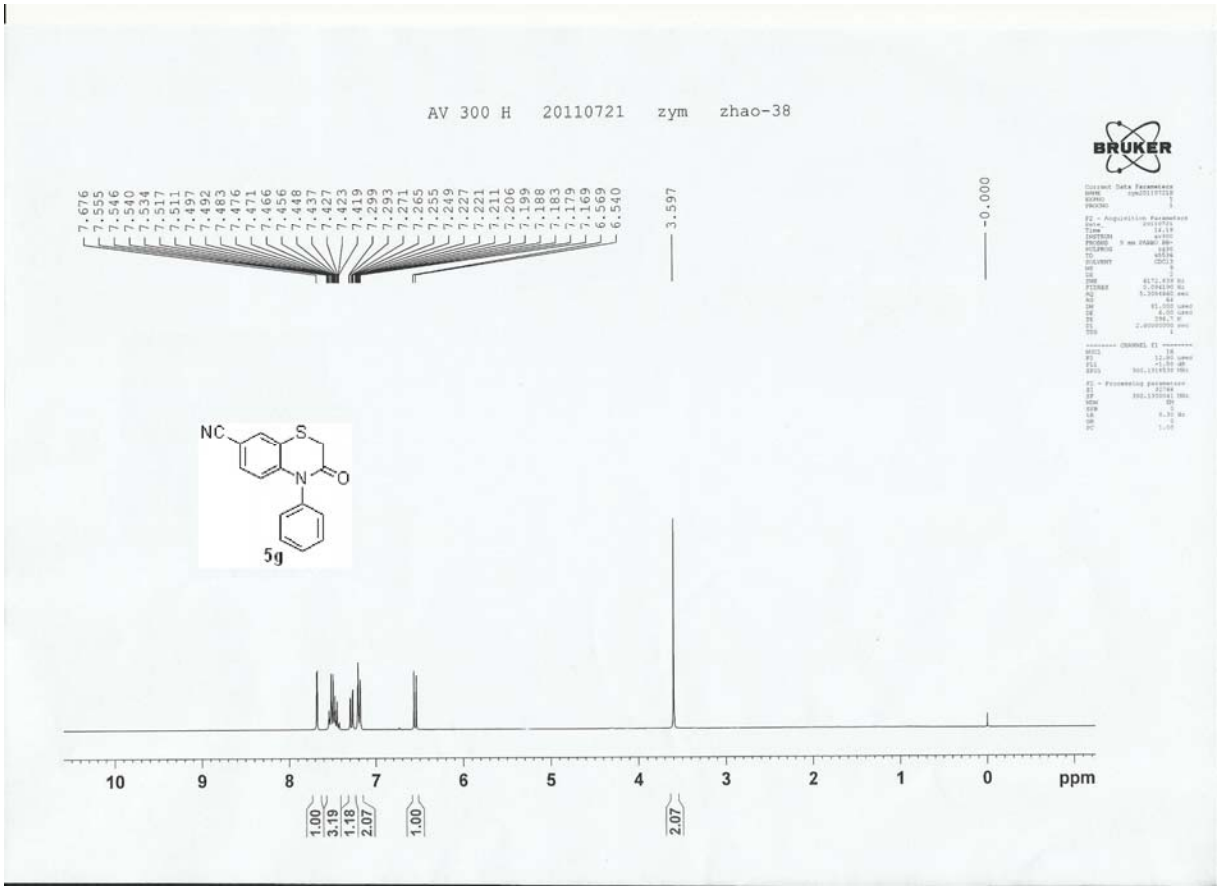
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BRUKER
7.676
7.555
7.546
7.540
7.534
7.517
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7.492
7.483
7.476
7.471
7.466
7.456
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7.255
7.249
7.227
7.221
7.211
7.206
7.199
7.188
7.183
7.179
7.169
6.569
6.540
3.597
-0.000
NC
S
N
O
5g
10 9 8 7 6 5 4 3 2 1 0 ppm
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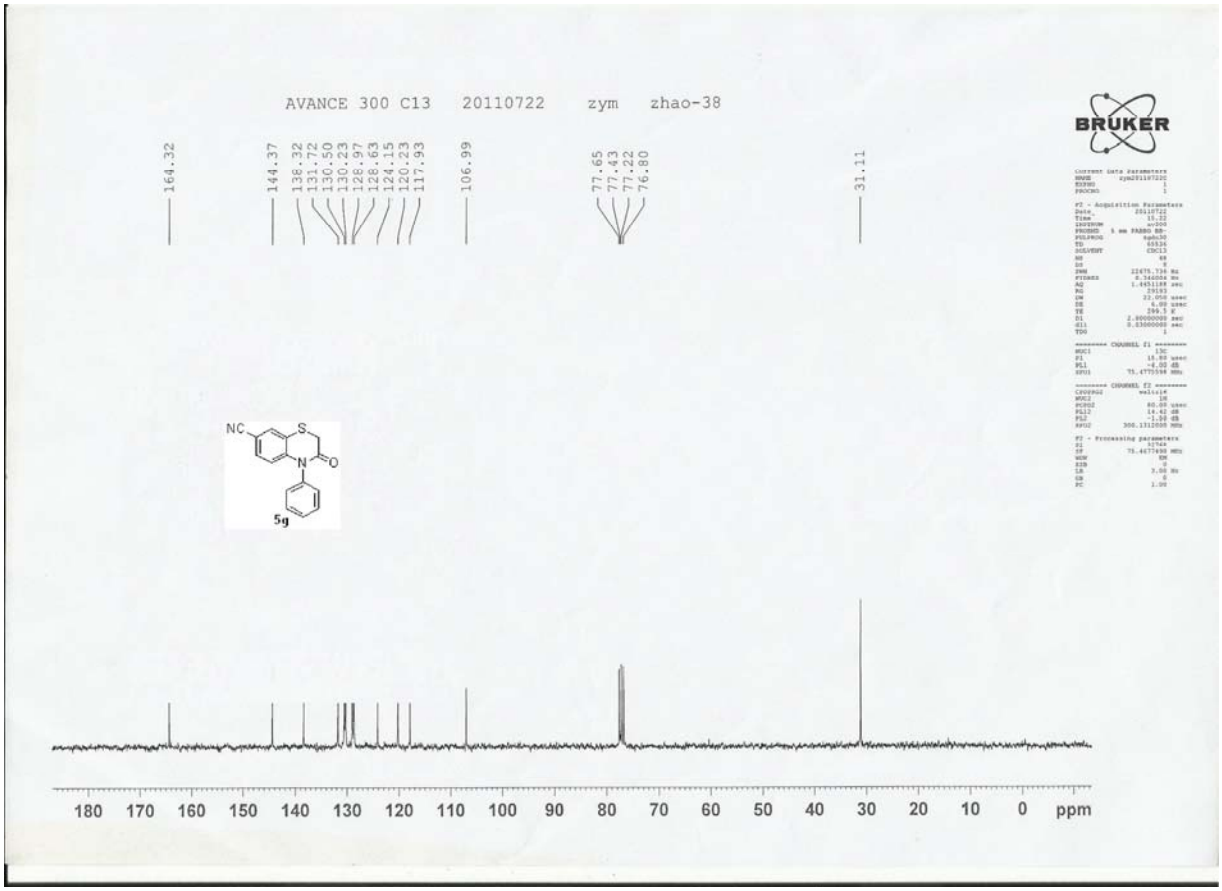
3.19
1.18
2.07
1.00
2.07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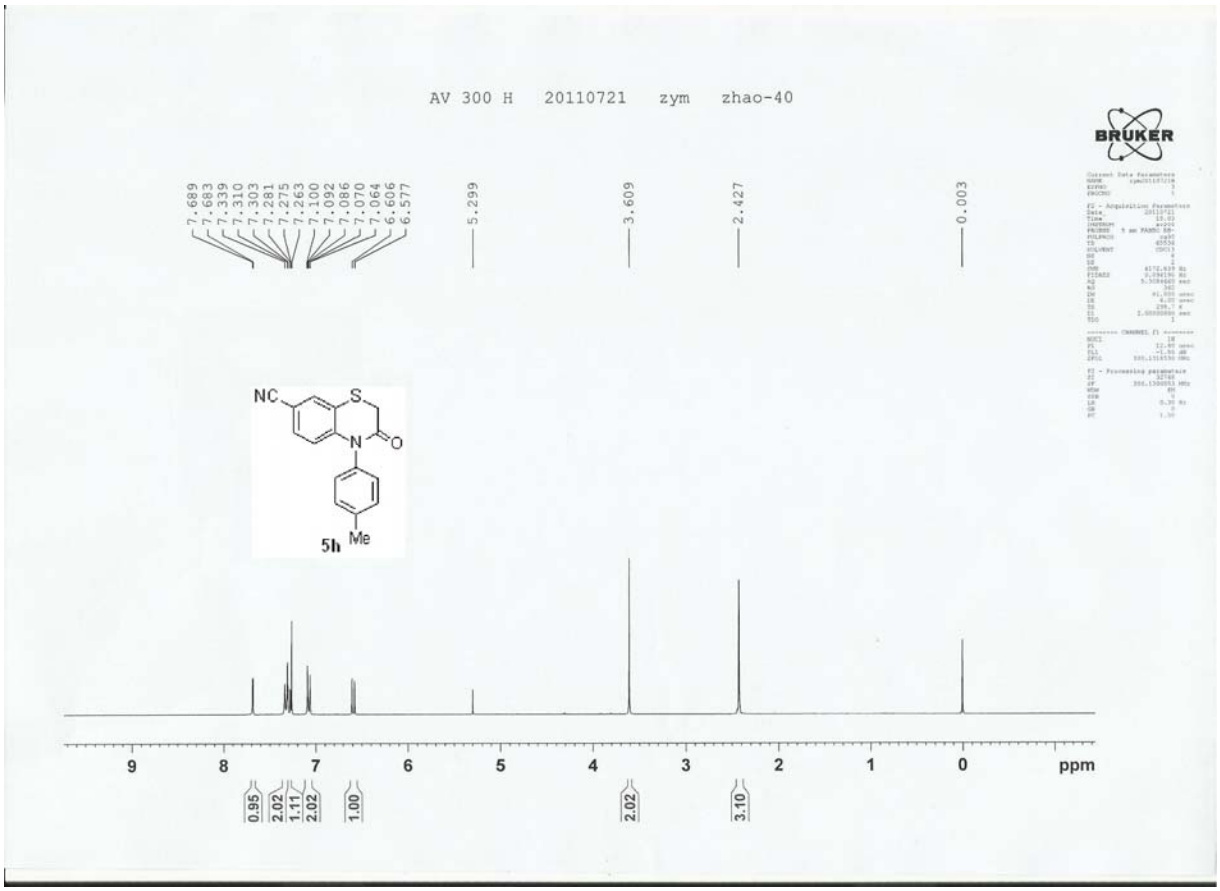
BRUKER
164.32
144.37
136.32
131.72
130.50
130.23
126.97
126.63
124.15
120.23
117.93
106.99
77.65
77.43
77.22
76.80
31.11
NC
S
N
O
5g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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BRUKER
7.689
7.683
7.339
7.310
7.303
7.281
7.275
7.263
7.100
7.092
7.086
7.070
7.064
6.606
6.577
5.299
3.609
2.427
0.003
NC
S
N
O
Me
5h
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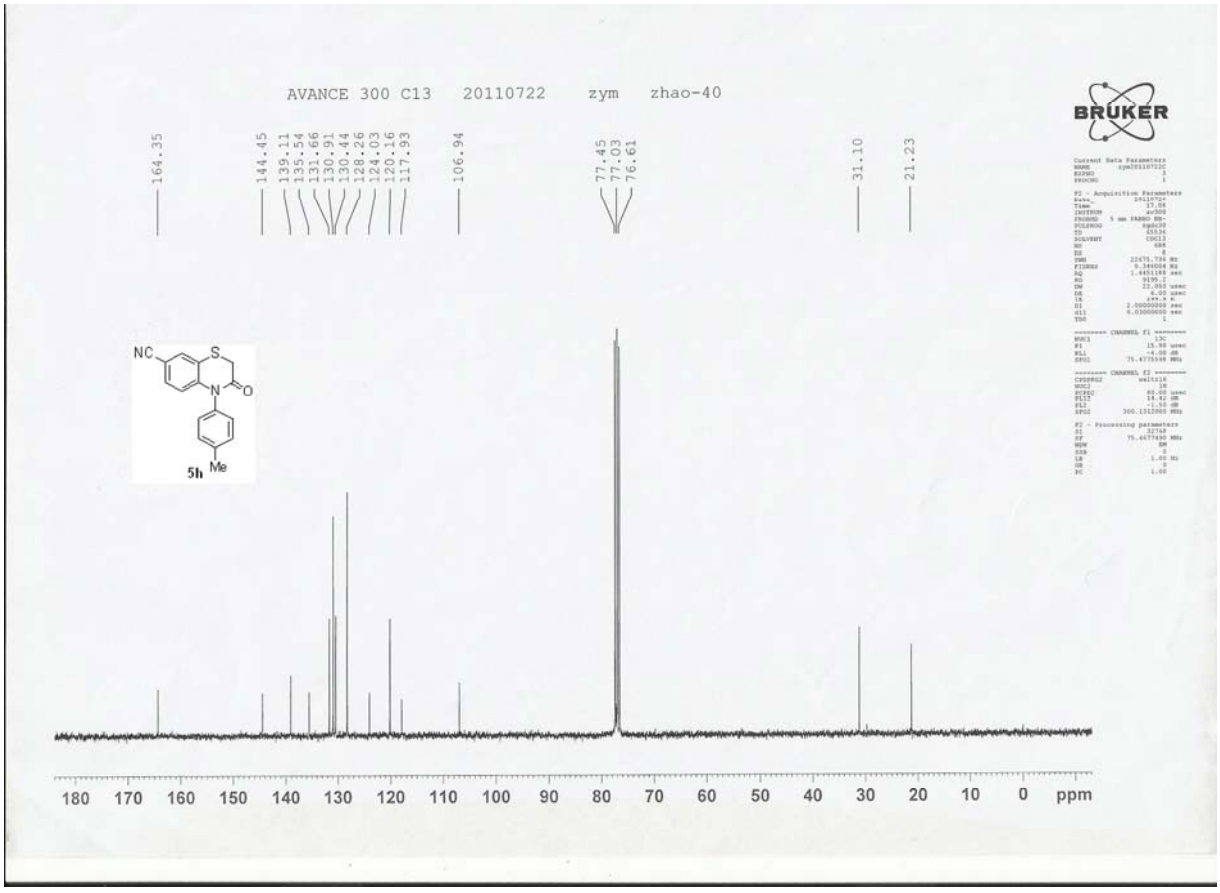
0.95
2.02
1.11
2.02
1.00
2.02
3.10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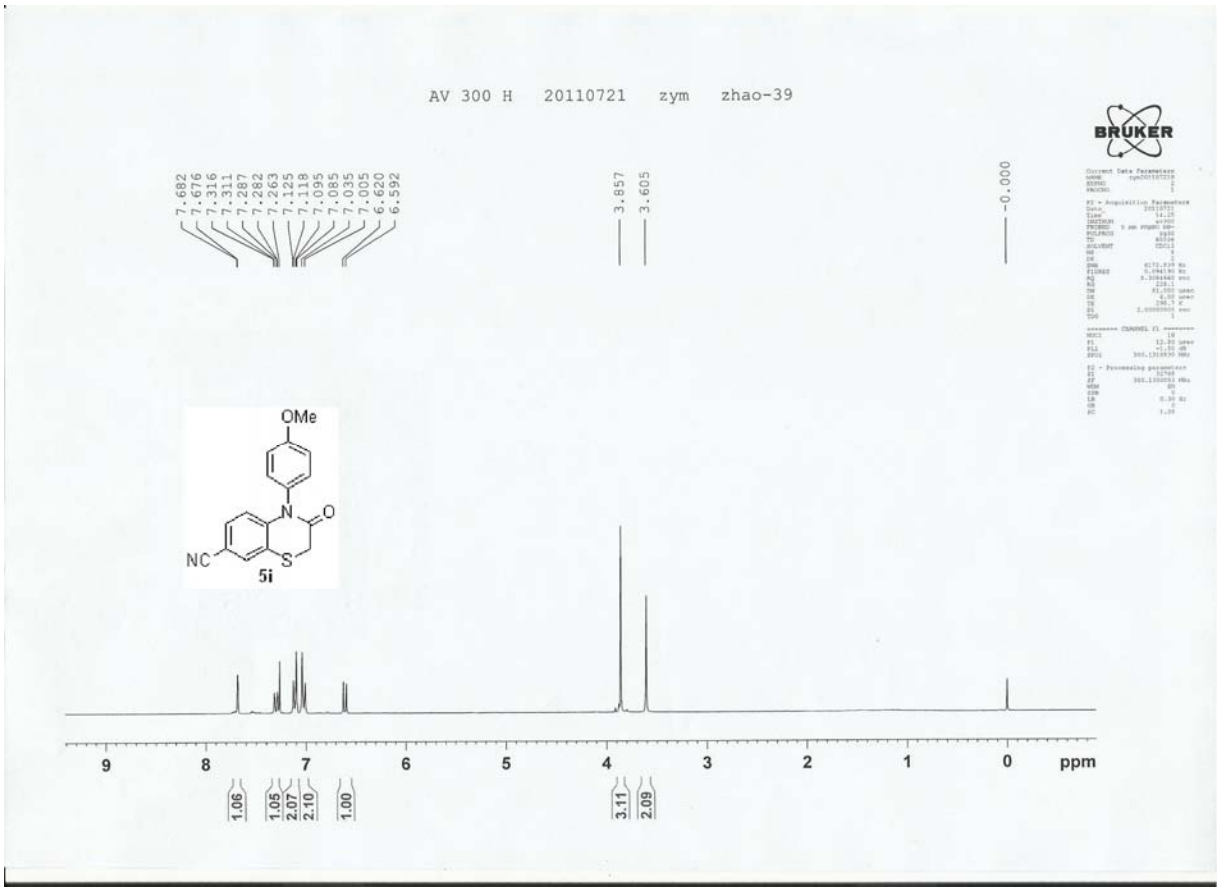
BRUKER
164.35
144.45
139.11
135.54
131.66
130.91
130.44
128.26
124.03
120.16
117.93
106.94
77.45
77.03
76.61
31.10
21.23
NC
S
N
O
Me
5h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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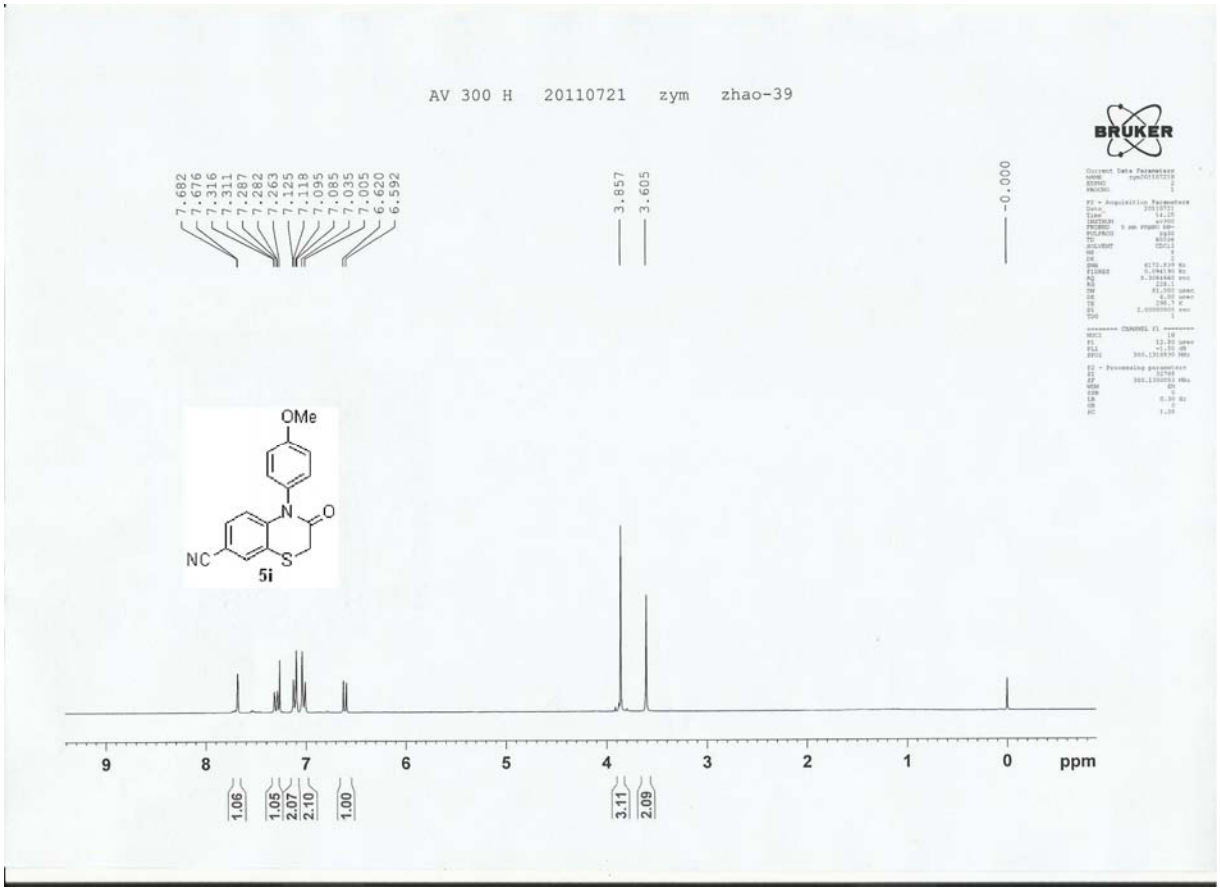
BRUKER
7.682
7.676
7.316
7.311
7.287
7.282
7.263
7.125
7.118
7.095
7.085
7.035
7.005
6.620
6.592
3.857
3.605
0.000
OMe
N
O
NC
S
5i
9 8 7 6 5 4 3 2 1 0 ppm
1.06
1.05
2.07
2.10
1.00
3.11
2.09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BRUKER
7.682
7.676
7.316
7.311
7.287
7.282
7.263
7.125
7.118
7.095
7.085
7.035
7.005
6.620
6.592
3.857
3.605
-0.000
OMe
N
O
NC
S
5i
9
8
7
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4
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2
1
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ppm
1.06
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2.07
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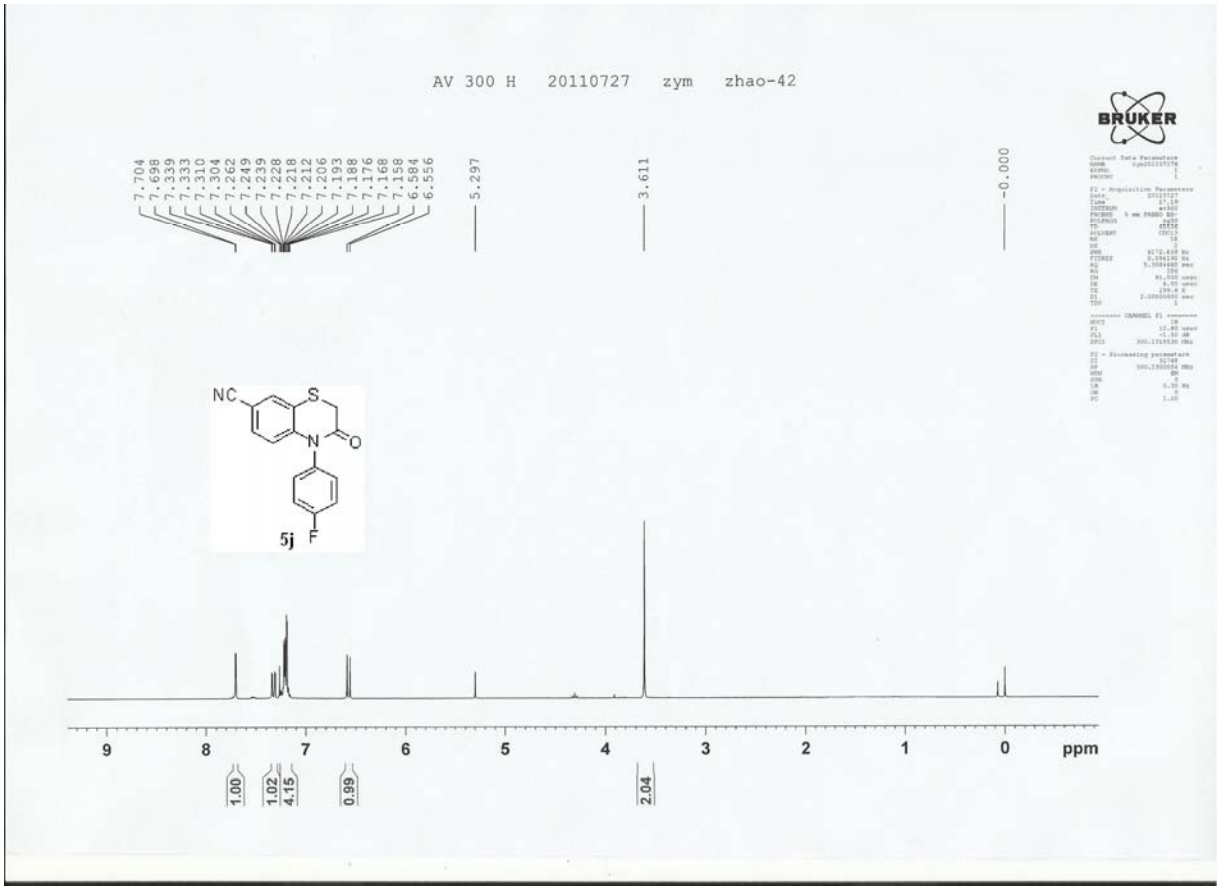
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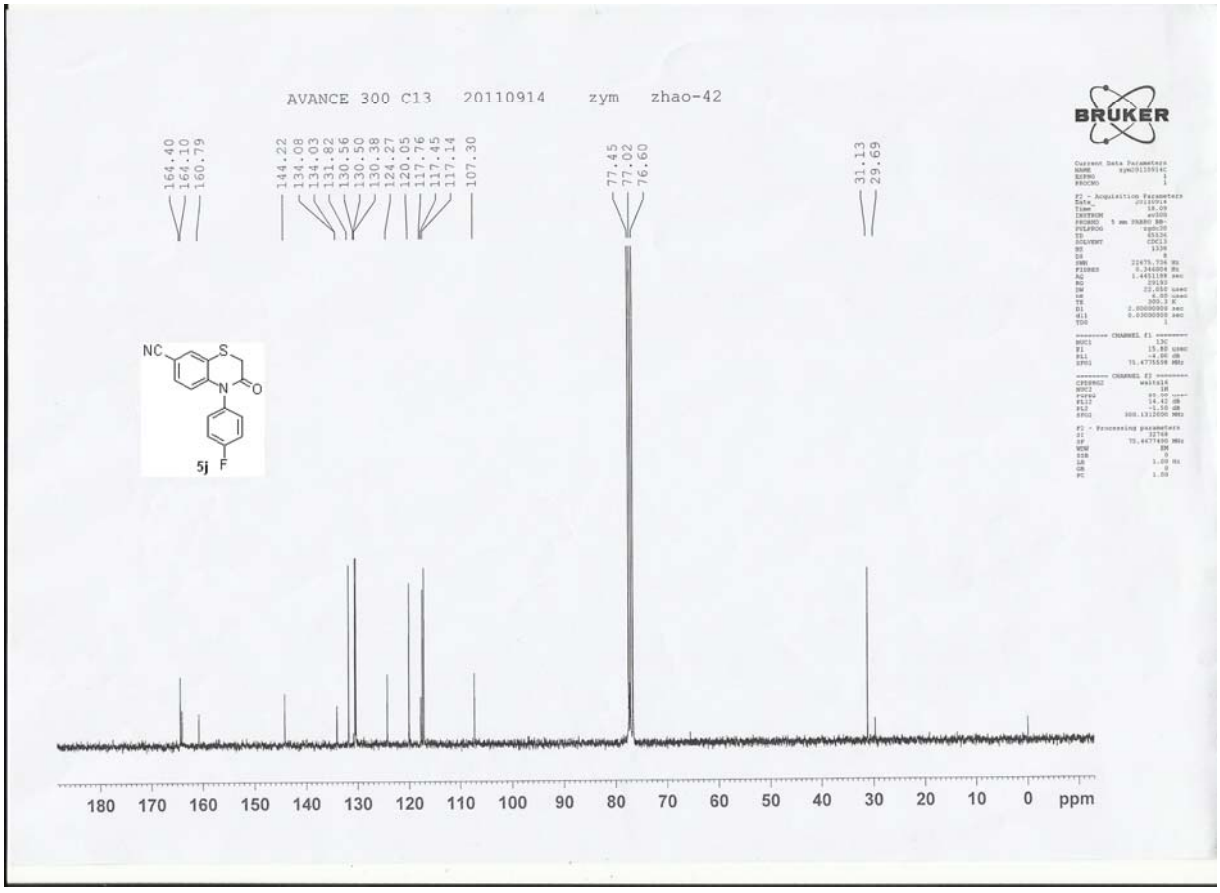
BRUKER
7.704
7.698
7.339
7.333
7.310
7.304
7.262
7.249
7.239
7.228
7.218
7.212
7.206
7.193
7.188
7.176
7.168
7.158
6.584
6.556
5.297
3.611
-0.000
NC
S
N
O
5j
F
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
4.15
0.99
2.04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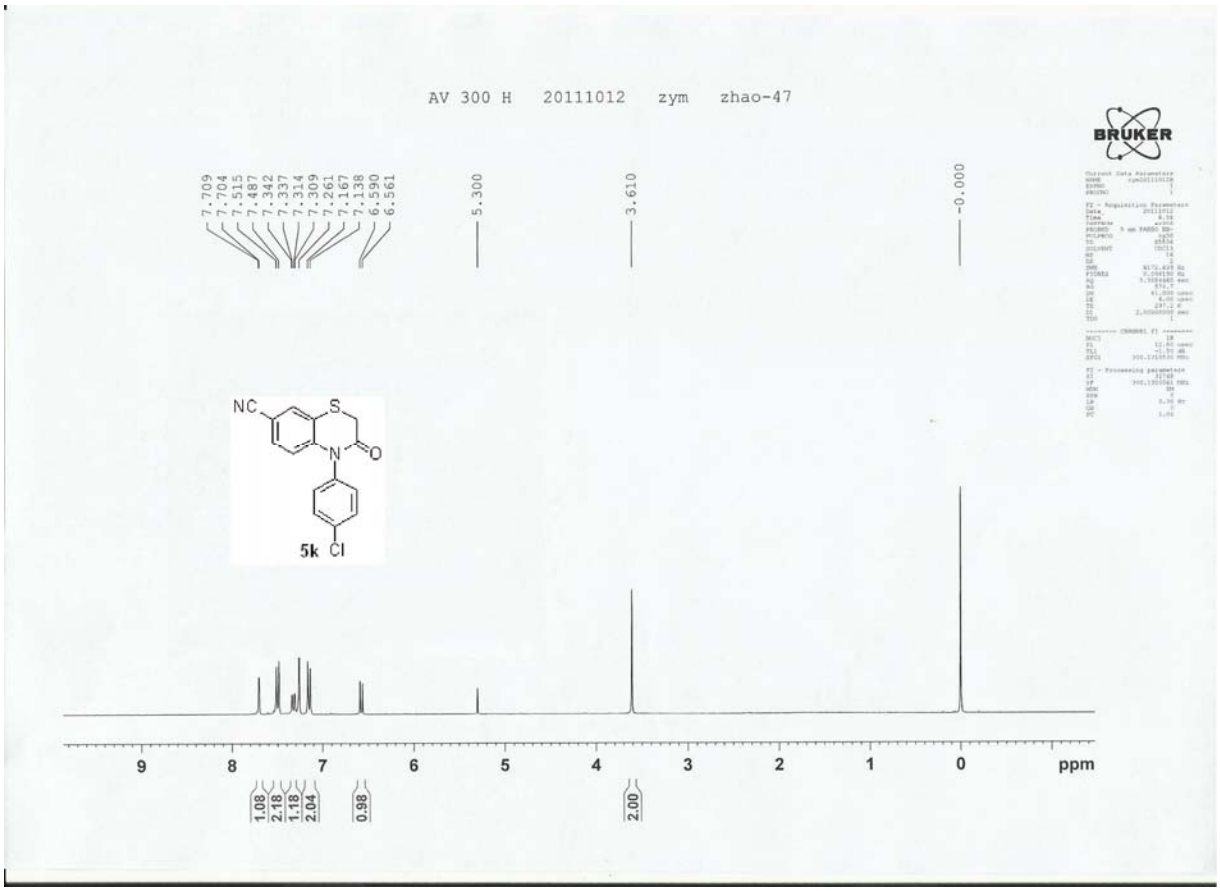
BRUKER
164.40
164.10
160.79
144.22
134.08
134.03
131.82
130.56
130.50
130.38
124.27
120.05
117.76
117.45
117.14
107.30
77.45
77.02
76.60
31.13
29.69
NC
S
N
O
5j F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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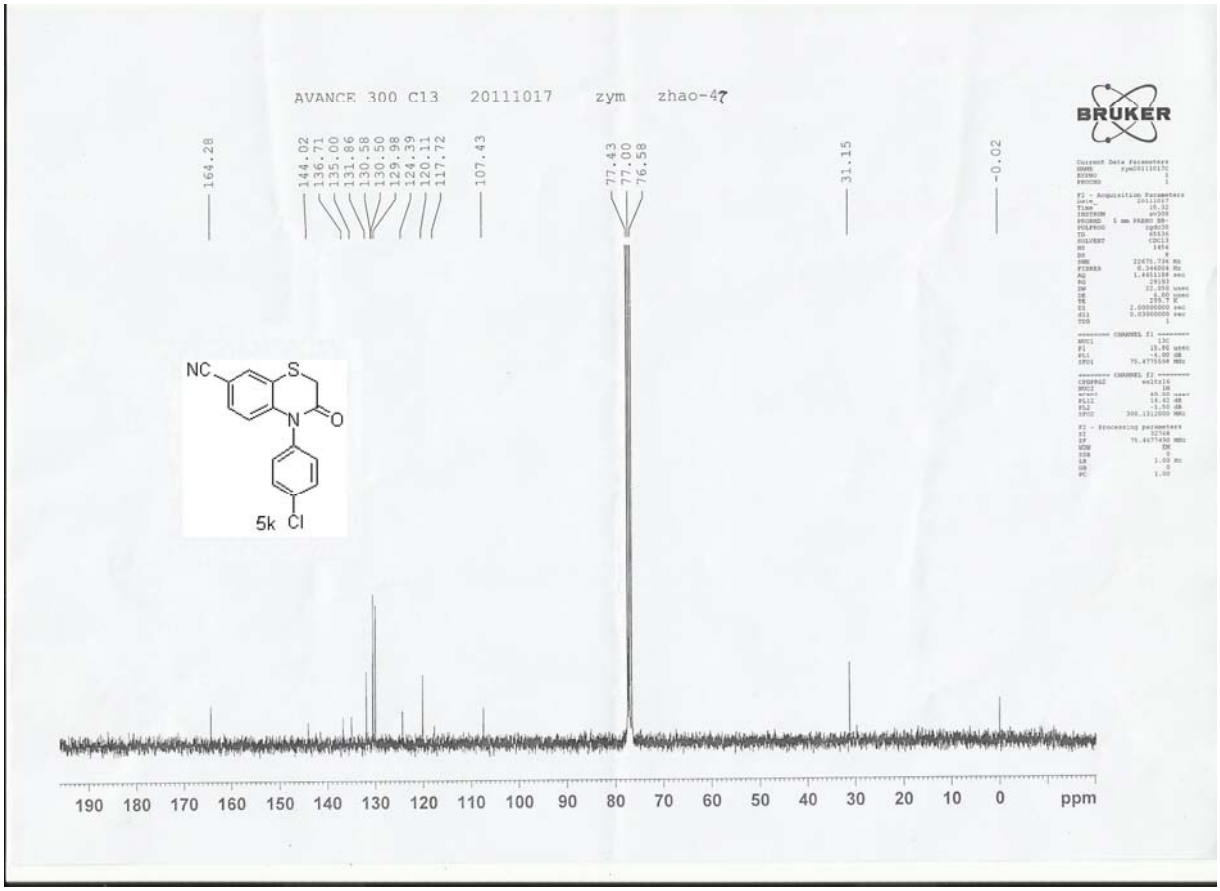
BRUKER
7.709
7.704
7.515
7.487
7.342
7.337
7.314
7.309
7.261
7.167
7.138
6.590
6.561
5.300
3.610
0.000
NC
S
N
O
5k Cl
9 8 7 6 5 4 3 2 1 0 ppm
1.08
2.18
1.18
2.04
0.98
2.00



2. X-ray structural data for product 5a

Crystal data

$C_{10}H_8N_2OS$
$M_r = 204.24$
Triclinic, P1
a = 8.3539 (13) Å
b = 9.2782 (14) Å
c = 13.883 (2) Å
α = 101.664 (2)°
β = 8.3539 (2)°
γ = 115.710 (2)°
$V = 942.9$ (2) $Å^3$

$F_{000} = 424$
$D_x = 1.539$ Mg m^{-3}
Mo Kα radiation
λ = 0.71073 Å
μ = 0.71073 Å
T = 273 K
0.01 × 0.01 × 0.01 mm
Z = 4

Data collection

Radiation source: fine-focus sealed tube
graphite
Absorption correction: multi-scan
SADABS

2522 reflections with $I > 2\sigma(I)$
Rint = 0.021
$\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$
h = -9→9

T_{min} = 0.997, T_{max} = 0.998
6606 measured reflections
3273 independent reflection

k = -11→11
l = -16→16

Refinement

Refinement on F^2

Least-suares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

S = 1.02
3273 reflections

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2 (F_o^2) + (0.0581P)^2 + 0.180P]$
where $P = (Fo^2 + 2Fc^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

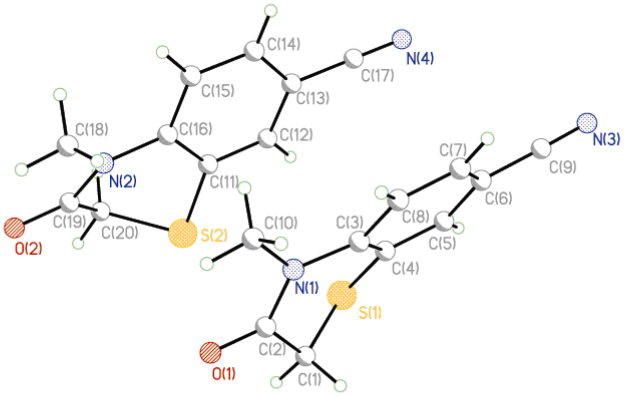


Figure 1.. X-ray structure of compound **5a**

3. Cartesian Coordinates and Absolute Energies for all optimized structures shown in Figure 2:

R:

C	-1.56899200	1.32741700	0.33128500
C	-0.37892200	0.61363100	0.36345100
C	-0.36363800	-0.76952300	0.09956500
C	-1.59307300	-1.36734500	-0.21971200
C	-2.78574900	-0.68096800	-0.26152500
C	-2.78453200	0.69534700	0.02314300
H	-1.55626200	2.39185600	0.53339600
H	-3.69891400	-1.20835000	-0.50576600
C	-4.00656800	1.42984000	-0.00842700
N	-5.00120500	2.02314400	-0.03190200
S	1.07405700	-1.78780800	0.14090000
C	2.33799500	-0.72238700	0.96854000
H	3.06656200	-1.46177200	1.30824400
H	1.86456800	-0.25413700	1.83216200
C	3.05645200	0.30014200	0.06077900
O	3.91678300	-0.14926400	-0.73891200
N	2.66381900	1.54035100	0.28079100
C	3.34853200	2.52927900	-0.53454100
H	4.43952100	2.52434500	-0.37841200
H	3.20028100	2.36556000	-1.61454000
H	2.97341100	3.52893100	-0.28532100
F	-1.62015400	-2.69976600	-0.49466000
H	0.56572300	1.13343600	0.54149500

Sum of electronic and zero-point Energies=-1068.735519

R':

C	1.93140100	0.01788300	1.07826200
C	0.68731000	-0.54683700	0.89470400
C	0.21526200	-0.97174900	-0.35428800
C	1.09673900	-0.82339800	-1.43776500
C	2.36150700	-0.27761500	-1.28650700
C	2.79147000	0.15760900	-0.02359300
H	2.22999500	0.33536900	2.06905700
H	0.75136000	-1.12092000	-2.42003200
H	3.01369200	-0.16480100	-2.14391800
C	4.08957000	0.72356500	0.14519200

N	5.14832700	1.17437100	0.27780900
S	-1.31328200	-1.80896500	-0.62655000
C	-2.59246900	-0.88827500	0.34225000
H	-2.43801500	-1.06787800	1.40593200
H	-3.51397300	-1.39653900	0.04672300
C	-2.76206200	0.62967900	0.09676300
O	-3.82165600	1.08731100	0.61087400
N	-1.79926000	1.22675700	-0.55643200
C	-1.98705700	2.65874800	-0.70936600
H	-2.91446500	2.90983200	-1.25045800
H	-2.05182600	3.18568500	0.25712400
H	-1.14337900	3.07920900	-1.26948200
F	-0.08679000	-0.71117200	1.99103300

Sum of electronic and zero-point Energies=-1068.726114

TS1:

C	1.84996100	-0.19789300	1.07678400
C	0.53473700	-0.52759300	0.90381400
C	-0.11720100	-0.60063800	-0.36057300
C	0.76217400	-0.45747200	-1.47431400
C	2.09663200	-0.12703900	-1.32789900
C	2.67579000	0.01859400	-0.05380800
H	2.24987800	-0.12774100	2.08114900
H	0.33895600	-0.57922200	-2.46358800
H	2.71493500	0.00358900	-2.20918900
C	4.04722500	0.34172400	0.09882200
N	5.17206500	0.60607000	0.22137800
S	-1.52218400	-1.73734800	-0.59414900
C	-2.88506500	-0.75471400	0.14157600
H	-3.02339100	-1.01936700	1.19170900
H	-3.79580800	-1.00516000	-0.40496800
C	-2.62884800	0.75967100	0.04720100
O	-3.55457700	1.53166500	0.37563600
N	-1.40858300	1.04339400	-0.35672400
C	-0.94139100	2.40561600	-0.35593300
H	-1.52109500	3.03384700	-1.04686000
H	-1.00802800	2.87422800	0.63667400
H	0.10560000	2.42199600	-0.67930700
F	-0.21977200	-0.75174600	2.01878600

Sum of electronic and zero-point Energies=-1068.718906

IM1:

C	1.87771700	0.04782800	1.07508800
C	0.52378500	0.06059800	0.96852800
C	-0.22748300	-0.04810600	-0.27089800
C	0.65022500	0.06330400	-1.43227100
C	2.01859200	0.05039200	-1.34058000
C	2.69032600	0.02653800	-0.09291900
H	2.32570000	0.06549500	2.06196500
H	0.16853500	0.07616700	-2.40343200
H	2.60833500	0.07767900	-2.25121500
C	4.09719600	0.03136300	-0.00687200
N	5.26049800	0.03573400	0.06238200
S	-1.23815000	-1.93196600	-0.33715000
C	-2.80930000	-1.14368100	0.10954500
H	-3.08034100	-1.32734500	1.15338000
H	-3.63299500	-1.48702400	-0.51935300
C	-2.69391000	0.36131400	-0.07056500
O	-3.68025400	1.09145300	0.00933900
N	-1.43403700	0.80839700	-0.32463600
C	-1.19837500	2.24574700	-0.39464500
H	-2.15778800	2.73632500	-0.54995900
H	-0.75020200	2.61379600	0.53502500
H	-0.51585300	2.46764800	-1.21693500
F	-0.23009100	0.09737700	2.11994700

Sum of electronic and zero-point Energies=-1068.734301

TS2:

C	1.73691800	-0.69965200	0.54910500
C	0.32675200	-0.53178000	0.51272700
C	-0.16953200	0.73169300	0.04652100
C	0.70250100	1.64352000	-0.53087600
C	2.08059100	1.41973200	-0.60446700
C	2.58582500	0.23516600	-0.04248100
H	2.12978100	-1.60077600	1.00062000
H	0.29990100	2.55535500	-0.95631600
H	2.74162500	2.14341700	-1.06137900
C	3.99817400	0.00765500	-0.03557400
N	5.14387700	-0.16508900	-0.03232400
S	-0.72688100	-1.97892500	-0.87537900
C	-2.32234900	-1.40213400	-0.19948700

H	-2.45918200	-1.80757800	0.80800300
H	-3.13417900	-1.78782600	-0.81674600
C	-2.59249700	0.09129400	-0.07912000
O	-3.76251500	0.48026400	-0.09643500
N	-1.56882400	1.00252700	0.09892400
C	-1.97917500	2.39797700	0.26529700
H	-2.93940800	2.42049700	0.77666400
H	-1.22299200	2.91782600	0.85336700
H	-2.10118600	2.90779100	-0.69754700
F	-0.31252900	-1.01676800	1.67942300

Sum of electronic and zero-point Energies=-1068.720420

TS3:

C	-1.54728500	0.55169200	0.66576200
C	-0.24149700	0.01782300	0.78333900
C	0.01434800	-1.25614700	0.19635700
C	-0.94280100	-1.84860900	-0.61510100
C	-2.20218700	-1.27864100	-0.81193100
C	-2.49058100	-0.07212700	-0.15247200
H	-1.79829100	1.44756500	1.21764400
H	-0.69004300	-2.78186500	-1.10662100
H	-2.94494000	-1.75553100	-1.43761200
C	-3.79489900	0.50437500	-0.28354700
N	-4.85271200	0.96224000	-0.39442600
S	1.65362900	-1.92054000	0.36020500
C	2.31867300	0.81905100	-0.53127000
O	3.28272700	1.55497900	-0.83575900
N	1.09762600	1.20769700	-0.19723000
C	0.86058100	2.62924200	-0.09865200
H	1.18146100	3.15548400	-1.00589300
H	-0.21375300	2.80214600	0.03545400
H	1.39263000	3.08969100	0.74693400
F	0.36135100	0.30191300	1.99557700
C	2.58114100	-0.69276600	-0.68131600
H	2.42235800	-0.95697700	-1.73032000
H	3.63117800	-0.86185000	-0.44241200

Sum of electronic and zero-point Energies=-1068.710382

P1:

C	1.76687400	-0.80785500	-0.39799500

C	0.41730400	-0.49828800	-0.48940400
C	-0.05135400	0.78865400	-0.10220700
C	0.89776200	1.70741700	0.39095200
C	2.24949300	1.39915400	0.45885200
C	2.70398600	0.13840200	0.05387400
H	2.10008900	-1.79657600	-0.68949700
H	0.57589100	2.68509300	0.72009700
H	2.95366800	2.13333000	0.83160800
C	4.09184000	-0.18167400	0.10856900
N	5.22256000	-0.43285600	0.14955200
S	-0.72781200	-1.65248400	-1.17194300
C	-2.16458600	-1.17639100	-0.16367300
H	-1.88095500	-1.59974900	1.38656500
H	-3.00713600	-1.81869400	-0.40274700
C	-2.49843300	0.21028700	-0.18539900
O	-3.62586500	0.68864300	-0.04413300
N	-1.38459900	1.15277700	-0.26419200
C	-1.74132200	2.55781300	-0.12490000
H	-2.77894400	2.66294300	-0.42935700
H	-1.65844800	2.91080800	0.91200500
H	-1.09679000	3.17061300	-0.76088700
F	-1.71673200	-1.92019200	2.33853900

Sum of electronic and zero-point Energies=-1068.761435

P2:

C	1.27382300	0.41937900	0.00871600
C	-0.07187800	0.02337100	-0.09263300
C	-0.38788700	-1.35097600	-0.13133800
C	0.62472500	-2.31472500	-0.13251800
C	1.95403100	-1.93278200	-0.09554700
C	2.26914700	-0.56555500	-0.00756300
H	1.54885200	1.50823300	0.14843800
H	0.35621400	-3.36489400	-0.15385600
H	2.74289300	-2.67544000	-0.10710300
C	3.65758800	-0.21208100	0.07367800
N	4.79685100	-0.01988100	0.12671700
S	-2.08297600	-1.88567500	-0.16000600
C	-2.38469100	0.82874200	0.17848800
O	-3.27316100	1.66083700	0.03056400
N	-1.08590200	1.01703800	-0.21304800
C	-0.72246500	2.30908000	-0.83870400
H	-0.42864600	2.12211000	-1.87672400

H	-1.60976100	2.93534000	-0.82049000
H	0.11784400	2.78133700	-0.30091300
F	1.75432500	3.05516400	0.48676200
C	-2.70217300	-0.49802400	0.85061500
H	-2.25761500	-0.55533700	1.84769800
H	-3.78376200	-0.58239400	0.92282400

Sum of electronic and zero-point Energies=-1068.758240