# Discovery of a novel and potent class of *F. tularensis* enoyl-reductase (FabI) inhibitors by molecular shape and electrostatic matching

## Supporting Information

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# Tables in Supporting Information

# 1. ROCS/EON Validation Results: Diphenyl Class

**Table S1. Diphenyl class validation: ROCS (Shape-only)/EON query combinations**

| EON(#n)+ ROCS | EF 1% | EON(#n)+ ROCS | EF 1% |
|---|---|---|---|
| #1+B EON_input | 46.45 | **#1+C EON_input** | **46.45** |
| #2+B EON_input | 46.45 | #2+C EON_input | 46.45 |
| #3+B EON_input | 46.45 | #3+C EON_input | 46.45 |
| #4+B EON_input | 46.45 | #4+C EON_input | 46.45 |
| #5+B EON_input | 46.45 | #5+C EON_input | 46.45 |

Left: Diphenyl class ROCS (B) #1 +#2 (Shape-only) query combines with EON queries (#n / n=1~5)

Right: Diphenyl class ROCS (C) #1 +#2+#3 (Shape-only) query combines with EON queries (#n / n=1~5)

All the ROCS (Shape-only) /EON query combination listed in table 1 show perfect results. Therefore, we eventually choose "#1+C EON_input" combination, the bold one in the right side of table 1, for the following ASDI production run, because ROCS (C) #1 +#2+#3 (Shape-only) query contains a larger shape than ROCS (B) #1 +#2 (Shape-only) query and #1 EON query contains the highest activity among all the other EON queries.

**Table S2. Diphenyl class validation: ROCS plus pharmacophore features without EON refinement**

| Diphenyl ROCS plus pharmacophore feature query | AUC | EF1% |
|---|---|---|
| Diphenyl_ROCS_pharmacophore_1 | 1 | 46.45 |
| Diphenyl_ROCS_pharmacophore_1+2 | 1 | 46.45 |
| Diphenyl_ROCS_pharmacophore_1+2+3 | 1 | 46.45 |
| Diphenyl_ROCS_pharmacophore_1+2+3+4 | 1 | 46.45 |
| Diphenyl_ROCS_pharmacophore_1+2+3+4+5 | 1 | 46.45 |

## 2. ROCS/EON Validation Results: Indole Class

**Table S3. Indole class validation: ROCS (Shape-only)/EON query combinations**

| EON(#n)+ ROCS | EF 1% | EON(#n)+ ROCS | EF 1% |
|---|---|---|---|
| #1+C EON_input | 0 | **#1+D EON_input** | **51** |
| #2+C EON_input | 0 | #2+D EON_input | 51 |
| #3+C EON_input | 0 | #3+D EON_input | 51 |
| #4+C EON_input | 0 | #4+D EON_input | 51 |
| #5+C EON_input | 0 | #5+D EON_input | 51 |

Left: Indole class ROCS (C) #1 +#2+#3 (Shape-only) query combines with EON queries (#n / n=1~5).

Right: Indole class ROCS (D) #1 +#2+#3 +#4 (Shape-only) query combines with EON queries (#n / n=1~5) .

All the ROCS (Shape-only) /EON query combination listed in the right part of table 3 show perfect results. Therefore, we eventually choose "#1+D EON_input" combination, the bold one in the right side of table 1, for the following ASDI production run, because #1 EON query contains the highest activity among all the other EON queries.

**Table S4. Indole class validation: ROCS plus pharmacophore features without EON refinement**

| Indole ROCS plus pharmacophore feature query | AUC | EF1% |
|---|---|---|
| Indole_ROCS_pharmacophore_1 | 0.994 | 51 |
| Indole_ROCS_pharmacophore_1+2 | 0.994 | 51 |
| Indole_ROCS_pharmacophore_1+2+3 | 0.994 | 51 |
| Indole_ROCS_pharmacophore_1+2+3+4 | 1 | 51 |
| Indole_ROCS_pharmacophore_1+2+3+4+5 | * | * |

* "Indole_ROCS_pharmacophore_1+2+3+4+5"query is the same as "Indole_ROCS_pharmacophore_1+2+3+4"query, so we did not perform Indole_ROCS_pharmacophore_1+2+3+4+5 validation run.

## 3. ROCS/EON Validation Results: Amide Class

**Table S5. Amide class validation: ROCS (Shape-only)/EON query combinations**

| EON(#n)+ ROCS | EF 1% | EON(#n)+ ROCS | EF 1% |
|---|---|---|---|
| #1+C EON_input | 14.67 | #1+D EON_input | 11 |
| **#2+C EON_input** | **18.33** | #2+D EON_input | 11 |
| #3+C EON_input | 14.67 | #3+D EON_input | 14.67 |
| #4+C EON_input | 11 | #4+D EON_input | 11 |
| #5+C EON_input | 18.33 | #5+D EON_input | 11 |

Left: Amide class ROCS (C) #1 +#2+#3 (Shape-only) query combines with EON queries (#n / n=1~5)

Right: Amide class ROCS (D) #1 +#2+#3 +#4 (Shape-only) query combines with EON queries (#n / n=1~5)

Both #2+C and #5+C in the left side of table 4 are the best ROCS (Shape-only) /EON query combinations for the amide class. Therefore, we eventually choose "#2+C EON_input" combination for the following ASDI production run because #2 amide EON query contains a higher activity than #5 amide EON query.

**Table S6. Amide class validation: ROCS plus pharmacophore features without EON refinement**

| Amide ROCS plus pharmacophore feature query | AUC | EF1% |
|---|---|---|
| Amide_ROCS_pharmacophore_1 | 0.987 | 22 |
| Amide_ROCS_pharmacophore_1+2 | 0.985 | 22 |
| Amide_ROCS_pharmacophore_1+2+3 | 0.992 | 22 |
| Amide_ROCS_pharmacophore_1+2+3+4 | 0.992 | 22 |
| Amide_ROCS_pharmacophore_1+2+3+4+5 | 0.943 | 22 |

## 4. ROCS/EON Validation Results: Imidazole Class

**Table S7. Imidazole class validation: ROCS (Shape-only)/EON query combinations**

| EON(#n)+ ROCS | EF 1% | EON(#n)+ ROCS | EF 1% |
|---|---|---|---|
| #1+A EON_input | 47.82 | #1+B EON_input | 11.96 |
| #2+A EON_input | 47.82 | #2+B EON_input | 11.96 |
| #3+A EON_input | 47.82 | #3+B EON_input | 11.96 |
| #4+A EON_input | 59.78 | #4+B EON_input | 11.96 |
| **#5+A EON_input** | **59.78** | #5+B EON_input | 11.96 |

Left: Imidazole class ROCS (A) #1 (Shape-only) query combines with EON queries (#n / n=1~5)

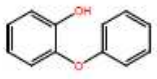
Right: Imidazole class ROCS (B) #1 +#2 (Shape-only) query combines with EON queries (#n / n=1~5)

Both #4+A and #5+A in the left side of table 4 are the best ROCS (Shape-only) /EON query combinations for the imidazole class. However, #5+A shows a better performance in the enrichment factor at 2% (data not shown) and the activity of imidazole #4 and #5 EON query is not significantly different ($IC_{50}$ to *E.coli* are 1.2μM and 1.9μM respectively). Therefore, we eventually choose "#5+A EON_input" combination for the following ASDI production run.

**Table S8. Imidazole class validation: ROCS (Shape-only)/EON query combinations**

| Imidazole ROCS plus pharmacophore feature query | AUC | EF 1% |
|---|---|---|
| Imidazole_ROCS_pharmacophore_1 | 1 | 59.78 |
| Imidazole_ROCS_pharmacophore_1+2 | * | * |
| Imidazole_ROCS_pharmacophore_1+2+3 | * | * |
| Imidazole_ROCS_pharmacophore_1+2+3+4 | * | * |
| Imidazole_ROCS_pharmacophore_1+2+3+4+5 | 0.379 | 0 |

## 5. Diphenyl Actives



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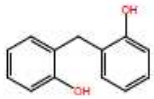

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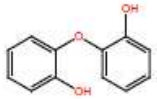

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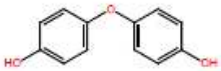

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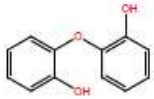

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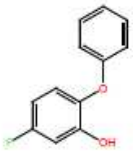

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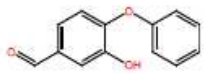

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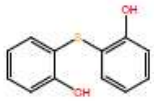

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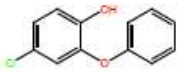

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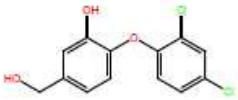

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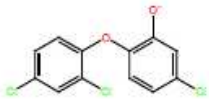

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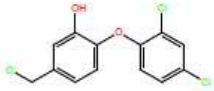
KI_ECOLI_NM: 1300.0



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## 6. Indole Actives

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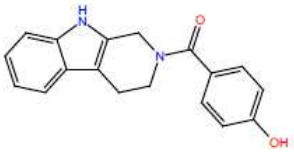

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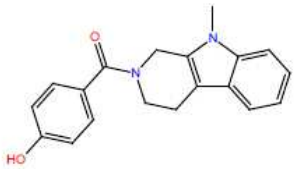
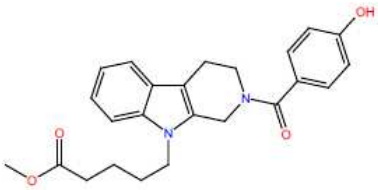


title: indole 7
Enzymologic: IC50 nM 1: 11000

title: indole 8
Enzymologic: IC50 nM 1: 34900



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Enzymologic: IC50 nM 1: 26800

title: indole 10
Enzymologic: IC50 nM 1: 27000

title: indole 11
Enzymologic: IC50 nM 1: 8800

title: indole 3
Enzymologic: IC50 nM 1: 4200

title: indole 12
Enzymologic: IC50 nM 1: 21400

title: indole 13
Enzymologic: IC50 nM 1: 4200

title: indole 14
Enzymologic: IC50 nM 1: 4500

title: indole 19
Enzymologic: IC50 nM 1: 2700

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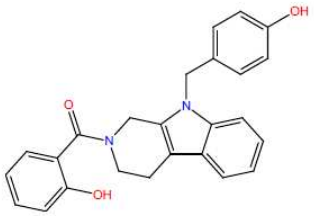

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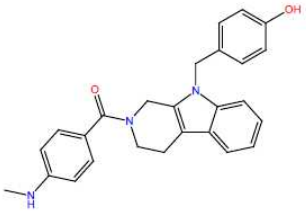

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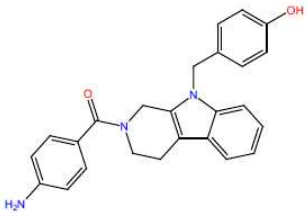

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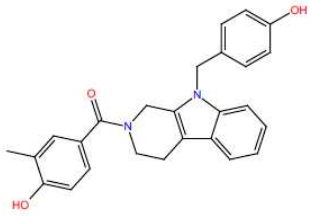

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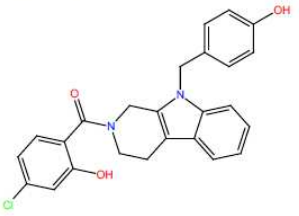

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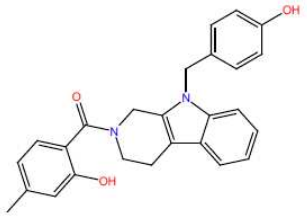
Enzymologic: IC50 nM 1: 6100



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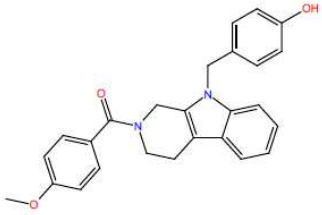
Enzymologic: IC50 nM 1: 8200



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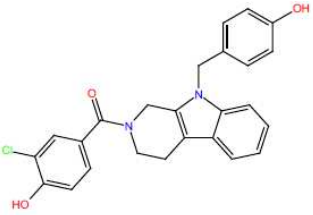
Enzymologic: IC50 nM 1: 35500



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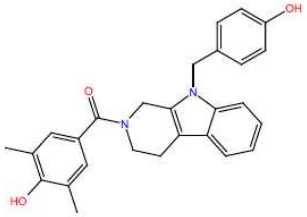

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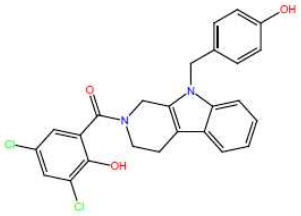

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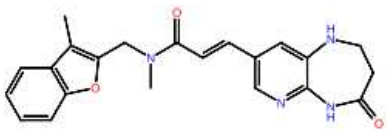
Enzymologic: IC50 nM 1: 9900

## 7. Amide Actives



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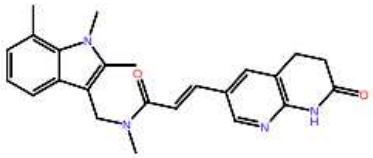

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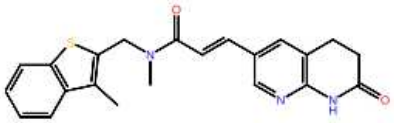
IC50_SAUREUS_NM: 20

title: pyridodiazepine9a
IC50_SAUREUS_NM: 26



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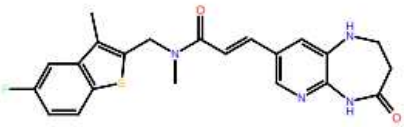

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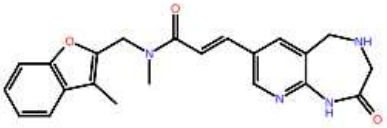
IC50_SAUREUS_NM: 31



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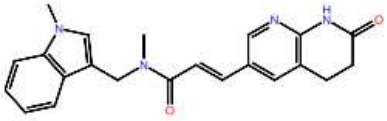
IC50_SAUREUS_NM: 48



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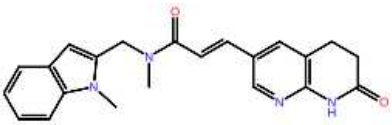

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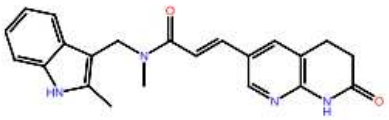
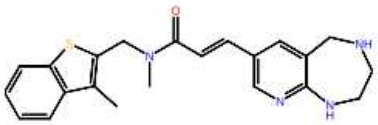
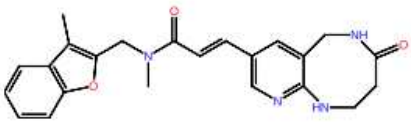


title: INDOLENAPHTHYRIDINONE30
IC50_SAUREUS_NM: 50



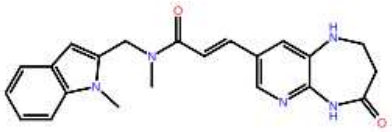
title: pyridodiazepine20a
IC50_SAUREUS_NM: 57

title: INDOLE NAPHTHYRIDINONE 31
IC50_SAUREUS_NM: 60

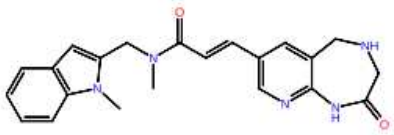


title: pyridodiazepine28
IC50_SAUREUS_NM: 61

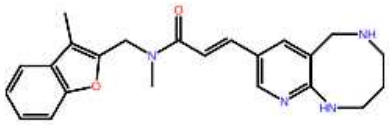
title: pyridodiazepine9b
IC50_SAUREUS_NM: 67



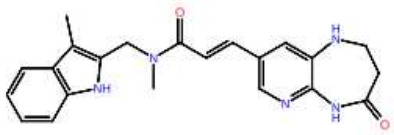
title: pyridodiazepine11b
IC50_SAUREUS_NM: 130



title: pyridodiazepine16c
IC50_SAUREUS_NM: 130

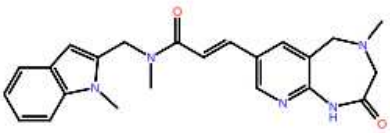


title: pyridodiazepine31
IC50_SAUREUS_NM: 170



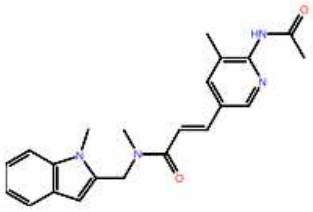
title: pyridodiazepine11c
IC50_SAUREUS_NM: 200

title: ACETAMIDO DERIV. 12
IC50_SAUREUS_NM: 300



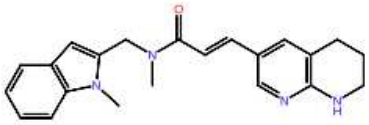
title: pyridodiazepin16a
IC50_SAUREUS_NM: 510

title: AMINOPYRIDINE 5
IC50_SAUREUS_NM: 910



title: ACETAMIDODERIV.13
IC50_SAUREUS_NM: 940

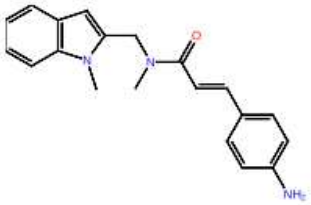
title: AMINOPYRIMIDINE DERIV. 10
IC50_SAUREUS_NM: 2200



title: PIPERIDINE 11
IC50_SAUREUS_NM: 2300

title: AMINOPYRIDINEDERIV.9
IC50_SAUREUS_NM: 2400

title: 1LX6_Ecoli_NAD_Benzamide_2.40A
IC50_SAUREUS_NM: 6700

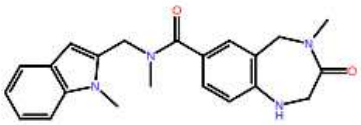


title: ACRYLAMIDE DERIV. 13
IC50_SAUREUS_NM: 11200

title: AMINOPYRIDINEDERIV.14
IC50_SAUREUS_NM: 14200

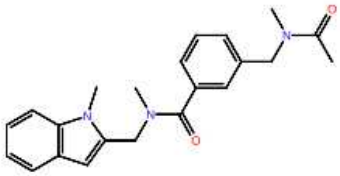
title: BENZAMIDEDERIV.7
IC50_SAUREUS_NM: 16300

title: 1,4-BENZODIAZEPINEDERIV.3
IC50_SAUREUS_NM: 16500



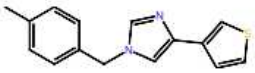
title: 1,4-BENZODIAZEPINEDERIV.4
IC50_SAUREUS_NM: 21200

title: AMINOPYRIDINEDERIV.11
IC50_SAUREUS_NM: 93700

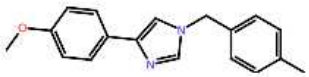


title: BENZAMIDEDERIV.6
IC50_SAUREUS_NM: 107000

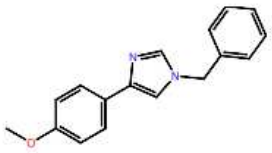
## 8. Imidazole Actives



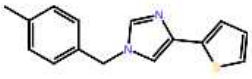
title: DISUBSTITUTEDIMIDAZOLE23
E_COLI_IC50_NM: 250



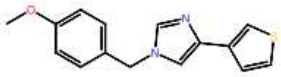
title: DISUBSTITUTEDIMIDAZOLE4
E_COLI_IC50_NM: 360



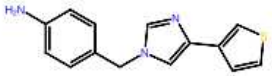
title: DISUBSTITUTEDIMIDAZOLE28
E_COLI_IC50_NM: 1130



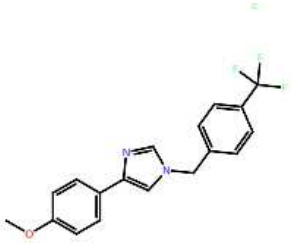
title: 1I2Z_Ecoli_NAD_BRL12654_2.80A
E_COLI_IC50_NM: 1240



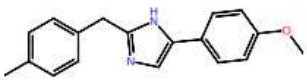
title: DISUBSTITUTEDIMIDAZOLE21
E_COLI_IC50_NM: 1900



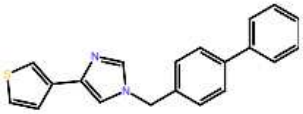
title: DISUBSTITUTED IMIDAZOLE 20
E_COLI_IC50_NM: 2030



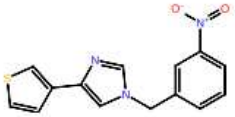
title: DISUBSTITUTEDIMIDAZOLE29
E_COLI_IC50_NM: 4070



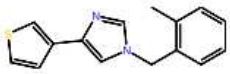
title: DISUBSTITUTEDIMIDAZOLE11
E_COLI_IC50_NM: 6620



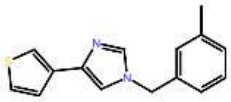
title: DISUBSTITUTEDIMIDAZOLE27
E_COLI_IC50_NM: 7660



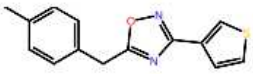
title: DISUBSTITUTEDIMIDAZOLE8
E_COLI_IC50_NM: 14700



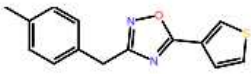
title: DISUBSTITUTEDIMIDAZOLE26
E_COLI_IC50_NM: 36500



title: DISUBSTITUTEDIMIDAZOLE25
E_COLI_IC50_NM: 42400



title: OXADIAZOLE33
E_COLI_IC50_NM: 50700



title: OXADIAZOLE 19
E_COLI_IC50_NM: 51000

## 9. Diphenyl Decoys

See separately attached .sdf file entitled “FabI_Diphenyl_Decoys_500.sdf“

## 10. Indole Decoys

See Separately attached .sdf file entitled “FabI_Indole_Decoys_1000.sdf“

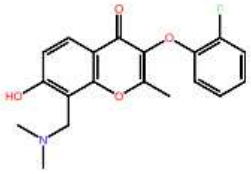
## 11. Amide Decoys

See separately attached .sdf file entitled “FabI_Amide_Decoys_533.sdf“

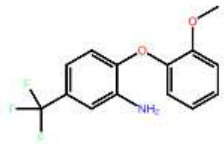
## 12. Imidazole Decoys

See separately attached .sdf file entitled “FabI_Imidazole_Decoys_529.sdf“

## 13. Diphenyl Virtual Screen, Compounds Ordered and Tested

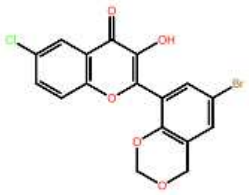


title: 250003954
Inhibition %25: 85% @ 100uM (55% @ 40uM)



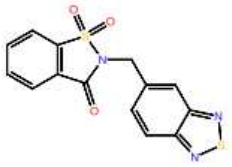
title: 650000242
Inhibition %25: 18% @ 100uM (3% @ 40uM)

title: 600003523
Inhibition %25: 17% @ 100uM (6% @ 40uM)

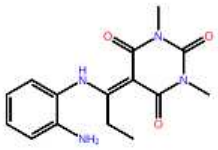


title: 100038212
Inhibition %25: 14% @ 100uM (0% @ 40uM)

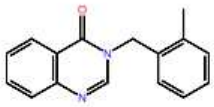
title: 150012092
Inhibition %25: 14% @ 100uM (0% @ 40uM)



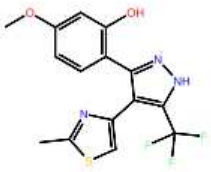
title: 650005614
Inhibition %25: 13% @ 100uM (5% @ 40uM)



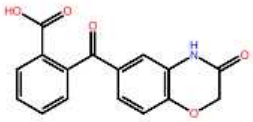
title: 800000443
Inhibition %25: 12% @ 100uM (14% @ 40uM)



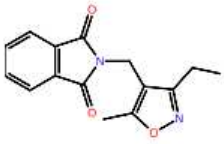
title: 600004374
Inhibition %25: 10% @ 100uM (0% @ 40uM)



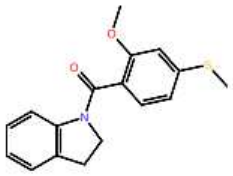
title: 100084666
Inhibition %25: 9% @ 100uM (6% @ 40uM)



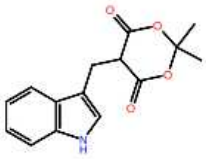
title: 600001343
Inhibition %25: 8% @ 100uM (0% @ 40uM)



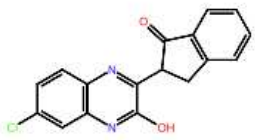
title: 100084635
Inhibition %25: 3% @ 100uM (0% @ 40uM)



title: 450000131
Inhibition %25: 1% @ 100uM (6% @ 40uM)

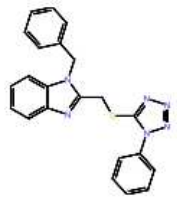


title: 100026264
Inhibition %25: 0% @ 100uM (0% @ 40uM)



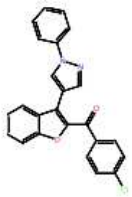
title: 100072943
Inhibition %25: 0% @ 100uM (0% @ 40uM)

# 14. Indole Virtual Screen, Compounds Ordered and Tested

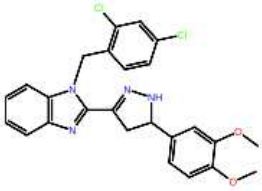


title: 600009538
Inhibition %25: 68% @ 100uM (42% @ 40uM)

title: 950017010
Inhibition %25: 57% @ 100uM (0% @ 40uM)



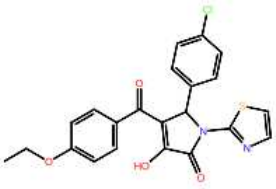
title: 600005310
Inhibition %25: 24% @ 100uM (26% @ 40uM)



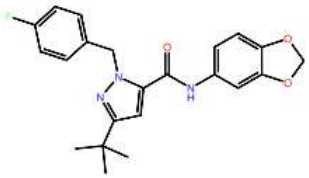
title: 100034909
Inhibition %25: 22% @ 100uM (25% @ 40uM)

title: 800003371
Inhibition %25: 21% @ 100uM (10% @ 40uM)

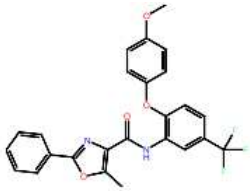
title: 900087852
Inhibition %25: 21% @ 100uM (8% @ 40uM)



title: 250002111
Inhibition %25: 18% @ 100uM (7% @ 40uM)

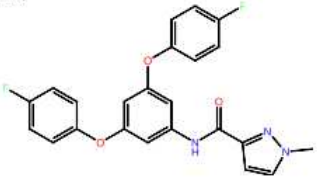


title: 650002560
Inhibition %25: 11% @ 100uM (0% @ 40uM)

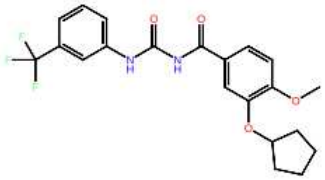


title: 650002232
Inhibition %25: 7% @ 100uM (0% @ 40uM)

title: 100047760
Inhibition %25: 3% @ 100uM (12% @ 40uM)

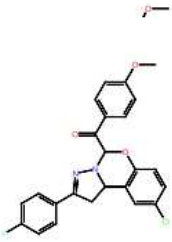


title: 600008452
Inhibition %25: 3% @ 100uM (0% @ 40uM)



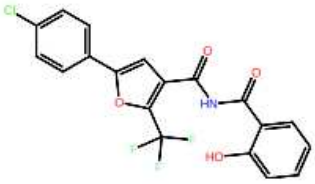
title: 650006798
Inhibition %25: 2% @ 100uM (0% @ 40uM)

title: 100039560
Inhibition %25: 0% @ 100uM (17% @ 40uM)



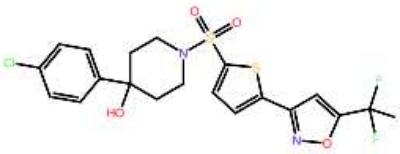
title: 100040675
Inhibition %25: 0% @ 100uM (0% @ 40uM

## 15. Amide Virtual Screen, Compounds Ordered and Tested

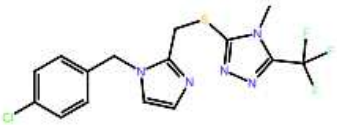


title: 650005744
Inhibition %25: 39% @ 100uM (100% @ 4...

title: 250002532
Inhibition %25: 23% @ 100uM (5% @ 40uM)



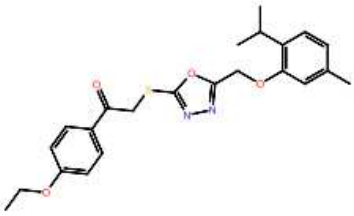
title: 650000871
Inhibition %25: 17% @ 100uM (10% @ 40uM)



title: 650006663
Inhibition %25: 13% @ 100uM (17% @ 40uM)

title: 800000798
Inhibition %25: 6% @ 100uM (1% @ 40uM)

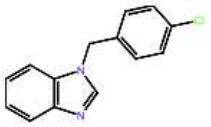
title: 100077132
Inhibition %25: 3% @ 100uM (12% @ 40uM)



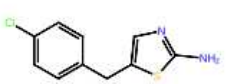
title: 100066729
Inhibition %25: 0% @ 100uM (15% @ 40uM)

title: 100041600
Inhibition %25: 0% @ 100uM (0% @ 40uM)

# 16. Imidazole Virtual Screen, Compounds Ordered and Tested

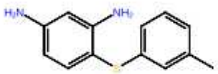


title: 100017167
Inhibition %25: 70% @ 100uM (94% @ 40uM)

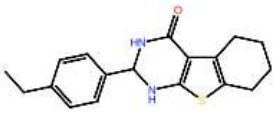


title: 100042025
Inhibition %25: 49% @ 100uM (45% @ 40uM)

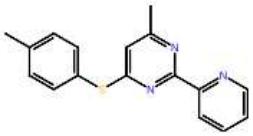
title: 100065143
Inhibition %25: 31% @ 100uM (0% @ 40uM)



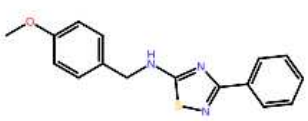
title: 100080858
Inhibition %25: 22% @ 100uM (11% @ 40uM)



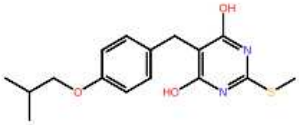
title: 400000213
Inhibition %25: 22% @ 100uM (0% @ 40uM)



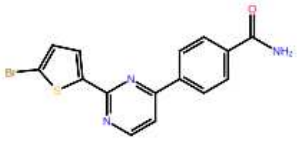
title: 650010595
Inhibition %25: 18% @ 100uM (23% @ 40uM)



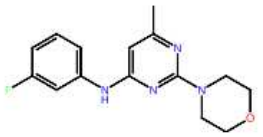
title: 650002962
Inhibition %25: 18% @ 100uM (3% @ 40uM)



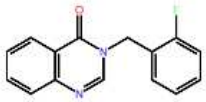
title: 600003750
Inhibition %25: 15% @ 100uM (0% @ 40uM)



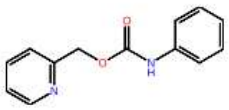
title: 650002630
Inhibition %25: 10% @ 100uM (11% @ 40uM)



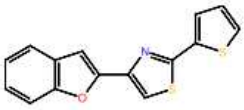
title: 800000418
Inhibition %25: 10% @ 100uM (0% @ 40uM)



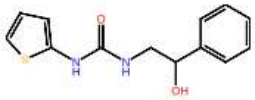
title: 100042452
Inhibition %25: 4% @ 100uM (15% @ 40uM)



title: 600001518
Inhibition %25: 3% @ 100uM (7% @ 40uM)

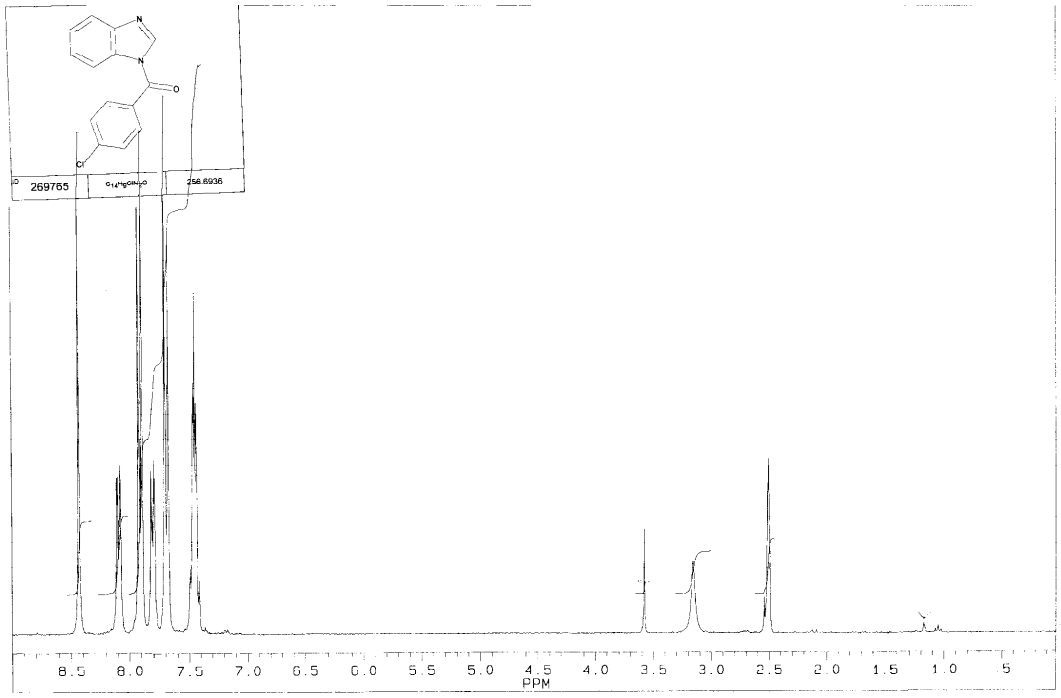


title: 650002616
Inhibition %25: 2% @ 100uM (0% @ 40uM)

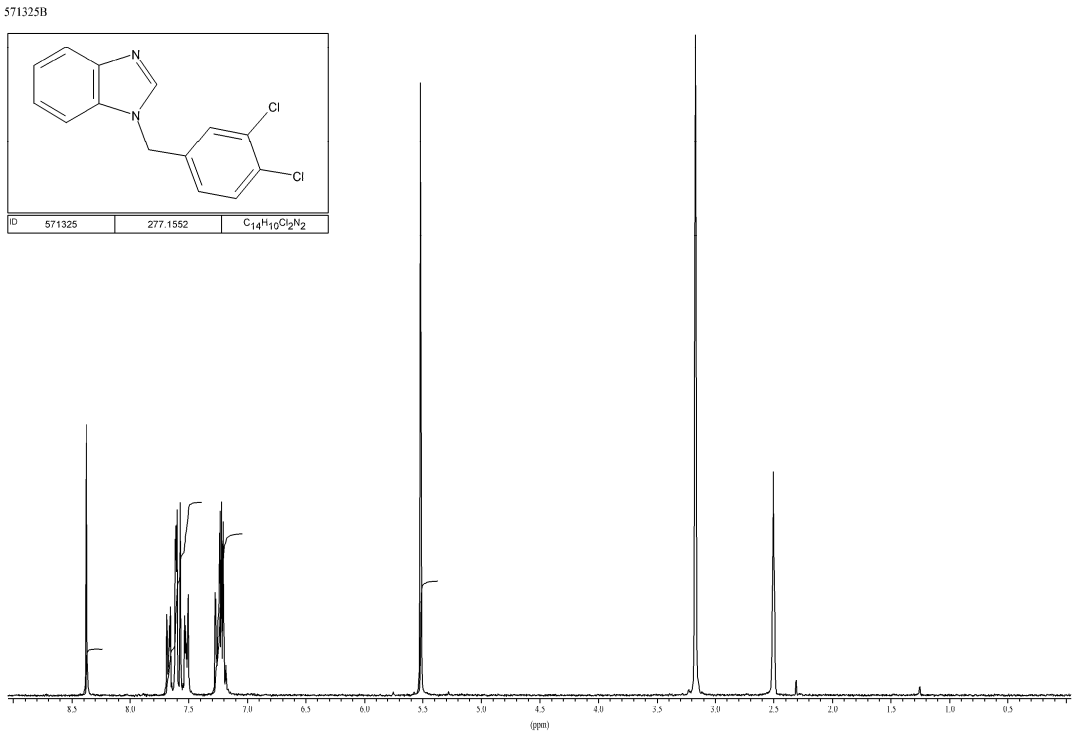


title: 650004123
Inhibition %25: 2% @ 100uM (0% @ 40uM)

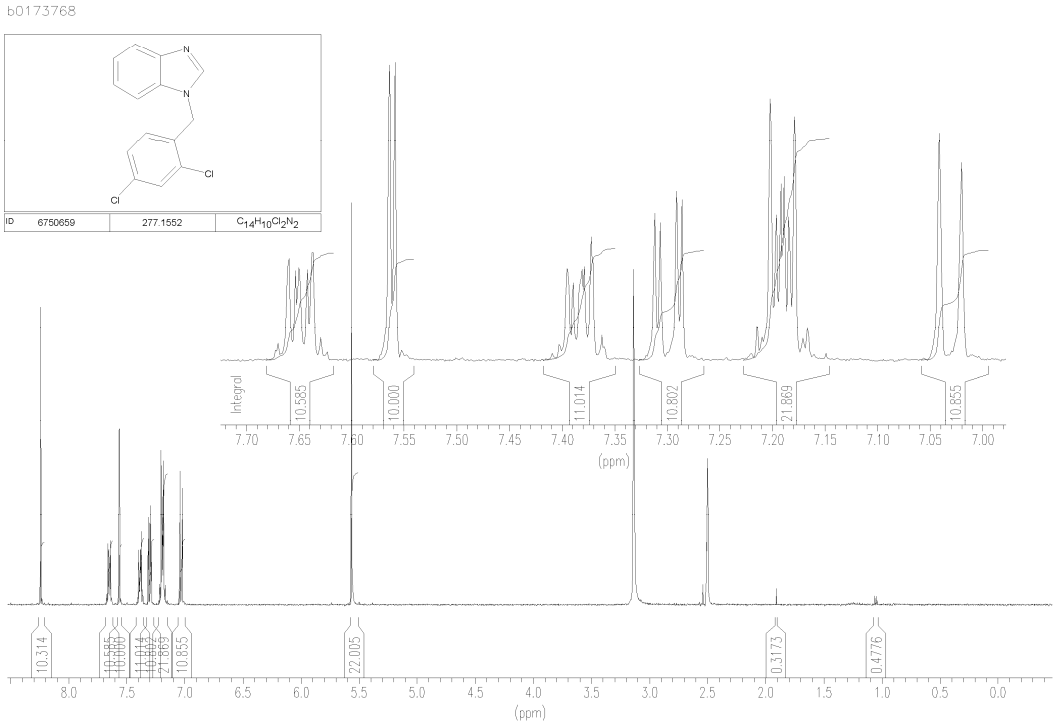
## 17. NMR Spectra for Published Compounds



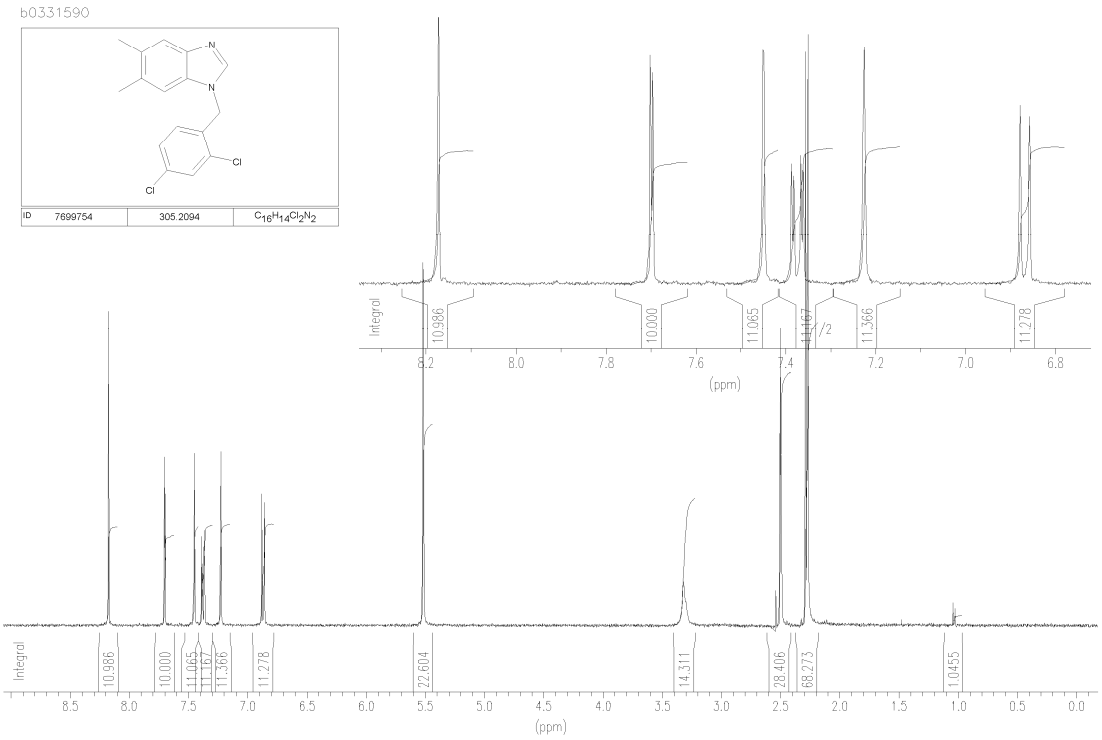

CB-5269765 NMR spectrum



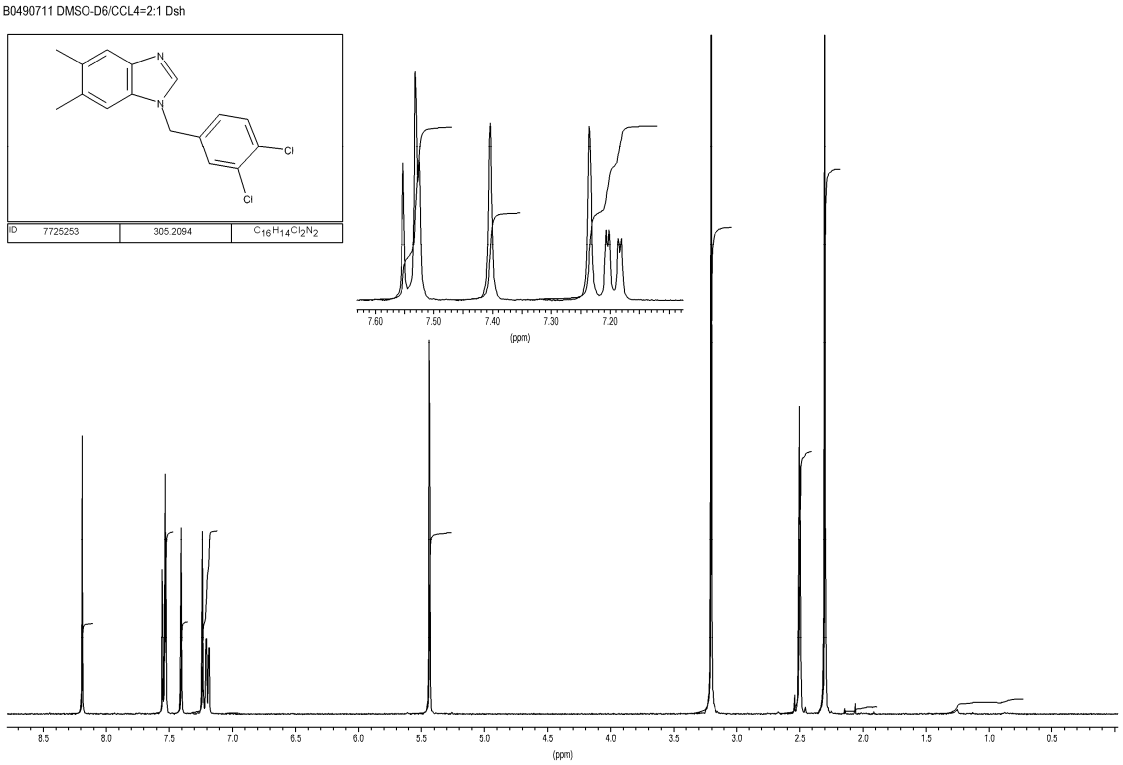

CB-5571325 NMR spectrum



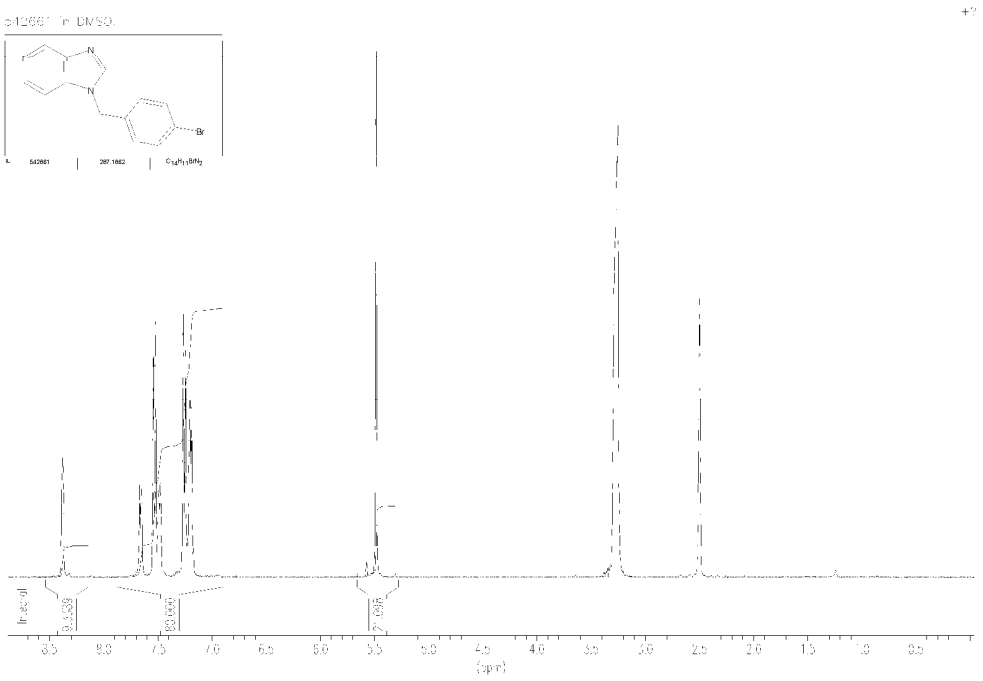

CB-6750659 NMR spectrum



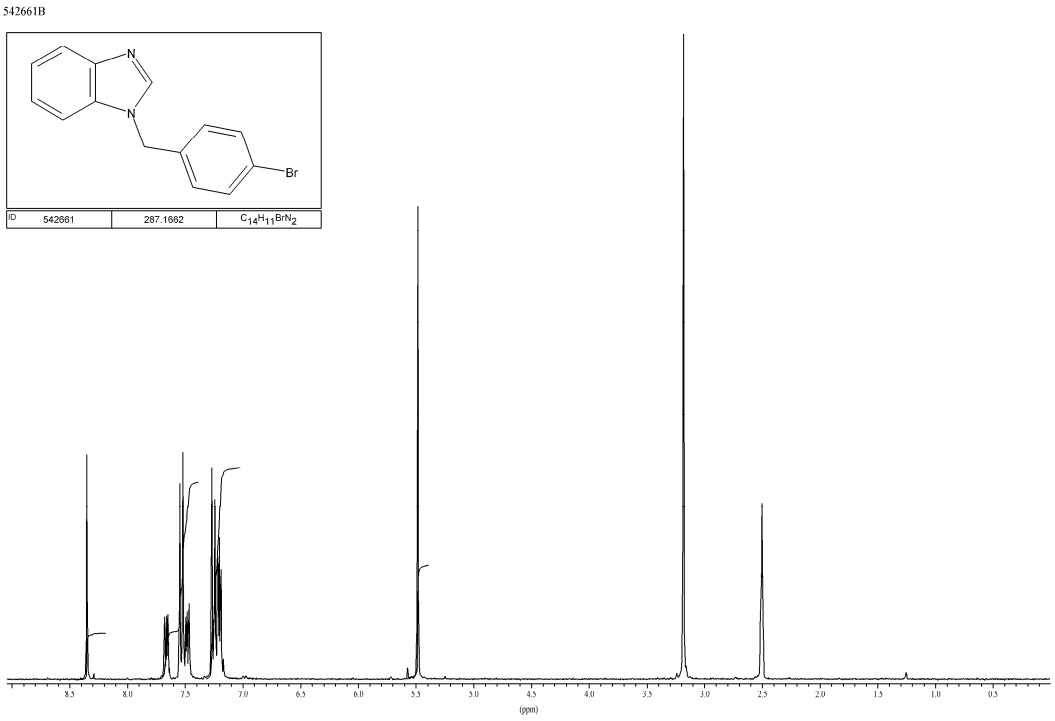

CB-7699754 NMR spectrum



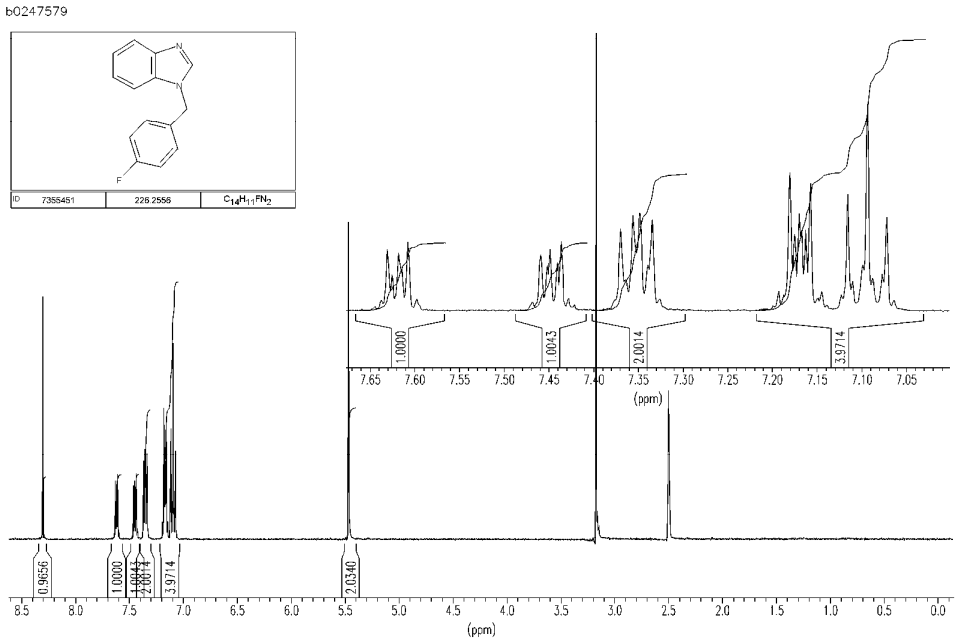

Cb-772532 NMR spectrum



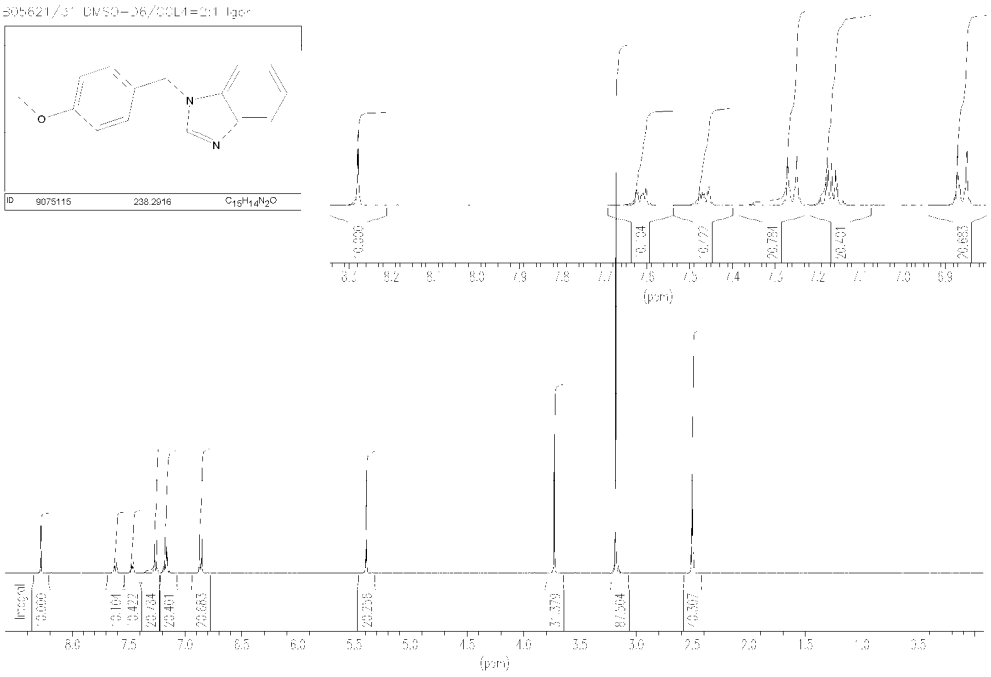

CB-5542661 NMR spectrum-1



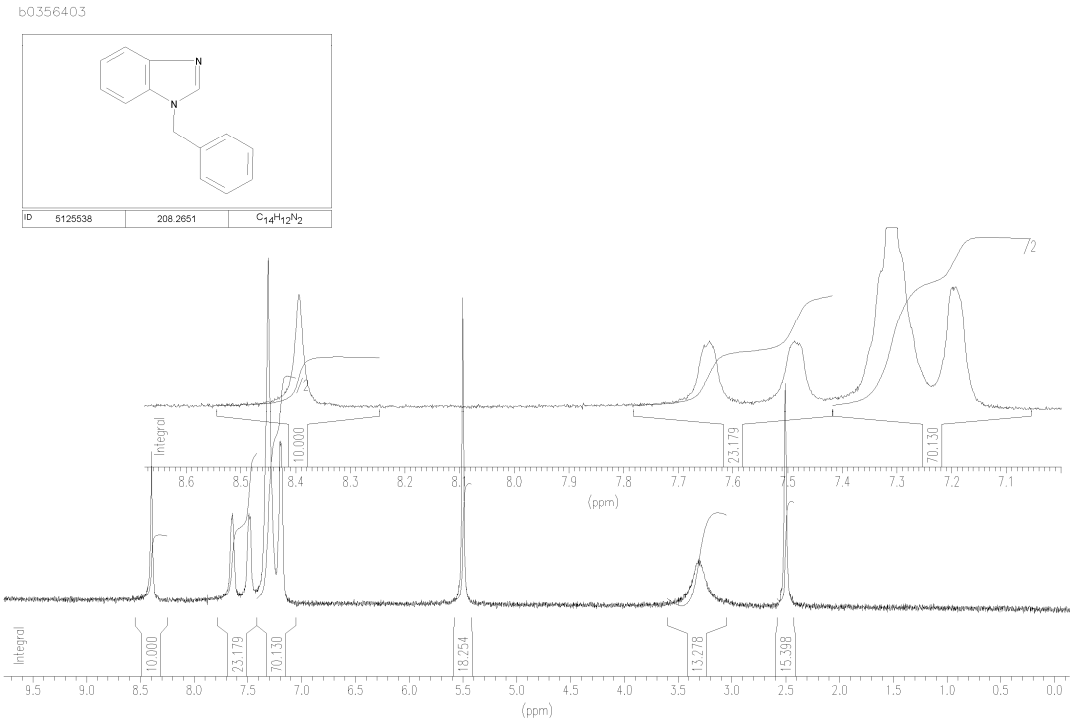

CB-5542661 NMR spectrum-2



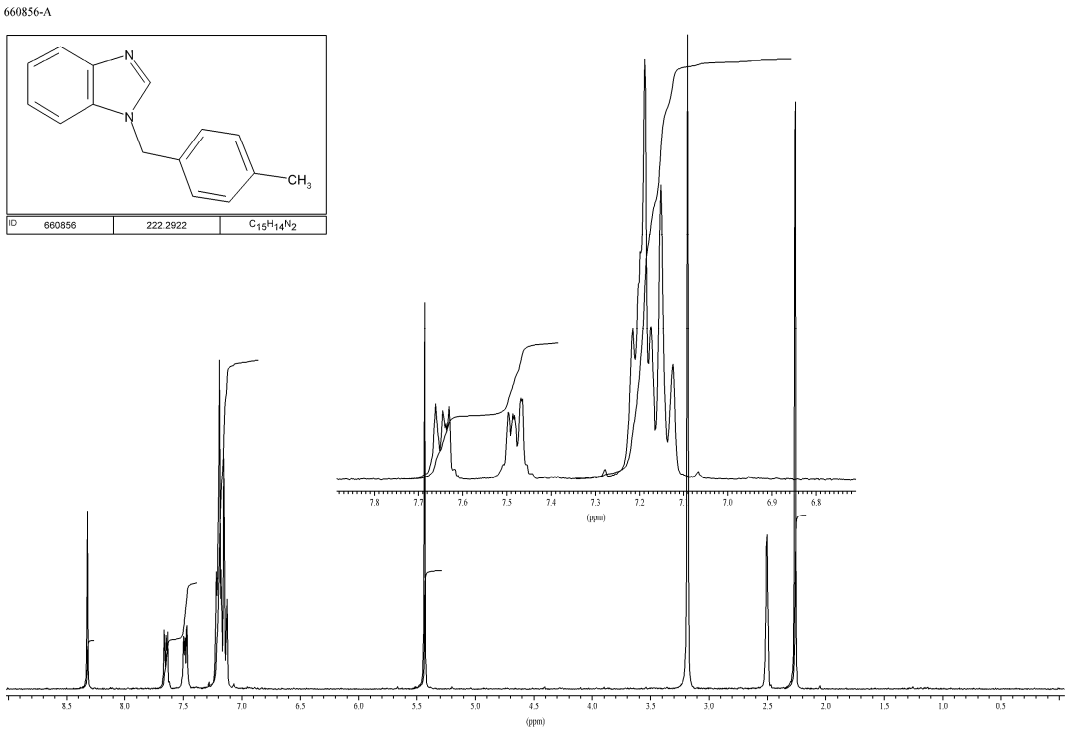
CB-7355451 NMR spectrum



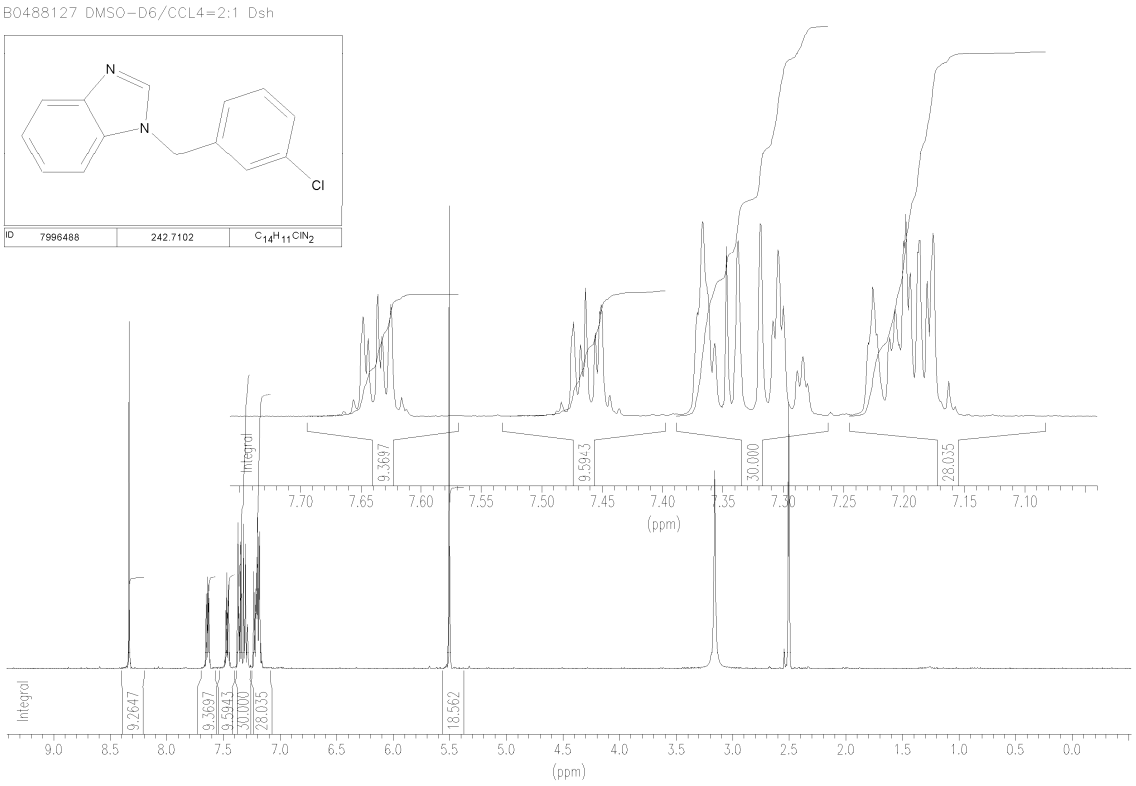

CB-9075115 NMR spectrum



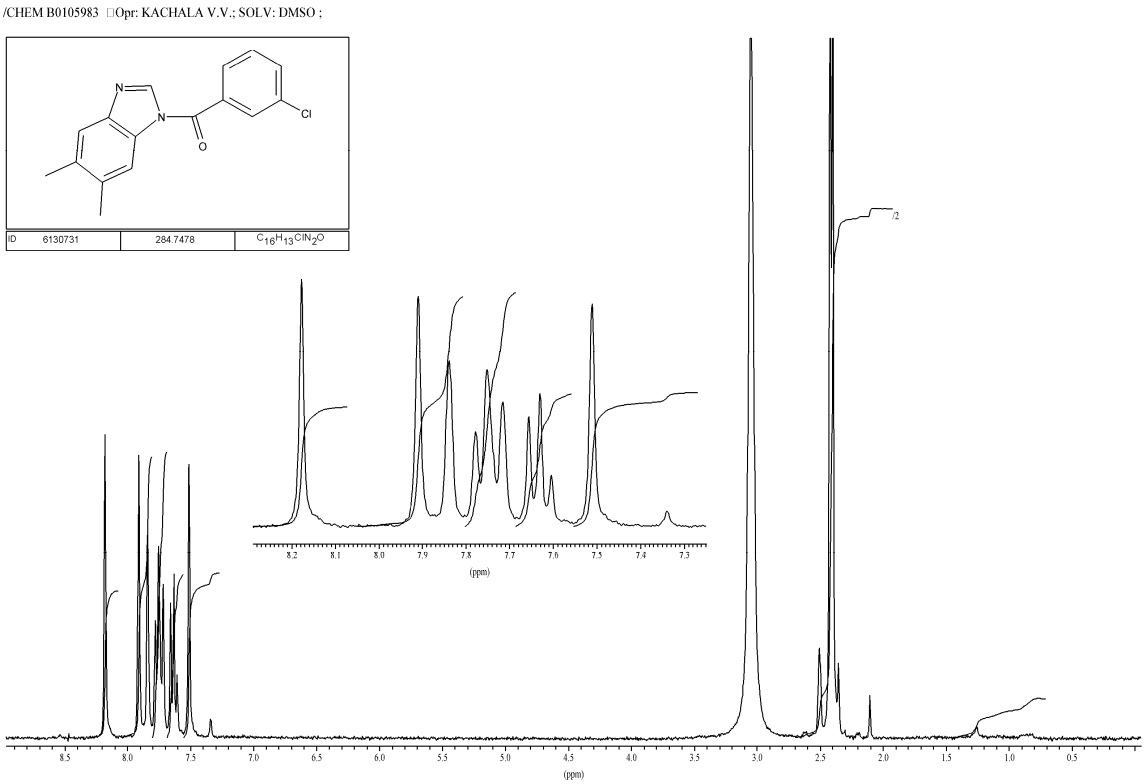

CB-5125538 NMR spectrum



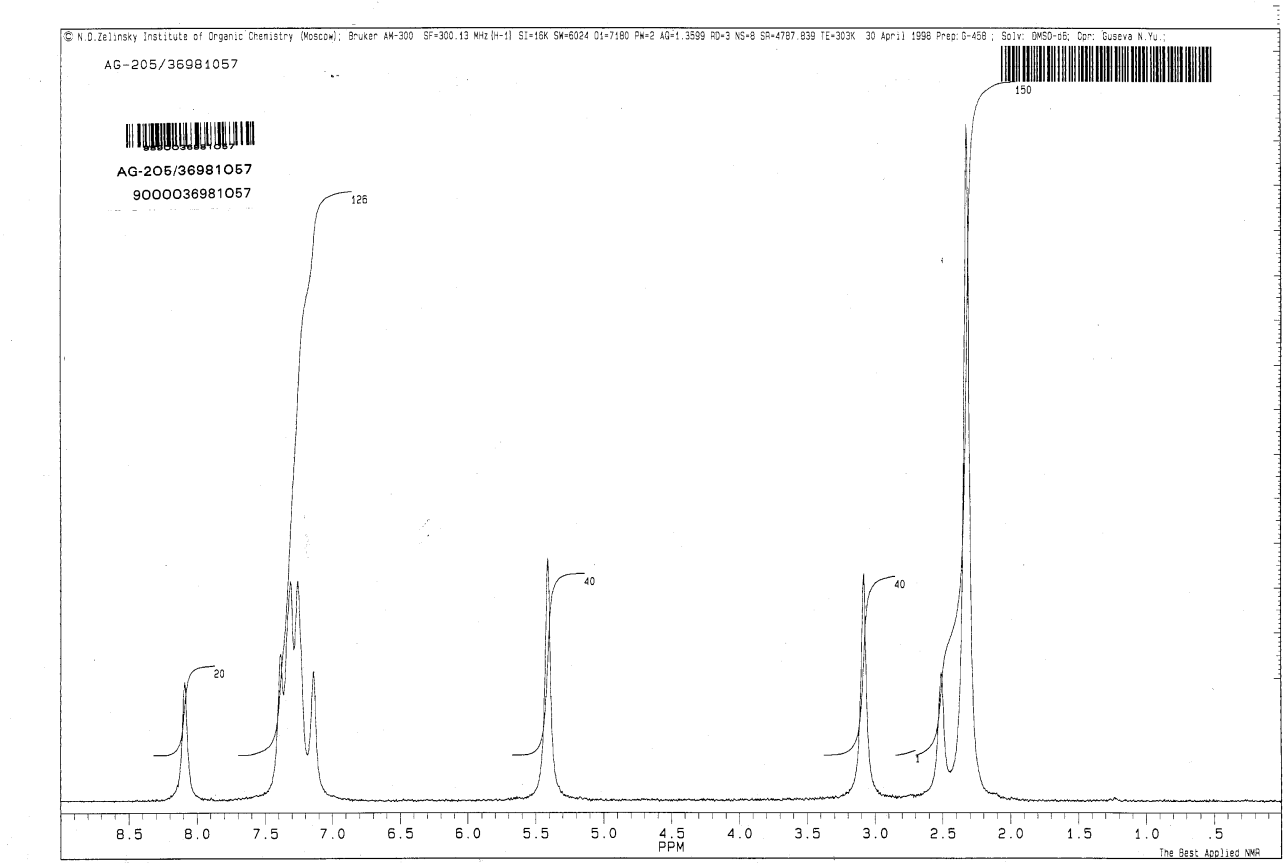

CB-5660856 NMR spectrum



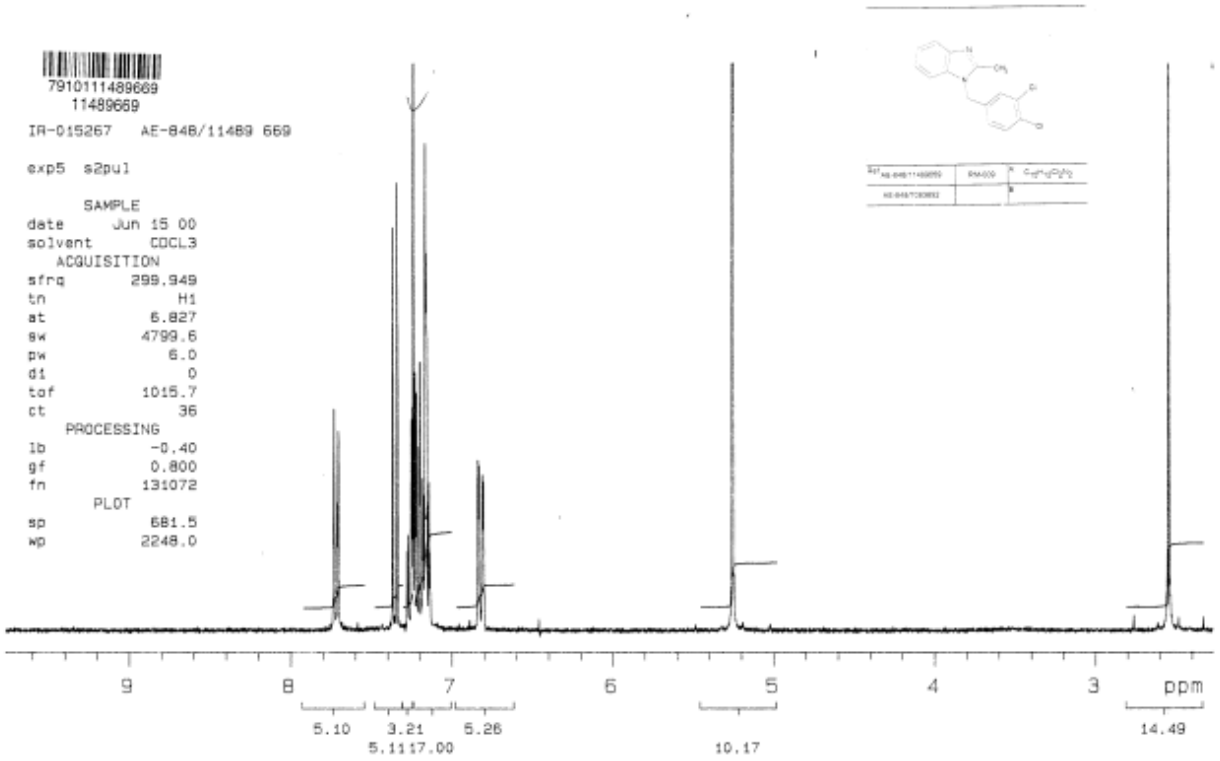

CB-7996488 NMR spectrum



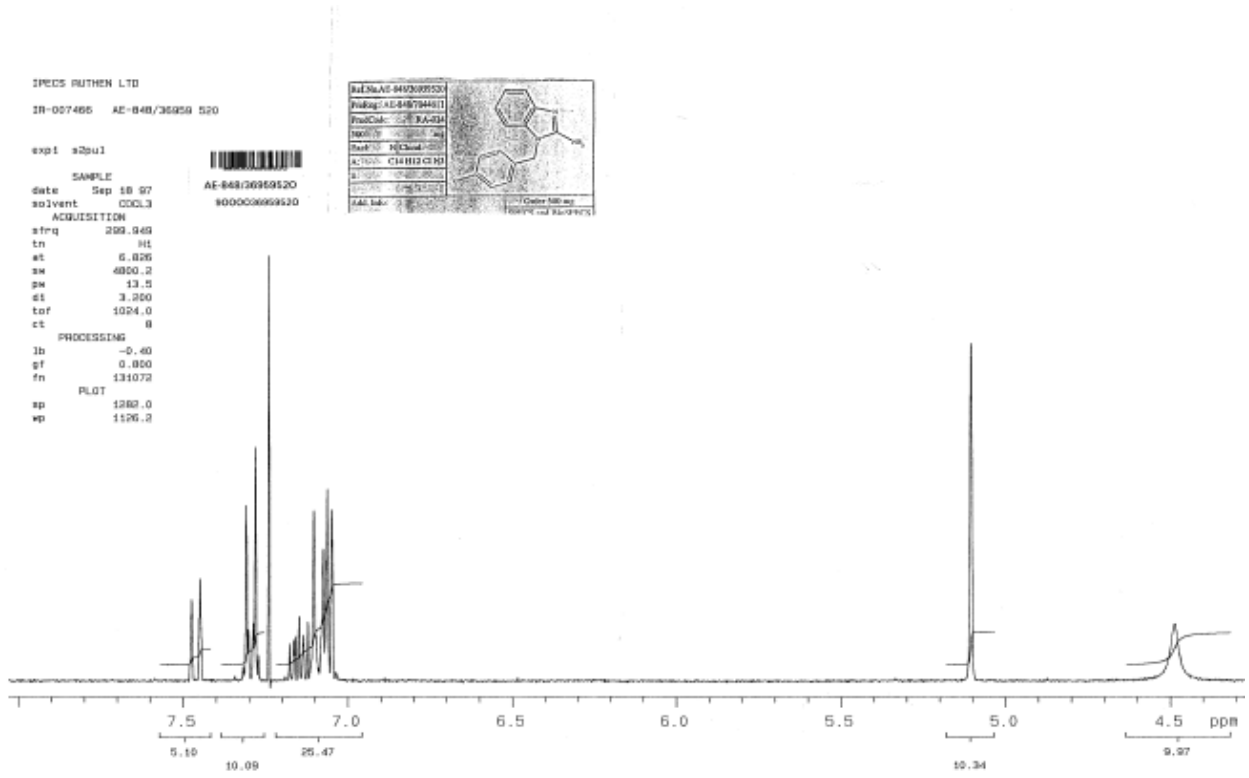

CB-6130731NMR spectrum




AG-205/36981057 NMR spectrum



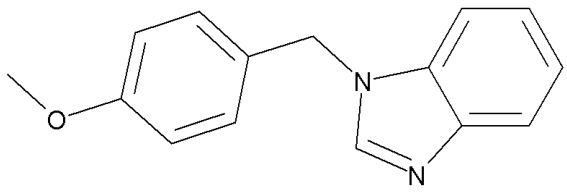

AE-848/11489669 NMR spectrum



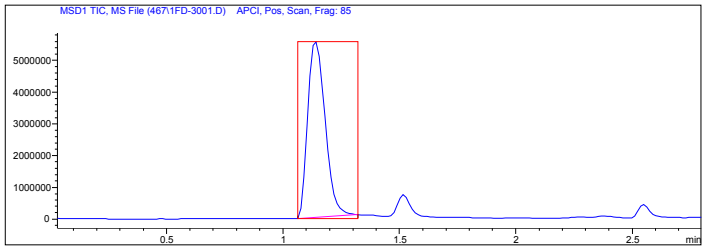

AE-848/36959520 NMR spectrum

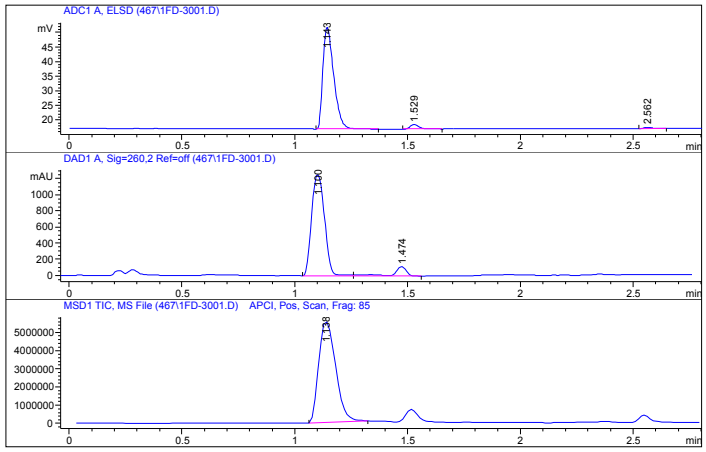
# 18. HPLC Analysis of Published Compounds

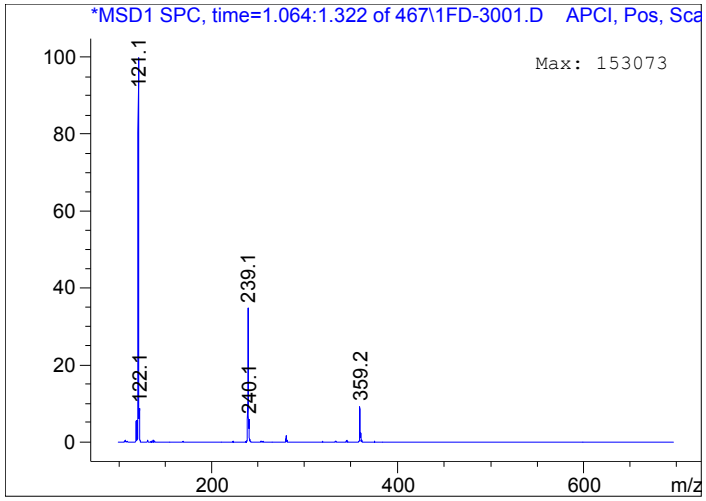
CH00562130



| ID | 9075115 | 238.2916 | $C_{15}H_{14}N_2O$ |
|---|---|---|---|



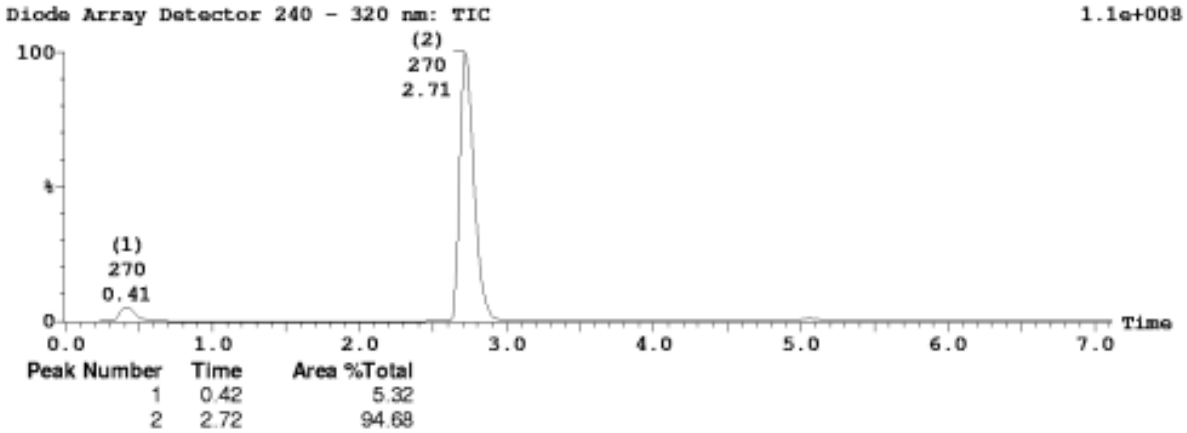




```
Data File C:\HPCHEM\1\DATA\467\1FD-3001.D
Sample Name: CH005621P1-F-04
Instrument 1 10/09/2006 13:34:47  LCMS#1
Column: Chromolith SpeedROD C18 50x4.6mm | 3.75ml/min
Gradient: "A"->@2.2min->"B"(Hold 0.5min)->@0.1min->"A"-
>PostRun
PMP1, Solvent A          : 0.1% TFA in AcN/Water (5:95)
PMP1, Solvent B          : 0.1% TFA in AcN
PMP1, Solvent C          : 10mM CH3COONH4 in AcN/Water
(2.5:75.5)
PMP1, Solvent D          : 10mM CH3COONH4 in AcN/Water (90:10)
Ionization mode             :    APCI Positive

Signal 1: ADC1 A, ELSD
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mV*s]      [mV]        %
----|-------|----|-------|----------|----------|--------|
   1   1.143 PP    0.0521  116.41392   34.76533  95.8423
   2   1.529 PP    0.0418    3.96096    1.49830   3.2610
   3   2.562 PP    0.0363    1.08921 4.64966e-1   0.8967
Totals :                   121.46409   36.72859


Signal 2: DAD1 A, Sig=260,2 Ref=off
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   1.100 PV    0.0643 4979.98828 1255.57410  91.5908
   2   1.474 VP    0.0568  457.22726  119.08273   8.4092
Totals :                  5437.21555 1374.65683


Signal 3: MSD1 TIC, MS File
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]                          %
----|-------|----|-------|----------|----------|--------|
   1   1.138 PBA   0.0880 2.90206e7  5.55998e6  100.0000
Totals :                  2.90206e7  5.55998e6
```

File:9900036981057 ID:AG-205/36981057 Description:C16H15ClN2
Instrument:LC/MS B Vial:1:93 Date:18-Jun-2004

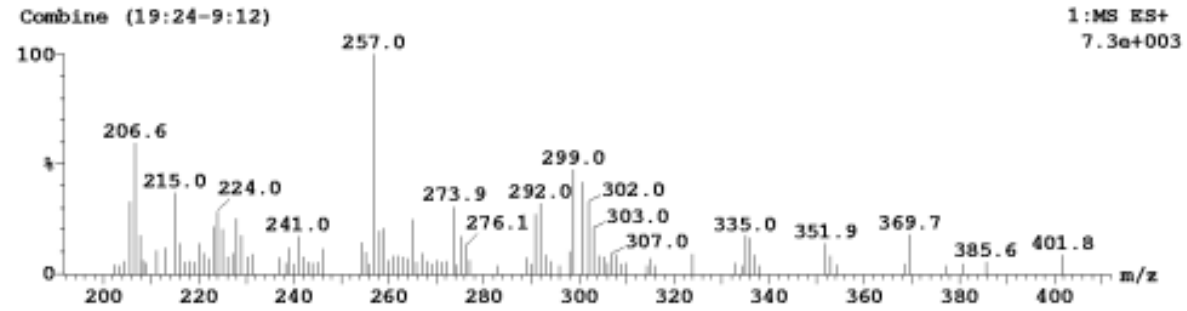
Printed: Fri Jun 18 13:46:13 2004

**Sample Report (continued):**

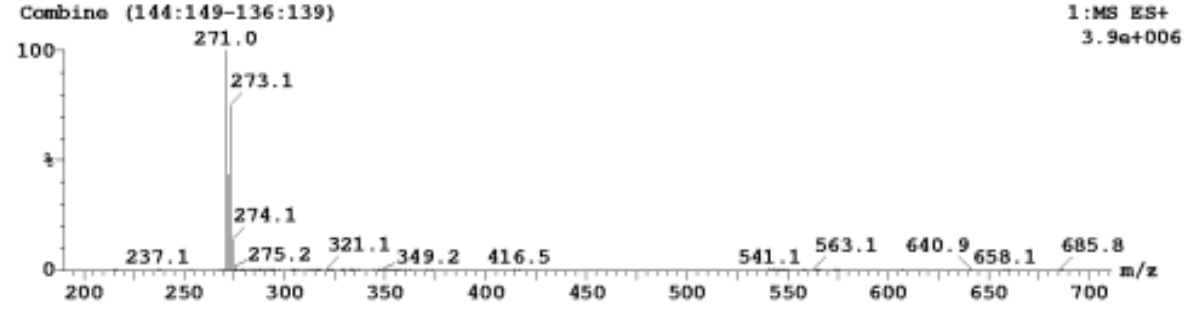



| Peak Number | Time | Area %Total |
|---|---|---|
| 1 | 0.42 | 5.32 |
| 2 | 2.72 | 94.68 |

| Peak ID | Time | Mass Found | BPM |
|---|---|---|---|
| 1 | 0.42 | 270.09 | 257 |

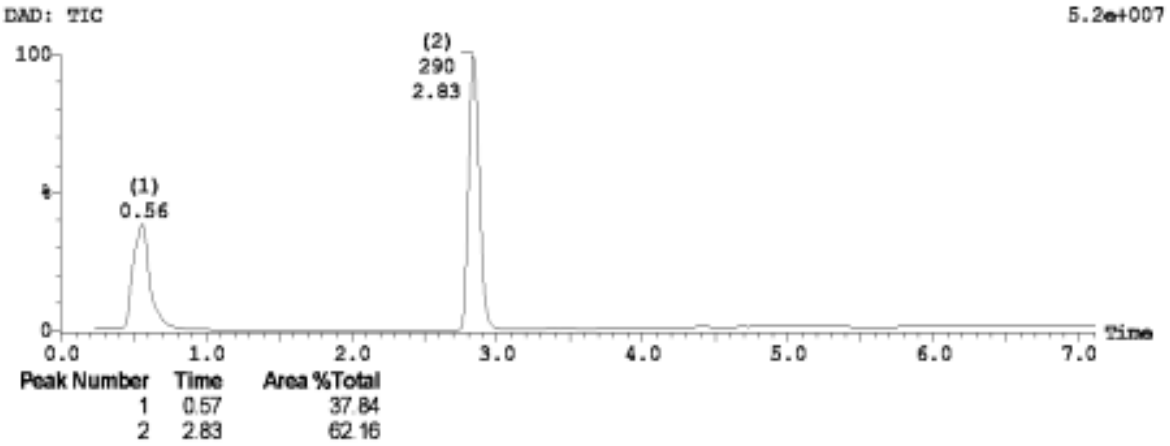



| Peak ID | Time | Mass Found | BPM |
|---|---|---|---|
| 2 | 2.72 | 270.09 | 271 |



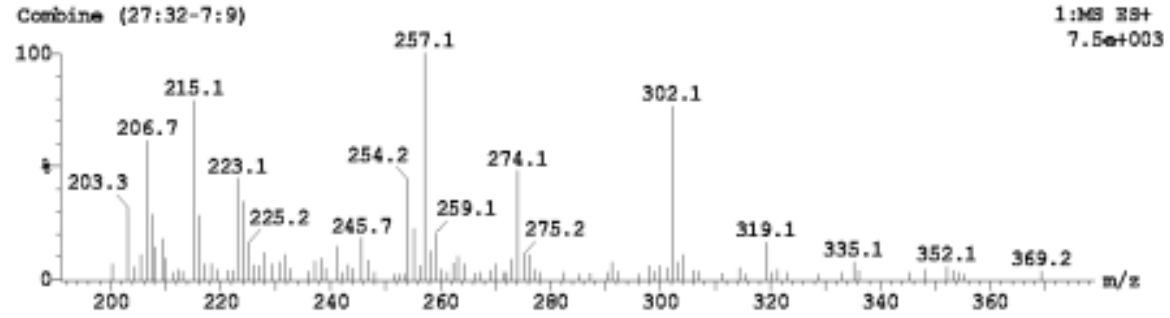

AG-205/36981057 LC-MS Spectrum

**Sample Report (continued):**

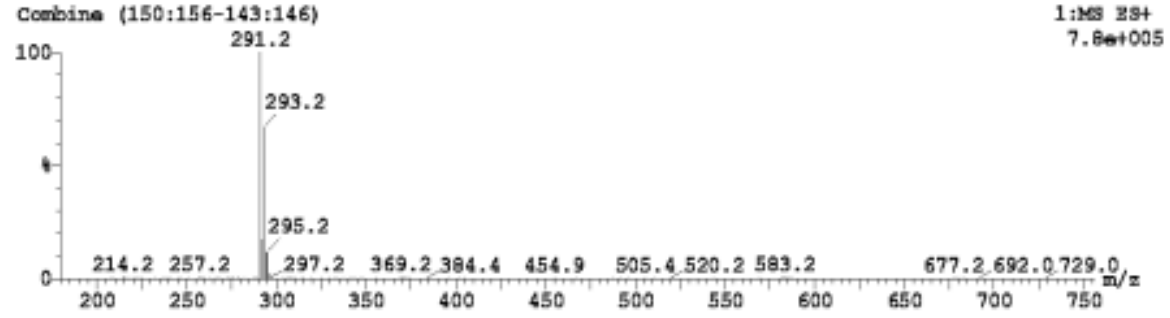



| Peak Number | Time | Area %Total |
|---|---|---|
| 1 | 0.57 | 37.84 |
| 2 | 2.83 | 62.16 |

| Peak ID | Time | Mass Found | BPM |
|---|---|---|---|
| 1 | 0.57 | 257.1 | |




| Peak ID | Time | Mass Found | BPM |
|---|---|---|---|
| 2 | 2.83 | 290.04 | 291.2 |




AE-848/11489669 Spectrum