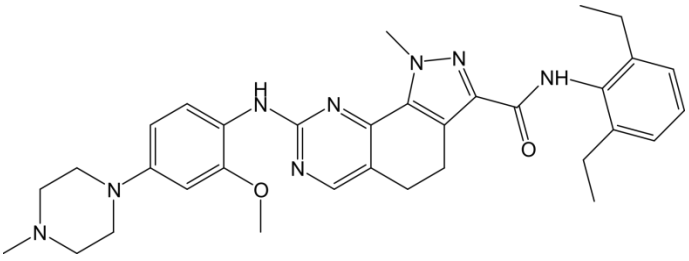
RGNCY-0015 (MPS1/TTK Inhibitor CPD-5)



Systematic Name:
N-(2,6-diethylphenyl)-8-((2-methoxy-4-(4-methylpiperazin-1-yl)phenyl)amino)-1-methyl-4,5-dihydro-1*H*-pyrazolo[4,3-*h*]quinazoline-3-carboxamide

Molecular Weight: 580.74

Molecular Formula: $C_{33}H_{40}N_8O_2$

SMILES:
COC1=CC(N2CCN(C)CC2)=CC=C1NC3=NC=C(CCC4=C5N(C)N=C4C(NC6=C(CC)C=CC=C6CC)=O)C5=N3

Batch No: R15-2-15

Purity: 99.1%

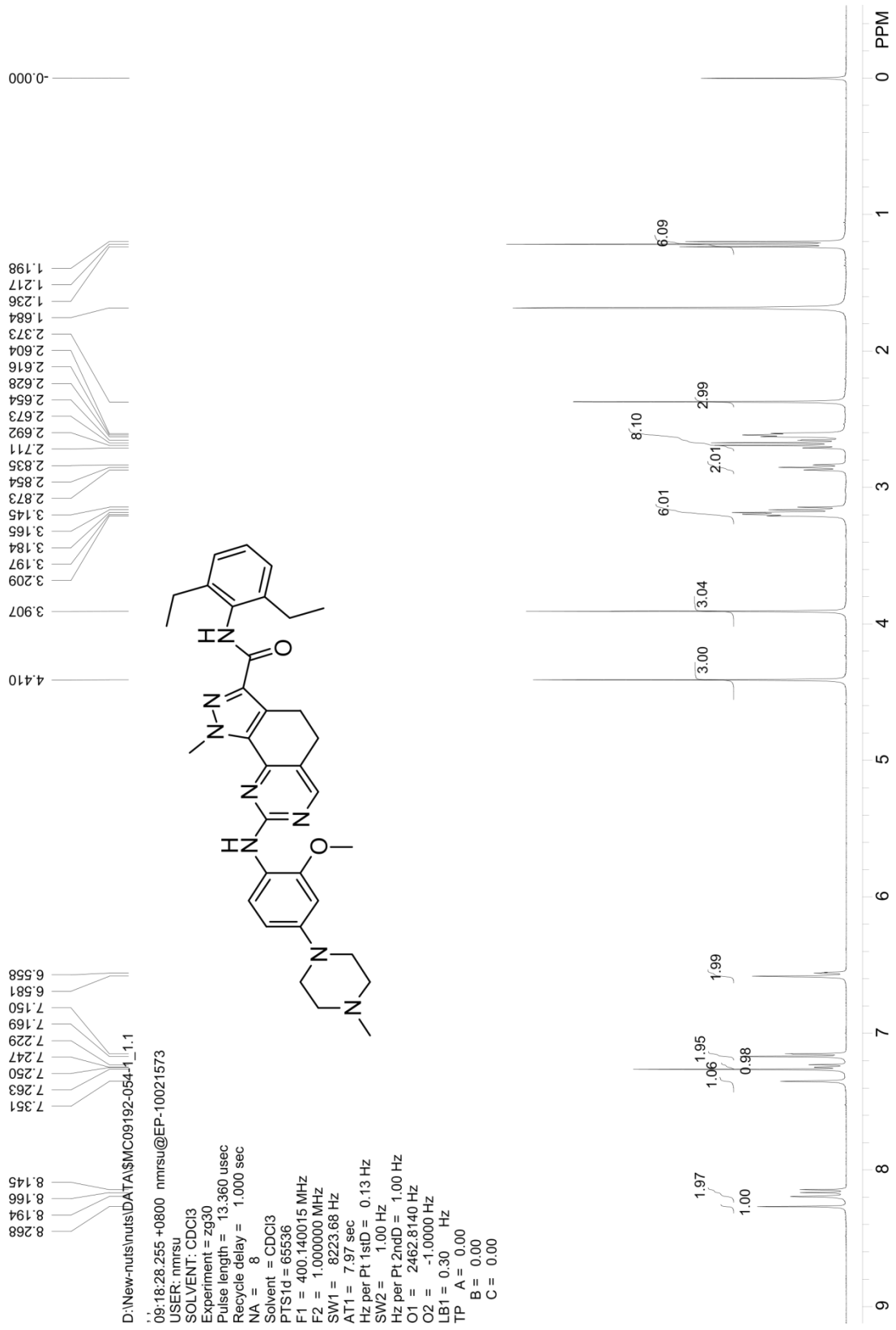
Description

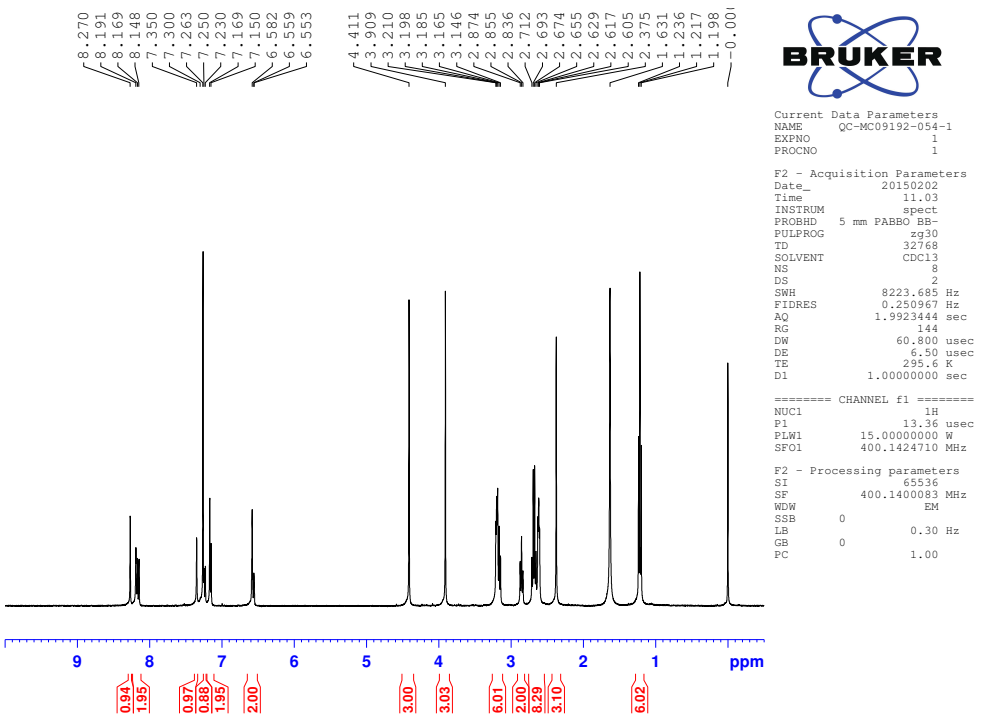
CPD-5 is a protein kinase inhibitor with activity against MPS1/TTK. It has an IC_{50} of 0.10 μM in cellular proliferation inhibition assay using A2780 cells.

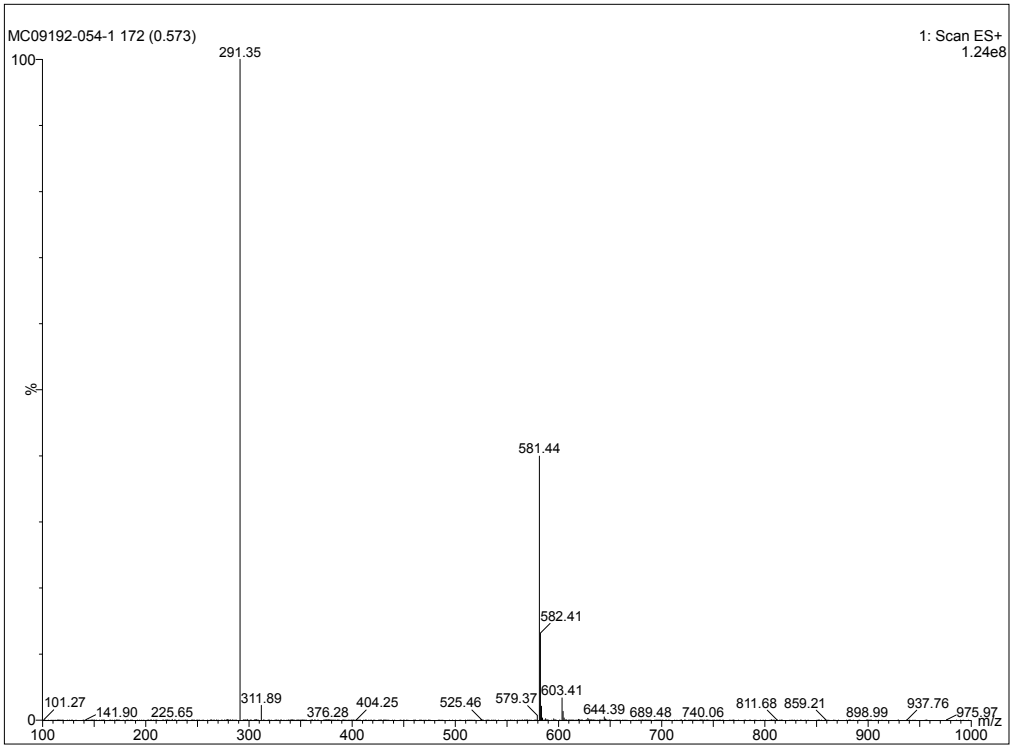
References

US Patent No. 20110105542 A1
Pyrazolo-quinazolines - Compound 5

NMR QC Data







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Data File D:\CHEM32\DATA\2015\150202\AM000006.D
Sample Name: QC-MC09192-054-1

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    Acq. Operator   : XXYAN                          Seq. Line :   6
    Acq. Instrument : HPLC-002(Agilent 1100 2#)       Location : Vial 15
    Injection Date  : 2/2/2015 11:39:25 AM                Inj :   1
                                                    Inj Volume : 1 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 3.5 µl
    Acq. Method     : D:\CHEM32\METHOD\N-C90D10.M
    Last changed    : 4/11/2014 11:24:19 AM by FFLIU
    Analysis Method : D:\CHEM32\METHOD\WAITING-WATERS.M
    Last changed    : 2/2/2015 12:14:31 PM by XXYAN
                      (modified after loading)
    Method Info     : Waters Sunfire  C18 5um 4.6*150mm column
                      Mobile phase: C: 0.03%TFA in H2O D: 0.03% TFA in ACN
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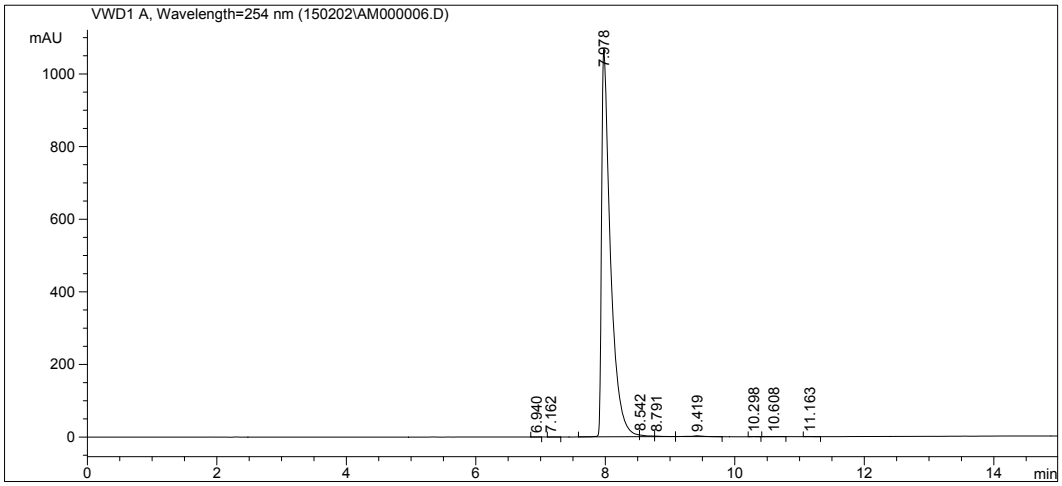


```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=254 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]  mAU   *s    [mAU   ]      %
    ----|-------|----|-------|----------|----------|--------|
       1   6.940 BV    0.0627 9.84830e-1 2.38793e-1 9.582e-3
       2   7.162 VB    0.0647 9.50441e-1 2.21357e-1 9.247e-3
       3   7.978 BV    0.1377 1.01917e4  1066.85510  99.1604
       4   8.542 VV B  0.1006   35.53906    4.58807   0.3458
       5   8.791 VB    0.1094   11.33023    1.46100   0.1102
       6   9.419 BB    0.1701   30.12338    2.34742   0.2931
       7  10.298 BB    0.0793    1.70432 3.46252e-1   0.0166
       8  10.608 BB    0.1459    4.08992 4.19049e-1   0.0398
       9  11.163 VB    0.0908    1.56734 2.44432e-1   0.0152

    Totals :                  1.02780e4  1076.72147

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