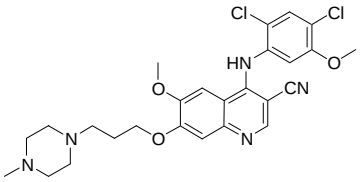
Certificate of Analysis

Axon Catalogue ID:	1407	**Batch Number:**	3
Product Name:	Bosutinib		
Alternative Name(s):	SKI 606		
IUPAC Name:	4-(2,4-Dichloro-5-methoxy-phenylamino)-6-methoxy-7-[3-(4-methyl-piperazin-1-yl)propoxy]quinoline-3-carbonitrile		
Structure:		**Amount:**	
CAS number:	380843-75-4	**MW:**	530.45
Batch Molecular Formula:	C26H29Cl2N5O3.3H2O	**Batch MW:**	584.48
Appearance:	Off-white solid		
TLC (R_f)**:**	0.1 DCM/MeOH (9:1)		
Chemical Purity:	100.0%		
Optical Purity (ee):			
1H-NMR (300 MHz):	Analytical data confirm chemical structure		
Mass Spec:	Analytical data confirm chemical structure		
Microanalysis:	C, H, and N fit within 0,4% of theoretical calculation		
Storage Conditions:	Store at +4°C		

Solubility Data:

Solvent	Solubility (mg/ml)	Solubility (mM)	Remarks
Water			Not Tested
0.1N NaOH (aq)			Not Tested
0.1N HCl (aq)	10.8	18.5	
DMSO	40.0	68.4	
EtOH			Not Tested

Remarks: Microanalysis: Calcd. C 53.43, H 6.04, N 11.98; Found: C 53.09, H 5.67, H 11.72.

Pfizer compound; Sold for research purposes under agreement from Pfizer Inc.

QC Date: 5/2/2013

The purity of Axon products is confirmed by HPLC, MS, NMR and/or microanalysis. Analytical data are available upon request. Request can be submitted by e-mail to info@axonmedchem.com indicating Axon Catalogue ID and Batch number.

Caution: Not fully tested. For research purposes only

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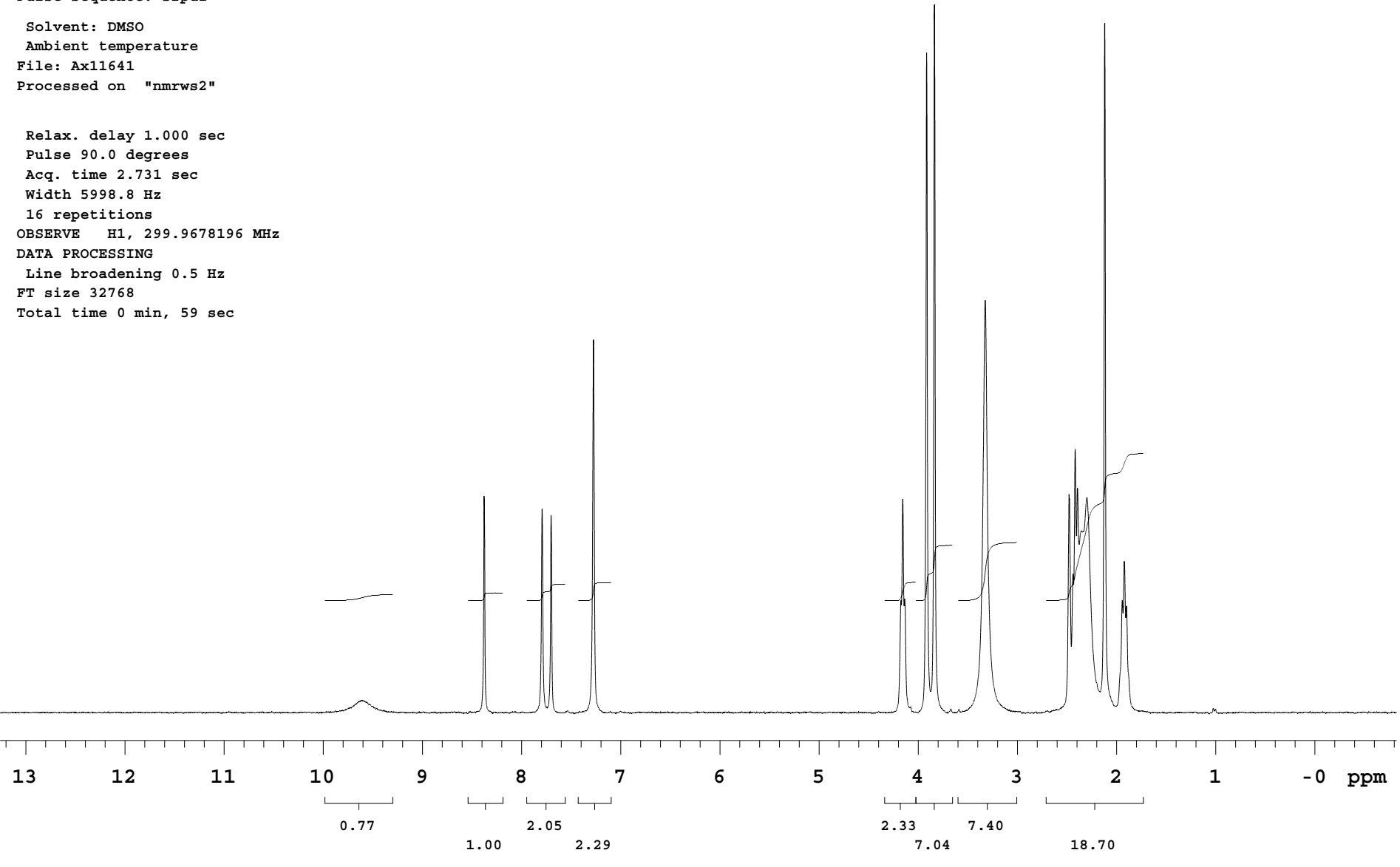
Ax11641 in DMSOd6 at 300 MHz

Pulse Sequence: s2pul

Solvent: DMSO
Ambient temperature
File: Ax11641
Processed on "nmrws2"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.731 sec
Width 5998.8 Hz
16 repetitions
OBSERVE H1, 299.9678196 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 0 min, 59 sec



Ax11641 in DMSOd6 at 300 MHz

Pulse Sequence: s2pul

INDEX	FREQUENCY	PPM	HEIGHT
1	2513.233	8.378	38.7
2	2337.487	7.792	36.4
3	2310.759	7.703	35.3
4	2182.245	7.275	66.7
5	1252.255	4.175	20.1
6	1246.763	4.156	38.2
7	1240.905	4.137	20.4
8	1174.634	3.916	118.0
9	1150.835	3.837	126.7
10	997.057	3.324	73.8
11	743.689	2.479	39.1
12	731.607	2.439	24.8
13	725.016	2.417	47.1
14	718.060	2.394	40.2
15	689.501	2.299	38.5
16	635.679	2.119	123.3
17	582.589	1.942	20.1
18	576.365	1.921	27.1
19	569.774	1.899	19.1

Axon Medchem BV
Biotech Center UMCG
Postbus 770
9700AT
Groningen
The Netherlands

Sample and Acquisition parameters

Sample and Acquisition Information

Sample Name: Ax11641-01
Date Acquired: 18/04/13
Used Method: Gradient B.lcm

Data file:Ax11641-01-01.lcd
Acquisition Time:23:09:51
Injection Volume: 2 ul

Comment:

System Parameters

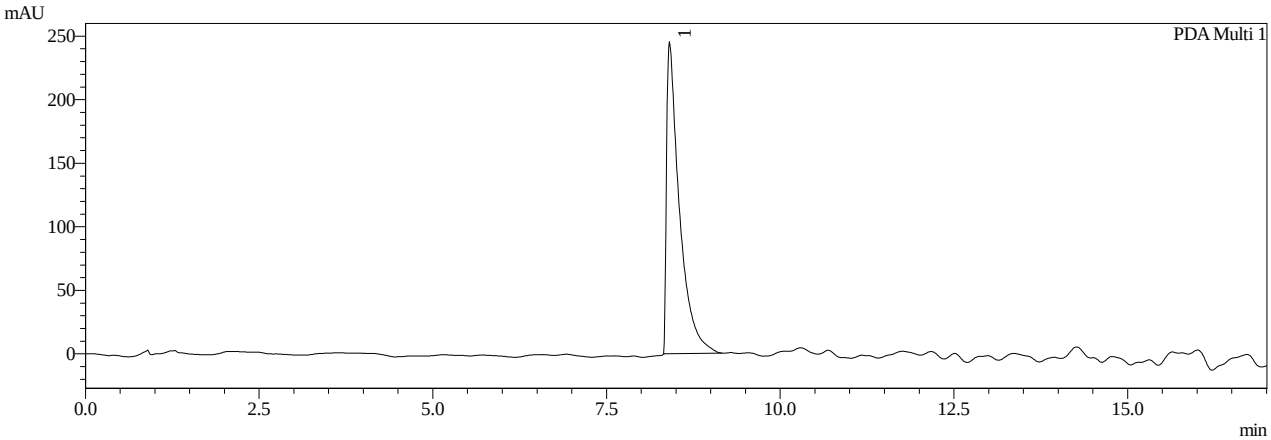
Probe type: ESI Type M

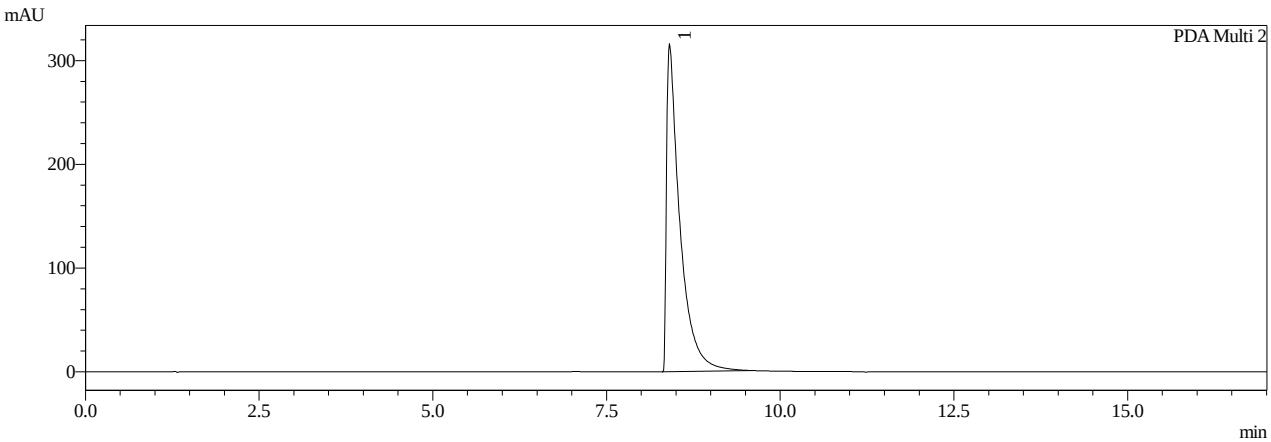
Flow: 1.000 ml/min
Buffer: B/C: 20.0/0.0 %
Concentration D: 20.0 %

Column Name: Luna 5u C18(2) 100A
Length x diameter - 100 x 4.6 mm

Oven Temperature: 40 °C

Chromatogram(s)





PDA Ch1 204nm 4nm

Peak#	Ret. Time (min.)	Area %
1	8.40	100.00
Total		100.00

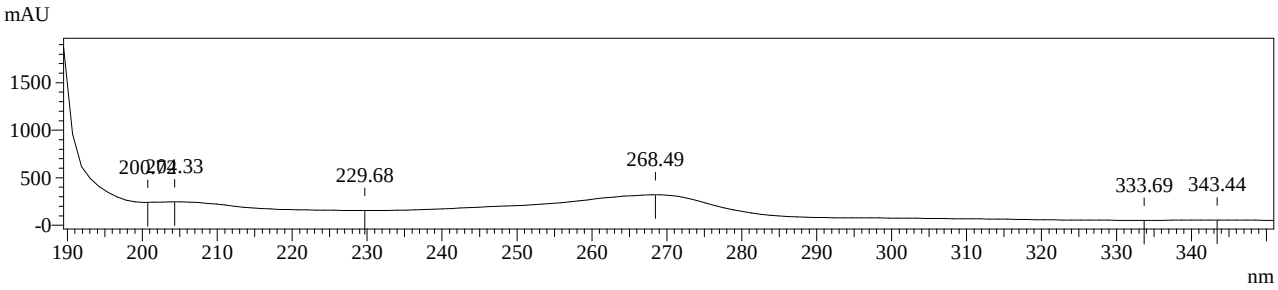
PDA Ch2 268nm 4nm

Peak#	Ret. Time (min.)	Area %
1	8.40	100.00
Total		100.00

PDA Ch3

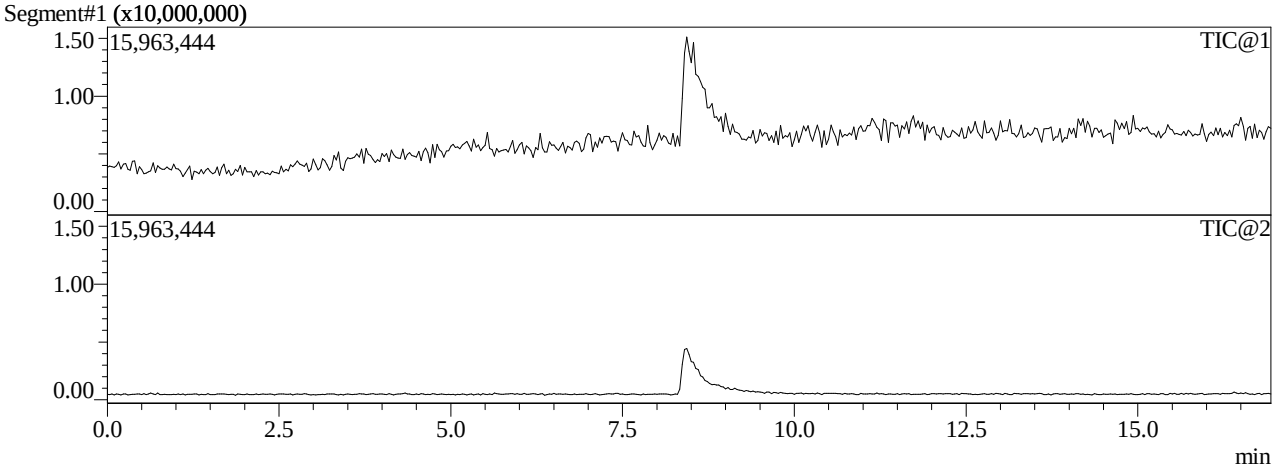
UV spectra

#: 1
Retention Time: 8.414
Maximum wavelength:268/204/343 nm



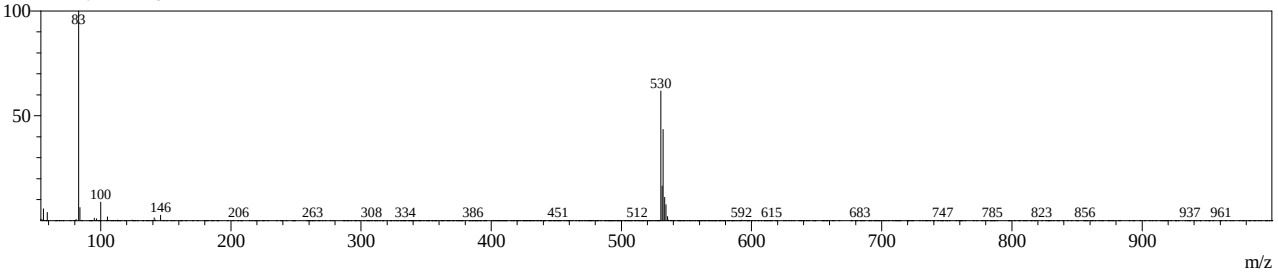
MS

TiC

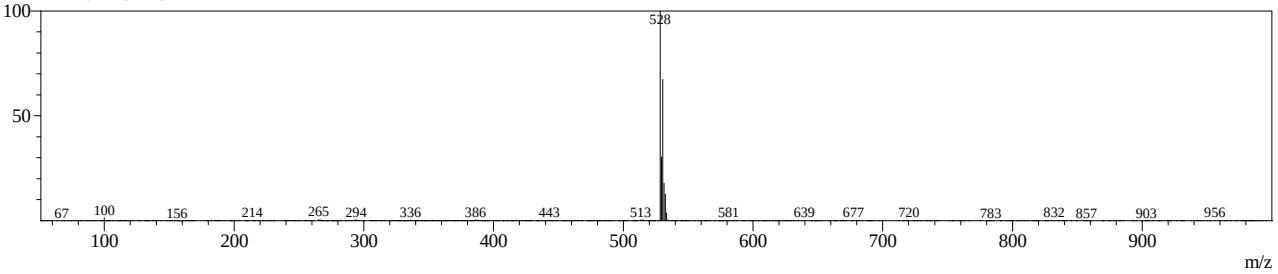


MS Spectrum Graph

#:1 Ret.Time:Averaged 8.267-9.300(Scan#:497-559)
Polarity:Pos Segment1 - Event1



#:2 Ret.Time:Averaged 8.283-9.317(Scan#:498-560)
Polarity:Neg Segment1 - Event2



Extended Method and Gradient Information

Mobile Phase Setup:
Mobile Phase A: Water
Mobile Phase B: Aqueous buffer pH 8
Mobile Phase C: Aqueous buffer pH 4
Mobile Phase D: Acetonitril

Pump Settings:

Pump Mode	:Low pressure gradient
Pump A	:LC-2010 Pump
Flow	:1.000 mL/min
B.Conc	:20.0 %
C.Conc	:0.0 %
D.Conc	:20.0 %
B.Curve	:0
C.Curve	:0
D.Curve	:0
PressMax	:250 bar
PressMin	:0 bar
LPGE Mode	:Auto

LC-Program:

Time	Unit	Command	Value	Comment
10.00	Pumps	Pump D Conc.	80	
17.00	Pumps	Pump D Conc.	80	
18.00	Pumps	Pump D Conc.	20	
22.00	Pumps	Pump B Conc.	20	
22.00	Pumps	Pump D Conc.	20	
22.00	Controller	Stop