Supplementary Information

Urea / thiourea as ammonia surrogate: A catalyst free synthesis of 2-substituted 2,3-dihydroquinazolin-4(1*H*)-ones / quinazoline-4(3*H*)-ones

P. Paradesi Naidu^{a,b}, Akula Raghunadh^a, K. Raghavendra Rao^a, Ramamohan Mekala^a, J. Moses Babu^c, B. R. Rao^a, V. Siddaiah^b, Manojit Pal^{d,*}

^a*Process Research and Development, Dr. Reddy's Laboratories Ltd., Bollaram, Jinnaram, Medak, Andhra Pradesh, India.*

^b*Organic Research Labs, Dept. of Organic Chemistry, Andhra University, Visakhapatnam-530 003, India.*

^c*Analytical Research, Custom Pharmaceutical Services, Dr. Reddy's Laboratories Ltd., Bollaramroad, Miyapur, Hyderabad-500049, India.*

^d*Dr. Reddy's Institute of Life Sciences, University of Hyderabad Campus, Hyderabad-500 046, India.*

E-mail: manojitpal@rediffmail.com (MP)

EXPERIMENTAL

All the reactants and reagents were used as received from various commercial sources without further purification or prepared as described in the literature. Reactions were stirred using Teflon-coated magnetic stirring bars. The progress of the reaction was monitored by using silica gel plates (Merck) and chloroform-methanol (9:1) as a solvent system. Iodine was used as a developing agent. Melting points (mp) were determined by using open capillaries on Thomas Hoover melting point apparatus and are uncorrected. An Agilent 1100 series LC system coupled to a triple quadrupole mass spectrometer (Agilent LC/MS/MS model 6410, Agilent Technologies Inc., Santa Clara, CA, USA) with electrospray ionization (ESI) Source was used and ES ionization was done in positive mode. The HRMS analysis has been performed on the Micromass LCT Premier XE mass spectrometer equipped with an ESI lock spray source for accurate mass values (Water Corporation, Milford, MA, USA). The NMR spectra were recorded using Varian mercury plus 400MHz FT NMR Spectrometer. The chemical shifts are reported as parts per million (δ ppm) with tetramethylsilane (TMS) as an internal standard. The coupling constants are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

Typical method for the synthesis of 2-(2-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one¹ (3a):

A mixture of isatoic anhydride **1** (3.0 mmol), 2-bromobenzaldehyde **2a** (3.3 mmol), urea (3.3 mmol) in EtOH (4.0 mL) was stirred at reflux for 6h under open air. The progress of the reaction was monitored by TLC. After completion of the reaction the mixture was concentrated under reduced pressure. The crude product obtained was crystallised from methanol to give the analytically pure compound as a colourless solid; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.19 (s, 1H, NH), 7.69-7.65 (m, 3H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 6.8 Hz, 1H), 6.98 (s, 1H, NH), 6.77 (d, *J* = 7.6 Hz, 1H), 6.74 (t, *J* = 8.0 Hz, 1H), 6.09 (s, 1H, CH); ¹³C NMR (DMSO-*d*₆, 100 MHz) 163.6, 147.7,

139.1, 133.4, 132.8, 130.7, 129.1, 128.1, 127.4, 122.2, 117.5, 114.7, 114.6, 66.4; HRMS (ESI): Calcd for $C_{14}H_{12}N_2OBr$, $(M+H)^+$ 303.0133, found 303.0140.

Synthesis of 2-(4-ethoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3b):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 4-ethoxy benzaldehyde **2b** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a colourless solid; 1H NMR (400 MHz, $DMSO-d_6$) δ 8.16 (br s, 1H, NH), 7.59 (d, $J = 7.6$ Hz, 1H), 7.38 (d, $J = 8.4$ Hz, 2H), 7.23-7.19 (t, $J = 8$ Hz, 1H), 6.99 (s, 1H, NH), 6.93 (d, $J = 8.8$ Hz, 2H), 6.74 (d, $J = 8$ Hz, 1H), 6.68 (t, $J = 7.2$ Hz, 1H), 5.68 (s, 1H, CH), 4.00 (q, $J = 6.8$ Hz, 2H), 1.31 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR ($DMSO-d_6$, 100 MHz) 163.6, 162.3, 161.2, 134.5, 133.2, 129.5 (2C), 128.1, 126.1, 125.8 (2C), 120.6, 114.3 (2C), 63.4, 14.5; HRMS (ESI): Calcd for $C_{16}H_{16}N_2O_2$ $(M+H)^+$ 267.1134, found 267.1122.

Synthesis of 2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one² (3c):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 2-chlorobenzaldehyde **2c** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a colourless solid; 1H NMR (400 MHz, $DMSO-d_6$) δ 8.21 (s, 1H, NH), 7.66 (d, $J = 6$ Hz, 2H), 7.50 (d, $J = 8$ Hz, 1H), 7.51 (m, $J = 4.2$ Hz, 2H), 7.26 (t, $J = 7.6$ Hz, 1H), 7.01 (s, 1H, NH), 6.77 (d, $J = 8.0$ Hz, 1H), 6.73 (t, $J = 7.2$ Hz, 1H), 6.13 (s, 1H, CH); ^{13}C NMR ($DMSO-d_6$, 100 MHz) 163.6, 147.7, 137.8, 133.4, 131.8, 130.2, 129.5, 128.7, 127.4, 127.3, 117.4, 114.6, 114.5, 63.6; HRMS (ESI): Calcd for $C_{14}H_{12}N_2OCl$ $(M+H)^+$ 259.0638, found 259.0633.

Synthesis of 2-(2-iodophenyl)-2,3-dihydroquinazolin-4(1H)-one (3d):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 2-iodobenzaldehyde **2d** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a colourless solid; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.15 (s, 1H, NH), 7.91 (d, $J = 7.2$ Hz, 1H), 7.70-7.66 (m, 2H), 7.47 (t, $J = 7.0$ Hz, 1H), 7.26 (t, $J = 7.2$ Hz, 1H), 7.18 (t, $J = 6.0$ Hz, 1H), 6.95 (s, 1H, NH), 6.77 (m, $J = 8.4$ Hz, 2H), 5.95 (s, 1H, CH); ^{13}C NMR ($\text{DMSO-}d_6$, 100 MHz) 163.6, 147.7, 139.1, 133.4, 132.8, 130.7, 129.1, 128.1, 127.4, 122.2, 119.5, 114.7, 114.6, 66.4; MS ($\text{M}^+ \text{H}^+$) 351 (100%).

Synthesis of 2-phenylquinazolin-4(3H)-one³ (**3e**):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), benzaldehyde **2e** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a pale yellow solid; ^1H NMR ($\text{DMSO-}d_6$ 400 MHz,) δ 12.54 (br s, 1H, NH), 8.15-8.25 (m, 3H), 7.85 (dd, $J = 7.2, 7.2$ Hz, 1H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.50-7.65 (m, 4H); ^{13}C NMR ($\text{DMSO-}d_6$, 100 MHz) 162.2, 152.3, 148.7, 134.6, 132.7, 131.3, 128.6 (2C), 127.7 (2C), 127.5, 126.6, 125.8, 120.9; HRMS (ESI): Calcd for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}$ ($\text{M}^+ \text{H}^+$) 223.0871, found 223.0867.

Synthesis of 2-(4-hydroxyphenyl)quinazolin-4(3H)-one (**3f**):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 4-hydroxybenzaldehyde **2f** (3.3 mmol) and urea (3.3 mmol) according to the procedure

described above and was isolated as a colourless solid; ^1H NMR (DMSO- d_6 , 400 MHz) δ 12.30 (s, 1H, NH), 10.14 (s, 1H, OH), 8.13-8.09 (m, J = 8.8 Hz, 3H), 7.80 (t, J = 7.2 Hz, 1H, Ar H), 7.68 (d, J = 8.4 Hz, 1H), 7.48 (t, J = 8.1 Hz, 1H), 6.9 (d, J = 8.8 Hz, 2H); ^{13}C NMR (DMSO- d_6 , 100 MHz) 169.0, 160.2, 158.4, 140.2, 135.2, 132.1, 129.4 (2C), 126.2 (2C), 125.2, 118.4, 116.2, 114.2; HRMS (ESI): Calcd for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}_2$ ($\text{M}^+ \text{H}^+$) 239.0821, found 239.0820.

Synthesis of 2-(4-fluorophenyl)quinazolin-4(3H)-one⁴ (3g):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 4-fluorobenzaldehyde **2g** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a white solid; ^1H NMR (DMSO- d_6 , 400 MHz) δ 12.57 (s, 1H, NH), 8.27 (t, J = 6.6 Hz, 2H), 8.16 (d, J = 7.6 Hz, 1H), 7.85 (t, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.53 (t, J = 7.2 Hz, 1H), 7.39 (t, J = 8.8 Hz, 2H); ^{13}C NMR (DMSO- d_6 , 100 MHz) 169.0, 166.2, 158.2, 142.6, 134.3, 131.1, 130.2, 129.1 (2C), 126.1 (2C), 118.1, 116.4, 115.6; HRMS (ESI): Calcd for $\text{C}_{14}\text{H}_{10}\text{N}_2\text{OF}$, ($\text{M}^+ \text{H}^+$) 241.0777, found 241.0787.

Synthesis of 2-(5-fluoro-1H-indol-3-yl)quinazolin-4(3H)-one (3h):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 5-fluoro-1H-indol-3-yl benzaldehyde **2f** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a pale yellow solid; ^1H NMR (DMSO- d_6 , 400 MHz) δ 12.19 (s, 1H, NH), 11.97 (s, 1H, NH), 8.61 (d, 1H), 8.40 (dd, J = 7 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.79 (m, J = 8.0 Hz, 2H), 7.52 (m, J = 7.8 Hz, 1H), 7.44 (t, J = 6.4 Hz, 1H), 7.08 (m, J = 6.8 Hz, 1H); ^{13}C NMR (DMSO- d_6 , 100 MHz) 150.0, 149.5,

134.4, 133.4, 130.7, 127.0, 125.7, 125.2, 120.4, 113.2, 113.1, 111.2, 110.7, 108.6, 107.2, 107.0; HRMS (ESI): Calcd for C₁₆H₁₁N₃OF, (M+ H)⁺ 280.0886, found 280.0896.

Synthesis of 2-(3-bromophenyl)quinazolin-4(3H)-one (3i):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 3-bromobenzaldehyde **3i** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a pale yellow solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 12.62 (s, 1H, NH), 8.38 (s, 1H), 8.22 (dd, *J* = 8.4, 8.8 Hz, 2H), 7.87 (t, *J* = 6.8 Hz, 1H), 7.84 (t, *J* = 7.2 Hz, 2H), 7.52 (m, *J* = 8.4 Hz, 2H); ¹³C NMR (DMSO-*d*₆, 100 MHz): 166.2, 163.6, 148.7, 139.6, 134.5, 132.8, 131.6, 129.3, 128.4, 127.2, 122.2, 119.5, 115.7, 114.8; HRMS (ESI): Calcd for C₁₄H₁₀N₂OBr, (M+ H)⁺ 300.9979, found 300.9985.

Synthesis of 2-(4-(dimethylamino)phenyl)quinazolin-4(3H)-one (3j):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 4-(dimethylamino)benzaldehyde **2j** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a colourless solid; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 12.17 (s, NH, 1H), 8.13 (d, *J* = 8.8 Hz, 2H), 8.10 (d, *J* = 6.8 Hz, 1H), 7.77 (t, *J* = 7.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.0 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 2H), 3.01 (s, 6H, 2Me); ¹³C NMR (DMSO-*d*₆, 100 MHz) 162.3, 152.2, 149.3, 134.3, 128.8 (2C), 126.9, 125.7 (2C), 125.3, 120.3, 118.7, 111.2 (2C), 38.8 (2C); HRMS (ESI): Calcd for C₁₆H₁₆N₃O, (M+ H)⁺ 266.1286, found 266.1293.

Synthesis of 2-(2,4-difluorophenyl)quinazolin-4(3H)-one (3k):

The title compound was prepared via the reaction of isatoic anhydride (3.0 mmol), 2,4-difluorobenzaldehyde **2k** (3.3 mmol) and urea (3.3 mmol) according to the procedure described above and was isolated as a colourless solid; ^1H NMR (DMSO- d_6 , 400 MHz) δ 12.58 (s, 1H, NH), 8.18 (d, $J = 7.2$ Hz, 1H), 7.88 (m, $J = 7.4$ Hz, 3H), 7.57 (t, $J = 7.2$ Hz, 1H), 7.47 (t, $J = 8.8$ Hz, 1H), 7.27 (t, $J = 6.4$ Hz, 1H); ^{13}C NMR (DMSO- d_6 , 100 MHz) 161.4, 149.1, 148.5, 134.6, 132.6, 127.4, 127.0, 125.8, 121.0, 119.0, 112.1, 111.8, 104.9, 104.6. HRMS (ESI): Calcd for $\text{C}_{14}\text{H}_9\text{N}_2\text{OF}_2$, ($\text{M} + \text{H}$) $^+$ 259.0694, found 259.0683.

REFERENCES

- [1] Wang, X.-S.; Yang, K.; Yao, C.-S.; Zhang, M.-M. *Synth. Commun.* **2010**, *40*, 2633.
- [2] Zeng, L.-Y.; Cai, C. *J. Heterocycl. Chem.* **2010**, *47*, 1035.
- [3] Heravi, M. M.; Tavakoli-Hoseini, N.; Bamoharram, F. F. *Synth. Commun.* **2011**, *41*, 707.
- [4] Wang, X.-S.; Yang, K.; Zhang, M.-M.; Yao, C.-S. *Synth. Commun.* **2010**, *40*, 2633.
- [5] Zhou, J.; Fang, J. *J. Org. Chem.* **2011**, *76*, 7730.

Copies of spectra

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

41 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-2 Br: 0-1

ISA-U-1

1: TOF MS ES+

130409003 10 (0.364) Cm (3.11-20.28x0.025)

2.75e+003

Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.0140	303.0133	0.7	2.3	9.5	132.6	C14 H12 N2 O Br

CEB-3 ISA-U-1 In DMF

NAME: 400MHz
 ACQ: 04/12/2012
 ANALYST: G. S. Smith
 DATE: 04th April 2012

CTC-3 ISA-U-1 1h 0450
 NMR-400MHz
 AR.No: M6413/642
 Analyst: Harikabu
 Date: 5th April 2013

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

58 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-4 O: 0-4

ISA-U-8

1: TOF MS ES+

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130409005 9 (0.338) Cm (9:12-16:25x0.025)

1.70e+003

Minimum:							
Maximum:	5.0	5.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
267.1122	267.1134	-1.2	-4.5	10.5	1219.7	C16 H15 N2 O2

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)

Elements Used:

C: 0-15 H: 0-15 N: 0-2 O: 0-2 Cl: 0-1

ISA-U-Cl

130107001 11 (0.299) Cm (11:18-13x0.010)

Gajanan
1: TOF MS ES+
5.69e+004

Minimum:

Maximum:

5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
259.0633	259.0638	-0.5	-1.9	9.5	181.0	C14 H12 N2 O Cl

C10-3 ISA-U-Cl in DMSO

400MHz
AR.No:ME6113/381
Analyst: Ganesh
Date: 4th Jan 2013.

TDC-219 3/BGX/182 Fz2 in DMSO

NMR-400MHz

AK No:MR1012/1751

Analyte: Haribabu

Date:17th Oct.2012

NUCLEUS : ¹H
PULP (Hz): 400.23
EXP : s2pul

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-4 O: 0-2

ISA-U-11

1: TOF MS ES+

130418036 16 (0.494) Cm (16.18-(1+28.35)x0.025)

6.59e+003

Minimum:				-5.0		
Maximum:	5.0	5.0		80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0867	223.0871	-0.4	-1.8	10.5	1.1	C14 H11 N2 O

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

34 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-25 N: 0-2 O: 0-4

ISA-U-7

1: TOF MS ES+

130314006 13 (0.365) Cm (13:17-(1.3+21.24))

6.93e+004

Minimum:				-5.0		
Maximum:	5.0	5.0		80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
239.0820	239.0821	-0.1	-0.4	10.5	24.5	C14 H11 N2 O2

CT0-3 ISA-U-7 in DMSO

NMR-400MHz

AR-Vol: B313/219

Analyst: Ganesh

Date: 4th March 2013

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-2 F: 0-1

ISA-U-9

1: TOF MS ES+

130430022 9 (0.297) Cm (8.12-15.21x0.025)

5.76e+003

Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
241.0787	241.0777	1.0	4.1	10.5	8.0	C14 H10 N2 O F

CT0-3 ISA-U-10/9 in DMSO

NMR-400MHz
Ac.No:ME0213/75
Analyst: Ganesh
Date: 1st March 2013

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-18 H: 0-18 N: 0-3 O: 0-1 F: 0-1

ISA-U-14

1: TOF MS ES+

130319003 12 (0.320) Cm (12:16-29.45)

1.44e+004

Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
280.0896	280.0886	1.0	3.6	12.5	1.1	C16 H11 N3 O F

CT0-3 ISA-U-14 in DMSO

HR=400MHz
AK.No:ME0513/2322
Analyst: Ganesh
Date: 26th March 2013

NMR-400MHz
AR.No:ME0313/2793
Analyst: Haribabu
Date: 29th March 2013

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-2 Br: 0-1

ISA-U-3-A

1: TOF MS ES+

130430023 13 (0.422) Cm (13:14)

2.38e+004

Minimum:				-5.0		
Maximum:	5.0	5.0		80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-PTT	Formula
300.9985	300.9976	0.9	3.0	10.5	51.0	C14 H10 N2 O Br

CTD-3 ISA-U-3 In DMSO

HRP-400MHz
AK.No:ME 0213/2457
Analyst: Bar Hada
Date:27th Feb, 2013

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

32 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-4 O: 0-2

ISA-U-16

1: TOF MS ES+

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Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

33 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 0-15 H: 0-15 N: 0-4 O: 0-2 F: 0-2

ISA-U-18

1: TOF MS ES+

130507006 6 (0.198) Cm (6.7)

6.12e+004

Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
259.0694	259.0683	1.1	4.2	10.5	172.6	C14 H9 N2 O F2

CT0-3 ISA-U-18 1n DMSO

NMR=400MHz

AR.No:ME0413/55

Analyst: Ganesh

Date: 01st April 2013

CTO-3 ISA-U-18 in DMSO

NMR-400MHz
AR.No:ME0413/650
Analyst: Haribabu
Date: 5th April 2013