

Characterization of 2C-B-BZP (dihydrochloride)

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2C-B-BZP (dihydrochloride), Cayman Item #14793 Batch #0453346

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Forendex

SWGDRUG

Wikipedia

Part 1. Cayman Chemical Company Data

Name: 2C-B-BZP (dihydrochloride)

Synonyms: 1-[(4-bromo-2,5-dimethoxyphenyl)methyl]-piperazine, dihydrochloride

CAS#: N/A

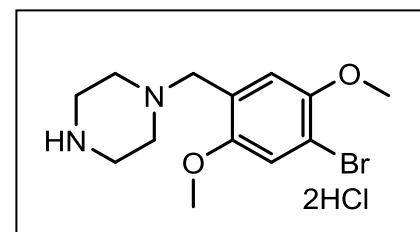
Molecular Formula: C₁₃H₁₉BrN₂O₂ • 2HCl

Molecular Weight: 388.1 g/mol

SMILES: BrC1=CC(OC)=C(CN2CCNCC2)C=C1OC.Cl.Cl

InChI Key: FNDWKKCHLQJPIL-UHFFFAOYSA-N

InChI: InChI=1S/C13H19BrN2O2.2ClH/c1-17-12-8-11(14)13(18-2)7-10(12)9-16-5-3-15-4-6-16;/h7-8,15H,3-6,9H2,1-2H3;2*1H



Background:

2C-B-BZP is a designer drug analogue of the US DEA Schedule I controlled stimulant BZP (N-benzylpiperazine).^{1,2} 2C-B-BZP differs from BZP in that the phenyl ring has methoxy groups in the 2 and 5 positions and a bromine in the 4 position.³ The specific 2,5-dimethoxy-4-bromo substitution pattern on the phenyl ring is also a key feature of the US DEA Schedule I controlled psychedelic phenethylamine 2C-B.⁴ The name "2C-B-BZP" reflects the fact that this designer drug contains key structural motifs from the two highly psychoactive controlled substances. The structure of 2C-B-BZP was elucidated in 2009 after it was detected in seized illicit drug products in Germany.³

1- Forensic Science International, 121, 47-56, 2001.

2- Neuropsychopharmacology, 30, 550-560, 2005.

3- Forensic Science International, 187, 87-96, 2009.

4- Br. J. Pharmacol. 141(7), 1167-1174, 2004.

Figure 1: Liquid Chromatography/Mass Spectrometry of 2C-B-BZP**Experiment Parameters:**

Thermo Scientific LTQ Orbitrap XL mass spectrometer

Flow injection with an eluent of methanol

Electrospray ionization (ESI) in positive mode

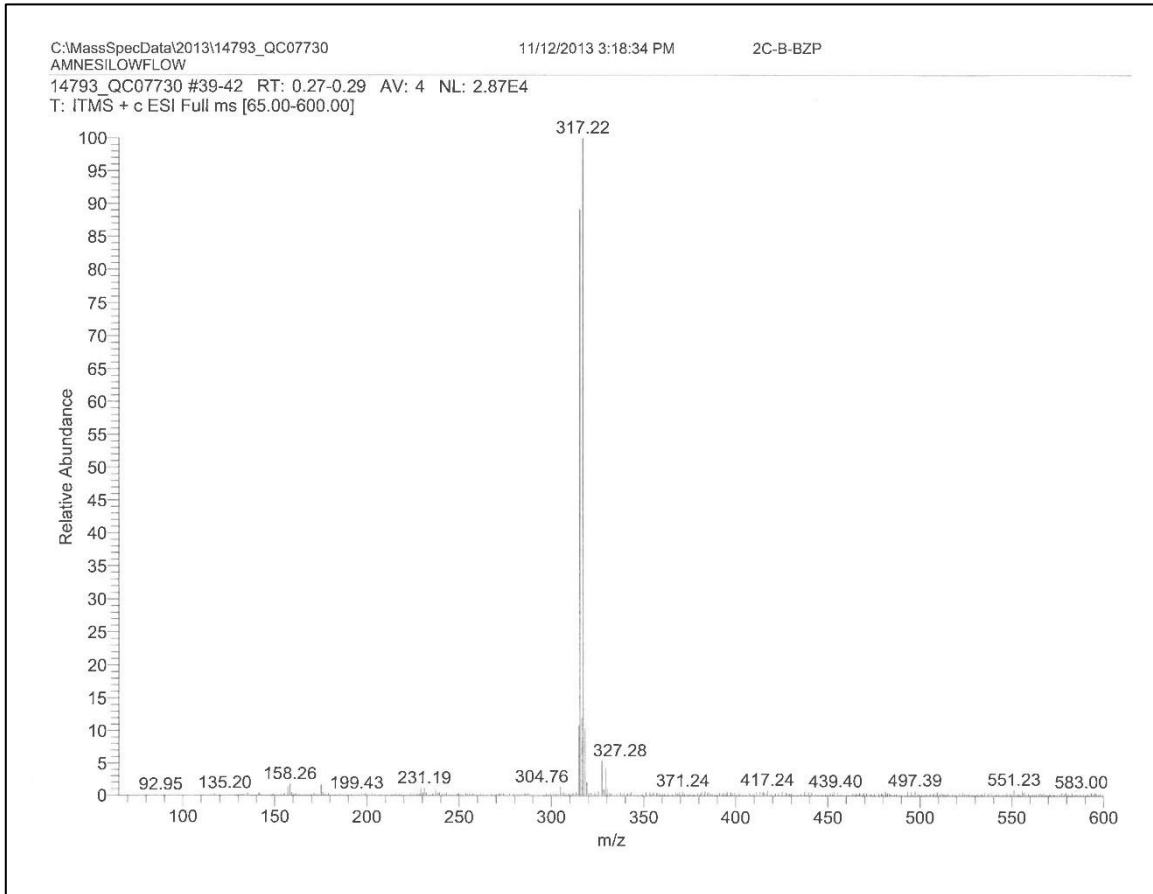
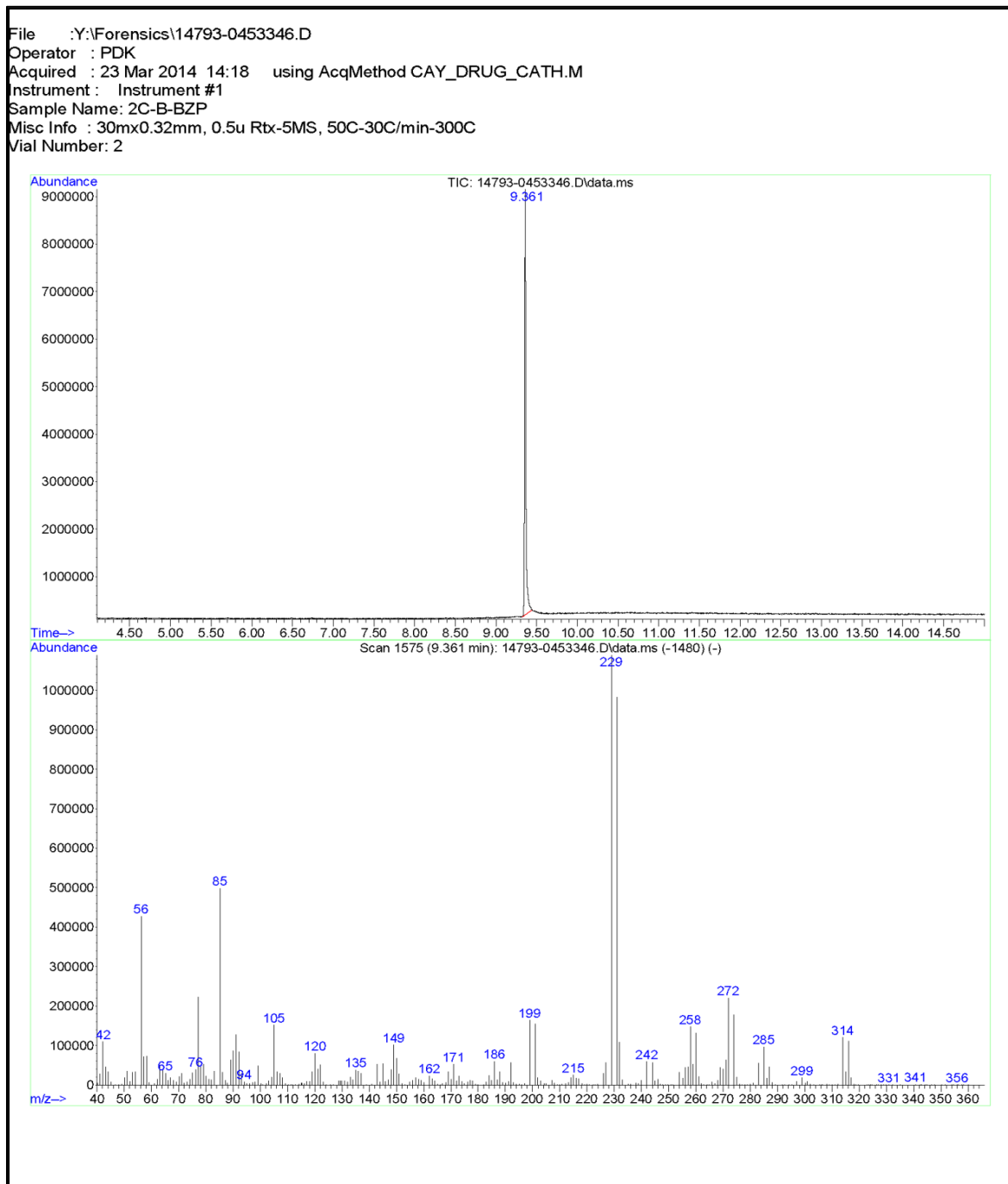
Resolution setting of 30 000 (FWHM) at m/z 400 and internal lock mass of 391.2843 for the $[M+H]^+$ for dioctyl phthalateFull scan: 65-600 m/z 

Figure 2. Gas Chromatography/Mass Spectrometry of 2C-B-BZP

Experiment Parameters:

Agilent 6890 GC/5973 MSD
 15:1 split, 1 mL/min He carrier gas
 300°C inlet
 30 m x 0.32 mm, 0.5 µm Rtx-5MS column
 240°C, ramp 10°C/min to 300°C (hold for 1 min, ramp, hold for 25 min)



Part 2. Georgia Bureau of Investigation Data

Name: 2C-B-BZP (dihydrochloride)

Synonyms: 1-[(4-bromo-2,5-dimethoxyphenyl)methyl]-piperazine, dihydrochloride; 4-bromo-2,5-dimethoxybenzylpiperazine; 4-bromo-2,5-dimethoxy-1-benzylpiperazine

CAS#: N/A

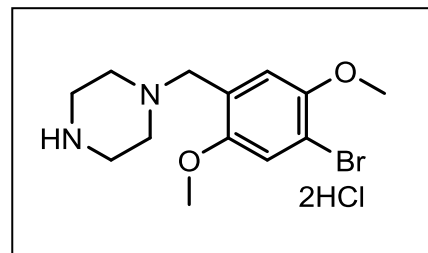
Molecular Formula: C₁₃H₁₉BrN₂O₂

Molecular Weight: 315.2085 g/mol (388.1 g/mol dihydrochloride)

SMILES: BrC1=CC(OC)=C(CN2CCNCC2)C=C1OC.Cl.Cl

InChI Key: FNDWKKCHLQJPIL-UHFFFAOYSA-N

InChI: InChI=1S/C13H19BrN2O2.2ClH/c1-17-12-8-11(14)13(18-2)7-10(12)9-16-5-3-15-4-6-16;;/h7-8,15H,3-6,9H2,1-2H3;2*1H



Gas chromatography / Mass spectrometry:

Sample Preparation: ~ 2mg/mL in EtOH

Instrument: Agilent 7890A gas chromatograph / 5975C mass spectrometer

GC Parameters Column: HP Ultra-1 12m × 200µm × 0.33µm

Carrier gas: Helium

Oven program: 1) initial temperature 70°C for 1 min.

2) ramp to 230°C at 30°C/min.

3) hold at 230°C for 1 min.

Injection parameters: 1µL injection; split ratio: 150:1

Inlet temperature: 275°C

Constant Pressure: 8 psi

MS Parameters Transfer Line temperature: 280°C

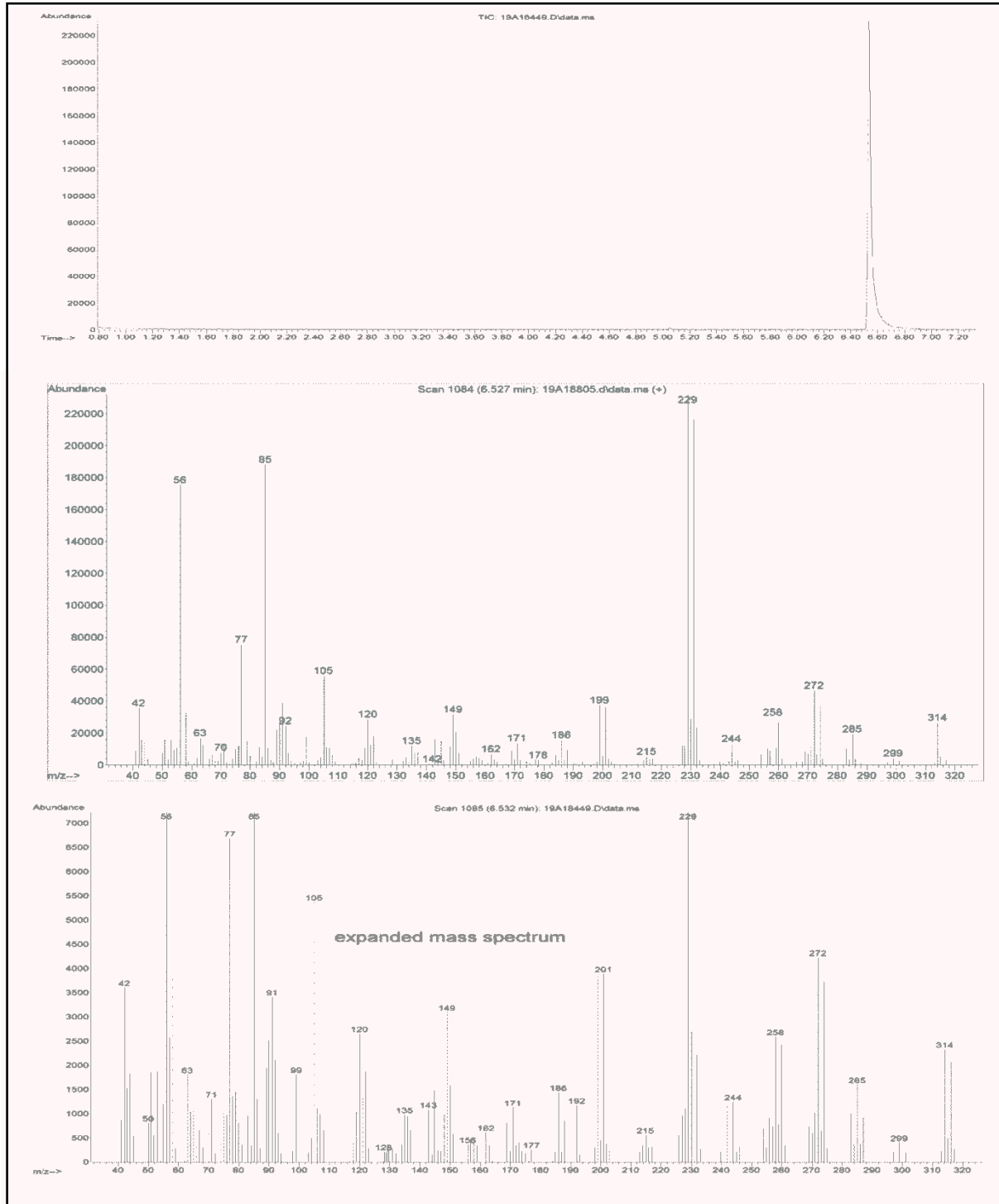
Source temperature: 230°C

Quad temperature: 150°C

Mass scan range: 40-500 amu

Tune file: stune

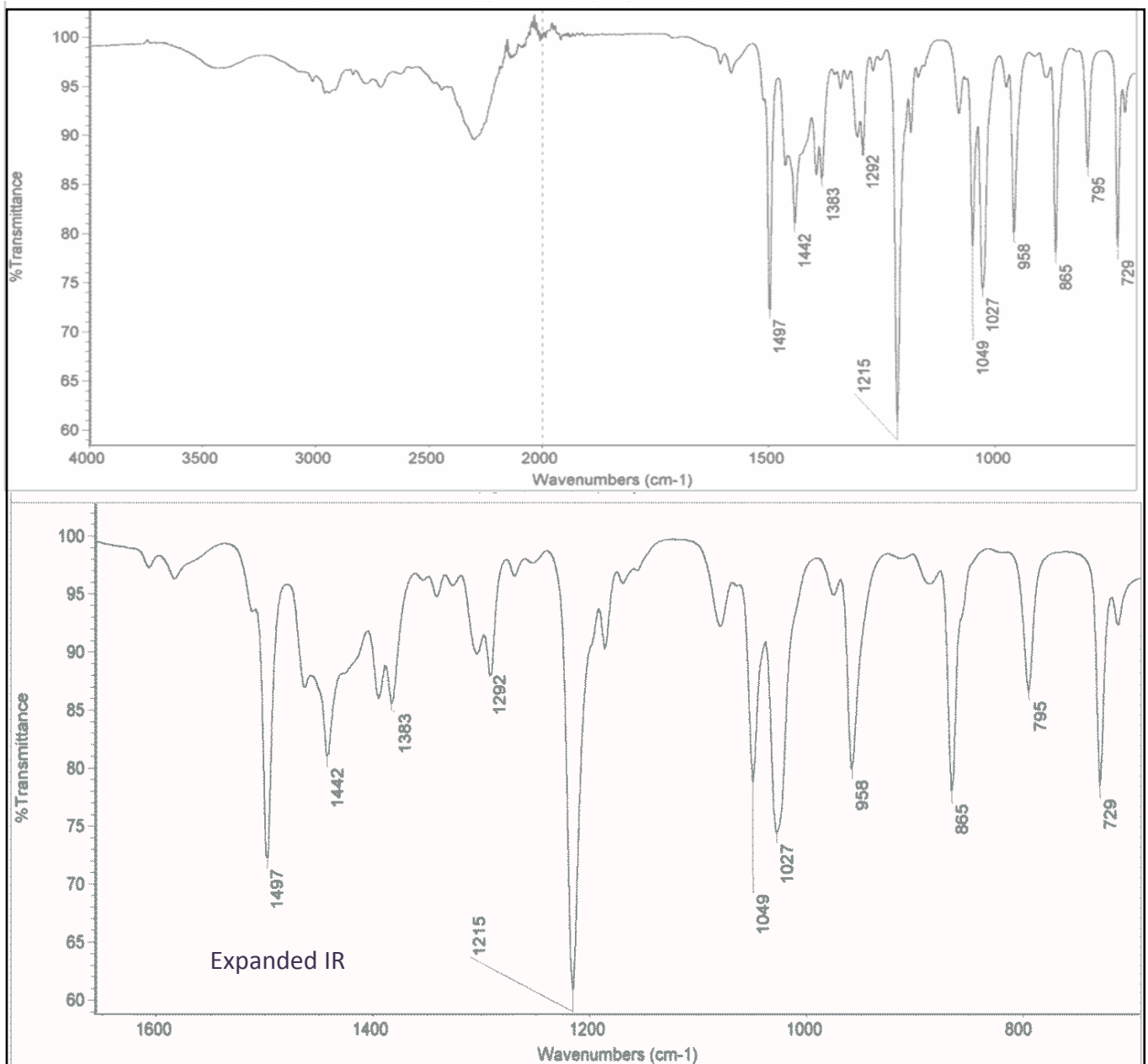
Figure 3: Gas Chromatography/Mass Spectrometry of 2C-B-BZP



Fourier Transform Infrared Spectroscopy

Instrument: Nicolet 4700 with diamond ATR attachment (3 bounce)
Scan parameters: Number of scans: 32
 Number of background scans: 32
 Resolution: 4cm^{-1}
 Sample gain: 8

Figure 4: FTIR of 2C-B-BZP



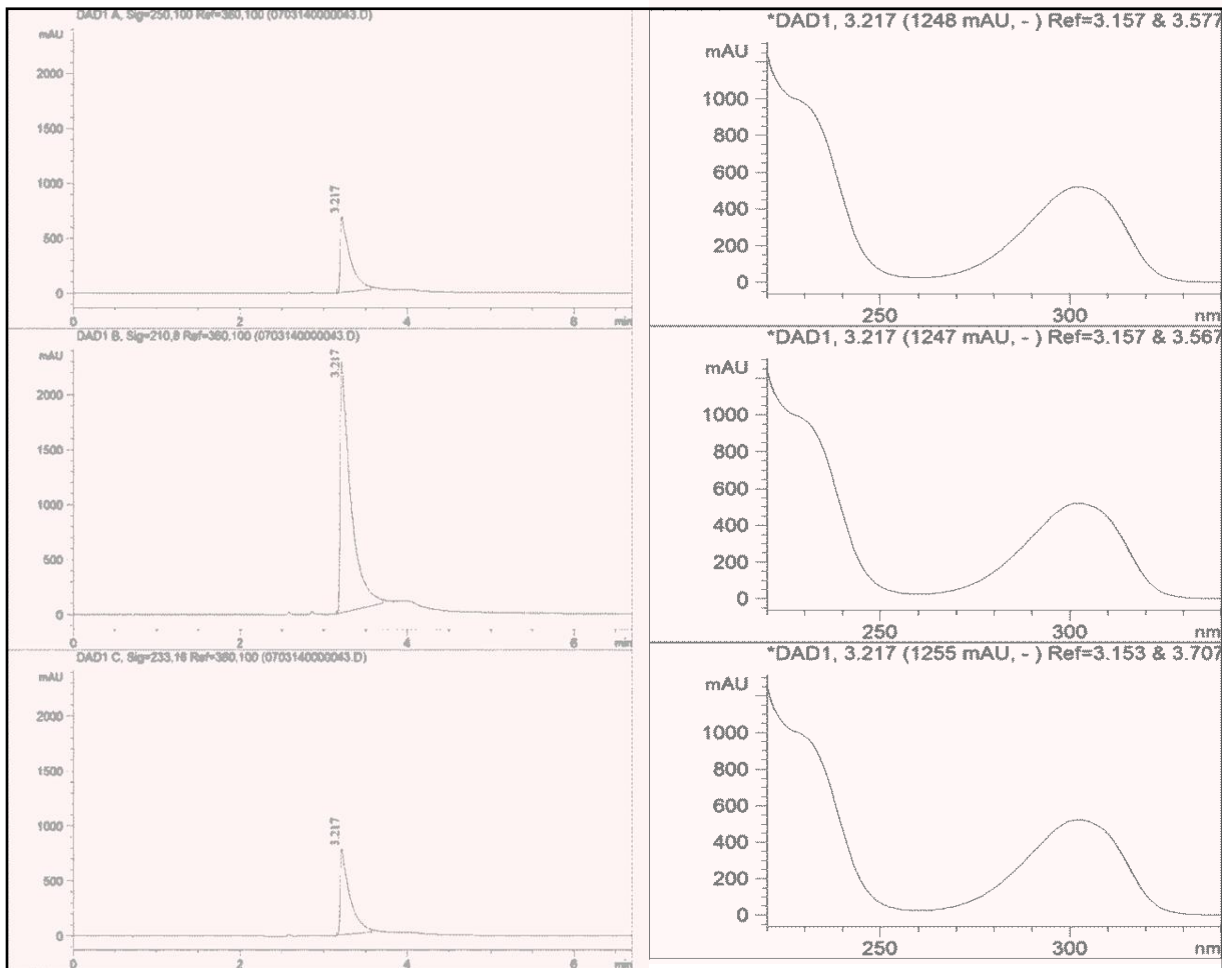
High Performance Liquid Chromatography (HPLC)

Instrument: Agilent 1260 Infinity
LC Parameters: Column: Zorbax Eclipse Plus C18 3.0 x 100mm 35-micron
 Column compartment: 40°C
 Mobile phase: A: Ammonium Phosphate buffer
 B: Acetonitrile

| Time | %A | %B | Flow |
|------|----|----|--------------|
| 0 | 95 | 5 | 1.000 mL/min |
| 0.67 | 95 | 5 | 1.000 mL/min |
| 0.68 | 85 | 15 | 1.000 mL/min |
| 2.00 | 85 | 15 | 1.000 mL/min |
| 6.70 | 15 | 85 | 1.000 mL/min |

UV Parameters: Scan: 220 – 340nm
 Step: 1.0nm
 Slitwidth: 4nm

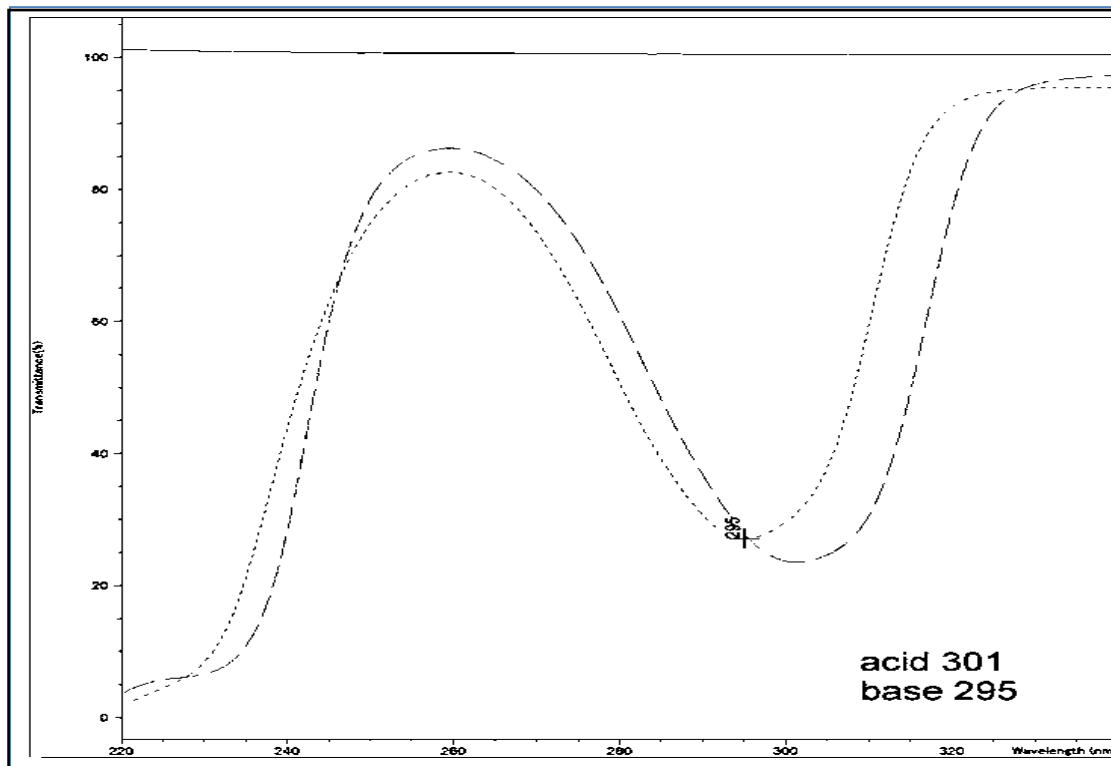
Figure 5. HPLC of 2C-B-BZP



Ultraviolet Spectrophotometry (UV)

Instrument: HP 8453
Parameters: source: deuterium lamp
Path length: 1cm
Transmittance
Wavelength range: 220 – 340nm
Integration time: 0.5 sec
Interval: 1nm

Figure 6. UV of 2C-B-BZP



Part 3. External Links

[Forendex link to 2C-B-BZP](#)

[SWGDRUG Monograph](#)

[Wikipedia link to 2C-B-BZP](#)