**Propargyl bromide as an excellent α -Bromoacetone equivalent:
Convenient and New route to α -aroylacetoness**

*Sakkarapalayam. M. Mahalingam, Indrapal Singh Aidhen**

*Department of Chemistry, Indian Institute of Technology Madras, Chennai - 600 036,
India*

E-mail: isingh@iitm.ac.in

Supporting information

Table of Contents

[A] Experimental section	S2
[B] ^1H NMR, ^{13}C NMR spectra	
(i) Compound 1g	S3-S4
(ii) Compound 3a	S5
(iii) Compound 3b	S6
(iv) Compound 4a	S7
(v) Compound 4b	S8
(vi) Compound 4e	S9
[C] High Resolution Mass spectra	
(i) Compound 3a	S10
(ii) Compound 4b	S10
(iii) Compound 4e	S11
[D] DEPT spectrum of 4a	S11

General Methods and Materials

All solvents were distilled before use. Anhydrous DMF prepared using standard procedure involving drying over CaH_2 and distillation under reduced pressure. Melting points were determined in capillary and are uncorrected. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded using deuteriochloroform (CDCl_3) as solvent and tetramethylsilane (TMS) as a reference. IR spectra were recorded using KBr pallet for solid samples and neat for liquid samples. Electron-Impact mass spectra and HRMS were accomplished at 70 eV. All the reactions were monitored by TLC on precoated silica-gel plates by developing the spots with iodine vapors or under UV-light absorbance.

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

smm-ips-1
DEPARTMENT OF CHEMISTRY, IITM

Q TOF MICRO
CE = 10eV
Cone = 21V

13-Jul-2005 17:36:27
1 sec scan

smmips-1 22 (1.719) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.80,LS 5); Cm (20:22)

5: TOF MS ES+
99.2

Minimum:				-1.5		
Maximum:	5.0	20.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
241.1331	241.1341	-1.0	-4.0	8.5	1	C15 H17 N2 O

Elemental Composition Report

Page 1

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

smmips6
DEPARTMENT OF CHEMISTRY, IITM

Q TOF MICRO
CE = 10eV
Cone = 21V
177.0912

14-Jul-2005 14:00:30
1 sec scan

smmips6 10 (0.773) AM (Cen,4, 80.00, Ar,5000.0,556.33,0.80,LS 5); Cm (10:17)

5: TOF MS ES+
297

Minimum:				-1.5		
Maximum:	5.0	20.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
177.0912	177.0916	-0.3	-1.7	5.5	1	C11 H13 O2

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

ips-smm3
DEPARTMENT OF CHEMISTRY, IITM

Q TOF MICRO
CE = 10eV
Cone = 21V

13-Jul-2005 17:49:15
1 sec scan

ipssmm3 6 (0.457) AM (Cen,4, 80.00, Ar,5000.0,556.32,0.80,LS 5)

5: TOF MS ES+
1.12e3

Minimum: -1.5
Maximum: 5.0 20.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
253.1072	253.1076	-0.4	-1.5	5.5	1	C13 H17 O5

Page 1