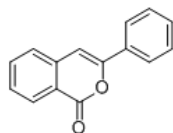


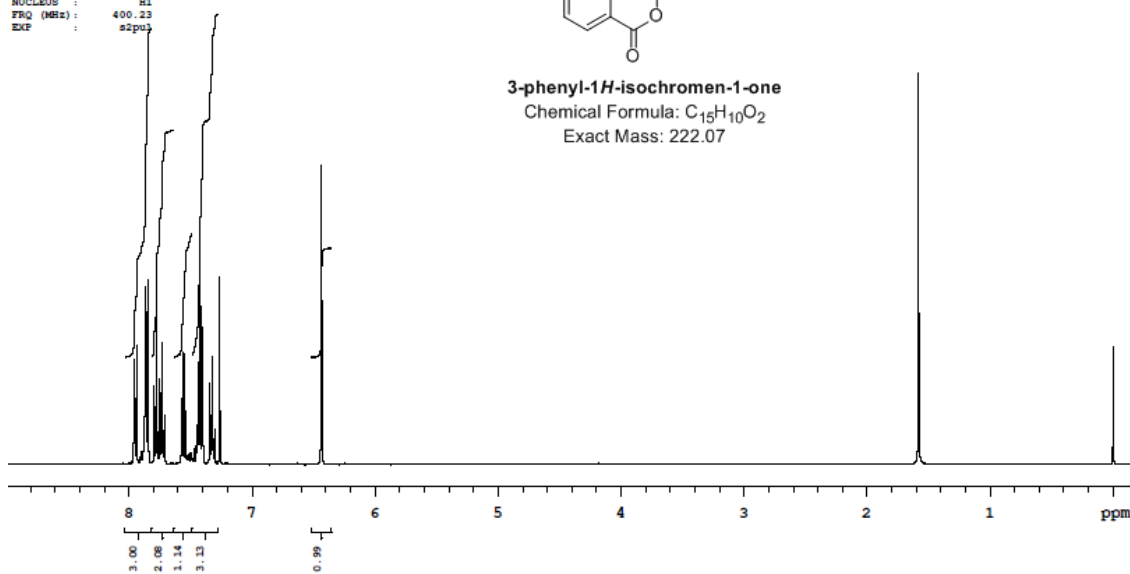
Copies of spectra

MNR-400MHz
AR.No:ME0812/1879
Analyst: Ganesh
Date: 23rd Aug. 2012

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul

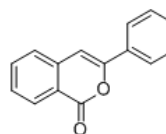


3-phenyl-1H-isochromen-1-one
Chemical Formula: C₁₅H₁₀O₂
Exact Mass: 222.07

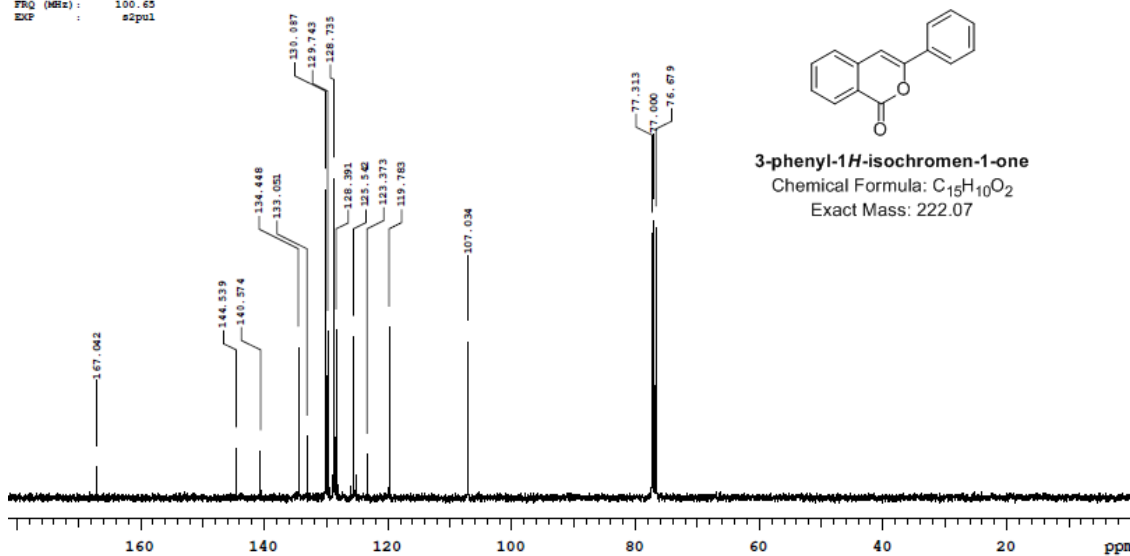


Analyst: Haribabu
Date: 3rd Sep. 2012

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul



3-phenyl-1H-isochromen-1-one
Chemical Formula: C₁₅H₁₀O₂
Exact Mass: 222.07



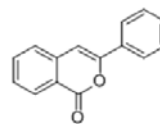
Elemental Composition Report

Page 1

Single Mass Analysis

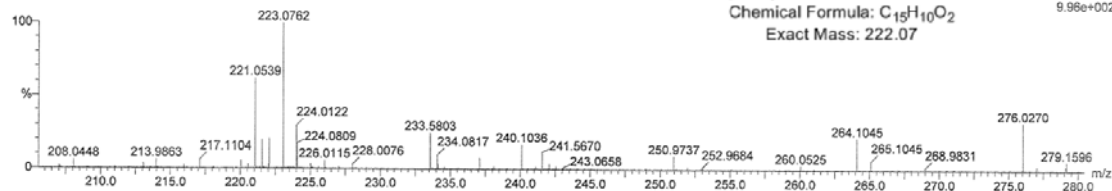
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 38 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
 Elements Used:
 C: 0-25 H: 0-28 N: 0-4 O: 0-2
 A508-VIKKY1-048
 UT1211_072 15 (0.278) Cm (14:16-57:61x0.010)



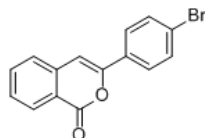
3-phenyl-1H-isochromen-1-one
 Chemical Formula: C₁₅H₁₀O₂
 Exact Mass: 222.07

1: TOF MS ES+
 9.98e+002

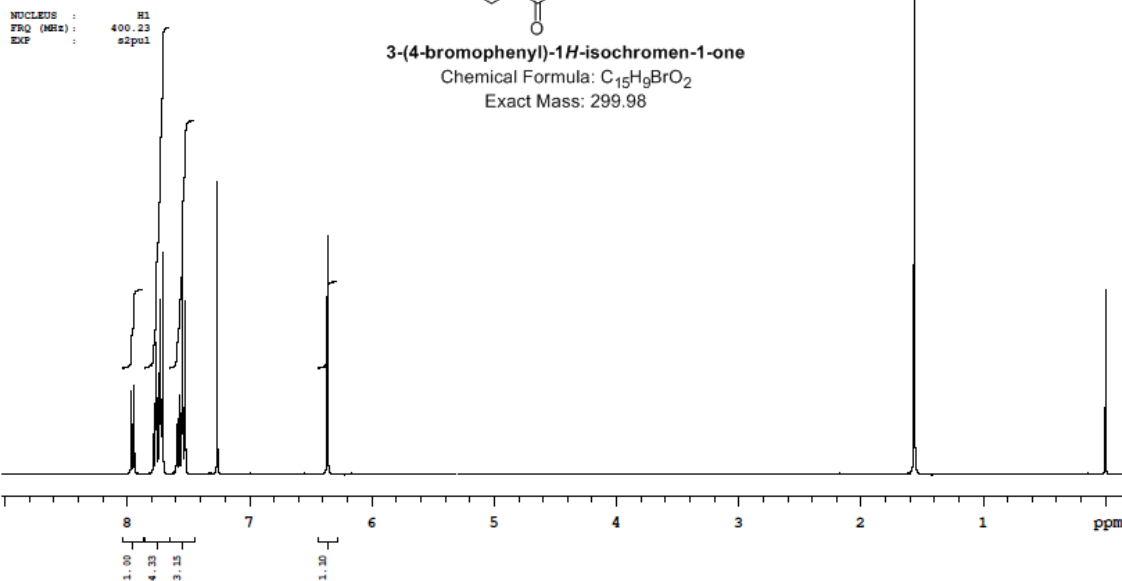


Minimum:	5.0	5.0	-1.5			
Maximum:			80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0762	223.0759	0.3	1.3	10.5	2.2	C15 H11 O2

TDC-J-04 A508-VIKKY5-053 in CDCl3
 NMR-400MHz
 AR.No:ME0912/751
 Analyst: Ganesh
 Date: 10 th Sep2012

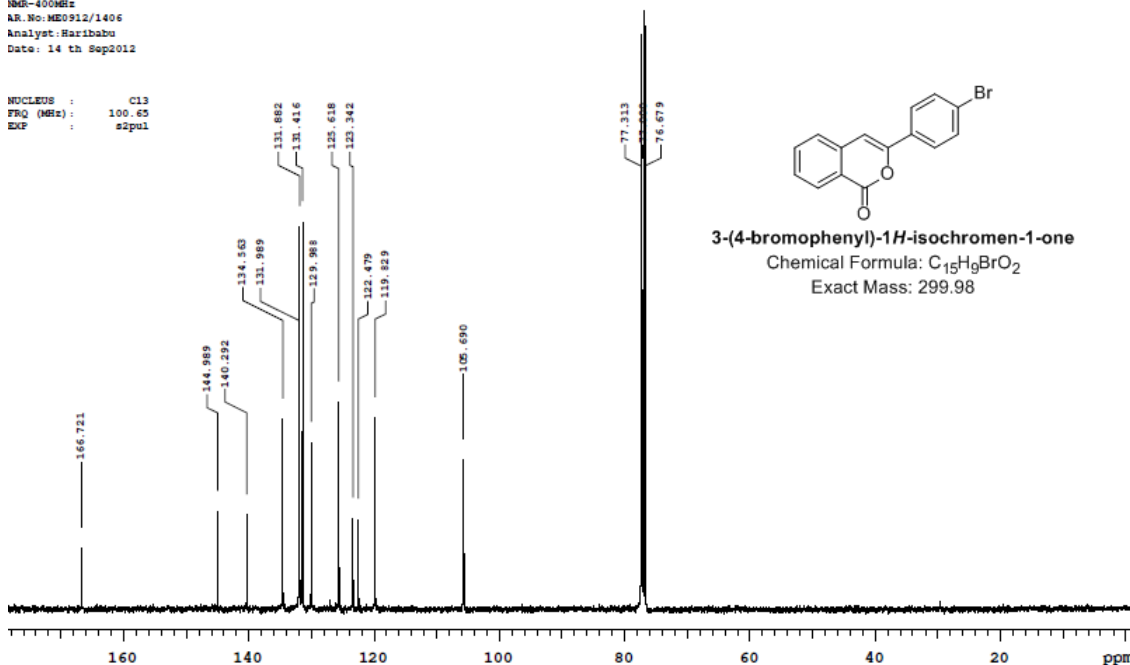


3-(4-bromophenyl)-1H-isochromen-1-one
 Chemical Formula: C₁₅H₉BrO₂
 Exact Mass: 299.98



NMR-400MHz
 AR.No:ME0912/1406
 Analyst:Haribabu
 Date: 14 th Sep2012

NUCLEUS : C13
 FREQ (MHz): 100.65
 EXP : s2pul



Elemental Composition Report

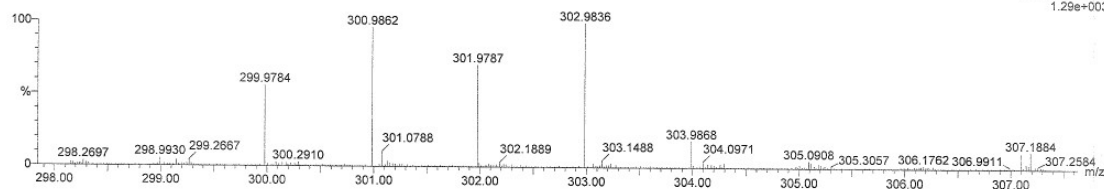
Page 1

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 = 2

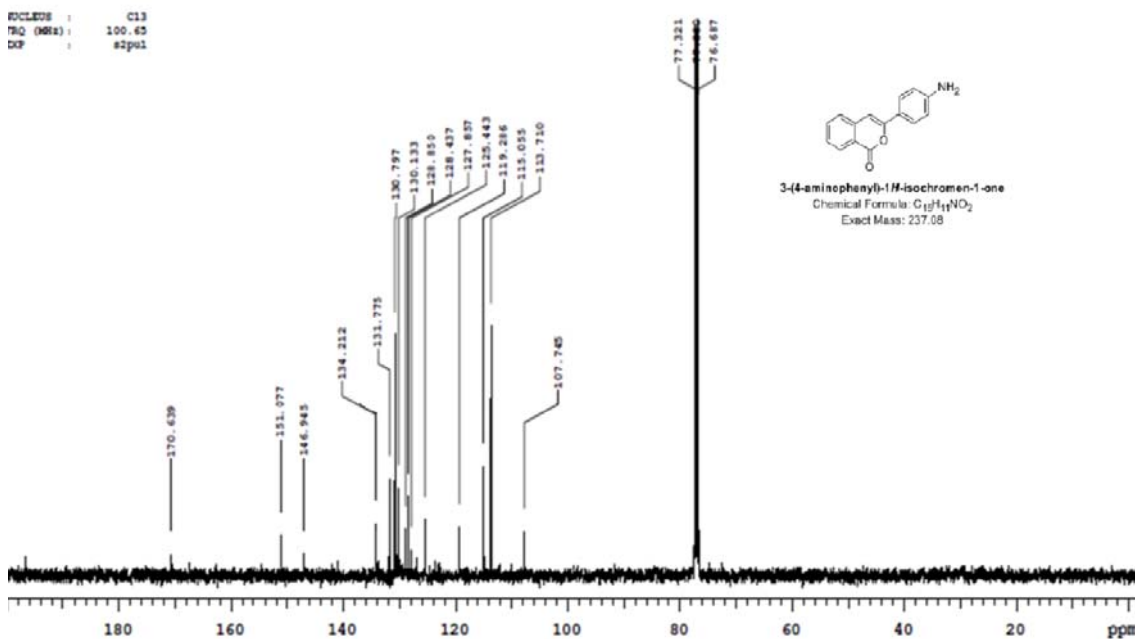
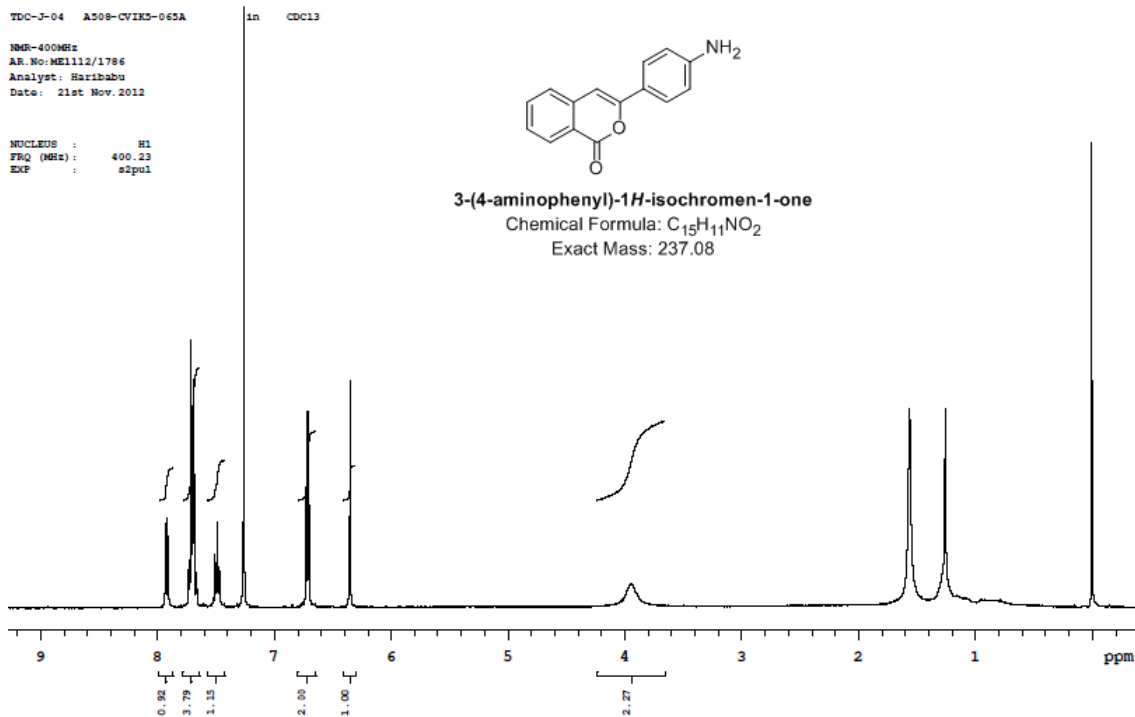
Monoisotopic Mass, Even Electron Ions
 6 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
 Elements Used:
 C: 0-20 H: 0-20 O: 0-2 Br: 0-1

A508/CV1K5/053B
 130211012 16 (0.292) Cm (6:28)



Gajanan
 1: TOF MS ES+
 1.29e+003

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
300.9862	300.9864	-0.2	-0.7	10.5	237.3	C15 H10 O2 Br

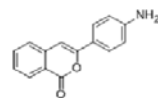


Elemental Composition Report

Single Mass Analysis

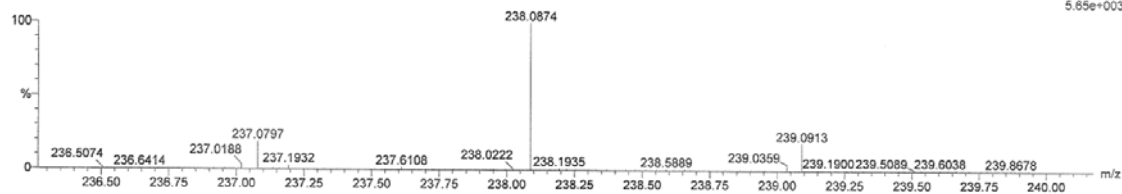
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 102 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: 0-1 O: 0-7 Cl: 0-2
 A508/CVIK15/065 A
 1: TOF MS ES+



3-(4-aminophenyl)-1H-isochromen-1-one
 Chemical Formula: C₁₅H₁₁NO₂
 Exact Mass: 237.08

UT1211_121 20 (0.367) Cm (15:28-57:77x0.010)

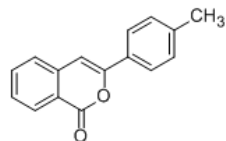


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
238.0874	238.0868	0.6	2.5	10.5	n/a	C15 H12 N O2

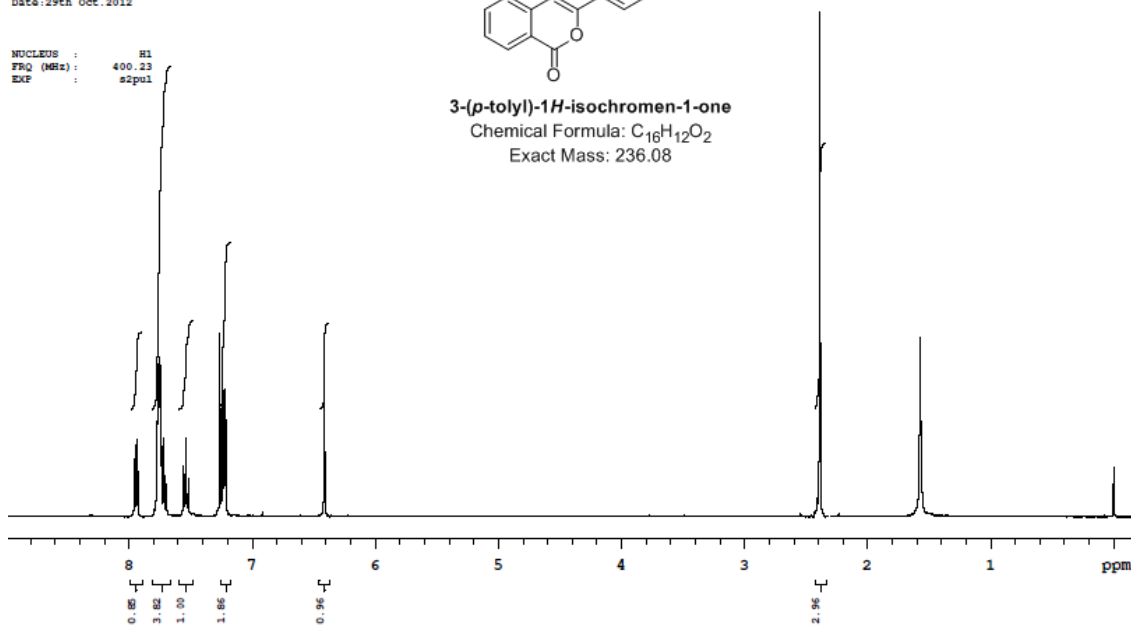
TDC-J-04 A508-CVIR8-072 in CDCl3

MR-400MHz
 AR.No:ME1012/2702
 Analyst:Ganesh
 Date:29th Oct. 2012

NUCLEUS : H1
 FRQ (MHz): 400.23
 EXP : s2pul



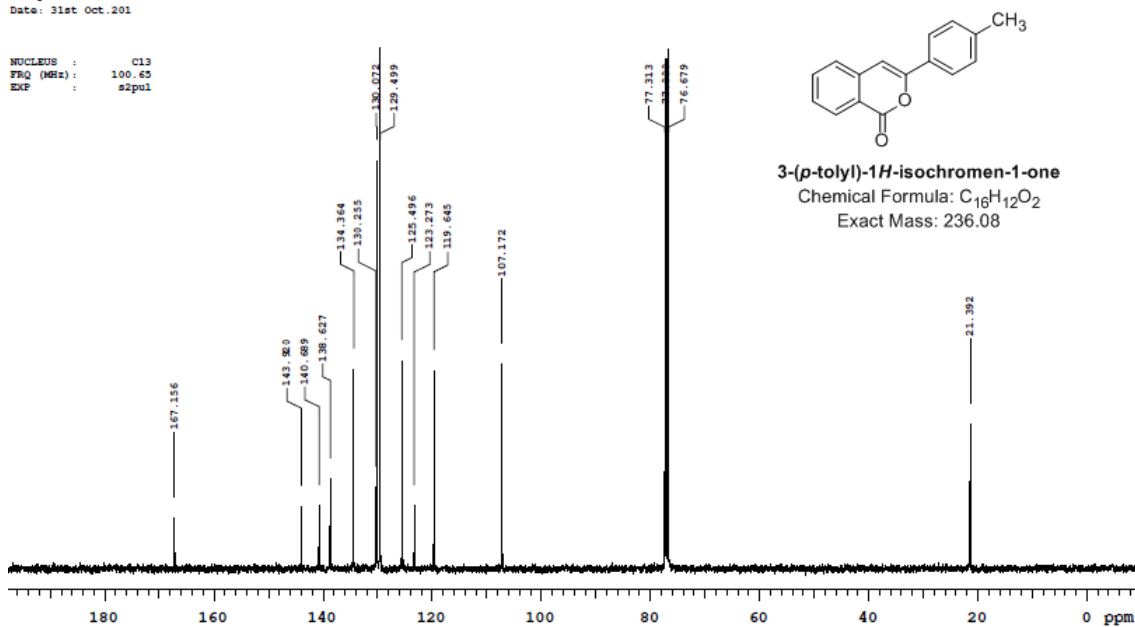
3-(p-tolyl)-1H-isochromen-1-one
 Chemical Formula: C₁₆H₁₂O₂
 Exact Mass: 236.08



TDC-J-04 A508-CVIK18-072 in CDCl3

MR-400MHz
 AR No: ME1012/3045
 Analyst: Ganesh
 Date: 31st Oct. 201

NUCLEUS : C13
 FREQ (MHz): 100.63
 EXP : s1pul

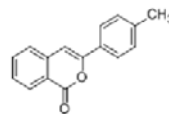


Elemental Composition Report

Single Mass Analysis

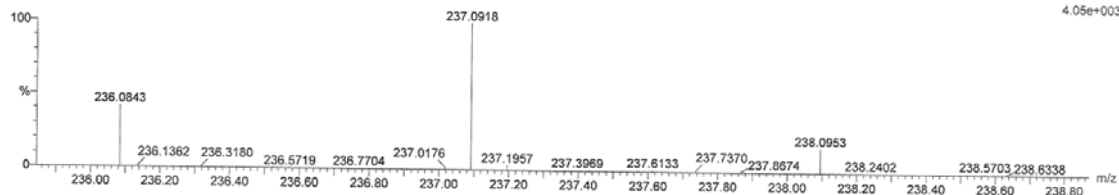
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 20 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
 Elements Used:
 C: 0-27 H: 0-30 O: 0-7
 A508/CVIK18/072
 1: TOF MS ES+



3-(p-tolyl)-1H-isochromen-1-one
 Chemical Formula: C₁₆H₁₂O₂
 Exact Mass: 236.08

Page 1



Minimum: -1.5
 Maximum: 80.0

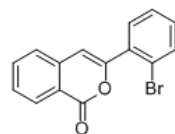
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
237.0918	237.0916	0.2	0.8	10.5	n/a	C ₁₆ H ₁₃ O ₂

UT1211_124 20 (0.366) Cm (20.27-45.71x0.010)

4.05e+003

NMR-400MHz
AR.No:ME1112/201
Analyst: Ganesh
Date:05th Nov.2012

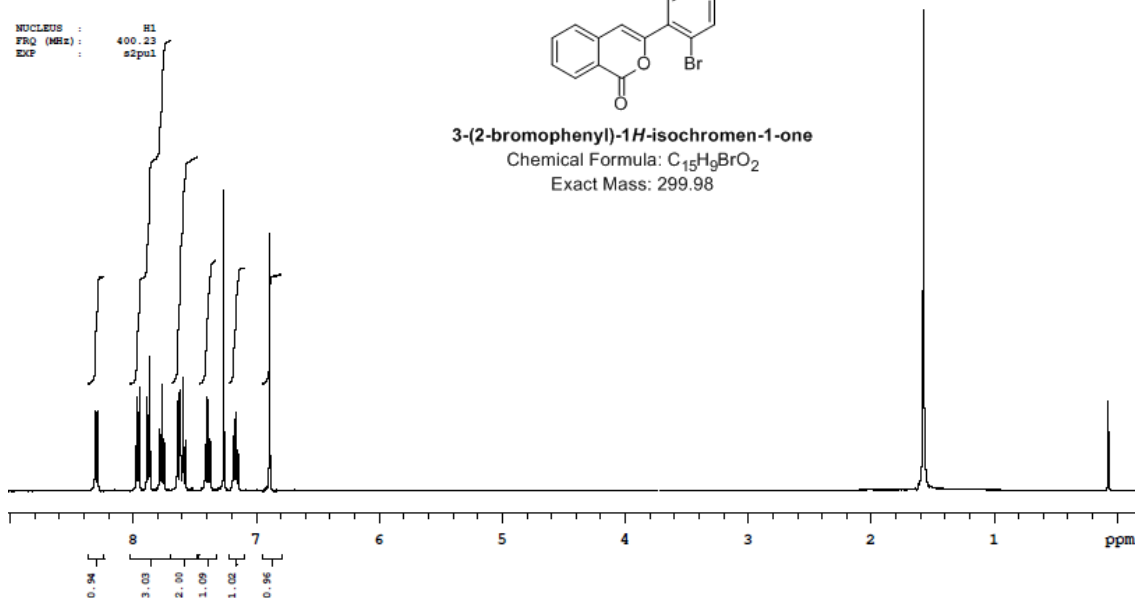
NUCLEUS : ¹H
FREQ (MHz) : 400.12
EXP : s2pul



3-(2-bromophenyl)-1H-isochromen-1-one

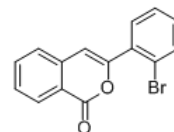
Chemical Formula: C₁₅H₉BrO₂

Exact Mass: 299.98



NMR-400MHz
AR.No:ME1112/272
Analyst: Haribabu
Date:09th Nov.2012

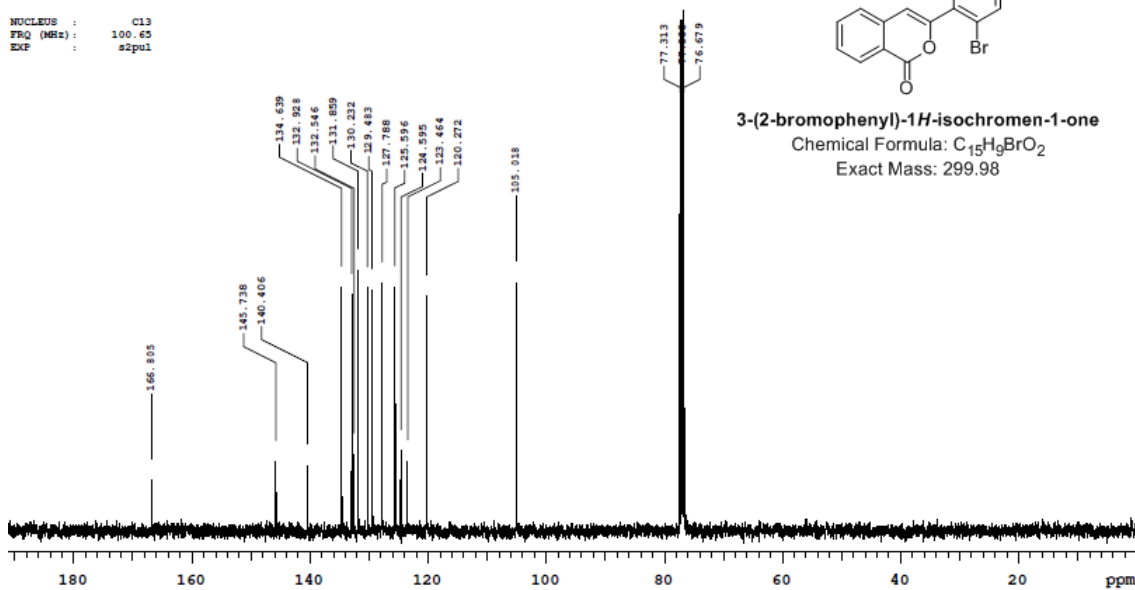
NUCLEUS : ¹³C
FREQ (MHz) : 100.63
EXP : s2pul



3-(2-bromophenyl)-1H-isochromen-1-one

Chemical Formula: C₁₅H₉BrO₂

Exact Mass: 299.98

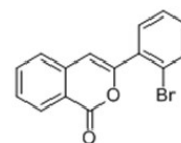


Elemental Composition Report

Page 1

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 = 2

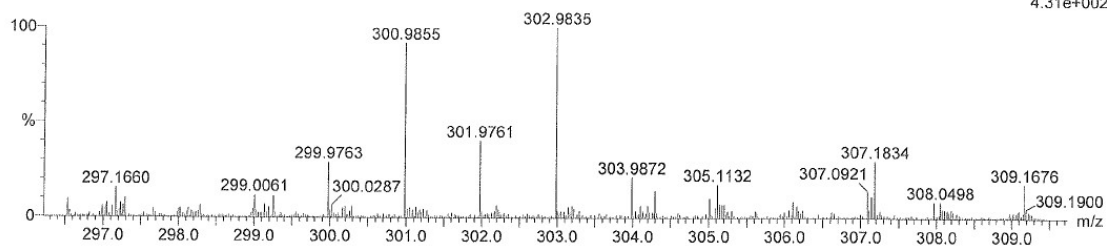


3-(2-bromophenyl)-1H-isochromen-1-one
 Chemical Formula: C₁₅H₉BrO₂
 Exact Mass: 299.98

Monoisotopic Mass, Even Electron Ions
 27 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
 Elements Used:
 C: 0-30 H: 0-30 O: 0-4 Br: 0-1

A508/CVIK19/073B
 130211014 19 (0.353) Cm (19.34)

Gajanan
 1: TOF MS ES+
 4.31e+002



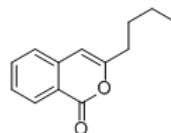
Minimum: -1.5
 Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
300.9855	300.9864	-0.9	-3.0	10.5	53.9	C15 H10 O2 Br

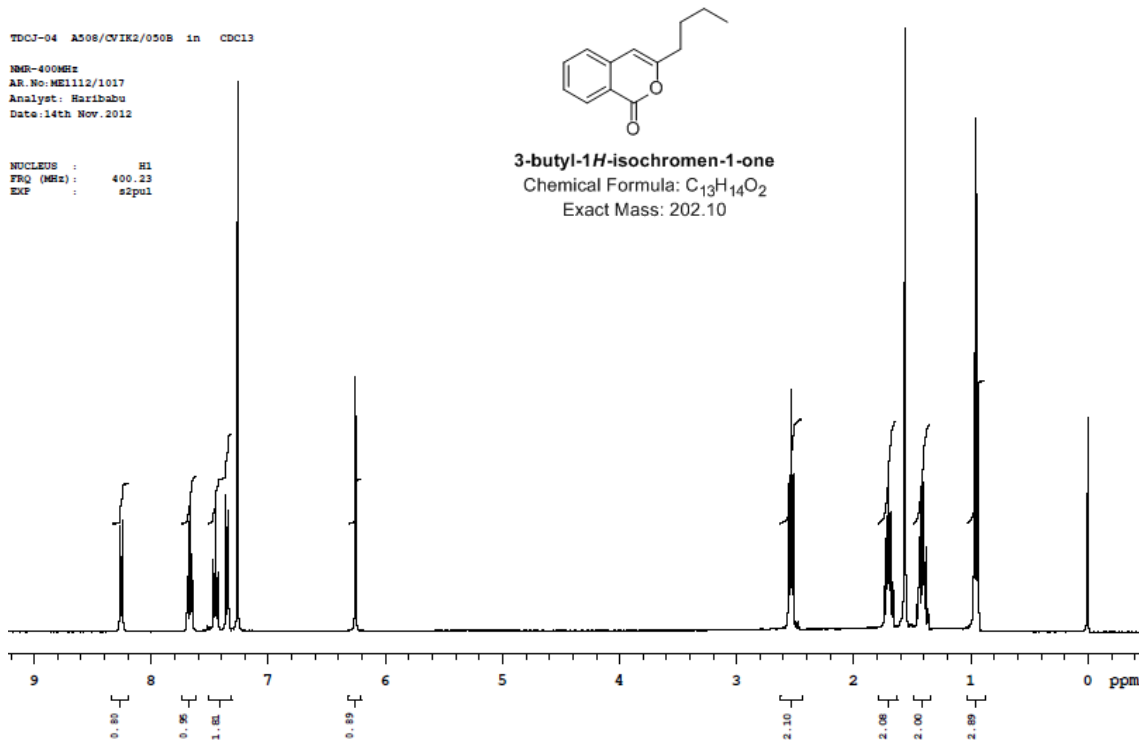
TDCJ-04 A508/CVIK2/050B in CDCl₃

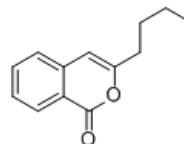
MR-400MHz
 AR.No: ME1112/1017
 Analyst: Haribabu
 Date: 14th Nov. 2012

NUCLEUS : H1
 FREQ (MHz): 400.23
 EXP : s2pul



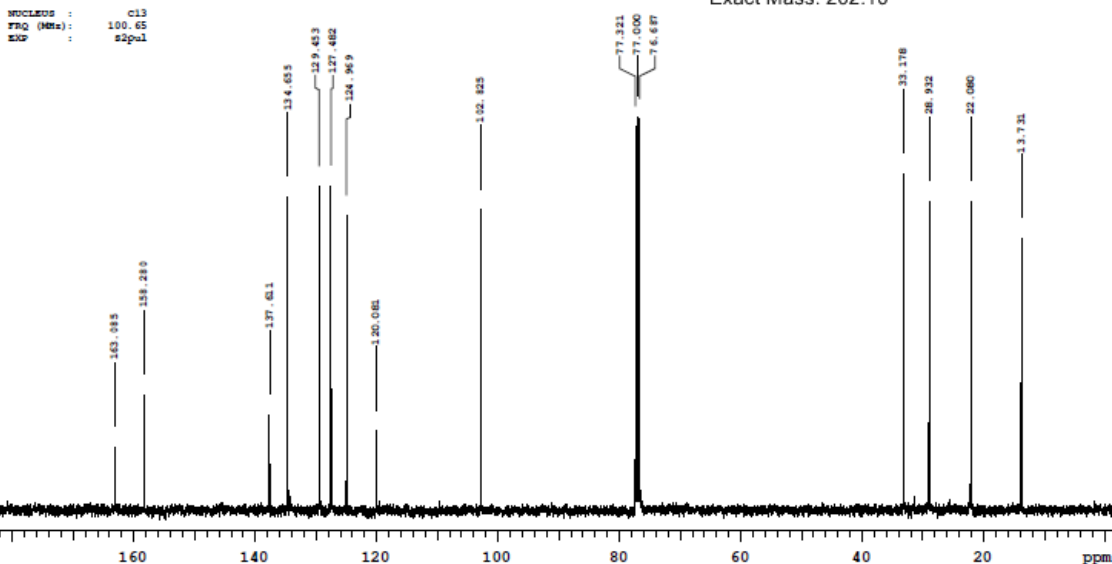
3-butyl-1H-isochromen-1-one
 Chemical Formula: C₁₃H₁₄O₂
 Exact Mass: 202.10





TQC-3-04 A508-CVIX2-050b in cdc13
 NMR-400MHz
 AN. NO: HELL12/1534
 Analyst: MArribabu
 Date: 19th Nov. 2012

3-butyl-1H-isochromen-1-one
 Chemical Formula: C₁₃H₁₄O₂
 Exact Mass: 202.10

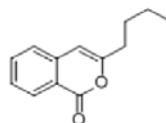


Elemental Composition Report

Page 1

Single Mass Analysis

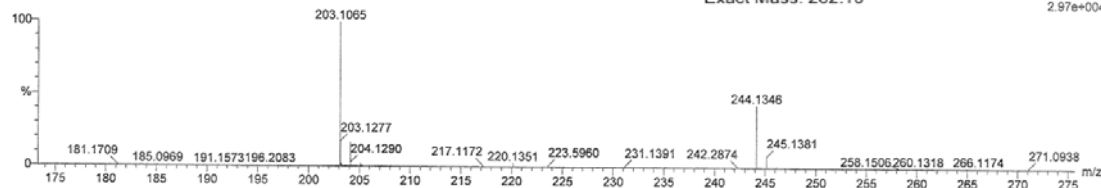
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



3-butyl-1H-isochromen-1-one
 Chemical Formula: C₁₃H₁₄O₂
 Exact Mass: 202.10

1: TOF MS ES+
 2.97e+004

Monoisotopic Mass, Even Electron Ions
 38 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
 Elements Used:
 C: 0-25 H: 0-28 N: 0-4 O: 0-2
 A508-VIKKY1-050 B
 UT1211_073 13 (0.251) Cm (13.22-69:79x0.010)

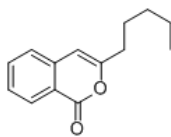


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
203.1065	203.1072	-0.7	-3.4	6.5	38.7	C13 H15 O2

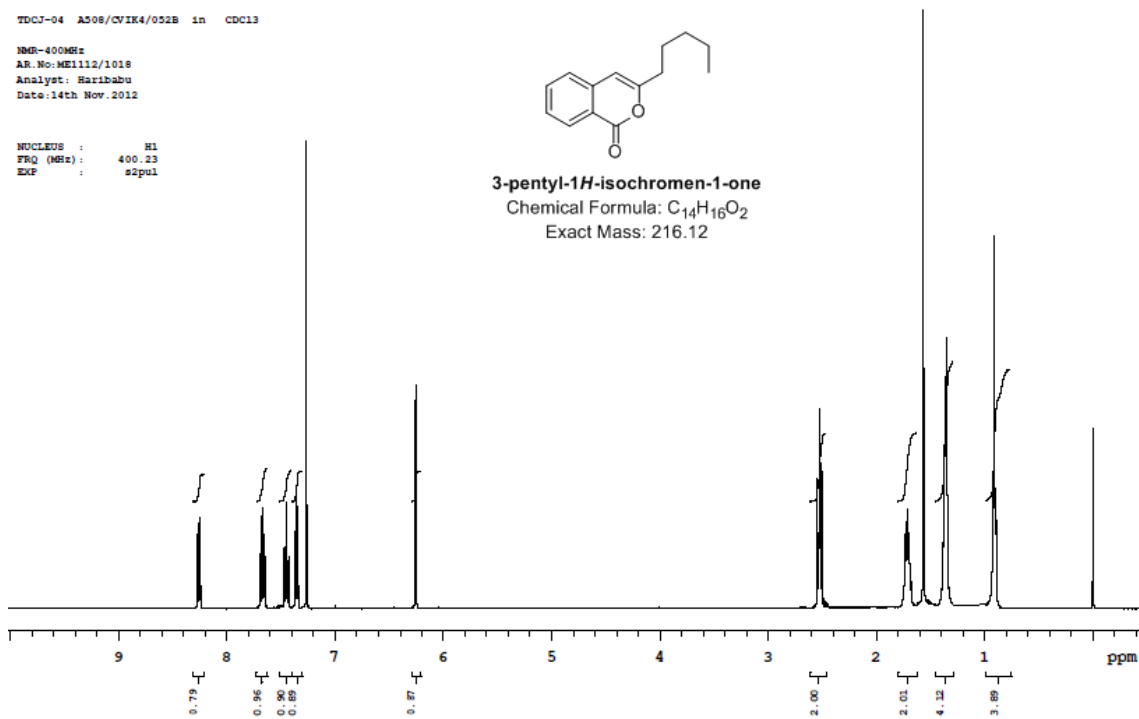
TDCJ-04 A508/CVIK4/052B in CDCl3

NMR-400MHz
AR.No:ME1112/1018
Analyst: Haribabu
Date:14th Nov.2012

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul



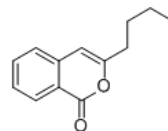
3-pentyl-1H-isochromen-1-one
Chemical Formula: C₁₄H₁₆O₂
Exact Mass: 216.12



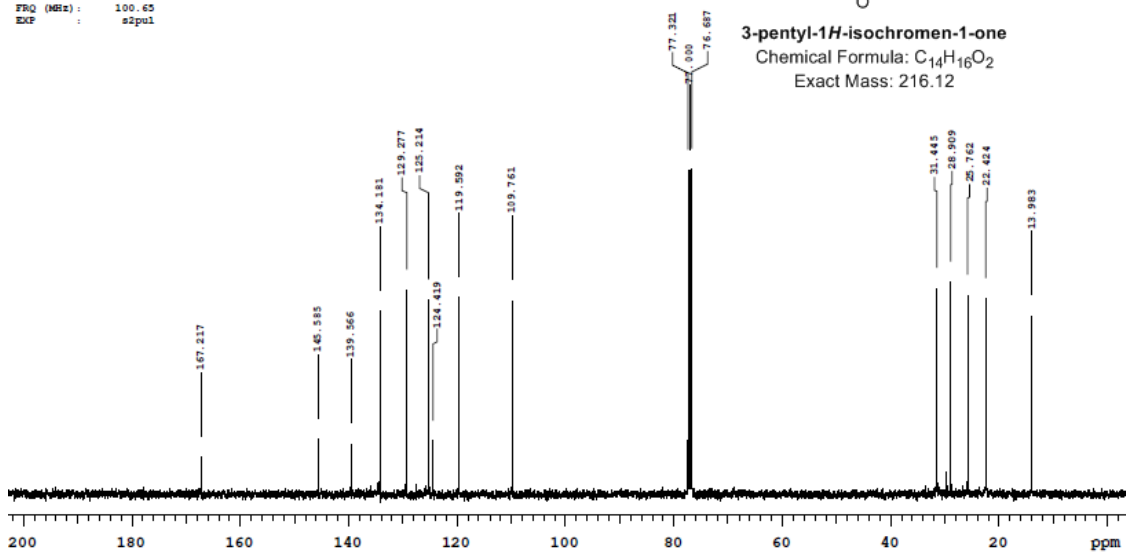
TDC-3-04 A508-CVIK4-052B1 in CDCl3

NMR-400MHz
AR.No:ME1112/2110
Analyst: Ganesh
Date: 23rd Nov.2012

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul



3-pentyl-1H-isochromen-1-one
Chemical Formula: C₁₄H₁₆O₂
Exact Mass: 216.12

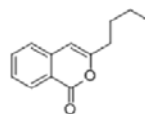


Elemental Composition Report

Single Mass Analysis

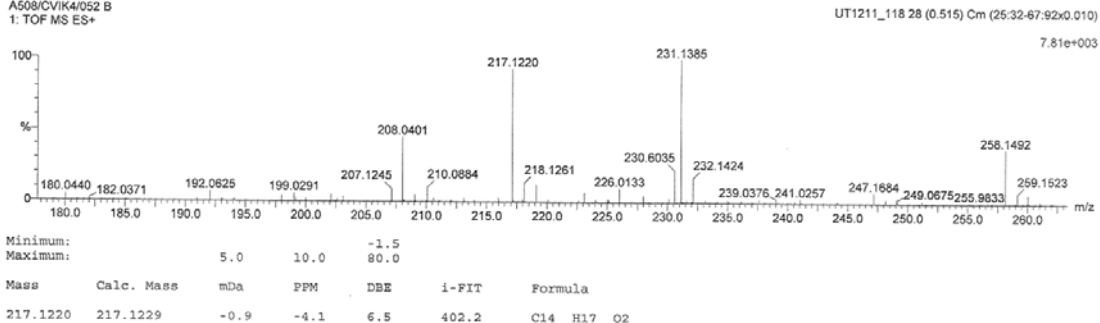
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
74 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: 0-3 O: 0-7
A508/CVIK4/052 B
1: TOF MS ES+



3-pentyl-1H-isochromen-1-one
Chemical Formula: C₁₄H₁₆O₂
Exact Mass: 216.12

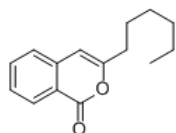
Page 1



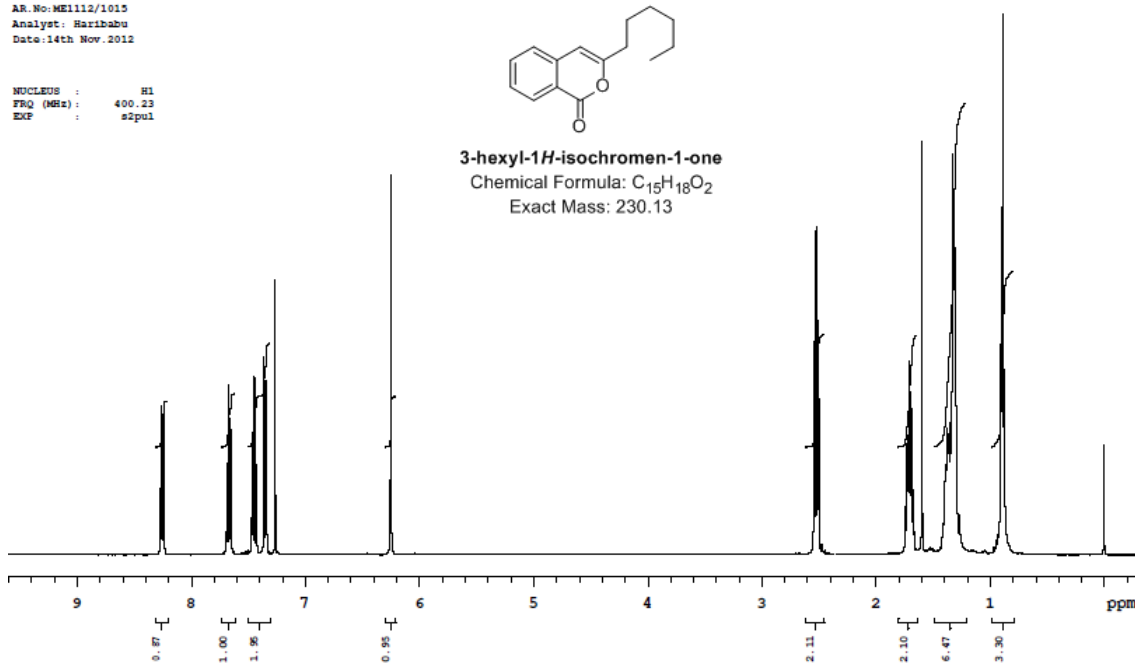
TDCJ-04 A508/CVIK3/051B in CDC13

NMR-400MHz
AR.No:ME1112/1015
Analyst: Haribabu
Date:14th Nov.2012

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul



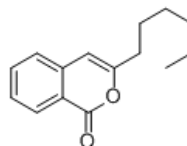
3-hexyl-1H-isochromen-1-one
Chemical Formula: C₁₅H₁₈O₂
Exact Mass: 230.13



TDC-J-04 A508-CVIX3-051a in cocl3

MSM-400MHz
 AN: NO: ME1112/1535
 Analyst: Maribabu
 Date: 19th Nov. 2012

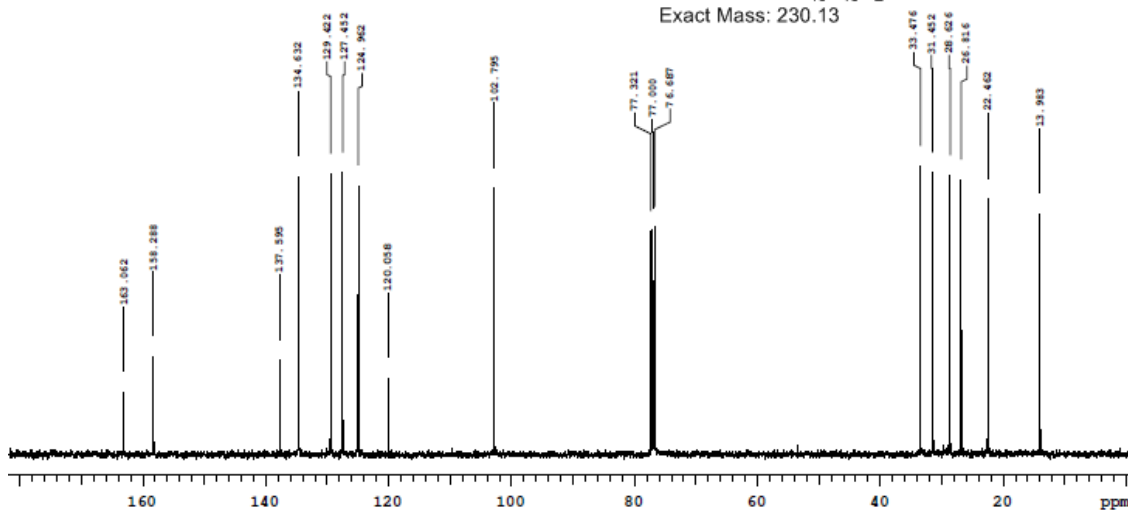
NUCLEUS : c13
 FREQ (MHz): 100.65
 EXP : sqpul



3-hexyl-1H-isochromen-1-one

Chemical Formula: C₁₅H₁₈O₂

Exact Mass: 230.13



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 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

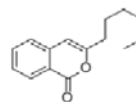
75 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-3 O: 0-7

A508/CVIX3/051 B

1: TOF MS ES+

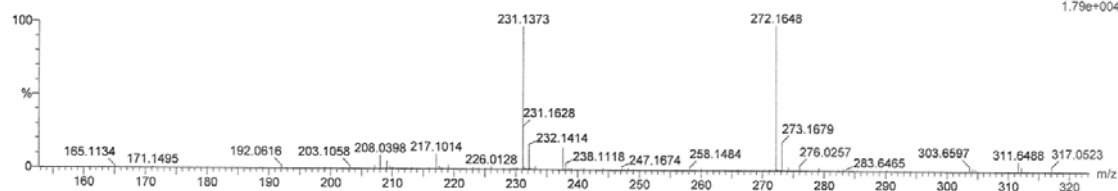


3-hexyl-1H-isochromen-1-one

Chemical Formula: C₁₅H₁₈O₂

Exact Mass: 230.13

UT1211_117 32 (0.587) Cm (32:36-85:92x0.010)



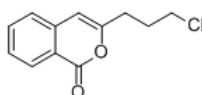
Minimum: -1.5
 Maximum: 5.0 10.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
231.1373	231.1385	-1.2	-5.2	6.5	8.9	C15 H19 O2

1.79e+004

TDC-J-04 A508-CVIK6-054C in CDCl3

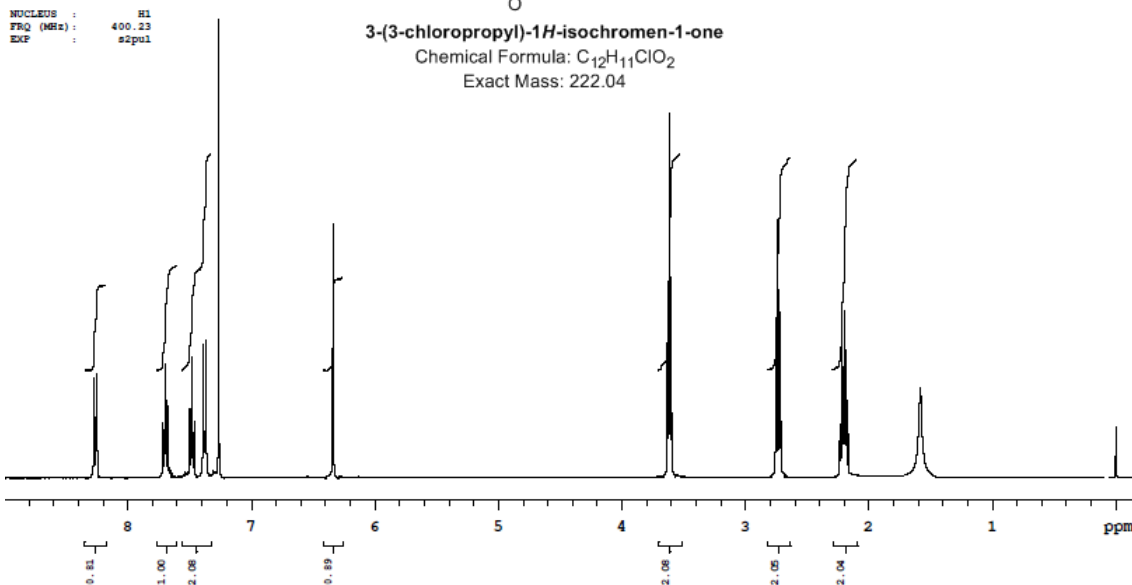
900MHz
AR.No:ME1112/1441
Analyst: Ganesh
Date: 19th Nov. 2012



3-(3-chloropropyl)-1H-isochromen-1-one

Chemical Formula: C₁₂H₁₁ClO₂

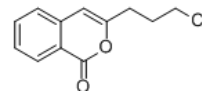
Exact Mass: 222.04



TDC-J-04 A508-CVIK6-054B in CDCl3

900MHz
AR.No:ME1112/2111
Analyst: Ganesh
Date: 23rd Nov. 2012

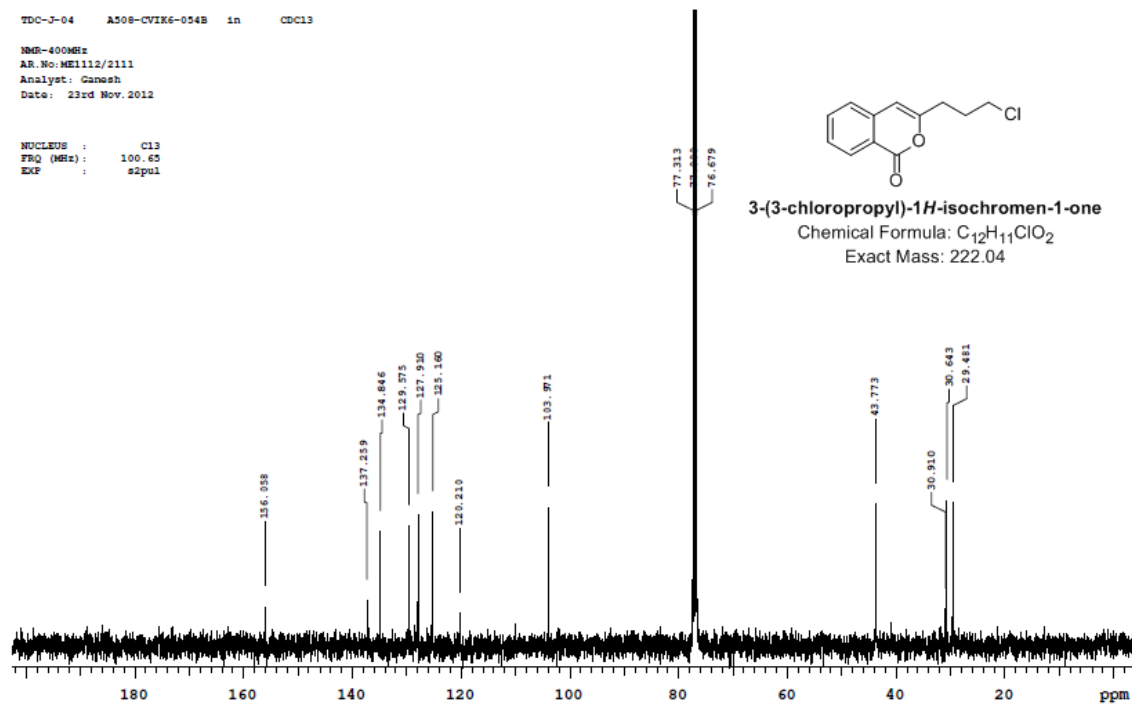
NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul



3-(3-chloropropyl)-1H-isochromen-1-one

Chemical Formula: C₁₂H₁₁ClO₂

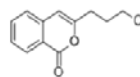
Exact Mass: 222.04



Elemental Composition Report

Single Mass Analysis

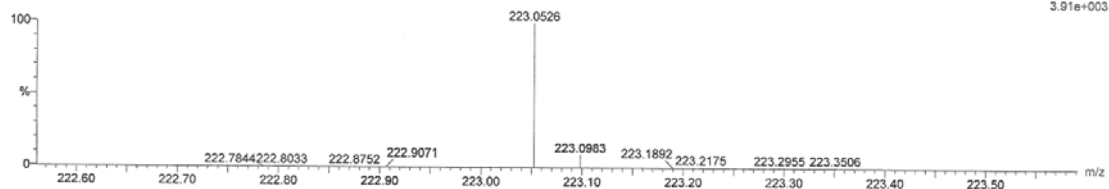
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



3-(3-chloropropyl)-1H-isochromen-1-one
 Chemical Formula: C₁₂H₁₁ClO₂
 Exact Mass: 222.04

Monoisotopic Mass, Even Electron Ions
 51 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 O: 0-7 Cl: 0-2
 A508/CV1K5/054 B
 1: TOF MS ES+

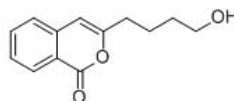
UT1211_119 21 (0.398) Cm (21:27-58:71x0.010)



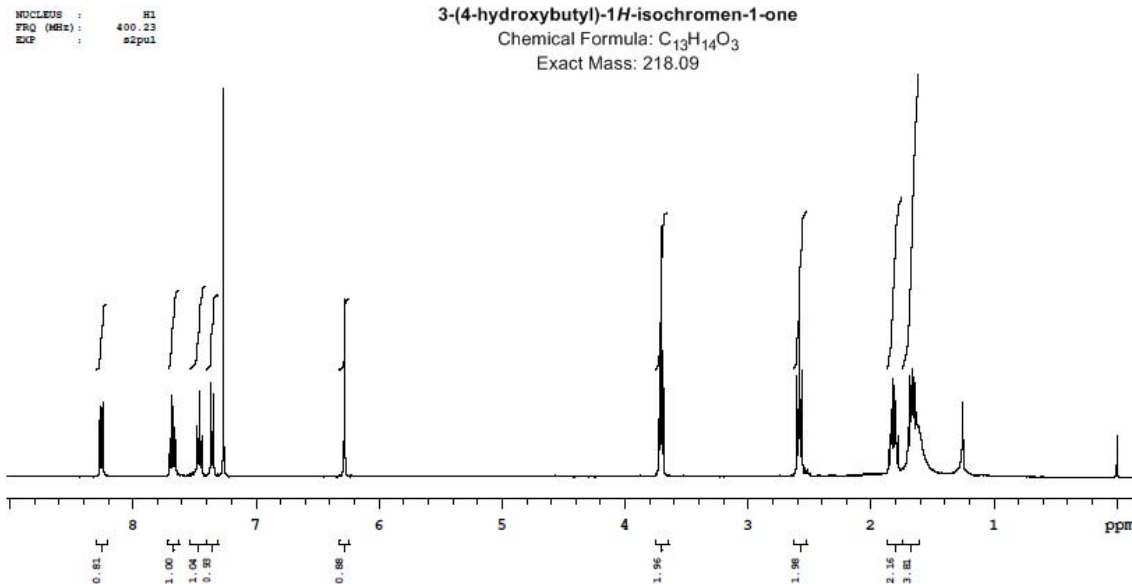
Mass	Calc. Mass	mDa	PPM	DBE	i-PIT	Formula
223.0526	223.0526	0.0	0.0	6.5	n/a	C12 H12 O2 Cl

TDC-J-04 A508-CV1K5-059B in CDCl3

NMR-400MHz
 AR.No: ME1112/1442
 Analyst: Ganesh
 Date: 19th Nov. 2012

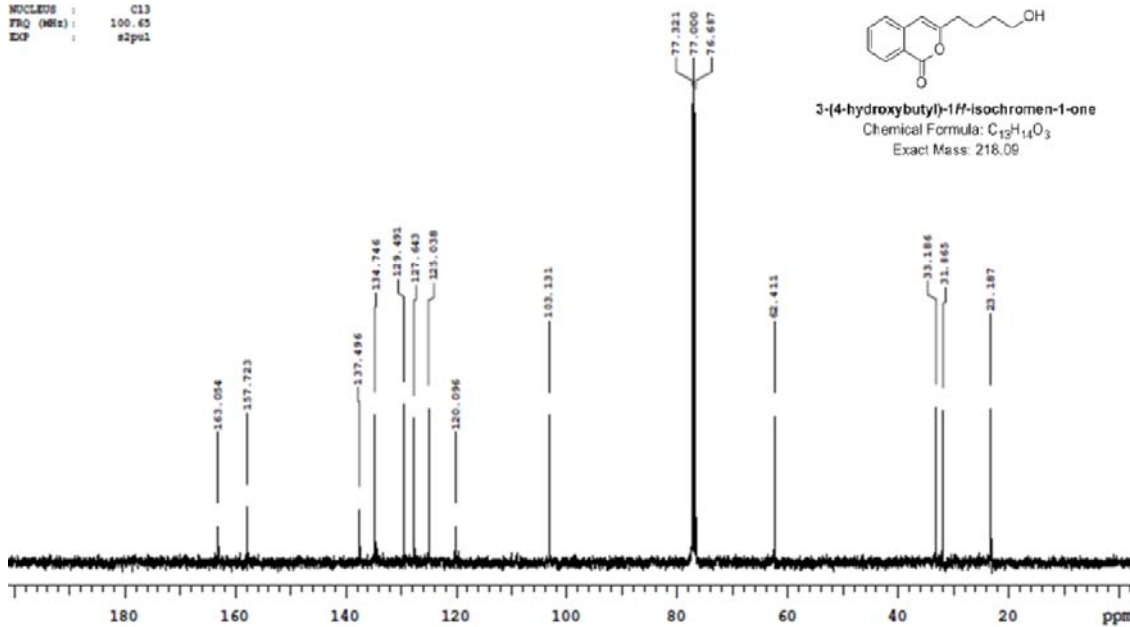


3-(4-hydroxybutyl)-1H-isochromen-1-one
 Chemical Formula: C₁₃H₁₄O₃
 Exact Mass: 218.09



WD-400MHz
 AR. No: NE1112/2114
 Analyst: Ganesh
 Date: 23rd Nov. 2012

NUCLEUS : C13
 FREQ (MHz): 100.63
 EXP : s2pul



Elemental Composition Report

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

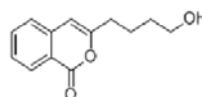
52 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-25 H: 0-25 O: 0-7 Cl: 0-2

A508/CV1K8/059 B

1: TOF MS ES+



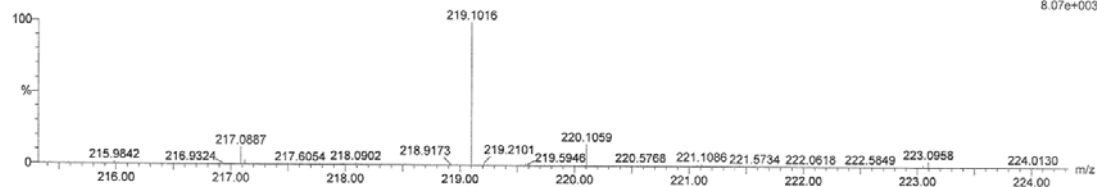
3-(4-hydroxybutyl)-1H-isochromen-1-one

Chemical Formula: C₁₃H₁₄O₃

Exact Mass: 218.09

UT1211_120 50 (0.931) Cm (47:53-94:104x0.010)

8.07e+003



Minimum:

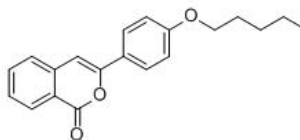
Maximum: 5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.1016	219.1021	-0.5	-2.3	6.5	0.4	C13 H15 O3

TDC-J-04 A508-CVIX10-060 in CDCl3

NMR-400MHz
AR.No:ME1112/1563
Analyst: Ganesh
Date: 20th Nov.2012

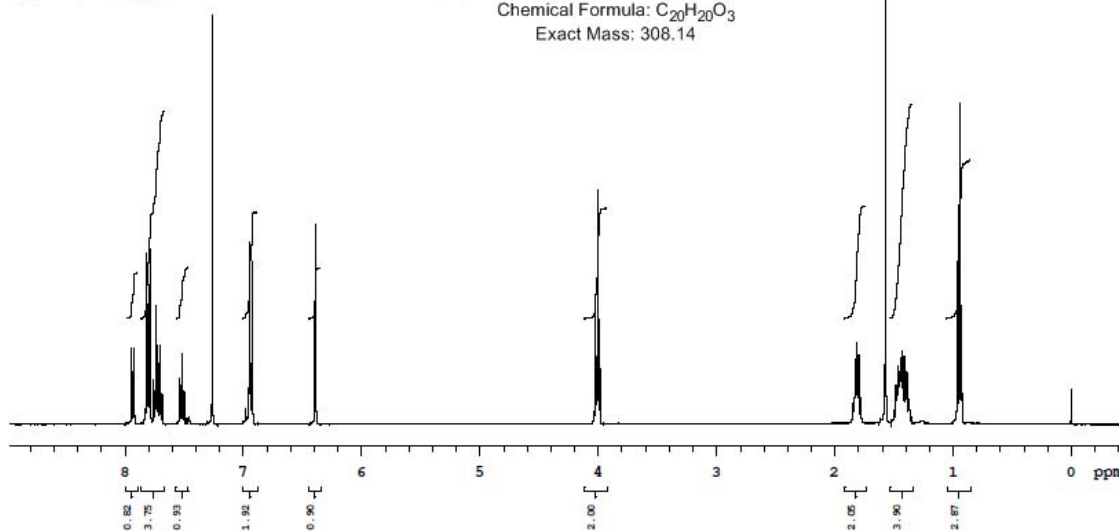
NUCLEUS : H1
FREQ (MHz): 400.23
EXP : s2pul



3-(4-(pentyloxy)phenyl)-1H-isochromen-1-one

Chemical Formula: C₂₀H₂₀O₃

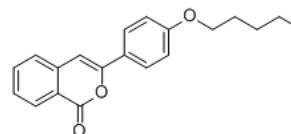
Exact Mass: 308.14



TDC-J-04 A508-CVIX10-060 in CDCl3

NMR-400MHz
AR.No:ME1112/2112
Analyst: Ganesh
Date: 23rd Nov.2012

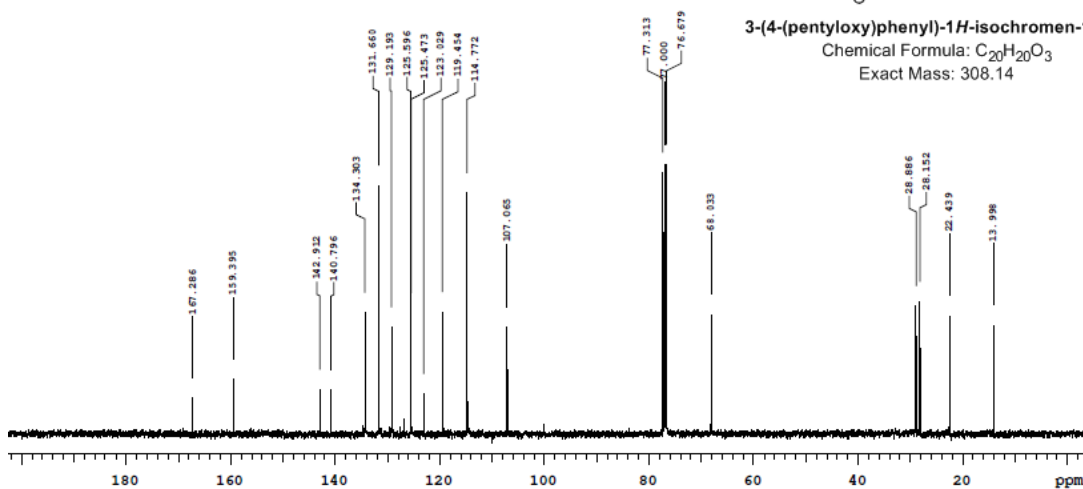
NUCLEUS : C13
FREQ (MHz): 100.63
EXP : s2pul



3-(4-(pentyloxy)phenyl)-1H-isochromen-1-one

Chemical Formula: C₂₀H₂₀O₃

Exact Mass: 308.14

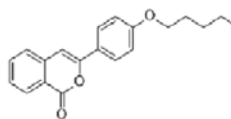


Elemental Composition Report

Page 1

Single Mass Analysis

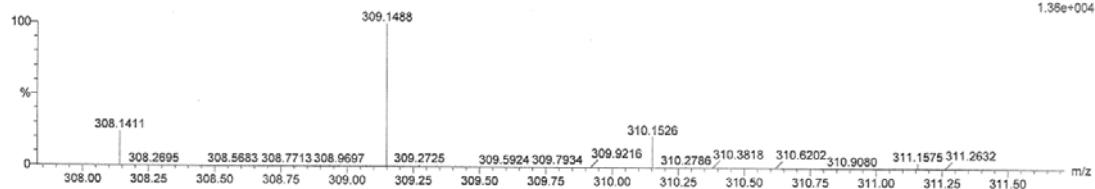
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



3-(4-(pentyloxy)phenyl)-1H-isochromen-1-one
 Chemical Formula: C₂₂H₂₂O₃
 Exact Mass: 308.14

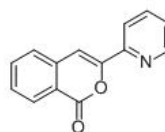
Monoisotopic Mass, Even Electron Ions
 18 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
 Elements Used:
 C: 0-25 H: 0-25 O: 0-7
 A508CVIK101060
 1: TOF MS ES+

UT1211_122.21 (0.400) Cm (17:25-68.88x0.010)

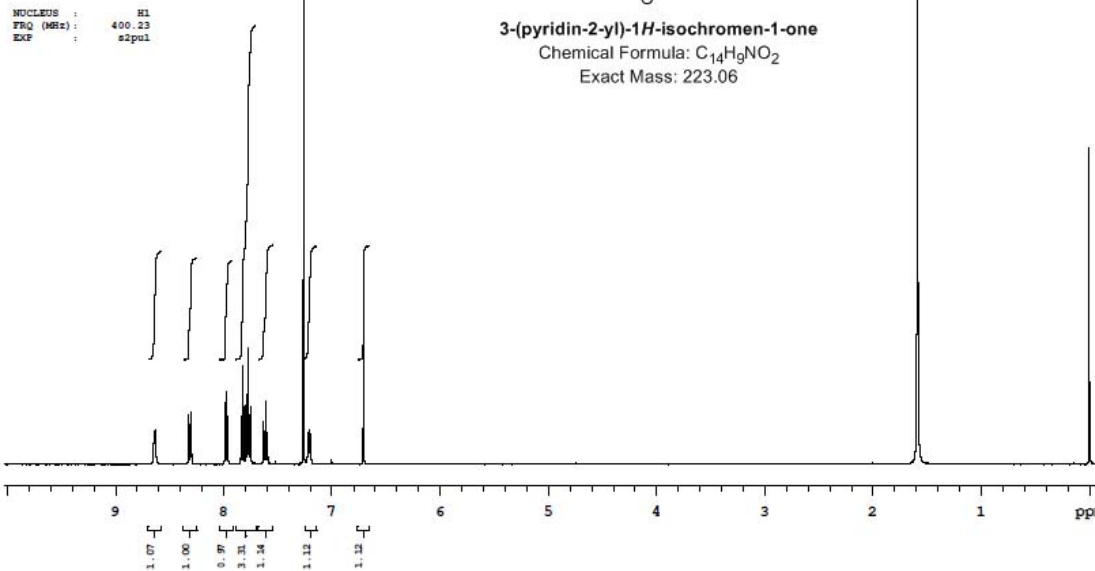


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
309.1488	309.1491	-0.3	-1.0	10.5	15.3	C20 H21 O3

TDC-J-04 A508-CVIX11-055 in cdcl3
 NMR-400MHz
 AR.No: ME912/876
 Analyst: Ganesh
 Date: 11 th Sep2012



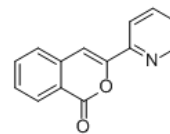
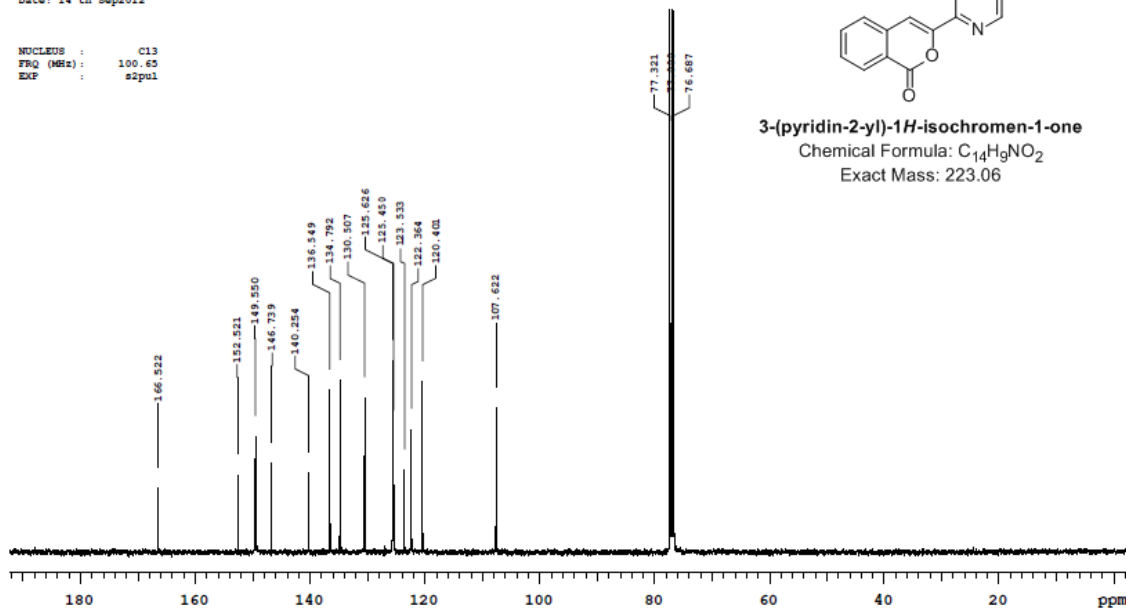
3-(pyridin-2-yl)-1H-isochromen-1-one
 Chemical Formula: C₁₄H₉NO₂
 Exact Mass: 223.06



TDCJ-04 A508/CVIK11/055 in CDCl3

NAME: 400MHz
 AR. No: ME0912/1405
 Analyst: Haribabu
 Date: 14 th Sep 2012

NUCLEUS : C13
 FREQ (MHz): 100.62
 EXP : zgpg1



3-(pyridin-2-yl)-1H-isochromen-1-one
 Chemical Formula: C₁₄H₉NO₂
 Exact Mass: 223.06

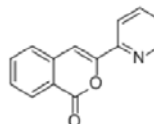
Elemental Composition Report

Page 1

Single Mass Analysis

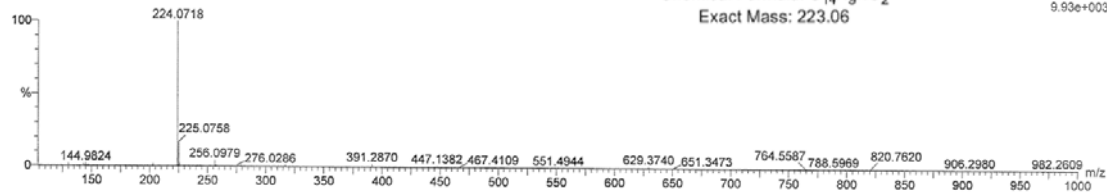
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 15 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
 Elements Used:
 C: 0-19 H: 0-10 N: 0-4 O: 0-2
 A508-VIKKY1-055
 UT1211_075 26 (0.486) Cm (26.28-73.79x0.010)



3-(pyridin-2-yl)-1H-isochromen-1-one
 Chemical Formula: C₁₄H₉NO₂
 Exact Mass: 223.06

1: TOF MS ES+
 9.93e+003

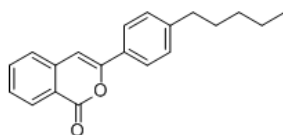


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
224.0718	224.0712	0.6	2.7	10.5	0.7	C14 H10 N O2

TDCJ-04 A508-CVIK12-056 in CDCl3

NMR-400MHz
AR.No:ME0912/875
Analyst: Ganesh
Date: 11 th Sep2012

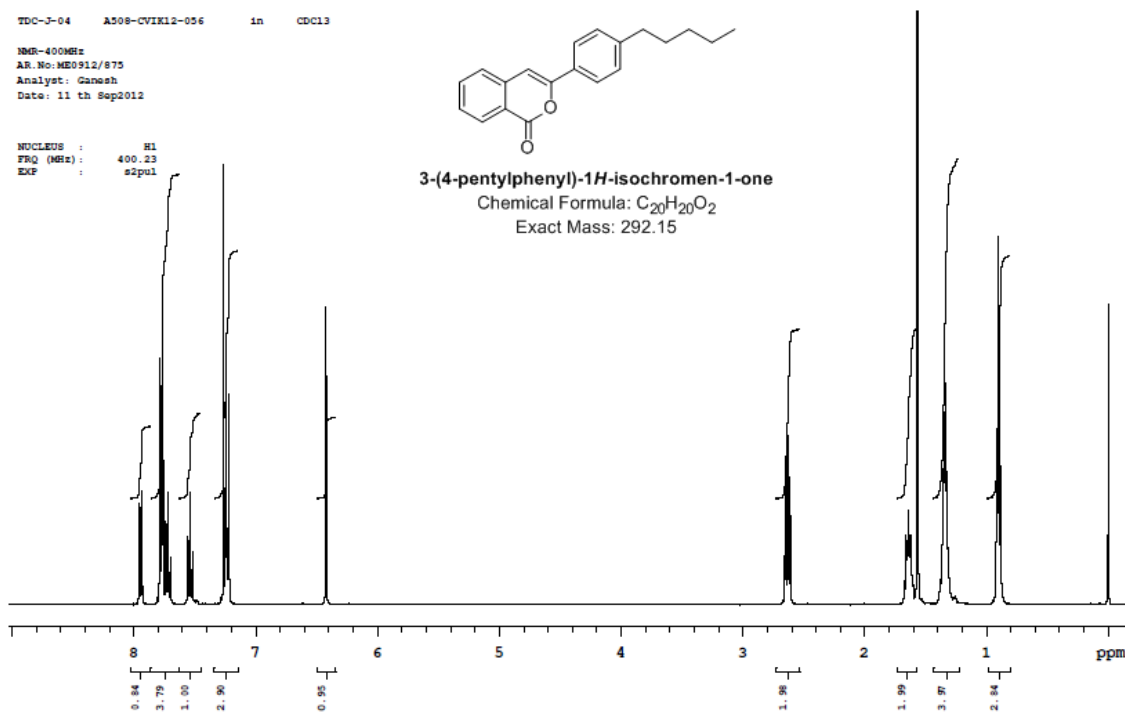
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul



3-(4-pentylphenyl)-1H-isochromen-1-one

Chemical Formula: C₂₀H₂₀O₂

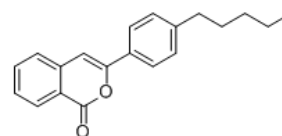
Exact Mass: 292.15



TDCJ-04 A508-CVIK12/056 in CDCl3

NMR-400MHz
AR.No:ME0912/1404
Analyst: Haribabu
Date: 14 th Sep2012

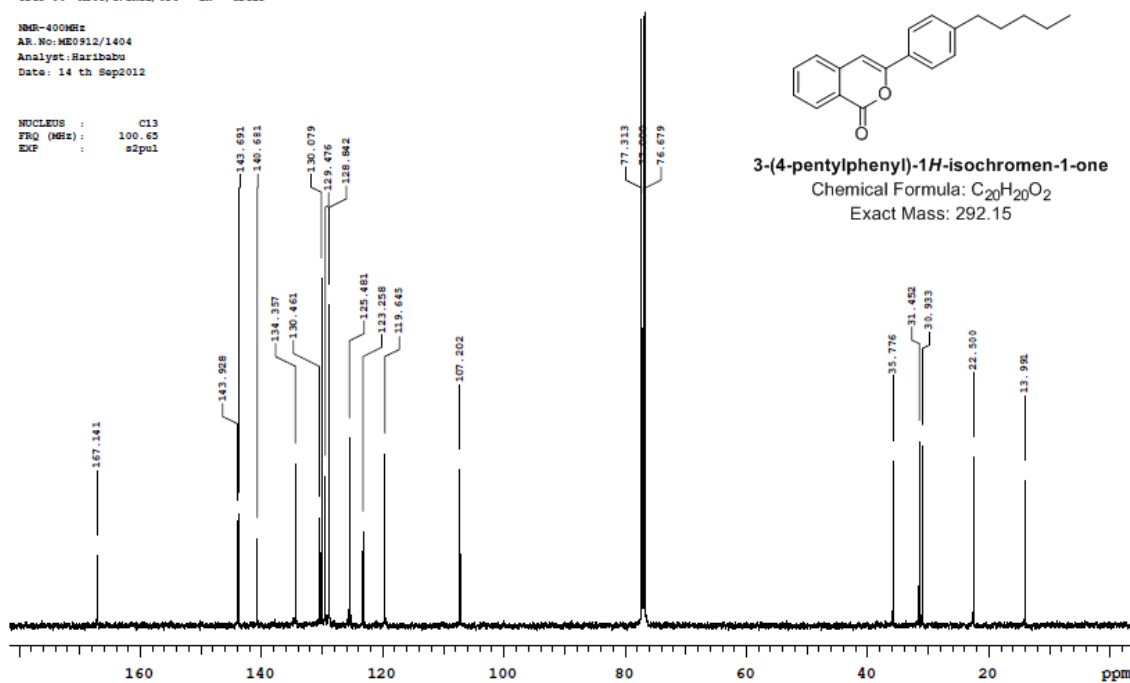
NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul



3-(4-pentylphenyl)-1H-isochromen-1-one

Chemical Formula: C₂₀H₂₀O₂

Exact Mass: 292.15



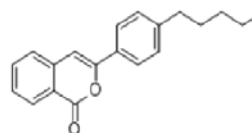
Elemental Composition Report

Page 1

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

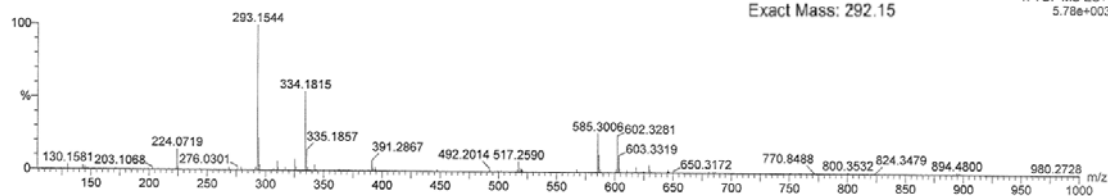
Monoisotopic Mass, Even Electron Ions
 3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
 Elements Used:
 C: 0-22 H: 0-22 O: 0-2
 A508-VIKKY1-056
 UT1211_076 17 (0.325) Cm (17:20-65:72x0.010)



3-(4-pentylphenyl)-1H-isochromen-1-one

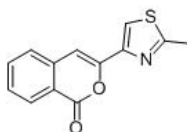
Chemical Formula: C₂₀H₂₀O₂
 Exact Mass: 292.15

1: TOF MS ES+
 5.78e+003



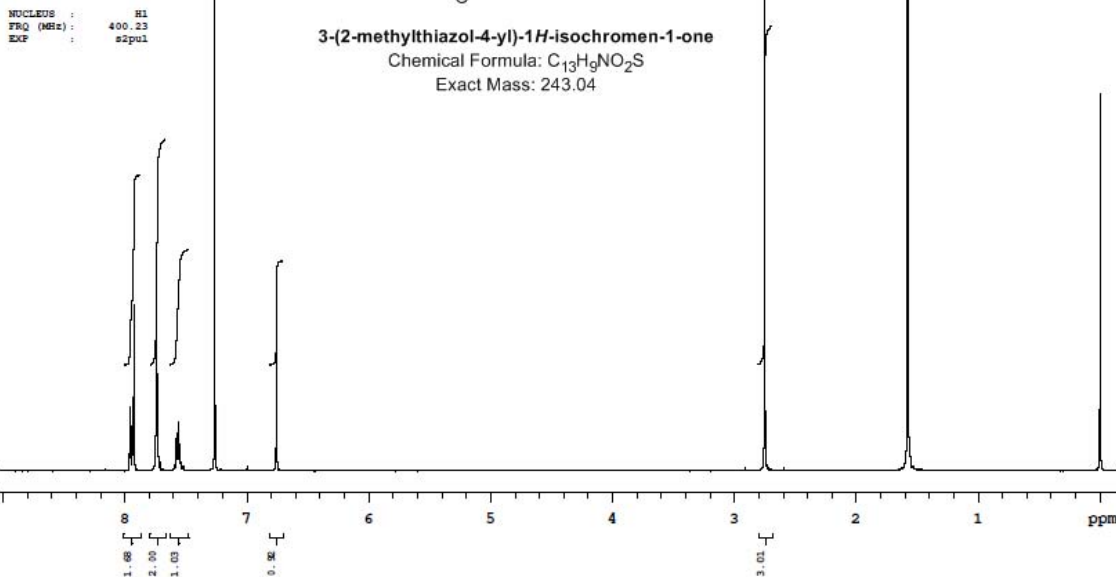
Mass	Calc. Mass	mDa	PPM	DBE	i-PIT	Formula
293.1544	293.1542	0.2	0.7	10.5	4.3	C ₂₀ H ₂₁ O ₂

TDC-J-04 A508-CVIXL3-057 in CDCl₃
 NMR-400MHz
 AR. No: ME0812/874
 Analyst: Ganesh
 Date: 11 th Sep2012



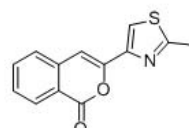
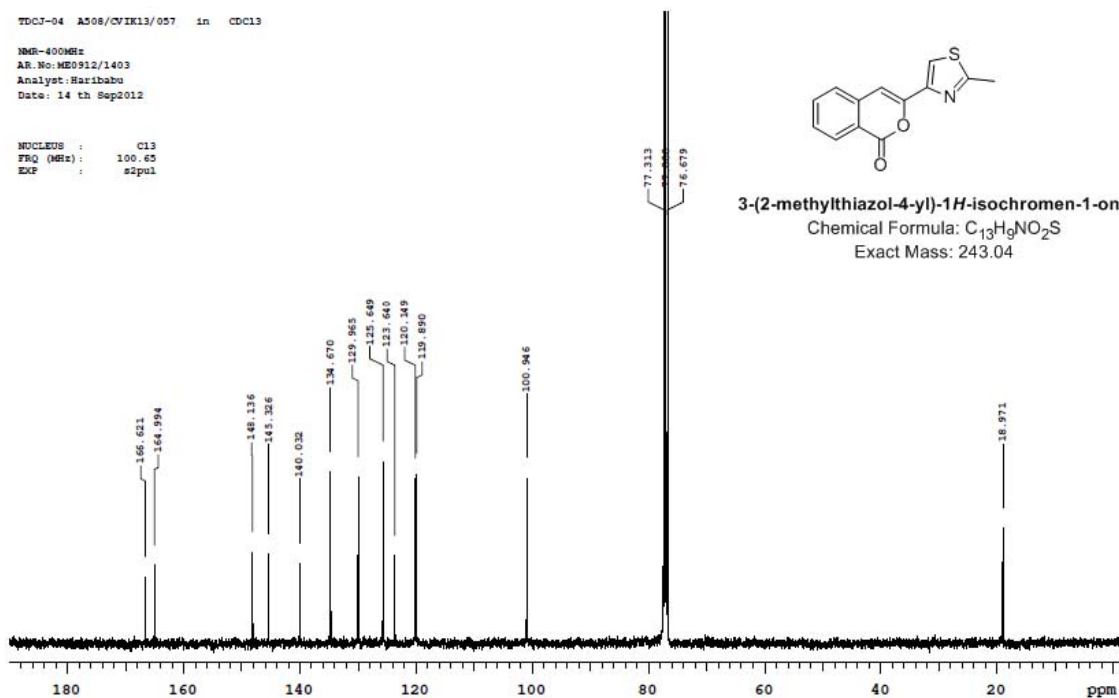
3-(2-methylthiazol-4-yl)-1H-isochromen-1-one

Chemical Formula: C₁₃H₉NO₂S
 Exact Mass: 243.04



TDCJ-04 A508/CV1K13/057 in CDCl3
 INM-400MS
 AR. No: ME0912/1403
 Analyst: Haribabu
 Date: 14 th Sep2012

NUCLEUS : C13
 FREQ (MHz) : 100.63
 EXP : s2pul



3-(2-methylthiazol-4-yl)-1H-isochromen-1-one
 Chemical Formula: C₁₃H₉NO₂S
 Exact Mass: 243.04

Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 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

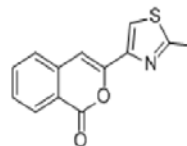
13 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

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

A508-VIKKY1-057

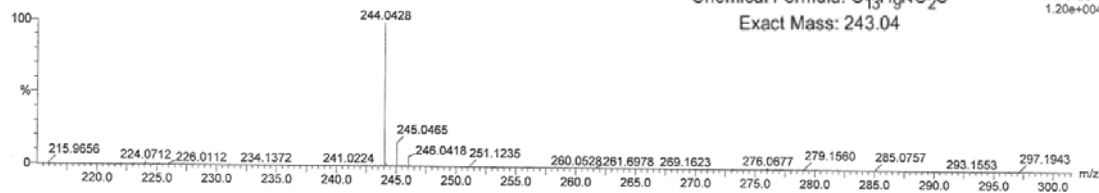
UT1211_077 31 (0.573) Cm (30.32-62.68x0.010)



3-(2-methylthiazol-4-yl)-1H-isochromen-1-one

Chemical Formula: C₁₃H₉NO₂S
 Exact Mass: 243.04

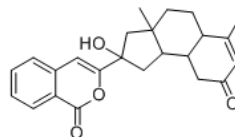
Page 1



Minimum:

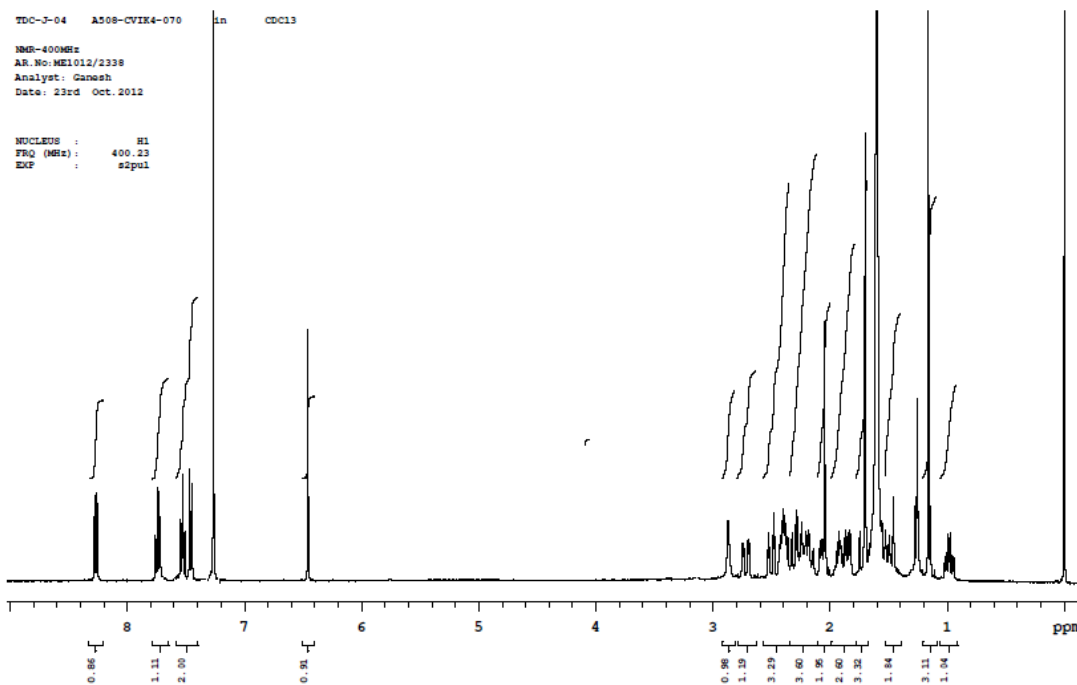
Maximum:

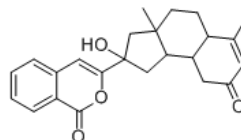
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
244.0428	244.0432	-0.4	-1.6	9.5	1.3	C13 H10 N O2 S



3-(2-hydroxy-3a,6-dimethyl-8-oxo-2,3,3a,4,5,5a,8,9,9a,9b-decahydro-1H-cyclopenta[a]naphthalen-2-yl)-1H-isochromen-1-one

Chemical Formula: C₂₄H₂₆O₄
Exact Mass: 378.18





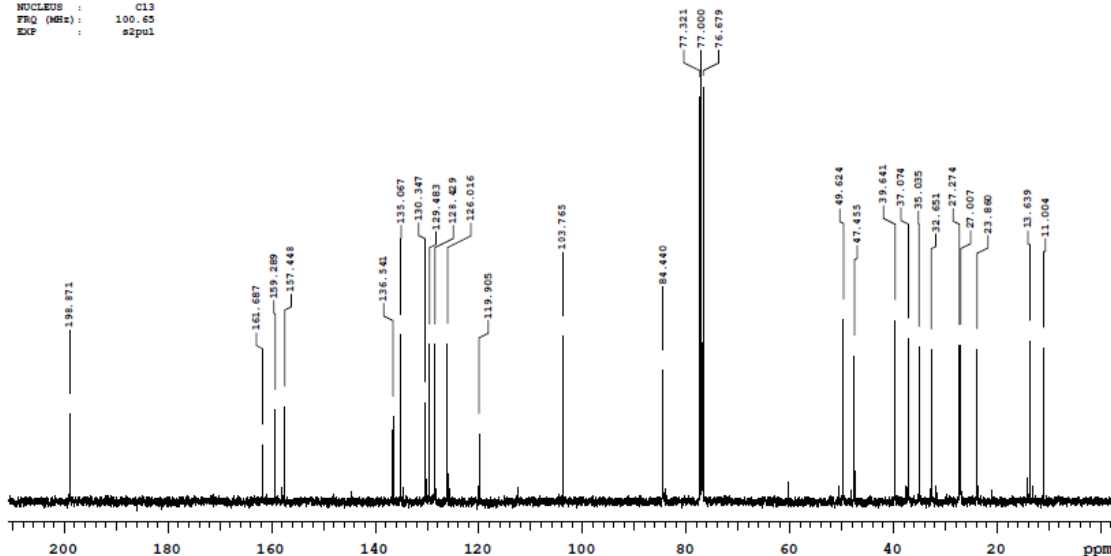
3-(2-hydroxy-3a,6-dimethyl-8-oxo-2,3,3a,4,5,5a,8,9,9a,9b-decahydro-1H-cyclopenta[a]naphthalen-2-yl)-1H-isochromen-1-one

Chemical Formula: C₂₄H₂₆O₄
 Exact Mass: 378.18

TDC-J-04 A508-CV1K14-070 in CDC13

MR: 400MHz
 AR.No: ME1112/564
 Analyst: Haribabu
 Date: 07th Nov. 2012

NUCLEUS : C13
 FREQ (MHz): 100.65
 EXP : s2pul

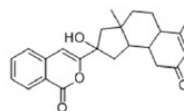


Elemental Composition Report

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 = 2

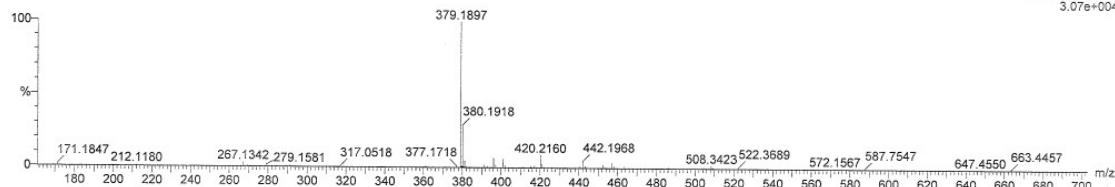
Monoisotopic Mass, Even Electron Ions
 12 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
 Elements Used:
 C: 0-30 H: 0-30 O: 0-4
 A508/CV1K14/070B
 1302110:3 30 (0.561) Cm (29:32)



3-(2-hydroxy-3a,6-dimethyl-8-oxo-2,3,3a,4,5,5a,8,9,9a,9b-decahydro-1H-cyclopenta[a]naphthalen-2-yl)-1H-isochromen-1-one

Chemical Formula: C₂₄H₂₆O₄
 Exact Mass: 378.18

Page 1



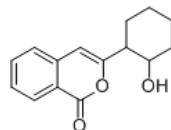
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.1897	379.1909	-1.2	-3.2	11.5	15.3	C ₂₄ H ₂₇ O ₄

Gajanan
 1: TOF MS ES+
 3.07e+004

TDC-J-04 A508-CVIK20-074 in CDCl3

NMR-400MHz
AR.No:ME1112/202
Analyst: Ganesh
Date:05th Nov.2012

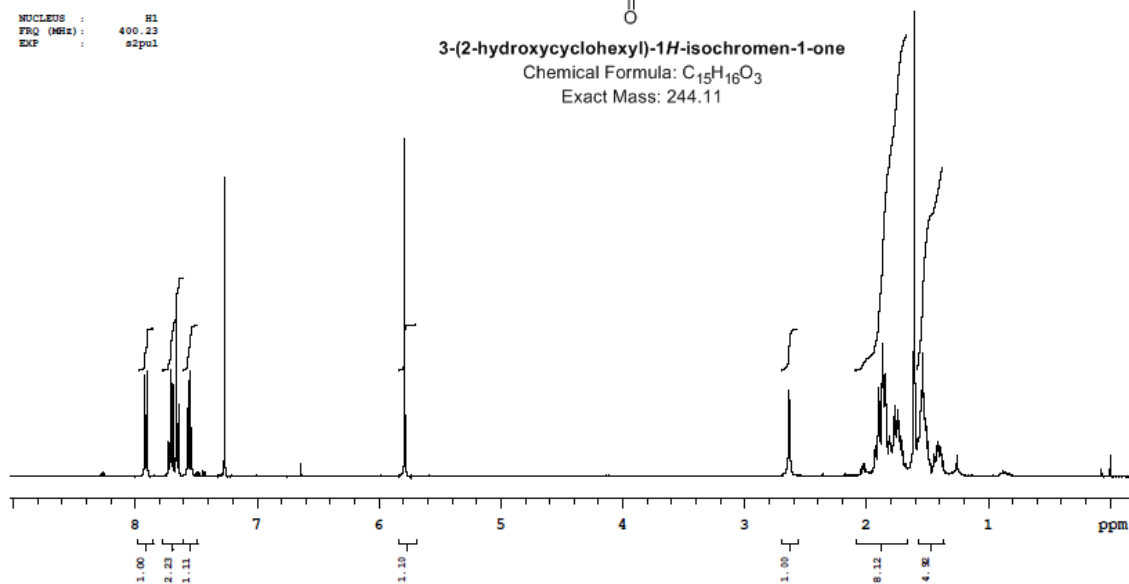
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul



3-(2-hydroxycyclohexyl)-1*H*-isochromen-1-one

Chemical Formula: C₁₅H₁₆O₃

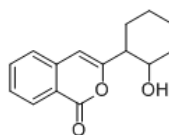
Exact Mass: 244.11



TDC-J-04 A508-CVIK20-074 in CDCl3

NMR-400MHz
AR.No:ME1112/870
Analyst: Haribabu
Date:09th Nov.2012

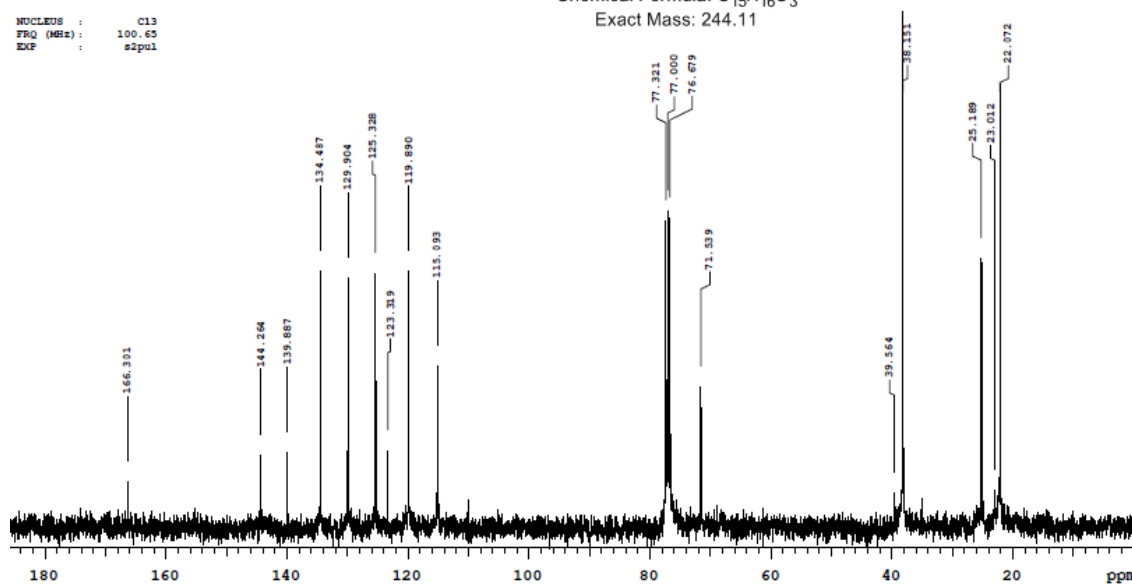
NUCLEUS : C13
FRQ (MHz): 100.63
EXP : s2pul



3-(2-hydroxycyclohexyl)-1*H*-isochromen-1-one

Chemical Formula: C₁₅H₁₆O₃

Exact Mass: 244.11



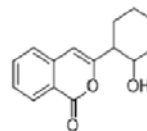
Elemental Composition Report

Page 1

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

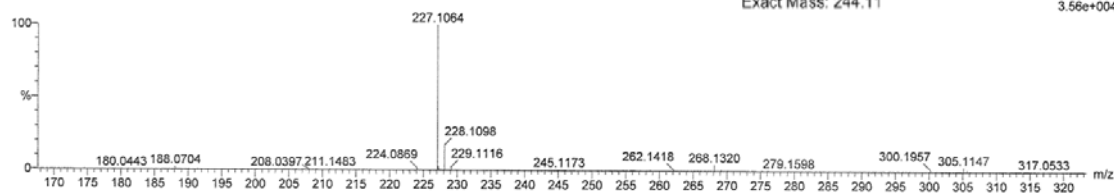
Monoisotopic Mass, Even Electron Ions
 9 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
 Elements Used:
 C: 0-20 H: 0-20 O: 0-4
 A508/CV1K20/074A
 130103004 13 (0.365) Cm (13.18)



3-(2-hydroxycyclohexyl)-1H-isochromen-1-one

Chemical Formula: C₁₅H₁₆O₃
 Exact Mass: 244.11

Gajanan
 1: TOF MS ES+
 3.56e+004

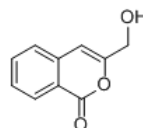


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
245.1173	245.1178	-0.5	-2.0	7.5	1.2	C15 H17 O3

TDC-J-04 A508-CV1K21-075 in CDCl3

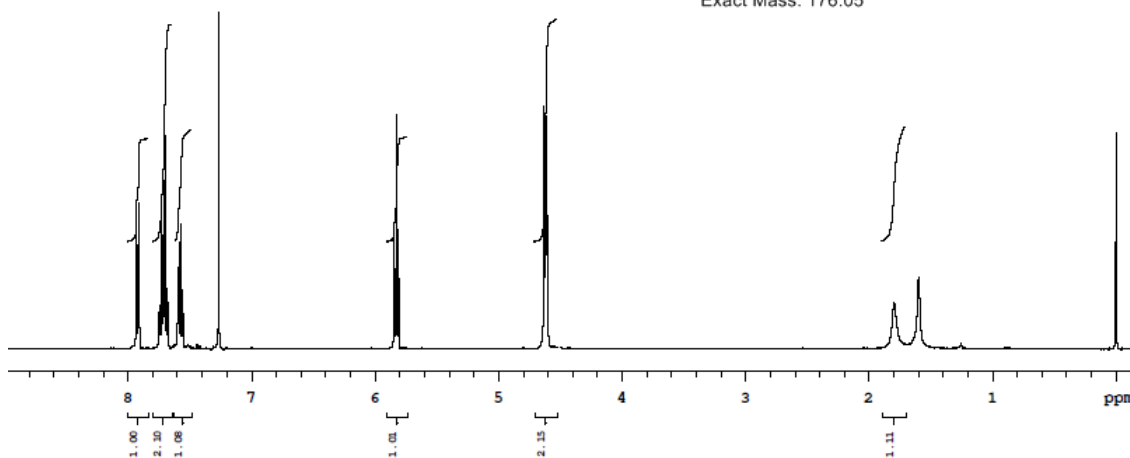
100-400MHz
 AR. No: ME1112/618
 Analyst: Ganesh
 Date: 08th Nov. 2012

NUCLEUS : H1
 FRQ (MHz): 400.23
 EXP : s2pul



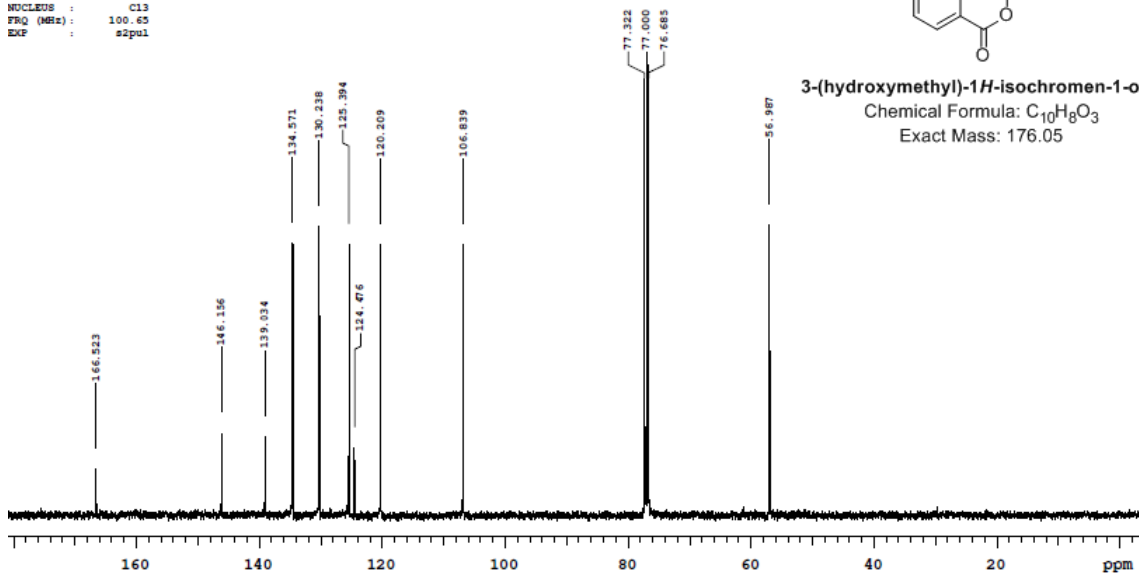
3-(hydroxymethyl)-1H-isochromen-1-one

Chemical Formula: C₁₀H₈O₃
 Exact Mass: 176.05



NMR-400MHz
 LR No: ME1112/964
 Analyst: Haribabu
 Date: 12th Nov. 2012

NUCLEUS : C13
 FREQ (MHz): 100.63
 EXP : zgpg30



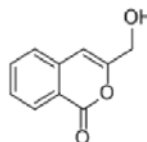
Elemental Composition Report

Page 1

Single Mass Analysis

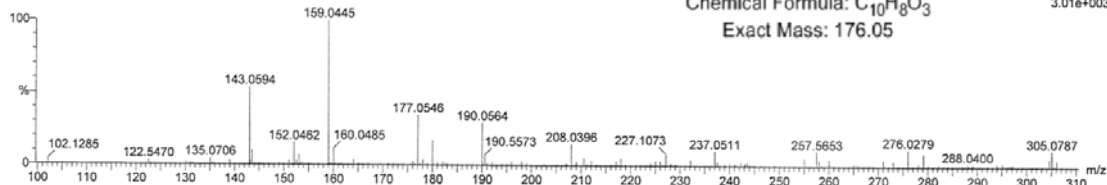
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 8 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
 Elements Used:
 C: 0-20 H: 0-20 O: 0-4
 A508/CVIK21/075A
 130103005 10 (0.278) Cm (8.12)

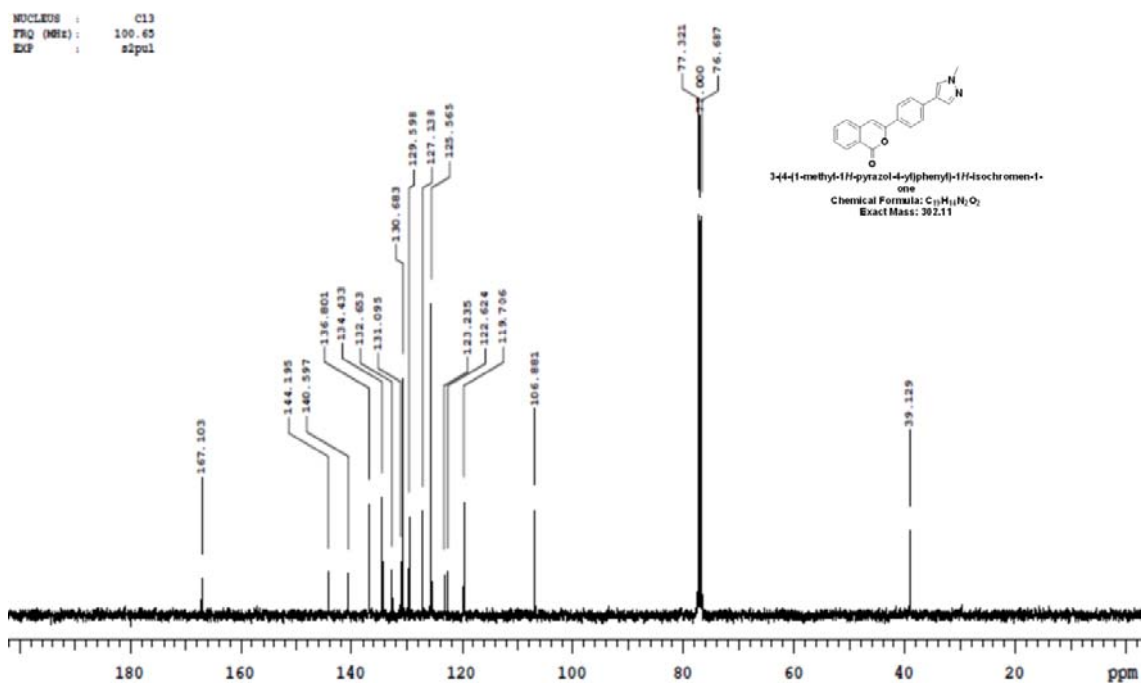
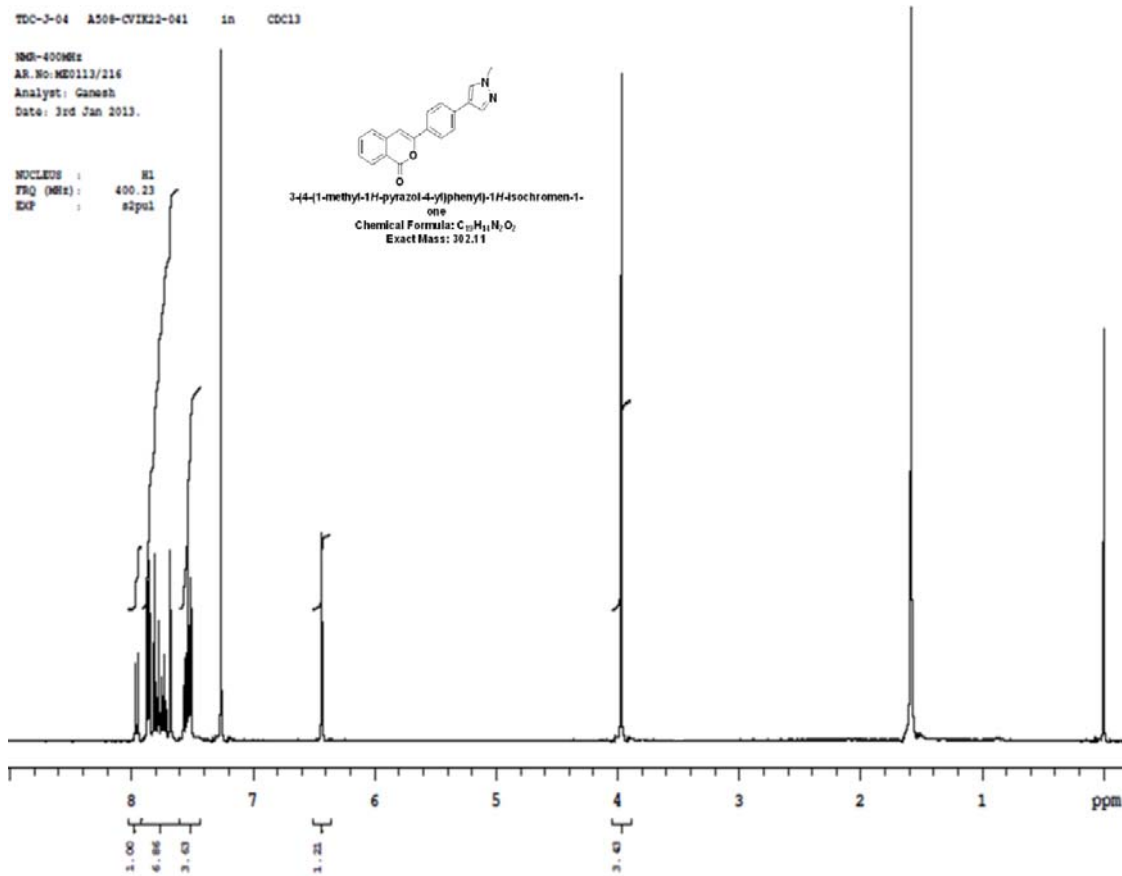


3-(hydroxymethyl)-1H-isochromen-1-one
 Chemical Formula: C₁₀H₈O₃
 Exact Mass: 176.05

Gajanan
 1: TOF MS ES+
 3.01e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
177.0546	177.0552	-0.6	-3.4	6.5	5.8	C10 H9 O3

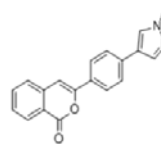


Elemental Composition Report

Page 1

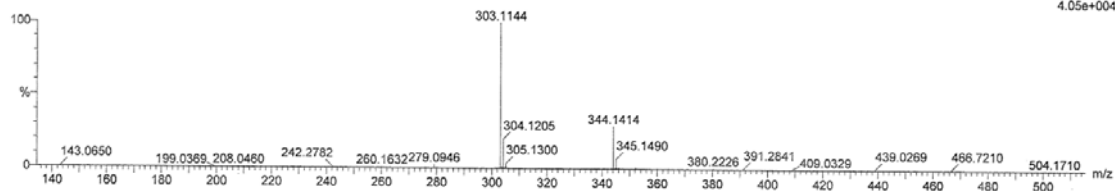
Single Mass Analysis

Tolerance = 5.0 PPM // DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



3-(4-(1-methyl-1H-pyrazol-4-yl)phenyl)-1H-isochromen-1-one
 Chemical Formula: C₁₉H₁₅N₂O₂
 Exact Mass: 302.11

Monoisotopic Mass, Even Electron Ions
 5 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
 Elements Used:
 C: 0-20 H: 0-20 N: 0-2 O: 0-2
 A508/CV1K22/041
 1: TOF MS ES+

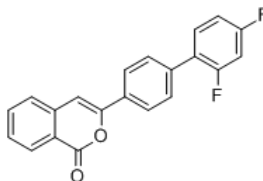


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.1144	303.1134	1.0	3.3	13.5	68.8	C ₁₉ H ₁₅ N ₂ O ₂

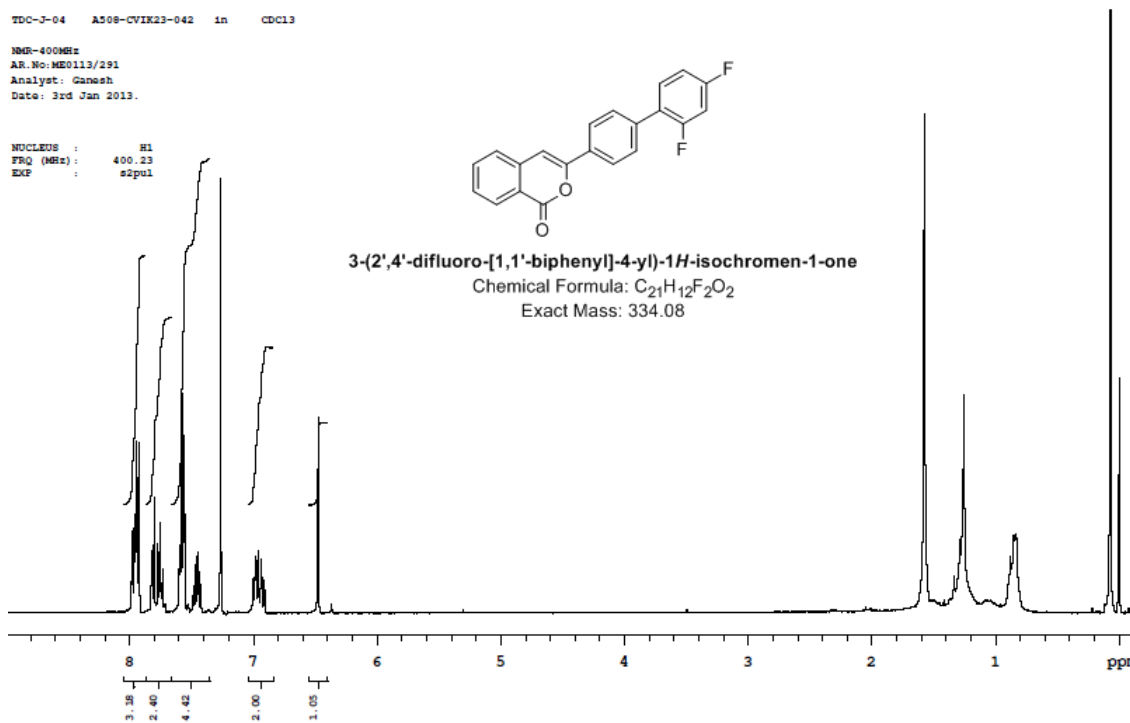
TDC-J-04 A508-CV1K23-042 in CDCl₃

NMR-400MHz
 AR.No:ME0113/291
 Analyst: Ganesh
 Date: 3rd Jan 2013.

NUCLEUS : H1
 FREQ (MHz): 400.23
 EXP : s2pul

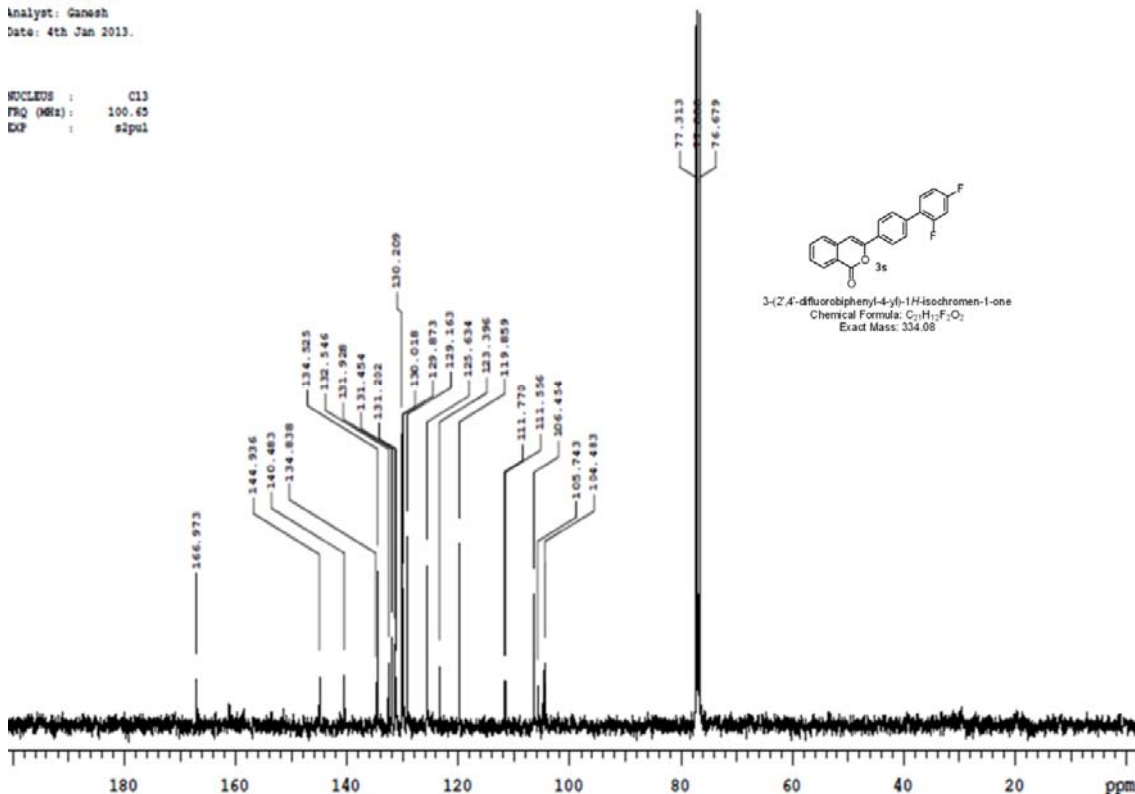


3-(2',4'-difluoro-[1,1'-biphenyl]-4-yl)-1H-isochromen-1-one
 Chemical Formula: C₂₁H₁₂F₂O₂
 Exact Mass: 334.08



MSD-400MHz
 LR. No: MS0113/461
 Analyst: Ganesh
 Date: 4th Jan 2013.

NUCLEUS : C13
 FREQ (MHz): 100.63
 EXP : sfpul

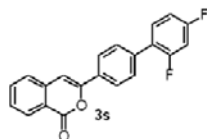


Elemental Composition Report

Single Mass Analysis

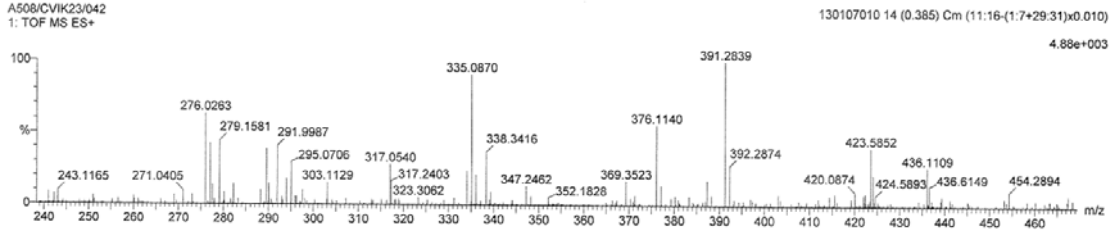
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 7 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
 Elements Used:
 C: 0-22 H: 0-30 O: 0-2 F: 0-2
 A508/CV/K23/042
 1: TOF MS ES+

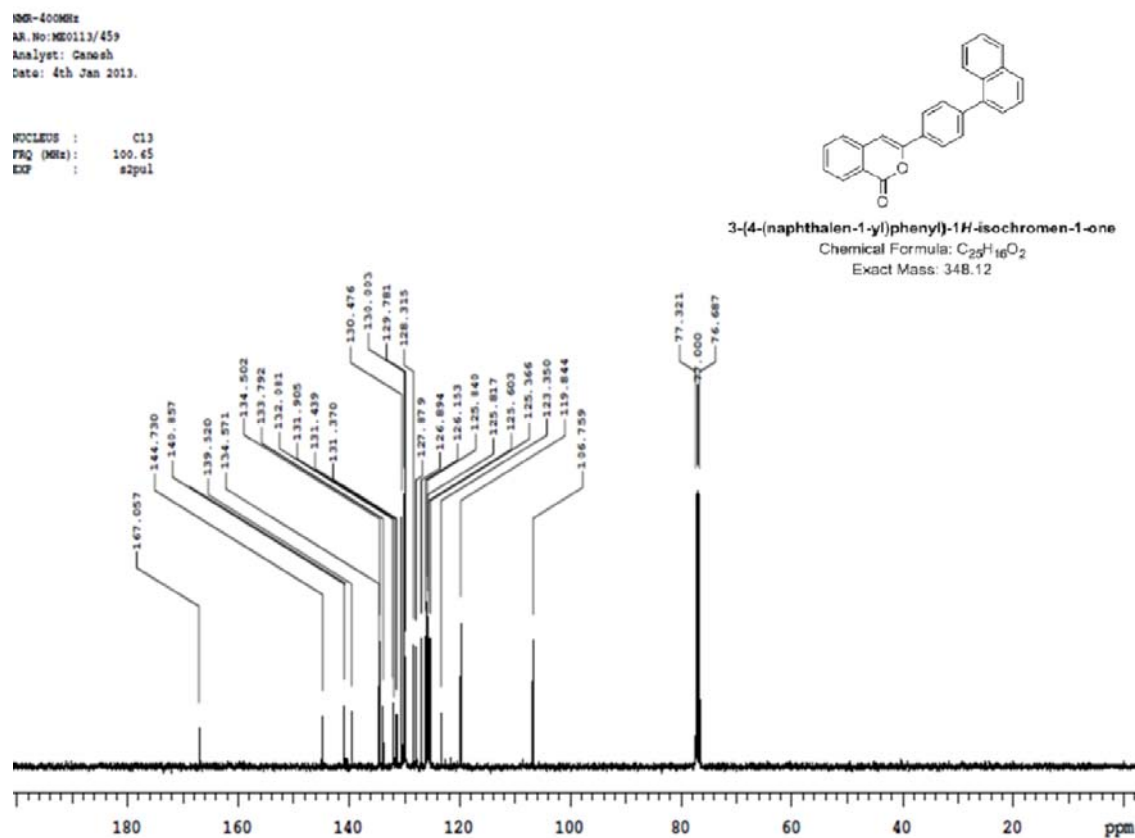
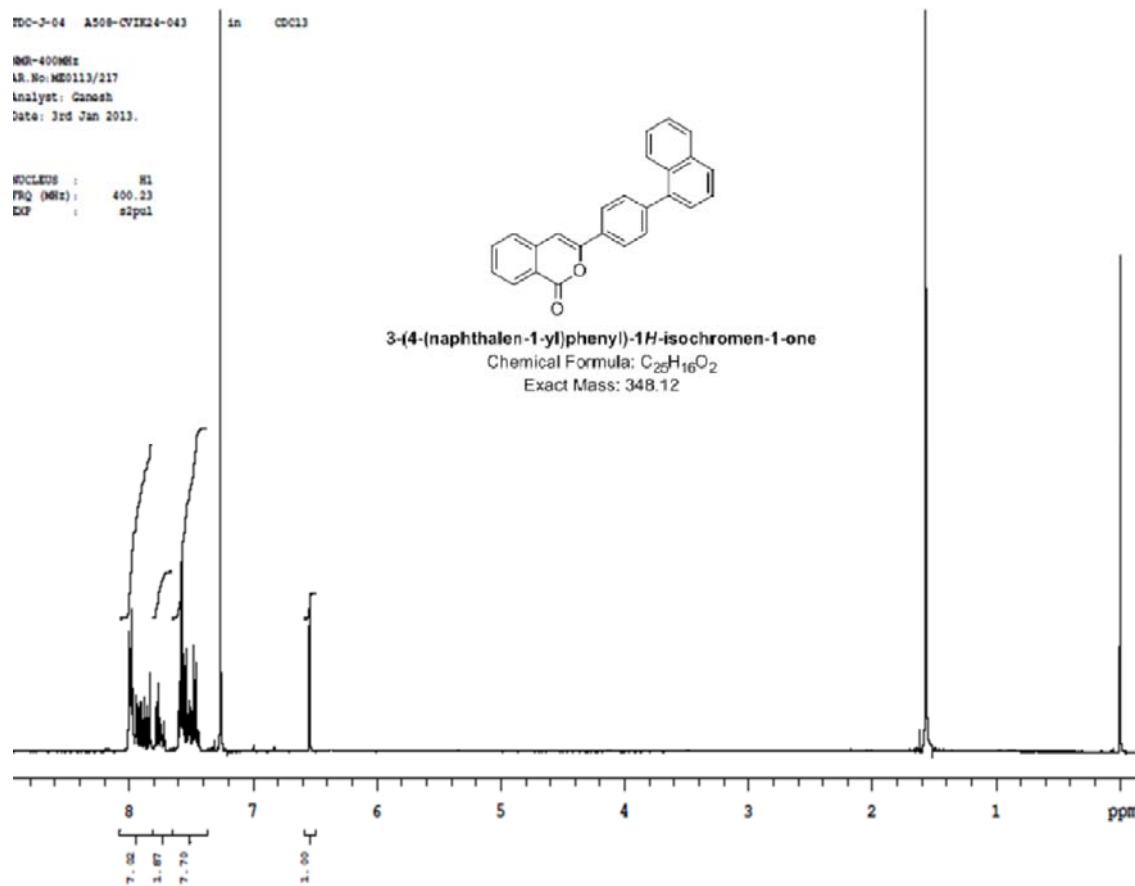


3-(2,4-difluorophenyl-4-yl)-1H-isochromen-1-one
 Chemical Formula: C₂₁H₁₃F₂O₂
 Exact Mass: 334.08

Page 1



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
335.0870	335.0884	-1.4	-4.2	14.5	1.0	C21 H13 O2 F2

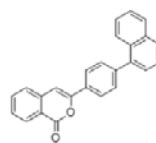


Elemental Composition Report

Page 1

Single Mass Analysis

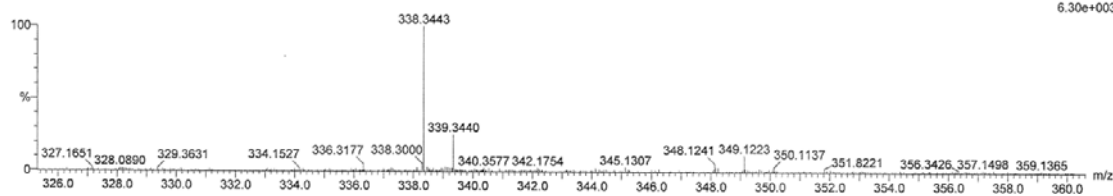
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



3-(4-(naphthalen-1-yl)phenyl)-1H-isochromen-1-one
 Chemical Formula: C₂₅H₁₆O₂
 Exact Mass: 348.12

Monoisotopic Mass, Even Electron Ions
 7 formula(e) evaluated with 1 results within limits (up to 8 best isotopic matches for each mass)
 Elements Used:
 C: 0-30 H: 0-25 O: 0-2
 A508/CVIK24/D43
 1: TOF MS ES+

130107011 11 (0.298) Cm (10:13)
 6.30e+003

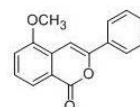


Mass	Calc. Mass	mDa	PPM	DBE	i-PIT	Formula
349.1223	349.1229	-0.6	-1.7	17.5	19.9	C ₂₅ H ₁₇ O ₂

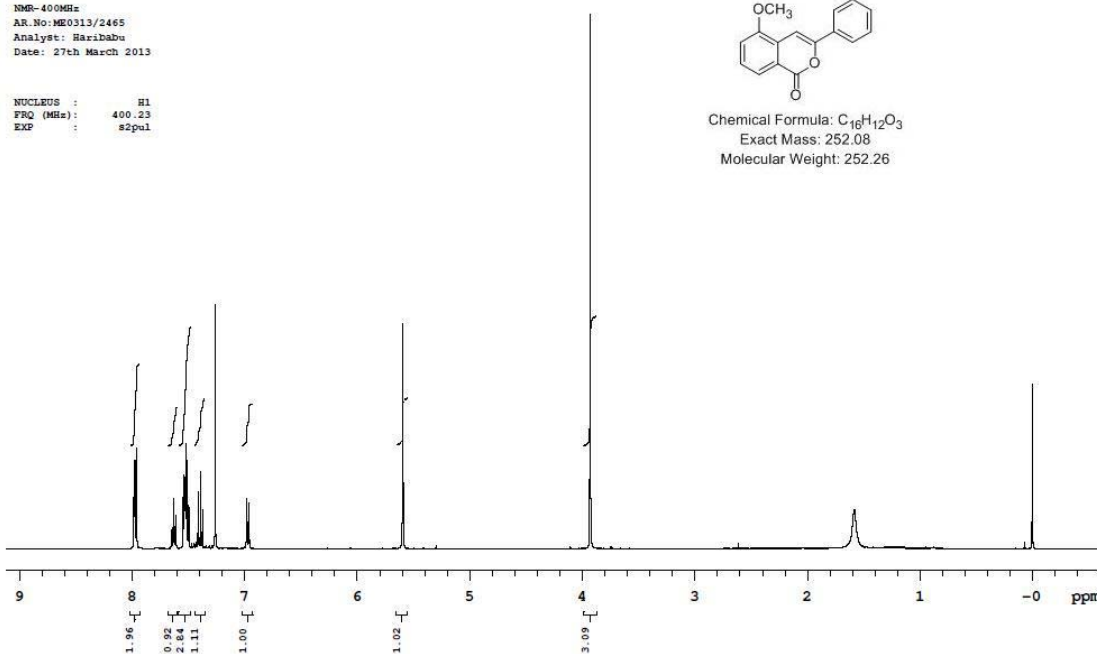
TDCJ-04 A508/CVIK26/026 in CDCl₃

NMR-400MHz
 AR.No:ME0313/2465
 Analyst: Haribabu
 Date: 27th March 2013

NUCLEUS : H1
 FRQ (MHz): 400.23
 EXP : s2pul



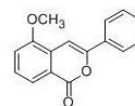
Chemical Formula: C₁₆H₁₂O₃
 Exact Mass: 252.08
 Molecular Weight: 252.26



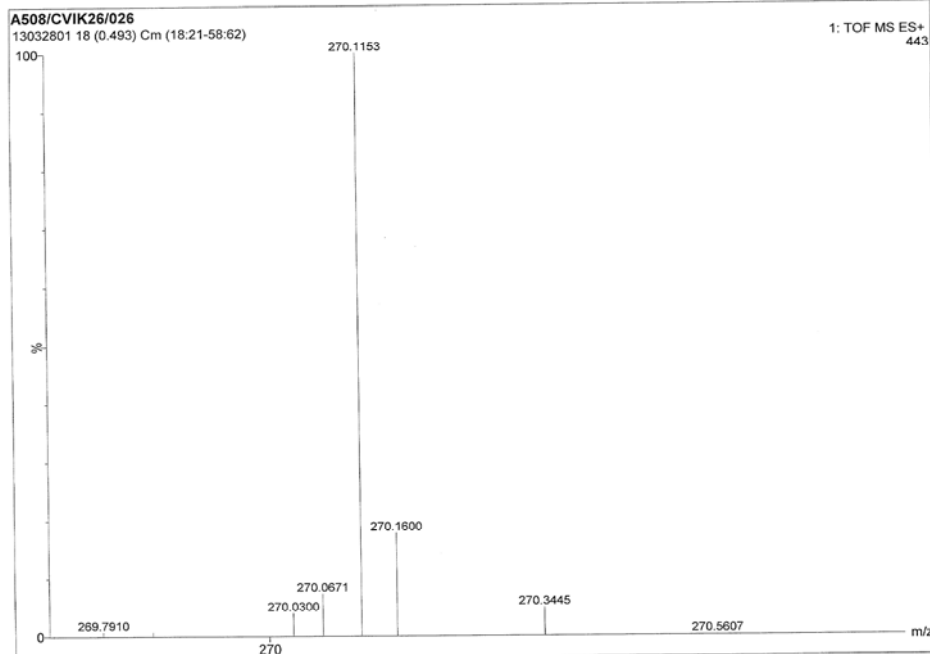
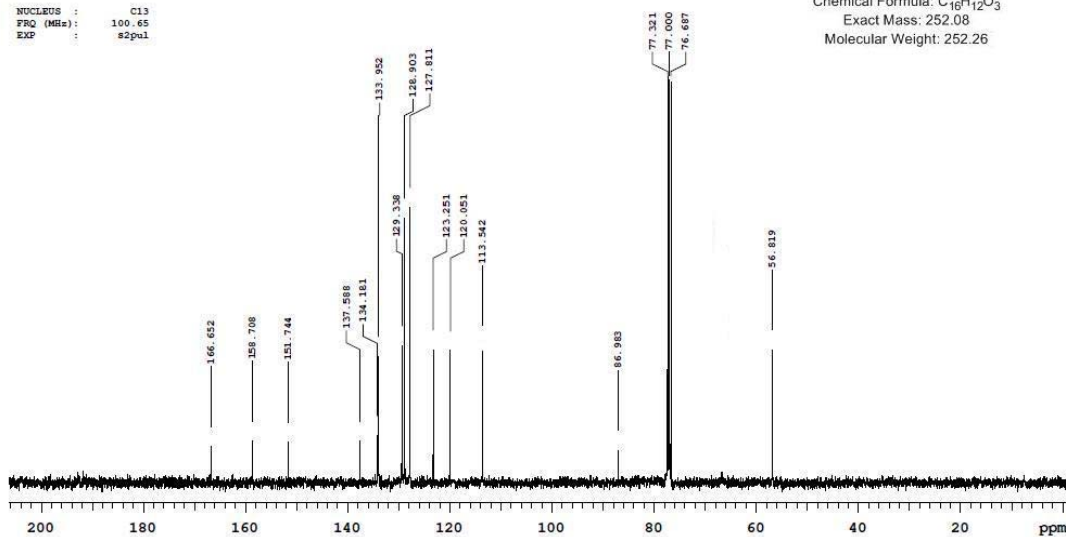
TDCJ-04 A508/CVIK26/026 in CDCl3

NMR-400MHz
AR.No:ME0313/2670
Analyst: Haribabu
Date: 28th March 2013

NUCLEUS : C13
FREQ (MHz) : 100.65
EXP : s2pul



Chemical Formula: C₁₆H₁₂O₃
Exact Mass: 252.08
Molecular Weight: 252.26



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 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

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

Elements Used:

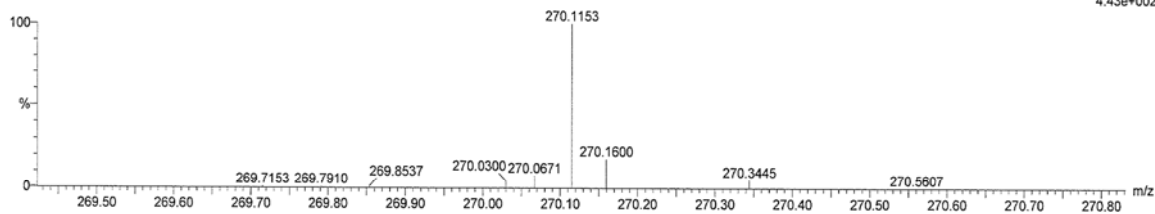
C: 10-20 H: 10-20 N: 0-2 O: 1-5

A508/CVIK26/026

1: TOF MS ES+

13032801 18 (0.493) Cm (18.21-58.62)

4.43e+002



Minimum: -5.0
Maximum: 5.0 10.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.1153	270.1130	2.3	8.5	9.5	n/a	C16 H16 N O3