

Iodine catalyzed one-pot four component synthesis of coumarinyl phosphoramidates via sequential addition of reactants.

Mohammed Imran Khan and Kalegowda Shivashankar*

P.G. Department of Chemistry, Central College Campus, Bangalore University, Bangalore- 560 001, Karnataka, India.

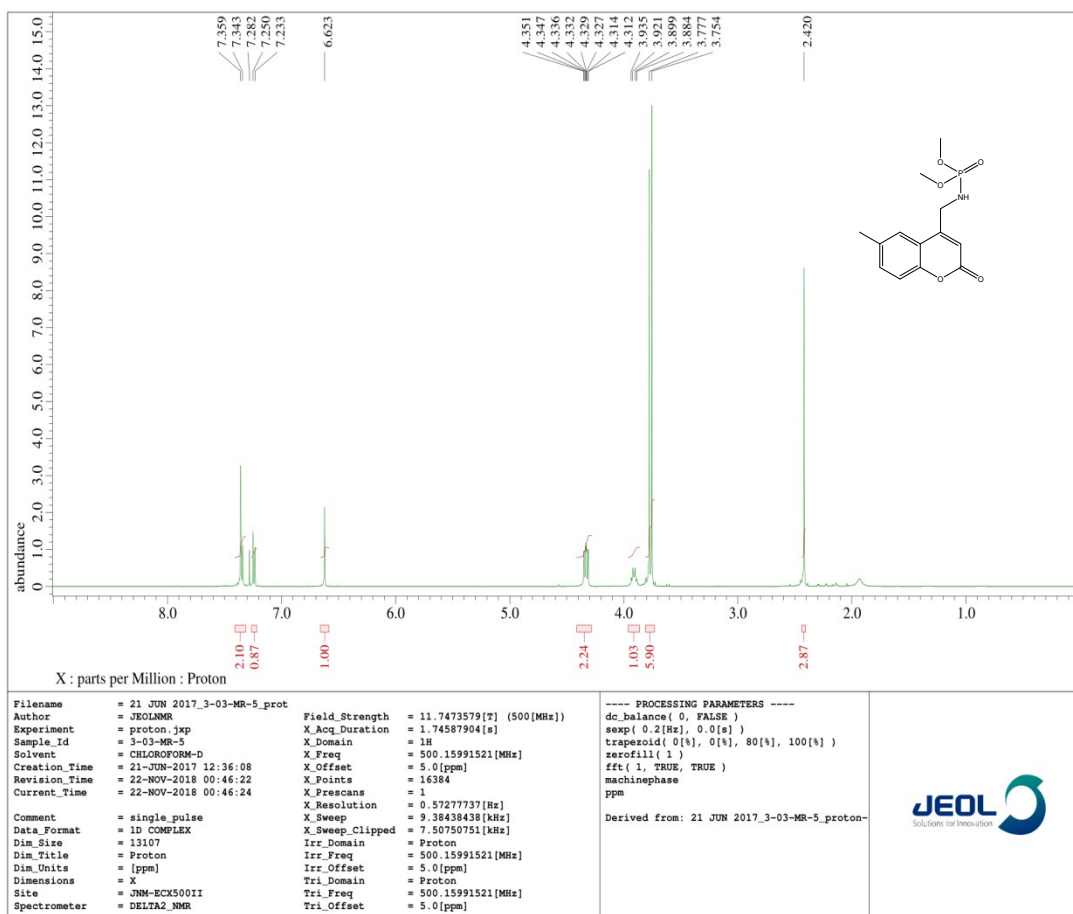
***Corresponding author.** *E-mail address:* shivashankark@gmail.com (K. Shivashankar)

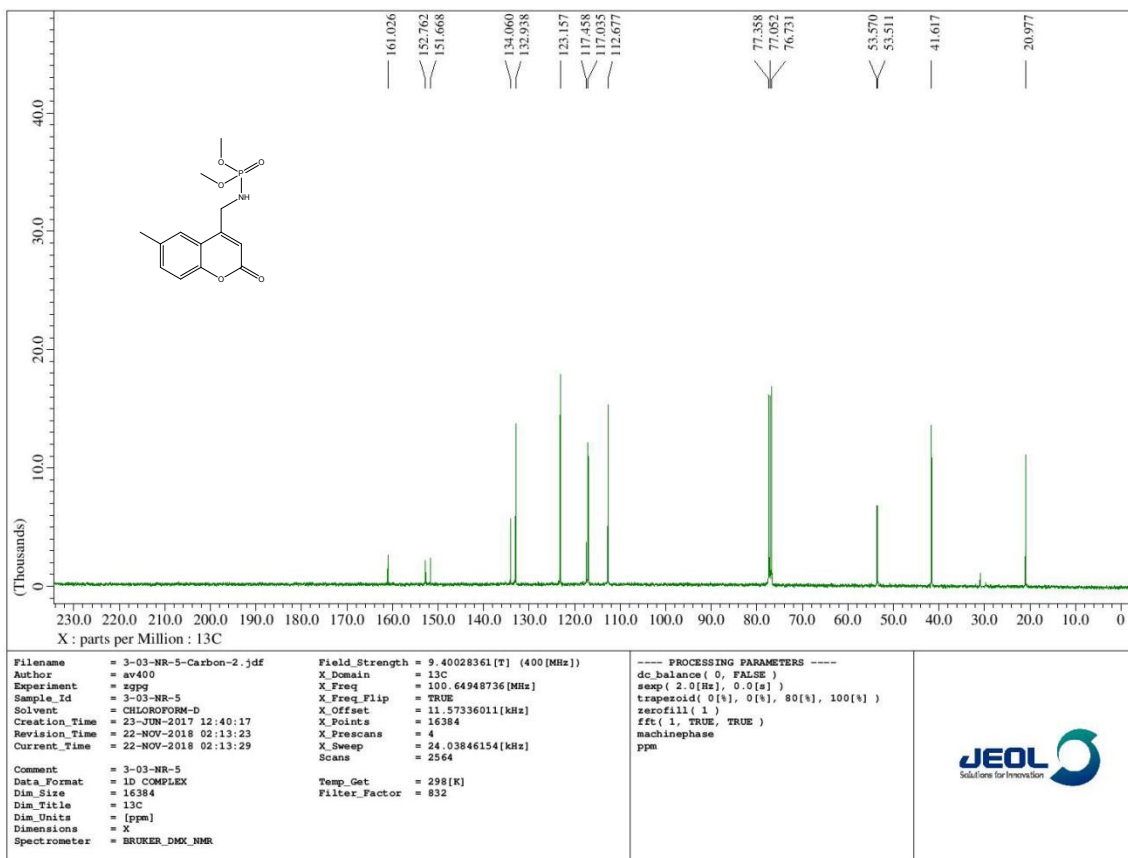
SUPPORTING FILES

Entry	Compounds	Spectra
S4	5a	¹ H
S5	5a	¹³ C
S6	5a	LC –MS
S7	5b	¹ H
S8	5b	¹³ C
S9	5b	HR-MS
S10	5c	¹ H
S11	5c	¹³ C
S12	5c	HR-MS
S13	5d	¹ H
S14	5d	¹³ C
S15	5d	HR-MS

cS16	5e	^1H
S17	5e	^{13}C
S18	5e	HR-MS
S19	5f	^1H
S20	5f	^{13}C
S21	5f	HR-MS
S22	5g	^1H
S23	5g	^{13}C
S24	5g	HR-MS
S25	5h	^1H
S26	5h	^{13}C
S27	5h	HR-MS
S28	5i	^1H
S29	5i	^{13}C
S30	5i	HR-MS
S31	5j	^1H
S32	5j	^{13}C
S33	5j	HR-MS
S34	5k	^1H

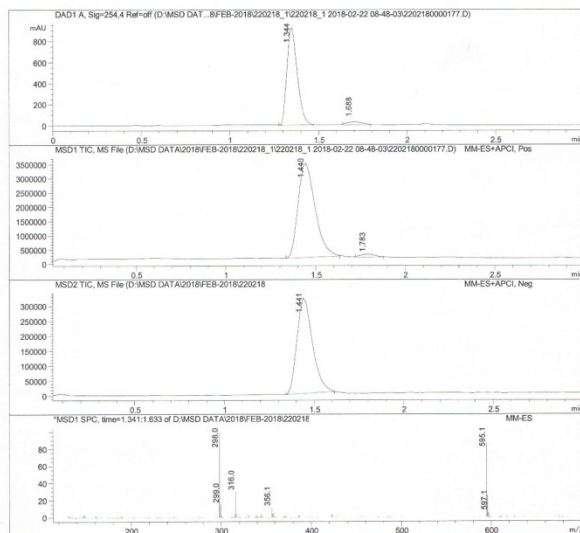
S35	5k	^{13}C
S36	5k	LC –MS
S37	5k	LC –MS
S38	5l	^1H
S39	5l	^{13}C
S40	5l	HR–MS
S41	5m	^1H
S42	5m	^{13}C
S43	5m	HR–MS
S44	5n	^1H
S45	5n	^{13}C
S46	5n	LC –MS
S47	5o	^1H
S48	5o	^{13}C
S49	5o	LC –MS
S50	5p	^1H
S51	5p	^{13}C
S52	5p	LC –MS





Pcode: Sample Id: PDA/MS (APCI+MODE AND APCI+MODE)
 Injection Date : 2/22/2018 10:18:46 PM Vial No. : P2-B-08
 Data file : D:\MSD DATA\2018\FEB-2018\220218_1\ -> Injection vol : 1µL

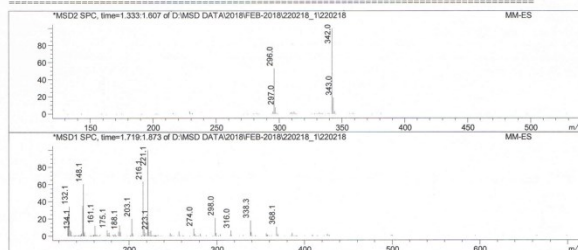
Method info : METHOD:34-100316, Flow rate:0.3 ml /min
 Ascentis Express C18 (50 mm X 2.1mm X 2.7µm)
 Mobile Phase (A) : 0.1% FORMIC ACID IN WATER
 MobilePhase (B) : ACN



Analysed By :

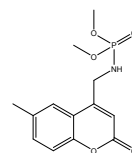
Instrument Code : Instrument 1

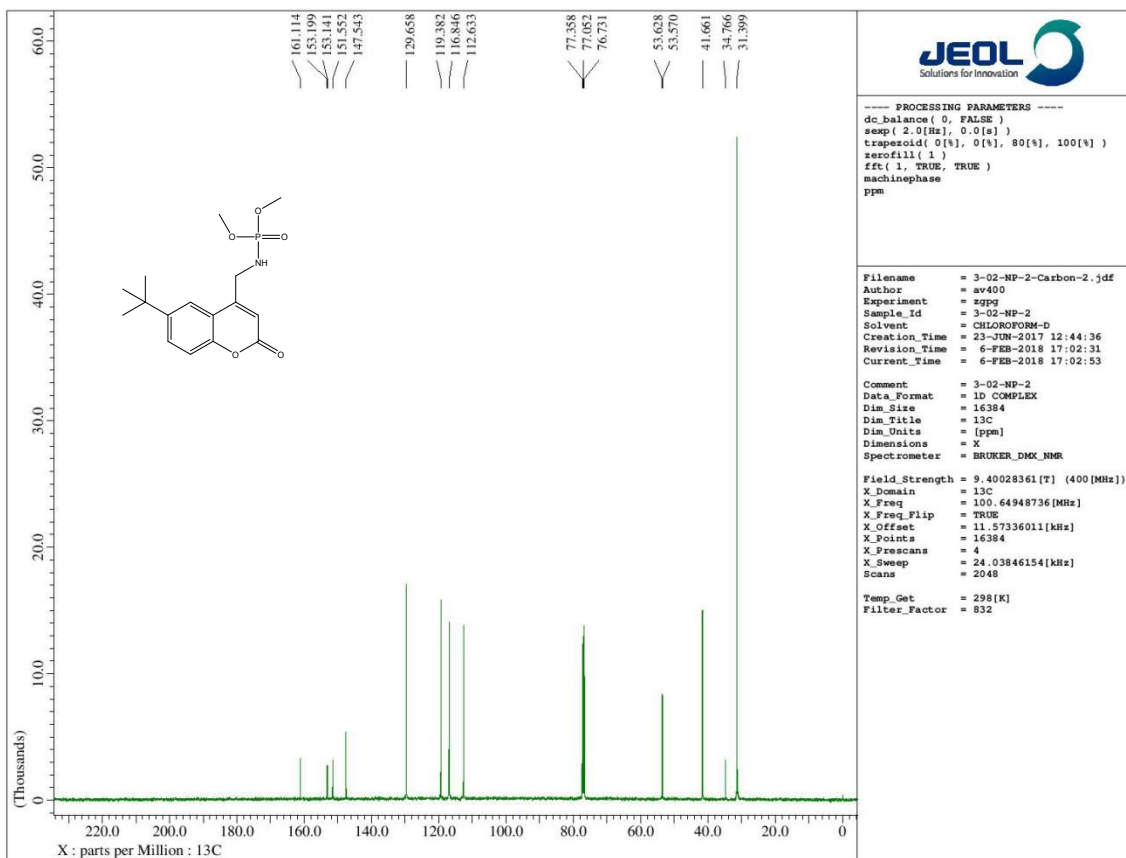
Page 1 of 2

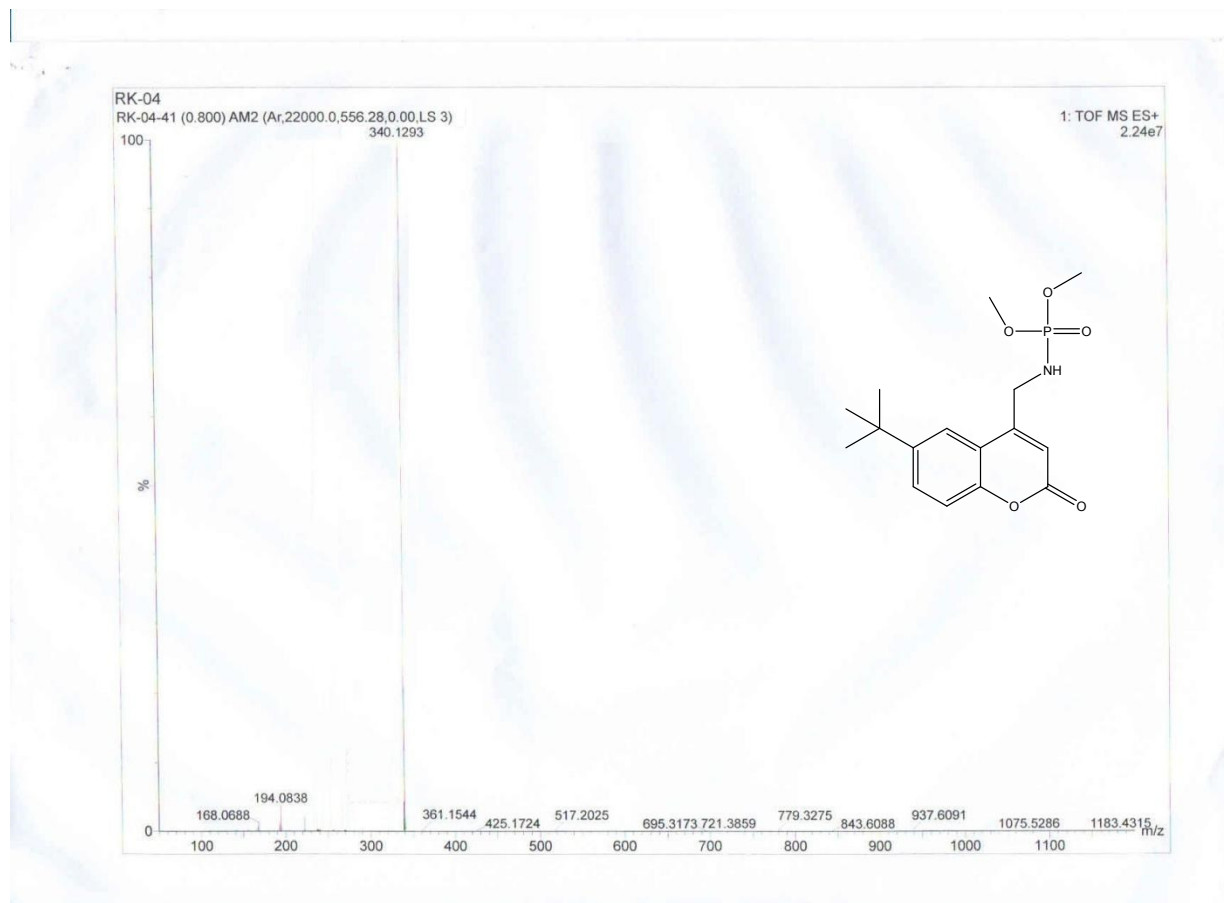


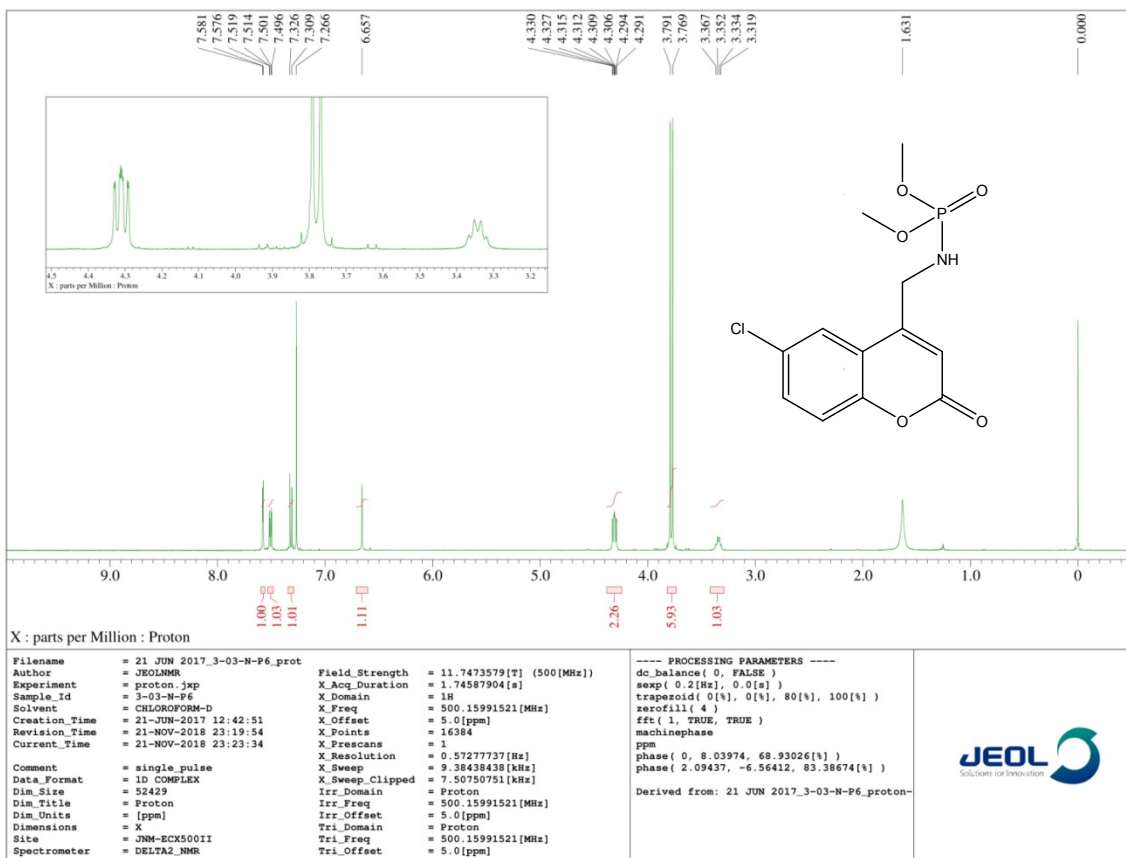
Compound Name	Area	Meas. R	Area %
	2.162e7	1.440	97.362
	5.860e5	1.783	2.638

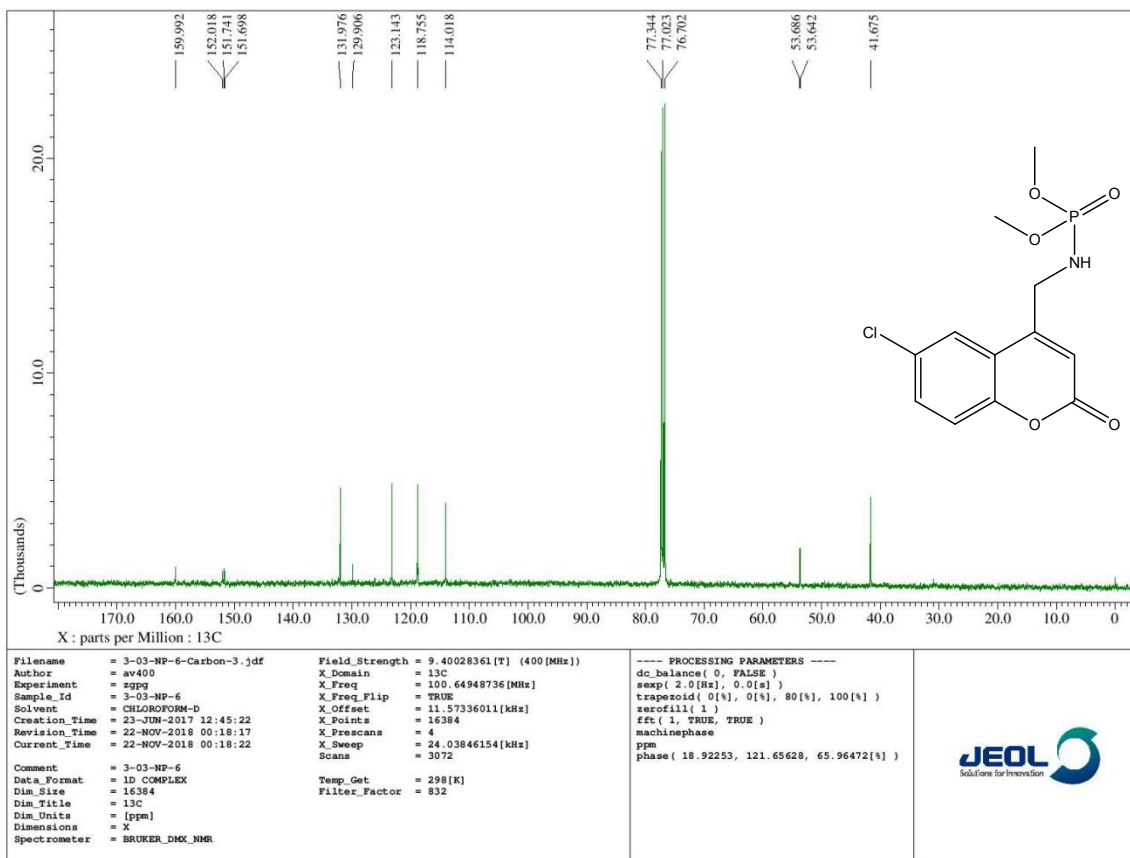
Compound Name	Area	Meas. R	Area %
	1.910e6	1.441	100.000

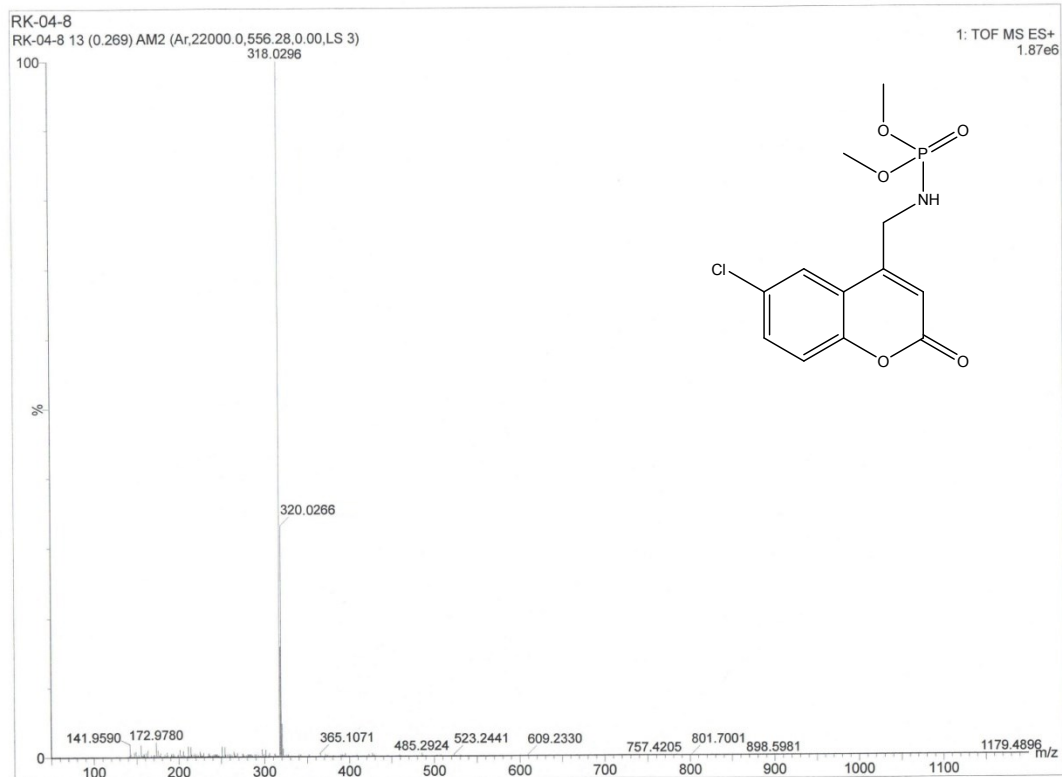


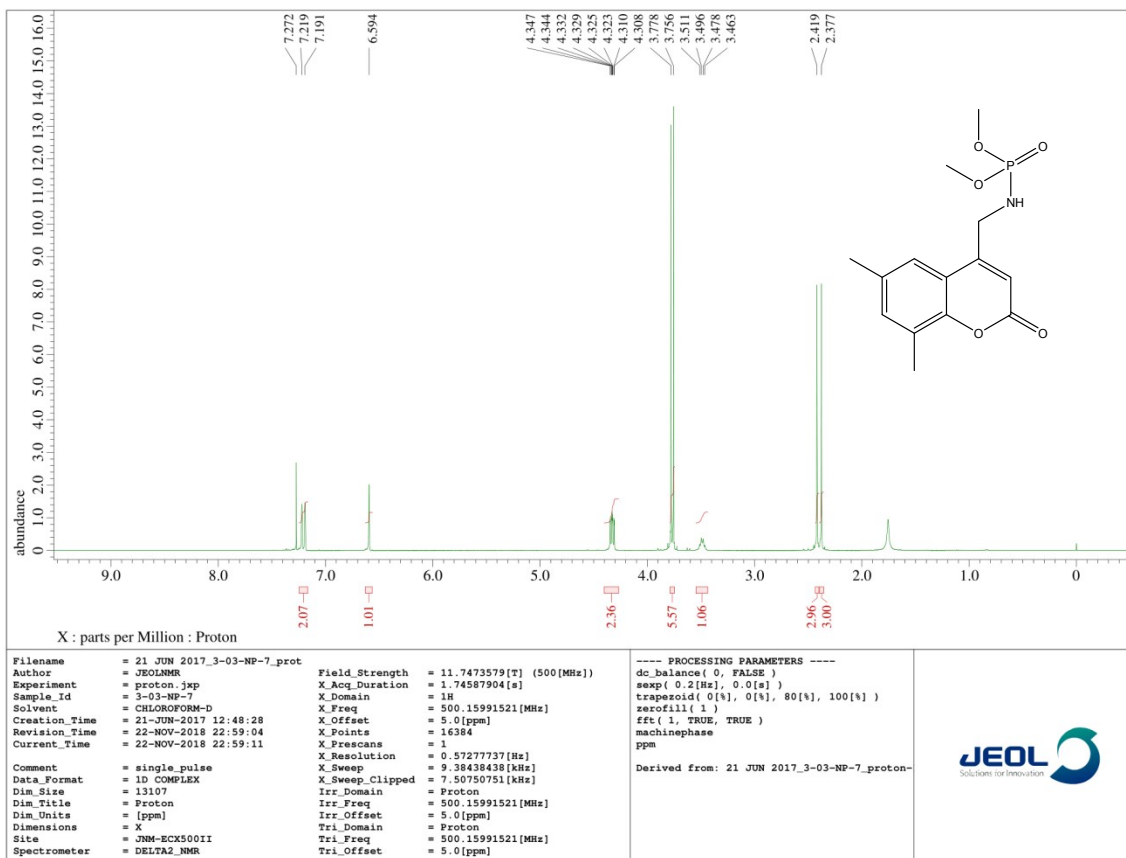


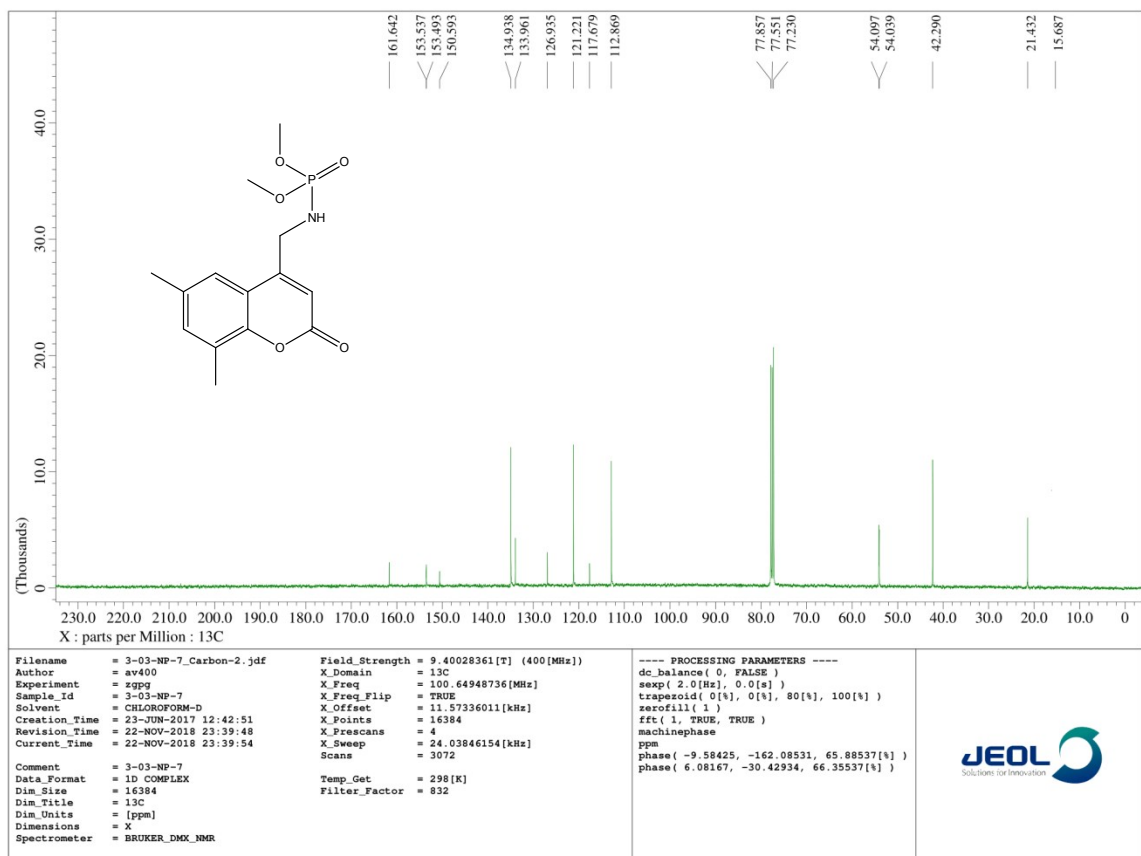


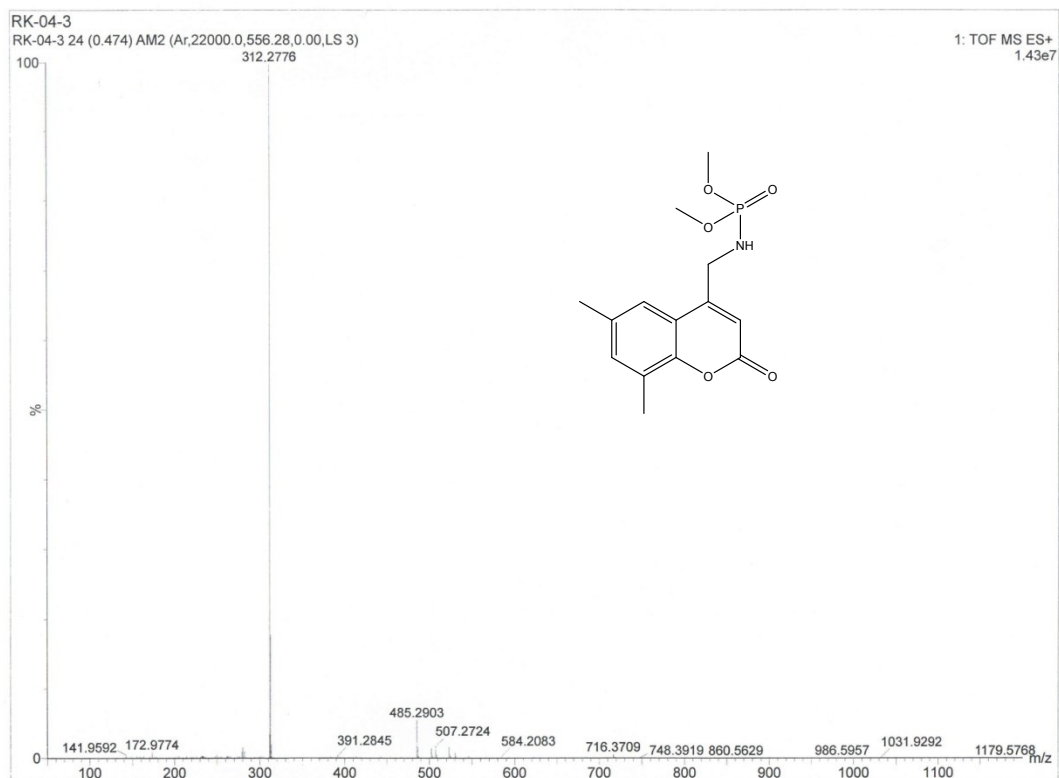


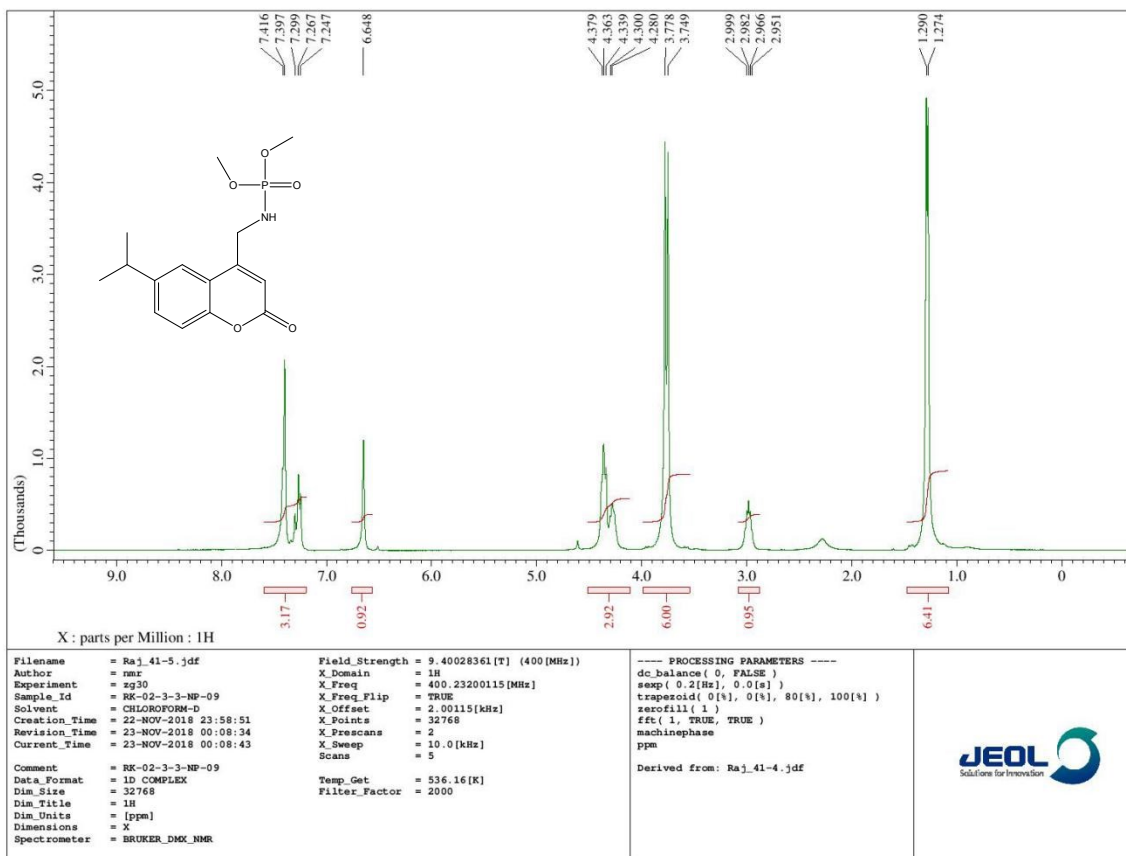


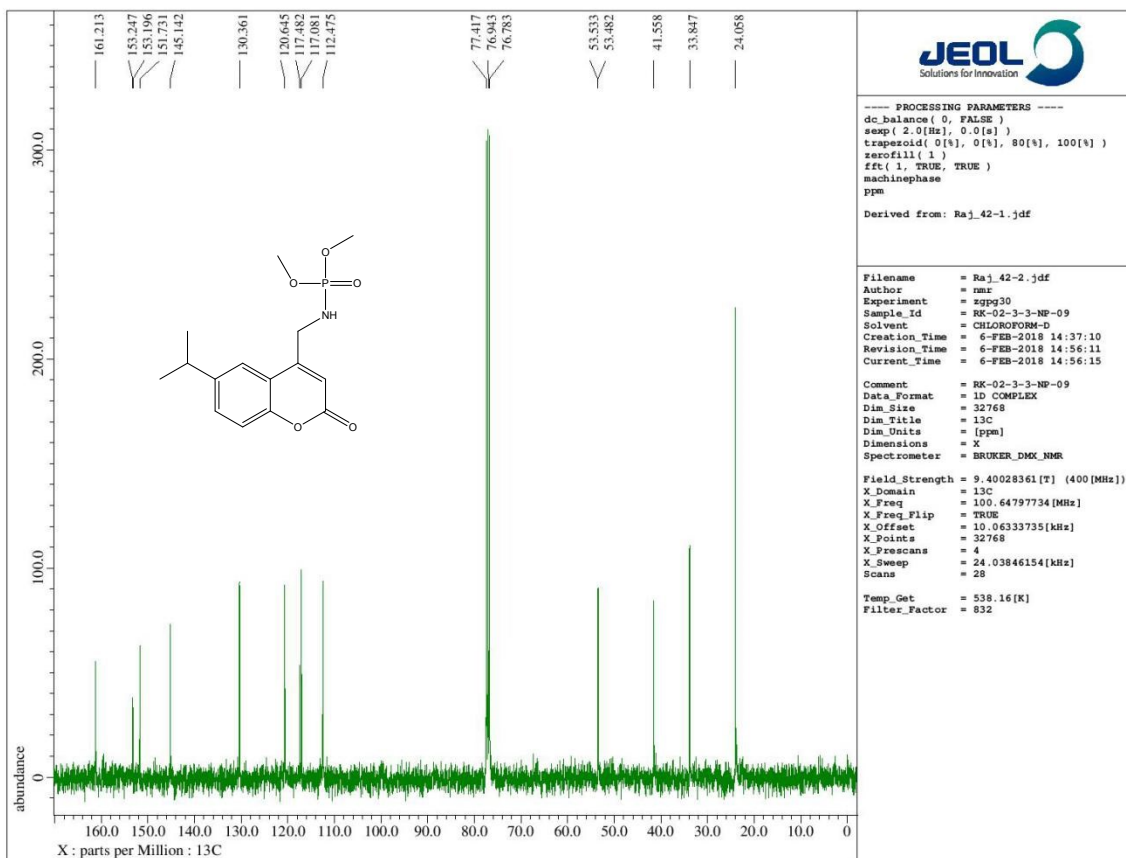


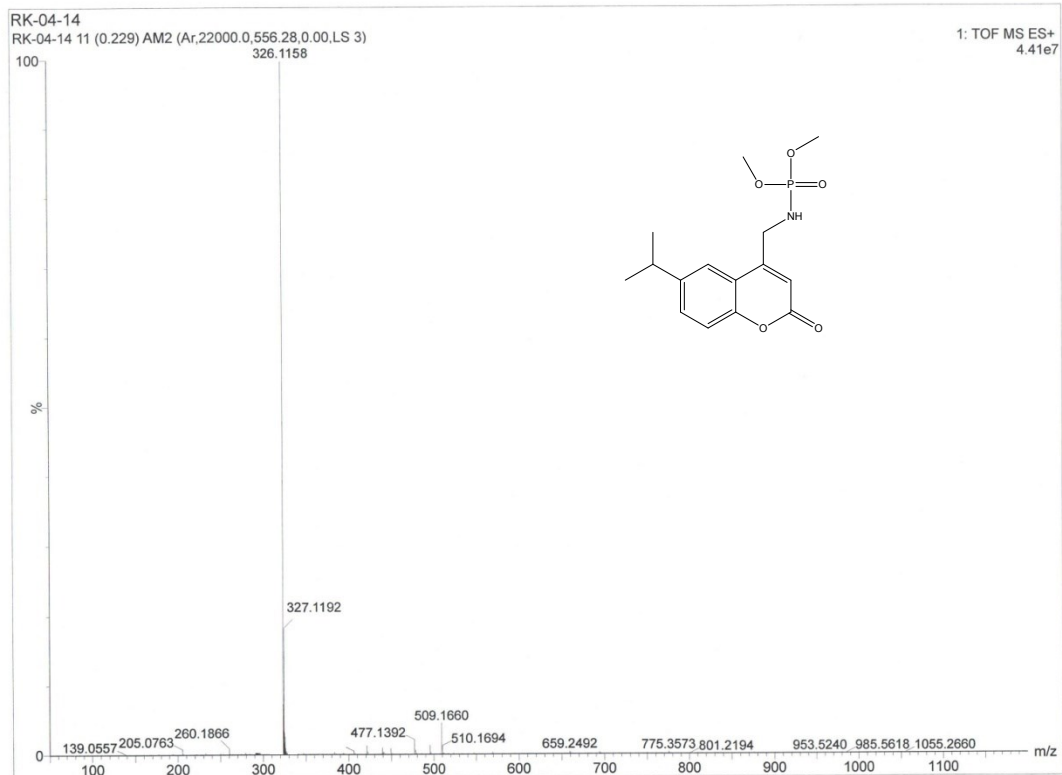


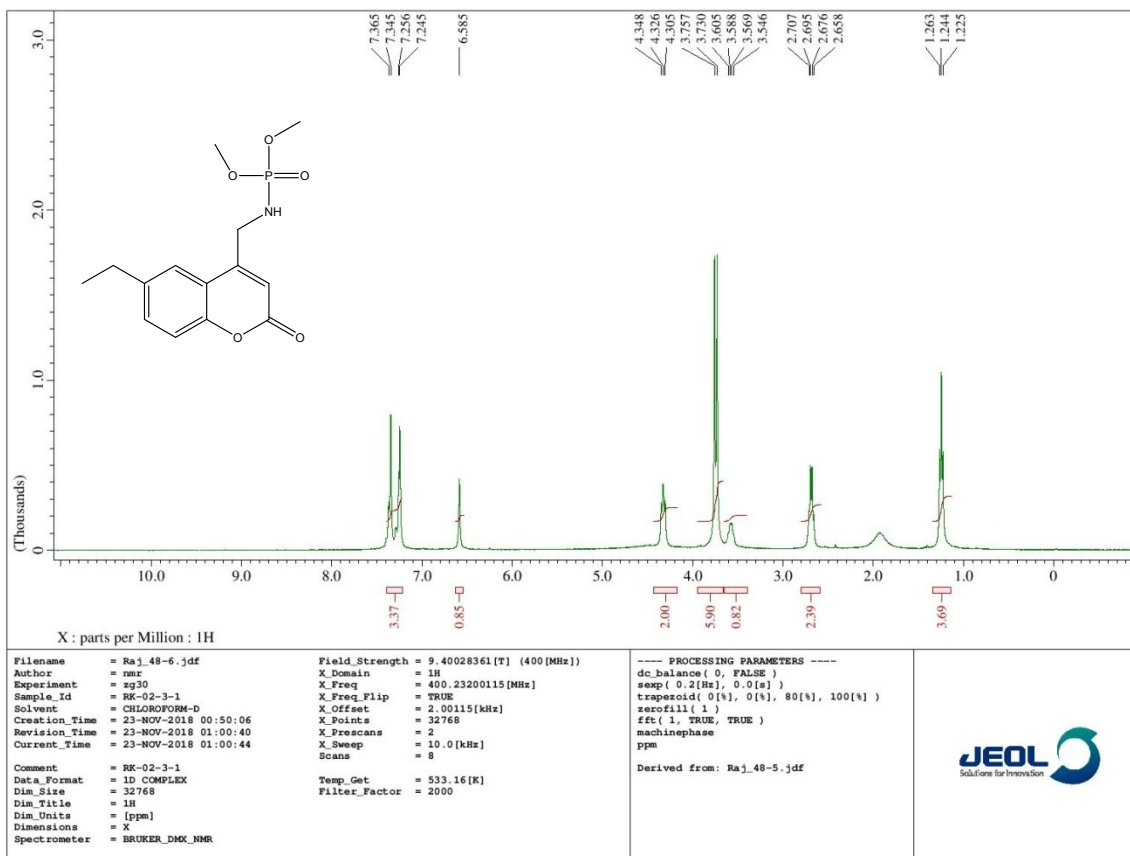


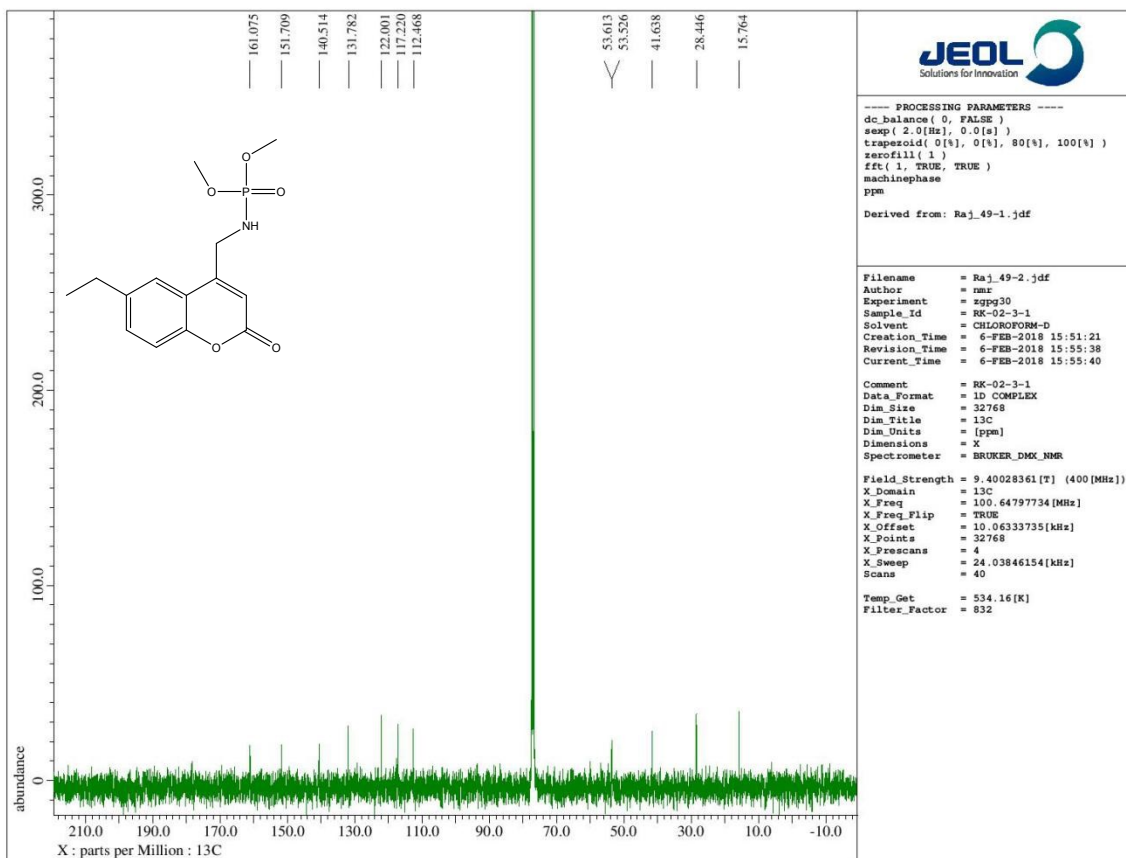


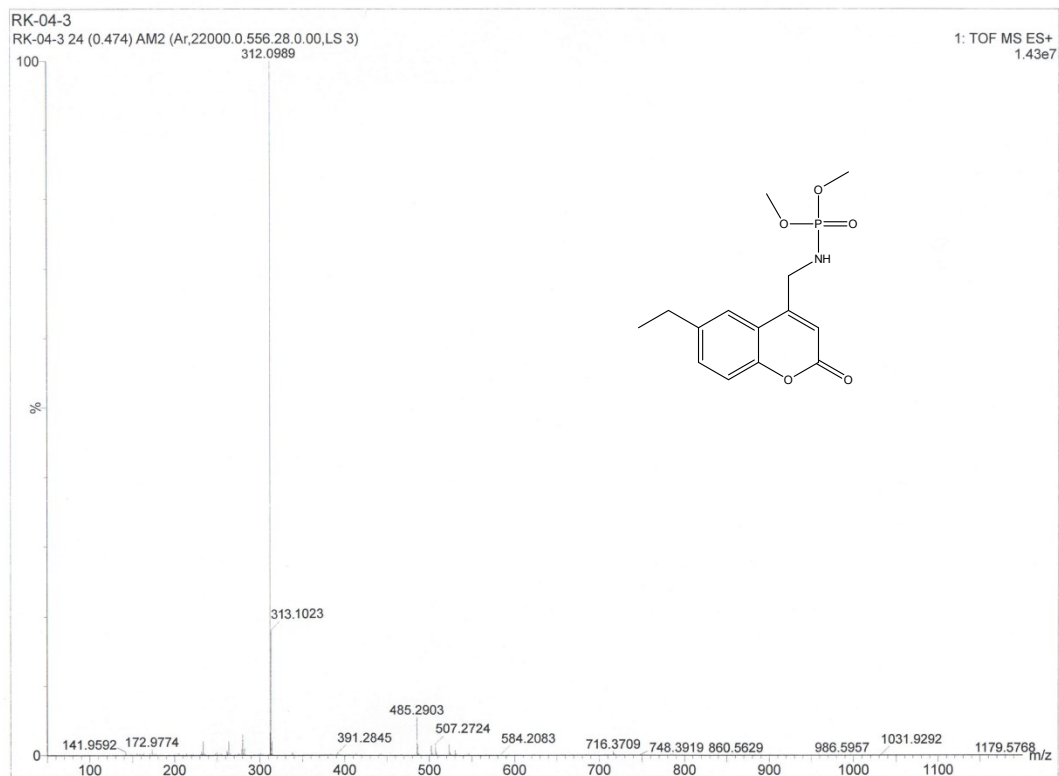


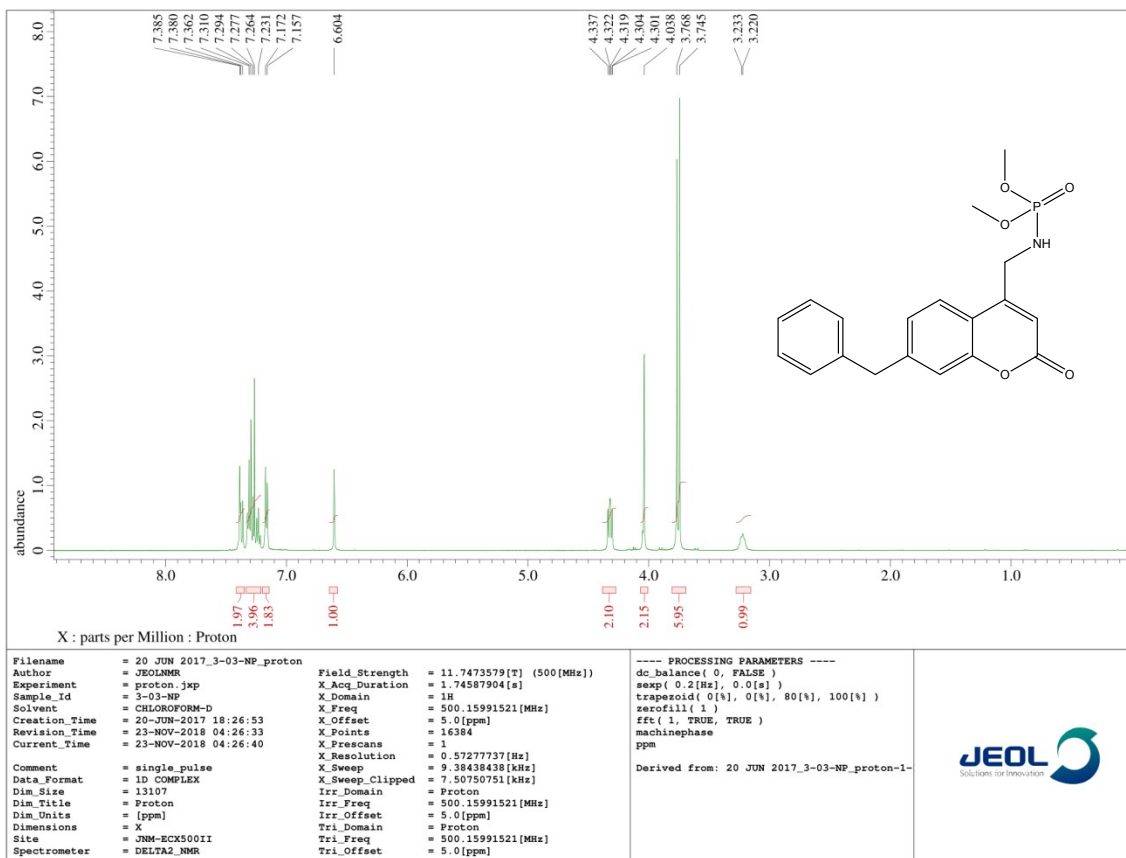


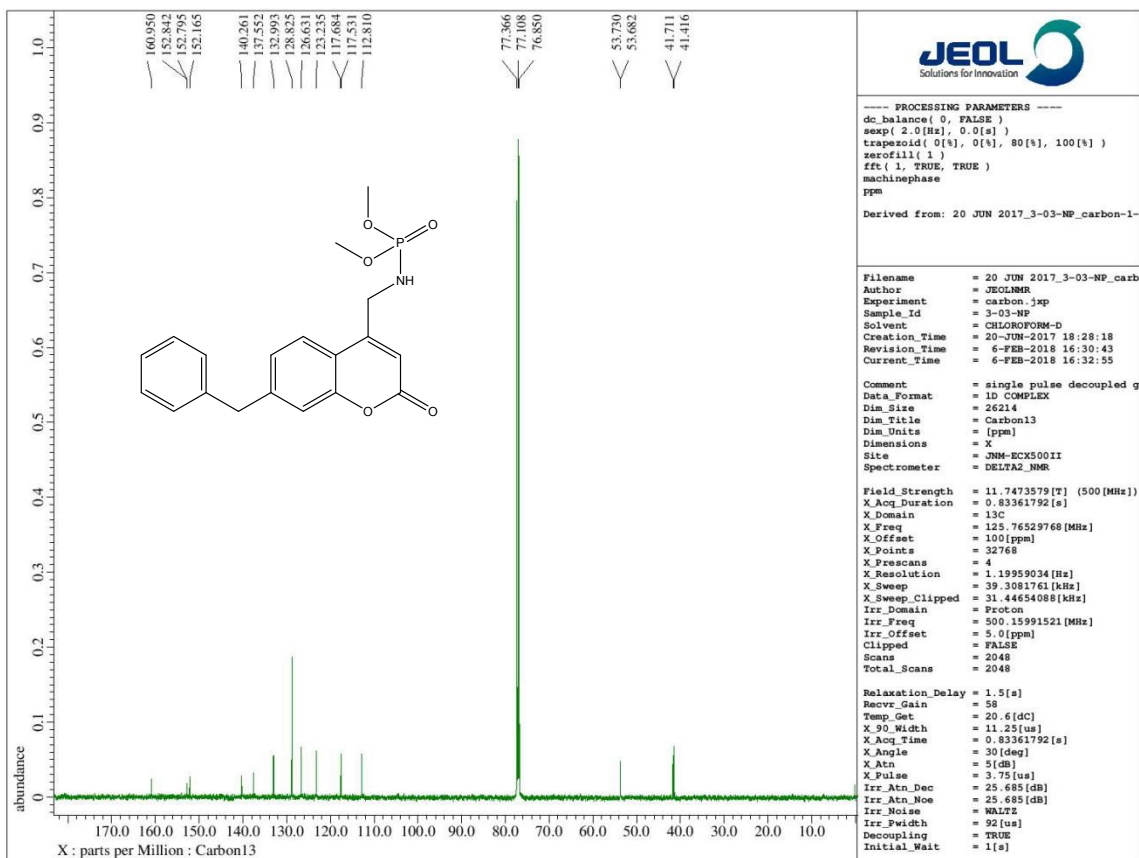


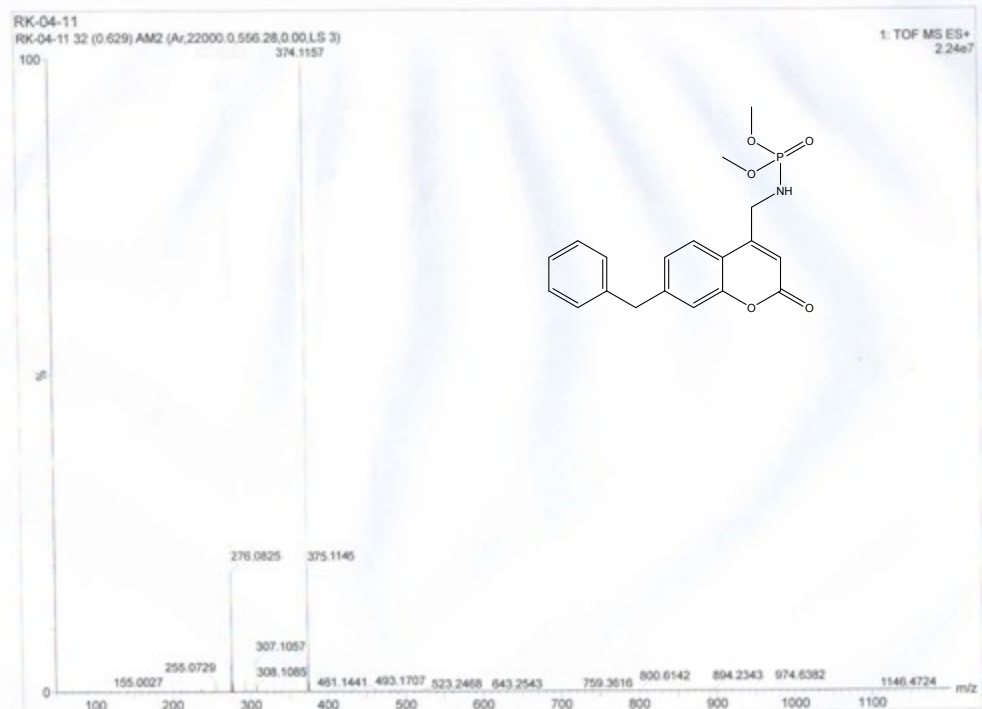


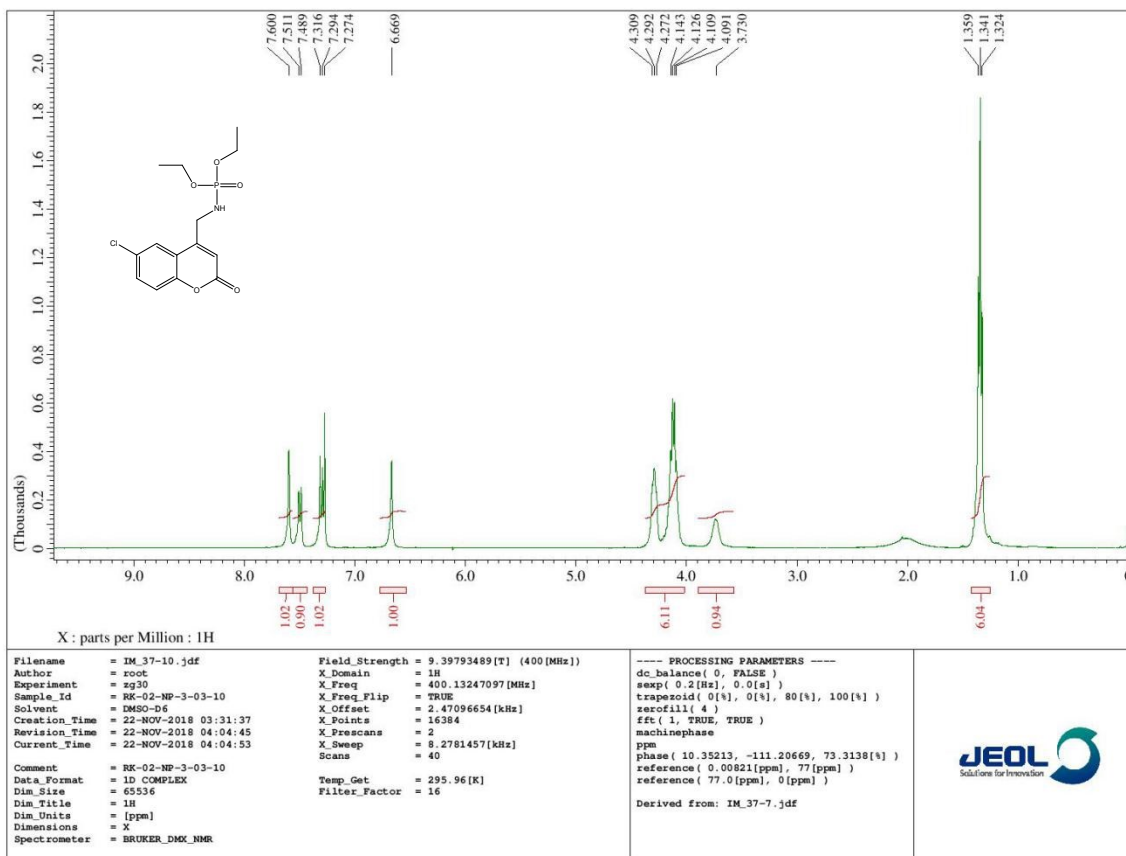


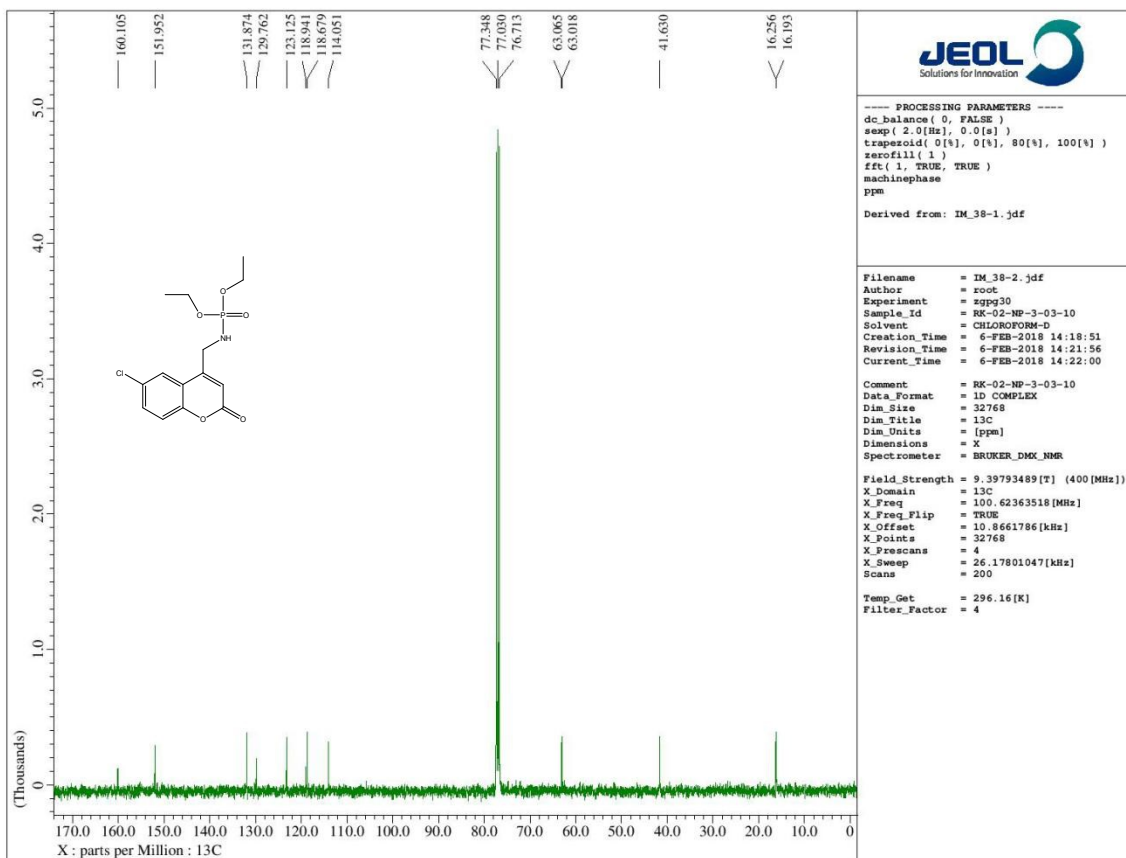


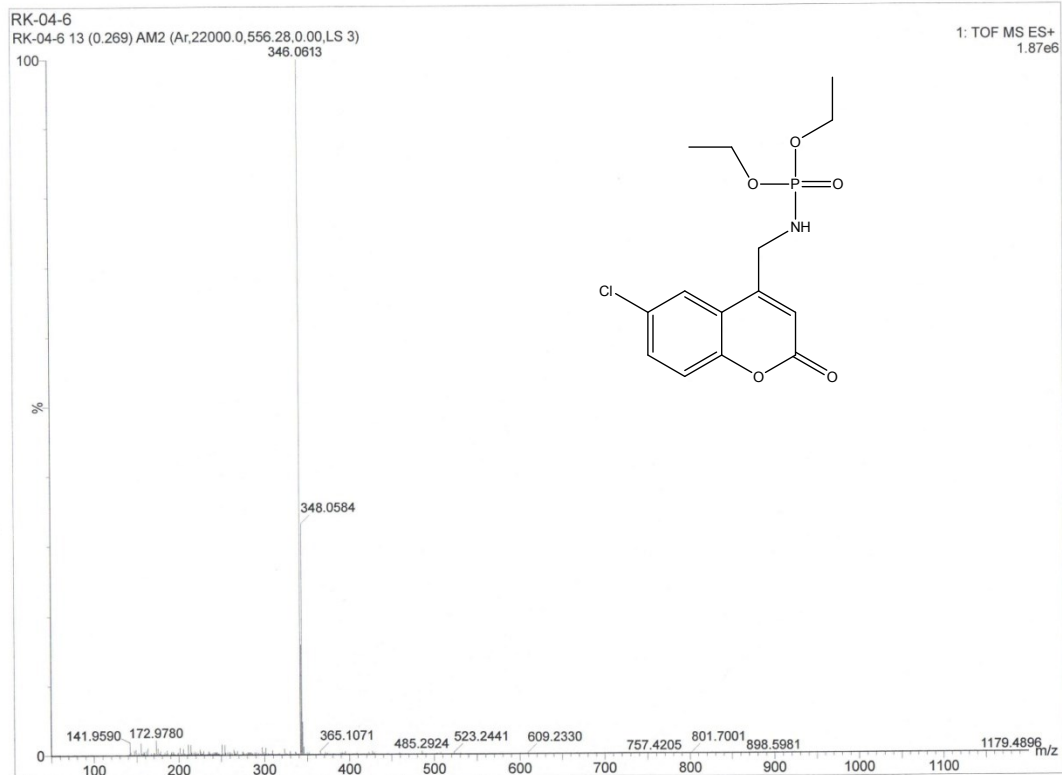


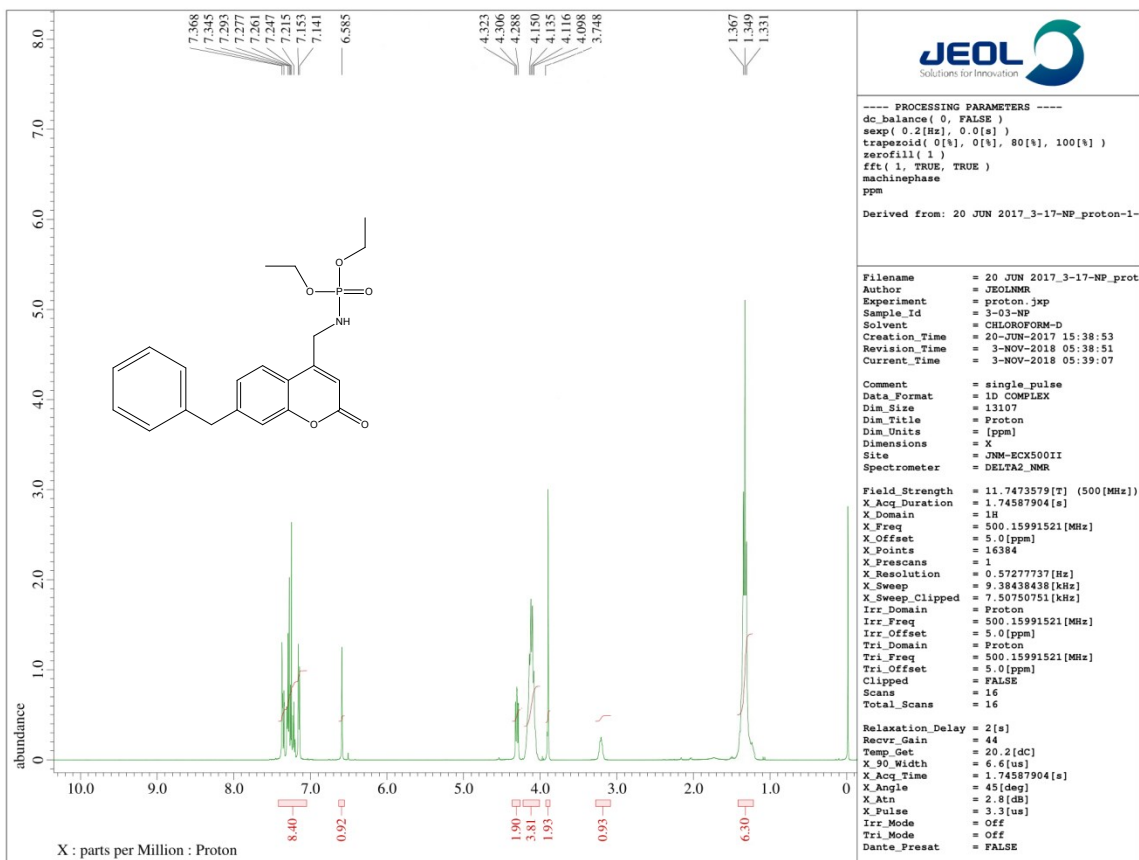


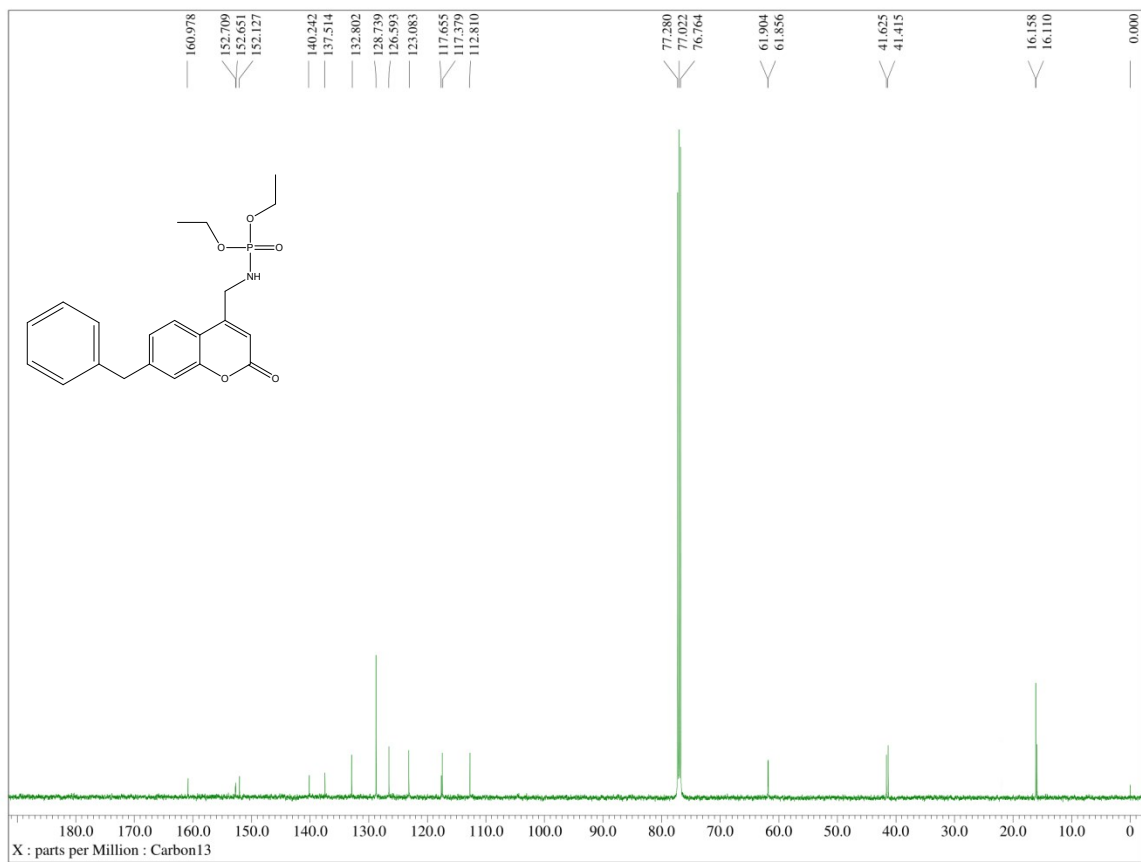






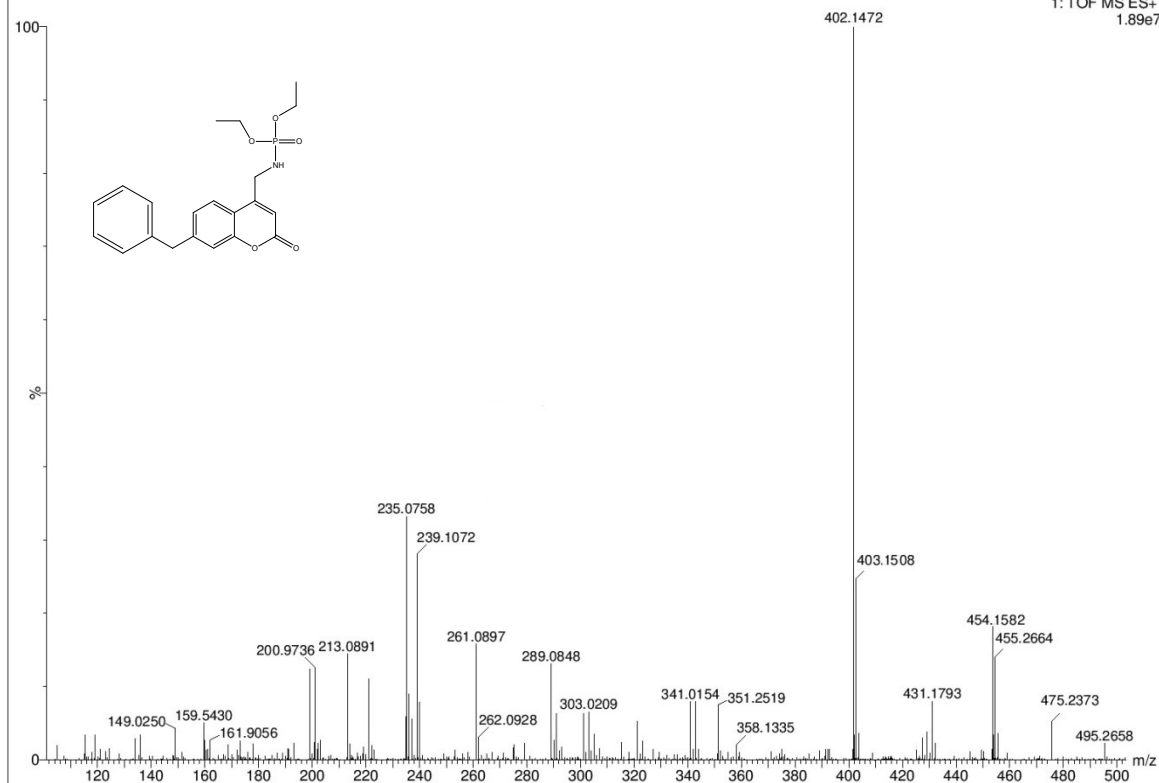


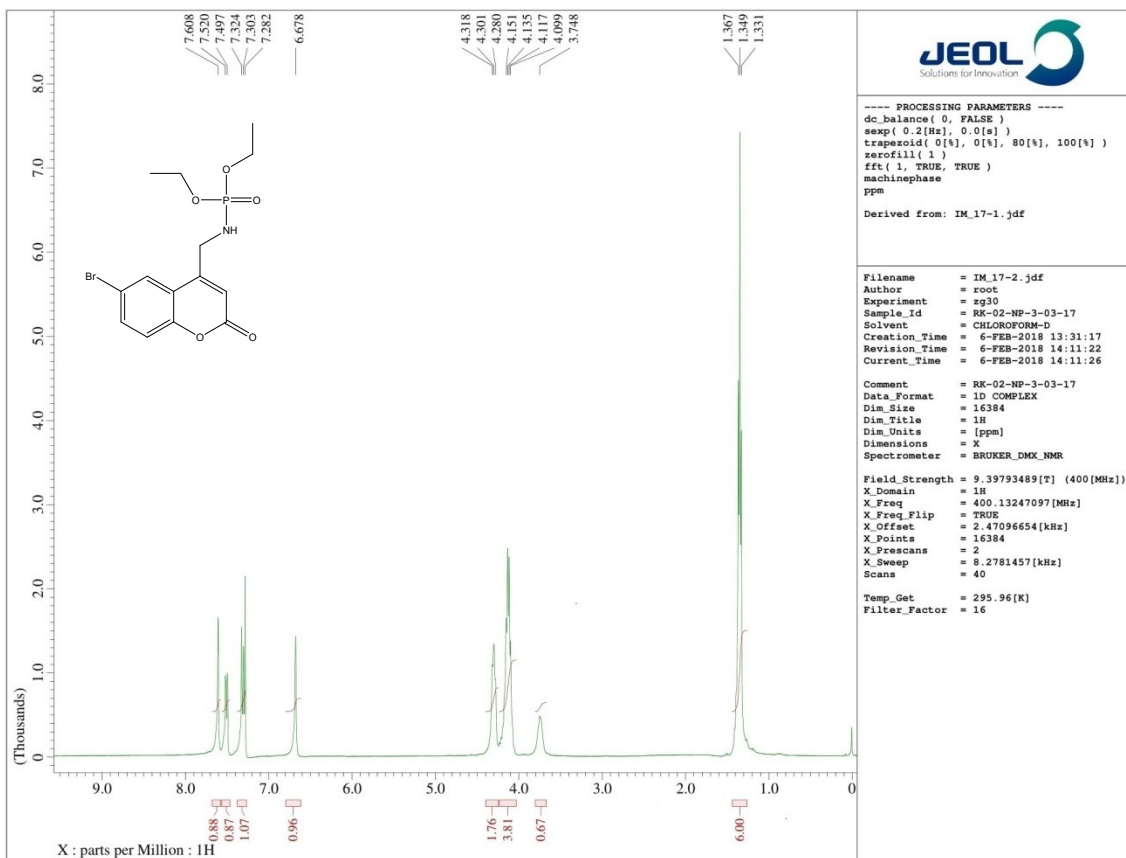


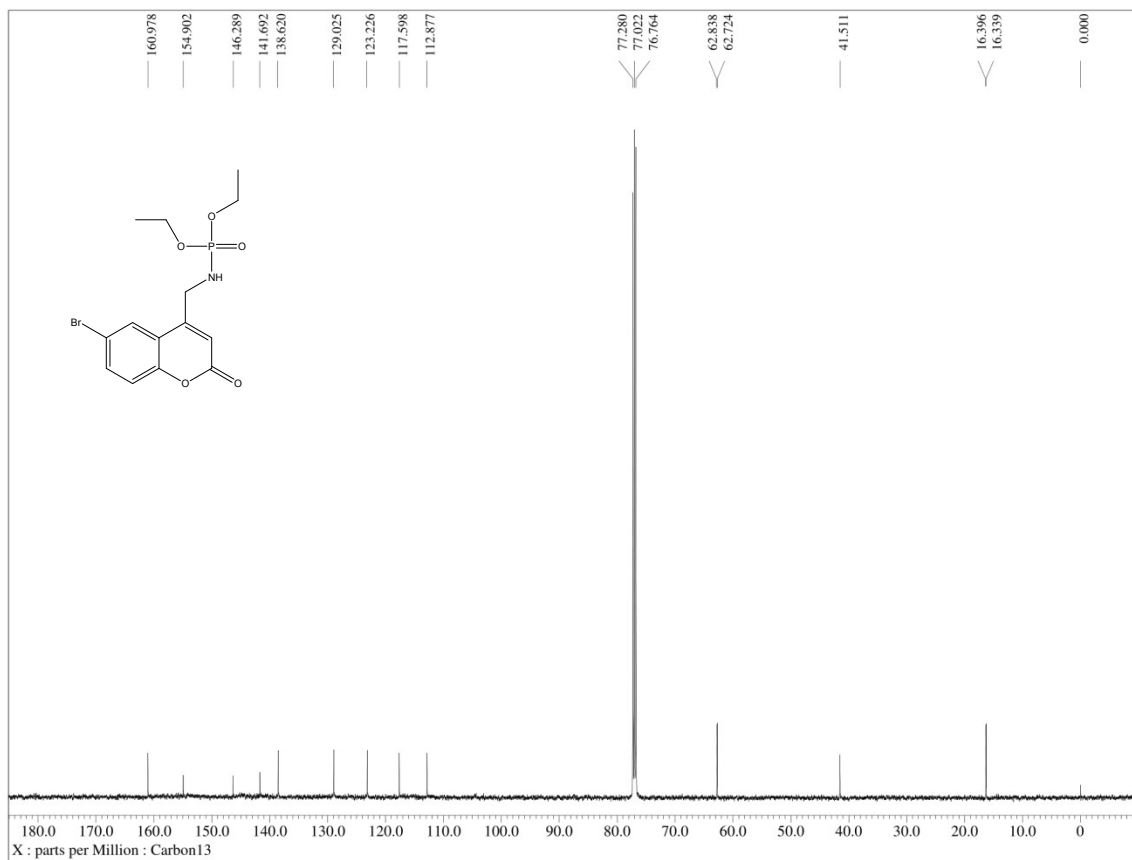


Sample ID: ANG

1: TOF MS ES+
1.89e7

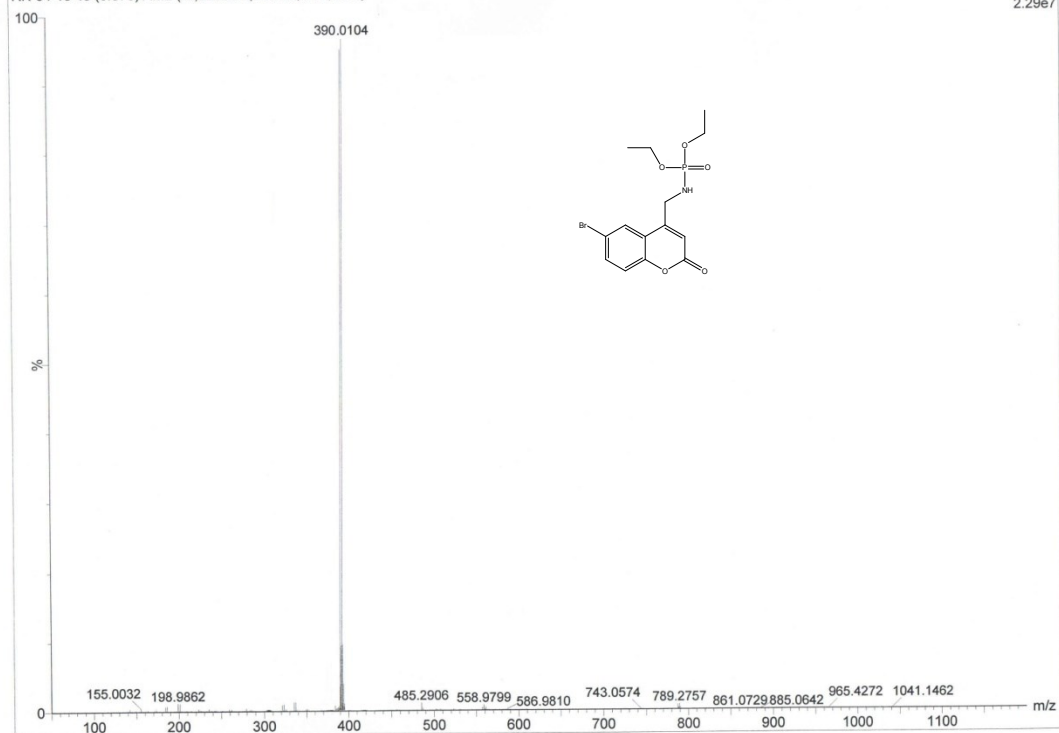




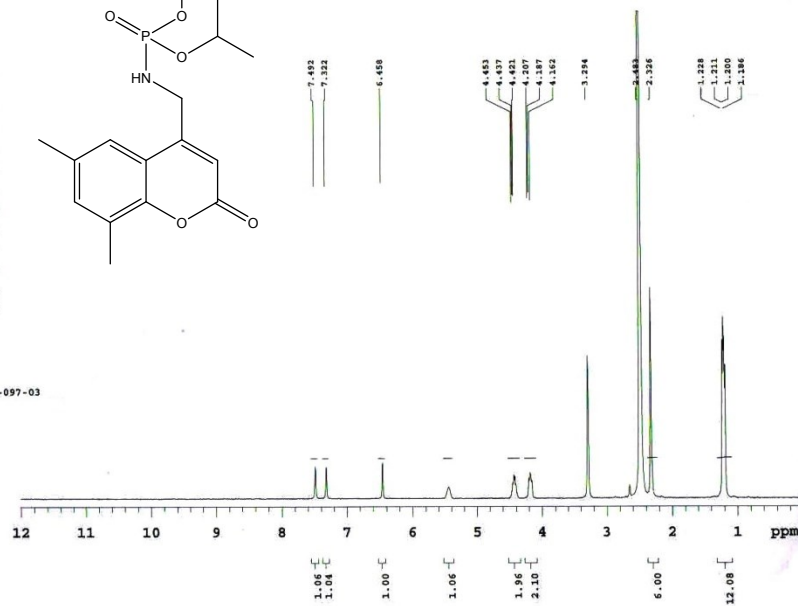
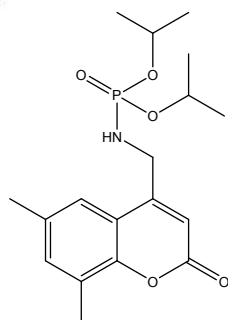


RK-04-13
RK-04-13 45 (0.875) AM2 (Ar,22000.0,556.28,0.00,LS 3)

1: TOF MS ES+
2.29e7



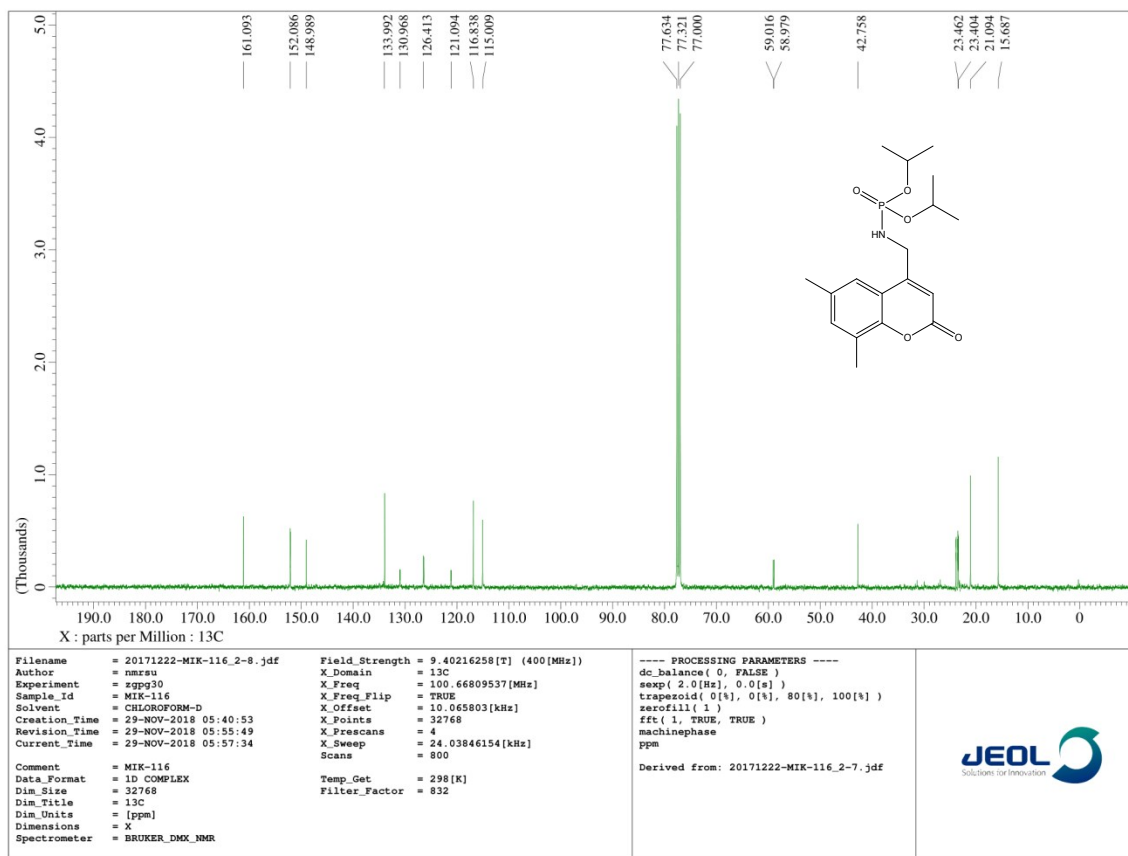
NUCLEUS : H1
 FRQ (MHz): 399.64
 AT (sec): 2.28
 SW (ppm): 17.98
 RD (sec): 1.00
 PW (usec): 6.05
 NT : 64
 Solvent : dmsd
 NP : 64
 LB (Hz): 1.0
 TEMP (K): 303.15
 EXP : s2pul
 DATE : Feb 23 2018
 TIME : 09:22:41



1H NMR REPORT

SAMPLE NAME : C-2044-097-03

Probe:ASW4Nclei



P.code&Sample Id:

Injection Date :

PDA/MS (APCI+MODE AND APCI-MODE)

Vial No. : P2-

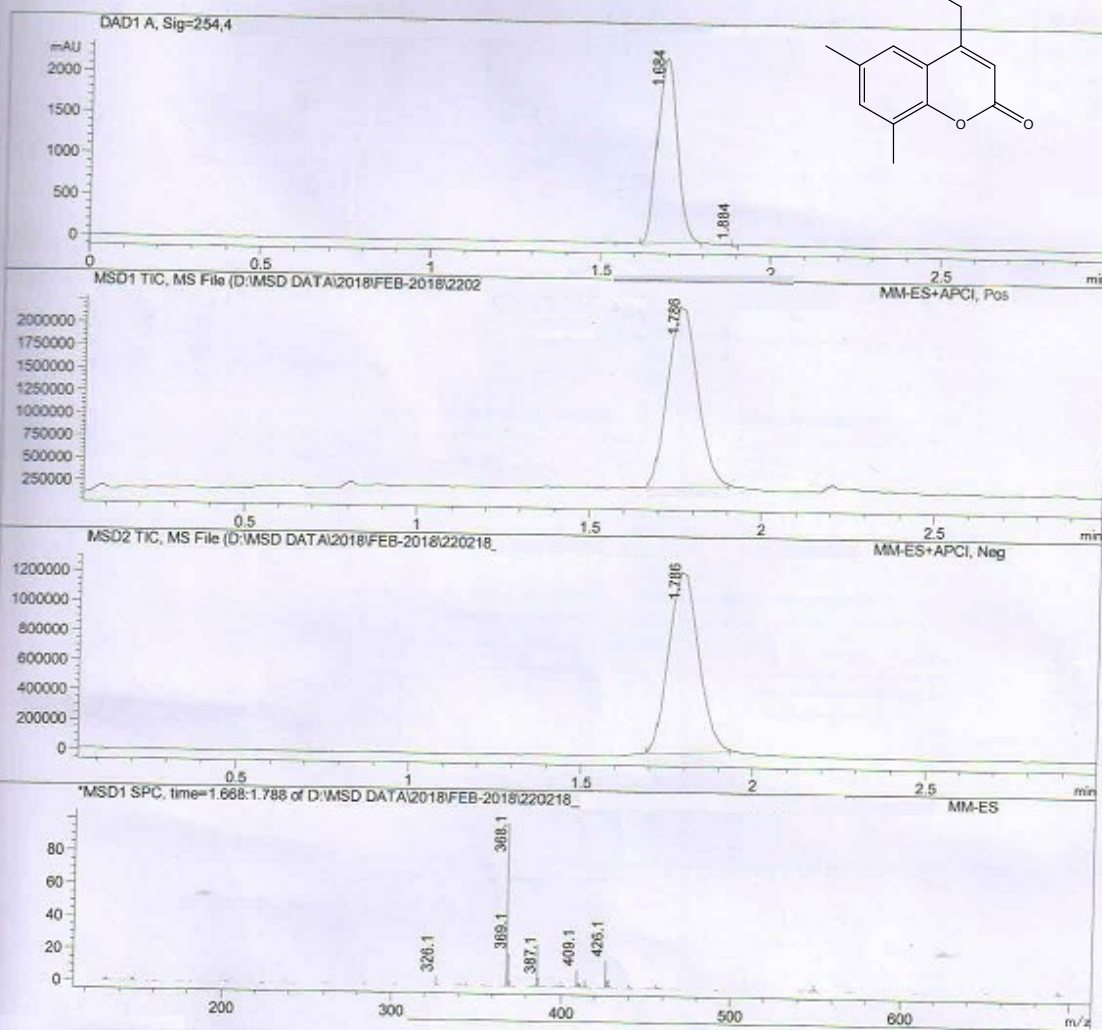
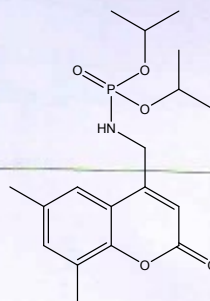
Injection vol : 1µL

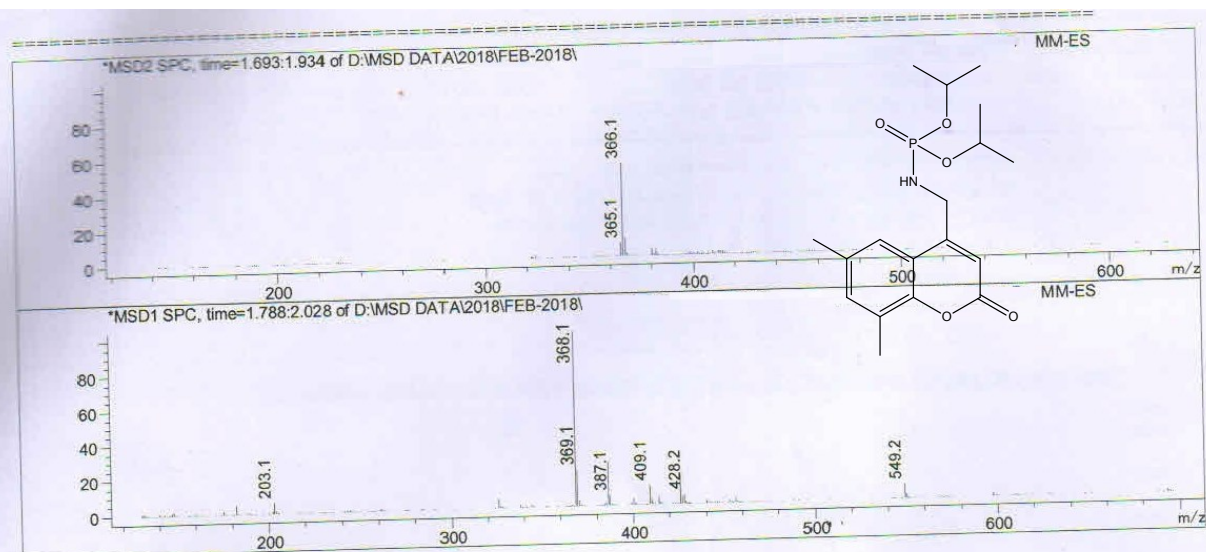
Method info : METHOD:34-100316, Flow rate:0.3 ml /min

Ascentis Express C18 (50 mm X 2.1mm X 2.7µm)

Mobile Phase (A) : 0.1%FORMIC ACID IN WATER

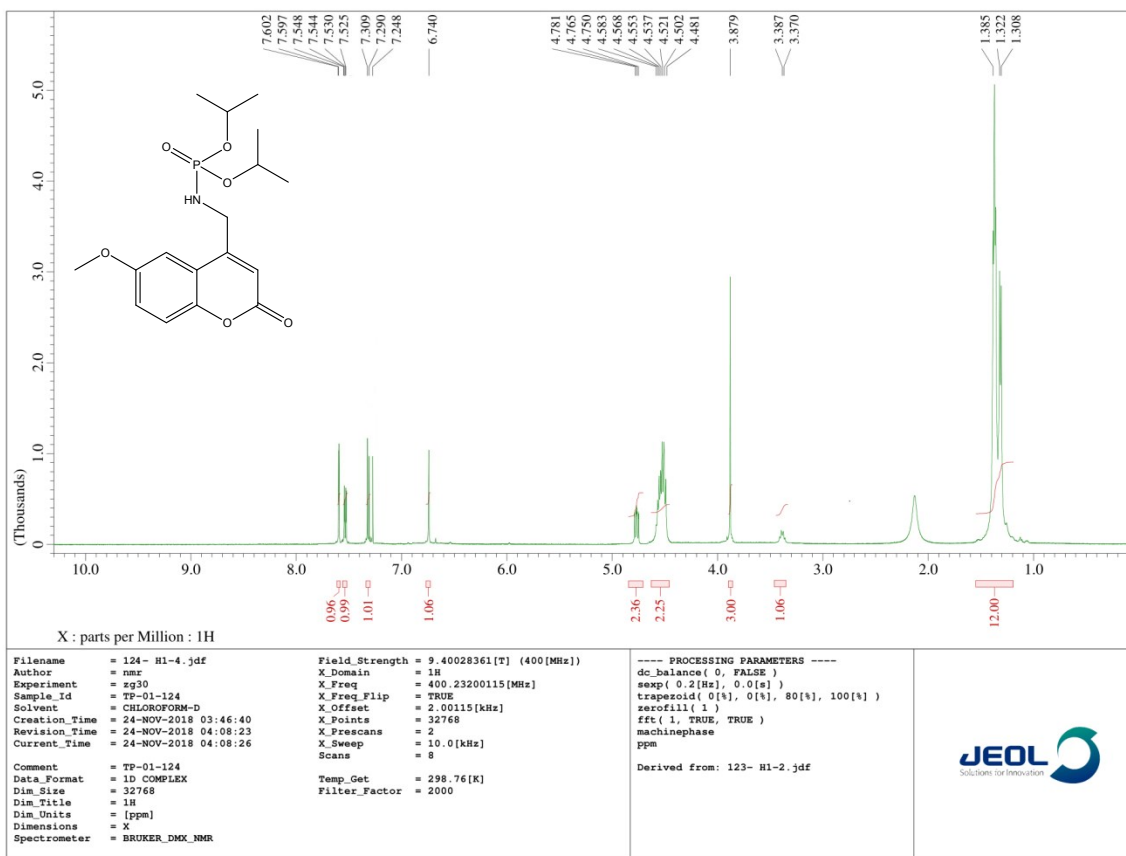
MobilePhase (B) : ACN

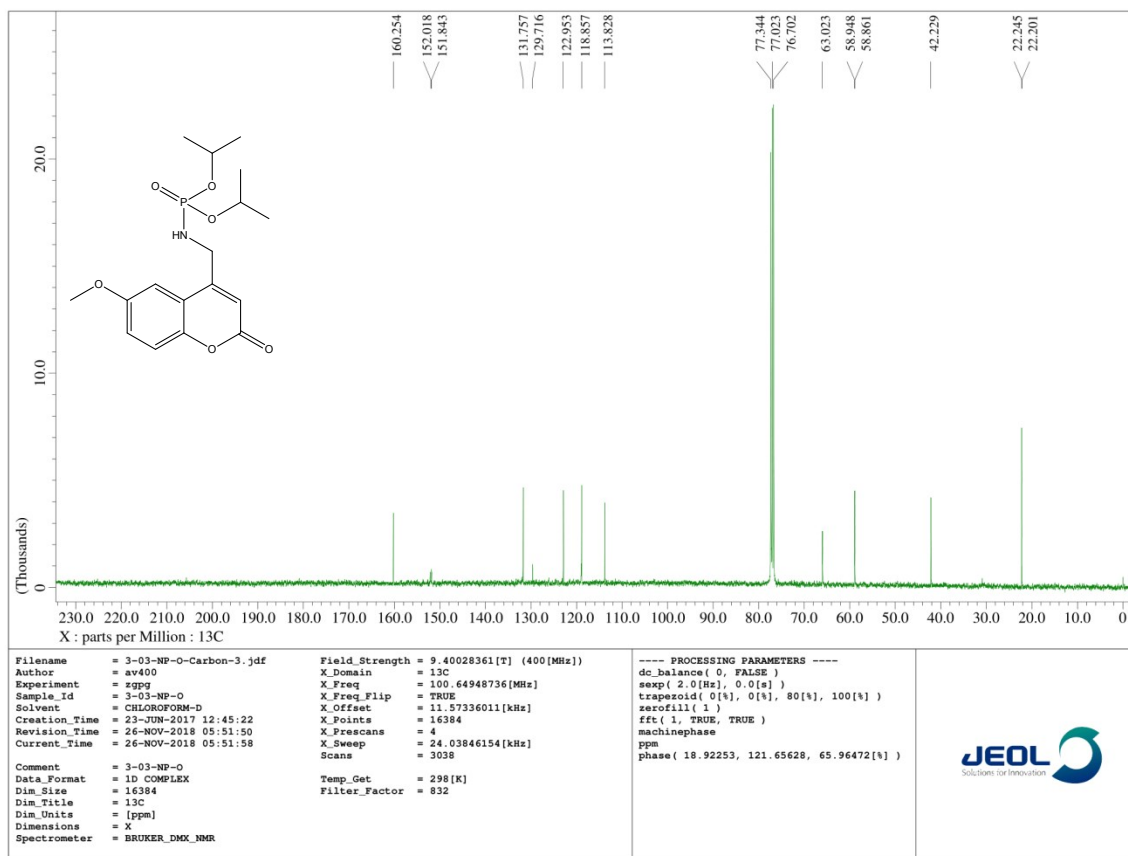


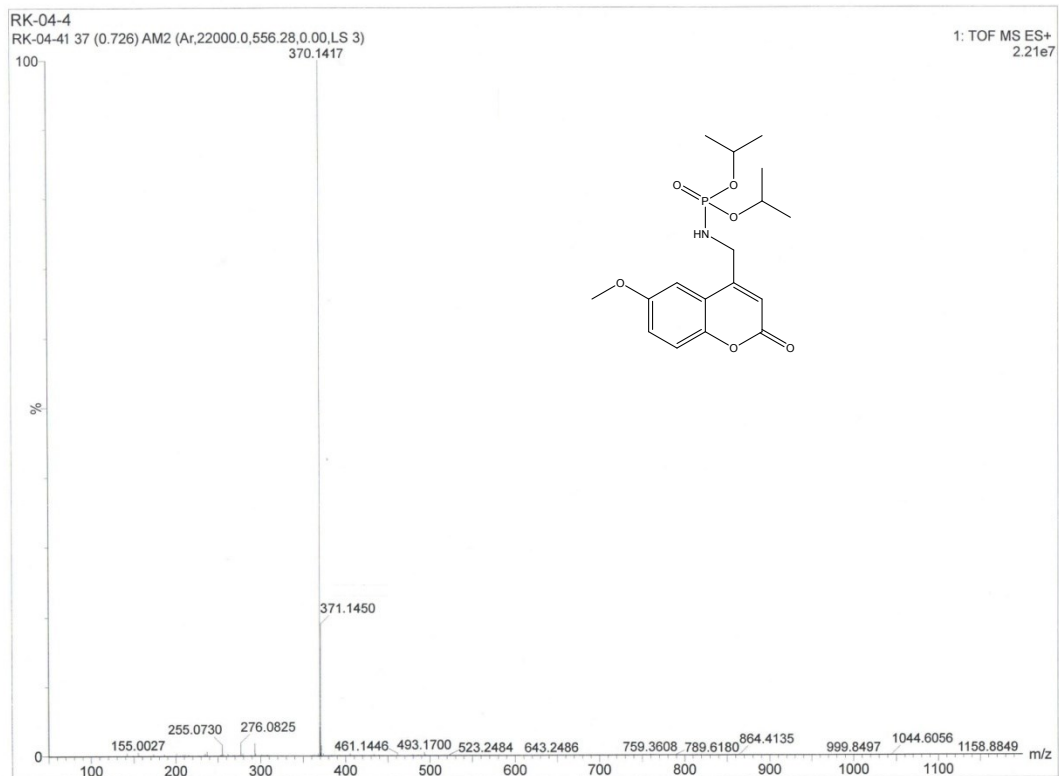


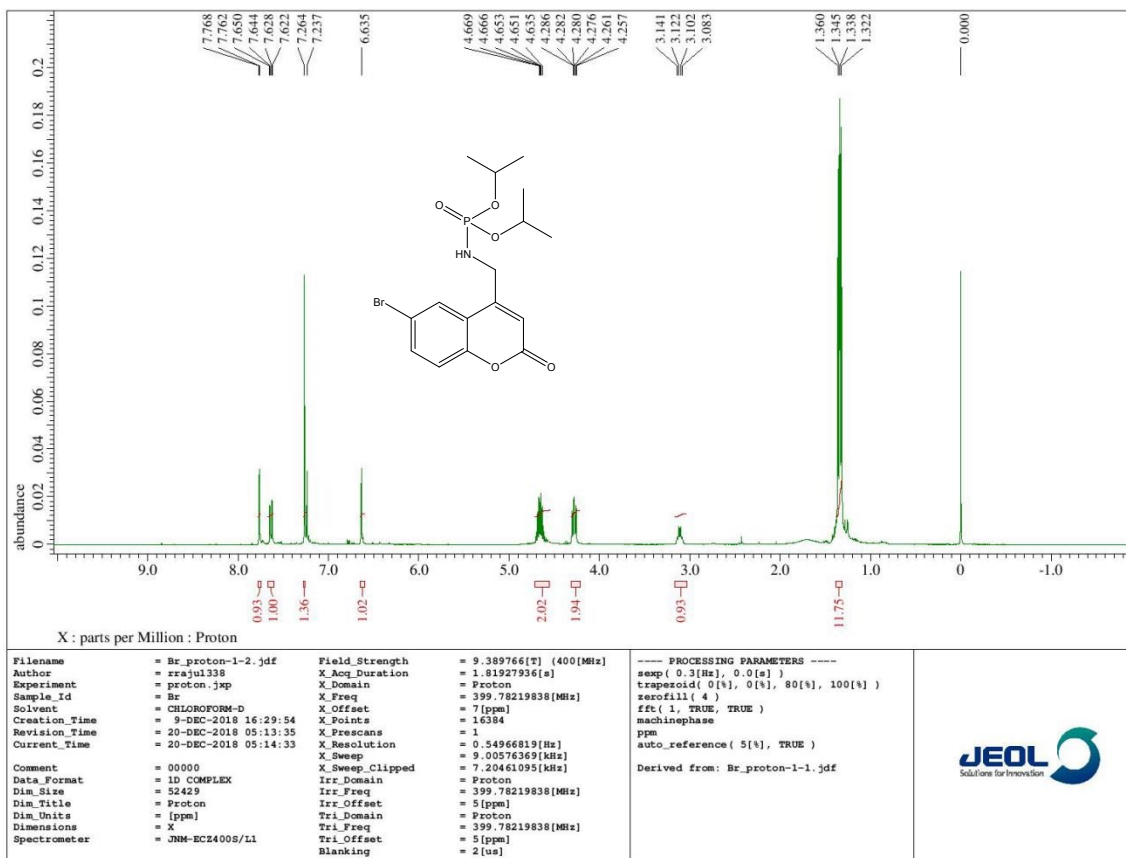
Compound Name	Area	Meas. R	Area %
	8.975e3	1.684	99.739
	23.516	1.884	0.261

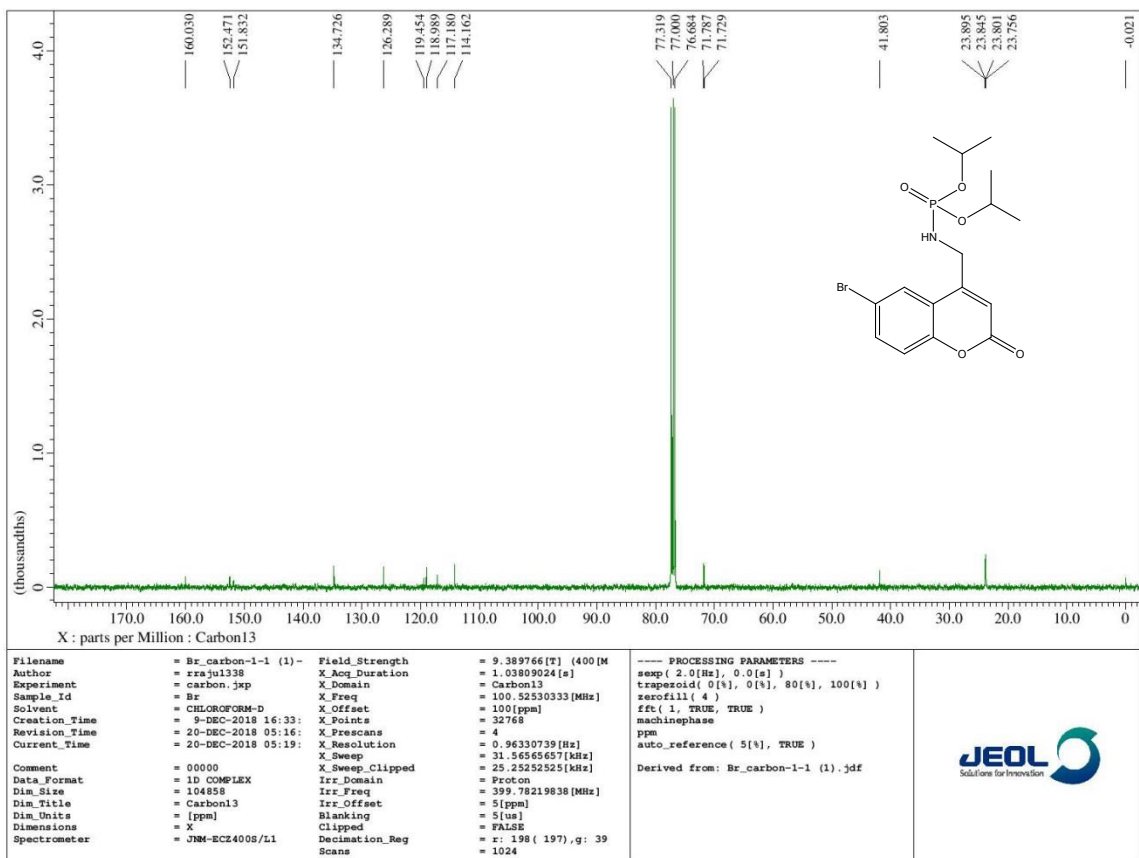
Compound Name	Area	Meas. R	Area %
	6.538e6	1.747	99.261
	1.126e7	1.847	00.739

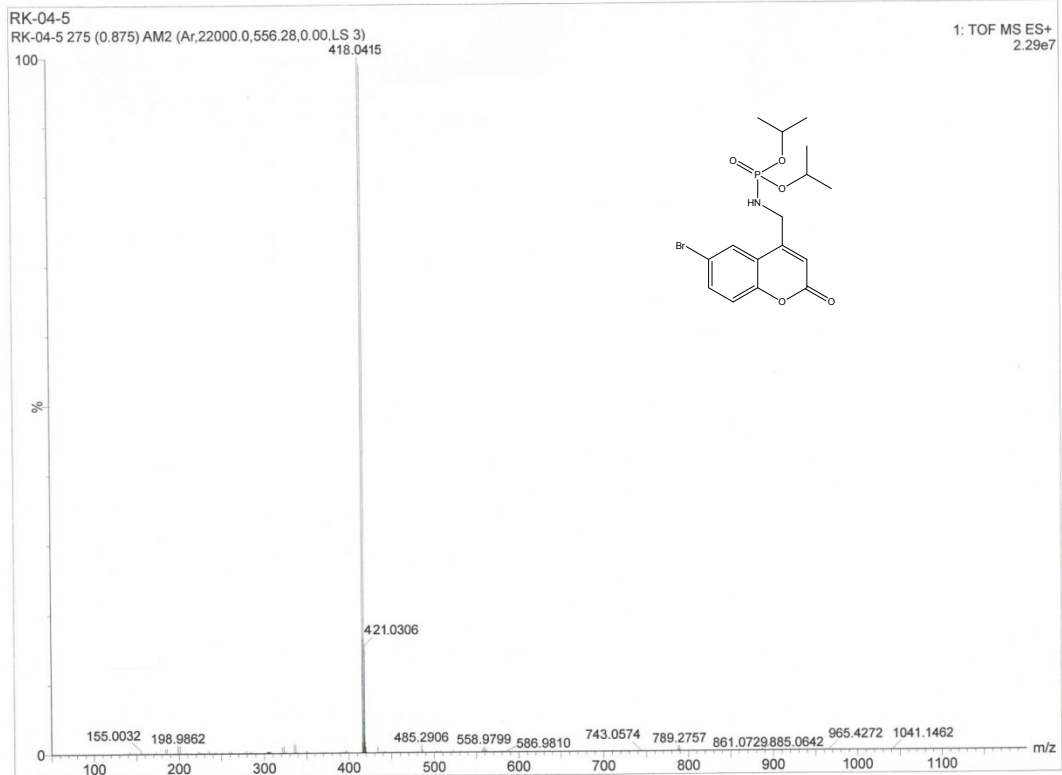




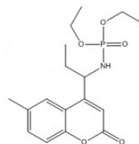




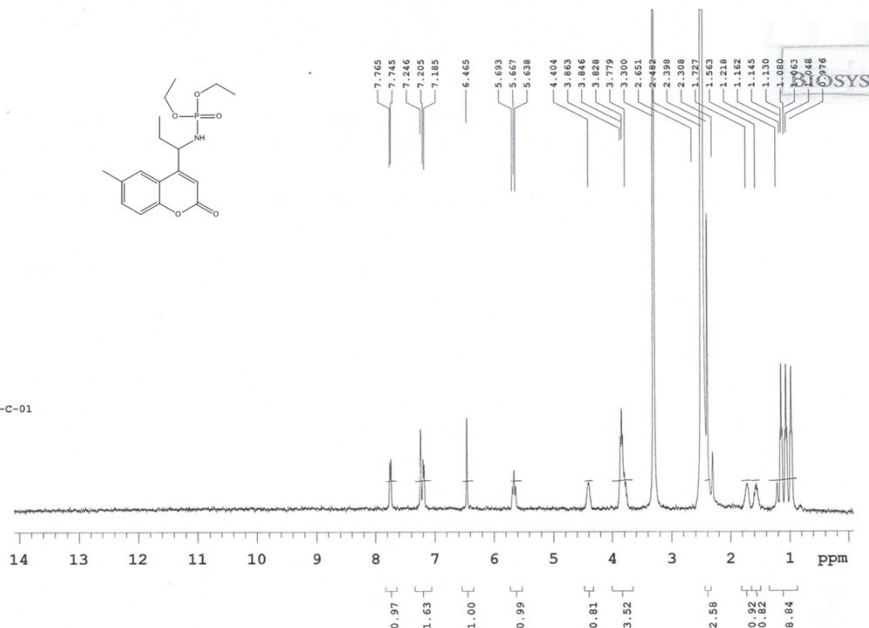


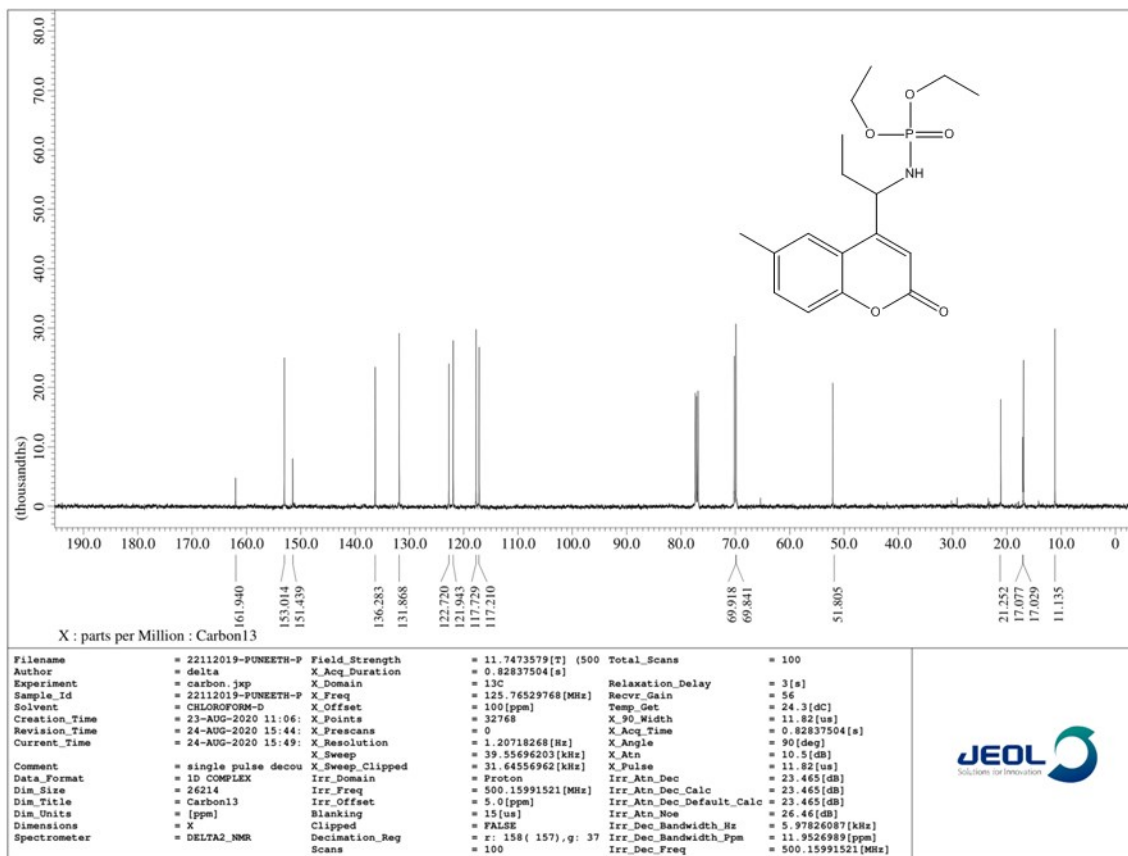


NUCLEUS : H1
 FRQ (MHz): 399.64
 AT (sec): 2.28
 SW (ppm): 17.98
 RD (sec): 1.00
 PW (usec): 5.00
 NT : 16
 Solvent : dmsd
 NP : 16
 LB (Hz): 1.0
 TEMP (K): 303.15
 EXP : s2pul
 DATE : Aug 21 2020
 TIME : 13:25:02



NMR REPORTS:
 PROJECT NAME: 113784-C-01
 PROBE: ATB
 Run Time: 00:08:00

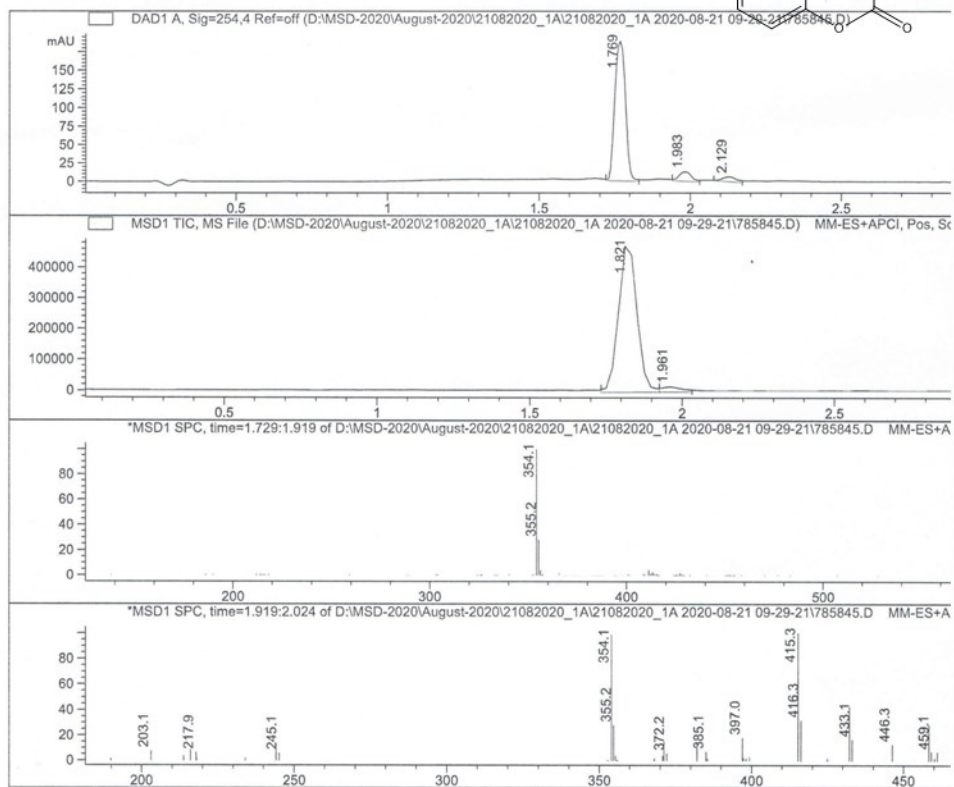
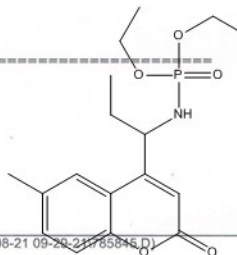




P.code&Sample Id: FZHIN1-113784-C-01 Instrument Code: Agilent LCMS
 Injection Date :21-08-2020 13:06:18 Vial No. : P2-F-09
 Data file :D:\MSD-2020\August-2020\21082020_1->
 Injection volume:0.8µL
 Run Time : 3.0 Minutes

Method info :

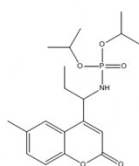
Analytical conditions: Flow rate :0.5ml
 Zorbax Eclipse plus C18 (50mm X 2.1 mm X 1.8 mic)
 Mobile phase (A) :0.1% Formic acid in water
 Mobile phase (B) :Acetonitrile
 T/%B:0/10.1.1/98,2.4/98,2.5/10,3/10



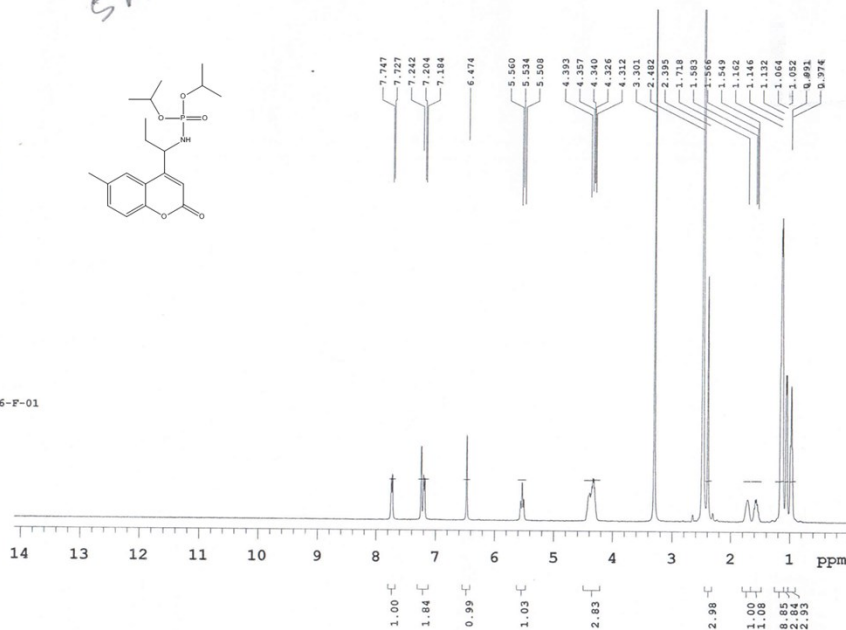
Compound Name	Area	Meas. R	Area %
	2.015e6	1.821	96.317
	7.707e4	1.961	3.683

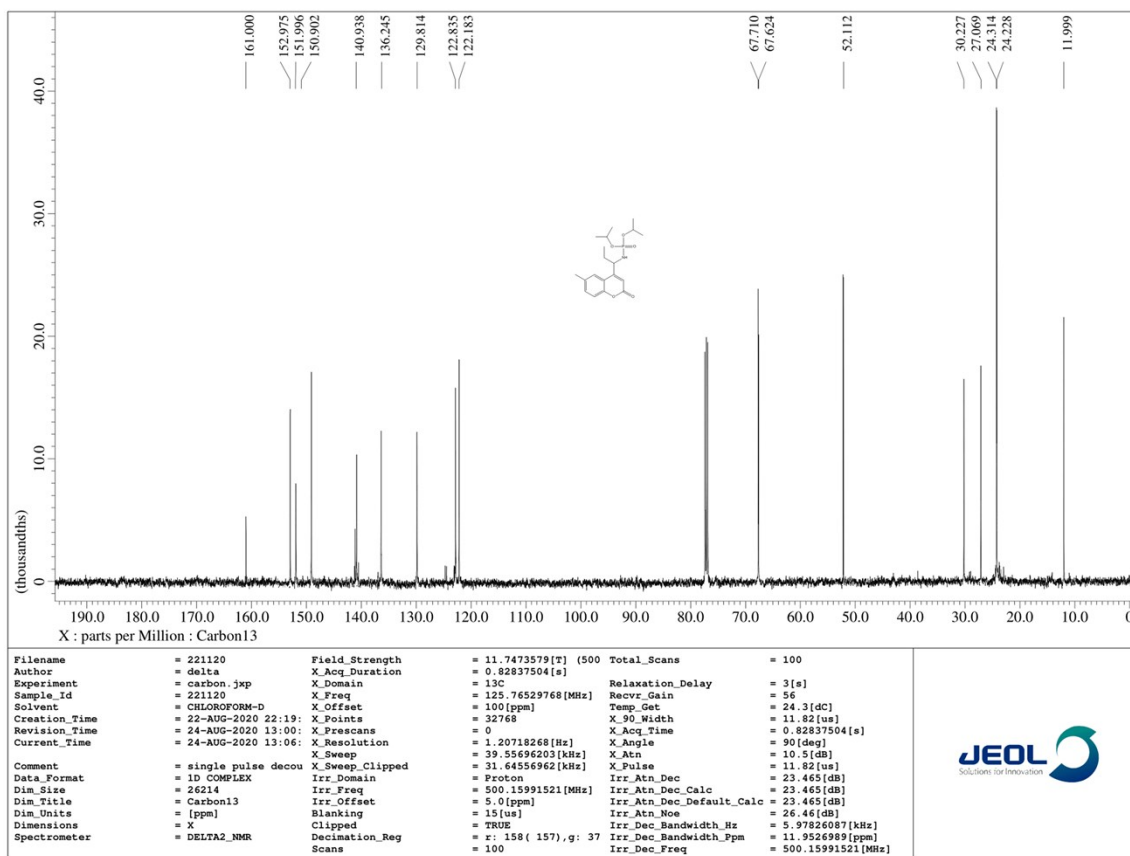
Analysed By : SYSTEM

NUCLEUS : H1
 FRQ (MHz): 399.64
 AT (sec): 2.28
 SW (ppm): 17.98
 RD (sec): 1.00
 PW (usec): 5.00
 NT : 16
 Solvent : dmsd
 NP : 16
 LB (Hz): 1.0
 TEMP (K): 303.15
 EXP : s2pul
 DATE : Aug 18 2020
 TIME : 15:00:15



NMR REPORTS:
 PROJECT NAME: 111256-F-01
 PROBE: ATB
 Run Time: 00:08:00





```

=====
P.code&Sample Id:111256-F-01                      Instrument Code: Agilent LCMS
Injection Date  :18-08-2020      14:03:56          Vial No.   :    P2-D-02
Data file      :D:\MSD-2020\August-2020\18082020_4->
Injection volume:1.0µL
Run Time       : 3.0 Minutes
=====

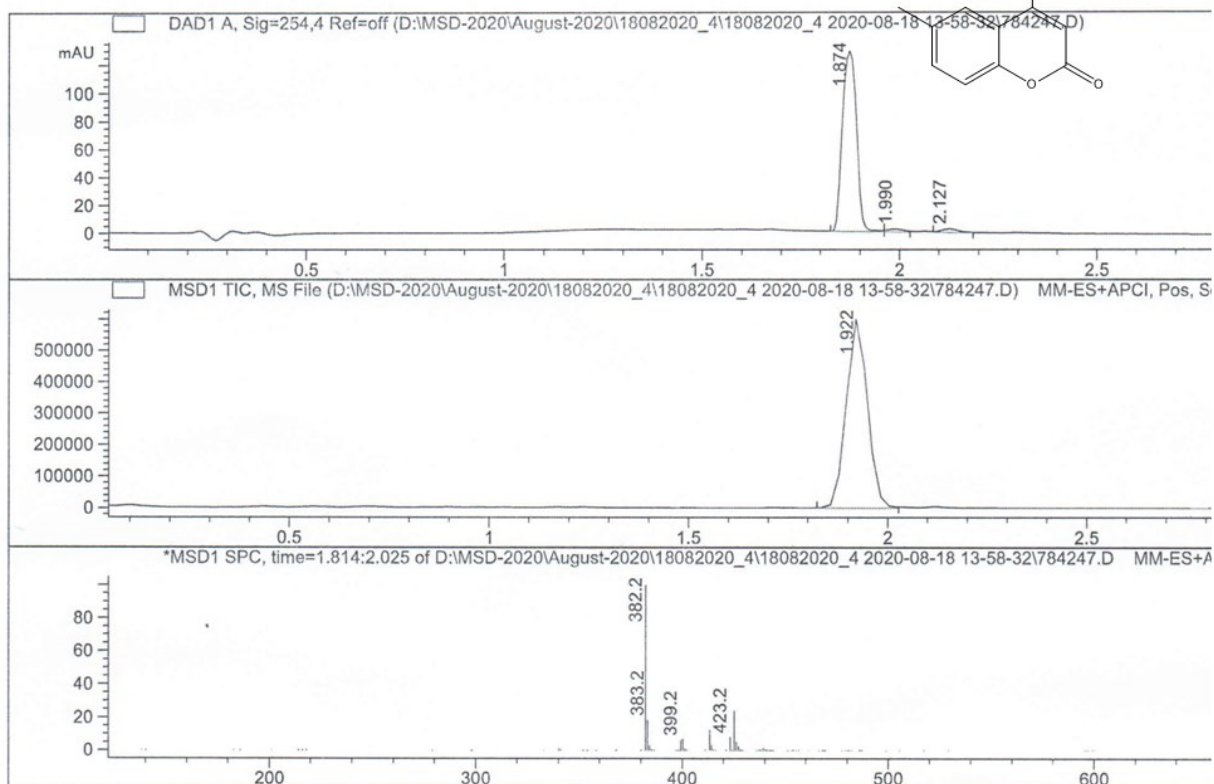
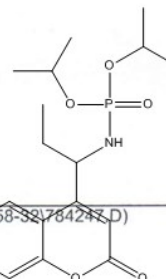
```

Method info :

```

Analytical conditions: Flow rate :0.5ml
Zorbax Eclipse plus C18 (50mm X 2.1 mm X 1.8 mic)
Mobile phase (A) :0.1% Formic acid in water
Mobile phase (B) :Acetonitrile
T/%B:0/10.1.1/98,2.4/98,2.5/10,3/10

```



Compound Name	Area	Meas. R	Area %
	318.729	1.874	96.105
	5.609	1.990	1.691
	7.309	2.127	2.204

Compound Name	Area	Meas. R	Area %
	2.214e6	1.922	100.000

Analysed By : SYSTEM

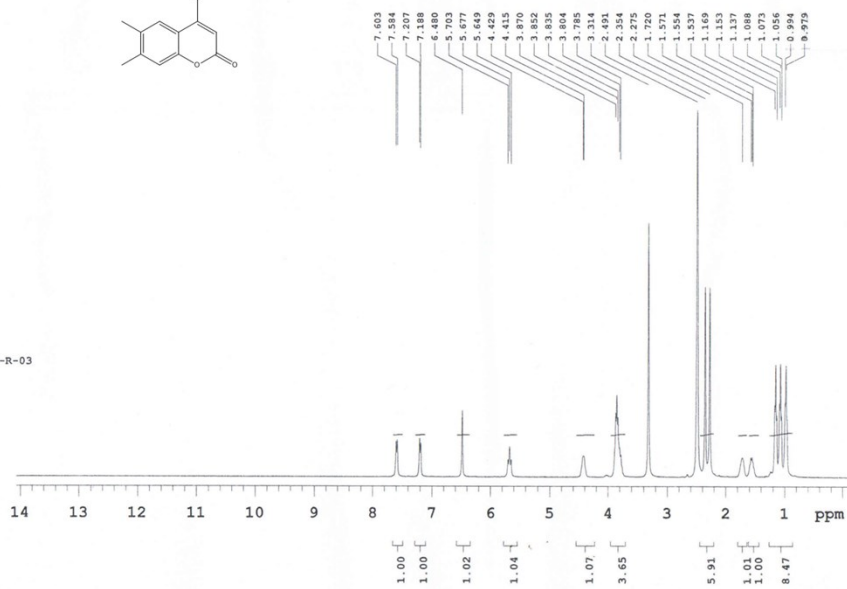
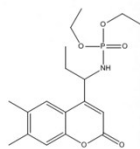
NUCLEUS : H1
 FREQ (MHz): 399.64
 AT (sec): 2.28
 SW (ppm): 17.98
 RD (sec): 1.00
 PW (usec): 5.00
 NT : 16
 Solvent : dmsd
 NP : 16
 LB (Hz): 1.0
 TEMP (K): 303.15
 EXP : s2pul
 DATE : Jun 19 2020
 TIME : 09:40:58

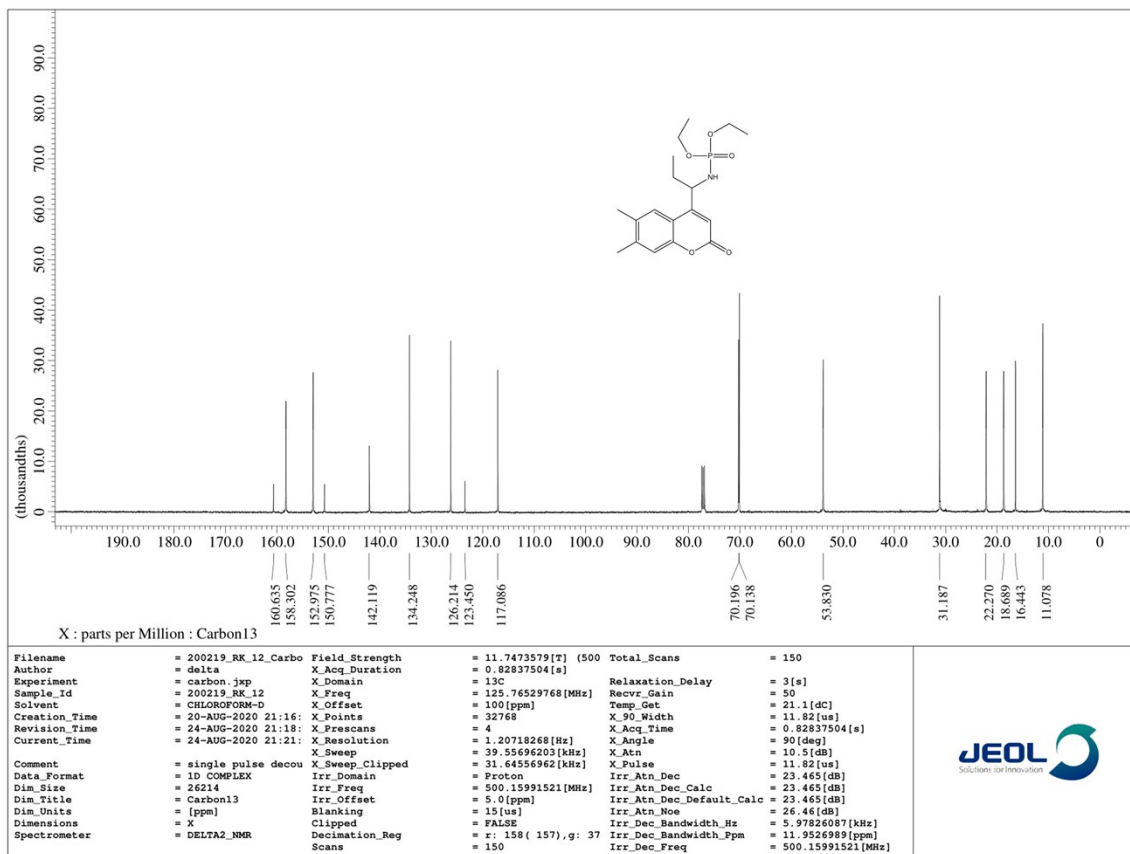
NMR REPORTS:

PROJECT NAME: 90500-R-03

PROBE: ATB

Run Time: 00:05:00

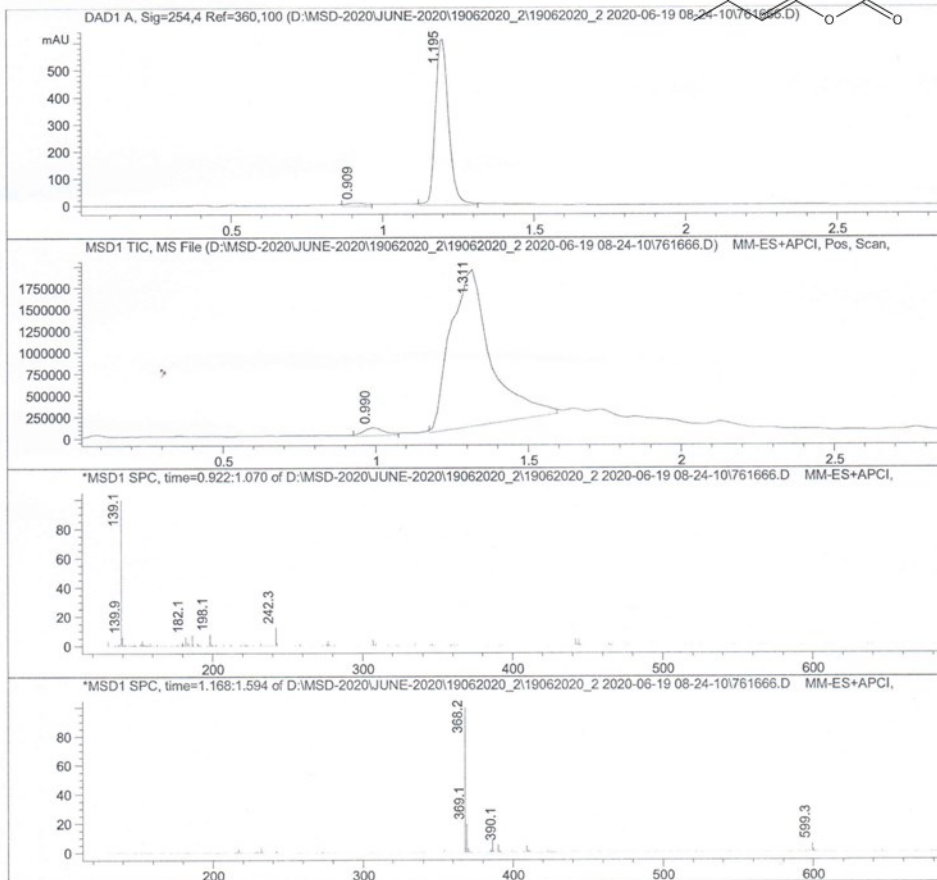
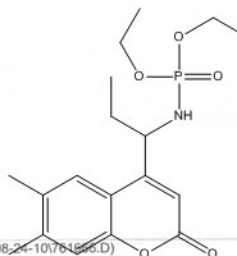




P.code&Sample Id: 90500-R-03 Instrument Code: Agilent LCMS1
 Injection Date : 6/19/2020 10:19:27 AM Vial No. : P2-C-05
 Data file : D:\MSD-2020\JUNE-2020\19062020_2-> Injection vol : 0.8µL
 Run Time: 3 Minutes

Method info :

Analytical Conditions :
 Column: Ascentis Exp C18 (50 mm X 2.1mm X 2.7 µm)
 Mobile Phase (A) : 0.1% Formic acid in water
 Mobile Phase (B) : Acetonitrile
 % of B: 0/20, 0.6/90, 2.5/90, 2.8/20, 3/20



Analysed By : AARIFA

Instrument Code : Instrument 1

Page 1 of 2