# Supporting Information

## Palladium-Catalyzed Direct *mono*-Aroylation of *O*-Arylmethyl and Aryl Substituted Acetoxime Ethers

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[b] School of Chemical Engineering & Technology, Xuzhou College of Industrial Technology, Xuzhou, 221006, P. R. China. Email: xzcitwcy@126.com.

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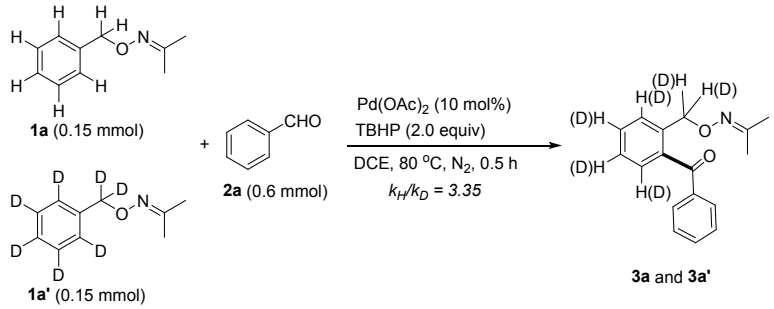
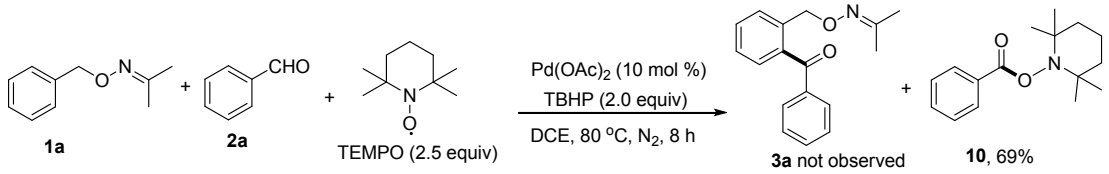
## 1. Kinetic isotope effect study (Scheme 4)




**Procedure:** A mixture of substrate **1a** (24.5 mg, 0.15 mmol), **1a´** (25.5 mg, 0.15 mmol), **2a** (63.7 mg, 0.6 mmol), $Pd(OAc)_2$ (6.7 mg, 10 mol %), TBHP (54.1 mg, 2.0 equiv) in DCE (2.5 mL) was charged in a glass sealed-tube and stirred under $N_2$ atmosphere at 80 °C for 0.5 h. Upon completion of the reaction, saturated brine (15 mL) and DCM (15 mL) were added to the mixture, then the aqueous layer was extracted with DCM (15 mL × 2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified *via* a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 40:1) to supply the product **3a** and **3a´** in 19.0 mg (about 23% yield). The product distribution ($k_H/k_D$ = 3.35) was analyzed by $^1$H NMR, see: section 4.6 (Copies of the spectra for **Scheme 4**).

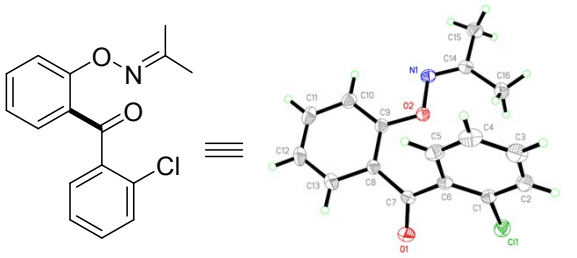
## 2. Inhibitation reaction of free radical




**Procedure:** A mixture of substrate **1a** (49.0 mg, 0.3 mmol), **2a** (63.7 mg, 0.6 mmol), $Pd(OAc)_2$ (6.7 mg, 10 mol %), TBHP (54.1 mg, 2.0 equiv) and TEMPO (117.2 mg, 2.5 equiv) in DCE (2.5 mL) was charged in a glass sealed-tube and stirred under $N_2$ atmosphere at 80 °C for 8 h. Upon completion of the reaction, saturated brine (15 mL) and DCM (15 mL) were added to the mixture, then the aqueous layer was extracted with DCM (15 mL × 2). The combined organic layer was dried over anhydrous $MgSO_4$. Finally, the solution was concentrated *in vacuo* to provide a crude product, which was further purified *via* a column chromatography on silica gel (eluents: petroleum ether/ethyl acetate = 40:1) to supply the TEMPO ester adduct **10** in 69% yield.

**2,2,6,6-Tetramethylpiperidin-1-yl benzoate (10)**: yellow oil, 108.2 mg (69% yield); $^1$H NMR (400 MHz, $CDCl_3$, ppm): $\delta$ 8.09 (d, $J$ = 7.2 Hz, 2H), 7.59 (t, $J$ = 7.2 Hz, 1H), 7.48 (t, $J$ = 7.6 Hz, 2H), 1.84−1.75 (m, 2H), 1.73−1.61 (m, 2H), 1.59−1.41 (m, 2H), 1.29 (s, 6H), 1.34 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): $\delta$ 166.5, 133.1, 129.9, 129.7 (2C), 128.7 (2C), 60.5 (2C), 39.2 (2C), 32.2 (2C), 21.0 (2C), 17.2; HRMS (EI): *m/z* $[M]^+$ calcd. for $C_{16}H_{23}NO_2$: 261.1729; found: 261.1730.

## 3. Crystallographic data for 6h




| | | |
|---|---|---|
| Bond precision: | C-C = 0.0059 Å | |
| Wavelength: | 1.54178 Å | |
| Unit cell dimensions: | a = 10.1392(4) Å | α= 90° |
| | b = 10.1392(4) Å | β= 90° |
| | c = 28.1205(16) Å | γ = 90° |
| Temperature: | 296 K | |
| | Calculated | Reported |
| Volume: | 2890.9(3) Å$^3$ | 2890.9(3) Å$^3$ |
| Space group: | P 41 | P 41 |
| Hall group | P 4w | P 4w |
| Moiety formula | $C_{16}H_{14}ClNO_2$ | $C_{16}H_{14}ClNO_2$ |
| Sum formula | $C_{16}H_{14}ClNO_2$ | $C_{16}H_{14}ClNO_2$ |
| Mr | 287.73 | 287.73 |
| Dx,g cm$^{-3}$ | 1.322 | 1.322 |
| z | 8 | 8 |
| Mu (mm$^{-1}$) | 2.344 | 2.344 |
| F000 | 1200.0 | 1200.0 |
| F000’ | 1206.13 | |
| h,k,lmax | 12,12,33 | 12,12,33 |
| Nref | 5318[ 2719] | 5263 |
| Tmin,Tmax | 0.627,0.656 | 0.512,0.753 |
| Tmin’ | 0.569 | |

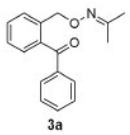
Correction method = # Reported T Limits: Tmin=0.512 Tmax=0.753

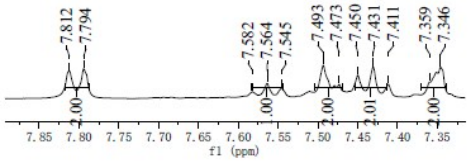
AbsCorr = ?

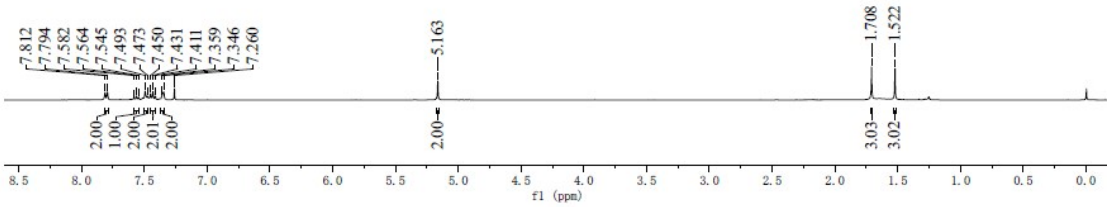
| | |
|---|---|
| Data completeness= 1.94/0.99 | Theta(max)= 68.464 |
| R(reflections)= 0.0390( 4470) | wR2(reflections)= 0.1010( 5263) |
| S = 1.021 | Npar= 365 |

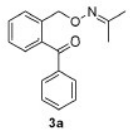
## 4. All Copies of Spectra

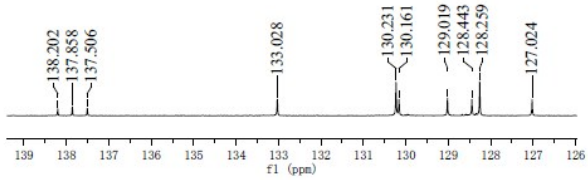
### 4.1 Copies of the spectra for Tables 2

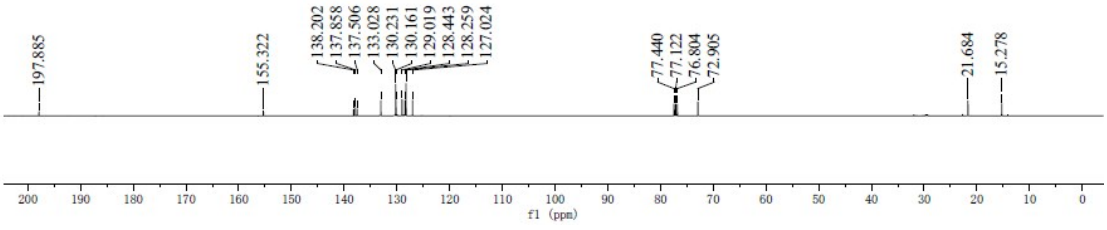


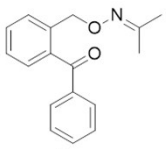



**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

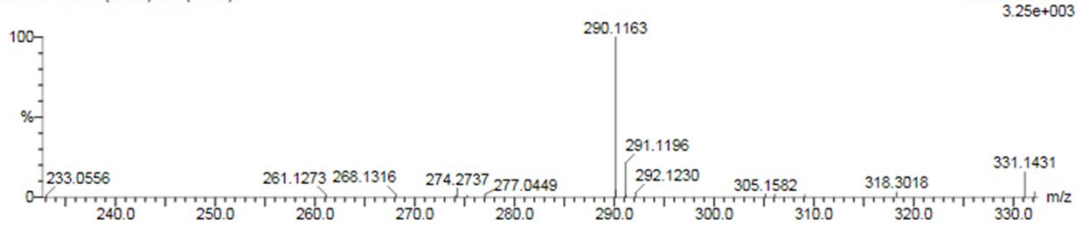
Monoisotopic Mass, Even Electron Ions
60 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-3 O: 0-4 Na: 0-1



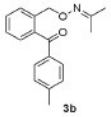
3a

YF-JI ECUST institute of Fine Chem 24-Jun-2016 20:55:43

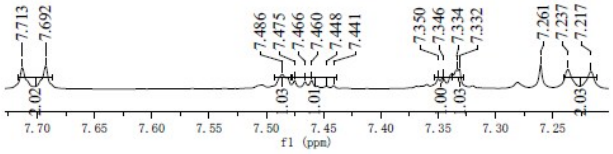
JYF-S-416 11 (0.422) Cm (11:12) 1: TOF MS ES+ 3.25e+003

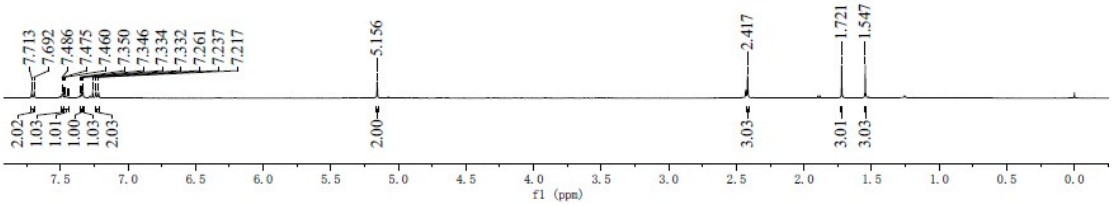


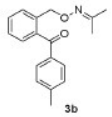

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 300.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 290.1163 | 290.1157 | 0.6 | 2.1 | 9.5 | 23.0 | 0.0 | C17 H17 N O2 Na |

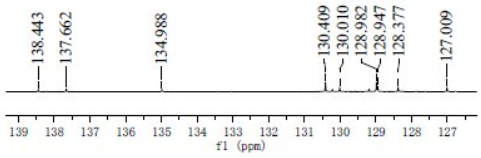


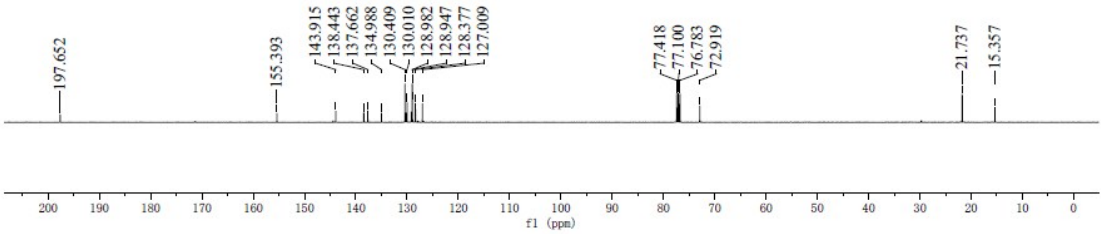
3b





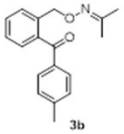




**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Even Electron Ions

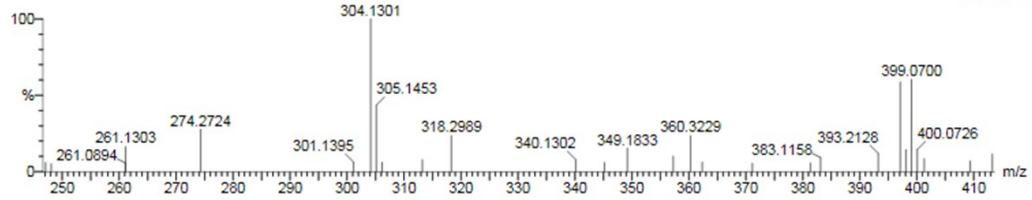
9 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

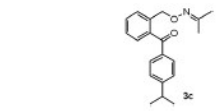
C: 0-18 H: 0-20 N: 0-1 O: 0-2 Na: 0-1

YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:59:07

JYF-S-611 35 (0.521) Cm (33:35) 1: TOF MS ES+ 2.02e+003




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1301 | 304.1313 | -1.2 | -3.9 | 9.5 | 23.6 | 0.0 | C18 H19 N O2 Na |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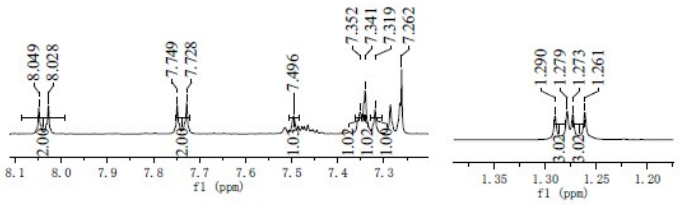
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8.028
7.749
7.728
7.496
7.352
7.341
7.319
7.262
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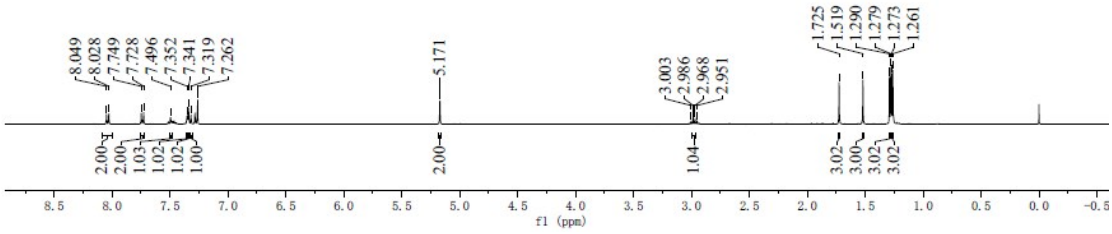
1.279
1.273
1.261
f1 (ppm)


8.049
8.028
7.749
7.728
7.496
7.352
7.341
7.319
7.262
5.171
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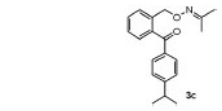
1.273
1.261
f1 (ppm)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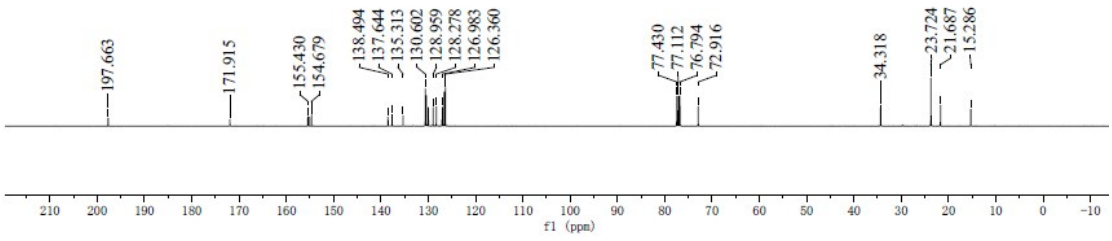
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128.959
128.278
126.983
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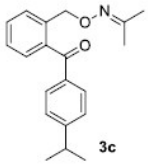
23.724
21.687
15.286
f1 (ppm)

Elemental Composition Report




Multiple Mass Analysis: 41 mass(es) processed

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

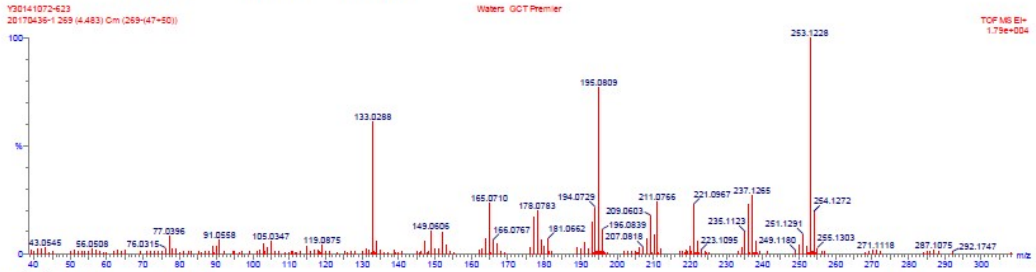
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

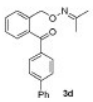
505 formula(e) evaluated with 39 results within limits (up to 50 closest results for each mass)

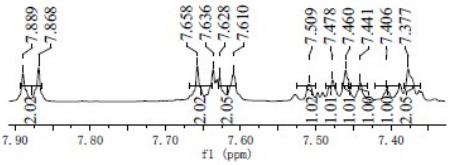
Elements Used:

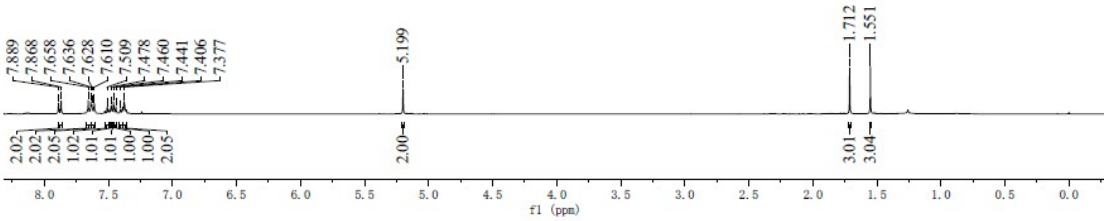
C: 0-20 H: 0-23 N: 0-1 O: 0-2

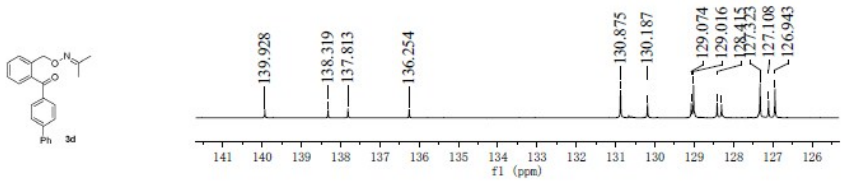


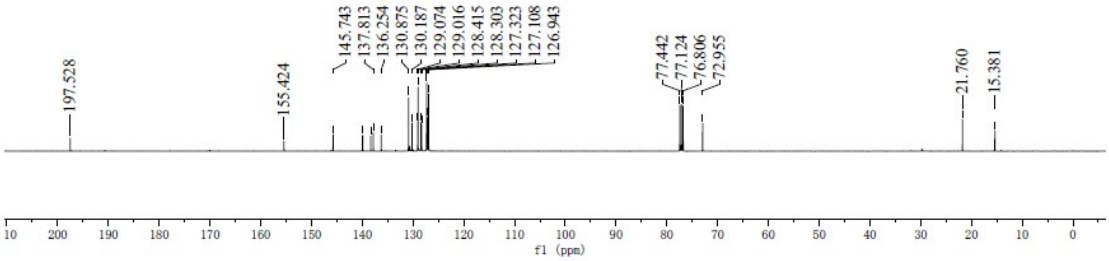

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 253.1228 | 100.00 | 253.1229 | -0.1 | -0.4 | 9.5 | 1.5 | C17H17 O2 |



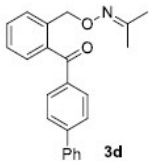






Elemental Composition Report




Multiple Mass Analysis: 42 mass(es) processed

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

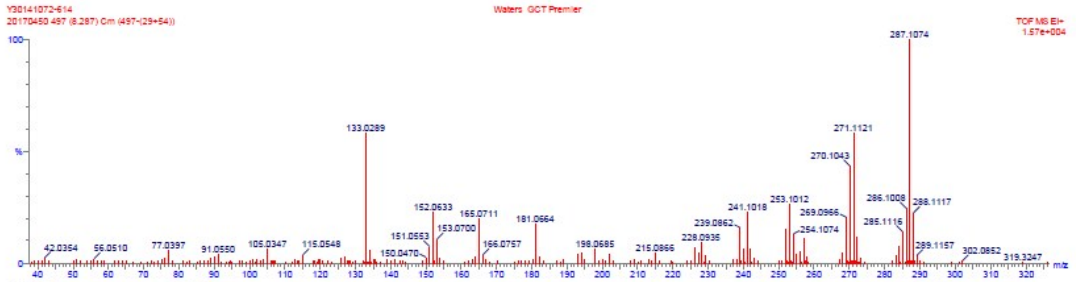
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

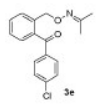
480 formula(e) evaluated with 41 results within limits (up to 50 closest results for each mass)

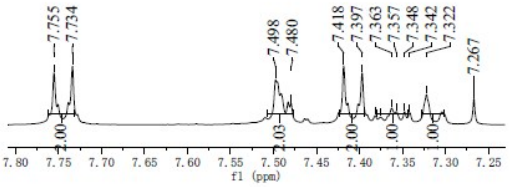
Elements Used:

C: 0-23 H: 0-21 N: 0-1 O: 0-2




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 287.1074 | 100.00 | 287.1072 | 0.2 | 0.7 | 13.5 | 3.3 | C20 H15 O2 |


3e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7.480
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7.397
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7.357
7.348
7.342
7.322
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2.03
2.00
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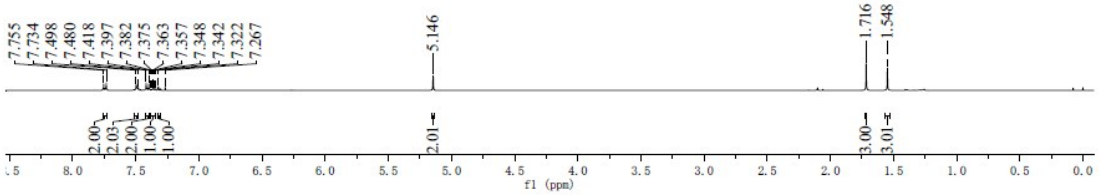
f1 (ppm)


7.755
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7.498
7.480
7.418
7.397
7.382
7.375
7.363
7.357
7.348
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7.267
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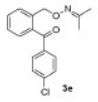
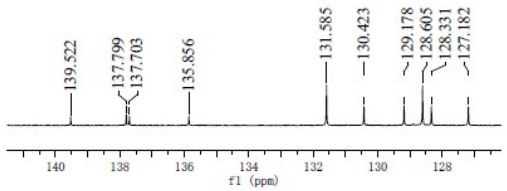
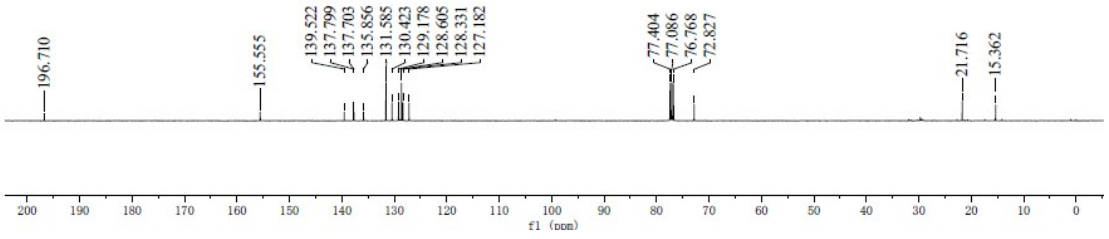
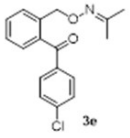
1.00
1.00
2.01
3.00
3.01
f1 (ppm)


3e


139.522
137.799
137.703
135.856
131.585
130.423
129.178
128.605
128.331
127.182
140 138 136 134 132 130 128
f1 (ppm)


196.710
155.555
139.522
137.799
137.703
135.856
131.585
130.423
129.178
128.605
128.331
127.182
77.404
77.086
76.768
72.827
21.716
15.362
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

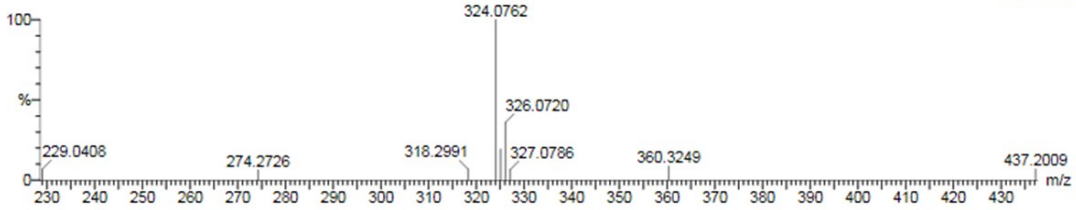
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



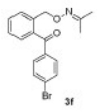

Monoisotopic Mass, Even Electron Ions
76 formula(e) evaluated with 4 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-40 N: 0-1 O: 0-5 Na: 0-1 Cl: 0-1

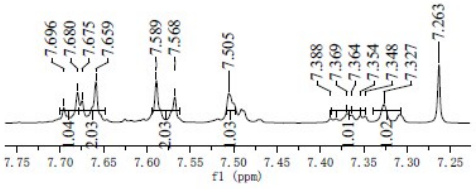
YF-JI ECUST institute of Fine Chem 05-Jan-2017 22:11:02

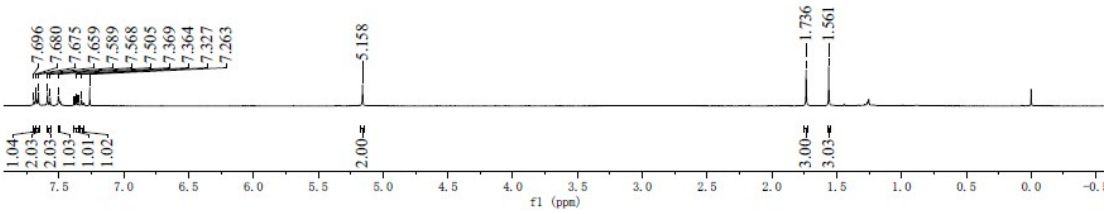
YF-S-518 8 (0.191) Cm (6:8) 1: TOF MS ES+ 2.31e+003

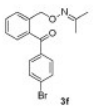


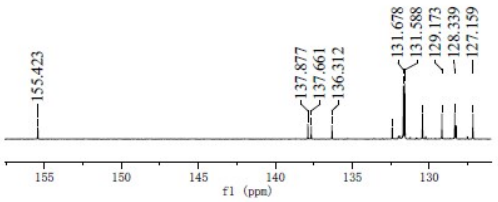

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum: | | | 30.0 | 50.0 | -1.5 | | | | | | | |
| Maximum: | | | | | 100.0 | | | | | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula | | | | | |
| 324.0762 | 324.0767 | -0.5 | -1.5 | 9.5 | 7.3 | 0.0 | C17 | H16 | N | O2 | Na | Cl |

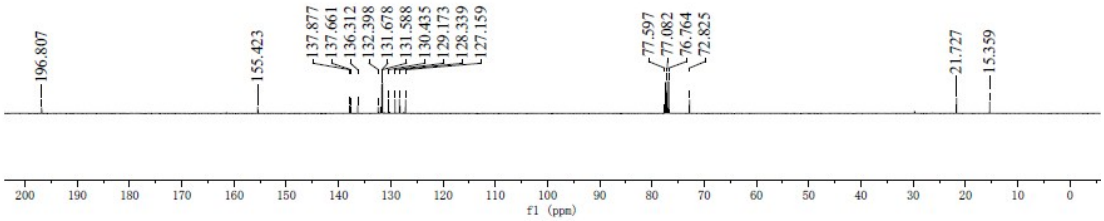


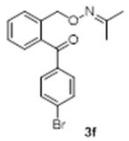





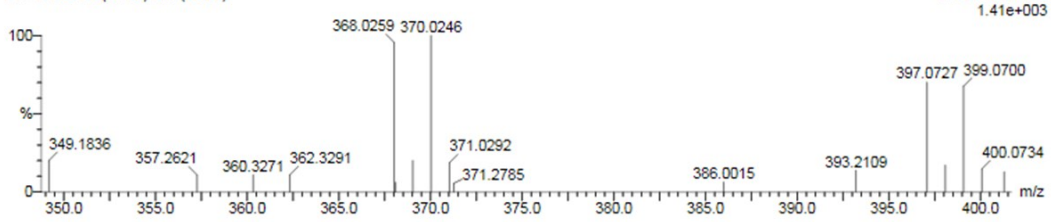




**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

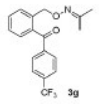


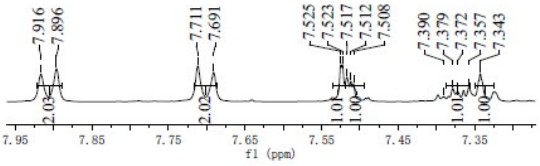

Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-1 O: 0-2 Na: 0-1 Br: 0-1

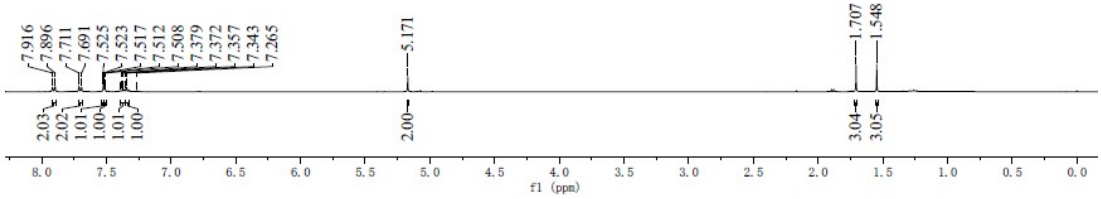
YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:46:00
JYF-S-606 56 (0.786) Cm (56:58) 1: TOF MS ES+ 1.41e+003

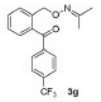


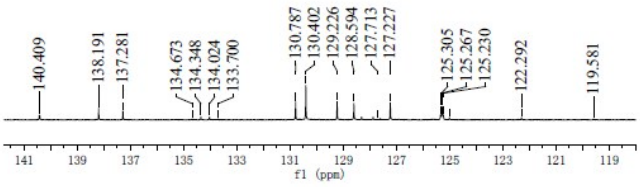

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 368.0259 | 368.0262 | -0.3 | -0.8 | 9.5 | 14.7 | 0.0 | C17 H16 N O2 Na Br |

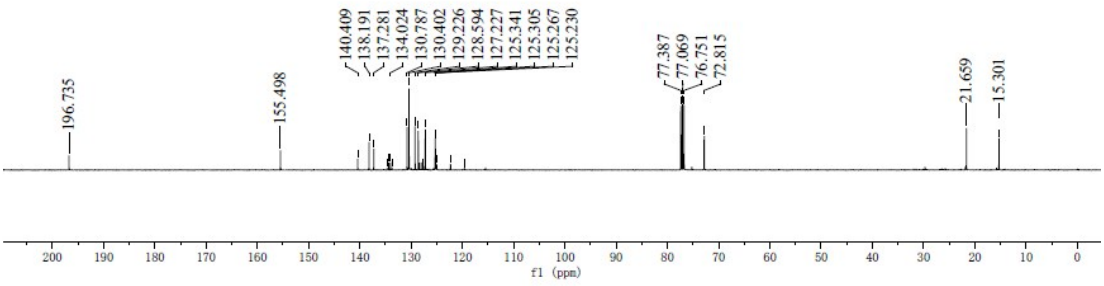

3g


7.916
7.896
7.711
7.691
7.525
7.523
7.517
7.512
7.508
7.390
7.379
7.372
7.357
7.343
2.03
2.02
1.01
1.00
1.01
1.00
7.95
7.85
7.75
7.65
7.55
7.45
7.35
f1 (ppm)

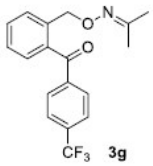

7.916
7.896
7.711
7.691
7.525
7.523
7.517
7.512
7.508
7.379
7.372
7.357
7.343
7.265
5.171
1.707
1.548
2.03
2.02
1.01
1.00
1.01
1.00
2.00
3.04
3.05
f1 (ppm)


3g


140.409
138.191
137.281
134.673
134.348
134.024
133.700
130.787
130.402
129.226
128.594
127.713
127.227
125.305
125.267
125.230
122.292
119.581
f1 (ppm)


196.735
155.498
140.409
138.191
137.281
134.024
130.787
130.402
129.226
128.594
127.227
125.341
125.305
125.267
125.230
77.387
77.069
76.751
72.815
21.659
15.301
f1 (ppm)

Elemental Composition Report



3g

Multiple Mass Analysis: 31 mass(es) processed

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

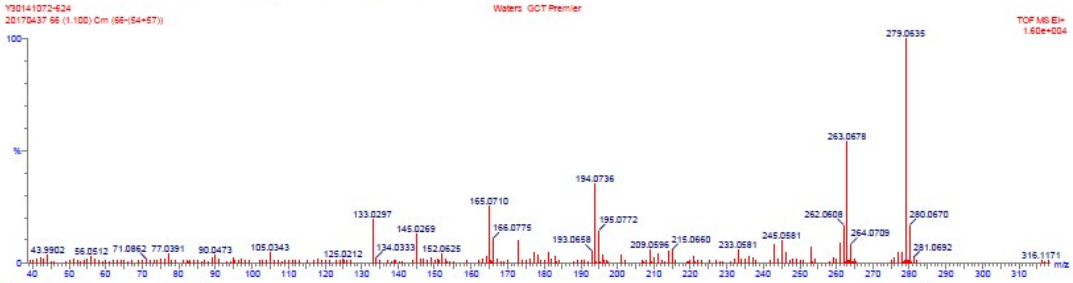
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

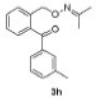
987 formula(e) evaluated with 76 results within limits (up to 50 closest results for each mass)

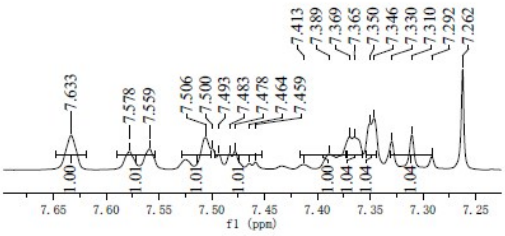
Elements Used:

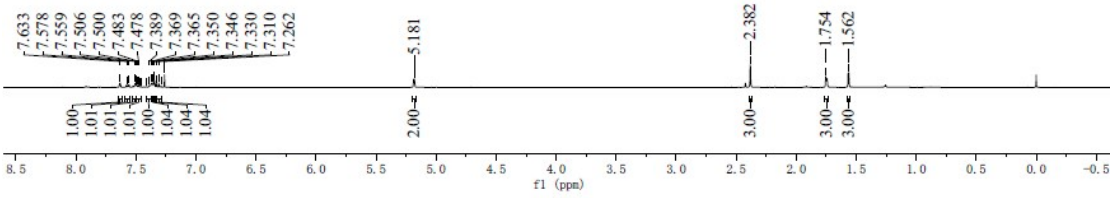
C: 0-18 H: 0-16 N: 0-1 O: 0-2 F: 0-3

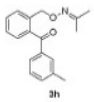


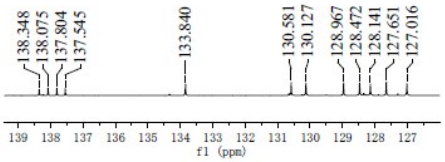

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 279.0635 | 100.00 | 279.0633 | 0.2 | 0.7 | 9.5 | 1.3 | C15 H10 O2 F3 |

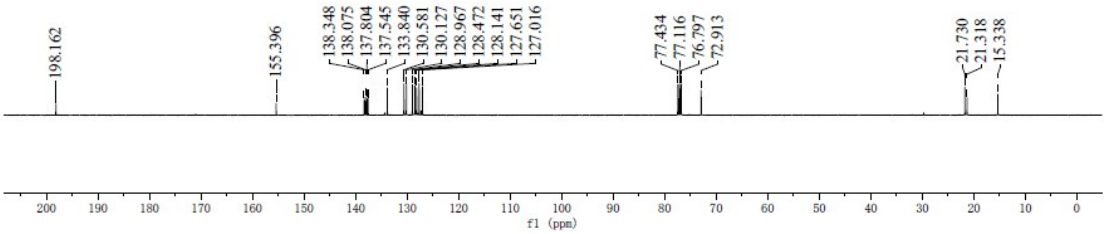

3h





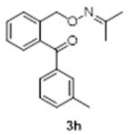




**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Even Electron Ions

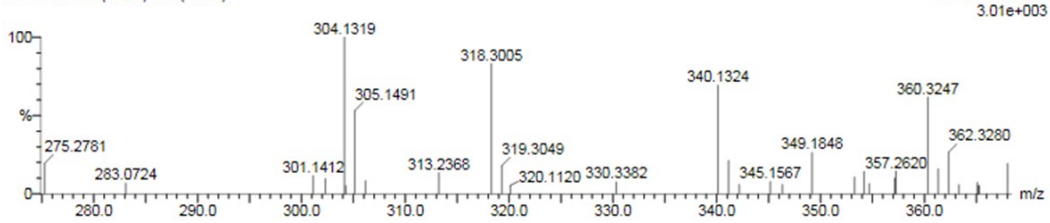
9 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

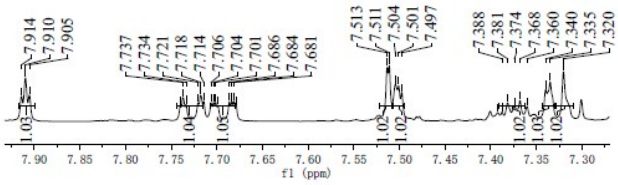
C: 0-18 H: 0-20 N: 0-1 O: 0-2 Na: 0-1

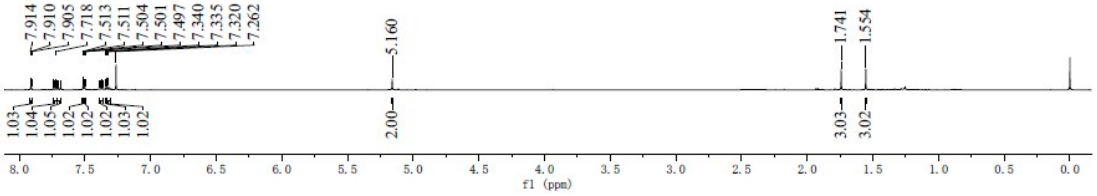
YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:55:25

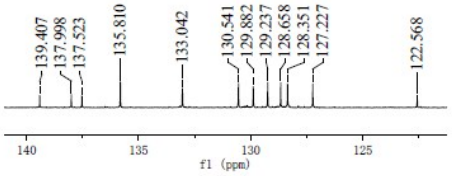
JYF-S-610 34 (0.509) Cm (28:35) 1: TOF MS ES+ 3.01e+003

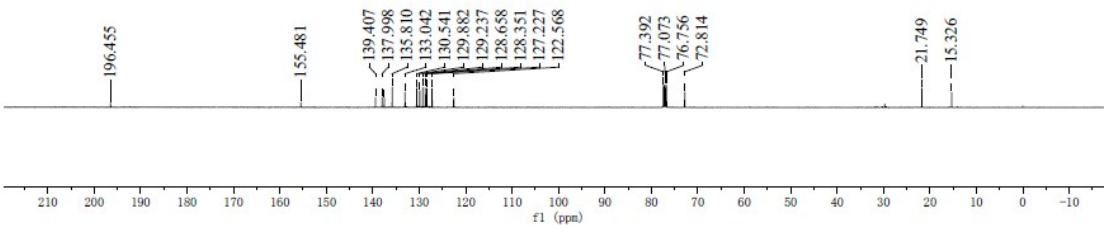



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1319 | 304.1313 | 0.6 | 2.0 | 9.5 | 37.2 | 0.0 | C18 H19 N O2 Na |

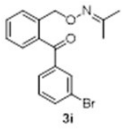

7.914
7.910
7.905
7.737
7.734
7.721
7.718
7.714
7.706
7.704
7.701
7.686
7.684
7.681
7.513
7.511
7.504
7.501
7.497
7.388
7.381
7.374
7.368
7.360
7.340
7.335
7.320
1.03
1.04
1.02
1.03
1.02
1.03
1.02
7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)


7.914
7.910
7.905
7.718
7.513
7.511
7.504
7.501
7.497
7.340
7.335
7.320
7.262
5.160
1.741
1.554
1.03
1.04
1.05
1.02
1.02
1.02
1.03
1.02
2.00
3.03
3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


139.407
137.998
137.523
135.810
133.042
130.541
129.882
129.237
128.658
128.351
127.227
122.568
140 135 130 125
f1 (ppm)

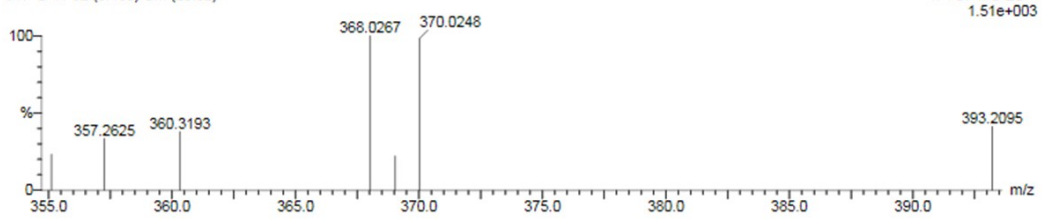

196.455
155.481
139.407
137.998
135.810
133.042
130.541
129.882
129.237
128.658
128.351
127.227
122.568
77.392
77.073
76.756
72.814
21.749
15.326
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

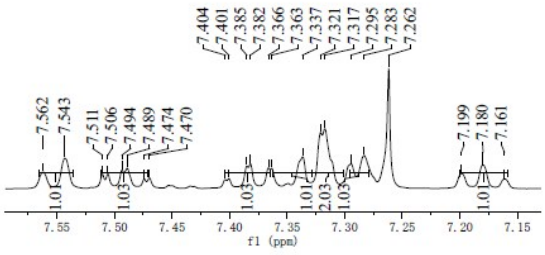


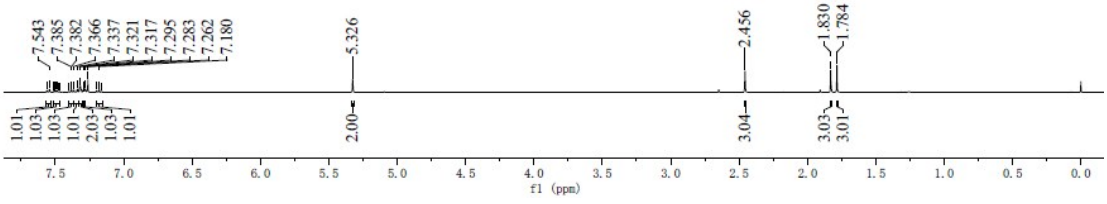

Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-16 N: 0-1 O: 0-2 Na: 0-1 Br: 0-1

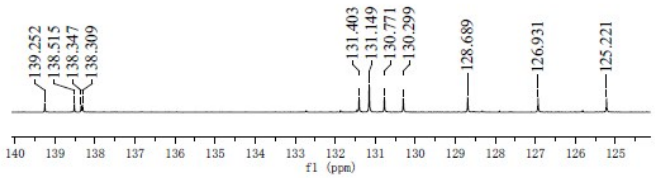
YF-JI ECUST institute of Fine Chem 18-Jan-2017 10:19:35
JYF-S-41 32 (0.488) Cm (28:32) 1: TOF MS ES+ 1.51e+003

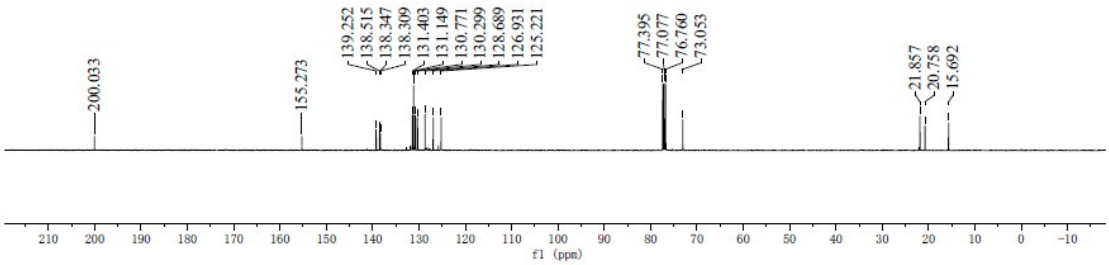



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 368.0267 | 368.0262 | 0.5 | 1.4 | 9.5 | 7.2 | 0.0 | C17 H16 N O2 Na Br |

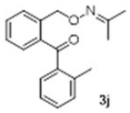





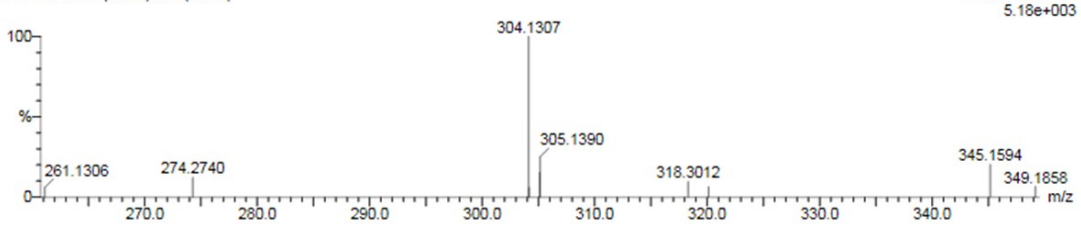




**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

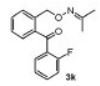


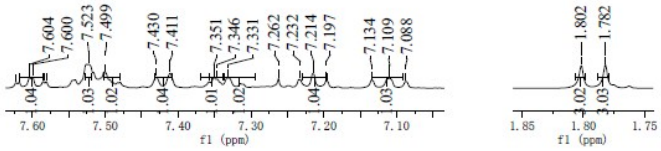
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-1 O: 0-2 Na: 0-1

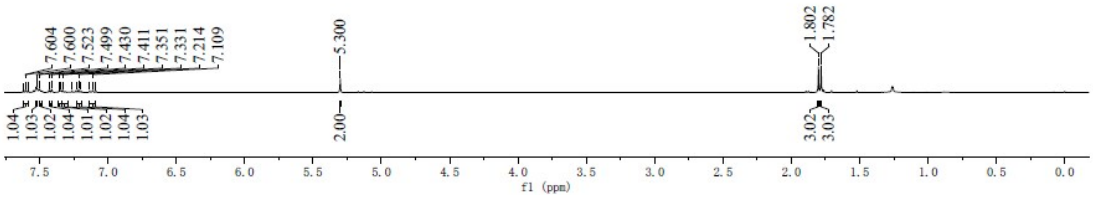
YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:38:47
JYF-S-603 43 (0.624) Cm (42:44) 1: TOF MS ES+ 5.18e+003



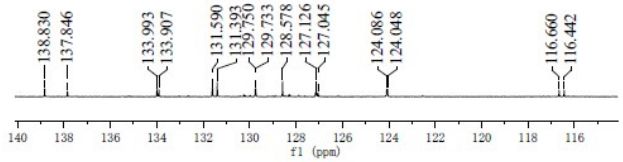

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1307 | 304.1313 | -0.6 | -2.0 | 9.5 | 53.2 | 0.0 | C18 H19 N O2 Na |

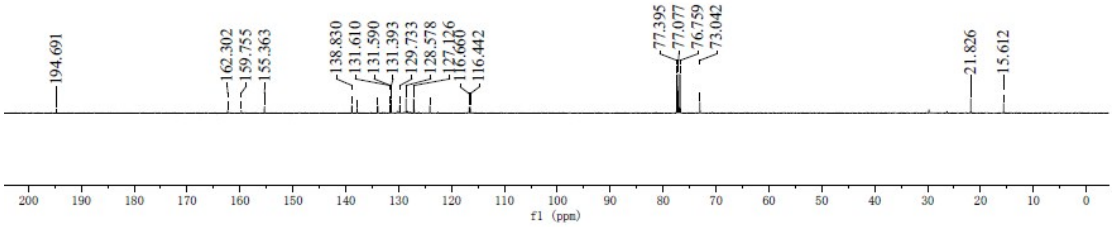

3k


7.604
7.600
7.523
7.499
7.430
7.411
7.351
7.346
7.331
7.262
7.232
7.214
7.197
7.134
7.109
7.088
1.802
1.782
f1 (ppm)

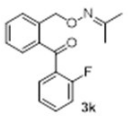

7.604
7.600
7.523
7.499
7.430
7.411
7.351
7.331
7.214
7.109
5.300
1.802
1.782
f1 (ppm)


3k


138.830
137.846
133.993
133.907
131.590
131.393
129.750
129.733
128.578
127.126
127.045
124.086
124.048
116.660
116.442
f1 (ppm)

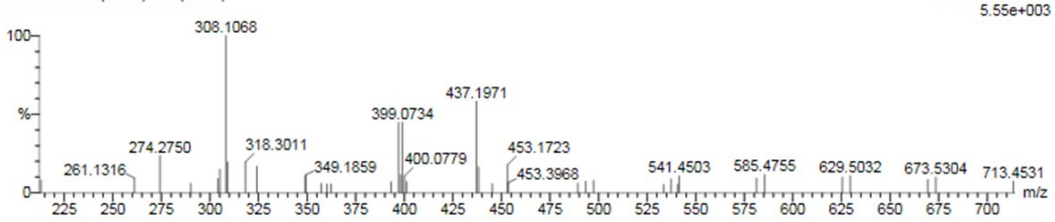

194.691
162.302
159.755
155.363
138.830
131.610
131.590
131.393
129.733
128.578
127.126
116.660
116.442
77.395
77.077
76.759
73.042
21.826
15.612
f1 (ppm)

**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

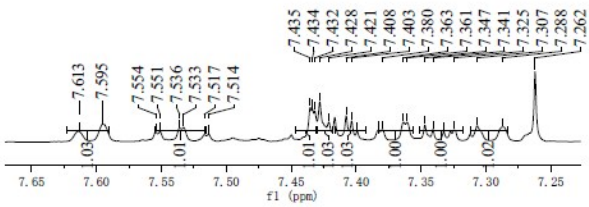


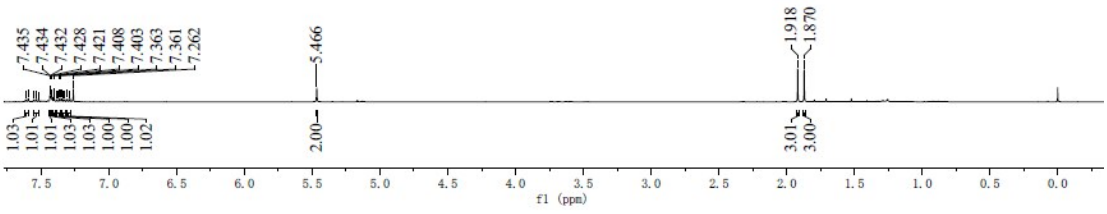

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-18 H: 0-20 N: 0-1 O: 0-2 Na: 0-1 F: 0-1

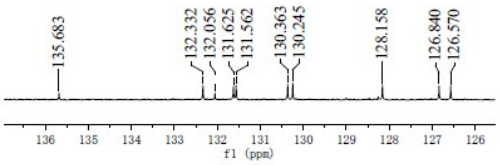
YF-JI ECUST institute of Fine Chem 06-Mar-2017 22:10:34
JYF-S-602 14 (0.269) Cm (10:16) 1: TOF MS ES+ 5.55e+003

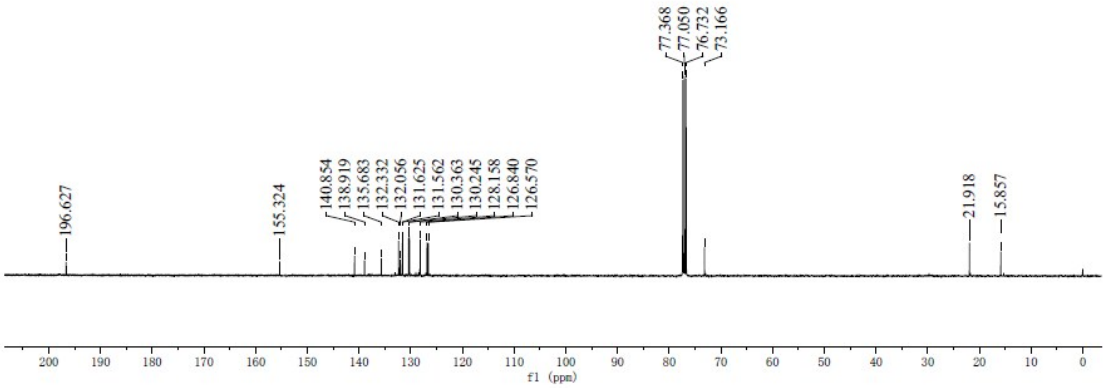



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 308.1068 | 308.1063 | 0.5 | 1.6 | 9.5 | 22.5 | 0.0 | C17 H16 N O2 Na F |



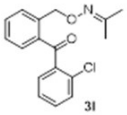




**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Even Electron Ions

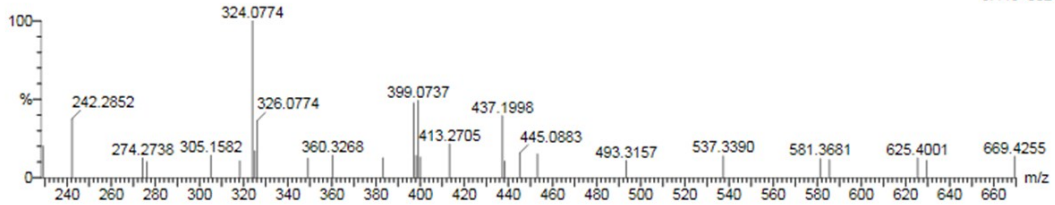
29 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-1 O: 0-3 Na: 0-1 Cl: 0-1

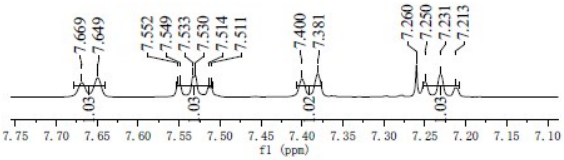
YF-JI ECUST institute of Fine Chem 06-Mar-2017 20:48:26

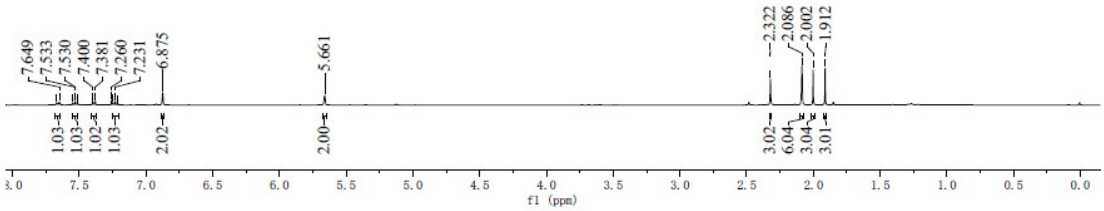
JYF-S-539 28 (0.451) Cm (28) 1: TOF MS ES+ 8.44e+002



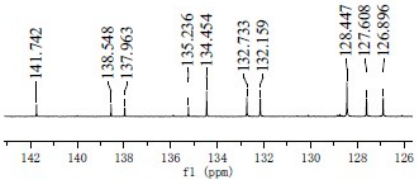

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 324.0774 | 324.0767 | 0.7 | 2.2 | 9.5 | 7.4 | 0.0 | C17 H16 N O2 Na Cl |

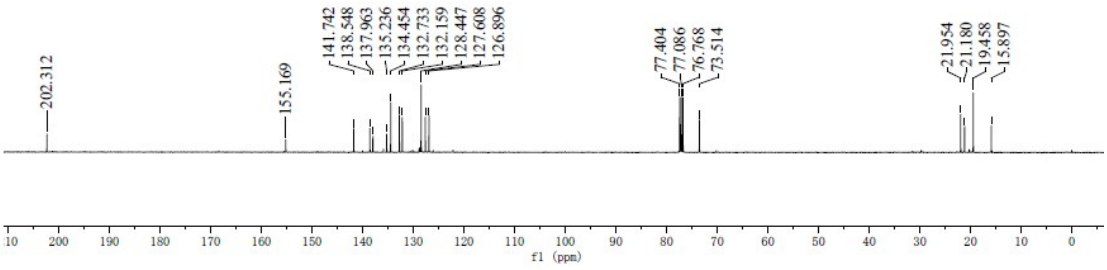

3m


7.669
7.649
7.552
7.549
7.533
7.530
7.514
7.511
7.400
7.381
7.260
7.250
7.231
7.213
1.03
1.03
1.02
1.03
f1 (ppm)

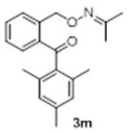

7.649
7.533
7.530
7.400
7.381
7.260
7.231
6.875
5.661
2.322
2.086
2.002
1.912
1.03
1.03
1.02
1.03
2.02
2.00
3.02
6.04
3.04
3.01
f1 (ppm)


3m


141.742
138.548
137.963
135.236
134.454
132.733
132.159
128.447
127.608
126.896
f1 (ppm)


202.312
155.169
141.742
138.548
137.963
135.236
134.454
132.733
132.159
128.447
127.608
126.896
77.404
77.086
76.768
73.514
21.954
21.180
19.458
15.897
f1 (ppm)

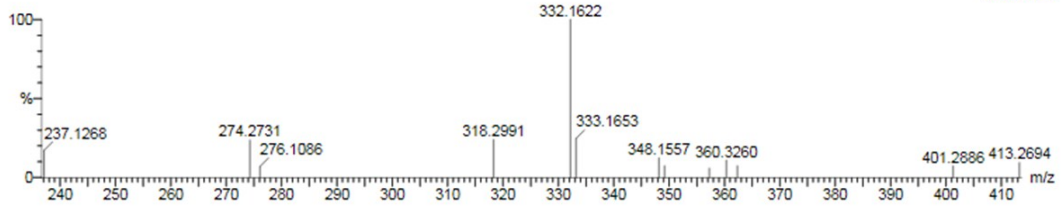
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



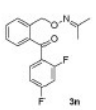

Monoisotopic Mass, Even Electron Ions
44 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-40 N: 0-1 O: 0-5 Na: 0-1

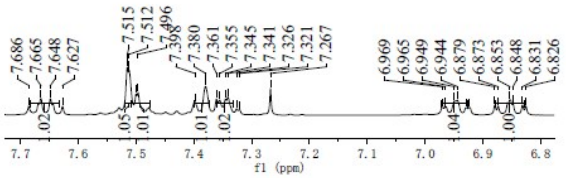
YF-JI ECUST institute of Fine Chem 05-Jan-2017 21:54:47

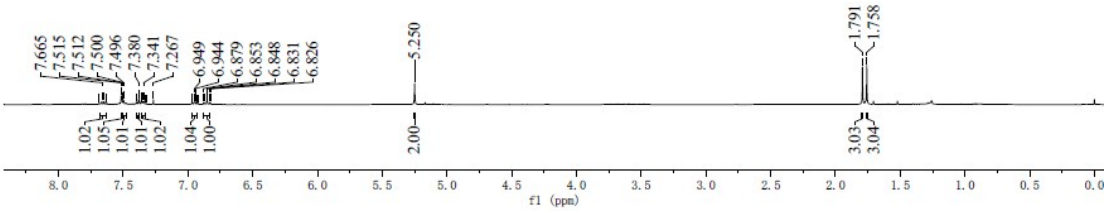
YF-S-521 36 (0.530) Cm (34:36) 1: TOF MS ES+ 2.22e+003

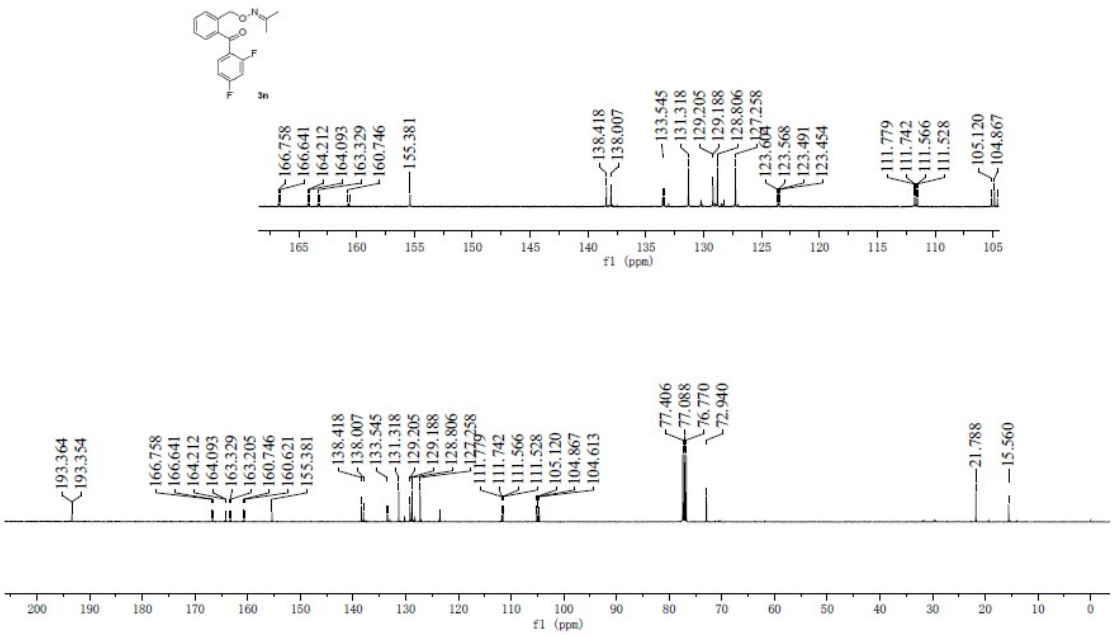



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 332.1622 | 332.1626 | -0.4 | -1.2 | 9.5 | 20.6 | 0.0 | C20 H23 N O2 Na |



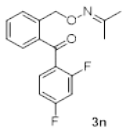





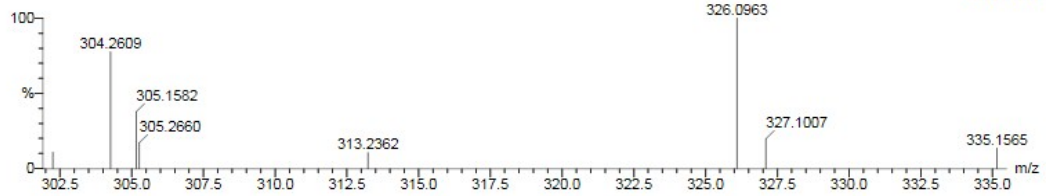

**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

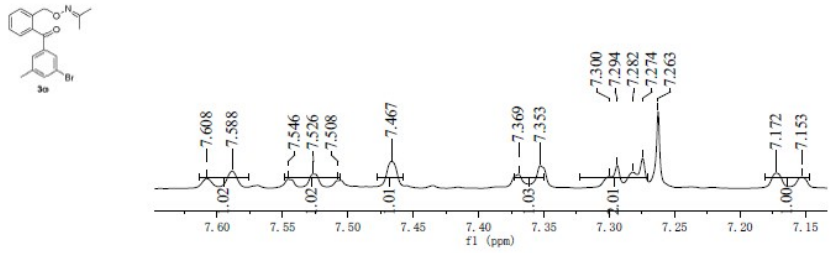


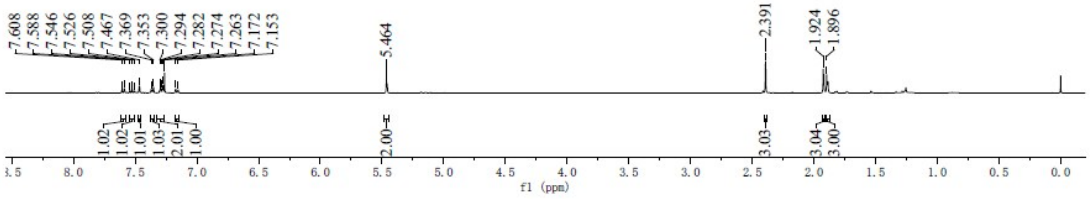

Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-16 N: 0-1 O: 0-2 F: 0-2 Na: 0-1

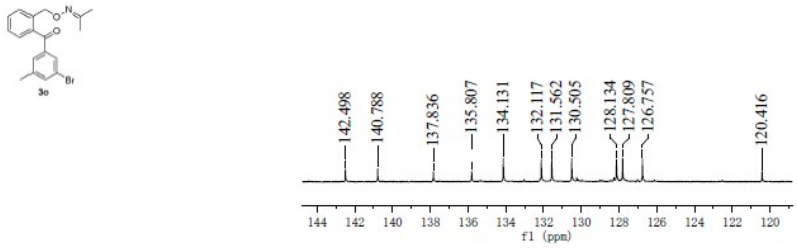
YF-JI ECUST institute of Fine Chem 18-Jan-2017 10:15:48
JYF-S-40 4 (0.149) Cm (4:6) 1: TOF MS ES+ 3.03e+003

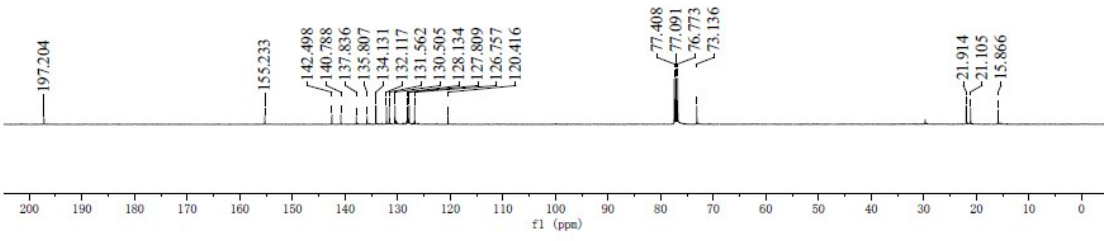



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 326.0963 | 326.0969 | -0.6 | -1.8 | 9.5 | 21.5 | 0.0 | C17 H15 N O2 F2 Na |

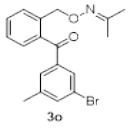

3o
7.608
7.588
7.546
7.526
7.508
7.467
7.369
7.353
7.300
7.294
7.282
7.274
7.263
7.172
7.153
1.02
1.02
1.01
1.03
2.01
1.00
f1 (ppm)


7.608
7.588
7.546
7.526
7.508
7.467
7.369
7.353
7.300
7.294
7.282
7.274
7.263
7.172
7.153
5.464
2.391
1.924
1.896
1.02
1.02
1.01
1.03
2.01
1.00
2.00
3.03
3.04
3.00
f1 (ppm)


3o
142.498
140.788
137.836
135.807
134.131
132.117
131.562
130.505
128.134
127.809
126.757
120.416
f1 (ppm)


197.204
155.233
142.498
140.788
137.836
135.807
134.131
132.117
131.562
130.505
128.134
127.809
126.757
120.416
77.408
77.091
76.773
73.136
21.914
21.105
15.866
f1 (ppm)

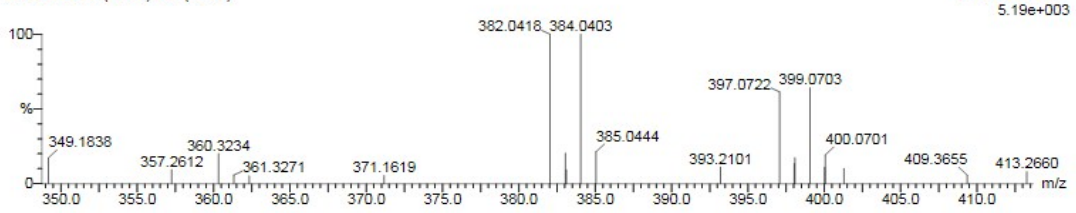
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



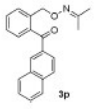
3o

Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-1 O: 0-2 Na: 0-1 Br: 0-1

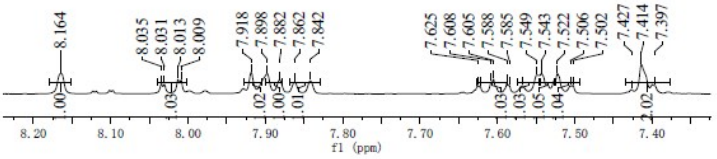
YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:42:02
JYF-S-605 26 (0.410) Cm (22:30) 1: TOF MS ES+ 5.19e+003

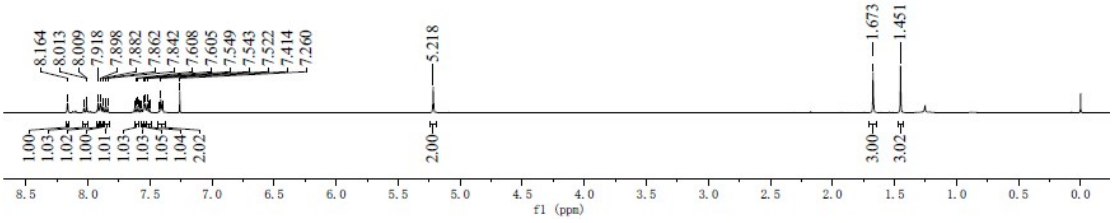


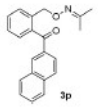

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 382.0418 | 382.0419 | -0.1 | -0.3 | 9.5 | 18.1 | 0.0 | C18 H18 N O2 Na Br |

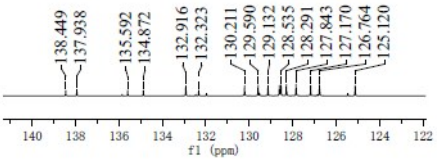


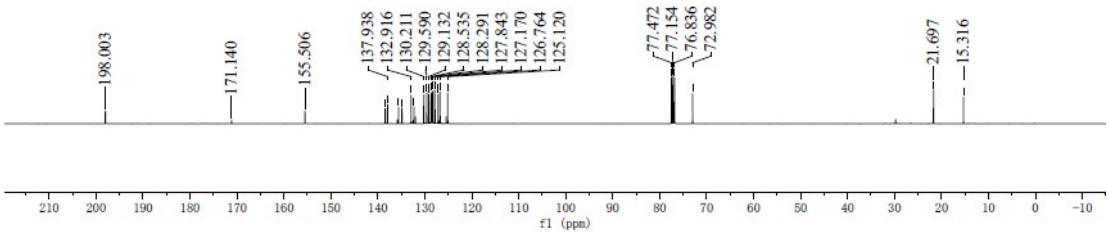
3p





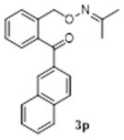




**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Even Electron Ions

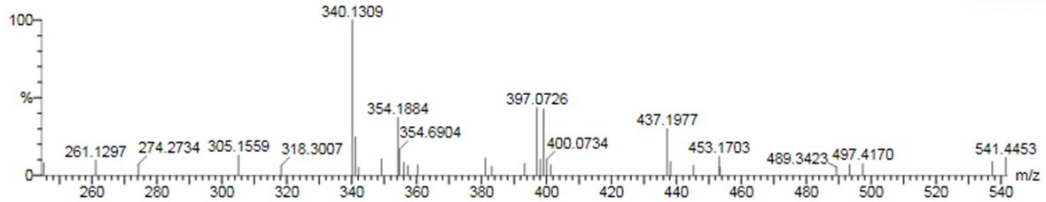
5 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

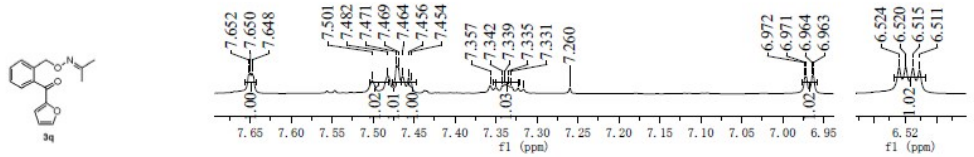
C: 0-22 H: 0-20 N: 0-1 O: 0-2 Na: 0-1

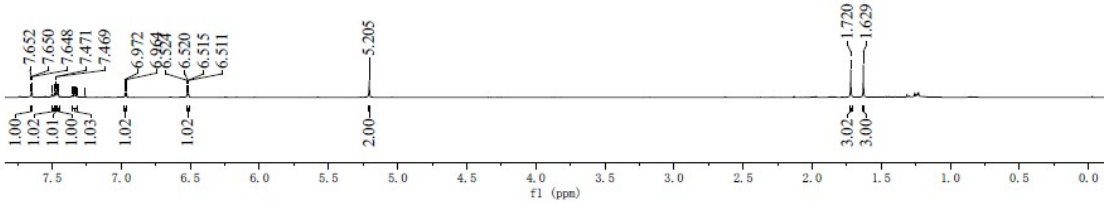
YF-JI ECUST institute of Fine Chem 06-Mar-2017 21:49:13

JYF-S-607 109 (1.433) Cm (108:113) 1: TOF MS ES+ 4.24e+003

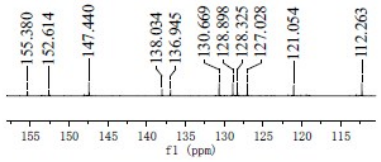


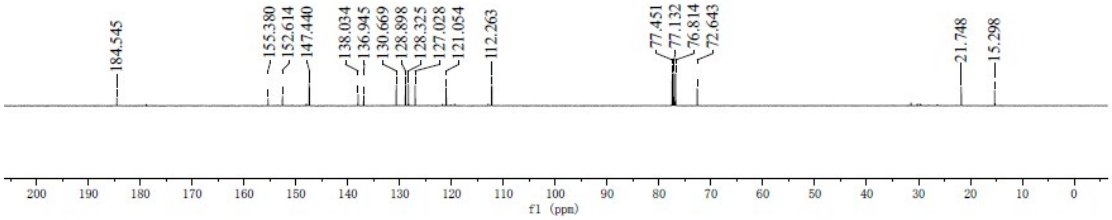

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 340.1309 | 340.1313 | -0.4 | -1.2 | 12.5 | 11.7 | 0.0 | C21 H19 N O2 Na |


3q
7.652
7.650
7.648
7.501
7.482
7.471
7.469
7.464
7.456
7.454
7.357
7.342
7.339
7.335
7.331
7.260
6.972
6.971
6.964
6.963
6.524
6.520
6.515
6.511
f1 (ppm)

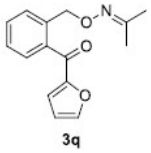

7.652
7.650
7.648
7.471
7.469
6.972
6.964
6.524
6.520
6.515
6.511
5.205
1.720
1.629
f1 (ppm)


3q


155.380
152.614
147.440
138.034
136.945
130.669
128.898
128.325
127.028
121.054
112.263
f1 (ppm)


184.545
155.380
152.614
147.440
138.034
136.945
130.669
128.898
128.325
127.028
121.054
112.263
77.451
77.132
76.814
72.643
21.748
15.298
f1 (ppm)

Elemental Composition Report



3q

Multiple Mass Analysis: 29 mass(es) processed

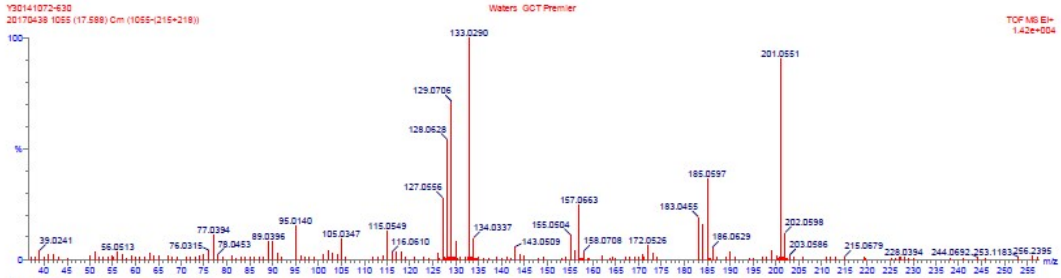
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions 315 formula(e) evaluated with 29 results within limits (up to 50 closest results for each mass)

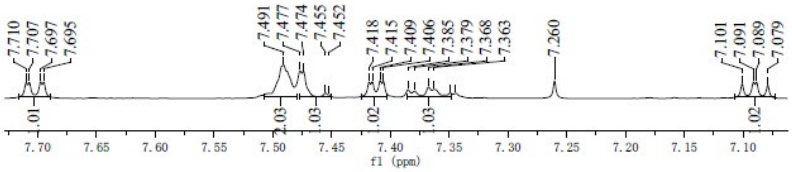
Elements Used:

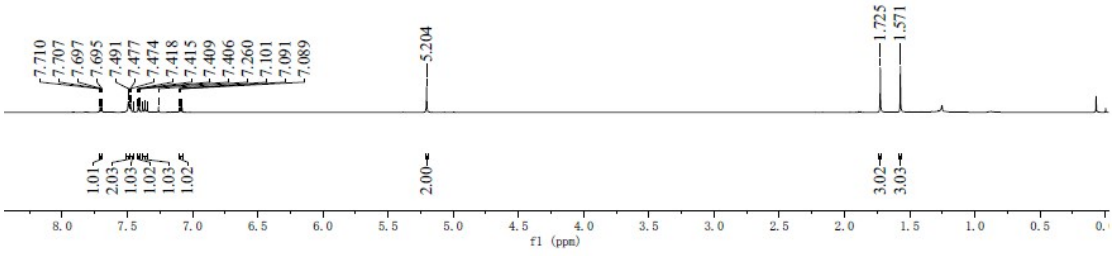
C: 0-15 H: 0-15 N: 0-1 O: 0-3

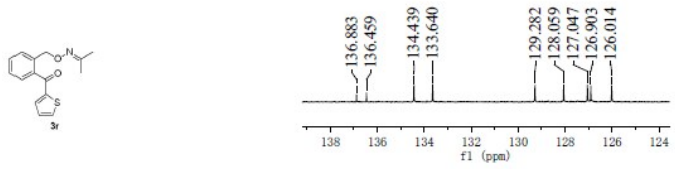


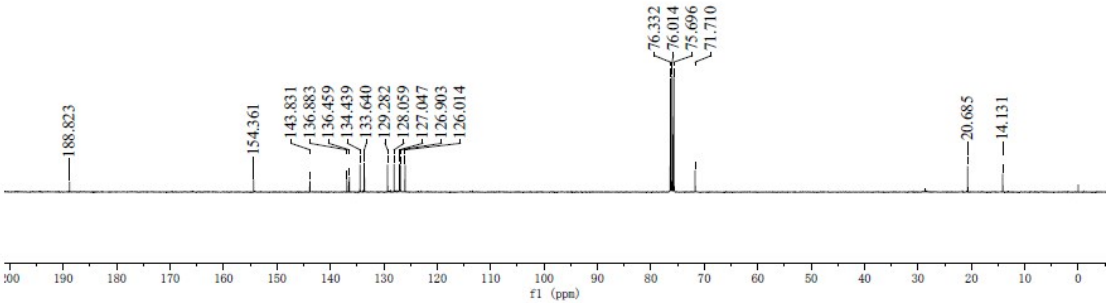

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 201.0551 | 90.10 | 201.0552 | -0.1 | -0.5 | 8.5 | 4.3 | C12 H9 O3 |

3r

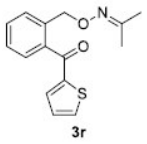





Elemental Composition Report




Multiple Mass Analysis: 29 mass(es) processed

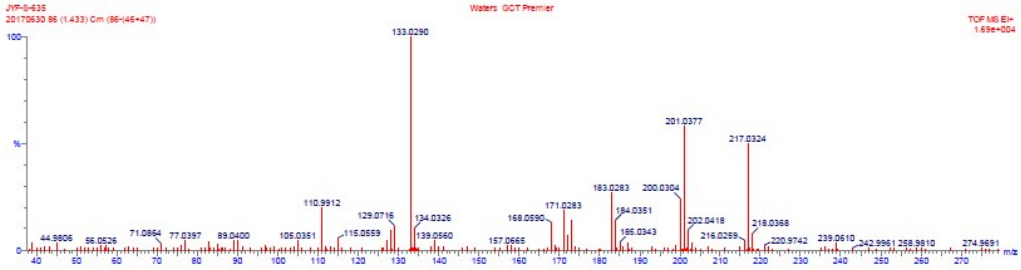
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions 466 formula(e) evaluated with 58 results within limits (up to 50 closest results for each mass)

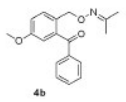
Elements Used:

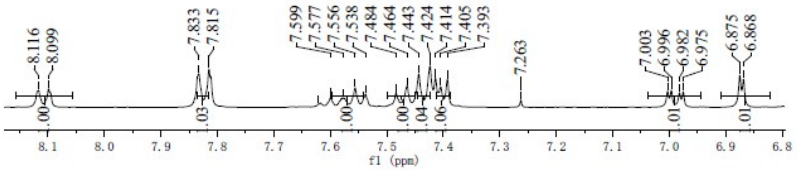
C: 0-15 H: 0-15 N: 0-1 O: 0-2 S: 0-1

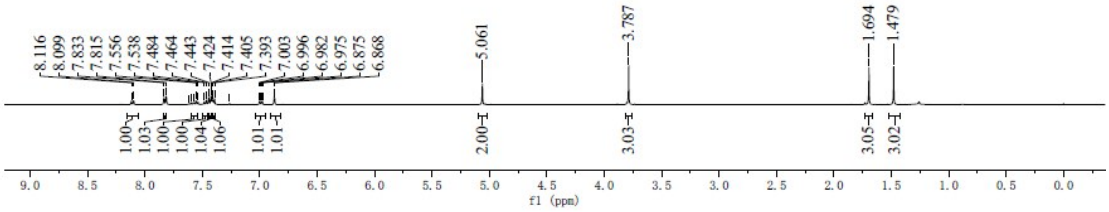


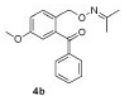

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 217.0324 | 49.74 | 217.0323 | 0.1 | 0.5 | 8.5 | 2777586.8 | C12H9O2S |

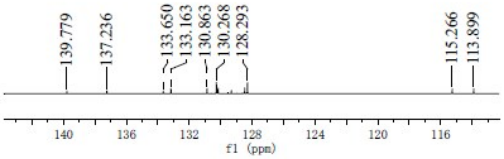
## 4.2 Copies of the spectra for Tables 3

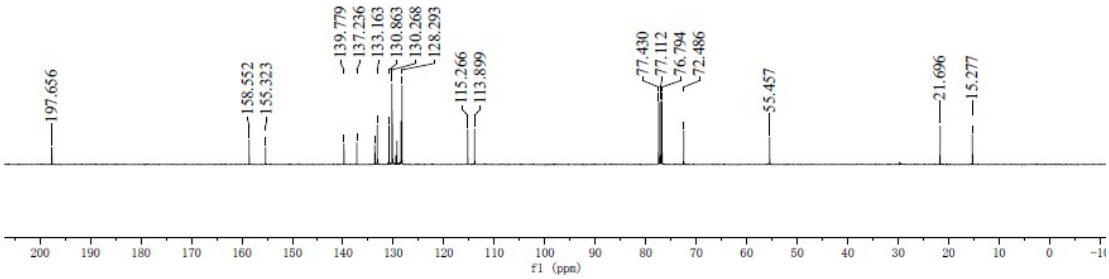


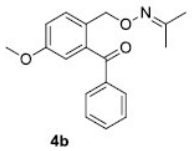



Elemental Composition Report



4b

Multiple Mass Analysis: 81 mass(es) processed

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

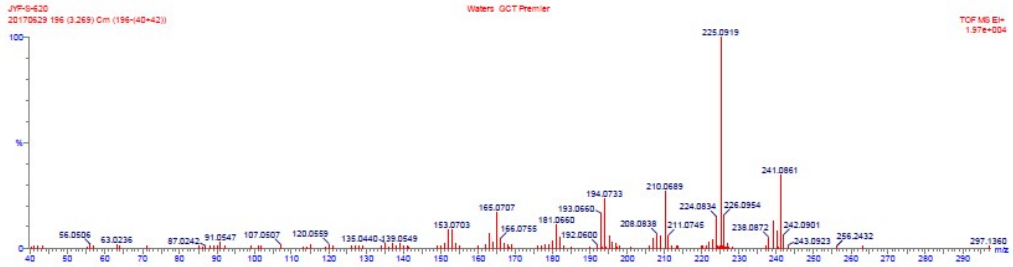
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions 1059 formula(e)

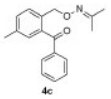
evaluated with 77 results within limits (up to 50 closest results for each mass)

Elements Used:

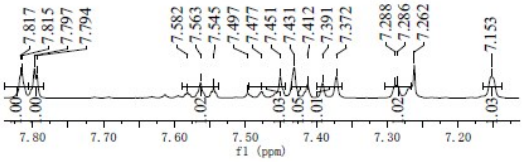
C: 0-18 H: 0-19 N: 0-1 O: 0-3

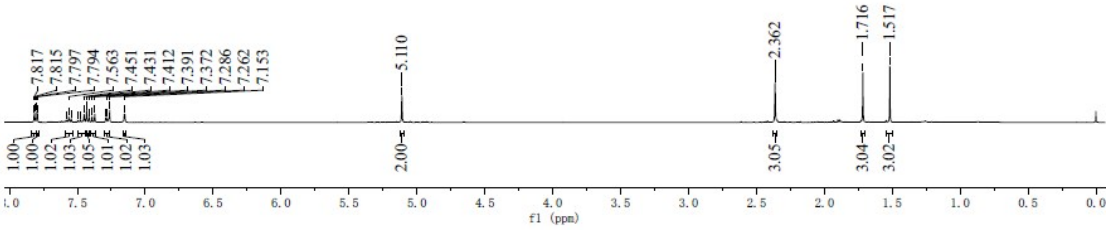


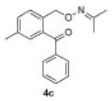

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 0.27 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 297.1360 | 0.28 | 297.1365 | -0.5 | -1.7 | 10.0 | 5546041.5 | C18H19NO3 |

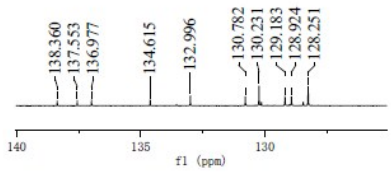


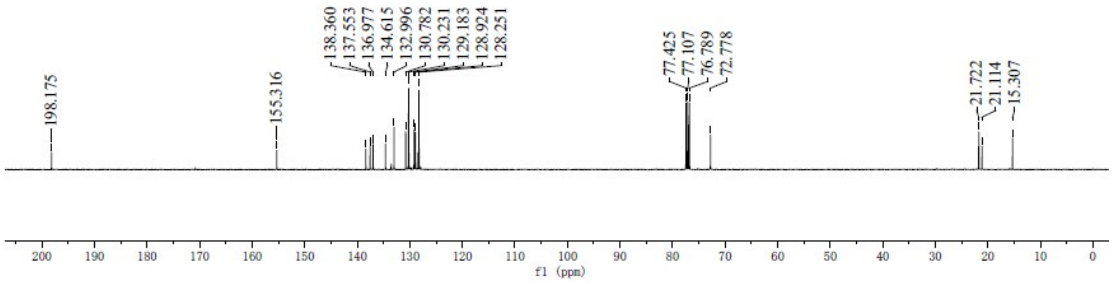
4c



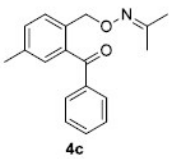






Elemental Composition Report




Multiple Mass Analysis: 25 mass(es) processed

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

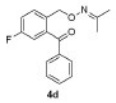
Element prediction: Off

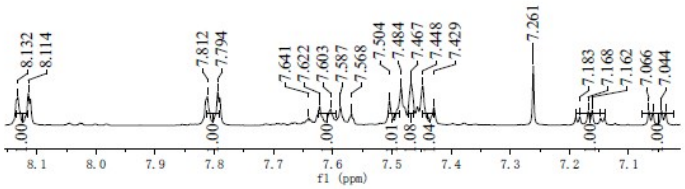
Monoisotopic Mass, Odd and Even Electron Ions 264 formula(e) evaluated with 24 results within limits (up to 50 closest results for each mass)

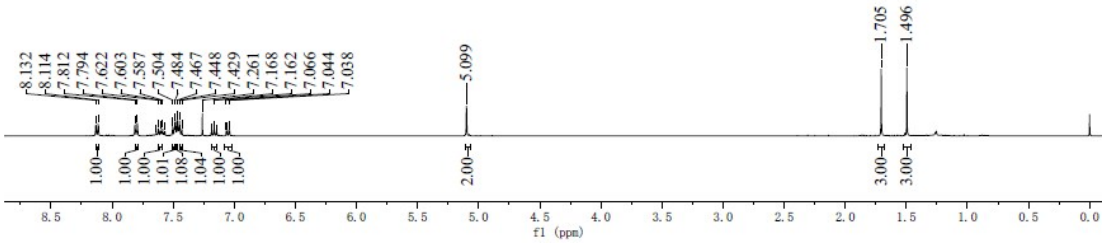
Elements Used:

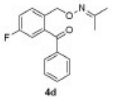
C: 0-18 H: 0-19 N: 0-1 O: 0-2

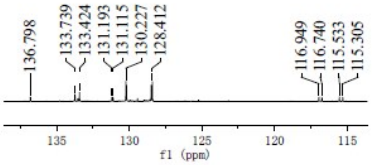

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 225.0917 | 100.00 | 225.0916 | 0.1 | 0.4 | 9.5 | 0.7 | C15H13O2 |

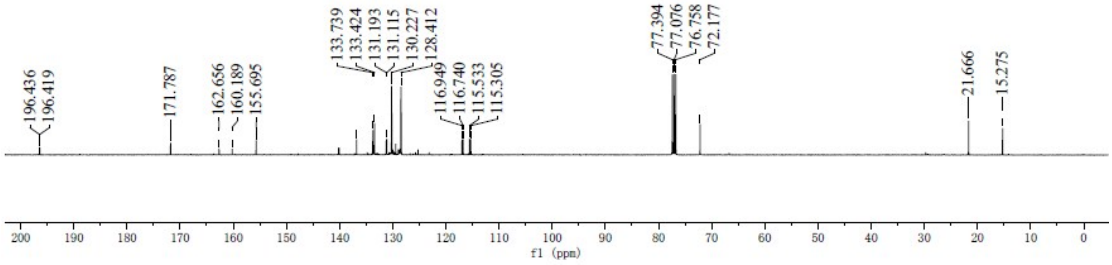

4d


8.132
8.114
7.812
7.794
7.641
7.622
7.603
7.587
7.568
7.504
7.484
7.467
7.448
7.429
7.261
7.183
7.168
7.162
7.066
7.044
f1 (ppm)

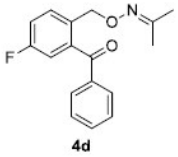

8.132
8.114
7.812
7.794
7.622
7.603
7.587
7.504
7.484
7.467
7.448
7.429
7.261
7.168
7.162
7.066
7.044
7.038
5.099
1.705
1.496
f1 (ppm)


4d


136.798
133.739
133.424
131.193
131.115
130.227
128.412
116.949
116.740
115.533
115.305
f1 (ppm)


196.436
196.419
171.787
162.656
160.189
155.695
133.739
133.424
131.193
131.115
130.227
128.412
116.949
116.740
115.533
115.305
77.394
77.076
76.758
72.177
21.666
15.275
f1 (ppm)

Elemental Composition Report



4d

Multiple Mass Analysis: 30 mass(es) processed

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

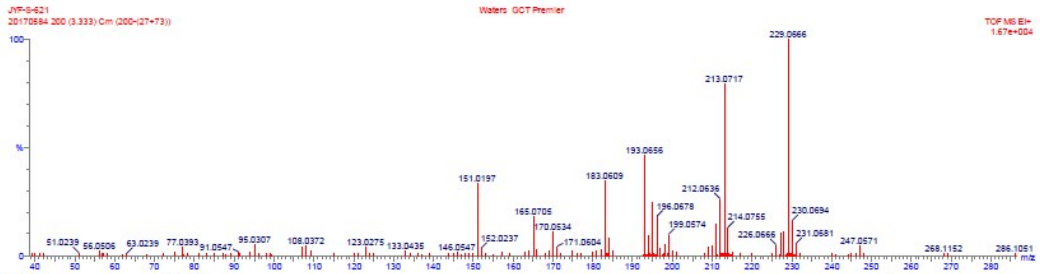
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

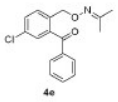
514 formula(e) evaluated with 51 results within limits (up to 50 closest results for each mass)

Elements Used:

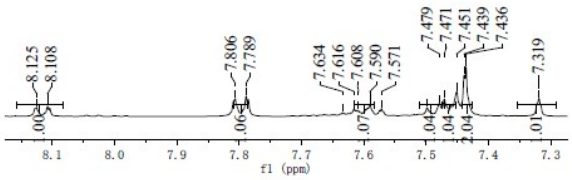
C: 0-17 H: 0-16 N: 0-1 O: 0-2 F: 0-1

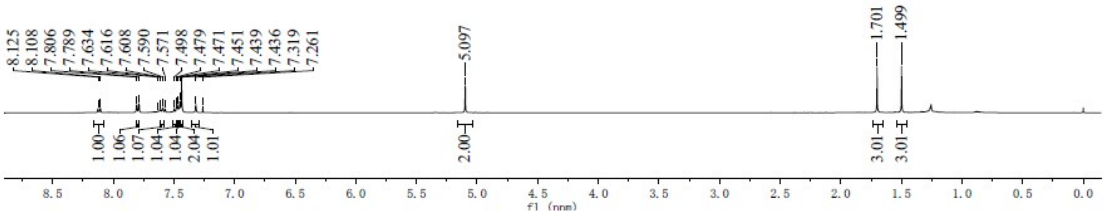


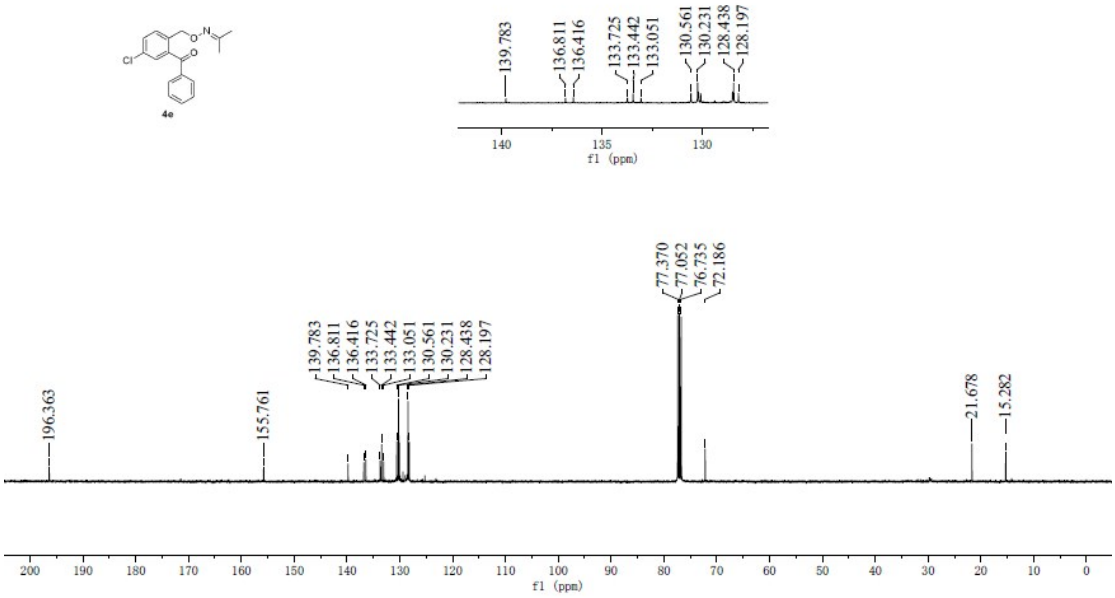

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 229.0666 | 100.00 | 229.0665 | 0.1 | 0.4 | 9.5 | 199.7 | C14H10O2F |



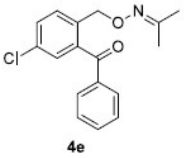
4e






Elemental Composition Report




Multiple Mass Analysis: 29 mass(es) processed

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

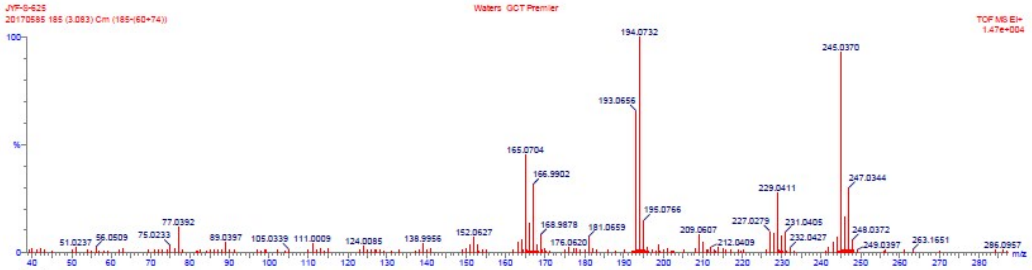
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

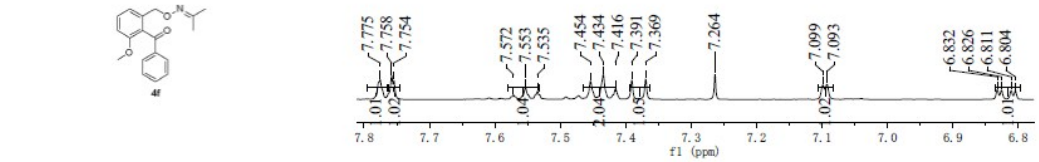
969 formula(e) evaluated with 75 results within limits (up to 50 closest results for each mass)

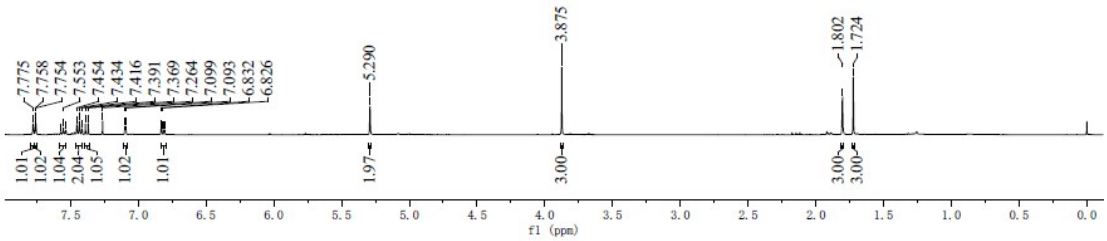
Elements Used:

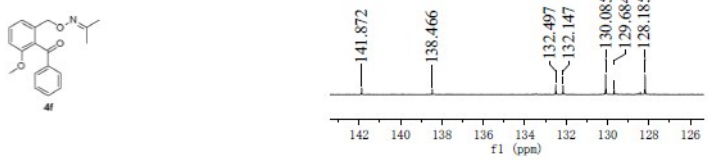
C: 0-17 H: 0-16 N: 0-1 O: 0-2 35Cl: 0-1 37Cl: 0-1

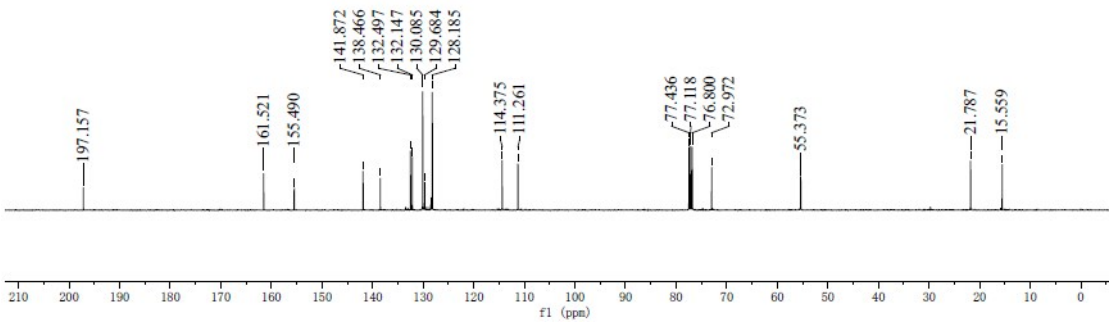



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 245.0370 | 92.51 | 245.0369 | 0.1 | 0.4 | 9.5 | 15.1 | C14H10O2 35Cl |

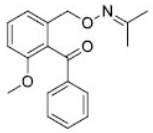

4f
7.775
7.758
7.754
7.572
7.553
7.535
7.454
7.434
7.416
7.391
7.369
7.264
7.099
7.093
6.832
6.826
6.811
6.804
f1 (ppm)


7.775
7.758
7.754
7.553
7.454
7.434
7.416
7.391
7.369
7.264
7.099
7.093
6.832
6.826
5.290
3.875
1.802
1.724
1.01
1.02
1.04
2.04
1.05
1.02
1.01
1.97
3.00
3.00
3.00
f1 (ppm)

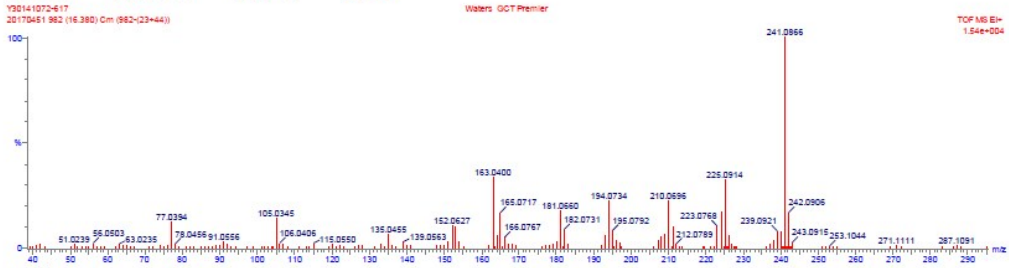

4f
141.872
138.466
132.497
132.147
130.085
129.684
128.185
f1 (ppm)


197.157
161.521
155.490
141.872
138.466
132.497
132.147
130.085
129.684
128.185
114.375
111.261
77.436
77.118
76.800
72.972
55.373
21.787
15.559
f1 (ppm)

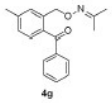
Elemental Composition Report
Multiple Mass Analysis: 27 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
367 formula(e) evaluated with 31 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-18 H: 0-19 N: 0-1 O: 0-3



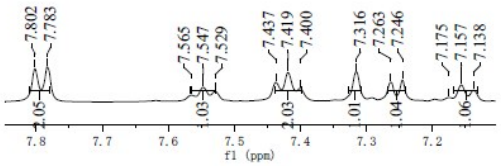
4f

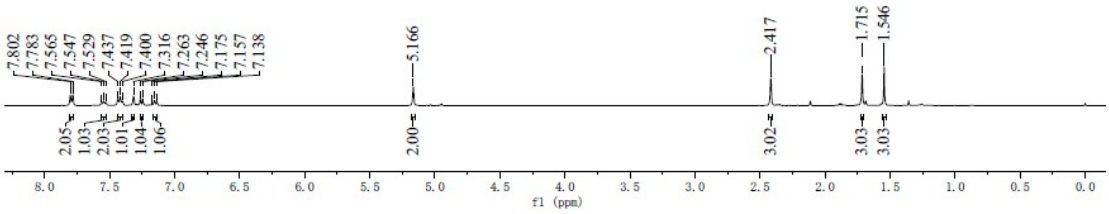


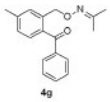

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 241.0866 | 100.00 | 241.0865 | 0.1 | 0.4 | 9.5 | 2.5 | C15H13O3 |

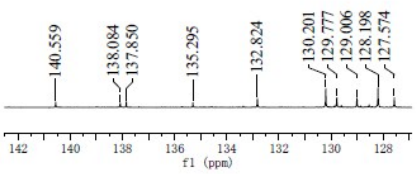


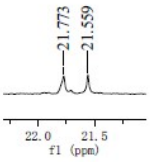
4g

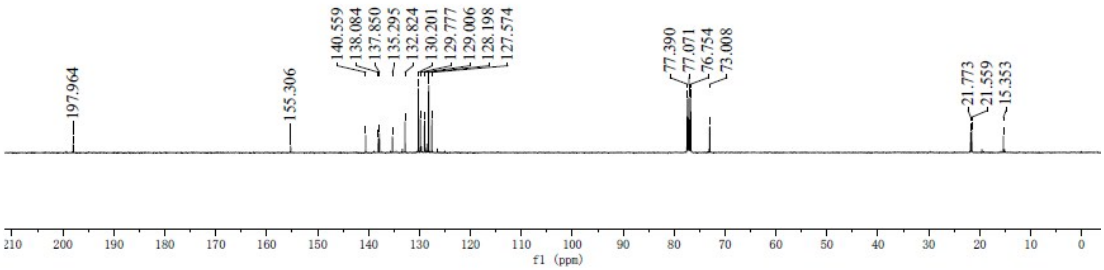




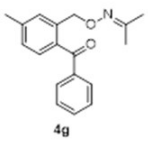




**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3




Monoisotopic Mass, Even Electron Ions

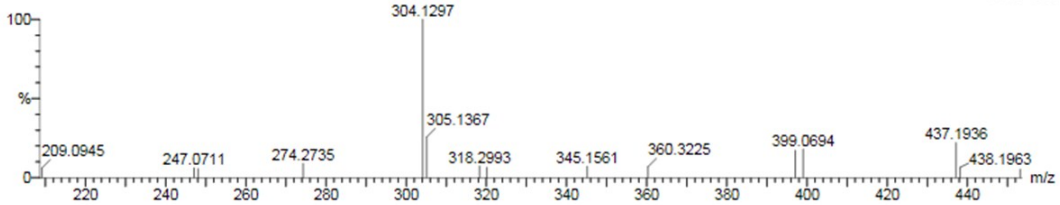
9 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

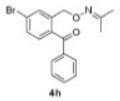
C: 0-18 H: 0-20 N: 0-1 O: 0-2 Na: 0-1

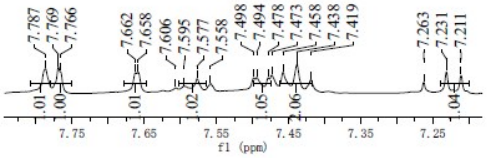
YF-JI ECUST institute of Fine Chem 06-Mar-2017 22:06:28

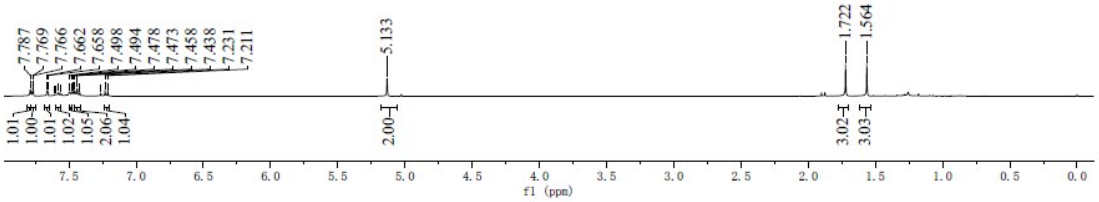
JYF-S-546 66 (0.907) Cm (66:68) 1: TOF MS ES+ 7.40e+003

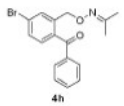


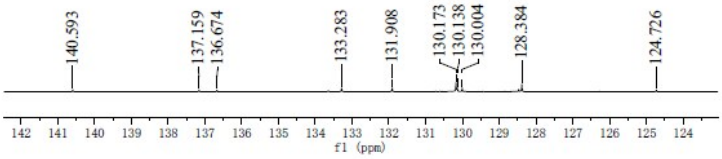

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1297 | 304.1313 | -1.6 | -5.3 | 9.5 | 29.0 | 0.0 | C18 H19 N O2 Na |

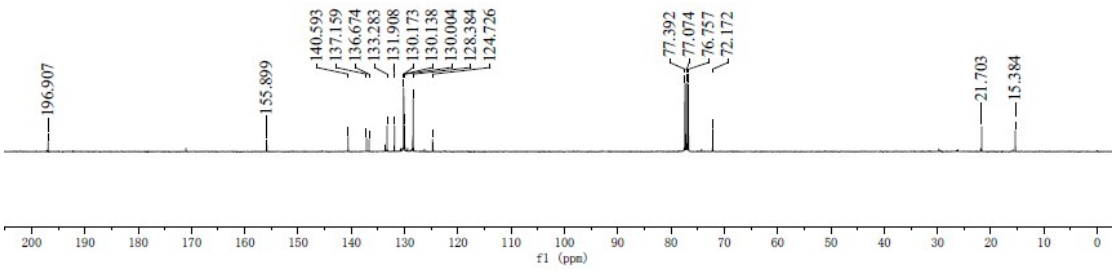

Br
O
N
O
4h


7.787
7.769
7.766
7.662
7.658
7.606
7.595
7.577
7.558
7.498
7.494
7.478
7.473
7.458
7.438
7.419
7.263
7.231
7.211
1.01
1.00
1.01
1.02
1.05
2.06
1.04
7.75
7.65
7.55
7.45
7.35
7.25
f1 (ppm)

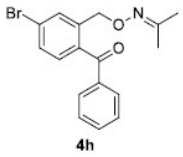

7.787
7.769
7.766
7.662
7.658
7.498
7.494
7.478
7.473
7.458
7.438
7.231
7.211
5.133
1.722
1.564
1.01
1.00
1.01
1.02
1.05
2.06
1.04
2.00
3.02
3.03
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Br
O
N
O
4h


140.593
137.159
136.674
133.283
131.908
130.173
130.138
130.004
128.384
124.726
142
141
140
139
138
137
136
135
134
133
132
131
130
129
128
127
126
125
124
f1 (ppm)


196.907
155.899
140.593
137.159
136.674
133.283
131.908
130.173
130.138
130.004
128.384
124.726
77.392
77.074
76.757
72.172
21.703
15.384
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Elemental Composition Report



4h

Multiple Mass Analysis: 44 mass(es) processed

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

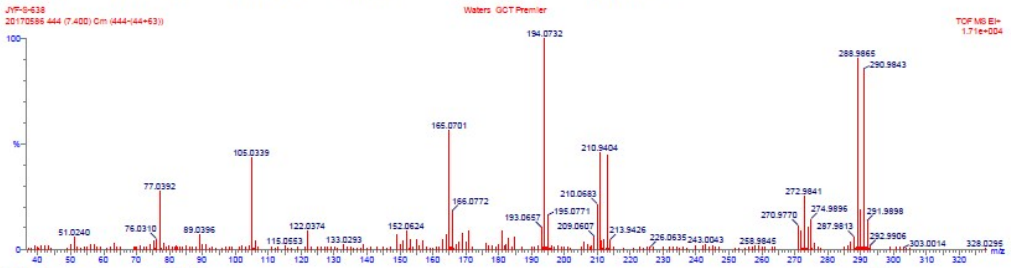
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

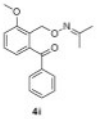
1189 formula(e) evaluated with 58 results within limits (up to 50 closest results for each mass)

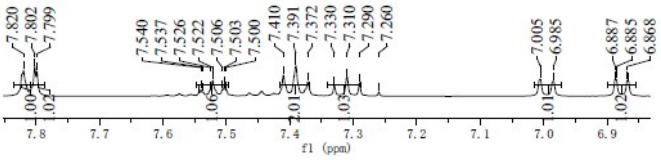
Elements Used:

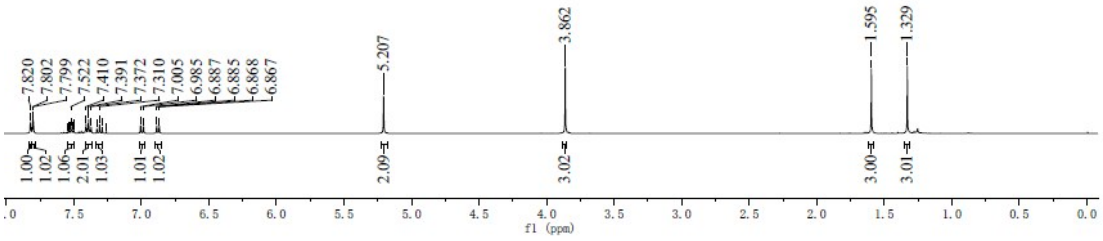
C: 0-17 H: 0-16 N: 0-1 O: 0-2 79Br: 0-1 81Br: 0-1

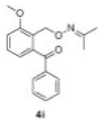



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 288.9865 | 90.44 | 288.9864 | 0.1 | 0.3 | 9.5 | 90.3 | C14H10O2 79Br |

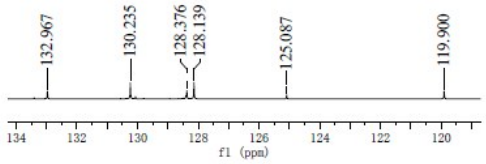

4i

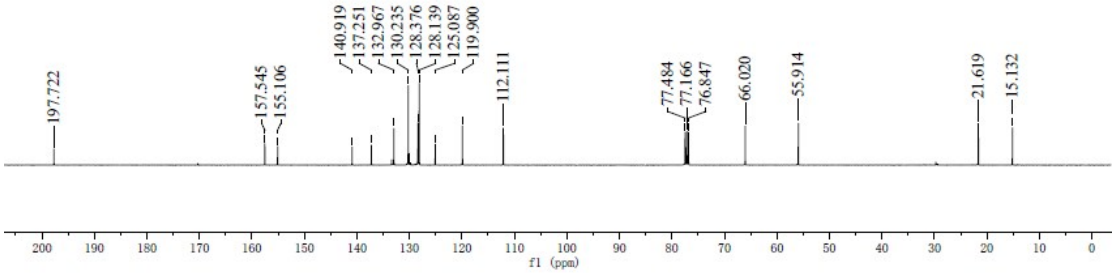




4i




Elemental Composition Report

Multiple Mass Analysis: 39 mass(es) processed

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

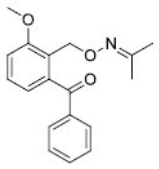
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

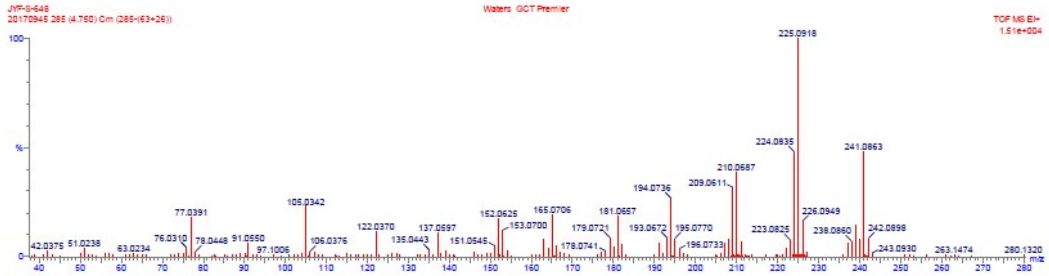
523 formula(e) evaluated with 41 results within limits (up to 50 closest results for each mass)

Elements Used:

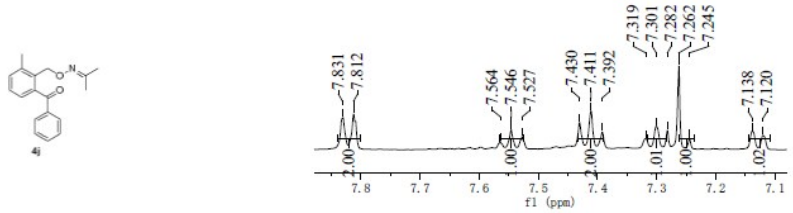
C: 0-18 H: 0-19 N: 0-1 O: 0-3

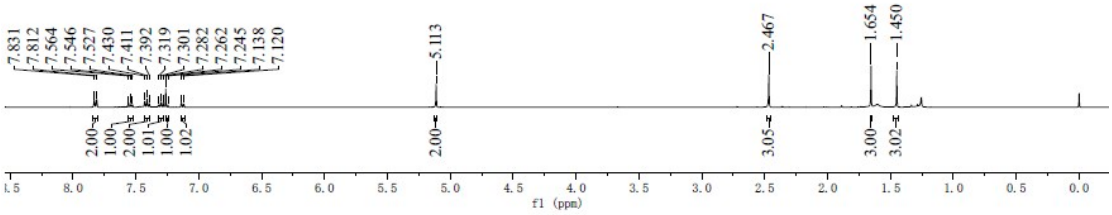


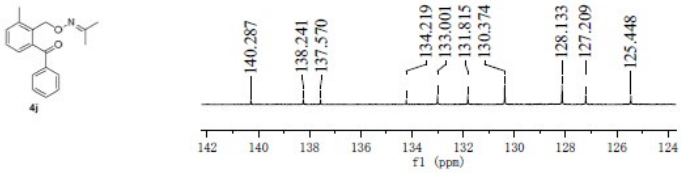
4i

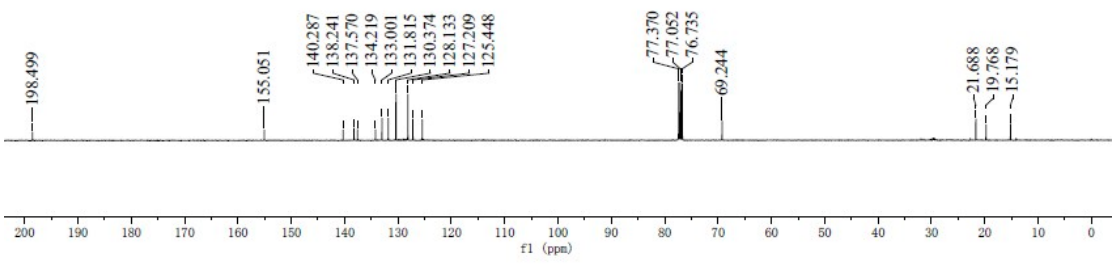



| Minimum: | 3.00 | | | | | | -1.5 |
|---|---|---|---|---|---|---|---|
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 241.0863 | 47.56 | 241.0865 | -0.2 | -0.8 | 9.5 | 0.3 | C15H13O3 |

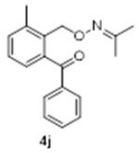

4j
7.831
7.812
7.564
7.546
7.527
7.430
7.411
7.392
7.319
7.301
7.282
7.262
7.245
7.138
7.120
2.00
1.00
2.00
1.01
1.00
1.02
f1 (ppm)


7.831
7.812
7.564
7.546
7.527
7.430
7.411
7.392
7.319
7.301
7.282
7.262
7.245
7.138
7.120
5.113
2.467
1.654
1.450
2.00
1.00
2.00
1.01
1.00
1.02
2.00
3.05
3.00
3.02
f1 (ppm)


4j
140.287
138.241
137.570
134.219
133.001
131.815
130.374
128.133
127.209
125.448
f1 (ppm)

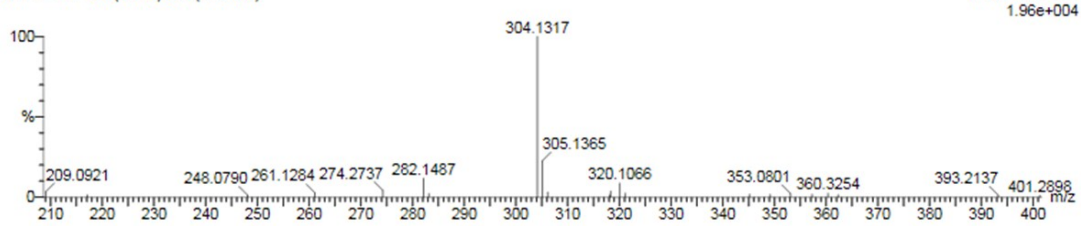

198.499
155.051
140.287
138.241
137.570
134.219
133.001
131.815
130.374
128.133
127.209
125.448
77.370
77.052
76.735
69.244
21.688
19.768
15.179
f1 (ppm)

**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

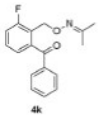


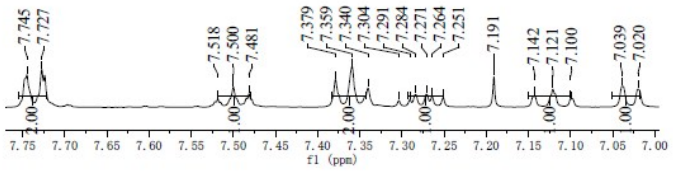

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-18 H: 0-40 N: 0-1 O: 0-2 Na: 0-1

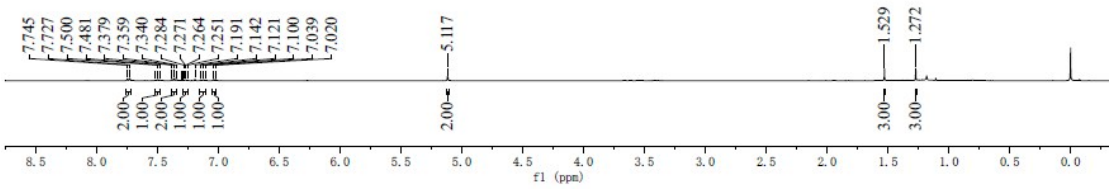
YF-JI ECUST institute of Fine Chem 07-Jul-2016 22:32:46
JYF-S-417 105 (0.740) Cm (101:109) 1: TOF MS ES+ 1.96e+004

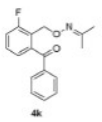


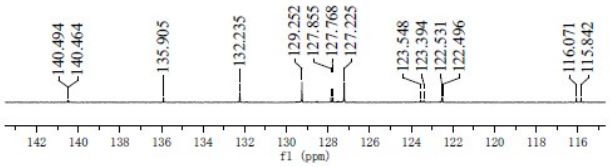

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 300.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1317 | 304.1313 | 0.4 | 1.3 | 9.5 | 15.5 | 0.0 | C18 H19 N O2 Na |

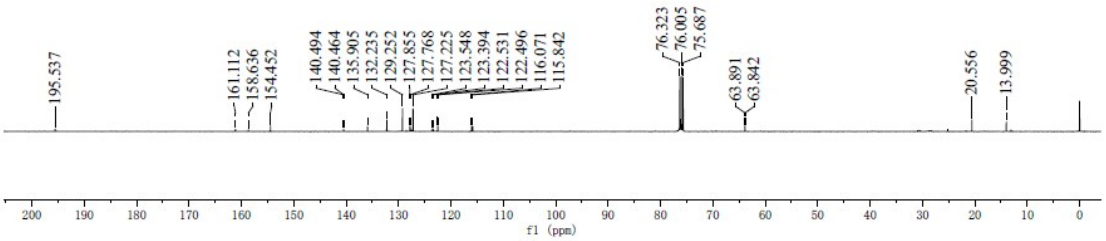


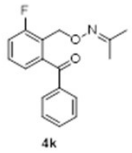





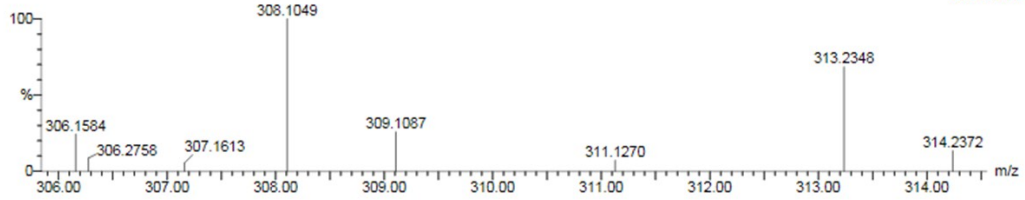




**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

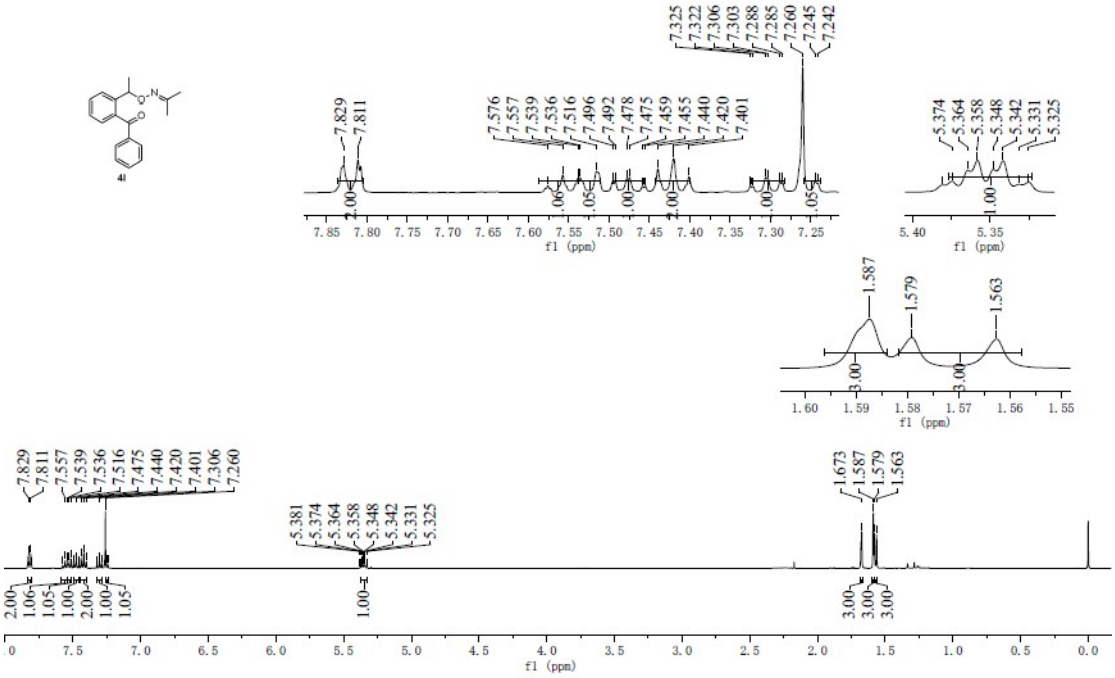


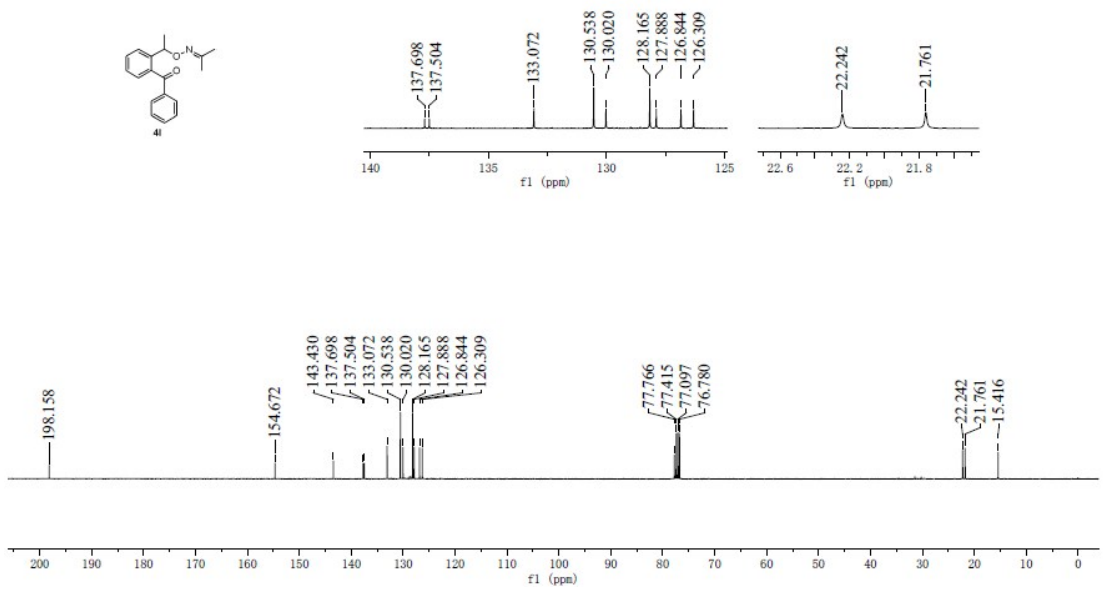

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-18 H: 0-20 N: 0-1 O: 0-2 Na: 0-1 F: 0-2

YF-JI ECUST institute of Fine Chem 06-Mar-2017 22:03:03
JYF-S-511 45 (0.640) Cm (40:46) 1: TOF MS ES+ 5.54e+002



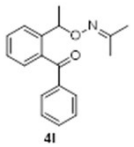

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 308.1049 | 308.1063 | -1.4 | -4.5 | 9.5 | 14.7 | 0.0 | C17 H16 N O2 Na F |


4l
7.829
7.811
7.576
7.557
7.539
7.536
7.516
7.496
7.492
7.478
7.475
7.459
7.455
7.440
7.420
7.401
7.325
7.322
7.306
7.303
7.288
7.285
7.260
7.245
7.242
5.374
5.364
5.358
5.348
5.342
5.331
5.325
1.587
1.579
1.563
f1 (ppm)


4l
137.698
137.504
133.072
130.538
130.020
128.165
127.888
126.844
126.309
22.242
21.761
f1 (ppm)


198.158
154.672
143.430
137.698
137.504
133.072
130.538
130.020
128.165
127.888
126.844
126.309
77.766
77.415
77.097
76.780
22.242
21.761
15.416
f1 (ppm)

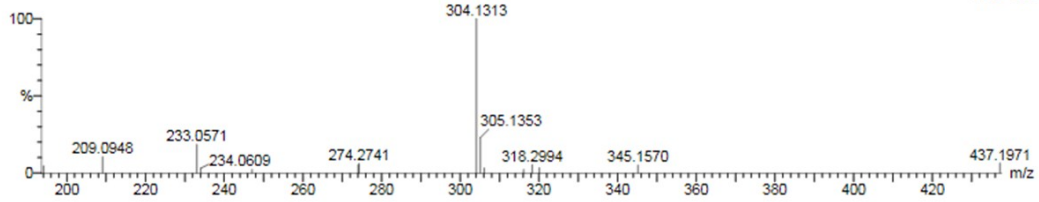
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



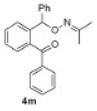

Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-40 N: 0-1 O: 0-5 Na: 0-1

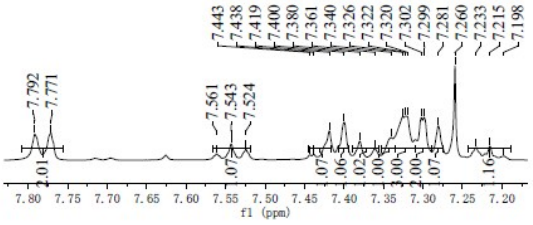
YF-JI ECUST institute of Fine Chem 05-Jan-2017 21:43:41

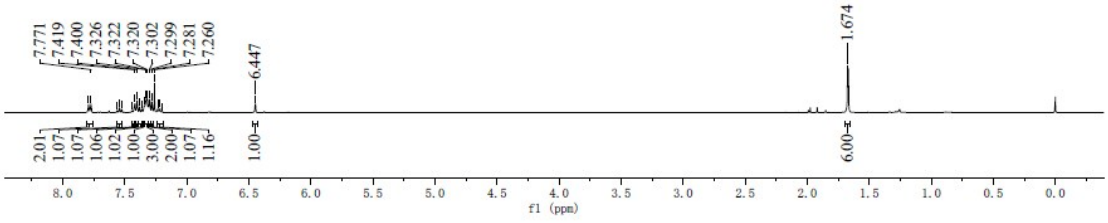
YF-S-520 46 (0.665) Cm (45:48) 1: TOF MS ES+ 7.96e+003

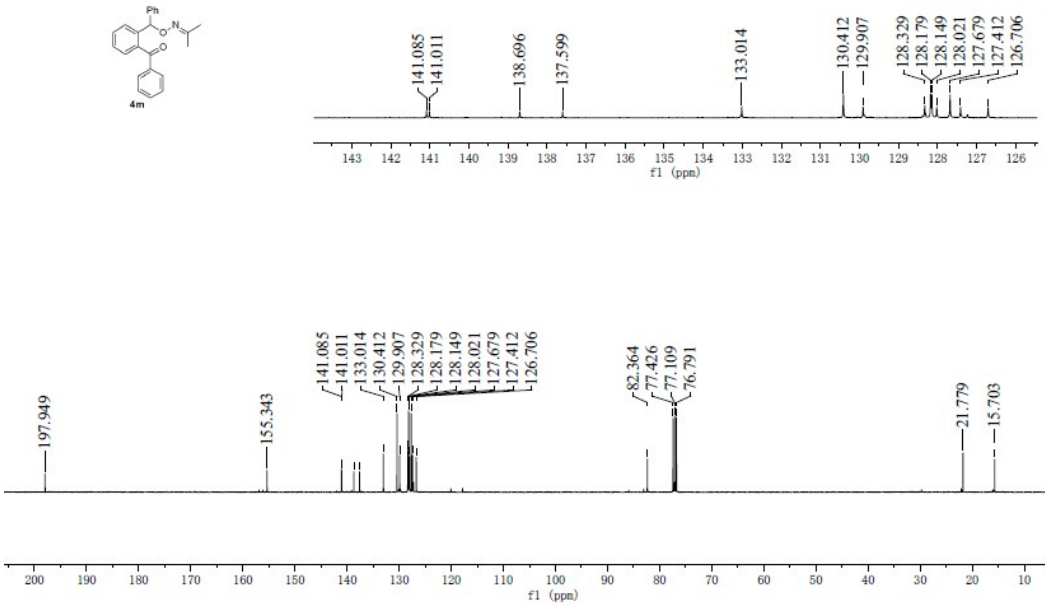



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 304.1313 | 304.1313 | 0.0 | 0.0 | 9.5 | 9.7 | 0.0 | C18 H19 N O2 Na |

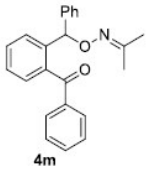





Elemental Composition Report




Multiple Mass Analysis: 25 mass(es) processed

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

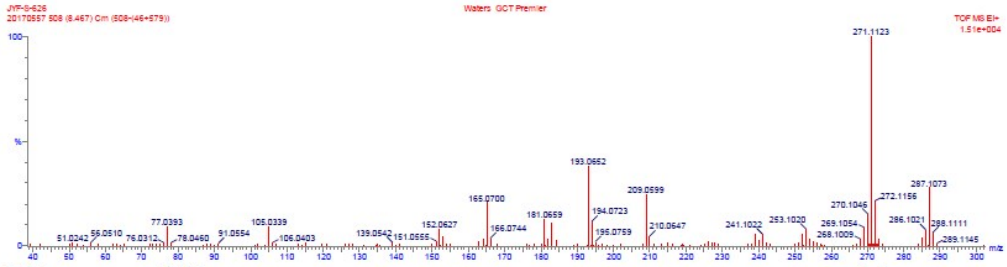
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

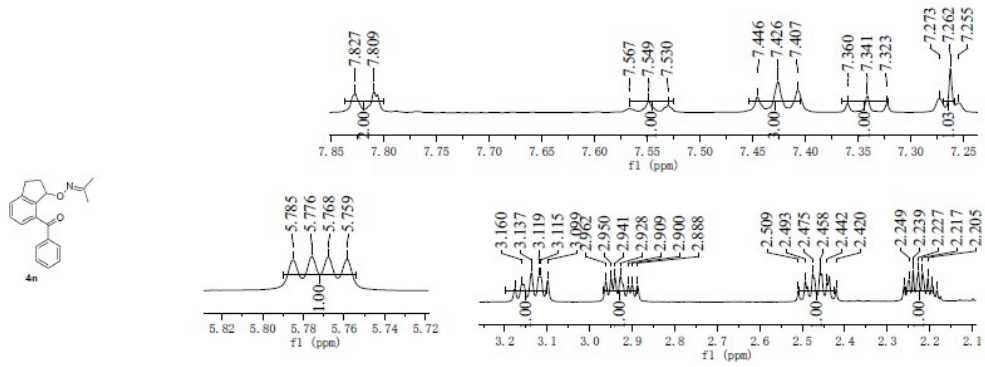
286 formula(e) evaluated with 24 results within limits (up to 50 closest results for each mass)

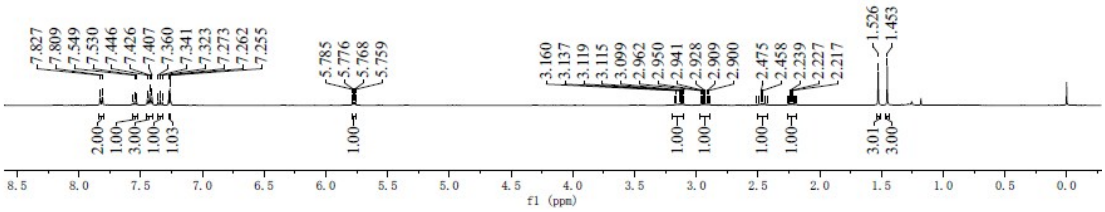
Elements Used:

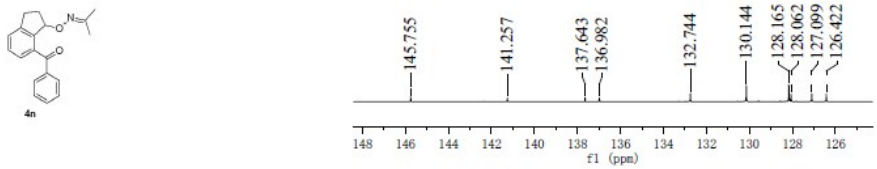
C: 0-23 H: 0-21 N: 0-1 O: 0-2

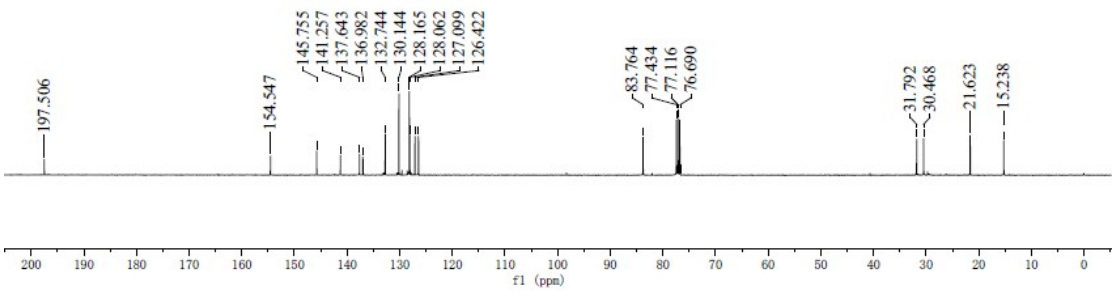



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | -1.5 | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 287.1073 | 27.27 | 287.1072 | 0.1 | 0.3 | 13.5 | 2.6 | C20H15O2 |

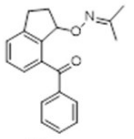

4n
7.827
7.809
7.567
7.549
7.530
7.446
7.426
7.407
7.360
7.341
7.323
7.273
7.262
7.255
5.785
5.776
5.768
5.759
3.160
3.137
3.119
3.115
3.099
2.962
2.950
2.941
2.928
2.909
2.900
2.888
2.509
2.493
2.475
2.458
2.442
2.420
2.249
2.239
2.227
2.217
2.205
f1 (ppm)


7.827
7.809
7.549
7.530
7.446
7.426
7.407
7.360
7.341
7.323
7.273
7.262
7.255
5.785
5.776
5.768
5.759
3.160
3.137
3.119
3.115
3.099
2.962
2.950
2.941
2.928
2.909
2.900
2.475
2.458
2.239
2.227
2.217
1.526
1.453
f1 (ppm)


4n
145.755
141.257
137.643
136.982
132.744
130.144
128.165
128.062
127.099
126.422
f1 (ppm)


197.506
154.547
145.755
141.257
137.643
136.982
132.744
130.144
128.165
128.062
127.099
126.422
83.764
77.434
77.116
76.690
31.792
30.468
21.623
15.238
f1 (ppm)

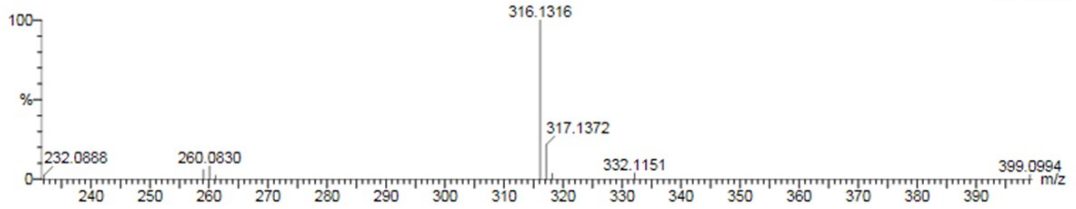
**Single Mass Analysis**
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



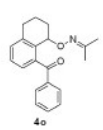

Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 3 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-40 N: 0-1 O: 0-5 Na: 0-1

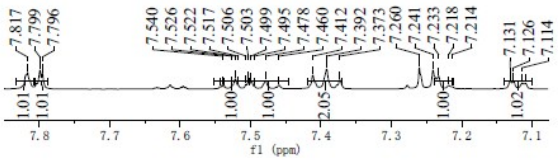
YF-JI ECUST institute of Fine Chem 05-Jan-2017 21:40:05

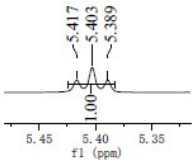
YF-S-519 25 (0.400) Cm (19:27) 1: TOF MS ES+ 1.79e+004

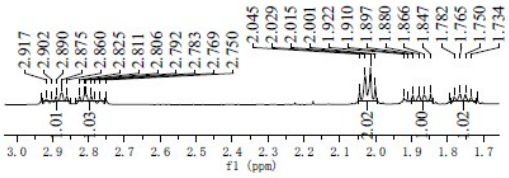


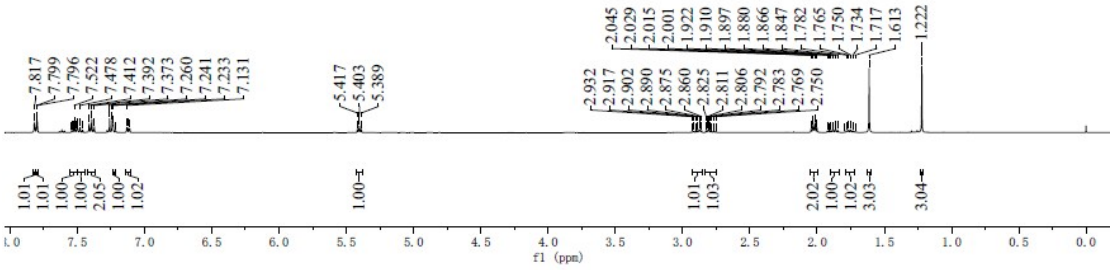

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | | |
| Maximum: | | 30.0 | 50.0 | 100.0 | | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | i-FIT (Norm) | Formula |
| 316.1316 | 316.1313 | 0.3 | 0.9 | 10.5 | 15.5 | 0.0 | C19 H19 N O2 Na |

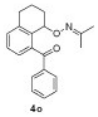


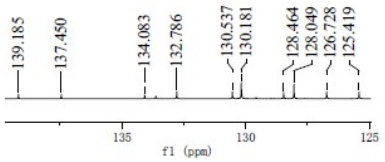



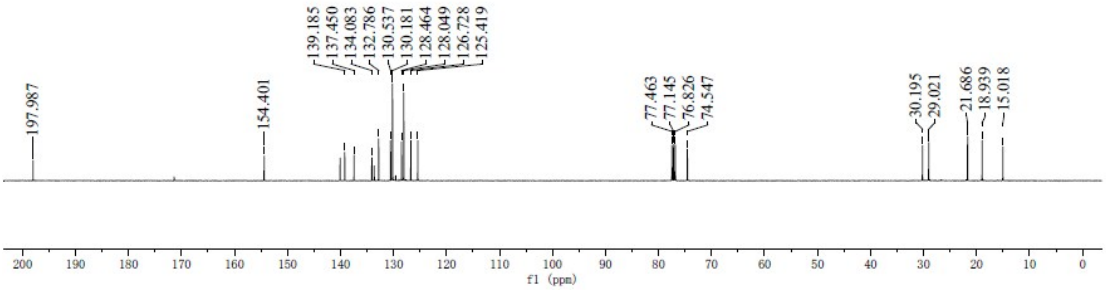



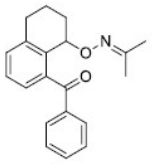






Elemental Composition Report




Multiple Mass Analysis: 17 mass(es) processed

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

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

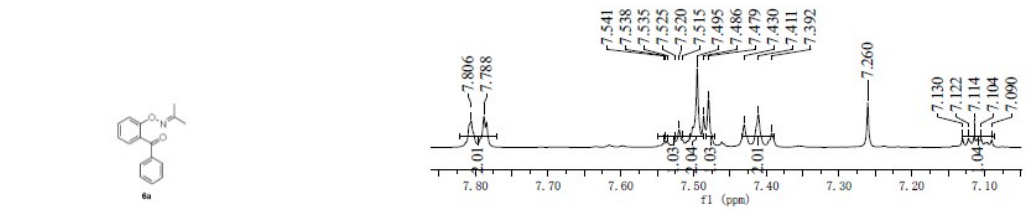
195 formula(e) evaluated with 17 results within limits (up to 50 closest results for each mass)

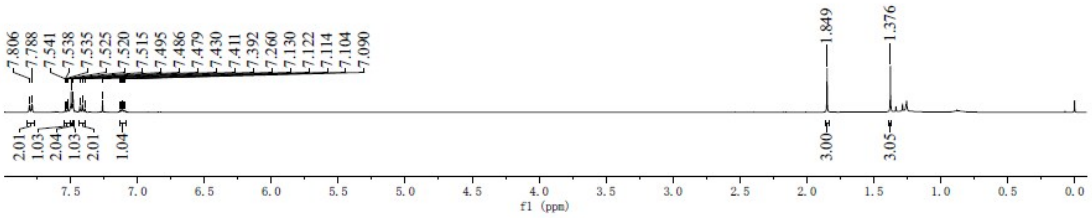
Elements Used:

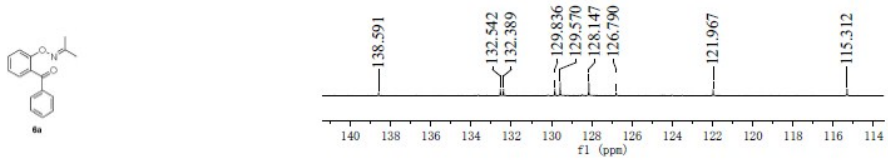
C: 0-20 H: 0-21 N: 0-1 O: 0-2

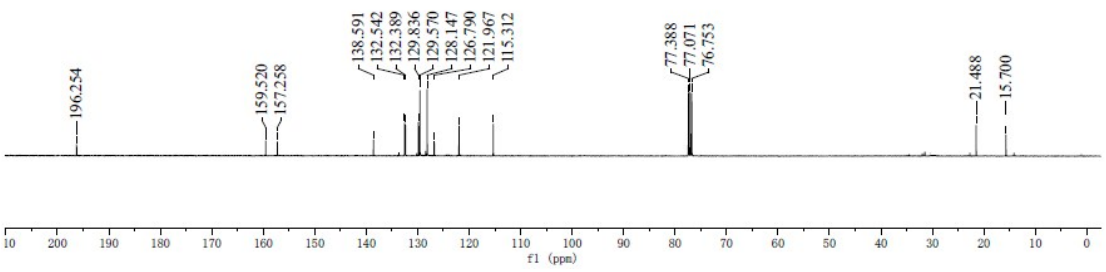

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 251.1073 | 9.88 | 251.1072 | 0.1 | 0.4 | 10.5 | 4.1 | C17 H15 O2 |

## 4.3 Copies of the spectra for Tables 4

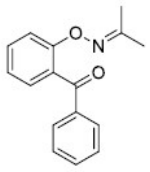


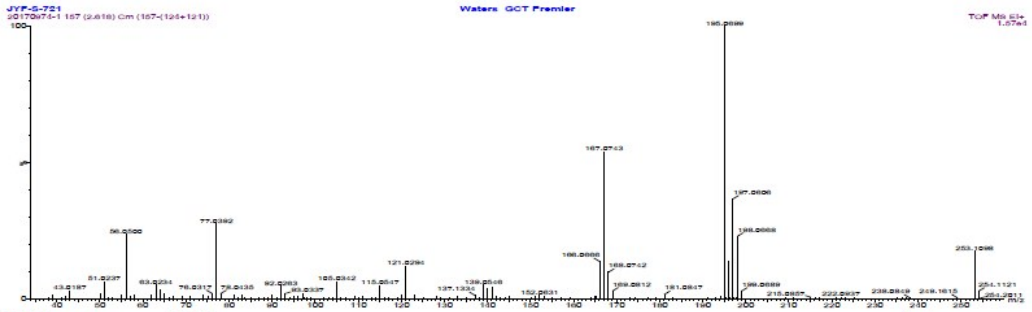



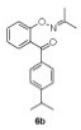
Elemental Composition Report
Multiple Mass Analysis: 24 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
195 formula(e) evaluated with 19 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-15 N: 0-1 O: 0-2



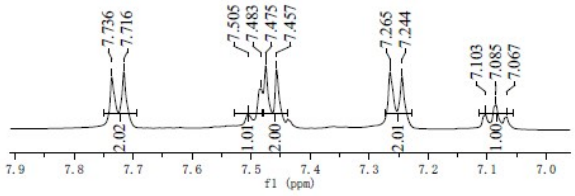
6a

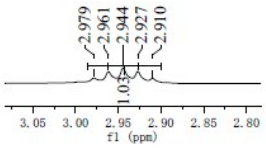


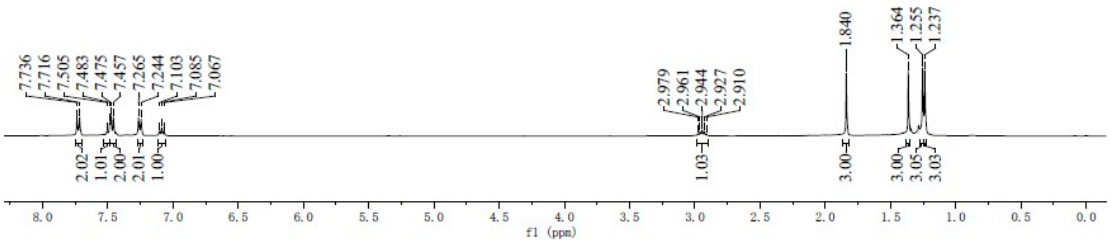
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 253.1098 | 17.66 | 253.1103 | -0.5 | -2.0 | 10.0 | 4.4 | C16H15NO2 |

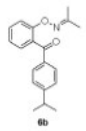


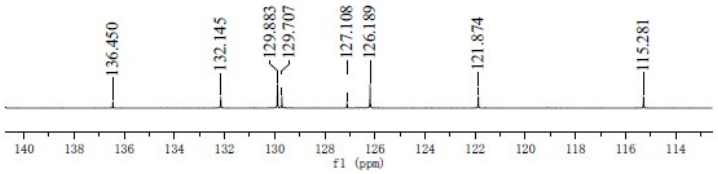
6b

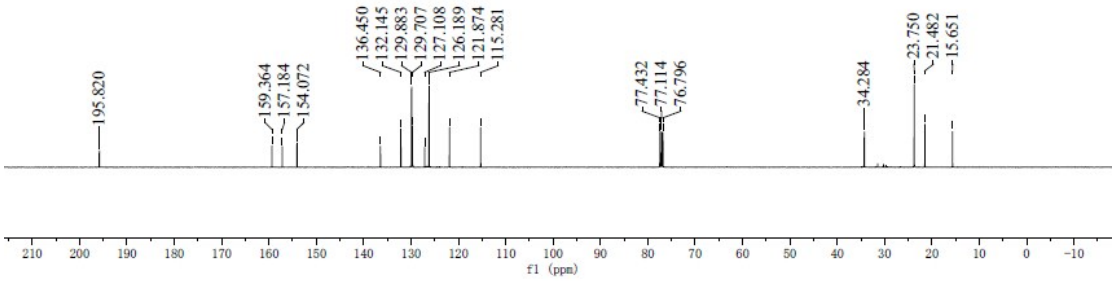





Elemental Composition Report

Multiple Mass Analysis: 45 mass(es) processed

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

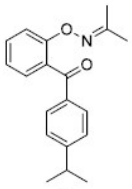
Element prediction: Off

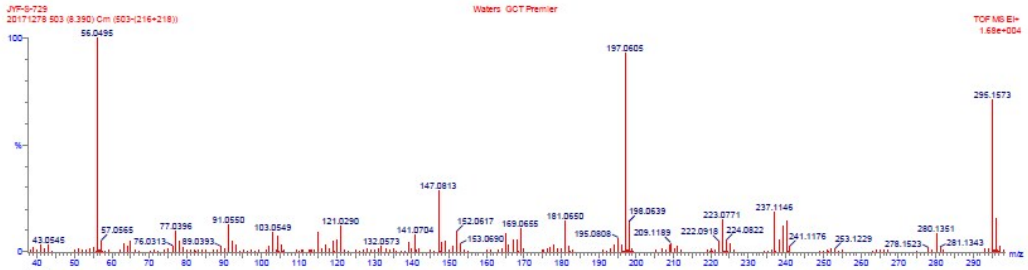
Monoisotopic Mass, Odd and Even Electron Ions

478 formula(e) evaluated with 42 results within limits (up to 50 closest results for each mass)

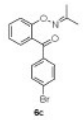
Elements Used:

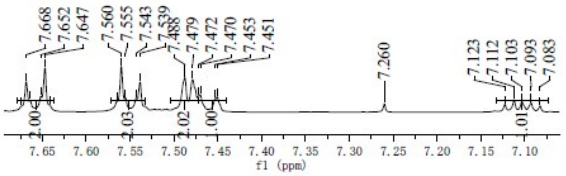
C: 0-19 H: 0-21 N: 0-1 O: 0-2

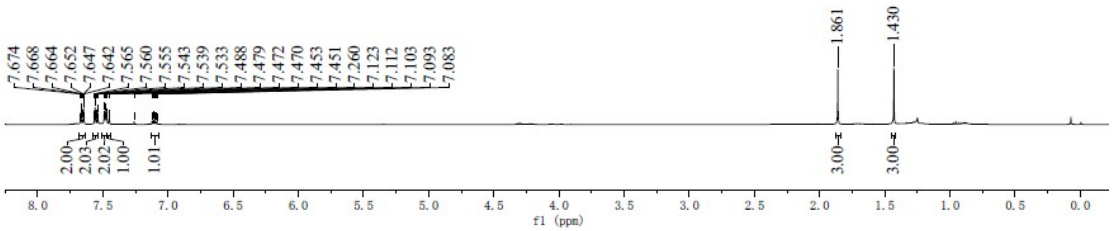


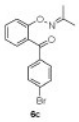



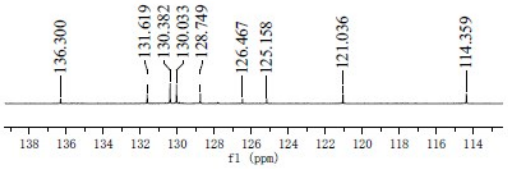

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 295.1573 | 70.72 | 295.1572 | 0.1 | 0.3 | 10.0 | 2.6 | C19H21NO2 |

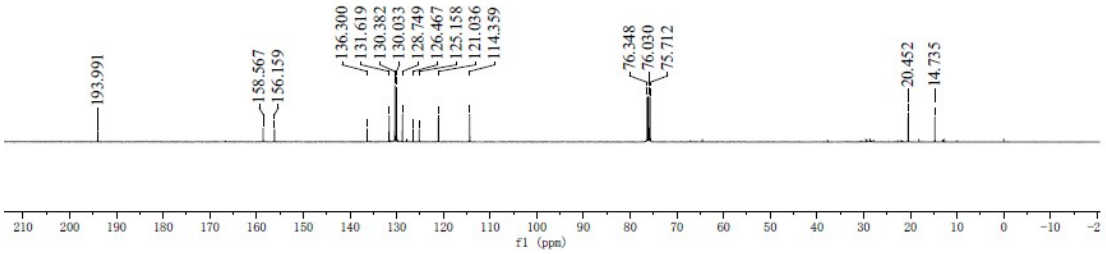



7.668
7.652
7.647
7.560
7.555
7.543
7.539
7.488
7.479
7.472
7.470
7.453
7.451
7.260
7.123
7.112
7.103
7.093
7.083
2.00
2.03
2.02
1.00
1.01
f1 (ppm)


7.674
7.668
7.664
7.652
7.647
7.642
7.565
7.560
7.555
7.543
7.539
7.533
7.488
7.479
7.472
7.470
7.453
7.451
7.260
7.123
7.112
7.103
7.093
7.083
1.861
1.430
2.00
2.03
2.02
1.00
1.01
3.00
3.00
f1 (ppm)




136.300
131.619
130.382
130.033
128.749
126.467
125.158
121.036
114.359
f1 (ppm)


193.991
158.567
156.159
136.300
131.619
130.382
130.033
128.749
126.467
125.158
121.036
114.359
76.348
76.030
75.712
20.452
14.735
f1 (ppm)

Elemental Composition Report

Multiple Mass Analysis: 44 mass(es) processed

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

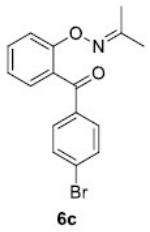
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

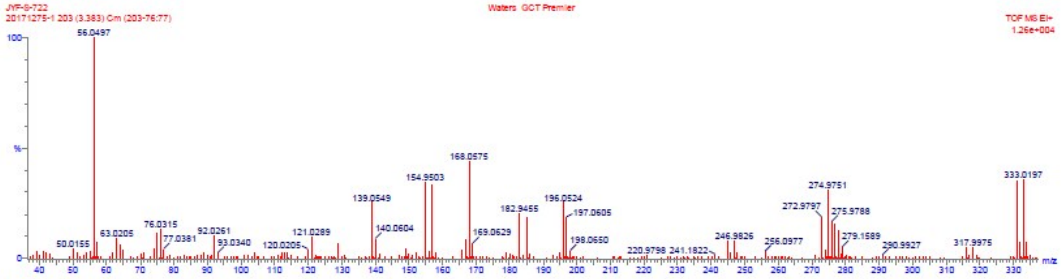
878 formula(e) evaluated with 49 results within limits (up to 50 closest results for each mass)

Elements Used:

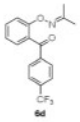
C: 0-16 H: 0-14 N: 0-1 O: 0-2 79Br: 0-1 81Br: 0-1

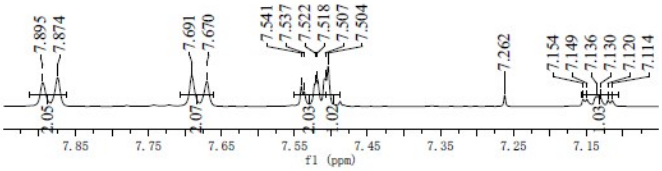


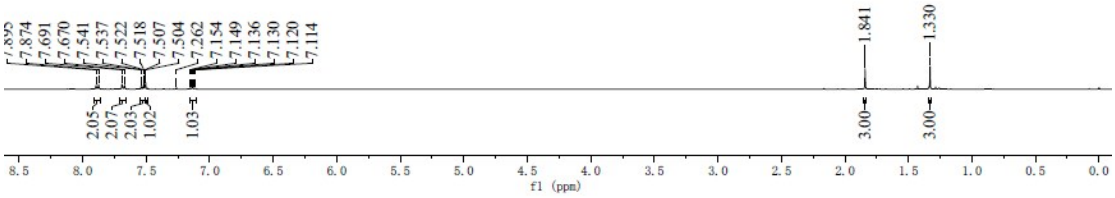

**6c**

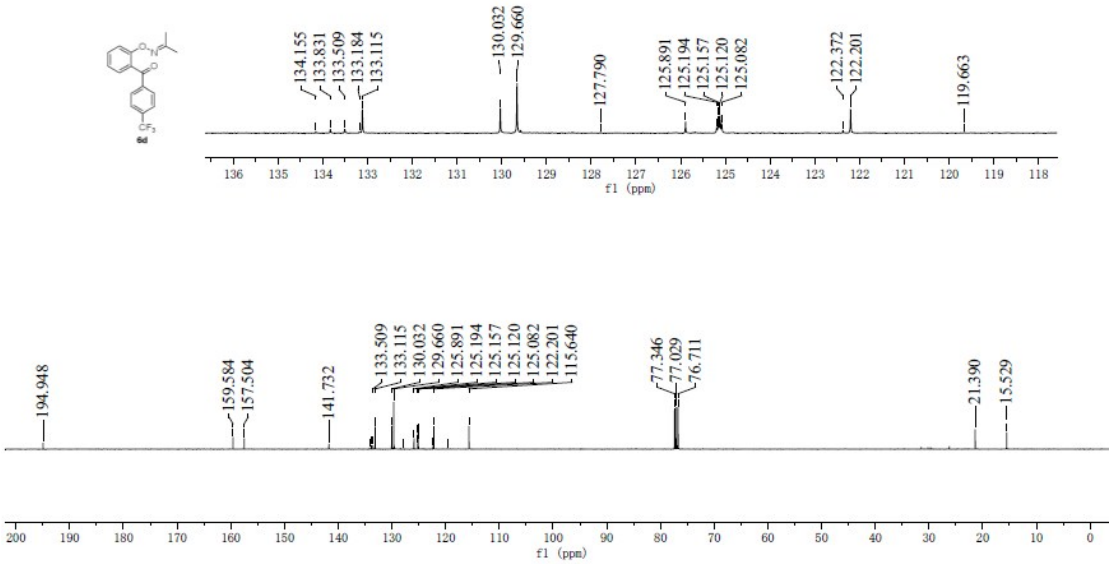



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 331.0211 | 34.60 | 331.0208 | 0.3 | 0.9 | 10.0 | 3.2 | C16H14NO2 79Br |
| 333.0197 | 35.08 | 333.0187 | 1.0 | 3.0 | 10.0 | 4.8 | C16H14NO2 81Br |






Elemental Composition Report

Multiple Mass Analysis: 38 mass(es) processed

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

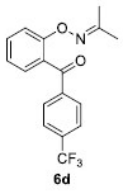
Element prediction: Off

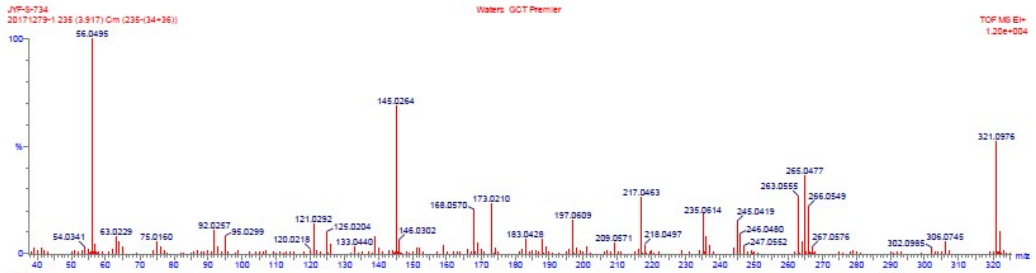
Monoisotopic Mass, Odd and Even Electron Ions

1011 formula(e) evaluated with 78 results within limits (up to 50 closest results for each mass)

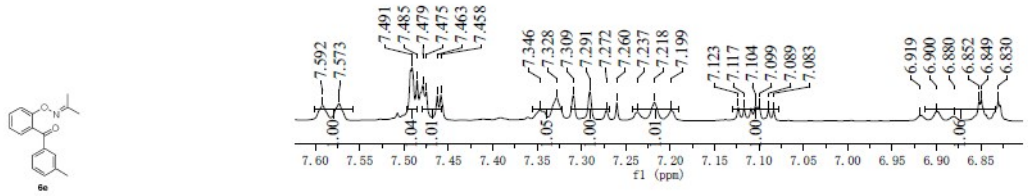
Elements Used:

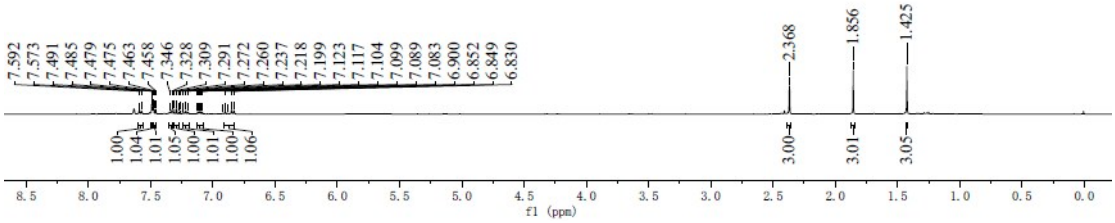
C: 0-17 H: 0-14 N: 0-1 O: 0-2 F: 0-3

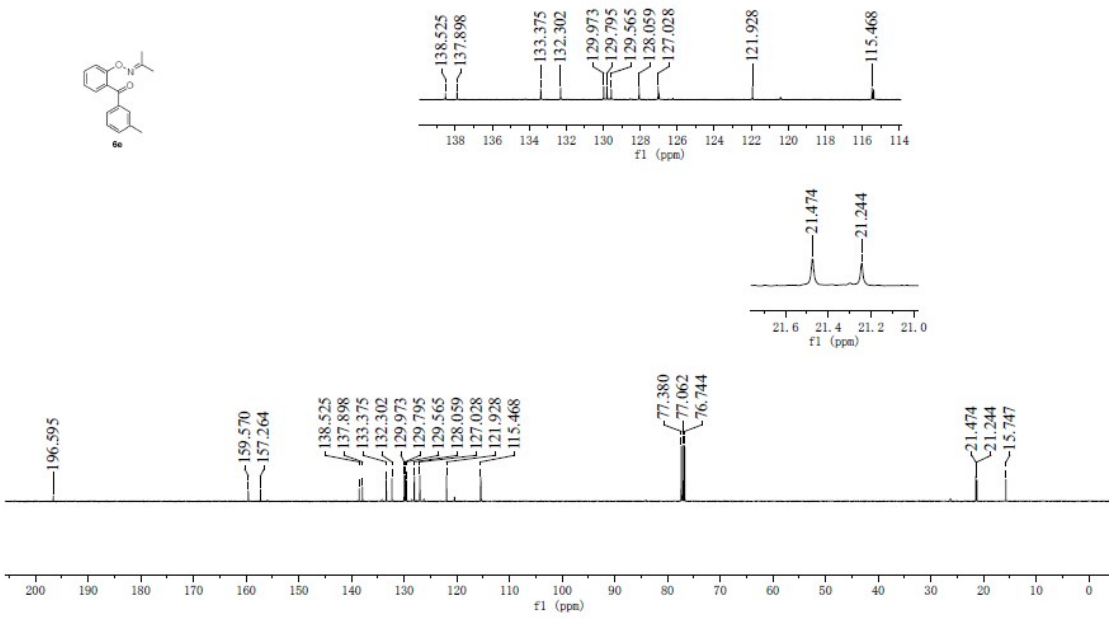



| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 321.0976 | 51.58 | 321.0977 | -0.1 | -0.3 | 10.0 | 0.0 | C17H14NO2F3 |


7.592
7.573
7.491
7.485
7.479
7.475
7.463
7.458
7.346
7.328
7.309
7.291
7.272
7.260
7.237
7.218
7.199
7.123
7.117
7.104
7.099
7.089
7.083
6.919
6.900
6.880
6.852
6.849
6.830
1.00
1.04
1.01
1.05
1.00
1.01
1.00
1.06
f1 (ppm)


7.592
7.573
7.491
7.485
7.479
7.475
7.463
7.458
7.346
7.328
7.309
7.291
7.272
7.260
7.237
7.218
7.199
7.123
7.117
7.104
7.099
7.089
7.083
6.900
6.852
6.849
6.830
2.368
1.856
1.425
3.00
3.01
3.05
f1 (ppm)


138.525
137.898
133.375
132.302
129.973
129.795
129.565
128.059
127.028
121.928
115.468
21.474
21.244
77.380
77.062
76.744
196.595
159.570
157.264
15.747
f1 (ppm)

Elemental Composition Report

Multiple Mass Analysis: 29 mass(es) processed

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

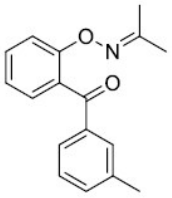
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

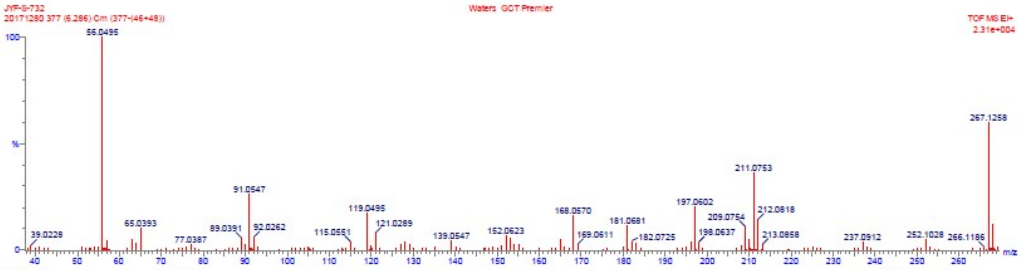
256 formula(e) evaluated with 27 results within limits (up to 50 closest results for each mass)

Elements Used:

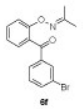
C: 0-17 H: 0-17 N: 0-1 O: 0-2



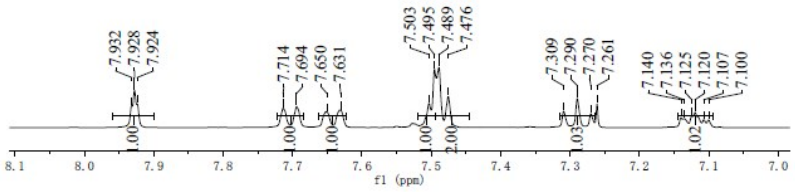
**6e**

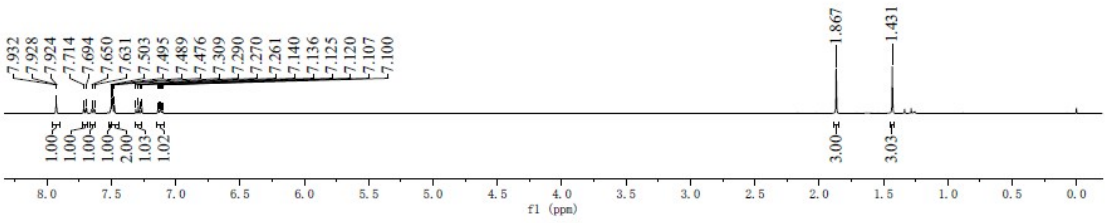


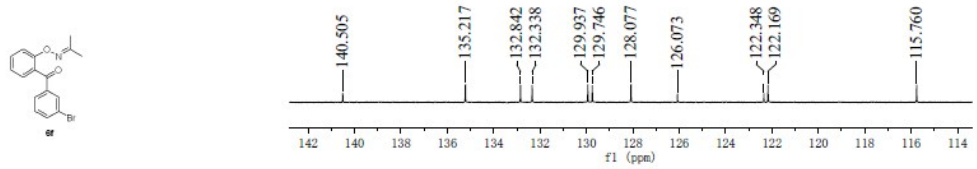

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | 3.00 | | | | | -1.5 |
| Maximum: | | 100.00 | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 267.1258 | 59.53 | 267.1259 | -0.1 | -0.4 | 10.0 | 0.5 | C17H17NO2 |

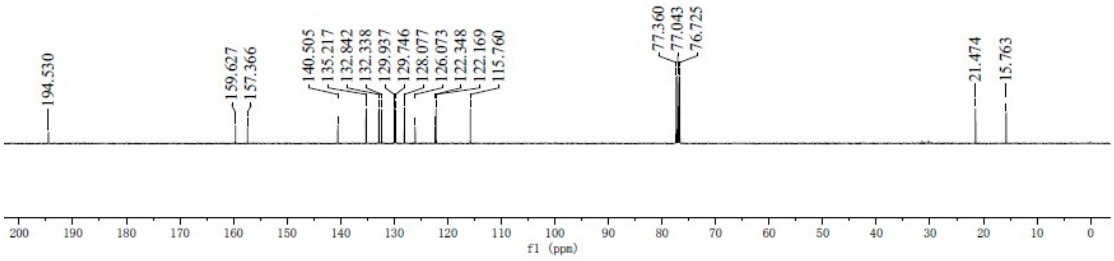


**6f**






Elemental Composition Report

Multiple Mass Analysis: 26 mass(es) processed

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

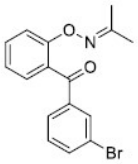
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

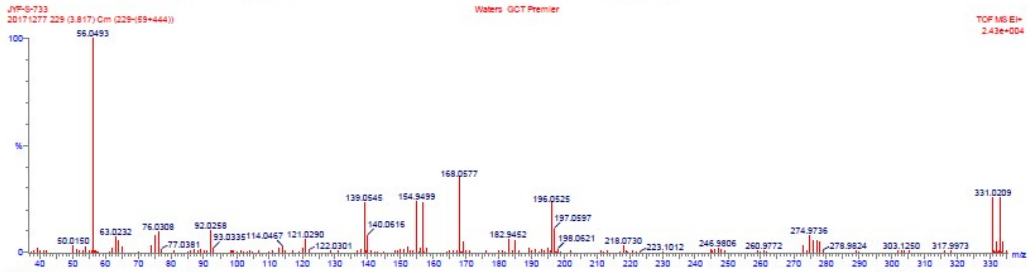
532 formula(e) evaluated with 30 results within limits (up to 50 closest results for each mass)

Elements Used:

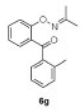
C: 0-16 H: 0-14 N: 0-1 O: 0-2 79Br: 0-1 81Br: 0-1

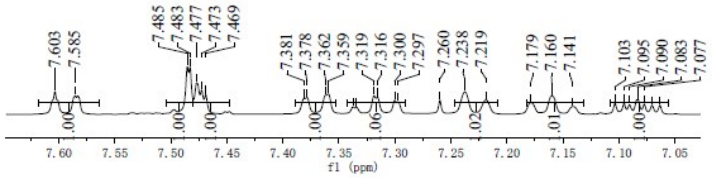


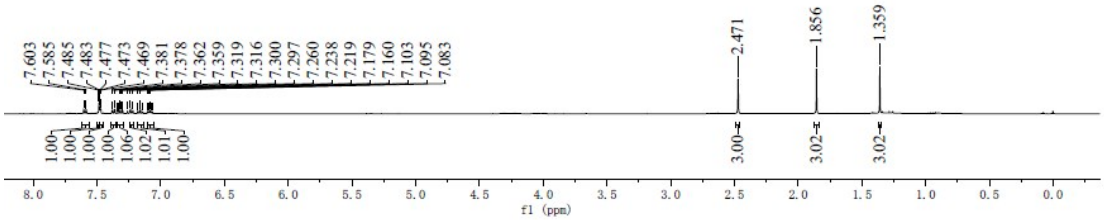

**6f**

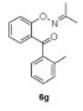


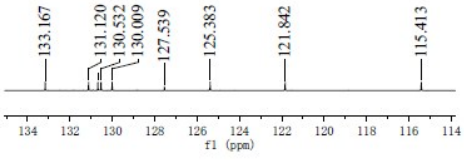

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 331.0209 | 25.30 | 331.0208 | 0.1 | 0.3 | 10.0 | 0.1 | C16H14NO2 79Br |
| 333.0195 | 25.27 | 333.0187 | 0.8 | 2.4 | 10.0 | 0.4 | C16H14NO2 81Br |

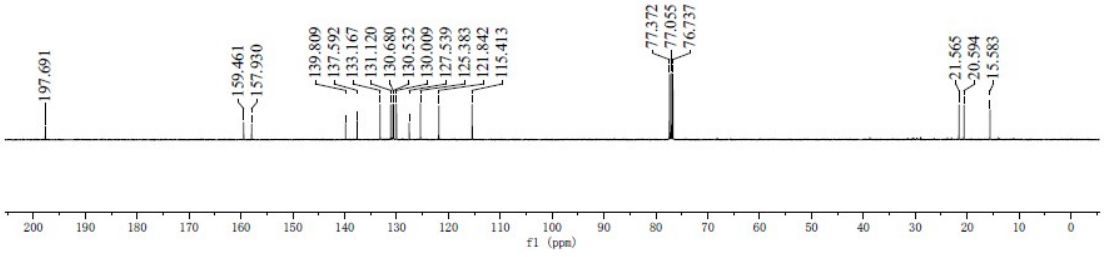

6g


7.603
7.585
7.485
7.483
7.477
7.473
7.469
7.381
7.378
7.362
7.359
7.319
7.316
7.300
7.297
7.260
7.238
7.219
7.179
7.160
7.141
7.103
7.095
7.090
7.083
7.077
f1 (ppm)


2.471
1.856
1.359
f1 (ppm)


6g


133.167
131.120
130.532
130.009
127.539
125.383
121.842
115.413
f1 (ppm)


197.691
159.461
157.930
139.809
137.592
133.167
131.120
130.680
130.532
130.009
127.539
125.383
121.842
115.413
77.372
77.055
76.737
21.565
20.594
15.583
f1 (ppm)

Elemental Composition Report

Multiple Mass Analysis: 32 mass(es) processed

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

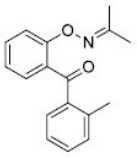
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

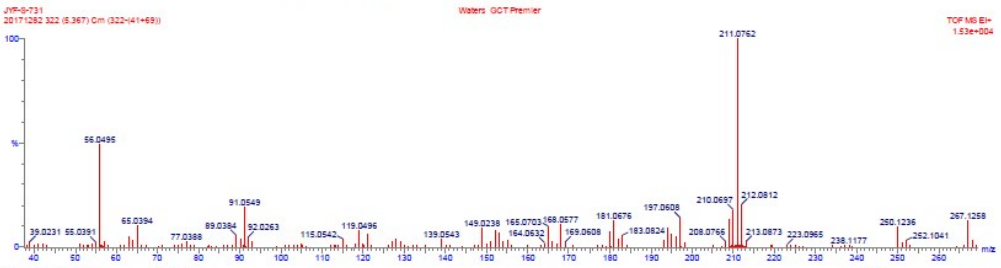
295 formula(e) evaluated with 30 results within limits (up to 50 closest results for each mass)

Elements Used:

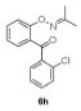
C: 0-17 H: 0-17 N: 0-1 O: 0-2



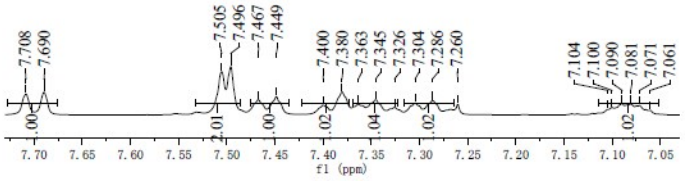
**6g**

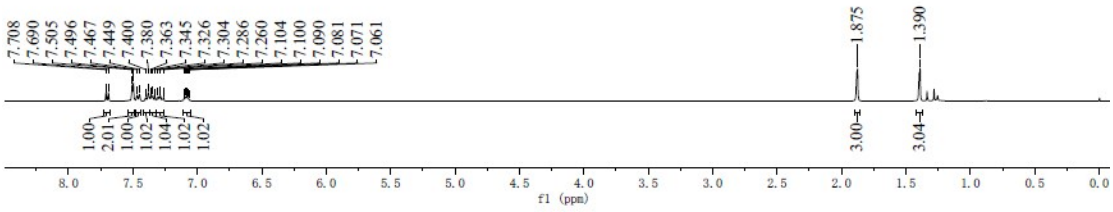


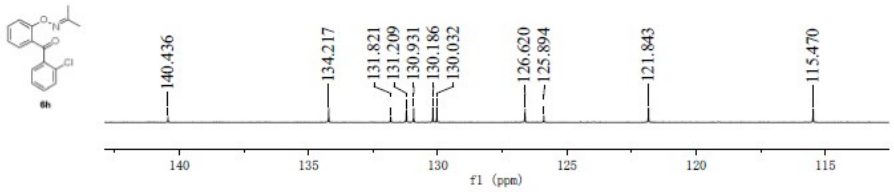

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 267.1258 | 12.61 | 267.1259 | -0.1 | -0.4 | 10.0 | 1.4 | C17H17NO2 |

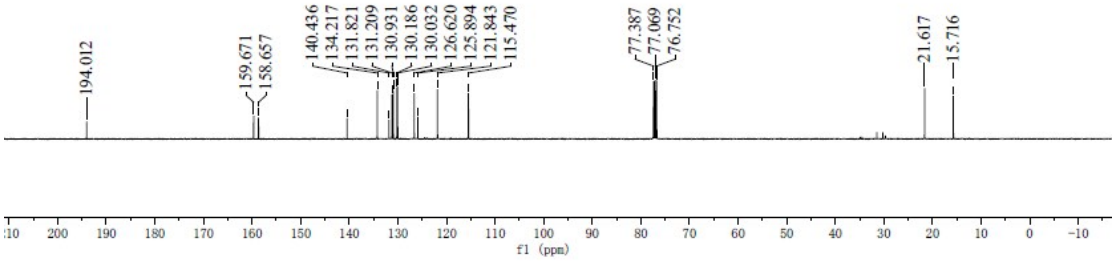


**6h**

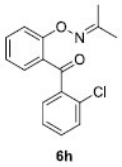





Elemental Composition Report




Multiple Mass Analysis: 32 mass(es) processed

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

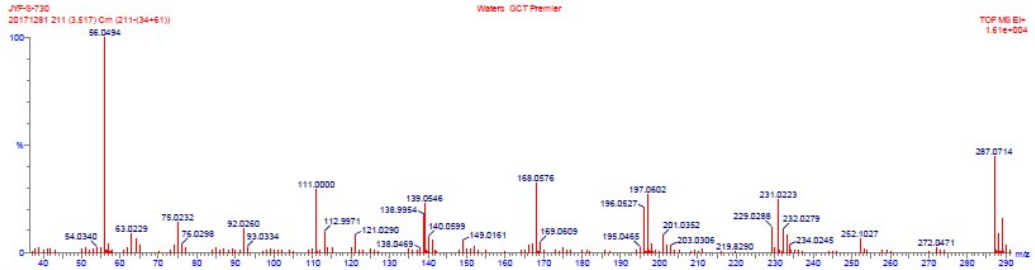
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

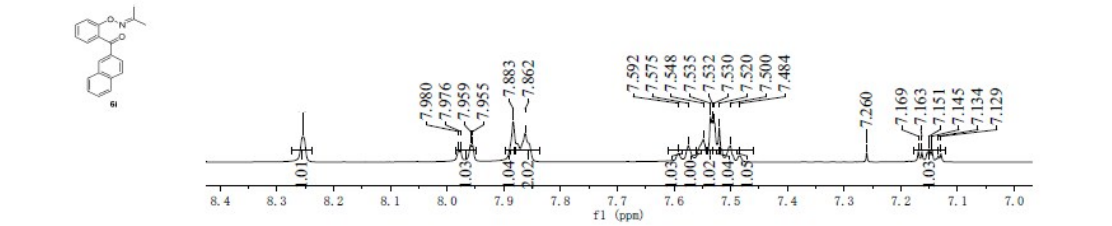
845 formula(e) evaluated with 62 results within limits (up to 50 closest results for each mass)

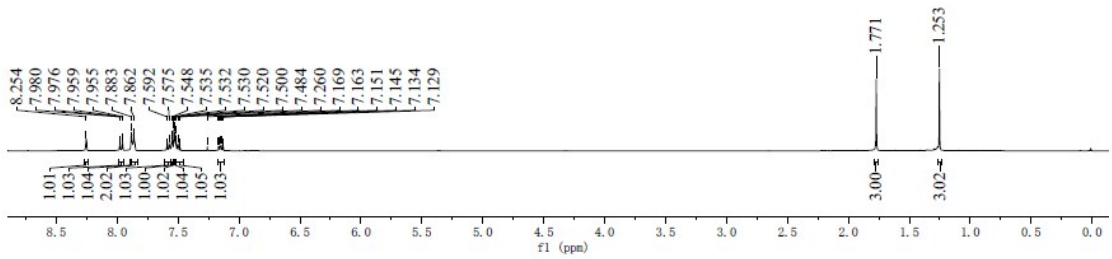
Elements Used:

C: 0-16 H: 0-14 N: 0-1 O: 0-2 35Cl: 0-1 37Cl: 0-1

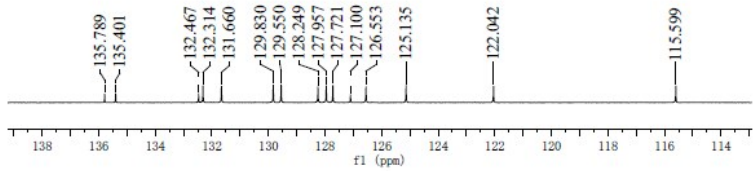


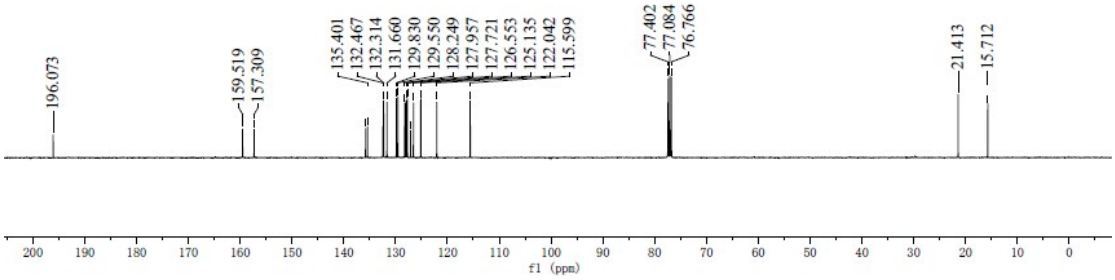

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 287.0714 | 44.63 | 287.0713 | 0.1 | 0.3 | 10.0 | 1.6 | C16H14NO2 35Cl |


6i
7.980
7.976
7.959
7.955
7.883
7.862
7.592
7.575
7.548
7.535
7.532
7.530
7.520
7.500
7.484
7.260
7.169
7.163
7.151
7.145
7.134
7.129
f1 (ppm)


8.254
7.980
7.976
7.959
7.955
7.883
7.862
7.592
7.575
7.548
7.535
7.532
7.530
7.520
7.500
7.484
7.260
7.169
7.163
7.151
7.145
7.134
7.129
1.771
1.253
f1 (ppm)


6k


135.789
135.401
132.467
132.314
131.660
129.830
129.550
128.249
127.957
127.721
127.100
126.553
125.135
122.042
115.599
f1 (ppm)


196.073
159.519
157.309
135.401
132.467
132.314
131.660
129.830
129.550
128.249
127.957
127.721
126.553
125.135
122.042
115.599
77.402
77.084
76.766
21.413
15.712
f1 (ppm)

Elemental Composition Report

Multiple Mass Analysis: 28 mass(es) processed

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

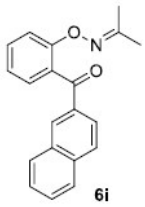
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

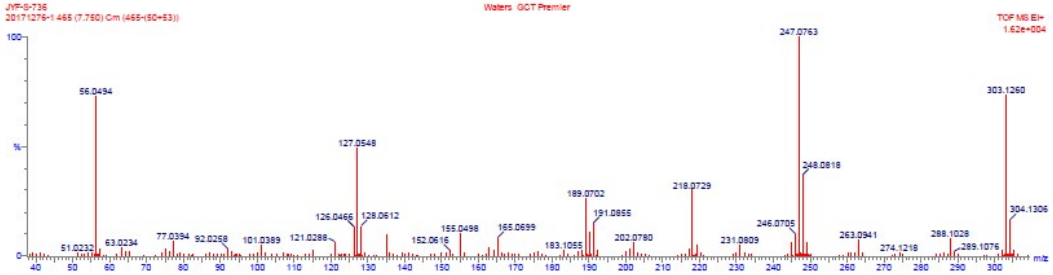
245 formula(e) evaluated with 27 results within limits (up to 50 closest results for each mass)

Elements Used:

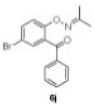
C: 0-20 H: 0-17 N: 0-1 O: 0-2



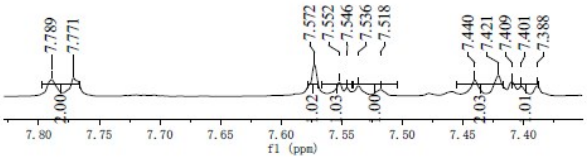

6i

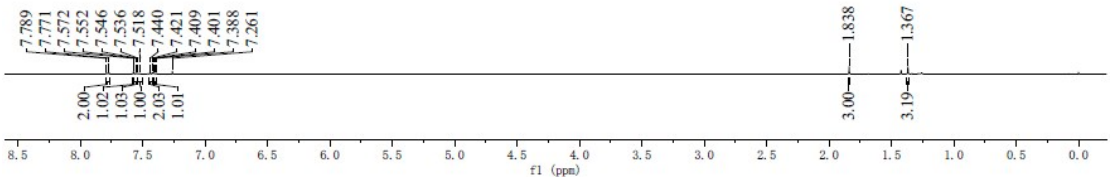


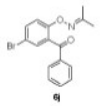

| Minimum: | 3.00 | | | | | -1.5 | |
|---|---|---|---|---|---|---|---|
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 303.1260 | 73.34 | 303.1259 | 0.1 | 0.3 | 13.0 | 4.1 | C20H17NO2 |

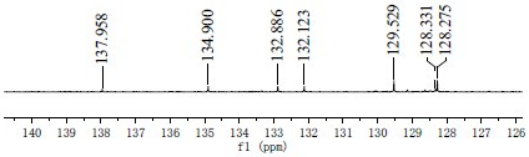


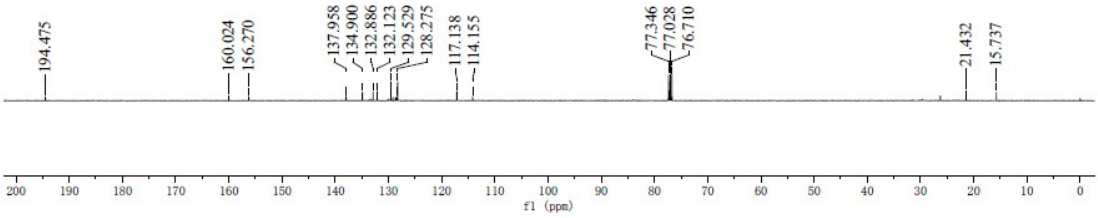

6i



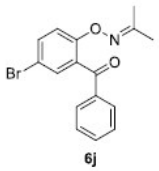







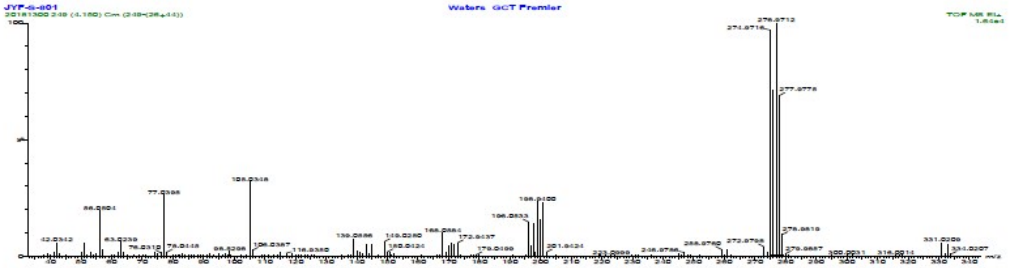




Elemental Composition Report

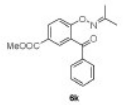


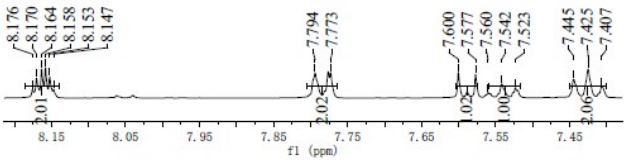

6j

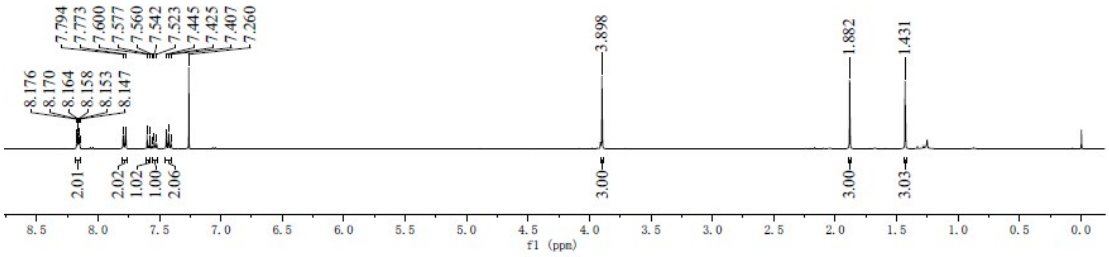
Multiple Mass Analysis: 29 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
665 formula(e) evaluated with 42 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-14 N: 0-1 O: 0-2 79Br: 0-1 81Br: 0-1

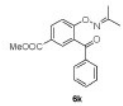


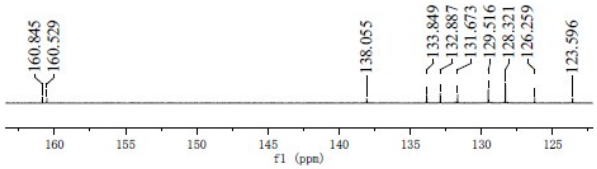

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | 5.0 | | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 331.0209 | 5.83 | 331.0208 | 0.1 | 0.3 | 10.0 | 2.9 | C16H14NO2 79Br |
| 333.0194 | 5.17 | 333.0187 | 0.7 | 2.1 | 10.0 | 2773107.3 | C16H14NO2 81Br |

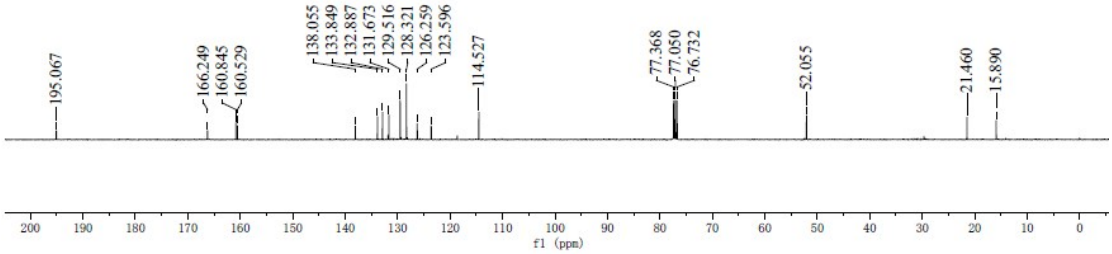

MeOOC
O
N
O
6k


8.176
8.170
8.164
8.158
8.153
8.147
7.794
7.773
7.600
7.577
7.560
7.542
7.523
7.445
7.425
7.407
2.01
2.02
1.02
1.00
2.06
8.15
8.05
7.95
7.85
7.75
7.65
7.55
7.45
f1 (ppm)


7.794
7.773
7.600
7.577
7.560
7.542
7.523
7.445
7.425
7.407
7.260
8.176
8.170
8.164
8.158
8.153
8.147
3.898
1.882
1.431
2.01
2.02
1.02
1.00
2.06
3.00
3.00
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


MeOOC
O
N
O
6k


160.845
160.529
138.055
133.849
132.887
131.673
129.516
128.321
126.259
123.596
160
155
150
145
140
135
130
125
f1 (ppm)


195.067
166.249
160.845
160.529
138.055
133.849
132.887
131.673
129.516
128.321
126.259
123.596
114.527
77.368
77.050
76.732
52.055
21.460
15.890
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Elemental Composition Report

Multiple Mass Analysis: 25 mass(es) processed

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

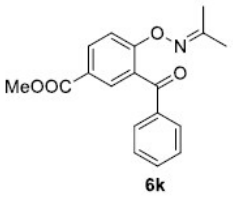
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

347 formula(e) evaluated with 34 results within limits (up to 50 closest results for each mass)

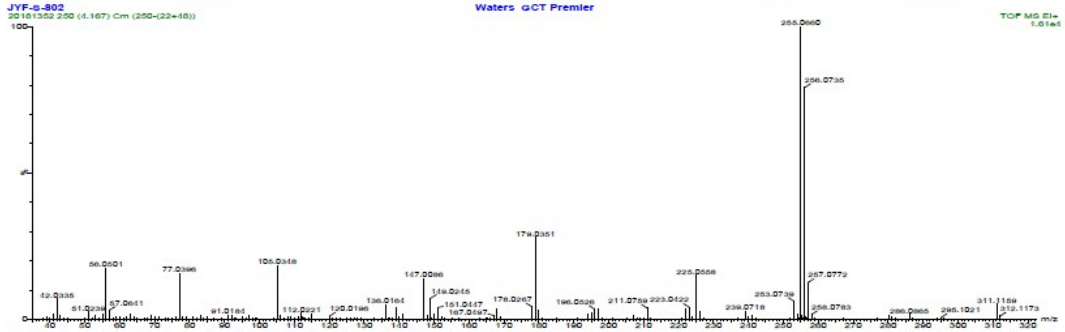
Elements Used:

C: 0-18 H: 0-17 N: 0-1 O: 0-4

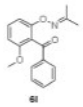


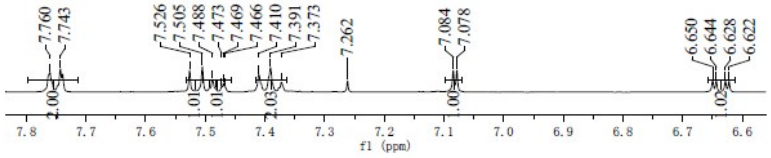
6k

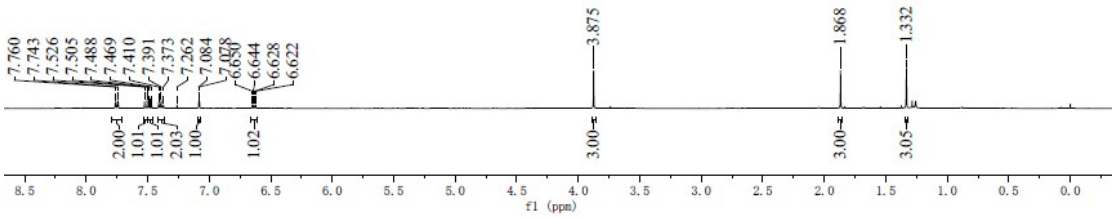
| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | -1.5 |
| Maximum: | 100.00 | | 5.0 | 10.0 | | 100.0 |

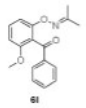


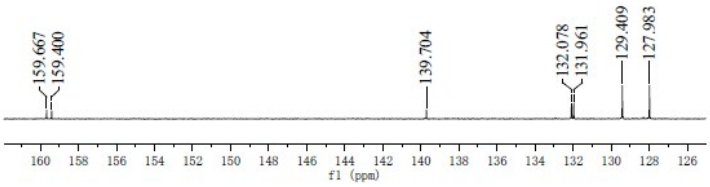

| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
|---|---|---|---|---|---|---|---|
| 311.1159 | 5.16 | 311.1158 | 0.1 | 0.3 | 11.0 | 0.2 | C18H17NO4 |

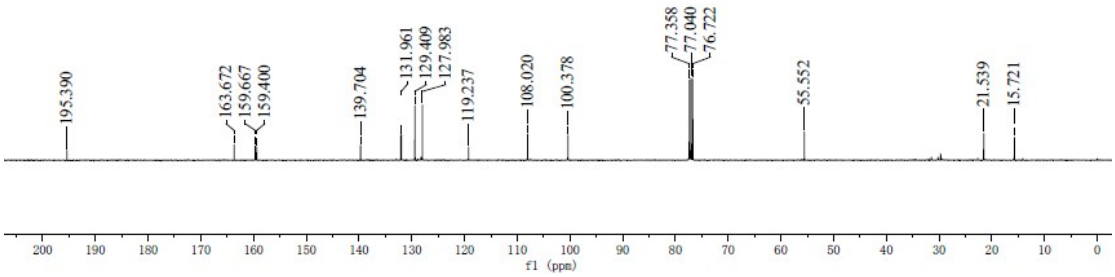

6l



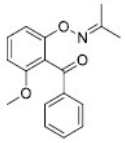







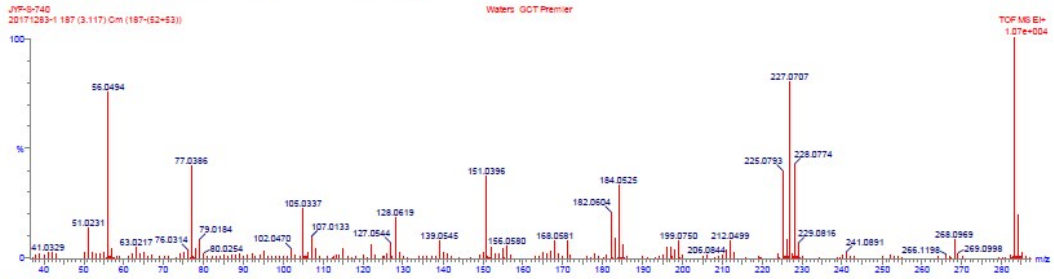

Elemental Composition Report



6l

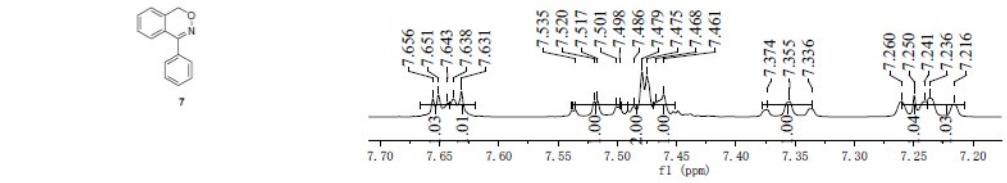
Multiple Mass Analysis: 40 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off

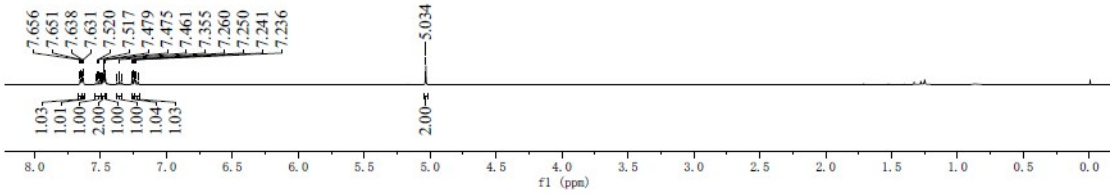
Monoisotopic Mass, Odd and Even Electron Ions
462 formula(e) evaluated with 41 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-17 H: 0-17 N: 0-1 O: 0-3

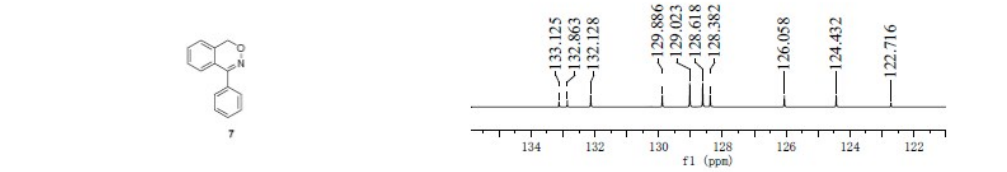


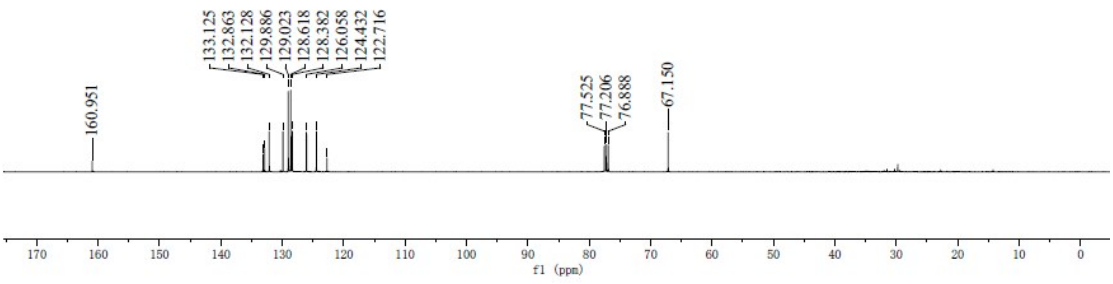

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | -1.5 | | |
| Maximum: | 100.00 | | | 5.0 | 10.0 | 100.0 | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 283.1209 | 100.00 | 283.1208 | 0.1 | 0.4 | 10.0 | 0.4 | C17H17NO3 |

## 4.4 Copies of the spectra for Scheme 2



Elemental Composition Report

Multiple Mass Analysis: 46 mass(es) processed

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

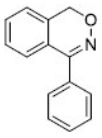
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

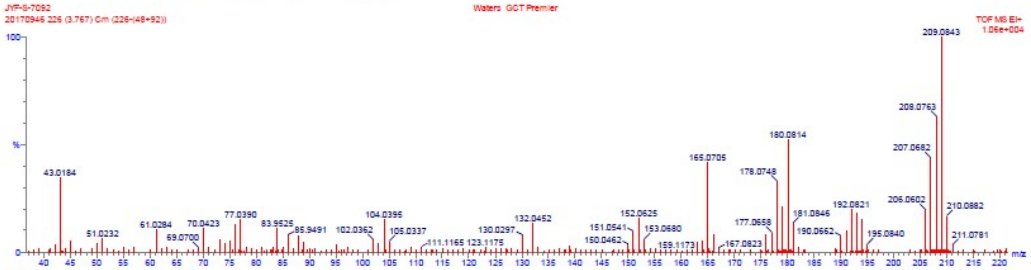
167 formula(e) evaluated with 39 results within limits (up to 50 closest results for each mass)

Elements Used:

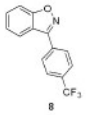
C: 0-14 H: 0-11 N: 0-1 O: 0-1



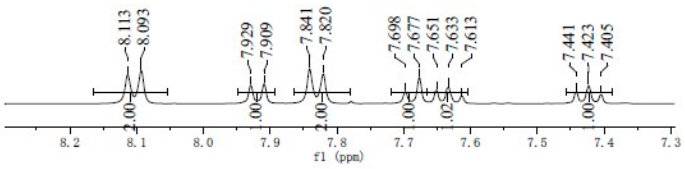
7

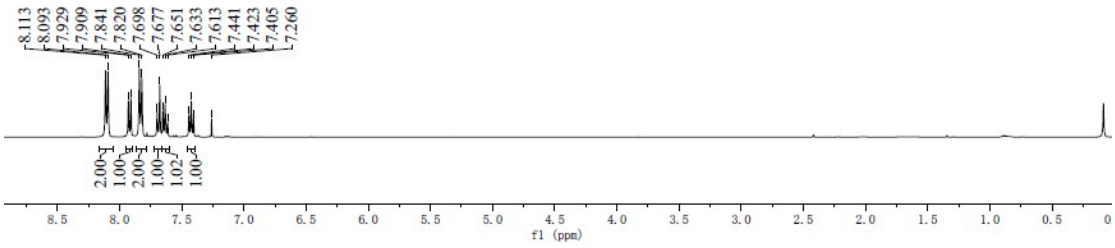


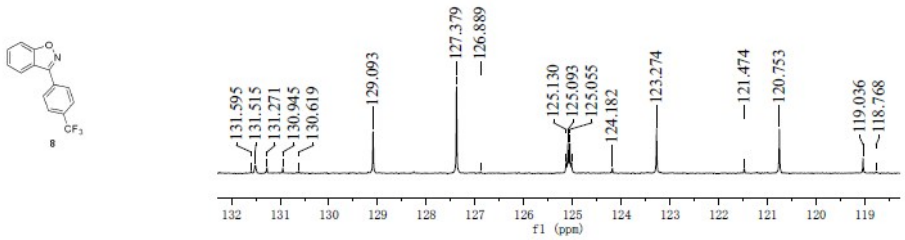

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 209.0843 | 100.00 | 209.0841 | 0.2 | 1.0 | 10.0 | 32.3 | C14H11NO |

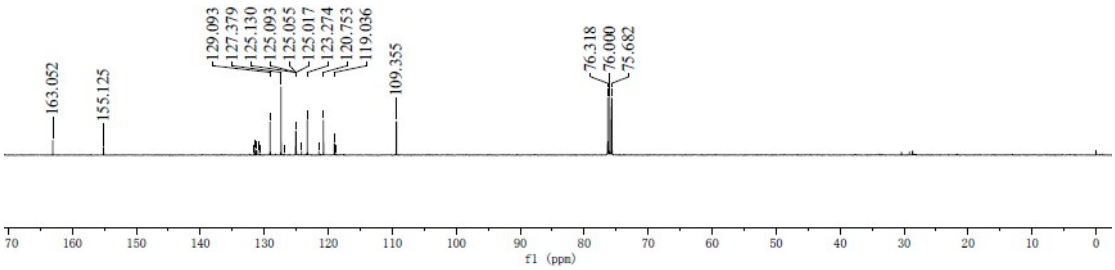


8






Elemental Composition Report

Multiple Mass Analysis: 18 mass(es) processed

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

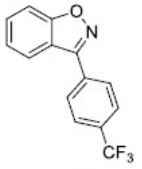
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

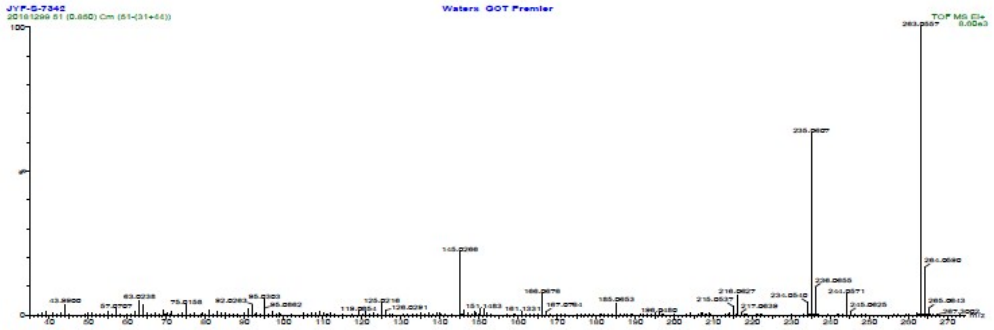
191 formula(e) evaluated with 23 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-14 H: 0-8 N: 0-1 O: 0-1 F: 0-3

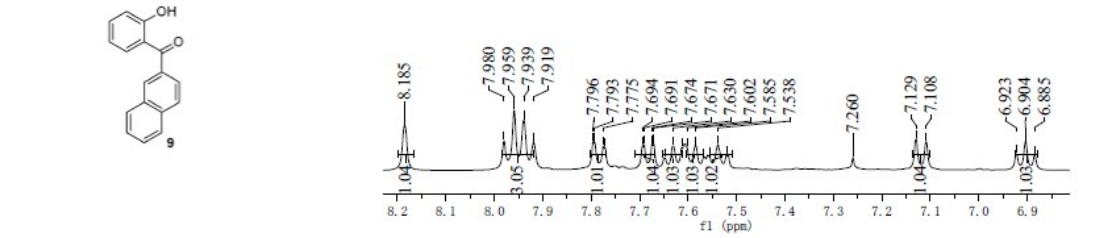


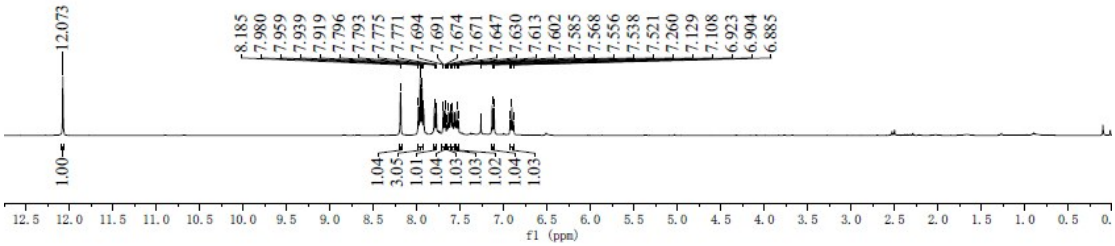
8

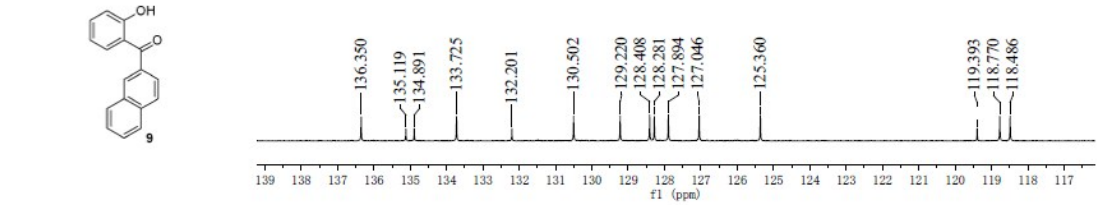


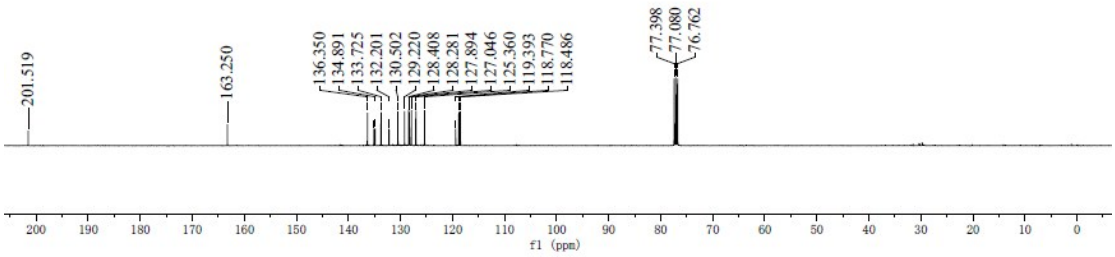

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | 3.00 | | | | | | -1.5 |
| Maximum: | 100.00 | | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 263.0557 | 100.00 | 263.0558 | -0.1 | -0.4 | 10.0 | 17.8 | C14H8NOF3 |

## 4.5 Copies of the spectra for Scheme 3

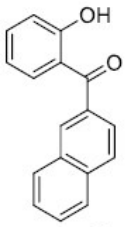


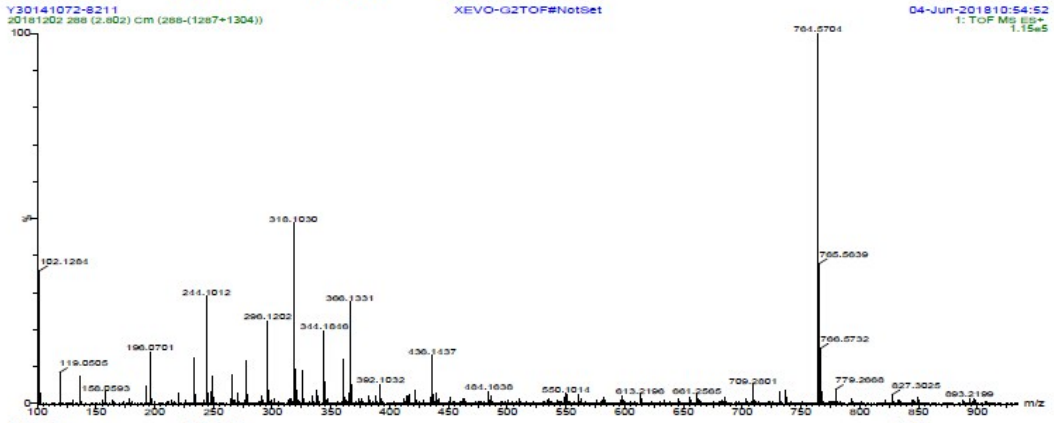



Elemental Composition Report
Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
470 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
12C: 0-50 13C: 0-1 H: 0-50 O: 0-6

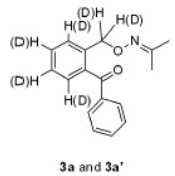



9

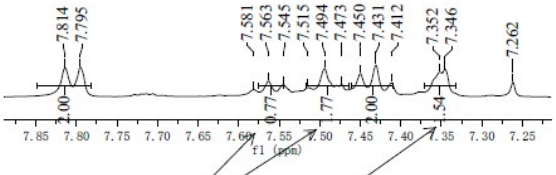



| Minimum: | 15.00 | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Maximum: | 100.00 | | | | 5.0 | 5.0 | 50.0 | | |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Norm | Conf(%) | Formula |
| 249.0918 | 100.00 | 249.0916 | 0.2 | 0.8 | 11.5 | 240.7 | n/a | n/a | 12C17H13O2 |

## 4.6 Copies of the spectra for Scheme 4

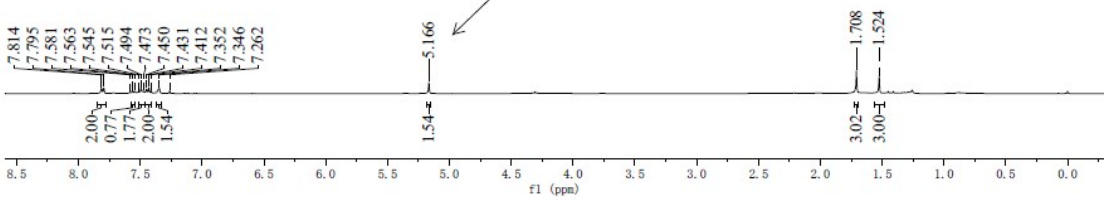



**3a** and **3a'**

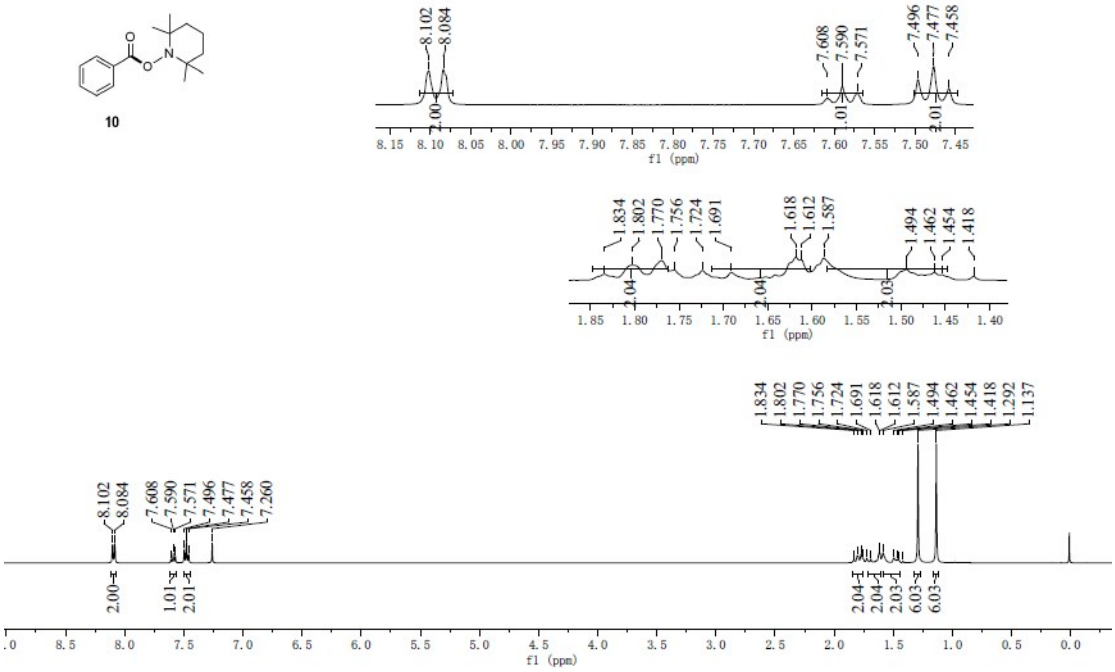


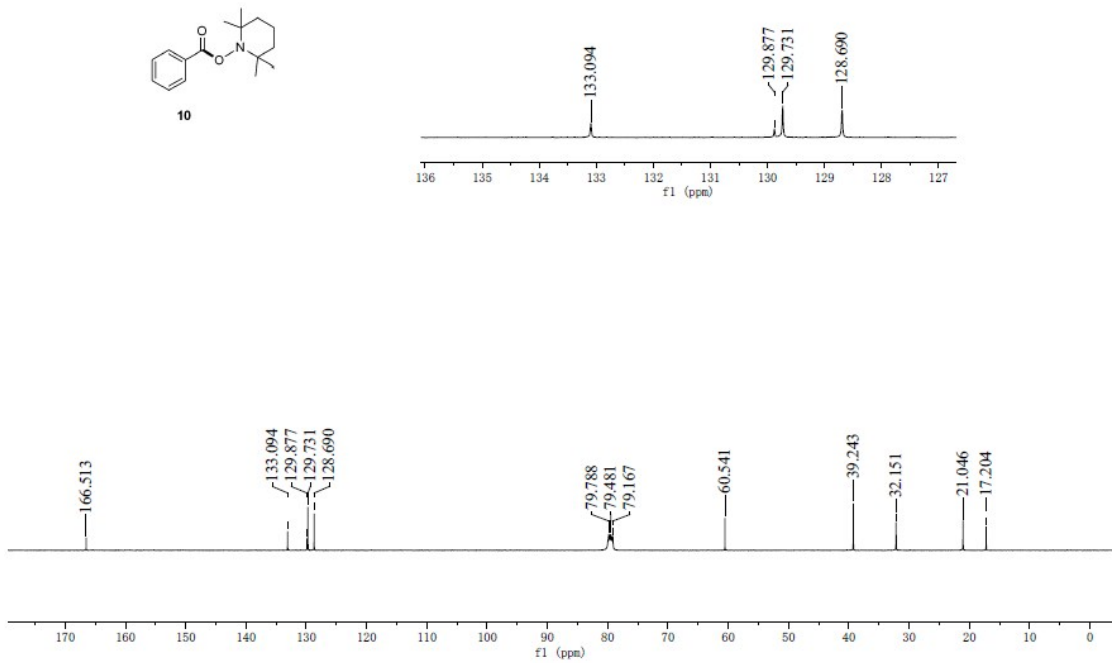

kH/kD = 0.77/0.23 = 3.35

kH/kD = 1.54/0.46 = 3.35

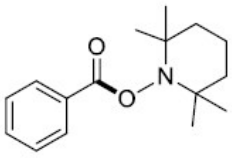


## 4.7 Copies of the spectra for TEMPO ester adduct 10

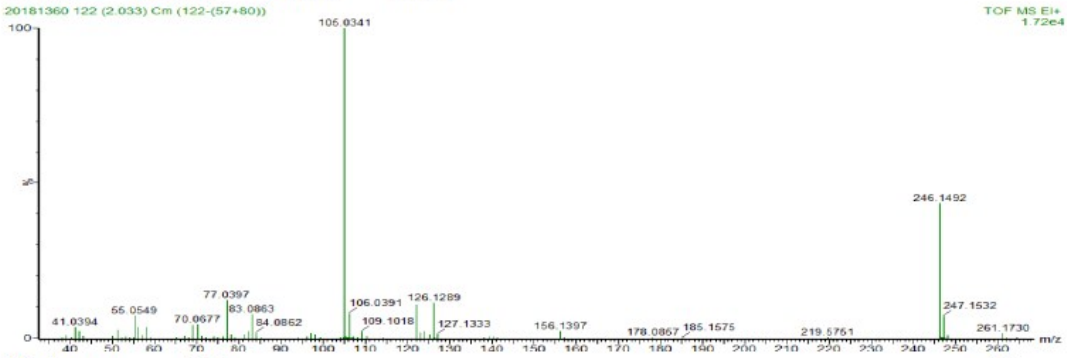


Elemental Composition Report
Multiple Mass Analysis: 24 mass(es) processed
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
239 formula(e) evaluated with 23 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-23 N: 0-1 O: 0-2



**10**




| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Minimum: | | 1.50 | | | | | -1.5 |
| Maximum: | | 100.00 | | | 5.0 | 10.0 | 100.0 |
| Mass | RA | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 261.1730 | 1.56 | 261.1729 | 0.1 | 0.4 | 6.0 | 2773021.8 | C16H23NO2 |