

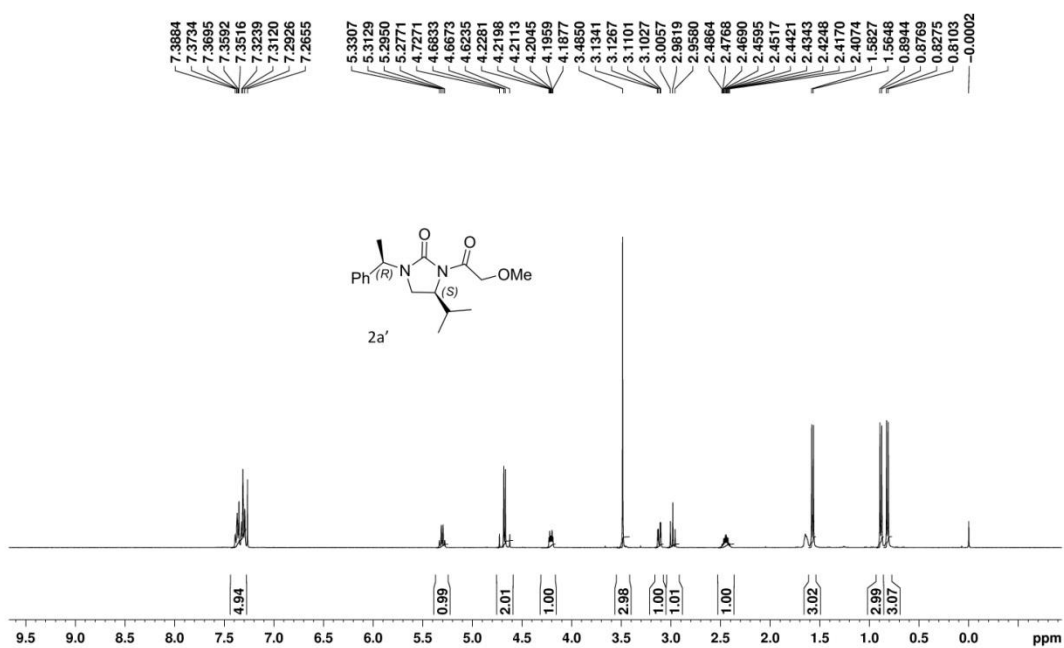
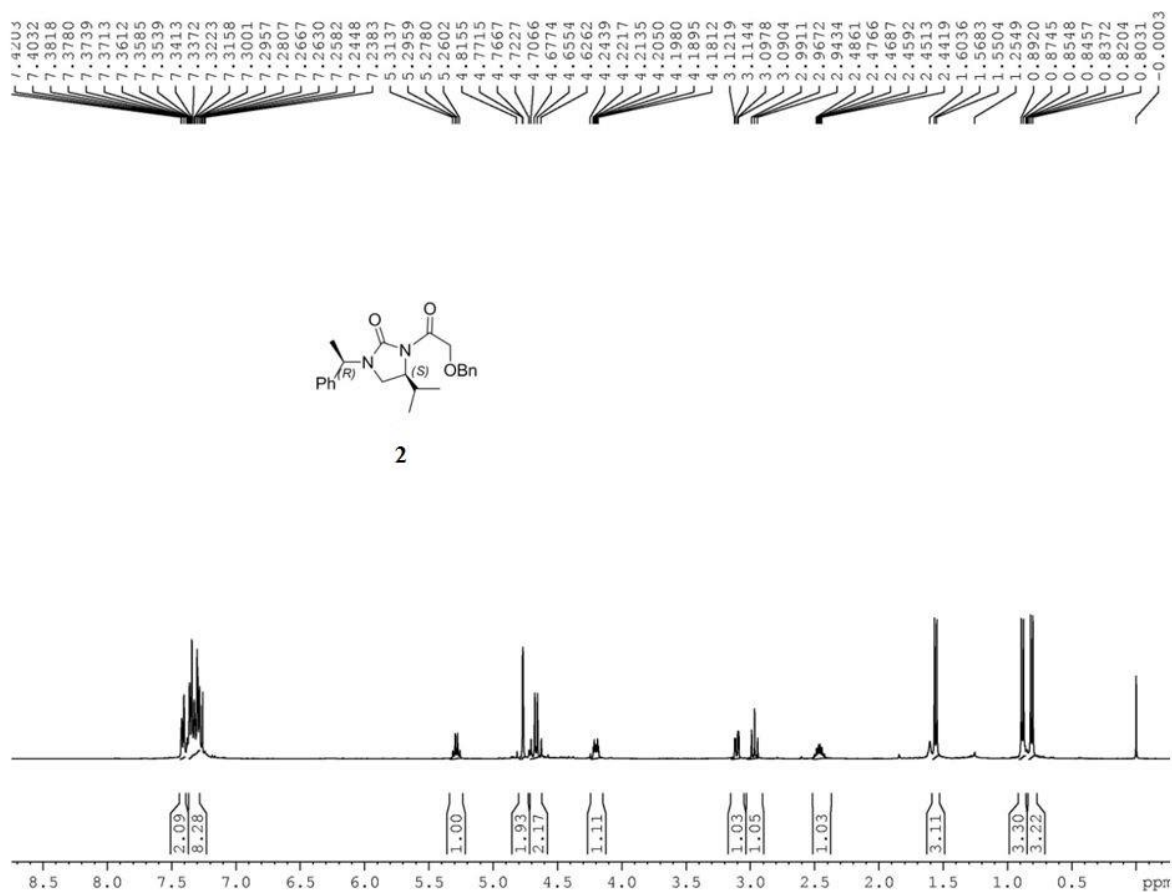
## Supporting Information

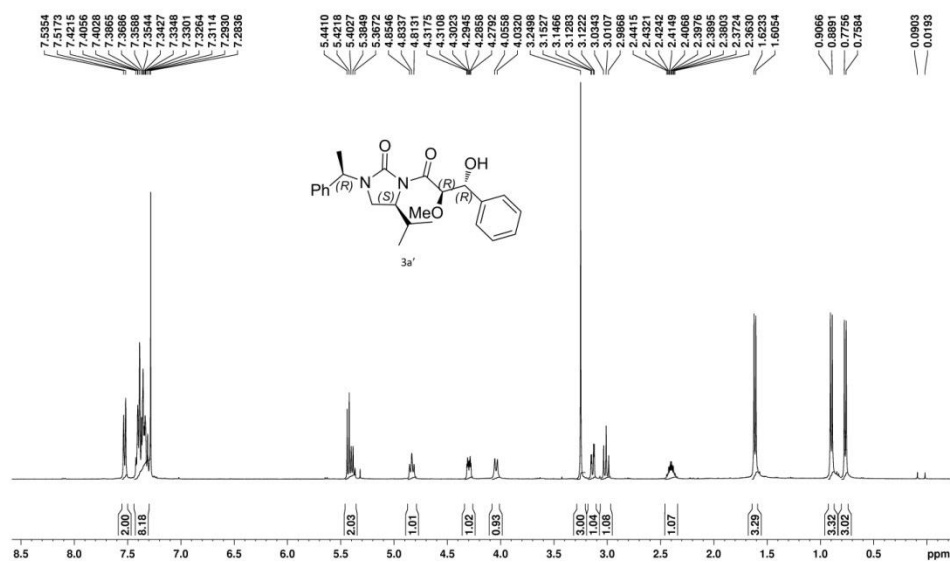
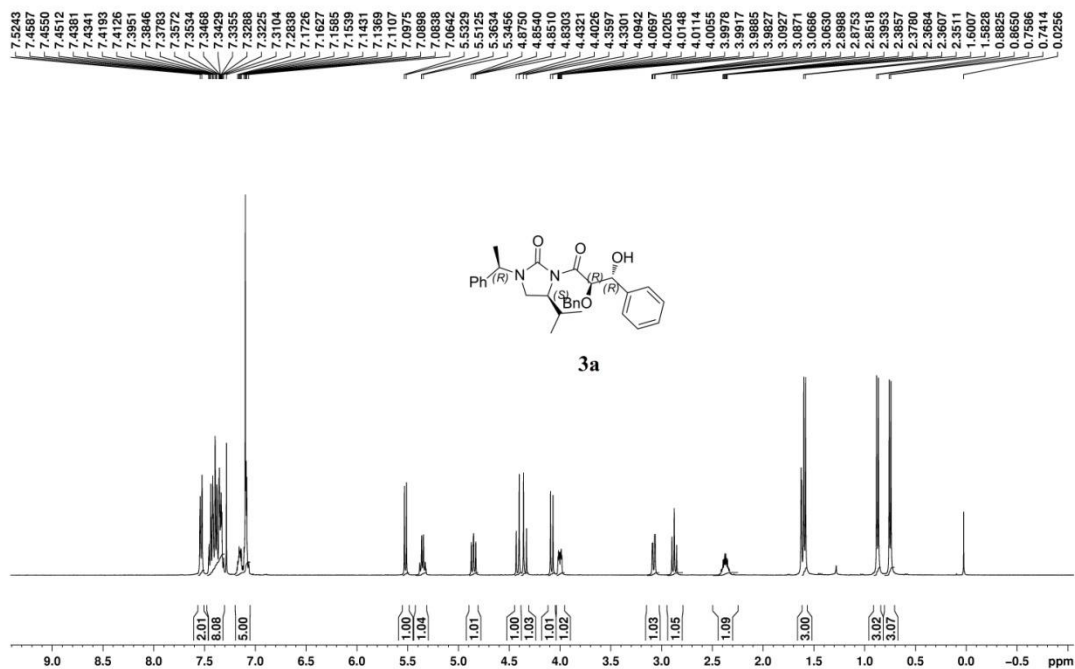
### ***Anti selective glycolate aldol reactions of (S)-4-isopropyl-1-[(R)-1-phenylethyl] imidazolidin-2-one: application towards the asymmetric synthesis of 8-4'-oxyneolignans***

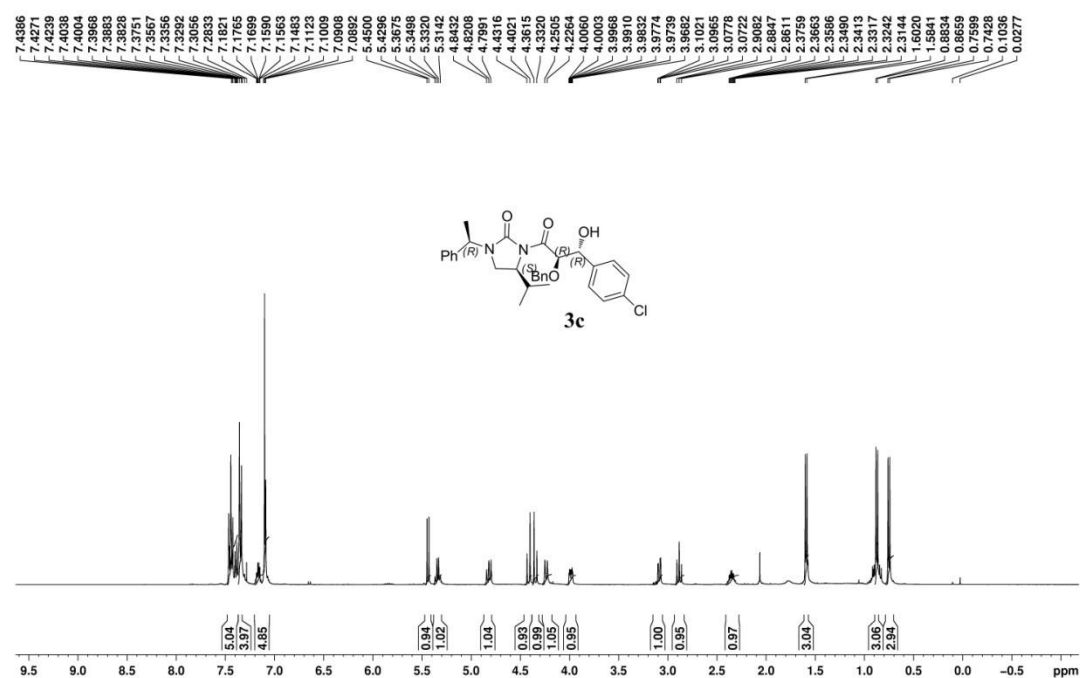
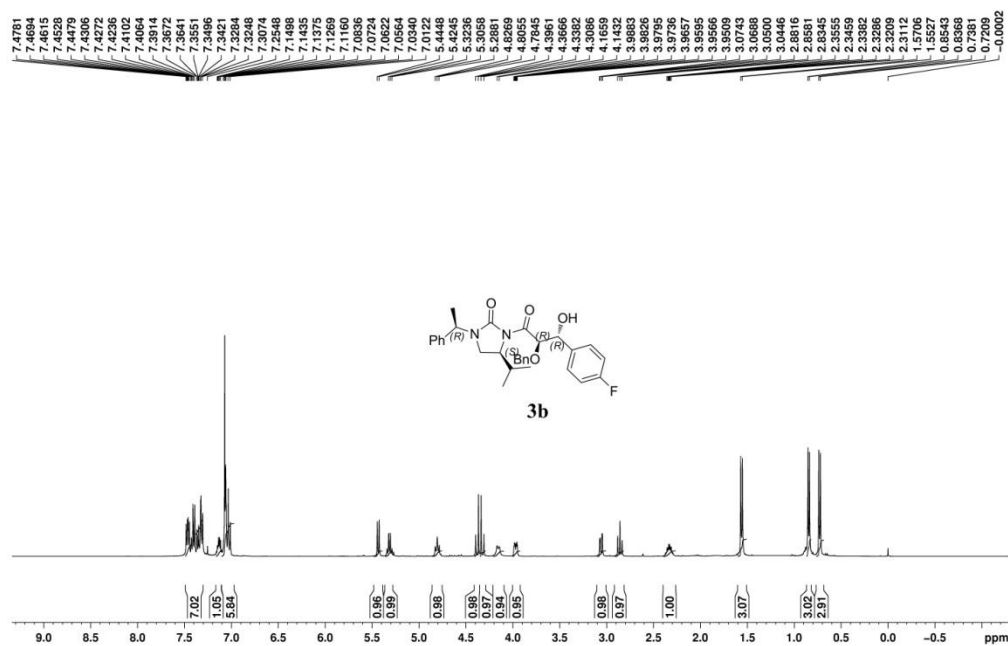
Mukesh Gangar, Avinash Ittuveetil, Sandeep Goyal, Anang Pal, Harikrishnan M., Vipin A. Nair\*

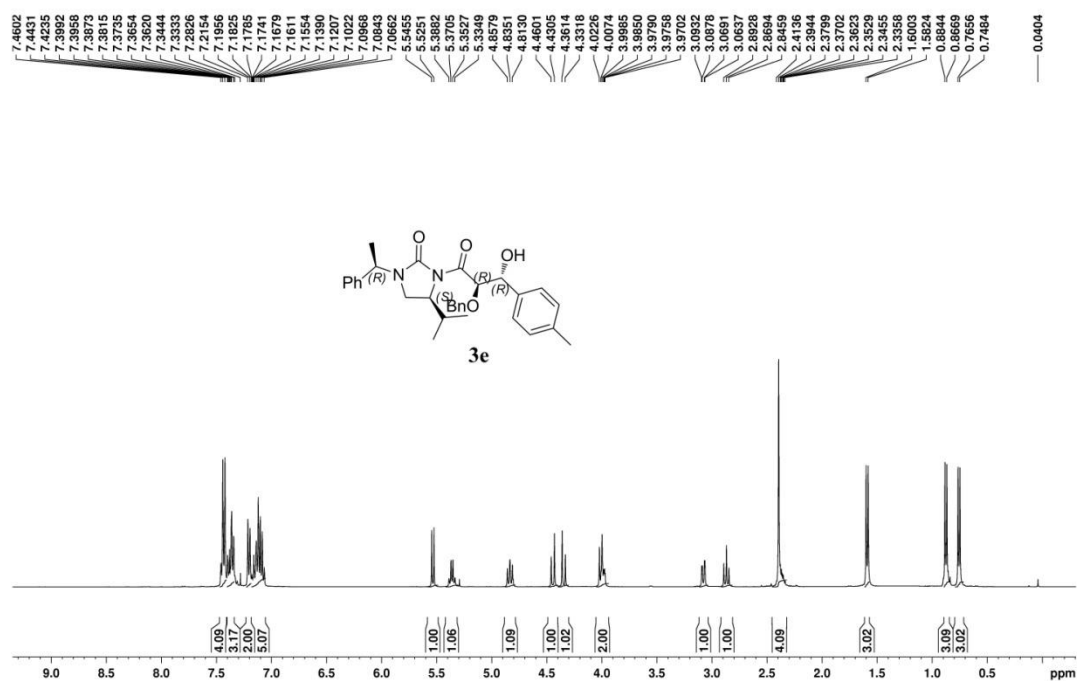
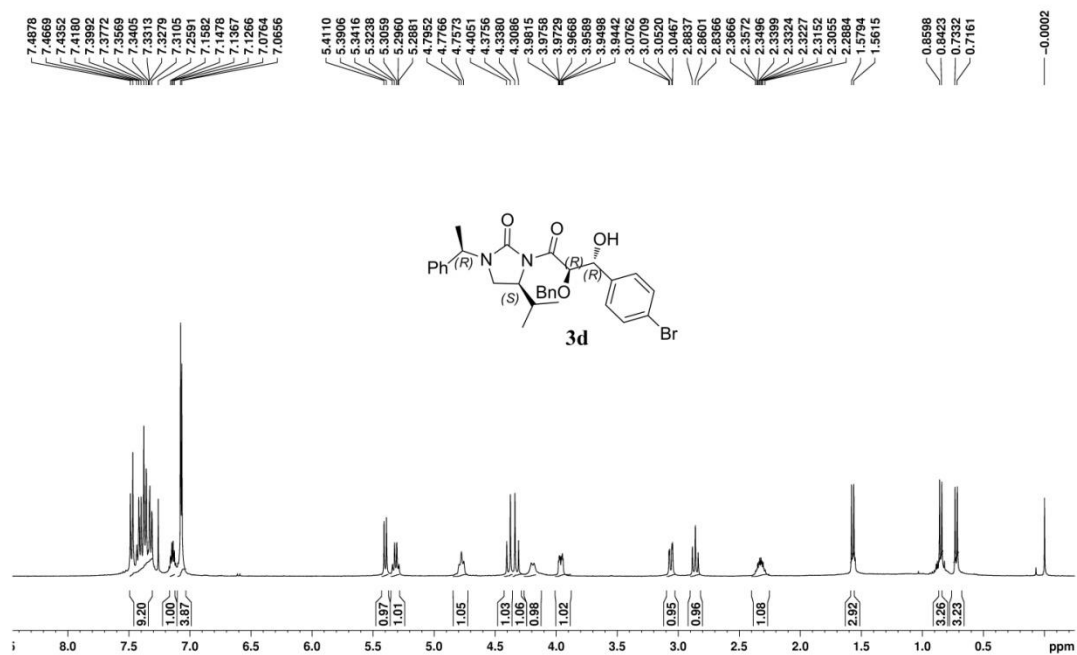
Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, Sector 67, Mohali, Punjab 160062, India

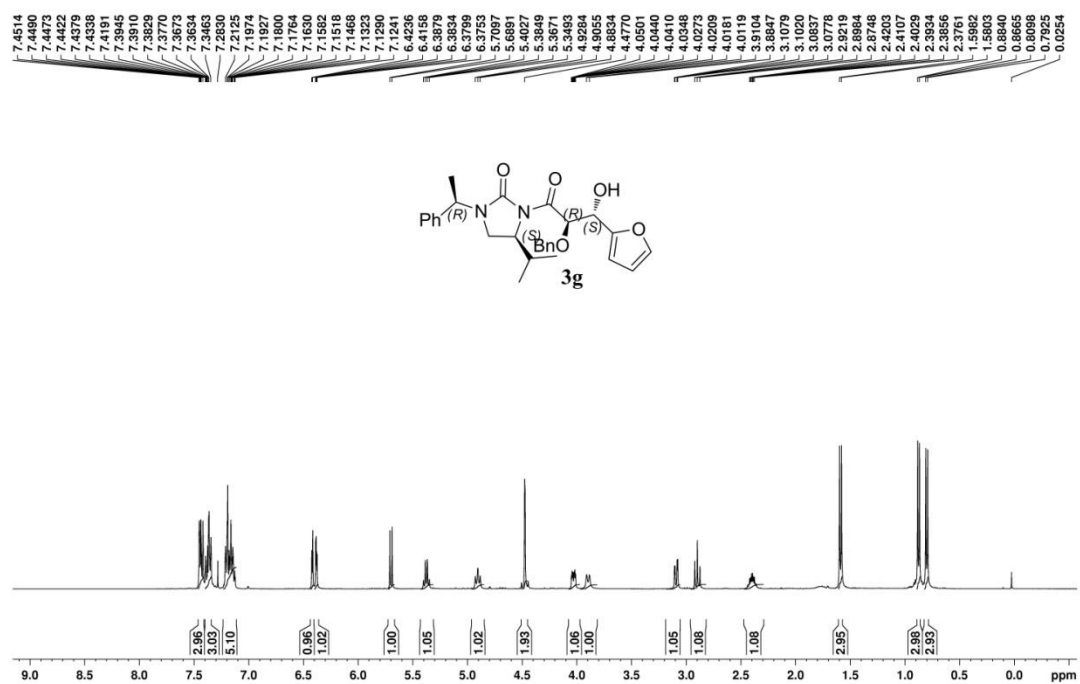
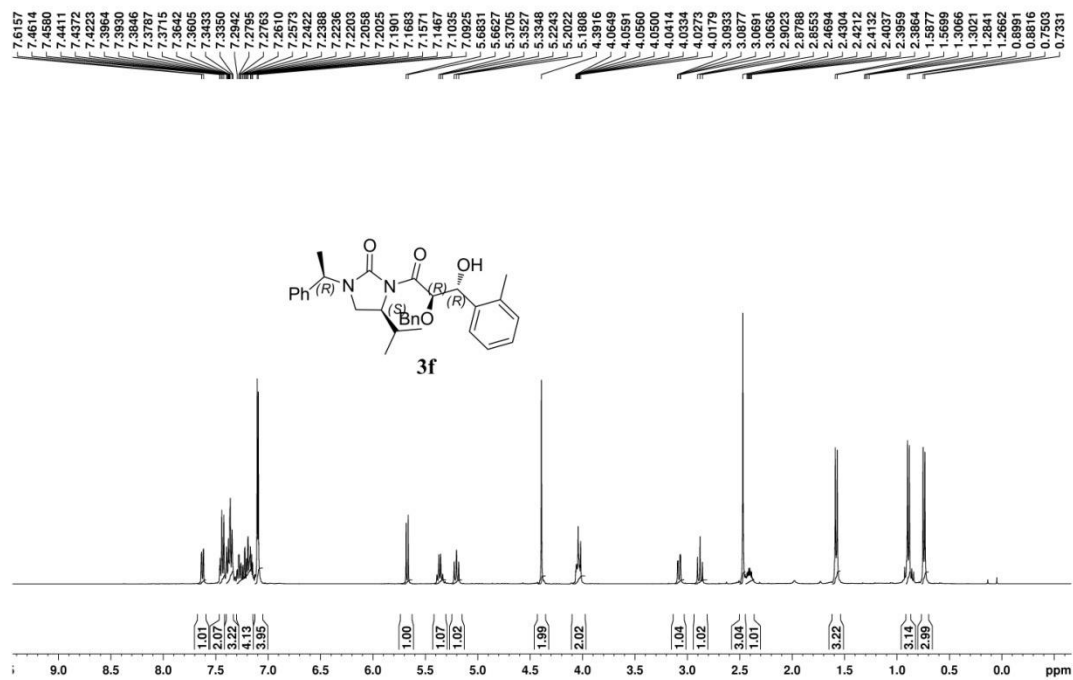
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| <b>Copies of <math>^{13}\text{C}</math> NMR Spectra</b> | <b>21 – 38</b> |
| <b>Copies of HRMS Spectra</b>                           | <b>39 - 70</b> |
| <b>Copies of IR Spectra</b>                             | <b>71 - 76</b> |

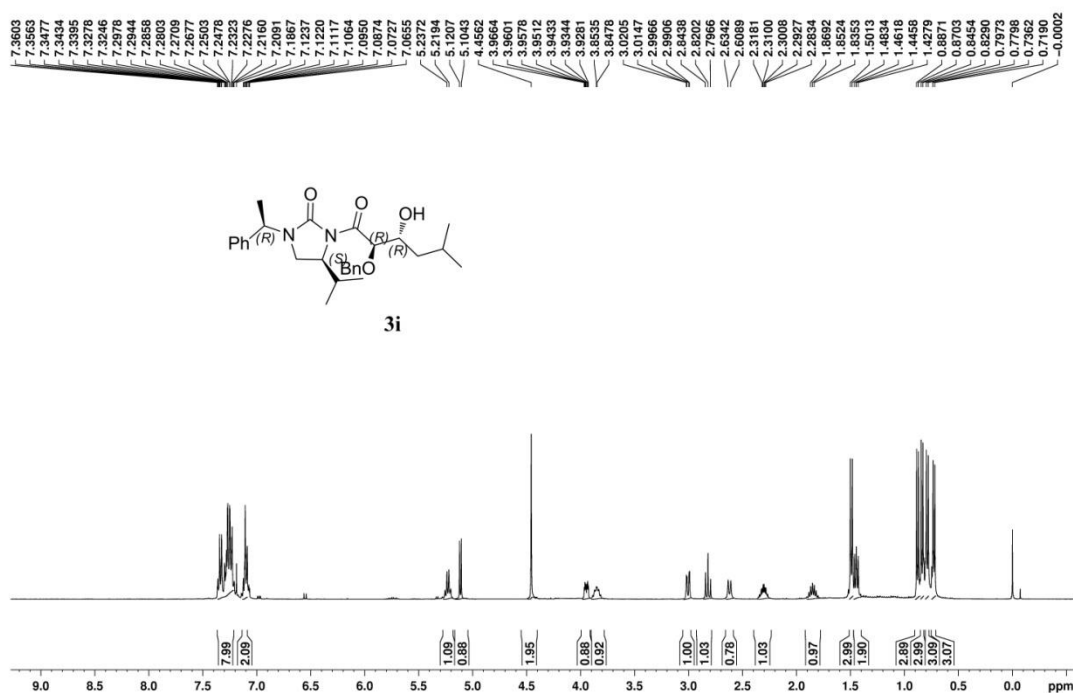
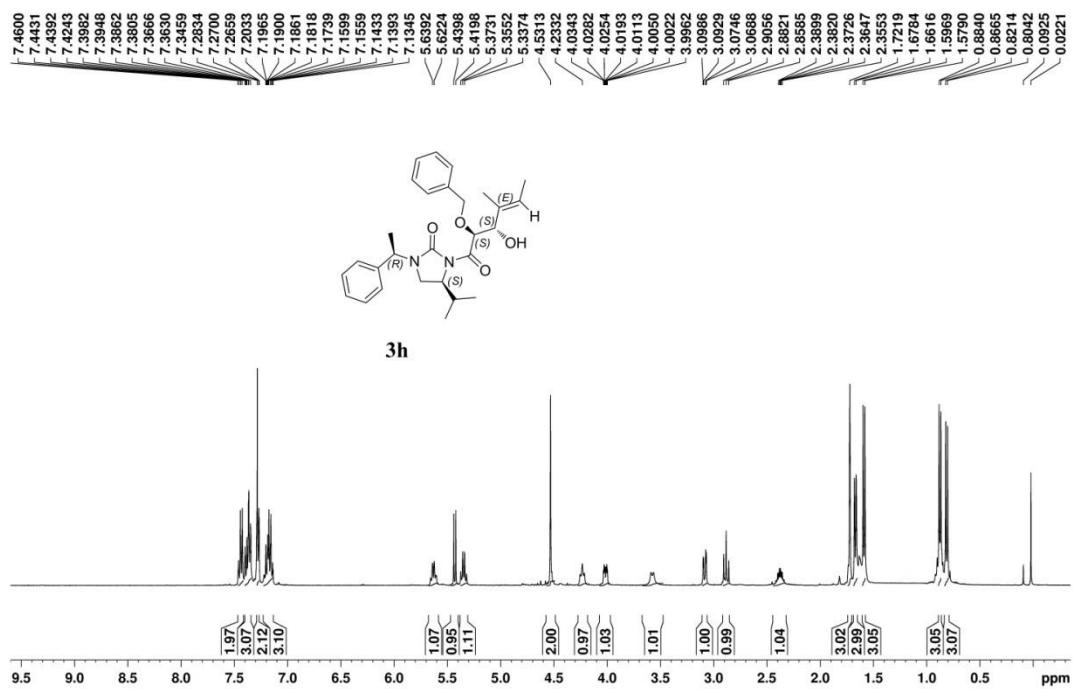


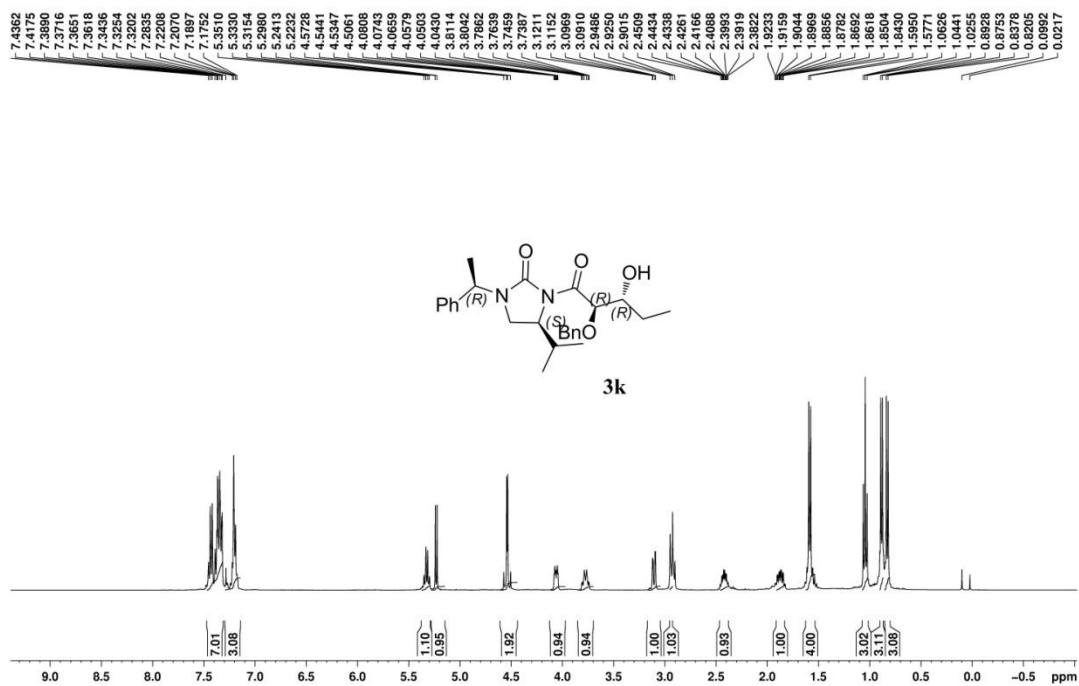
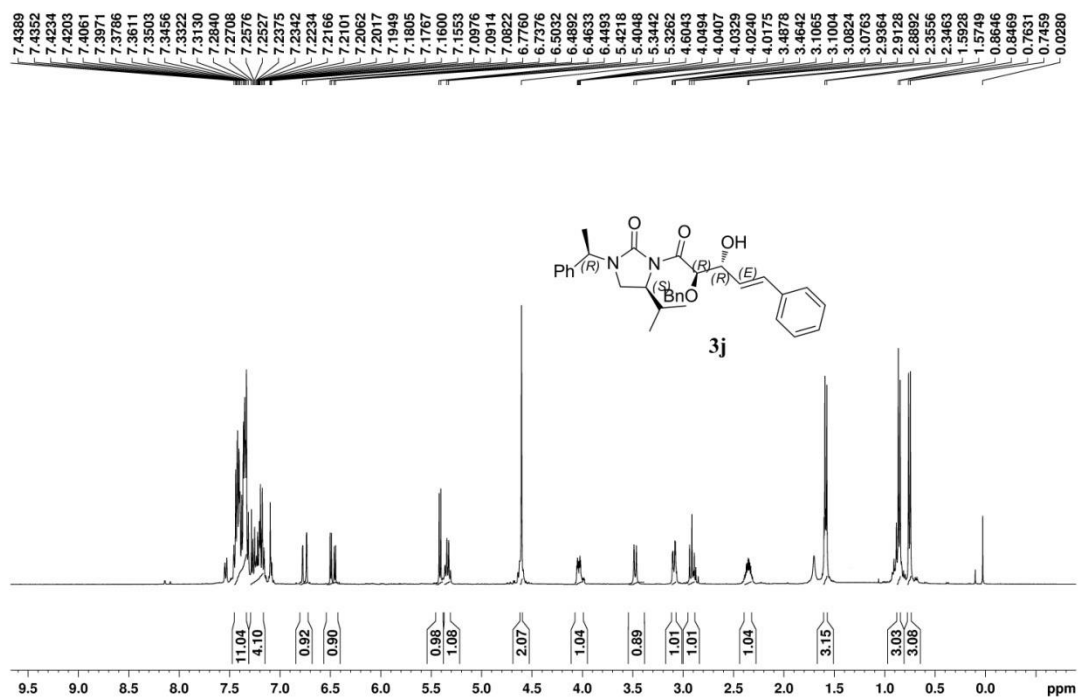


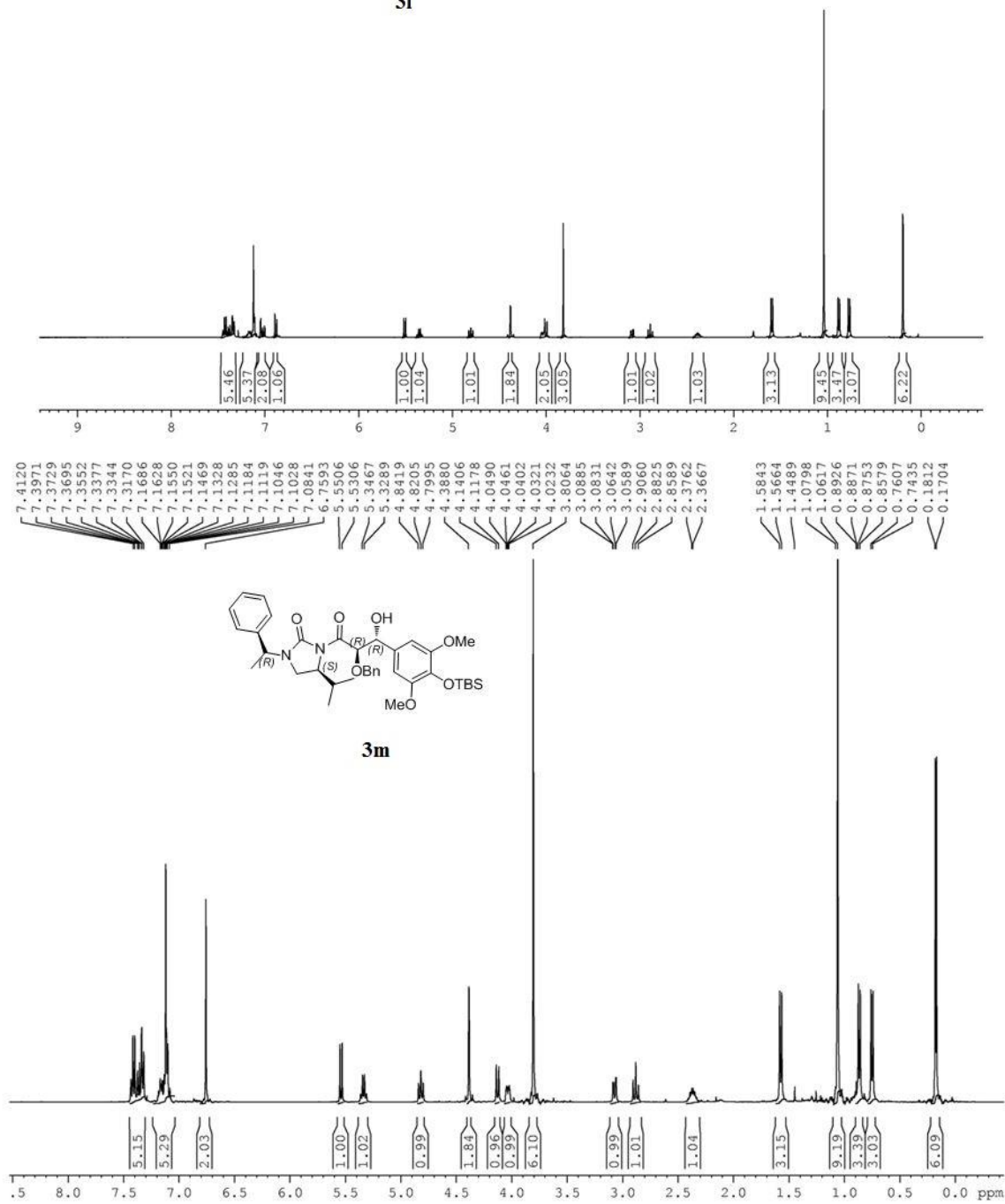
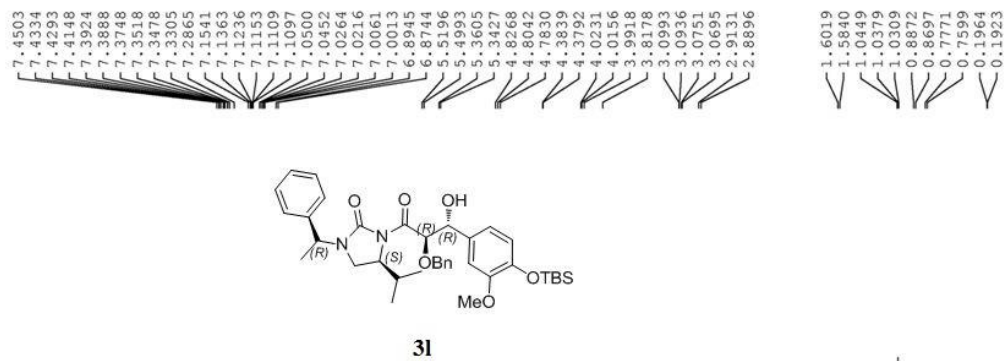


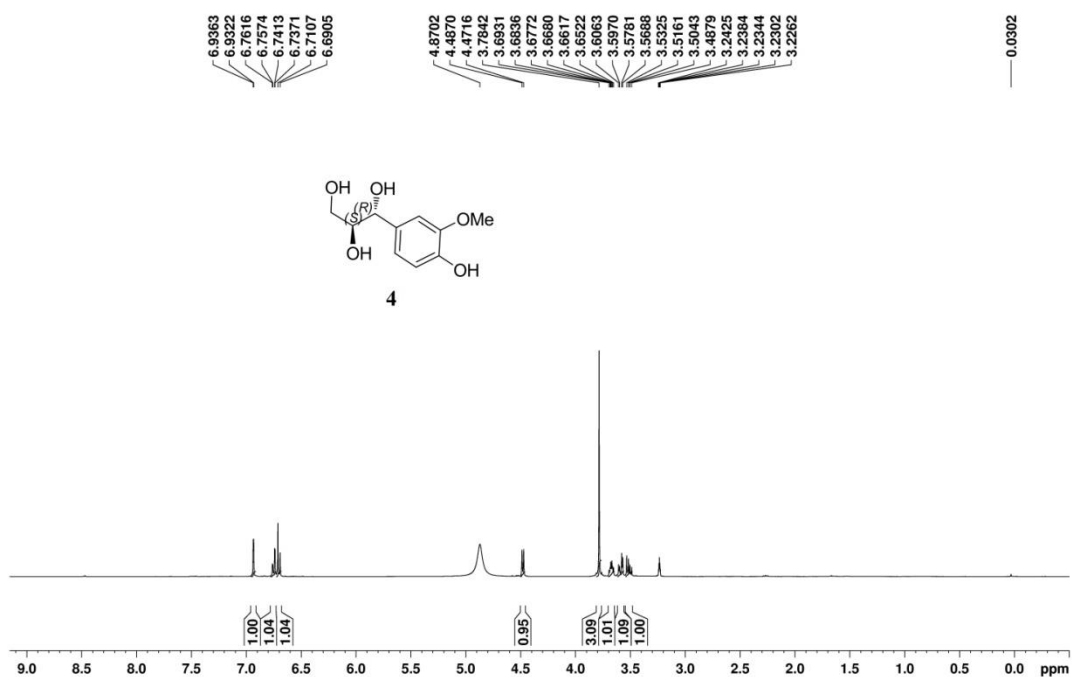
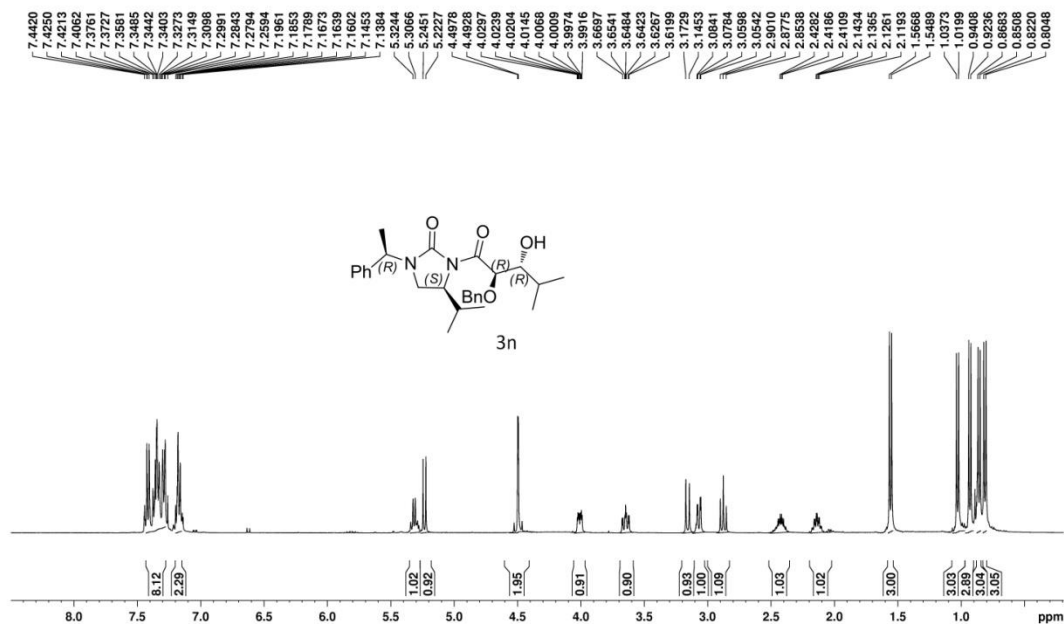


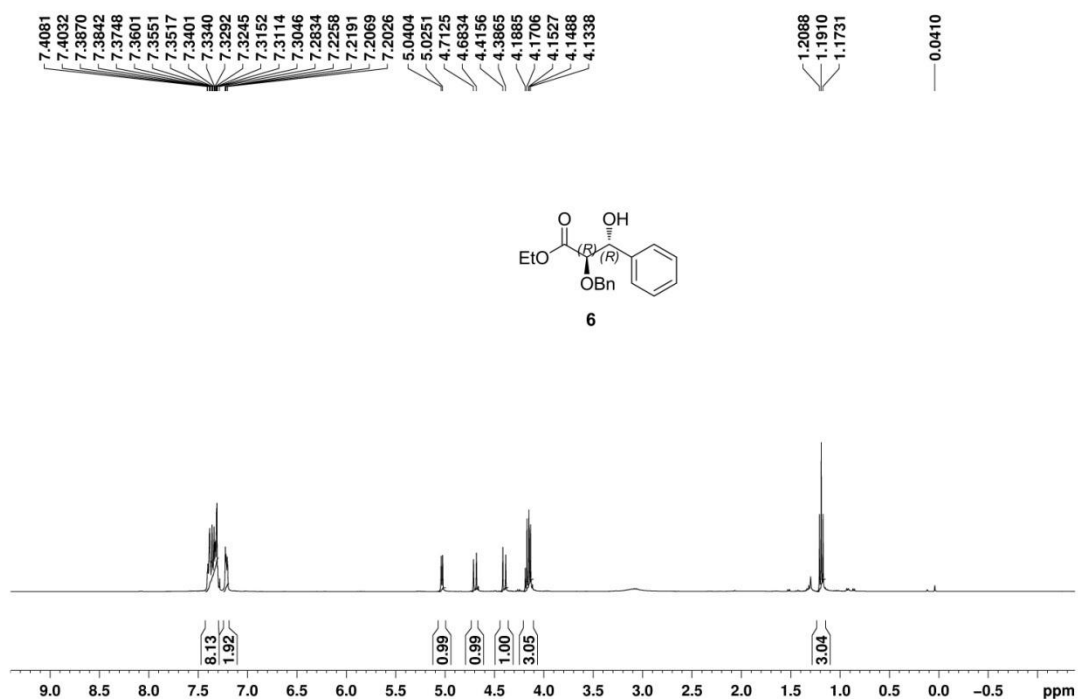
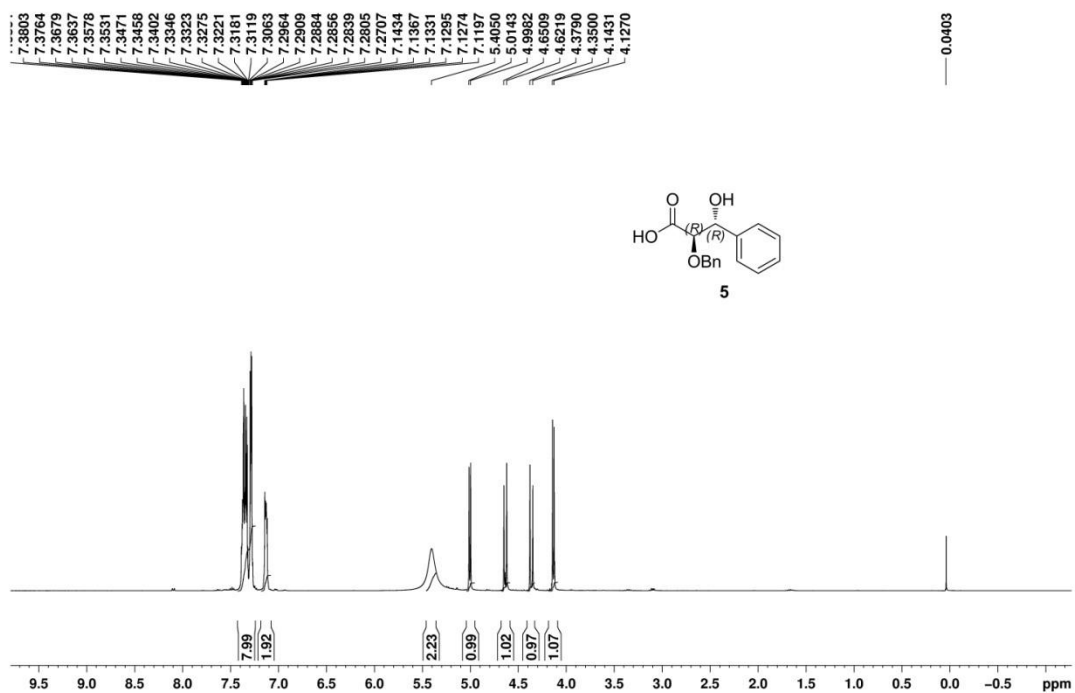


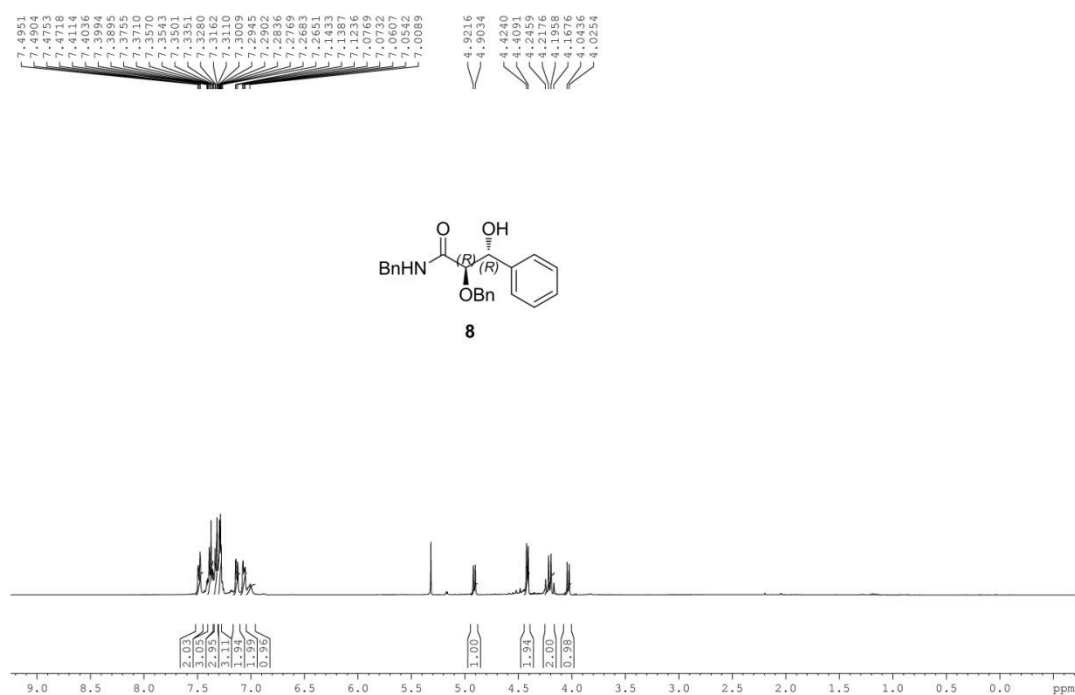
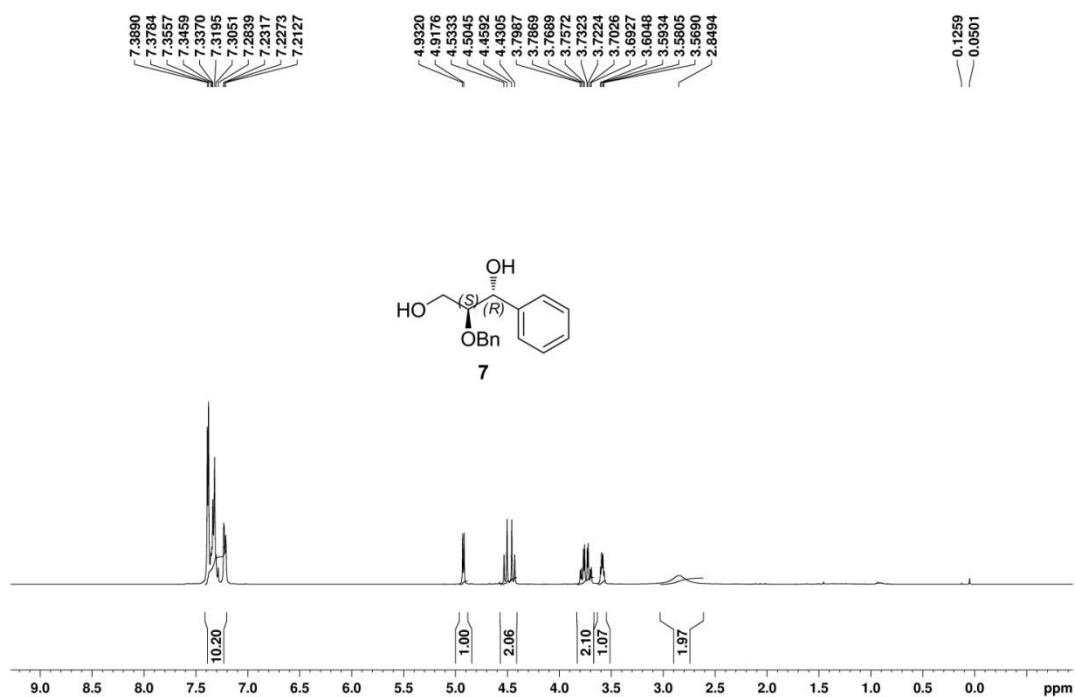




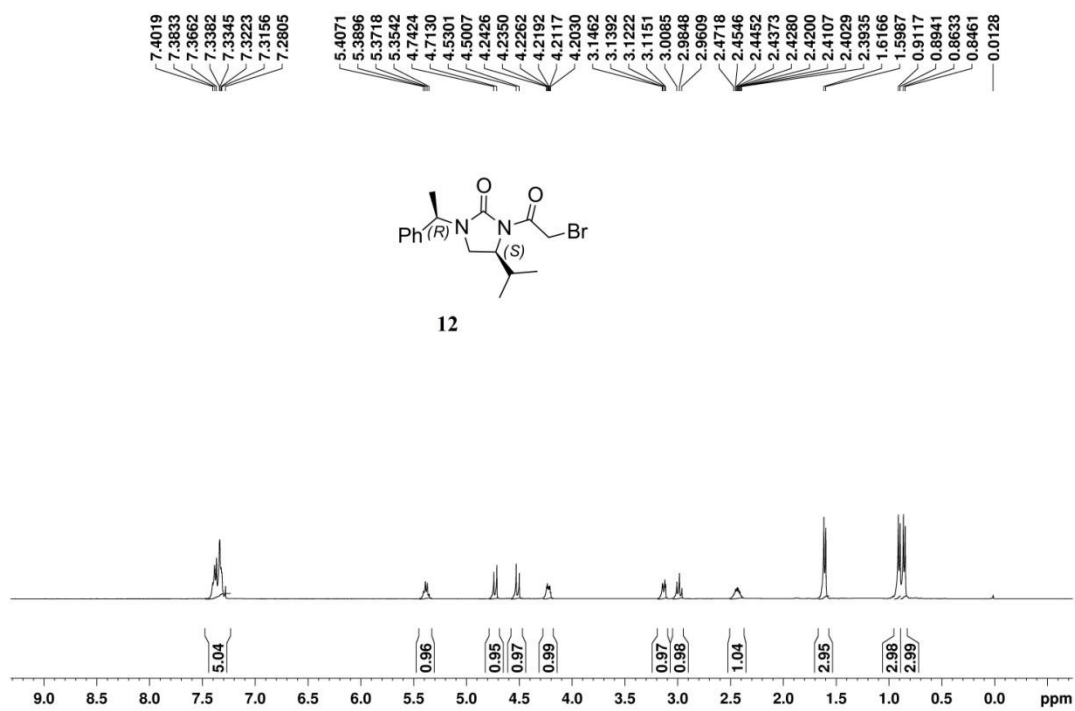
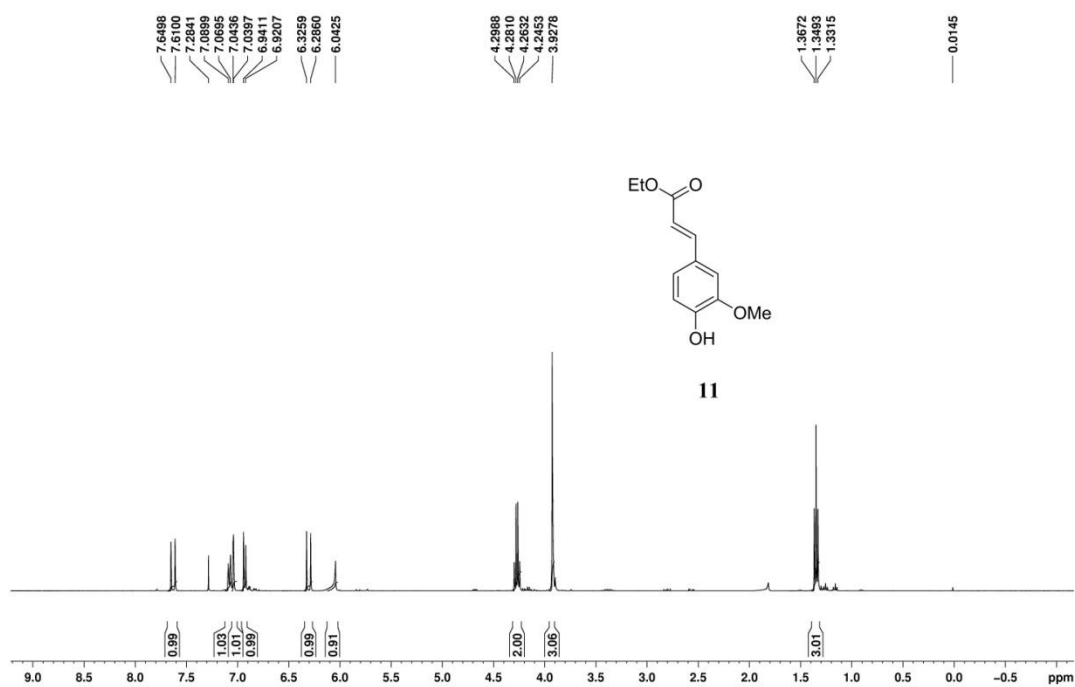


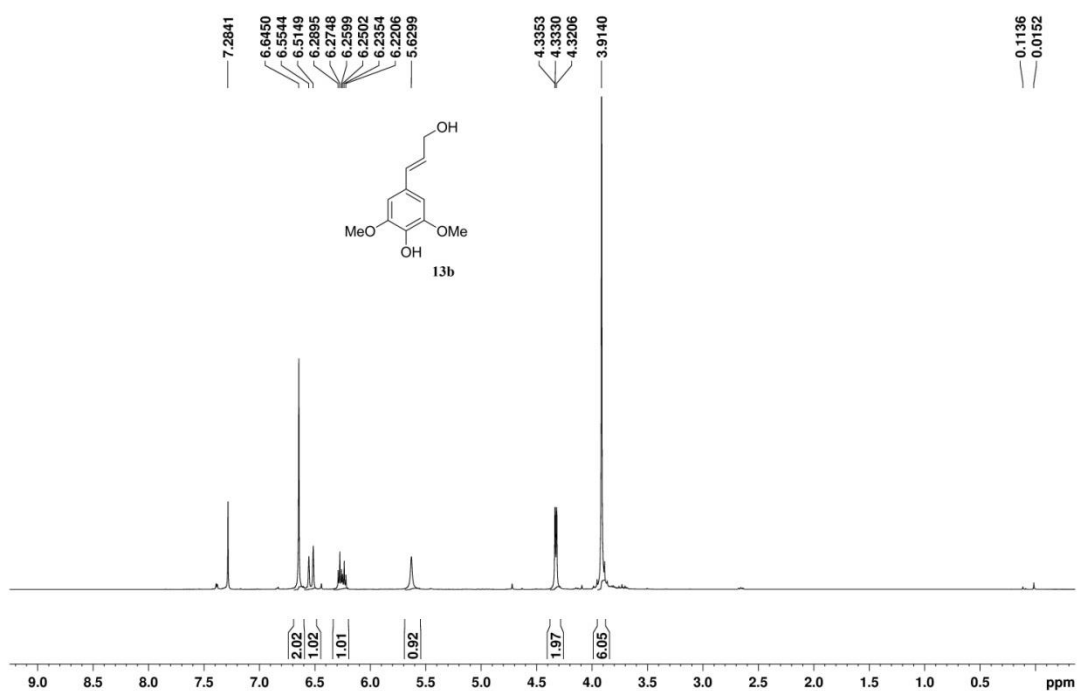
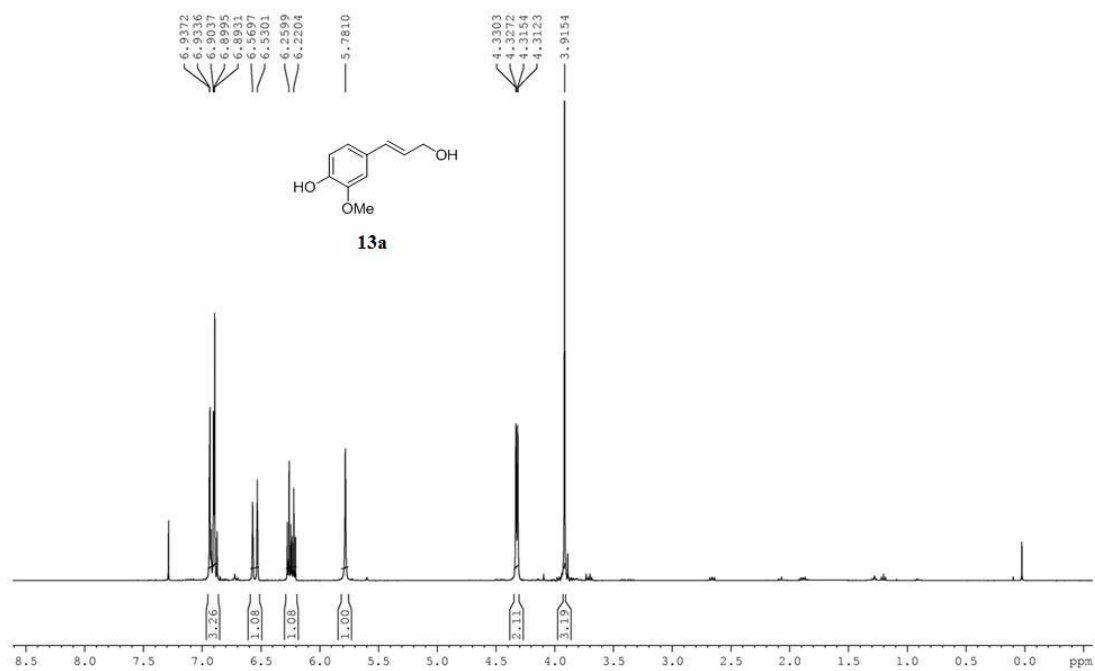


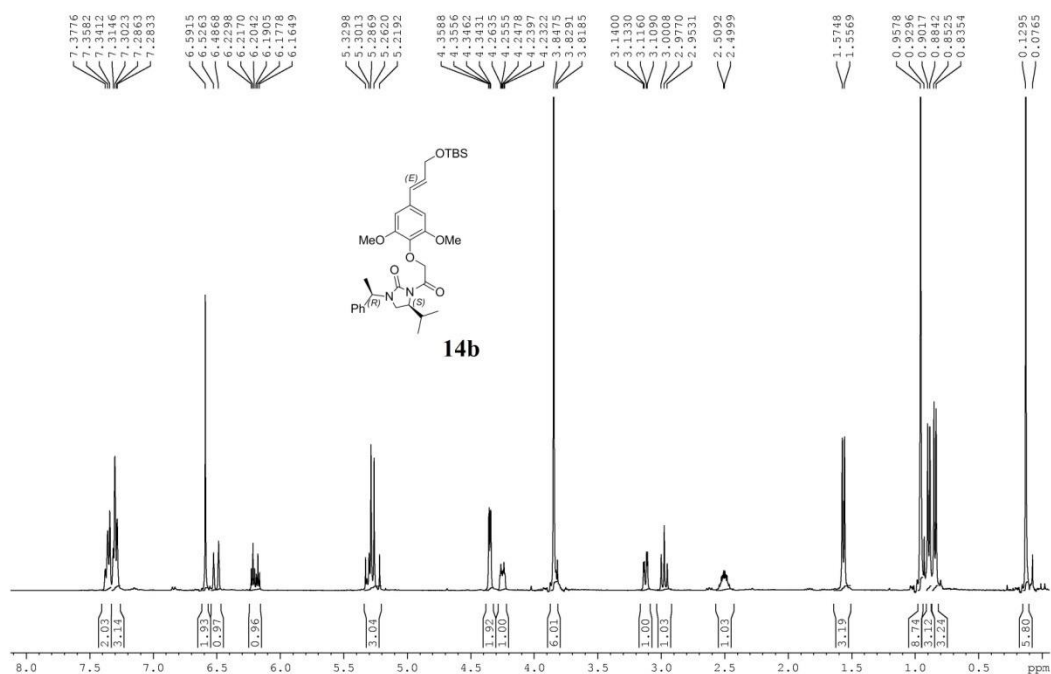
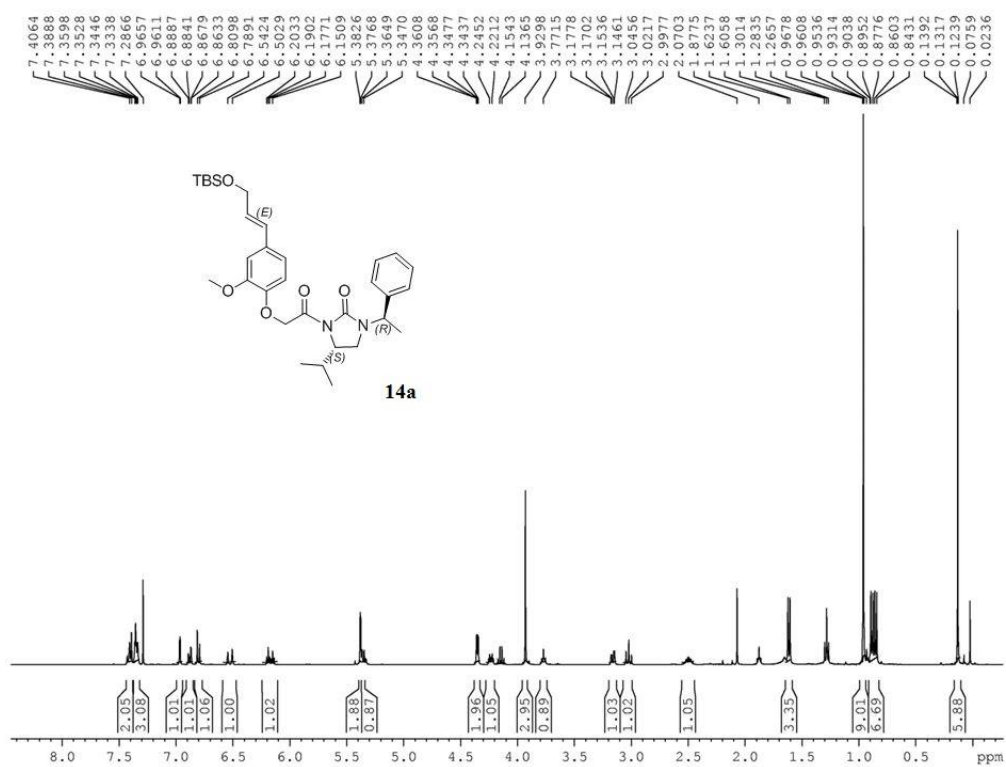


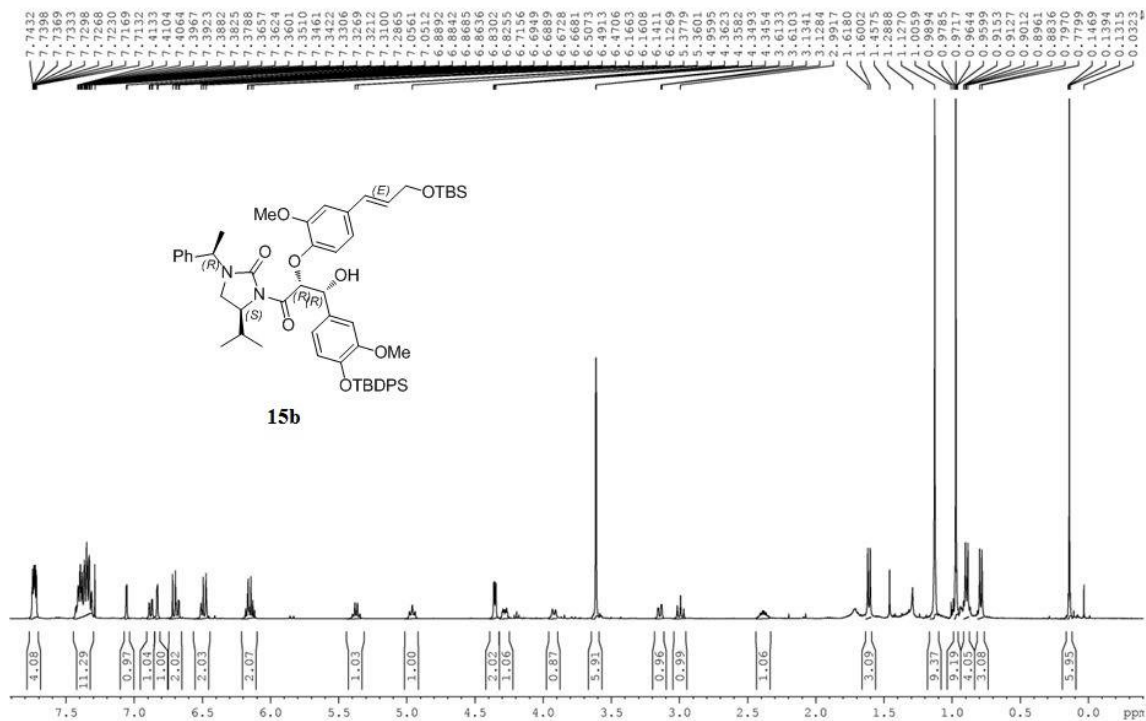
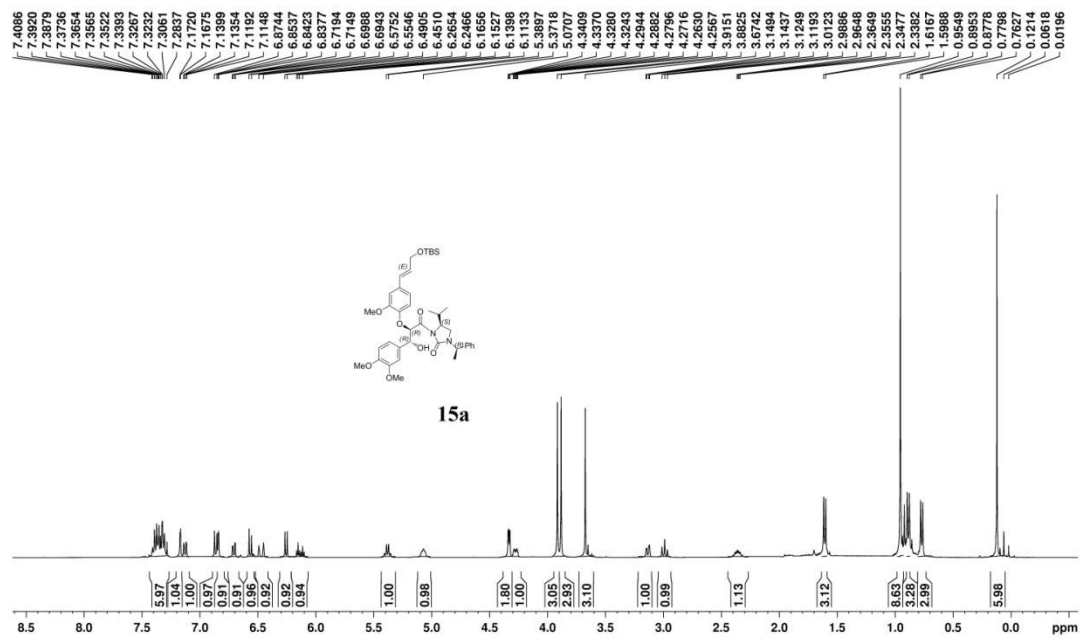


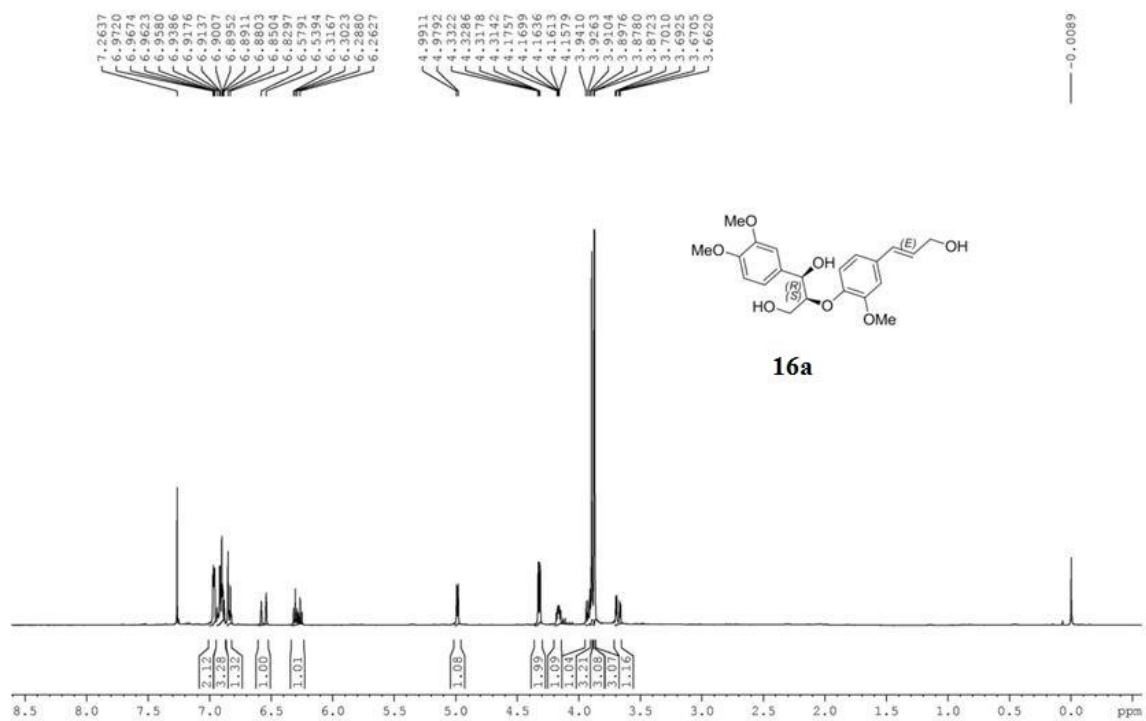
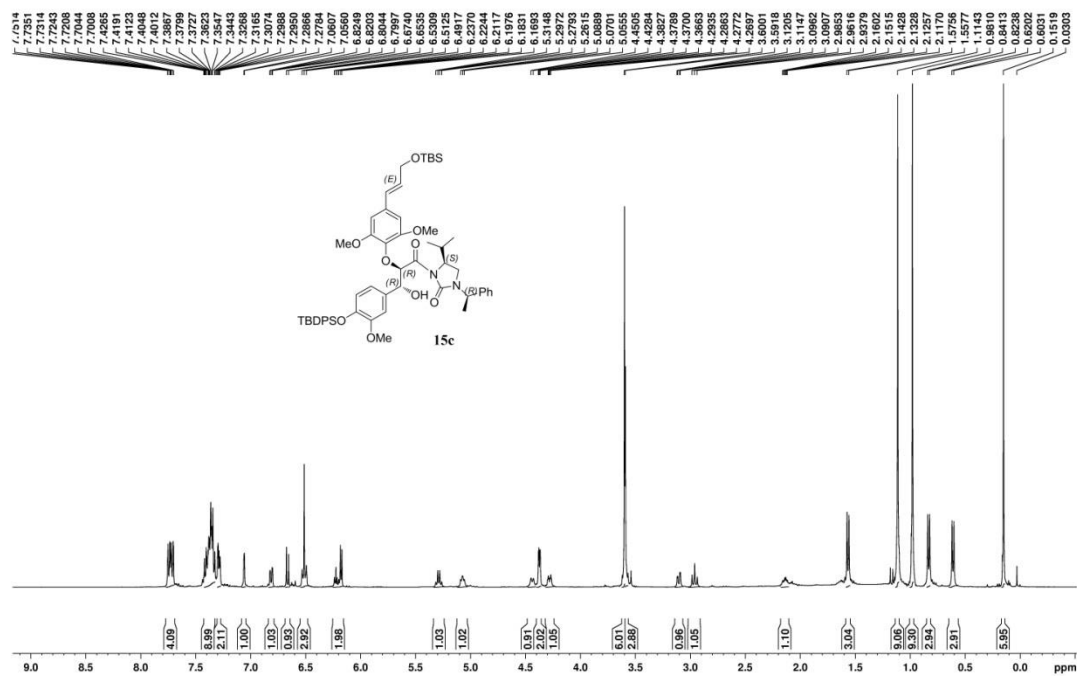


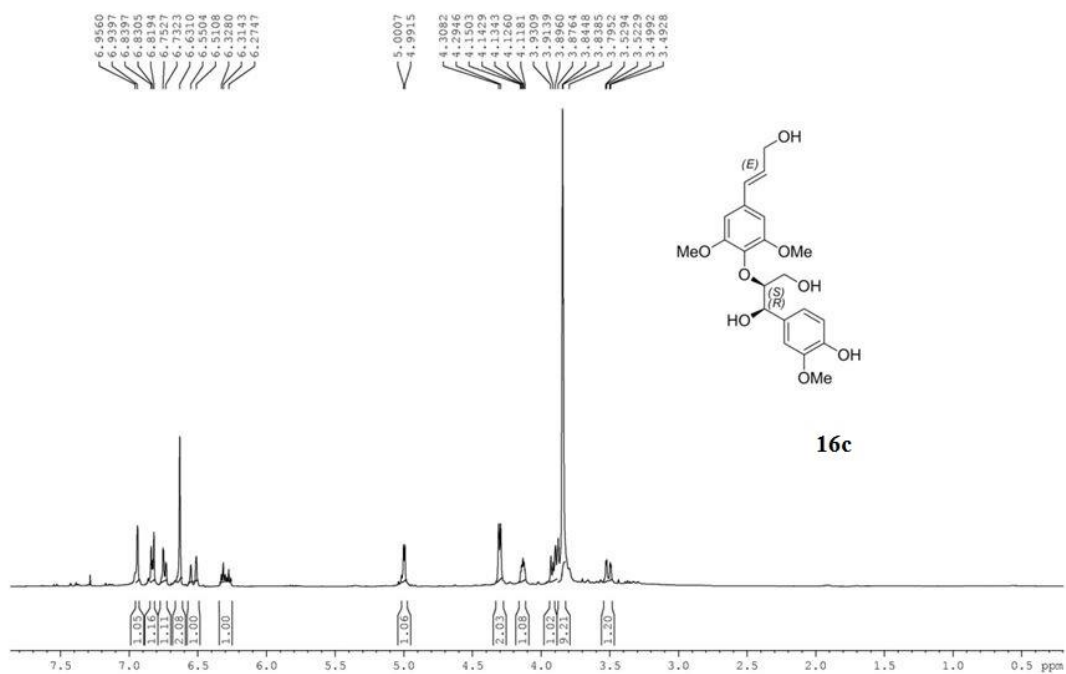
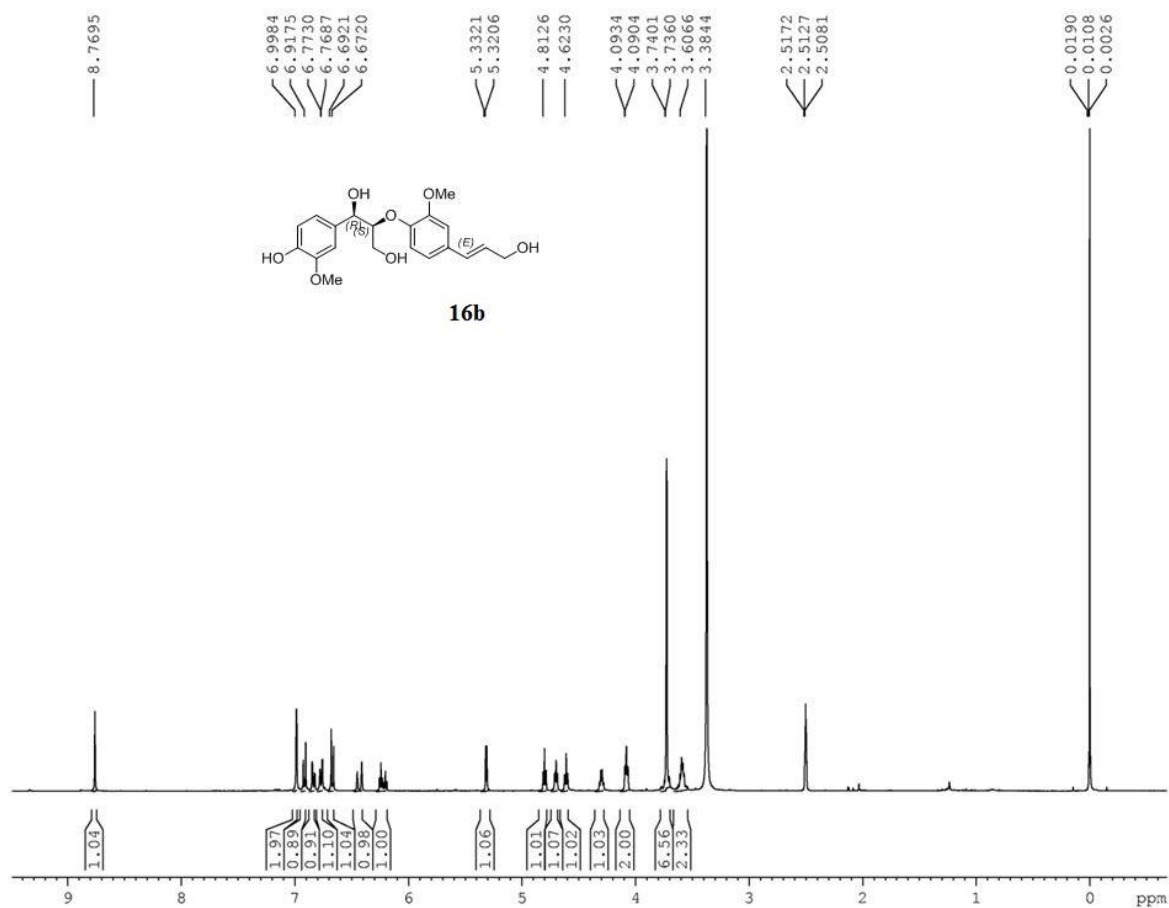


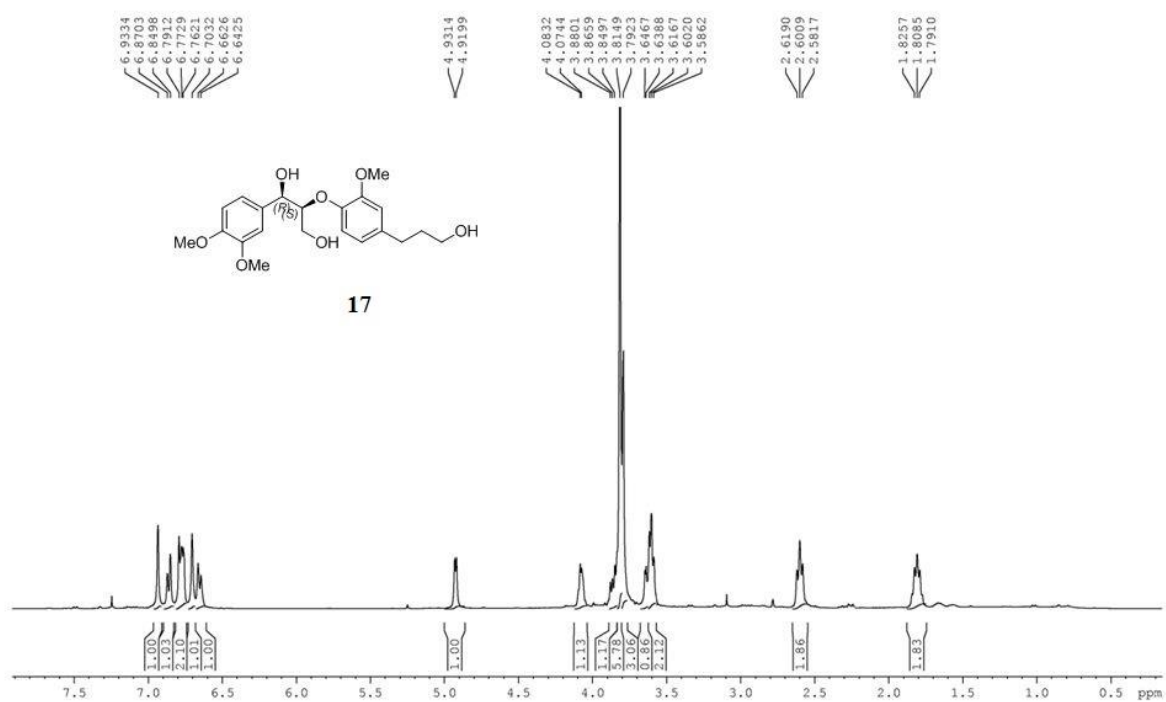




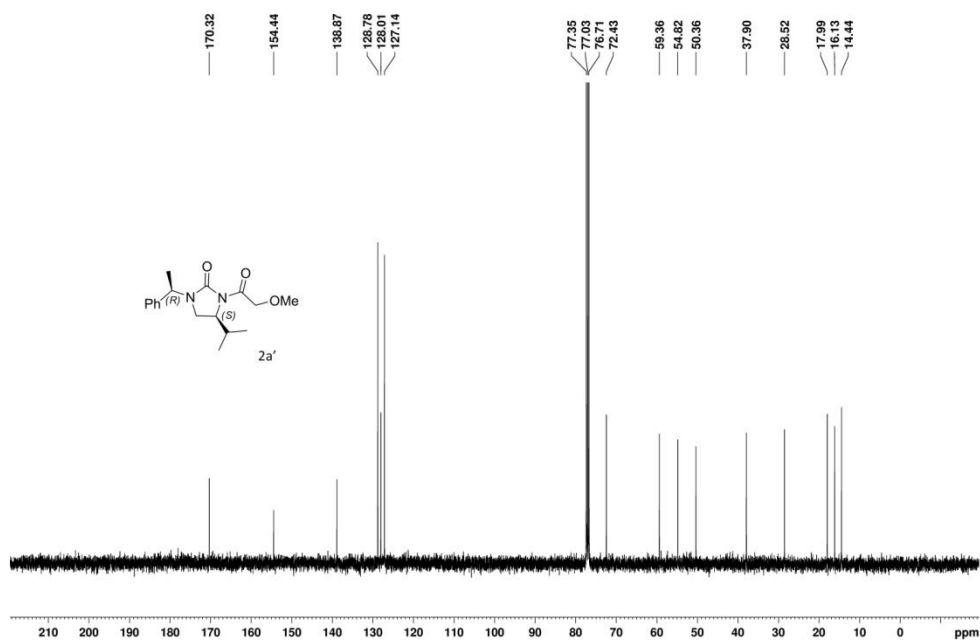
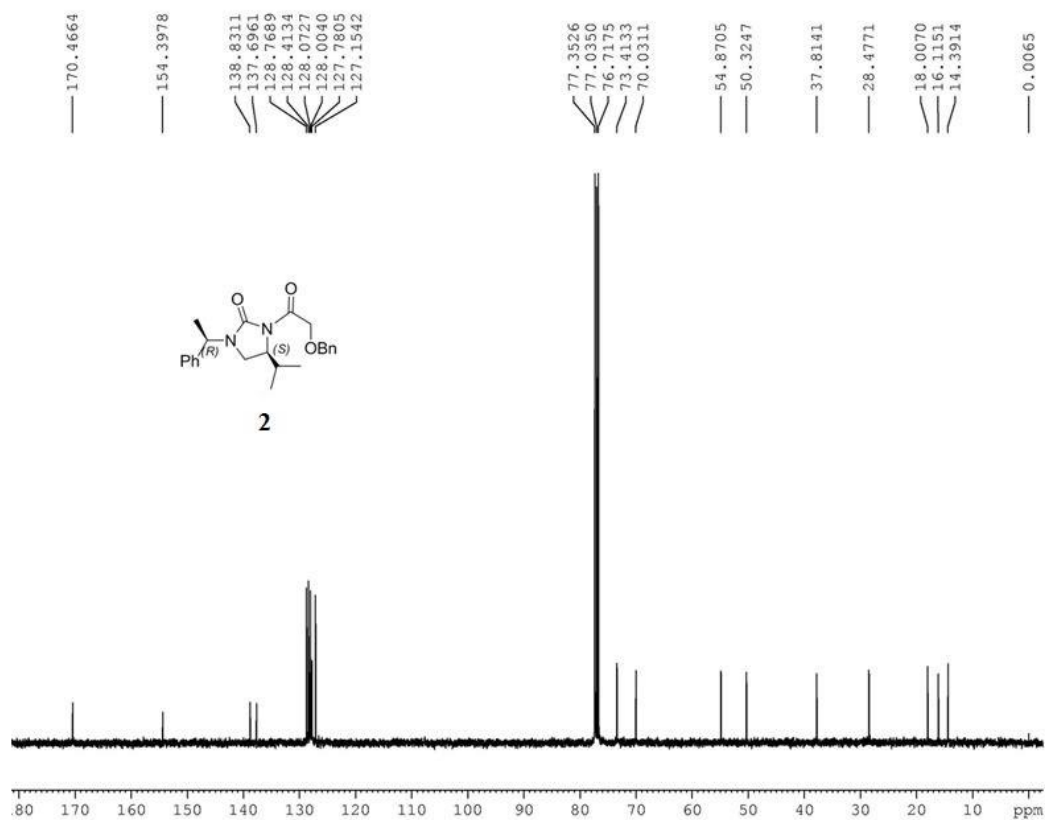


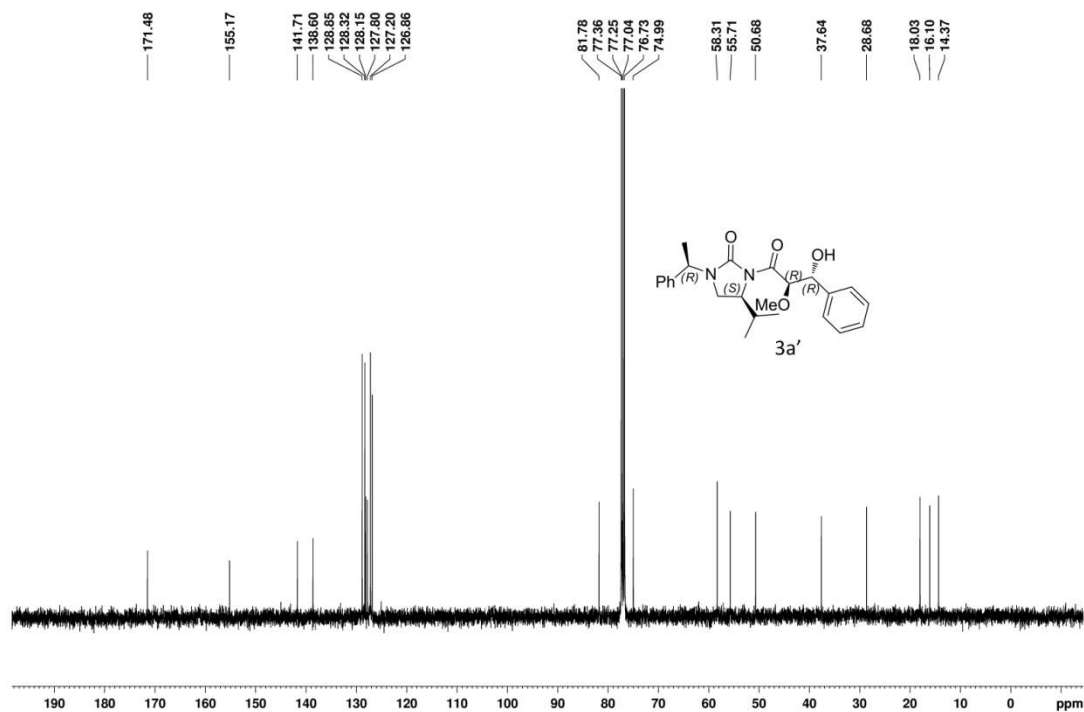
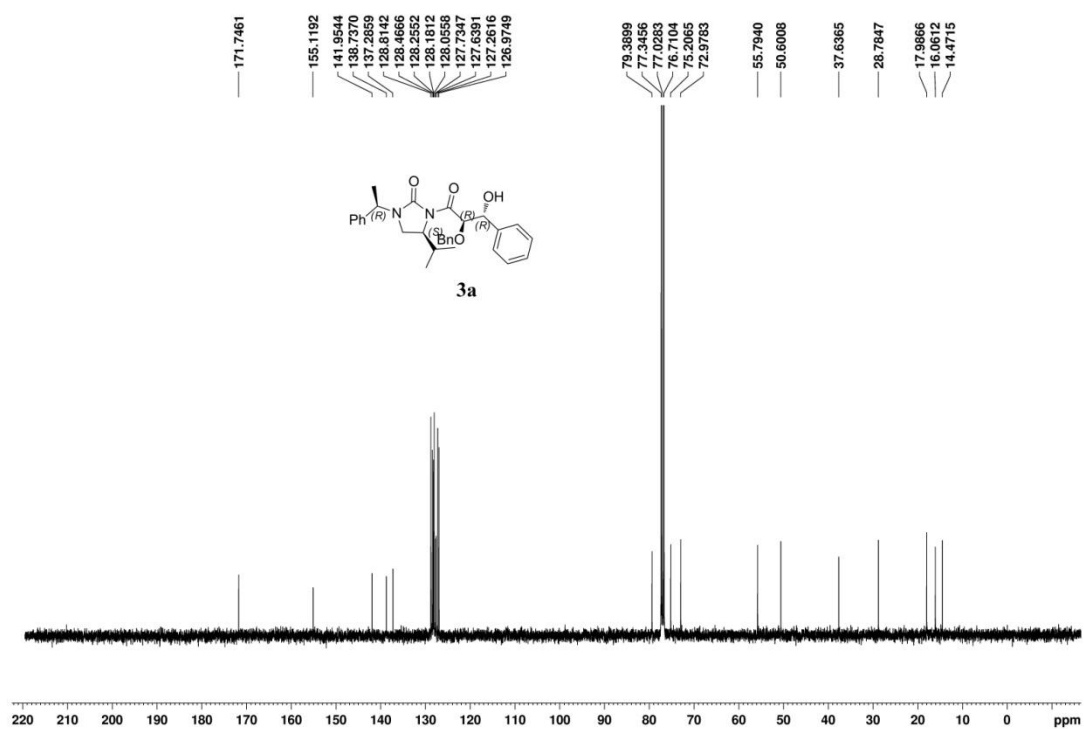


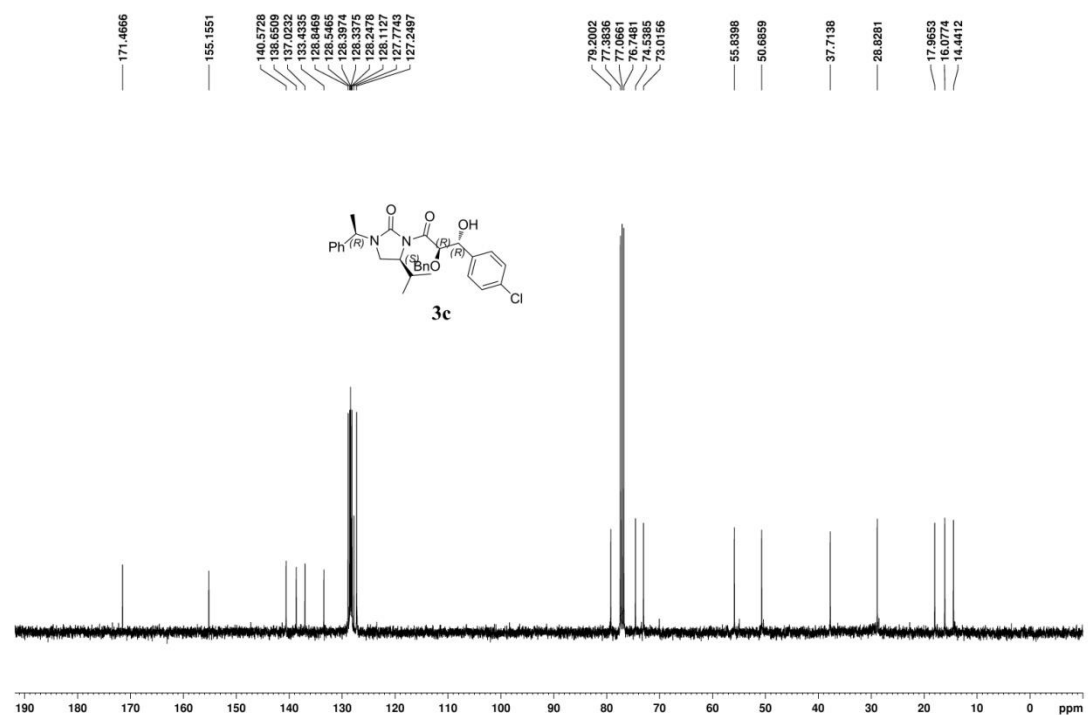
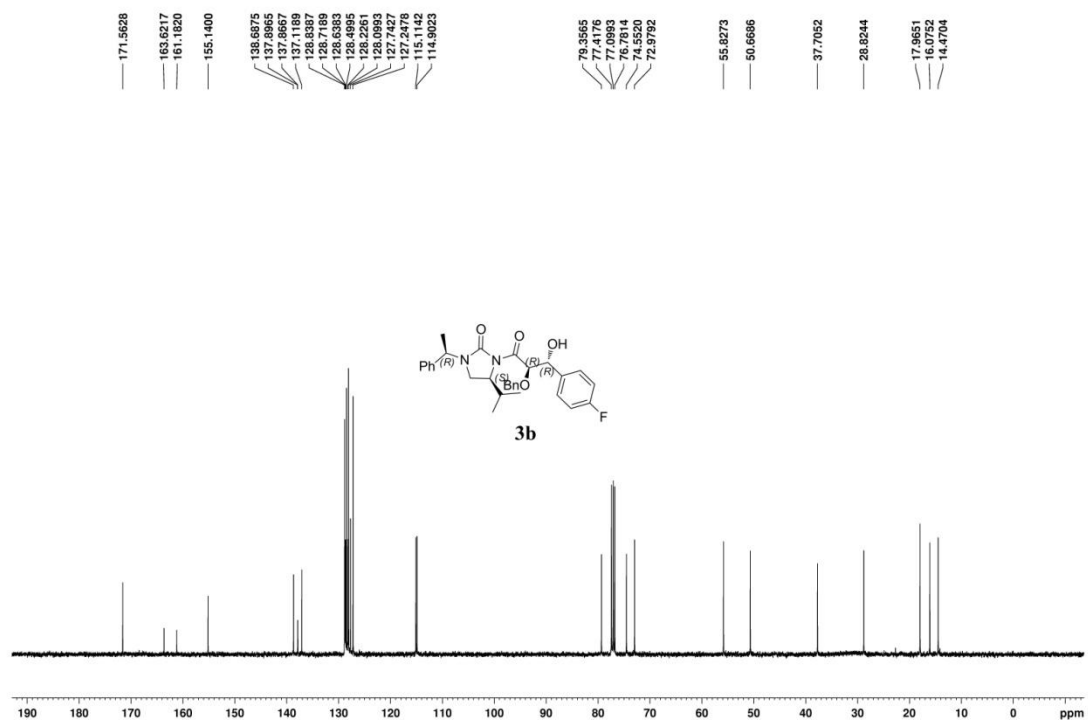


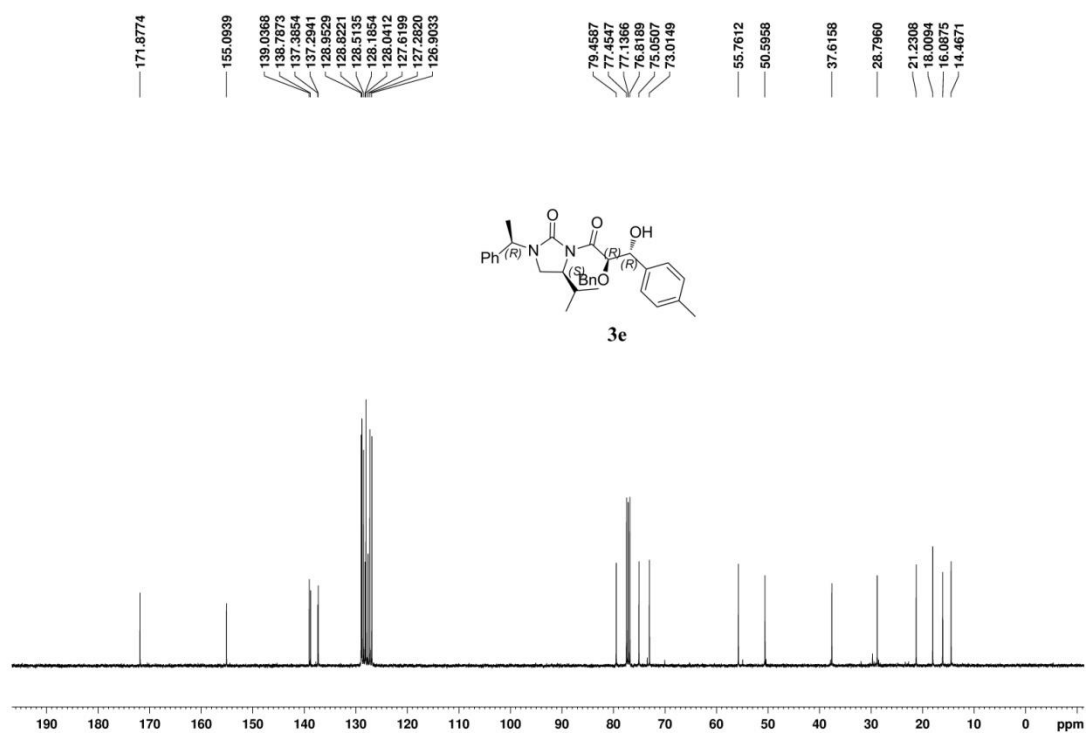
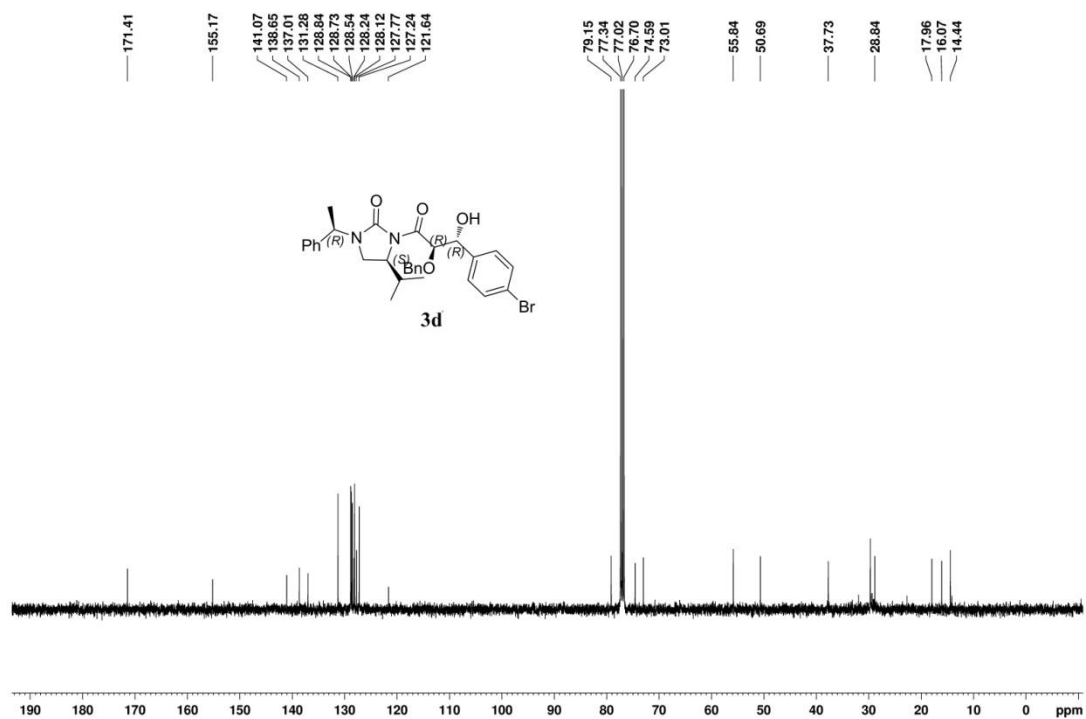


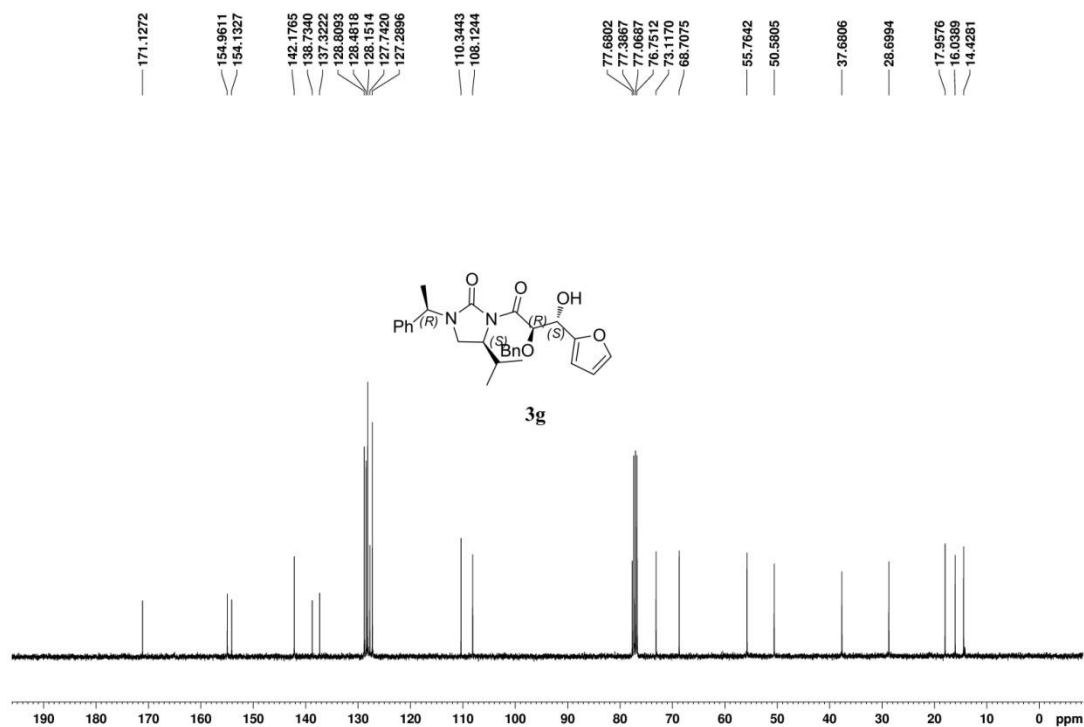
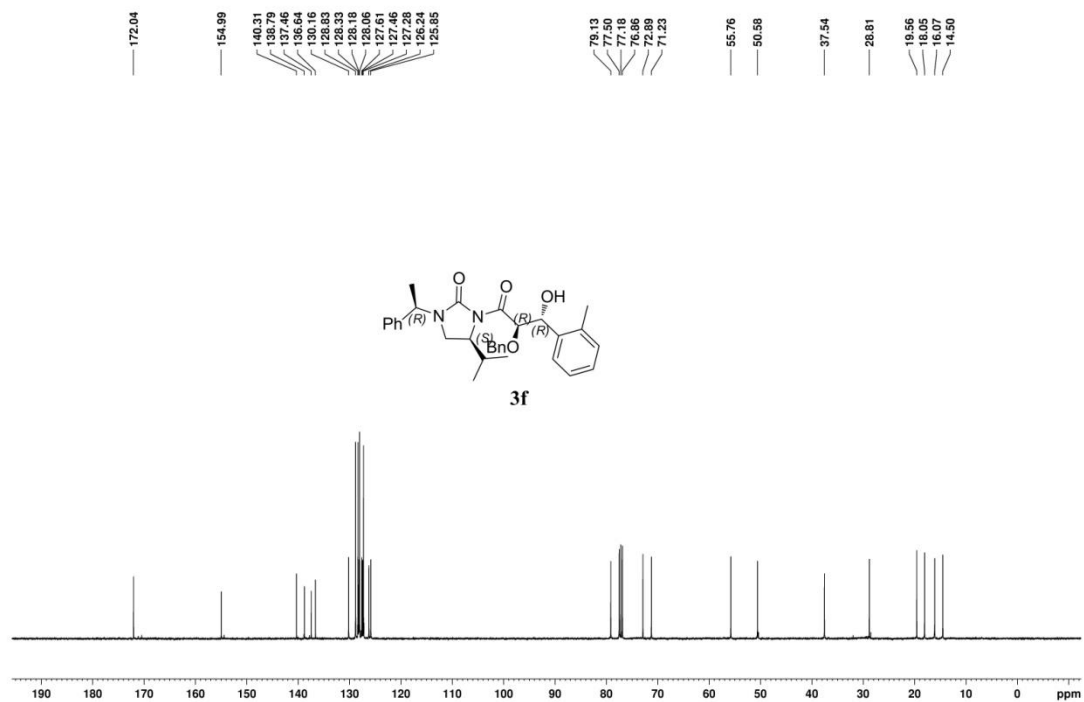
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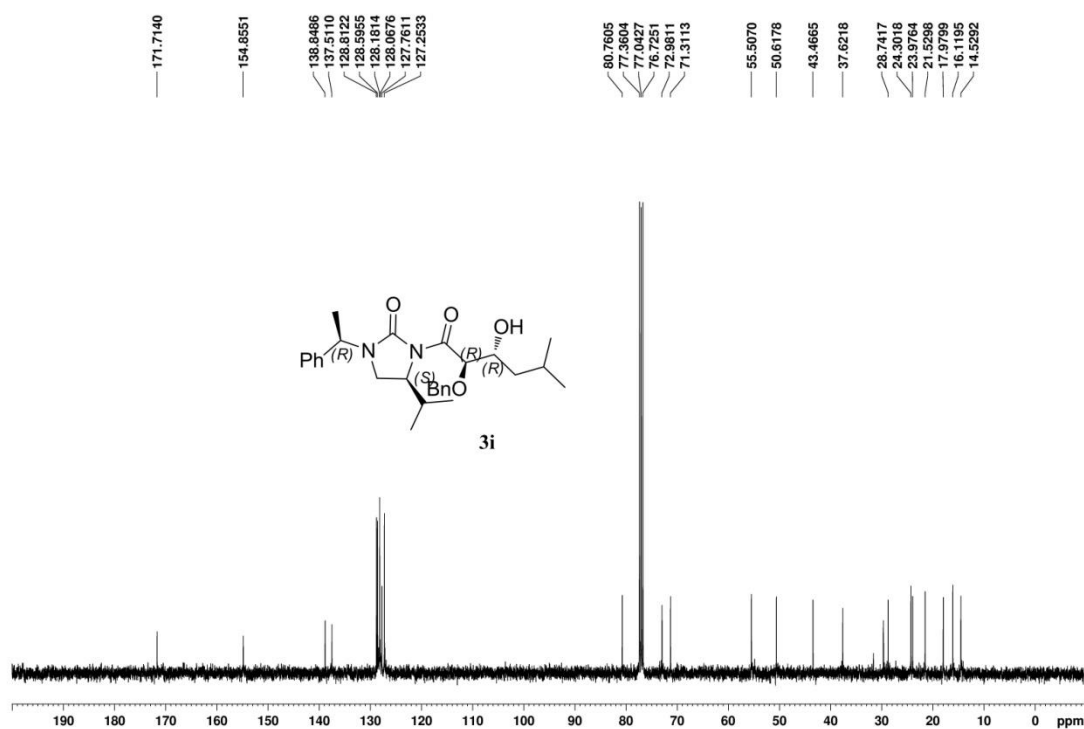
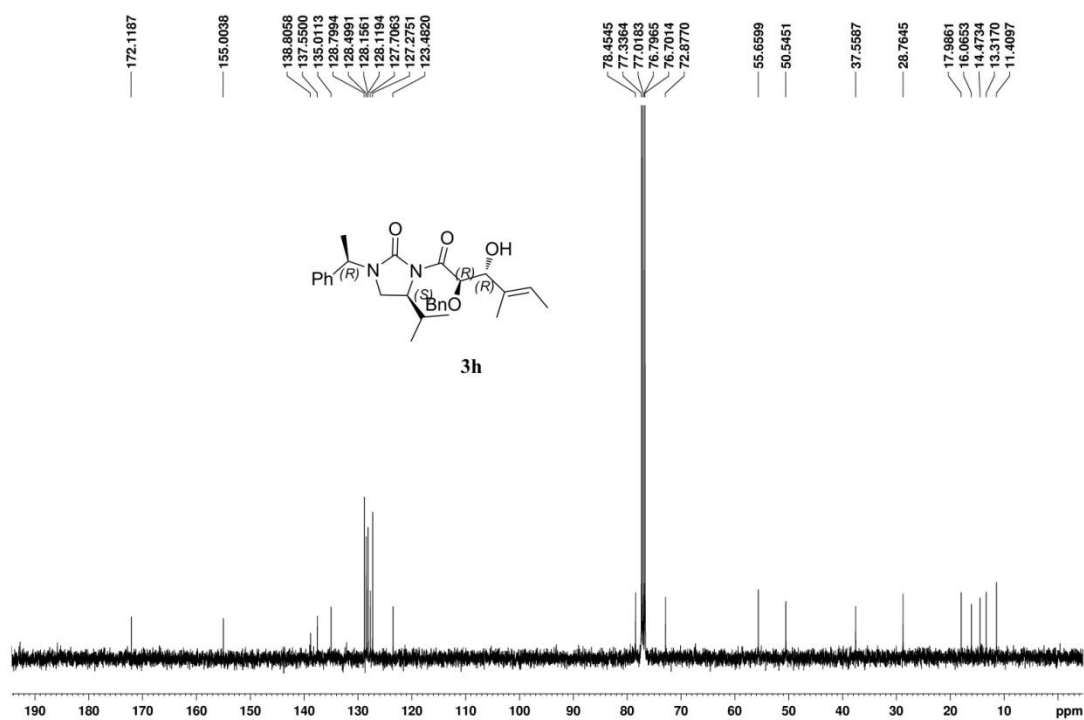


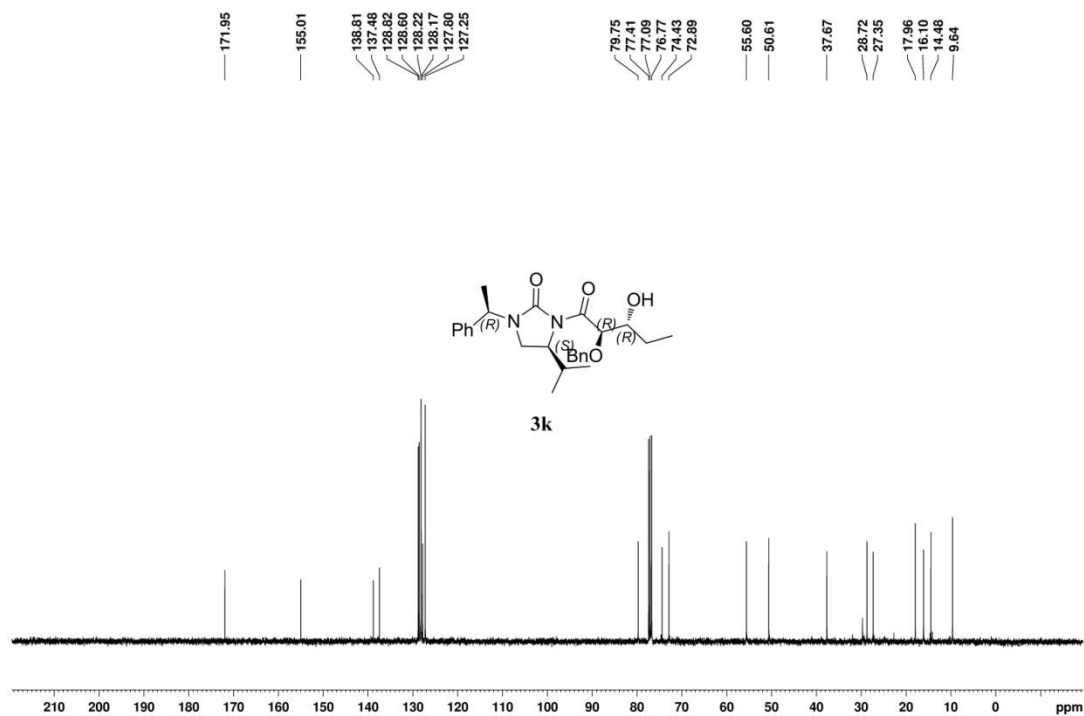
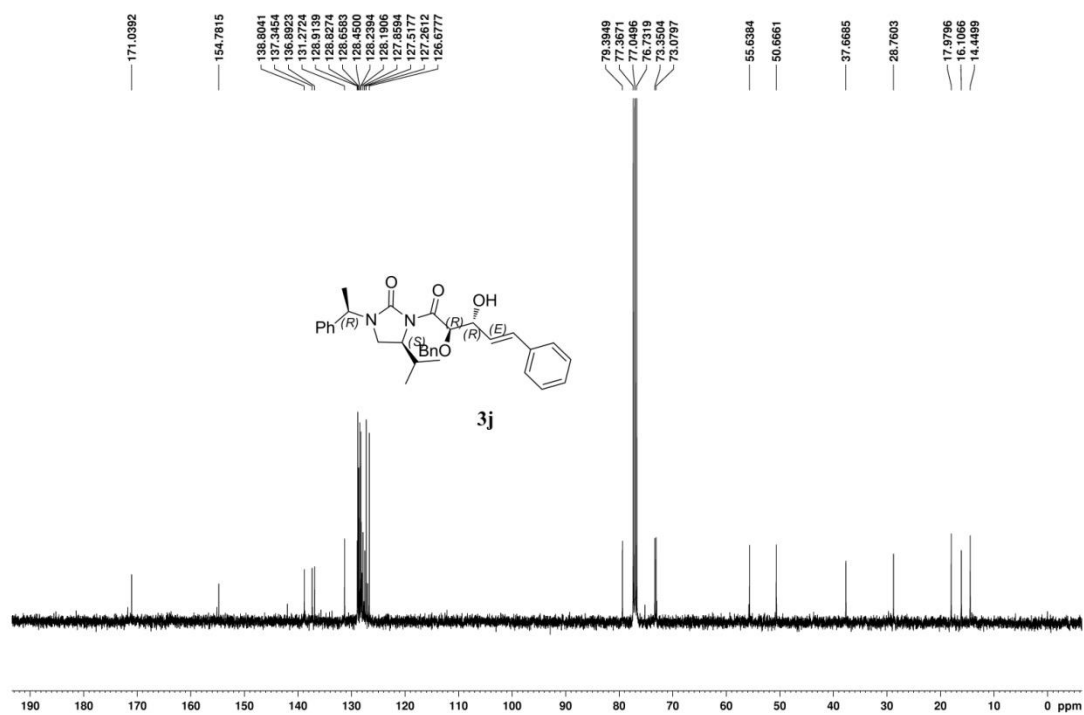


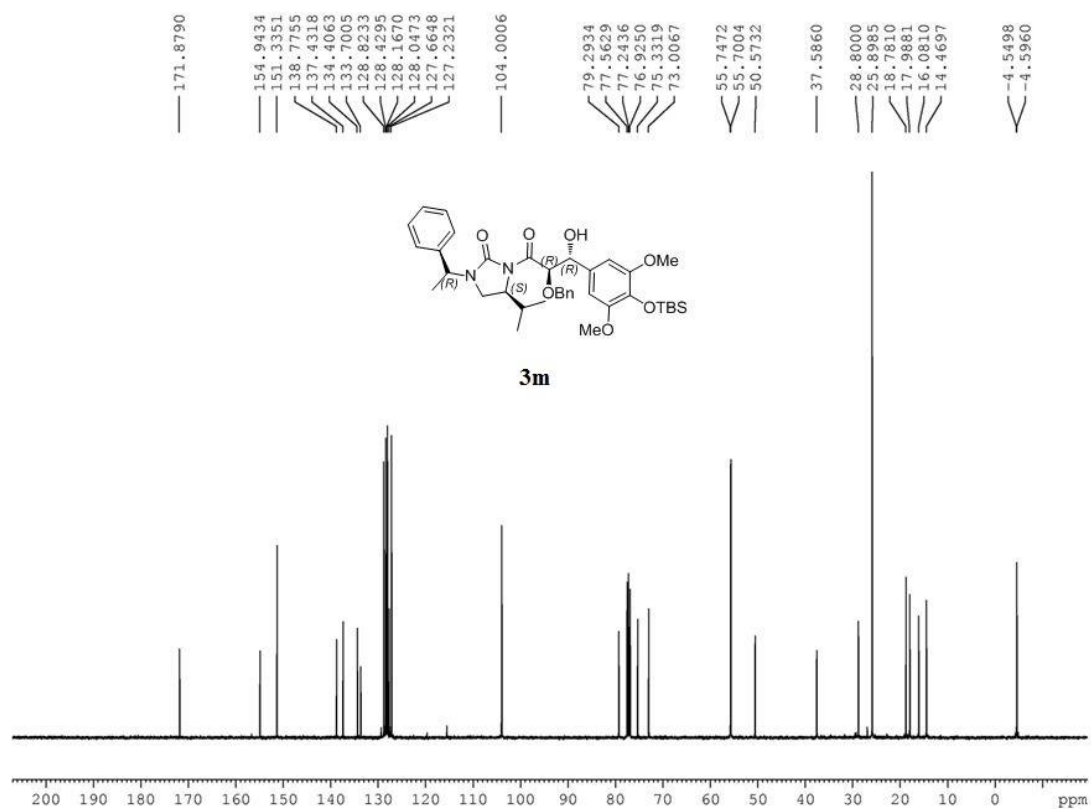
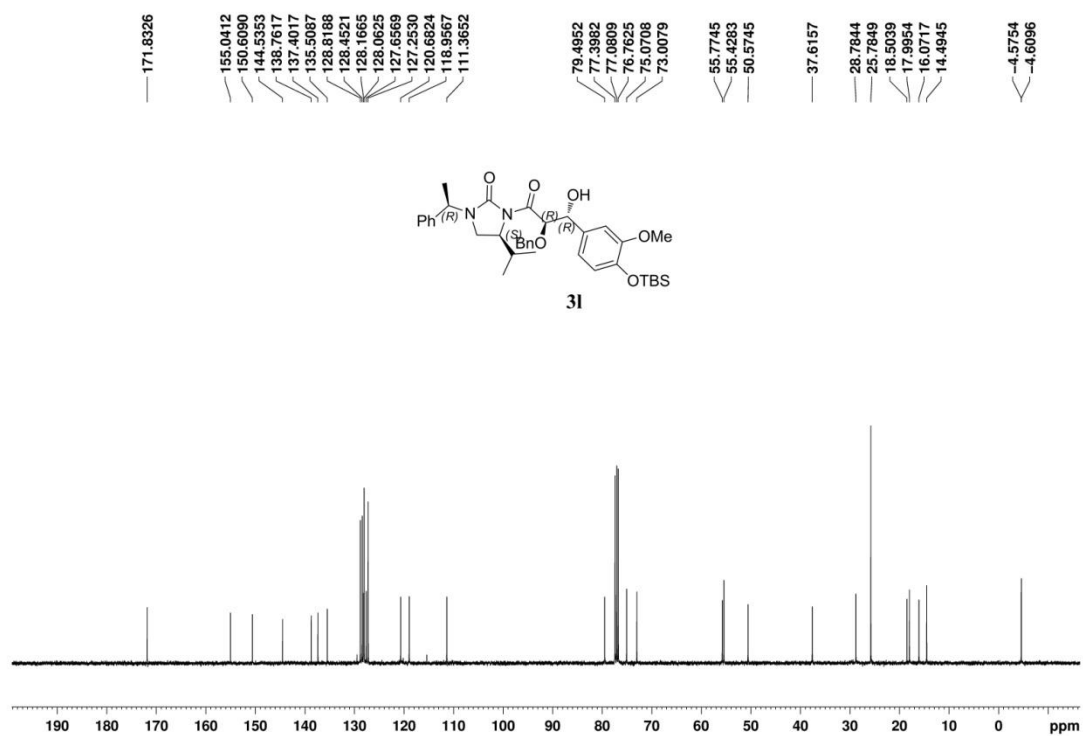


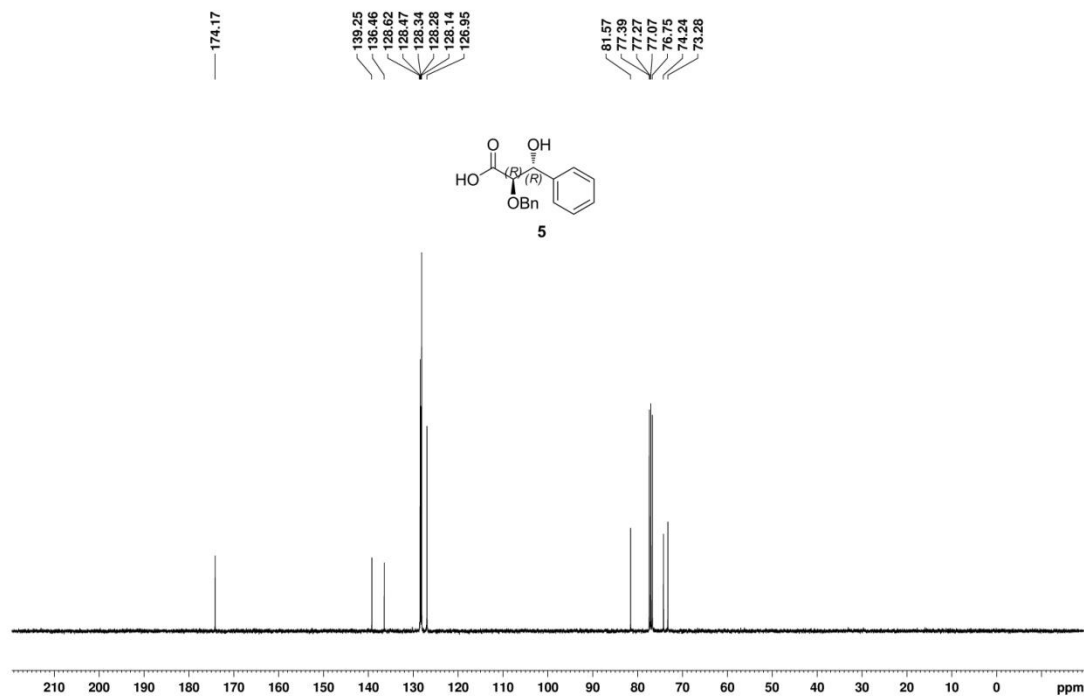
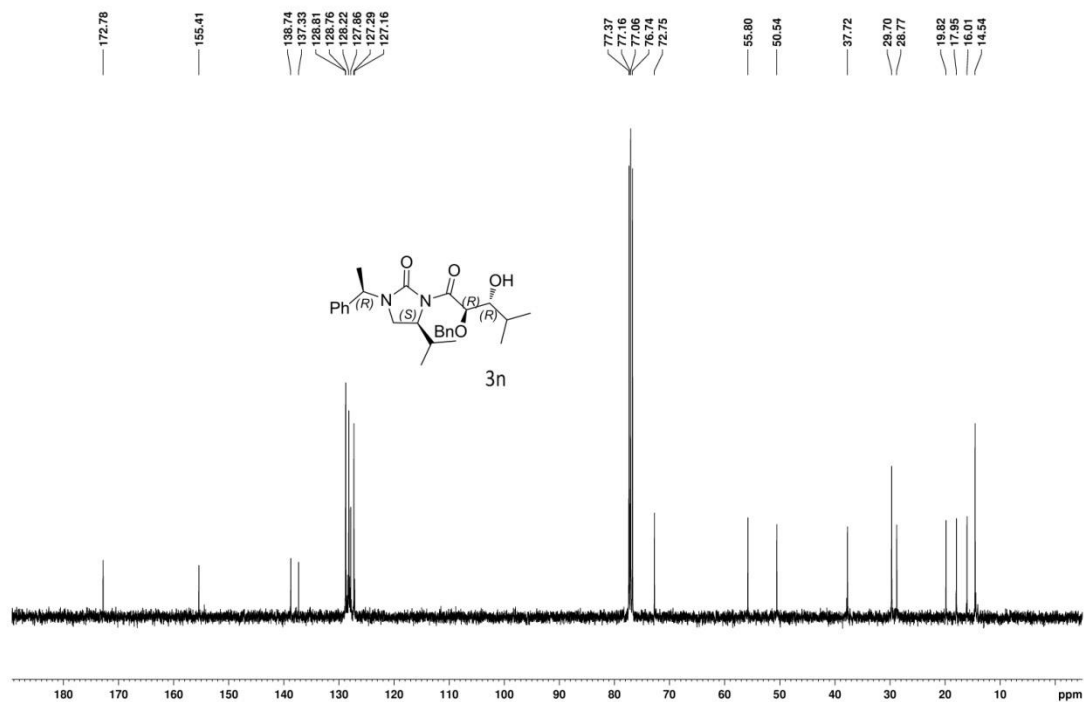


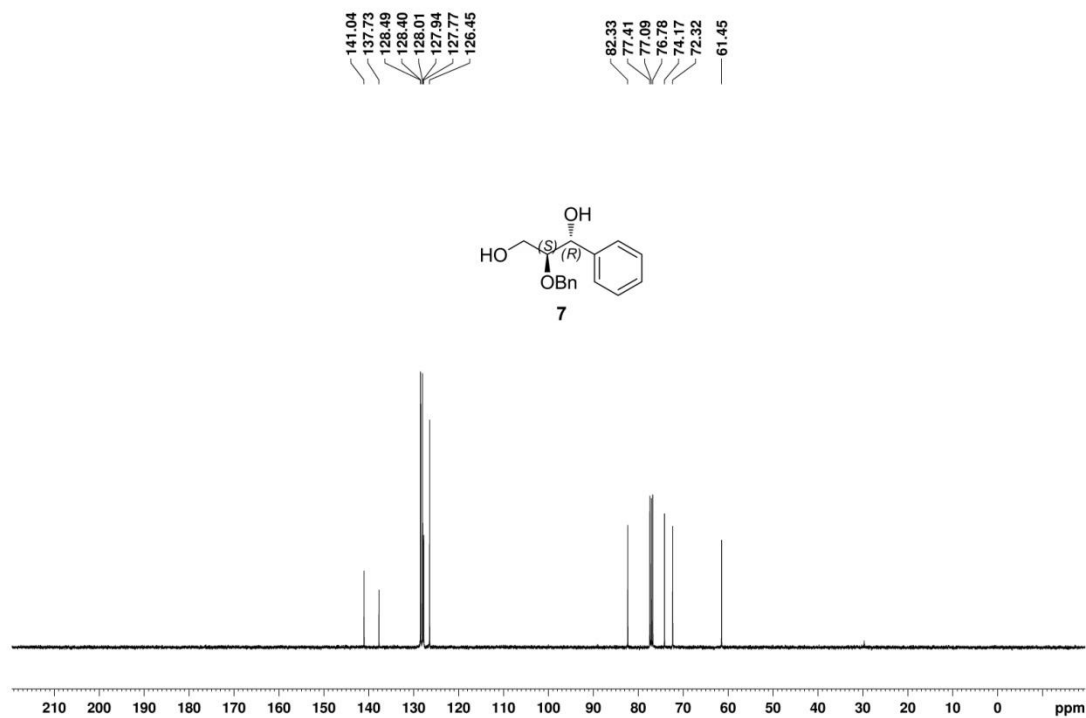
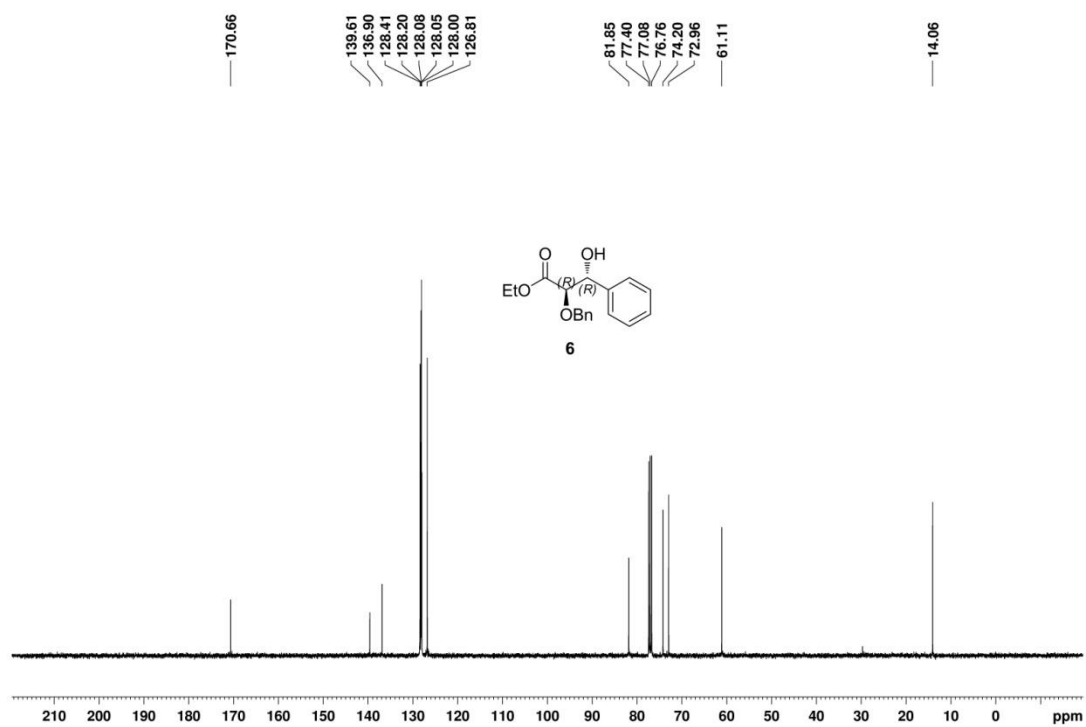


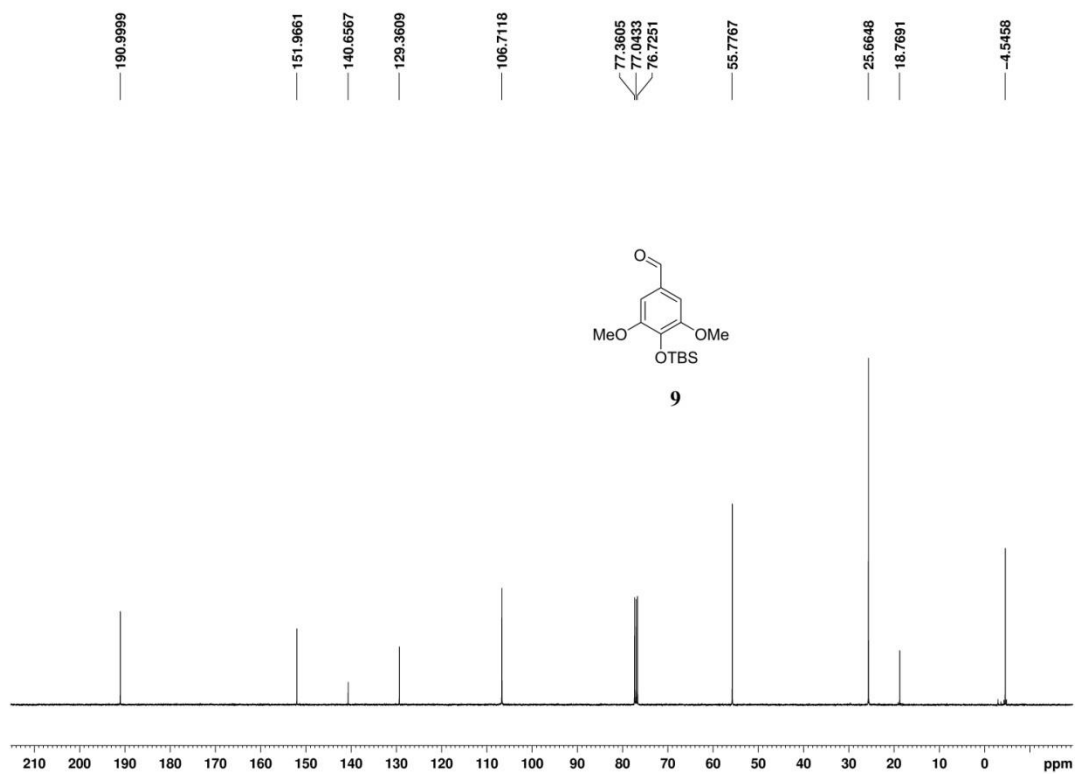
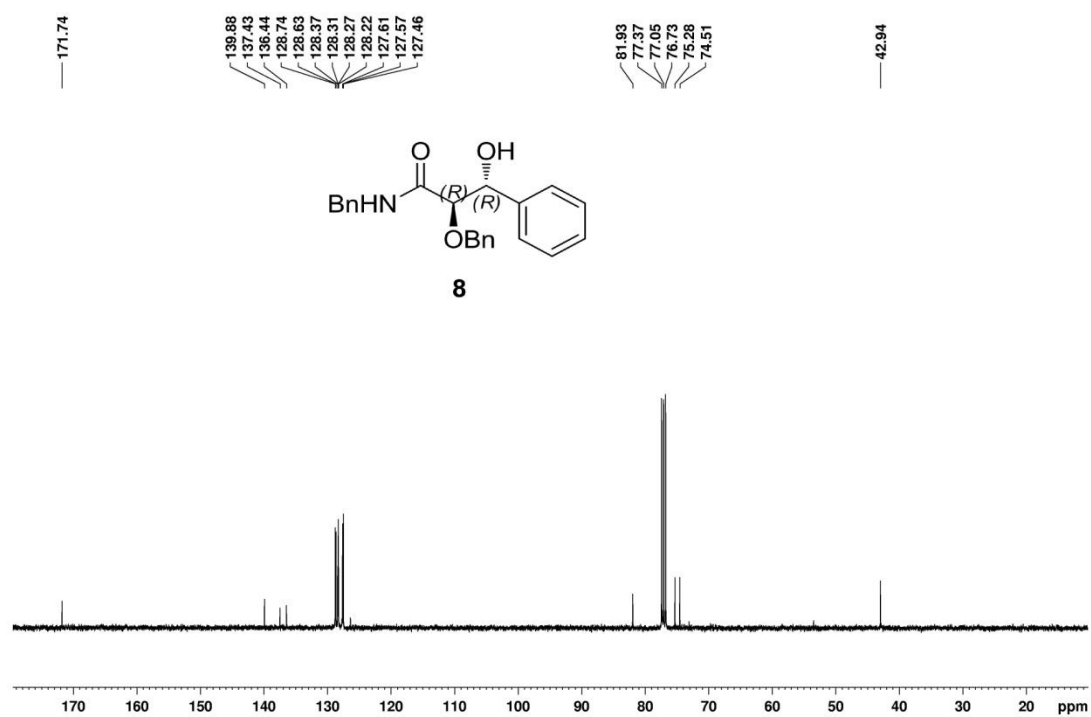


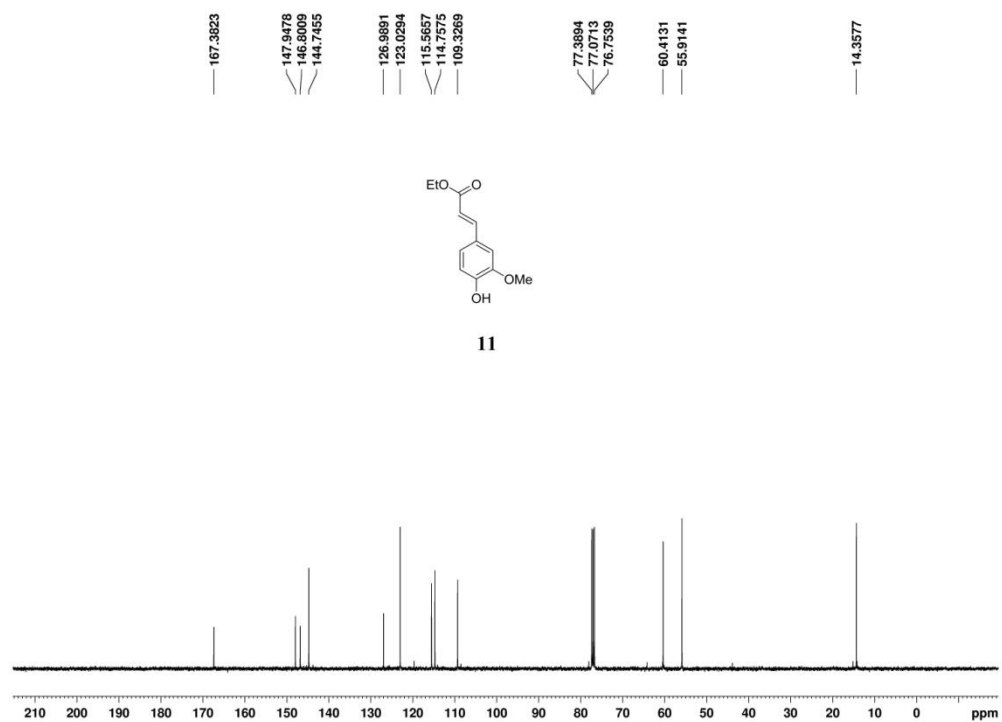
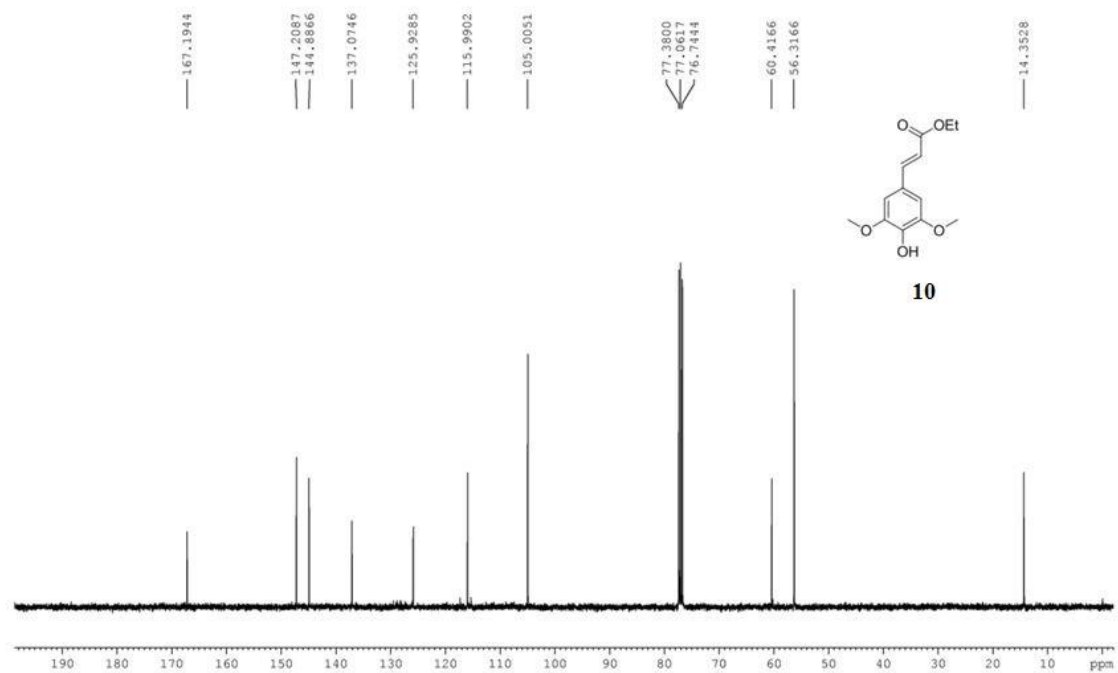


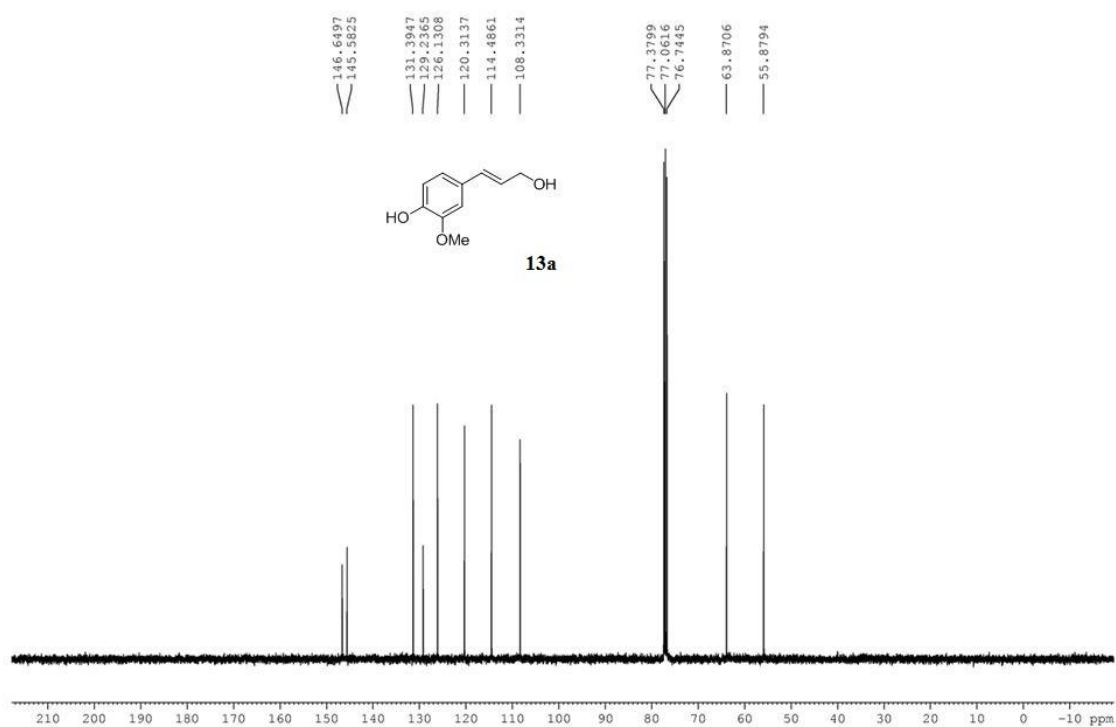
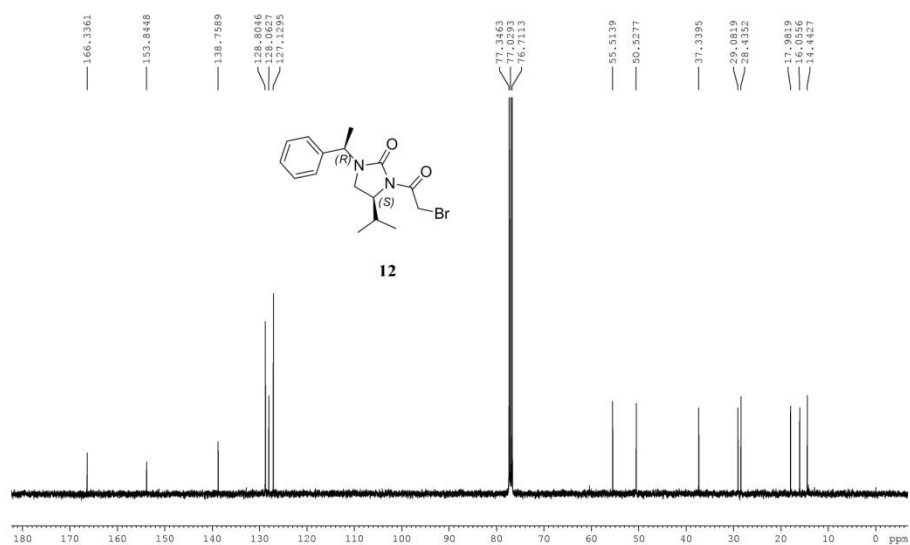


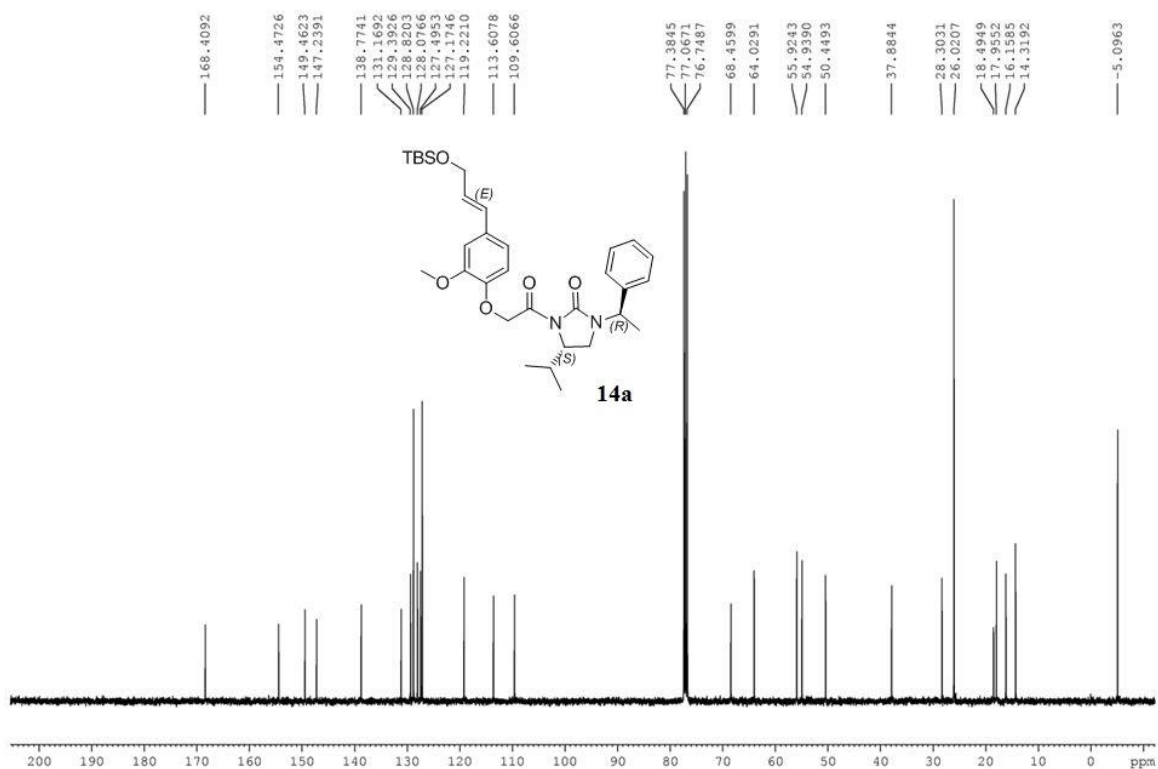
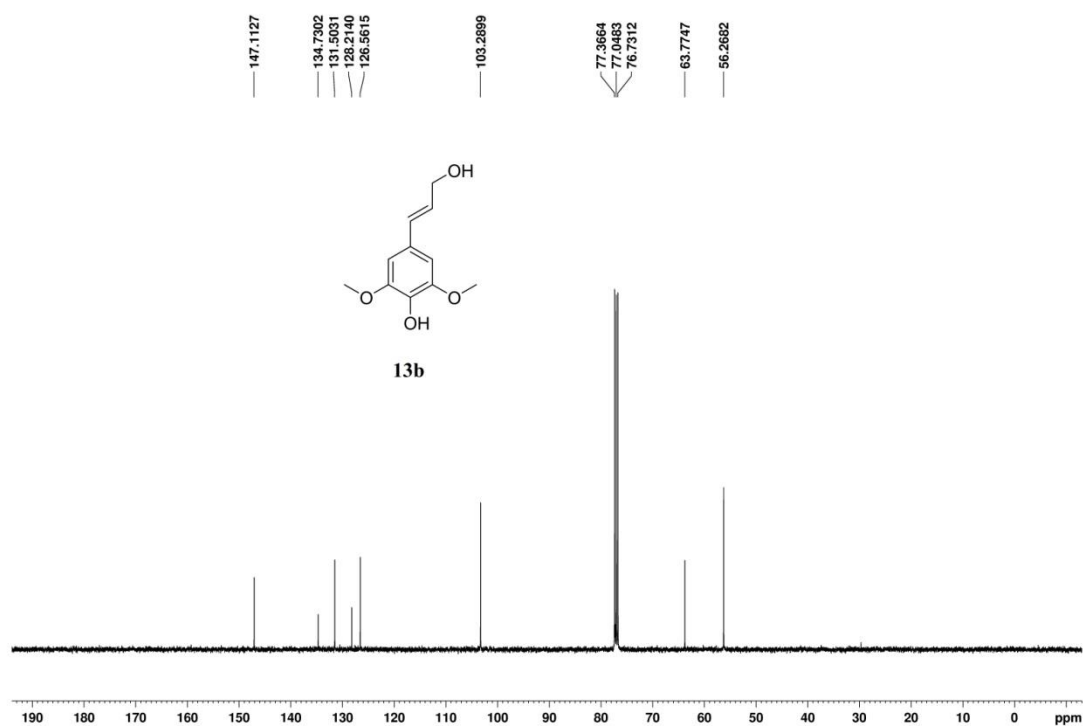


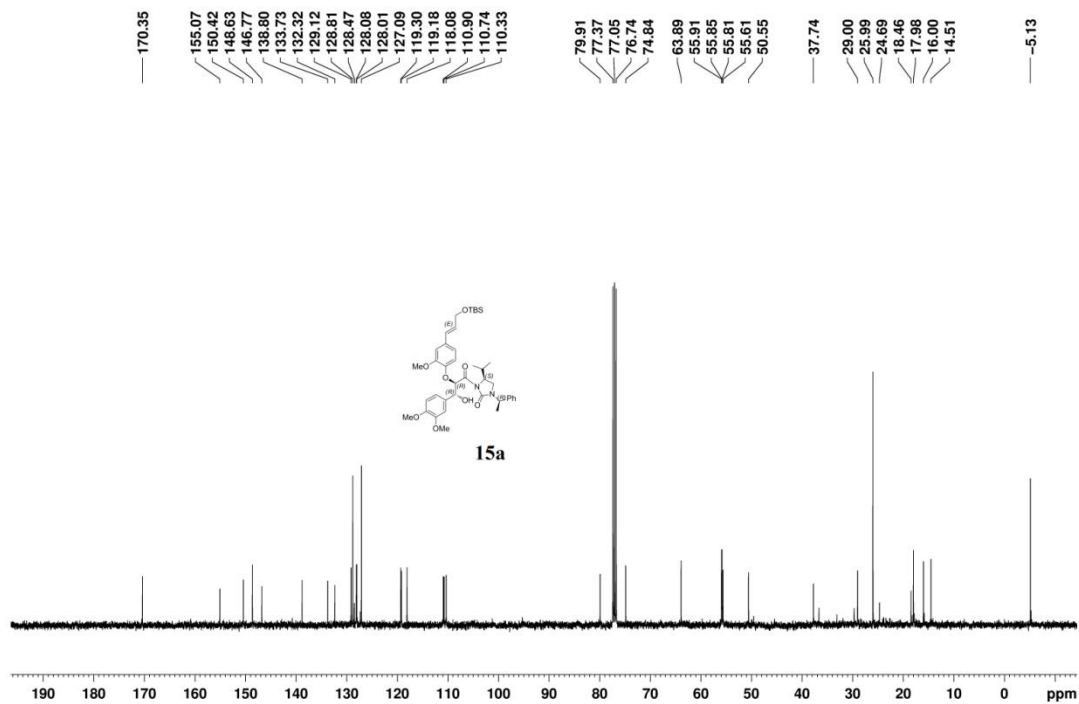
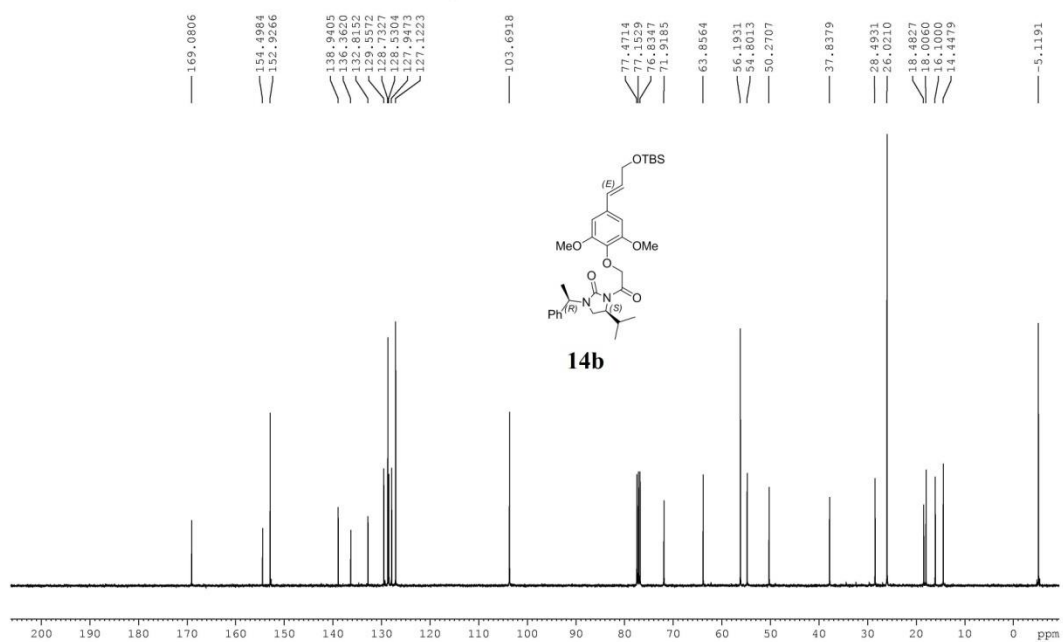


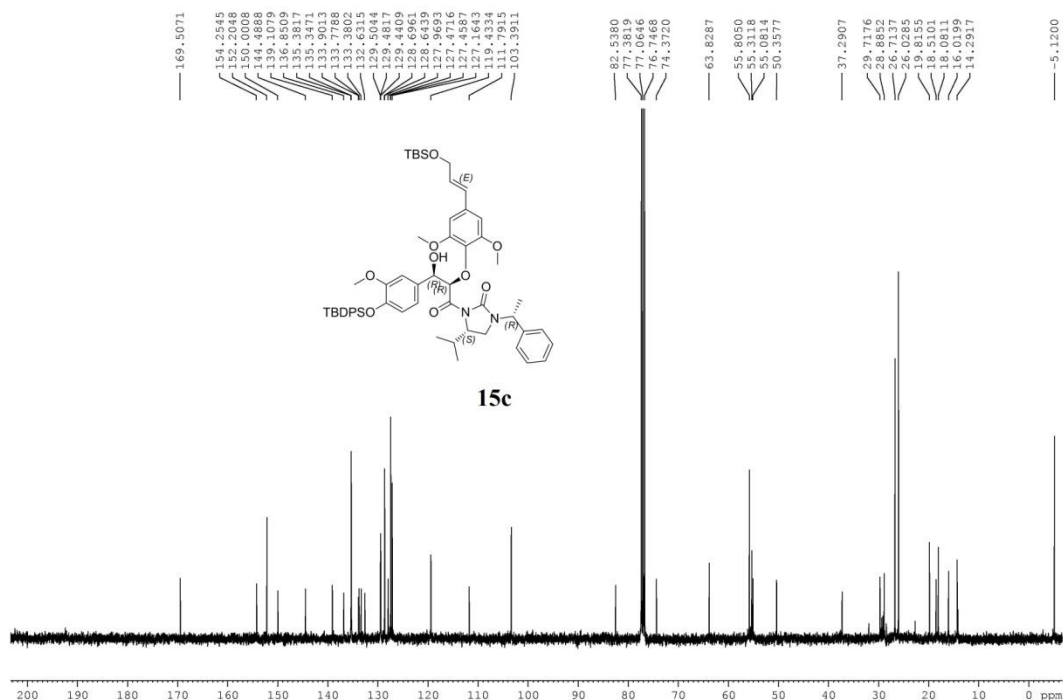
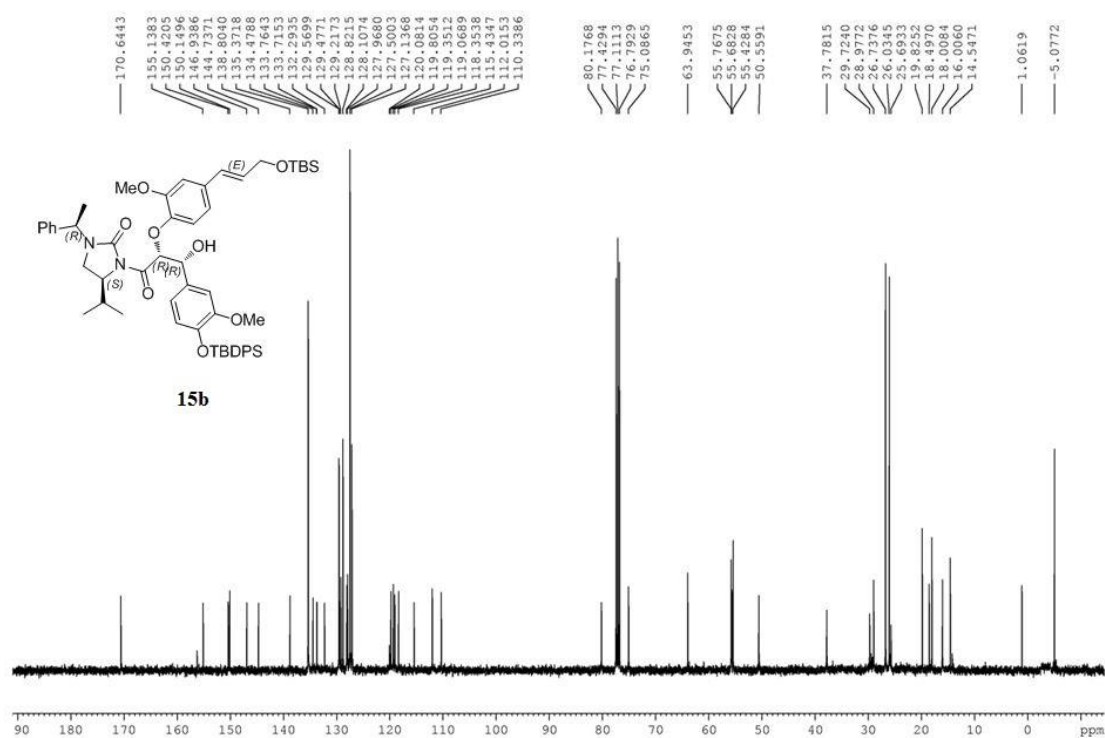


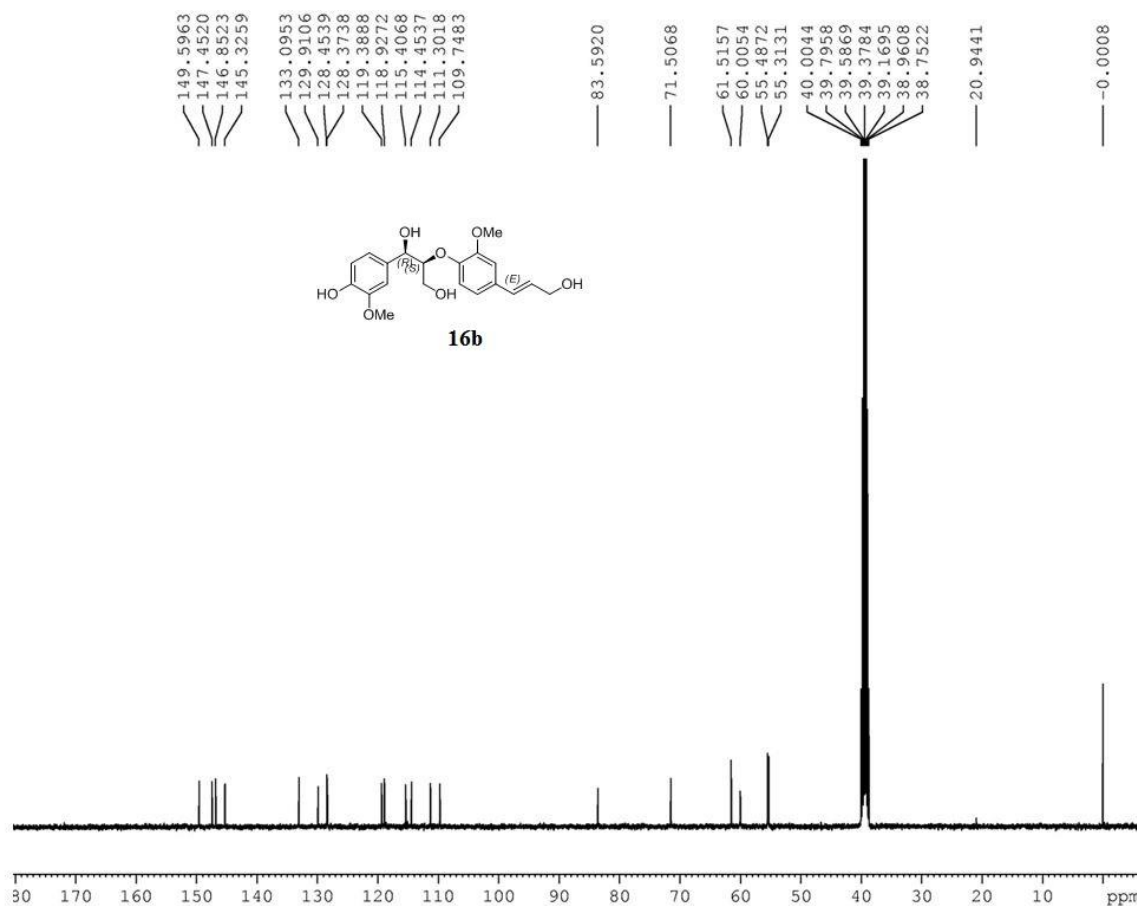
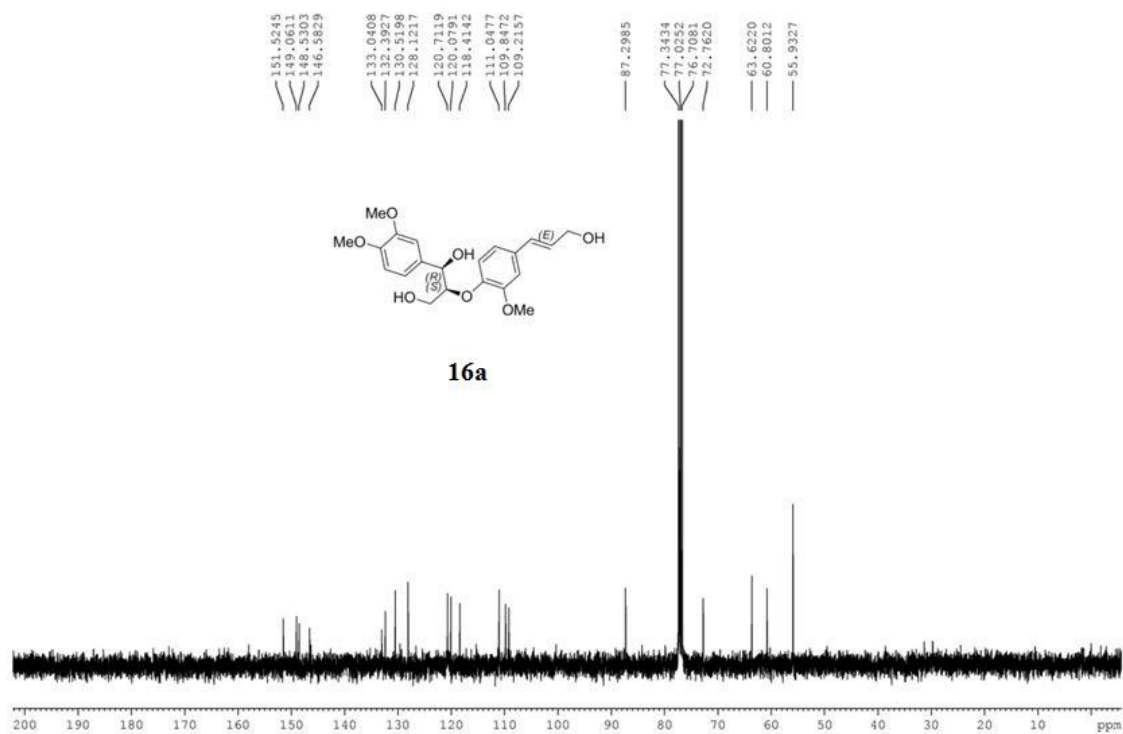


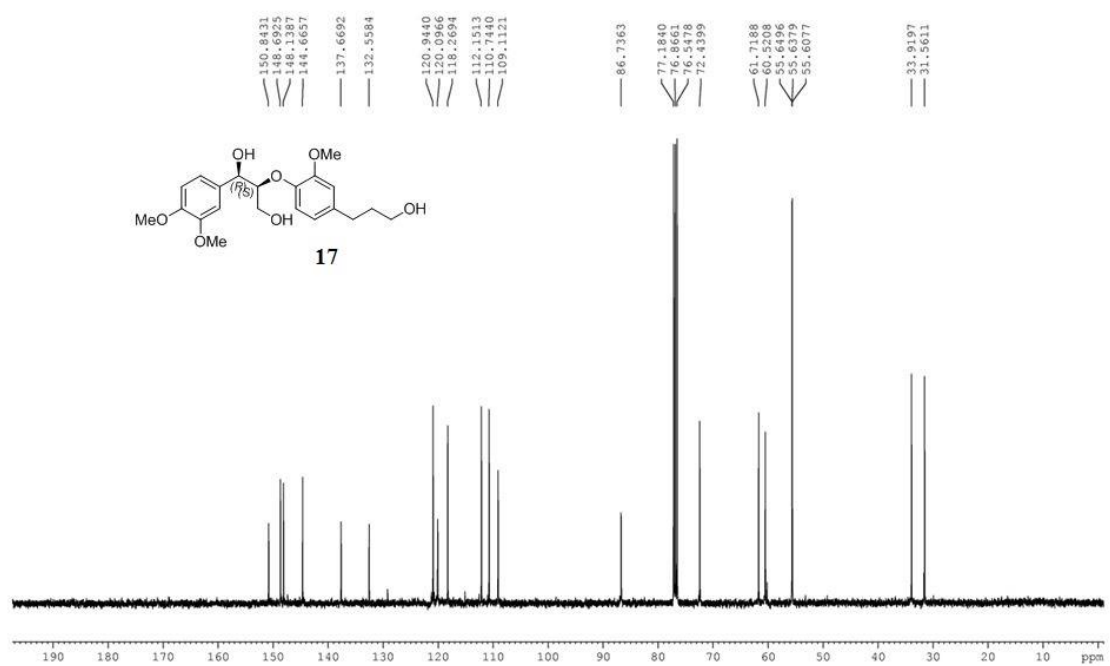
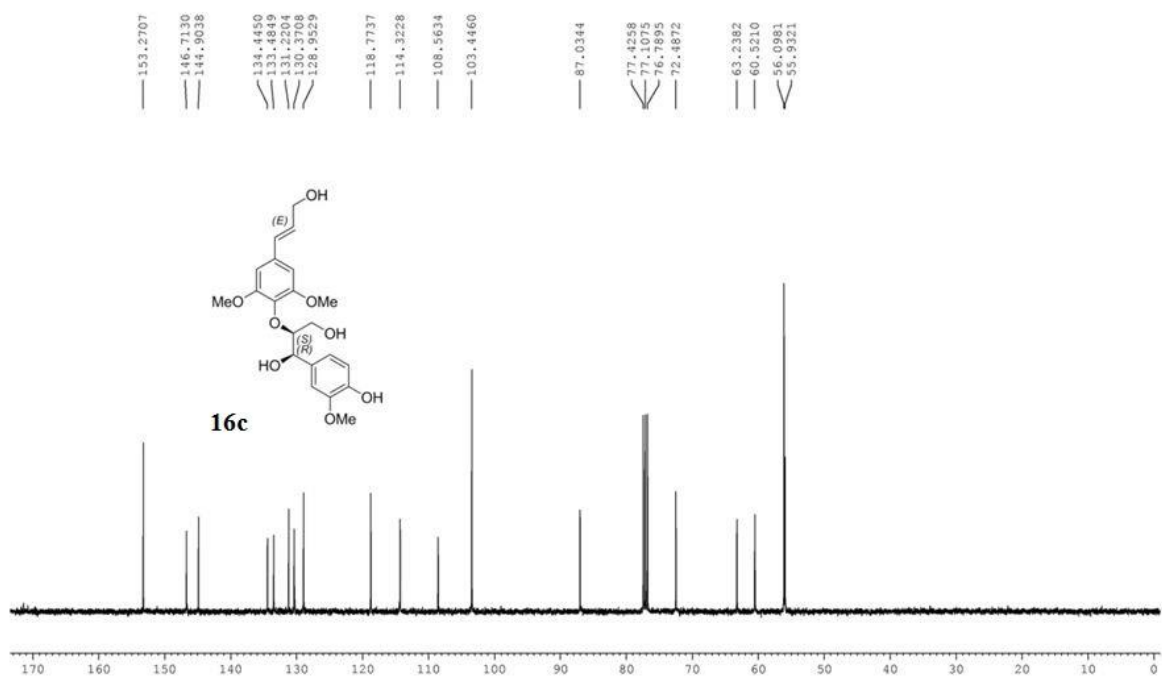












## Copies of HRMS Spectra

### Mass Spectrum List Report

#### Analysis Info

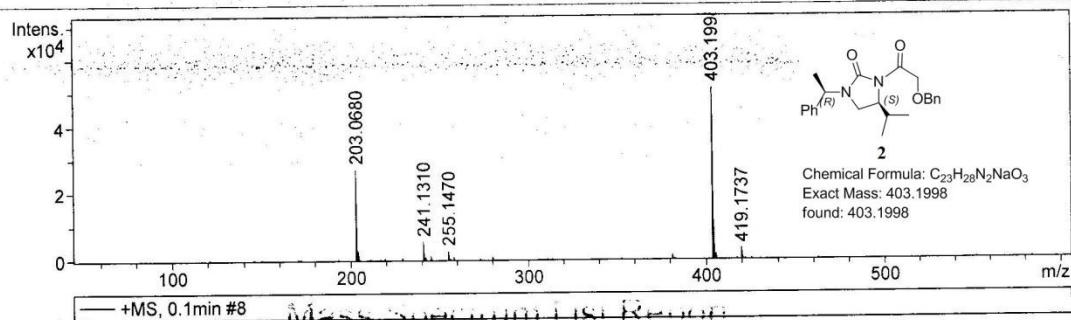
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 Method sodium formate tune\_low.m  
 Sample Name 12-02-14-DGK-046  
 Comment

Acquisition Date 2/14/2012 4:52:38 PM

Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

#### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.4 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| # | m/z      | Res.  | S/N   | I     | FWHM   |
|---|----------|-------|-------|-------|--------|
| 1 | 203.0680 | 22336 | 412.1 | 27152 | 0.0091 |
| 2 | 241.1310 | 22048 | 100.2 | 5673  | 0.0109 |
| 3 | 255.1470 | 23980 | 61.6  | 2794  | 0.0106 |
| 4 | 403.1998 | 23353 | 471.4 | 51253 | 0.0173 |
| 5 | 419.1737 | 25100 | 45.0  | 3241  | 0.0167 |

# Mass Spectrum List Report

## Analysis Info

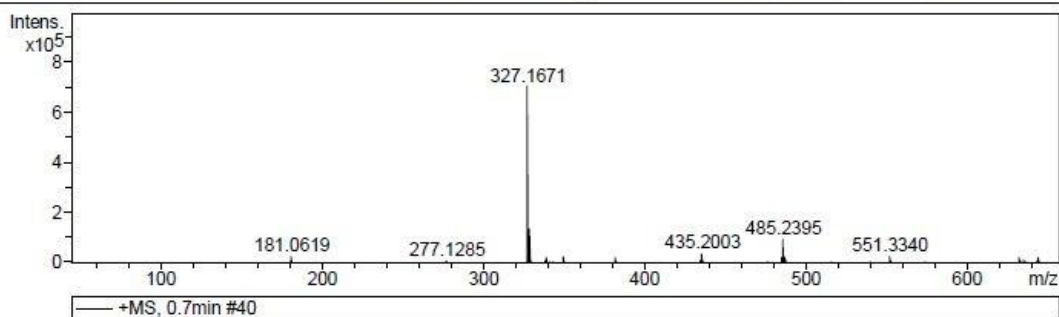
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Method UPLC HRMS LOW.m  
Sample Name MGG-73  
Comment

Acquisition Date 9/22/2016 4:14:05 PM

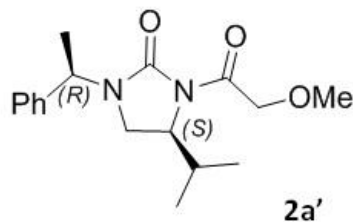
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 650 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N     | I      | FWHM   |
|----|----------|-------|---------|--------|--------|
| 1  | 180.0653 | 13814 | 720.0   | 6998   | 0.0130 |
| 2  | 181.0619 | 14013 | 3063.5  | 29867  | 0.0129 |
| 3  | 277.1285 | 15165 | 716.4   | 10105  | 0.0183 |
| 4  | 327.1671 | 14678 | 31259.2 | 703256 | 0.0223 |
| 5  | 328.1704 | 14955 | 6067.3  | 135290 | 0.0219 |
| 6  | 329.1739 | 14469 | 732.5   | 16199  | 0.0228 |
| 7  | 338.1378 | 15058 | 557.7   | 11333  | 0.0225 |
| 8  | 339.1340 | 15422 | 1216.0  | 24450  | 0.0220 |
| 9  | 341.1833 | 15090 | 220.7   | 4358   | 0.0226 |
| 10 | 343.1417 | 14564 | 387.7   | 7493   | 0.0236 |
| 11 | 349.1488 | 15572 | 1460.8  | 26434  | 0.0224 |
| 12 | 350.1525 | 15414 | 277.5   | 4979   | 0.0227 |
| 13 | 381.1751 | 15670 | 1782.0  | 24297  | 0.0243 |
| 14 | 382.1784 | 14890 | 348.8   | 4713   | 0.0257 |
| 15 | 434.2040 | 15723 | 596.8   | 8695   | 0.0276 |
| 16 | 435.2003 | 15729 | 2546.0  | 37363  | 0.0277 |
| 17 | 436.2036 | 15261 | 490.4   | 7263   | 0.0286 |
| 18 | 484.2430 | 15646 | 1331.7  | 22319  | 0.0310 |
| 19 | 485.2395 | 15857 | 5817.8  | 96413  | 0.0306 |
| 20 | 486.2428 | 15717 | 1387.0  | 22736  | 0.0309 |
| 21 | 515.3342 | 15931 | 395.0   | 4665   | 0.0323 |
| 22 | 551.3340 | 15942 | 1727.4  | 26326  | 0.0346 |
| 23 | 552.3373 | 15495 | 604.8   | 9282   | 0.0356 |
| 24 | 631.3446 | 15876 | 1303.9  | 23901  | 0.0398 |
| 25 | 632.3479 | 15954 | 508.1   | 9428   | 0.0396 |
| 26 | 634.3705 | 15549 | 697.6   | 13242  | 0.0408 |
| 27 | 635.3743 | 15114 | 279.2   | 5328   | 0.0420 |
| 28 | 642.3152 | 15910 | 589.7   | 11240  | 0.0404 |



Chemical formula: C<sub>17</sub>H<sub>24</sub>N<sub>2</sub>NaO<sub>3</sub>

Exact Mass: 327.1685

Found: 327.1671

# Mass Spectrum List Report

## Analysis Info

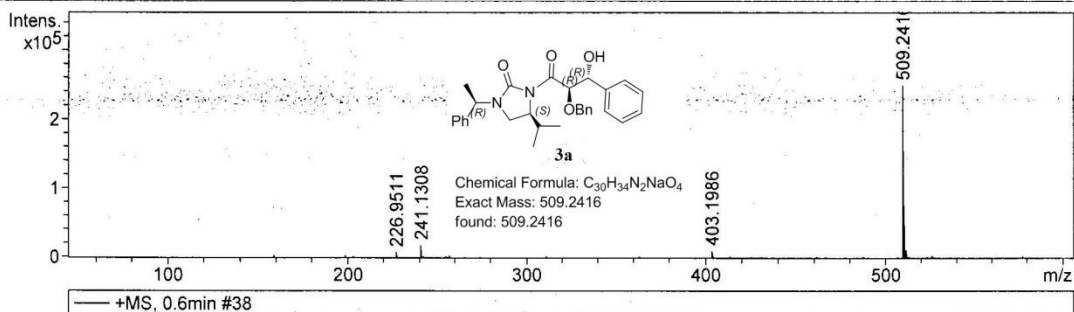
Analysis Name D:\Data\vipin\12-02-14-DGK-085.d  
Method sodium formate tune\_low.m  
Sample Name 12-02-14-DGK-085  
Comment

Acquisition Date 2/15/2012 10:40:02 AM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.4 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #   | m/z      | Res.  | S/N    | I      | FWHM   |
|-----|----------|-------|--------|--------|--------|
| 1   | 226.9511 | 24378 | 106.3  | 7730   | 0.0093 |
| 2   | 241.1308 | 25262 | 238.1  | 18519  | 0.0095 |
| 3   | 403.1986 | 25838 | 225.0  | 10696  | 0.0156 |
| ⇒ 4 | 509.2416 | 24657 | 1329.8 | 249017 | 0.0207 |

## Mass Spectrum List Report

### Analysis Info

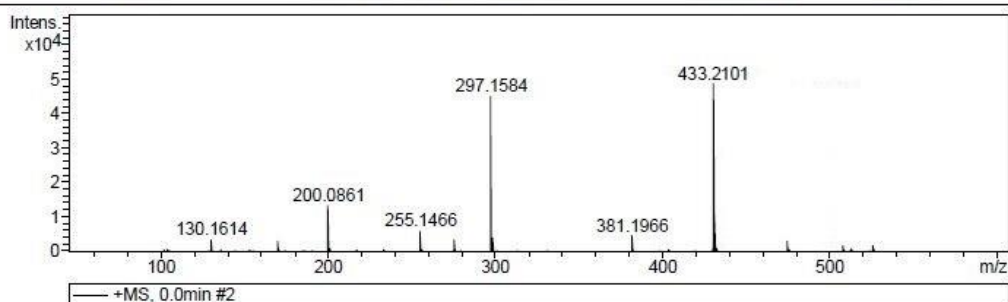
Analysis Name D:\Data\vipin\14-03-31-AT-104.d  
 Method sodium formate tune\_low.m  
 Sample Name AT-104  
 Comment

Acquisition Date 9/21/2016 2:52:17 PM

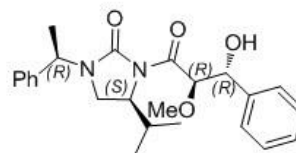
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N   | I     | FWHM   |
|----|----------|-------|-------|-------|--------|
| 1  | 102.1352 | 14878 | 16.3  | 624   | 0.0069 |
| 2  | 104.1140 | 12860 | 19.9  | 780   | 0.0081 |
| 3  | 130.1614 | 17074 | 66.1  | 3450  | 0.0076 |
| 4  | 136.1136 | 15378 | 12.4  | 686   | 0.0089 |
| 5  | 153.1384 | 15822 | 13.6  | 737   | 0.0097 |
| 6  | 170.0960 | 16076 | 63.8  | 3327  | 0.0106 |
| 7  | 200.0861 | 17018 | 178.9 | 13543 | 0.0118 |
| 8  | 201.0897 | 16916 | 13.7  | 1048  | 0.0119 |
| 9  | 255.1466 | 16911 | 82.1  | 5988  | 0.0151 |
| 10 | 275.1759 | 16559 | 33.4  | 3591  | 0.0166 |
| 11 | 297.1584 | 17110 | 427.2 | 45038 | 0.0174 |
| 12 | 298.1611 | 16281 | 39.3  | 4047  | 0.0183 |
| 13 | 381.1966 | 17473 | 97.3  | 4663  | 0.0218 |
| 14 | 382.1997 | 15183 | 17.1  | 836   | 0.0252 |
| 15 | 403.1765 | 16404 | 12.1  | 727   | 0.0246 |
| 16 | 433.2101 | 18188 | 374.3 | 48572 | 0.0273 |
| 17 | 497.2295 | 19175 | 72.6  | 9682  | 0.0259 |
| 18 | 507.2588 | 19755 | 11.6  | 1968  | 0.0257 |
| 19 | 525.2221 | 17966 | 14.7  | 1881  | 0.0292 |



**3a'**

Chemical formula:  $C_{24}H_{30}N_2NaO_4$

Exact Mass: 433.2103

Found: 433.2101

# Mass Spectrum List Report

## Analysis Info

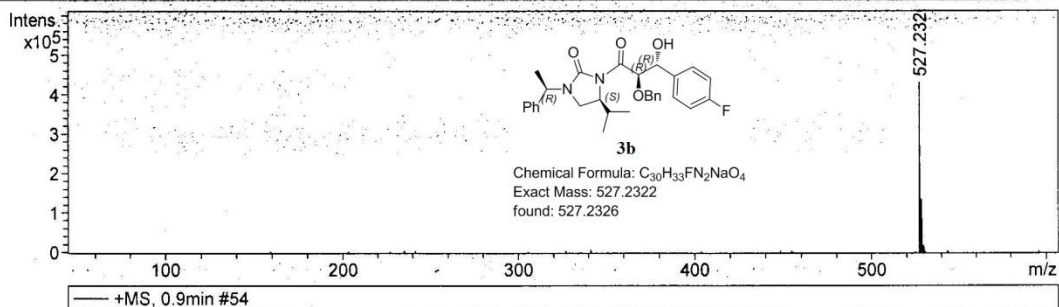
Analysis Name D:\Data\vipin\120-02-16-DGK-89.d  
Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-89  
Comment

Acquisition Date 2/16/2012 1:41:01 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.4 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| # | m/z      | Res.  | S/N    | I      | FWHM   |
|---|----------|-------|--------|--------|--------|
| 1 | 527.2326 | 24523 | 2537.1 | 429674 | 0.0215 |
| 2 | 528.2357 | 25165 | 821.6  | 135190 | 0.0210 |
| 3 | 529.2380 | 26699 | 129.2  | 20639  | 0.0198 |

# Mass Spectrum List Report

## Analysis Info

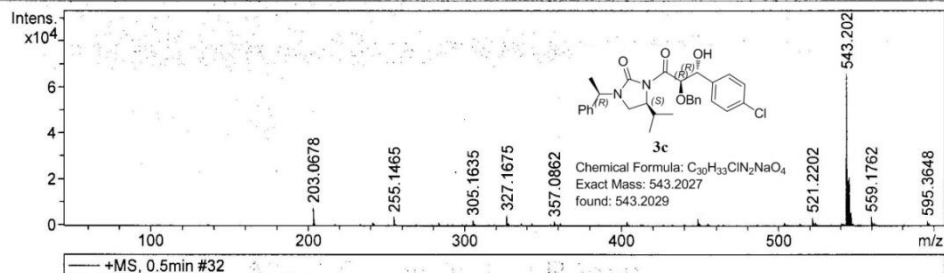
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Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-98  
Comment

Acquisition Date 2/16/2012 4:14:10 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 600 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



| #  | m/z      | Res.  | S/N   | I     | FWHM   |
|----|----------|-------|-------|-------|--------|
| 1  | 203.0678 | 23797 | 177.6 | 7698  | 0.0085 |
| 2  | 255.1465 | 23730 | 74.9  | 3719  | 0.0108 |
| 3  | 305.1635 | 25891 | 40.4  | 2309  | 0.0118 |
| 4  | 327.1675 | 25931 | 78.5  | 4441  | 0.0126 |
| 5  | 357.0862 | 25528 | 36.9  | 1680  | 0.0140 |
| 6  | 448.2570 | 26865 | 68.8  | 3065  | 0.0167 |
| 7  | 521.2202 | 26865 | 48.2  | 3619  | 0.0194 |
| 8  | 543.2029 | 26499 | 503.0 | 65568 | 0.0205 |
| 9  | 544.2058 | 27346 | 148.0 | 19664 | 0.0199 |
| 10 | 545.2010 | 25464 | 152.4 | 20625 | 0.0214 |
| 11 | 546.2032 | 26619 | 41.3  | 5697  | 0.0205 |
| 12 | 559.1762 | 26948 | 31.5  | 3686  | 0.0207 |
| 13 | 560.1793 | 26069 | 10.6  | 1212  | 0.0215 |
| 14 | 561.1744 | 24886 | 13.2  | 1468  | 0.0226 |
| 15 | 595.3648 | 27744 | 53.2  | 2204  | 0.0215 |

# Mass Spectrum List Report

## Analysis Info

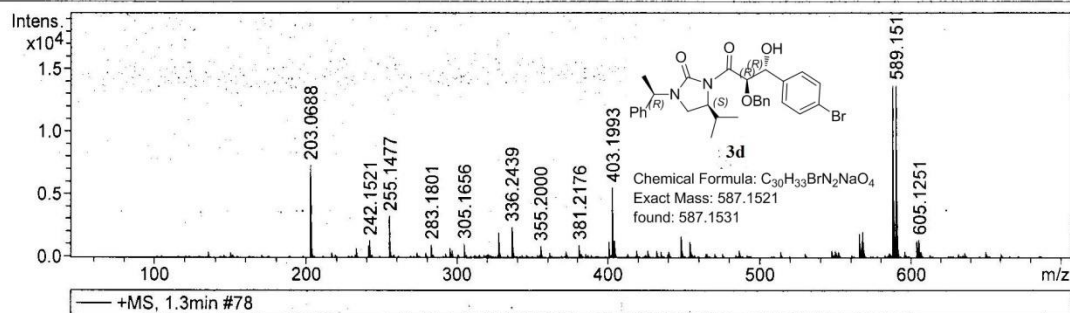
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Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-96  
Comment

Acquisition Date 2/16/2012 3:30:09 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 700 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



| #  | m/z      | Res.  | S/N   | I     | FWHM   |
|----|----------|-------|-------|-------|--------|
| 1  | 203.0688 | 23354 | 185.3 | 7294  | 0.0087 |
| 2  | 242.1521 | 25172 | 30.4  | 1306  | 0.0096 |
| 3  | 255.1477 | 23895 | 78.5  | 3276  | 0.0107 |
| 4  | 283.1801 | 26459 | 25.6  | 992   | 0.0107 |
| 5  | 305.1656 | 27638 | 24.2  | 1036  | 0.0110 |
| 6  | 327.1683 | 27078 | 41.0  | 1982  | 0.0121 |
| 7  | 336.2439 | 29039 | 50.5  | 2405  | 0.0116 |
| 8  | 355.2000 | 27017 | 21.6  | 893   | 0.0131 |
| 9  | 381.2176 | 27243 | 25.8  | 988   | 0.0140 |
| 10 | 403.1993 | 27123 | 109.7 | 5550  | 0.0149 |
| 11 | 448.2570 | 27121 | 36.2  | 1651  | 0.0165 |
| 12 | 454.1985 | 27546 | 29.1  | 1247  | 0.0165 |
| 13 | 567.1688 | 27947 | 30.2  | 2043  | 0.0203 |
| 14 | 587.1531 | 26396 | 137.4 | 13664 | 0.0222 |
| 15 | 588.1561 | 28241 | 45.1  | 4556  | 0.0208 |
| 16 | 589.1513 | 26284 | 133.3 | 13684 | 0.0224 |
| 17 | 590.1544 | 28241 | 43.5  | 4529  | 0.0209 |
| 18 | 591.1571 | 28040 | 7.2   | 765   | 0.0211 |
| 19 | 605.1251 | 26905 | 15.2  | 1409  | 0.0225 |

# Mass Spectrum List Report

## Analysis Info

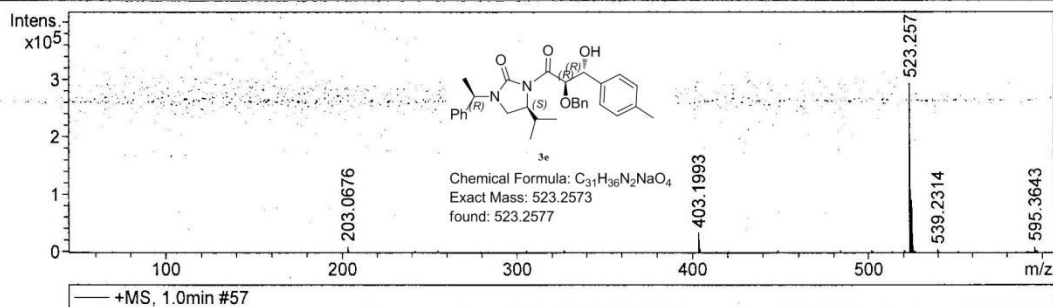
Analysis Name D:\Data\vipin\120-02-16-DGK-92.d  
Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-92  
Comment

Acquisition Date 2/16/2012 2:17:49 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 600 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



| # | m/z      | Res.  | S/N    | I      | FWHM   |
|---|----------|-------|--------|--------|--------|
| 1 | 203.0676 | 24910 | 234.5  | 10429  | 0.0082 |
| 2 | 241.1308 | 24168 | 64.7   | 2940   | 0.0100 |
| 3 | 255.1465 | 23841 | 88.0   | 3965   | 0.0107 |
| 4 | 403.1993 | 26653 | 382.0  | 33867  | 0.0151 |
| 5 | 523.2577 | 25109 | 1924.5 | 293648 | 0.0208 |
| 6 | 524.2606 | 25910 | 604.5  | 90320  | 0.0202 |
| 7 | 525.2629 | 26843 | 99.8   | 14598  | 0.0196 |
| 8 | 539.2314 | 27857 | 53.4   | 5461   | 0.0194 |
| 9 | 595.3643 | 26778 | 118.9  | 10379  | 0.0222 |

## Mass Spectrum List Report

### Analysis Info

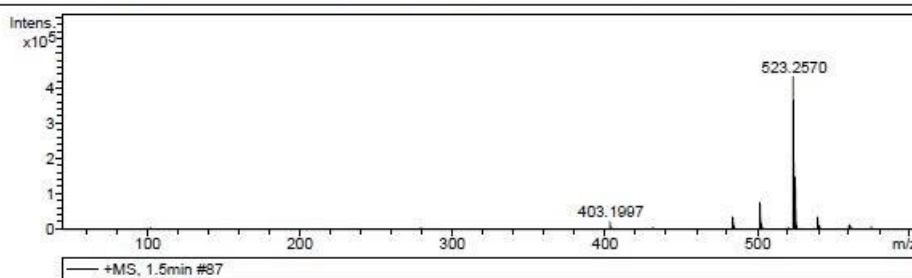
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 Method UPLC HRMS LOW.m  
 Sample Name HA-05  
 Comment

Acquisition Date 6/8/2016 3:30:38 PM

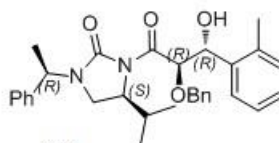
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 102.1260 | 13787 | 134.7  | 5253   | 0.0074 |
| 2  | 233.1648 | 18007 | 63.6   | 2461   | 0.0129 |
| 3  | 279.1202 | 18209 | 76.2   | 4875   | 0.0153 |
| 4  | 288.1256 | 18424 | 48.6   | 3382   | 0.0156 |
| 5  | 403.1997 | 19179 | 290.3  | 23927  | 0.0210 |
| 6  | 404.2029 | 18988 | 76.3   | 6130   | 0.0213 |
| 7  | 431.2413 | 19626 | 235.4  | 5506   | 0.0220 |
| 8  | 483.2648 | 20391 | 1249.8 | 37516  | 0.0237 |
| 9  | 484.2681 | 20682 | 414.8  | 13078  | 0.0234 |
| 10 | 501.2752 | 19466 | 1374.2 | 78021  | 0.0258 |
| 11 | 502.2785 | 20124 | 452.9  | 26406  | 0.0250 |
| 12 | 503.2816 | 18948 | 80.3   | 4820   | 0.0266 |
| 13 | 518.3016 | 20076 | 49.1   | 3088   | 0.0258 |
| 14 | 520.2481 | 20113 | 108.3  | 6470   | 0.0259 |
| 15 | 520.7504 | 19760 | 75.2   | 4443   | 0.0264 |
| 16 | 523.2570 | 19839 | 7836.5 | 432051 | 0.0264 |
| 17 | 524.2604 | 20602 | 2774.6 | 148917 | 0.0254 |
| 18 | 525.2634 | 19201 | 466.8  | 24389  | 0.0274 |
| 19 | 526.2665 | 19392 | 67.7   | 3456   | 0.0271 |
| 20 | 528.2355 | 20452 | 76.8   | 3694   | 0.0258 |
| 21 | 528.7363 | 20870 | 57.2   | 2716   | 0.0253 |
| 22 | 539.2310 | 19932 | 1145.6 | 36428  | 0.0271 |
| 23 | 540.2347 | 20029 | 403.2  | 12237  | 0.0270 |
| 24 | 541.2338 | 18460 | 155.6  | 4502   | 0.0293 |
| 25 | 559.3287 | 20460 | 245.7  | 10456  | 0.0273 |
| 26 | 560.3457 | 17485 | 339.4  | 15273  | 0.0320 |
| 27 | 561.3504 | 18800 | 119.7  | 5677   | 0.0299 |
| 28 | 574.3645 | 19900 | 117.8  | 9282   | 0.0289 |
| 29 | 575.3691 | 19498 | 45.8   | 3722   | 0.0295 |
| 30 | 602.3963 | 20540 | 46.0   | 4946   | 0.0293 |



**3f**

Chemical formula : C<sub>31</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>Na

Exact Mass : 523.2573

Found : 523.2570

# Mass Spectrum List Report

## Analysis Info

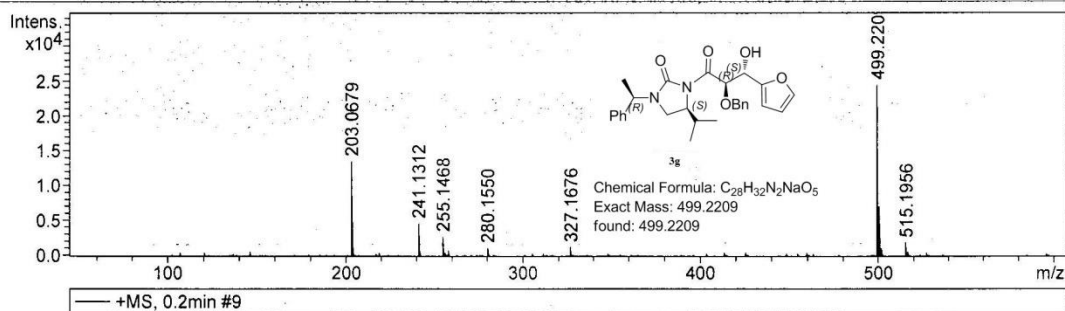
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Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-90  
Comment

Acquisition Date 2/16/2012 1:55:36 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 600 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



| # | m/z      | Res.  | S/N   | I     | FWHM   |
|---|----------|-------|-------|-------|--------|
| 1 | 203.0679 | 25527 | 264.2 | 13473 | 0.0080 |
| 2 | 241.1312 | 23537 | 83.8  | 4648  | 0.0102 |
| 3 | 255.1468 | 25170 | 53.6  | 2763  | 0.0101 |
| 4 | 280.1550 | 25143 | 32.2  | 1197  | 0.0111 |
| 5 | 327.1676 | 26495 | 44.6  | 1233  | 0.0123 |
| 6 | 499.2209 | 26664 | 656.4 | 24404 | 0.0187 |
| 7 | 500.2238 | 27160 | 185.7 | 7022  | 0.0184 |
| 8 | 501.2267 | 27011 | 30.7  | 1180  | 0.0186 |
| 9 | 515.1956 | 25802 | 45.0  | 1916  | 0.0200 |

# Mass Spectrum List Report

## Analysis Info

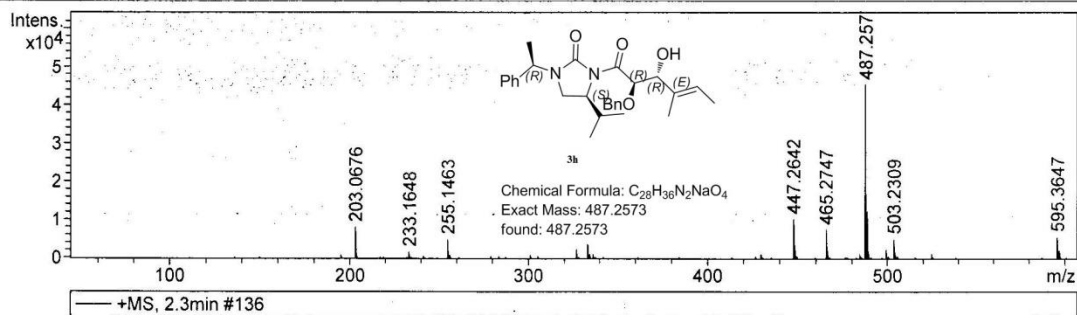
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Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-93  
Comment

Acquisition Date 2/16/2012 2:34:09 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive  
Focus Not active Set Capillary 4500 V  
Scan Begin 50 m/z Set End Plate Offset 500 V  
Scan End 600 m/z Set Collision Cell RF 300.0 Vpp  
Set Nebulizer 0.4 Bar  
Set Dry Heater 180 °C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Source



| #  | m/z      | Res.  | S/N   | I     | FWHM   |
|----|----------|-------|-------|-------|--------|
| 1  | 203.0676 | 24414 | 180.6 | 8108  | 0.0083 |
| 2  | 233.1648 | 25508 | 30.4  | 1730  | 0.0091 |
| 3  | 255.1463 | 23315 | 87.6  | 4992  | 0.0109 |
| 4  | 333.2169 | 25588 | 102.1 | 5984  | 0.0130 |
| 5  | 447.2642 | 26946 | 122.2 | 10268 | 0.0166 |
| 6  | 465.2747 | 26471 | 57.1  | 7601  | 0.0176 |
| 7  | 487.2573 | 26498 | 349.1 | 45222 | 0.0184 |
| 8  | 488.2603 | 25957 | 96.8  | 12319 | 0.0188 |
| 9  | 489.2625 | 26264 | 15.5  | 1939  | 0.0186 |
| 10 | 503.2309 | 26606 | 54.1  | 5099  | 0.0189 |
| 11 | 595.3647 | 27285 | 95.3  | 5591  | 0.0218 |

## Mass Spectrum List Report

### Analysis Info

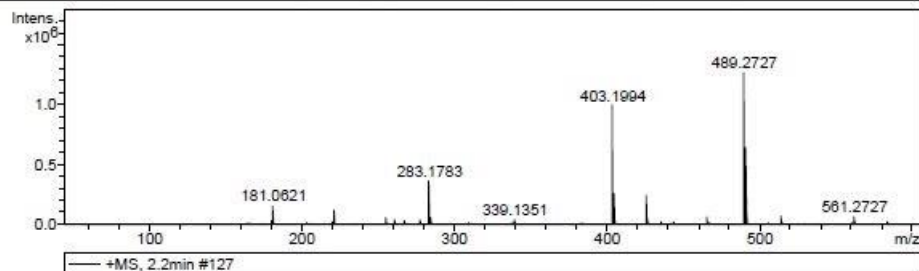
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 Method UPLC HRMS LOW.m  
 Sample Name MG-23  
 Comment

Acquisition Date 6/13/2016 11:47:55 AM

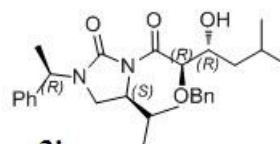
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N     | I       | FWHM   |
|----|----------|-------|---------|---------|--------|
| 1  | 164.9207 | 15550 | 799.8   | 18771   | 0.0106 |
| 2  | 180.0657 | 16217 | 1355.6  | 38461   | 0.0111 |
| 3  | 181.0621 | 15683 | 5547.8  | 157821  | 0.0115 |
| 4  | 220.0584 | 16020 | 900.9   | 28531   | 0.0137 |
| 5  | 221.0547 | 16550 | 3987.0  | 126555  | 0.0134 |
| 6  | 255.1470 | 17112 | 1729.9  | 62670   | 0.0149 |
| 7  | 261.0473 | 16709 | 1147.8  | 44330   | 0.0156 |
| 8  | 267.0397 | 17330 | 746.5   | 30650   | 0.0154 |
| 9  | 277.1291 | 17851 | 1006.6  | 45433   | 0.0155 |
| 10 | 283.1783 | 17545 | 7644.2  | 363594  | 0.0161 |
| 11 | 284.1815 | 17689 | 1268.3  | 60860   | 0.0161 |
| 12 | 309.0503 | 17825 | 481.7   | 19535   | 0.0173 |
| 13 | 338.1386 | 17959 | 607.8   | 18991   | 0.0188 |
| 14 | 339.1351 | 18019 | 1288.8  | 39979   | 0.0188 |
| 15 | 403.1994 | 17686 | 13805.8 | 997415  | 0.0228 |
| 16 | 404.2028 | 19258 | 3702.1  | 265630  | 0.0210 |
| 17 | 405.2059 | 19273 | 506.8   | 36143   | 0.0210 |
| 18 | 425.1815 | 18694 | 3987.0  | 244061  | 0.0227 |
| 19 | 426.1848 | 19458 | 988.5   | 60038   | 0.0219 |
| 20 | 435.2020 | 18978 | 450.9   | 25361   | 0.0229 |
| 21 | 443.1922 | 19572 | 366.3   | 25236   | 0.0226 |
| 22 | 465.1741 | 19622 | 558.1   | 65020   | 0.0237 |
| 23 | 489.2727 | 14087 | 12649.7 | 1269698 | 0.0347 |
| 24 | 490.2757 | 19279 | 6560.2  | 642760  | 0.0254 |
| 25 | 491.2790 | 19380 | 1051.1  | 100502  | 0.0254 |
| 26 | 513.2839 | 19780 | 1571.4  | 73455   | 0.0259 |
| 27 | 514.2871 | 19019 | 482.3   | 22521   | 0.0270 |
| 28 | 561.2727 | 19706 | 1718.8  | 67372   | 0.0285 |
| 29 | 562.2760 | 19324 | 500.6   | 19461   | 0.0291 |
| 30 | 583.2551 | 19478 | 806.5   | 25348   | 0.0299 |



**3i**

Chemical formula : C<sub>28</sub>H<sub>38</sub>N<sub>2</sub>O<sub>4</sub>Na

Exact Mass : 489.2729

Found : 489.2727

# Mass Spectrum List Report

## Analysis Info

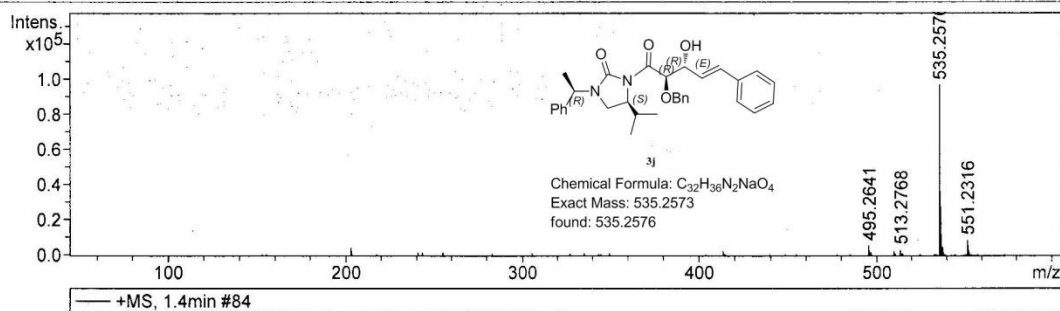
Analysis Name D:\Data\vipin\12-02-14-DGK-088.d  
Method sodium formate tune\_low.m  
Sample Name 12-02-14-DGK-088  
Comment

Acquisition Date 2/15/2012 11:07:18 AM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar  
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 600 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



| # | m/z      | Res.  | S/N   | I     | FWHM   |
|---|----------|-------|-------|-------|--------|
| 1 | 495.2641 | 26844 | 120.8 | 5552  | 0.0184 |
| 2 | 509.2408 | 26031 | 50.1  | 2865  | 0.0196 |
| 3 | 513.2768 | 23789 | 52.9  | 3394  | 0.0216 |
| 4 | 535.2576 | 25146 | 743.0 | 96233 | 0.0213 |
| 5 | 551.2316 | 25457 | 54.9  | 8851  | 0.0217 |

# Mass Spectrum List Report

## Analysis Info

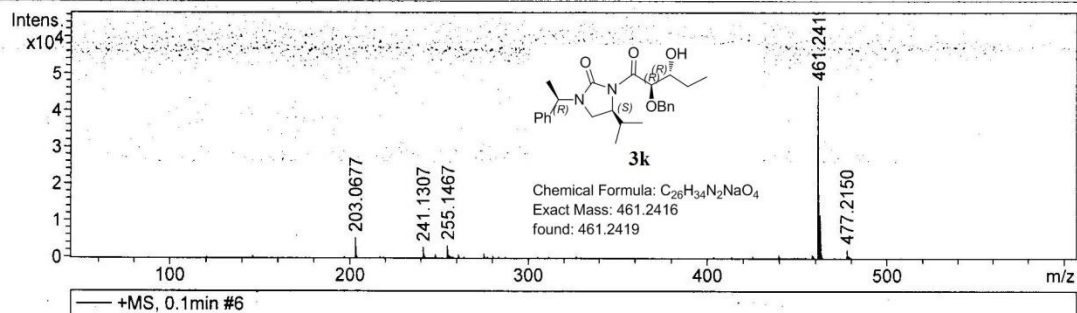
Analysis Name D:\Data\vipin\120-02-16-DGK-97-B.d  
Method sodium formate tune\_low.m  
Sample Name 120-02-16-DGK-97  
Comment

Acquisition Date 2/16/2012 4:45:10 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.4 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| # | m/z      | Res.  | S/N   | I     | FWHM   |
|---|----------|-------|-------|-------|--------|
| 1 | 203.0677 | 25029 | 141.1 | 5500  | 0.0081 |
| 2 | 241.1307 | 24354 | 54.5  | 3055  | 0.0099 |
| 3 | 248.1117 | 28056 | 14.0  | 829   | 0.0088 |
| 4 | 255.1467 | 23258 | 59.7  | 3387  | 0.0110 |
| 5 | 461.2419 | 26840 | 907.1 | 46814 | 0.0172 |
| 6 | 462.2446 | 26064 | 222.1 | 11674 | 0.0177 |
| 7 | 463.2477 | 26404 | 32.2  | 1725  | 0.0175 |
| 8 | 477.2150 | 27374 | 41.1  | 2495  | 0.0174 |

## Mass Spectrum List Report

### Analysis Info

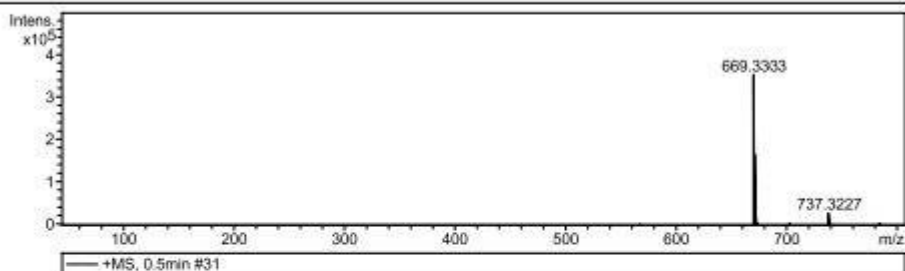
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 Method tune\_high.m  
 Sample Name AR-24  
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Acquisition Date 3/26/2014 2:55:07 PM

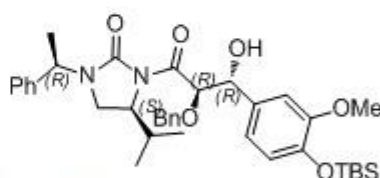
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 7.0 l/min |
| Scan End    | 800 m/z    | Set Collision Cell RF | 2500.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N     | I      | FWHM   |
|----|----------|-------|---------|--------|--------|
| 1  | 430.9151 | 17503 | 49.0    | 663    | 0.0246 |
| 2  | 475.3259 | 18982 | 81.5    | 1188   | 0.0250 |
| 3  | 498.9019 | 19270 | 59.8    | 864    | 0.0259 |
| 4  | 505.2302 | 25334 | 69.2    | 993    | 0.0199 |
| 5  | 566.8900 | 20146 | 127.0   | 1866   | 0.0281 |
| 6  | 619.3190 | 18893 | 101.4   | 1554   | 0.0328 |
| 7  | 620.3211 | 20123 | 42.3    | 656    | 0.0308 |
| 8  | 629.3415 | 20761 | 95.8    | 1531   | 0.0303 |
| 9  | 630.3443 | 19793 | 39.7    | 655    | 0.0318 |
| 10 | 634.8769 | 20086 | 76.0    | 1355   | 0.0316 |
| 11 | 669.3333 | 16326 | 12077.6 | 350755 | 0.0410 |
| 12 | 670.3395 | 16283 | 5684.7  | 166984 | 0.0412 |
| 13 | 671.3401 | 17111 | 1824.4  | 54205  | 0.0392 |
| 14 | 672.3402 | 19466 | 270.7   | 8145   | 0.0345 |
| 15 | 673.3412 | 17259 | 27.5    | 851    | 0.0390 |
| 16 | 683.3510 | 15504 | 13.5    | 430    | 0.0441 |
| 17 | 685.3085 | 20284 | 37.7    | 1151   | 0.0338 |
| 18 | 686.3100 | 22344 | 18.9    | 581    | 0.0307 |
| 19 | 701.4950 | 21092 | 101.5   | 2604   | 0.0333 |
| 20 | 702.4978 | 19935 | 35.6    | 913    | 0.0352 |
| 21 | 702.8647 | 22065 | 100.3   | 2536   | 0.0319 |
| 22 | 737.3227 | 19906 | 1536.2  | 26994  | 0.0370 |
| 23 | 738.3249 | 21875 | 572.4   | 10057  | 0.0338 |
| 24 | 739.3252 | 19871 | 124.2   | 2191   | 0.0372 |
| 25 | 740.3259 | 17897 | 21.3    | 388    | 0.0414 |
| 26 | 770.8509 | 19819 | 94.8    | 1621   | 0.0389 |
| 27 | 783.4098 | 21895 | 277.7   | 4675   | 0.0358 |



Chemical formula :  $C_{37}H_{50}N_2O_6SiNa$

Exact Mass : 669.3336

Found : 669.3333

## Mass Spectrum List Report

### Analysis Info

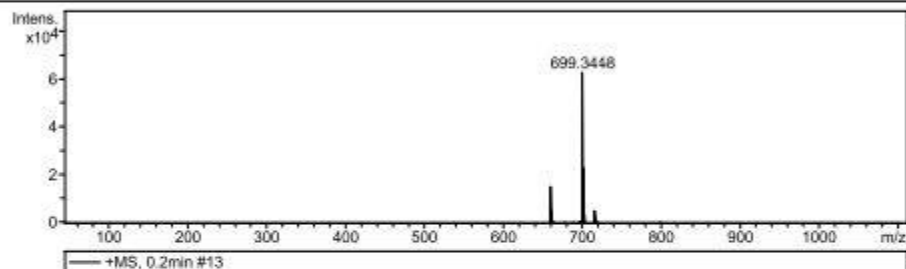
Analysis Name D:\Data\vipin\14-03-28-AR-25.d  
 Method tune\_high.m  
 Sample Name AR-25  
 Comment

Acquisition Date 3/28/2014 1:54:01 PM

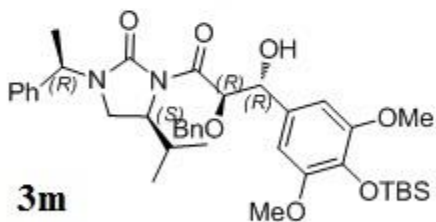
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 7.0 l/min |
| Scan End    | 1100 m/z   | Set Collision Cell RF | 2500.0 Vpp | Set Divert Valve | Source    |



| #  | m/z       | Res.  | S/N   | I     | FWHM   |
|----|-----------|-------|-------|-------|--------|
| 1  | 659.3523  | 21397 | 192.3 | 15255 | 0.0308 |
| 2  | 660.3551  | 20447 | 58.3  | 4679  | 0.0323 |
| 3  | 661.3551  | 20035 | 12.3  | 1003  | 0.0330 |
| 4  | 699.3448  | 19289 | 529.2 | 62650 | 0.0363 |
| 5  | 700.3480  | 21361 | 192.4 | 22962 | 0.0328 |
| 6  | 701.3479  | 21088 | 34.3  | 4126  | 0.0333 |
| 7  | 715.3182  | 22491 | 38.3  | 5136  | 0.0318 |
| 8  | 716.3209  | 18298 | 12.0  | 1616  | 0.0391 |
| 9  | 798.4522  | 18017 | 36.7  | 687   | 0.0443 |
| 10 | 799.4543  | 17149 | 19.6  | 364   | 0.0466 |
| 11 | 1027.0248 | 26828 | 11.4  | 185   | 0.0383 |
| 12 | 1034.5119 | 24238 | 12.1  | 206   | 0.0427 |
| 13 | 1035.0145 | 19660 | 14.3  | 244   | 0.0526 |
| 14 | 1035.5168 | 18168 | 11.3  | 193   | 0.0570 |



Chemical formula :  $C_{38}H_{52}N_2O_7SiNa$

Exact Mass : 699.3441

Found : 699.3448

# Mass Spectrum List Report

## Analysis Info

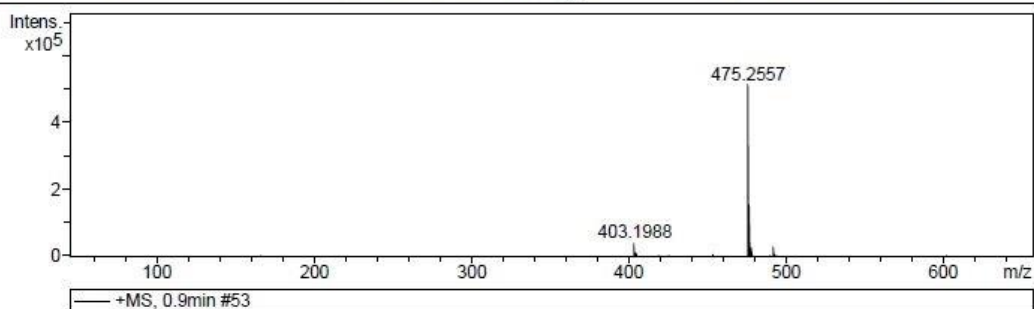
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Method UPLC HRMS LOW.m  
Sample Name ALD-04R  
Comment

Acquisition Date 9/22/2016 4:02:51 PM

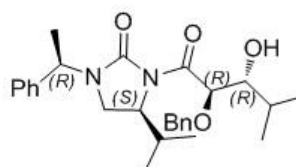
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 650 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N     | I      | FWHM   |
|----|----------|-------|---------|--------|--------|
| 1  | 102.1277 | 12314 | 135.8   | 1863   | 0.0083 |
| 2  | 166.0977 | 13327 | 179.6   | 3147   | 0.0125 |
| 3  | 233.1643 | 13698 | 117.6   | 2367   | 0.0170 |
| 4  | 345.2164 | 14917 | 144.4   | 1175   | 0.0231 |
| 5  | 381.2168 | 14523 | 116.5   | 1185   | 0.0262 |
| 6  | 403.1988 | 15585 | 3940.9  | 40966  | 0.0259 |
| 7  | 404.2023 | 15472 | 1008.7  | 10466  | 0.0261 |
| 8  | 405.2055 | 14983 | 150.7   | 1565   | 0.0270 |
| 9  | 419.1731 | 14444 | 278.6   | 2793   | 0.0290 |
| 10 | 425.1806 | 15262 | 257.9   | 2548   | 0.0279 |
| 11 | 453.2746 | 15237 | 253.6   | 6977   | 0.0297 |
| 12 | 454.2775 | 15657 | 78.4    | 2231   | 0.0290 |
| 13 | 472.2506 | 14487 | 34.5    | 1486   | 0.0326 |
| 14 | 475.2557 | 16015 | 11808.8 | 513315 | 0.0297 |
| 15 | 475.4764 | 5248  | 51.1    | 2240   | 0.0906 |
| 16 | 475.5563 | 6071  | 35.7    | 1568   | 0.0783 |
| 17 | 475.7591 | 5423  | 24.1    | 1066   | 0.0877 |
| 18 | 476.2590 | 16262 | 3526.8  | 154222 | 0.0293 |
| 19 | 477.2624 | 16044 | 581.5   | 25591  | 0.0297 |
| 20 | 478.2649 | 15737 | 73.6    | 3269   | 0.0304 |
| 21 | 489.2705 | 15393 | 115.0   | 5421   | 0.0318 |
| 22 | 490.2730 | 15181 | 37.3    | 1775   | 0.0323 |
| 23 | 491.2308 | 15732 | 618.2   | 29407  | 0.0312 |
| 24 | 492.2340 | 15725 | 184.8   | 8845   | 0.0313 |
| 25 | 493.2323 | 14783 | 73.7    | 3550   | 0.0334 |
| 26 | 529.2463 | 15232 | 52.0    | 2288   | 0.0347 |
| 27 | 583.2546 | 16177 | 64.9    | 1031   | 0.0361 |
| 28 | 600.3074 | 15643 | 96.0    | 976    | 0.0384 |



3n

Chemical formula: C<sub>27</sub>H<sub>36</sub>N<sub>2</sub>NaO<sub>4</sub>

Exact Mass: 475.2573

Found: 475.2557

# Mass Spectrum List Report

## Analysis Info

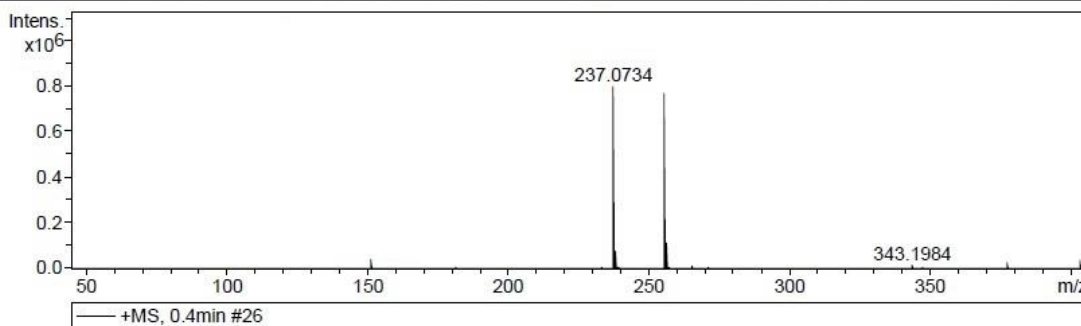
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Method sodium formate tune\_low.m  
Sample Name RS-A-3  
Comment

Acquisition Date 7/8/2013 2:34:35 PM

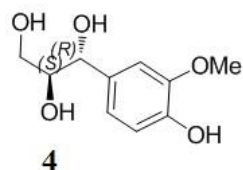
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 400 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #    | m/z      | Res.  | S/N    | I      | FWHM   |
|------|----------|-------|--------|--------|--------|
| 1    | 129.1038 | 16510 | 55.4   | 1048   | 0.0078 |
| 2    | 137.0608 | 18213 | 37.6   | 800    | 0.0075 |
| 3    | 151.0843 | 18731 | 1571.6 | 39950  | 0.0081 |
| 4    | 152.0871 | 18392 | 58.2   | 1496   | 0.0083 |
| 5    | 181.0933 | 18370 | 130.1  | 4315   | 0.0099 |
| 6    | 195.1087 | 19060 | 36.0   | 1131   | 0.0102 |
| 7    | 198.1280 | 18537 | 34.9   | 1081   | 0.0107 |
| 8    | 209.1241 | 19558 | 20.4   | 851    | 0.0107 |
| 9    | 233.1637 | 18891 | 25.8   | 5977   | 0.0123 |
| ⇒ 10 | 237.0734 | 15780 | 2542.8 | 796234 | 0.0150 |
| 11   | 238.0761 | 17166 | 236.8  | 79093  | 0.0139 |
| 12   | 239.0775 | 18754 | 17.5   | 6211   | 0.0127 |
| 13   | 255.1470 | 15991 | 1681.9 | 770168 | 0.0160 |
| 14   | 256.1499 | 17217 | 262.0  | 115491 | 0.0149 |
| 15   | 257.1518 | 17597 | 11.2   | 4730   | 0.0146 |
| 16   | 265.1037 | 19156 | 36.6   | 10525  | 0.0138 |
| 17   | 271.1203 | 18734 | 33.2   | 6132   | 0.0145 |
| 18   | 273.0337 | 21768 | 16.7   | 2547   | 0.0125 |
| 19   | 279.0833 | 19606 | 23.9   | 3282   | 0.0142 |
| 20   | 285.1560 | 18573 | 16.3   | 2014   | 0.0154 |
| 21   | 291.1789 | 19600 | 15.5   | 1694   | 0.0149 |
| 22   | 292.1303 | 21005 | 12.6   | 1349   | 0.0139 |
| 23   | 299.1711 | 17814 | 23.6   | 2189   | 0.0168 |
| 24   | 301.1414 | 15237 | 10.8   | 977    | 0.0198 |
| 25   | 325.1885 | 18774 | 13.4   | 1040   | 0.0173 |
| 26   | 343.1984 | 20474 | 113.3  | 14068  | 0.0168 |
| 27   | 344.2015 | 19951 | 15.6   | 1972   | 0.0173 |
| 28   | 347.1569 | 20494 | 40.2   | 5325   | 0.0169 |
| 29   | 359.1912 | 18927 | 11.1   | 1682   | 0.0190 |



Chemical Formula: C<sub>10</sub>H<sub>14</sub>NaO<sub>5</sub>  
Exact Mass: 237.0739  
found: 237.0734

# Mass Spectrum List Report

## Analysis Info

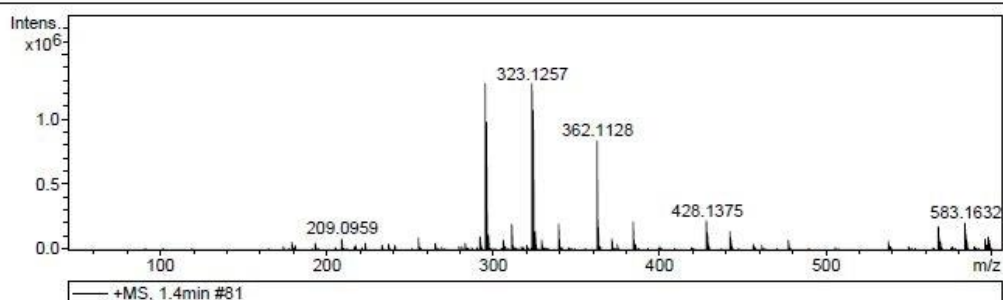
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Method UPLC HRMS LOW.m  
Sample Name AV-03  
Comment

Acquisition Date 6/6/2016 1:56:48 PM

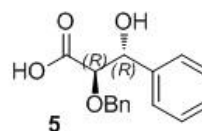
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N    | I       | FWHM   |
|----|----------|-------|--------|---------|--------|
| 1  | 209.0959 | 16718 | 1323.2 | 85579   | 0.0125 |
| 2  | 255.1459 | 17662 | 924.5  | 95708   | 0.0144 |
| 3  | 292.0851 | 18214 | 354.5  | 97958   | 0.0160 |
| 4  | 295.0944 | 8927  | 4461.5 | 1274282 | 0.0331 |
| 5  | 296.0969 | 17652 | 3402.2 | 982894  | 0.0168 |
| 6  | 297.0991 | 18711 | 403.9  | 118182  | 0.0159 |
| 7  | 306.1008 | 18552 | 224.0  | 72181   | 0.0165 |
| 8  | 311.0659 | 16878 | 597.5  | 201913  | 0.0184 |
| 9  | 323.1257 | 8976  | 3381.6 | 1274802 | 0.0360 |
| 10 | 324.1279 | 17433 | 2825.1 | 1074243 | 0.0186 |
| 11 | 325.1309 | 18904 | 371.2  | 141818  | 0.0172 |
| 12 | 329.0693 | 18613 | 214.7  | 76674   | 0.0177 |
| 13 | 339.0988 | 18260 | 689.8  | 201798  | 0.0186 |
| 14 | 362.1128 | 17434 | 5763.9 | 837395  | 0.0208 |
| 15 | 363.1159 | 18610 | 1332.4 | 190755  | 0.0195 |
| 16 | 371.0796 | 18230 | 606.4  | 80663   | 0.0204 |
| 17 | 384.0949 | 18823 | 1859.0 | 216196  | 0.0204 |
| 18 | 428.1375 | 18754 | 1723.4 | 223165  | 0.0228 |
| 19 | 428.6391 | 19772 | 943.3  | 122733  | 0.0217 |
| 20 | 442.1533 | 19760 | 1051.9 | 140007  | 0.0224 |
| 21 | 442.6549 | 19205 | 556.6  | 73769   | 0.0230 |
| 22 | 477.1216 | 19580 | 876.4  | 78042   | 0.0244 |
| 23 | 537.3941 | 20743 | 887.1  | 70164   | 0.0259 |
| 24 | 567.1963 | 19017 | 1056.5 | 182739  | 0.0298 |
| 25 | 568.1992 | 18984 | 392.7  | 69797   | 0.0299 |
| 26 | 583.1632 | 21438 | 837.2  | 205270  | 0.0272 |
| 27 | 583.6650 | 21010 | 485.7  | 120280  | 0.0278 |
| 28 | 595.2263 | 18864 | 334.3  | 86839   | 0.0316 |



Chemical formula : C<sub>16</sub>H<sub>16</sub>O<sub>4</sub>Na  
Exact Mass : 295.0945  
Found : 295.0944

# Mass Spectrum List Report

## Analysis Info

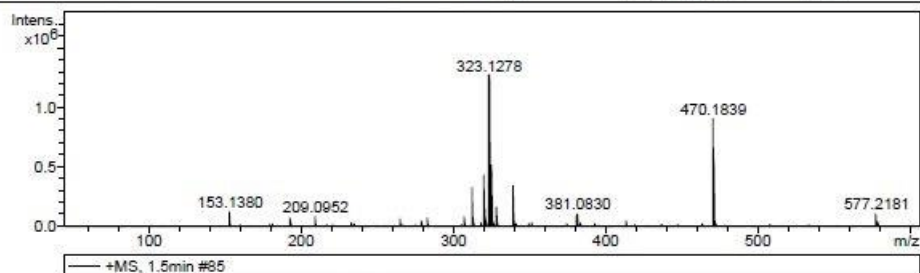
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Method UPLC HRMS LOW.m  
Sample Name MG-403  
Comment

Acquisition Date 6/6/2016 10:41:12 AM

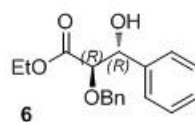
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -600 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N    | I       | FWHM   |
|----|----------|-------|--------|---------|--------|
| 1  | 153.1380 | 15646 | 3999.8 | 128057  | 0.0098 |
| 2  | 193.0857 | 16492 | 1579.5 | 75124   | 0.0117 |
| 3  | 209.0952 | 16755 | 1610.6 | 86387   | 0.0125 |
| 4  | 265.1215 | 18057 | 856.7  | 65739   | 0.0147 |
| 5  | 279.1557 | 17900 | 896.7  | 52917   | 0.0156 |
| 6  | 283.1319 | 18532 | 980.8  | 74183   | 0.0153 |
| 7  | 307.1509 | 18548 | 255.6  | 82270   | 0.0166 |
| 8  | 312.1274 | 18626 | 848.5  | 325529  | 0.0168 |
| 9  | 312.6288 | 17935 | 397.6  | 155200  | 0.0174 |
| 10 | 313.1282 | 17463 | 203.8  | 80974   | 0.0179 |
| 11 | 320.1161 | 18674 | 895.1  | 433317  | 0.0171 |
| 12 | 320.6179 | 18607 | 324.4  | 159262  | 0.0172 |
| 13 | 321.1147 | 14213 | 121.1  | 60398   | 0.0226 |
| 14 | 323.1278 | 5981  | 2442.9 | 1274614 | 0.0540 |
| 15 | 323.3085 | 14598 | 316.0  | 165873  | 0.0221 |
| 16 | 323.3838 | 14372 | 346.7  | 182242  | 0.0225 |
| 17 | 323.5418 | 19066 | 608.1  | 320695  | 0.0170 |
| 18 | 323.8903 | 13401 | 119.5  | 63757   | 0.0242 |
| 19 | 324.1276 | 10661 | 2381.9 | 1272776 | 0.0304 |
| 20 | 325.1305 | 18860 | 953.1  | 517335  | 0.0172 |
| 21 | 328.1020 | 18649 | 332.3  | 167261  | 0.0176 |
| 22 | 328.6039 | 18770 | 131.0  | 65200   | 0.0175 |
| 23 | 339.0982 | 18376 | 973.6  | 345570  | 0.0185 |
| 24 | 340.1017 | 19409 | 173.9  | 59527   | 0.0175 |
| 25 | 381.0830 | 19423 | 2059.3 | 109692  | 0.0196 |
| 26 | 413.1712 | 19054 | 723.0  | 49003   | 0.0217 |
| 27 | 470.1839 | 19739 | 4831.6 | 909517  | 0.0238 |
| 28 | 470.6855 | 19977 | 2958.9 | 562094  | 0.0236 |
| 29 | 471.1868 | 20137 | 986.4  | 189124  | 0.0234 |
| 30 | 577.2181 | 20345 | 1579.1 | 107247  | 0.0284 |



Chemical formula : C<sub>18</sub>H<sub>20</sub>O<sub>4</sub>Na  
Exact Mass : 323.1259  
Found : 323.1278

# Mass Spectrum List Report

## Analysis Info

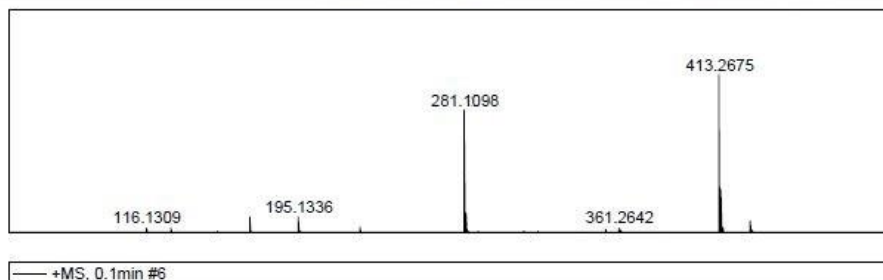
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Method sodium formate tune\_low.m  
Sample Name NKP-02  
Comment

Acquisition Date 1/6/2014 3:21:21 PM

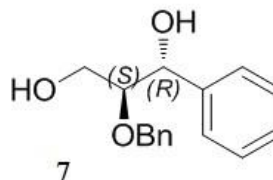
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 500 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 116.1309 | 16481 | 153.6  | 3210   | 0.0070 |
| 2  | 129.0424 | 17174 | 124.9  | 2760   | 0.0075 |
| 3  | 153.1321 | 17997 | 58.1   | 799    | 0.0085 |
| 4  | 170.0748 | 15695 | 418.4  | 11284  | 0.0108 |
| 5  | 171.0772 | 19001 | 17.5   | 486    | 0.0090 |
| 6  | 195.1336 | 15353 | 325.4  | 11302  | 0.0127 |
| 7  | 196.1366 | 18022 | 23.7   | 819    | 0.0109 |
| 8  | 227.1610 | 17327 | 148.4  | 3599   | 0.0131 |
| 9  | 281.1098 | 15188 | 1301.5 | 87154  | 0.0185 |
| 10 | 282.2130 | 16039 | 210.4  | 13786  | 0.0176 |
| 11 | 283.2151 | 17337 | 14.0   | 894    | 0.0163 |
| 12 | 288.1208 | 17827 | 13.0   | 742    | 0.0162 |
| 13 | 301.1402 | 18380 | 11.8   | 453    | 0.0164 |
| 14 | 309.2038 | 17582 | 13.5   | 412    | 0.0176 |
| 15 | 312.0763 | 16844 | 25.1   | 738    | 0.0185 |
| 16 | 319.2167 | 15208 | 18.2   | 488    | 0.0210 |
| 17 | 323.2197 | 17649 | 19.3   | 487    | 0.0183 |
| 18 | 339.1665 | 19569 | 17.8   | 420    | 0.0173 |
| 19 | 353.2301 | 19099 | 11.9   | 461    | 0.0185 |
| 20 | 354.2259 | 16919 | 52.0   | 2074   | 0.0209 |
| 21 | 361.2642 | 18610 | 67.2   | 3193   | 0.0194 |
| 22 | 362.1723 | 18358 | 36.5   | 1772   | 0.0197 |
| 23 | 362.2661 | 18704 | 12.6   | 612    | 0.0194 |
| 24 | 413.2675 | 14737 | 2383.2 | 112524 | 0.0280 |
| 25 | 414.2709 | 15414 | 625.2  | 30723  | 0.0269 |
| 26 | 415.2724 | 18671 | 77.3   | 3949   | 0.0222 |
| 27 | 429.2407 | 16721 | 108.2  | 8020   | 0.0257 |
| 28 | 430.2441 | 18520 | 19.2   | 1389   | 0.0232 |
| 29 | 465.3555 | 17207 | 25.1   | 375    | 0.0270 |
| 30 | 471.2238 | 16882 | 25.3   | 350    | 0.0279 |



Chemical formula : C<sub>16</sub>H<sub>18</sub>O<sub>3</sub>Na  
Exact Mass : 281.1154  
Found : 281.1098

# Mass Spectrum List Report

## Analysis Info

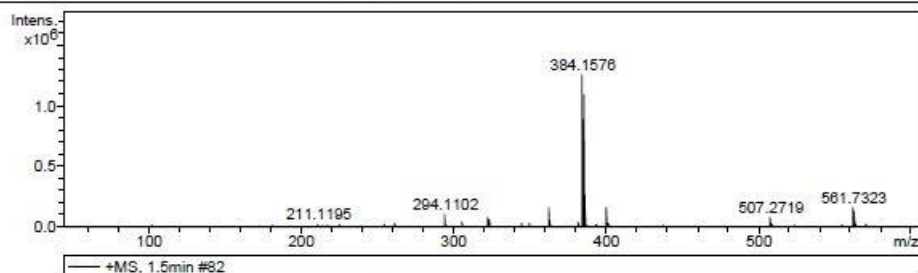
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Method UPLC HRMS LOW.m  
Sample Name HA-23  
Comment

Acquisition Date 6/13/2016 10:45:06 AM

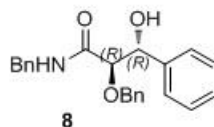
Operator VIKAS GROVER  
Instrument / Ser# maXis 40

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 250 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 5.0 l/min |
| Scan End    | 600 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N    | I       | FWHM   |
|----|----------|-------|--------|---------|--------|
| 1  | 211.1195 | 10711 | 826.2  | 28750   | 0.0197 |
| 2  | 217.1047 | 17040 | 562.8  | 19985   | 0.0127 |
| 3  | 225.1386 | 17436 | 764.4  | 27216   | 0.0129 |
| 4  | 254.1176 | 17525 | 654.6  | 24273   | 0.0145 |
| 5  | 261.1311 | 17643 | 921.6  | 36069   | 0.0148 |
| 6  | 294.1102 | 18017 | 2171.6 | 110285  | 0.0163 |
| 7  | 305.1572 | 17813 | 667.0  | 38283   | 0.0171 |
| 8  | 322.2278 | 18657 | 1234.3 | 83321   | 0.0173 |
| 9  | 323.1255 | 18087 | 978.9  | 66616   | 0.0179 |
| 10 | 344.1646 | 18797 | 528.6  | 37517   | 0.0183 |
| 11 | 349.1833 | 17588 | 440.8  | 31503   | 0.0199 |
| 12 | 362.1751 | 18851 | 2297.7 | 166465  | 0.0192 |
| 13 | 363.1783 | 18944 | 559.9  | 43005   | 0.0192 |
| 14 | 381.1488 | 19729 | 243.2  | 39278   | 0.0193 |
| 15 | 381.6504 | 19739 | 121.1  | 19899   | 0.0193 |
| 16 | 384.1576 | 9771  | 7170.0 | 1257051 | 0.0393 |
| 17 | 384.4386 | 17729 | 151.4  | 26826   | 0.0217 |
| 18 | 384.8099 | 20275 | 307.0  | 54556   | 0.0190 |
| 19 | 385.1603 | 16735 | 6071.3 | 1093076 | 0.0230 |
| 20 | 386.1638 | 19388 | 947.2  | 175071  | 0.0199 |
| 21 | 393.2094 | 19570 | 104.4  | 22832   | 0.0201 |
| 22 | 400.1312 | 19547 | 663.2  | 162703  | 0.0205 |
| 23 | 401.1347 | 19294 | 158.4  | 38013   | 0.0208 |
| 24 | 507.2719 | 20317 | 1443.3 | 85120   | 0.0250 |
| 25 | 508.2754 | 20647 | 435.2  | 25851   | 0.0246 |
| 26 | 561.7323 | 19550 | 2113.2 | 161940  | 0.0287 |
| 27 | 562.2339 | 20386 | 1692.1 | 128682  | 0.0276 |
| 28 | 562.7354 | 19699 | 652.7  | 49286   | 0.0286 |
| 29 | 569.7190 | 19652 | 371.2  | 25009   | 0.0290 |
| 30 | 570.2208 | 19921 | 298.8  | 19968   | 0.0286 |



Chemical formula : C<sub>23</sub>H<sub>23</sub>NO<sub>3</sub>Na  
Exact Mass : 384.1576  
Found : 384.1576

## Mass Spectrum List Report

### Analysis Info

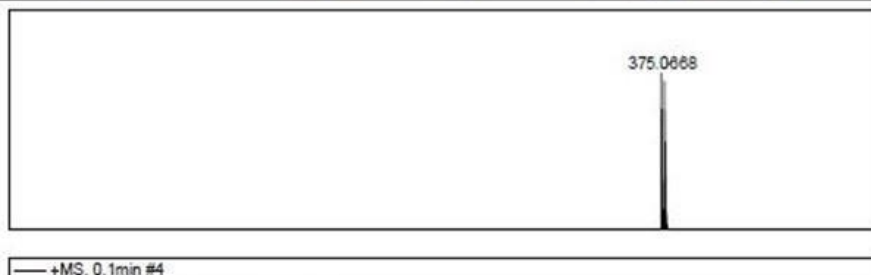
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 Method sodium formate tune\_low.m  
 Sample Name NK-73  
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Acquisition Date 4/11/2014 2:18:51 PM

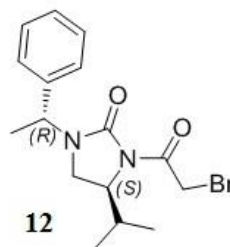
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 500 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 142.1234 | 15021 | 14.9   | 141    | 0.0095 |
| 2  | 156.1379 | 20672 | 12.1   | 127    | 0.0076 |
| 3  | 226.9507 | 15023 | 16.4   | 173    | 0.0151 |
| 4  | 235.9701 | 10972 | 12.5   | 136    | 0.0215 |
| 5  | 292.0314 | 16877 | 17.2   | 213    | 0.0173 |
| 6  | 294.0301 | 15021 | 15.9   | 207    | 0.0198 |
| 7  | 315.9948 | 17987 | 22.2   | 312    | 0.0176 |
| 8  | 317.9912 | 15920 | 15.4   | 210    | 0.0200 |
| 9  | 364.1029 | 16610 | 12.0   | 166    | 0.0219 |
| 10 | 366.1014 | 16982 | 10.9   | 154    | 0.0216 |
| 11 | 367.0636 | 22622 | 19.9   | 289    | 0.0162 |
| 12 | 369.0633 | 17567 | 10.5   | 242    | 0.0210 |
| 13 | 375.0668 | 15686 | 1143.4 | 123721 | 0.0248 |
| 14 | 376.0506 | 18395 | 138.9  | 15620  | 0.0212 |
| 15 | 377.0648 | 15207 | 1006.3 | 117450 | 0.0257 |
| 16 | 392.0487 | 18199 | 121.2  | 14668  | 0.0215 |



Chemical formula : C<sub>16</sub>H<sub>21</sub>BrN<sub>2</sub>O<sub>2</sub>Na

Exact Mass : 375.0684

Found : 375.0668

## Mass Spectrum List Report

### Analysis Info

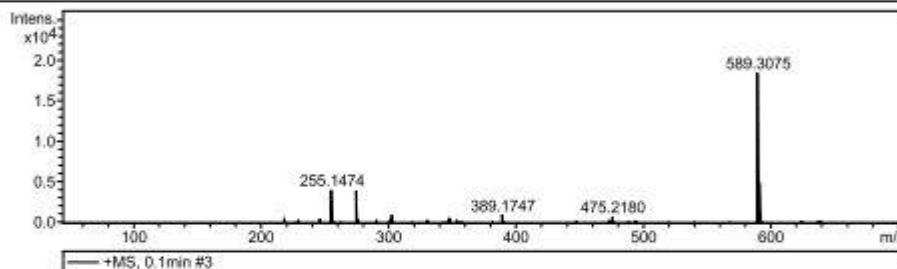
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 Method sodium formate tune\_low.m  
 Sample Name MG-21  
 Comment

Acquisition Date 3/14/2014 3:05:05 PM

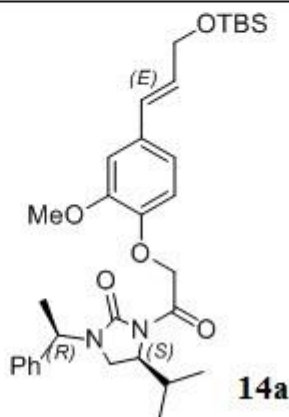
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 700 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N   | I     | FWHM   |
|----|----------|-------|-------|-------|--------|
| 1  | 218.2133 | 16348 | 22.1  | 570   | 0.0133 |
| 2  | 229.1237 | 18349 | 11.5  | 379   | 0.0125 |
| 3  | 246.2436 | 13863 | 11.3  | 479   | 0.0178 |
| 4  | 255.1474 | 17351 | 94.5  | 4083  | 0.0147 |
| 5  | 256.1509 | 18606 | 15.2  | 659   | 0.0138 |
| 6  | 274.2746 | 16219 | 88.1  | 3975  | 0.0169 |
| 7  | 275.2777 | 17281 | 11.2  | 506   | 0.0159 |
| 8  | 302.3047 | 17405 | 24.7  | 946   | 0.0174 |
| 9  | 330.3369 | 18103 | 14.4  | 337   | 0.0182 |
| 10 | 347.1801 | 16832 | 25.9  | 621   | 0.0206 |
| 11 | 353.2653 | 14711 | 13.3  | 323   | 0.0240 |
| 12 | 389.1747 | 17369 | 44.0  | 955   | 0.0224 |
| 13 | 447.1878 | 14176 | 11.0  | 239   | 0.0315 |
| 14 | 473.2028 | 16929 | 17.6  | 439   | 0.0280 |
| 15 | 475.2180 | 17342 | 30.2  | 745   | 0.0274 |
| 16 | 589.3075 | 18832 | 183.9 | 18471 | 0.0313 |
| 17 | 590.3097 | 17421 | 48.2  | 4954  | 0.0339 |
| 18 | 591.3116 | 15216 | 11.8  | 1235  | 0.0389 |



Chemical formula : C<sub>32</sub>H<sub>46</sub>N<sub>2</sub>O<sub>5</sub>SiNa

Exact Mass : 589.3074

Found : 589.3075

## Mass Spectrum List Report

### Analysis Info

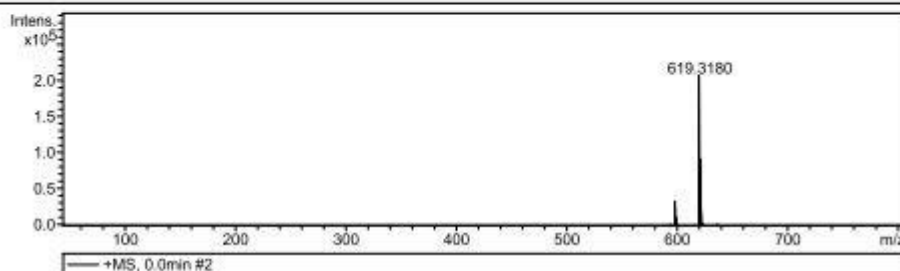
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 Sample Name AR-21  
 Comment

Acquisition Date 3/26/2014 2:50:51 PM

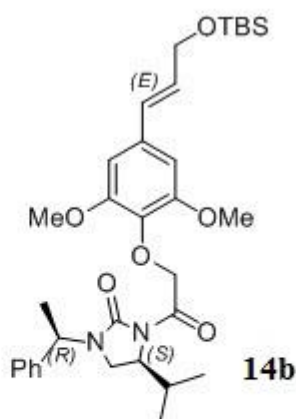
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 7.0 l/min |
| Scan End    | 800 m/z    | Set Collision Cell RF | 2500.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 503.2161 | 19587 | 49.4   | 681    | 0.0257 |
| 2  | 505.2303 | 25235 | 62.1   | 856    | 0.0200 |
| 3  | 506.2328 | 34074 | 21.0   | 293    | 0.0149 |
| 4  | 593.3008 | 22773 | 59.5   | 1175   | 0.0261 |
| 5  | 594.3017 | 20163 | 22.8   | 459    | 0.0295 |
| 6  | 597.3342 | 25283 | 1653.3 | 33682  | 0.0236 |
| 7  | 598.3369 | 26442 | 505.9  | 10401  | 0.0228 |
| 8  | 599.3409 | 19972 | 118.5  | 2462   | 0.0300 |
| 9  | 600.3440 | 15641 | 22.1   | 469    | 0.0384 |
| 10 | 616.3094 | 25419 | 24.4   | 586    | 0.0242 |
| 11 | 616.6103 | 21295 | 22.1   | 533    | 0.0290 |
| 12 | 619.3180 | 20017 | 8393.0 | 204182 | 0.0309 |
| 13 | 620.3203 | 22088 | 3737.0 | 91590  | 0.0281 |
| 14 | 621.3226 | 22433 | 1063.3 | 26257  | 0.0277 |
| 15 | 622.3251 | 18434 | 140.4  | 3498   | 0.0338 |
| 16 | 623.3269 | 22666 | 27.7   | 701    | 0.0275 |
| 17 | 635.2926 | 18290 | 61.9   | 1550   | 0.0347 |
| 18 | 636.2958 | 20377 | 28.8   | 723    | 0.0312 |
| 19 | 637.2951 | 15281 | 12.6   | 319    | 0.0417 |
| 20 | 653.3220 | 20853 | 35.7   | 825    | 0.0313 |
| 21 | 654.3248 | 22124 | 13.7   | 320    | 0.0296 |
| 22 | 656.4053 | 26742 | 20.2   | 463    | 0.0245 |
| 23 | 661.6086 | 22989 | 16.0   | 359    | 0.0288 |
| 24 | 670.4233 | 22016 | 22.8   | 485    | 0.0305 |
| 25 | 677.3578 | 22948 | 18.5   | 381    | 0.0295 |
| 26 | 695.3325 | 22808 | 35.9   | 700    | 0.0305 |
| 27 | 698.4552 | 27503 | 34.4   | 666    | 0.0254 |
| 28 | 699.4577 | 26958 | 14.7   | 289    | 0.0259 |



Chemical formula : C<sub>33</sub>H<sub>48</sub>N<sub>2</sub>O<sub>6</sub>SiNa

Exact Mass : 619.3175

Found : 619.3180

## Mass Spectrum List Report

### Analysis Info

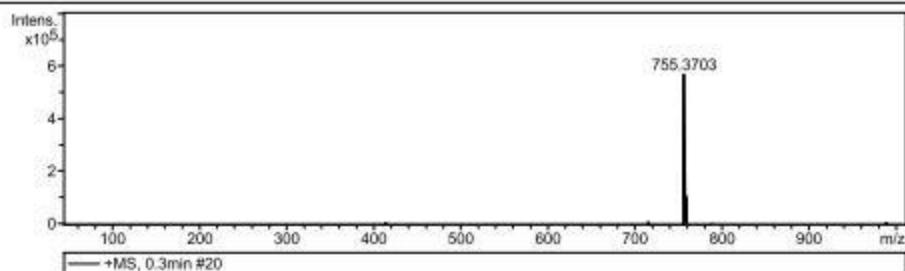
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 Sample Name ARW-L1-P  
 Comment

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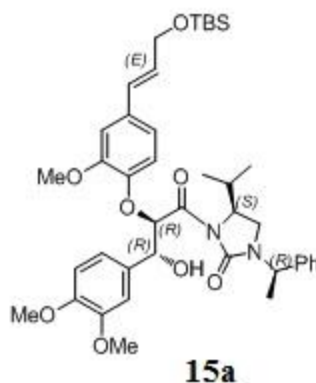
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 0.4 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1000 m/z   | Set Collision Cell RF | 1200.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 255.1310 | 13889 | 58.9   | 945    | 0.0184 |
| 2  | 353.2265 | 18207 | 27.6   | 917    | 0.0194 |
| 3  | 355.2422 | 20548 | 58.7   | 1983   | 0.0173 |
| 4  | 389.1743 | 19776 | 44.0   | 1842   | 0.0197 |
| 5  | 413.1565 | 22958 | 30.4   | 1307   | 0.0180 |
| 6  | 413.2660 | 21062 | 156.5  | 6729   | 0.0196 |
| 7  | 414.2894 | 17005 | 26.6   | 1141   | 0.0244 |
| 8  | 453.3196 | 16390 | 18.3   | 756    | 0.0277 |
| 9  | 455.3338 | 18281 | 30.9   | 1277   | 0.0249 |
| 10 | 471.3267 | 18664 | 19.4   | 755    | 0.0253 |
| 11 | 613.2510 | 21280 | 30.2   | 866    | 0.0288 |
| 12 | 639.2859 | 21200 | 78.5   | 2413   | 0.0302 |
| 13 | 640.2884 | 17956 | 24.0   | 740    | 0.0357 |
| 14 | 641.2804 | 19092 | 29.8   | 920    | 0.0336 |
| 15 | 715.3764 | 19168 | 221.2  | 10846  | 0.0373 |
| 16 | 716.3786 | 21513 | 100.4  | 4949   | 0.0333 |
| 17 | 717.3816 | 21259 | 26.2   | 1355   | 0.0337 |
| 18 | 755.3703 | 17145 | 2682.0 | 569378 | 0.0441 |
| 19 | 756.3734 | 17046 | 1325.9 | 287101 | 0.0444 |
| 20 | 757.3760 | 16711 | 490.3  | 108251 | 0.0453 |
| 21 | 758.3775 | 18956 | 104.6  | 23540  | 0.0400 |
| 22 | 759.3794 | 18651 | 12.5   | 2858   | 0.0407 |
| 23 | 787.3593 | 18902 | 10.2   | 2984   | 0.0417 |
| 24 | 801.4106 | 20978 | 10.2   | 2338   | 0.0382 |
| 25 | 823.3570 | 21998 | 18.7   | 2476   | 0.0374 |
| 26 | 971.5495 | 17573 | 11.1   | 769    | 0.0553 |
| 27 | 987.5384 | 21598 | 138.5  | 9730   | 0.0457 |



Chemical formula : C<sub>42</sub>H<sub>58</sub>N<sub>2</sub>O<sub>9</sub>SiNa  
 Exact Mass : 755.3704  
 Found : 755.3703

## Mass Spectrum List Report

### Analysis Info

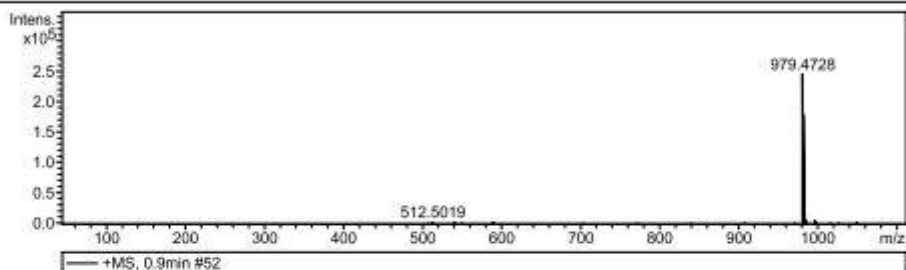
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 Sample Name MG-86  
 Comment

Acquisition Date 12/10/2013 4:46:58 PM

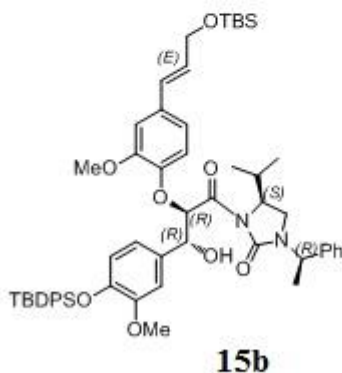
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 7.0 l/min |
| Scan End    | 1100 m/z   | Set Collision Cell RF | 2500.0 Vpp | Set Divert Valve | Source    |



| #  | m/z       | Res.  | S/N    | I      | FWHM   |
|----|-----------|-------|--------|--------|--------|
| 1  | 507.2685  | 19528 | 41.1   | 1905   | 0.0260 |
| 2  | 512.5019  | 17863 | 86.6   | 4041   | 0.0287 |
| 3  | 513.5048  | 18820 | 23.4   | 1091   | 0.0273 |
| 4  | 522.5954  | 16510 | 21.4   | 1013   | 0.0317 |
| 5  | 537.3929  | 19376 | 19.4   | 934    | 0.0277 |
| 6  | 540.5330  | 18496 | 71.2   | 3445   | 0.0292 |
| 7  | 541.5362  | 19028 | 24.1   | 1168   | 0.0285 |
| 8  | 550.6272  | 19136 | 24.6   | 1204   | 0.0288 |
| 9  | 568.5645  | 16635 | 22.5   | 1126   | 0.0342 |
| 10 | 589.3053  | 19658 | 57.6   | 2769   | 0.0300 |
| 11 | 702.8615  | 20900 | 39.2   | 1796   | 0.0336 |
| 12 | 770.8492  | 21111 | 83.9   | 1903   | 0.0365 |
| 13 | 838.8365  | 20624 | 123.8  | 2126   | 0.0407 |
| 14 | 906.8252  | 18769 | 75.7   | 1537   | 0.0483 |
| 15 | 969.7365  | 19026 | 48.9   | 1760   | 0.0510 |
| 16 | 974.8107  | 17962 | 30.6   | 1164   | 0.0543 |
| 17 | 979.4728  | 15624 | 6305.9 | 245881 | 0.0627 |
| 18 | 980.4757  | 15527 | 4544.7 | 178798 | 0.0631 |
| 19 | 981.4780  | 15244 | 2237.2 | 88808  | 0.0644 |
| 20 | 982.4797  | 17331 | 797.0  | 31931  | 0.0567 |
| 21 | 983.4796  | 19349 | 152.9  | 6195   | 0.0508 |
| 22 | 984.4816  | 15609 | 22.3   | 930    | 0.0631 |
| 23 | 995.4465  | 19040 | 151.3  | 6763   | 0.0523 |
| 24 | 996.4485  | 20002 | 95.0   | 4287   | 0.0498 |
| 25 | 997.4508  | 15825 | 40.2   | 1840   | 0.0630 |
| 26 | 1015.5402 | 20114 | 31.0   | 1282   | 0.0505 |
| 27 | 1016.5414 | 20974 | 23.6   | 974    | 0.0485 |



Chemical formula :  $C_{56}H_{72}N_2O_8Si_2Na$

Exact Mass : 979.4725

Found : 979.4728

## Mass Spectrum List Report

### Analysis Info

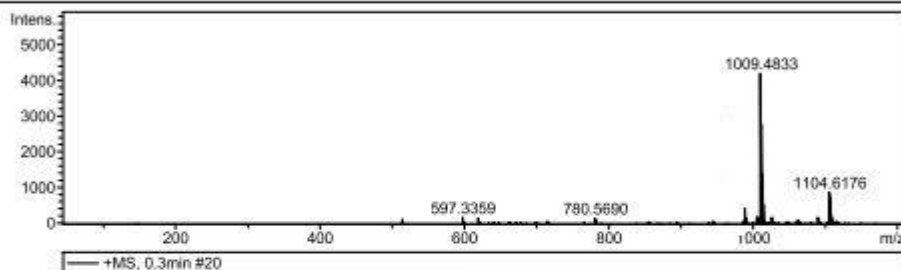
Analysis Name: D:\Data\vipin\14-03-26-AR-22.d  
 Method: tune\_high.m  
 Sample Name: AR-22  
 Comment:

Acquisition Date: 3/26/2014 3:15:03 PM

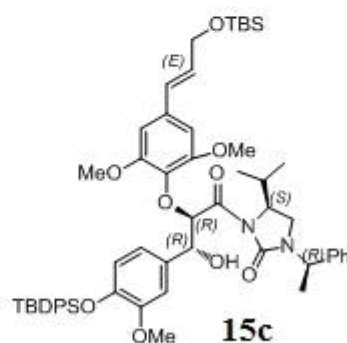
Operator: VIKAS GROVER  
 Instrument / Ser#: maXis 40

### Acquisition Parameter

|             |            |                       |            |                  |           |
|-------------|------------|-----------------------|------------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive   | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4200 V     | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V     | Set Dry Gas      | 7.0 l/min |
| Scan End    | 1200 m/z   | Set Collision Cell RF | 2500.0 Vpp | Set Divert Valve | Source    |



| #  | m/z       | Res.  | S/N   | I    | FWHM   |
|----|-----------|-------|-------|------|--------|
| 1  | 513.2259  | 26007 | 15.0  | 143  | 0.0197 |
| 2  | 513.7314  | 18846 | 10.8  | 103  | 0.0273 |
| 3  | 597.3359  | 15942 | 15.4  | 174  | 0.0375 |
| 4  | 619.3182  | 13933 | 11.4  | 135  | 0.0444 |
| 5  | 780.5690  | 16712 | 16.0  | 160  | 0.0417 |
| 6  | 969.4913  | 20917 | 380.1 | 2928 | 0.0463 |
| 7  | 970.4929  | 22531 | 263.2 | 2036 | 0.0431 |
| 8  | 971.4988  | 19945 | 140.4 | 1091 | 0.0487 |
| 9  | 972.5027  | 15875 | 46.9  | 368  | 0.0613 |
| 10 | 988.5063  | 16253 | 30.0  | 250  | 0.0542 |
| 11 | 989.5145  | 16255 | 17.9  | 151  | 0.0609 |
| 12 | 1004.5258 | 17271 | 23.3  | 205  | 0.0582 |
| 13 | 1005.5294 | 19697 | 16.7  | 148  | 0.0510 |
| 14 | 1006.5273 | 12053 | 18.0  | 160  | 0.0835 |
| 15 | 1009.4833 | 22862 | 476.1 | 4189 | 0.0441 |
| 16 | 1010.4854 | 22835 | 317.0 | 2799 | 0.0443 |
| 17 | 1011.4895 | 19780 | 151.0 | 1339 | 0.0511 |
| 18 | 1012.4940 | 21670 | 64.0  | 569  | 0.0467 |
| 19 | 1013.4990 | 14259 | 15.7  | 142  | 0.0711 |
| 20 | 1025.4606 | 25281 | 22.1  | 196  | 0.0406 |



Chemical formula : C<sub>57</sub>H<sub>74</sub>N<sub>2</sub>O<sub>9</sub>Si<sub>2</sub>Na

Exact Mass : 1009.4831

Found : 1009.4833

## Mass Spectrum List Report

### Analysis Info

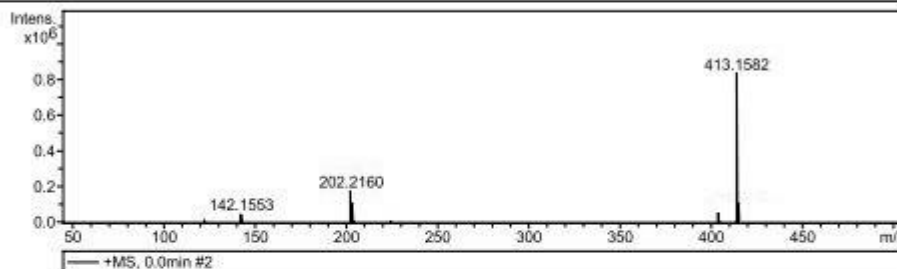
Analysis Name D:\Data\vipin\14-01-30-MG-12.d  
 Method sodium formate tune\_low.m  
 Sample Name MG-12  
 Comment

Acquisition Date 1/30/2014 9:30:55 AM

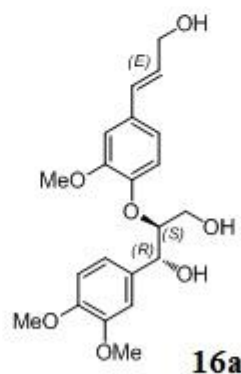
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 500 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N    | I      | FWHM   |
|----|----------|-------|--------|--------|--------|
| 1  | 122.0525 | 15038 | 195.7  | 19862  | 0.0081 |
| 2  | 142.1553 | 14489 | 380.0  | 48271  | 0.0098 |
| 3  | 143.1581 | 15551 | 19.6   | 2510   | 0.0092 |
| 4  | 146.1502 | 14471 | 15.3   | 2018   | 0.0101 |
| 5  | 184.2040 | 14956 | 34.0   | 2740   | 0.0123 |
| 6  | 186.2189 | 15359 | 13.5   | 1322   | 0.0121 |
| 7  | 188.1989 | 15490 | 21.9   | 2527   | 0.0121 |
| 8  | 202.2160 | 15869 | 678.1  | 160848 | 0.0151 |
| 9  | 203.2189 | 14702 | 432.2  | 105990 | 0.0138 |
| 10 | 204.2209 | 15201 | 15.8   | 4019   | 0.0134 |
| 11 | 224.1976 | 16237 | 51.2   | 12390  | 0.0138 |
| 12 | 403.4264 | 17855 | 279.1  | 57186  | 0.0226 |
| 13 | 404.4291 | 17144 | 44.6   | 9289   | 0.0236 |
| 14 | 413.1582 | 13383 | 3527.4 | 834455 | 0.0260 |
| 15 | 414.1608 | 18099 | 108.2  | 26024  | 0.0229 |
| 16 | 415.1649 | 15977 | 14.8   | 3603   | 0.0260 |



Chemical formula : C<sub>21</sub>H<sub>26</sub>O<sub>7</sub>Na

Exact Mass : 413.1576

Found : 413.1582

## Mass Spectrum List Report

### Analysis Info

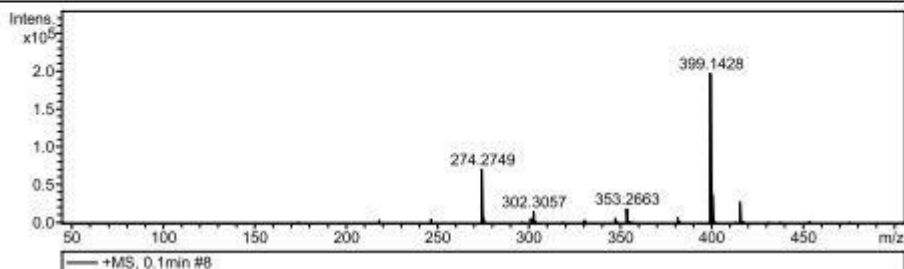
Analysis Name D:\Data\vipin\14-03-14-MG-22.d  
 Method sodium formate tune\_low.m  
 Sample Name MG-22  
 Comment

Acquisition Date 3/14/2014 3:09:55 PM

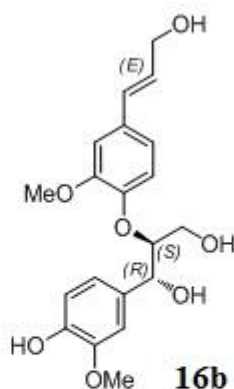
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 500 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source    |



| #  | m/z      | Res.  | S/N   | I      | FWHM   |
|----|----------|-------|-------|--------|--------|
| 1  | 174.1232 | 15735 | 73.0  | 1946   | 0.0111 |
| 2  | 218.2101 | 16568 | 115.3 | 4291   | 0.0132 |
| 3  | 246.2425 | 16429 | 108.3 | 5631   | 0.0150 |
| 4  | 247.0937 | 15978 | 16.7  | 883    | 0.0155 |
| 5  | 255.1468 | 14434 | 13.7  | 833    | 0.0177 |
| 6  | 274.2749 | 15358 | 887.6 | 71312  | 0.0179 |
| 7  | 275.2778 | 17142 | 88.0  | 7144   | 0.0161 |
| 8  | 296.2563 | 16143 | 20.0  | 1841   | 0.0184 |
| 9  | 301.1411 | 16853 | 63.5  | 6014   | 0.0179 |
| 10 | 302.3057 | 17159 | 165.7 | 15786  | 0.0176 |
| 11 | 303.3089 | 17271 | 20.7  | 1987   | 0.0176 |
| 12 | 318.3002 | 17646 | 18.4  | 1567   | 0.0180 |
| 13 | 330.3366 | 17427 | 60.8  | 4487   | 0.0190 |
| 14 | 331.3394 | 14631 | 10.4  | 754    | 0.0226 |
| 15 | 347.1813 | 16824 | 81.2  | 6838   | 0.0206 |
| 16 | 348.1836 | 16326 | 13.8  | 1180   | 0.0213 |
| 17 | 353.2663 | 17898 | 211.8 | 19705  | 0.0197 |
| 18 | 354.2696 | 16183 | 24.6  | 2329   | 0.0219 |
| 19 | 356.3514 | 18043 | 18.2  | 1773   | 0.0198 |
| 20 | 381.2977 | 17214 | 49.5  | 8211   | 0.0222 |
| 21 | 399.1428 | 14645 | 889.8 | 197265 | 0.0273 |
| 22 | 400.1452 | 17763 | 175.8 | 38488  | 0.0225 |
| 23 | 401.1478 | 16010 | 15.2  | 3284   | 0.0251 |
| 24 | 413.1568 | 15502 | 12.1  | 2206   | 0.0267 |
| 25 | 415.1157 | 17938 | 156.4 | 27736  | 0.0231 |
| 26 | 416.1186 | 16864 | 18.8  | 3289   | 0.0247 |
| 27 | 437.1927 | 15974 | 18.8  | 2127   | 0.0274 |
| 28 | 453.1666 | 16814 | 36.9  | 2340   | 0.0270 |



Chemical formula : C<sub>20</sub>H<sub>24</sub>O<sub>9</sub>Na

Exact Mass : 399.1420

Found : 399.1428

### Analysis Info

Acquisition Date 3/26/2014 3:20:15 PM

Operator VIKAS GROVER  
Instrument / Ser# maXis 40

### Acquisition Parameter

Mass spectrum showing relative intensity (0 to 6000+) versus m/z (50 to 450). The base peak is at m/z 429.1520. Other labeled peaks include m/z 122.0584, 202.2164, and 395.1357. The x-axis is labeled 'm/z' and the y-axis is labeled 'Intens.'.

**16c**

69 | 7 6

## Mass Spectrum List Report

### Analysis Info

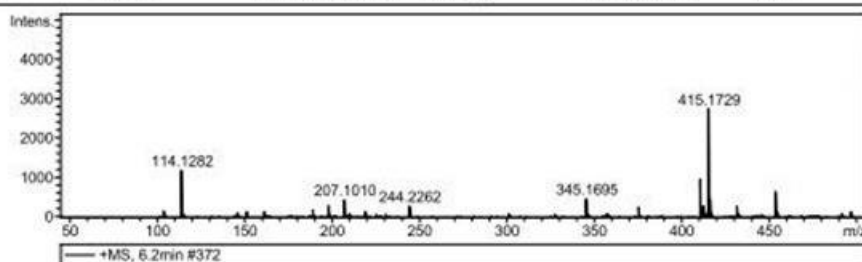
Analysis Name D:\Data\vipin\AR-17\_1-B,3\_01\_97.d  
 Method HIGH FLOW DIRECT INJECTION LOW MASS.m  
 Sample Name AR-17  
 Comment

Acquisition Date 4/22/2014 12:13:18 PM

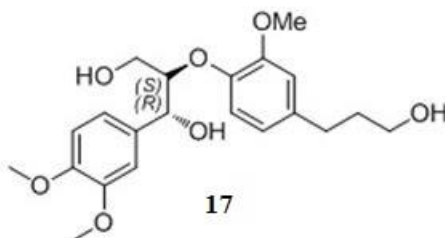
Operator VIKAS GROVER  
 Instrument / Ser# maXis 40

### Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 1.2 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 7.0 l/min |
| Scan End    | 500 m/z    | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Waste     |



| #  | m/z      | Res.  | S/N  | I    | FWHM   |
|----|----------|-------|------|------|--------|
| 1  | 104.0713 | 15198 | 15.4 | 166  | 0.0068 |
| 2  | 114.1282 | 17746 | 94.7 | 1196 | 0.0064 |
| 3  | 151.0759 | 17568 | 10.1 | 152  | 0.0086 |
| 4  | 161.0591 | 15140 | 10.2 | 156  | 0.0106 |
| 5  | 189.0907 | 14641 | 11.0 | 184  | 0.0129 |
| 6  | 198.1260 | 18212 | 17.6 | 313  | 0.0109 |
| 7  | 207.1010 | 16266 | 24.3 | 455  | 0.0127 |
| 8  | 244.2262 | 16135 | 22.4 | 291  | 0.0151 |
| 9  | 345.1695 | 17261 | 29.5 | 478  | 0.0200 |
| 10 | 375.1795 | 18171 | 15.0 | 255  | 0.0206 |
| 11 | 410.2176 | 16225 | 30.4 | 961  | 0.0253 |
| 12 | 415.1729 | 17121 | 81.1 | 2744 | 0.0242 |
| 13 | 416.1754 | 14079 | 13.2 | 454  | 0.0296 |
| 14 | 453.3442 | 15382 | 25.5 | 645  | 0.0295 |



Chemical formula : C<sub>21</sub>H<sub>28</sub>O<sub>7</sub>Na

Exact Mass : 415.1733

Observed : 415.1729

## Copies of IR Spectra

