

Diastereoselective syntheses of 3-aryl-5-(arylalkyl)-6-methyl-1-(1-phenylethyl)thioxotetrahydropyrimidin-4(1*H*)-ones: A stereochemical perspective from endo and exocyclic chiral centres

Varun Kumar^a, Pallepogu Raghavaiah^b, Shaikh M. Mobin^c and Vipin A. Nair^{a*}

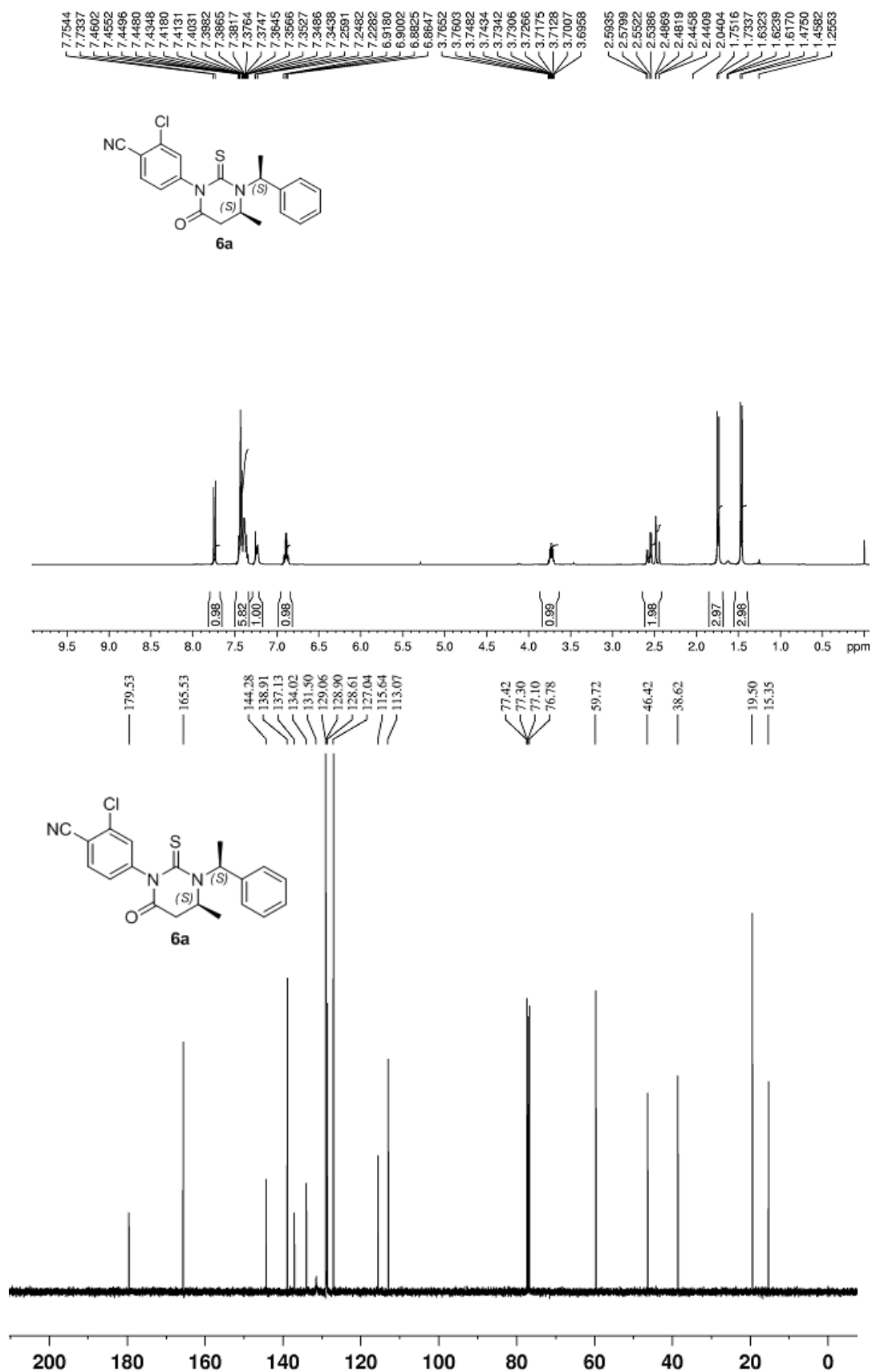
^a Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, Sector 67, Mohali, Punjab 160 062, India;

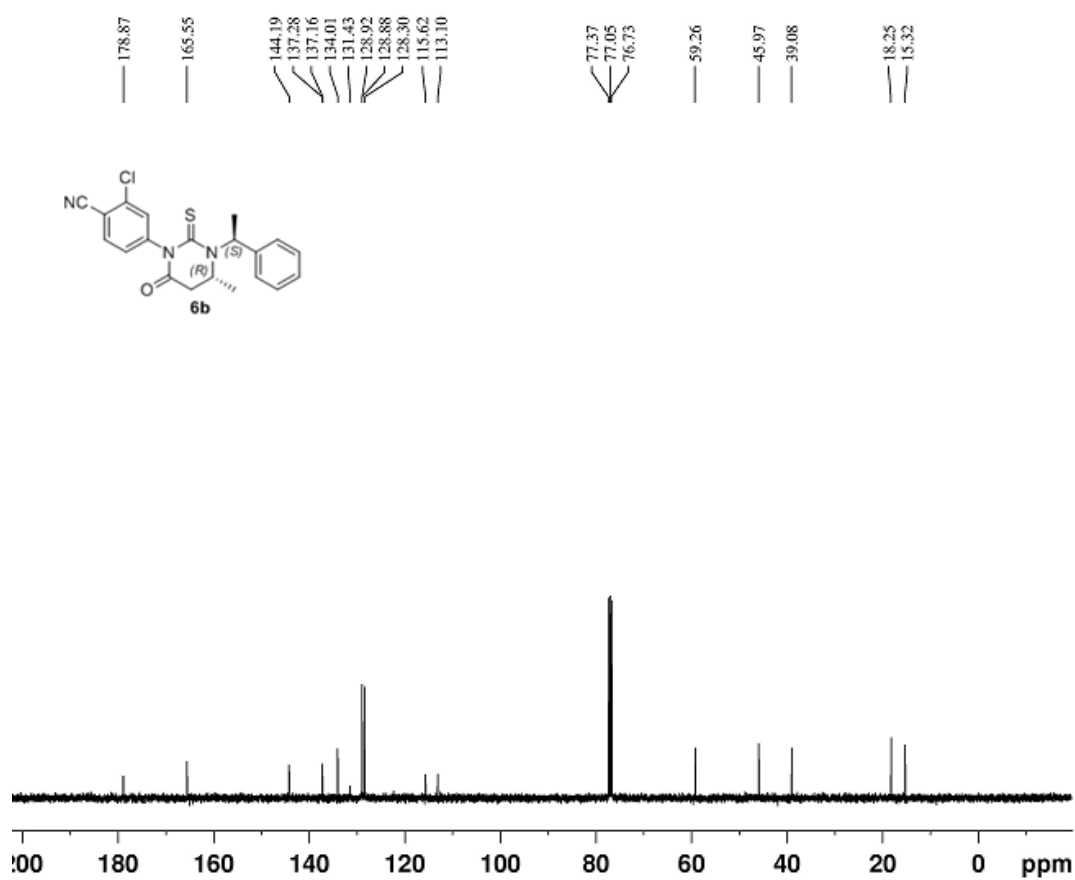
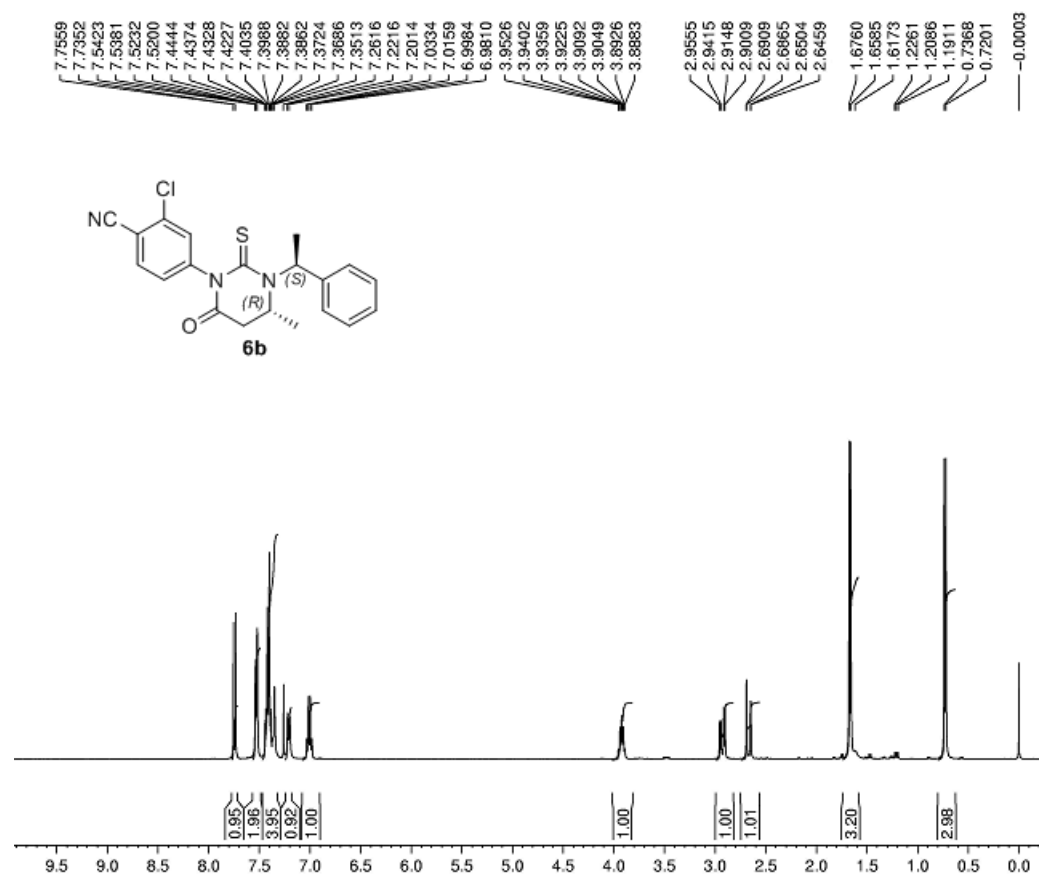
^b National Single Crystal X-ray Diffractometer Facility, School of Chemistry, University of Hyderabad, Hyderabad 500 046, India;

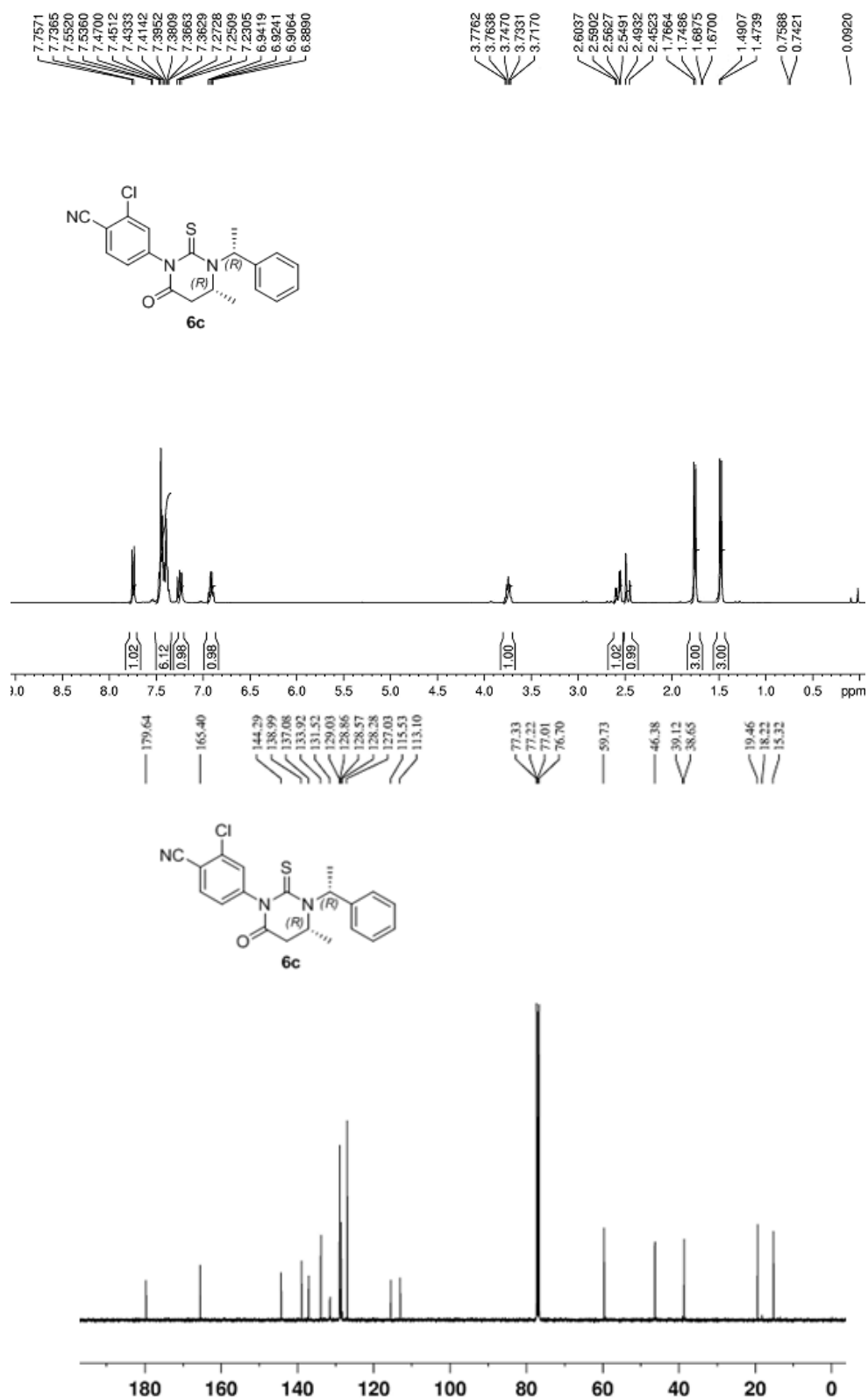
^c National Single Crystal X-ray Diffraction Facility, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India.

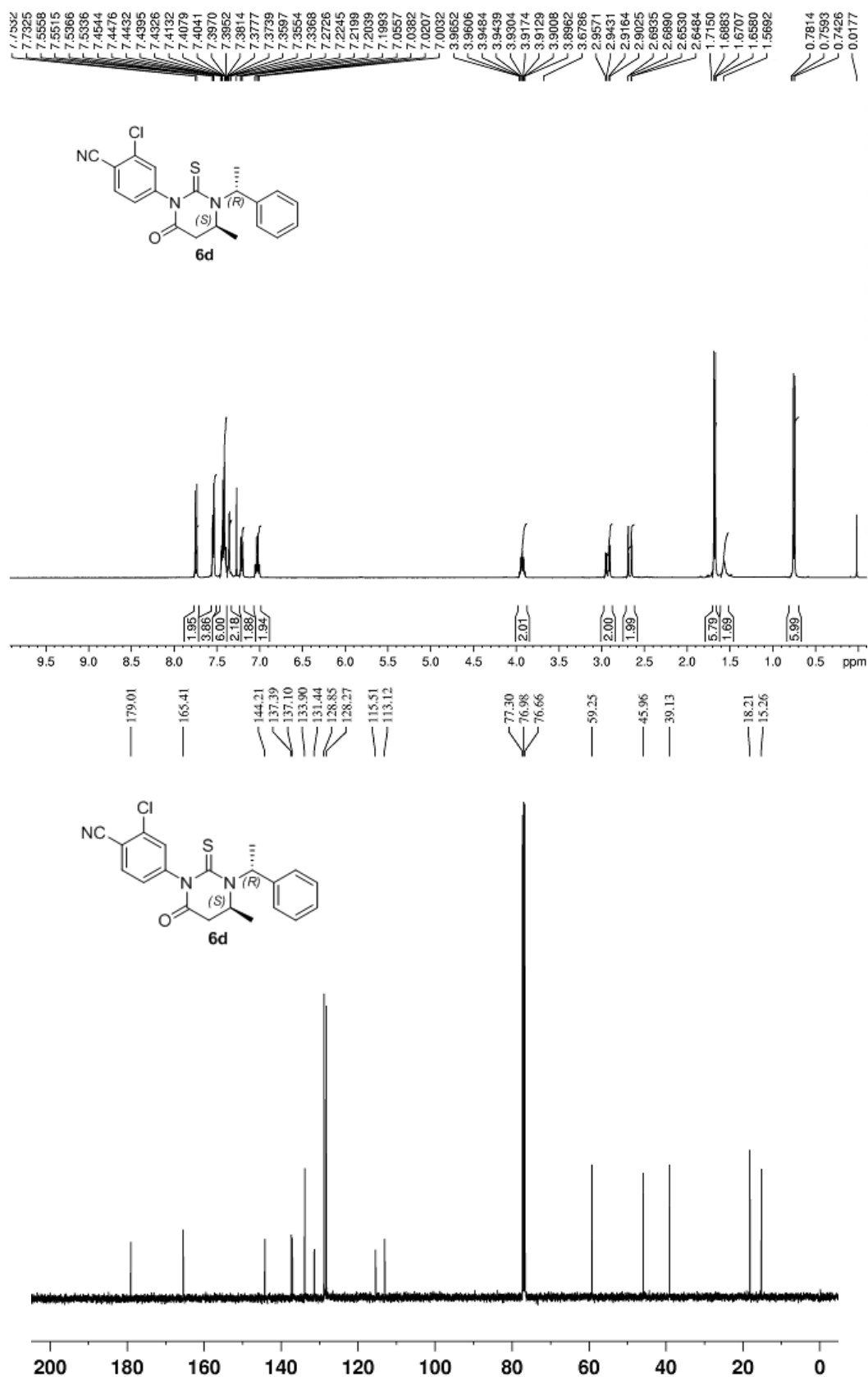
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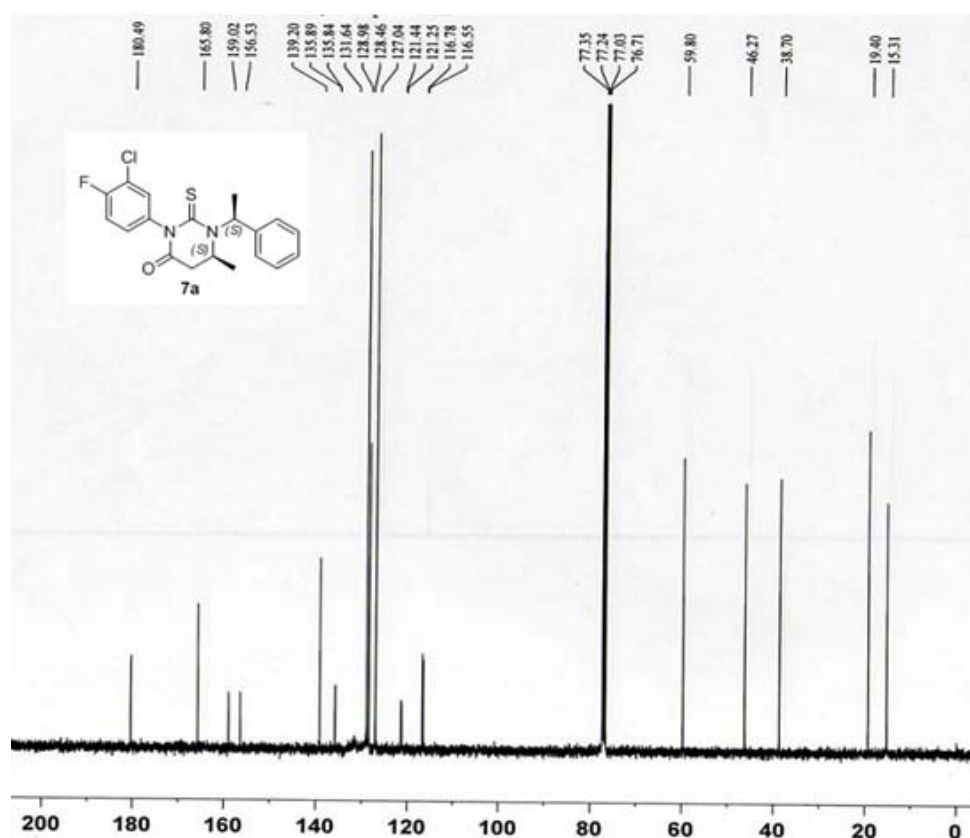
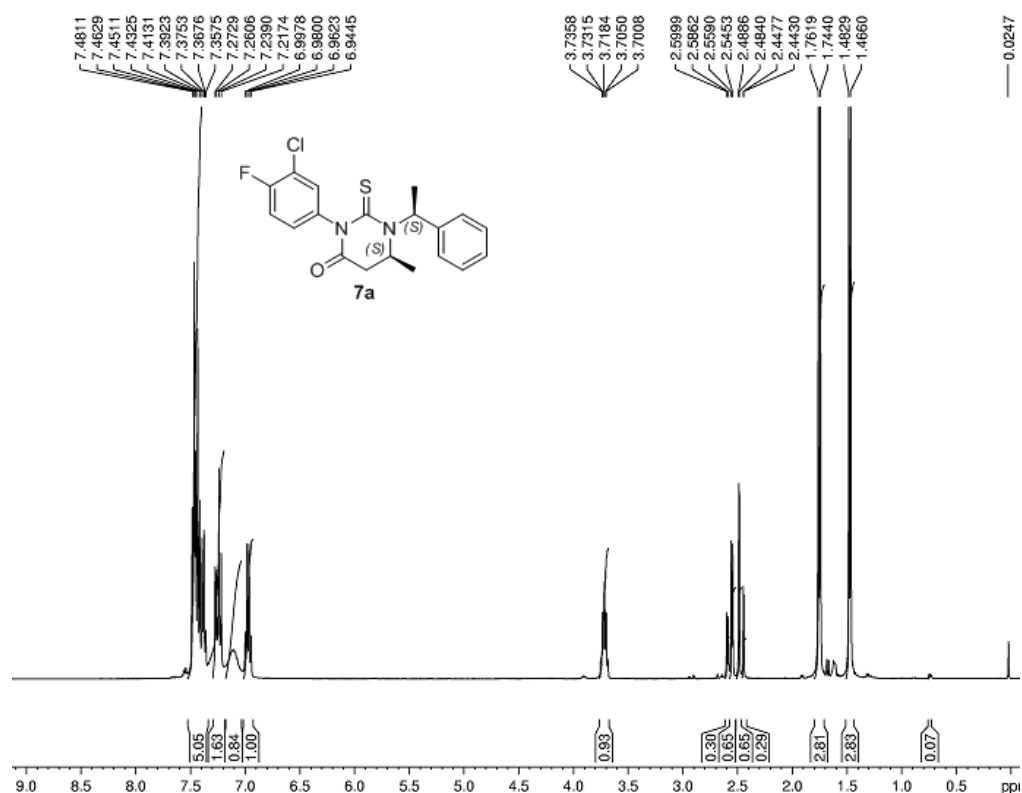
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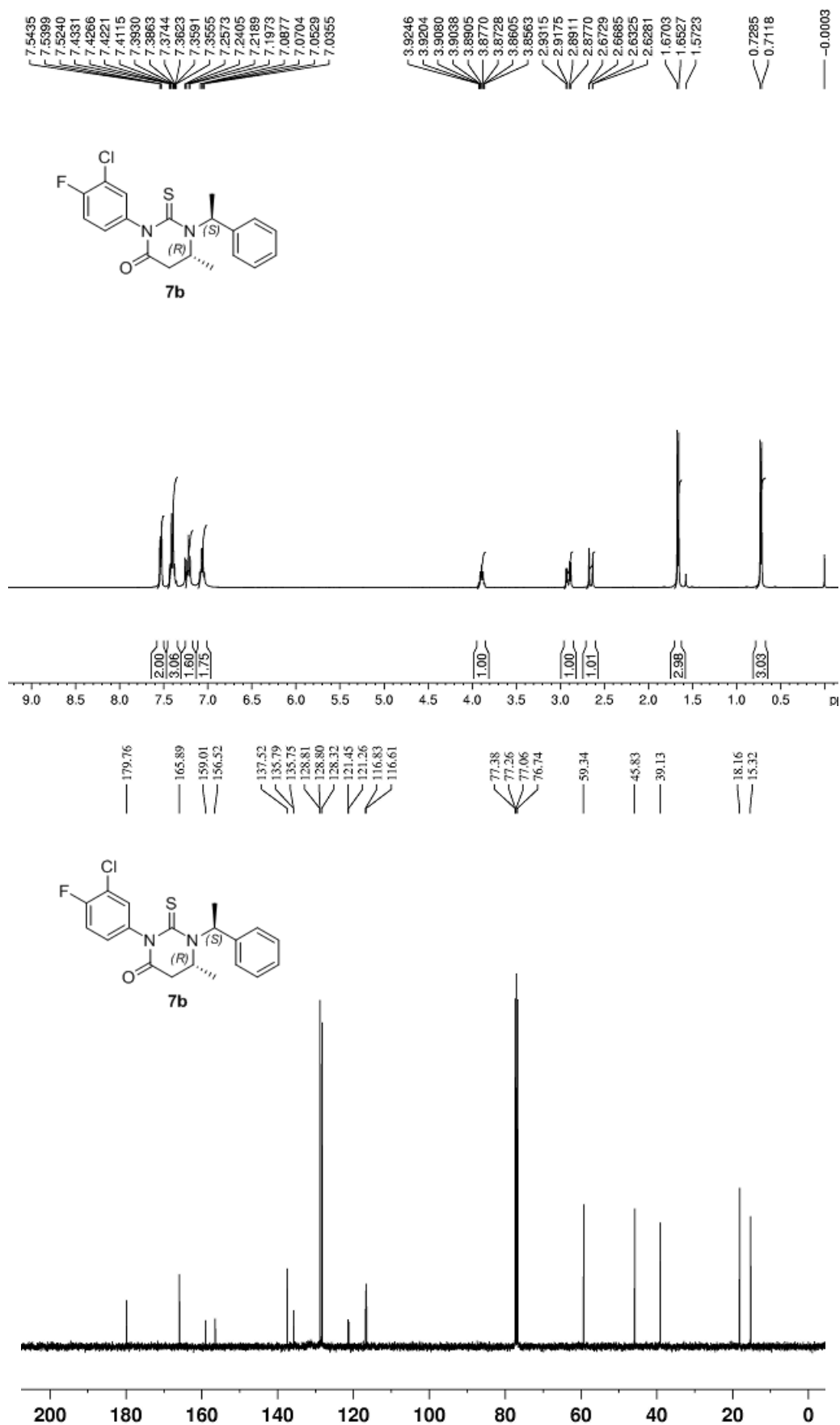


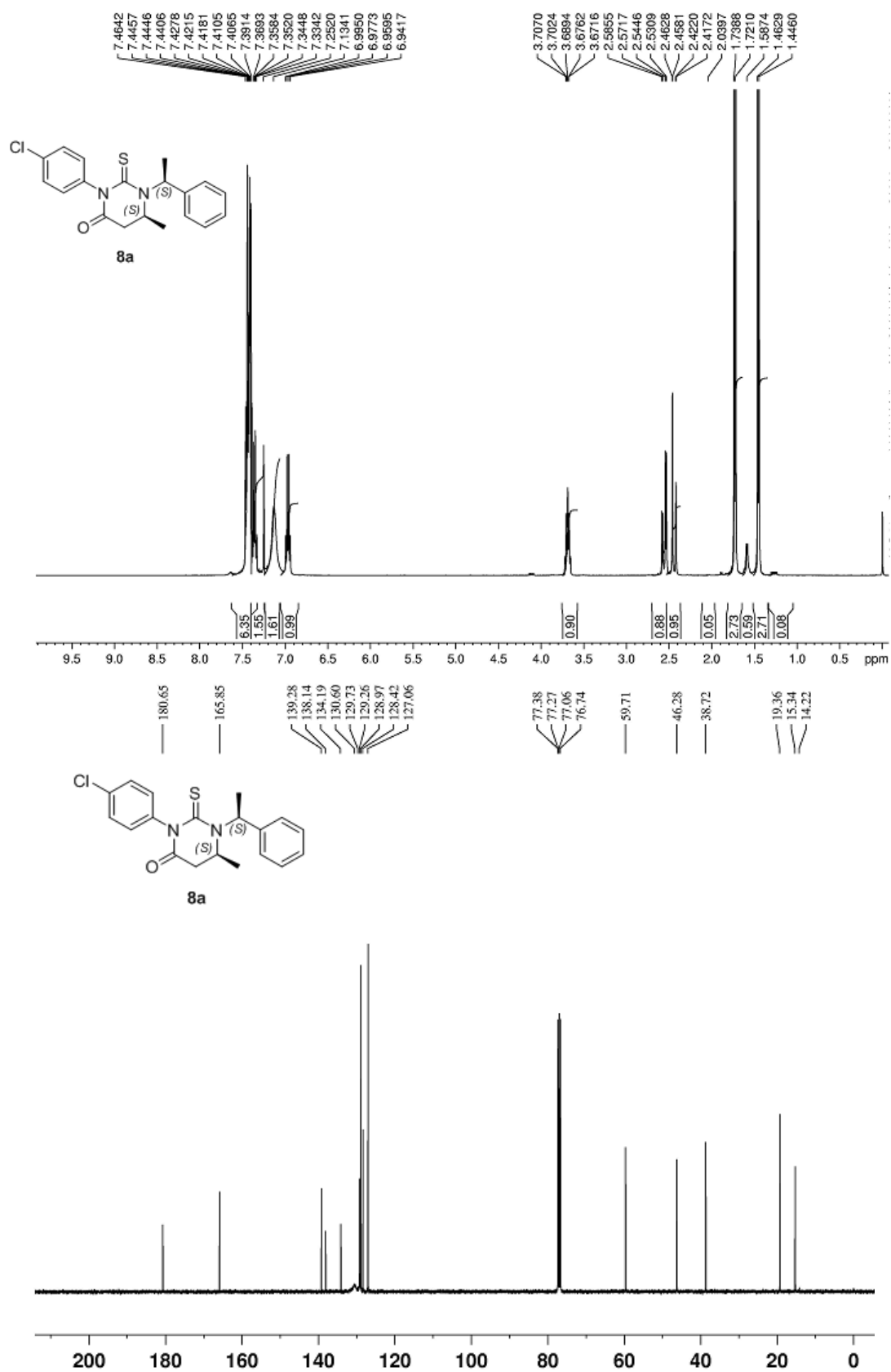


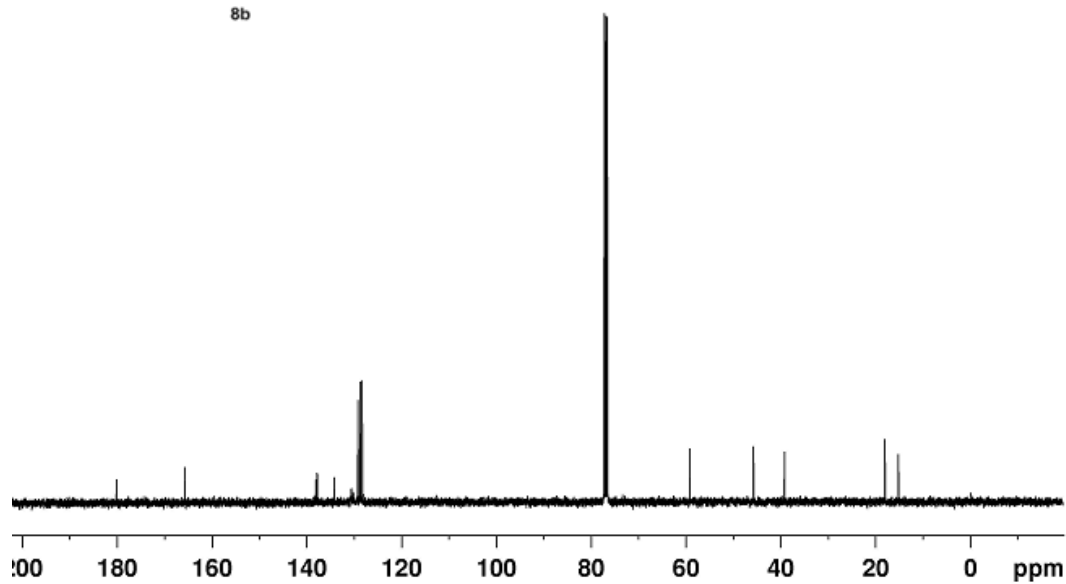
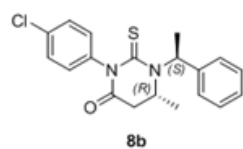
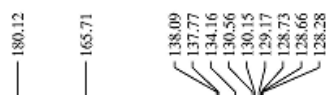
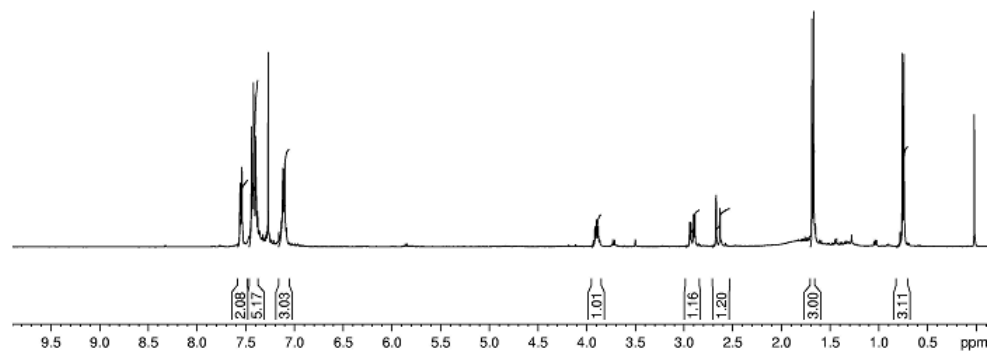
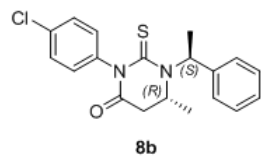


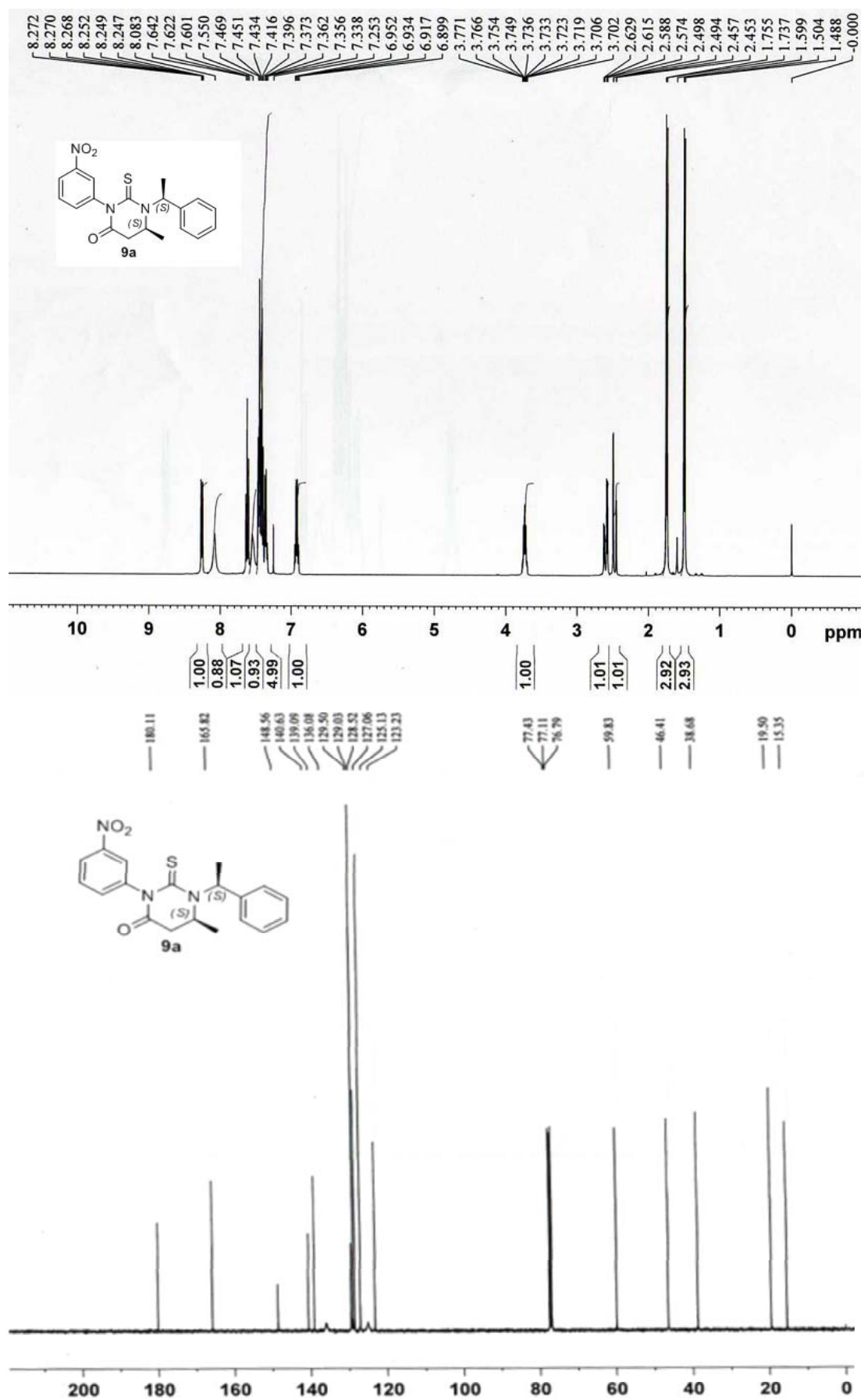


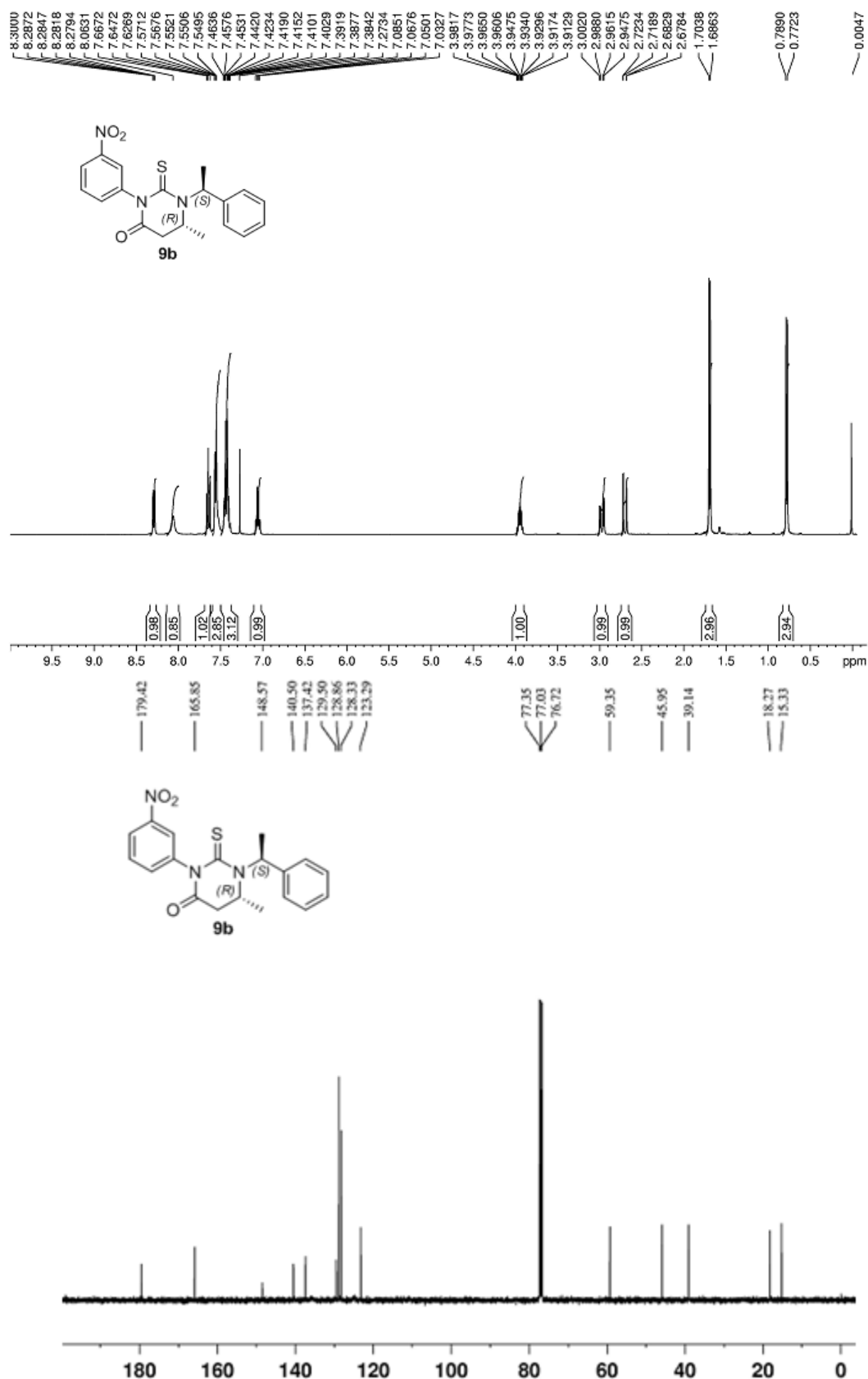


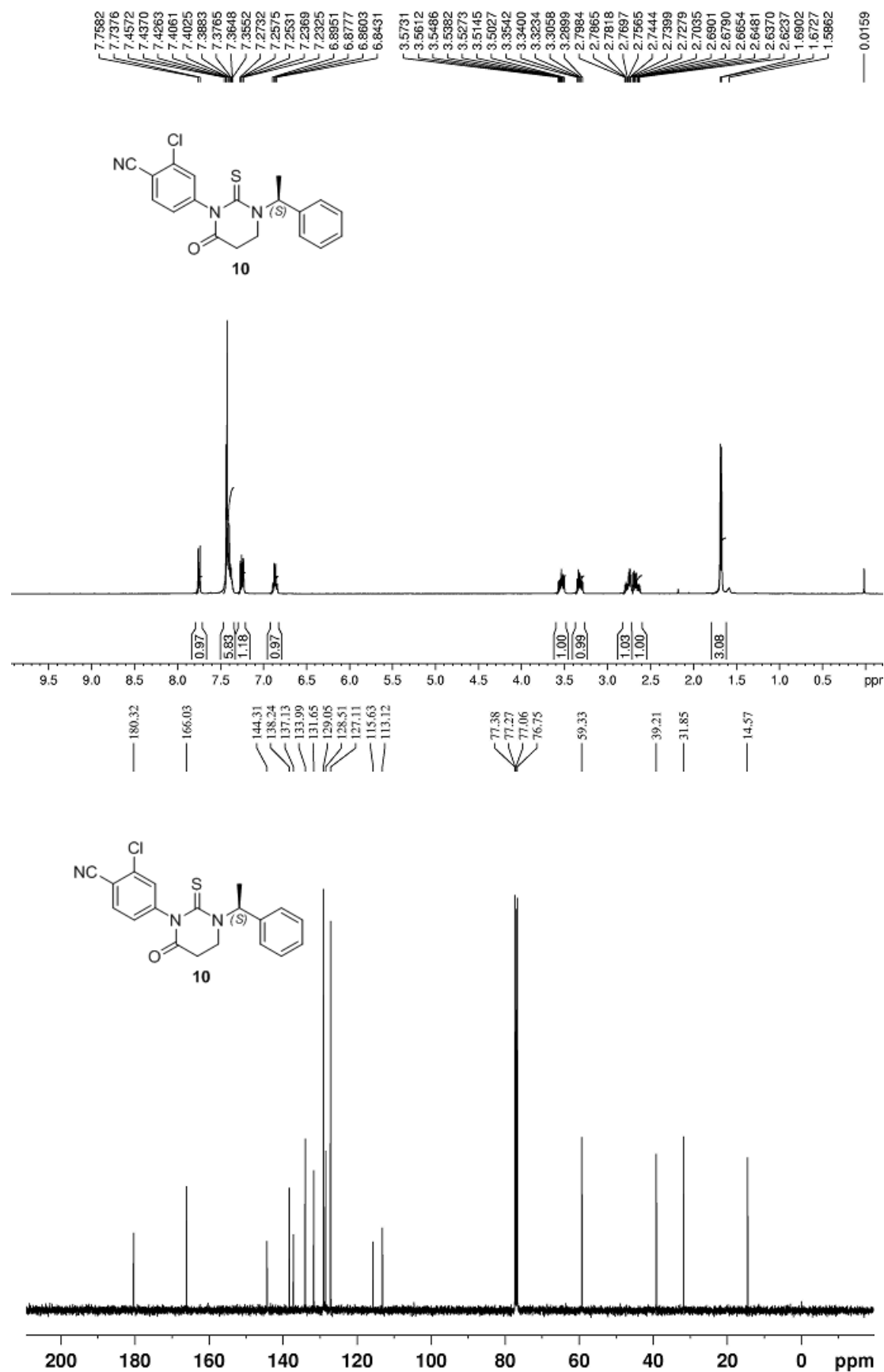


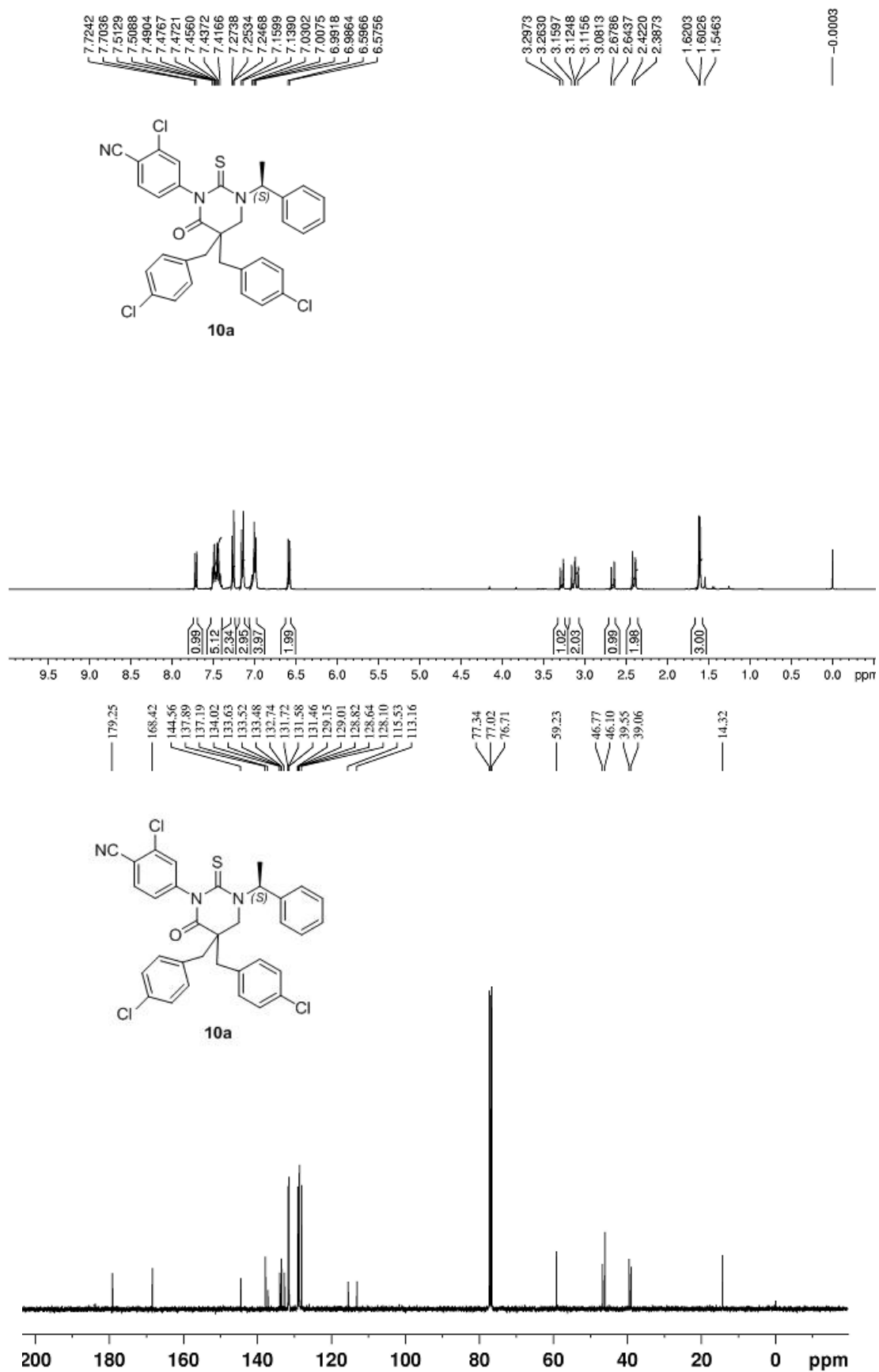


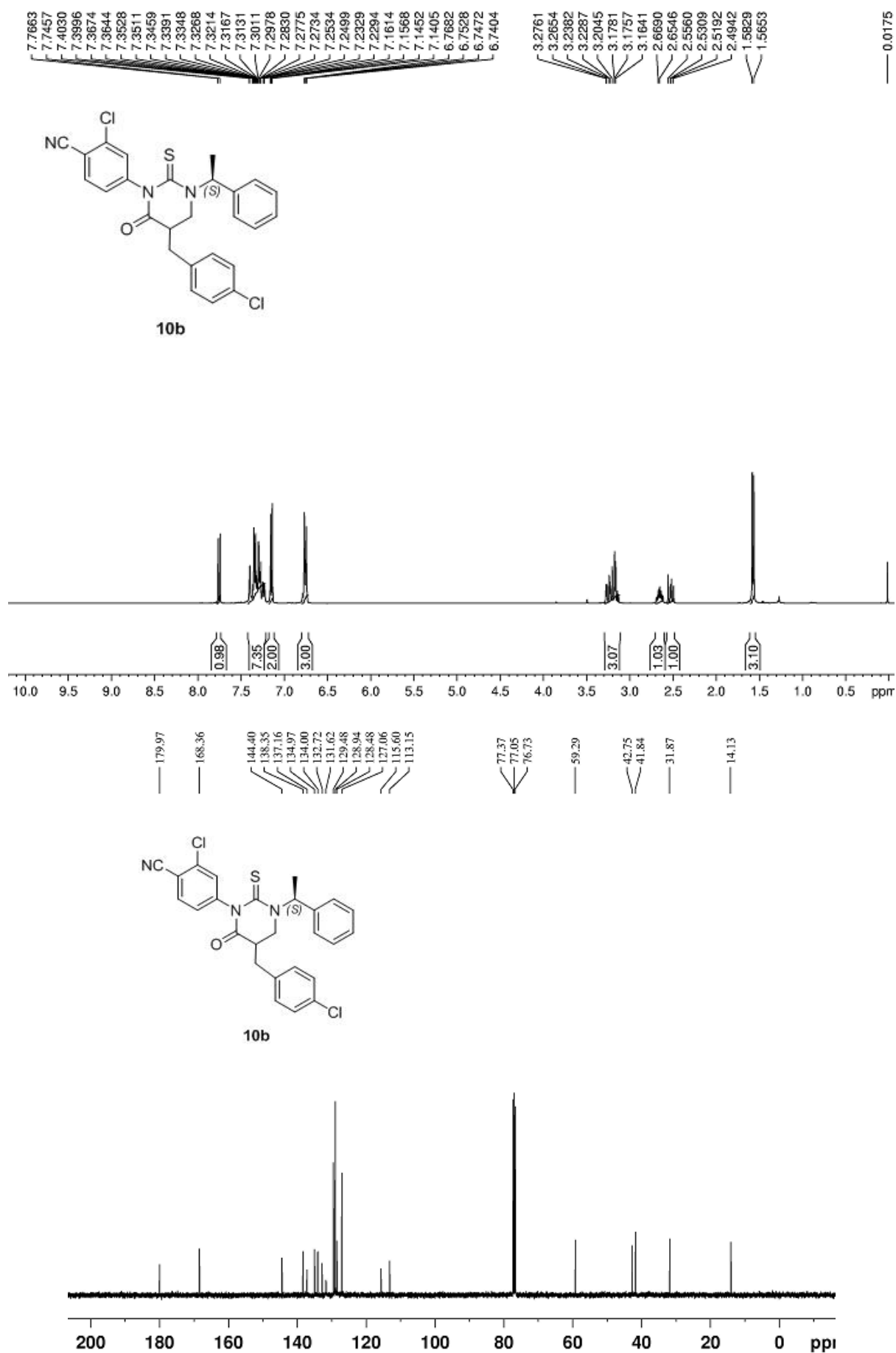


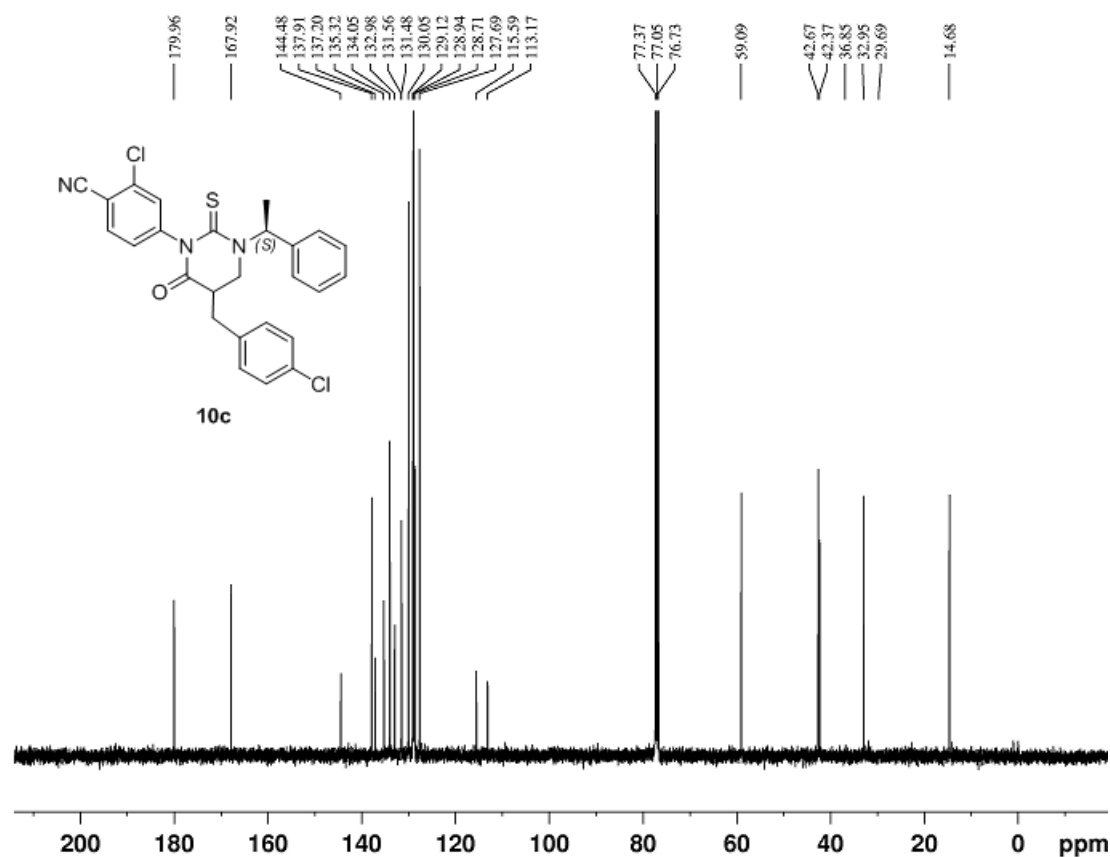
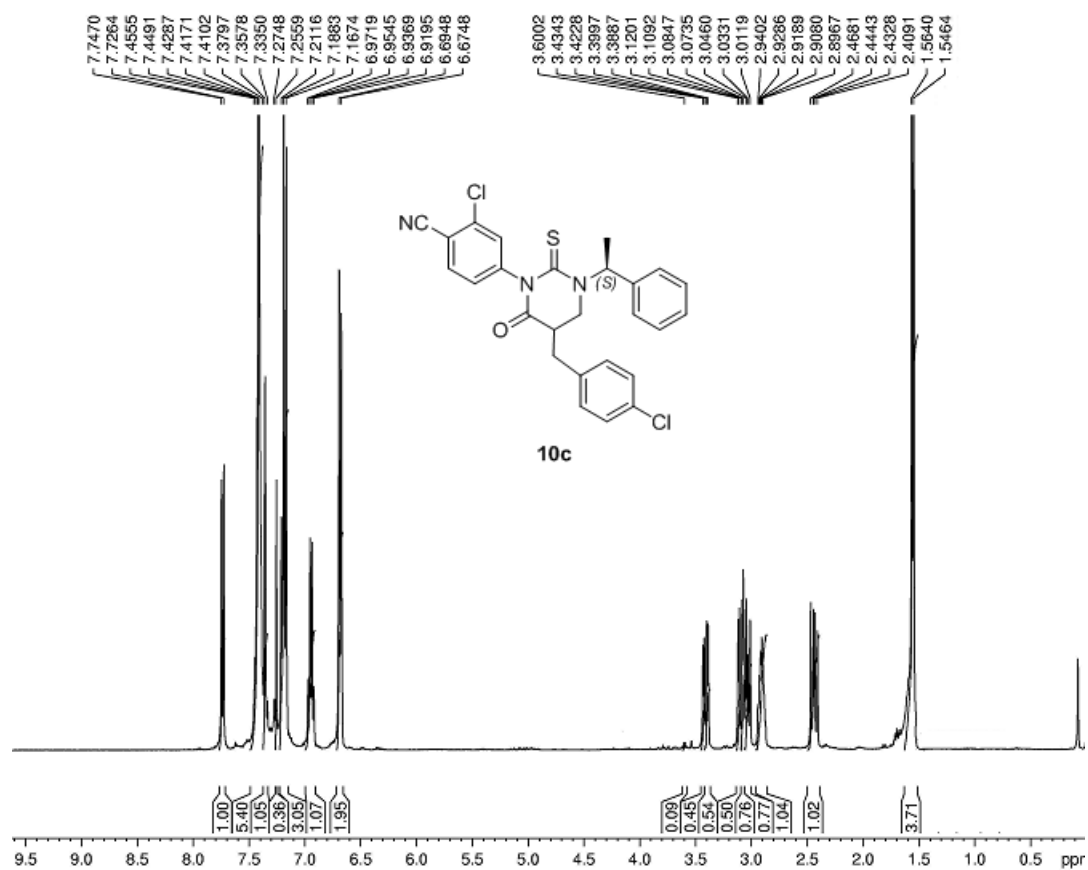


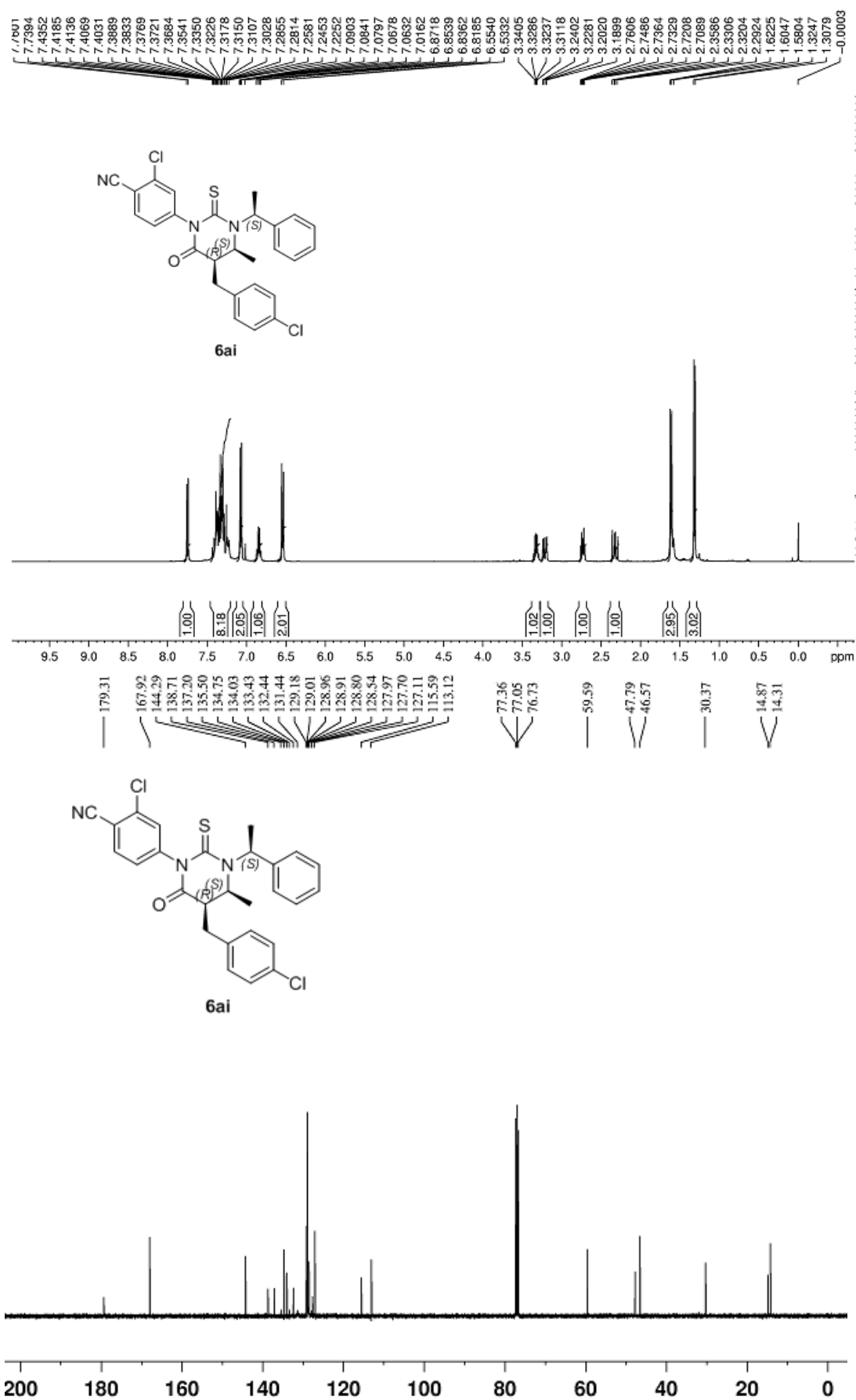


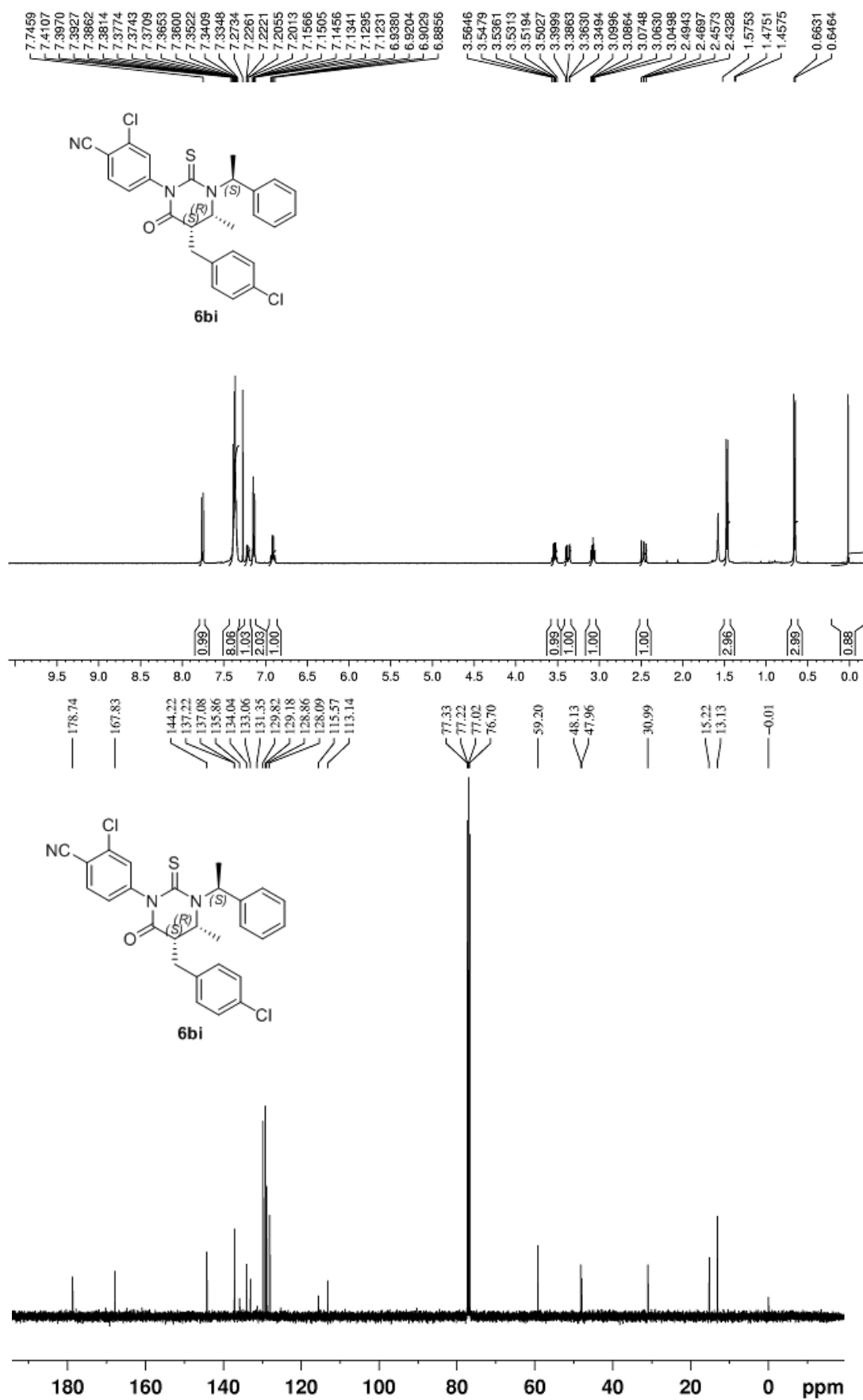


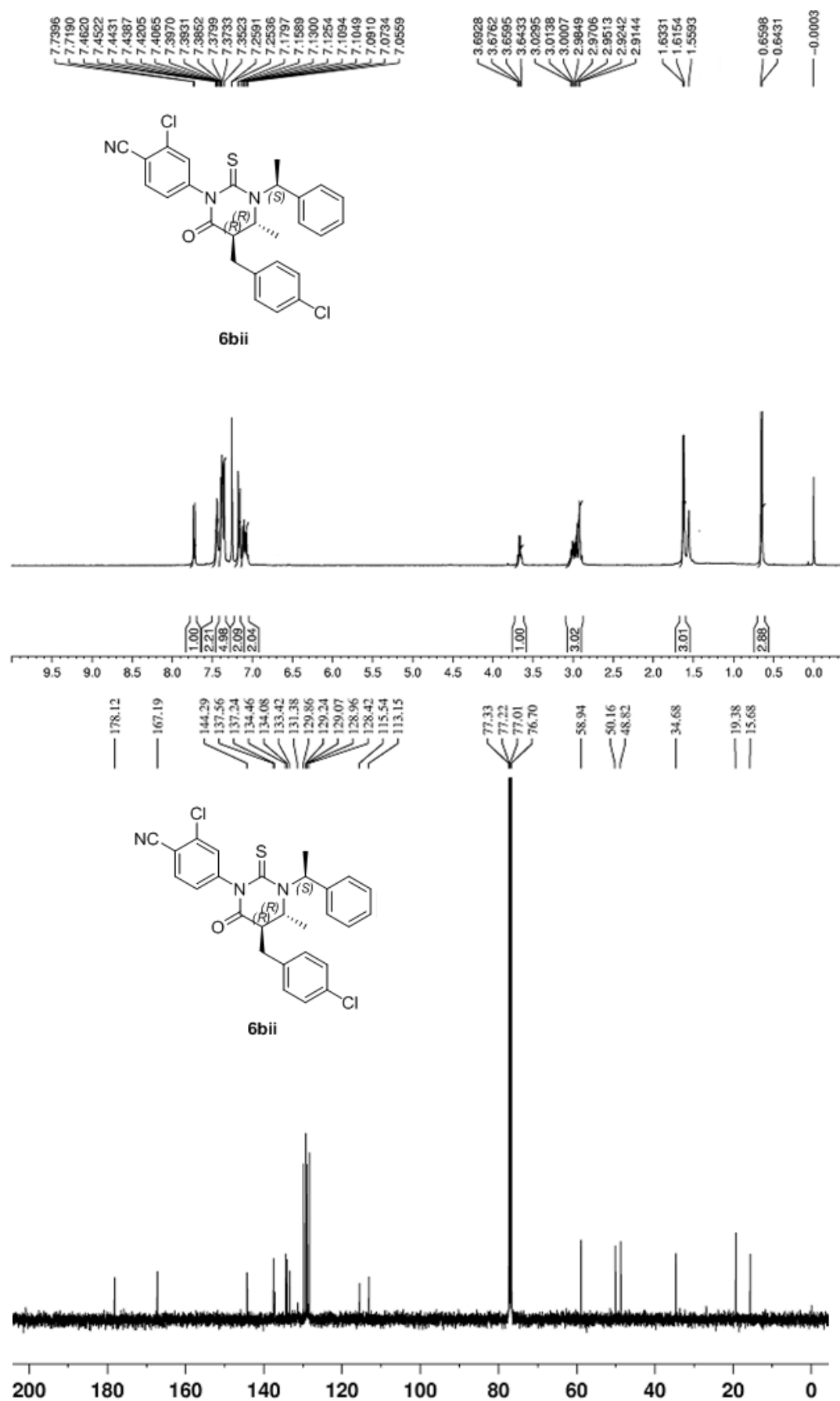


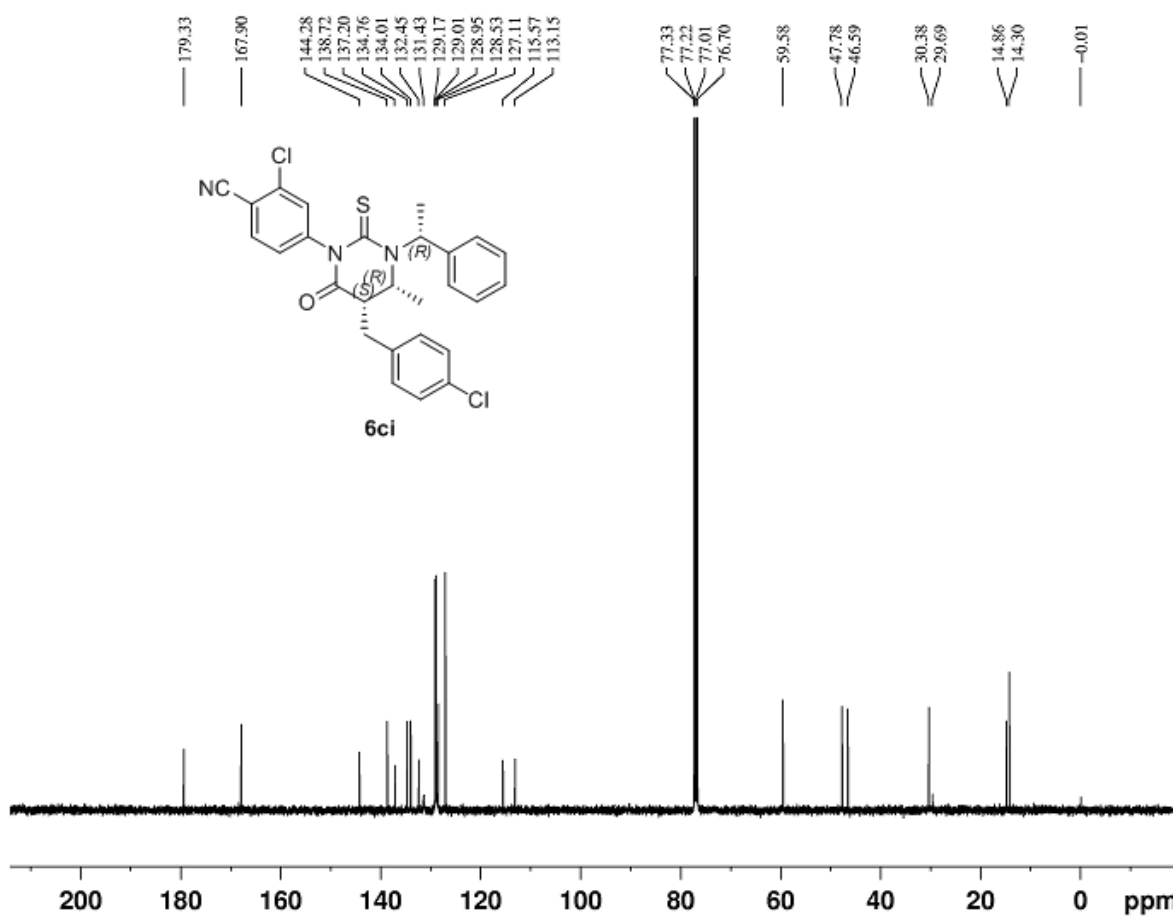
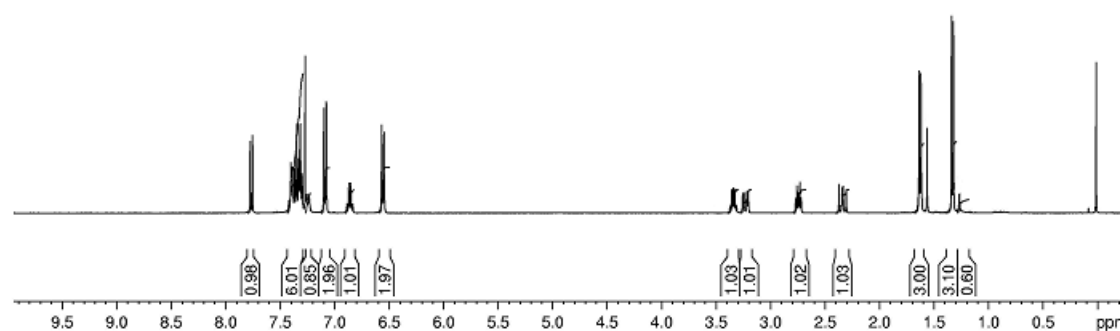
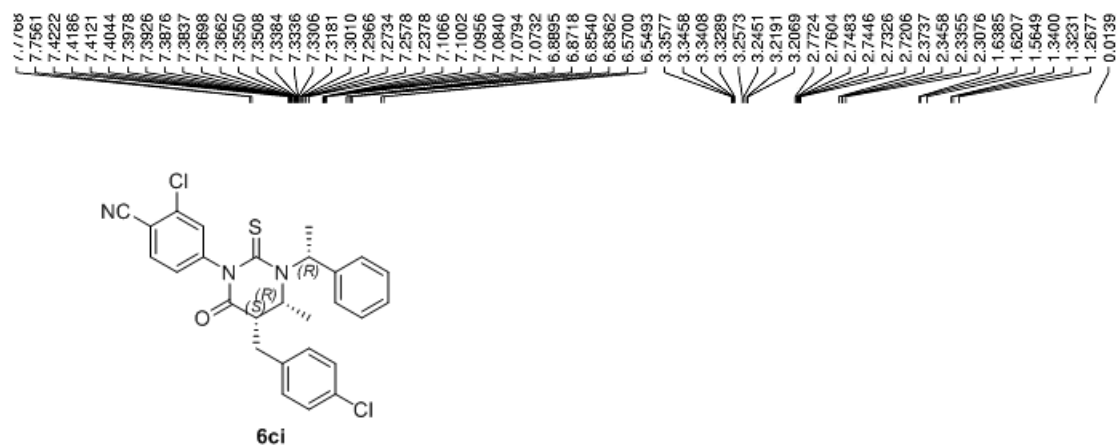


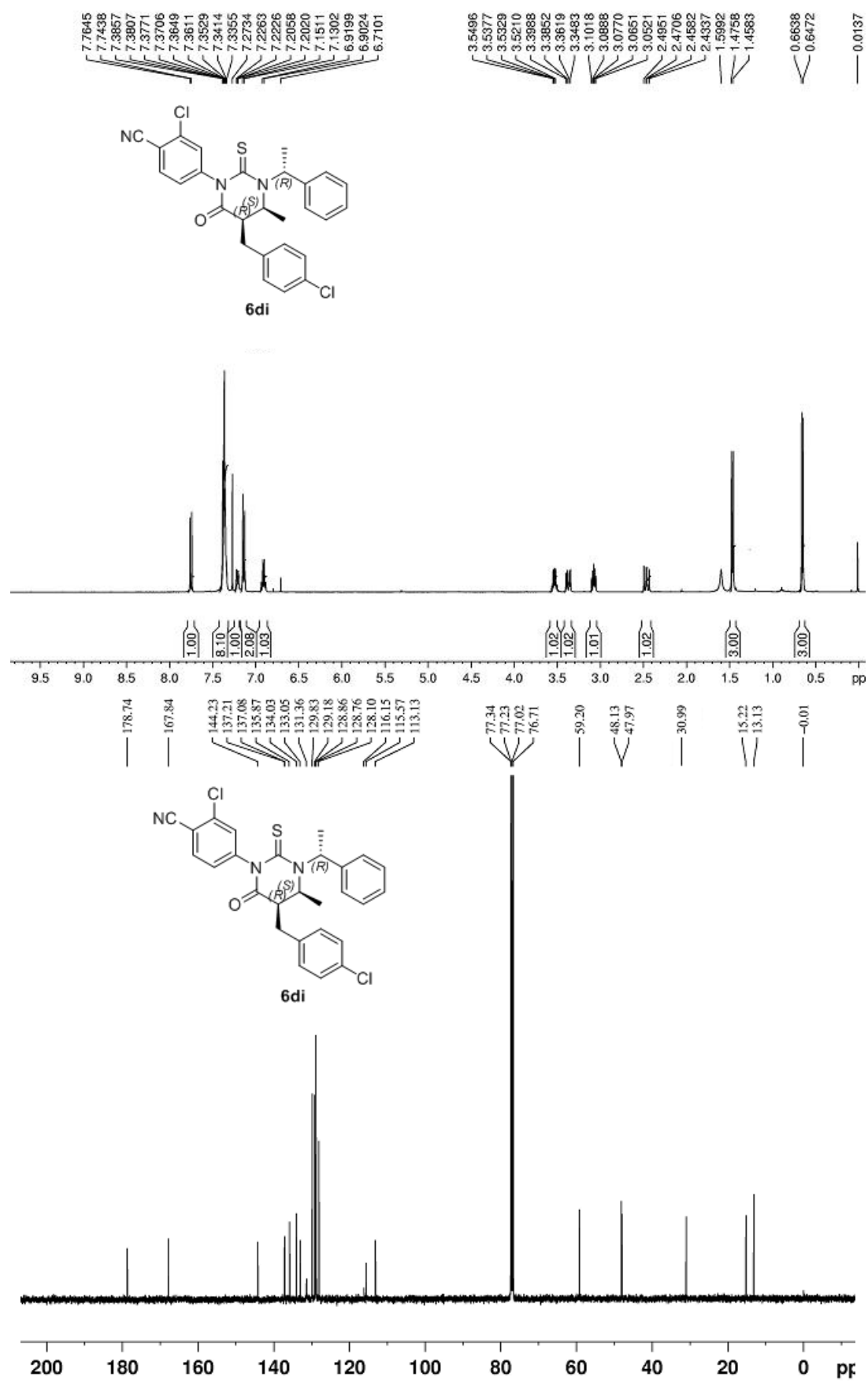


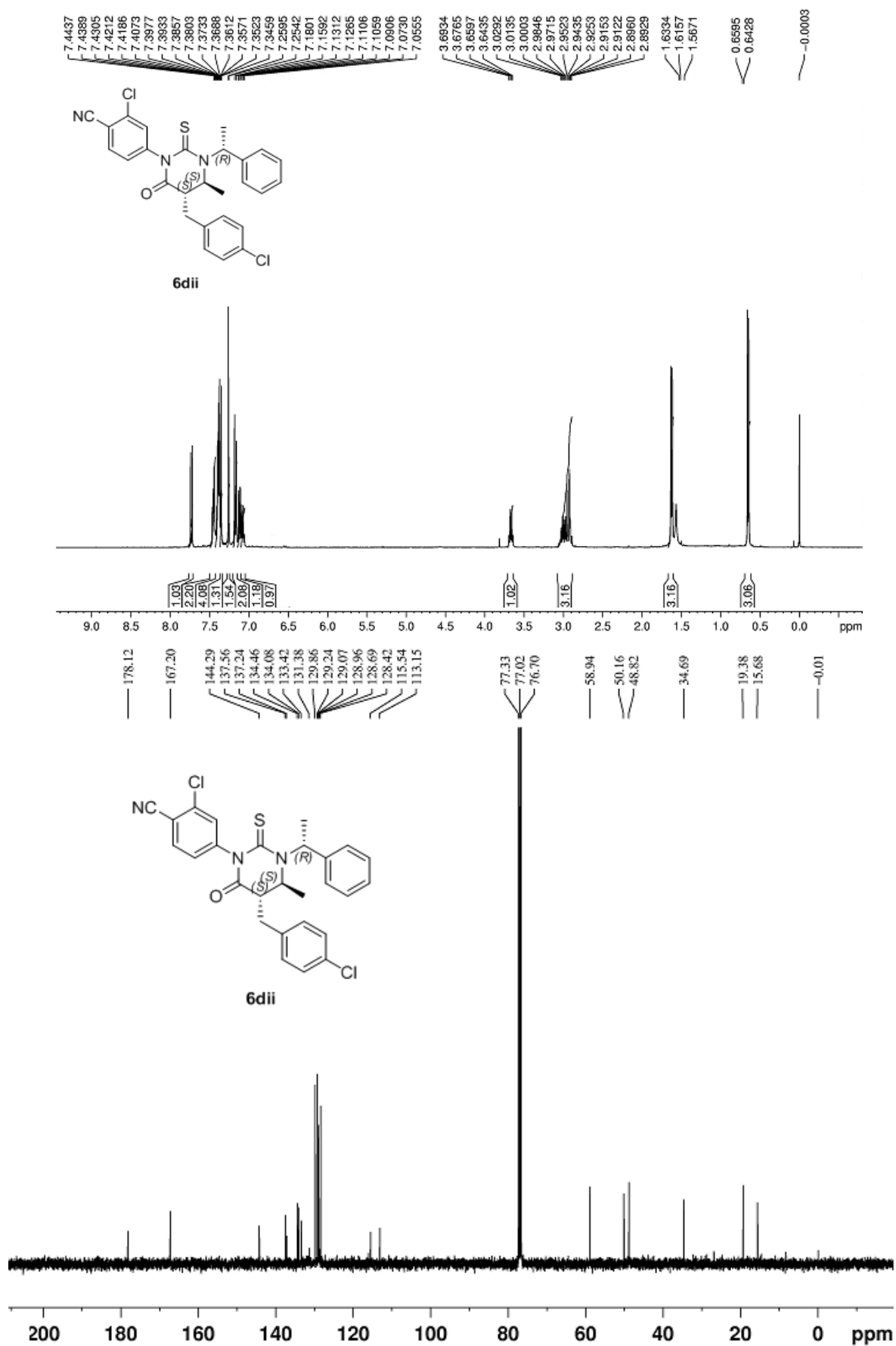


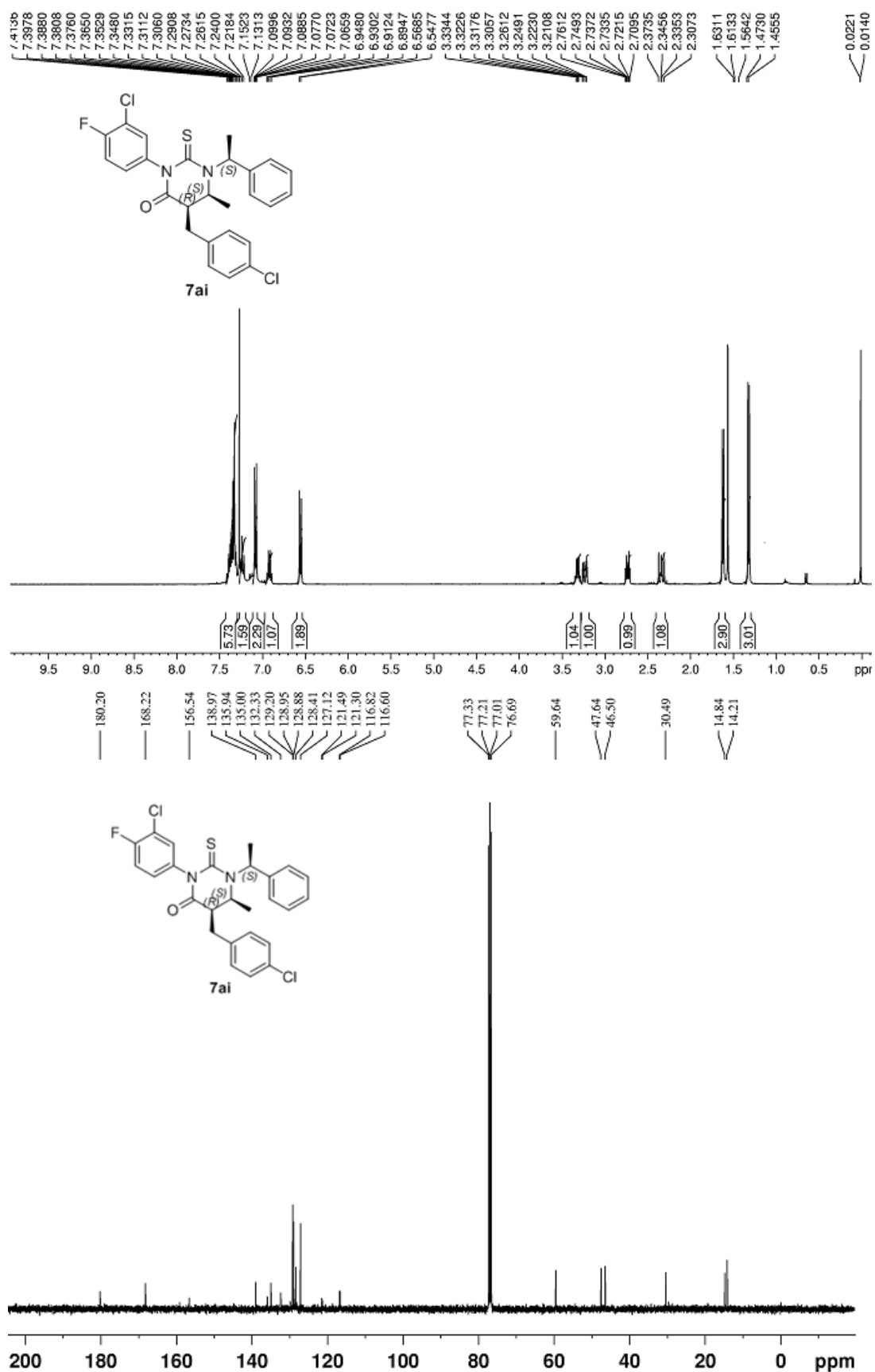


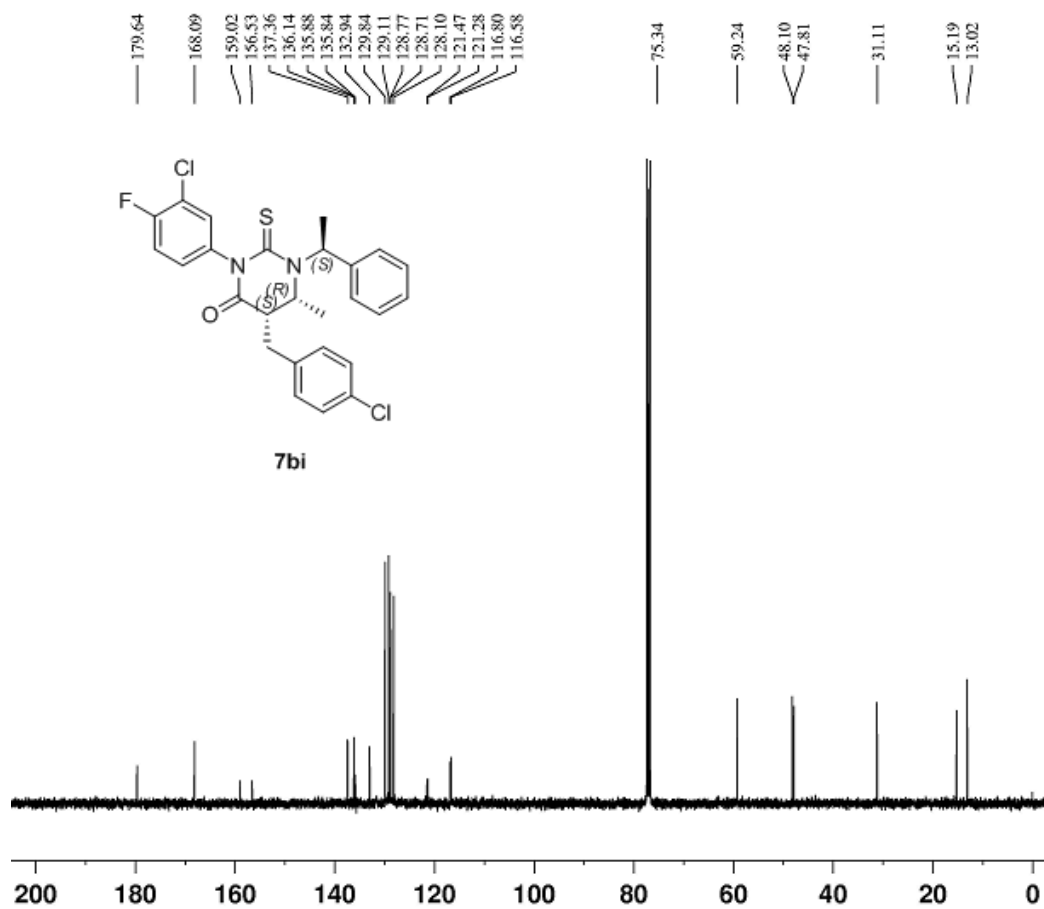
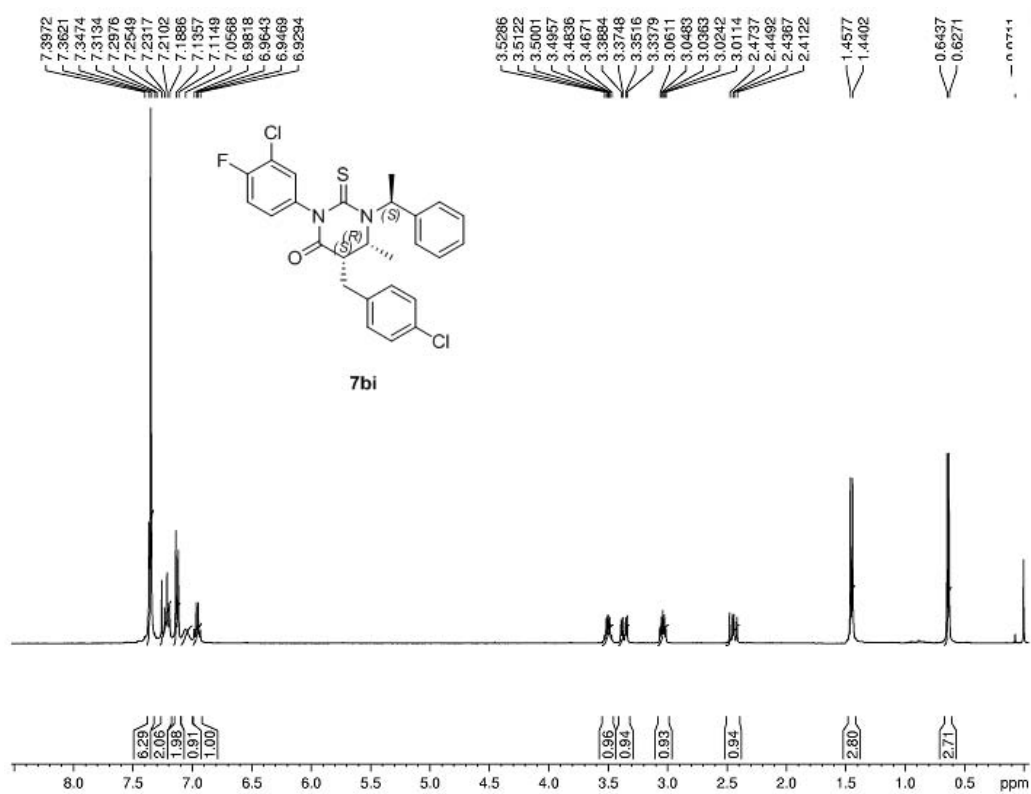


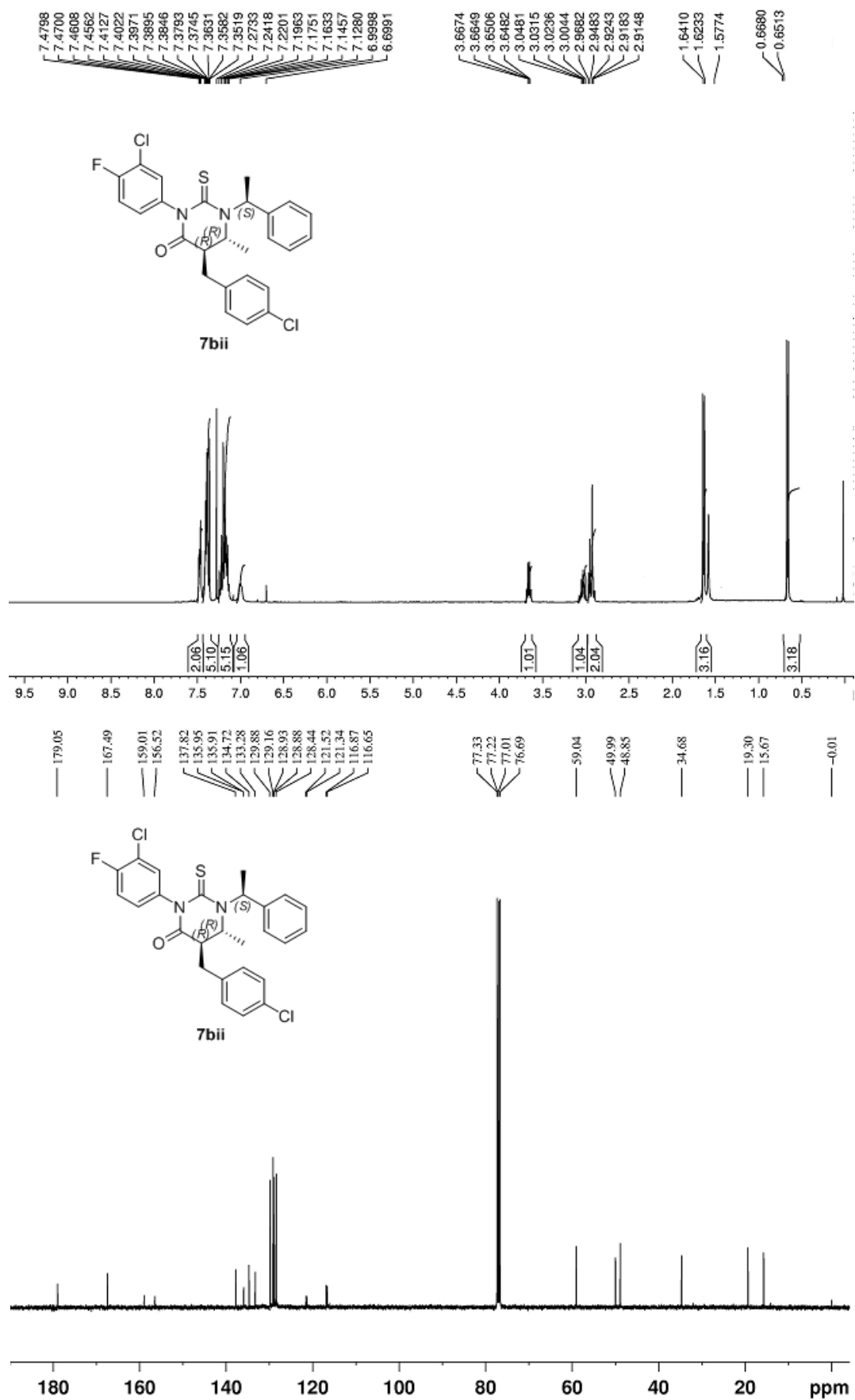


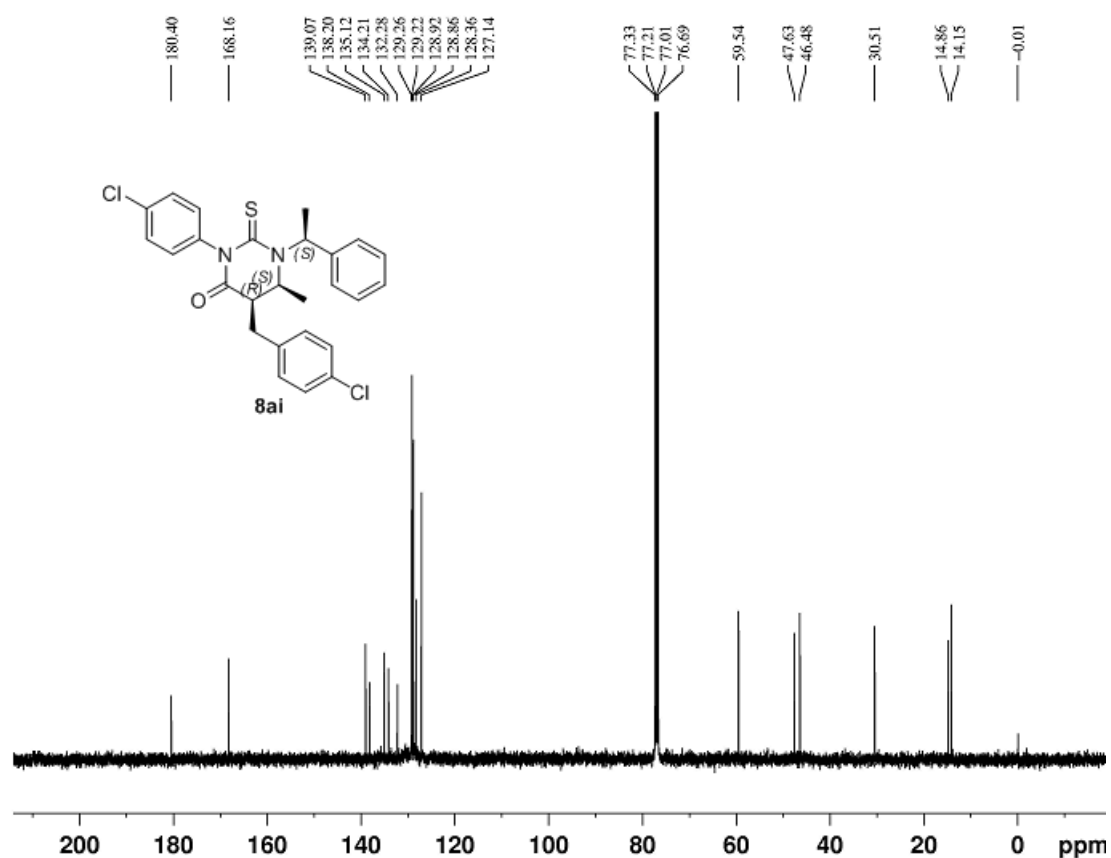
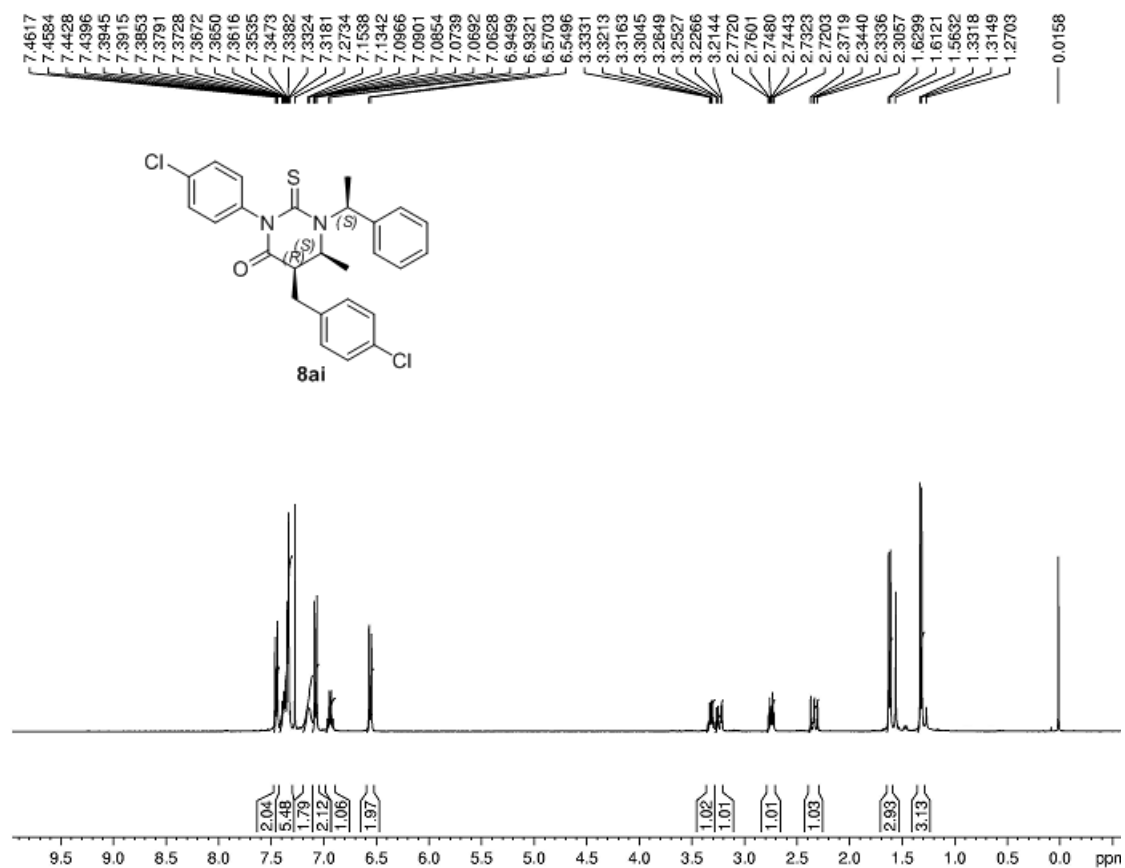


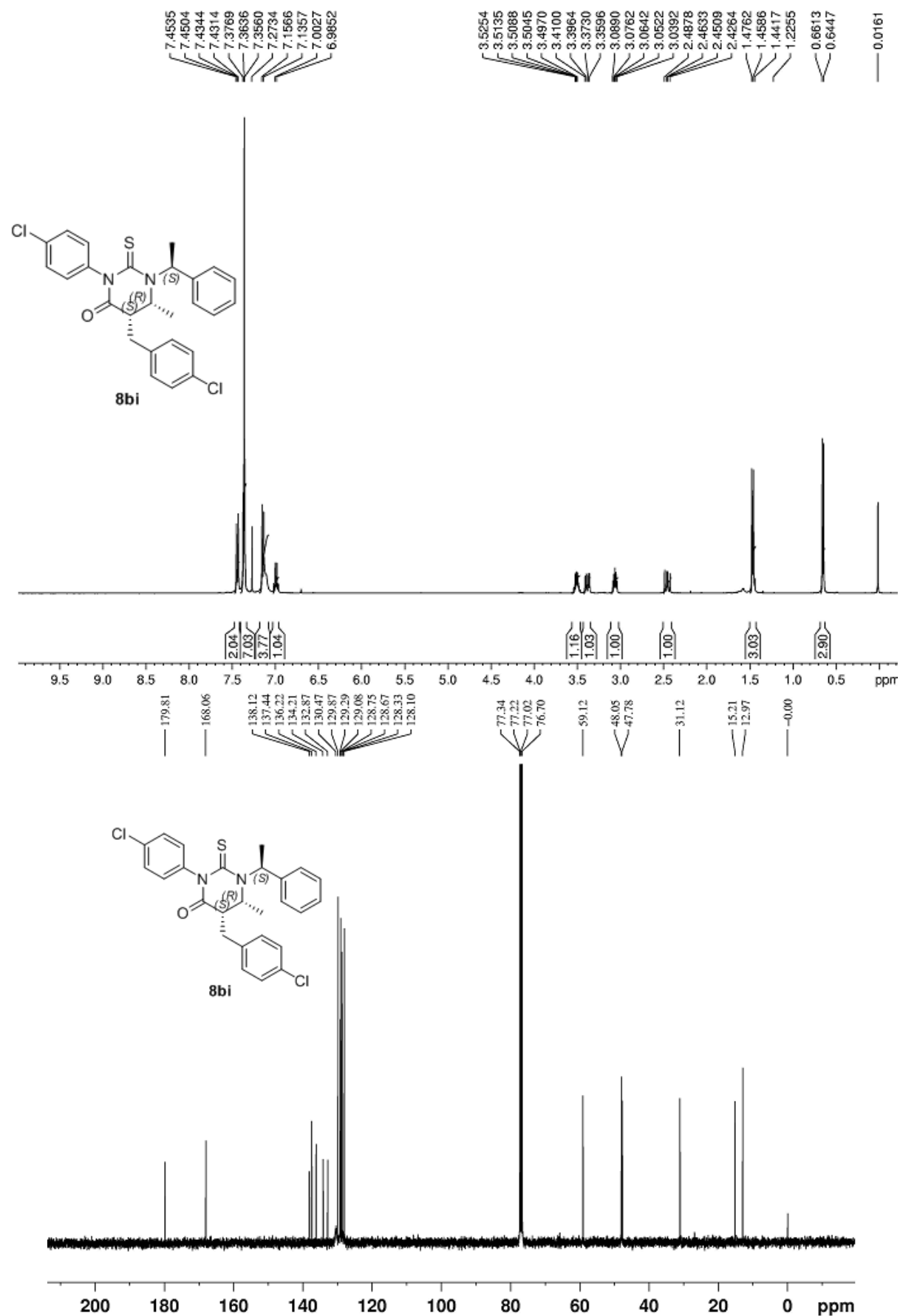


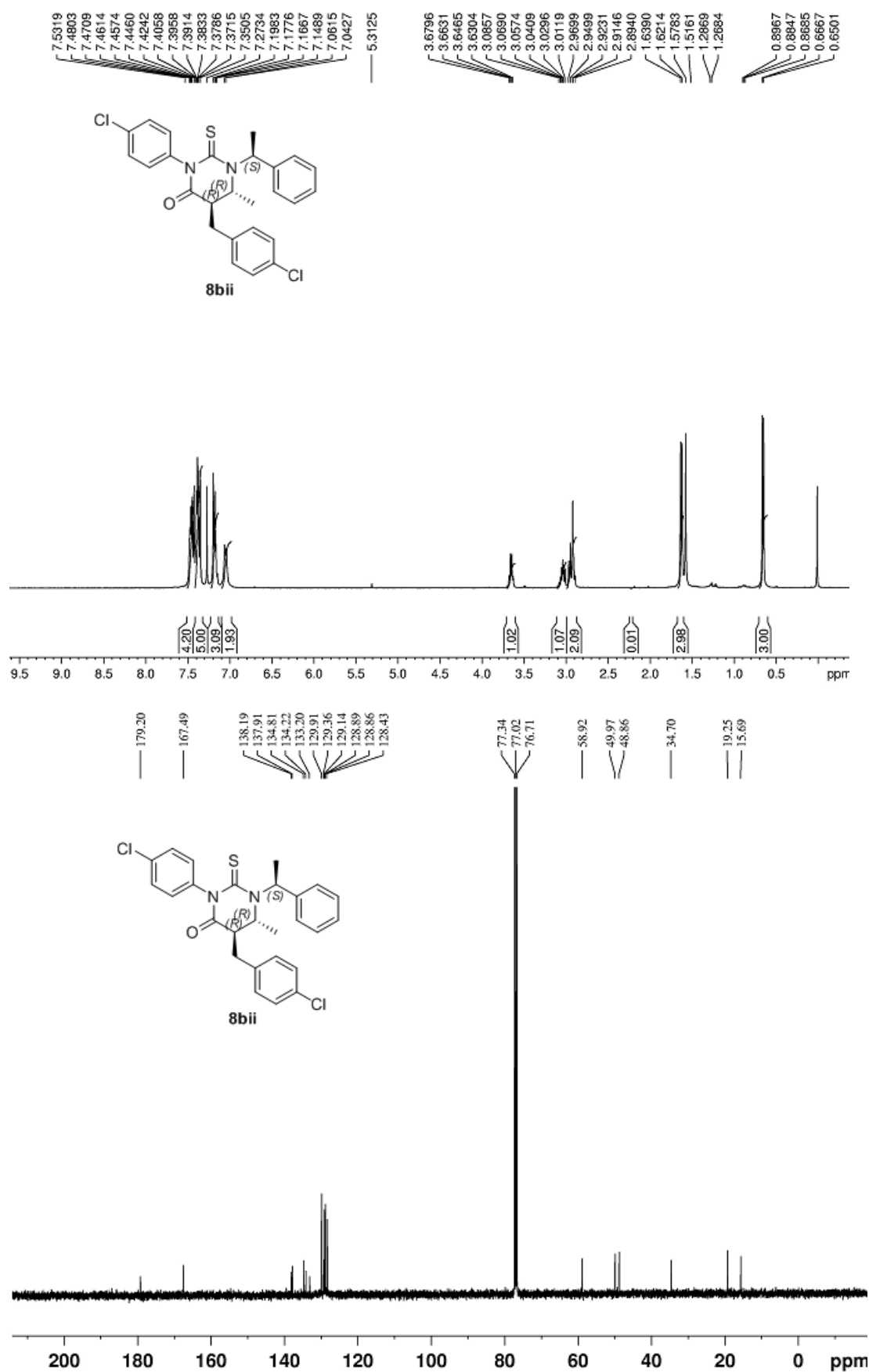


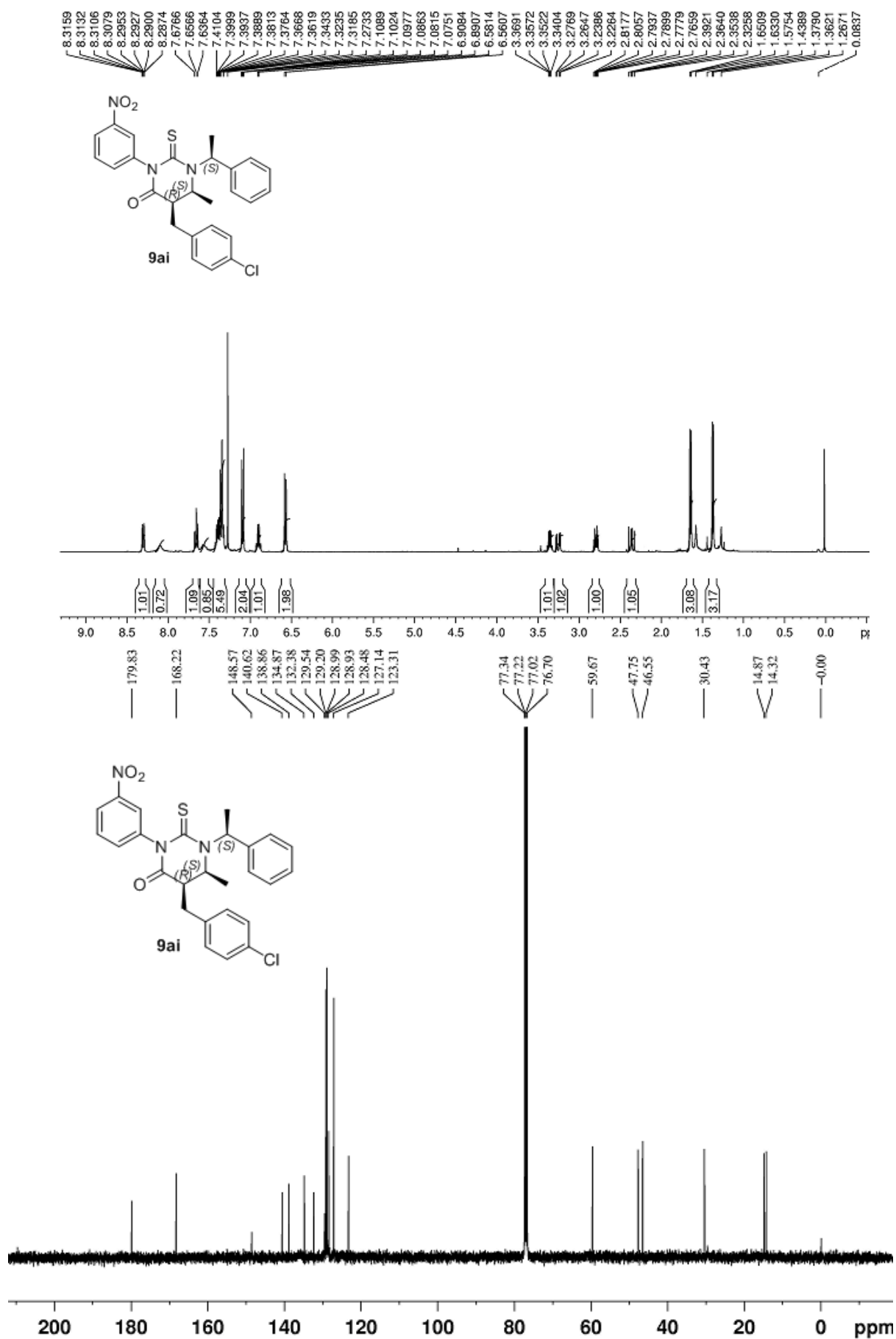


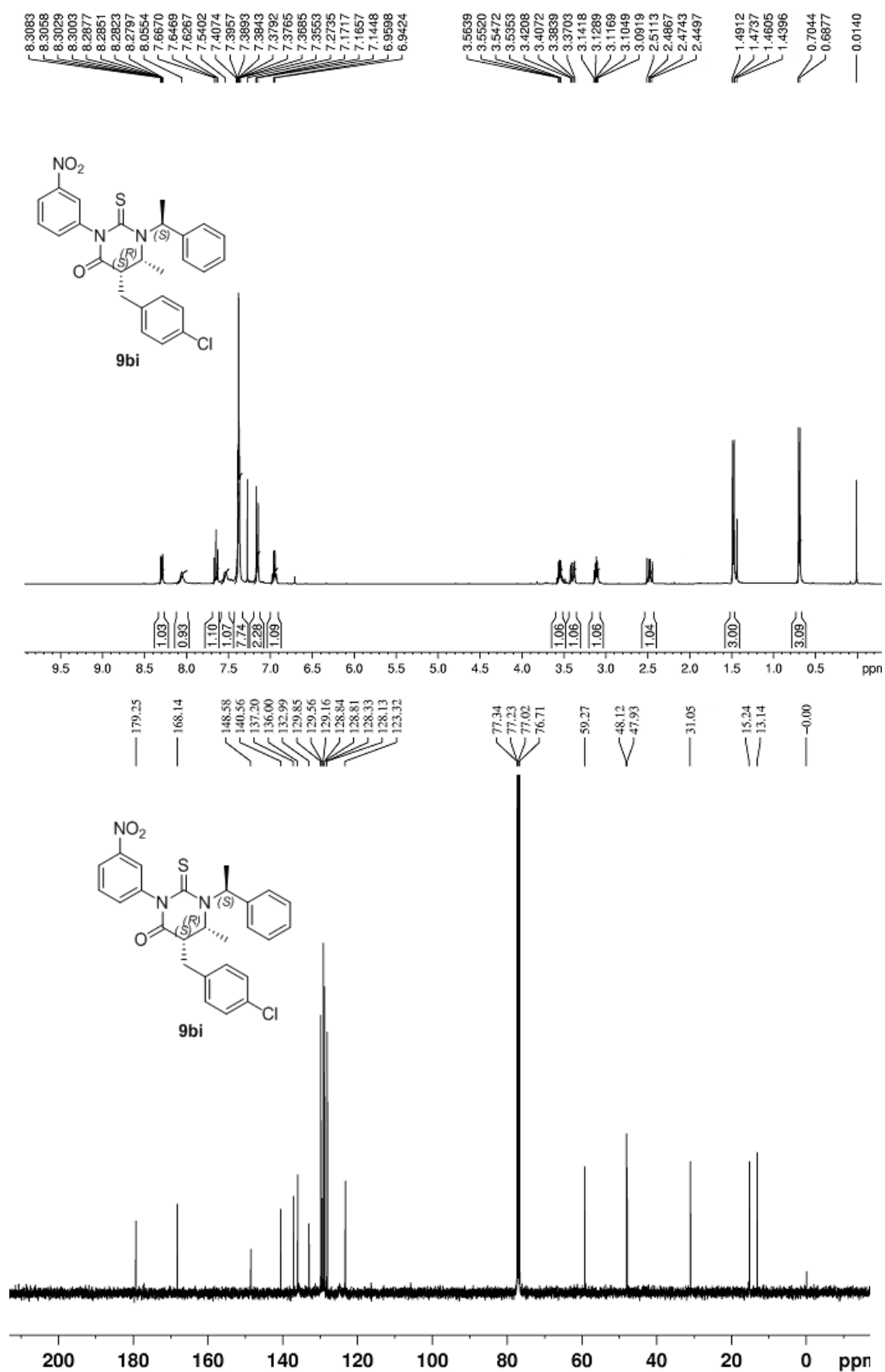


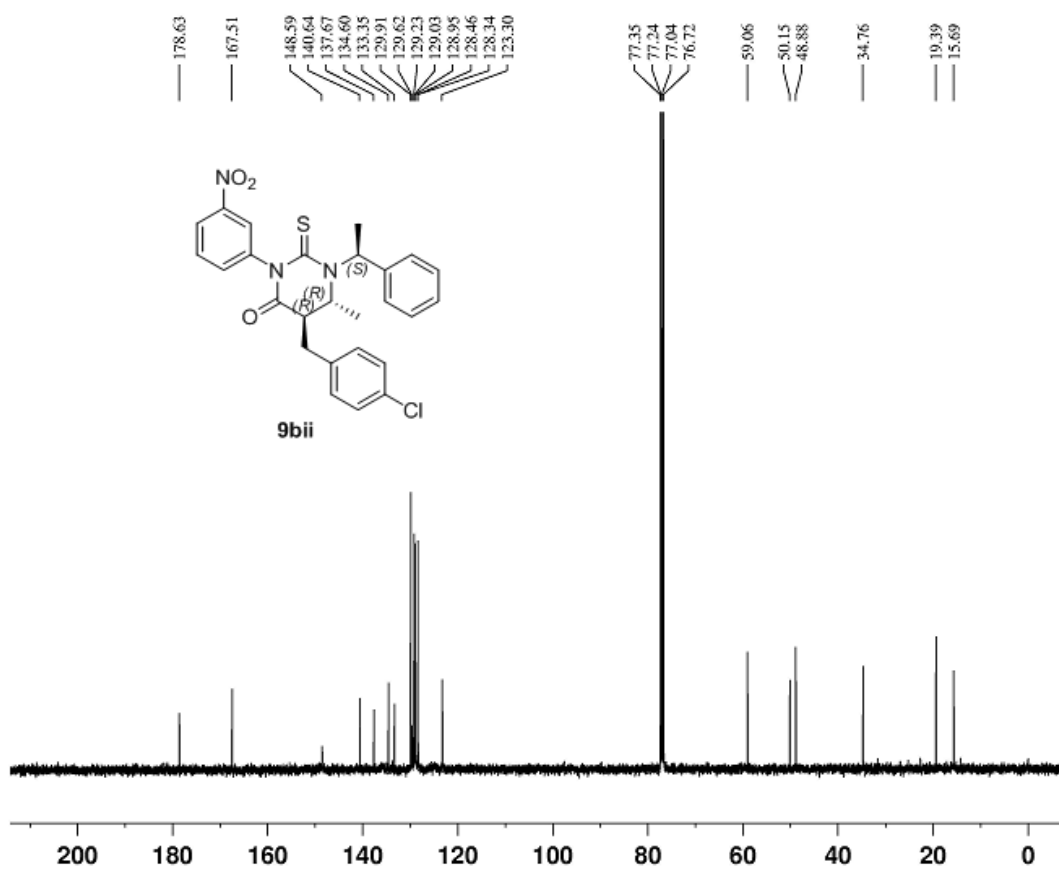
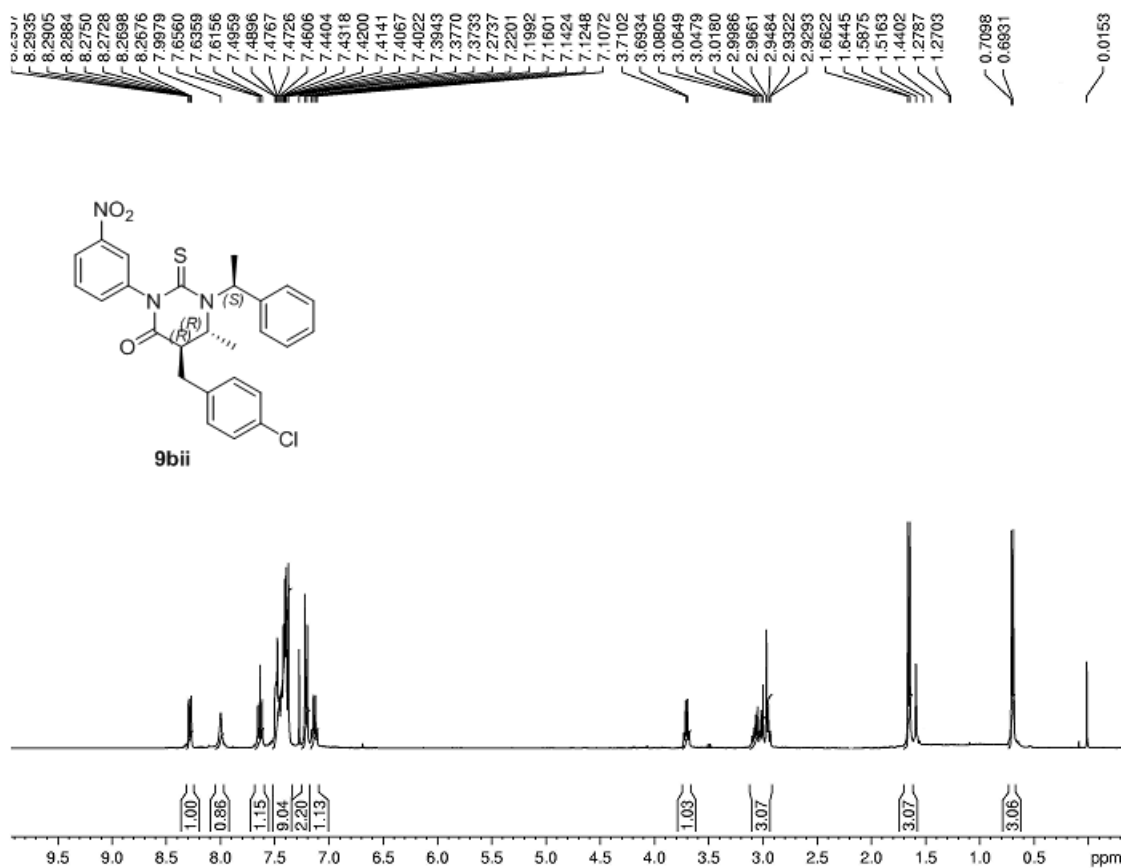


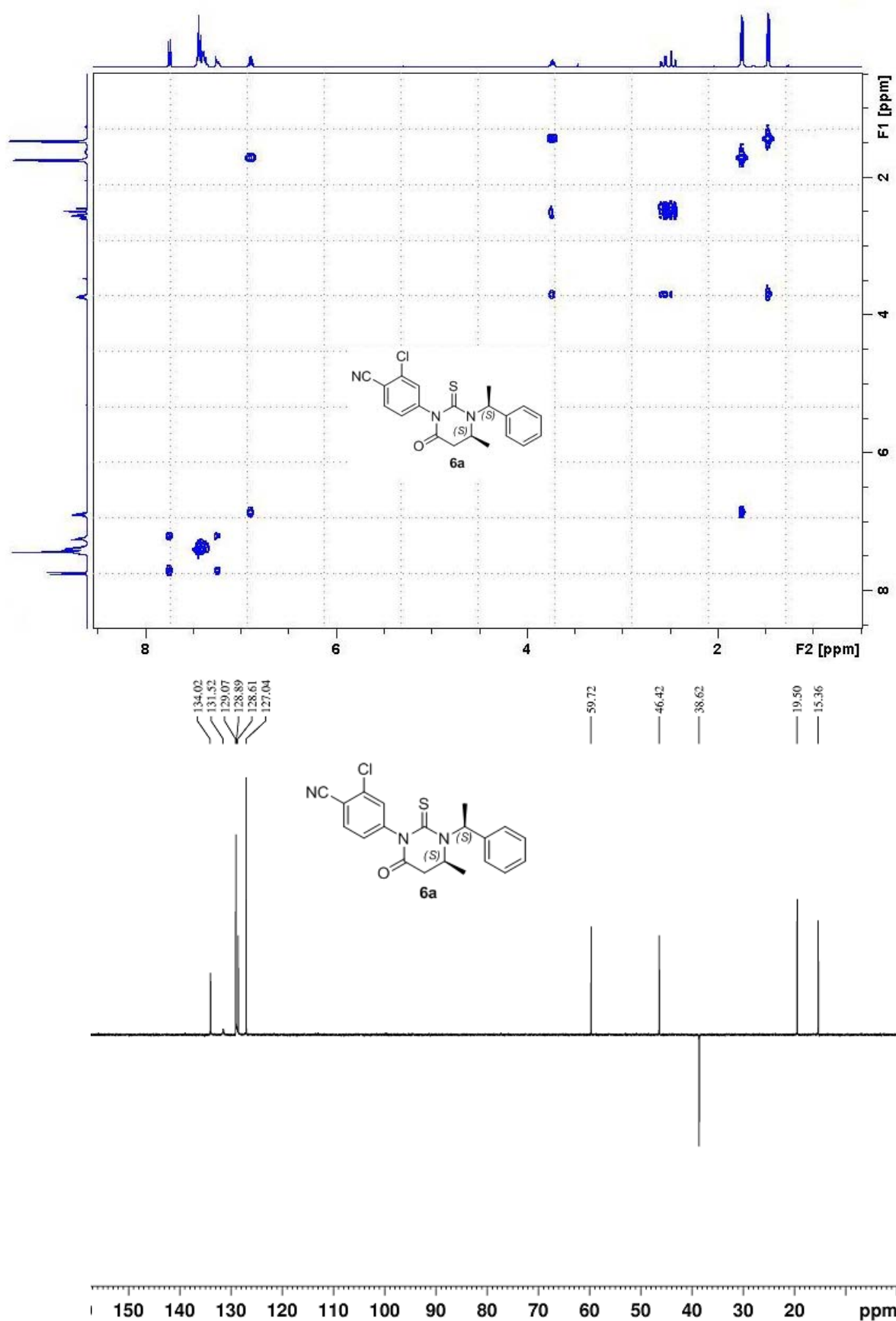


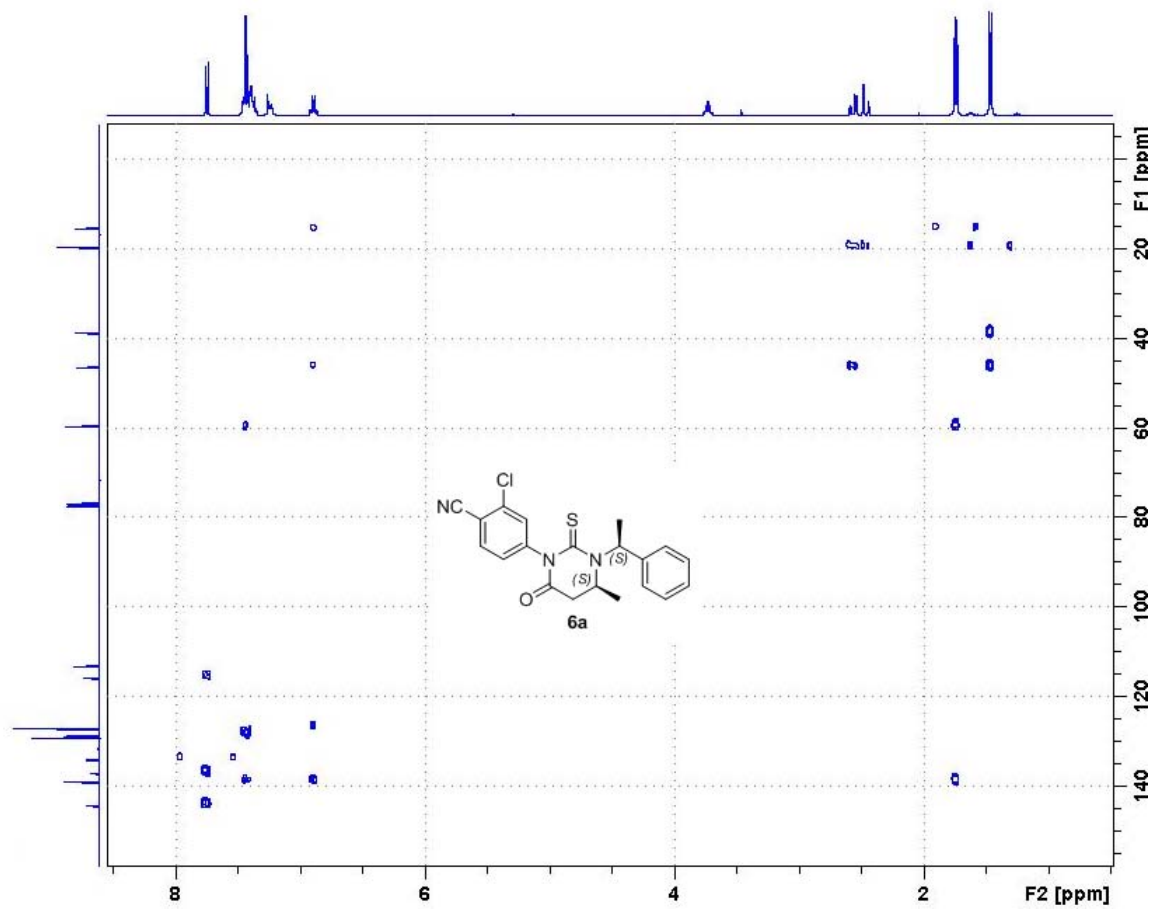


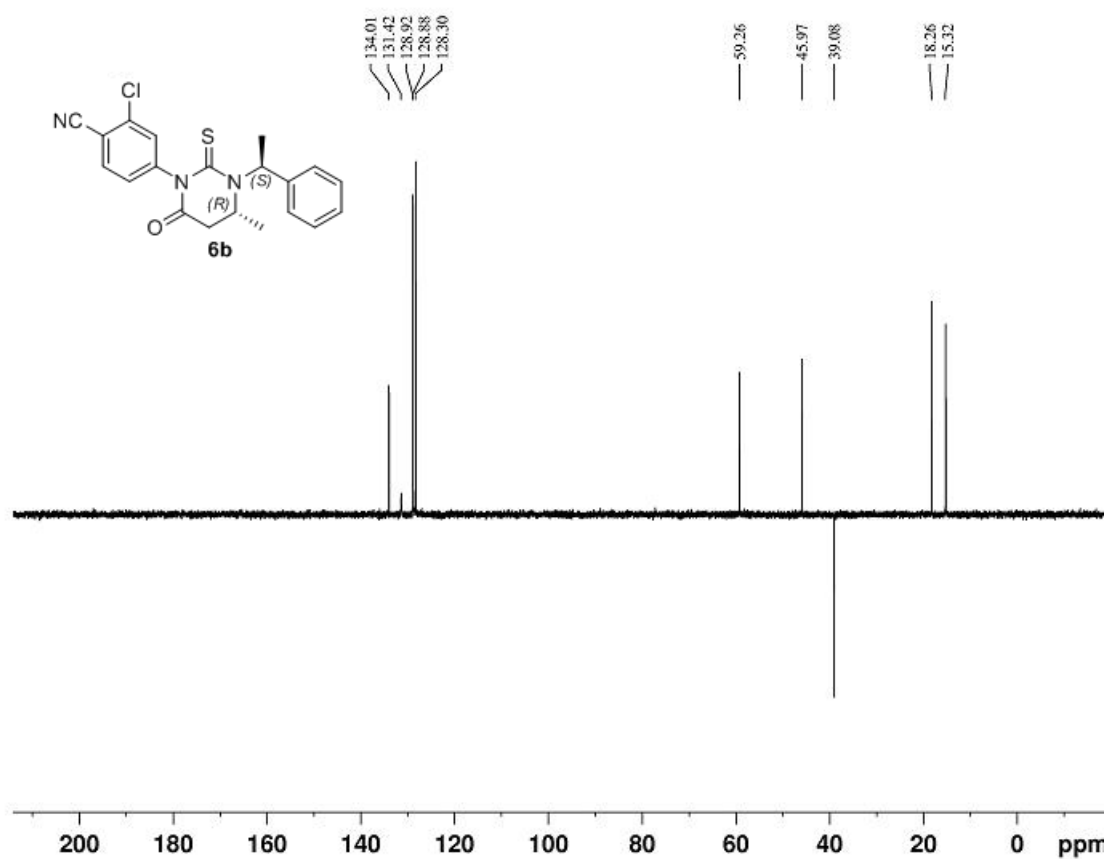
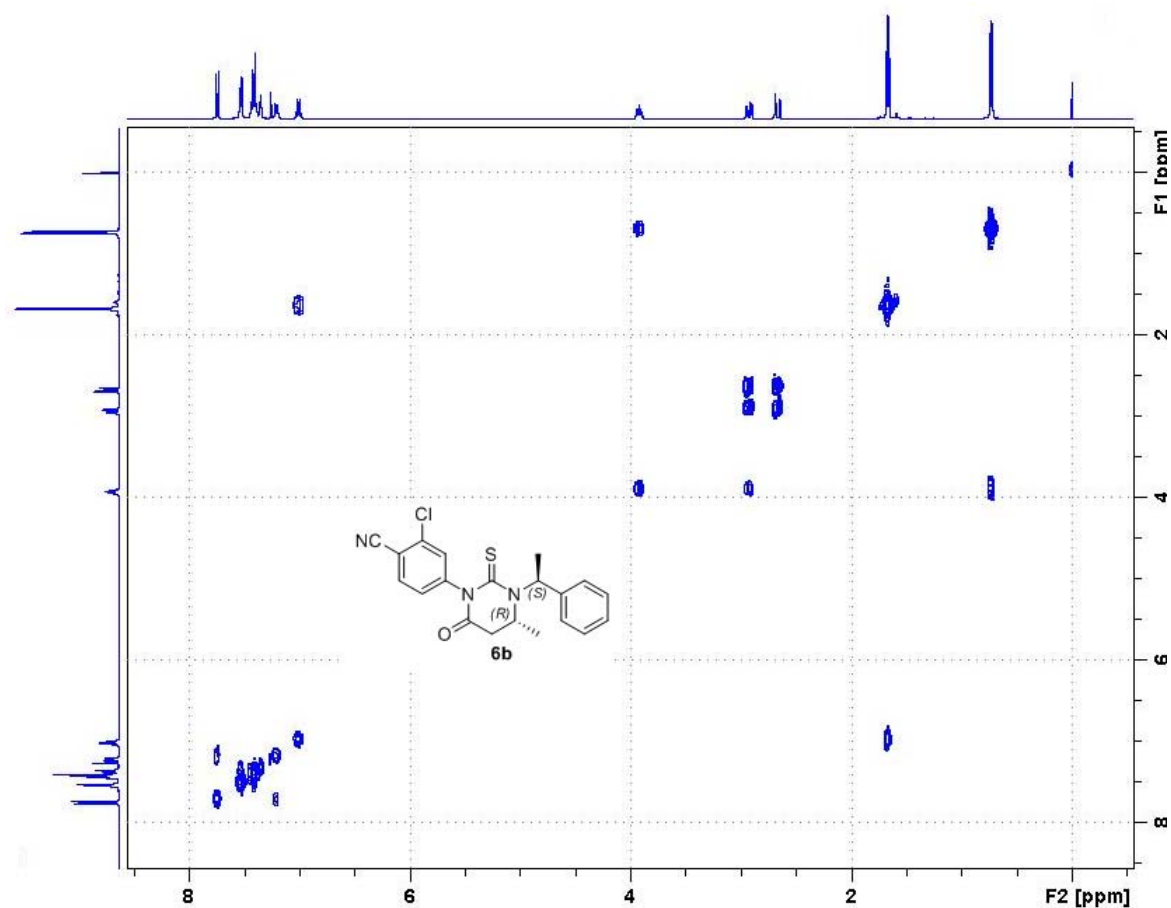


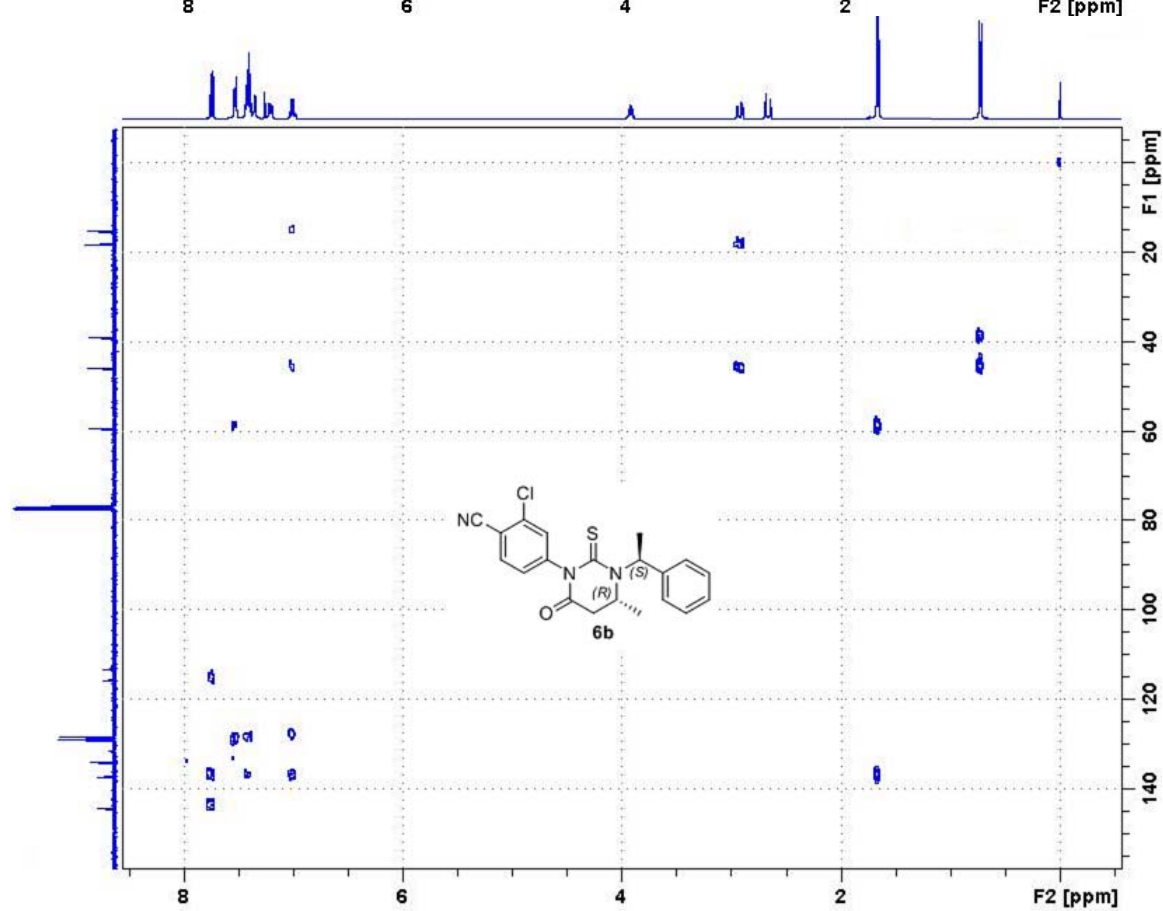
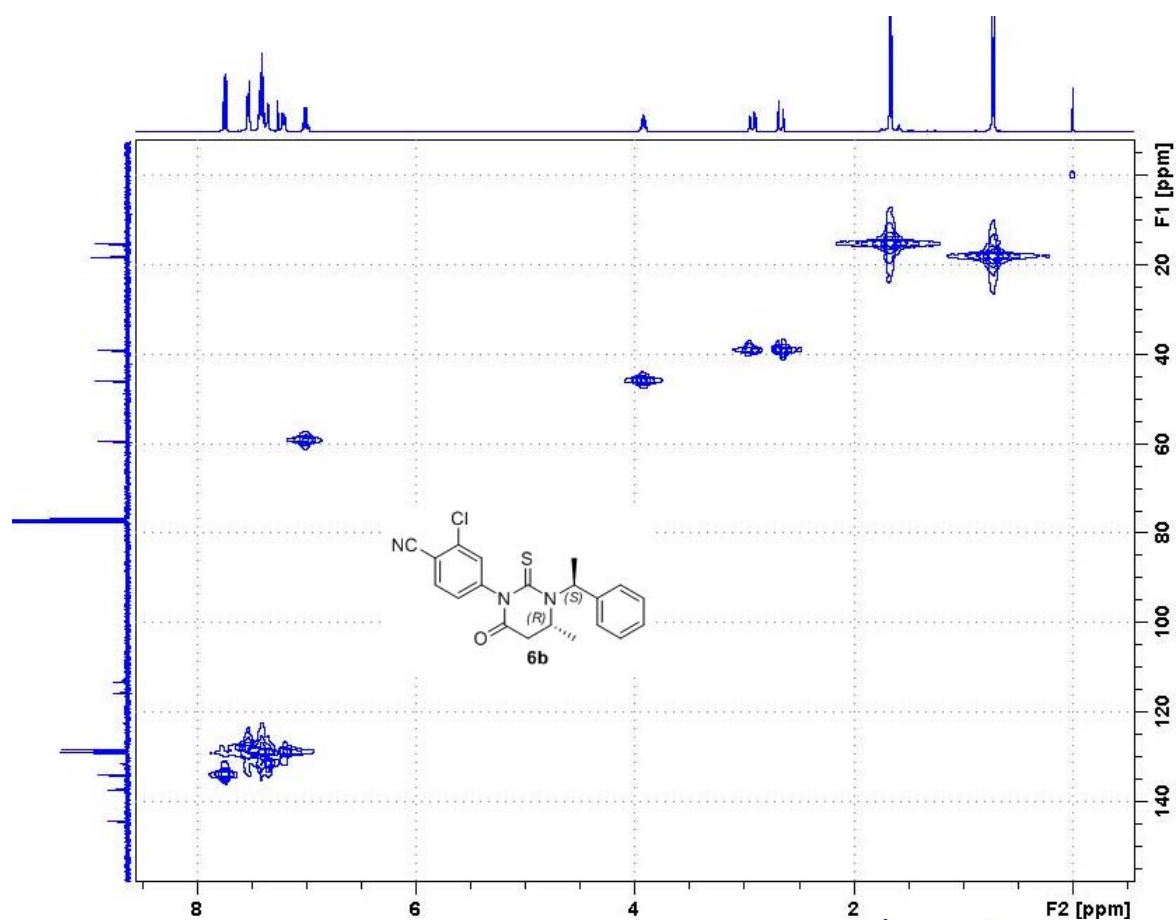


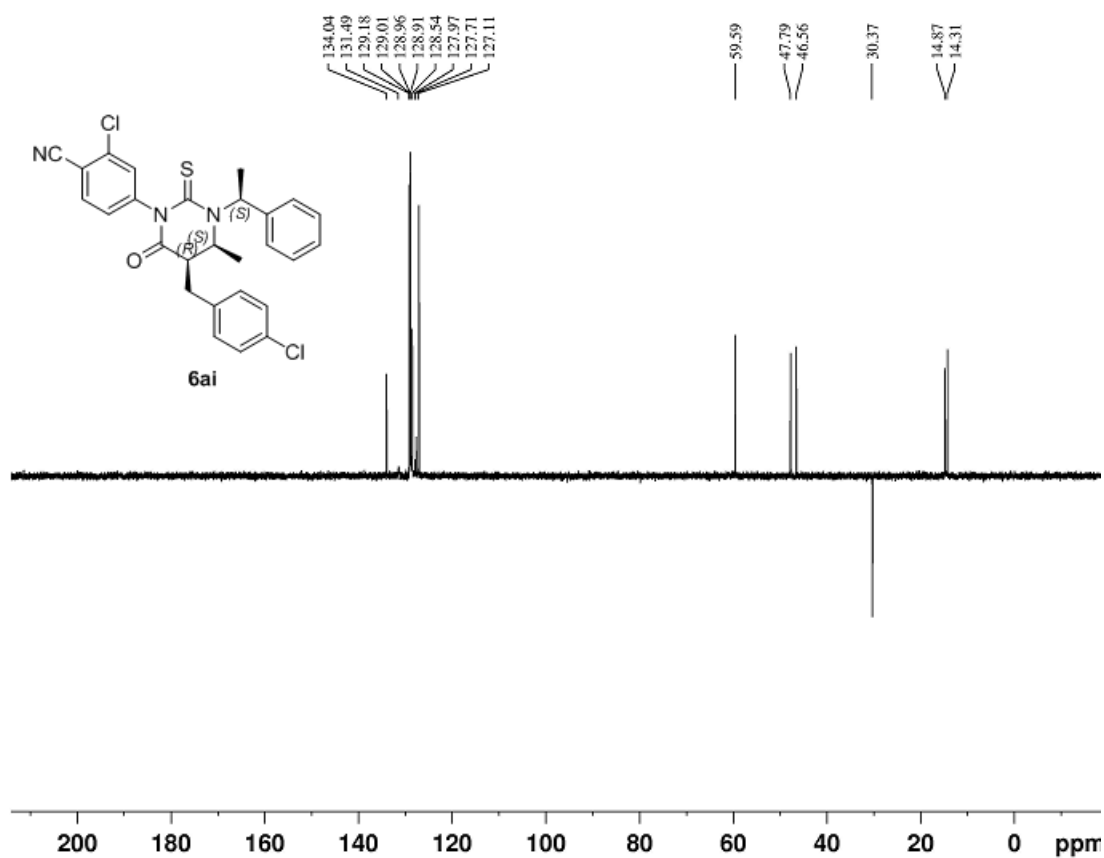
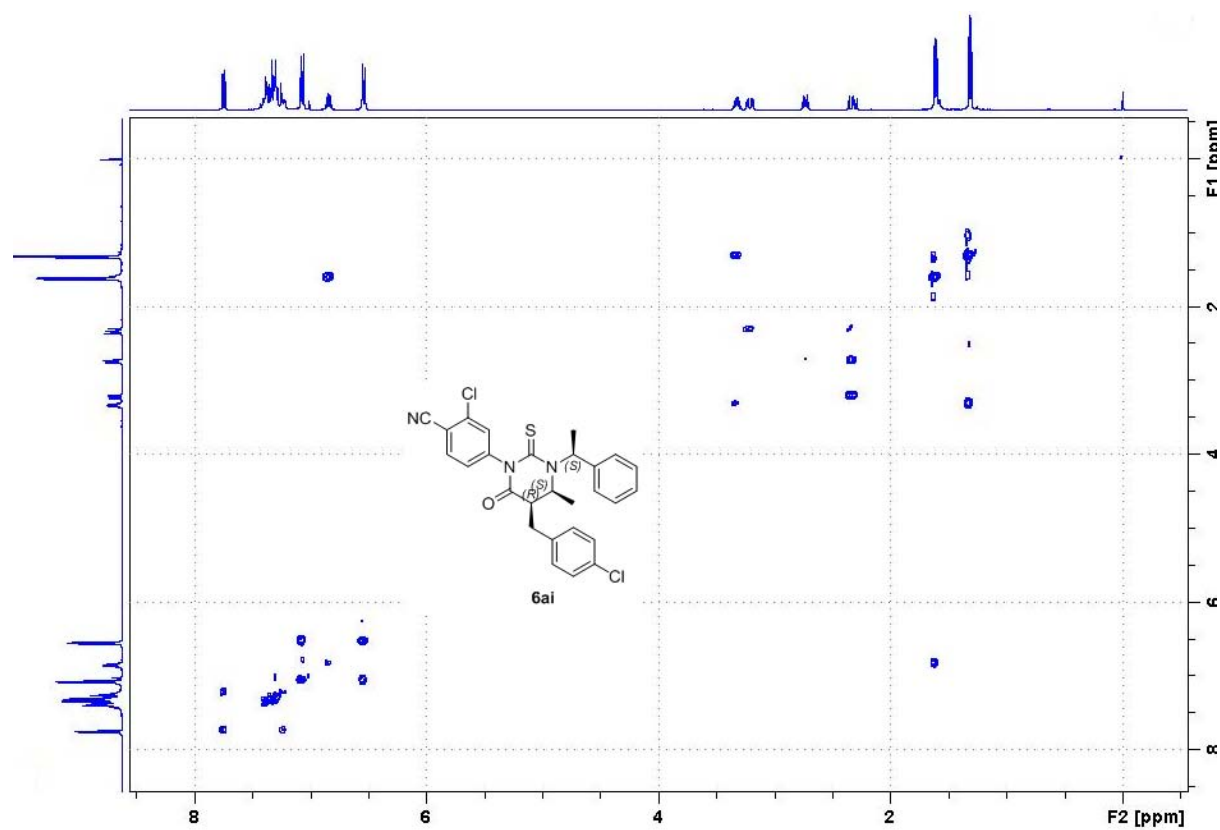


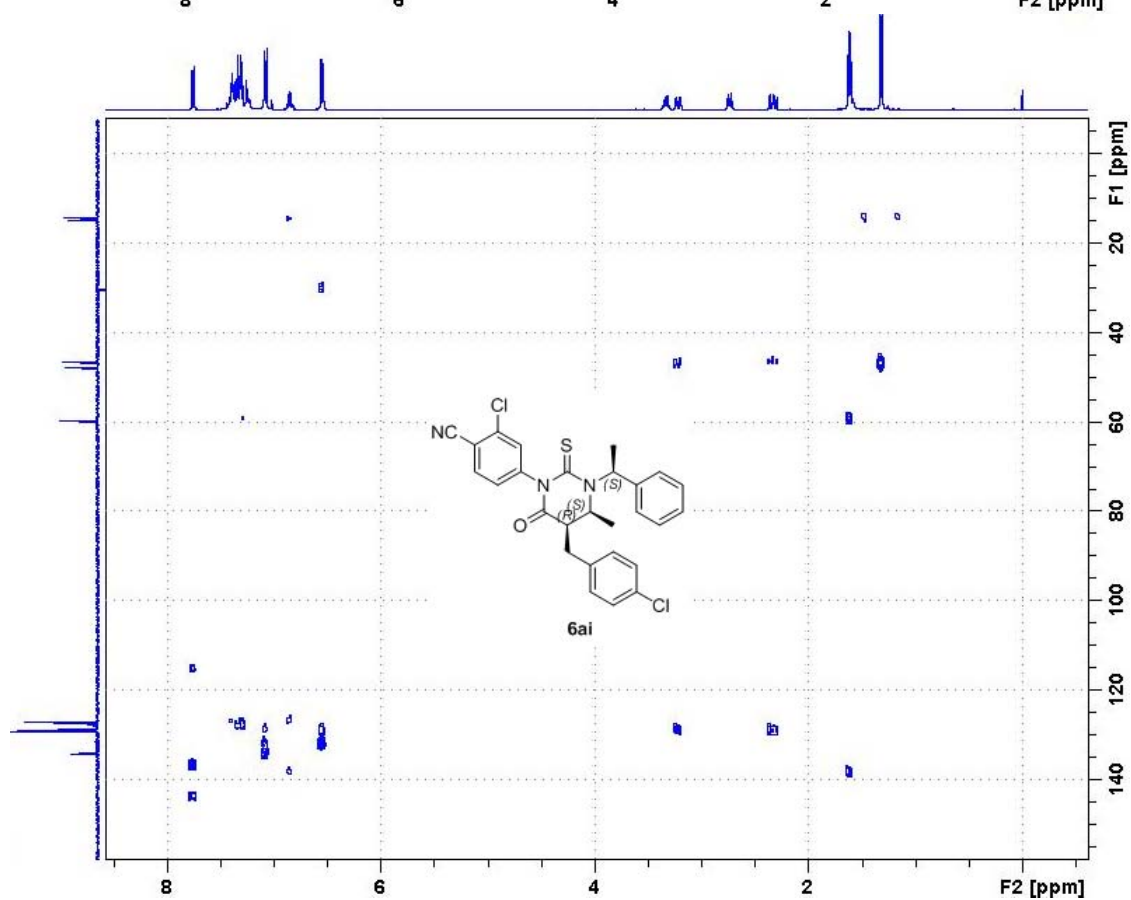
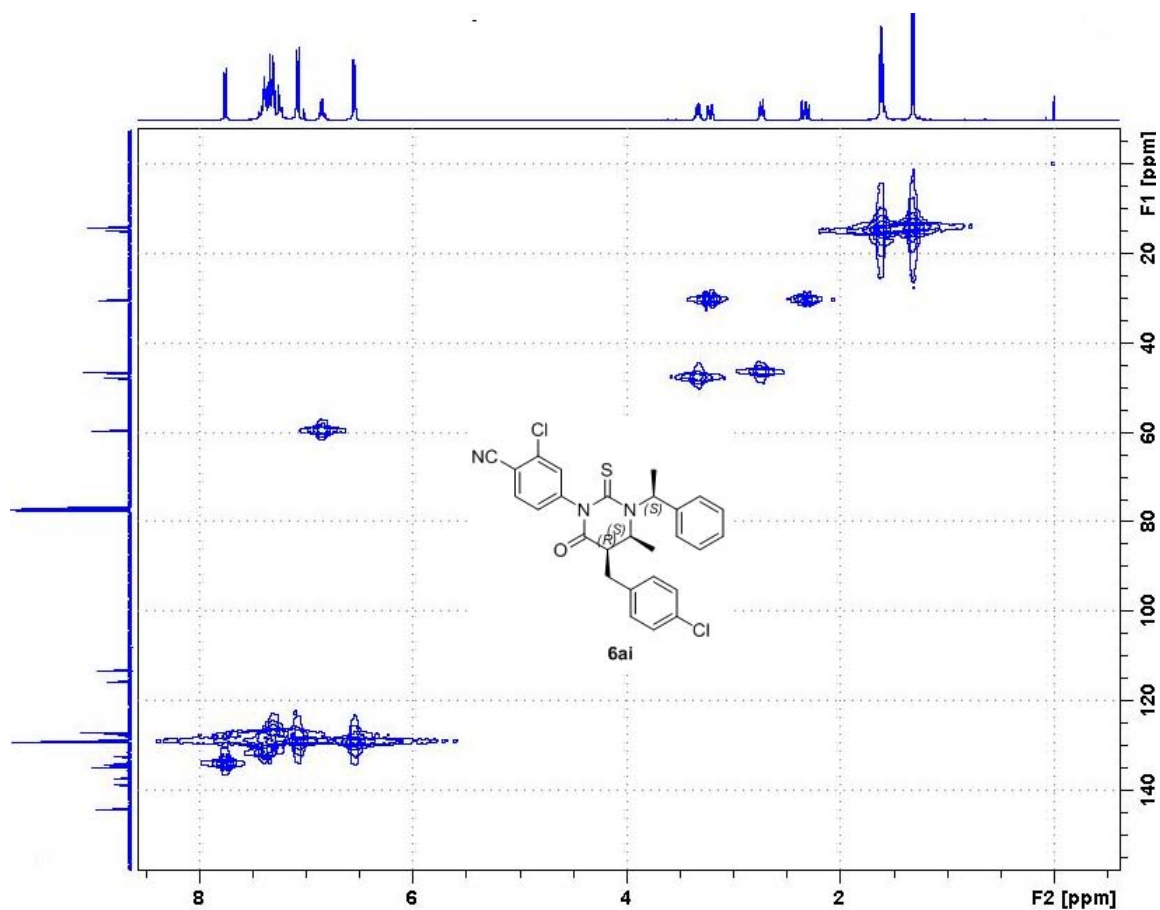


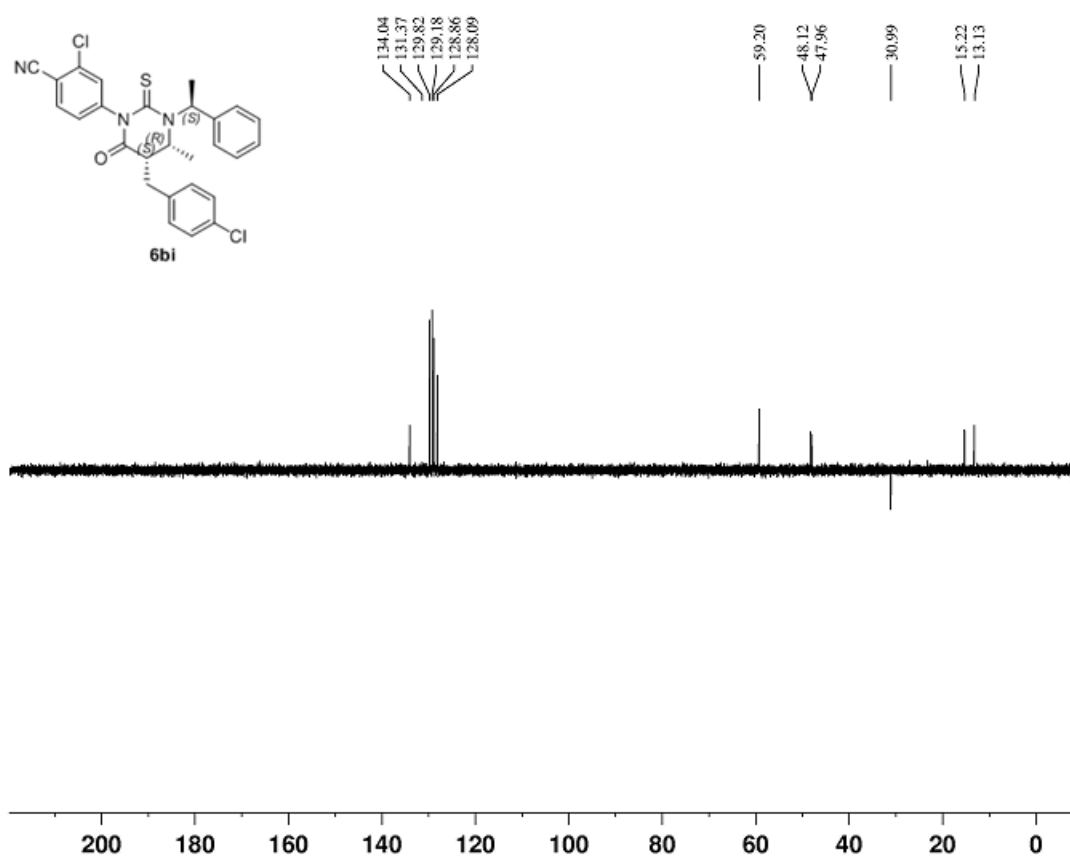
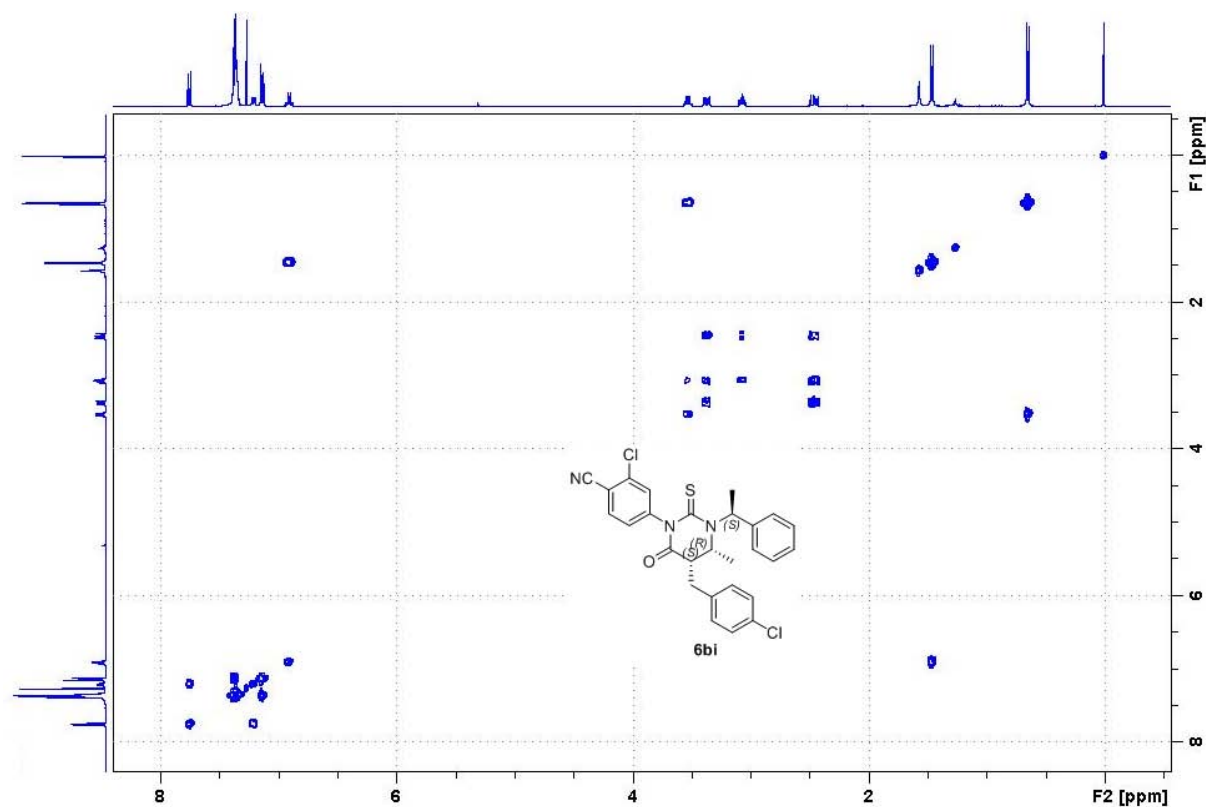


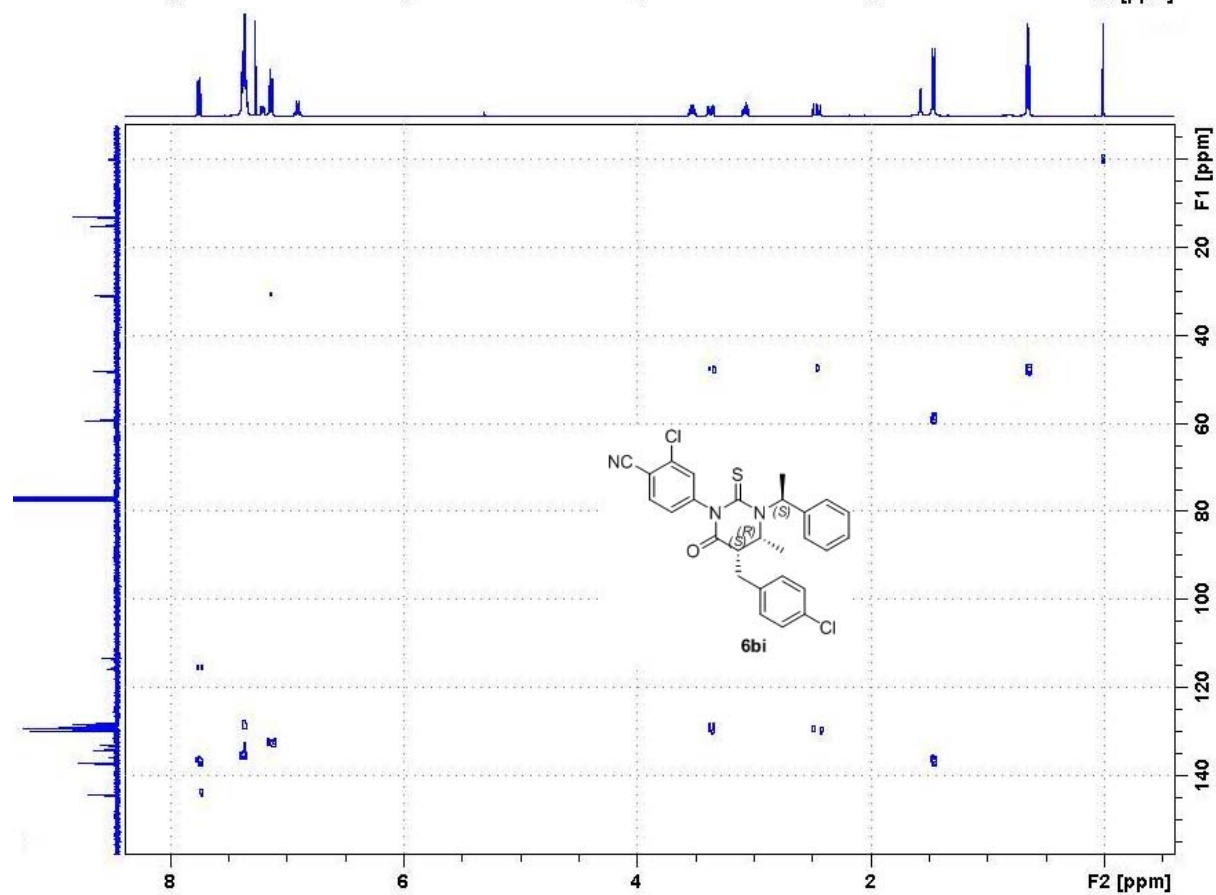
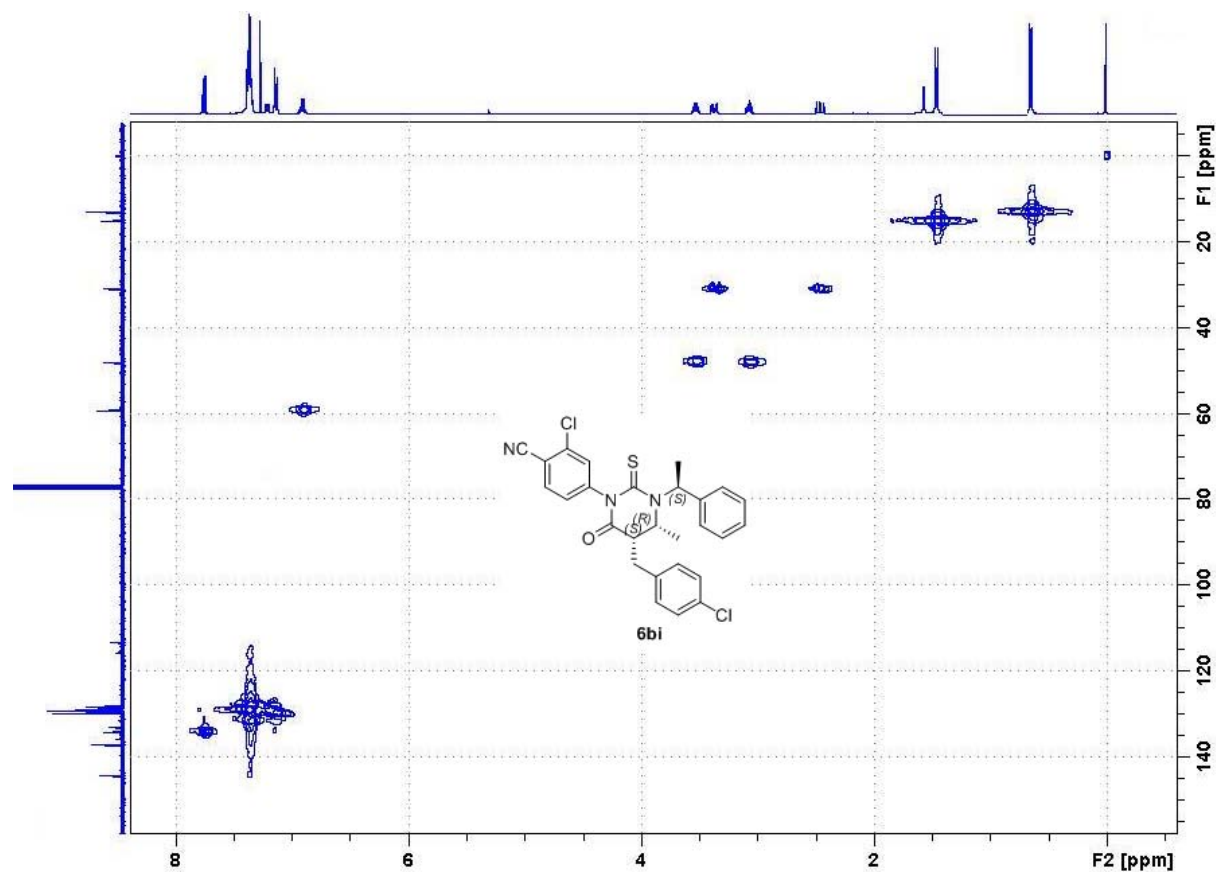


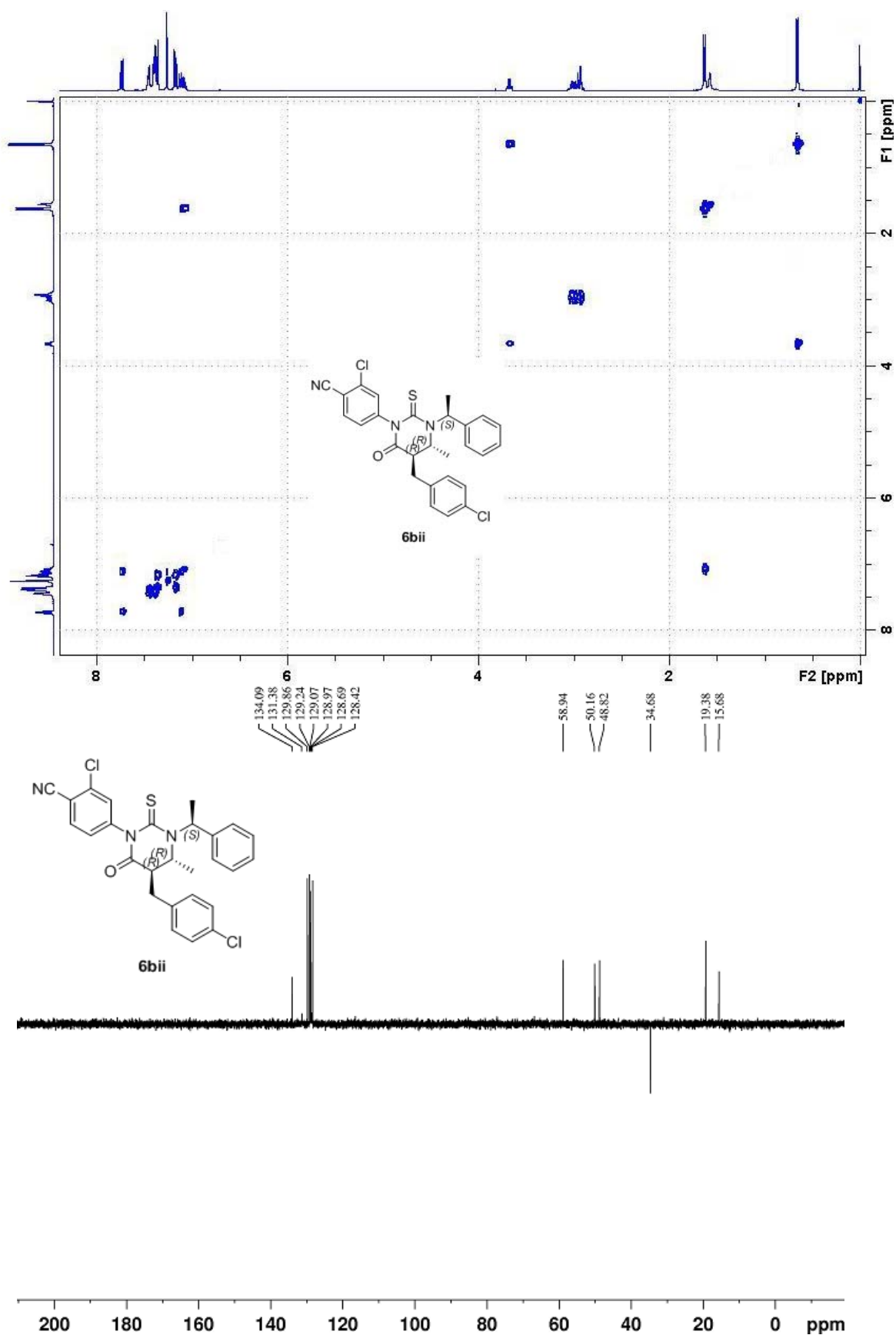


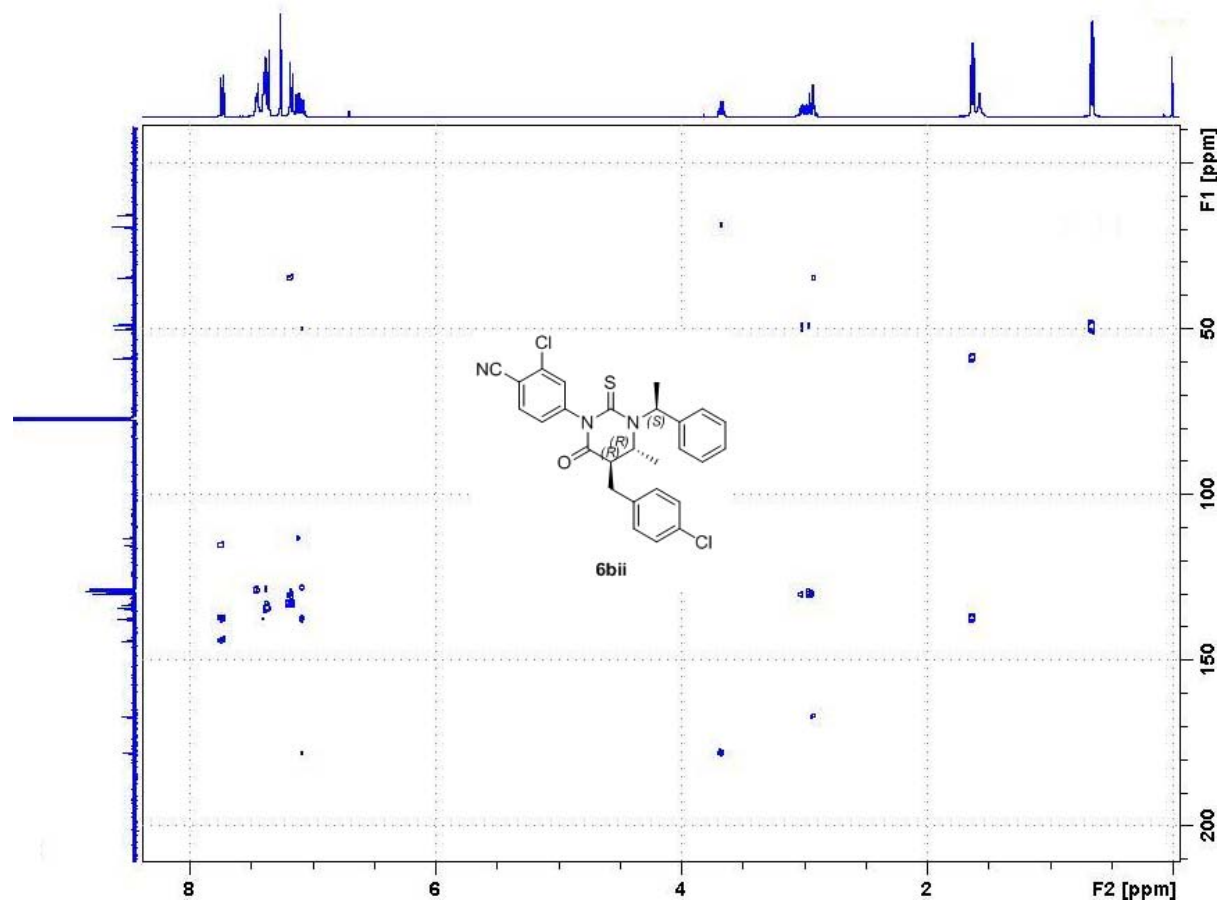
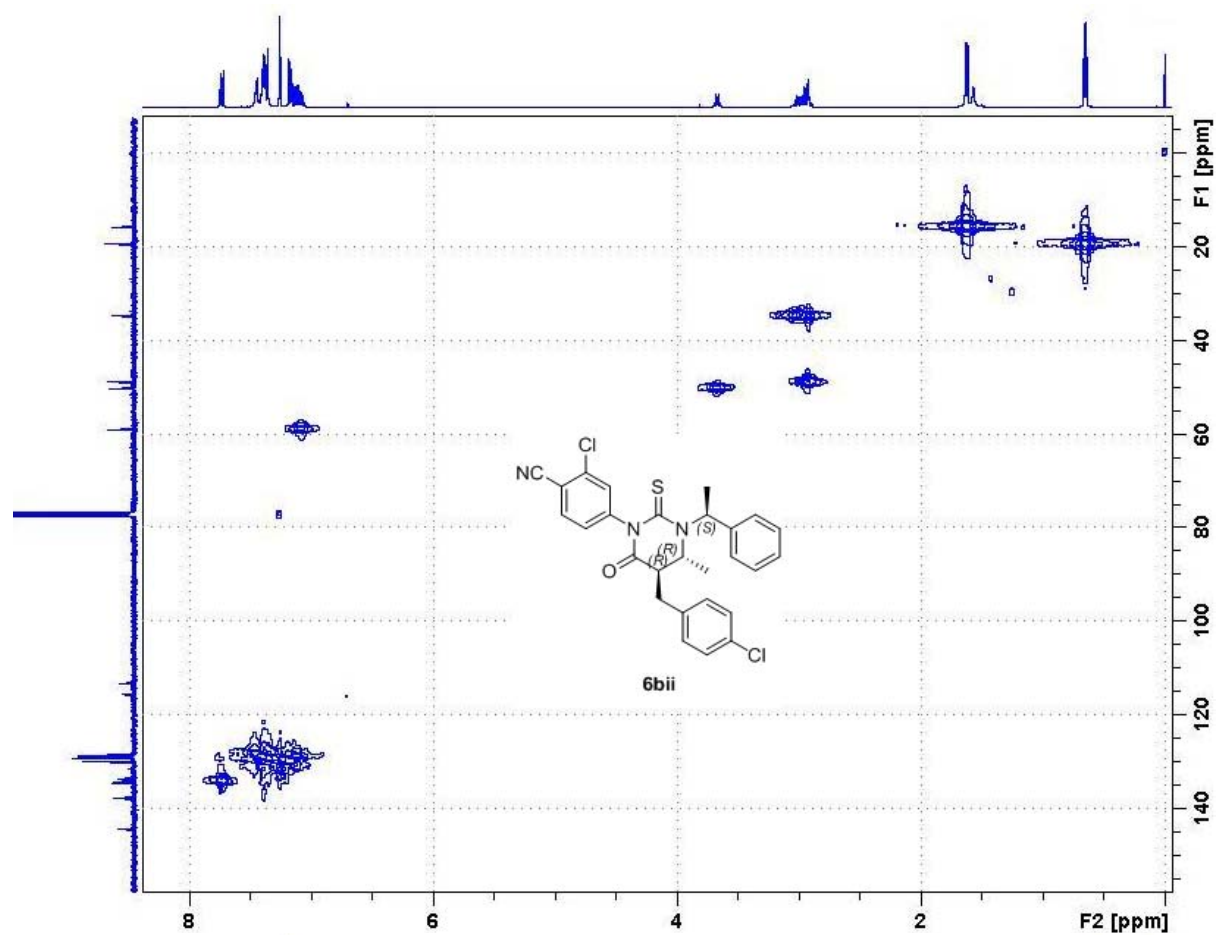


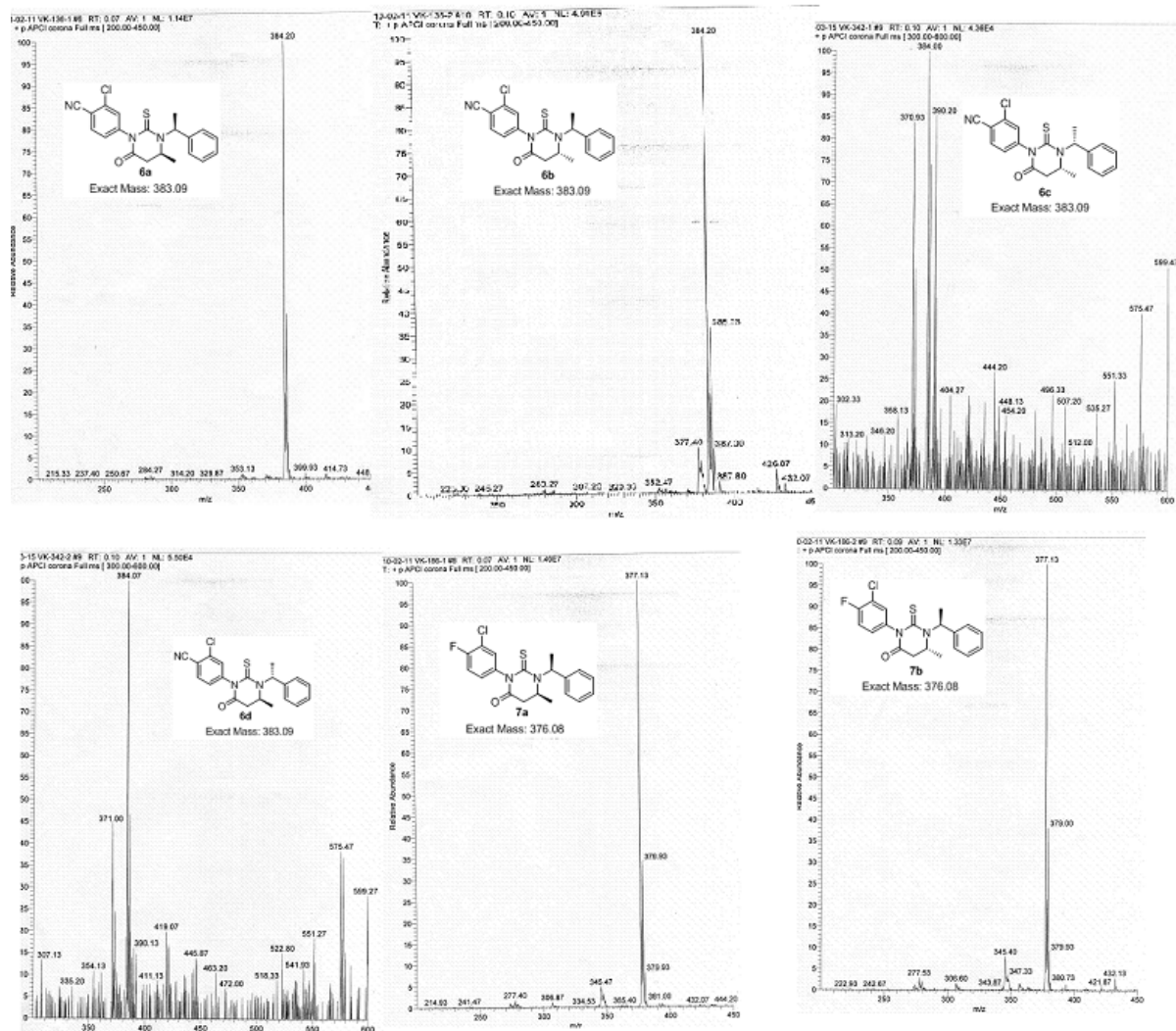


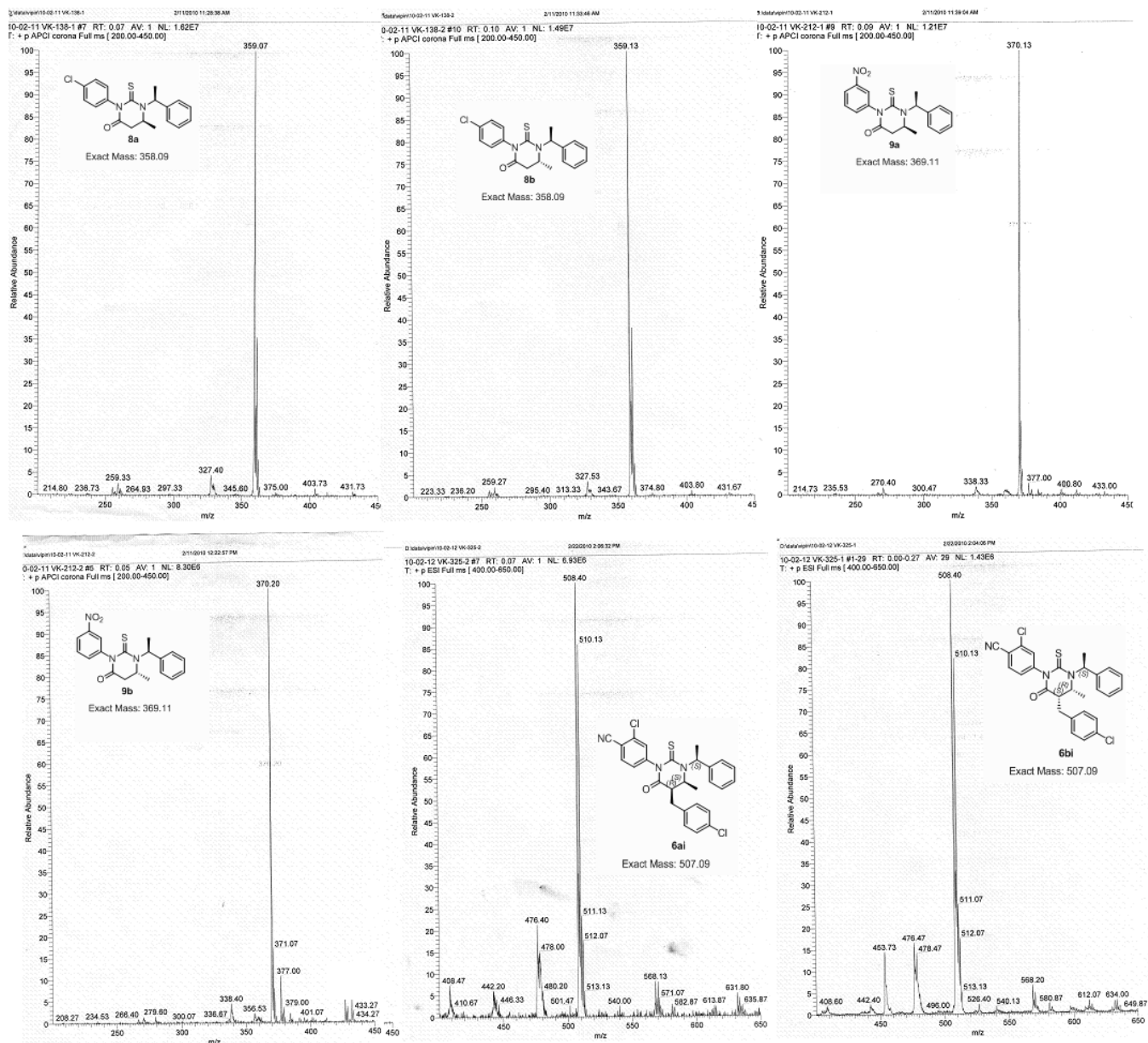


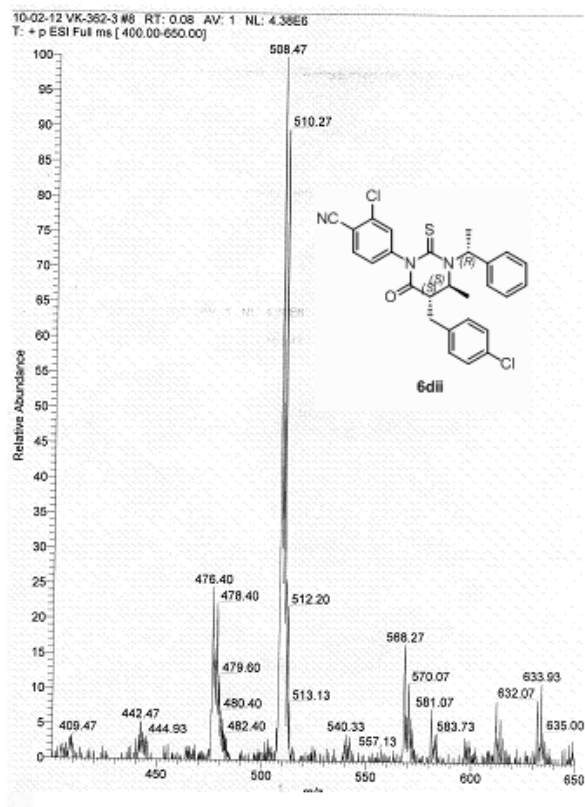
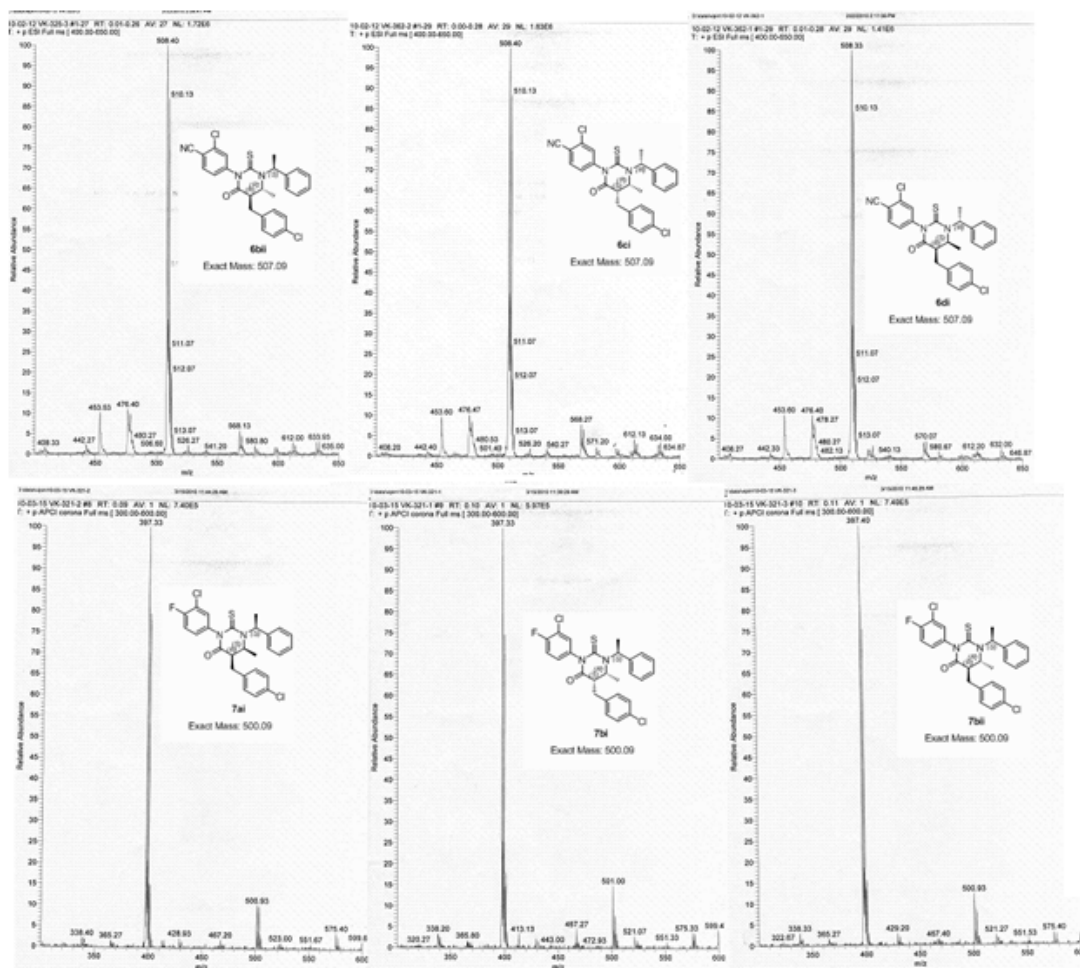


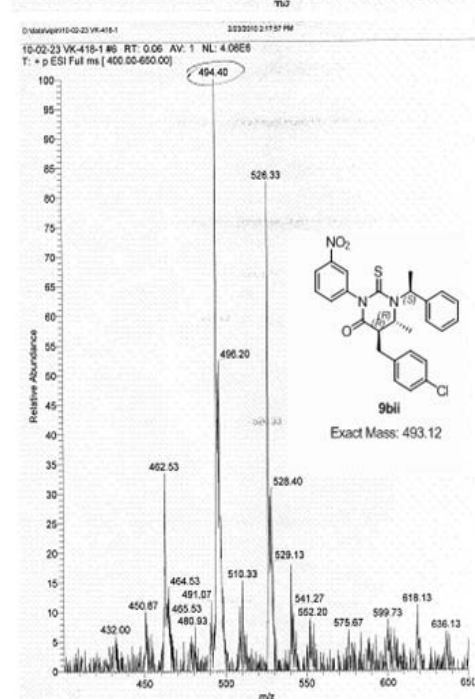
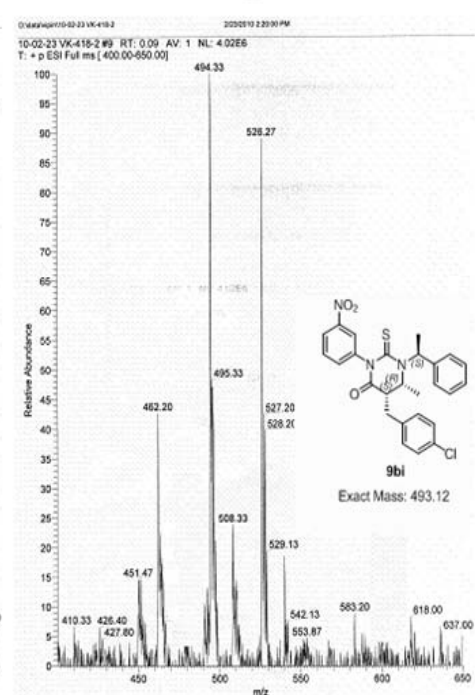
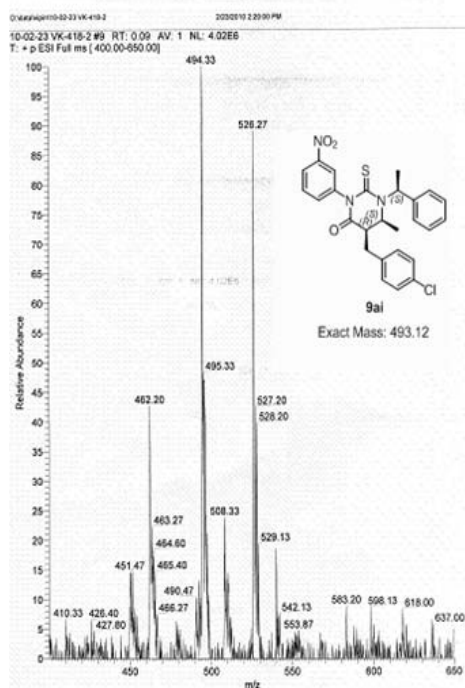
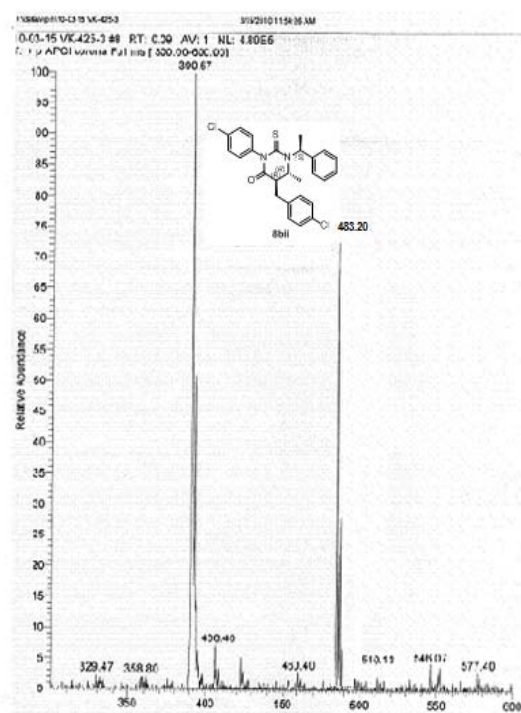
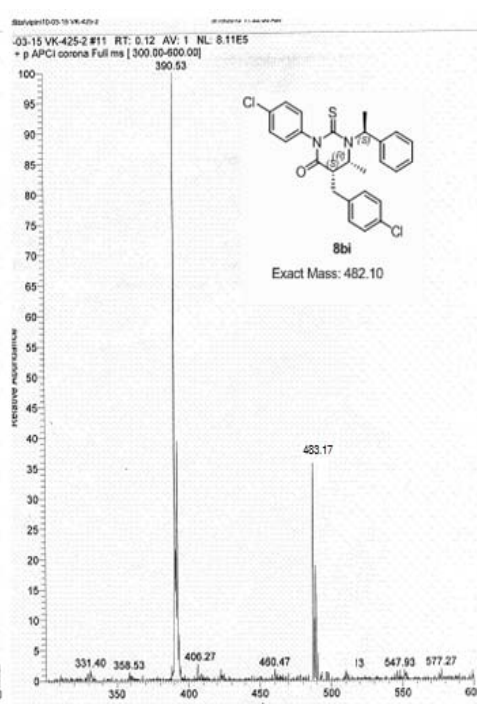
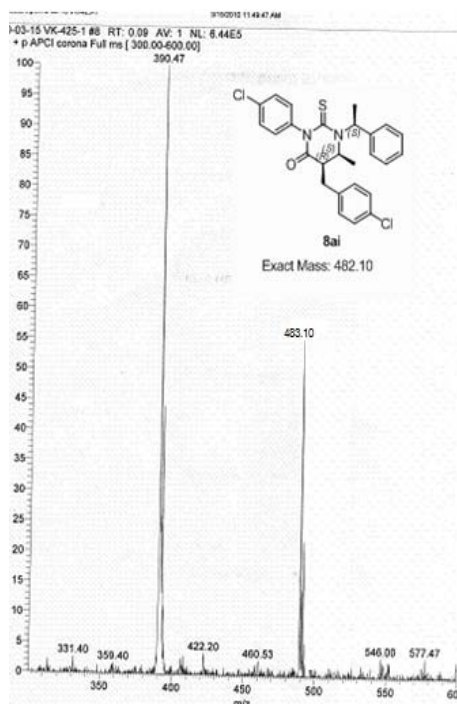


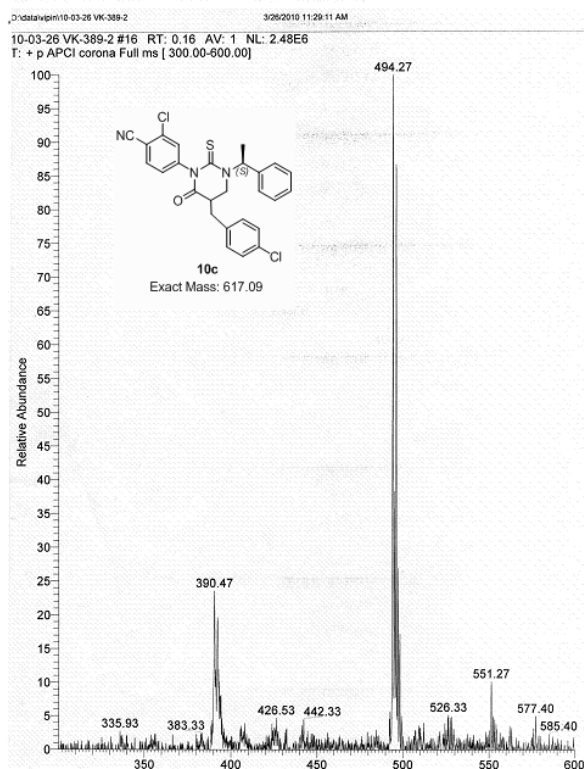
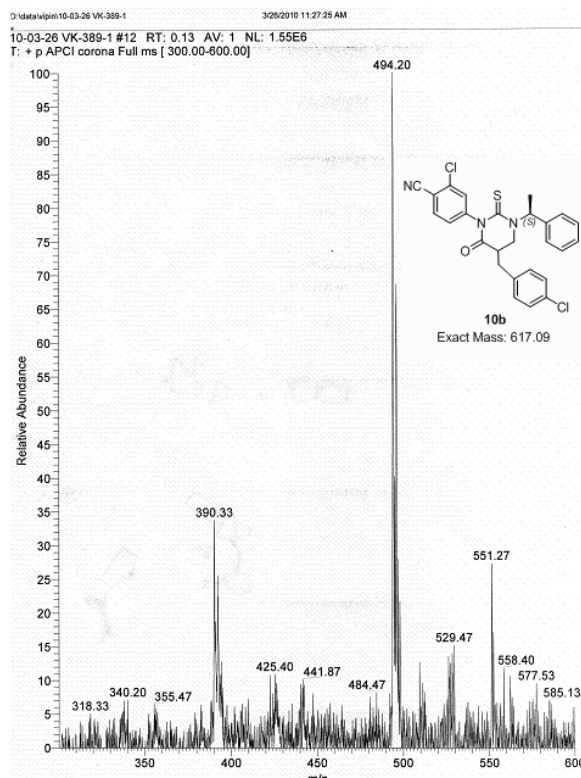
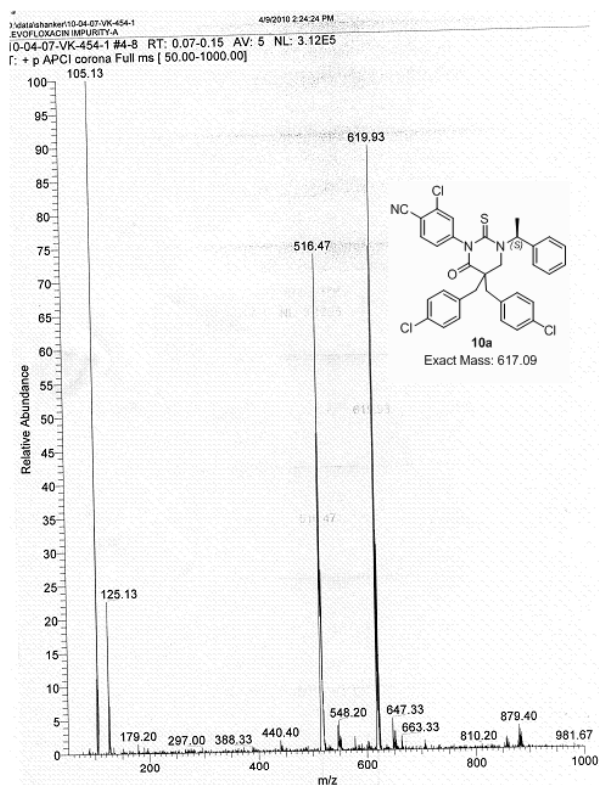
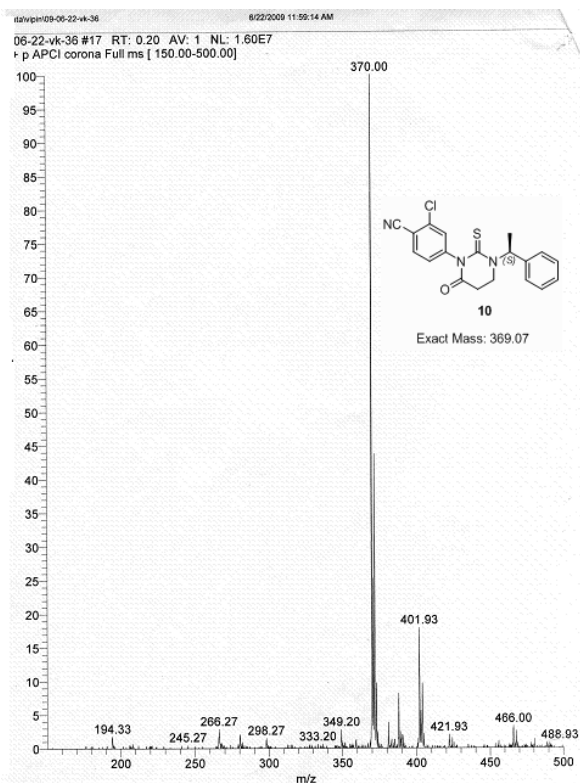




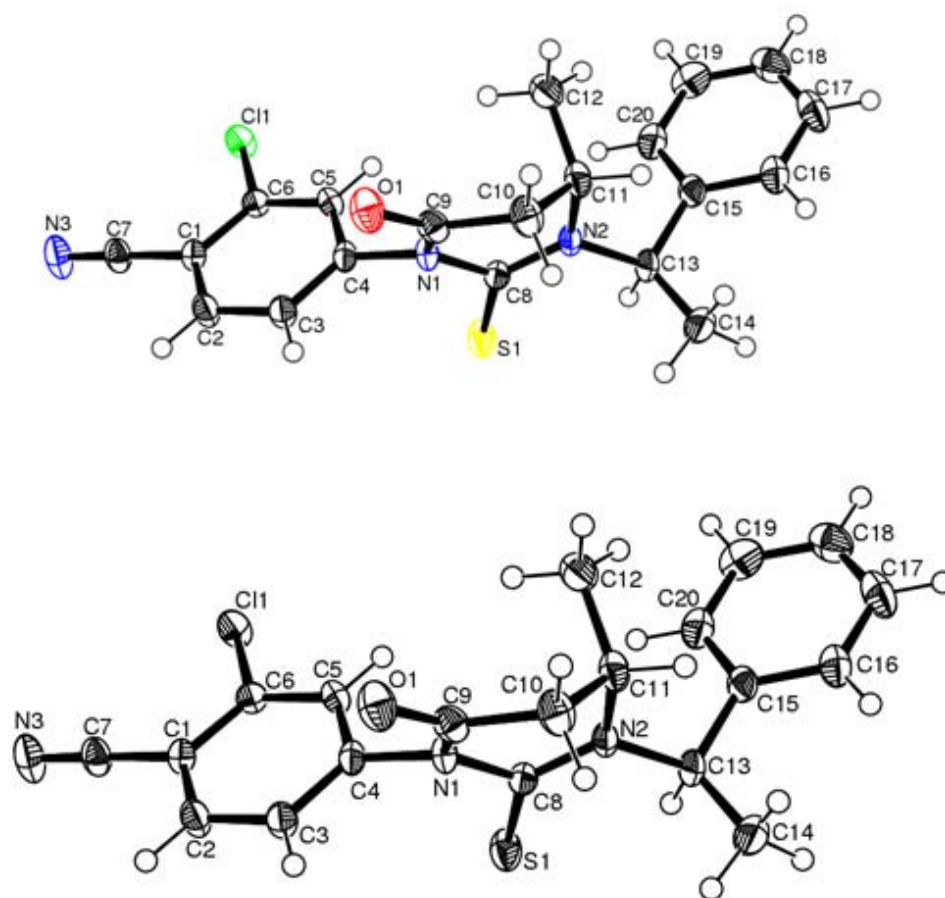




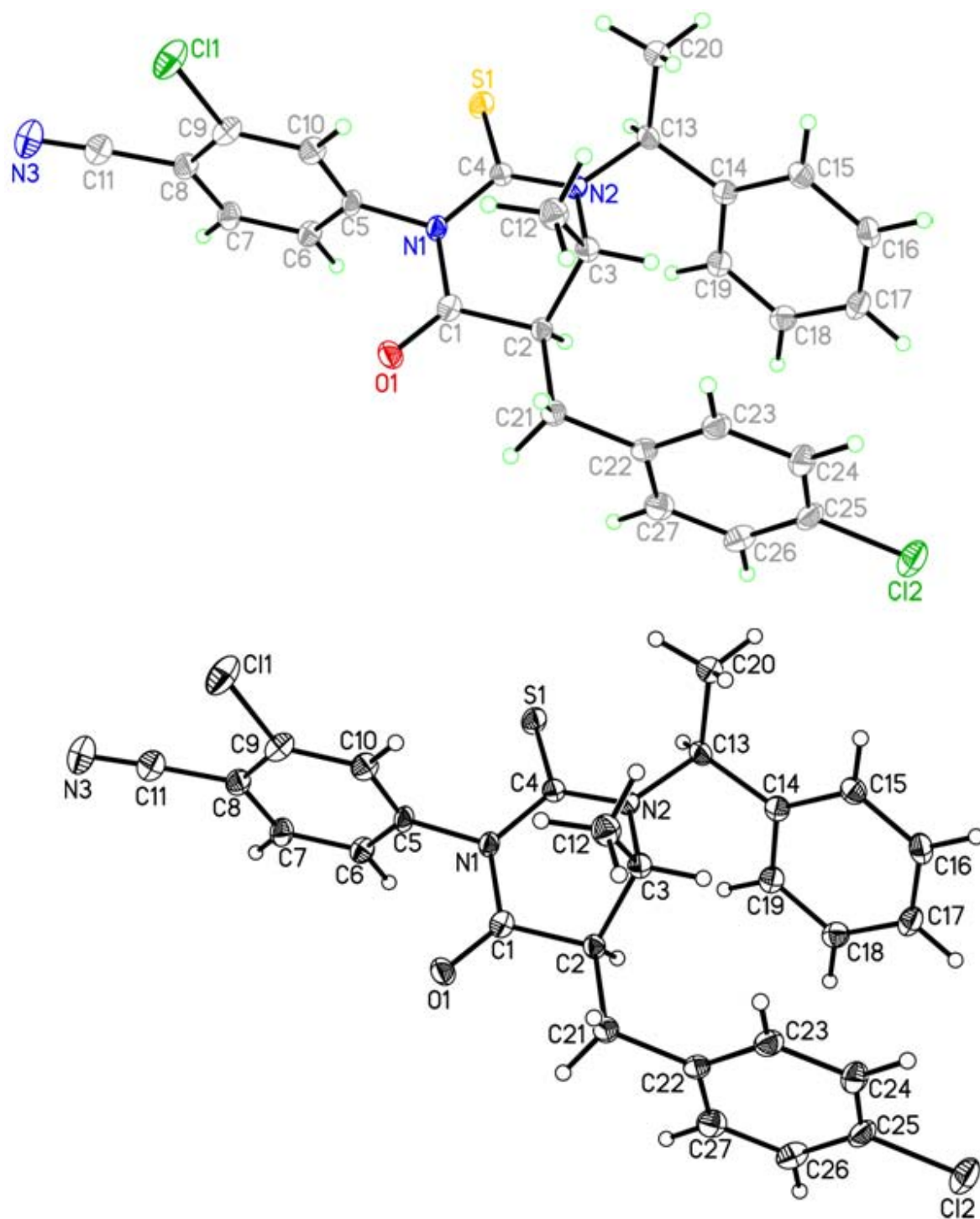




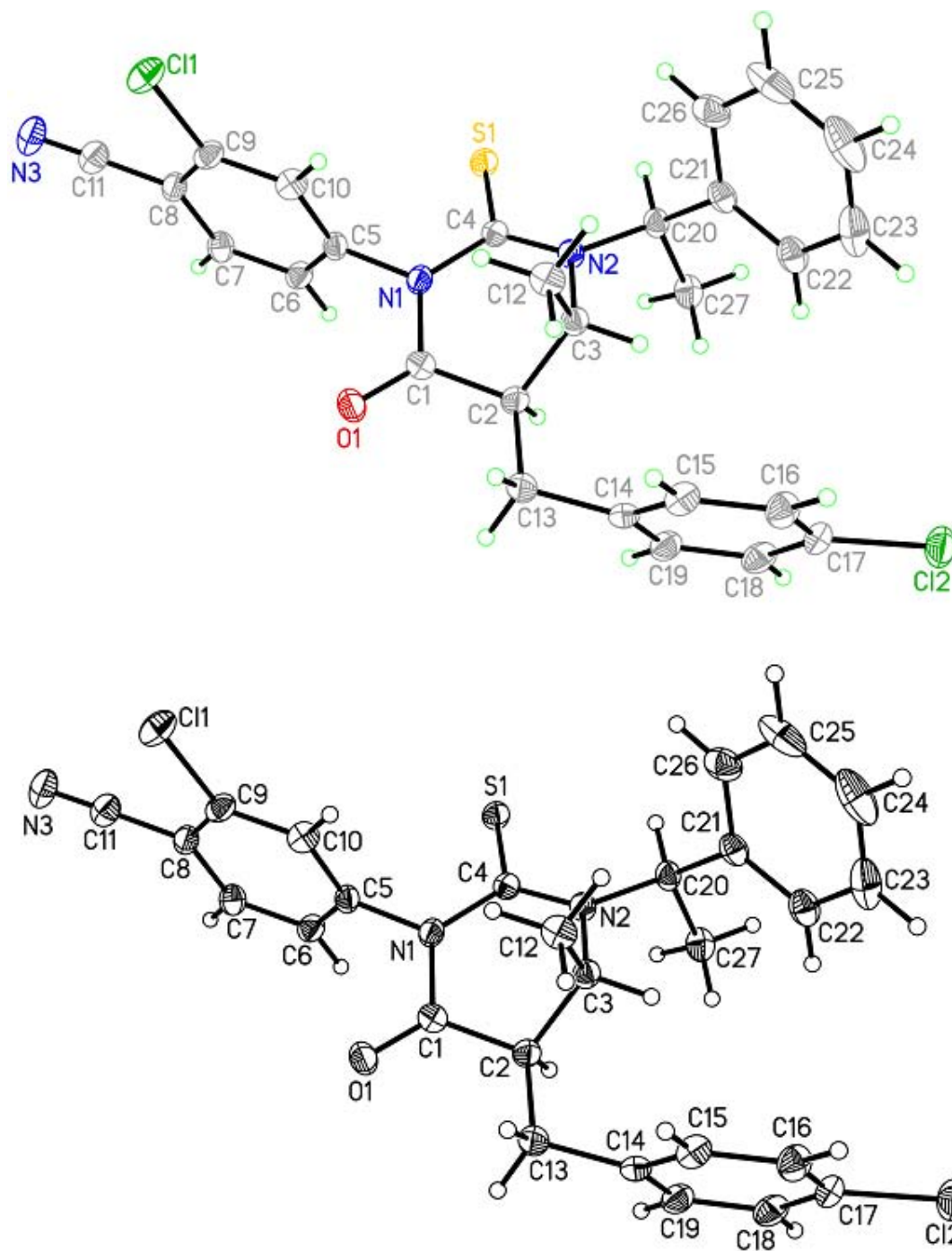
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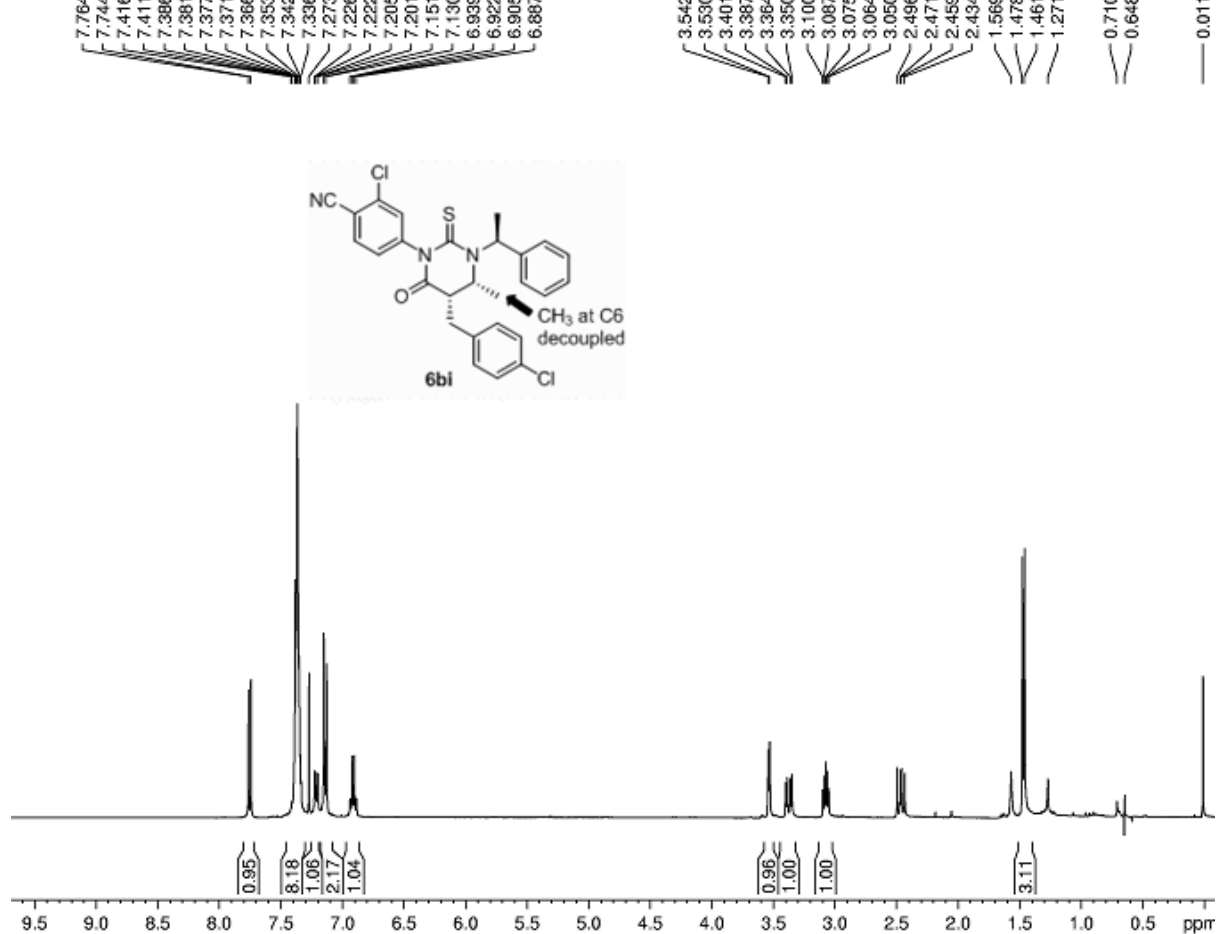
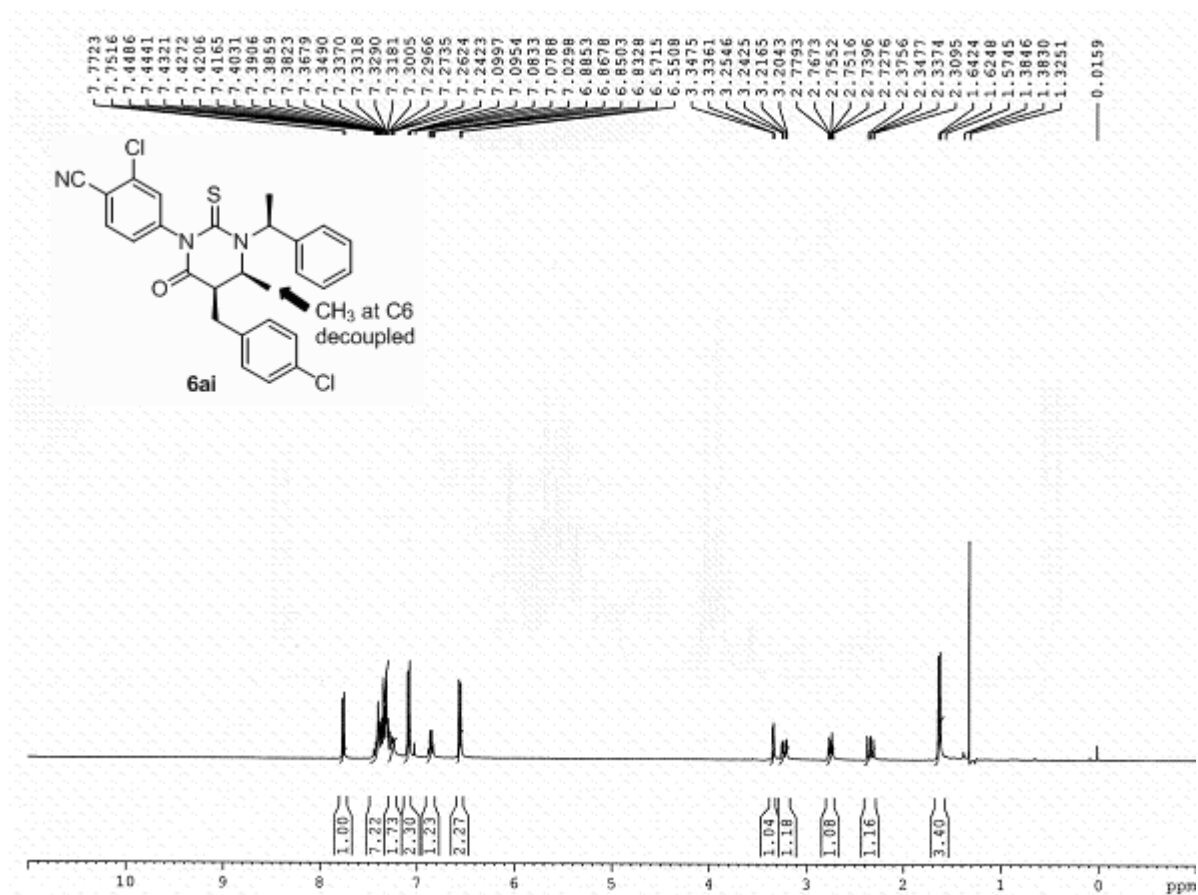
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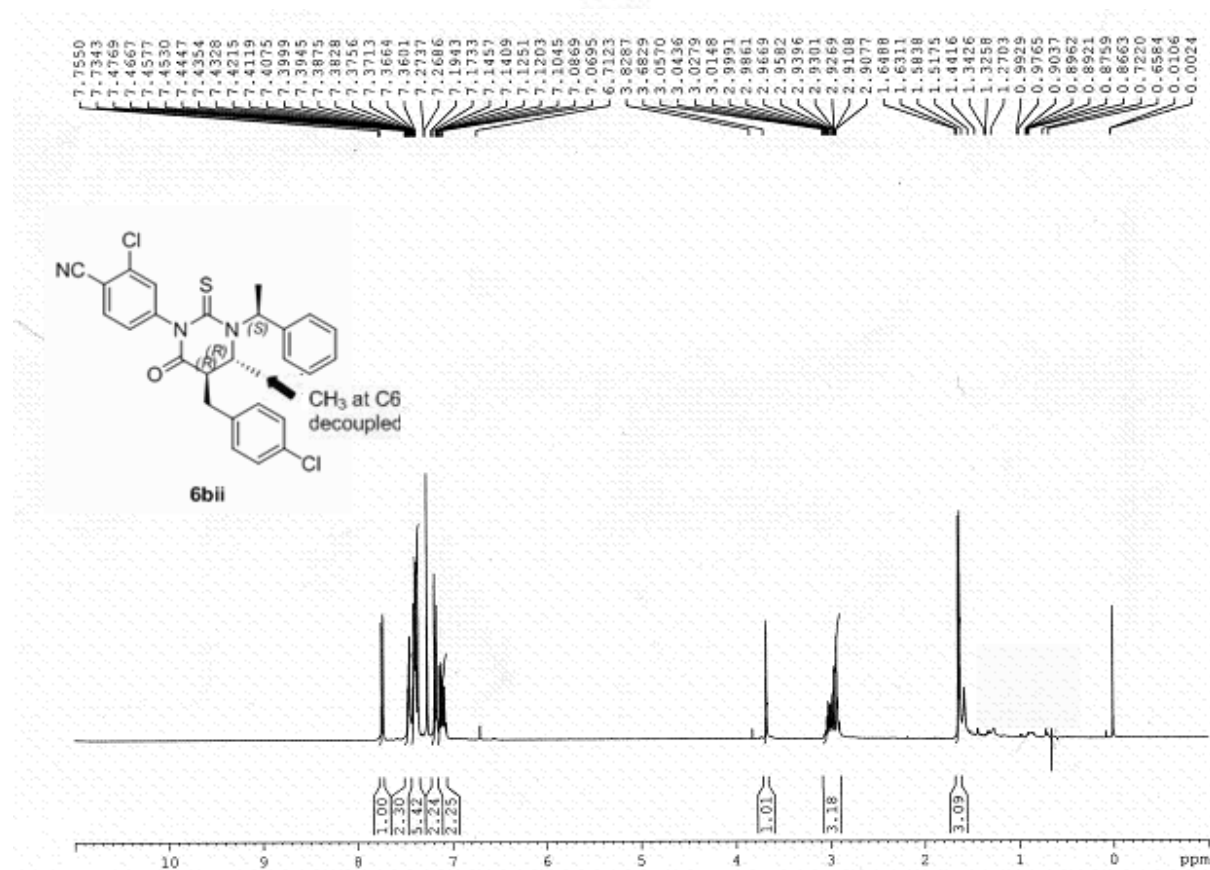


ORTEP diagram of compound **6ai**



ORTEP diagram of compound **6di**





Mass Spectrum List Report

Analysis Info

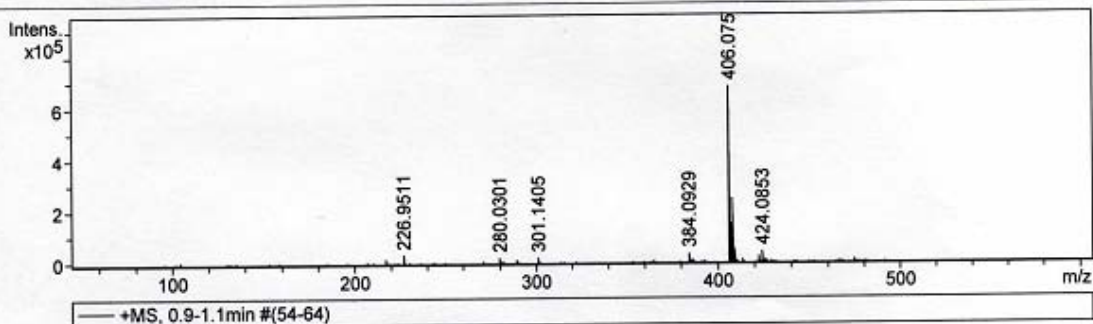
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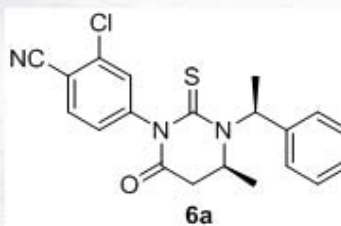
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

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| 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 |



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| 2 | 226.9511 | 23652 | 4330.9 | 32076 | 0.0096 |
| 3 | 270.9769 | 26339 | 728.6 | 8057 | 0.0103 |
| 4 | 280.0301 | 24934 | 1611.5 | 20773 | 0.0112 |
| 5 | 289.1533 | 25799 | 692.1 | 9898 | 0.0112 |
| 6 | 301.1405 | 26219 | 1723.8 | 22378 | 0.0115 |
| 7 | 384.0929 | 25068 | 912.5 | 34735 | 0.0153 |
| 8 | 406.0757 | 22348 | 13085.1 | 679592 | 0.0182 |
| 9 | 407.0785 | 22022 | 2940.1 | 150213 | 0.0185 |
| 10 | 407.5373 | 20028 | 0.2 | 9 | 0.0203 |
| 11 | 408.0731 | 21015 | 4947.9 | 248640 | 0.0194 |
| 12 | 409.0752 | 24048 | 1034.8 | 51124 | 0.0170 |
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Exact Mass: 383.0859
[M+Na]⁺ = 406.0757

Mass Spectrum List Report

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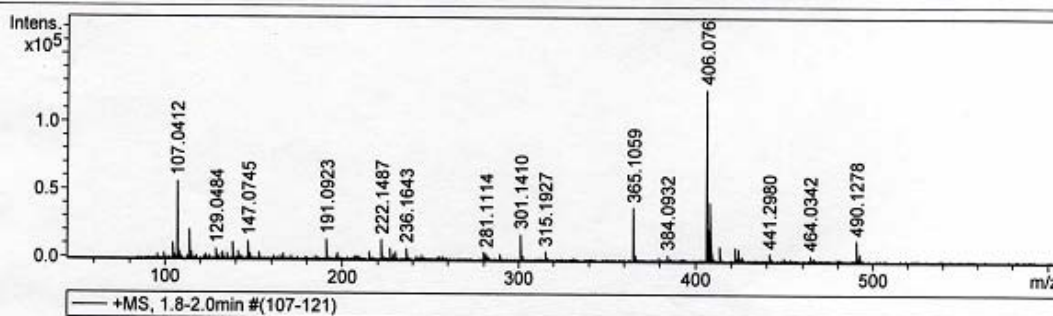
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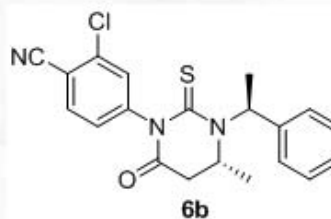
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Instrument / Ser# maXis 40

Acquisition Parameter

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|-------------|------------|-----------------------|-----------|------------------|-----------|
| 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 | 107.0412 | 16913 | 5452.3 | 56321 | 0.0063 |
| 2 | 114.0541 | 24261 | 1769.4 | 20615 | 0.0047 |
| 3 | 129.0484 | 19200 | 459.4 | 6651 | 0.0067 |
| 4 | 138.0644 | 12439 | 243.7 | 3943 | 0.0111 |
| 5 | 147.0745 | 19810 | 827.2 | 12469 | 0.0074 |
| 6 | 191.0923 | 21145 | 1053.5 | 14184 | 0.0090 |
| 7 | 222.1487 | 23998 | 871.4 | 14222 | 0.0093 |
| 8 | 227.0564 | 22703 | 470.0 | 7583 | 0.0100 |
| 9 | 236.1643 | 23738 | 518.8 | 8187 | 0.0099 |
| 10 | 281.1114 | 25303 | 299.1 | 4984 | 0.0111 |
| 11 | 289.1536 | 24827 | 221.9 | 3756 | 0.0116 |
| 12 | 301.1410 | 24587 | 1113.0 | 18375 | 0.0122 |
| 13 | 315.1927 | 24431 | 382.0 | 6121 | 0.0129 |
| 14 | 365.1059 | 24120 | 2216.9 | 38375 | 0.0151 |
| 15 | 384.0932 | 26103 | 189.4 | 4064 | 0.0147 |
| 16 | 406.0762 | 22830 | 5242.7 | 125386 | 0.0178 |
| 17 | 413.2665 | 26302 | 444.3 | 10118 | 0.0157 |
| 18 | 422.0496 | 26199 | 427.8 | 9142 | 0.0161 |
| 19 | 441.2980 | 27014 | 258.3 | 5085 | 0.0163 |
| 20 | 464.0342 | 26870 | 167.9 | 3981 | 0.0173 |
| 21 | 490.1278 | 24819 | 733.1 | 14933 | 0.0197 |



Exact Mass: 383.0859

$[M+Na]^+ = 406.0757$

Mass Spectrum List Report

Analysis Info

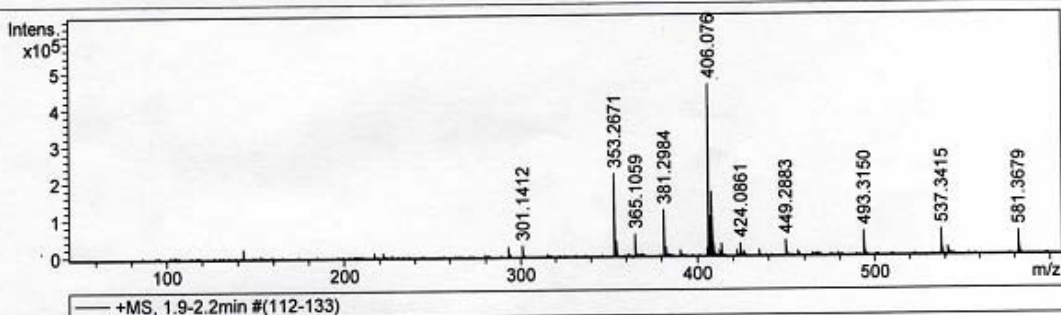
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Method tune_low.m
Sample Name VK-6C
Comment

Acquisition Date 5/18/2010 9:12:31 AM

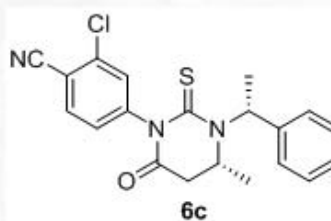
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 301.1412 | 25222 | 1721.1 | 28534 | 0.0119 |
| 2 | 353.2671 | 21332 | 8035.1 | 219458 | 0.0166 |
| 3 | 365.1059 | 23981 | 1662.4 | 57945 | 0.0152 |
| 4 | 381.2984 | 22623 | 2268.6 | 122849 | 0.0169 |
| 5 | 406.0766 | 22036 | 6780.4 | 460465 | 0.0184 |
| 6 | 407.0791 | 23017 | 1565.9 | 104244 | 0.0177 |
| 7 | 408.0738 | 21600 | 2592.2 | 169127 | 0.0189 |
| 8 | 424.0861 | 25886 | 746.2 | 32726 | 0.0164 |
| 9 | 434.2567 | 27256 | 436.5 | 13216 | 0.0159 |
| 10 | 449.2883 | 24885 | 1637.2 | 41502 | 0.0181 |
| 11 | 493.3150 | 24964 | 3193.3 | 63447 | 0.0198 |
| 12 | 537.3415 | 24270 | 3458.3 | 66391 | 0.0221 |
| 13 | 581.3679 | 25384 | 3856.7 | 60525 | 0.0229 |



Exact Mass: 383.0859
[M+Na]⁺ = 406.0757

Mass Spectrum List Report

Analysis Info

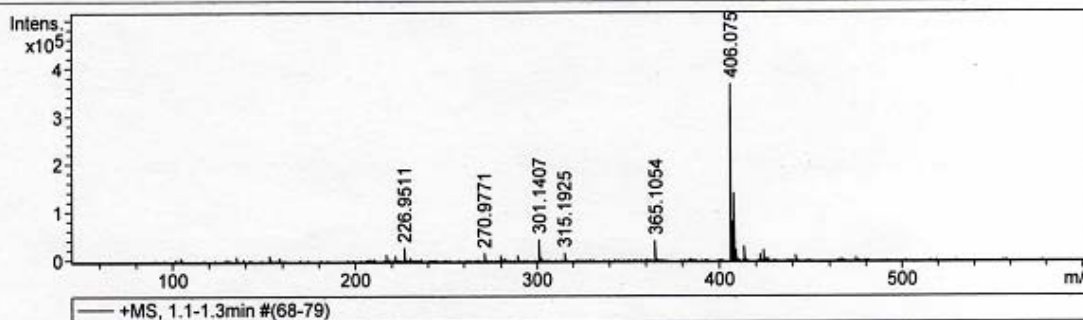
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Method tune_low.m
Sample Name VK-6D
Comment

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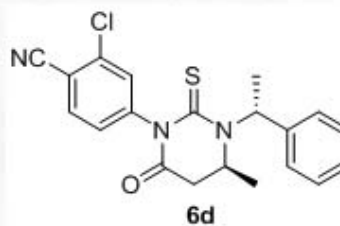
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

| | | | | | |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 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 | 216.9221 | 23575 | 1058.4 | 14406 | 0.0092 |
| 2 | 222.1482 | 24114 | 764.1 | 10312 | 0.0092 |
| 3 | 226.9511 | 23111 | 2019.7 | 27040 | 0.0098 |
| 4 | 270.9771 | 24866 | 779.0 | 14509 | 0.0109 |
| 5 | 280.0300 | 24253 | 542.2 | 11474 | 0.0115 |
| 6 | 289.1533 | 25200 | 426.9 | 9886 | 0.0115 |
| 7 | 301.1407 | 23263 | 2058.3 | 44379 | 0.0129 |
| 8 | 315.1925 | 25593 | 797.0 | 15695 | 0.0123 |
| 9 | 365.1054 | 25035 | 1634.3 | 40958 | 0.0146 |
| 10 | 406.0759 | 21406 | 8650.4 | 364845 | 0.0190 |
| 11 | 407.0786 | 23370 | 1967.2 | 81763 | 0.0174 |
| 12 | 408.0733 | 21749 | 3404.0 | 139404 | 0.0188 |
| 13 | 409.0752 | 24177 | 584.8 | 23589 | 0.0169 |
| 14 | 413.2662 | 25509 | 775.2 | 29280 | 0.0162 |
| 15 | 424.0854 | 26135 | 756.0 | 23553 | 0.0162 |



Exact Mass: 383.0859
[M+Na]⁺ = 406.0757

Mass Spectrum List Report

Analysis Info

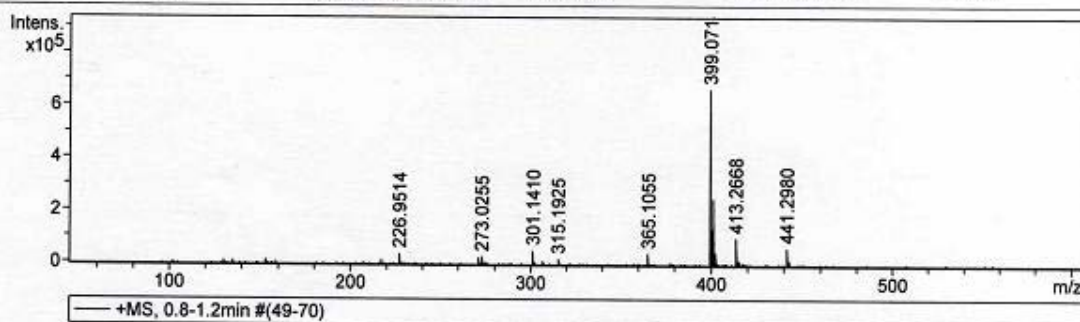
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Sample Name VK-7A
Comment

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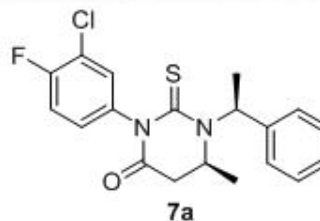
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

| | | | | | |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 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 | 216.9224 | 24162 | 997.9 | 14650 | 0.0090 |
| 2 | 226.9514 | 21619 | 2589.2 | 38926 | 0.0105 |
| 3 | 273.0255 | 23866 | 944.4 | 26389 | 0.0114 |
| 4 | 301.1410 | 23823 | 1527.6 | 50307 | 0.0126 |
| 5 | 306.2786 | 25800 | 322.1 | 10247 | 0.0119 |
| 6 | 315.1925 | 25230 | 602.3 | 17992 | 0.0125 |
| 7 | 365.1055 | 24714 | 1189.5 | 40844 | 0.0148 |
| 8 | 399.0714 | 22088 | 8970.9 | 663240 | 0.0181 |
| 9 | 400.0741 | 21798 | 1828.3 | 136265 | 0.0184 |
| 10 | 401.0687 | 21351 | 3405.0 | 249804 | 0.0188 |
| 11 | 402.0708 | 24055 | 646.5 | 46671 | 0.0167 |
| 12 | 413.2668 | 23115 | 1680.9 | 99251 | 0.0179 |
| 13 | 441.2980 | 23977 | 2093.6 | 62927 | 0.0184 |



Exact Mass: 376.0812

$[M+Na]^+ = 399.0710$

Mass Spectrum List Report

Analysis Info

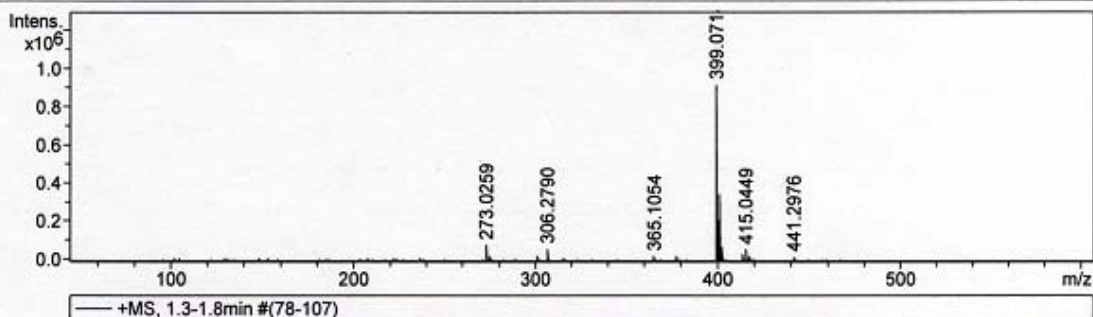
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Method tune_low.m
Sample Name VK-7B
Comment

Acquisition Date 5/18/2010 9:34:30 AM

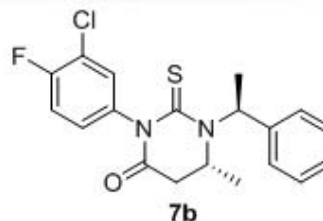
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 273.0259 | 22239 | 4195.1 | 78721 | 0.0123 |
| 2 | 301.1407 | 23603 | 1149.3 | 24631 | 0.0128 |
| 3 | 306.2790 | 22919 | 2758.6 | 57310 | 0.0134 |
| 4 | 365.1054 | 25552 | 878.9 | 21797 | 0.0143 |
| 5 | 377.0884 | 25870 | 475.7 | 19750 | 0.0146 |
| 6 | 399.0714 | 21187 | 12628.1 | 911532 | 0.0188 |
| 7 | 400.0743 | 22057 | 2881.8 | 210006 | 0.0181 |
| 8 | 401.0688 | 20366 | 4844.8 | 345916 | 0.0197 |
| 9 | 402.0711 | 23180 | 1024.9 | 71651 | 0.0173 |
| 10 | 415.0449 | 24707 | 1116.5 | 56582 | 0.0168 |
| 11 | 441.2976 | 25595 | 955.9 | 16642 | 0.0172 |



Exact Mass: 376.0812

$[M+Na]^+ = 399.0710$

Mass Spectrum List Report

Analysis Info

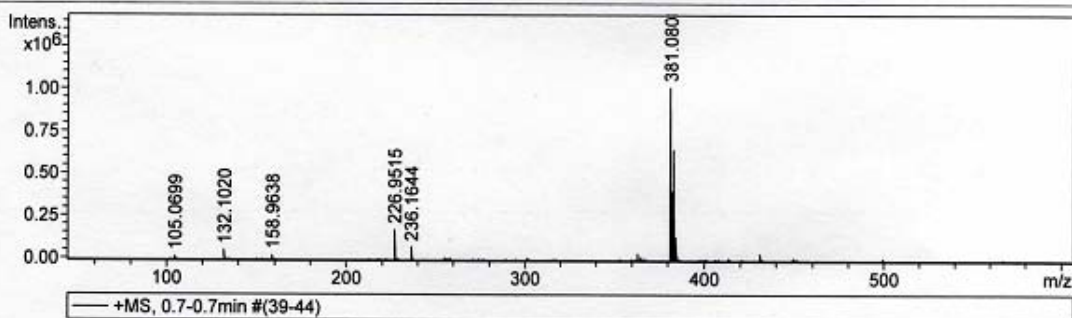
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Method tune_low.m
Sample Name VK-8A
Comment

Acquisition Date 5/18/2010 11:20:28 AM

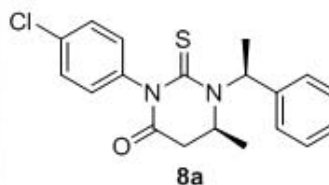
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 105.0699 | 22485 | 14985.7 | 17886 | 0.0047 |
| 2 | 132.1020 | 21091 | 19221.6 | 53716 | 0.0063 |
| 3 | 158.9638 | 20022 | 7052.5 | 24794 | 0.0079 |
| 4 | 226.9515 | 21127 | 17351.7 | 174327 | 0.0107 |
| 5 | 236.1644 | 21732 | 7108.3 | 76277 | 0.0109 |
| 6 | 381.0808 | 15636 | 22423.0 | 1011544 | 0.0244 |
| 7 | 382.0833 | 21791 | 8751.8 | 400401 | 0.0175 |
| 8 | 383.0776 | 20273 | 13848.9 | 642375 | 0.0189 |
| 9 | 384.0802 | 21153 | 2917.8 | 137207 | 0.0182 |



Exact Mass: 358.0907

$[M+Na]^+ = 381.0805$

Mass Spectrum List Report

Analysis Info

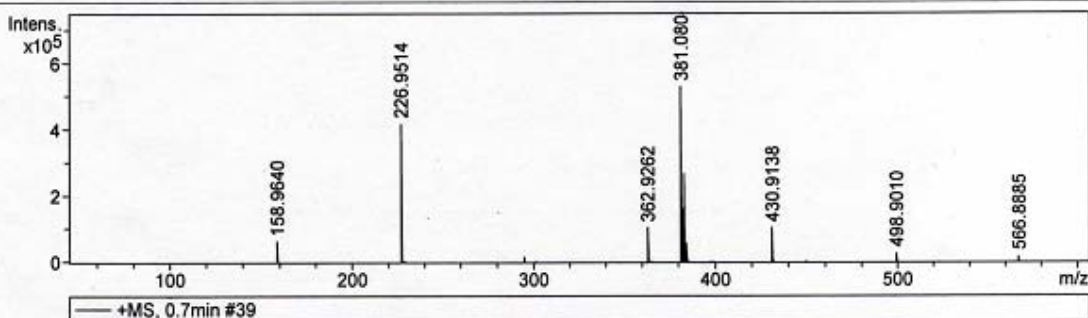
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Method tune_low.m
Sample Name VK-8B
Comment

Acquisition Date 5/18/2010 11:44:01 AM

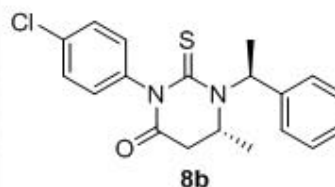
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 158.9640 | 20911 | 2484.3 | 63564 | 0.0076 |
| 2 | 226.9514 | 19886 | 6959.9 | 417687 | 0.0114 |
| 3 | 362.9262 | 23217 | 1316.3 | 104131 | 0.0156 |
| 4 | 381.0804 | 17470 | 2672.7 | 527155 | 0.0218 |
| 5 | 382.0830 | 21910 | 797.3 | 162450 | 0.0174 |
| 6 | 383.0775 | 20655 | 1281.1 | 269326 | 0.0185 |
| 7 | 384.0800 | 22107 | 261.5 | 56670 | 0.0174 |
| 8 | 385.0762 | 18526 | 47.3 | 10549 | 0.0208 |
| 9 | 430.9138 | 23202 | 954.8 | 105667 | 0.0186 |
| 10 | 498.9010 | 26446 | 1100.1 | 28711 | 0.0189 |
| 11 | 566.8885 | 25833 | 803.1 | 17893 | 0.0219 |



Exact Mass: 358.0907

$[M+Na]^+ = 381.0805$

Mass Spectrum List Report

Analysis Info

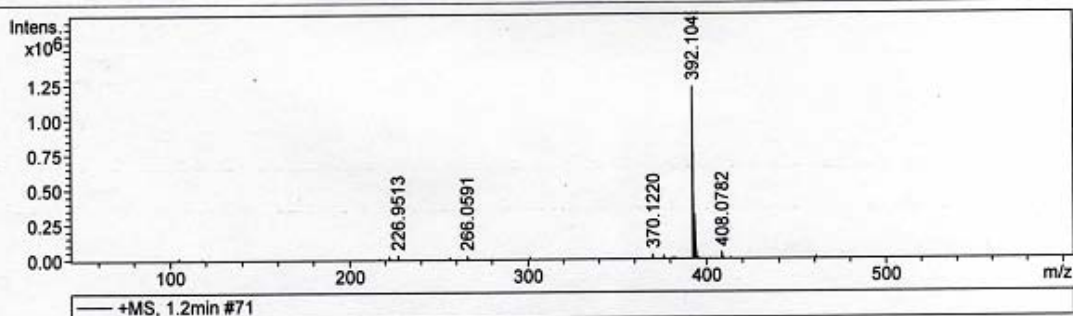
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Method tune_low.m
Sample Name vk-9a
Comment

Acquisition Date 5/19/2010 12:31:51 PM

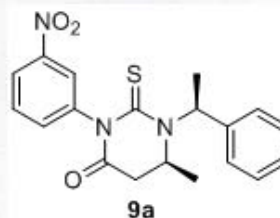
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 222.1486 | 26078 | 119.4 | 26176 | 0.0085 |
| 2 | 226.9513 | 23528 | 148.6 | 31578 | 0.0096 |
| 3 | 256.1304 | 25072 | 106.8 | 18635 | 0.0102 |
| 4 | 266.0591 | 25419 | 178.4 | 29446 | 0.0105 |
| 5 | 301.1407 | 26525 | 143.1 | 17017 | 0.0114 |
| 6 | 370.1220 | 25635 | 145.8 | 37371 | 0.0144 |
| 7 | 376.1270 | 26288 | 79.3 | 24815 | 0.0143 |
| 8 | 392.1049 | 19133 | 2655.2 | 1228859 | 0.0205 |
| 9 | 393.1077 | 21480 | 679.4 | 320817 | 0.0183 |
| 10 | 394.1042 | 18477 | 175.6 | 84559 | 0.0213 |
| 11 | 408.0782 | 24894 | 111.6 | 48412 | 0.0164 |



Exact Mass: 369.1147

$[M+Na]^+ = 392.1045$

Mass Spectrum List Report

Analysis Info

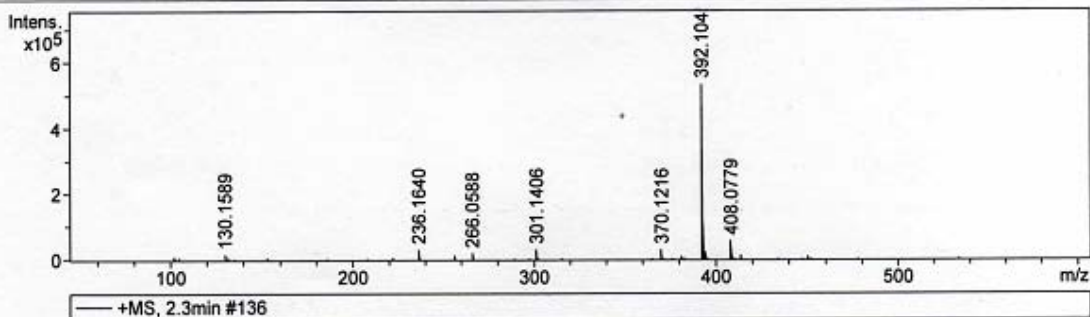
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Sample Name VK-9B
Comment

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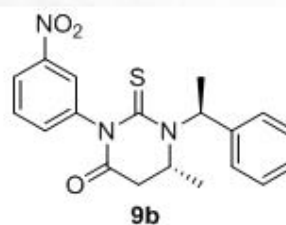
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

| | | | | | |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 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 | 130.1589 | 23574 | 2082.5 | 17959 | 0.0055 |
| 2 | 236.1640 | 25121 | 1654.4 | 32158 | 0.0094 |
| 3 | 256.1300 | 25340 | 712.1 | 16035 | 0.0101 |
| 4 | 266.0588 | 25523 | 954.1 | 21368 | 0.0104 |
| 5 | 301.1406 | 24515 | 1473.1 | 31942 | 0.0123 |
| 6 | 370.1216 | 25398 | 898.1 | 30007 | 0.0146 |
| 7 | 392.1045 | 22323 | 10163.7 | 532185 | 0.0176 |
| 8 | 408.0779 | 24355 | 1137.9 | 58296 | 0.0168 |



Exact Mass: 369.1147

$[M+Na]^+ = 392.1045$

Mass Spectrum List Report

Analysis Info

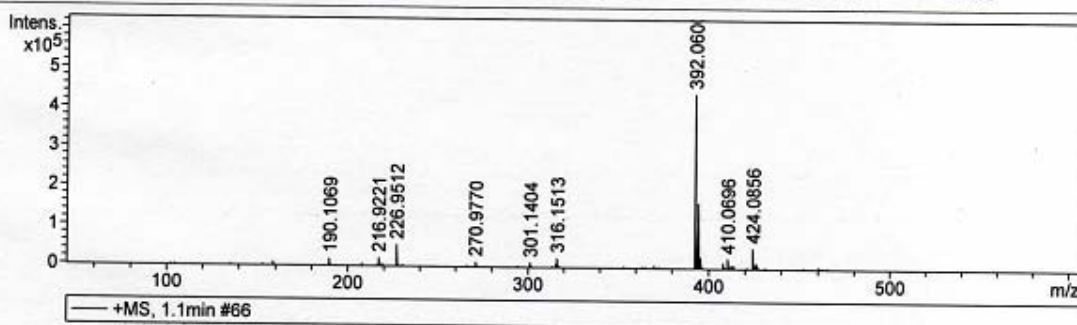
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Method tune_low.m
Sample Name VK-10
Comment

Acquisition Date 5/18/2010 1:35:54 PM

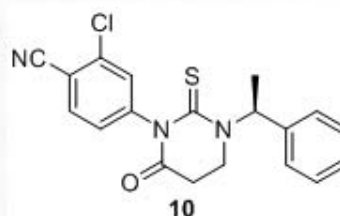
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 190.1069 | 21558 | 2686.4 | 18663 | 0.0088 |
| 2 | 216.9221 | 25943 | 2145.4 | 21612 | 0.0084 |
| 3 | 226.9512 | 21601 | 5648.2 | 54440 | 0.0105 |
| 4 | 270.9770 | 26859 | 1159.7 | 13468 | 0.0102 |
| 5 | 301.1404 | 25256 | 798.8 | 11855 | 0.0119 |
| 6 | 316.1513 | 25675 | 1572.0 | 24721 | 0.0123 |
| 7 | 392.0600 | 22371 | 9356.1 | 441772 | 0.0175 |
| 8 | 393.0626 | 23284 | 1978.9 | 95433 | 0.0169 |
| 9 | 394.0573 | 22062 | 3383.5 | 166556 | 0.0179 |
| 10 | 395.0593 | 25095 | 562.5 | 28254 | 0.0157 |
| 11 | 410.0696 | 27161 | 547.5 | 25956 | 0.0151 |
| 12 | 424.0856 | 25611 | 189.3 | 52682 | 0.0166 |



Exact Mass: 369.0703

[M+Na]⁺ = 392.0601

Mass Spectrum List Report

Analysis Info

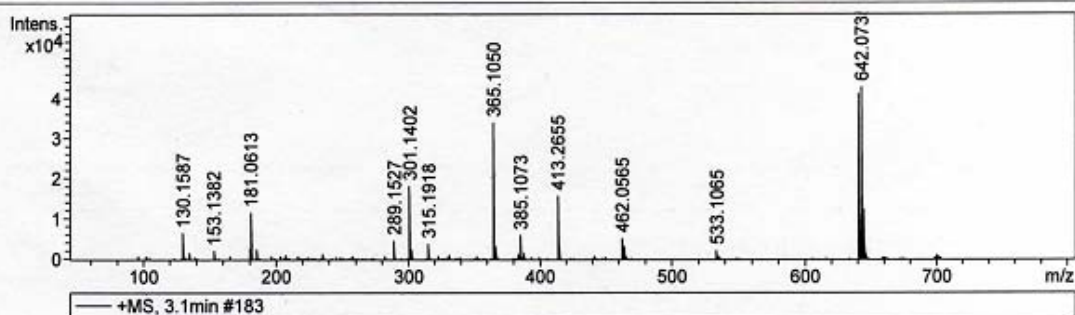
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Method tune_low.m
Sample Name VK-10A
Comment

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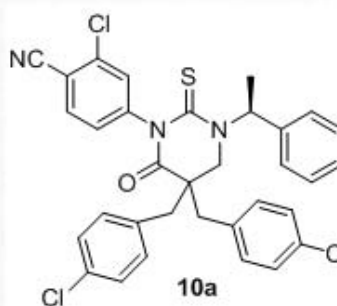
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

| | | | | | |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|-------|-------|--------|
| 1 | 130.1587 | 20234 | 90.2 | 6628 | 0.0064 |
| 2 | 153.1382 | 20883 | 27.2 | 2231 | 0.0073 |
| 3 | 181.0613 | 22741 | 138.1 | 11688 | 0.0080 |
| 4 | 289.1527 | 27025 | 63.2 | 4754 | 0.0107 |
| 5 | 301.1402 | 24593 | 216.8 | 18337 | 0.0122 |
| 6 | 315.1918 | 24455 | 41.5 | 3968 | 0.0129 |
| 7 | 365.1050 | 26120 | 286.9 | 33968 | 0.0140 |
| 8 | 385.1073 | 25972 | 54.7 | 6034 | 0.0148 |
| 9 | 399.0692 | 32334 | 5.3 | 505 | 0.0123 |
| 10 | 413.2655 | 26137 | 196.6 | 15757 | 0.0158 |
| 11 | 414.2687 | 28864 | 47.0 | 3720 | 0.0144 |
| 12 | 462.0565 | 28766 | 99.0 | 5371 | 0.0161 |
| 13 | 533.1065 | 27726 | 77.5 | 2352 | 0.0192 |
| 14 | 640.0760 | 26728 | 900.6 | 40918 | 0.0239 |
| 15 | 641.0786 | 26070 | 251.4 | 11311 | 0.0246 |
| 16 | 642.0735 | 25873 | 960.6 | 42789 | 0.0248 |
| 17 | 643.0755 | 26208 | 260.0 | 11467 | 0.0245 |
| 18 | 644.0708 | 24884 | 286.5 | 12507 | 0.0259 |
| 19 | 645.0725 | 26072 | 72.8 | 3145 | 0.0247 |
| 20 | 646.0690 | 24610 | 34.1 | 1459 | 0.0263 |
| 21 | 647.0683 | 25671 | 9.1 | 384 | 0.0252 |



Exact Mass: 617.0862
[M+Na]⁺ = 640.0760

Mass Spectrum List Report

Analysis Info

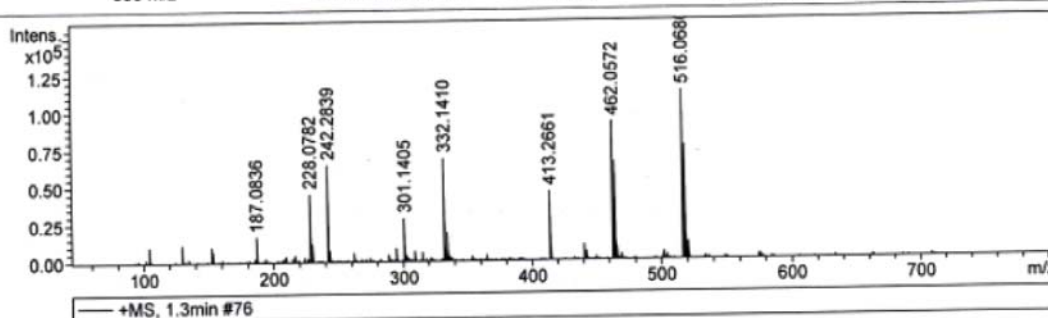
Analysis Name D:\Data\vipin\10-05-18-VK-10B.d
Method tune_low.m
Sample Name VK-10B
Comment

Acquisition Date 5/18/2010 2:39:14 PM

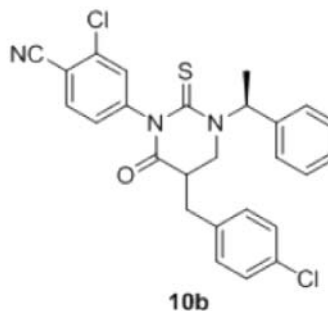
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 187.0836 | 22909 | 1352.8 | 16542 | 0.0082 |
| 2 | 228.0782 | 24547 | 2346.7 | 45375 | 0.0093 |
| 3 | 242.2839 | 23894 | 3383.0 | 64496 | 0.0101 |
| 4 | 301.1405 | 24175 | 1053.2 | 28747 | 0.0125 |
| 5 | 332.1410 | 24090 | 2103.4 | 68748 | 0.0138 |
| 6 | 413.2661 | 25711 | 1657.5 | 46152 | 0.0161 |
| 7 | 462.0572 | 23682 | 2797.0 | 92261 | 0.0195 |
| 8 | 463.0598 | 27211 | 631.2 | 20891 | 0.0170 |
| 9 | 464.0544 | 24964 | 1977.5 | 65674 | 0.0186 |
| 10 | 516.0680 | 24486 | 2943.6 | 112464 | 0.0211 |
| 11 | 517.0707 | 26952 | 713.8 | 27333 | 0.0192 |
| 12 | 518.0655 | 24400 | 1987.9 | 76303 | 0.0212 |
| 13 | 519.0677 | 27323 | 429.3 | 16517 | 0.0190 |



Exact Mass: 493.0782

$[M+Na]^+ = 516.0680$

Mass Spectrum List Report

Analysis Info

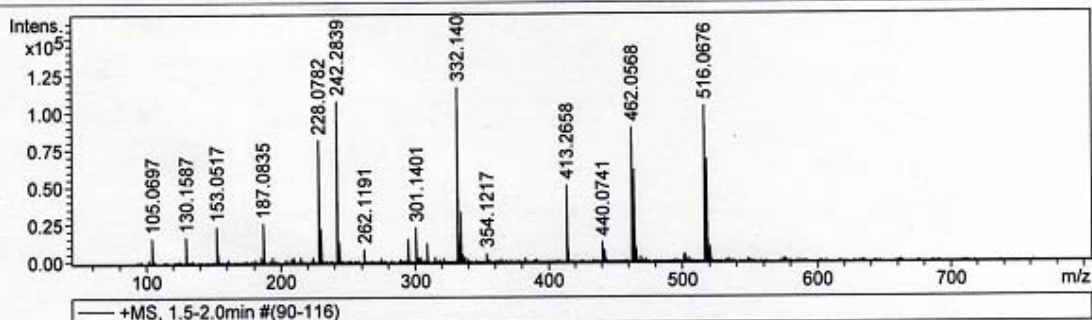
Analysis Name D:\Data\vipin\10-05-18-VK-10C.d
Method tune_low.m
Sample Name VK-10C
Comment

Acquisition Date 5/18/2010 3:11:01 PM

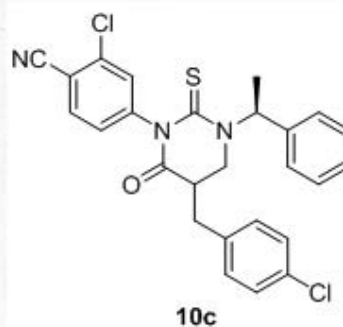
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 105.0697 | 23556 | 6368.8 | 16098 | 0.0045 |
| 2 | 130.1587 | 25510 | 3637.7 | 16927 | 0.0051 |
| 3 | 153.0517 | 25267 | 3210.9 | 24008 | 0.0061 |
| 4 | 187.0835 | 23527 | 2002.4 | 26043 | 0.0080 |
| 5 | 228.0782 | 23134 | 4095.7 | 81613 | 0.0099 |
| 6 | 242.2839 | 22172 | 5713.4 | 107838 | 0.0109 |
| 7 | 262.1191 | 25820 | 506.9 | 8823 | 0.0102 |
| 8 | 295.1140 | 25477 | 643.3 | 15294 | 0.0116 |
| 9 | 301.1401 | 25161 | 903.4 | 23235 | 0.0120 |
| 10 | 309.1297 | 26783 | 437.1 | 12368 | 0.0115 |
| 11 | 332.1409 | 23018 | 3794.9 | 116922 | 0.0144 |
| 12 | 354.1217 | 27000 | 232.4 | 5874 | 0.0131 |
| 13 | 413.2658 | 25787 | 2246.1 | 51200 | 0.0160 |
| 14 | 440.0741 | 26533 | 524.9 | 13052 | 0.0166 |
| 15 | 462.0568 | 24277 | 3351.9 | 89662 | 0.0190 |
| 16 | 516.0676 | 24658 | 3350.6 | 103859 | 0.0209 |
| 17 | 517.0701 | 26471 | 776.2 | 24116 | 0.0195 |
| 18 | 518.0649 | 24135 | 2205.5 | 68691 | 0.0215 |
| 19 | 519.0671 | 26711 | 477.5 | 14907 | 0.0194 |
| 20 | 520.0623 | 25431 | 322.1 | 10082 | 0.0204 |



10c

Exact Mass: 493.0782

$[M+Na]^+ = 516.0680$

Mass Spectrum List Report

Analysis Info

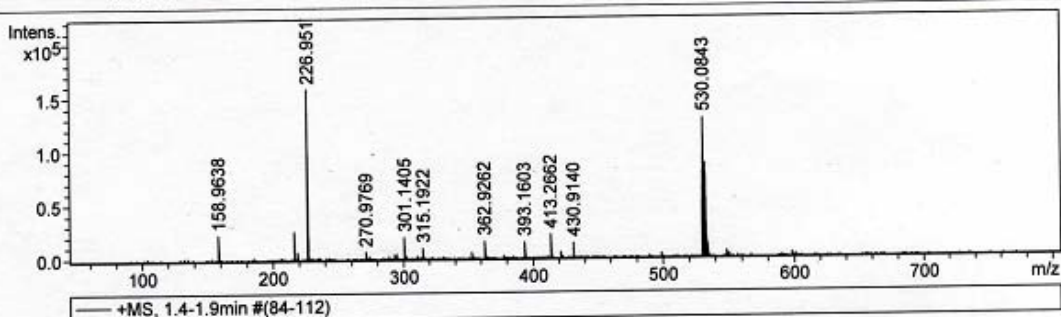
Analysis Name D:\Data\vipin\10-05-18-VK-6AI-R.d
Method tune_low.m
Sample Name VK-6AI-R
Comment

Acquisition Date 5/18/2010 3:45:31 PM

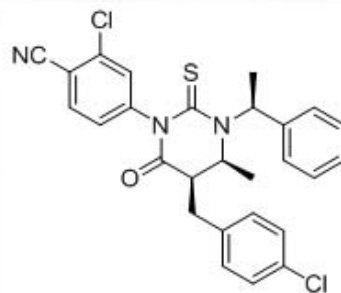
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 158.9638 | 21846 | 8250.7 | 22641 | 0.0073 |
| 2 | 216.9223 | 22164 | 2434.6 | 25679 | 0.0098 |
| 3 | 226.9517 | 21152 | 14037.7 | 157461 | 0.0107 |
| 4 | 270.9769 | 26383 | 673.2 | 6388 | 0.0103 |
| 5 | 301.1405 | 25903 | 1799.6 | 20350 | 0.0116 |
| 6 | 315.1922 | 26342 | 803.2 | 9840 | 0.0120 |
| 7 | 352.8970 | 26163 | 437.9 | 5939 | 0.0135 |
| 8 | 362.9262 | 24705 | 1159.0 | 16015 | 0.0147 |
| 9 | 393.1603 | 26482 | 1077.8 | 15380 | 0.0148 |
| 10 | 413.2662 | 27188 | 1500.8 | 21679 | 0.0152 |
| 11 | 430.9140 | 26302 | 1000.8 | 14093 | 0.0164 |
| 12 | 530.0843 | 24544 | 5990.7 | 128468 | 0.0216 |
| 13 | 531.0868 | 26444 | 1544.8 | 32751 | 0.0201 |
| 14 | 532.0817 | 24149 | 4169.2 | 87388 | 0.0220 |
| 15 | 533.0842 | 26392 | 978.7 | 20277 | 0.0202 |
| 16 | 534.0792 | 24840 | 641.7 | 13140 | 0.0215 |
| 17 | 535.0814 | 25095 | 134.8 | 2728 | 0.0213 |



6ai

Exact Mass: 507.0939

$[M+Na]^+ = 530.0837$

Mass Spectrum List Report

Analysis Info

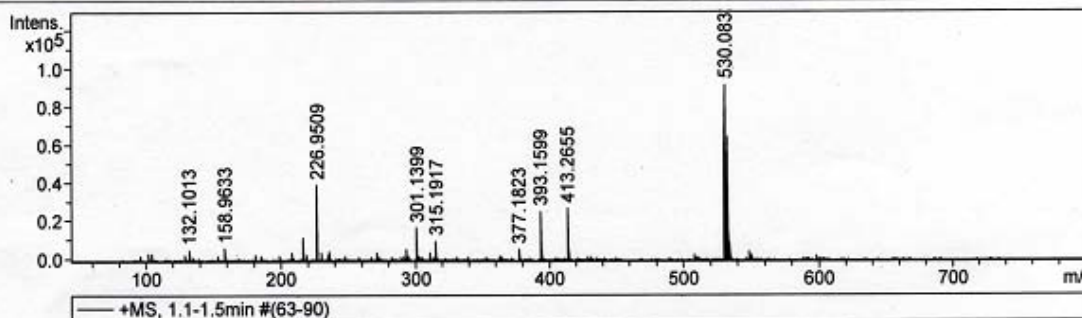
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Method tune_low.m
Sample Name VK-6BI
Comment

Acquisition Date 5/18/2010 4:07:52 PM

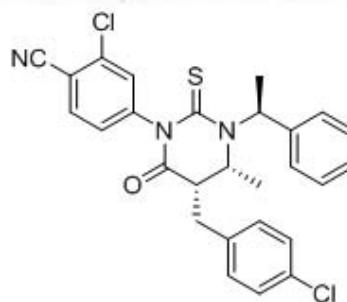
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 132.1013 | 26731 | 2269.6 | 5292 | 0.0049 |
| 2 | 158.9633 | 26791 | 2009.3 | 6251 | 0.0059 |
| 3 | 216.9217 | 24733 | 1264.0 | 11427 | 0.0088 |
| 4 | 226.9509 | 22647 | 4053.9 | 39159 | 0.0100 |
| 5 | 282.2777 | 25803 | 139.3 | 1383 | 0.0109 |
| 6 | 293.0802 | 24490 | 547.2 | 5800 | 0.0120 |
| 7 | 301.1399 | 25572 | 1499.6 | 16647 | 0.0118 |
| 8 | 315.1917 | 25582 | 833.9 | 9987 | 0.0123 |
| 9 | 377.1823 | 25639 | 441.7 | 5500 | 0.0147 |
| 10 | 393.1599 | 25745 | 2038.4 | 25445 | 0.0153 |
| 11 | 413.2655 | 26260 | 2137.2 | 26759 | 0.0157 |
| 12 | 530.0832 | 24034 | 5106.4 | 91350 | 0.0221 |
| 13 | 531.0856 | 26889 | 1340.0 | 23673 | 0.0198 |
| 14 | 532.0805 | 24927 | 3656.9 | 63801 | 0.0213 |
| 15 | 533.0828 | 26630 | 846.2 | 14577 | 0.0200 |
| 16 | 534.0780 | 24245 | 529.8 | 9009 | 0.0220 |
| 17 | 548.0916 | 27157 | 312.4 | 4344 | 0.0202 |



6bi

Exact Mass: 507.0939
[M+Na]⁺ = 530.0837

Mass Spectrum List Report

Analysis Info

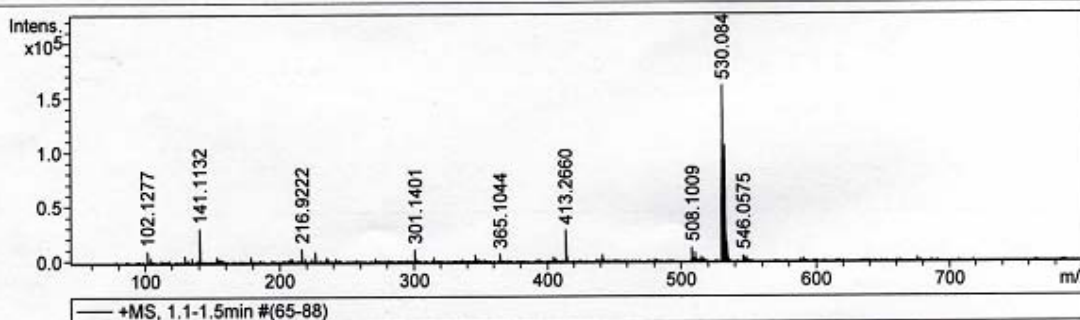
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Method tune_low.m
Sample Name VK-6BII
Comment

Acquisition Date 5/18/2010 4:37:26 PM

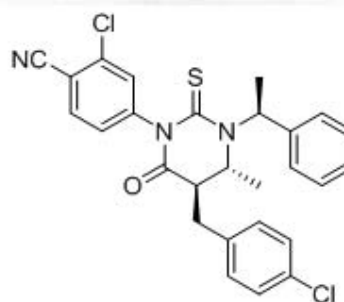
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 102.1277 | 17509 | 2403.2 | 9678 | 0.0058 |
| 2 | 141.1132 | 19889 | 4655.2 | 30394 | 0.0071 |
| 3 | 216.9222 | 25952 | 943.6 | 12089 | 0.0084 |
| 4 | 301.1401 | 26524 | 758.0 | 11449 | 0.0114 |
| 5 | 315.1917 | 26245 | 226.6 | 3636 | 0.0120 |
| 6 | 365.1044 | 25857 | 440.8 | 6610 | 0.0141 |
| 7 | 413.2660 | 26377 | 1642.8 | 28207 | 0.0157 |
| 8 | 508.1009 | 27814 | 440.8 | 12147 | 0.0183 |
| 9 | 510.0983 | 27813 | 286.3 | 8118 | 0.0183 |
| 10 | 511.1012 | 26485 | 69.7 | 2004 | 0.0193 |
| 11 | 512.0960 | 24051 | 45.4 | 1323 | 0.0213 |
| 12 | 514.1053 | 27678 | 131.9 | 3952 | 0.0186 |
| 13 | 516.1084 | 16700 | 83.9 | 2579 | 0.0309 |
| 14 | 518.1137 | 18280 | 27.5 | 867 | 0.0283 |
| 15 | 530.0841 | 24219 | 4816.5 | 159828 | 0.0219 |
| 16 | 531.0865 | 25258 | 1254.5 | 41092 | 0.0210 |
| 17 | 532.0814 | 23003 | 3275.3 | 105904 | 0.0231 |
| 18 | 533.0836 | 26321 | 824.8 | 26318 | 0.0203 |
| 19 | 534.0789 | 25747 | 556.1 | 17509 | 0.0207 |
| 20 | 535.0806 | 26911 | 119.6 | 3714 | 0.0199 |
| 21 | 539.3253 | 21253 | 3.1 | 91 | 0.0254 |
| 22 | 546.0575 | 27816 | 194.4 | 5135 | 0.0196 |
| 23 | 804.6421 | 20677 | 9.3 | 73 | 0.0389 |



6bii

Exact Mass: 507.0939

$[M+Na]^+ = 530.0837$

Mass Spectrum List Report

Analysis Info

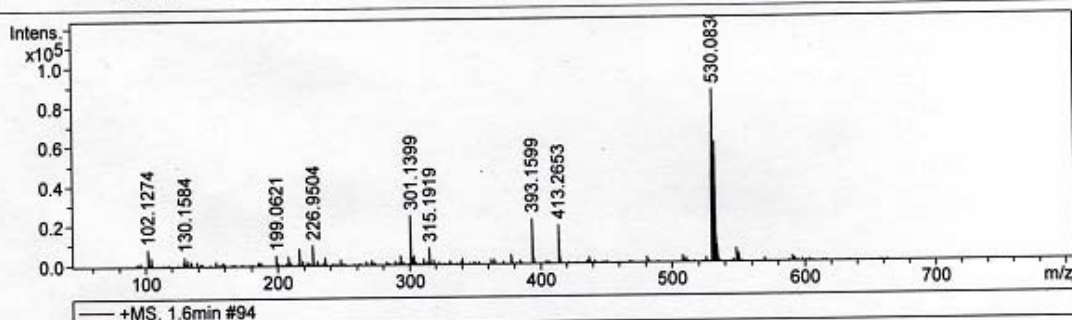
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Method tune_low.m
Sample Name VK-6ci
Comment

Acquisition Date 5/19/2010 9:24:16 AM

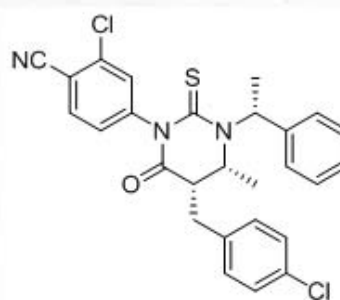
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|-------|--------|
| 1 | 102.1274 | 18195 | 2584.0 | 8276 | 0.0056 |
| 2 | 130.1584 | 22899 | 970.7 | 4816 | 0.0057 |
| 3 | 185.1138 | 22844 | 252.0 | 1990 | 0.0081 |
| 4 | 199.0621 | 23180 | 503.4 | 4943 | 0.0086 |
| 5 | 208.1322 | 23544 | 432.9 | 4792 | 0.0088 |
| 6 | 216.9217 | 22813 | 709.0 | 8708 | 0.0095 |
| 7 | 226.9504 | 24680 | 771.8 | 10130 | 0.0092 |
| 8 | 301.1399 | 24101 | 1468.2 | 24491 | 0.0125 |
| 9 | 315.1919 | 24461 | 473.5 | 8486 | 0.0129 |
| 10 | 393.1599 | 25644 | 1223.2 | 22526 | 0.0153 |
| 11 | 413.2653 | 25918 | 1059.7 | 19121 | 0.0159 |
| 12 | 530.0830 | 24546 | 3220.0 | 86460 | 0.0216 |
| 13 | 531.0855 | 26537 | 809.7 | 21536 | 0.0200 |
| 14 | 531.5046 | 28885 | 3.2 | 84 | 0.0184 |
| 15 | 532.0806 | 25067 | 2286.4 | 60239 | 0.0212 |
| 16 | 533.0829 | 27021 | 527.7 | 13770 | 0.0197 |
| 17 | 534.0778 | 24584 | 328.7 | 8501 | 0.0217 |
| 18 | 535.0800 | 26050 | 74.5 | 1906 | 0.0205 |
| 19 | 548.0920 | 25701 | 312.6 | 6973 | 0.0213 |



6ci

Exact Mass: 507.0939
[M+Na]⁺ = 530.0837

Mass Spectrum List Report

Analysis Info

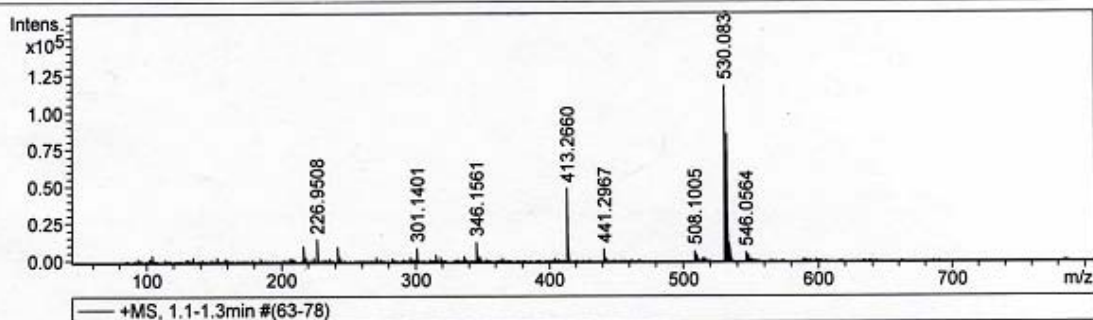
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Method tune_low.m
Sample Name VK-6di-r
Comment

Acquisition Date 5/19/2010 9:42:11 AM

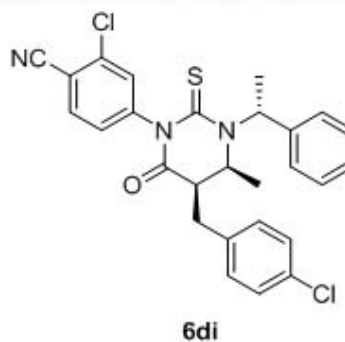
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 216.9220 | 22947 | 970.1 | 10064 | 0.0095 |
| 2 | 226.9508 | 23475 | 1356.5 | 14707 | 0.0097 |
| 3 | 242.0933 | 23910 | 944.0 | 9820 | 0.0101 |
| 4 | 301.1401 | 24257 | 797.8 | 8895 | 0.0124 |
| 5 | 315.1919 | 25069 | 374.4 | 4480 | 0.0126 |
| 6 | 346.1561 | 26841 | 1156.7 | 12948 | 0.0129 |
| 7 | 413.2660 | 25414 | 4084.8 | 48903 | 0.0163 |
| 8 | 441.2967 | 27099 | 747.6 | 8442 | 0.0163 |
| 9 | 508.1005 | 26759 | 388.0 | 6871 | 0.0190 |
| 10 | 530.0834 | 23193 | 5369.7 | 117587 | 0.0229 |
| 11 | 531.0859 | 26742 | 1506.6 | 32578 | 0.0199 |
| 12 | 532.0808 | 24227 | 4003.2 | 85471 | 0.0220 |
| 13 | 533.0830 | 26864 | 948.7 | 19996 | 0.0198 |
| 14 | 534.0781 | 24506 | 572.4 | 11909 | 0.0218 |
| 15 | 546.0564 | 27166 | 316.2 | 5542 | 0.0201 |



Exact Mass: 507.0939
[M+Na]⁺ = 530.0837

Mass Spectrum List Report

Analysis Info

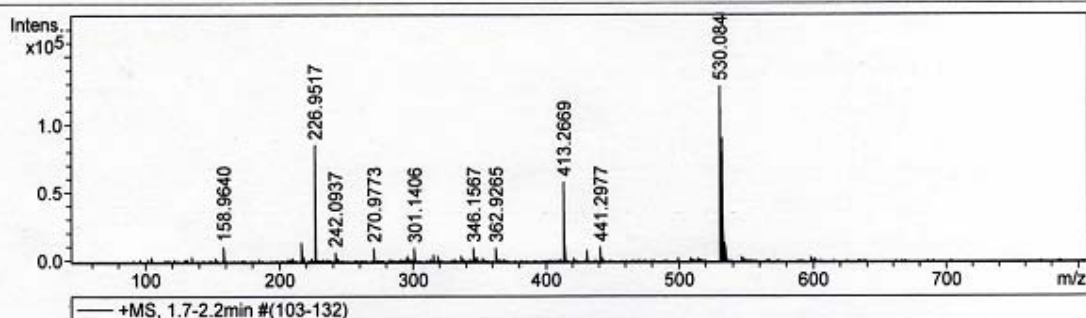
Analysis Name D:\Data\vipin\10-05-19-VK-6dii.d
Method tune_low.m
Sample Name VK-6dii
Comment

Acquisition Date 5/19/2010 9:53:41 AM

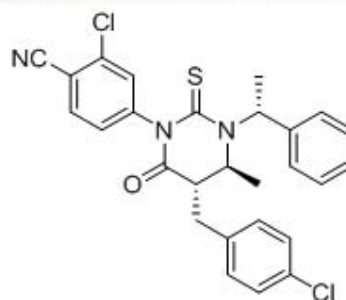
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 158.9640 | 22629 | 3888.5 | 10782 | 0.0070 |
| 2 | 216.9224 | 22666 | 1358.6 | 13473 | 0.0096 |
| 3 | 226.9517 | 21790 | 8145.1 | 85155 | 0.0104 |
| 4 | 242.0937 | 25410 | 691.7 | 6668 | 0.0095 |
| 5 | 270.9773 | 24969 | 1221.3 | 9874 | 0.0109 |
| 6 | 301.1406 | 25128 | 994.2 | 9403 | 0.0120 |
| 7 | 315.1926 | 24648 | 490.8 | 5003 | 0.0128 |
| 8 | 346.1567 | 26801 | 976.0 | 9768 | 0.0129 |
| 9 | 362.9265 | 24000 | 1020.5 | 9740 | 0.0151 |
| 10 | 413.2669 | 24311 | 4872.3 | 57892 | 0.0170 |
| 11 | 430.9142 | 23432 | 692.7 | 8353 | 0.0184 |
| 12 | 441.2977 | 26965 | 936.1 | 10282 | 0.0164 |
| 13 | 530.0846 | 23757 | 6407.6 | 127748 | 0.0223 |
| 14 | 531.0872 | 26268 | 1765.9 | 34745 | 0.0202 |
| 15 | 532.0822 | 23903 | 4661.9 | 90521 | 0.0223 |
| 16 | 533.0843 | 27024 | 1137.7 | 21795 | 0.0197 |
| 17 | 534.0795 | 24646 | 709.8 | 13414 | 0.0217 |



6dii

Exact Mass: 507.0939

[M+Na]⁺ = 530.0837

Mass Spectrum List Report

Analysis Info

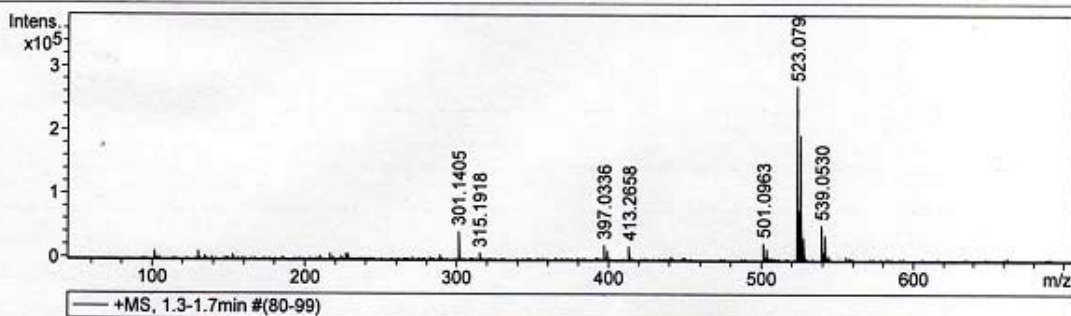
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Method tune_low.m
Sample Name vk-7ai
Comment

Acquisition Date 5/19/2010 1:55:43 PM

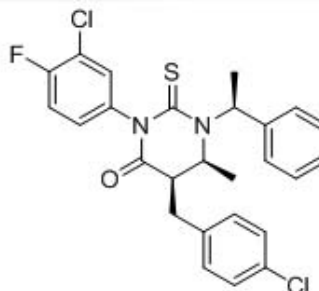
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 301.1405 | 25329 | 2557.1 | 43471 | 0.0119 |
| 2 | 315.1918 | 27653 | 558.6 | 9167 | 0.0114 |
| 3 | 397.0336 | 27608 | 1297.1 | 22636 | 0.0144 |
| 4 | 413.2658 | 26387 | 1092.1 | 20405 | 0.0157 |
| 5 | 501.0963 | 26822 | 628.1 | 25529 | 0.0187 |
| 6 | 523.0792 | 22635 | 7482.9 | 269964 | 0.0231 |
| 7 | 524.0820 | 24864 | 2173.2 | 77216 | 0.0211 |
| 8 | 525.0767 | 22978 | 5519.5 | 193119 | 0.0229 |
| 9 | 526.0790 | 26252 | 1438.6 | 49548 | 0.0200 |
| 10 | 527.0740 | 25177 | 998.5 | 33851 | 0.0209 |
| 11 | 528.0753 | 27047 | 180.4 | 6016 | 0.0195 |
| 12 | 528.4821 | 27651 | 2.7 | 91 | 0.0191 |
| 13 | 539.0530 | 26105 | 1949.7 | 53380 | 0.0206 |
| 14 | 540.0555 | 27020 | 409.3 | 10982 | 0.0200 |
| 15 | 541.0505 | 26119 | 1461.3 | 38420 | 0.0207 |



7ai

Exact Mass: 500.0892

[M+Na]⁺ = 523.0790

Mass Spectrum List Report

Analysis Info

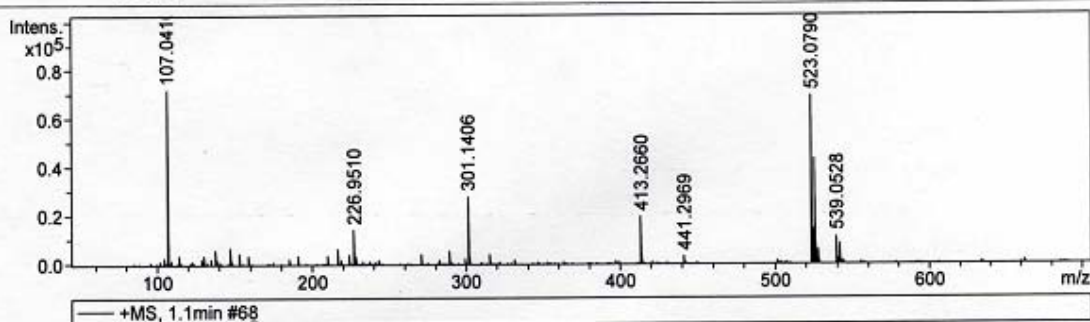
Analysis Name D:\Data\vipin\10-05-19-VK-7bi.d
Method tune_low.m
Sample Name vk-7bi
Comment

Acquisition Date 5/19/2010 2:04:10 PM

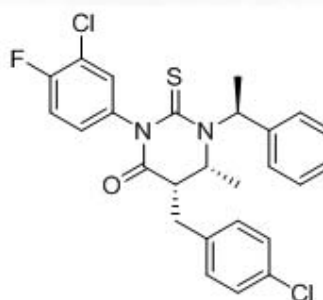
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 700 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|-------|-------|--------|
| 1 | 107.0410 | 17763 | 254.7 | 71839 | 0.0060 |
| 2 | 226.9510 | 25789 | 126.7 | 14352 | 0.0088 |
| 3 | 301.1406 | 26063 | 209.2 | 27967 | 0.0116 |
| 4 | 413.2660 | 26955 | 206.8 | 19413 | 0.0153 |
| 5 | 441.2969 | 27281 | 44.3 | 3226 | 0.0162 |
| 6 | 523.0790 | 25617 | 755.1 | 68892 | 0.0204 |
| 7 | 524.0816 | 26429 | 156.8 | 14266 | 0.0198 |
| 8 | 525.0764 | 25085 | 477.2 | 43313 | 0.0209 |
| 9 | 526.0786 | 27355 | 96.1 | 8696 | 0.0192 |
| 10 | 527.0739 | 25244 | 65.6 | 5920 | 0.0209 |
| 11 | 528.0761 | 26454 | 14.5 | 1309 | 0.0200 |
| 12 | 539.0528 | 26509 | 130.3 | 11399 | 0.0203 |
| 13 | 541.0502 | 26919 | 96.2 | 8373 | 0.0201 |



7bi

Exact Mass: 500.0892

$[M+Na]^+ = 523.0790$

Mass Spectrum List Report

Analysis Info

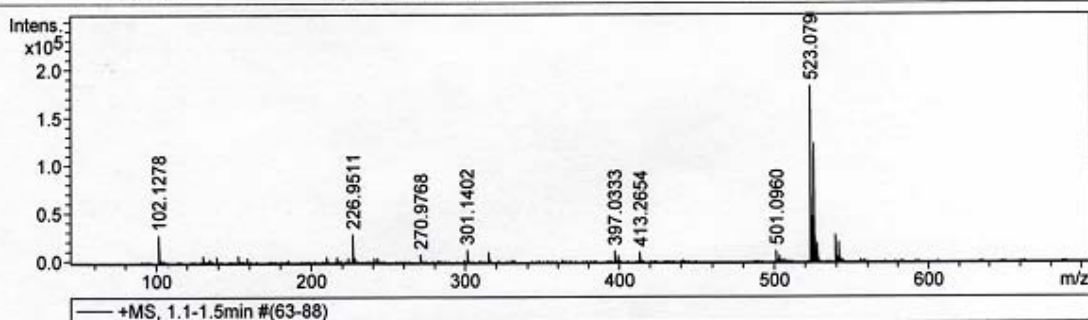
Analysis Name D:\Data\vipin\10-05-19-VK-7bii.d
Method tune_low.m
Sample Name vk-7bii
Comment

Acquisition Date 5/19/2010 2:11:04 PM

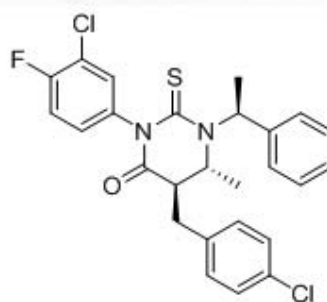
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 102.1278 | 17768 | 12887.1 | 27467 | 0.0057 |
| 2 | 226.9511 | 23895 | 3136.8 | 28434 | 0.0095 |
| 3 | 270.9768 | 26345 | 654.7 | 7325 | 0.0103 |
| 4 | 301.1402 | 26898 | 1153.6 | 12435 | 0.0112 |
| 5 | 331.1860 | 25097 | 253.2 | 2510 | 0.0132 |
| 6 | 397.0333 | 27744 | 1049.8 | 10855 | 0.0143 |
| 7 | 413.2654 | 27493 | 888.6 | 9912 | 0.0150 |
| 8 | 501.0960 | 27887 | 435.2 | 10989 | 0.0180 |
| 9 | 523.0790 | 23347 | 8204.8 | 181858 | 0.0224 |
| 10 | 524.0817 | 24868 | 2113.9 | 46086 | 0.0211 |
| 11 | 525.0765 | 22656 | 5731.6 | 122884 | 0.0232 |
| 12 | 526.0787 | 25824 | 1334.2 | 28119 | 0.0204 |
| 13 | 527.0738 | 25239 | 942.0 | 19518 | 0.0209 |
| 14 | 539.0527 | 26508 | 1701.6 | 27848 | 0.0203 |
| 15 | 540.0553 | 25950 | 346.4 | 5543 | 0.0208 |
| 16 | 541.0503 | 26514 | 1293.7 | 20236 | 0.0204 |



7bii

Exact Mass: 500.0892

[M+Na]⁺ = 523.0790

Mass Spectrum List Report

Analysis Info

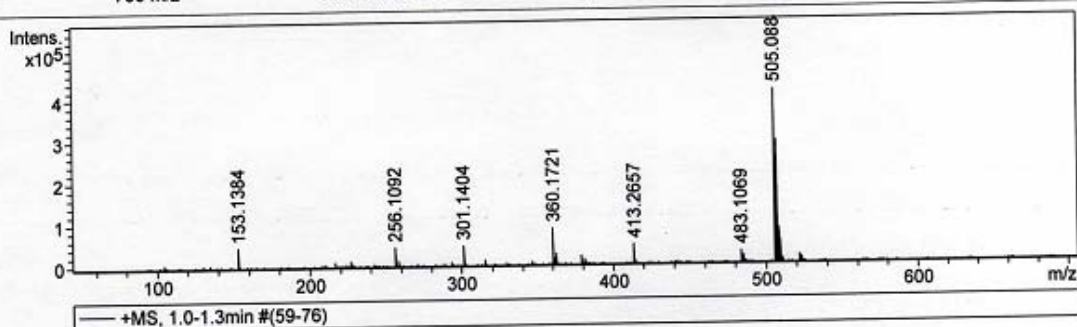
Analysis Name D:\Data\vipin\10-05-19-VK-8ai.d
Method tune_low.m
Sample Name vk-8ai
Comment

Acquisition Date 5/19/2010 2:19:23 PM

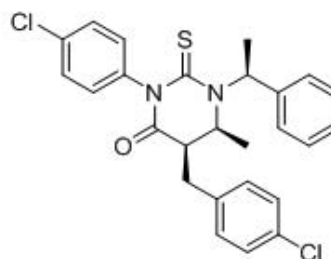
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 153.1384 | 20911 | 6861.9 | 45963 | 0.0073 |
| 2 | 256.1092 | 22426 | 2651.5 | 44796 | 0.0114 |
| 3 | 301.1404 | 24832 | 2450.9 | 47638 | 0.0121 |
| 4 | 360.1721 | 23392 | 3112.3 | 86810 | 0.0154 |
| 5 | 413.2657 | 25880 | 2178.9 | 46428 | 0.0160 |
| 6 | 483.1069 | 24669 | 771.8 | 29253 | 0.0196 |
| 7 | 505.0884 | 22223 | 6945.8 | 413441 | 0.0227 |
| 8 | 506.0912 | 22907 | 1954.7 | 118278 | 0.0221 |
| 9 | 507.0859 | 21956 | 4781.2 | 292075 | 0.0231 |
| 10 | 508.0883 | 24501 | 1358.1 | 81428 | 0.0207 |
| 11 | 509.0833 | 23406 | 930.4 | 54736 | 0.0217 |
| 12 | 510.0849 | 26628 | 183.6 | 10595 | 0.0192 |



8ai

Exact Mass: 482.0986

$[M+Na]^+ = 505.0884$

Mass Spectrum List Report

Analysis Info

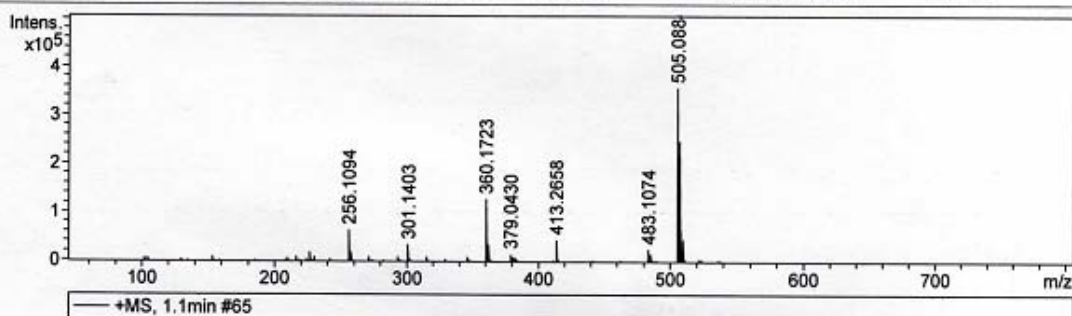
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Method tune_low.m
Sample Name VK-8bi
Comment

Acquisition Date 5/19/2010 10:15:08 AM

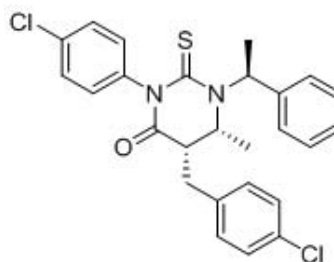
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 256.1094 | 22438 | 3938.1 | 63511 | 0.0114 |
| 2 | 301.1403 | 25115 | 1824.5 | 34729 | 0.0120 |
| 3 | 360.1723 | 22991 | 4706.2 | 127550 | 0.0157 |
| 4 | 379.0430 | 26307 | 502.7 | 14655 | 0.0144 |
| 5 | 413.2658 | 25781 | 1954.8 | 43934 | 0.0160 |
| 6 | 483.1074 | 24632 | 1073.4 | 24812 | 0.0196 |
| 7 | 505.0884 | 22569 | 4357.3 | 355447 | 0.0224 |
| 8 | 506.0912 | 24157 | 3270.7 | 103841 | 0.0209 |
| 9 | 507.0858 | 22166 | 7694.5 | 247167 | 0.0229 |
| 10 | 508.0882 | 24692 | 2031.4 | 66018 | 0.0206 |
| 11 | 509.0833 | 23842 | 1395.6 | 45876 | 0.0214 |



8bi

Exact Mass: 482.0986

$[M+Na]^+ = 505.0884$

Mass Spectrum List Report

Analysis Info

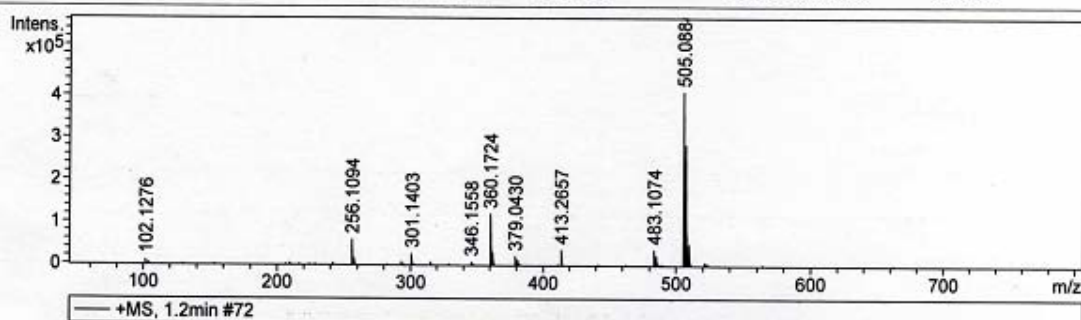
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Method tune_low.m
Sample Name VK-8bii
Comment

Acquisition Date 5/19/2010 10:32:57 AM

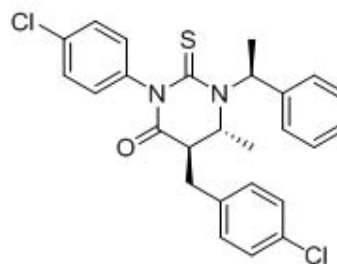
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|---------|--------|--------|
| 1 | 102.1276 | 24196 | 4106.6 | 12289 | 0.0042 |
| 2 | 256.1094 | 22262 | 3679.0 | 61338 | 0.0115 |
| 3 | 301.1403 | 25927 | 1356.9 | 27792 | 0.0116 |
| 4 | 315.1912 | 27087 | 363.3 | 7632 | 0.0116 |
| 5 | 329.1713 | 26654 | 167.0 | 3780 | 0.0123 |
| 6 | 346.1558 | 26219 | 336.2 | 8950 | 0.0132 |
| 7 | 360.1724 | 23157 | 4072.0 | 121783 | 0.0156 |
| 8 | 379.0430 | 24952 | 689.6 | 22241 | 0.0152 |
| 9 | 413.2657 | 26016 | 1516.6 | 38443 | 0.0159 |
| 10 | 483.1074 | 23425 | 1243.0 | 37934 | 0.0206 |
| 11 | 505.0884 | 22864 | 10281.1 | 411035 | 0.0221 |
| 12 | 506.0912 | 23348 | 2888.5 | 116726 | 0.0217 |
| 13 | 507.0858 | 22391 | 6994.5 | 285646 | 0.0226 |
| 14 | 508.0882 | 24723 | 1904.5 | 78596 | 0.0206 |
| 15 | 509.0833 | 22721 | 1249.7 | 52108 | 0.0224 |
| 16 | 510.0846 | 25606 | 231.7 | 9761 | 0.0199 |
| 17 | 521.0623 | 25276 | 200.1 | 9374 | 0.0206 |



8bii

Exact Mass: 482.0986

$[M+Na]^+ = 505.0884$

Mass Spectrum List Report

Analysis Info

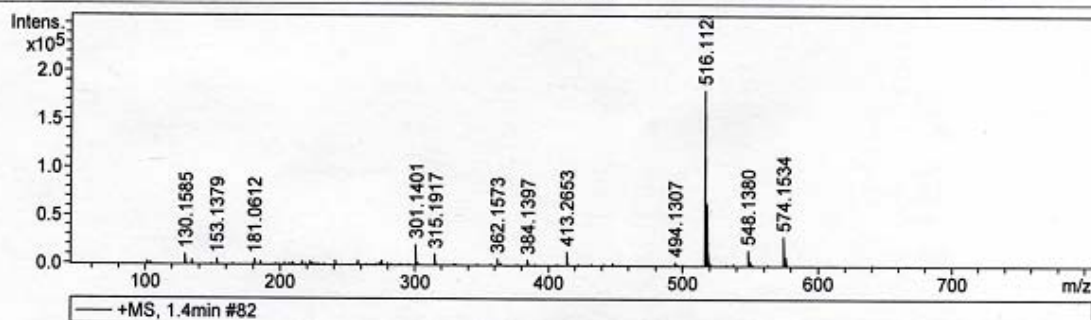
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Method tune_low.m
Sample Name VK-9ai
Comment

Acquisition Date 5/19/2010 11:54:22 AM

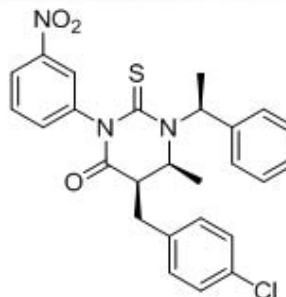
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 130.1585 | 24734 | 110.3 | 10317 | 0.0053 |
| 2 | 153.1379 | 26165 | 61.3 | 5723 | 0.0059 |
| 3 | 181.0612 | 27024 | 59.2 | 5840 | 0.0067 |
| 4 | 301.1401 | 24720 | 158.5 | 21706 | 0.0122 |
| 5 | 315.1917 | 25323 | 82.2 | 11823 | 0.0124 |
| 6 | 362.1573 | 25602 | 65.2 | 6930 | 0.0141 |
| 7 | 384.1397 | 26753 | 64.5 | 6066 | 0.0144 |
| 8 | 413.2653 | 27058 | 150.2 | 14431 | 0.0153 |
| 9 | 494.1307 | 25683 | 52.2 | 4165 | 0.0192 |
| 10 | 516.1128 | 22799 | 1649.4 | 181441 | 0.0226 |
| 11 | 517.1152 | 23992 | 411.0 | 45779 | 0.0216 |
| 12 | 518.1102 | 22577 | 574.6 | 64787 | 0.0229 |
| 13 | 519.1120 | 26827 | 122.7 | 14001 | 0.0194 |
| 14 | 548.1380 | 27407 | 143.4 | 16546 | 0.0200 |
| 15 | 574.1534 | 26547 | 289.4 | 30416 | 0.0216 |



9ai

Exact Mass: 493.1227

$[M+Na]^+ = 516.1125$

Mass Spectrum List Report

Analysis Info

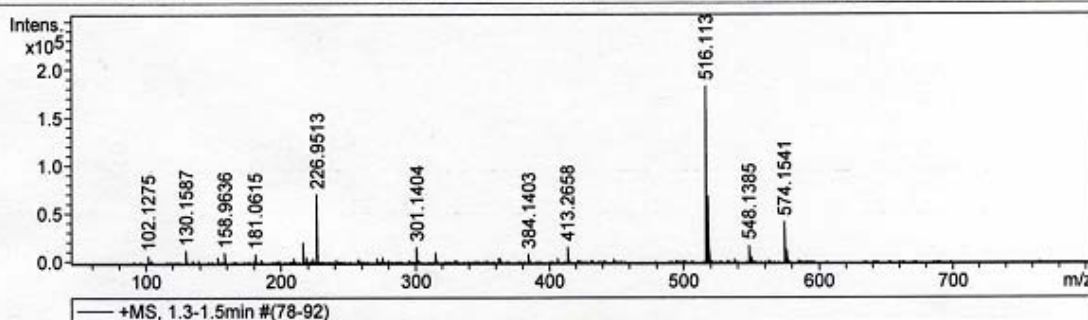
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Method tune_low.m
Sample Name VK-9bi
Comment

Acquisition Date 5/19/2010 12:03:34 PM

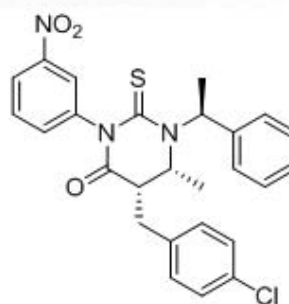
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 102.1275 | 24063 | 5497.7 | 7078 | 0.0042 |
| 2 | 130.1587 | 23754 | 5620.5 | 12128 | 0.0055 |
| 3 | 158.9636 | 20129 | 2849.1 | 10013 | 0.0079 |
| 4 | 181.0615 | 25700 | 1593.9 | 8592 | 0.0070 |
| 5 | 216.9221 | 26310 | 2025.7 | 20739 | 0.0082 |
| 6 | 226.9513 | 20971 | 6521.1 | 70731 | 0.0108 |
| 7 | 301.1404 | 24677 | 1493.1 | 16315 | 0.0122 |
| 8 | 315.1921 | 25074 | 871.3 | 10026 | 0.0126 |
| 9 | 384.1403 | 26183 | 772.1 | 8764 | 0.0147 |
| 10 | 413.2658 | 26580 | 1312.5 | 16368 | 0.0155 |
| 11 | 516.1133 | 22330 | 8770.2 | 182118 | 0.0231 |
| 12 | 517.1157 | 25122 | 2340.1 | 49302 | 0.0206 |
| 13 | 518.1108 | 23687 | 3207.6 | 68556 | 0.0219 |
| 14 | 519.1127 | 26733 | 665.0 | 14417 | 0.0194 |
| 15 | 548.1385 | 26922 | 906.5 | 17618 | 0.0204 |
| 16 | 574.1541 | 26833 | 2914.4 | 41254 | 0.0214 |



9bi

Exact Mass: 493.1227

[M+Na]⁺ = 516.1125

Mass Spectrum List Report

Analysis Info

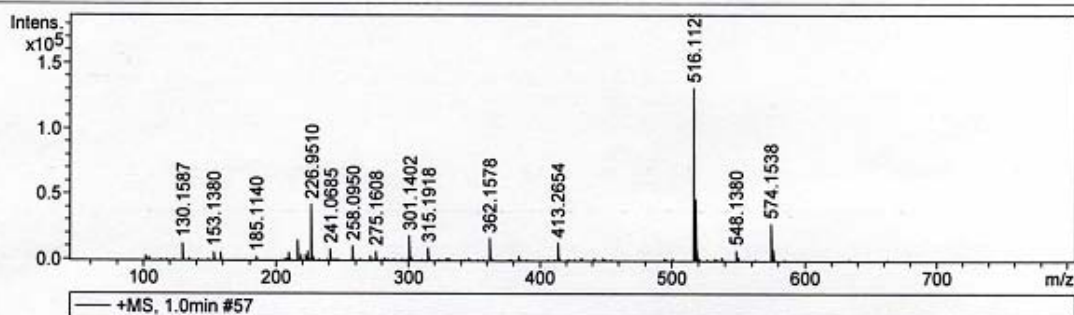
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Method tune_low.m
Sample Name vk-9bii
Comment

Acquisition Date 5/19/2010 12:15:43 PM

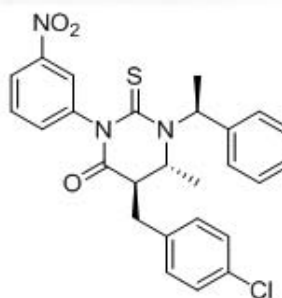
Operator VIKAS GROVER
Instrument / Ser# maXis 40

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 | 800 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |



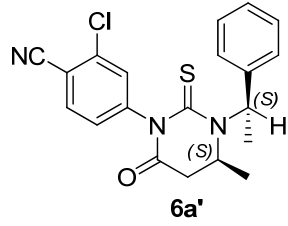
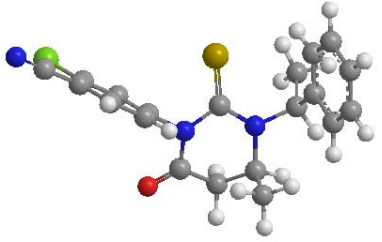
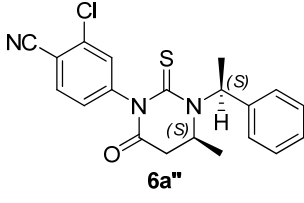
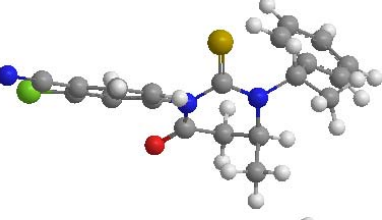
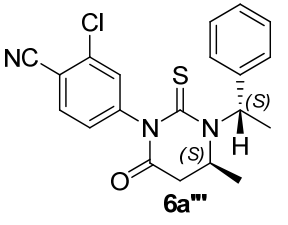
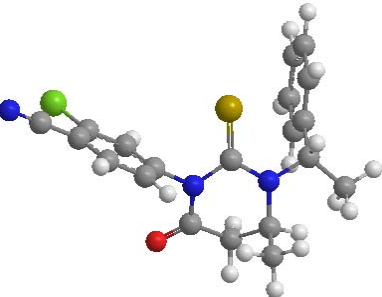
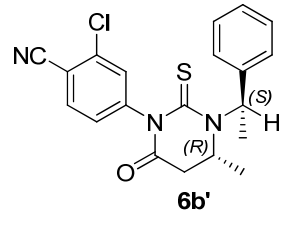
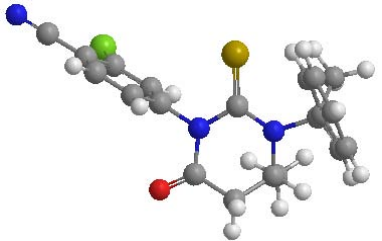
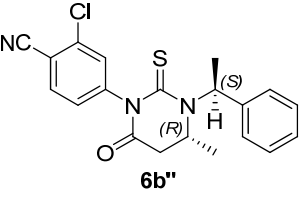
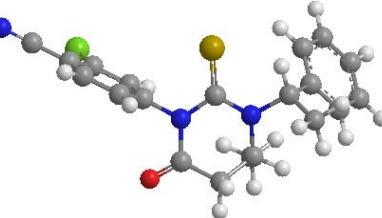
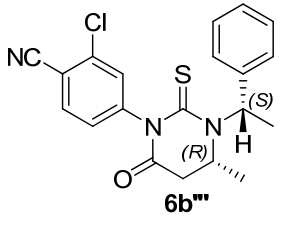
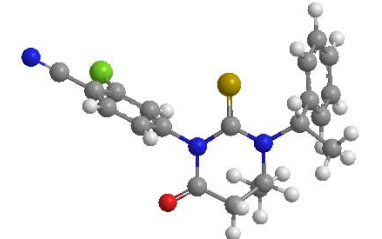
| # | m/z | Res. | S/N | I | FWHM |
|----|----------|-------|--------|--------|--------|
| 1 | 130.1587 | 19565 | 3702.8 | 12985 | 0.0067 |
| 2 | 153.1380 | 20861 | 1410.4 | 6505 | 0.0073 |
| 3 | 158.9634 | 23560 | 1242.7 | 6080 | 0.0067 |
| 4 | 185.1140 | 22473 | 353.7 | 2716 | 0.0082 |
| 5 | 210.1017 | 22286 | 514.6 | 6022 | 0.0094 |
| 6 | 216.9220 | 24040 | 1218.5 | 15599 | 0.0090 |
| 7 | 226.9510 | 23205 | 3058.6 | 42035 | 0.0098 |
| 8 | 241.0685 | 24780 | 634.8 | 8886 | 0.0097 |
| 9 | 258.0950 | 26008 | 774.6 | 11080 | 0.0099 |
| 10 | 275.1608 | 26838 | 486.0 | 7106 | 0.0103 |
| 11 | 301.1402 | 25762 | 1217.3 | 18479 | 0.0117 |
| 12 | 315.1918 | 25033 | 630.7 | 9765 | 0.0126 |
| 13 | 362.1578 | 26300 | 1112.1 | 16847 | 0.0138 |
| 14 | 413.2654 | 25906 | 871.3 | 13610 | 0.0160 |
| 15 | 516.1129 | 22968 | 4478.8 | 131261 | 0.0225 |
| 16 | 517.1155 | 25268 | 1554.5 | 33227 | 0.0205 |
| 17 | 518.1103 | 24109 | 2168.6 | 46836 | 0.0215 |
| 18 | 519.1122 | 26688 | 434.8 | 9488 | 0.0195 |
| 19 | 548.1380 | 27137 | 405.9 | 8097 | 0.0202 |
| 20 | 574.1538 | 26304 | 1791.1 | 28317 | 0.0218 |



9bii

Exact Mass: 493.1227

[M+Na]⁺ = 516.1125

| Entry | Conformation | 3-dimensional representation | Total Energy Kcal/mol |
|-------|---|--|--------------------------|
| 01 |  <p>6a'</p> |  | -90576.3225 |
| 02 |  <p>6a''</p> |  | -90578.7543 |
| 03 |  <p>6a'''</p> |  | -90565.4083 |
| 04 |  <p>6b'</p> |  | -90575.9313 |
| 05 |  <p>6b''</p> |  | -90580.2530 |
| 06 |  <p>6b'''</p> |  | -90577.8479 |