

Electrochemical bottom-up synthesis of Chiral Carbon Dots and their application as Nano-Organocatalysts in a stereoselective Mannich reaction in water

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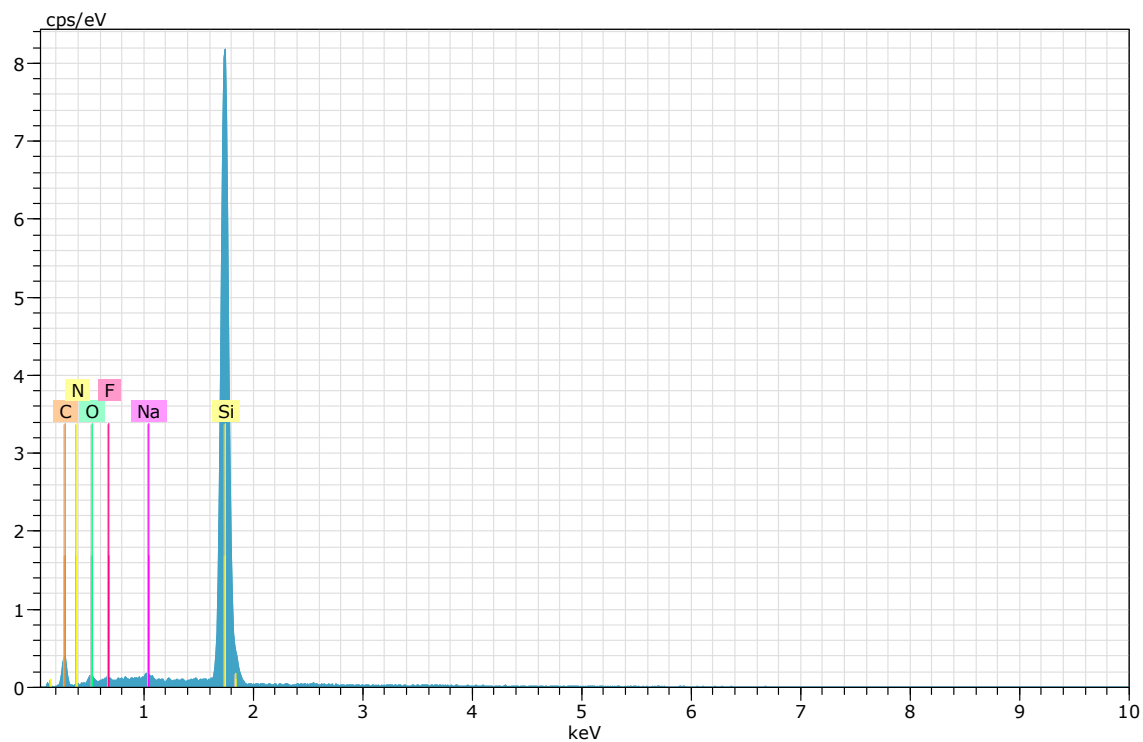
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Energy Dispersive X-ray (EDX) analysis

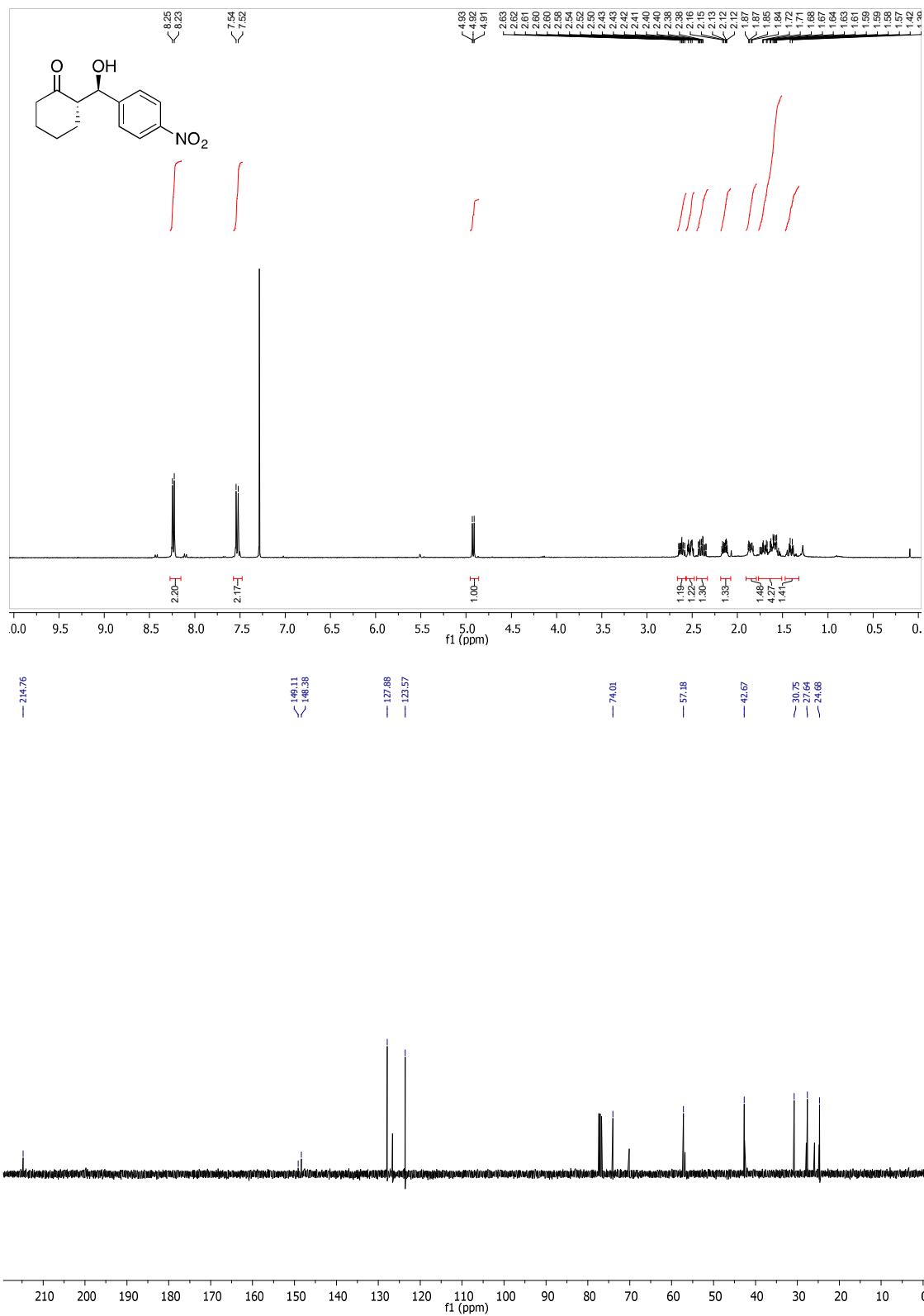


Spectrum: CD101_ 3

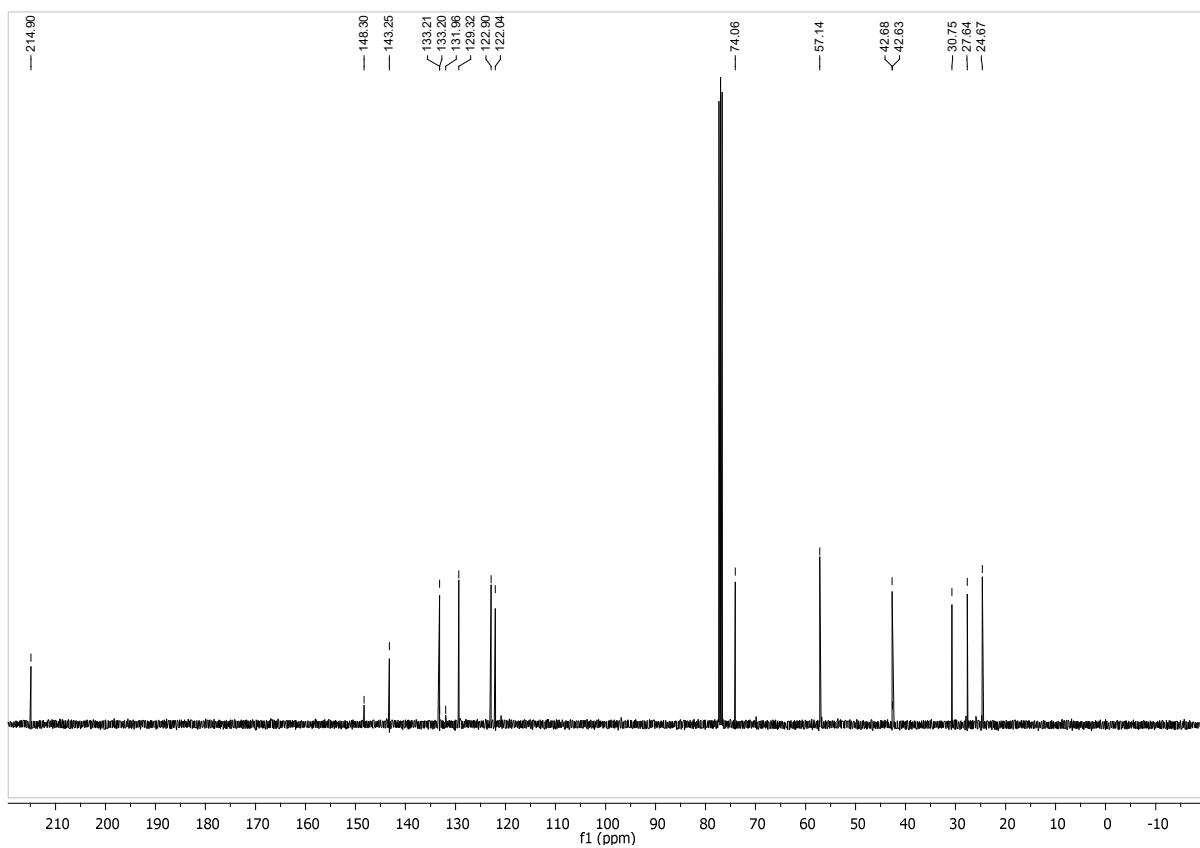
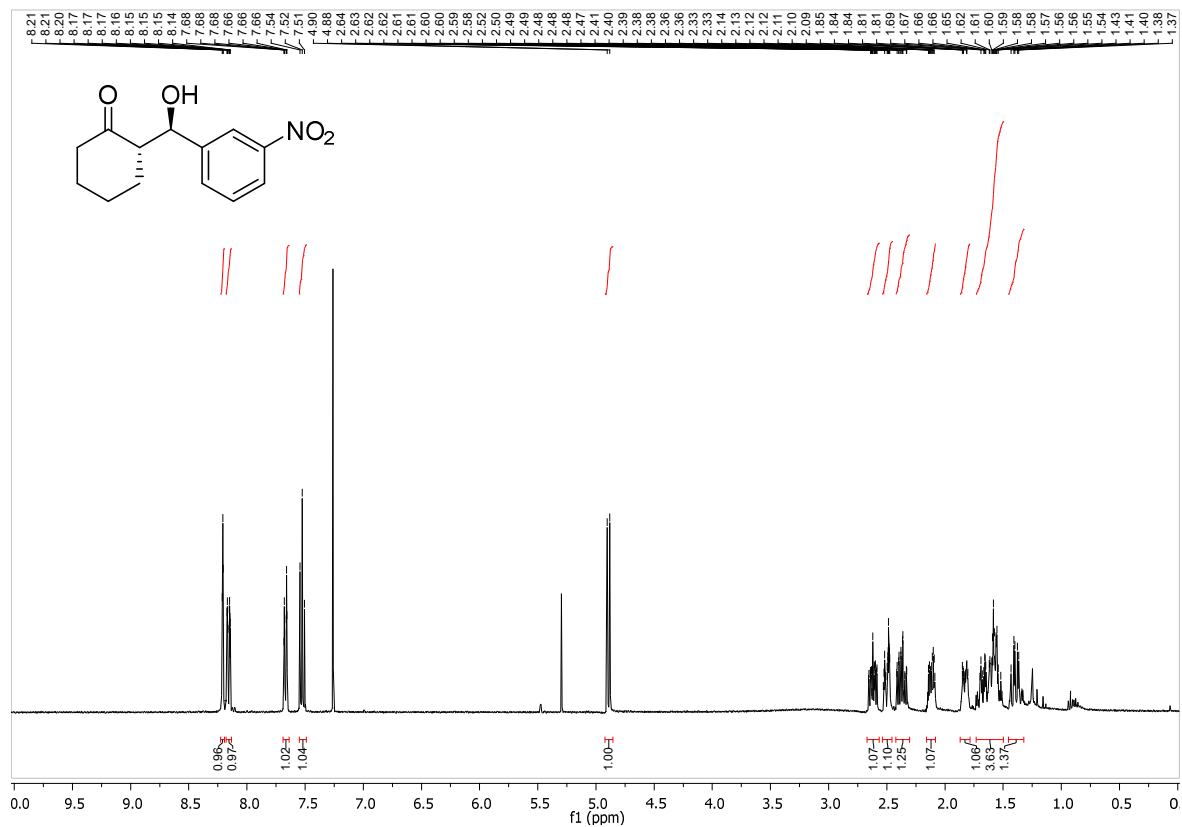
| Element | Series | unn. C [wt.%] | norm. C [wt.%] | Atom. C [at.%] | Error (1 Sigma) [wt.%] |
|----------|----------|------------------|-------------------|-------------------|---------------------------|
| Silicon | K-series | 0.00 | 0.00 | 0.00 | 0.00 |
| Carbon | K-series | 1.11 | 45.01 | 54.37 | 0.30 |
| Oxygen | K-series | 0.68 | 27.38 | 24.83 | 0.24 |
| Fluorine | K-series | 0.31 | 12.52 | 9.56 | 0.15 |
| Sodium | K-series | 0.27 | 10.89 | 6.87 | 0.05 |
| Nitrogen | K-series | 0.10 | 4.21 | 4.36 | 0.12 |
| Total: | | 2.47 | 100.00 | 100.00 | |

NMR SPECTRA

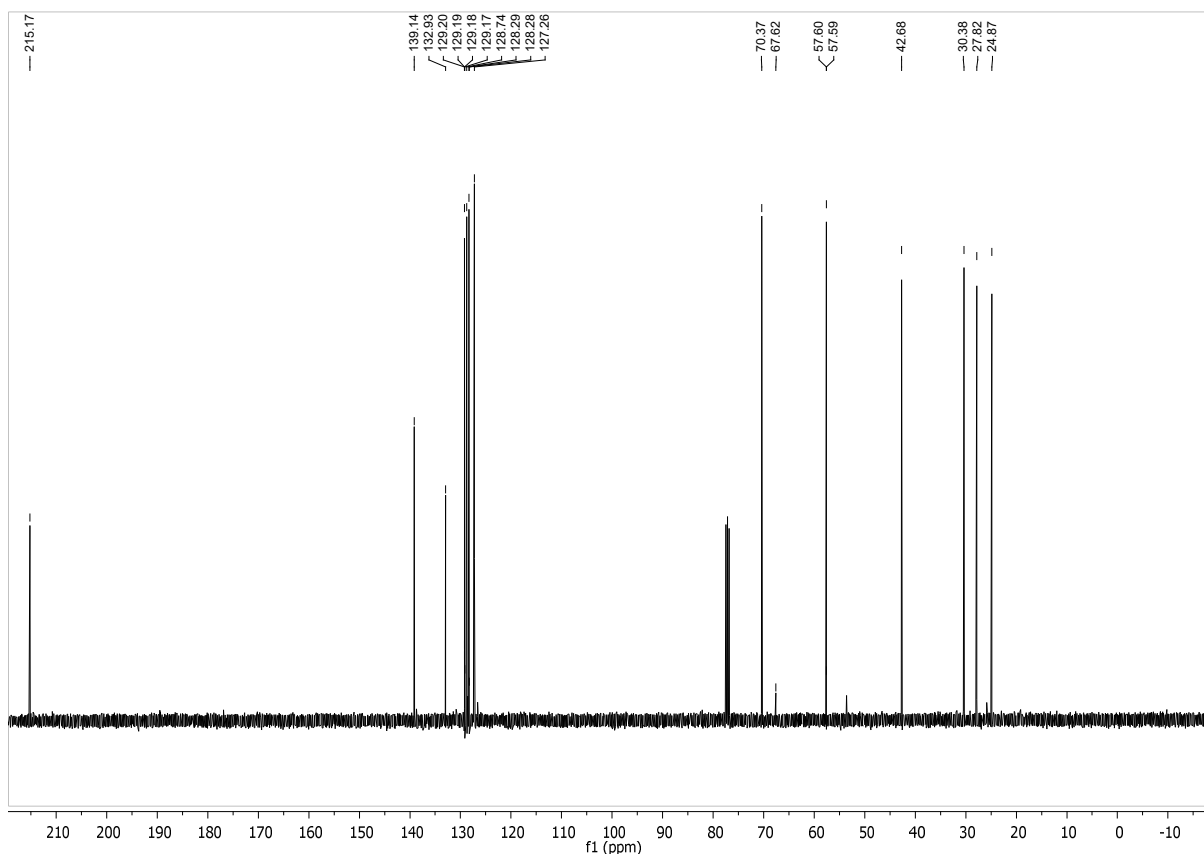
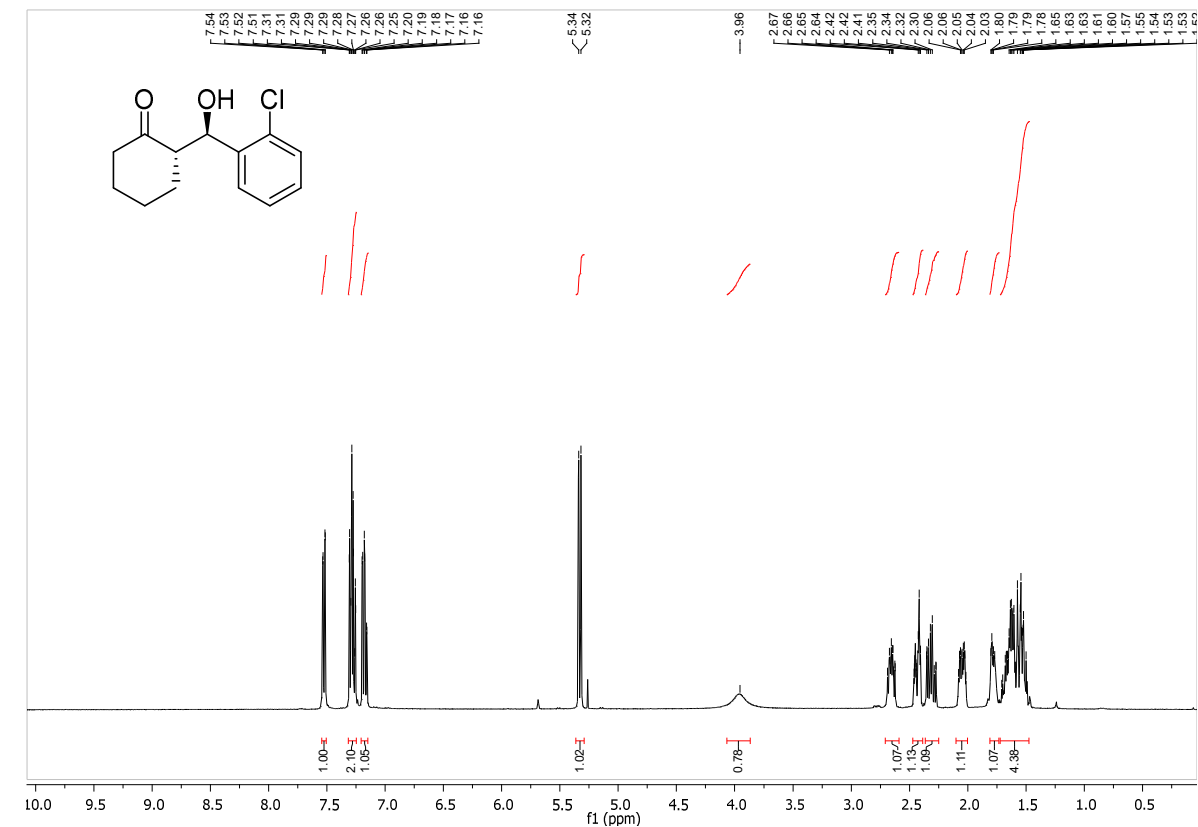
(S)-2-((R)-hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one (3a)



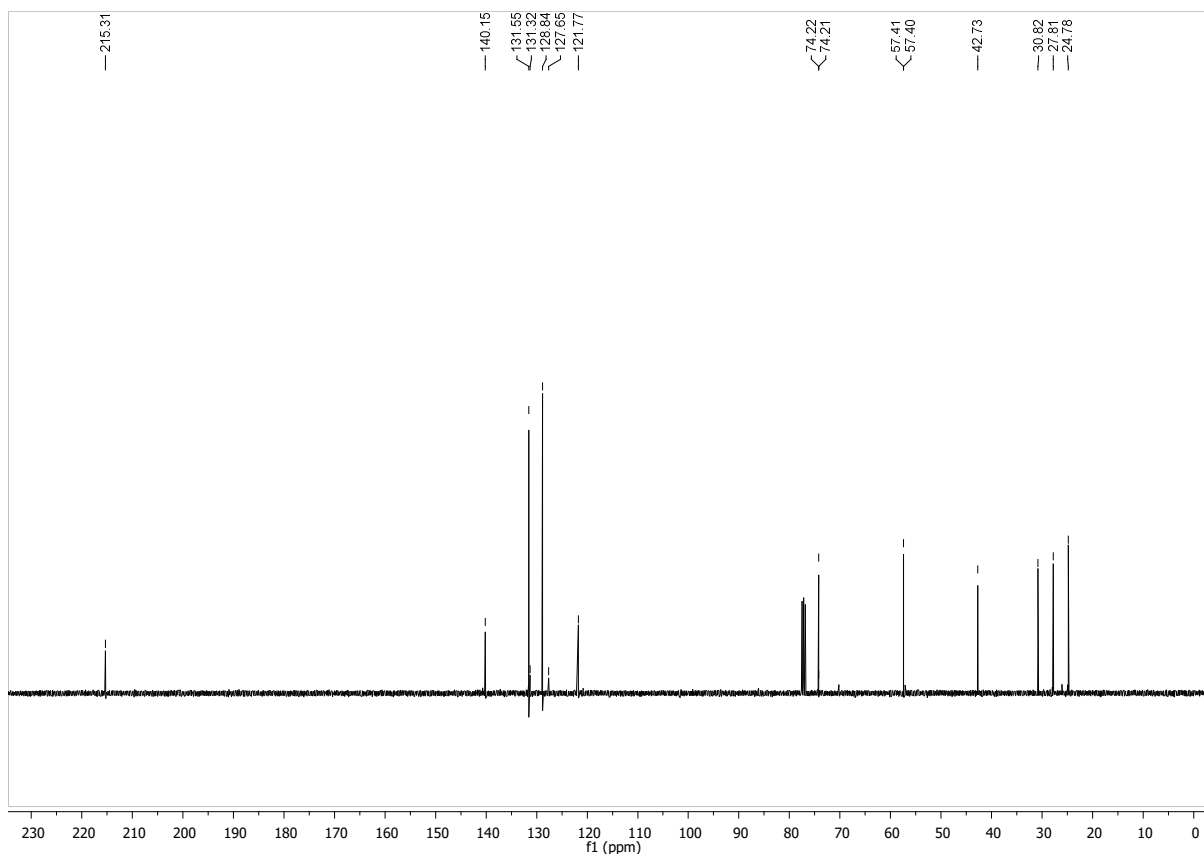
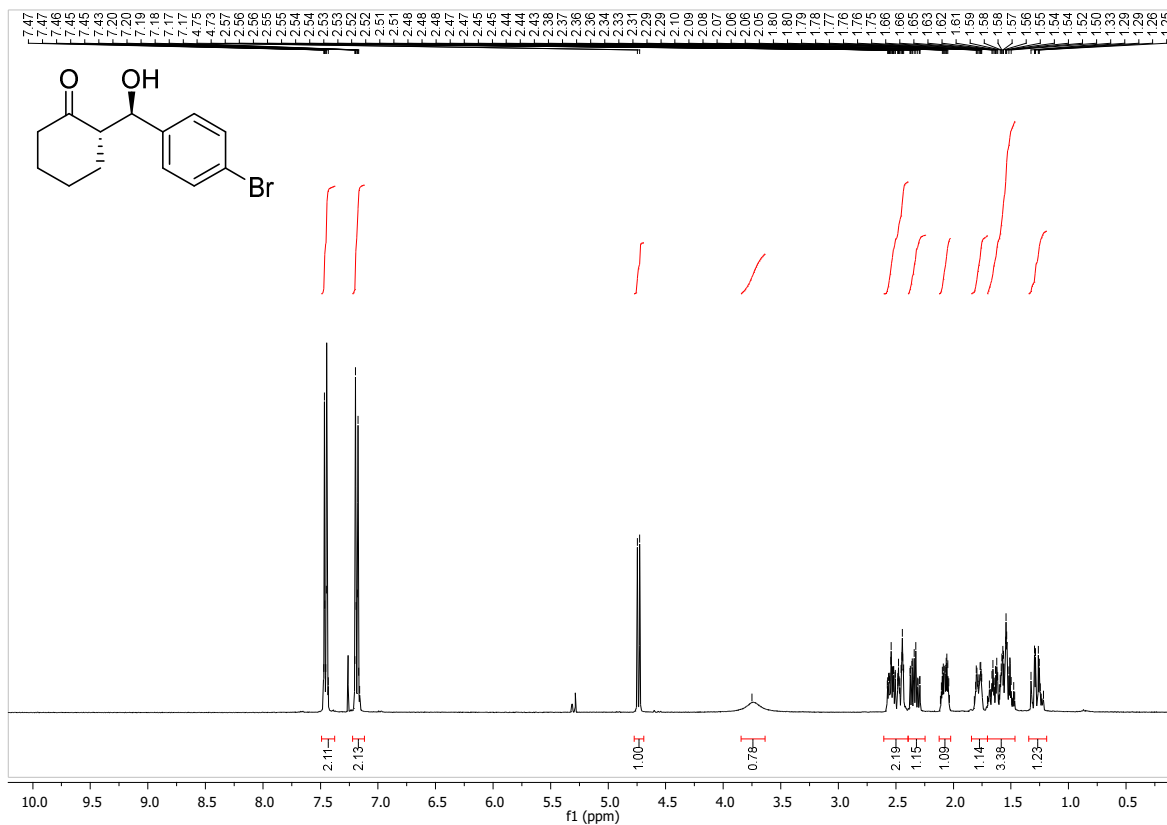
***(S)*-2-((*R*)-hydroxy(3-nitrophenyl)methyl)cyclohexan-1-one (3b)**



(S)-2-((R)-(2-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one (3c)



(S)-2-((R)-(4-bromophenyl)(hydroxy)methyl)cyclohexan-1-one (3d)

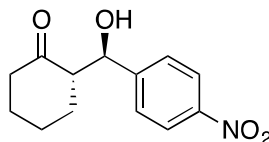


HPLC DATA

(S)-2-((*R*)-hydroxy(4-nitrophenyl)methyl)cyclohexan-1-one (*X*)



Analysis Report

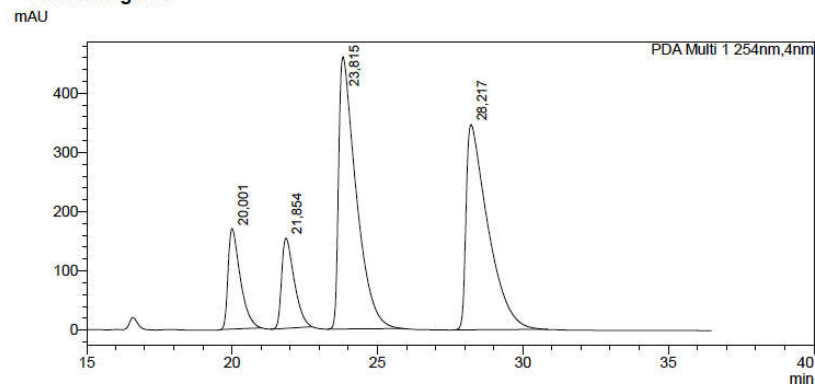


<Sample Information>

Sample Name : CD65
Sample ID : CD65
Data Filename : CD65.lcd
Method Filename : H-PrOH_95-5_1mlmin.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 1 uL
Date Acquired : 17/03/2022 17:09:44
Date Processed : 17/03/2022 17:58:10

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

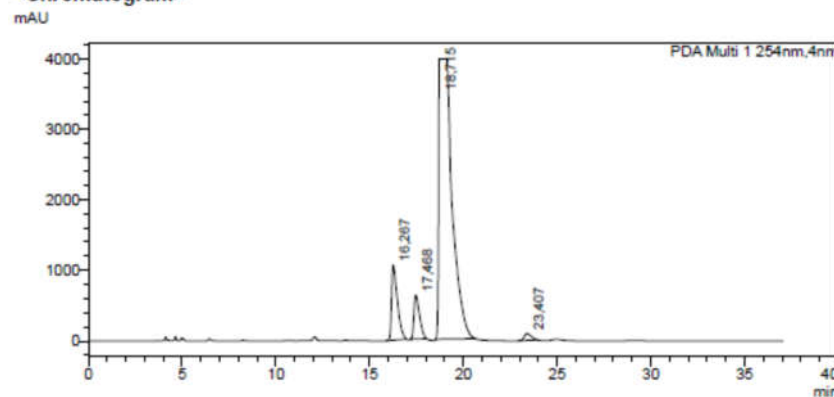
| Peak# | Ret. Time | Area | Height | Area% |
|-------|-----------|----------|---------|---------|
| 1 | 20.001 | 4950415 | 169548 | 10.548 |
| 2 | 21.854 | 4598570 | 152293 | 9.799 |
| 3 | 23.815 | 19254976 | 459733 | 41.029 |
| 4 | 28.217 | 18126578 | 346597 | 38.624 |
| Total | | 46930538 | 1128171 | 100.000 |

<Sample Information>

Sample Name : CD 103
Sample ID : CD 103
Data Filename : CD 103.lcd
Method Filename : Hex_iPro_95_5.lcm
Batch Filename :
Vial # : 1-1
Injection Volume : 1 uL
Date Acquired : 30/06/2022 14:51:05
Date Processed : 01/07/2022 13:31:13

Sample Type : Unknown
Acquired by : System Administrator
Processed by : System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

| Peak# | Ret. Time | Area | Height | Area% |
|-------|-----------|-----------|---------|---------|
| 1 | 16.267 | 22864421 | 1059916 | 9.767 |
| 2 | 17.468 | 12910651 | 622412 | 5.515 |
| 3 | 18.715 | 195899067 | 3975108 | 83.680 |
| 4 | 23.407 | 2430270 | 94067 | 1.038 |
| Total | | 234104409 | 5751503 | 100.000 |

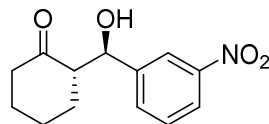
(S)-2-((R)-hydroxy(3-nitrophenyl)methyl)cyclohexan-1-one (3b)

<Sample Information>

Sample Name : CD 113 con C4D6 0,5
 Sample ID : CD 113 con C4D6 0,5
 Data Filename : CD 113 con C4D6 0,5.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 20/07/2022 13:17:02
 Date Processed : 20/07/2022 17:47:50

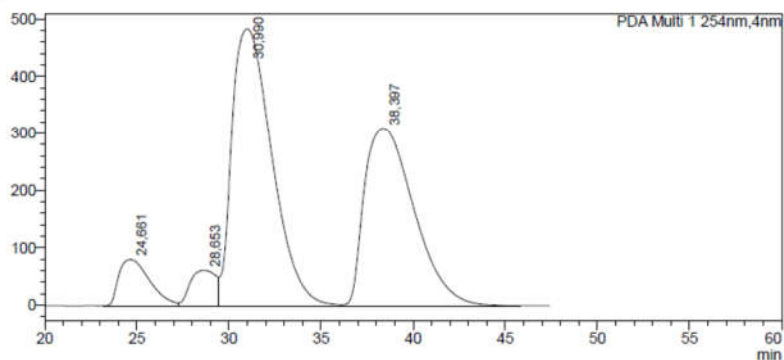
Sample Type : Unknown

Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>

mAU



<Peak Table>

| PDA Ch1 254nm | | | | |
|---------------|-----------|-----------|--------|---------|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 24.661 | 9396329 | 80658 | 6.413 |
| 2 | 28.653 | 5950630 | 61819 | 4.061 |
| 3 | 30.990 | 73076041 | 483790 | 49.874 |
| 4 | 38.397 | 58097332 | 309518 | 39.651 |
| Total | | 146520332 | 935785 | 100,000 |

<Sample Information>

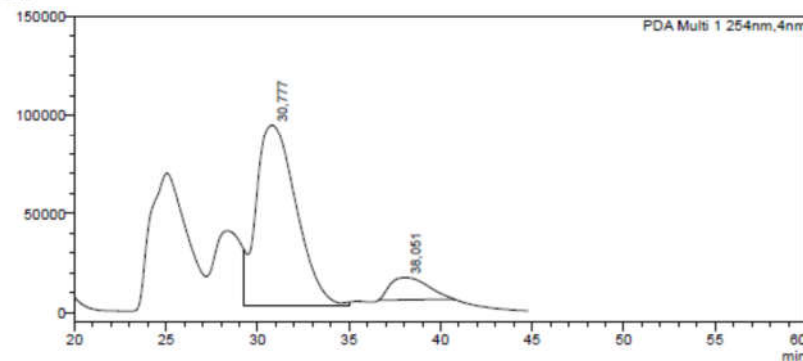
Sample Name : CD 112 0,5 p2
 Sample ID : CD 112 0,5 p2
 Data Filename : CD 112 chiral 0,5 p2.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 20/07/2022 15:12:14
 Date Processed : 20/07/2022 15:57:06

Sample Type : Unknown

Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>

uAU



<Peak Table>

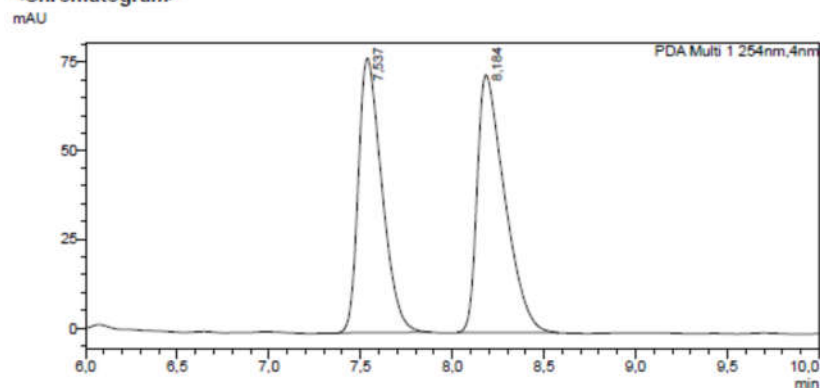
| PDA Ch1 254nm | | | |
|---------------|-----------|----------|--------|
| Peak# | Ret. Time | Area | Height |
| 1 | 30.777 | 14003083 | 91706 |
| 2 | 38.051 | 1630231 | 11252 |
| Total | | 15633313 | 102958 |

(S)-2-((R)-(2-chlorophenyl)(hydroxy)methyl)cyclohexan-1-one (3c)

<Sample Information>

Sample Name : CD115
 Sample ID : CD115
 Data Filename : CD115.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 18/07/2022 15:04:15
 Date Processed : 18/07/2022 15:40:59
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



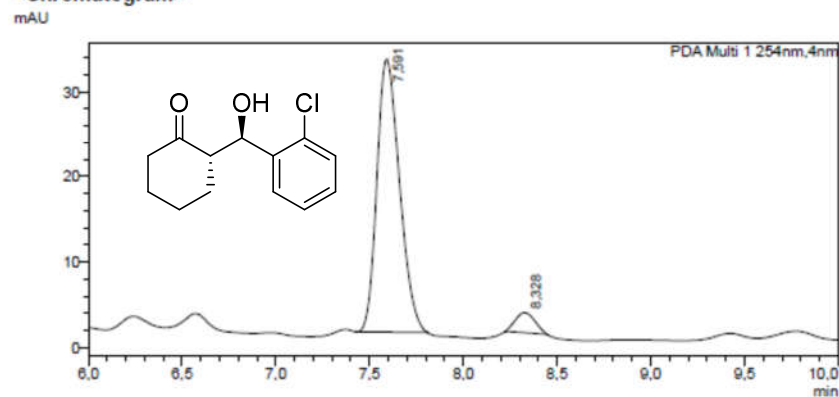
<Peak Table>

| PDA Ch1 254nm | | | | |
|---------------|-----------|---------|--------|---------|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 7.537 | 692475 | 77270 | 47.779 |
| 2 | 8.184 | 756865 | 72722 | 52.221 |
| Total | | 1449339 | 149992 | 100.000 |

<Sample Information>

Sample Name : CD114
 Sample ID : CD114
 Data Filename : CD114.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 18/07/2022 15:22:09
 Date Processed : 18/07/2022 15:39:00
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

| PDA Ch1 254nm | | | | |
|---------------|-----------|--------|--------|---------|
| Peak# | Ret. Time | Area | Height | Area% |
| 1 | 7.591 | 268441 | 32012 | 94.017 |
| 2 | 8.328 | 17083 | 2350 | 5.983 |
| Total | | 285523 | 34362 | 100.000 |

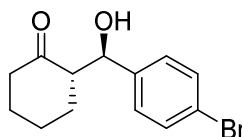
(S)-2-((R)-(4-bromophenyl)(hydroxy)methyl)cyclohexan-1-one (3d)

<Sample Information>

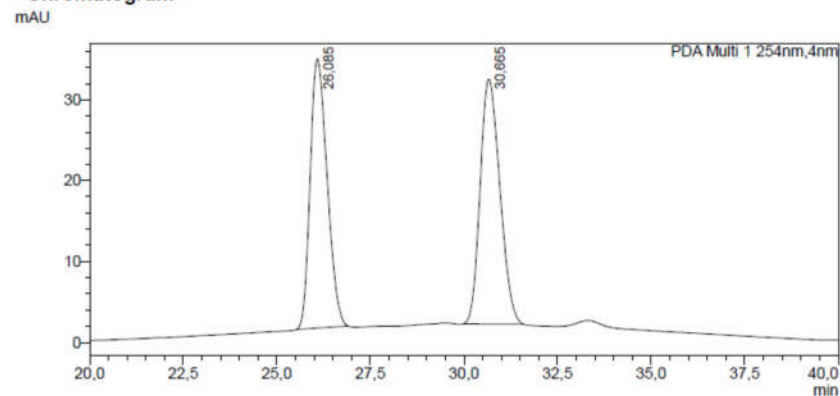
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 Sample ID : CD 120COL
 Data Filename : CD 120COL.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 25/07/2022 13:23:58
 Date Processed : 25/07/2022 15:11:34

Sample Type : Unknown

Acquired by : System Administrator
 Processed by : System Administrator



<Chromatogram>



<Peak Table>

| Peak# | Ret. Time | Area | Height | Area% |
|-------|-----------|---------|--------|---------|
| 1 | 26.085 | 1046305 | 33285 | 48.548 |
| 2 | 30.665 | 1108904 | 30281 | 51.452 |
| Total | | 2155209 | 63566 | 100.000 |

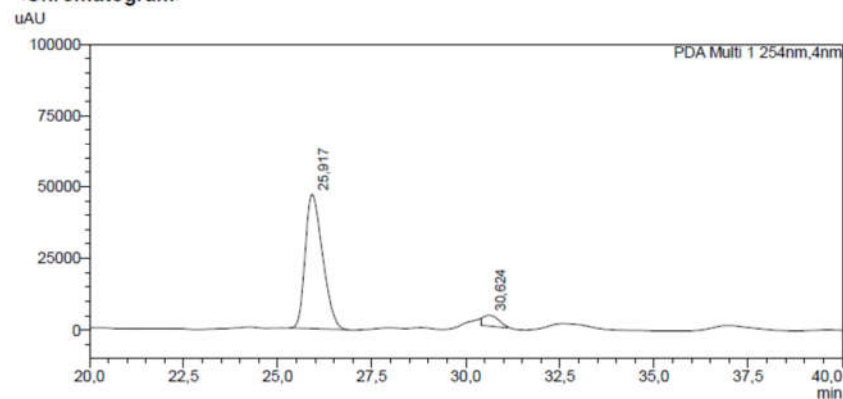
<Sample Information>

Sample Name : CD 119EST chir
 Sample ID : CD 119EST chir
 Data Filename : CD 119EST chir.lcd
 Method Filename : Hex_iPro_95_5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 25/07/2022 14:06:54
 Date Processed : 25/07/2022 15:15:26

Sample Type : Unknown

Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

| Peak# | Ret. Time | Area | Height | Area% |
|-------|-----------|---------|--------|---------|
| 1 | 25.917 | 1504360 | 46681 | 93.324 |
| 2 | 30.624 | 107616 | 3777 | 6.676 |
| Total | | 1611976 | 50458 | 100.000 |