

Qualitative Analysis Report

Data Filename HF_Cu_II_1-Iso_8Aug22.d

Sample Type Sample

Instrument Name QTOF

Acq Method Test_DL_Pos.m

IRM Calibration Status Success

Comment Reran complexation reaction under N2 and anhydrous MeCN. Random paptide column present

Sample Name HF_C1_Cu_II_1-Iso

Position P1-A2

User Name

Acquired Time 8/8/2022 10:23:11 AM (UTC-04:00)

DA Method Default.m

Sample Group

Stream Name LC 1

Info.

Acquisition Time 8/8/2022 10:23:11 AM (UTC-04:00)

QTOF Driver Version 10.01.00

Acquisition SW 6200 series TOF/6500 series

Version Q-TOF 10.1 (48.0)

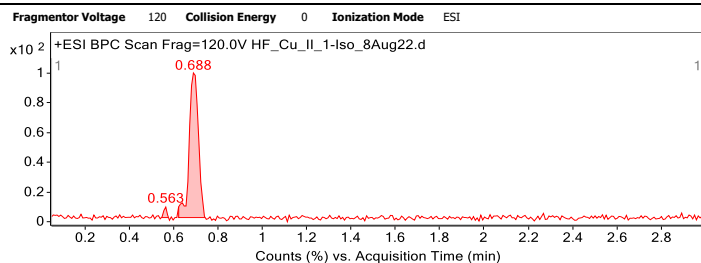
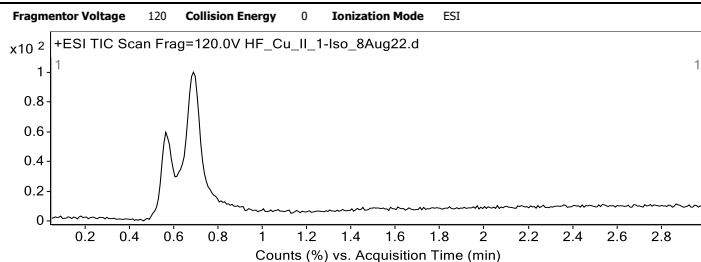
QTOF Firmware 25.809

Version

Tune Mass Range 3200

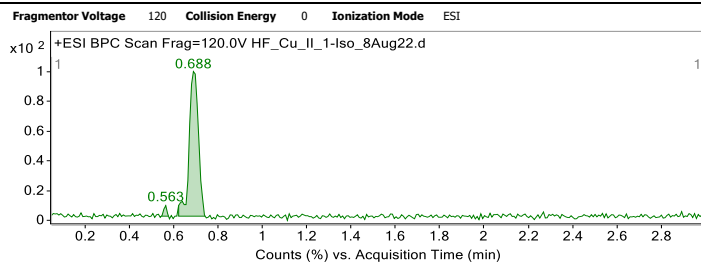
Max.

Chromatograms



Integration Peak List

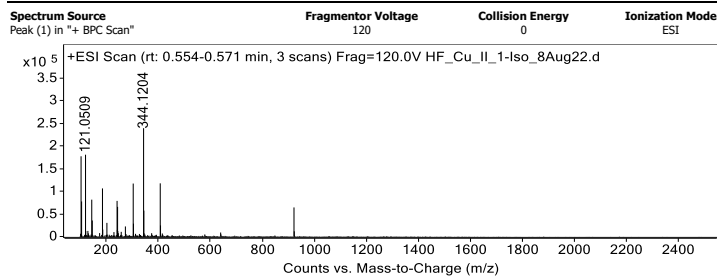
| Peak | Start | RT | End | Height | Area | Area % |
|------|-------|-------|-------|------------|------------|--------|
| 1 | 0.543 | 0.563 | 0.575 | 79998.37 | 73459.5 | 2.29 |
| 2 | 0.621 | 0.688 | 0.741 | 1098595.34 | 3206549.35 | 100 |



Integration Peak List

| Peak | Start | RT | End | Height | Area | Area % |
|------|-------|-------|-------|------------|------------|--------|
| 1 | 0.543 | 0.563 | 0.575 | 79998.37 | 73459.5 | 2.29 |
| 2 | 0.621 | 0.688 | 0.741 | 1098595.34 | 3206549.35 | 100 |

Spectra

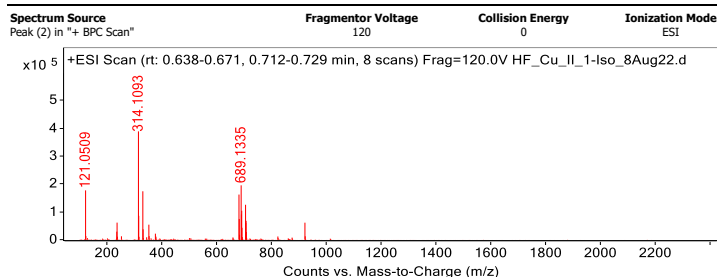


Peak List

| m/z | Abund |
|----------|-----------|
| 103.9555 | 177048.58 |
| 121.0509 | 180539.55 |
| 304.3004 | 116870.93 |
| 344.1204 | 239050.98 |

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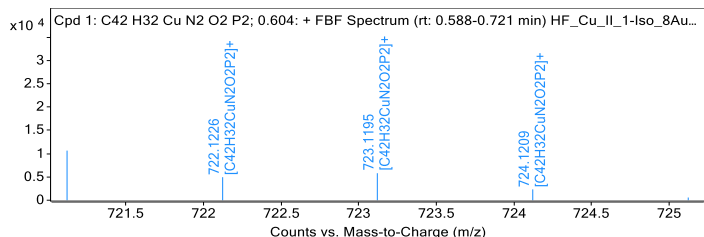
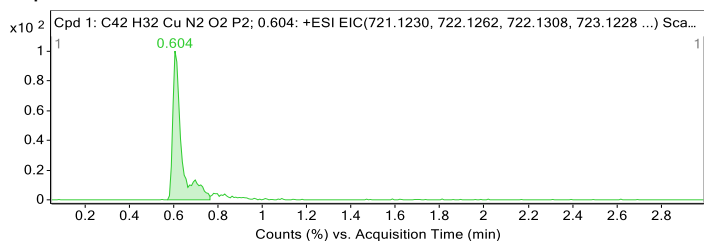
408.1186 117325.46



Peak List

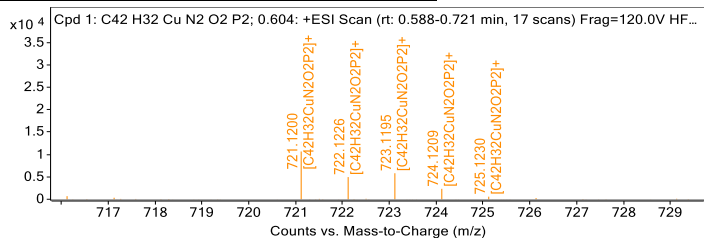
| m/z | Abund |
|----------|-----------|
| 121.0509 | 176772.59 |
| 314.1093 | 388526.25 |
| 330.1047 | 173564.81 |
| 681.1838 | 161776.61 |
| 689.1335 | 194891.42 |

Compounds



Peak List

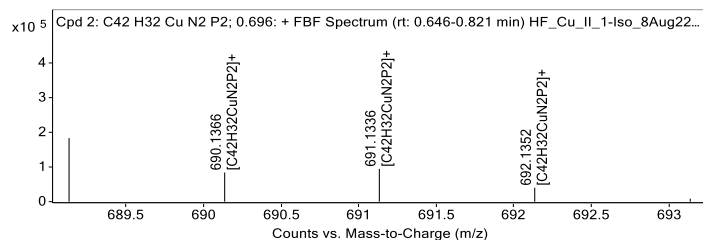
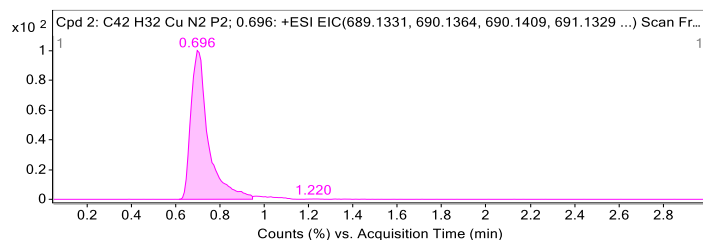
| m/z | z | Abund | Formula | Ion |
|----------|---|----------|----------------|-----|
| 721.12 | 1 | 10653.05 | C42H32CuN2O2P2 | M+ |
| 722.1226 | 1 | 4945.74 | C42H32CuN2O2P2 | M+ |
| 723.1195 | 1 | 5801.48 | C42H32CuN2O2P2 | M+ |
| 724.1209 | 1 | 2328.66 | C42H32CuN2O2P2 | M+ |
| 725.123 | 1 | 576.25 | C42H32CuN2O2P2 | M+ |



Peak List

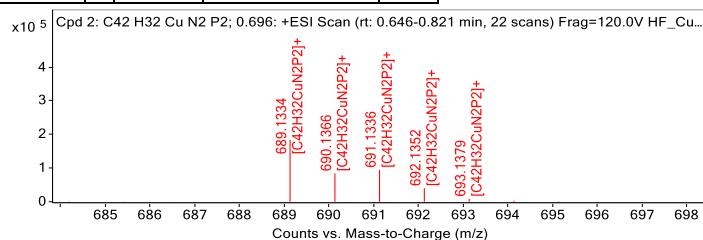
| m/z | z | Abund | Formula | Ion |
|----------|---|----------|----------------|-----|
| 721.12 | 1 | 10653.05 | C42H32CuN2O2P2 | M+ |
| 722.1226 | 1 | 4945.74 | C42H32CuN2O2P2 | M+ |
| 723.1195 | 1 | 5801.48 | C42H32CuN2O2P2 | M+ |
| 724.1209 | 1 | 2328.66 | C42H32CuN2O2P2 | M+ |
| 725.123 | 1 | 576.25 | C42H32CuN2O2P2 | M+ |

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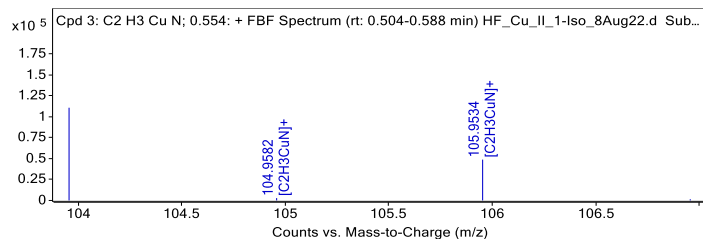
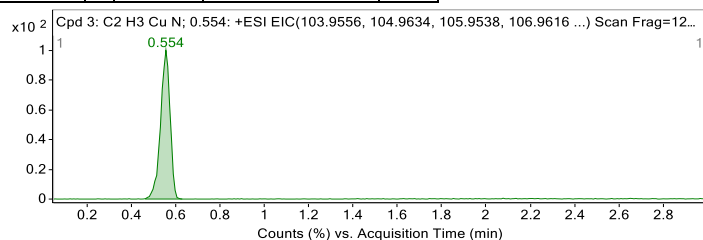
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|--------------|-----|
| 689.1334 | 1 | 183604.22 | C42H32CuN2P2 | M+ |
| 690.1366 | 1 | 84206.49 | C42H32CuN2P2 | M+ |
| 691.1336 | 1 | 94749.55 | C42H32CuN2P2 | M+ |
| 692.1352 | 1 | 40236.19 | C42H32CuN2P2 | M+ |
| 693.1379 | 1 | 8752.54 | C42H32CuN2P2 | M+ |



Peak List

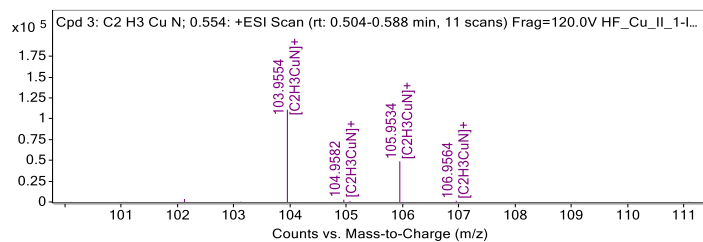
| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|--------------|-----|
| 689.1334 | 1 | 183604.22 | C42H32CuN2P2 | M+ |
| 690.1366 | 1 | 84206.49 | C42H32CuN2P2 | M+ |
| 691.1336 | 1 | 94749.55 | C42H32CuN2P2 | M+ |
| 692.1352 | 1 | 40236.19 | C42H32CuN2P2 | M+ |
| 693.1379 | 1 | 8752.54 | C42H32CuN2P2 | M+ |



Peak List

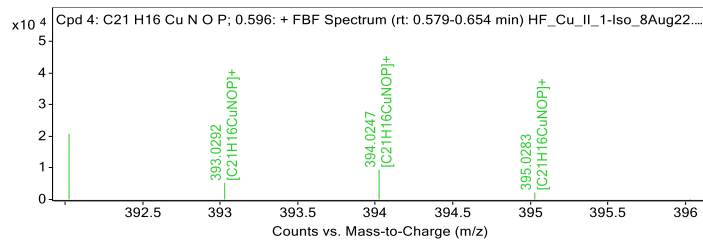
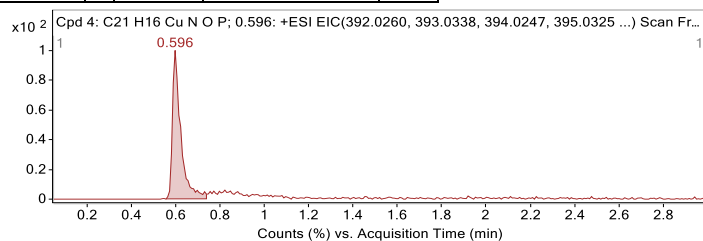
| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|---------|-----|
| 103.9554 | 1 | 110845.55 | C2H3CuN | M+ |
| 104.9582 | 1 | 2810.8 | C2H3CuN | M+ |
| 105.9534 | 1 | 48822.1 | C2H3CuN | M+ |
| 106.9564 | 1 | 1454.22 | C2H3CuN | M+ |

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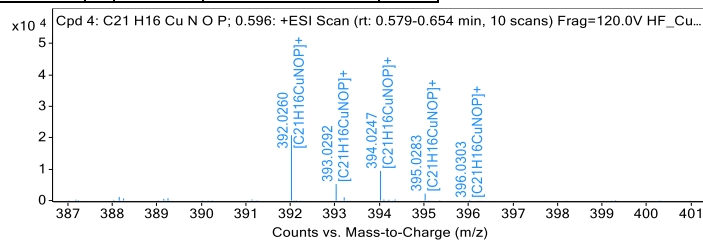
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|-----------------------------------|-----|
| 103.9554 | 1 | 110845.55 | C ₂ H ₃ CuN | M+ |
| 104.9582 | 1 | 2810.8 | C ₂ H ₃ CuN | M+ |
| 105.9534 | 1 | 48822.1 | C ₂ H ₃ CuN | M+ |
| 106.9564 | 1 | 1454.22 | C ₂ H ₃ CuN | M+ |



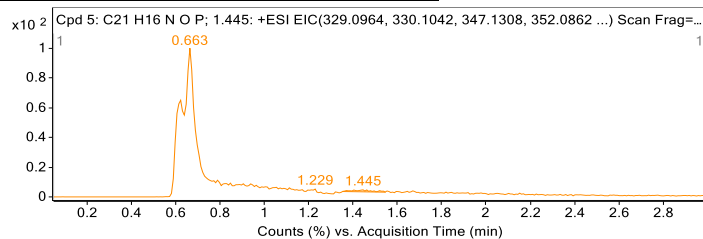
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|---------------------------------------|-----|
| 392.026 | 1 | 20782.75 | C ₂₁ H ₁₆ CuNOP | M+ |
| 393.0292 | 1 | 5235.91 | C ₂₁ H ₁₆ CuNOP | M+ |
| 394.0247 | 1 | 9411.81 | C ₂₁ H ₁₆ CuNOP | M+ |
| 395.0283 | 1 | 2218.18 | C ₂₁ H ₁₆ CuNOP | M+ |
| 396.0303 | 1 | 205.37 | C ₂₁ H ₁₆ CuNOP | M+ |

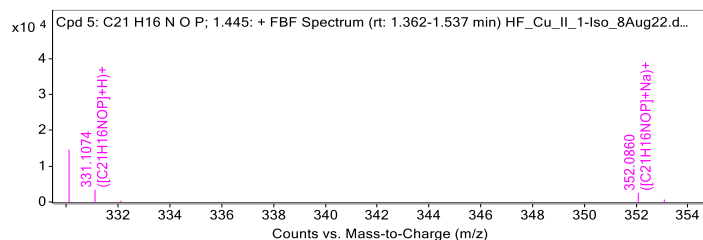


Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|---------------------------------------|-----|
| 392.026 | 1 | 20782.75 | C ₂₁ H ₁₆ CuNOP | M+ |
| 393.0292 | 1 | 5235.91 | C ₂₁ H ₁₆ CuNOP | M+ |
| 394.0247 | 1 | 9411.81 | C ₂₁ H ₁₆ CuNOP | M+ |
| 395.0283 | 1 | 2218.18 | C ₂₁ H ₁₆ CuNOP | M+ |
| 396.0303 | 1 | 205.37 | C ₂₁ H ₁₆ CuNOP | M+ |

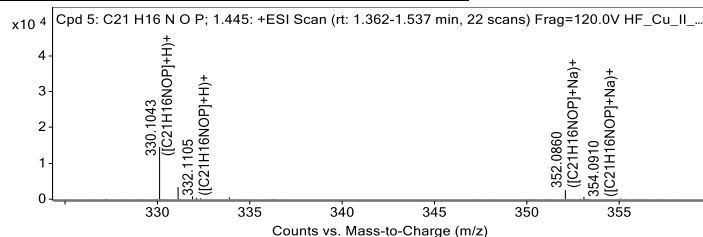


Qualitative Analysis Report



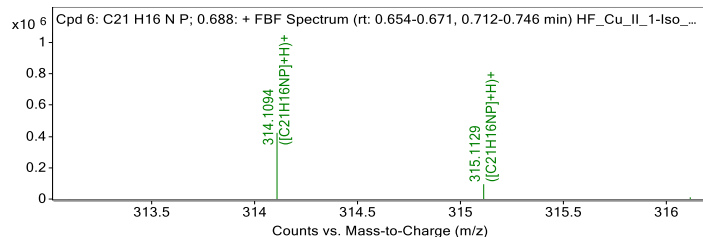
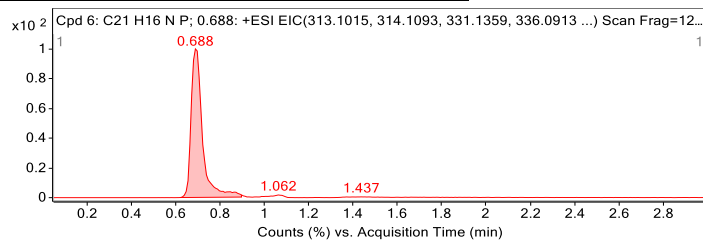
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|-------------------------------------|---------|
| 330.1043 | 1 | 14552.77 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 331.1074 | 1 | 3401.55 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 332.1105 | 1 | 383.51 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 352.086 | 1 | 2529.69 | C ₂₁ H ₁₆ NOP | (M+Na)+ |
| 353.0893 | 1 | 669.03 | C ₂₁ H ₁₆ NOP | (M+Na)+ |
| 354.091 | 1 | 32.84 | C ₂₁ H ₁₆ NOP | (M+Na)+ |



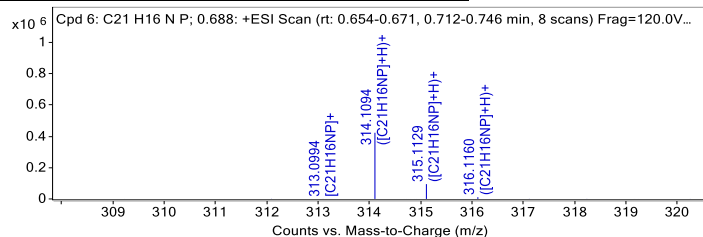
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|-------------------------------------|---------|
| 330.1043 | 1 | 14552.77 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 331.1074 | 1 | 3401.55 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 332.1105 | 1 | 383.51 | C ₂₁ H ₁₆ NOP | (M+H)+ |
| 352.086 | 1 | 2529.69 | C ₂₁ H ₁₆ NOP | (M+Na)+ |
| 353.0893 | 1 | 669.03 | C ₂₁ H ₁₆ NOP | (M+Na)+ |
| 354.091 | 1 | 32.84 | C ₂₁ H ₁₆ NOP | (M+Na)+ |



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|------------------------------------|--------|
| 313.0994 | 1 | 371.44 | C ₂₁ H ₁₆ NP | M+ |
| 314.1094 | 1 | 422514.84 | C ₂₁ H ₁₆ NP | (M+H)+ |
| 315.1129 | 1 | 94561.46 | C ₂₁ H ₁₆ NP | (M+H)+ |
| 316.116 | 1 | 11095.66 | C ₂₁ H ₁₆ NP | (M+H)+ |

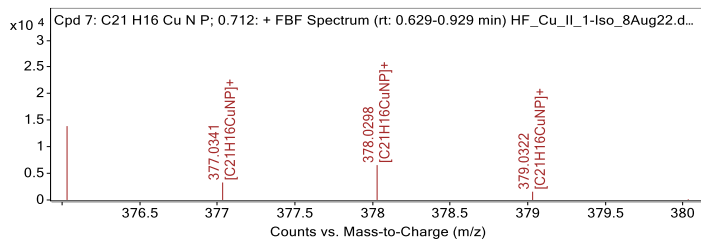
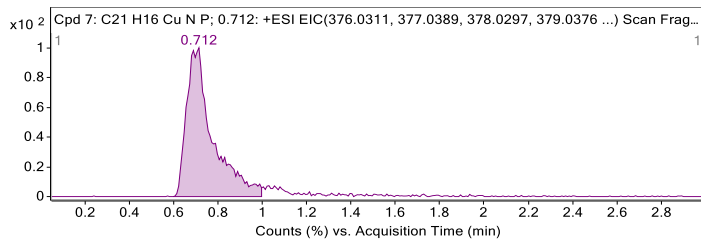


Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|--------|------------------------------------|-----|
| 313.0994 | 1 | 371.44 | C ₂₁ H ₁₆ NP | M+ |

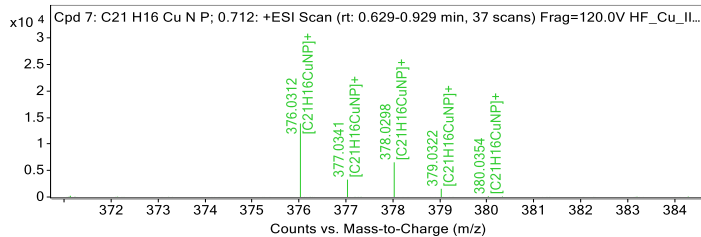
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| | | | | |
|----------|---|-----------|----------|--------|
| 314.1094 | 1 | 422514.84 | C21H16NP | (M+H)+ |
| 315.1129 | 1 | 94561.46 | C21H16NP | (M+H)+ |
| 316.116 | 1 | 11095.66 | C21H16NP | (M+H)+ |



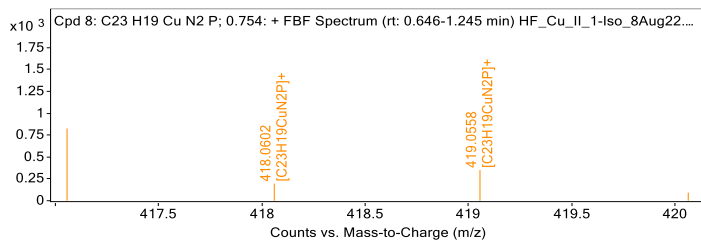
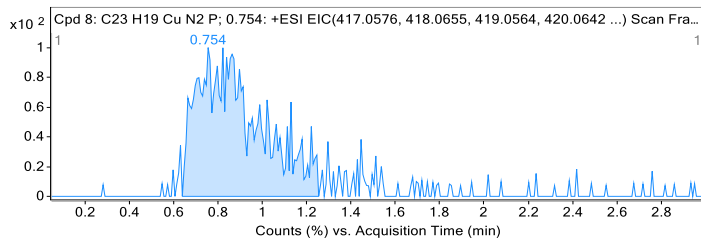
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|-----|
| 376.0312 | 1 | 13888.54 | C21H16CuNP | M+ |
| 377.0341 | 1 | 3287.75 | C21H16CuNP | M+ |
| 378.0298 | 1 | 6554.68 | C21H16CuNP | M+ |
| 379.0322 | 1 | 1553.48 | C21H16CuNP | M+ |
| 380.0354 | 1 | 131.16 | C21H16CuNP | M+ |



Peak List

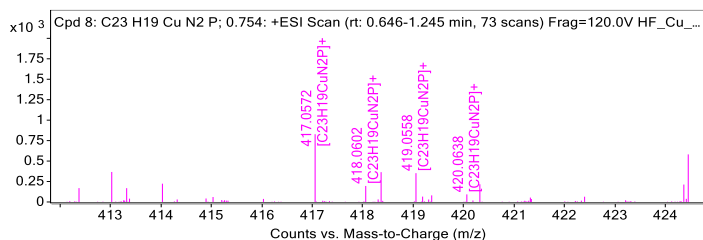
| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|-----|
| 376.0312 | 1 | 13888.54 | C21H16CuNP | M+ |
| 377.0341 | 1 | 3287.75 | C21H16CuNP | M+ |
| 378.0298 | 1 | 6554.68 | C21H16CuNP | M+ |
| 379.0322 | 1 | 1553.48 | C21H16CuNP | M+ |
| 380.0354 | 1 | 131.16 | C21H16CuNP | M+ |



Peak List

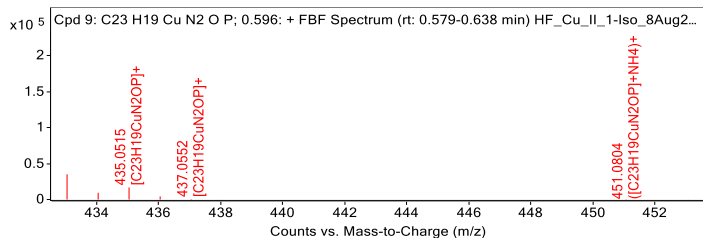
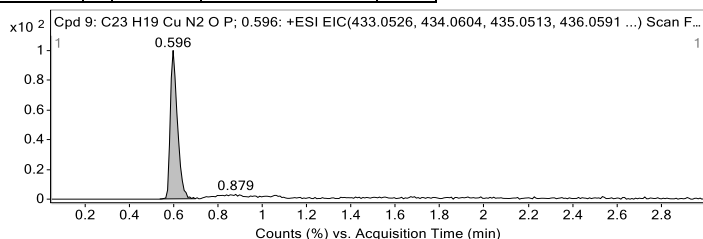
| m/z | z | Abund | Formula | Ion |
|----------|---|--------|-------------|-----|
| 417.0572 | 1 | 826.13 | C23H19CuN2P | M+ |
| 418.0602 | 1 | 195.35 | C23H19CuN2P | M+ |
| 419.0558 | 1 | 351.24 | C23H19CuN2P | M+ |
| 420.0638 | 1 | 92.44 | C23H19CuN2P | M+ |

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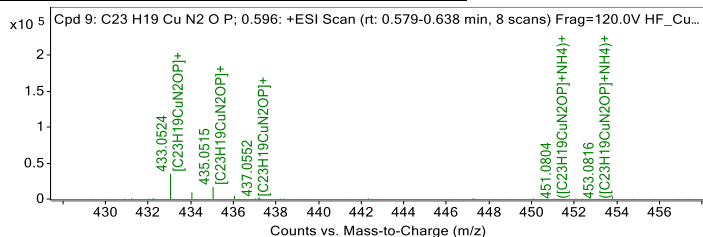
Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|--------|-------------|-----|
| 417.0572 | 1 | 826.13 | C23H19CuN2P | M+ |
| 418.0602 | 1 | 195.35 | C23H19CuN2P | M+ |
| 419.0558 | 1 | 351.24 | C23H19CuN2P | M+ |
| 420.0638 | 1 | 92.44 | C23H19CuN2P | M+ |



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|--------------|----------|
| 433.0524 | 1 | 35121.56 | C23H19CuN2OP | M+ |
| 434.0555 | 1 | 9407.71 | C23H19CuN2OP | M+ |
| 435.0515 | 1 | 16823.3 | C23H19CuN2OP | M+ |
| 436.0543 | 1 | 4334.02 | C23H19CuN2OP | M+ |
| 437.0552 | 1 | 621.03 | C23H19CuN2OP | M+ |
| 438.0638 | 1 | 29.55 | C23H19CuN2OP | M+ |
| 451.0804 | 1 | 438.8 | C23H19CuN2OP | (M+NH4)+ |
| 453.0816 | 1 | 99.05 | C23H19CuN2OP | (M+NH4)+ |



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|--------------|----------|
| 433.0524 | 1 | 35121.56 | C23H19CuN2OP | M+ |
| 434.0555 | 1 | 9407.71 | C23H19CuN2OP | M+ |
| 435.0515 | 1 | 16823.3 | C23H19CuN2OP | M+ |
| 436.0543 | 1 | 4334.02 | C23H19CuN2OP | M+ |
| 437.0552 | 1 | 621.03 | C23H19CuN2OP | M+ |
| 438.0638 | 1 | 29.55 | C23H19CuN2OP | M+ |
| 451.0804 | 1 | 438.8 | C23H19CuN2OP | (M+NH4)+ |
| 453.0816 | 1 | 99.05 | C23H19CuN2OP | (M+NH4)+ |

--- End Of Report ---