

Supporting Information

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Chemical Composition and Anthelmintic Activity of the Peruvian Endemic Species *Chuquiraga weberbaueri* “Amaro” on Sheep Fasciolosis

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181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 12 (1.589)

1: ScanWave MS ES-
6.56e7

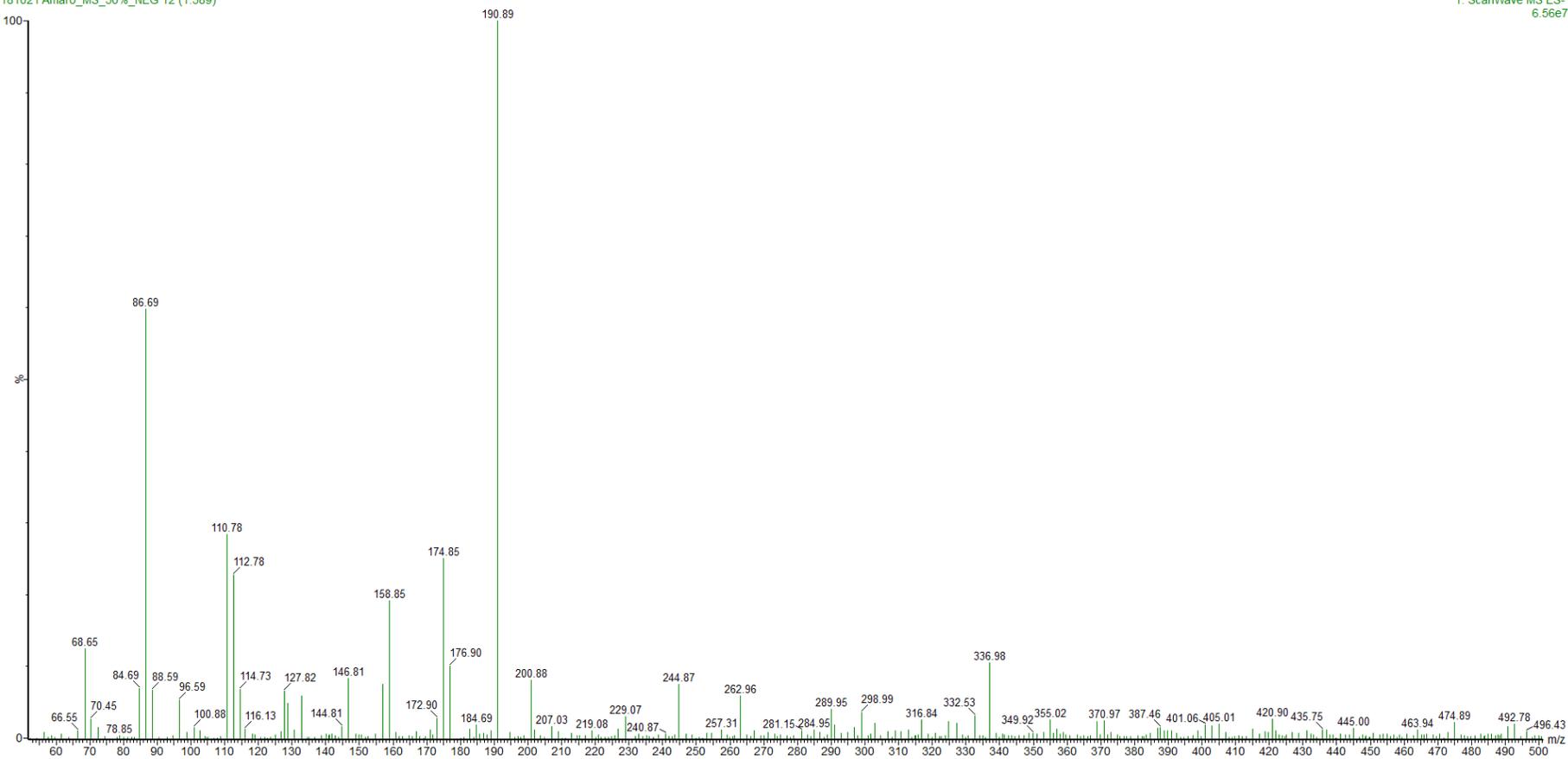


Figure S1: MS-ESI(-) of Substance 1

181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50%_NEG 34 (1.601)

2: Auto Daughters 190.89ES-
5.52e5



Figure S2: MS/MS-ESI(-) of Substance 1

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 18 (1.907)

1: ScanWave MS ES-
3.83e7

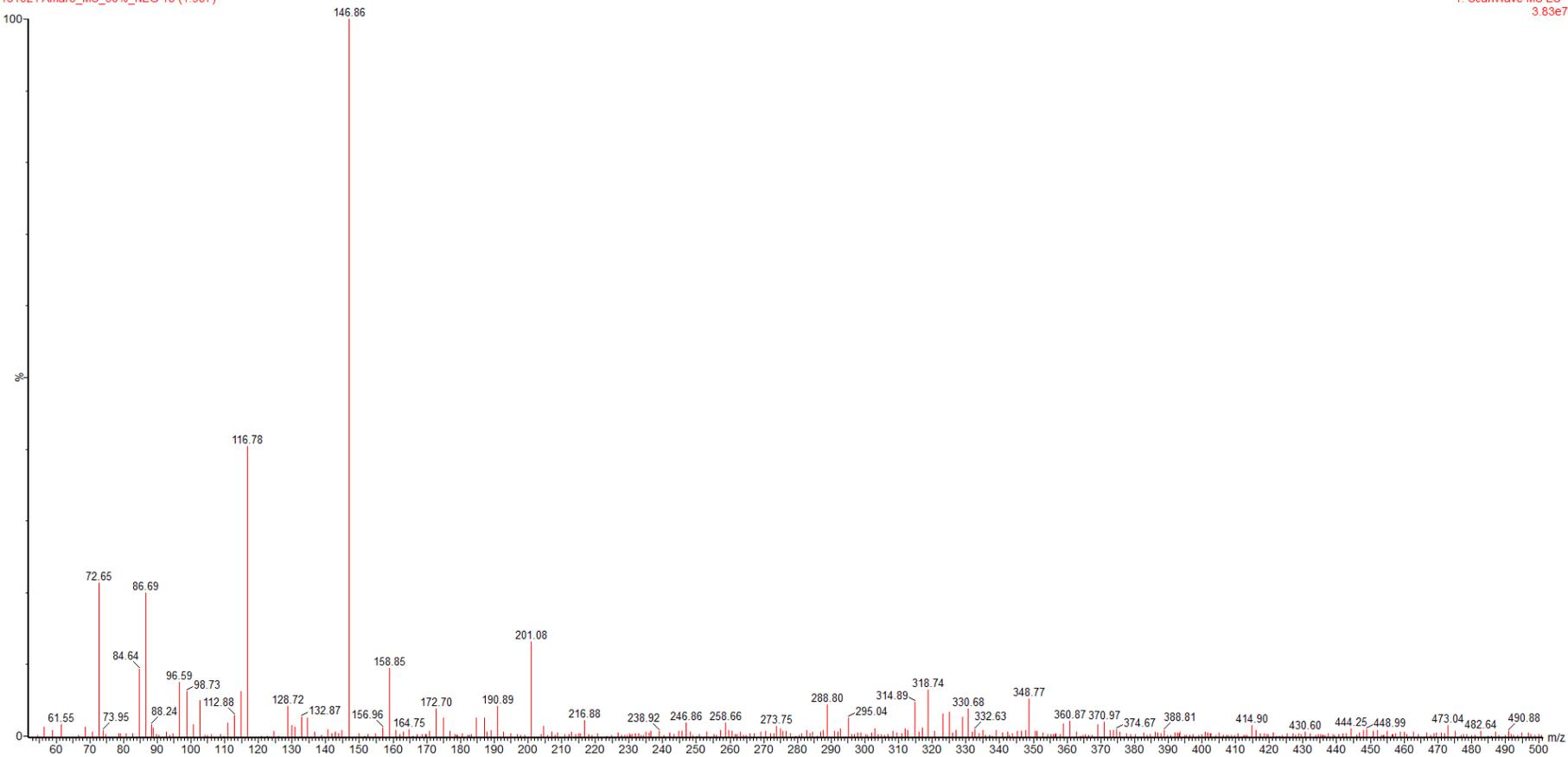


Figure S3: MS-ESI(-) of Substance 2

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 51 (1.895)

2: Auto Daughters 146.79ES-
5.08e5



Figure S4: MS/MS-ESI(-) of Substance 2

181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50%_NEG 23 (2.172)

1: ScanWave MS ES-
1.97e7

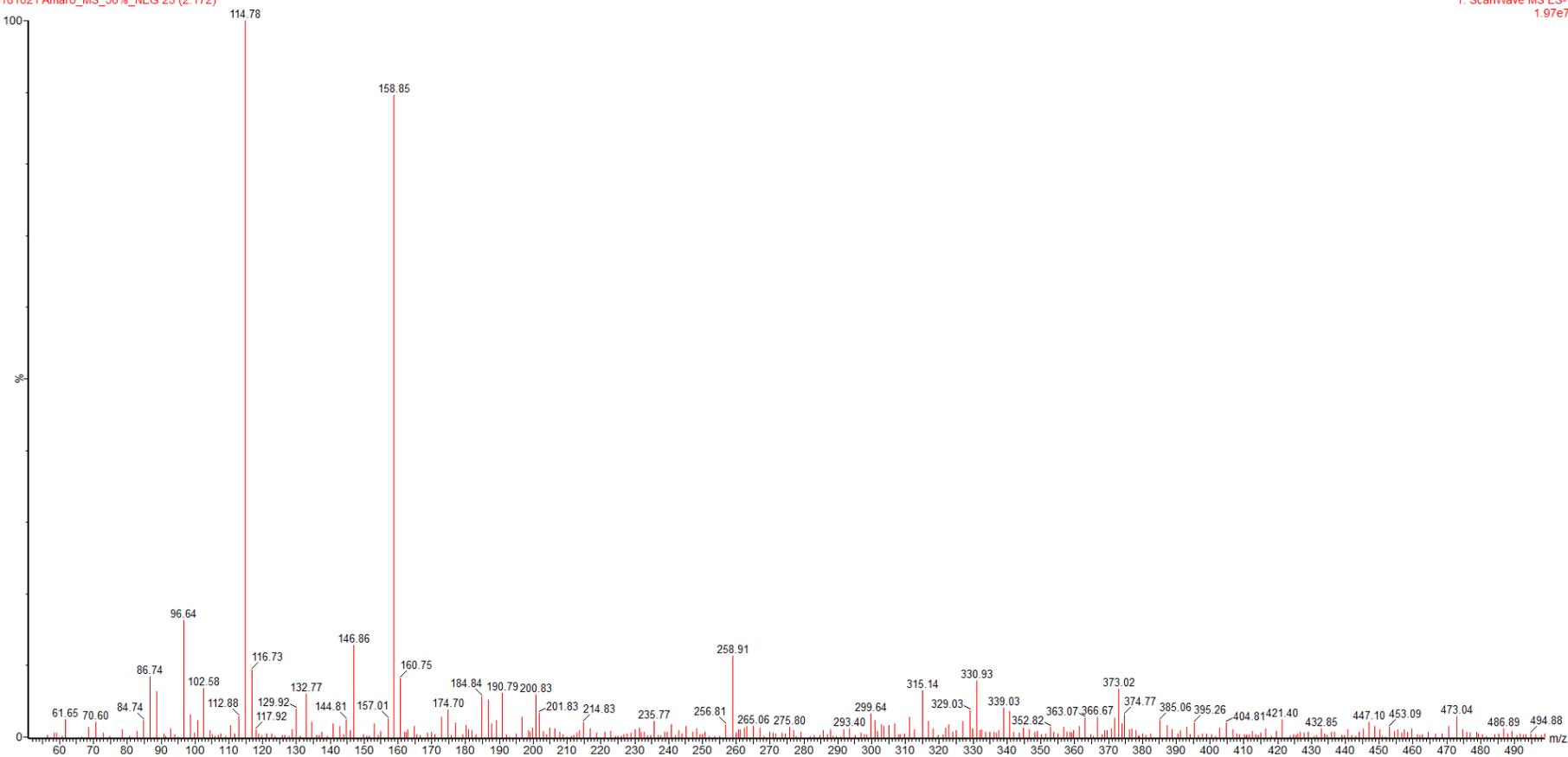


Figure S5: MS-ESI(-) of Substance 3

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181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50%_NEG 88 (5.615)

1: ScanWave MS ES-
6.19e7

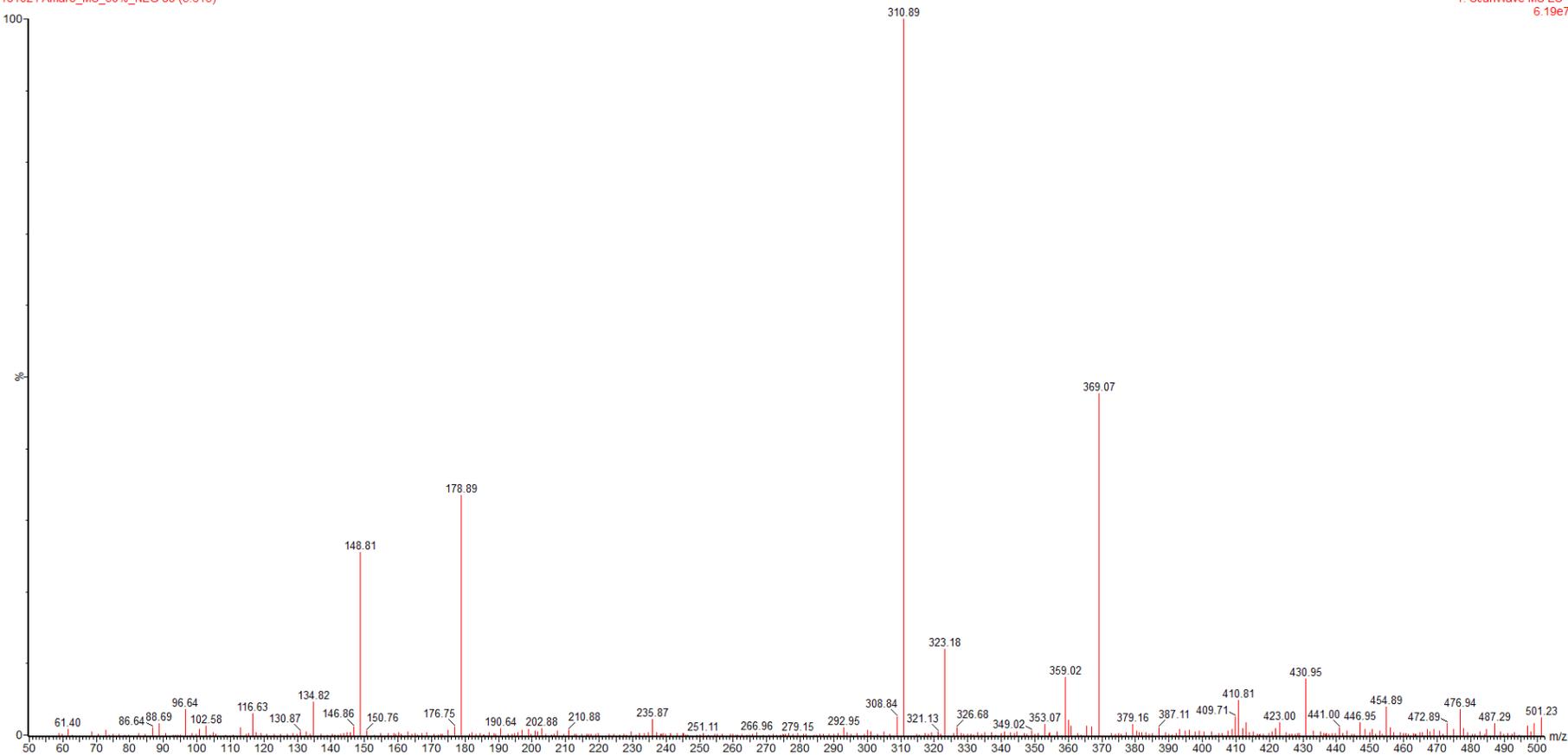


Figure S6: MS-ESI(-) of Substance 4

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 263 (5.641)

2: Auto Daughters 310.89ES-
9.00e6

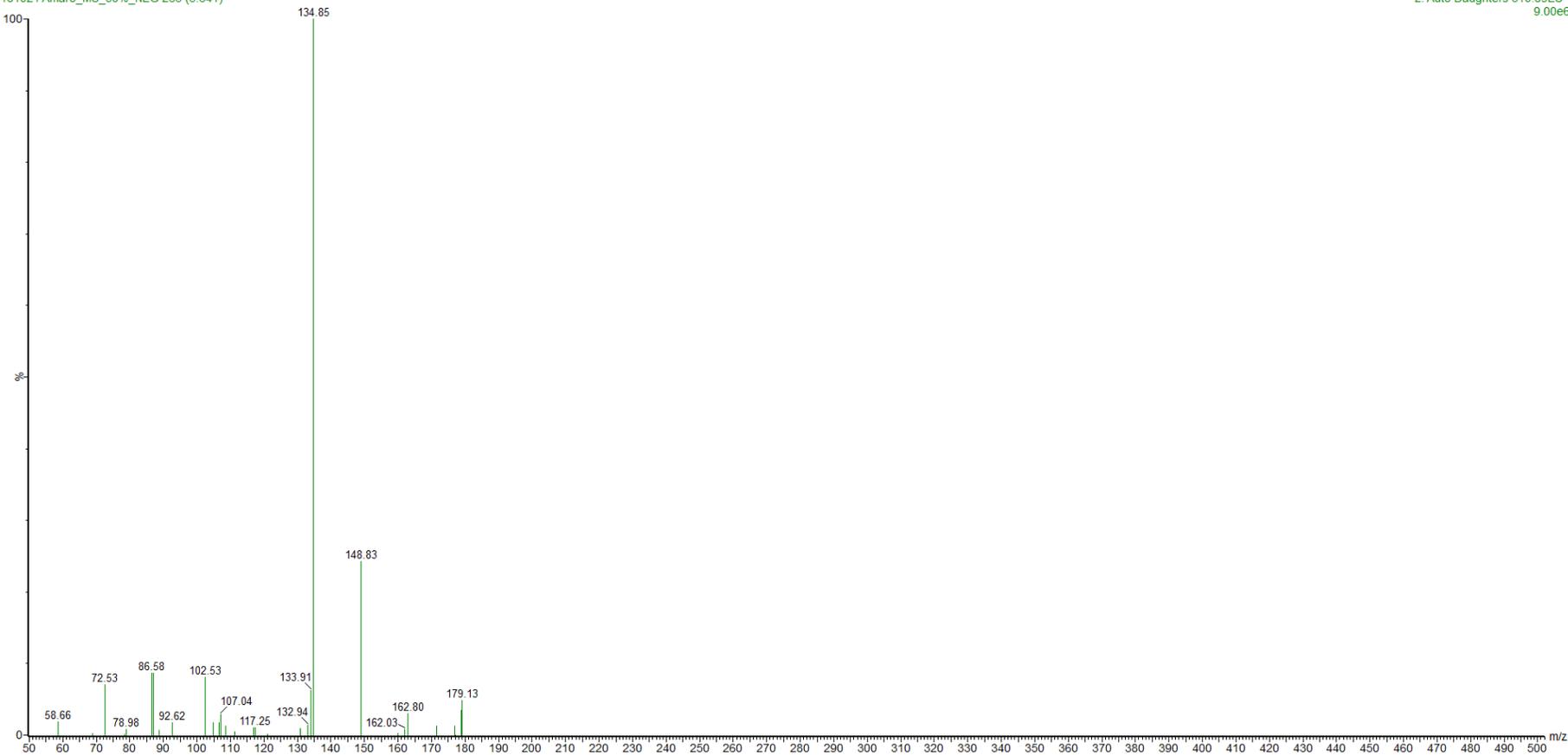


Figure S7: MS/MS-ESI(-) of Substance 4

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 100 (6.250)

1: ScanWave MS ES-
5.00e7

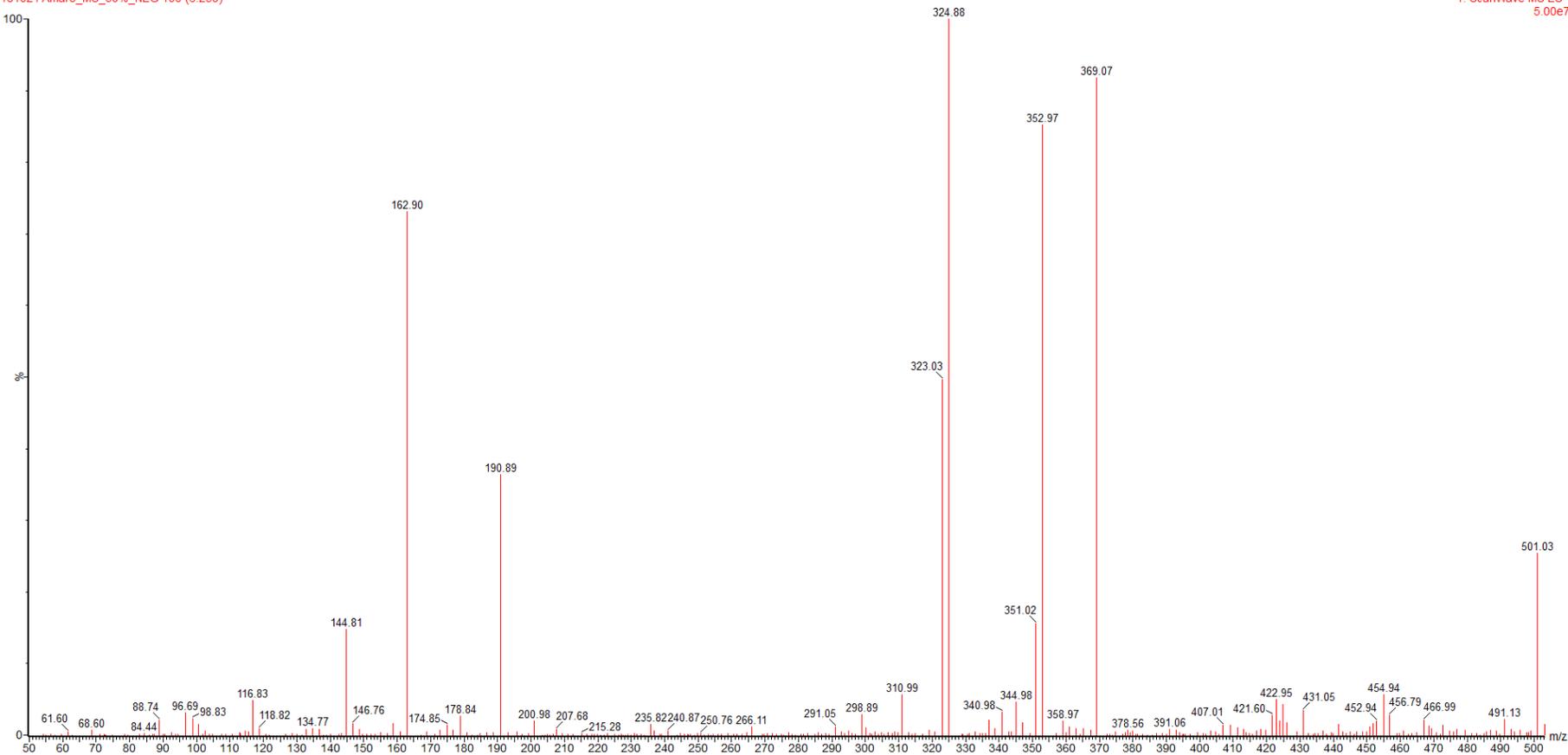


Figure S8: MS-ESI(-) of Substance 5

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 298 (6.262)

2: Auto Daughters 324.88ES-
6.26e6

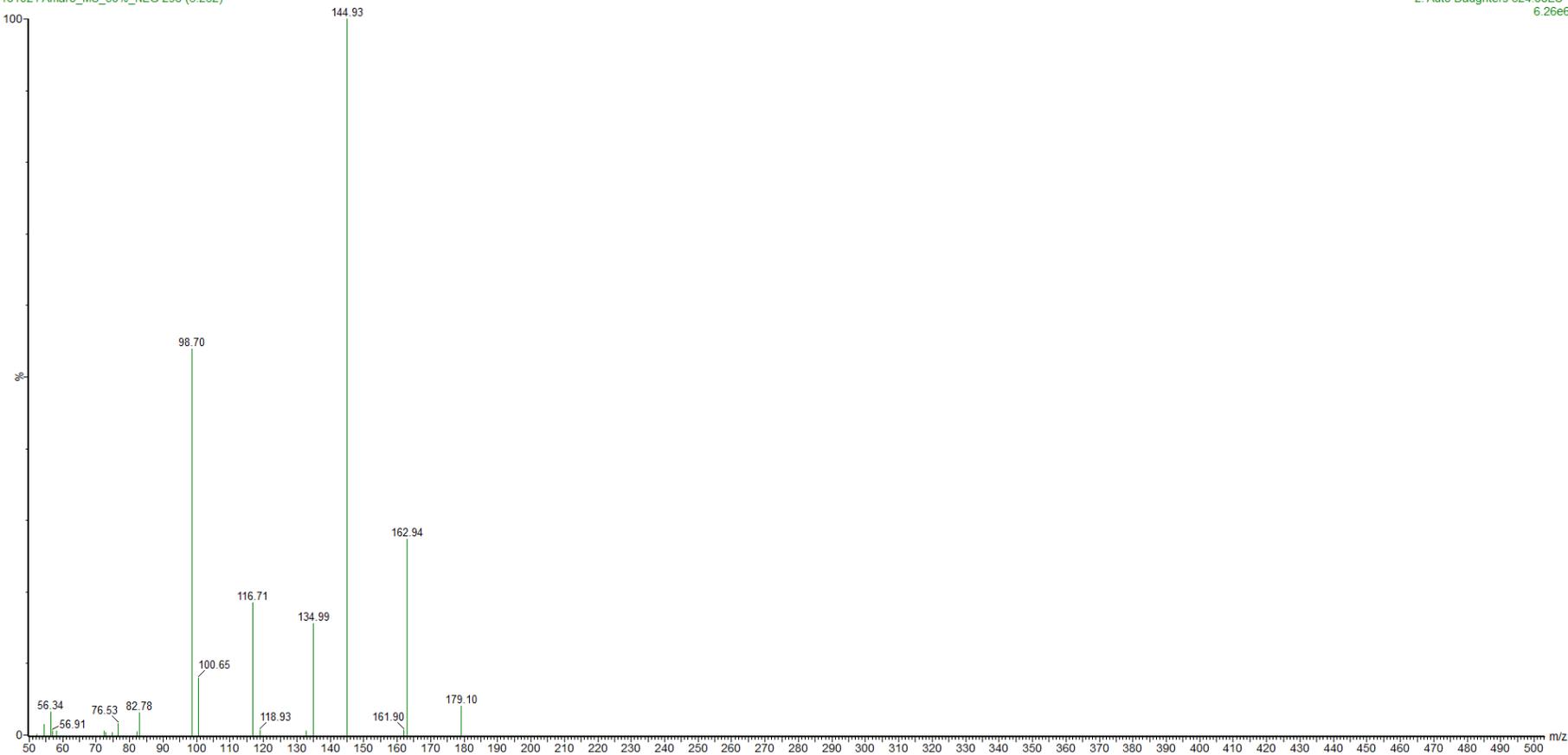


Figure S9: MS/MS-ESI(-) of Substance 5

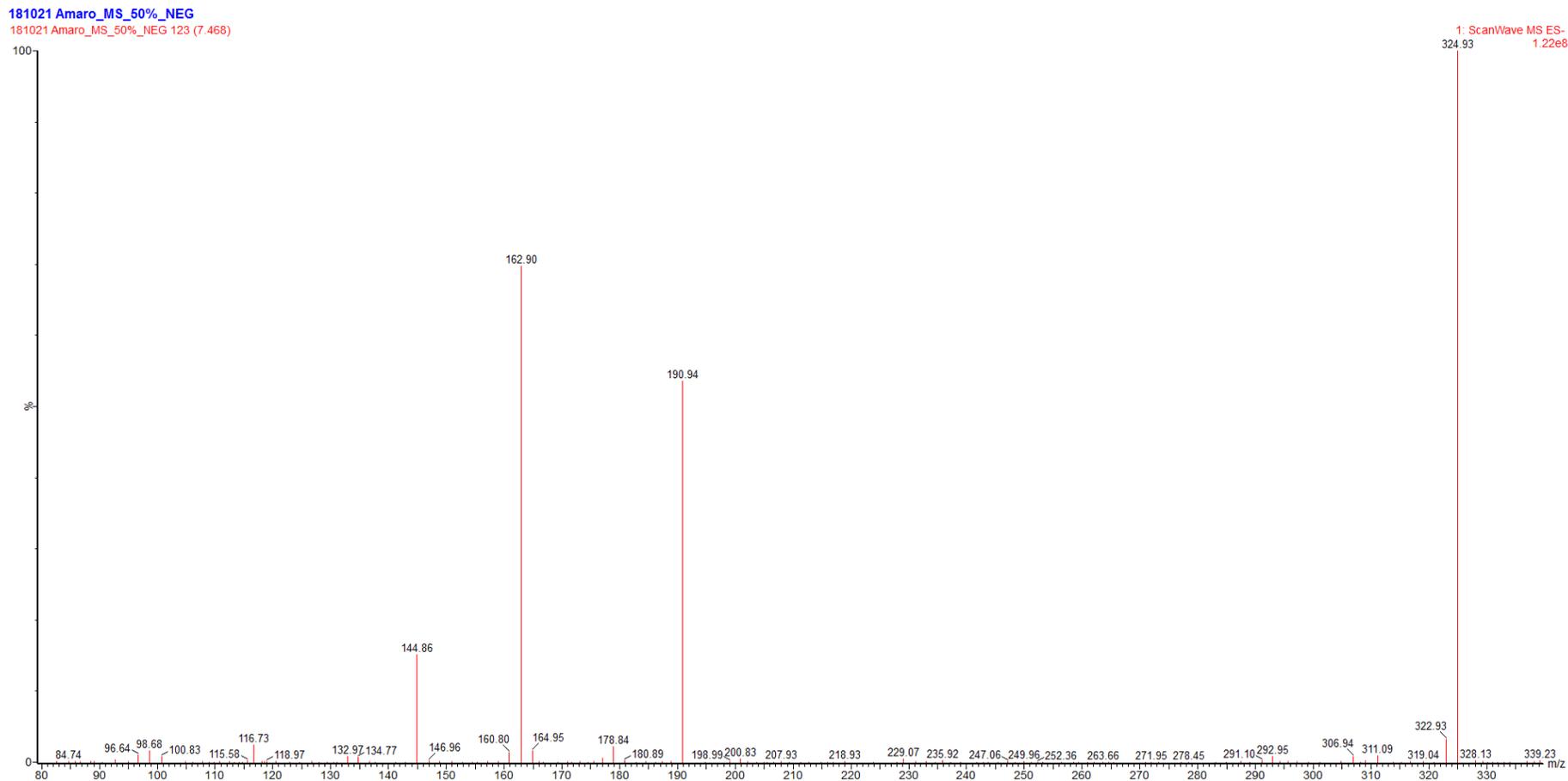


Figure S10: MS-ESI(-) of Substance 6

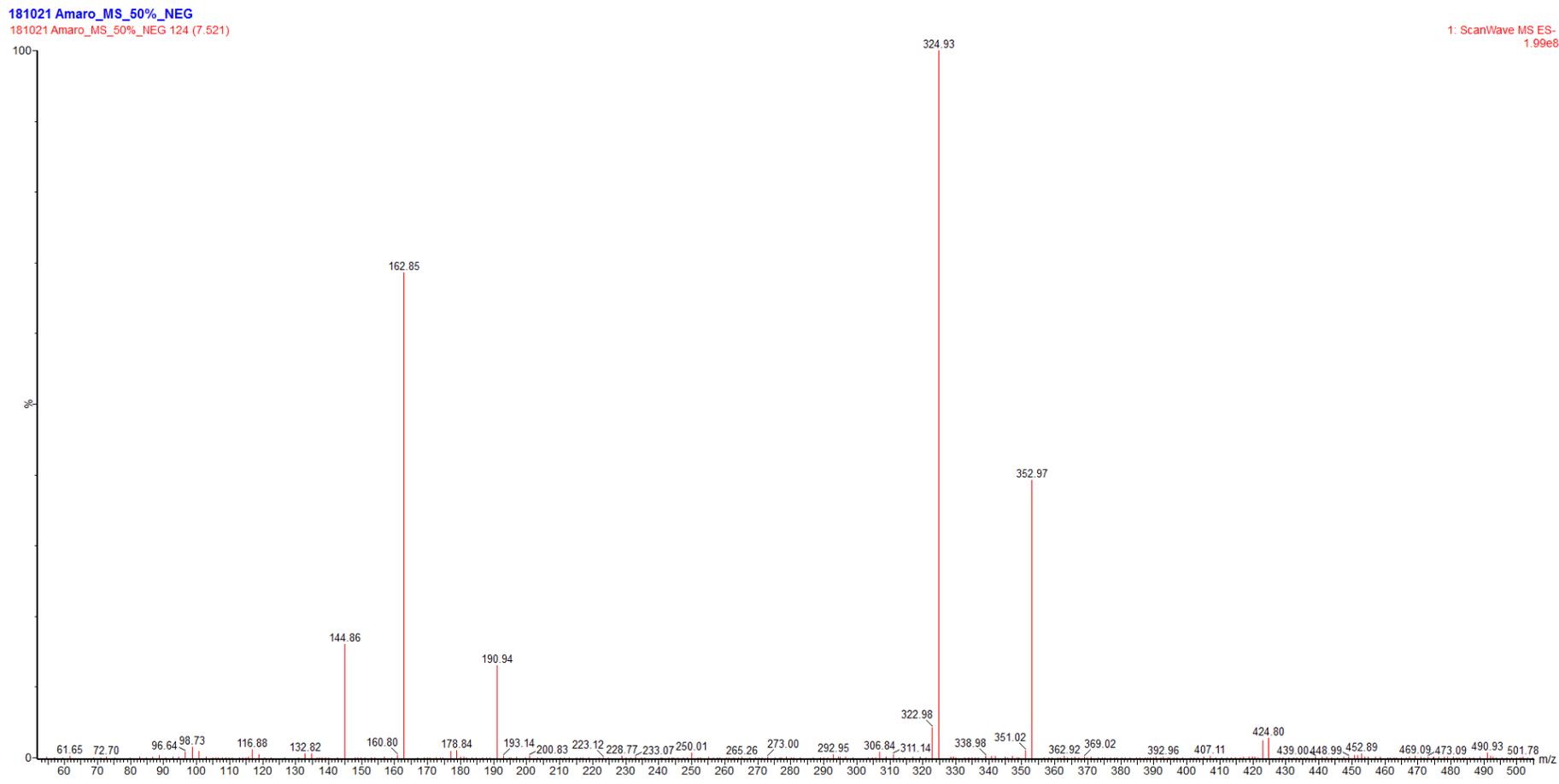


Figure S11: MS-ESI(-) of Substance 7

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Figure S12: MS/MS-ESI(-) of Substance 7

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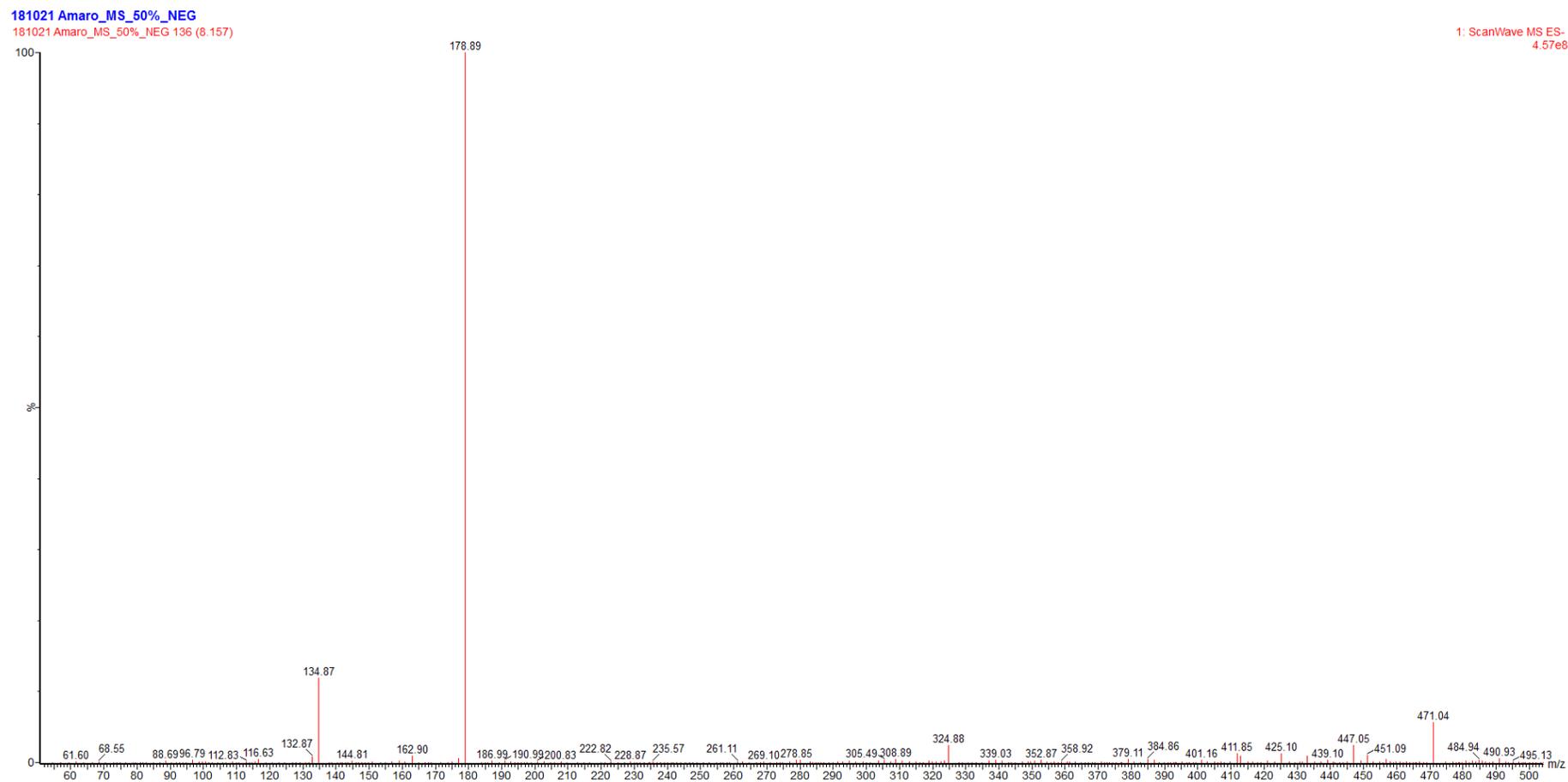


Figure S13: MS-ESI(-) of Substance 8

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Figure S14: MS/MS-ESI(-) of Substance 8

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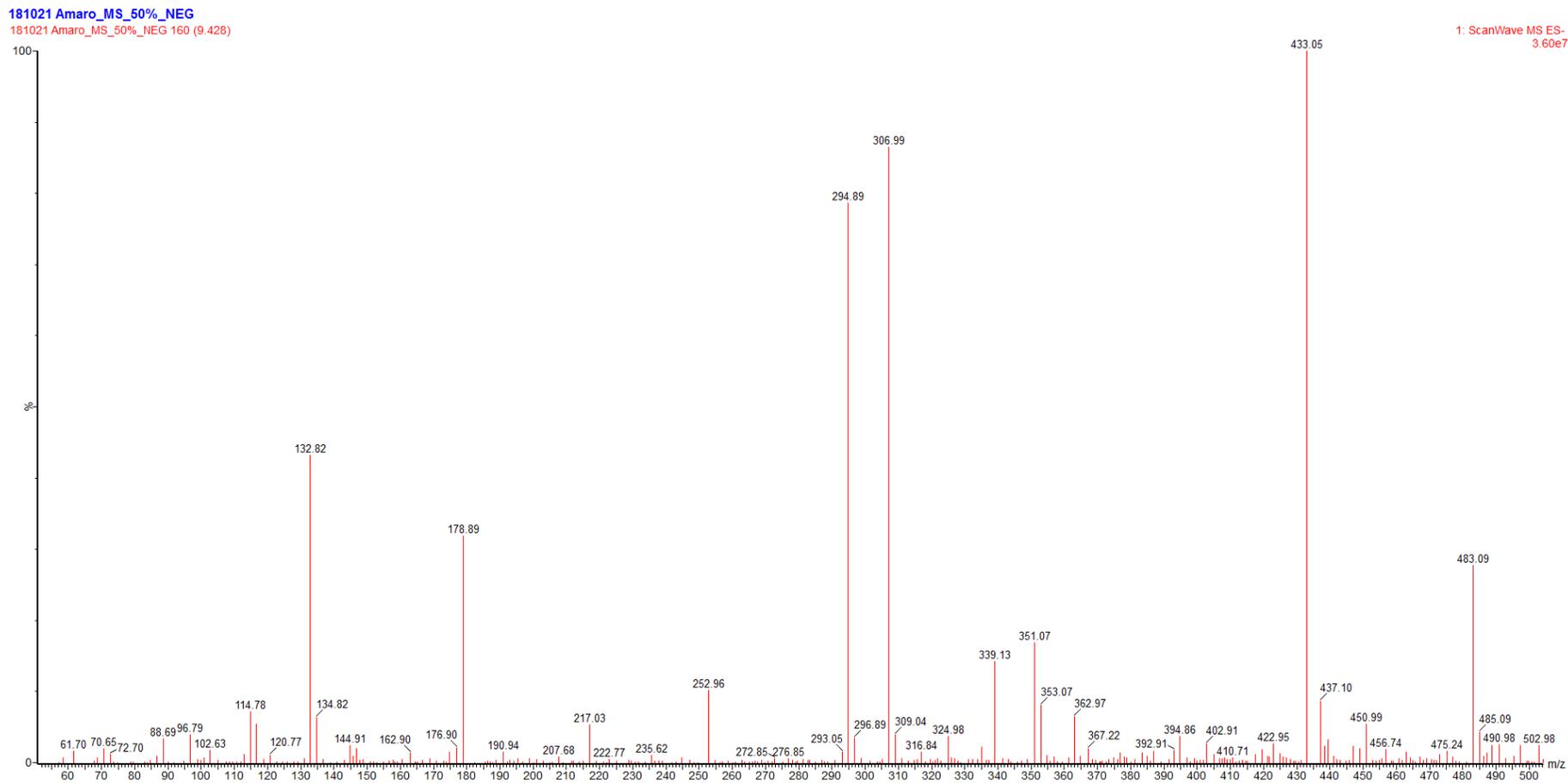


Figure S15: MS-ESI(-) of Substance 9

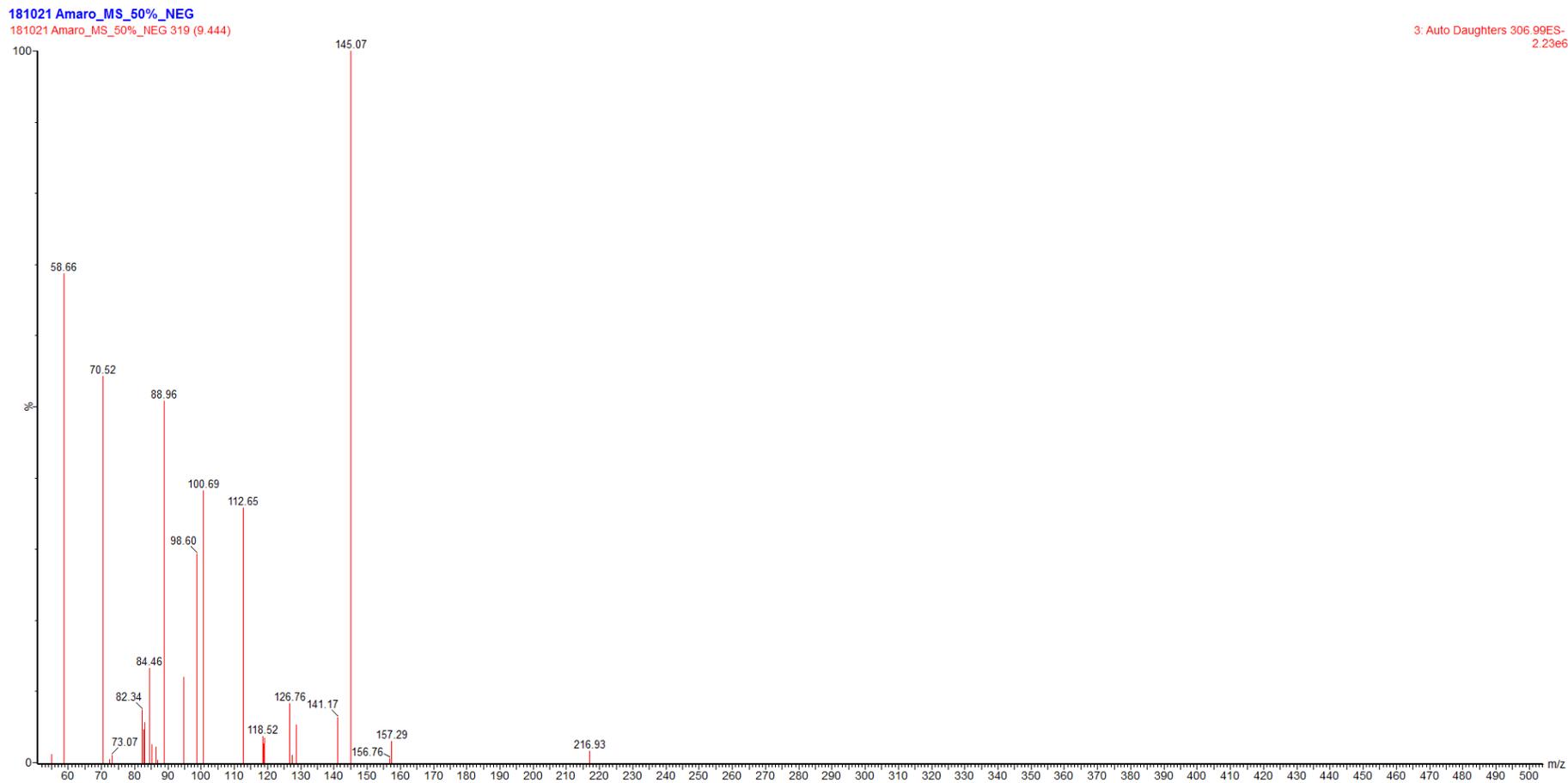


Figure S16: MS/MS-ESI(-) of Substance 9

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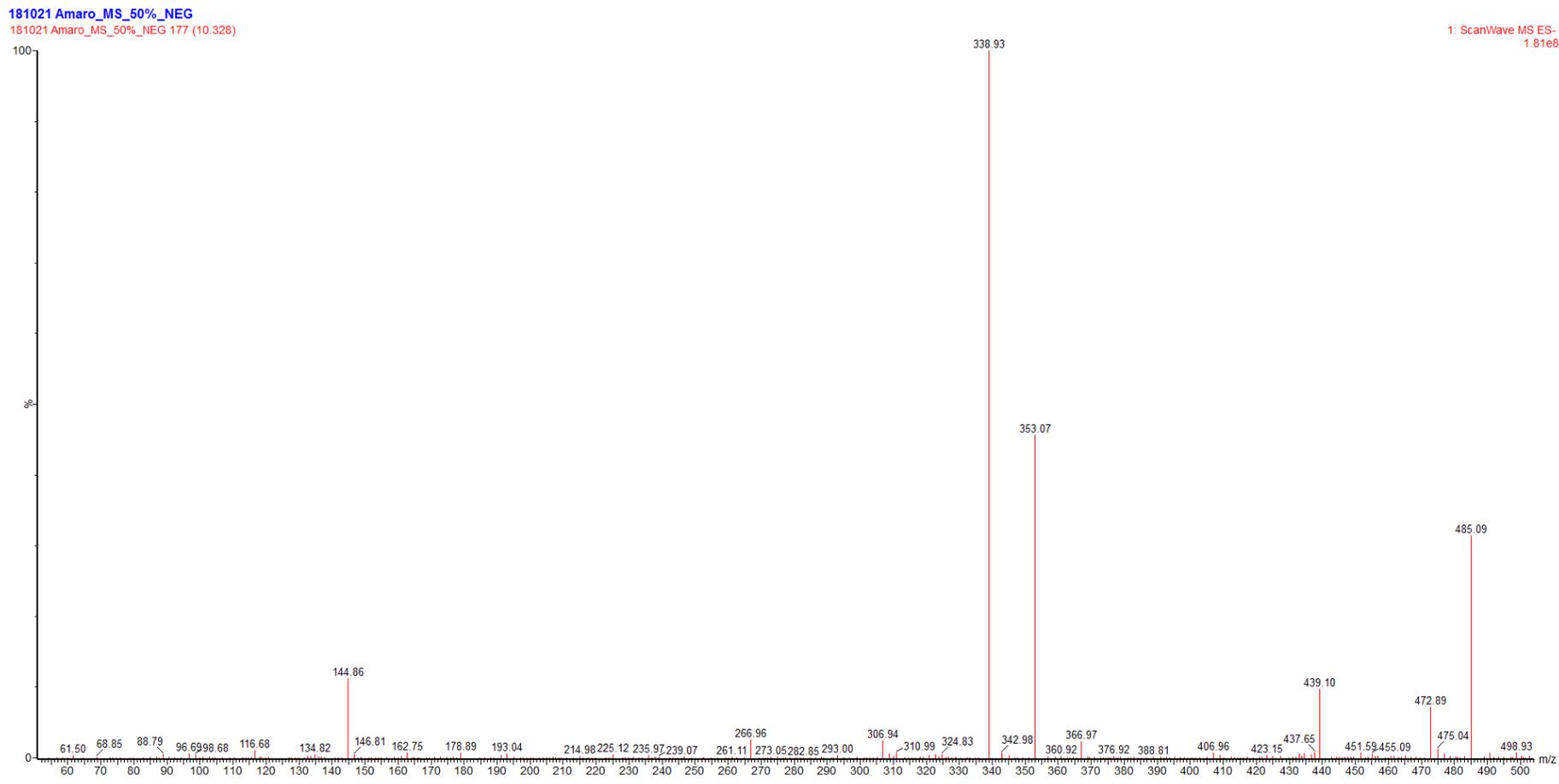


Figure S17: MS-ESI(-) of Substance 10

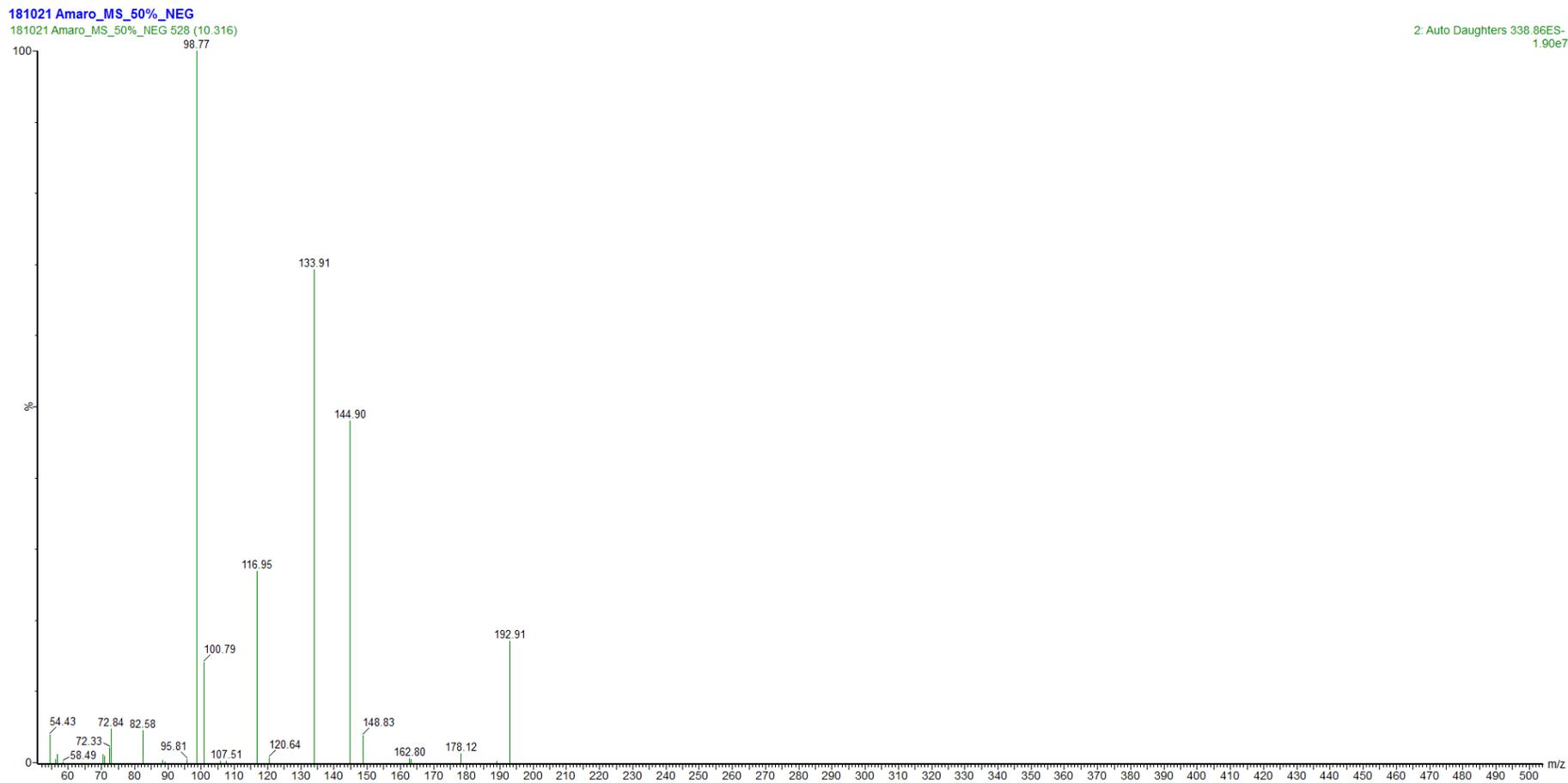


Figure S18: MS/MS-ESI(-) of Substance 10

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Figure S19: MS-ESI(-) of Substance 11

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Figure S20: MS/MS-ESI(-) of Substance 11

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181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50__NEG 211 (12.129)

1: ScanWave MS ES-
1.52e7

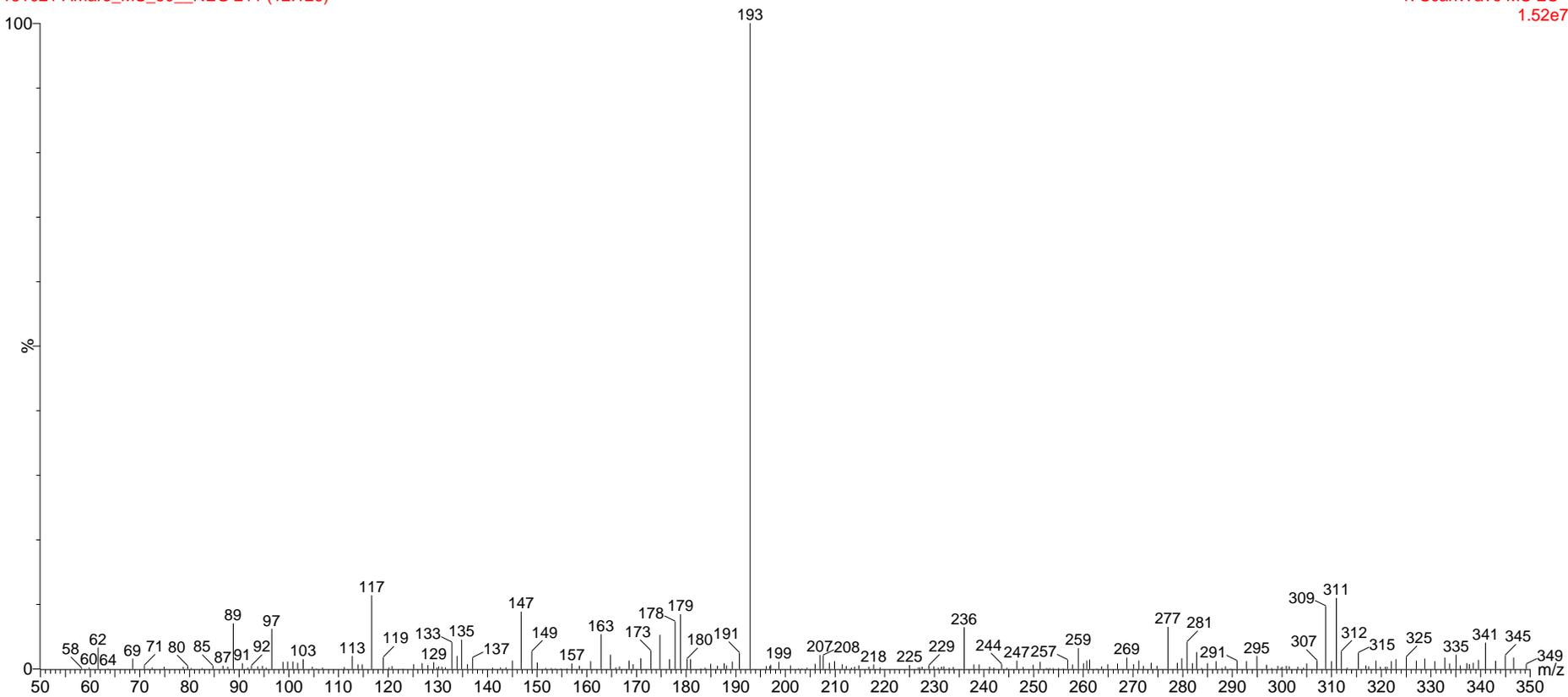


Figure S21: MS-ESI(-) of Substance 12

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50__NEG 218 (12.500)

1: ScanWave MS ES-
9.79e7

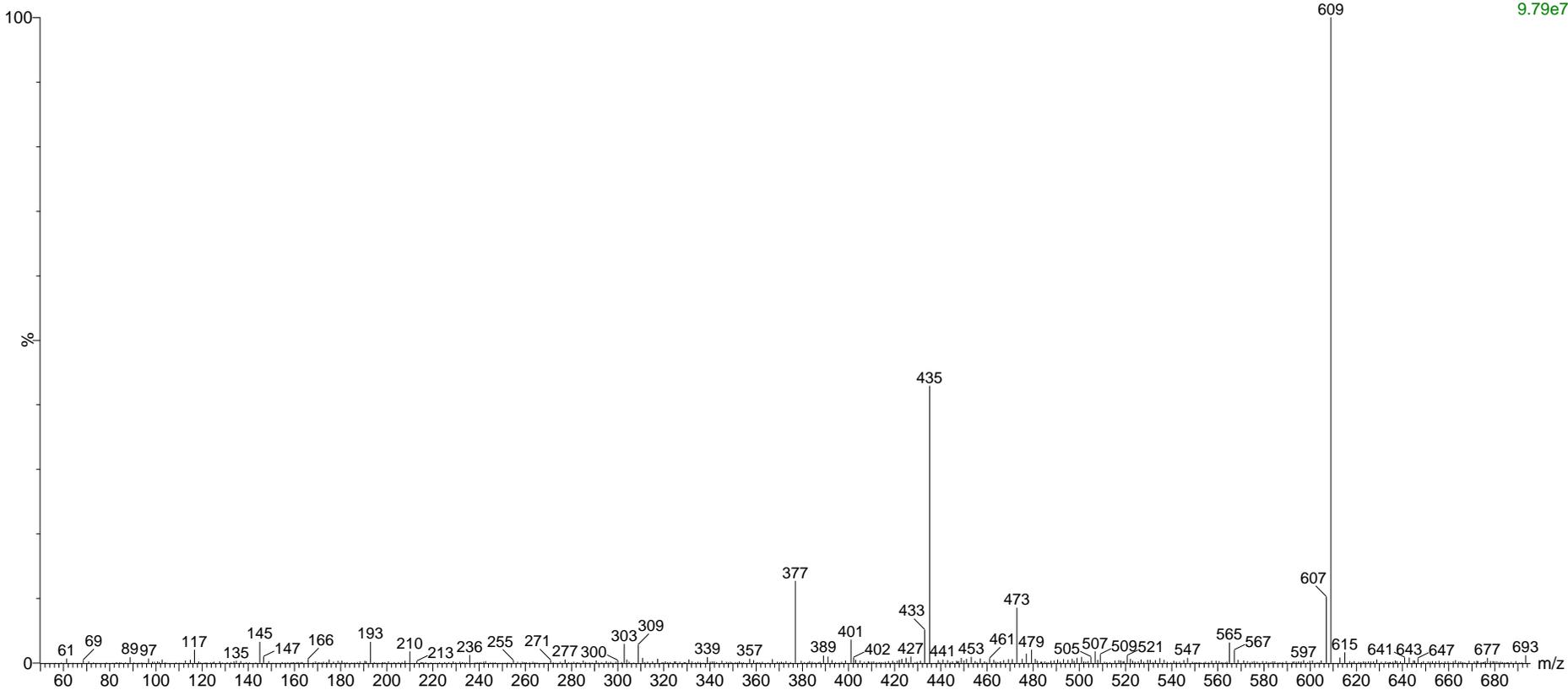


Figure S22: MS-ESI(-) of Substance 13

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50__NEG 654 (12.541)

2: Auto Daughters 608.87ES-
2.93e7

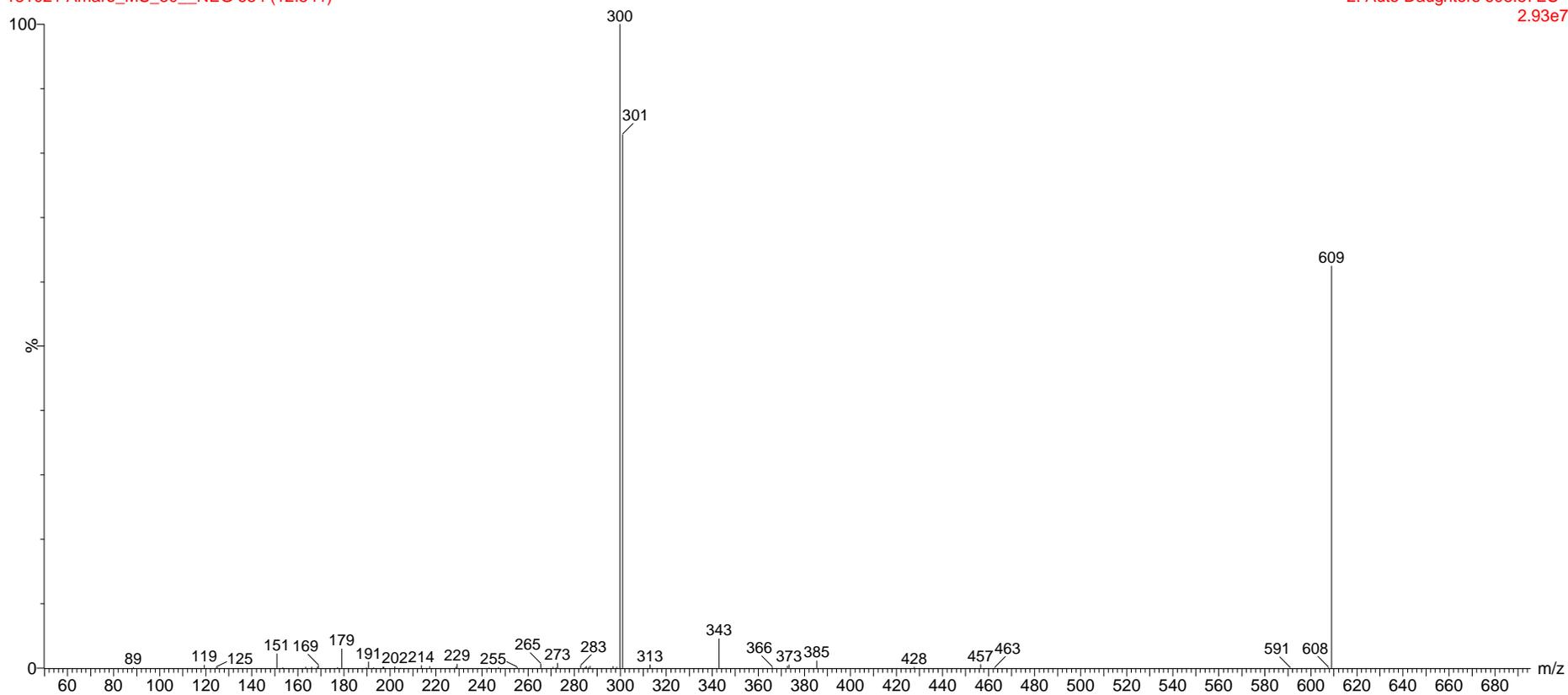


Figure S23: MS/MS-ESI(-) of Substance 13

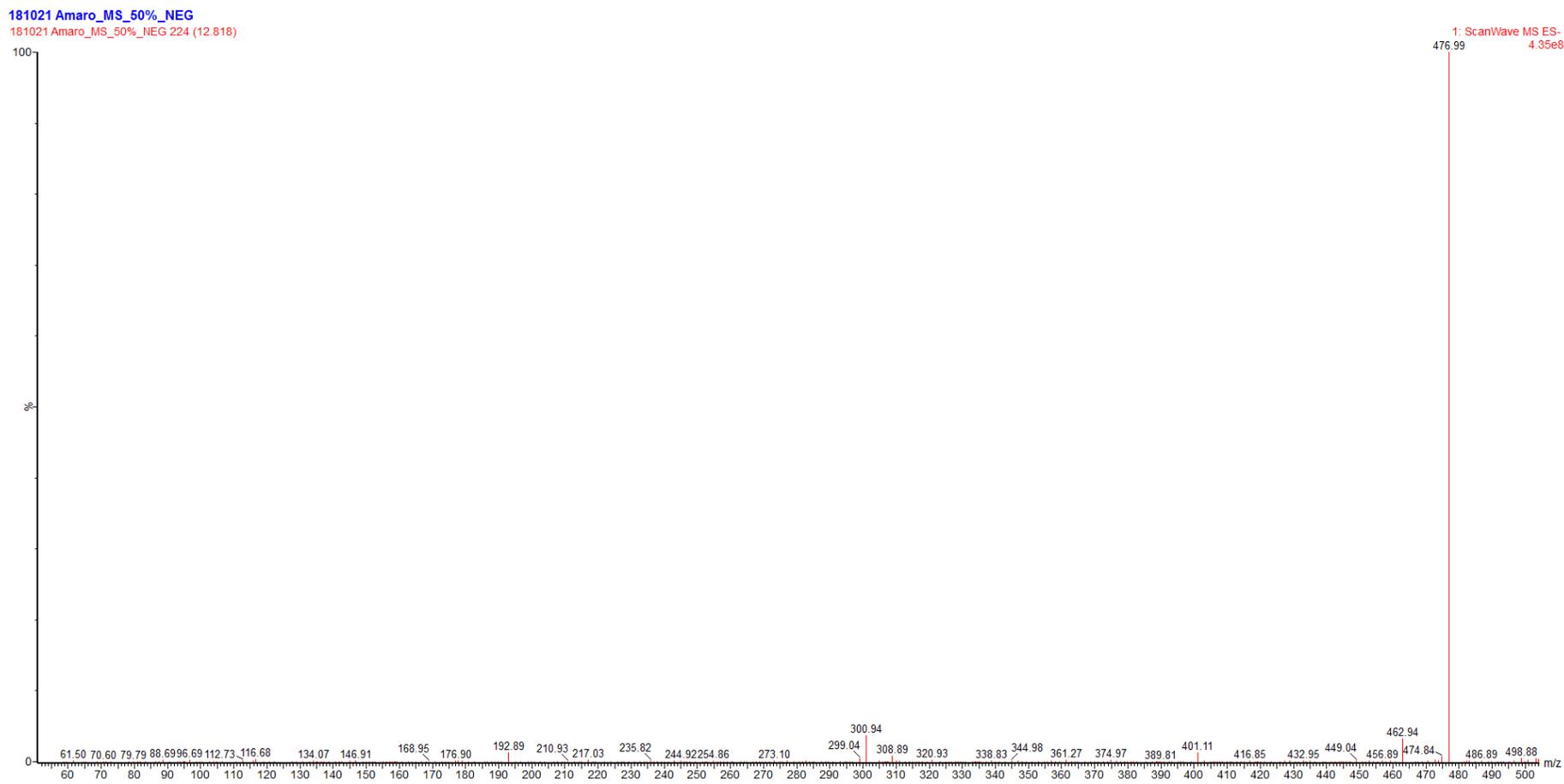


Figure S24: MS-ESI(-) of Substance 14

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 670 (12.829)

2: Auto Daughters 476.99ES-
1.57e8

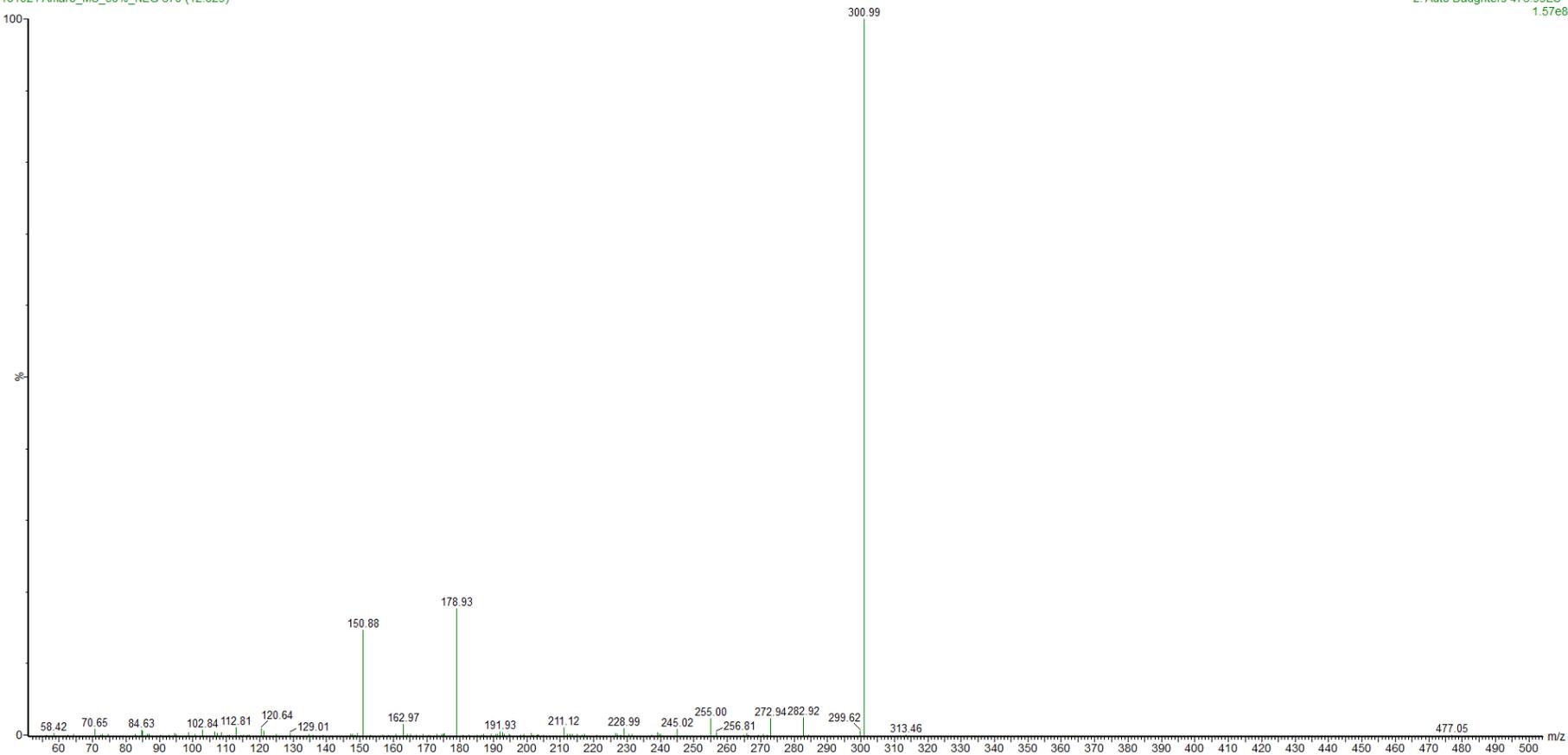


Figure S25: MS/MS-ESI(-) of Substance 14

181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50%_NEG 251 (14.248)



Figure S26: MS-ESI(-) of Substance 15

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 750 (14.236)

2: Auto Daughters 514.87ES-
1.08e8

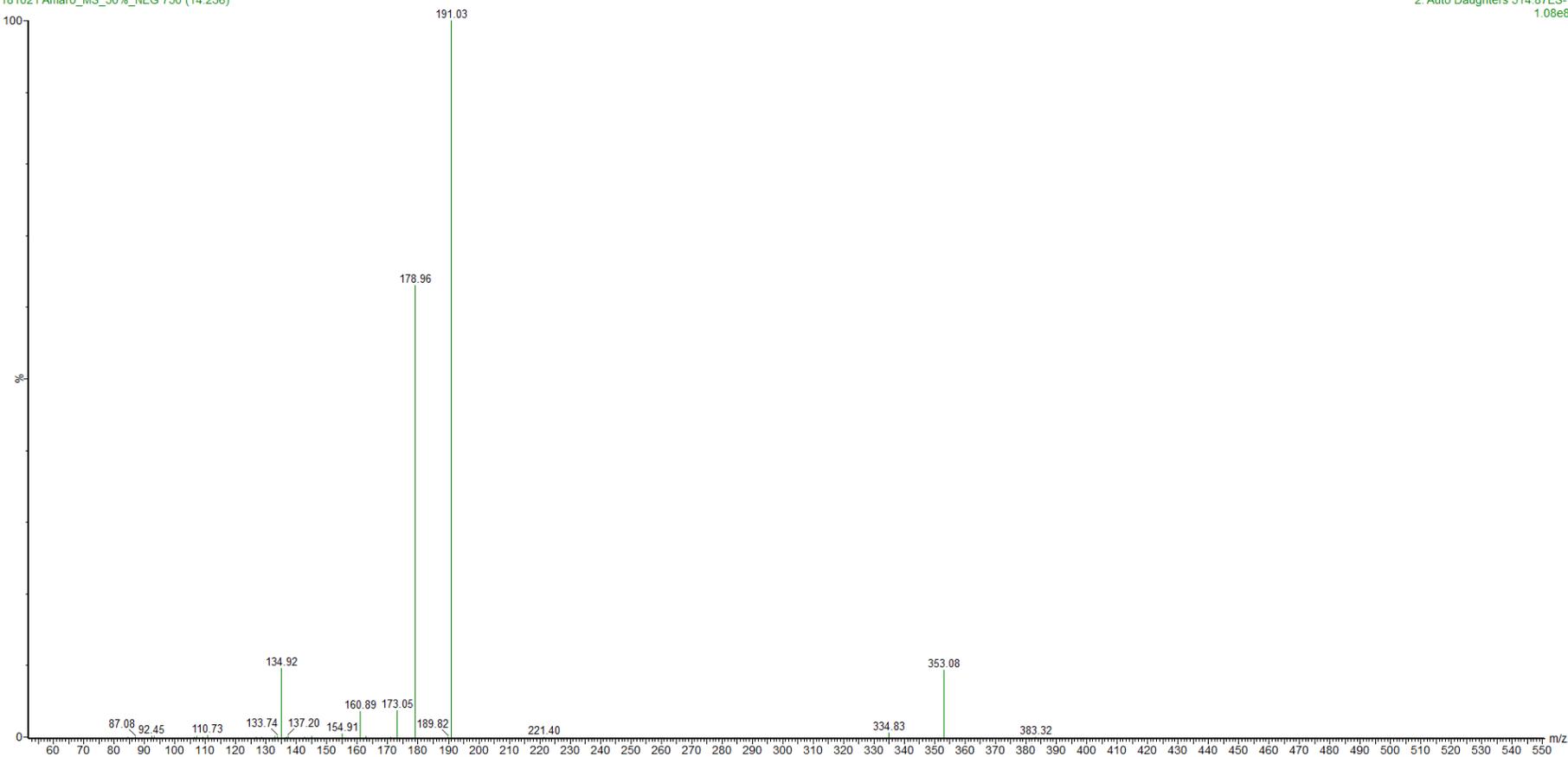


Figure S27: MS/MS-ESI(-) of Substance 15

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 254 (14.407)

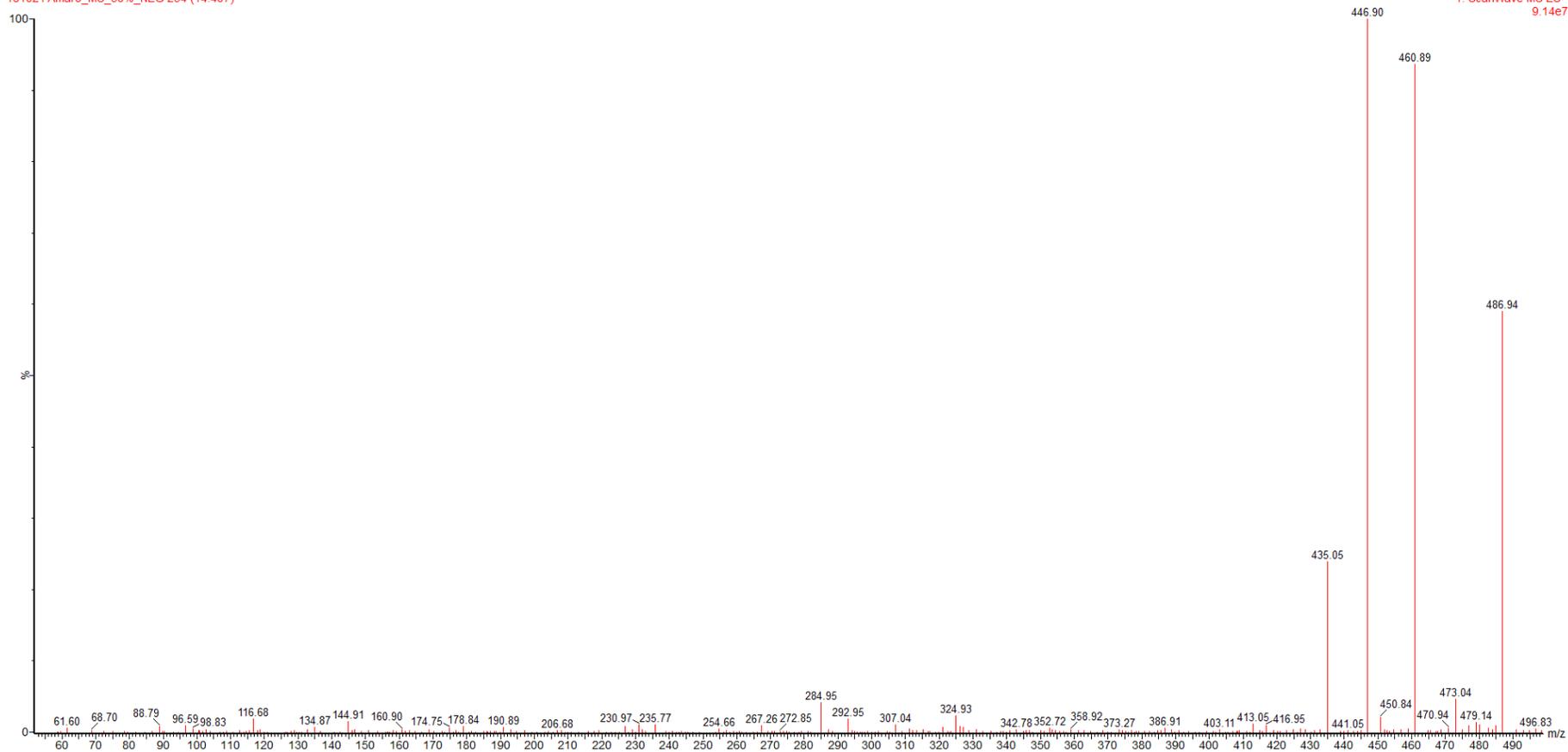


Figure S28: MS-ESI(-) of Substance 16

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 760 (14.418)

2: Auto Daughters 446.90ES-
3.17e7

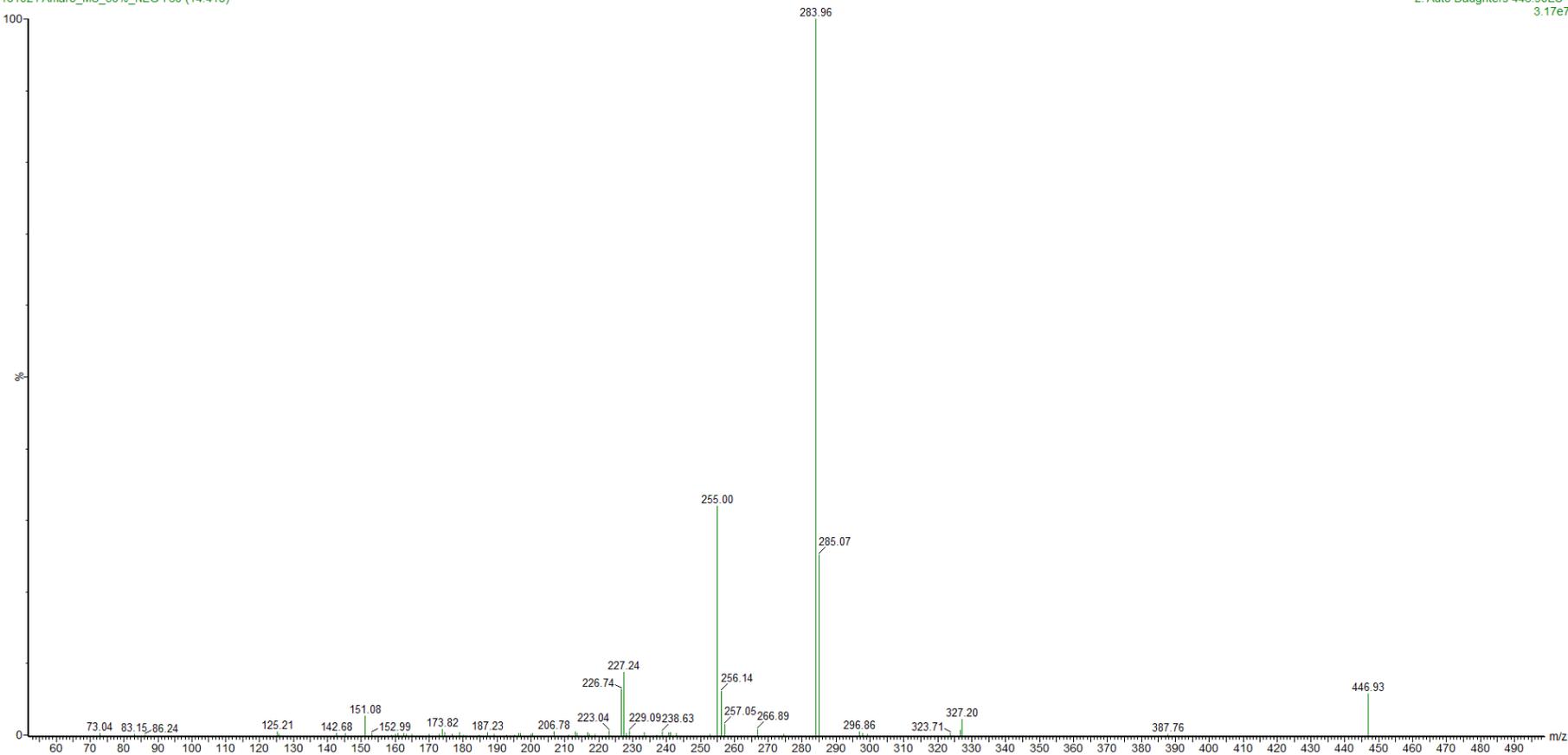


Figure S29: MS/MS-ESI(-) of Substance 16

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 261 (14.777)



Figure S30: MS-ESI(-) of Substance 17

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 780 (14.766)

2: Auto Daughters 486.82ES-
1.15e8

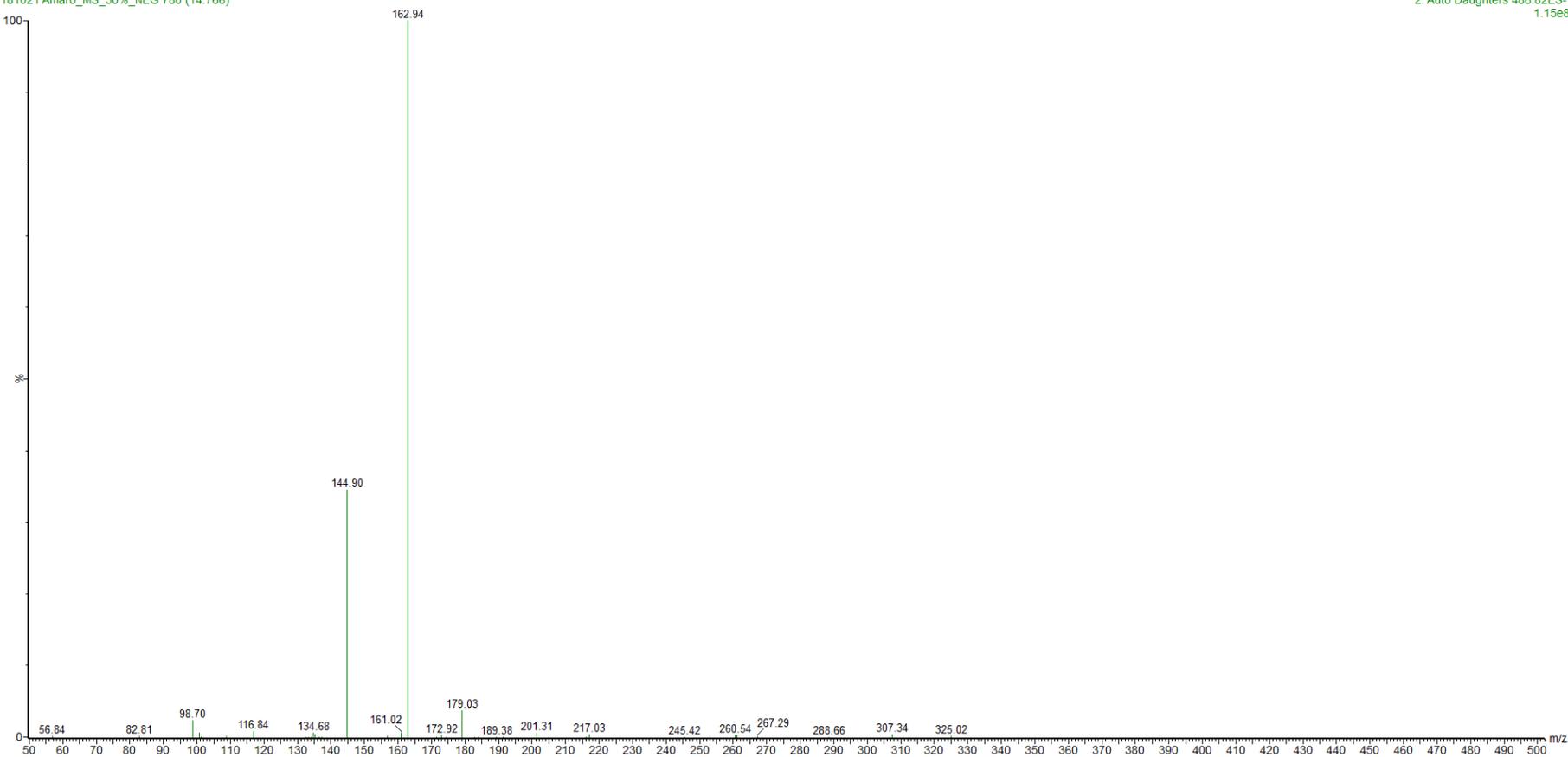


Figure S31: MS/MS-ESI(-) of Substance 17

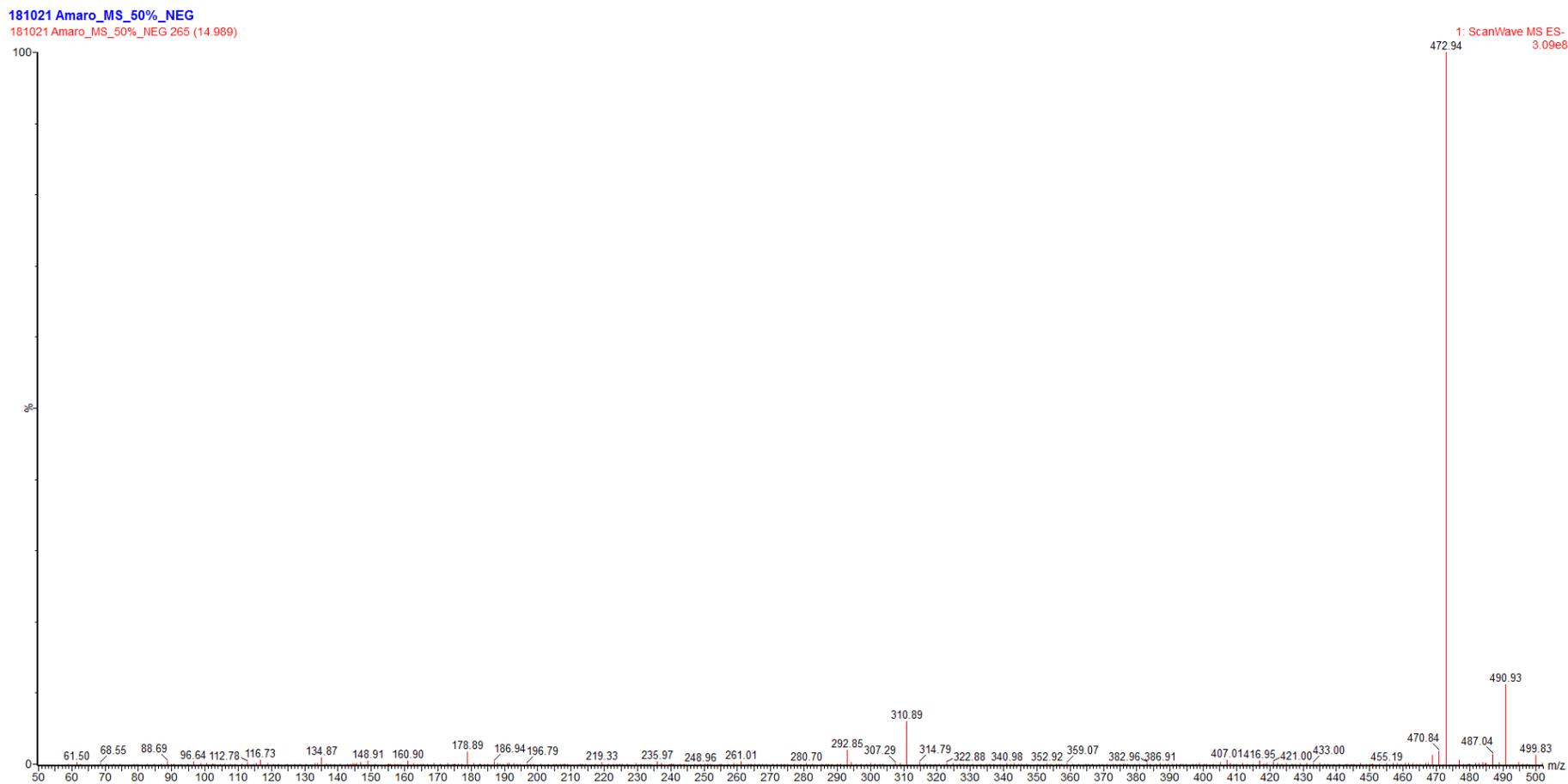


Figure S32: MS-ESI(-) of Substance 18

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 792 (14.977)

2: Auto Daughters 472.82ES-
8.84e7

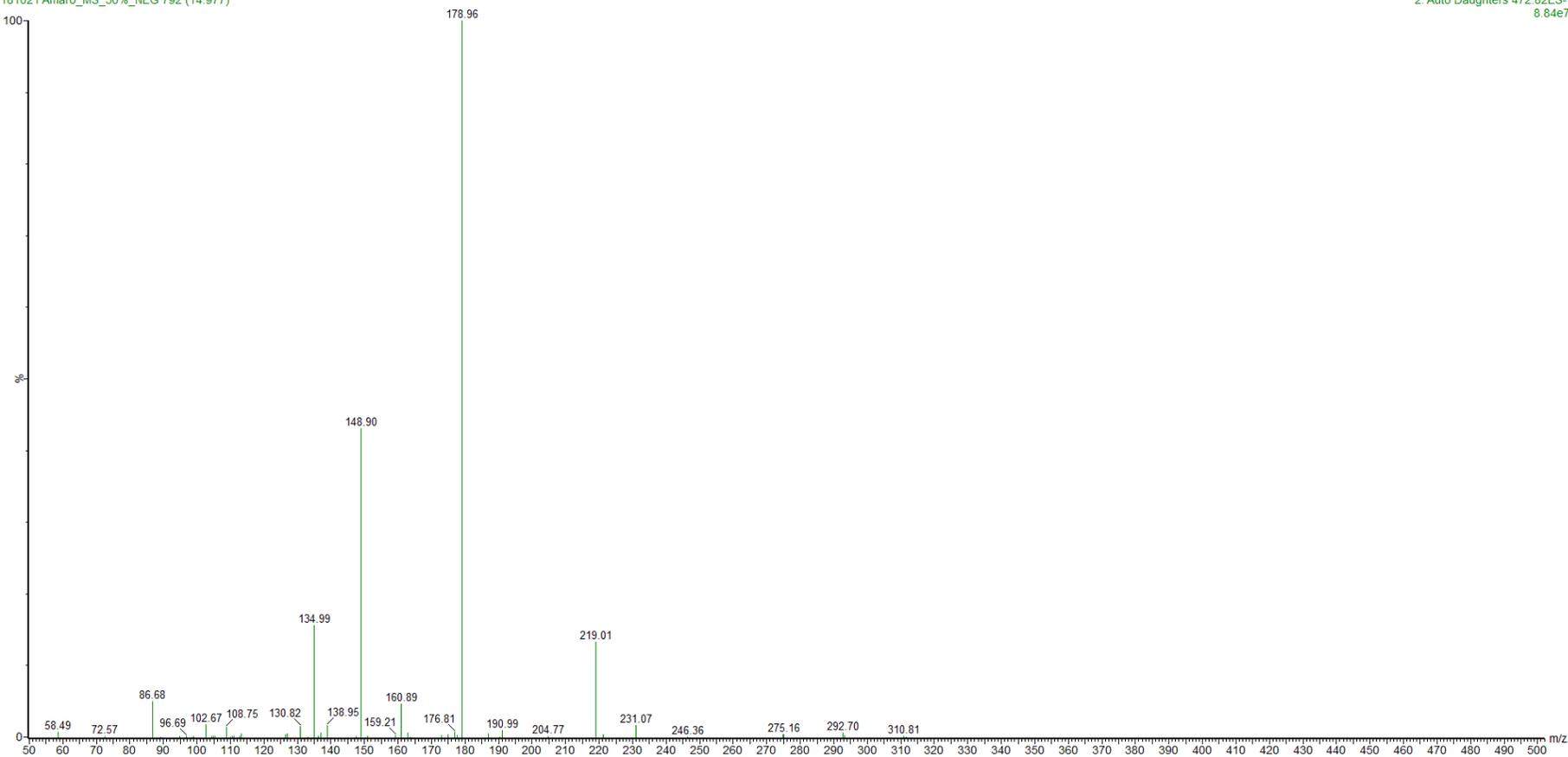


Figure S33: MS/MS-ESI(-) of Substance 18

181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50%_NEG 310 (17.373)

1: ScanWave MS ES-
2.33e8

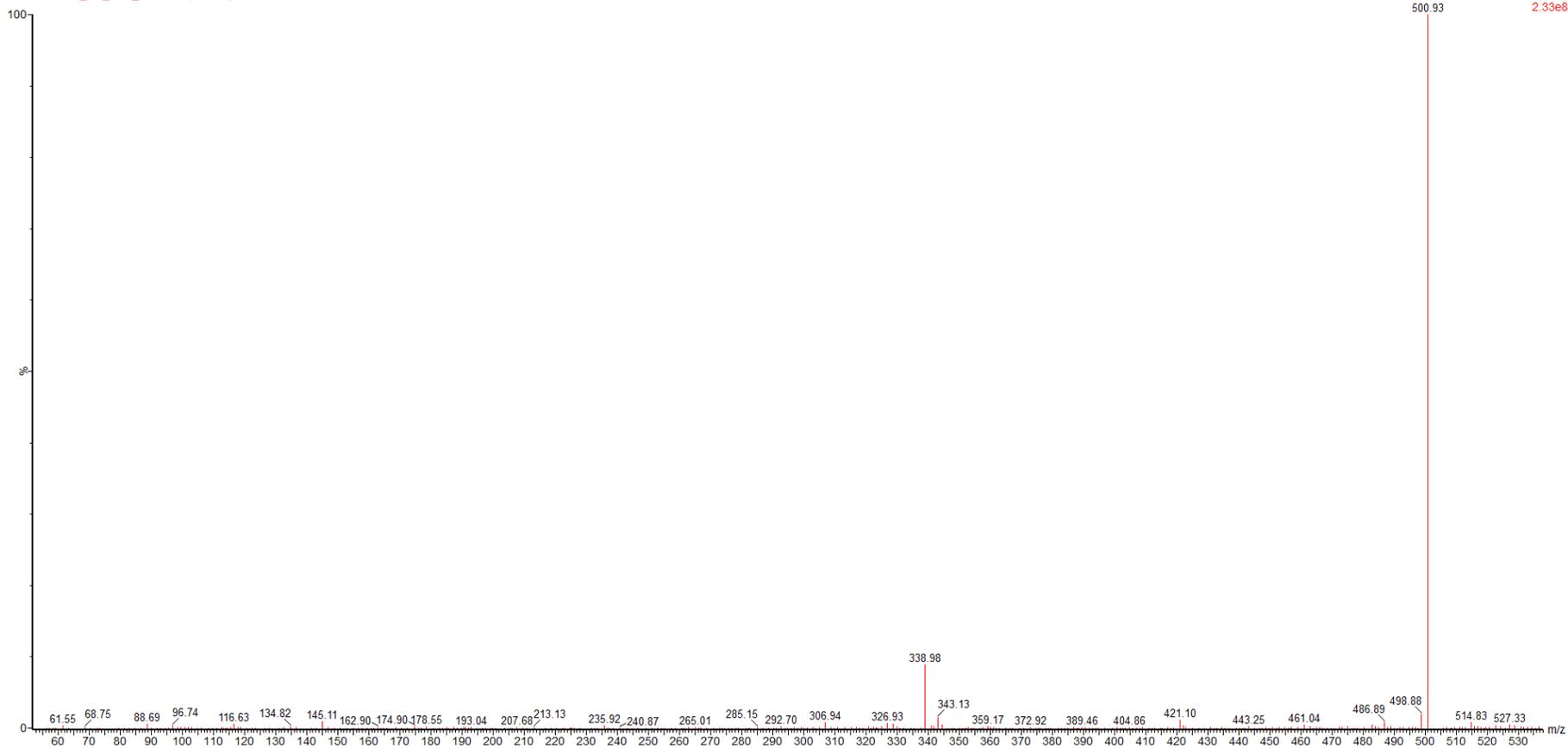


Figure S34: MS-ESI(-) of Substance 19

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 927 (17.361)

2: Auto Daughters 500.87ES-
7.96e7

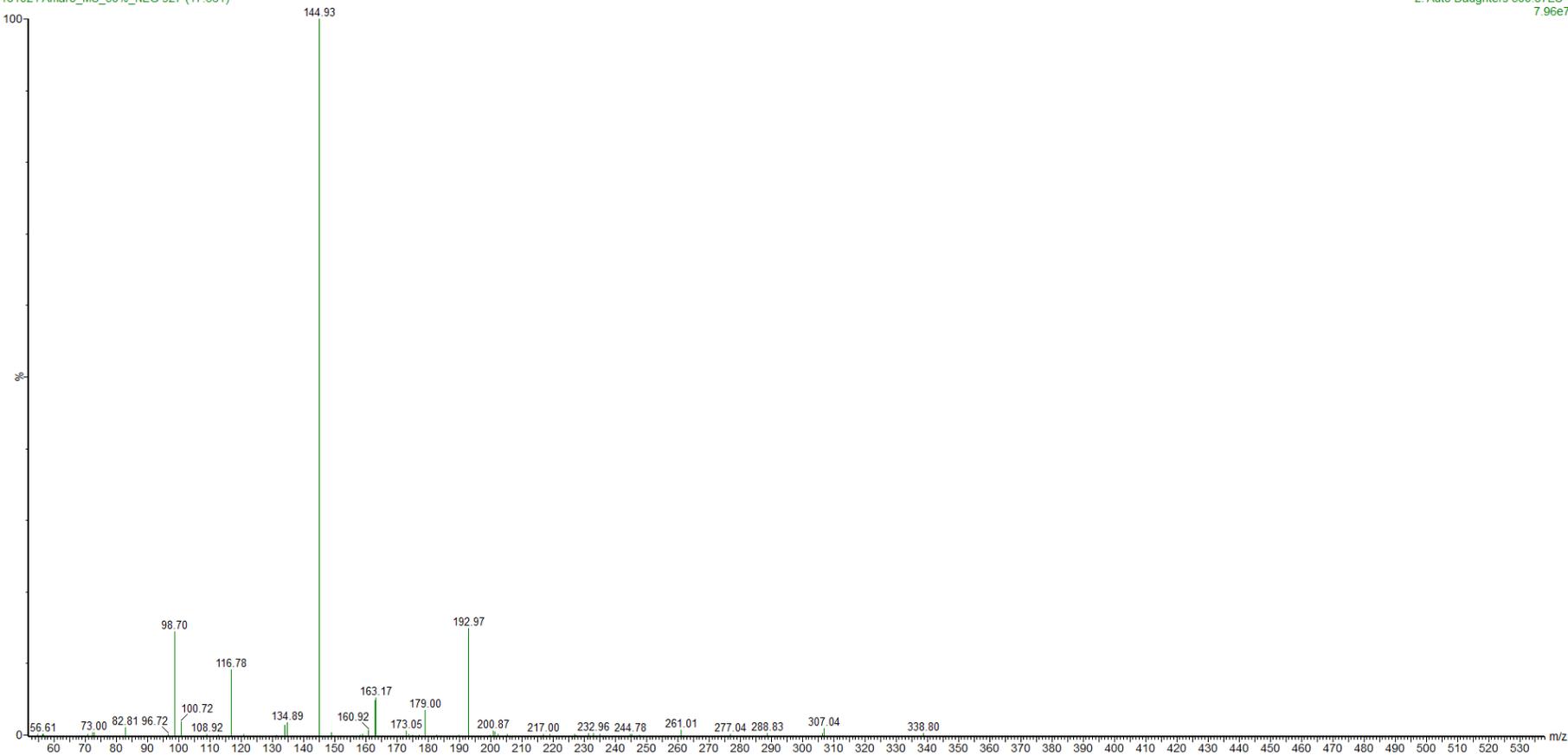


Figure S35: MS/MS-ESI(-) of Substance 19

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 318 (17.797)



Figure S36: MS-ESI(-) of Substance 20

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 951 (17.785)

2: Auto Daughters 486.82ES-
1.37e7

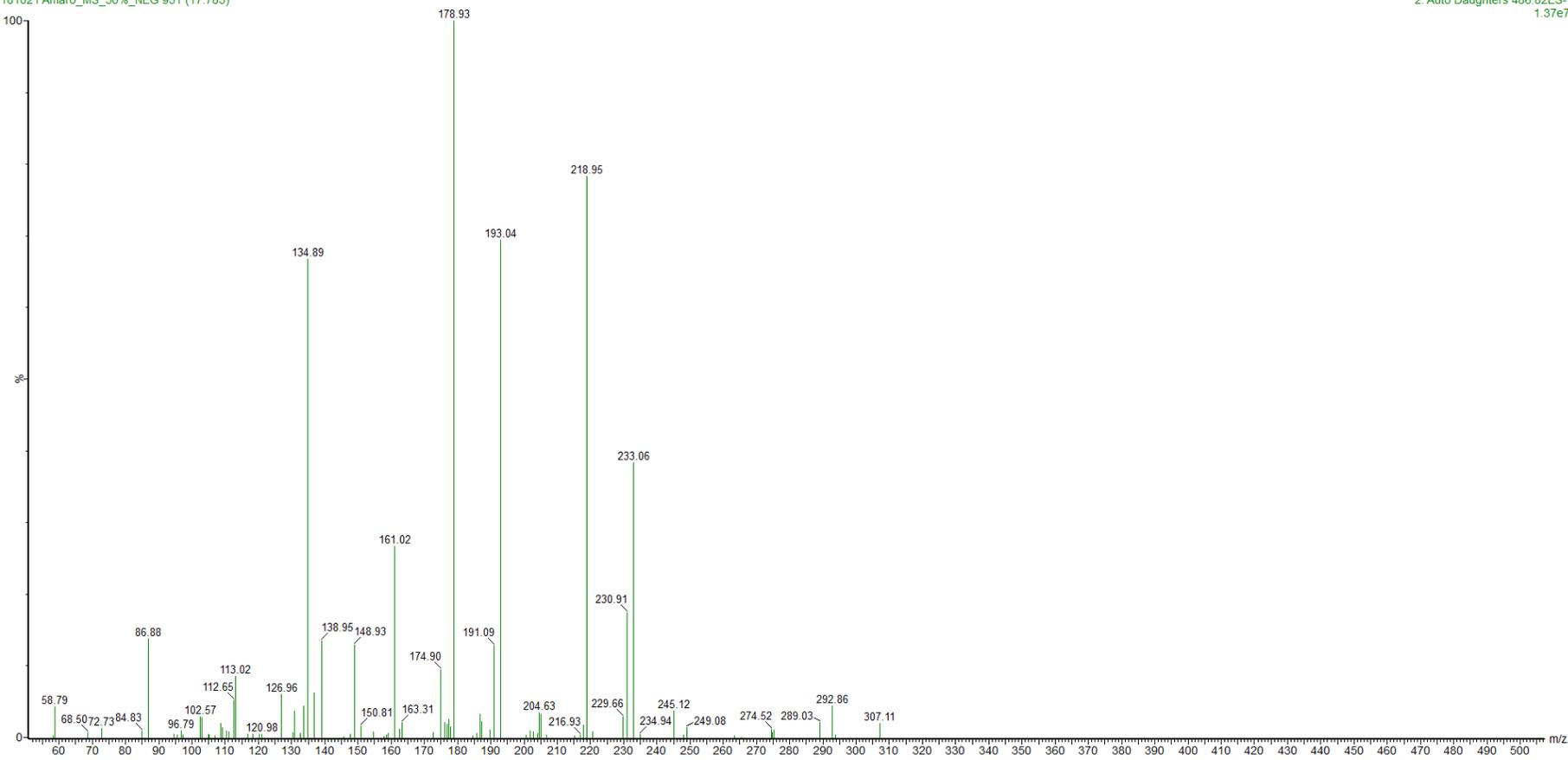


Figure S37: MS/MS-ESI(-) of Substance 20

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 334 (18.644)

1: ScanWave MS ES-
1.17e8

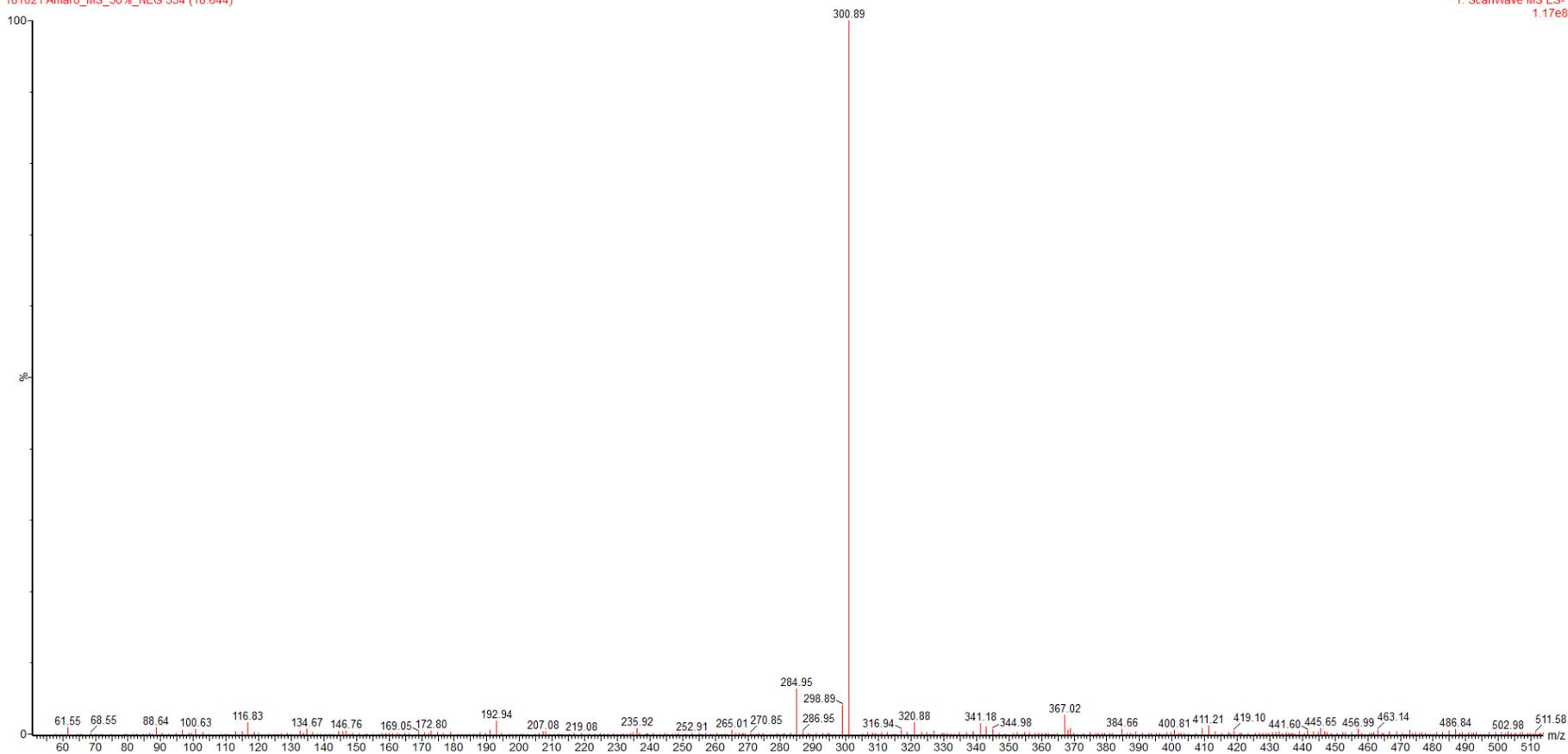


Figure S38: MS-ESI(-) of Substance 21

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 999 (18.633)

2: Auto Daughters 300.83ES-
1.52e7



Figure S39: MS/MS-ESI(-) of Substance 21

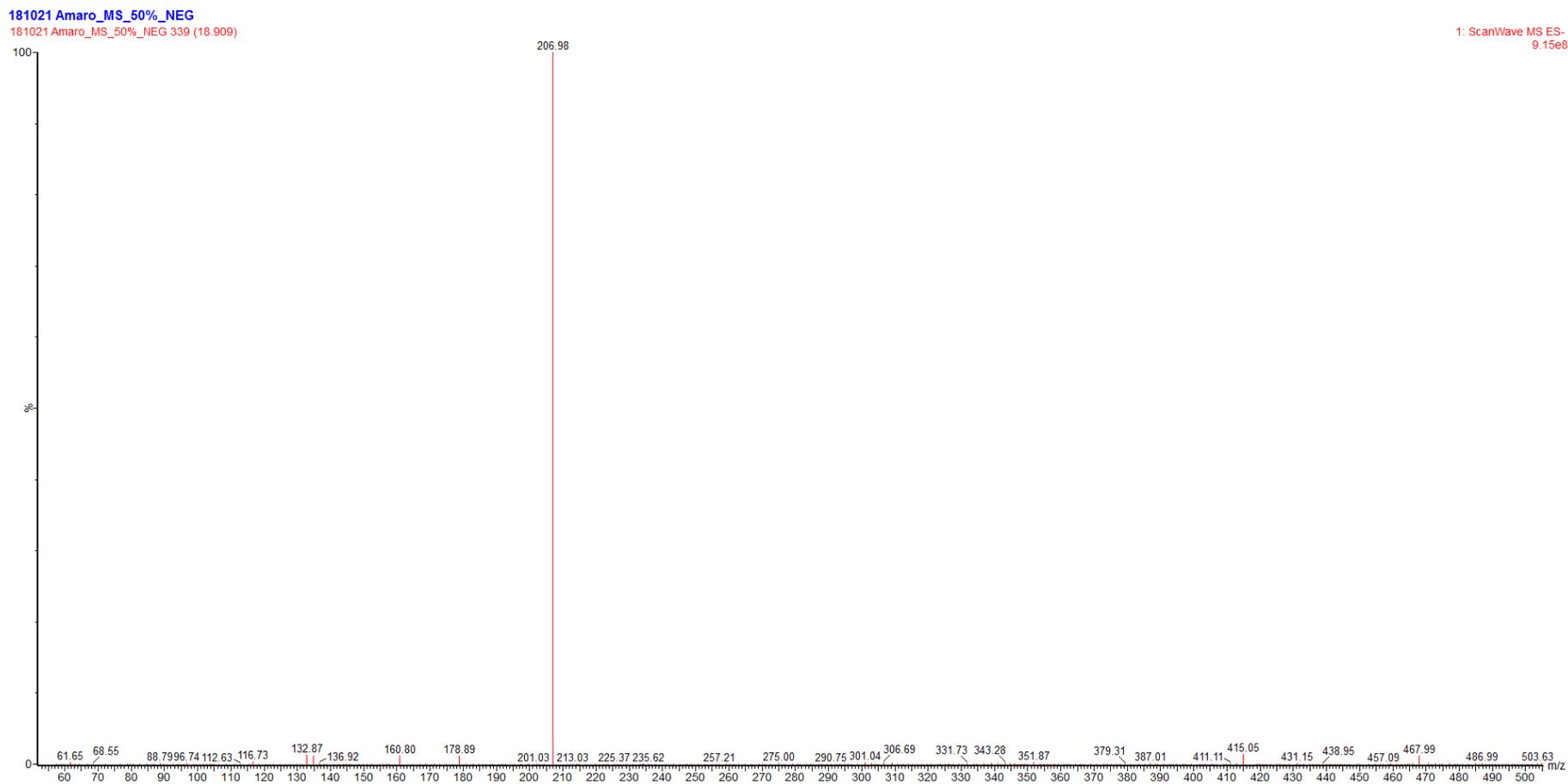


Figure S40: MS-ESI(-) of Substance 22

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 1014 (18.897)

2: Auto Daughters 206.84ES-
1.64e8

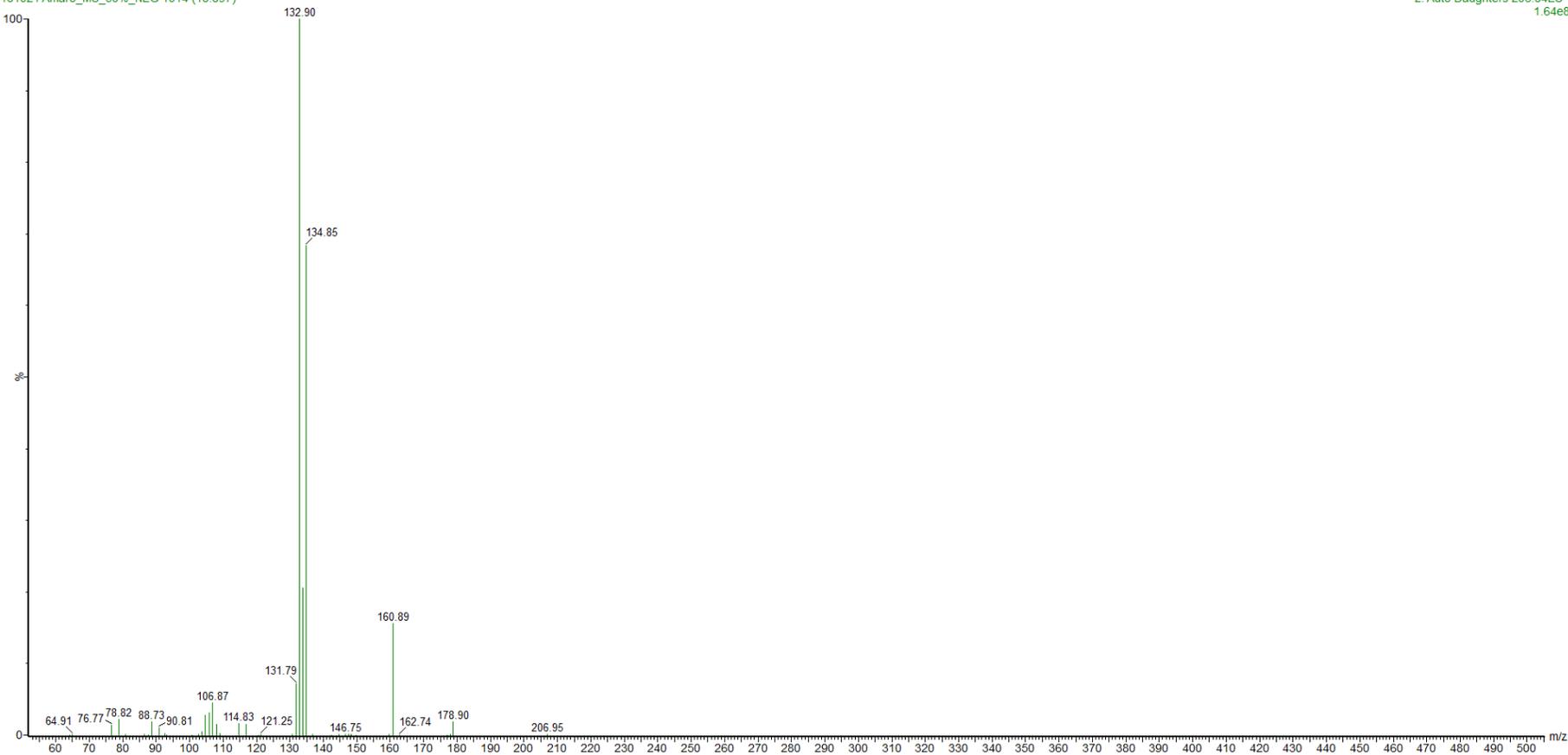


Figure S41: MS/MS-ESI(-) of Substance 22

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 342 (19.068)

1: ScanWave MS ES-
9.21e7

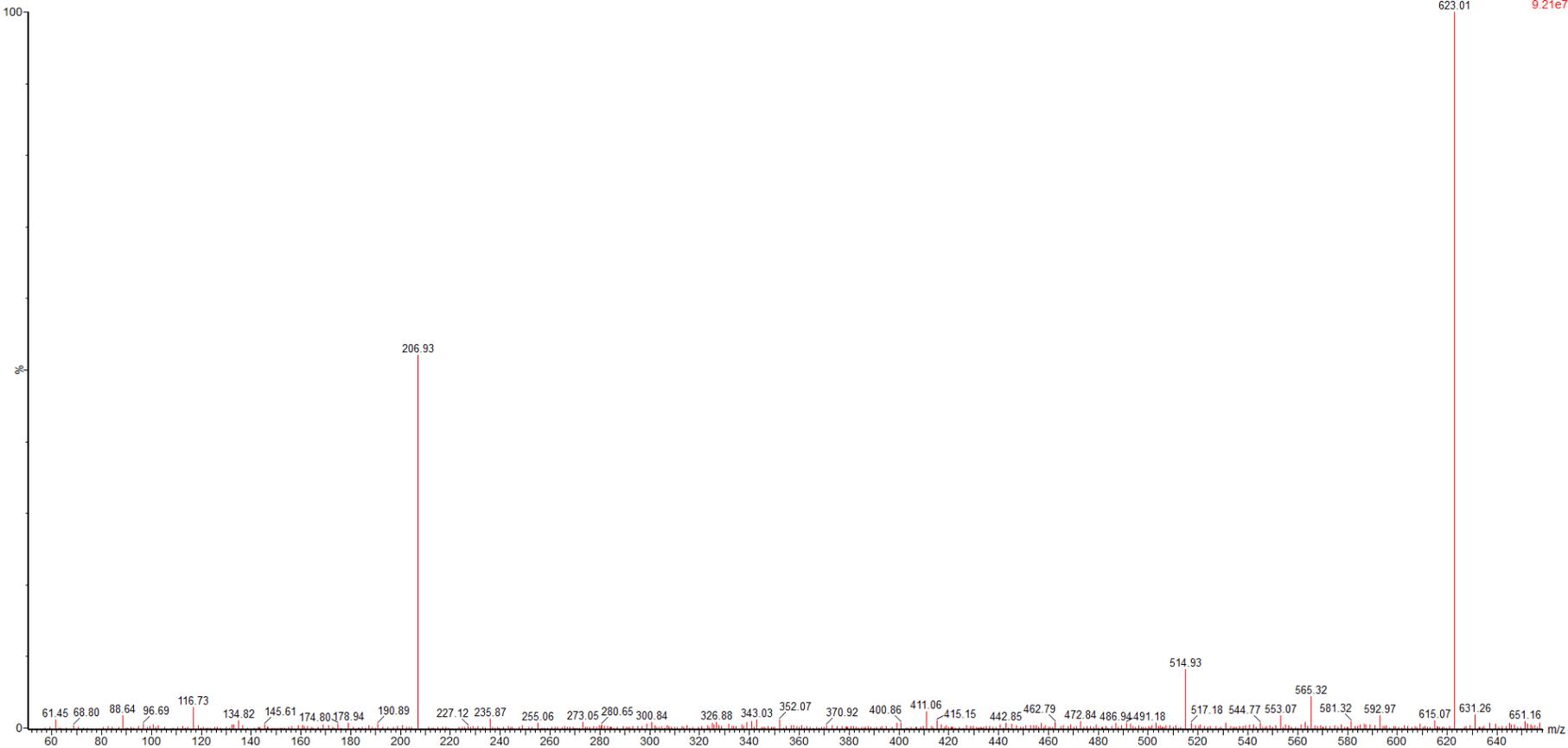


Figure S42: MS-ESI(-) of Substance 23

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 1024 (19.080)

2: Auto Daughters 623.01ES-
3.47e7

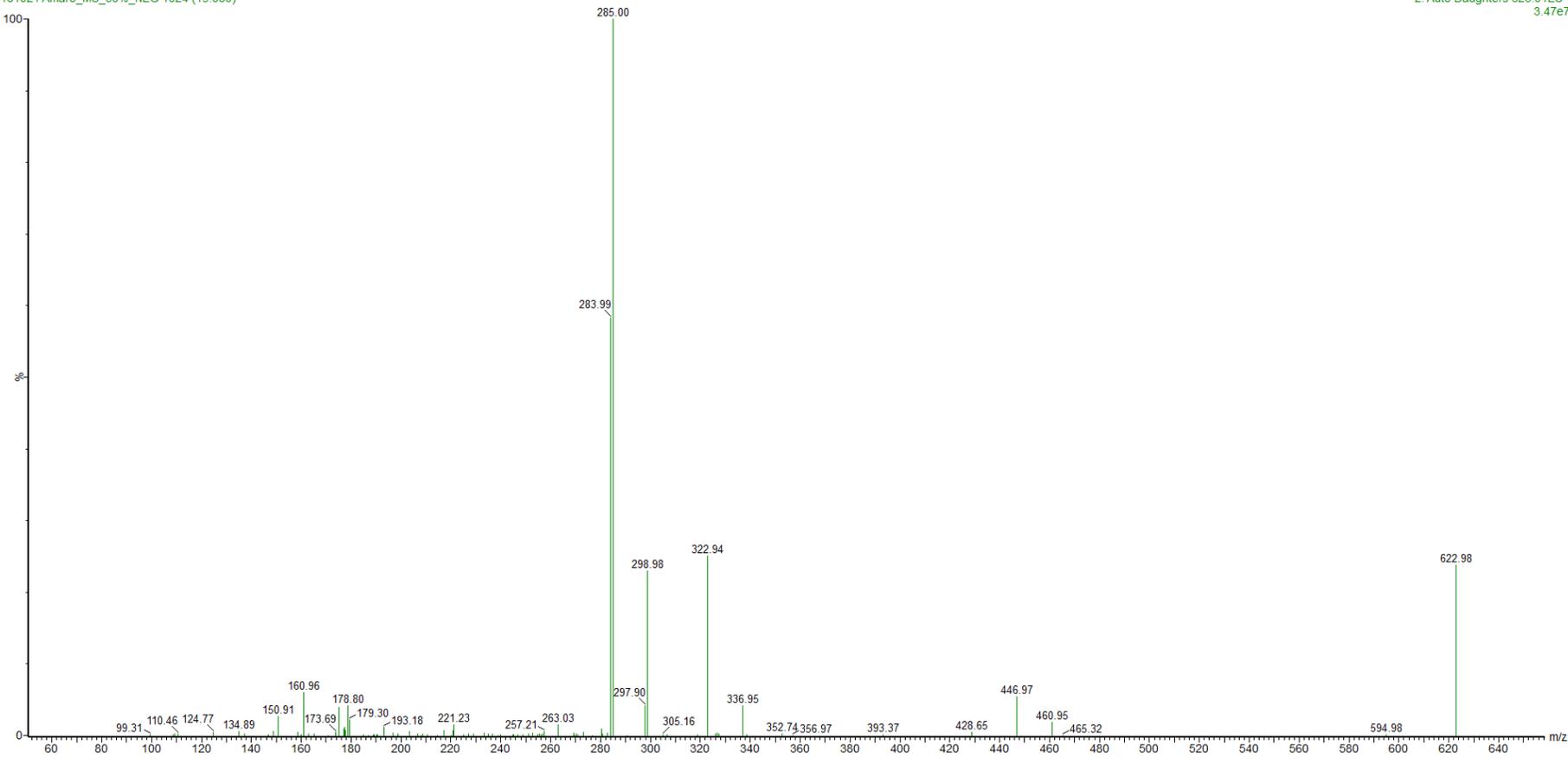


Figure S43: MS/MS-ESI(-) of Substance 23

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 363 (20.181)

1: ScanWave MS ES-
5.94e7

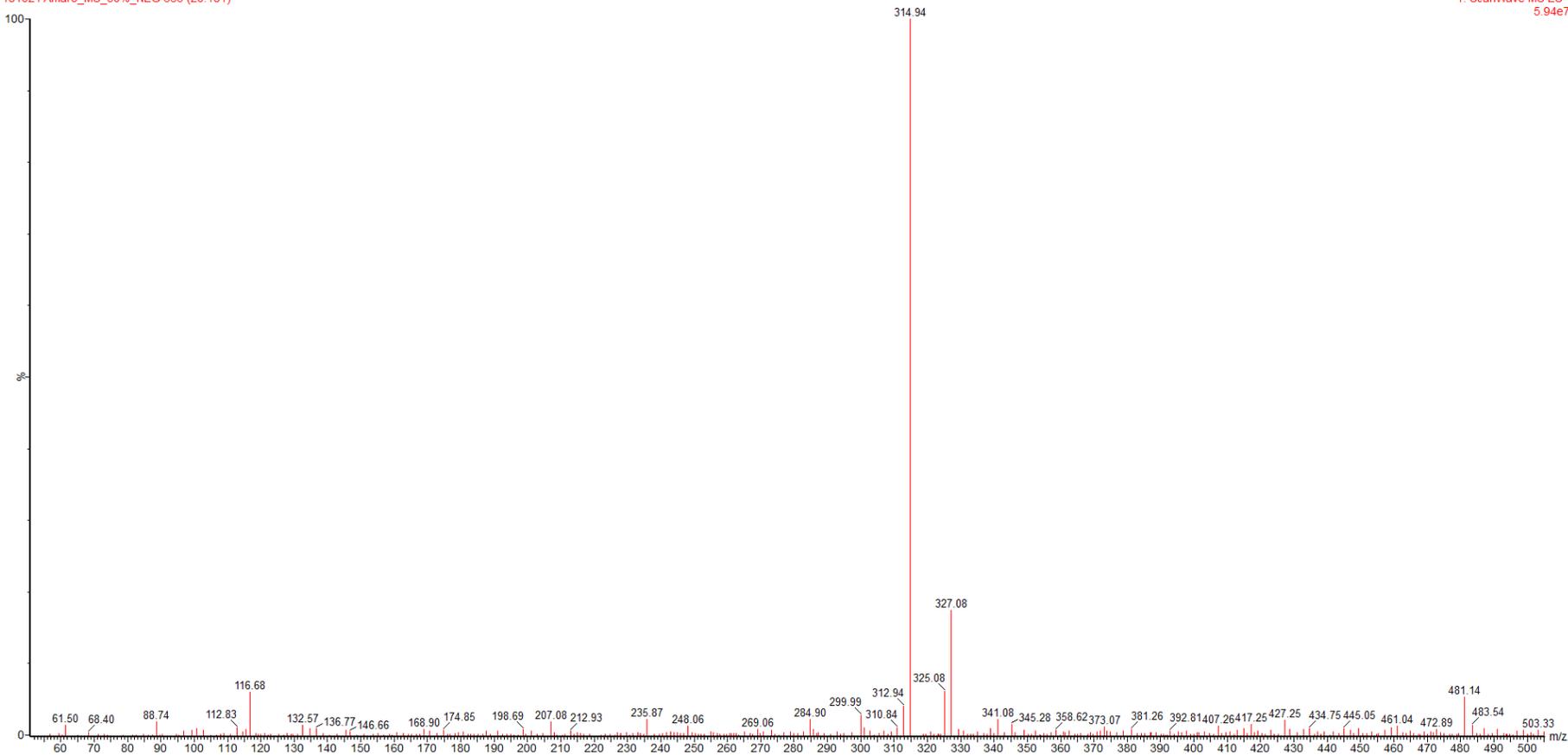


Figure S44: MS-ESI(-) of Substance 24

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50%_NEG 373 (20.712)

1: ScanWave MS ES-
2.94e7

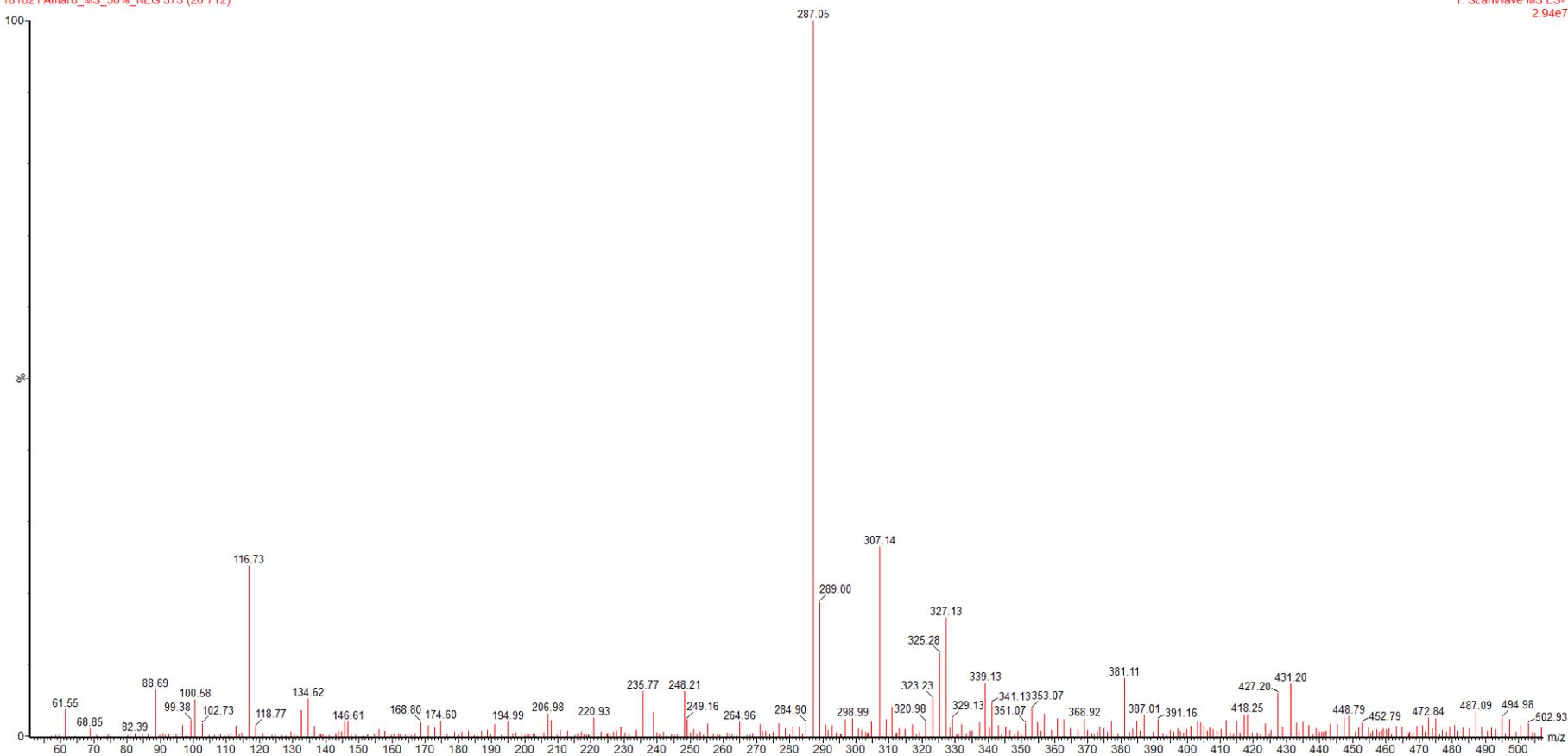


Figure S45: MS-ESI(-) of Substance 25

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50__NEG 354 (19.704)

1: ScanWave MS ES-
6.30e6

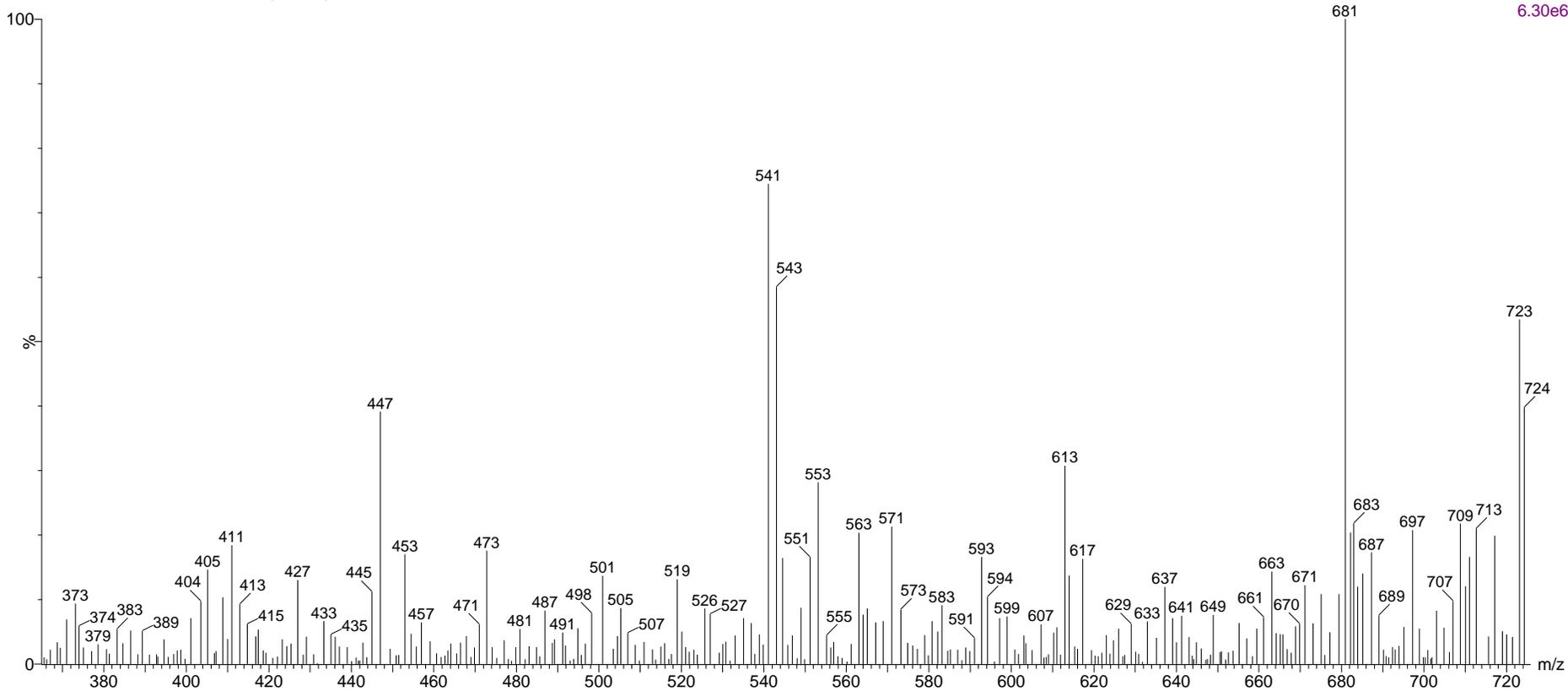


Figure S46: MS-ESI(-) of Substance D1

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50__NEG 361 (20.076)

1: ScanWave MS ES-
3.73e7

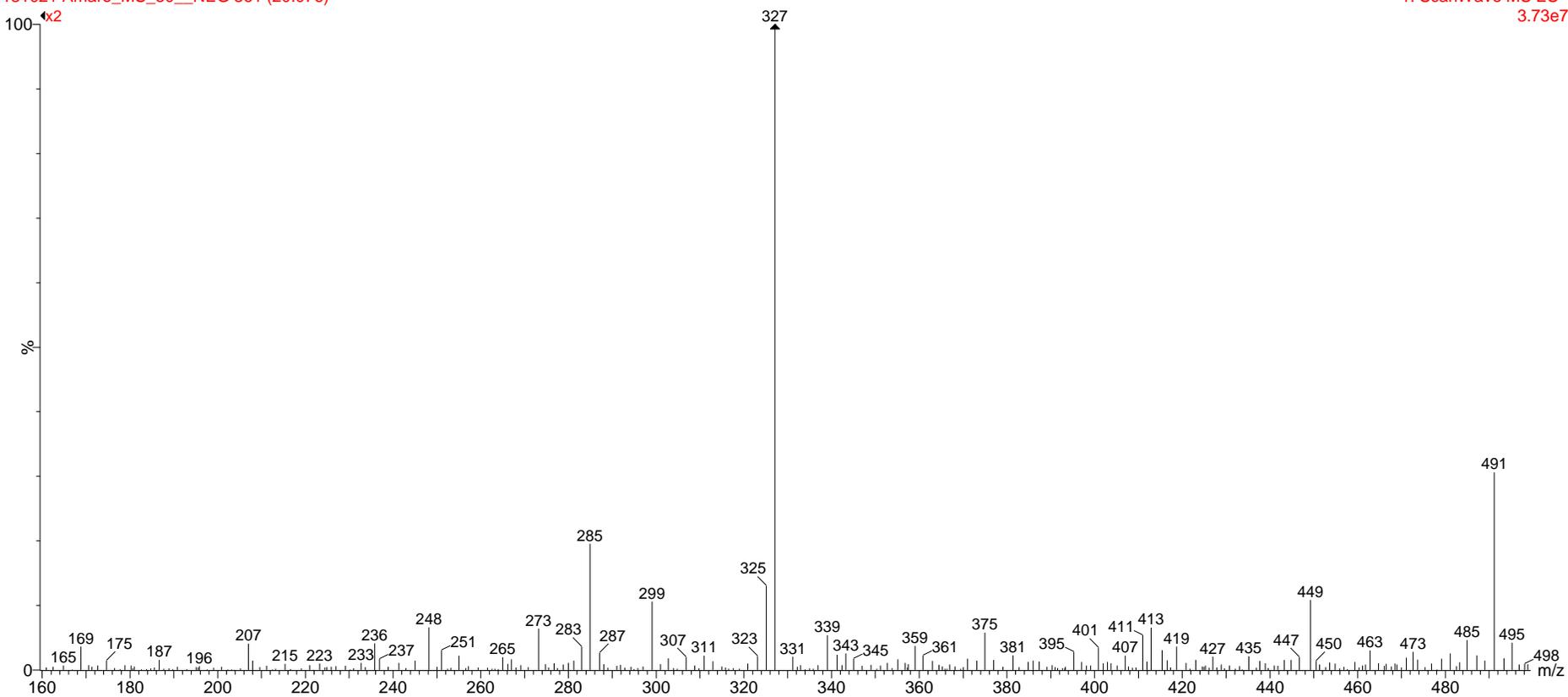


Figure S47: MS-ESI(-) of Substance D2

181021 Amaro_MS_50%_NEG

181021 Amaro_MS_50__NEG 367 (20.394)

1: ScanWave MS ES-
1.38e8

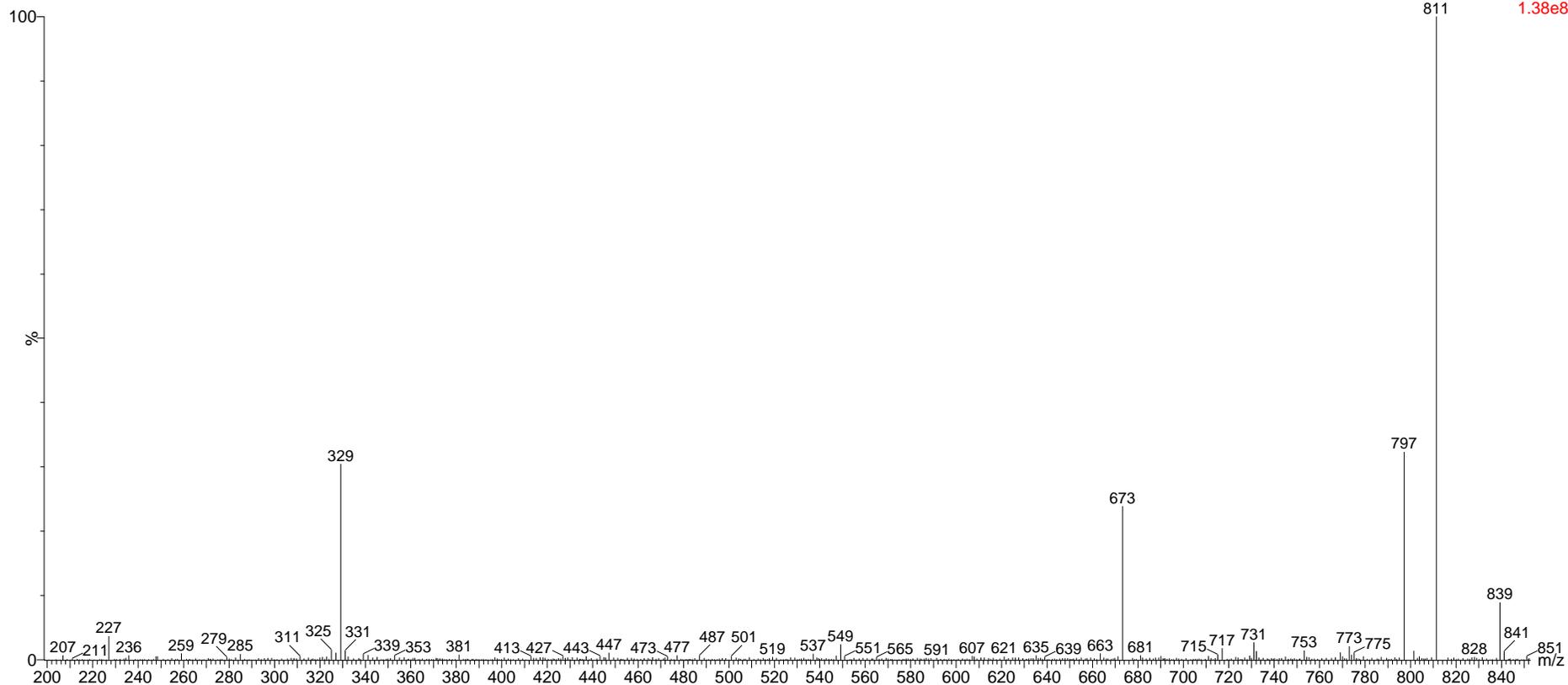


Figure S48: MS-ESI(-) of Substance D3

181021 Amaro_MS_50%_NEG
181021 Amaro_MS_50__NEG 368 (20.447)

1: ScanWave MS ES-
7.67e6

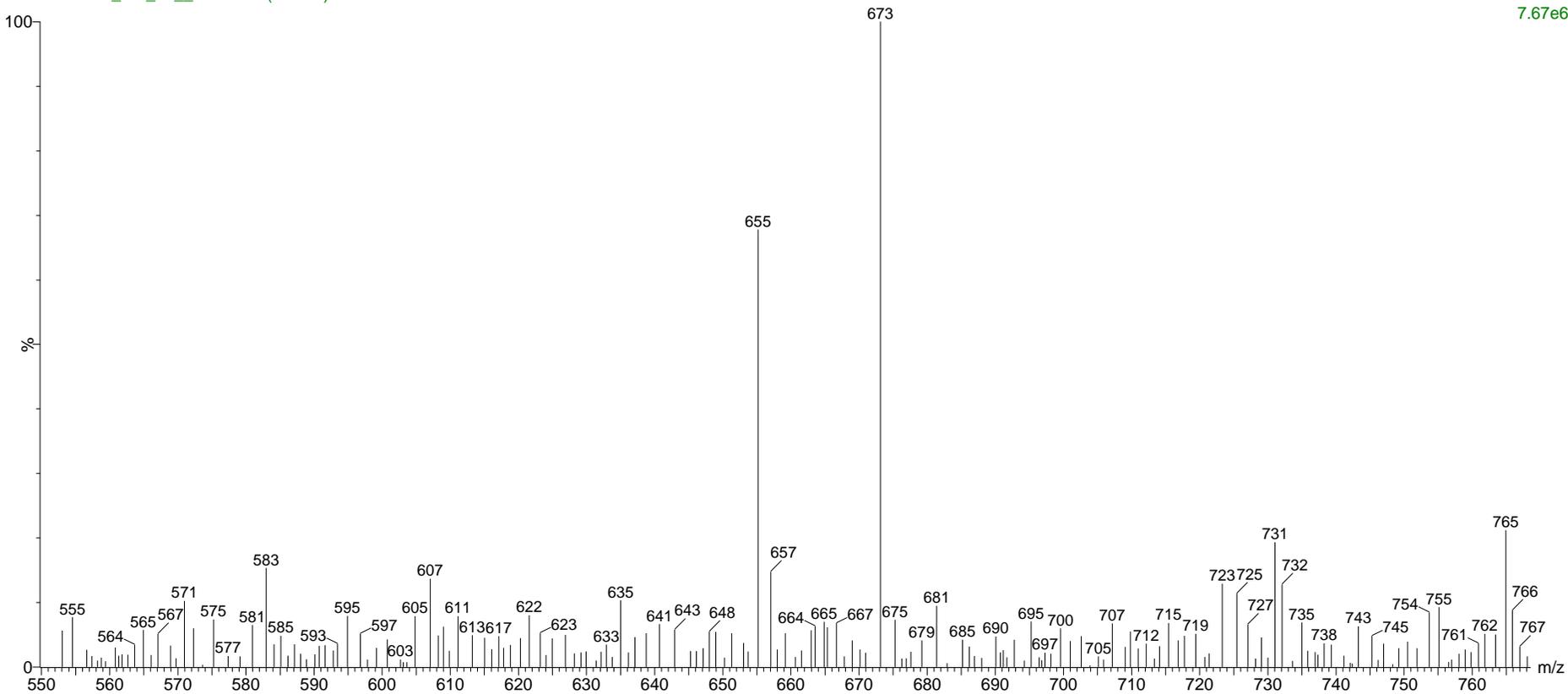


Figure S49: MS-ESI(-) of Substance D4

Compound name: ACIDO CLOROGENICO (1)
Correlation coefficient: $r = 0.998742$, $r^2 = 0.997486$
Calibration curve: $556625 * x + -4552.93$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: $1/x$, Axis trans: None

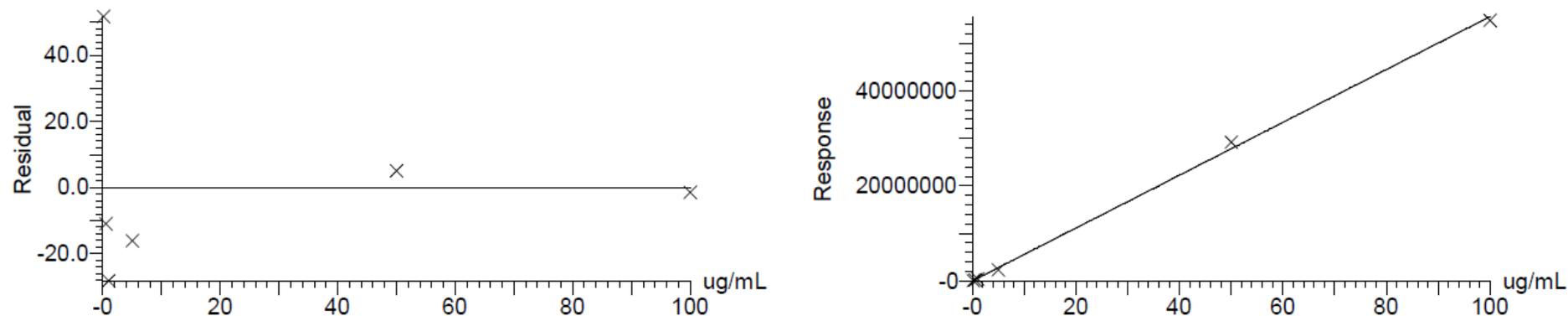


Figure S50: Chlorogenic Acid Calibration Curve 1

Dataset: C:\MassLynx\2021Tesistas.PRO\210823_CURVAACIDOCLOGENICO_1.qld

Last Altered: Monday, August 21, 2023 17:31:16 SA Pacific Standard Time

Printed: Monday, August 21, 2023 17:33:13 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesistas.PRO\MethDB\190823_acido clorogenico.mdb 21 Aug 2023 17:31:16

Calibration: 21 Aug 2023 17:31:16

Sample Name: 190823_STAC_PR_1_3_P Sample Name: 190823_STAC_PR1_POS Sample Name: 190823_STAC_PR2_POS

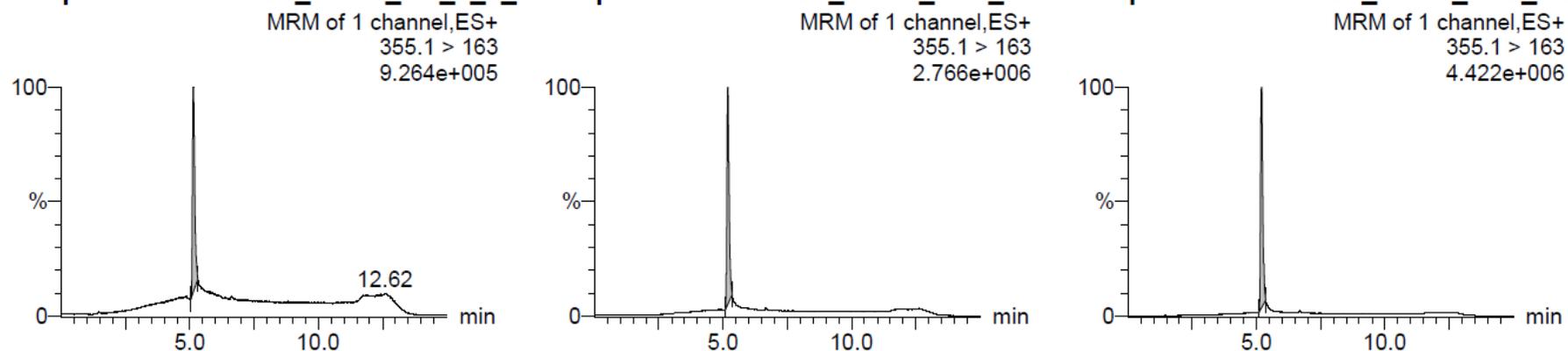
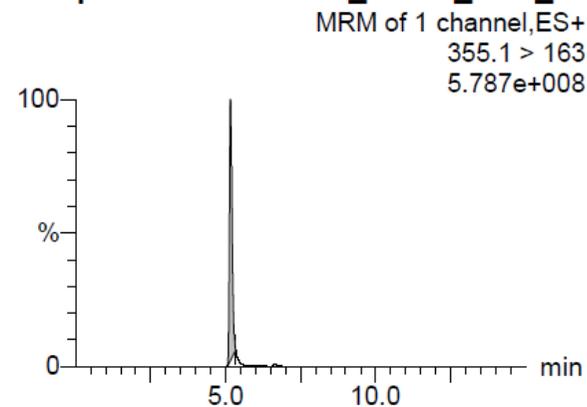
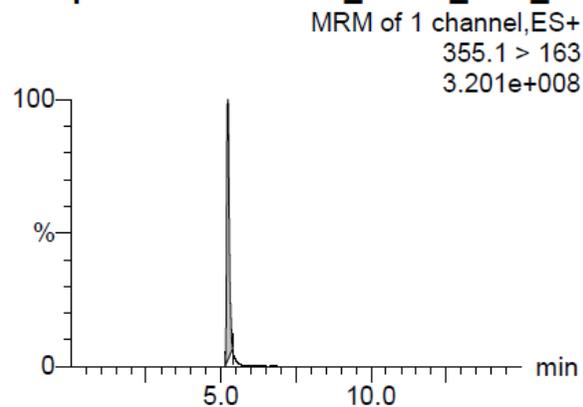
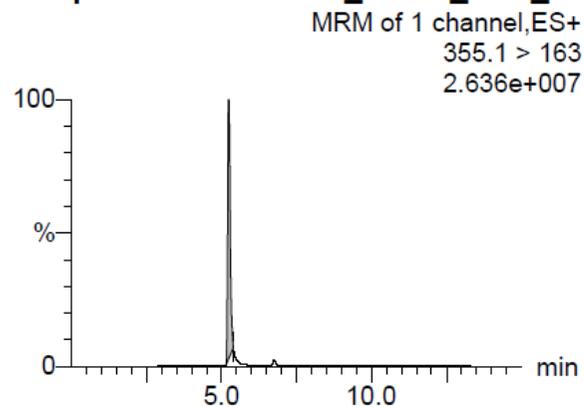
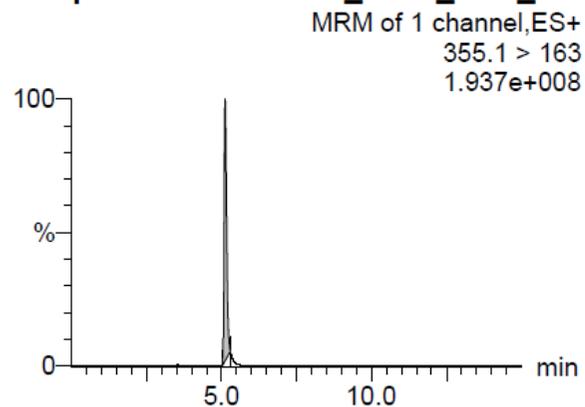


Figure S51: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 1, 2, and 3 (Curve 1)

Sample Name: 190823_STAC_PR3_POS Sample Name: 190823_STAC_PR4_POS Sample Name: 190823_STAC_PR5_POS



Sample Name: 190823_MAC_PR6_POS



Sample Name: 190823_DEC_PR7_POS

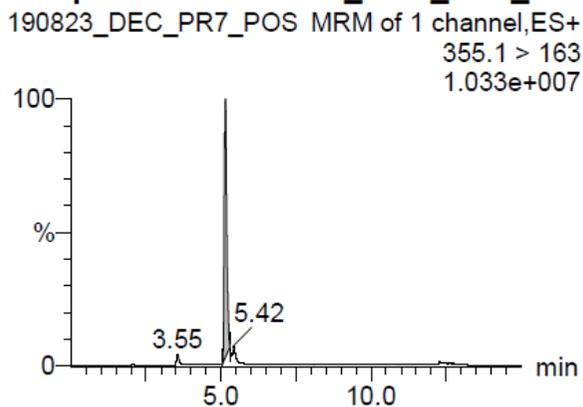


Figure S52: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 4, 5, and 6 (Curve 1); Hydroethanolic Extract 1 and Aqueous Extract 1

| | # Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|-------------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 190823_STAC_... | Standard | 0.100 | 5.1366 | 79897.891 | | 79897.891 | bb | 0.152 | 51.7 |
| 2 | 2 190823_STAC_... | Standard | 0.500 | 5.1800 | 243268.641 | | 243268.641 | bb | 0.445 | -11.0 |
| 3 | 3 190823_STAC_... | Standard | 1.000 | 5.1945 | 394913.063 | | 394913.063 | bb | 0.718 | -28.2 |
| 4 | 4 190823_STAC_... | Standard | 5.000 | 5.2393 | 2329791.750 | | 2329791.750 | bb | 4.194 | -16.1 |
| 5 | 5 190823_STAC_... | Standard | 50.000 | 5.2225 | 29220226.0... | | 29220226.0... | bb | 52.504 | 5.0 |
| 6 | 6 190823_STAC_... | Standard | 100.000 | 5.1585 | 54871988.0... | | 54871988.0... | bb | 98.588 | -1.4 |
| 7 | 7 190823_MAC_P... | Analyte | | 5.1198 | 17492622.0... | | 17492622.0... | bb | 31.434 | |
| 8 | 8 190823_DEC_P... | Analyte | | 5.1408 | 895424.063 | | 895424.063 | bb | 1.617 | |

Figure S53: Quantify of Chlorogenic Acid in Hydroethanolic Extract 1 and Aqueous Extract 1 (Curve 1)

Compound name: ACIDO CLOROGENICO (1)
Correlation coefficient: $r = 0.999049$, $r^2 = 0.998099$
Calibration curve: $562968 * x + 11478.5$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: $1/x$, Axis trans: None

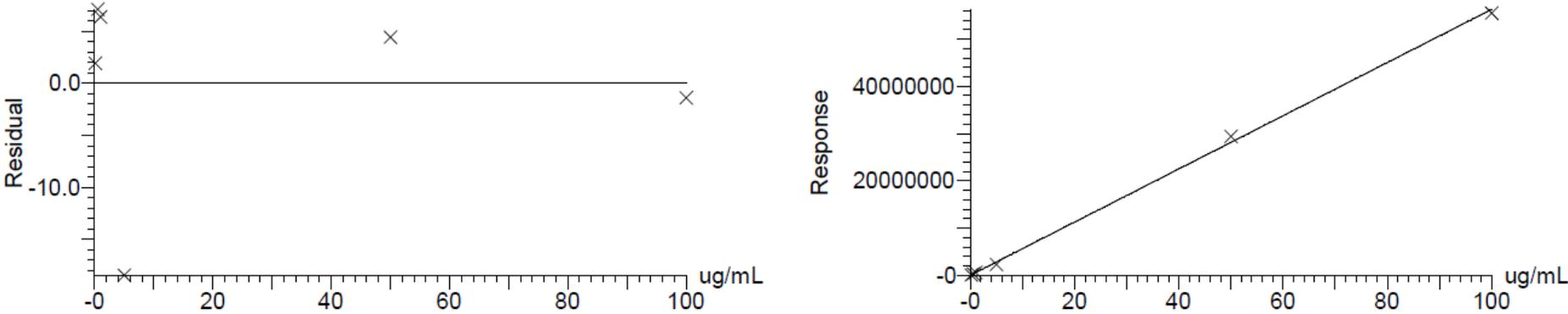


Figure S54: Chlorogenic Acid Calibration Curve 2

Dataset: C:\MassLynx\2021Tesisas.PRO\210823_CURVAACIDOCLOGENICO_2.qld

Last Altered: Monday, August 21, 2023 17:34:22 SA Pacific Standard Time

Printed: Monday, August 21, 2023 17:35:11 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesisas.PRO\MethDB\190823_acido clorogenico.mdb 21 Aug 2023 17:34:22

Calibration: 21 Aug 2023 17:34:22

Sample Name: 190823_STAC_PR_1_3_2_Sample Name: 190823_STAC_PR1_2_PCSample Name: 190823_STAC_PR2_2_POS

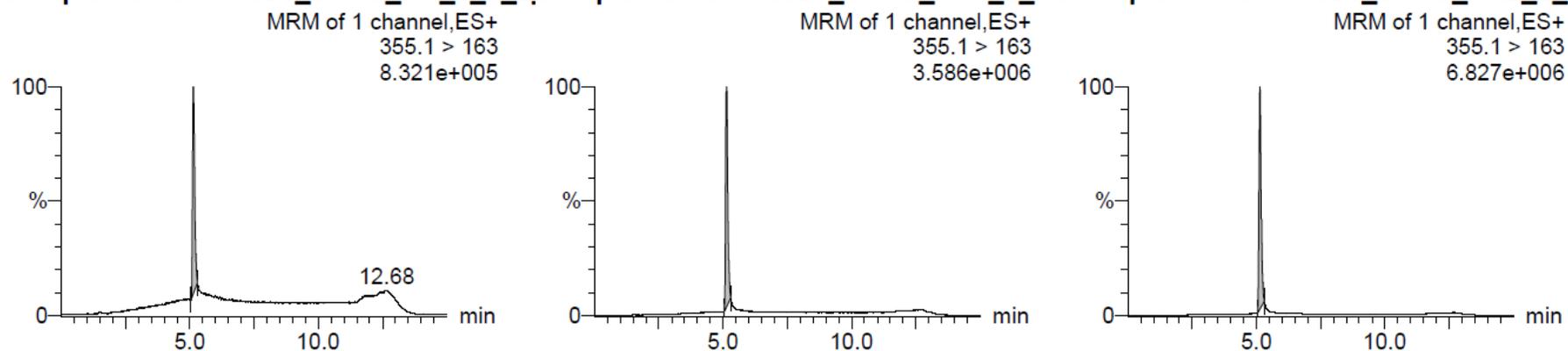
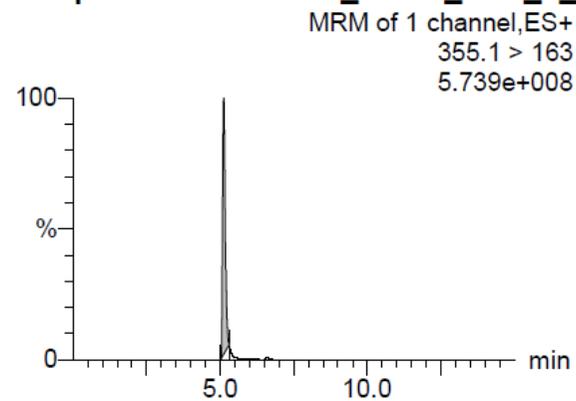
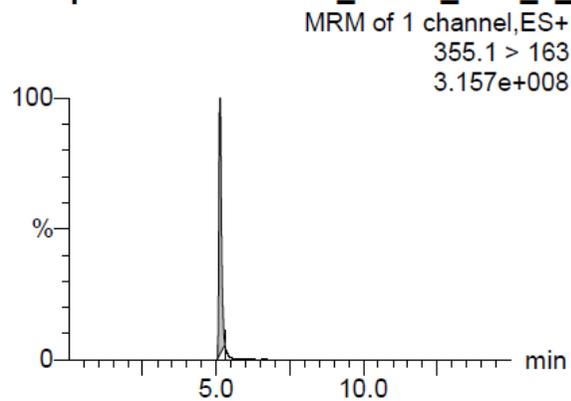
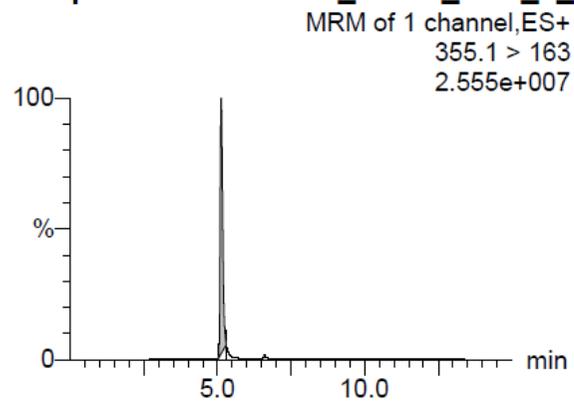


Figure S55: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 1, 2, and 3(Curve 2)

Sample Name: 190823_STAC_PR3_2_PC Sample Name: 190823_STAC_PR4_2_PC Sample Name: 190823_STAC_PR5_2_POS



Sample Name: 190823_MAC_PR6_2_PO Sample Name: 190823_DEC_PR7_2_POS

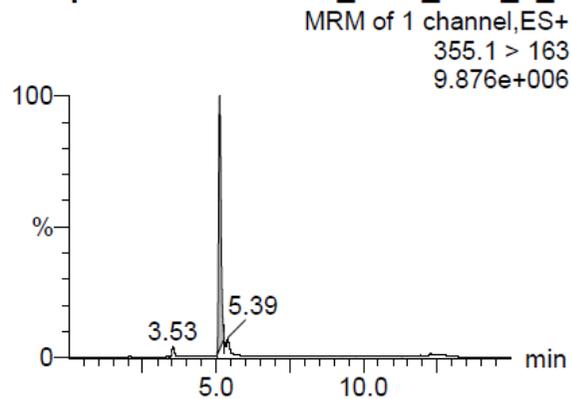
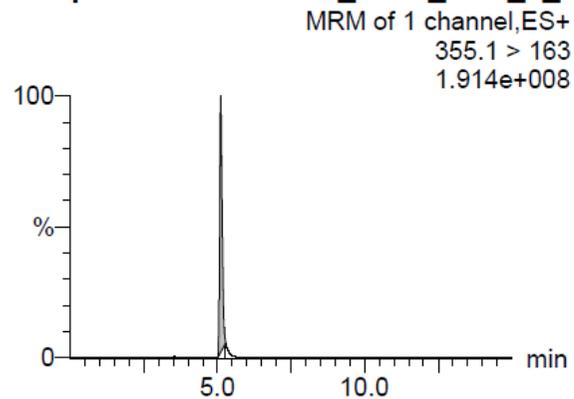


Figure S56: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 4, 5, and 6 (Curve 2); Hydroethanolic Extract 2 and Aqueous Extract 2

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|-----------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 190823_STAC_... | Standard | 0.100 | 5.1361 | 68863.273 | | 68863.273 | bb | 0.102 | 1.9 |
| 2 | 2 | 190823_STAC_... | Standard | 0.500 | 5.1305 | 312949.031 | | 312949.031 | bb | 0.536 | 7.1 |
| 3 | 3 | 190823_STAC_... | Standard | 1.000 | 5.1319 | 610334.063 | | 610334.063 | bb | 1.064 | 6.4 |
| 4 | 4 | 190823_STAC_... | Standard | 5.000 | 5.1268 | 2307404.500 | | 2307404.500 | bb | 4.078 | -18.4 |
| 5 | 5 | 190823_STAC_... | Standard | 50.000 | 5.1236 | 29402018.0... | | 29402018.0... | bb | 52.206 | 4.4 |
| 6 | 6 | 190823_STAC_... | Standard | 100.000 | 5.1175 | 55528056.0... | | 55528056.0... | bb | 98.614 | -1.4 |
| 7 | 7 | 190823_MAC_P... | Analyte | | 5.1091 | 17297620.0... | | 17297620.0... | bb | 30.705 | |
| 8 | 8 | 190823_DEC_P... | Analyte | | 5.1105 | 858223.125 | | 858223.125 | bb | 1.504 | |

Figure S57: Quantify of Chlorogenic Acid in Hydroethanolic Extract 2 and Aqueous Extract 2 (Curve 2)

Compound name: ACIDO CLOROGENICO (1)
Correlation coefficient: $r = 0.999867$, $r^2 = 0.999734$
Calibration curve: $524147 * x + -33459.9$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

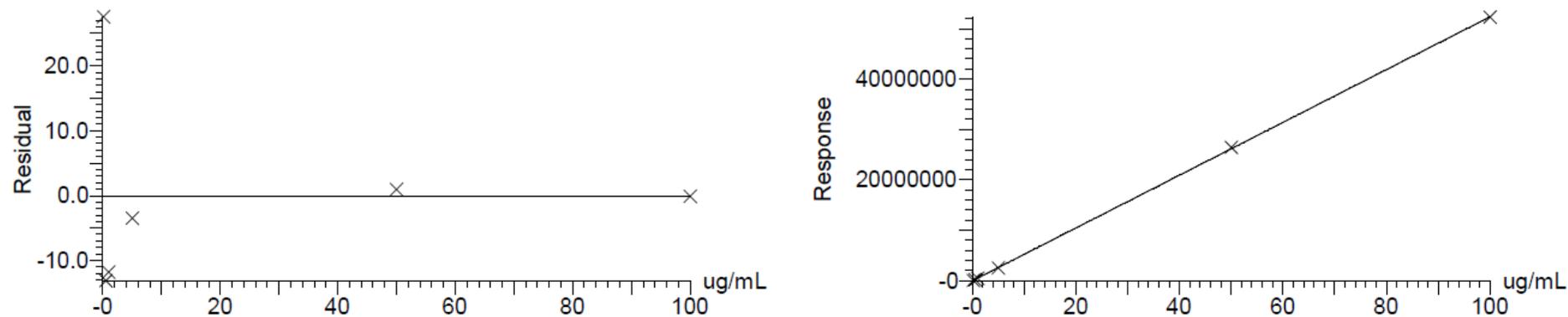


Figure S58: Chlorogenic Acid Calibration Curve 3

Dataset: Untitled

Last Altered: Monday, August 21, 2023 17:35:34 SA Pacific Standard Time

Printed: Monday, August 21, 2023 17:35:46 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesistas.PRO\MethDB\190823_acido clorogenico.mdb 21 Aug 2023 17:35:34

Calibration: 21 Aug 2023 17:35:34

Sample Name: 190823_STAC_PR_1_3_3_Sample Name: 190823_STAC_PR1_3_PCSample Name: 190823_STAC_PR2_3_POS

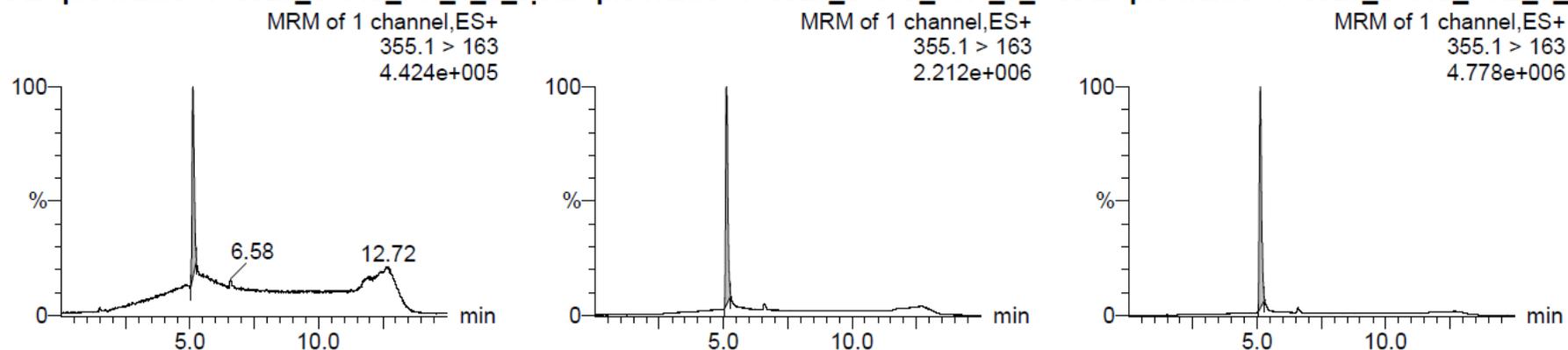
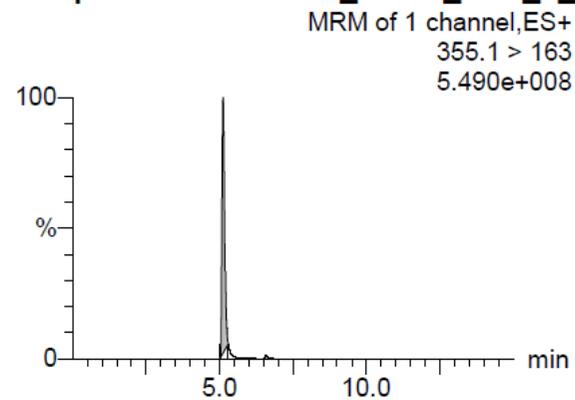
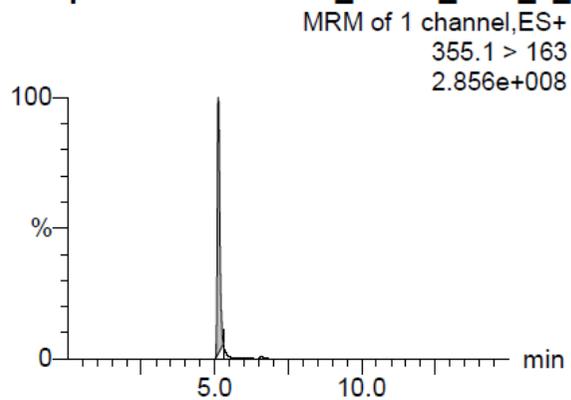
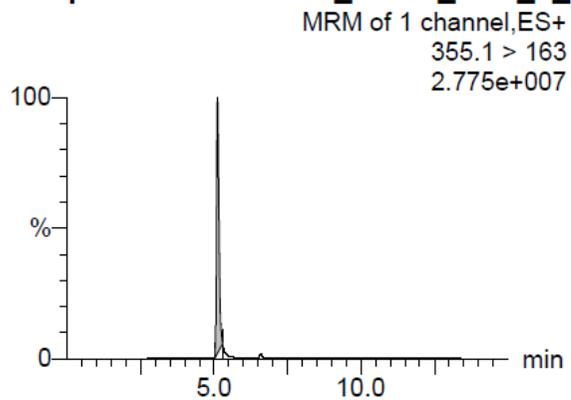


Figure S59: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 1, 2, and 3 (Curve 3)

Sample Name: 190823_STAC_PR3_3_PC Sample Name: 190823_STAC_PR4_3_PC Sample Name: 190823_STAC_PR5_3_POS



Sample Name: 190823_MAC_PR6_3_PO Sample Name: 190823_DEC_PR7_3_POS

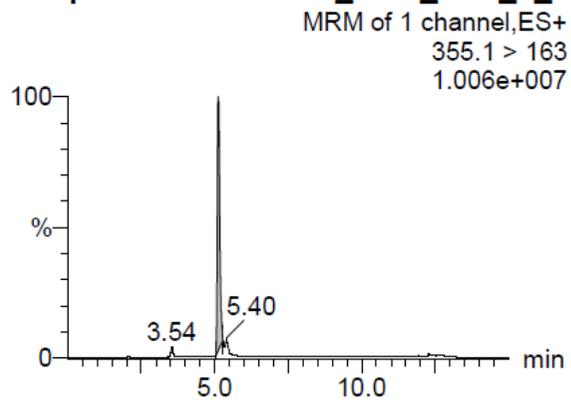
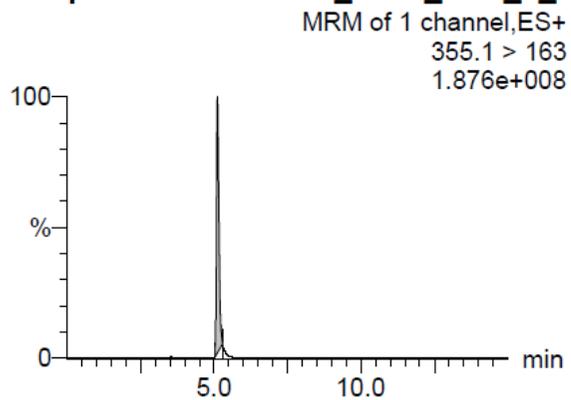


Figure S60: UHPLC-ESI-MRM/MS of Chlorogenic Acid Standards 4, 5, and 6 (Curve 3); Hydroethanolic Extract 3 and Aqueous Extract 3

| | # Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|-------------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 190823_STAC_... | Standard | 0.100 | 5.1166 | 33399.672 | | 33399.672 | bb | 0.128 | 27.6 |
| 2 | 2 190823_STAC_... | Standard | 0.500 | 5.1147 | 194224.922 | | 194224.922 | bb | 0.434 | -13.1 |
| 3 | 3 190823_STAC_... | Standard | 1.000 | 5.1184 | 429023.063 | | 429023.063 | bb | 0.882 | -11.8 |
| 4 | 4 190823_STAC_... | Standard | 5.000 | 5.1170 | 2496041.500 | | 2496041.500 | bb | 4.826 | -3.5 |
| 5 | 5 190823_STAC_... | Standard | 50.000 | 5.1184 | 26424958.0... | | 26424958.0... | bb | 50.479 | 1.0 |
| 6 | 6 190823_STAC_... | Standard | 100.000 | 5.1166 | 52303020.0... | | 52303020.0... | bb | 99.851 | -0.1 |
| 7 | 7 190823_MAC_P... | Analyte | | 5.1161 | 16999852.0... | | 16999852.0... | bb | 32.497 | |
| 8 | 8 190823_DEC_P... | Analyte | | 5.1185 | 878478.250 | | 878478.250 | bb | 1.740 | |

Figure S61: Quantify of Chlorogenic Acid in Hydroethanolic Extract 3 and Aqueous Extract 3 (Curve 3)

Compound name: RUTINA
Correlation coefficient: $r = 0.999462$, $r^2 = 0.998925$
Calibration curve: $877034 * x + 45598.5$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: $1/x$, Axis trans: None

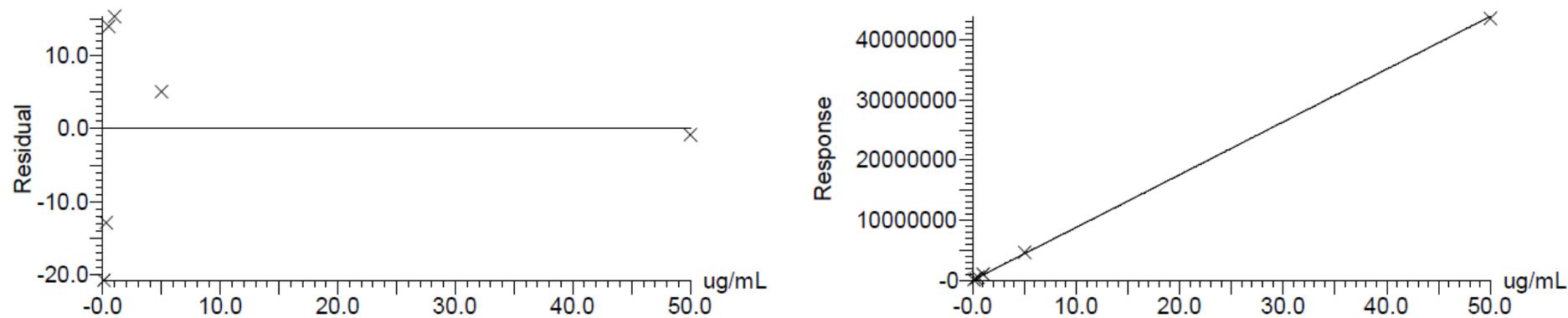


Figure S62: Rutin Calibration Curve 1

Quantify Compound Report MassLynx V4.2 SCN1007

RESULTADOS DE LABORATORIO

Dataset: C:\MassLynx\2021Tesisas.PRO\210823_CURVARUTINA_3 opcional.qld

Last Altered: Wednesday, August 23, 2023 08:35:01 SA Pacific Standard Time

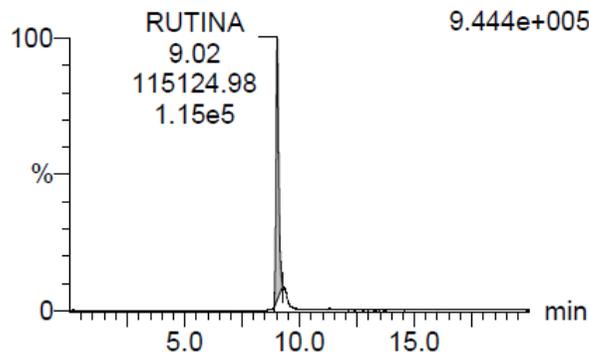
Printed: Wednesday, August 23, 2023 08:36:19 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesisas.PRO\MethDB\210823_RUTINA_2.mdb 21 Aug 2023 16:00:41

Calibration: 23 Aug 2023 08:35:01

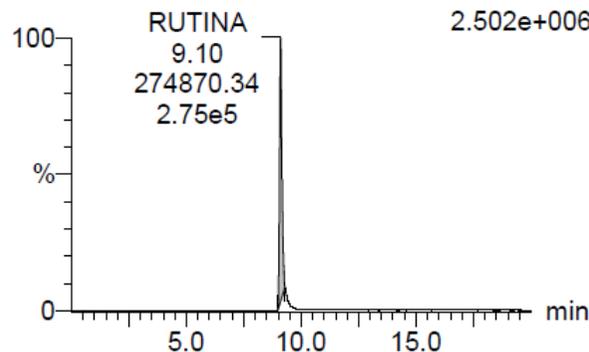
Sample Name: 130823_STR_P6_POS

130823_STR_P6_POS MRM of 1 channel,ES+
611.3 > 303.1
9.444e+005



Sample Name: 130823_STR_P6_1_POS

MRM of 1 channel,ES+
611.3 > 303.1
2.502e+006



Sample Name: 130823_STR_P7_POS

130823_STR_P7_POS MRM of 1 channel,ES+
611.3 > 303.1
4.282e+006

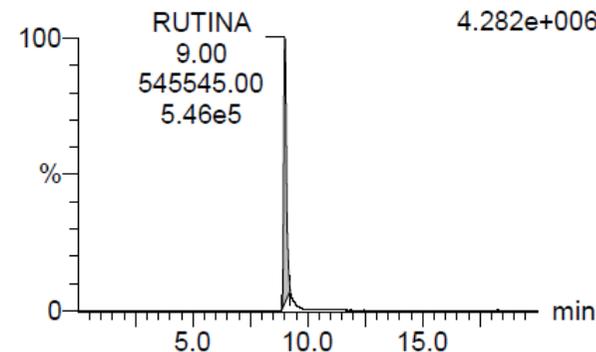
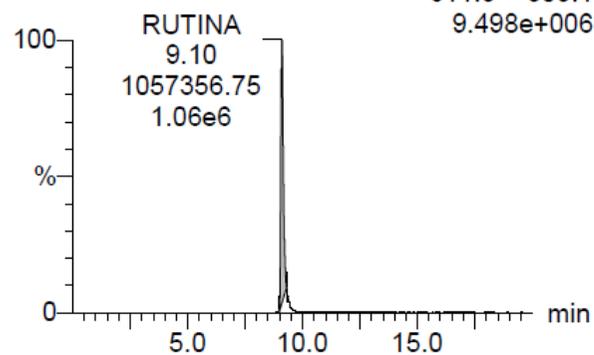


Figure S63: UHPLC-ESI-MRM/MS of Rutin Standards 1, 2, and 3 (Curve 1)

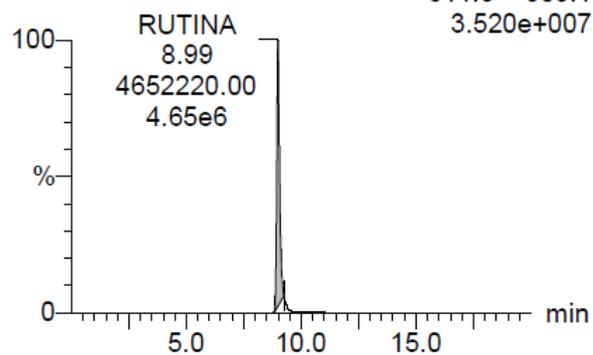
Sample Name: 130823_STR_P8_POS

130823_STR_P8_POS MRM of 1 channel,ES+
611.3 > 303.1
9.498e+006



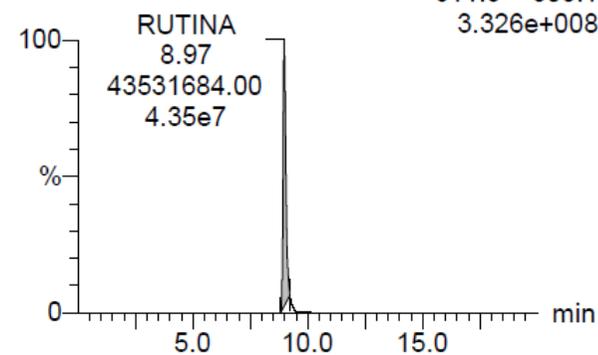
Sample Name: 130823_STR_P8_1_POS

MRM of 1 channel,ES+
611.3 > 303.1
3.520e+007



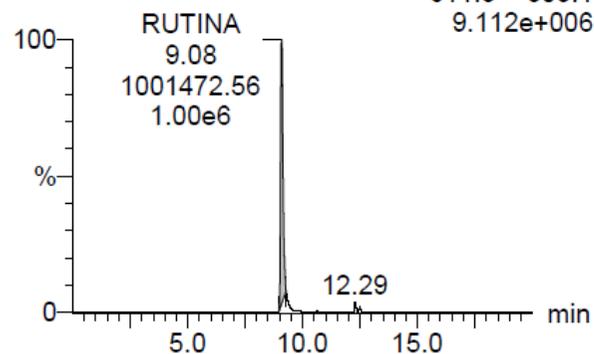
Sample Name: 130823_STR_P9_POS

130823_STR_P9_POS MRM of 1 channel,ES+
611.3 > 303.1
3.326e+008



Sample Name: 130823_MACR_POS

130823_MACR_POS MRM of 1 channel,ES+
611.3 > 303.1
9.112e+006



Sample Name: 130823_DECR_POS

130823_DECR_POS MRM of 1 channel,ES+
611.3 > 303.1
5.589e+006

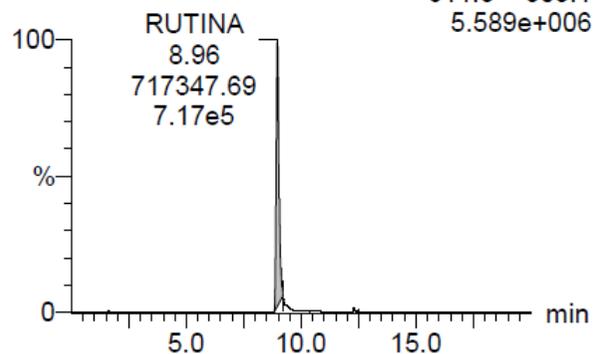


Figure S64: UHPLC-ESI-MRM/MS of Rutin Standards 4, 5, and 6 (Curve 1); Hydroethanolic Extract 1 and Aqueous Extract 1

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|-----------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 130823_STR_P... | Standard | 0.100 | 9.0215 | 115124.984 | | 115124.984 | bb | 0.079 | -20.7 |
| 2 | 2 | 130823_STR_P... | Standard | 0.300 | 9.0989 | 274870.344 | | 274870.344 | bb | 0.261 | -12.9 |
| 3 | 3 | 130823_STR_P... | Standard | 0.500 | 9.0033 | 545545.000 | | 545545.000 | bb | 0.570 | 14.0 |
| 4 | 4 | 130823_STR_P... | Standard | 1.000 | 9.0962 | 1057356.750 | | 1057356.750 | bb | 1.154 | 15.4 |
| 5 | 5 | 130823_STR_P... | Standard | 5.000 | 8.9879 | 4652220.000 | | 4652220.000 | bb | 5.253 | 5.1 |
| 6 | 6 | 130823_STR_P... | Standard | 50.000 | 8.9734 | 43531684.0... | | 43531684.0... | bb | 49.583 | -0.8 |
| 7 | 7 | 130823_MACR_... | Analyte | | 9.0840 | 1001472.563 | | 1001472.563 | bb | 1.090 | |
| 8 | 8 | 130823_DECR_... | Analyte | | 8.9622 | 717347.688 | | 717347.688 | bb | 0.766 | |

Figure S65: Quantify of Rutin in Hydroethanolic Extract 1 and Aqueous Extract 1 (Curve 1)

Compound name: RUTINA

Correlation coefficient: $r = 0.997567$, $r^2 = 0.995140$

Calibration curve: $1.04364e+006 * x + 91038.9$

Response type: External Std, Area

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

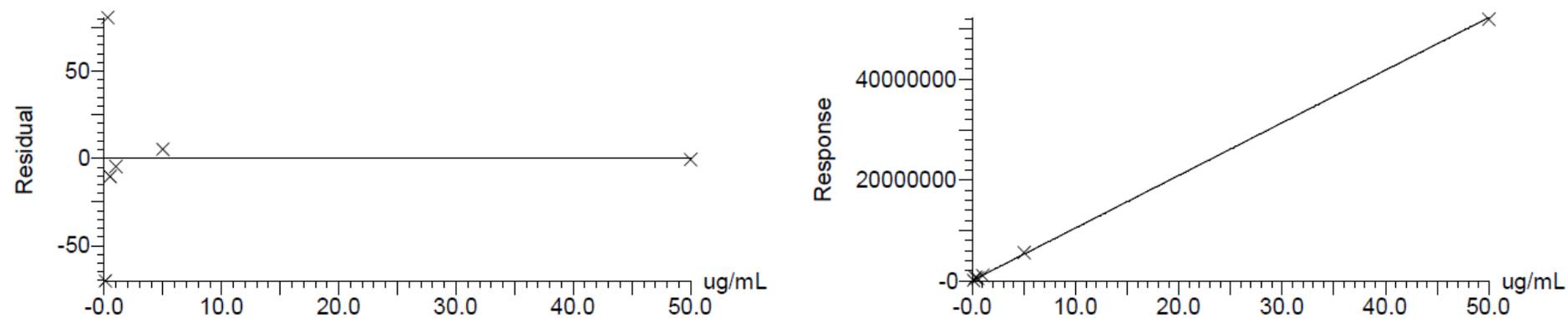
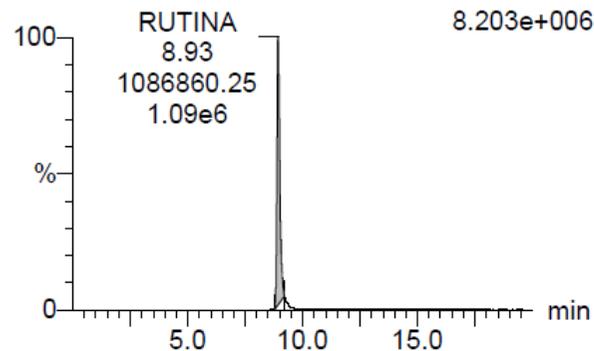


Figure S66: Rutin Calibration Curve 2

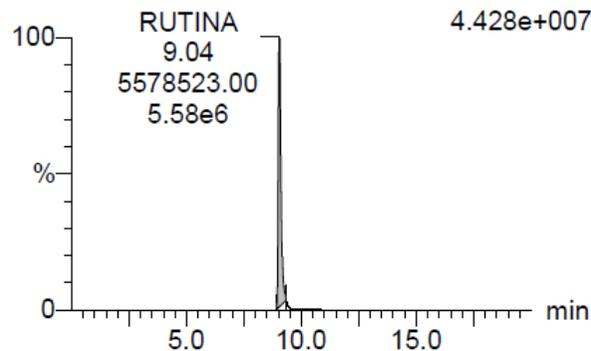
Sample Name: 140823_ST8R_1_POS

140823_ST8R_1_POS MRM of 1 channel,ES+
611.3 > 303.1
8.203e+006



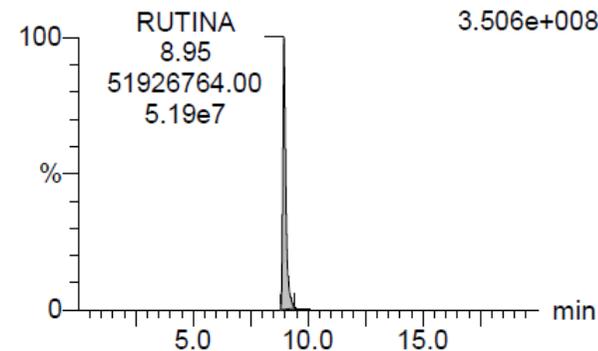
Sample Name: 140823_ST8R_3_POS

140823_ST8R_3_POS MRM of 1 channel,ES+
611.3 > 303.1
4.428e+007



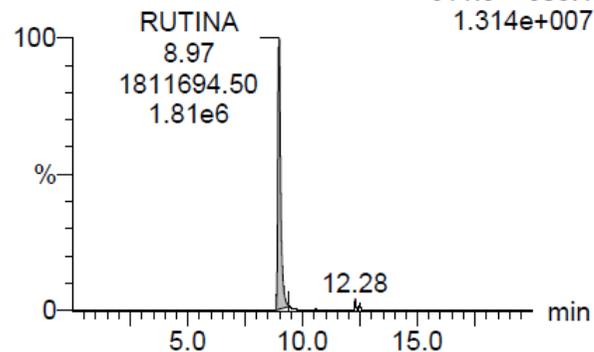
Sample Name: 140823_ST9R_1_POS

140823_ST9R_1_POS MRM of 1 channel,ES+
611.3 > 303.1
3.506e+008



Sample Name: 140823_MAC_1_POS

140823_MAC_1_POS MRM of 1 channel,ES+
611.3 > 303.1
1.314e+007



Sample Name: 140823_DEC_1_POS

140823_DEC_1_POS MRM of 1 channel,ES+
611.3 > 303.1
7.678e+006

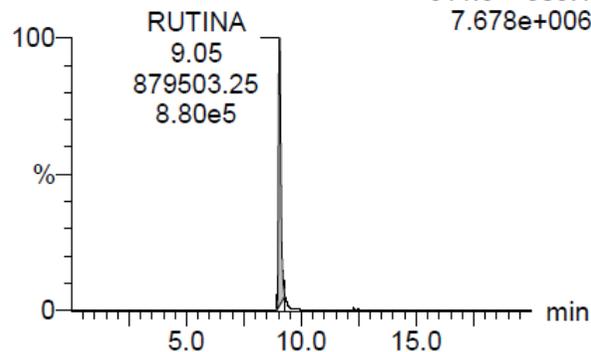


Figure S68: UHPLC-ESI-MRM/MS of Rutin Standards 4, 5, and 6 (Curve 2); Hydroethanolic Extract 2 and Aqueous Extract 2

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|------------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 140823_ST6R_1... | Standard | 0.100 | 8.9240 | 122219.648 | | 122219.648 | bb | 0.030 | -70.1 |
| 2 | 2 | 140823_ST6R_3... | Standard | 0.300 | 8.9748 | 656584.438 | | 656584.438 | bb | 0.542 | 80.6 |
| 3 | 3 | 140823_ST7R_1... | Standard | 0.500 | 8.9837 | 558466.375 | | 558466.375 | bb | 0.448 | -10.4 |
| 4 | 4 | 140823_ST8R_1... | Standard | 1.000 | 8.9286 | 1086860.250 | | 1086860.250 | bb | 0.954 | -4.6 |
| 5 | 5 | 140823_ST8R_3... | Standard | 5.000 | 9.0392 | 5578523.000 | | 5578523.000 | bb | 5.258 | 5.2 |
| 6 | 6 | 140823_ST9R_1... | Standard | 50.000 | 8.9496 | 51926764.0... | | 51926764.0... | bb | 49.668 | -0.7 |
| 7 | 7 | 140823_MAC_1... | Analyte | | 8.9683 | 1811694.500 | | 1811694.500 | bb | 1.649 | |
| 8 | 8 | 140823_DEC_1... | Analyte | | 9.0462 | 879503.250 | | 879503.250 | bb | 0.755 | |

Figure S69: Quantify of Rutin in Hydroethanolic Extract 2 and Aqueous Extract 2 (Curve 2)

Compound name: RUTINA
Correlation coefficient: $r = 0.967644$, $r^2 = 0.936335$
Calibration curve: $838429 * x + -15613.6$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: $1/x$, Axis trans: None

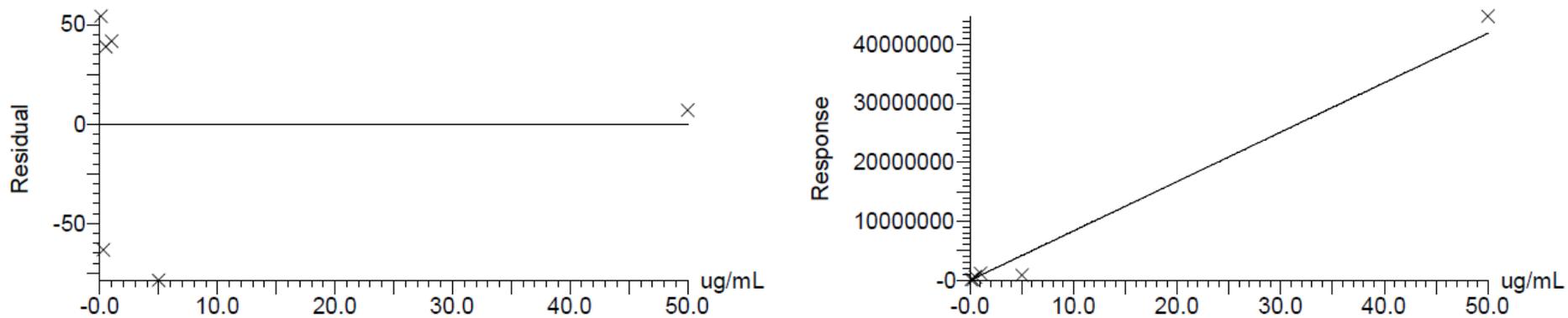


Figure S70: Rutin Calibration Curve 3

Quantify Compound Report MassLynx V4.2 SCN1007
RESULTADOS DE LABORATORIO

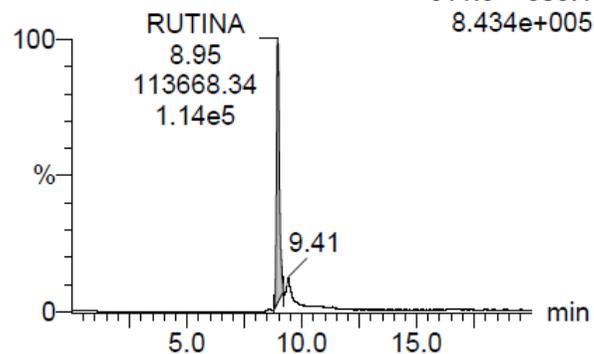
Dataset: C:\MassLynx\2021Tesisas.PRO\210823_CURVARUTINA_3.qld

Last Altered: Tuesday, August 22, 2023 17:08:53 SA Pacific Standard Time
Printed: Tuesday, August 22, 2023 17:11:58 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesisas.PRO\MethDB\210823_RUTINA_3.mdb 22 Aug 2023 16:20:47
Calibration: 22 Aug 2023 17:08:53

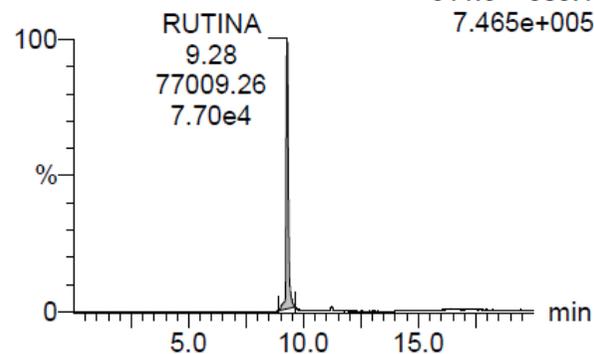
Sample Name: 140823_ST6R_POS

140823_ST6R_POS MRM of 1 channel,ES+
611.3 > 303.1
8.434e+005



Sample Name: 140823_ST6R_2_POS

140823_ST6R_2_POS MRM of 1 channel,ES+
611.3 > 303.1
7.465e+005



Sample Name: 140823_ST7R_POS

140823_ST7R_POS MRM of 1 channel,ES+
611.3 > 303.1
4.486e+006

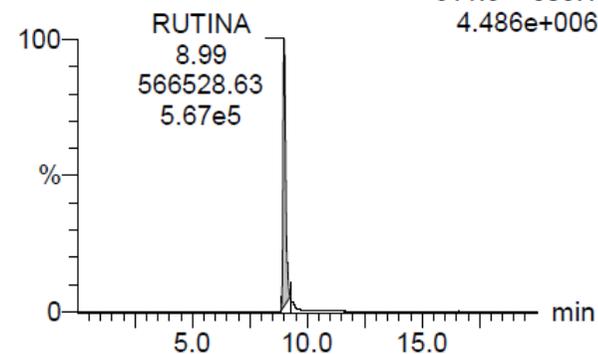
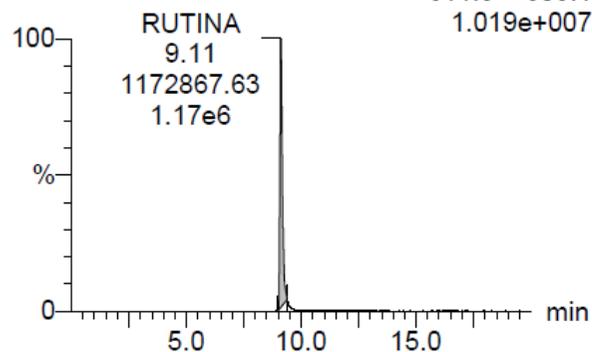


Figure S71: UHPLC-ESI-MRM/MS of Rutin Standards 1, 2, and 3 (Curve 3)

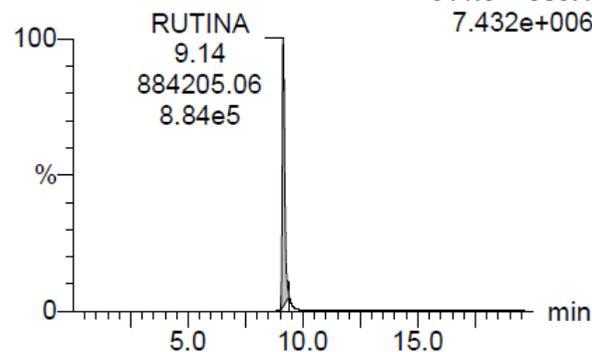
Sample Name: 140823_ST8R_POS

140823_ST8R_POS MRM of 1 channel,ES+
611.3 > 303.1
1.019e+007



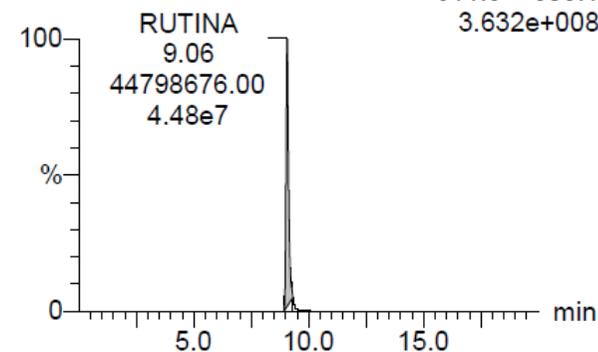
Sample Name: 140823_ST8R_2_POS

140823_ST8R_2_POS MRM of 1 channel,ES+
611.3 > 303.1
7.432e+006



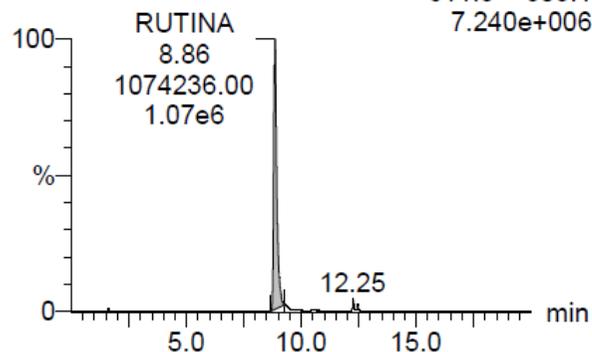
Sample Name: 140823_ST9R_POS

140823_ST9R_POS MRM of 1 channel,ES+
611.3 > 303.1
3.632e+008



Sample Name: 140823_MAC_POS

040823_MAC_POS MRM of 1 channel,ES+
611.3 > 303.1
7.240e+006



Sample Name: 140823_DEC_POS

040823_DEC_POS MRM of 1 channel,ES+
611.3 > 303.1
5.996e+006

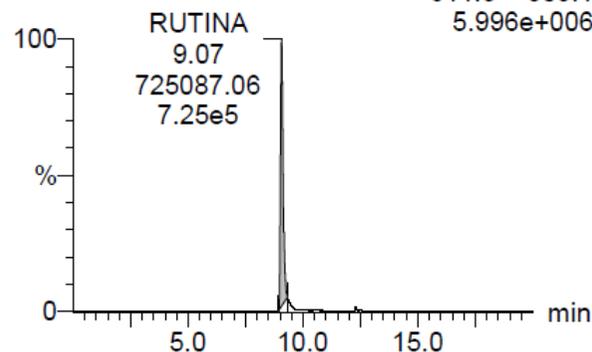


Figure S72: UHPLC-ESI-MRM/MS of Rutin Standards 4, 5, and 6 (Curve 3); Hydroethanolic Extract 3 and Aqueous Extract 3

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|------------------|----------|-----------|--------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 140823_ST6R_... | Standard | 0.100 | 8.9473 | 113668.336 | | 113668.336 | bb | 0.154 | 54.2 |
| 2 | 2 | 140823_ST6R_2... | Standard | 0.300 | 9.2812 | 77009.258 | | 77009.258 | bb | 0.110 | -63.2 |
| 3 | 3 | 140823_ST7R_... | Standard | 0.500 | 8.9907 | 566528.625 | | 566528.625 | bb | 0.694 | 38.9 |
| 4 | 4 | 140823_ST8R_... | Standard | 1.000 | 9.1120 | 1172867.625 | | 1172867.625 | bb | 1.418 | 41.8 |
| 5 | 5 | 140823_ST8R_2... | Standard | 5.000 | 9.1391 | 884205.063 | | 884205.063 | bb | 1.073 | -78.5 |
| 6 | 6 | 140823_ST9R_... | Standard | 50.000 | 9.0574 | 44798676.0... | | 44798676.0... | bb | 53.450 | 6.9 |
| 7 | 7 | 140823_MAC_P... | Analyte | | 8.8554 | 1074236.000 | | 1074236.000 | bb | 1.300 | |
| 8 | 8 | 140823_DEC_P... | Analyte | | 9.0677 | 725087.063 | | 725087.063 | bb | 0.883 | |

Figure S73: Quantify of Rutin in Hydroethanolic Extract 3 and Aqueous Extract 3 (Curve 3)

Compound name: QUERCETINA
Correlation coefficient: $r = 0.987189$, $r^2 = 0.974541$
Calibration curve: $243505 * x + 1534.36$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

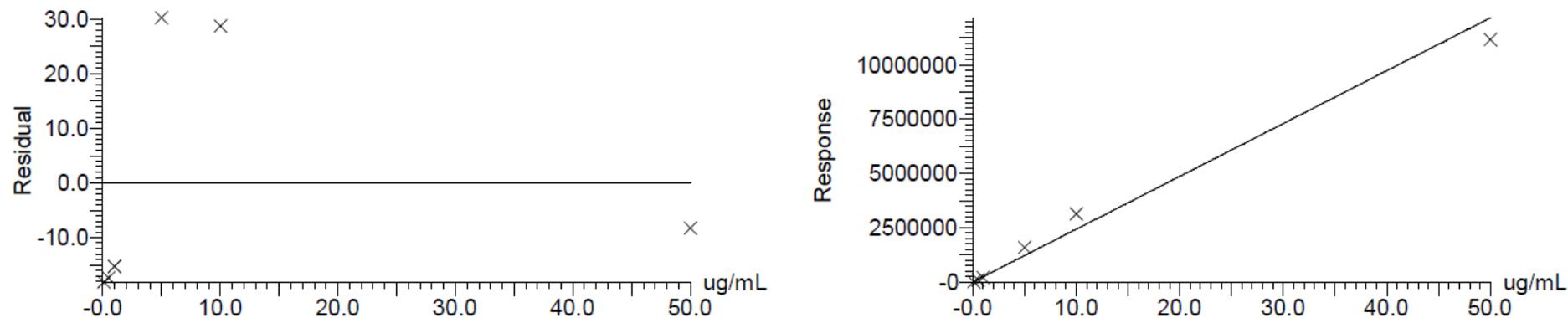


Figure S74: Quercetin Calibration Curve 1

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RESULTADOS DE LABORATORIO

Dataset: C:\MassLynx\2021Tesisas.PRO\230823_CURVADEQUERCETINA_1_CASI.qld

Last Altered: Wednesday, August 23, 2023 17:18:42 SA Pacific Standard Time

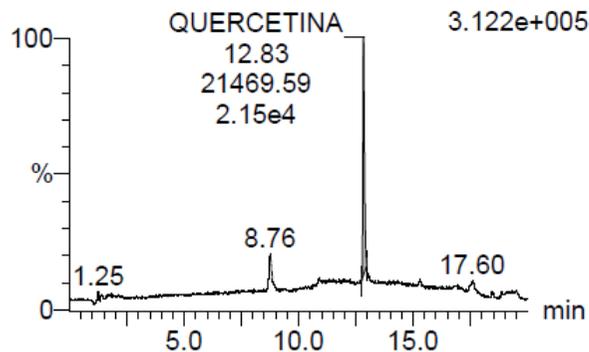
Printed: Wednesday, August 23, 2023 17:19:20 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesisas.PRO\MethDB\230823_QUERCETINA_1.mdb 23 Aug 2023 16:16:23

Calibration: 23 Aug 2023 17:18:42

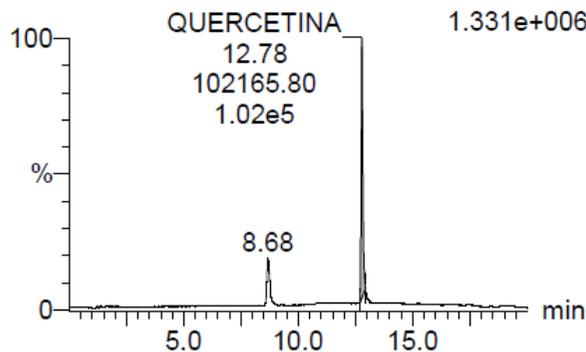
Sample Name: 040823_ST6_POS

040823_ST6_POS MRM of 1 channel,ES+
303.1 > 153
3.122e+005



Sample Name: 040823_ST7_POS

040823_ST7_POS MRM of 1 channel,ES+
303.1 > 153
1.331e+006



Sample Name: 040823_ST8_POS

040823_ST8_POS MRM of 1 channel,ES+
303.1 > 153
2.700e+006

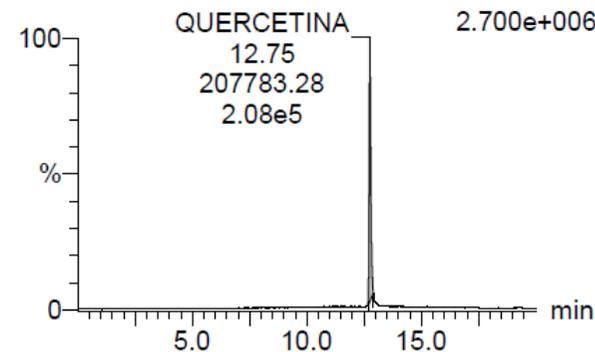
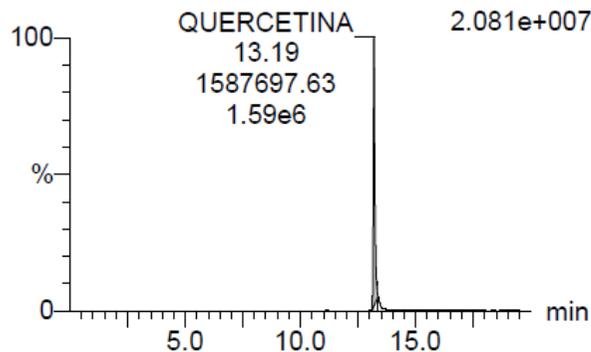


Figure S75: UHPLC-ESI-MRM/MS of Quercetin Standards 1, 2, and 3 (Curve 1)

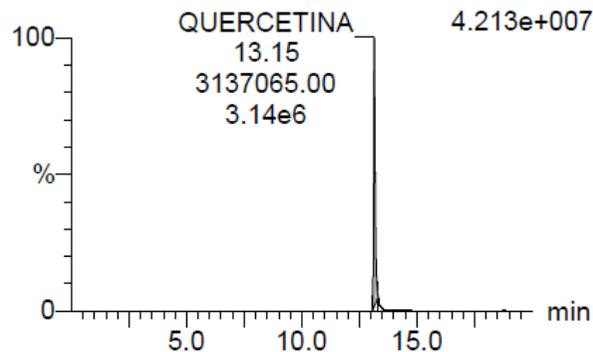
Sample Name: 040823_ST8_1_POS

040823_ST8_1_POS MRM of 1 channel,ES+
303.1 > 153
2.081e+007



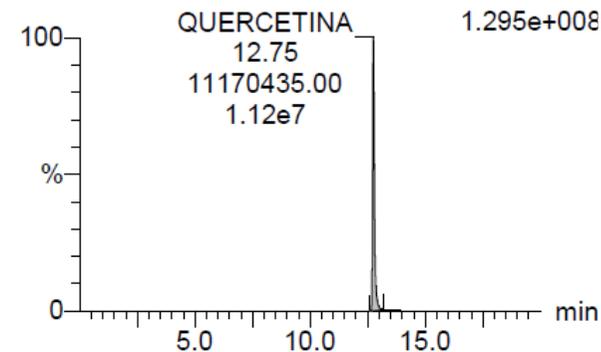
Sample Name: 040823_ST8_2_POS

040823_ST8_2_POS MRM of 1 channel,ES+
303.1 > 153
4.213e+007



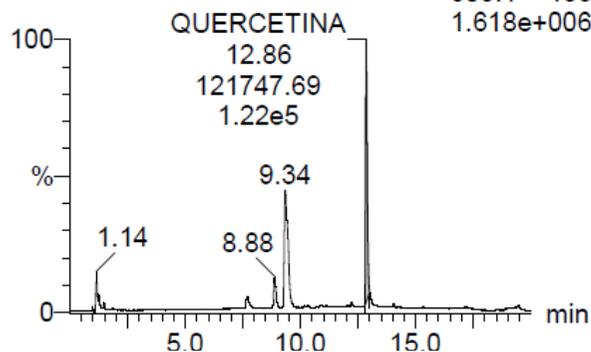
Sample Name: 040823_ST9_POS

040823_ST9_POS MRM of 1 channel,ES+
303.1 > 153
1.295e+008



Sample Name: 040823_MAC_POS

040823_MAC_POS MRM of 1 channel,ES+
303.1 > 153
1.618e+006



Sample Name: 040823_DEC_POS

040823_DEC_POS MRM of 1 channel,ES+
303.1 > 153
2.156e+005

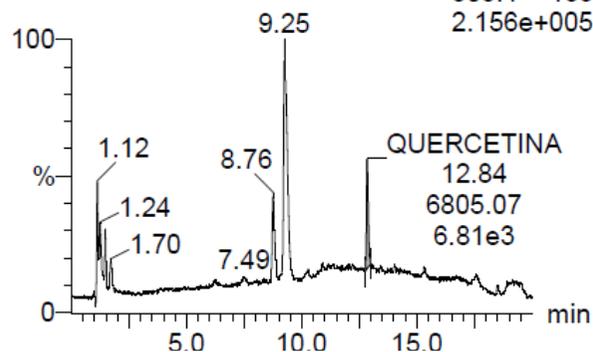


Figure S76: UHPLC-ESI-MRM/MS of Quercetin Standards 4, 5, and 6 (Curve 1); Hydroethanolic Extract 1 and Aqueous Extract 1

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|------------------|----------|-----------|---------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 040823_ST6_POS | Standard | 0.100 | 12.8312 | 21469.594 | | 21469.594 | bb | 0.082 | -18.1 |
| 2 | 2 | 040823_ST7_POS | Standard | 0.500 | 12.7752 | 102165.805 | | 102165.805 | bb | 0.413 | -17.3 |
| 3 | 3 | 040823_ST8_POS | Standard | 1.000 | 12.7496 | 207783.281 | | 207783.281 | bb | 0.847 | -15.3 |
| 4 | 4 | 040823_ST8_1_... | Standard | 5.000 | 13.1886 | 1587697.625 | | 1587697.625 | bb | 6.514 | 30.3 |
| 5 | 5 | 040823_ST8_2_... | Standard | 10.000 | 13.1471 | 3137065.000 | | 3137065.000 | bb | 12.877 | 28.8 |
| 6 | 6 | 040823_ST9_POS | Standard | 50.000 | 12.7458 | 11170435.0... | | 11170435.0... | bb | 45.867 | -8.3 |
| 7 | 7 | 040823_MAC_P... | Analyte | | 12.8564 | 121747.688 | | 121747.688 | bb | 0.494 | |
| 8 | 8 | 040823_DEC_P... | Analyte | | 12.8401 | 6805.068 | | 6805.068 | bb | 0.022 | |

Figure S77: Quantify of Quercetin in Hydroethanolic Extract 1 and Aqueous Extract 1 (Curve 1)

Compound name: QUERCETINA
Correlation coefficient: $r = 0.985111$, $r^2 = 0.970444$
Calibration curve: $227933 * x + -1969.34$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: $1/x$, Axis trans: None

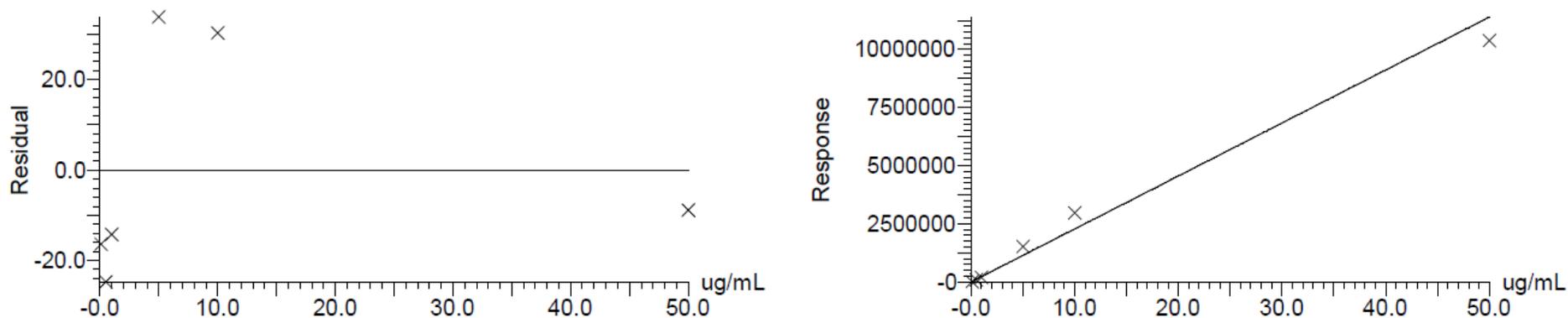


Figure S78: Quercetin Calibration Curve 2

Quantify Compound Report MassLynx V4.2 SCN1007

RESULTADOS DE LABORATORIO

Dataset: C:\MassLynx\2021Tesistas.PRO\230823_CURVADEQUERCETINA_2.qld

Last Altered: Wednesday, August 23, 2023 18:06:04 SA Pacific Standard Time

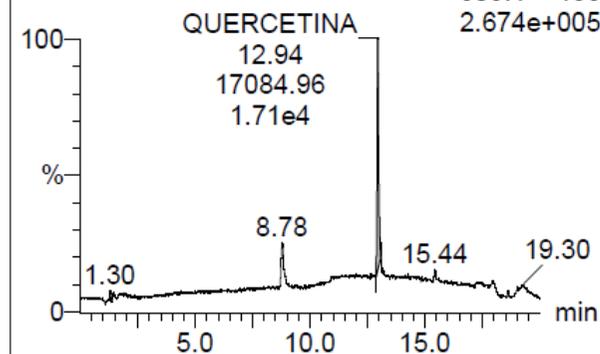
Printed: Wednesday, August 23, 2023 18:06:52 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesistas.PRO\MethDB\230823_QUERCETINA_1.mdb 23 Aug 2023 17:19:51

Calibration: 23 Aug 2023 18:06:04

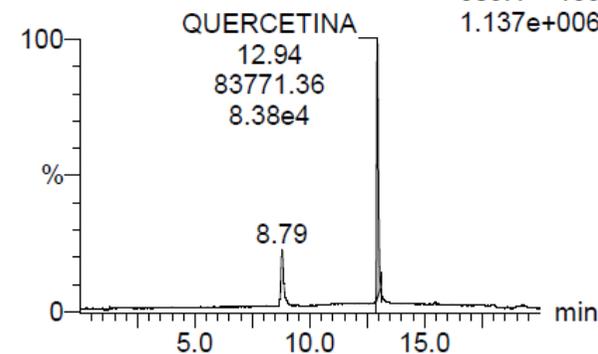
Sample Name: 130823_ST6_POS

130823_ST6_POS MRM of 1 channel,ES+
303.1 > 153
2.674e+005



Sample Name: 130823_ST7_POS

130823_ST7_POS MRM of 1 channel,ES+
303.1 > 153
1.137e+006



Sample Name: 130823_ST8_POS

130823_ST8_POS MRM of 1 channel,ES+
303.1 > 153
2.398e+006

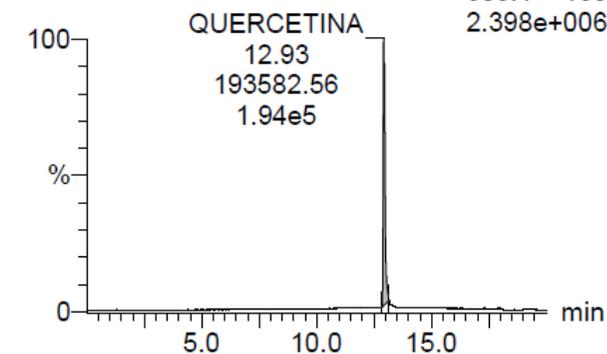
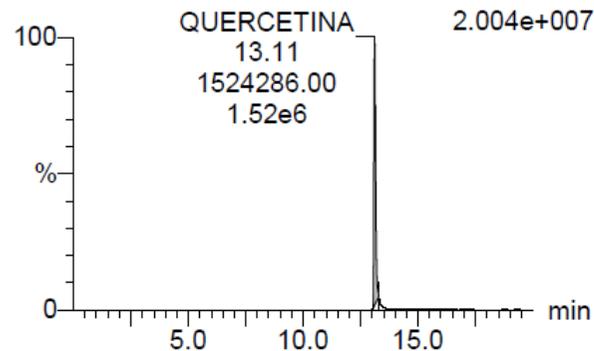


Figure S79: UHPLC-ESI-MRM/MS of Quercetin Standards 1, 2, and 3 (Curve 2)

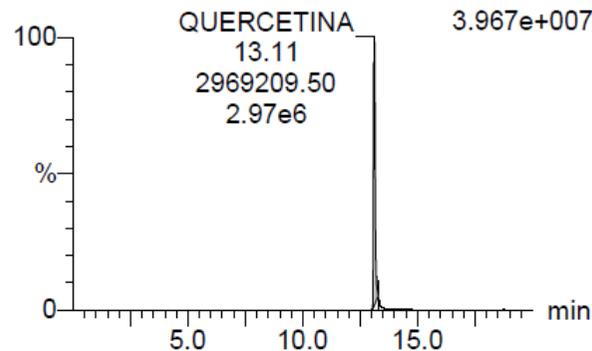
Sample Name: 130823_ST8_5_5_POS

130823_ST8_5_5_POS MRM of 1 channel,ES+
303.1 > 153
2.004e+007



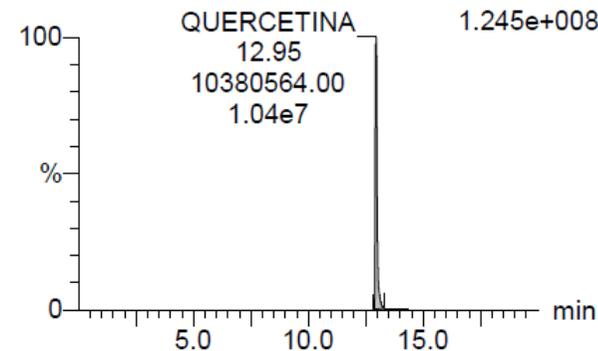
Sample Name: 130823_ST8_6_6_POS

130823_ST8_6_6_POS MRM of 1 channel,ES+
303.1 > 153
3.967e+007



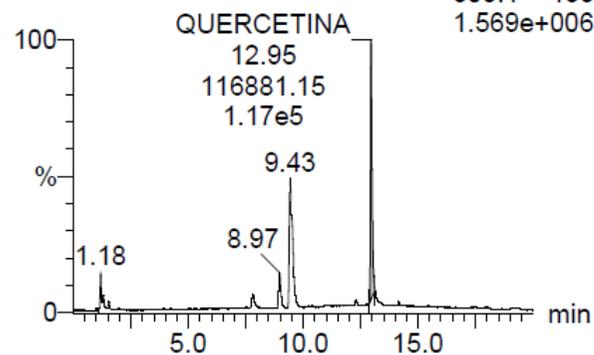
Sample Name: 130823_ST9_POS

130823_ST9_POS MRM of 1 channel,ES+
303.1 > 153
1.245e+008



Sample Name: 130823_MAC_POS

040823_MAC_POS MRM of 1 channel,ES+
303.1 > 153
1.569e+006



Sample Name: 130823_DEC_POS

040823_DEC_POS MRM of 1 channel,ES+
303.1 > 153
1.932e+005

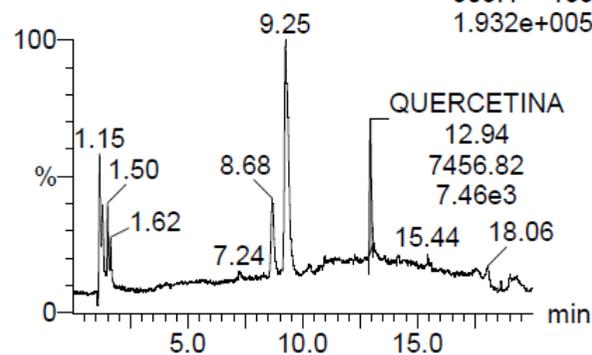


Figure S80: UHPLC-ESI-MRM/MS of Quercetin Standards 4, 5, and 6 (Curve 2); Hydroethanolic Extract 2 and Aqueous Extract 2

| | # | Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|---|------------------|----------|-----------|---------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 | 130823_ST6_POS | Standard | 0.100 | 12.9418 | 17084.963 | | 17084.963 | bb | 0.084 | -16.4 |
| 2 | 2 | 130823_ST7_POS | Standard | 0.500 | 12.9358 | 83771.359 | | 83771.359 | bb | 0.376 | -24.8 |
| 3 | 3 | 130823_ST8_POS | Standard | 1.000 | 12.9288 | 193582.563 | | 193582.563 | bb | 0.858 | -14.2 |
| 4 | 4 | 130823_ST8_5_... | Standard | 5.000 | 13.1093 | 1524286.000 | | 1524286.000 | bb | 6.696 | 33.9 |
| 5 | 5 | 130823_ST8_6_... | Standard | 10.000 | 13.1103 | 2969209.500 | | 2969209.500 | bb | 13.035 | 30.4 |
| 6 | 6 | 130823_ST9_POS | Standard | 50.000 | 12.9479 | 10380564.0... | | 10380564.0... | bb | 45.551 | -8.9 |
| 7 | 7 | 130823_MAC_P... | Analyte | | 12.9539 | 116881.148 | | 116881.148 | bb | 0.521 | |
| 8 | 8 | 130823_DEC_P... | Analyte | | 12.9381 | 7456.821 | | 7456.821 | bb | 0.041 | |

Figure S81: Quantify of Quercetin in Hydroethanolic Extract 2 and Aqueous Extract 2 (Curve 2)

Compound name: QUERCETINA
Correlation coefficient: $r = 0.999100$, $r^2 = 0.998201$
Calibration curve: $287785 * x + -20219.6$
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

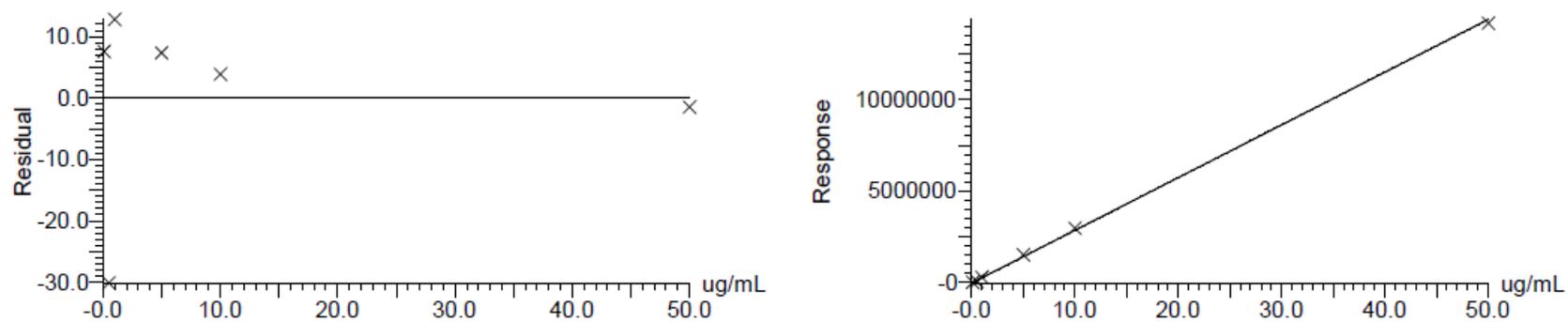


Figure S82: Quercetin Calibration Curve 3

Quantify Compound Report MassLynx V4.2 SCN1007
RESULTADOS DE LABORATORIO

Dataset: C:\MassLynx\2021Tesisas.PRO\230823_CURVAQUERCETINA_3.qld

Last Altered: Wednesday, August 23, 2023 17:27:56 SA Pacific Standard Time

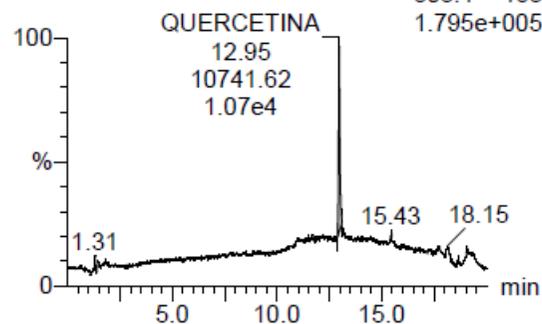
Printed: Wednesday, August 23, 2023 17:29:05 SA Pacific Standard Time

Method: C:\MassLynx\2021Tesisas.PRO\MethDB\230823_QUERCETINA_1.mdb 23 Aug 2023 17:19:51

Calibration: 23 Aug 2023 17:27:56

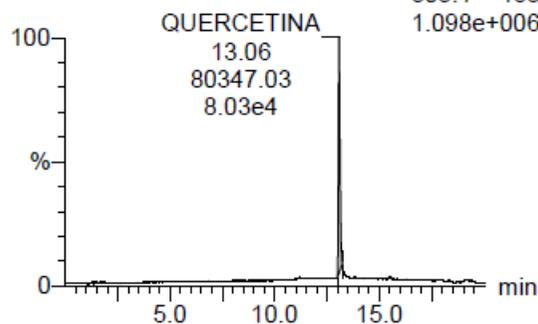
Sample Name: 130823_ST6_2_POS

130823_ST6_2_POS MRM of 1 channel,ES+
303.1 > 153
1.795e+005



Sample Name: 130823_ST7_2_POS

130823_ST7_2_POS MRM of 1 channel,ES+
303.1 > 153
1.098e+006



Sample Name: 130823_ST8_2_POS

130823_ST8_2_POS MRM of 1 channel,ES+
303.1 > 153
3.995e+006

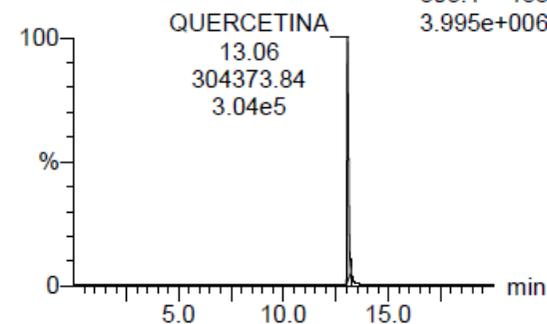
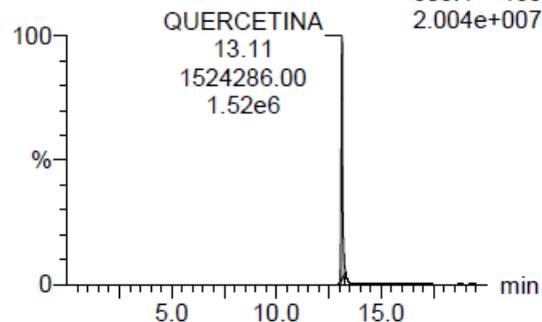


Figure S83: UHPLC-ESI-MRM/MS of Quercetin Standards 1, 2, and 3 (Curve 3)

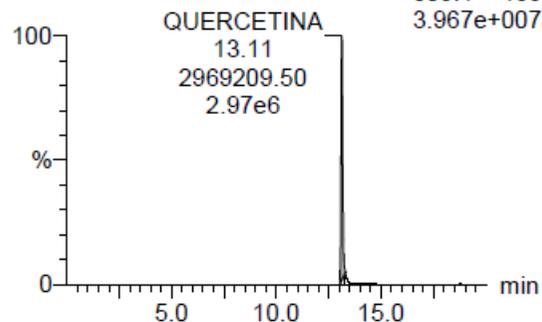
Sample Name: 130823_ST8_5_5_POS

130823_ST8_5_5_POS MRM of 1 channel,ES+
303.1 > 153



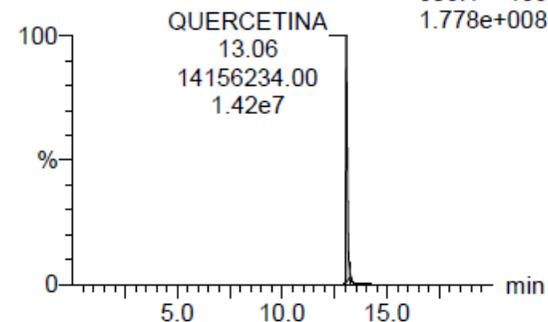
Sample Name: 130823_ST8_6_6_POS

130823_ST8_6_6_POS MRM of 1 channel,ES+
303.1 > 153



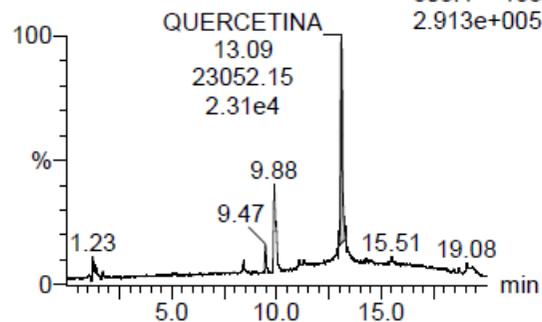
Sample Name: 130823_ST9_2_POS

130823_ST9_2_POS MRM of 1 channel,ES+
303.1 > 153



Sample Name: 130823_MAC_2_POS

130823_MAC_2_POS MRM of 1 channel,ES+
303.1 > 153



Sample Name: 130823_DEC_2_POS

130823_DEC_2_POS MRM of 1 channel,ES+
303.1 > 153

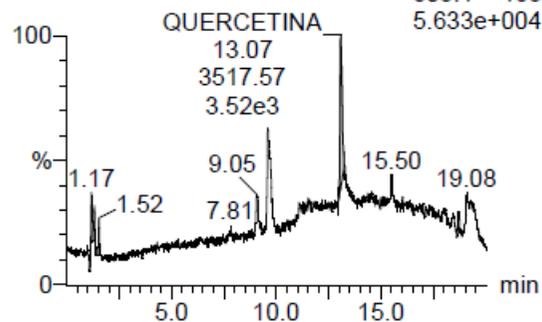


Figure S84: UHPLC-ESI-MRM/MS of Quercetin Standards 4, 5, and 6 (Curve 3); Hydroethanolic Extract 3 and Aqueous Extract 3

| | # Name | Type | Std. Conc | RT | Area | IS Area | Response | Primary Flags | ug/mL | %Dev |
|---|--------------------|----------|-----------|---------|---------------|---------|---------------|---------------|--------|-------|
| 1 | 1 130823_ST6_2_... | Standard | 0.100 | 12.9512 | 10741.620 | | 10741.620 | bb | 0.108 | 7.6 |
| 2 | 2 130823_ST7_2_... | Standard | 0.500 | 13.0636 | 80347.031 | | 80347.031 | bb | 0.349 | -30.1 |
| 3 | 3 130823_ST8_2_... | Standard | 1.000 | 13.0580 | 304373.844 | | 304373.844 | bb | 1.128 | 12.8 |
| 4 | 4 130823_ST8_5_... | Standard | 5.000 | 13.1093 | 1524286.000 | | 1524286.000 | bb | 5.367 | 7.3 |
| 5 | 5 130823_ST8_6_... | Standard | 10.000 | 13.1103 | 2969209.500 | | 2969209.500 | bb | 10.388 | 3.9 |
| 6 | 6 130823_ST9_2_... | Standard | 50.000 | 13.0608 | 14156234.0... | | 14156234.0... | bb | 49.260 | -1.5 |
| 7 | 7 130823_MAC_2... | Analyte | | 13.0878 | 23052.154 | | 23052.154 | bb | 0.150 | |
| 8 | 8 130823_DEC_2... | Analyte | | 13.0687 | 3517.569 | | 3517.569 | bb | 0.082 | |

Figure S85: Quantify of Quercetin in Hydroethanolic Extract 3 and Aqueous Extract 3 (Curve 3)