SUPPLEMENTARY INFORMATION

Modulation of i-Motif Thermal Stability by Insertion of Anthraquinone Monomers

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Circular Dichroism (CD) spectral analysis of human telomeric DNA (ON1) and anthraquinone-modified i-motif variants (ON2-ON33, Fig. S1-S3):

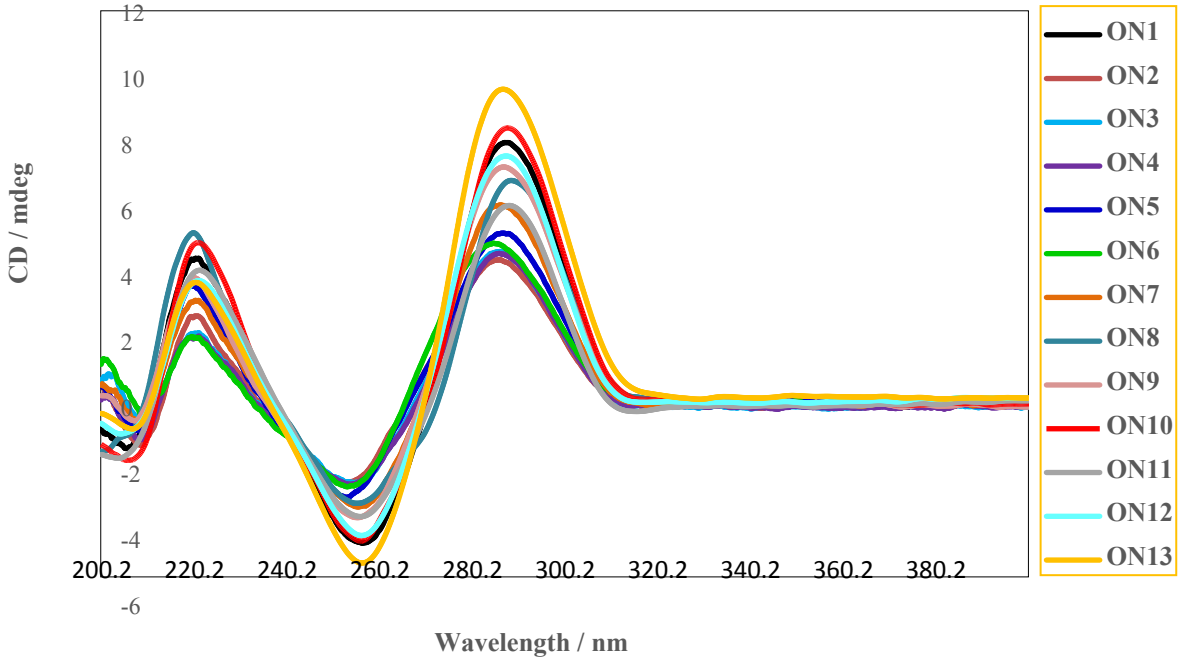


Figure S1. Circular dichroism (CD) spectra of human telomeric i-motif DNA (**ON1**) and anthraquinone-modified i-motif variants (**ON2-ON13**) measured at 20 ºC. For sample composition see table 1.

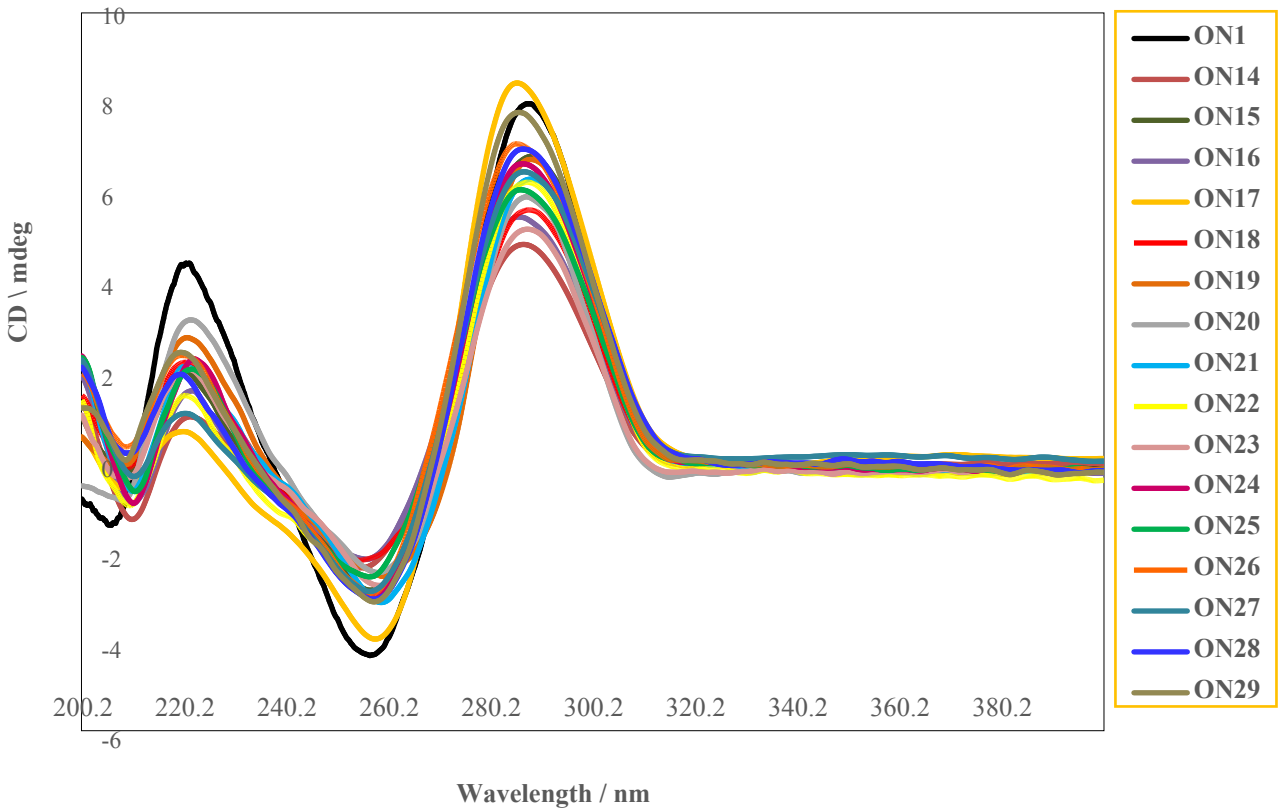


Figure S2. CD spectra of human telomeric i-motif DNA **(ON1)** and anthraquinone-modified i-motif variants **(ON14-ON29)** measured at 20 ºC. For sample composition see table 1.

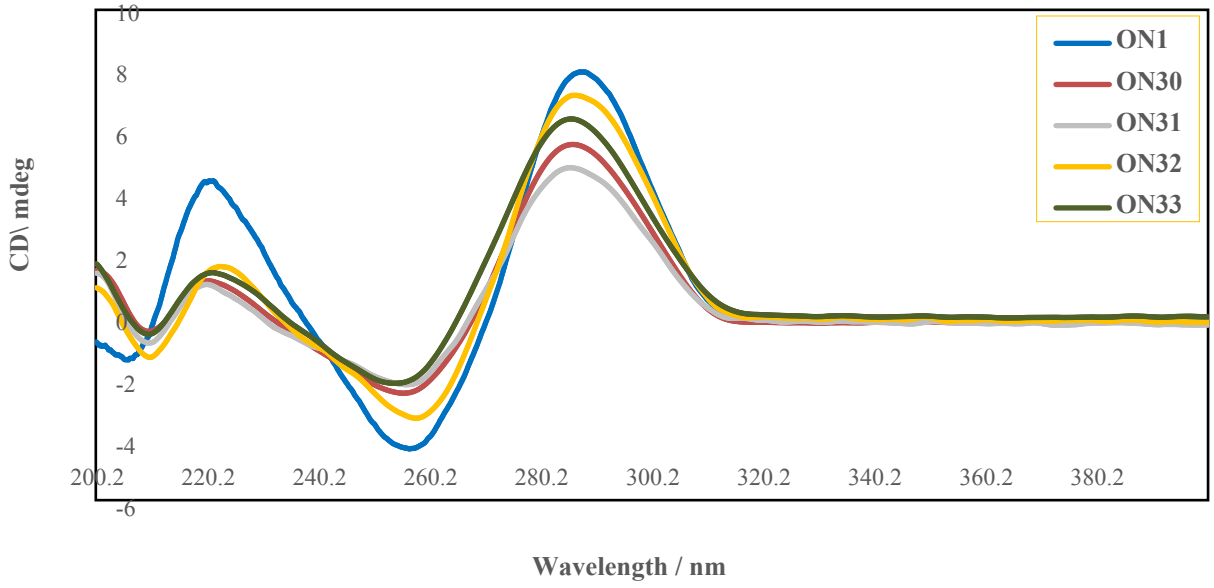


Figure S3. CD spectra of human telomeric i-motif DNA **(ON1)** and anthraquinone-modified i-motif variants **(ON30-ON33)** measured at 20 ºC. For sample composition see table 1.

Normalized UV absorption melting curves and first derivatives of human telomeric i-motif DNA (ON1) and anthraquinone-modified i-motif variants (ON2-ON33, Fig S4-S6):

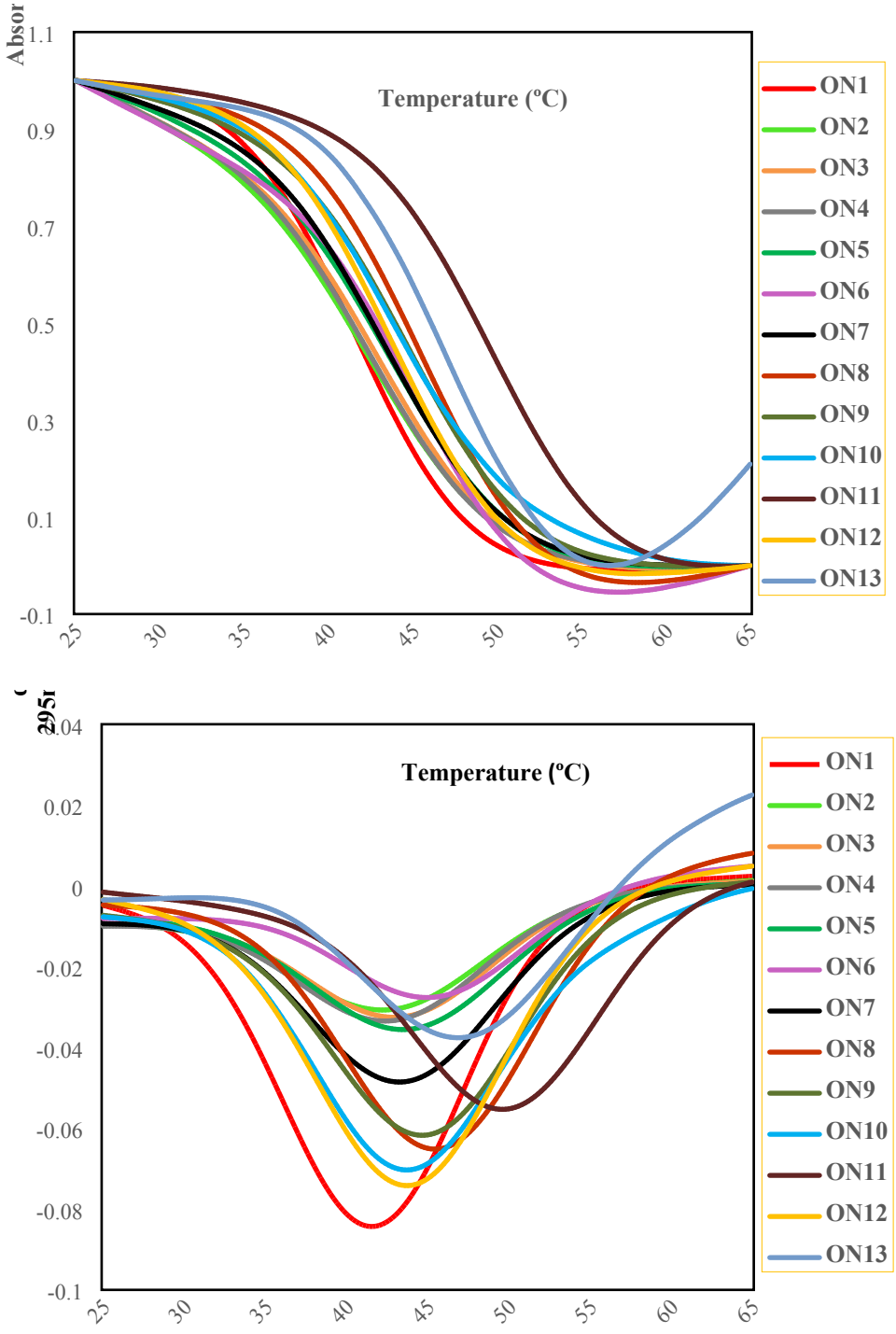


Figure S4. Normalized UV absorption melting curves (Up) and first derivatives (Down) versus temperature difference (0.5 ºC/min) from 25-65 ºC for i–motifs (**ON1-ON13)** at 295 nm (4 µM) in potassium buffer (100 mM KCl + 20 mM K_2HPO_4 (pH= 5.5) and 1 mM K_2EDTA). Melting temperatures are within the uncertainty ± 0.5 °C as determined by repetitive experiments and T_m values were calculated taking an average of the two melting curves.

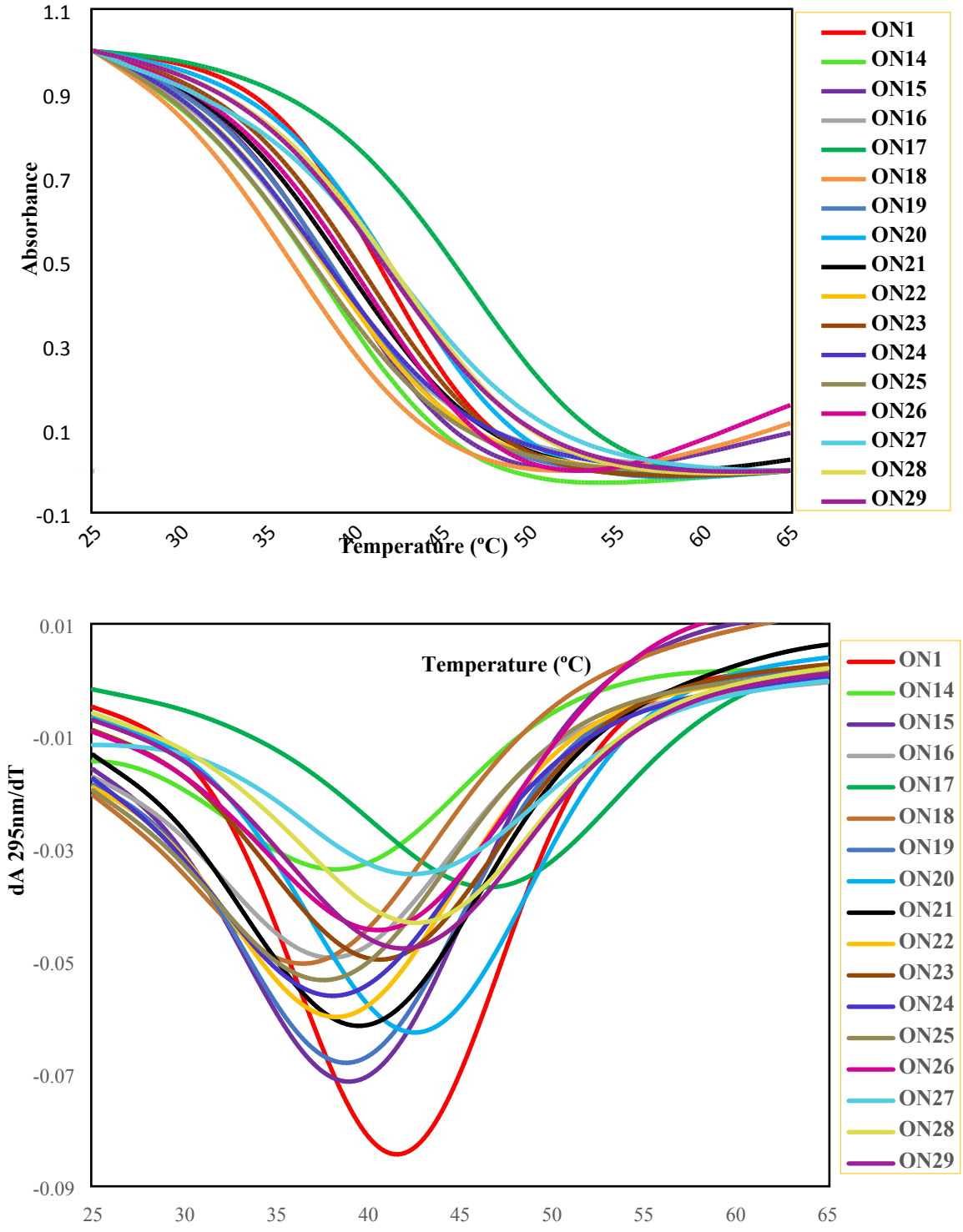
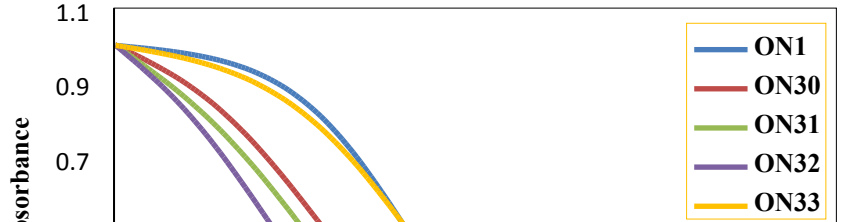


Figure S5. Normalized UV absorption melting curves (Up) and first derivatives (Down) versus temperature difference (0.5 ºC/min) from 25-65 ºC for i–motifs (**ON1** and **ON14-ON29)** at 295 nm (4 µM) in potassium buffer (100 mM KCl + 20 mM K_2HPO_4 (pH= 5.5) and 1 mM K_2EDTA). Melting temperatures are within the uncertainty ± 0.5 °C as determined by repetitive experiments and T_m values were calculated taking an average of the two melting curves.



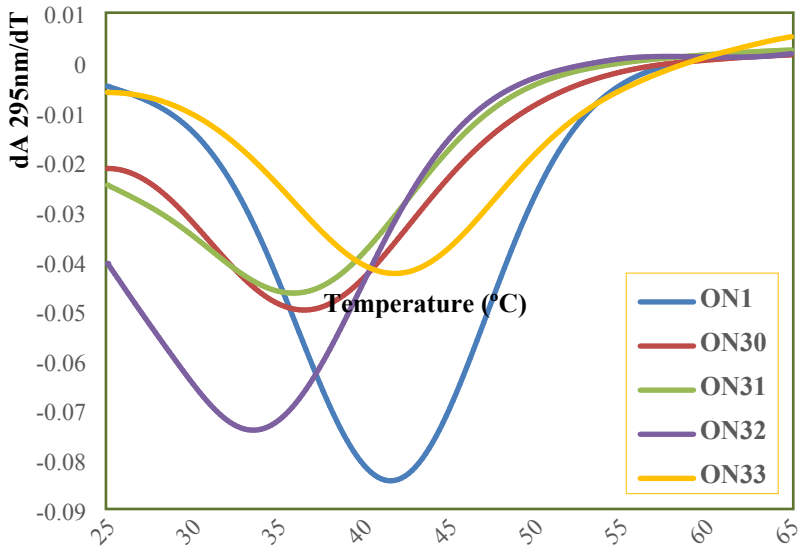


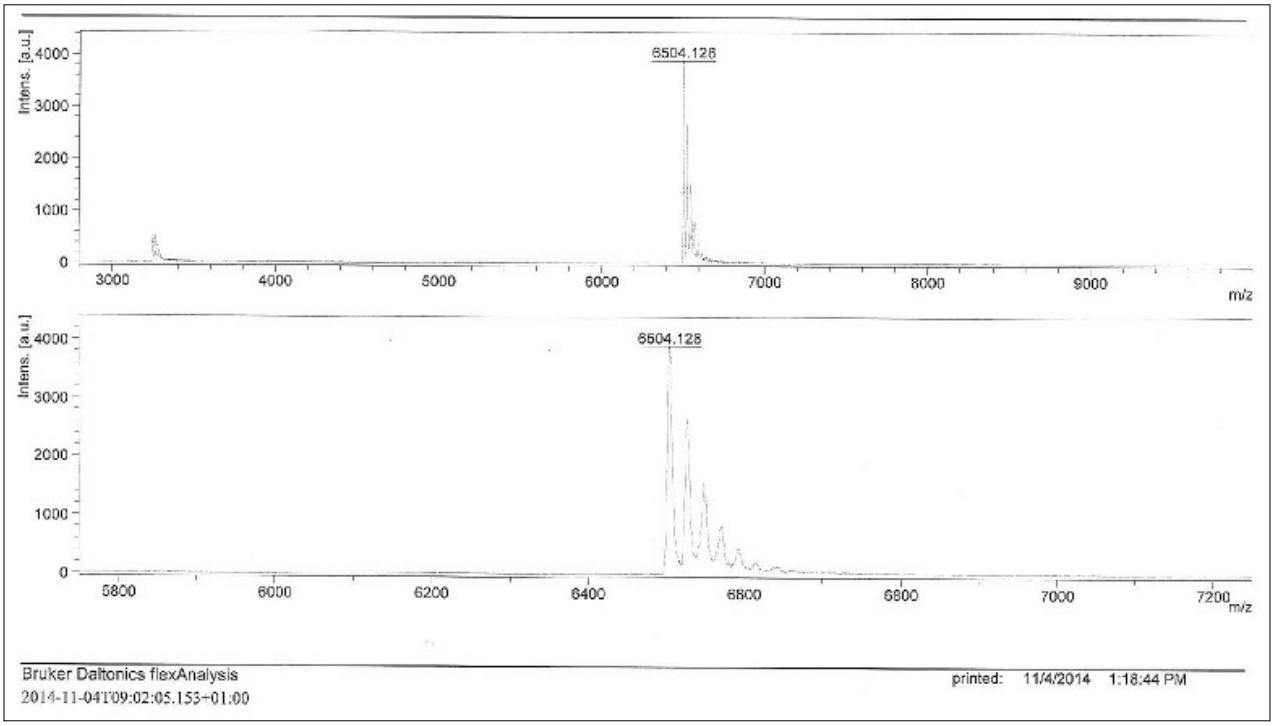
Figure S6. Normalized UV absorption melting curves (Up) and first derivatives (Down) versus temperature difference (0.5 ºC/min) from 25-65 ºC for i–motifs (**ON1** and **ON30-ON33)** at 295 nm (4 µM) in potassium buffer (100 mM KCl + 20 mM K_2HPO_4 (pH= 5.5) and 1 mM K_2EDTA). Melting temperatures are within the uncertainty ± 0.5 °C as determined by repetitive experiments and T_m values were calculated taking an average of the two melting curves.

Table S1. MALDI-TOF mass spectrometry data (calculated and found mass) of i-Motifs

Oligo	bases replaced	Sequence	M_{calcd}	M_{found}
ON1	wild type	5'-CCC TAA CCC TAA CCC TAA CCC T-3'	6504.44	6504.13
ON2	T_{10}	5'-CCC TAA CCC **H_{18}**AA CCC TAA CCC T-3'	6617.43	6618.68
ON3	A_{11}	5'-CCC TAA CCC T**H_{18}**A CCC TAA CCC T-3'	6608.43	6608.07
ON4	A_{12}	5'-CCC TAA CCC TA**H_{18}** CCC TAA CCC T-3'	6608.43	6609.25
ON5	T_{10}	5'-CCC TAA CCC **H_{14}**AA CCC TAA CCC T-3'	6617.43	6617.38
ON6	A_{11}	5'-CCC TAA CCC T**H_{14}**A CCC TAA CCC T-3'	6608.43	6608.94
ON7	A_{12}	5'-CCC TAA CCC TA**H_{14}** CCC TAA CCC-T-3'	6608.43	6608.07
ON8	T_{10}	5'-CCC TAA CCC **H_{15}**AA CCC TAA CCC T-3'	6617.43	6618.29
ON9	A_{11}	5'-CCC TAA CCC T**H_{15}**A CCC TAA CCC T-3'	6608.43	6609.22
ON10	A_{12}	5'-CCC TAA CCC TA**H_{15}** CCC TAA CCC T-3'	6608.43	6609.30
ON11	T_{10}	5'-CCC TAA CCC **H_{26}**AA CCC TAA CCC T-3'	6617.43	6617.49
ON12	A_{11}	5'-CCC TAA CCC T**H_{26}**A CCC TAA CCC T-3'	6608.43	6608.65
ON13	A_{12}	5'-CCC TAA CCC TA**H_{26}** CCC TAA CCC-T-3'	6608.43	6608.36
ON14	A_6T_{16}	5'-CCC TA**H_{18}** CCC TAA CCC **H_{18}**AA CCC T-3'	6721.56	6722.74
ON15	A_6T_{16}	5'-CCC TA**H_{14}** CCC TAA CCC **H_{14}**AA CCC T-3'	6721.56	6722.85
ON16	A_6T_{16}	5'-CCC TA**H_{15}** CCC TAA CCC **H_{15}**AA CCC T-3'	6721.56	6728.08
ON17	A_6T_{16}	5'-CCC TA**H_{26}** CCC TAA CCC **H_{26}**AA CCC T-3'	6721.56	6721.66
ON18	A_6T_{16}	5'-CCC TA**H_{18}** CCC TAA CCC **H_{14}**AA CCC T-3'	6721.56	6723.44
ON19	A_6T_{16}	5'-CCC TA**H_{18}** CCC TAA CCC **H_{15}**AA CCC T-3'	6721.56	6725.84
ON20	A_6T_{16}	5'-CCC TA**H_{18}** CCC TAA CCC **H_{26}**AA CCC T-3'	6721.56	6721.66
ON21	A_6T_{16}	5'-CCC TA**H_{14}** CCC TAA CCC **H_{18}**AA CCC T-3'	6721.56	6722.85
ON22	A_6T_{16}	5'-CCC TA**H_{14}** CCC TAA CCC **H_{15}**AA CCC T-3'	6721.56	6724.04
ON23	A_6T_{16}	5'-CCC TA**H_{14}** CCC TAA CCC **H_{26}**AA CCC T-3'	6721.56	6722.76
ON24	A_6T_{16}	5'-CCC TA**H_{15}** CCC TAA CCC **H_{18}**AA CCC T-3'	6721.56	6723.74
ON25	A_6T_{16}	5'-CCC TA**H_{15}** CCC TAA CCC **H_{14}**AA CCC-T-3'	6721.56	6722.26
ON26	A_6T_{16}	5'-CCC TA**H_{15}** CCC TAA CCC **H_{26}**AA CCC T-3'	6721.56	6722.18
ON27	A_6T_{16}	5'-CCC TA**H_{26}** CCC TAA CCC **H_{18}**AA CCC T-3'	6721.56	6719.88
ON28	A_6T_{16}	5'-CCC TA**H_{26}** CCC TAA CCC **H_{14}**AA CCC T-3'	6721.56	6722.26
ON29	A_6T_{16}	5'-CCC TA**H_{26}** CCC TAA CCC **H_{15}**AA CCC T-3'	6721.56	6718.12
ON30	A_{18}	5'-CCC TAA CCC TAA CCC TA**H_{18}** CCC T-3'	6608.43	6608.28
ON31	A_{18}	5'-CCC TAA CCC TAA CCC TA**H_{14}** CCC-T-3'	6608.43	6612.98
ON32	A_{18}	5'-CCC TAA CCC TAA CCC TA**H_{15}** CCC T-3'	6608.43	6608.36
ON33	A_{18}	5'-CCC TAA CCC TAA CCC TA**H_{26}** CCC T-3'	6608.43	6609.83

Maldi-TOF Mass Spectrometry Data of Oligonucleotides (ON1-ON33)

ON1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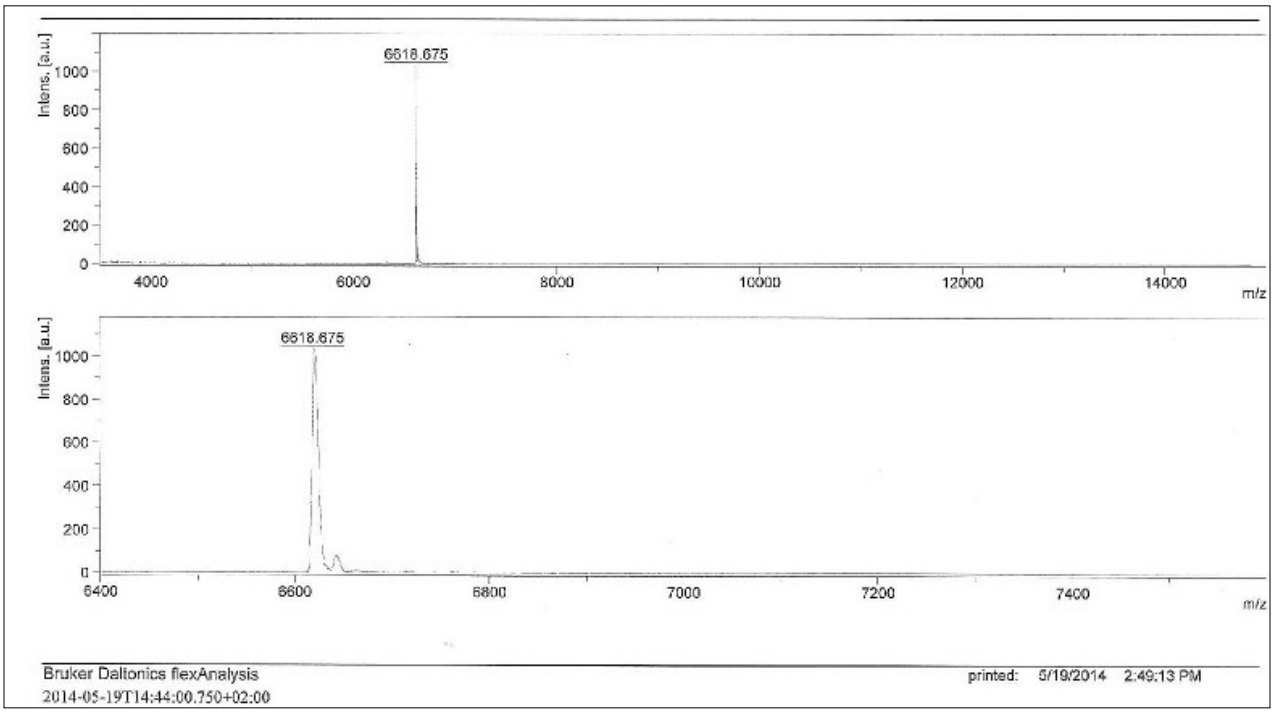
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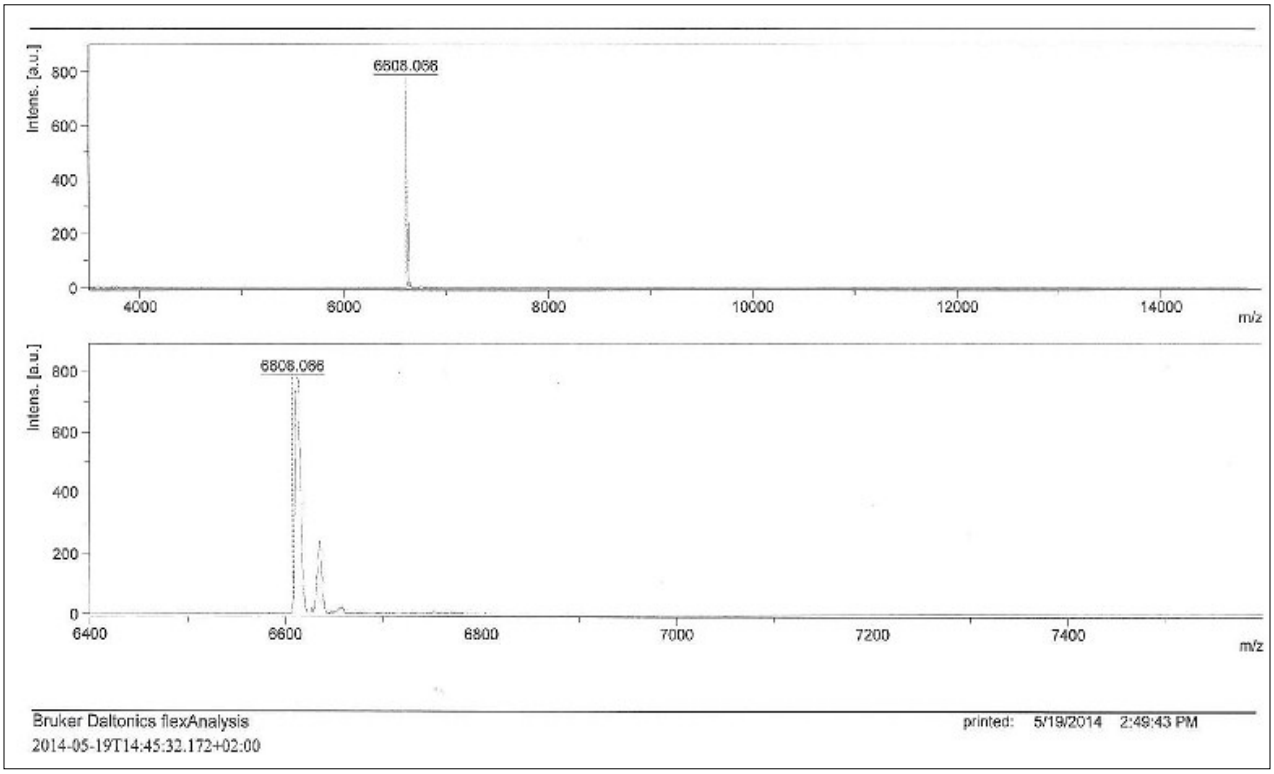
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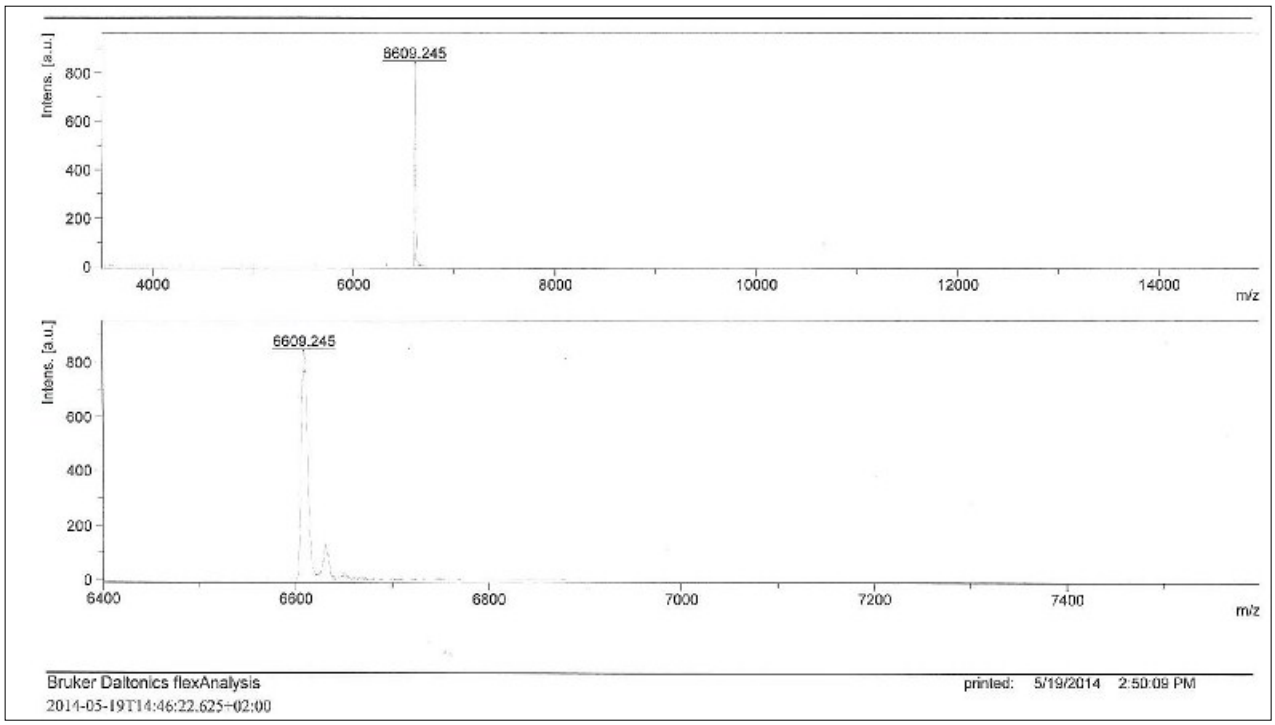
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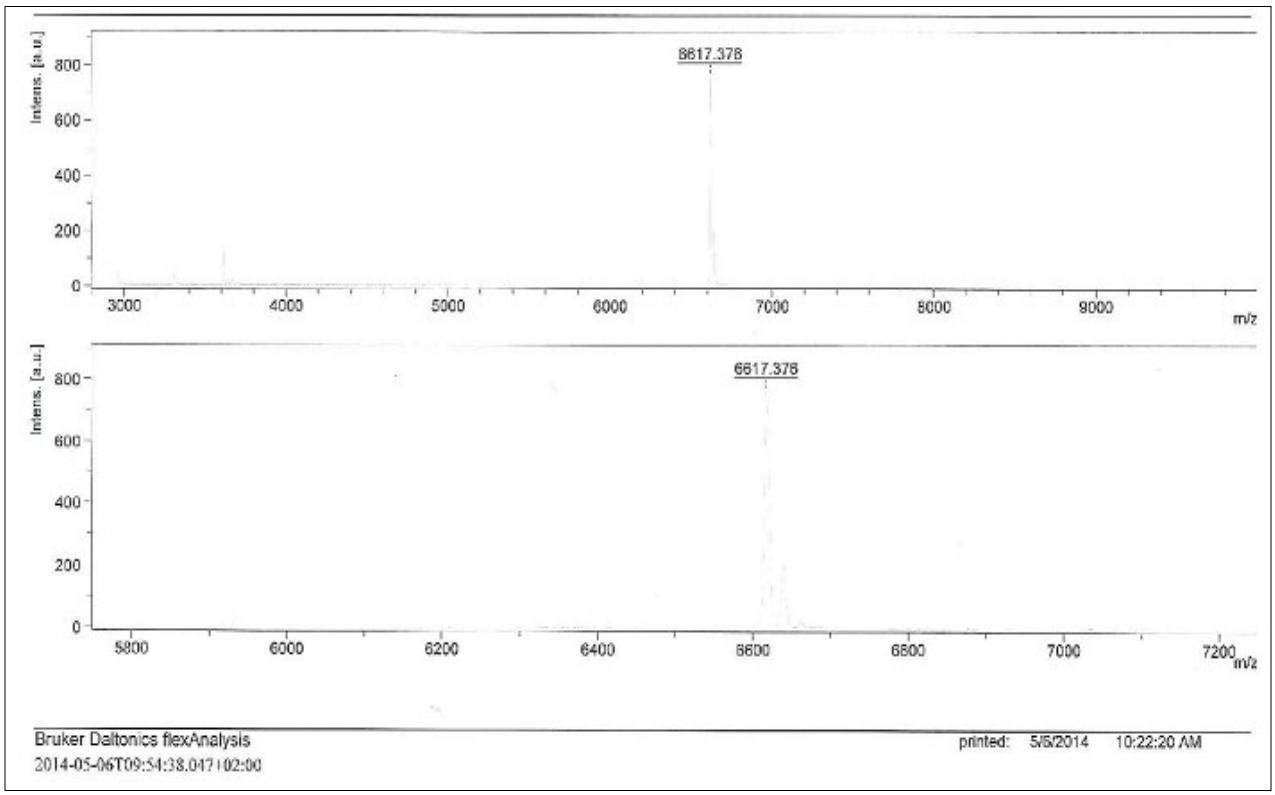
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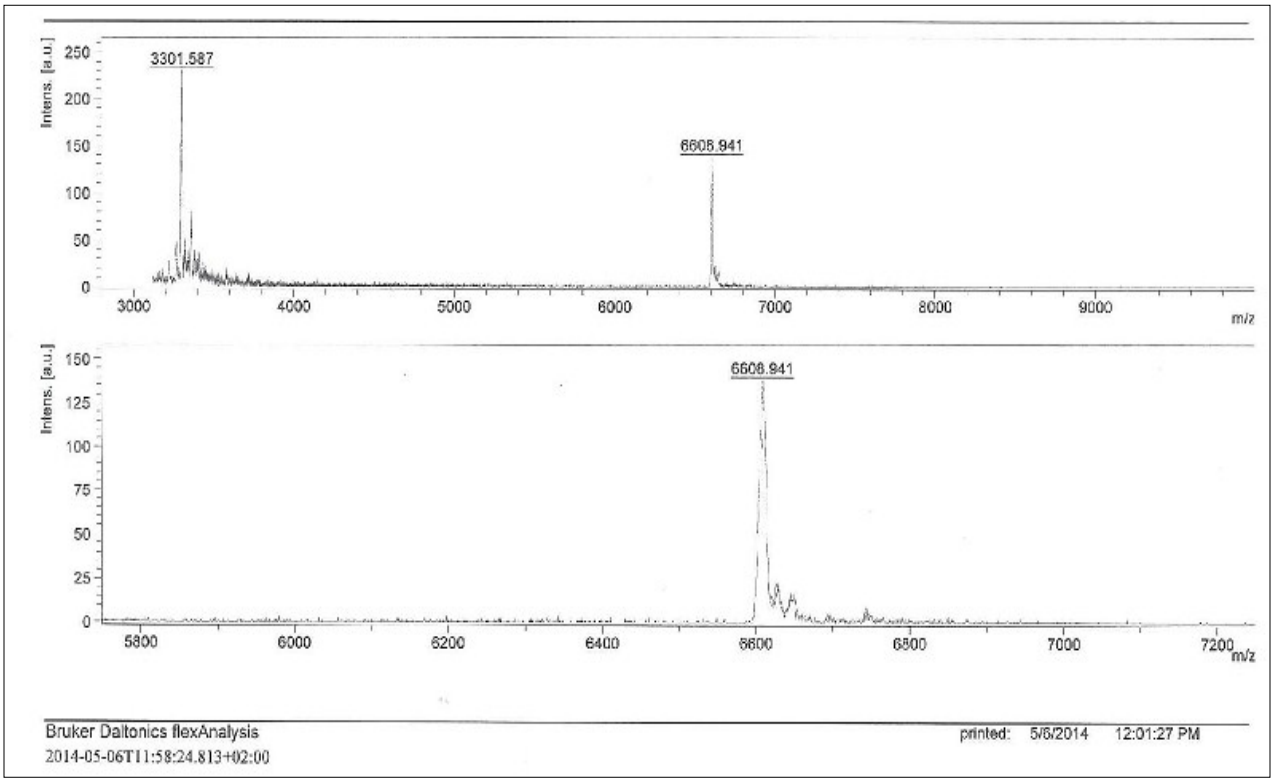
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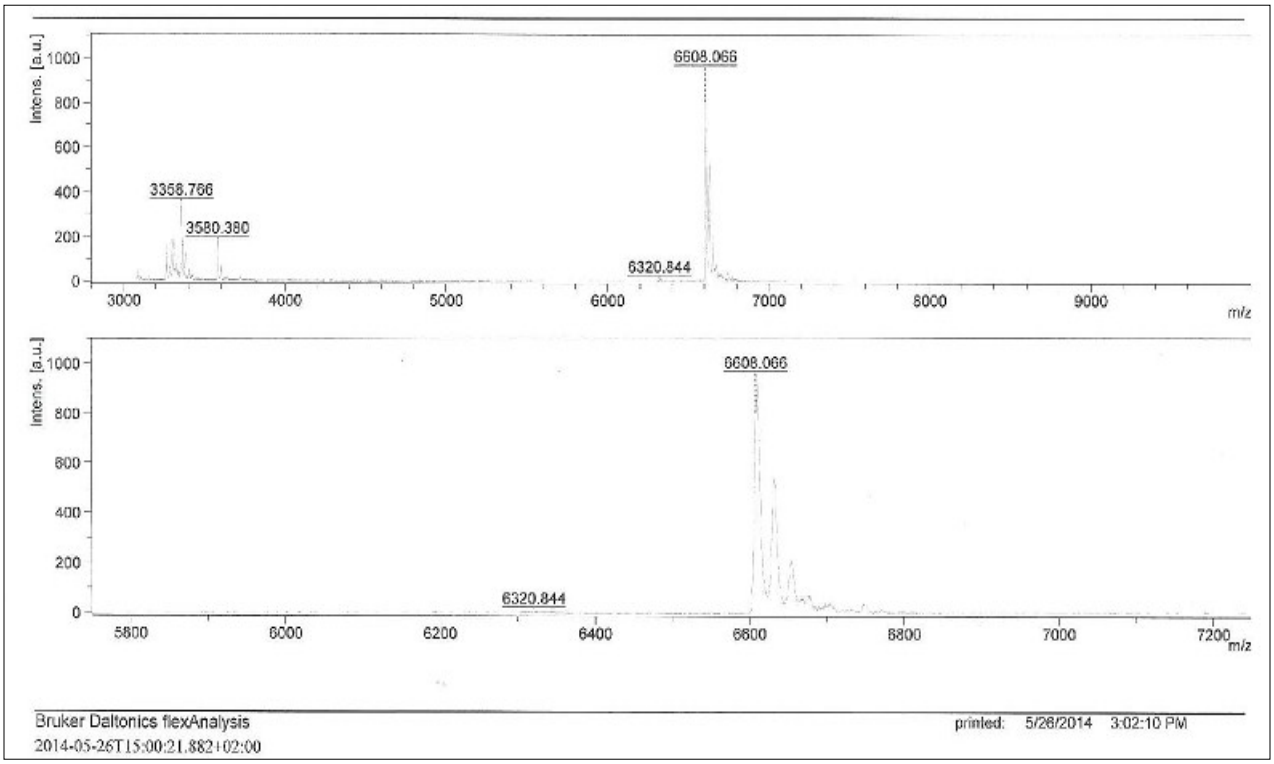
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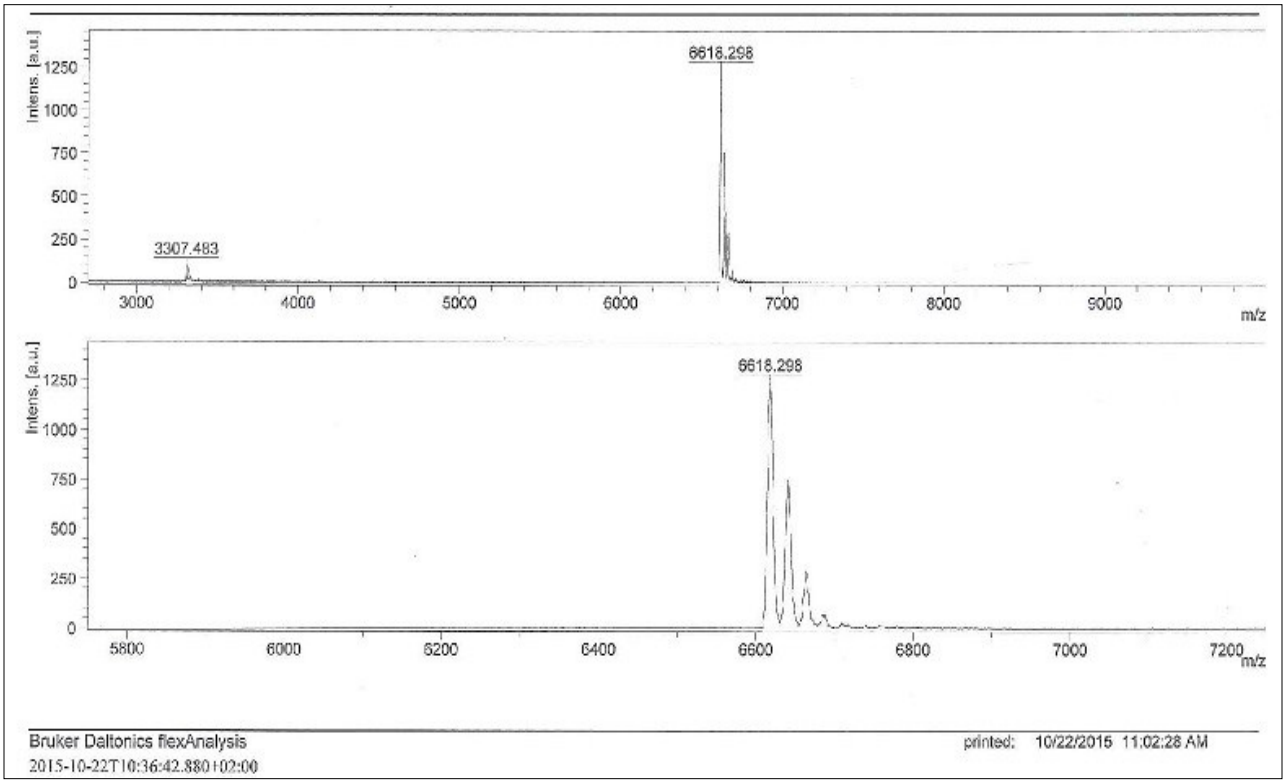
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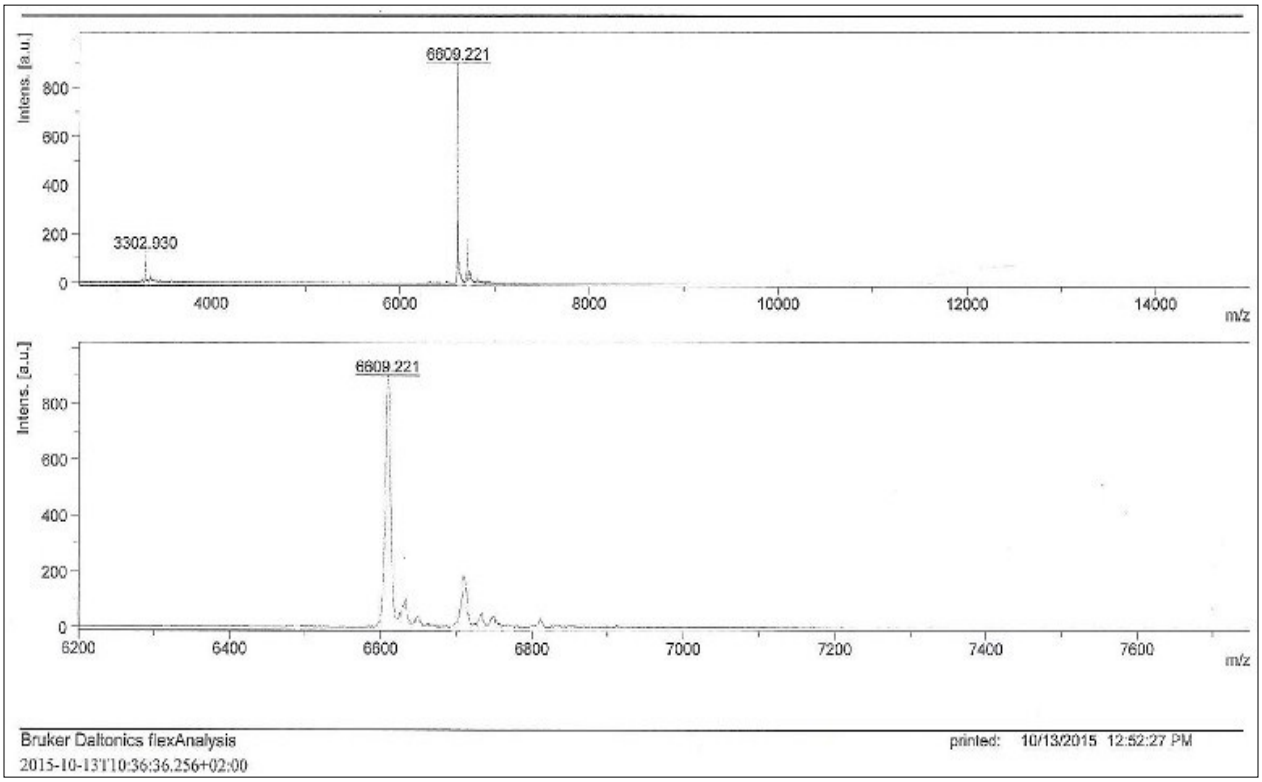
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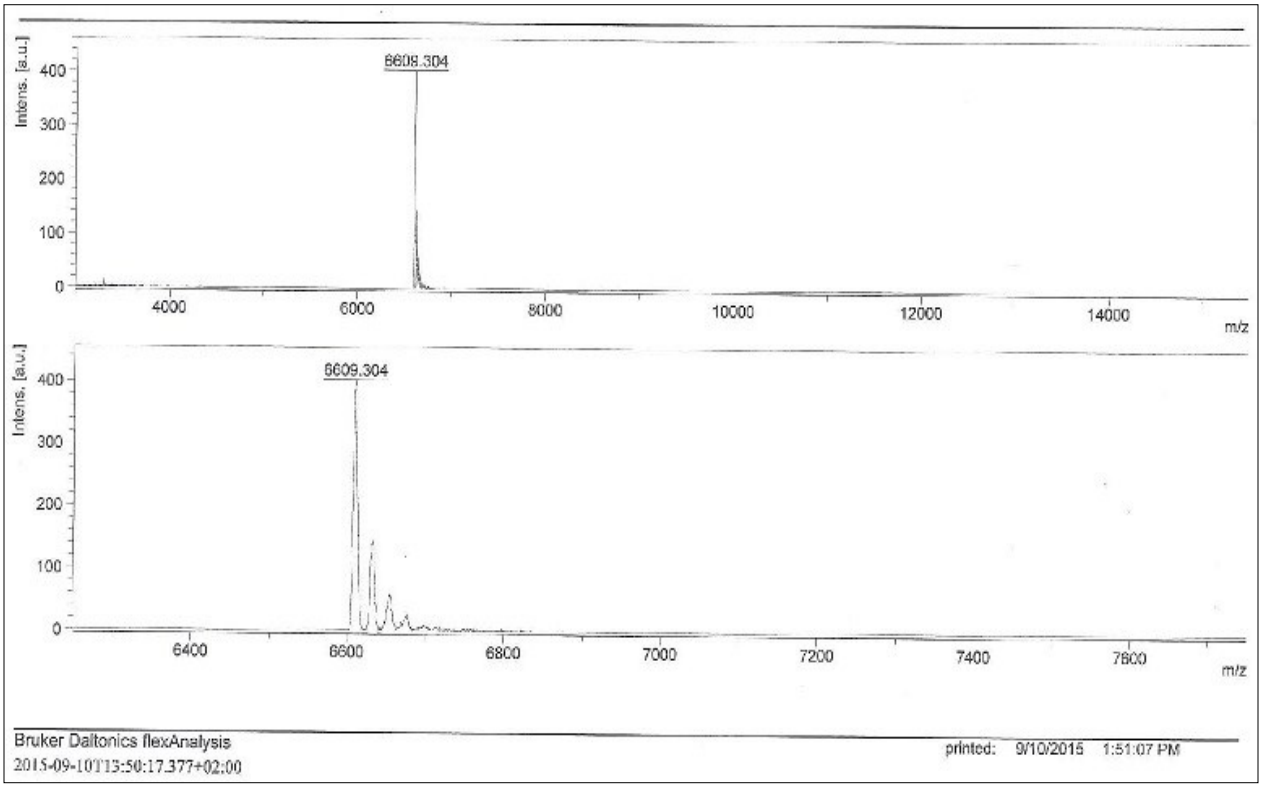
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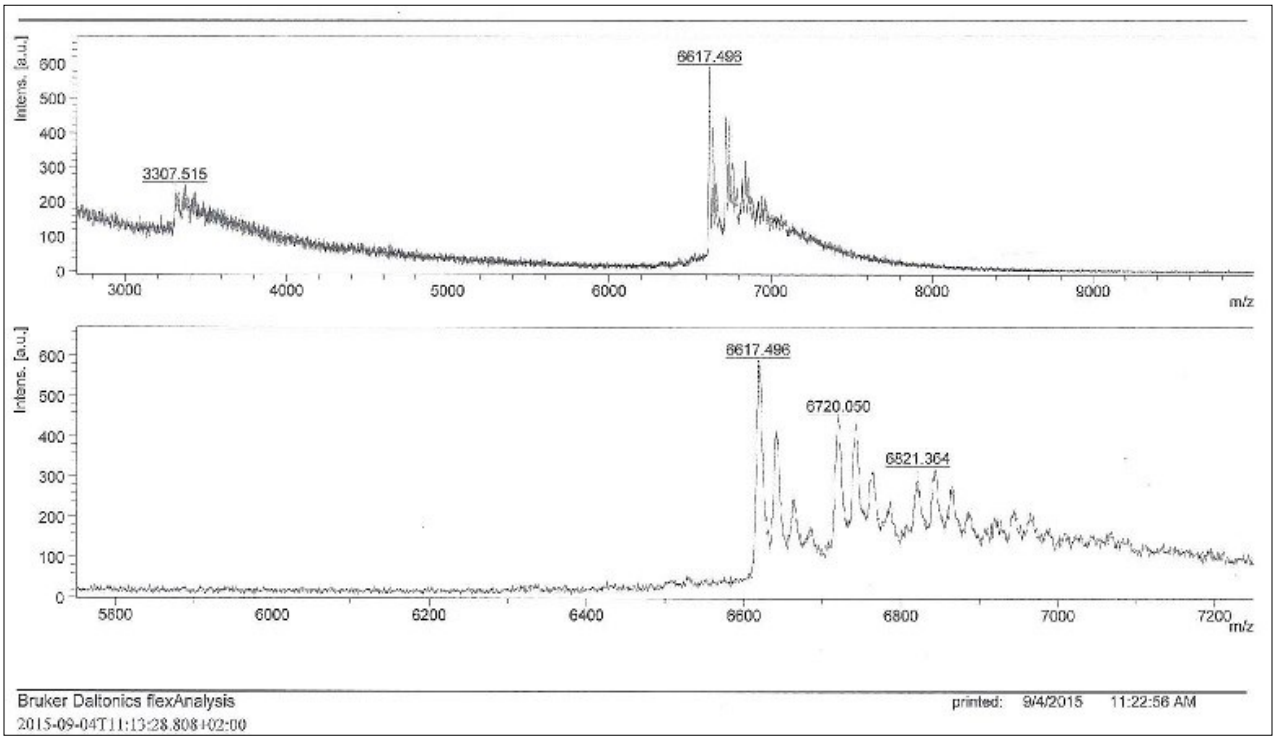
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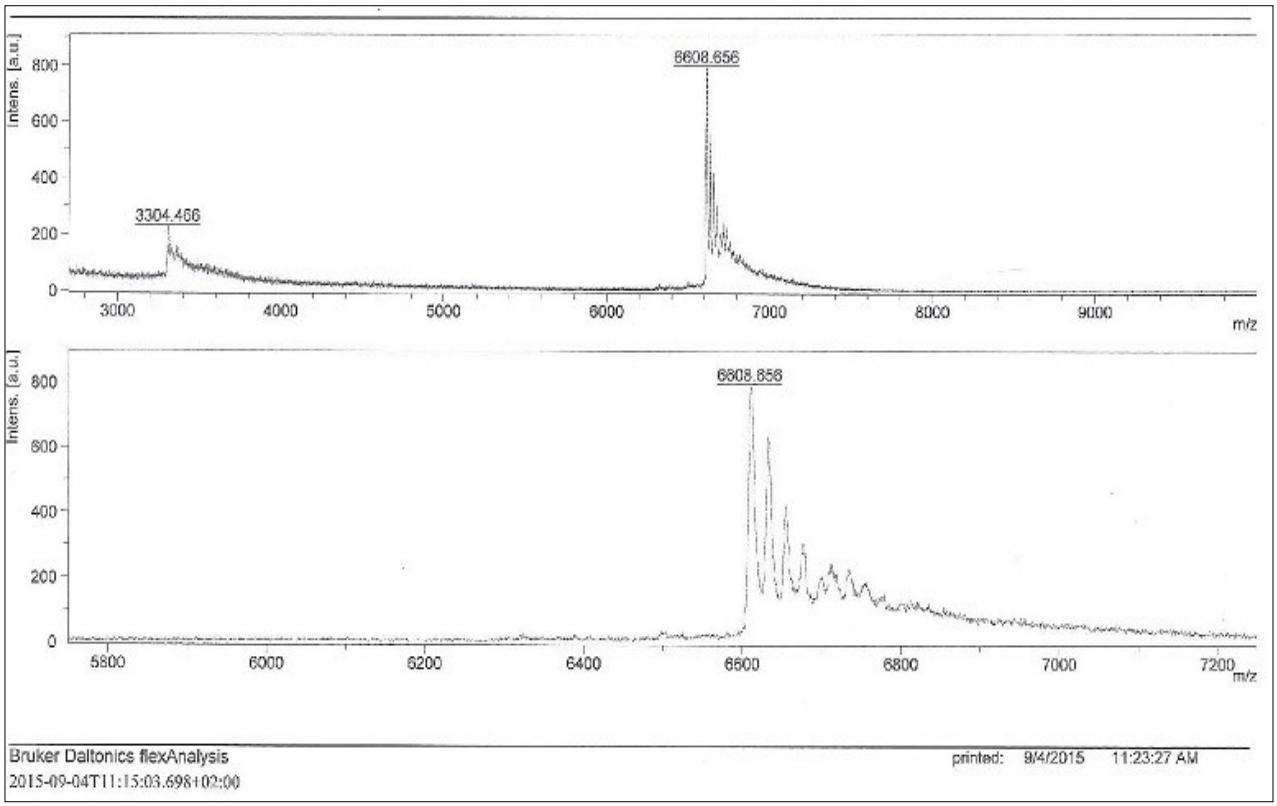
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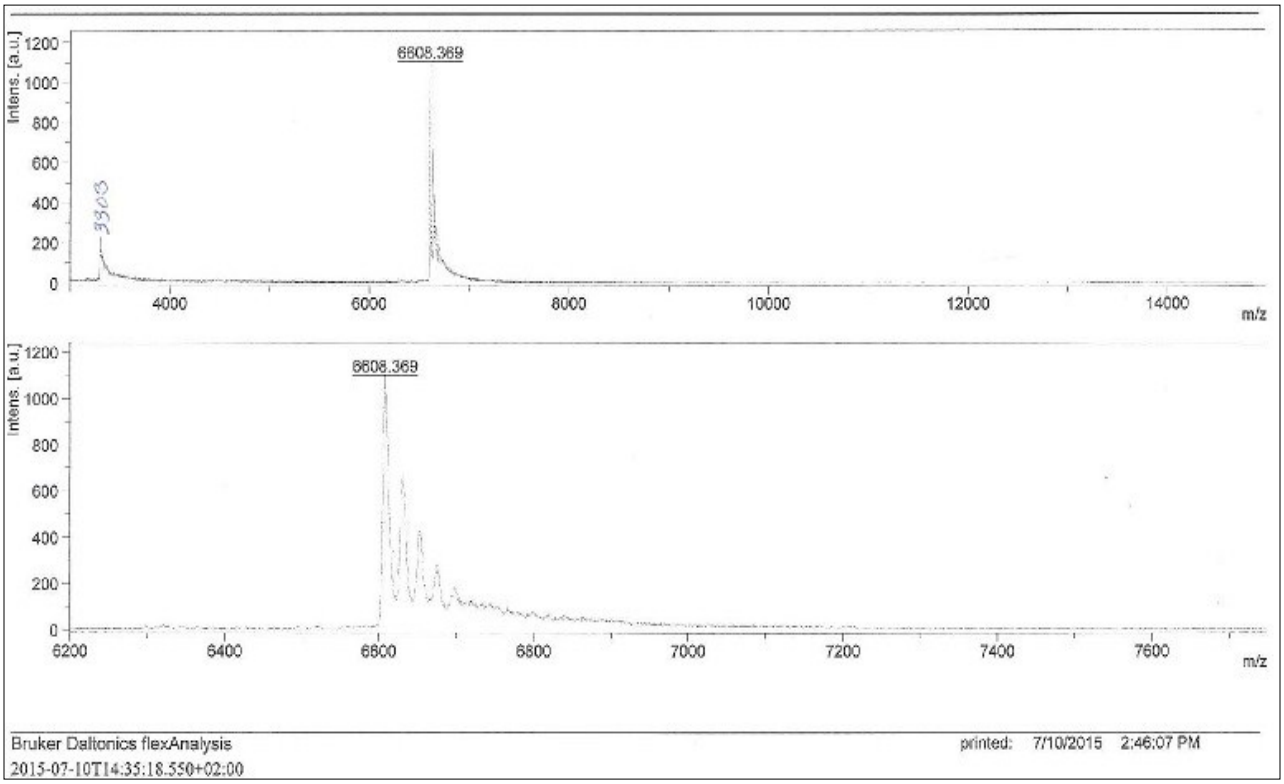
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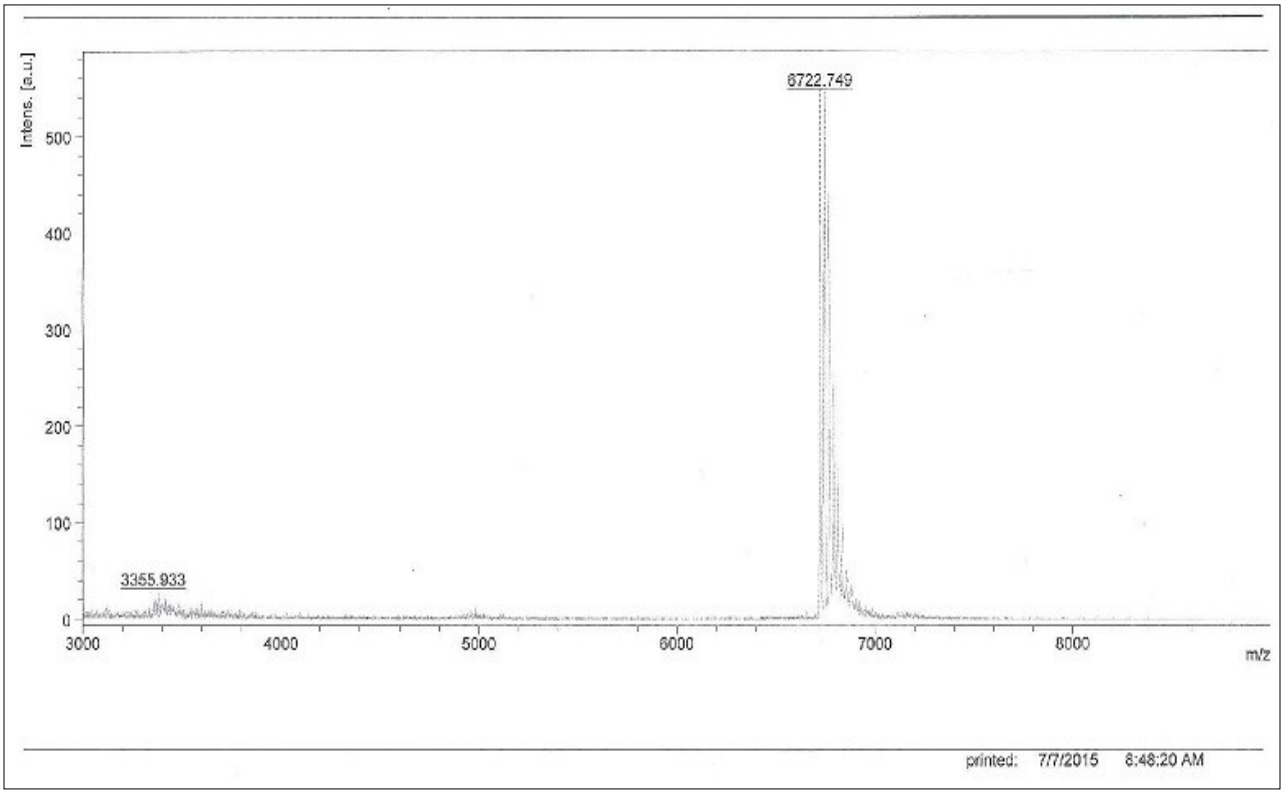
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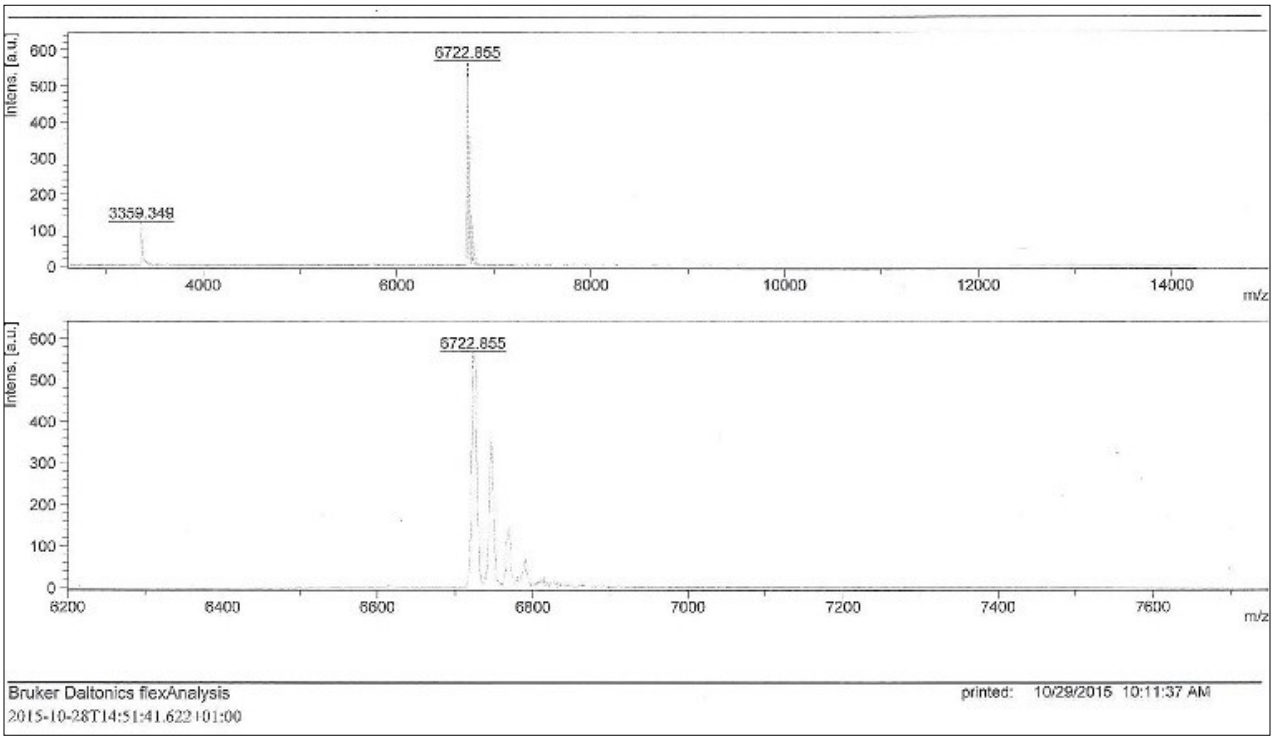
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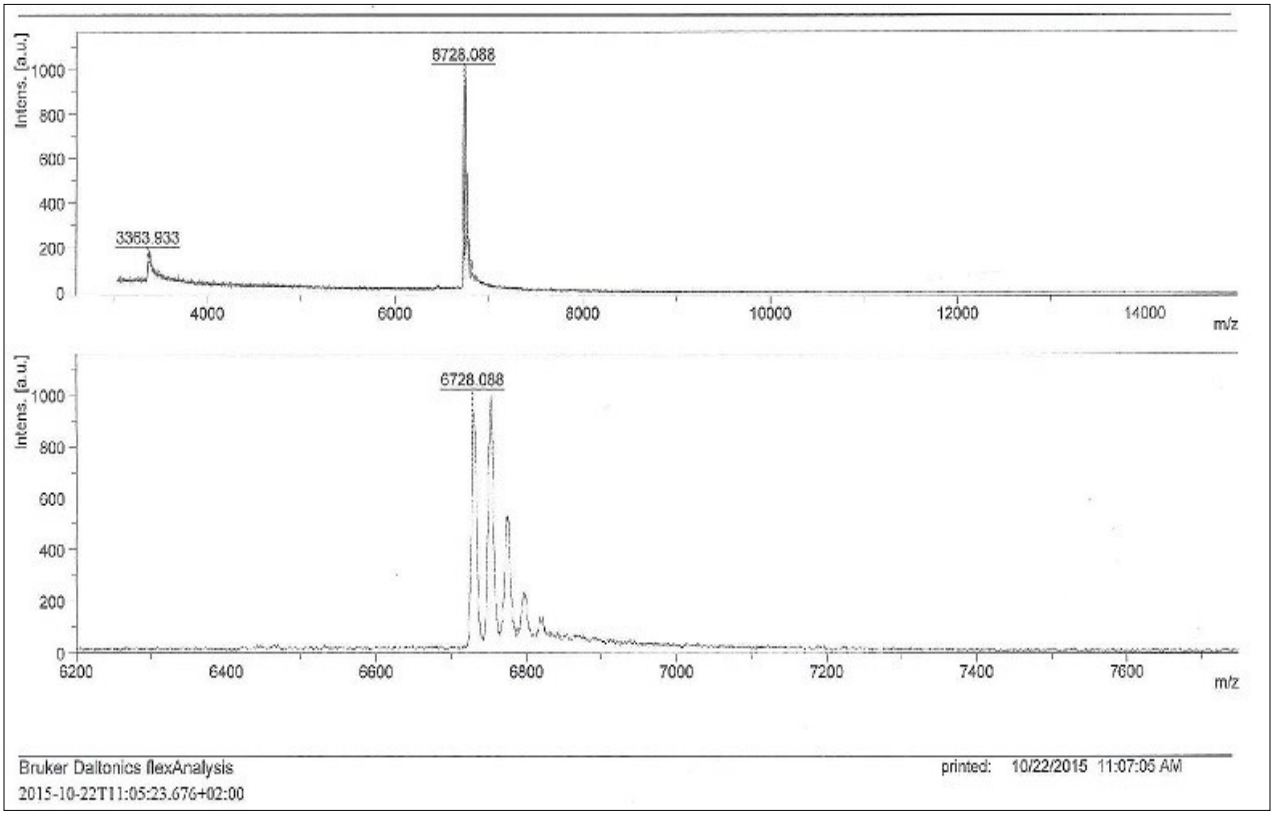
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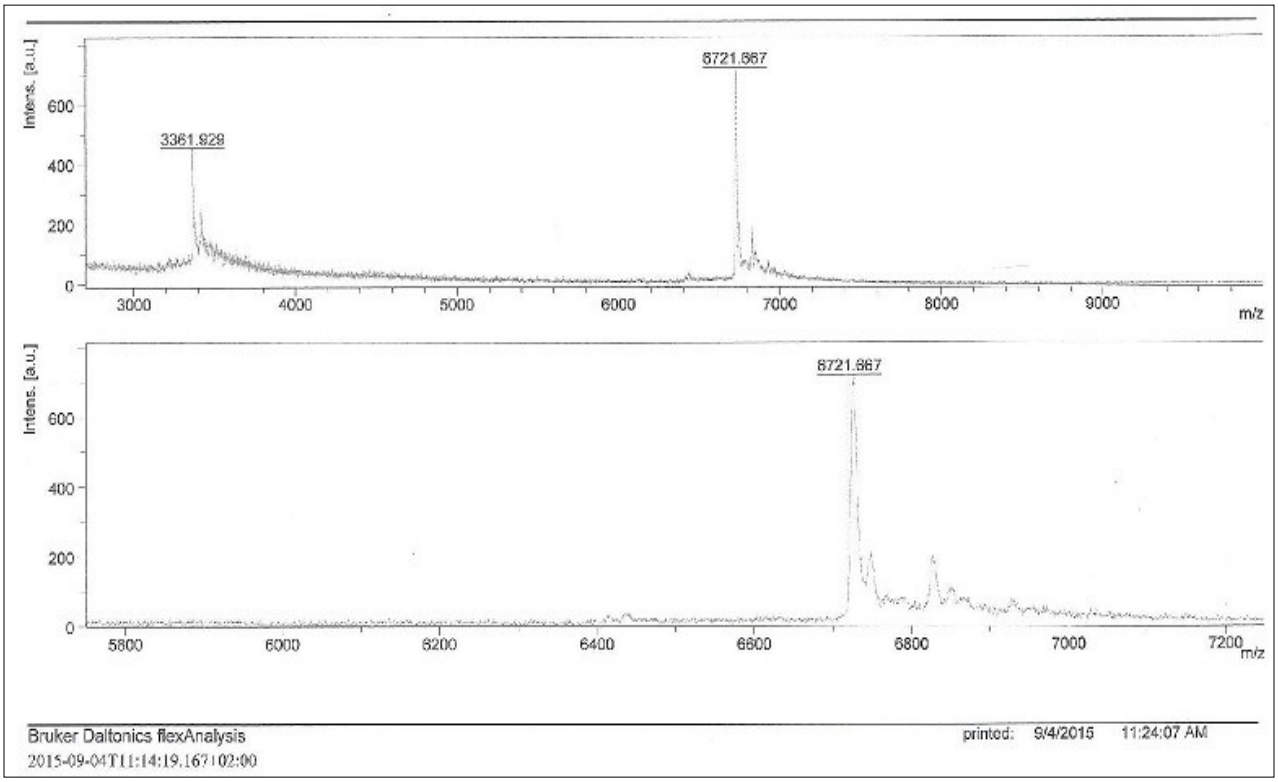
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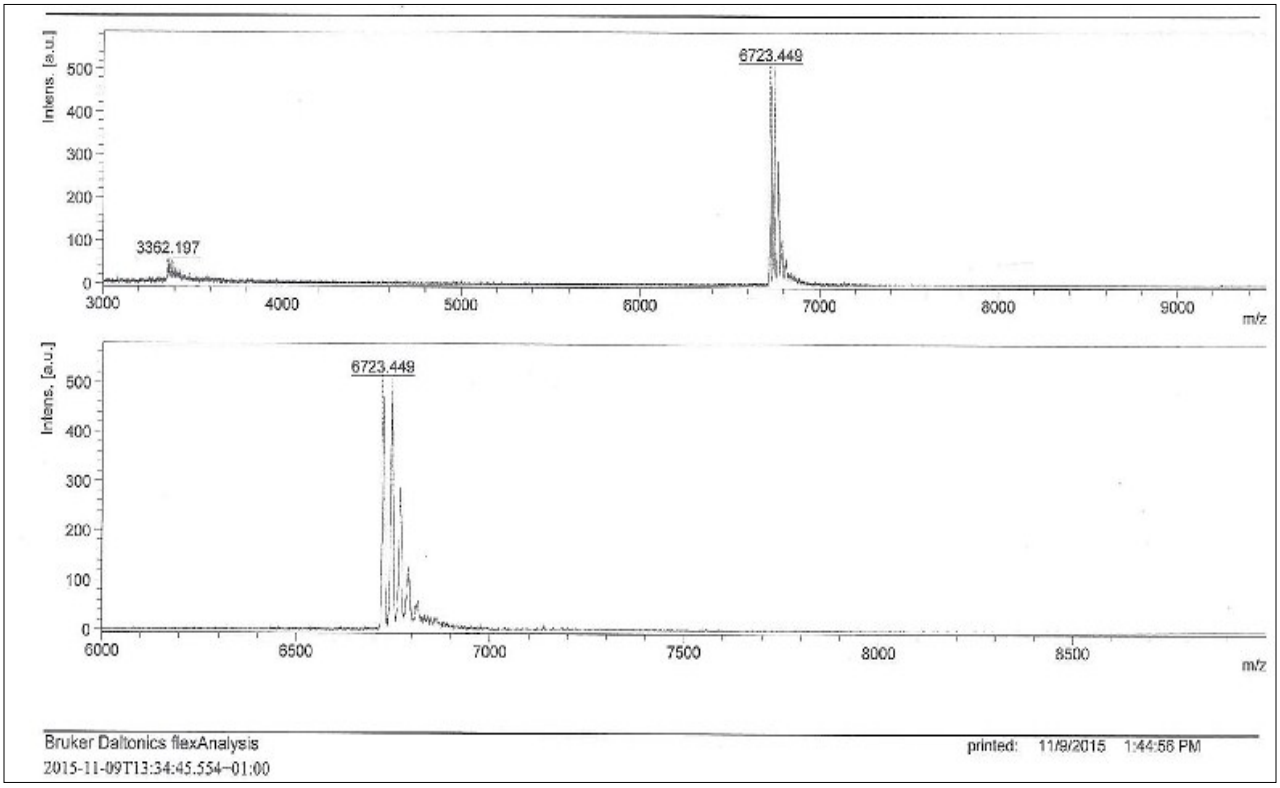
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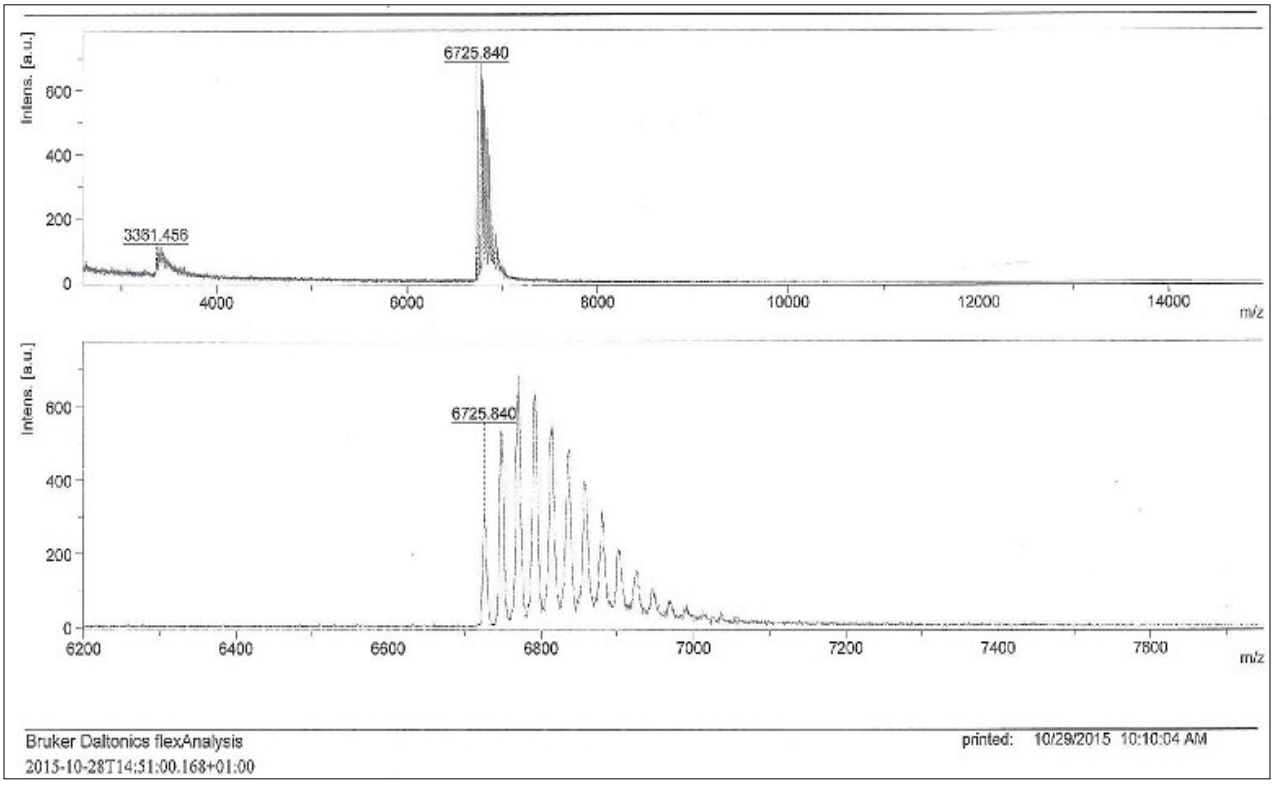
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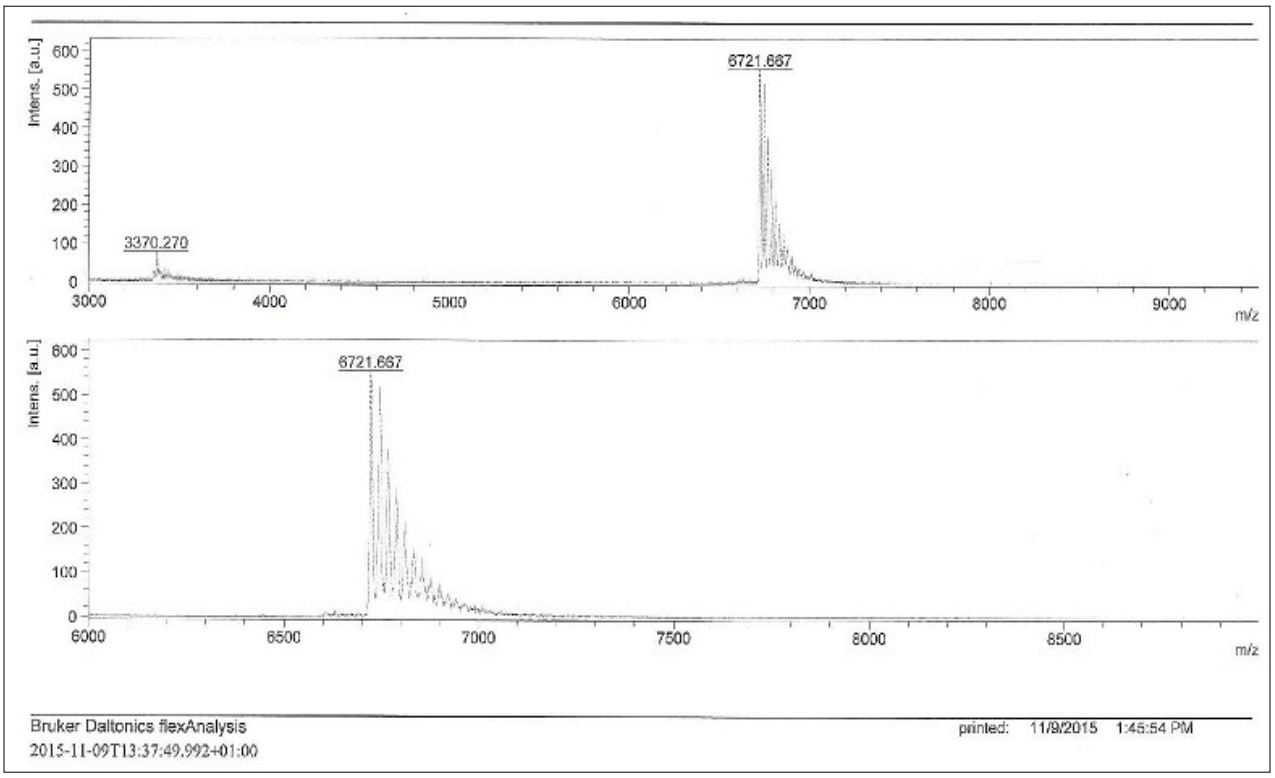
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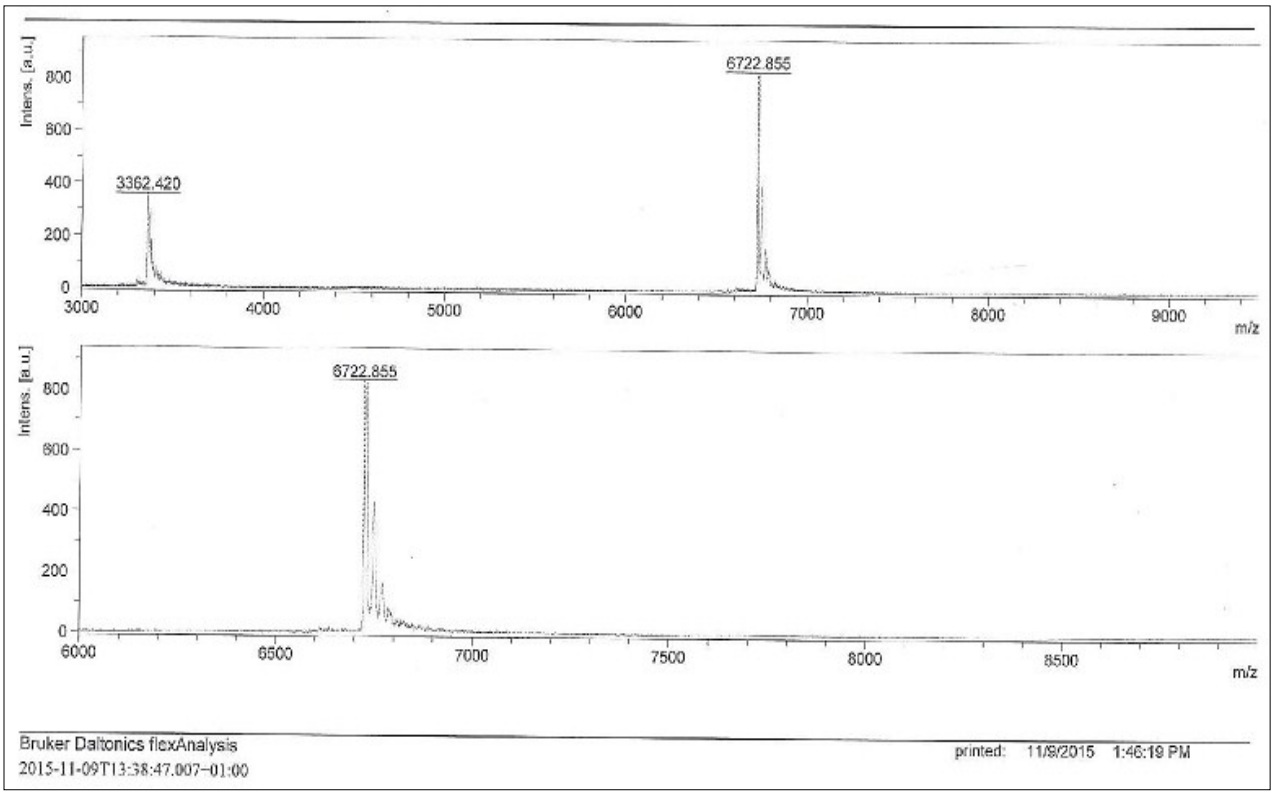
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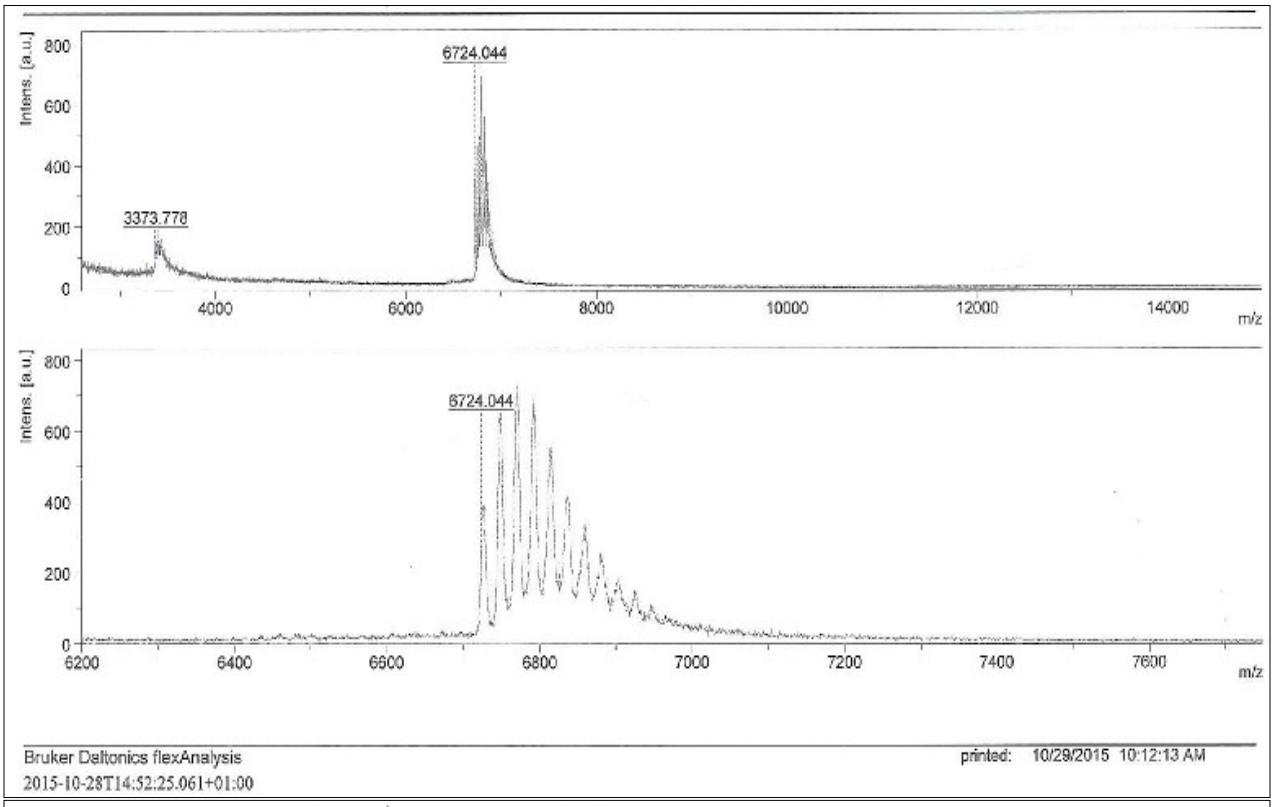
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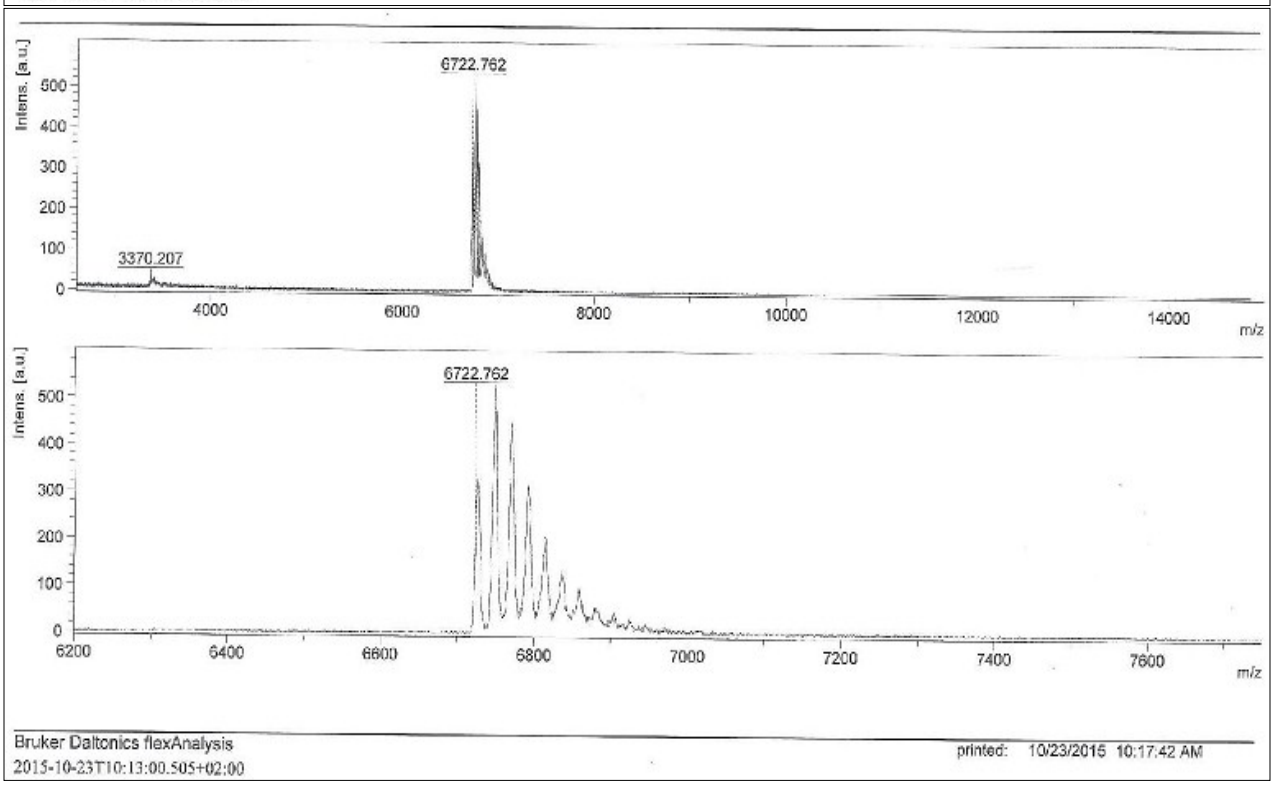
Intens. [a.u.]
6722.762
3370.207
m/z
6722.762
Bruker Daltonics flexAnalysis
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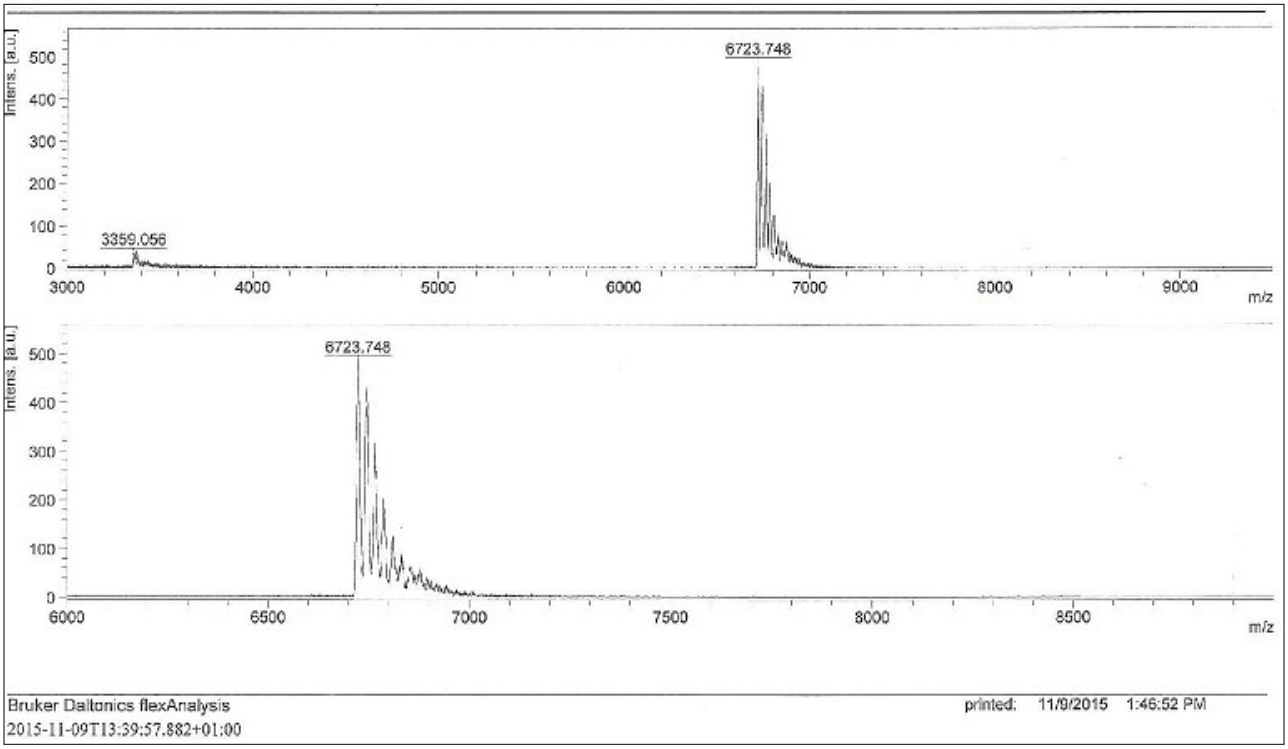
ON24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6723.748
3359.056
m/z
6723.748
Bruker Daltonics flexAnalysis
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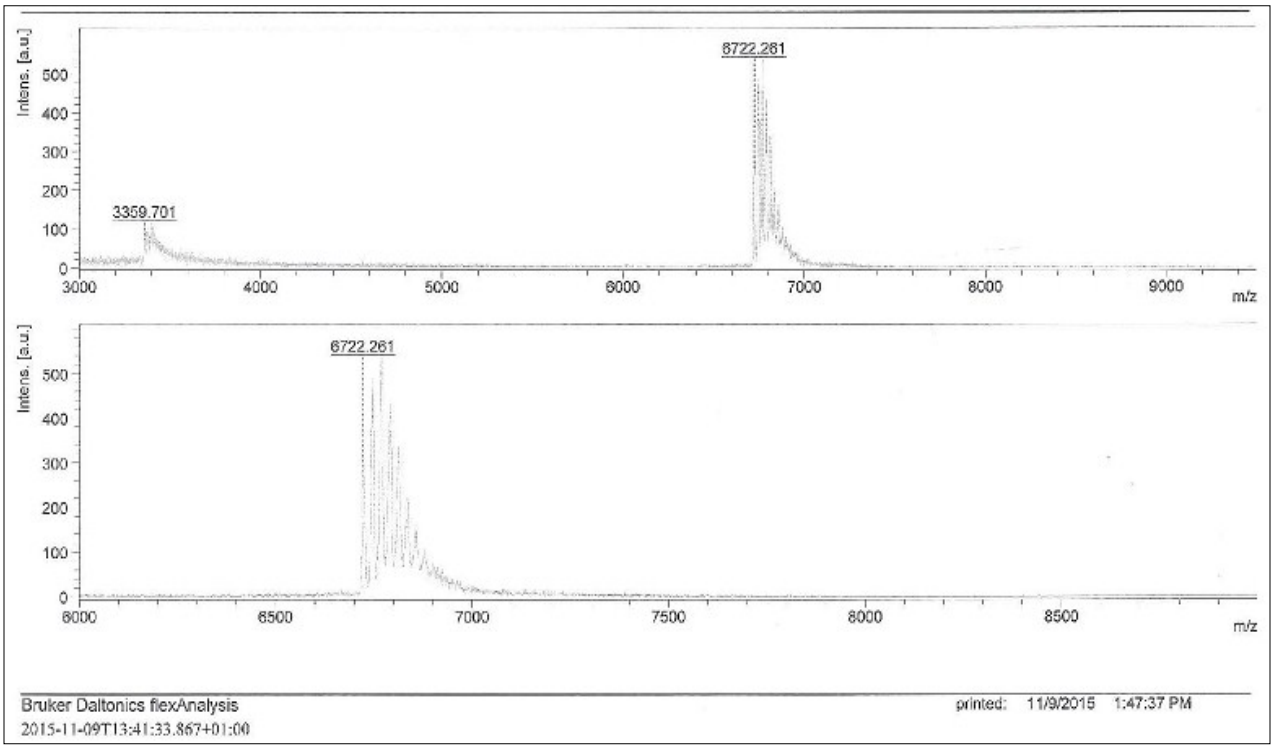
ON25


Intens. [a.u.]
8722.261
3359.701
m/z
6722.261
Bruker Daltonics flexAnalysis
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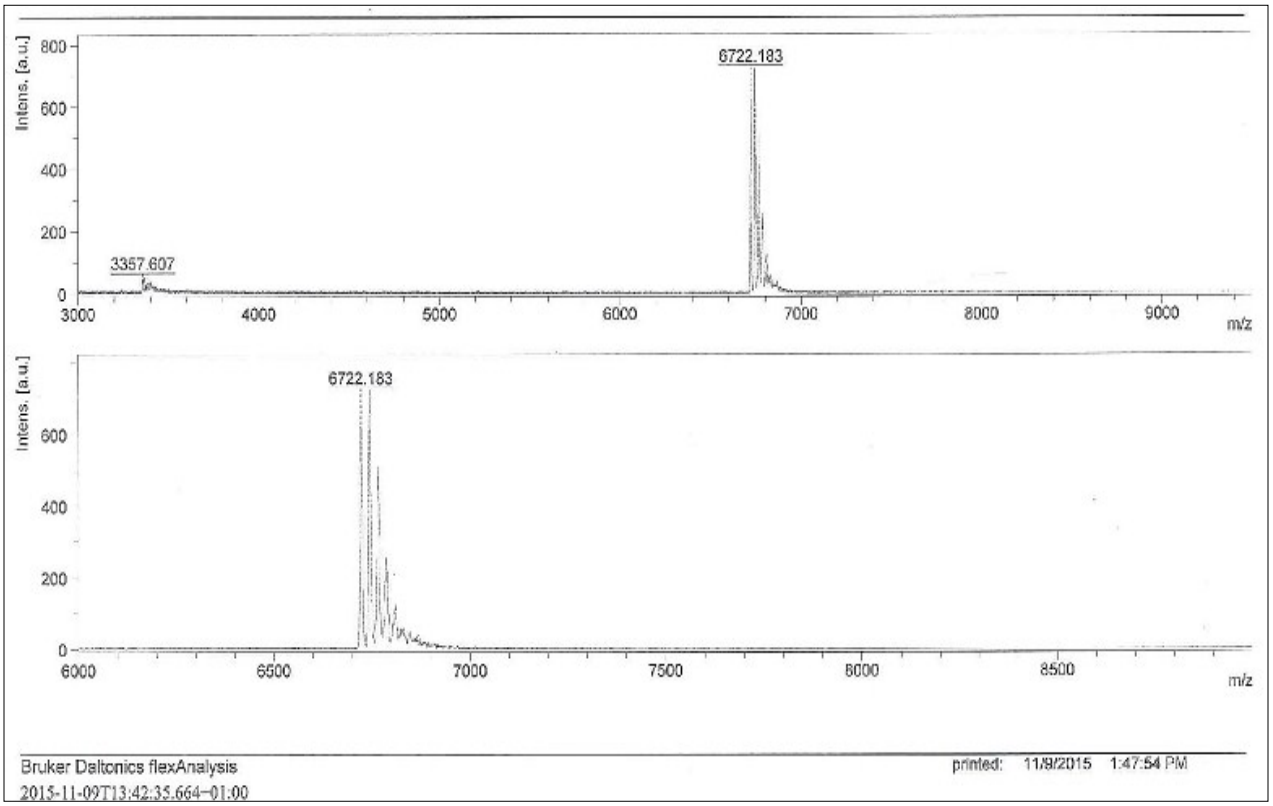
2015-11-09T13:41:33.867+01:00

ON26


Intens. [a.u.]
6722.183
3357.607
m/z
6722.183
Bruker Daltonics flexAnalysis
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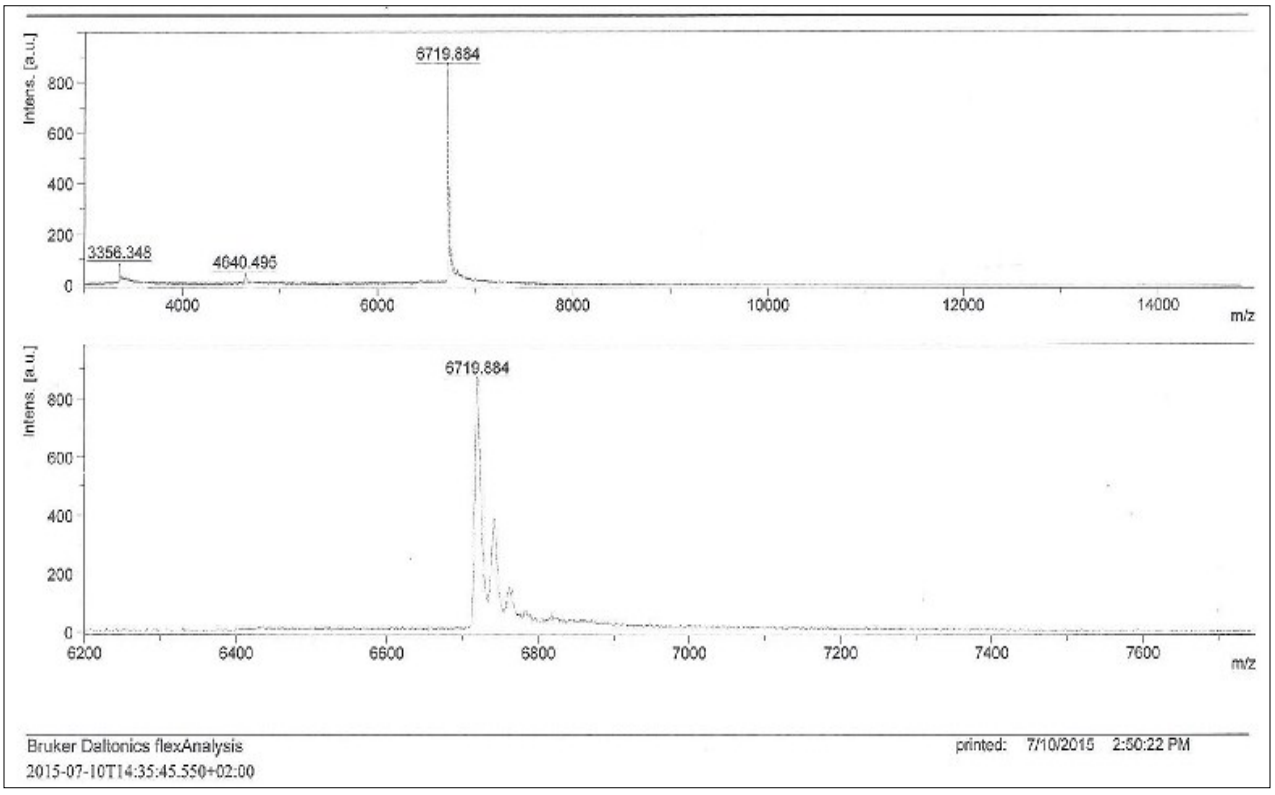
ON27


Intens. [a.u.]
6719.884
3356.348
4640.495
m/z
6719.884
Bruker Daltonics flexAnalysis
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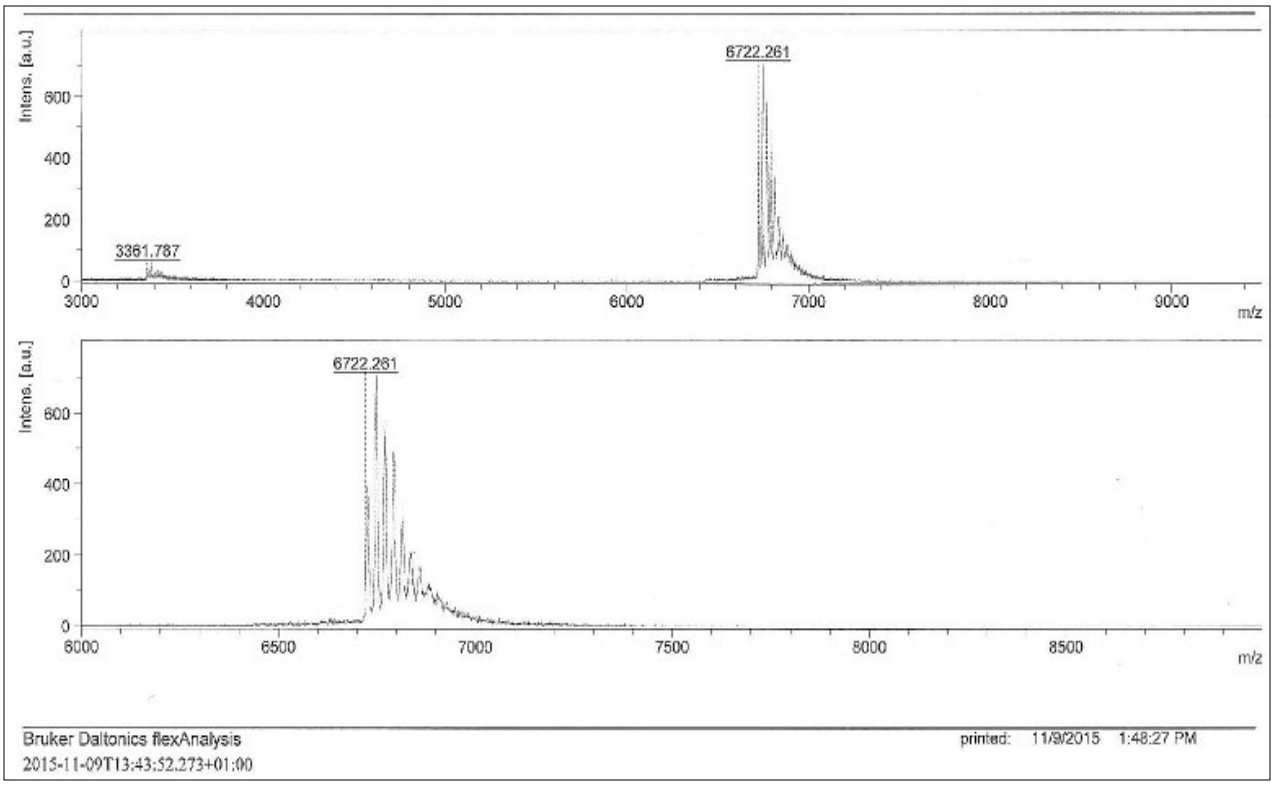
2015-07-10T14:35:45.550+02:00

ON28


Intens. [a.u.]
6722.261
3361.787
m/z
Intens. [a.u.]
6722.261
m/z
Bruker Daltonics flexAnalysis
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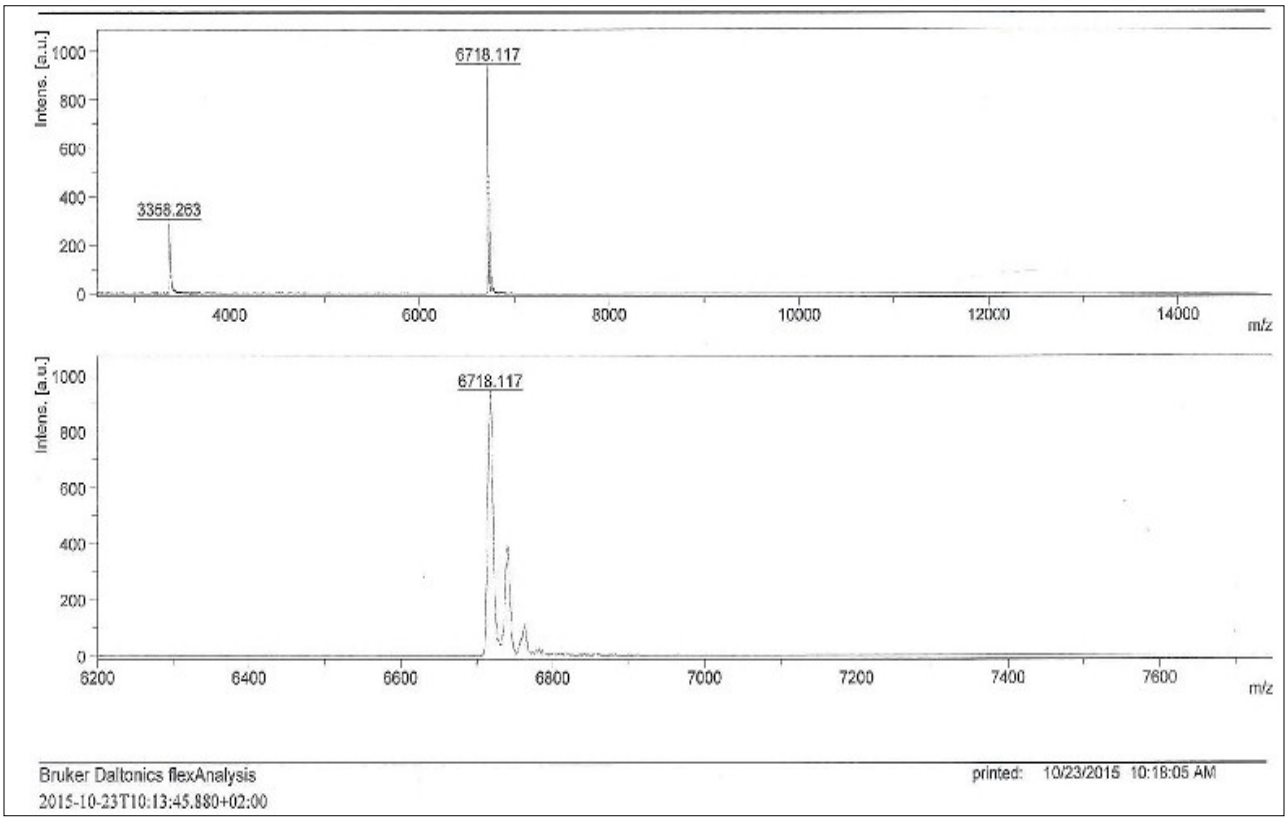
2015-11-09T13:43:52.273+01:00

ON29


Intens. [a.u.]
6718.117
3358.263
m/z
Intens. [a.u.]
6718.117
m/z
Bruker Daltonics flexAnalysis
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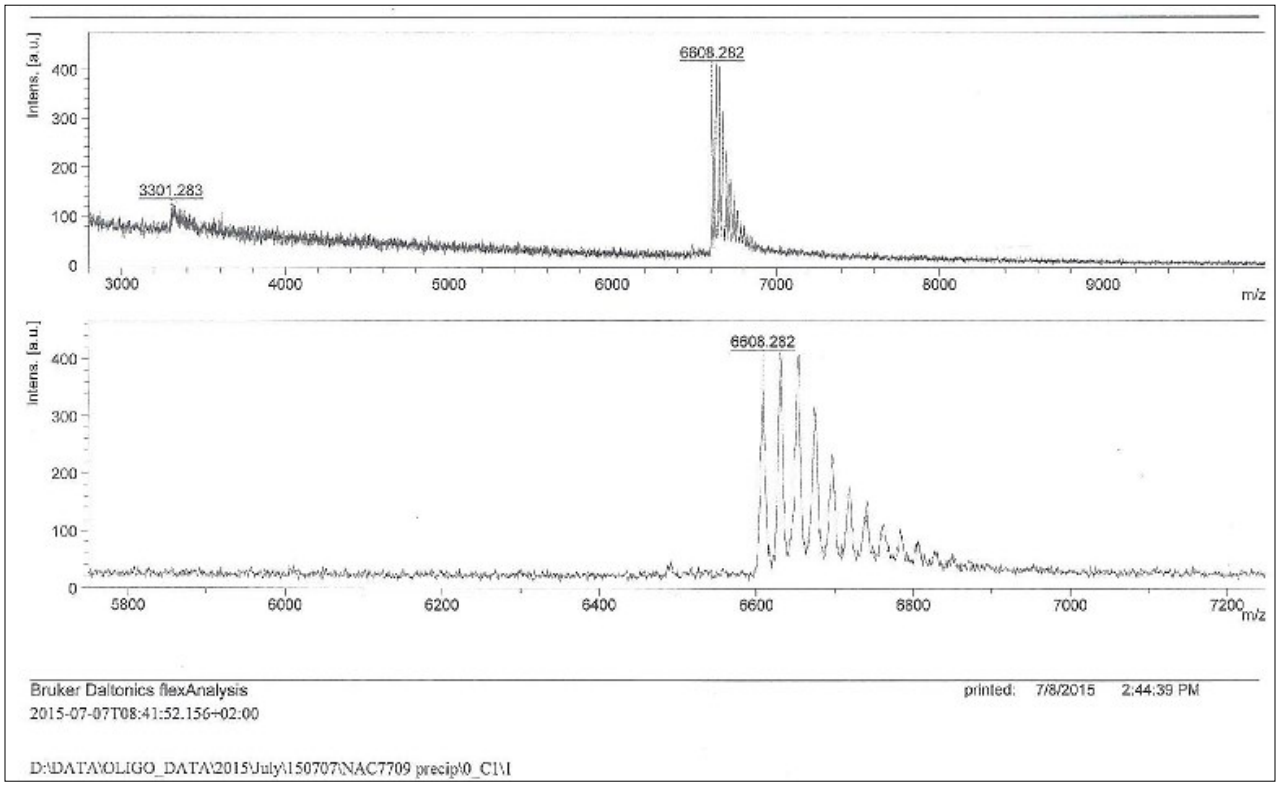
2015-10-23T10:13:45.880+02:00

ON30


Intens. [a.u.]
6608.282
3301.283
m/z
Intens. [a.u.]
6608.282
m/z
Bruker Daltonics flexAnalysis
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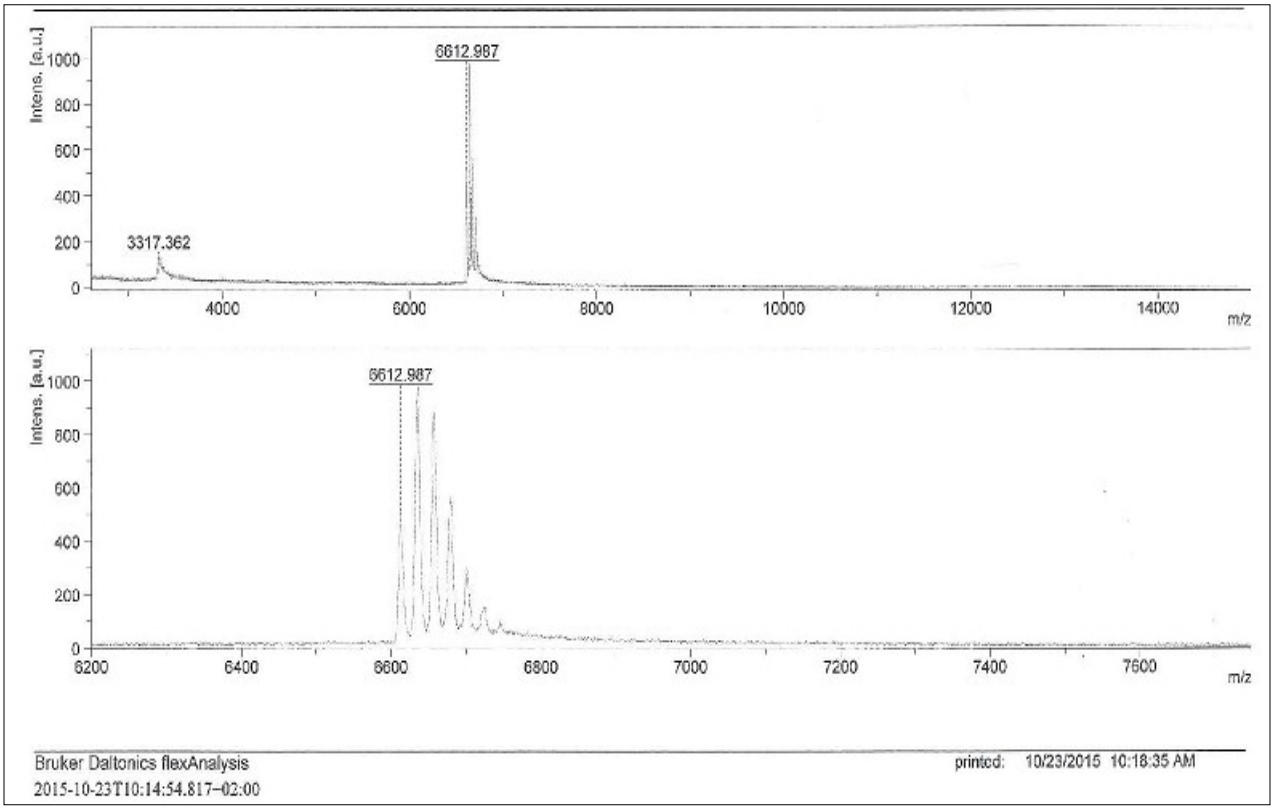
ON31


Intens. [a.u.]
6612.987
3317.362
m/z
Intens. [a.u.]
6612.987
m/z
Bruker Daltonics flexAnalysis
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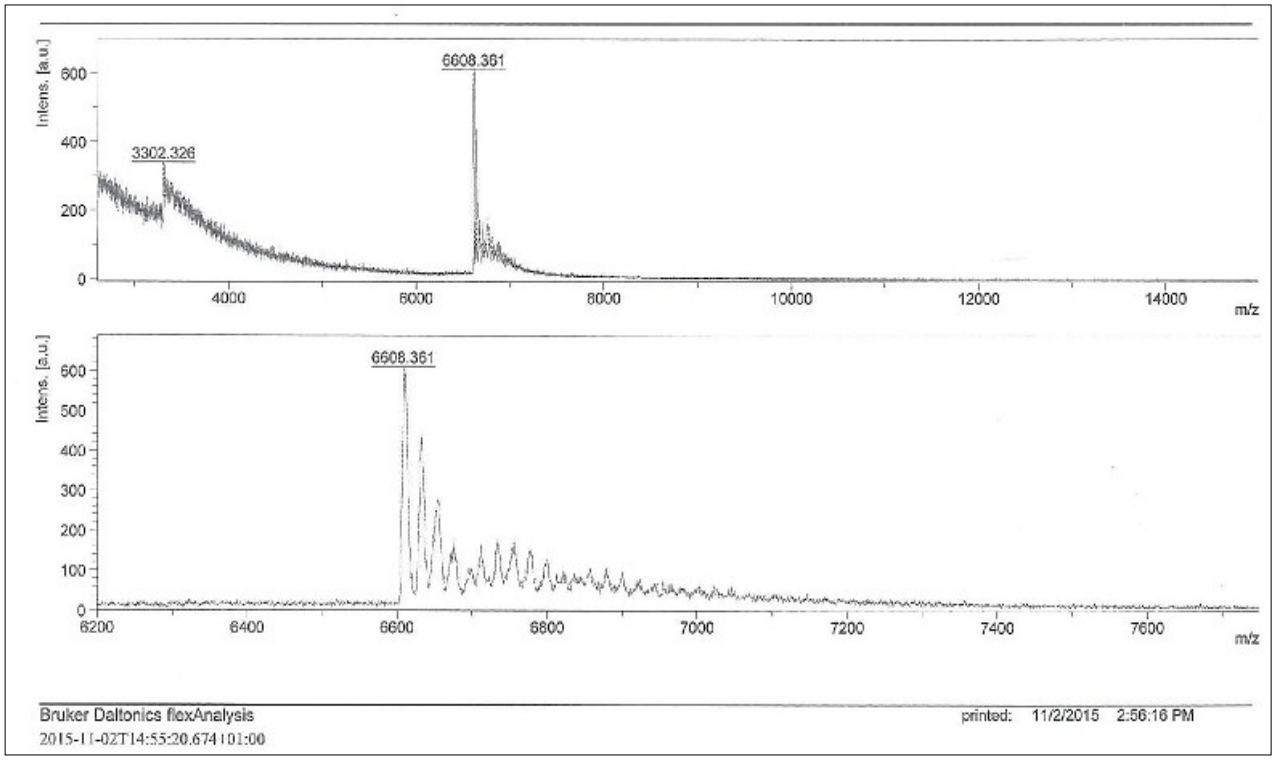
2015-10-23T10:14:54.817-02:00

ON32


Intens. [a.u.]
6608.361
3302.326
m/z
6608.361
Bruker Daltonics flexAnalysis
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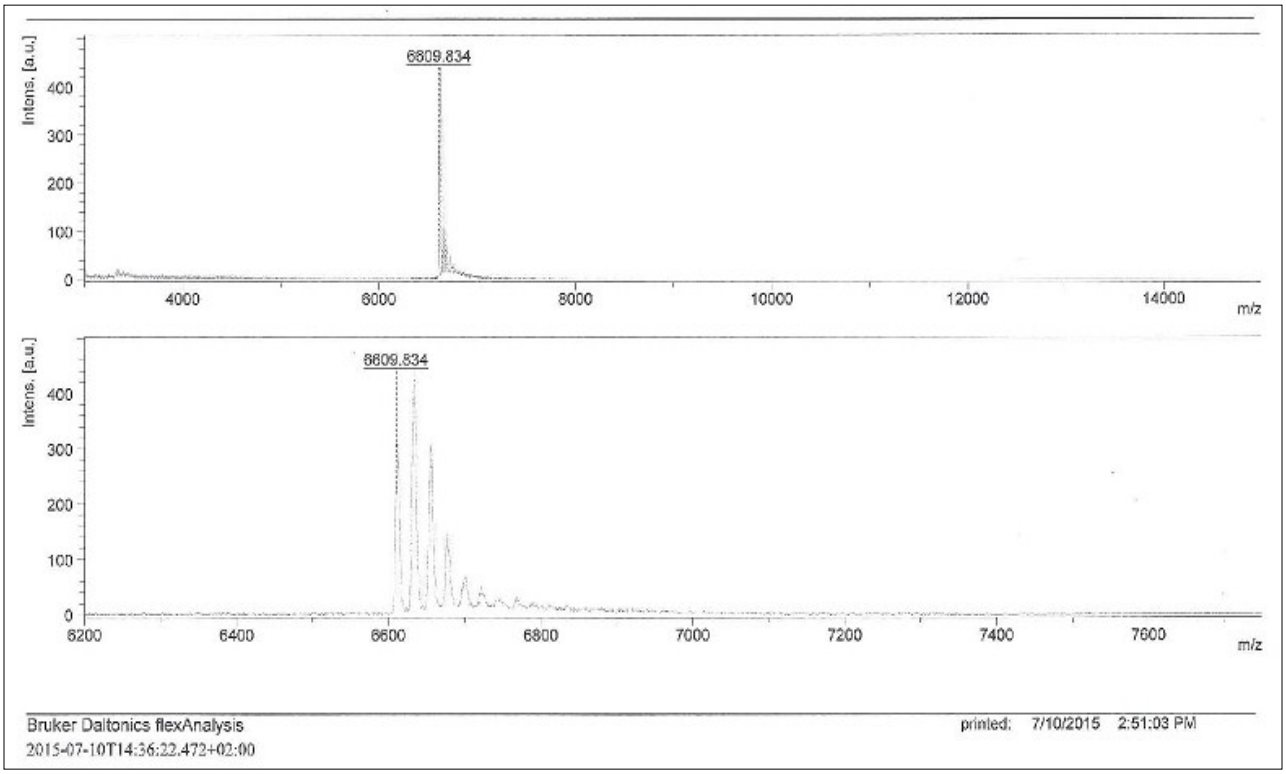
2015-11-02T14:55:20.674101:00

ON33


Intens. [a.u.]
6609.834
m/z
6609.834
Bruker Daltonics flexAnalysis
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2015-07-10T14:36:22.472+02:00