

Guanidine Functionalized Anthranilamides as Effective Antibacterials with Biofilm Disruption Activity

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Contents

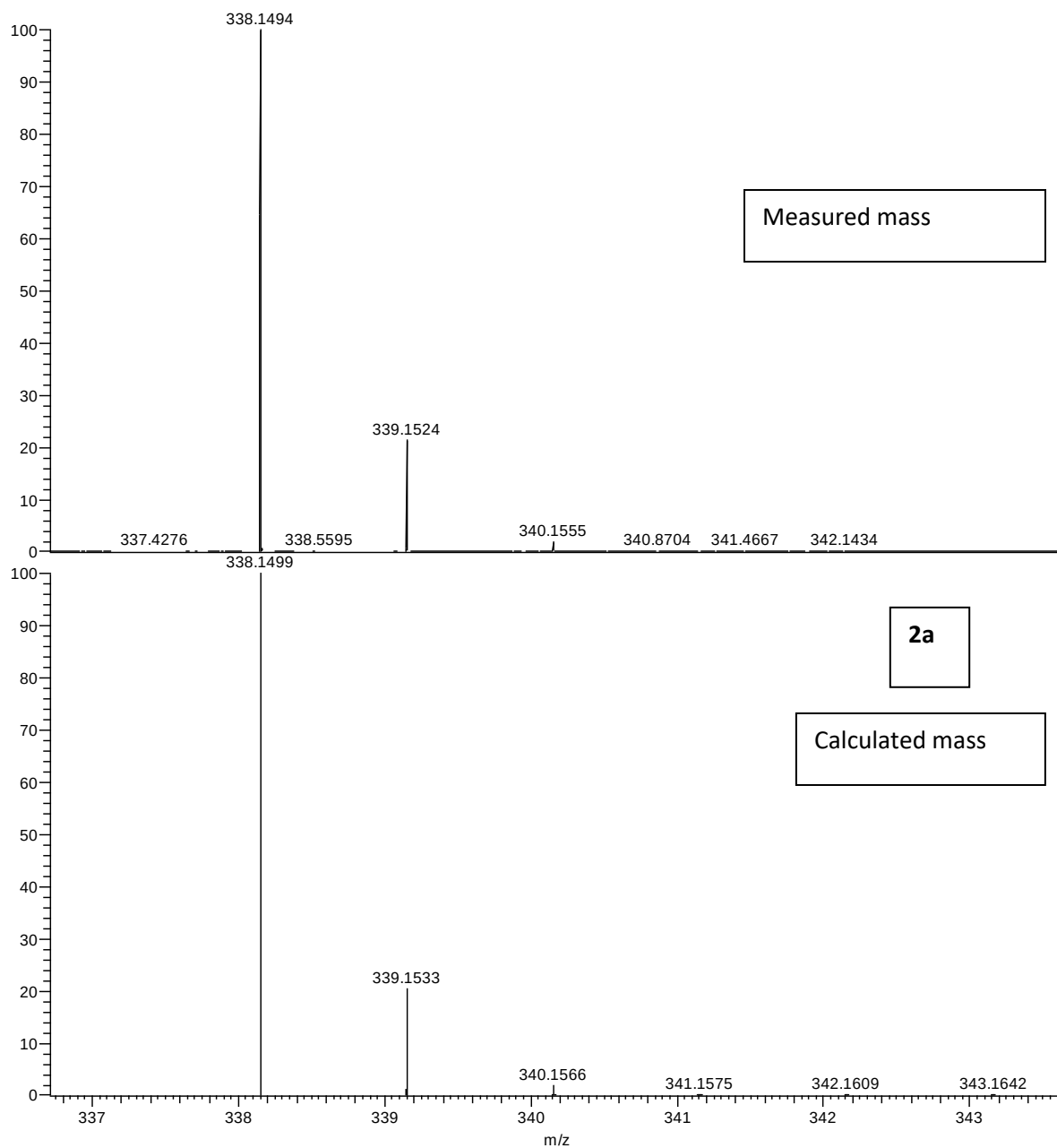
HRMS of Methyl (2-aminobenzoyl)-L-tryptophanate (2a).....	4
HRMS of Methyl (2-amino-5-fluorobenzoyl)-L-tryptophanate (2b).....	5
HRMS of Methyl (2-amino-5-chlorobenzoyl)-L-tryptophanate (2c).....	6
HRMS of Methyl (2-amino-5-bromobenzoyl)-L-tryptophanate (2d).....	7
HRMS of Methyl (2-amino-5-methoxybenzoyl)-L-tryptophanate (2e).....	8
HRMS of Methyl (2-(2-naphthamido)benzoyl)-L-tryptophanate (3a).....	9
HRMS of Methyl (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophanate (3b).....	10
HRMS of Methyl (2-(2-naphthamido)-5-chlorobenzoyl)-L-tryptophanate (3c).....	11
HRMS of Methyl (2-(2-naphthamido)-5-bromobenzoyl)-L-tryptophanate (3d).....	12
HRMS of Methyl (2-(2-naphthamido)-5-methoxybenzoyl)-L-tryptophanate (3e).....	13
HRMS of (2-(2-naphthamido)benzoyl)-L-tryptophan (4a).....	14
HRMS of (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophan (4b).....	15
HRMS of (2-(2-naphthamido)-5-chlorobenzoyl)-L-tryptophan (4c).....	16
HRMS of (2-(2-naphthamido)-5-bromobenzoyl)-L-tryptophan (4d).....	17
HRMS of (2-(2-naphthamido)-5-methoxybenzoyl)-L-tryptophan (4e).....	18
HRMS of <i>tert</i> -butyl (S)-(2-(2-(2-(2-naphthamido)benzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)ethyl)carbamate (5a).....	19
HRMS of <i>tert</i> -butyl (S)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)ethyl)carbamate (5b).....	20

HRMS of <i>tert</i> -butyl (S)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)ethyl)carbamate (5c).....	21
HRMS of <i>tert</i> -butyl (S)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)ethyl)carbamate (5d)	22
HRMS of <i>tert</i> -butyl (S)-(2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)ethyl)carbamate (5e)	23
HRMS of (S)- <i>N</i> -(2-((1-((2-dibocguanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6a).....	24
HRMS of (S)- <i>N</i> -(4-fluoro-2-((1-((2-dibocguanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6b)	25
HRMS of (S)- <i>N</i> -(4-chloro-2-((1-((2-dibocguanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6c)	26
HRMS of (S)- <i>N</i> -(4-bromo-2-((1-((2-dibocguanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6d)	27
HRMS of (S)- <i>N</i> -(4-methoxy-2-((1-((2-dibocguanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (6e).....	28
HRMS of (S)- <i>N</i> -(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (7a).....	29
HRMS of (S)- <i>N</i> -(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-fluorophenyl)-2-naphthamide (7b).....	30
HRMS of (S)- <i>N</i> -(4-chloro-2-((1-((2-(dimethylamino)ethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (7c)	31
HRMS of (S)- <i>N</i> -(4-bromo-2-((1-((2-(dimethylamino)ethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (7d)	32
HRMS of (S)- <i>N</i> -(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (7e).....	33
HRMS of (S)- <i>N</i> -(2-((1-((2-aminoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (8a)	34
HRMS of (S)- <i>N</i> -(2-((1-((2-aminoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-fluorophenyl)-2-naphthamide (8b).....	35
HRMS of (S)- <i>N</i> -(2-((1-((2-aminoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-chlorophenyl)-2-naphthamide (8c).....	36
HRMS of (S)- <i>N</i> -(2-((1-((2-aminoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-bromophenyl)-2-naphthamide (8d).....	37
HRMS of (S)- <i>N</i> -(2-((1-((2-aminoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (8e).....	38

HRMS of (S)-N-(2-((1-((2-guanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (9a)	39
HRMS of (S)-N-(4-fluoro-2-((1-((2-guanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (9b)	40
HRMS of (S)-N-(4-chloro-2-((1-((2-guanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (9c)	41
HRMS of (S)-N-(4-bromo-2-((1-((2-guanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (9d)	42
HRMS of (S)-N-(2-((1-((2-guanidinoethyl)amino)-3-(1 <i>H</i> -indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (9e).....	43
HRMS of (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N</i> -dimethylethan-1-aminium chloride (10a).....	44
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N</i> -dimethylethan-1-aminium chloride (10b)	45
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N</i> -dimethylethan-1-aminium chloride (10c).....	46
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N</i> -dimethylethan-1-aminium (10d)	47
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N</i> -dimethylethan-1-aminium (10e).....	48
HRMS of (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N,N</i> -trimethylethan-1-aminium iodide (11a).....	49
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N,N</i> -trimethylethan-1-aminium iodide (11b).....	50
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N,N</i> -trimethylethan-1-aminium (11c)	51
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N,N</i> -trimethylethan-1-aminium iodide (11d).....	52
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1 <i>H</i> -indol-3-yl)propanamido)- <i>N,N,N</i> -trimethylethan-1-aminium iodide (11e).....	53

** The HRMS data indicates both the found mass and calculated mass. The calculated mass is below the found mass*

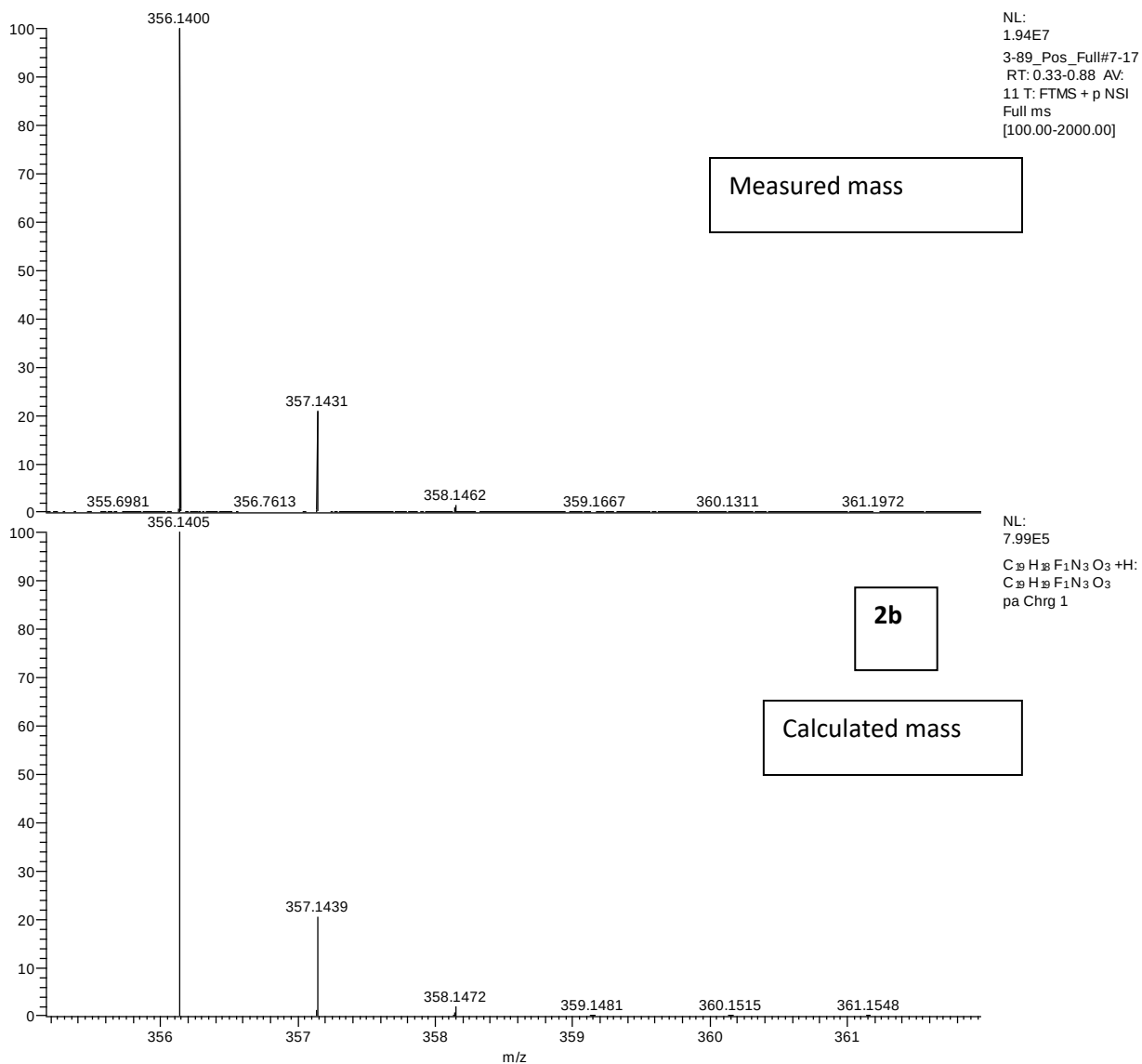
HRMS of Methyl (2-aminobenzoyl)-L-tryptophanate (**2a**)



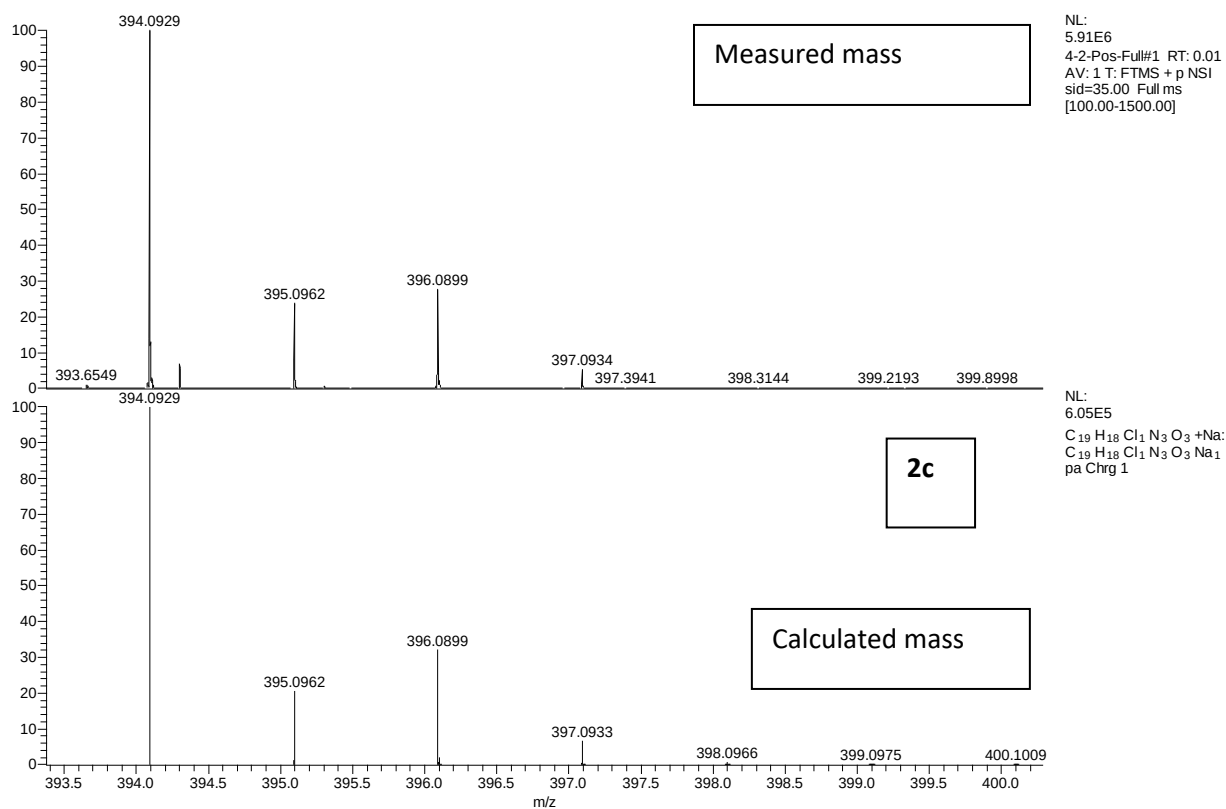
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10 RT: 0.24-0.52
AV: 6 T: FTMS + p
NSI Full ms
[100.00-2000.00]

NL:
7.98E5
C₂₀H₁₉N₃O₃ + H:
C₂₀H₂₀N₃O₃
pa Chrg 1

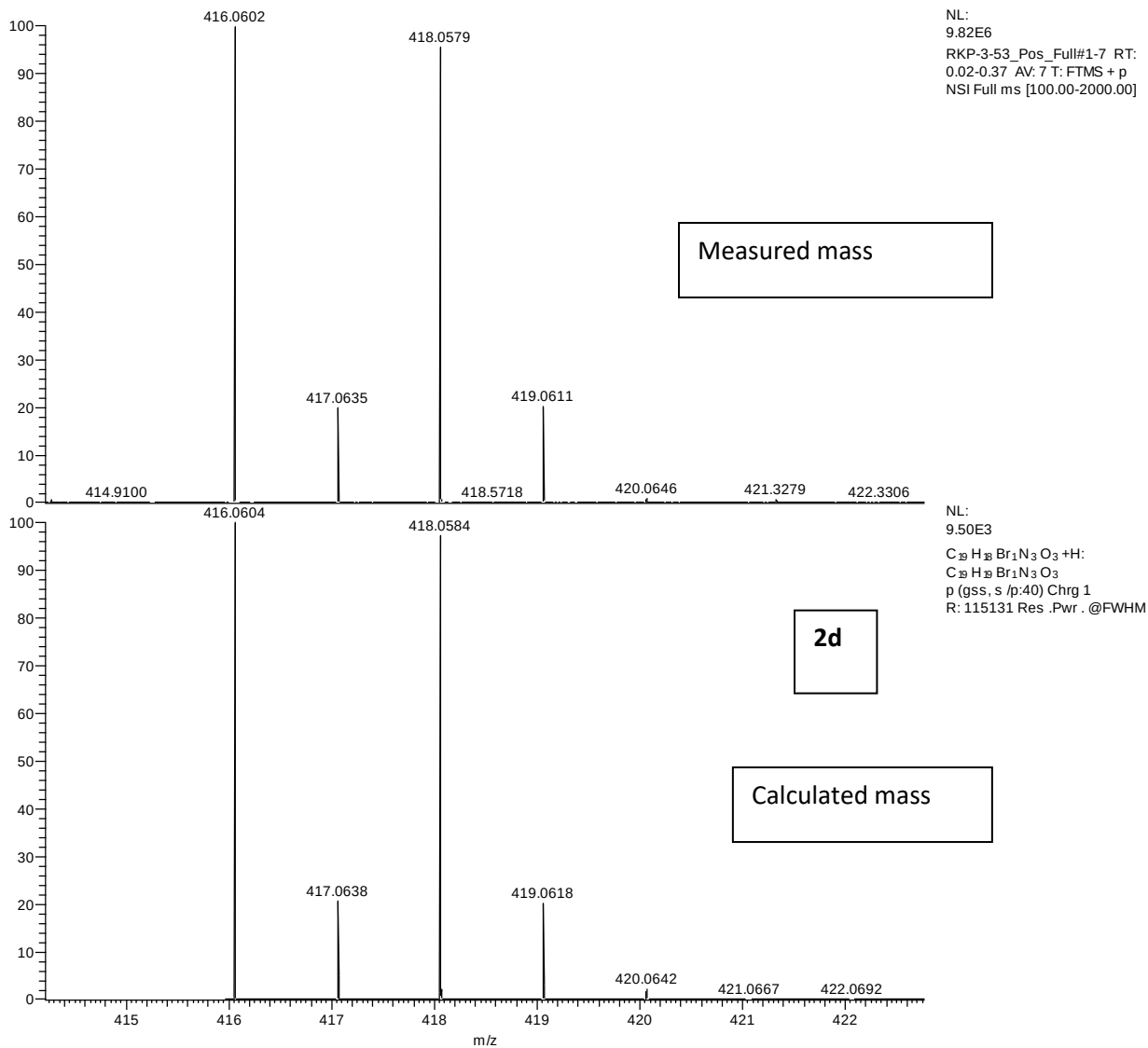
HRMS of Methyl (2-amino-5-fluorobenzoyl)-*L*-tryptophanate (2b)



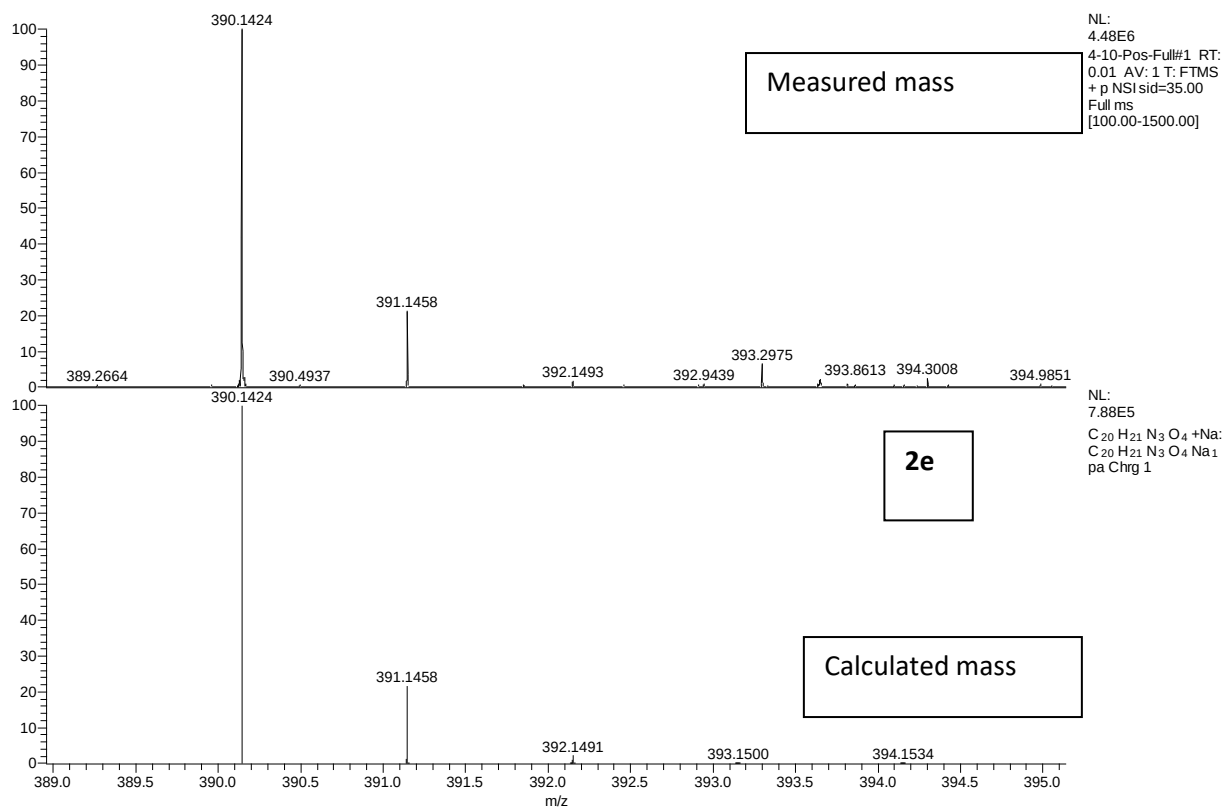
HRMS of Methyl (2-amino-5-chlorobenzoyl)-L-tryptophanate (2c)



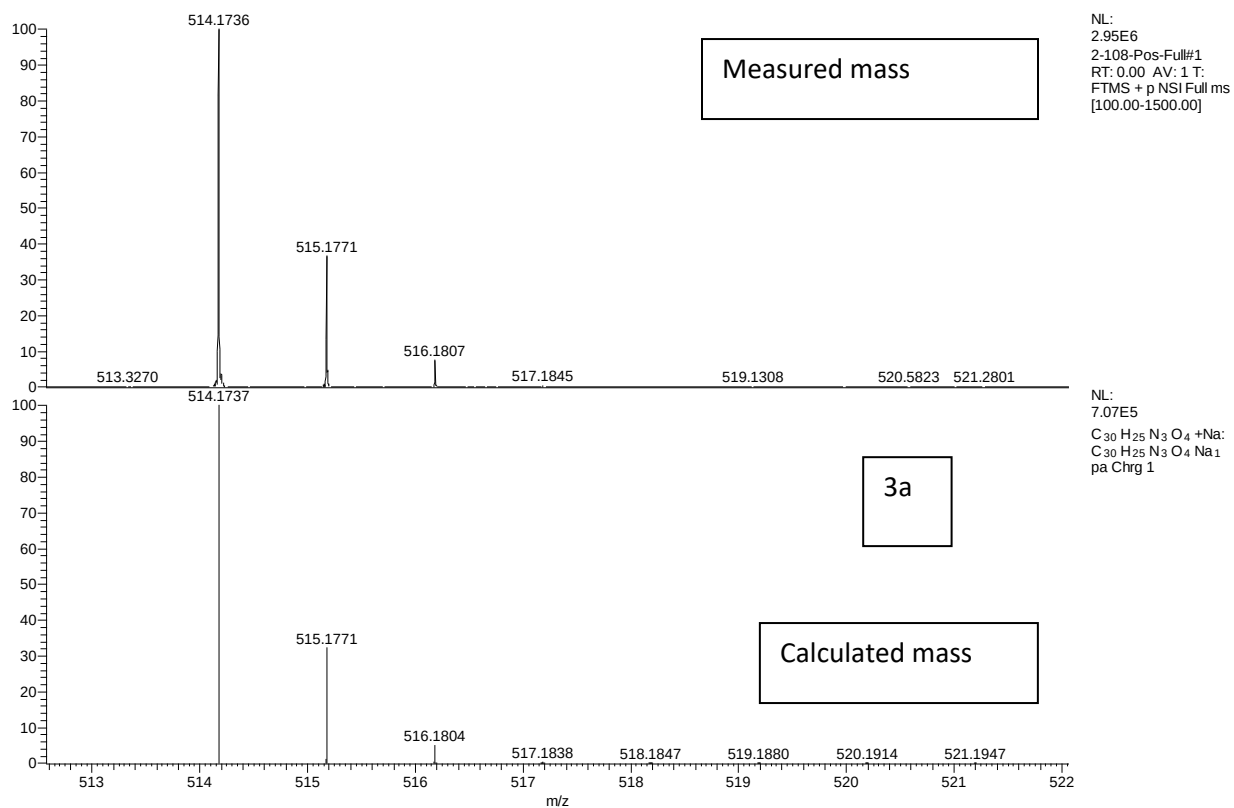
HRMS of Methyl (2-amino-5-bromobenzoyl)-L-tryptophanate (2d)



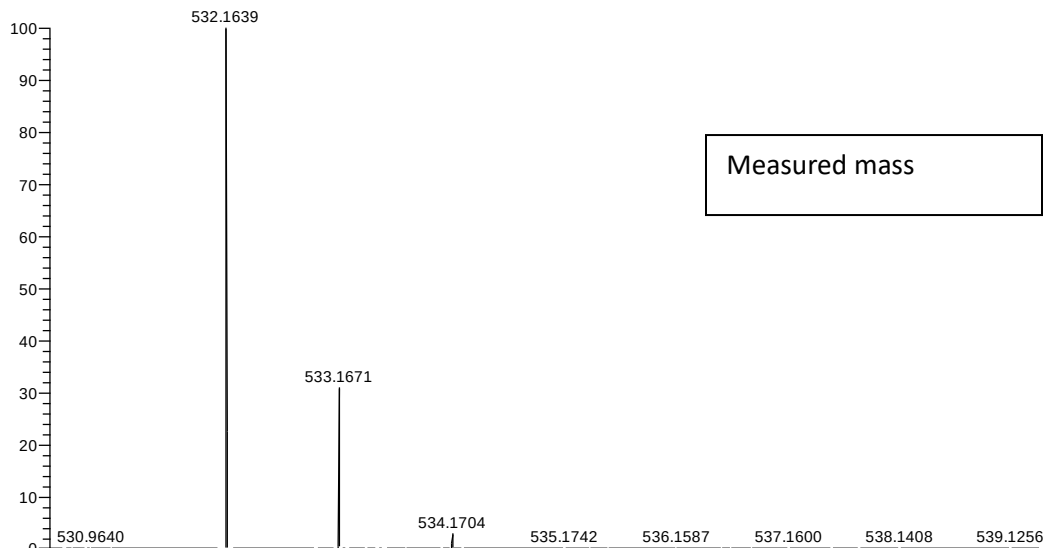
HRMS of Methyl (2-amino-5-methoxybenzoyl)-*L*-tryptophanate (**2e**)



HRMS of Methyl (2-(2-naphthamido)benzoyl)-*L*-tryptophanate (**3a**)

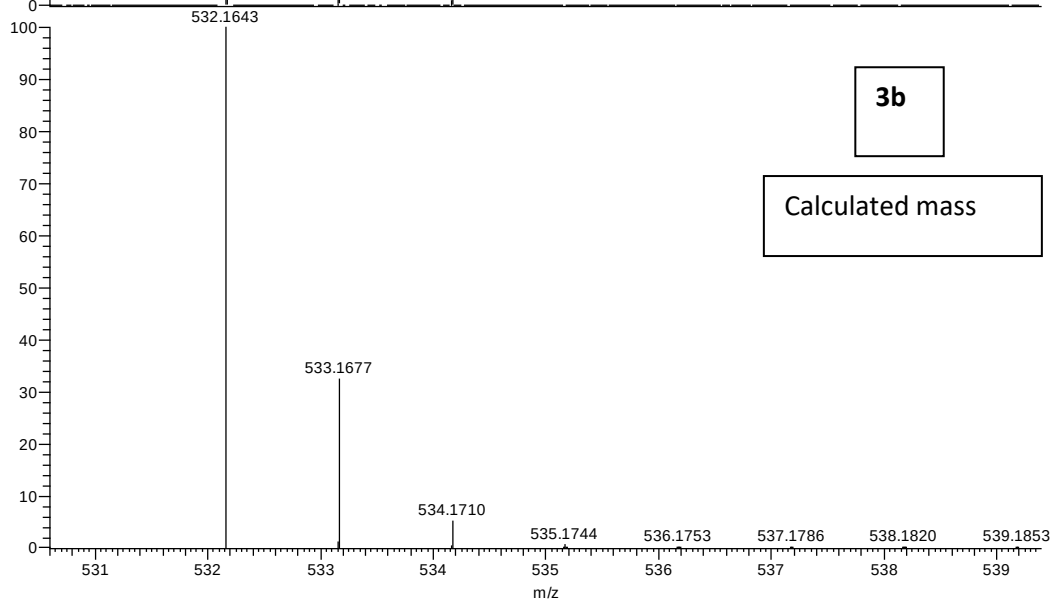


HRMS of Methyl (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophanate (**3b**)



NL:
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RT: 0.47-0.80 AV: 7 T:
FTMS + p NSI Full ms
[100.00-2000.00]

Measured mass

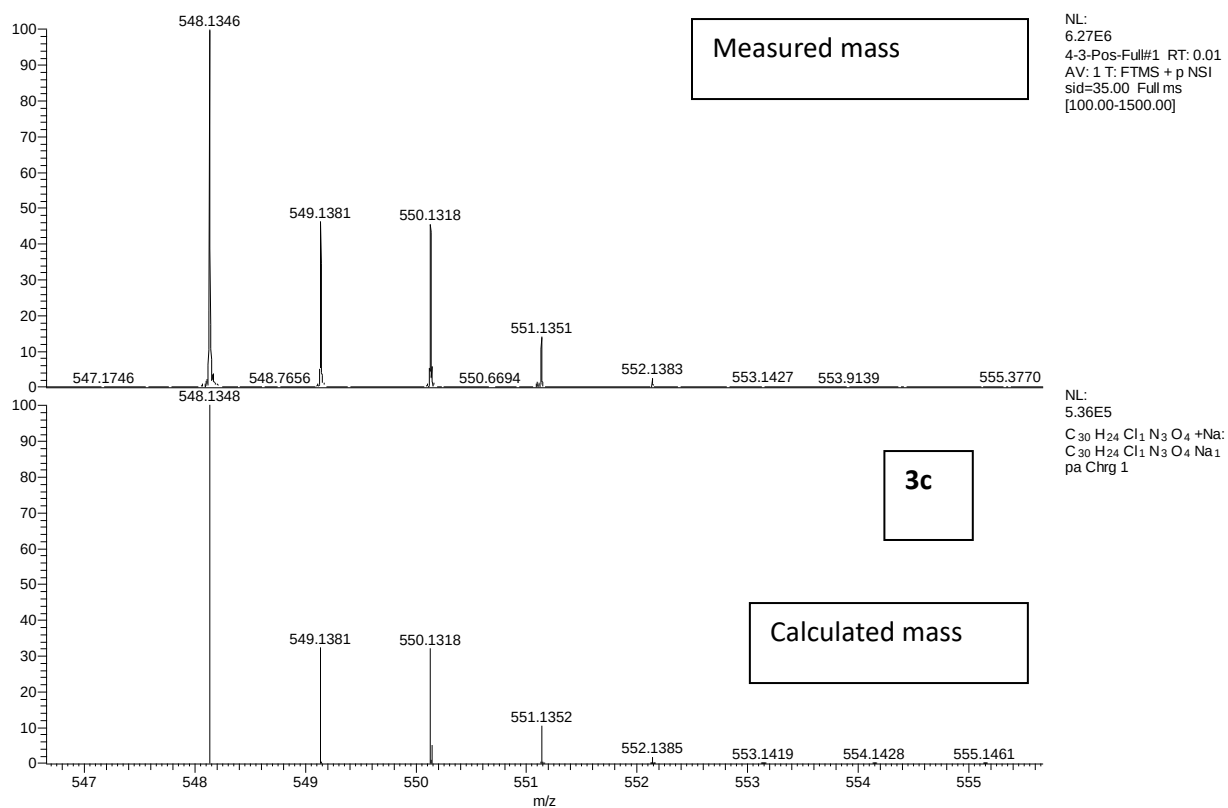


NL:
7.07E5
C₃₀ H₂₄ F₁ N₃ O₄ +Na:
C₃₀ H₂₄ F₁ N₃ O₄ Na₁
pa Chrg 1

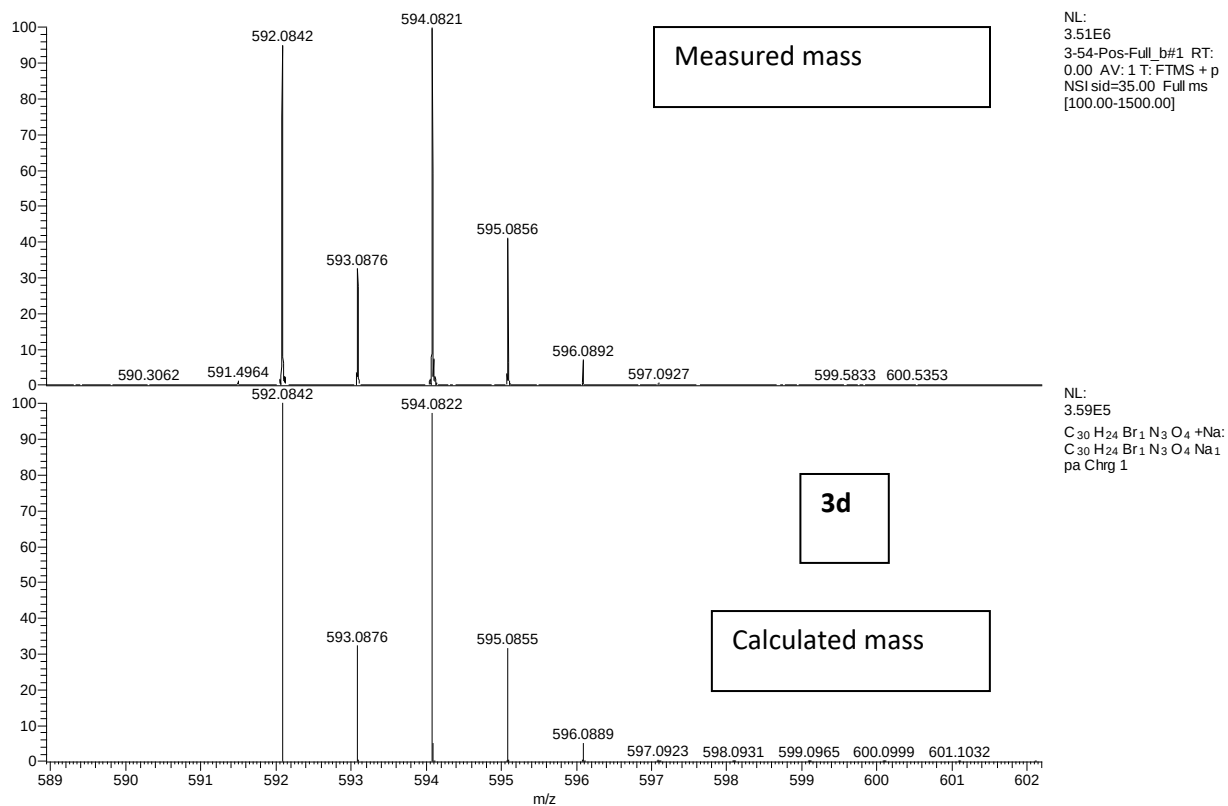
3b

Calculated mass

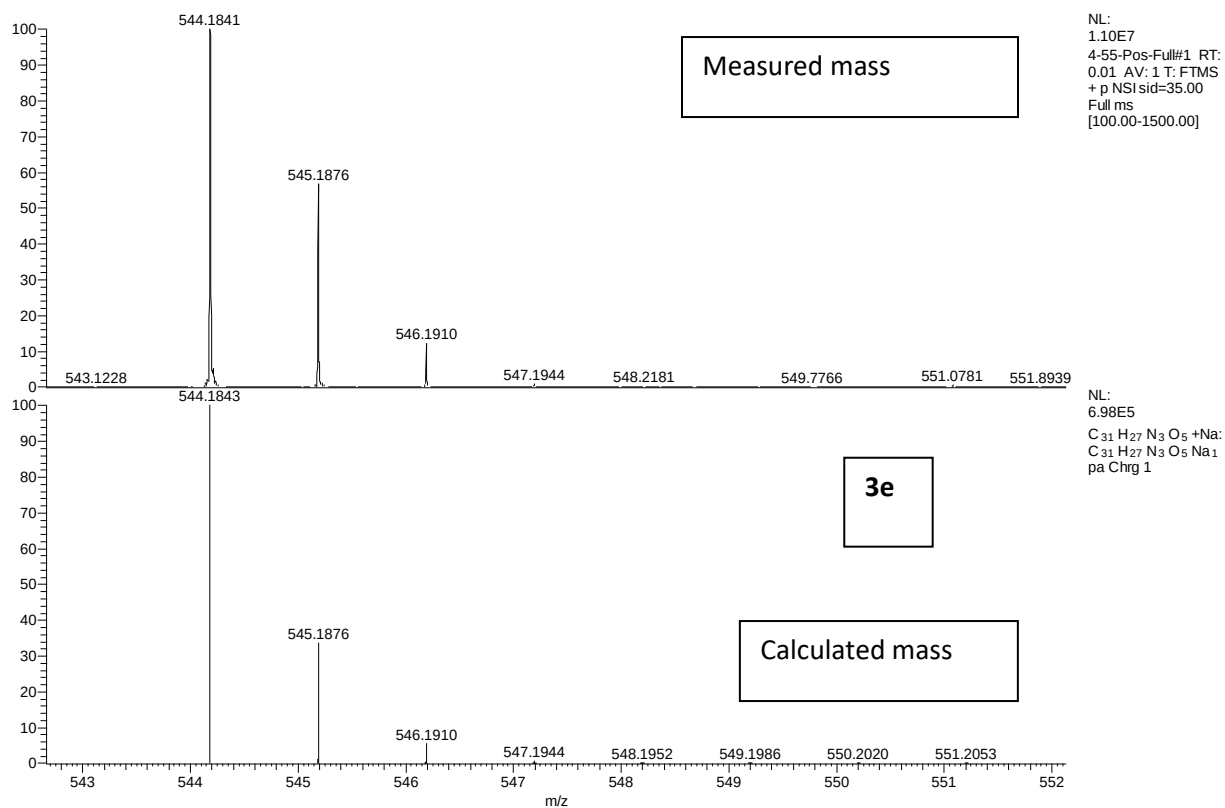
HRMS of Methyl (2-(2-naphthamido)-5-chlorobenzoyl)-L-tryptophanate (**3c**)



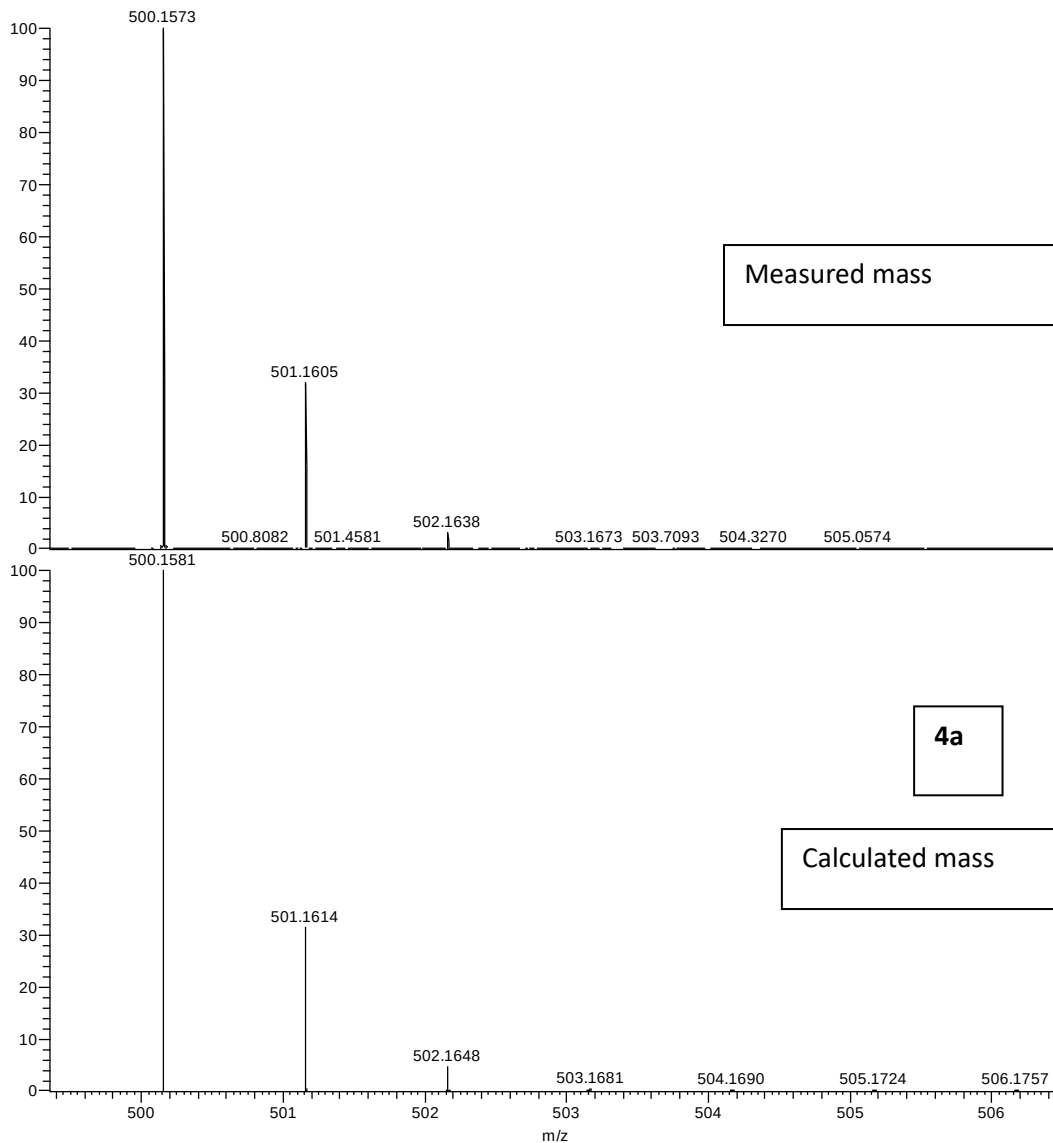
HRMS of Methyl (2-(2-naphthamido)-5-bromobenzoyl)-L-tryptophanate (**3d**)



HRMS of Methyl (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophanate (**3e**)



HRMS of (2-(2-naphthamido)benzoyl)-L-tryptophan (**4a**)

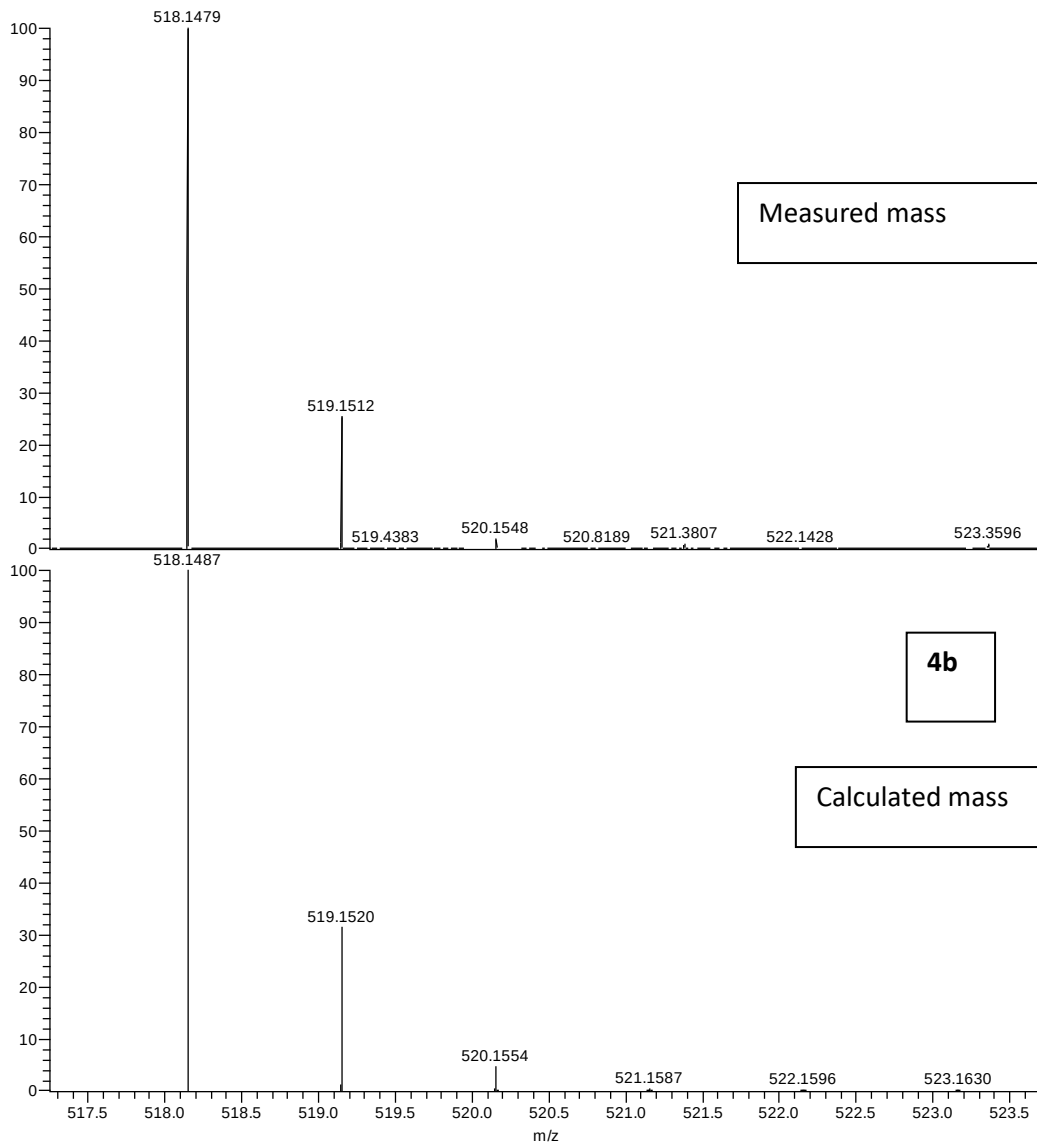


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NSI Full ms
[100.00-2000.00]

NL:
7.15E5
C₂₉H₂₃N₃O₄+Na:
C₂₉H₂₃N₃O₄Na₁
pa Chrg 1

4a

HRMS of (2-(2-naphthamido)-5-fluorobenzoyl)-L-tryptophan (**4b**)

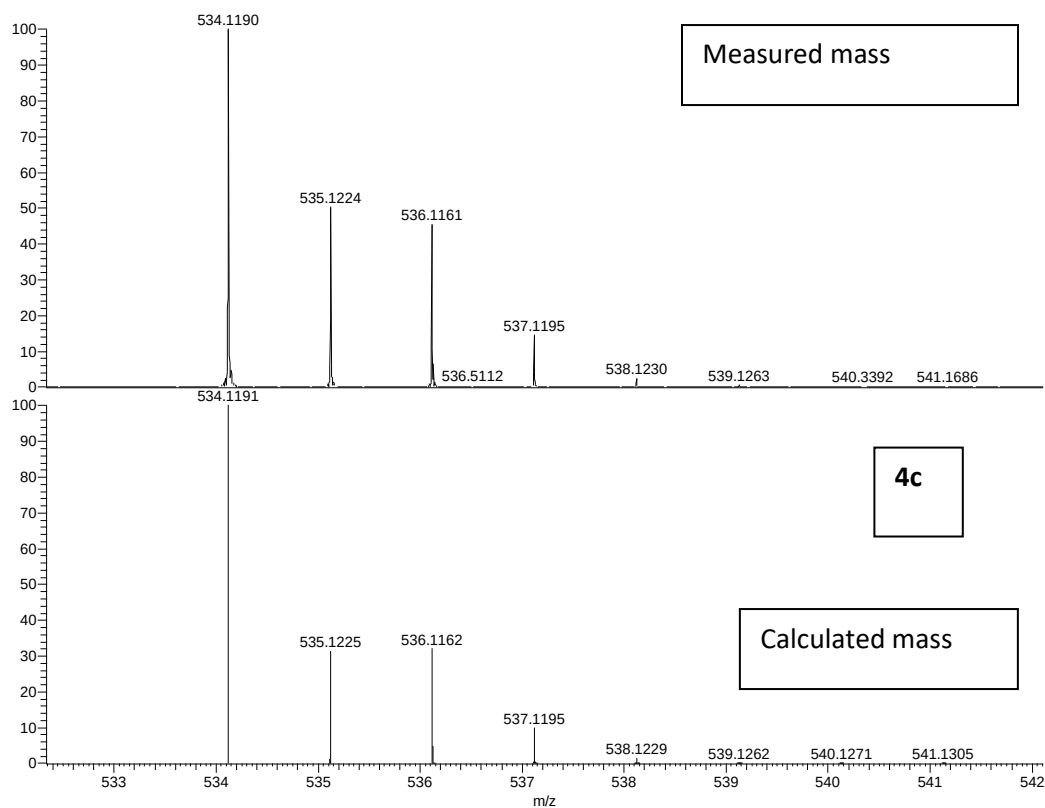


NL:
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3-100_Pos_Full#5-9
RT: 0.23-0.45 AV: 5 T:
FTMS + p NSI Full ms
[100.00-2000.00]

NL:
7.15E5
C₂₉H₂₂F₁N₃O₄+Na:
C₂₉H₂₂F₁N₃O₄Na₁
pa Chrg 1

4b

HRMS of (2-(2-naphthamido)-5-chlorobenzoyl)-*L*-tryptophan (**4c**)



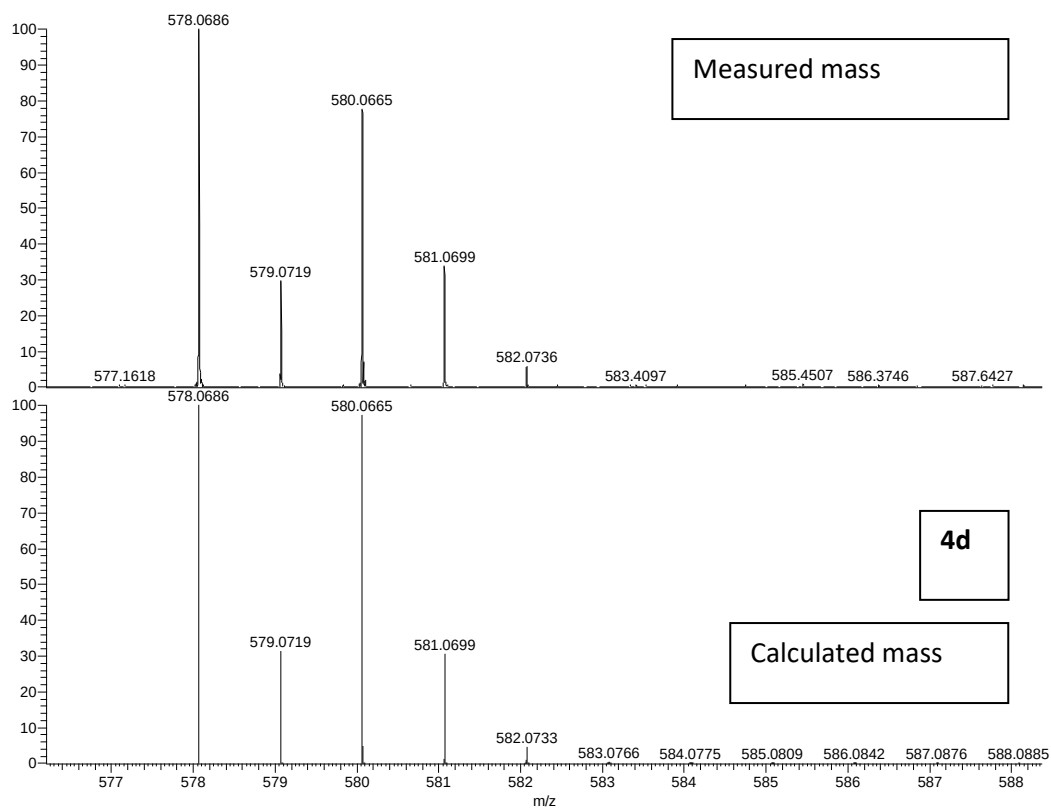
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AV: 1 T: FTMS + p NSI
sid=35.00 Full ms
[100.00-1500.00]

NL:
5.42E5
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C₂₉ H₂₂ Cl₁ N₃ O₄ Na₁
pa Chrg 1

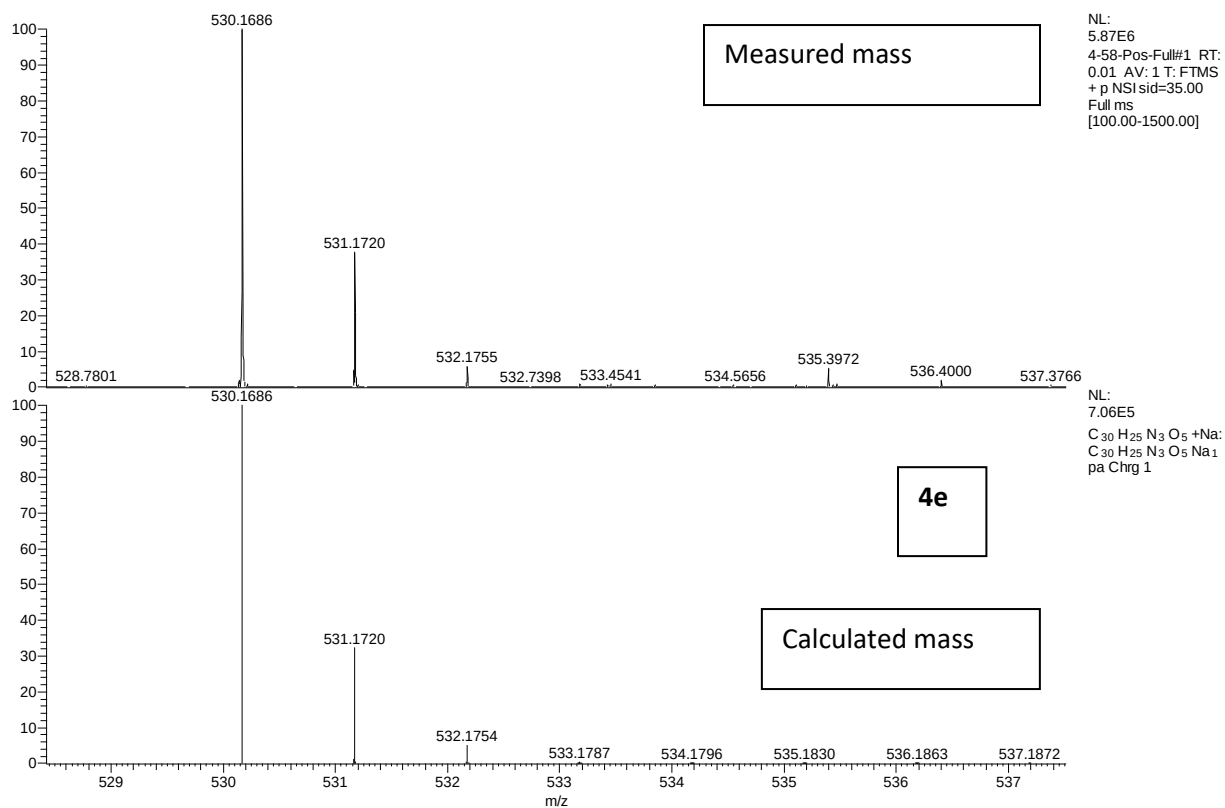
4c

Calculated mass

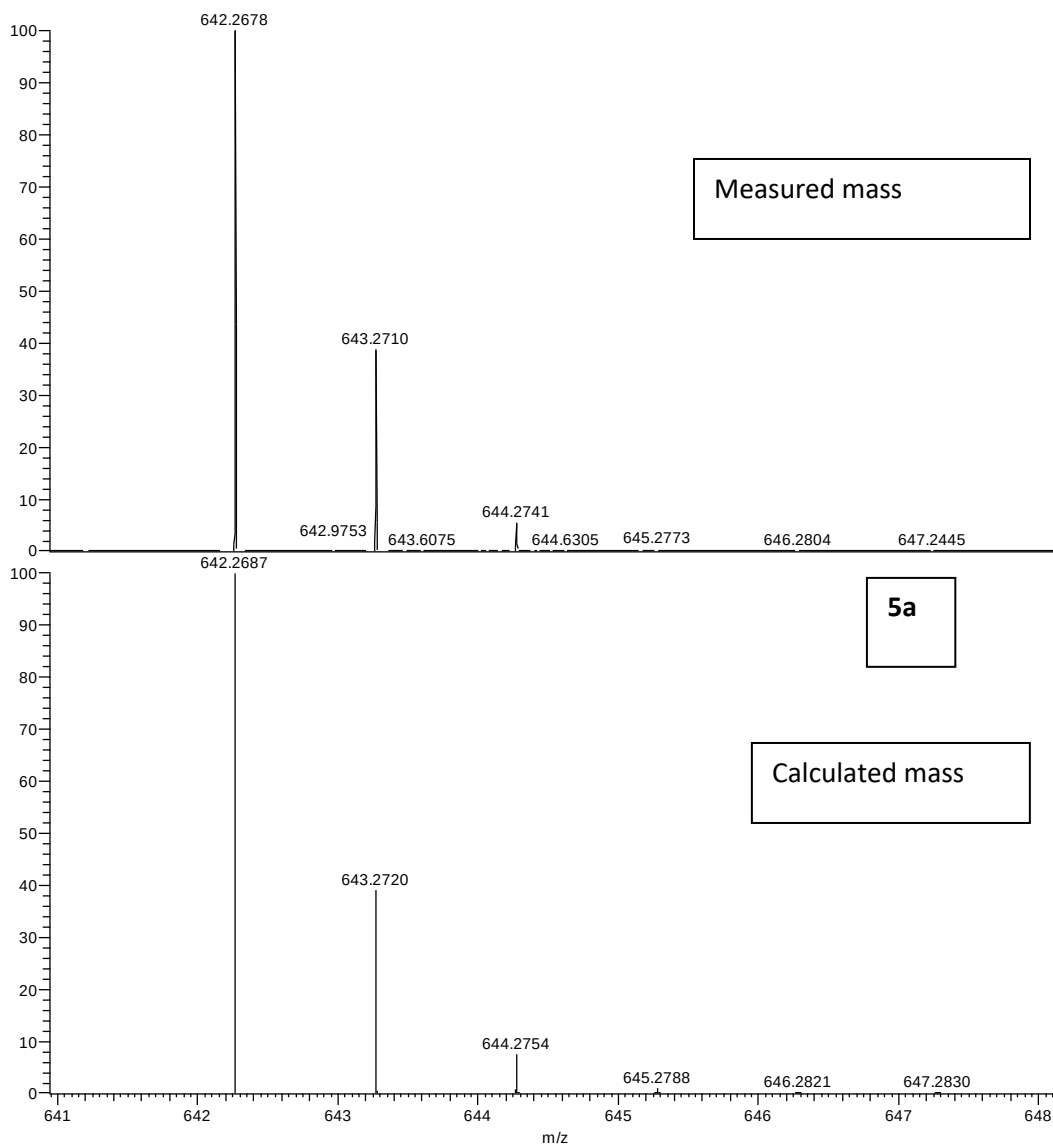
HRMS of (2-(2-naphthamido)-5-bromobenzoyl)-L-tryptophan (**4d**)



HRMS of (2-(2-naphthamido)-5-methoxybenzoyl)-*L*-tryptophan (**4e**)



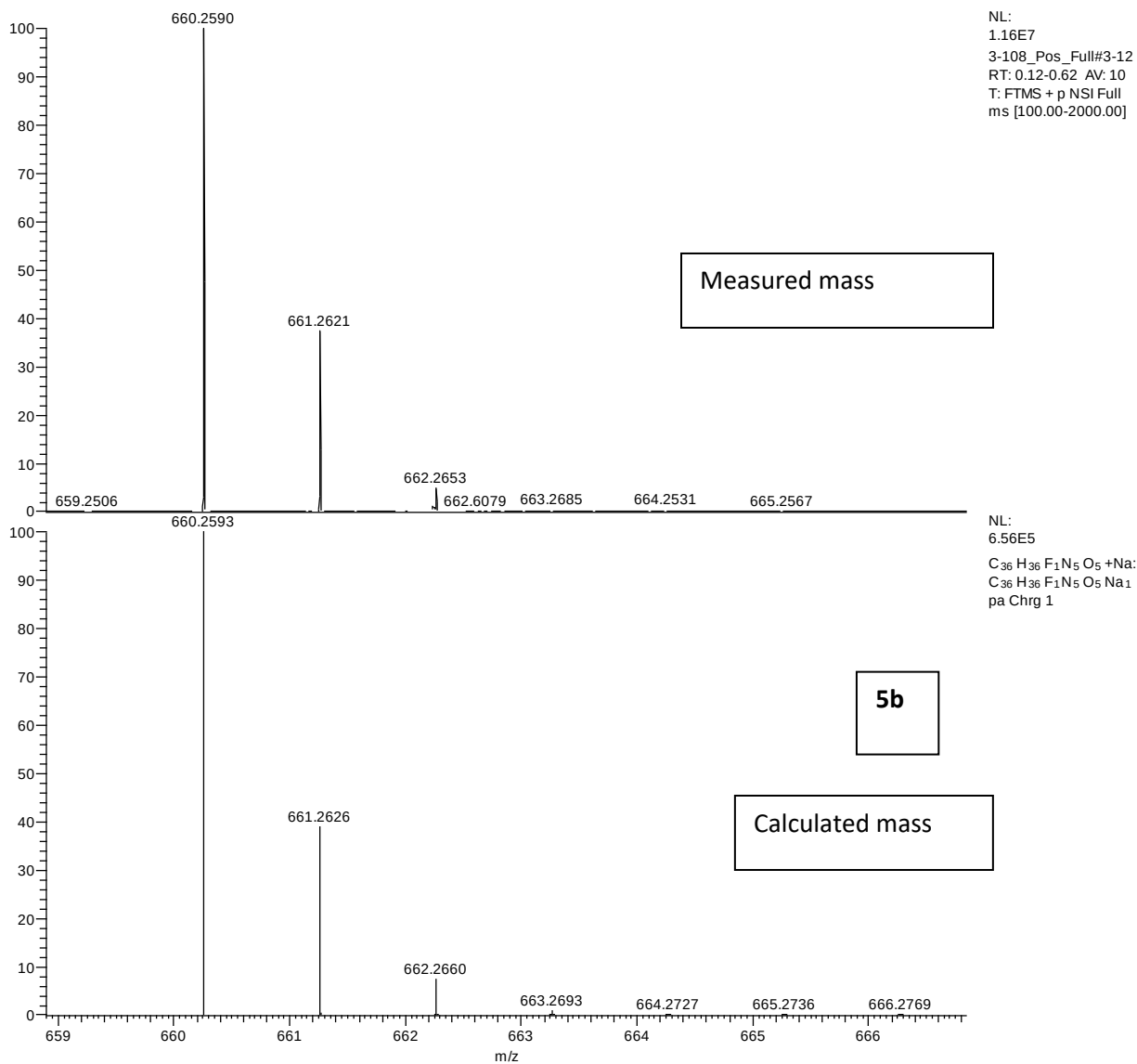
HRMS of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5a**)



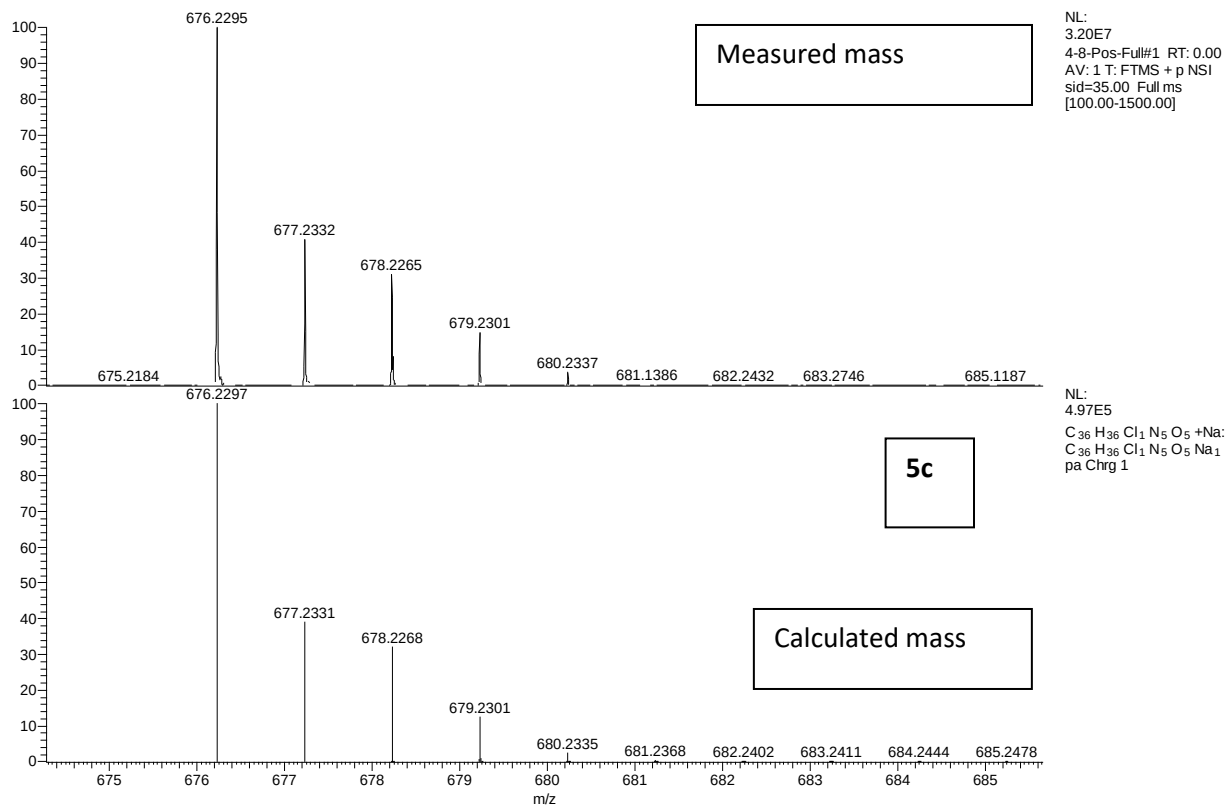
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NSI Full ms
[100.00-2000.00]

NL:
6.56E5
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C₃₆H₃₇N₅O₅Na₁
pa Chrg 1

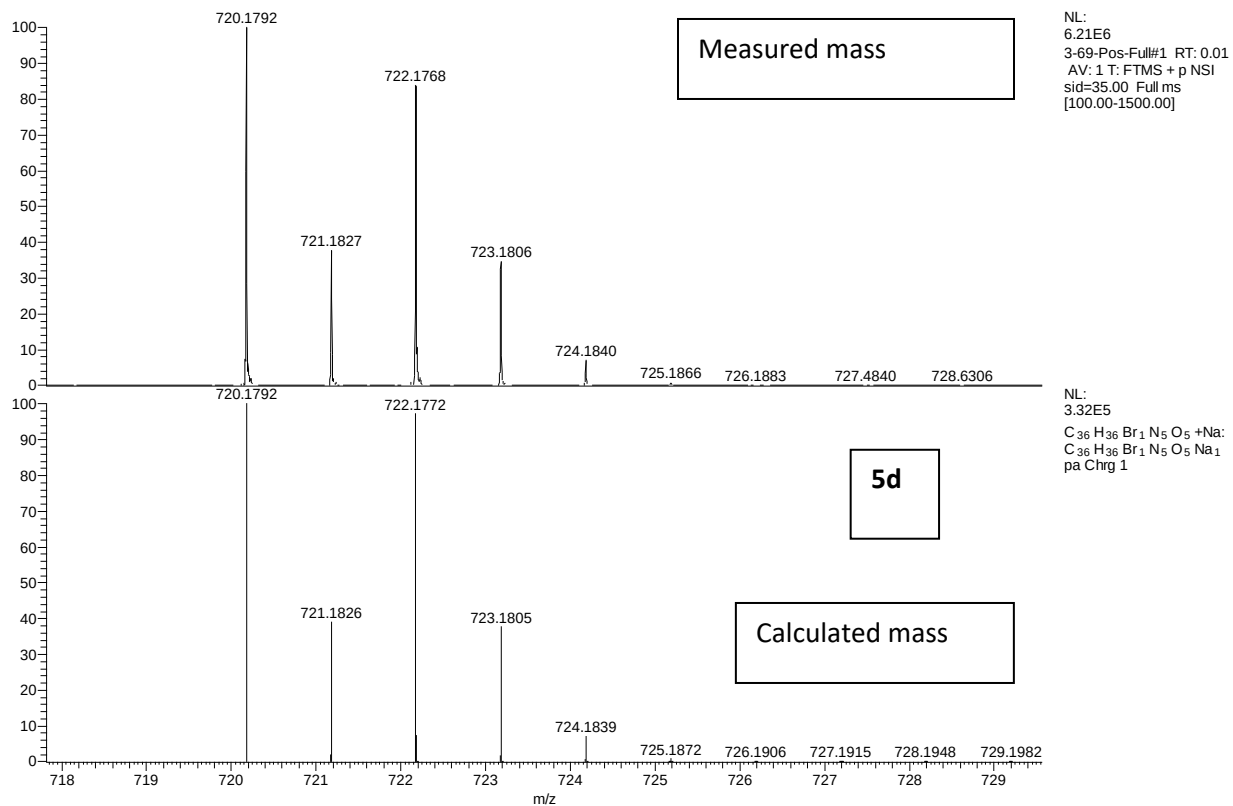
HRMS of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5b**)



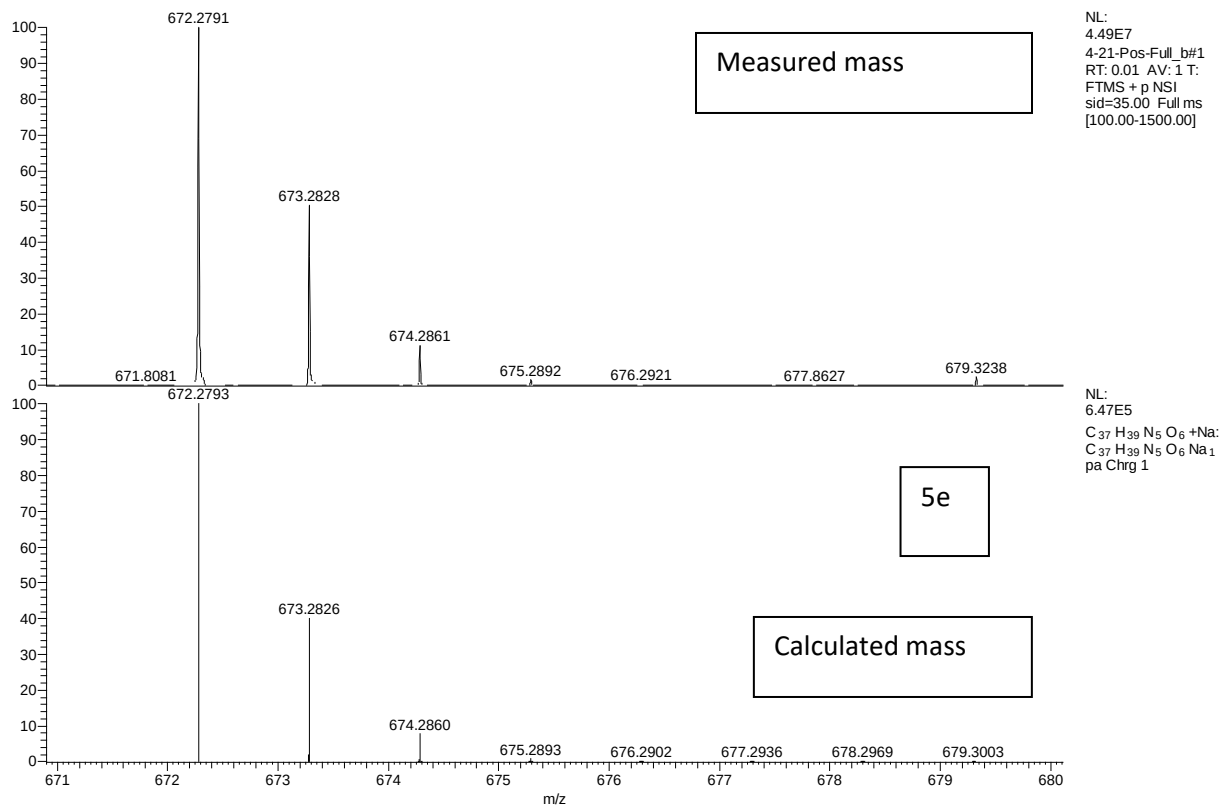
HRMS of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5c**)



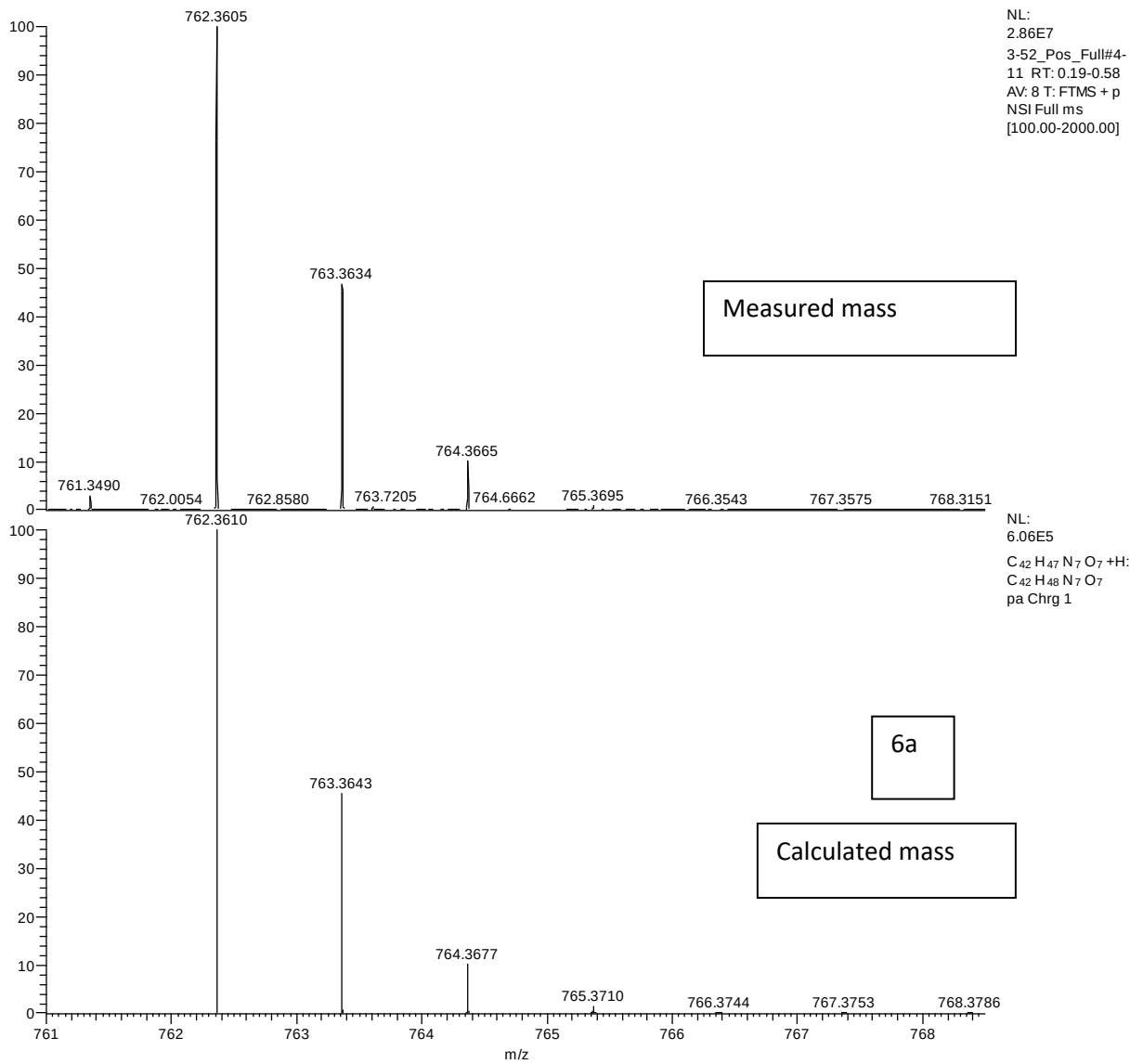
HRMS of *tert*-butyl (S)-(2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5d**)



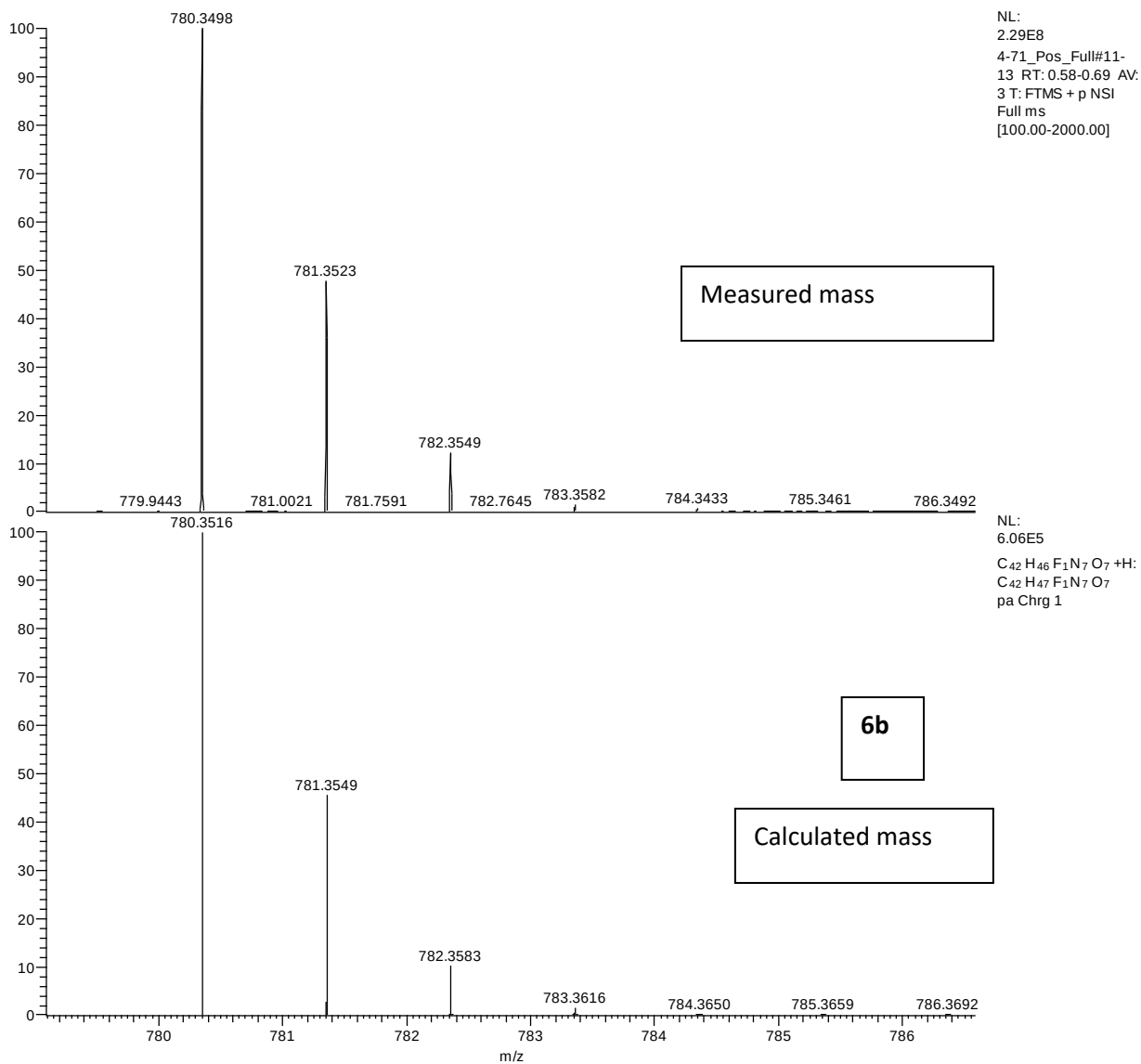
HRMS of *tert*-butyl (*S*)-(2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1*H*-indol-3-yl)propanamido)ethyl)carbamate (**5e**)



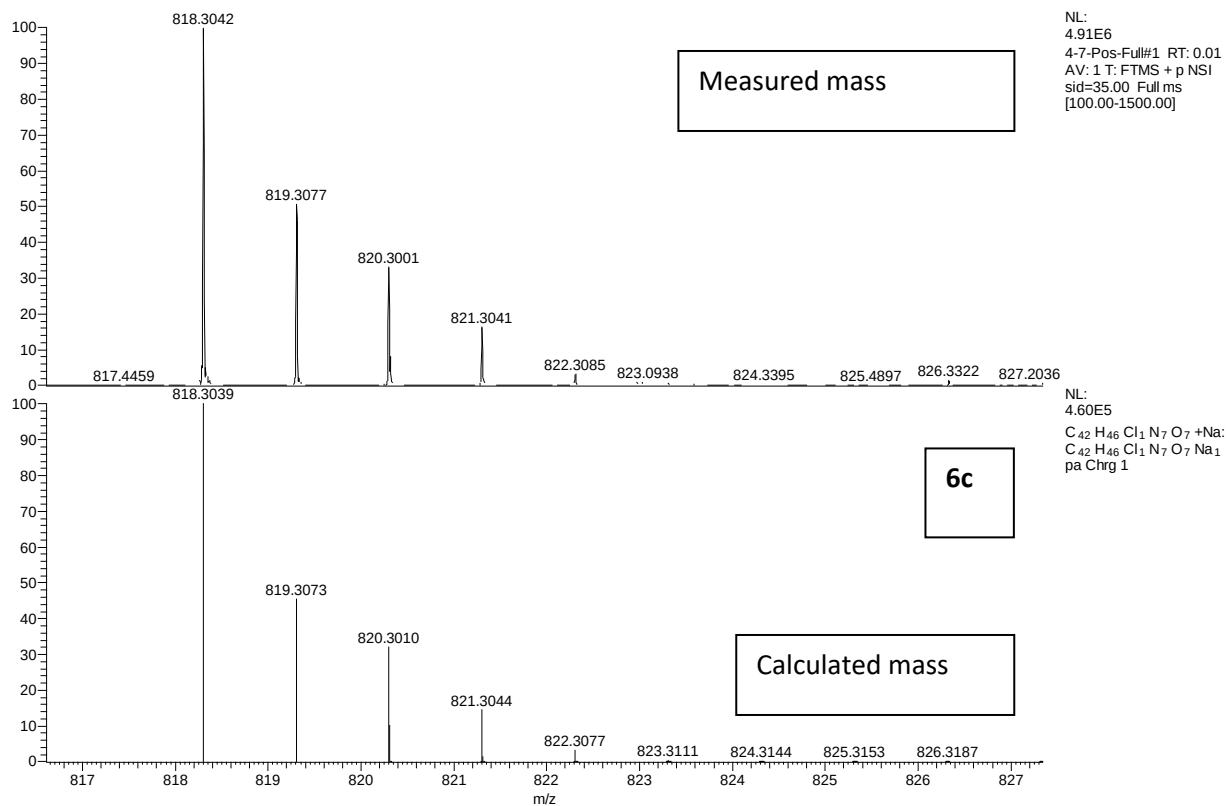
HRMS of (S)-N-(2-((1-((2-dibocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6a**)



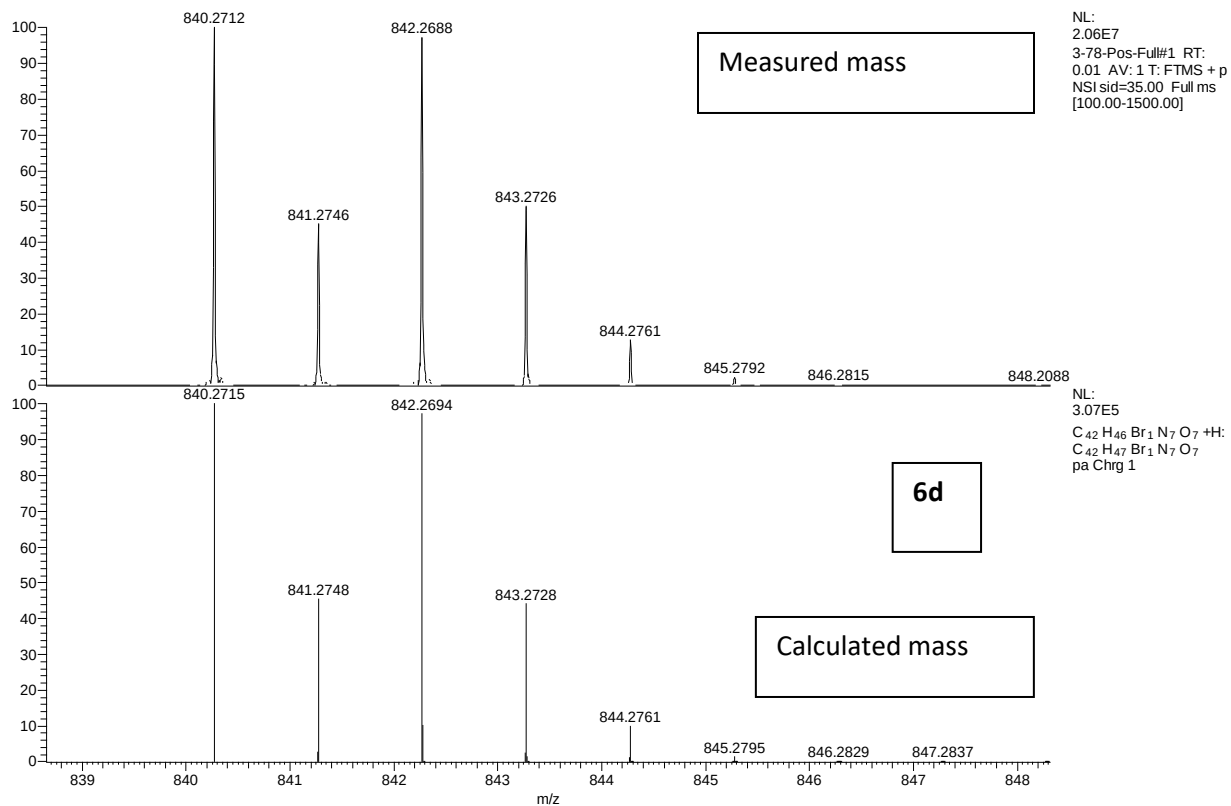
HRMS of (S)-N-(4-fluoro-2-(((1-((2-dibocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6b**)



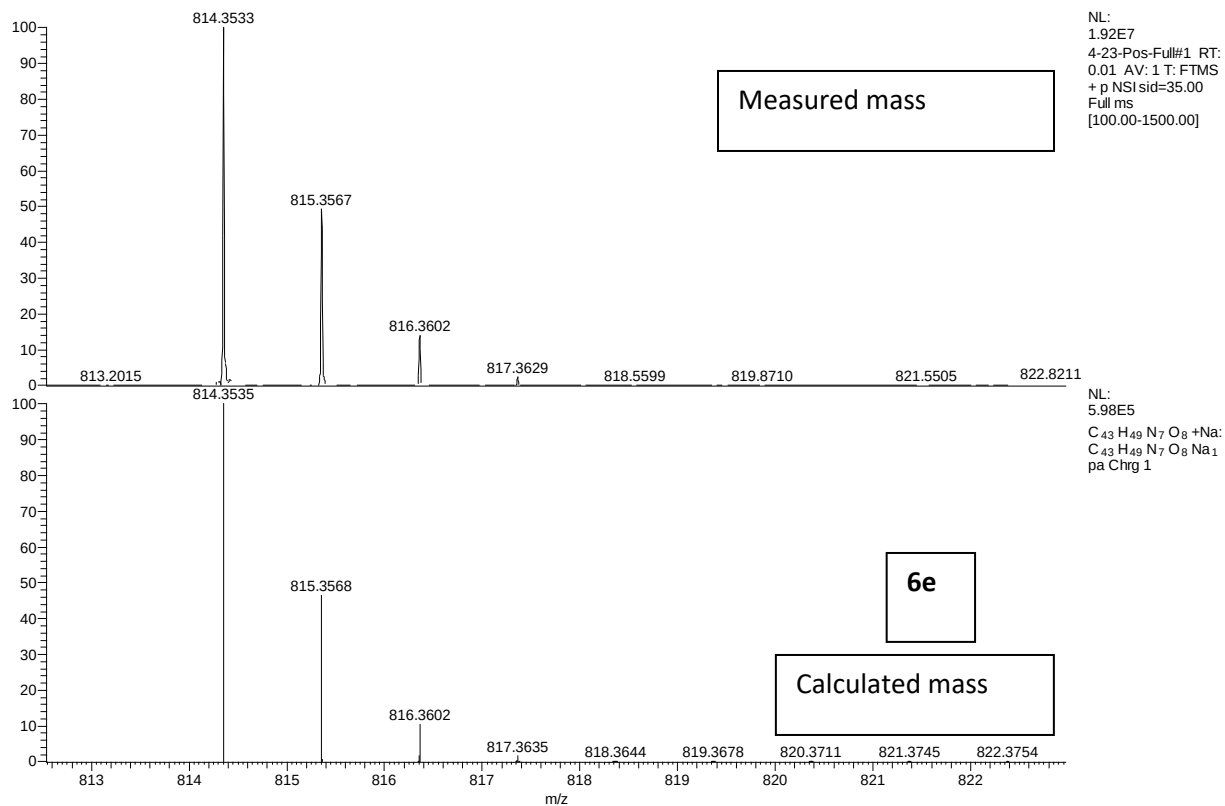
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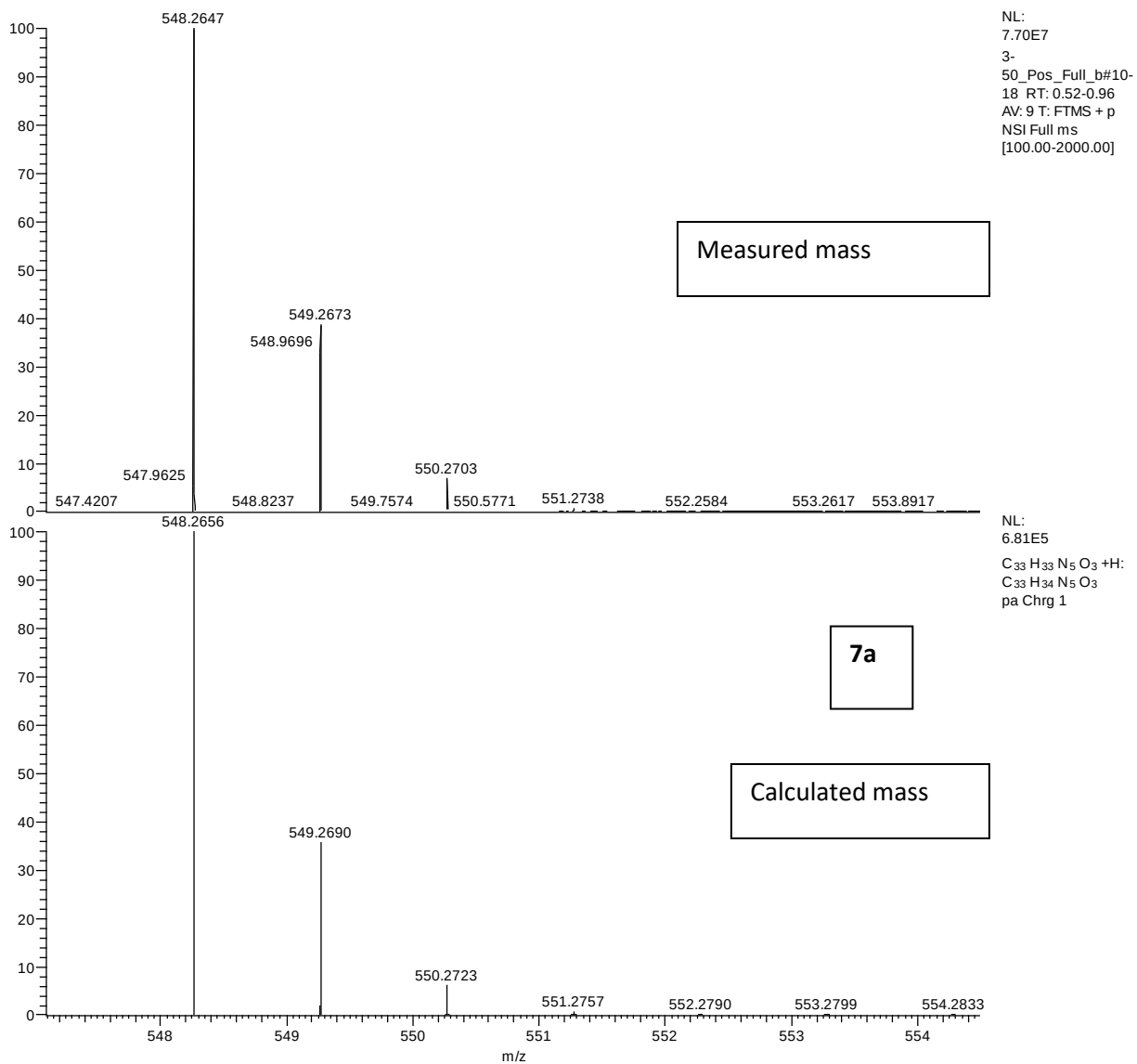
HRMS of (S)-N-(4-bromo-2-((1-((2-dibocguanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**6d**)



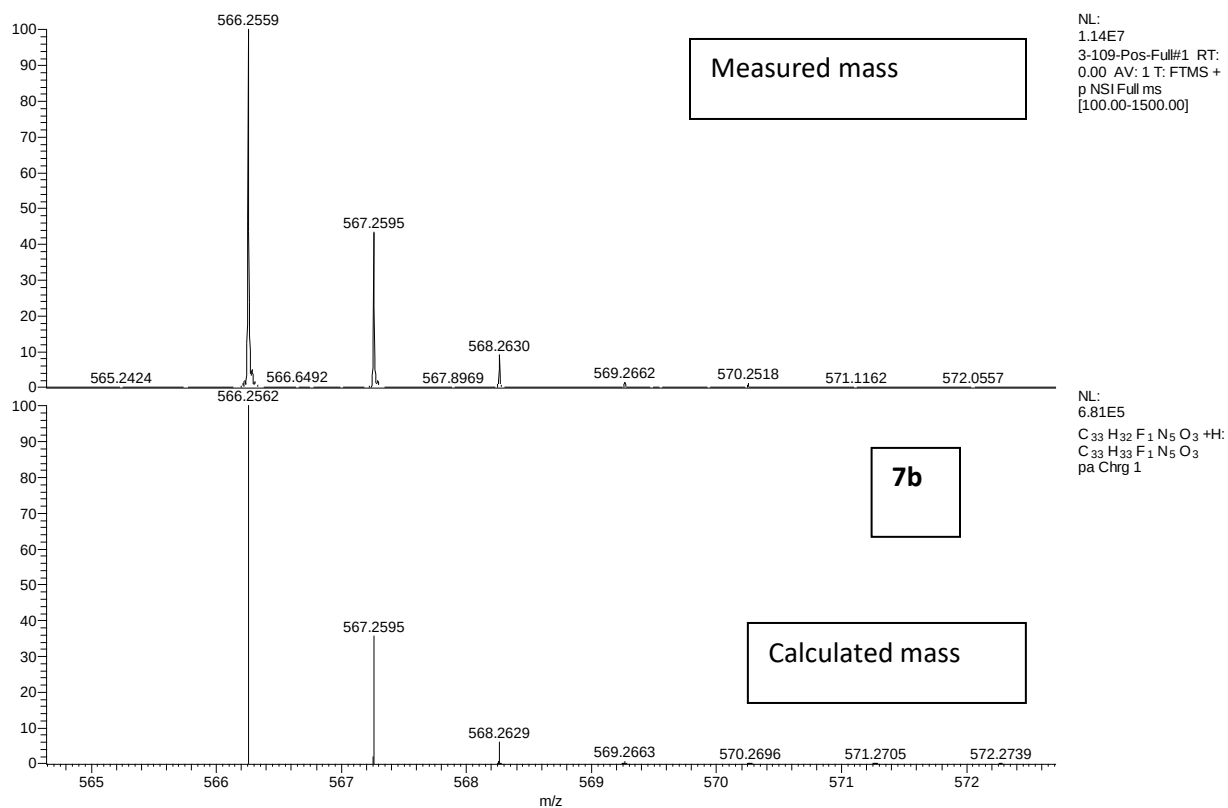
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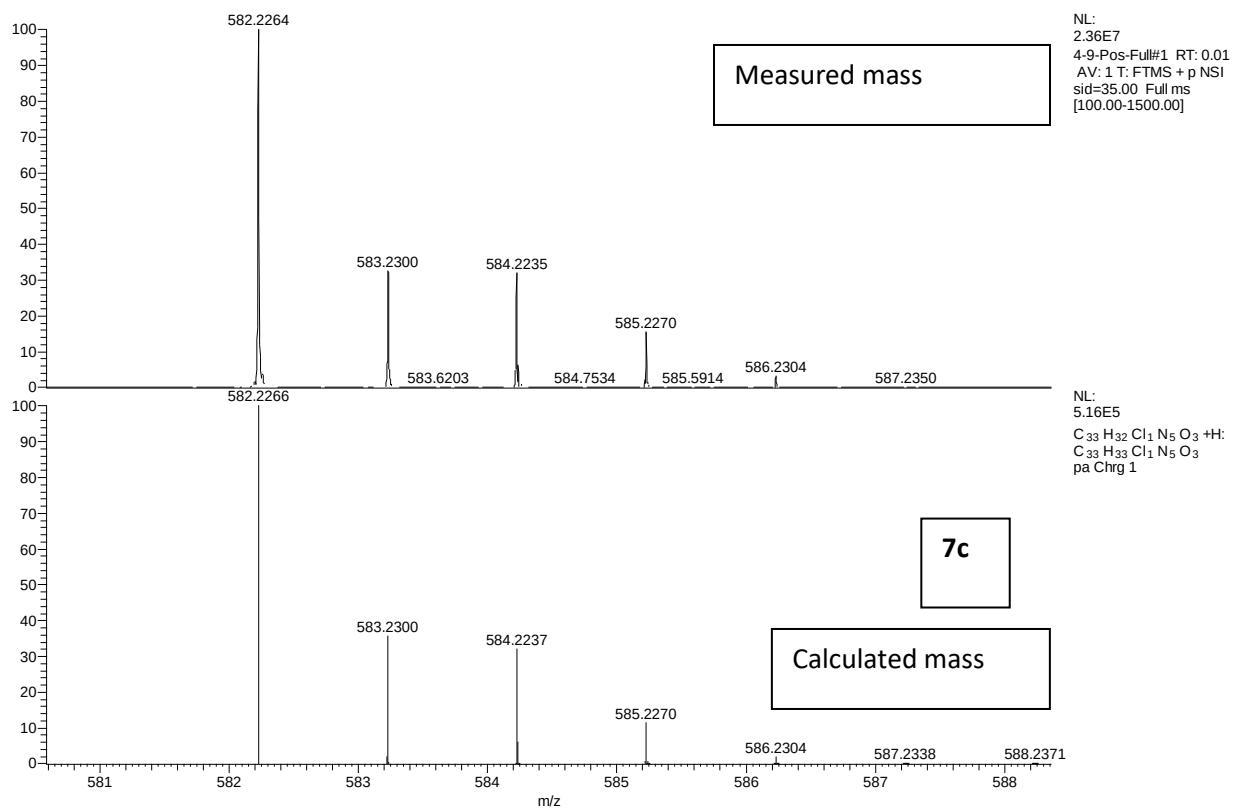
HRMS of (S)-N-(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**7a**)



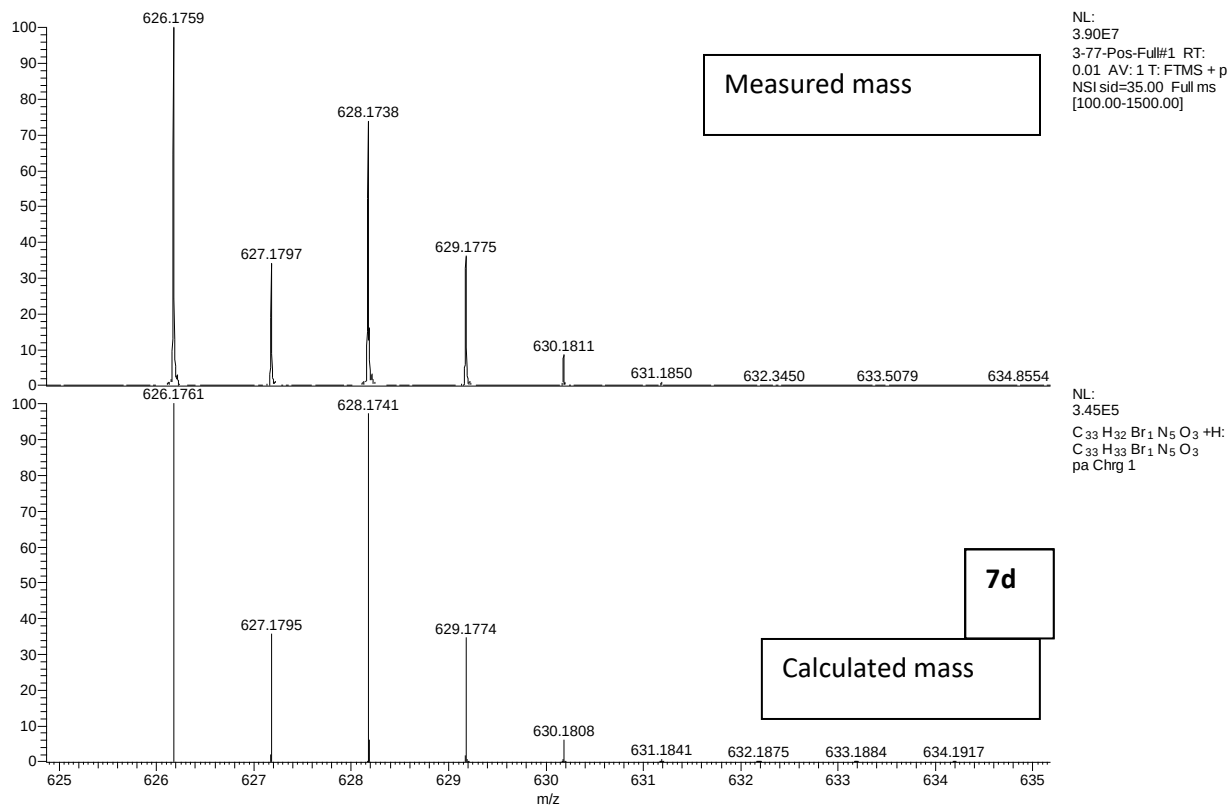
HRMS of (S)-N-(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-fluorophenyl)-2-naphthamide (**7b**)



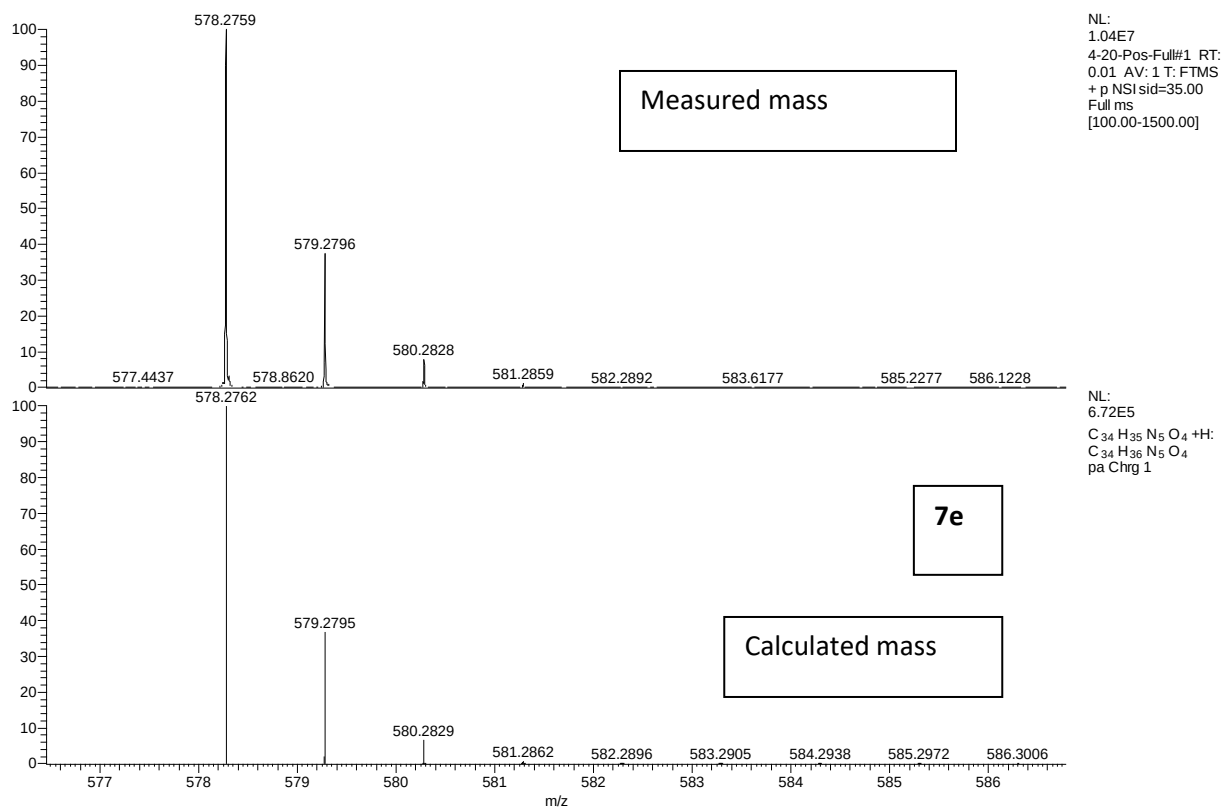
HRMS of (S)-N-(4-chloro-2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**7c**)



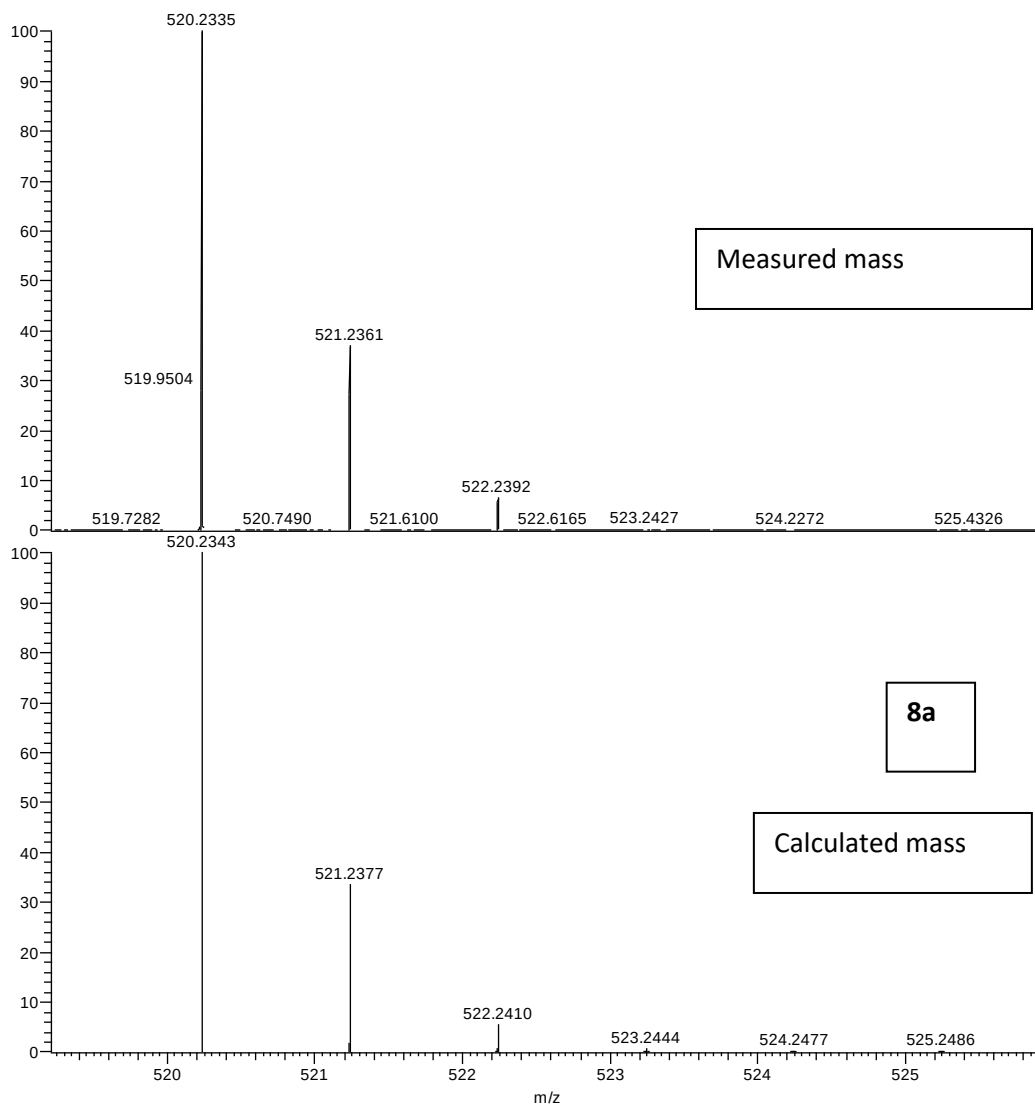
HRMS of (S)-N-(4-bromo-2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**7d**)



HRMS of (S)-N-(2-((1-((2-(dimethylamino)ethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (**7e**)



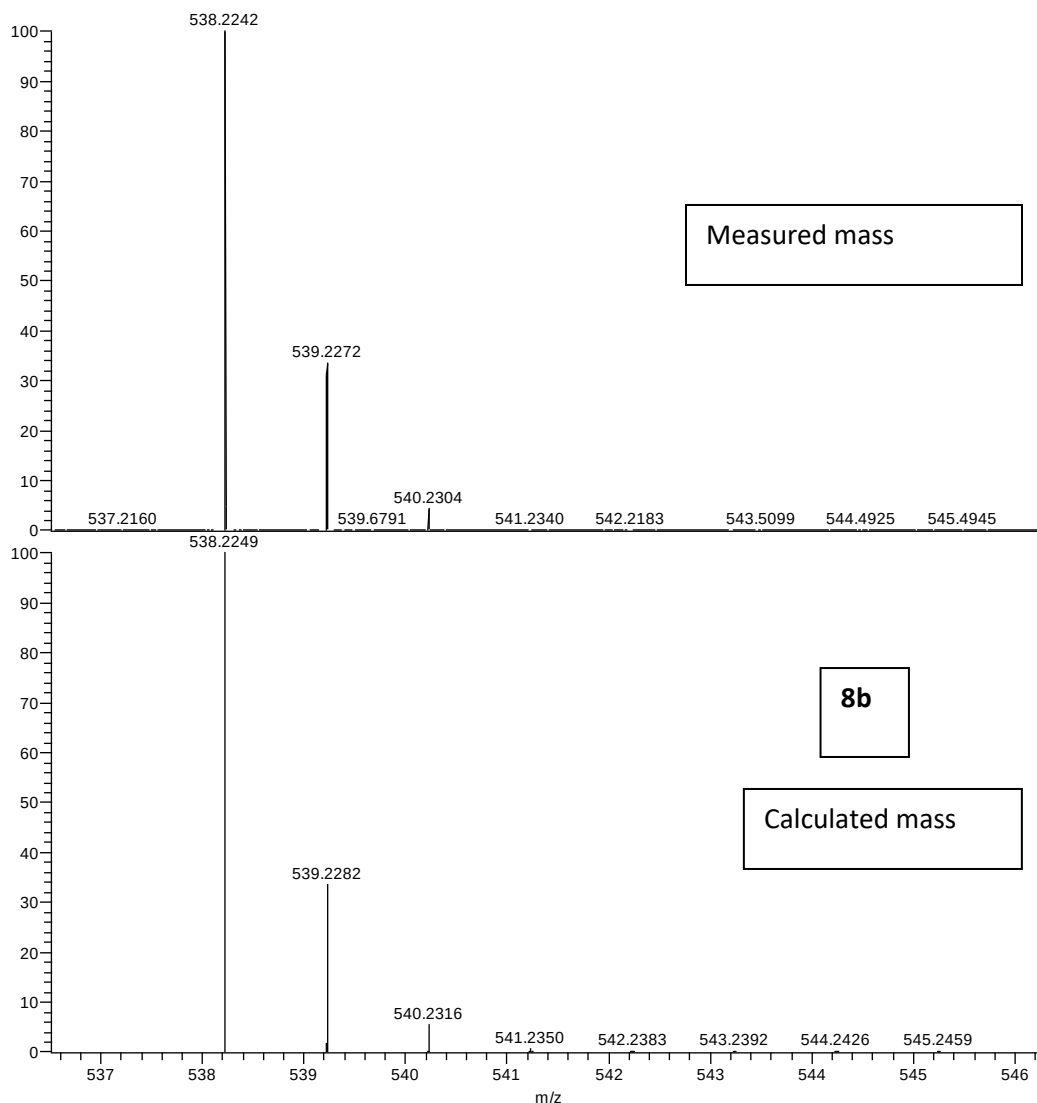
HRMS of (S)-N-(2-((1-((2-aminoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**8a**)



NL:
1.16E8
Sample_4-
46_Pos_Full#12-14
RT: 0.63-0.74 AV: 3 T:
FTMS + p NSI Full ms
[100.00-2000.00]

NL:
6.96E5
C₃₁H₂₉N₅O₃ + H:
C₃₁H₃₀N₅O₃
pa Chrg 1

HRMS of (S)-N-(2-((1-((2-aminoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-fluorophenyl)-2-naphthamide (**8b**)

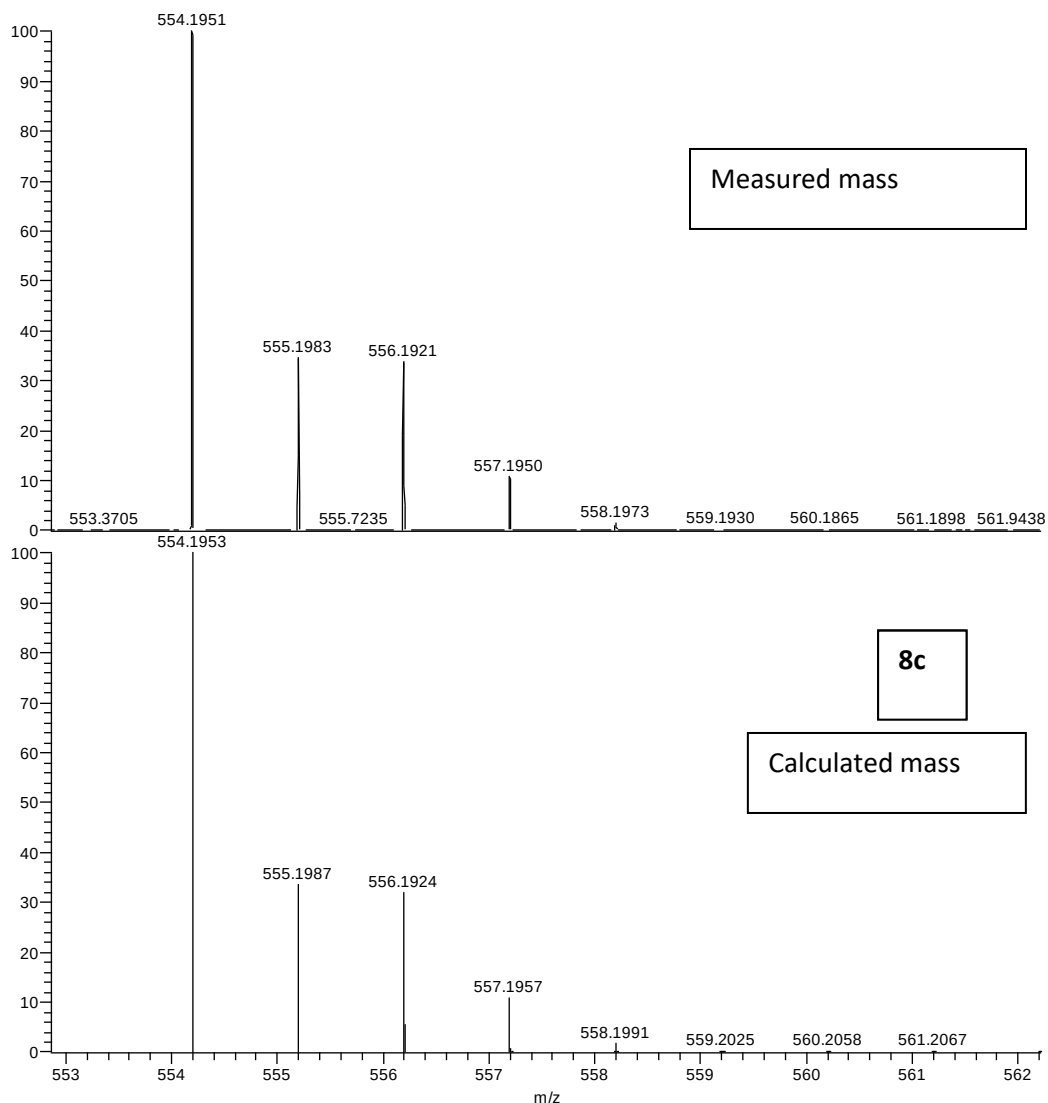


NL:
2.76E7
Sample_3-
117_Pos_Full#4-7
RT: 0.19-0.36 AV: 4 T:
FTMS + p NSI Full ms
[100.00-2000.00]

NL:
6.96E5
C₃₁H₂₈F₁N₅O₃ + H:
C₃₁H₂₉F₁N₅O₃
pa Chrg 1

8b

HRMS of (S)-N-(2-((1-((2-aminoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-chlorophenyl)-2-naphthamide (**8c**)



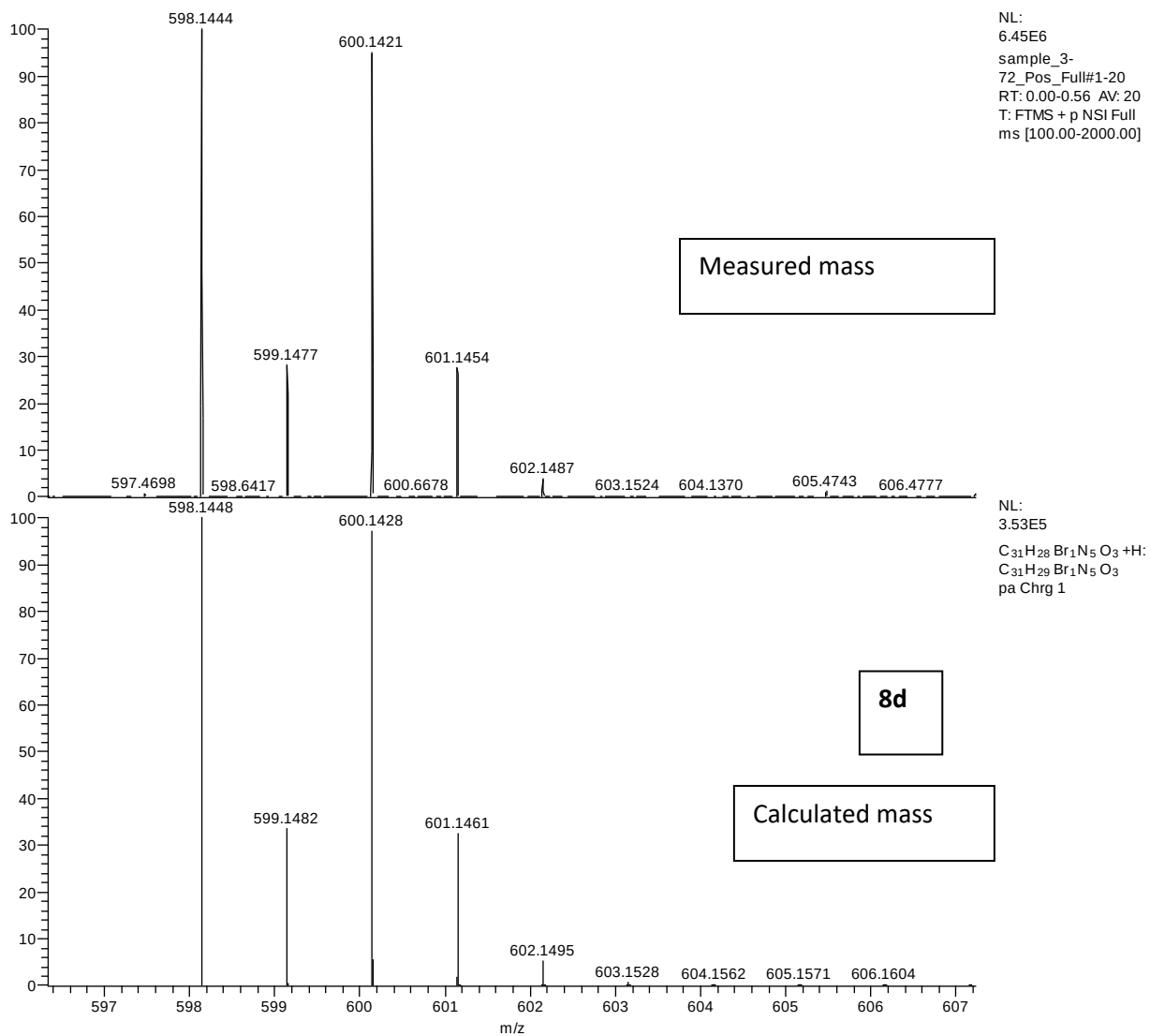
NL:
3.10E7
sample_4-
13_Pos_Full#11-20
RT: 0.30-0.57 AV: 10
T: FTMS + p NSI Full
ms [100.00-2000.00]

NL:
5.27E5
C₃₁H₂₈ClN₅O₃ +H:
C₃₁H₂₉ClN₅O₃
pa Chrg 1

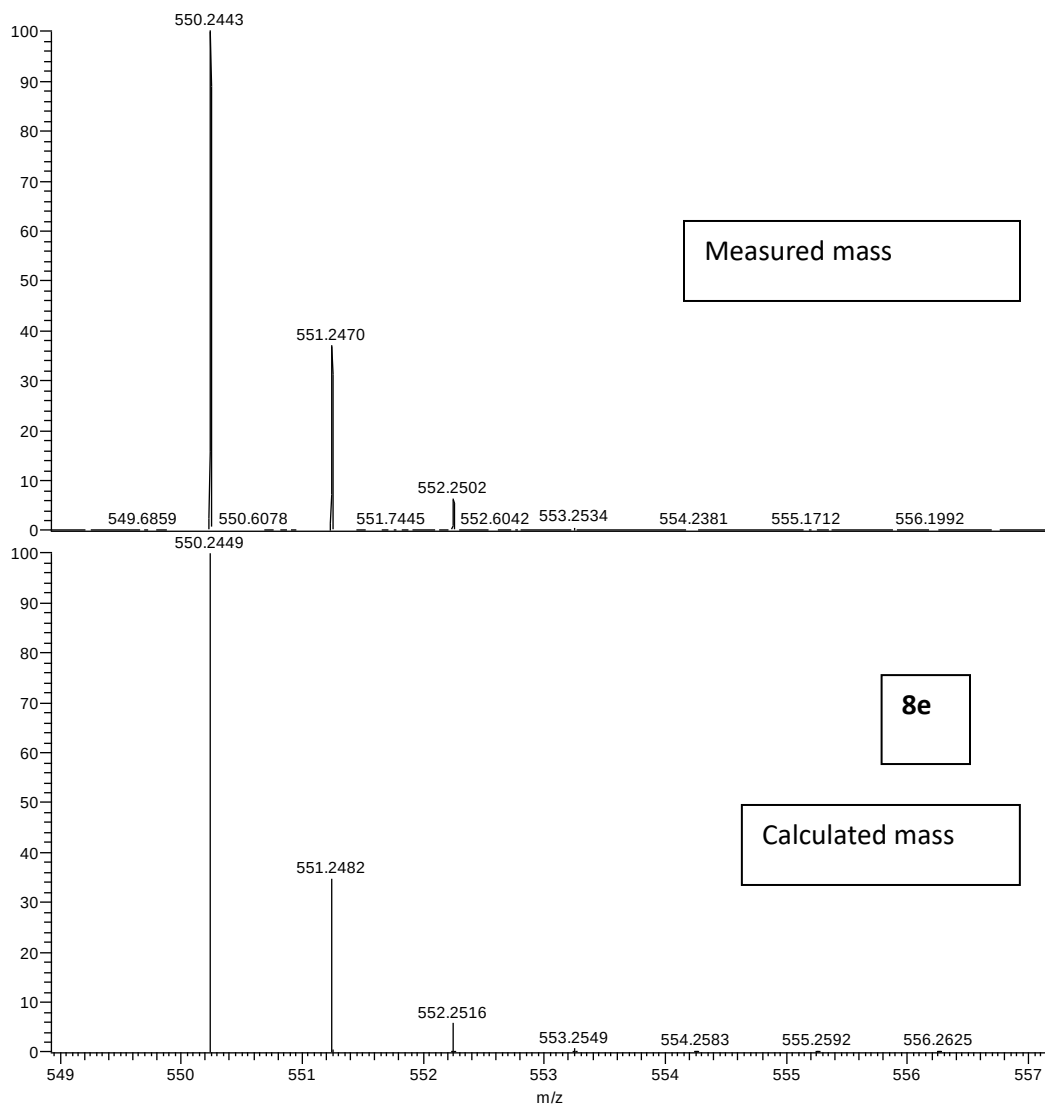
8c

Calculated mass

HRMS of (S)-N-(2-((1-((2-aminoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-bromophenyl)-2-naphthamide (**8d**)



HRMS of (S)-N-(2-((1-((2-aminoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (**8e**)

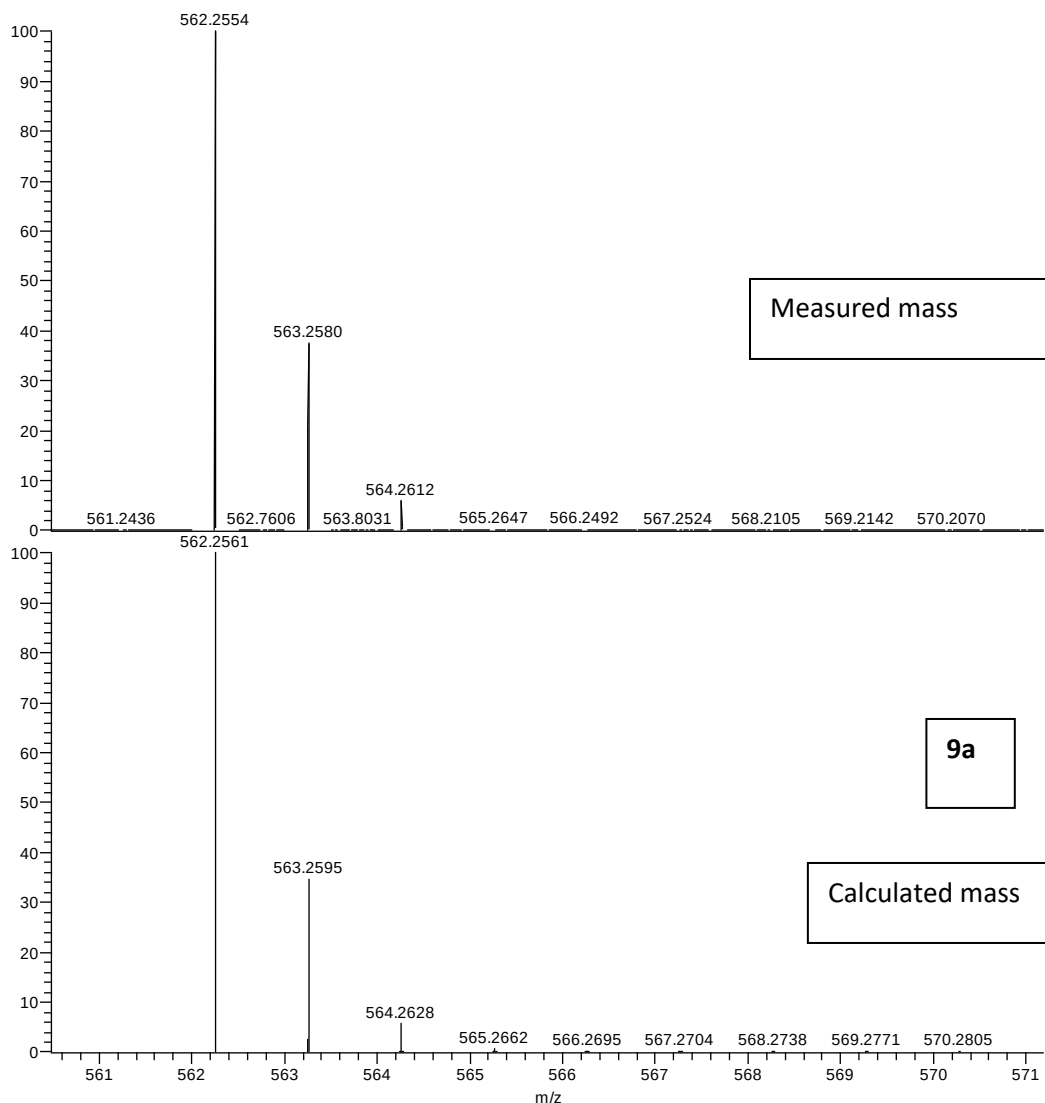


NL:
1.19E8
sample_4-
64_Pos_Full#5-8
RT: 0.13-0.21 AV: 4
T: FTMS + p NSI Full
ms [100.00-2000.00]

NL:
6.87E5
C₃₂H₃₁N₅O₄ +H:
C₃₂H₃₂N₅O₄
pa Chrg 1

8e

HRMS of (S)-N-(2-((1-((2-guanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**9a**)

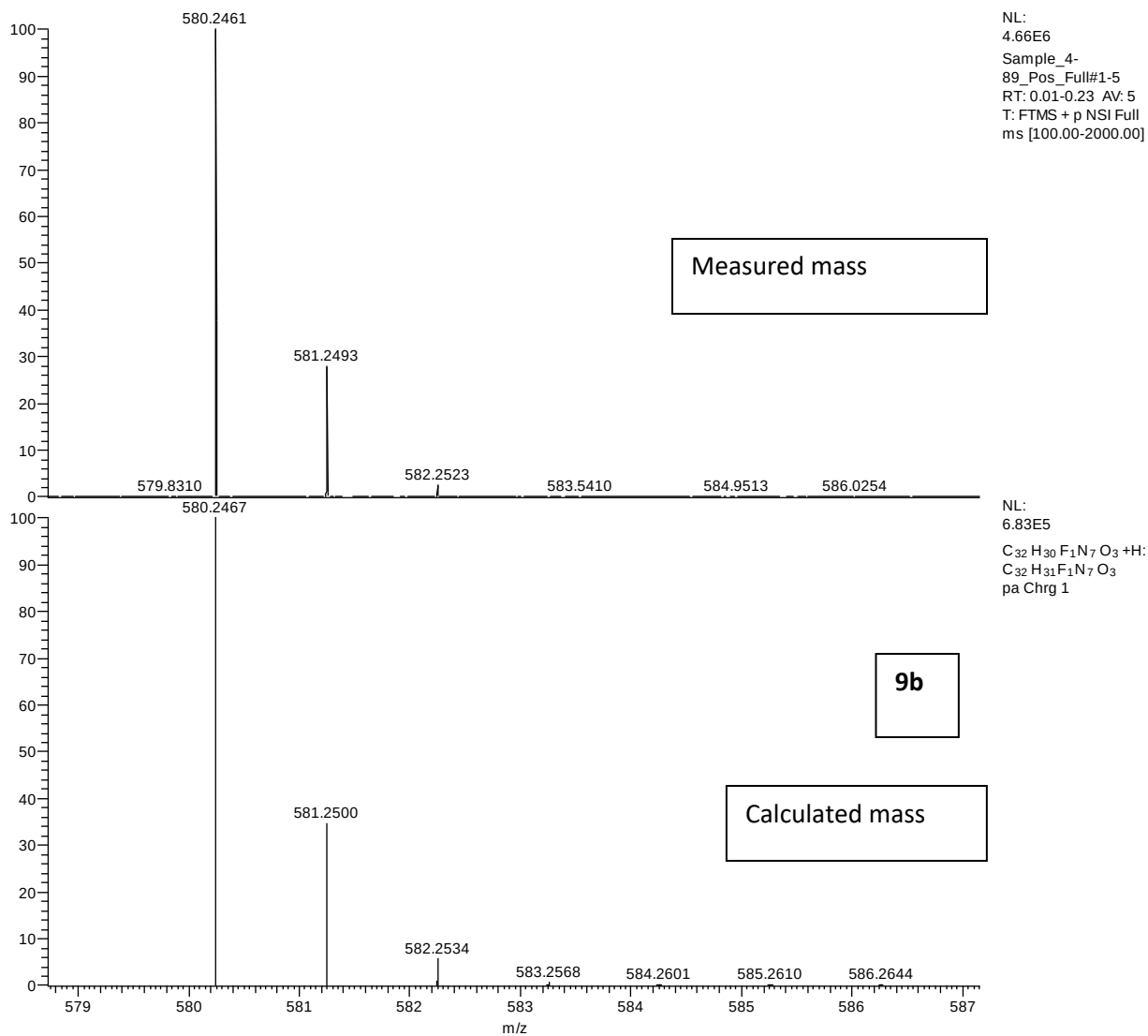


NL:
7.40E7
Sample_4-
56_Pos_Full#4-10
RT: 0.19-0.52 AV: 7 T:
FTMS + p NSI Full ms
[100.00-2000.00]

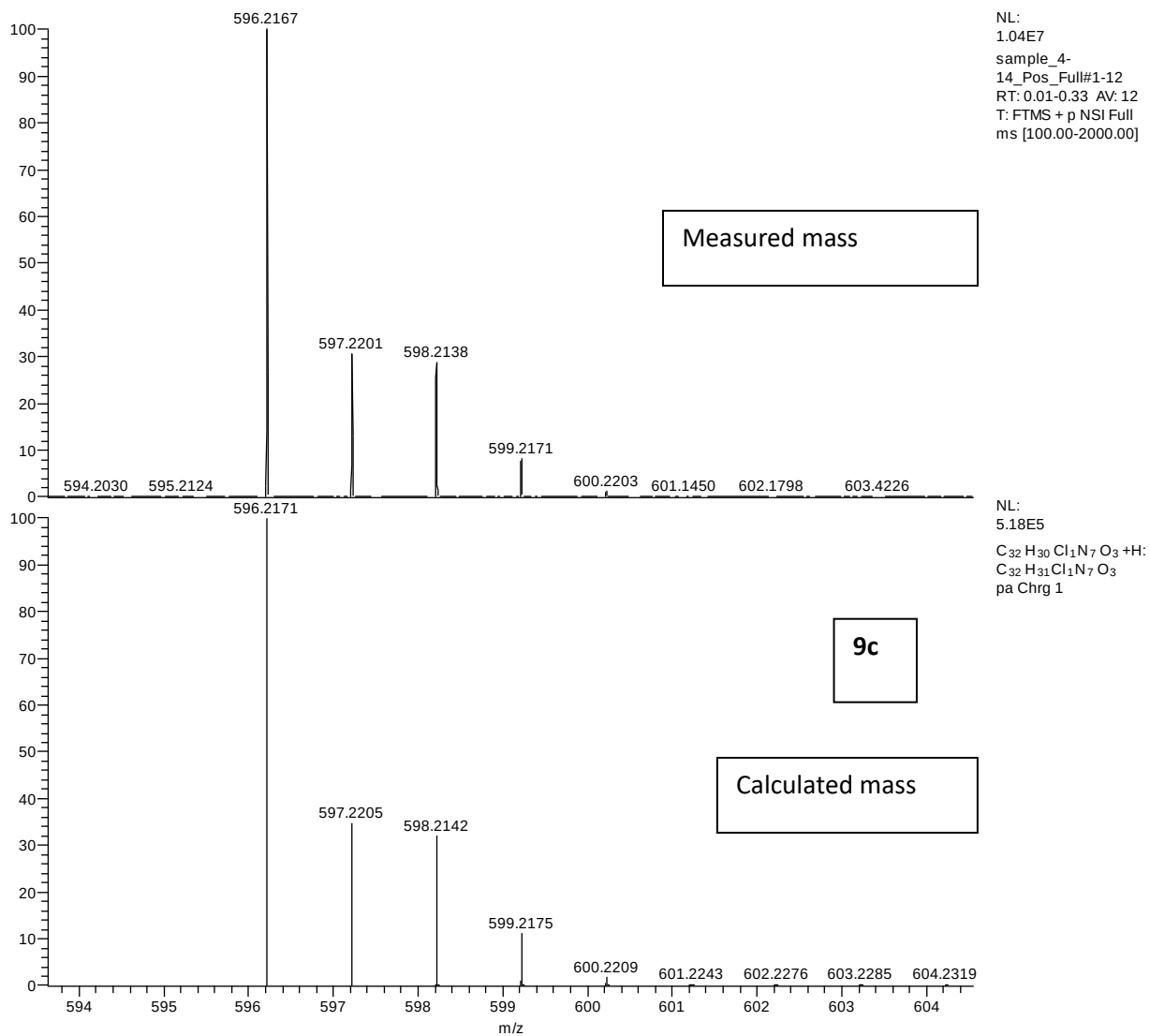
NL:
6.83E5
C₃₂H₃₁N₇O₃ + H:
C₃₂H₃₂N₇O₃
pa Chrg 1

9a

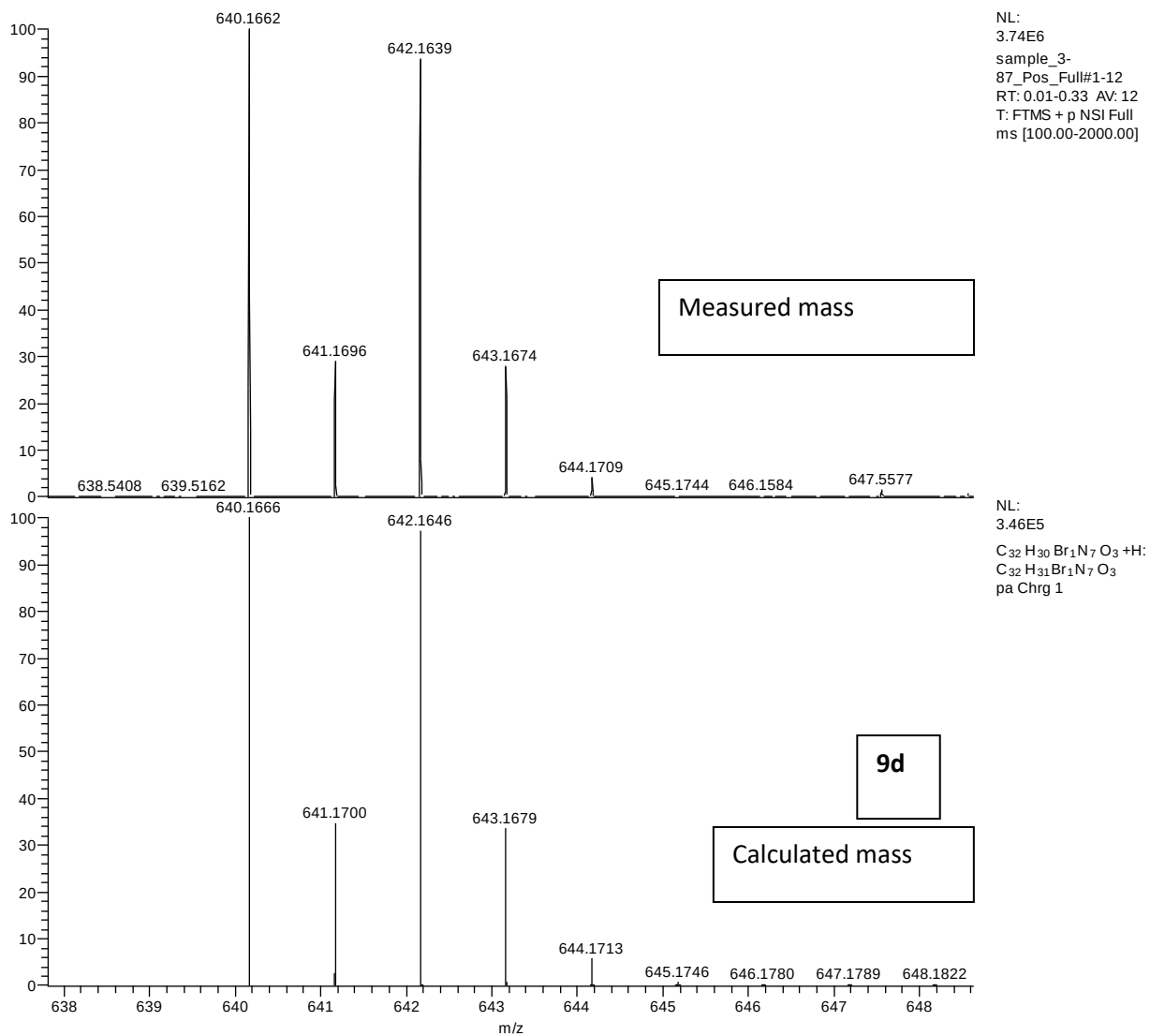
HRMS of (S)-N-(4-fluoro-2-((1-((2-guanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**9b**)



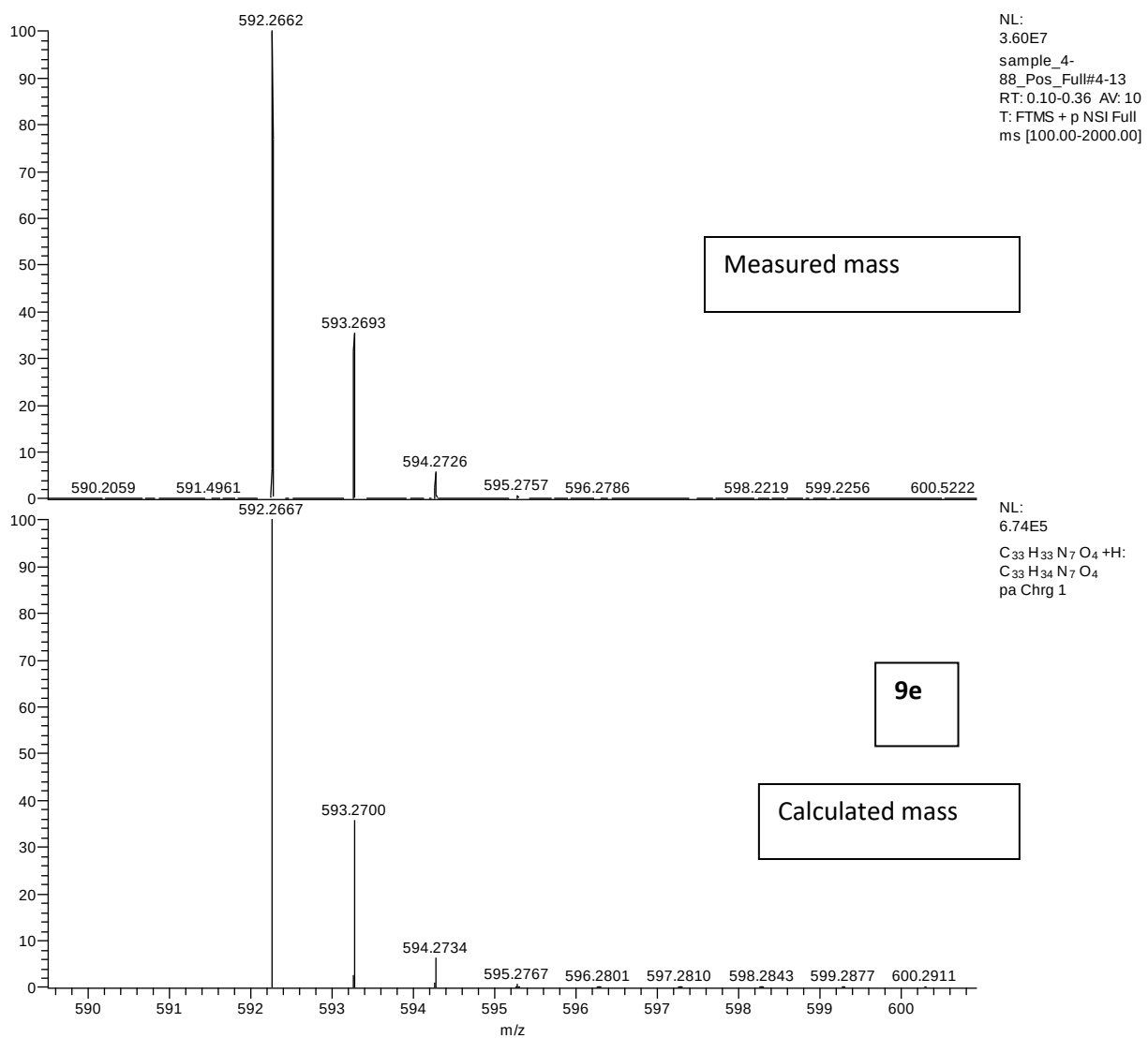
HRMS of (S)-N-(4-chloro-2-((1-((2-guanidinoethyl)amino)-3-(1H-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**9c**)



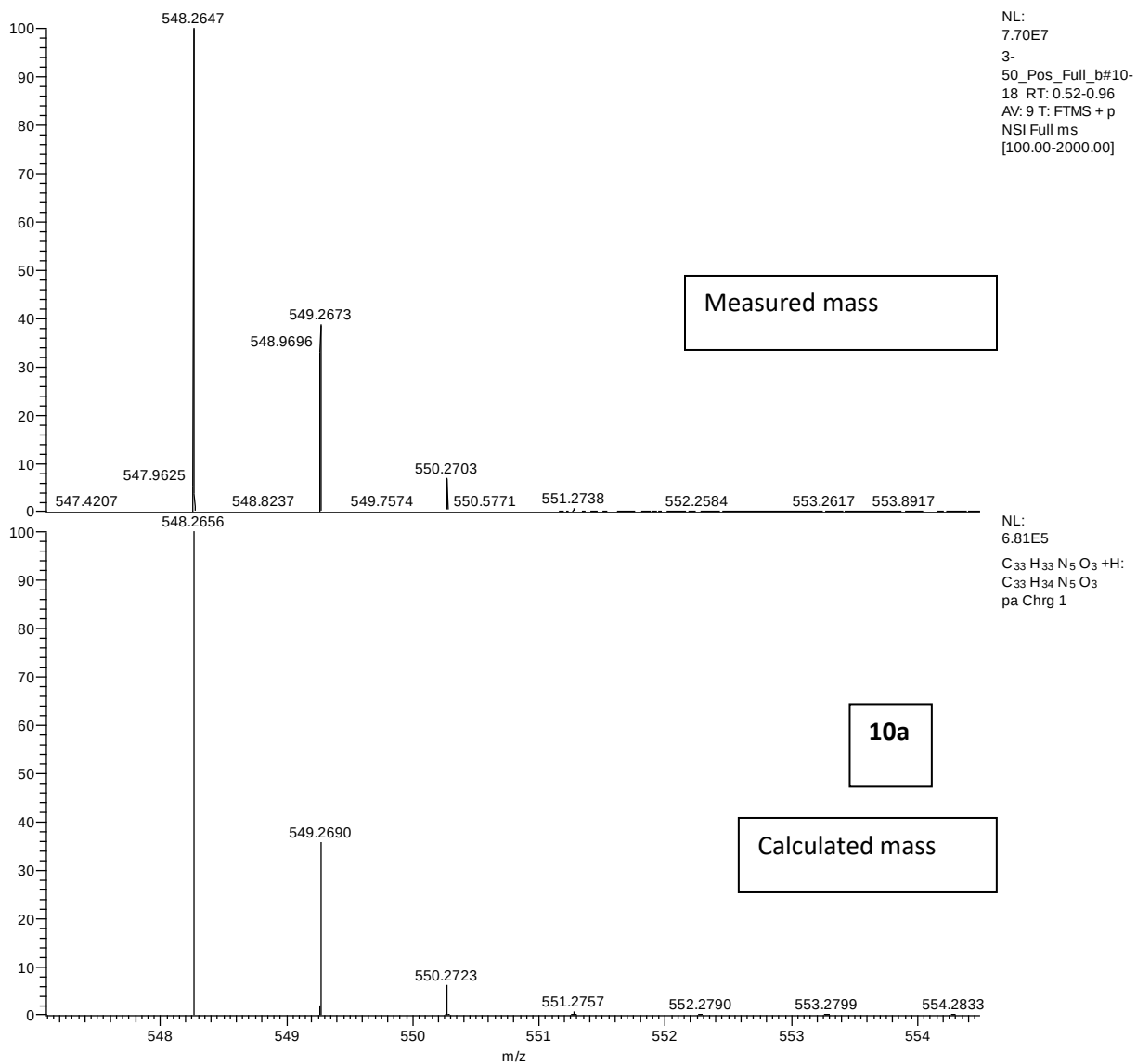
HRMS of (S)-N-(4-bromo-2-((1-((2-guanidinoethyl)amino)-3-(1H-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)phenyl)-2-naphthamide (**9d**)



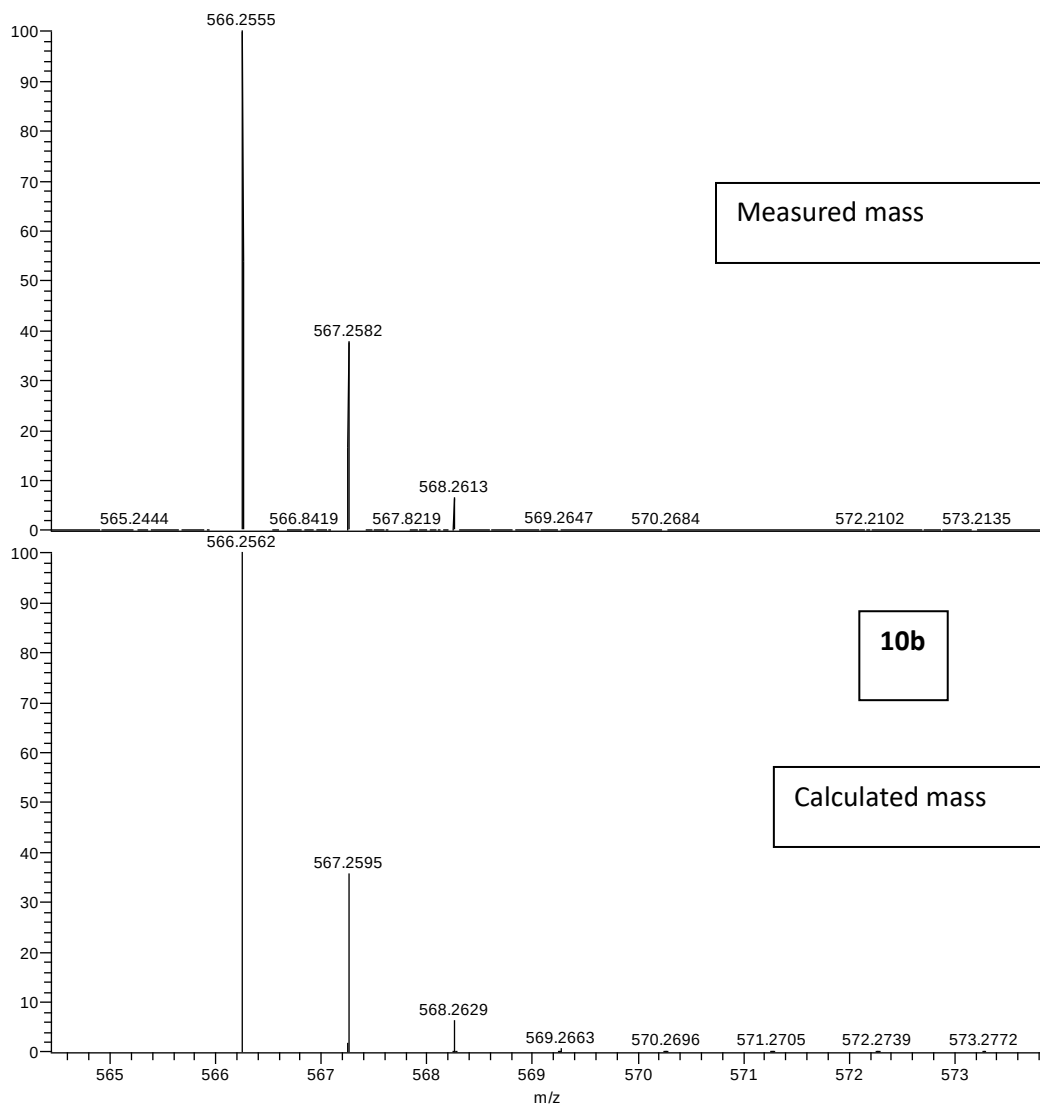
HRMS of (S)-N-(2-((1-((2-guanidinoethyl)amino)-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)carbamoyl)-4-methoxyphenyl)-2-naphthamide (**9e**)



HRMS of (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium chloride (**10a**)



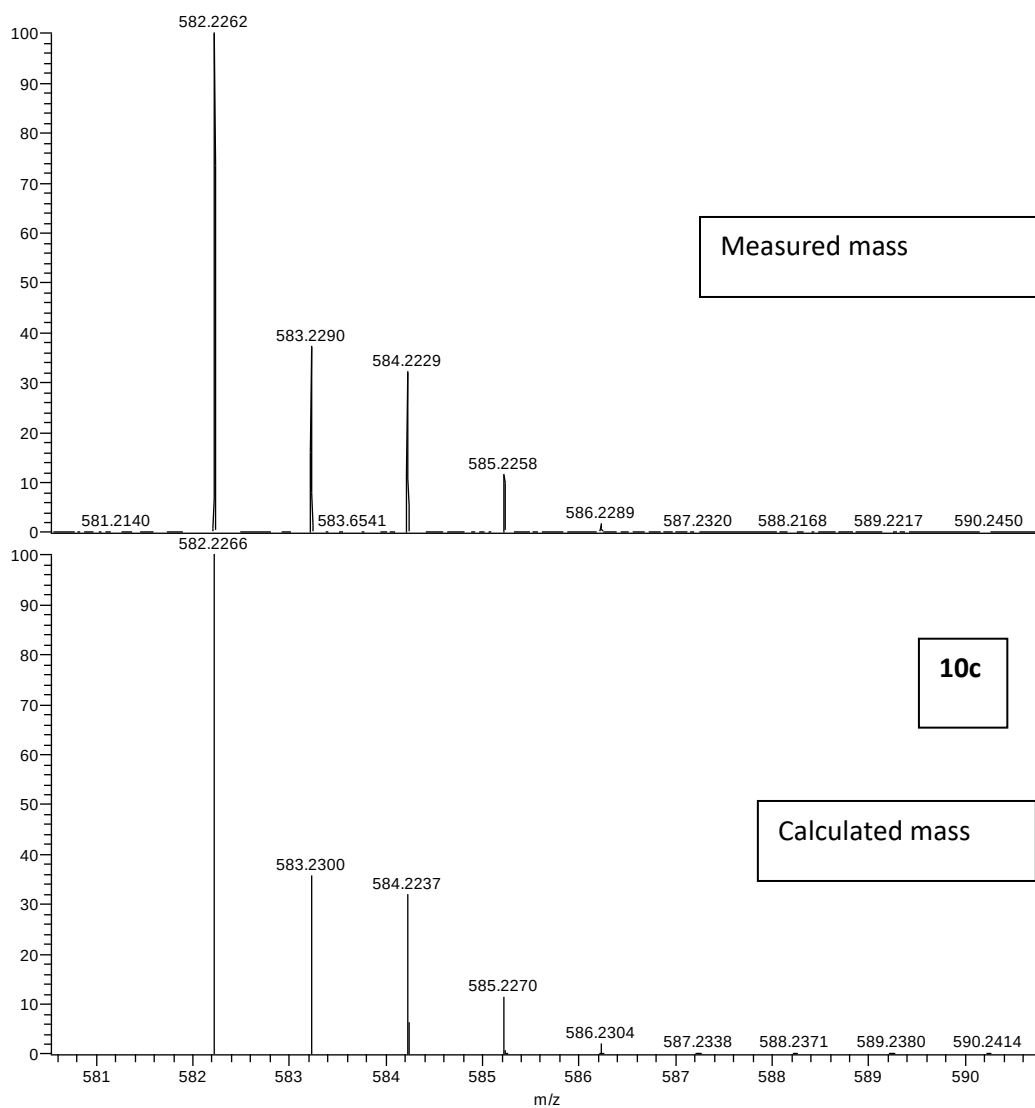
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium chloride (**10b**)



NL:
9.91E7
Sample_4-
45_Pos_Full#15-17
RT: 0.80-0.91 AV: 3 T:
FTMS + p NSI Full ms
[100.00-2000.00]

NL:
6.81E5
C₃₃H₃₂F₁N₅O₃+H:
C₃₃H₃₃F₁N₅O₃
pa Chrg 1

HRMS of (S)-2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium chloride (**10c**)

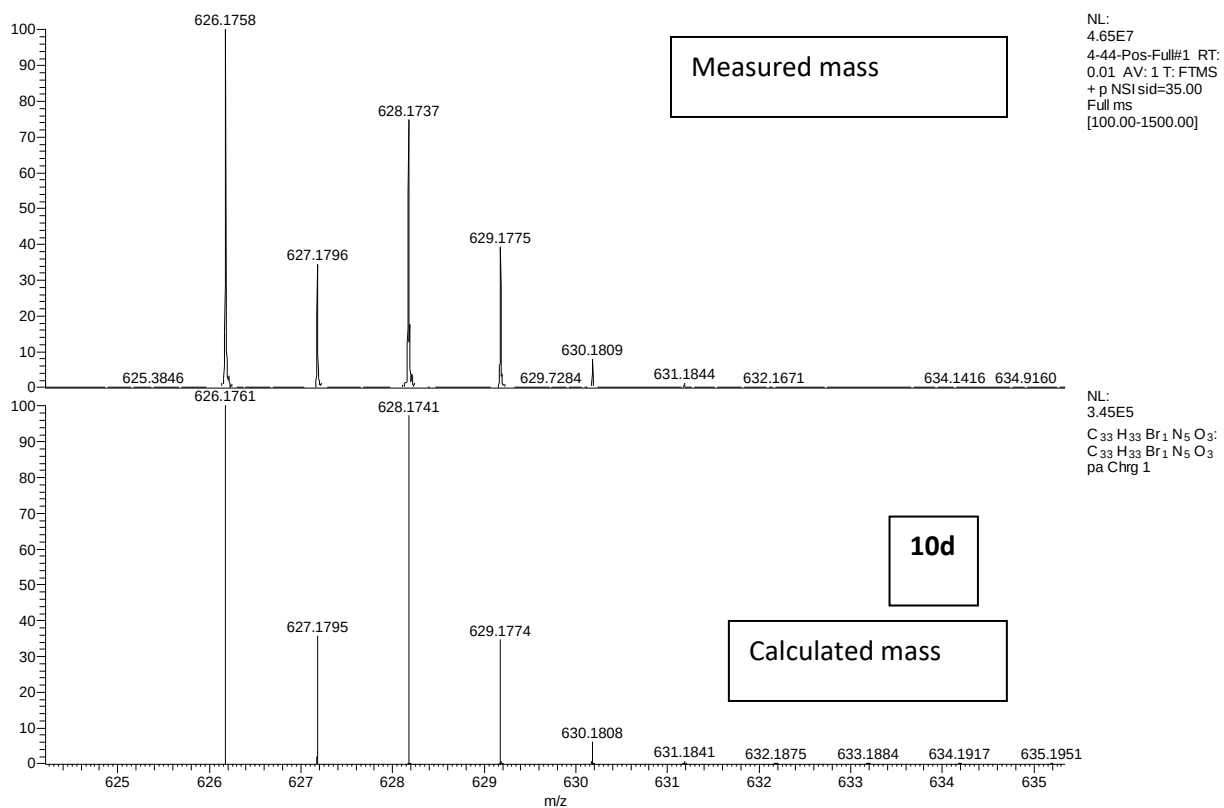


NL:
5.88E7
sample_4-
40_Pos_Full#1-34
RT: 0.01-0.97 AV: 34
T: FTMS + p NSI Full
ms [100.00-2000.00]

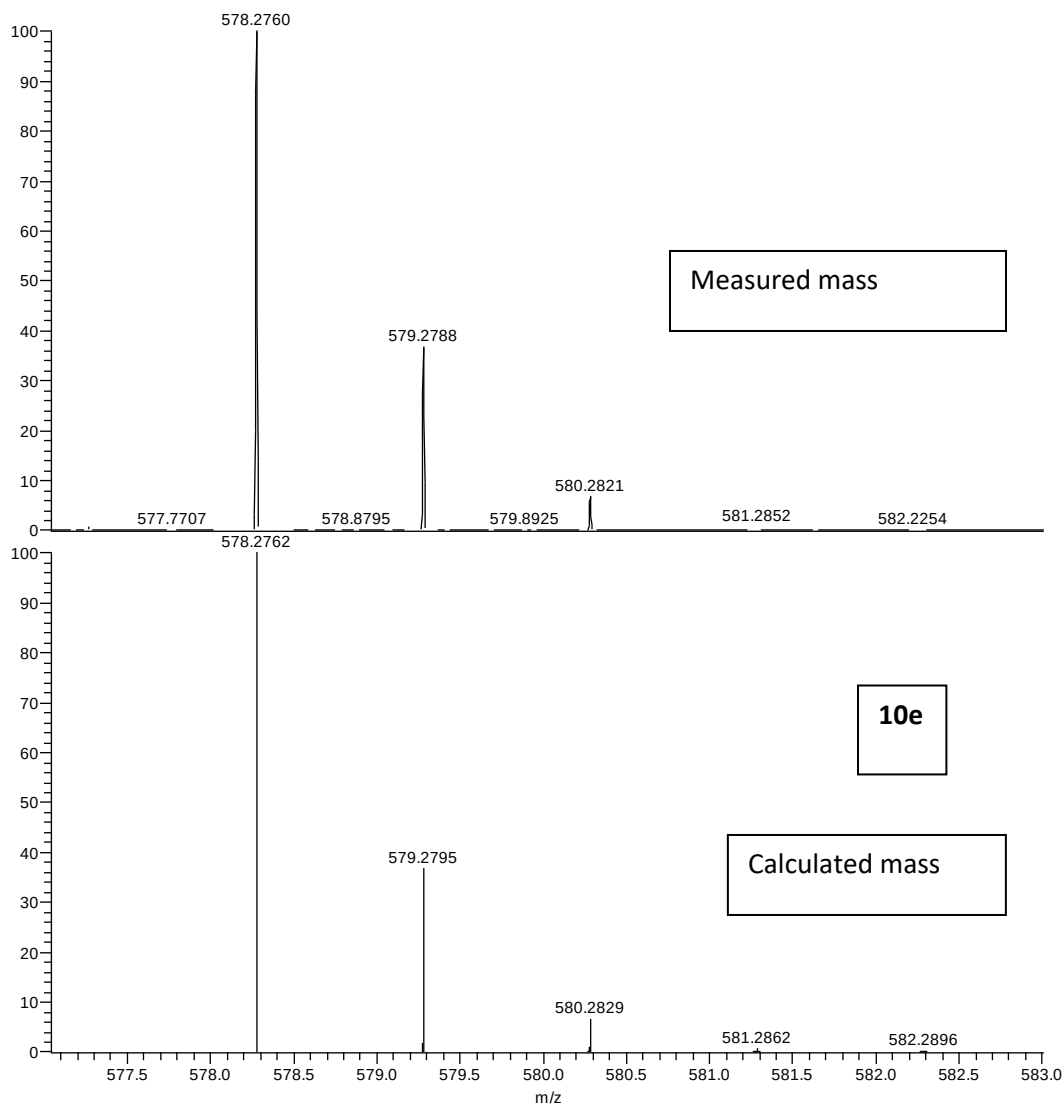
NL:
5.16E5
C₃₃H₃₃Cl₁N₅O₃⁺
C₃₃H₃₃Cl₁N₅O₃
pa Chrg 1

10c

HRMS of (S)-2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium (**10d**)



HRMS of (S)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N*-dimethylethan-1-aminium (**10e**)

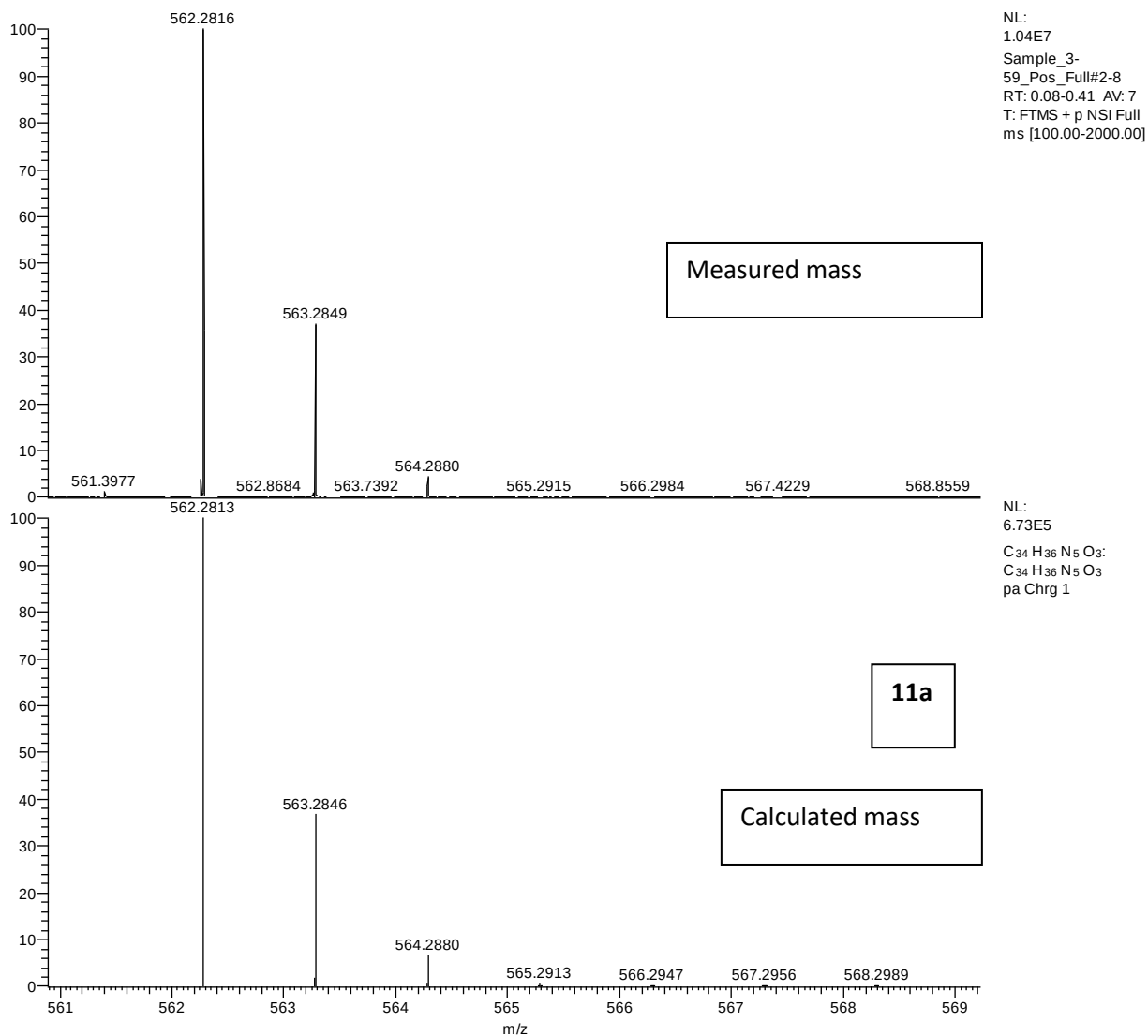


NL:
6.10E7
sample_4-
74_Pos_Full#9-15
RT: 0.24-0.42 AV: 7 T:
FTMS + p NSI Full ms
[100.00-2000.00]

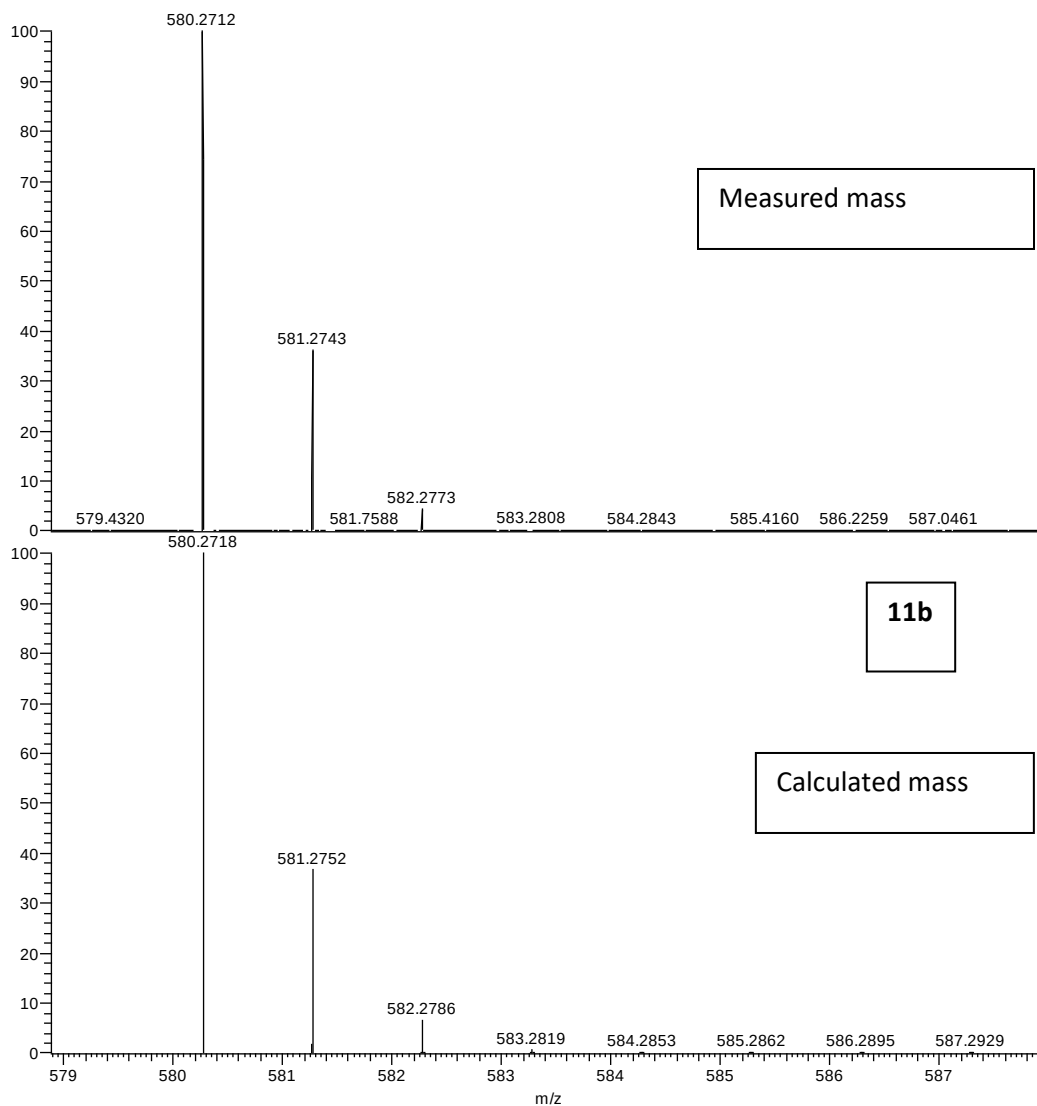
NL:
6.72E5
C₃₄H₃₅N₅O₄+H:
C₃₄H₃₆N₅O₄
pa Chrg 1

10e

HRMS of (S)-2-(2-(2-(2-naphthamido)benzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11a**)



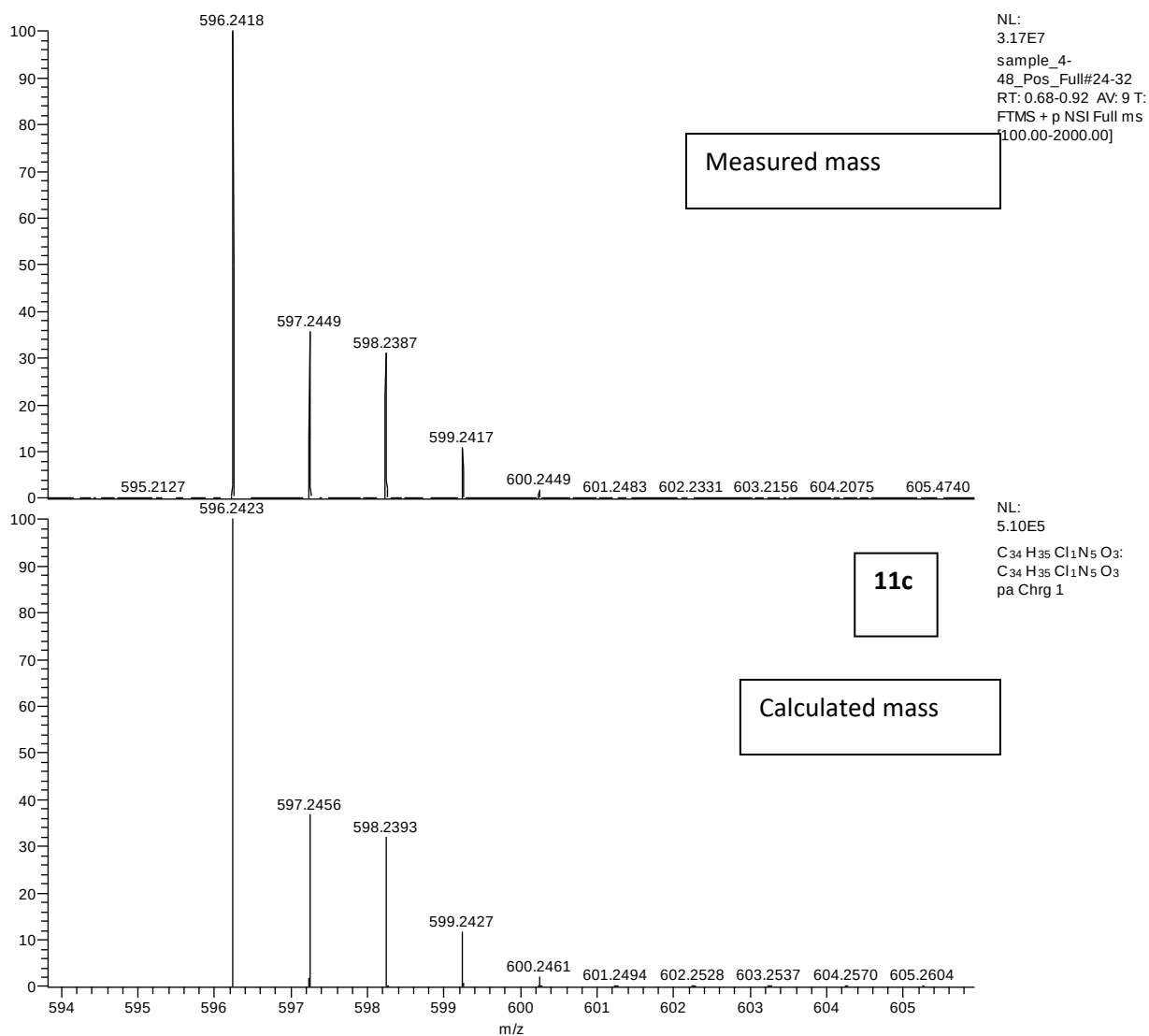
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-fluorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11b**)



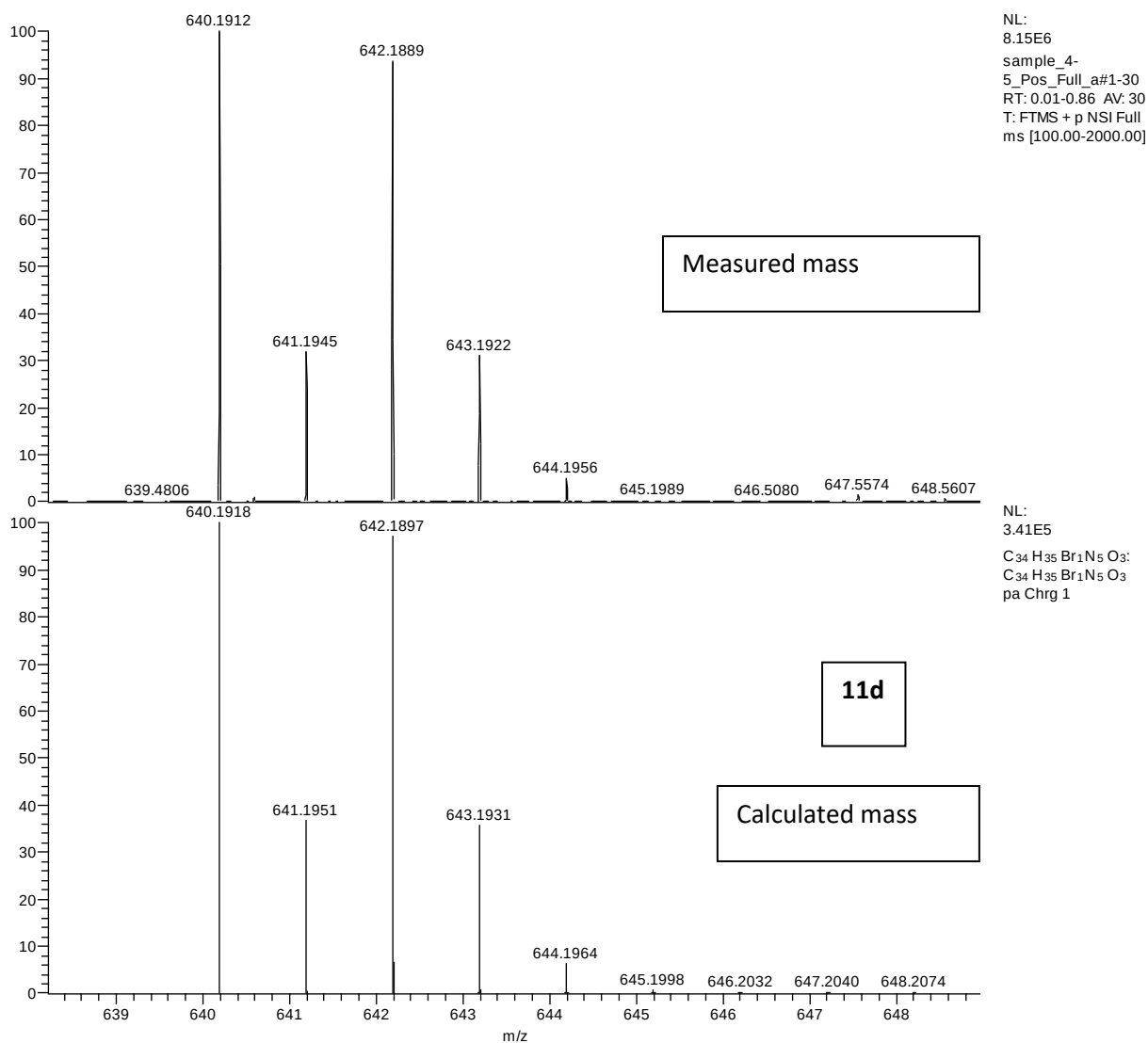
NL:
1.39E7
Sample_3-
118_Pos_Full#1-4
RT: 0.01-0.17 AV: 4 T:
FTMS + p NSI Full ms
[100.00-2000.00]

NL:
6.73E5
C₃₄H₃₅F₁N₅O₃:
C₃₄H₃₅F₁N₅O₃
pa Chrg 1

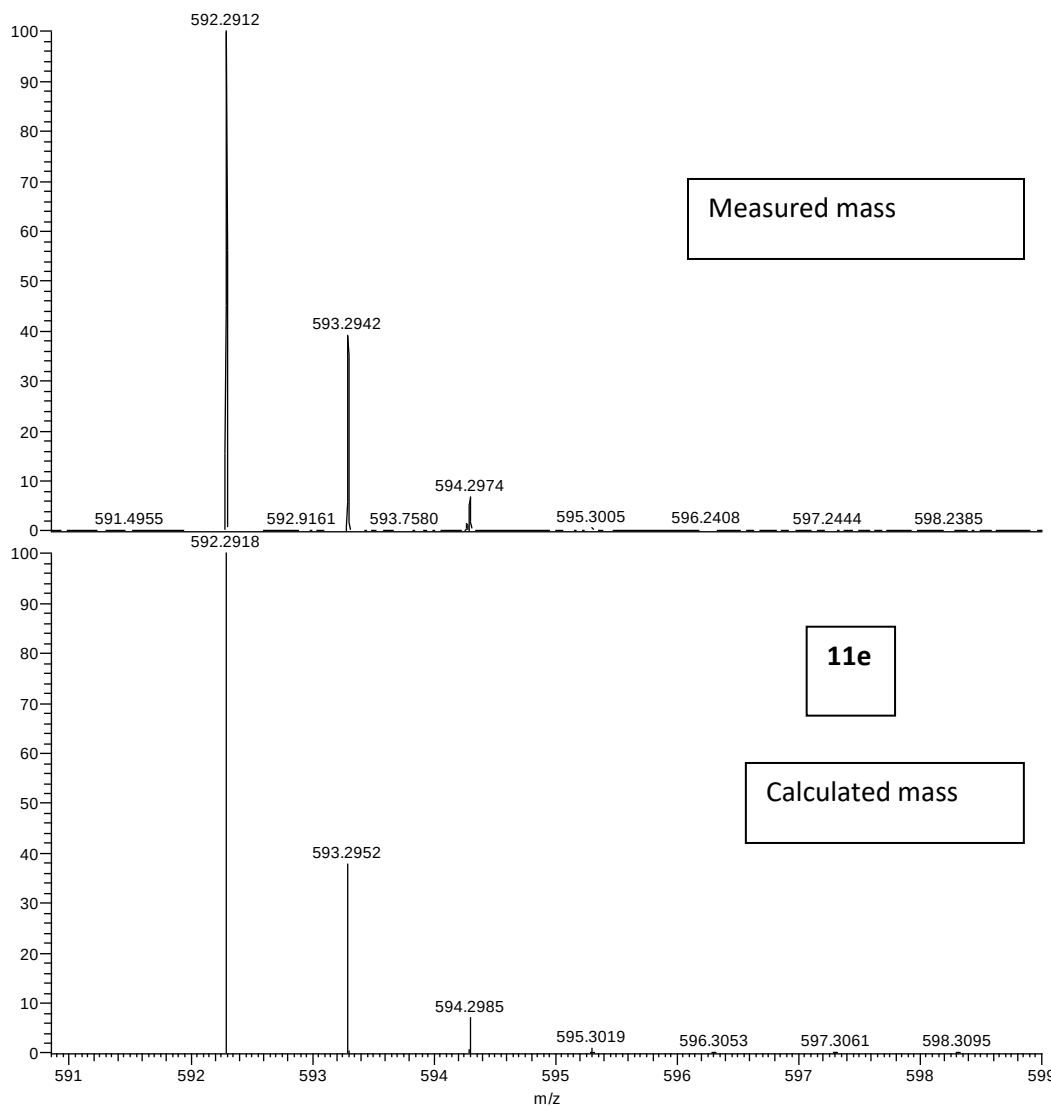
HRMS of (S)-2-(2-(2-(2-naphthamido)-5-chlorobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium (**11c**)



HRMS of (S)-2-(2-(2-(2-naphthamido)-5-bromobenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11d**)



HRMS of (S)-2-(2-(2-(2-naphthamido)-5-methoxybenzamido)-3-(1*H*-indol-3-yl)propanamido)-*N,N,N*-trimethylethan-1-aminium iodide (**11e**)



NL:
4.05E7
sample_4-
68_Pos_Full#9-25
RT: 0.25-0.71 AV: 17
T: FTMS + p NSI Full
ms [100.00-2000.00]

NL:
6.64E5
C₃₅H₃₈N₅O₄:
C₃₅H₃₈N₅O₄
pa Chrg 1