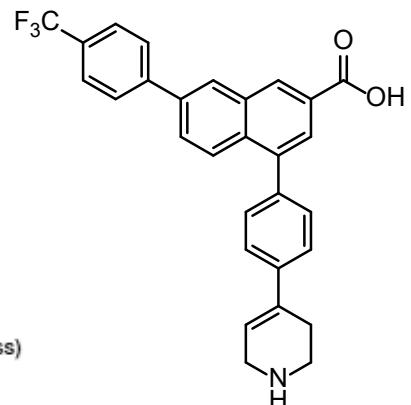


4-(4-(1,2,3,6-Tetrahydropyridin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**3**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

88 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

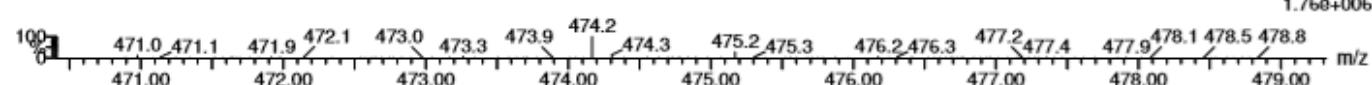
Elements Used:

C: 0-150 H: 0-200 N: 1-1 O: 0-40 F: 3-3

JYH-09MAY18-037-2 120 (2.046) AM2 (Ar,22000.0,0.00,0.00); ABS

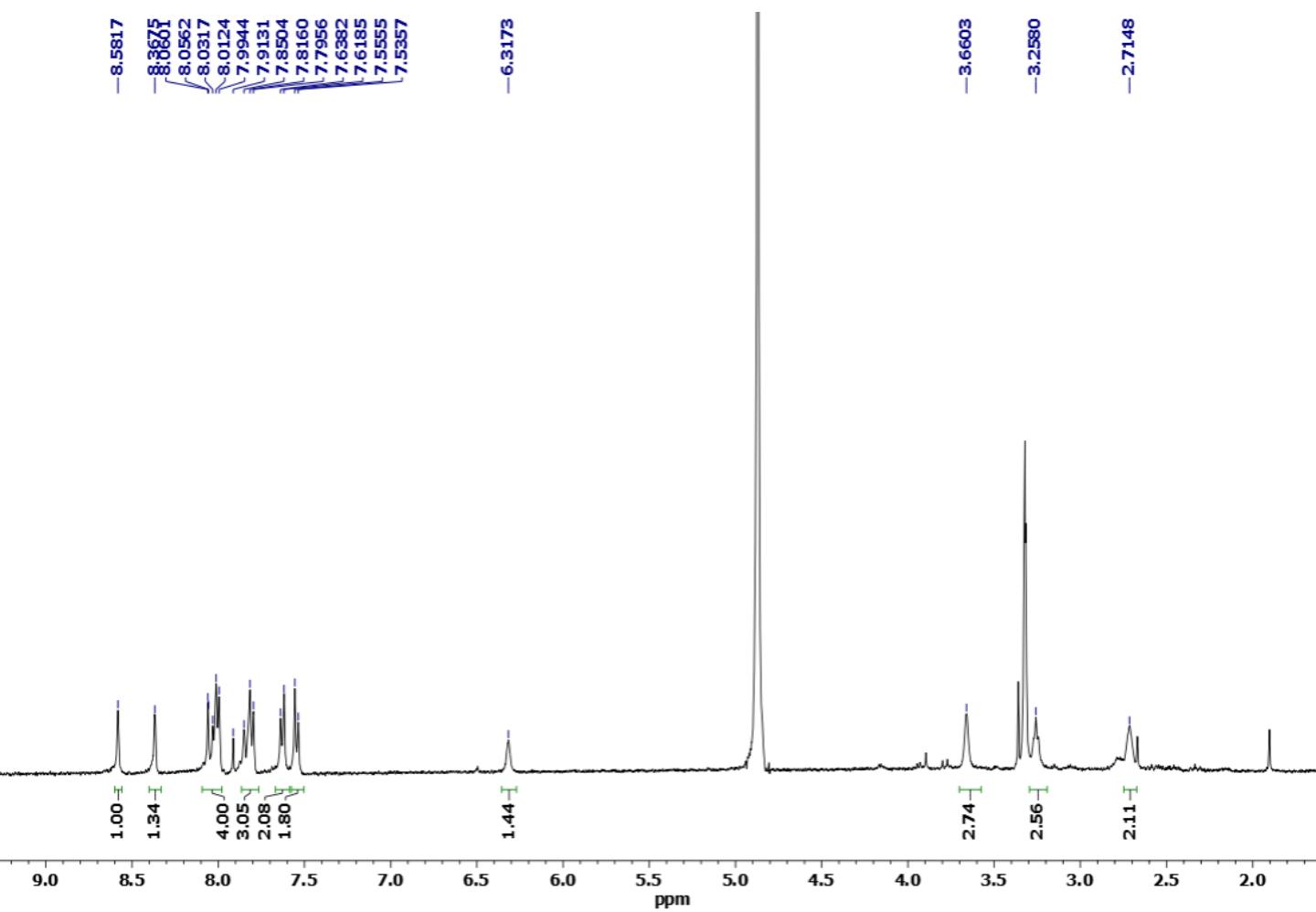
TOF MS ES+

1.768+006

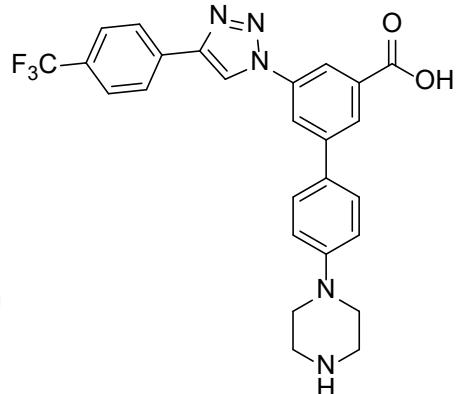


Minimum: -1.5
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
474.1683	474.1681	0.2	0.4	17.5	431.0	n/a	n/a	C ₂₉ H ₂₃ N O ₂ F ₃



4'-(Piperazin-1-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carboxylic acid (4)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

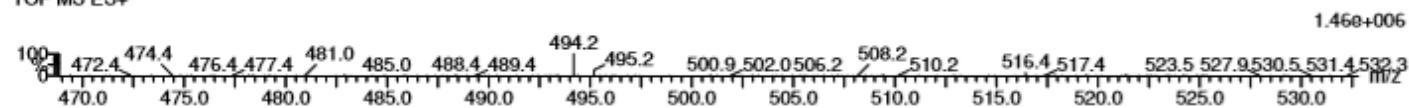
80 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 5-5 O: 0-40 F: 3-3

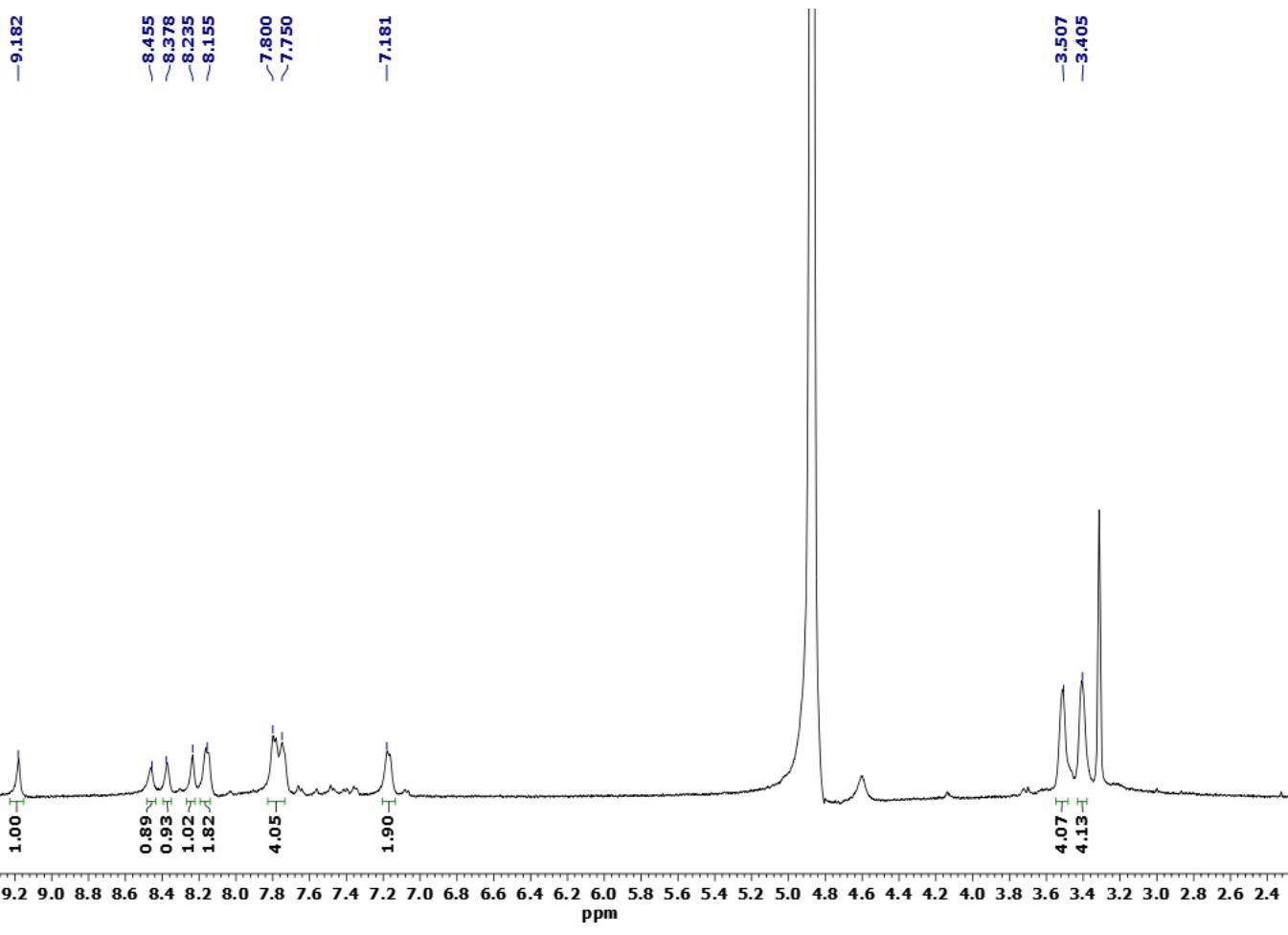
JYH-18AUG18-100-2 317 (5.379) AM2 (Ar,42000.0,0.00,0.00); ABS

TOF MS ES+

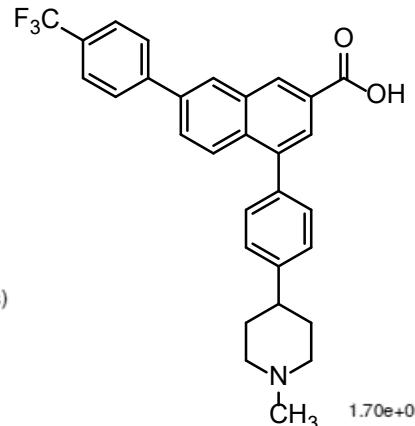


Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
494.1807	494.1804	0.3	0.6	16.5	94.0	n/a	n/a	C26 H23 N5 O2 F3



4-(4-(1-Methylpiperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid
(5)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

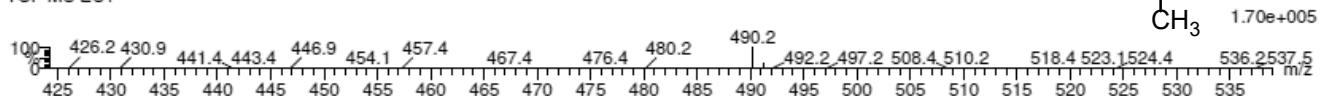
94 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-60 H: 0-200 N: 1-1 O: 0-40 F: 3-3

YJ-09JAN18-V-62 154 (2.621) AM (Cen,5, 50.00, Ht,10000.0,0.00,0.70); Sm (SG, 1x2.00); Sb (15,10.00)

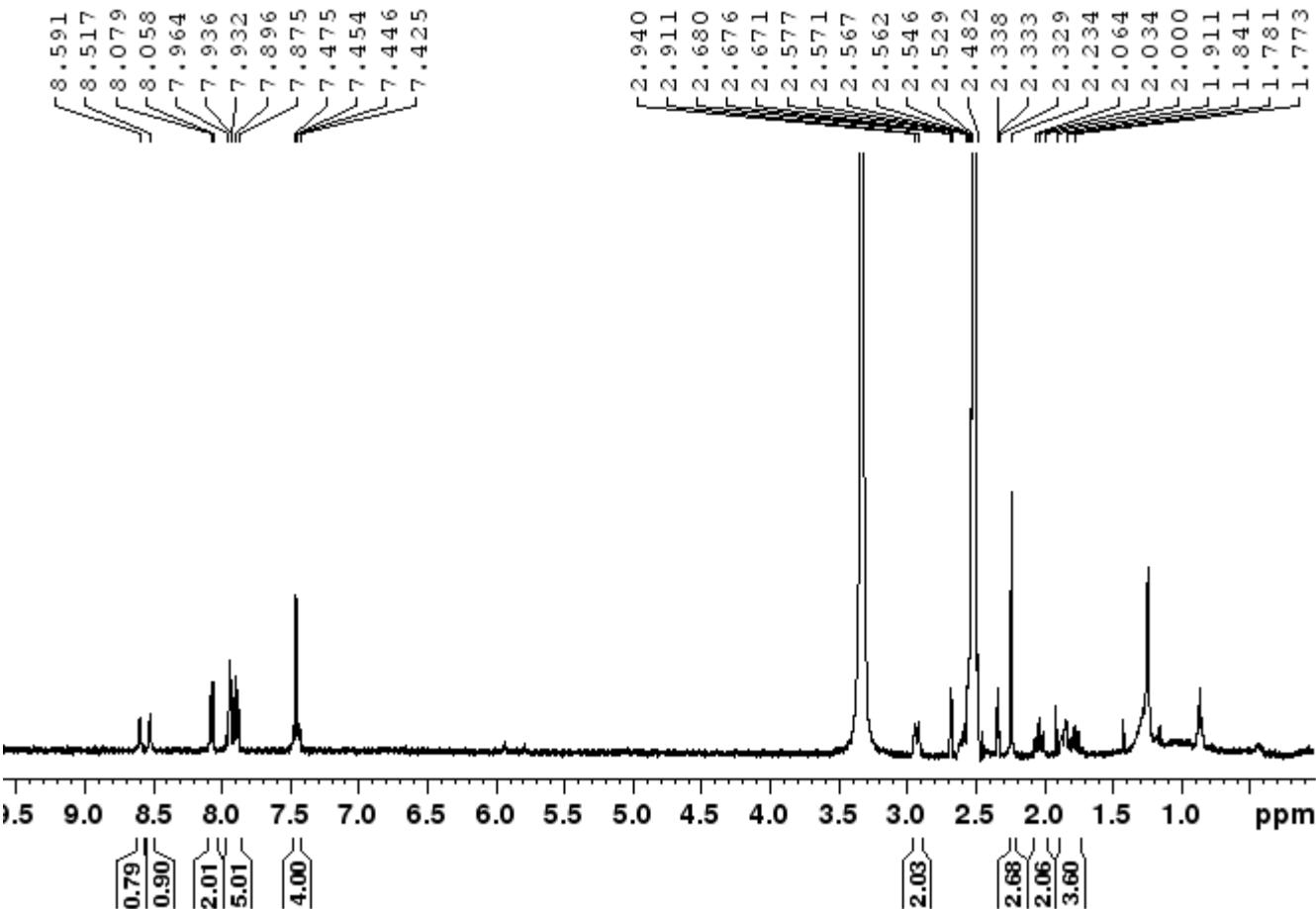
TOF MS ES+



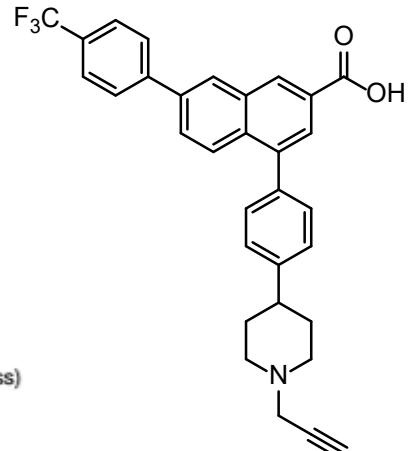
Minimum: -1.5
 Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

490.2001	490.1994	0.7	1.4	16.5	252.8	1.680	18.63	C30 H27 N O2 F3
	490.2053	-5.2	-10.6	7.5	251.4	0.206	81.37	C23 H31 N O7 F3



4-(4-(1-(Prop-2-yn-1-yl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (6a**)**



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

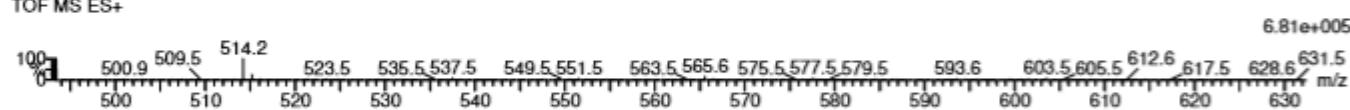
103 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-120 H: 0-200 N: 1-1 O: 0-40 F: 3-3

JYH-02APR18-017 4 (0.084) AM (Cen,5, 50.00, Ht,10000.0,0.00,0.70); Sm (SG, 1x2.00); Sb (15,10.00)

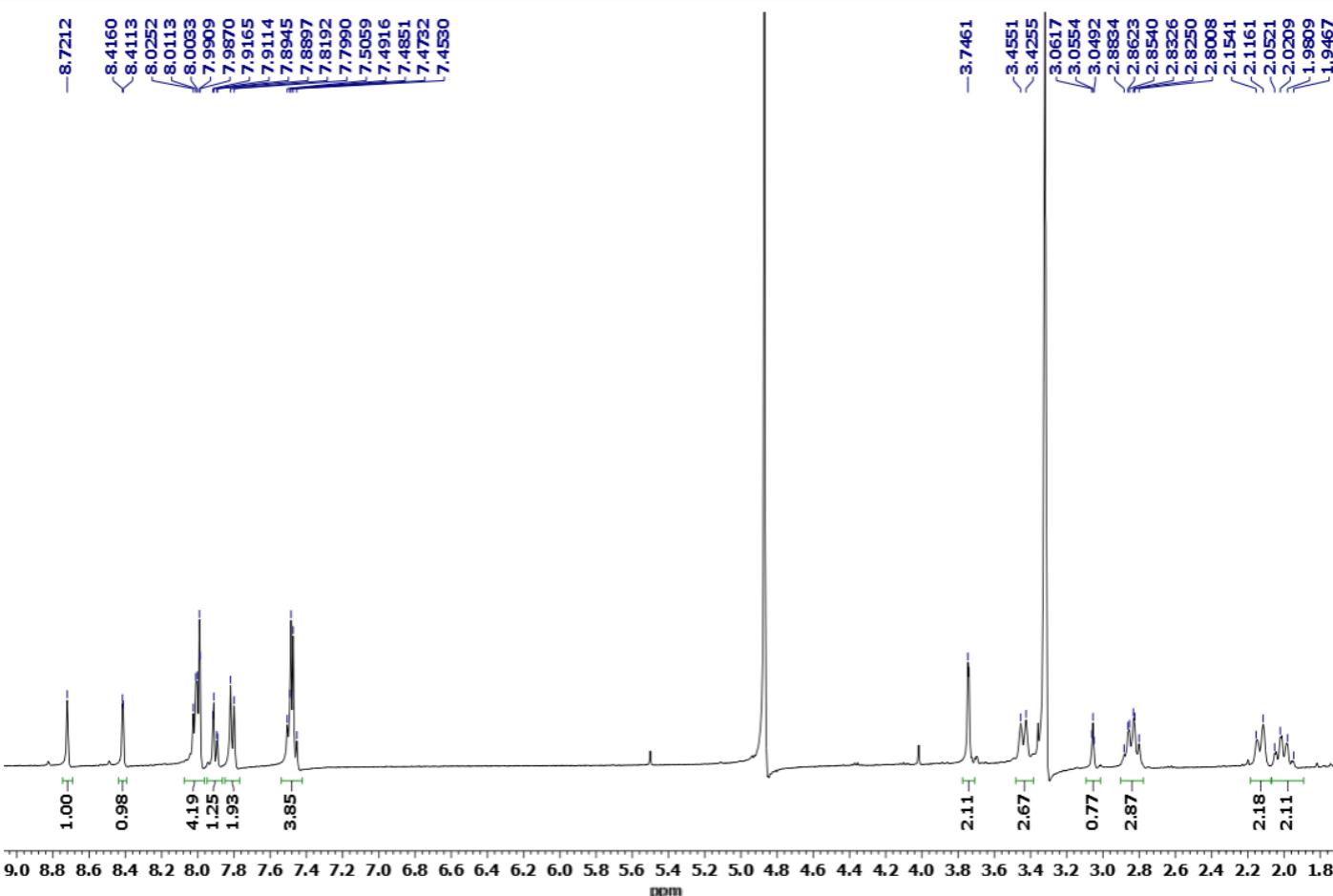
TOF MS ES+



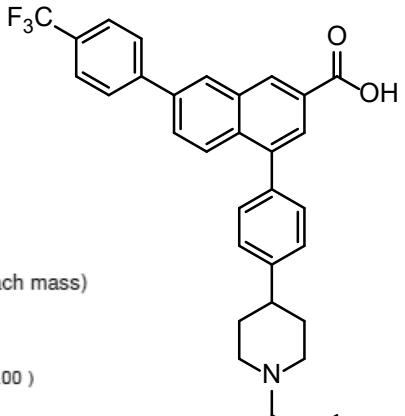
Minimum: -1.5
Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	I-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

514.2001	514.1994	0.7	1.4	18.5	374.0	0.623	53.64	C ₃₂ H ₂₇ N ₀ O ₂ F ₃
	514.2053	-5.2	-10.1	9.5	374.1	0.769	46.36	C ₂₅ H ₃₁ N ₀ O ₇ F ₃



4-(4-(1-Propylpiperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**6b**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

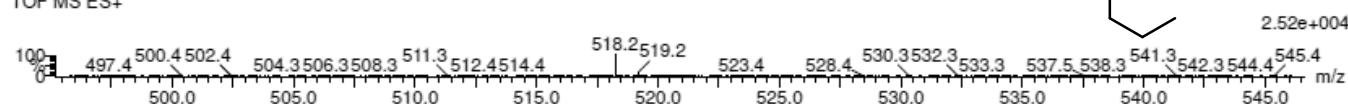
Monoisotopic Mass, Even Electron Ions

104 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

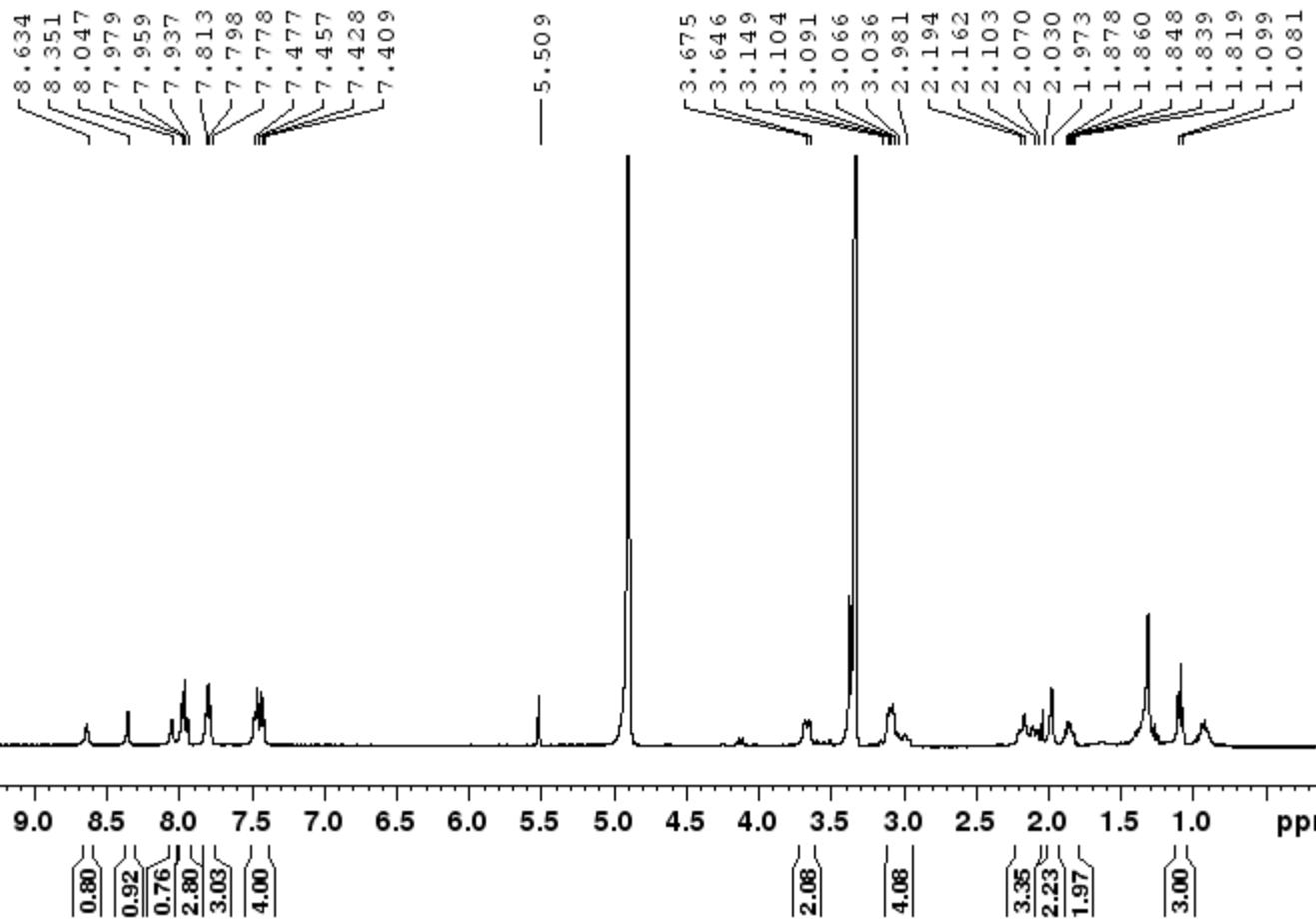
C: 0-150 H: 0-300 N: 1-1 O: 0-100 F: 3-3

YJ-20DEC17-V-56 99 (1.691) AM (Cen,3, 50.00, Ht,10000.0,0.00,0.70); Sm (SG, 1x2.00); Sb (15,10.00)
TOF MS ES+

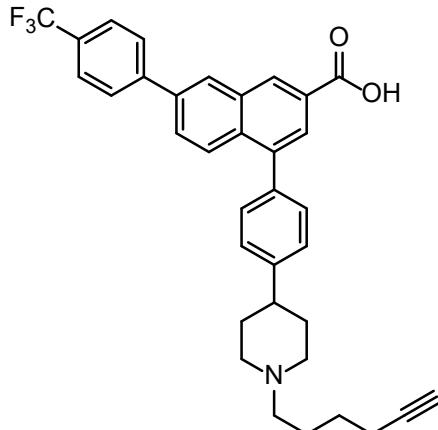


Minimum: -1.5
Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
518.2301	518.2307	-0.6	-1.2	16.5	505.6	4.681	0.93	C32 H31 N O2 F3
	518.2366	-6.5	-12.5	7.5	503.3	2.401	9.07	C25 H35 N O7 F3
	518.2213	8.8	17.0	3.5	501.0	0.105	90.01	C21 H35 N O10 F3



4-(4-(1-(Hex-5-yn-1-yl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**7a**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

116 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

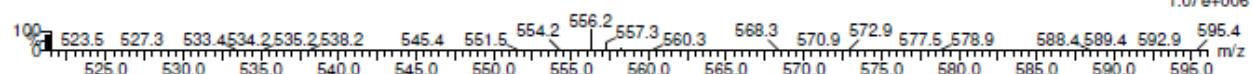
Elements Used:

C: 0-100 H: 0-250 N: 1-1 O: 0-60 F: 3-3

JYH-26JUL19-254-HPLC-2 181 (3.079) AM2 (Ar,25000.0,0.00,0.00); ABS

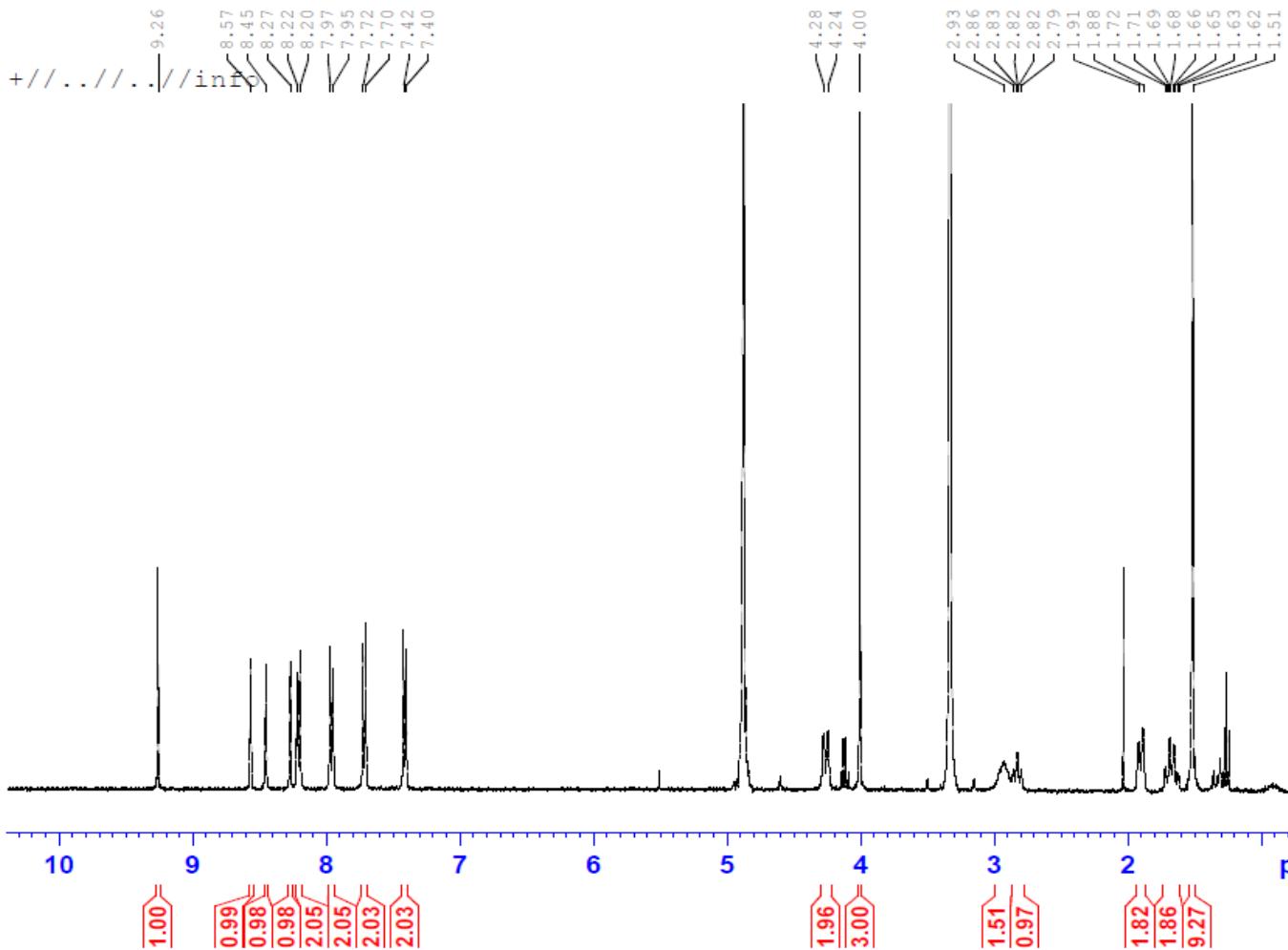
TOF MS ES+

1.07e+006

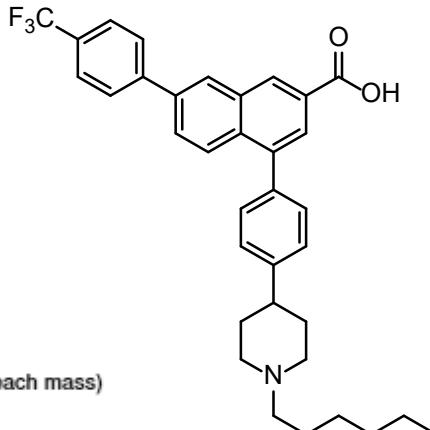


Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
556.2470	556.2463	0.7	1.3	18.5	387.6	n/a	n/a	C35 H33 N O2 F3



4-(4-(1-Hexylpiperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**7b**) $\text{FeCl}_3 \quad \hat{\wedge}$



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mPa. / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of Isotope peaks used for I-FIT = 3

Monoisotopic Mass: Even Electron Ions

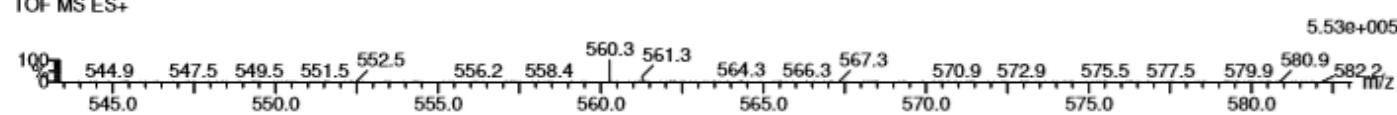
116 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

The ionizing elements used:

Elements used:

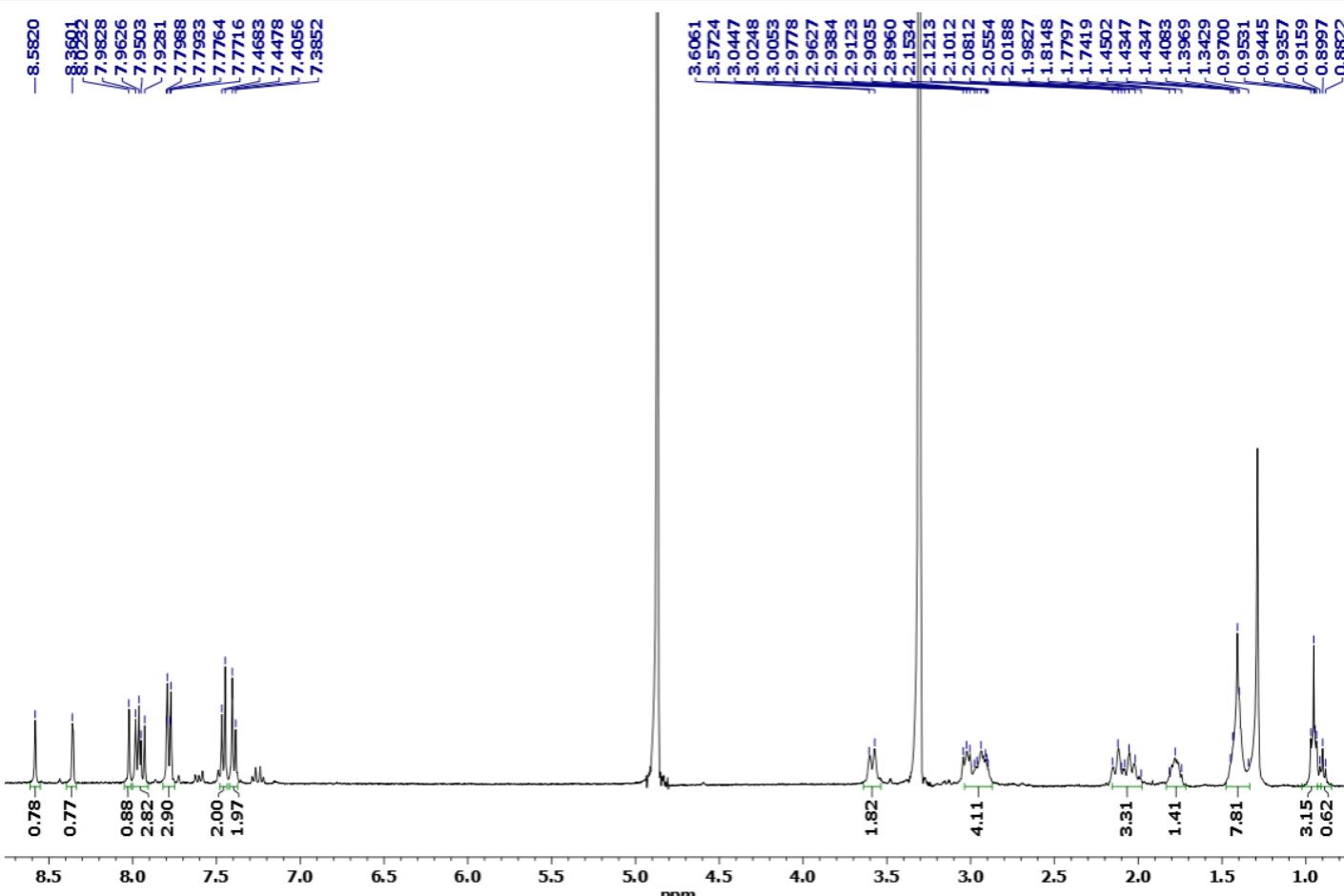
IMH-DRMAR18-004-2-182 (2,205) AM (Can-5, 20, 20, Ht-10000, 0, 0, 00, 0, 70); Sca (SG, 1-2, 20); Sh (15, 10, 00).

JYH-08MAR1
TOE MSG FG

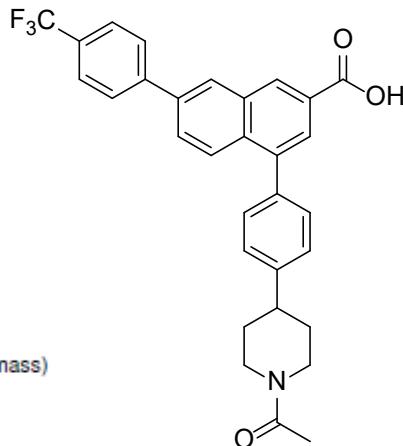


Minimum: -1.5
Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
560.2782	560.2776	0.6	1.1	16.5	202.5	0.386	67.99	C35 H37 N O2 F3
	560.2835	-5.3	-9.5	7.5	203.4	1.355	25.81	C28 H41 N O7 F3
	560.2683	9.9	17.7	3.5	204.9	2.780	6.20	C24 H41 N O10 F3



4-(4-(1-(Acetyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (8)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

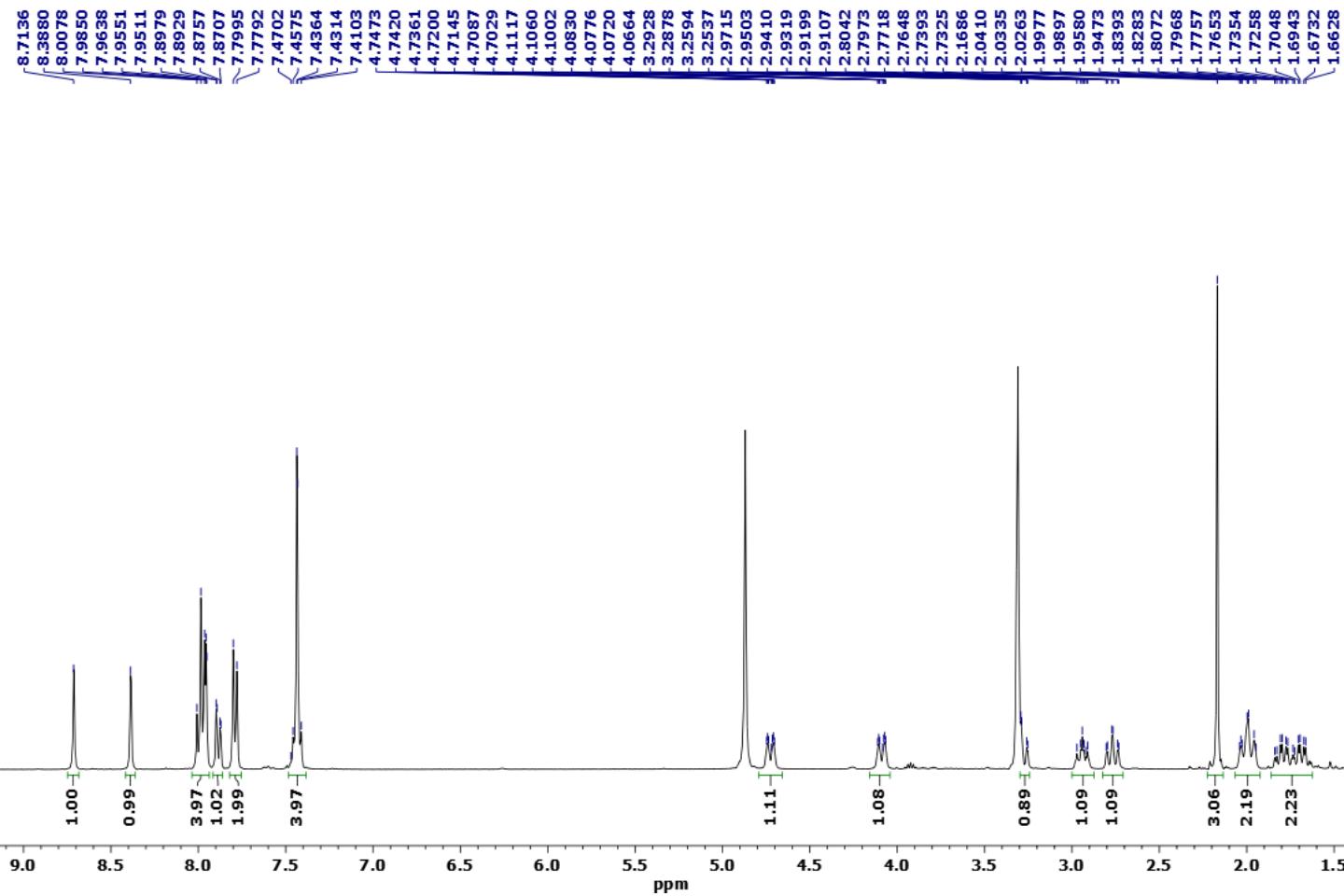
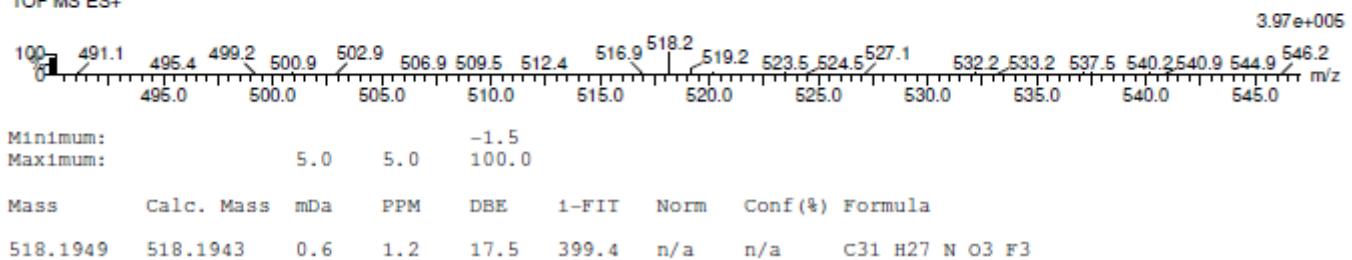
104 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

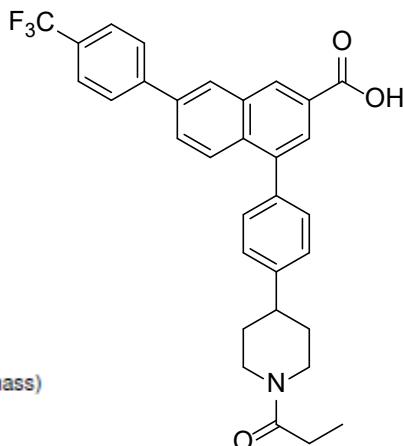
C: 0-100 H: 0-250 N: 1-1 O: 0-60 F: 3-3

JYH-16MAY19-223 96 (1.641) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+



4-(4-(1-(Propionyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**9**).



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

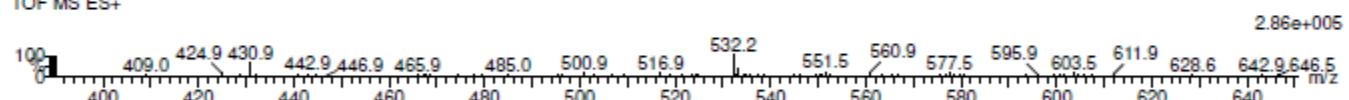
105 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-250 N: 1-1 O: 0-60 F: 3-3

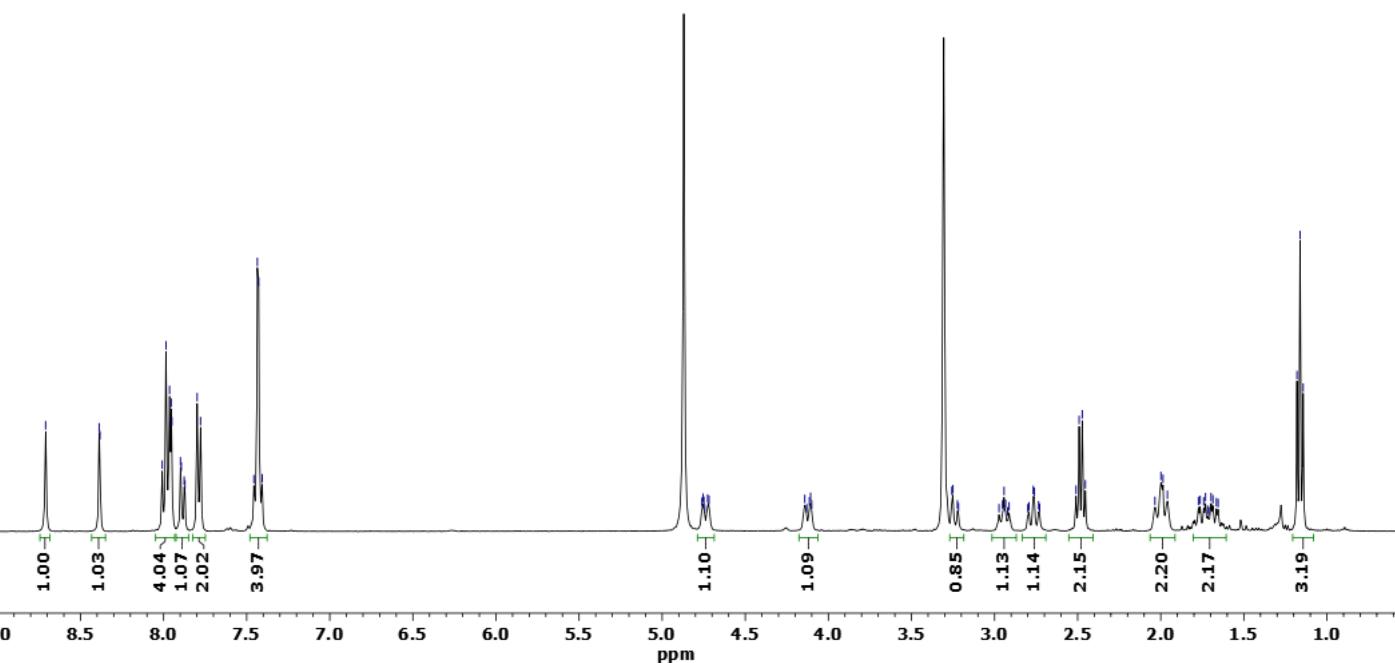
JYH-17MAY19-227 239 (4.060) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+



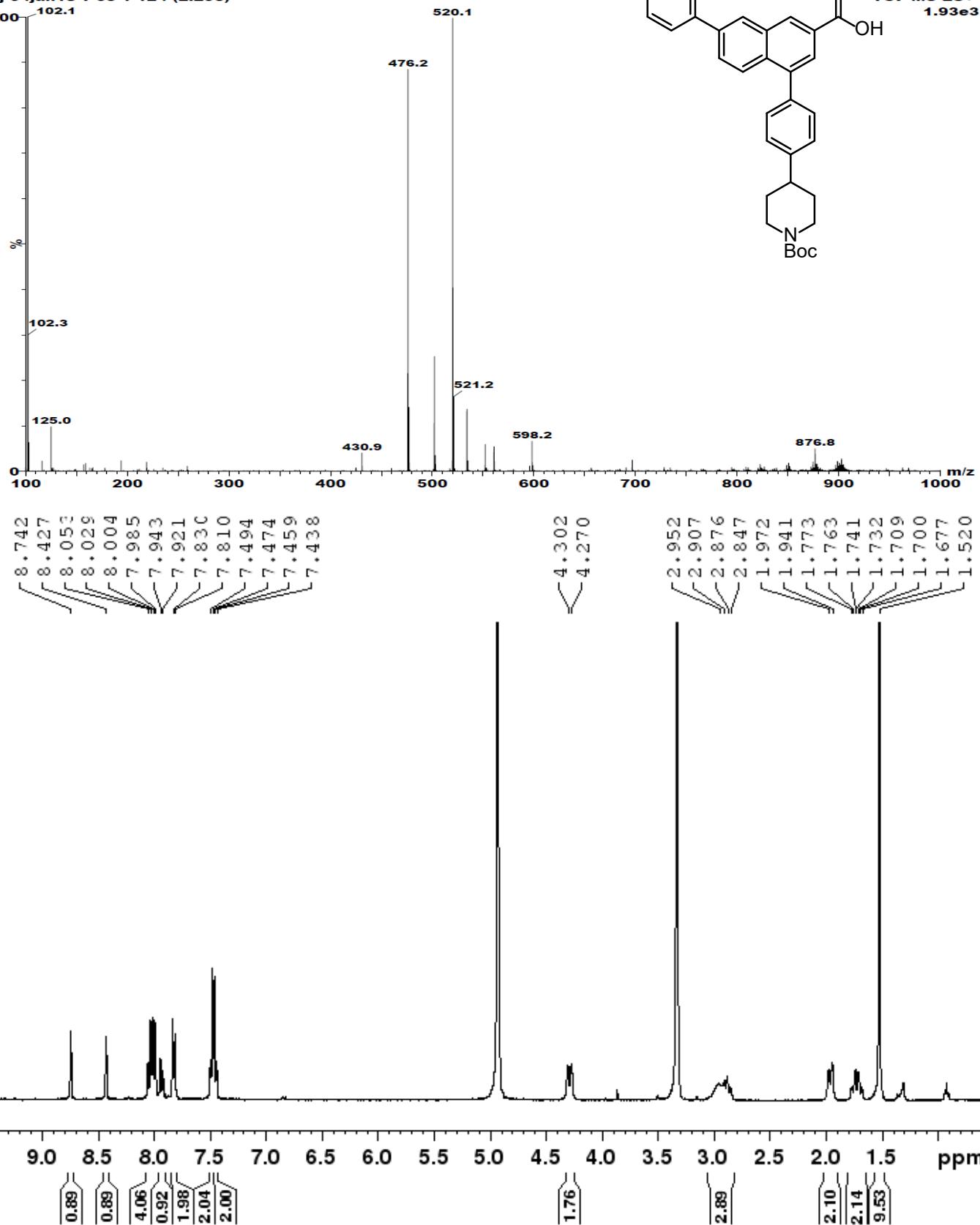
Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Norm	Conf (%)	Formula
532.2102	532.2100	0.2	0.4	17.5	359.2	n/a	n/a	C32 H29 N O3 F3

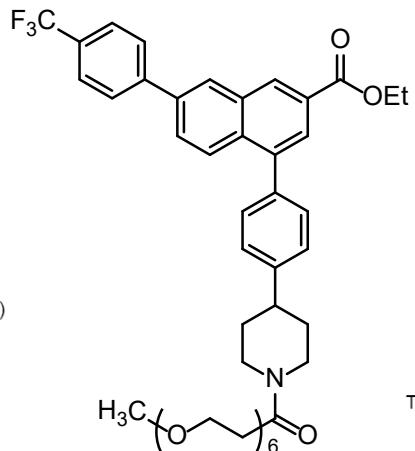


4-(4-(1-Propylpiperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**10**)

04-Jan-2018
yj-04jan18-v-63-1 124 (2.293)



Ethyl 4-(4-(1-(2,5,8,11,14,17-hexaoxaicosan-20-oyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoate (11)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

161 formula(e) evaluated with 4 results within limits (up to 19 closest results for each mass)

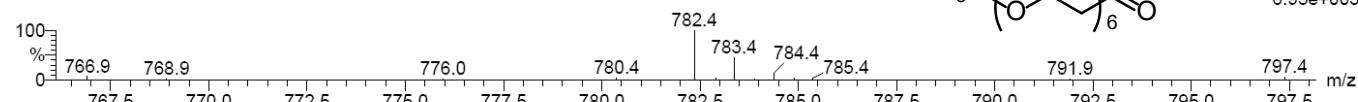
Elements Used:

C: 0-100 H: 0-200 N: 1-1 O: 0-20 F: 3-3

14-Dec-2017

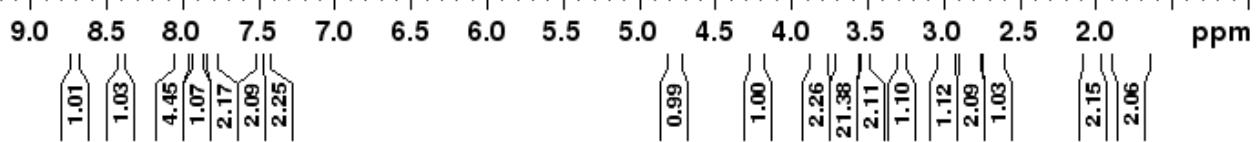
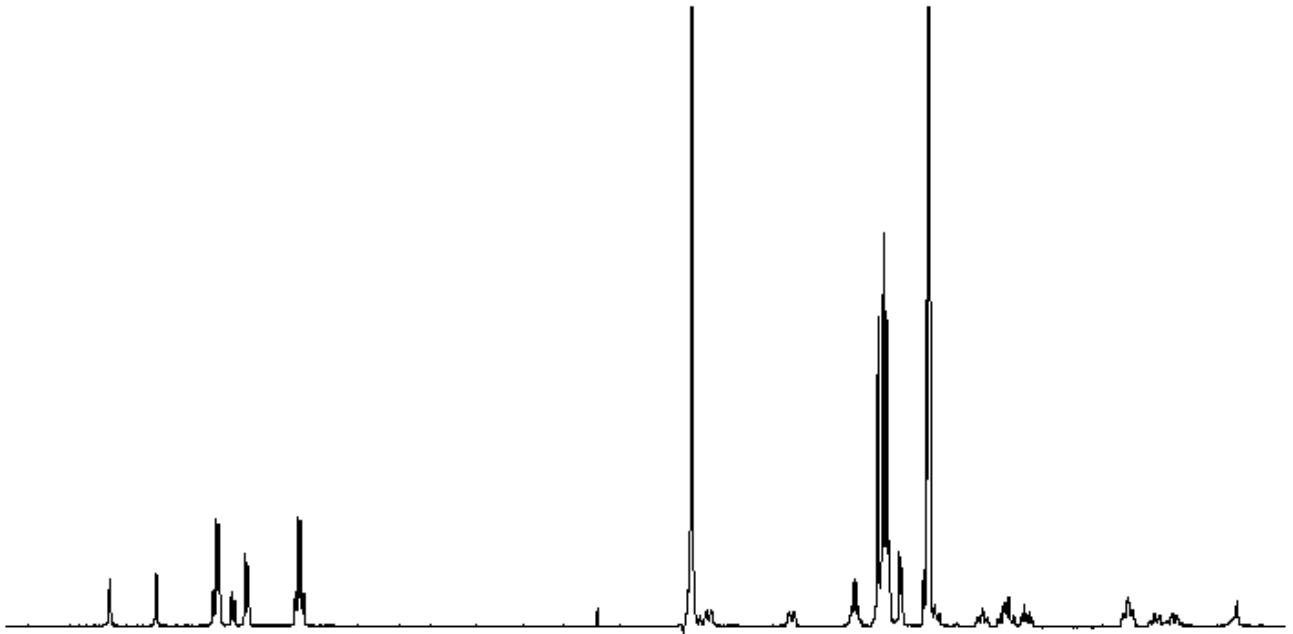
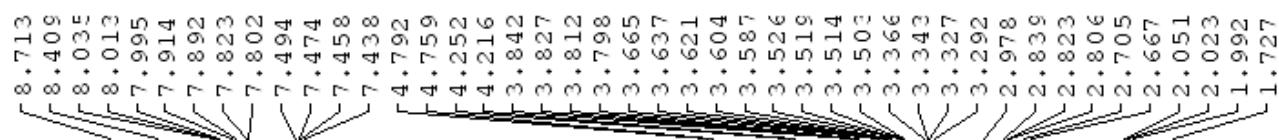
yj-14dec17-v-53 169 (3.125) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

TOF MS ES+
6.95e+003



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
782.3530	782.3516	1.4	1.8	17.5	14.5	C43 H51 N O9 F3
	782.3575	-4.5	-5.8	8.5	14.4	C36 H55 N O14 F3
	782.3457	7.3	9.3	26.5	83.1	C50 H47 N O4 F3
	782.3610	-8.0	-10.2	30.5	139.1	C54 H47 N O F3



4-(4-(1-(1-Amino-3,6,9,12,15,18-hexaoxahenicosan-21-oyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (12)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

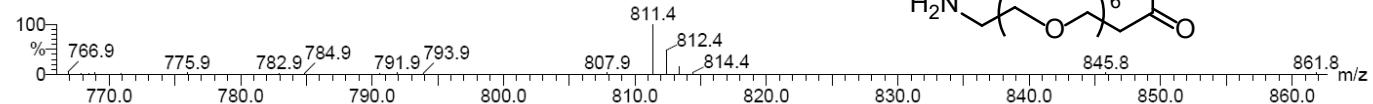
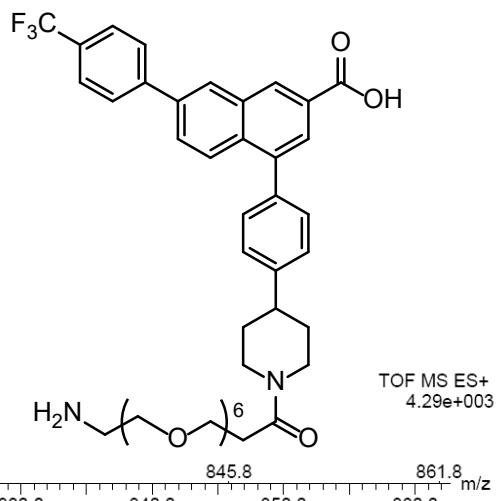
161 formula(e) evaluated with 4 results within limits (up to 19 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 2-2 O: 0-20 F: 3-3

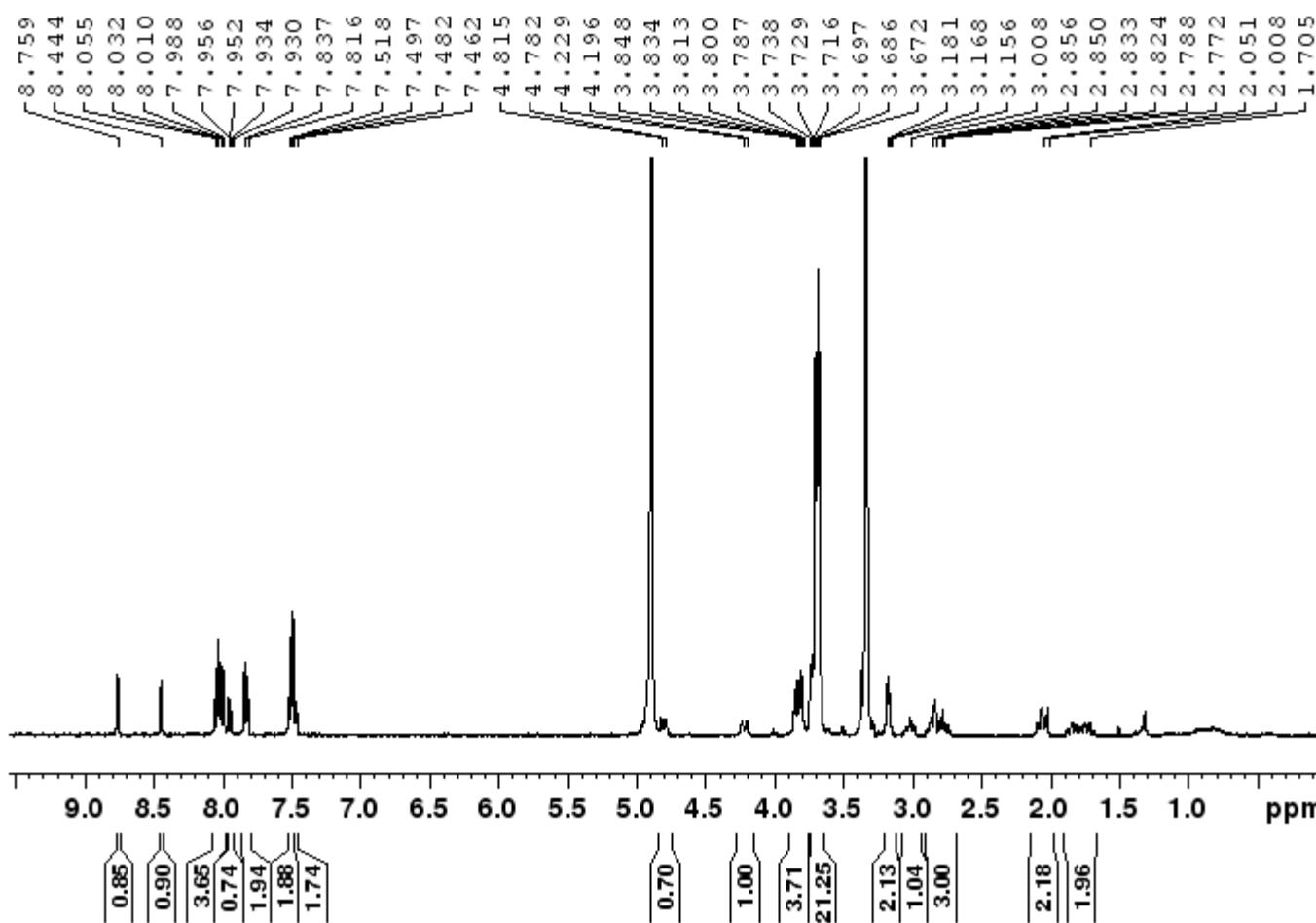
11-Dec-2017

yj-11dec17-v-49 95 (1.757) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

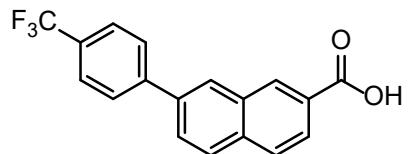


Minimum:		-2.0
Maximum:	10.0	10.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
811.3793	811.3781	1.2	1.5	17.5	2.6	C44 H54 N2 O9 F3
	811.3840	-4.7	-5.8	8.5	14.5	C37 H58 N2 O14 F3
	811.3723	7.0	8.6	26.5	33.3	C51 H50 N2 O4 F3
	811.3875	-8.2	-10.1	30.5	67.4	C55 H50 N2 O F3



4-(4-(1-(2-Oxo-6,9,12,15,18,21-hexaoxa-3-azatetracosan-24-oyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (13)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

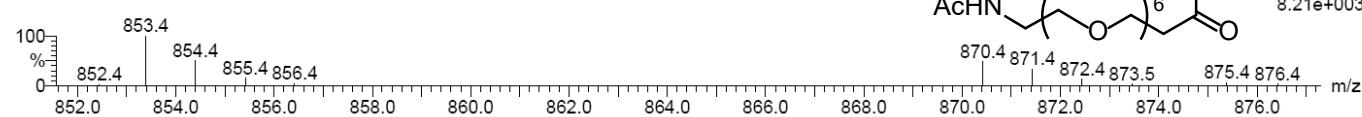
175 formula(e) evaluated with 5 results within limits (up to 19 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 2-2 O: 0-20 F: 3-3

13-Dec-2017

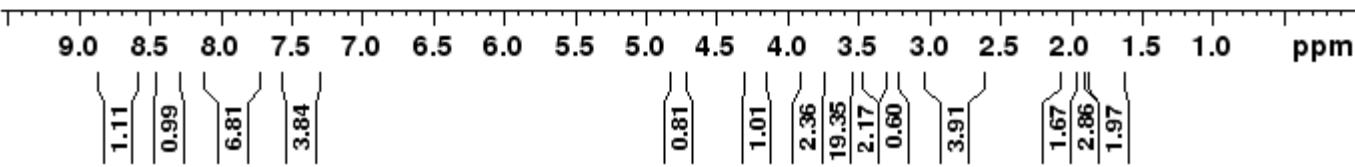
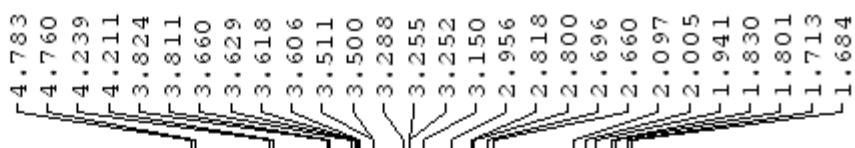
yi-13dec17-v-52 99 (1.831) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
------	------------	-----	-----	-----	-------	---------

853.3893	853.3887	0.6	0.7	18.5	7.1	C46 H56 N2 O10 F3
	853.3946	-5.3	-6.2	9.5	19.8	C39 H60 N2 O15 F3
	853.3828	6.5	7.6	27.5	73.8	C53 H52 N2 O5 F3
	853.3981	-8.8	-10.3	31.5	134.9	C57 H52 N2 O2 F3
	853.3793	10.0	11.7	5.5	75.3	C35 H60 N2 O18 F3



4-(4-(1-(2,2-Dimethyl-4-oxo-3,8,11,14,17,20,23-heptaoxa-5-azahexacosan-26-oyl)piperidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (**14**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

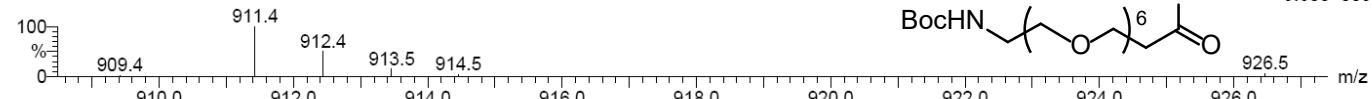
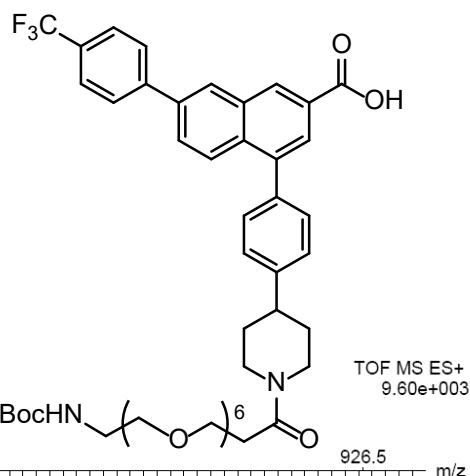
188 formula(e) evaluated with 5 results within limits (up to 19 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 2-2 O: 0-20 F: 3-3

07-Dec-2017

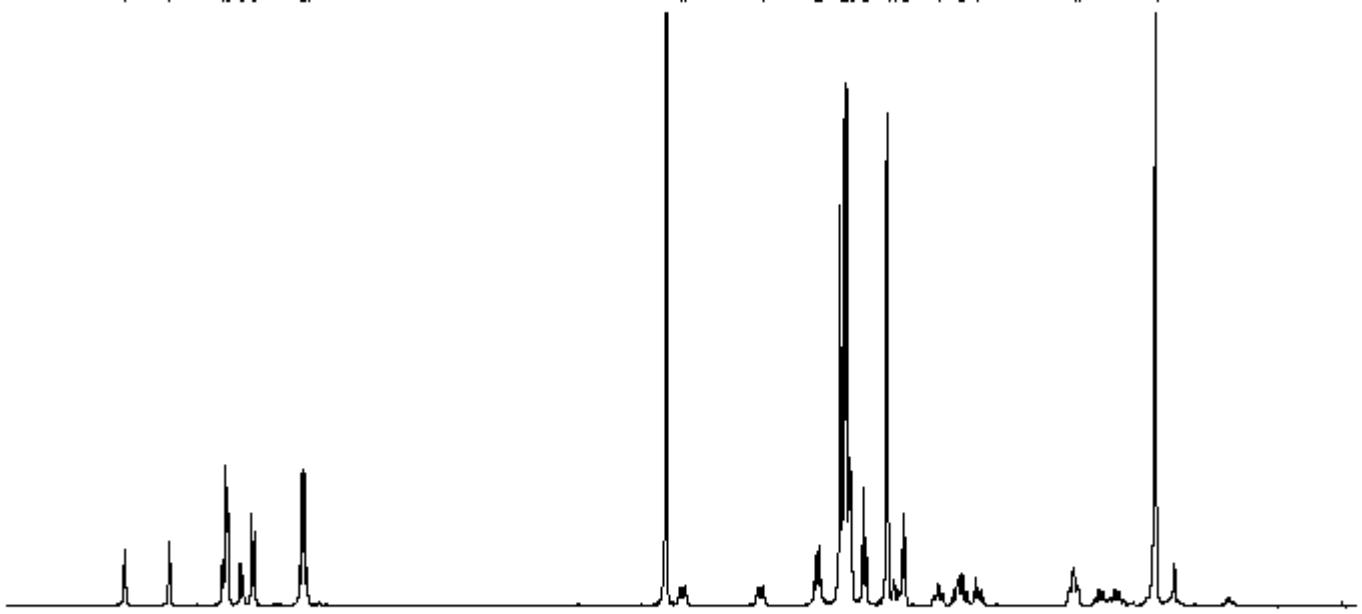
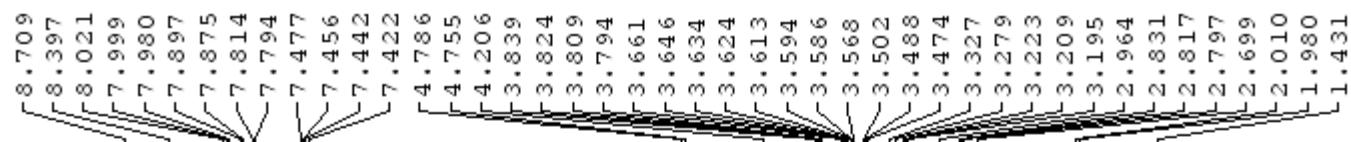
ijy-07dec17-v-48-2 226 (4.179) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
------	------------	-----	-----	-----	-------	---------

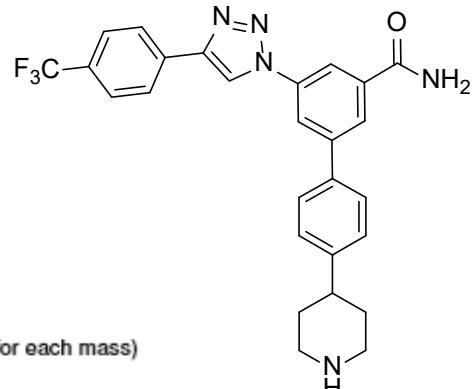
911.4300	911.4306	-0.6	-0.7	18.5	49.9	C49 H62 N2 O11 F3
	911.4247	5.3	5.8	27.5	179.5	C56 H58 N2 O6 F3
	911.4364	-6.4	-7.0	9.5	5.7	C42 H66 N2 O16 F3
	911.4212	8.8	9.7	5.5	34.8	C38 H66 N2 O19 F3
	911.4400	-10.0	-11.0	31.5	275.9	C60 H58 N2 O3 F3



0.90
0.94
4.03
0.97
2.00
2.04
1.97

0.90
0.89
2.08
21.72
2.07
0.79
1.89
0.86
0.86
0.86
9.03

4'-(Piperidin-4-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carboxamide (15)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

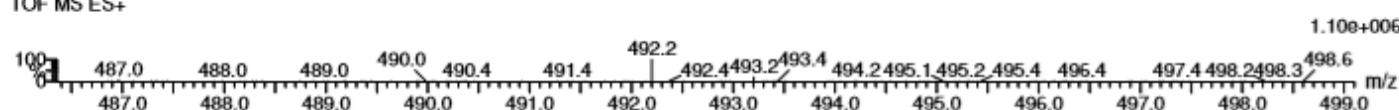
77 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 5-5 O: 0-50 F: 3-3

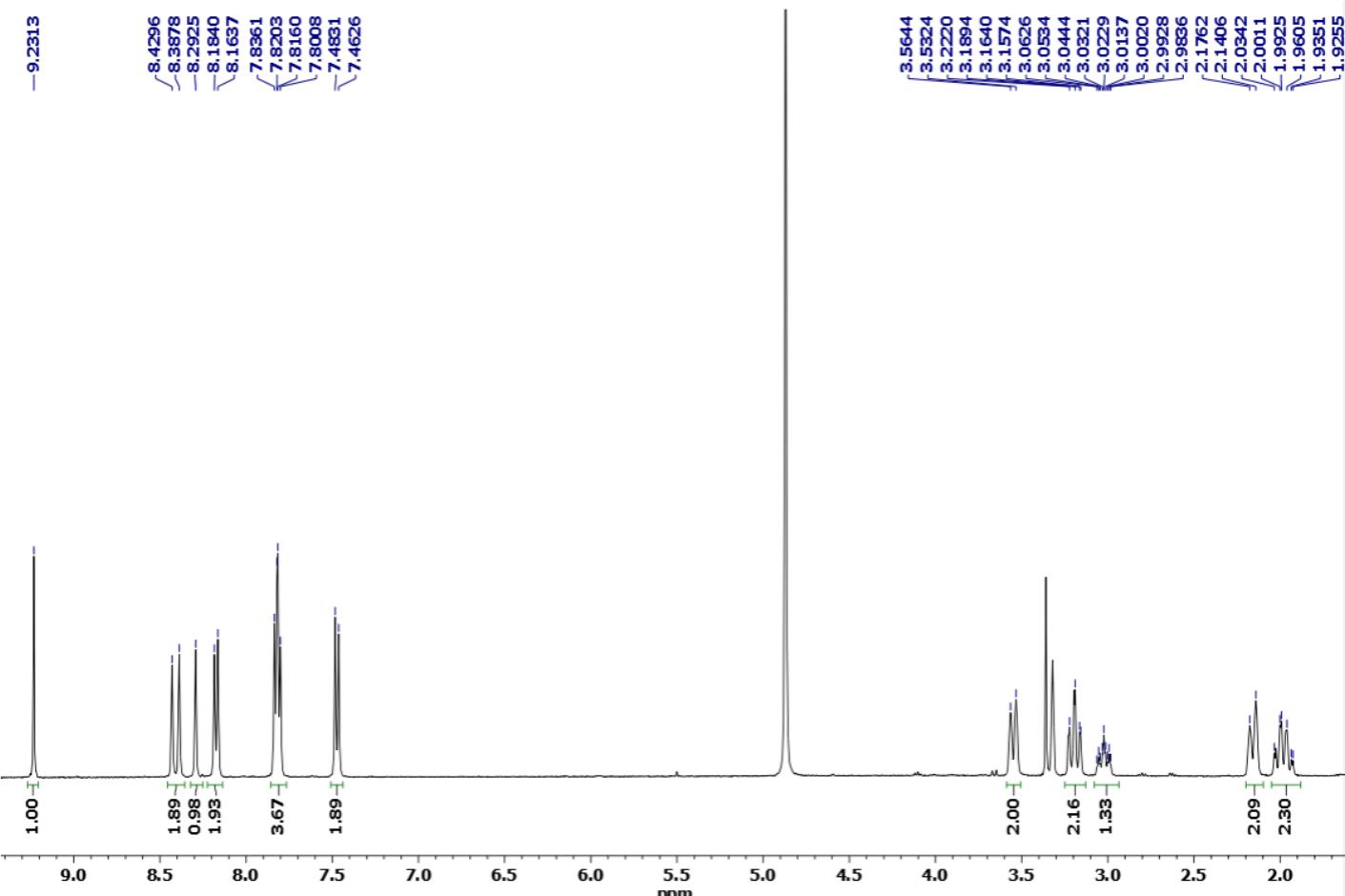
JYH-12APR18-025 137 (2.334) AM (Cen,5, 50.00, Ht,10000.0,0.00,0.70); Sm (SG, 1x2.00); Sb (15,10.00); Cm ((135+137))

TOF MS ES+

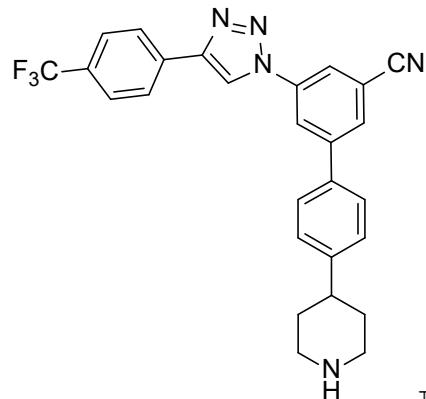


Minimum: -1.5
Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
492.2013	492.2011	0.2	0.4	16.5	258.0	2.166	11.46	C27 H25 N5 O F3
	492.2070	-5.7	-11.6	7.5	256.7	0.855	42.54	C20 H29 N5 O6 F3
	492.1917	9.6	19.5	3.5	256.6	0.777	46.00	C16 H29 N5 O9 F3



4'-(Piperidin-4-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carbonitrile (16)



Elemental Composition Report

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 19 closest results for each mass)

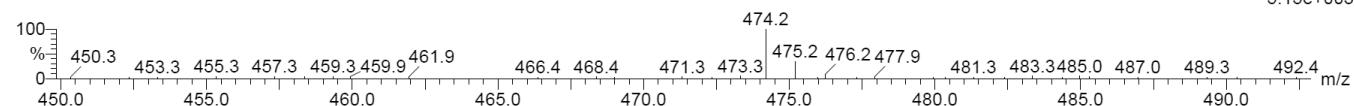
Elements Used:

C: 0-100 H: 0-200 N: 5-5 F: 3-3

08-Nov-2017

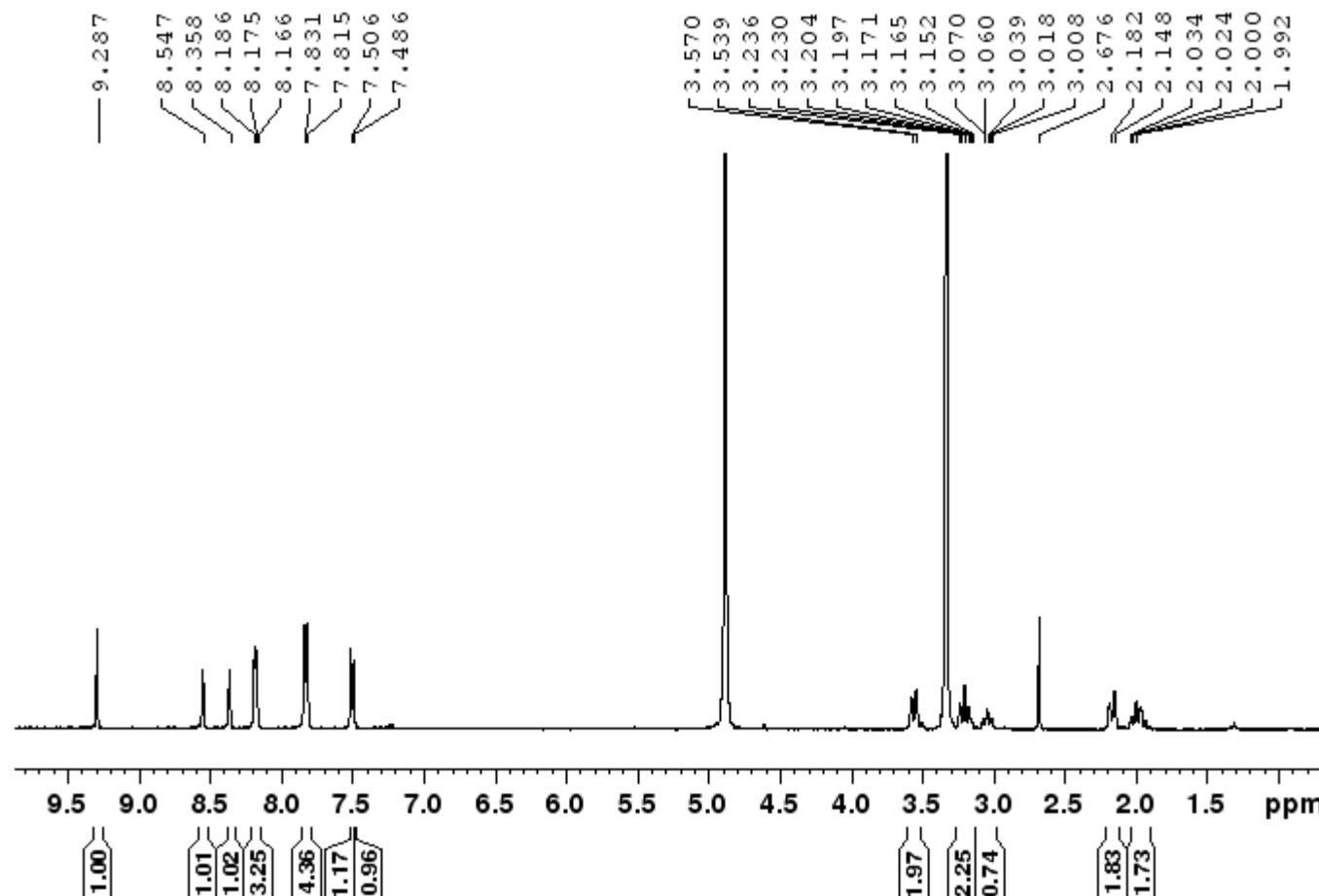
yj-08nov17-v-24 166 (3.070) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)

TOF MS ES+
5.15e+003



Minimum: -2.0
Maximum: 30.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
474.1912	474.1906	0.6	1.3	17.5	41.2	C27 H23 N5 F3



4-(4-(Quinuclidin-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoic acid (17)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

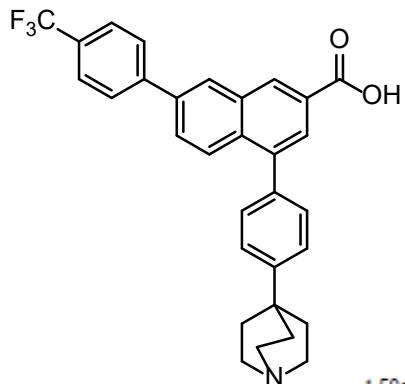
98 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

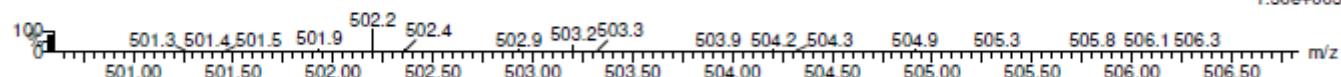
C: 0-100 H: 0-200 N: 1-1 O: 0-60 F: 3-3

JYH-15JAN19-170F 153 (2.605) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+

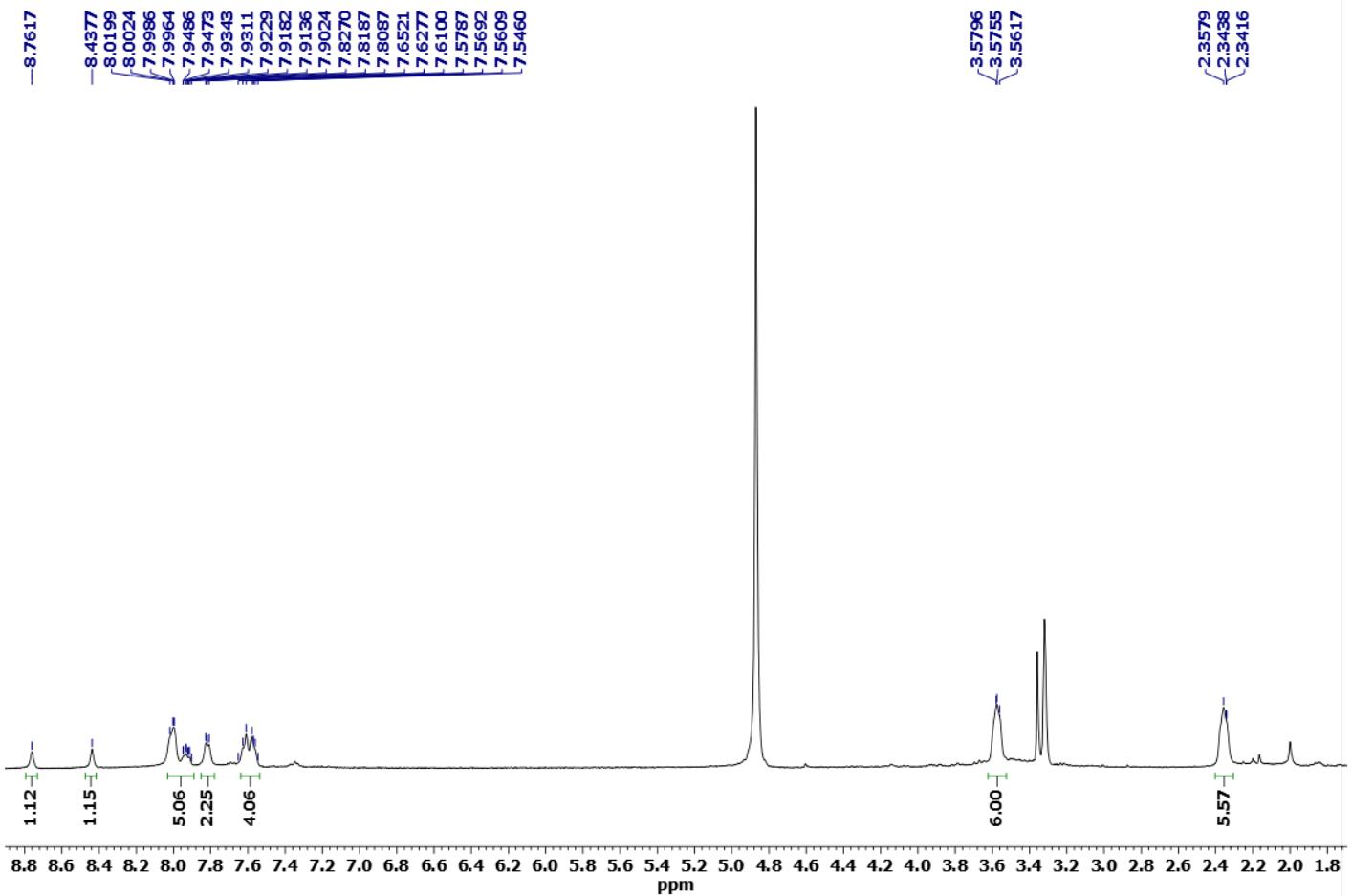


1.50e+005

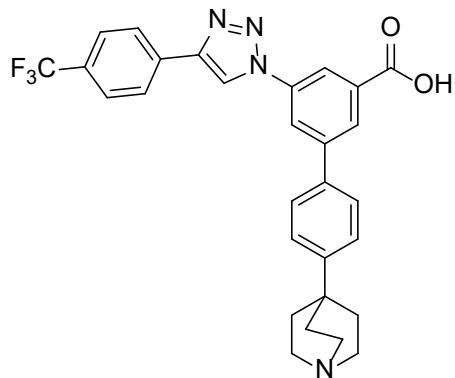


Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Norm	Conf (%)	Formula
502.1993	502.1994	-0.1	-0.2	17.5	359.0	n/a	n/a	C31 H27 N O2 F3



4'-(Quinuclidin-4-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carboxylic acid (**18**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

88 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

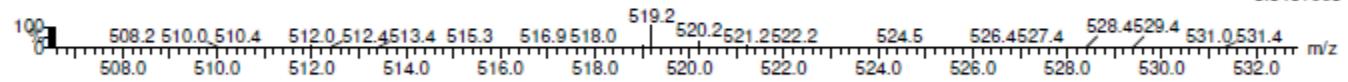
Elements Used:

C: 0-150 H: 0-200 N: 4-4 O: 0-60 F: 3-3

JYH-28MAR19-200 101 (1.725) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+

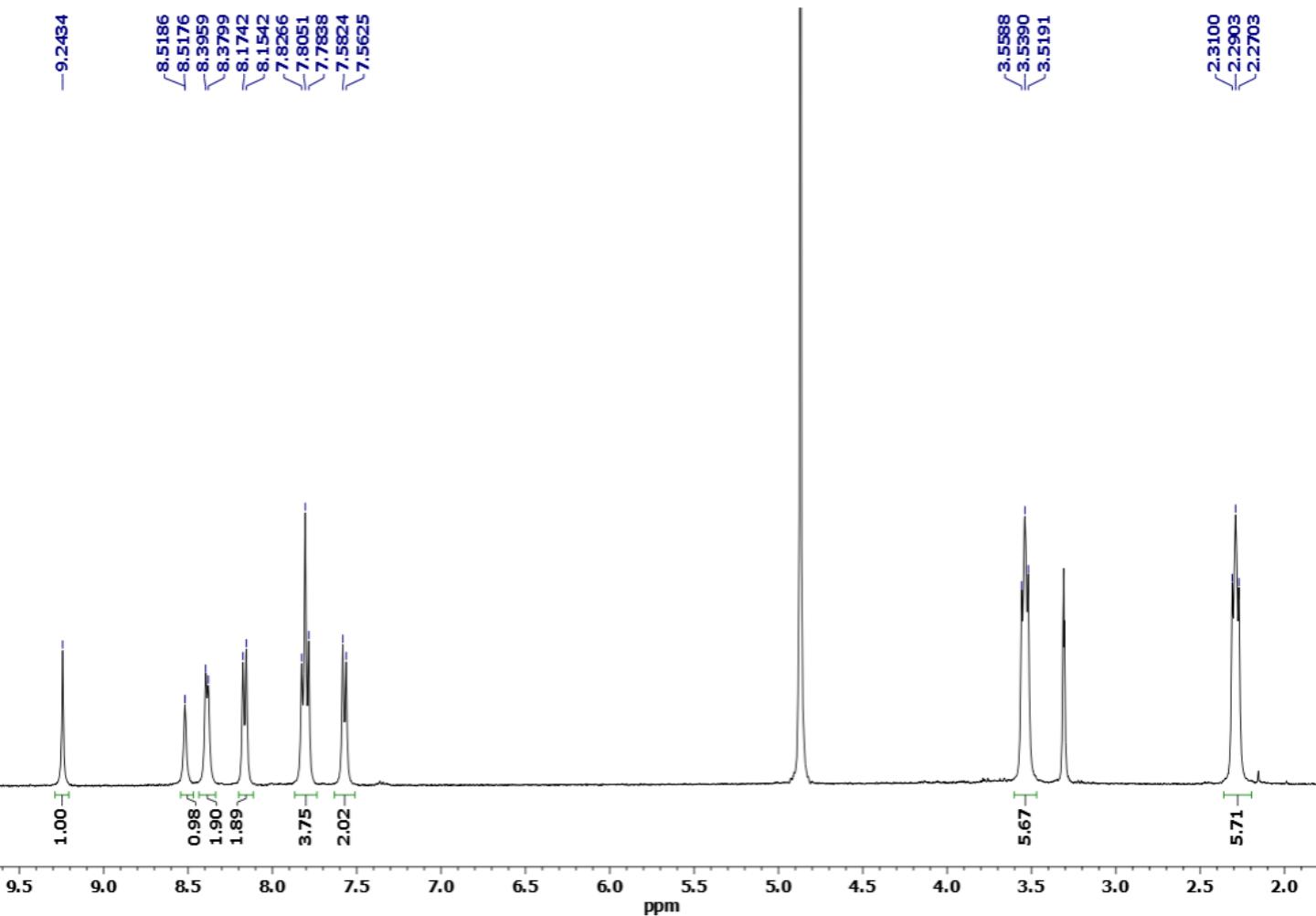
5.64e+005



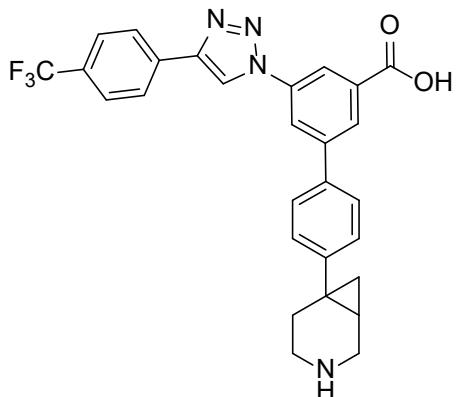
Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

519.2013	519.2008	0.5	1.0	17.5	429.5	n/a	n/a	C ₂₉ H ₂₆ N ₄ O ₂ F ₃
----------	----------	-----	-----	------	-------	-----	-----	--



4'-(3-Azabicyclo[4.1.0]heptan-6-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carboxylic acid (**19**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

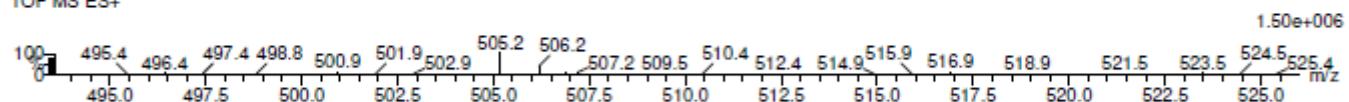
87 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-110 H: 0-200 N: 4-4 O: 0-40 F: 3-3

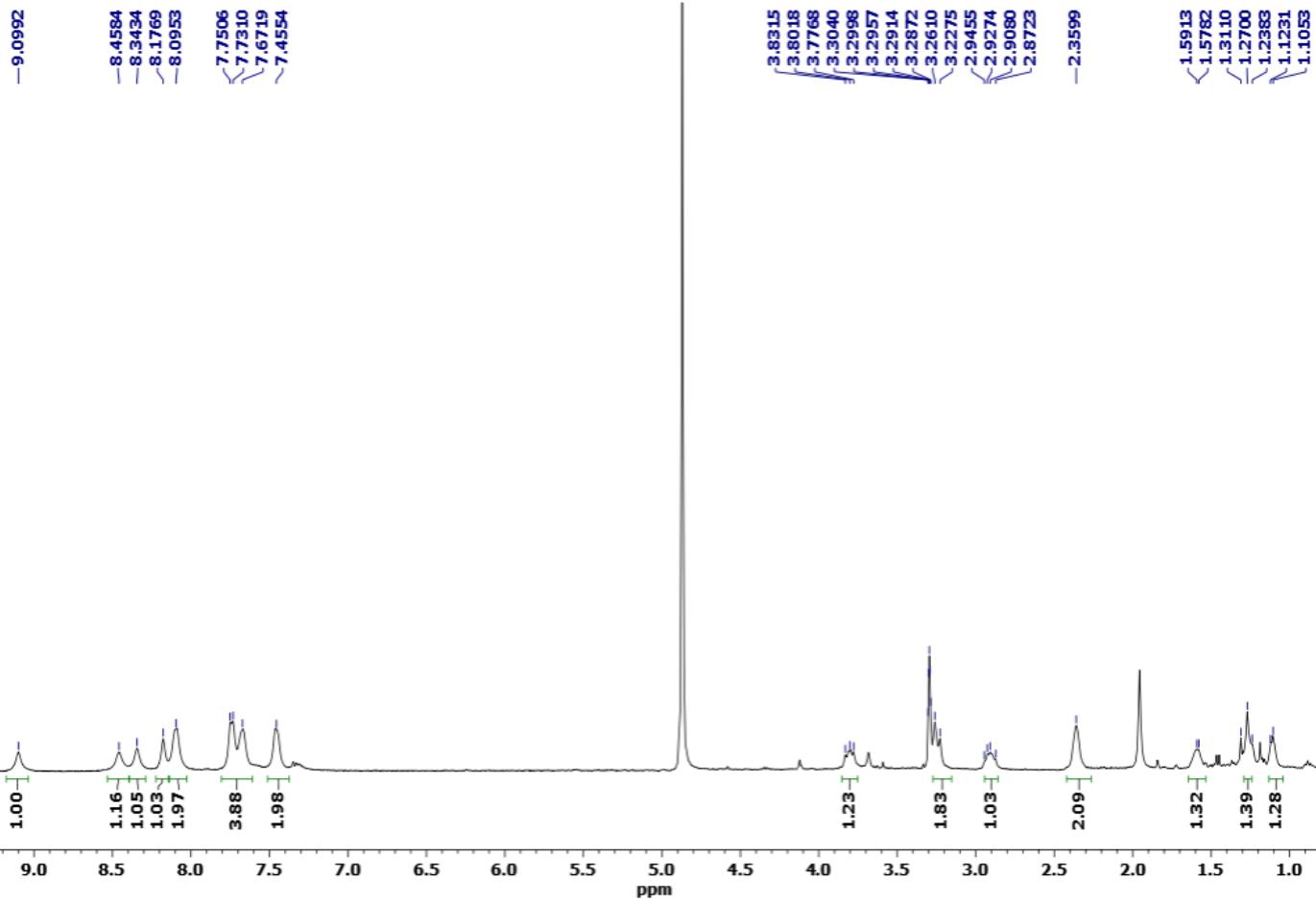
JYH-23JAN19-175-1 125 (2.131) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+

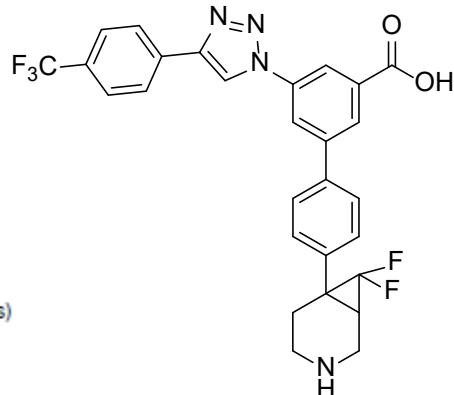


Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
505.1848	505.1851	-0.3	-0.6	17.5	519.3	n/a	n/a	C28 H24 N4 O2 F3



4'-(7,7-Difluoro-3-azabicyclo[4.1.0]heptan-6-yl)-5-(4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)-[1,1'-biphenyl]-3-carboxylic acid (**20**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

79 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

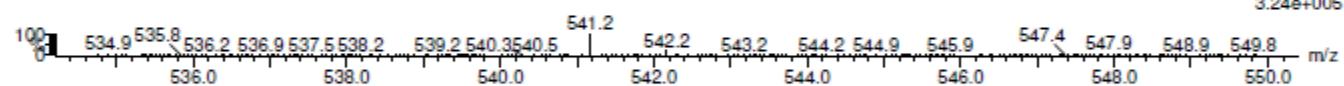
Elements Used:

C: 0-100 H: 0-200 N: 4-4 O: 0-60 F: 5-5

JYH-28FEB19-190 384 (6.513) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+

3.24e+005



Minimum: -1.5
Maximum: 20.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

541.1668	541.1663	0.5	0.9	17.5	354.4	2.369	9.35	C ₂₈ H ₂₂ N ₄ O ₂ F ₅
	541.1722	-5.4	-10.0	8.5	353.0	1.052	34.93	C ₂₁ H ₂₆ N ₄ O ₇ F ₅
	541.1569	9.9	18.3	4.5	353.1	1.073	34.21	C ₁₇ H ₂₆ N ₄ O ₁₀ F ₅
	541.1780	-11.2	-20.7	-0.5	354.1	2.133	11.84	C ₁₄ H ₃₀ N ₄ O ₁₂ F ₅
	541.1510	15.8	29.2	13.5	354.3	2.337	9.66	C ₂₄ H ₂₂ N ₄ O ₅ F ₅

9.1915
8.5057
8.3615
8.3168
8.1425
8.1280
<7.7783
<7.7777
<7.7572
<7.5850
<7.5664
3.9519
3.9221
3.8932
3.7350
3.4194
3.3852
3.0099
2.6332
2.5964
2.5151
2.2851

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

—

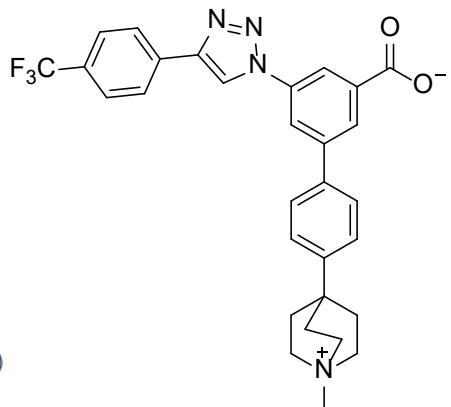
—

—

—

—

4-(4-(1-methylquinuclidin-1-i um-4-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-2-naphthoate
(21)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

99 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

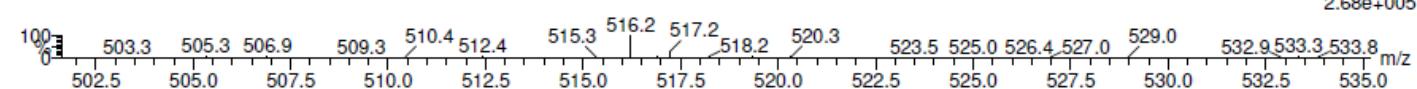
Elements Used:

C: 0-100 H: 0-250 N: 1-1 O: 0-60 F: 3-3

JYH-03MAY19-MRS-4616-HPLC 131 (2.233) AM2 (Ar,25000.0,0.00,0.00); ABS

TOF MS ES+

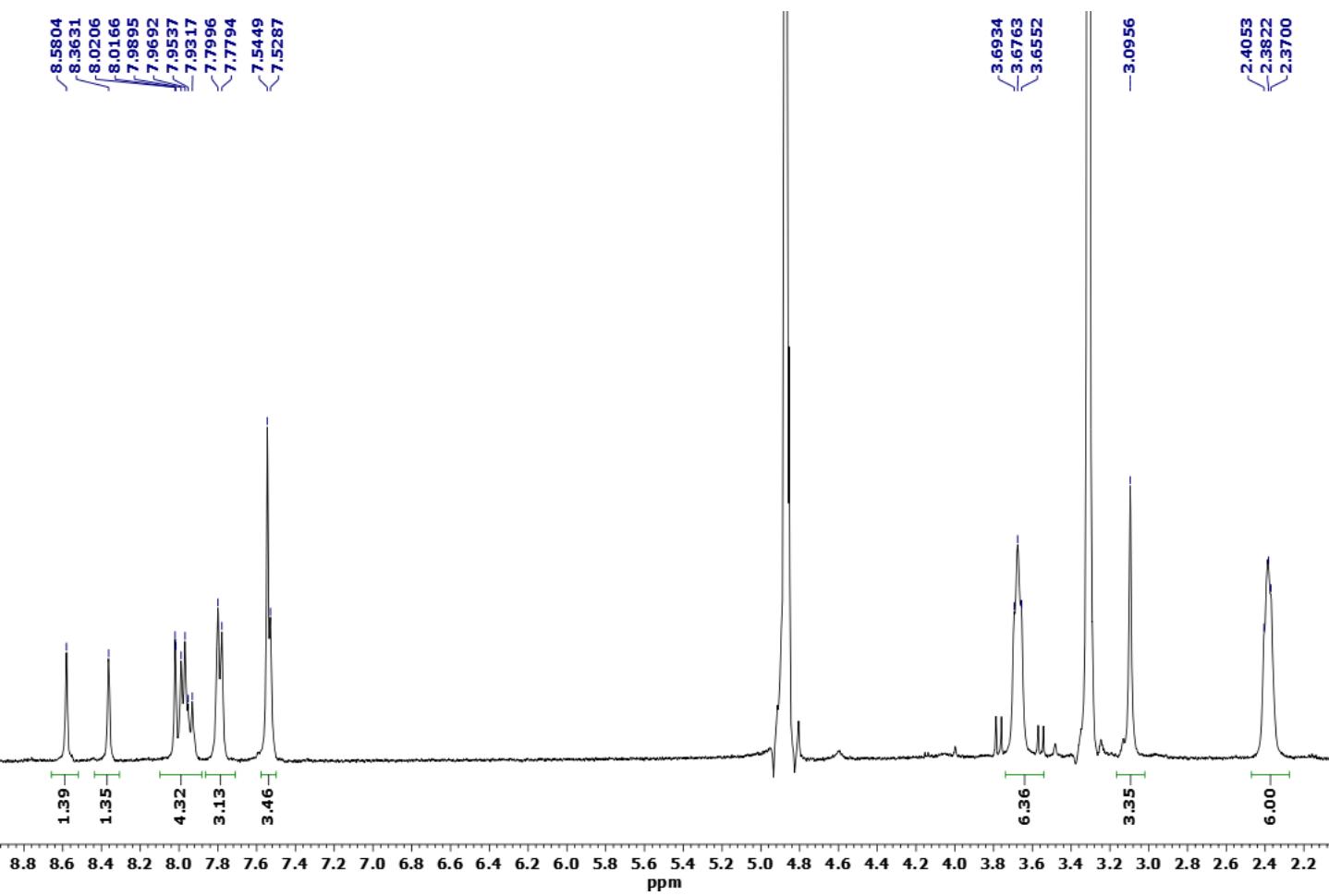
2.68e+005



Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

516.2159	516.2150	0.9	1.7	17.5	379.8	n/a	n/a	C32 H29 N O2 F3
----------	----------	-----	-----	------	-------	-----	-----	-----------------



4'-Carbamoyl-5-(1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)-[1,1'-biphenyl]-3-carboxylic acid (24)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

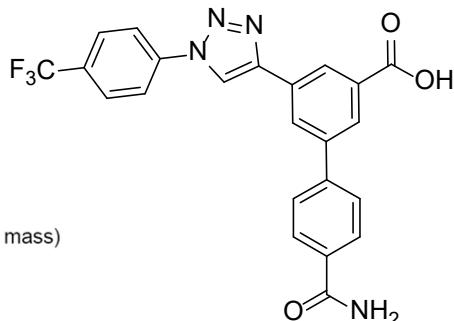
71 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

Elements Used:

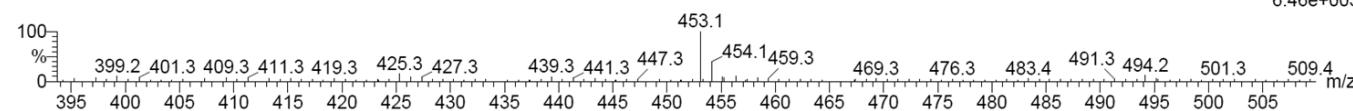
C: 0-100 H: 0-200 N: 4-4 O: 0-40 F: 3-3

02-Aug-2017

yj-02aug17-iv-43 158 (2.922) Cn (Cen,5, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

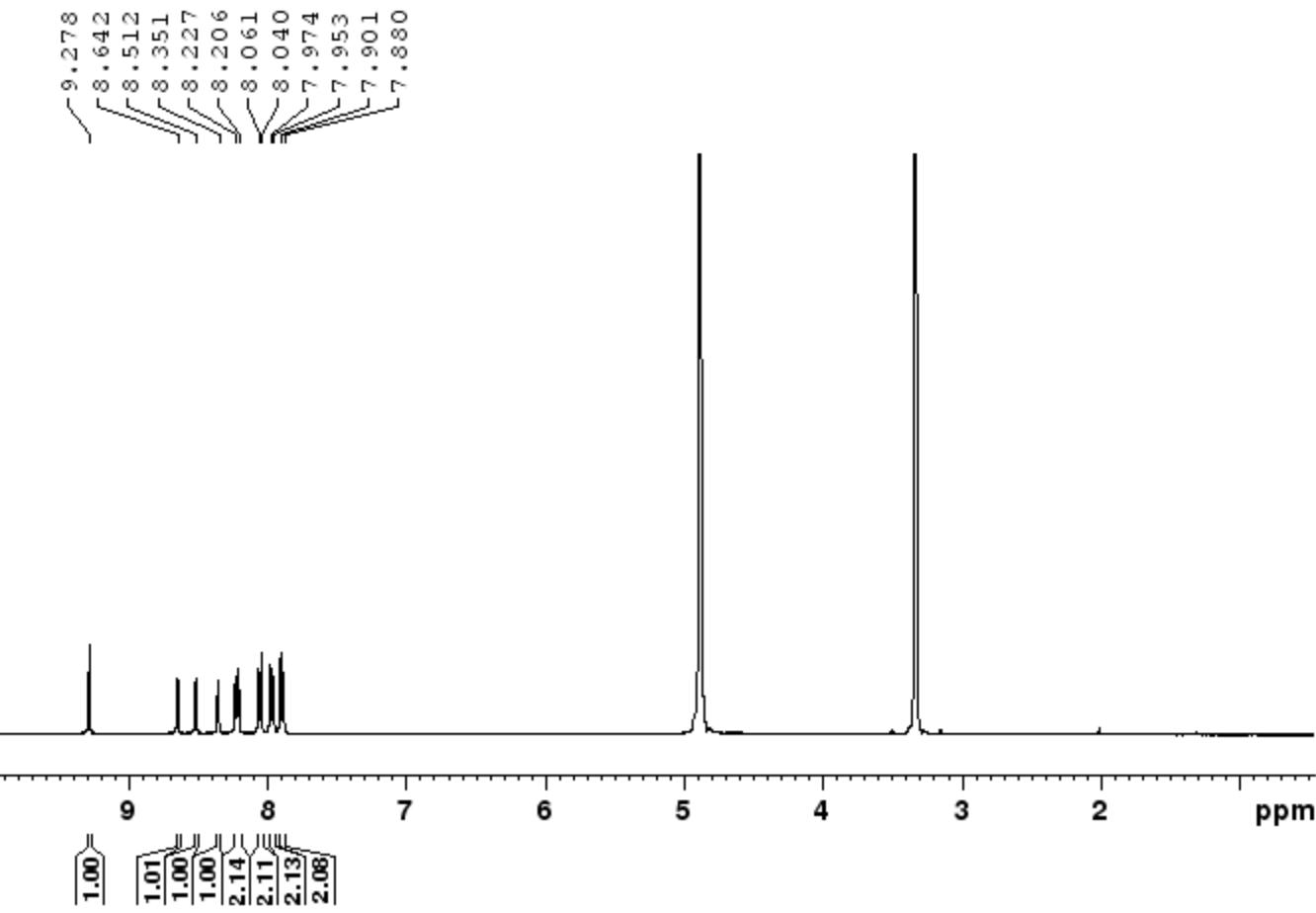


TOF MS ES+
6.46e+003



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
453.1169	453.1175	-0.6	-1.3	16.5	155.1	C23	H16	N4	O3	F3	
	453.1233	-6.4	-14.1	7.5	364.0	C16	H20	N4	O8	F3	
	453.1081	8.8	19.4	3.5	541.6	C12	H20	N4	O11	F3	



4'-(Piperidin-4-yl)-5-(1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)-[1,1'-biphenyl]-3-carboxylic acid (**25**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

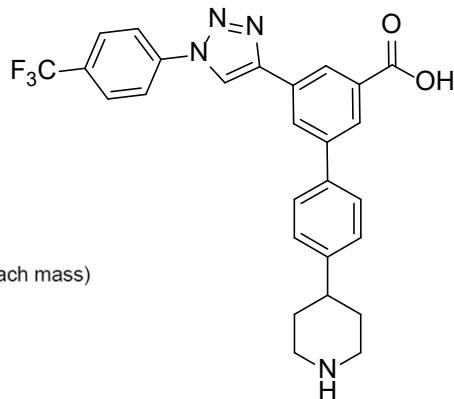
84 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

Elements Used:

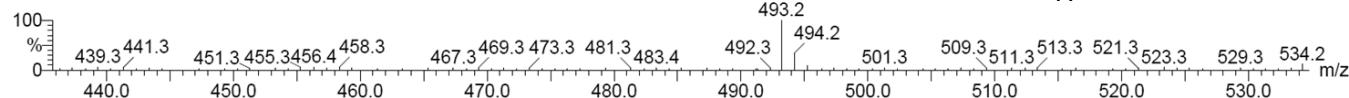
C: 0-100 H: 0-200 N: 4-4 O: 0-40 F: 3-3

25-Jul-2017

yj-25Jul17-iv-29-2 118 (2.182) Cn (Cen,5, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5,00)

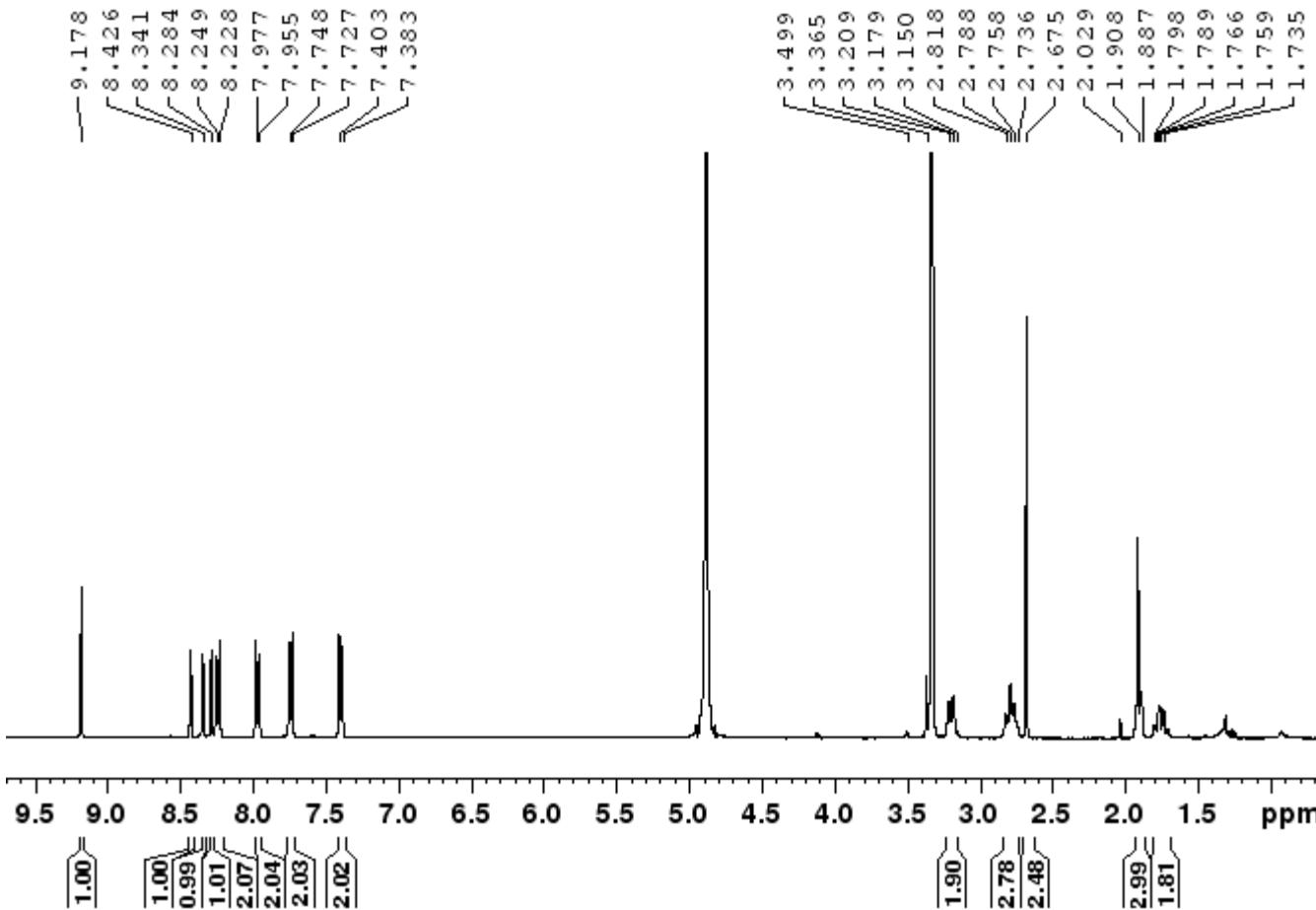


TOF MS ES+
8.33e+003

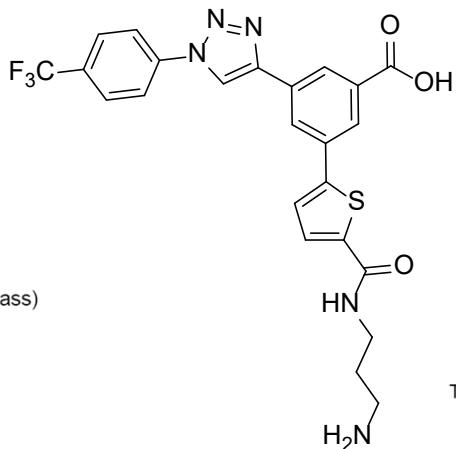


Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
493.1856	493.1851	0.5	1.0	16.5	55.9	C27 H24 N4 O2 F3
	493.1910	-5.4	-10.9	7.5	168.1	C20 H28 N4 O7 F3



3-((3-Aminopropyl)carbamoyl)thiophen-2-yl)-5-(1-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-4-yl)benzoic acid (**26**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

76 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

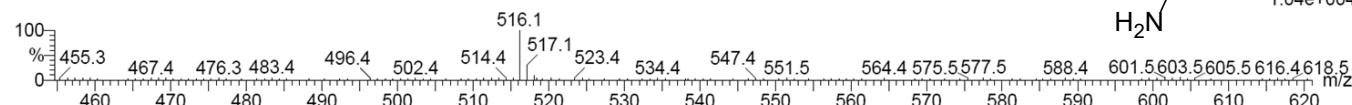
Elements Used:

C: 0-100 H: 0-200 N: 5-5 O: 0-40 F: 3-3 32S: 1-1

02-Aug-2017

yj-02aug17-iv-41-2 102 (1.886) Cn (Cen,5, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)

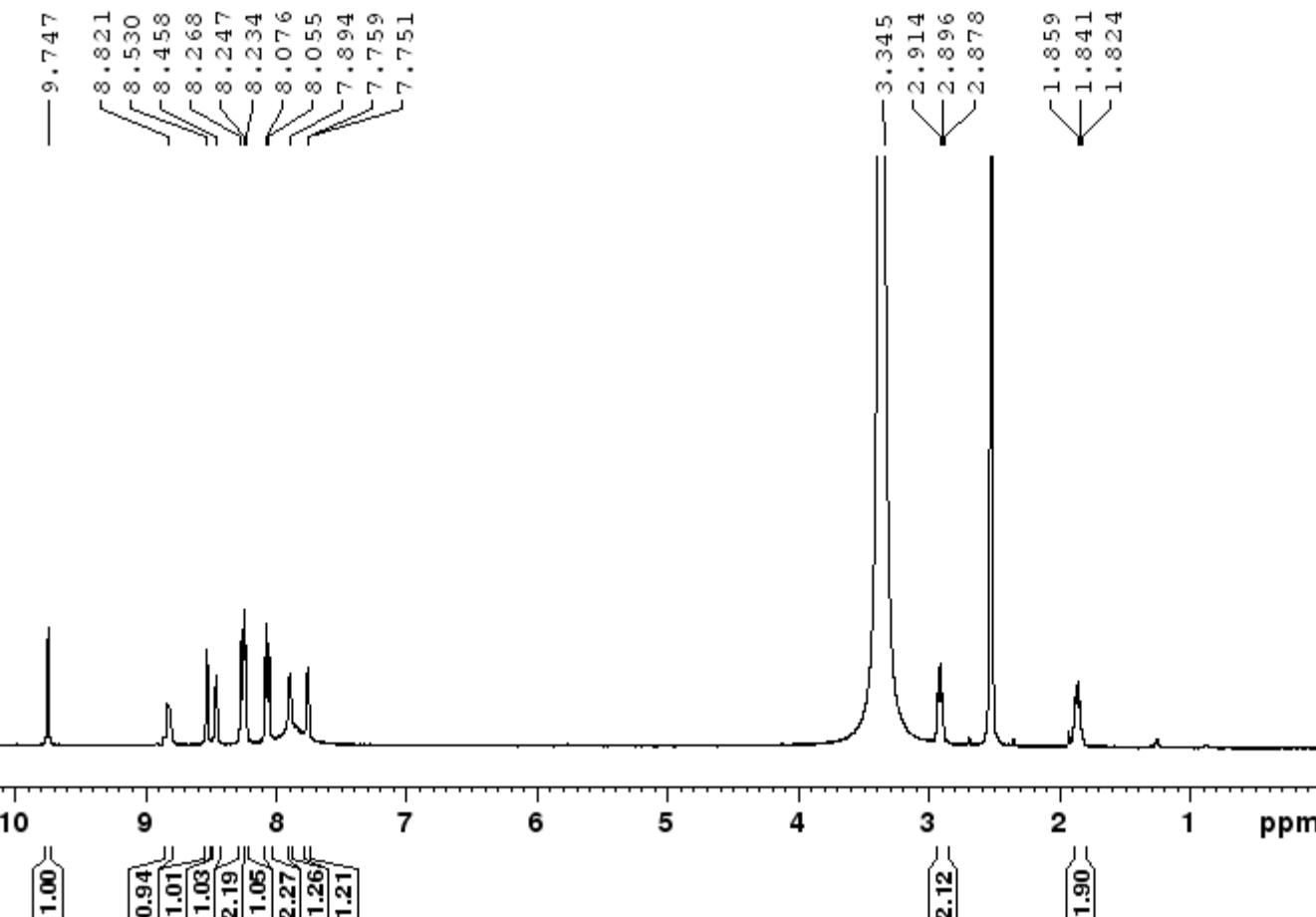
TOF MS ES+
1.04e+004



Minimum: -2.0
Maximum: 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
------	------------	-----	-----	-----	-------	---------

516.1316	516.1317	-0.1	-0.2	15.5	127.7	C24 H21 N5 O3 F3 32S
	516.1376	-6.0	-11.6	6.5	279.5	C17 H25 N5 O8 F3 32S
	516.1223	9.3	18.0	2.5	465.8	C13 H25 N5 O11 F3 32S



4'-carbamoyl-5-(4-(trifluoromethyl)benzamido)-[1,1'-biphenyl]-3-carboxylic acid (27)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

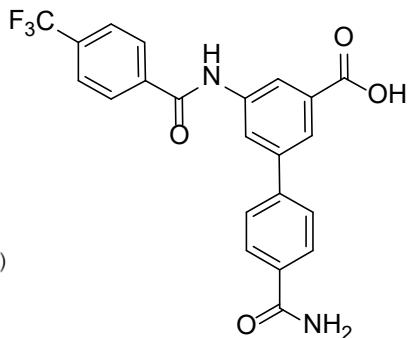
68 formula(e) evaluated with 2 results within limits (up to 19 closest results for each mass)

Elements Used:

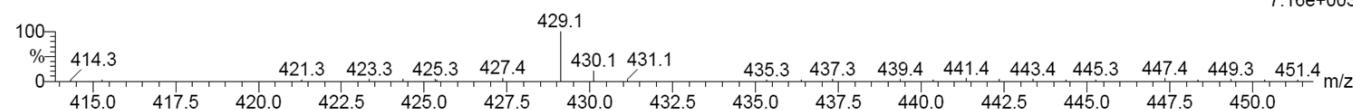
C: 0-90 H: 0-200 N: 2-2 O: 0-20 F: 3-3

18-Oct-2017

yj-18oct17-v-01 126 (2.330) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)

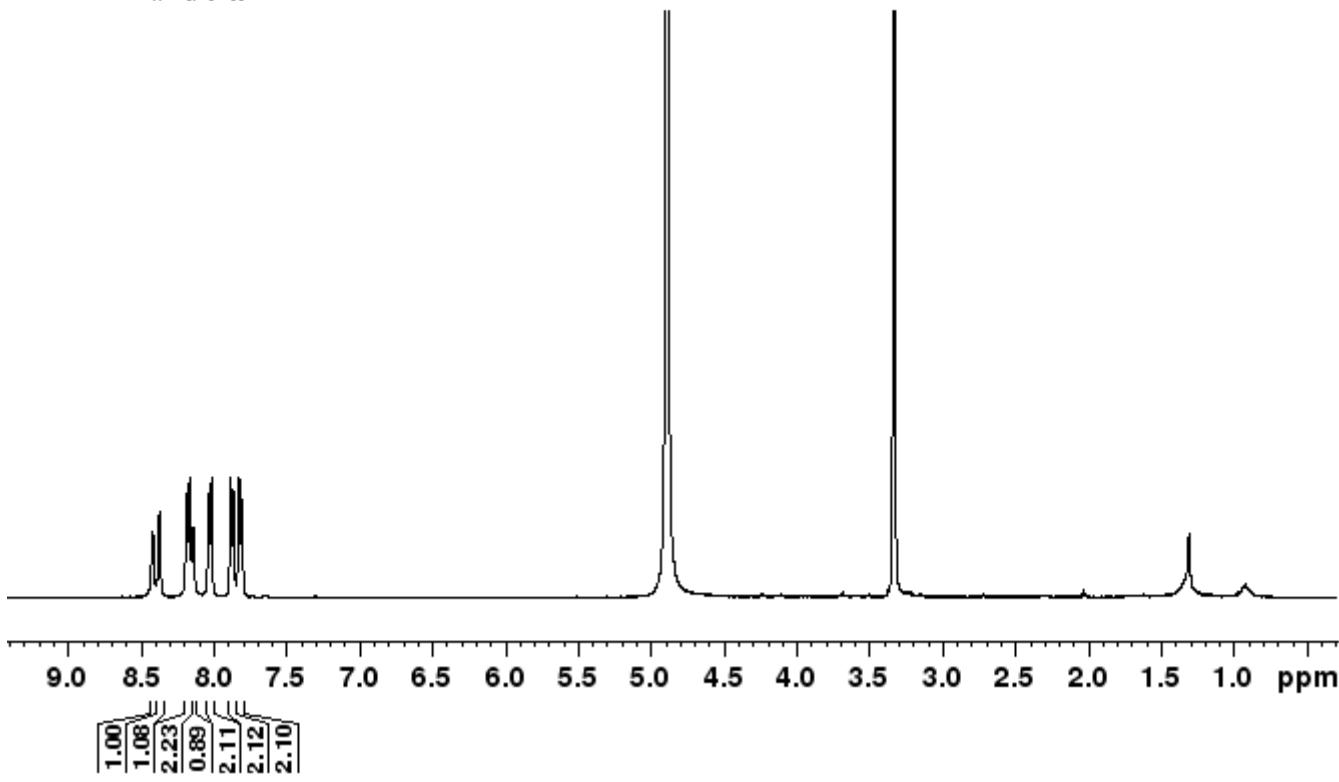
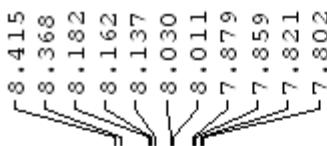


TOF MS ES+
7.16e+003

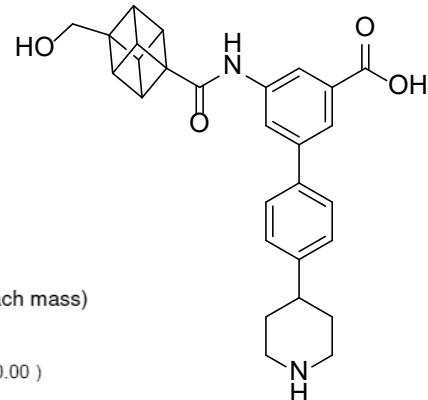


Minimum: -2.0
Maximum: 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
429.1069	429.1062	0.7	1.6	14.5	49.1	C22 H16 N2 O4 F3
	429.1121	-5.2	-12.1	5.5	13.4	C15 H20 N2 O9 F3



5-(4-(Hydroxymethyl)cubane-1-carboxamido)-4'-(piperidin-4-yl)-[1,1'-biphenyl]-3-carboxylic acid (**28**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

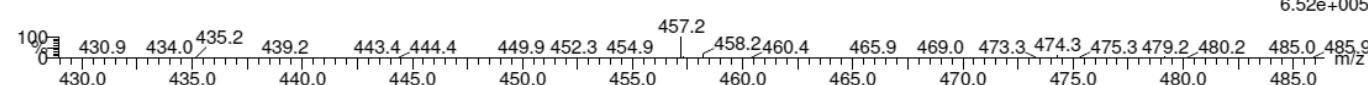
100 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-110 H: 0-300 N: 2-2 O: 0-65

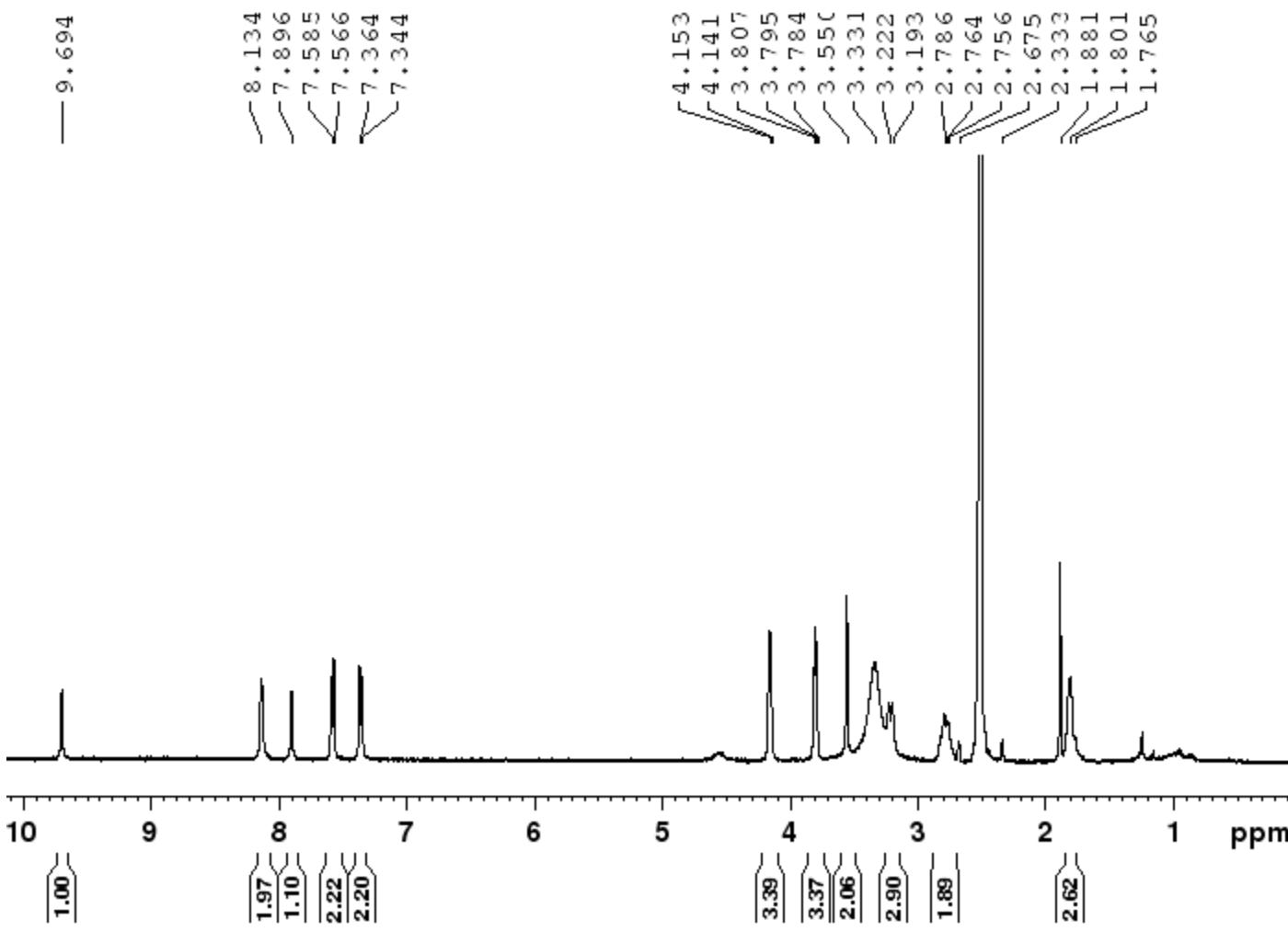
YJ-05FEB18-V-38-126 (2.148) AM (Cen.5, 50.00, Ht.10000.0.0.00,0.70); Sm (SG, 1x2.00); Sb (15.10.00)

TOF MS ES+ 86

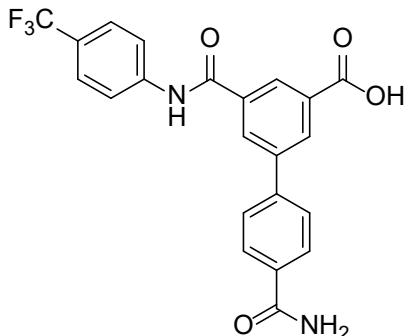


Minimum: -1.5
Maximum: 10.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
457.2129	457.2127	0.2	0.4	15.5	330.0	0.919	39.88	C28 H29 N2 O4
	457.2186	-5.7	-12.5	6.5	329.8	0.712	49.06	C21 H33 N2 O9
	457.2033	9.6	21.0	2.5	331.3	2.202	11.06	C17 H33 N2 O12



4'-Carbamoyl-5-((4-(trifluoromethyl)phenyl)carbamoyl)-[1,1'-biphenyl]-3-carboxylic acid (**29**)



Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

68 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

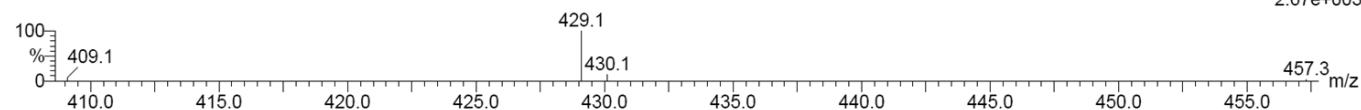
Elements Used:

C: 0-100 H: 0-200 N: 2-2 O: 0-20 F: 3-3

27-Nov-2017

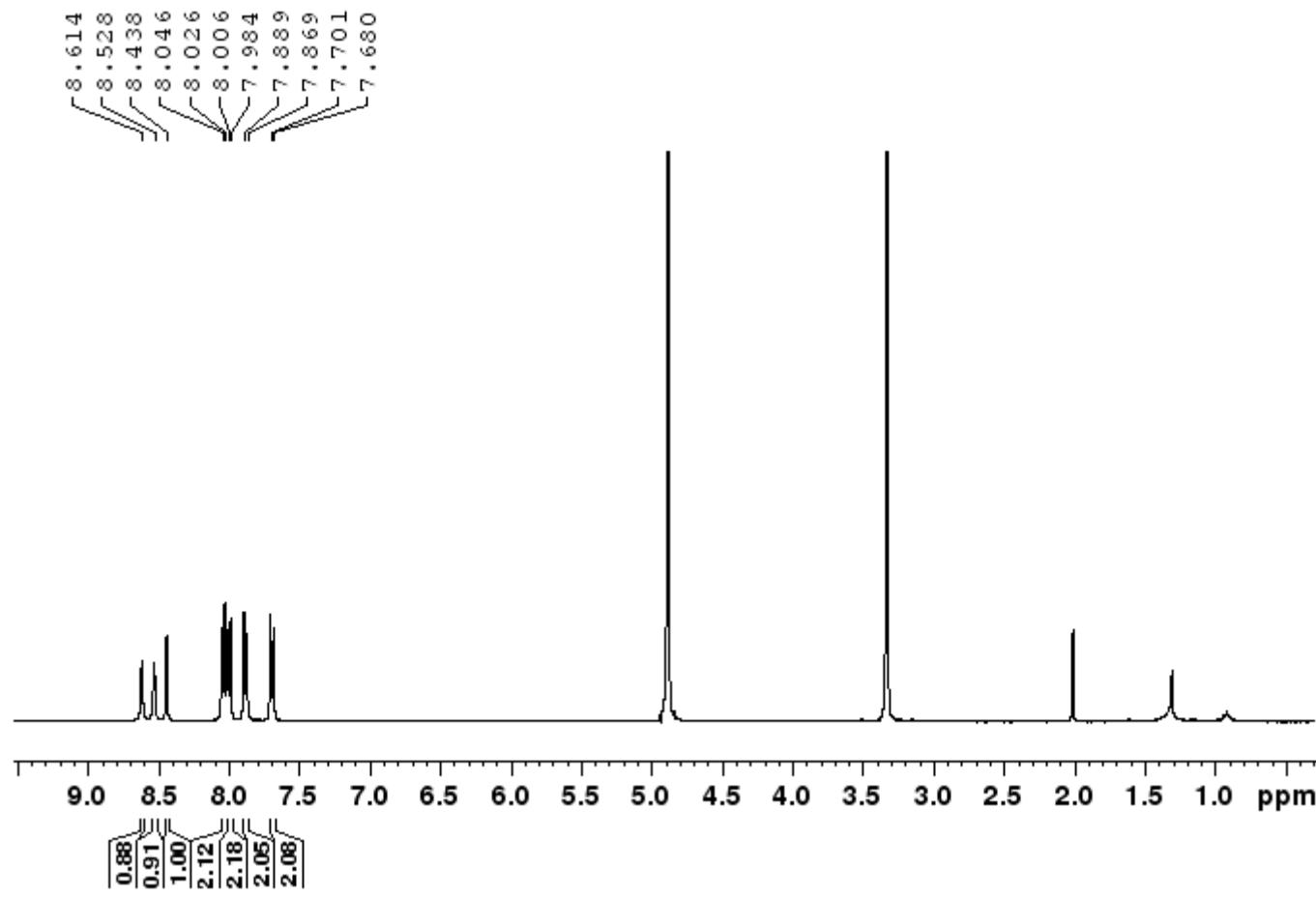
yj-27nov17-v-40 88 (1.627) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5,00); Cm (88-22x10.000)

TOF MS ES+
2.67e+003



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
429.1065	429.1062	0.3	0.7	14.5	n/a	C22 H16 N2 O4 F3
	429.1121	-5.6	-13.1	5.5	n/a	C15 H20 N2 O9 F3
	429.0968	9.7	22.6	1.5	n/a	C11 H20 N2 O12 F3



4'-Carbamoyl-5-(5-(trifluoromethyl)-1H-indol-2-yl)-[1,1'-biphenyl]-3-carboxylic acid (**30**)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

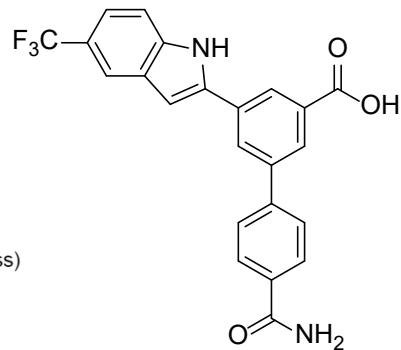
67 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

Elements Used:

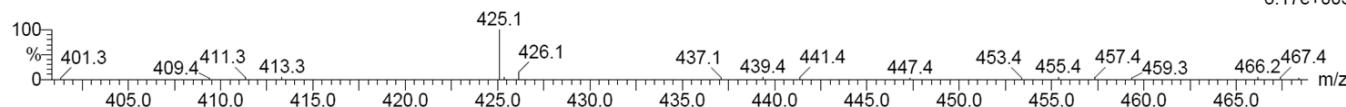
C: 0-90 H: 0-200 N: 2-2 O: 0-20 F: 3-3

23-Oct-2017

yj-23oct17-v-11 79 (1.461) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

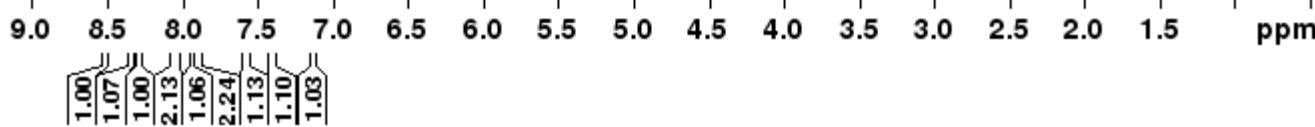
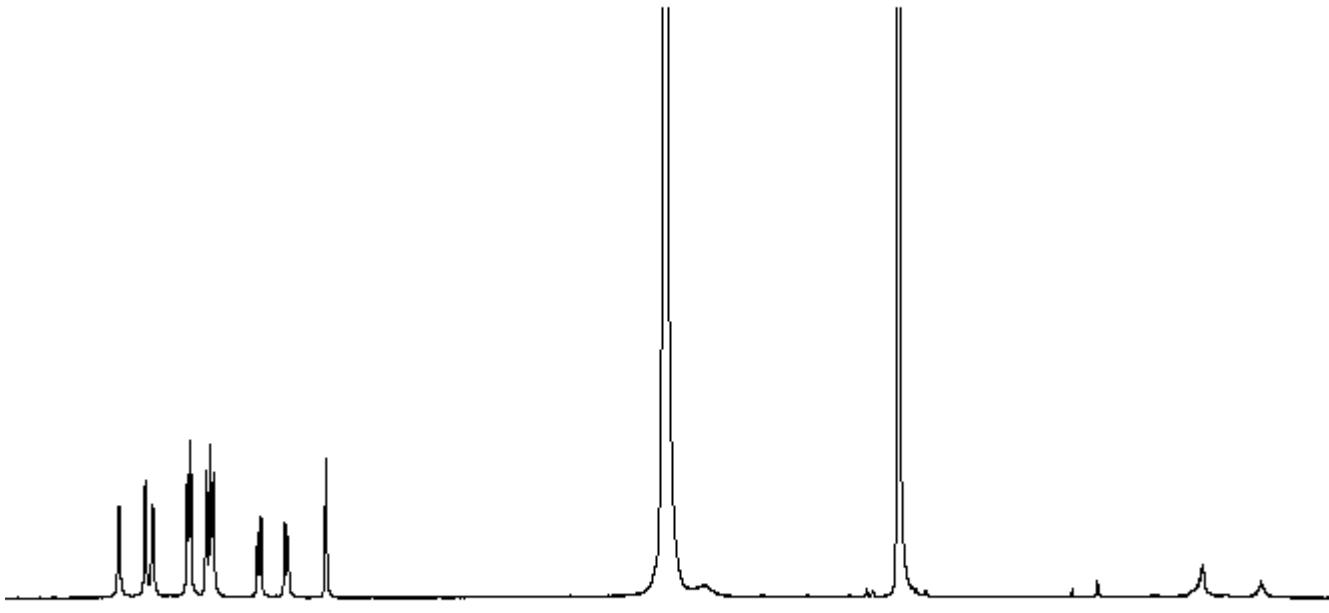
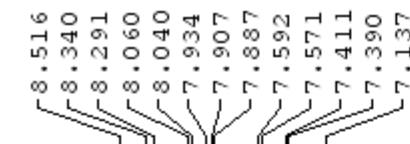


TOF MS ES+
8.17e+003



Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
425.1112	425.1113	-0.1	-0.2	15.5	n/a	C23 H16 N2 O3 F3
	425.1172	-6.0	-14.1	6.5	n/a	C16 H20 N2 O8 F3
	425.1019	9.3	21.9	2.5	n/a	C12 H20 N2 O11 F3



4'-Carbamoyl-5-(6-(trifluoromethyl)-1*H*-indol-2-yl)-[1,1'-biphenyl]-3-carboxylic acid (31)

Elemental Composition Report

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass. Even Electron Ions

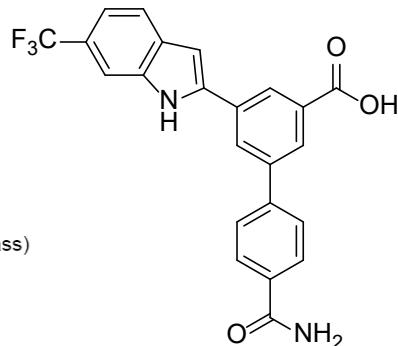
67 formula(e) evaluated with 9 results within limits (up to 19 closest results for each mass)

Elements Used:

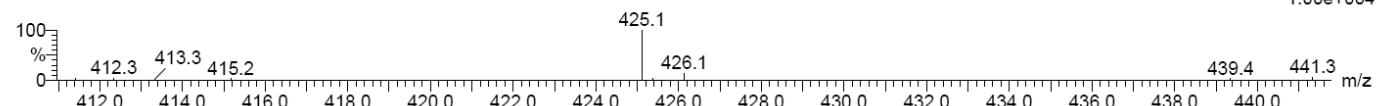
C: 0-100 H: 0-200 N: 2-2 O: 0-20 F: 3-3

15-Nov-2017

yj-15nov17-v-28 221 (4.087) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

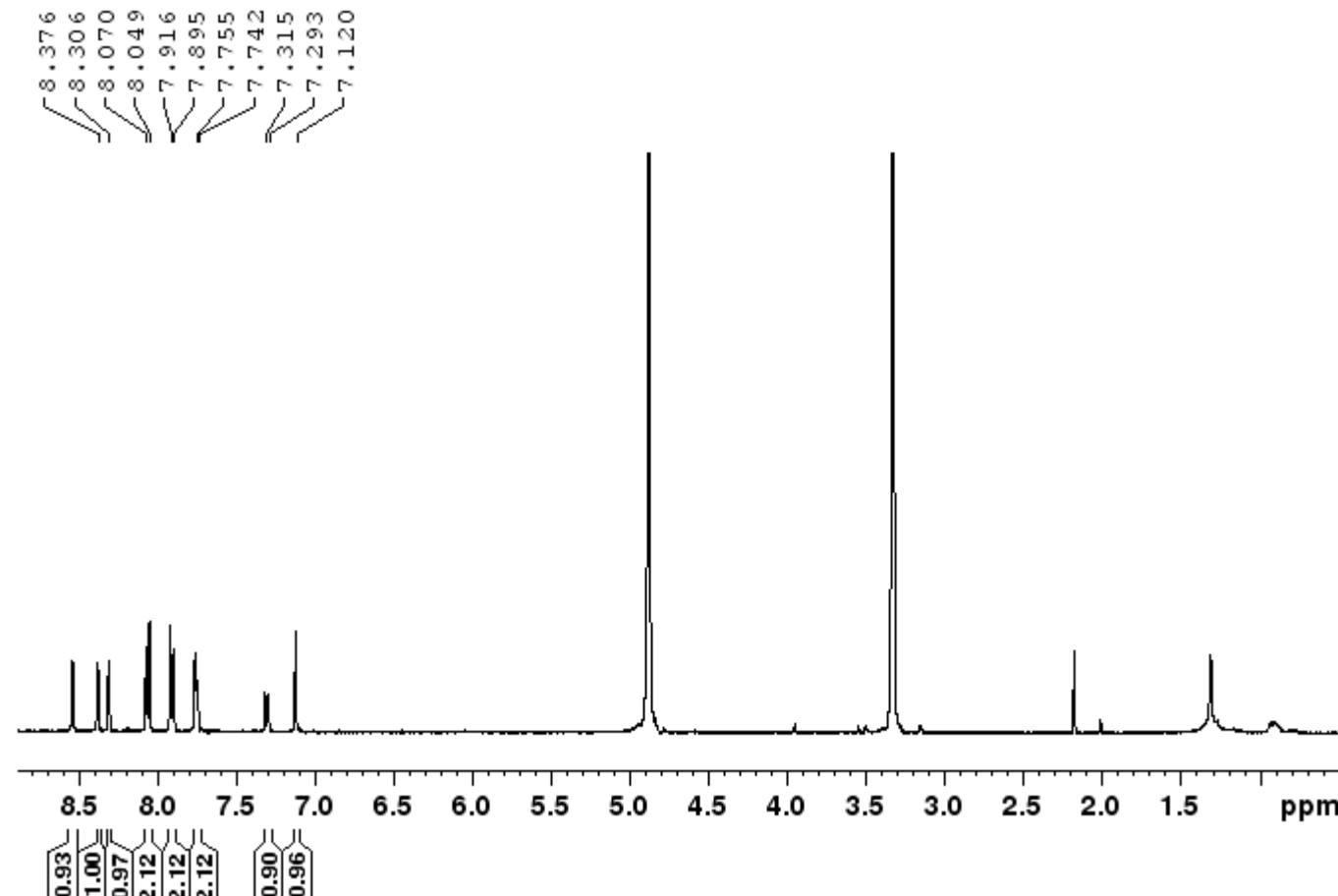


TOF MS ES+
1.00e+004



Minimum: -2.0
Maximum: 30.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
425.1108	425.1113	-0.5	-1.2	15.5	n/a	C23	H16	N2	O3	F3
	425.1172	-6.4	-15.1	6.5	n/a	C16	H20	N2	O8	F3
	425.1019	8.9	20.9	2.5	n/a	C12	H20	N2	O11	F3
	425.0960	14.8	34.8	11.5	n/a	C19	H16	N2	O6	F3
	425.1266	-15.8	-37.2	19.5	n/a	C27	H16	N2	F3	
	425.0902	20.6	48.5	20.5	n/a	C26	H12	N2	O	F3
	425.1324	-21.6	-50.8	10.5	n/a	C20	H20	N2	O5	F3
	425.0867	24.1	56.7	-1.5	n/a	C8	H20	N2	O14	F3
	425.1383	-27.5	-64.7	1.5	n/a	C13	H24	N2	O10	F3



4'-Carbamoyl-5-(5-(trifluoromethyl)-1*H*-benzo[d]imidazol-2-yl)-[1,1'-biphenyl]-3-carboxylic acid (32)

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

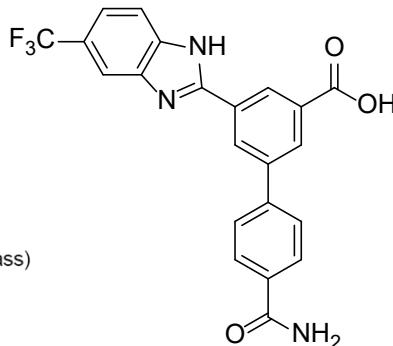
67 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

Elements Used:

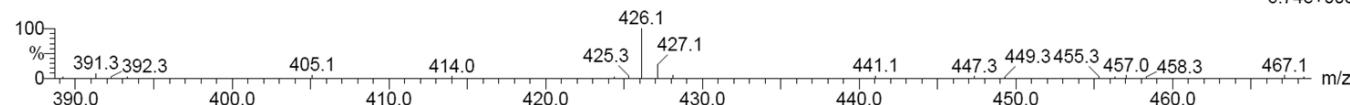
C: 0-100 H: 0-200 N: 3-3 O: 0-20 F: 3-3

02-Nov-2017

yj-02nov17-v-17 246 (4.549) Cn (Cen,3, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)

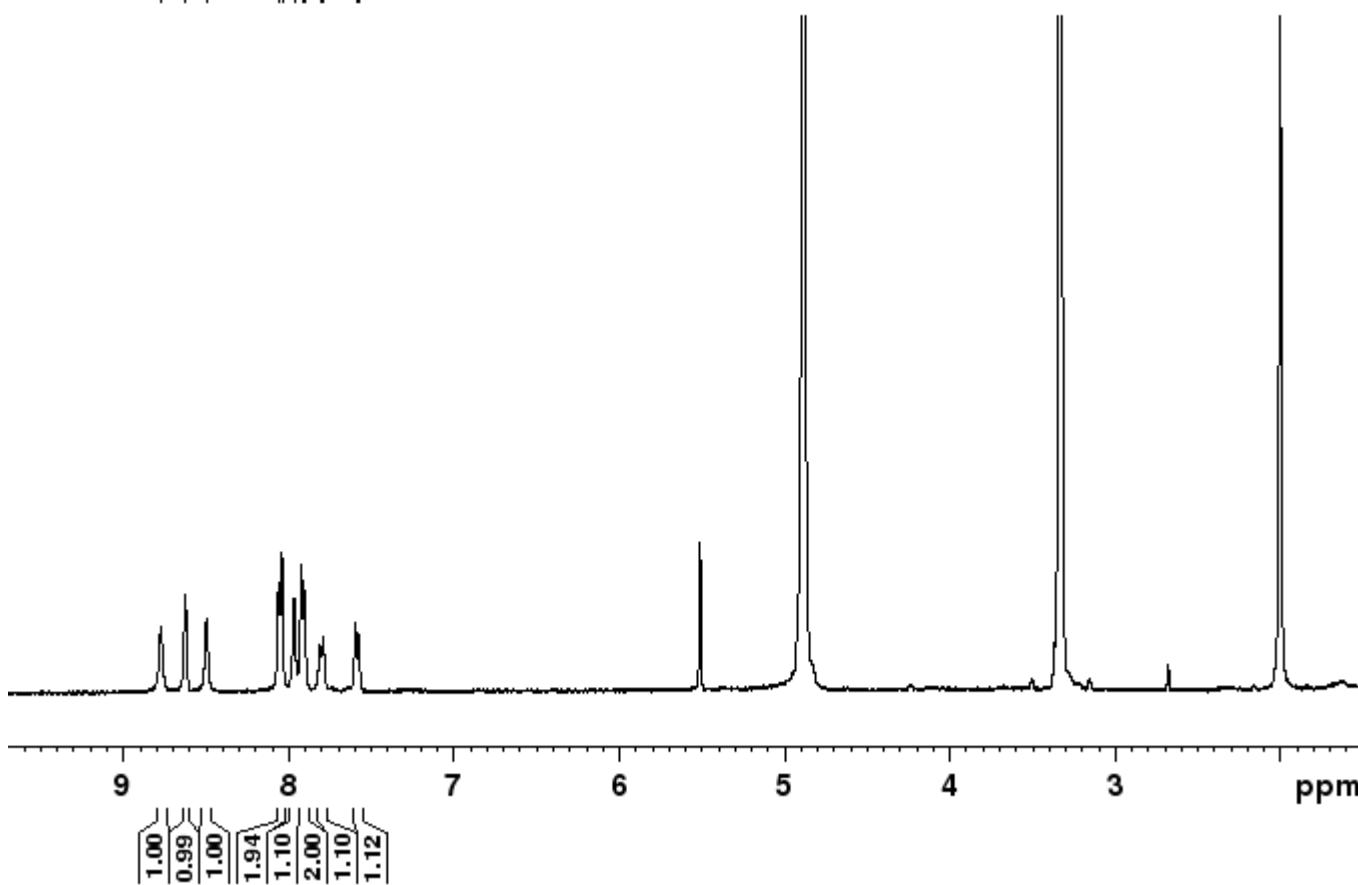


TOF MS ES+
6.74e+003

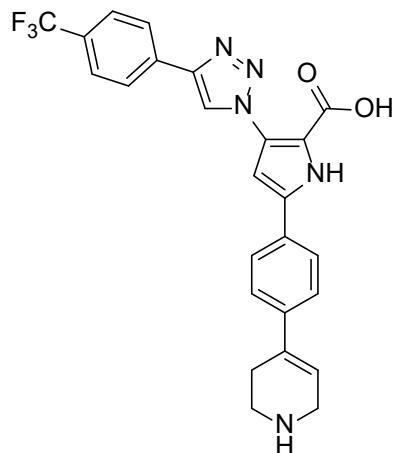


Minimum: -2.0
Maximum: 10.0 10.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.1063	426.1066	-0.3	-0.7	15.5	16.7	C22 H15 N3 O3 F3
	426.1124	-6.1	-14.3	6.5	94.6	C15 H19 N3 O8 F3
	426.0972	9.1	21.4	2.5	222.6	C11 H19 N3 O11 F3



5-(4-(1,2,3,6-Tetrahydropyridin-4-yl)phenyl)-3-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazol-1-yl)-1*H*-pyrrole-2-carboxylic acid (33)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

73 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 5-5 O: 0-60 F: 3-3

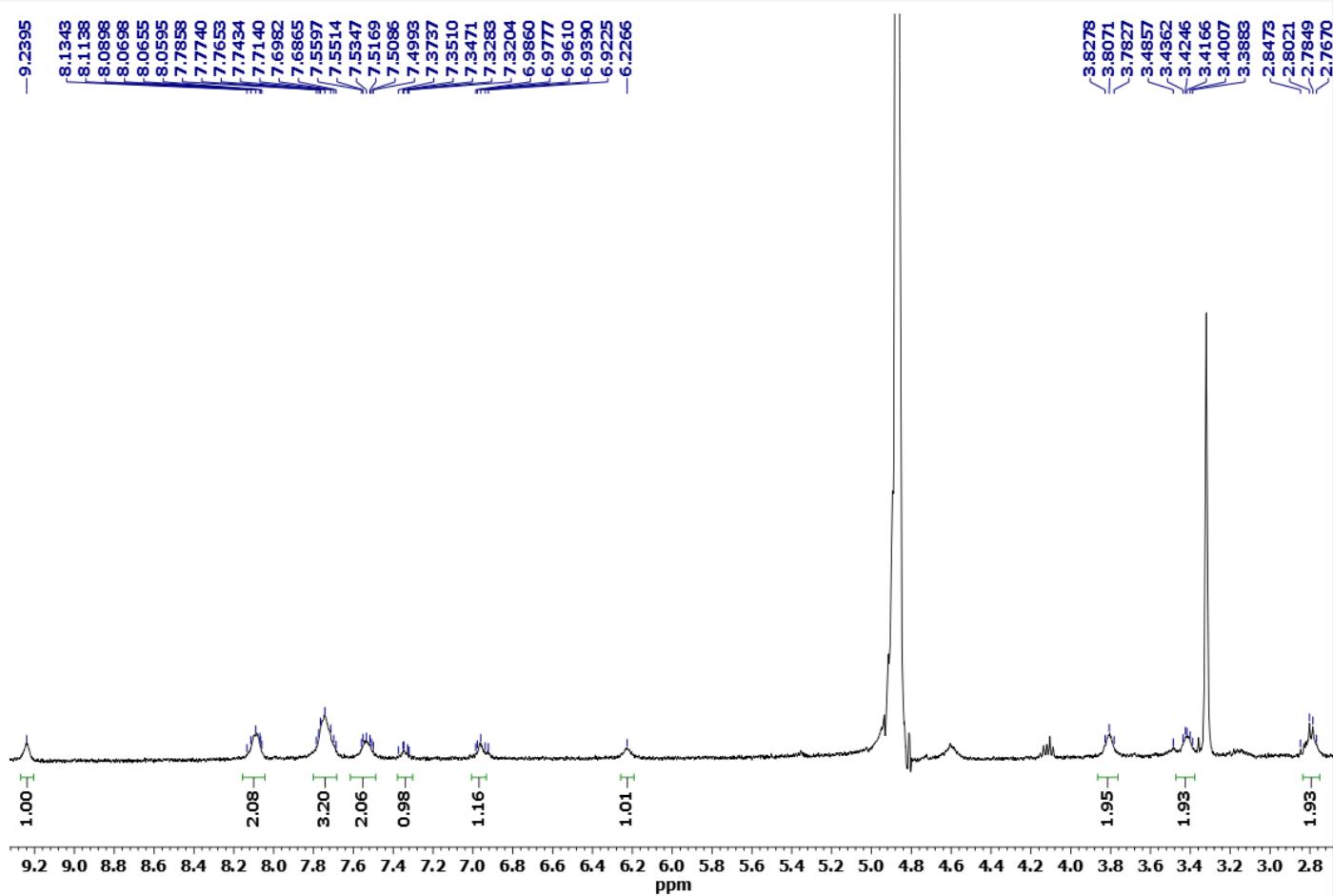
JYH-04JUN18-054-2-1 150 (2.554) AM2 (Ar,22000.0,0.00,0.00); ABS

TOF MS ES+

Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass Calc. Mass mDa PPM DBE

480.1649 480.1647 0.2 0.4 16.5 184.1 n/a n/a C25 H21 N5 O2 F3



2-methyl-4'-(piperidin-4-yl)-5-(1-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)-[1,1'-biphenyl]-3-carboxylic acid (34)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

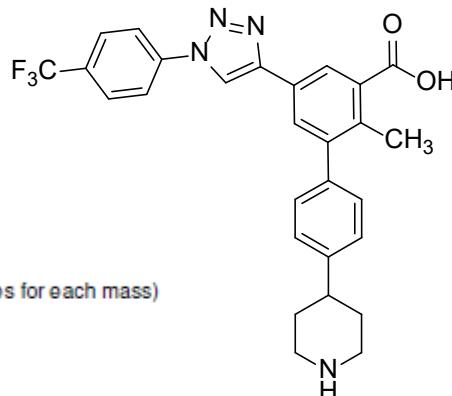
83 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

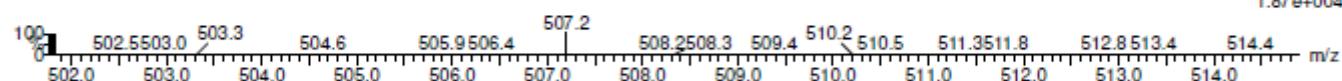
C: 0-100 H: 0-200 N: 4-4 O: 0-40 F: 3-3

JYH-21MAY18-051-2 424 (7.191) AM2 (Ar,22000.0,0.00,0.00); ABS

TOF MS ES+



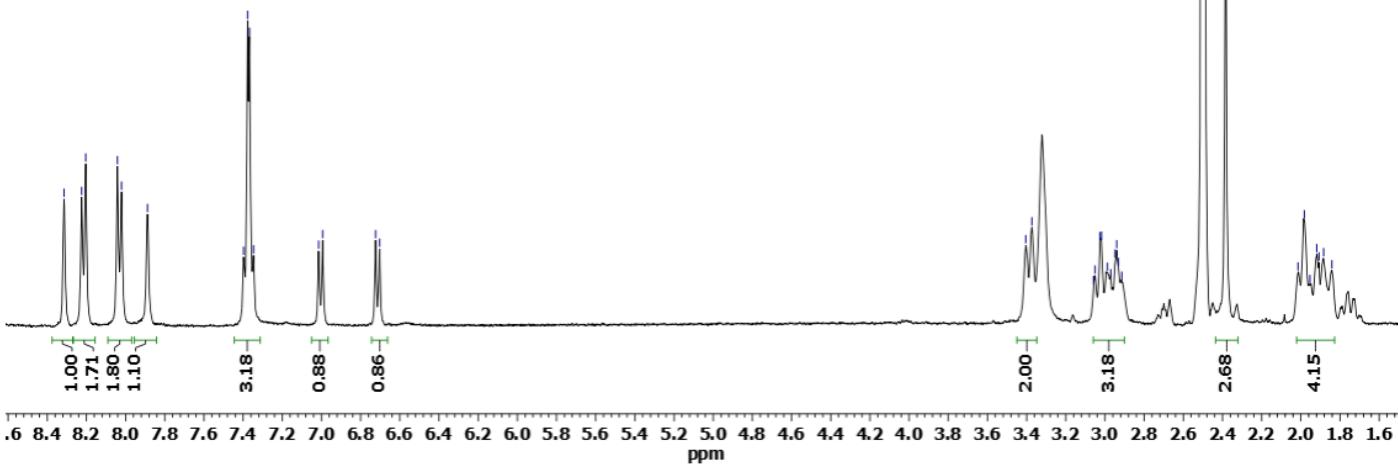
1.87e+004



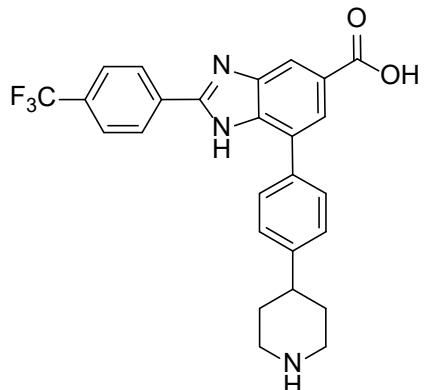
Minimum: -1.5
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	Norm	Conf (%)	Formula
------	------------	-----	-----	-----	-------	------	----------	---------

507.2009	507.2008	0.1	0.2	16.5	85.5	n/a	n/a	C28 H26 N4 O2 F3
----------	----------	-----	-----	------	------	-----	-----	------------------



7-(4-(Piperidin-4-yl)phenyl)-2-(4-(trifluoromethyl)phenyl)-1H-benzo[d]imidazole-5-carboxylic acid (35)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

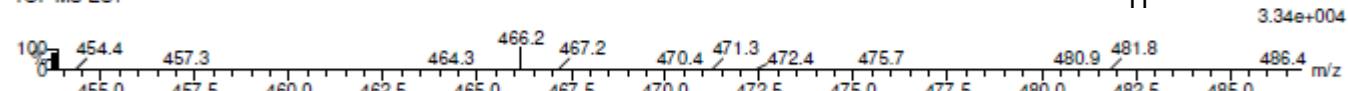
77 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-100 H: 0-200 N: 3-3 O: 0-40 F: 3-3

JYH-23AUG18-106-2 153 (2.605) AM2 (Ar,42000.0,0.00,0.00); ABS

TOF MS ES+



Minimum: -1.5
Maximum: 5.0 5.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
466.1747	466.1742	0.5	1.1	15.5	33.0	n/a	n/a	C26 H23 N3 O2 F3

