

Supplementary materials

Novel Cecropin-4 Derived Peptides against Methicillin-Resistant *Staphylococcus aureus*

Jian Peng ^{1,2#}, Biswajit Mishra ^{1#}, Rajamohammed Khader ¹, LewisOscar Felix ¹ and Eleftherios Mylonakis ^{1,*}

¹Infectious Diseases Division, Rhode Island Hospital, Warren Alpert Medical School of Brown University, Providence, RI 02903, USA; jian_peng@brown.edu (J.P.); biswajit_mishra@brown.edu (B.M.); rajamohammed_khader@brown.edu (R.K.); lewis_oscar_felix_raj_lucas@brown.edu (L.F.)

²Immune Cells and Antibody Engineering Research Center of Guizhou Province, Key Laboratory of Biology and Medical Engineering, School of Biology and Engineering/School of Basic Medical Sciences, Guizhou Medical University, Guiyang 550025, P.R. China

Both the authors have contributed equally

*Correspondence: emylonakis@lifespan.org

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Table S1. The physicochemical properties of Cec4 derived peptides

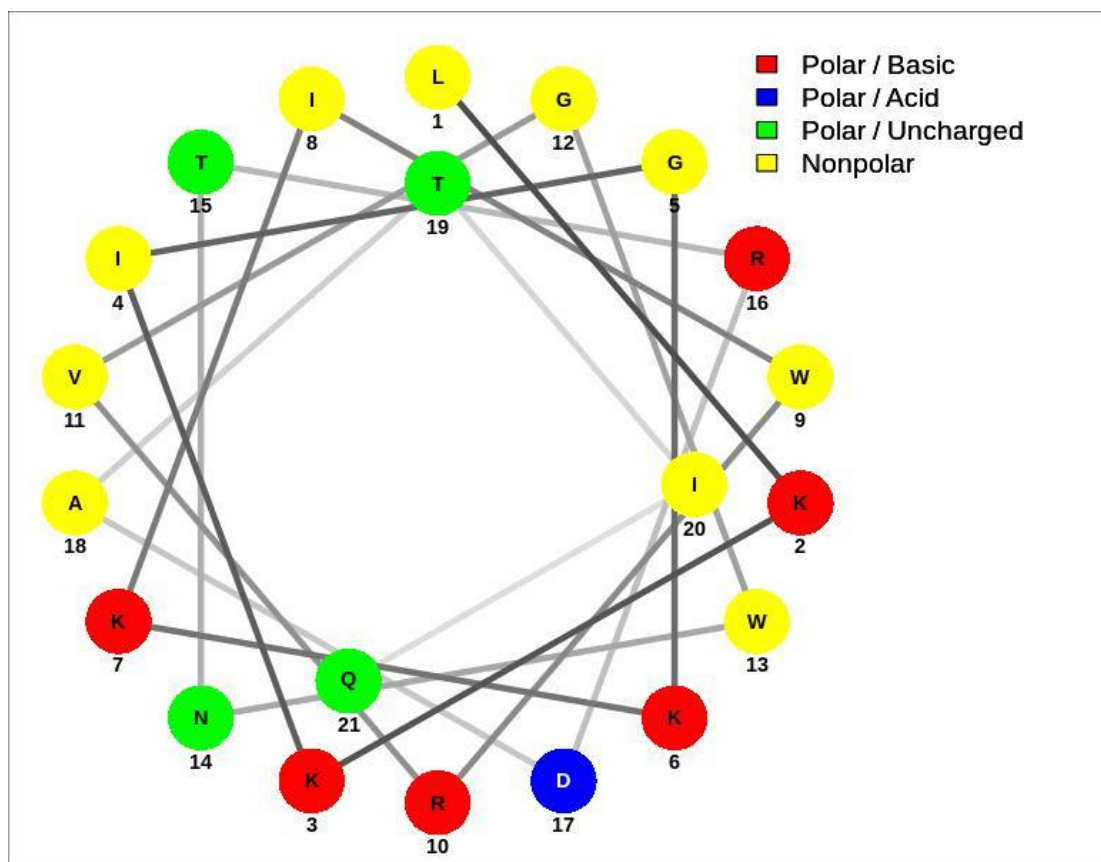
No	Amino acids	Molecular weight (Da)	Theoretical pI	GRAVY	Aliphatic index	Hydrophobicity	Net charge at pH 7.0
Cec4	41	4333.1	10.66	-0.356	95.37	42.2	6
C1	21	2512	11.17	-0.752	92.89	35.47	5
C2	16	1983.44	12.03	-0.9	91.25	31.52	6
C3	16	2068.54	12.03	-0.912	91.25	35.85	6
C4	12	1425.83	11.33	-0.4	121.67	24.37	5
C5	16	2126.58	12.02	-0.725	91.25	43.76	5
C6	16	2184.62	12.02	-0.537	91.25	51.05	4
C7	12	1483.87	11.26	-0.15	121.67	33.41	4
C8	12	1541.91	11.17	0.1	121.67	40.74	3
C9	16	2126.58	12.02	-0.725	91.25	43.29	5
C10	16	2184.62	12.02	-0.537	91.25	51.11	4
C11	12	1483.87	11.26	-0.15	121.67	32.75	4
C12	12	1541.91	11.17	0.1	121.67	40.69	3
C13	16	2255.75	12.02	-0.756	91.25	50.17	5
C14	16	2255.75	12.02	-0.756	91.25	52.97	5
C15	16	2384.91	12.02	-0.787	91.25	60.85	5
C16	16	2326.87	12.03	-0.975	91.25	52.25	6
C17	16	2182.69	12.02	-0.463	115.62	48.46	5
C18	16	2182.69	12.02	-0.463	115.62	51.73	5
C19	16	2238.8	12.02	-0.2	140	57.9	5
C20	16	2180.76	12.03	-0.388	140	49.19	6
C21	16	2442.95	12.02	-0.6	91.25	67.65	4
C22	16	2384.91	12.02	-0.787	91.25	59.08	5
C23	16	2296.84	12.02	-0.013	140	64.91	4
C24	16	2238.8	12.02	-0.2	140	56.25	5

Note: Isoelectric point (pI), Grand average of hydropathicity (GRAVY), amino acid (AA).

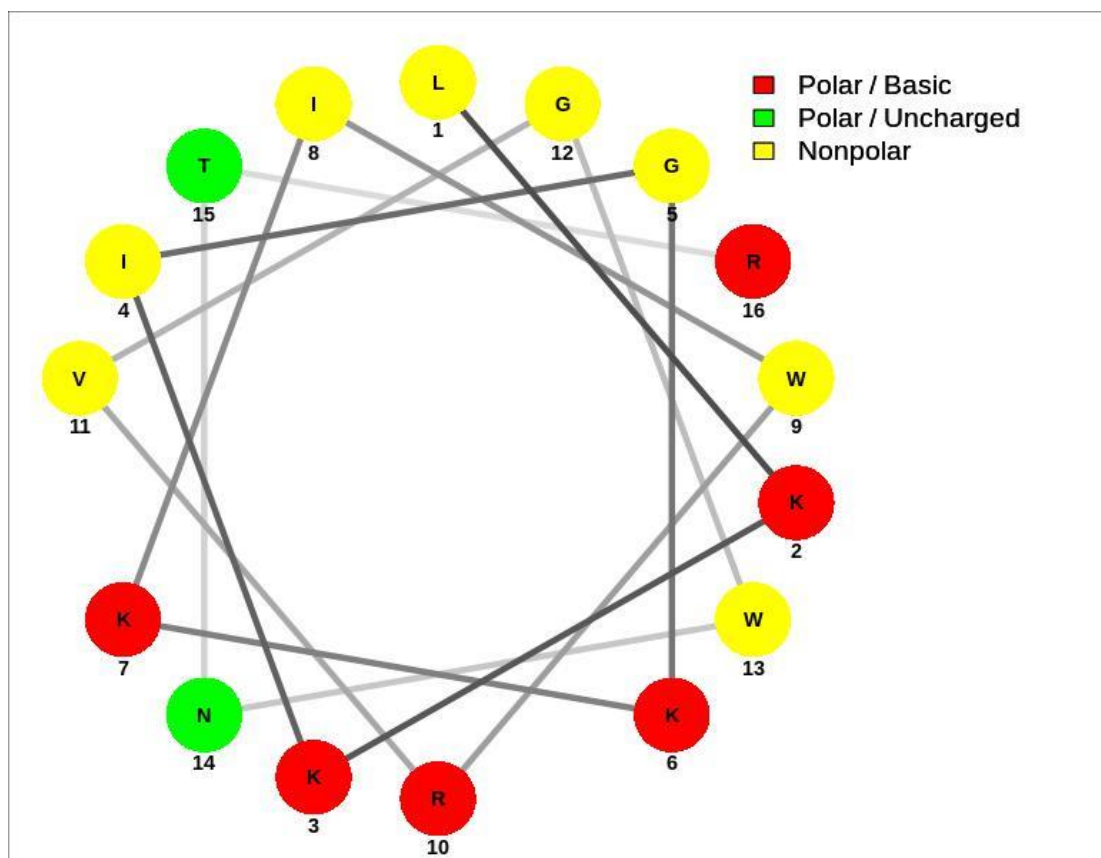
Table S2. The qPCR primers of bacterial virulence genes

Gene	Function	Sequence of primer	Size of product (bp)
<i>agrA</i>	Regulator of gene expression	F: 5' -TGATAATCCTTATGAGGTGCTT-3' R: 5' -CACTGTGACTCGTAACGAAAA-3'	164
<i>Spa</i>	Surface protein for bacterial aggregation	F: 5' -GCGCAACACGATGAAGCTCAACAA-3' R: 5' -ACGTTAGCACTTTGGCTTGGATCA-3	125
<i>Fnb-A</i>	Surface protein	F: 5' -ACTTGATTTTGTGTAGCCTTTTT-3' R: 5' -GAAGAAGCACCAAAAAGCAGTA-3'	185
<i>Fnb-B</i>	Surface protein	F: 5' -CGTTATTTGTAGTTGTTTGTGTT-3' R: 5' - TGGAATGGGACAAGAAAAAGAA-3'	118
<i>Clf-1</i>	Surface protein	F: 5' -CGGTTTTGGACTACTCAGCA-3' R: 5' - GCTACTGCCGATAAACTA-3'	151
<i>srrA</i>	Regulator of gene expression	F: 5' -AGCATGTGTGGGAGGTATGA-3' R: 5' -TGCAATCAAATATGATGTGAAGAA-3'	118

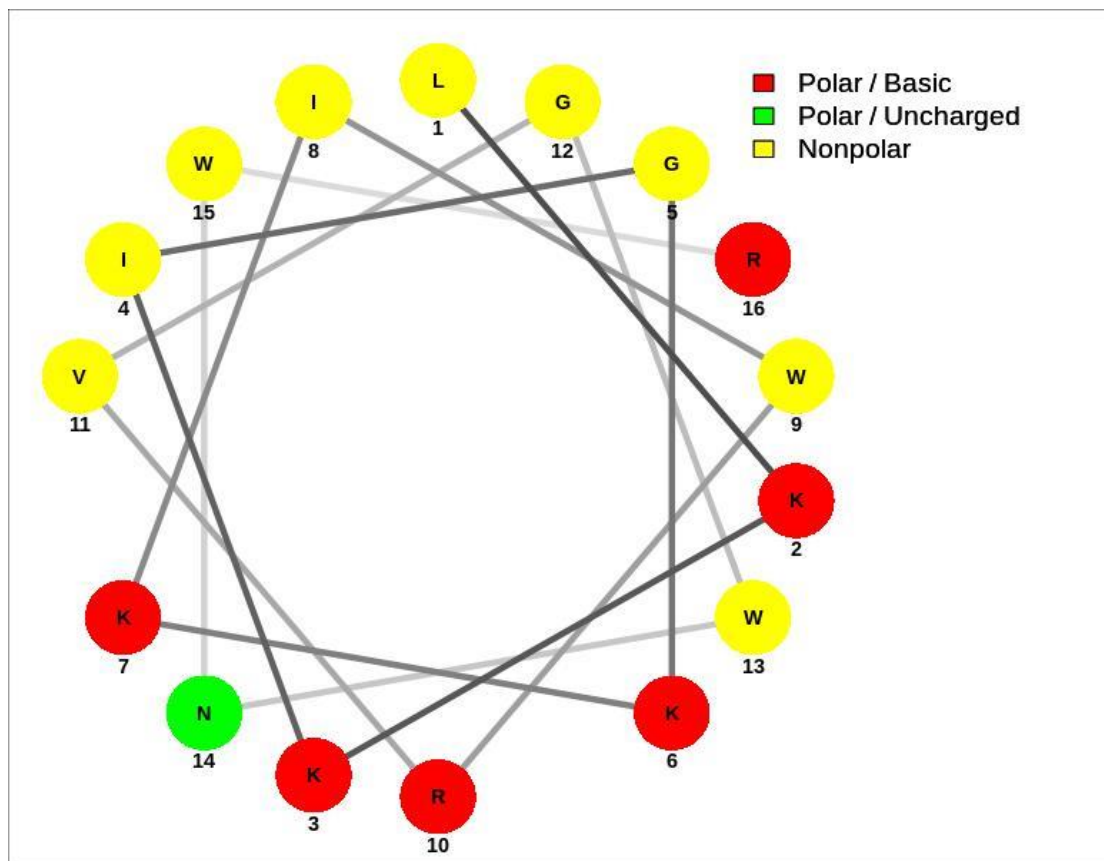
Figure S1. The helical wheels of synthetic peptides
C1



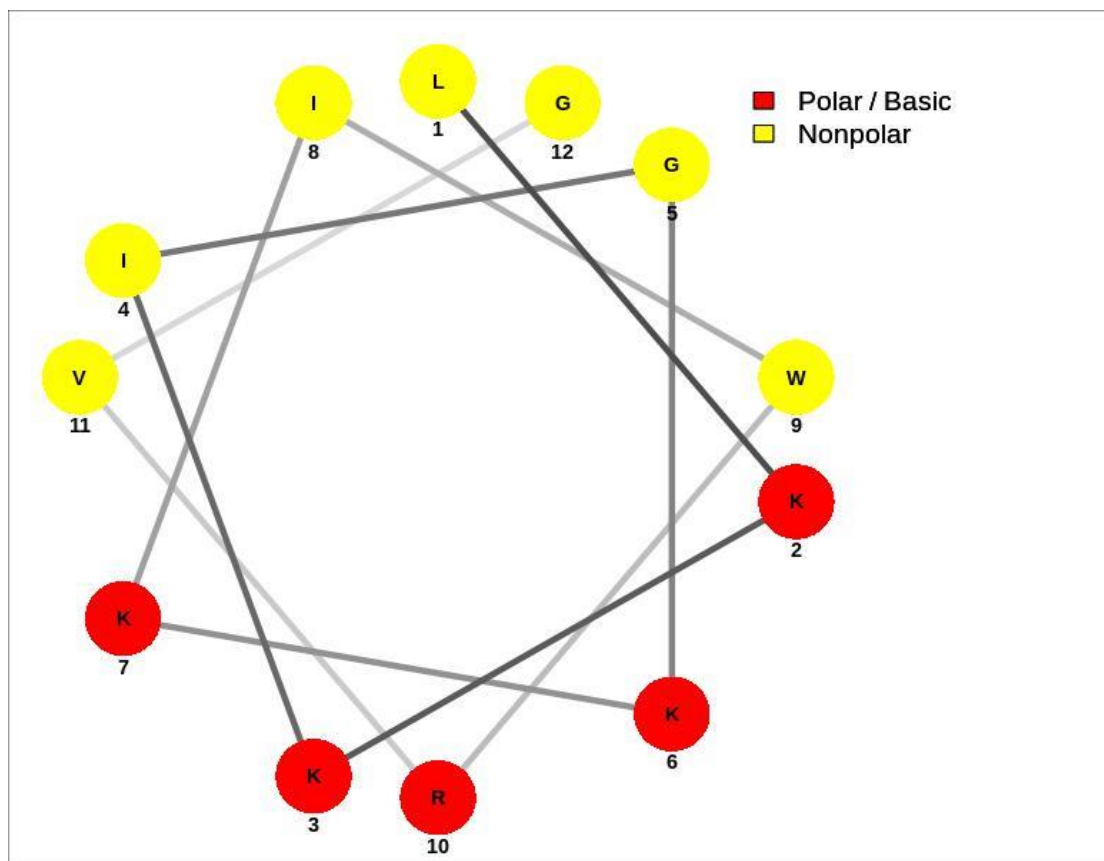
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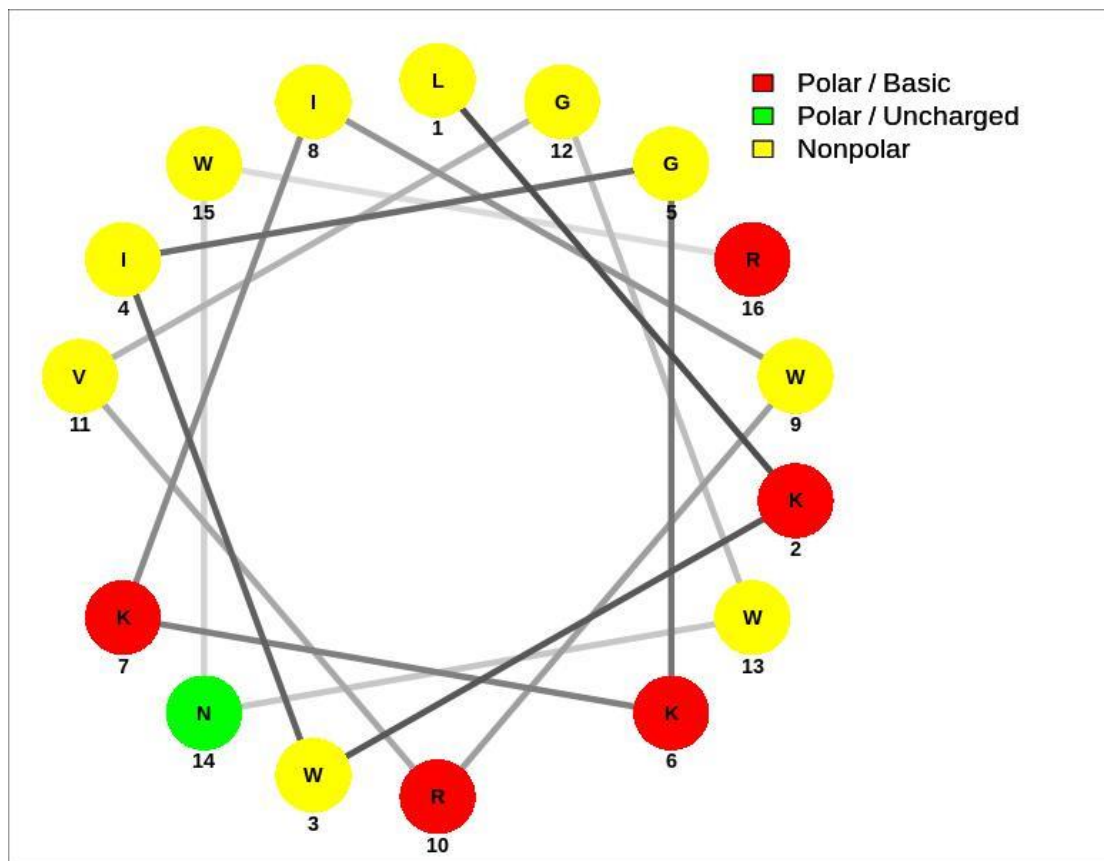
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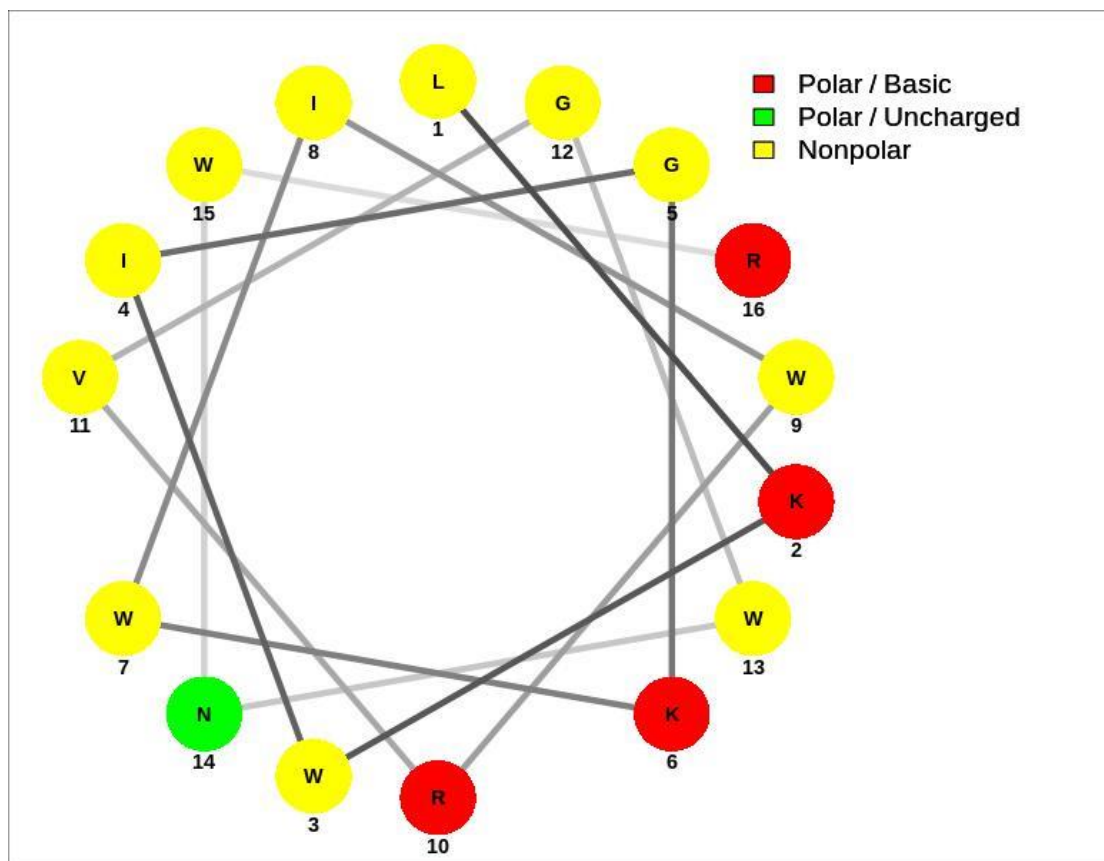
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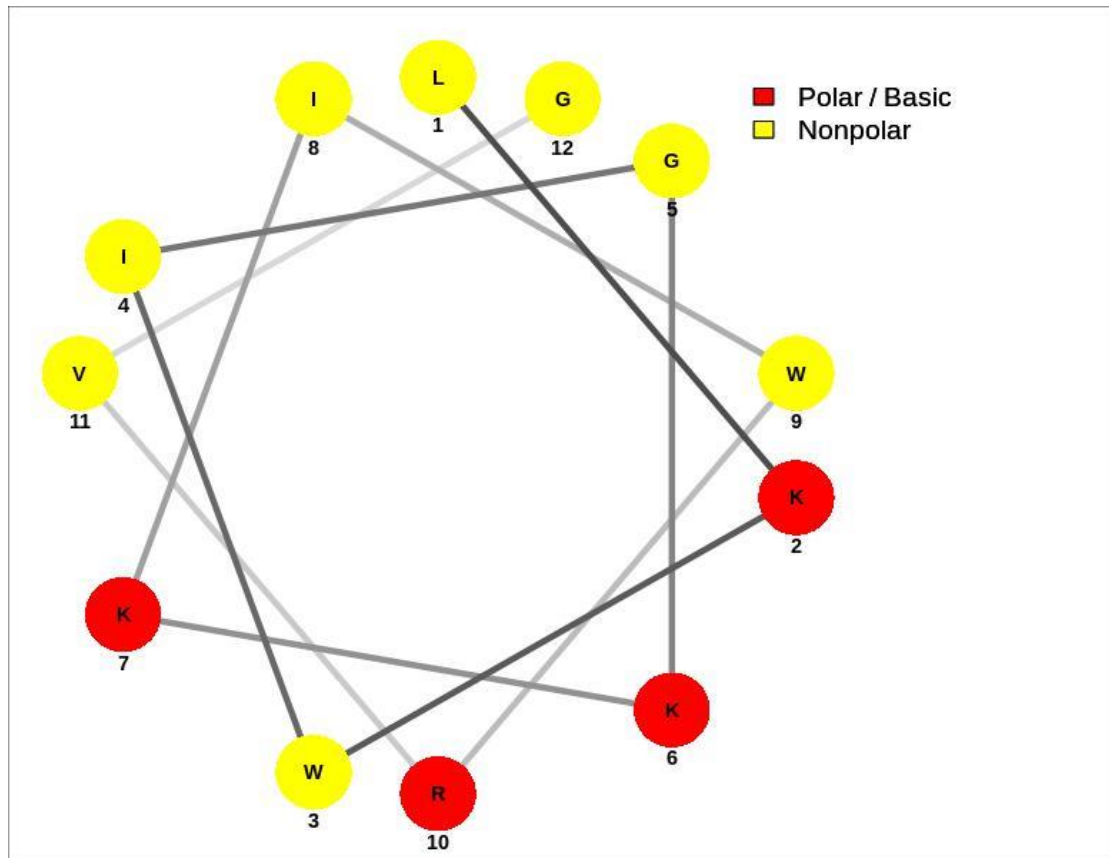
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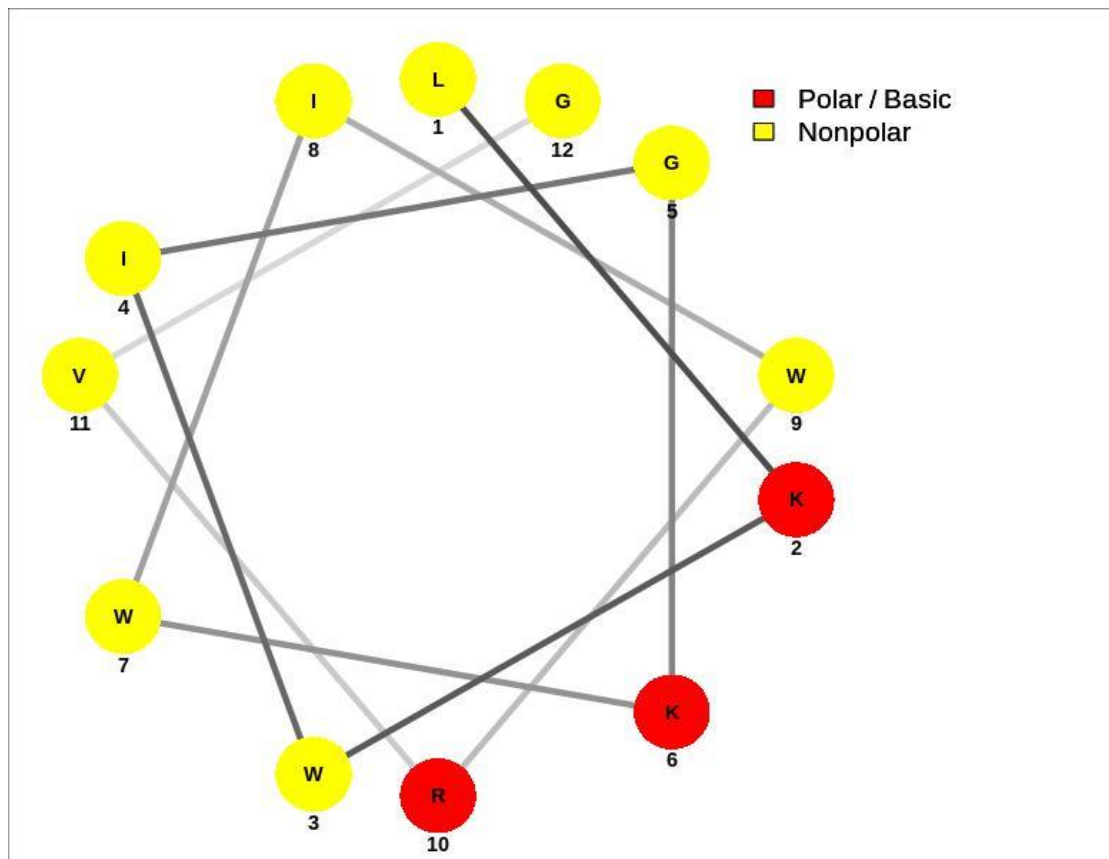
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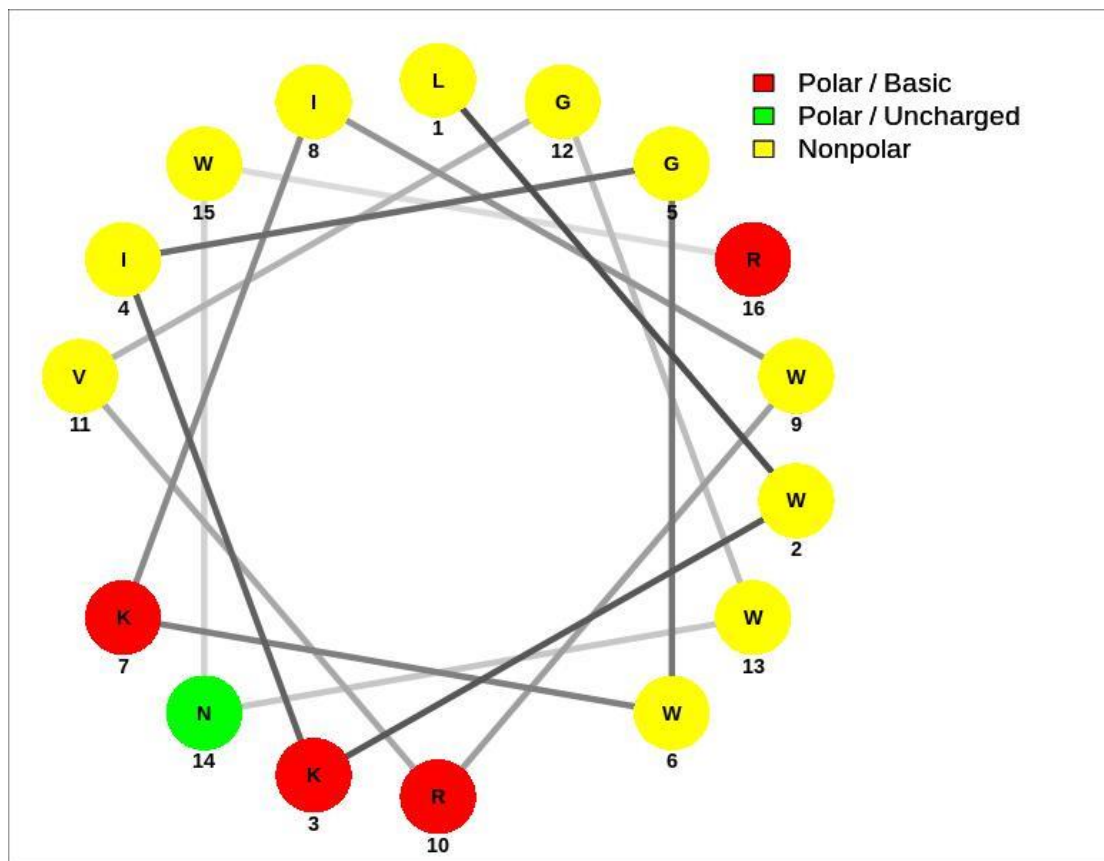
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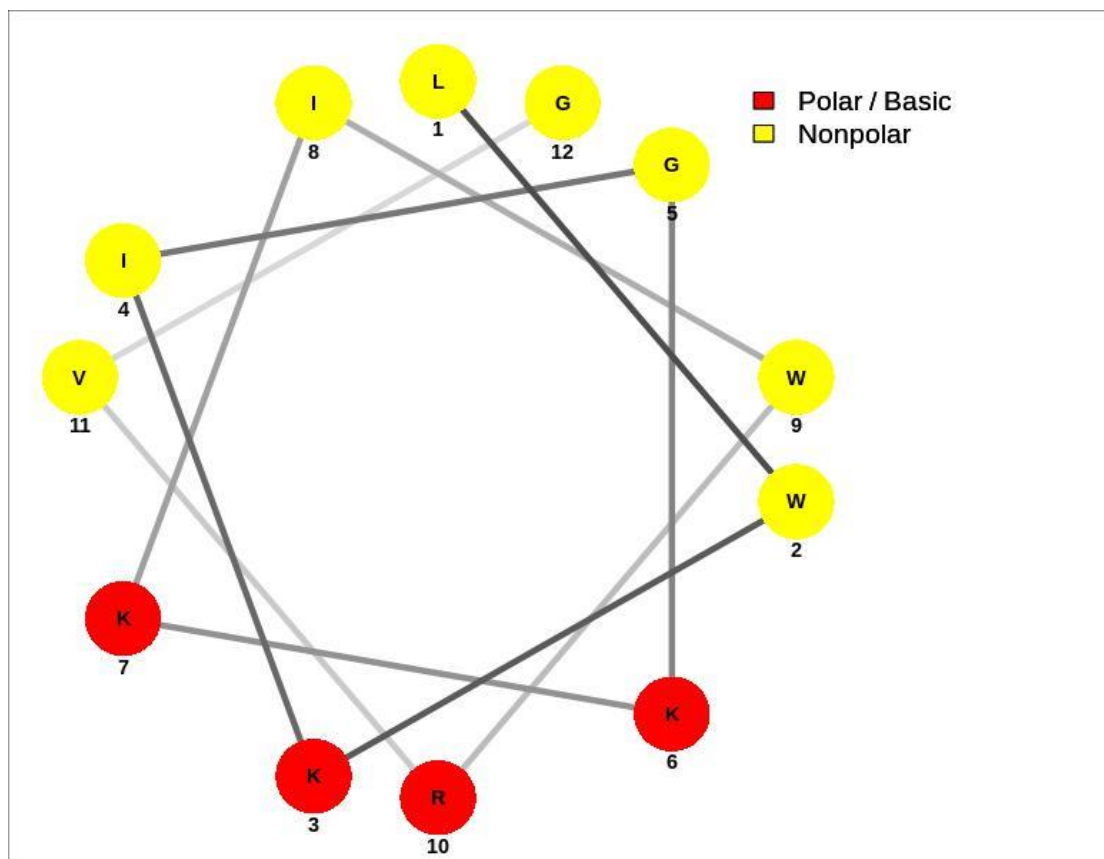
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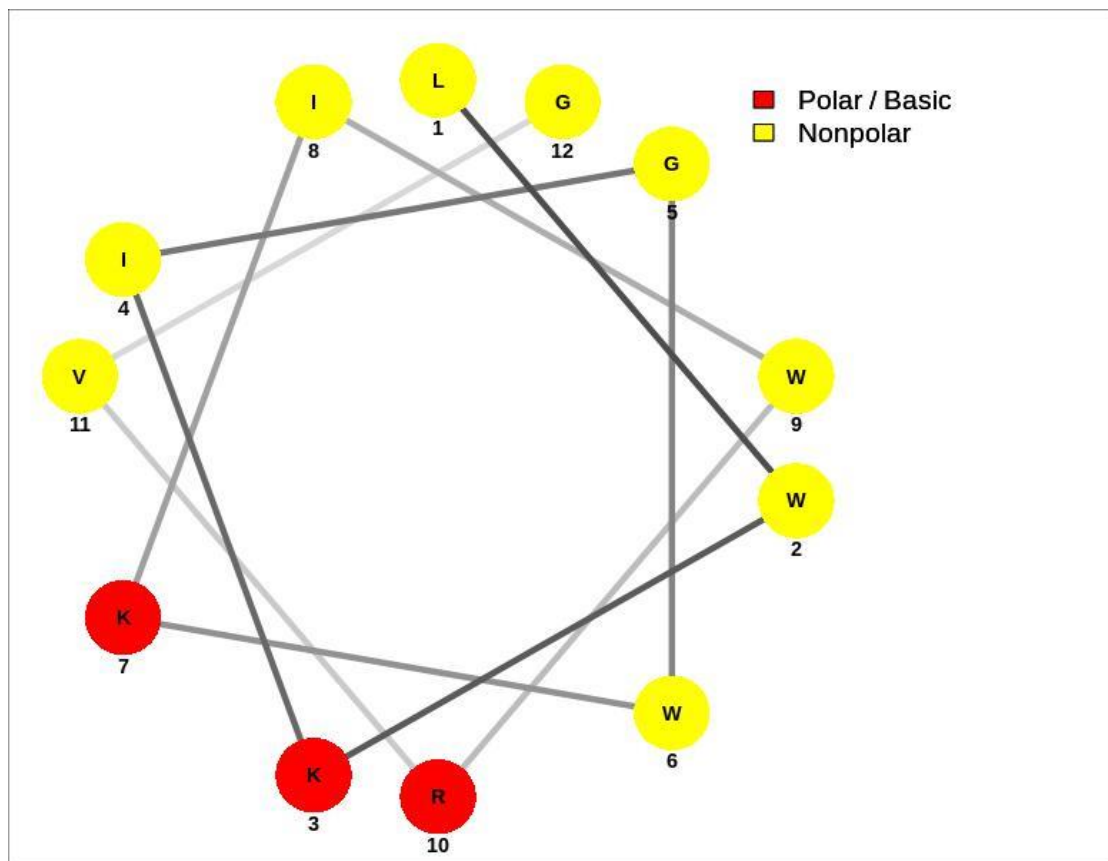
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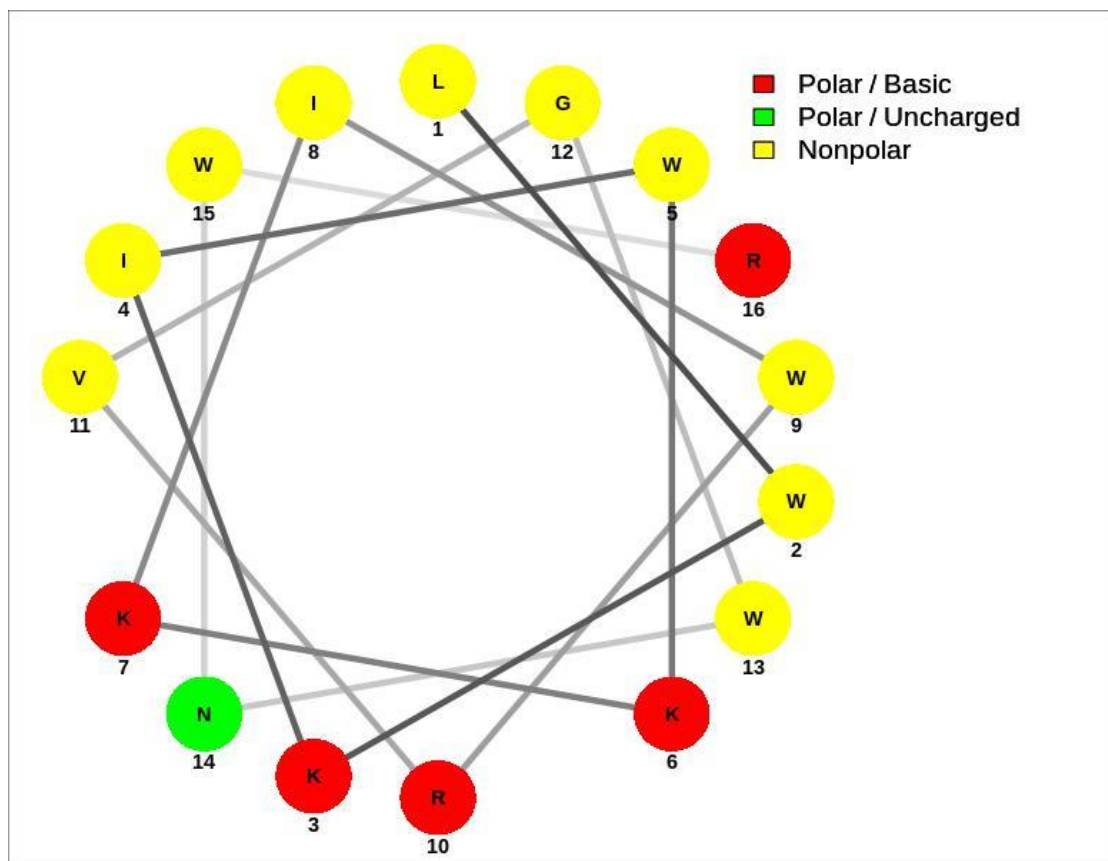
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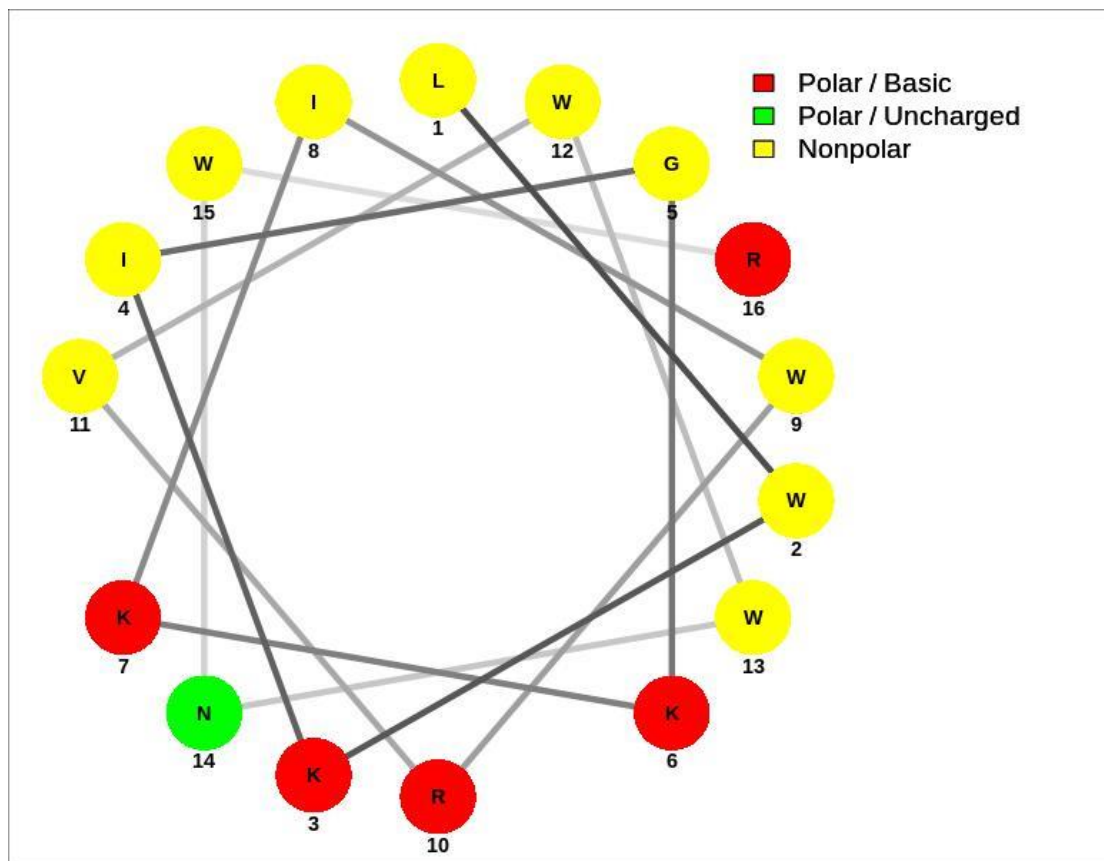
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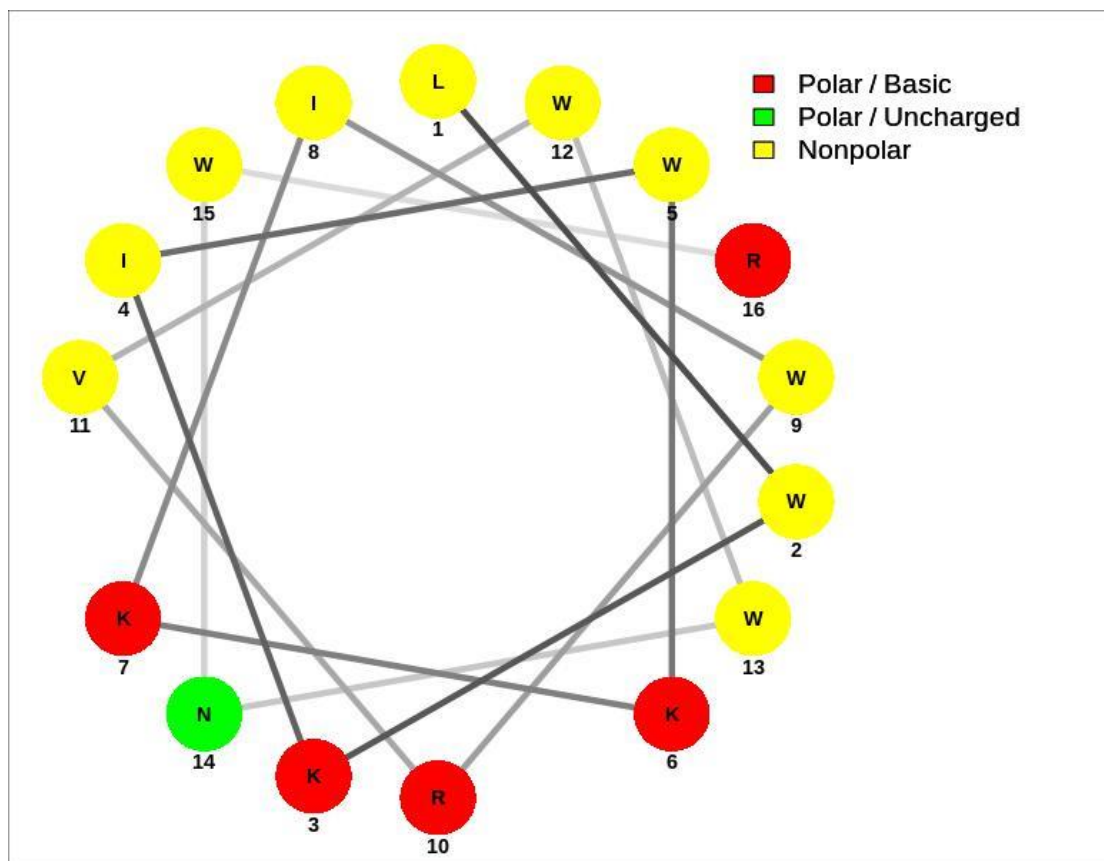
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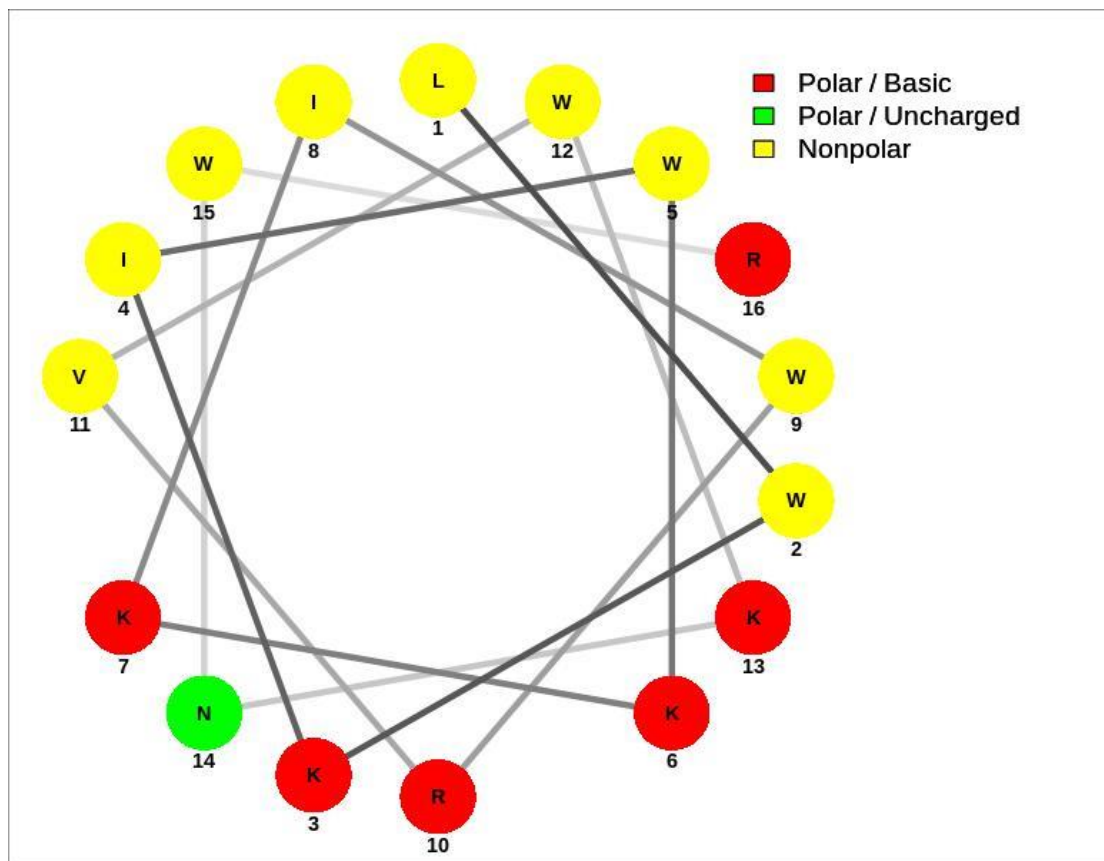
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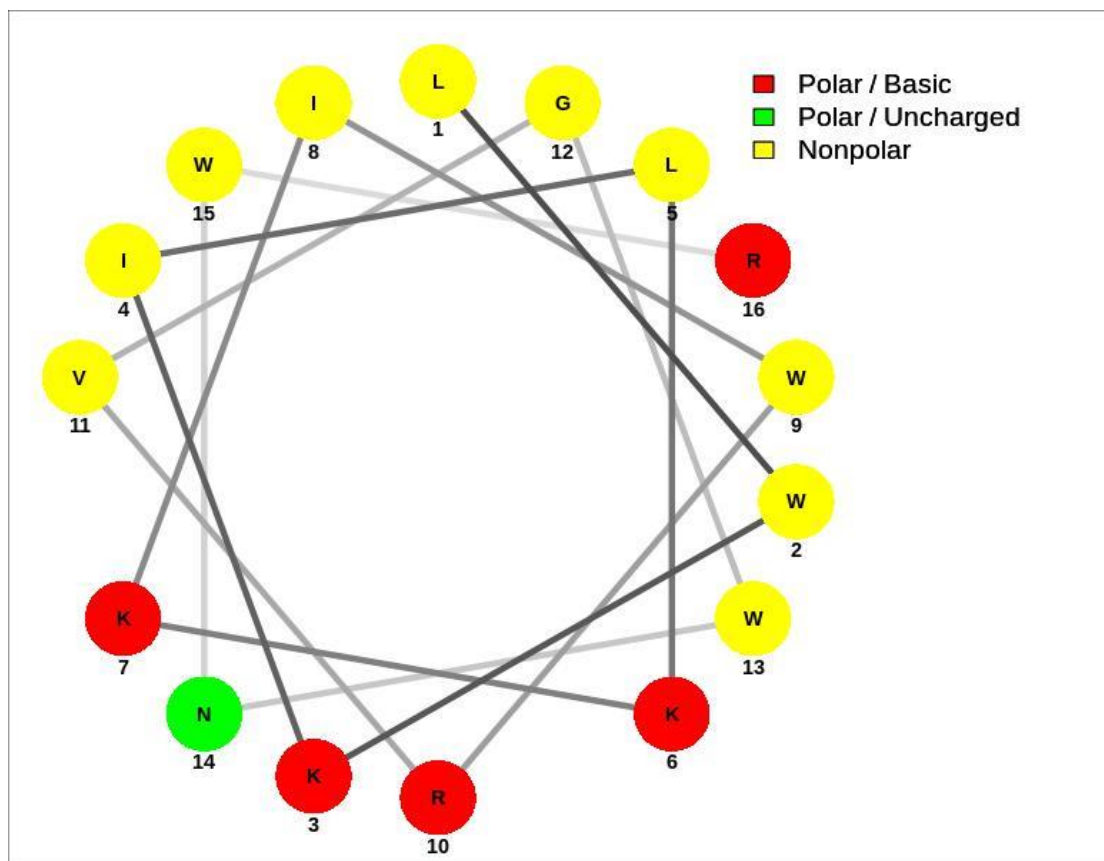
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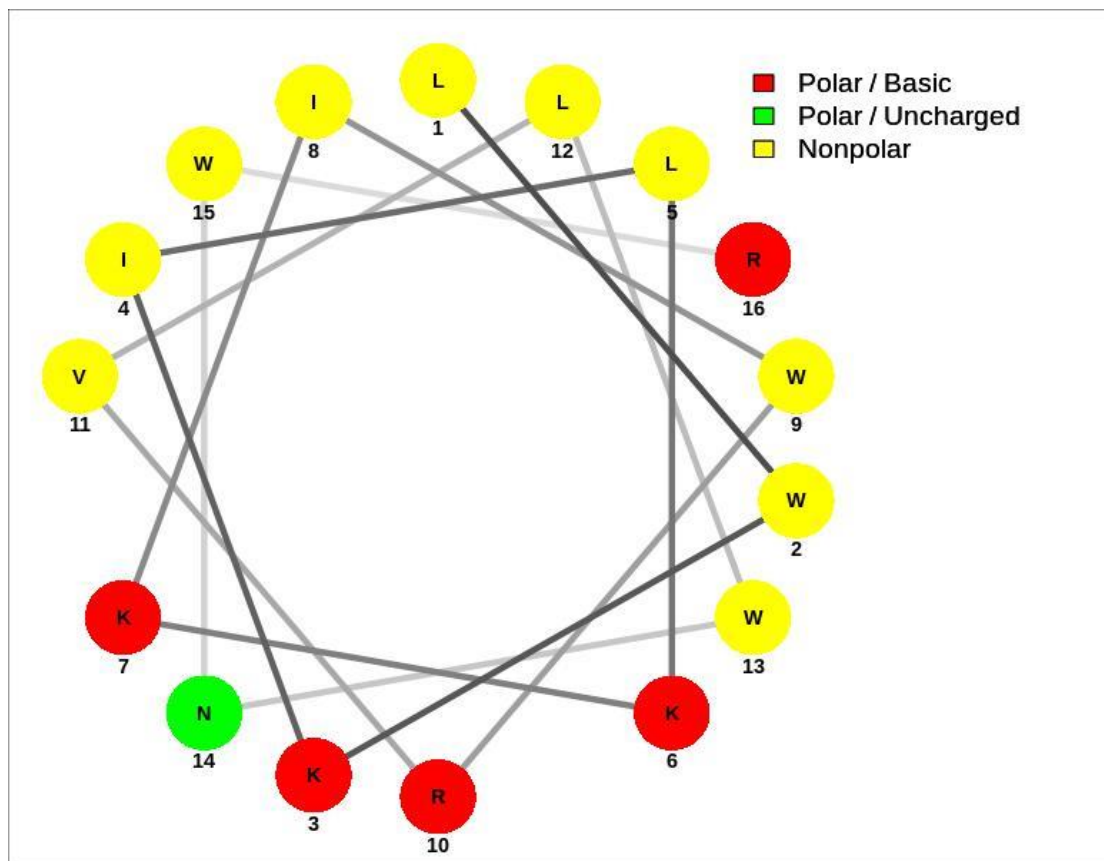
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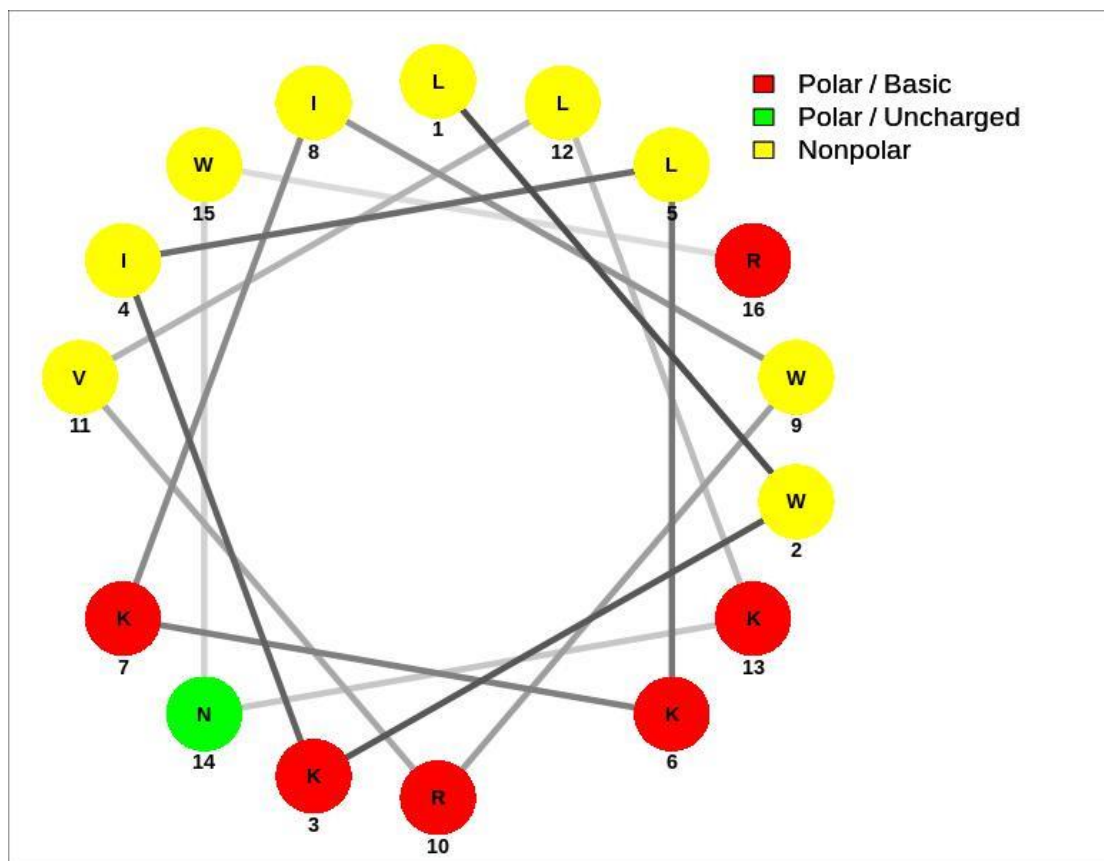
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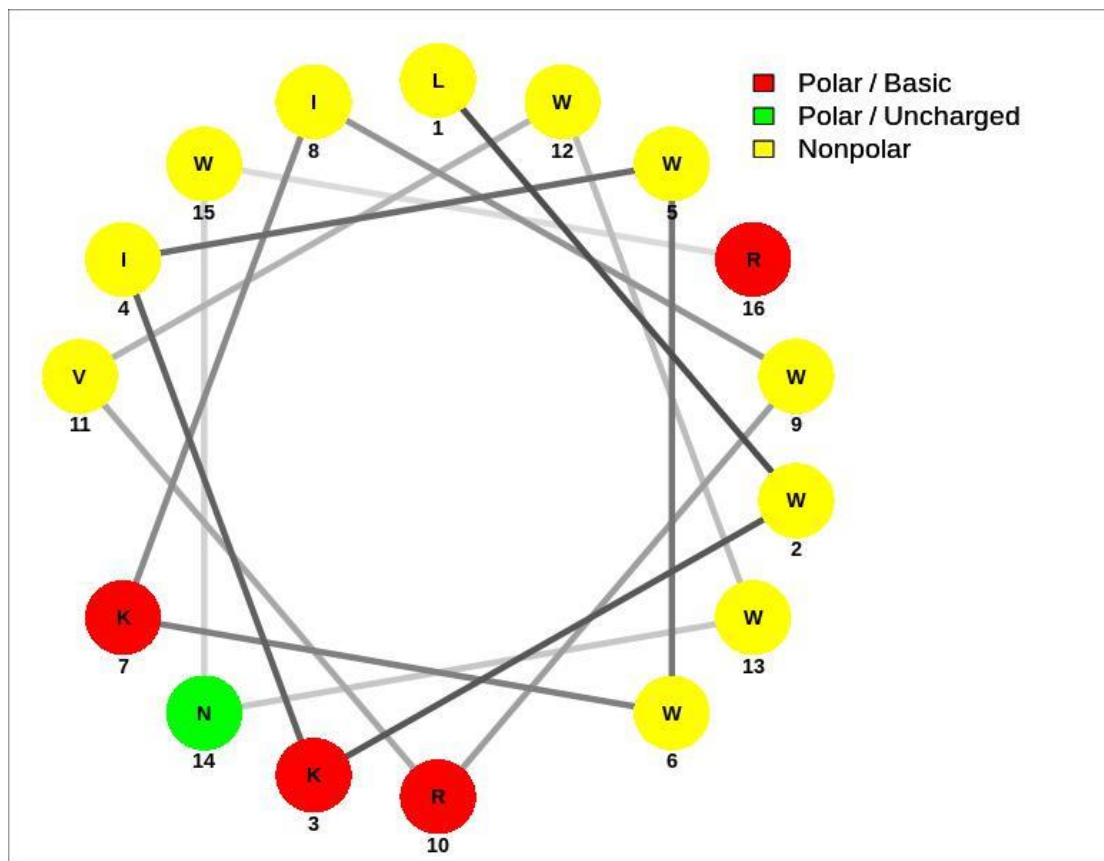
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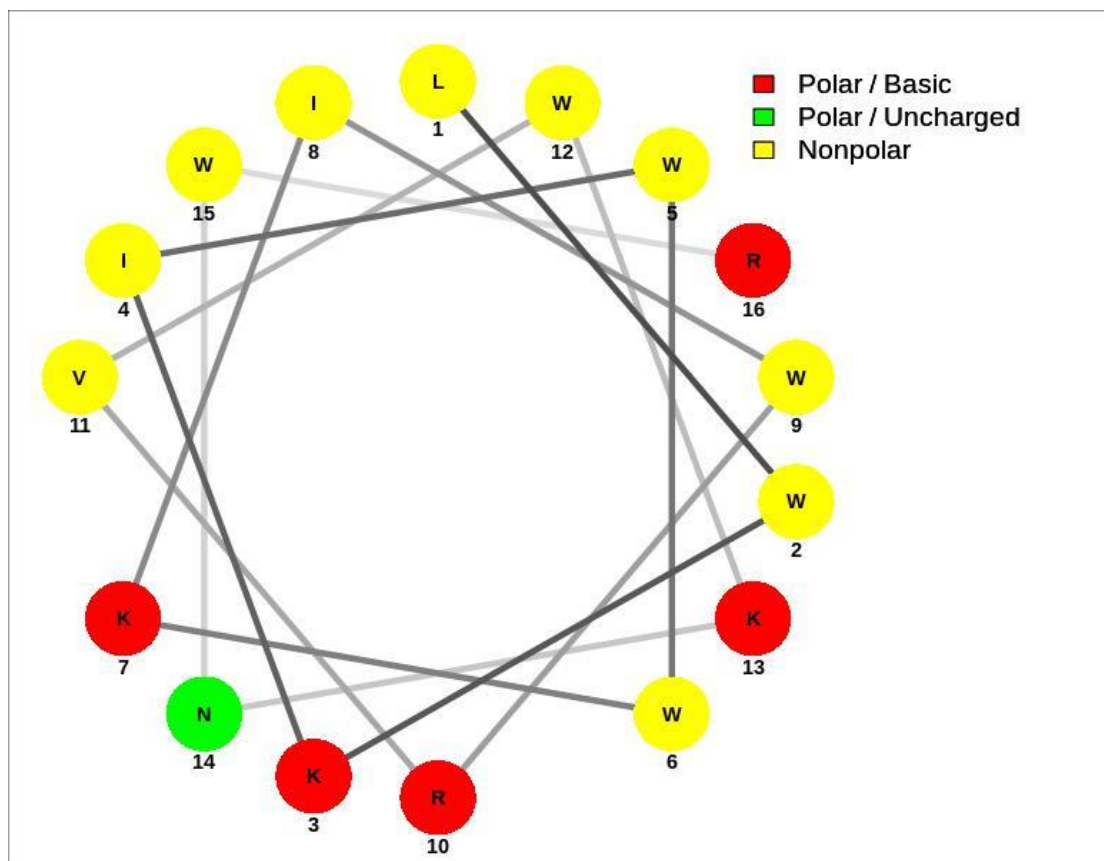
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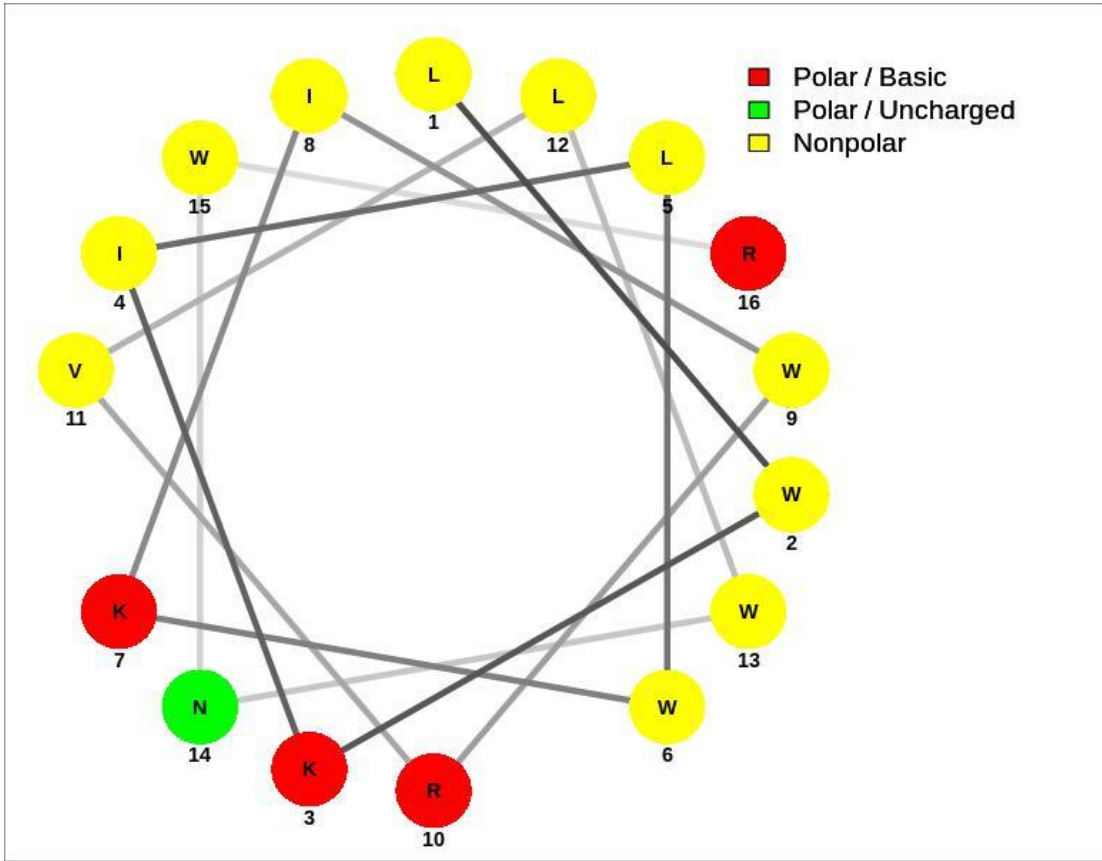
C21



C22



C23



C24

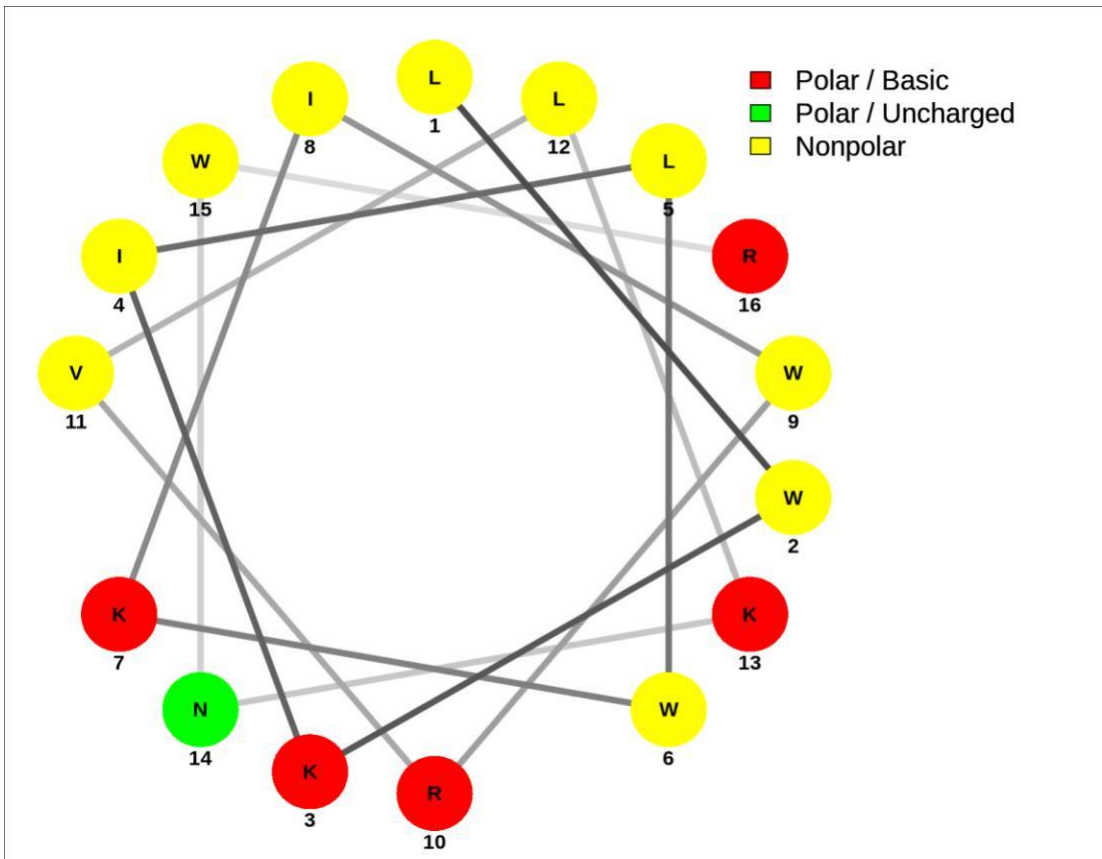
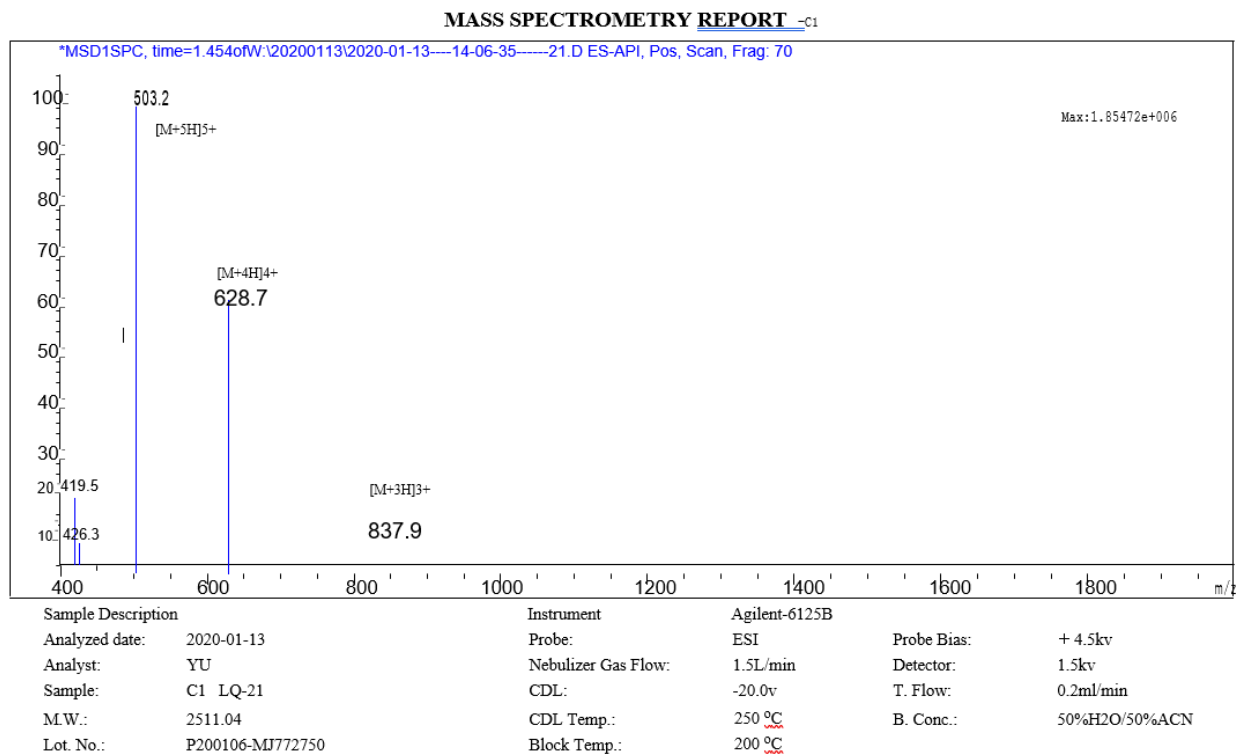


Figure S2. The MS and HPLC information of synthetic peptides





HPLC REPORT -C1

Product Name: C1 LQ-21

Instrument No: 0200194

Lot No : P200106-MJ772750

Column : 4.6*250mm C18

Solvent A : 0.1% Trifluoroacetic in 100% Acetonitrile

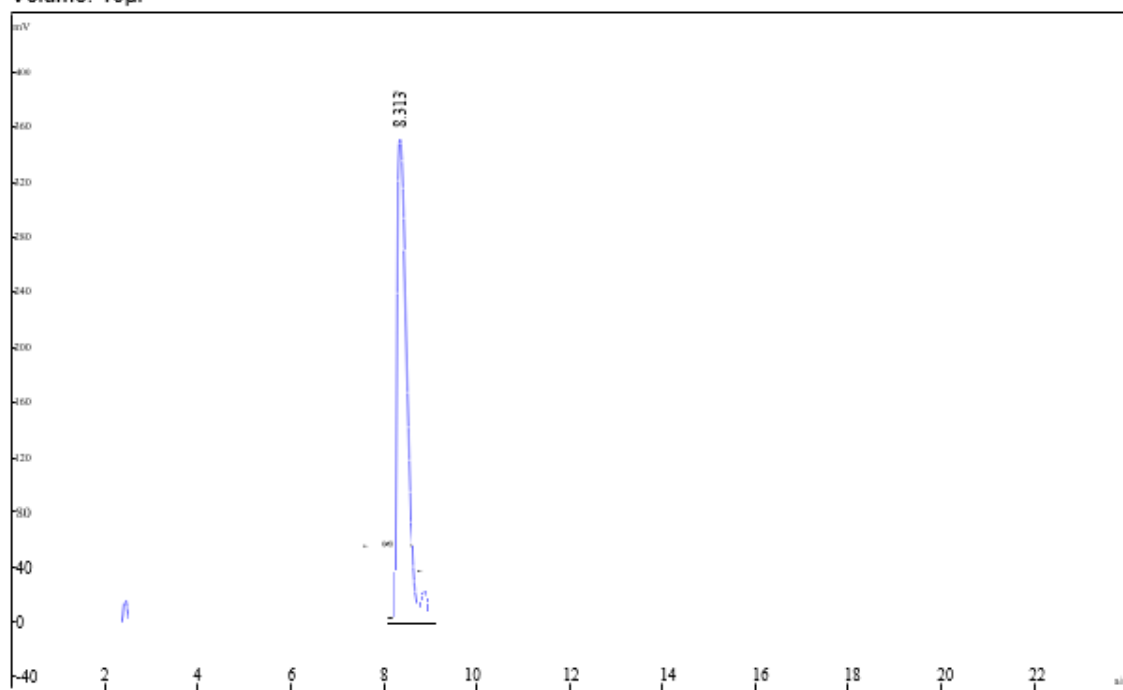
Solvent B : 0.1% Trifluoroacetic in 100% Water

Gradient :
 A B
 0.01min 20% 80%
 25min 45% 55%
 25.01min 100% 0%
 30.0min STOP

Flow rate : 1.0ml/min

Wavelength : 220nm

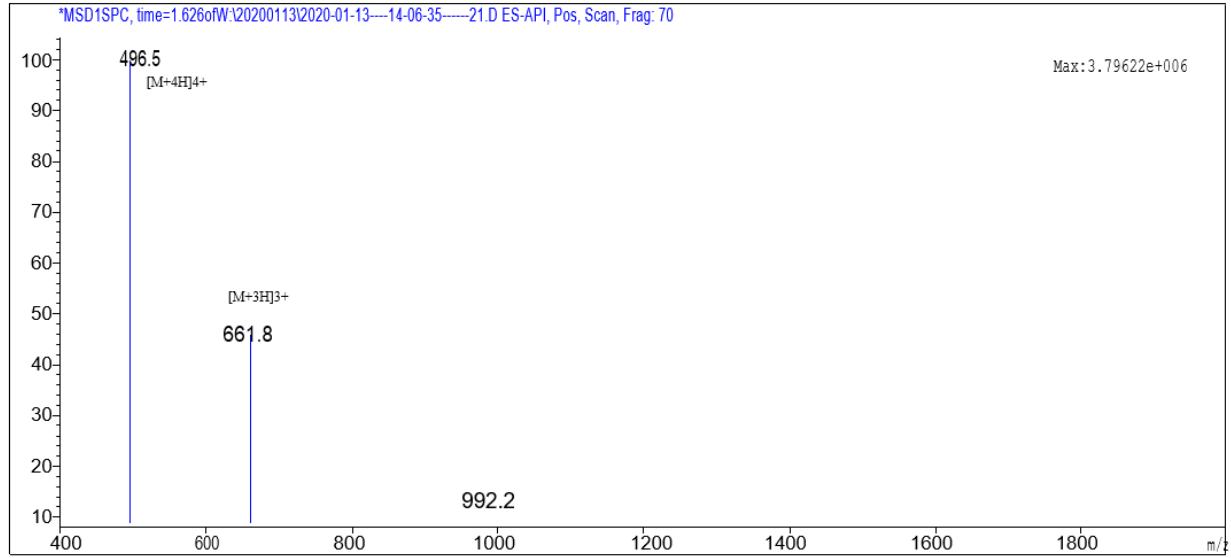
Volume: 10µl



Rank	Time	Name	Conc.	Area	Height
1	8.205		0.07226	3340	2492
2	8.313		95.98	4436853	348374
3	8.849		3.946	182381	19720
Total			100	4622574	370586

MASS SPECTROMETRY REPORT

-C2



Sample Description

Analyzed date: 2020-01-13
 Analyst: YU
 Sample: C2 LR-16
 M.W.: 1982.47
 Lot. No.: P200106-MJ772751

Instrument

Agilent-6125B
 Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 CDL: -20.0v
 CDL Temp.: 250 °C
 Block Temp.: 200 °C

Probe Bias: + 4.5kv
 Detector: 1.5kv
 T. Flow: 0.2ml/min
 B. Conc.: 50%H₂O/50%ACN

HPLC REPORT ^{-C2}

Product Name: C2 LR-16

Instrument No: 0200194

Lot No : P200106-MJ772751

Column : 4.6*250mm C18

Solvent A : 0.1% Trifluoroacetic in 100% Acetonitrile

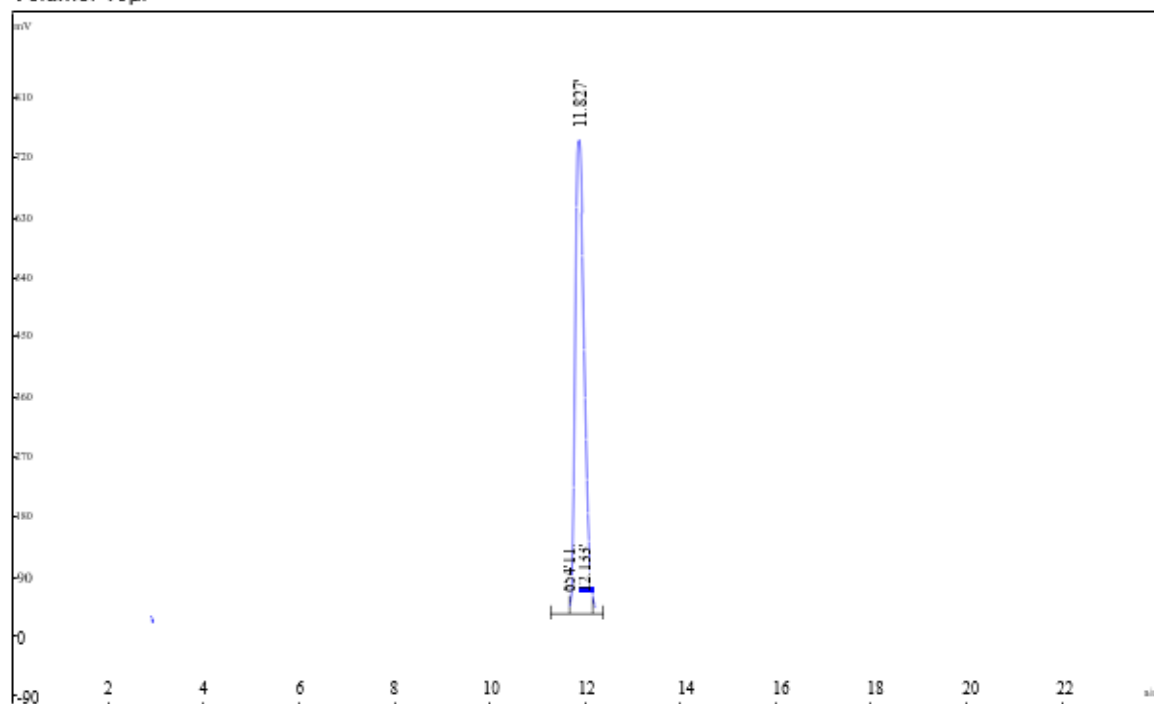
Solvent B : 0.1% Trifluoroacetic in 100% Water

Gradient	:	A	B
	0.01min	16%	84%
	25min	41%	59%
	25.01min	100%	0%
	30.0min	STOP	

Flow rate : 1.0ml/min

Wavelength : 220nm

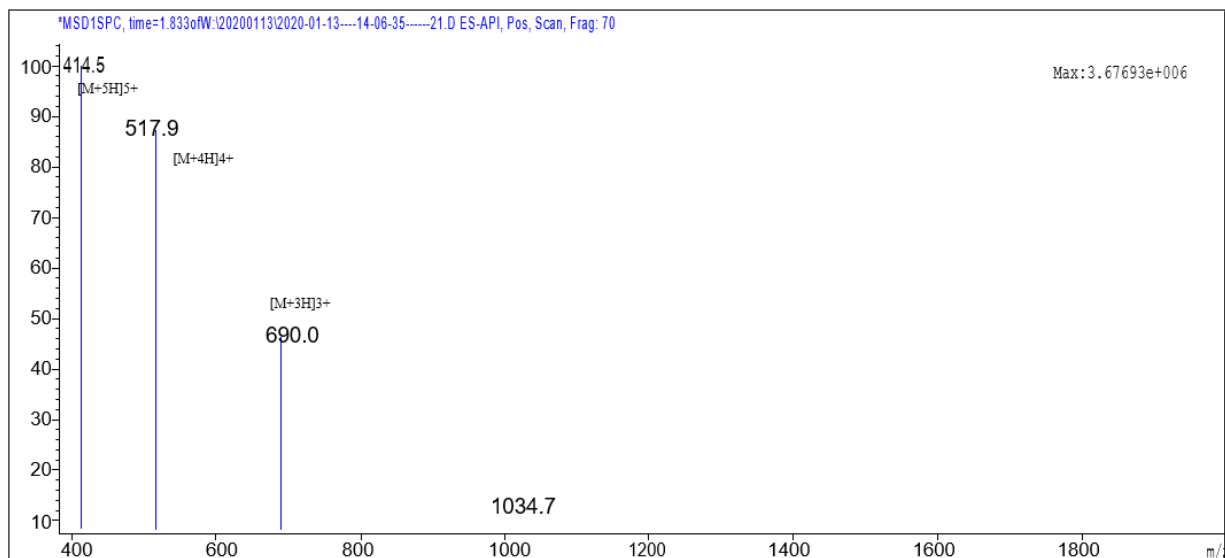
Volume: 10µl



Rank	Time	Name	Conc.	Area	Height
1	11.654		1.683	148100	14151
2	11.827		97.84	8609738	711574
3	12.133		0.4731	41628	13487
Total			100	8799466	739212

MASS SPECTROMETRY REPORT

-C3



Sample Description

Analyzed date: 2020-01-13
 Analyst: YU
 Sample: C3 LR-16
 M.W.: 2067.58
 Lot. No.: P200106-MJ772752

Instrument

Agilent-6125B
 Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 CDL: -20.0v
 CDL Temp.: 250 °C
 Block Temp.: 200 °C

Probe Bias:

+ 4.5kv
 Detector: 1.5kv
 T. Flow: 0.2ml/min
 B. Conc.: 50%H₂O/50%ACN

HPLC REPORT -C3

Product Name:C3 LR-16

Instrument No: 0200194

Lot No :P200106-MJ772752

Column :4.6*250mm C18

Solvent A :0.1%Trifluoroacetic in 100% Acetonitrile

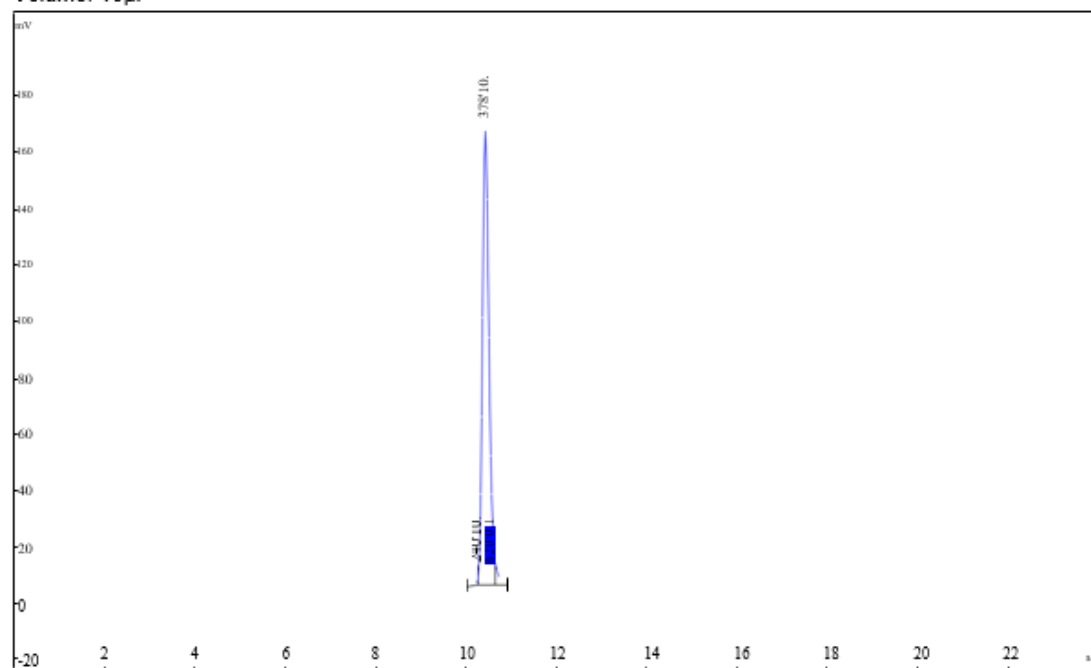
Solvent B :0.1%Trifluoroacetic in 100% Water

Gradient	:	A	B	
		0.01min	21%	79%
		25min	46%	54%
		25.01min	100%	0%
		30.0min	STOP	

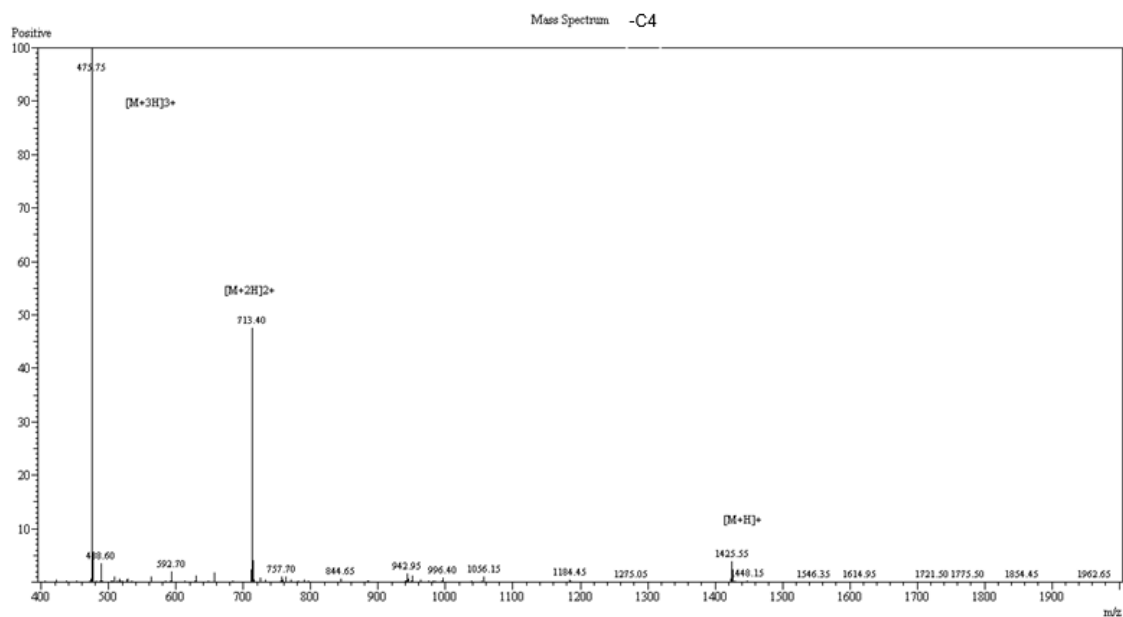
Flow rate :1.0ml/min

Wavelength :220nm

Volume: 10µl



Rank	Time	Name	Conc.	Area	Height
1	10.240		0.6636	10208	4521
2	10.378		97.75	1503781	161147
3	10.620		1.584	24374	5448
Total			100	1538363	171116



Sample Information
Date and Time : 2020-1-10 10:17:28
User : CHAO
Sample : CT4 LG-12
Inj. Volume : 1
MW : 1424.86
Lot No. : P200106-MJ772753

Probe:	ESI	Probe bias:	-3.5kv
Nebulizer Gas Flow:	1.5L/min	Detector:	1.0kv
DL:	-20.0v	T. Flow:	0.2ml/min
DL Temp:	250°C	B. conc:	50%H2O/50%ACN
Block Temp:	200°C		

HPLC -C4

Sample Description:

Analyst: YSC

Structure: C4 LG-12

Lot NO: P200106-MJ772753

Number: 0200193

Column: 250*4.6mm Boston Green ODS-AQ

Solvent A: 0.1%TFA in 100%water

Solvent B: 0.1%TFA in 100%acetonitrile

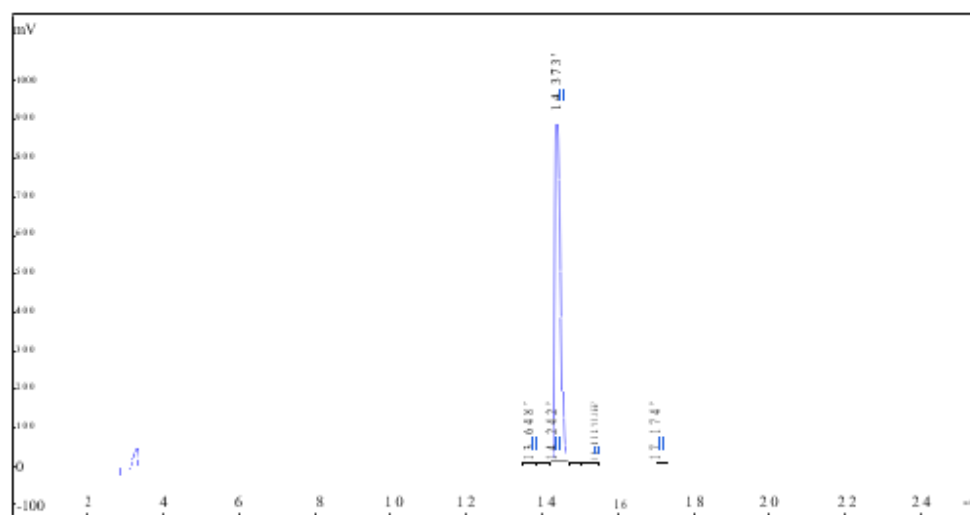
<u>Gradient</u>	A	B
0.1min	88	12
25min	63	37
25.01min	0	100
30min	0	100

Flow rate: 1.0ml/min

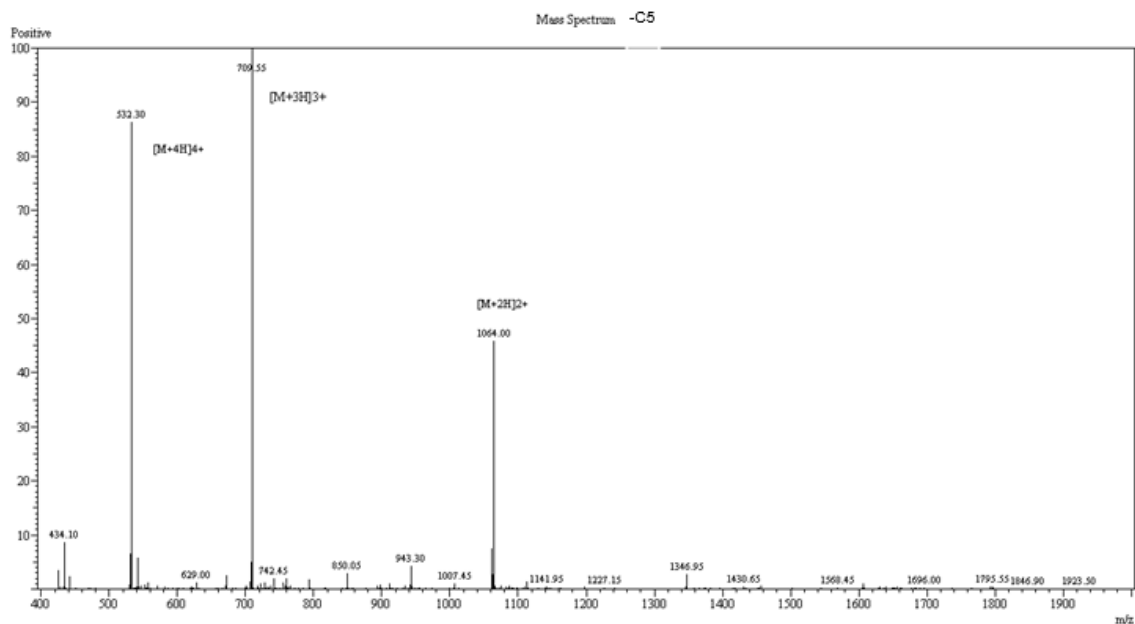
Wavelength(nm): 220

Volume: 10ul

File opened: D:\2020 HPLC\lg-12-f 772753 200113.hw, where



Rank	Time	Conc.	Area	Height
1	13.648	0.4177	35391	5086
2	14.242	0.3492	29584	3645
3	14.373	97.6	8269514	873551
4	14.832	0.5624	47647	4250
5	15.166	0.8562	72540	8631
6	17.174	0.2126	18009	2708
Total		100	8472685	897871



Sample Information
Date and Time : 2020-1-10 10:17:28
User : CHAO
Sample : CT5 LR-16
Inj. Volume : 1
MW : 2125.62
Lot No. : P200106-MJ772754

Probe: ESI
Nebulizer Gas Flow: 1.5L/min
DL: -20.0v
DL Temp: 250°C
Block Temp: 200°C
Probe bias: -3.5kv
Detector: 1.0kv
T. Flow: 0.2ml/min
B. conc: 50%H₂O/50%ACN

HPLC -C5

Sample Description:

Analyst: YSC

Structure: C5 LR-16

Lot NO: P200106-MJ772754

Number: 0200193

Column: 250*4.6mm Boston Green ODS-AQ

Solvent A: 0.1%TFA in 100%water

Solvent B: 0.1%TFA in 100%acetonitrile

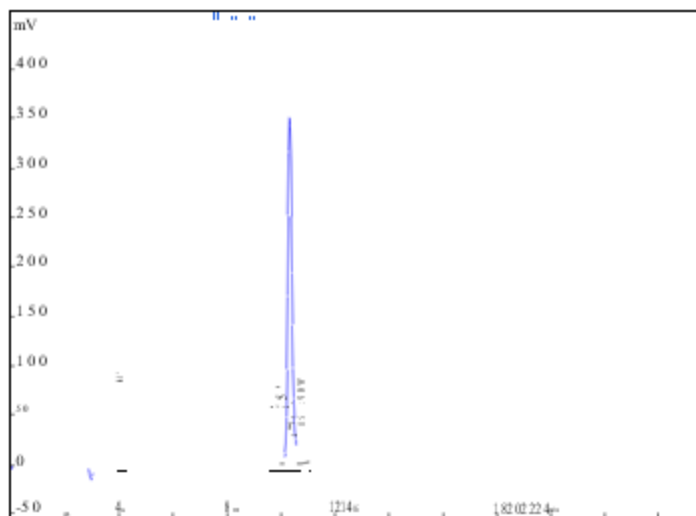
<u>Gradient:</u>	A	B
0.1min	80	20
25min	55	45
25.01min	0	100
30min	0	100

Flow rate: 1.0ml/min

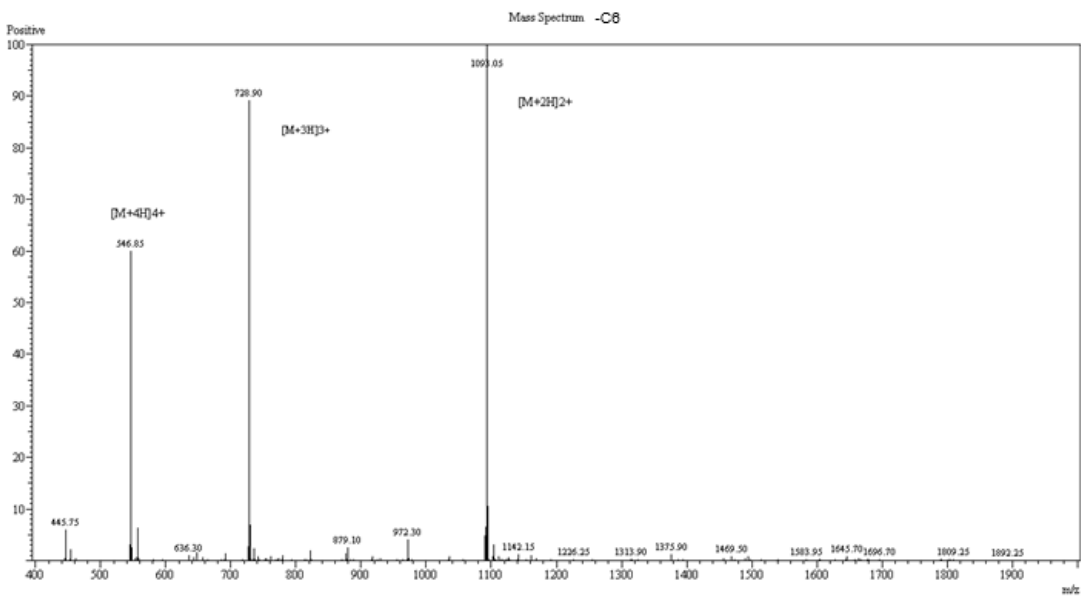
Wavelength(nm): 220

Volume: 10ul

File opened: D:\2020 HPLC\LR-16-F 772754 200113.hw, where



Rank	Time	Conc.	Area	Height
1	4.041	1.053	39379	4898
2	9.841	0.554	20719	2056
3	10.105	0.9643	36066	7942
4	10.279	95.15	3558855	348839
5	10.590	1.775	66385	12908
6	10.750	0.5015	18756	2746
Total		100	3740160	379389



Sample Information
Date and Time : 2020-1-10 10:17:28
User : CHAO
Sample : CT6 LR-16
Inj. Volume : 1
MW : 2183.66
Lot No. : P200106-MJ772755

Probe: ESI
Nebulizer Gas Flow: 1.5L/min
DL: -20.0v
DL Temp: 250°C
Block Temp: 200°C
Probe bias: -3.5kv
Detector: 1.0kv
T. Flow: 0.2ml/min
B. conc: 50%H₂O/50%ACN

HPLC -C6

Sample Description:

Analyst: YSC

Structure: C6 LR-16

Lot NO: P200106-MJ772755

Number: 0200193

Column: 250*4.6mm Boston Green ODS-AQ

Solvent A: 0.1%TFA in 100%water

Solvent B: 0.1%TFA in 100%acetonitrile

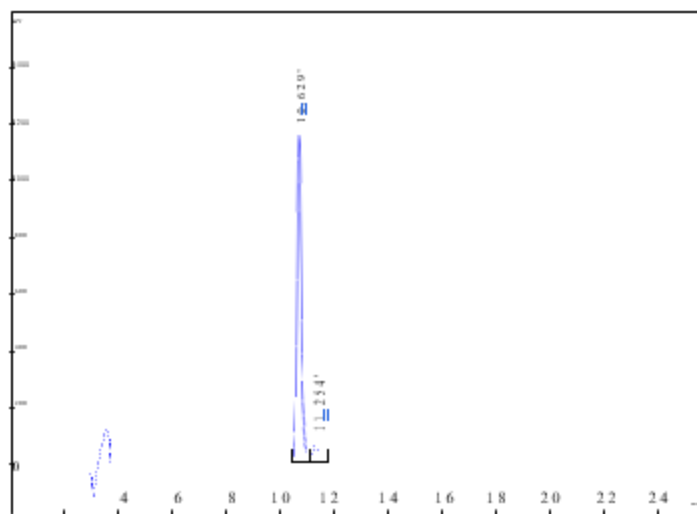
Gradient:	A	B
0.1min	75	25
25min	50	50
25.01min	0	100
30min	0	100

Flow rate: 1.0ml/min

Wavelength(nm): 220

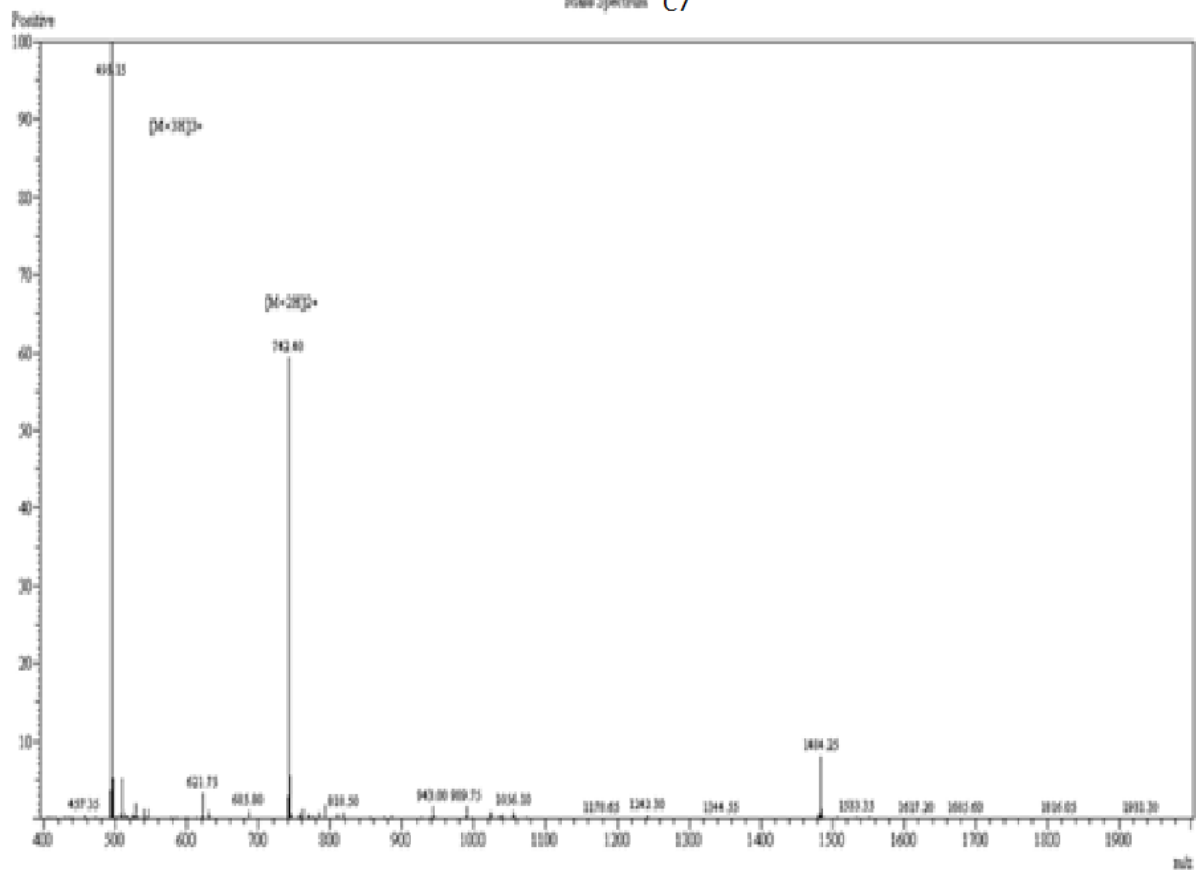
Volume: 10ul

File opened: D:\2020 HPLC\LR-16-F 772755 200113.hw, where



Rank	Time	Conc.	Area	Height
1	10.629	95.19	12285170	1135126
2	11.254	4.807	620363	49419
Total		100	12905533	1184545

Mass Spectrum C7



Sample Information

Date and Time : 2020-1-10 10:17:28
 User : CHAO
 Sample : CT7 LG-12
 Inj. Volume : 1
 MW : 1452.90
 Lot No. : P200106-MJ772756

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C

Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H2O/50%ACN

HPLC -C7

Sample Description:

Analyst: YSC

Structure: C7 LG-12

Lot NO: P200106-MJ772756

Number: 0200193

Column: 250*4.6mm Boston Green ODS-AQ

Solvent A: 0.1%TFA in 100%water

Solvent B: 0.1%TFA in 100%acetonitrile

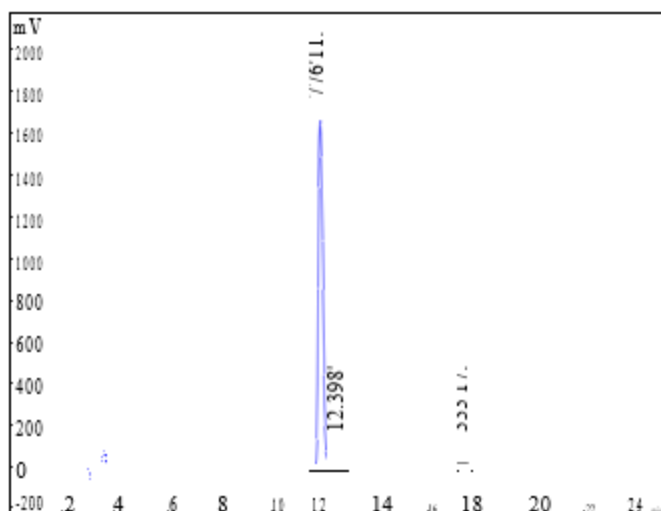
Gradient	A	B
0.1min	82	18
25min	57	43
25.01min	0	100
30min	0	100

Flow rate: 1.0ml/min

Wavelength(nm): 220

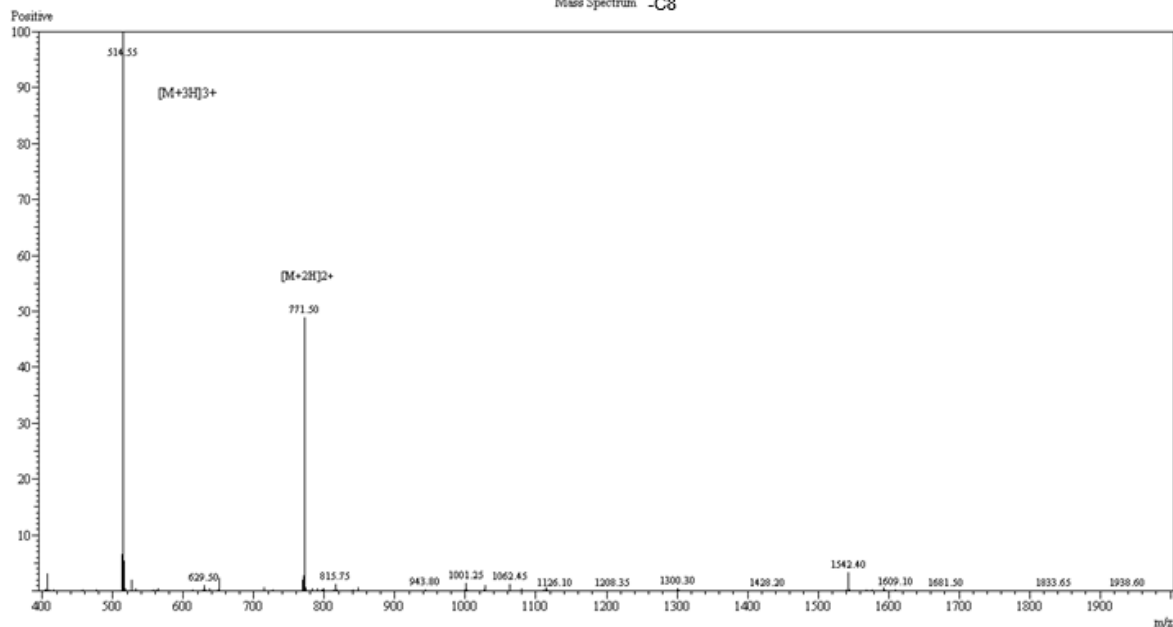
Volume: 10ul

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Rank	Time	Conc.	Area	Height
1	11.776	98.29	18104182	1647984
2	12.398	1.333	245526	17448
3	17.333	0.3786	69734	8281
Total		100	18419442	1673713

Mass Spectrum -C8



Sample Information
 Date and Time : 2020-1-10 9:34:35
 User : CHAO
 Sample : CT8 LG-12
 Inj. Volume : 1
 MW : 1540.94
 Lot No. : P200106-MJ772757

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C
 Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H₂O/50%ACN

REPORT -C8

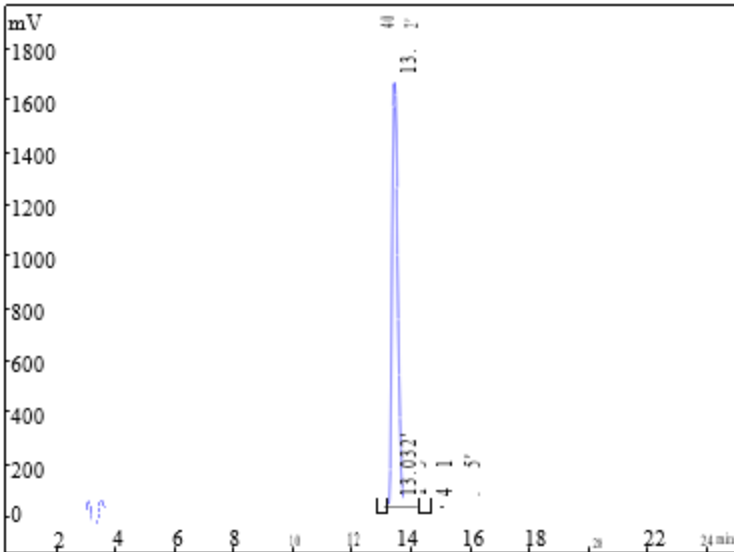
Sample Description:

Structure : C8 LG-12
 Number : 010250011
 Lot No : P200106-MJ772757
 Column : 4.6×250mm, Kromasil 100-5C18
 Solvent A : 0.1% trifluoroacetic in 100% acetonitrile
 Solvent B : 0.1% trifluoroacetic in 100% water
 Gradient :
 0.01min 30% 70%
 25min 55% 45%
 25.1min 100% 0%
 30min STOP

Flow rate : 1.0 mL/min

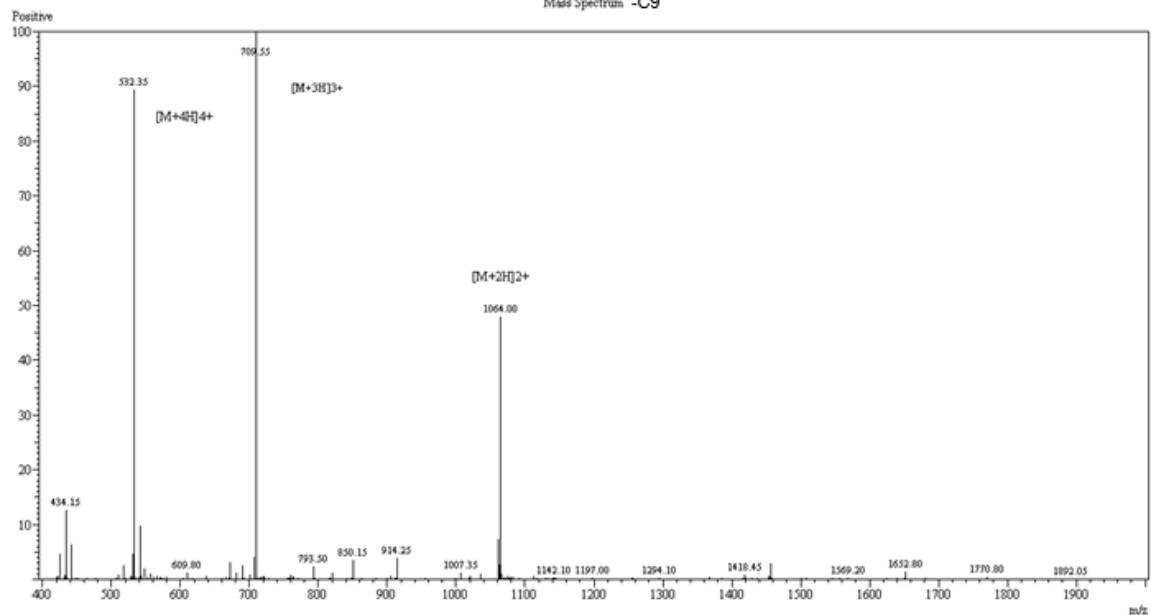
Wavelength : 220nm

Volume : 5ul



Rank	Time	Conc.	Area	Height
1	13.032	0.07746	15879	1457
2	13.402	99.74	20446309	1630245
3	14.515	0.1841	37739	2304
Total		100	20499927	1634006

Mass Spectrum -C9

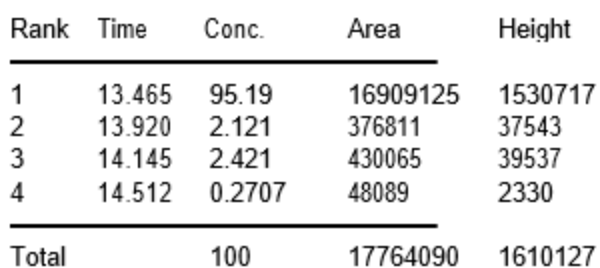


Sample Information
 Date and Time : 2020-1-13 12:23:10
 User : CHAO
 Sample : CT9 LR-16
 Inj. Volume : 1
 MW : 2125.62
 Lot No. : P200106-MJ772758

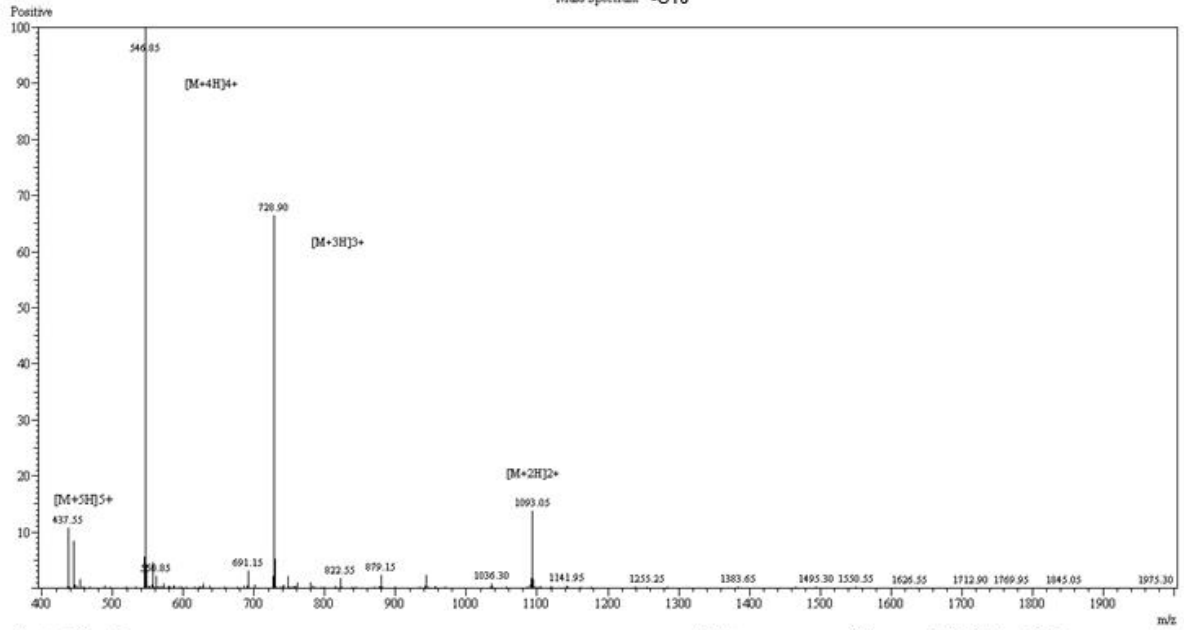
Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C
 Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H2O/50%ACN

Sample Description:

Volume : 5ul



Mass Spectrum -C10



Sample Information
 Date and Time : 2020-1-9 9:55:14
 User : CHAO
 Sample : CT10 LR-16
 Inj. Volume : 1
 MW : 2183.66
 Lot No. : P200106-MJ772759

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C

Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H₂O/50%ACN

REPORT -C10

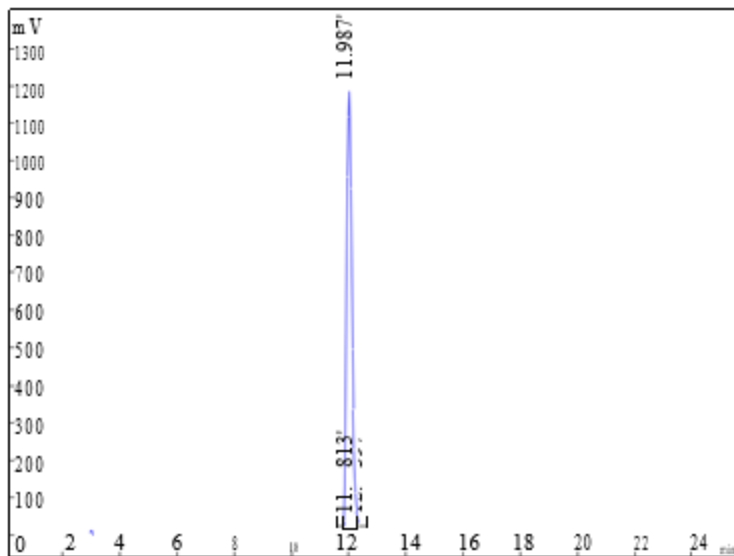
Sample Description:

Structure : C10 LR-16
 Number : 010250011
 Lot No : P200106-MJ772759
 Column : 4.6×250mm, Kromasil 100-5C18
 Solvent A : 0.1% trifluoroacetic in 100% acetonitrile
 Solvent B : 0.1% trifluoroacetic in 100% water
 Gradient :
 A B
 0.01min 23% 77%
 25min 48% 52%
 25.1min 100% 0%
 30min STOP

Flow rate : 1.0 mL/min

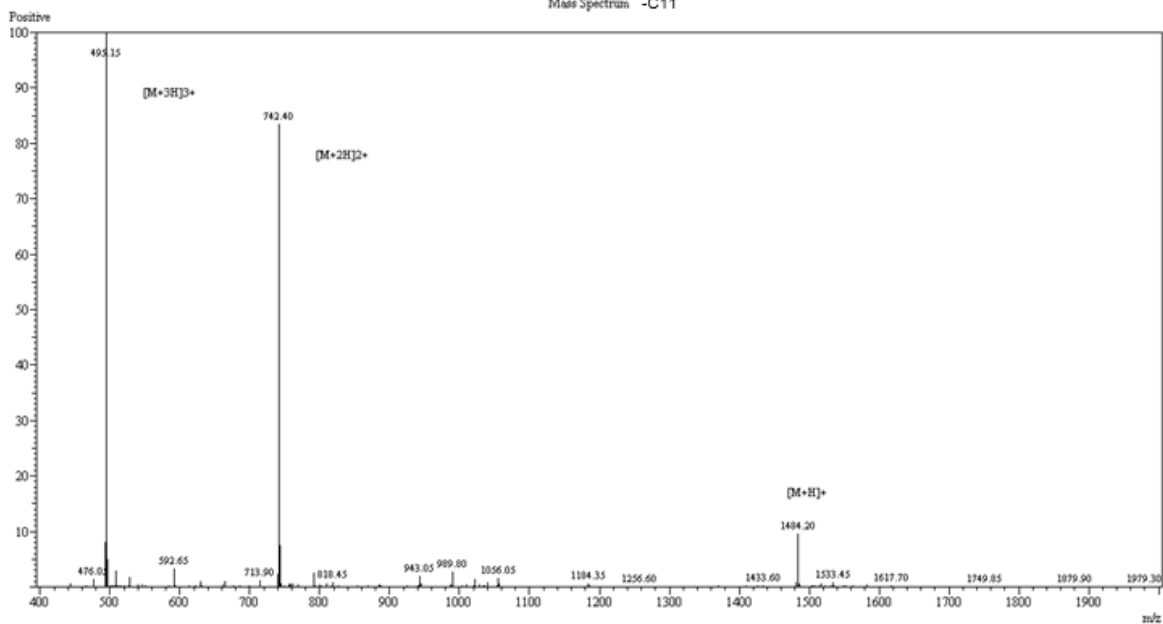
Wavelength : 220nm

Volume : 5ul



Rank	Time	Conc.	Area	Height
1	11.813	0.05078	6674	3423
2	11.987	99.88	13127402	1163632
3	12.397	0.06902	9071	2290
Total		100	13143147	1169345

Mass Spectrum -C11



Sample Information
 Date and Time : 2020-1-10 11:52:37
 User : CHAO
 Sample : CT11 LG-12
 Inj. Volume : 1
 MW : 1482.90
 Lot No. : P200106-MJ772761

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C
 Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H2O/50%ACN

REPORT -C11

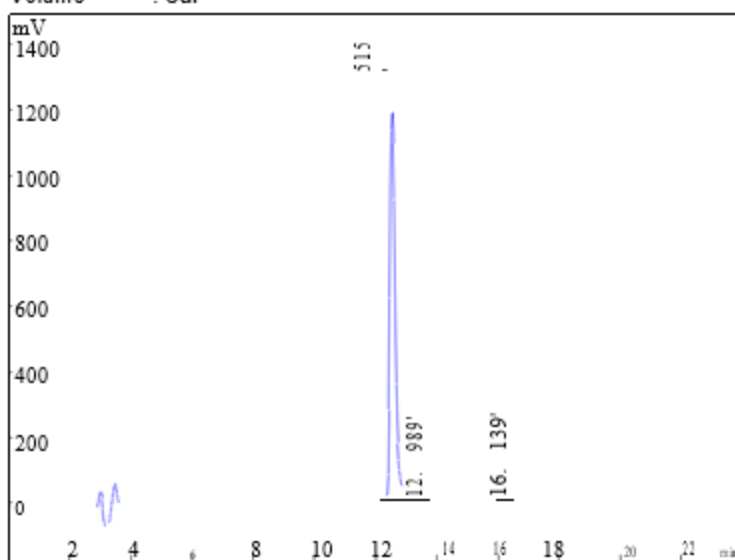
Sample Description:

Structure : C11 LG-12
 Number : 010250011
 Lot No : P200106-MJ772761
 Column : 4.6×250mm, Kromasil 100-5C18
 Solvent A : 0.1% trifluoroacetic in 100% acetonitrile
 Solvent B : 0.1% trifluoroacetic in 100% water
 Gradient :
 0.01min A B
 25min 40% 60%
 25.1min 100% 0%
 30min STOP

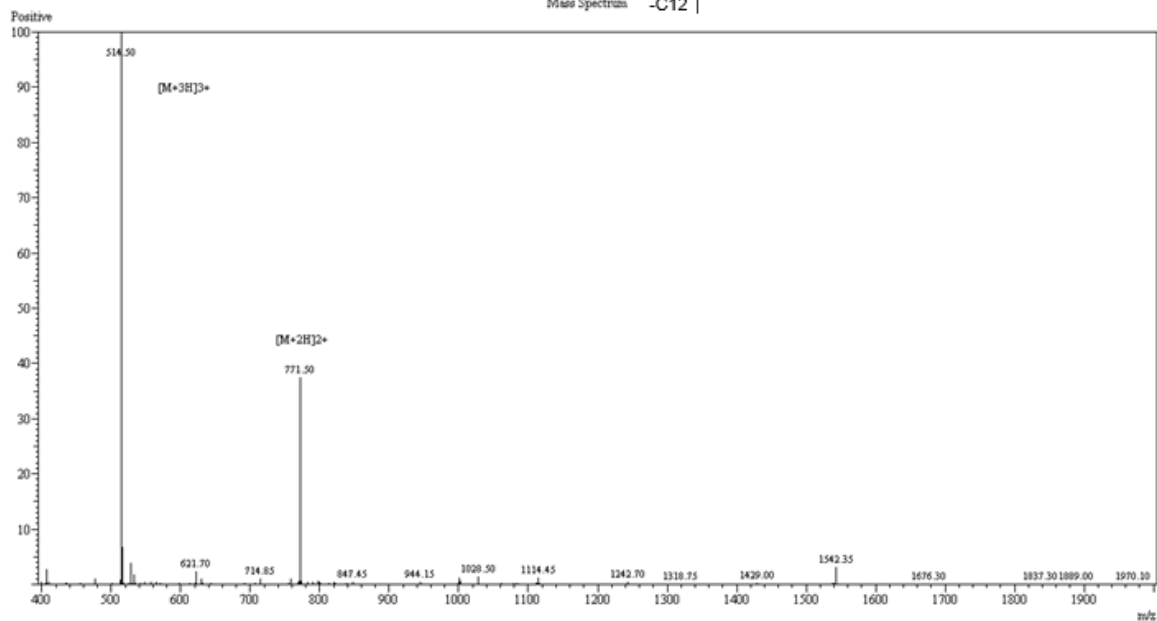
Flow rate : 1.0 mL/min

Wavelength : 220nm

Volume : 5ul



Rank	Time	Conc.	Area	Height
1	12.515	97.18	12279866	1171072
2	12.989	1.335	168682	16519
3	16.139	1.487	187850	16220
Total		100	12636398	1203811



Sample Information

Date and Time : 2020-1-9 9:55:14
User : CHAO
Sample : CT12 LG-12
Inj. Volume : 1
MW : 1540.94
Lot No. : P200106-MJ772762

Probe: ESI
Nebulizer Gas Flow: 1.5L/min
DL: -20.0v
DL Temp: 250°C
Block Temp: 200°C

Probe bias: -3.5kv
Detector: 1.0kv
T. Flow: 0.2ml/min
B. conc: 50%H2O/50%ACN

HPLC
REPORT -C12

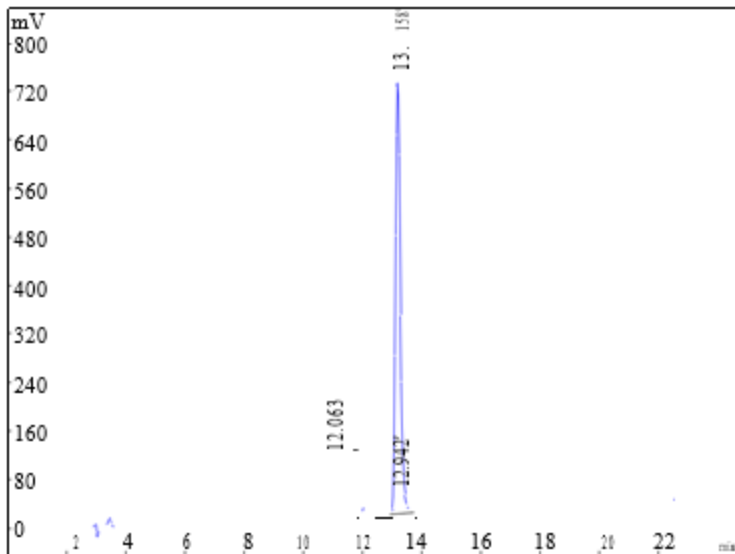
Sample Description:

Structure	C12 LG-12		
Number	010250011		
Lot No	P200106-MJ772762		
Column	4.6×250mm, Kromasil 100-5C18		
Solvent A	0.1% trifluoroacetic in 100% acetonitrile		
Solvent B	0.1% trifluoroacetic in 100% water		
Gradient		A	B
	0.01min	23%	77%
	25min	48%	52%
	25.1min	100%	0%
	30min	STOP	

Flow rate : 1.0 mL/min

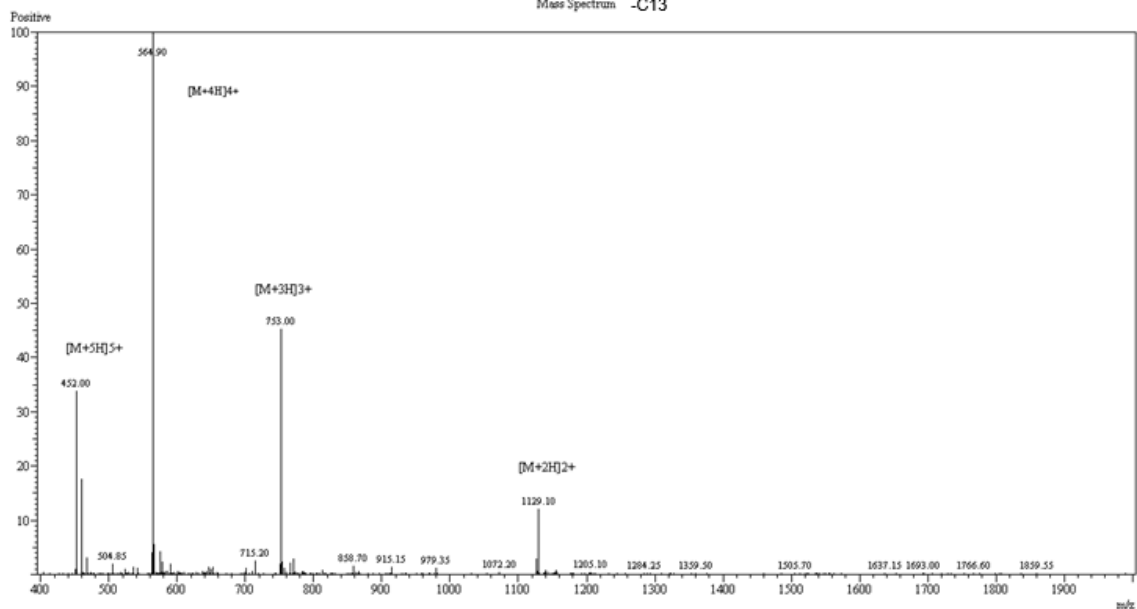
Wavelength : 220nm

Volume : 5ul



Rank	Time	Conc.	Area	Height
1	12.063	1.973	149559	15778
2	12.942	0.5075	38476	3629
3	13.158	97.52	7393997	711646
Total		100	7582032	731053

Mass Spectrum -C13



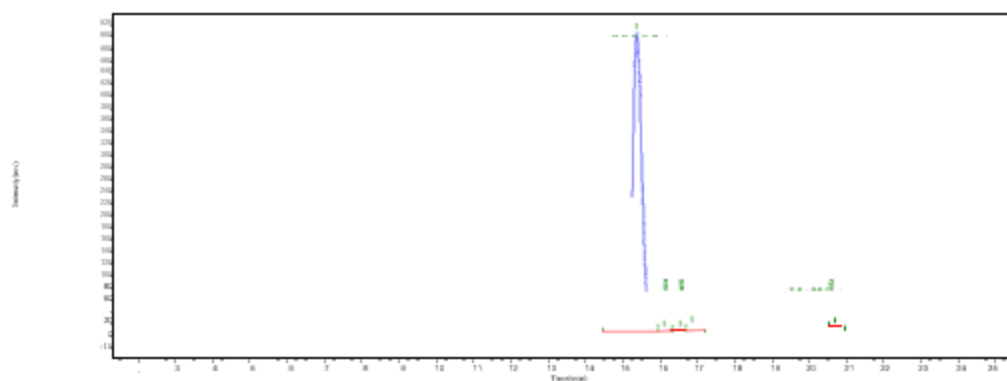
Sample Information
 Date and Time : 2020-2-21 15:27:44
 User : CHAO
 Sample : LR-16
 Inj. Volume : 1
 MW : 2255.9
 Lot No. : P200211-MJ781299

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C

Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H2O/50%ACN

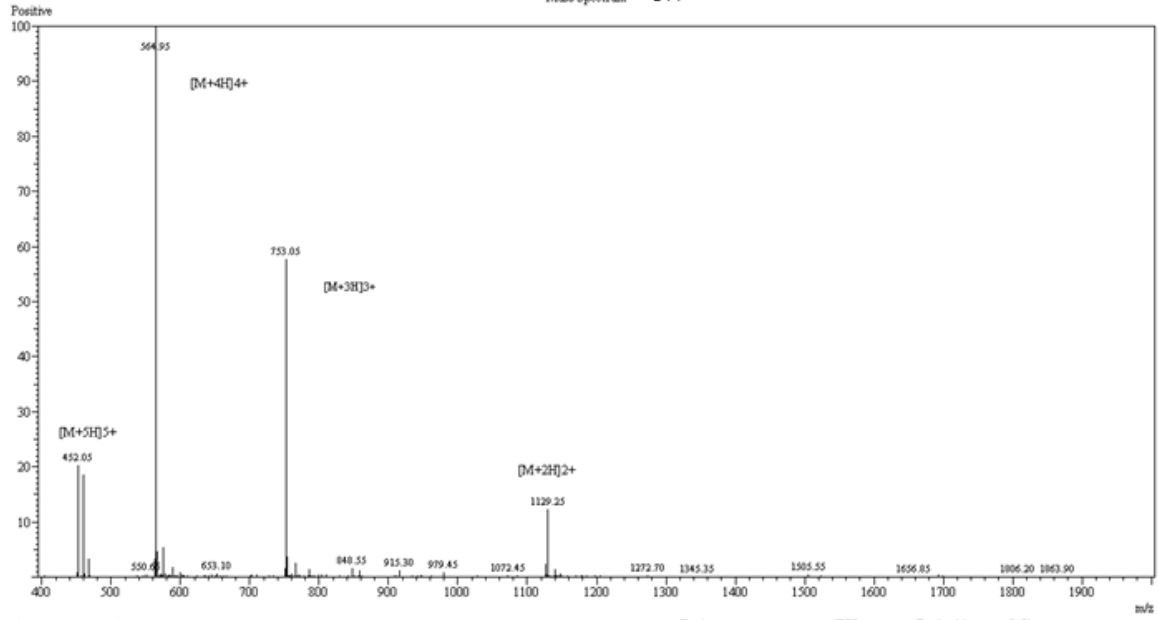
HPLC REPORT -C13

Structure : LR-16
 Number : 010250011
 Lot No : P200211-MJ781299
 Column : 4.6×250mm, Kromasil 100-5C18
 Solvent A : 0.1% trifluoroacetic in 100% acetonitrile
 Solvent B : 0.1% trifluoroacetic in 100% water
 Gradient :
 A B
 0.01min 25% 75%
 25min 50% 50%
 25.1min 100% 0%
 30min STOP
 Flow rate : 1.0 mL/min
 Wavelength : 220nm
 Volume : 5ul



Peak No.	Ret Time	Height	Area	Conc.
1	15.372	505074.031	8256661.500	95.2012
2	16.133	6648.099	117775.125	1.3580
3	16.533	6634.114	104721.688	1.2075
4	16.863	13236.716	148107.047	1.7077
5	20.707	5123.034	45587.508	0.5256
Total				100.0000

Mass Spectrum -C14



Sample Information
 Date and Time : 2020-2-21 9:42:46
 User : CHAO
 Sample : LR-16
 Inj. Volume : 1
 MW : 2255.90
 Lot No. : P200211-MJ781300

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C
 Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H₂O/50%ACN

HPLC -C14

Sample Description:

Analyst:YSC

Structure:LR-16

Lot NO.:P200211-MJ781300

Number:0200193

Column:250*4.6mm, Boston Green ODS-AQ

Solvent A:0.1%TFA in 100%water

Solvent B:0.1%TFA in 100%acetonitrile

Gradient :

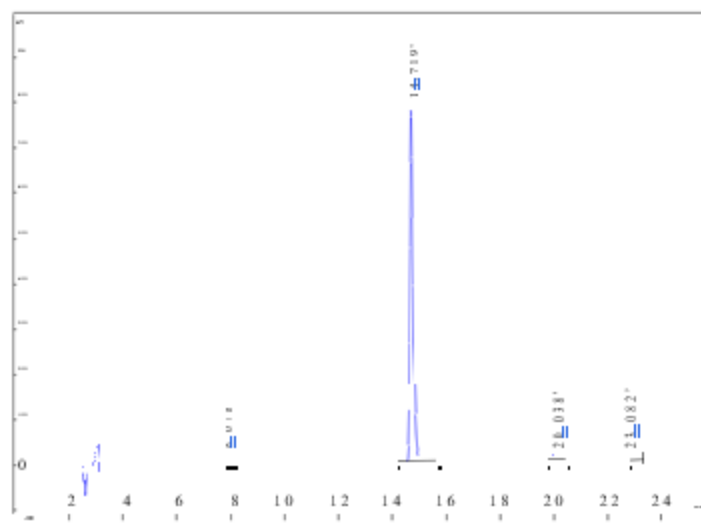
	A	B
0.1min	75	25
25min	50	50
25.01min	0	100
30min	0	100

Flow rate:1.0ml/min

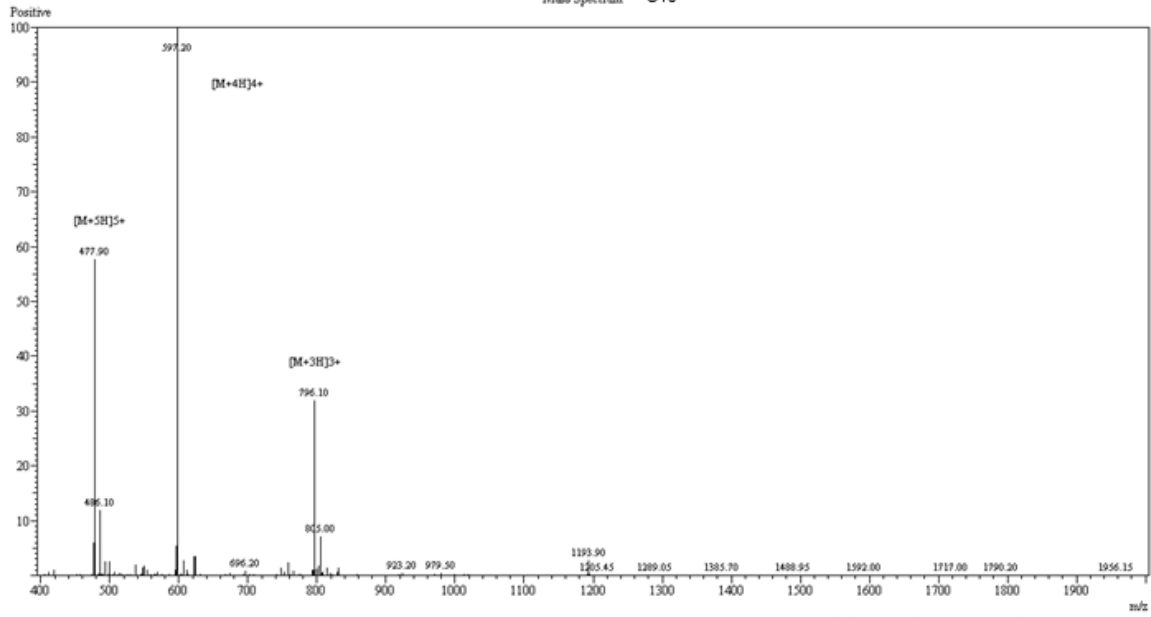
Wavelength(nm):220

Volume:10ul

File opened: D:\2020 HPLC\LR-16-F 781300 200221.hw, where



Rank	Time	Conc.	Area	Height
1	8.078	1.48	105399	11826
2	14.719	95.32	6787298	773221
3	20.038	2.09	148802	15692
4	23.082	1.109	78945	6547
Total		100	7120444	807286



Sample Information

Date and Time : 2020-2-20 10:02:03
User : CHAO
Sample : LR-16
Inj. Volume : 1
MW : 2385.05
Lot No. : P200211-MJ781301

Probe: ESI
Nebulizer Gas Flow: 1.5L/min
DL: -20.0v
DL Temp: 250°C
Block Temp: 200°C
Probe bias: -3.5kv
Detector: 1.0kv
T. Flow: 0.2ml/min
B. conc: 50%H₂O/50%ACN

HPLC

-C15

Sample Description:

Analyst:YSC

Structure:LR-16

Lot NO.:P200211-MJ781301

Number:0200193

Column:250*4.6mm, Boston Green ODS-AQ

Solvent A:0.1%TFA in 100%water

Solvent B:0.1%TFA in 100%acetonitrile

Gradient :

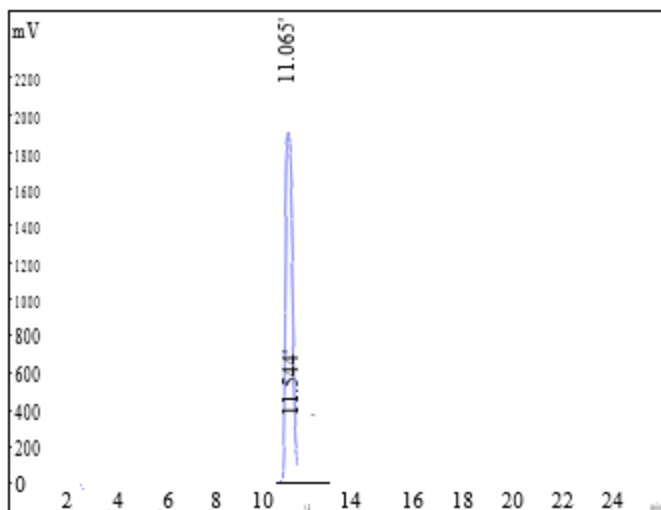
	A	B
0.1min	72	28
25min	47	53
25.01min	0	100
30min	0	100

Flow rate:1.0ml/min

Wavelength(nm):220

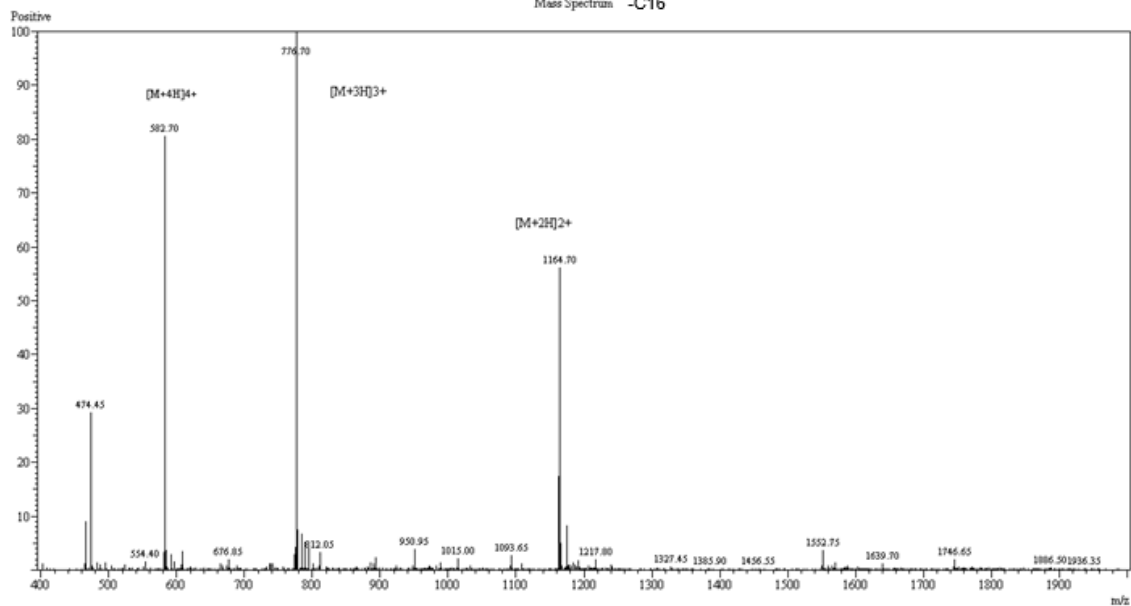
Volume:10ul

File opened: D:\2020\LR-16-F 781301 200220.hw, where



Rank	Time	Conc.	Area	Height
1	11.065	95.39	33221322	1891078
2	11.544	1.612	561229	42355
3	11.946	1.172	408038	24898
4	12.151	1.825	635470	22013
Total		100	34826059	1980344

Mass Spectrum -C16



Sample Information
 Date and Time : 2020-2-21 15:27:44
 User : CHAO
 Sample : LR-16
 Inj. Volume : 1
 MW : 2327.02
 Lot No. : P200211-MJ781302

Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C
 Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H₂O/50%ACN

HPLC REPORT -C16

Structure: LR-16

Number : 010250011

Lot No : P200211-MJ781302

Column : 4.6×250mm,Kromasil 100-5C18

Solvent A: 0.1% trifluoroacetic in 100% acetonitrile

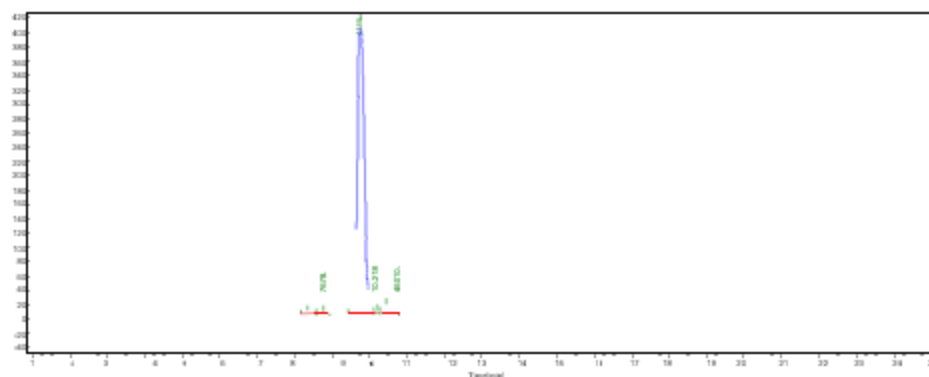
Solvent B: 0.1% trifluoroacetic in 100% water

Gradient	:	A	B
0.01min		20%	80%
25min		45%	55%
25.1min		100%	0%
30min		STOP	

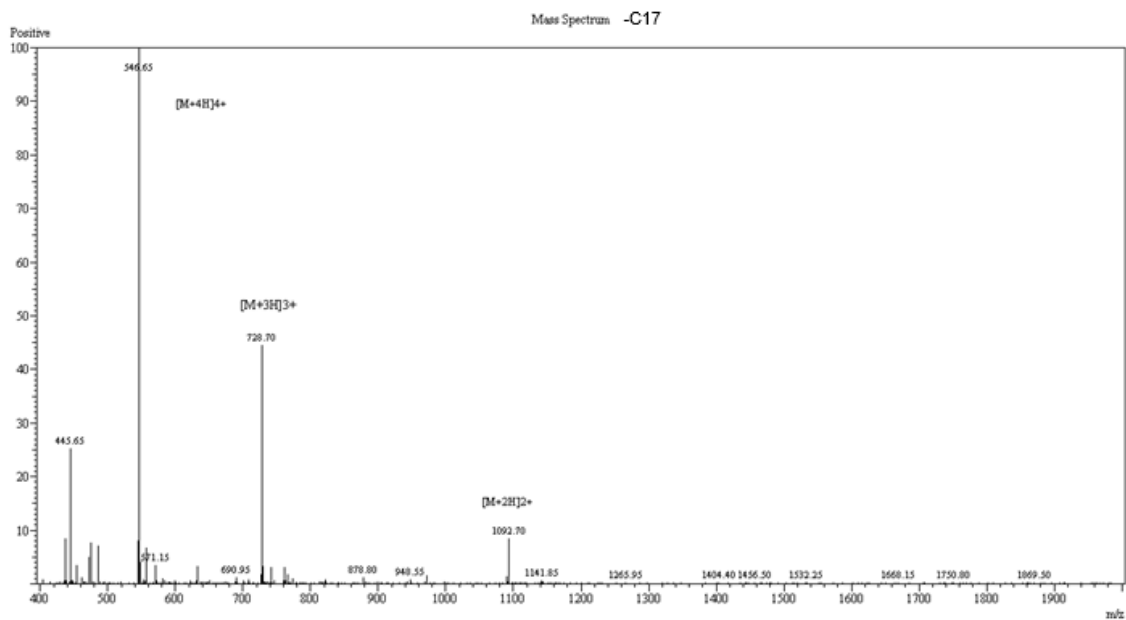
Flow rate : 1.0 mL/min

Wavelength : 220nm

Volume : 5ul



Peak No.	Ret Time	Height	Area	Conc.
1	8.347	3069.753	29357.186	0.5490
2	8.767	1570.017	15336.174	0.2868
3	9.775	409044.438	5160713.000	96.5070
4	10.218	3022.122	25842.918	0.4833
5	10.460	11414.246	116253.805	2.1740
Total				100.0000



Sample Information
Date and Time : 2020-2-21 9:42:46
User : CHAO
Sample : LR-16
Inj. Volume : 1
MW : 2182.85
Lot No. : P200211-MJ781303

Probe: ESI
Nebulizer Gas Flow: 1.5L/min
DL: -20.0v
DL Temp: 250°C
Block Temp: 200°C
Probe bias: -3.5kv
Detector: 1.0kv
T. Flow: 0.2ml/min
B. conc: 50%H₂O/50%ACN

HPLC -C17

Sample Description:

Analyst:YSC

Structure:LR-16

Lot NO. :P200211-MJ781303

Number:0200193

Column:250*4.6mm, Boston Green ODS-AQ

Solvent A:0.1%TFA in 100%water

Solvent B:0.1%TFA in 100%acetonitrile

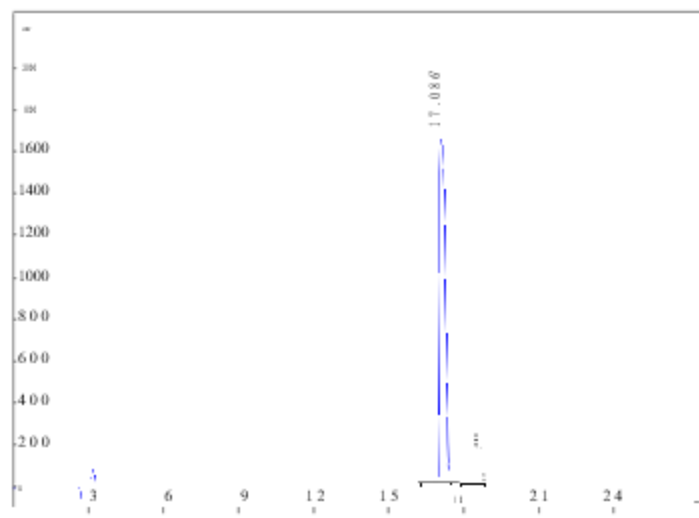
Gradient :	A	B
0.1min	80	20
25min	55	45
25.01min	0	100
30min	0	100

Flow rate:1.0ml/min

Wavelength(nm):220

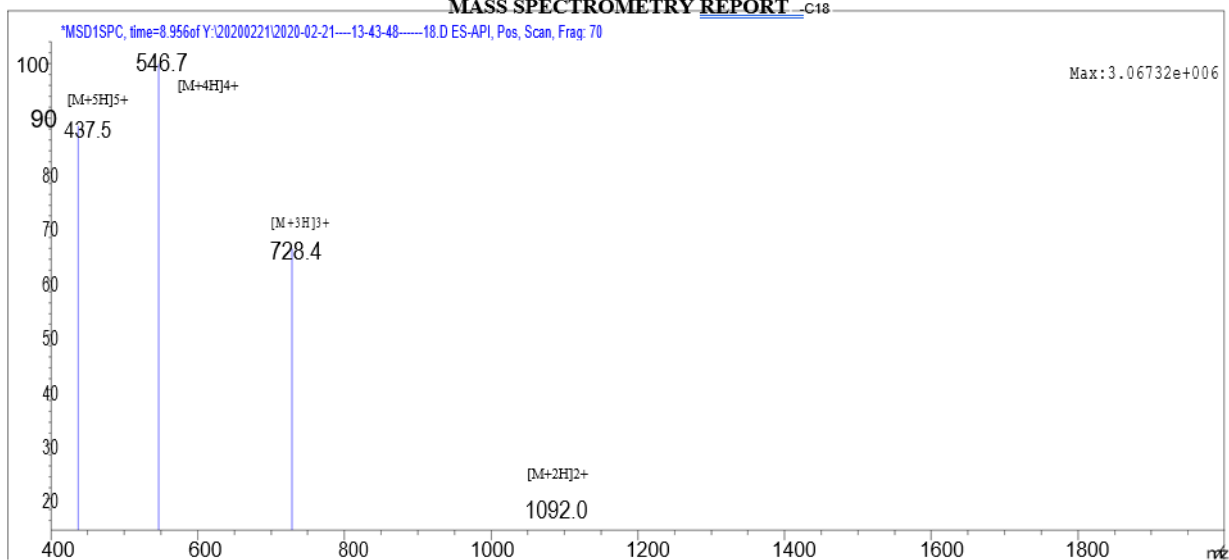
Volume:10ul

File opened: D:\2020 HPLC\LR-16-F 781303 200221(20200221 20:51:59).hw, where



Rank	Time	Conc.	Area	Height
1	17.086	99.09	24899485	1636224
2	17.880	0.9064	227739	11594
Total		100	25127224	1647818

MASS SPECTROMETRY REPORT C18



Sample Description

Analyzed date: 2020-02-21
 Analyst: YU
 Sample: LR-16
 M.W.: 2182.85
 Lot No.: P200211-MJ781304

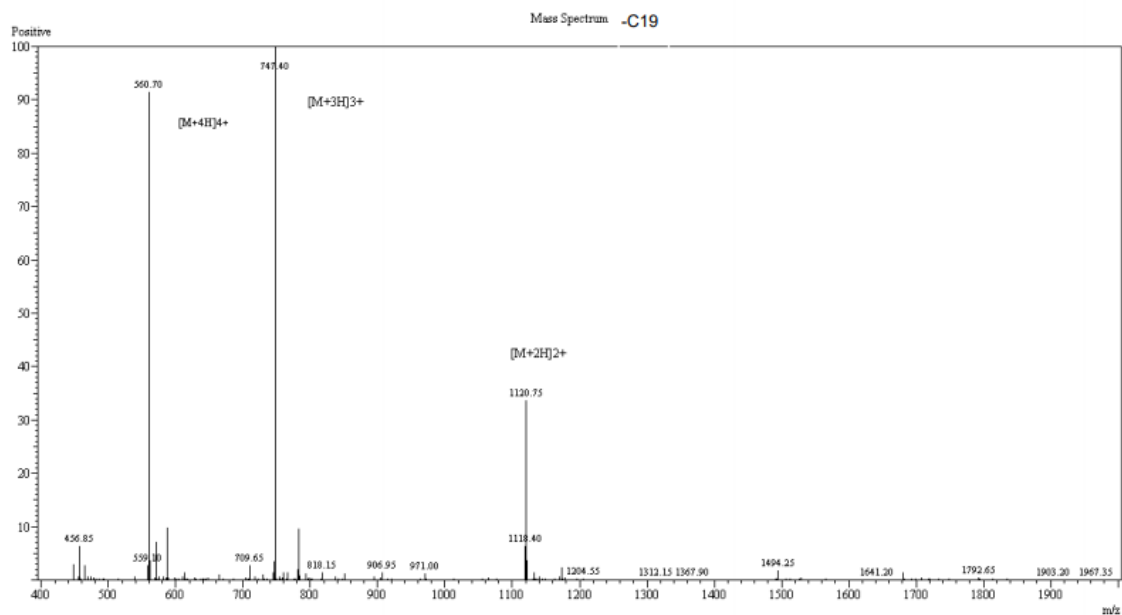
Instrument

Agilent-6125B
 Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 CDL: -20.0v
 CDL Temp.: 250 °C
 Block Temp.: 200 °C

Probe Bias: +4.5kv
 Detector: 1.5kv
 T. Flow: 0.2ml/min
 B. Conc.: 50%H₂O/50%ACN

100



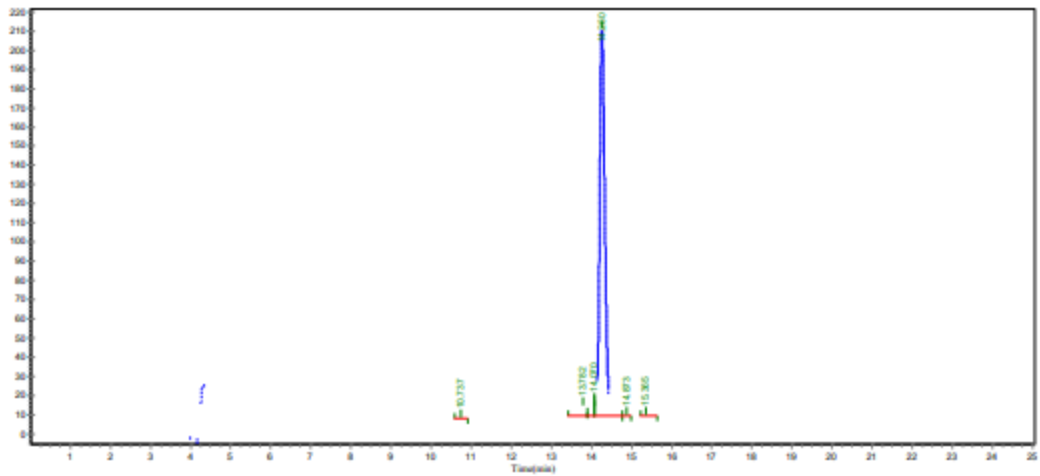


Sample Information
Date and Time : 2020-2-21 9:24:34
User : CHAO
Sample : LR-16
Inj. Volume : 1
MW : 2238.95
Lot No. : P200211-MJ781305

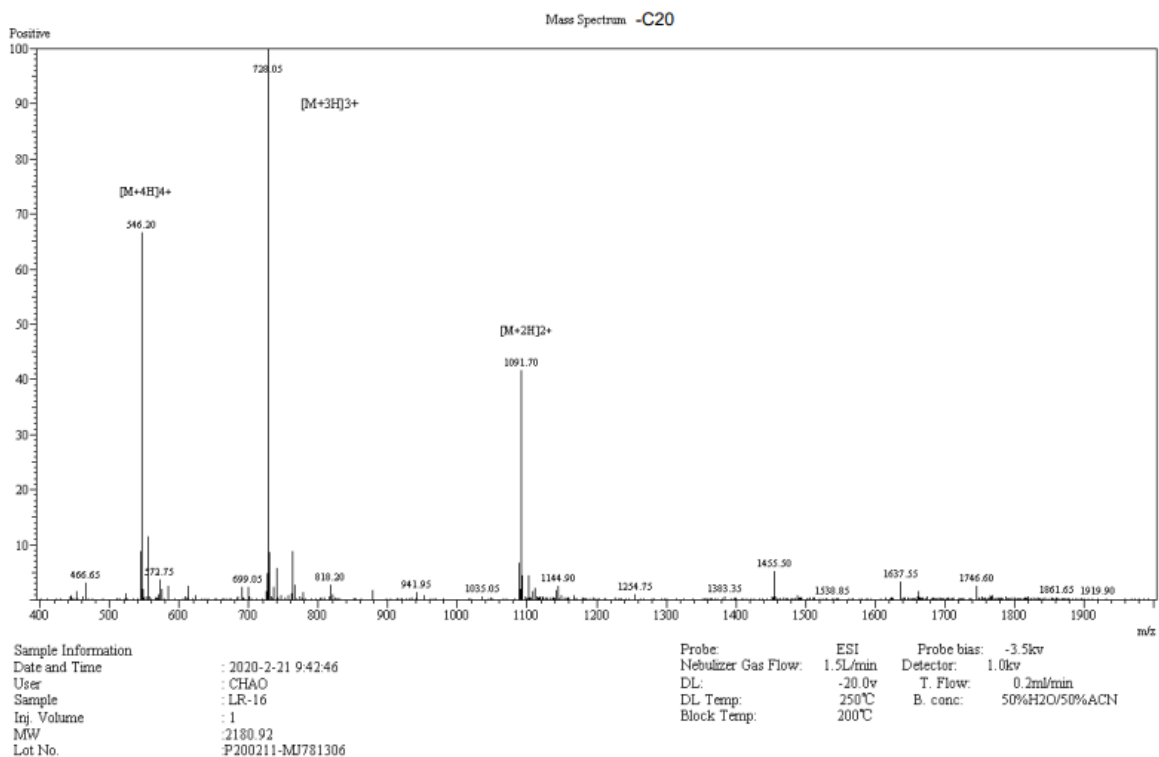
Probe:	ESI	Probe bias:	-3.5kv
Nebulizer Gas Flow:	1.5L/min	Detector:	1.0kv
DL:	-20.0v	T. Flow:	0.2ml/min
DL Temp:	250°C	B. conc:	50%H2O/50%ACN
Block Temp:	200°C		

-C19

Structure	: LR-16		
Number	: 010250011		
Lot No	: P200211-MJ781305		
Column	: 4.6×250mm,Sincochrom ODS-BP 5		
Solvent A	: 0.1% trifluoroacetic in 100% acetonitrile		
Solvent B	: 0.1% trifluoroacetic in 100% water		
Gradient		A	B
	0.01min	37%	63%
	25min	62%	38%
	25.1min	100%	0%
	30min	STOP	
Flow rate	: 1.0 mL/min		
Wavelength	: 220nm		
Volume	: 5ul		



Peak No.	Ret Time	Height	Area	Conc..
1	10.737	379.749	2989.092	0.1562
2	13.782	5546.957	44716.340	2.3364
3	14.070	7557.202	35563.609	1.8582
4	14.260	201991.625	1824847.500	95.3487
5	14.873	438.334	2991.183	0.1563
6	15.365	382.416	2760.492	0.1442
Total				100.0000



HPLC -C20

Sample Description:

Analyst:YSC

Structure:LR-16

Lot NO.:P200211-MJ781306

Number:0200193

Column:250*4.6mm, Boston Green ODS-AQ

Solvent A:0.1%TFA in 100%water

Solvent B:0.1%TFA in 100%acetonitrile

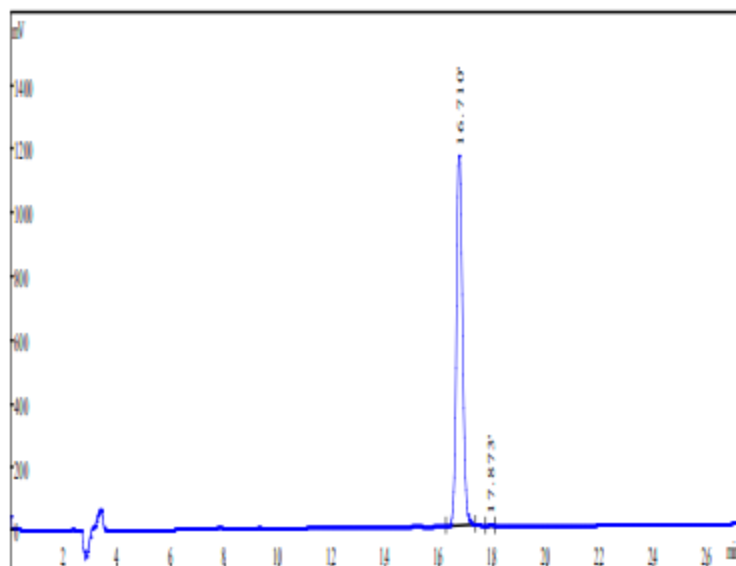
Gradient :	A	B
0.1min	72	28
25min	47	53
25.01min	0	100
30min	0	100

Flow rate:1.0ml/min

Wavelength(nm):220

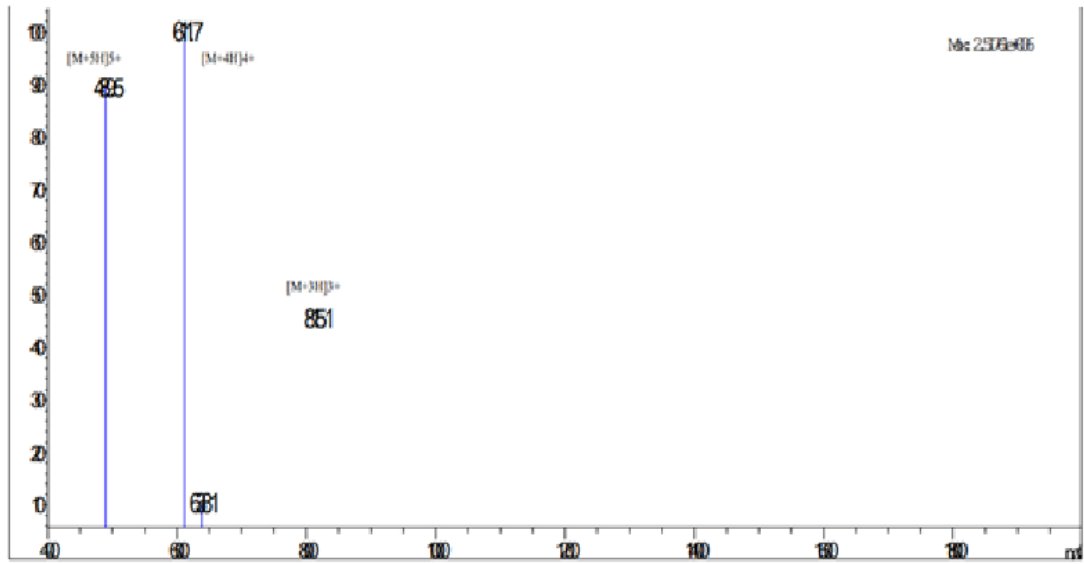
Volume:10ul

File opened: D:\2020\lr-16-f 781306 200221.hw, where



Rank	Time	Conc.	Area	Height
1	16.710	99.75	17259829	1164325
2	17.873	0.2534	43846	5362
Total		100	17303675	1169687

MASS SPECTROMETRY REPORT C21



Sample Description

Analyzed date: 2020-02-20
 Analyst: YU
 Sample: LR-16
 M.W.: 2443.08
 Lot. No.: P200211-MJ781307

Instrument

Agilent-6125B
 Probe: ESI
 Nebulizer Gas Flow: 1.5L/min
 CDL: -20.0v
 CDL Temp.: 250 °C
 Block Temp.: 200 °C

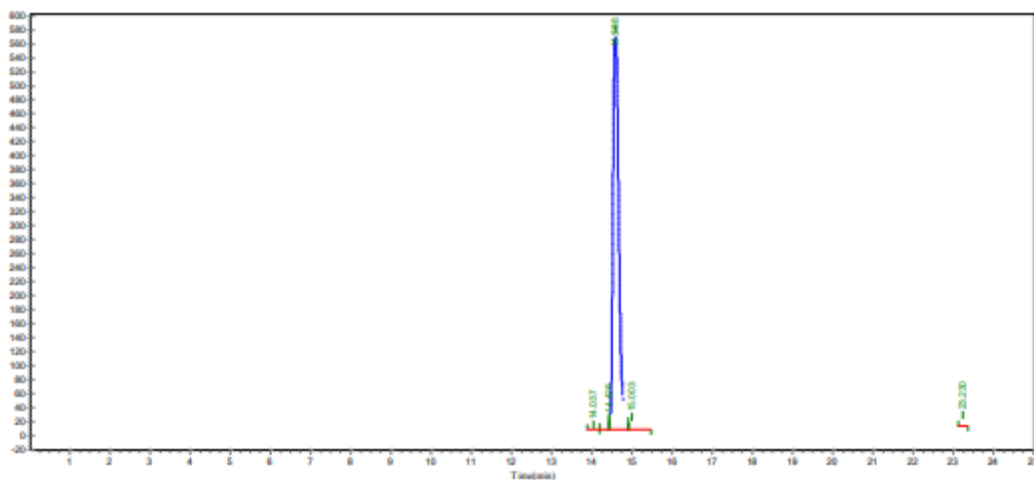
Probe Bias: +4.5kv
 Detector: 1.5kv
 T. Flow: 0.2ml/min
 B. Conc.: 50%H₂O/50%ACN

-C21

0.01min	32%	68%
25min	57%	43%
25.1min	100%	0%
30min	STOP	

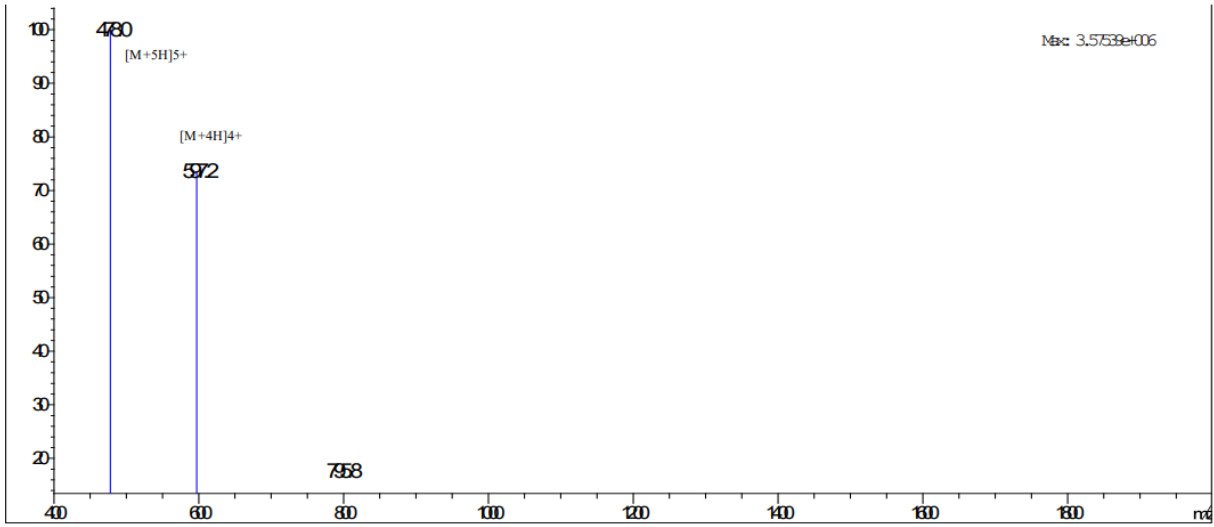
Wavelength : 220nm

: 5ul



Peak No.	Ret Time	Height	Area	Conc..
1	14.037	1349.542	15164.871	0.2547
2	14.428	10651.179	57934.039	0.9730
3	14.588	566633.000	5682708.500	95.4367
4	15.003	11920.900	130646.016	2.1941
5	23.230	9561.931	67972.742	1.1415
Total				100.0000

MASS SPECTROMETRY REPORT -C22



Sample Description	Instrument	Agilent-6125B
Analyzed date: 2020-02-29	Probe:	ESI
Analyst: YU	Nebulizer Gas Flow:	1.5L/min
Sample: LR-16	CDL:	-20.0v
M.W.: 2385.05	CDL Temp.:	250 °C
Lot. No.: P200211-MJ781308	Block Temp.:	200 °C
	Probe Bias:	+4.5kv
	Detector:	1.5kv
	T. Flow:	0.2ml/min
	B. Conc.:	50%H2O/50%ACN

REPORT -C22

Sample Description:

Structure : LR-16

Number : 0200046

Analyst : HCM

Lot# : P200211-MJ781308

Column : 4.6mm*250mm, Venusil XBP-C18

Solvent A : 0.1% trifluoroacetic in 100% acetonitrile

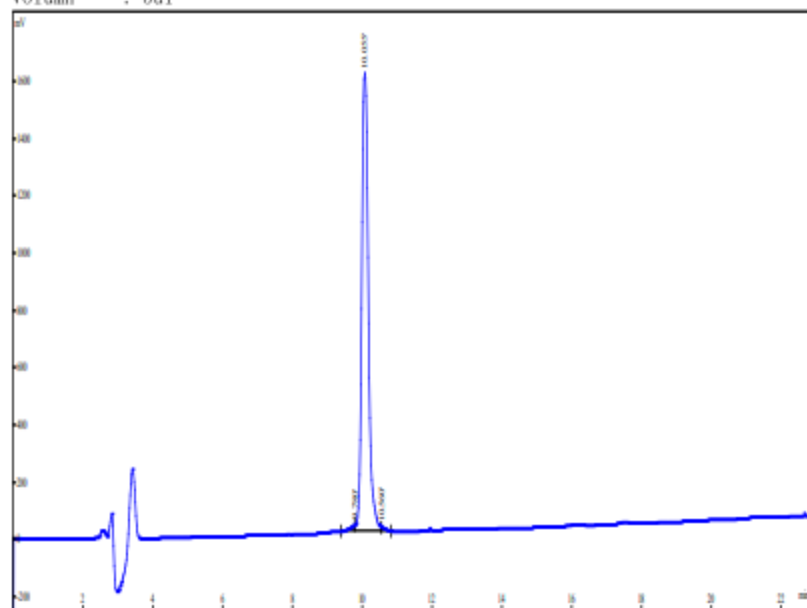
Solvent B : 0.1% trifluoroacetic in 100% water

Gradient	A	B
0.01min	32%	68%
25min	57%	43%
25.1min	100%	0%
30.0min	STOP	

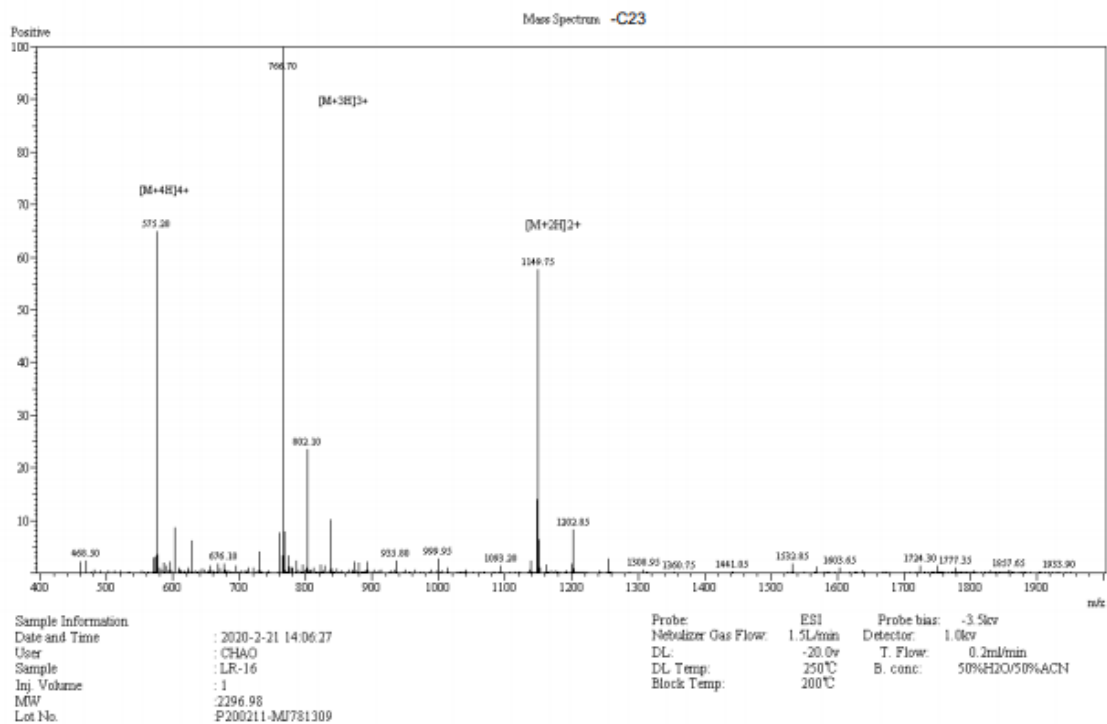
Flow rate : 1.0ml/min

Wavelength : 220nm

Volumn : 5ul



Rank	Time	Conc.	Area	Height
1	9.780	1.051	224028	23373
2	10.055	98.61	21029795	1603747
3	10.560	0.3382	72126	11790
Total		100	21325949	1638910



Structure : LR-16

Number : 010250011

Lot No :P200211-MJ781309

Column : 4.6×250mm,Kromasil 100-5C18

Solvent A : 0.1% trifluoroacetic in 100% acetonitrile

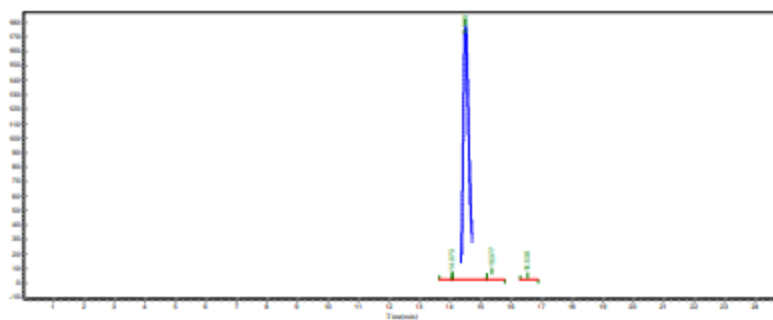
Solvent B : 0.1% trifluoroacetic in 100% water

Gradient	:	A	B
	0.01min	40%	60%
	25min	65%	35%
	25.1min	100%	0%
	30min	STOP	

Flow rate : 1.0 mL/min

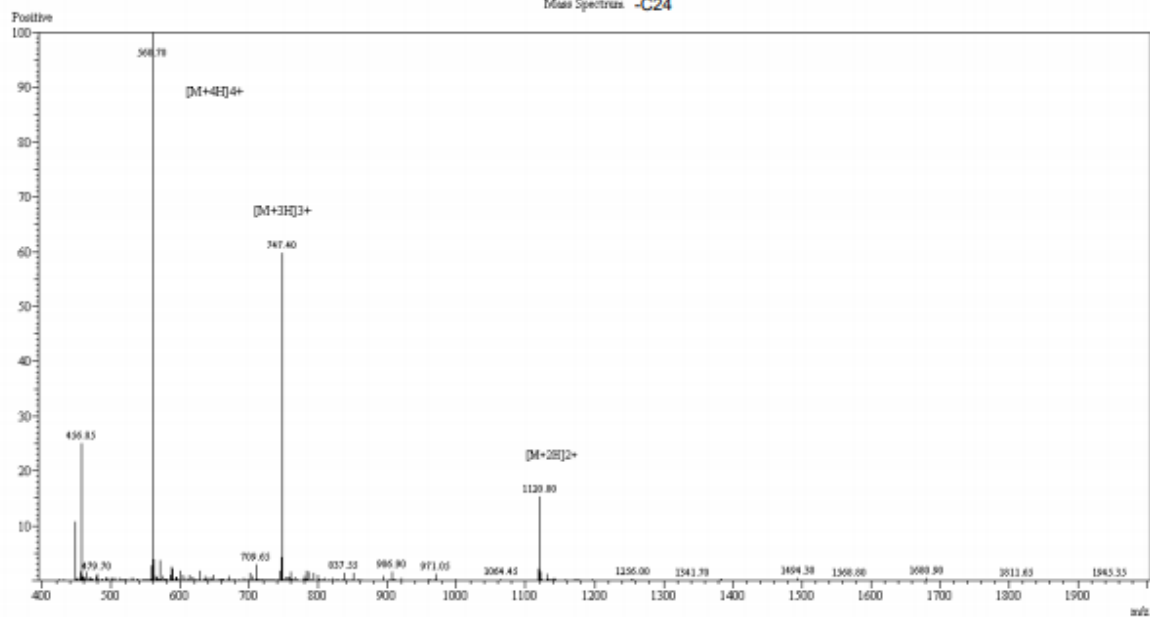
Wavelength : 220nm

Volume : 5ul



Peak No.	Ret Time	Height	Area	Conc.
1	14.073	1825.672	18094.828	0.7174
2	14.503	176059.781	2443543.500	96.8809
3	15.377	4032.513	50059.551	1.9847
4	16.538	723.222	10515.502	0.4169
Total				100.0000

Mass Spectra -C24



Sample Information

Date and Time : 2020-2-20 8:35:04
 User : CHAO
 Sample : LR-16
 Inj Volume : 1
 MW : 2238.95
 Lot No. : P200211-MJ781310

Probe

Nebulizer Gas Flow: 1.5L/min
 DL: -20.0v
 DL Temp: 250°C
 Block Temp: 200°C

ESI

Probe bias: -3.5kv
 Detector: 1.0kv
 T. Flow: 0.2ml/min
 B. conc: 50%H₂O/50%ACN

HPLC REPORT -C24

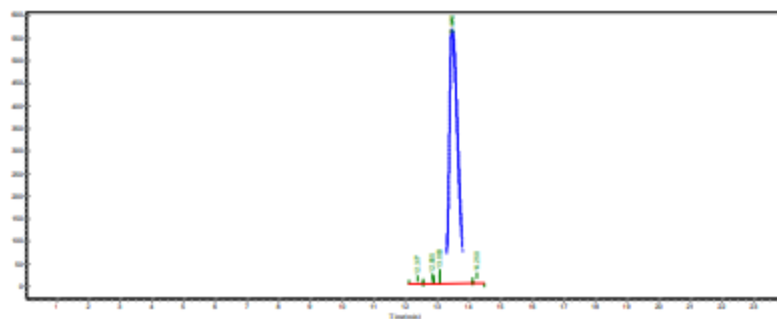
Structure : LR-16
 Number : 010250011
 Lot No : P200211-MJ781310
 Column : 4.6×250mm,Kromasil 100-5C18
 Solvent A : 0.1% trifluoroacetic in 100% acetonitrile
 Solvent B : 0.1% trifluoroacetic in 100% water
 Gradient :

	A	B
0.01min	33%	67%
25min	58%	42%
25.1min	100%	0%
30min	STOP	

Flow rate : 1.0 mL/min

Wavelength : 220nm

Volume : 5ul



Peak No.	Ret Time	Height	Area	Conc.
1	12.377	5375.193	79238.063	0.7020
2	12.855	9943.389	137947.328	1.2222
3	13.083	19111.195	148997.516	1.3201
4	13.478	575532.500	10801205.000	95.6957
5	14.250	11149.404	119639.859	1.0600
Total				100.0000