Fig. 1

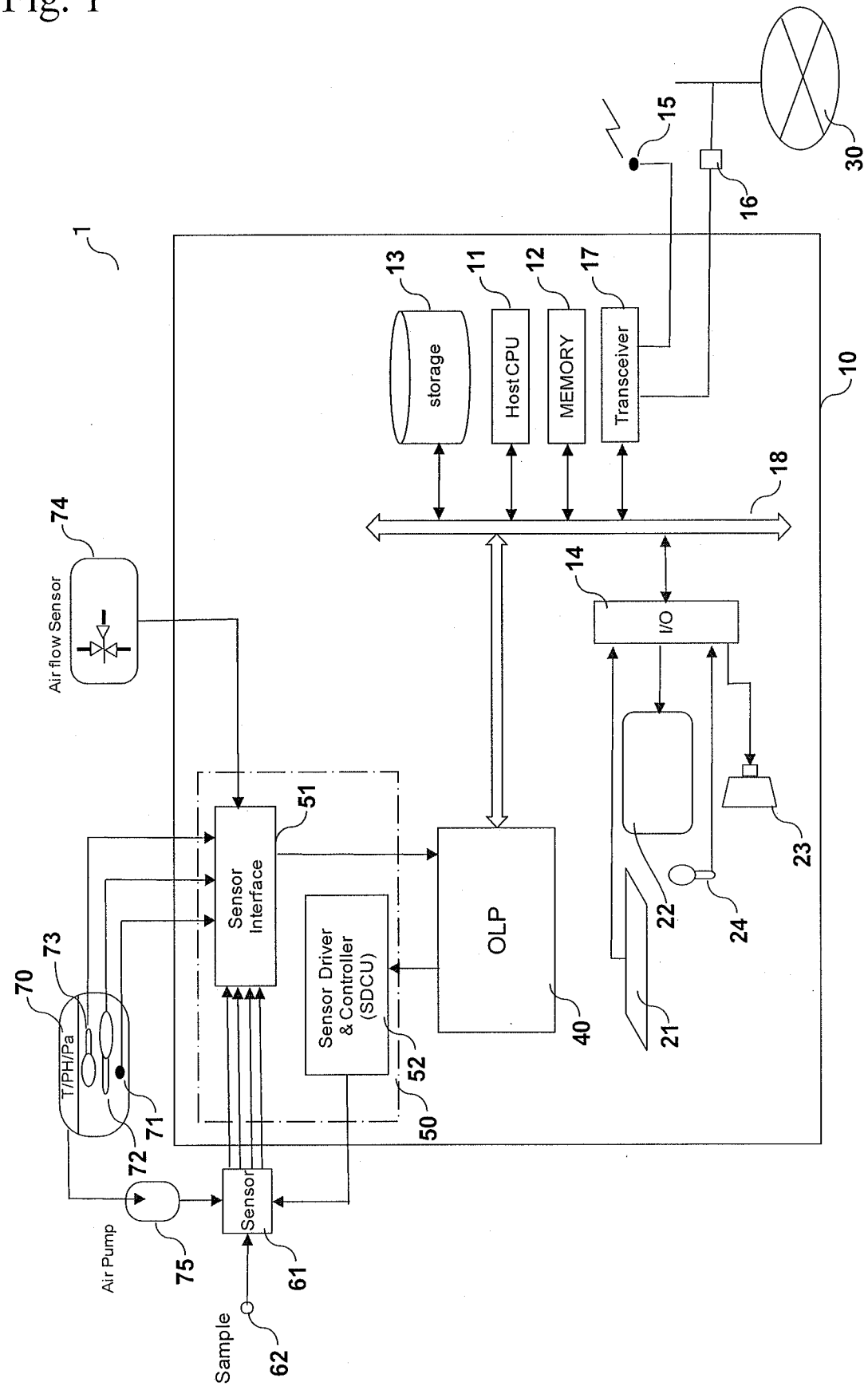

1
10
13
storage
11
Host CPU
12
MEMORY
17
Transceiver
15
16
30
18
14
I/O
74
Air flow Sensor
51
Sensor Interface
OLP
40
Sensor Driver & Controller (SDCU)
52
50
70
73
T/PH/Pa
71
72
Sensor
61
Air Pump
75
Sample
62
21
22
23
24

Fig. 2

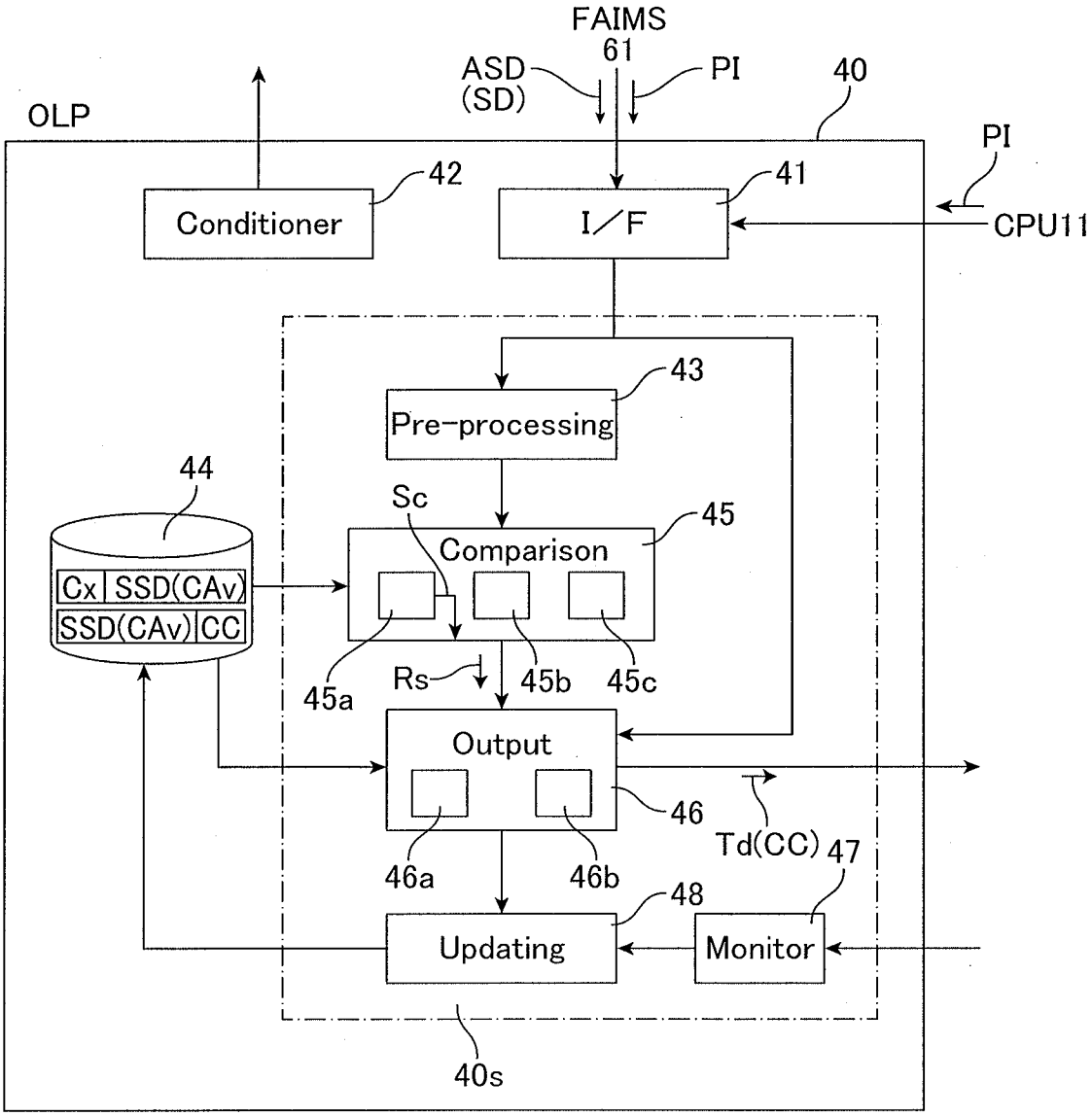

FAIMS
61
ASD
(SD)
PI
40
OLP
PI
42
41
Conditioner
I／F
CPU11
43
Pre-processing
44
Sc
45
Comparison
Cx
SSD(CAv)
SSD(CAv)
CC
45a
Rs
45b
45c
Output
46
Td(CC)
47
46a
46b
48
Updating
Monitor
40s

Fig. 3

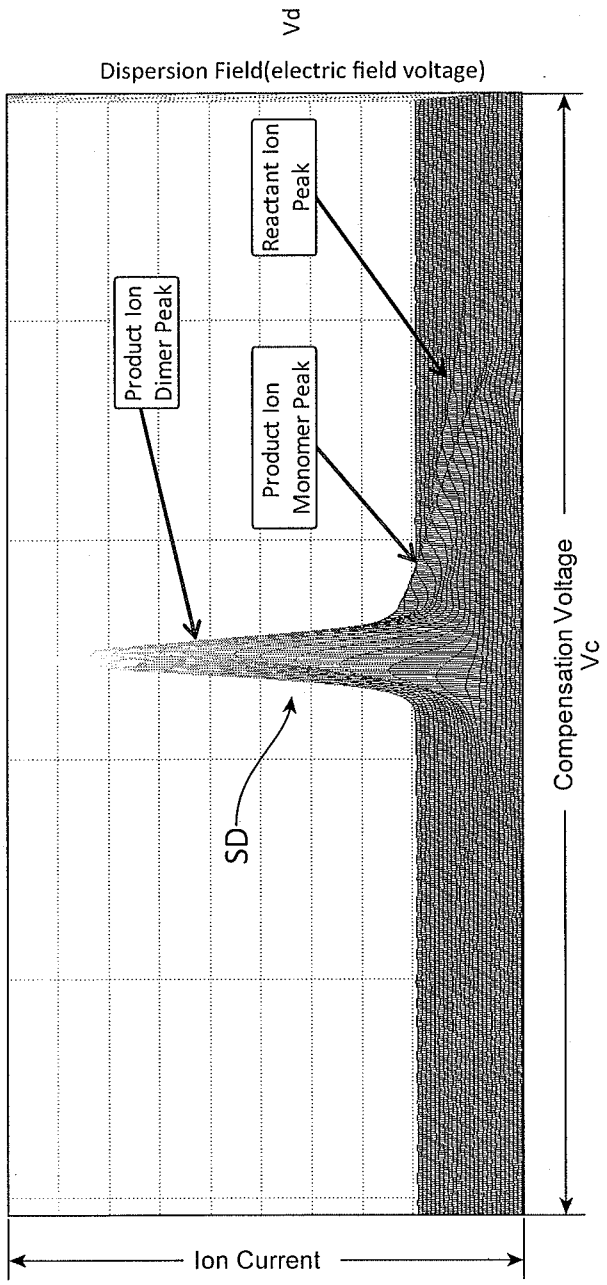

Vd
Dispersion Field(electric field voltage)
Reactant Ion Peak
Product Ion Dimer Peak
Product Ion Monomer Peak
SD
Compensation Voltage Vc
Ion Current

Fig. 4

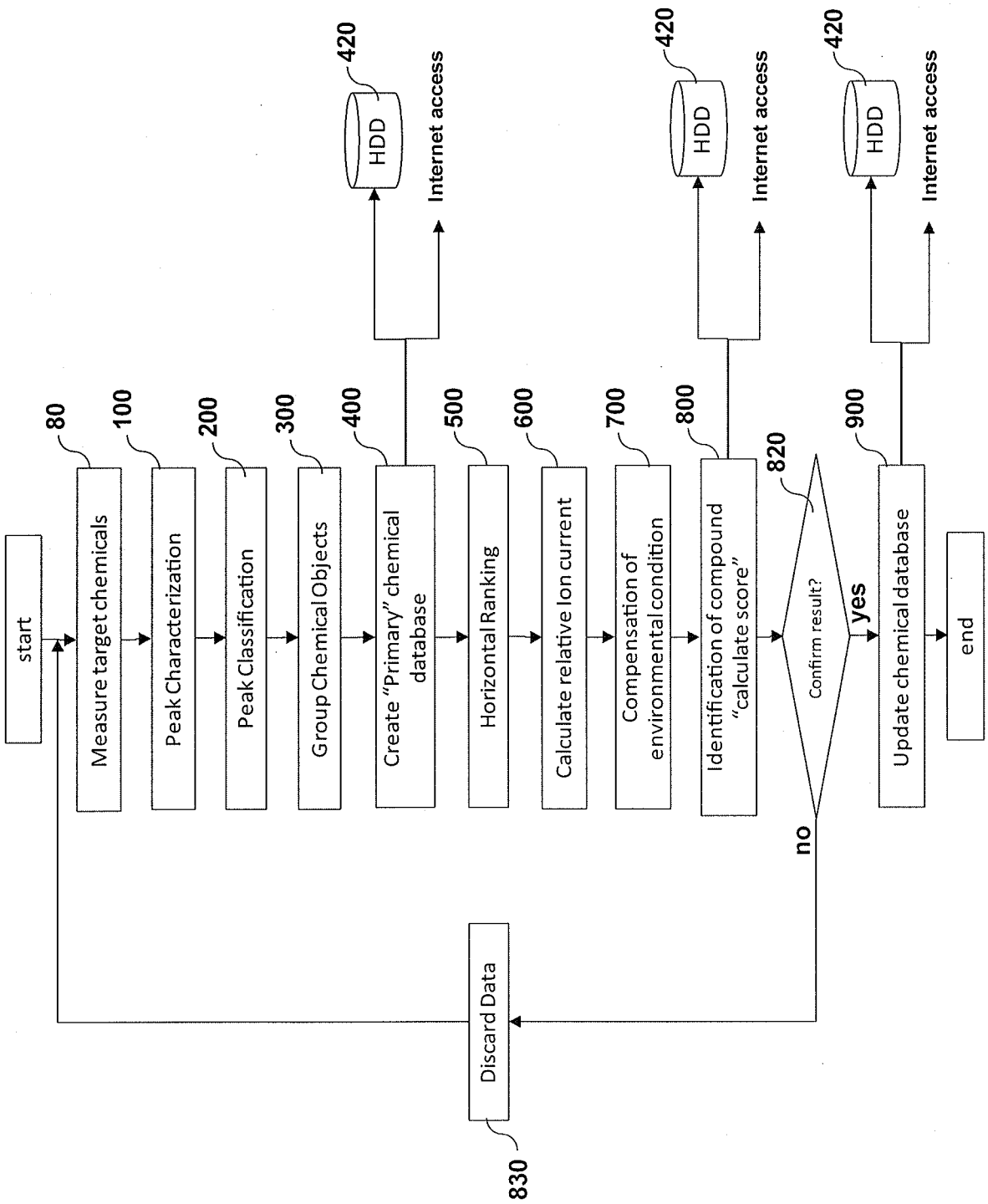

start
Measure target chemicals
80
Peak Characterization
100
Peak Classification
200
Group Chemical Objects
300
Create "Primary" chemical database
400
HDD
420
Internet access
Horizontal Ranking
500
Calculate relative Ion current
600
Compensation of environmental condition
700
Identification of compound "calculate score"
800
HDD
420
Internet access
Confirm result?
820
yes
no
Update chemical database
900
HDD
420
Internet access
end
Discard Data
830

Fig. 5

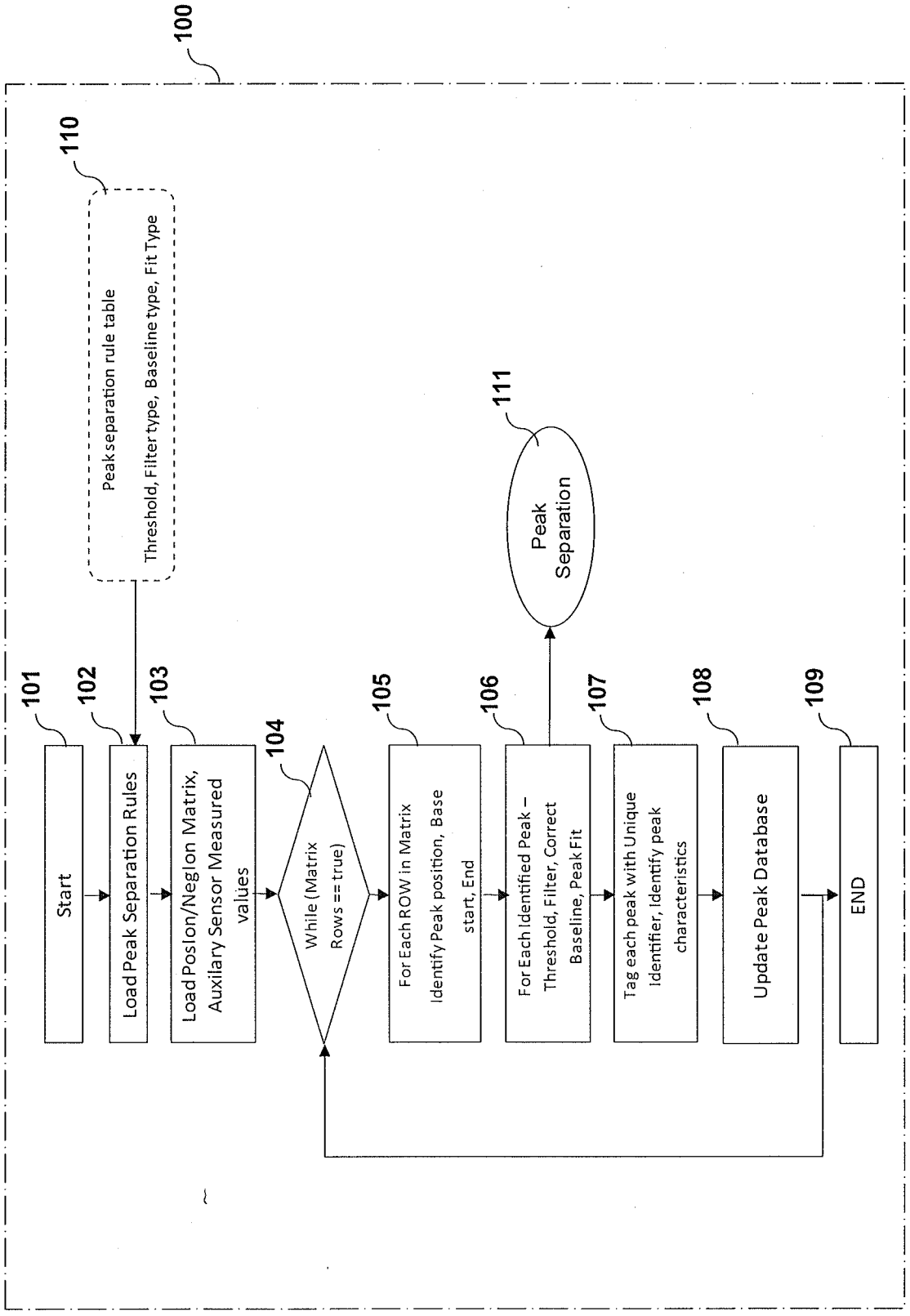

100
110
Peak separation rule table
Threshold, Filter type, Baseline type, Fit Type
111
Peak Separation
101
Start
102
Load Peak Separation Rules
103
Load Poslon/Neglon Matrix, Auxilary Sensor Measured values
104
While (Matrix Rows == true)
105
For Each ROW in Matrix Identify Peak position, Base start, End
106
For Each Identified Peak – Threshold, Filter, Correct Baseline, Peak Fit
107
Tag each peak with Unique Identifier, Identify peak characteristics
108
Update Peak Database
109
END

Fig. 6

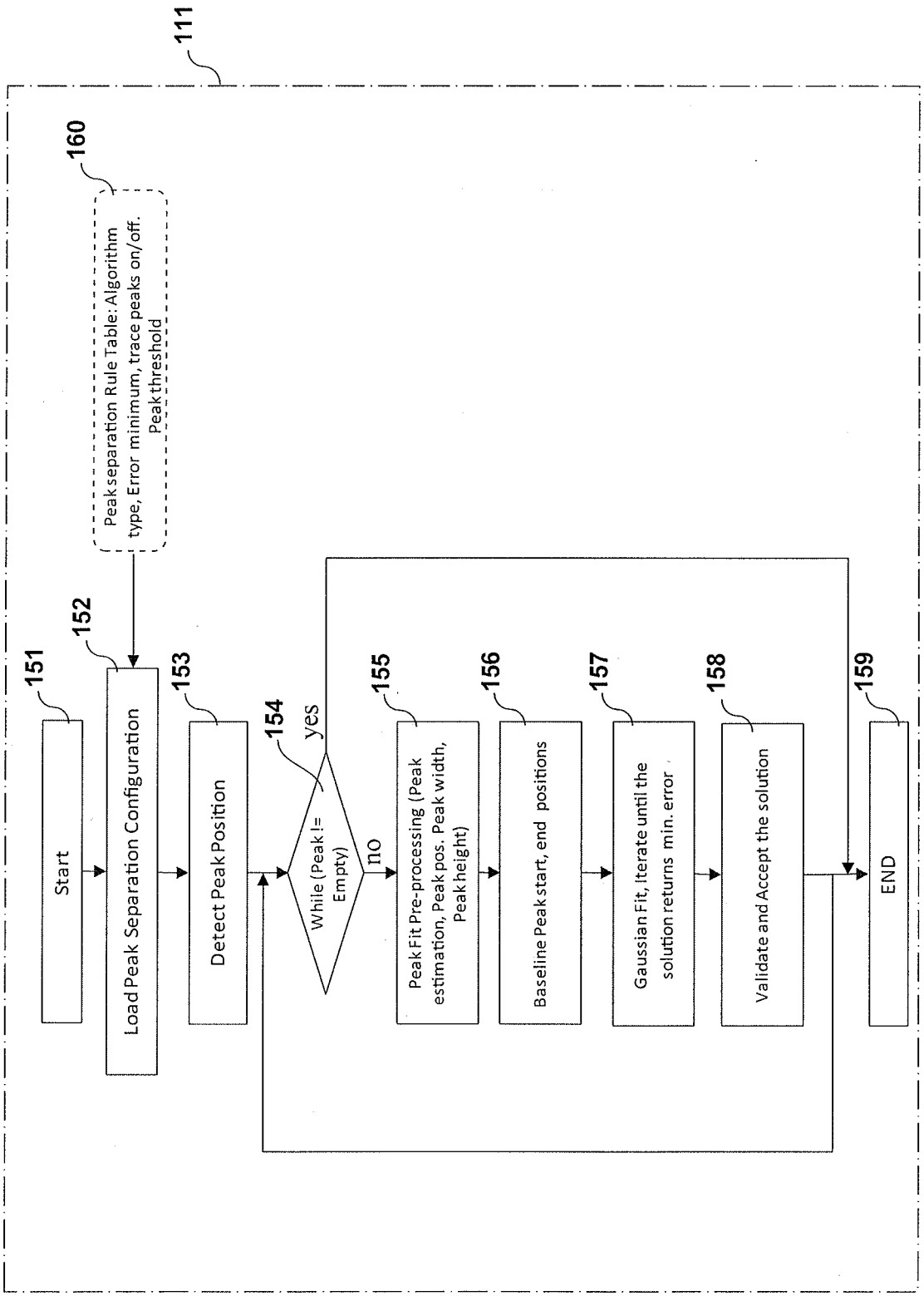

111
160
Peak separation Rule Table: Algorithm type, Error minimum, trace peaks on/off. Peak threshold
151
Start
152
Load Peak Separation Configuration
153
Detect Peak Position
154
While (Peak != Empty)
yes
no
155
Peak Fit Pre-processing (Peak estimation, Peak pos. Peak width, Peak height)
156
Baseline Peak start, end positions
157
Gaussian Fit, Iterate until the solution returns min. error
158
Validate and Accept the solution
159
END

Fig. 7

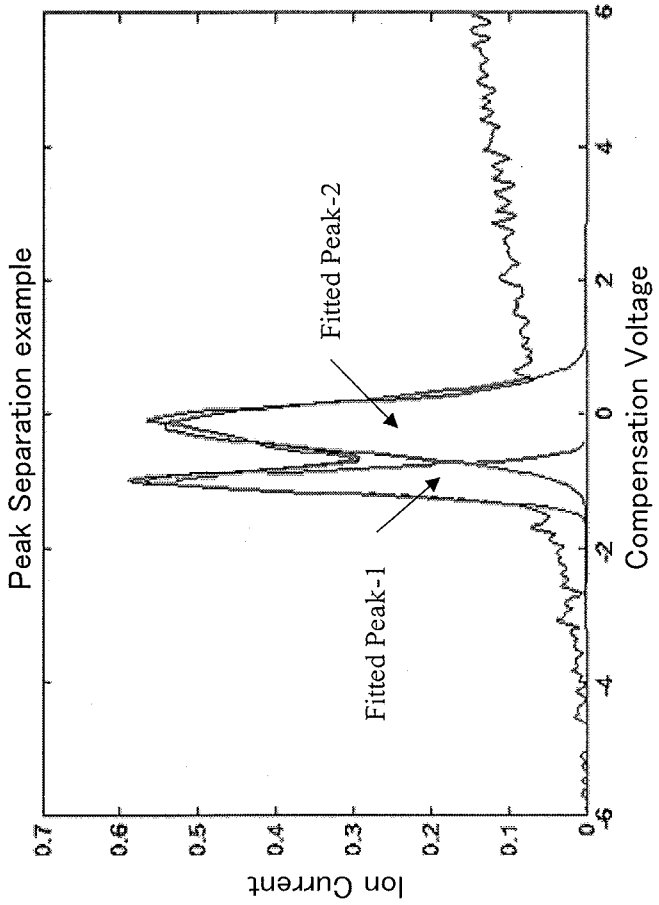

Peak Separation example
Fitted Peak-2
Fitted Peak-1
Ion Current
Compensation Voltage
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-6
-4
-2
0
2
4
6

Fig. 8

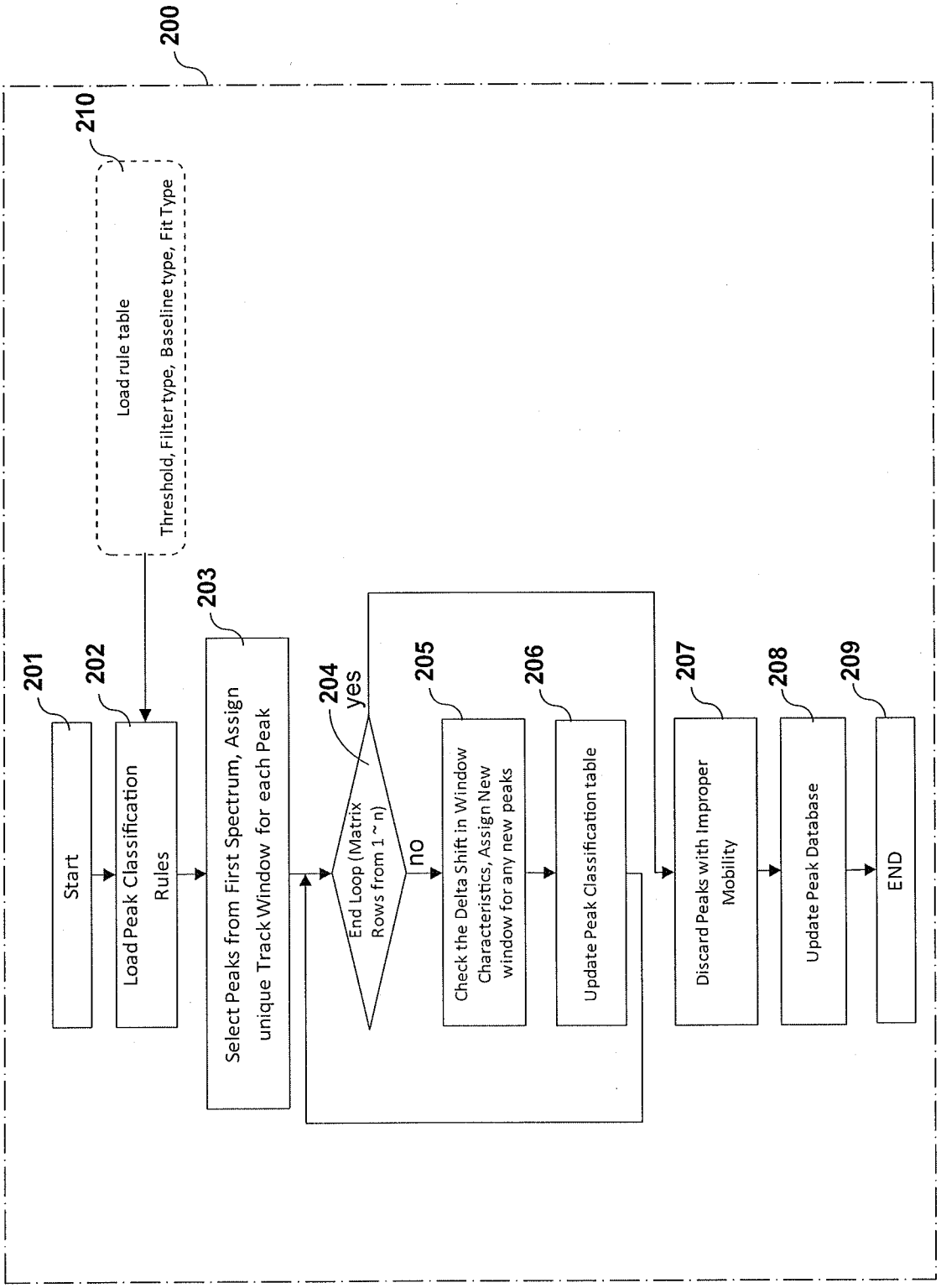

200
210
Load rule table
Threshold, Filter type, Baseline type, Fit Type
201
Start
202
Load Peak Classification Rules
203
Select Peaks from First Spectrum, Assign unique Track Window for each Peak
204
End Loop (Matrix Rows from 1 ~ n)
yes
no
205
Check the Delta Shift in Window Characteristics, Assign New window for any new peaks
206
Update Peak Classification table
207
Discard Peaks with Improper Mobility
208
Update Peak Database
209
END

Fig. 9

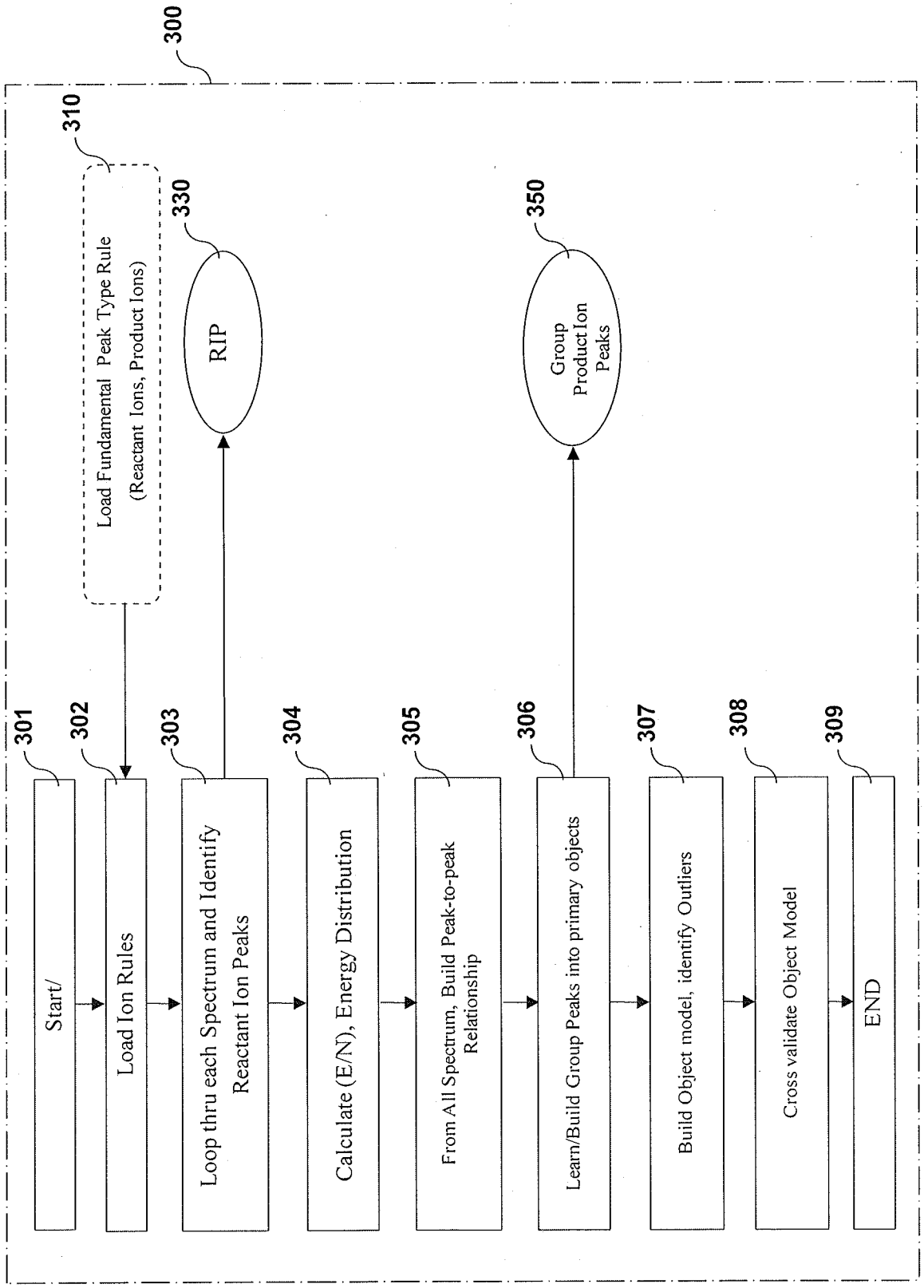

300
310
Load Fundamental Peak Type Rule
(Reactant Ions, Product Ions)
330
RIP
350
Group
Product Ion
Peaks
301
Start/
302
Load Ion Rules
303
Loop thru each Spectrum and Identify
Reactant Ion Peaks
304
Calculate (E/N), Energy Distribution
305
From All Spectrum, Build Peak-to-peak
Relationship
306
Learn/Build Group Peaks into primary objects
307
Build Object model, identify Outliers
308
Cross validate Object Model
309
END

Fig. 10

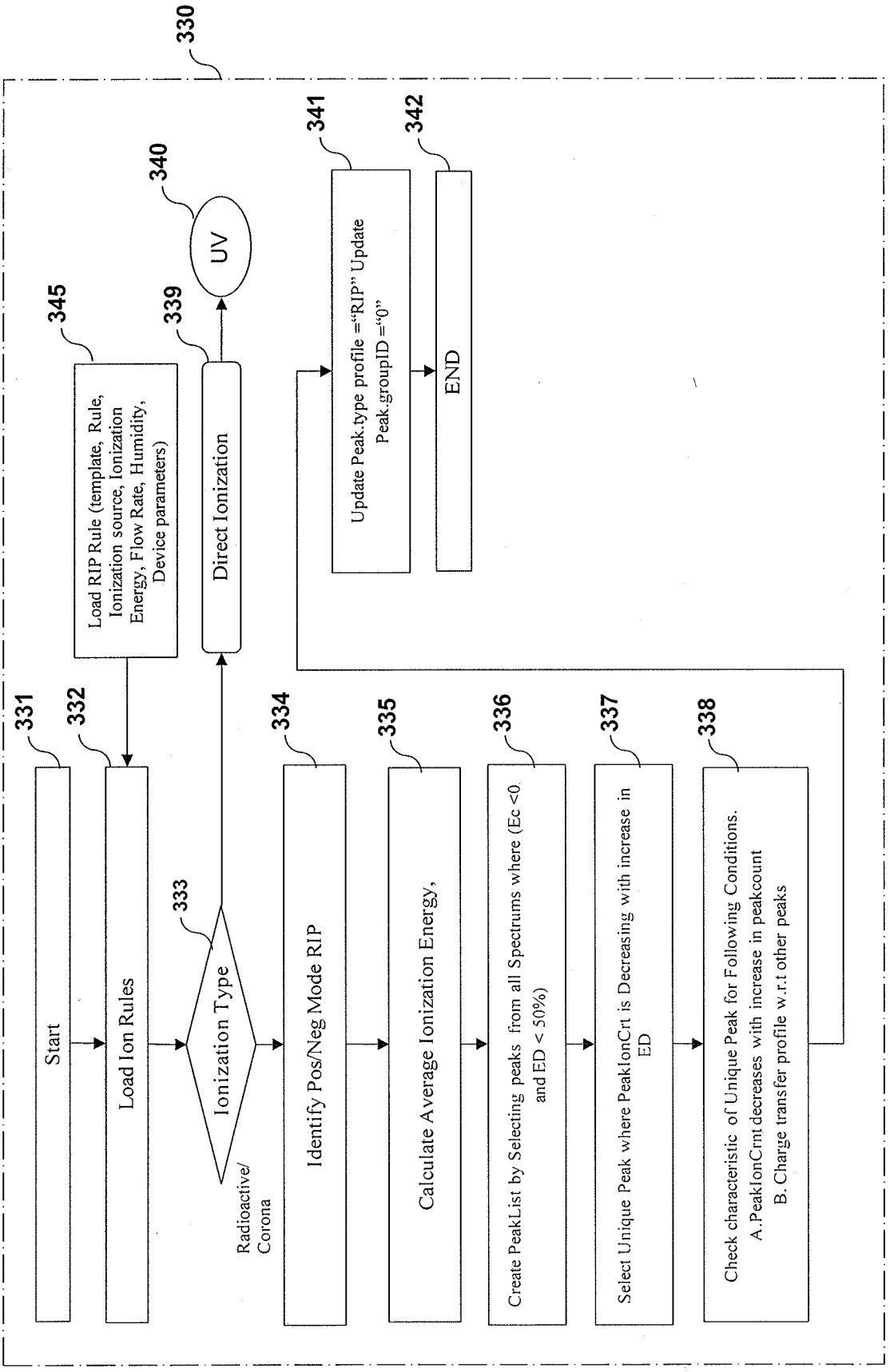

330
331
Start
332
Load Ion Rules
333
Ionization Type
Radioactive/
Corona
334
Identify Pos/Neg Mode RIP
335
Calculate Average Ionization Energy,
336
Create PeakList by Selecting peaks from all Spectrums where (Ec <0 and ED < 50%)
337
Select Unique Peak where PeakIonCrt is Decreasing with increase in ED
338
Check characteristic of Unique Peak for Following Conditions.
A. PeakIonCrnt decreases with increase in peakcount
B. Charge transfer profile w.r.t other peaks
339
Direct Ionization
340
UV
341
Update Peak.type profile ="RIP" Update Peak.groupID ="0"
342
END
345
Load RIP Rule (template, Rule, Ionization source, Ionization Energy, Flow Rate, Humidity, Device parameters)

Fig. 11

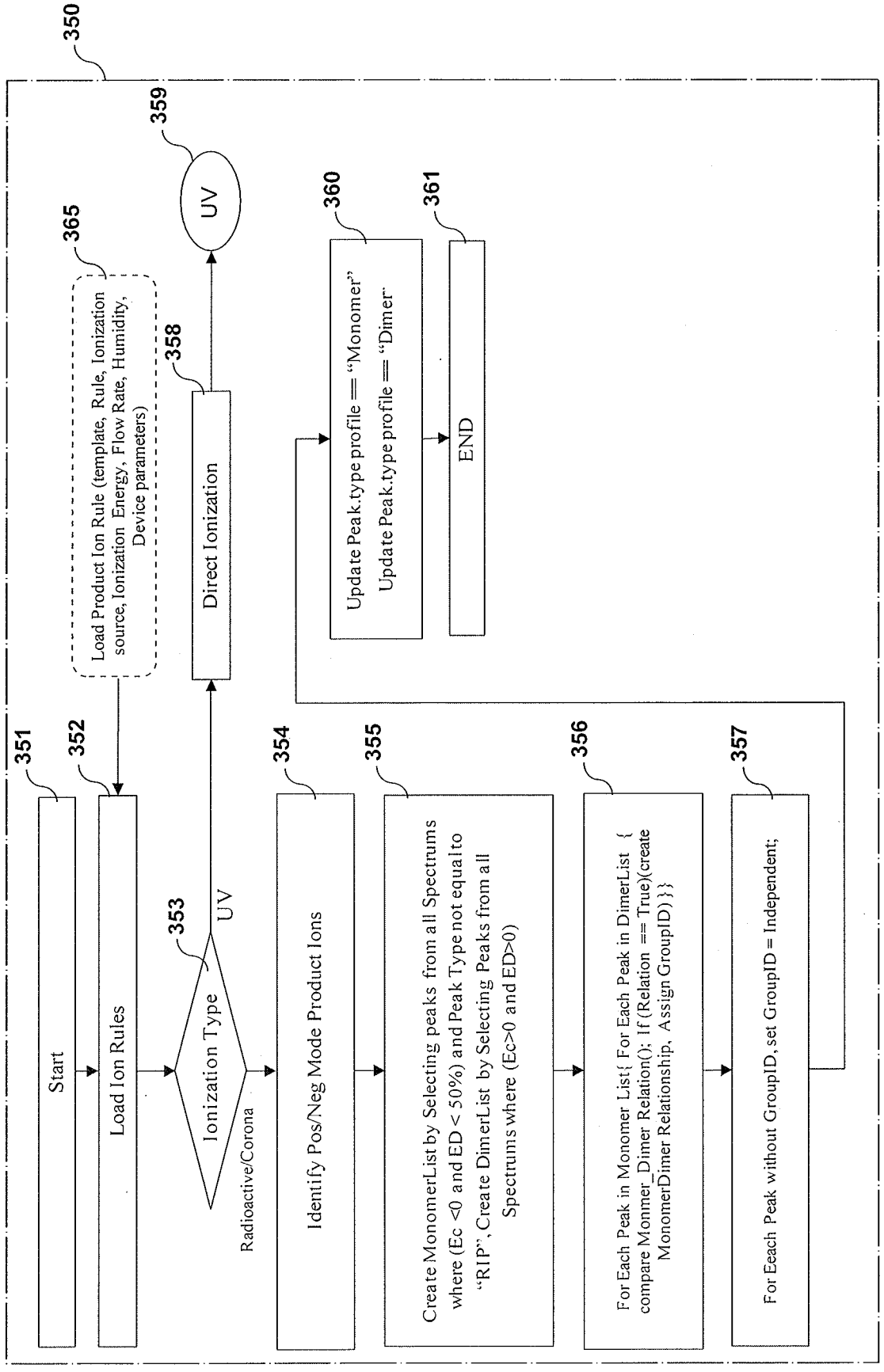

350
Start
351
Load Ion Rules
352
Load Product Ion Rule (template, Rule, Ionization source, Ionization Energy, Flow Rate, Humidity, Device parameters)
365
Ionization Type
353
UV
Radioactive/Corona
Direct Ionization
358
UV
359
Identify Pos/Neg Mode Product Ions
354
Create MonomerList by Selecting peaks from all Spectrums where (Ec <0 and ED < 50%) and Peak Type not equal to "RIP", Create DimerList by Selecting Peaks from all Spectrums where (Ec>0 and ED>0)
355
For Each Peak in Monomer List{ For Each Peak in DimerList { compare Monmer_Dimer Relation(); If (Relation == True)(create MonomerDimer Relationship, Assign GroupID) }}
356
For Eeach Peak without GroupID, set GroupID = Independent;
357
Update Peak.type profile == "Monomer"
Update Peak.type profile == "Dimer"
360
END
361

Fig. 12

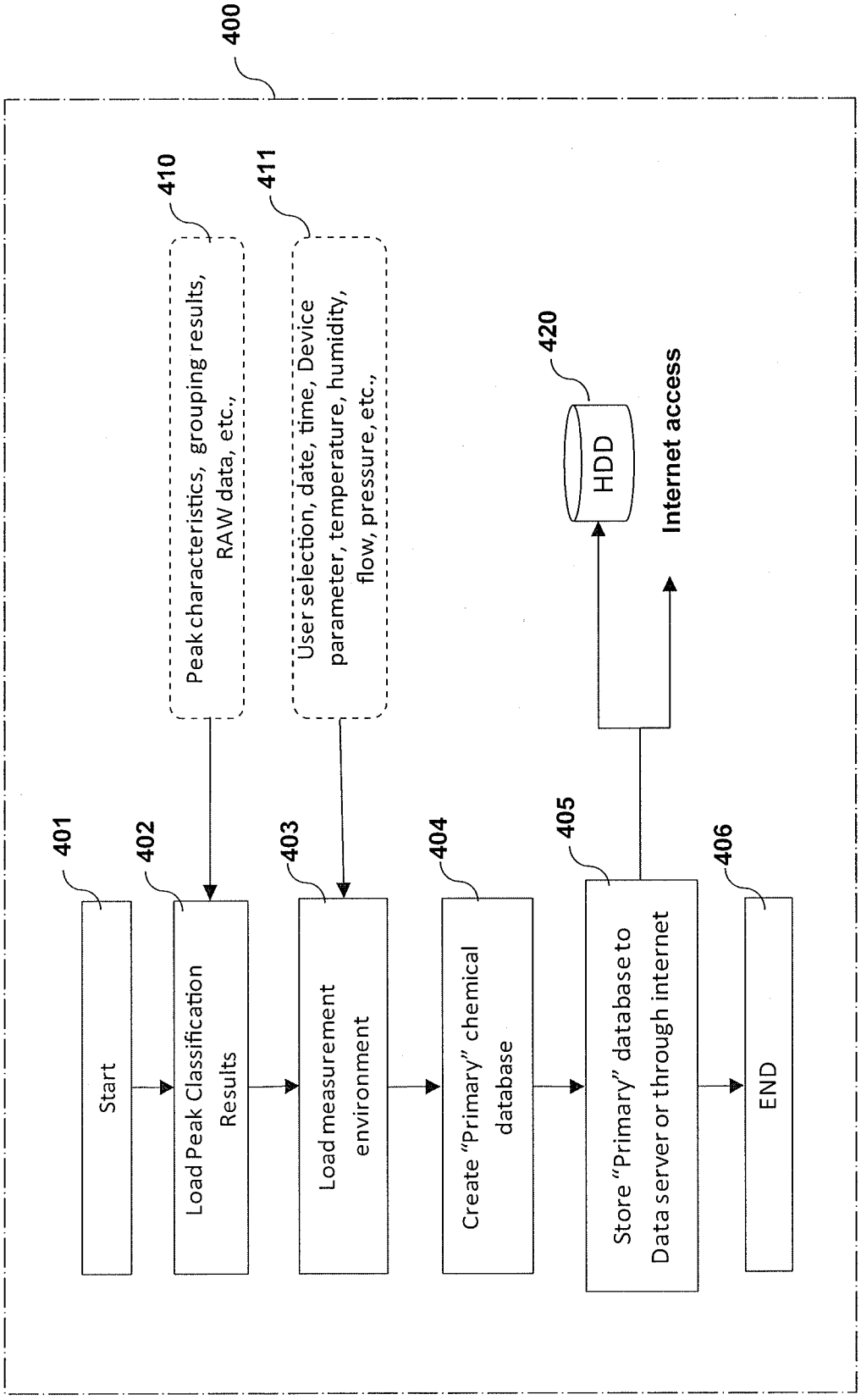

400
410
411
Peak characteristics, grouping results, RAW data, etc.,
User selection, date, time, Device parameter, temperature, humidity, flow, pressure, etc.,
420
HDD
Internet access
401
402
403
404
405
406
Start
Load Peak Classification Results
Load measurement environment
Create "Primary" chemical database
Store "Primary" database to Data server or through internet
END

Fig. 13

450

No.	Category	Contents	Remarks
1	Application Profile Database	Olfaction/Health/Sequrity/Scientific	
2	Profile Specific Data	Spectrum Ranking	*
3		Rule based Chemical Object Tree	**
4		Relationship Index Generation	**
5		Chemical family and AMU based classification tree	**
6		Supervised and Unsupervised Learning Process	
7		Application profile associated Database	
8	Sensor Independent Data	Chemical Objects	**
9		Ion mobility	*
10		Calibration	
11		Environmental Model	
12	Sensor Dependent Data	Disp. Voltage	
13		Compensation Voltage	
14		Ion Current	
15		Peak Position	
16		FWHM(Full width of half maximum)	
17		Peak Current	
18		Linearity	
19		Temperature	
20		Humidity	
21		Pressure	
22		Flo Rate	
23		Ionization Ratio	**

Fig. 14

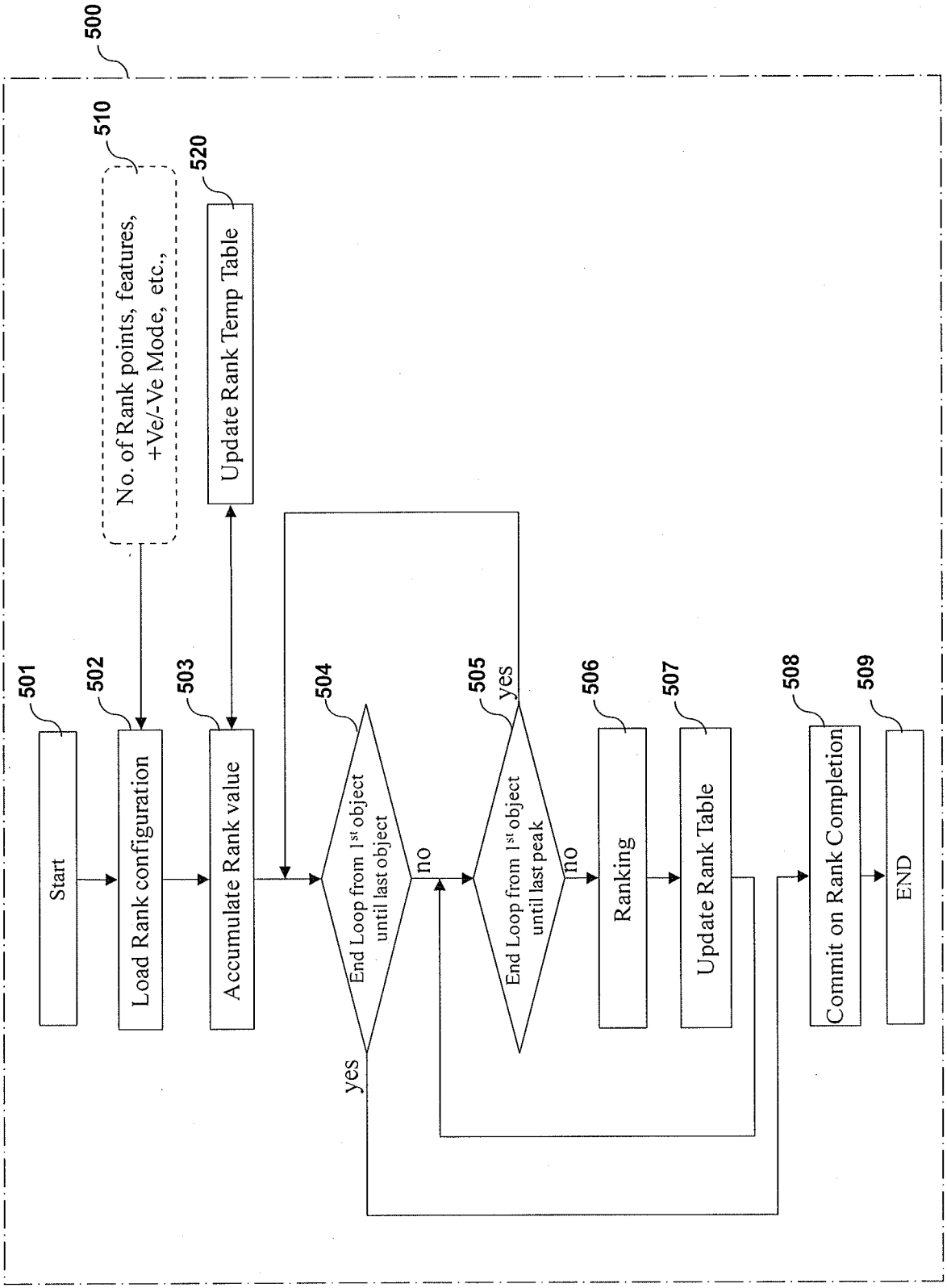

500
510
No. of Rank points, features, +Ve/-Ve Mode, etc.,
520
Update Rank Temp Table
501
Start
502
Load Rank configuration
503
Accumulate Rank value
504
End Loop from 1st object until last object
yes
no
505
End Loop from 1st object until last peak
yes
no
506
Ranking
507
Update Rank Table
508
Commit on Rank Completion
509
END

Fig. 15

451

No.	Vd	Vc	Ion current	FWHM	Ranking	example
1	Vd-1	Vc-11	Icurrent-11	FWHM-11	W-11	0.5
2		Vc-12	Icurrent-12	FWHM-12	W-12	0.6
3	Vd-2	Vc-21	Icurrent-21	FWHM-21	W-21	0.6
4		Vc-22	Icurrent-22	FWHM-22	W-22	0.7
5		Vc-23	Icurrent-23	FWHM-23	W-23	0.4
6	Vd-3	Vc-31	Icurrent-31	FWHM-31	W-31	1.2
7		Vc-32	Icurrent-32	FWHM-32	W-32	1.75
8		Vc-33	Icurrent-33	FWHM-33	W-33	0.6
9	Vd-4	Vc-41	Icurrent-41	FWHM-41	W-41	1.3
10		Vc-42	Icurrent-42	FWHM-42	W-42	1.8
11		Vc-43	Icurrent-43	FWHM-43	W-43	0.8
12	Vd-5	Vc-51	Icurrent-51	FWHM-51	W-51	1.1
13		Vc-52	Icurrent-52	FWHM-52	W-52	1.7
14	Vd-6	Vc-61	Icurrent-61	FWHM-61	W-61	0.9
15		Vc-62	Icurrent-62	FWHM-62	W-62	1.4
16	Vd-7	Vc-71	Icurrent-71	FWHM-71	W-71	0.7
17		Vc-72	Icurrent-72	FWHM-72	W-72	1.1
18	Vd-8	Vc-81	Icurrent-81	FWHM-81	W-81	0.9
19	Vd-9	Vc-91	Icurrent-91	FWHM-91	W-91	0.7

Fig. 16

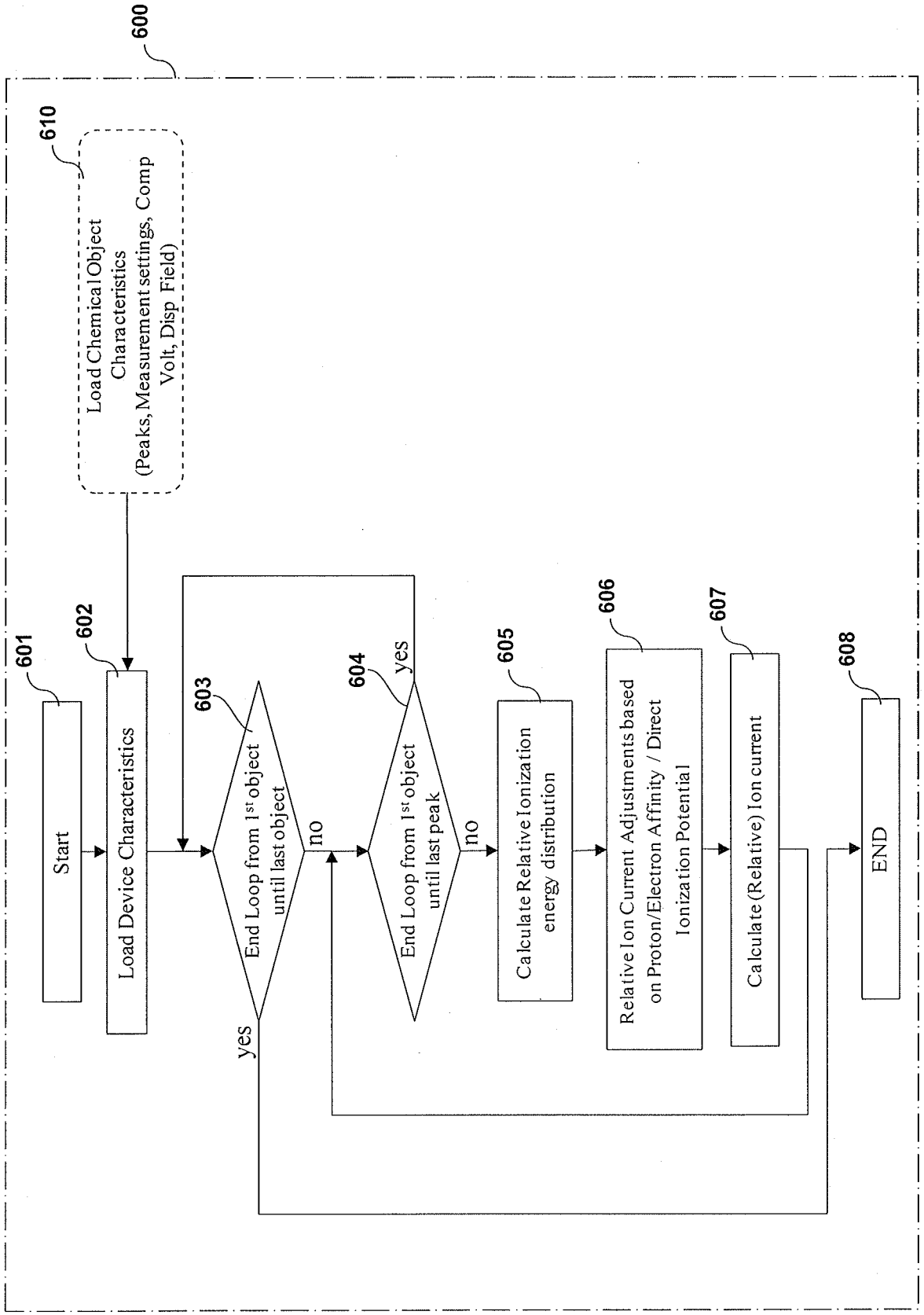

600
610
Load Chemical Object Characteristics (Peaks, Measurement settings, Comp Volt, Disp Field)
601
Start
602
Load Device Characteristics
603
End Loop from 1st object until last object
no
yes
604
End Loop from 1st object until last peak
no
yes
605
Calculate Relative Ionization energy distribution
606
Relative Ion Current Adjustments based on Proton/Electron Affinity / Direct Ionization Potential
607
Calculate (Relative) Ion current
608
END

Fig. 17

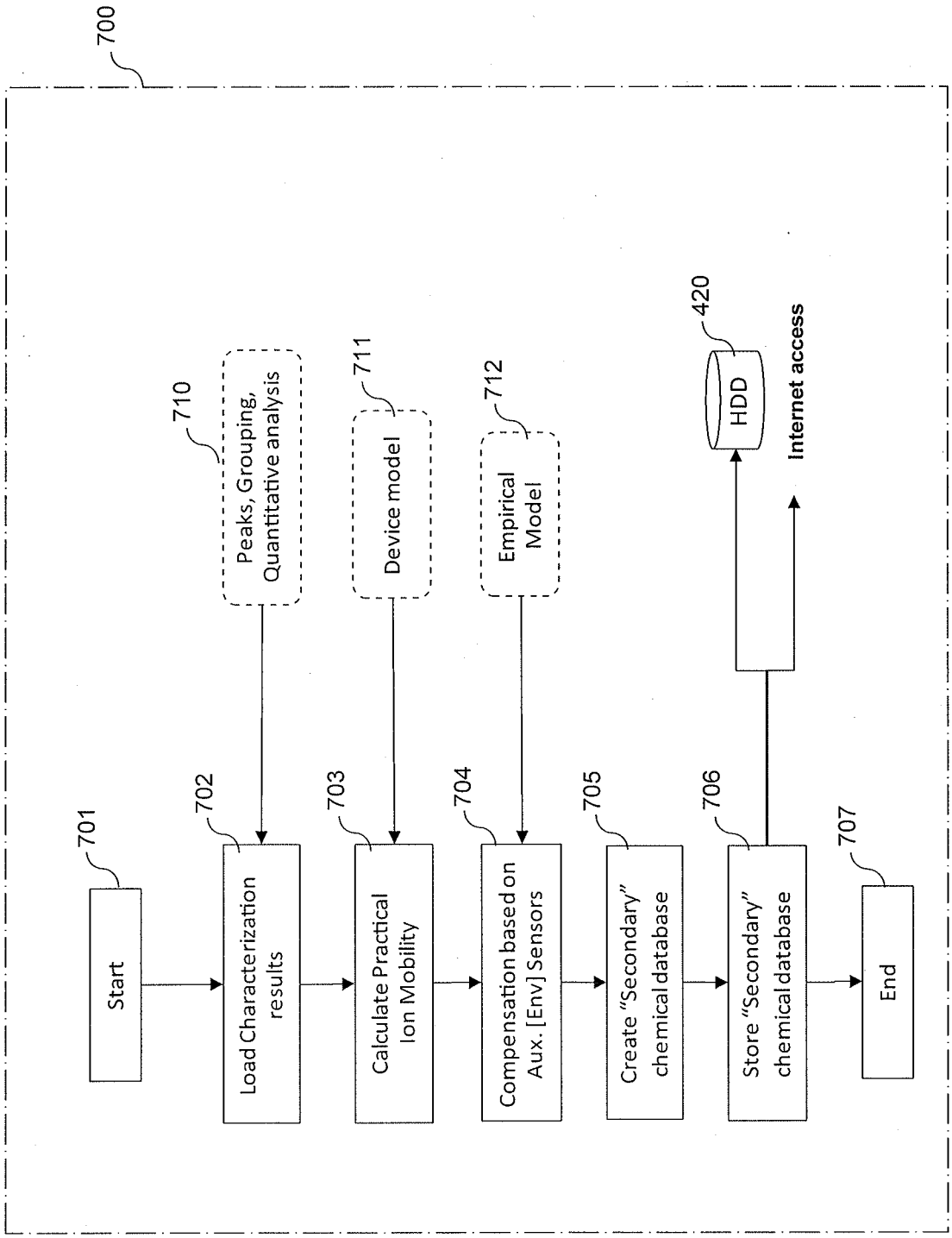

700
701
Start
702
Load Characterization results
703
Calculate Practical Ion Mobility
704
Compensation based on Aux. [Env] Sensors
705
Create "Secondary" chemical database
706
Store "Secondary" chemical database
707
End
710
Peaks, Grouping, Quantitative analysis
711
Device model
712
Empirical Model
420
HDD
Internet access

Fig. 18

1801

Air Pressure [%]	Ion Current [relative value]	FWHM [relative value]
20	I_{20}	W_{20}
40	I_{40}	W_{40}
60	I_{60}	W_{60}
80	I_{80}	W_{80}

Fig. 19

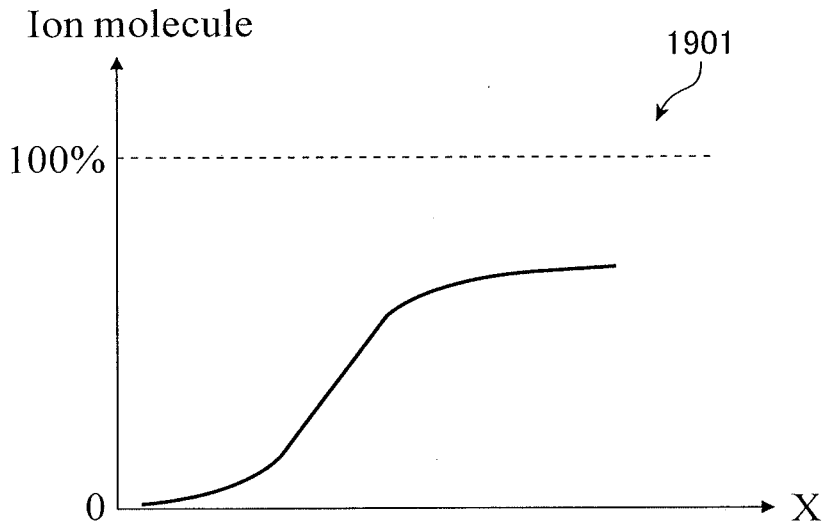


Fig. 20

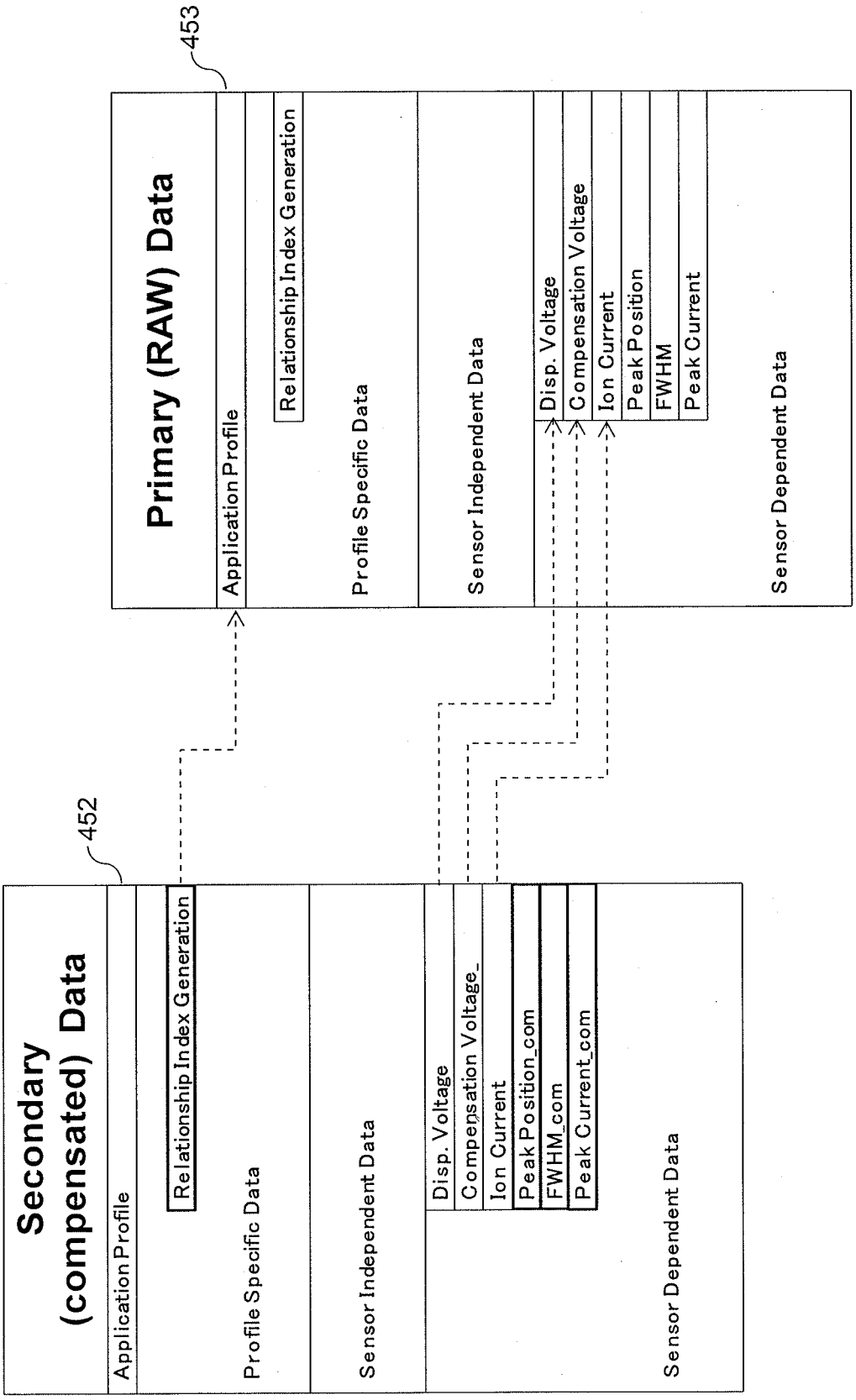

Primary (RAW) Data
453
Application Profile
Relationship Index Generation
Profile Specific Data
Sensor Independent Data
Disp. Voltage
Compensation Voltage
Ion Current
Peak Position
FWHM
Peak Current
Sensor Dependent Data
Secondary (compensated) Data
452
Application Profile
Relationship Index Generation
Profile Specific Data
Sensor Independent Data
Disp. Voltage
Compensation Voltage_
Ion Current
Peak Position_com
FWHM_com
Peak Current_com
Sensor Dependent Data

Fig. 21

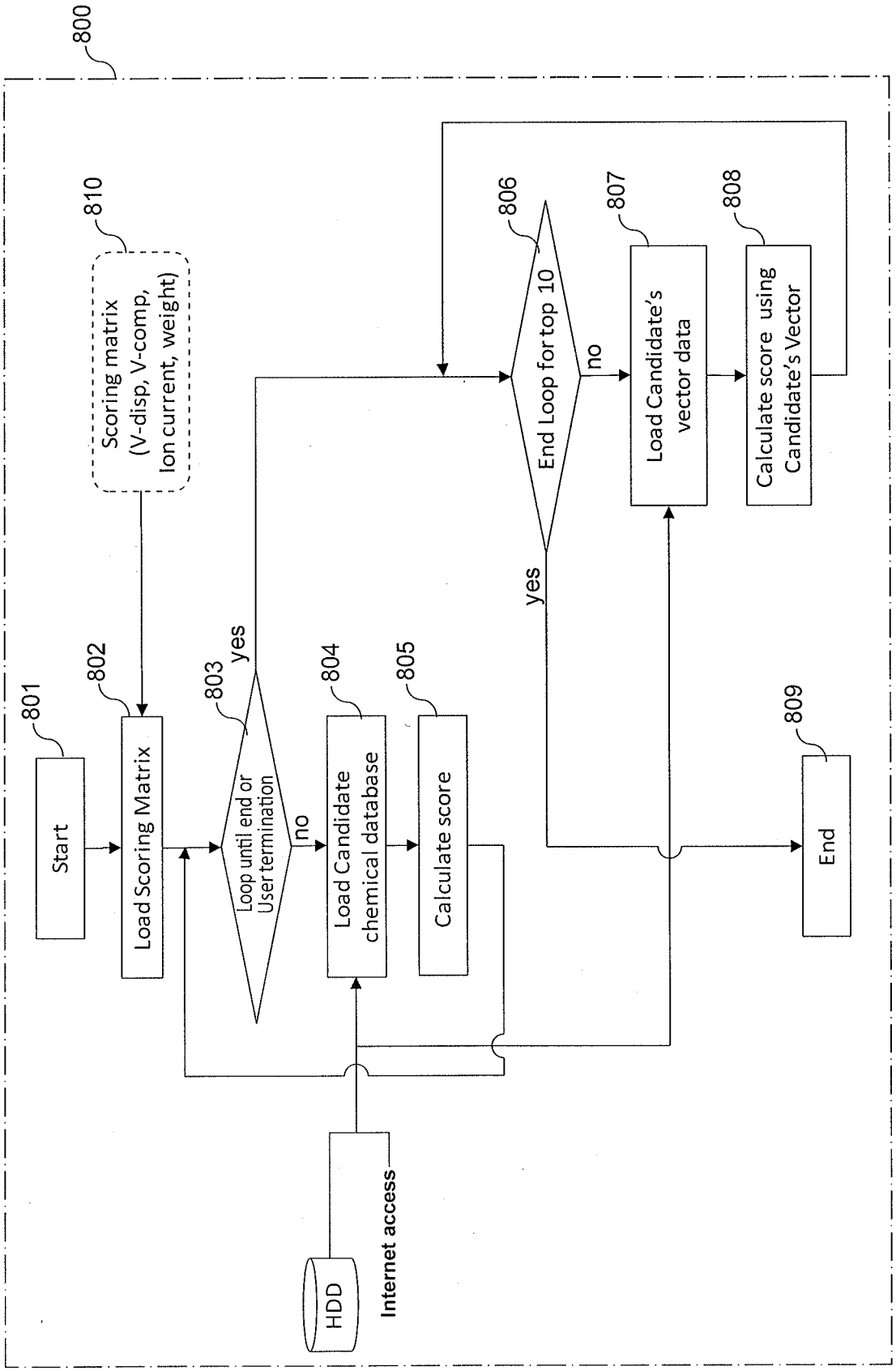

800
Start
801
Load Scoring Matrix
802
Scoring matrix
(V-disp, V-comp,
Ion current, weight)
810
Loop until end or
User termination
803
yes
no
Load Candidate
chemical database
804
Calculate score
805
End Loop for top 10
806
yes
no
Load Candidate's
vector data
807
Calculate score using
Candidate's Vector
808
End
809
HDD
Internet access

Fig. 22

454

No.	Vd	Vc	Ion current	FWHM	Weight
1	Vd-3	Vc-31	Icurrent-31	FWHM-31	W-31
2		Vc-32	Icurrent-32	FWHM-32	W-32
3	Vd-4	Vc-41	Icurrent-41	FWHM-41	W-41
4		Vc-42	Icurrent-42	FWHM-42	W-42
5	Vd-5	Vc-51	Icurrent-51	FWHM-51	W-51
6		Vc-52	Icurrent-52	FWHM-52	W-52
7	Vd-6	Vc-61	Icurrent-61	FWHM-61	W-61
8		Vc-62	Icurrent-62	FWHM-62	W-62
9	Vd-7	Vc-72	Icurrent-72	FWHM-72	W-72
10	Vd-8	Vc-81	Icurrent-81	FWHM-81	W-81

Fig. 23

455

No.	Vd	Vc	Ion current	FWHM	Ranking
1	Vd-1	Vc-11	Icurrent-11	FWHM-11	W-11
2	Vd-2	Vc-21	Icurrent-21	FWHM-21	W-21
3	Vd-3	Vc-31	Icurrent-31	FWHM-31	W-31
4		Vc-32	Icurrent-32	FWHM-32	W-32
5	Vd-4	Vc-41	Icurrent-41	FWHM-41	W-41
6		Vc-42	Icurrent-42	FWHM-42	W-42
7	Vd-5	Vc-51	Icurrent-51	FWHM-51	W-51
8		Vc-52	Icurrent-52	FWHM-52	W-52
9	Vd-6	Vc-62	Icurrent-62	FWHM-62	W-62
10		Vc-72	Icurrent-72	FWHM-72	W-72

Fig. 24

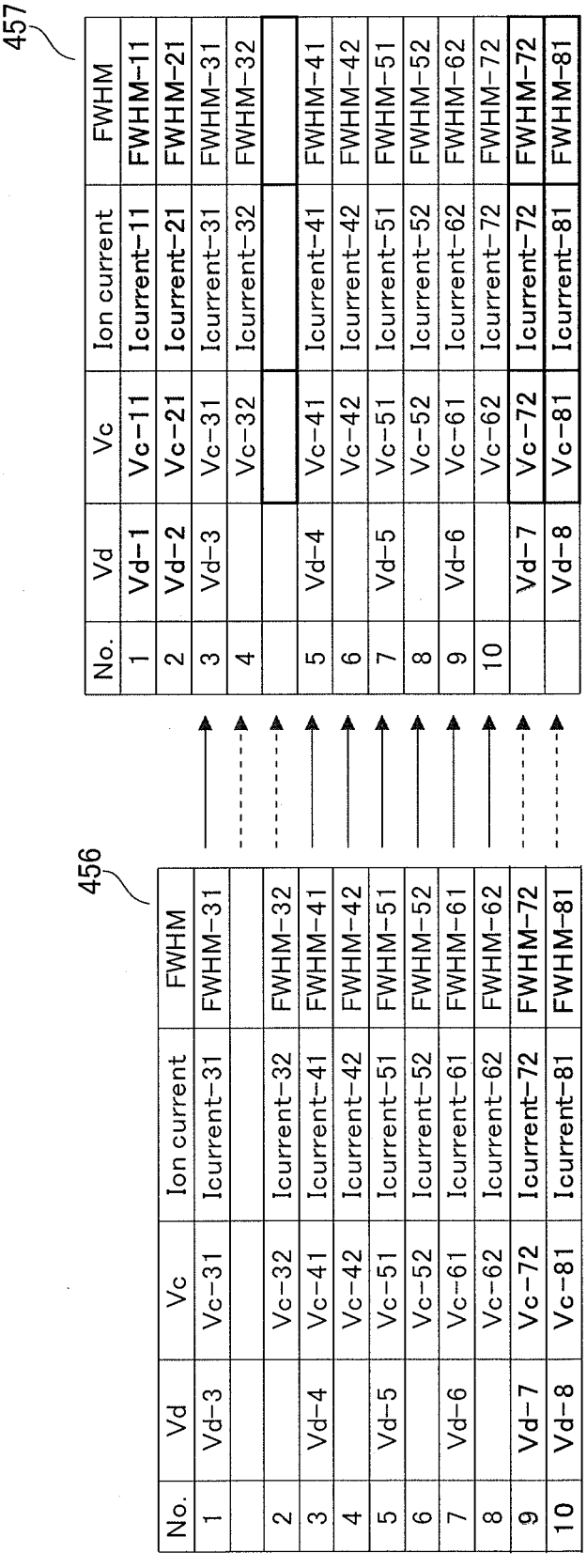
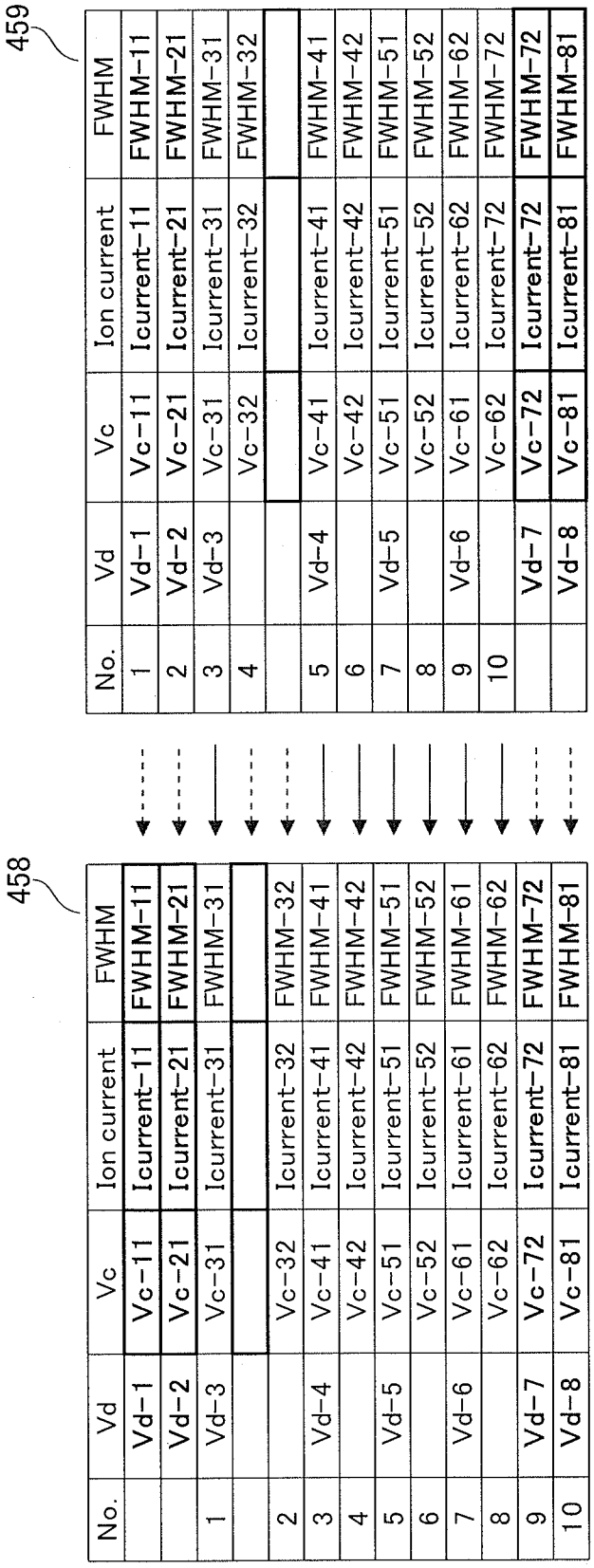

456
457
No. Vd Vc Ion current FWHM
1 Vd-3 Vc-31 Icurrent-31 FWHM-31
2 Vc-32 Icurrent-32 FWHM-32
3 Vd-4 Vc-41 Icurrent-41 FWHM-41
4 Vc-42 Icurrent-42 FWHM-42
5 Vd-5 Vc-51 Icurrent-51 FWHM-51
6 Vc-52 Icurrent-52 FWHM-52
7 Vd-6 Vc-61 Icurrent-61 FWHM-61
8 Vc-62 Icurrent-62 FWHM-62
9 Vd-7 Vc-72 Icurrent-72 FWHM-72
10 Vd-8 Vc-81 Icurrent-81 FWHM-81
No. Vd Vc Ion current FWHM
1 Vd-1 Vc-11 Icurrent-11 FWHM-11
2 Vd-2 Vc-21 Icurrent-21 FWHM-21
3 Vd-3 Vc-31 Icurrent-31 FWHM-31
4 Vc-32 Icurrent-32 FWHM-32
5 Vd-4 Vc-41 Icurrent-41 FWHM-41
6 Vc-42 Icurrent-42 FWHM-42
7 Vd-5 Vc-51 Icurrent-51 FWHM-51
8 Vc-52 Icurrent-52 FWHM-52
9 Vd-6 Vc-61 Icurrent-61 FWHM-62
10 Vc-62 Icurrent-72 FWHM-72
Vd-7 Vc-72 Icurrent-72 FWHM-72
Vd-8 Vc-81 Icurrent-81 FWHM-81

Fig. 25



458

No.	Vd	Vc	Ion current	FWHM
	Vd-1	Vc-11	Icurrent-11	FWHM-11
	Vd-2	Vc-21	Icurrent-21	FWHM-21
1	Vd-3	Vc-31	Icurrent-31	FWHM-31
2		Vc-32	Icurrent-32	FWHM-32
3	Vd-4	Vc-41	Icurrent-41	FWHM-41
4		Vc-42	Icurrent-42	FWHM-42
5	Vd-5	Vc-51	Icurrent-51	FWHM-51
6		Vc-52	Icurrent-52	FWHM-52
7	Vd-6	Vc-61	Icurrent-61	FWHM-61
8		Vc-62	Icurrent-62	FWHM-62
9	Vd-7	Vc-72	Icurrent-72	FWHM-72
10	Vd-8	Vc-81	Icurrent-81	FWHM-81

459

No.	Vd	Vc	Ion current	FWHM
1	Vd-1	Vc-11	Icurrent-11	FWHM-11
2	Vd-2	Vc-21	Icurrent-21	FWHM-21
3	Vd-3	Vc-31	Icurrent-31	FWHM-31
4		Vc-32	Icurrent-32	FWHM-32
5	Vd-4	Vc-41	Icurrent-41	FWHM-41
6		Vc-42	Icurrent-42	FWHM-42
7	Vd-5	Vc-51	Icurrent-51	FWHM-51
8		Vc-52	Icurrent-52	FWHM-52
9	Vd-6	Vc-61	Icurrent-61	FWHM-62
10		Vc-62	Icurrent-72	FWHM-72
	Vd-7	Vc-72	Icurrent-72	FWHM-72
	Vd-8	Vc-81	Icurrent-81	FWHM-81

Fig. 26

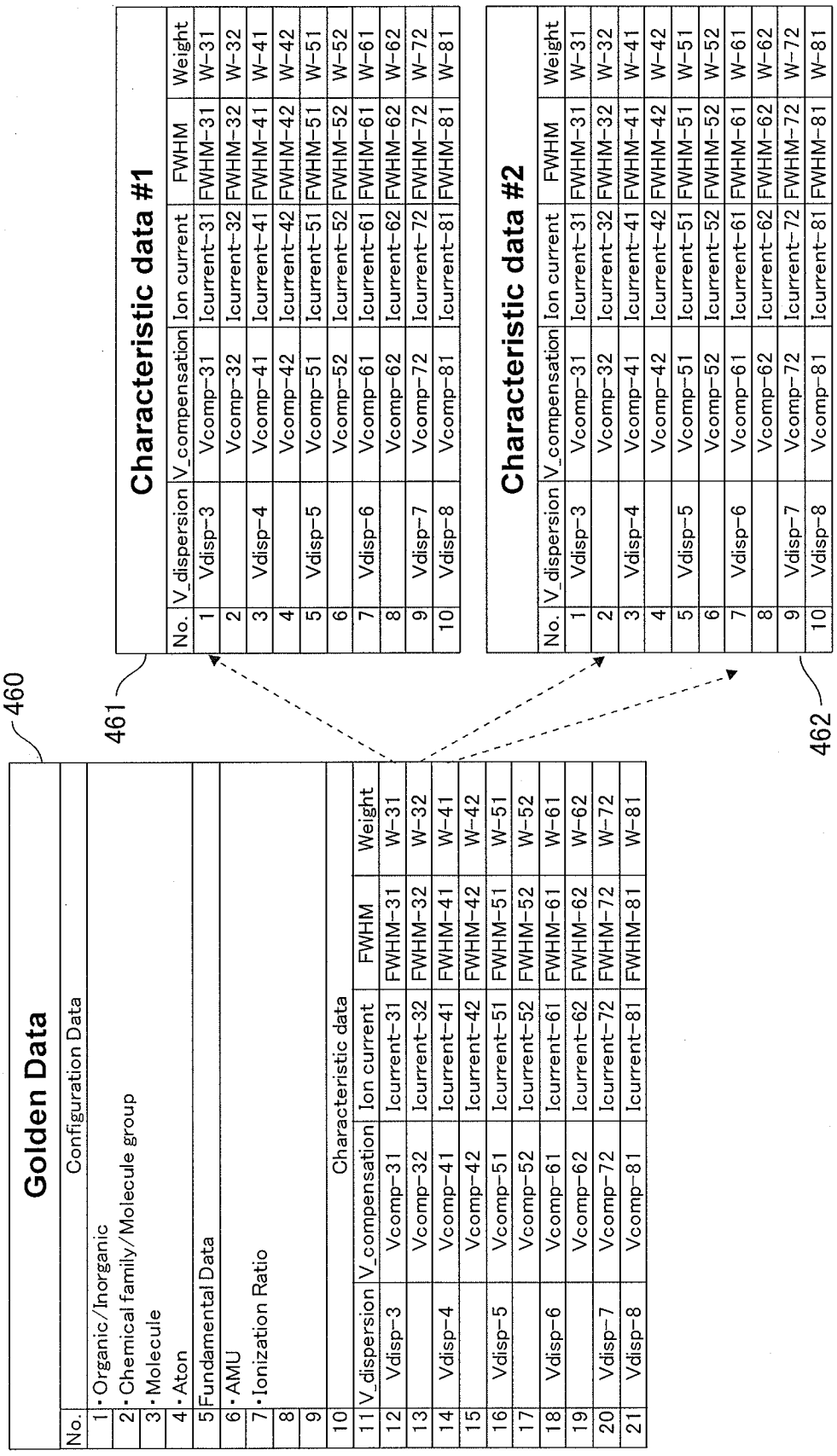
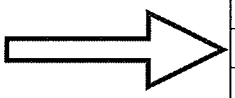

460
461
462
Golden Data
No.
Configuration Data
1 • Organic/Inorganic
2 • Chemical family/Molecule group
3 • Molecule
4 • Aton
5 Fundamental Data
6 • AMU
7 • Ionization Ratio
8
9
10 Characteristic data
11 V_dispersion V_compensation Ion current FWHM Weight
12 Vdisp-3 Vcomp-31 Icurrent-31 FWHM-31 W-31
13 Vcomp-32 Icurrent-32 FWHM-32 W-32
14 Vdisp-4 Vcomp-41 Icurrent-41 FWHM-41 W-41
15 Vcomp-42 Icurrent-42 FWHM-42 W-42
16 Vdisp-5 Vcomp-51 Icurrent-51 FWHM-51 W-51
17 Vcomp-52 Icurrent-52 FWHM-52 W-52
18 Vdisp-6 Vcomp-61 Icurrent-61 FWHM-61 W-61
19 Vcomp-62 Icurrent-62 FWHM-62 W-62
20 Vdisp-7 Vcomp-72 Icurrent-72 FWHM-72 W-72
21 Vdisp-8 Vcomp-81 Icurrent-81 FWHM-81 W-81
Characteristic data #1
No. V_dispersion V_compensation Ion current FWHM Weight
1 Vdisp-3 Vcomp-31 Icurrent-31 FWHM-31 W-31
2 Vcomp-32 Icurrent-32 FWHM-32 W-32
3 Vdisp-4 Vcomp-41 Icurrent-41 FWHM-41 W-41
4 Vcomp-42 Icurrent-42 FWHM-42 W-42
5 Vdisp-5 Vcomp-51 Icurrent-51 FWHM-51 W-51
6 Vcomp-52 Icurrent-52 FWHM-52 W-52
7 Vdisp-6 Vcomp-61 Icurrent-61 FWHM-61 W-61
8 Vcomp-62 Icurrent-62 FWHM-62 W-62
9 Vdisp-7 Vcomp-72 Icurrent-72 FWHM-72 W-72
10 Vdisp-8 Vcomp-81 Icurrent-81 FWHM-81 W-81
Characteristic data #2
No. V_dispersion V_compensation Ion current FWHM Weight
1 Vdisp-3 Vcomp-31 Icurrent-31 FWHM-31 W-31
2 Vcomp-32 Icurrent-32 FWHM-32 W-32
3 Vdisp-4 Vcomp-41 Icurrent-41 FWHM-41 W-41
4 Vcomp-42 Icurrent-42 FWHM-42 W-42
5 Vdisp-5 Vcomp-51 Icurrent-51 FWHM-51 W-51
6 Vcomp-52 Icurrent-52 FWHM-52 W-52
7 Vdisp-6 Vcomp-61 Icurrent-61 FWHM-61 W-61
8 Vcomp-62 Icurrent-62 FWHM-62 W-62
9 Vdisp-7 Vcomp-72 Icurrent-72 FWHM-72 W-72
10 Vdisp-8 Vcomp-81 Icurrent-81 FWHM-81 W-81

Fig. 27



Vertical Ranking

463

Chemical compound	Idenfied number
A	Na
B	Nb
C	Nc
D	Nd
E	Ne
F	Nf
G	Ng
H	Nh
I	Ni
J	Nj
K	Nk
L	Nl
M	Nm
N	Nn

Fig. 28

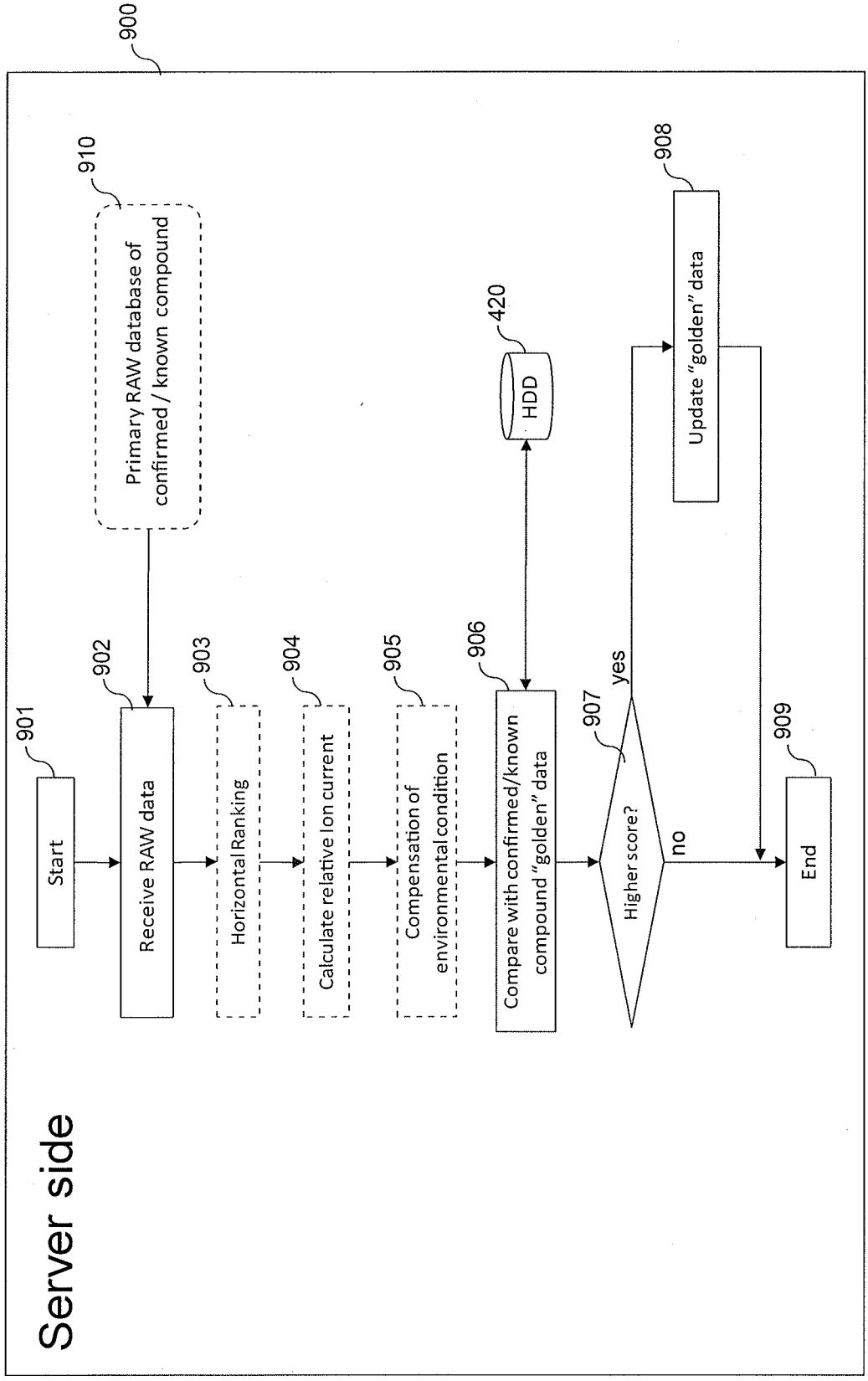

900
Server side
910
Primary RAW database of confirmed / known compound
420
HDD
908
Update "golden" data
901
Start
902
Receive RAW data
903
Horizontal Ranking
904
Calculate relative Ion current
905
Compensation of environmental condition
906
Compare with confirmed/known compound "golden" data
907
Higher score?
yes
no
909
End

Fig. 29

2901

(a)

Vd[%]	P-Xylene	M-Xylene	O-Xylene	Sample-A
40	0.17	-0.35	0.1	0.11
60	0.38	0.25	0.275	0.37
70	0.52	0.36	0.43	0.54
75	0.68	0.49	0.57	0.68
80	0.8	0.58	0.69	0.79
90	1.20	0.78	1.00	1.16

Table1 Positive Ion mobility (represented as Vc)

2902

(b)

Vd[%]	P-Xylene	M-Xylene	O-Xylene	Sample-A
60	-0.28	0	-0.06	-0.28
70	-0.38	-0.16	-0.27	-0.44
75	-0.56	-0.22	-0.41	-0.64
80	-0.66	-0.42	-0.5	-0.78
90	-1.77	-0.7	-0.9	-1.3

Table2 Negative Ion mobility (represented as Vc)

Fig. 30

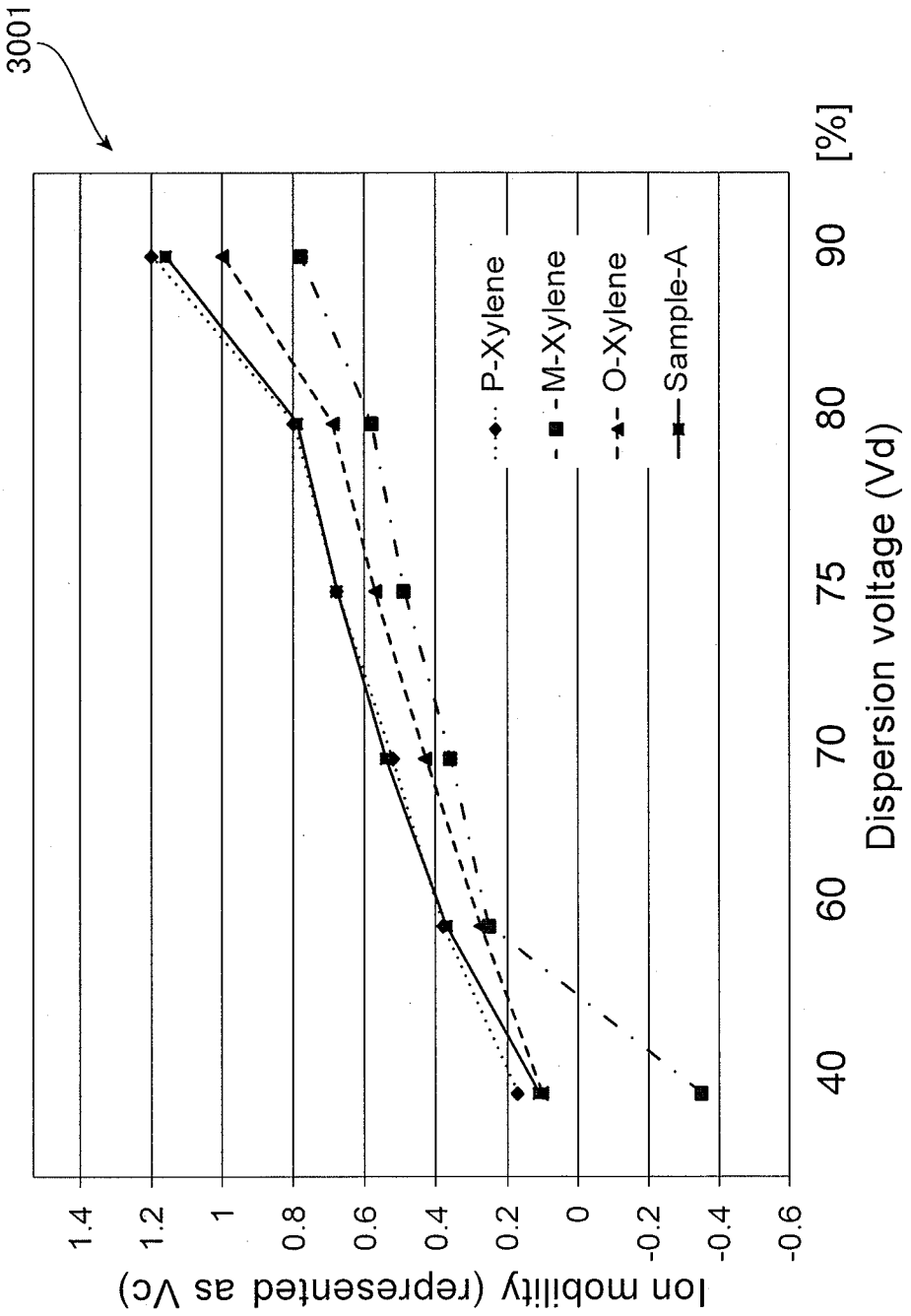

3001
Ion mobility (represented as Vc)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
40
60
70
75
80
90
[%]
Dispersion voltage (Vd)
P-Xylene
M-Xylene
O-Xylene
Sample-A

Fig. 31

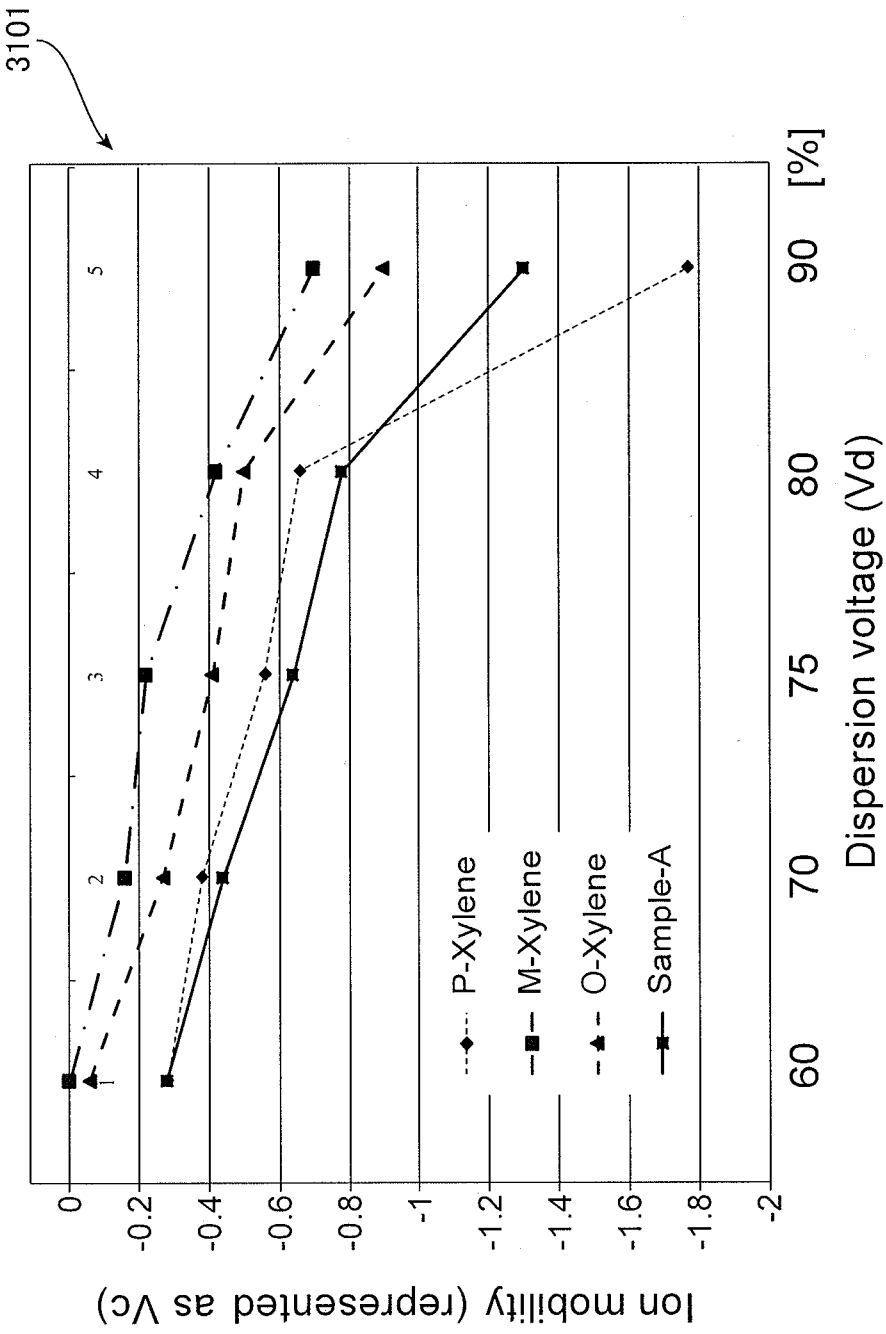

3101
Ion mobility (represented as Vc)
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-1.8
-2
1
2
3
4
5
60
70
75
80
90
[%]
Dispersion voltage (Vd)
P-Xylene
M-Xylene
O-Xylene
Sample-A

Fig. 32

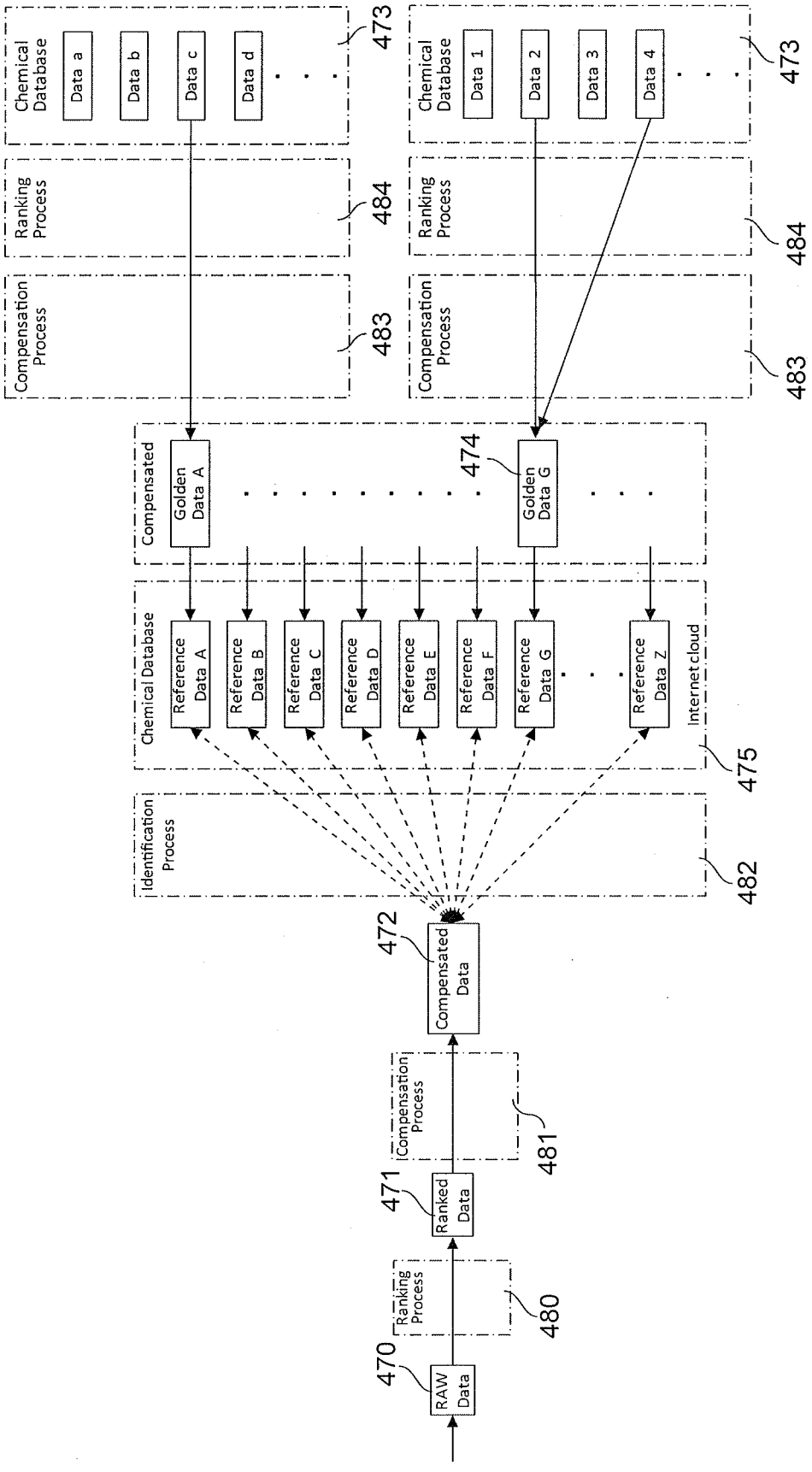

Chemical Database
Data a
Data b
Data c
Data d
473
Ranking Process
484
Compensation Process
483
Chemical Database
Data 1
Data 2
Data 3
Data 4
473
Ranking Process
484
Compensation Process
483
Compensated
Golden Data A
474
Golden Data G
Chemical Database
Reference Data A
Reference Data B
Reference Data C
Reference Data D
Reference Data E
Reference Data F
Reference Data G
Reference Data Z
Internet cloud
475
Identification Process
482
472
Compensated Data
Compensation Process
481
471
Ranked Data
Ranking Process
480
470
RAW Data

Fig. 33

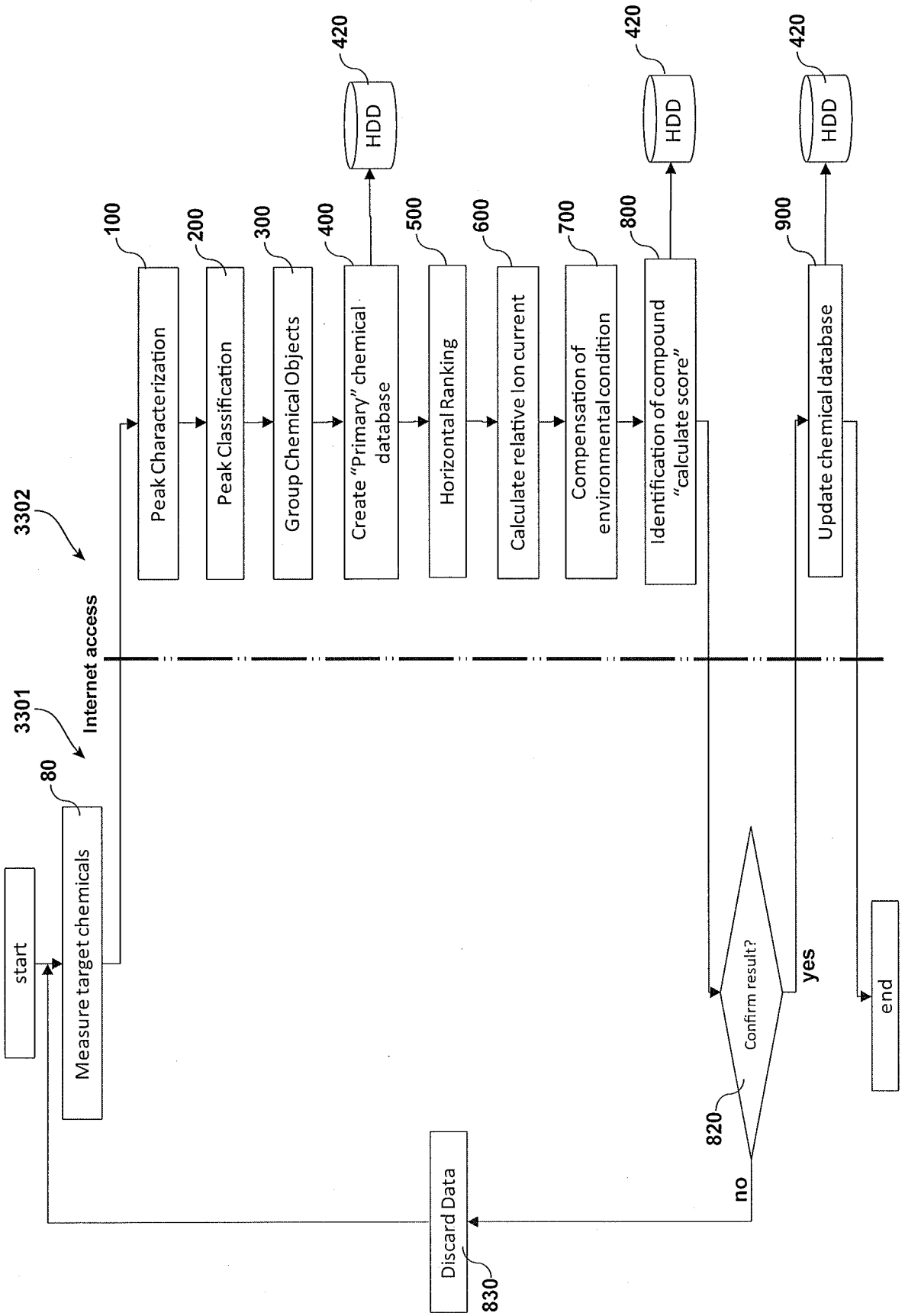

start
Measure target chemicals
80
3301
Internet access
3302
100
Peak Characterization
200
Peak Classification
300
Group Chemical Objects
400
Create "Primary" chemical database
420
HDD
500
Horizontal Ranking
600
Calculate relative Ion current
700
Compensation of environmental condition
800
Identification of compound "calculate score"
420
HDD
900
Update chemical database
420
HDD
end
Confirm result?
820
yes
no
Discard Data
830

Fig. 34

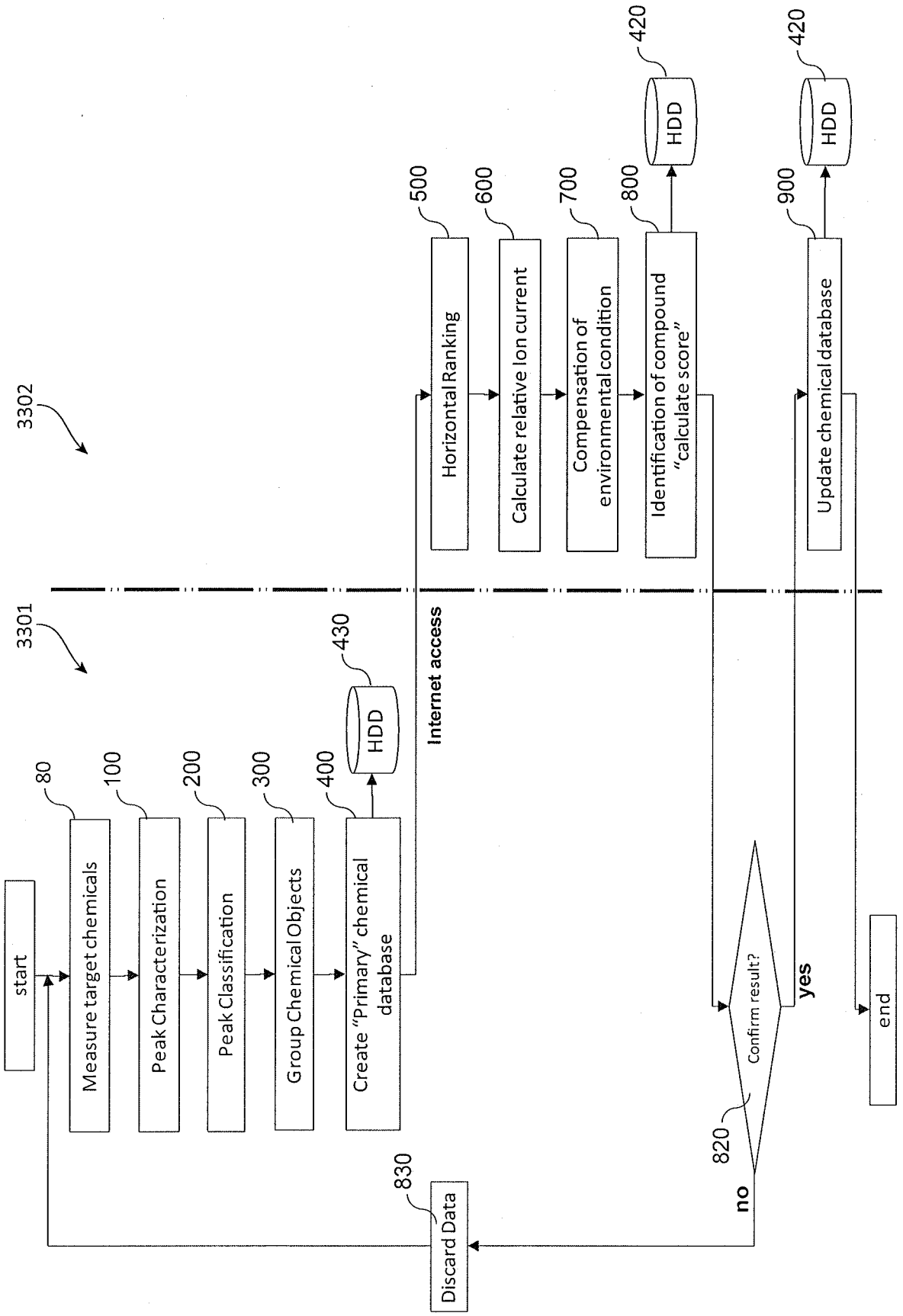
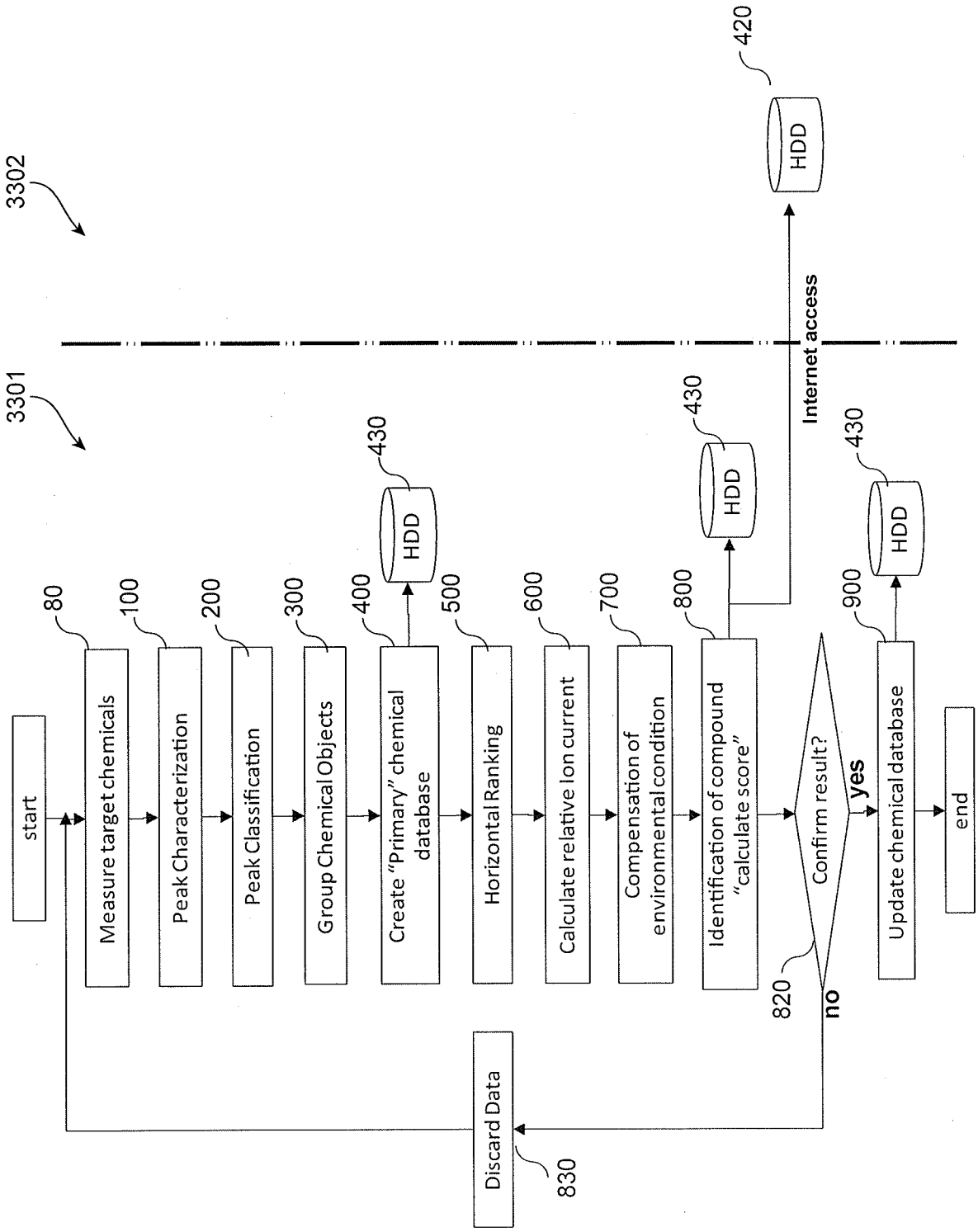

3302
3301
start
Measure target chemicals
80
Peak Characterization
100
Peak Classification
200
Group Chemical Objects
300
Create "Primary" chemical database
400
HDD
430
Internet access
Horizontal Ranking
500
Calculate relative Ion current
600
Compensation of environmental condition
700
Identification of compound "calculate score"
800
HDD
420
Update chemical database
900
HDD
420
Confirm result?
820
yes
no
Discard Data
830
end

Fig. 35


3302
3301
420
HDD
Internet access
430
HDD
430
HDD
430
HDD
start
80
Measure target chemicals
100
Peak Characterization
200
Peak Classification
300
Group Chemical Objects
400
Create "Primary" chemical database
500
Horizontal Ranking
600
Calculate relative Ion current
700
Compensation of environmental condition
800
Identification of compound "calculate score"
820
Confirm result?
yes
no
900
Update chemical database
end
Discard Data
830