Supporting Information File

New bicyclic pyridine based hybrids linked to 1,2,3-triazole unit: synthesis *via* click reaction and evaluation of neurotropic activity and molecular docking

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Samvel Sirakanyan – shnnr@mail.ru

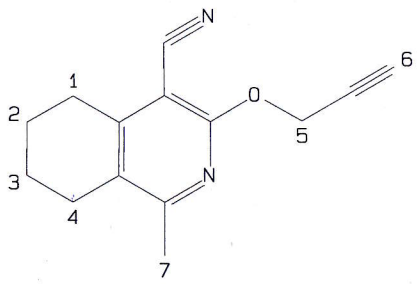
The copies of ^{1}H, ^{13}C NMR and MS spectra of all new synthesized compounds

2b

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Oct 4 2021

T20-145

NOCI_21 t20-145



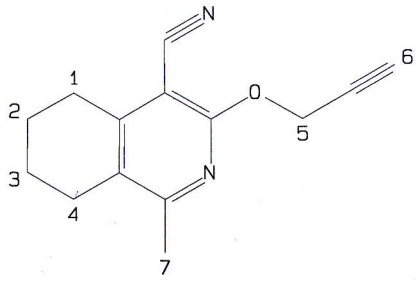
$C_{14}H_{14}N_2O$

2b

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 288, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 4 2021

T20-145

NOCI_21 t20-145



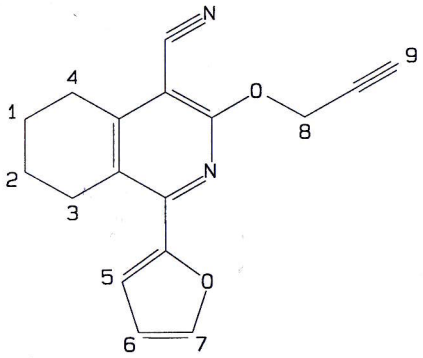
$C_{14}H_{14}N_2O$

2d

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Sep 26 2018

HA-997

SAMV_18 ha-997



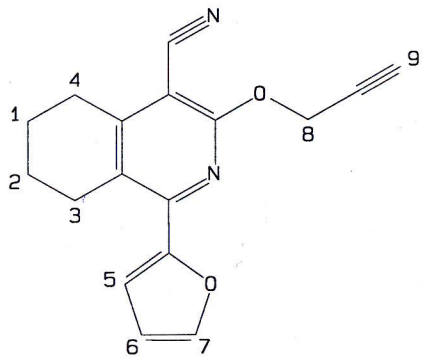
$C_{17}H_{14}N_2O_2$

2d

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 176, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Sep 26 2018

HA-997

SAMV_18 ha-997



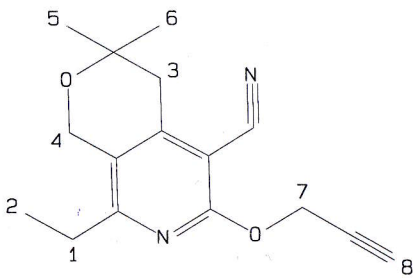
$C_{17}H_{14}N_2O_2$

2f

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Feb 27 2019

HA-1017

SAMV_19 ha-1017



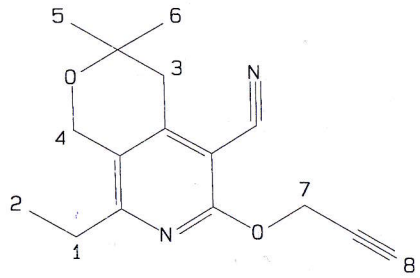
$C_{16}H_{18}N_2O_2$

2f

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 288, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Feb 27 2019

HA-1017

SAMV_19 ha-1017



$C_{16}H_{18}N_2O_2$

2g

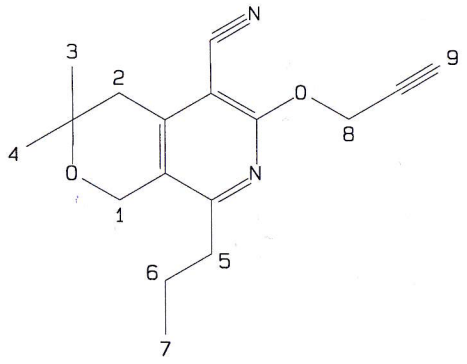
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 25 2019

HA-1023

SAMV_19 ha-1023



$C_{17}H_{20}N_2O_2$

2g

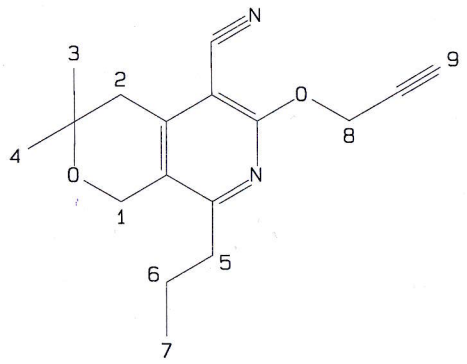
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 256, np = 32000, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 25 2019

SAMV_19 ha-1023

HA-1023



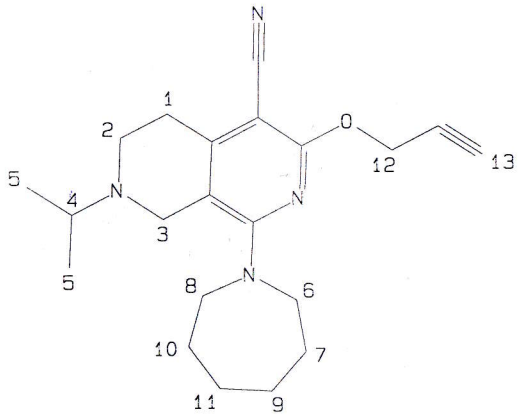
$C_{17}H_{20}N_2O_2$

2k

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 May 5 2021

S12-003

ANUSH_TEMA s12-003



$C_{21}H_{28}N_4O$

2h

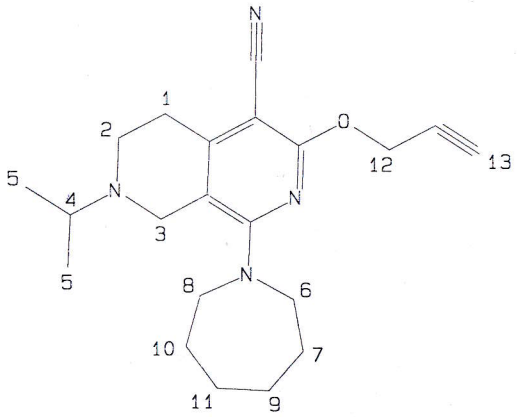
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 800, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

May 6 2021

S12-003

ANUSH_TEMA s12-003



$C_{21}H_{28}N_4O$

2i

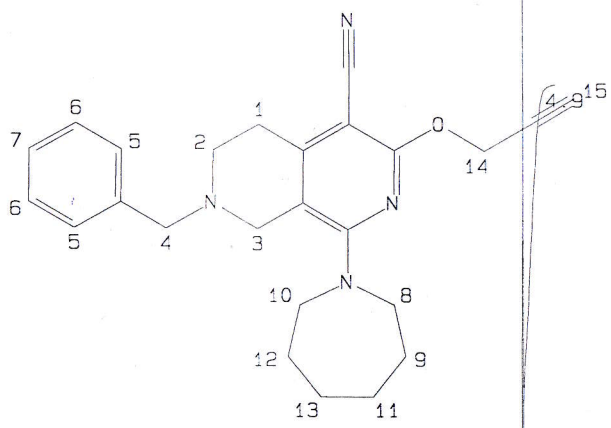
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Aug 5 2021

S12-030

NOCI_21 s12-030

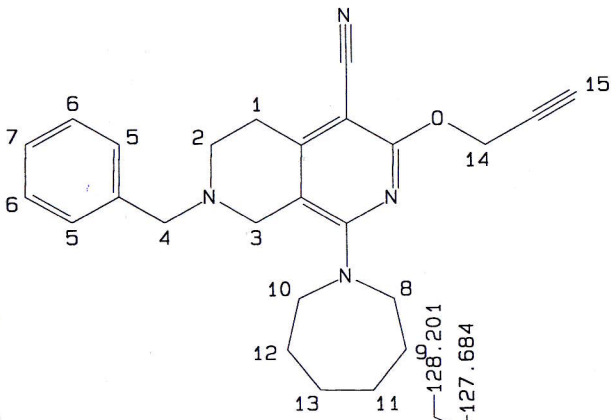


$C_{25}H_{28}N_4O$

2i

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 624, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Aug 5 2021

S12-030 NOCI_21 s12-030



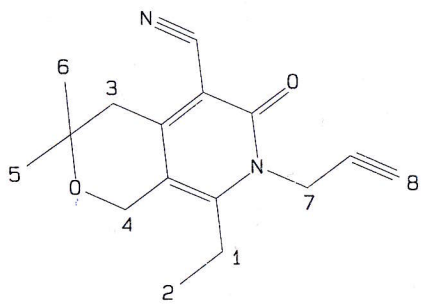
$C_{25}H_{28}N_4O$

3f

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Apr 22 2019

HA-1017-1

SAMV_19 ha-1017-1



$C_{16}H_{18}N_2O_2$

3f

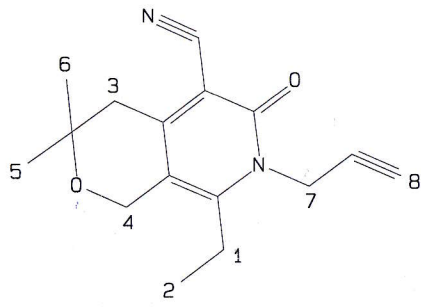
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 256, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Apr 22 2019

HA-1017-1

SAMV_19 ha-1017-1



$C_{16}H_{18}N_2O_2$

5a

Future

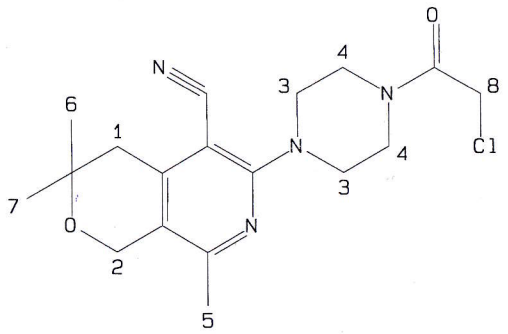
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 13 2019

HE-439

SAMV_19 he-439



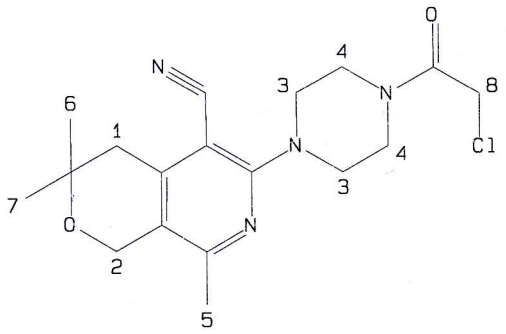
$C_{18}H_{23}ClN_4O_2$

5Q

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 432, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Mar 13 2019

HE-439

SAMV_19 he-439



$C_{18}H_{23}ClN_4O_2$

95.474

93.44

48.11

47.56

164.229
159.109
155.355
147.752
119.522
115.470
69.040
59.188
45.114
41.158
40.802
40.333
40.050
39.775
39.500
39.225
38.942
38.667
37.720
25.733
20.969

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

6a

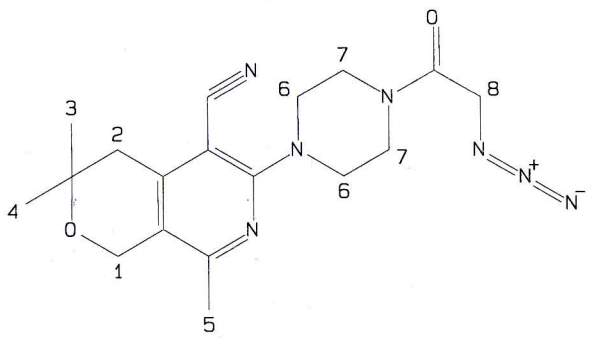
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 29 2019

HA-1028

SAMV_19 ha-1028



$C_{18}H_{23}N_7O_2$

6a

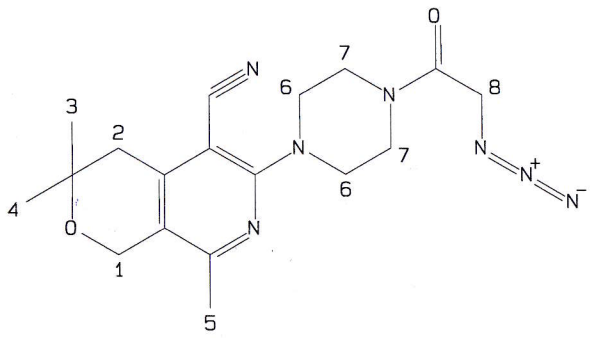
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 128, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 29 2019

HA-1028

SAMV_19 ha-1028



$C_{18}H_{23}N_7O_2$

95.499
93.331
69.064
59.204
49.579
47.969
47.597
43.844
41.037
40.058
39.775
39.500
39.225
38.950
37.737
25.749
20.993
165.361
159.109
155.396
147.776
119.482
115.534

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

7a

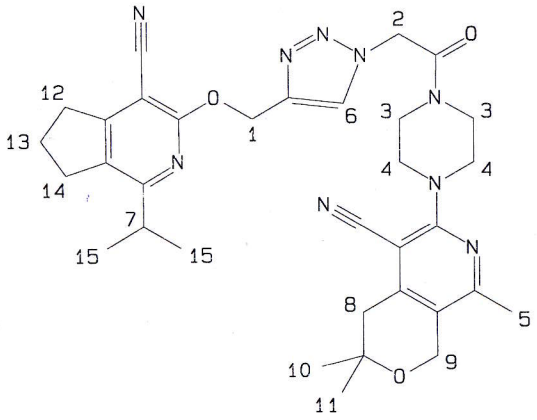
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Apr 22 2019

HA-1035

SAMV_19 ha-1035



$C_{33}H_{39}N_9O_3$

7a

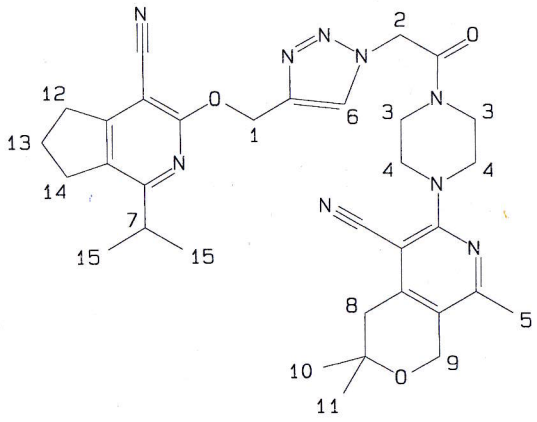
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt=416, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3

Apr 22 2019

HA-1035

SAMV_19 ha-1035



$C_{33}H_{39}N_9O_3$

95.474

93.242

89.739

69.040

59.641

59.609

59.188

50.347

47.945

47.920

47.492

43.973

41.207

40.333

40.050

39.775

39.492

39.217

38.942

37.729

32.697

32.002

28.677

25.733

23.889

20.993

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155.388

147.744

141.791

129.593

125.192

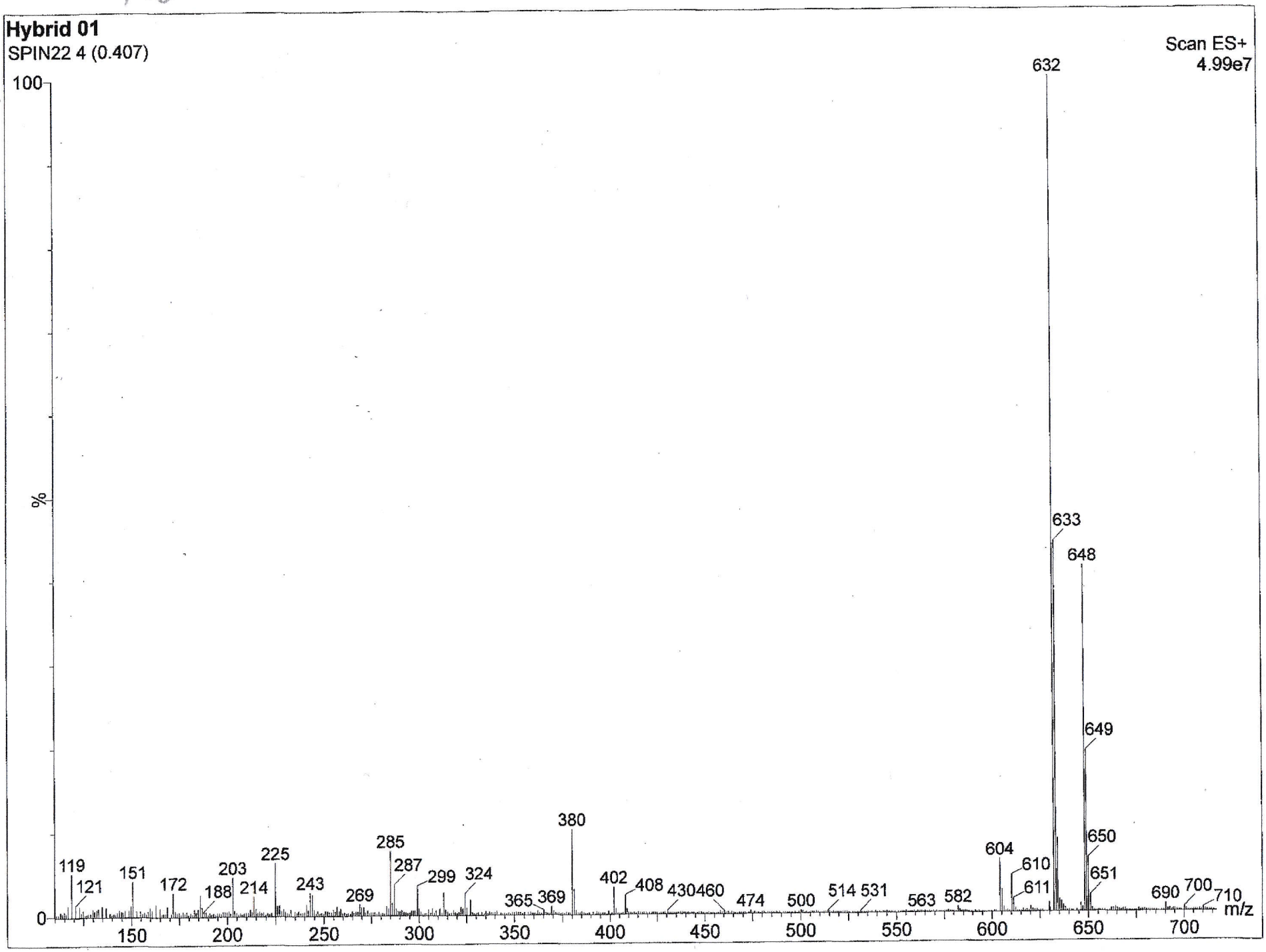
119.417

115.551

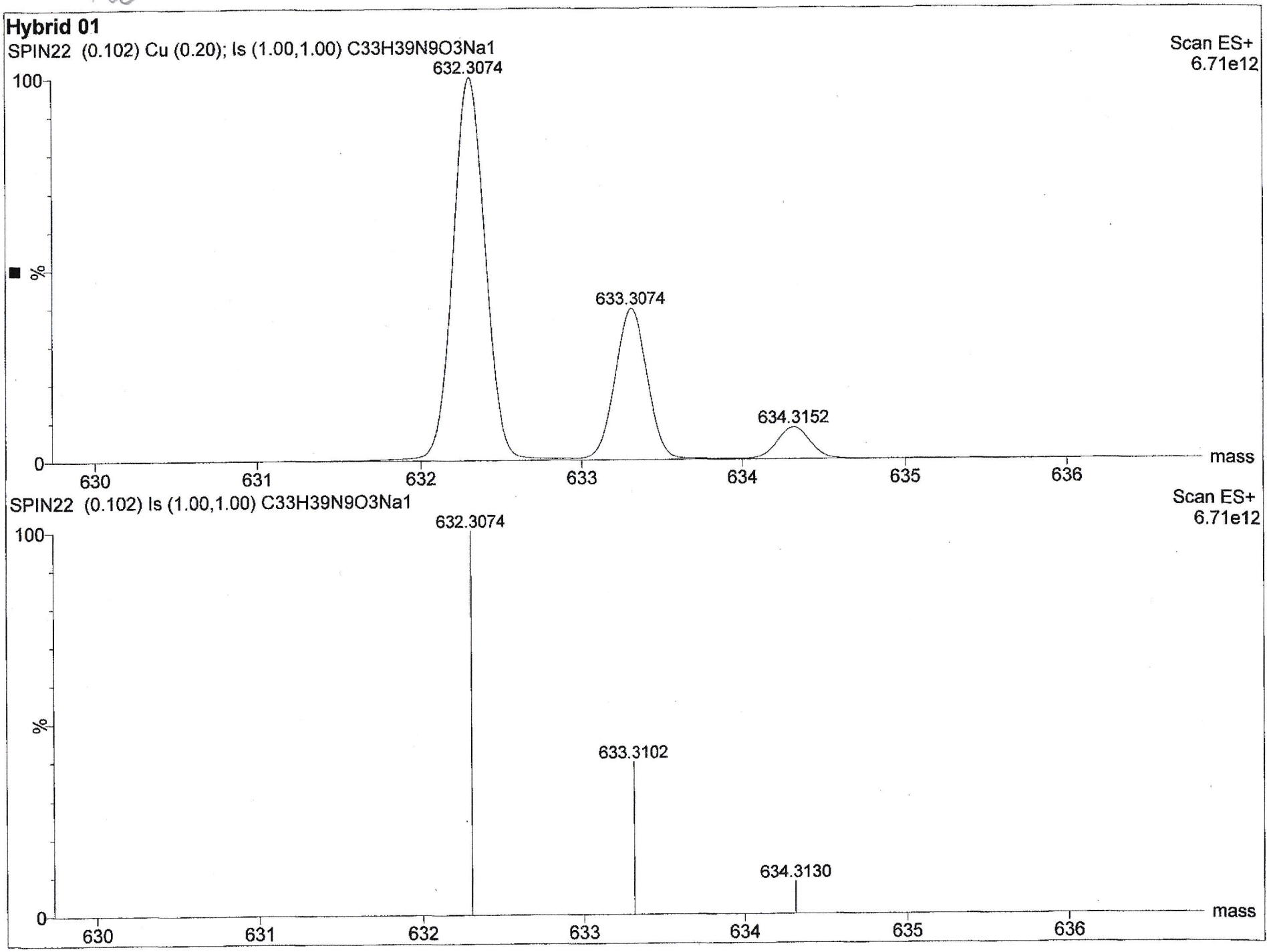
113.812

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

7a


Hybrid 01
SPIN22 4 (0.407)
Scan ES+
4.99e7
100
%
0
632
633
648
649
650
651
604
610
611
380
285
287
299
324
225
203
214
188
243
269
119
121
151
172
365
369
402
408
430460
474
500
514
531
563
582
690
700
710
m/z
150
200
250
300
350
400
450
500
550
600
650
700

7a


Hybrid 01
SPIN22 (0.102) Cu (0.20); Is (1.00,1.00) C33H39N9O3Na1
Scan ES+
6.71e12
100
%
0
632.3074
633.3074
634.3152
630
631
632
633
634
635
636
mass
SPIN22 (0.102) Is (1.00,1.00) C33H39N9O3Na1
Scan ES+
6.71e12
100
%
0
632.3074
633.3102
634.3130
630
631
632
633
634
635
636
mass

7c

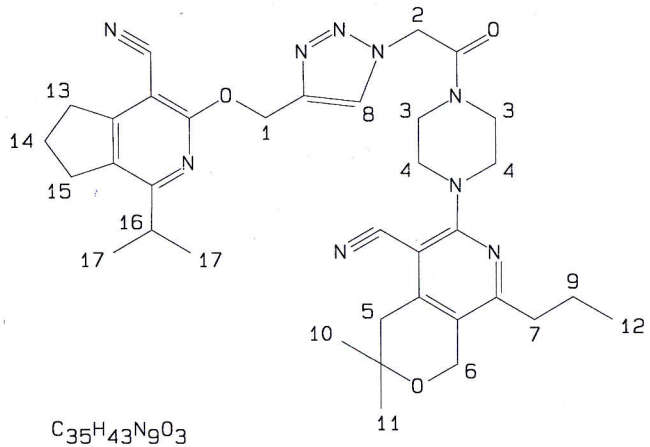
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 28 2019

HA-1026

SAMV_19 ha-1026



$C_{35}H_{43}N_9O_3$

7c

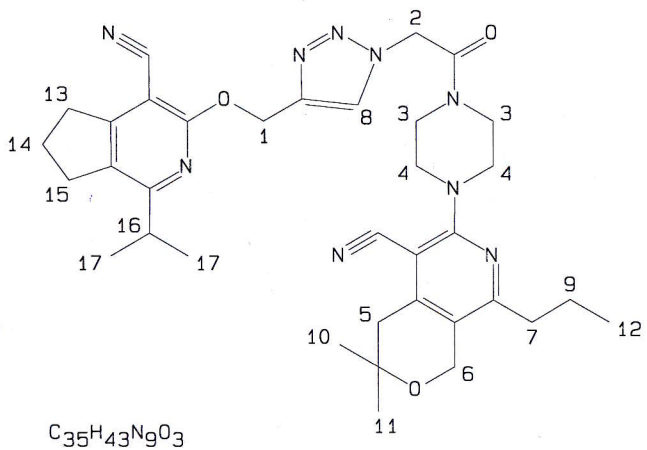
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 2544, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 28 2019

SAMV_19 ha-1026

HA-1026

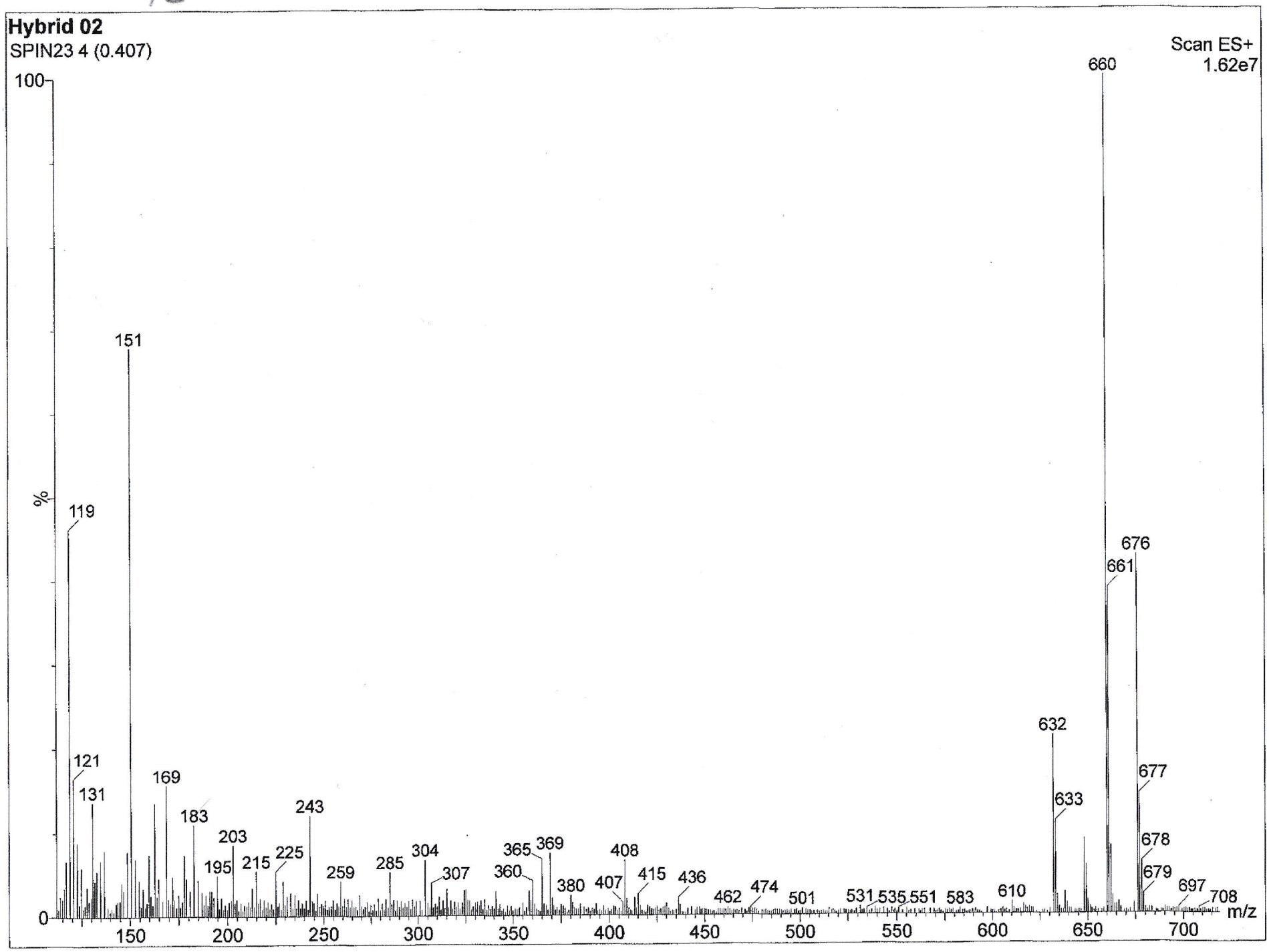


$C_{35}H_{43}N_9O_3$

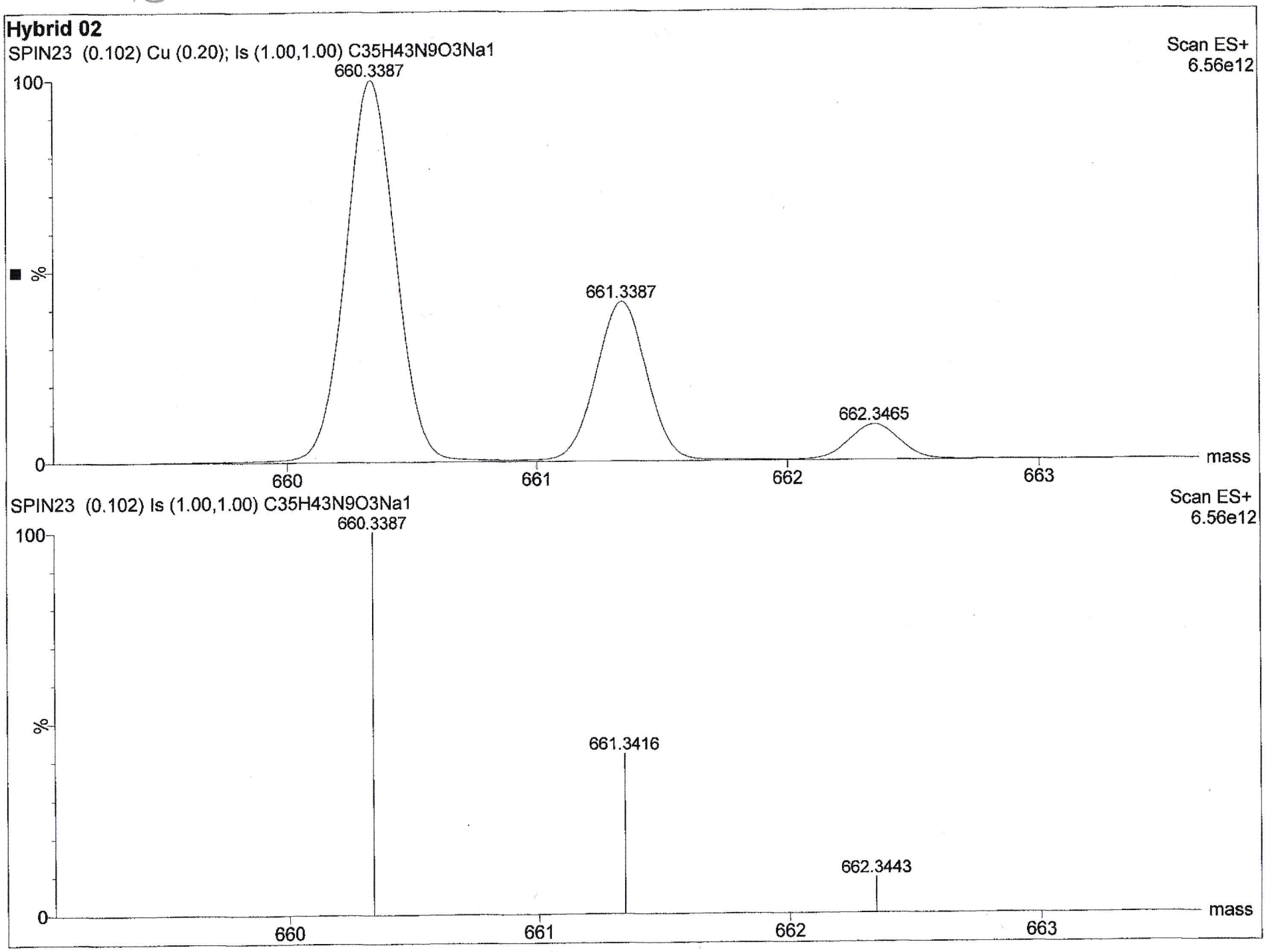
95.474
95.361
58.945
40.058
39.856
39.775
39.500
39.225
38.942
38.667
37.882
35.197
32.697
32.010
28.677
25.741
23.897
20.613
20.006
13.535
163.768
161.228
161.009
159.060
158.542
147.962
141.791
129.585
125.184
119.077
115.567
95.329
93.185
68.975
59.657
50.339
40.333
162,61
113,82
89,76
47,97
47,40
43,96
41,20

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

4c


Hybrid 02
SPIN23 4 (0.407)
Scan ES+
1.62e7
100
%
0
660
151
119
676
661
632
121
131
169
677
633
183
243
203
678
225
195
215
304
365
369
408
679
259
285
307
360
380
407
415
436
462
474
501
531
535
551
583
610
697
708
m/z
150
200
250
300
350
400
450
500
550
600
650
700

7c


Hybrid 02
SPIN23 (0.102) Cu (0.20); Is (1.00,1.00) C35H43N9O3Na1
Scan ES+
6.56e12
100
%
0
660.3387
661.3387
662.3465
660
661
662
663
mass
SPIN23 (0.102) Is (1.00,1.00) C35H43N9O3Na1
Scan ES+
6.56e12
100
%
0
660.3387
661.3416
662.3443
660
661
662
663
mass

7d

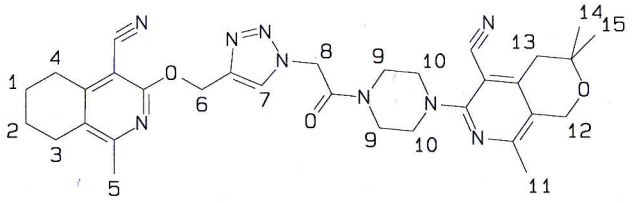
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

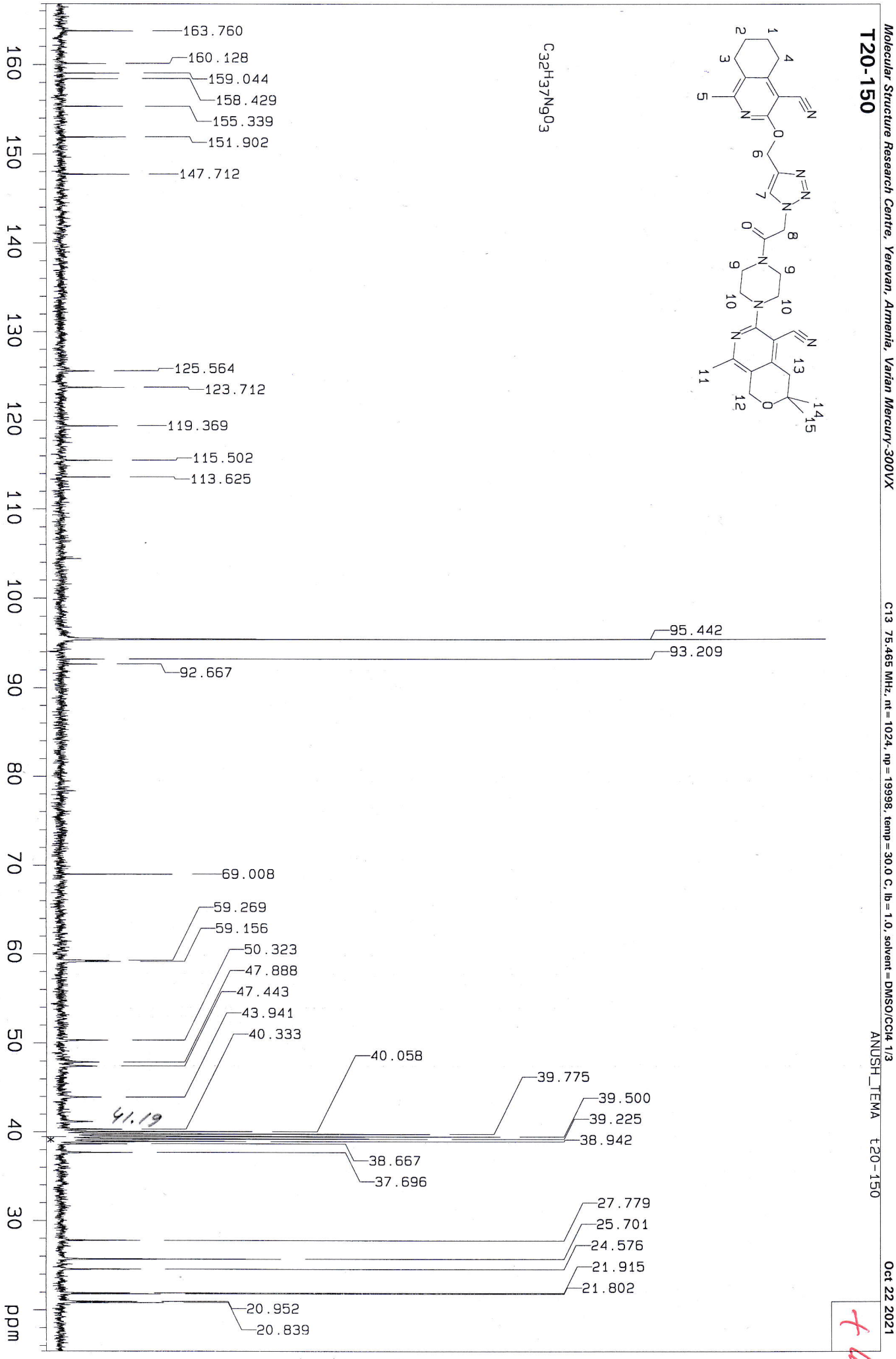
Oct 22 2021

T20-150

ANUSH_TEMA t20-150



$C_{32}H_{37}N_9O_3$


T20-150
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX
C32H37N9O3
C13 75.465 MHz, nt = 1024, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3
ANUSH_TEMA t20-150
Oct 22 2021
163.760
160.128
159.044
158.429
155.339
151.902
147.712
125.564
123.712
119.369
115.502
113.625
95.442
93.209
92.667
69.008
59.269
59.156
50.323
47.888
47.443
43.941
40.333
41.19
40.058
39.775
39.500
39.225
38.942
38.667
37.696
27.779
25.701
24.576
21.915
21.802
20.952
20.839
ppm

7e

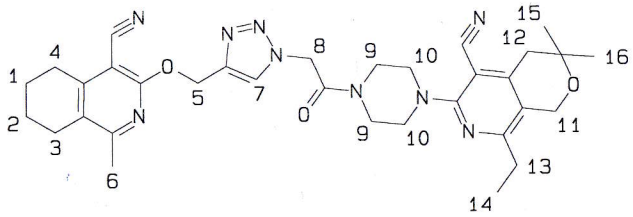
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO

Feb 23 2022

T20-171

NOCI_22 t20-171



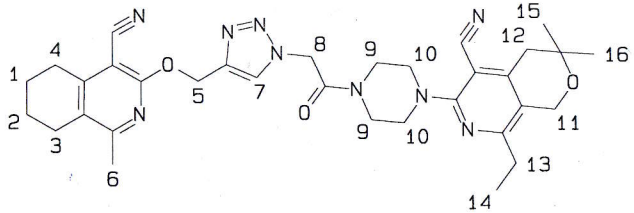
$C_{33}H_{39}N_9O_3$

7e

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 720, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Feb 23 2022

T20-171

NOCI_22 t20-171



$C_{33}H_{39}N_9O_3$

95.474
95.361
93.031
92.700
68.975
59.309
58.824
50.339
47.904
47.395
43.949
41.207
41.182
40.333
40.058
39.775
39.500
39.225
38.942
38.667
37.858
27.812
26.445
25.741
24.617
21.947
21.842
20.872
10.874
163.784
160.160
159.376
159.117
158.453
151.934
147.849
125.508
123.745
118.754
115.583
113.650

160 140 120 100 80 60 40 20 ppm

7f

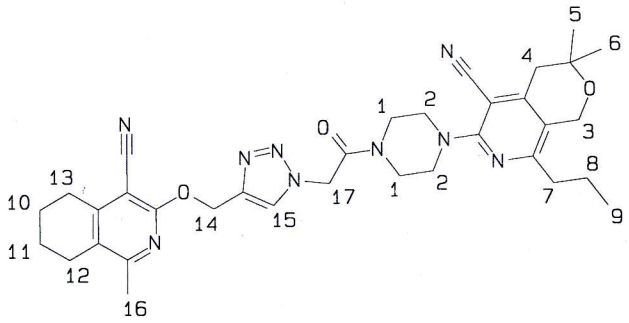
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO

Feb 16 2022

T20-169

ANUSH_TEMA t20-169



$C_{34}H_{41}N_9O_3$

7f

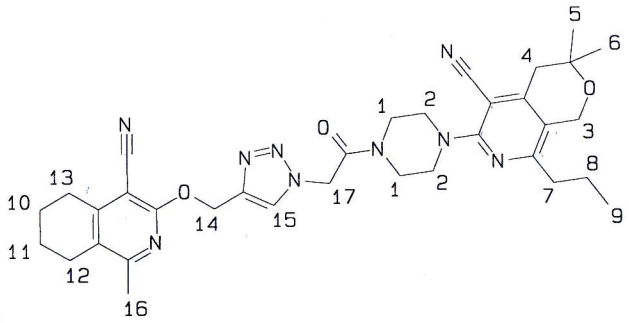
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 720, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Feb 16 2022

ANUSH_TEMA t20-169

T20-169



$C_{34}H_{41}N_9O_3$

95.450, 95.313, 93.137, 92.676, 68.935, 59.285, 58.913, 50.315, 47.937, 47.912, 47.378, 43.949, 43.916, 41.182, 41.150, 40.925, 40.050, 39.775, 39.662, 39.621, 39.500, 39.379, 39.346, 39.217, 38.942, 38.667, 37.850, 35.173, 27.787, 25.709, 24.592, 21.923, 21.818, 20.847, 19.974, 13.495

163.743, 160.136, 159.020, 158.502, 158.429, 151.910, 147.922, 125.540, 125.508, 123.720, 119.029, 115.534, 113.625

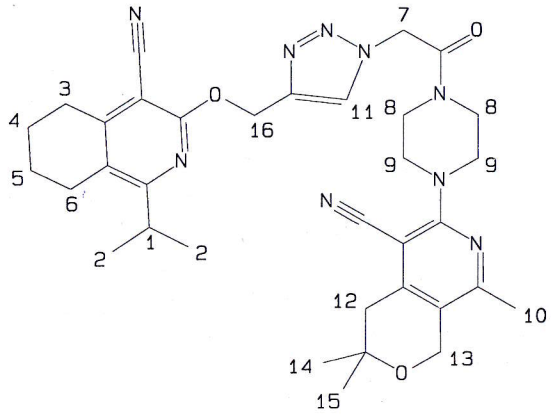
160 140 120 100 80 60 40 20 ppm

19

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 May 13 2019

HA-1040

NOCI_19 ha-1040



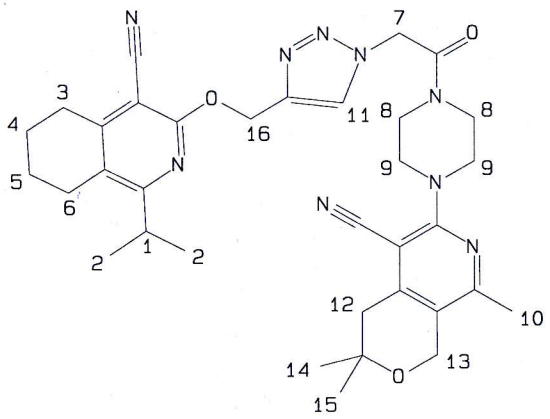
$C_{34}H_{41}N_9O_3$

79

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt=512, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3 May 13 2019

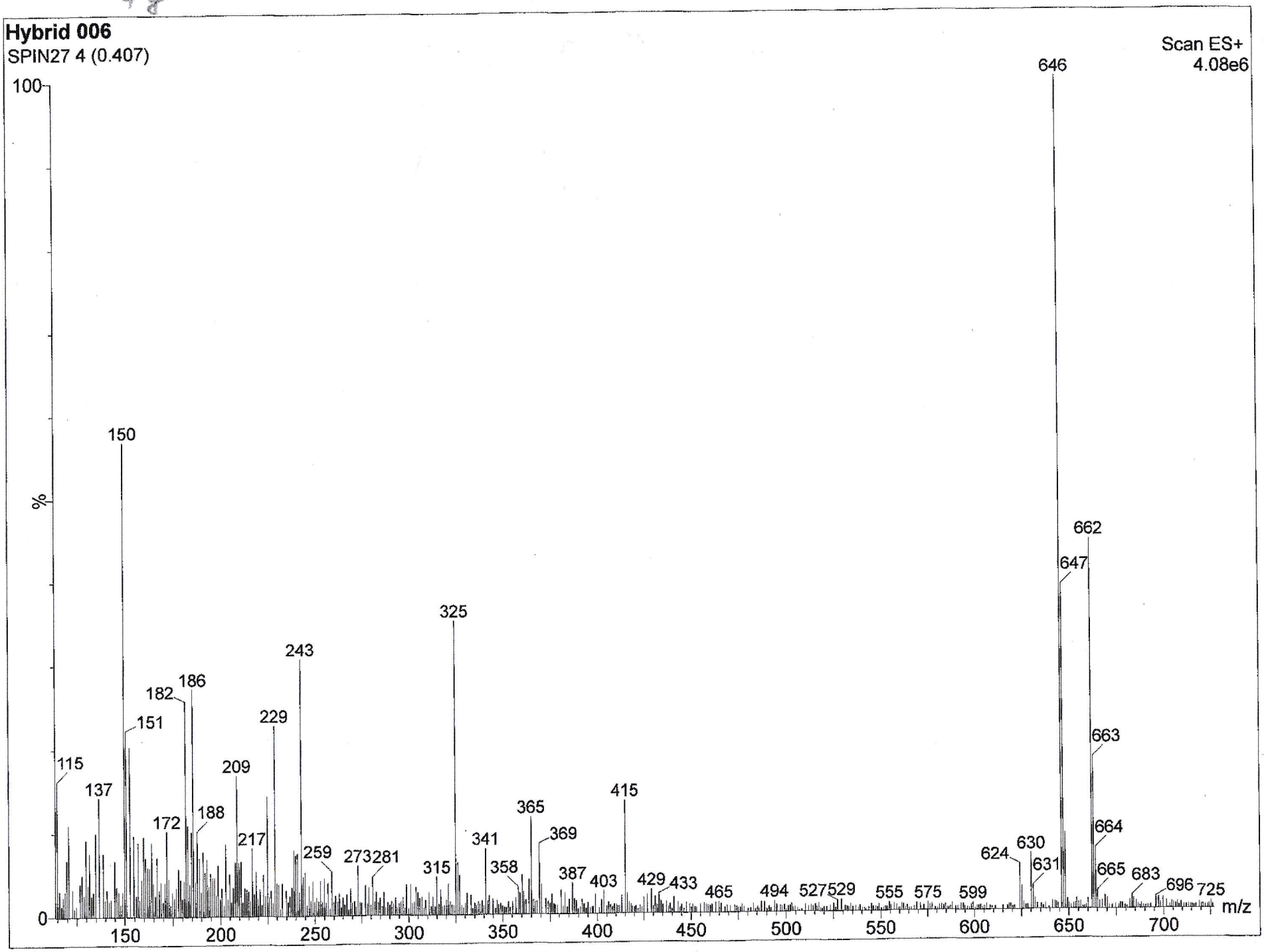
NOCI_19 ha-1040

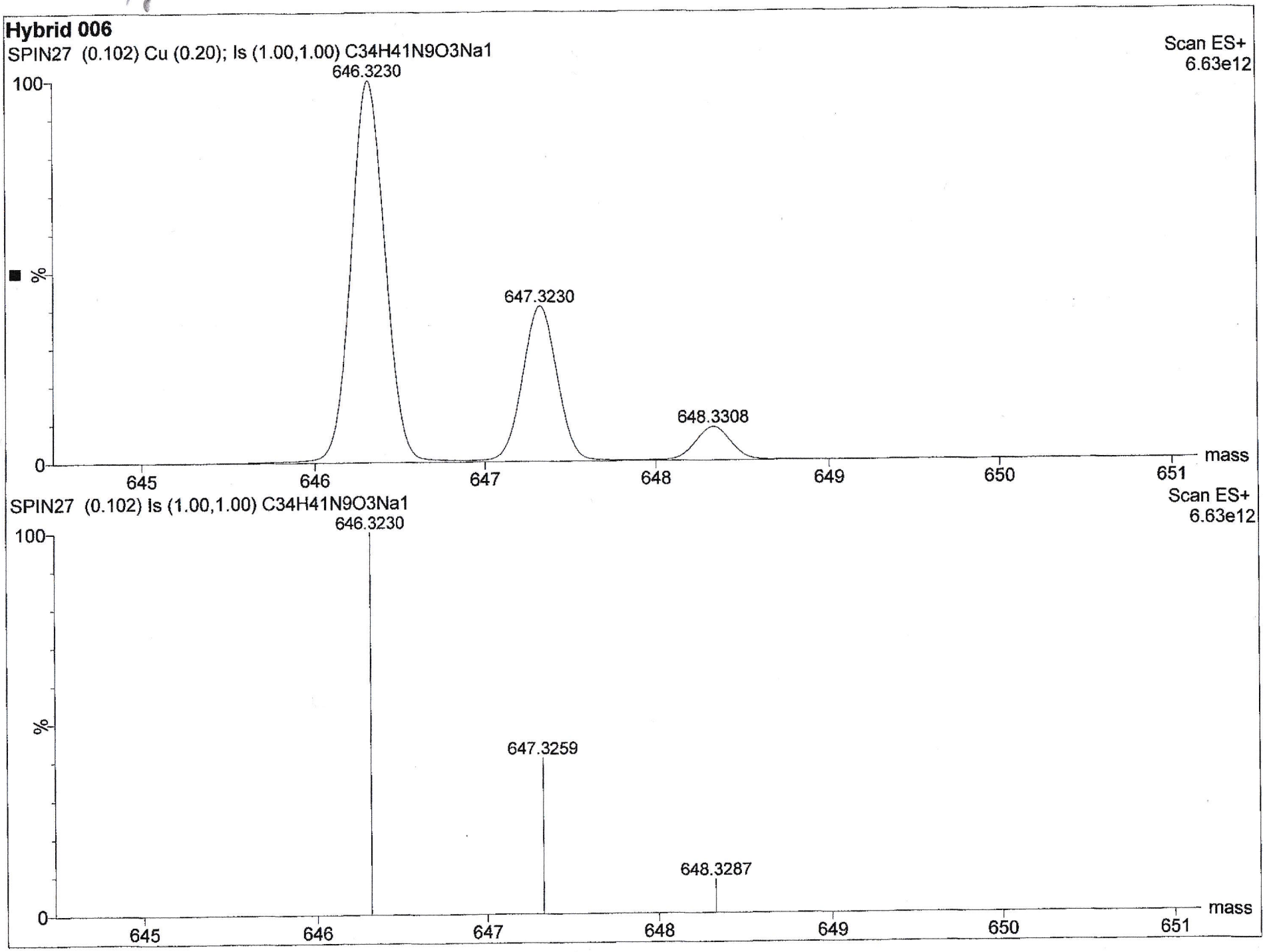
HA-1040



$C_{34}H_{41}N_9O_3$

78


Hybrid 006
SPIN27 4 (0.407)
Scan ES+
4.08e6
100
%
0
646
662
647
663
664
325
243
150
186
182
229
151
209
115
137
172
188
217
259
273
281
315
341
358
365
369
387
403
415
429
433
465
494
527
529
555
575
599
624
630
631
665
683
696
725
m/z
150
200
250
300
350
400
450
500
550
600
650
700


Hybrid 006
SPIN27 (0.102) Cu (0.20); Is (1.00,1.00) C34H41N9O3Na1
Scan ES+
6.63e12
100
%
0
646.3230
647.3230
648.3308
645
646
647
648
649
650
651
mass
SPIN27 (0.102) Is (1.00,1.00) C34H41N9O3Na1
Scan ES+
6.63e12
100
%
0
646.3230
647.3259
648.3287
645
646
647
648
649
650
651
mass

7i

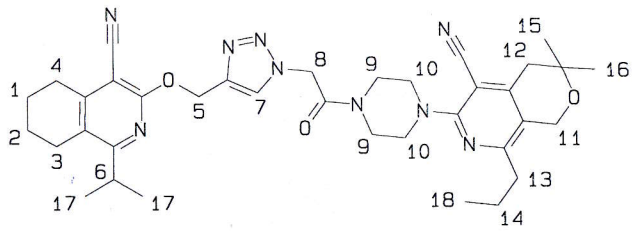
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 2 2022

NOCI_22 t20-170

T20-170



$C_{36}H_{45}N_9O_3$

7i

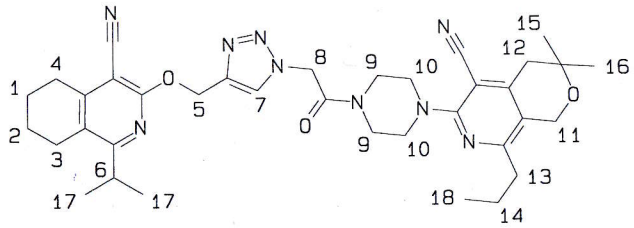
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 784, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 2 2022

NOCI_22 t20-170

T20-170



$C_{36}H_{45}N_9O_3$

95.466
93.153
92.692
166.025
163.735
160.468
159.036
158.518
152.516
147.938
141.89
125.112
122.224
119.053
115.551
113.690
68.951
59.180
58.937
50.323
47.937
47.387
43.941
41.182
40.333
40.058
39.775
39.500
39.225
38.942
38.667
37.866
35.181
30.344
28.103
25.725
23.808
21.964
20.880
20.823
19.990
13.511

160 140 120 100 80 60 40 20 ppm

7j

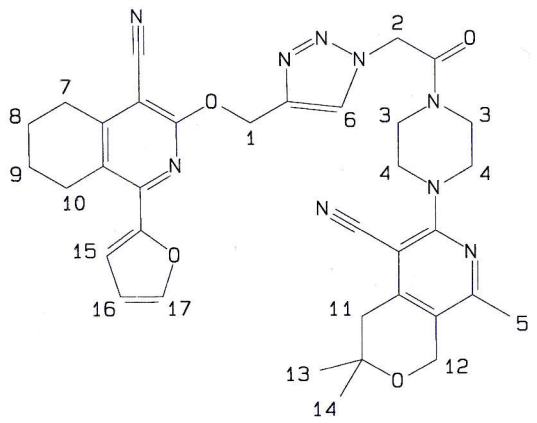
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Apr 17 2019

HA-1033

SAMV_19 ha-1033



$C_{35}H_{37}N_9O_4$

7i

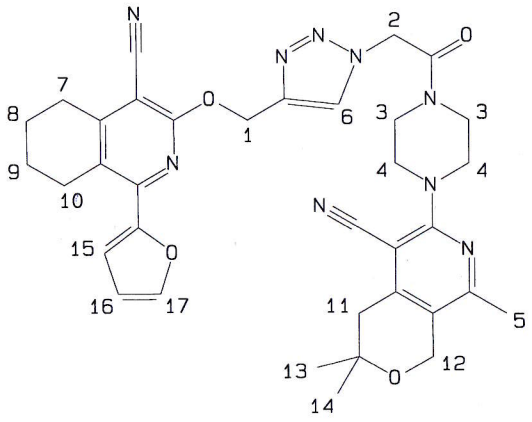
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 528, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Apr 17 2019

SAMV_19 ha-1033

HA-1033

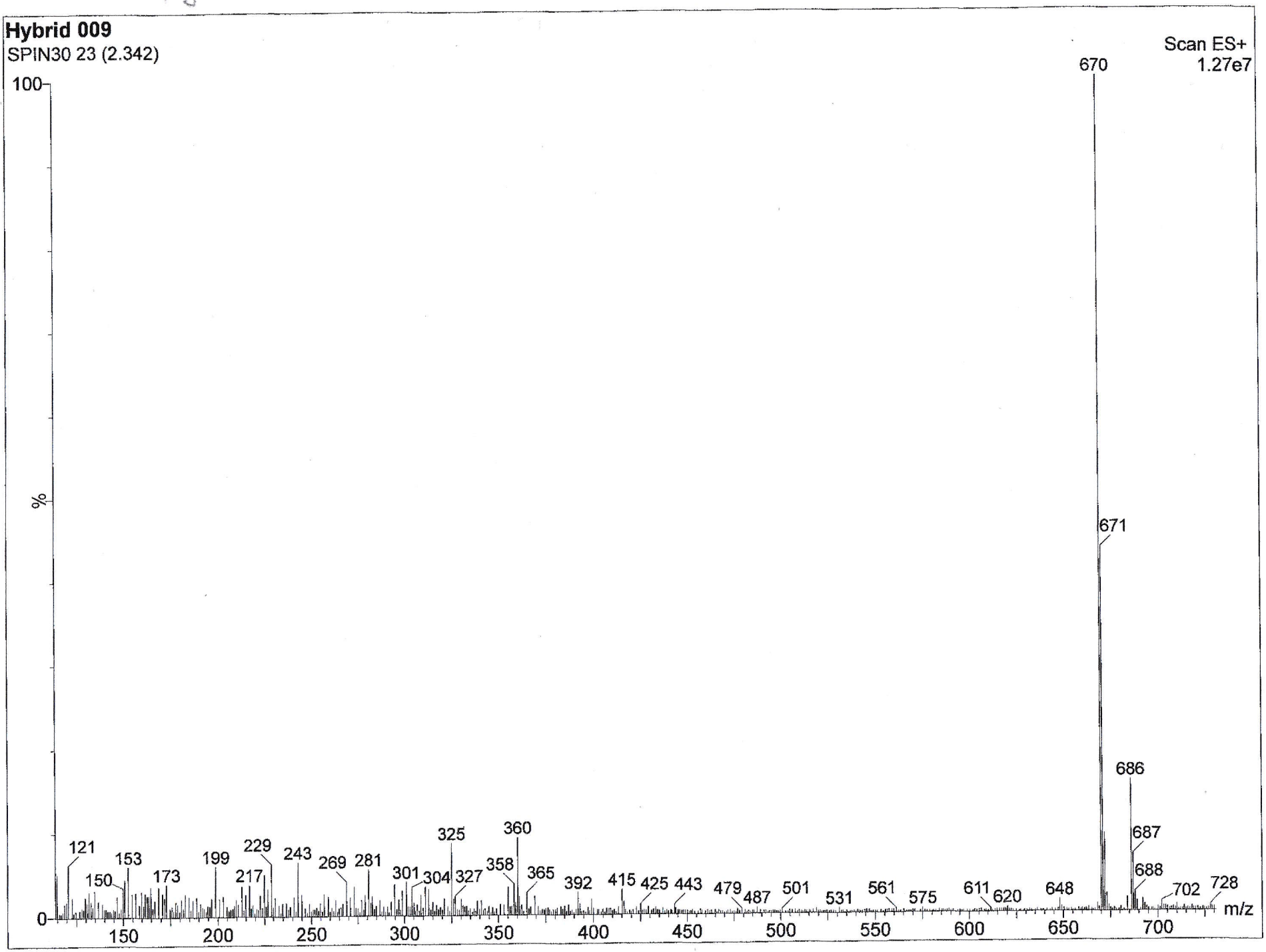


$C_{35}H_{37}N_9O_4$

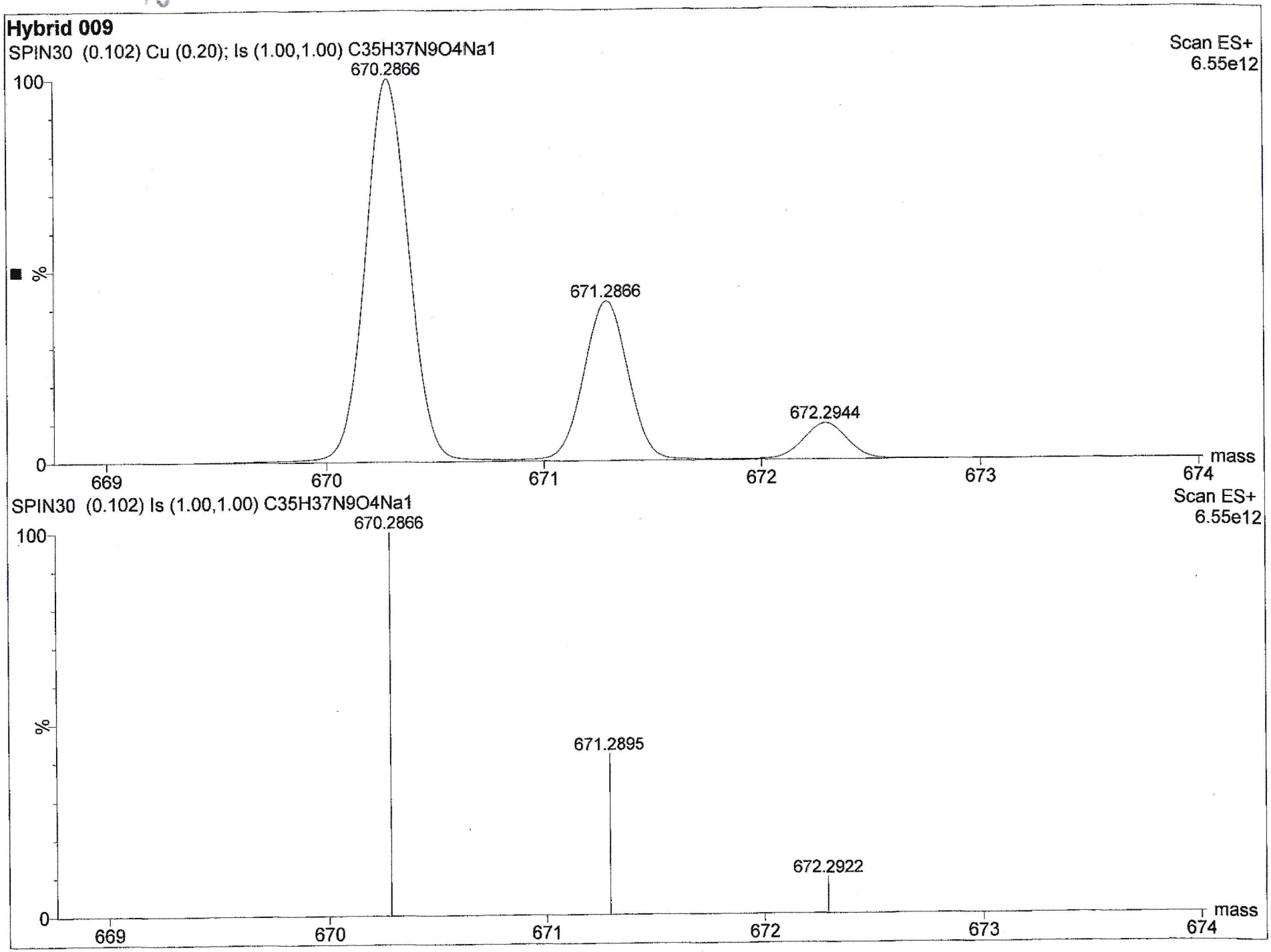
95.482
93.598
93.218
69.048
59.455
59.196
50.387
47.912
47.484
47.467
43.965
41.215
40.333
40.058
39.783
39.500
39.225
38.942
38.667
37.720
28.459
25.741
25.490
21.931
21.001
20.621
163.800
159.715
159.076
155.404
154.158
152.589
147.744
146.531
144.193
141.27
125.597
122.111
119.409
115.567
114.394
113.634
111.603

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

7j


Hybrid 009
SPIN30 23 (2.342)
Scan ES+
1.27e7
100
%
0
670
671
686
687
688
702
728
121
150
153
173
199
217
229
243
269
281
301
304
325
327
358
360
365
392
415
425
443
479
487
501
531
561
575
611
620
648
m/z
150
200
250
300
350
400
450
500
550
600
650
700

7j

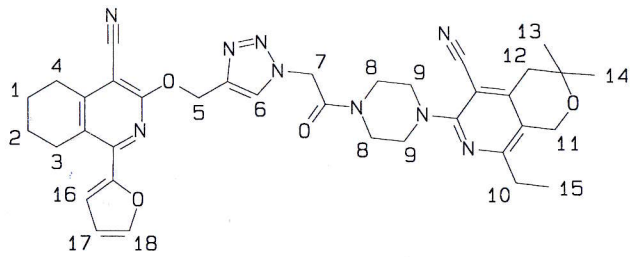

Hybrid 009
SPIN30 (0.102) Cu (0.20); Is (1.00,1.00) C35H37N9O4Na1
Scan ES+
6.55e12
100
%
0
670.2866
671.2866
672.2944
669
670
671
672
673
674
mass
SPIN30 (0.102) Is (1.00,1.00) C35H37N9O4Na1
Scan ES+
6.55e12
100
%
0
670.2866
671.2895
672.2922
669
670
671
672
673
674
mass

7k

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 **Feb 11 2022**

T20-166

ANUSH_TEMA t20-166



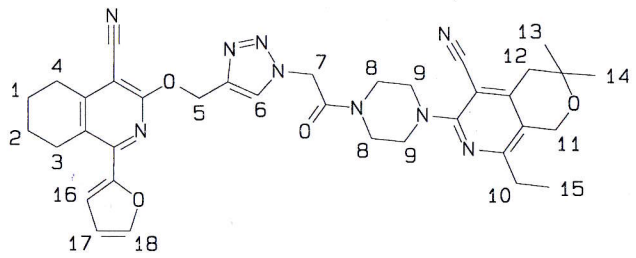
$C_{36}H_{39}N_9O_4$

7k

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 560, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Feb 11 2022

T20-166

ANUSH_TEMA t20-166



$C_{36}H_{39}N_9O_4$

95.458
95.377
39.775
39.500
39.225
38.942
38.667
37.834
28.443
26.429
25.725
40.058
25.474
21.915
20.605
10.858
163.768
159.707
159.376
159.092
154.142
152.581
147.833
146.523
144.161
125.589
122.103
118.746
115.599
114.370
113.609
111.579
93.590
92.983
68.967
59.439
58.808
50.363
47.872
47.362
43.949
41.191
41.158
40.333

141.79

160 140 120 100 80 60 40 20 ppm

7e

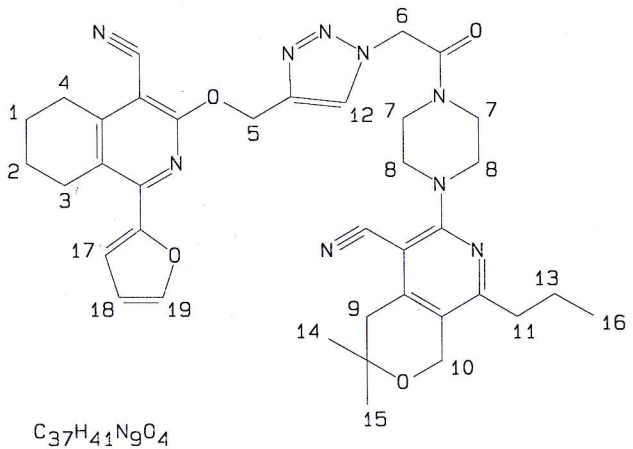
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 21 2019

HA-1025

SAMV_19 ha-1025



$C_{37}H_{41}N_9O_4$

7l

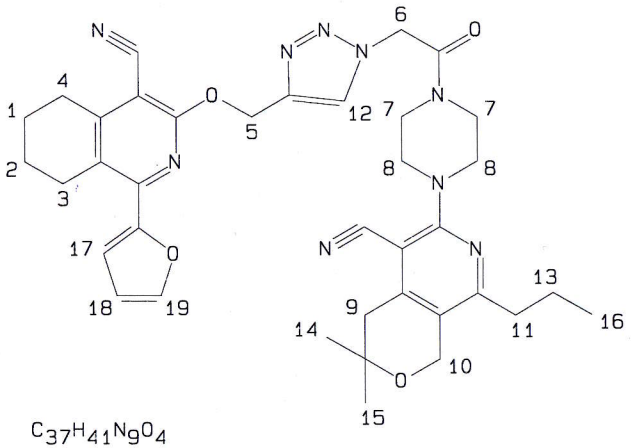
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 1296, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 21 2019

SAMV_19 ha-1025

HA-1025

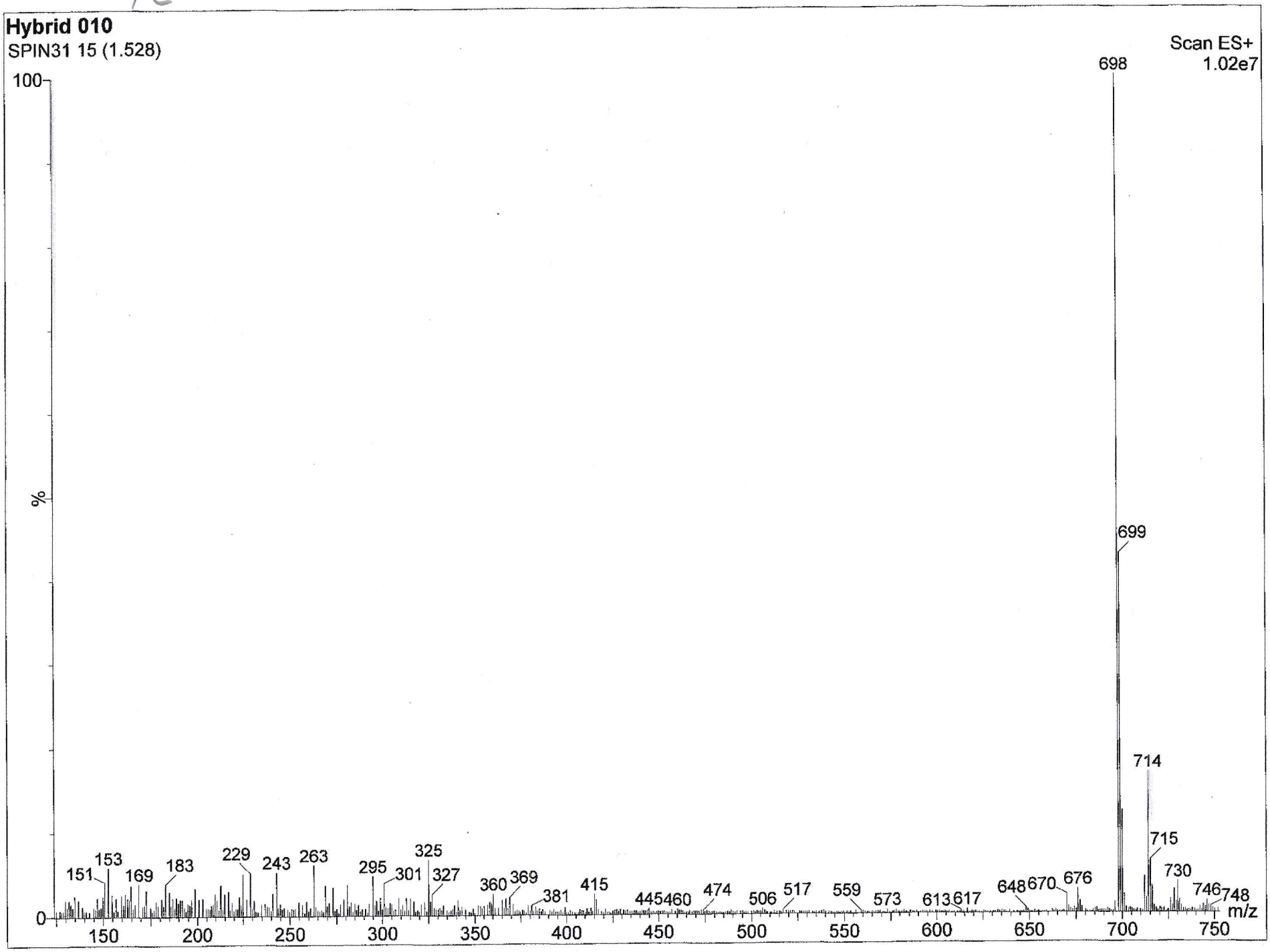


$C_{37}H_{41}N_9O_4$

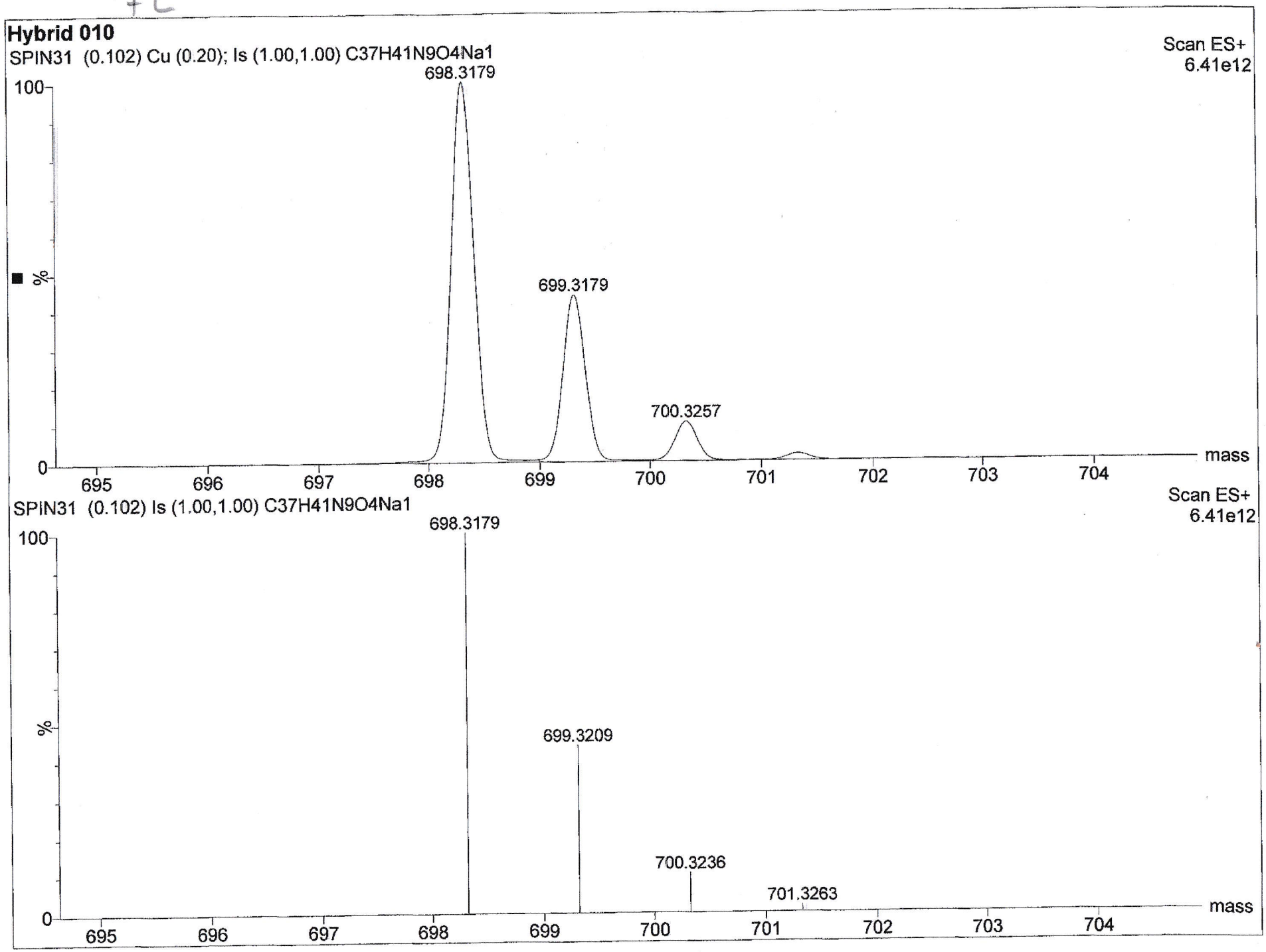
95.474
40.050
39.775
39.500
39.217
38.942
38.667
37.874
35.197
28.459
25.733
25.490
21.939
20.629
20.006
13.535
40.333
68.967
59.455
58.945
163.776
159.044
158.551
154.158
152.597
147.954
144.169
146.55
135.58 br.
122.119
119.061
115.58
114.378
113.62
111.595
93.61
93.145
50.37
47.93
47.41
43.96
41.21

160 140 120 100 80 60 40 20 ppm

7e


Hybrid 010
SPIN31 15 (1.528)
Scan ES+
1.02e7
100
%
0
698
699
714
715
730
746
748
151
153
169
183
229
243
263
295
301
325
327
360
369
381
415
445460
474
506
517
559
573
613617
648
670
676
150
200
250
300
350
400
450
500
550
600
650
700
750
m/z

7e


Hybrid 010
SPIN31 (0.102) Cu (0.20); Is (1.00,1.00) C37H41N9O4Na1
Scan ES+
6.41e12
698.3179
699.3179
700.3257
100
%
0
mass
695
696
697
698
699
700
701
702
703
704
SPIN31 (0.102) Is (1.00,1.00) C37H41N9O4Na1
Scan ES+
6.41e12
698.3179
699.3209
700.3236
701.3263

7m

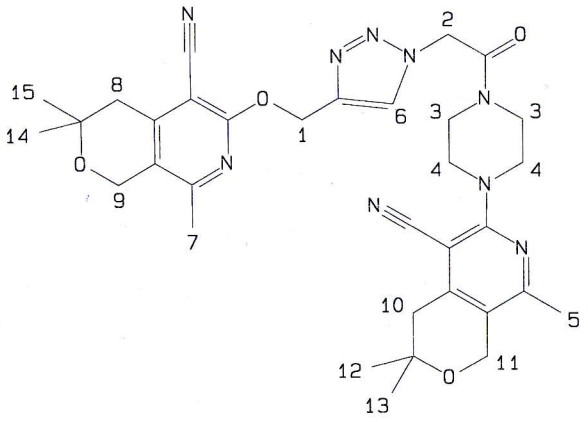
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Apr 12 2019

HA-1032

SAMV_19 ha-1032



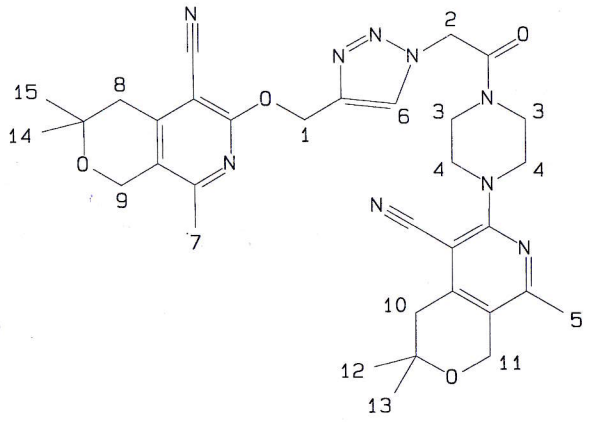
$C_{33}H_{39}N_9O_4$

7m

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 656, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Apr 12 2019

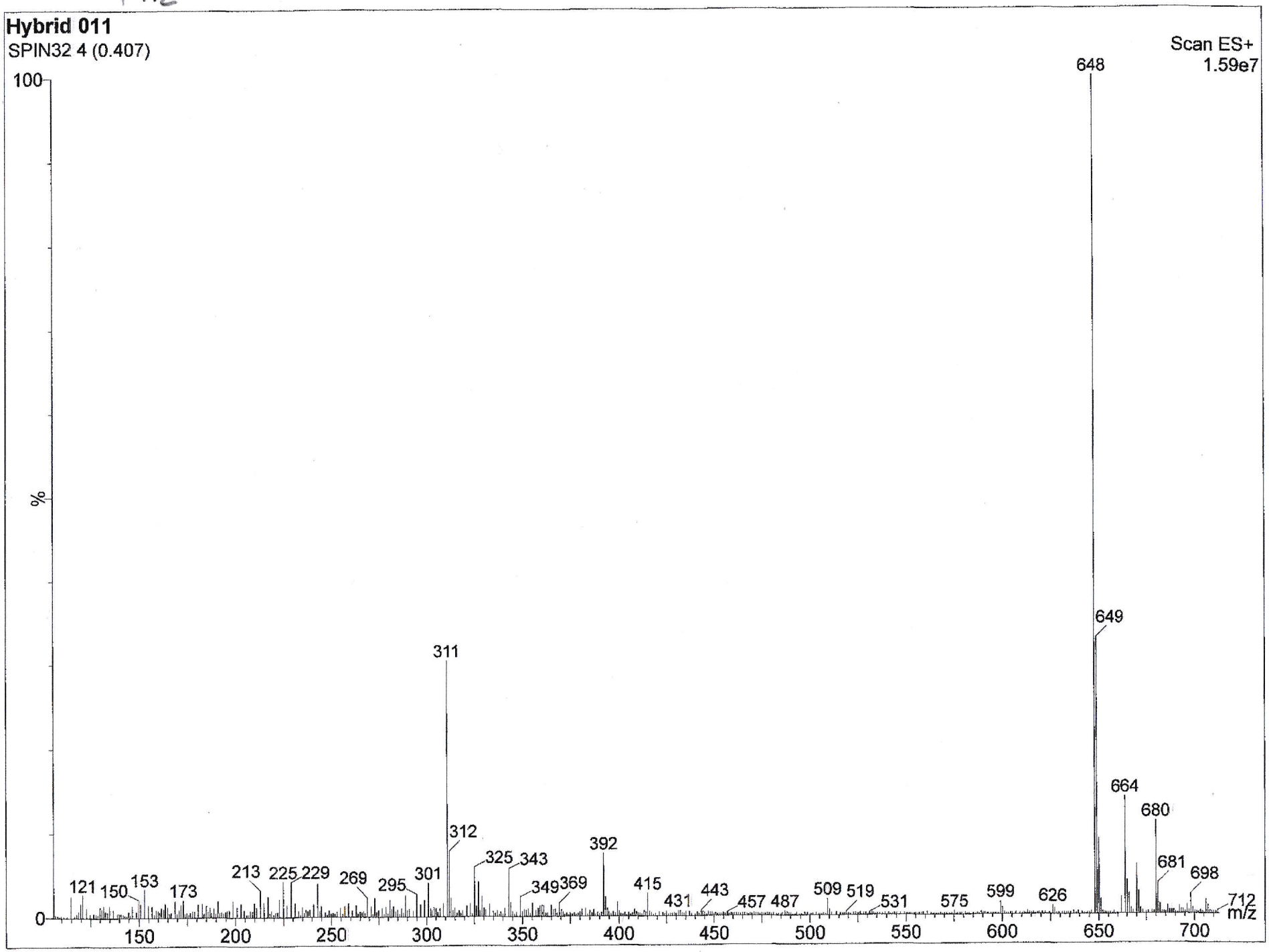
HA-1032

SAMV_19 ha-1032

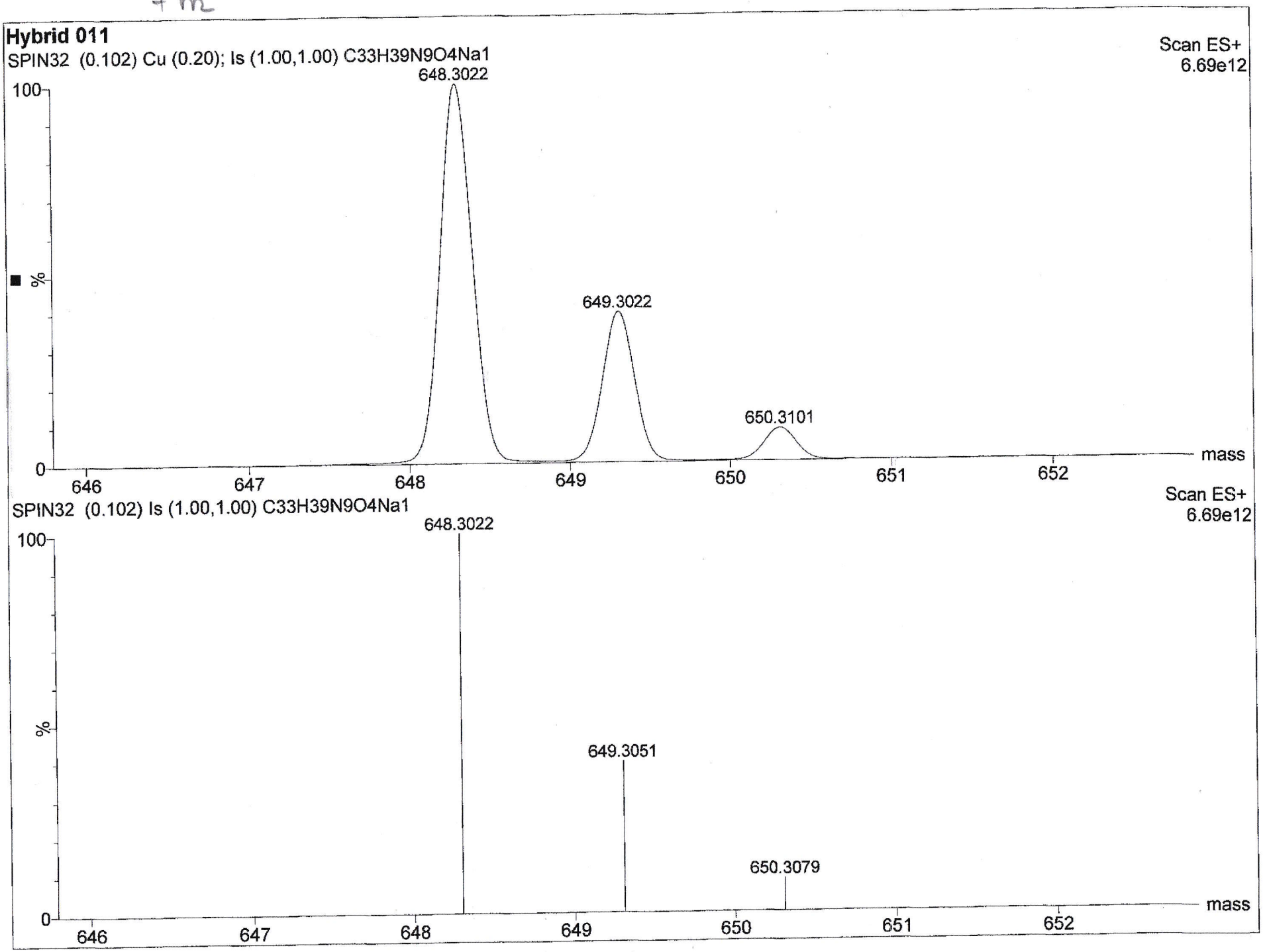


$C_{33}H_{39}N_9O_4$

7 m2


Hybrid 011
SPIN32 4 (0.407)
Scan ES+
1.59e7
100
%
0
121
150
153
173
213
225
229
269
295
301
311
312
325
343
349
369
392
415
431
443
457
487
509
519
531
575
599
626
648
649
664
680
681
698
712
150
200
250
300
350
400
450
500
550
600
650
700
m/z

7m


Hybrid 011
SPIN32 (0.102) Cu (0.20); Is (1.00,1.00) C33H39N9O4Na1
Scan ES+
6.69e12
100
%
0
648.3022
649.3022
650.3101
646
647
648
649
650
651
652
mass
SPIN32 (0.102) Is (1.00,1.00) C33H39N9O4Na1
Scan ES+
6.69e12
100
%
0
648.3022
649.3051
650.3079
646
647
648
649
650
651
652
mass

7n

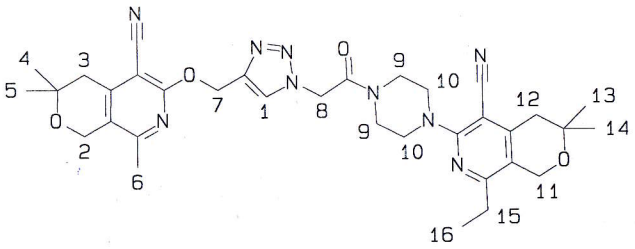
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 11 2022

NOCI_22 t20-176

T20-176



$C_{34}H_{41}N_9O_4$

7n

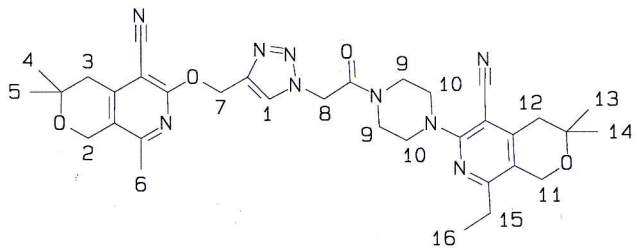
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 480, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Mar 11 2022

NOCI_22 t20-176

T20-176



$C_{34}H_{41}N_9O_4$

7p

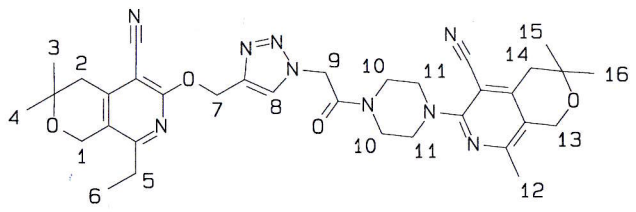
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

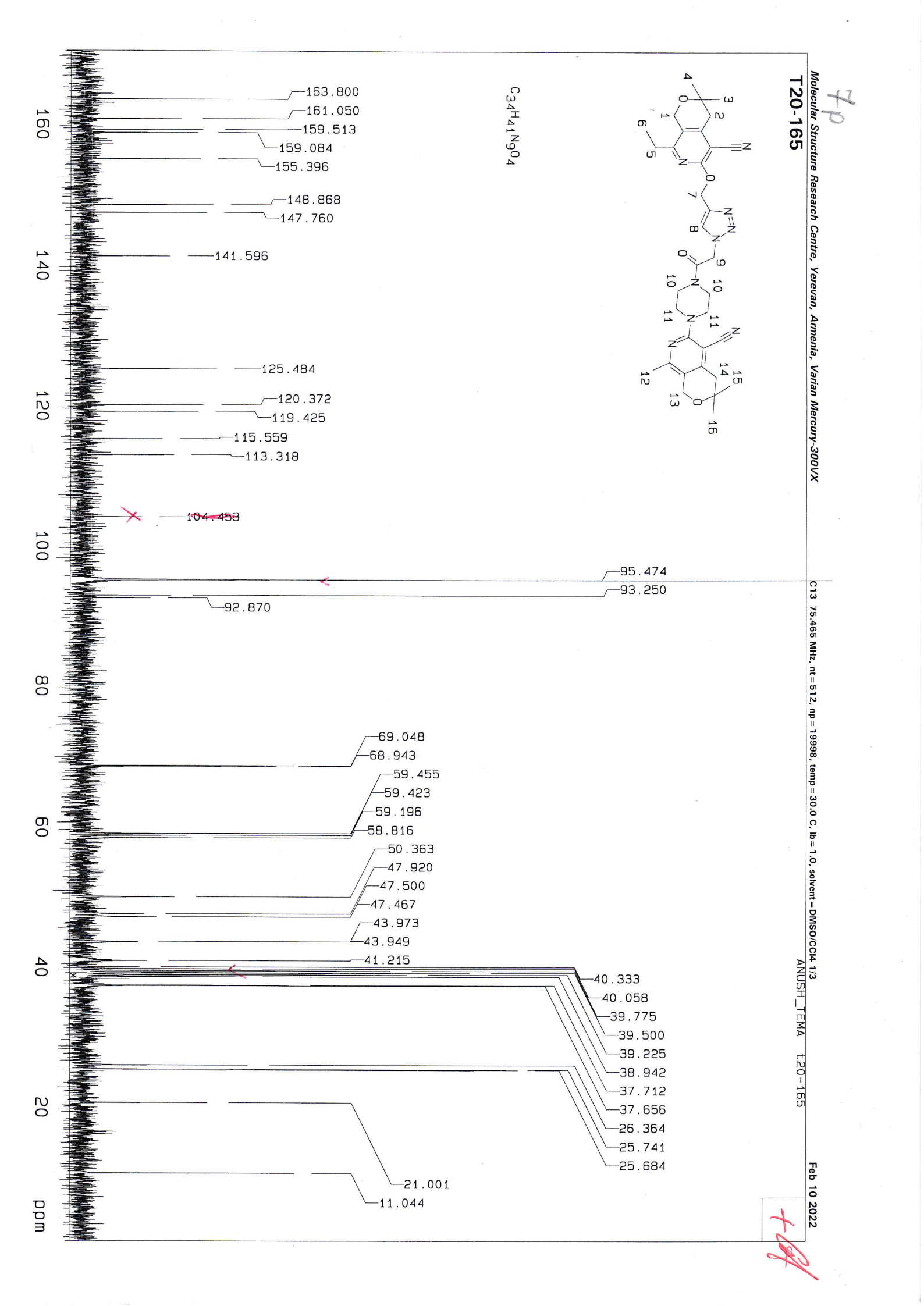
Feb 10 2022

T20-165

ANUSH_TEMA t20-165



$C_{34}H_{41}N_9O_4$

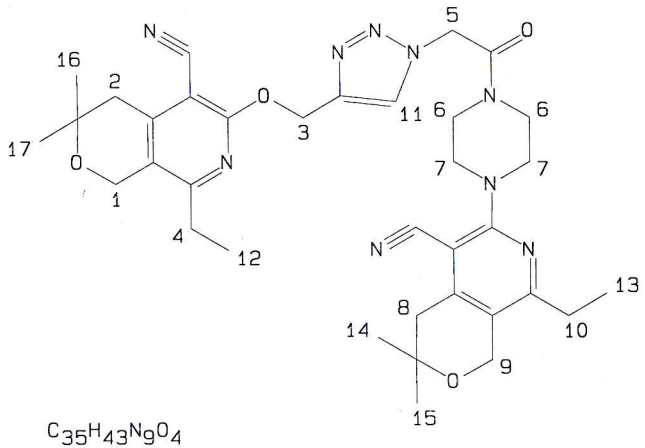

T20-165
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX
$C_{34}H_{41}N_9O_4$
C13 75.465 MHz, nt = 512, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3
ANUSH_TEMA t20-165
Feb 10 2022
163.800
161.050
159.513
159.084
155.396
148.868
147.760
141.596
125.484
120.372
119.425
115.559
113.318
104.453
95.474
93.250
92.870
69.048
68.943
59.455
59.423
59.196
58.816
50.363
47.920
47.500
47.467
43.973
43.949
41.215
40.333
40.058
39.775
39.500
39.225
38.942
37.712
37.656
26.364
25.741
25.684
21.001
11.044
160
140
120
100
80
60
40
20
ppm

79

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Mar 7 2019

HA-1018

NOCI_19 ha-1018



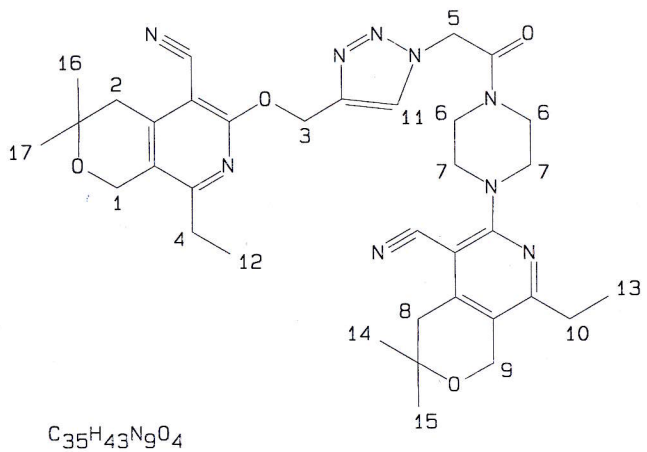
$C_{35}H_{43}N_9O_4$

79

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 1008, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Mar 7 2019

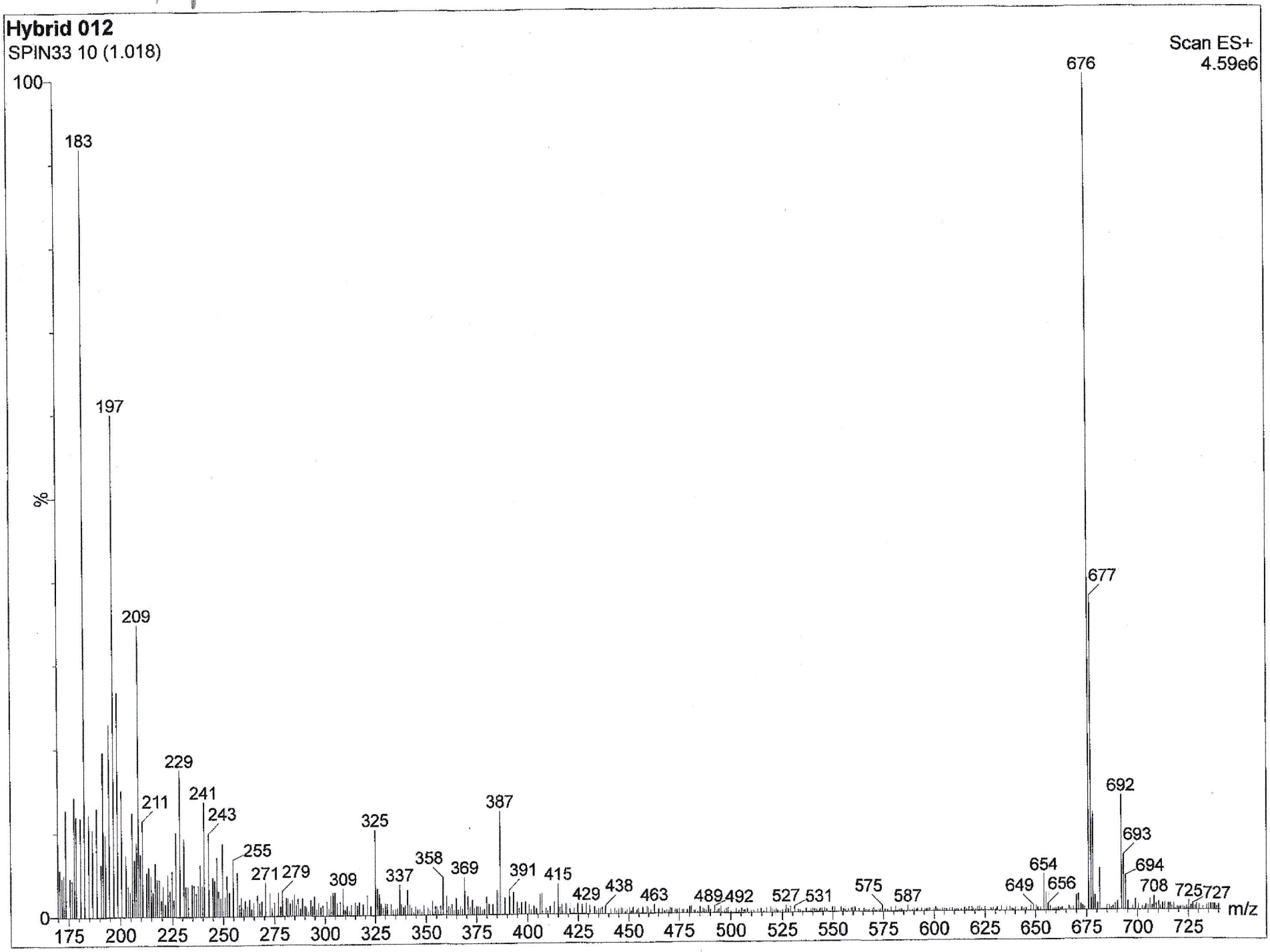
HA-1018

NOCI_19 ha-1018

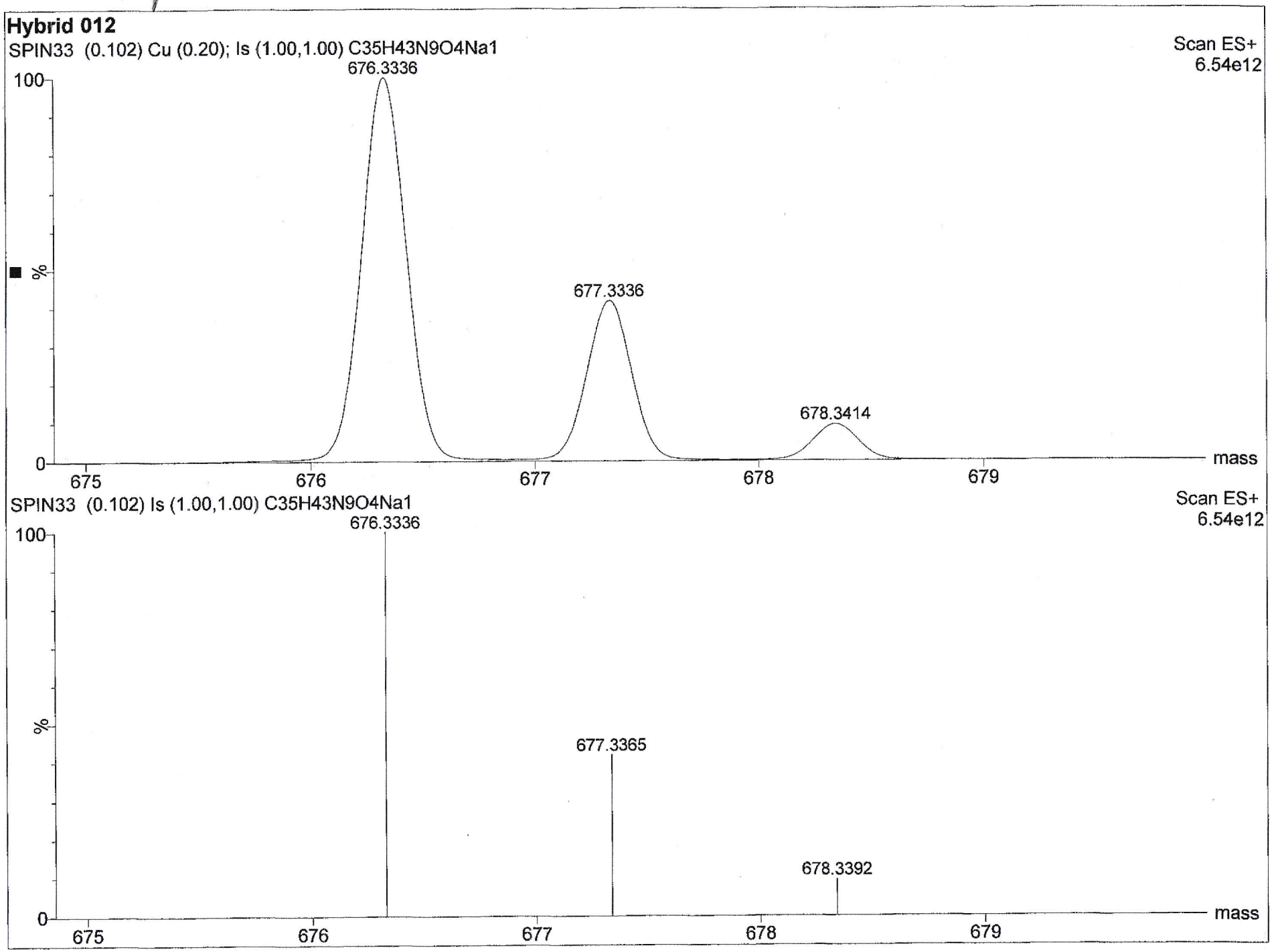


$C_{35}H_{43}N_9O_4$

7 g


Hybrid 012
SPIN33 10 (1.018)
Scan ES+
4.59e6
100
%
0
183
197
209
211
229
241
243
255
271
279
309
325
337
358
369
387
391
415
429
438
463
489
492
527
531
575
587
649
654
656
676
677
692
693
694
708
725
727
m/z
175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725

7g

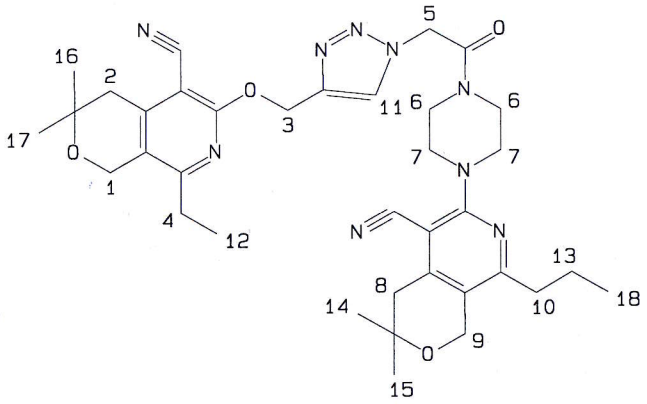

Hybrid 012
SPIN33 (0.102) Cu (0.20); Is (1.00,1.00) C35H43N9O4Na1
Scan ES+
6.54e12
676.3336
677.3336
678.3414
100
%
0
675
676
677
678
679
mass
SPIN33 (0.102) Is (1.00,1.00) C35H43N9O4Na1
Scan ES+
6.54e12
676.3336
677.3365
678.3392
100
%
0
675
676
677
678
679
mass

7z

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Mar 13 2019

HA-1020

SAMV_19 ha-1020



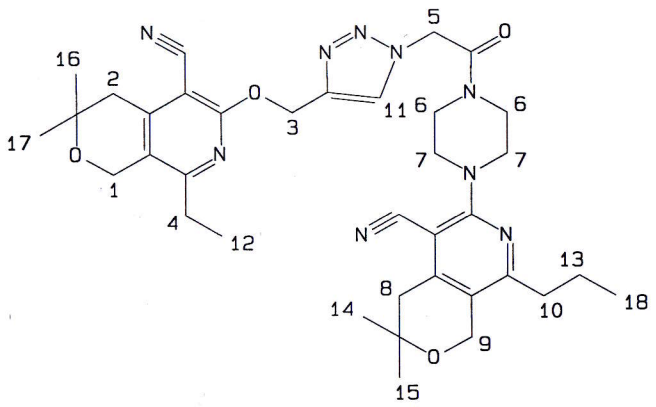
$C_{36}H_{45}N_9O_4$

7z

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt = 816, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Mar 13 2019

SAMV_19 ha-1020

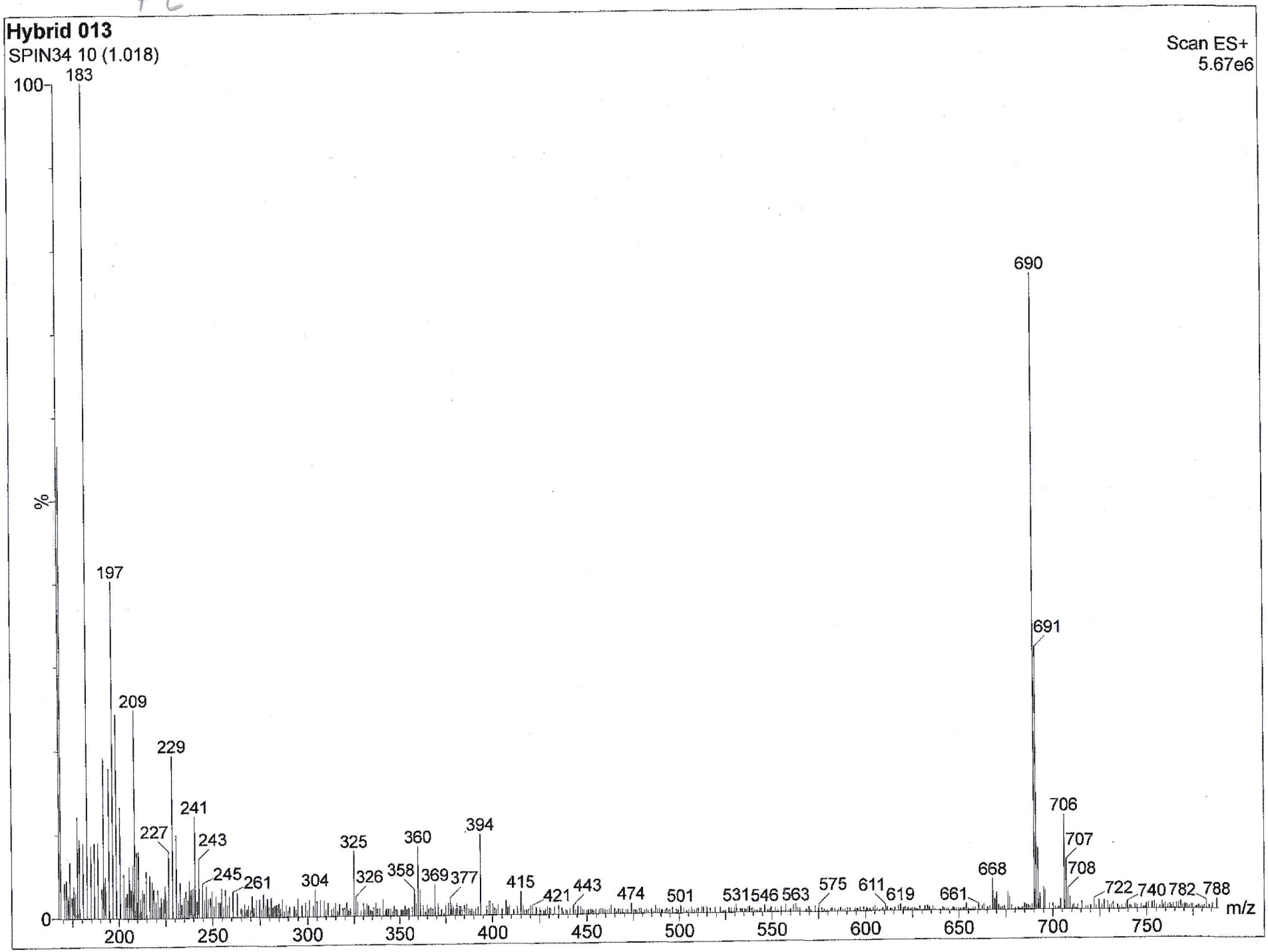
HA-1020



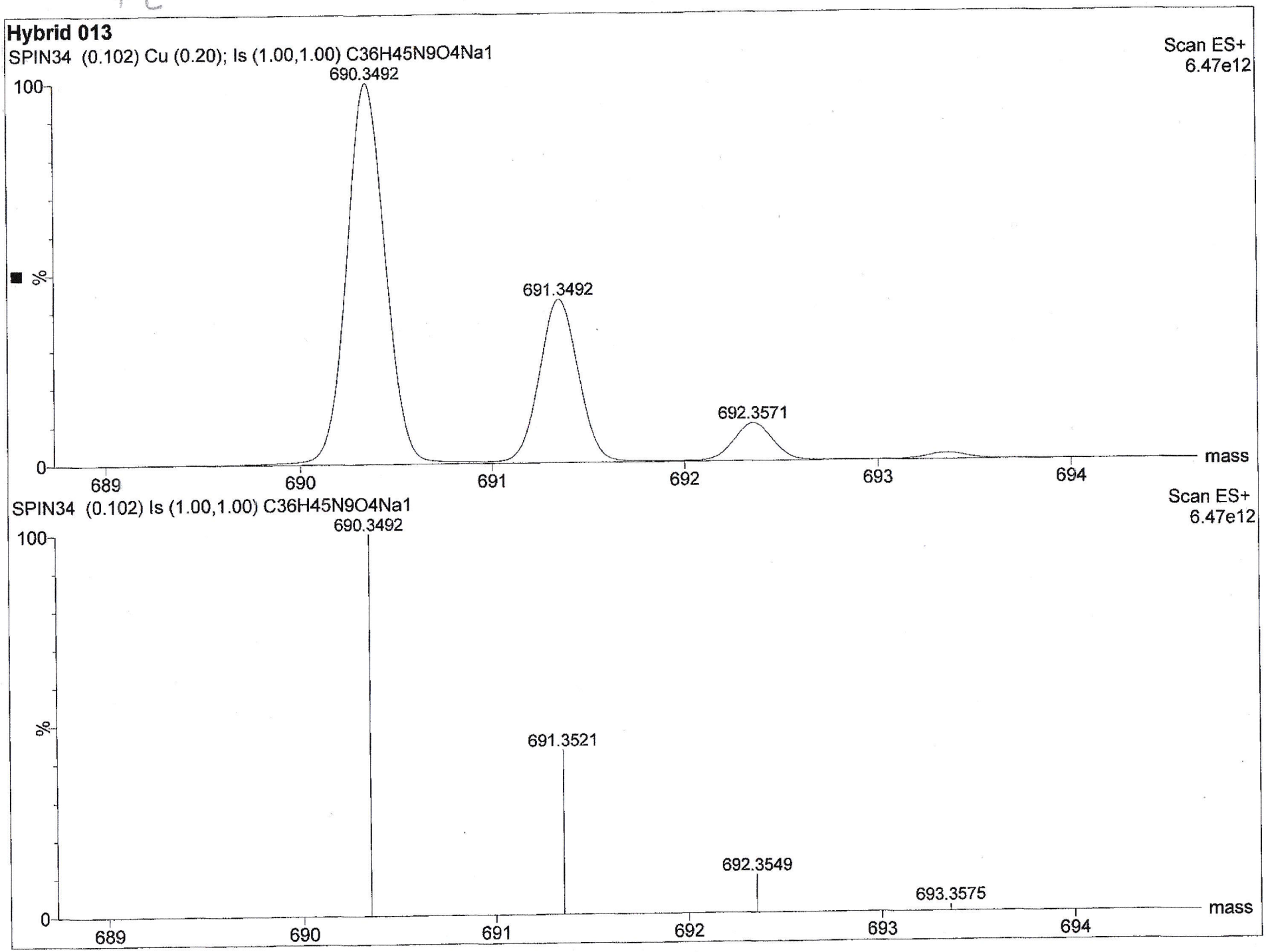
$C_{36}H_{45}N_9O_4$

95.482
95.393
39.783
39.508
39.225
38.950
38.667
37.882
37.704
35.197
26.364
25.741
25.684
40.058
68.975
68.943
59.455
58.945
58.816
50.355
47.985
47.961
47.403
43.973
40.341
20.006
13.535
11.044
163.776
161.058
159.497
159.052
158.542
148.868
147.962
141.596
125.459
120.372
119.085
115.575
113.302
95.596
95.369
95.337
93.177
92.886

160 140 120 100 80 60 40 20 ppm


Hybrid 013
SPIN34 10 (1.018)
Scan ES+
5.67e6
100
%
0
183
197
209
229
241
227
243
245
261
304
325
326
358
360
369
377
394
415
421
443
474
501
531
546
563
575
611
619
661
668
690
691
706
707
708
722
740
782
788
200
250
300
350
400
450
500
550
600
650
700
750
m/z

4c

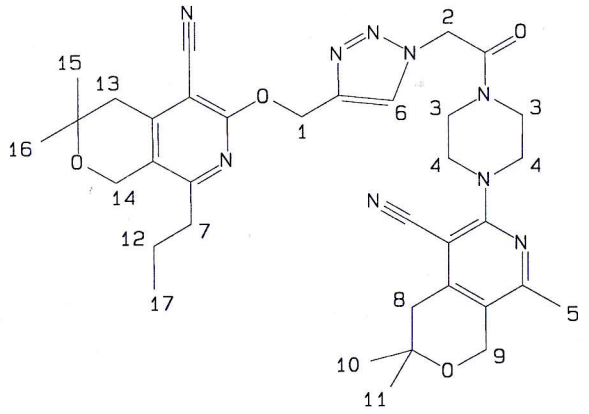

Hybrid 013
SPIN34 (0.102) Cu (0.20); Is (1.00,1.00) C36H45N9O4Na1
Scan ES+
6.47e12
100
%
0
690.3492
691.3492
692.3571
689
690
691
692
693
694
mass
SPIN34 (0.102) Is (1.00,1.00) C36H45N9O4Na1
Scan ES+
6.47e12
100
%
0
690.3492
691.3521
692.3549
693.3575
689
690
691
692
693
694
mass

7s

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Apr 30 2019

HA-1038

SAMV_19 ha-1038



$C_{35}H_{43}N_9O_4$

653.7742

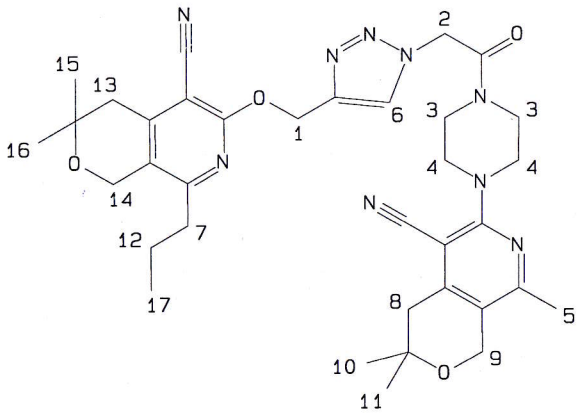
7s

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt=896, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3 Apr 30 2019

SAMV_19 ha-1038

+ CAF

HA-1038

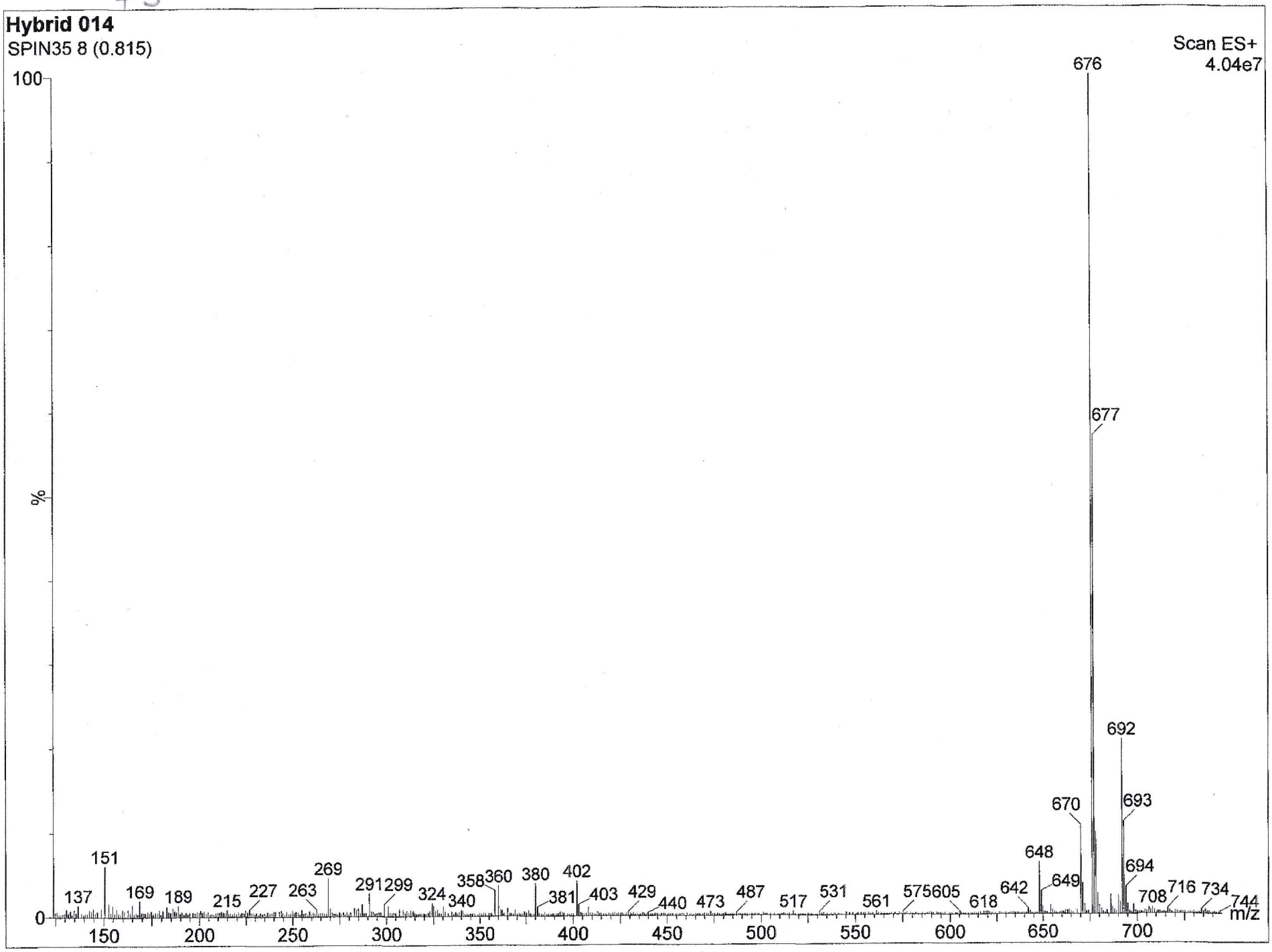


$C_{35}H_{43}N_9O_4$

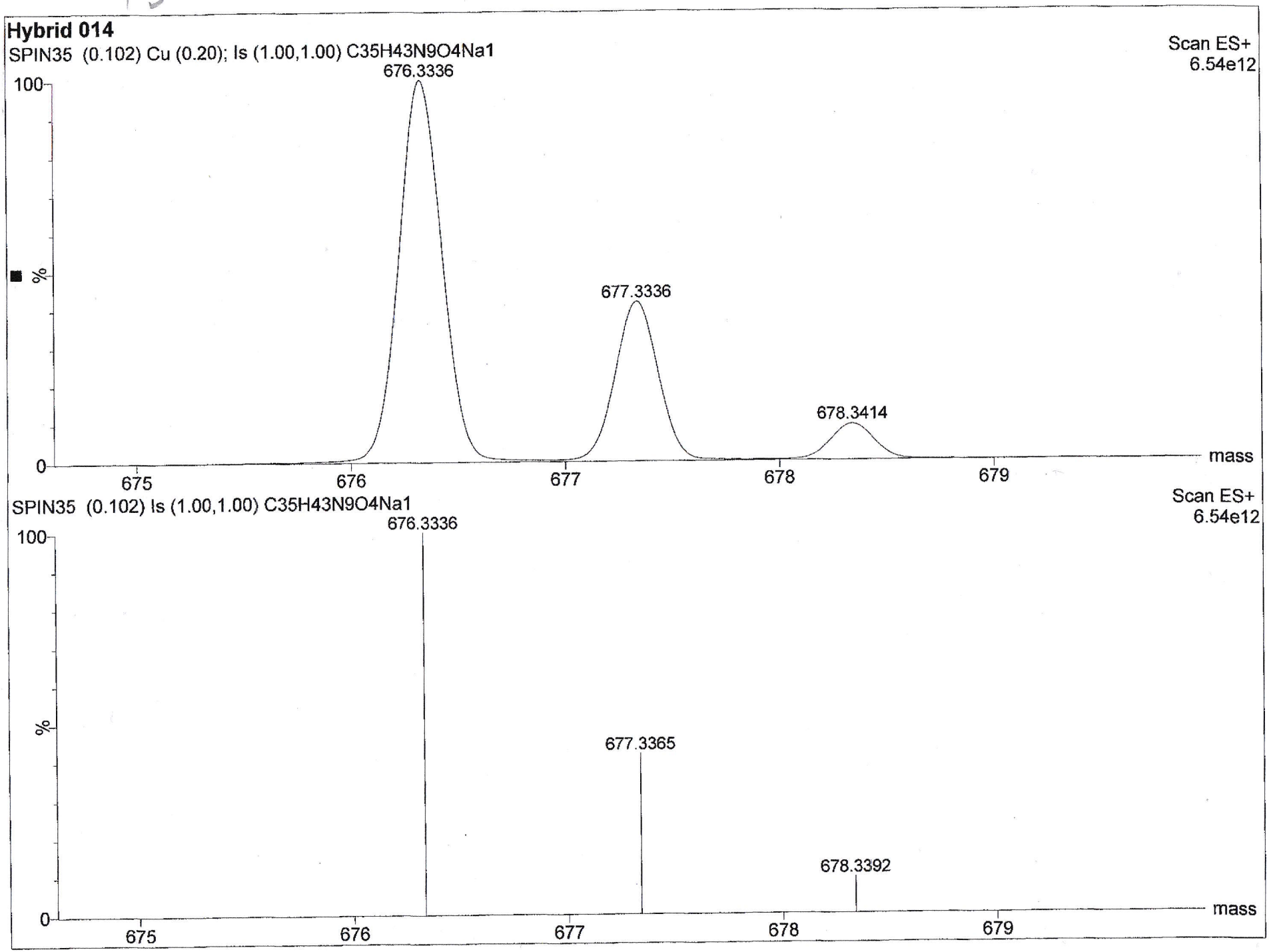
95.474
93.258
92.942
69.048
68.935
59.504
59.196
58.953
50.371
47.945
47.484
43.981
41.223
40.325
40.058
39.775
39.500
39.225
38.942
38.675
37.729
35.067
25.741
25.676
21.001
20.168
13.527
163.800
160.945
159.092
158.648
155.404
148.965
147.760
141.564
125.443
120.679
119.441
115.567
113.310

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

7s


Hybrid 014
SPIN35 8 (0.815)
Scan ES+
4.04e7
100
%
0
676
677
692
693
670
694
648
649
642
708
716
734
744
151
137
169
189
215
227
263
269
291
299
324
340
358
360
380
381
402
403
429
440
473
487
517
531
561
575
605
618
m/z
150
200
250
300
350
400
450
500
550
600
650
700

7s


Hybrid 014
SPIN35 (0.102) Cu (0.20); Is (1.00,1.00) C35H43N9O4Na1
Scan ES+
6.54e12
100
%
0
676.3336
677.3336
678.3414
675
676
677
678
679
mass
SPIN35 (0.102) Is (1.00,1.00) C35H43N9O4Na1
Scan ES+
6.54e12
100
%
0
676.3336
677.3365
678.3392
675
676
677
678
679
mass

77

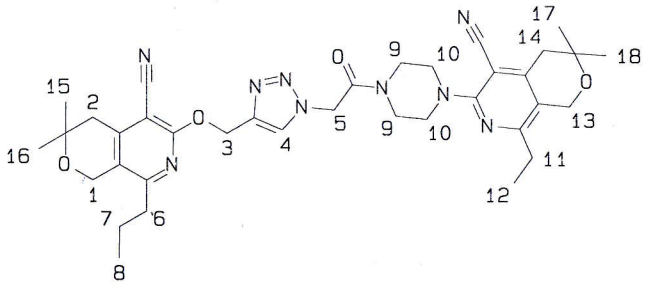
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Mar 3 2022

T20-172

NOCI_22 t20-172



$C_{36}H_{45}N_9O_4$

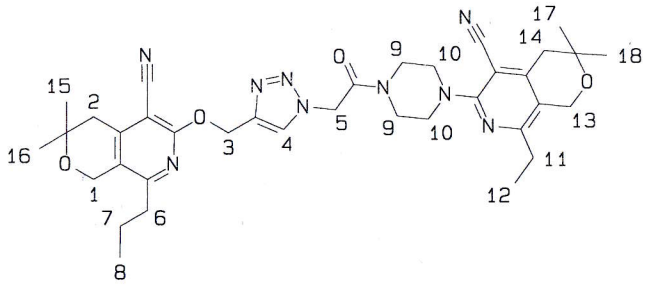
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.465 MHz, nt = 720, np = 19998, temp = 30.0 C, lb = 2.0, solvent = DMSO/CCl4 1/3

Mar 3 2022

T20-172

NOCI_22 t20-172



$C_{36}H_{45}N_9O_4$

95.474
93.048
92.959
163.776
160.945
159.384
159.133
158.631
148.957
147.865
141.572
125.411
120.671
118.778
115.591
113.294
68.984
68.935
59.520
58.953
58.824
50.355
47.920
47.387
41.191
40.333
40.058
43.98
39.775
39.500
39.371
39.225
38.942
38.667
37.858
37.729
35.067
26.453
25.749
25.668
25.587
20.168
13.519
10.882

160 140 120 100 80 60 40 20 ppm

7u

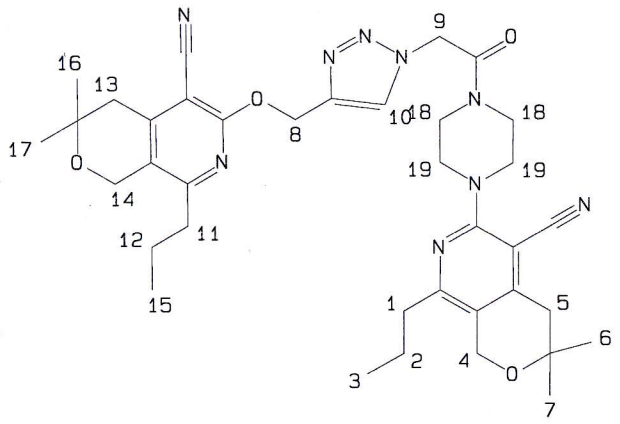
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.088 MHz, nt = 16, np = 32000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Apr 5 2019

HA-1029

NOCI_19 ha-1029



$C_{37}H_{47}N_9O_4$

681.8273

1.0
3.8
3.9
8.0
4.1
6.6
4.1
12.0
6.1

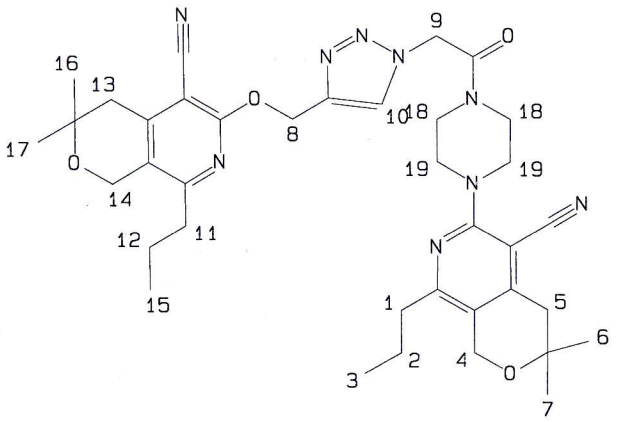
8 7 6 5 4 3 2 1 ppm

7u

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX C13 75.465 MHz, nt=672, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3 Apr 5 2019

HA-1029

NOCI_19 ha-1029

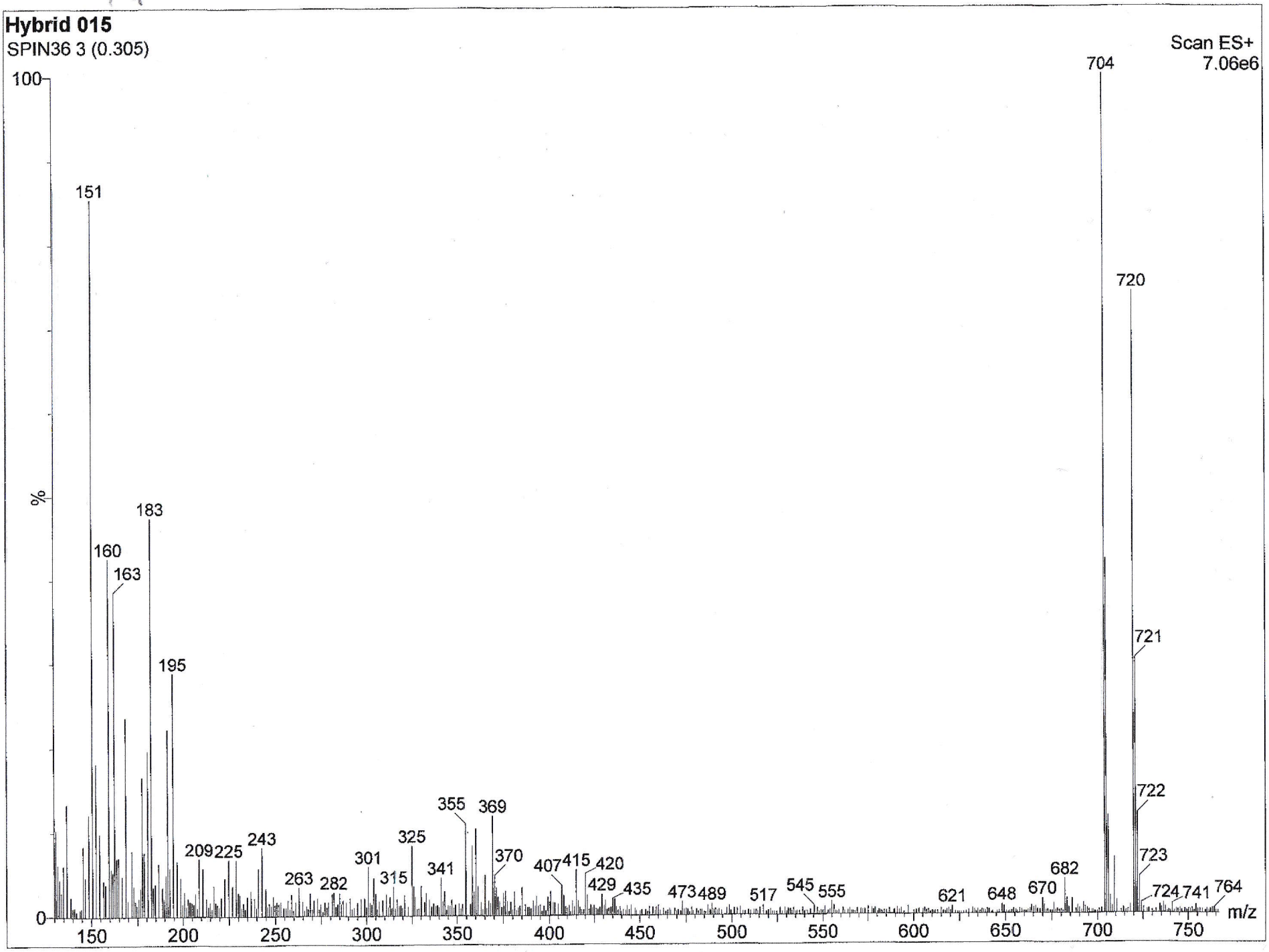


$C_{37}H_{47}N_9O_4$

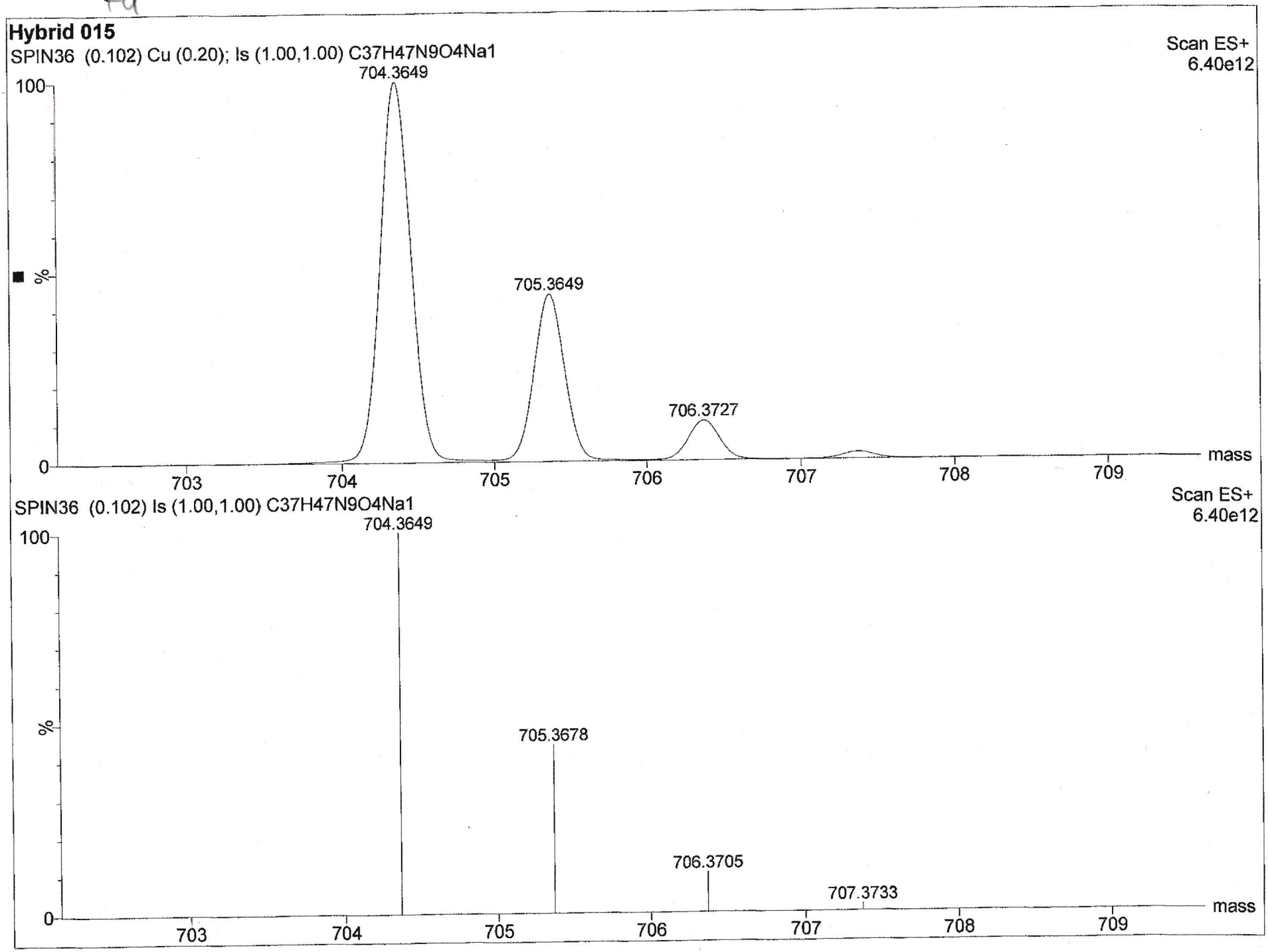
95.482
93.17
92.94
68.975
68.935
59.512
58.953
50.355
40.333
40.058
39.775
39.500
39.225
38.942
37.882
37.729
35.197
35.067
25.741
25.709
25.676
20.168
20.006
13.535
163.776
159.060
158.639
158.551
148.957
147.962
141.572
125.427
120.671
119.085
115.583
113.302
160.94
47.98
42.41
43.97
41.19

160 140 120 100 80 60 40 20 ppm

74


Hybrid 015
SPIN36 3 (0.305)
Scan ES+
7.06e6
100
%
0
151
183
160
163
195
209
225
243
263
282
301
315
325
341
355
369
370
407
415
420
429
435
473
489
517
545
555
621
648
670
682
704
720
721
722
723
724
741
764
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750

Hybrid 015


SPIN36 (0.102) Cu (0.20); Is (1.00,1.00) C37H47N9O4Na1
Scan ES+
6.40e12
100
%
0
704.3649
705.3649
706.3727
703
704
705
706
707
708
709
mass
SPIN36 (0.102) Is (1.00,1.00) C37H47N9O4Na1
Scan ES+
6.40e12
100
%
0
704.3649
705.3678
706.3705
707.3733
703
704
705
706
707
708
709
mass