Electronic Supplementary Material (ESI) for RSC Advances.

Multicomponent synthesis of hydrazino depsipeptides

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Supporting Information

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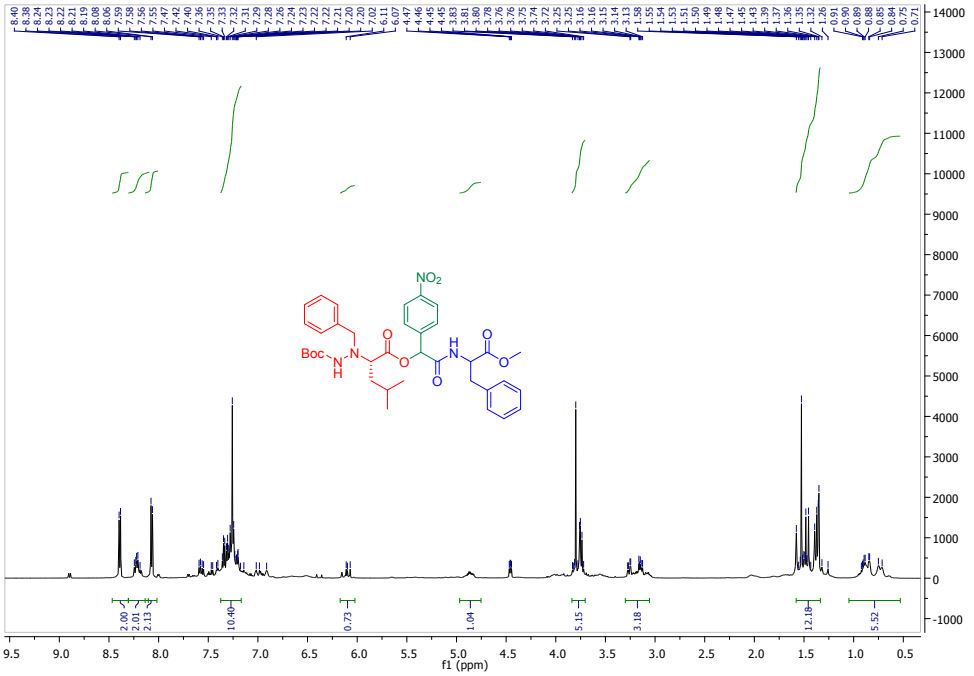
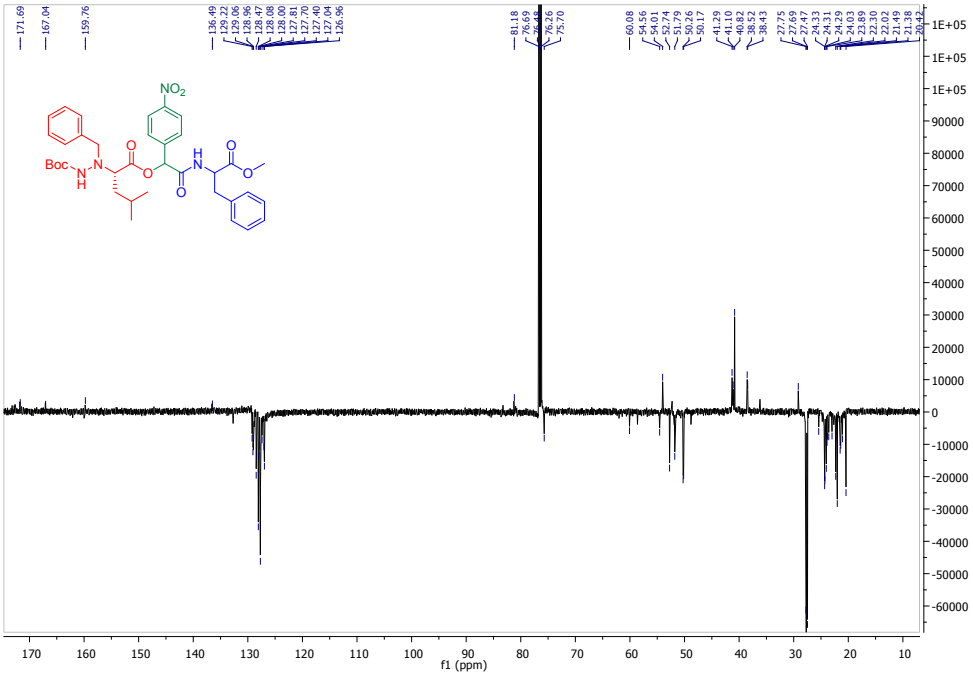
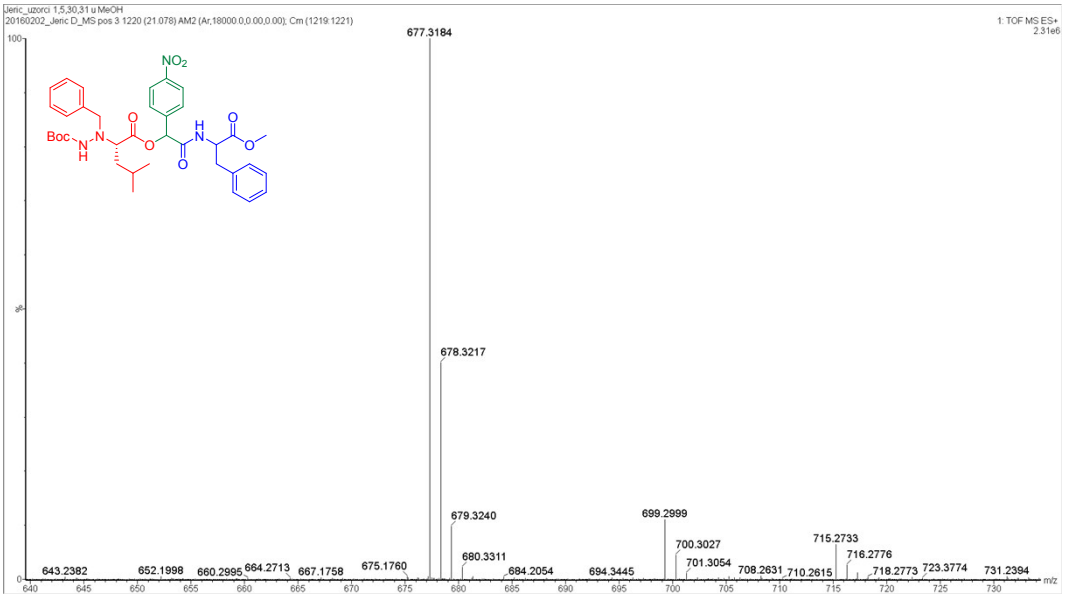
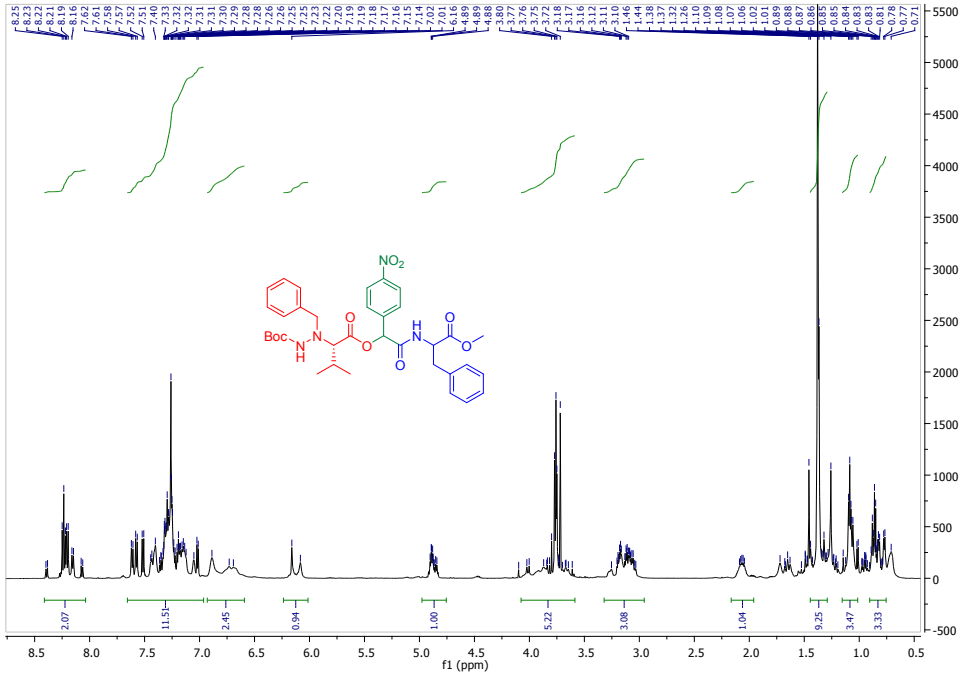
Compound **1**

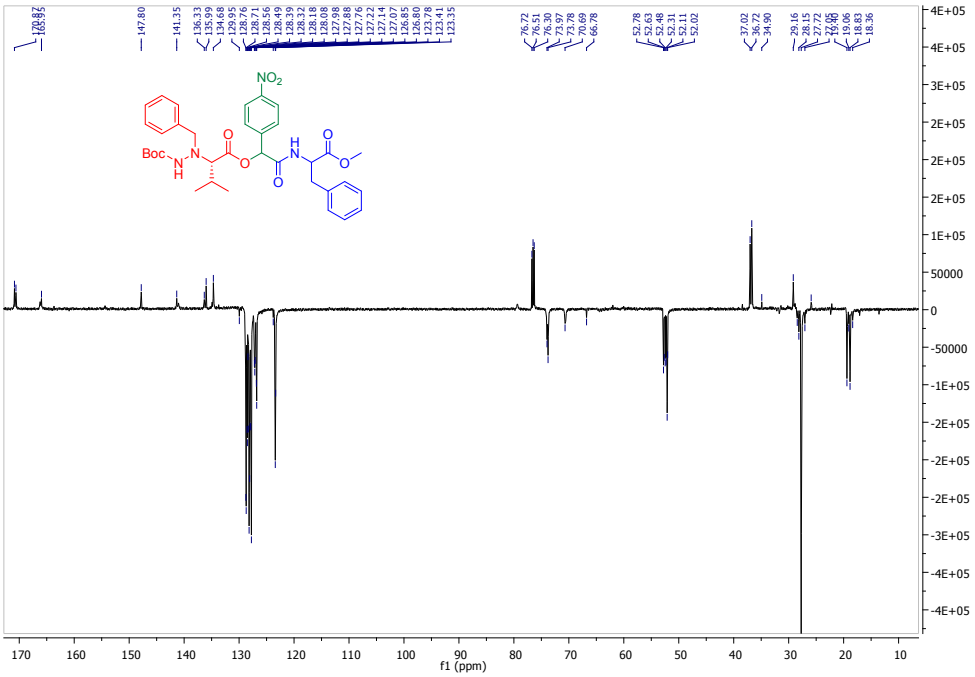


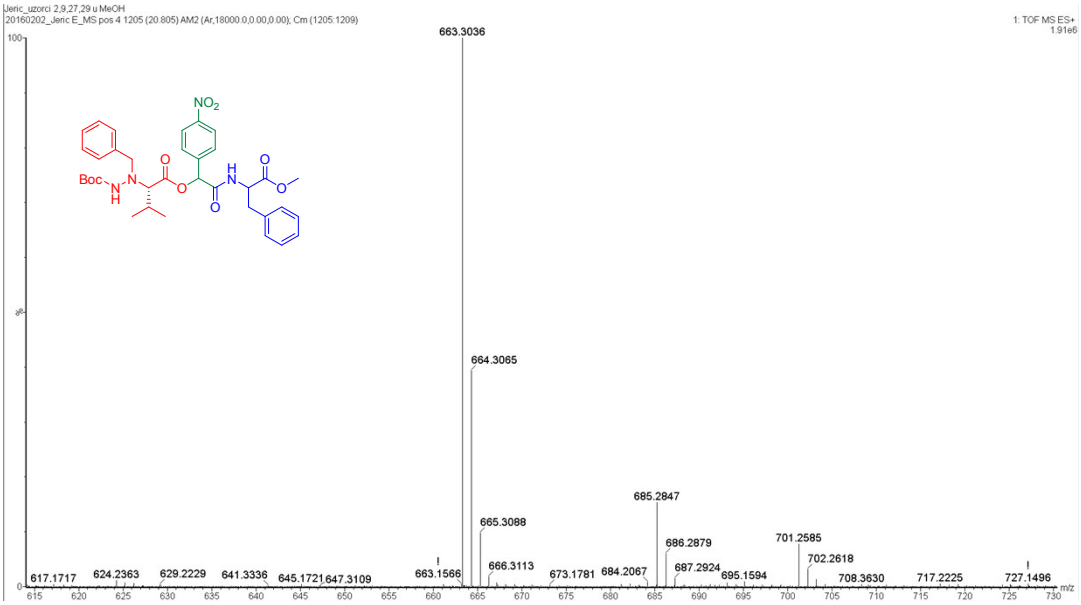



Jeric_uzorci 1,5,30,31 u MeOH
20160202_Jeric D_MS pos 3 1220 (21.078) AM2 (Ar,18000.0,0.00,0.00); Cm (1219:1221)
1: TOF MS ES+
2.31e6
677.3184
678.3217
679.3240
699.2999
700.3027
701.3054
715.2733
716.2776
680.3311
643.2382
652.1998
660.2995
664.2713
667.1758
675.1760
684.2054
694.3445
708.2631
710.2615
718.2773
723.3774
731.2394
m/z

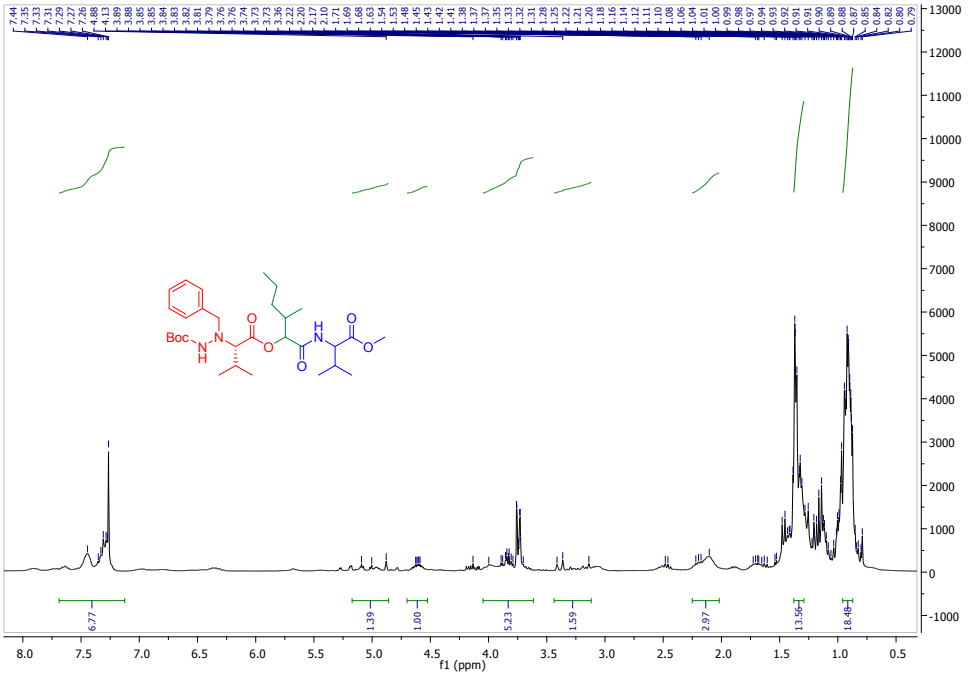
Compound **2**

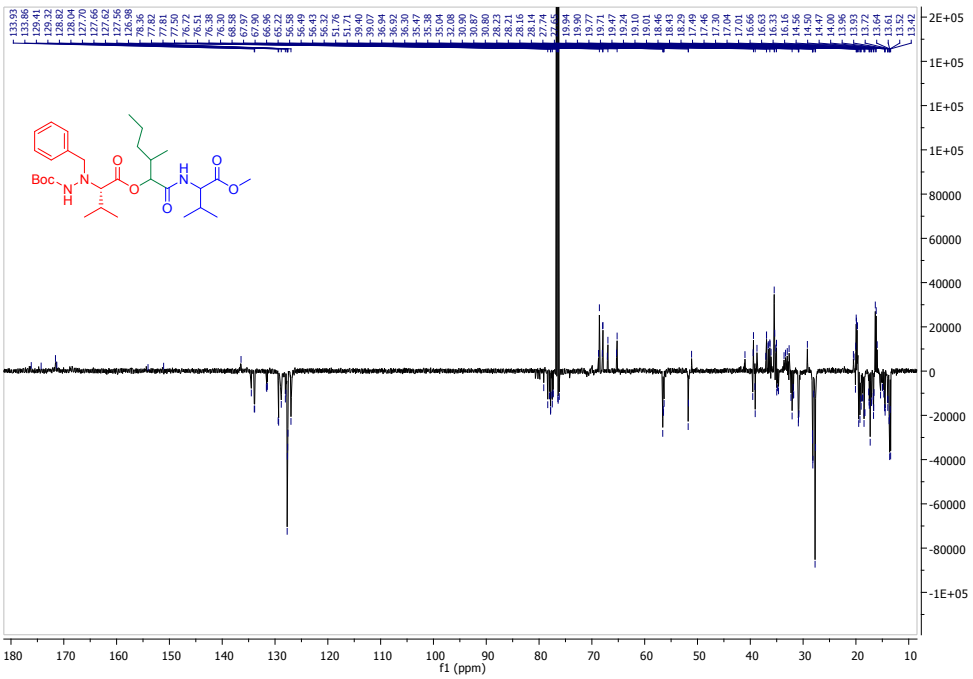

f1 (ppm)

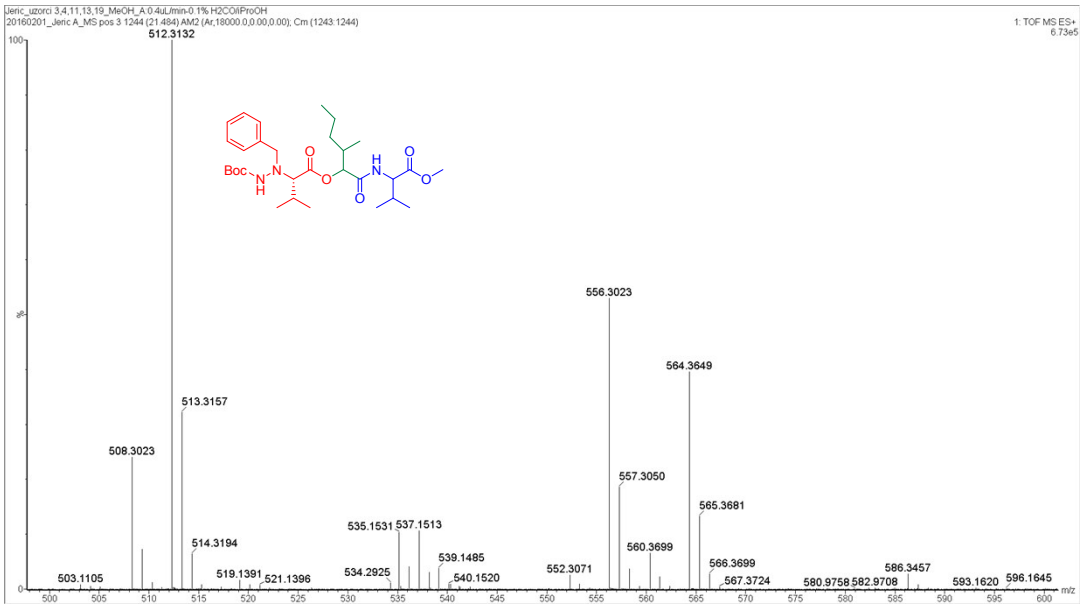

NO2
Boc
N
H
O
O
O
O
N
H
O
O
f1 (ppm)


Jeric_uzorci 2,9,27,29 u MeOH
20160202_Jeric E_MS pos 4 1205 (20.805) AM2 (Ar,18000.0,0.00,0.00); Cm (1205:1209)
1: TOF MS ES+
1.91e6
663.3036
664.3065
685.2847
665.3088
686.2879
701.2585
702.2618
666.3113
687.2924
617.1717
624.2363
629.2229
641.3336
645.1721
647.3109
663.1566
673.1781
684.2067
695.1594
708.3630
717.2225
727.1496
NO2
Boc
N
H
O
O
O
O
N
H
O
O
m/z

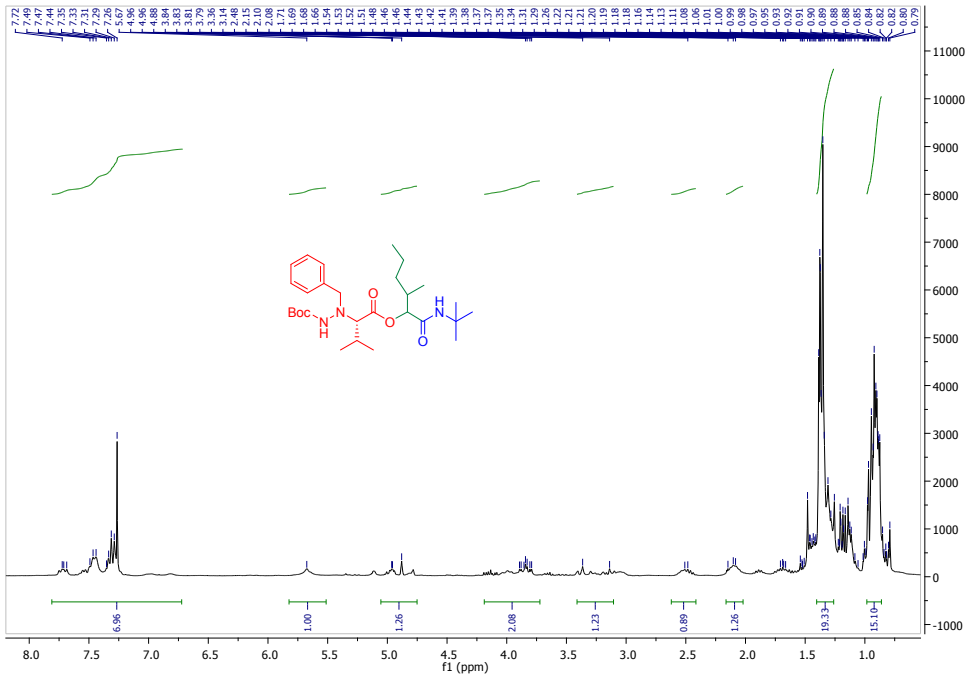
Compound **3**

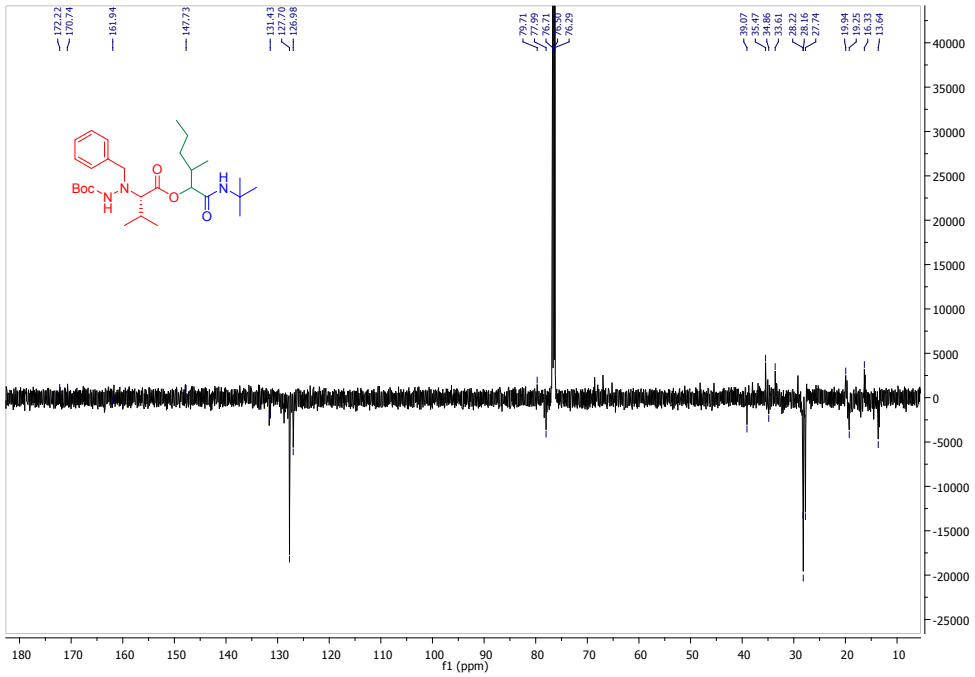


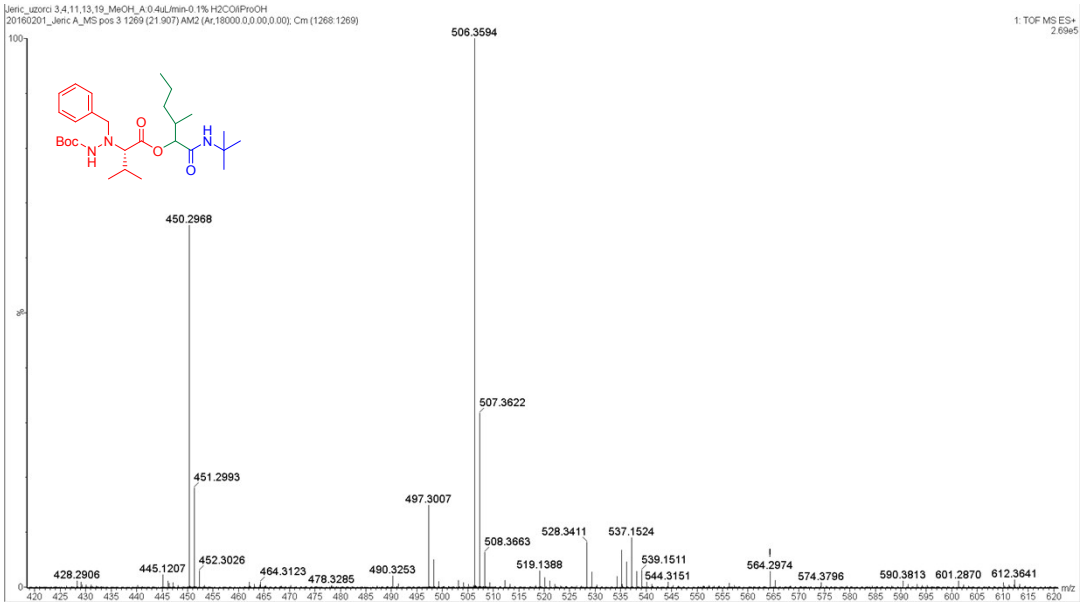



Jeric_uzorci 3,4,11,13,19_MeOH_A 0.4uL/min-0.1% H2COOPro0H
20160201_Jeric A_MS pos 3 1244 (21.484) AM2 (Ar,18000.0,0.00,0.00); Cm (1243:1244)
1: TOF MS ES+
6.73e5
512.3132
556.3023
564.3649
513.3157
508.3023
557.3050
565.3681
535.1531
537.1513
514.3194
560.3699
539.1485
566.3699
552.3071
586.3457
503.1105
519.1391
521.1396
534.2925
540.1520
567.3724
580.9758
582.9708
593.1620
596.1645
m/z

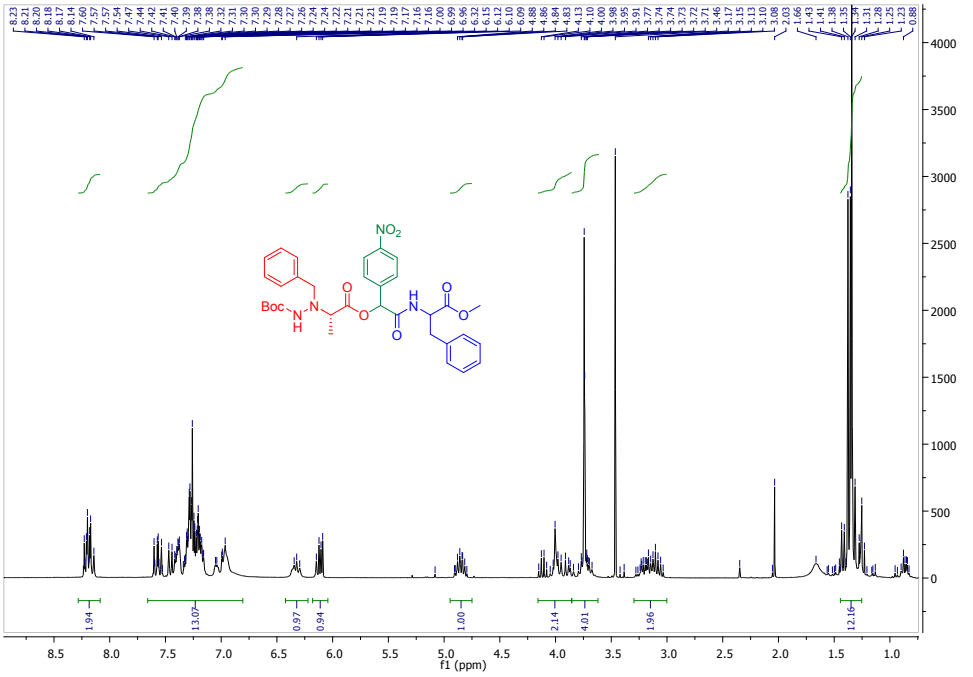
Compound **4**

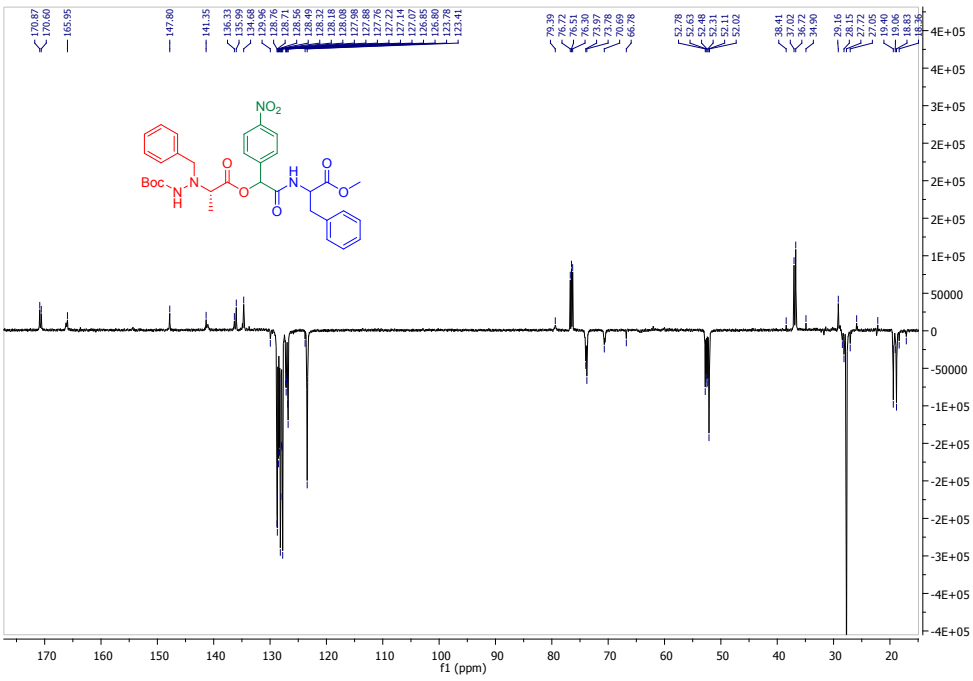

f1 (ppm)

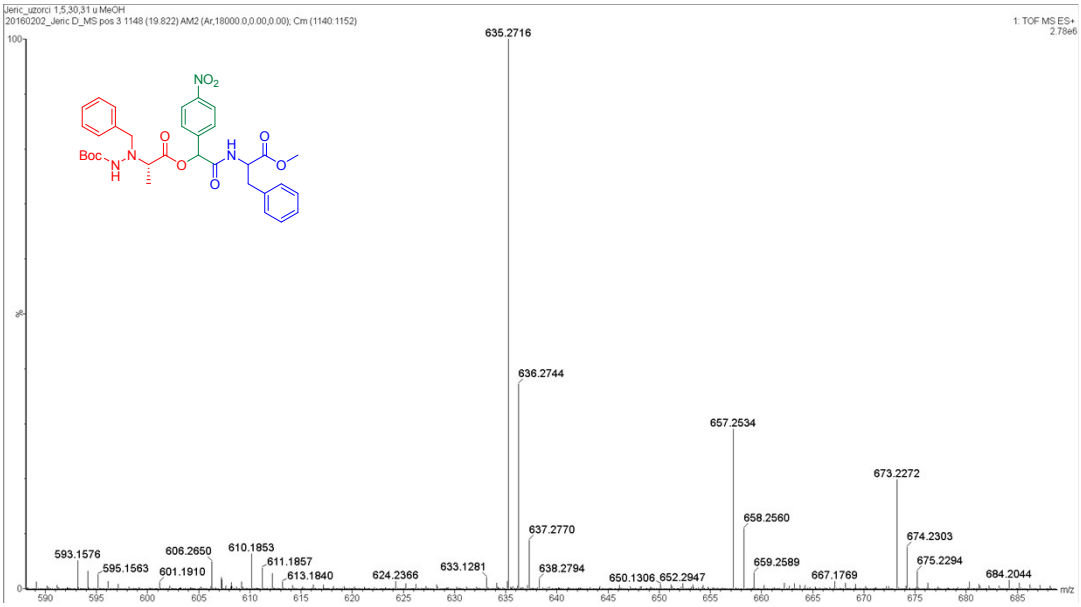

172.22
170.74
161.94
147.73
131.43
127.70
126.98
79.71
77.98
76.71
76.50
76.29
39.07
35.47
34.86
33.61
28.22
28.16
27.74
19.94
19.25
16.33
13.64
Boc
f1 (ppm)


Jeric_uzorci 3,4,11,13,19_MeOH_A 0.4uL/min-0.1% H2CO/ProOH
20160201_Jeric A_MS pos 3 1269 (21.907) AM2 (Ar,18000.0,0.00,0.00); Cm (1268:1269)
1: TOF MS ES+
2.69e5
506.3594
450.2968
507.3622
451.2993
497.3007
508.3663
528.3411
537.1524
539.1511
544.3151
519.1388
564.2974
574.3796
590.3813
601.2870
612.3641
428.2906
445.1207
452.3026
464.3123
478.3285
490.3253
Boc
m/z

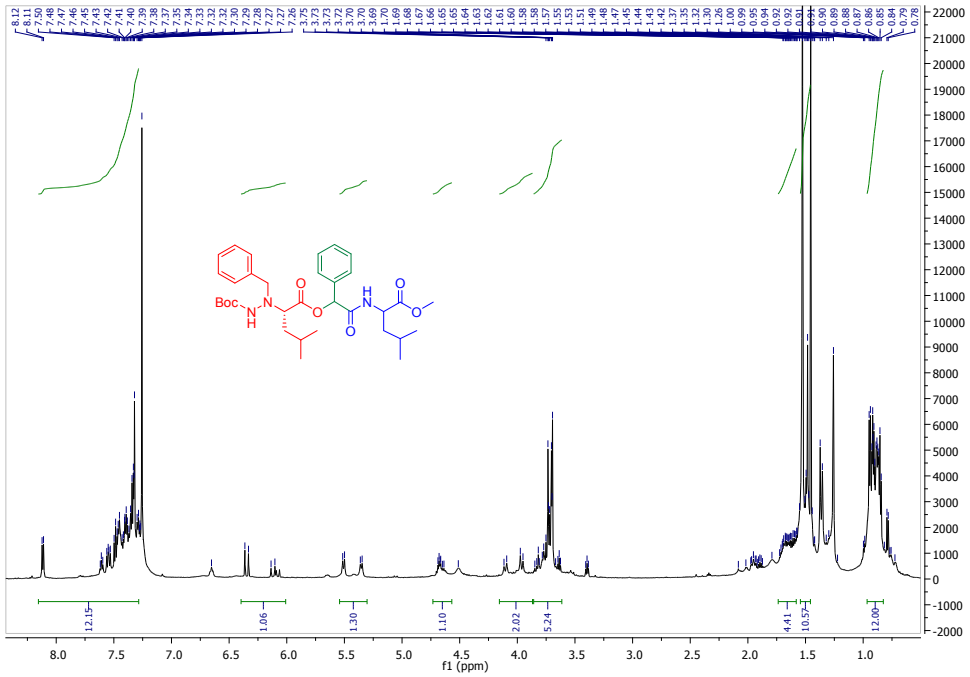
Compound **5**

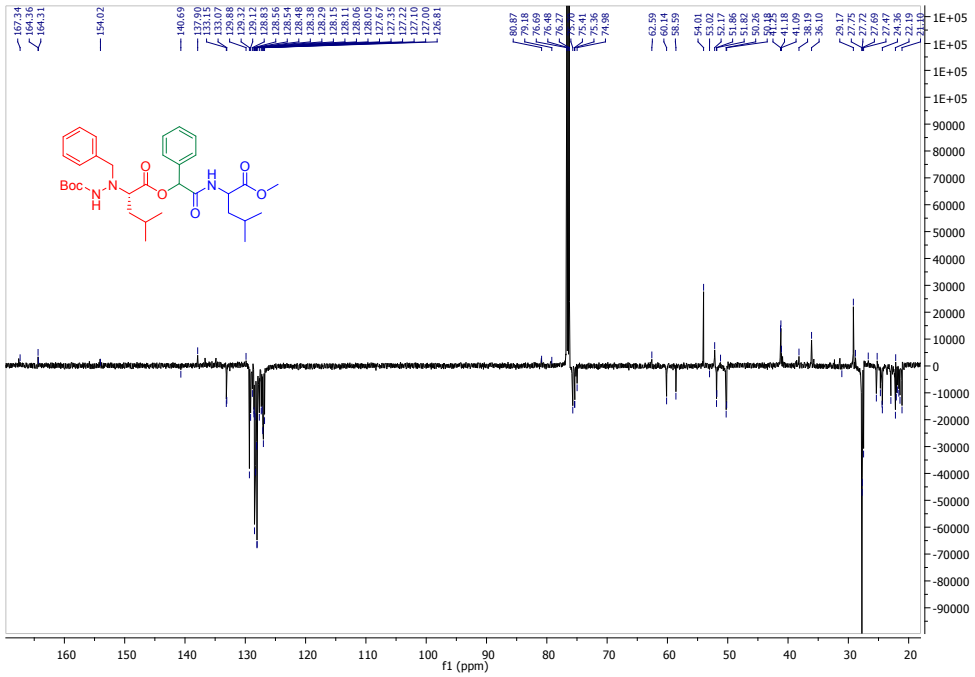

NO2
Boc
N
H
O
O
O
O
H
N
O
O
1.94
13.07
0.97
0.94
1.00
2.14
4.01
1.96
12.16
f1 (ppm)

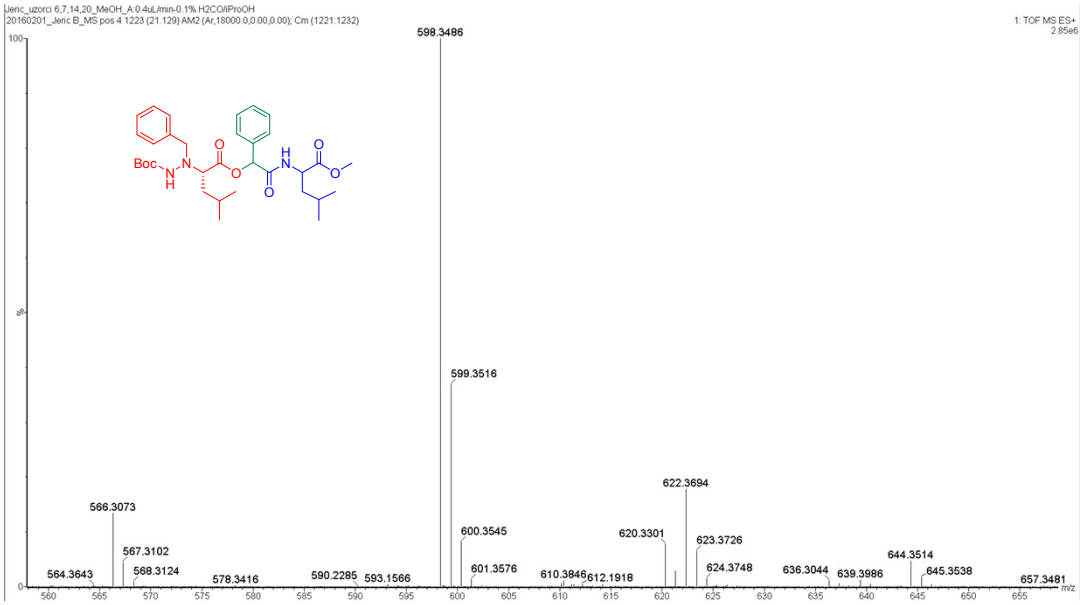

NO2
Boc
N
H
O
O
O
O
H
N
O
f1 (ppm)


Jeric_uzorci 1,5,30,31 u MeOH
20160202_Jeric D_MS pos 3 1148 (19.822) AM2 (Ar,18000.0,0.00,0.00); Cm (1140:1152)
1: TOF MS ES+
2.78e6
635.2716
636.2744
657.2534
673.2272
658.2560
637.2770
674.2303
675.2294
684.2044
593.1576
595.1563
606.2650
601.1910
610.1853
611.1857
613.1840
624.2366
633.1281
638.2794
650.1306
652.2947
659.2589
667.1769
m/z

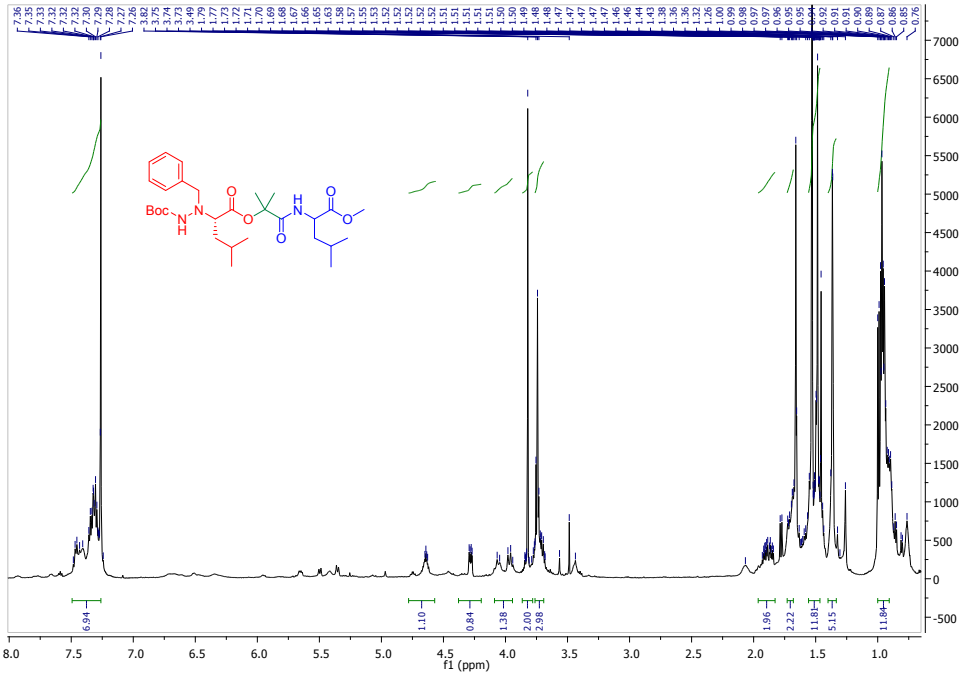
Compound **6**

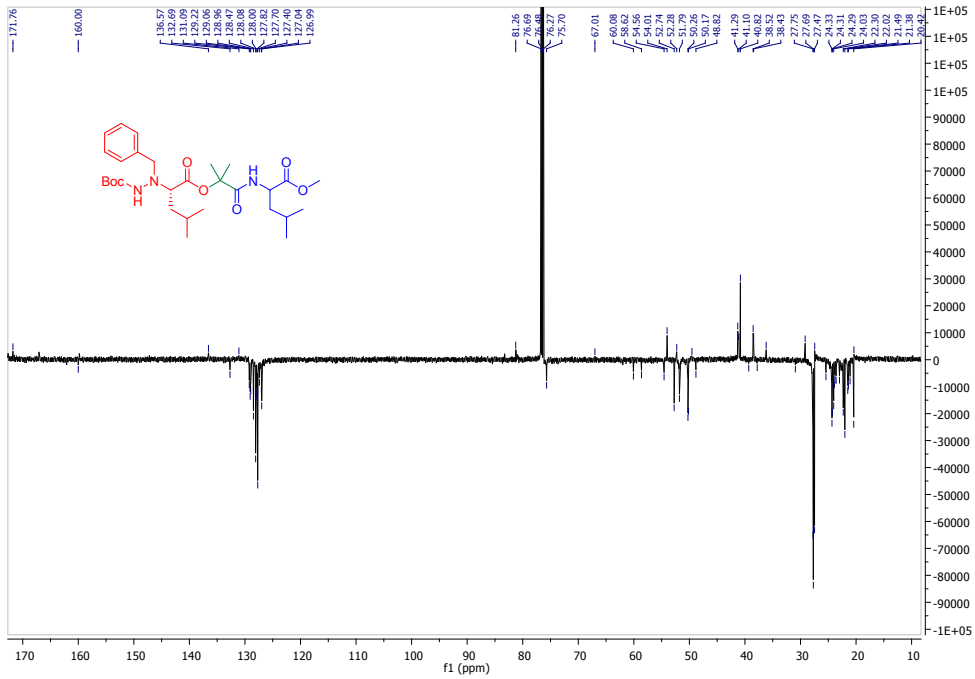

f1 (ppm)

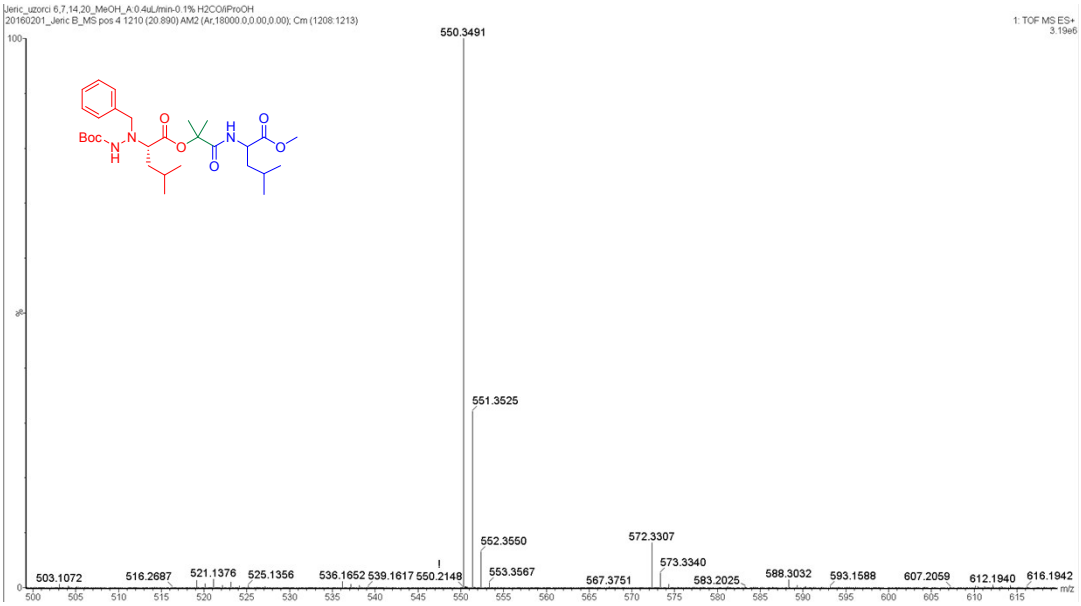

f1 (ppm)


598.3486
599.3516
622.3694
566.3073
600.3545
620.3301
623.3726
567.3102
624.3748
644.3514
564.3643
568.3124
601.3576
636.3044
639.3986
645.3538
578.3416
590.2285
593.1566
610.3846
612.1918
657.3481
m/z

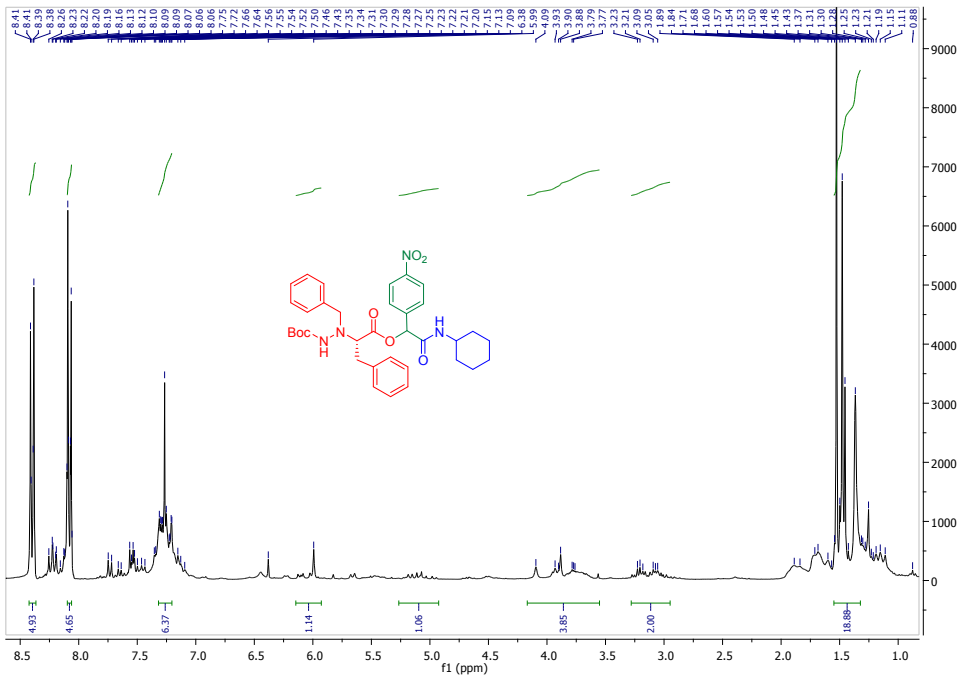
Compound **7**

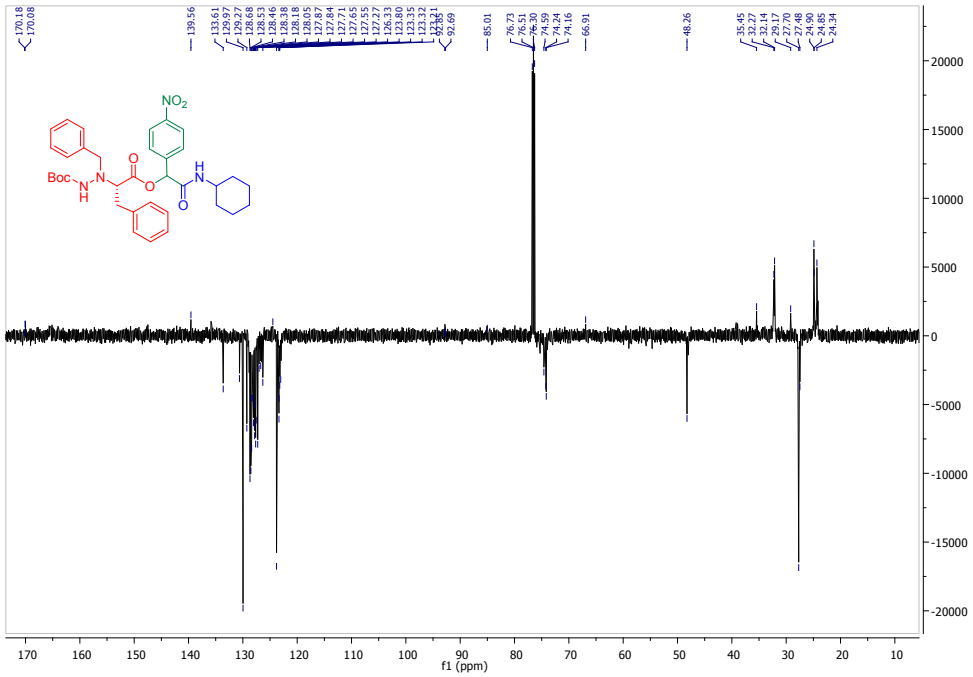


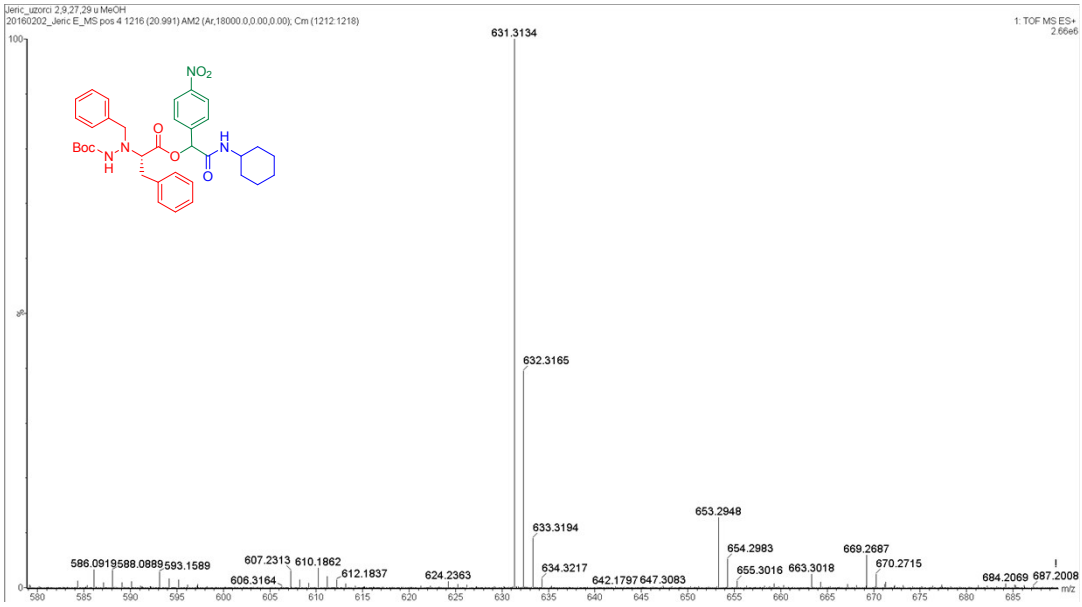



Jeric_uzorci 6,7,14,20_MeOH_A 0.4uL/min-0.1% H2CO/iProOH
20160201_Jeric B_MS pos 4 1210 (20.890) AM2 (Ar,18000.0,0.00,0.00); Cm (1208:1213)
1: TOF MS ES+
3.19e6
100
%
0
550.3491
551.3525
552.3550
553.3567
572.3307
573.3340
503.1072
516.2687
521.1376
525.1356
536.1652
539.1617
550.2148
567.3751
583.2025
588.3032
593.1588
607.2059
612.1940
616.1942
m/z
Boc
N
H
O
O
O
N
H
O
O

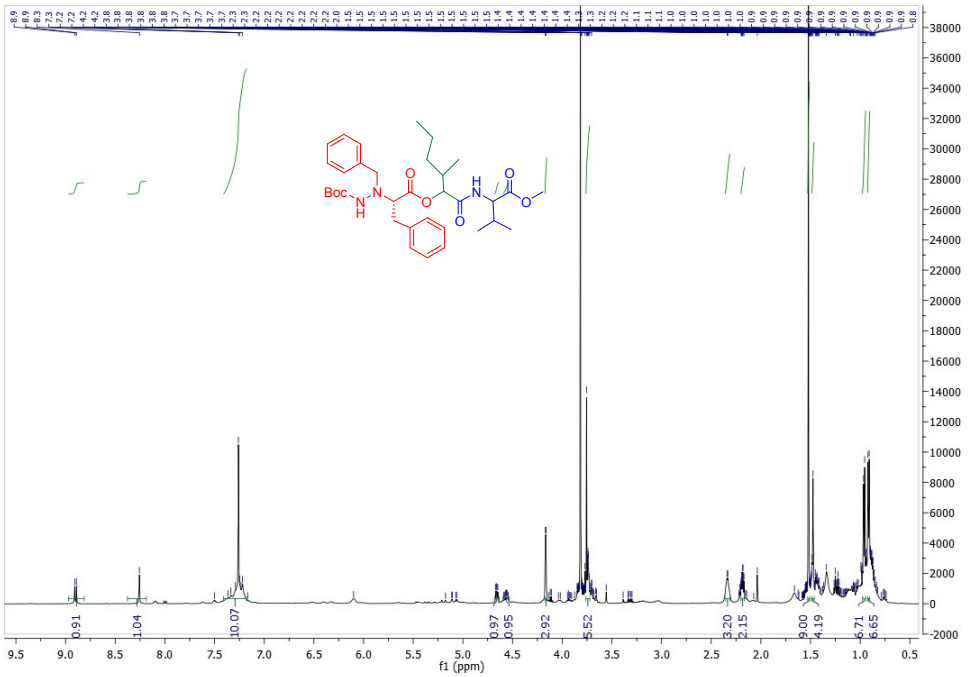
Compound **9**

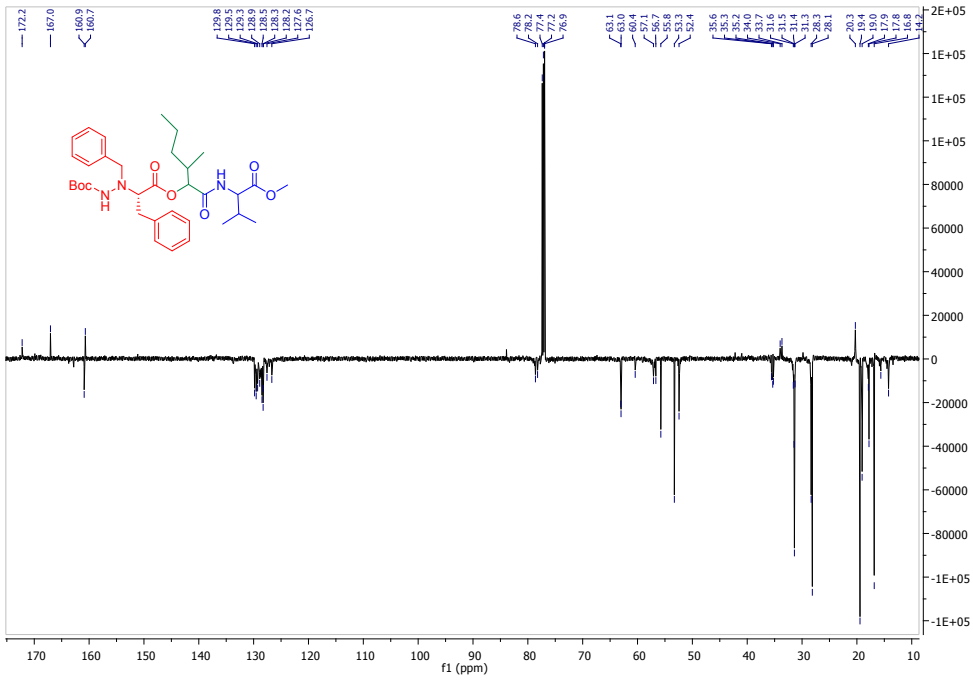

NO2
Boc
N
H
O
O
O
N
H
O
4.93
4.65
6.37
1.14
1.06
3.85
2.00
18.88
f1 (ppm)

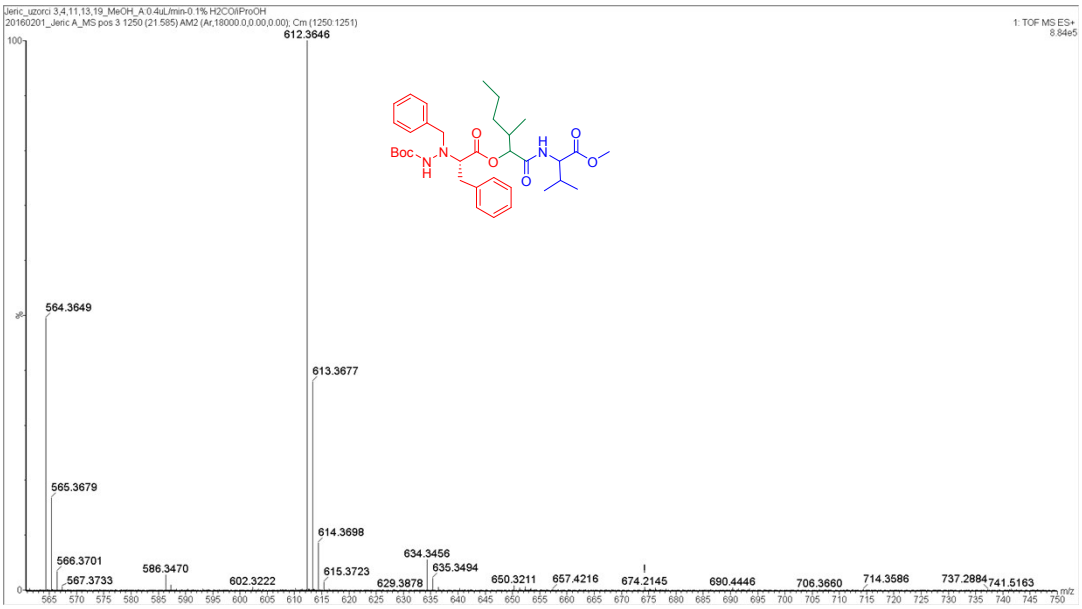

170.18
170.08
139.56
133.61
129.97
129.27
128.68
128.53
128.46
128.38
128.18
128.05
127.87
127.84
127.71
127.65
127.55
127.27
126.33
123.80
123.55
123.32
123.21
92.85
92.69
85.01
76.73
76.51
76.30
74.59
74.24
74.16
66.91
48.26
35.45
32.27
32.14
29.17
27.70
27.48
24.90
24.85
24.34
NO2
Boc
N
H
O
O
O
H
N
O
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


Jeric_uzorci 2,9,27,29 u MeOH
20160202_Jeric E_MS pos 4 1216 (20.991) AM2 (Ar,18000.0,0.00,0.00); Cm (1212:1218)
1: TOF MS ES+
2.66e6
100
%
0
631.3134
632.3165
633.3194
653.2948
654.2983
669.2687
670.2715
634.3217
655.3016
663.3018
642.1797
647.3083
684.2069
687.2008
586.0919
588.0889
593.1589
607.2313
610.1862
606.3164
612.1837
624.2363
NO2
Boc
N
H
O
O
O
H
N
O
580
585
590
595
600
605
610
615
620
625
630
635
640
645
650
655
660
665
670
675
680
685
m/z

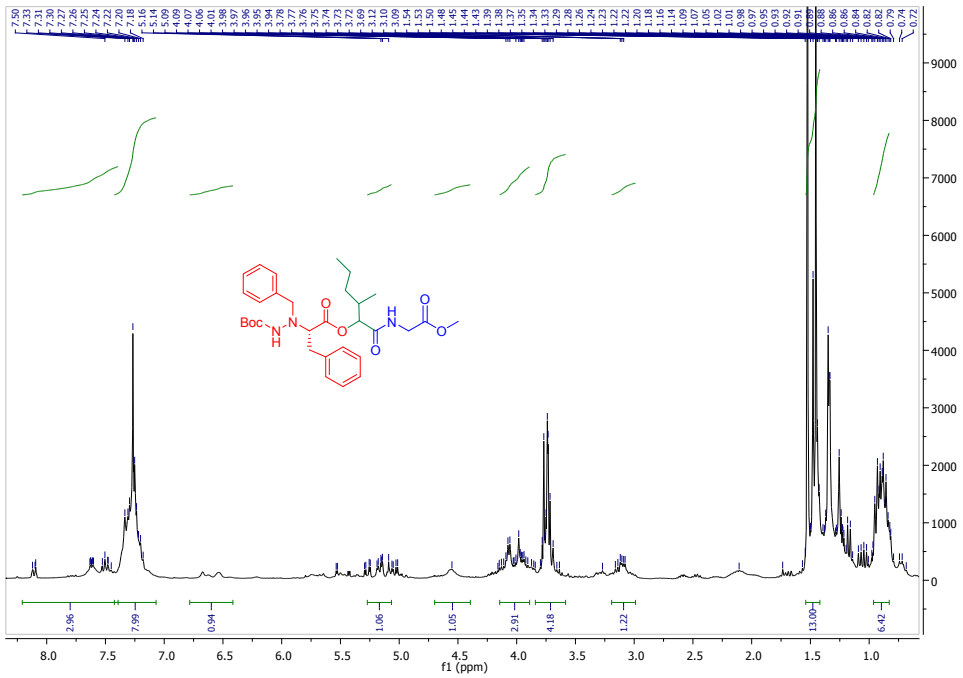
Compound **11**

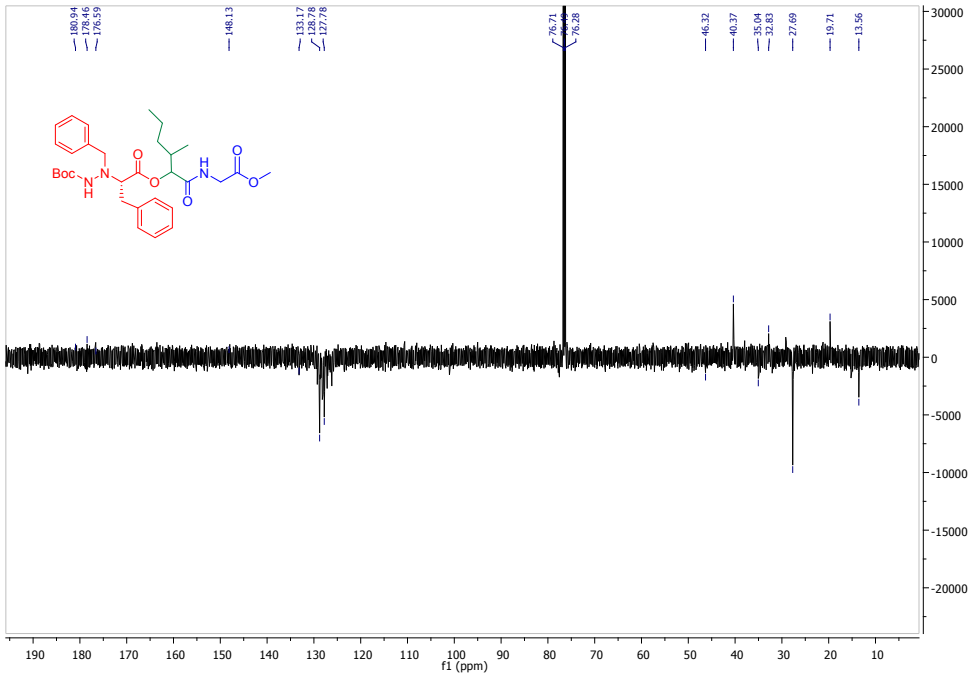

Boc
N
H
O
O
O
O
O
H
N
O
O
0.91
1.04
10.07
0.97
0.95
2.92
5.52
3.20
2.15
9.00
4.19
6.71
6.65
f1 (ppm)

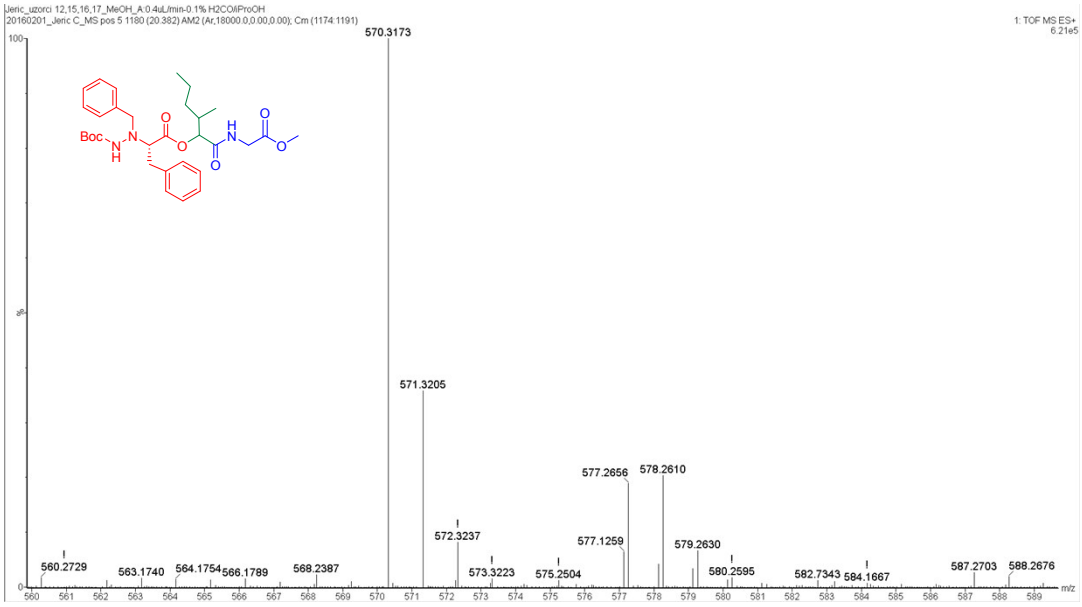

Boc
N
H
O
O
O
O
O
H
N
O
O
f1 (ppm)


Jeric_uzorci 3,4,11,13,19_MeOH_A 0.4uL/min-0.1% H2CO/iPrOH
20160201_Jeric A_MS pos 3 1250 (21.585) AM2 (Ar,18000.0,0.00,0.00); Cm (1250:1251)
1: TOF MS ES+
8.84e5
612.3646
564.3649
613.3677
565.3679
614.3698
566.3701
567.3733
586.3470
602.3222
615.3723
629.3878
634.3456
635.3494
650.3211
657.4216
674.2145
690.4446
706.3660
714.3586
737.2884
741.5163
m/z

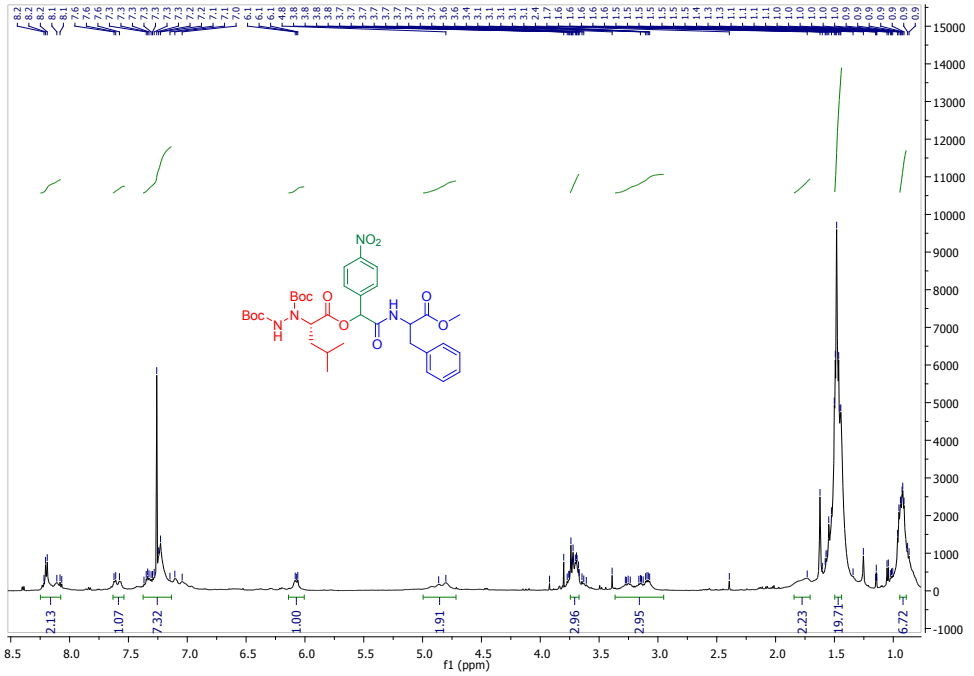
Compound **12**

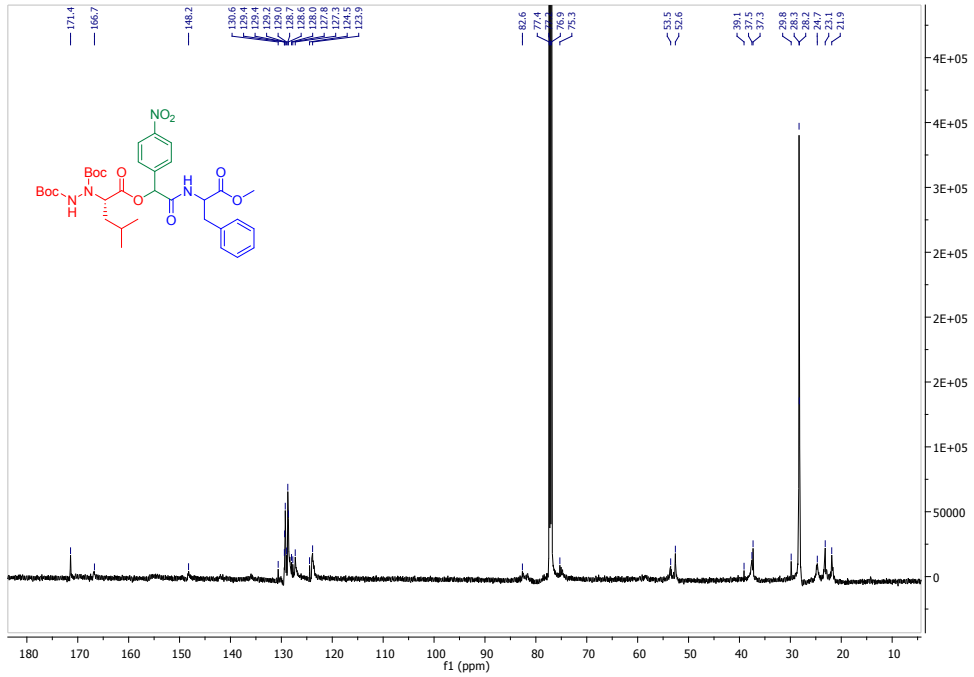

f1 (ppm)

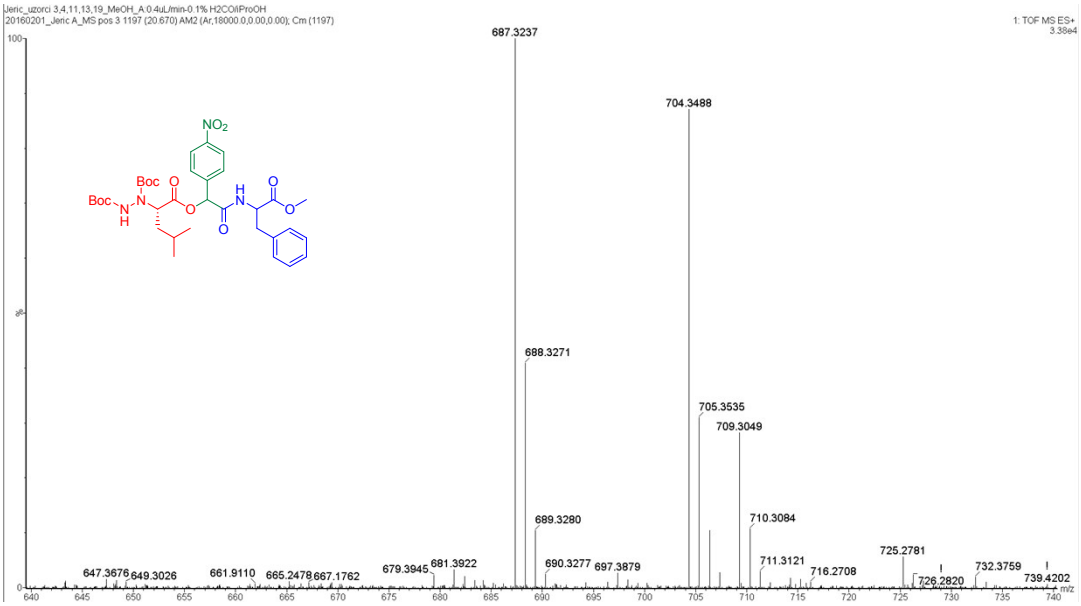

180.94
178.46
176.59
148.13
133.17
128.78
127.78
76.71
76.28
46.32
40.37
35.04
32.83
27.69
19.71
13.56
Boc
f1 (ppm)


Jeric_uzorci 12,15,16,17_MeOH_A:0.4uL/min-0.1% H2COl/ProOH
20160201_Jeric C_MS pos 5 1180 (20.382) AM2 (Ar,18000.0,0.00,0.00); Cm (1174:1191)
1: TOF MS ES+
6.21e5
570.3173
571.3205
577.2656
578.2610
572.3237
577.1259
579.2630
560.2729
563.1740
564.1754
566.1789
568.2387
573.3223
575.2504
580.2595
582.7343
584.1667
587.2703
588.2676
Boc
m/z

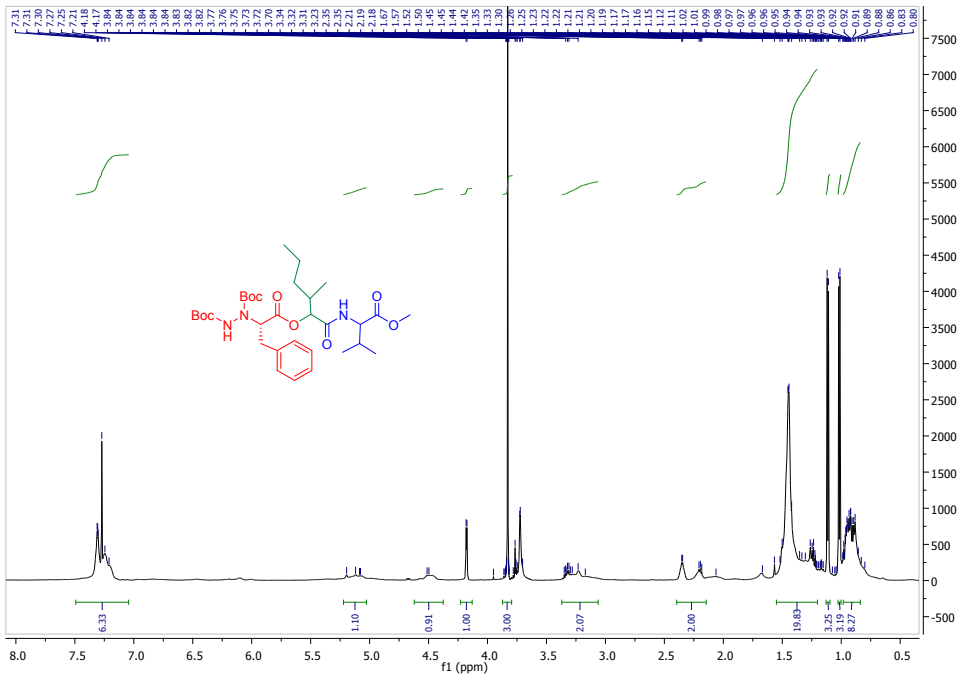
Compound **13**

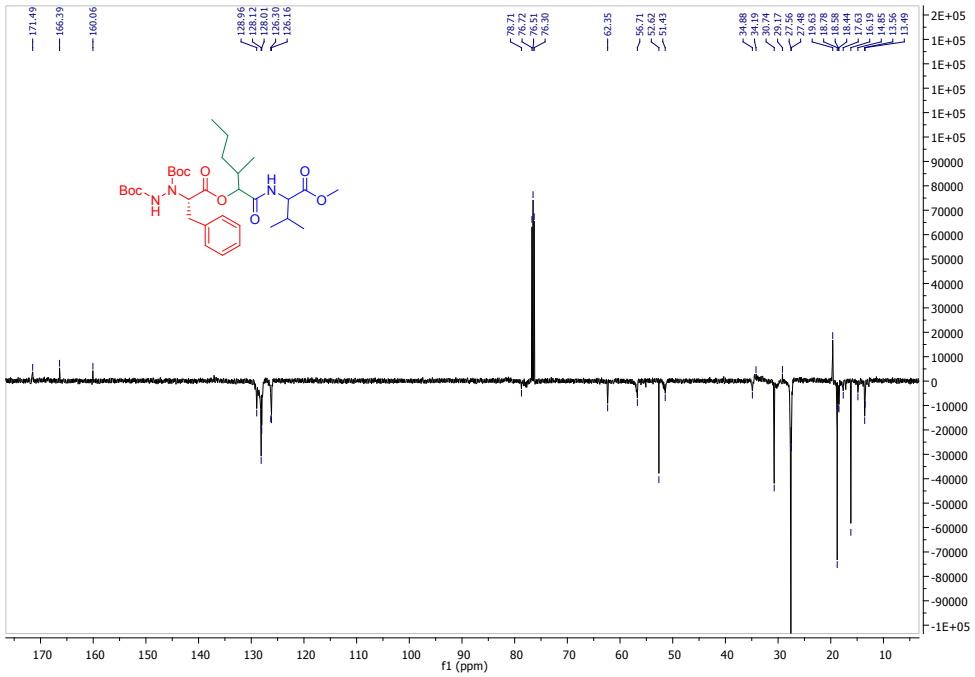

NO2
Boc
Boc
2.13
1.07
7.32
1.00
1.91
2.96
2.95
2.23
19.71
6.72
f1 (ppm)

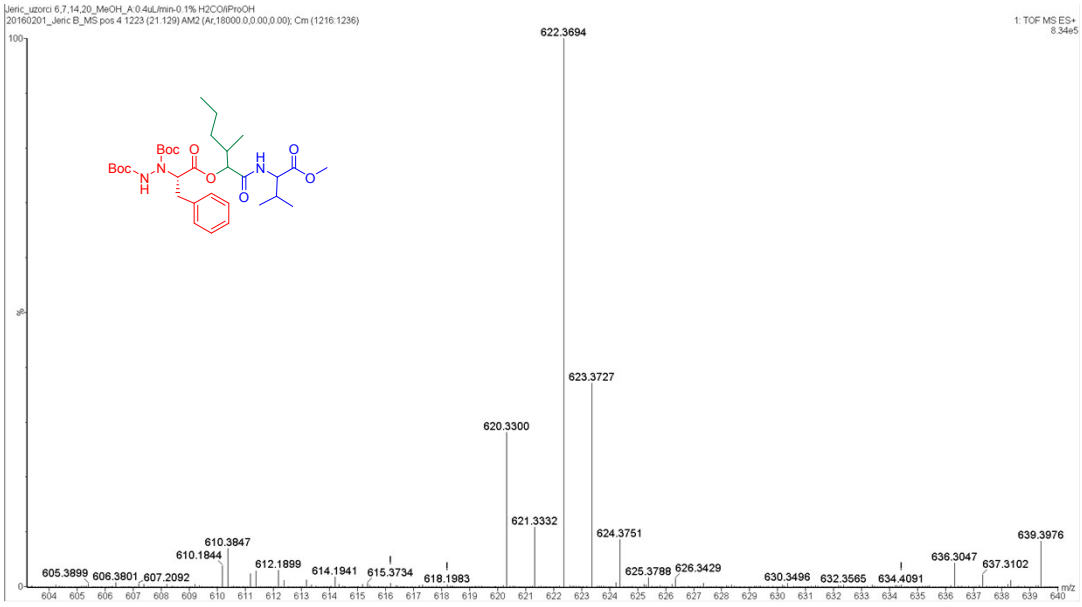

171.4
166.7
148.2
130.6
130.4
129.4
129.2
129.0
128.7
128.6
128.0
127.8
127.3
124.5
123.9
82.6
77.4
77.2
76.9
75.3
53.5
52.6
39.1
37.5
37.3
29.8
28.3
28.2
24.7
23.1
21.9
NO2
Boc
Boc
f1 (ppm)


Jeric_uzorci 3,4,11,13,19_MeOH_A 0.4uL/min-0.1% H2CO/PrOH
20160201_Jeric A_MS pos 3 1197 (20.670) AM2 (Ar,18000.0,0.00,0.00); Cm (1197)
1: TOF MS ES+
3.38e4
687.3237
704.3488
688.3271
705.3535
709.3049
689.3280
710.3084
690.3277
697.3879
711.3121
716.2708
725.2781
726.2820
732.3759
739.4202
647.3676
649.3026
661.9110
665.2478
667.1762
679.3945
681.3922
m/z

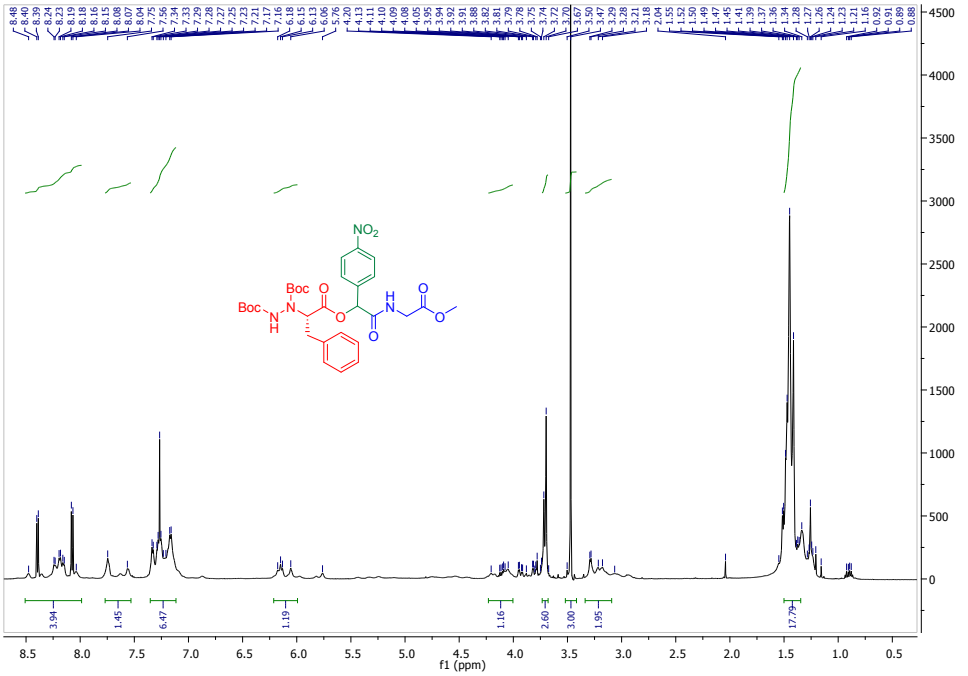
Compound **14**

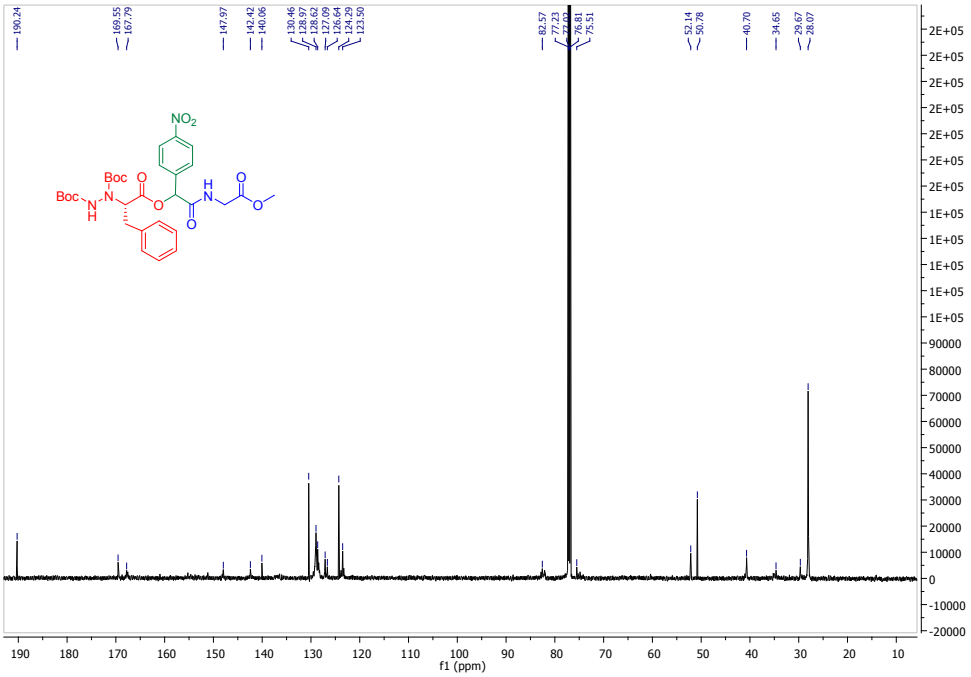

f1 (ppm)

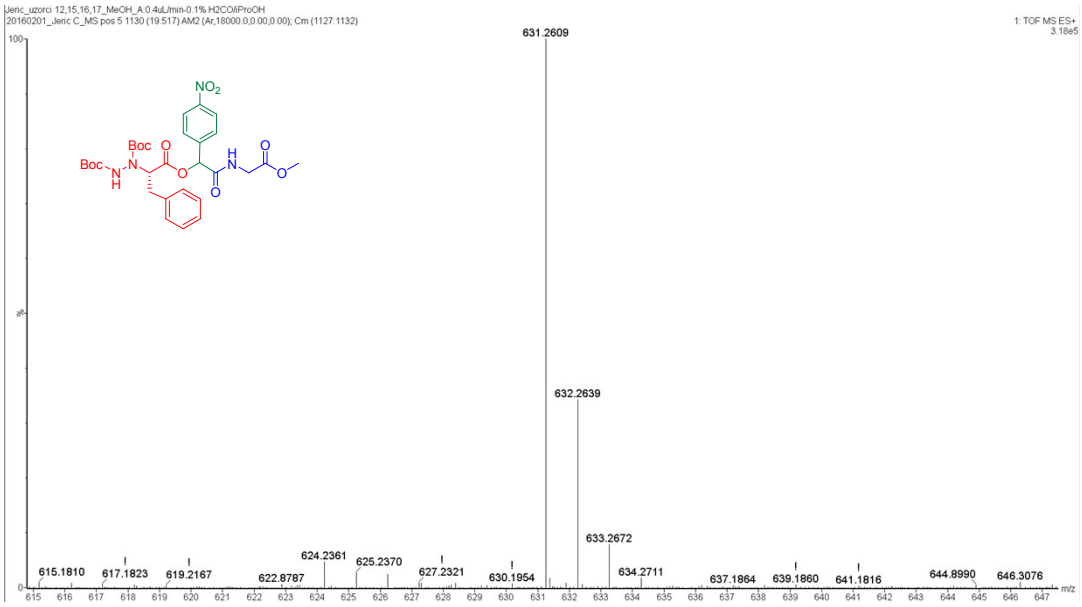

171.49
166.39
160.06
128.96
128.12
128.01
126.30
126.16
78.71
77.22
76.51
76.30
62.35
56.71
52.62
51.43
34.88
34.19
30.74
29.17
27.56
27.48
19.63
18.78
18.58
18.44
17.03
16.19
14.85
13.56
13.49
Boc
Boc
f1 (ppm)


Jeric_uzorci 6,7,14,20_MeOH_A 0.4uL/min-0.1% H2CO/iProOH
20160201_Jeric B_MS pos 4 1223 (21.129) AM2 (Ar,18000.0,0.00,0.00); Cm (1216:1236)
1: TOF MS ES+
8.34e5
622.3694
623.3727
620.3300
621.3332
624.3751
610.3847
610.1844
612.1899
614.1941
615.3734
618.1983
605.3899
606.3801
607.2092
625.3788
626.3429
630.3496
632.3565
634.4091
636.3047
637.3102
639.3976
Boc
Boc
m/z

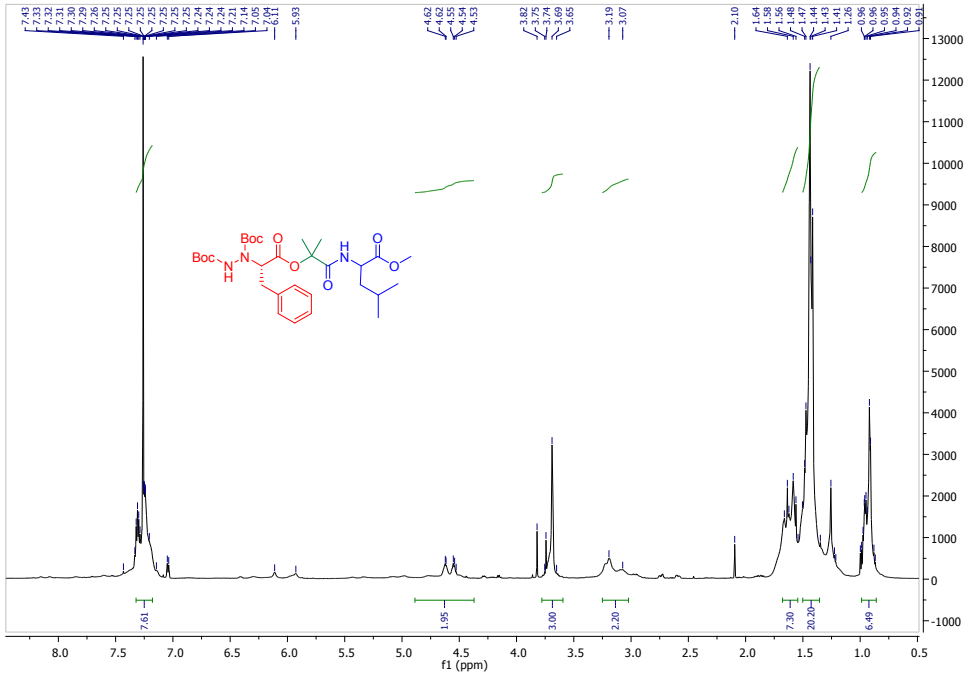
Compound **15**

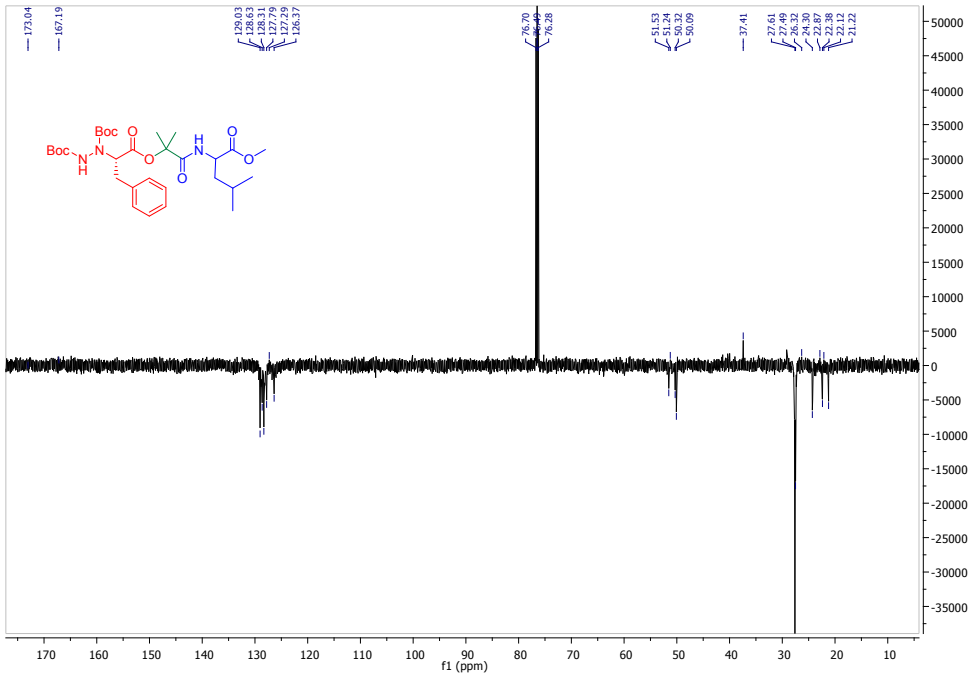


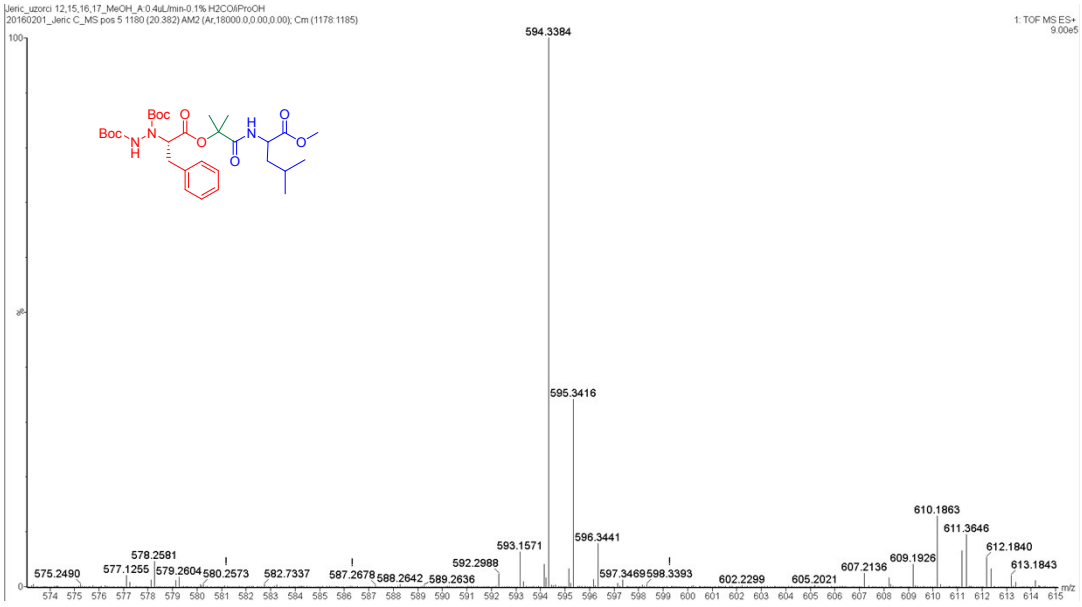



Jeric_uzorci 12,15,16,17_MeOH_A:0.4uL/min-0.1%H2COOiProOH
20160201_Jeric C_MS pos 5 1130 (19.517) AM2 (Ar,18000.0,0.00,0.00); Cm (1127:1132)
1: TOF MS ES+
3.18e5
631.2609
632.2639
633.2672
634.2711
624.2361
625.2370
627.2321
630.1954
622.8787
615.1810
617.1823
619.2167
637.1864
639.1860
641.1816
644.8990
646.3076
m/z

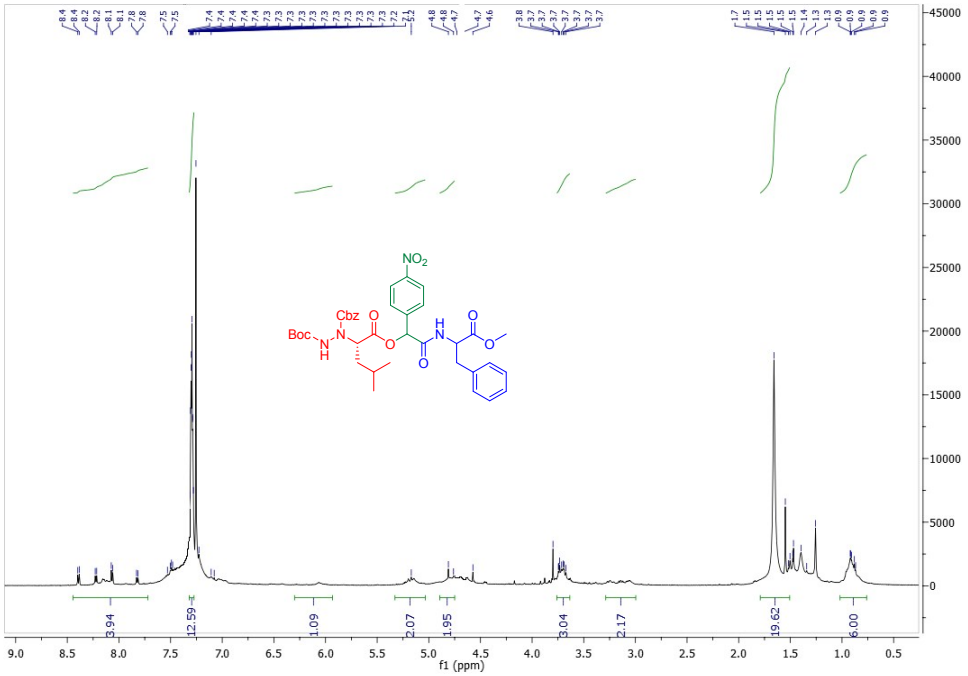
Compound **16**

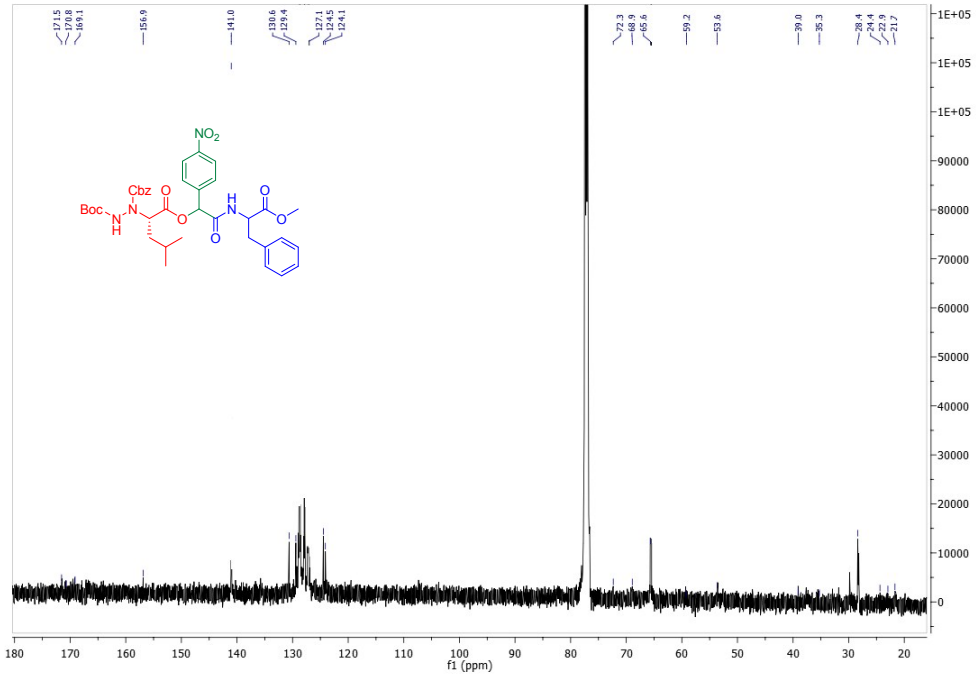

f1 (ppm)

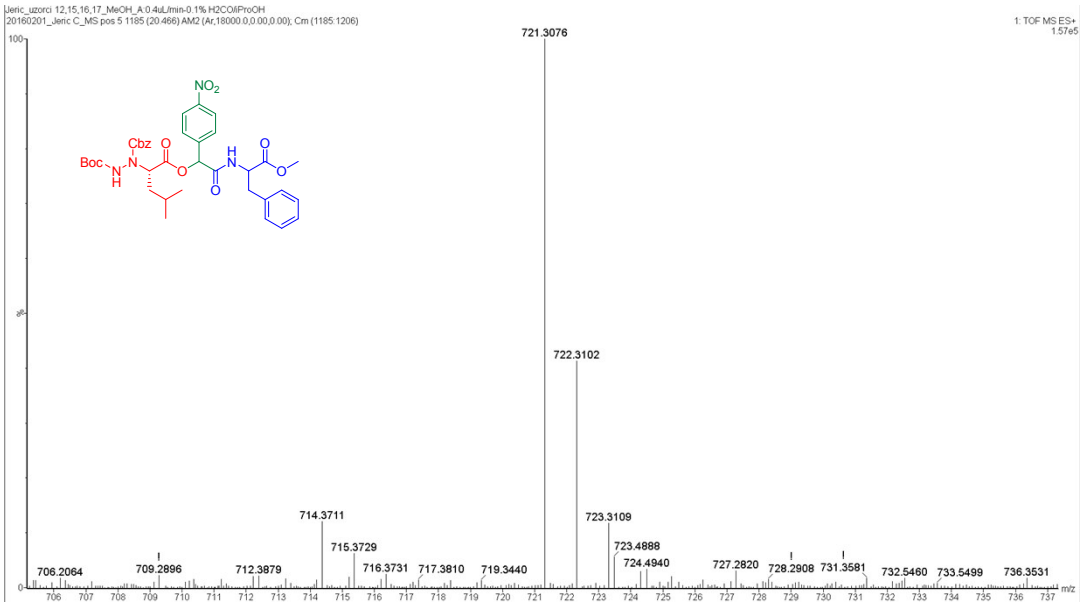

173.04
167.19
129.03
128.63
128.31
127.79
127.39
126.37
76.70
76.48
76.28
51.53
51.24
50.32
50.09
37.41
27.61
27.49
26.32
24.30
22.87
22.38
22.12
21.22
Boc
Boc
f1 (ppm)


Jeric_uzorci 12,15,16,17_MeOH_A:0.4uL/min-0.1% H2COl/ProOH
20160201_Jeric C_MS pos 5 1180 (20.382) AM2 (Ar,18000.0,0.00,0.00); Cm (1178:1185)
1: TOF MS ES+
9.00e5
Boc
Boc
594.3384
595.3416
596.3441
593.1571
592.2988
578.2581
577.1255
579.2604
580.2573
582.7337
587.2678
588.2642
589.2636
575.2490
597.3469
598.3393
602.2299
605.2021
607.2136
609.1926
610.1863
611.3646
612.1840
613.1843
m/z

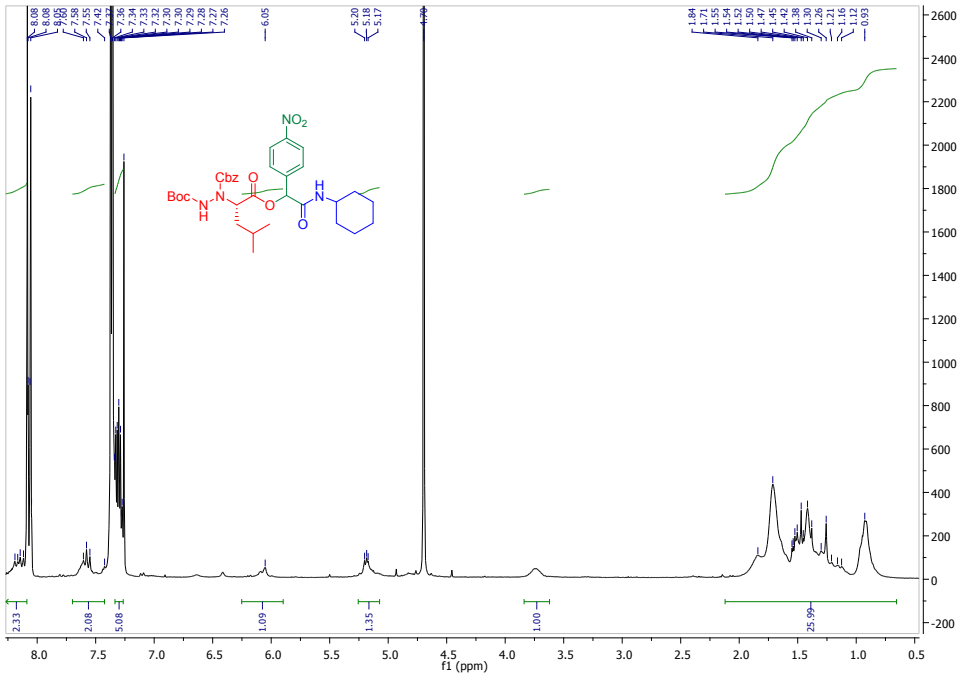
Compound **17**

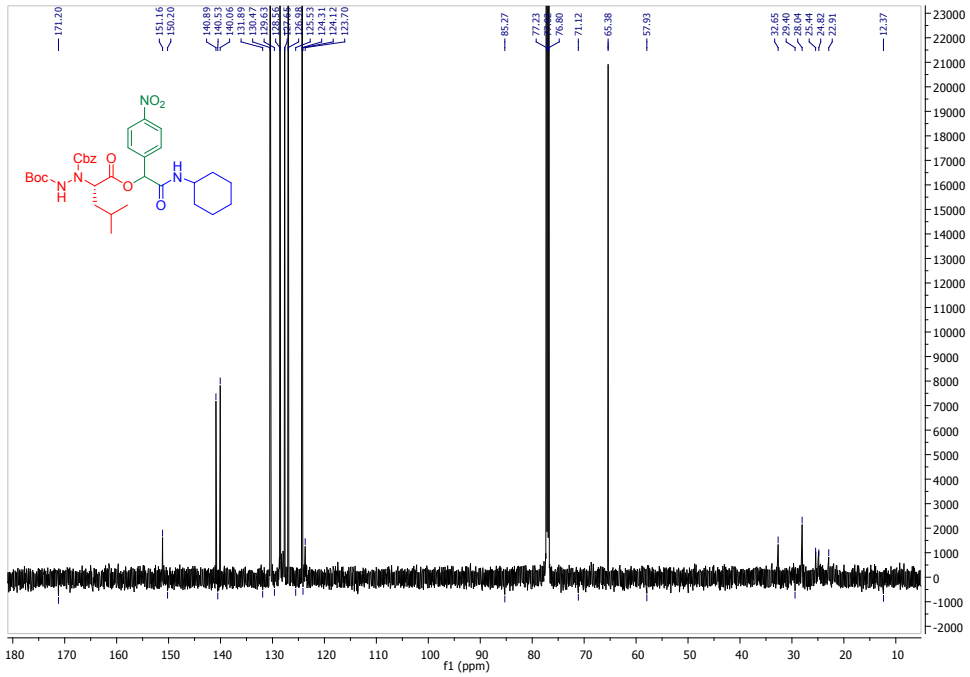


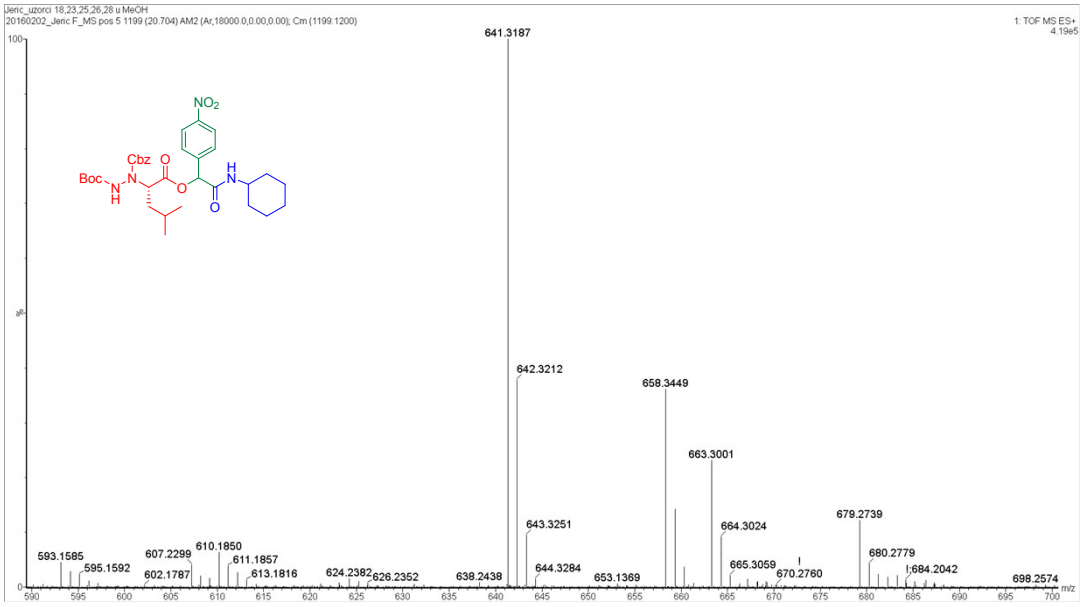



Jeric_uzorci 12,15,16,17_MeOH_A 0.4uL/min-0.1% H2CO/iProOH
20160201_Jeric C_MS pos 5 1185 (20.466) AM2 (Ar,18000.0,0.00,0.00); Cm (1185:1206)
1: TOF MS ES+
1.57e5
721.3076
722.3102
723.3109
714.3711
715.3729
716.3731
717.3810
719.3440
706.2064
709.2896
712.3879
723.4888
724.4940
727.2820
728.2908
731.3581
732.5460
733.5499
736.3531
m/z

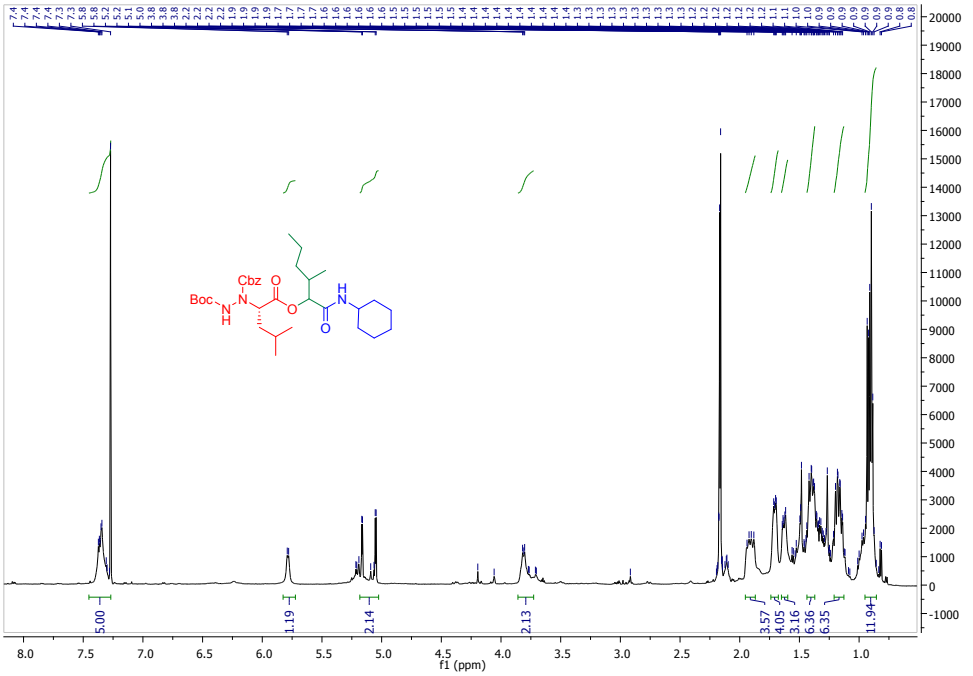
Compound **18**

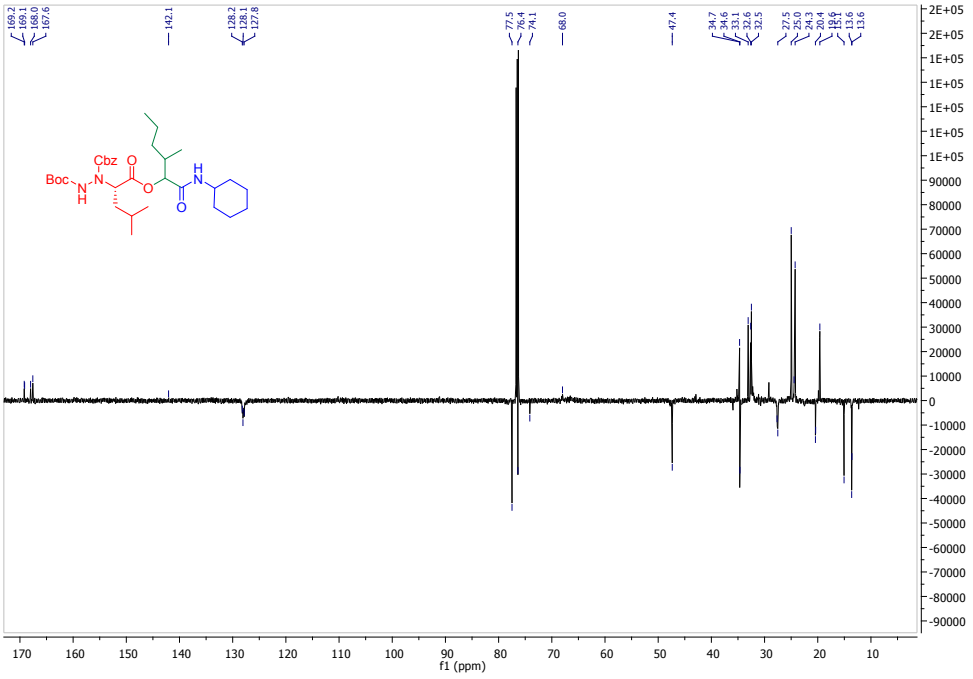

f1 (ppm)

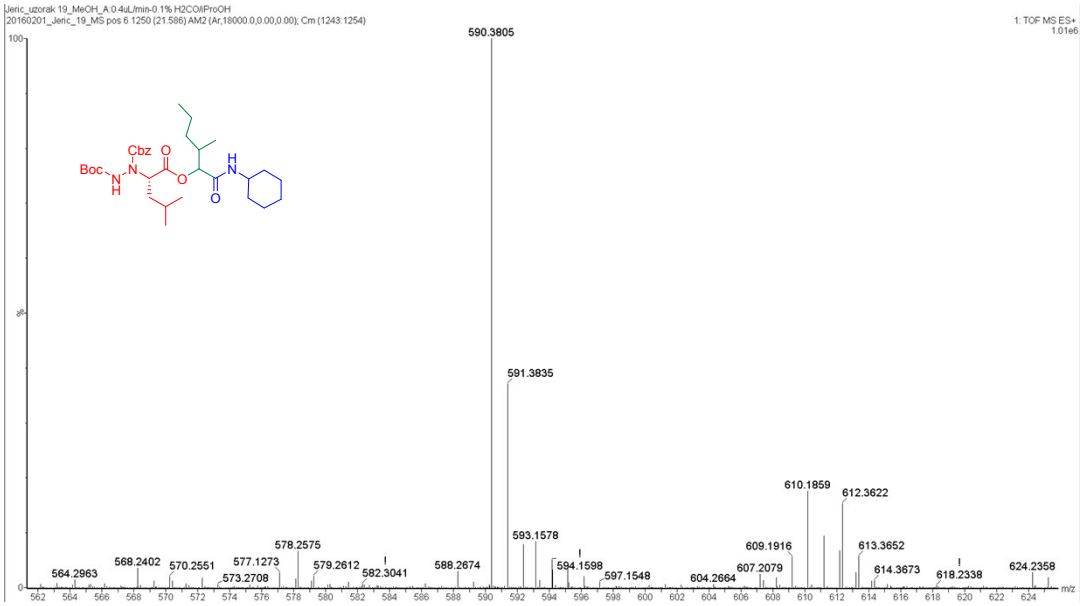

171.20
151.16
150.20
140.89
140.53
140.16
131.89
130.47
129.63
125.53
124.31
124.12
123.70
85.27
77.23
76.80
71.12
65.38
57.93
32.65
29.40
28.04
25.44
24.82
22.91
12.37
NO2
Cbz
Boc
f1 (ppm)


Jeric_uzorci 18,23,25,26,28 u MeOH
20160202_Jerc F_MS pos 5 1199 (20.704) AM2 (Ar,18000.0,0.00,0.00); Cm (1199:1200)
1: TOF MS ES+
4.19e5
641.3187
642.3212
658.3449
663.3001
643.3251
664.3024
679.2739
680.2779
684.2042
698.2574
593.1585
595.1592
607.2299
610.1850
611.1857
602.1787
613.1816
624.2382
626.2352
638.2438
644.3284
653.1369
665.3059
670.2760
NO2
Cbz
Boc
m/z

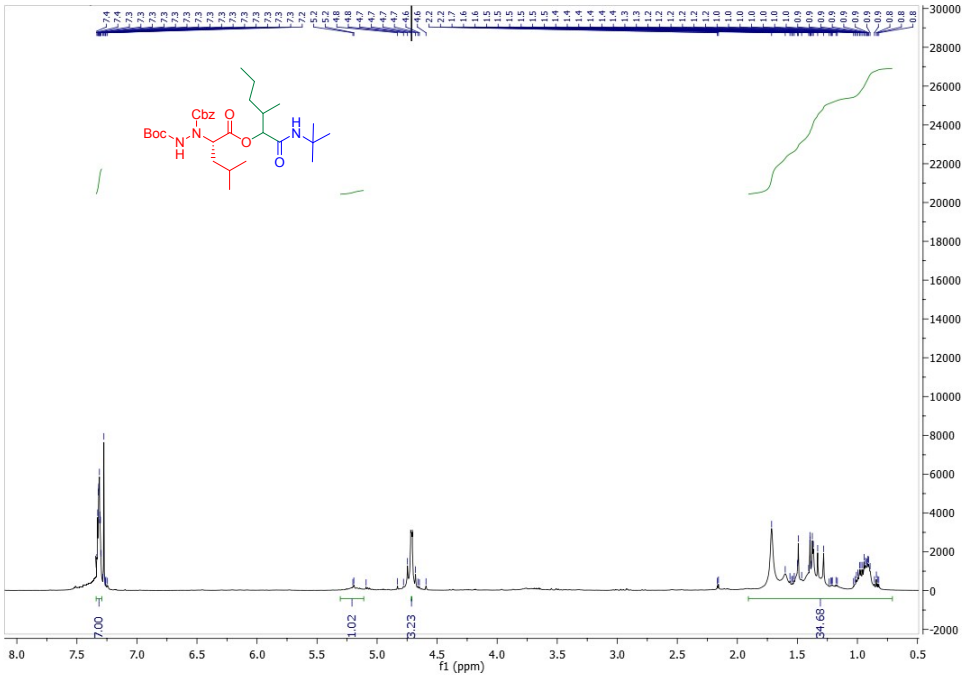
Compound **19**

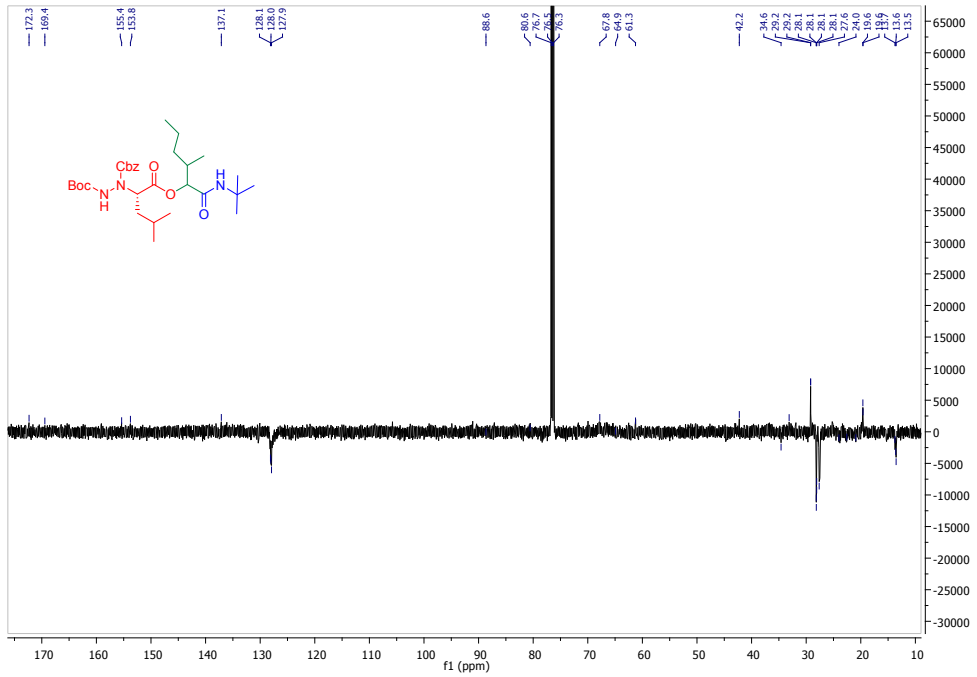


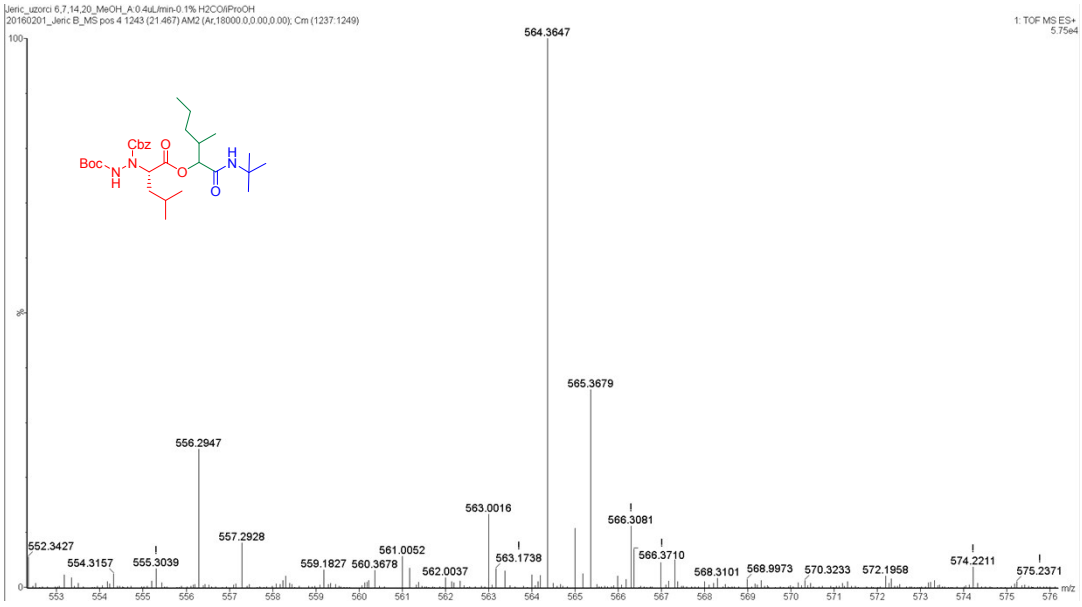



Jeric_uzorak 19_MeOH_A 0.4uL/min-0.1% H2COllProOH
20160201_Jeric_19_MS pos 6 1250 (21.586) AM2 (Ar,18000.0,0.00,0.00); Cm (1243:1254)
1: TOF MS ES+
1.01e6
590.3805
591.3835
610.1859
612.3622
593.1578
578.2575
609.1916
613.3652
568.2402
570.2551
577.1273
579.2612
582.3041
588.2674
594.1598
597.1548
607.2079
614.3673
624.2358
564.2963
573.2708
604.2664
618.2338
m/z

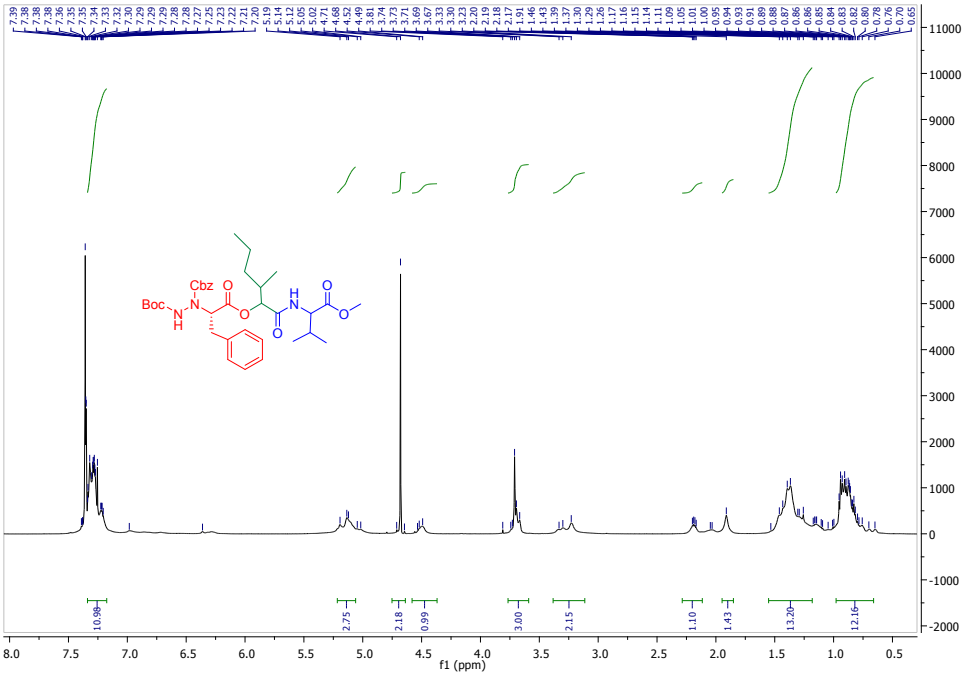
Compound **20**

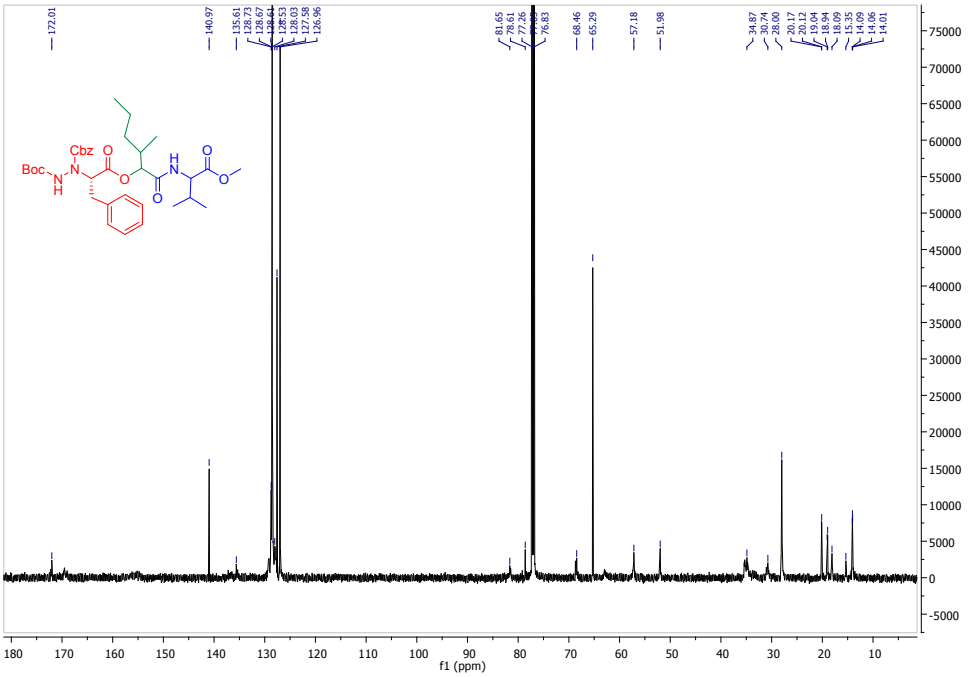

7.00
1.02
3.23
34.68
f1 (ppm)

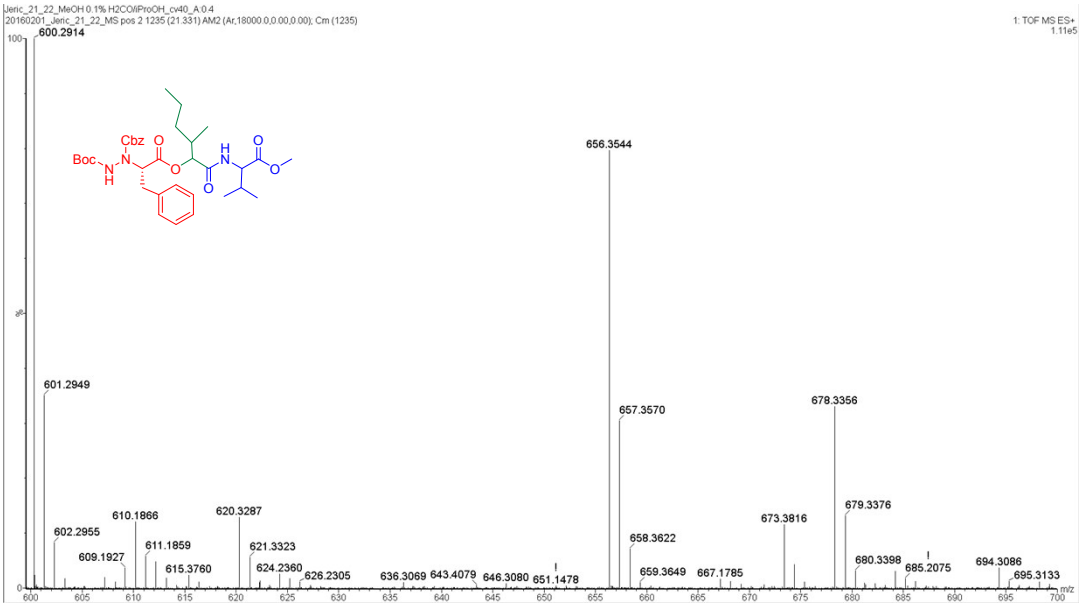

172.3
169.4
155.4
153.8
137.1
128.1
128.0
127.9
88.6
80.6
76.7
76.5
76.3
67.8
64.9
61.3
42.2
34.6
29.2
29.2
28.1
28.1
28.1
27.6
24.0
19.6
13.6
13.5
Cbz
Boc
f1 (ppm)


Jeric_uzorci 6,7,14,20_MeOH_A:0.4uL/min-0.1% H2CO/ProOH
20160201_Jeric B_MS pos 4 1243 (21.467) AM2 (Ar,18000.0,0.00,0.00); Cm (1237:1249)
1: TOF MS ES+
5.75e4
564.3647
565.3679
556.2947
563.0016
566.3081
557.2928
561.0052
563.1738
566.3710
552.3427
554.3157
555.3039
559.1827
560.3678
562.0037
568.3101
568.9973
570.3233
572.1958
574.2211
575.2371
Cbz
Boc
m/z

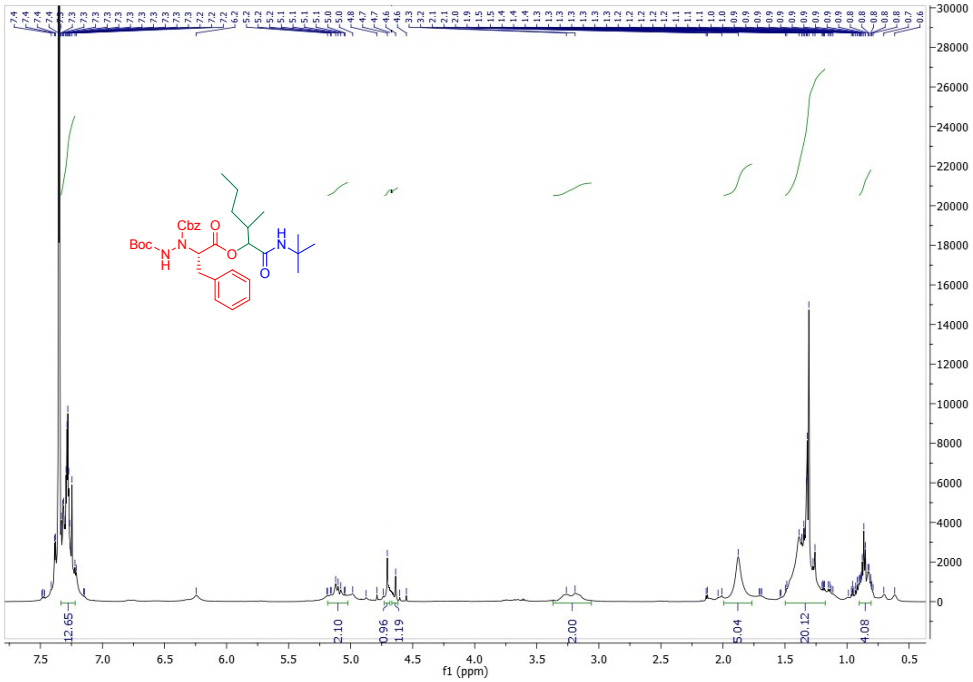
Compound **21**

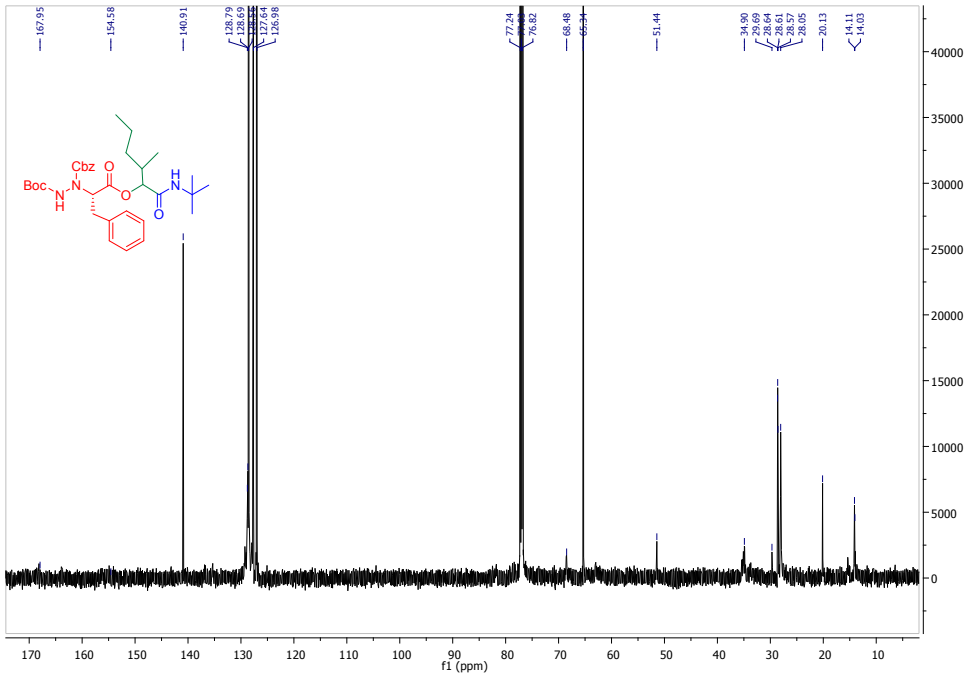

Cbz
Boc
N
H
O
O
O
O
O
N
H
O
O
10.99
2.75
2.18
0.99
3.00
2.15
1.10
1.43
13.20
12.16
f1 (ppm)

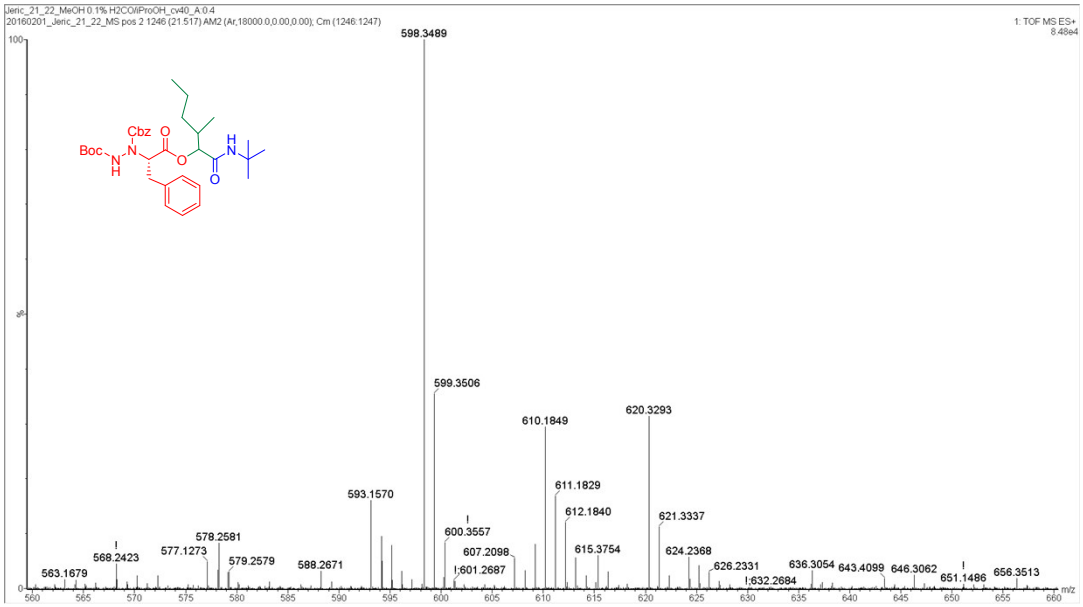

172.01
140.97
135.61
128.73
128.67
128.53
128.03
127.58
126.96
81.65
78.61
77.26
76.83
68.46
65.29
57.18
51.98
34.87
30.74
28.00
20.17
20.12
19.04
18.94
18.09
15.35
14.09
14.06
14.01
Cbz
Boc
N
H
O
O
O
O
O
N
H
O
O
f1 (ppm)


Jeric_21_22_MeOH 0.1% H2CO/iProOH_cv40_A 0.4
20160201_Jeric_21_22_MS pos 2 1235 (21.331) AM2 (Ar,18000.0,0.00,0.00); Cm (1235)
1: TOF MS ES+
1.11e5
600.2914
601.2949
602.2955
609.1927
610.1866
611.1859
615.3760
620.3287
621.3323
624.2360
626.2305
636.3069
643.4079
646.3080
651.1478
656.3544
657.3570
658.3622
659.3649
667.1785
673.3816
678.3356
679.3376
680.3398
685.2075
694.3086
695.3133
Cbz
Boc
m/z

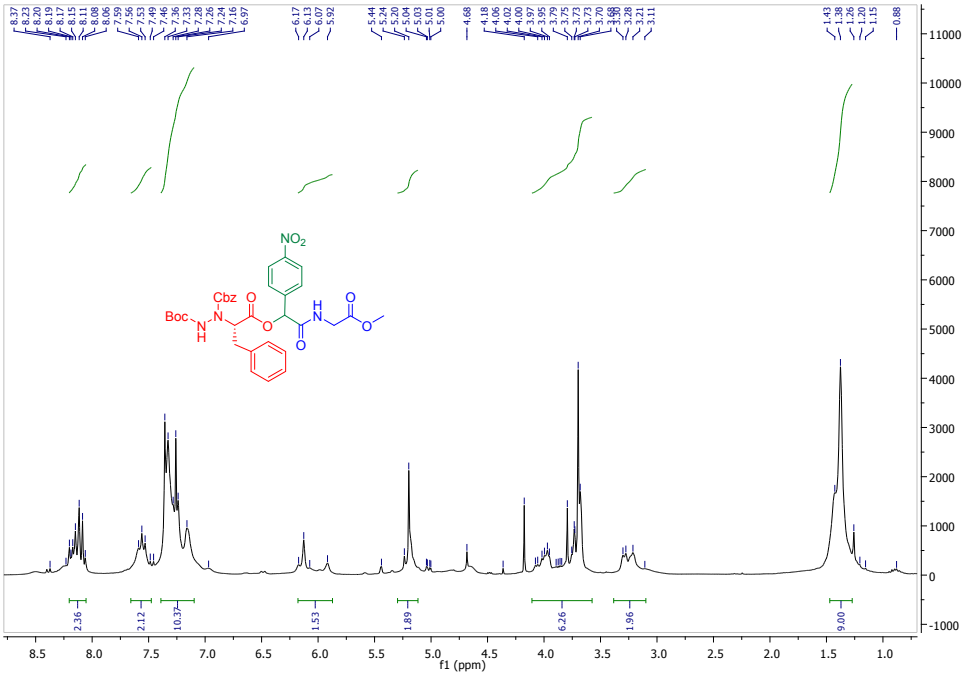
Compound **22**

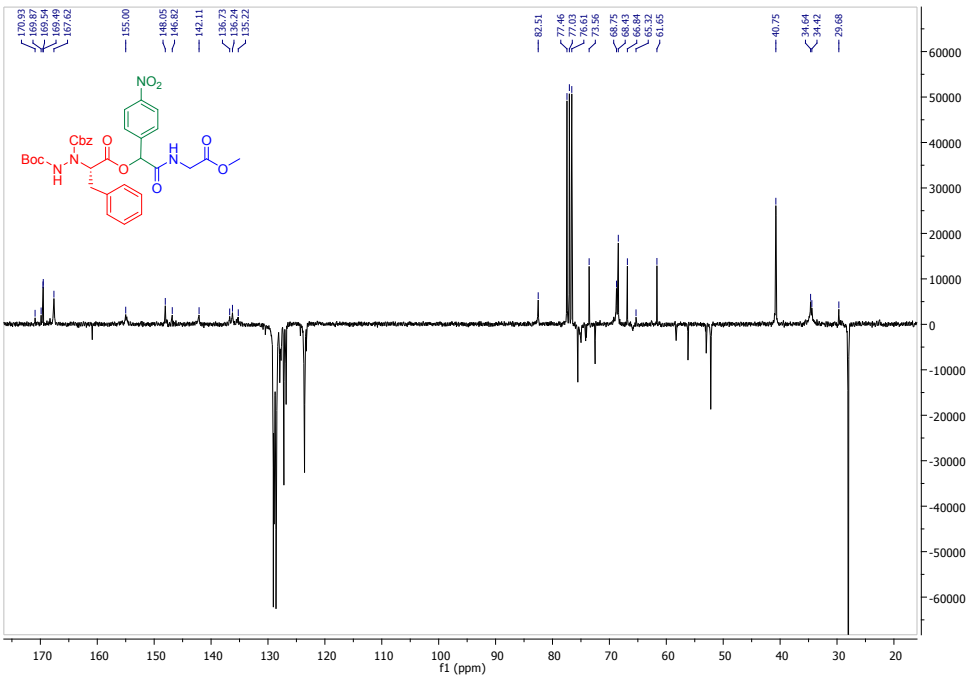

Cbz
Boc
12.65
2.10
0.96
1.19
2.00
5.04
20.12
4.08
f1 (ppm)

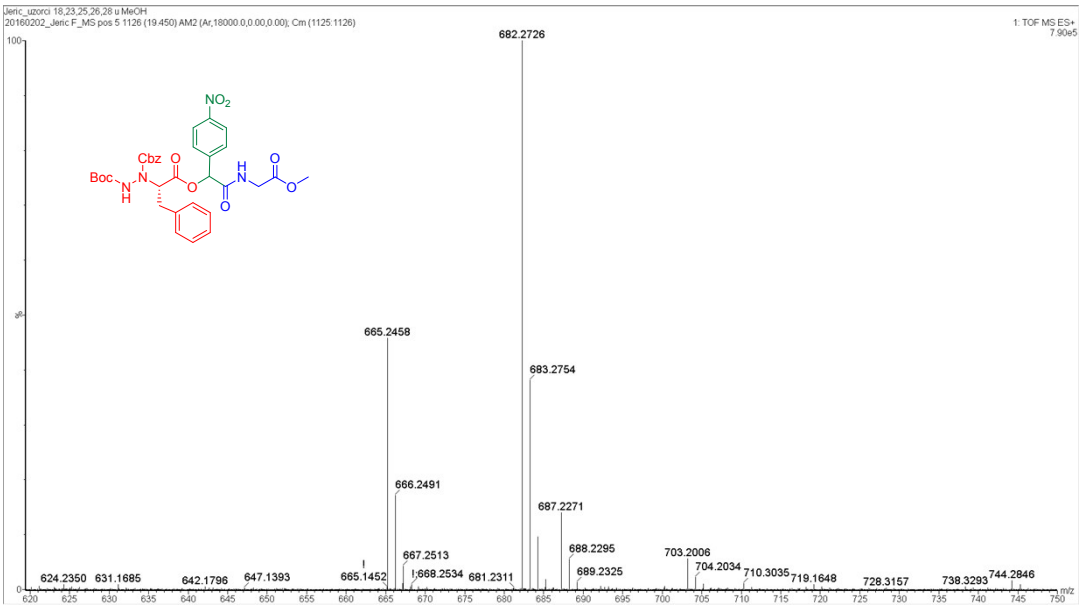

167.95
154.58
140.91
128.79
128.69
128.55
127.64
126.98
77.24
76.82
68.48
65.31
51.44
34.90
29.69
28.64
28.61
28.57
28.05
20.13
14.11
14.03
Cbz
Boc
f1 (ppm)


Jeric_21_22_MeOH 0.1% H2CO/iPrOH_cv40_A 0.4
20160201_Jeric_21_22_MS pos 2 1246 (21.517) AM2 (Ar,18000.0,0.00,0.00); Cm (1246:1247)
1: TOF MS ES+
8.48e4
598.3489
599.3506
610.1849
620.3293
611.1829
612.1840
621.3337
593.1570
600.3557
607.2098
615.3754
624.2368
578.2581
577.1273
568.2423
579.2579
588.2671
563.1679
601.2687
626.2331
632.2684
636.3054
643.4099
646.3062
651.1486
656.3513
m/z
Cbz
Boc

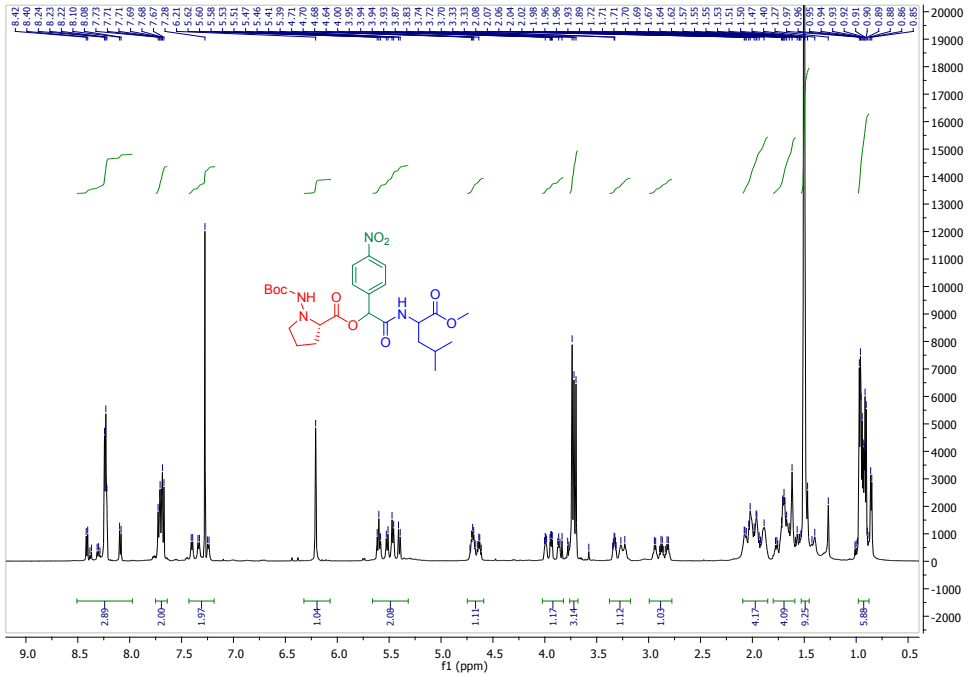
Compound **23**

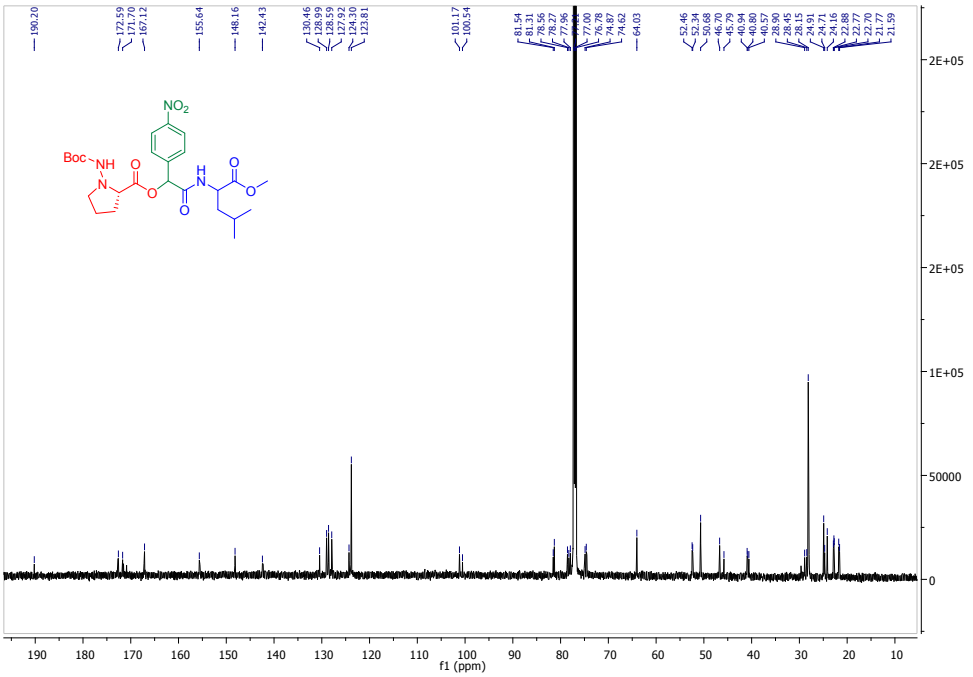

8.37
8.23
8.20
8.19
8.17
8.15
8.11
8.08
8.06
7.59
7.56
7.53
7.49
7.46
7.36
7.33
7.28
7.26
7.24
7.16
6.97
6.17
6.13
6.07
5.92
5.44
5.24
5.20
5.04
5.03
5.01
5.00
4.68
4.18
4.06
4.02
4.00
3.97
3.95
3.79
3.75
3.73
3.70
3.68
3.65
3.28
3.21
3.11
1.43
1.38
1.26
1.20
1.15
0.88
NO2
Cbz
Boc
2.36
2.12
10.37
1.53
1.89
6.26
1.96
9.00
f1 (ppm)

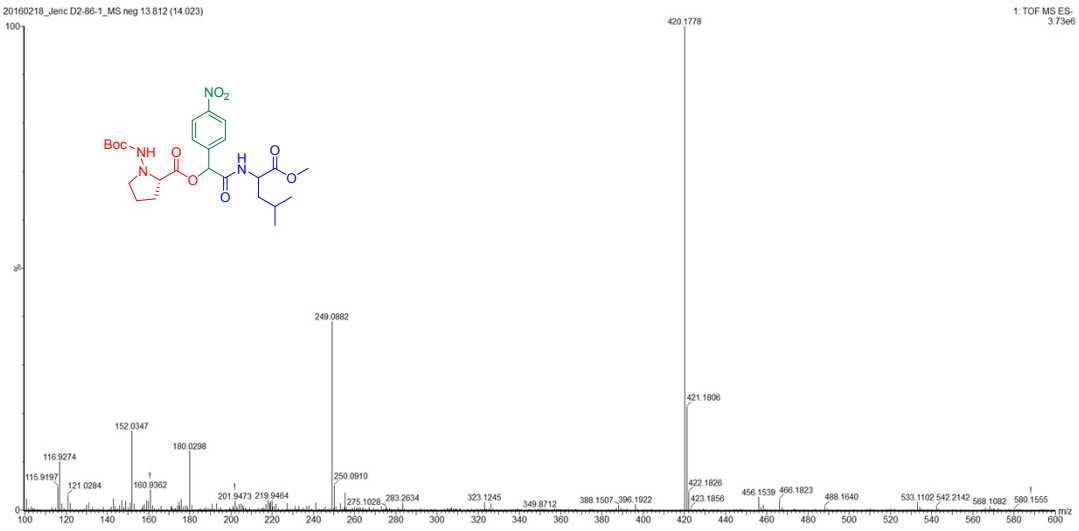

170.93
169.87
169.34
168.49
167.62
155.00
148.05
146.82
142.11
136.73
136.24
135.22
82.51
77.46
77.03
76.61
73.56
68.75
68.43
66.84
65.32
61.65
40.75
34.64
34.42
29.68
NO2
Cbz
Boc
f1 (ppm)


Jeric_uzorci 18,23,25,26,28 u MeOH
20160202_Jeric F_MS pos 5 1126 (19.450) AM2 (Ar,18000.0,0.00,0.00); Cm (1125:1126)
1: TOF MS ES+
7.90e5
682.2726
665.2458
683.2754
666.2491
687.2271
667.2513
688.2295
703.2006
704.2034
624.2350
631.1685
642.1796
647.1393
665.1452
668.2534
681.2311
689.2325
710.3035
719.1648
728.3157
738.3293
744.2846
NO2
Cbz
Boc
m/z

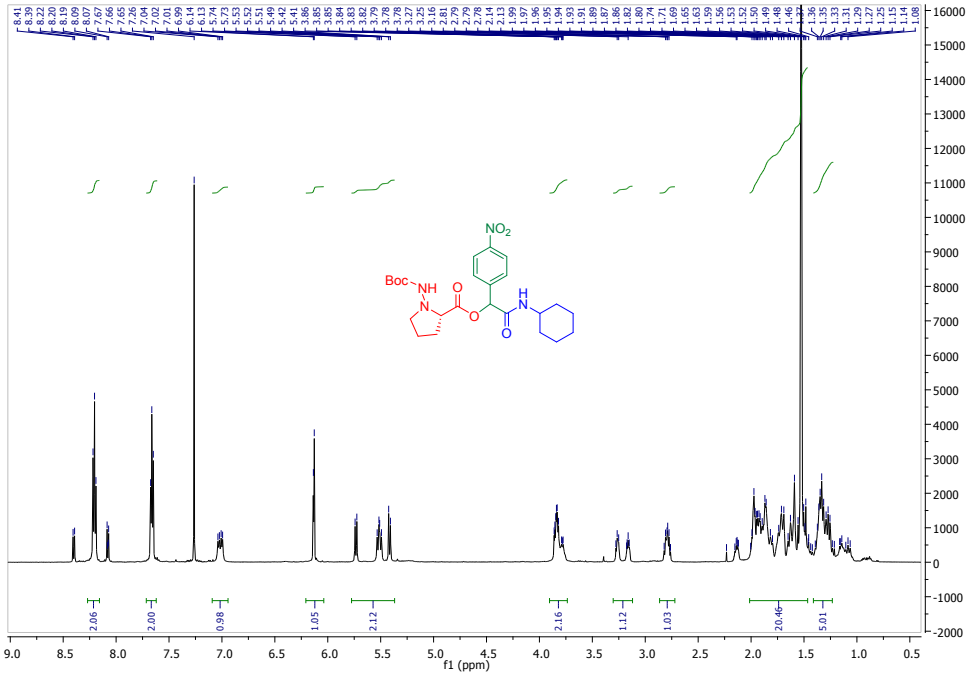
Compound **25**

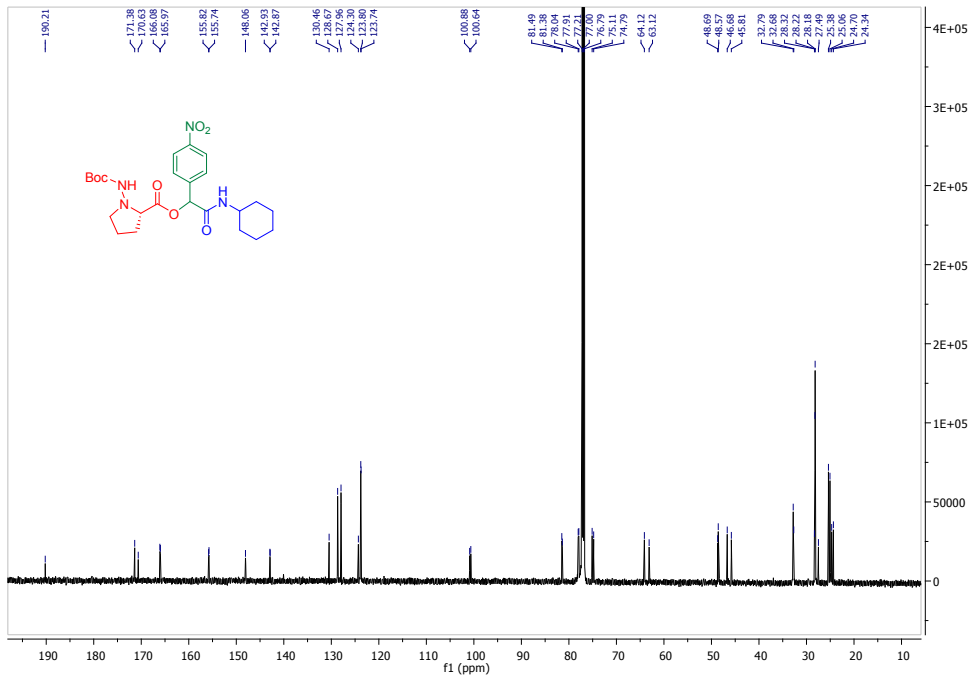

NO2
Boc
NH
f1 (ppm)

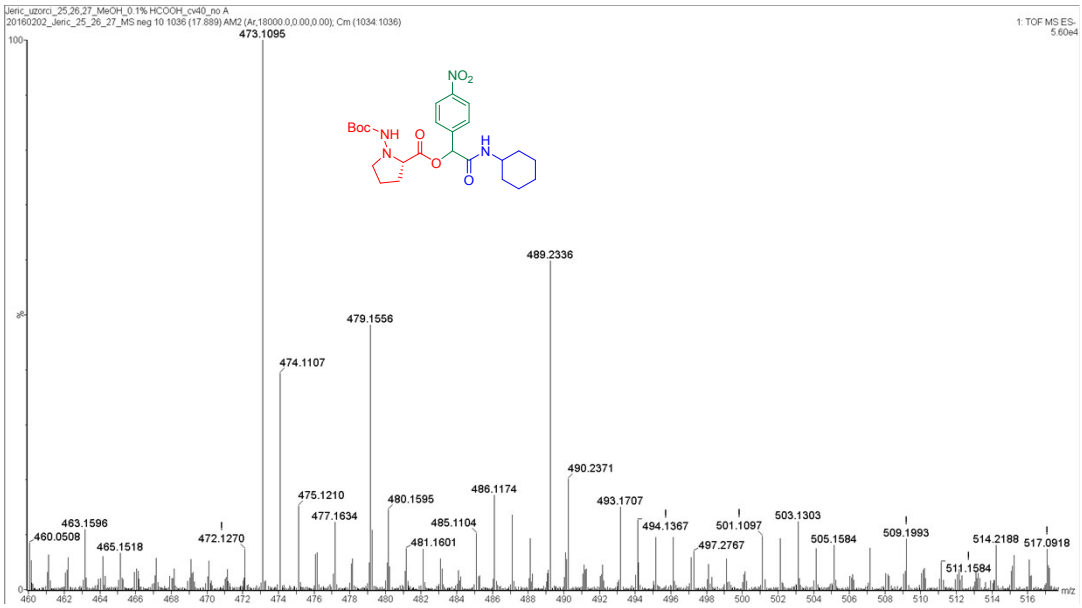

190.20
172.59
171.70
167.12
155.64
148.16
142.43
130.46
128.99
128.59
127.92
124.30
123.81
101.17
100.54
81.54
81.31
78.56
78.27
77.36
77.00
76.78
74.87
74.62
64.03
52.46
52.34
50.68
46.70
45.79
40.94
40.80
40.57
28.90
28.45
28.15
24.91
24.71
24.16
22.88
22.77
22.70
21.77
21.59
NO2
Boc
NH
2E+05
2E+05
2E+05
1E+05
50000
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


20160218_Jeric D2-86-1_MS neg 13.812 (14.023)
1: TOF MS ES-
3.73e6
100
%
0
NO2
Boc
NH
420.1778
249.0882
421.1806
152.0347
180.0298
116.9274
115.9197
121.0284
160.9362
250.0910
201.9473
219.9464
275.1026
283.2634
323.1245
349.8712
388.1507
396.1922
422.1826
423.1856
456.1539
466.1823
488.1640
533.1102
542.2142
568.1082
580.1555
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
m/z

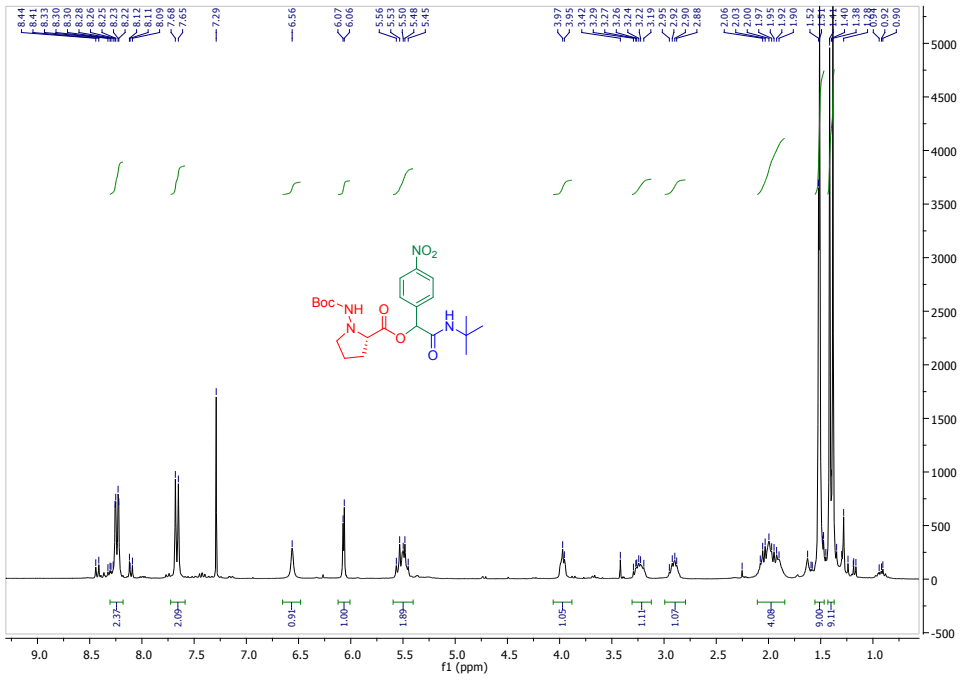
Compound **26**

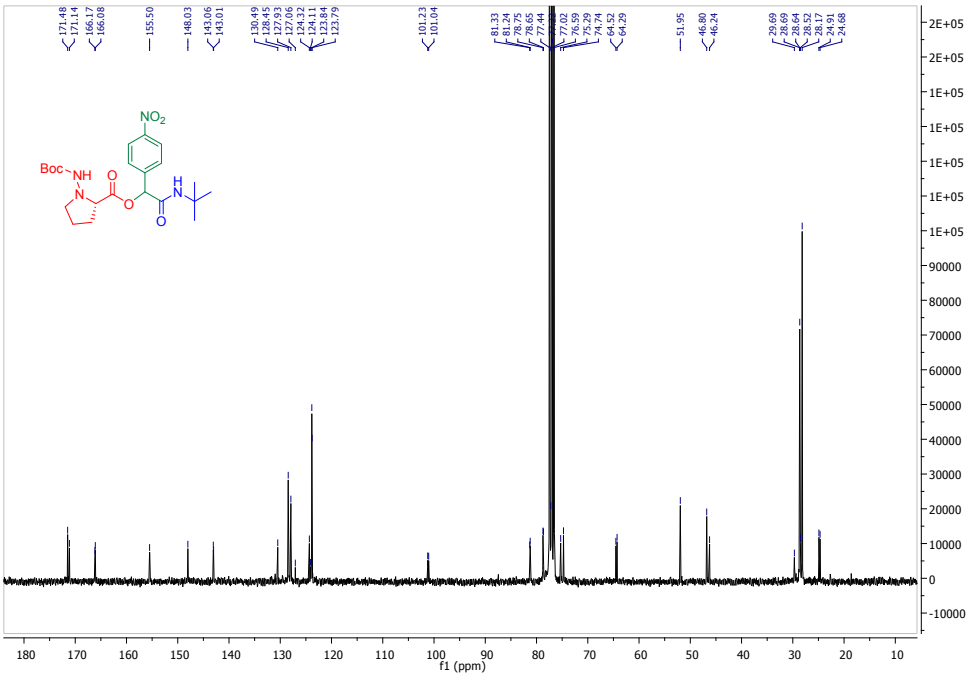


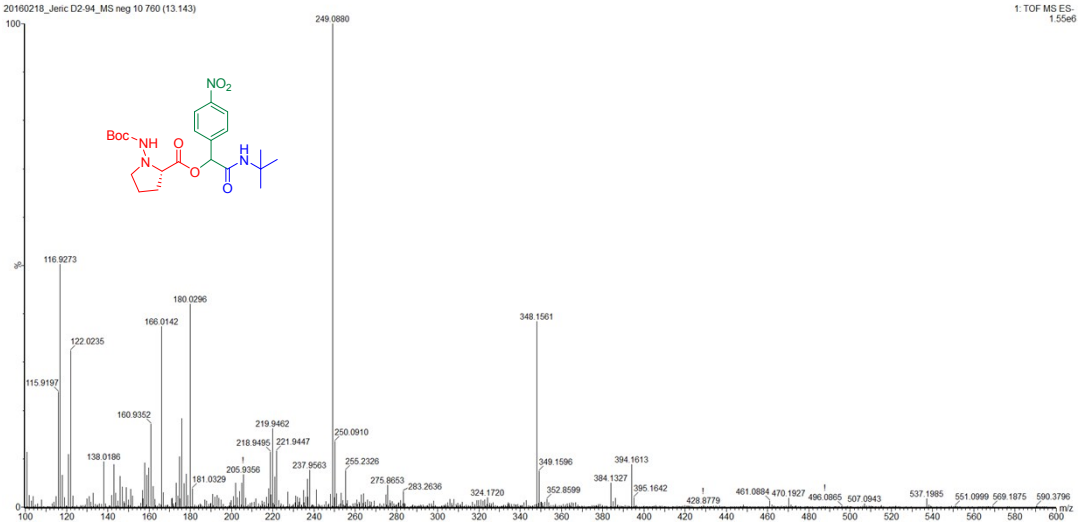



Jeric_uzorci_25,26,27_MeOH_0.1% HCOOH_cv40_no A
20160202_Jeric_25_26_27_MS neg 10 1036 (17.899) AM2 (Ar,18000.0,0.00,0.00); Cm (1034:1036)
1: TOF MS ES-
5.60e4
473.1095
489.2336
479.1556
474.1107
490.2371
475.1210
480.1595
486.1174
493.1707
477.1634
485.1104
494.1367
501.1097
503.1303
463.1596
460.0508
472.1270
465.1518
481.1601
497.2767
505.1584
509.1993
514.2188
517.0918
511.1584
m/z

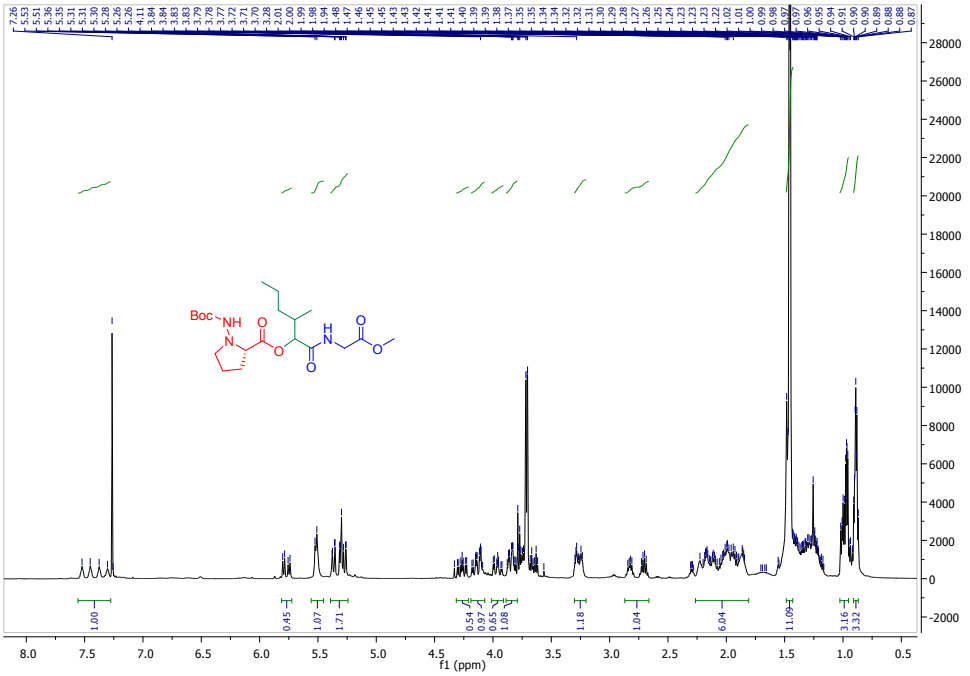
Compound **27**

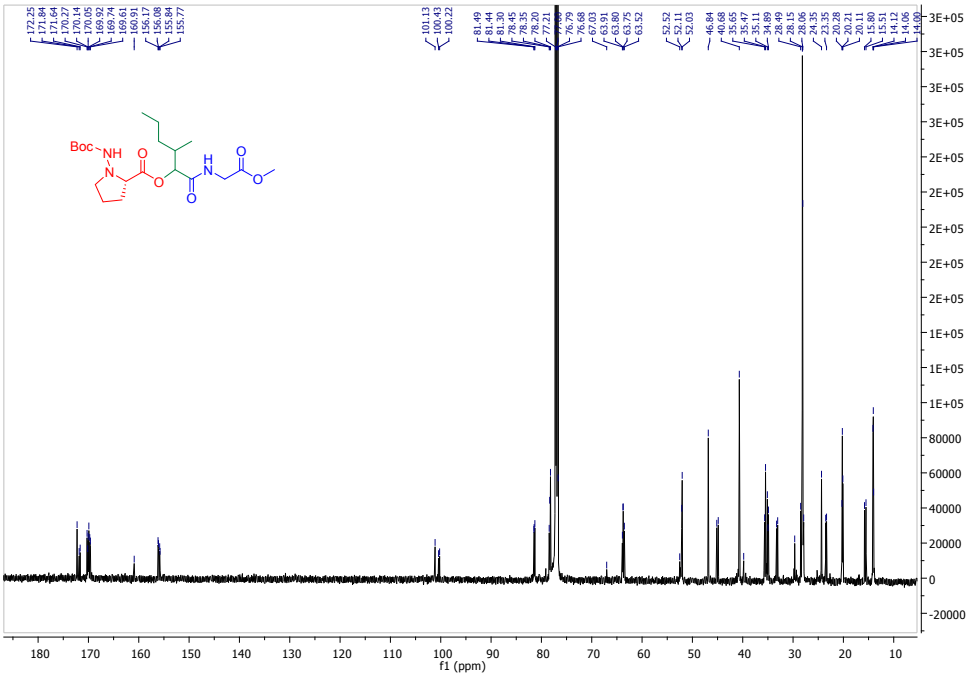

f1 (ppm)

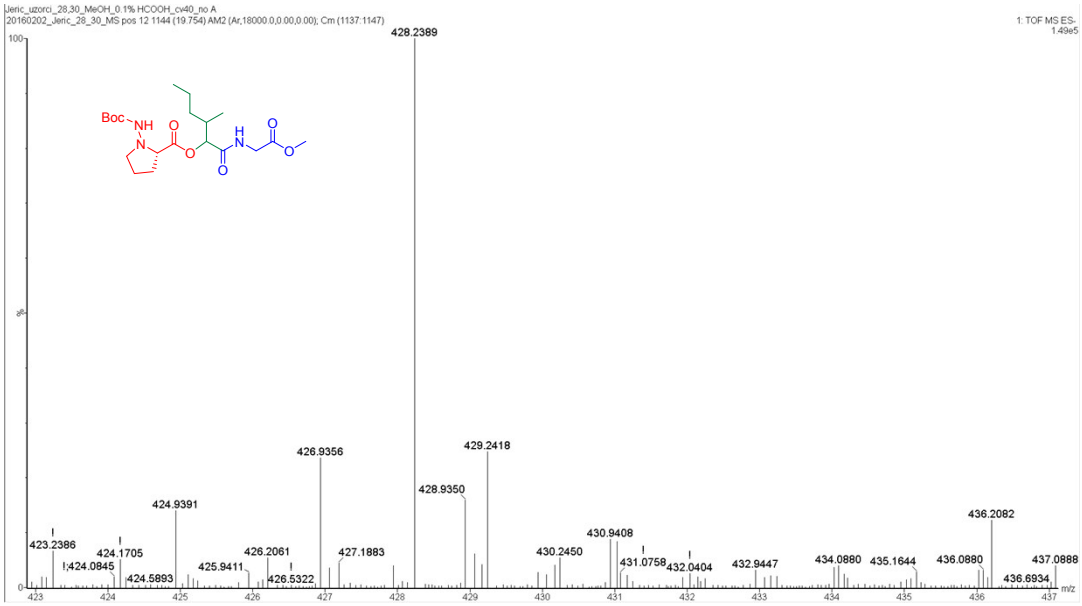

171.48
171.14
166.17
166.08
155.50
148.03
143.06
143.01
130.49
128.45
127.93
127.06
124.32
124.11
123.84
123.79
101.23
101.04
81.33
81.24
78.75
78.65
77.44
77.02
76.59
75.29
74.74
64.52
64.29
51.95
46.80
46.24
29.69
29.68
28.64
28.52
28.17
24.91
24.68
NO2
Boc
NH
N
O
O
H
N
O
2E+05
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


20160218_Jeric D2-94_MS neg 10 760 (13.143)
1: TOF MS ES-
1.55e6
100
%
0
NO2
Boc
NH
N
O
O
H
N
O
249.0880
116.9273
180.0296
166.0142
122.0235
348.1561
115.9197
160.9352
219.9462
218.9495
221.9447
250.0910
138.0186
237.9563
255.2326
205.9356
181.0329
349.1596
394.1613
275.8653
283.2636
384.1327
395.1642
324.1720
352.8599
428.8779
461.0884
470.1927
496.0865
507.0943
537.1985
551.0999
569.1875
590.3796
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
m/z

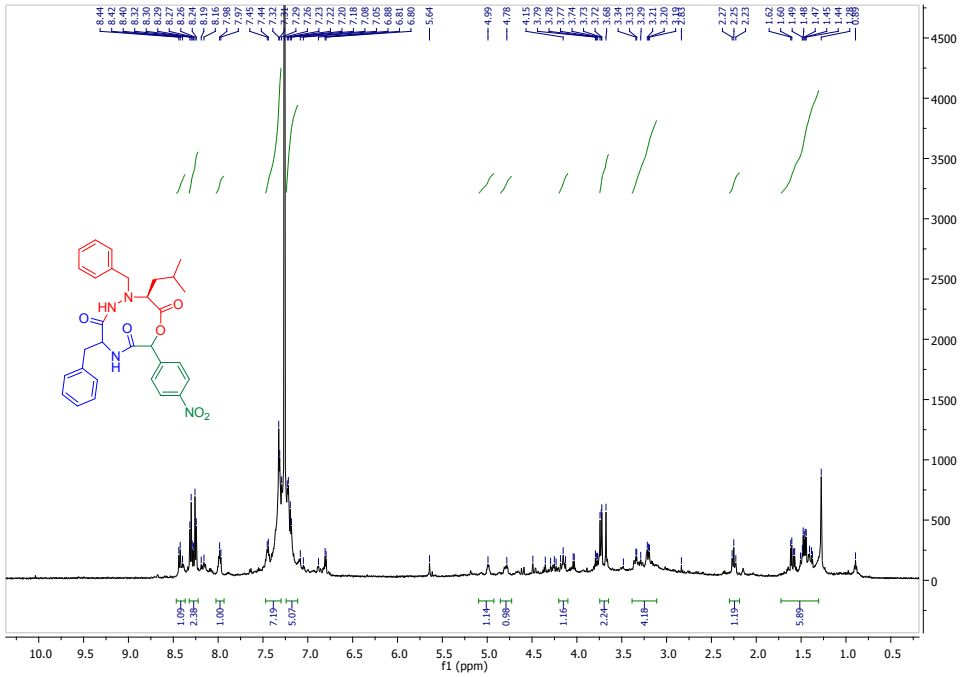
Compound **28**

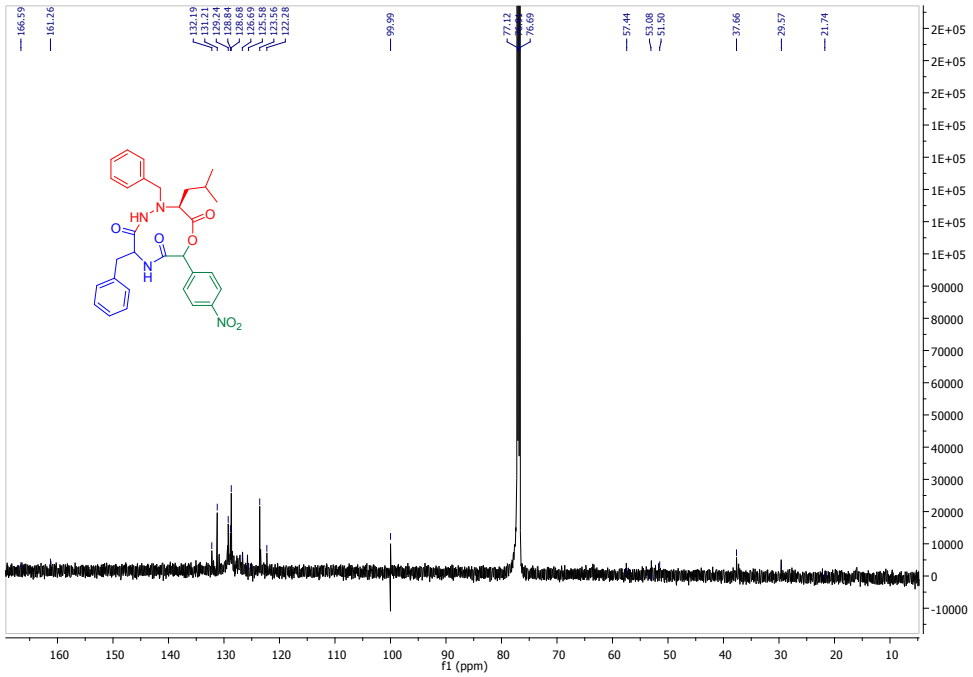


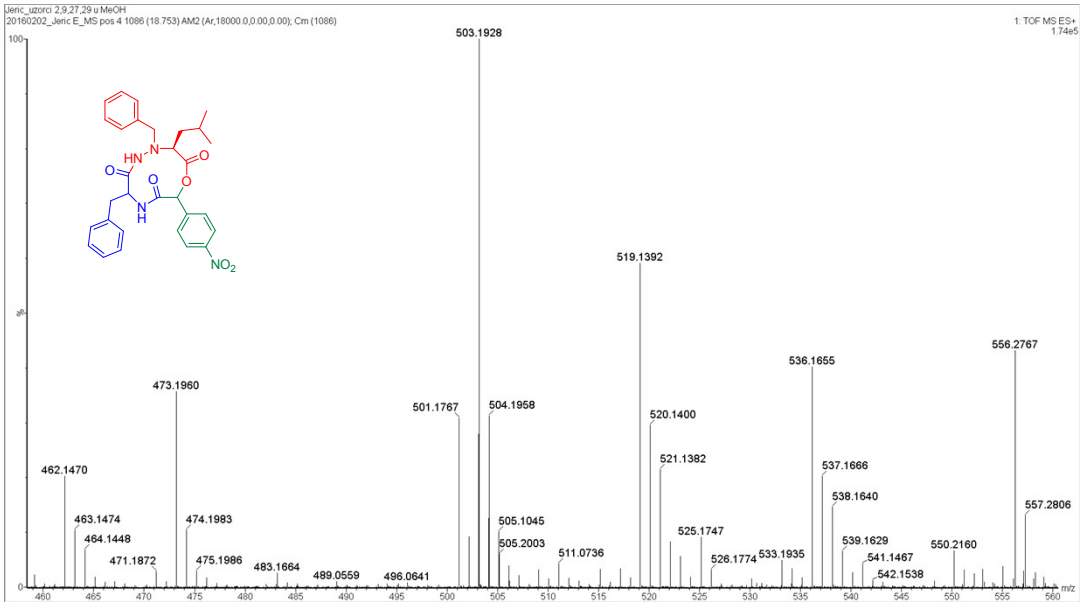



Jeric_uzorci_28,30_MeOH_0.1% HCOOH_cv40_no A
20160202_Jeric_28_30_MS pos 12 1144 (19.754) AM2 (Ar,18000.0,0.00,0.00); Cm (1137:1147)
1: TOF MS ES+
1.49e5
428.2389
429.2418
426.9356
428.9350
424.9391
436.2082
430.9408
423.2386
424.1705
424.0845
426.2061
427.1883
430.2450
431.0758
432.0404
432.9447
434.0880
435.1644
436.0880
437.0888
424.5893
425.9411
426.5322
436.6934
m/z

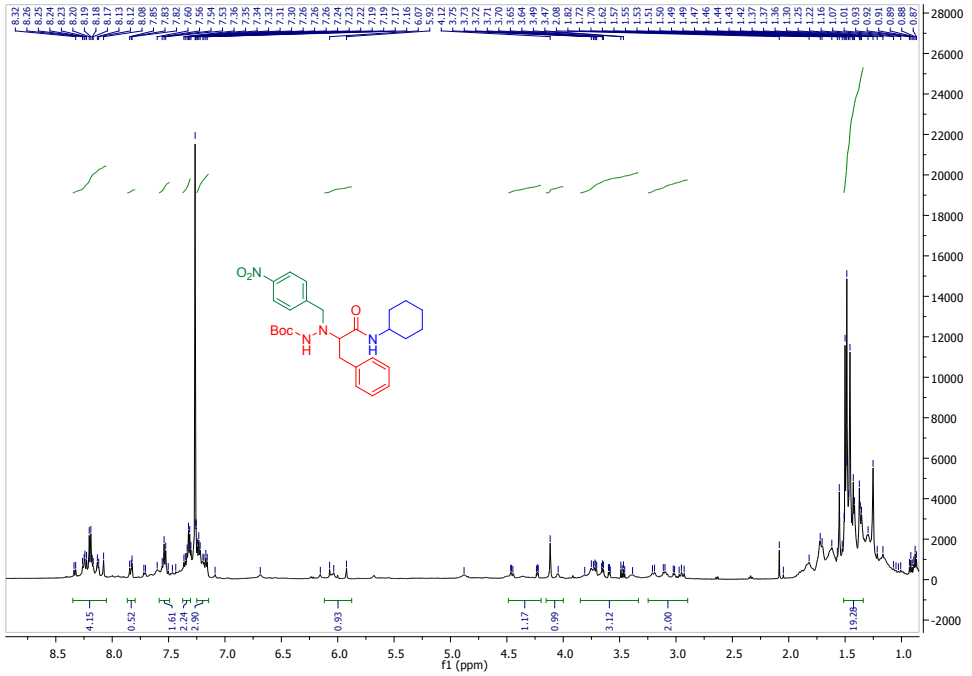
Compound **29**

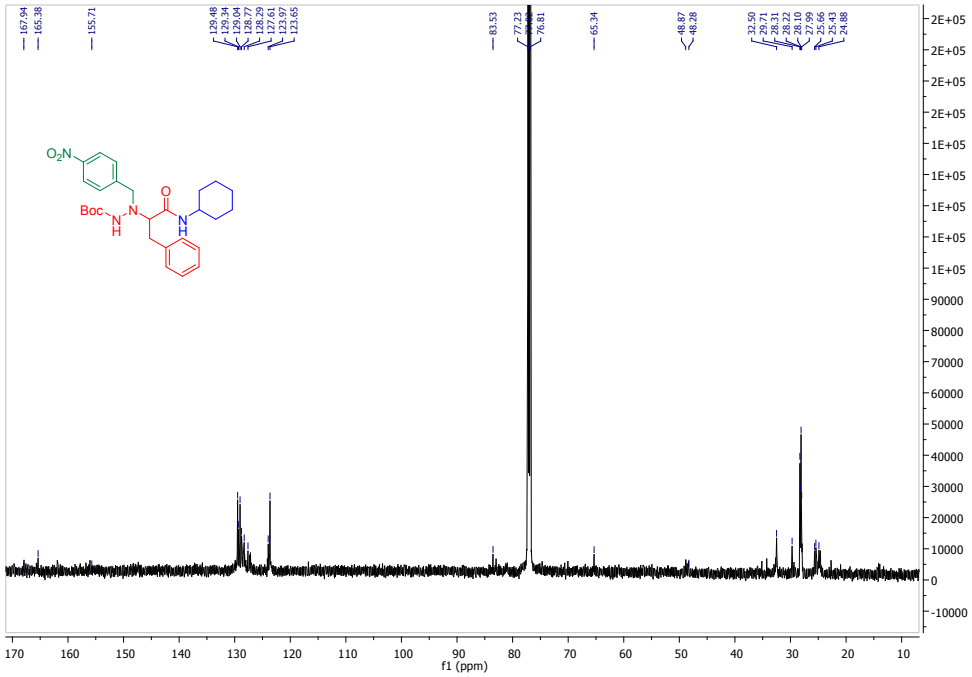

f1 (ppm)

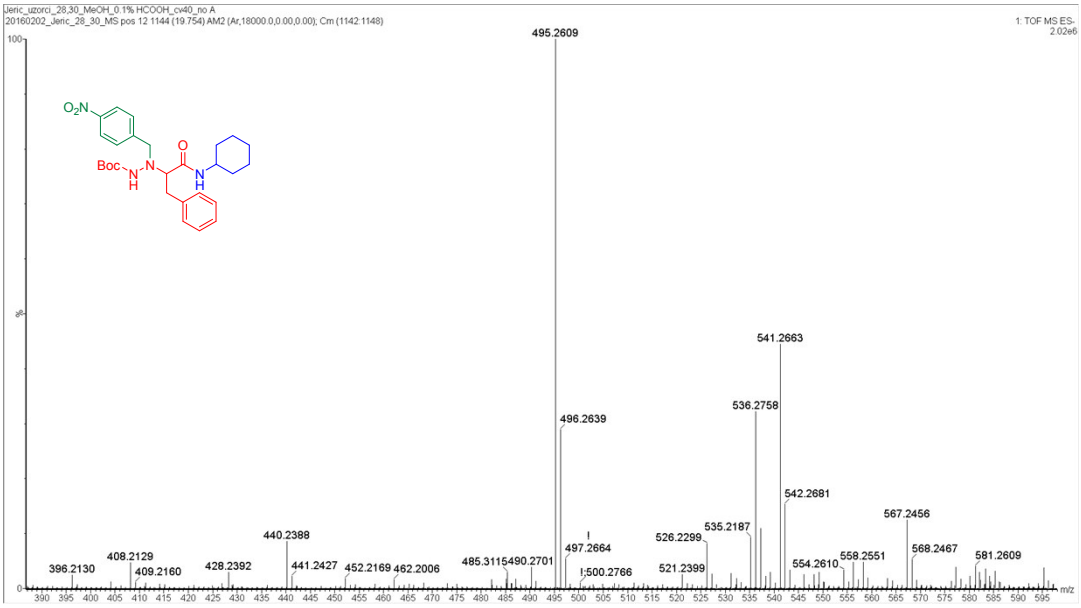

166.59
161.26
132.19
131.21
129.24
128.84
128.68
126.69
125.58
123.56
122.28
99.99
77.12
76.69
57.44
53.08
51.50
37.66
29.57
21.74
f1 (ppm)


Jeric_uzorci 2,9,27,29 u MeOH
20160202_Jeric E_MS pos 4 1086 (18.753) AM2 (Ar,18000.0,0.00,0.00); Cm (1086)
1: TOF MS ES+
503.1928
519.1392
556.2767
536.1655
473.1960
501.1767
504.1958
520.1400
521.1382
462.1470
537.1666
538.1640
557.2806
463.1474
474.1983
505.1045
505.2003
525.1747
464.1448
539.1629
550.2160
471.1872
475.1986
511.0736
526.1774
533.1935
541.1467
483.1664
542.1538
489.0559
496.0641
m/z

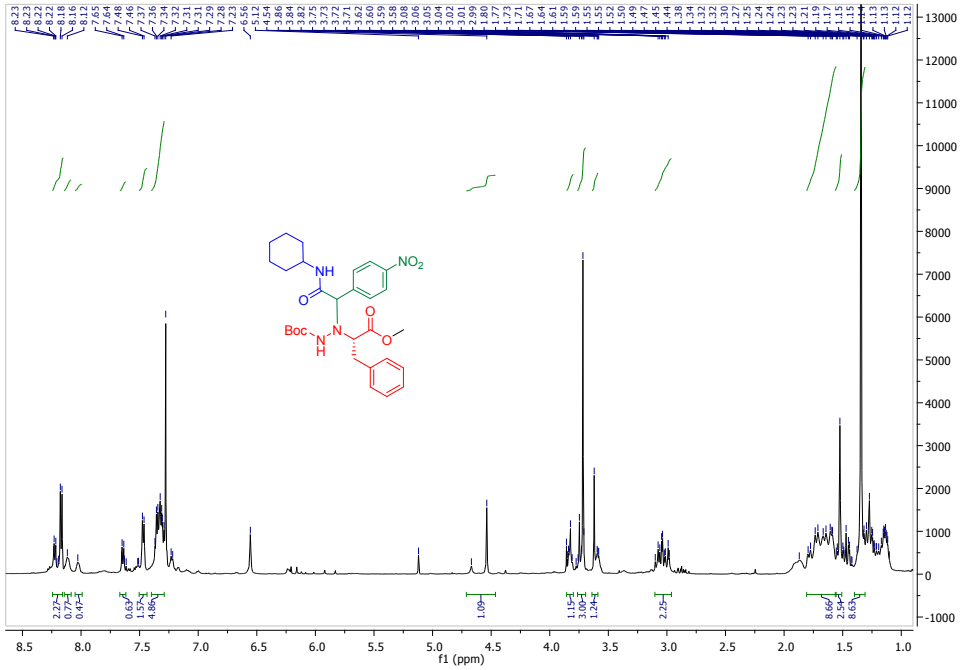
Compound **30**

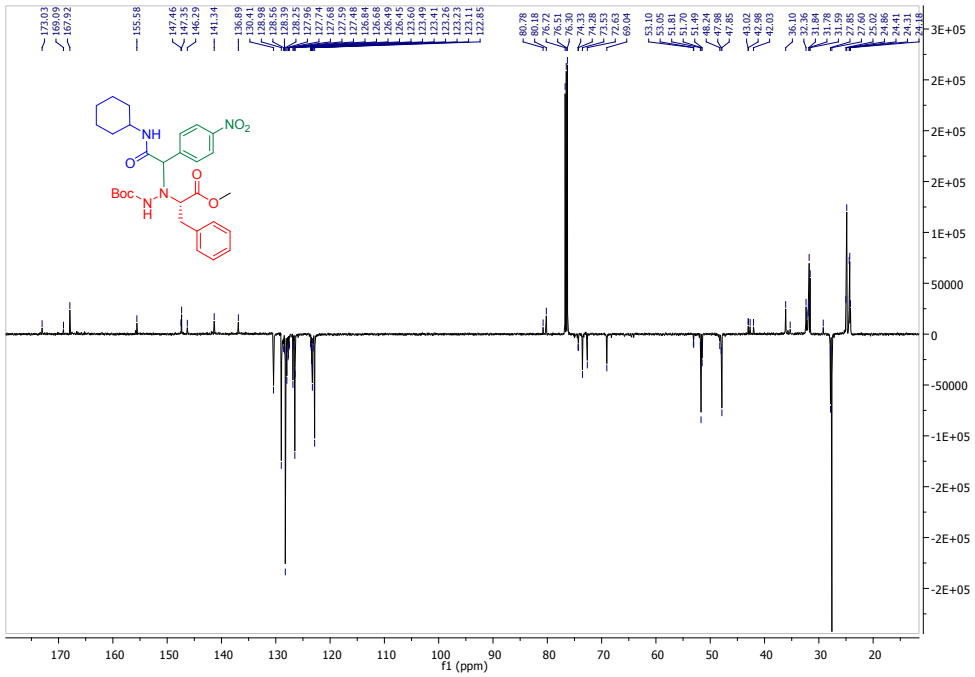


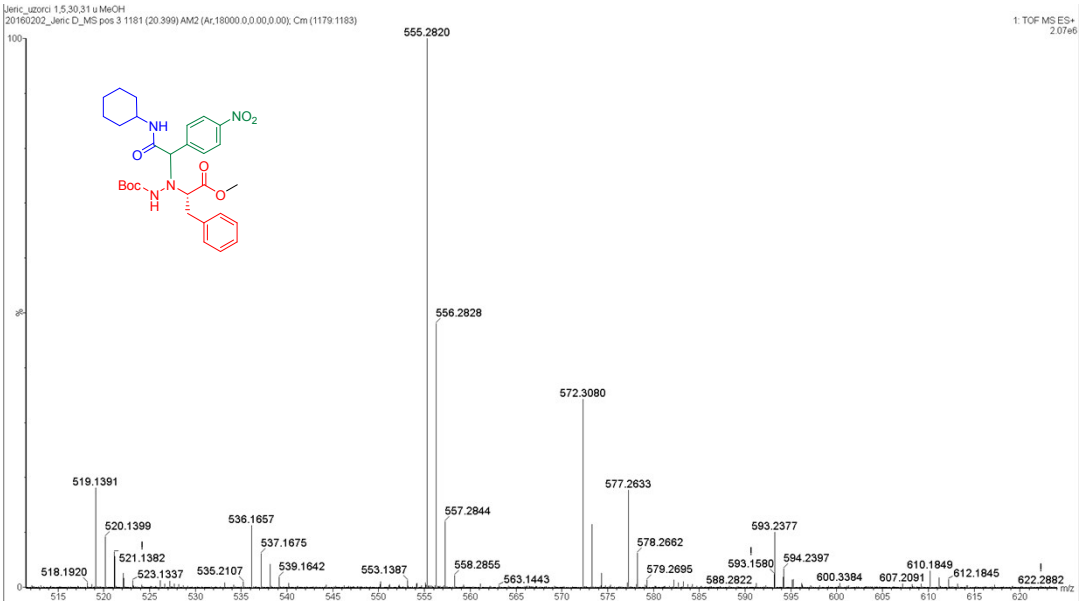



Jeric_uzorci_28.30_MeOH_0.1% HCOOH_cv40_no A
20160202_Jeric_28_30_MS pos 12 1144 (19.754) AM2 (Ar,18000.0,0.00,0.00); Cm (1142:1148)
1: TOF MS ES+
2.02e6
100
%
0
O2N
Boc
N
H
O
N
H
495.2609
541.2663
536.2758
496.2639
542.2681
567.2456
535.2187
526.2299
440.2388
497.2664
568.2467
581.2609
408.2129
396.2130
409.2160
428.2392
441.2427
452.2169
462.2006
485.3115
490.2701
500.2766
521.2399
554.2610
558.2551
390 395 400 405 410 415 420 425 430 435 440 445 450 455 460 465 470 475 480 485 490 495 500 505 510 515 520 525 530 535 540 545 550 555 560 565 570 575 580 585 590 595
m/z

Compound **31**


NH
O
NO2
Boc
N
H
O
O
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)


NO2
NH
O
Boc
N
H
O
O
f1 (ppm)


Jeric_uzorci 1,5,30,31 u MeOH
20160202_Jeric D_MS pos 3 1181 (20.399) AM2 (Ar,18000.0,0.00,0.00); Cm (1179:1183)
1: TOF MS ES+
2.07e6
555.2820
556.2828
572.3080
519.1391
577.2633
557.2844
536.1657
520.1399
593.2377
537.1675
578.2662
521.1382
539.1642
553.1387
558.2855
579.2695
594.2397
610.1849
518.1920
523.1337
535.2107
563.1443
593.1580
588.2822
600.3384
607.2091
612.1845
622.2882
m/z

Cartesian coordinates of minima and transition state for the rate-determining step of the reaction (in Angstroms)

Imidate-acid cluster, R^1 = benzyl

Atomic Number	X	Y	Z
6	-6.382391	2.243541	-0.633406
6	-6.159477	1.127014	0.181363
6	-6.485651	1.216479	1.538382
6	-7.007295	2.393152	2.073959
6	-7.212788	3.500980	1.254086
6	-6.903426	3.422136	-0.102948
6	-5.536861	-0.127253	-0.400079
7	-4.066873	-0.109599	-0.440595
7	-3.626963	0.913772	-1.276046
6	-2.511281	0.650686	-2.040061
8	-2.060301	1.783968	-2.590026
6	-0.834182	1.653349	-3.324204
6	-3.412660	-0.154771	0.882084
6	-3.836634	-1.399272	1.676325
6	-4.009741	-2.702250	0.917287
6	-4.907612	-3.643478	1.432869
6	-5.096135	-4.877563	0.814200
6	-4.386866	-5.185876	-0.344334
6	-3.496393	-4.251409	-0.870491
6	-3.304691	-3.017952	-0.249472
6	-1.884979	-0.107206	0.744725
8	-1.158290	-1.048368	1.006121
8	-1.444940	1.085509	0.388001
8	-2.009977	-0.442981	-2.194717
8	1.116521	0.921745	-0.377426
6	1.864252	0.610022	0.516697
8	1.476901	-1.921053	1.075146
6	1.593683	-1.676926	2.453875
6	1.863317	-0.211857	2.771412
8	1.401822	0.673743	1.793521
6	3.349735	0.328944	0.364427
6	4.101198	1.587759	0.847551
6	3.676086	2.914092	0.249897
6	3.681600	4.045548	1.073116
6	3.339415	5.299384	0.572602
6	2.978002	5.436508	-0.765983
6	2.960315	4.313678	-1.591164
6	3.306972	3.058361	-1.093633
7	2.322141	0.167196	3.874481
6	2.457142	1.579233	4.186171
7	3.648122	-0.032852	-1.014070
7	2.885412	-1.129879	-1.414527
6	2.019405	-0.968700	-2.469192
8	1.217542	-2.045561	-2.533086
6	0.337473	-2.087787	-3.660982
6	5.076891	-0.245129	-1.315505
6	5.775524	-1.265537	-0.437453
6	5.488401	-2.630828	-0.567190
6	6.090060	-3.566809	0.270866
6	6.998122	-3.155280	1.246110
6	7.308782	-1.803453	1.370259
6	6.699578	-0.868858	0.533451
8	2.016572	-0.047807	-3.255085
1	0.551597	-1.754420	0.814215

1	-0.472106	1.051229	0.188654
1	2.420536	-2.268541	2.853189
1	0.676143	-1.961843	2.982652
1	3.498384	1.774993	4.459688
1	1.849247	1.794413	5.069130
1	3.613939	-0.491700	1.055591
1	5.169466	1.424580	0.683342
1	3.979366	1.632330	1.935280
1	3.263002	2.187038	-1.741303
1	2.705689	6.410369	-1.161063
1	3.349959	6.164806	1.228056
1	3.960223	3.942513	2.120107
1	-3.672742	0.743522	1.472961
1	-2.945891	-4.477741	-1.778759
1	-5.799099	-5.591162	1.233351
1	-5.469520	-3.405524	2.334186
1	-2.627431	-2.298391	-0.696685
1	-4.774628	-1.180132	2.196277
1	-3.084865	-1.544040	2.459992
1	2.155925	2.247324	3.372190
1	-4.531503	-6.143178	-0.835726
1	2.669882	4.409031	-2.633054
1	5.101124	-0.552205	-2.363765
1	5.581573	0.724209	-1.254648
1	2.643593	-1.829582	-0.715169
1	-0.133591	-3.069109	-3.619145
1	-0.418585	-1.307428	-3.573266
1	0.907959	-1.972891	-4.585467
1	-3.680690	1.869048	-0.924925
1	-5.858361	-0.263246	-1.435949
1	-5.844909	-1.014282	0.159640
1	-0.585384	2.662139	-3.648919
1	-0.041976	1.247744	-2.691564
1	-0.978657	1.000545	-4.188043
1	-6.347282	0.350677	2.181745
1	-7.258746	2.441887	3.129046
1	-7.620679	4.417801	1.668013
1	-7.073953	4.276823	-0.750504
1	-6.150955	2.179212	-1.693950
1	6.964071	0.181992	0.627142
1	8.026876	-1.473872	2.114894
1	7.468164	-3.885646	1.897230
1	5.856373	-4.620795	0.155725
1	4.797445	-2.958530	-1.338393

Imidate-acid cluster, R^1 = Boc

Atomic Number	X	Y	Z
6	-1.975760	1.966993	-2.274005
6	-3.221335	1.354086	-2.117079
6	-4.266240	2.093900	-1.555563
6	-4.069945	3.409454	-1.142190
6	-2.823706	4.011770	-1.305895
6	-1.779740	3.286913	-1.878216
6	-3.466423	-0.066922	-2.564990
6	-3.219976	-1.159652	-1.501094
7	-3.837362	-0.848712	-0.191752
6	-5.214244	-0.734477	-0.165432
6	-1.735029	-1.498362	-1.395305
8	-0.912244	-1.074763	-2.184613

8	-1.453734	-2.382433	-0.453439
7	-3.194908	-0.987745	1.017425
6	-2.049822	-0.265029	1.266052
8	-1.489866	-0.722662	2.389223
6	-0.232638	-0.124841	2.744572
8	-1.621660	0.627742	0.568386
8	1.077204	-1.836105	0.173619
6	1.996601	-1.971886	-0.595614
8	1.718808	-0.654116	-2.868782
6	2.073617	-1.787489	-3.622640
6	2.601681	-2.895648	-2.733237
8	1.923517	-2.977120	-1.508183
6	3.334876	-1.277796	-0.466344
7	3.197906	0.169152	-0.295840
7	1.976276	0.787548	-0.453443
6	1.590215	1.682274	0.530108
8	0.688662	2.519872	0.008635
6	-0.035052	3.346938	0.923565
7	3.470714	-3.721370	-3.095360
6	3.895058	-4.798716	-2.219248
6	4.086310	-1.990560	0.698413
6	3.485242	-1.817449	2.069469
6	3.691868	-0.634477	2.783390
6	3.169564	-0.479020	4.065256
6	2.442798	-1.511658	4.654693
6	2.222501	-2.693409	3.948506
6	2.737890	-2.839643	2.662669
6	4.354530	0.922501	-0.378071
8	5.462902	0.421780	-0.352628
8	4.074158	2.222125	-0.473469
6	5.065197	3.220793	-0.075454
6	6.205798	3.261624	-1.085705
8	2.009141	1.697321	1.665092
6	4.254795	4.511021	-0.105188
6	5.540667	2.916792	1.342187
1	0.778655	-0.729429	-2.617667
1	-0.472720	-2.415658	-0.317977
1	2.856901	-1.522685	-4.335015
1	1.211258	-2.179127	-4.177691
1	4.946094	-4.635001	-1.962353
1	3.842169	-5.736269	-2.777442
1	3.923579	-1.455876	-1.373328
1	5.107127	-1.604828	0.678941
1	4.132402	-3.056166	0.439592
1	4.261621	0.172748	2.331894
1	2.044747	-1.394888	5.658529
1	1.652599	-3.500708	4.398449
1	2.564229	-3.763022	2.113724
1	-3.686120	-2.085449	-1.874273
1	-0.803544	3.744417	-2.010890
1	-4.893648	3.967990	-0.706525
1	-5.248190	1.636298	-1.459114
1	-1.154139	1.399177	-2.701034
1	-4.501243	-0.166750	-2.892640
1	-2.819407	-0.308952	-3.412013
1	3.304204	-4.887630	-1.302082
1	-2.669588	5.041481	-0.995341
1	3.332217	0.451451	4.600343
1	1.766175	1.072751	-1.405052
1	-0.141851	4.322181	0.447484
1	-1.016313	2.894130	1.078675
1	0.514738	3.437879	1.861486
1	-3.195494	-1.920603	1.413775

1	-0.013815	-0.488412	3.746193
1	0.546554	-0.444163	2.048636
1	-0.313783	0.963066	2.736606
1	6.127947	3.761745	1.713798
1	4.673071	2.777647	1.996430
1	6.164216	2.020966	1.370246
1	6.869575	4.097076	-0.842542
1	6.778947	2.333991	-1.068309
1	5.808789	3.418987	-2.093048
1	4.891256	5.357841	0.165775
1	3.848776	4.681073	-1.106293
1	3.424391	4.448633	0.604430
8	-5.670902	-0.461821	1.056772
8	-5.892071	-0.880500	-1.166207
6	-7.094070	-0.206348	1.266179
6	-7.155659	0.102037	2.757871
6	-7.534009	1.006360	0.450279
6	-7.911500	-1.453365	0.941217
1	-8.545669	1.293336	0.752880
1	-6.864594	1.850150	0.647055
1	-7.536900	0.787973	-0.618631
1	-8.187336	0.317909	3.049121
1	-6.797607	-0.752531	3.338507
1	-6.532802	0.968926	2.993835
1	-8.946414	-1.294020	1.259357
1	-7.899902	-1.670580	-0.126992
1	-7.515210	-2.314018	1.489113

Transition state, R^1 = benzyl

Atomic Number	X	Y	Z
6	6.083932	-2.035029	-0.068418
6	5.845686	-0.701467	0.286034
6	6.432503	-0.207220	1.455139
6	7.223552	-1.024887	2.261006
6	7.441108	-2.353949	1.904147
6	6.873326	-2.856665	0.734120
6	4.936025	0.163824	-0.564368
7	3.502772	0.001951	-0.276525
7	3.093935	-1.290422	-0.588933
6	1.850056	-1.426741	-1.173303
8	1.515506	-2.715077	-1.226151
6	0.216571	-2.991016	-1.784411
6	3.082638	0.480556	1.054091
6	3.426487	1.963663	1.249876
6	3.224379	2.912821	0.080462
6	3.972816	4.095550	0.077935
6	3.816638	5.050608	-0.924221
6	2.901079	4.831643	-1.950972
6	2.159580	3.651748	-1.964207
6	2.318017	2.692921	-0.963833
6	1.583915	0.234534	1.245230
8	0.799419	1.210292	1.233168
8	1.231145	-0.974772	1.454384
8	1.172217	-0.509099	-1.587343
8	-1.025094	-1.321297	0.738075
6	-1.997465	-0.665949	1.191059
8	-1.600729	1.000883	1.261283
6	-2.166133	1.525864	2.451665
6	-2.636483	0.309198	3.224231

8	-2.240395	-0.830761	2.577946
6	-3.310459	-0.608602	0.423723
6	-4.035229	-1.969817	0.476171
6	-3.366175	-3.124123	-0.231665
6	-2.803787	-4.170019	0.504426
6	-2.262101	-5.283632	-0.135361
6	-2.274034	-5.360353	-1.526843
6	-2.804695	-4.307305	-2.271061
6	-3.347839	-3.196800	-1.628768
7	-3.256975	0.358970	4.312948
6	-3.650923	-0.879406	4.965950
7	-3.192654	-0.135846	-0.958617
7	-1.991616	0.439192	-1.337844
6	-1.491774	0.131906	-2.577489
8	-0.643781	1.107099	-2.961205
6	0.128880	0.799165	-4.120623
6	-4.354035	0.665189	-1.389573
6	-4.479542	1.991257	-0.670064
6	-3.686990	3.086215	-1.038319
6	-3.728855	4.272244	-0.306513
6	-4.578604	4.388222	0.793494
6	-5.394354	3.316326	1.152614
6	-5.341395	2.128503	0.424370
8	-1.782550	-0.834034	-3.248158
1	-0.488664	1.060095	1.249284
1	0.129047	-1.164876	1.233120
1	-3.000251	2.190139	2.206501
1	-1.408954	2.070353	3.023466
1	-4.645469	-0.744858	5.396046
1	-2.960648	-1.080668	5.791222
1	-3.932116	0.094858	0.999665
1	-5.028322	-1.812077	0.038371
1	-4.198073	-2.222143	1.530066
1	-3.734853	-2.369318	-2.214879
1	-1.859421	-6.230112	-2.028481
1	-1.836020	-6.090877	0.452872
1	-2.795332	-4.113348	1.590732
1	3.574887	-0.105469	1.852459
1	1.443744	3.467212	-2.759711
1	4.410287	5.959514	-0.902502
1	4.689688	4.273440	0.877523
1	1.747339	1.772000	-1.023142
1	4.469470	2.037935	1.573271
1	2.827461	2.318710	2.096109
1	-3.653035	-1.745229	4.295309
1	2.771288	5.570845	-2.735565
1	-2.794296	-4.343571	-3.356307
1	-4.248818	0.806546	-2.469885
1	-5.252903	0.060784	-1.224090
1	-1.734398	1.341490	-0.950168
1	0.706255	1.696803	-4.338352
1	0.797268	-0.035382	-3.900922
1	-0.525506	0.549582	-4.958359
1	3.342066	-2.038298	0.057144
1	5.052738	-0.088263	-1.621474
1	5.183188	1.222702	-0.448898
1	0.138889	-4.075490	-1.792046
1	-0.563548	-2.551692	-1.157930
1	0.140002	-2.583642	-2.794626
1	6.284505	0.834269	1.730190
1	7.673104	-0.622197	3.163496
1	8.058221	-2.991950	2.528984
1	7.050944	-3.887369	0.442741

1	5.653344	-2.424217	-0.987877
1	-5.985353	1.296897	0.704024
1	-6.070212	3.402874	1.997852
1	-4.613796	5.313618	1.359770
1	-3.104553	5.109852	-0.601756
1	-3.041218	3.013881	-1.910822

Transition state, R^1 = Boc

Atomic Number	X	Y	Z
6	-4.189182	2.243907	-1.434548
6	-3.165821	1.562896	-2.100951
6	-1.952639	2.220670	-2.315309
6	-1.760989	3.523362	-1.864191
6	-2.779963	4.186993	-1.182971
6	-3.997187	3.542376	-0.969013
6	-3.393399	0.152155	-2.585667
6	-3.118415	-0.965224	-1.554223
7	-3.764600	-0.723938	-0.244911
7	-3.119524	-0.827026	0.967185
6	-2.007411	-0.049971	1.206169
8	-1.624687	0.855137	0.497570
6	-1.633654	-1.277167	-1.410088
8	-1.303883	-2.129866	-0.516859
8	-0.830453	-0.767502	-2.224235
6	-5.144514	-0.679221	-0.230101
8	-5.803735	-0.829923	-1.242864
8	-5.625570	-0.463440	0.993794
6	-7.062704	-0.290946	1.195465
6	-7.156151	-0.044235	2.696789
6	-7.554056	0.928264	0.420048
6	-7.810037	-1.565022	0.812051
8	-1.421920	-0.471038	2.329115
6	-0.175936	0.164486	2.656979
8	0.961104	-1.737796	0.137040
6	1.911140	-1.943001	-0.662270
8	1.537319	-1.231282	-2.200227
6	1.880373	-2.173986	-3.202479
6	2.324612	-3.410372	-2.448172
8	2.030767	-3.270205	-1.116121
6	3.279789	-1.336640	-0.386186
7	3.235491	0.129582	-0.346192
7	2.047091	0.815729	-0.448551
6	1.755339	1.781082	0.496507
8	2.246819	1.858405	1.598914
7	2.835639	-4.419800	-2.984295
6	3.211984	-5.558609	-2.161539
6	3.910629	-1.994368	0.862898
6	3.250084	-1.735430	2.193929
6	3.547644	-0.577327	2.915573
6	3.010790	-0.373675	4.185859
6	2.176516	-1.334014	4.753898
6	1.854933	-2.484435	4.033053
6	2.386034	-2.678054	2.760741
6	4.433720	0.800877	-0.494351
8	5.505508	0.226520	-0.465110
8	4.236323	2.108571	-0.668463
6	5.307562	3.059319	-0.370958
6	4.589612	4.400059	-0.465137
6	5.814443	2.818134	1.047641

6	6.409949	2.949044	-1.418178
8	0.838024	2.604847	-0.024501
6	0.162242	3.489497	0.872489
1	0.444026	-1.026764	-2.175238
1	-0.195707	-2.059036	-0.225295
1	2.687591	-1.788548	-3.828660
1	1.008438	-2.405300	-3.822415
1	2.462570	-6.346161	-2.286231
1	3.295099	-5.318484	-1.096473
1	3.927693	-1.611034	-1.229579
1	4.945733	-1.646121	0.892015
1	3.936573	-3.072266	0.665549
1	4.207513	0.168706	2.481208
1	1.769943	-1.184261	5.750036
1	1.194300	-3.231241	4.463063
1	2.134942	-3.574738	2.198667
1	-3.549358	-1.892119	-1.964703
1	-0.808467	4.015781	-2.039029
1	-4.802216	4.055258	-0.450519
1	-5.151110	1.755620	-1.293405
1	-1.149810	1.697960	-2.826823
1	-4.431499	0.040891	-2.900577
1	-2.756407	-0.056561	-3.448960
1	4.163693	-5.949640	-2.526090
1	-2.630205	5.202545	-0.827244
1	3.251565	0.533729	4.731075
1	1.747716	1.040387	-1.391128
1	0.111036	4.462488	0.381922
1	-0.843877	3.093660	1.028744
1	0.714812	3.566200	1.810250
1	-3.062423	-1.762408	1.354071
1	0.025113	-0.105055	3.690605
1	0.617220	-0.217431	2.008747
1	-0.265027	1.246408	2.551718
1	6.482514	3.635727	1.334159
1	4.967677	2.797051	1.741628
1	6.364586	1.877783	1.118611
1	7.141961	3.746410	-1.256556
1	6.914450	1.984305	-1.354057
1	5.987895	3.068032	-2.420690
1	5.293797	5.213585	-0.270029
1	4.164765	4.534641	-1.463904
1	3.780355	4.446573	0.269786
1	-8.589277	1.140637	0.704028
1	-6.943601	1.801374	0.672651
1	-7.514984	0.758105	-0.657015
1	-8.199999	0.112369	2.982340
1	-6.765105	-0.903248	3.248954
1	-6.576969	0.840548	2.973965
1	-8.854464	-1.473927	1.125856
1	-7.776197	-1.737554	-0.263903
1	-7.372496	-2.424671	1.329257

Dioxolan-acid cluster, R^1 = benzyl

Atomic Number	X	Y	Z
6	6.071049	-2.170875	0.064358
6	5.859331	-0.816492	0.349590
6	6.481339	-0.266928	1.474989
6	7.281430	-1.050135	2.305745

6	7.472411	-2.400065	2.018270
6	6.869054	-2.958236	0.892084
6	4.941880	0.012511	-0.527690
7	3.513909	-0.102634	-0.194112
7	3.076169	-1.408313	-0.386247
6	1.831368	-1.572428	-0.957008
8	1.491845	-2.861663	-0.944302
6	0.221603	-3.169524	-1.548507
6	3.133575	0.469838	1.108162
6	3.510643	1.955007	1.213616
6	3.326867	2.858677	0.004802
6	4.085587	4.035132	-0.021638
6	3.945361	4.967344	-1.046461
6	3.031723	4.733331	-2.071552
6	2.281425	3.559263	-2.062057
6	2.428404	2.618185	-1.042161
6	1.641203	0.229338	1.342103
8	0.877027	1.281358	1.124078
8	1.213375	-0.844970	1.733073
8	1.159825	-0.675740	-1.422125
8	-1.316713	-1.420601	0.773759
6	-2.265274	-0.574919	1.197754
8	-1.737411	0.747840	1.395596
6	-2.398725	1.354117	2.502518
6	-2.964768	0.171832	3.254626
8	-2.734866	-0.946131	2.504047
6	-3.473698	-0.518503	0.260164
6	-4.231615	-1.854944	0.154939
6	-3.532975	-3.009216	-0.524869
6	-3.137459	-4.125519	0.217891
6	-2.579977	-5.239127	-0.407139
6	-2.403799	-5.244996	-1.790272
6	-2.766738	-4.123823	-2.535572
6	-3.331991	-3.014461	-1.908712
7	-3.536942	0.221122	4.370227
6	-4.040921	-1.011907	4.956357
7	-3.190274	0.042447	-1.067422
7	-1.900039	0.477226	-1.321126
6	-1.352658	0.184377	-2.546970
8	-0.384741	1.079309	-2.826376
6	0.432787	0.725034	-3.941723
6	-4.211689	1.000912	-1.524966
6	-4.257344	2.280541	-0.716290
6	-3.293588	3.281047	-0.901898
6	-3.273603	4.410062	-0.084413
6	-4.232901	4.569045	0.916023
6	-5.218798	3.598653	1.087899
6	-5.225537	2.463003	0.278186
8	-1.693580	-0.711299	-3.286756
1	-0.074719	1.031358	1.221954
1	-0.494765	-1.320838	1.301381
1	-3.185985	2.034383	2.157906
1	-1.669933	1.902199	3.102852
1	-4.999006	-0.803365	5.437141
1	-3.348054	-1.345406	5.735456
1	-4.154487	0.168968	0.787071
1	-5.157848	-1.637401	-0.391624
1	-4.529404	-2.148483	1.167238
1	-3.589945	-2.137641	-2.493209
1	-1.975197	-6.113656	-2.282140
1	-2.288068	-6.101581	0.184719
1	-3.273436	-4.121718	1.297034
1	3.630643	-0.073541	1.931767

1	1.561792	3.371158	-2.853360
1	4.546482	5.871502	-1.041619
1	4.796072	4.227238	0.780326
1	1.847927	1.701457	-1.078750
1	4.557789	2.018285	1.526042
1	2.933532	2.371426	2.047940
1	-4.164393	-1.822408	4.230153
1	2.908480	5.457007	-2.871448
1	-2.611297	-4.106112	-3.610306
1	-3.997621	1.204968	-2.578899
1	-5.181732	0.493002	-1.480195
1	-1.570038	1.326394	-0.872409
1	1.238690	1.457489	-3.964346
1	0.842497	-0.275100	-3.795675
1	-0.150030	0.761150	-4.865048
1	3.338470	-2.113042	0.301346
1	5.026889	-0.305071	-1.570170
1	5.208676	1.071924	-0.482662
1	0.162886	-4.255119	-1.541520
1	-0.594421	-2.735590	-0.966398
1	0.181999	-2.781603	-2.568881
1	6.354788	0.790391	1.695161
1	7.759370	-0.604360	3.172655
1	8.096385	-3.011928	2.662086
1	7.025683	-4.005899	0.654299
1	5.611939	-2.604186	-0.820895
1	-5.998952	1.709776	0.414866
1	-5.979368	3.722768	1.852538
1	-4.220573	5.451605	1.547712
1	-2.515020	5.171516	-0.236936
1	-2.562454	3.183385	-1.701409

Dioxolan-acid cluster, R^1 = Boc

Atomic Number	X	Y	Z
6	-4.244853	2.289429	-1.331459
6	-3.239892	1.658094	-2.070353
6	-2.041119	2.339929	-2.288979
6	-1.845179	3.617265	-1.771857
6	-2.844573	4.229965	-1.018257
6	-4.047496	3.561229	-0.799033
6	-3.481742	0.282305	-2.641929
6	-3.212252	-0.918117	-1.705954
7	-3.803618	-0.773987	-0.358025
7	-3.102059	-0.991044	0.803809
6	-2.020573	-0.185337	1.091519
8	-1.714503	0.809821	0.473502
6	-1.747081	-1.316855	-1.584281
8	-1.390320	-2.269372	-0.908011
8	-0.918219	-0.606926	-2.324913
6	-5.180035	-0.698741	-0.281726
8	-5.879425	-0.744938	-1.277614
8	-5.605218	-0.572803	0.973790
6	-7.028252	-0.388139	1.251986

6	-7.050882	-0.253663	2.770065
6	-7.526357	0.894647	0.591994
6	-7.818001	-1.615731	0.807576
8	-1.372191	-0.688716	2.144072
6	-0.169002	0.001085	2.520587
8	1.117869	-1.873103	0.161252
6	2.087437	-1.970268	-0.762847
8	1.656566	-1.433116	-2.026461
6	2.210732	-2.221003	-3.076288
6	2.555478	-3.522770	-2.392292
8	2.372544	-3.342597	-1.048441
6	3.387119	-1.292945	-0.316573
7	3.259162	0.170105	-0.317429
7	2.028097	0.784500	-0.378452
6	1.733481	1.775688	0.542909
8	2.270938	1.920361	1.616484
7	2.936330	-4.569258	-2.965957
6	3.255384	-5.744269	-2.169284
6	3.982947	-1.896619	0.969727
6	3.288081	-1.638498	2.284646
6	3.513342	-0.447004	2.976842
6	2.964518	-0.244510	4.242736
6	2.197919	-1.242859	4.839915
6	1.952572	-2.430919	4.150174
6	2.488526	-2.620252	2.879169
6	4.414266	0.906124	-0.496345
8	5.517503	0.395716	-0.455658
8	4.139032	2.192827	-0.715013
6	5.155746	3.215384	-0.466585
6	4.356079	4.506907	-0.585652
6	5.704846	3.051606	0.947641
6	6.242087	3.137312	-1.532978
8	0.747477	2.525754	0.040470
6	0.070858	3.412505	0.936152
1	0.004163	-0.928026	-2.179684
1	0.281071	-2.254584	-0.179853
1	3.102832	-1.742170	-3.494276
1	1.464230	-2.362348	-3.859593
1	2.474137	-6.494793	-2.321665
1	3.344256	-5.538875	-1.097687
1	4.114208	-1.524161	-1.106763
1	5.004382	-1.509738	1.025643
1	4.057234	-2.975975	0.798727
1	4.123557	0.327971	2.521432
1	1.786279	-1.094878	5.834150
1	1.347588	-3.210323	4.603865
1	2.296087	-3.545312	2.340923
1	-3.684716	-1.793719	-2.176194
1	-0.904486	4.129681	-1.953211
1	-4.838706	4.035912	-0.225781
1	-5.198221	1.785705	-1.188972
1	-1.252729	1.859866	-2.860693
1	-4.525967	0.203175	-2.948304
1	-2.864702	0.131075	-3.532401
1	4.191991	-6.168107	-2.538118
1	-2.691458	5.225502	-0.611073
1	3.147120	0.691049	4.762497
1	1.675446	0.965669	-1.312204
1	0.051068	4.397037	0.465829
1	-0.945541	3.032201	1.057231
1	0.602094	3.459825	1.887855
1	-2.999323	-1.959707	1.084906
1	0.087319	-0.376468	3.506951

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1        0.628140   -0.237534    1.813480
1       -0.346051    1.077540    2.551977
1        6.315052    3.924553    1.197682
1        4.875128    2.988532    1.659258
1        6.324726    2.157323    1.034045
1        6.936399    3.973265   -1.402681
1        6.795345    2.200359   -1.457757
1        5.796502    3.213236   -2.529585
1        5.013658    5.366931   -0.431105
1        3.903445    4.584719   -1.578283
1        3.561555    4.528069    0.166369
1       -8.542463    1.104779    0.939426
1       -6.885598    1.734919    0.878677
1       -7.539661    0.803884   -0.495241
1       -8.078799   -0.110716    3.114402
1       -6.644790   -1.154769    3.237643
1       -6.449879    0.603518    3.085045
1       -8.850398   -1.521558    1.158001
1       -7.820049   -1.715250   -0.278214
1       -7.388049   -2.518613    1.252214
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Table S1. Energies (*E,* in a.u.), number of imaginary frequencies (NImag) and zero point vibrational energies (*ZPE,* in a.u.), obtained at M06-2X/6-31+G(d,p) level of theory, for stationary points of the rate-determining step of the reaction.

Stationary point	*E*	NImag	*ZPE*
Imidate cluster R^1=benzyl	–2463.132550	0	0.811167
Imidate cluster R^1=Boc	–2614.029636	0	0.846435
Transition state R^1=benzyl	–2463.114539	1	0.806555
Transition state R^1=Boc	–2614.0120882	1	0.841466
Dioxolan cluster R^1=benzyl	–2463.1393237	0	0.812941
Dioxolan cluster R^1=Boc	–2614.038251	0	0.848135

Cartesian coordinates of non-productive conformers of imidate cluster (in Angstroms)

Non-productive conformer 1 of imidate-acid cluster, R^1 = benzyl

Atomic Number	X	Y	Z
6	2.956902	2.451691	-2.250715
6	3.629406	2.640129	-1.038247
6	4.172230	3.900781	-0.759800
6	4.063388	4.948017	-1.669743
6	3.398360	4.749859	-2.879296
6	2.845429	3.503714	-3.160808
6	3.849009	1.543346	-0.013847
6	2.908501	0.325687	-0.013816
7	2.952807	-0.477088	-1.231509
7	2.251764	-1.666285	-1.045236
6	1.161326	-1.962515	-1.803470
8	0.658577	-3.137787	-1.400324
6	-0.541758	-3.558248	-2.046276
6	1.482662	0.837236	0.191074
8	1.158209	1.232235	1.463175
6	1.729449	0.649794	2.591671
6	1.361853	-0.809534	2.800159
8	1.119594	-1.492568	1.595543
8	0.702377	1.053793	-0.689683
7	2.365686	1.307228	3.452918
6	2.576562	2.735066	3.295220
6	4.279920	-0.723314	-1.821117
6	5.319325	-1.390757	-0.936293
6	5.142324	-2.692921	-0.449999
6	6.104102	-3.283423	0.367448
6	7.269565	-2.592242	0.696015
6	7.472474	-1.309645	0.192584
6	6.502539	-0.718150	-0.614734
8	0.735883	-1.316818	-2.749269
6	-1.687086	-0.279396	-0.743054
8	-1.542892	0.019199	-2.019961
6	-2.763987	0.557825	-0.060277
7	-3.891212	-0.325433	0.250480
6	-2.184067	1.257975	1.175985
6	-1.964857	0.479766	2.464682
6	-2.224718	-0.884472	2.649702
6	-2.044653	-1.469000	3.907349
6	-1.596848	-0.717329	4.990927
6	-1.309717	0.636441	4.809326
6	-1.492428	1.220427	3.559215
8	-1.035629	-1.131160	-0.167175
1	0.191457	-1.402725	1.313239
1	-0.732041	-0.427541	-2.370673
1	2.192746	-1.293798	3.318373
1	0.486481	-0.832991	3.458447
1	3.643950	2.944856	3.412323
1	2.059732	3.248460	4.111815
1	3.195481	-0.282589	0.860449
1	4.874504	1.169385	-0.085976
1	3.778089	1.980623	0.988807
1	2.497889	1.493049	-2.473371
1	3.306595	5.562994	-3.592735
1	4.492383	5.917078	-1.433196
1	4.687268	4.060811	0.185666
1	2.222760	3.141180	2.341272
1	2.315171	3.342264	-4.094337

1	4.085334	-1.334792	-2.706939
1	4.660514	0.239292	-2.178383
1	2.292870	-2.115995	-0.132519
1	-0.716050	-4.573475	-1.692206
1	-1.370874	-2.910996	-1.748409
1	-0.417393	-3.540377	-3.130837
1	6.674298	0.279083	-1.015487
1	8.384632	-0.769083	0.425747
1	8.019293	-3.055602	1.329655
1	5.947934	-4.291648	0.738815
1	4.258176	-3.256791	-0.730719
1	-3.057719	1.338712	-0.780824
1	-2.829134	2.111843	1.415541
1	-1.227058	1.693964	0.863394
1	-1.266421	2.276883	3.422891
1	-0.942117	1.235285	5.637228
1	-1.463363	-1.179788	5.964074
1	-2.260779	-2.526126	4.029866
1	-2.580410	-1.493706	1.826026
6	-5.061840	0.319789	0.862208
7	-4.232080	-1.111973	-0.836218
1	-4.501518	-0.693336	-1.722680
1	-5.727917	-0.492556	1.168051
1	-4.715751	0.820181	1.771971
6	-5.783154	1.286139	-0.053049
6	-5.462523	2.647368	-0.065690
6	-6.080370	3.518961	-0.960117
6	-7.032773	3.038427	-1.857306
6	-7.369706	1.685794	-1.848469
6	-6.750195	0.818330	-0.950604
1	-4.729400	3.032257	0.639304
1	-5.820099	4.572926	-0.955057
1	-7.514338	3.716162	-2.555189
1	-8.118571	1.306587	-2.536978
1	-7.023519	-0.234380	-0.935923
6	-4.096583	-2.469618	-0.750388
8	-4.404100	-3.021115	-1.946552
8	-3.767504	-3.098462	0.229055
6	-4.342569	-4.446382	-1.976068
1	-4.597956	-4.728665	-2.996106
1	-3.337930	-4.790288	-1.720671
1	-5.055031	-4.874020	-1.267530

Non-productive conformer 1 of imidate-acid cluster, R^1 = Boc

Atomic Number	X	Y	Z
6	3.871266	1.859661	-1.784650
6	3.948528	2.678748	-0.654640
6	4.236202	4.036485	-0.831182
6	4.451143	4.568420	-2.100127
6	4.368343	3.743692	-3.220102
6	4.074845	2.391512	-3.056420
6	3.758078	2.170428	0.759257
6	2.777349	1.001689	0.990735
7	3.259934	-0.360264	0.764335
6	4.557436	-0.737748	0.439873
8	5.397646	0.032676	0.028814
6	1.502303	1.212984	0.169582
8	0.688033	2.229483	0.585186

6	0.594219	2.610377	1.923840
7	0.861773	3.770387	2.324070
6	1.329852	4.785698	1.396212
8	1.241617	0.640305	-0.847619
6	-0.033765	1.564428	2.828697
8	0.256421	0.249144	2.424619
7	2.392636	-1.320468	1.227383
6	1.870456	-2.267555	0.411721
8	2.029277	-2.328474	-0.799166
8	1.192974	-3.161083	1.138479
6	0.436215	-4.114032	0.390696
8	4.716087	-2.050229	0.618429
6	5.815740	-2.748039	-0.047427
6	7.150712	-2.336089	0.563551
6	5.505283	-4.209146	0.255948
6	5.746277	-2.483919	-1.548650
6	-0.981289	-1.018734	-1.034988
8	-0.229080	-1.422092	-2.038043
6	-2.225936	-0.269372	-1.503613
6	-2.180873	1.159121	-0.922889
6	-2.682415	1.428167	0.482983
6	-2.833262	2.776212	0.844263
6	-3.339640	3.143284	2.088093
6	-3.709190	2.159302	3.007526
6	-3.541296	0.818723	2.670327
6	-3.024291	0.451278	1.424451
7	-3.383832	-1.106060	-1.148863
7	-3.159348	-2.469270	-1.184656
6	-3.401099	-3.184800	-0.018926
8	-3.477405	-2.727355	1.092876
6	-4.715214	-0.722732	-1.212159
8	-3.476242	-4.490567	-0.324032
6	-3.709220	-5.348562	0.795224
8	-0.713970	-1.188938	0.140087
1	-0.406457	-0.089523	1.797258
1	0.639055	-1.742952	-1.686868
1	0.358668	1.718442	3.836580
1	-1.112067	1.755787	2.848660
1	2.195508	5.286712	1.839239
1	0.543644	5.539622	1.289752
1	2.493721	1.051929	2.049339
1	4.723406	1.893696	1.189985
1	3.364704	2.993764	1.366850
1	3.640051	0.805048	-1.678324
1	4.527725	4.152945	-4.212976
1	4.676628	5.624527	-2.212855
1	4.295259	4.685606	0.040430
1	-2.158412	-0.181892	-2.594576
1	-3.813884	0.037568	3.373894
1	-3.447414	4.194545	2.338012
1	-2.553036	3.548717	0.129753
1	-2.911080	-0.602565	1.201450
1	-2.740867	1.810083	-1.598173
1	-1.129676	1.471117	-0.986435
1	1.592719	4.402752	0.404495
1	-4.113722	2.438508	3.975529
1	4.004221	1.741404	-3.923042
1	2.159389	-1.332722	2.213077
1	0.050692	-4.817677	1.126573
1	-0.388857	-3.611878	-0.121381
1	1.075767	-4.622785	-0.332986
1	-3.471907	-2.939124	-2.029510
1	-3.739689	-6.357384	0.387663

1	-2.902662	-5.247857	1.524356
1	-4.658476	-5.094954	1.271044
1	6.271930	-4.851420	-0.186272
1	5.485623	-4.378015	1.336325
1	4.531637	-4.482548	-0.161078
1	6.438812	-3.156467	-2.063755
1	4.731253	-2.681110	-1.908233
1	6.018232	-1.453705	-1.785024
1	7.942803	-2.968739	0.150933
1	7.378037	-1.292562	0.344059
1	7.127520	-2.479161	1.648266
8	-4.818890	0.576139	-1.492056
8	-5.623658	-1.507082	-1.040579
6	-6.086264	1.282812	-1.289723
6	-5.726660	2.717879	-1.654858
6	-7.153921	0.736581	-2.232806
6	-6.486810	1.183291	0.177756
1	-7.390204	1.778597	0.342981
1	-6.694229	0.149297	0.461389
1	-5.688020	1.579247	0.813931
1	-8.030414	1.390648	-2.193097
1	-6.778865	0.730425	-3.261019
1	-7.450451	-0.274797	-1.955117
1	-6.606887	3.357757	-1.546958
1	-4.941032	3.091289	-0.990958
1	-5.377947	2.773860	-2.690487

Non-productive conformer 2 of imidate-acid cluster, R^1 = benzyl

Atomic Number	X	Y	Z
6	-4.840582	-0.922764	-2.756825
6	-3.850051	-1.618611	-2.056745
6	-4.022130	-2.980341	-1.810040
6	-5.160274	-3.643727	-2.270444
6	-6.140878	-2.945352	-2.970744
6	-5.979840	-1.579836	-3.211856
6	-2.607878	-0.901000	-1.581595
7	-2.963737	0.305713	-0.826088
7	-3.802858	0.109858	0.276604
6	-3.864918	-1.032120	1.028367
8	-3.088101	-1.963402	1.048152
6	-1.914128	1.297529	-0.624546
6	-2.417694	2.741677	-0.815083
6	-3.632833	3.085929	0.010339
6	-4.909585	3.011671	-0.556052
6	-6.048861	3.243324	0.214121
6	-5.922655	3.562569	1.565141
6	-4.653151	3.660134	2.133726
6	-3.516969	3.426429	1.362284
6	-1.101617	1.135596	0.654441
8	-1.039575	-0.114414	1.059988
8	-0.508410	2.050935	1.204494
8	-4.982519	-0.976841	1.790999
6	-5.194268	-2.119428	2.615454
8	2.034128	3.128683	1.324395
6	2.630834	3.808638	0.251240
6	2.843925	2.942892	-0.970554
7	3.841032	3.093641	-1.722906
6	3.961941	2.441170	-3.012364
8	1.735540	2.142358	-1.216786

6	1.790168	0.801171	-1.490258
8	0.855307	0.320135	-2.072451
6	3.011993	0.011696	-0.993544
7	3.258396	0.206370	0.419057
7	2.153328	0.192967	1.239807
6	2.116696	-0.765955	2.226467
8	2.942045	-1.614079	2.450618
6	2.936553	-1.466797	-1.441994
6	2.170951	-2.418865	-0.547966
6	2.825703	-3.521983	0.003914
6	2.152036	-4.417142	0.833844
6	0.808655	-4.210647	1.137665
6	0.138749	-3.111478	0.595584
6	0.815202	-2.237905	-0.253115
6	4.466931	0.857221	0.918893
8	0.962245	-0.623014	2.935118
6	0.778297	-1.596563	3.971890
1	1.074287	3.059341	1.190161
1	3.607265	4.179495	0.569397
1	2.027894	4.673883	-0.058471
1	4.210564	3.207699	-3.750609
1	3.061505	1.912211	-3.348089
1	3.877660	0.439721	-1.510616
1	3.972176	-1.816534	-1.500071
1	2.525553	-1.490265	-2.457760
1	3.881856	-3.674515	-0.207323
1	0.283241	-4.901690	1.791105
1	-0.909098	-2.923774	0.824383
1	0.283547	-1.394183	-0.676781
1	4.804141	1.740432	-2.983120
1	2.682709	-5.265663	1.255234
1	1.732902	1.096795	1.459878
1	-0.211055	-1.402624	4.383279
1	0.837991	-2.599874	3.546036
1	1.546274	-1.471813	4.737076
1	-0.411965	-0.209879	1.809597
1	-1.167424	1.119967	-1.410390
1	-2.658291	2.856138	-1.876231
1	-1.589934	3.418722	-0.583501
1	-2.529271	3.493756	1.810366
1	-4.547265	3.917702	3.183255
1	-6.806984	3.741918	2.168588
1	-7.032443	3.174393	-0.240864
1	-5.008748	2.755366	-1.608524
1	-4.668288	0.635551	0.236689
1	-6.132580	-1.933377	3.135842
1	-5.265461	-3.022368	2.004905
1	-4.376289	-2.233697	3.330572
1	-2.029288	-0.550144	-2.443667
1	-1.977391	-1.586767	-1.004001
1	-3.265609	-3.513967	-1.240600
1	-5.282870	-4.704754	-2.074795
1	-7.029045	-3.459899	-3.324919
1	-6.742992	-1.030557	-3.755106
1	-4.709637	0.142421	-2.933833
1	4.504172	0.628101	1.989009
6	5.683932	0.284232	0.234957
1	4.452772	1.950791	0.810636
6	6.496493	1.075955	-0.576605
6	7.602095	0.517296	-1.222924
6	7.893922	-0.834368	-1.059806
6	7.079595	-1.630621	-0.249501
6	5.978032	-1.075187	0.393219

1	6.254641	2.129346	-0.707923
1	8.232219	1.138736	-1.852097
1	8.753042	-1.270228	-1.560521
1	7.307856	-2.684444	-0.119660
1	5.322888	-1.680829	1.018011

Non-productive conformer 2 of imidate-acid cluster, R^1 = Boc

Atomic Number	X	Y	Z
6	-4.180066	3.158865	-0.160528
6	-2.797260	3.086665	0.047640
6	-2.265469	3.653270	1.210818
6	-3.096819	4.265840	2.147180
6	-4.474523	4.317168	1.937835
6	-5.015672	3.764308	0.777479
6	-1.933467	2.330428	-0.930830
6	-1.775881	0.846812	-0.549986
7	-3.033161	0.224459	-0.160532
7	-3.416073	0.282418	1.159252
6	-3.691005	-0.916781	1.789628
8	-3.450885	-2.019768	1.363918
6	-0.711613	0.614743	0.510549
8	-0.696804	-0.619536	0.979012
8	0.089617	1.469118	0.840909
6	-3.913584	-0.167808	-1.144394
8	-3.598698	-0.211863	-2.318558
8	-5.108138	-0.469210	-0.628339
6	-6.080423	-1.219252	-1.419514
6	-5.455357	-2.529724	-1.889139
6	-7.189505	-1.484006	-0.408373
6	-6.587611	-0.362271	-2.574525
8	-4.264776	-0.656493	2.979077
6	-4.591250	-1.813343	3.748449
7	2.520837	-0.467923	0.482025
6	2.638195	-1.525543	1.356887
8	3.366443	-2.481718	1.266144
7	3.336963	-0.466337	-0.631577
6	4.719903	-0.380051	-0.532388
8	5.088840	-0.114585	0.716149
6	6.499351	-0.193846	1.098703
6	6.443666	0.064779	2.599173
6	2.711161	-0.333796	-1.934494
6	1.763106	0.870499	-1.962105
8	2.175353	2.032978	-1.370797
6	3.483322	2.376217	-1.028048
7	4.474904	2.450607	-1.793361
6	4.417076	2.165723	-3.212008
6	2.065060	-1.602330	-2.521839
6	0.944937	-2.260885	-1.747273
6	-0.400728	-1.994507	-2.026652
6	-1.412649	-2.622773	-1.303806
6	-1.099417	-3.531970	-0.296182
6	0.236103	-3.835693	-0.040658
6	1.248068	-3.214396	-0.772423
8	0.679540	0.854520	-2.475977
8	1.754632	-1.330515	2.367794
6	1.742773	-2.362196	3.360785
8	5.443053	-0.512437	-1.498618
6	7.028439	-1.594345	0.807816
6	7.292185	0.895865	0.384119

6	3.552977	2.895325	0.394445
8	2.672474	2.255448	1.283424
1	1.748330	2.421604	1.036316
1	4.569706	2.734671	0.756231
1	3.364800	3.977599	0.362812
1	4.898897	2.992693	-3.739016
1	3.402007	2.040269	-3.610576
1	3.538228	-0.086035	-2.606378
1	2.886867	-2.316302	-2.642045
1	1.712826	-1.337142	-3.523985
1	2.286212	-3.471359	-0.583509
1	-1.894970	-3.990439	0.282049
1	-2.449874	-2.391565	-1.523593
1	-0.657373	-1.290352	-2.814070
1	5.006421	1.264054	-3.408845
1	0.496744	-4.572434	0.715020
1	2.401810	0.450294	0.926887
1	1.030456	-2.032567	4.115080
1	1.423844	-3.304250	2.910433
1	2.737928	-2.478155	3.792745
1	8.017729	-1.704509	1.262272
1	6.357008	-2.341603	1.241392
1	7.113092	-1.770369	-0.265589
1	8.310742	0.915839	0.784187
1	7.333152	0.716116	-0.690498
1	6.834949	1.875007	0.556811
1	7.454734	0.058443	3.015469
1	5.985274	1.037393	2.801358
1	5.852724	-0.710875	3.094870
1	0.090996	-0.745527	1.545210
1	-1.415002	0.304877	-1.430415
1	-2.392131	2.354496	-1.924021
1	-0.934605	2.765579	-1.014275
1	-1.195494	3.591774	1.385578
1	-2.668247	4.698100	3.046287
1	-5.121733	4.789161	2.670478
1	-6.086074	3.807449	0.599923
1	-4.603817	2.731667	-1.067627
1	-3.988685	1.079197	1.427876
1	-8.003926	-2.037308	-0.883894
1	-6.803050	-2.073189	0.428457
1	-7.584275	-0.540210	-0.021443
1	-6.238979	-3.178455	-2.292001
1	-4.709329	-2.359035	-2.667200
1	-4.982494	-3.037220	-1.041557
1	-7.409203	-0.883163	-3.076010
1	-6.967500	0.591589	-2.194824
1	-5.794414	-0.170336	-3.297806
1	-5.044585	-1.436883	4.663807
1	-5.293485	-2.447367	3.202710
1	-3.689850	-2.387269	3.973110

Non-productive conformer 3 of imidate-acid cluster, R^1 = Boc

Atomic Number	X	Y	Z
6	3.259756	3.938574	1.987853
6	3.615149	2.609905	1.768679
6	4.250697	2.223746	0.583559
6	4.557699	3.208932	-0.359546
6	4.209763	4.540695	-0.139518
6	3.550867	4.909145	1.031264
6	4.649692	0.783472	0.337031
6	3.520282	-0.266205	0.244448
6	2.614082	-0.302282	1.462384
8	1.439685	-0.037027	1.478141
7	2.695660	-0.160897	-0.945534
7	2.103033	1.044540	-1.210876
6	2.587031	1.783292	-2.262290
8	1.793421	2.841593	-2.464103
6	2.232869	3.734151	-3.487011
6	2.356337	-1.234384	-1.740590
8	1.492253	-1.161743	-2.607239
8	3.075040	-2.305620	-1.447900
6	2.894172	-3.575952	-2.165407
6	1.483170	-4.107083	-1.946191
6	3.225339	-3.377033	-3.639851
6	3.918586	-4.474597	-1.484386
8	3.303494	-0.689645	2.564136
6	2.617496	-1.446908	3.520337
6	1.674889	-2.497900	2.955869
8	2.046527	-2.885858	1.653460
7	2.821996	-1.322874	4.749760
6	3.690113	-0.280133	5.263951
8	3.595233	1.530712	-2.883877
8	-0.559507	-0.228665	-1.157743
6	-0.722844	-1.039438	-0.132438
6	-1.672895	-0.491865	0.923681
8	-0.126532	-2.095354	-0.002178
1	1.314402	-2.692651	1.044651
1	1.716308	-3.349575	3.640267
1	0.660787	-2.085200	2.977907
1	4.045595	0.422306	4.503285
1	4.551878	-0.752675	5.743905
1	3.991572	-1.250260	0.214050
1	5.212623	0.713541	-0.598763
1	5.309124	0.449159	1.146225
1	5.060885	2.924067	-1.280123
1	3.274078	5.944726	1.202076
1	2.757908	4.215154	2.909926
1	3.402123	1.873741	2.539741
1	3.147458	0.266328	6.039200
1	4.455864	5.291803	-0.884758
1	1.164216	1.207612	-0.860434
1	1.480267	4.519296	-3.529968
1	3.209667	4.150959	-3.229353
1	2.302713	3.211696	-4.443086
1	1.406800	-5.094323	-2.412546
1	1.279339	-4.211405	-0.877159
1	0.733836	-3.447897	-2.385303
1	3.245259	-4.353737	-4.132779
1	2.482763	-2.747732	-4.131773
1	4.212229	-2.917239	-3.747119
1	3.873227	-5.477699	-1.917230
1	4.928270	-4.078036	-1.624208

1	3.707371	-4.539876	-0.413169
1	0.096439	-0.606267	-1.802613
7	-2.767076	0.249208	0.311737
6	-2.170787	-1.570729	1.906076
1	-1.071962	0.235572	1.483399
6	-3.369869	1.257513	1.034352
7	-3.338105	-0.245174	-0.838226
8	-4.486048	1.674142	0.432413
8	-2.914115	1.666874	2.084545
6	-5.104261	2.938054	0.824522
6	-6.197130	3.108287	-0.224161
6	-5.701668	2.812773	2.222199
6	-4.079712	4.063834	0.720256
1	-6.269224	3.719164	2.454669
1	-6.386410	1.959562	2.262154
1	-4.919926	2.681370	2.971173
1	-4.592130	5.025311	0.821320
1	-3.322178	3.984493	1.501197
1	-3.590865	4.027185	-0.258250
1	-6.758367	4.026592	-0.030527
1	-5.753342	3.168351	-1.222291
1	-6.888088	2.260794	-0.196030
1	-4.144796	-0.852071	-0.713959
6	-3.367339	0.593115	-1.939607
8	-4.155569	0.037281	-2.878937
8	-2.781086	1.639188	-2.057469
6	-4.249468	0.783005	-4.092286
1	-4.895753	0.198143	-4.744473
1	-4.683538	1.767046	-3.901780
1	-3.261019	0.906699	-4.538962
1	-2.482909	-1.054009	2.818645
6	-3.323628	-2.368400	1.350439
1	-1.333269	-2.227059	2.153493
6	-4.637566	-1.946528	1.582697
6	-5.714567	-2.608819	0.994232
6	-5.488316	-3.711115	0.170435
6	-4.183366	-4.149457	-0.052151
6	-3.108328	-3.481690	0.531937
1	-4.815521	-1.086290	2.225661
1	-6.727710	-2.265629	1.180998
1	-6.323855	-4.228077	-0.290911
1	-4.000563	-5.010196	-0.688240
1	-2.089967	-3.811275	0.343230

Table S2. Energies (*E,* in a.u.), number of imaginary frequencies (NImag) and zero point vibrational energies (*ZPE,* in a.u.), obtained at M06-2X/6-31+G(d,p) level of theory, for non-productive conformers of imidate cluster.

Conformer	*E*	NImag	*ZPE*
Non-productive 1 R^1=benzyl	–2463.1372861	0	0.811567
Non-productive 1 R^1=Boc	–2614.031873	0	0.846247
Non-productive 2 R^1=benzyl	–2463.1360802	0	0.810805
Non-productive 2 R^1=Boc	–2614.0497288	0	0.847305
Non-productive 3 R^1=Boc	–2614.0525049	0	0.845971