

Supporting Information

Thiazolidinedione-Based Structure Modification of Lupeol Provides Thiazolidinedione-Conjugated Derivatives as Potent Agents against Hepatocarcinoma Cells through a Mitochondria-Mediated Apoptotic Pathway

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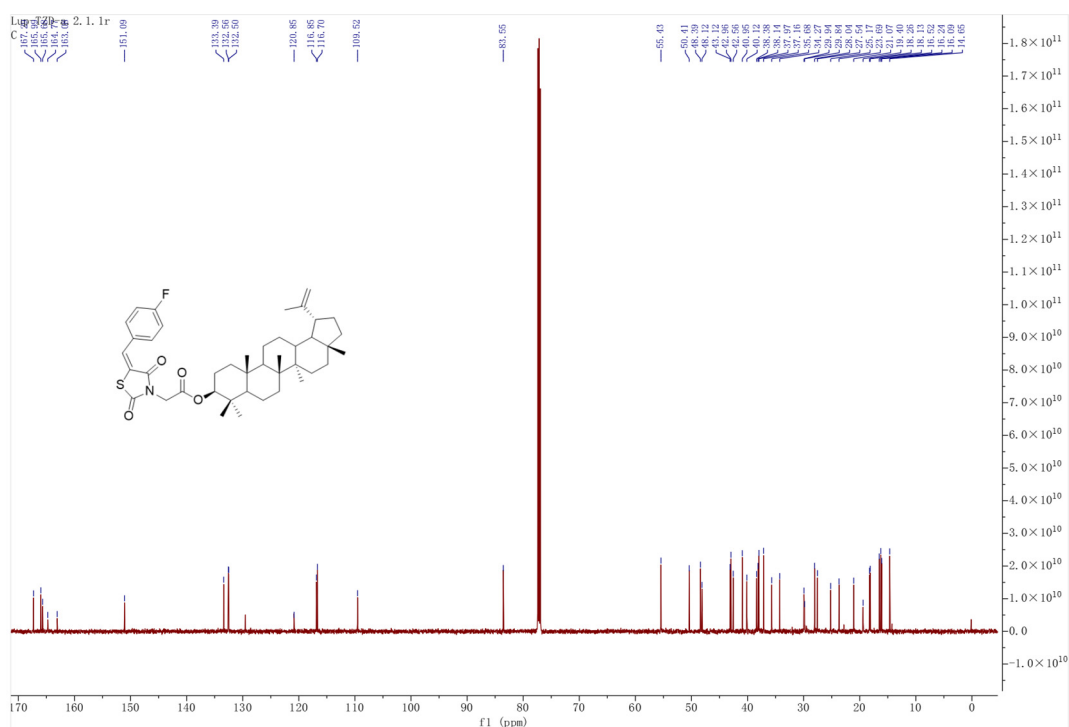
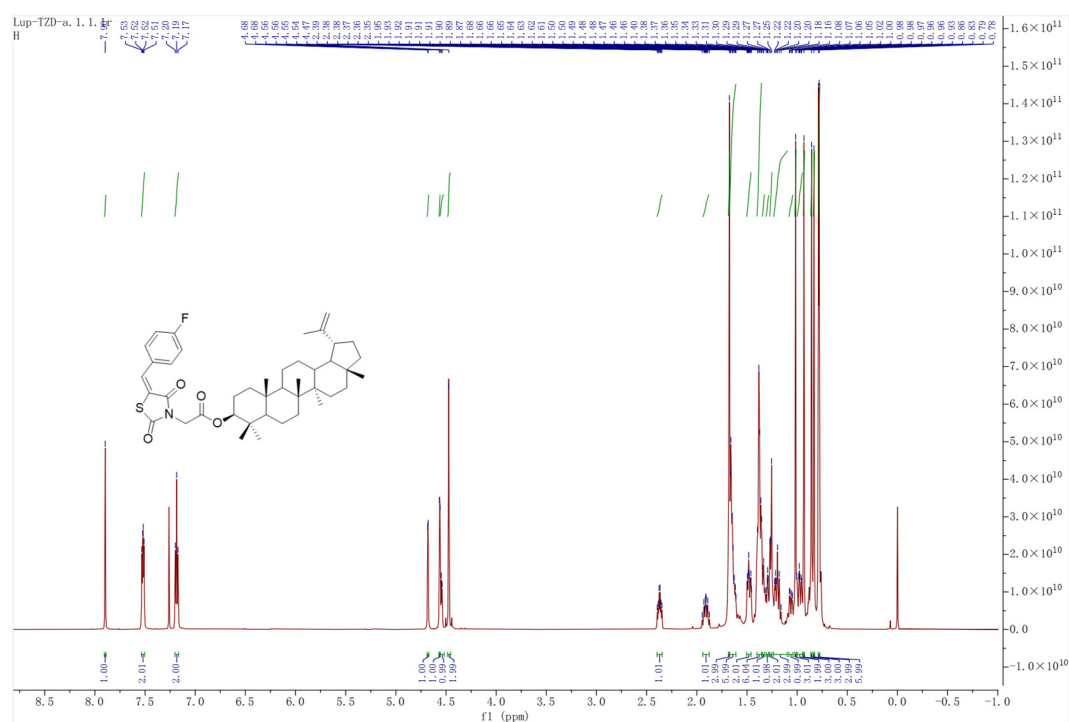
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** Corresponding author.*

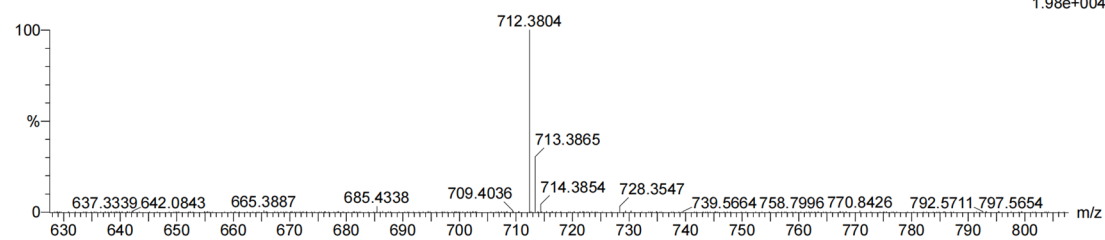
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¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6a

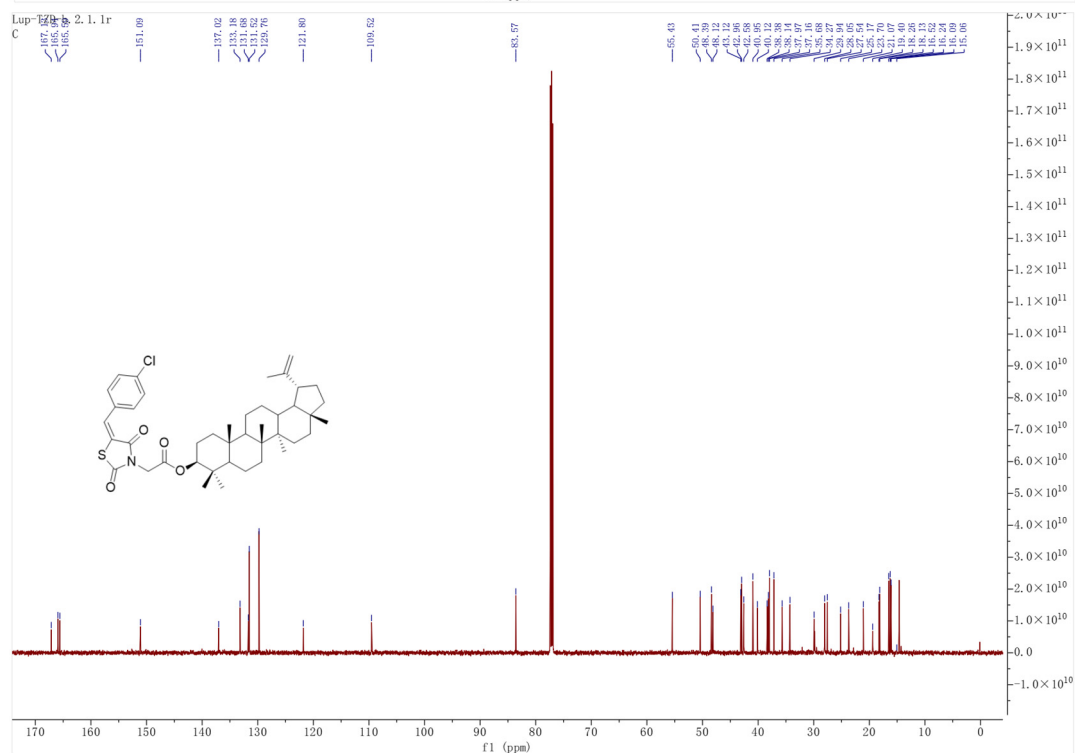
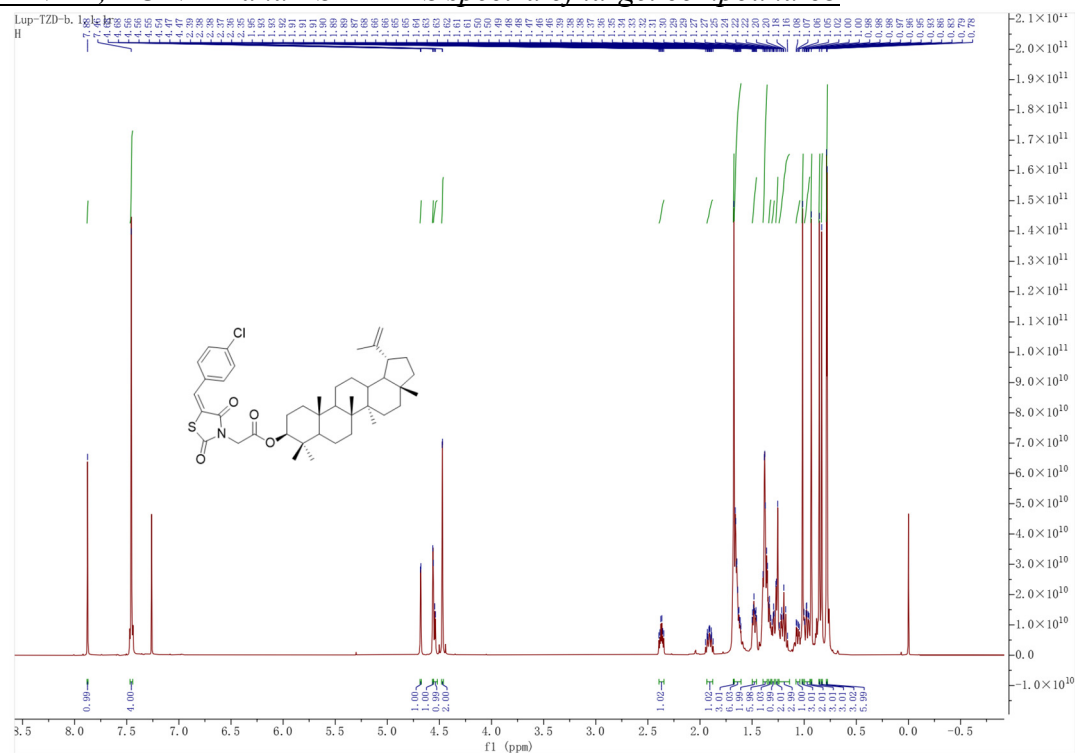


15
240120-13-EP-TZD-A 46 (0.221)

1: TOF MS ES+
1.98e+004

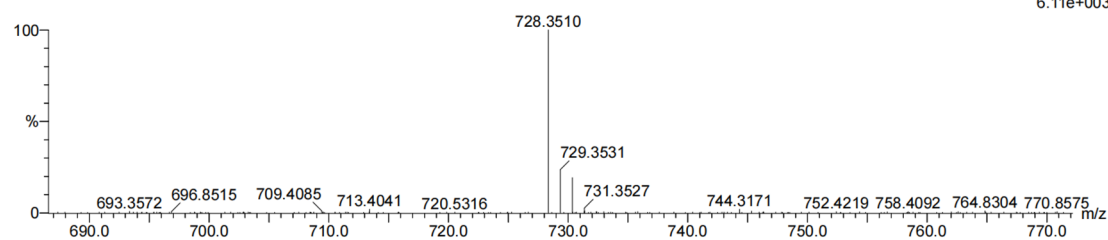


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6b

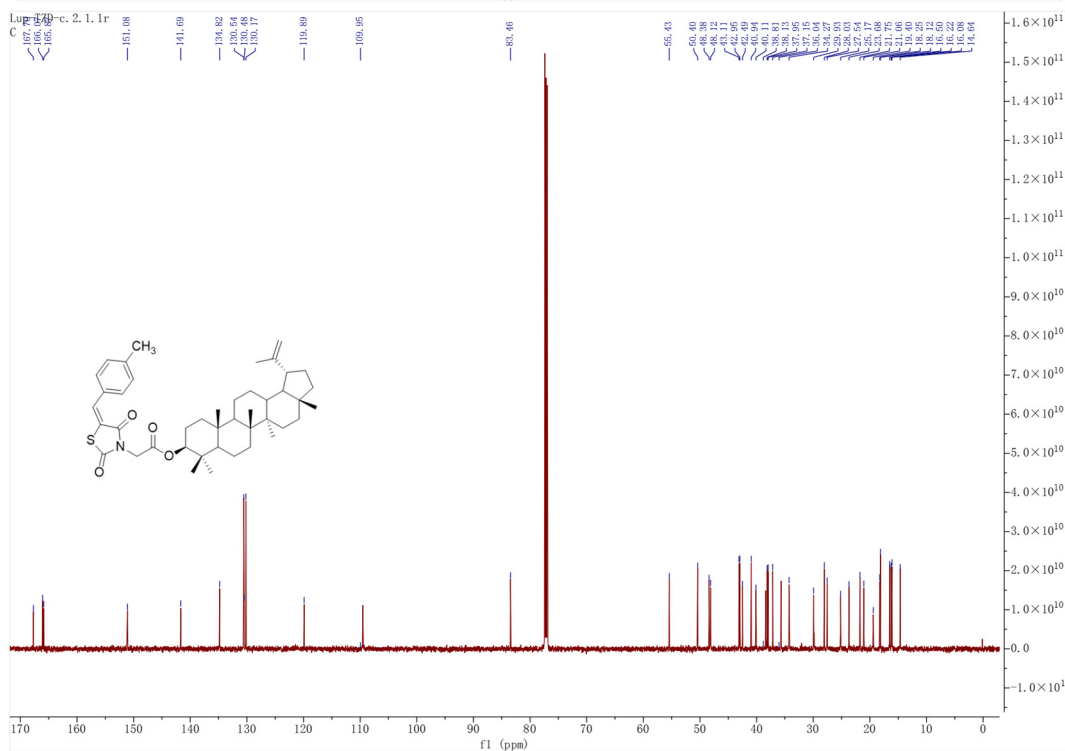
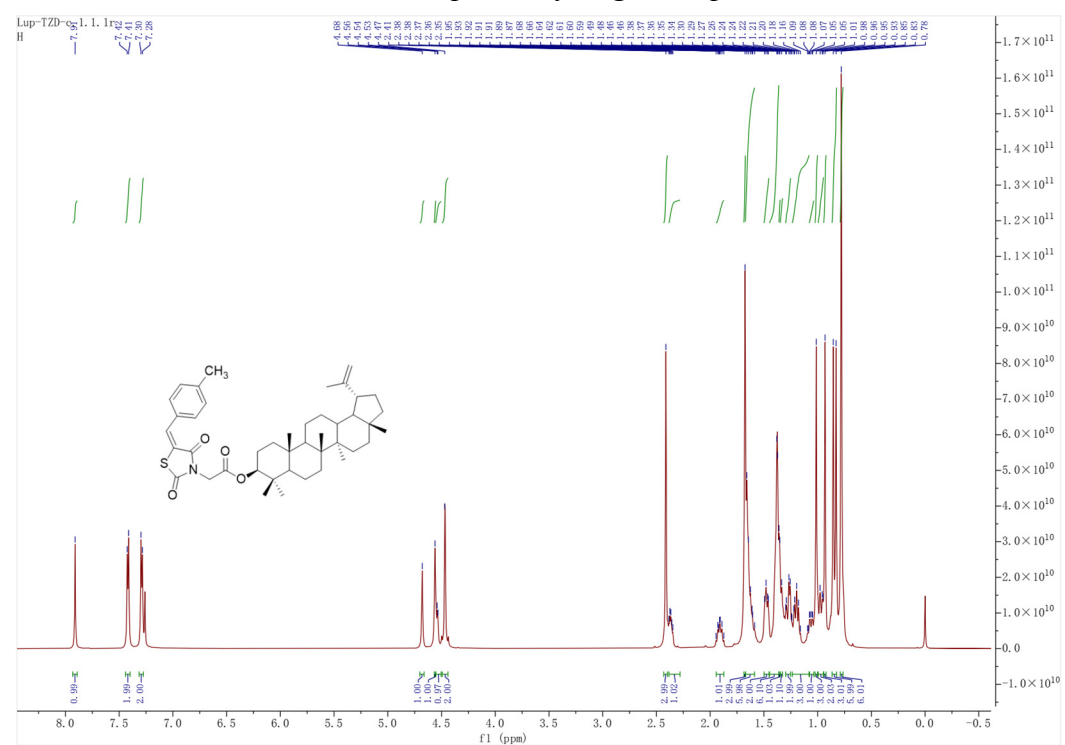


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240120-13-EP-TZD-B 57 (0.260)

1: TOF MS ES+
6.11e+003

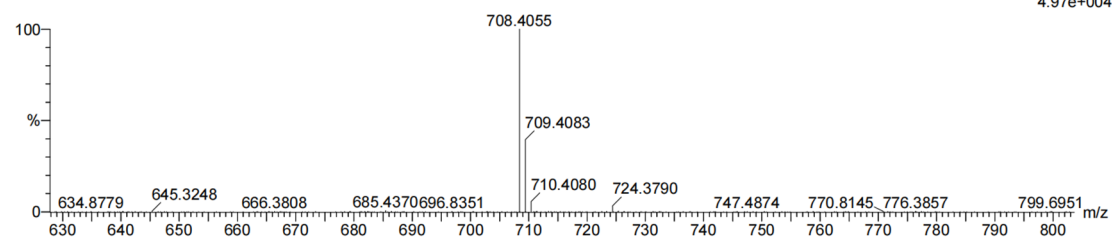


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6c

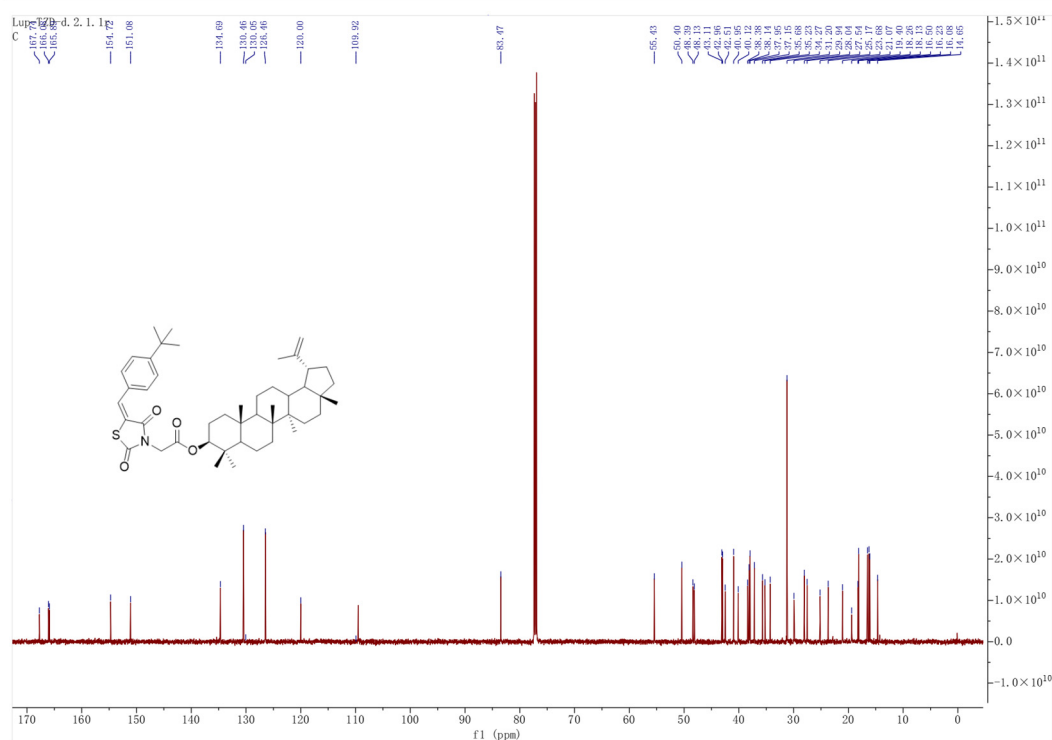
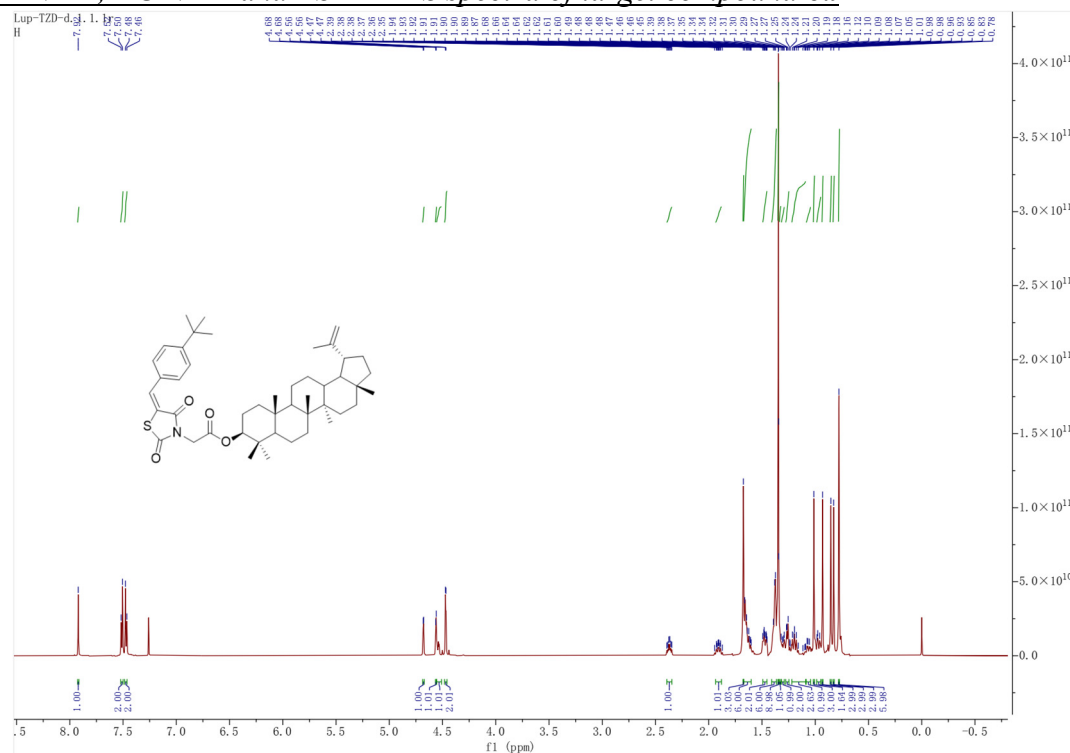


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240120-13-EP-TZD-C 57 (0.260)

1: TOF MS ES+
4.97e+004

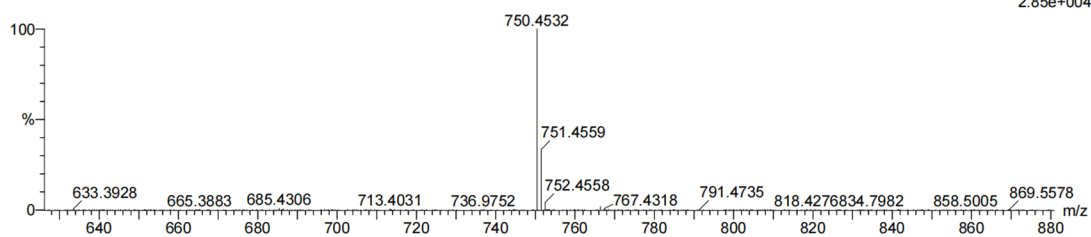


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6d

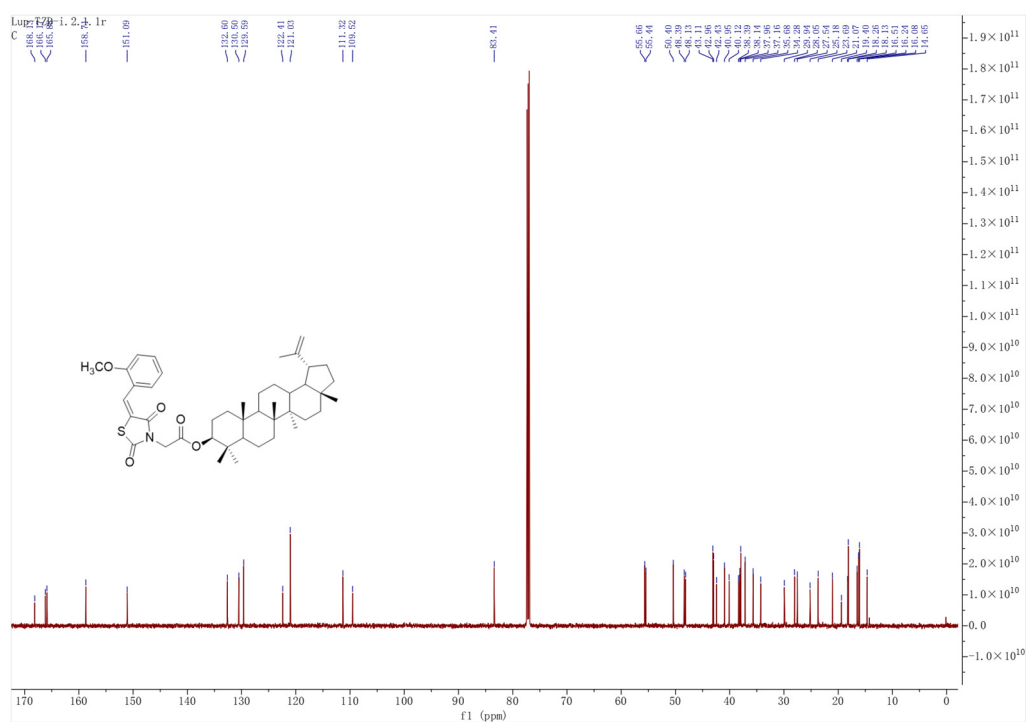
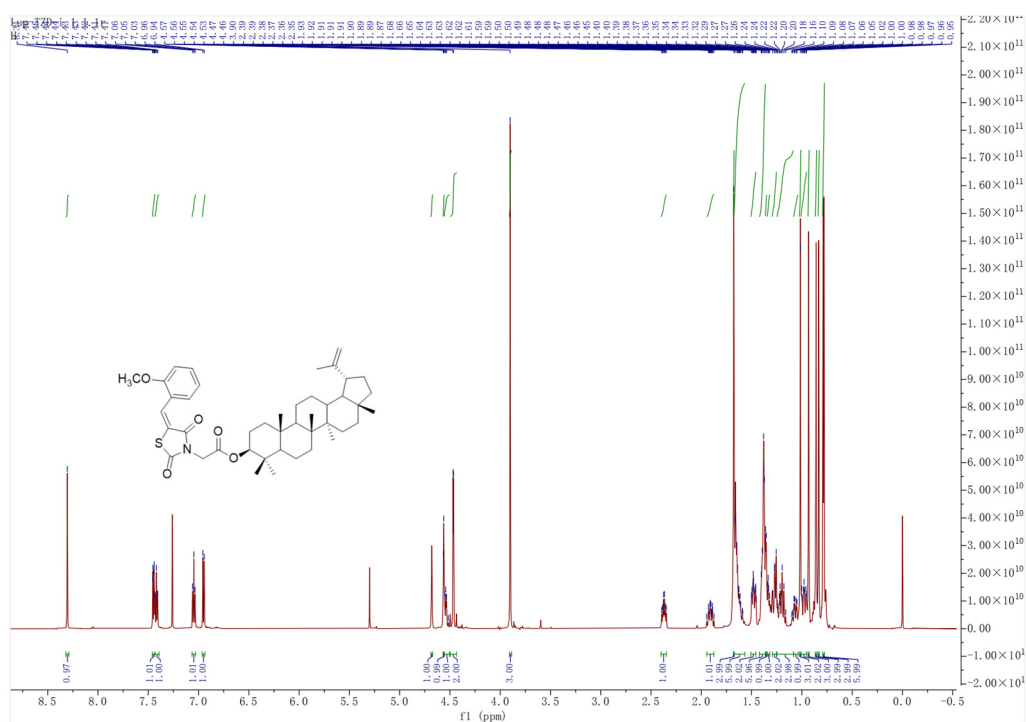


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240120-13-EP-TZD-D 74 (0.321)

1: TOF MS ES+
2.85e+004

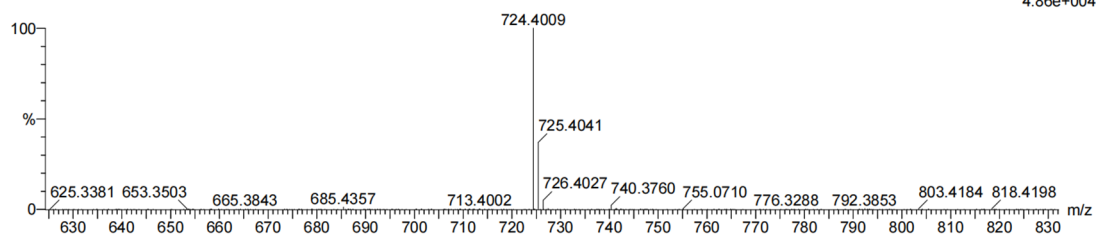


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6e

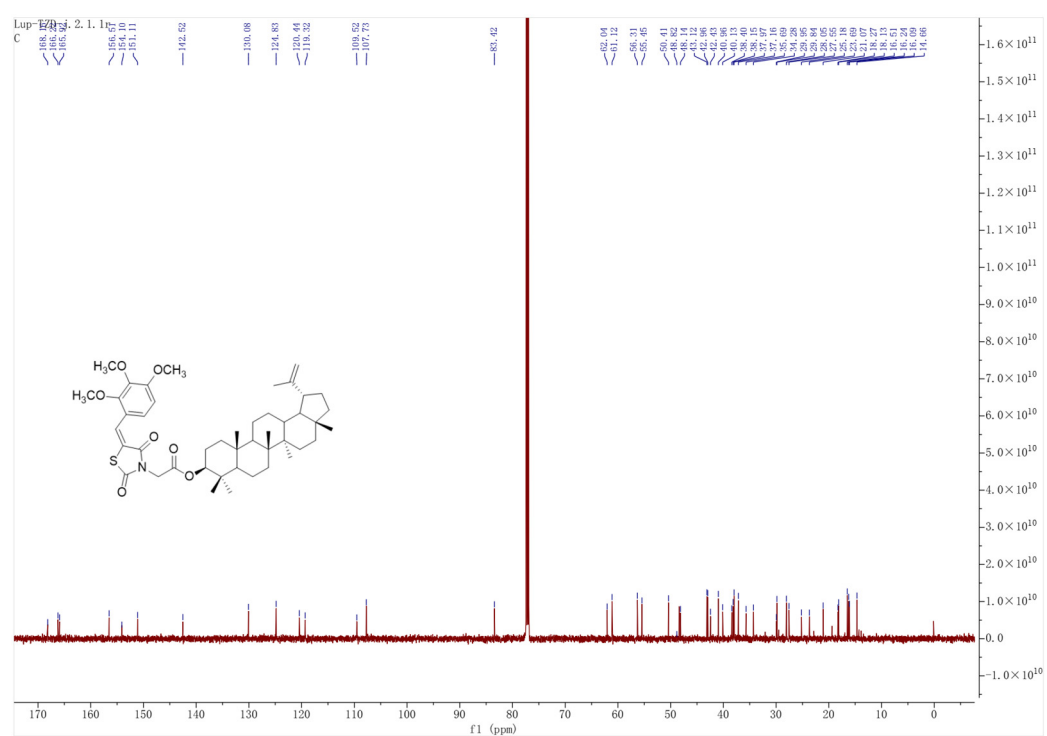
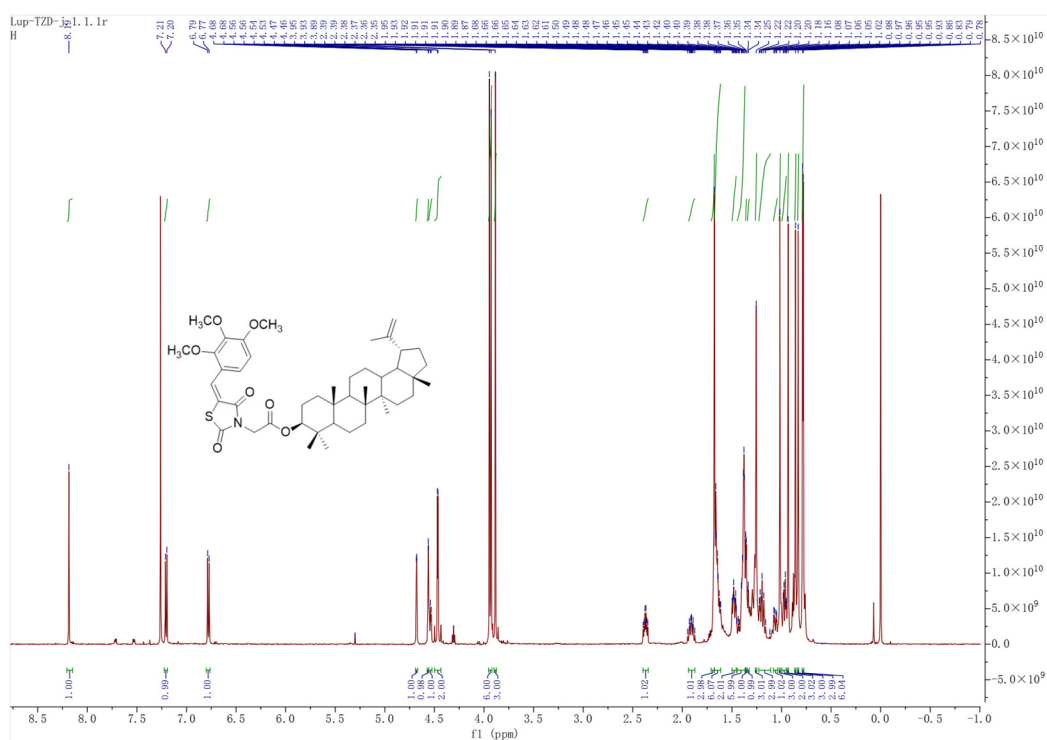


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240120-13-EP-TZD-I 47 (0.224)

1: TOF MS ES+
4.86e+004

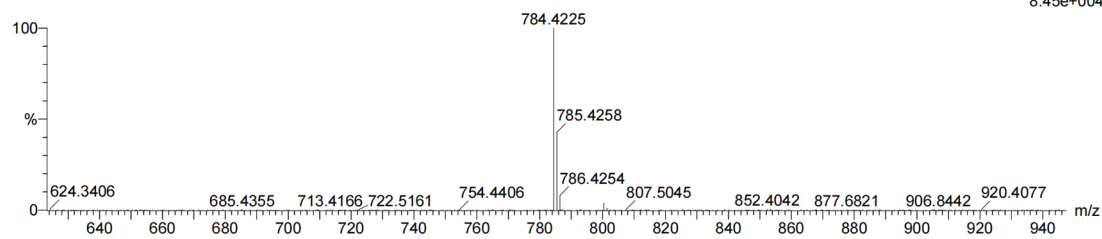


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6f

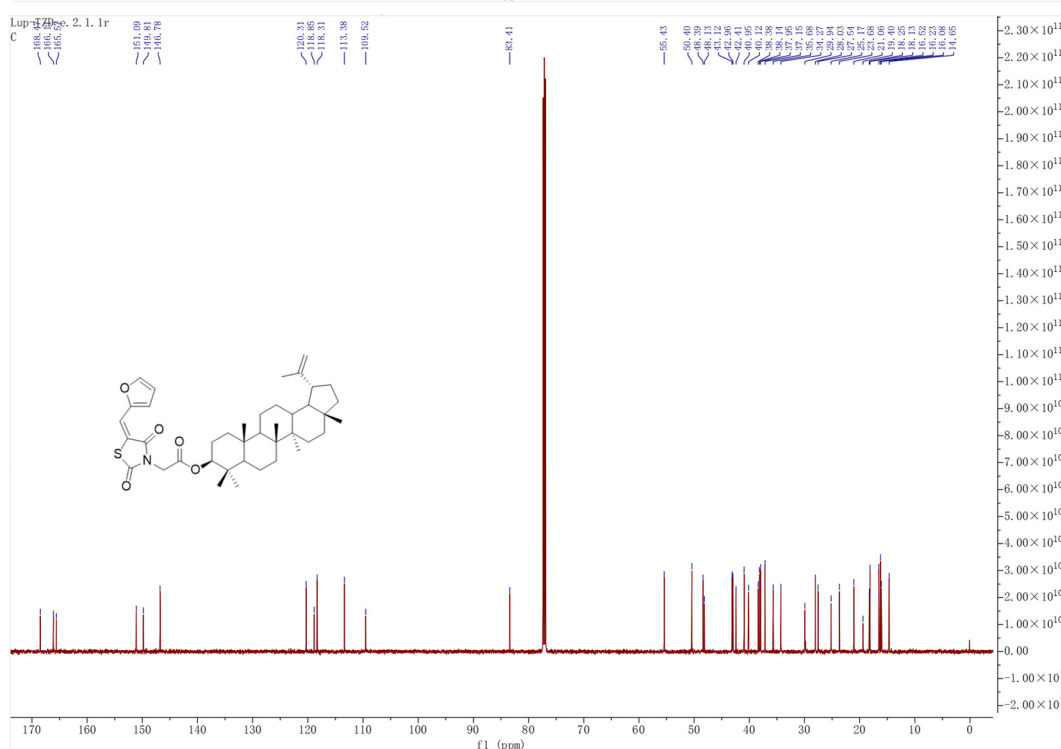
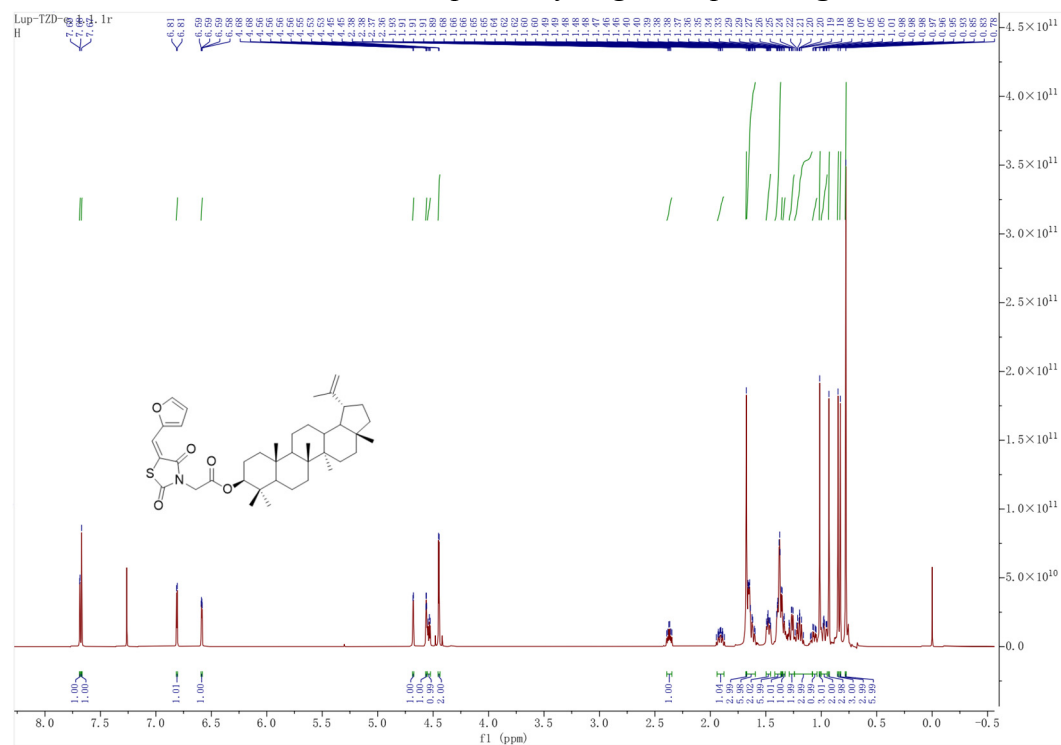


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1: TOF MS ES+
8.45e+004

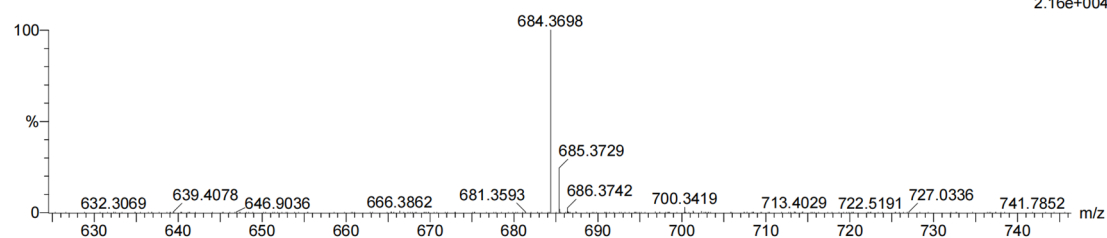


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6g

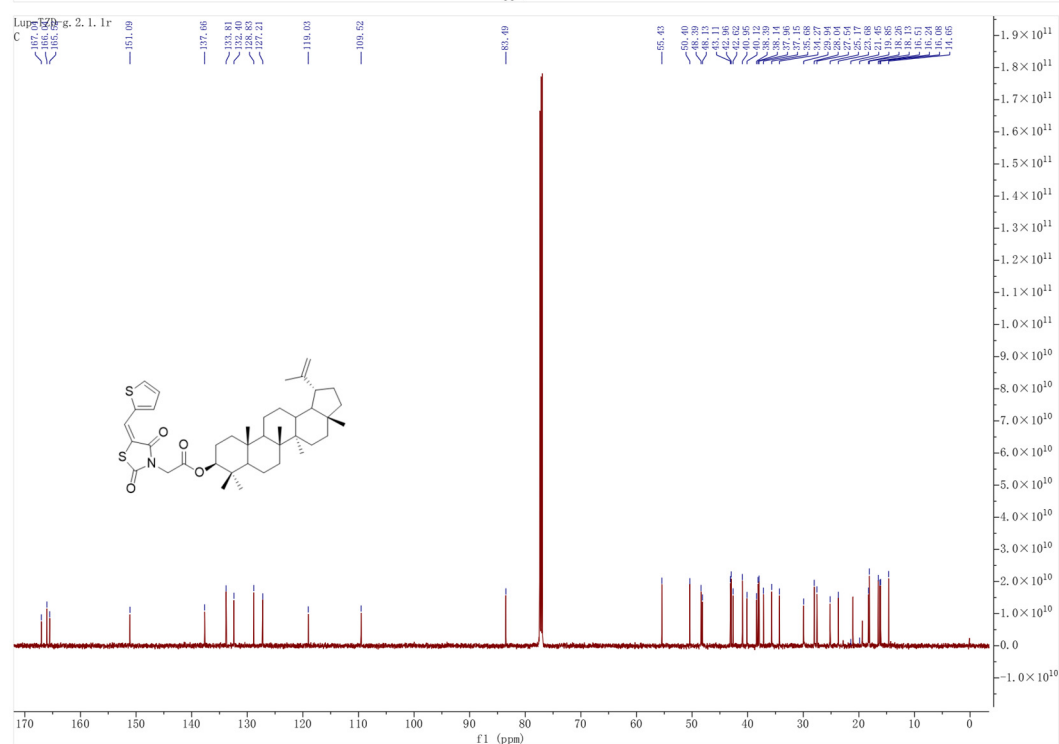
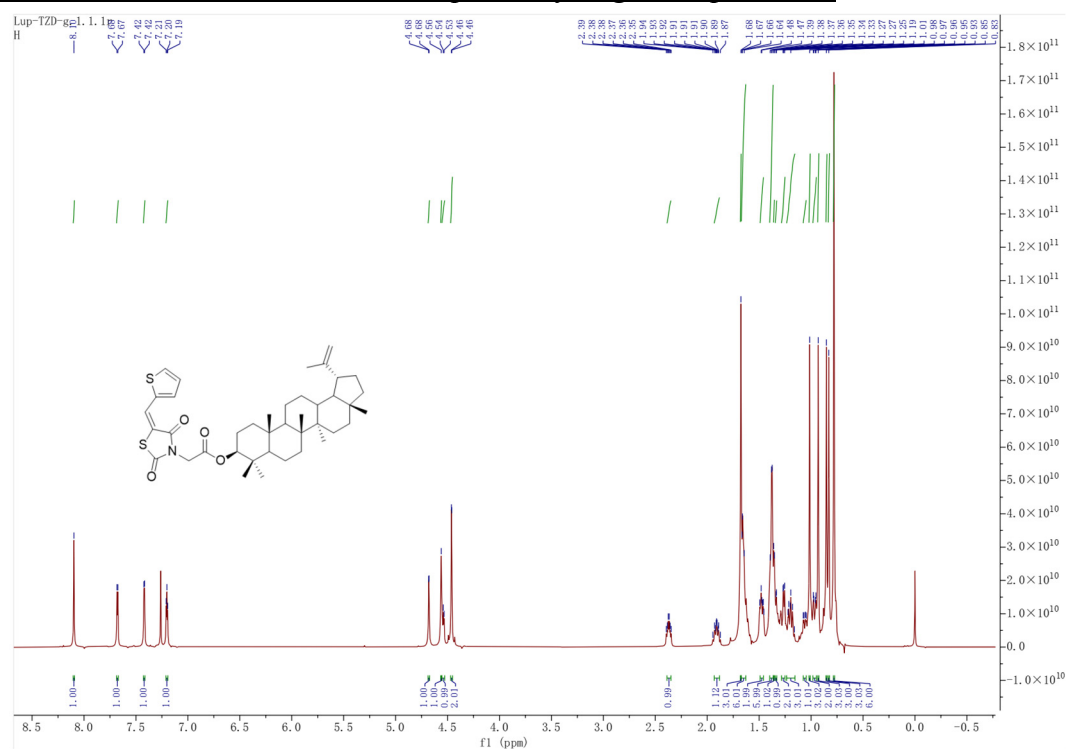


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240120-13-EP-TZD-E 40 (0.180)

1: TOF MS ES+
2.16e+004

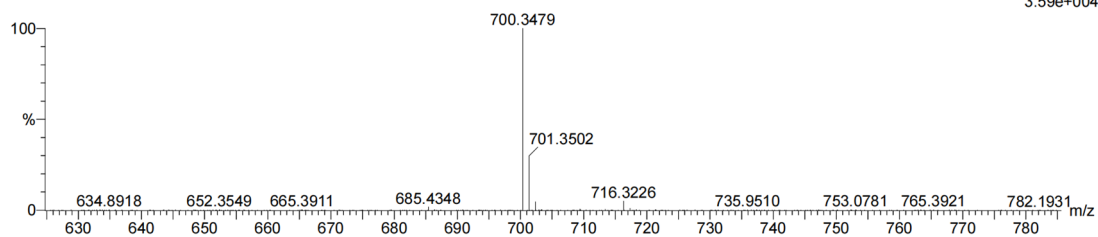


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6h

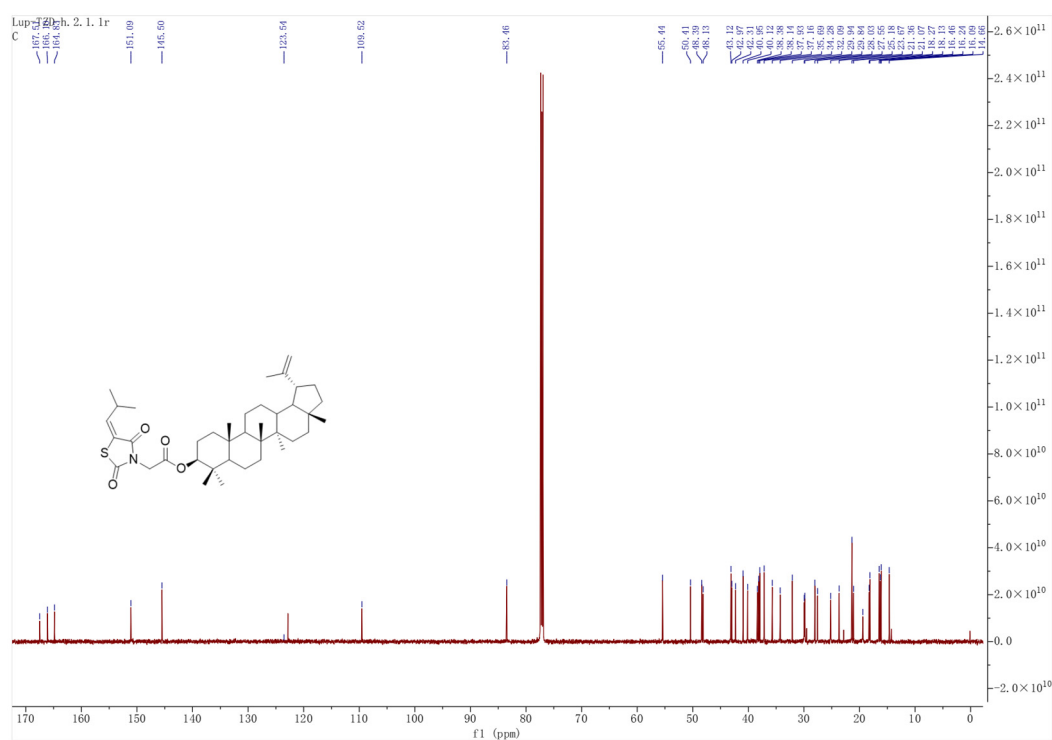
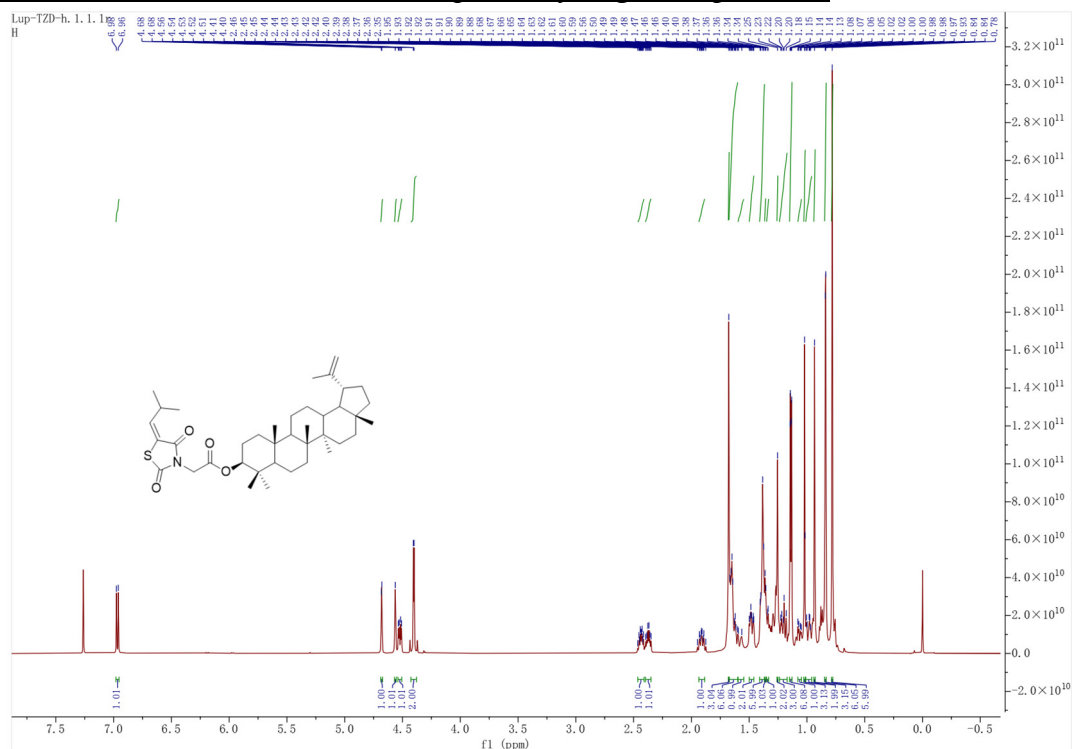


25
240120-13-EP-TZD-G 47 (0.224)

1: TOF MS ES+
3.59e+004

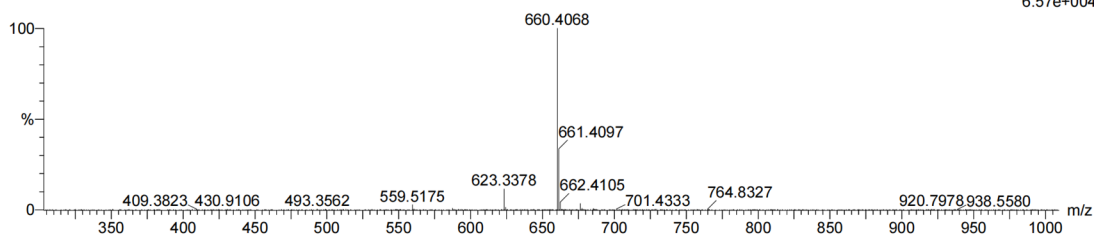


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 6i

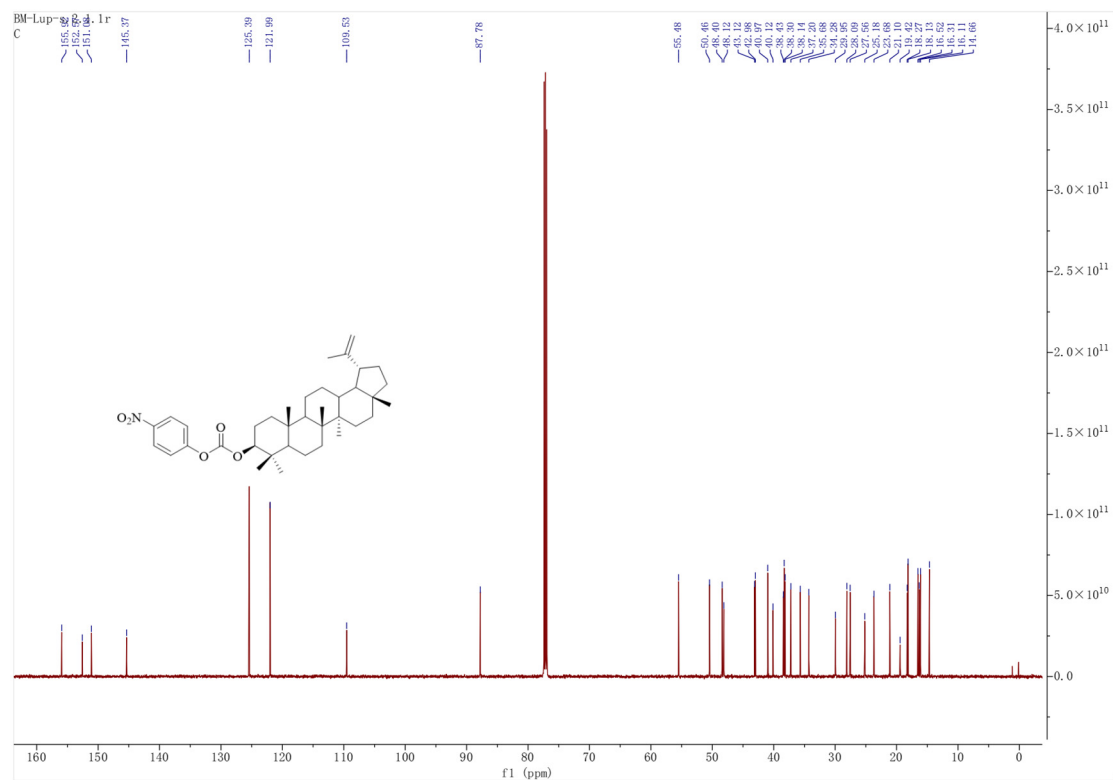
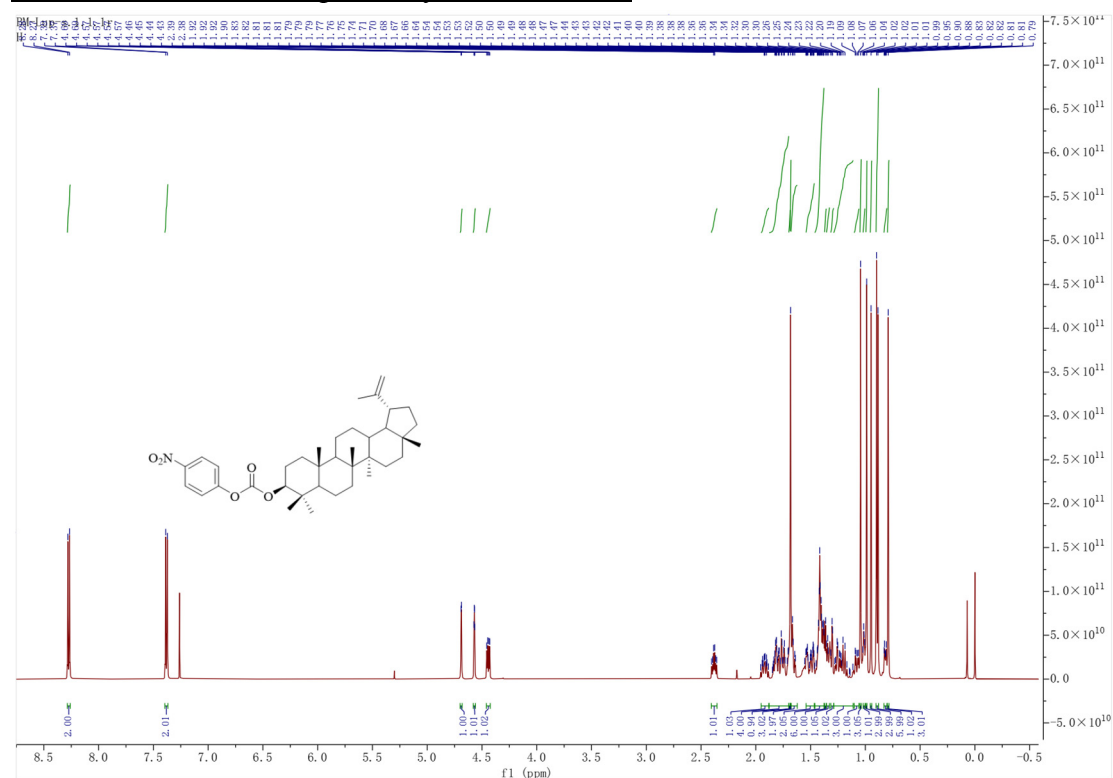


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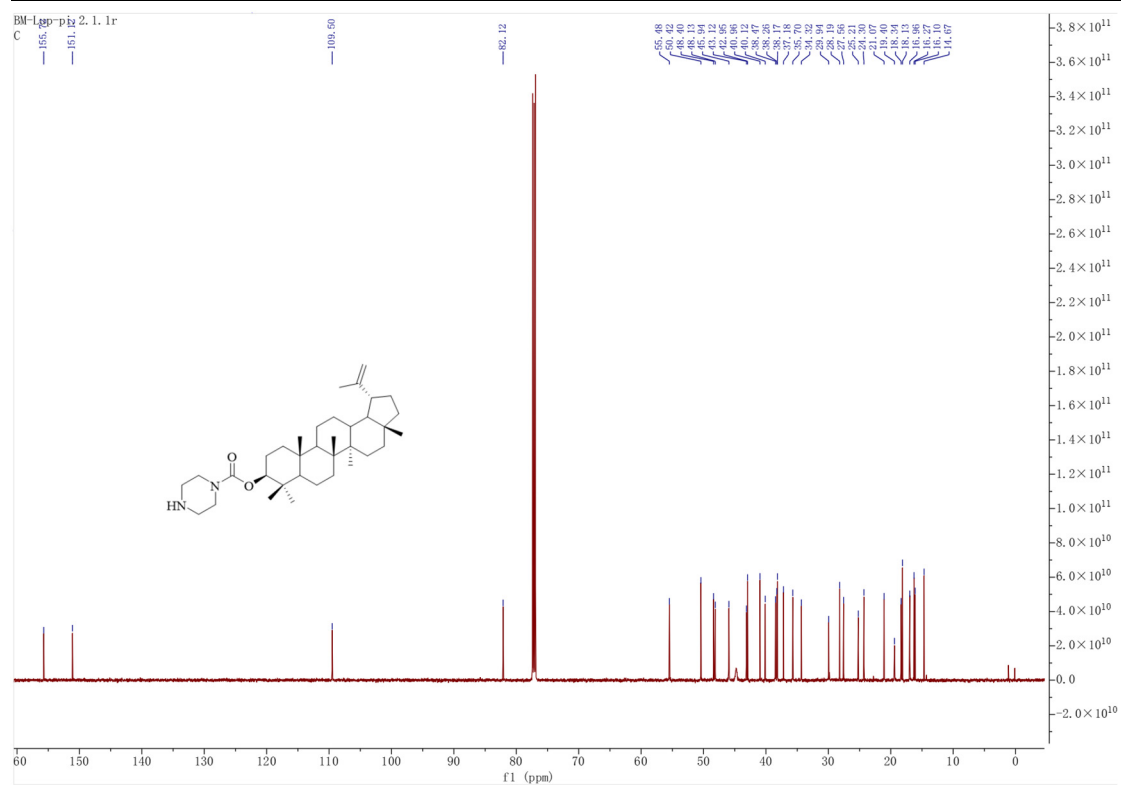
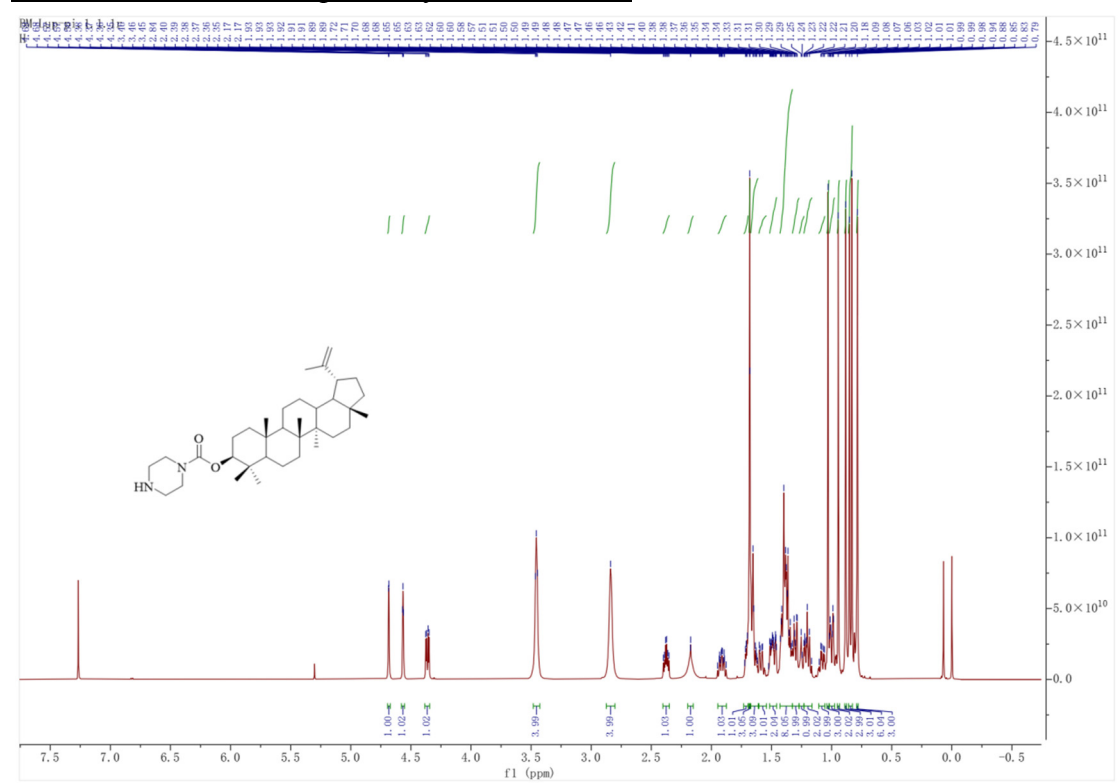
1: TOF MS ES+
6.57e+004



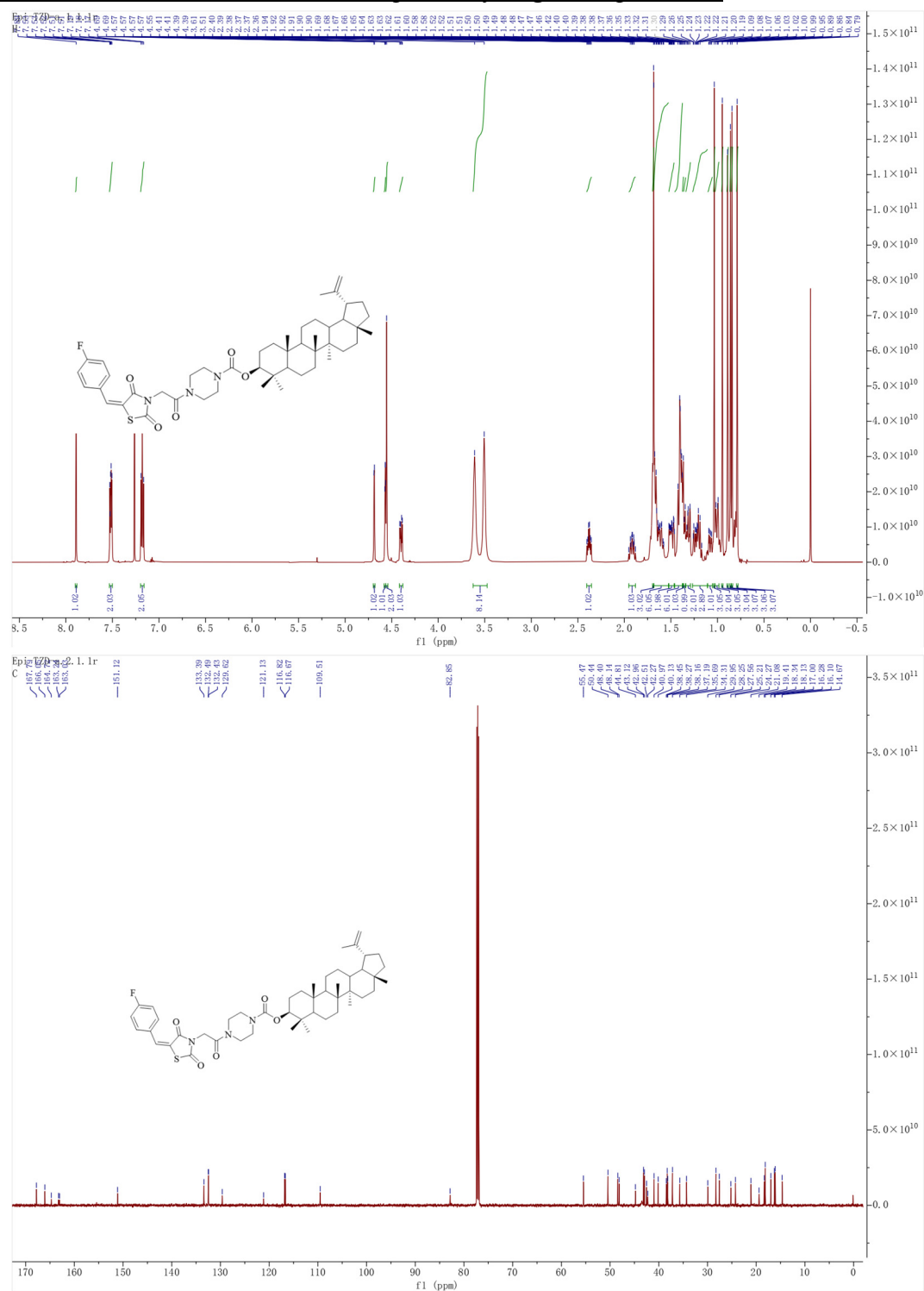
¹H NMR and ¹³C NMR spectra of intermediate 7



¹H NMR and ¹³C NMR spectra of intermediate 8

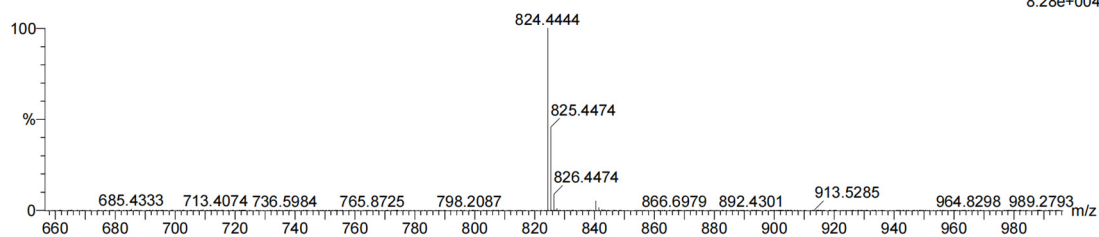


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9a

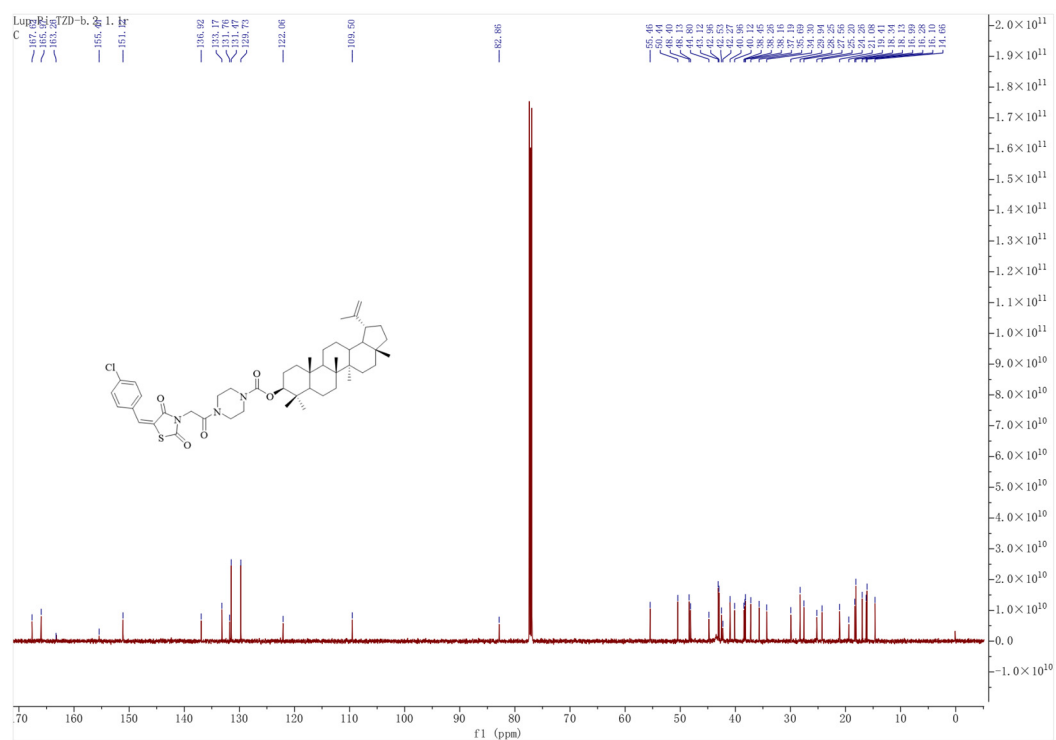
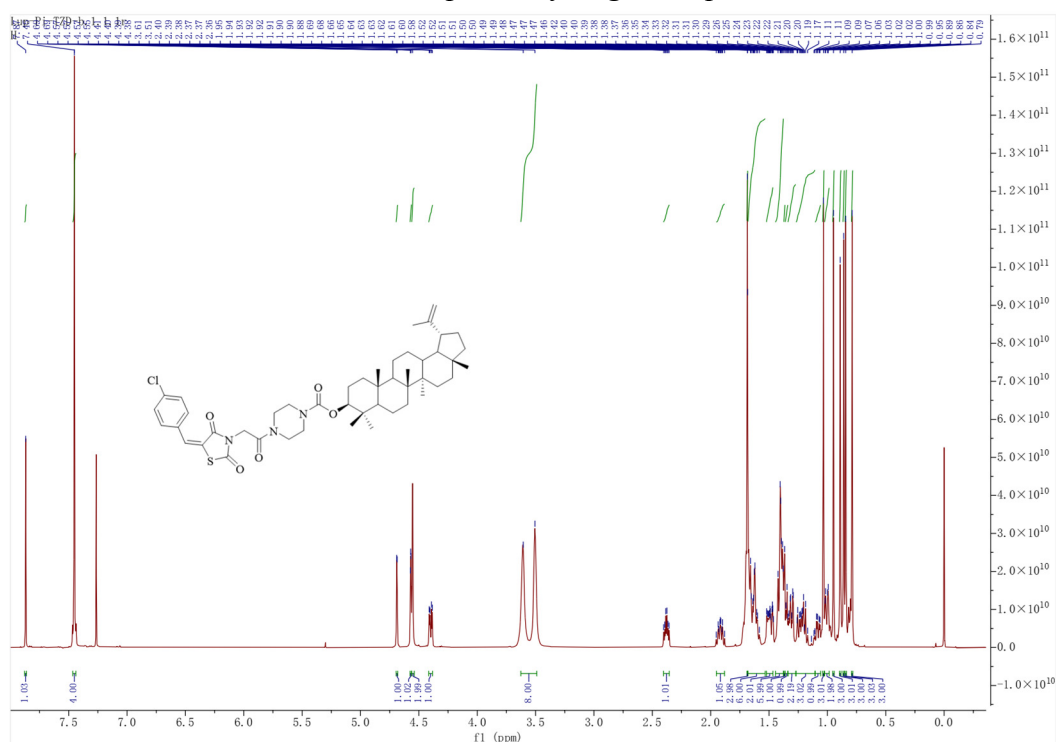


10
240107-5-LUP-PI-TZD-A 37 (0.162)

1: TOF MS ES+
8.28e+004

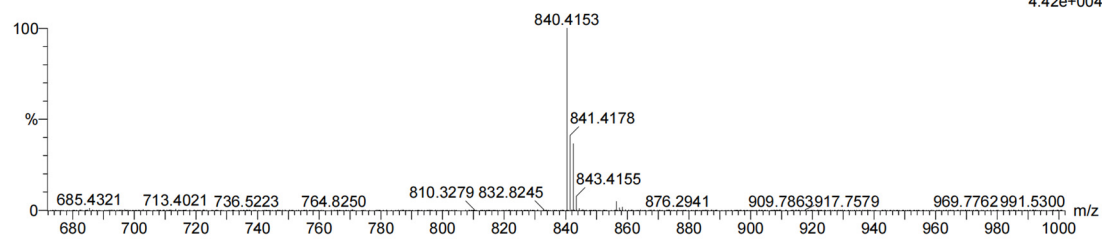


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9b

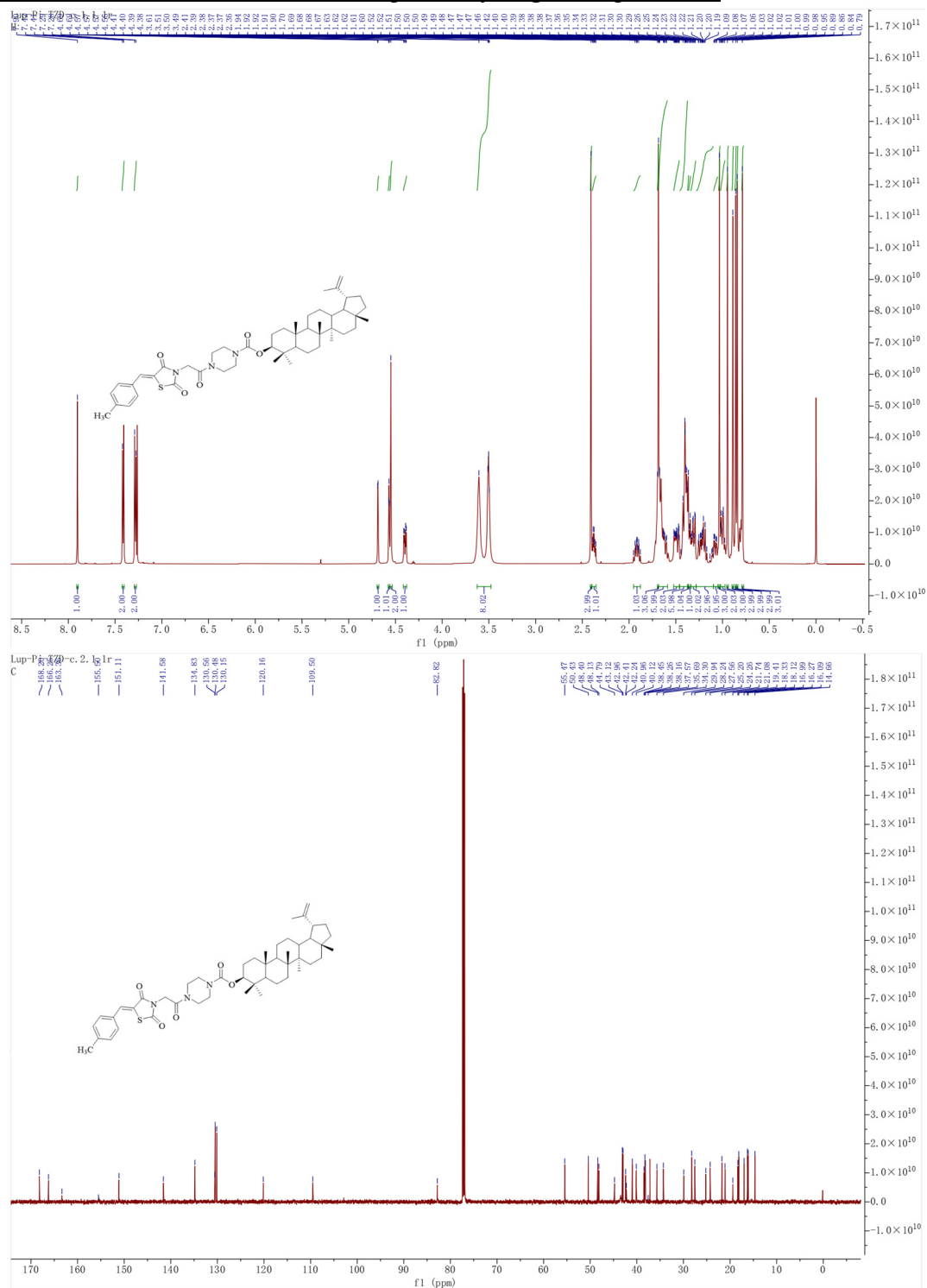


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1: TOF MS ES+
4.42e+004

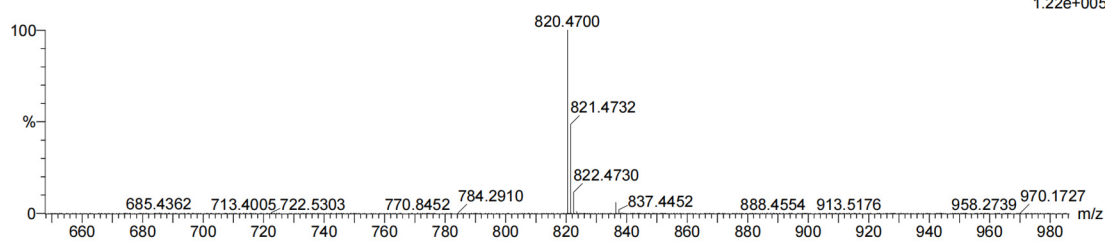


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9c

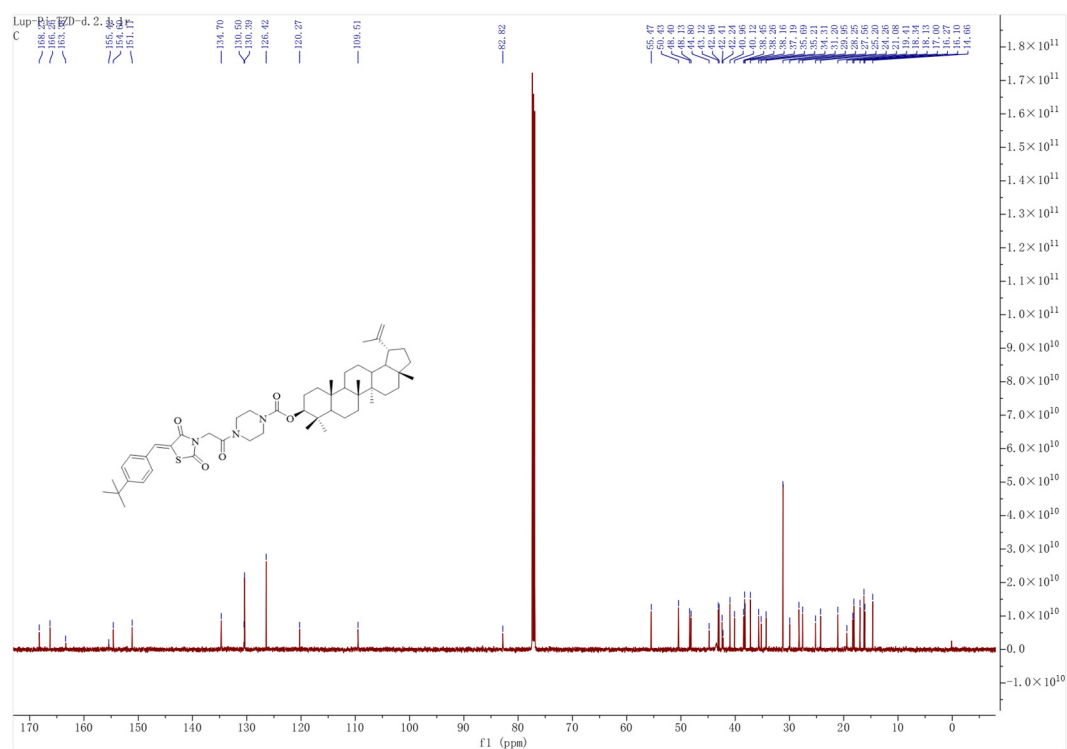
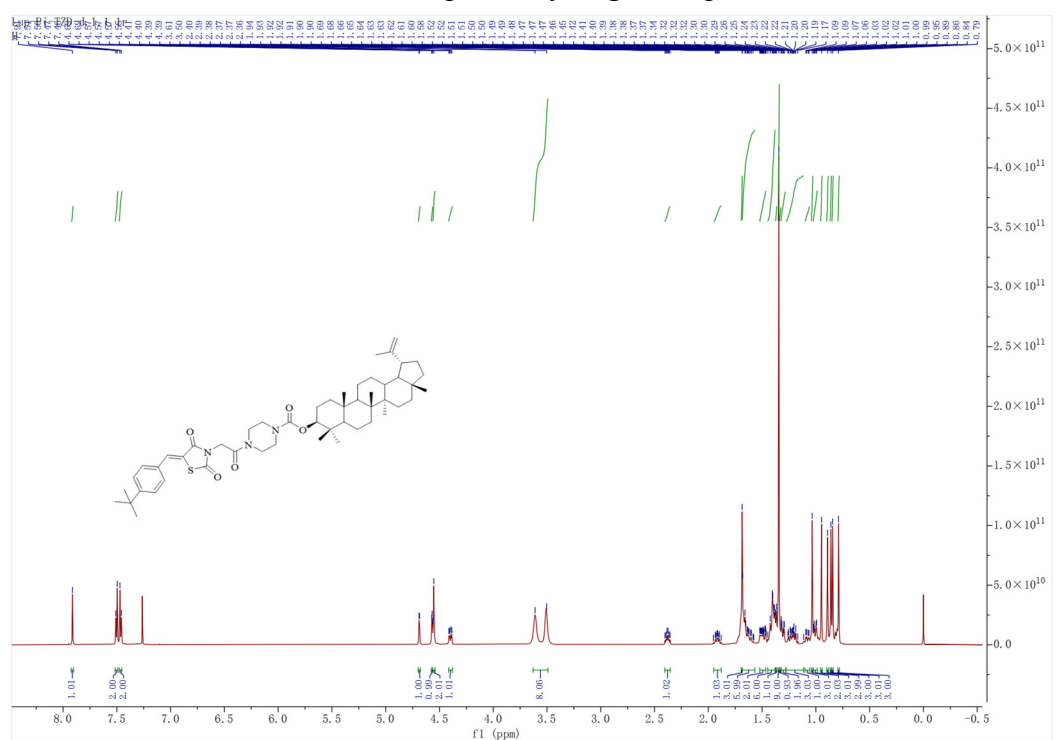


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240107-5-LUP-PI-TZD-C 42 (0.180)

1: TOF MS ES+
1.22e+005

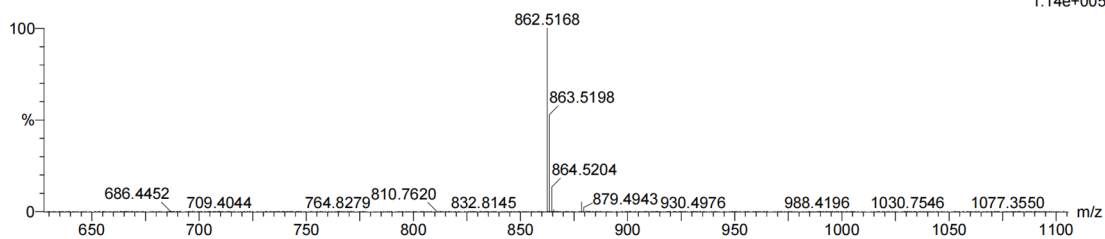


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9d

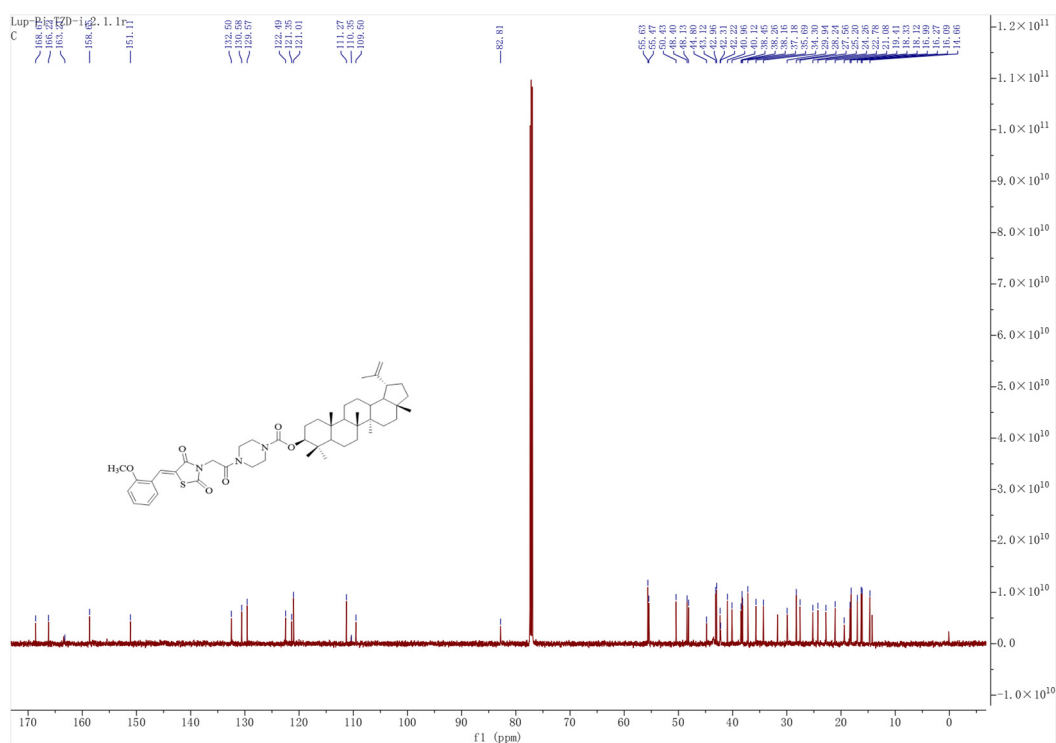
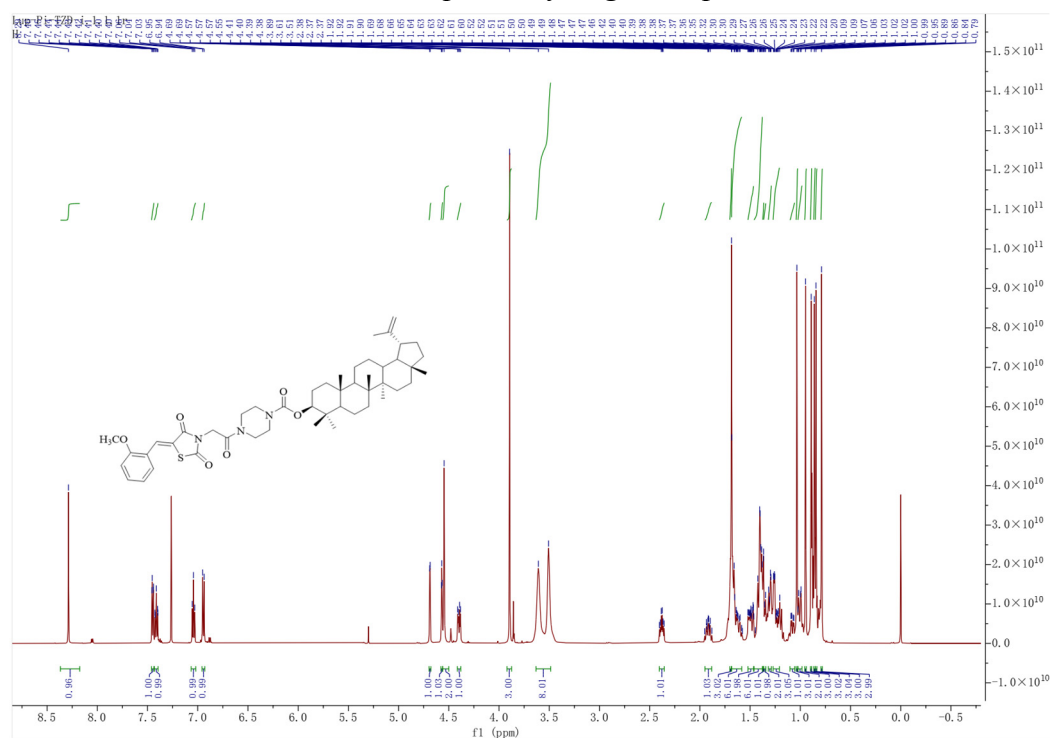


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1: TOF MS ES+
1.14e+005

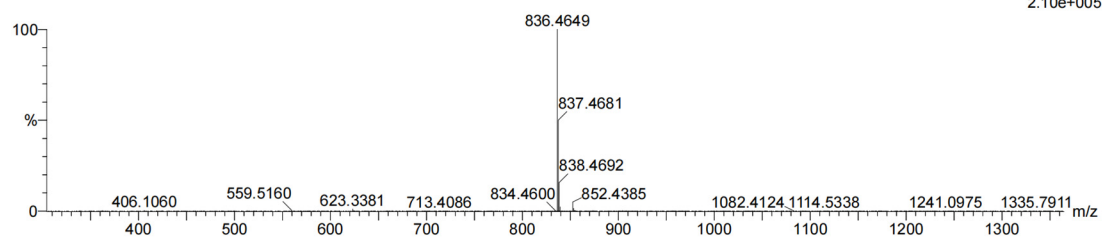


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9e

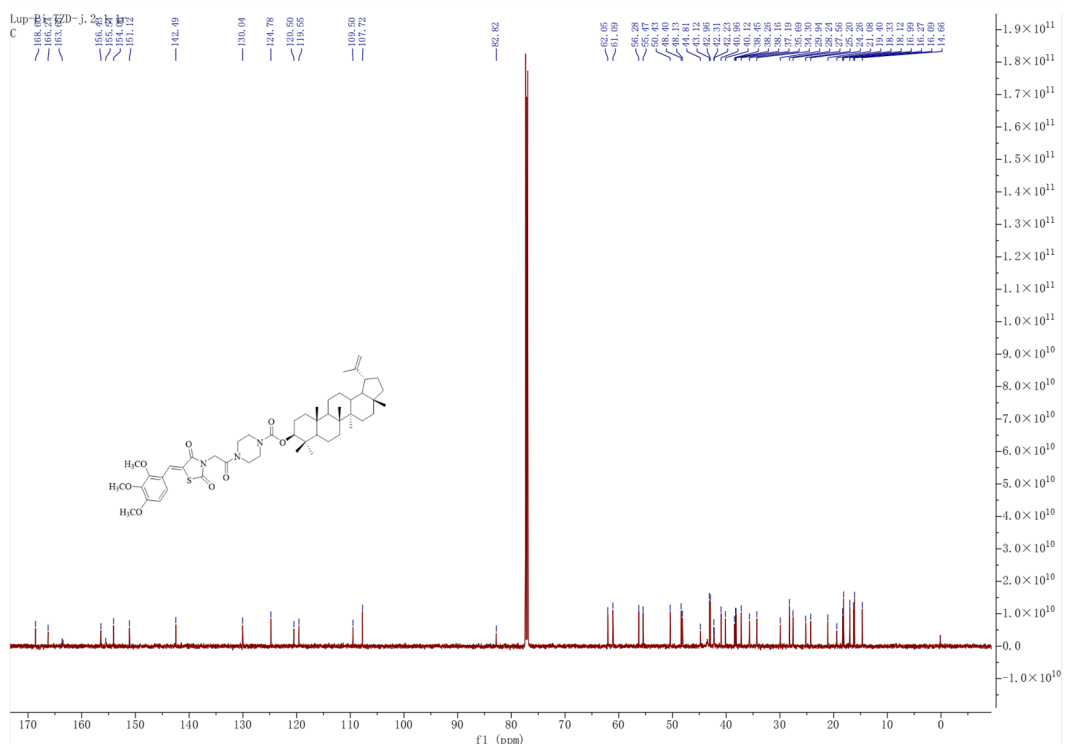
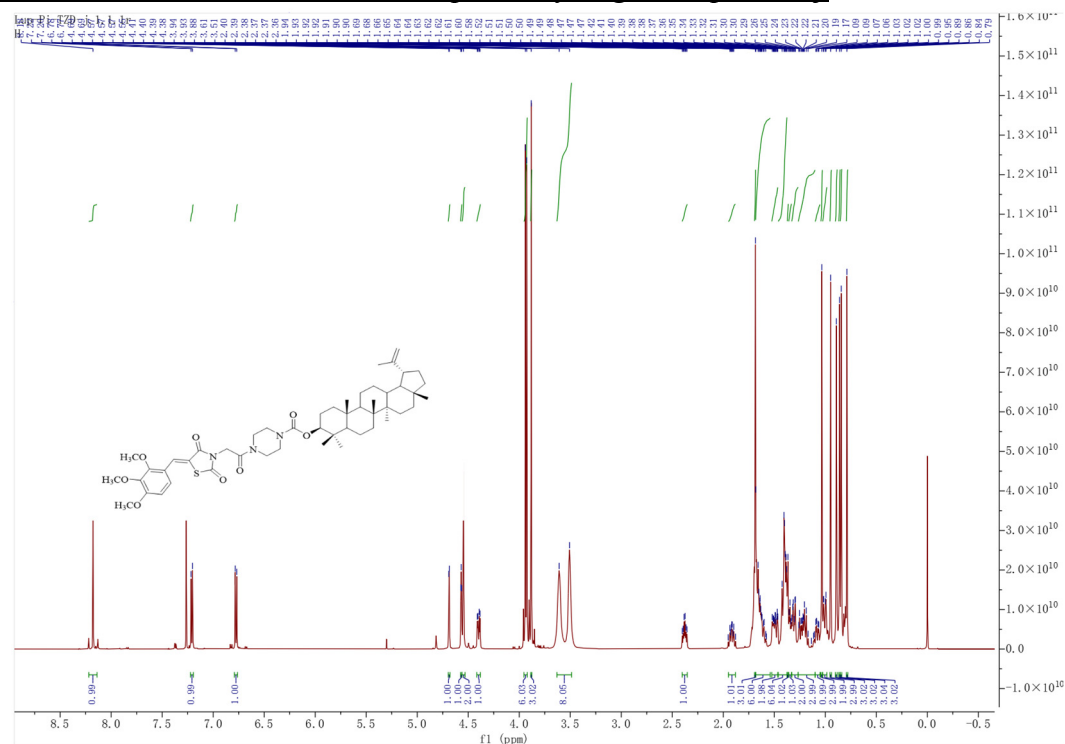


11
240107-5-LUP-PI-TZD-I 37 (0.162)

1: TOF MS ES+
2.10e+005

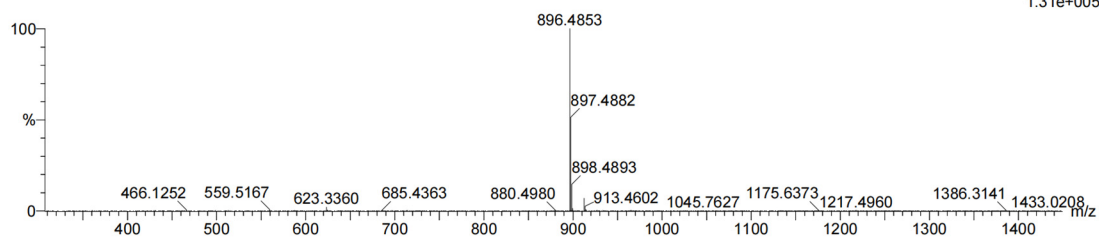


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9f

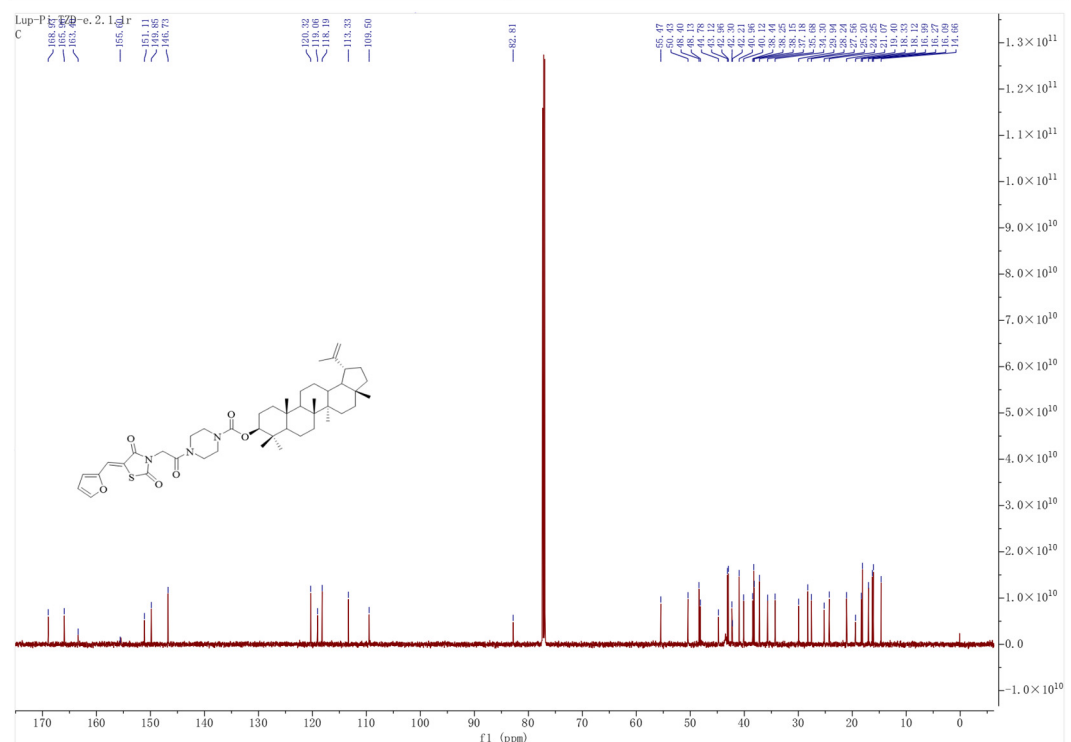
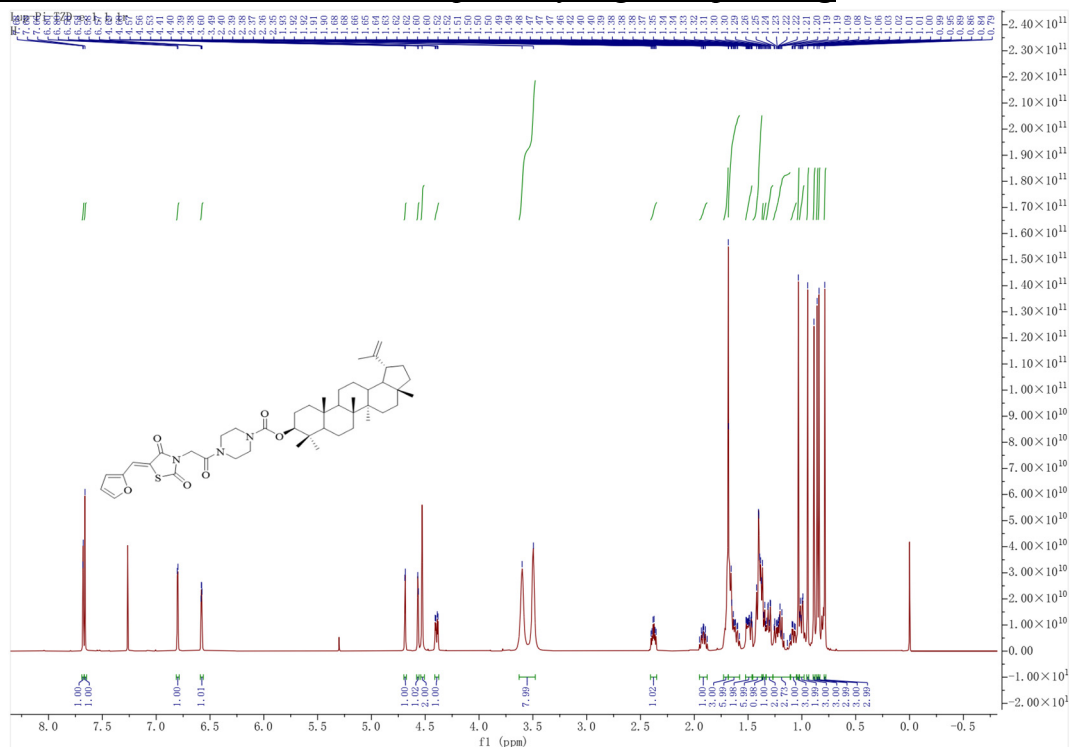


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240107-5-LUP-PI-TZD-J 37 (0.162)

1: TOF MS ES+
1.31e+005

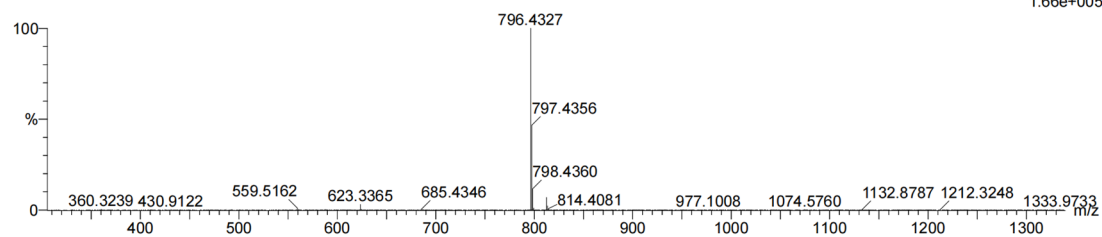


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9g

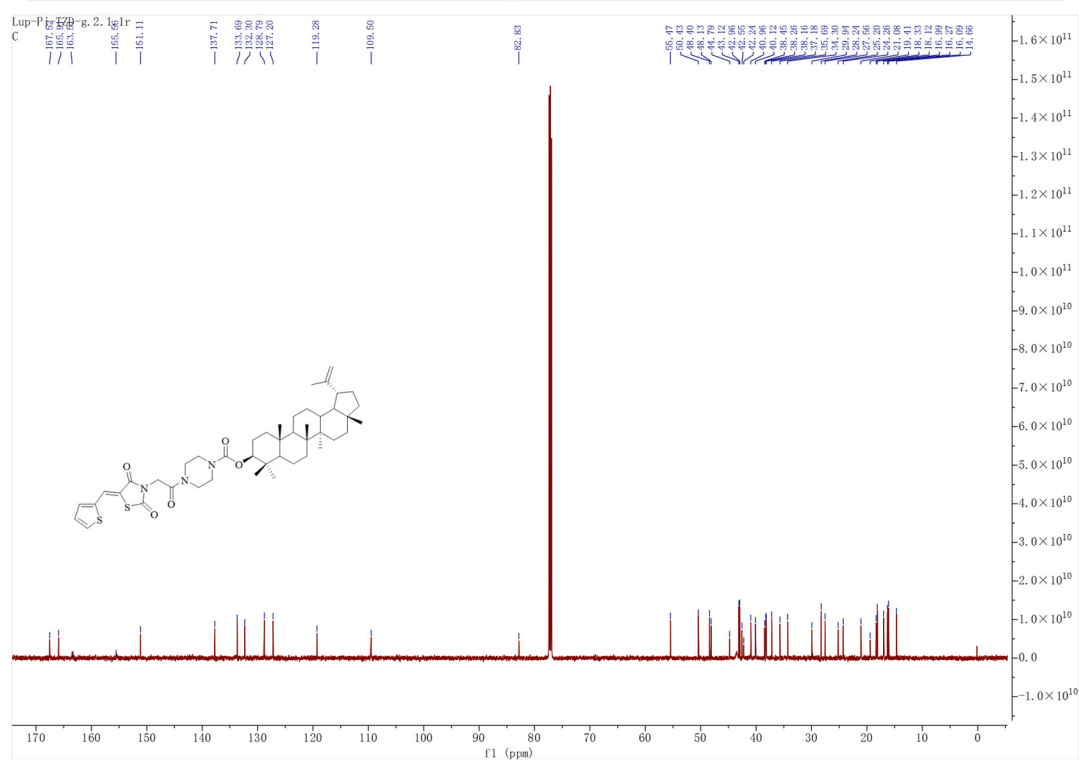
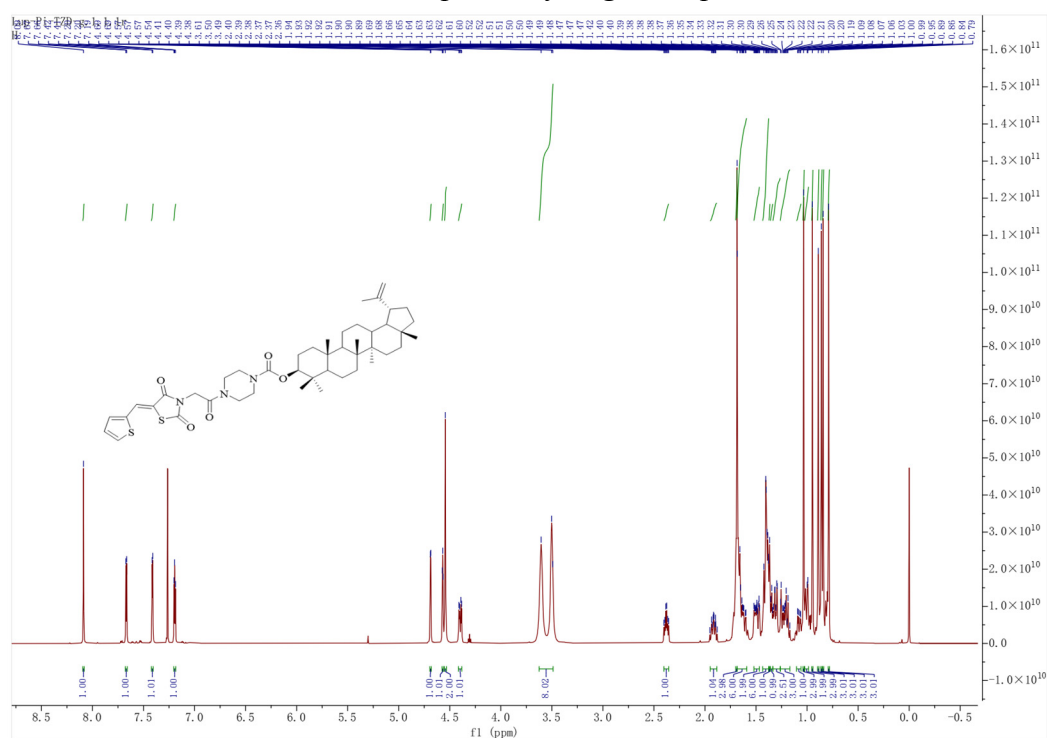


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1: TOF MS ES+
1.66e+005

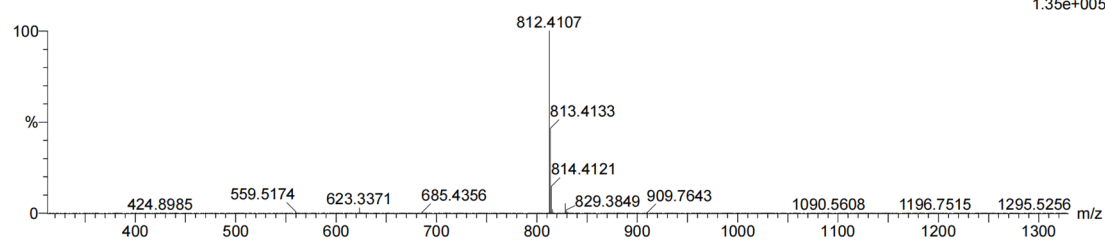


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9h

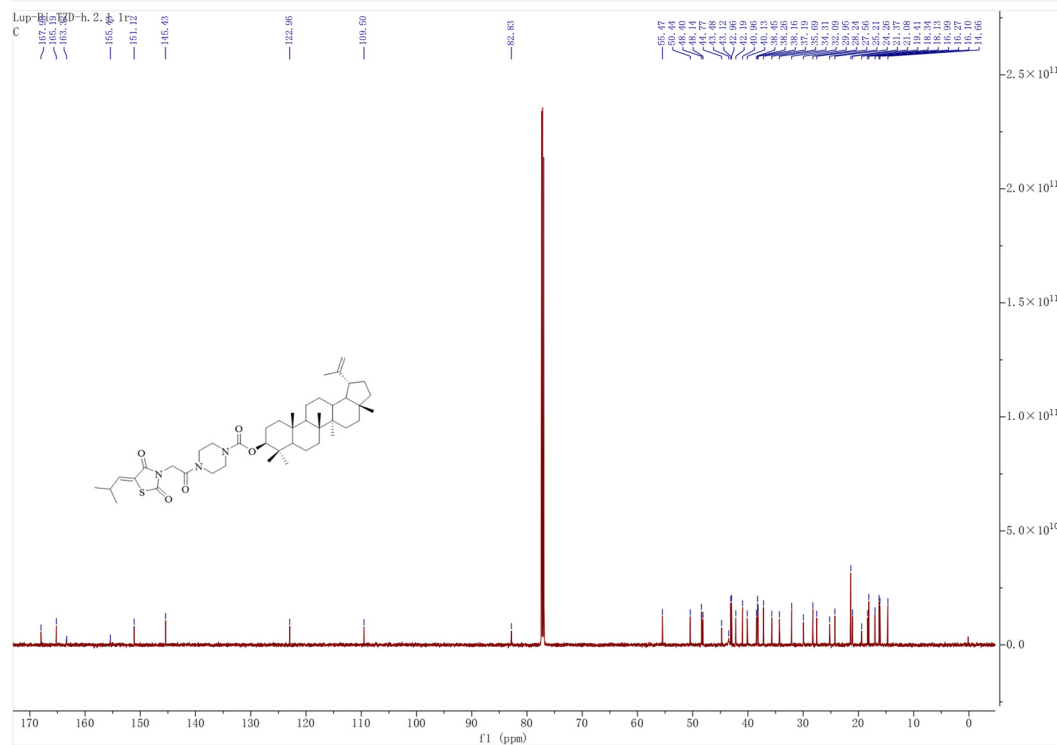
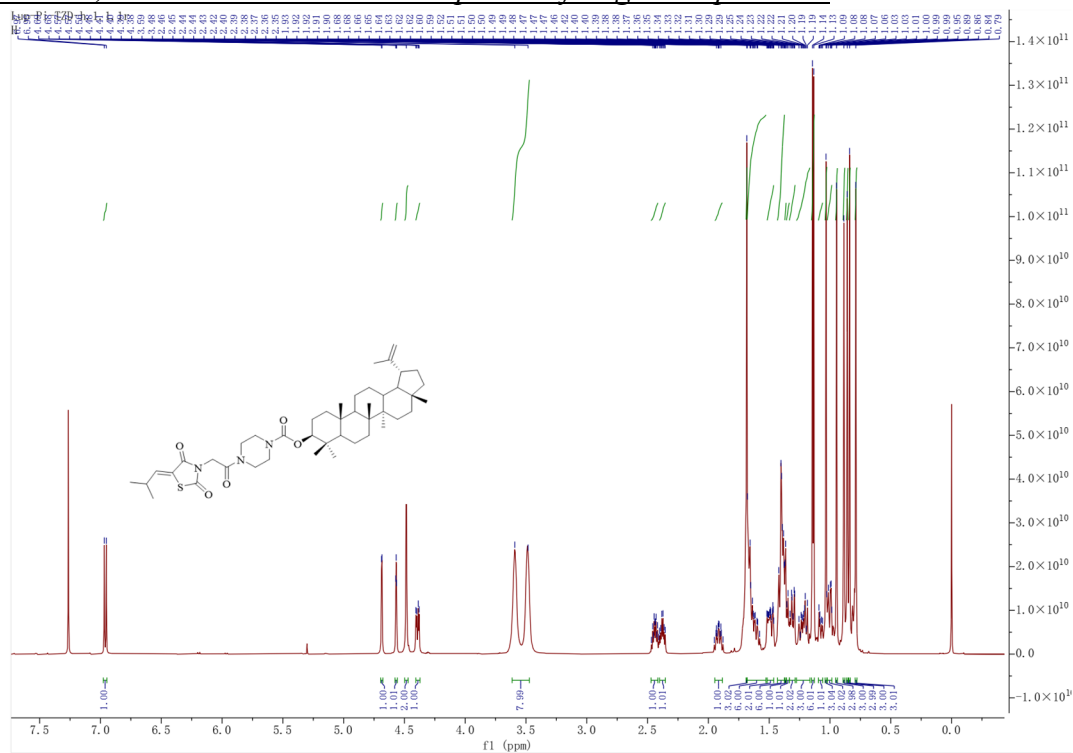


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1: TOF MS ES+
1.35e+005

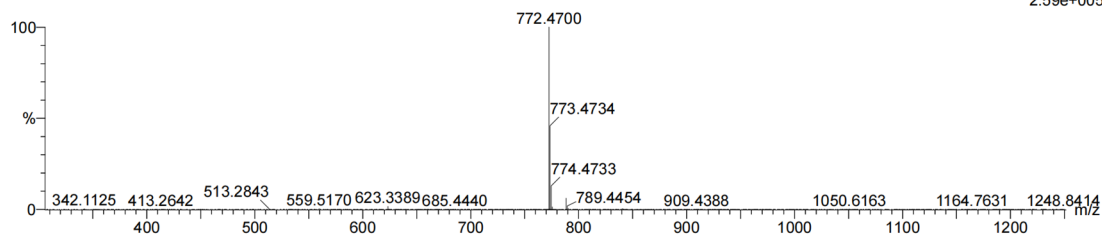


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 9i

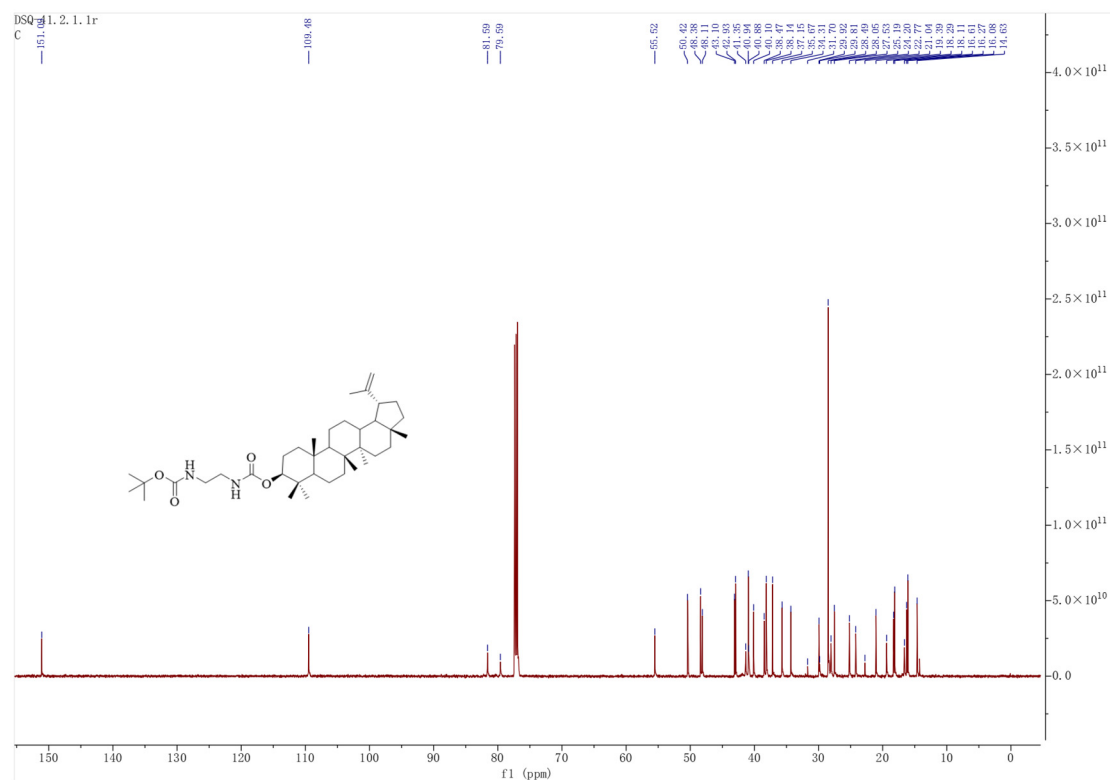
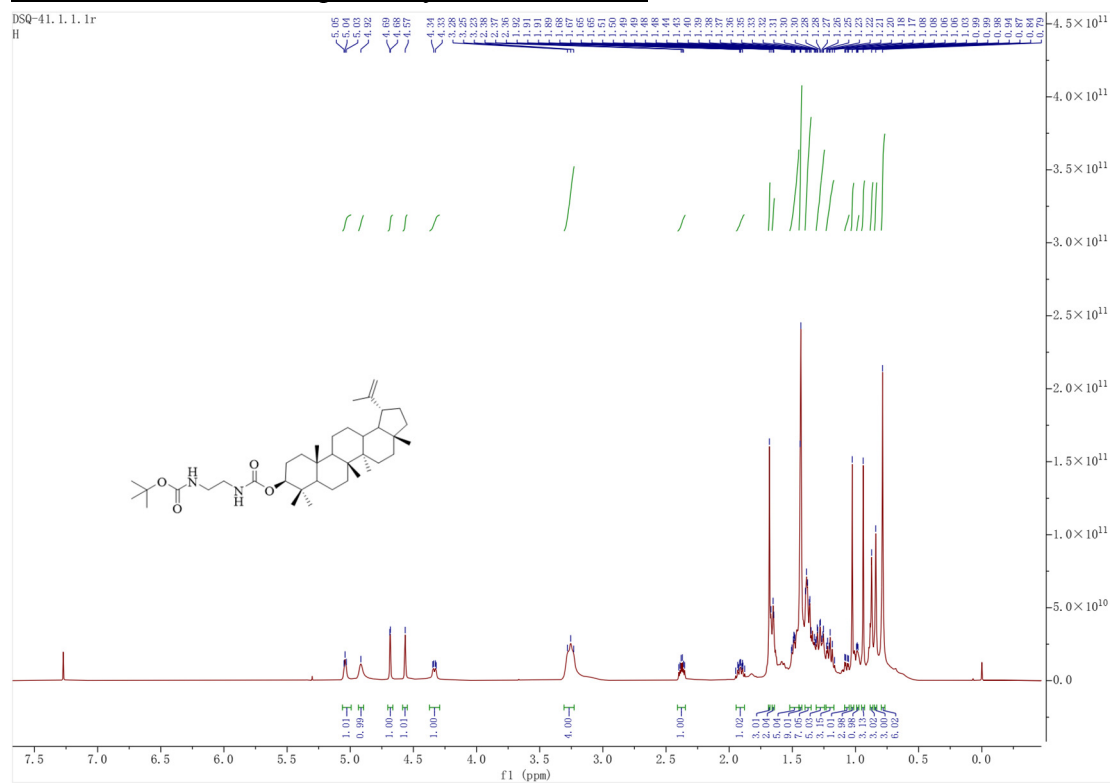


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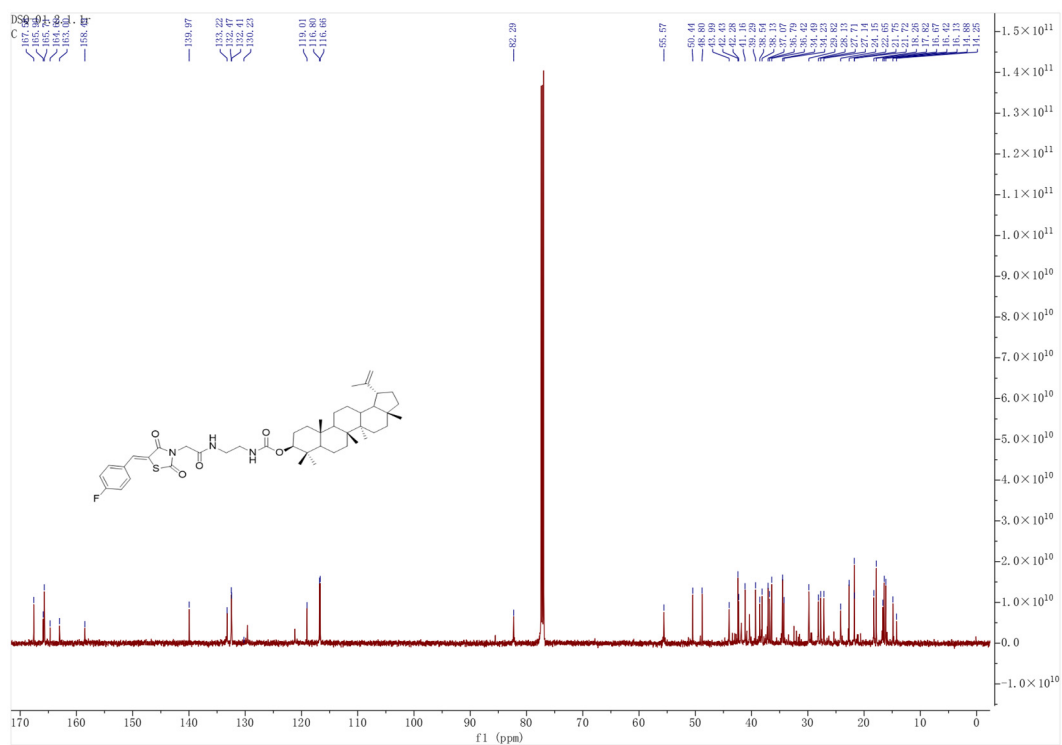
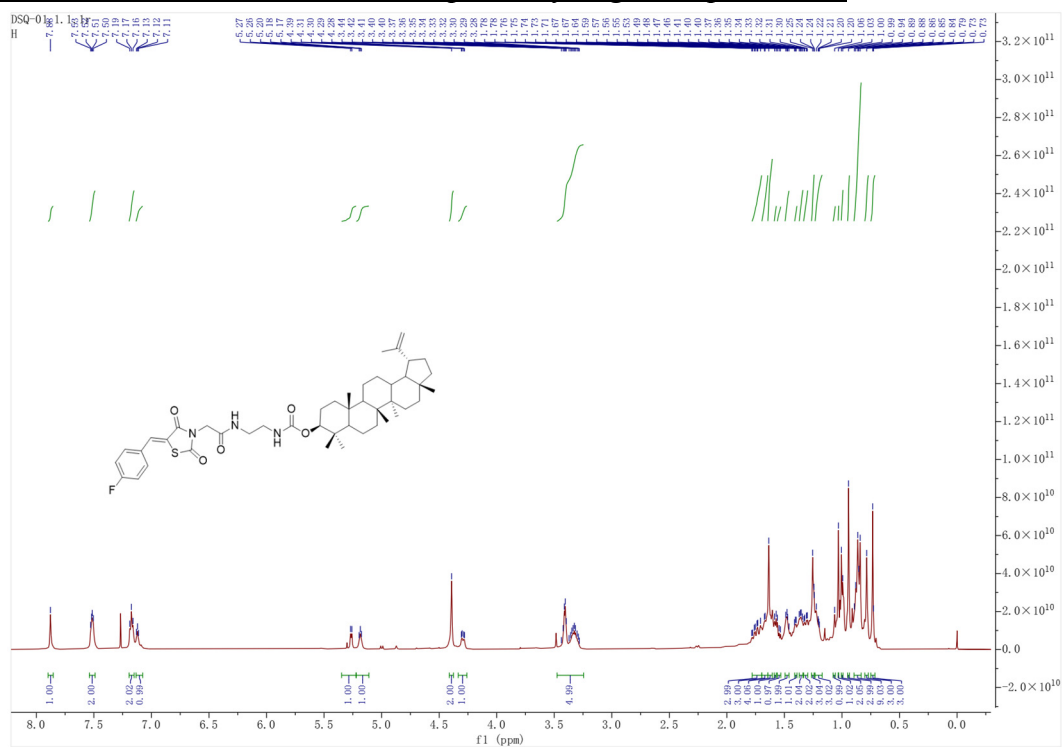
1: TOF MS ES+
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¹H NMR and ¹³C NMR spectra of intermediate 10

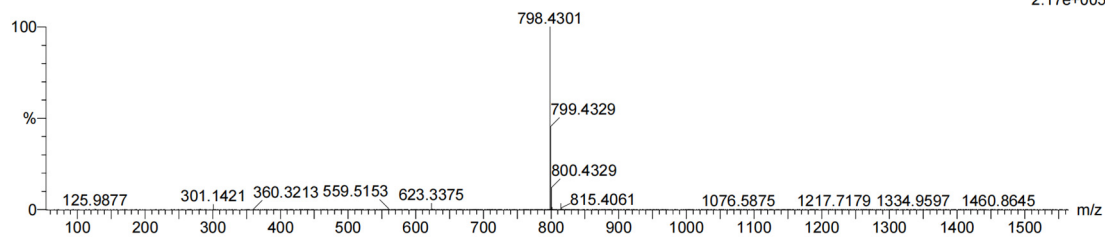


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12a

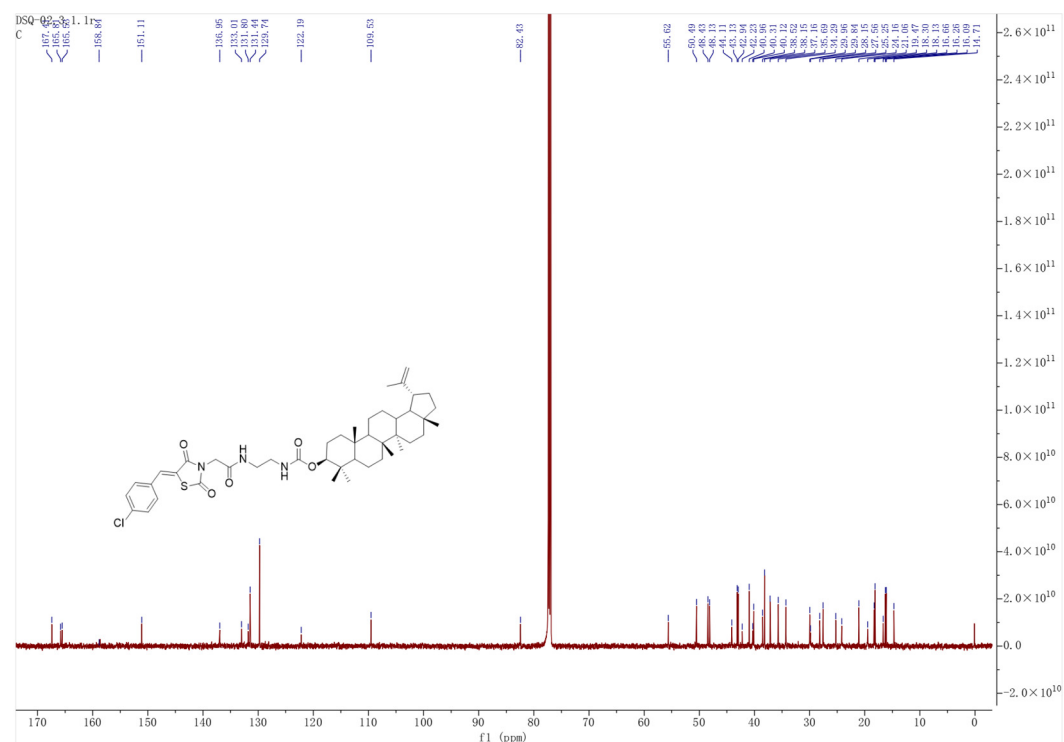
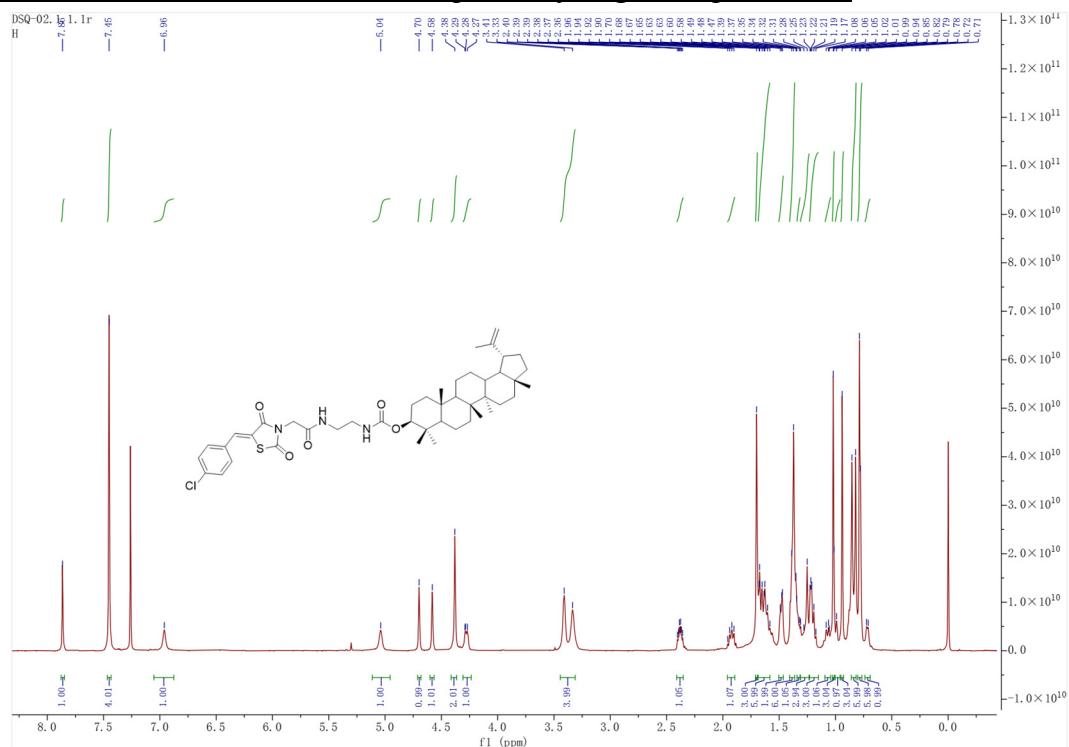


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1: TOF MS ES+
2.17e+005

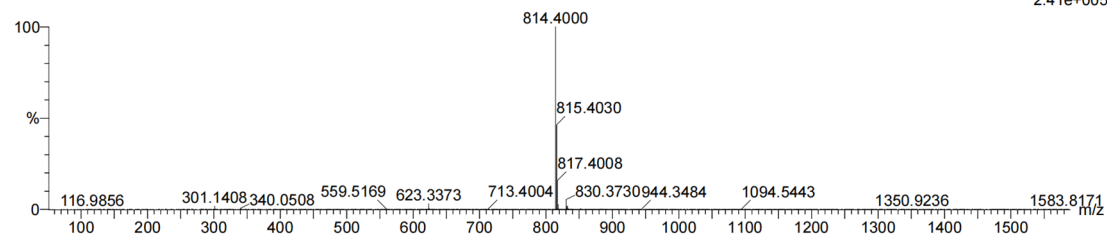


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12b

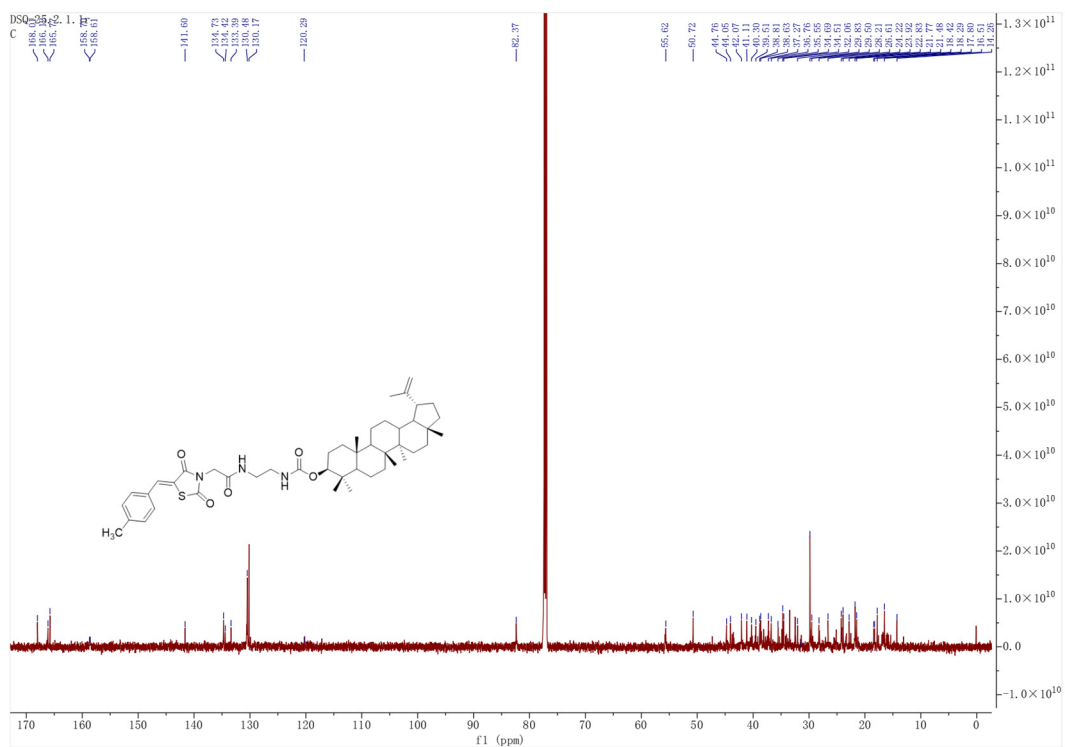
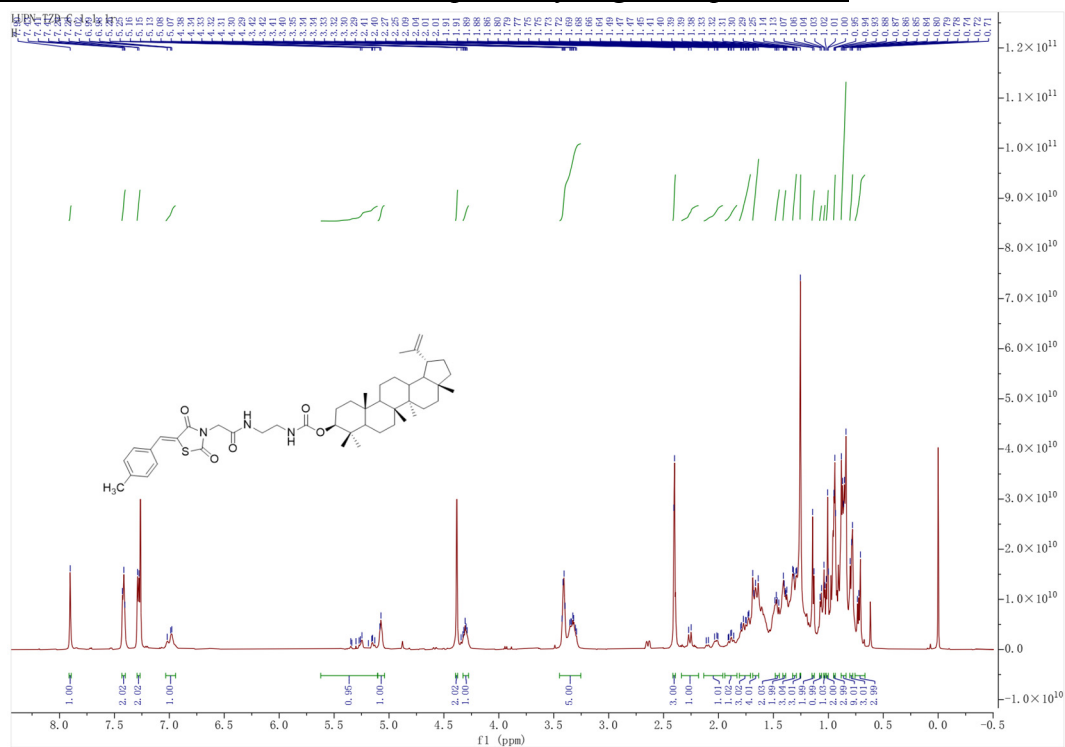


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240107-5-LUP-TZD-B 39 (0.169)

1: TOF MS ES+
2.41e+005

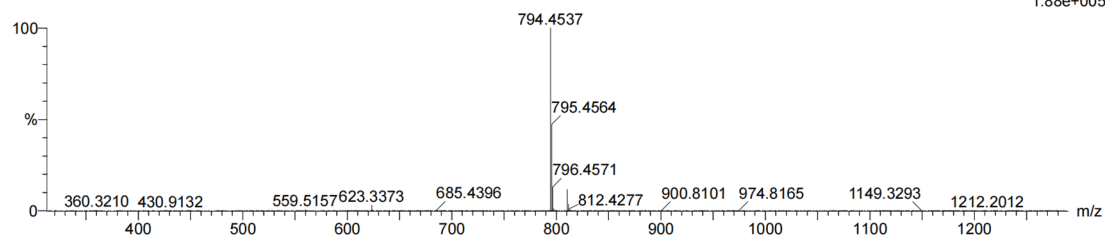


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12c

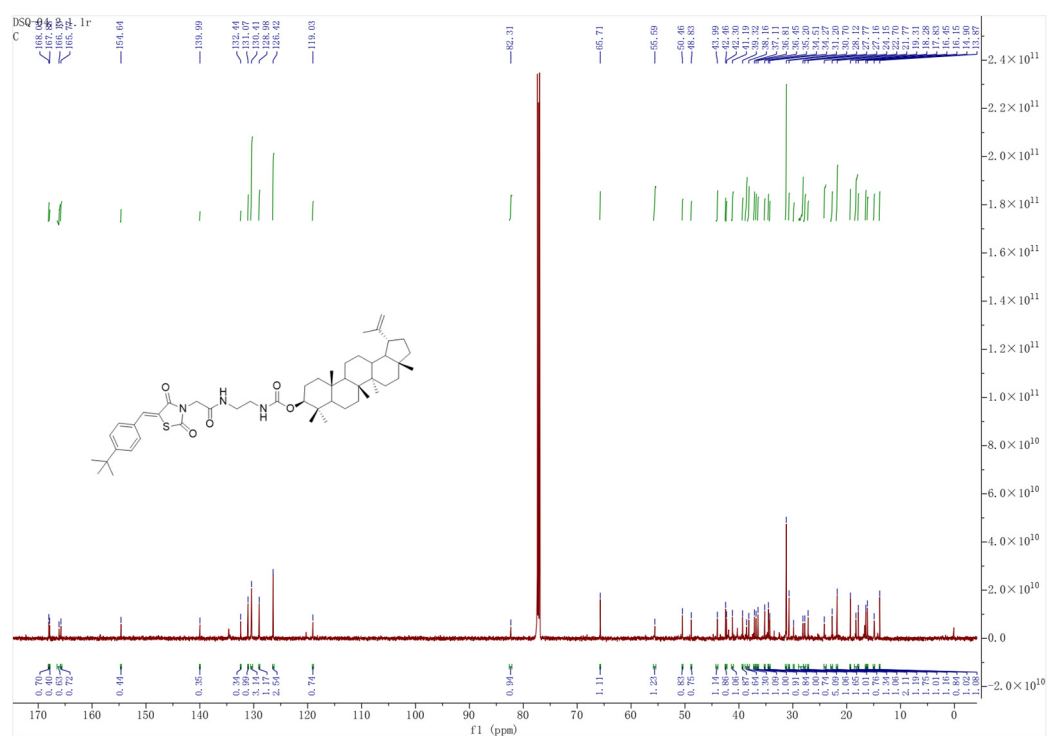
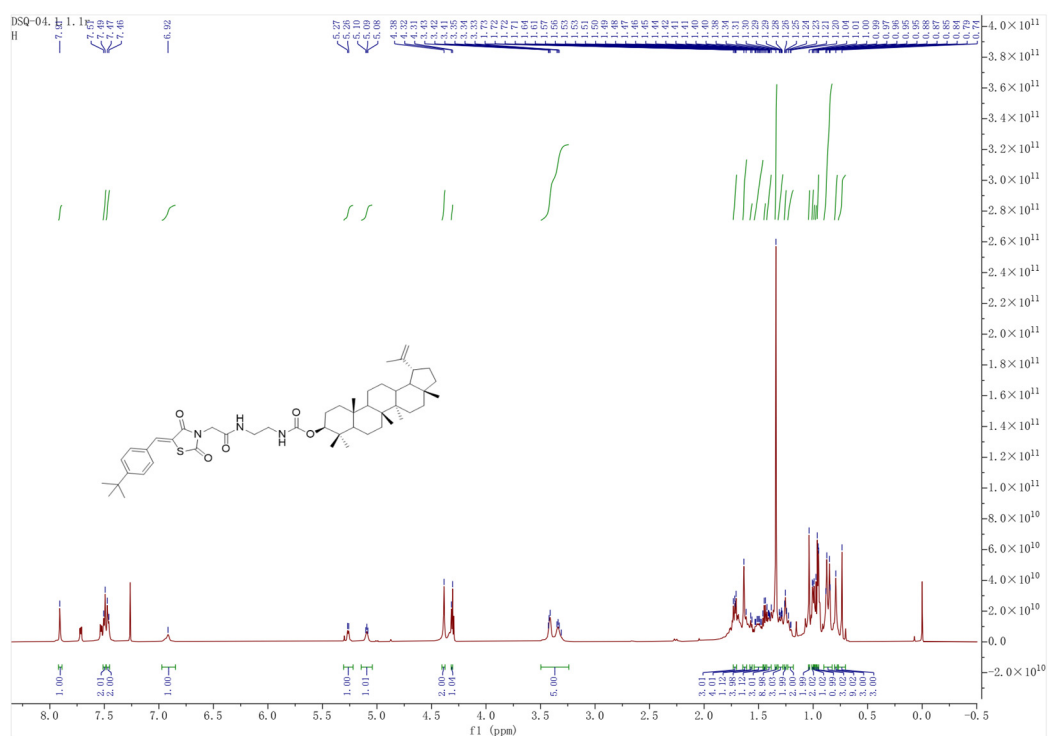


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240107-5-LUP-TZD-C 46 (0.194)

1: TOF MS ES+
1.88e+005

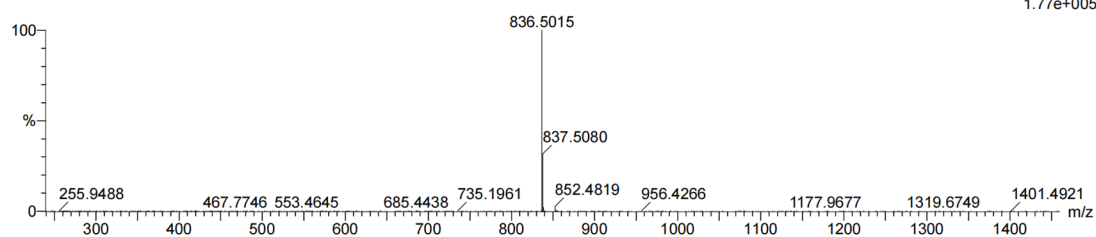


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12d

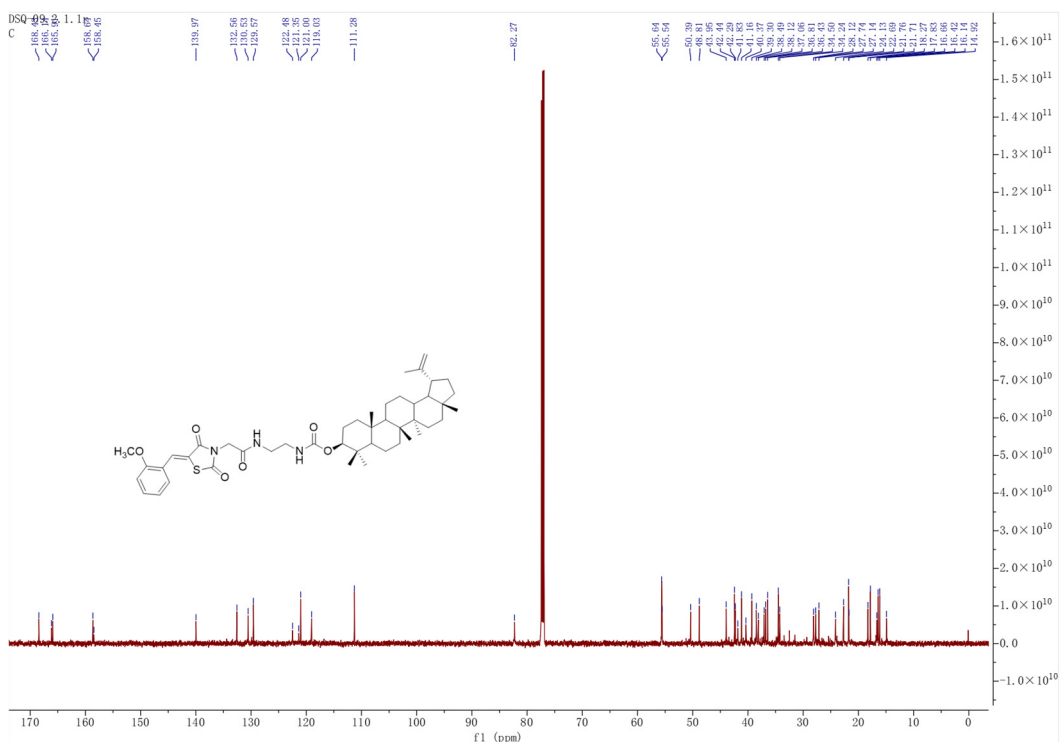
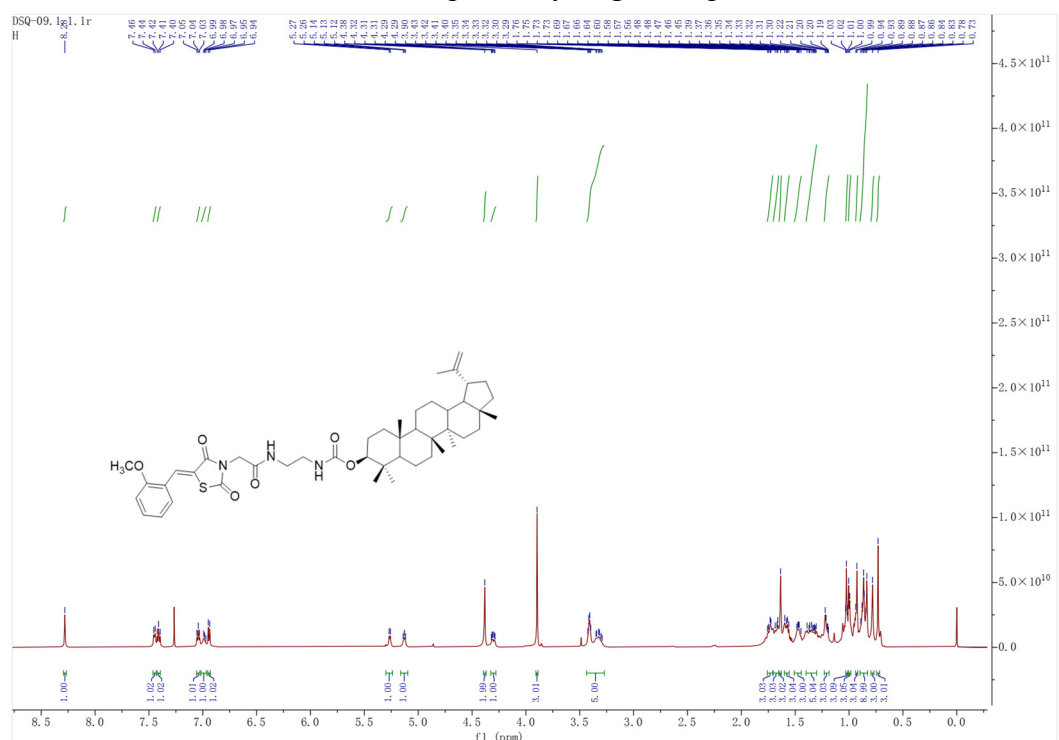


6
231202-15-LUPN-TZD-D 1 (0.037)

1: TOF MS ES+
1.77e+005

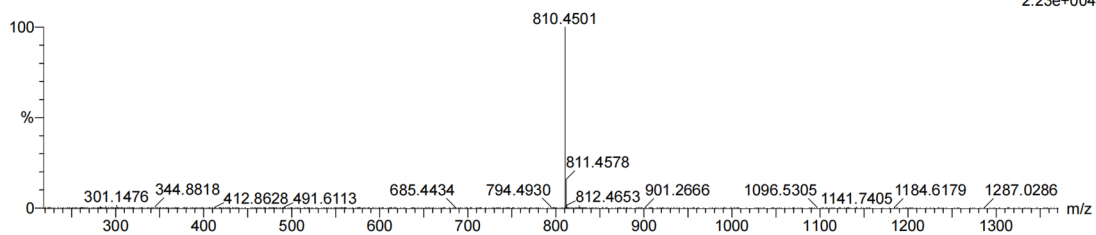


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12e

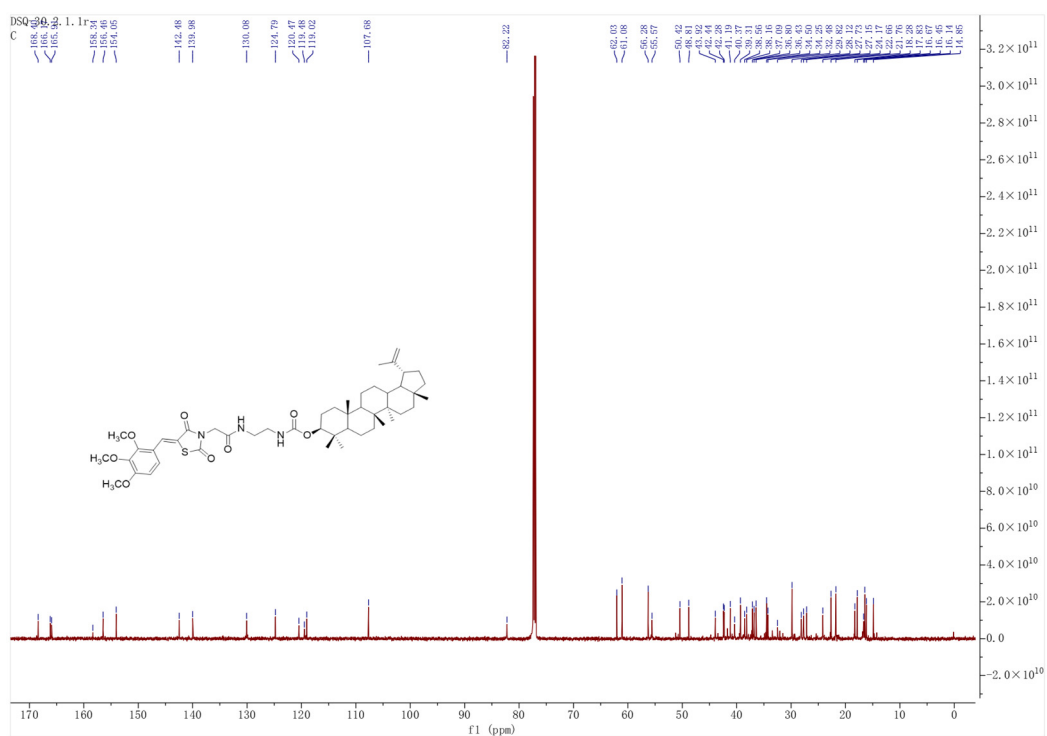
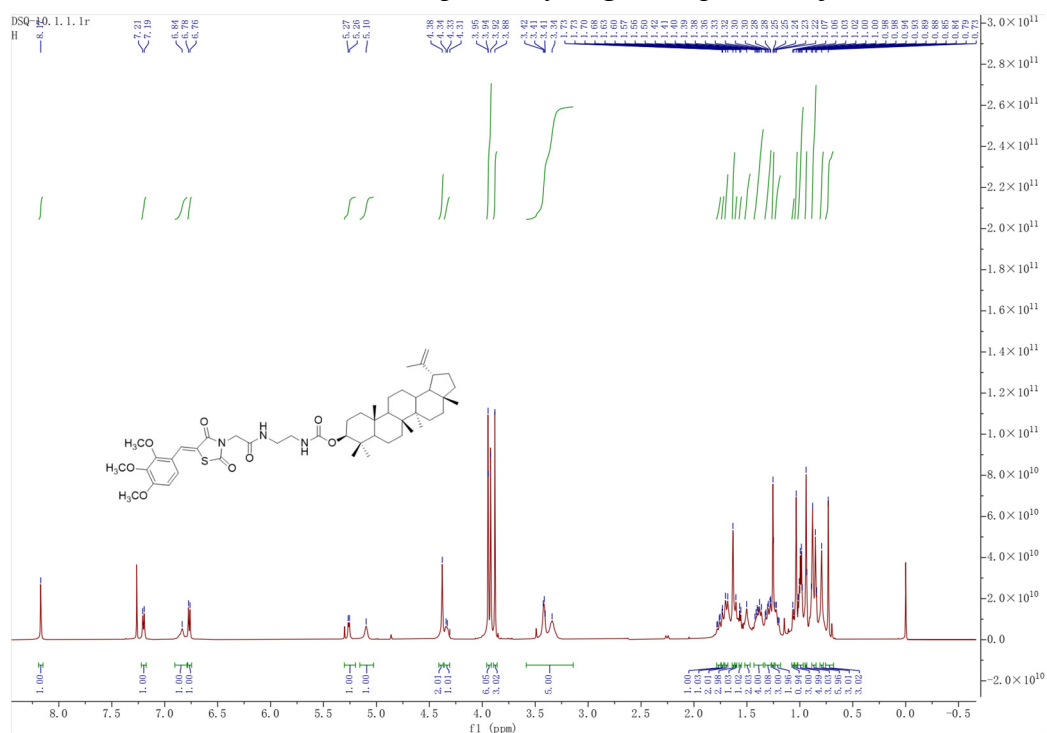


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231202-15-LUPN-TZD-I 93 (0.929)

1: TOF MS ES+
2.23e+004

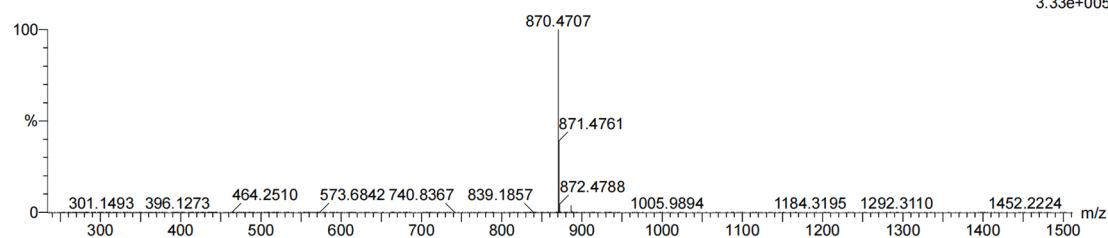


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12f

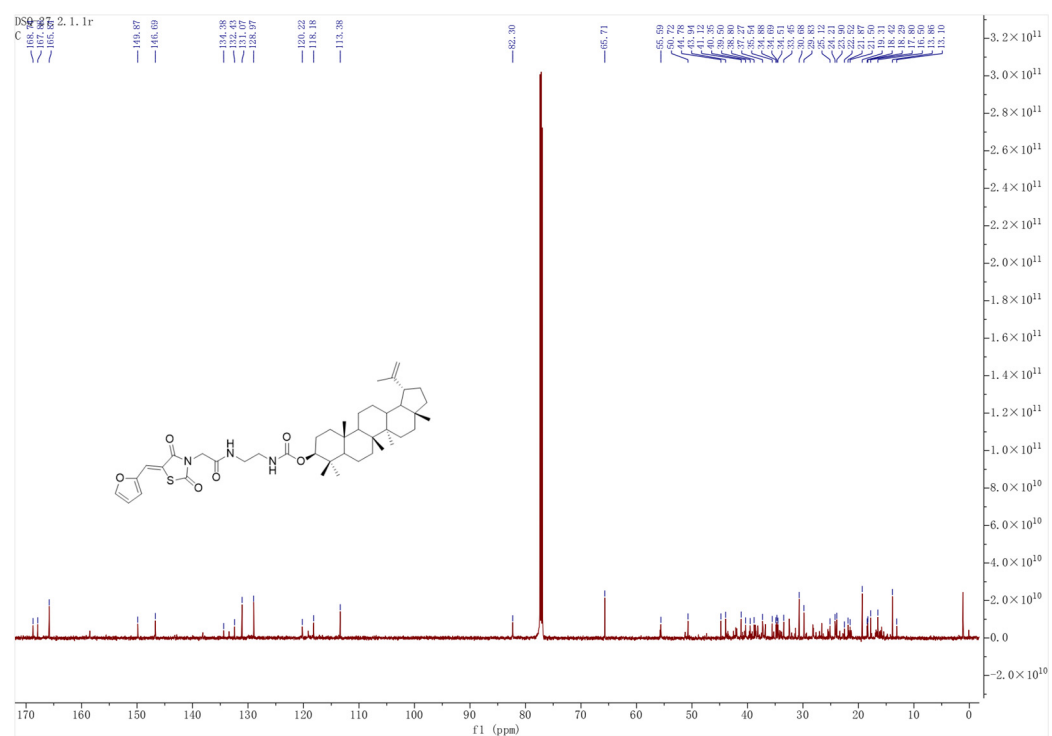
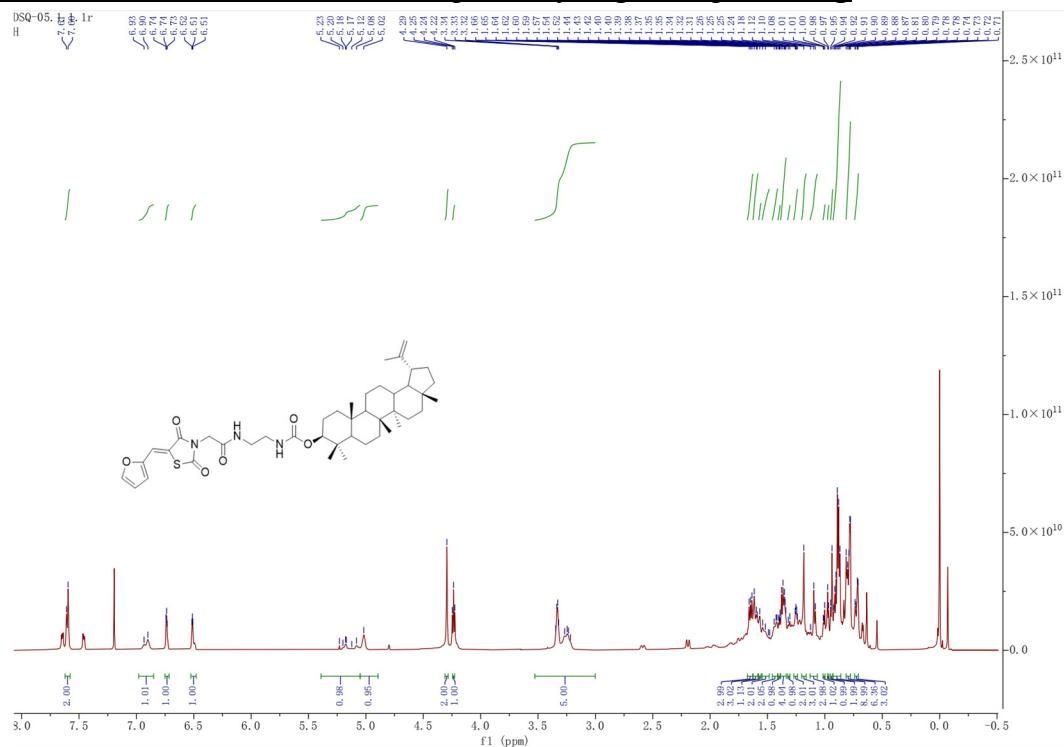


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231202-15-LUPN-TZD-J 92 (0.920)

1: TOF MS ES+
3.33e+005

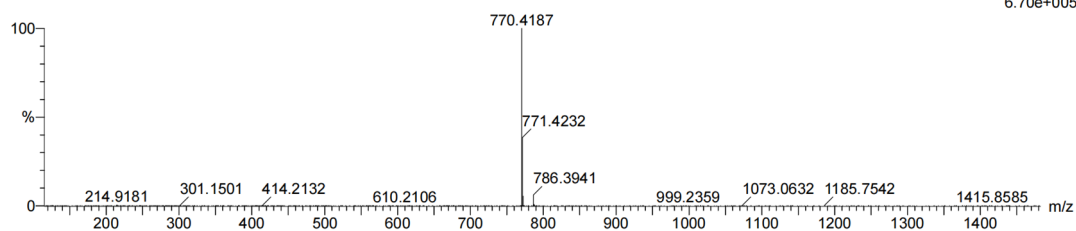


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12g

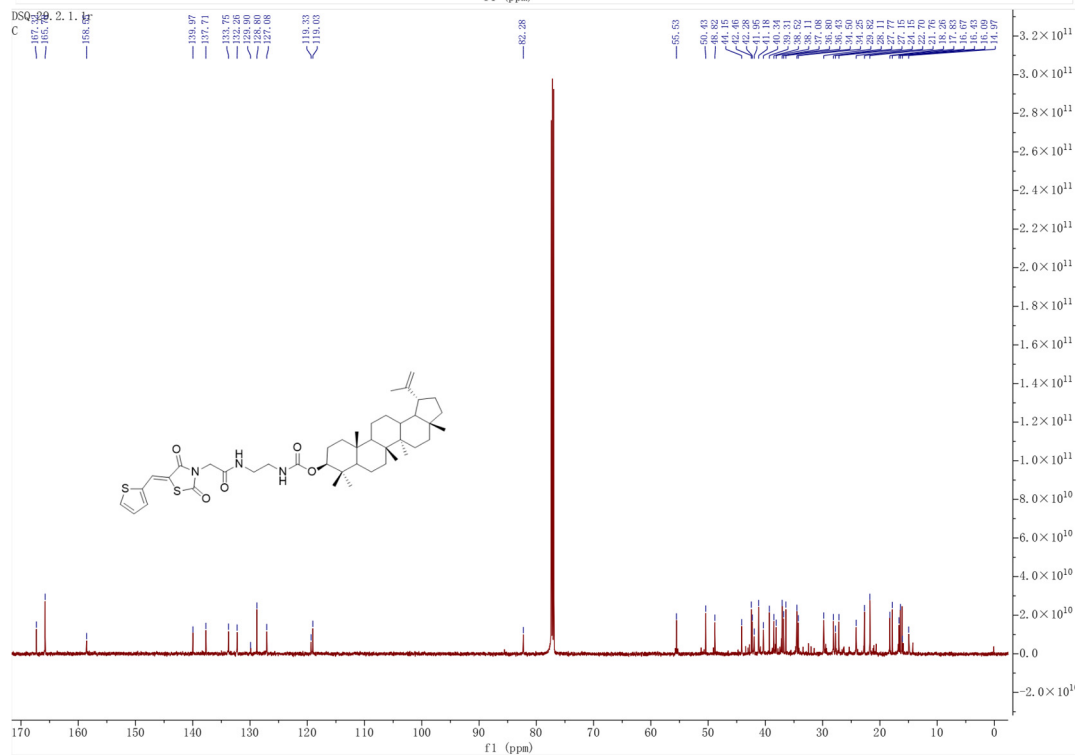
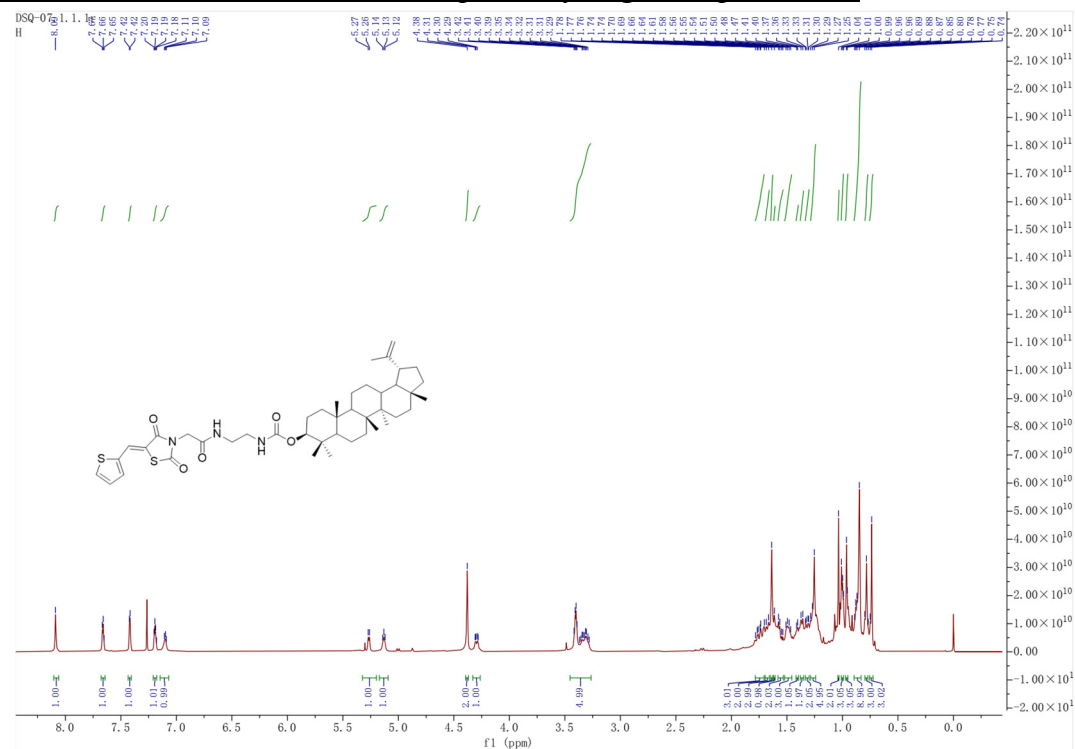


6
231202-15-LUPN-TZD-E 83 (0.832)

1: TOF MS ES+
6.70e+005

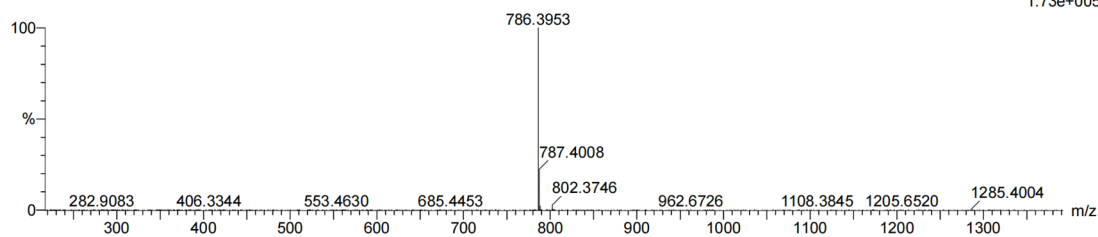


¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12h

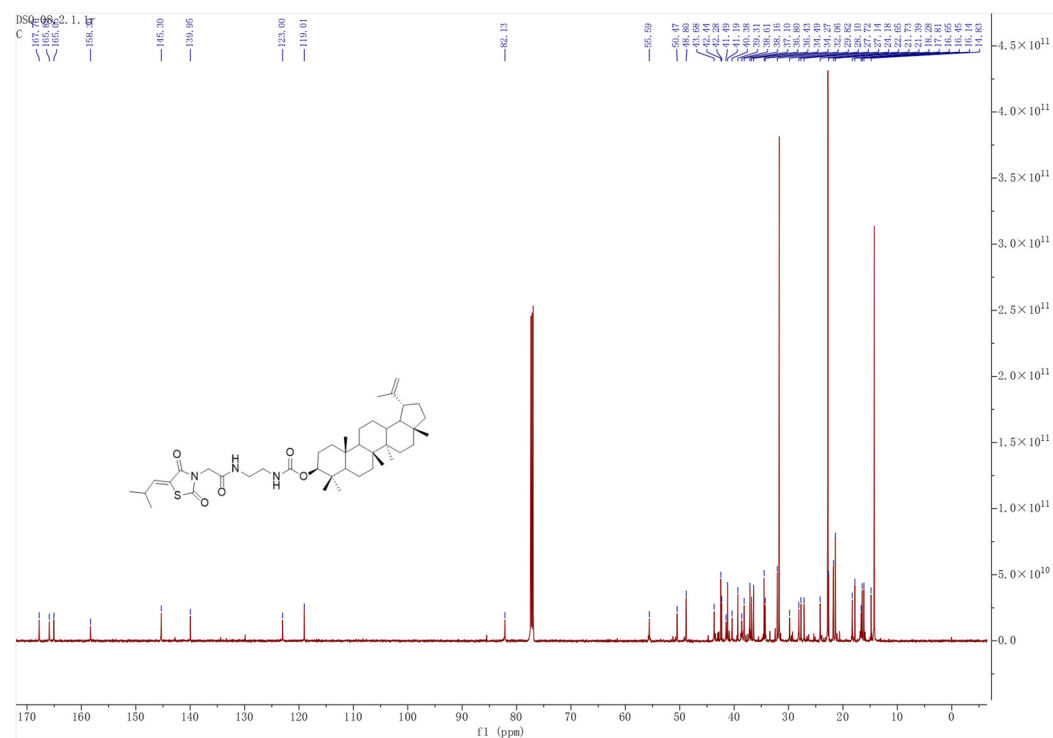
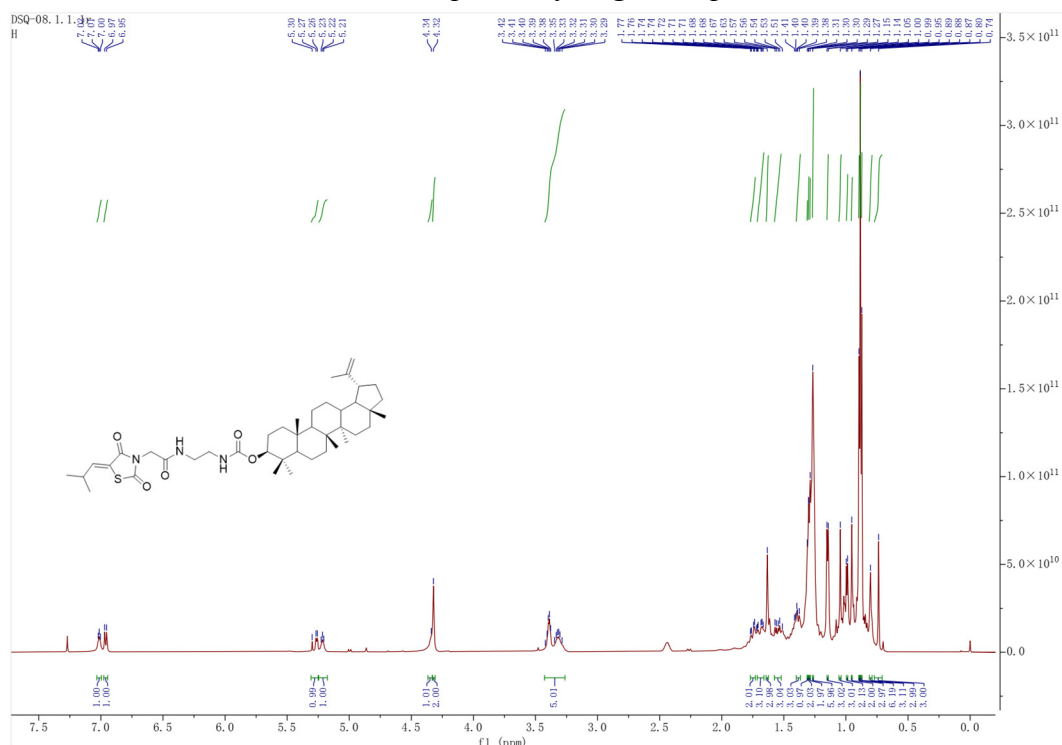


6
231202-15-LUPN-TZD-G 98 (0.972)

1: TOF MS ES+
1.73e+005



¹H NMR, ¹³C NMR and ESI-HRMS spectra of target compound 12i



6
231202-15-LUPN-TZD-H 100 (0.989)

1: TOF MS ES+
1.55e+005

