

Supporting Information

Synthesis and discovery of 18 β -glycyrrhetic acid derivatives inhibiting cancer stem cell properties in ovarian cancer cells

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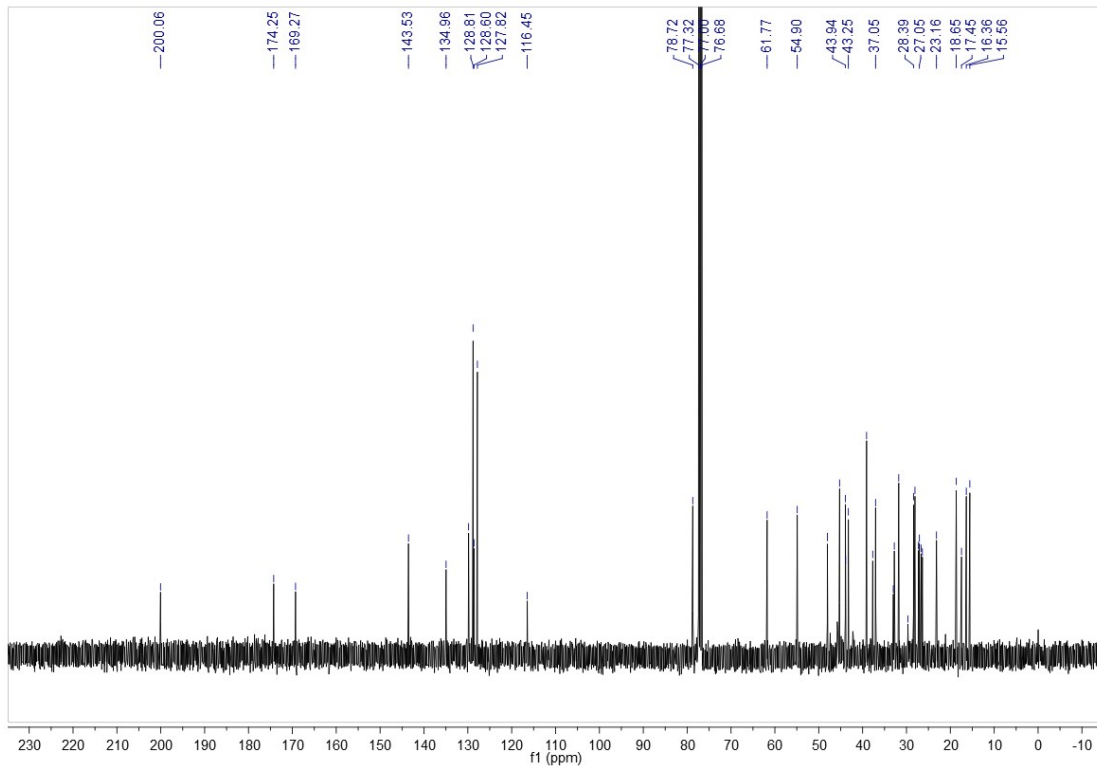
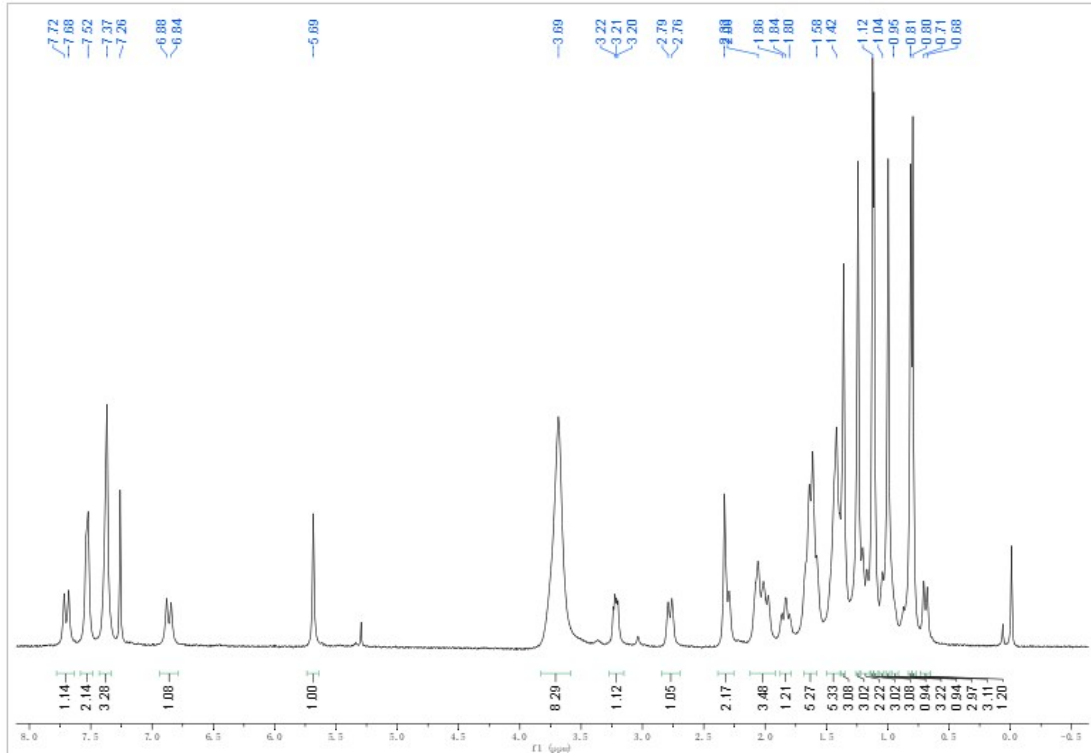
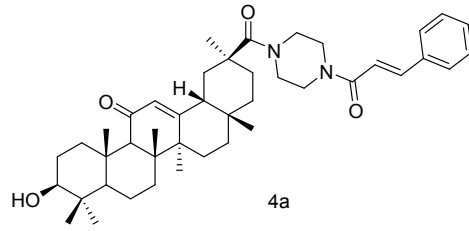
1. Purity of the target compounds 4a-4i and 7a-7i

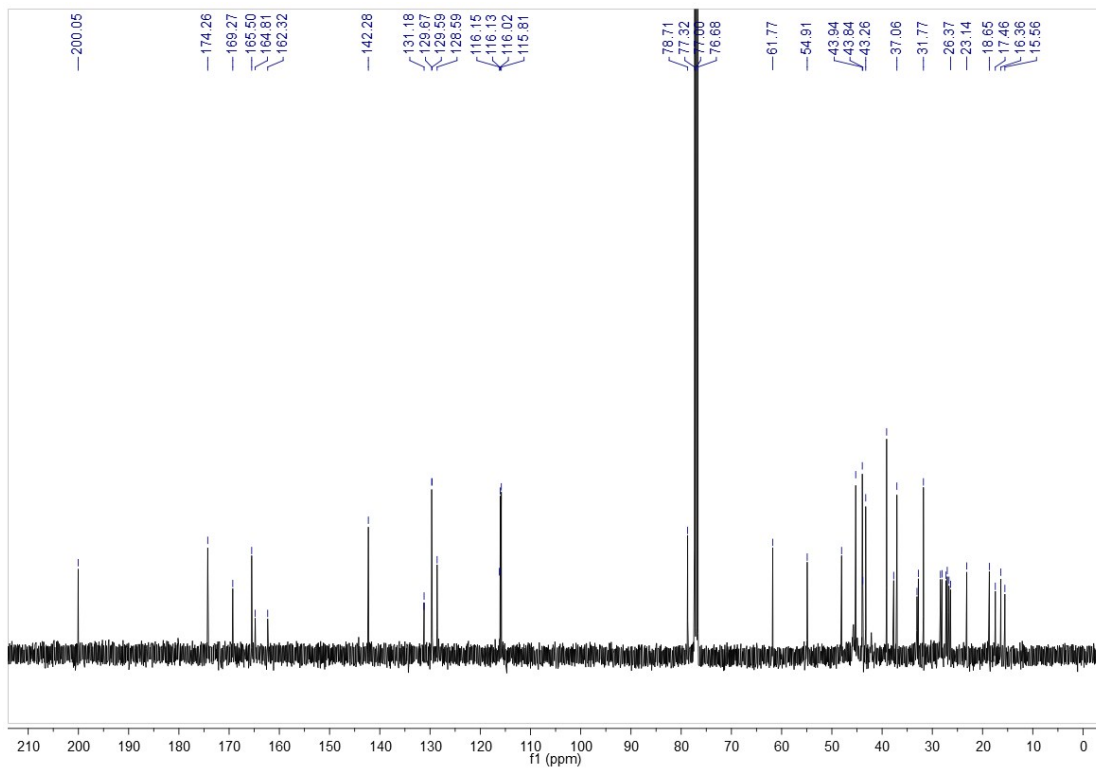
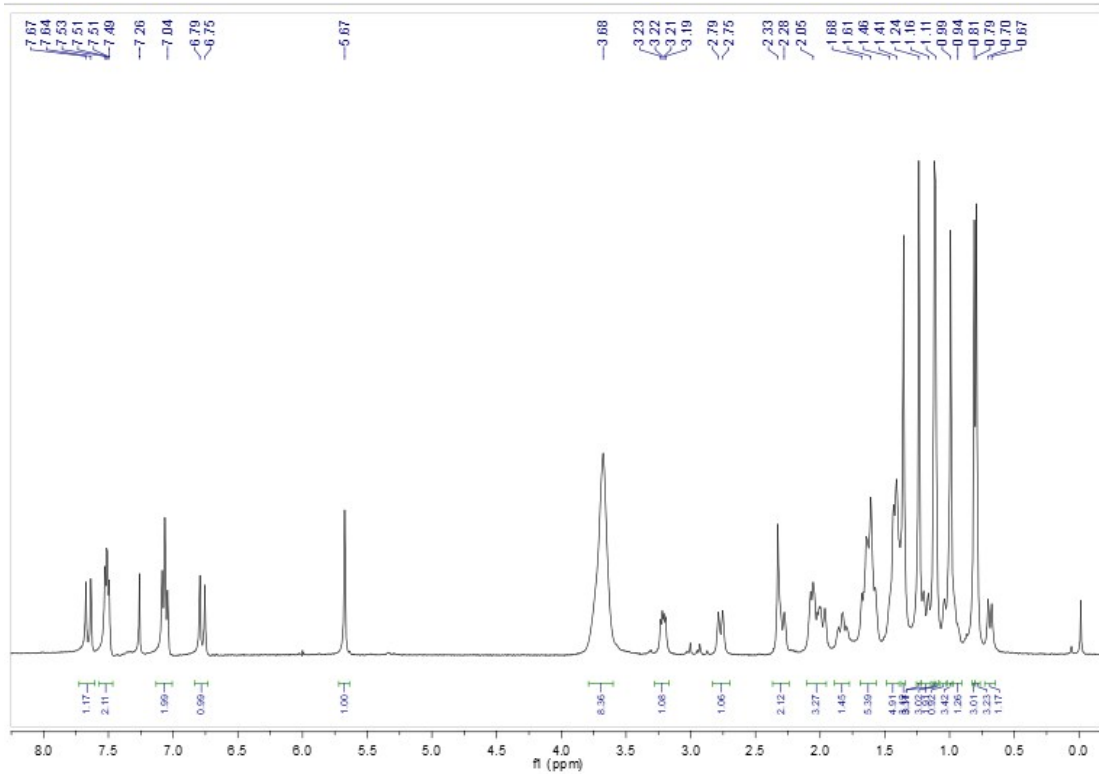
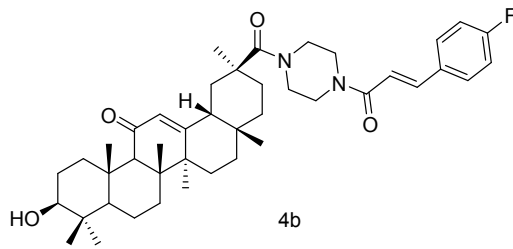
Instrumental equipment and conditions: An Agilent 1260 HPLC (Waldbronn, Germany) with diode array detection (DAD) was employed for chromatographic analyses. The column employed was an Agilent Eclipse Plus C18 (250 × 4.6 mm, 5 μm). The mobile phase used methanol and water (85:15 v/v) with a flow rate of 1.0 mLmin⁻¹, and the column temperature was held at 25 °C. The injection volume was set at 10 μL with detection wavelength of 283 nm.

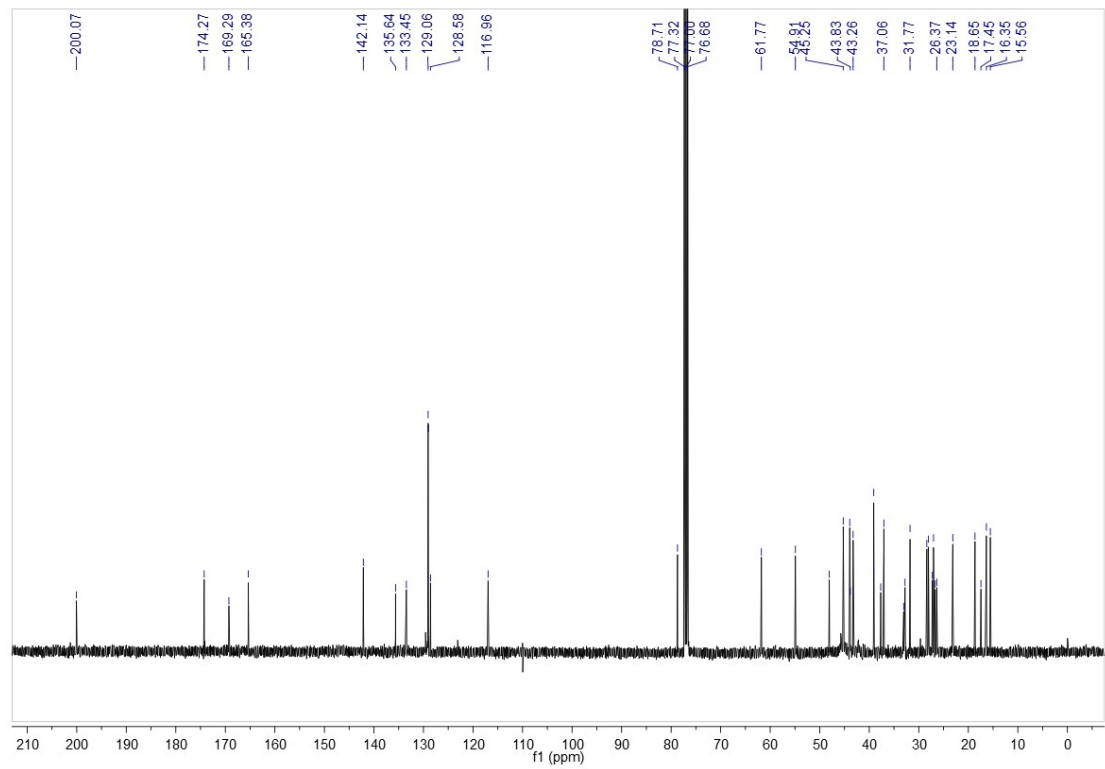
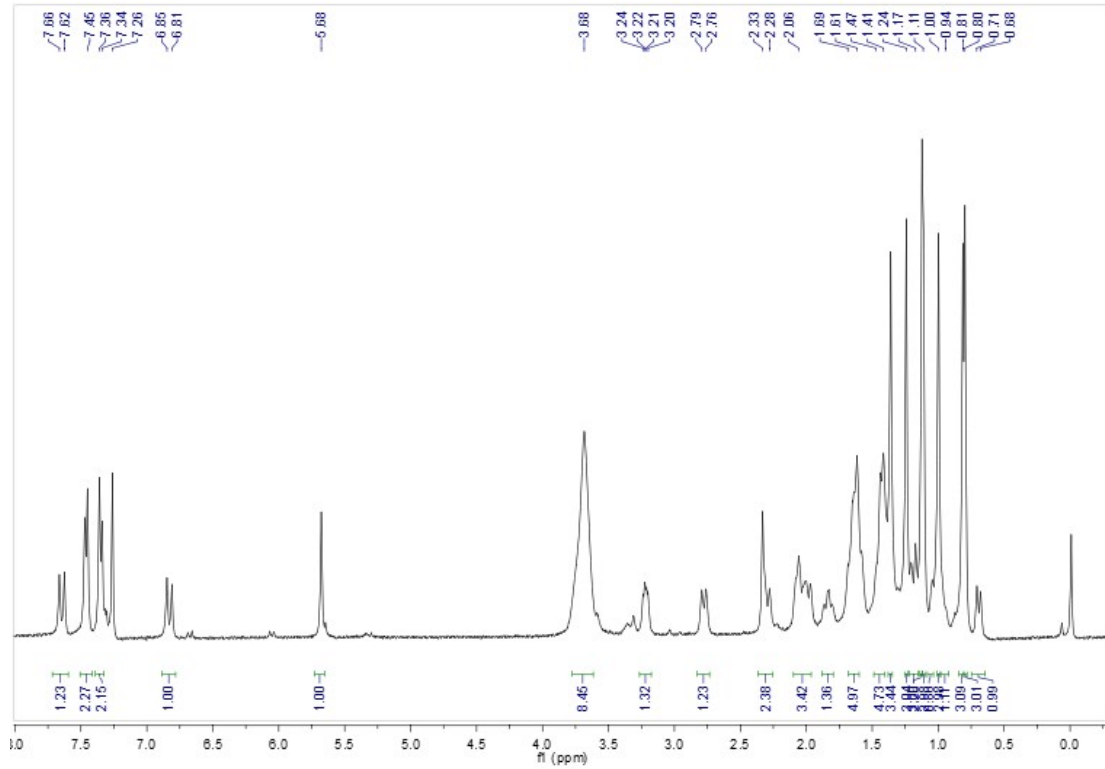
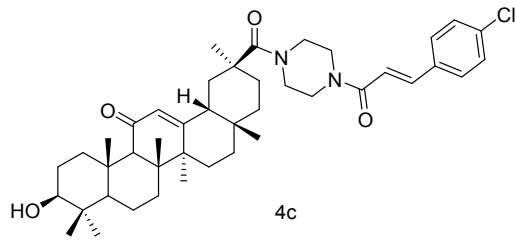
Table S1. Purity of the target compounds **4a-4i** and **7a-7i**

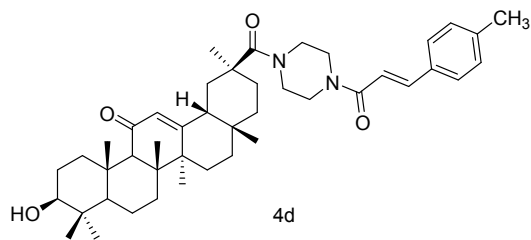
Compounds	t _R (min)	Purity (%)
4a	14.214	96.45
4b	14.364	98.72
4c	9.369	99.45
4d	18.244	99.68
4e	14.272	98.69
4f	10.649	99.70
4g	12.303	98.20
4h	15.154	97.52
4i	14.220	97.60
7a	12.713	99.59
7b	12.669	99.20
7c	16.682	99.86
7d	16.266	97.57
7e	14.819	98.71
7f	12.499	99.35
7g	10.980	98.97
7h	13.250	99.07
7i	15.614	99.84

2. NMR data of the target compounds 4a-4i and 7a-7i

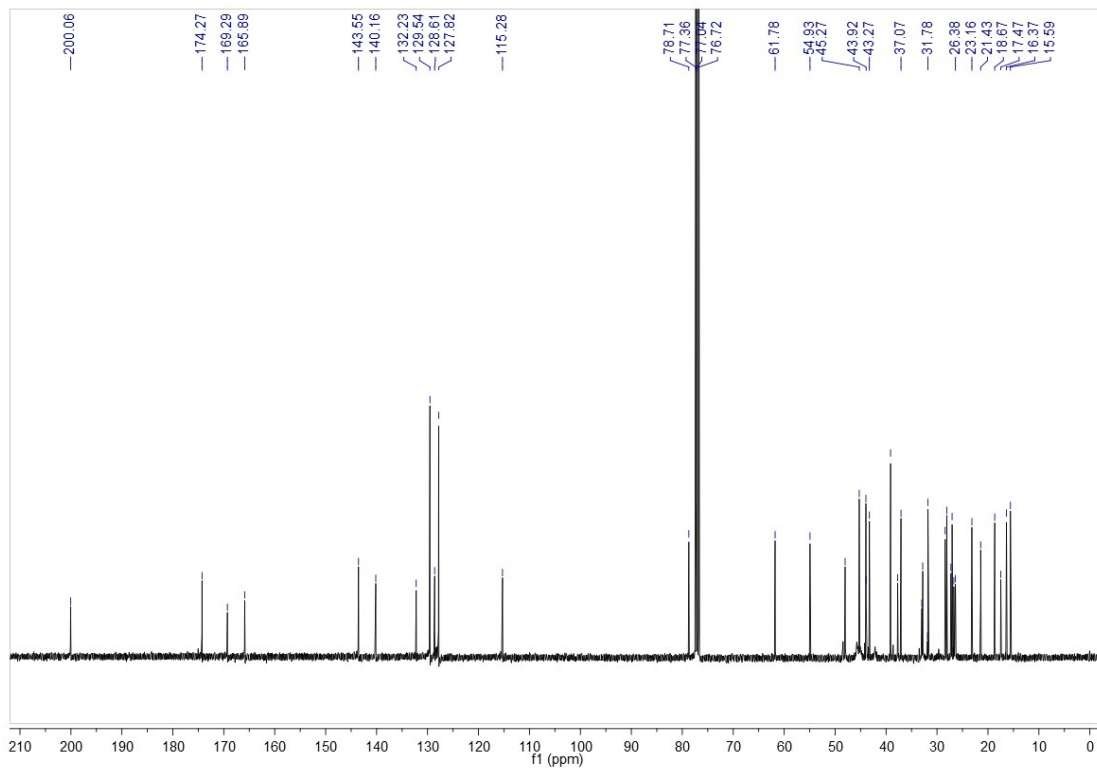
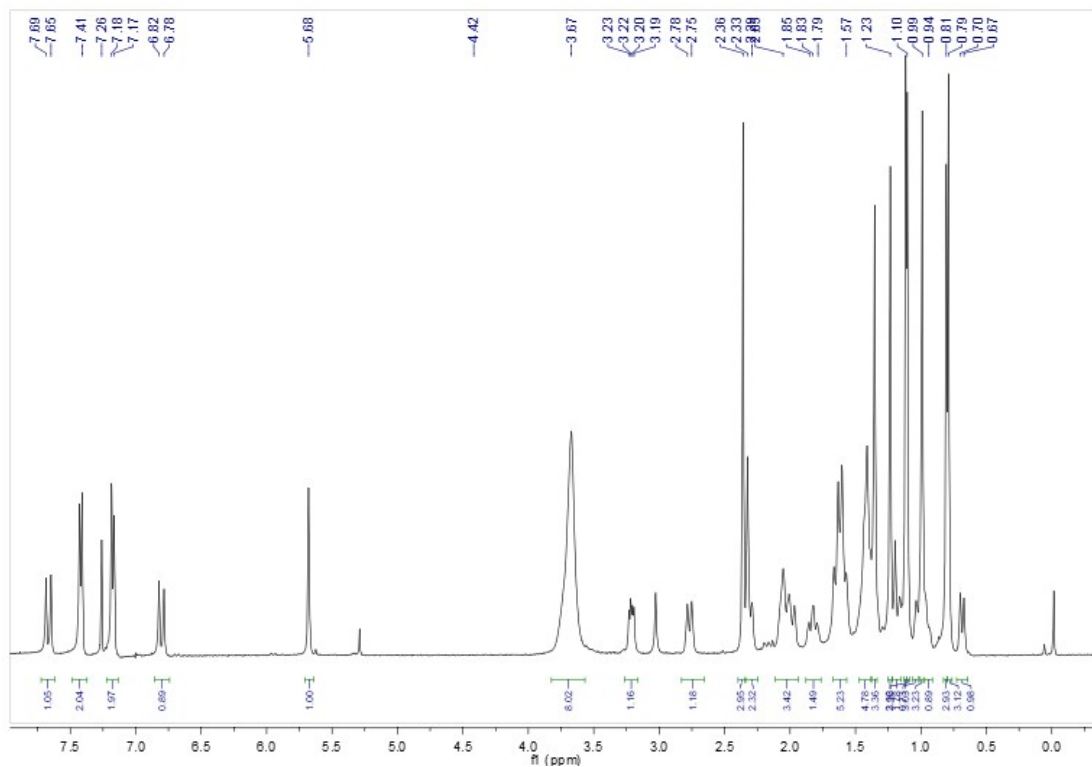


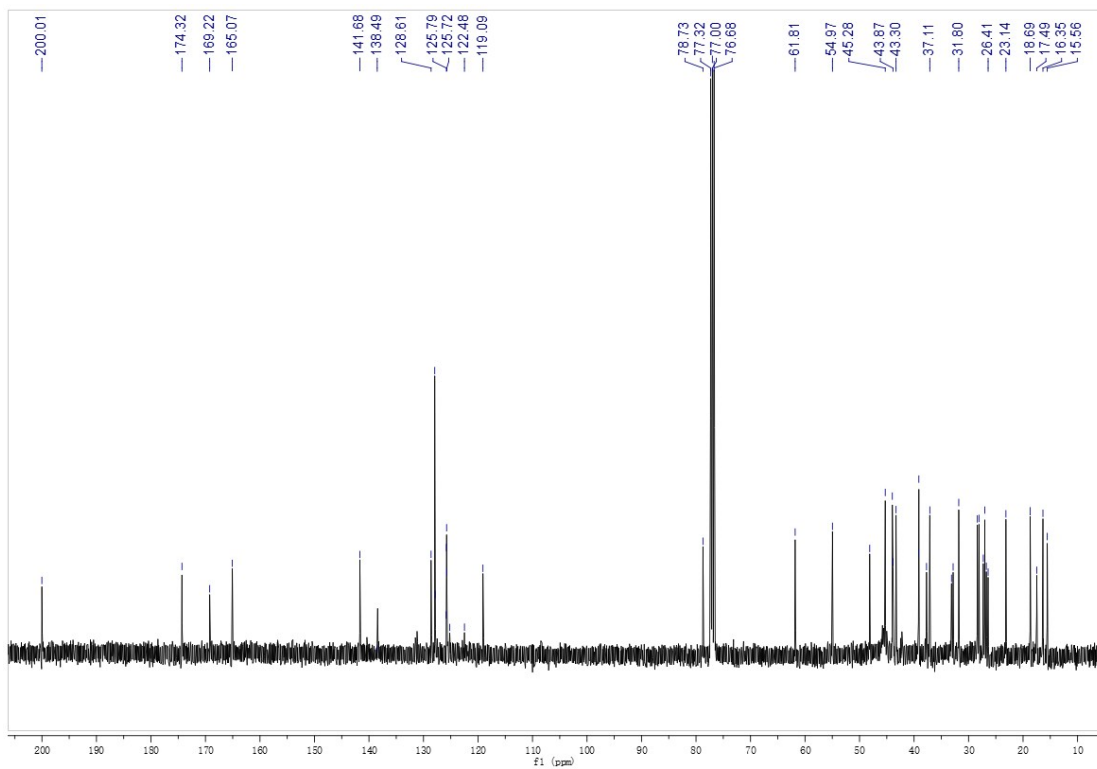
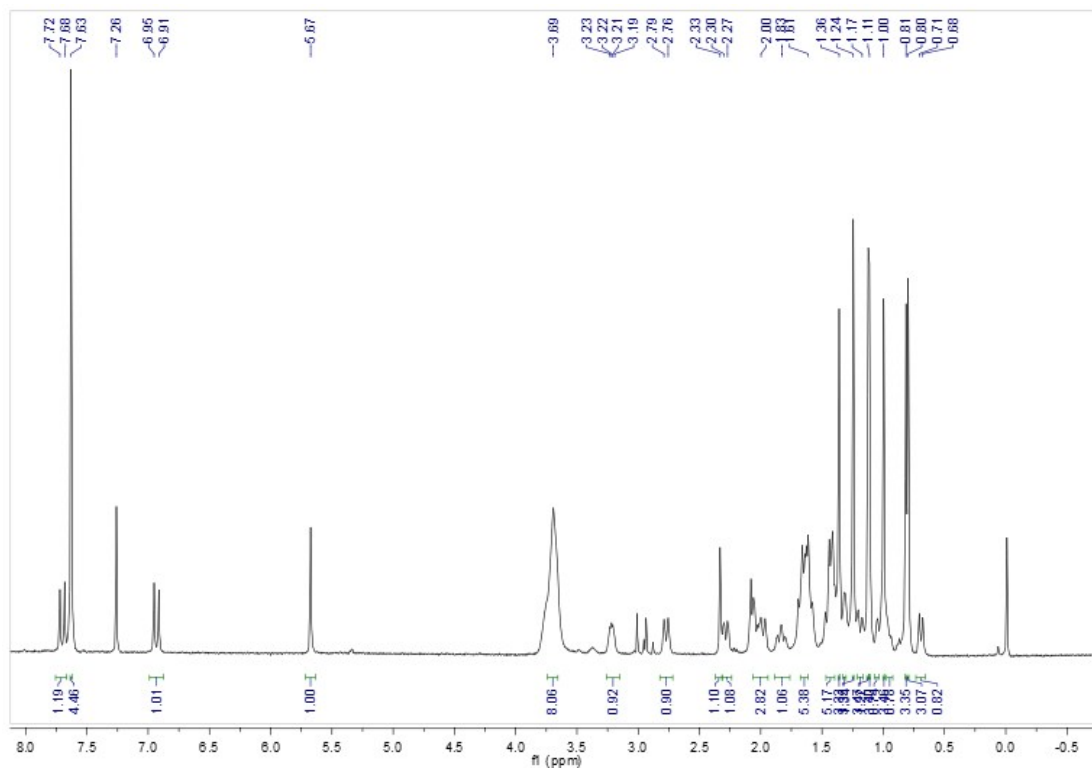
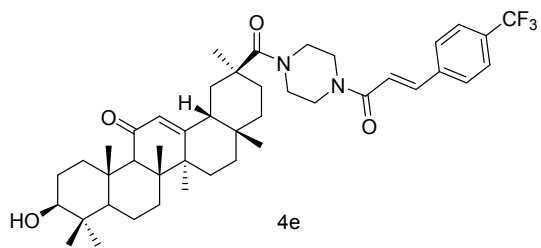


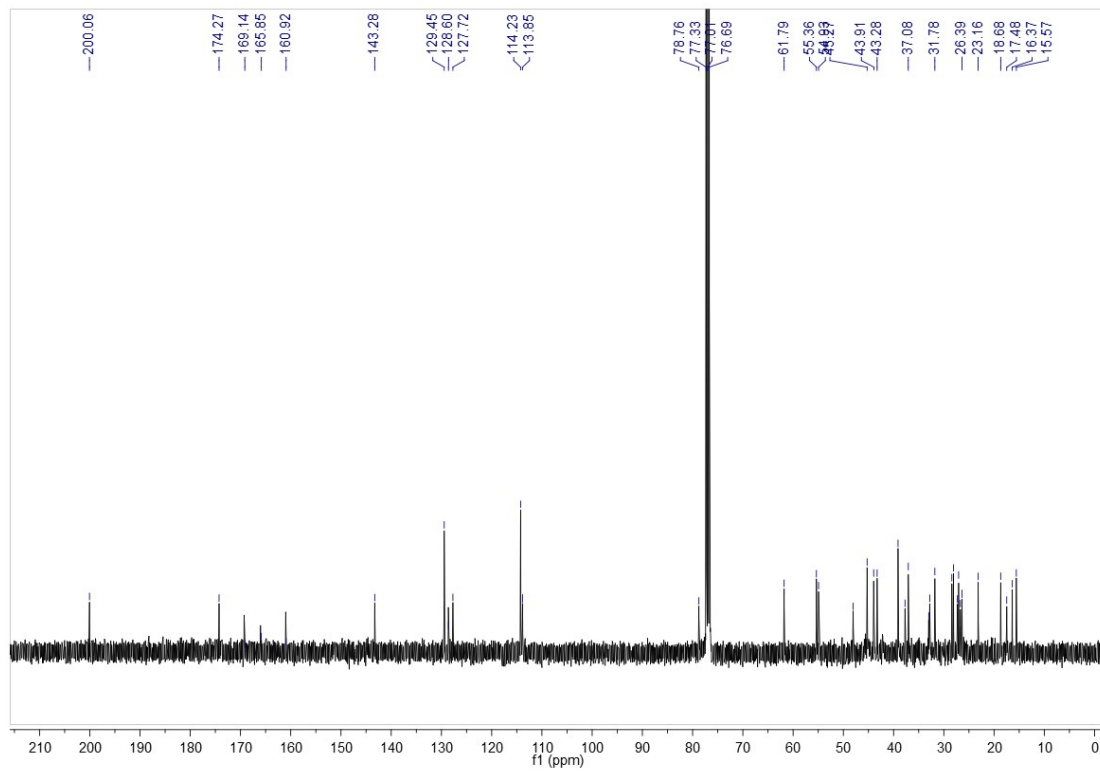
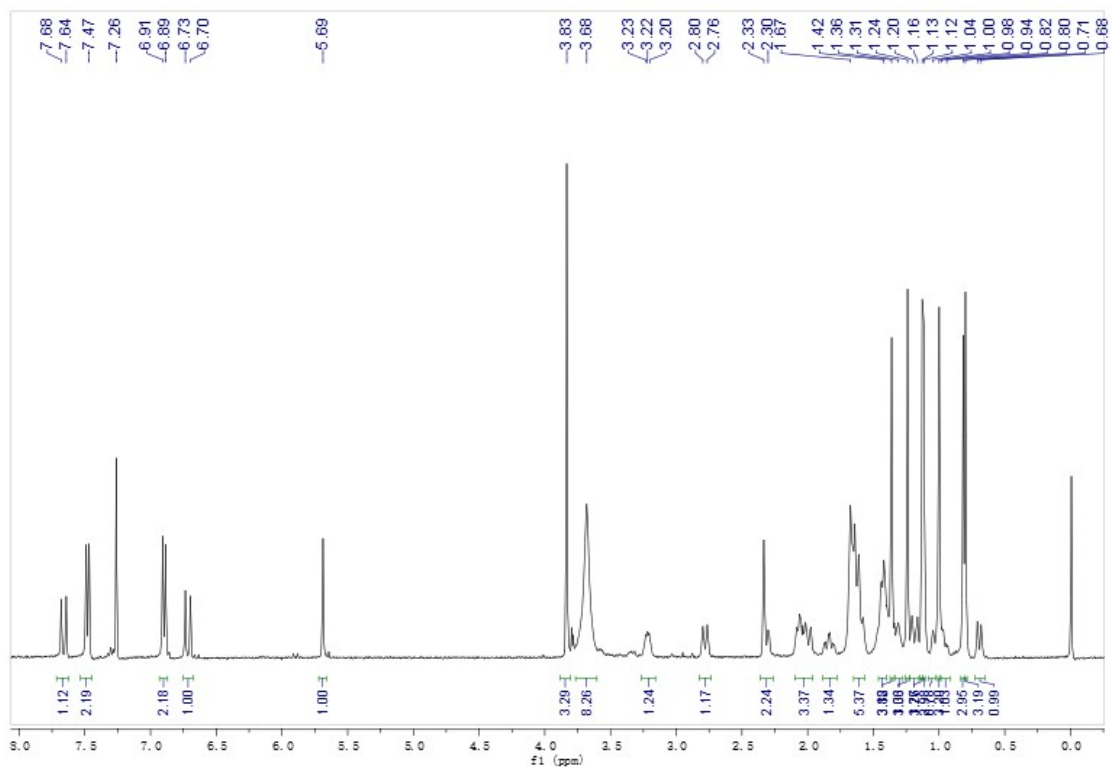
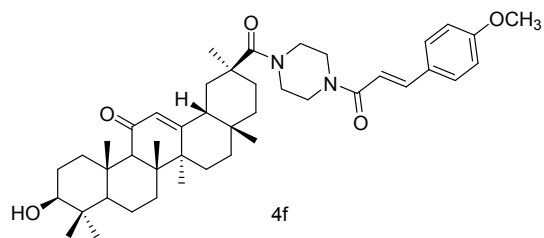


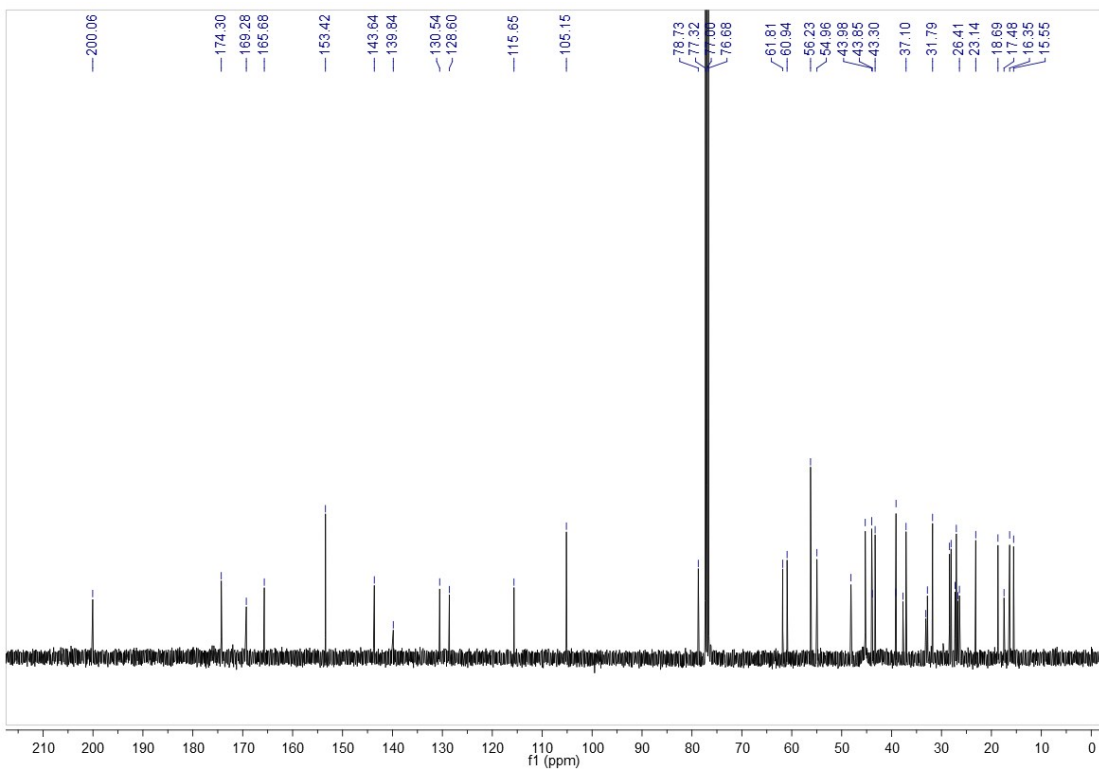
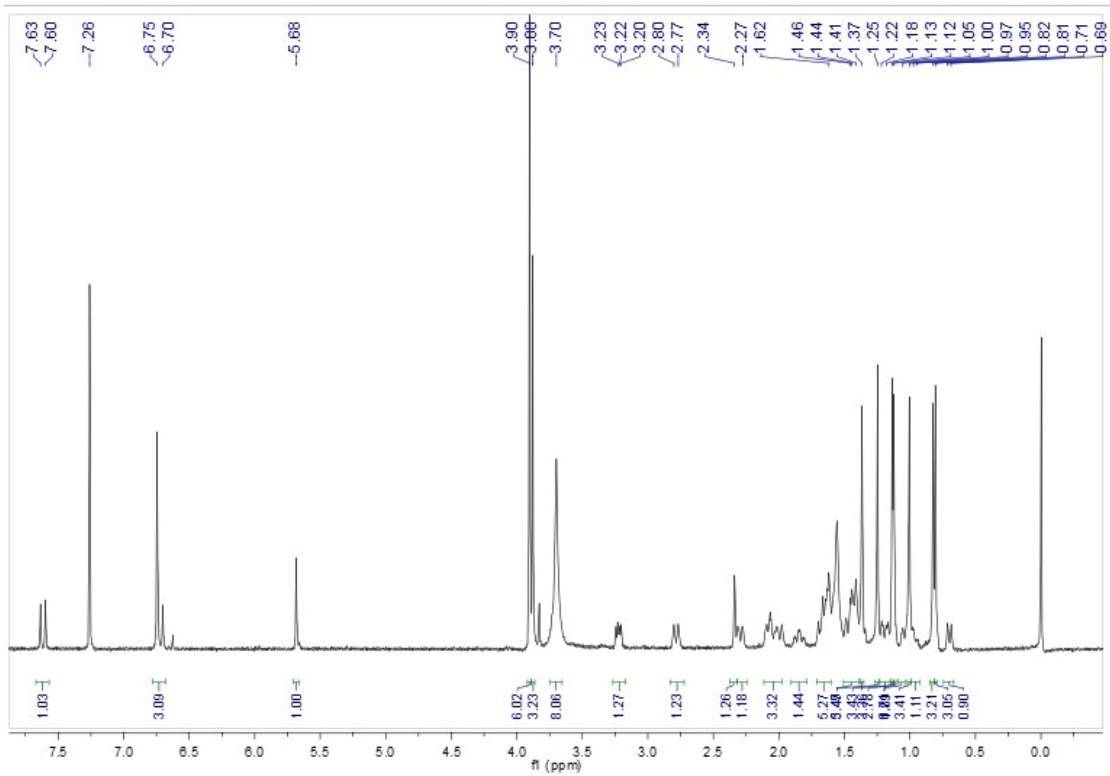
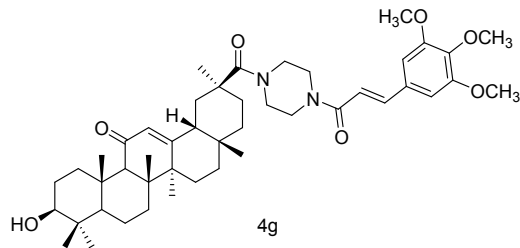


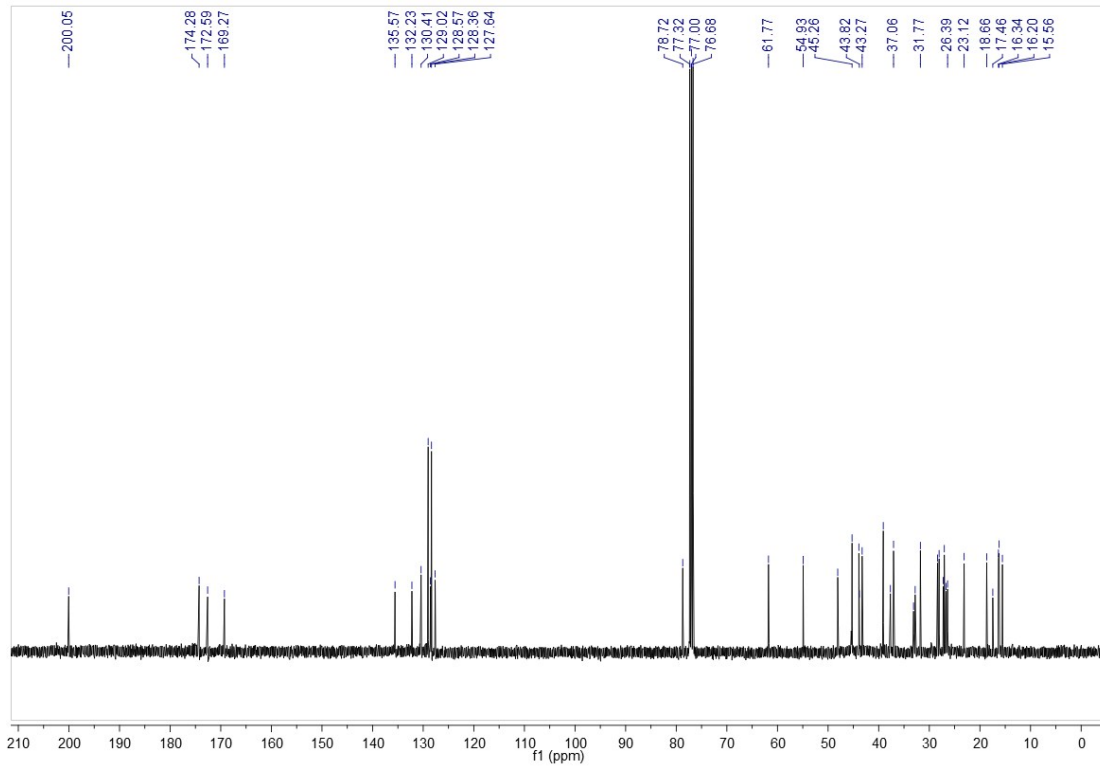
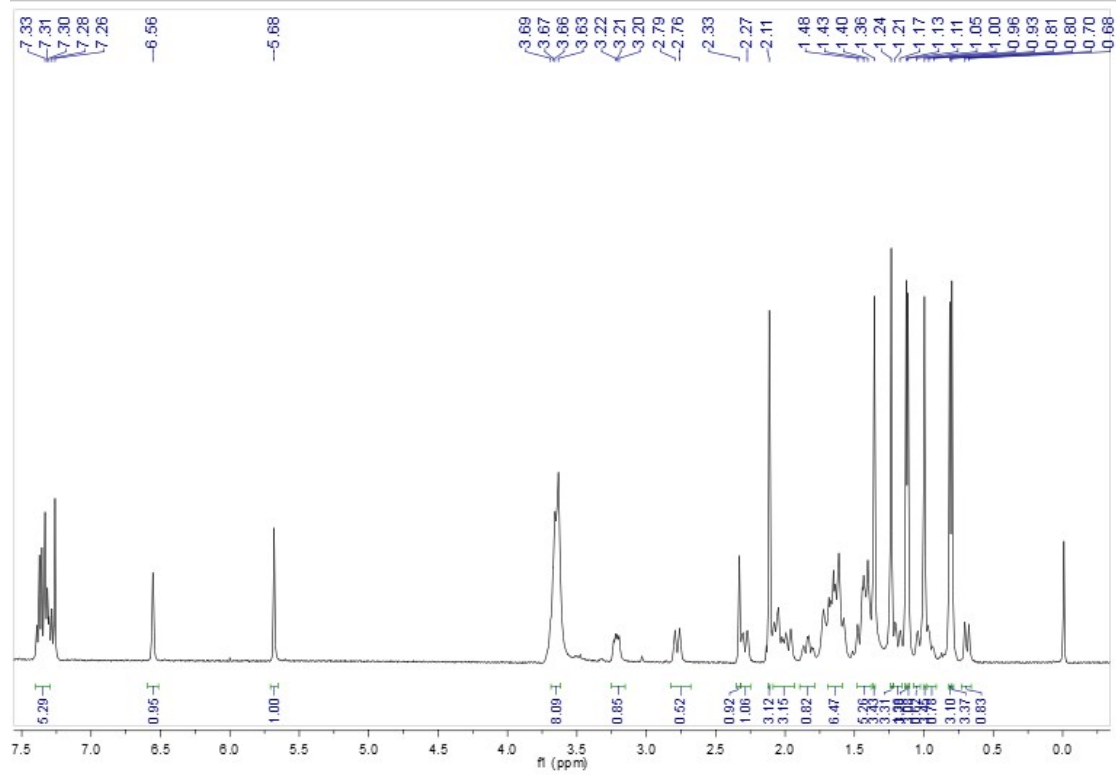
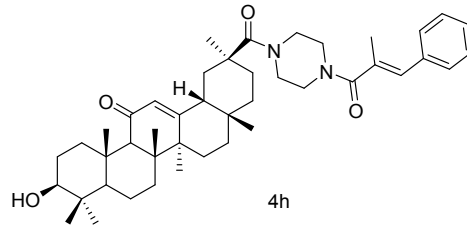
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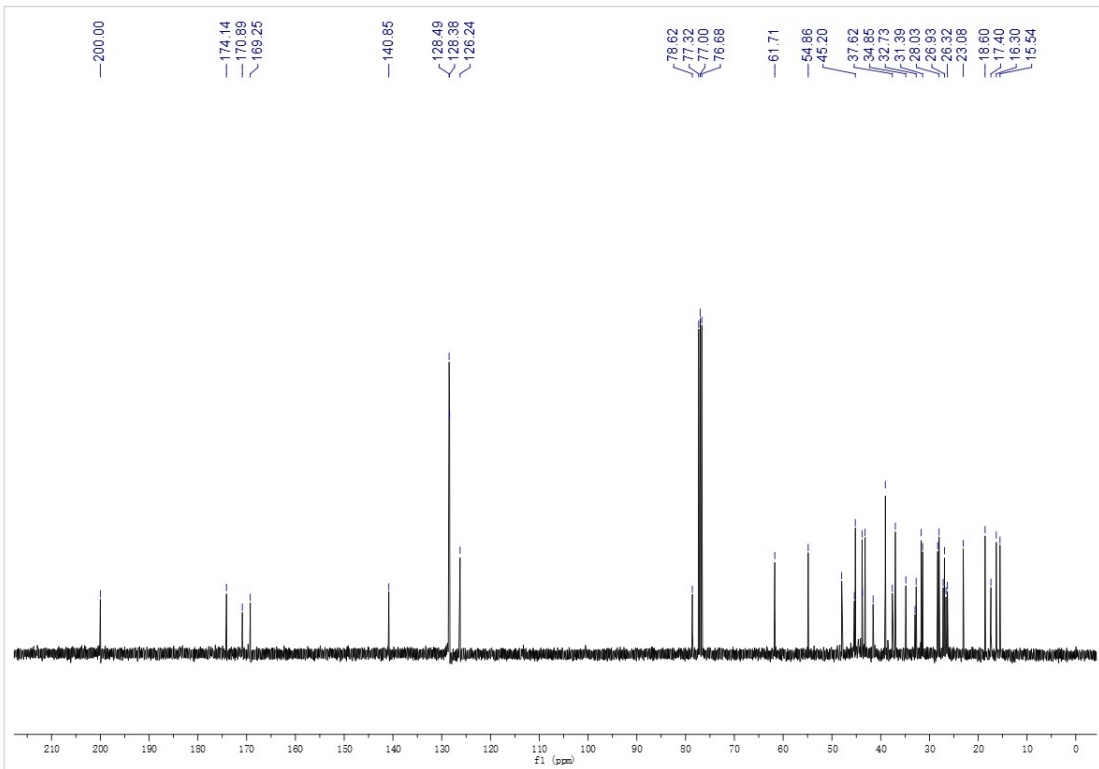
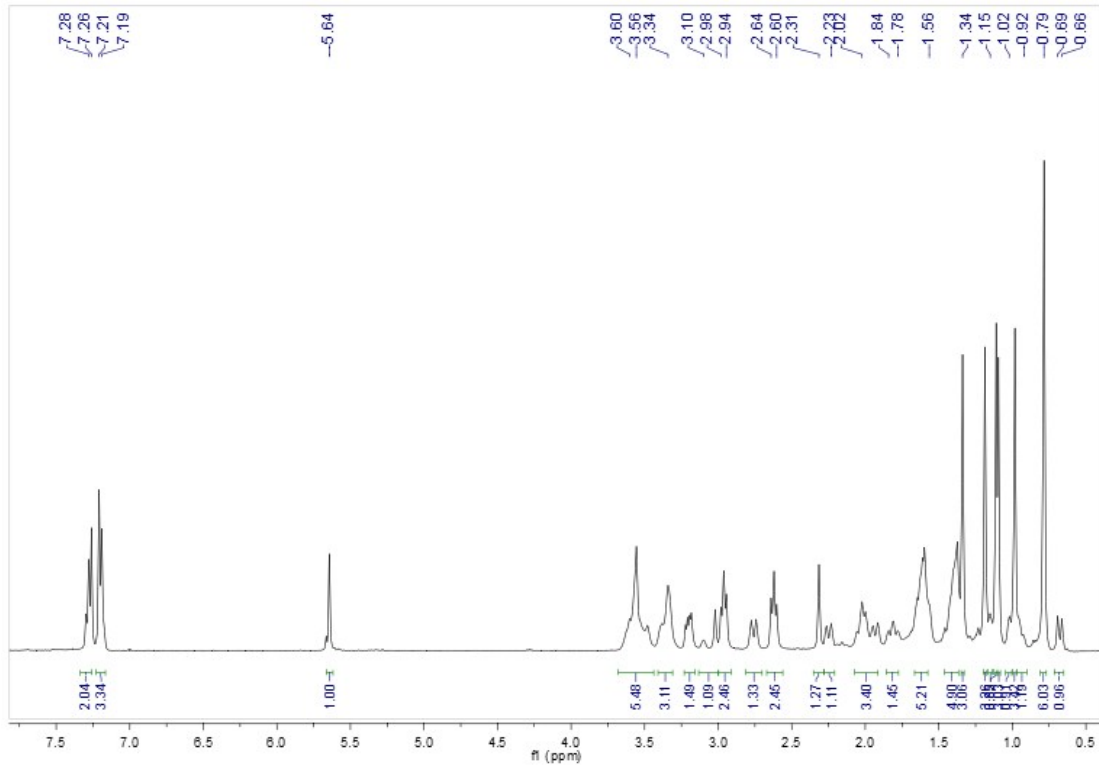
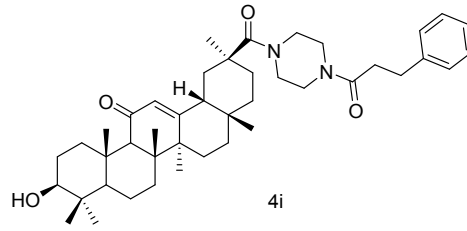


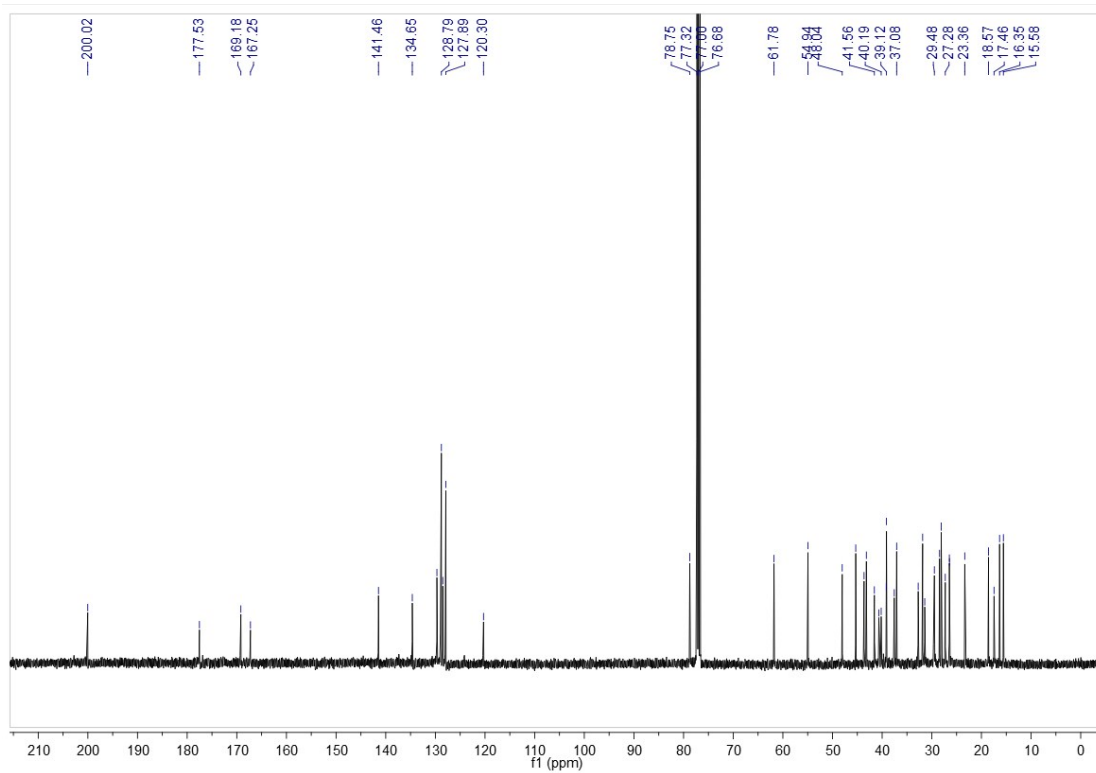
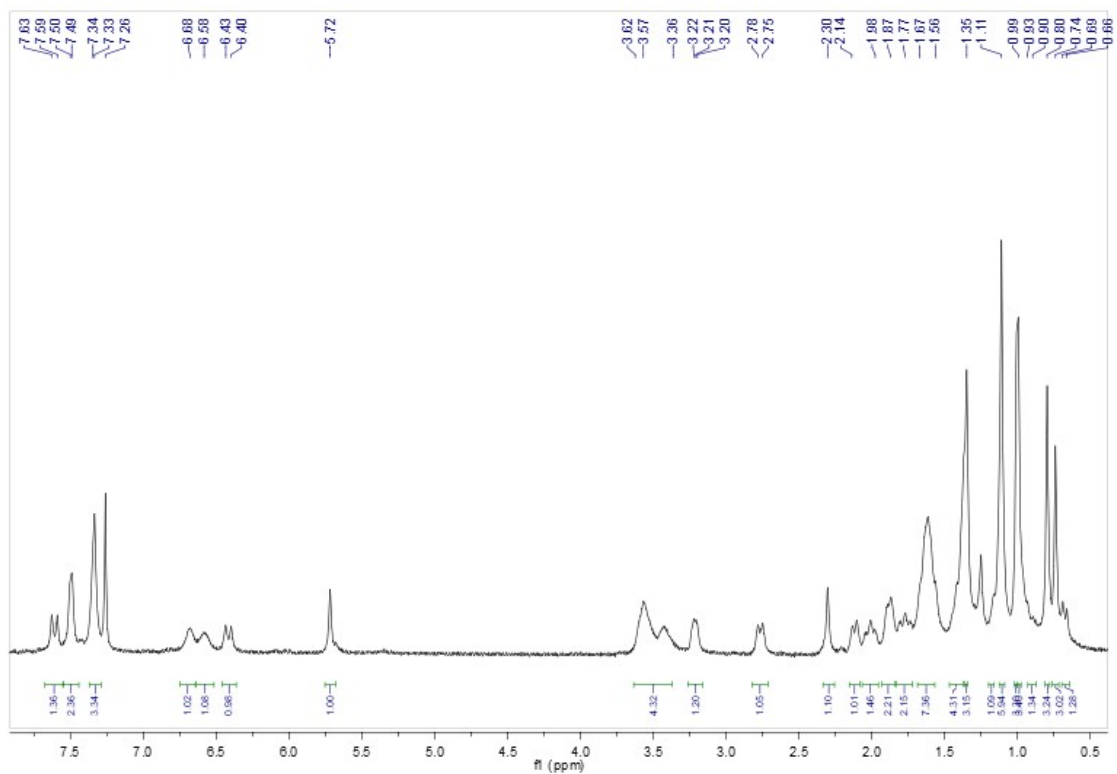
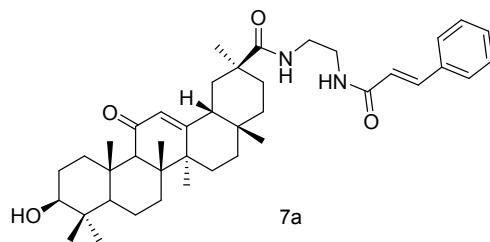


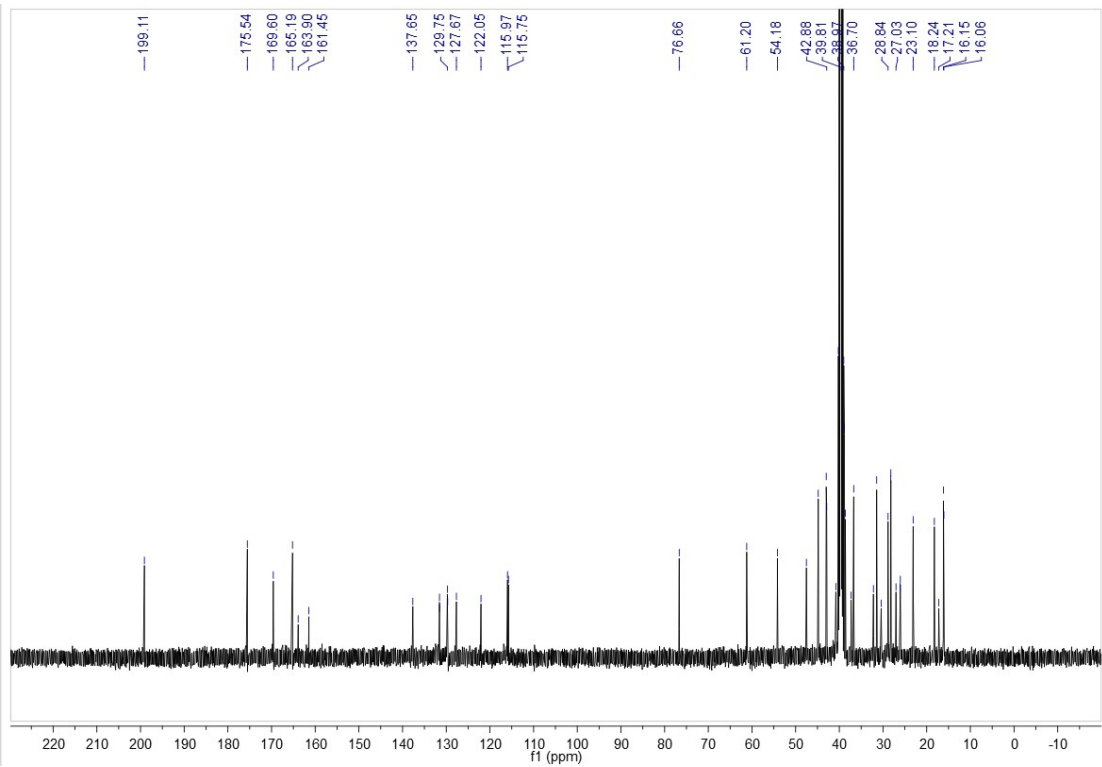
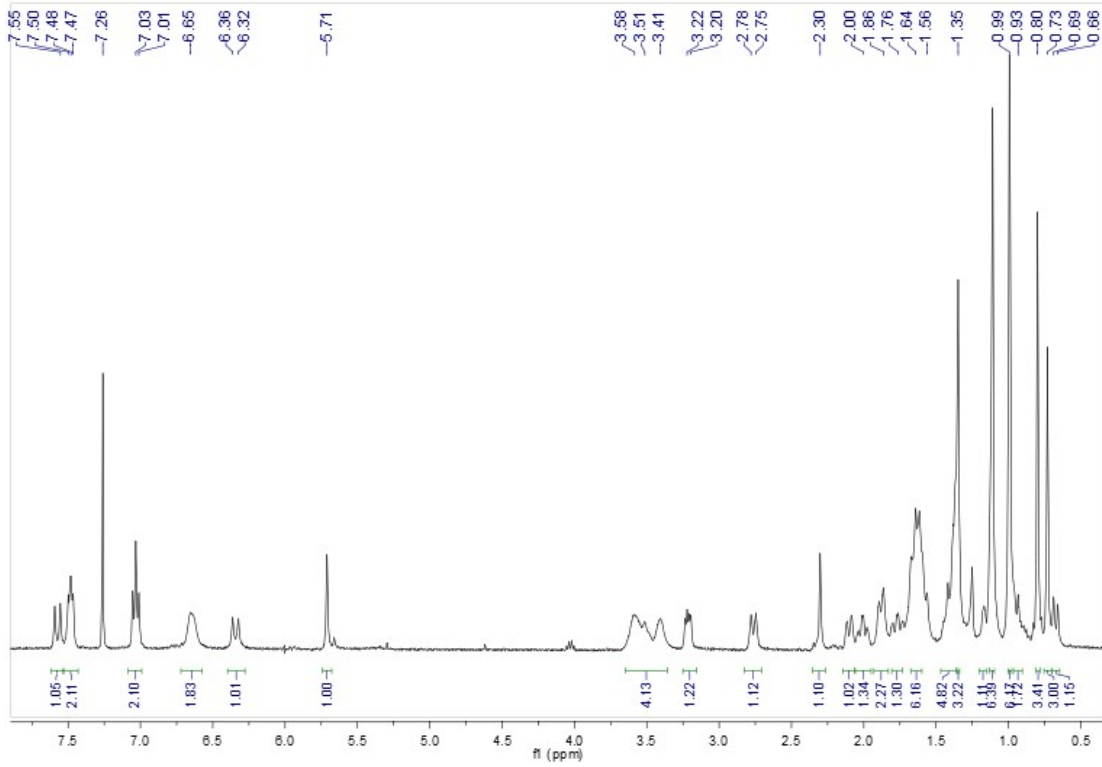
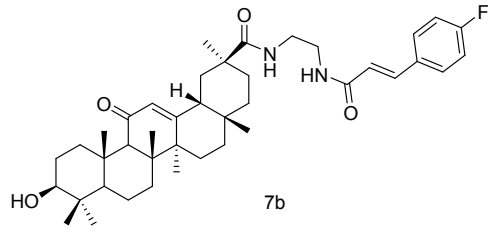


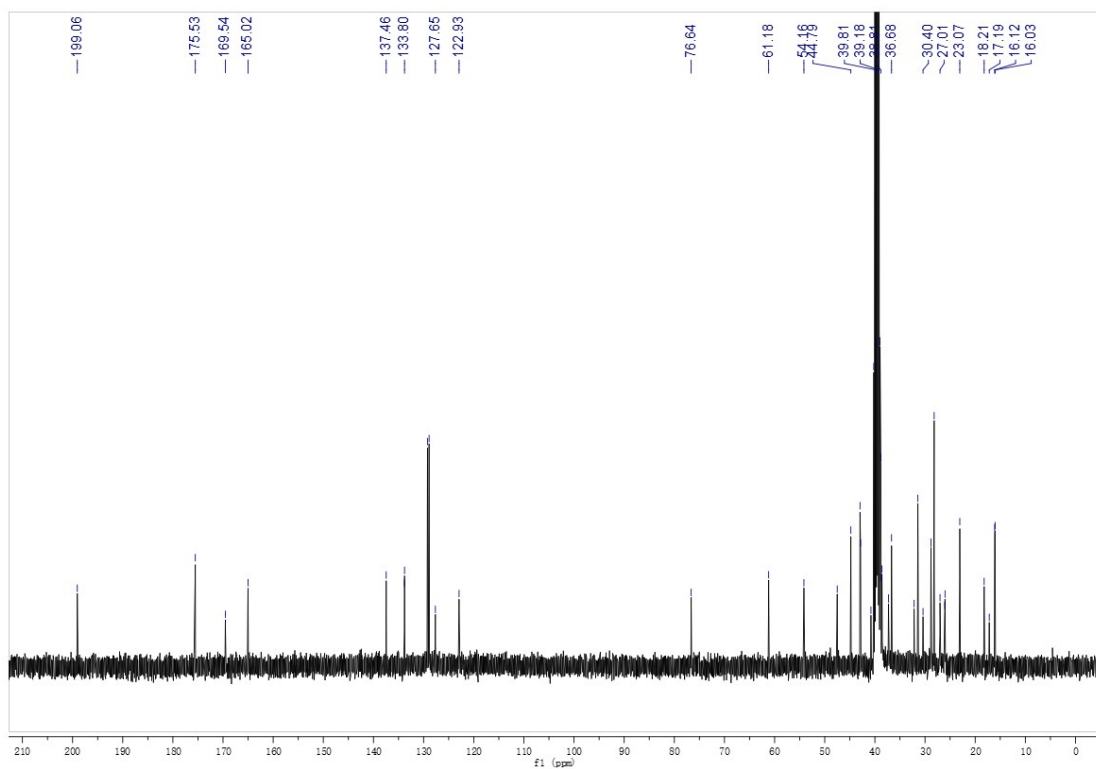
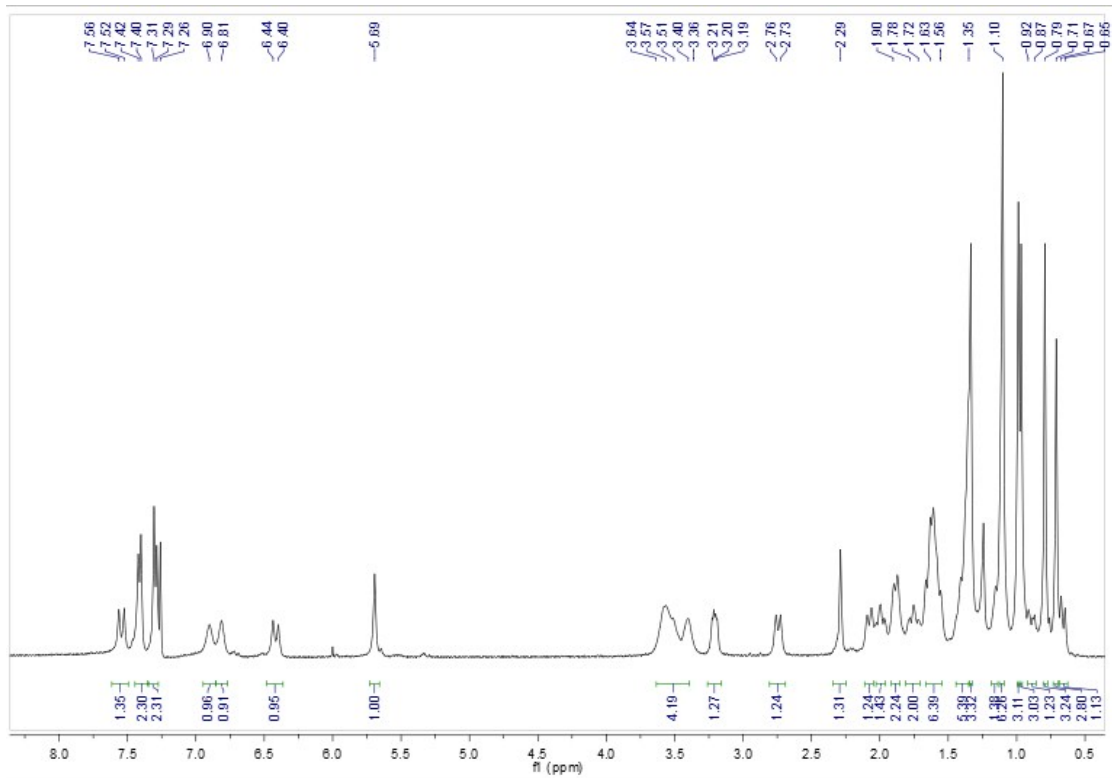
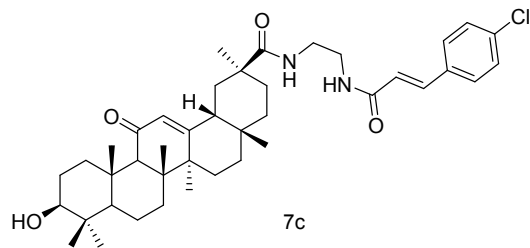


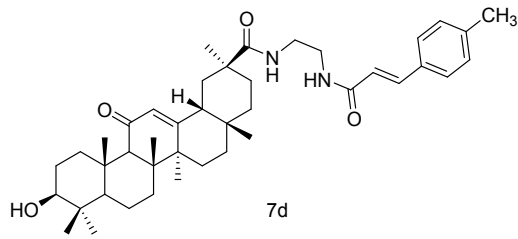




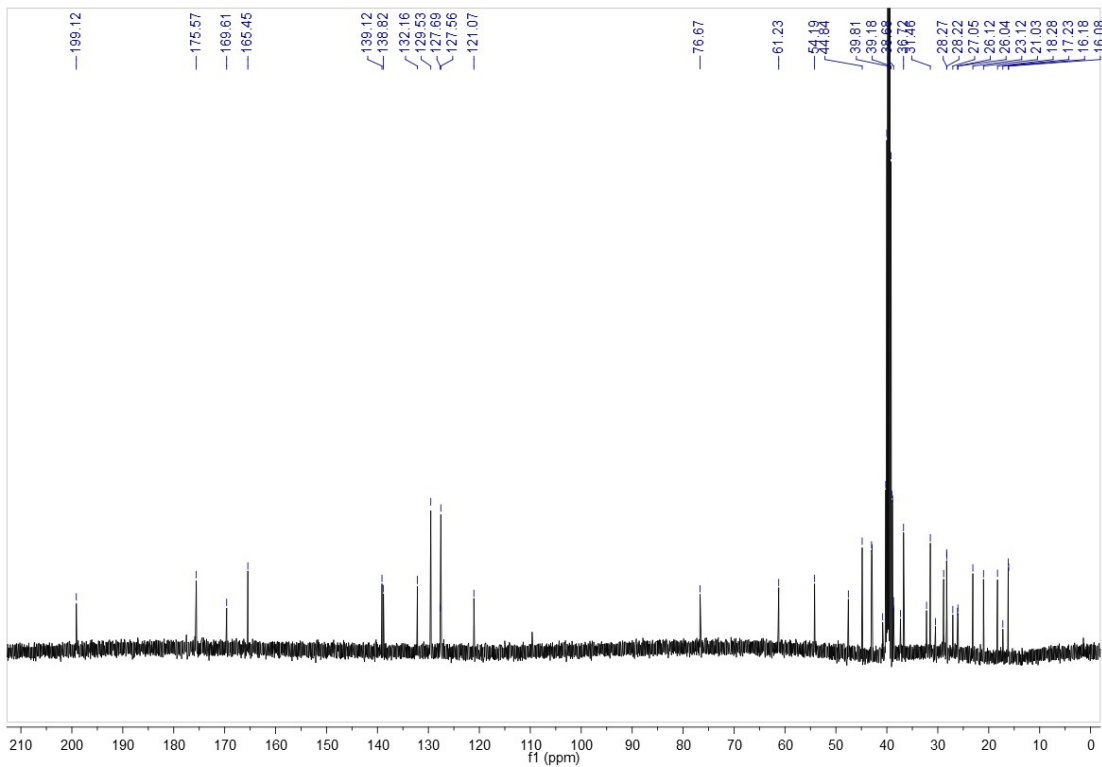
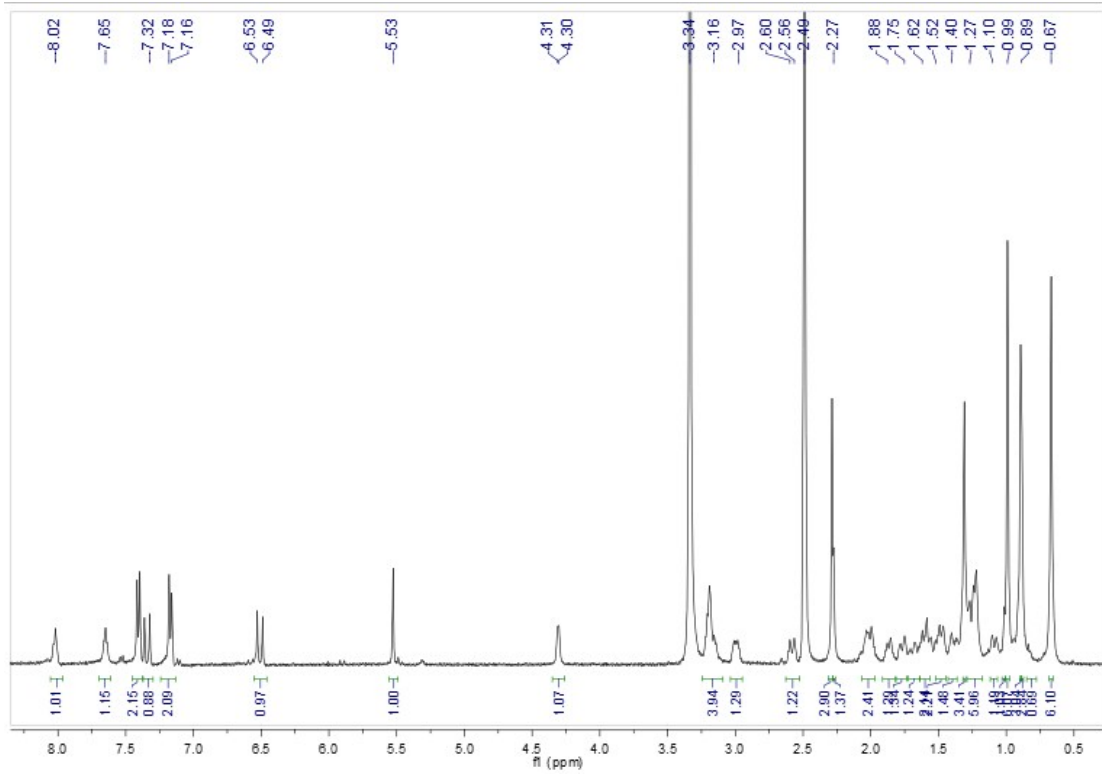


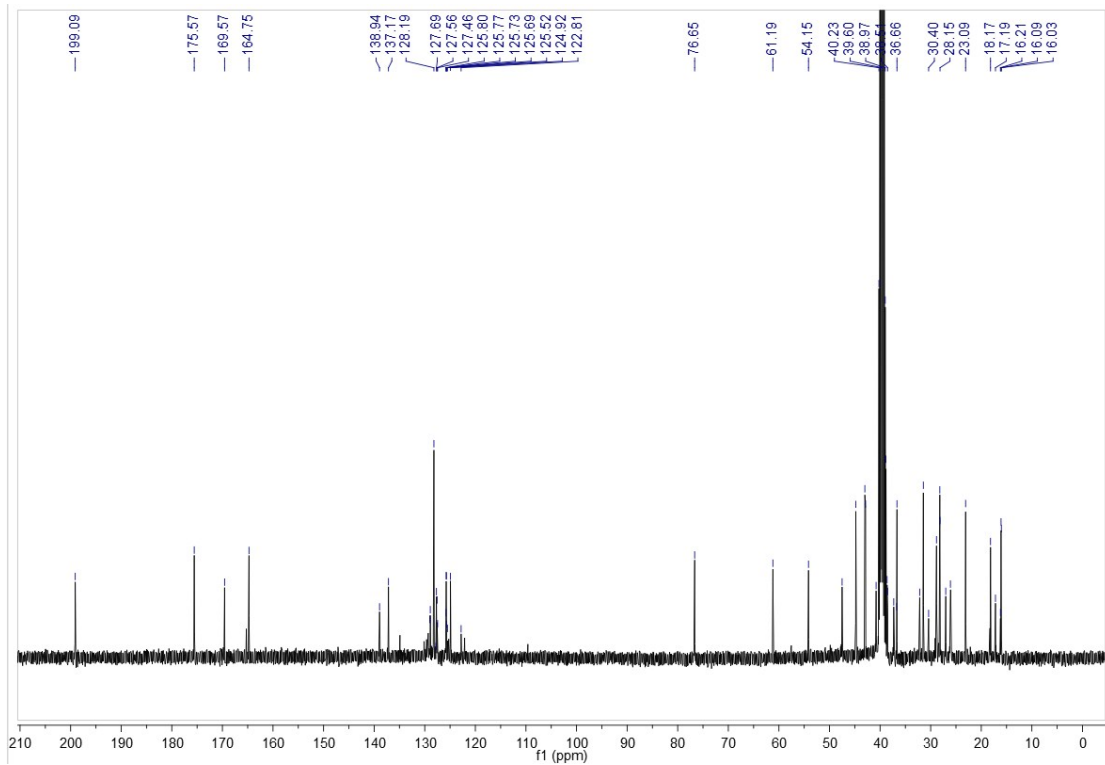
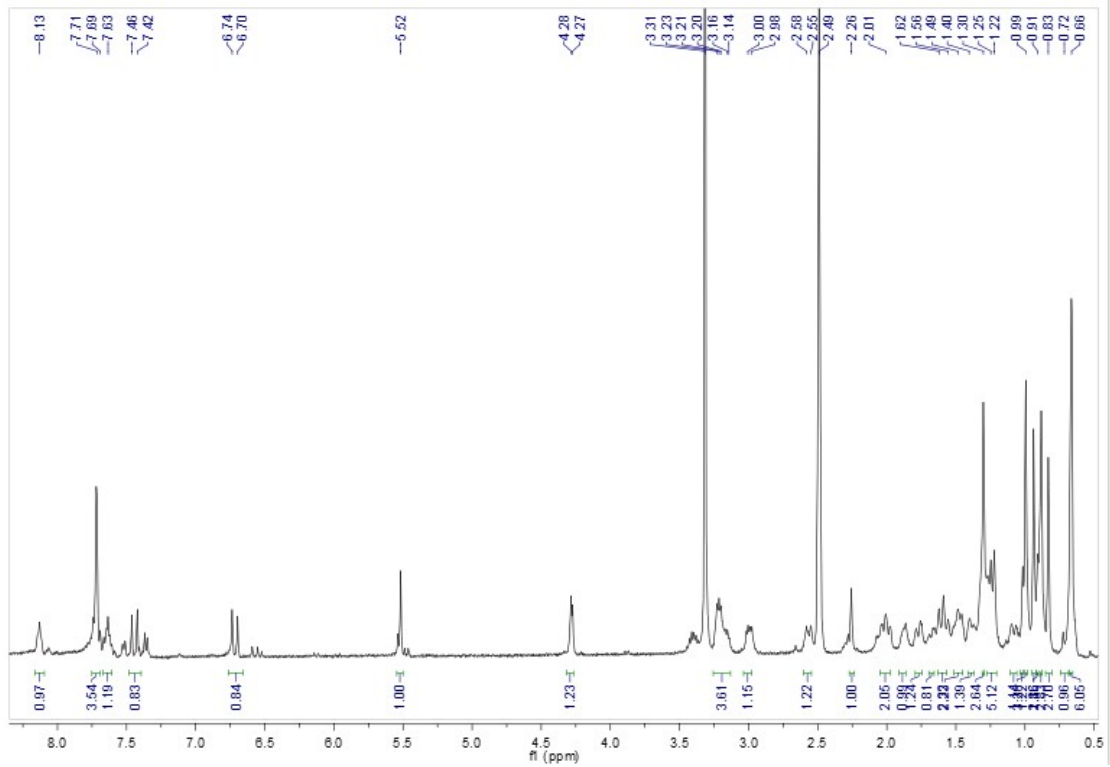
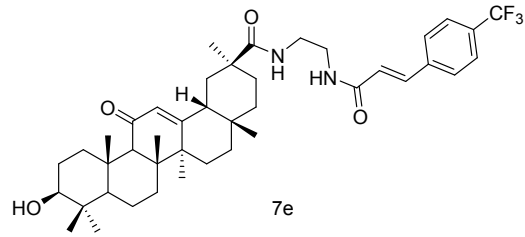


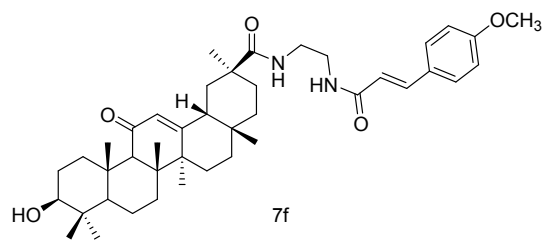




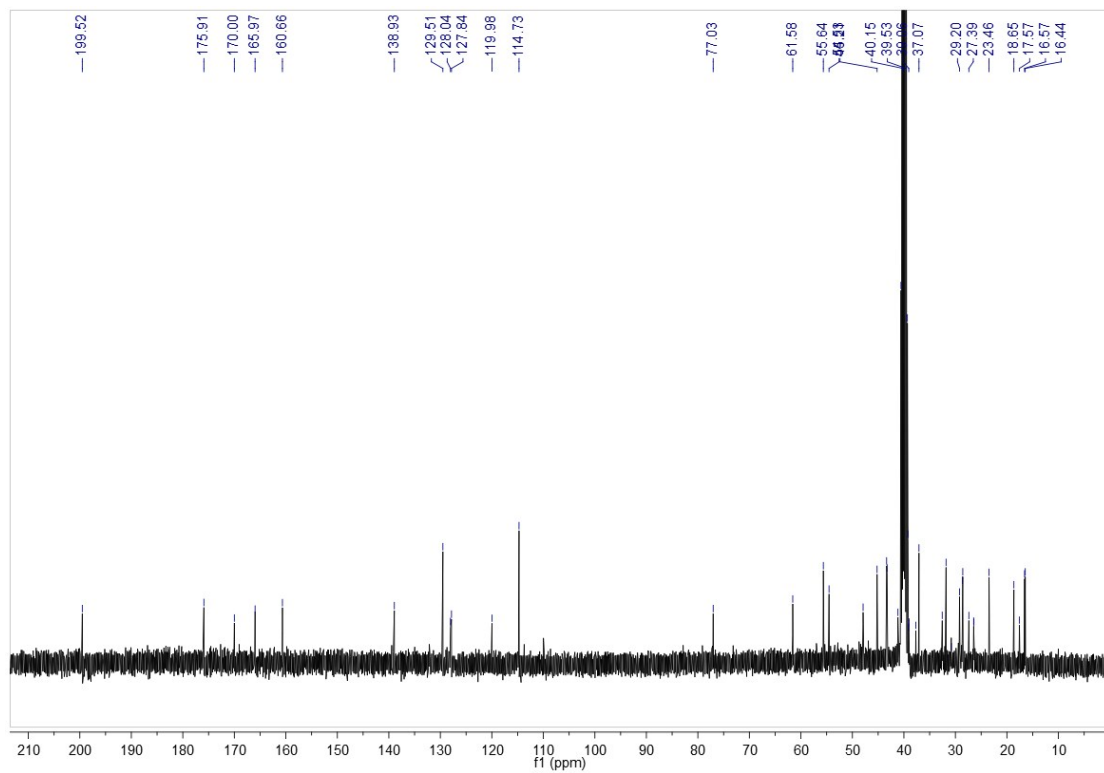
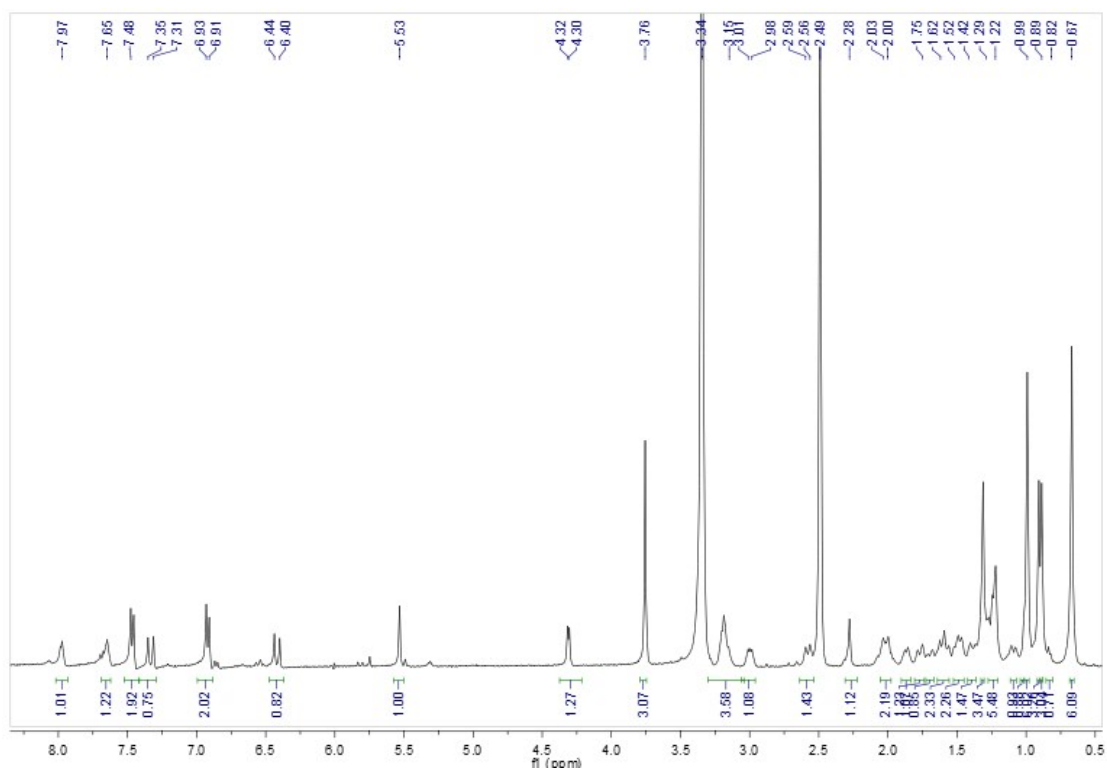
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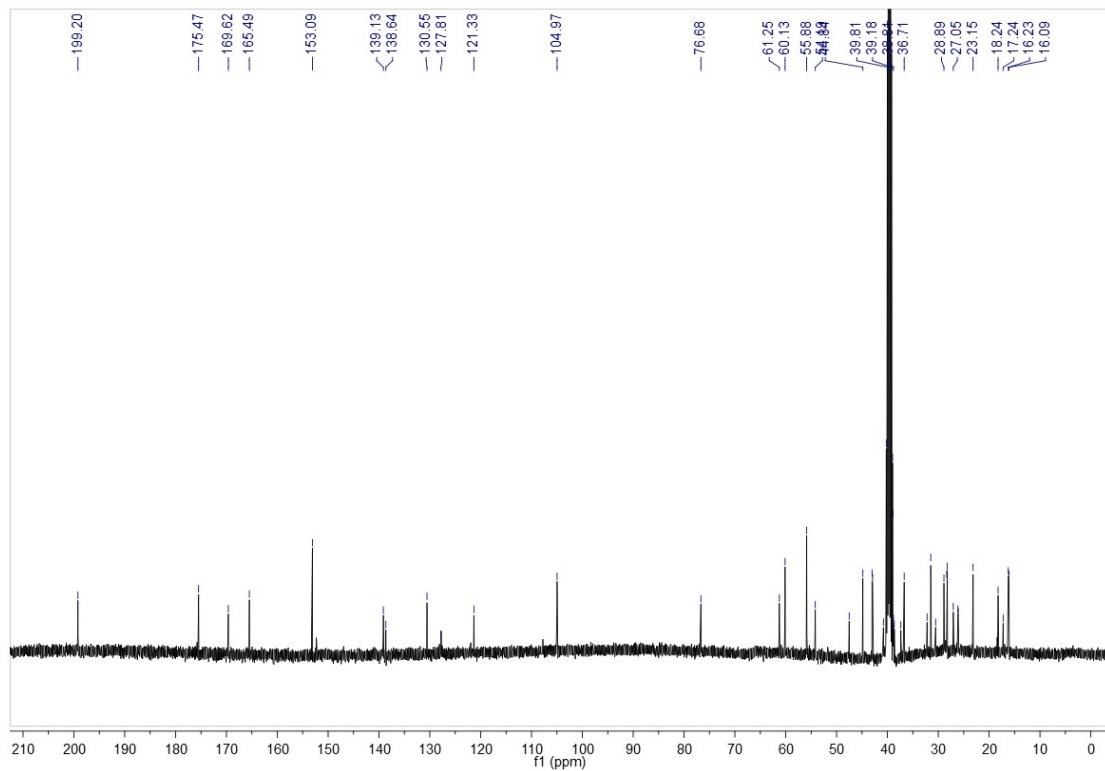
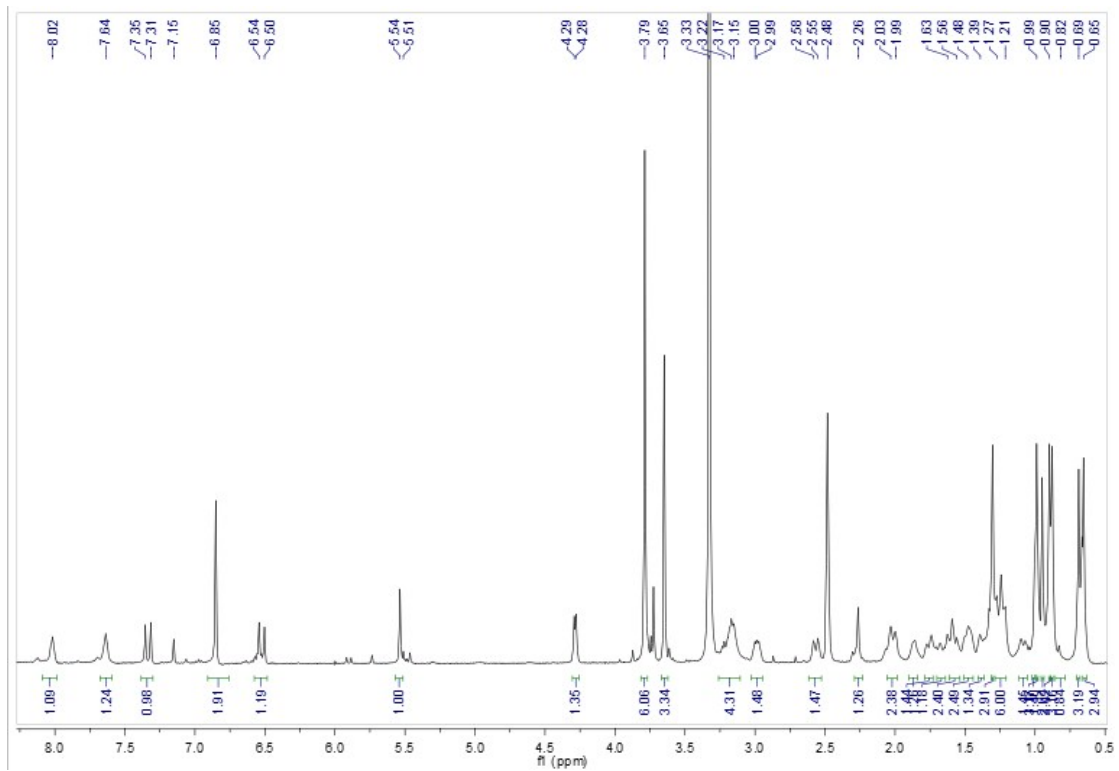
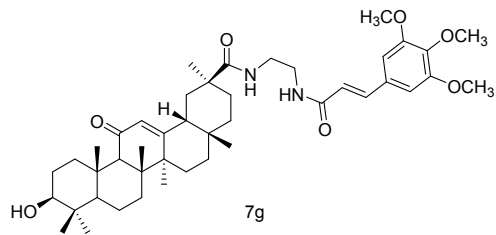


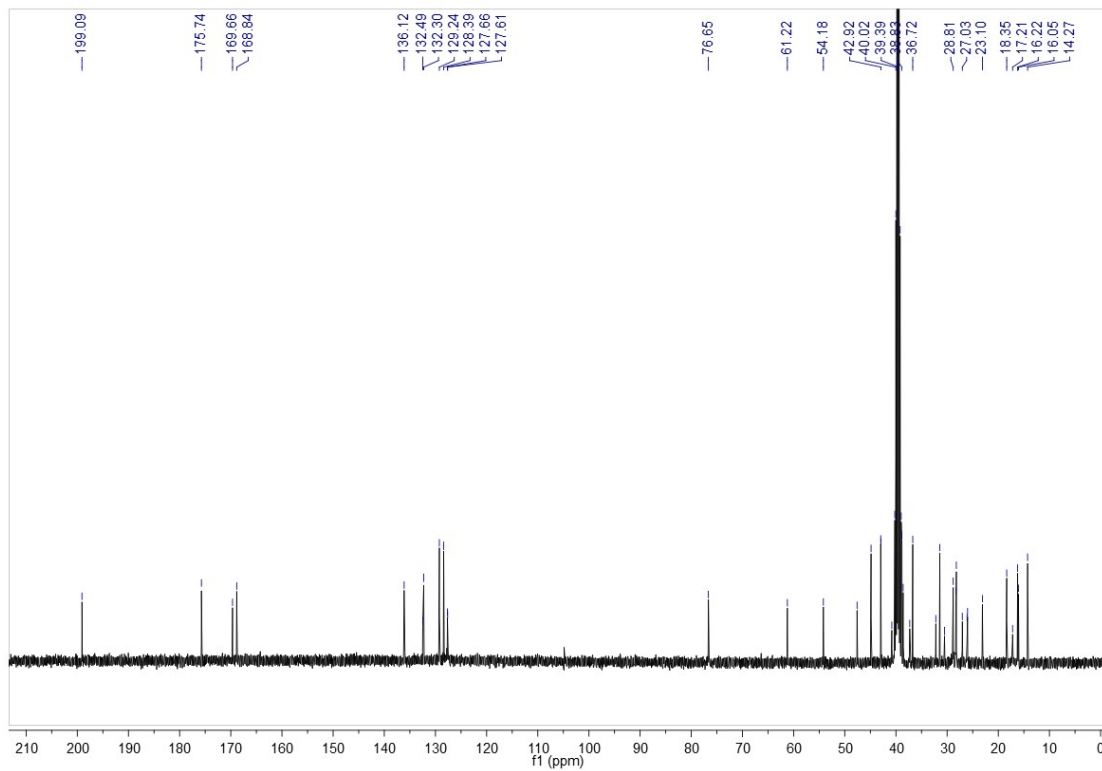
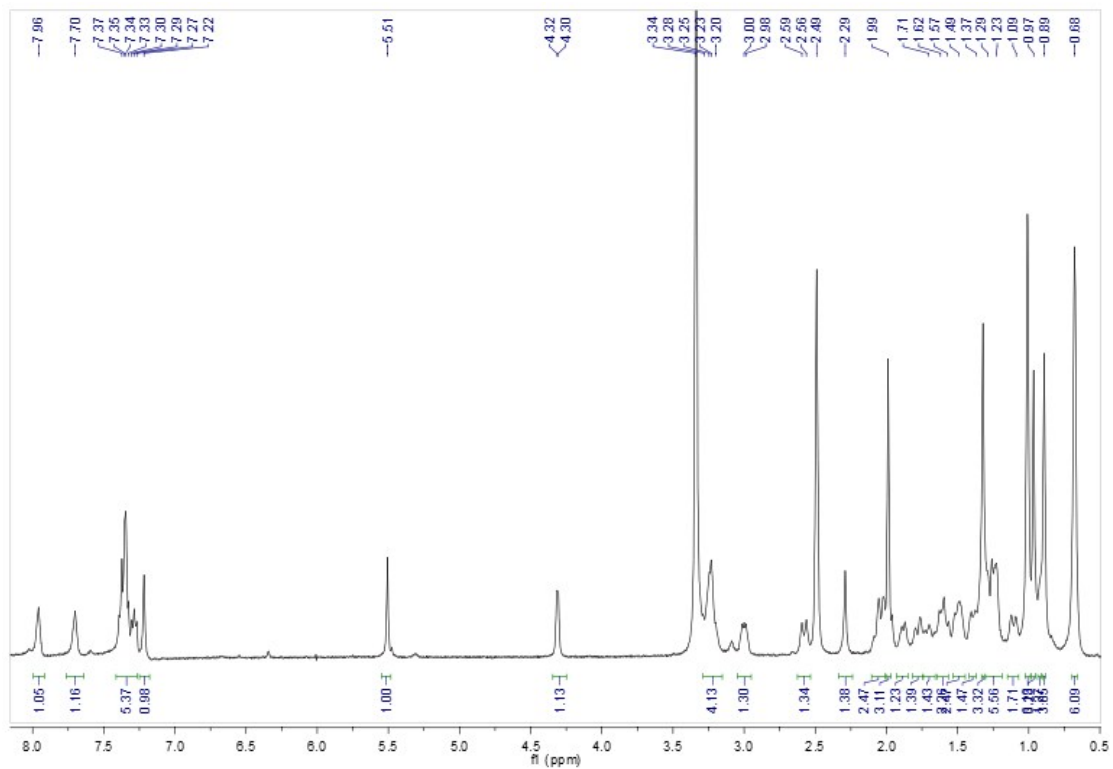
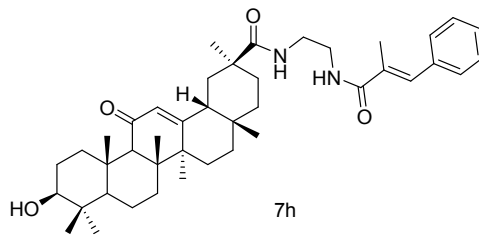


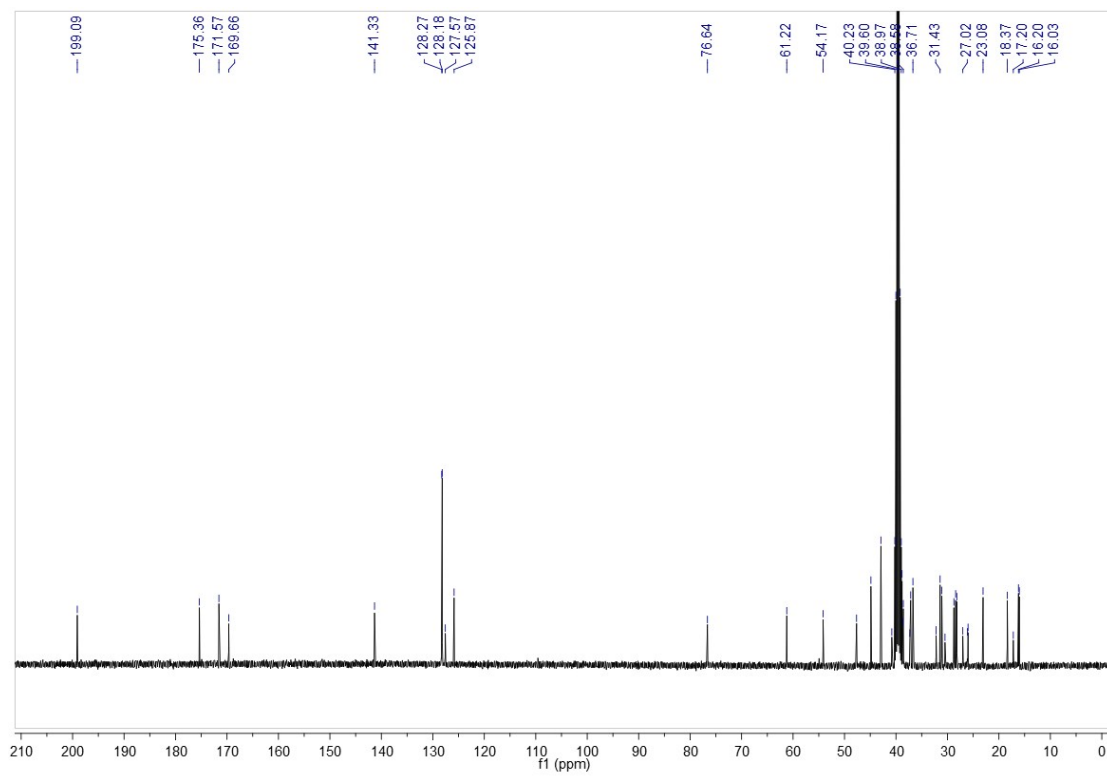
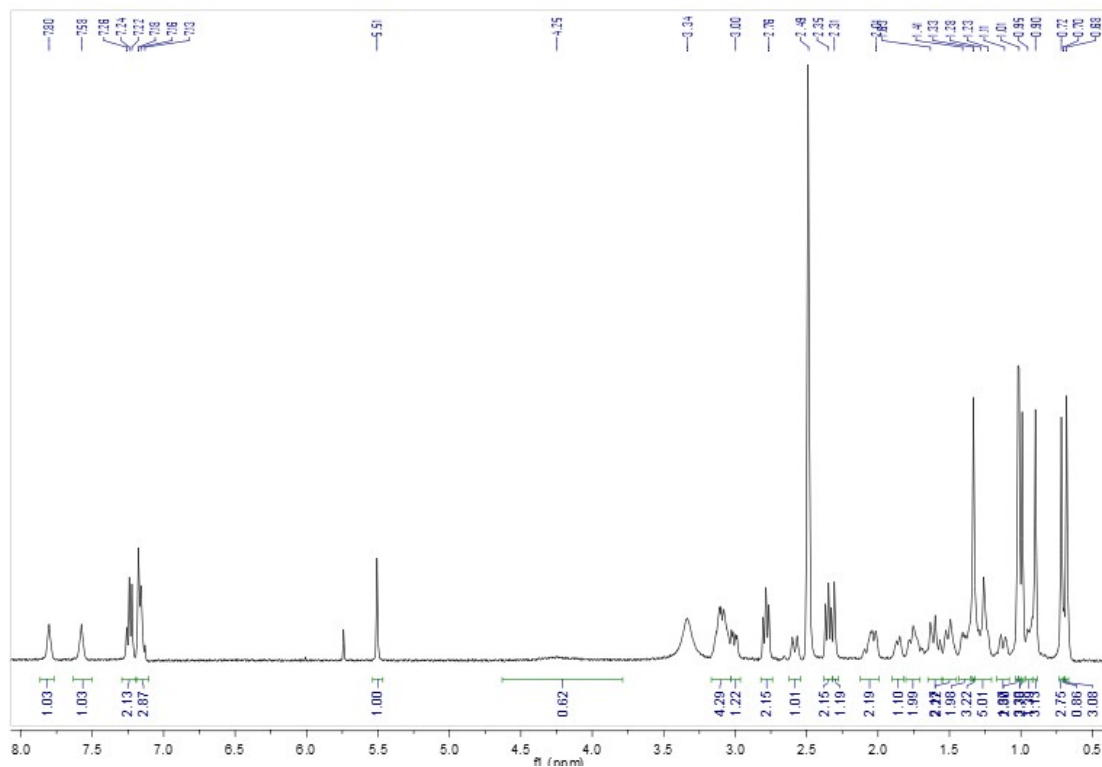
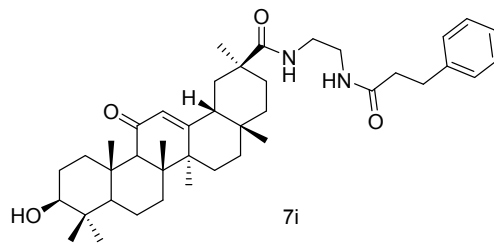


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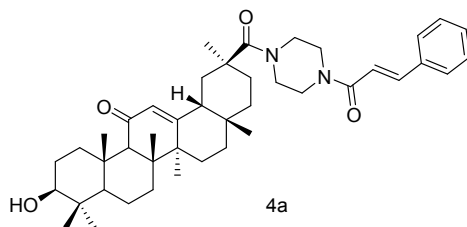




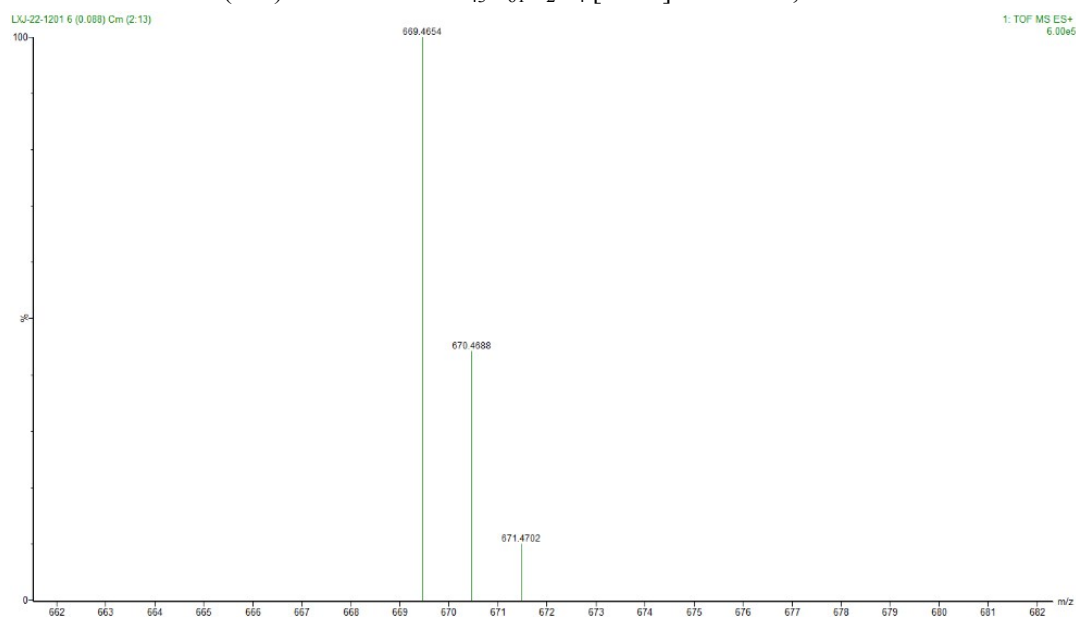


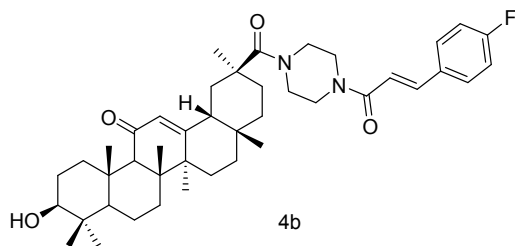


3. HRMS data of the target compounds 4a-4i and 7a-7i

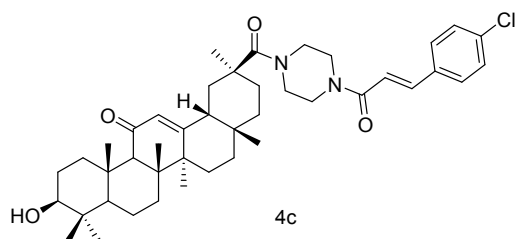
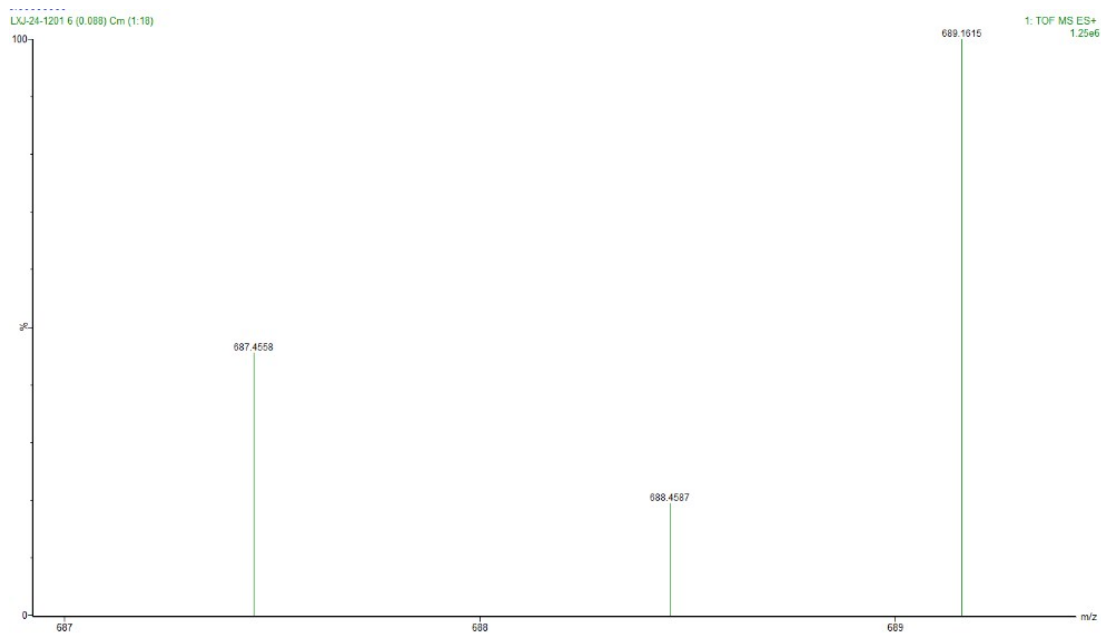


HRMS (ESI): m/z calcd for C₄₃H₆₁N₂O₄ [M+H]⁺ 669.4631, found 669.4654

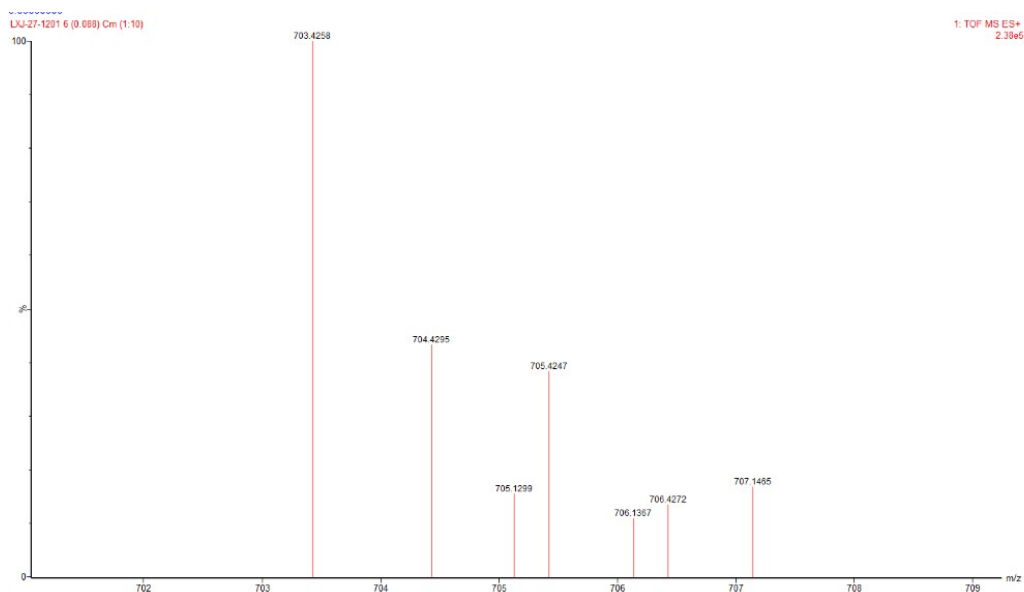


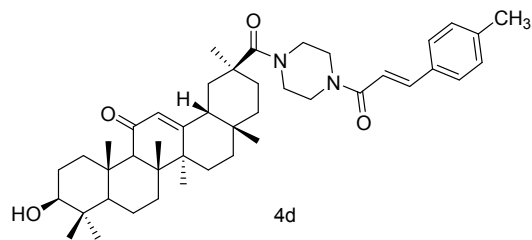


HRMS (ESI): m/z calcd for $C_{43}H_{60}FN_2O_4$ $[M+H]^+$ 687.4537, found 687.4558

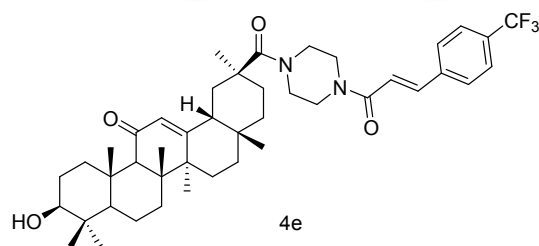
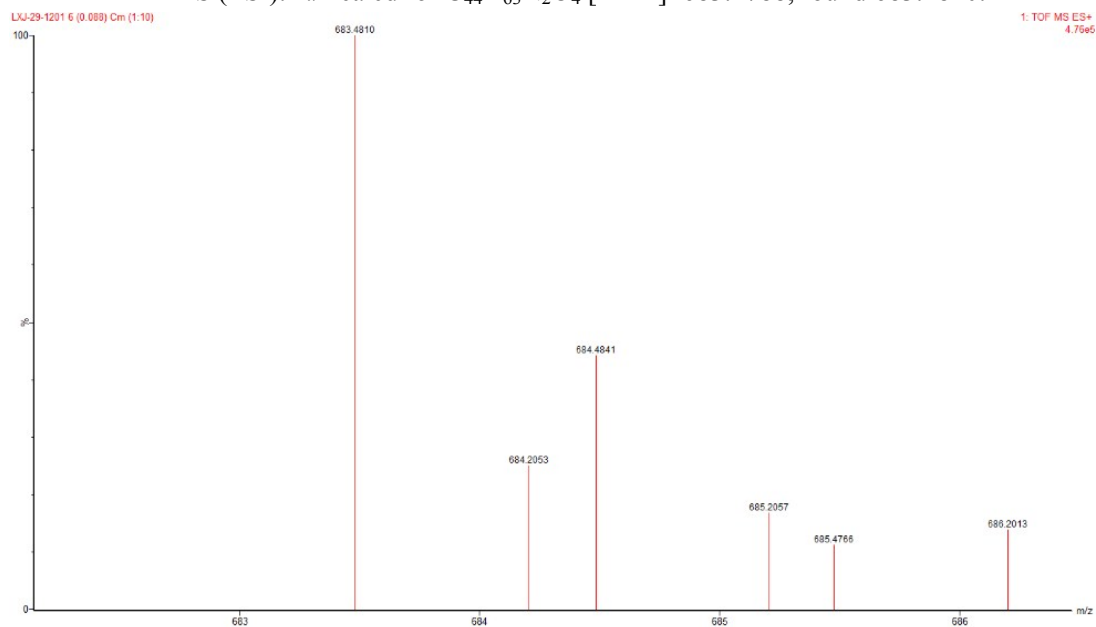


HRMS (ESI): m/z calcd for $C_{43}H_{60}ClN_2O_4$ $[M+H]^+$ 703.4242, found 703.4258

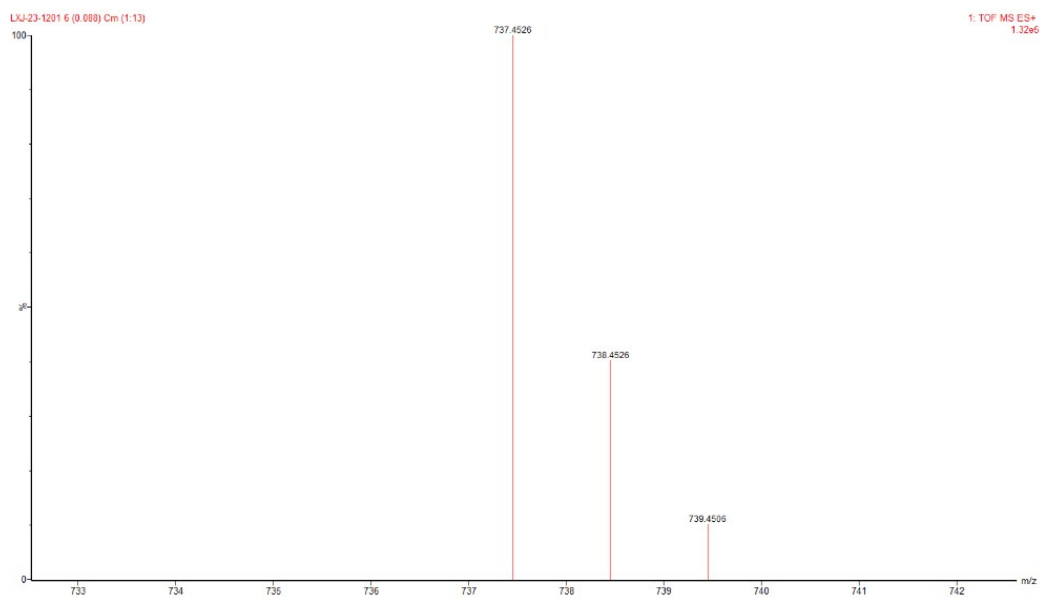


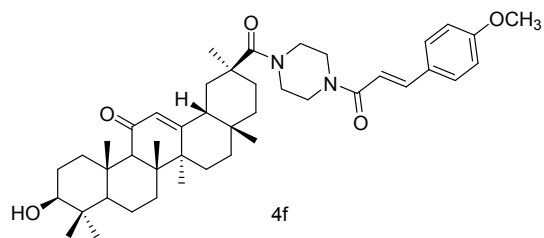


HRMS (ESI): m/z calcd for $C_{44}H_{63}N_2O_4$ $[M+H]^+$ 683.4788, found 683.4810.

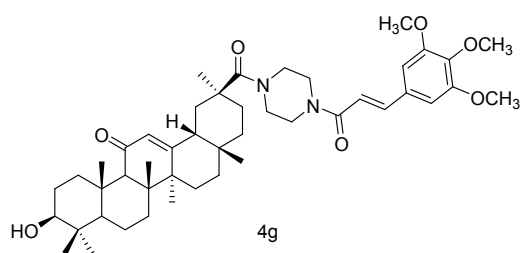
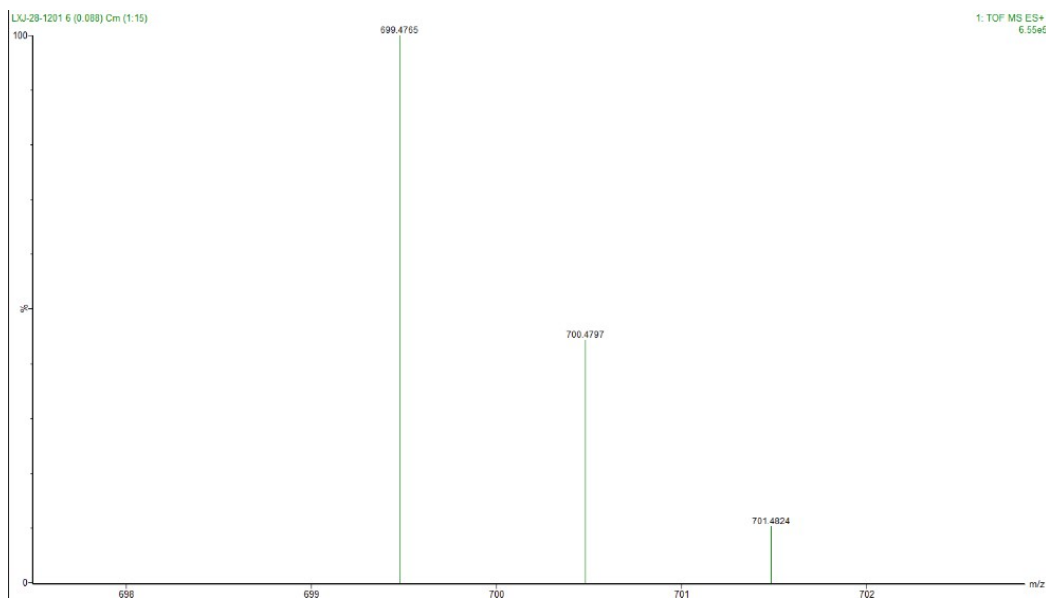


HRMS (ESI): m/z calcd for $C_{44}H_{60}F_3N_2O_4$ $[M+H]^+$ 737.4505, found 737.4526

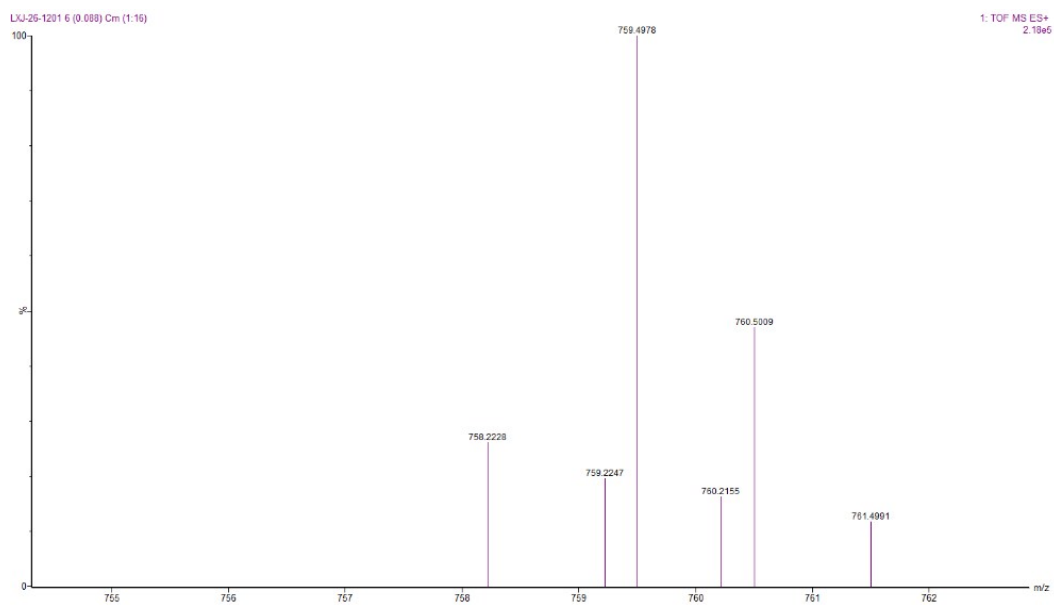


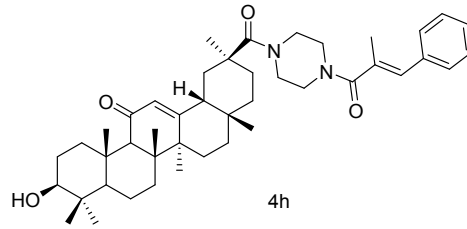


HRMS (ESI): m/z calcd for $C_{44}H_{63}N_2O_5$ $[M+H]^+$ 699.4737, found 699.4765

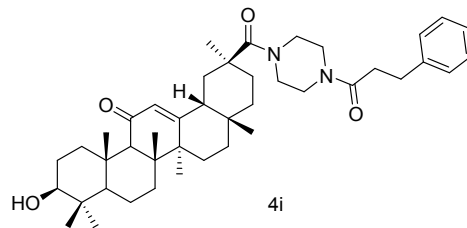
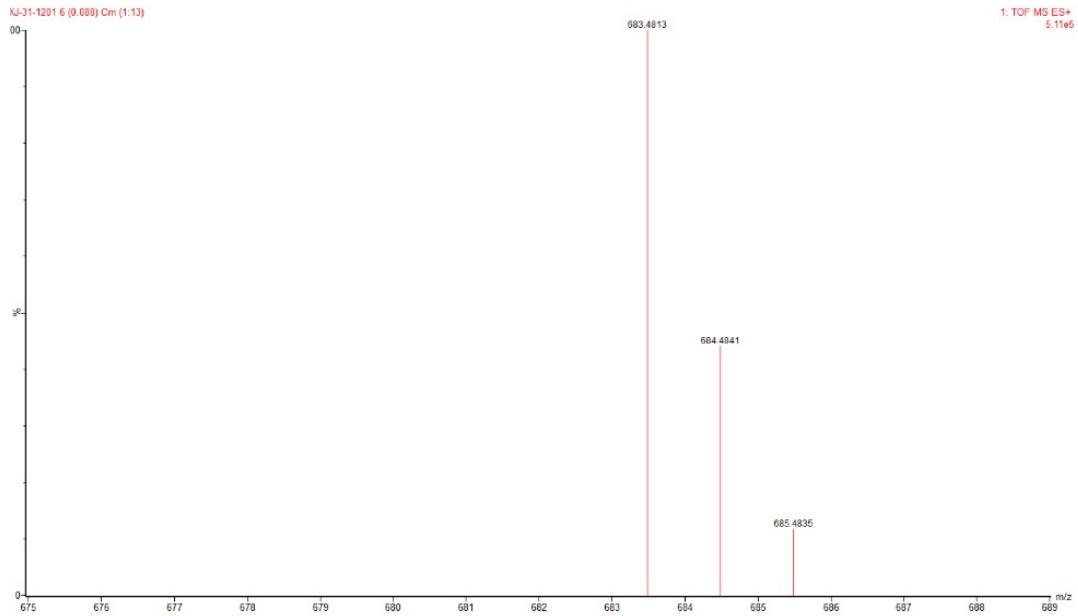


HRMS (ESI): m/z calcd for $C_{46}H_{67}N_2O_7$ $[M+H]^+$ 759.4948, found 759.4978

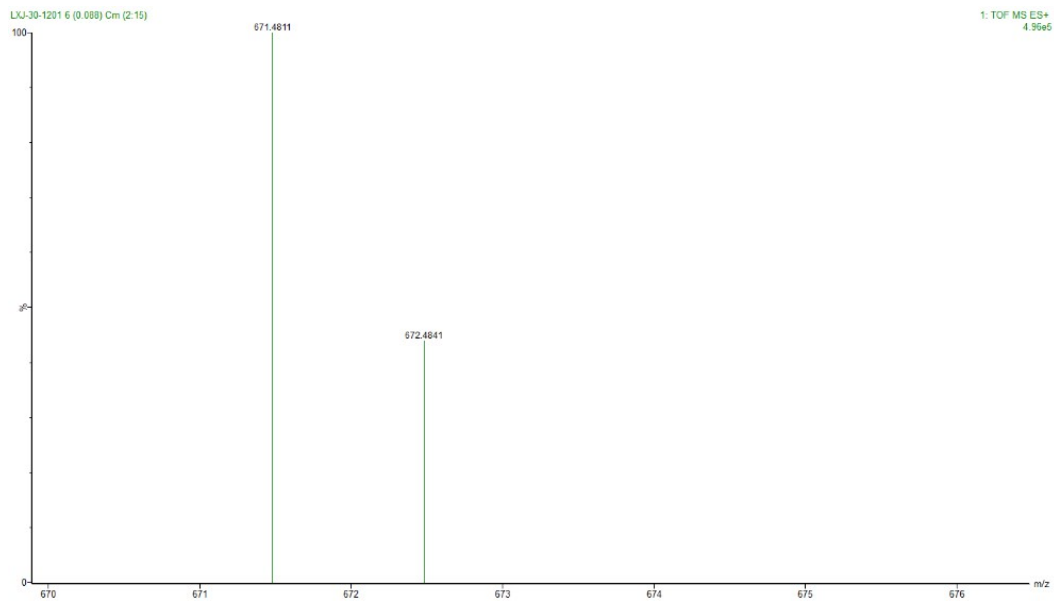


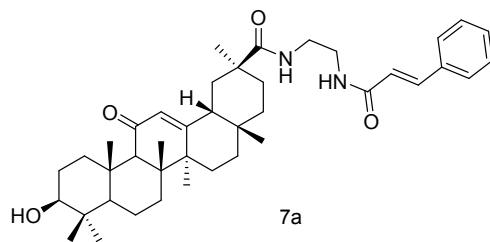


HRMS (ESI): m/z calcd for $C_{44}H_{63}N_2O_4$ $[M+H]^+$ 683.4788, found 683.4813

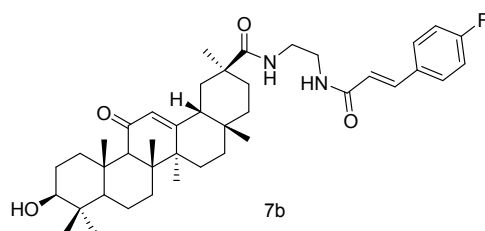
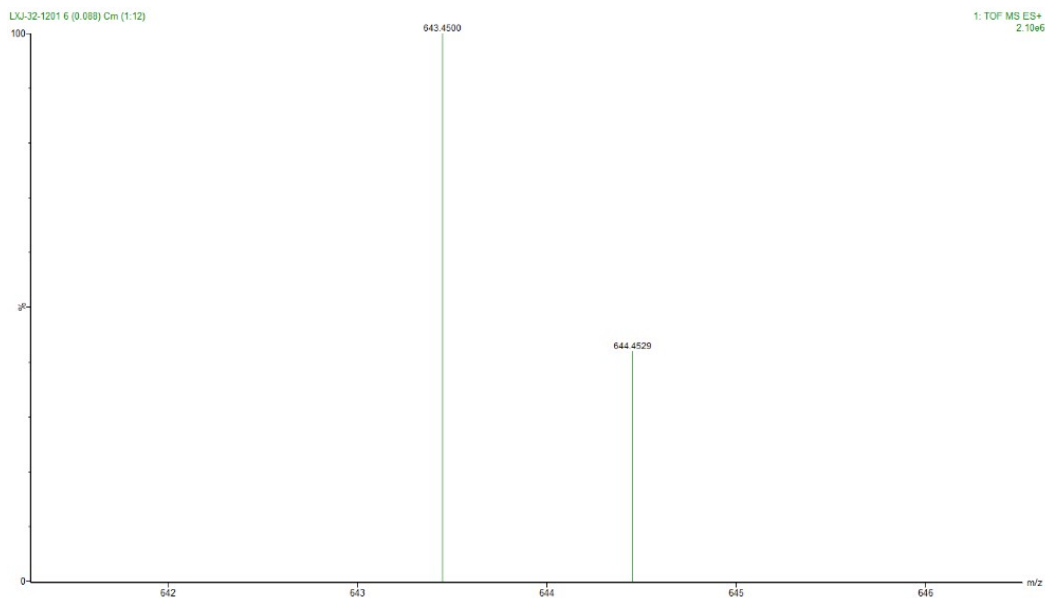


HRMS (ESI): m/z calcd for $C_{43}H_{63}N_2O_4$ $[M+H]^+$ 671.4788, found 671.4811

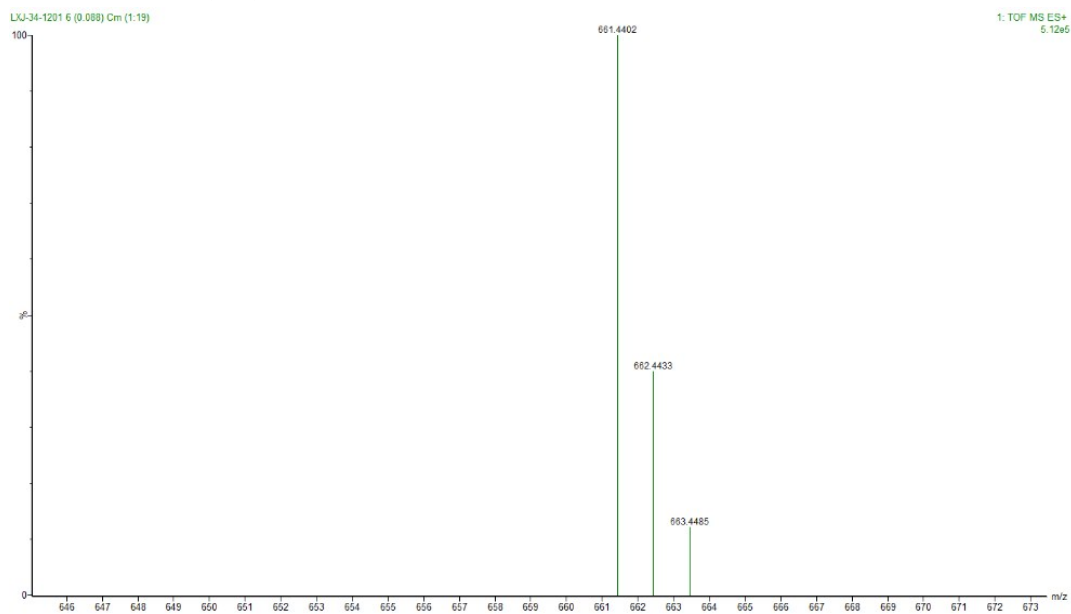


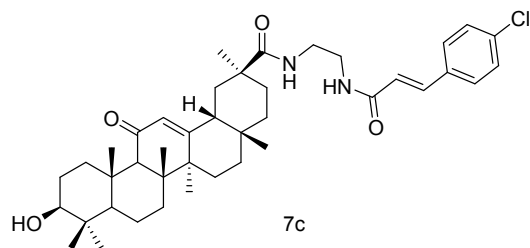


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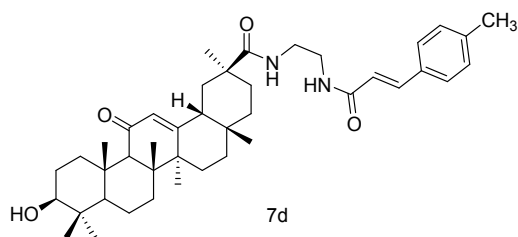
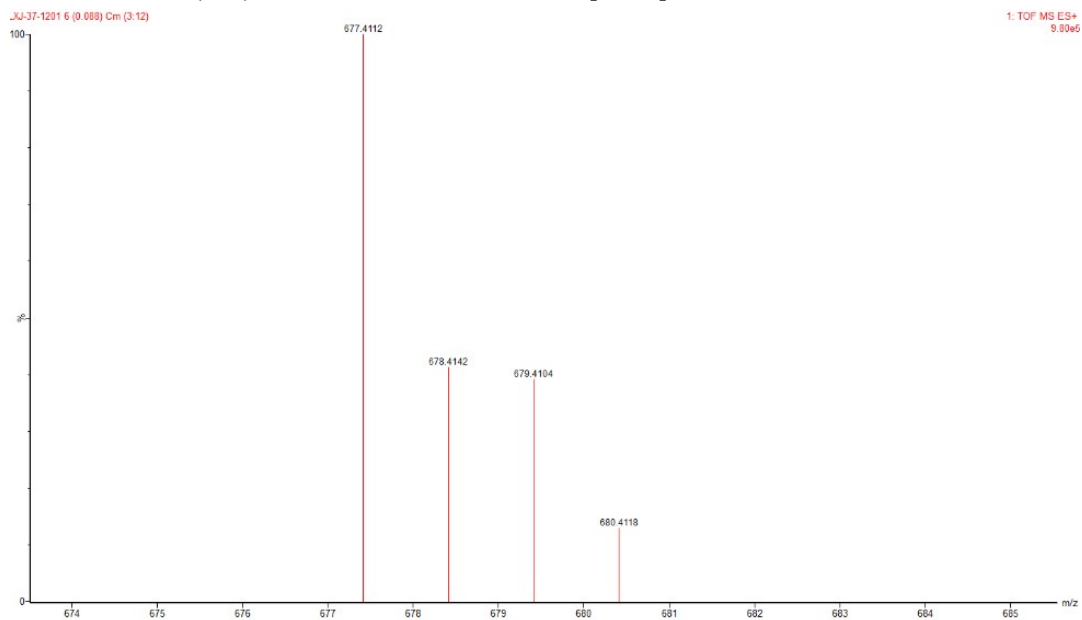


HRMS (ESI): m/z calcd for $C_{41}H_{58}FN_2O_4$ $[M+H]^+$ 661.4381, found 661.4402

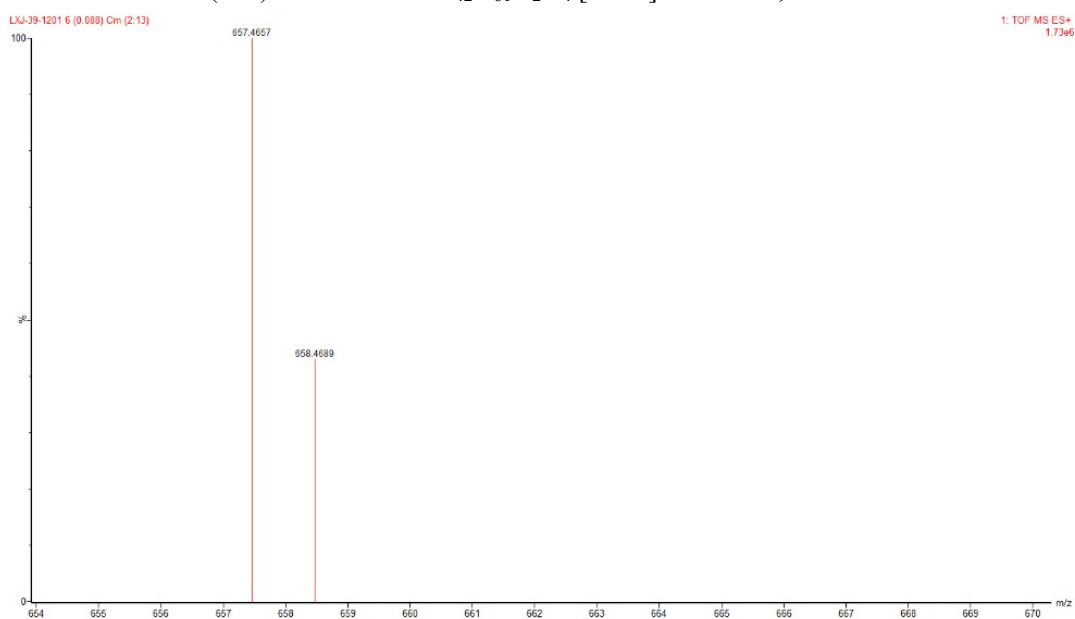


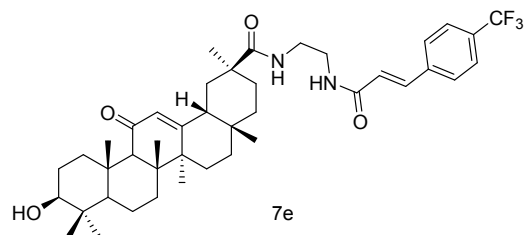


HRMS (ESI): m/z calcd for $C_{41}H_{58}ClN_2O_4$ $[M+H]^+$ 677.4085, found 677.4112

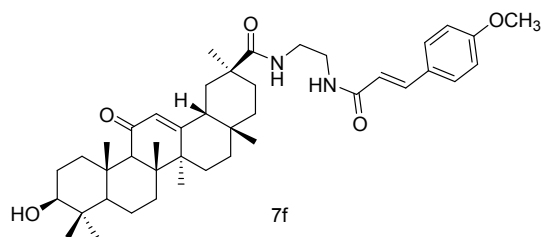
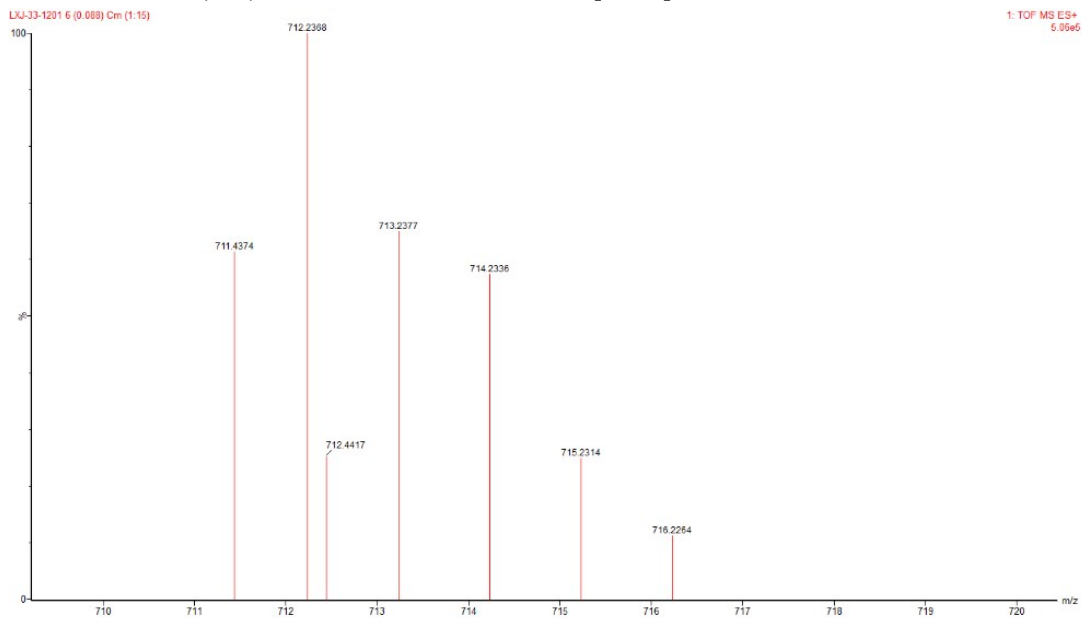


HRMS (ESI): m/z calcd for $C_{42}H_{61}N_2O_4$ $[M+H]^+$ 657.4631, found 657.4657

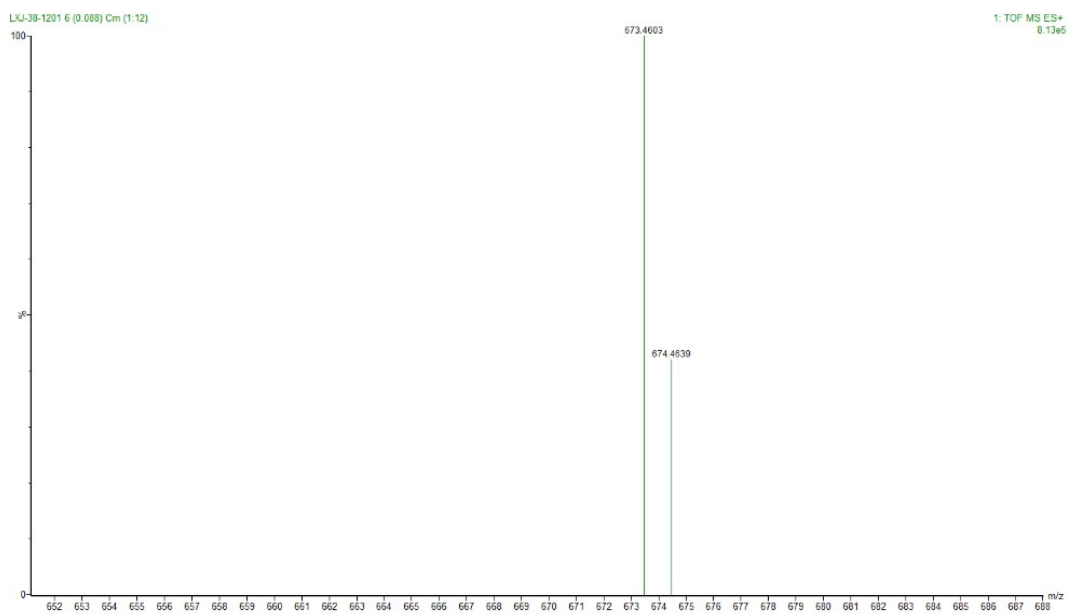


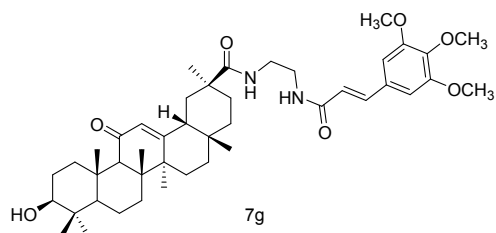


HRMS (ESI): m/z calcd for $C_{42}H_{58}F_3N_2O_4$ $[M+H]^+$ 711.4349, found 711.4374

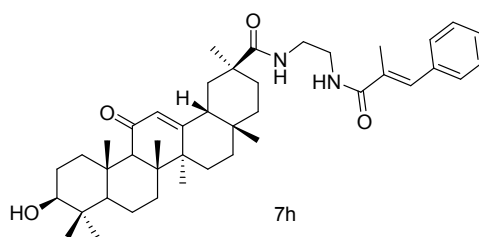
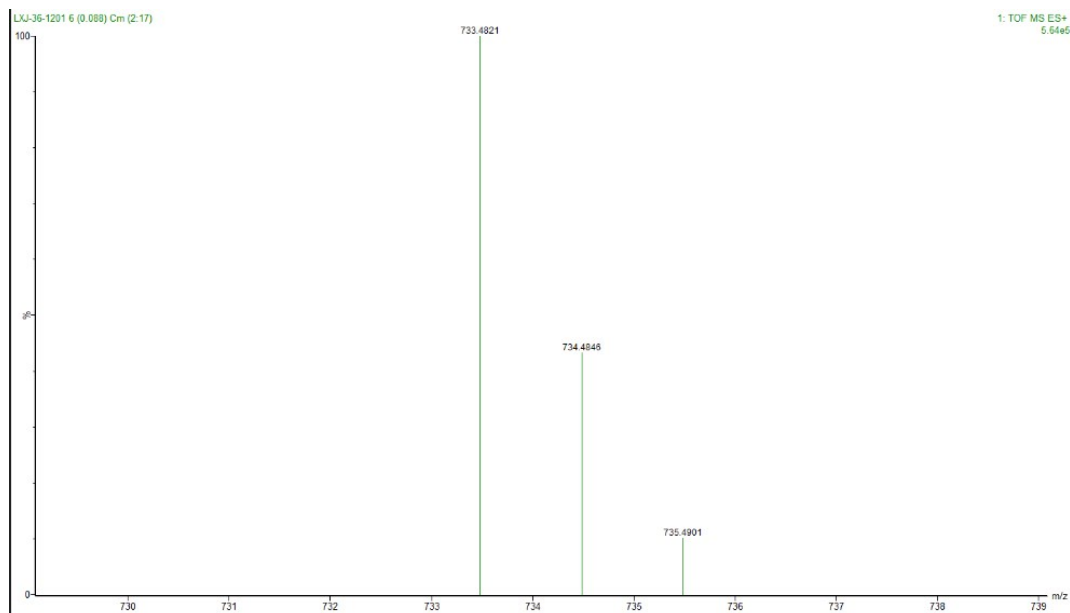


HRMS (ESI): m/z calcd for $C_{42}H_{61}N_2O_5$ $[M+H]^+$ 673.4580, found 673.4603

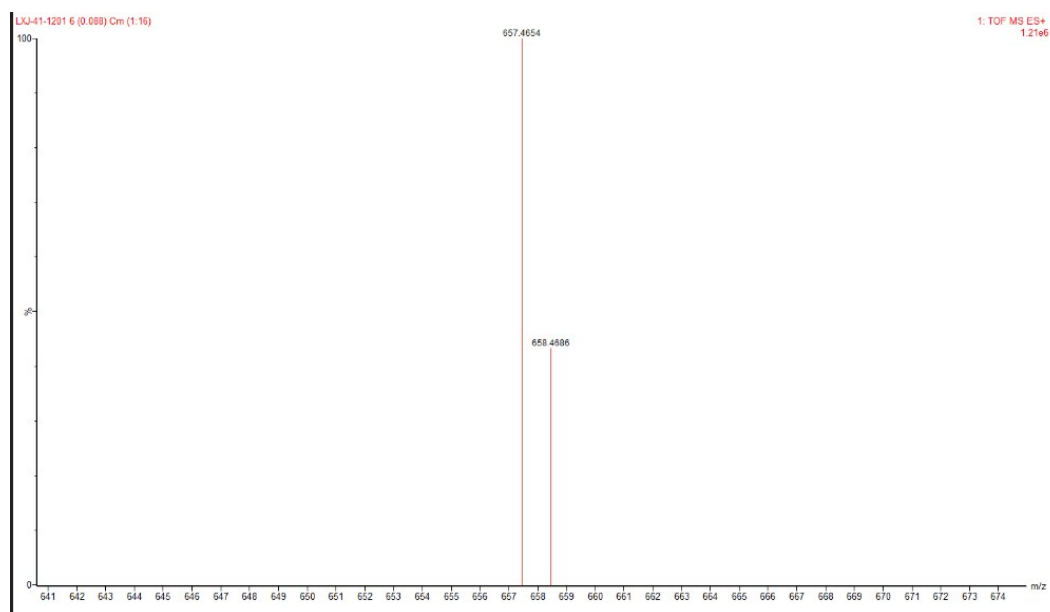


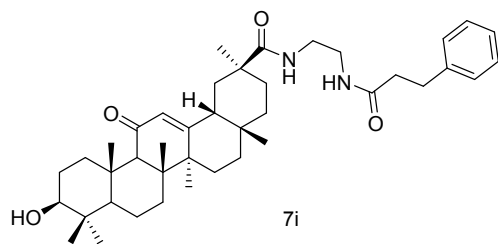


HRMS (ESI): m/z calcd for $C_{44}H_{65}N_2O_7$ $[M+H]^+$ 733.4792, found 733.4821



HRMS (ESI): m/z calcd for $C_{42}H_{61}N_2O_4$ $[M+H]^+$ 657.4631, found 657.4654





HRMS (ESI): m/z calcd for $C_{41}H_{61}N_2O_4$ $[M+H]^+$ 645.4631, found 645.4659

