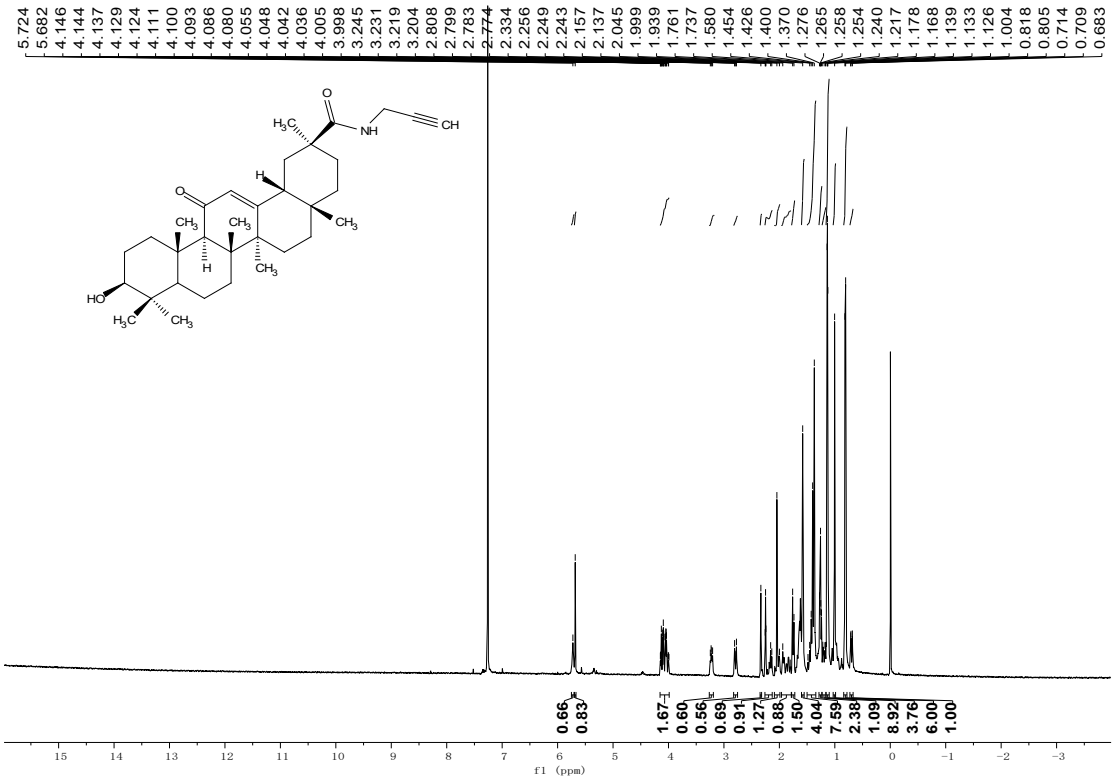
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis, structural characterization, docking studies and bioactivities of carbon monoxide release molecules based on triphenylphosphonium-glycyrrhetinic acid derivatives

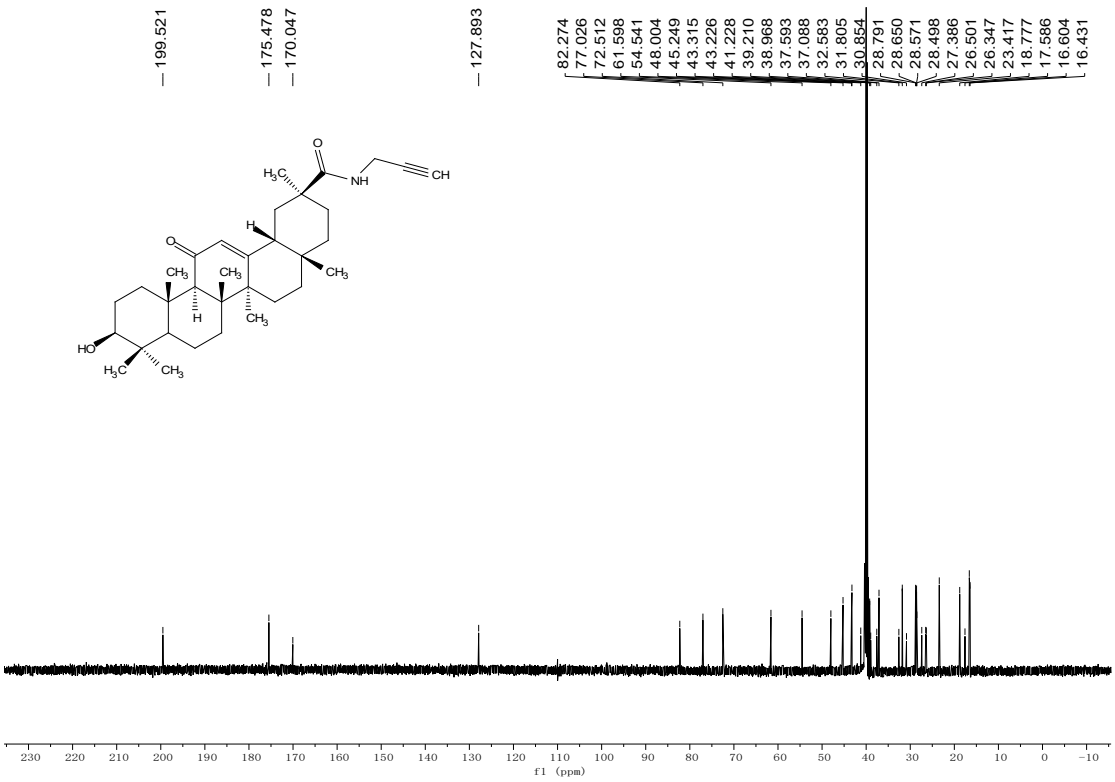
Hua-Peng Liu, † [a,b*] Ming-Zhe Ren, † [b] Yu-Jie Chen,[b] Sheng-Yan Zhao,[b] Yuan Liao,[b] Xi-Cun Wang,[b,*]

SI-Figure 1 The ^{1}H-NMR spectra of **Alkynyl-GA**(400 MHz, Chloroform-d)

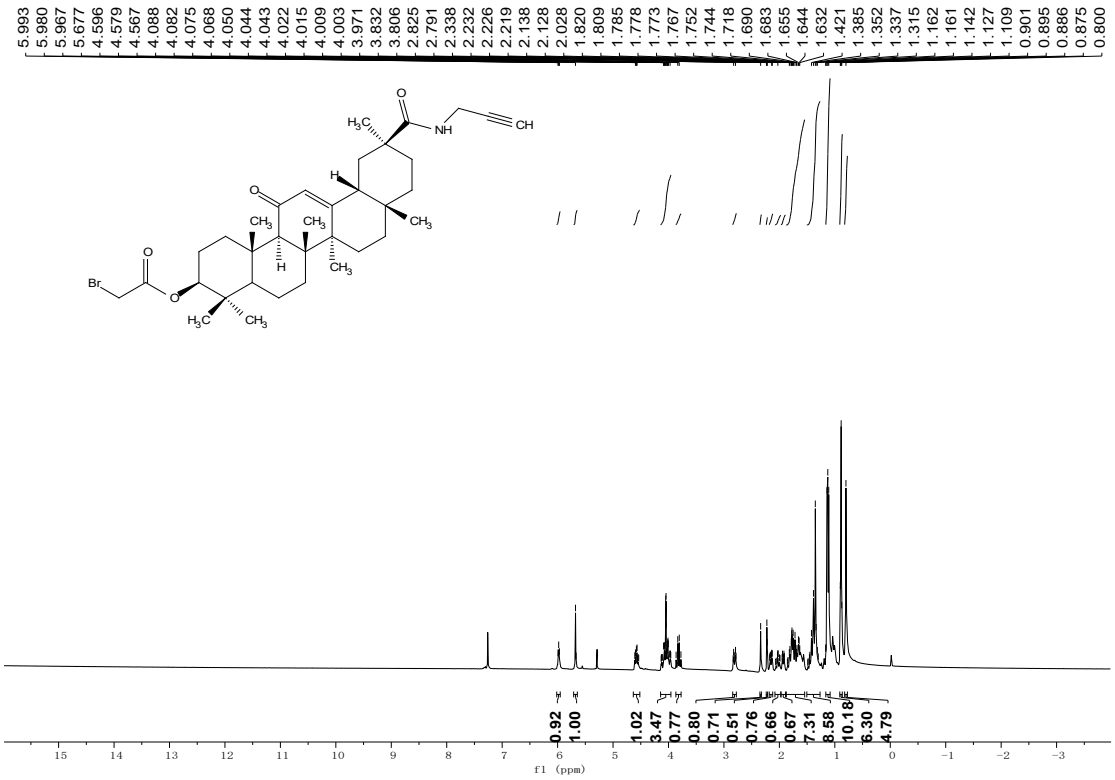


SI-Figure 2 The ^{13}C-NMR spectra of **Alkynyl-GA** (151 MHz, DMSO-d6)

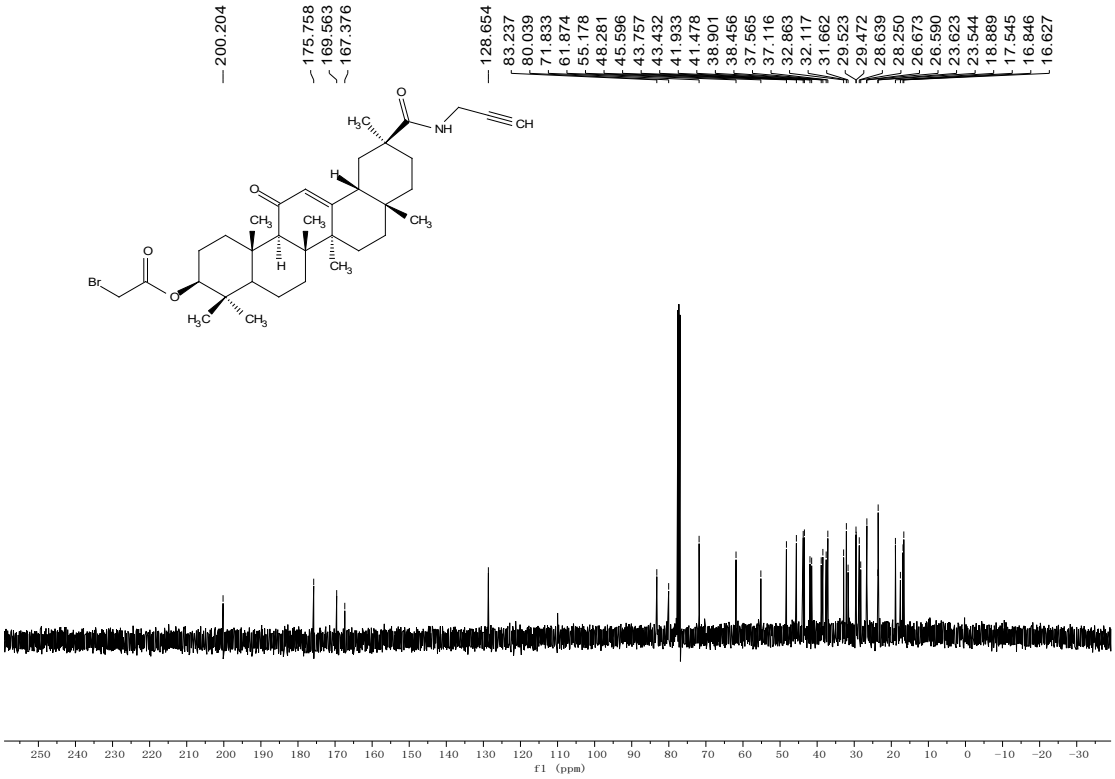
[a] College of Medical Engineering& the Key Laboratory for Medical Functional Nanomaterials, Jining Medical University, Shandong Jining, 272067, P. R. China.[b] College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu 730070, P. R. China,
† These authors equally contributed to this work.
* Corresponding author: E-mail: wangxicun@nwnu.edu.cn (Xicun Wang), liuhuapeng2021@mail.jnmc.edu.cn（Huapeng Liu）



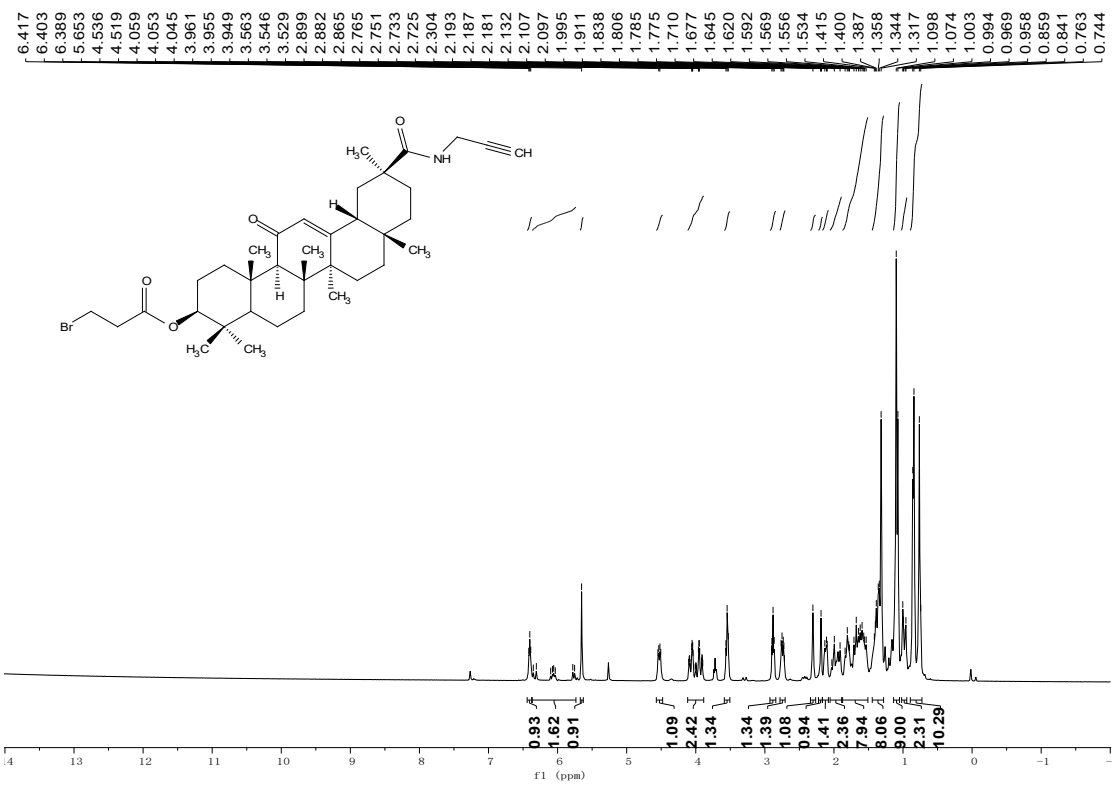
SI-Figure 3 The ^{1}H-NMR spectra of **1a** (400 MHz, Chloroform-d)



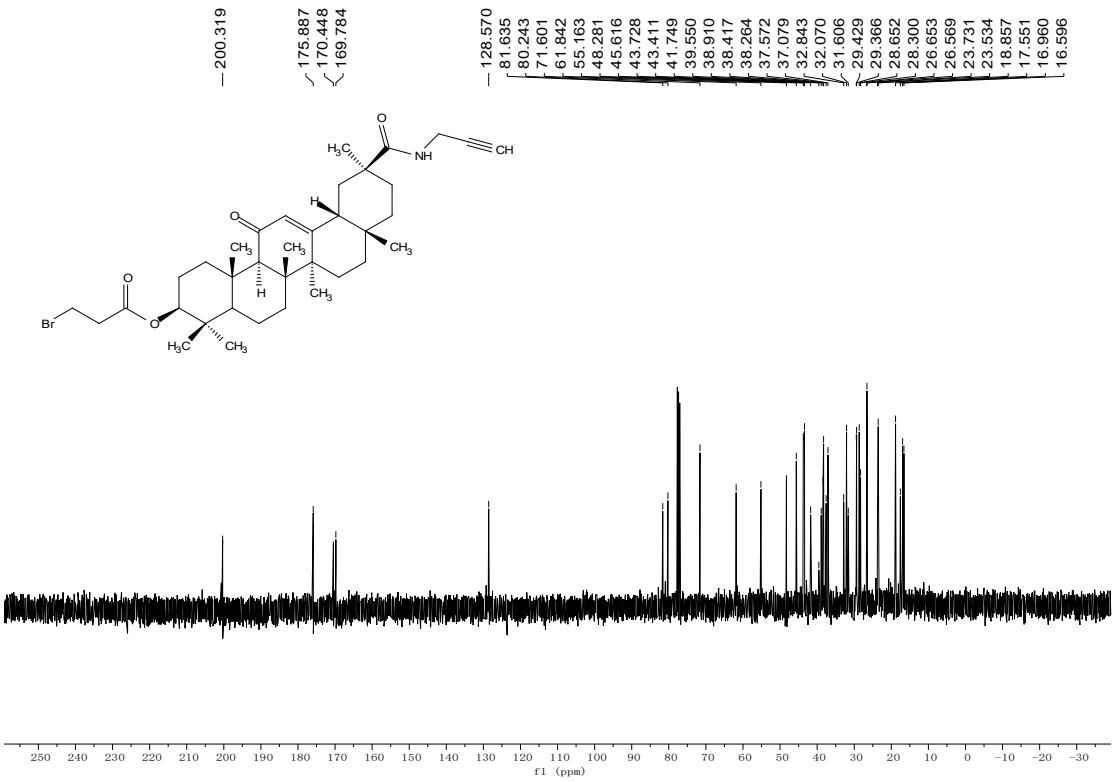
SI-Figure 4 The ^{13}C-NMR spectra of **1a** (101 MHz, Chloroform-d)



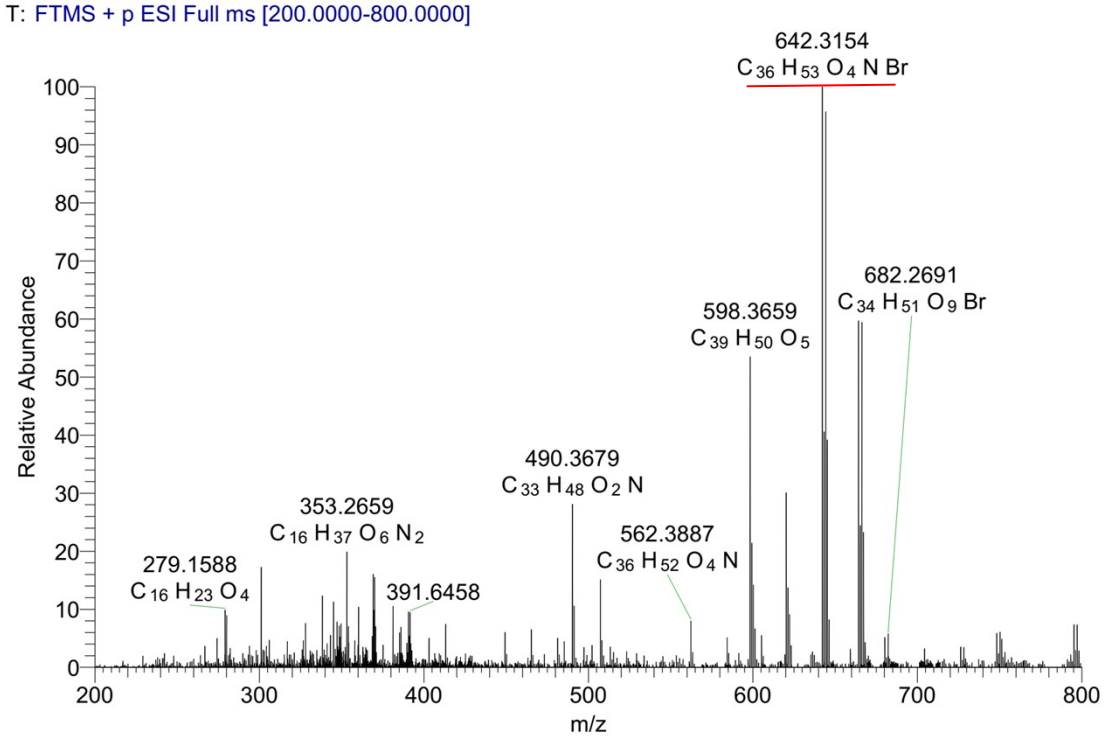
SI-Figure 5 The ^{1}H-NMR spectra of **2a** (400 MHz, Chloroform-d)



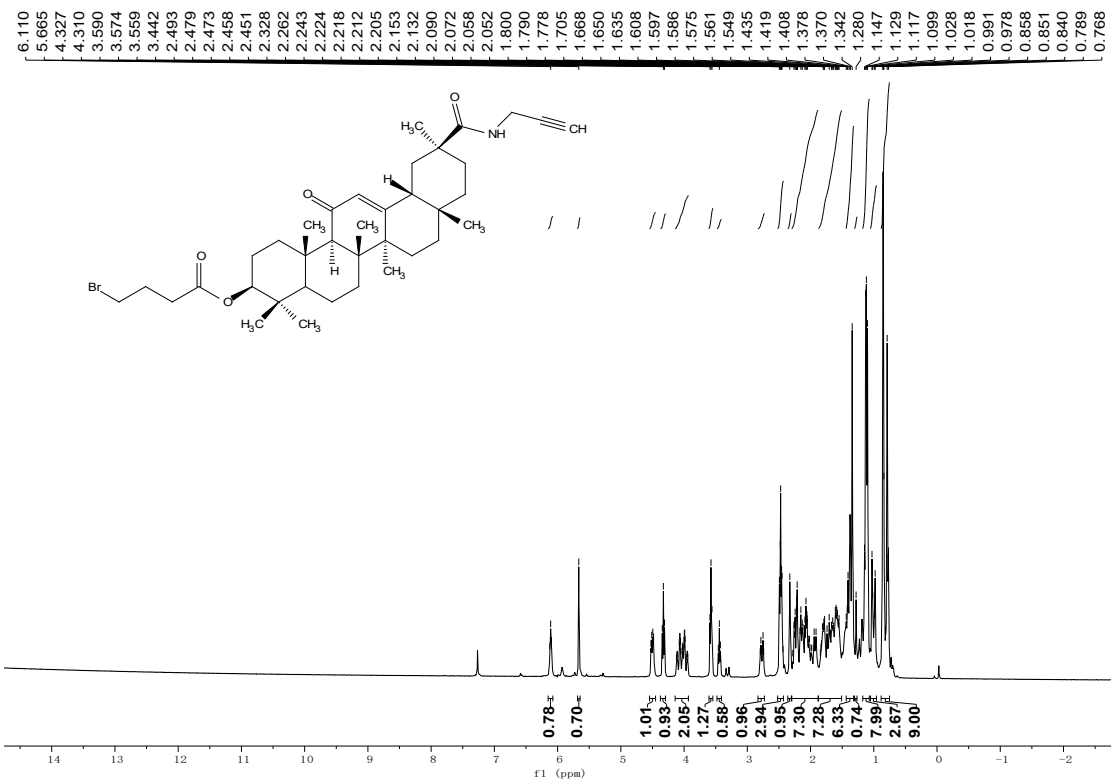
SI-Figure 6 The ^{13}C-NMR spectra of **2a** (101 MHz, Chloroform-d)



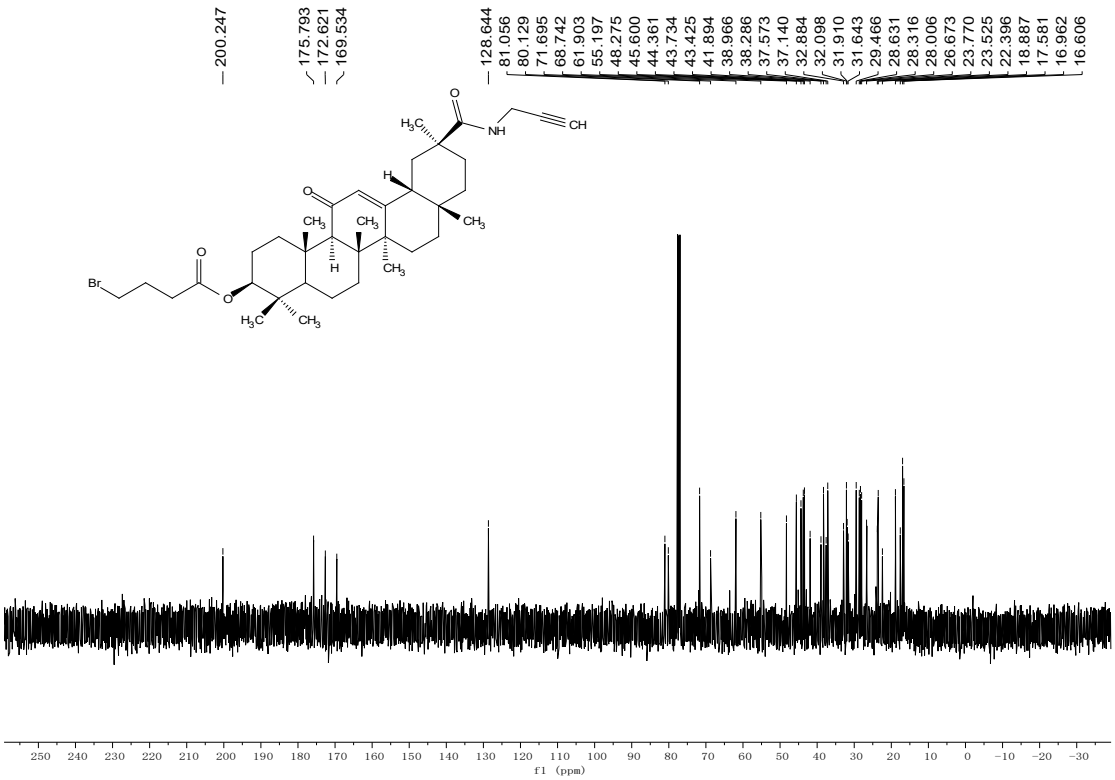
SI-Figure 7 The ESI-HRMS spectra of **2a**



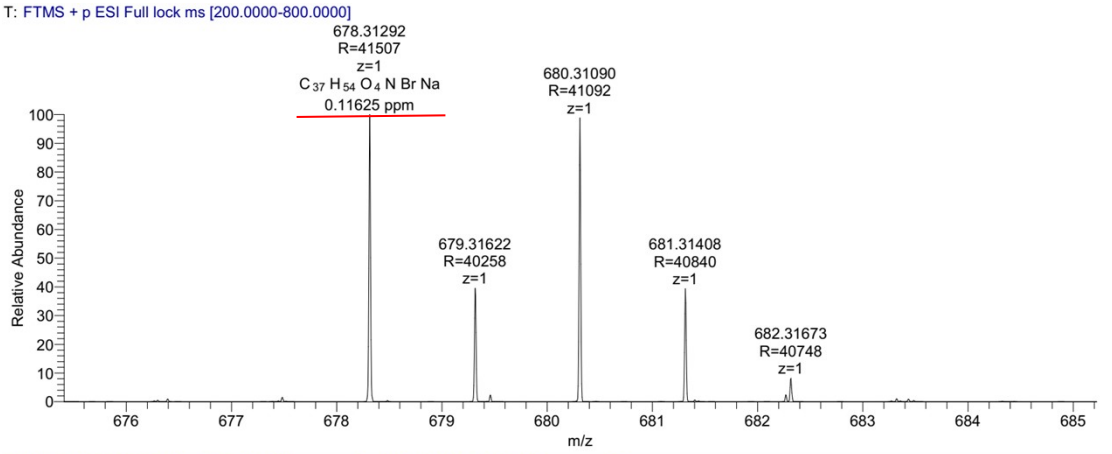
SI-Figure 8 The ^{1}H-NMR spectra of **3a** (400 MHz, Chloroform-d)



SI-Figure 9 The ^{13}C-NMR spectra of **3a** (101 MHz, Chloroform-d)



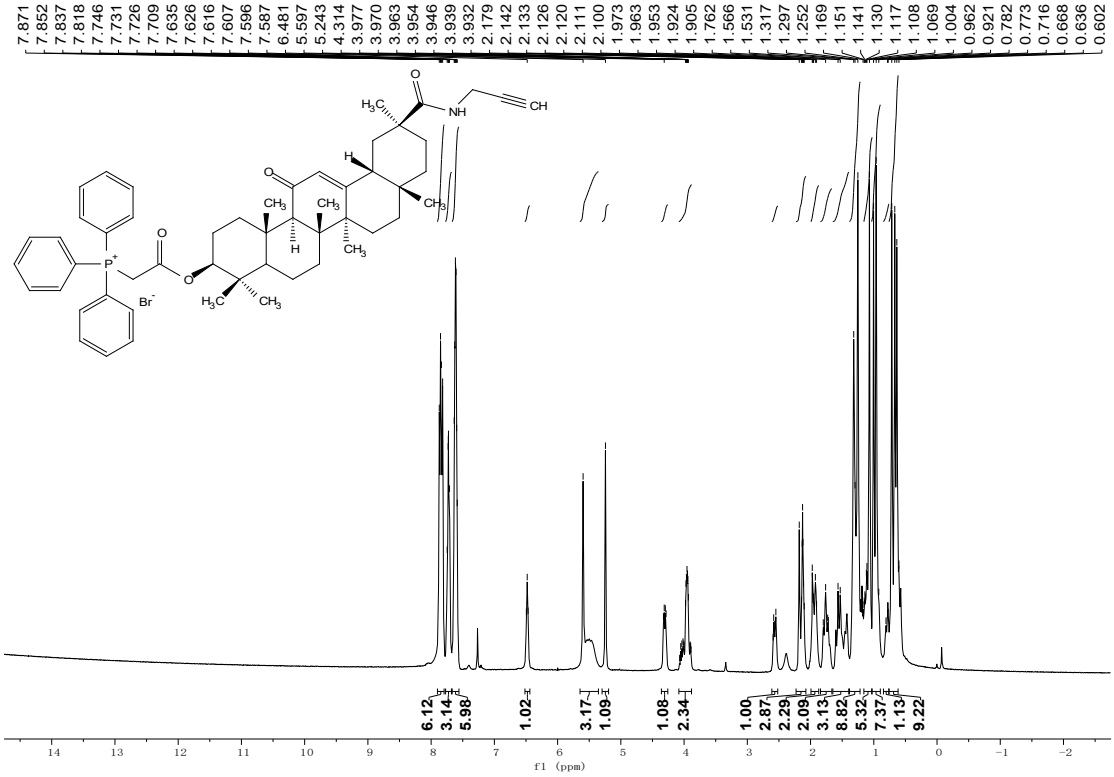
SI-Figure 10 The ESI-HRMS spectra of **3a**



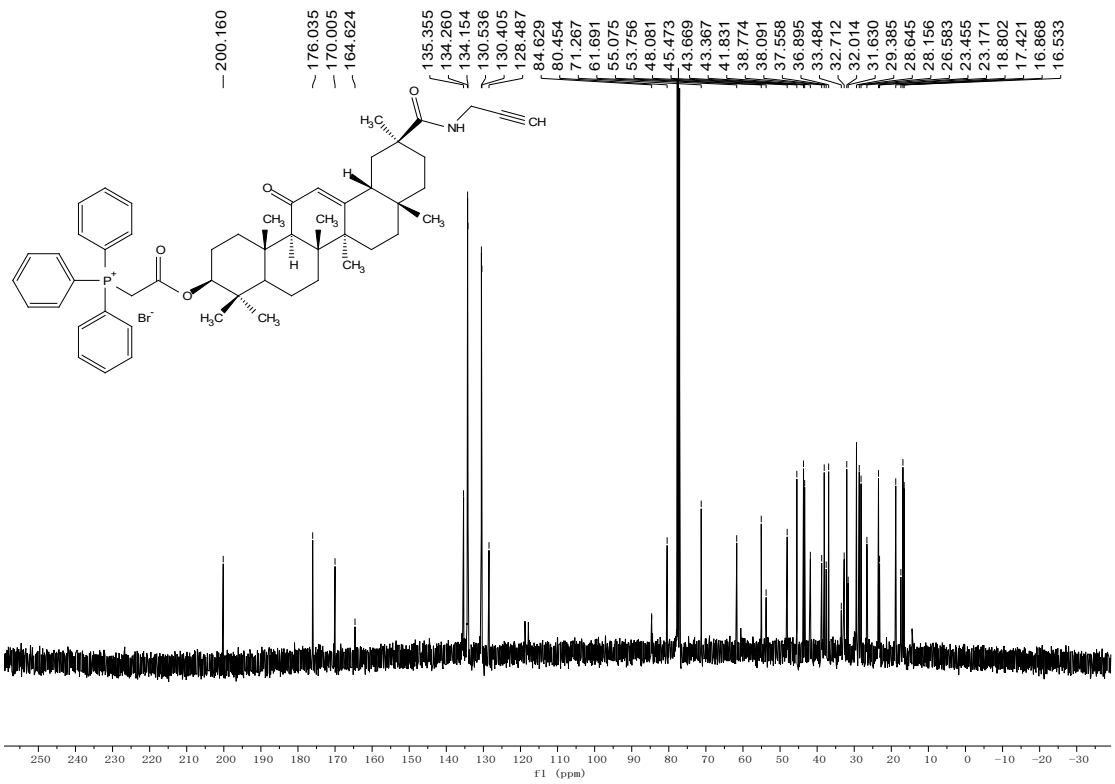
WXC-LIUHUAPENG-56#35-99 RT: 0.15578-0.44104 AV: 65
T: FTMS + p ESI Full lock ms [200.0000-800.0000]
m/z= 675.40842-685.22216

m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
678.31292	2408762.0	100.00	41506.51	1.00	0.12	$C_{37}H_{54}O_4NBrNa$
679.31622	966021.9	40.10	40258.05	1.00		
680.31090	2380580.0	98.83	41091.95	1.00		
681.31408	951169.8	39.49	40839.99	1.00		
682.31673	200193.2	8.31	40748.00	1.00		

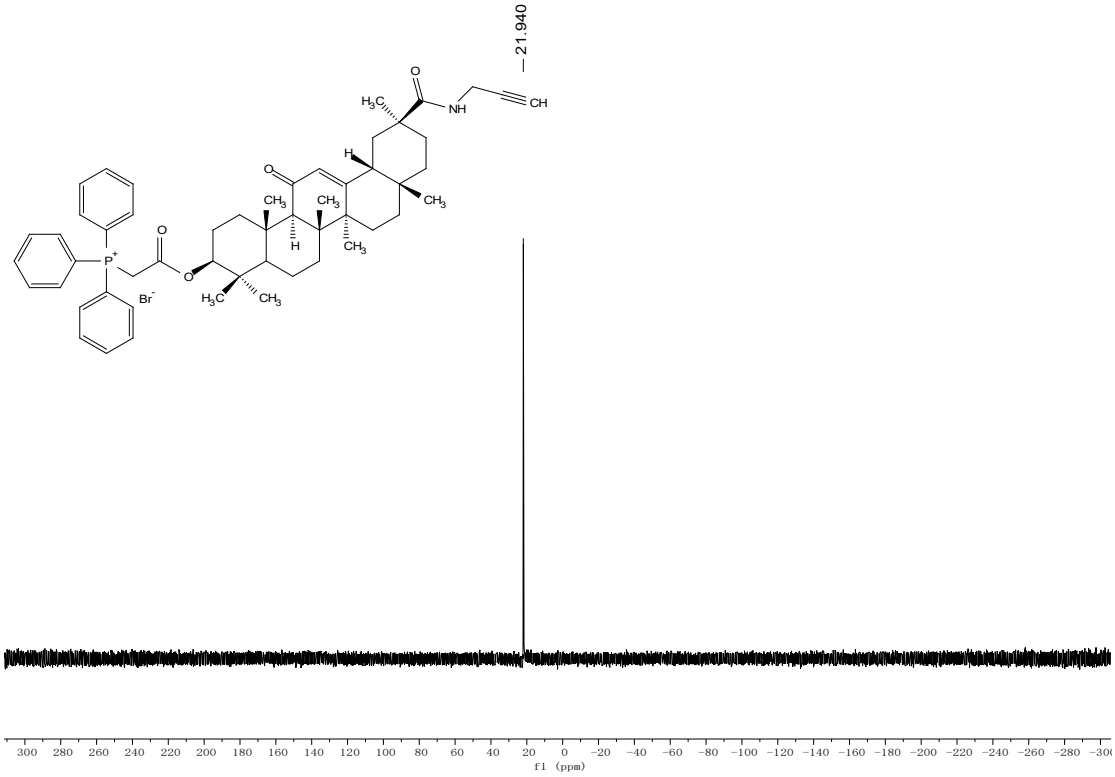
SI-Figure 11 The ^{1}H-NMR spectra of **1b** (400 MHz, Chloroform-d)



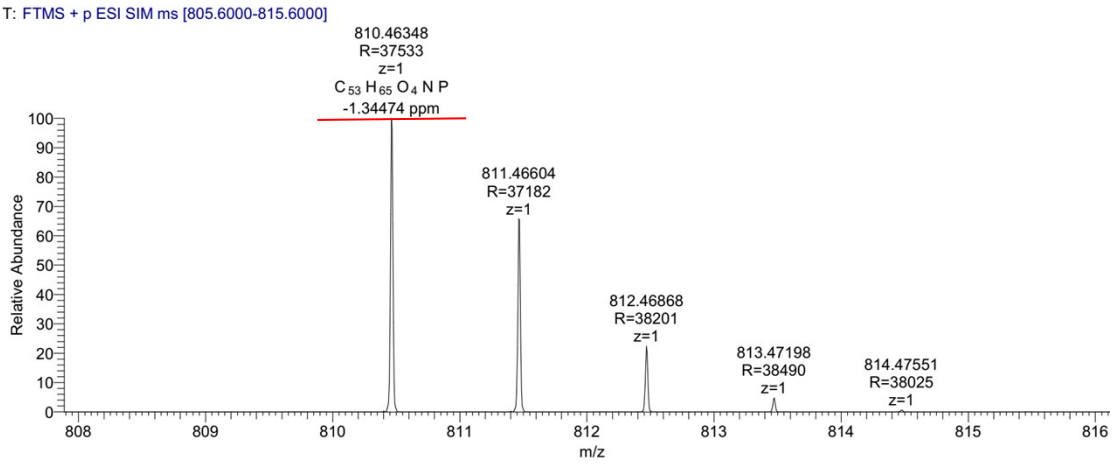
SI-Figure 12 The ^{13}C-NMR spectra of **1b** (101 MHz, Chloroform-d)



SI-Figure 13 The ^{31}P -NMR spectra of **1b** (162MHz, $CDCl_3$)



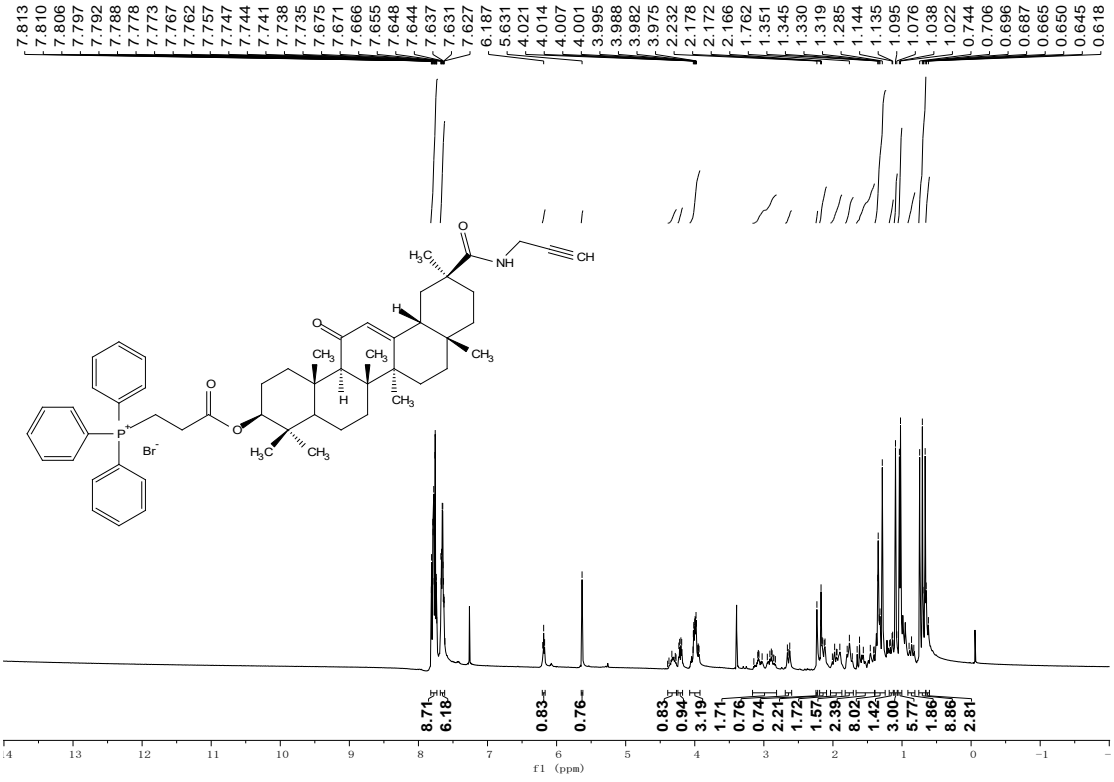
SI-Figure 14 The ESI-HRMS spectra of **1b**



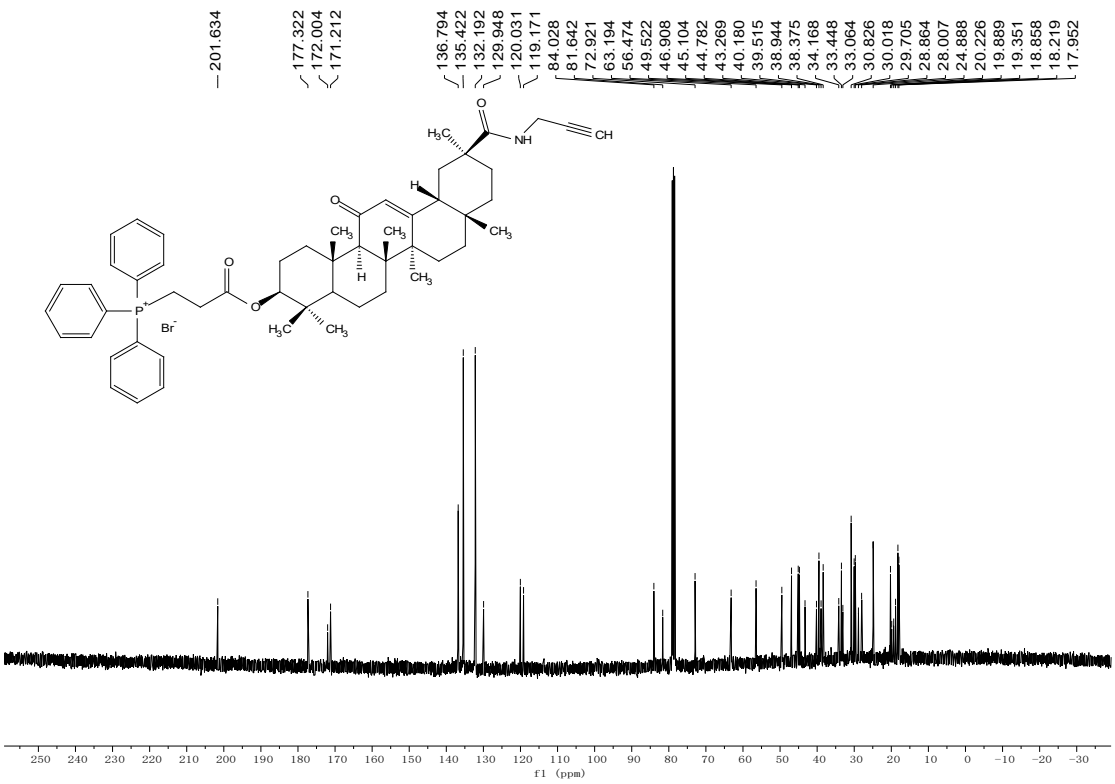
WXC-LIUHUAPENG-40#102-128 RT: 0.45484-0.57073 AV: 27
T: FTMS + p ESI SIM ms [805.6000-815.6000]
m/z= 807.88711-816.19644

m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
810.46348	1713143040.0	100.00	37532.88	1.00	-1.34	$C_{53}H_{65}O_4NP$
811.46604	1139326592.0	66.51	37181.58	1.00		
812.46868	378312512.0	22.08	38201.01	1.00		
813.47198	80049528.0	4.67	38489.99	1.00		
814.47551	11049324.0	0.64	38025.42	1.00		

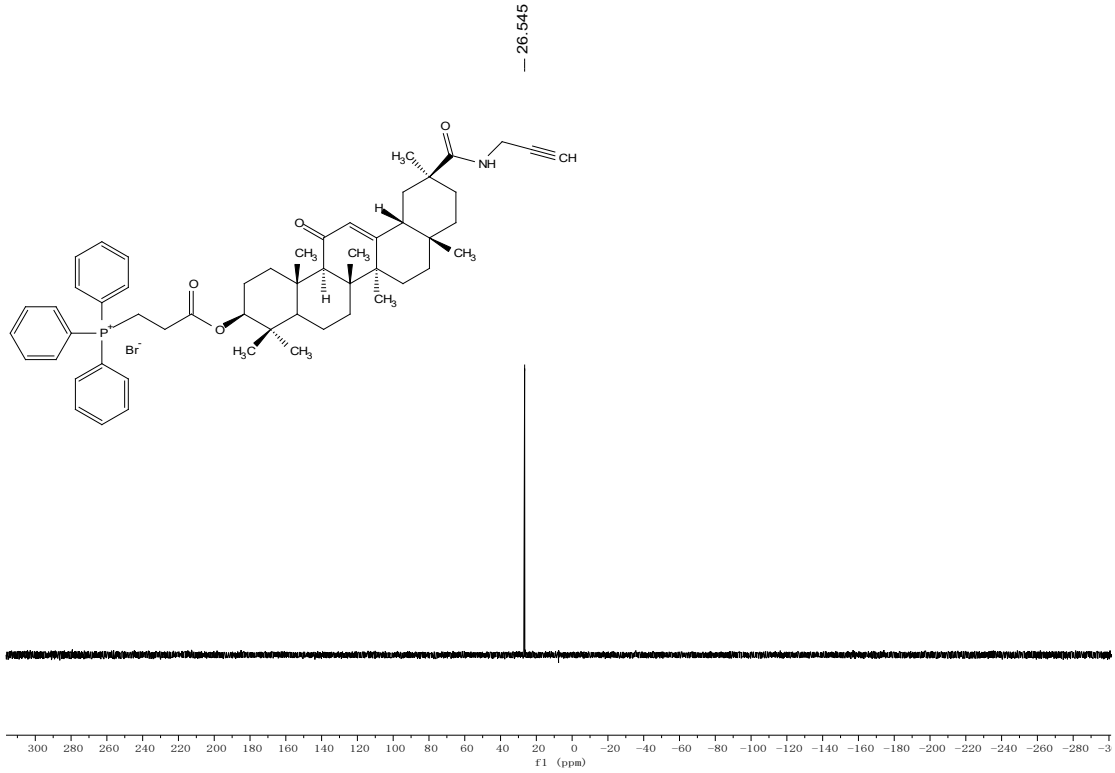
SI-Figure 15 The ^{1}H-NMR spectra of **2b** (400 MHz, Chloroform-d)



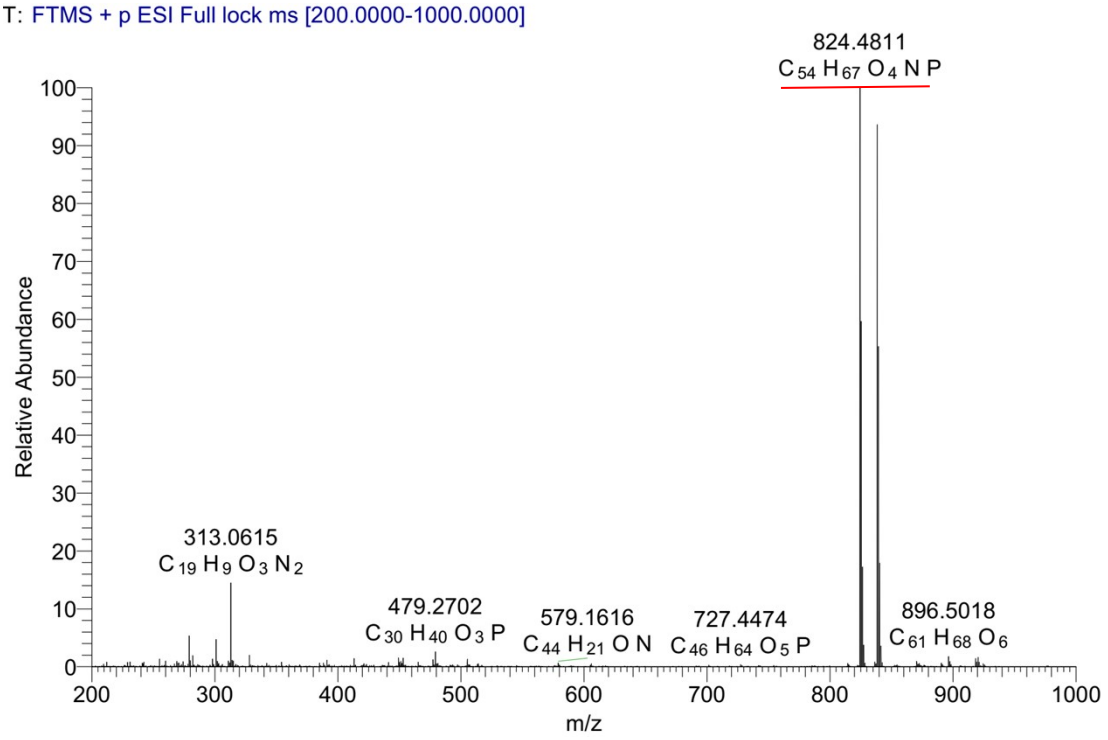
SI-Figure 16 The ^{13}C-NMR spectra of **2b** (101 MHz, Chloroform-d)



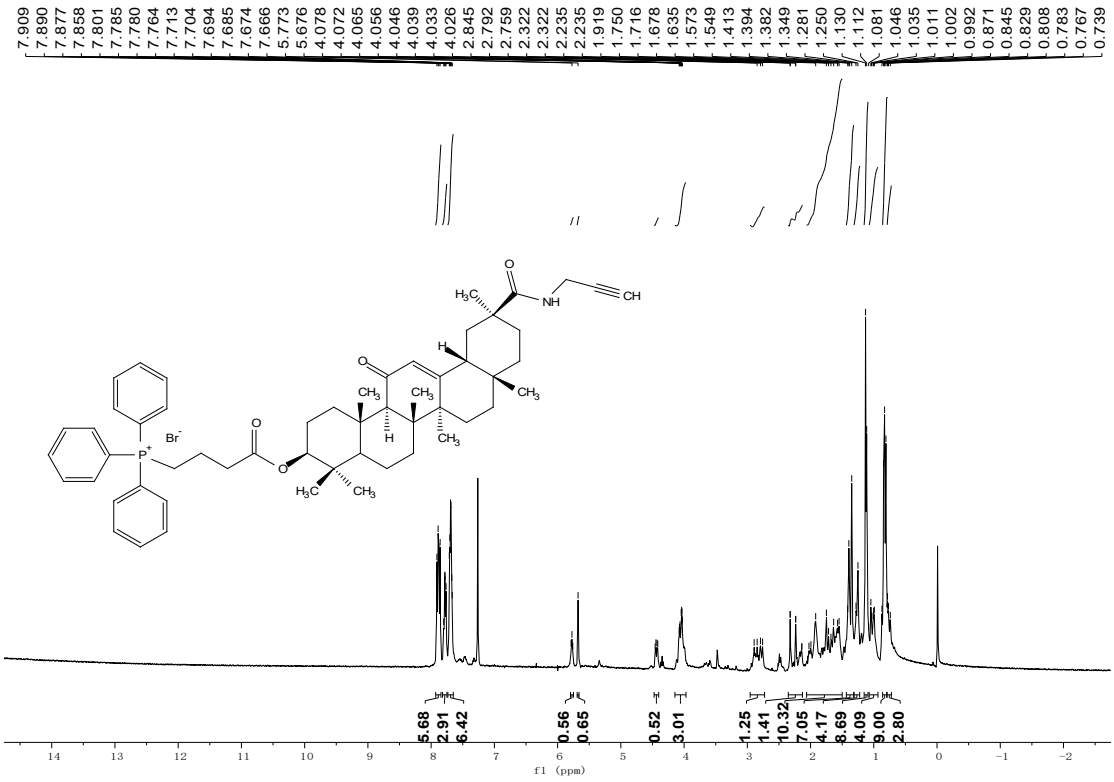
SI-Figure 17 The ^{31}P -NMR spectra of **2b** (162MHz, DMSO-d^6)



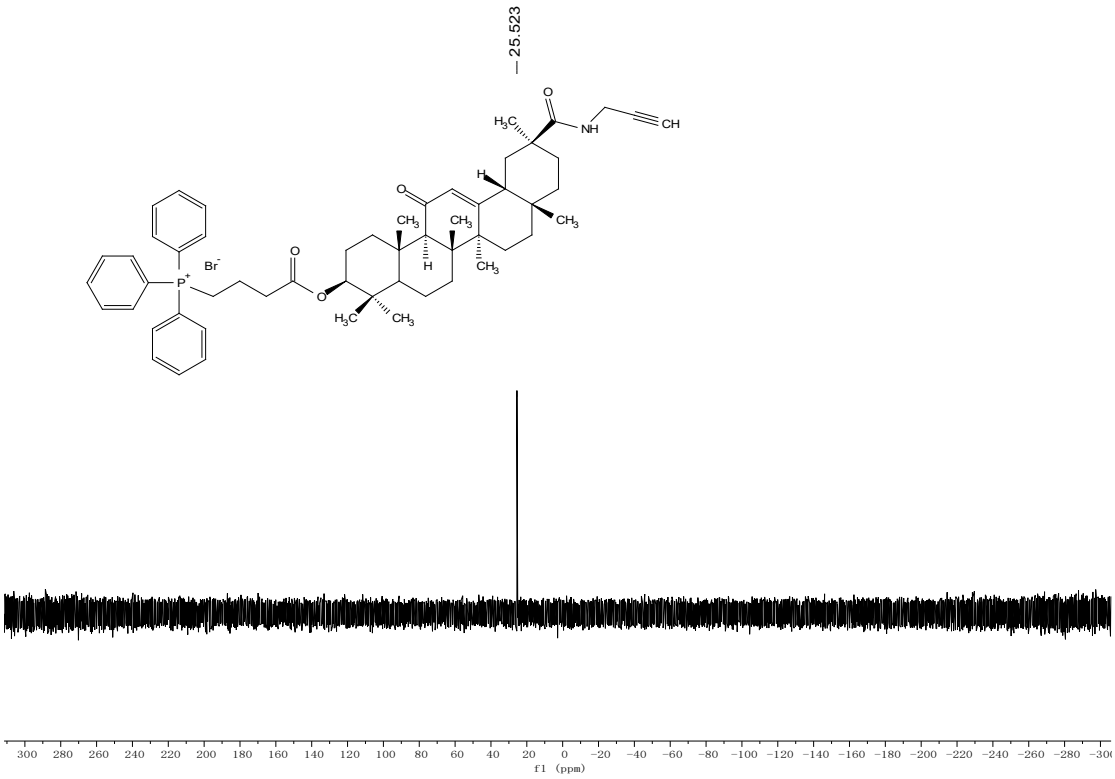
SI-Figure 18 The ESI-HRMS spectra of **2b**



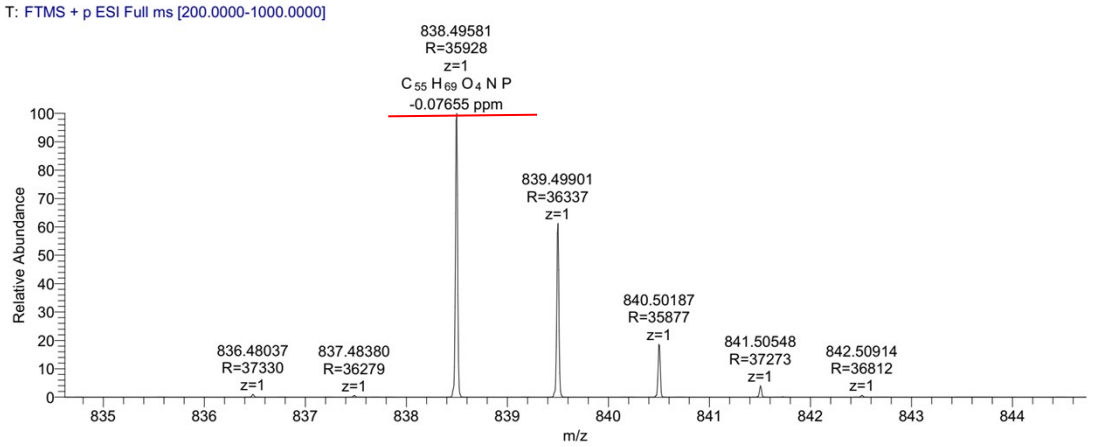
SI-Figure 19 The [1]H-NMR spectra of **3b** (400 MHz, Chloroform-d)



SI-Figure 20 The [31]P -NMR spectra of **3b** (162MHz, DMSO-d[6])



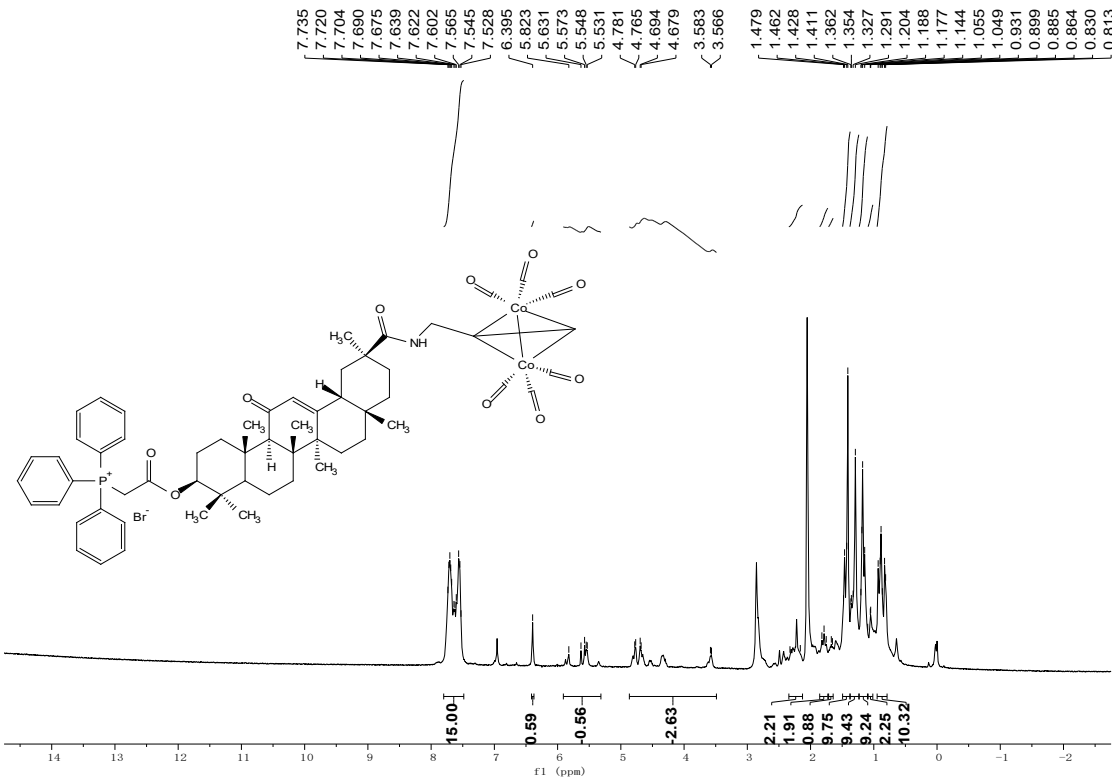
SI-Figure 21 The ESI-HRMS spectra of **3b**



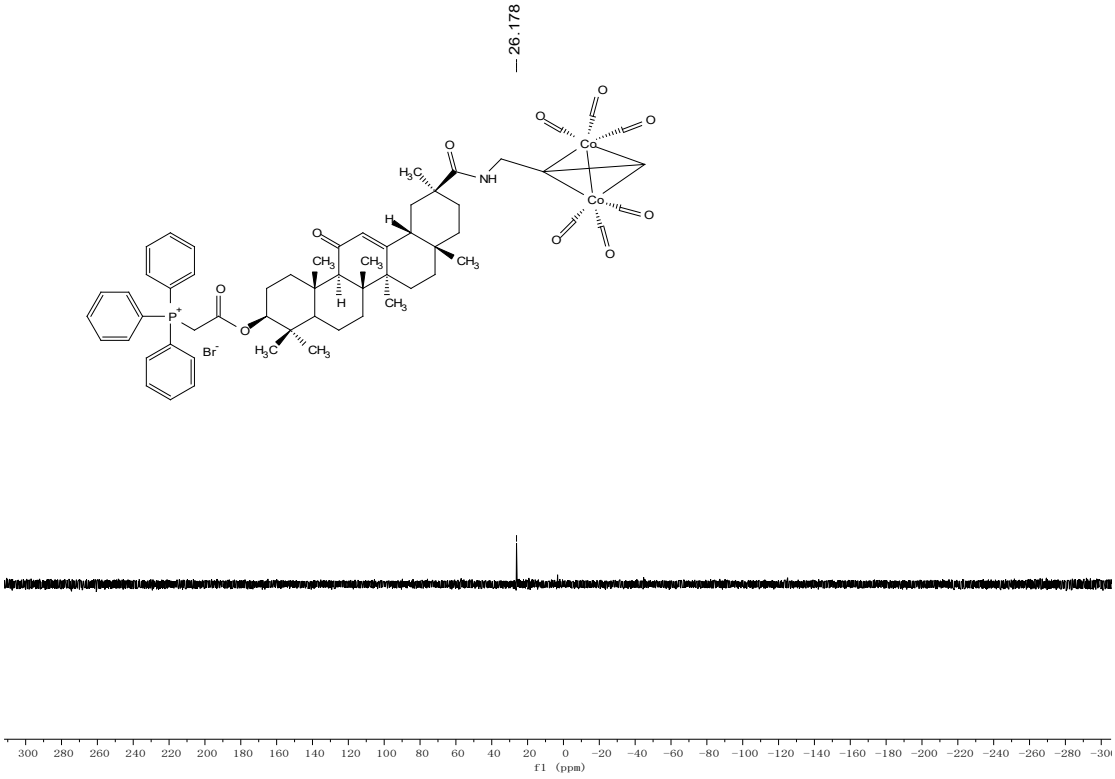
WXC-LIUHUAPENG-54#62-98 RT: 0.27612-0.43658 AV: 37
T: FTMS + p ESI Full ms [200.0000-1000.0000]
m/z= 834.61722-844.72806

m/z	Intensity	Relative	Resolution	Charge	Delta (ppm)	Composition
836.48037	2372263.8	0.97	37329.66	1.00		
838.49581	243771904.0	100.00	35927.69	1.00	-0.08	C55 H69 O4 N P
839.49901	147664960.0	60.58	36337.15	1.00		
840.50187	45579964.0	18.70	35877.41	1.00		
841.50548	9644352.0	3.96	37273.24	1.00		

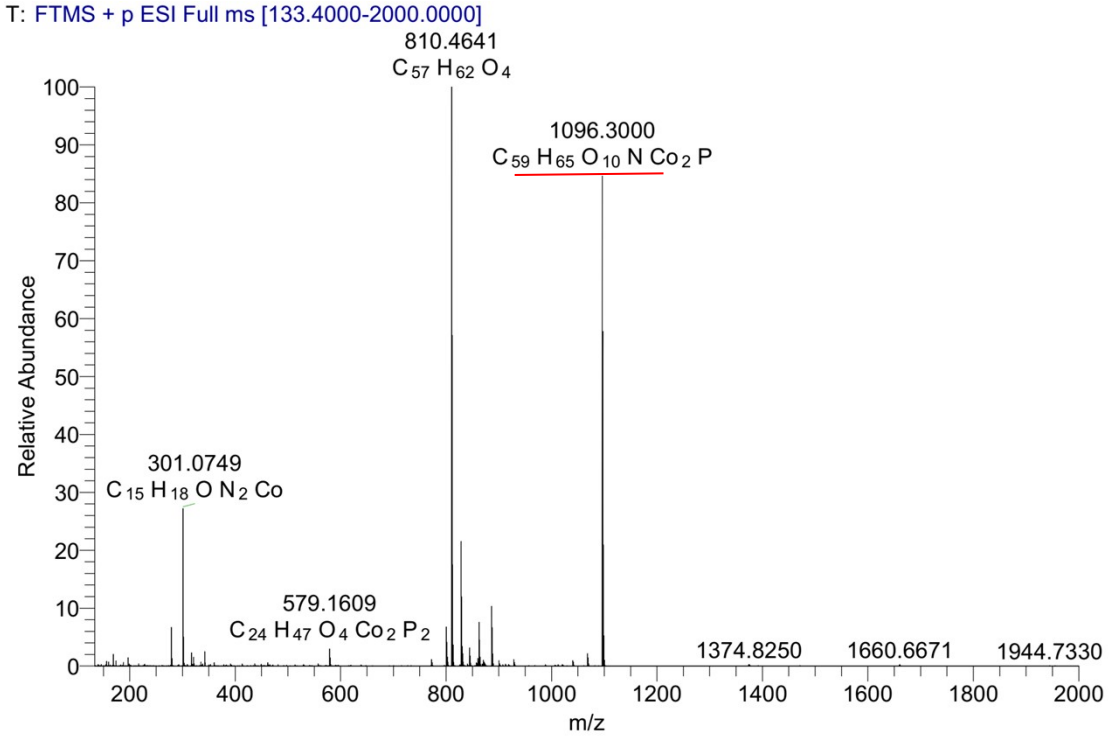
SI-Figure 22 The ^{1}H-NMR spectra of **complex 1** (400 MHz, Acetone-d^{6})



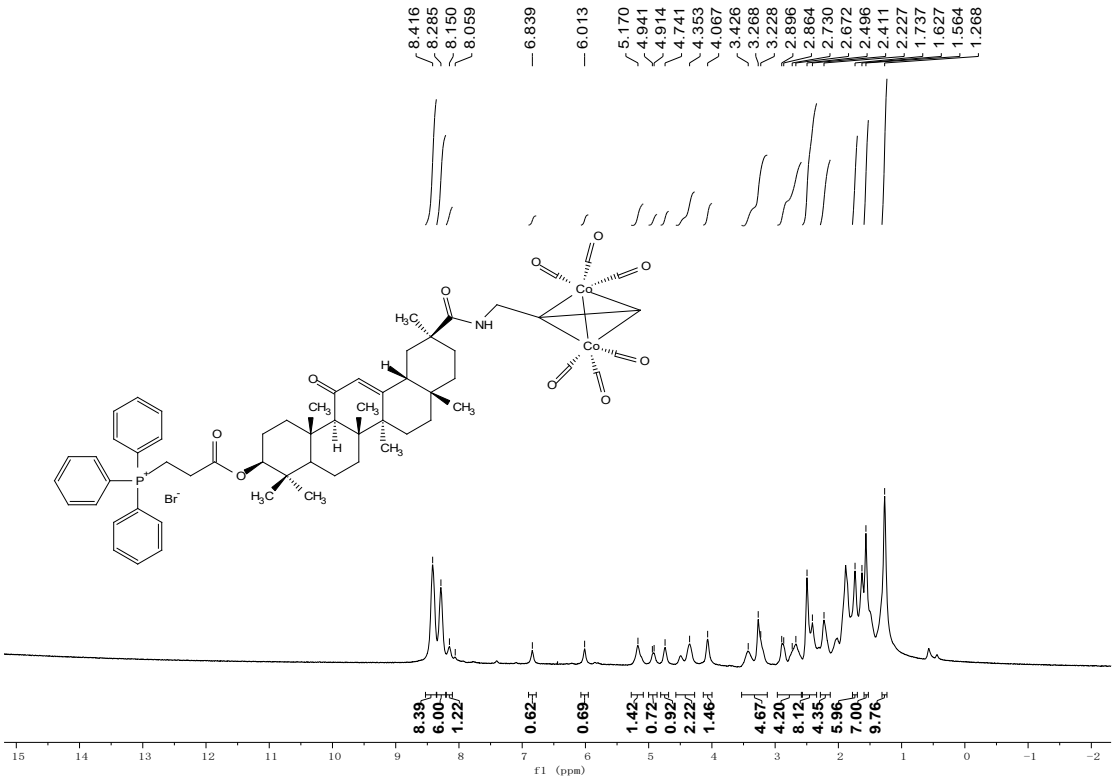
SI-Figure 23 The ^{31}P -NMR spectra of **complex 1**(162MHz, Acetone-d^6)



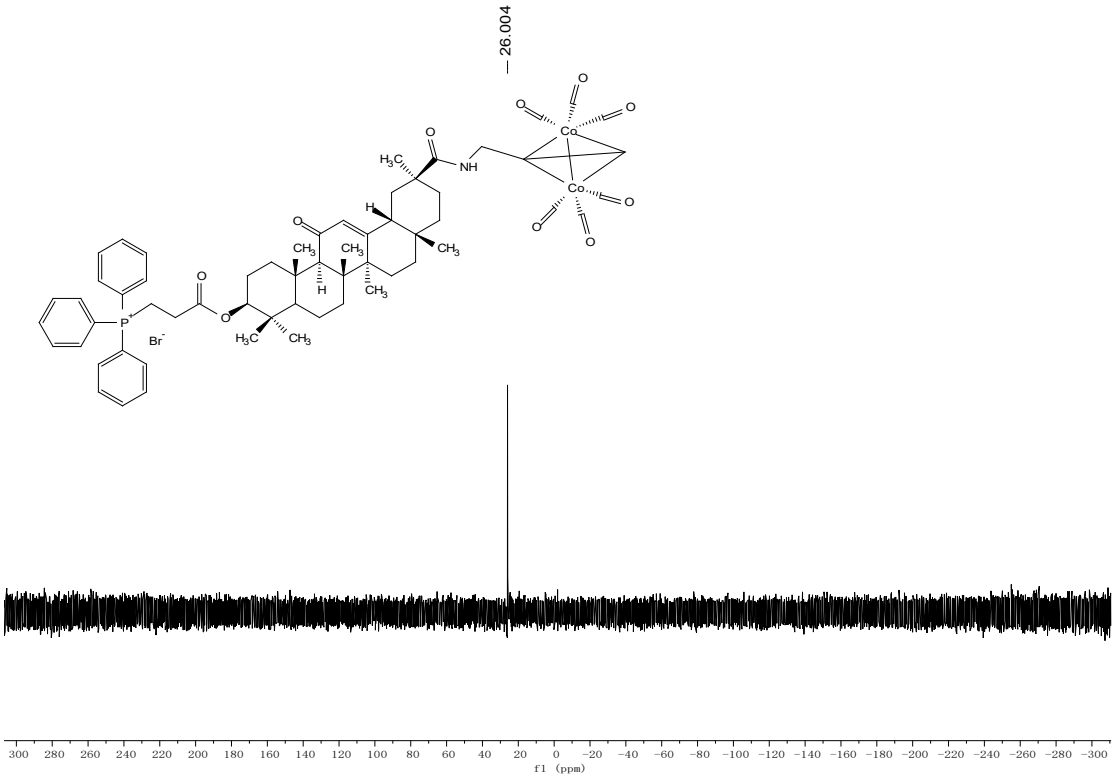
SI-Figure 24 The ESI-HRMS spectra of **1**



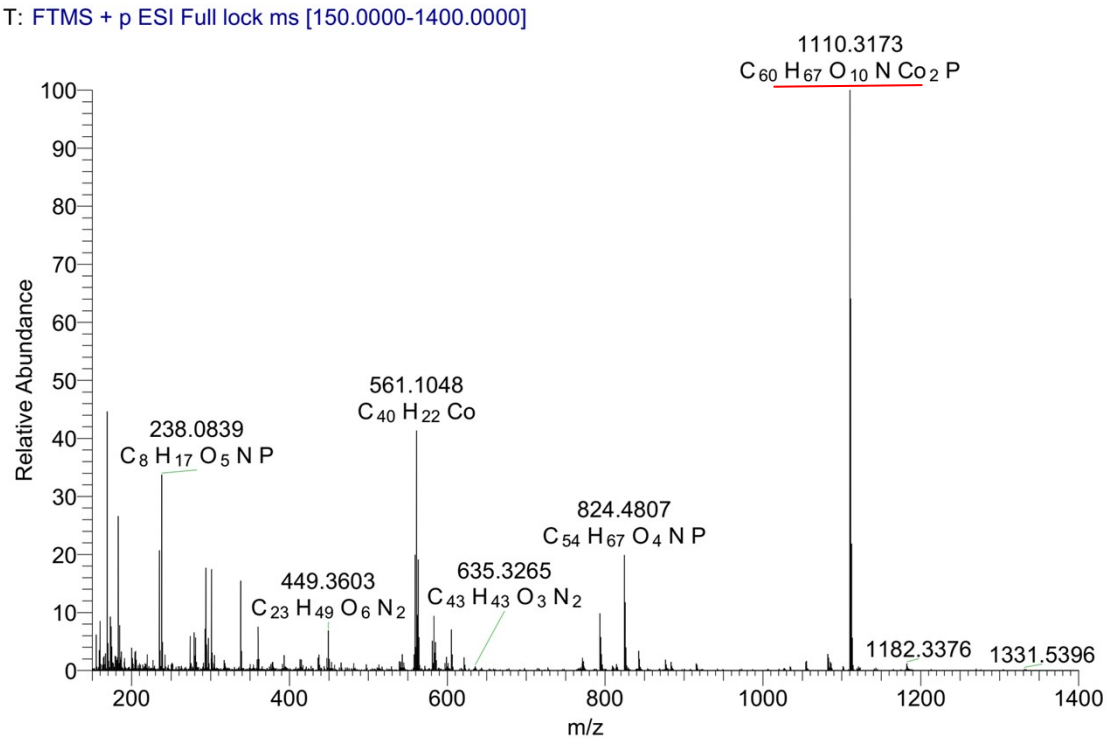
SI-Figure 25 The ^{1}H-NMR spectra of **complex 2** (400 MHz, Acetone-d^{6})



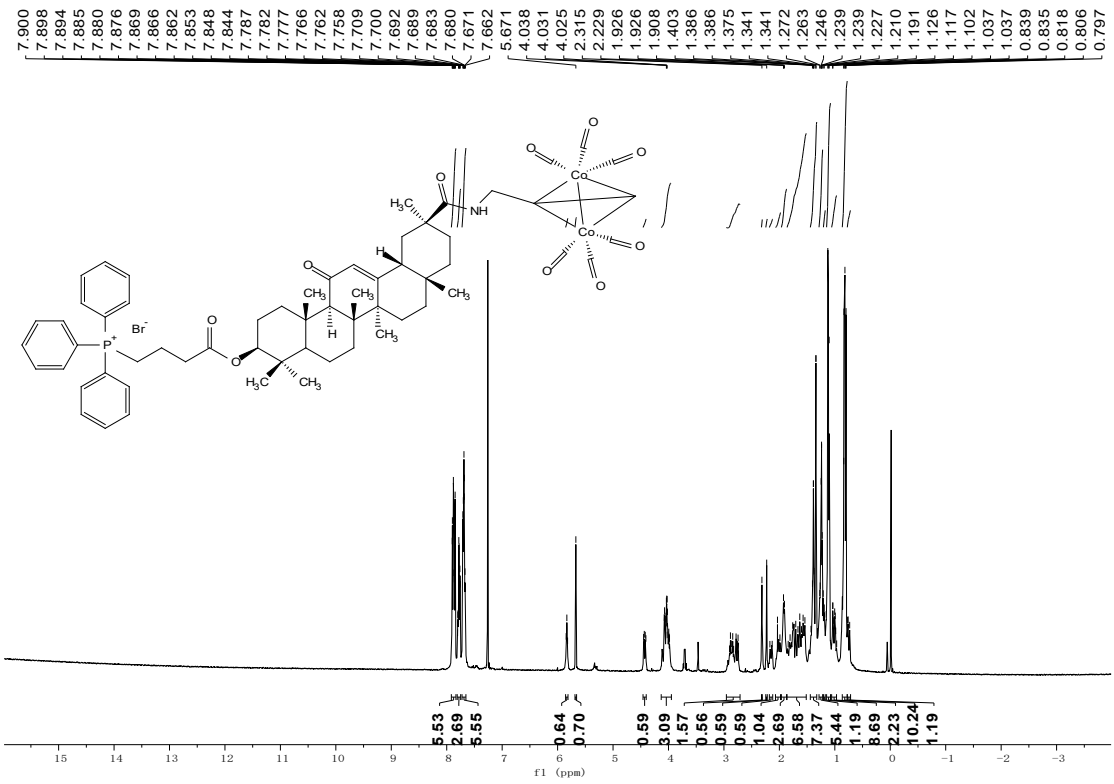
SI-Figure 26 The ^{31}P -NMR spectra of **complex 2** (162MHz, Acetone-d^{6})



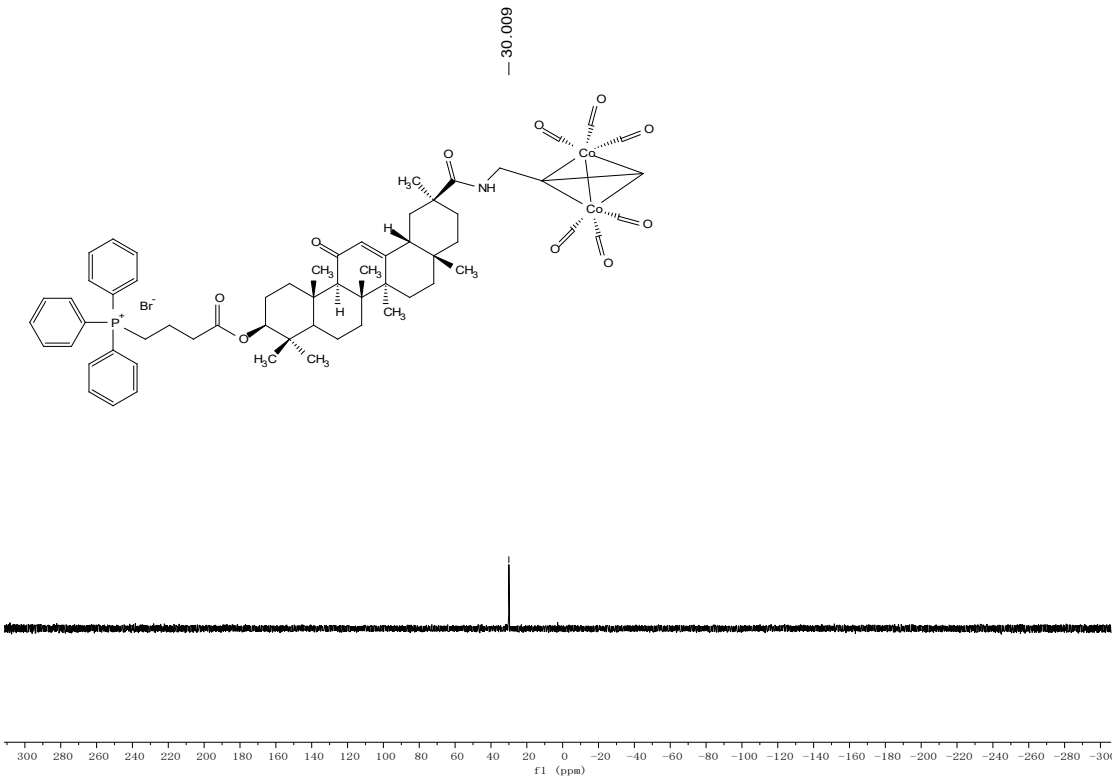
SI-Figure 27 The ESI-HRMS spectra of **2**



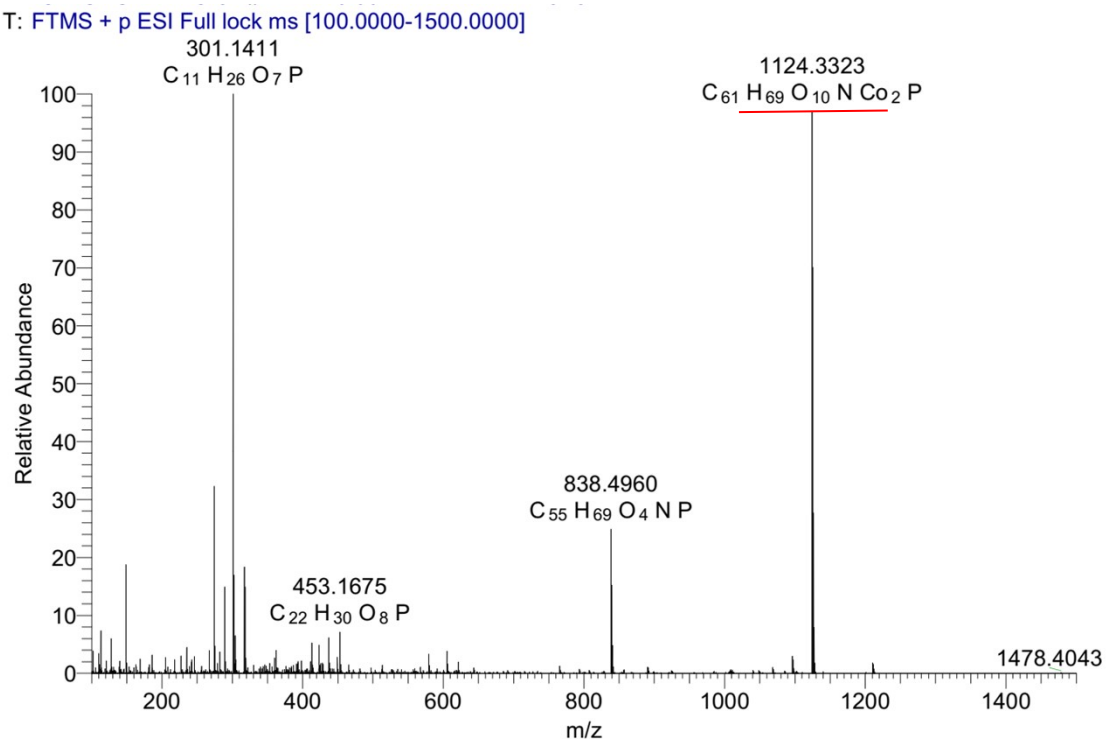
SI-Figure 28 The ^{1}H-NMR spectra of **complex 3** (400 MHz, Chloroform-d)



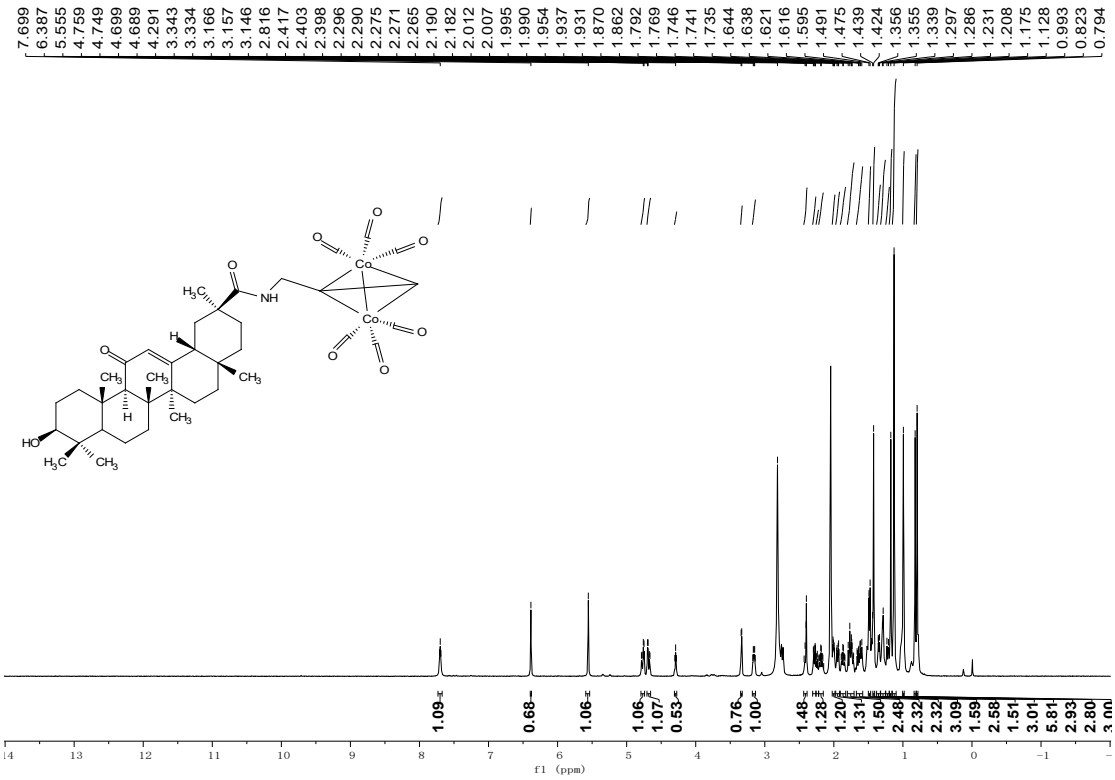
SI-Figure 29 The ^{31}P -NMR spectra of **complex 3** (162MHz, Acetone-d^6)



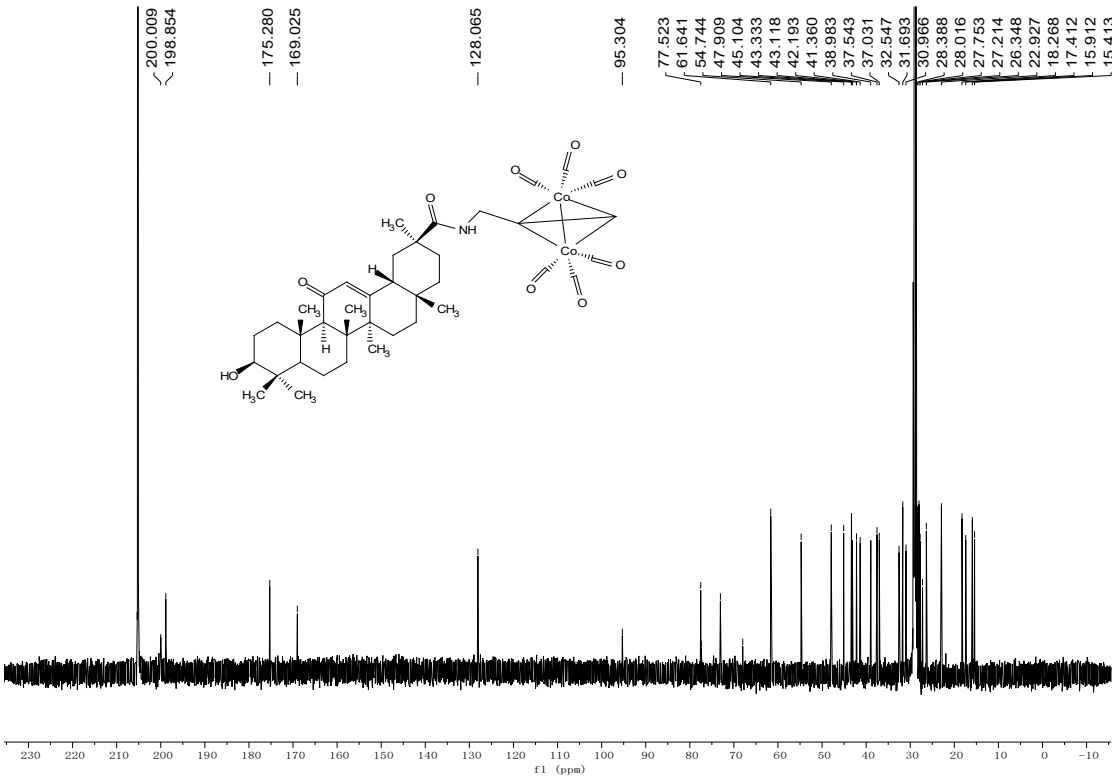
SI-Figure 30 The ESI-HRMS spectra of **3**



SI-Figure 31 The ^{1}H-NMR spectra of **Co-Alkynyl-GA** (600 MHz, Acetone-d^{6})



SI-Figure 32 The ^{31}P -NMR spectra of **Co-Alkynyl-GA** (151 MHz, Acetone-d^{6})



SI-Figure 33 The ESI-HRMS spectra of **Co-Alkynyl-GA**