

Discovery of a Dual-Acting Inhibitor of Interleukin-1 β and STATs for the Treatment of Inflammatory Bowel Disease

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Supporting Information

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1. The in vitro cytotoxicity profile for 10v

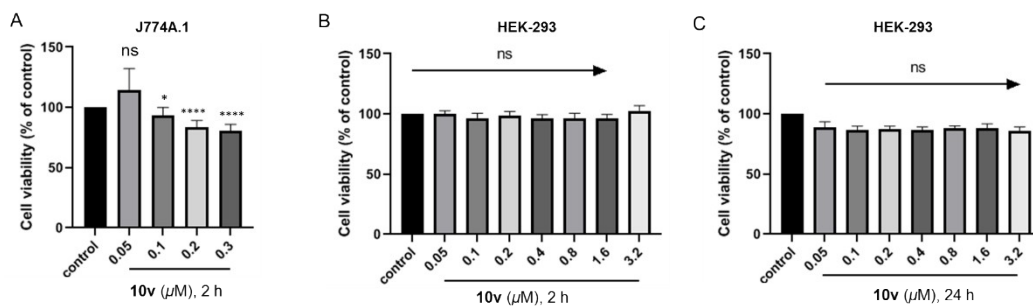
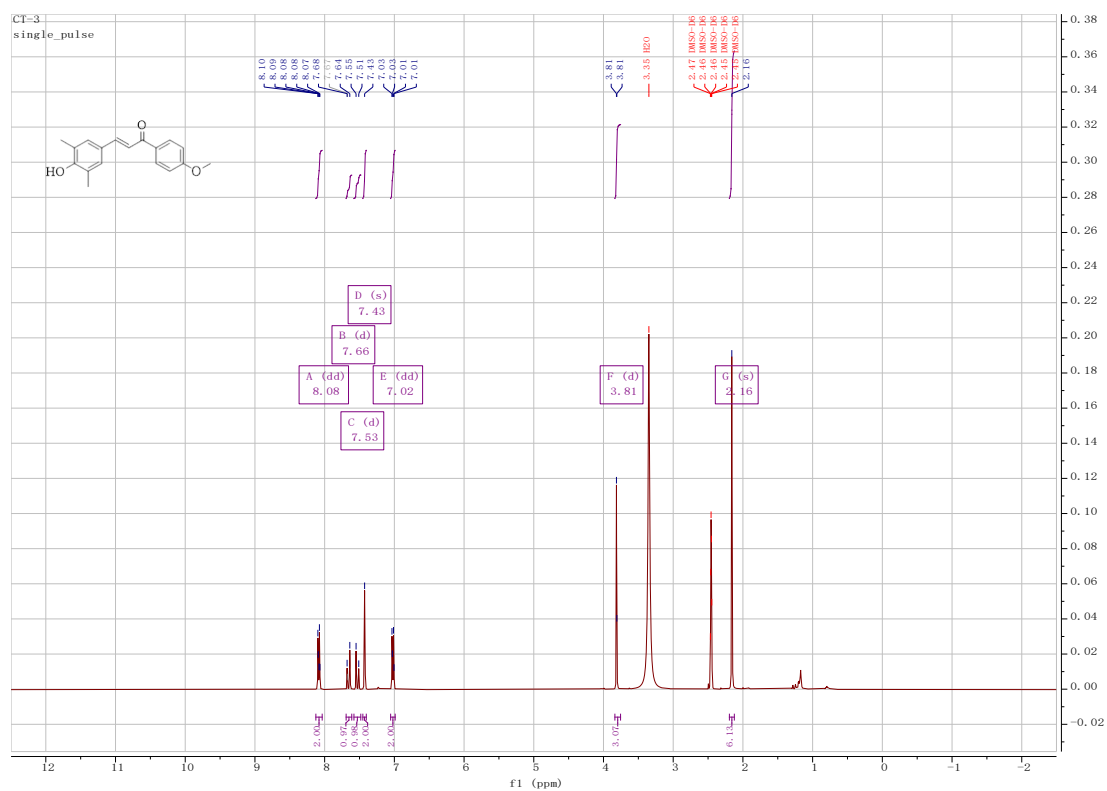
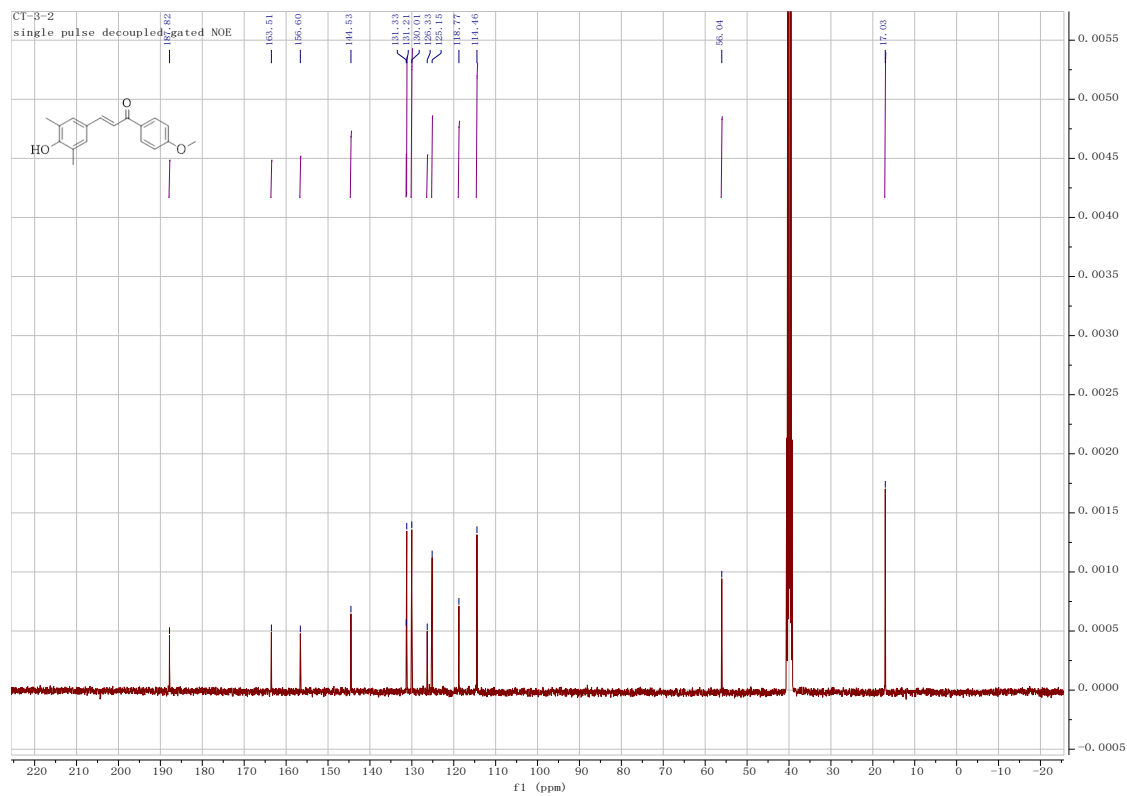


Figure S1. The cell viability detection of 10v using CCK8 assay.

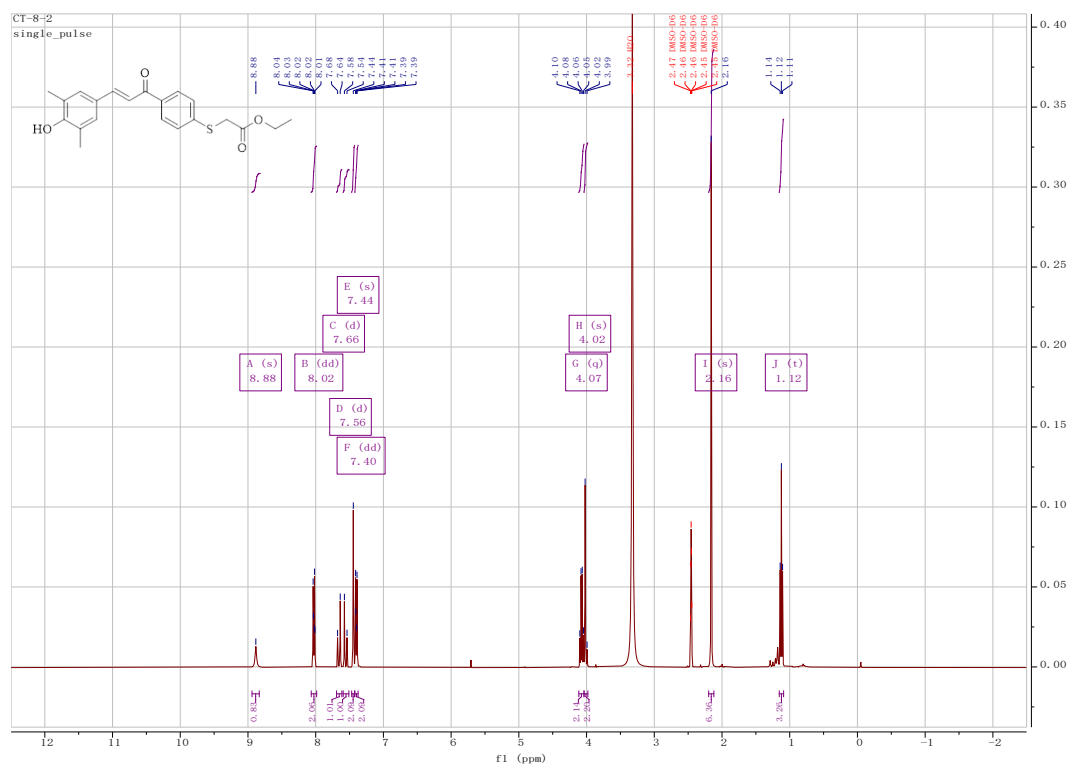
¹H NMR spectrum of **10b** in DMSO



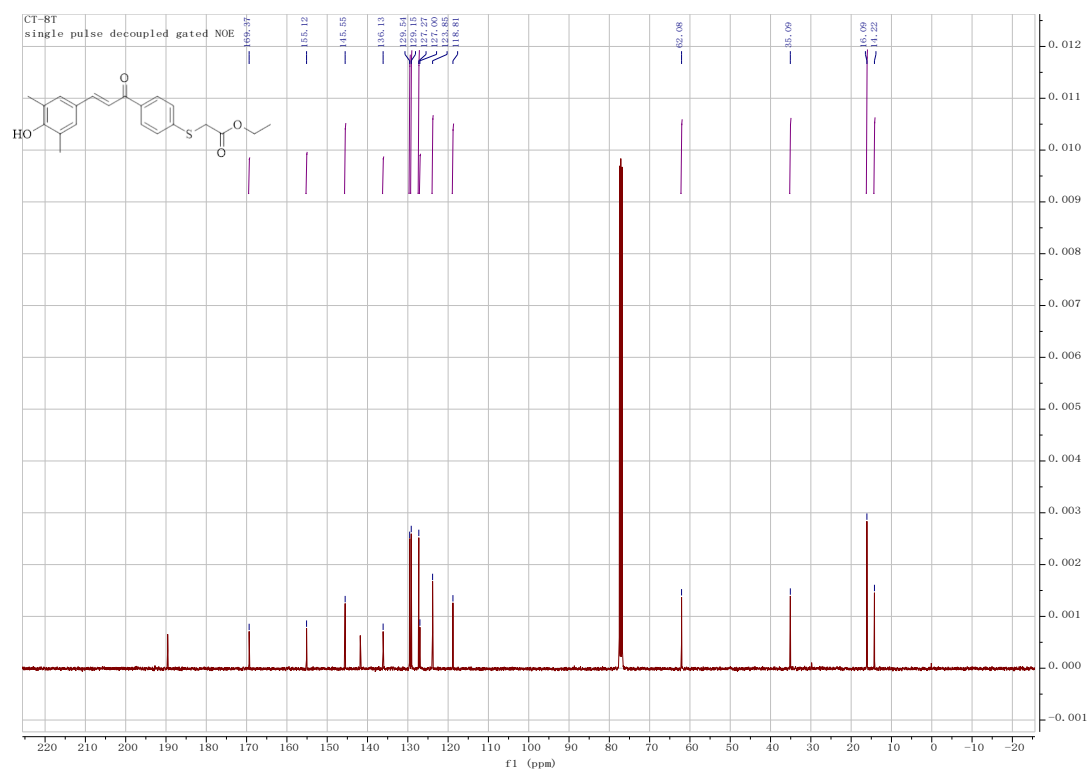
¹³C NMR spectrum of **10b** in DMSO



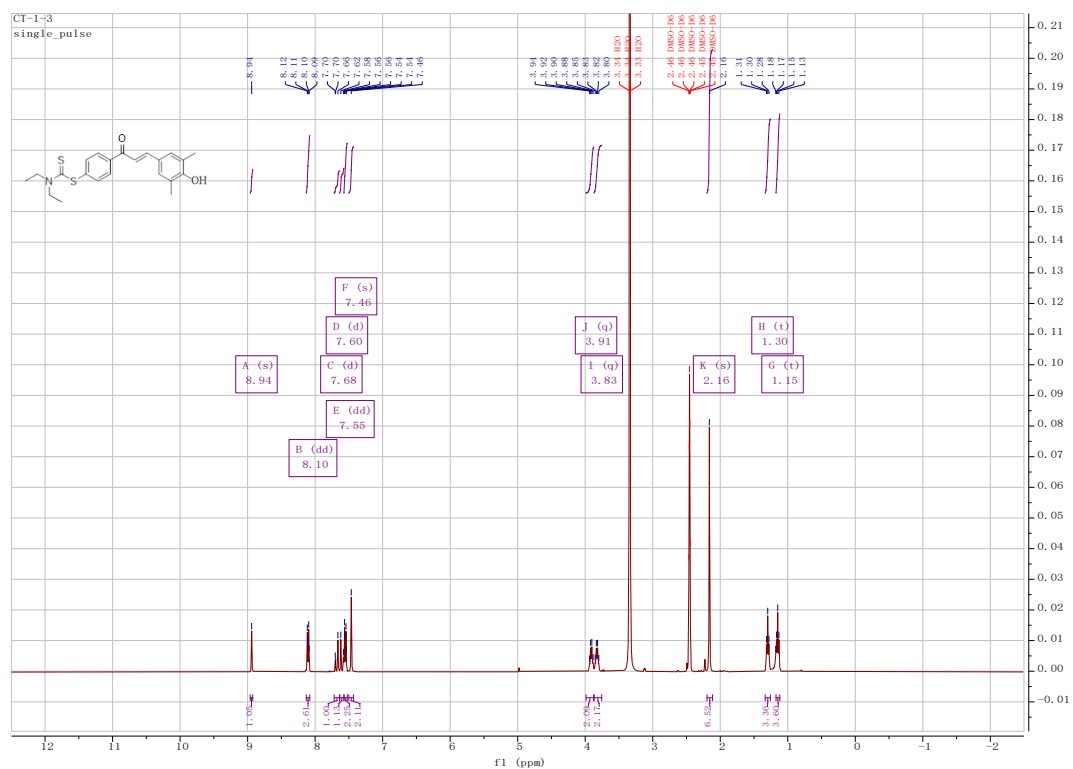
¹HNMR spectrum of 10c in DMSO



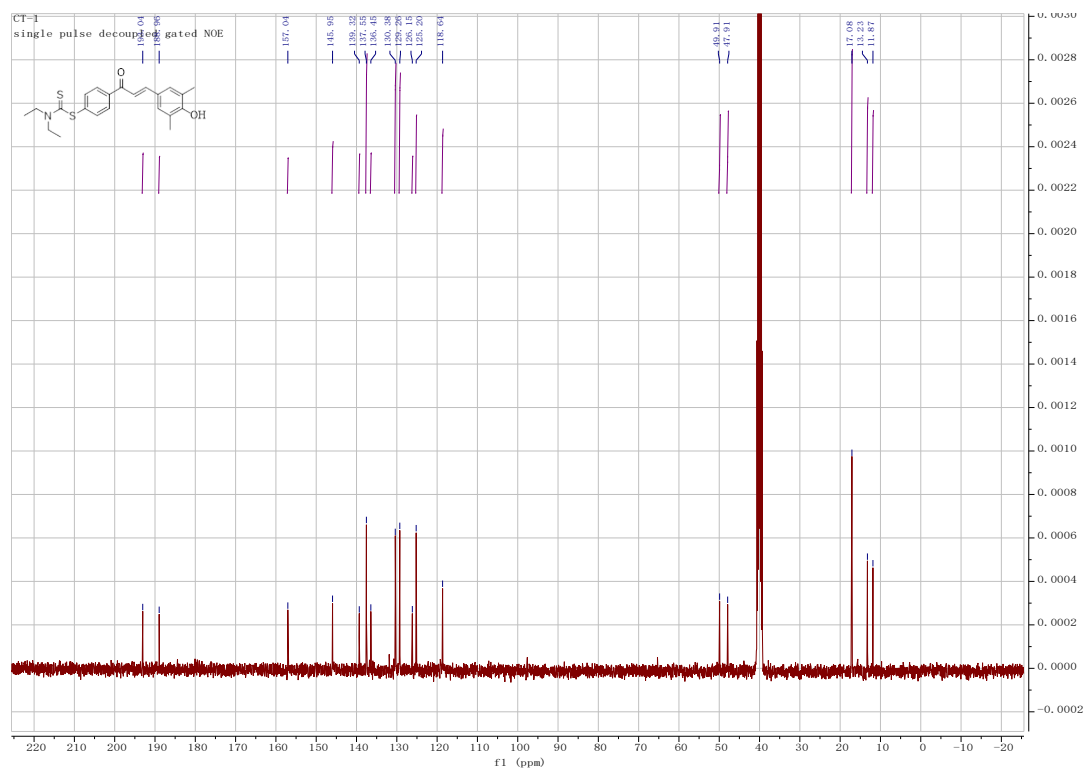
¹³CNMR spectrum of 10c in DMSO



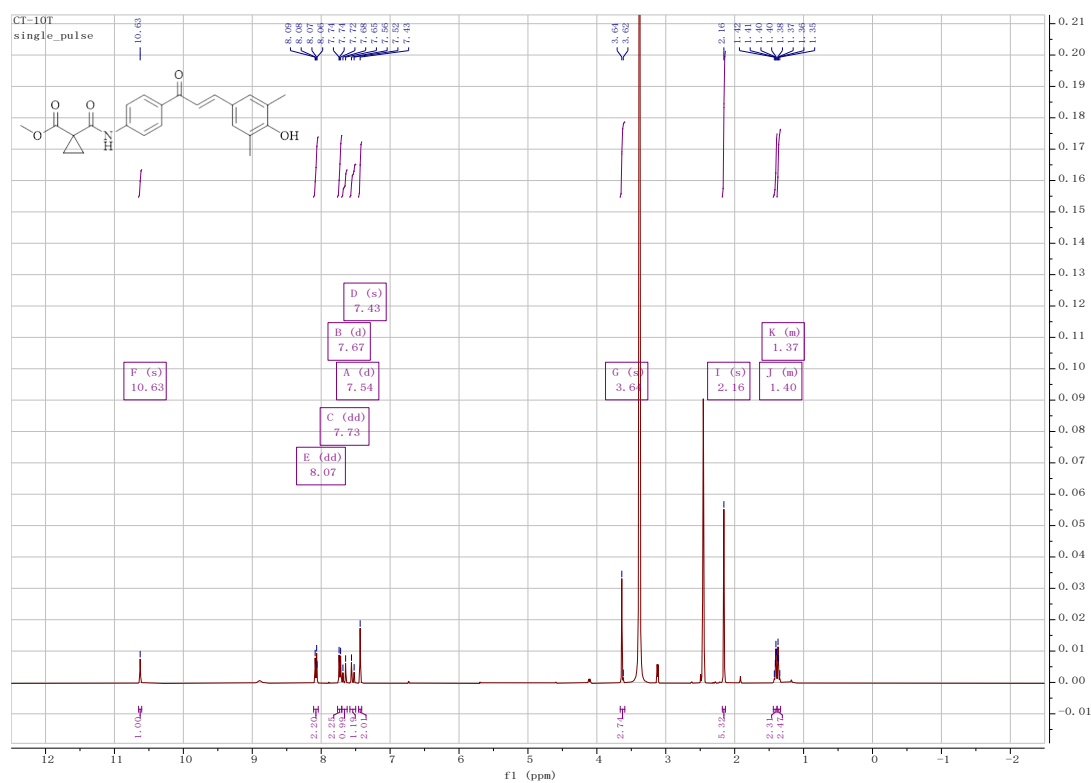
¹H NMR spectrum of **10d** in DMSO



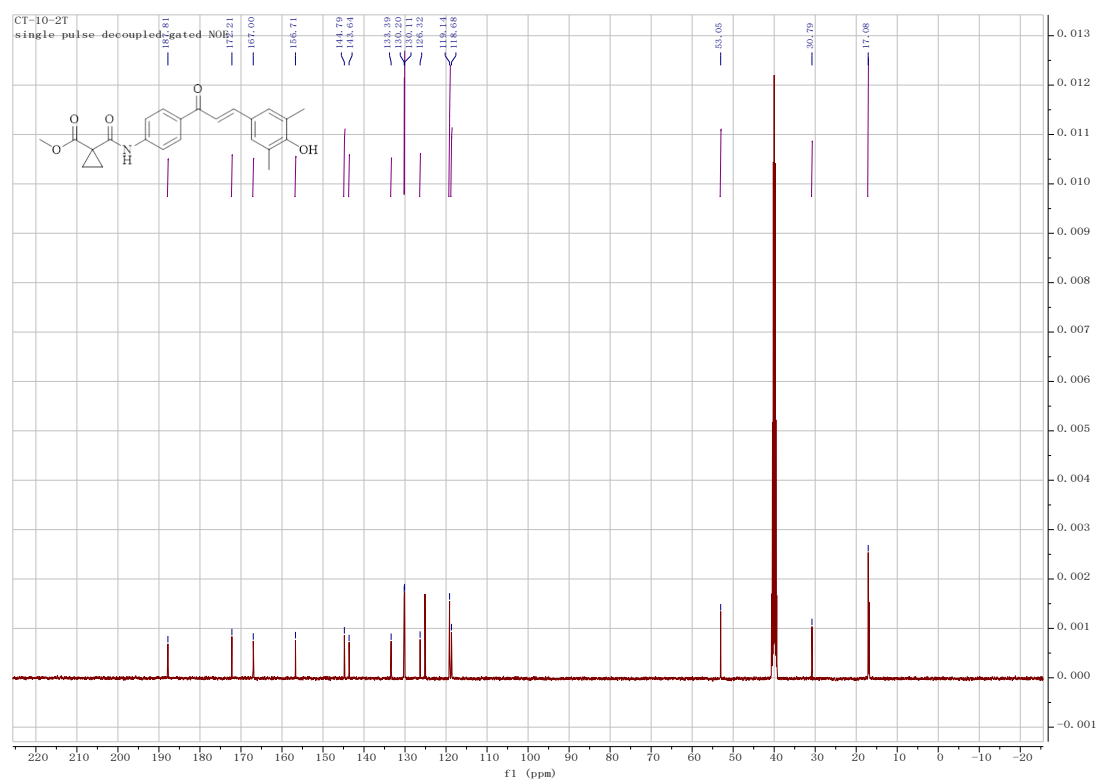
¹³C NMR spectrum of **10d** in DMSO



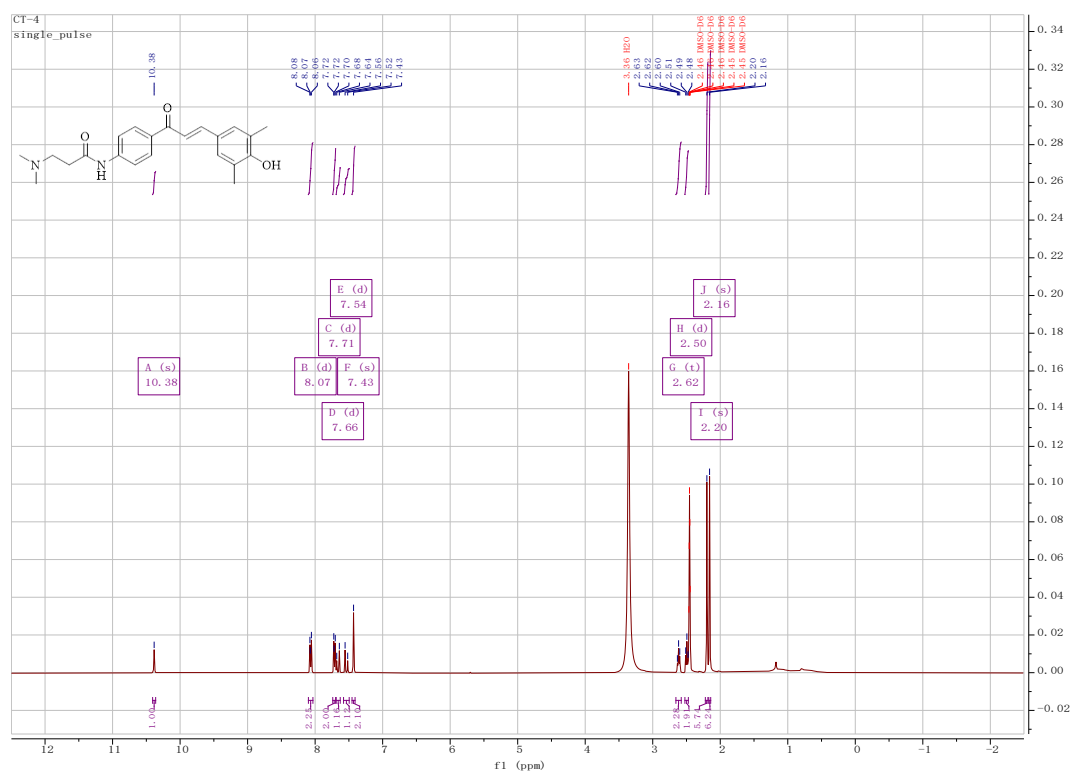
¹H NMR spectrum of **10f** in DMSO



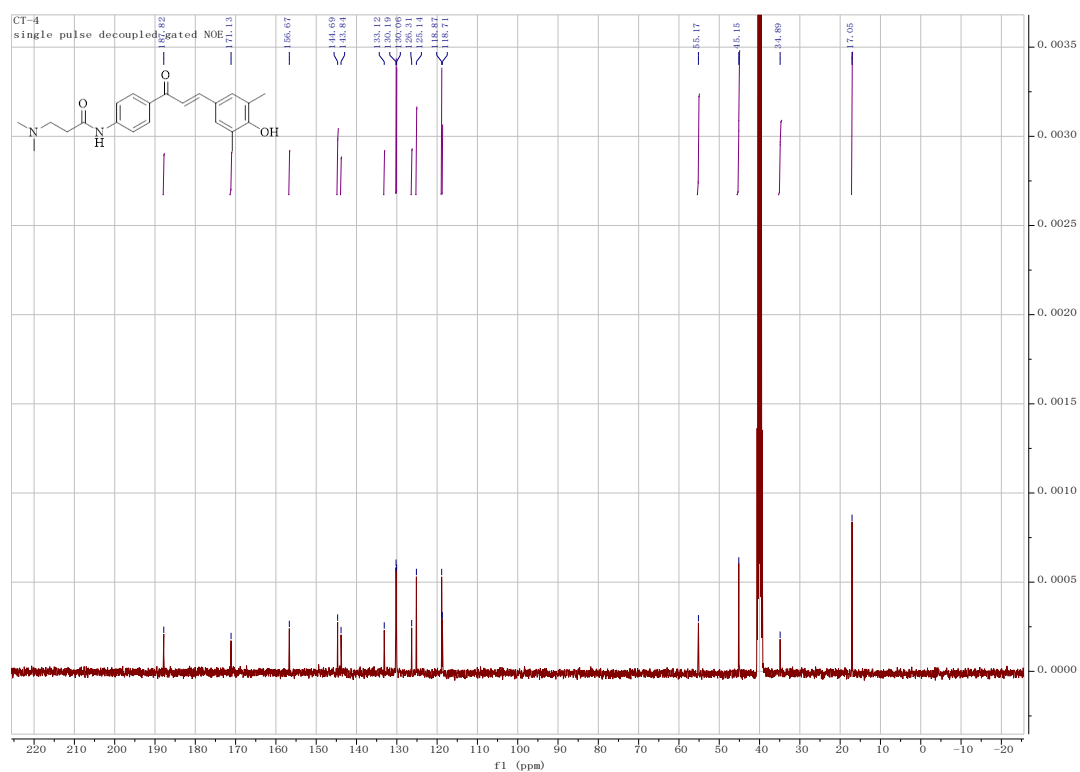
¹³C NMR spectrum of **10f** in DMSO



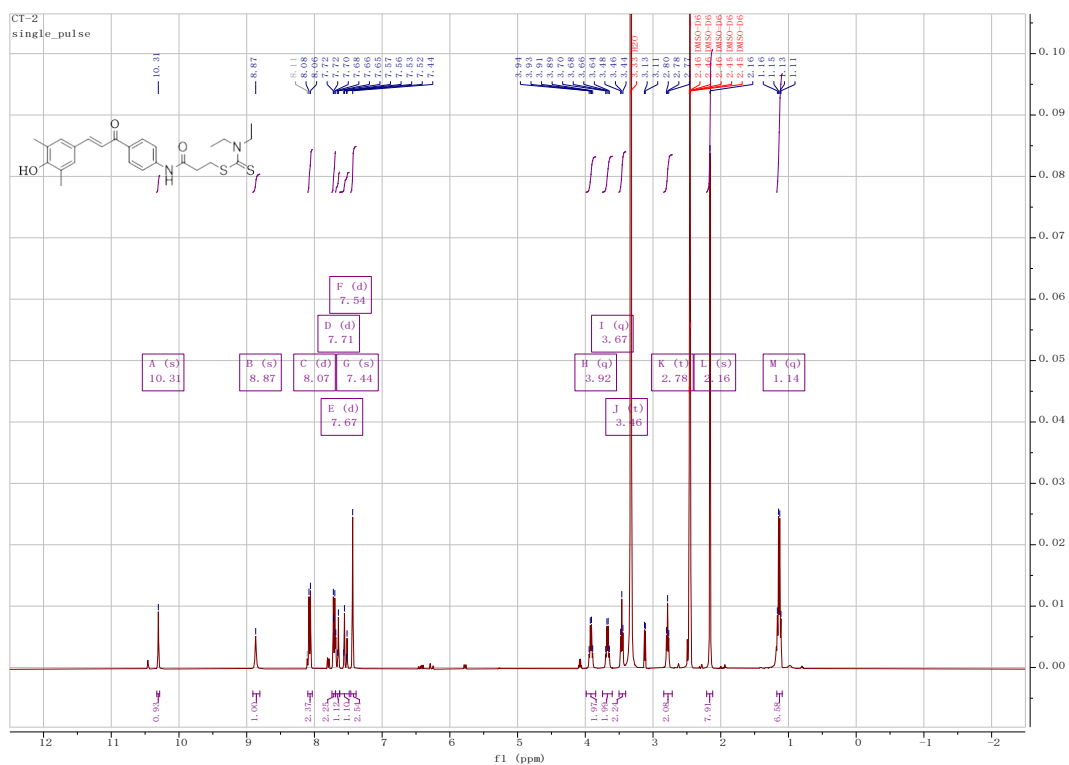
¹H NMR spectrum of **10h** in DMSO



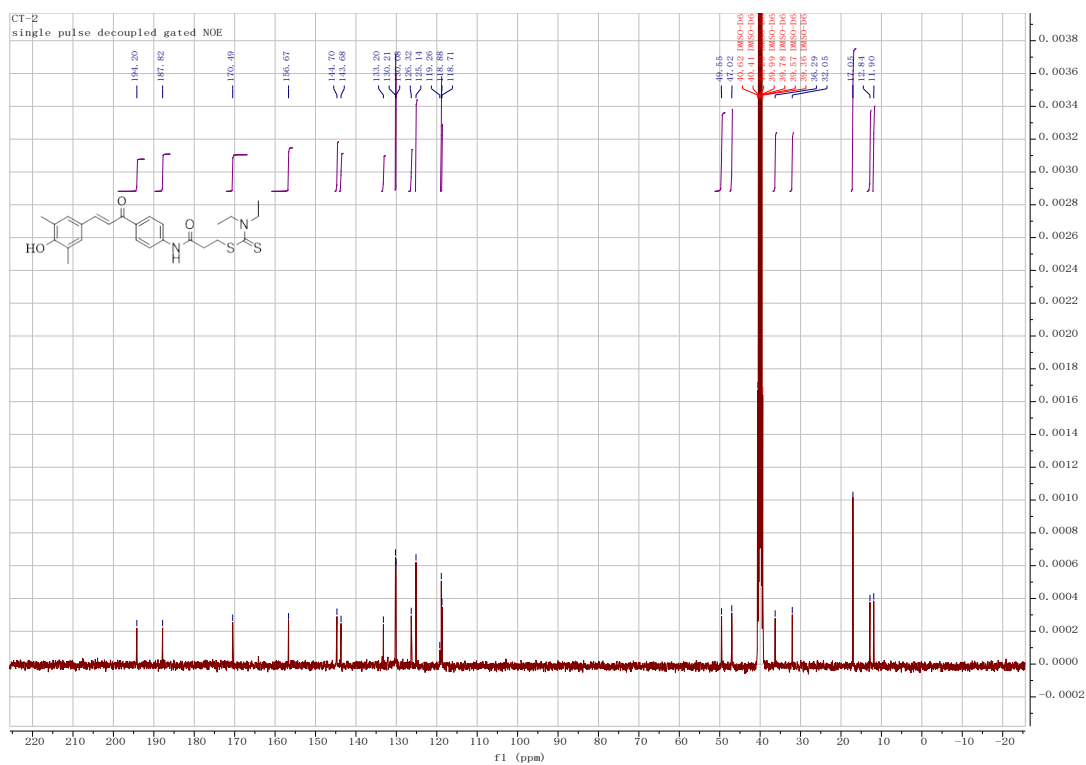
¹³C NMR spectrum of **10h** in DMSO



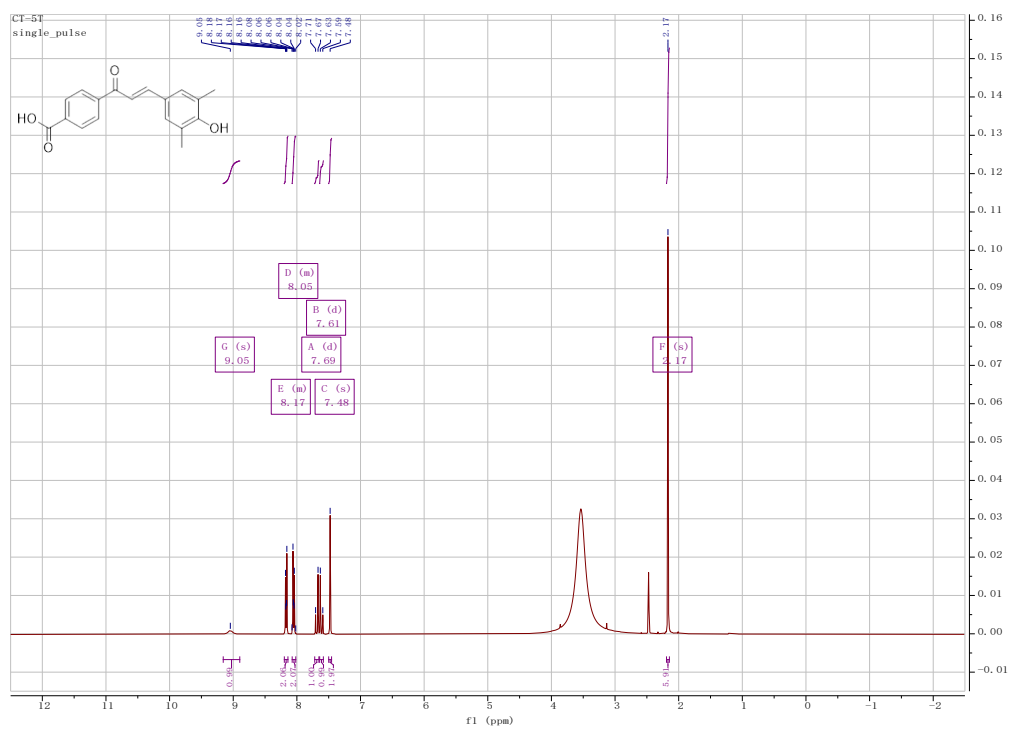
¹H NMR spectrum of **10i** in DMSO



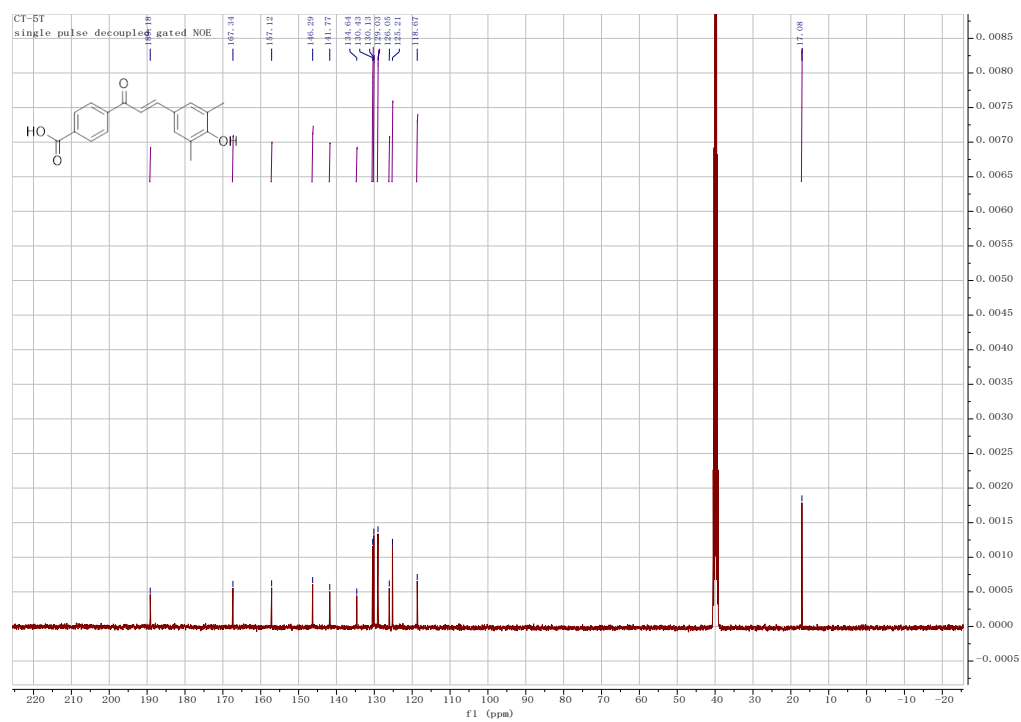
¹³C NMR spectrum of **10i** in DMSO



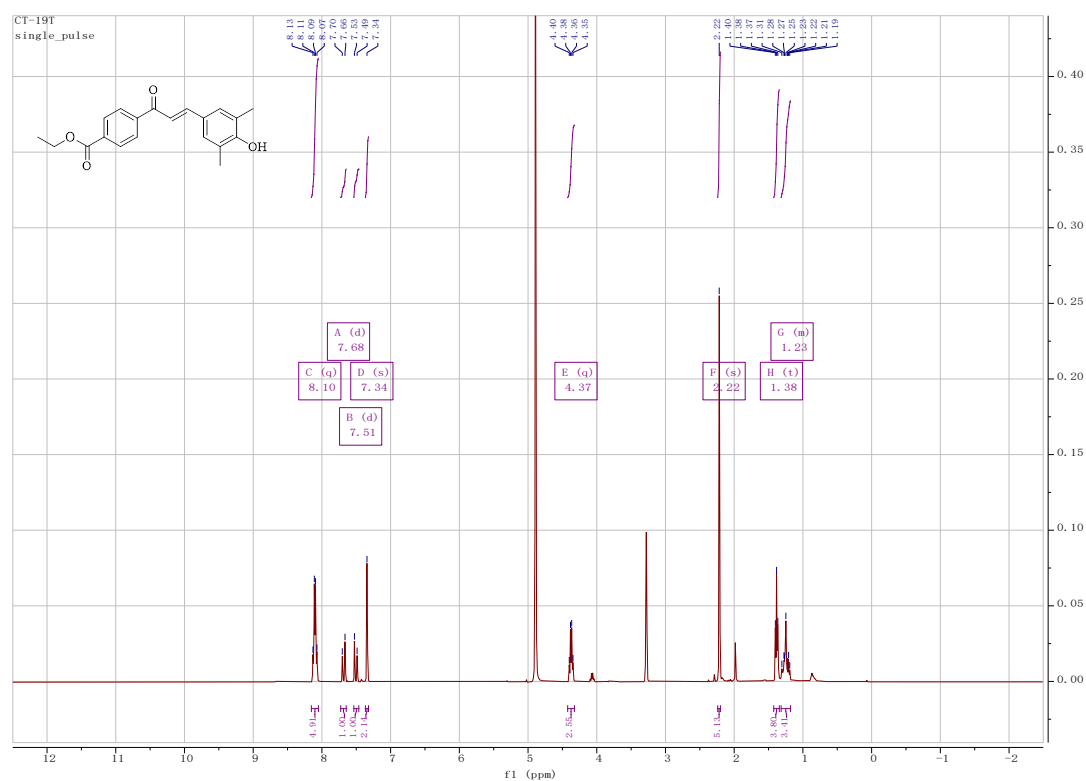
^1H NMR spectrum of **10j** in DMSO



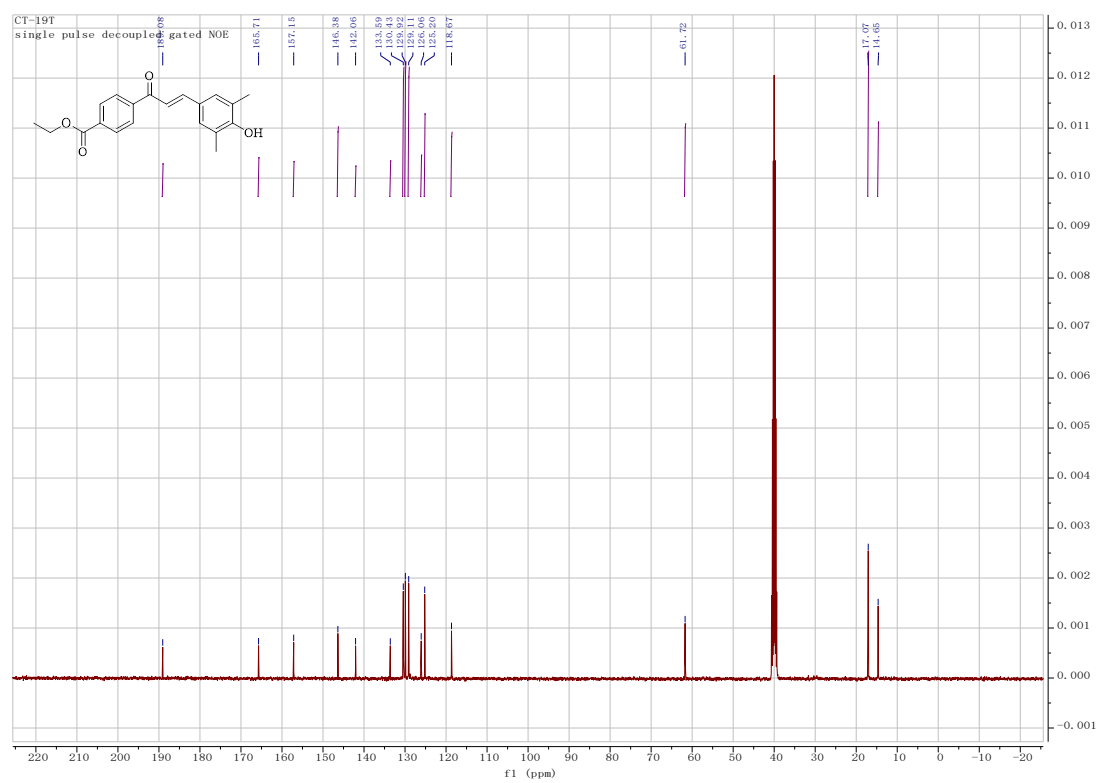
^{13}C NMR spectrum of **10j** in DMSO



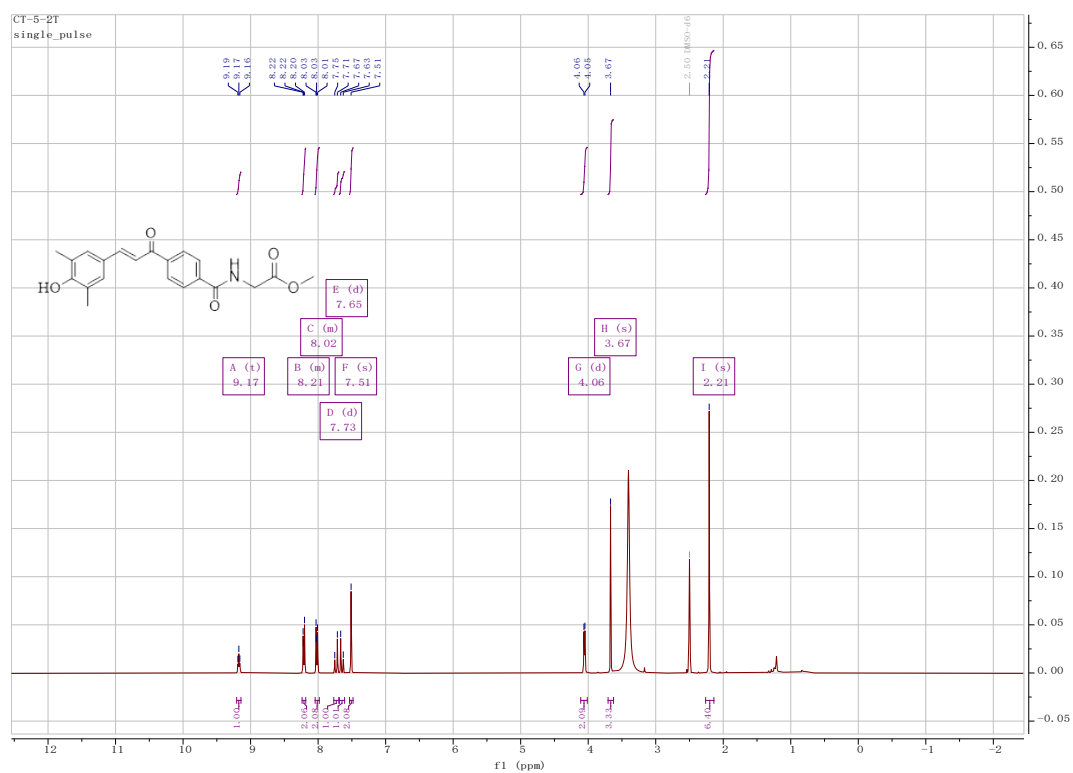
¹H NMR spectrum of **10k** in CD₃OD



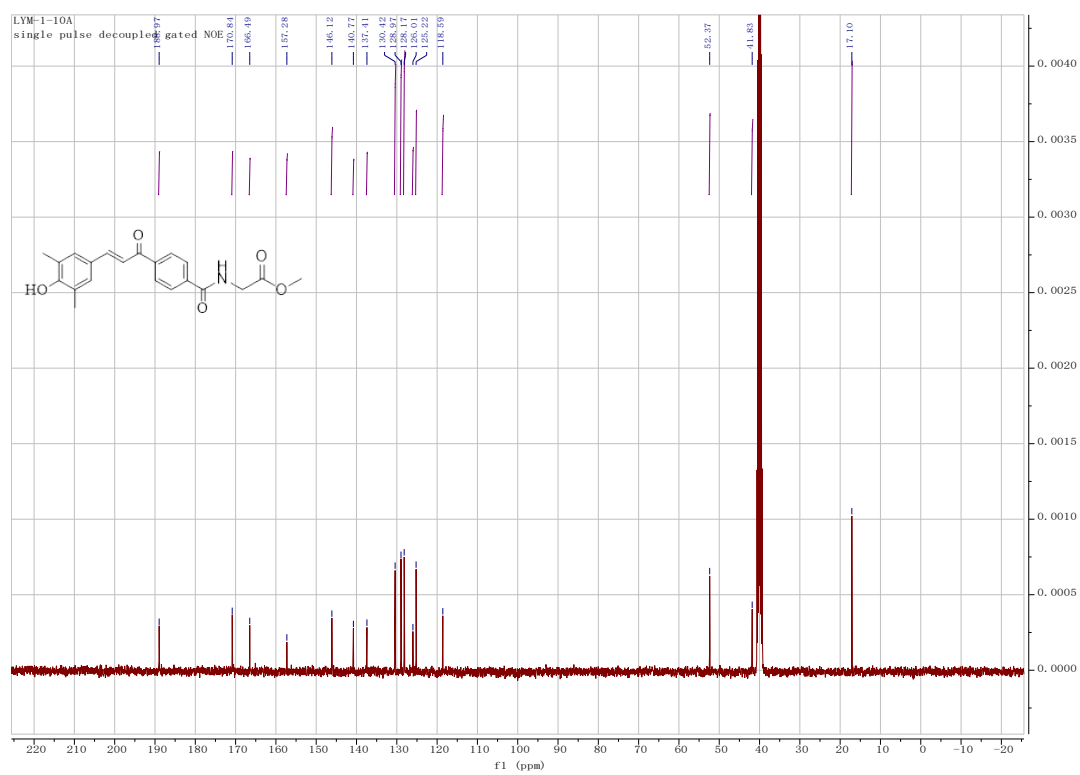
¹³C NMR spectrum of **10k** in DMSO



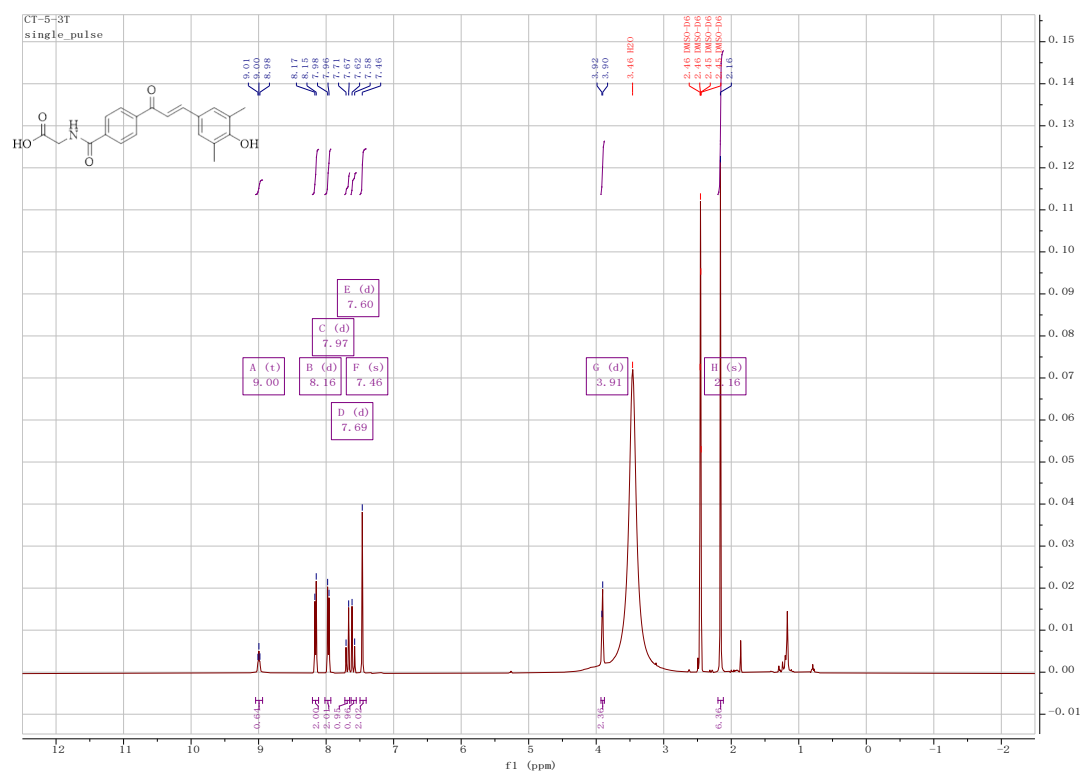
¹H NMR spectrum of **101** in DMSO



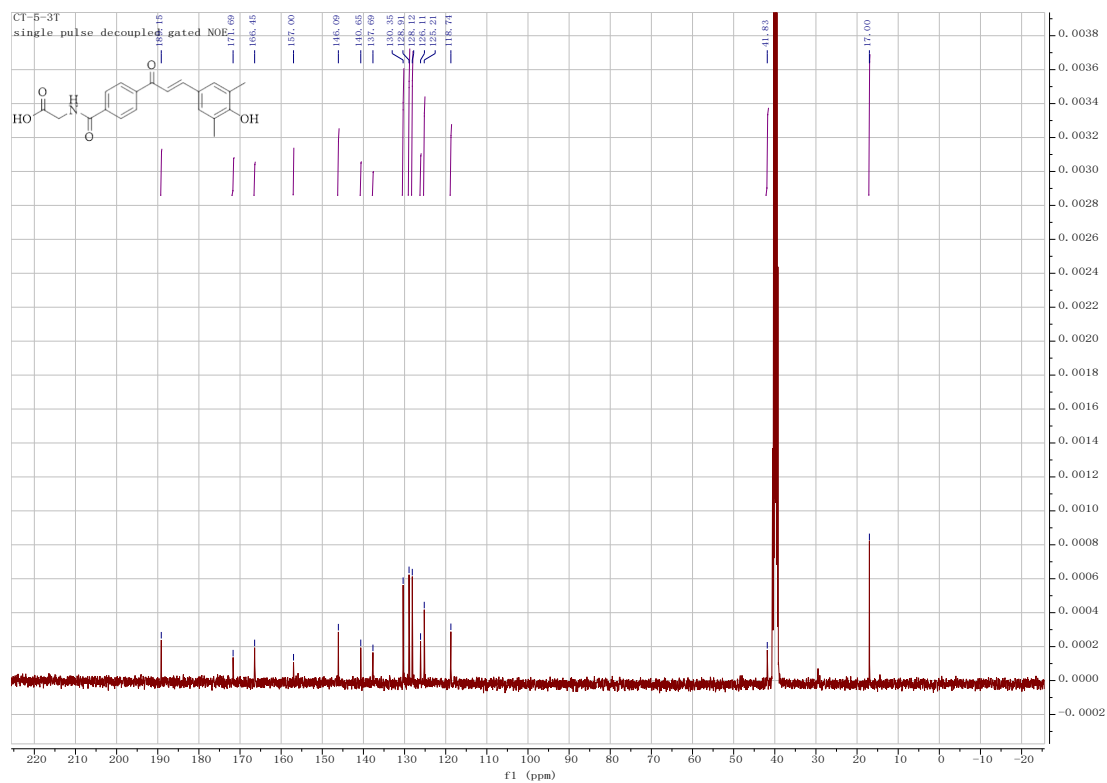
¹³C NMR spectrum of **101** in DMSO



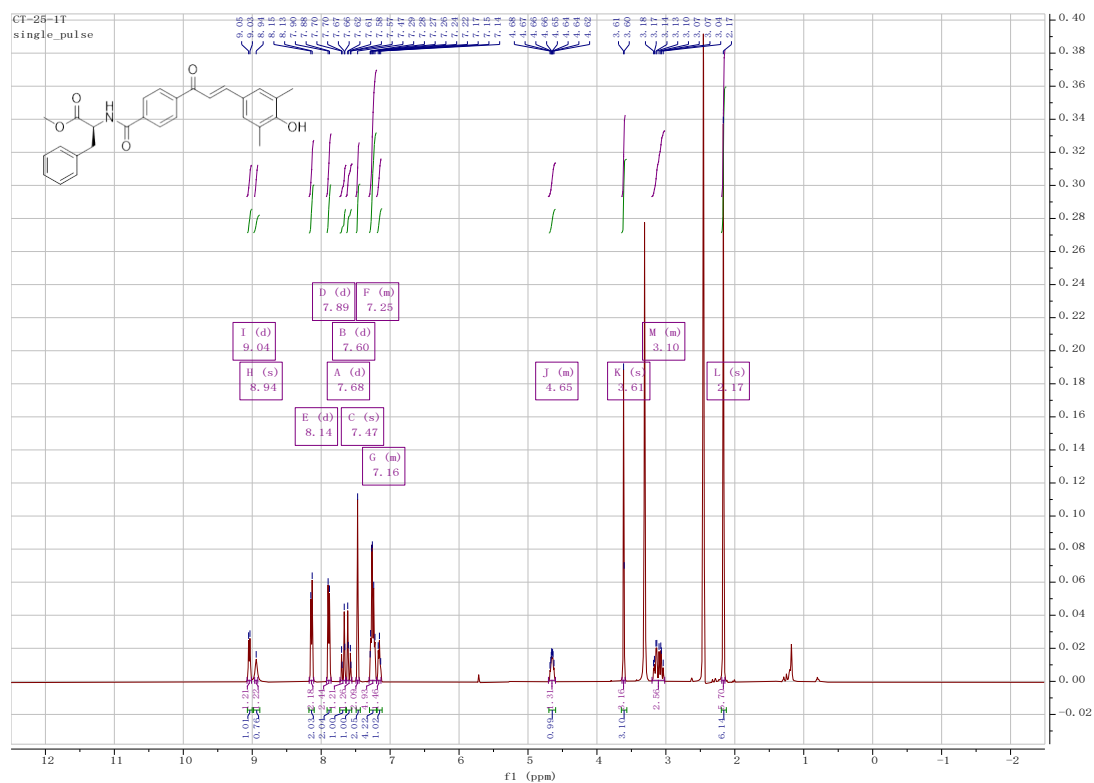
¹HNMR spectrum of **10m** in DMSO



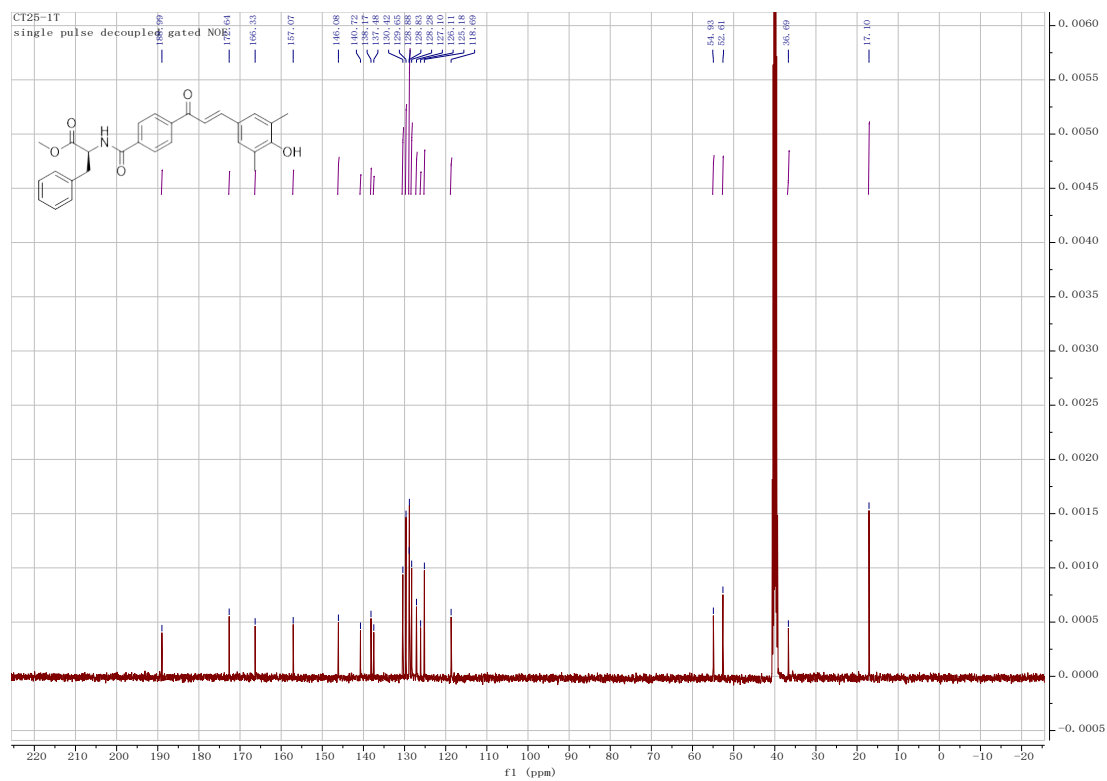
¹³CNMR spectrum of **10m** in DMSO



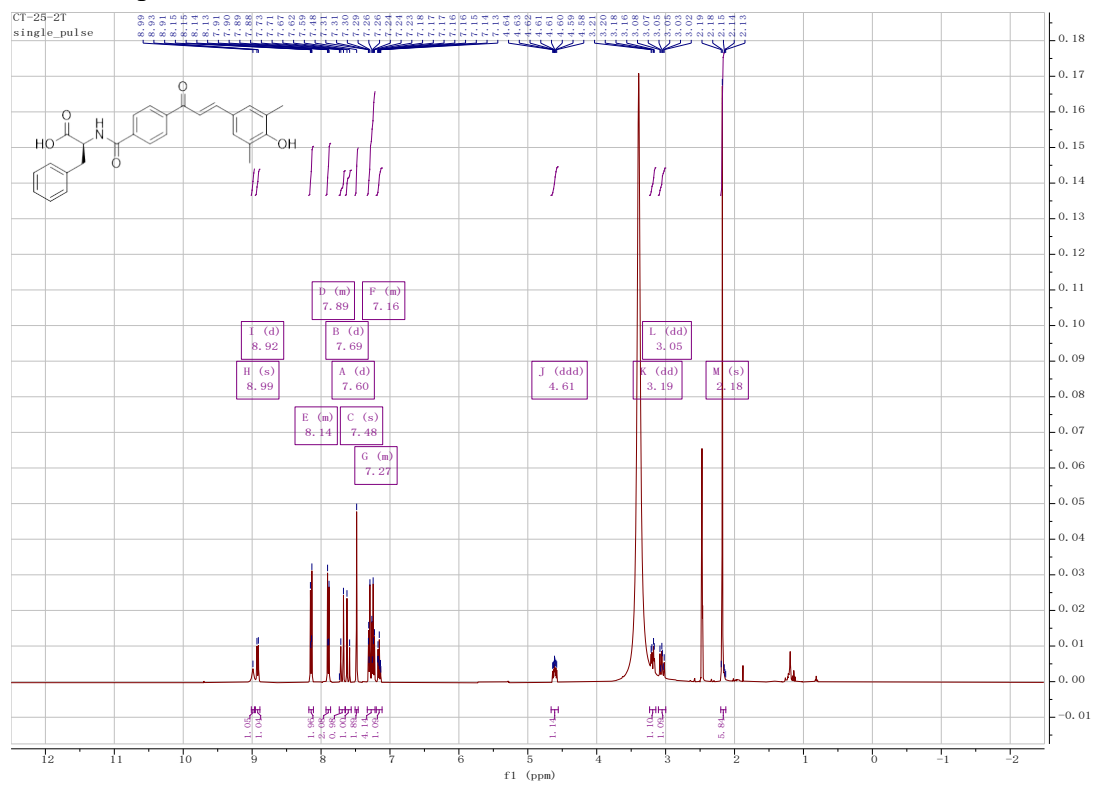
¹H NMR spectrum of **10n** in DMSO



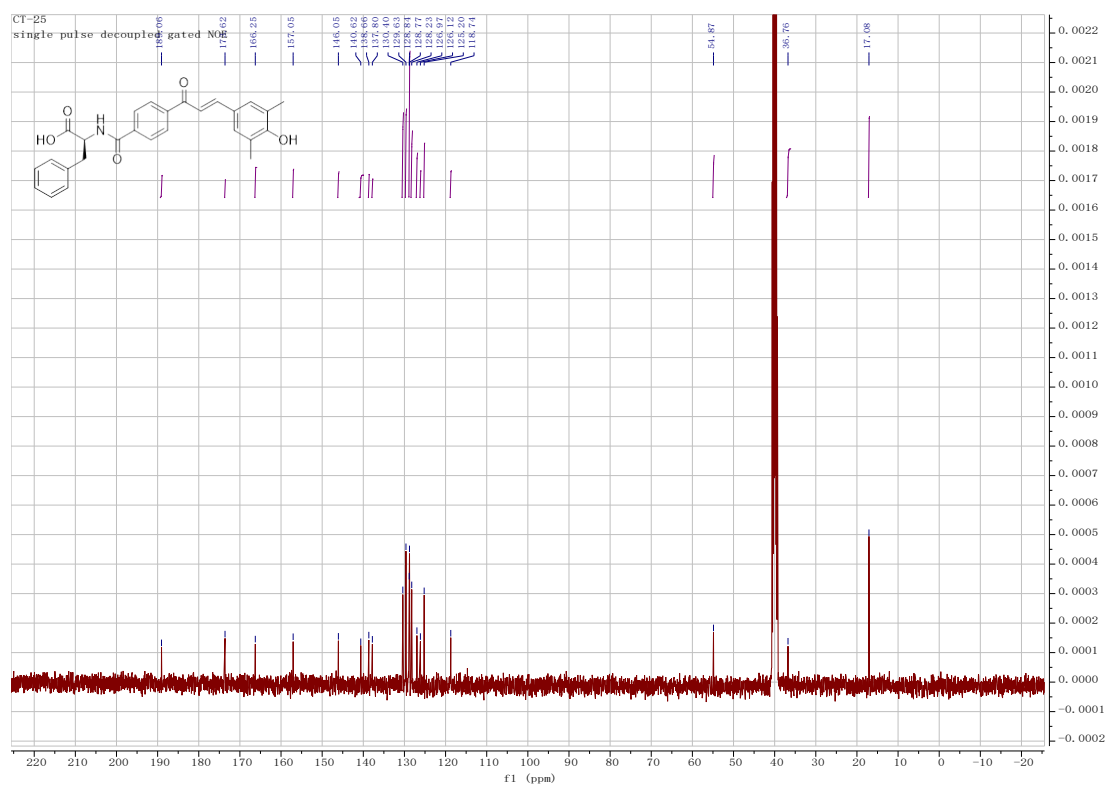
¹³C NMR spectrum of **10n** in DMSO



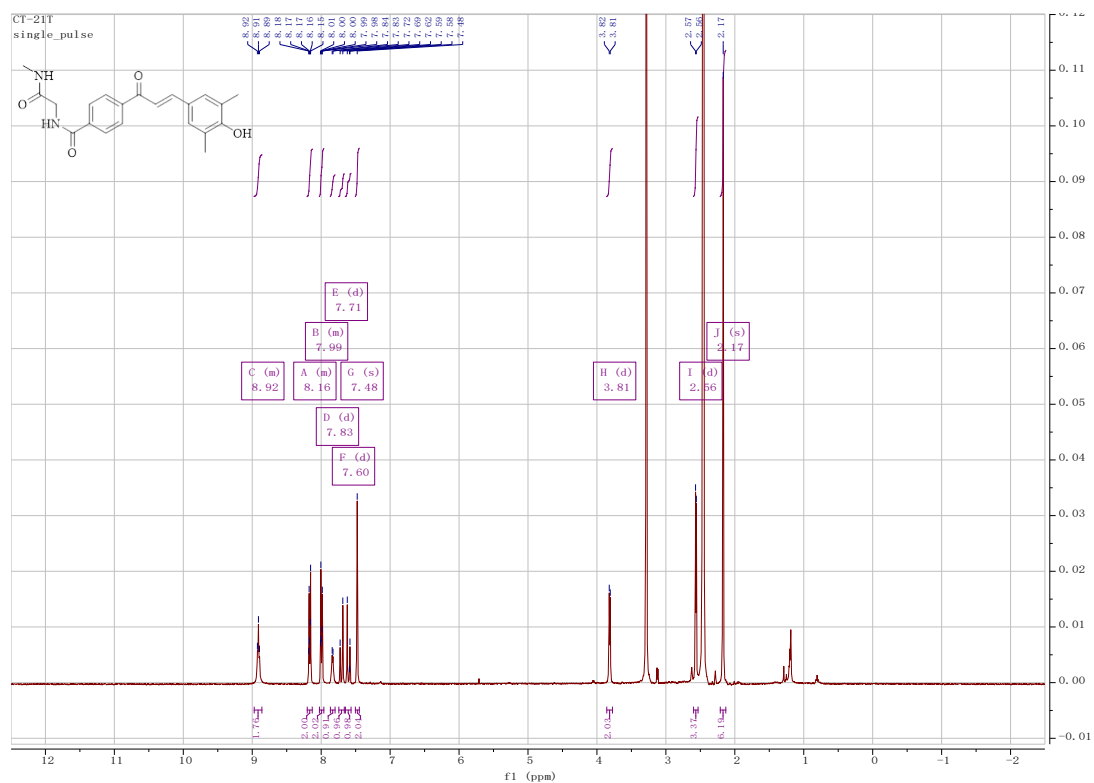
¹H NMR spectrum of **10o** in DMSO



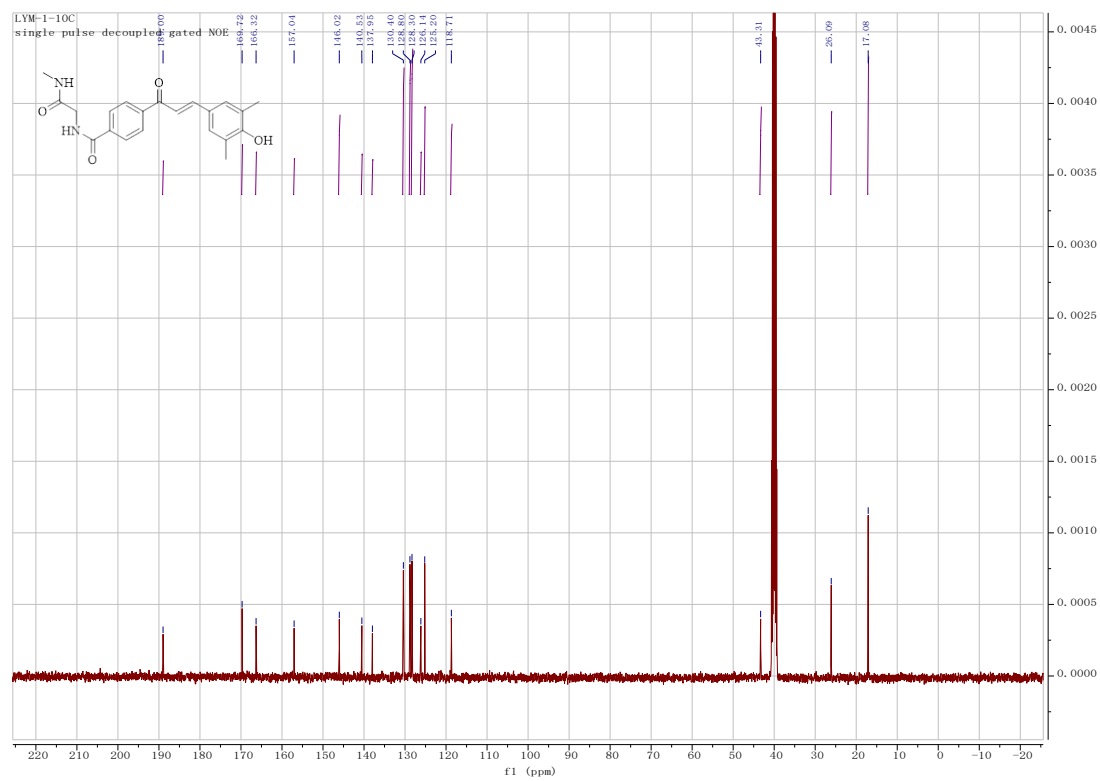
¹³C NMR spectrum of **10o** in DMSO



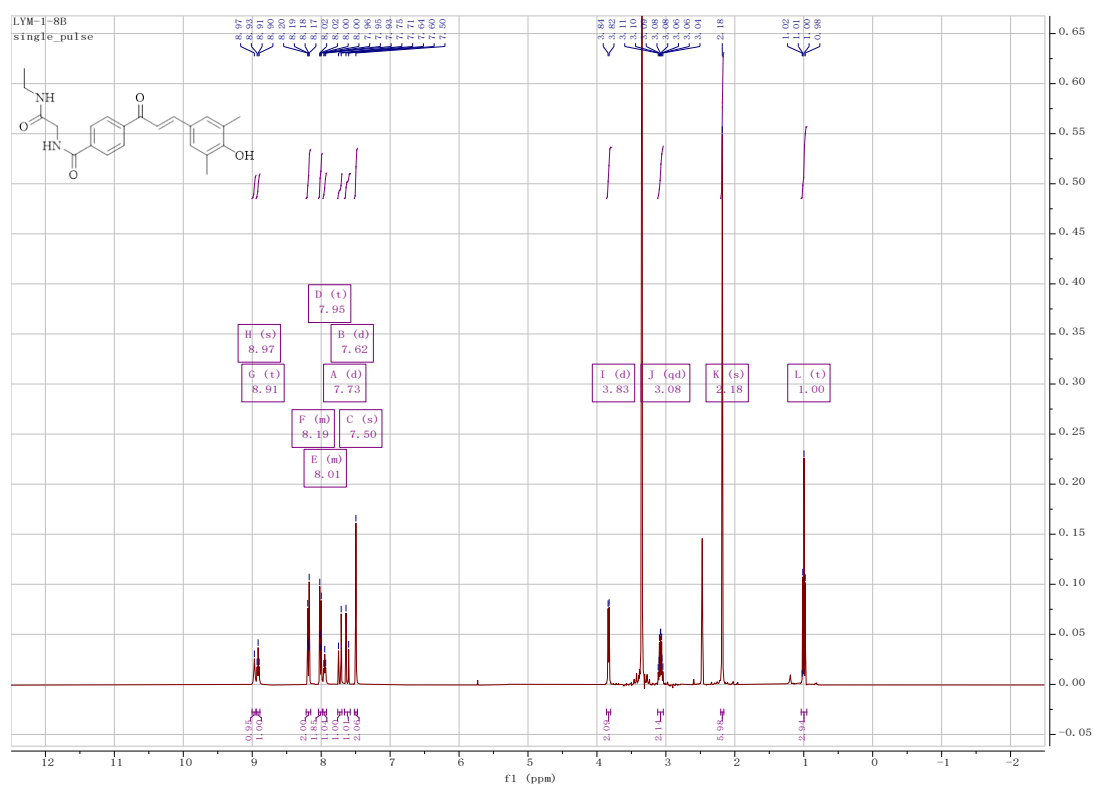
¹H NMR spectrum of **10p** in DMSO



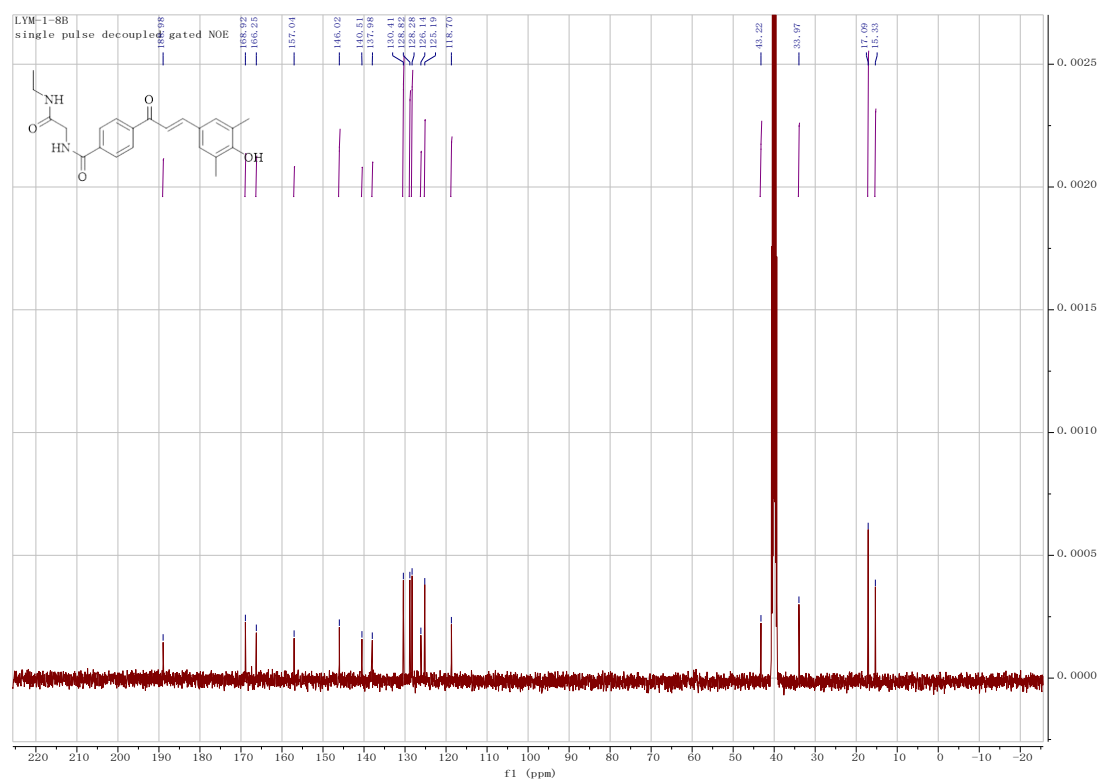
¹³C NMR spectrum of **10p** in DMSO



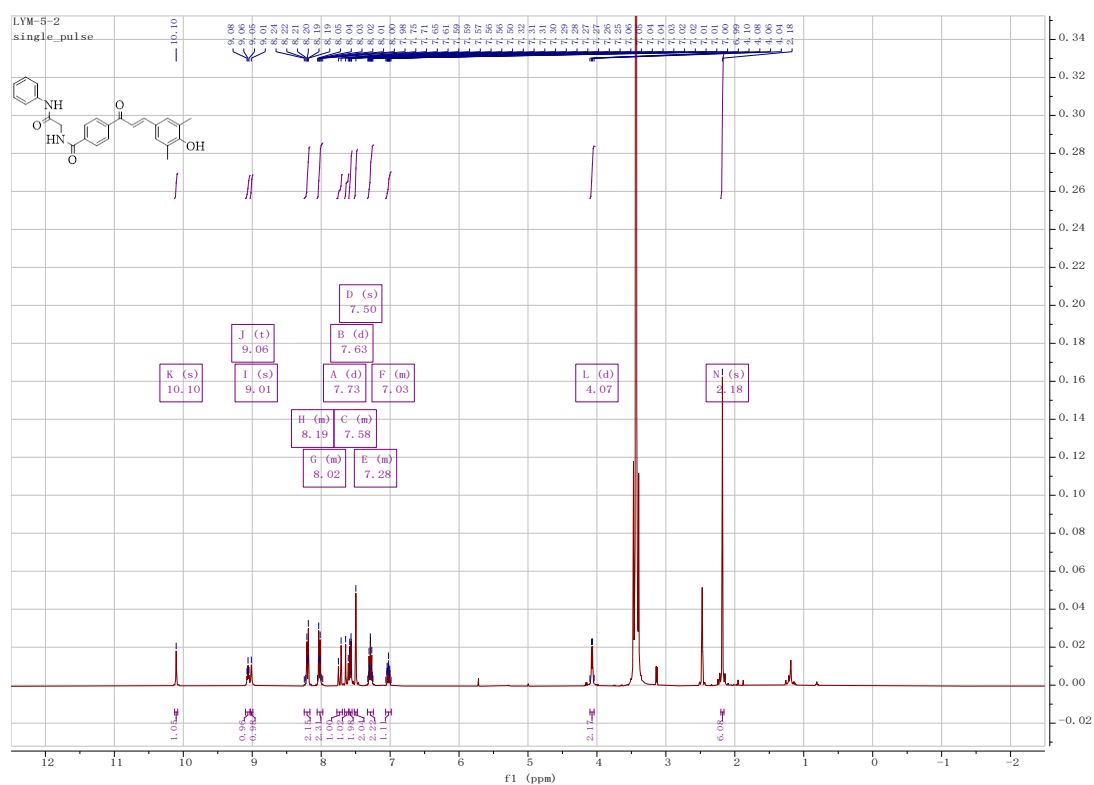
¹H NMR spectrum of **10q** in DMSO



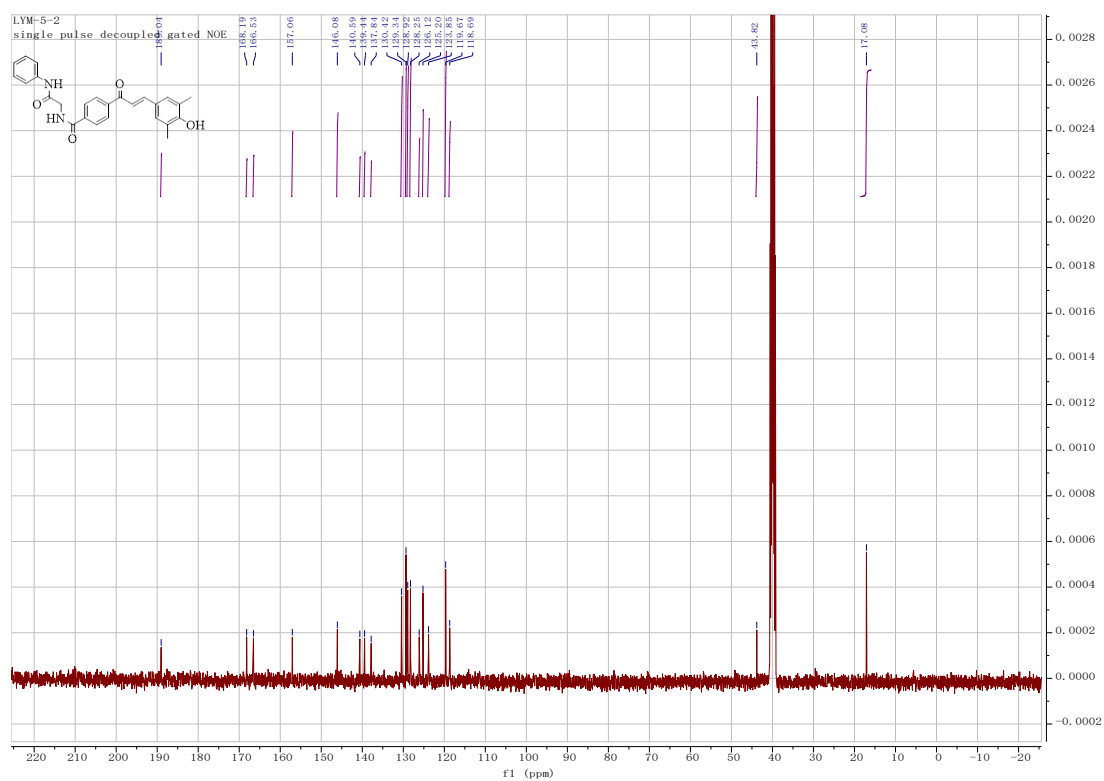
¹³C NMR spectrum of **10q** in DMSO



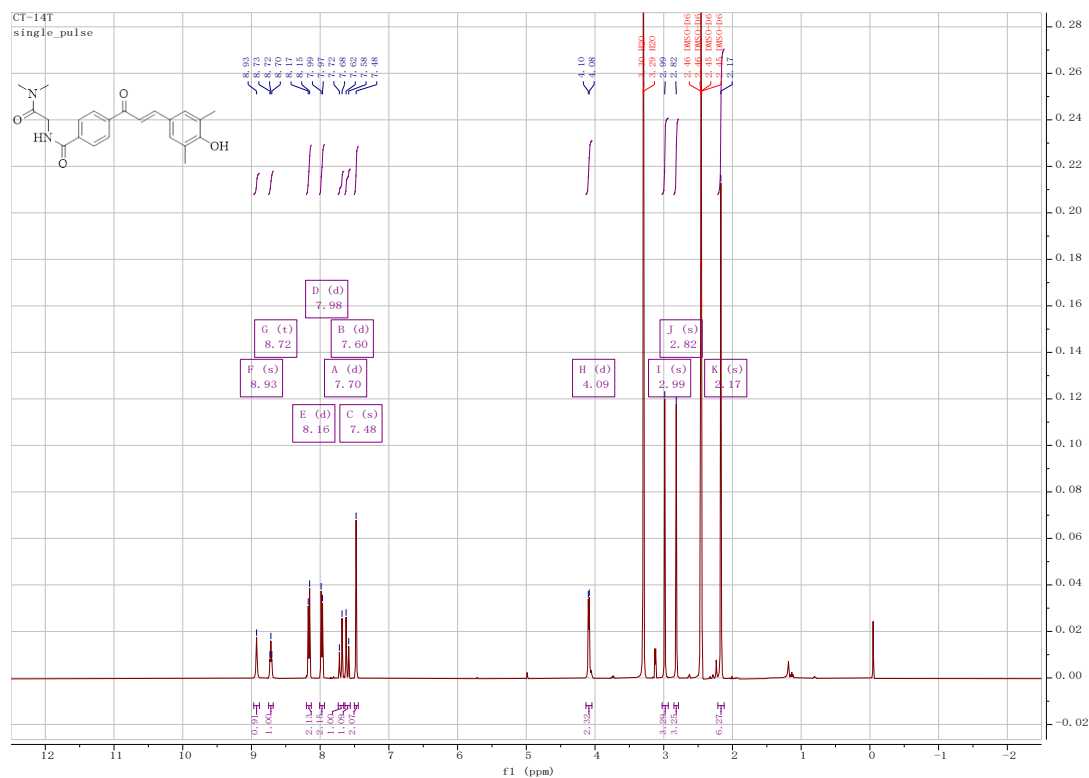
¹H NMR spectrum of **10r** in DMSO



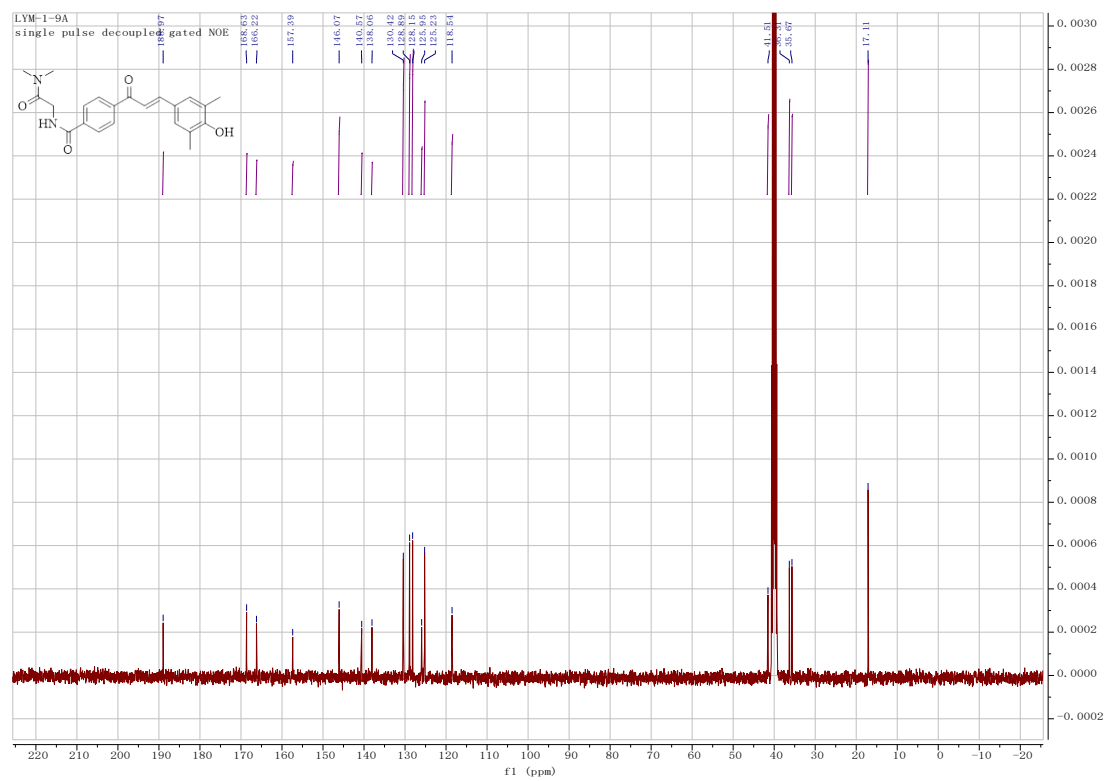
¹³C NMR spectrum of **10r** in DMSO



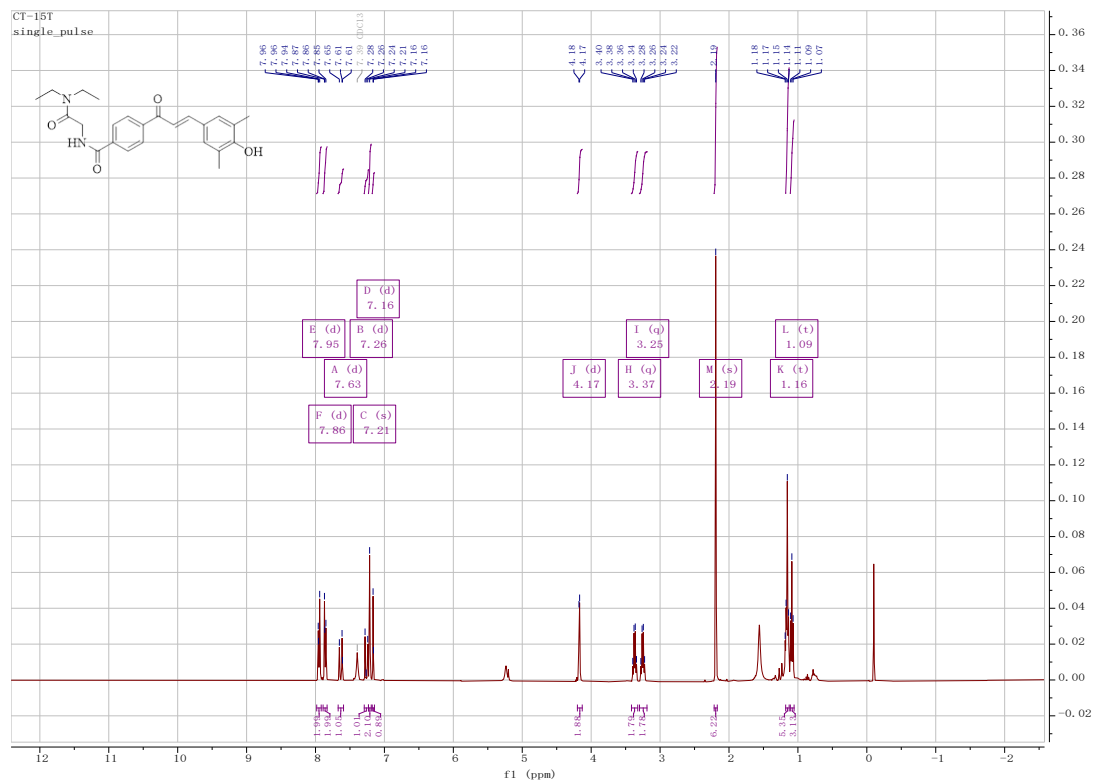
¹H NMR spectrum of 10s in DMSO



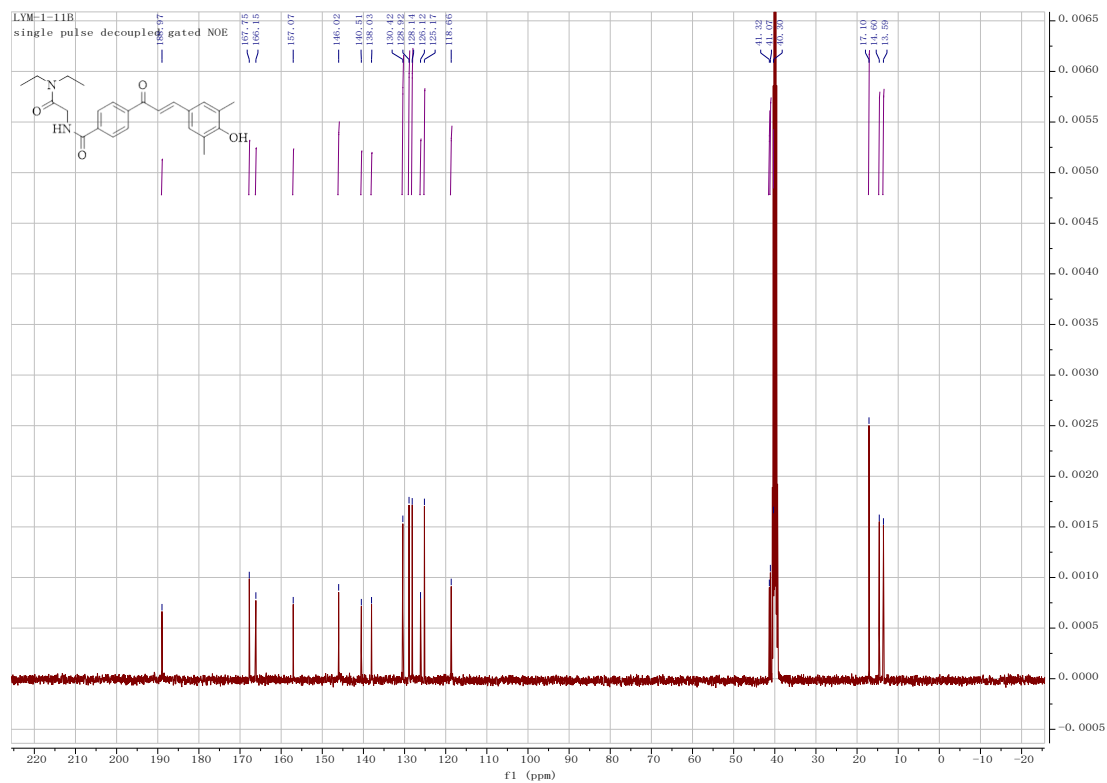
¹³C NMR spectrum of 10s in DMSO



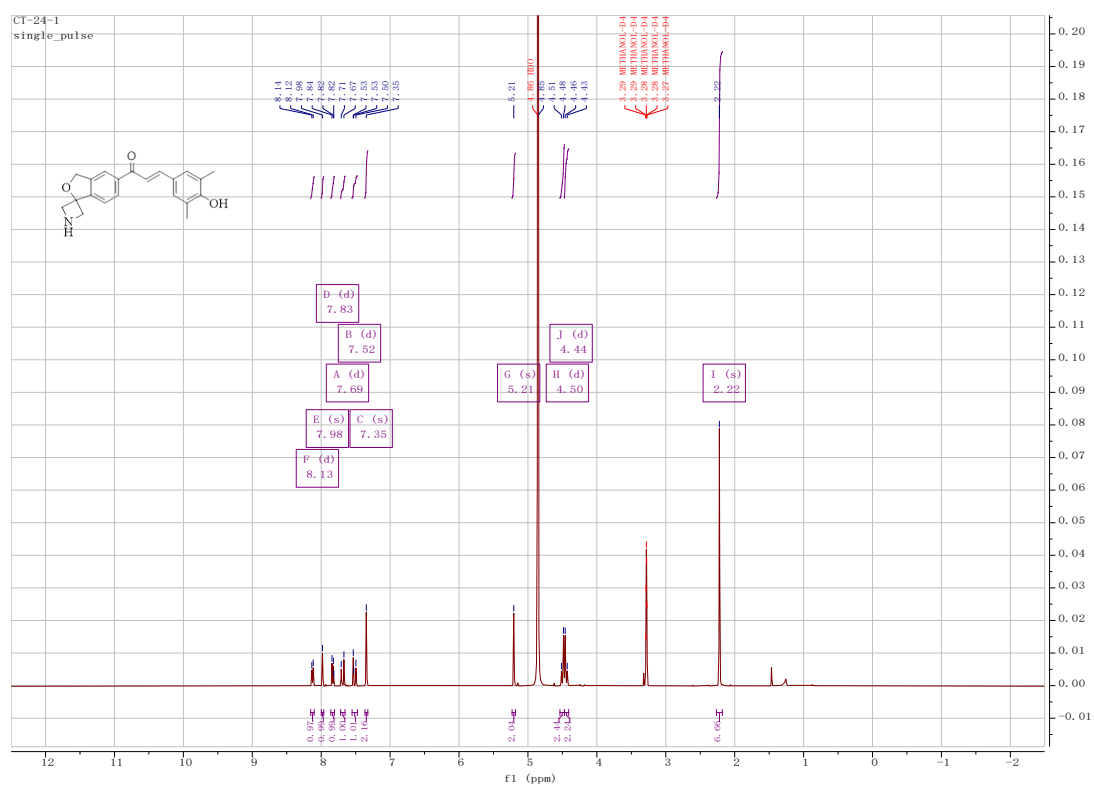
¹HNMR spectrum of **10t** in CDCl₃



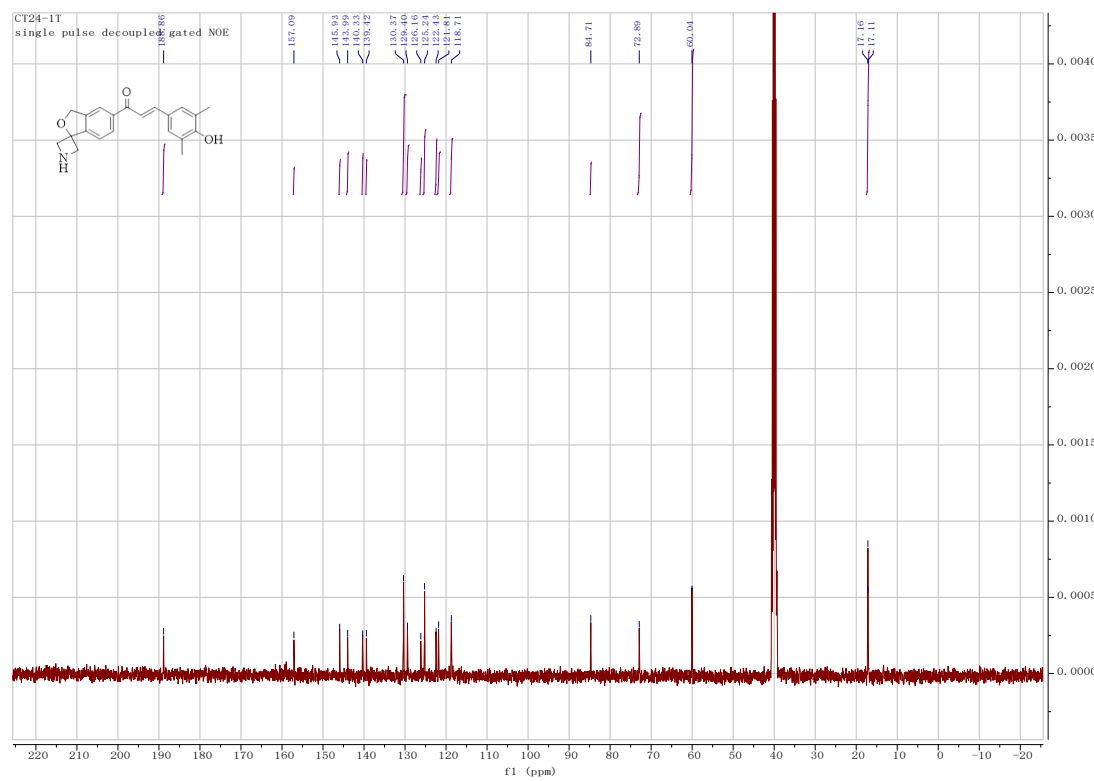
¹³CNMR spectrum of **10t** in DMSO



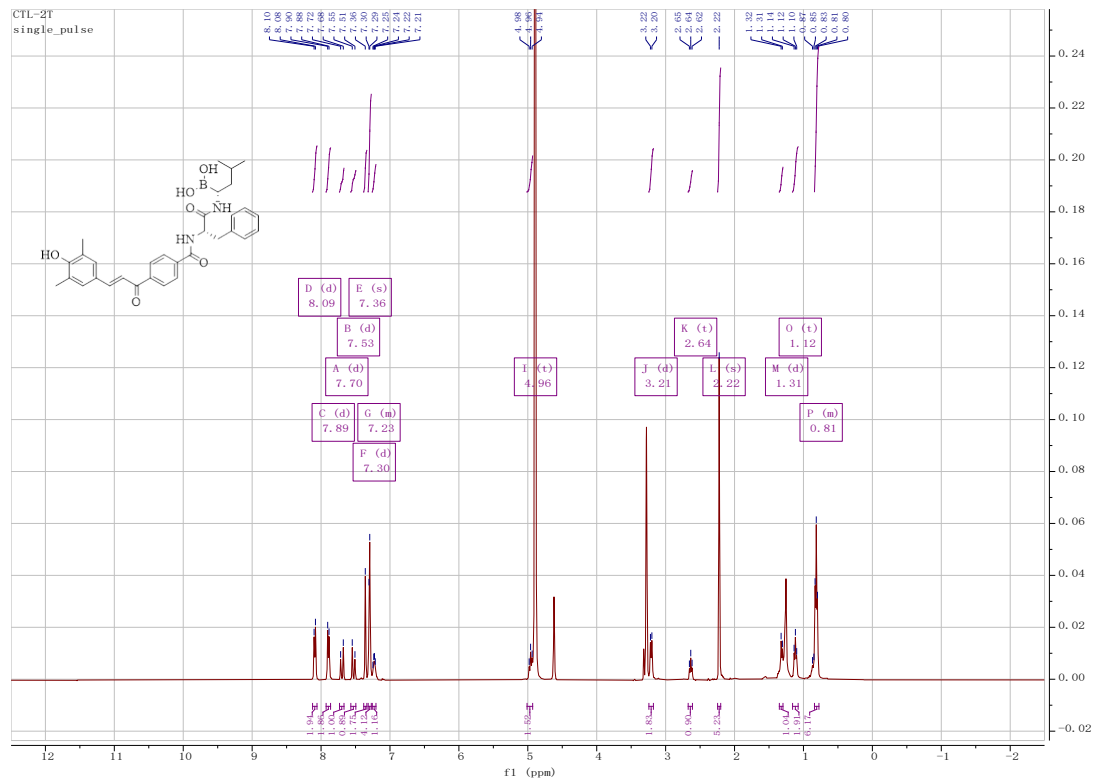
¹H NMR spectrum of **10u** in CD₃OD



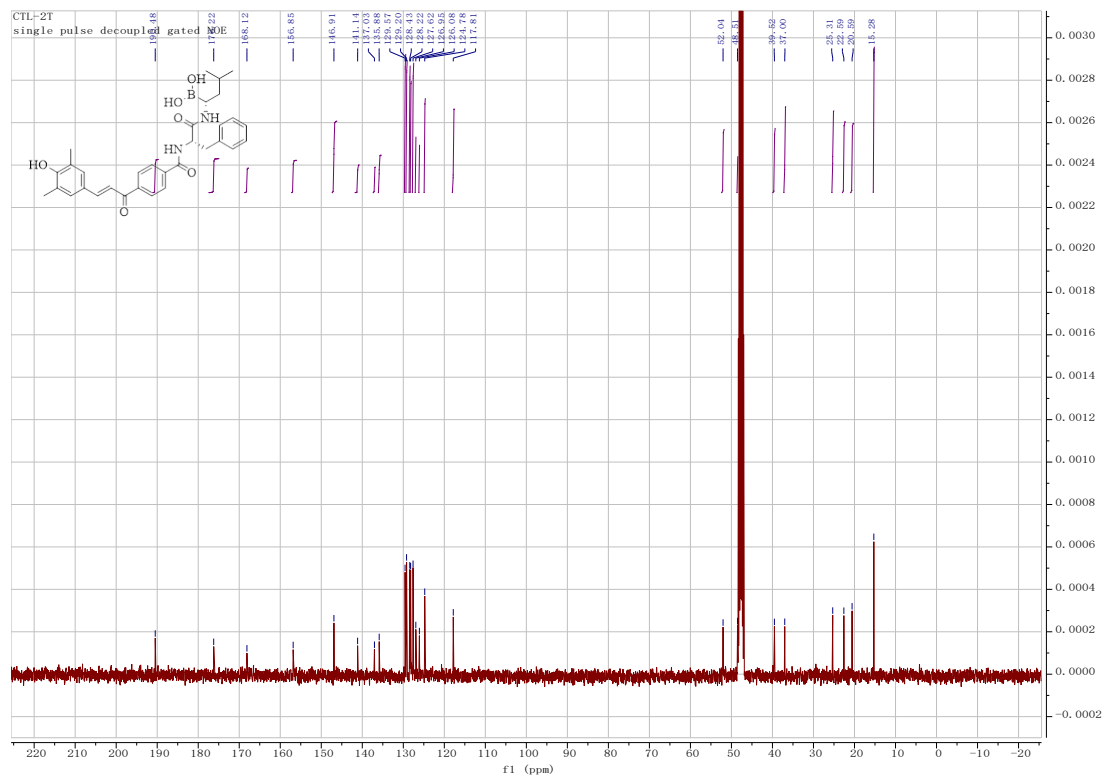
¹³C NMR spectrum of **10u** in DMSO



¹H NMR spectrum of **10v** in CD₃OD



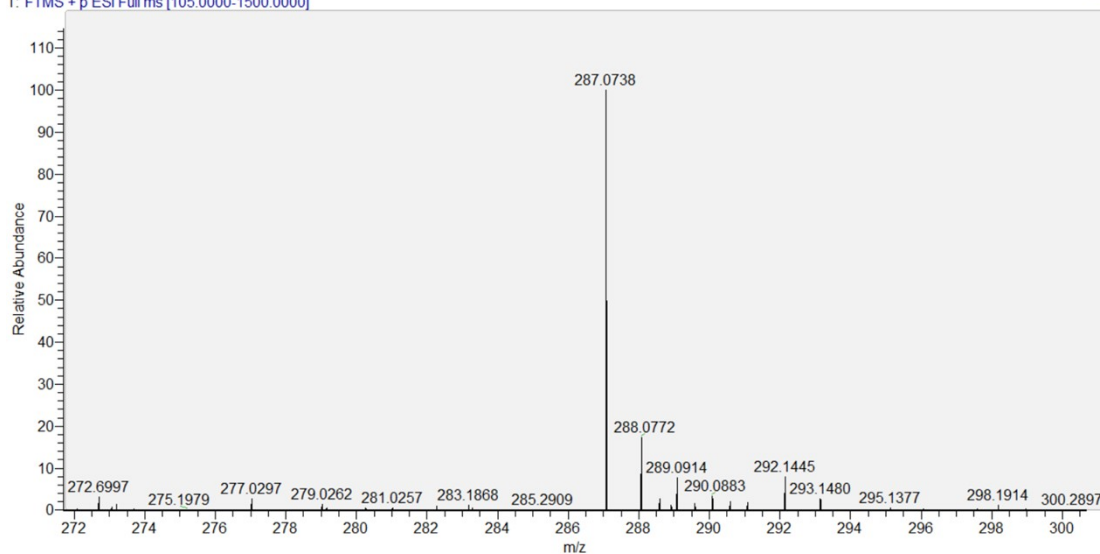
¹³C NMR spectrum of **10v** in CD₃OD



2. Copies of the HRMS

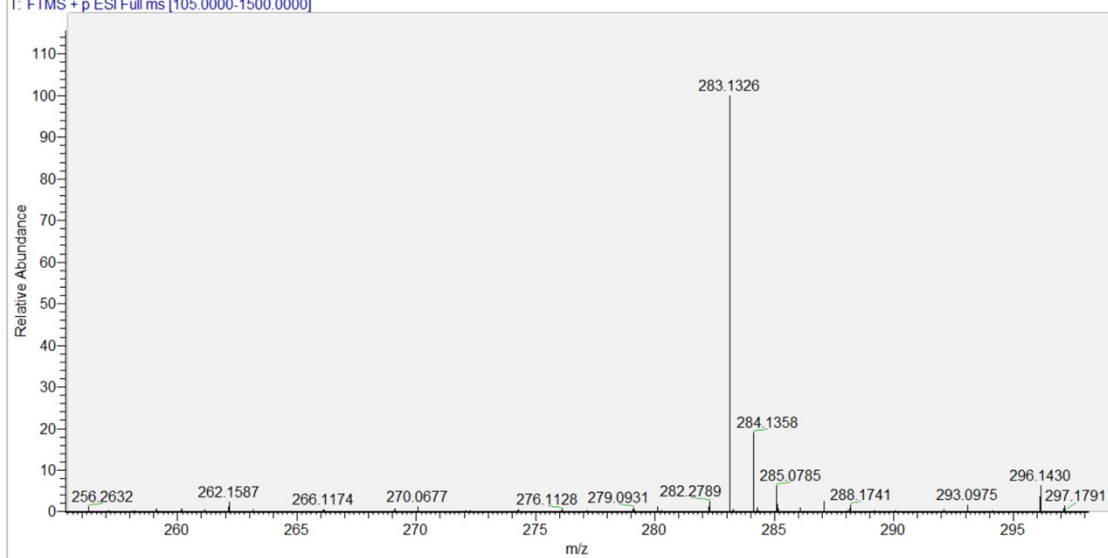
Mass spectrometry of 5

YY-15 #29-38 RT: 0.13-0.17 AV: 10 SB: 12 0.09-0.14 NL: 1.62E7
T: FTMS + p.ESI Full ms [105.0000-1500.0000]



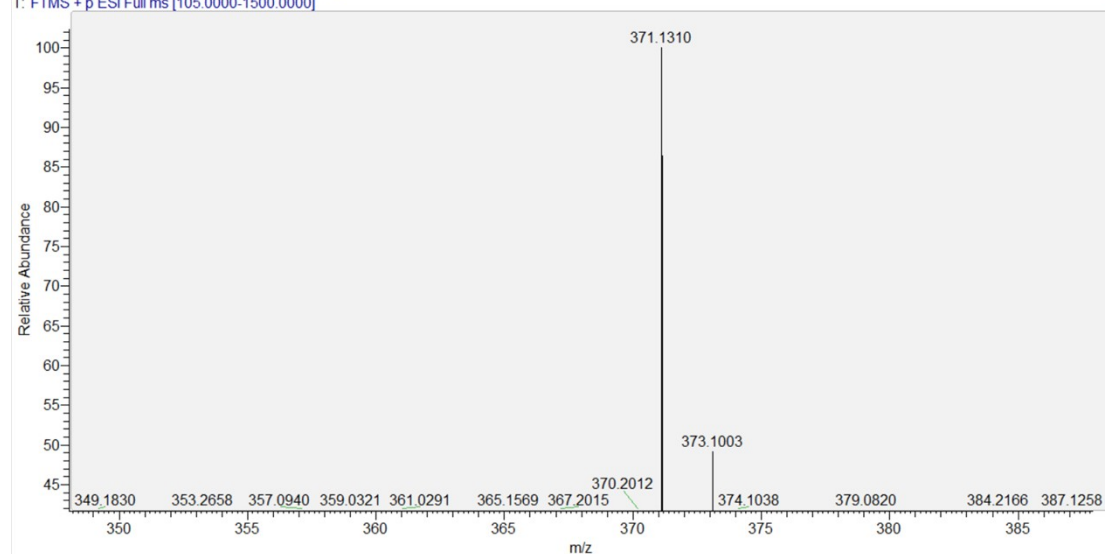
Mass spectrometry of 10b

ZXX34 #27-36 RT: 0.12-0.16 AV: 10 NL: 5.61E8
T: FTMS + p.ESI Full ms [105.0000-1500.0000]



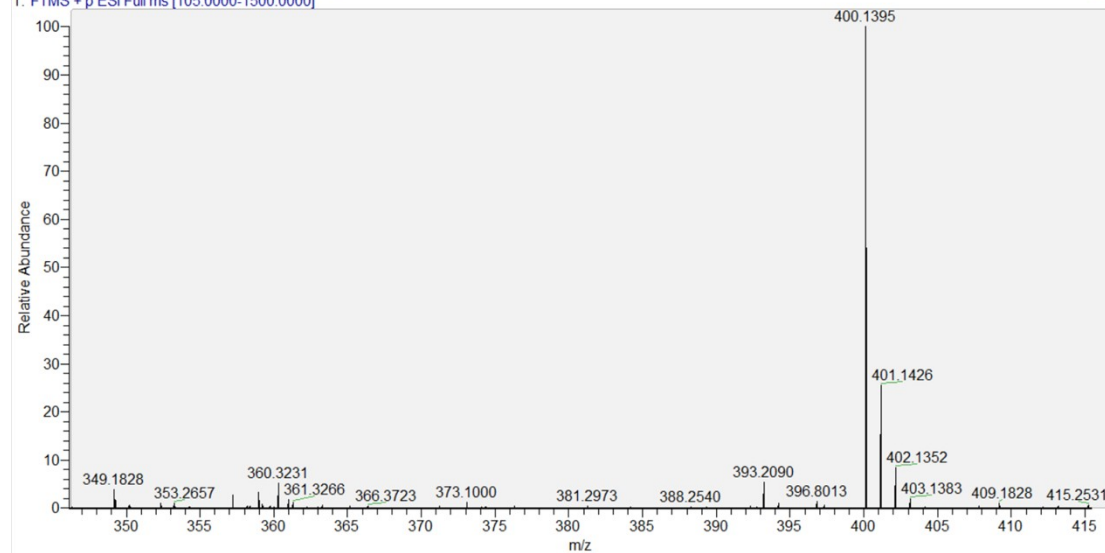
Mass spectrometry of 10c

ZXX36 #18-28 RT: 0.08-0.12 AV: 11 NL: 5.80E8
T: FTMS + p ESI Full ms [105.0000-1500.0000]



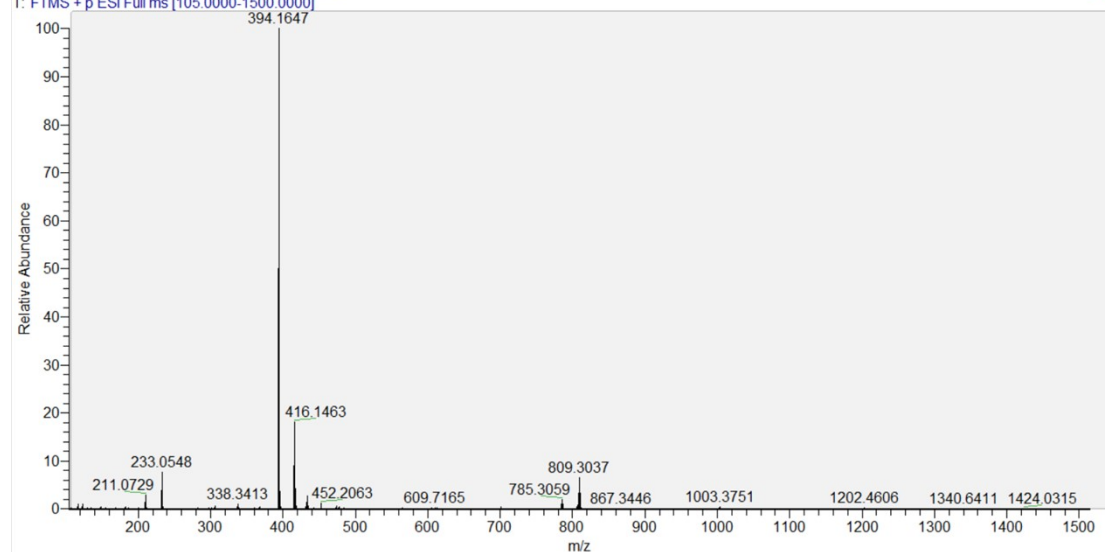
Mass spectrometry of 10d

ZXX32 #20-30 RT: 0.09-0.13 AV: 11 NL: 1.75E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



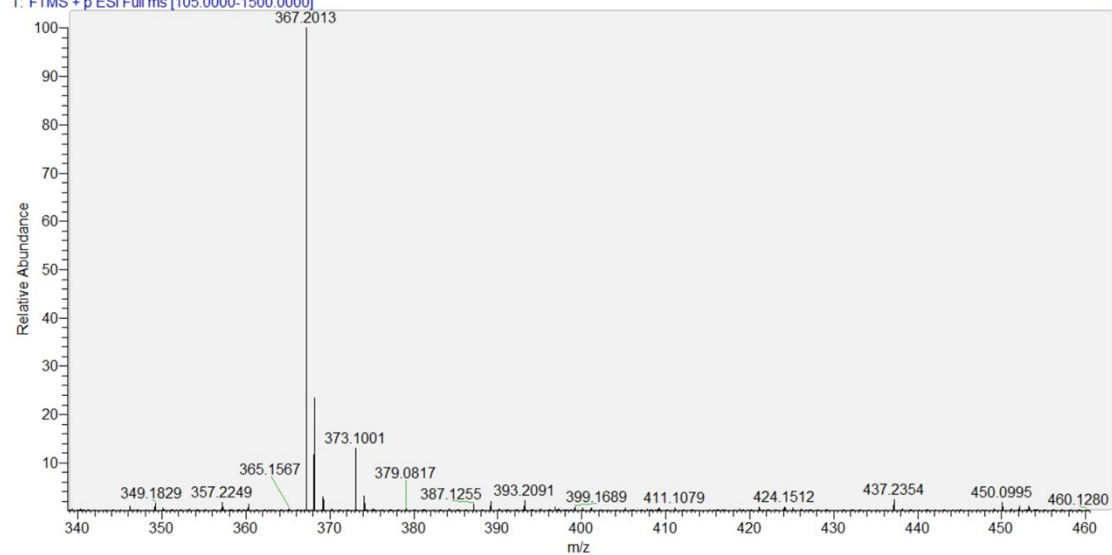
Mass spectrometry of 10f

YYY-19#28-43 RT: 0.12-0.19 AV: 16 NL: 1.76E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



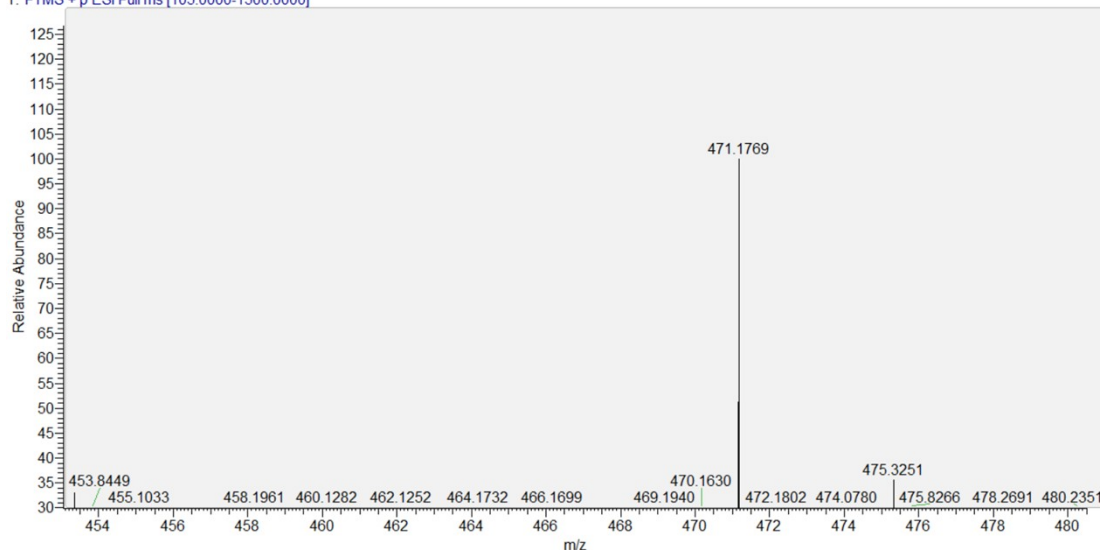
Mass spectrometry of 10h

ZXX35#19-28 RT: 0.08-0.12 AV: 10 NL: 2.49E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



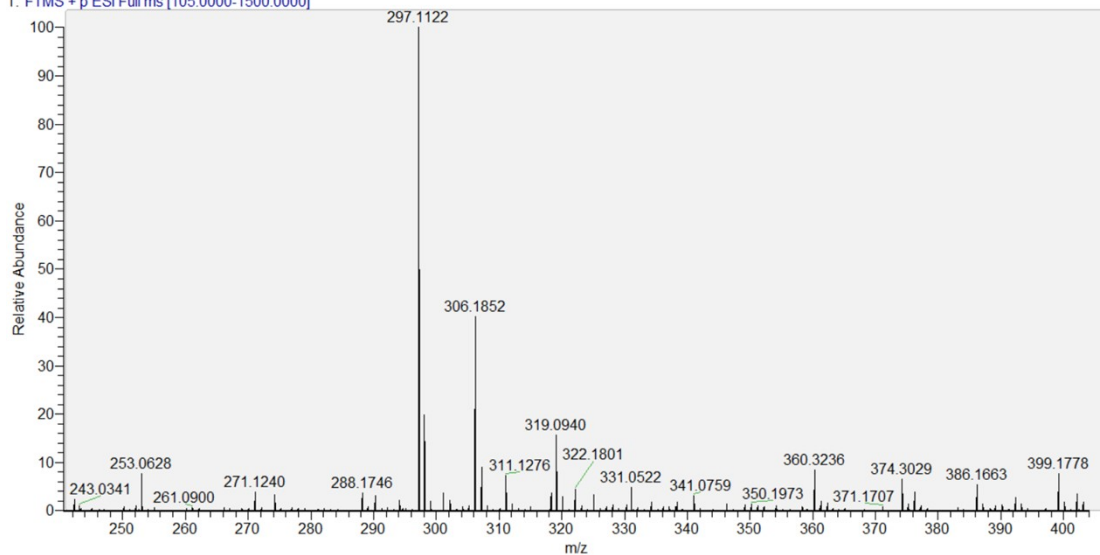
Mass spectrometry of 10i

ZXX33 #21-35 RT: 0.09-0.15 AV: 15 NL: 2.75E7
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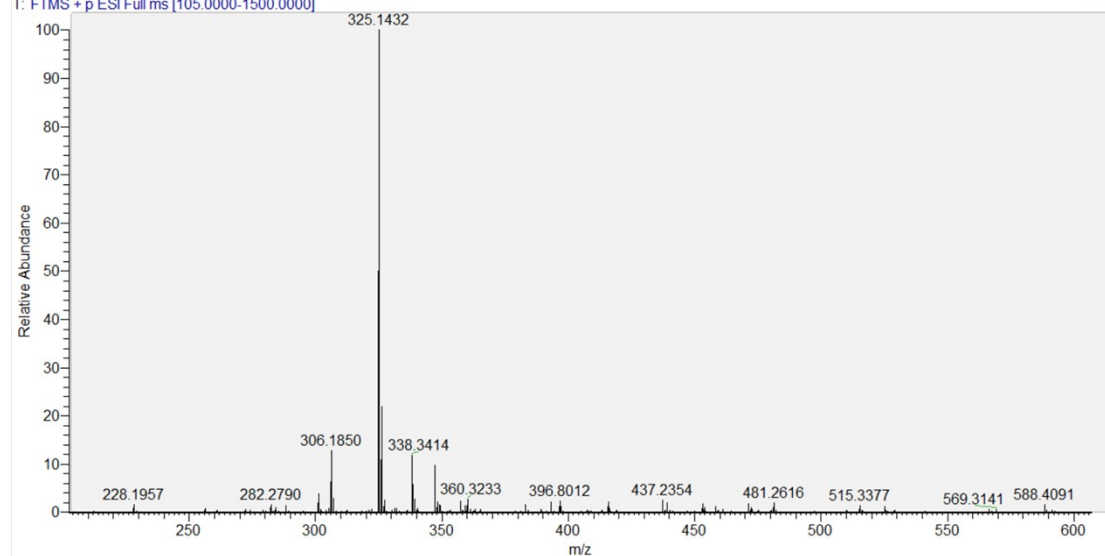
Mass spectrometry of 10j

YYY-16 #17-29 RT: 0.07-0.13 AV: 13 NL: 3.74E8
T: FTMS → p ESI Full ms [105.0000-1500.0000]



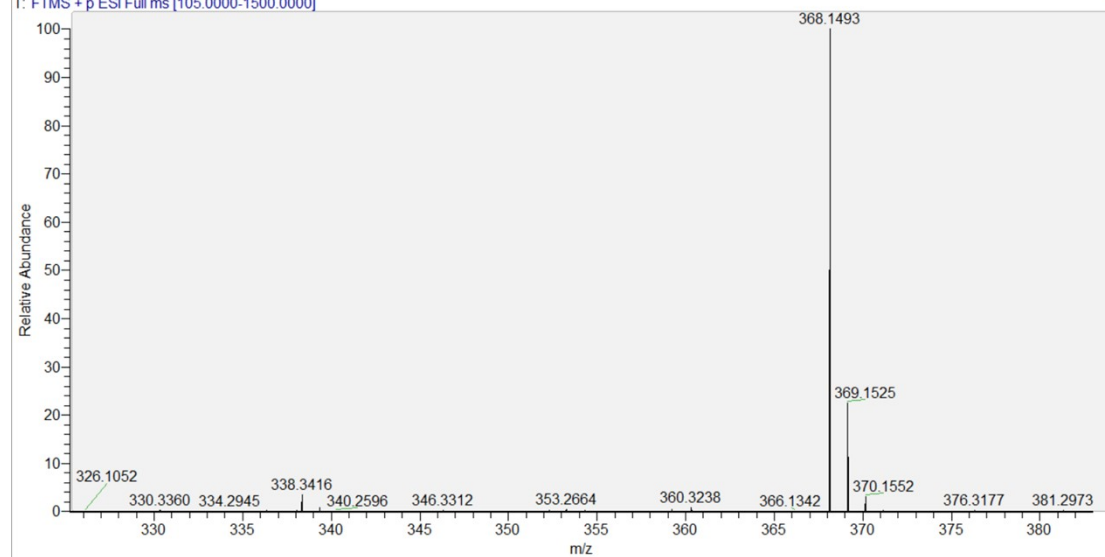
Mass spectrometry of 10k

ZXX40 #20-27 RT: 0.09-0.12 AV: 8 NL: 2.29E9
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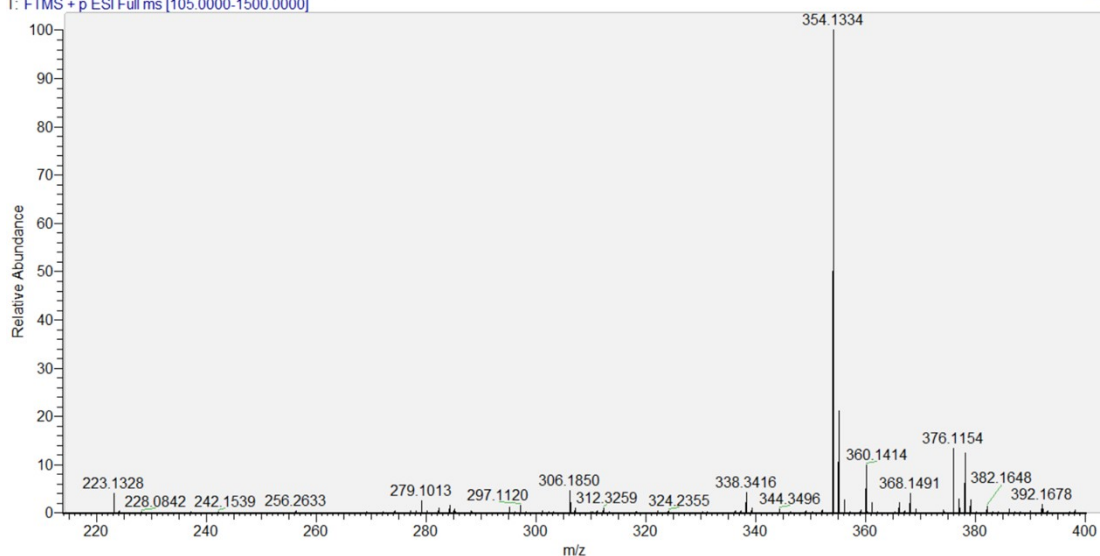
Mass spectrometry of 10l

YYY:17 #17-31 RT: 0.07-0.14 AV: 15 NL: 2.36E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



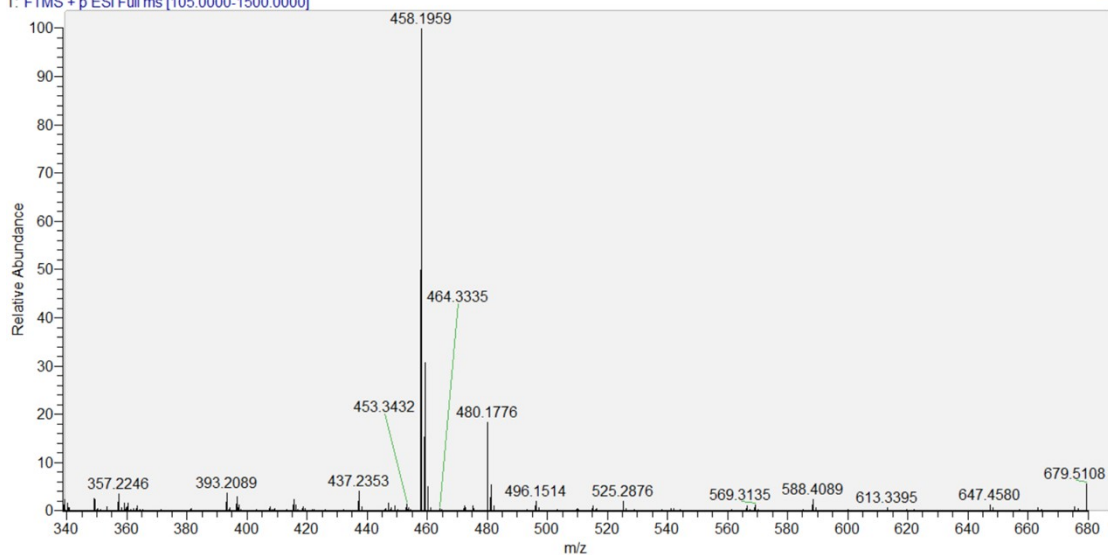
Mass spectrometry of 10m

YYY-18 #18-31 RT: 0.08-0.14 AV: 14 NL: 9.12E8
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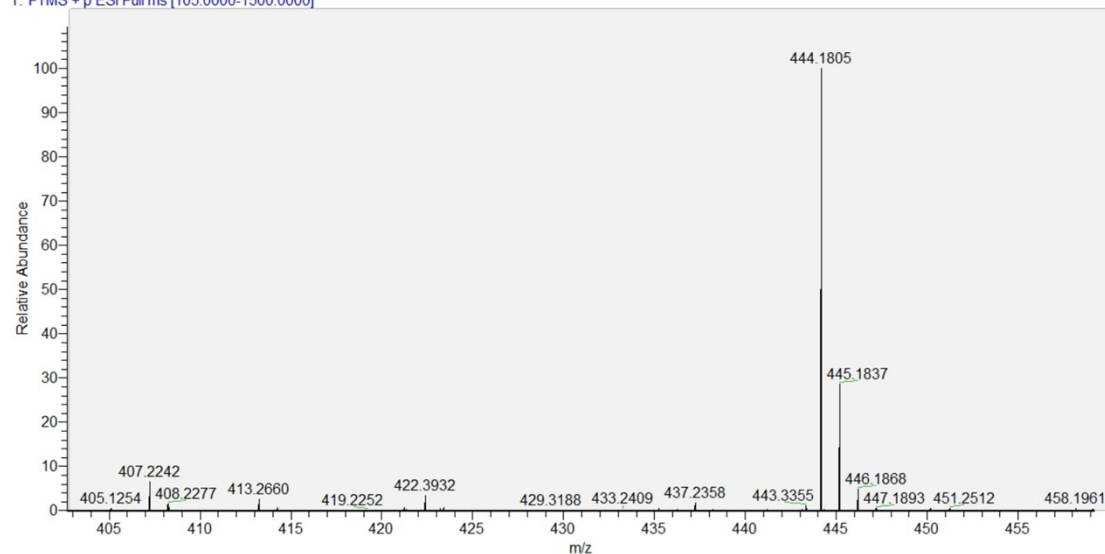
Mass spectrometry of 10n

ZXX12 #19-28 RT: 0.08-0.12 AV: 10 NL: 1.37E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



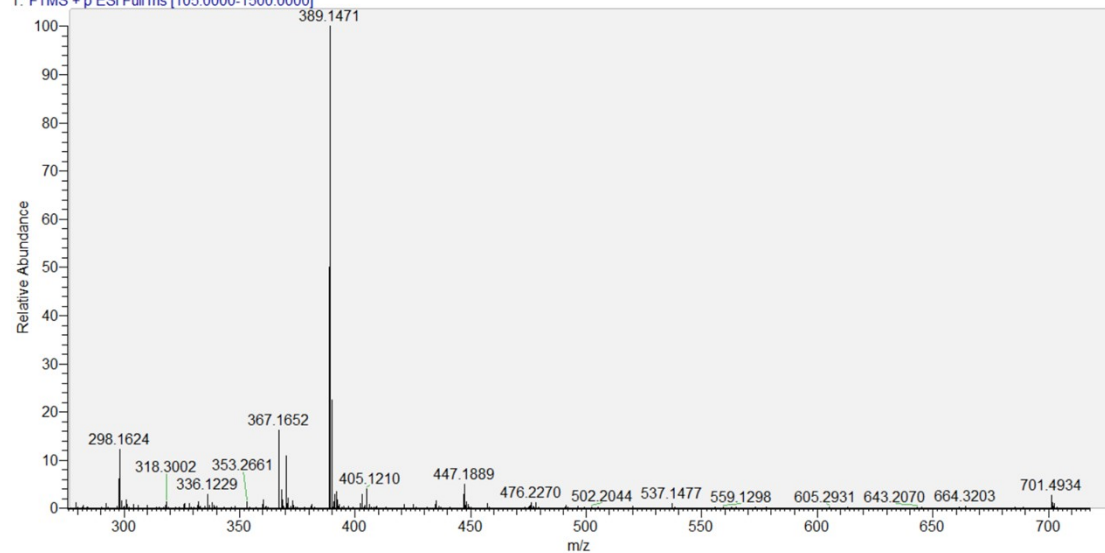
Mass spectrometry of 10o

YYY-25 #15-29 RT: 0.07-0.14 AV: 15 NL: 2.56E8
T: FTMS + p ESI Full ms [105.0000-1500.0000]



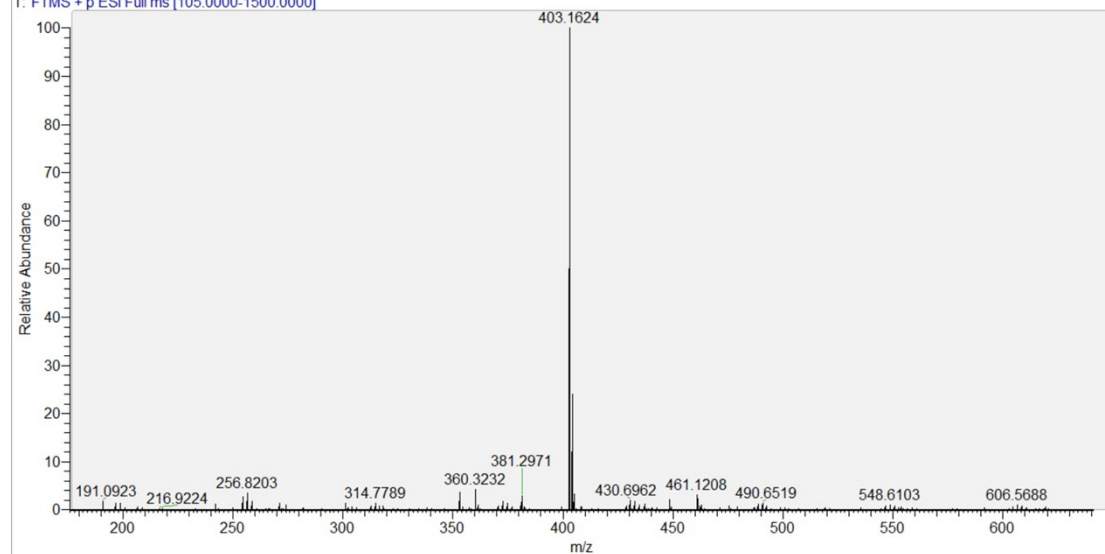
Mass spectrometry of 10p

YYY-23 #16-28 RT: 0.07-0.12 AV: 13 NL: 1.21E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



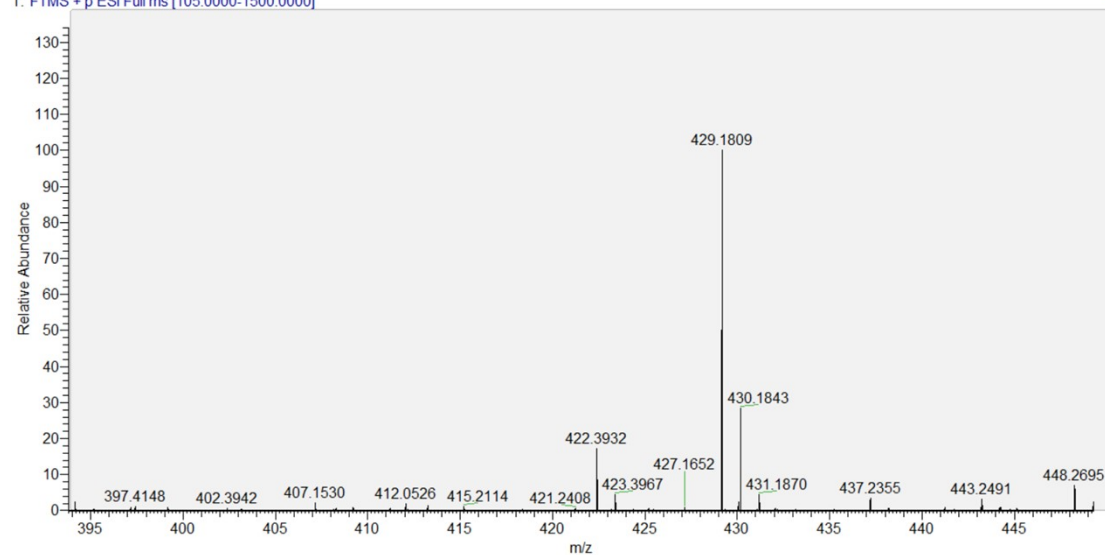
Mass spectrometry of 10q

YYY-22 #17-28 RT: 0.07-0.12 AV: 12 NL: 1.21E9
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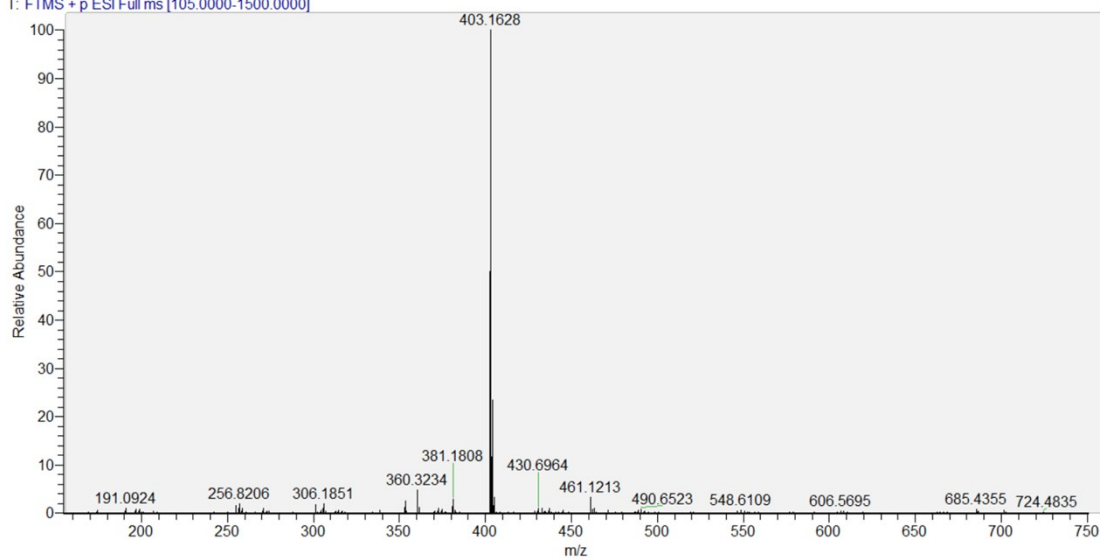
Mass spectrometry of 10r

YYY-24 #17-29 RT: 0.07-0.13 AV: 13 NL: 1.29E8
T: FTMS + p ESI Full ms [105.0000-1500.0000]



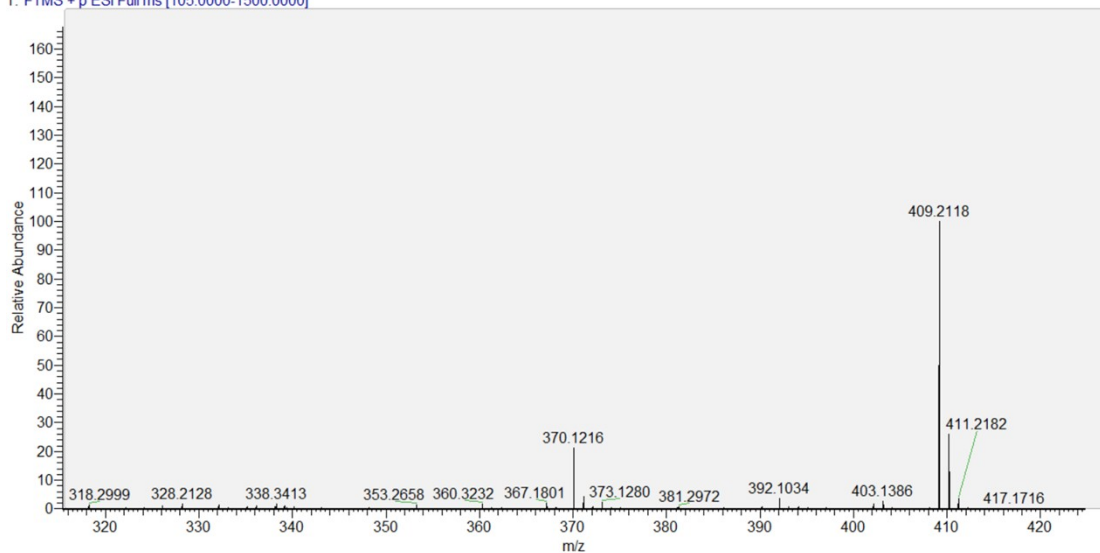
Mass spectrometry of 10s

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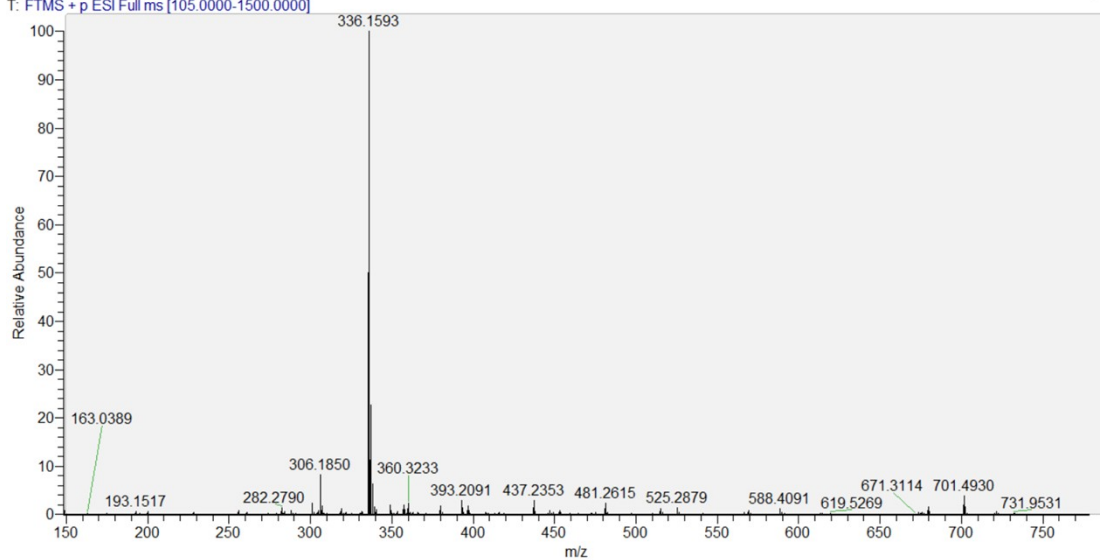
Mass spectrometry of 10t

YYY-21 #16-29 RT: 0.07-0.13 AV: 14 NL: 1.09E9
T: FTMS + p ESI Full ms [105.0000-1500.0000]



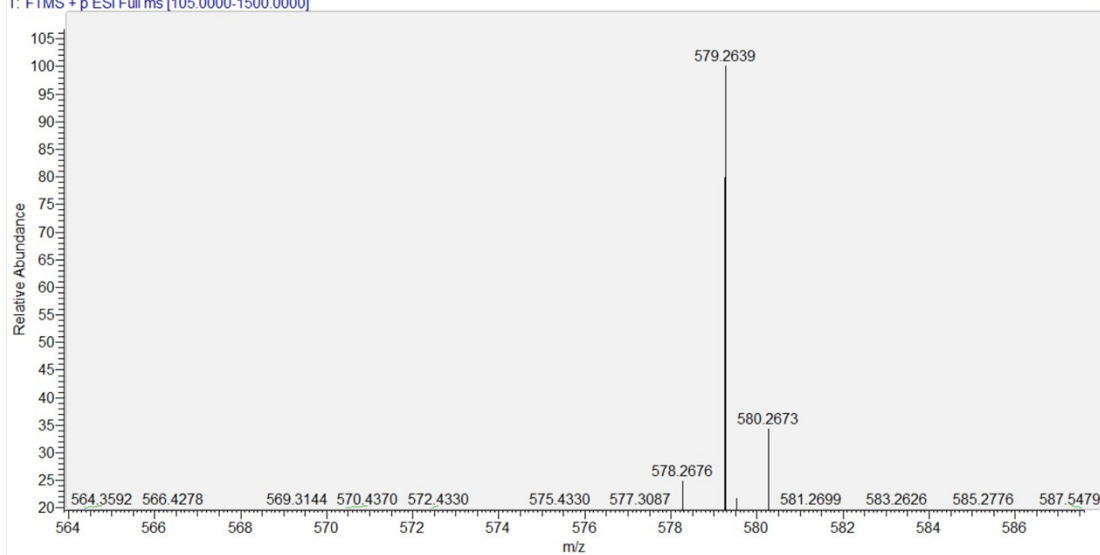
Mass spectrometry of 10u

ZXX41 #18-28 RT: 0.08-0.12 AV: 11 NL: 2.52E9
T: FTMS → p ESI Full ms [105.0000-1500.0000]



Mass spectrometry of 10v

ZXX27 #30-40 RT: 0.13-0.18 AV: 11 NL: 8.51E6
T: FTMS → p ESI Full ms [105.0000-1500.0000]



4. HPLC spectrum of 10v

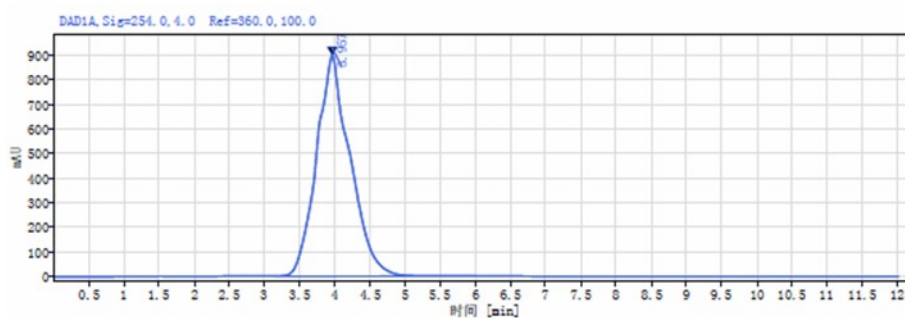
Instrument: Agilent 1290

Detector: UV (254 nM)

Column SB-C18 (25 cm × 0.46 cm, 5 μm)

Eluent: CH₃OH/H₂O (80/20 to 95/5, v/v), containing 0.1% formic acid.

Flow rate: 1.0 mL/min



Integration Results for DAD1A, Sig=254.0, 4.0 Ref=360.0, 100.0

Peak	RetTime	Area	%Area	Height	Type
1	3.957	29884.57	100%	895.12	VB