Supplementary Information

Design, Synthesis, and Biological Evaluation of Procaine-Based Triazole-Isoxazoline Hybrids as Selective PI3K/mTOR Inhibitors for Esophageal Cancer Therapy: An *in-vitro*, and *in-vivo* study

Yinliang Sheng,[1] Bin Wu,[1] Feng Li,[1] Chunyang Zhang[1]

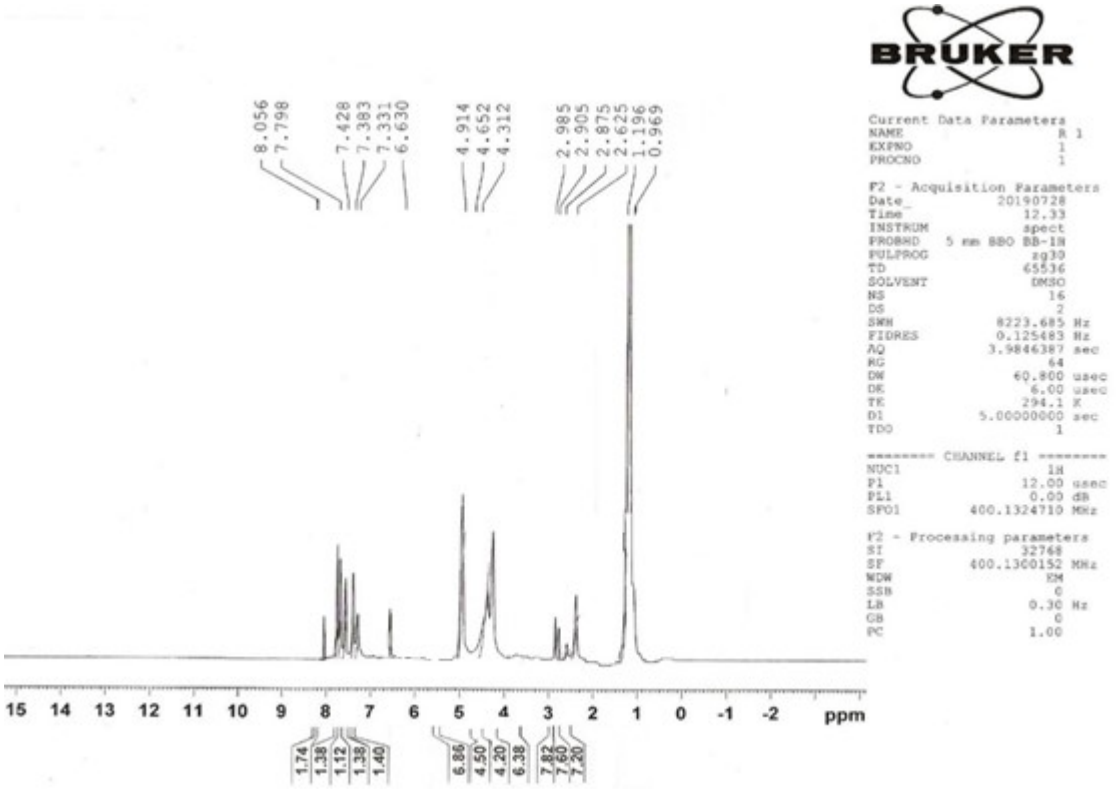
[1]Department of Thoracic Surgery, The First Affiliated Hospital of Zhengzhou University, Zhengzhou 450052, China

Corresponding author

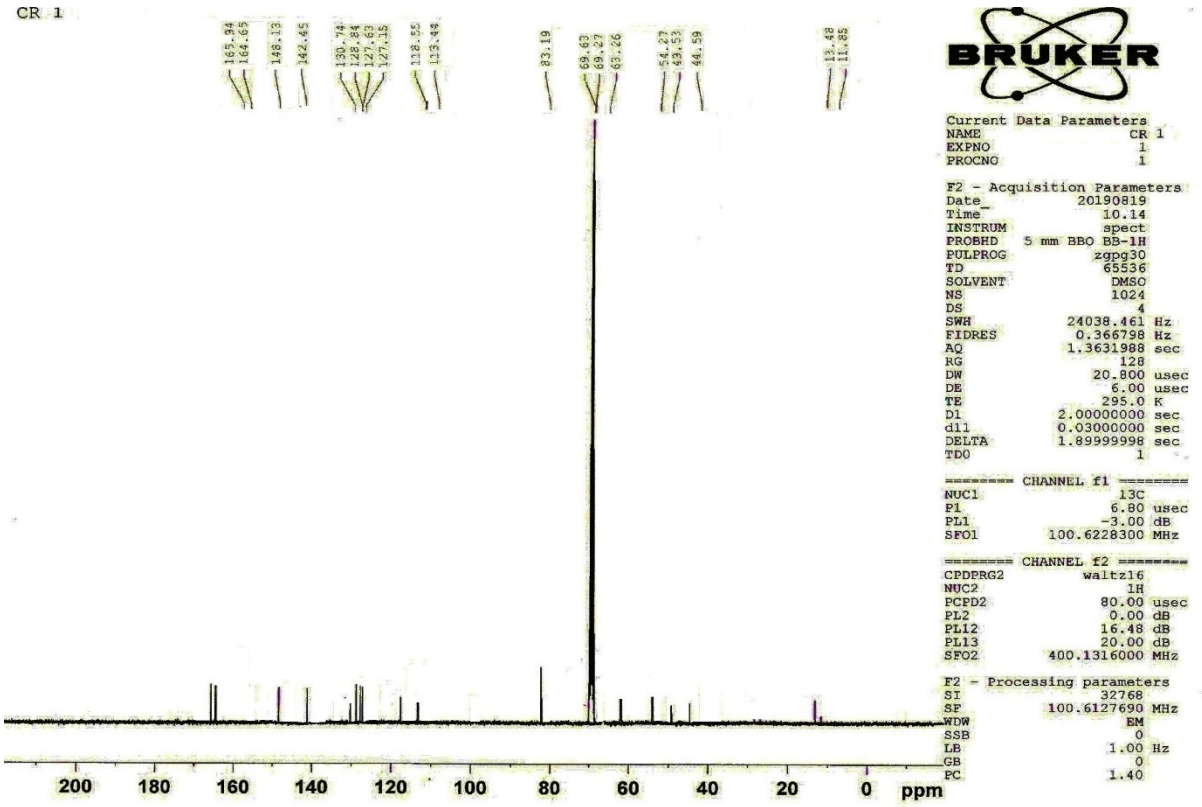
Chunyang Zhang

Email: zcy198200@outlook.com

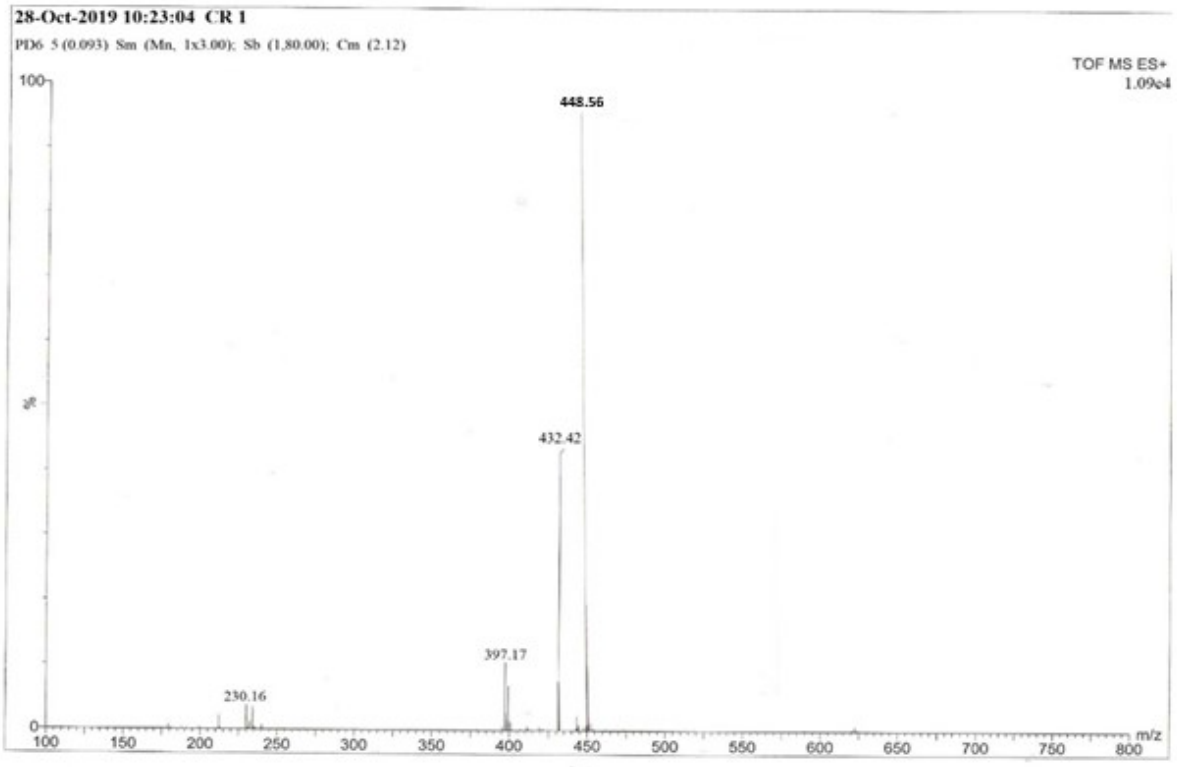
^{1}H NMR of 8a



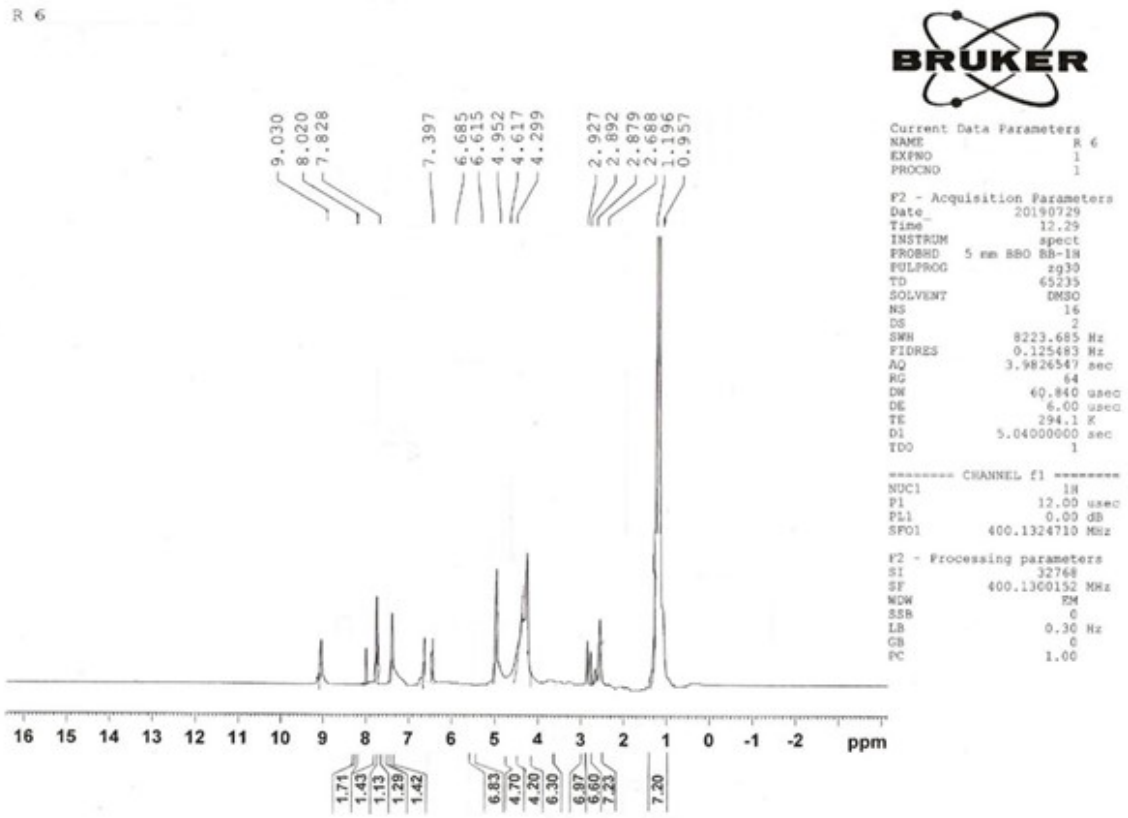
^{13}C NMR of 8a



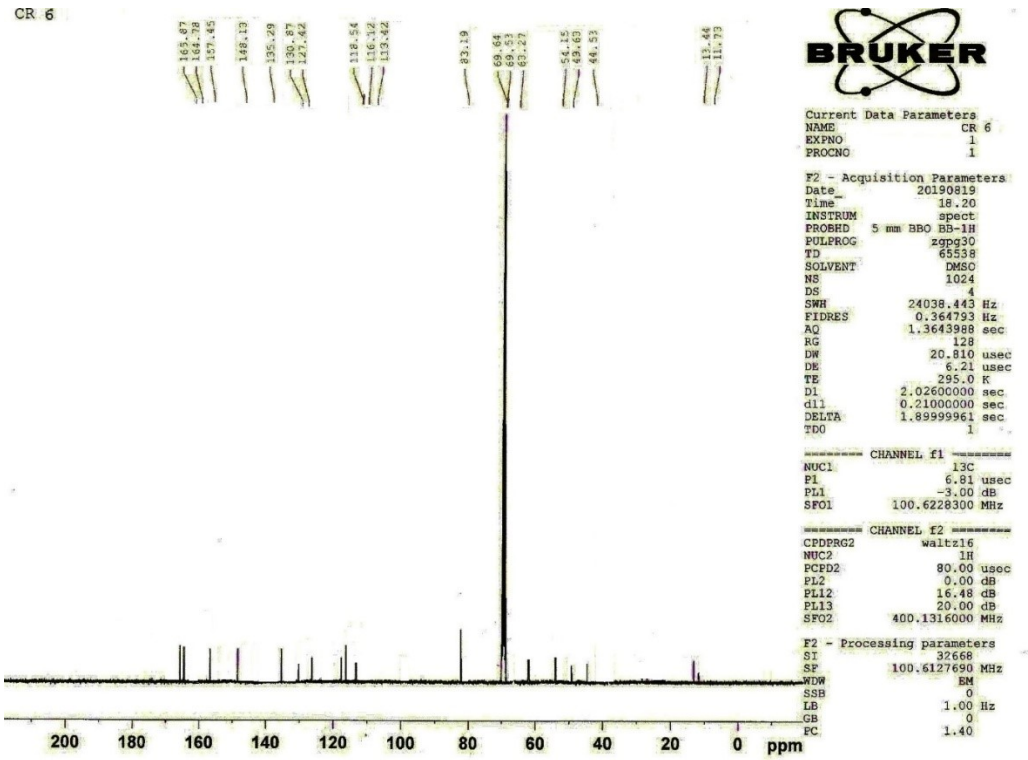
Mass of 8a


28-Oct-2019 10:23:04 CR 1
PD6 5 (0.093) Sm (Mn, 1x3.00); Sb (1,80.00); Cm (2.12)
TOF MS ES+
1.09e4
100
%
0
448.56
432.42
397.17
230.16
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

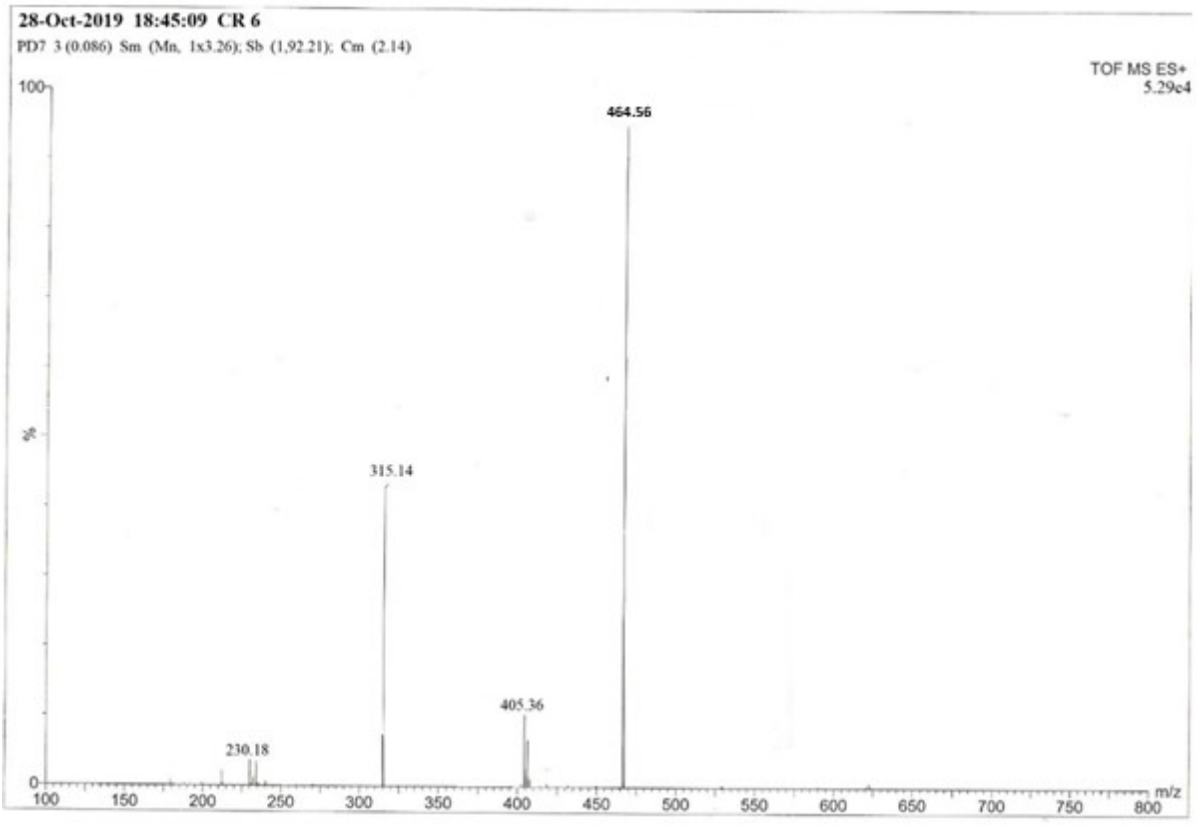
^{1}H NMR of 8b



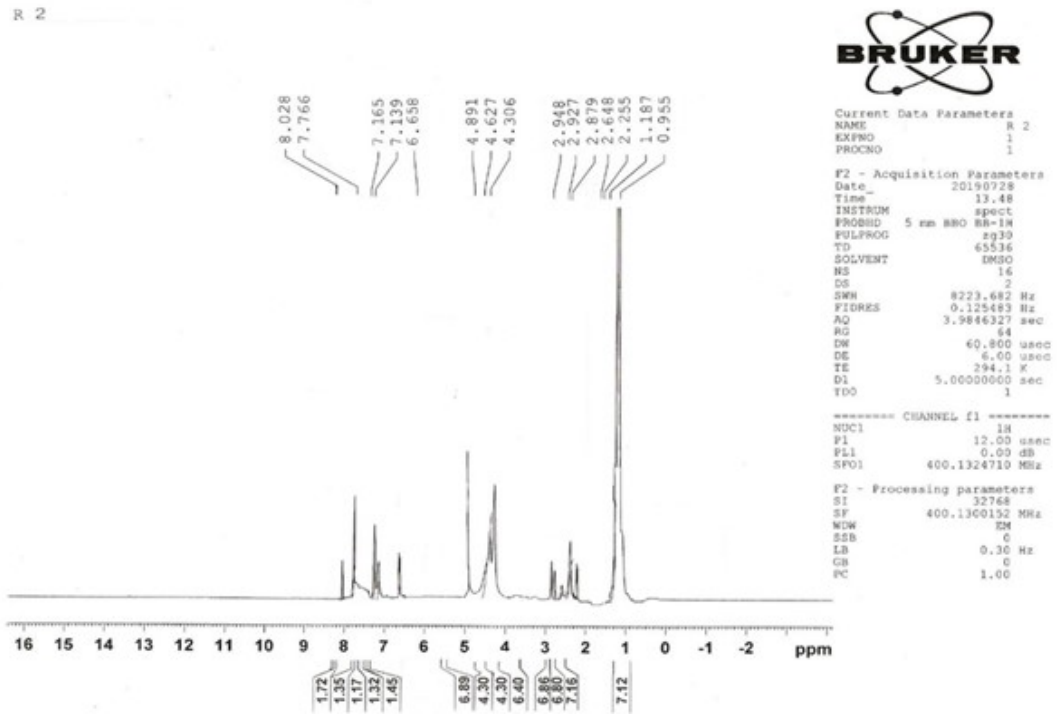
^{13}C NMR of 8b



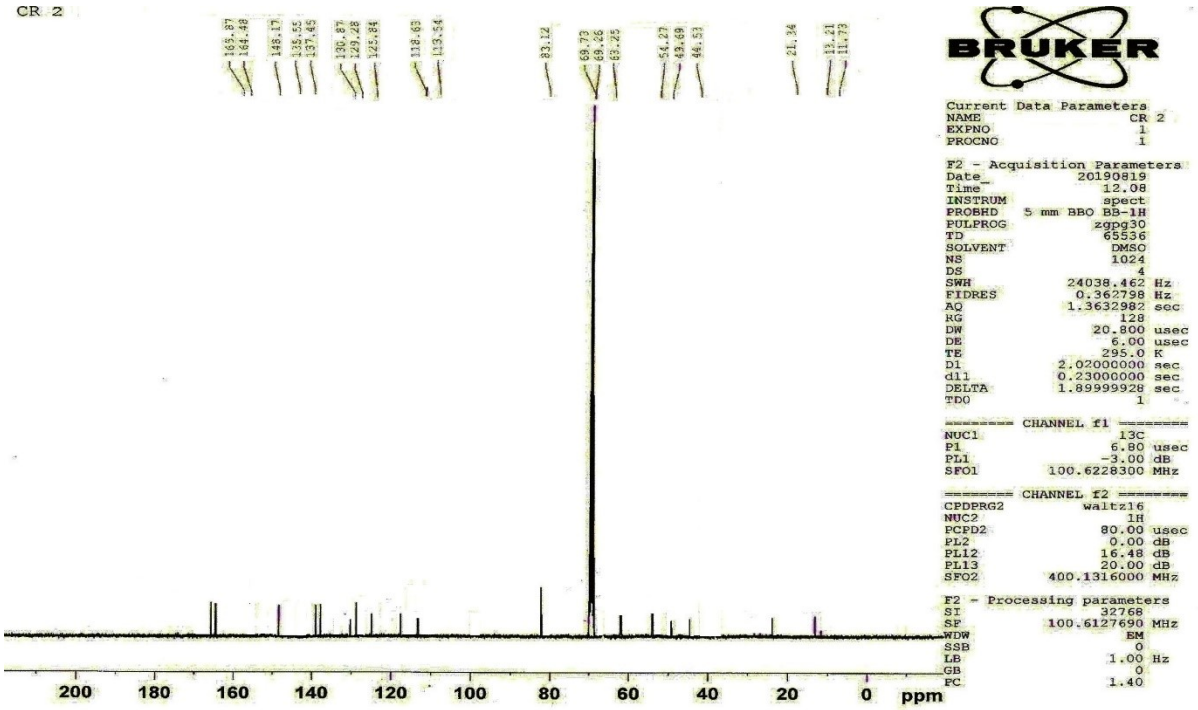
Mass of 8b


28-Oct-2019 18:45:09 CR 6
PD7 3 (0.086) Sm (Mn, 1x3.26); Sb (1,92.21); Cm (2.14)
TOF MS ES+
5.29e4
100
%
0
464.56
315.14
405.36
230.18
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

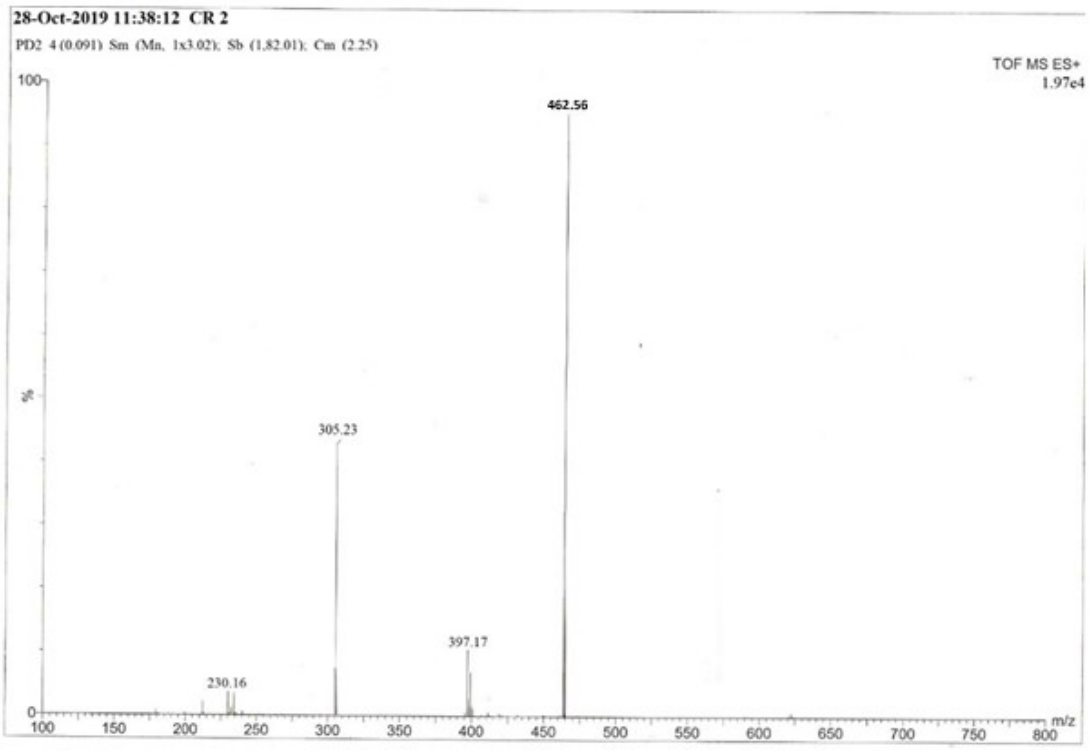
^{1}H NMR of 8c



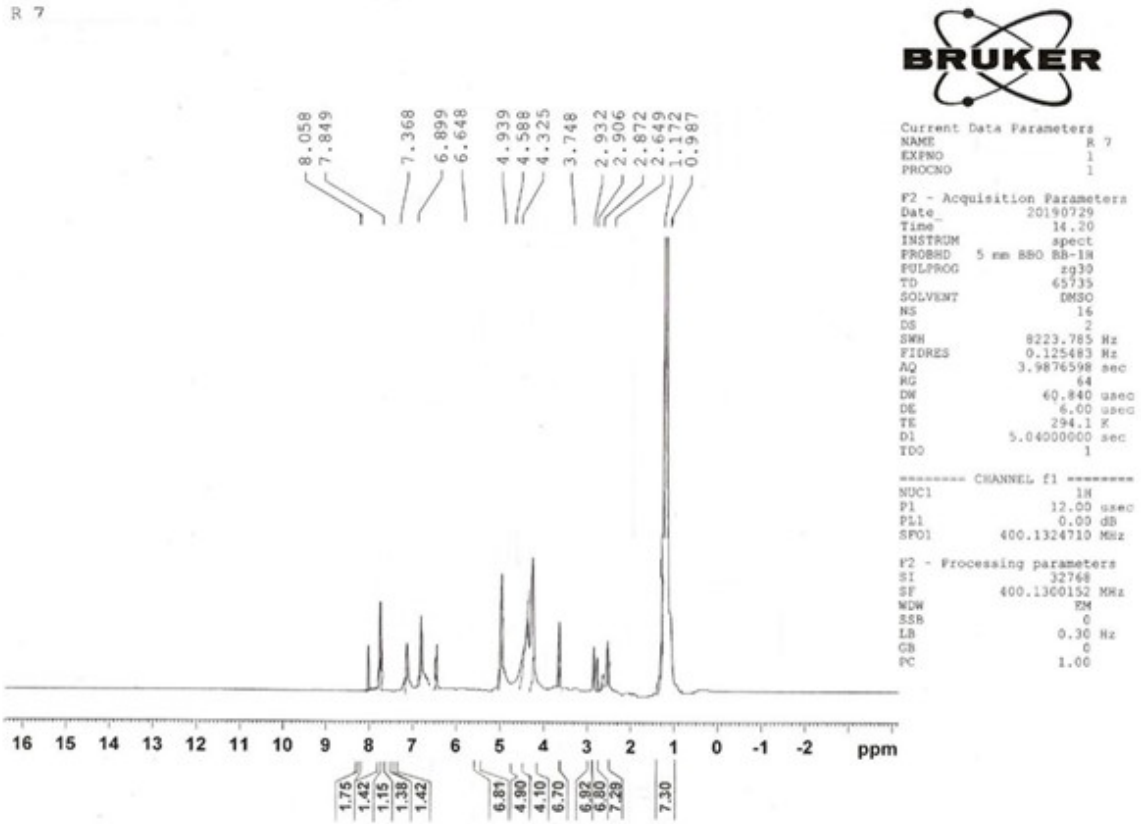
^{13}C NMR of 8c



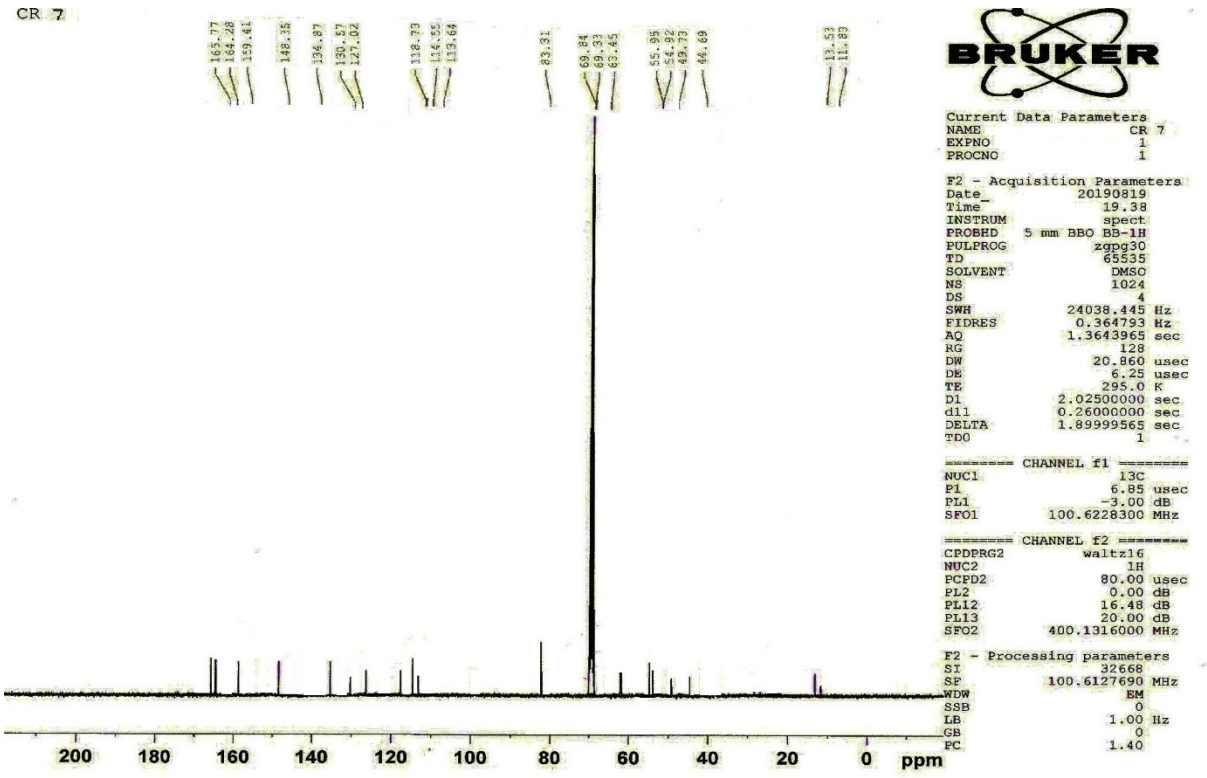
Mass of 8c


28-Oct-2019 11:38:12 CR 2
PD2 4 (0.091) Sm (Mn, 1x3.02); Sb (1,82.01); Cm (2.25)
TOF MS ES+
1.97e4
100
%
0
462.56
305.23
397.17
230.16
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

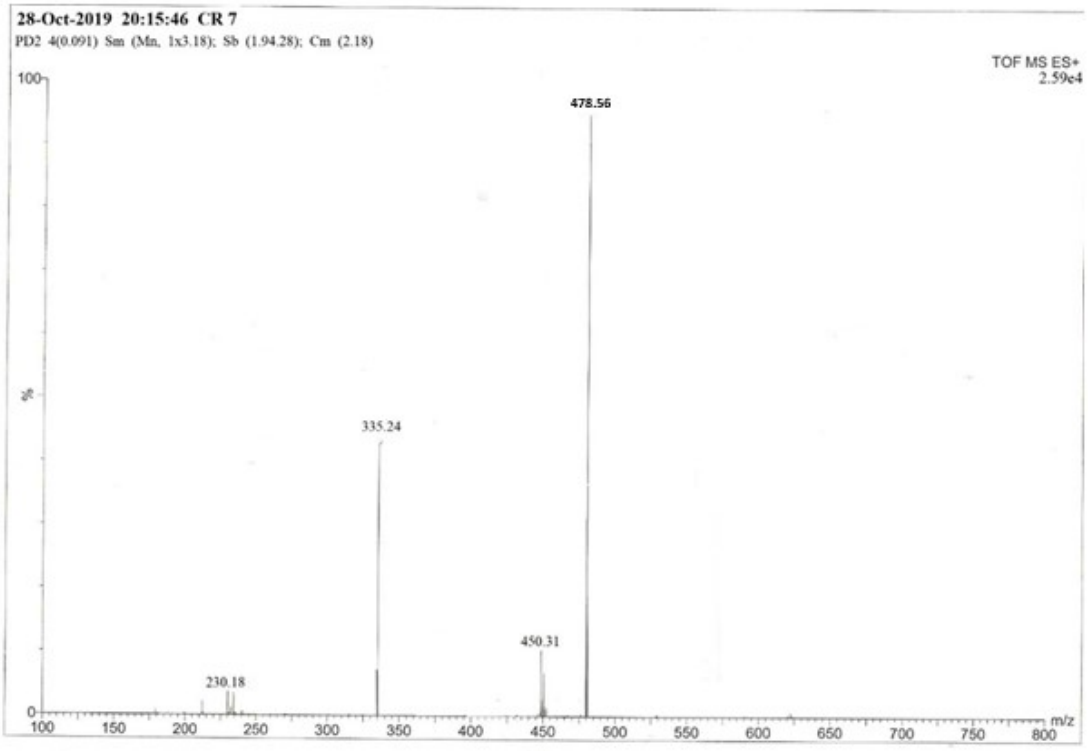
^{1}H NMR of 8d



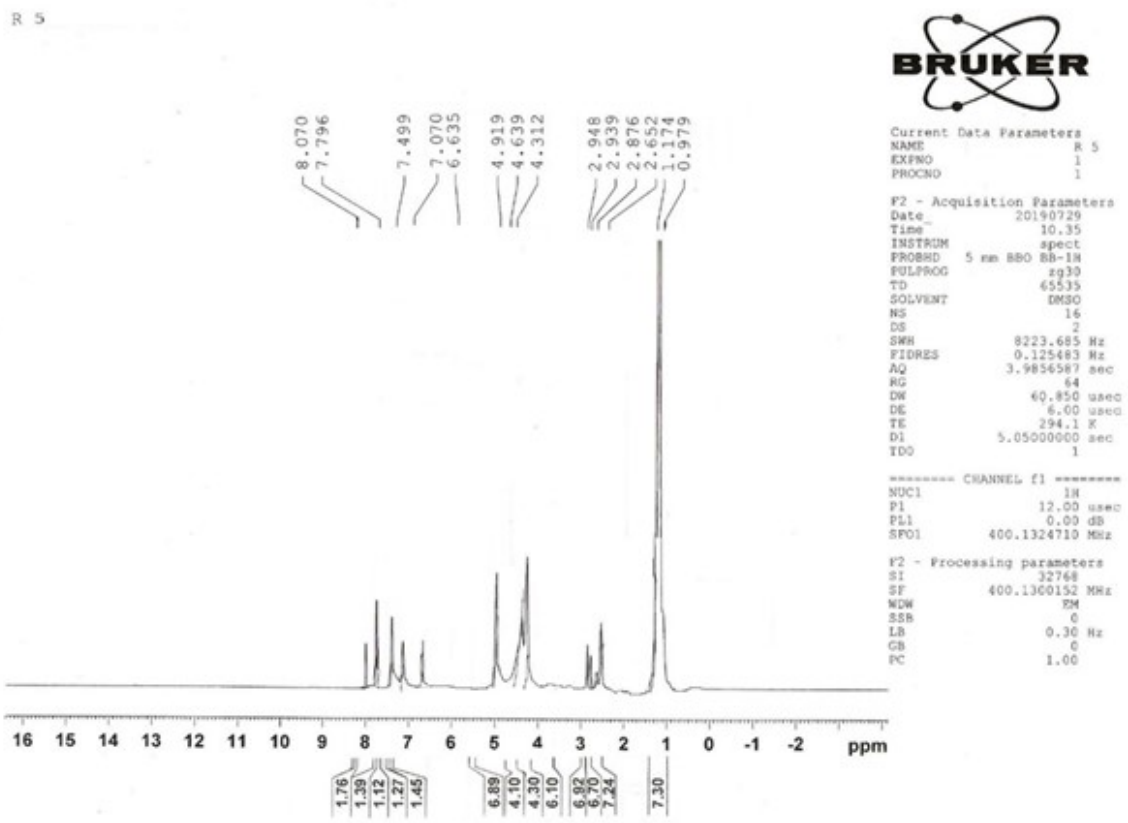
^{13}C NMR of 8d



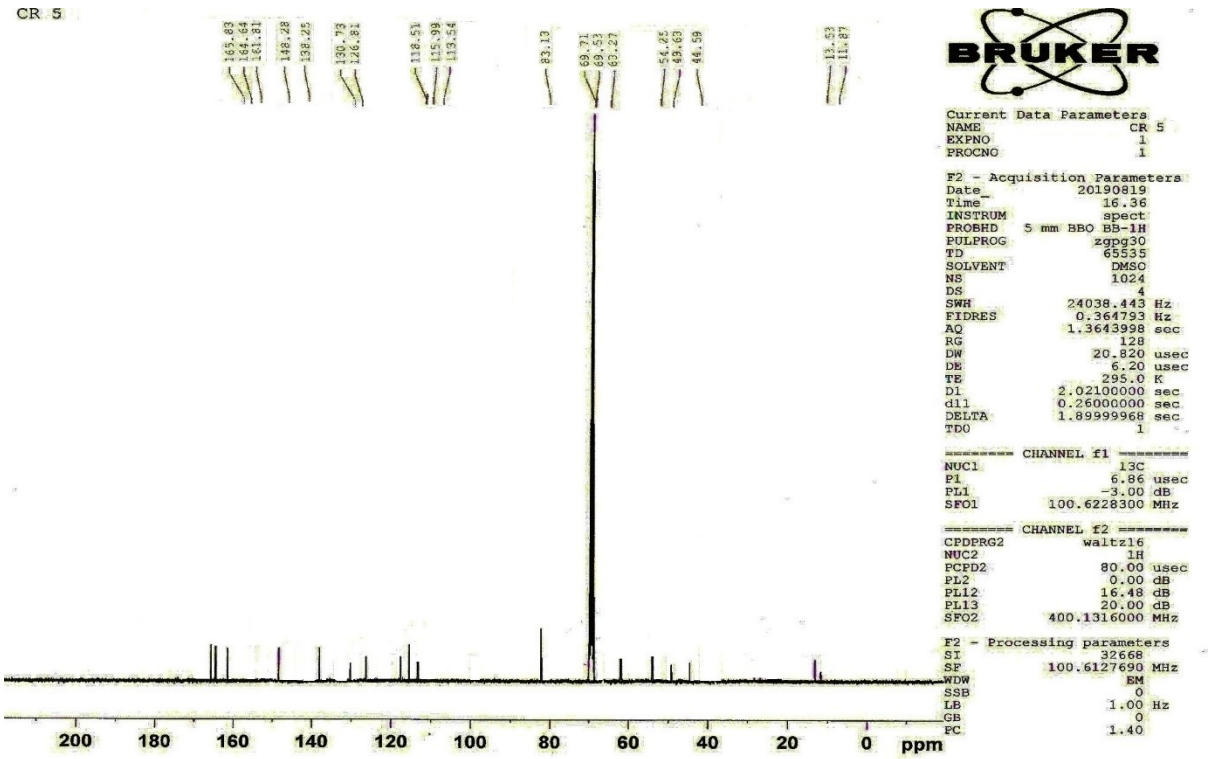
Mass of 8d


28-Oct-2019 20:15:46 CR 7
PD2 4(0.091) Sm (Mn, 1x3.18); Sb (1.94.28); Cm (2.18)
TOF MS ES+
2.59e4
100
%
0
478.56
335.24
450.31
230.18
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

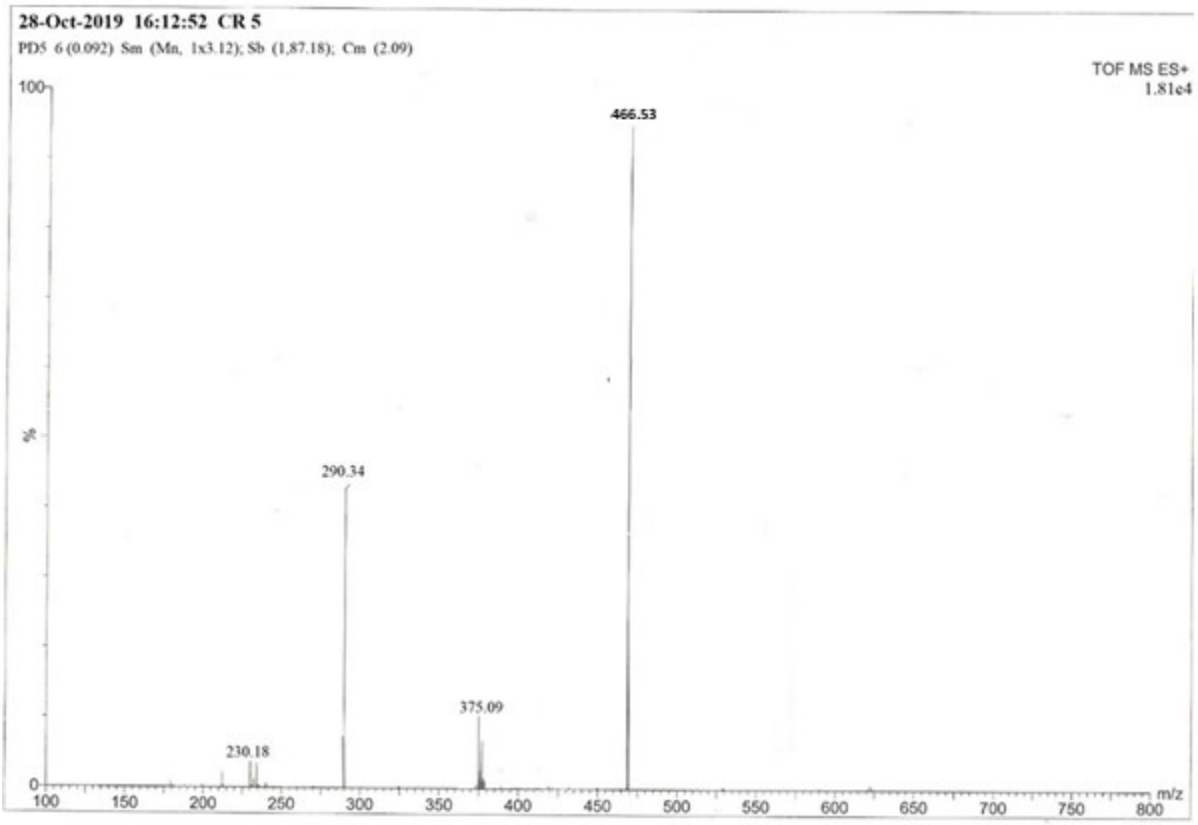
^{1}H NMR of 8e



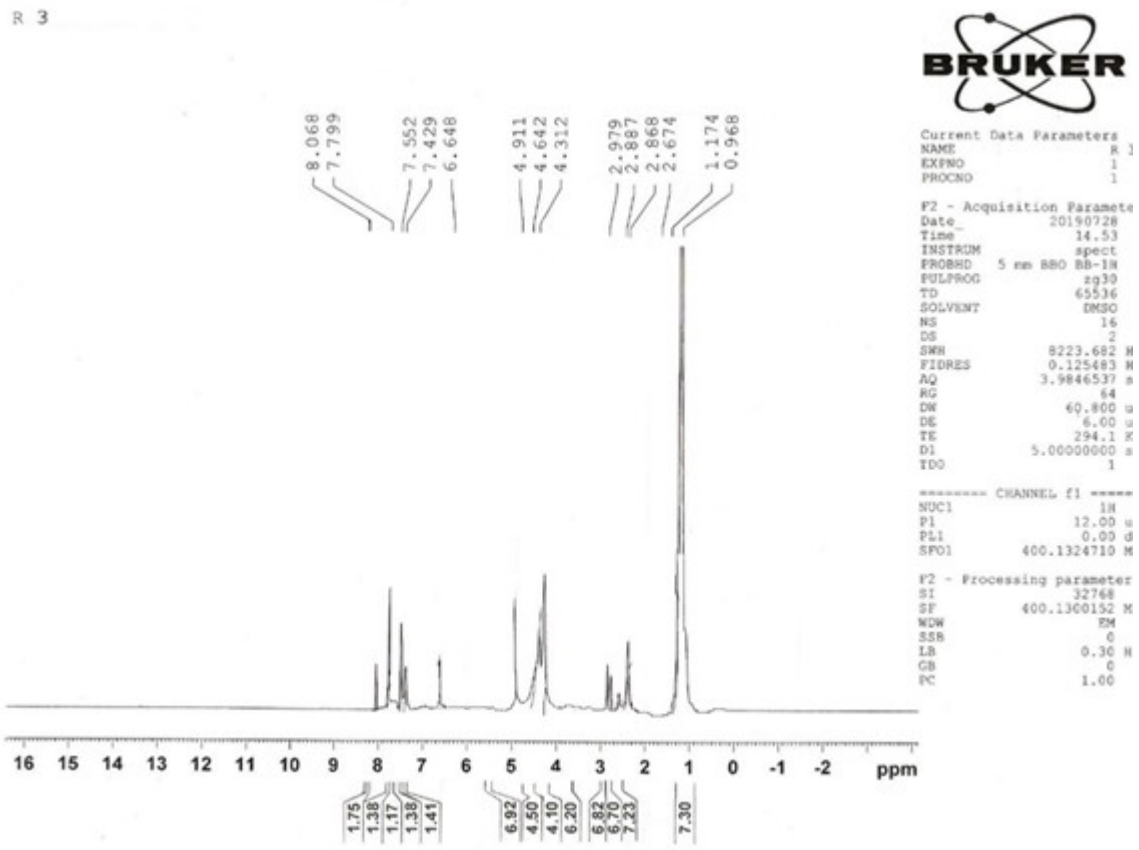
^{13}C NMR of 8e



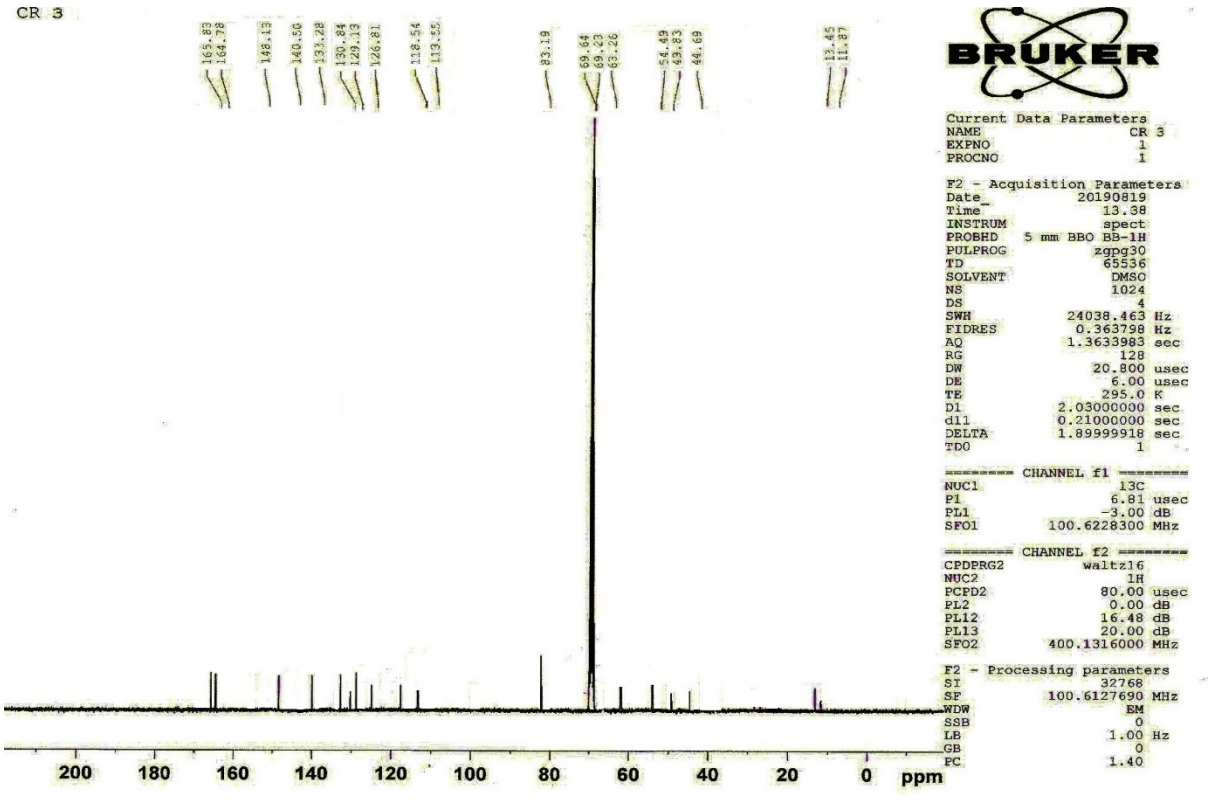
Mass of 8e


28-Oct-2019 16:12:52 CR 5
PD5 6 (0.092) Sm (Mn, 1x3.12); Sb (1,87.18); Cm (2.09)
TOF MS ES+
1.81e4
100
%
0
466.53
290.34
375.09
230.18
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
m/z

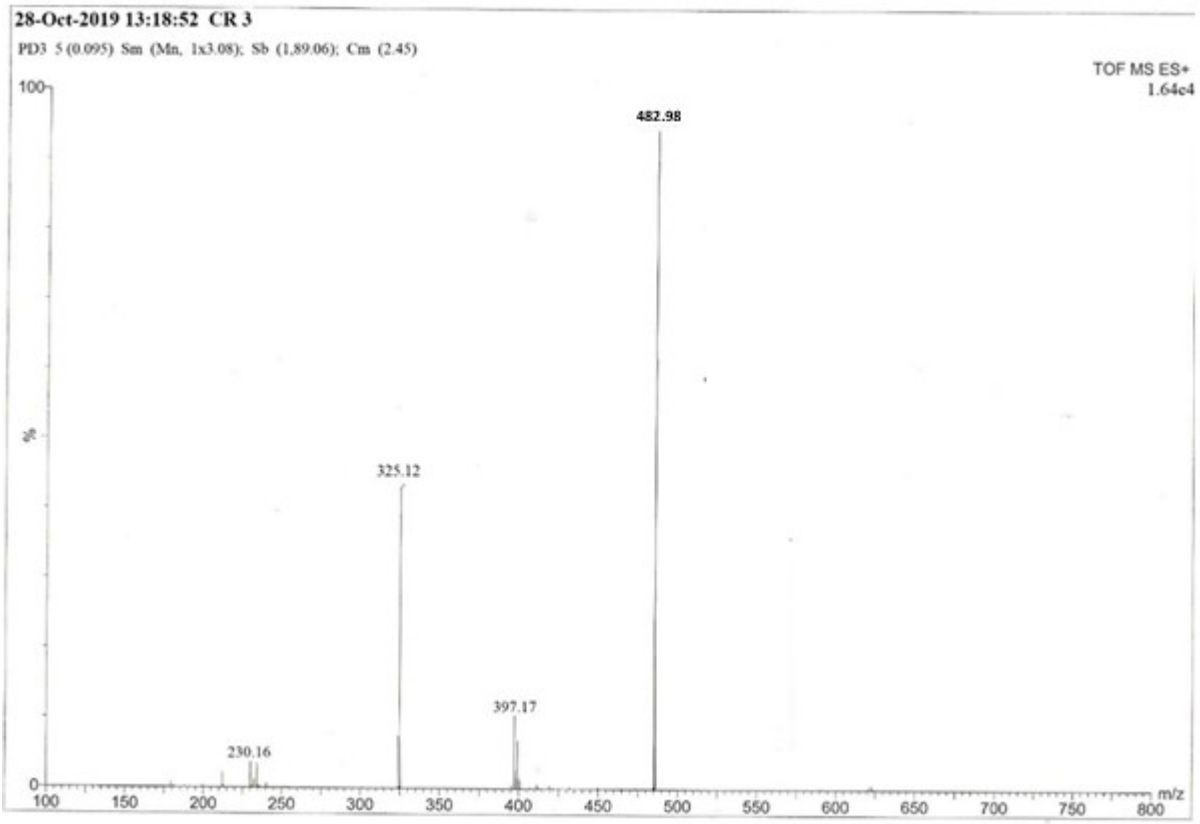
^{1}H NMR of 8f



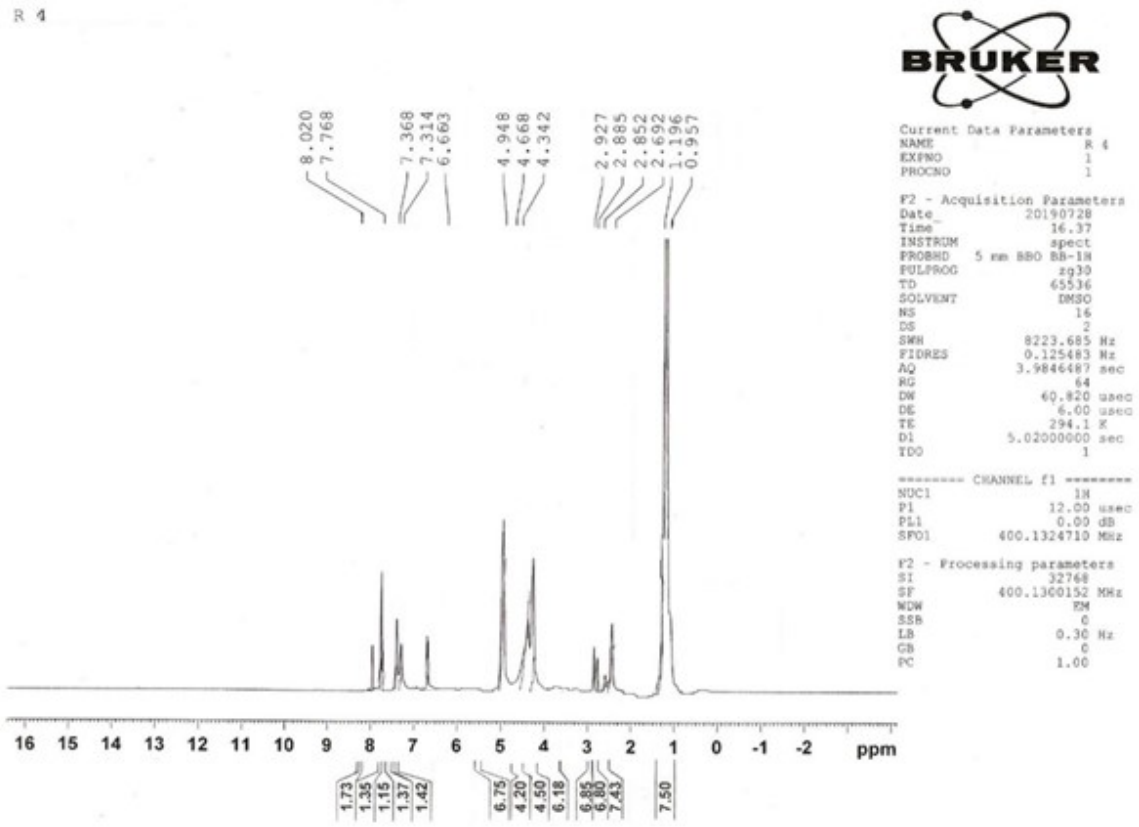
^{13}C NMR of 8f



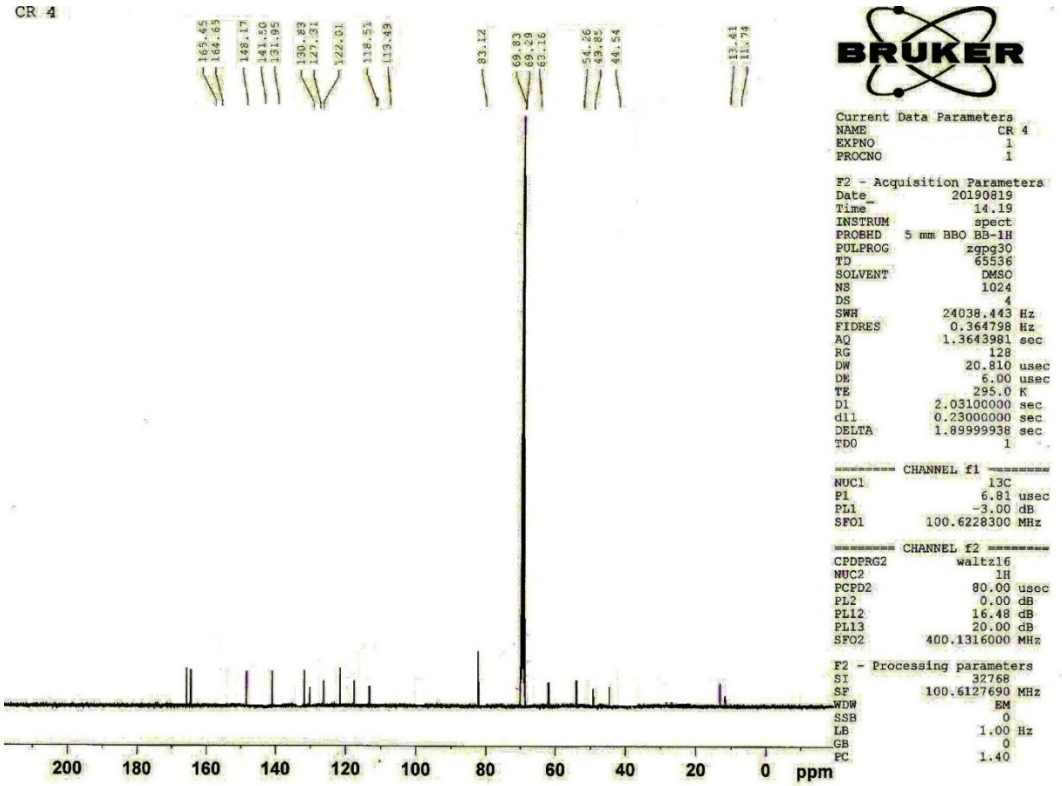
Mass of 8f


28-Oct-2019 13:18:52 CR 3
PD3 5 (0.095) Sm (Mn, 1x3.08); Sb (1,89.06); Cm (2.45)
TOF MS ES+
1.64e4
100
%
0
482.98
325.12
397.17
230.16
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

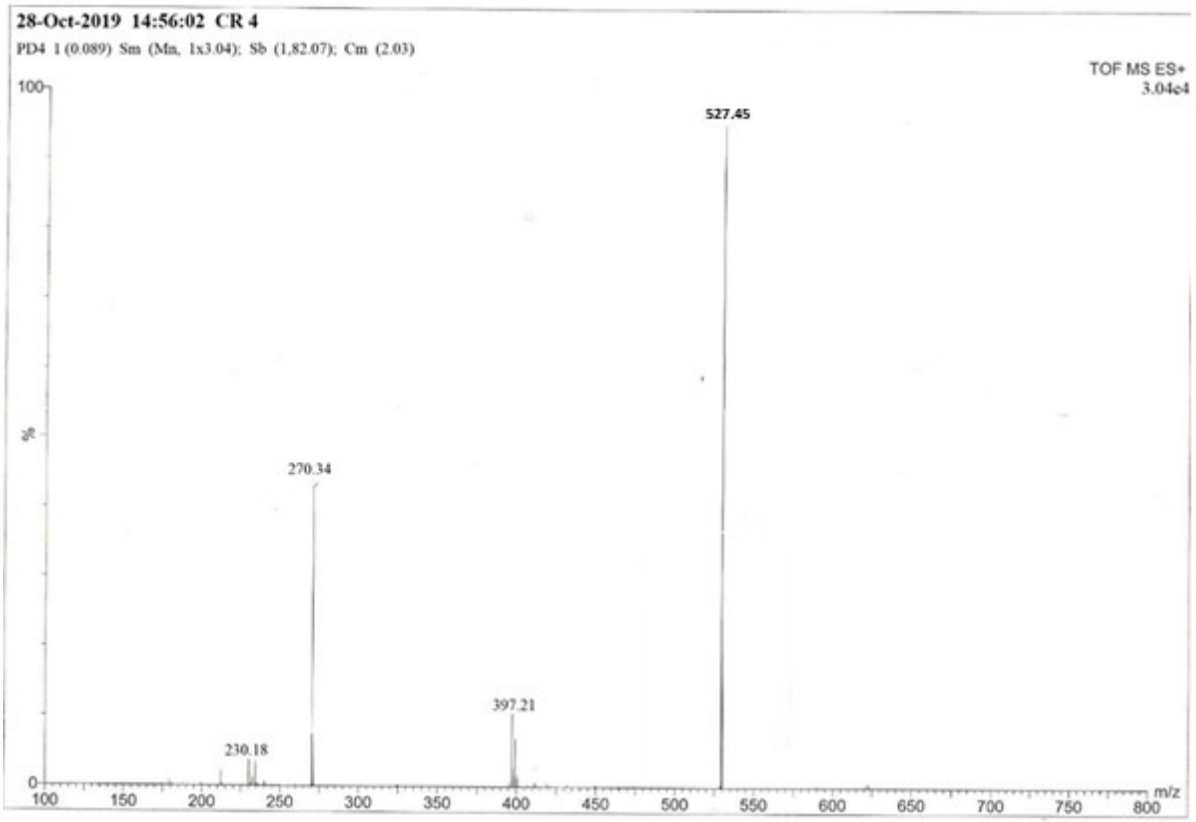
^{1}H NMR of 8g



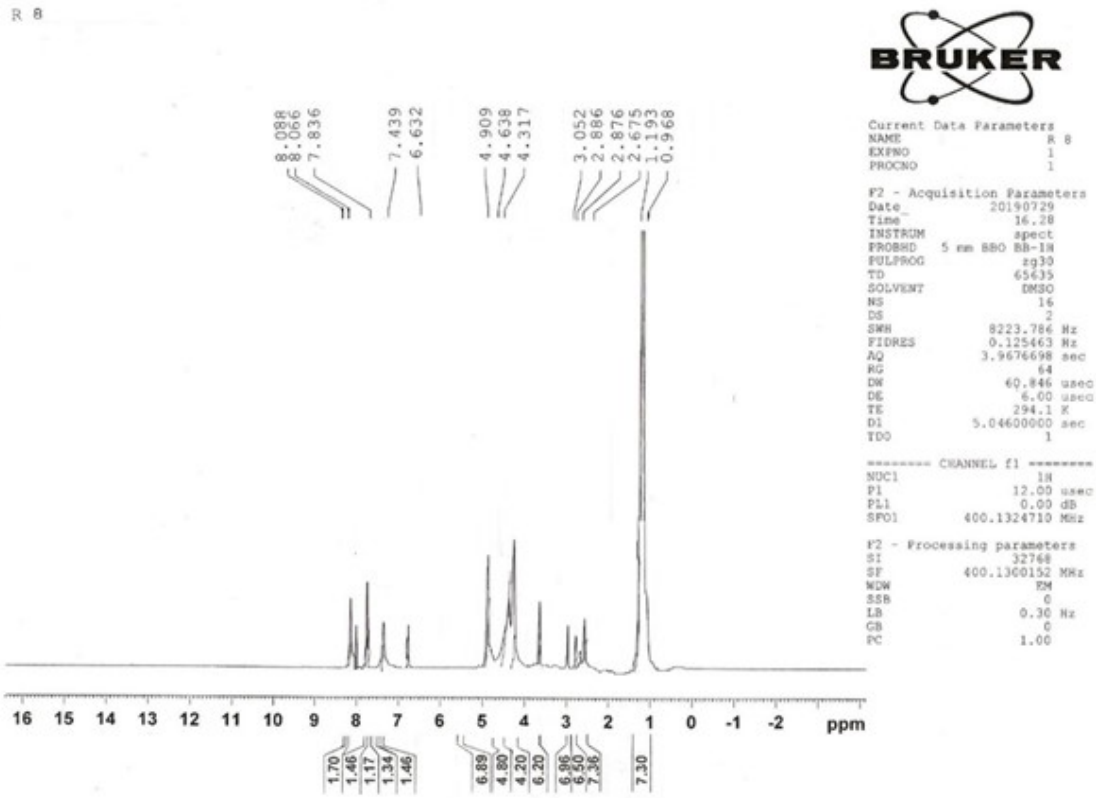
^{13}C NMR of 8g



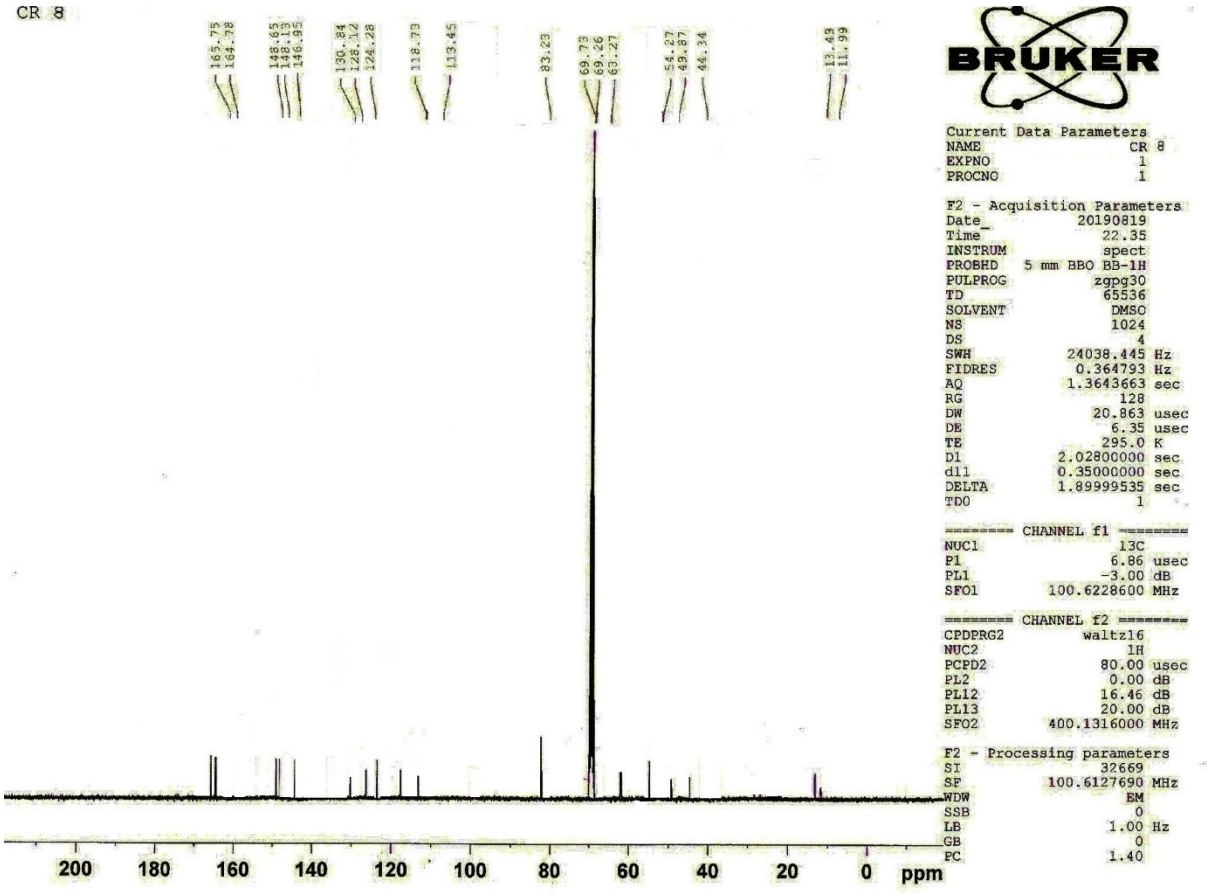
Mass of 8g


28-Oct-2019 14:56:02 CR 4
PD4 1 (0.089) Sm (Mn, 1x3.04); Sb (1,82.07); Cm (2.03)
TOF MS ES+
3.04e4
100
%
0
527.45
270.34
397.21
230.18
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

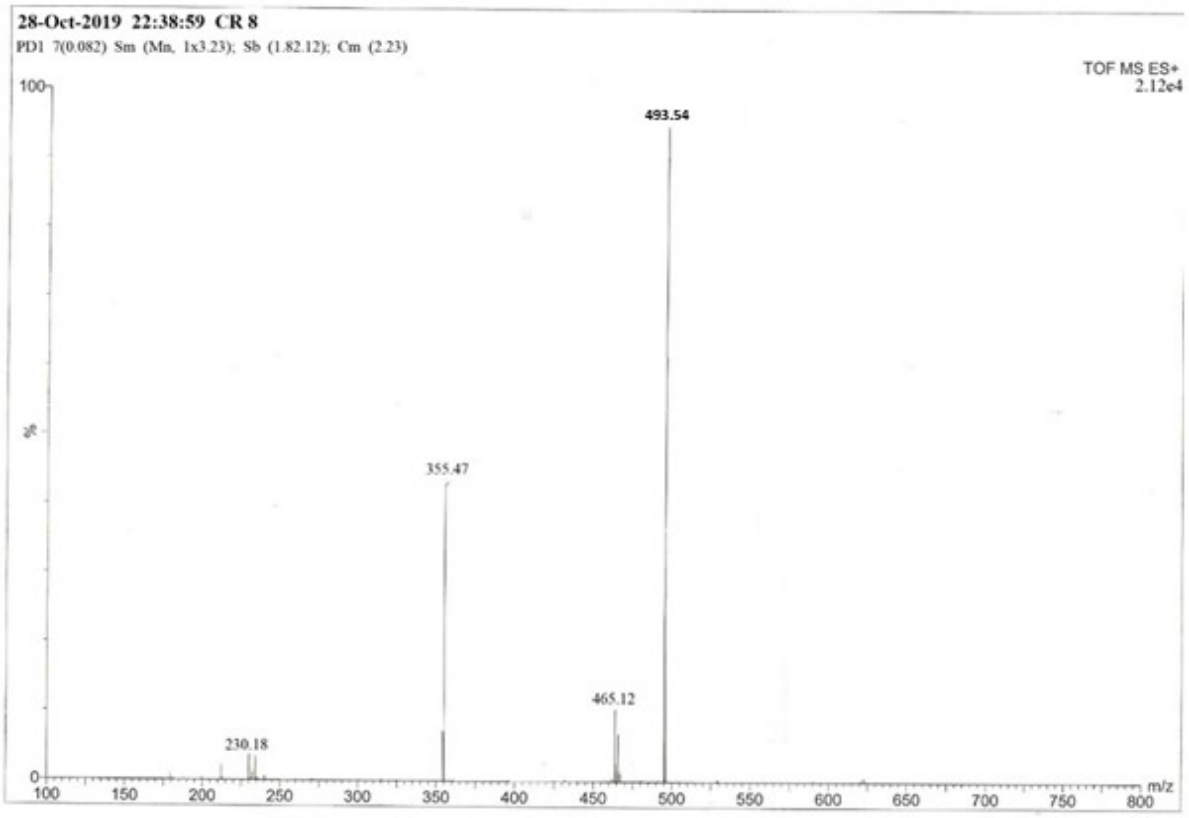
^{1}H NMR of 8h



^{13} C NMR of 8h



Mass of 8h


28-Oct-2019 22:38:59 CR 8
PD1 7(0.082) Sm (Mn, 1x3.23); Sb (1.82.12); Cm (2.23)
TOF MS ES+
2.12e4
100
%
0
493.54
355.47
465.12
230.18
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z