



Supporting Information

for

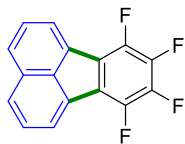
Mono or double Pd-catalyzed C–H bond functionalization for the annulative π -extension of 1,8-dibromonaphthalene: a one pot access to fluoranthene derivatives

Nahed Ketata, Linhao Liu, Ridha Ben Salem and Henri Doucet

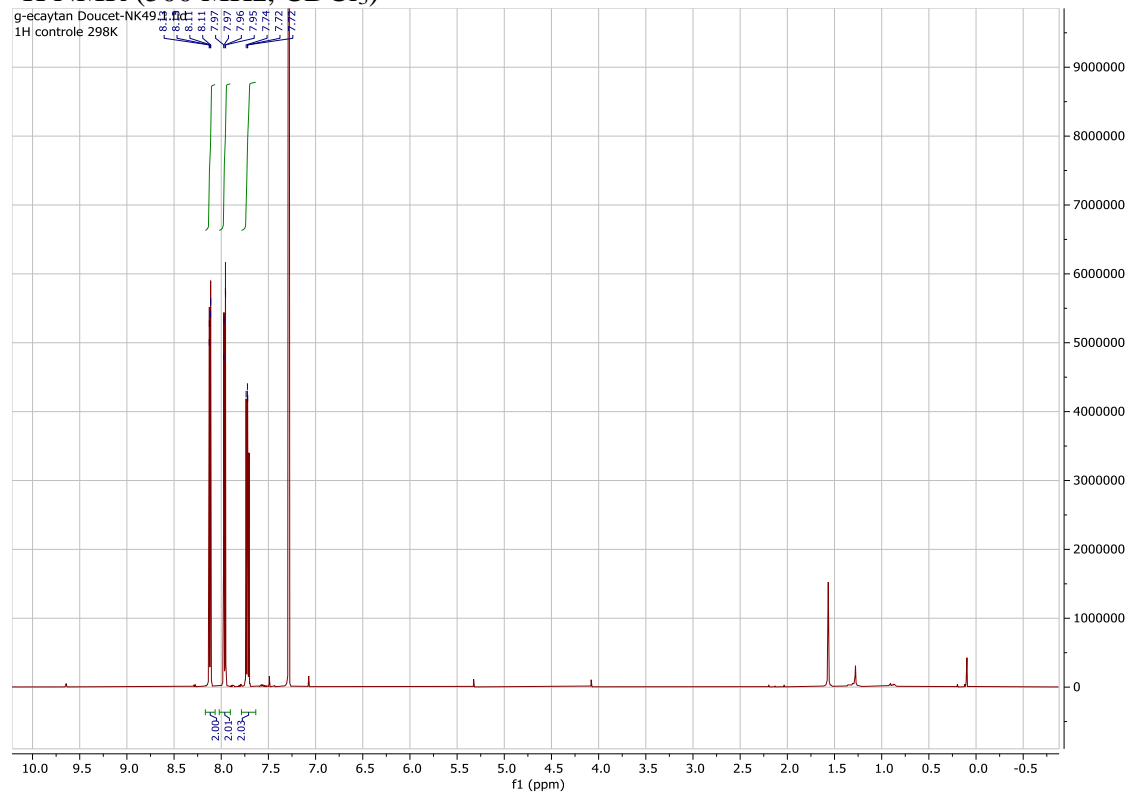
Beilstein J. Org. Chem. **2024**, *20*, 427–435. [doi:10.3762/bjoc.20.37](https://doi.org/10.3762/bjoc.20.37)

Copies of ^1H , ^{19}F , and ^{13}C NMR spectra

7,8,9,10-Tetrafluorofluoranthene (1)



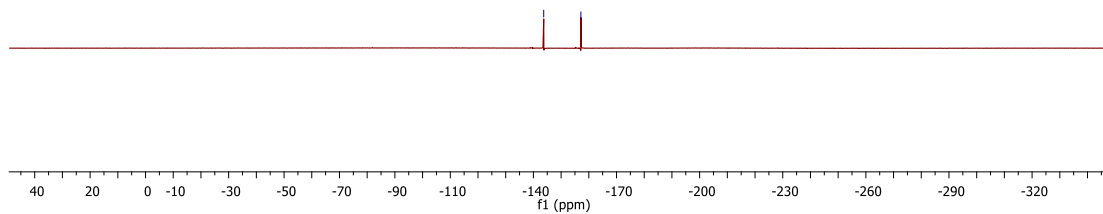
^1H NMR (500 MHz, CDCl_3)



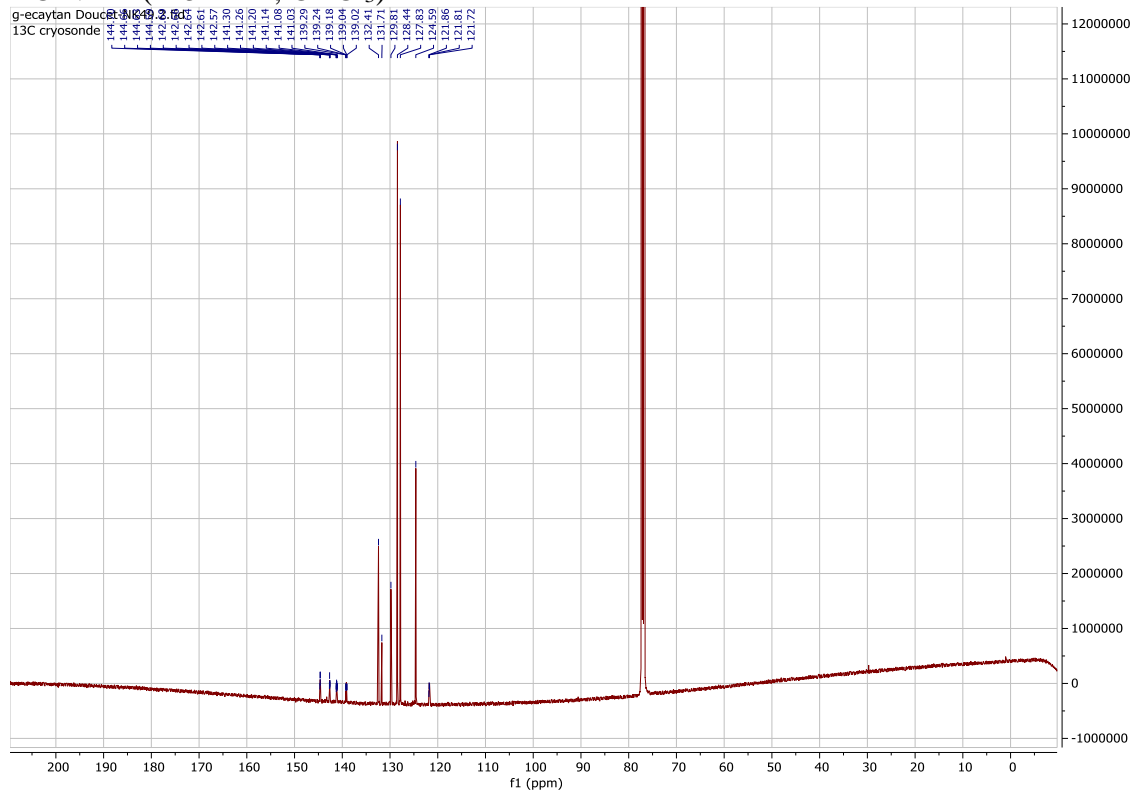
^{19}F NMR (376 MHz, CDCl_3)

nketata nk49f

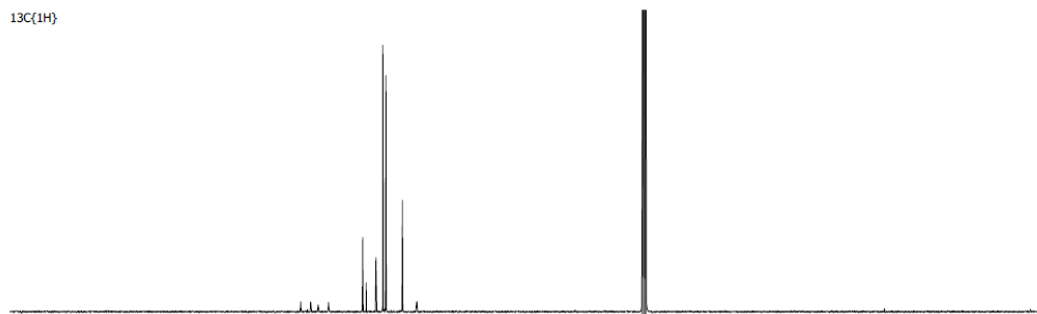
-143.72
-157.14



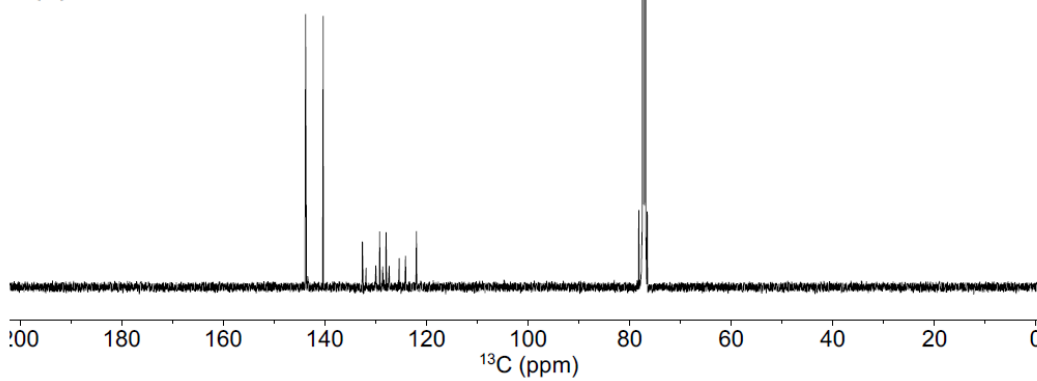
¹³C NMR (125 MHz, CDCl₃)



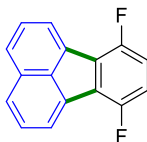
¹³C{¹H}



¹³C{¹⁹F}

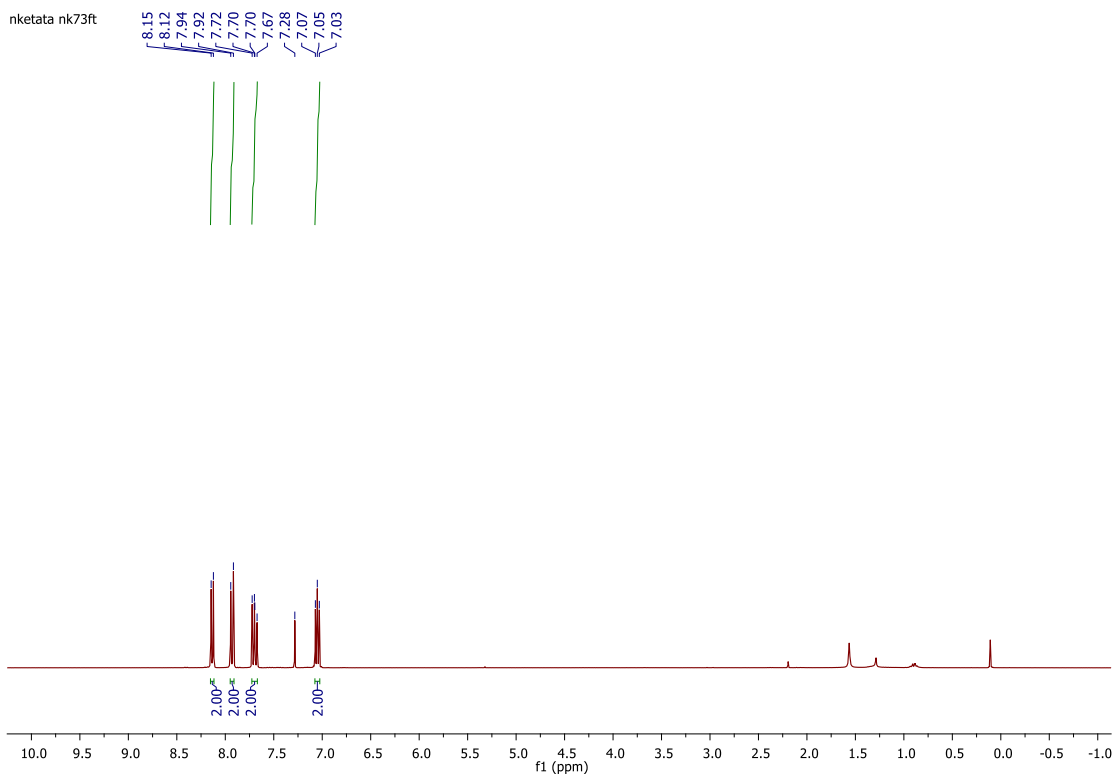


7,10-Difluorofluoranthene (2)



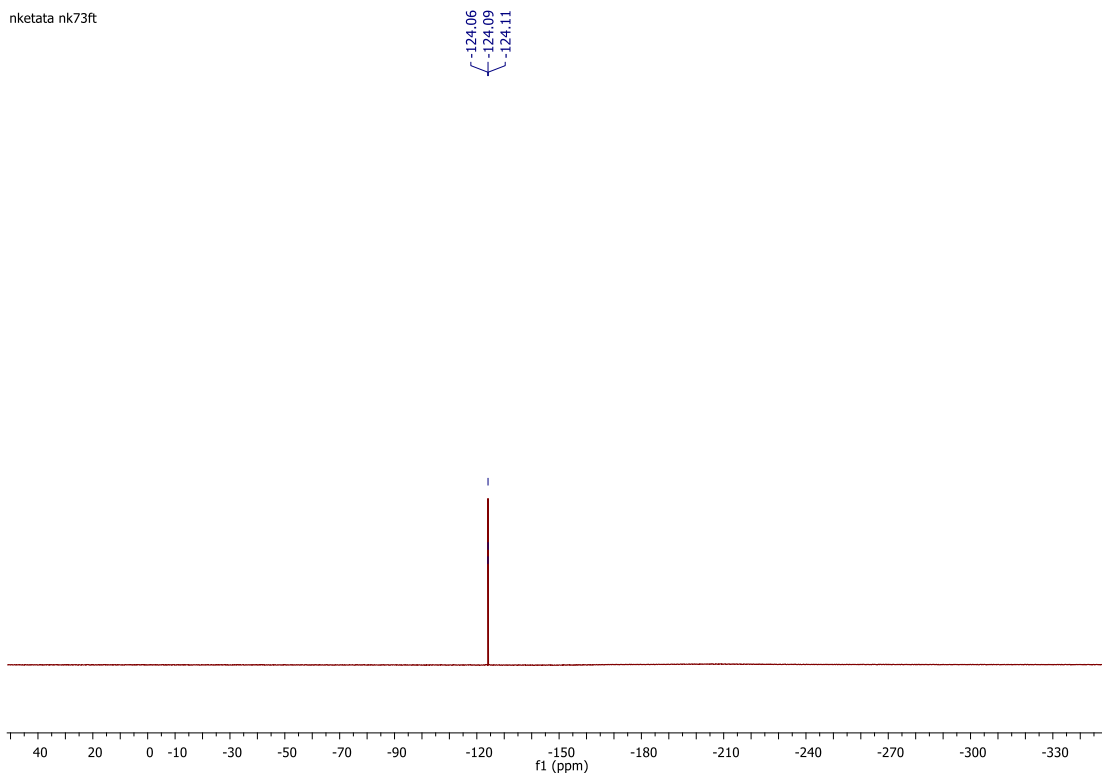
^1H NMR (400 MHz, CDCl_3)

nketata nk73ft



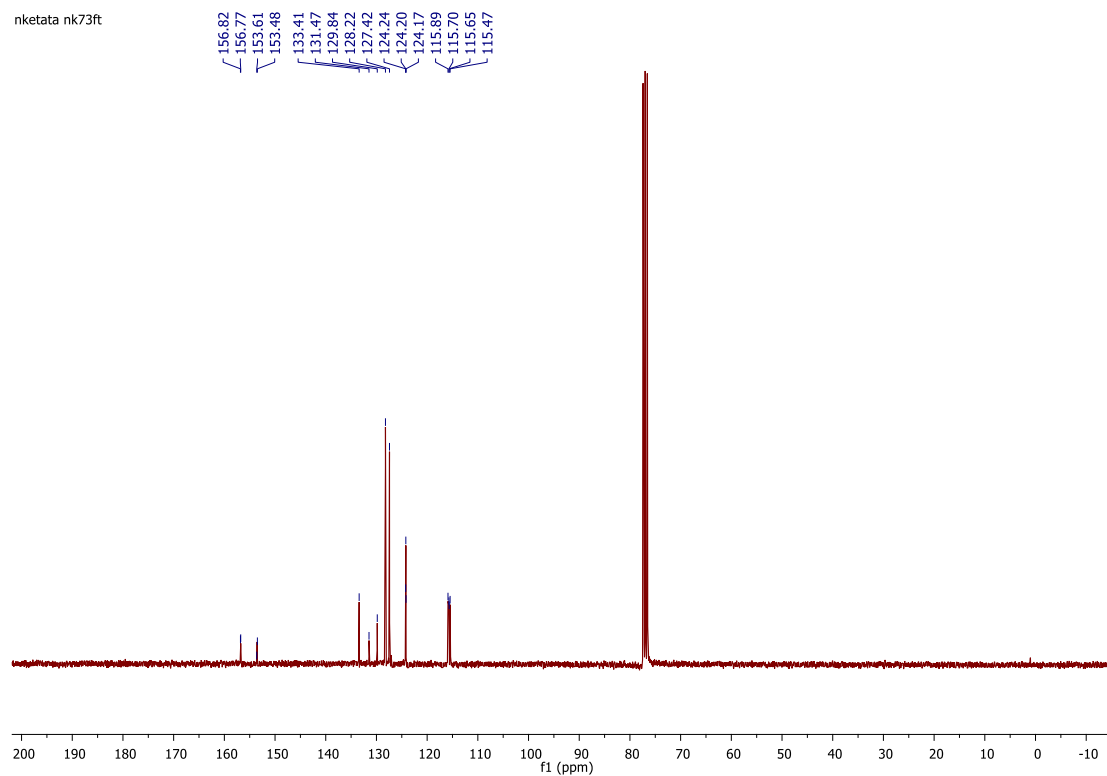
^{19}F NMR (376 MHz, CDCl_3)

nketata nk73ft

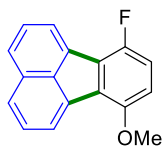


¹³C NMR (100 MHz, CDCl₃)

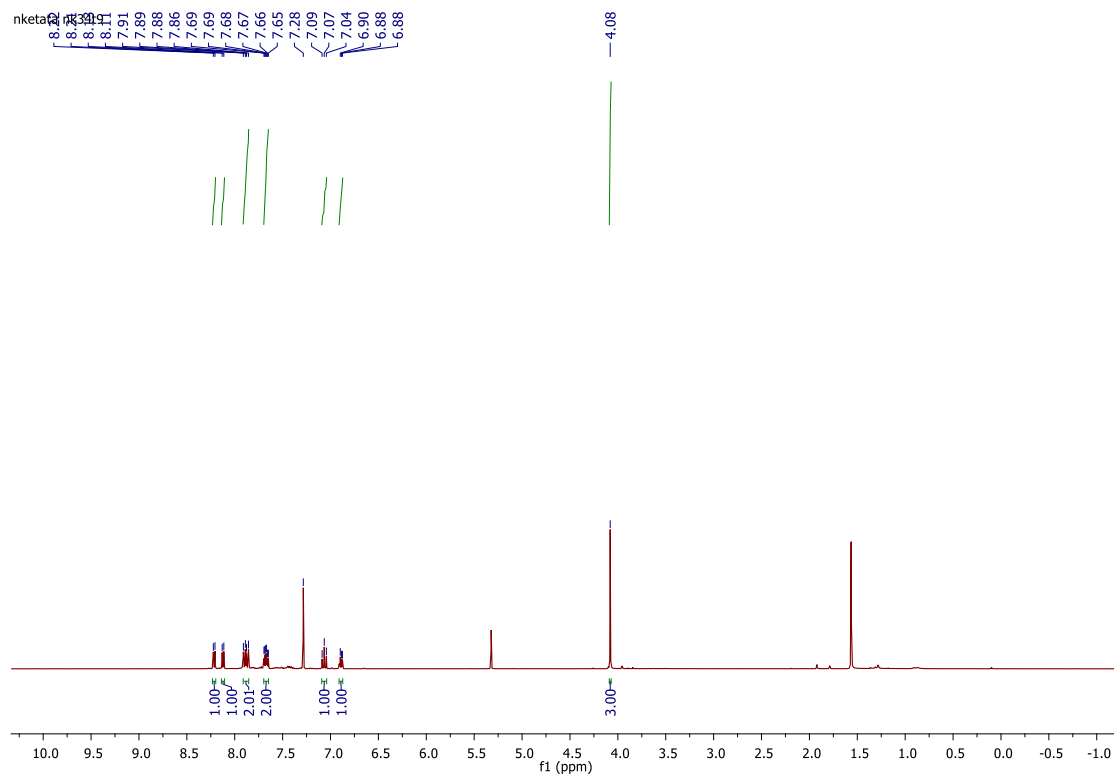
nketata nk73ft



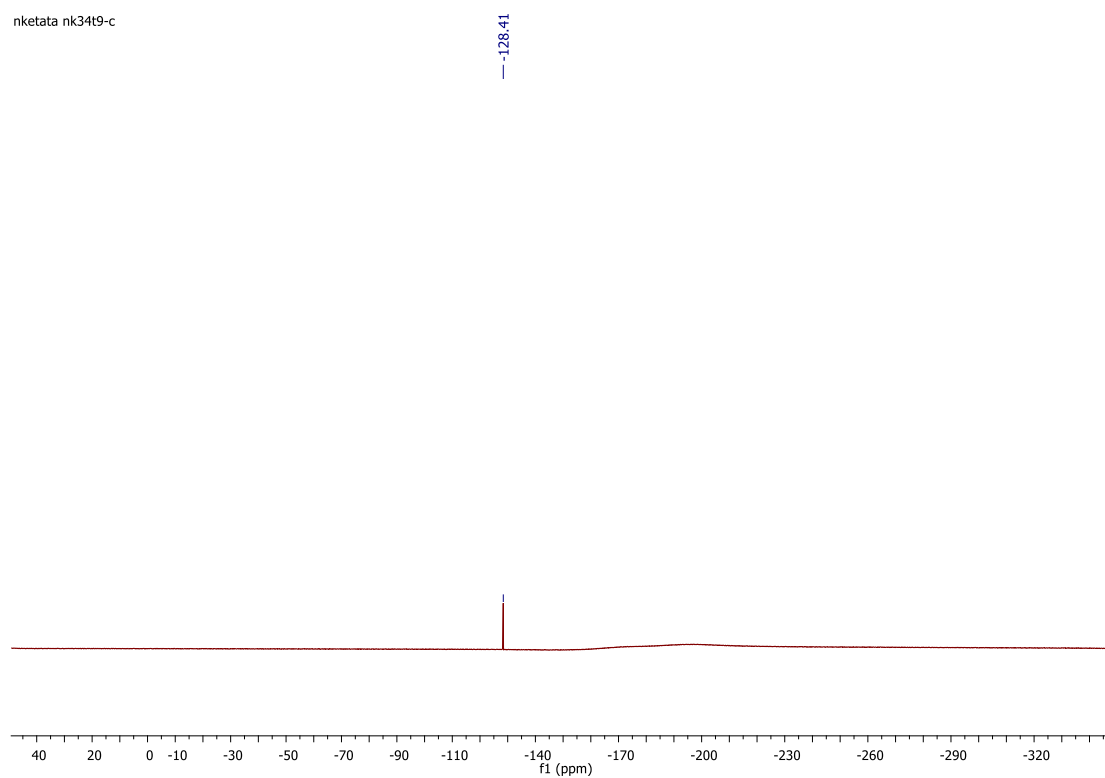
7-Fluoro-10-methoxyfluoranthene (3)



¹H NMR (400MHz, CDCl₃)

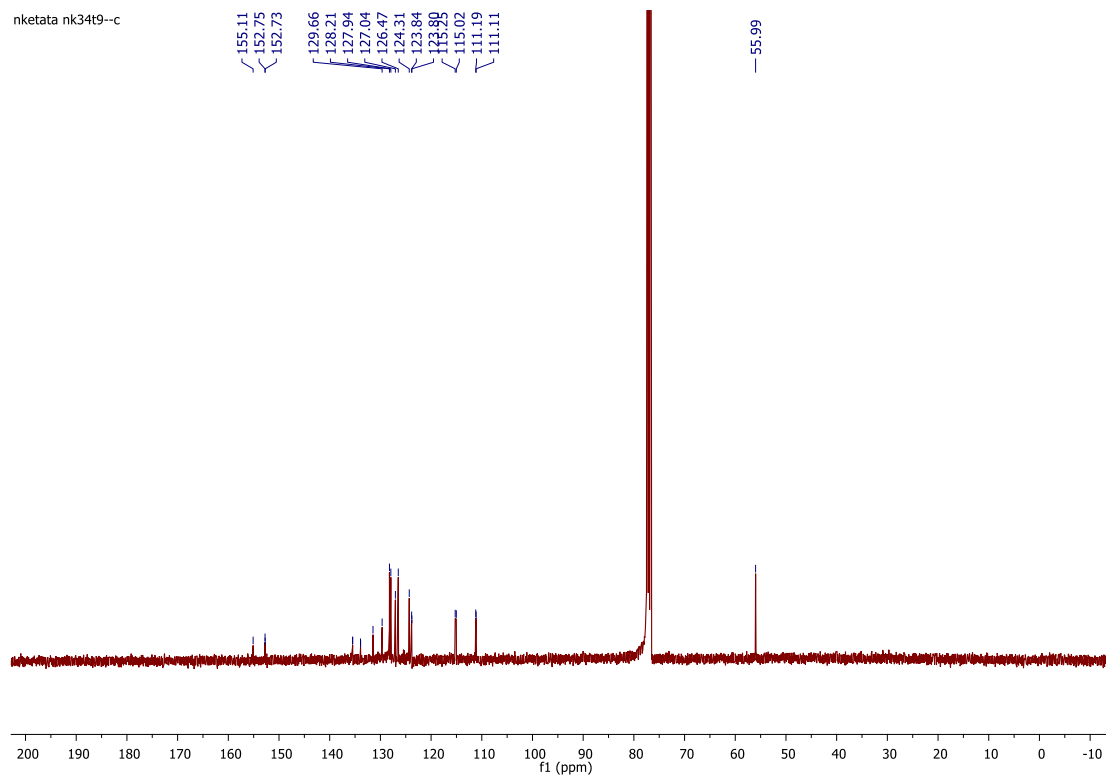


¹⁹F NMR (376 MHz, CDCl₃)

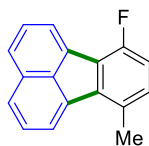


¹³C NMR (100 MHz, CDCl₃)

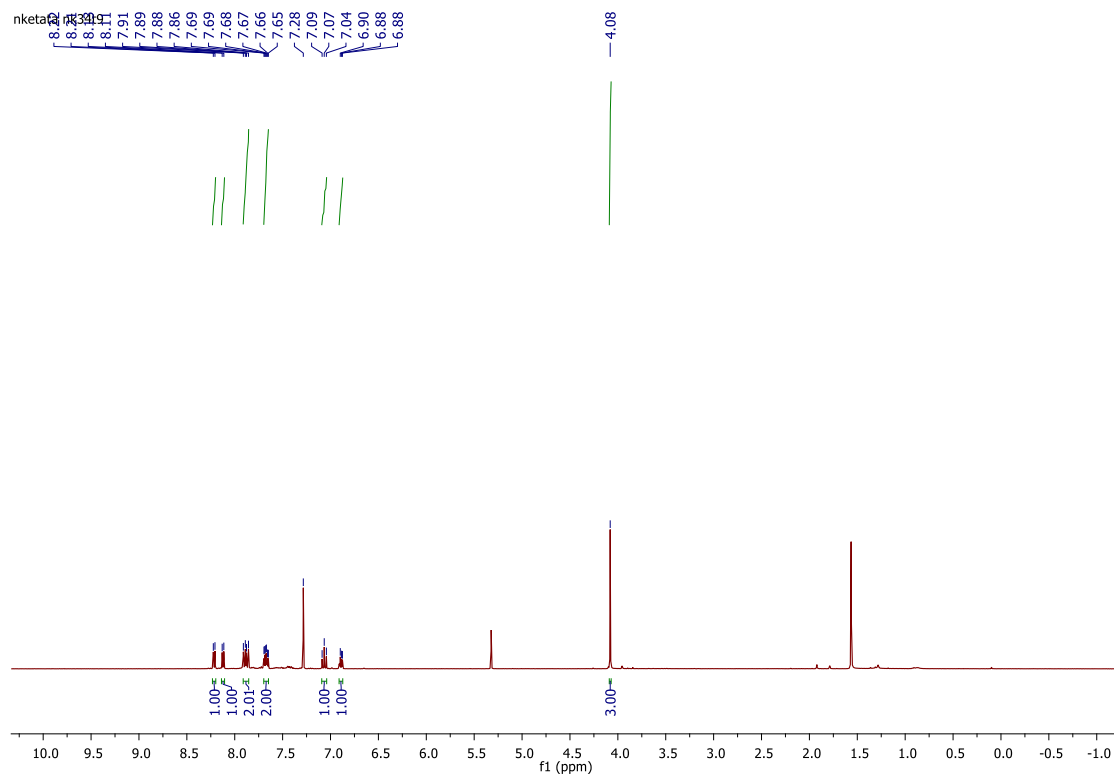
nketata nk34t9--c



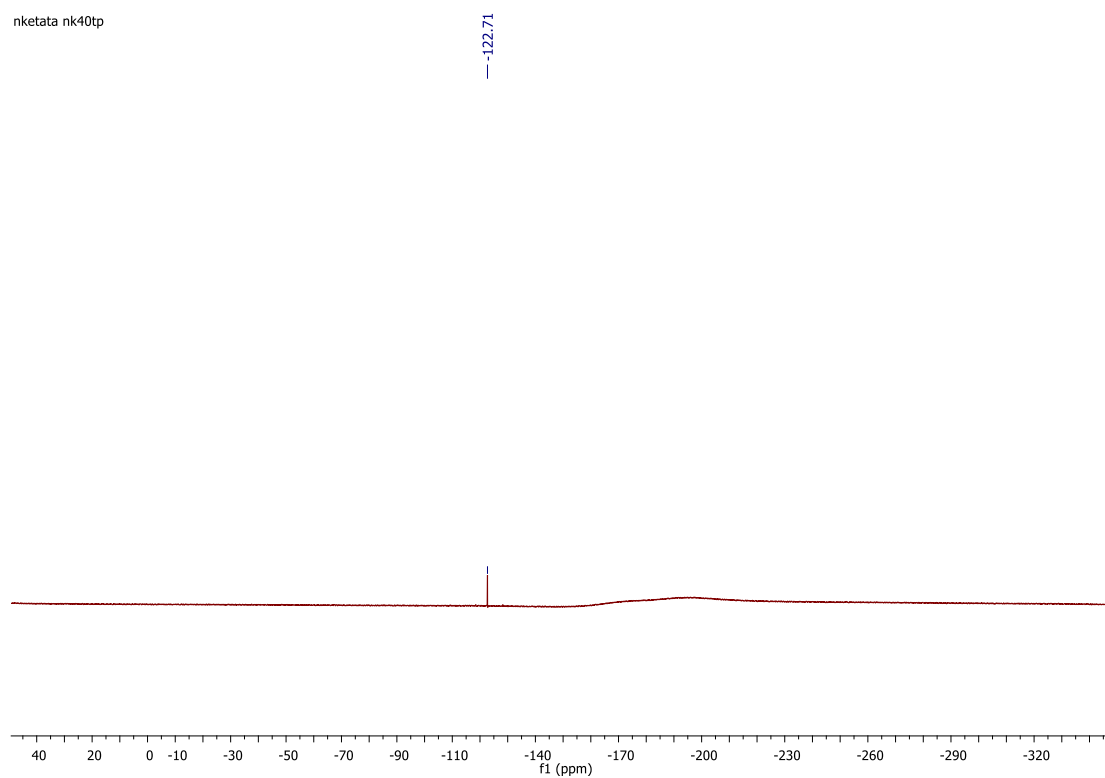
7-Fluoro-10-methylfluoranthene (4)



$^1\text{H NMR}$ (400MHz, CDCl_3)

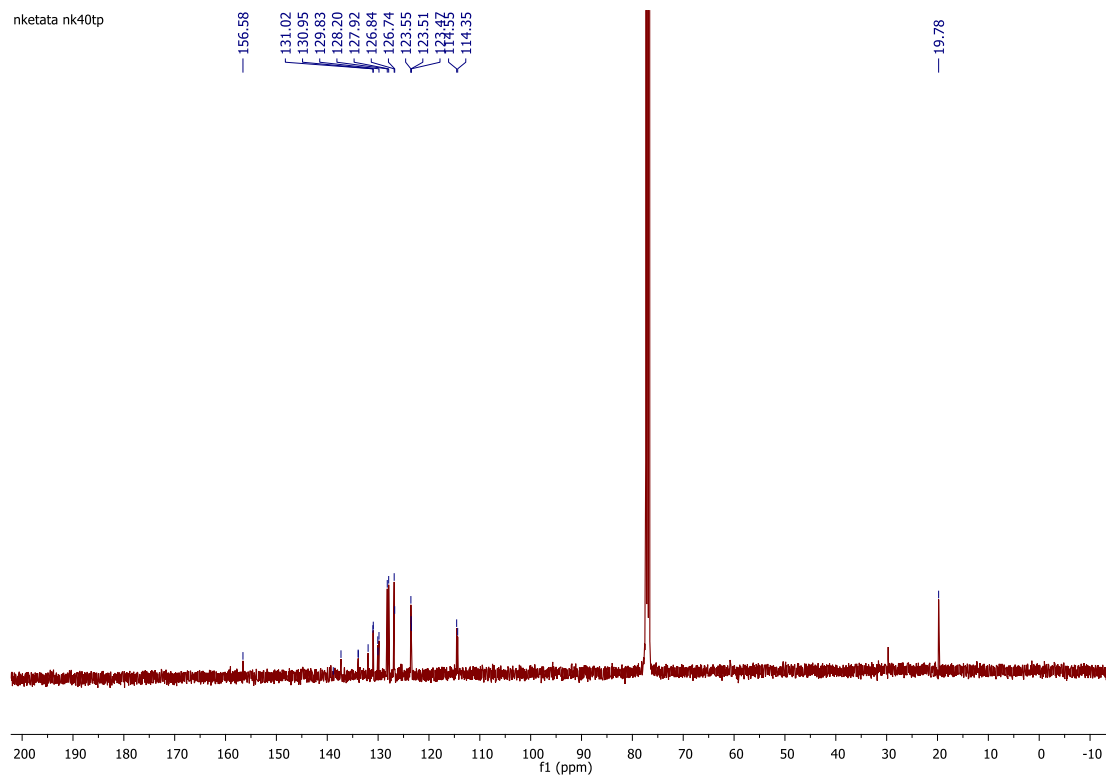


$^{19}\text{F NMR}$ (376 MHz, CDCl_3)

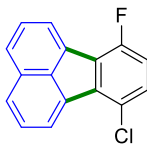


^{13}C NMR (100 MHz, CDCl_3)

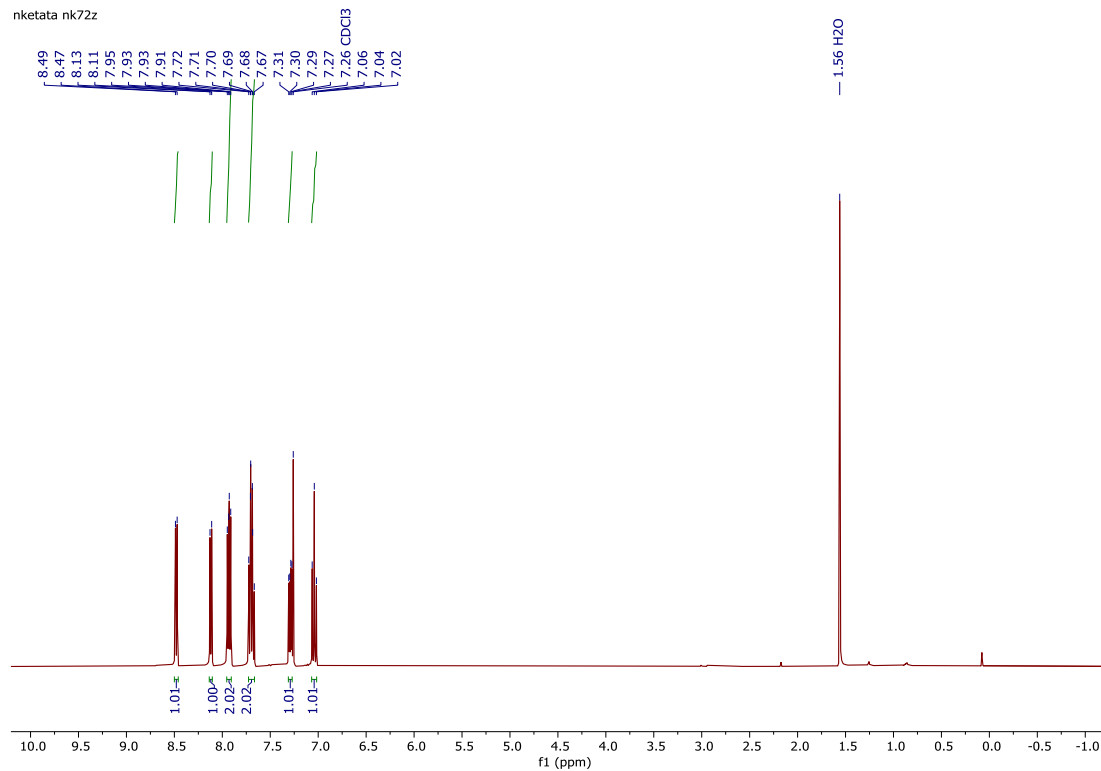
nketata nk40tp



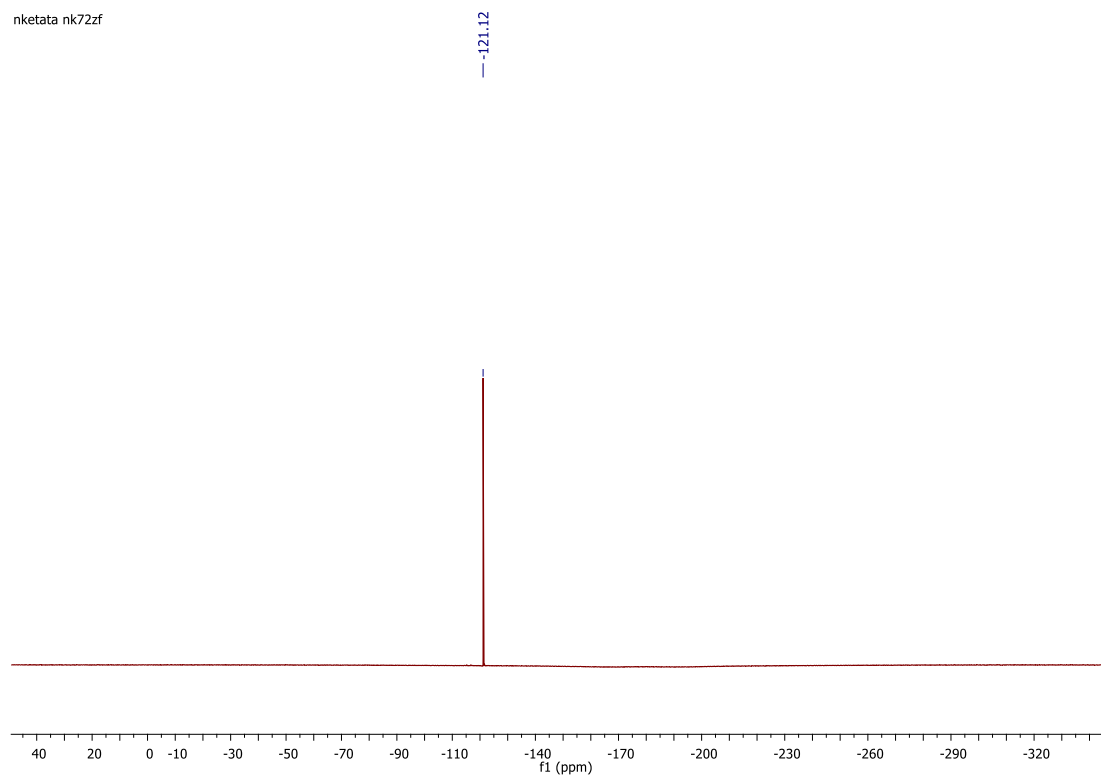
7-Chloro-10-fluorofluoranthene (5)



¹H NMR (400MHz, CDCl₃)

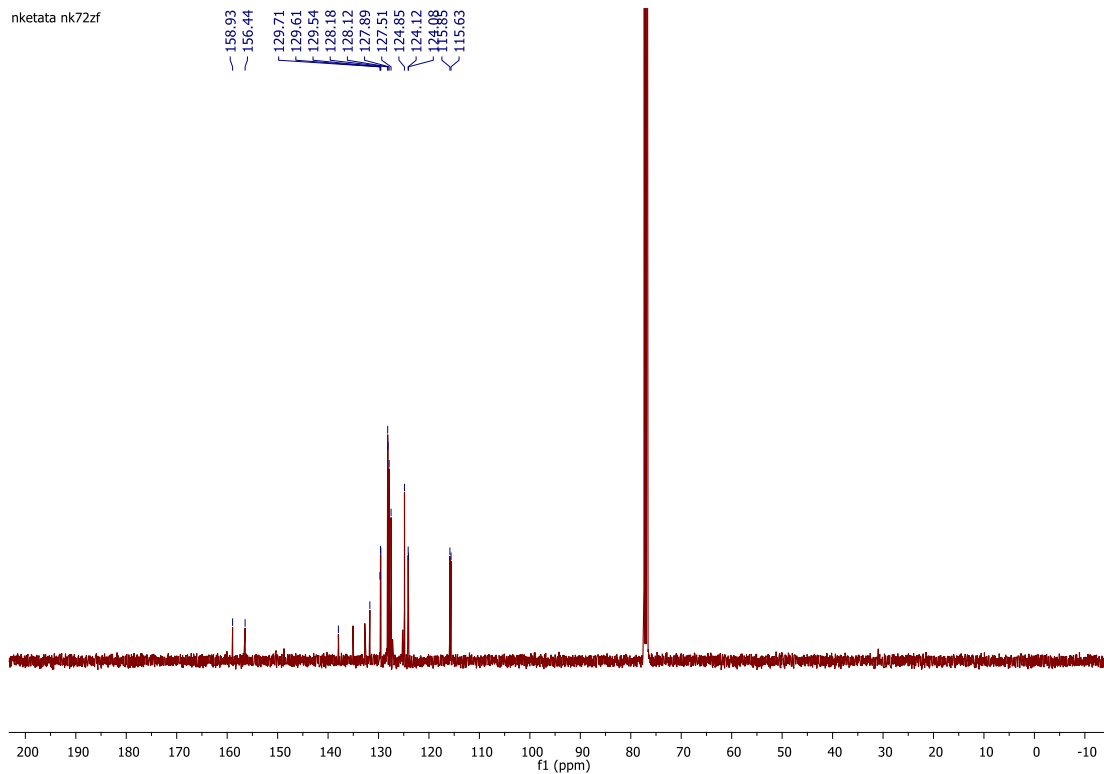


¹⁹F NMR (376 MHz, CDCl₃)

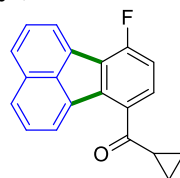


^{13}C NMR (100 MHz, CDCl_3)

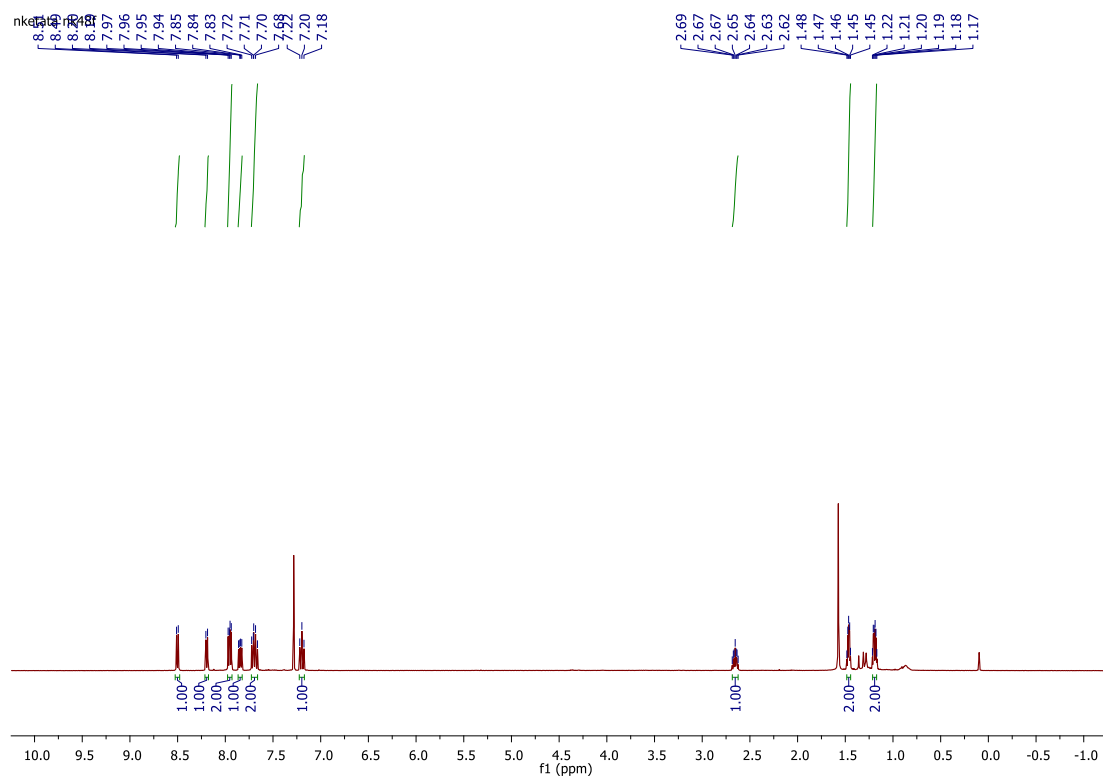
nketata nk72zf



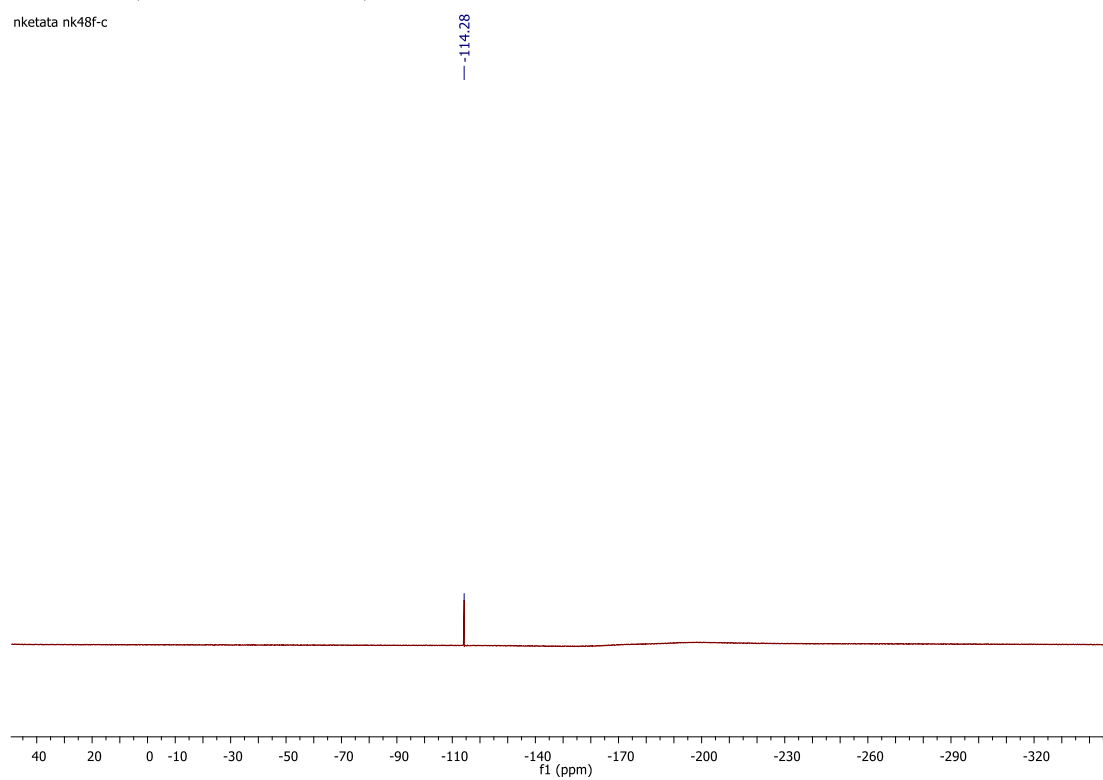
Cyclopropyl(10-fluorofluoranthren-7-yl)methanone (6)



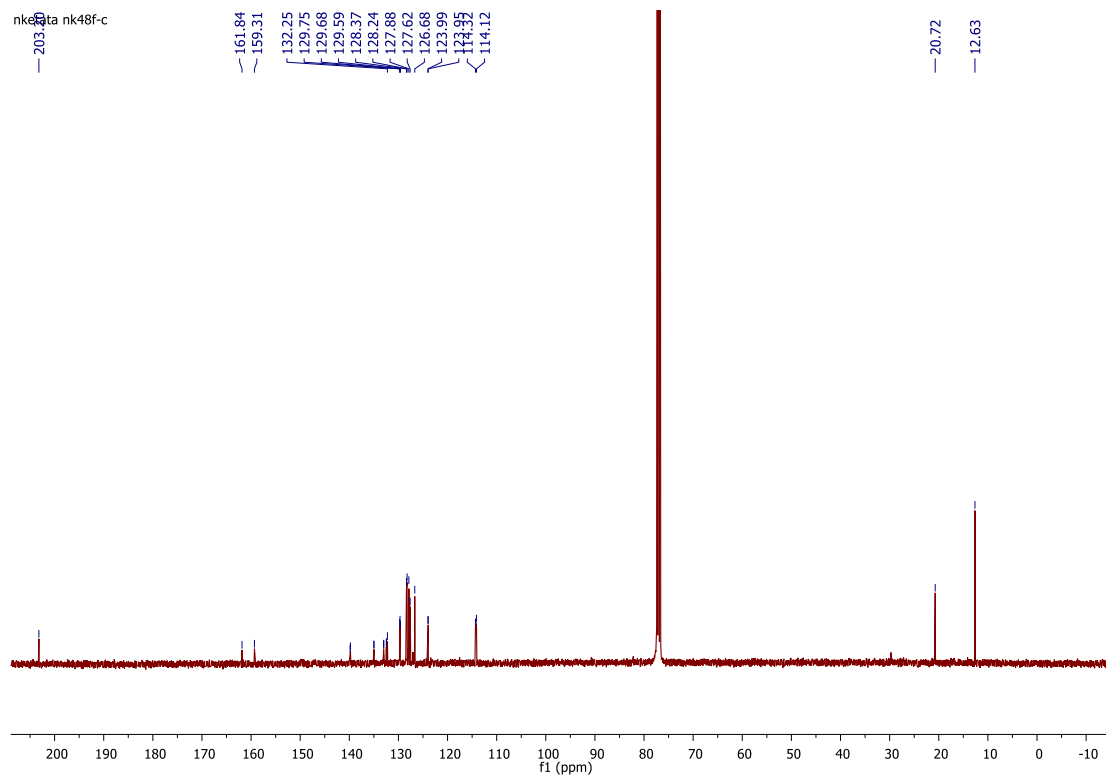
$^1\text{H NMR}$ (400MHz, CDCl_3)



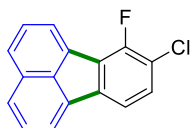
$^{19}\text{F NMR}$ (376 MHz, CDCl_3)



¹³C NMR (100 MHz, CDCl₃)

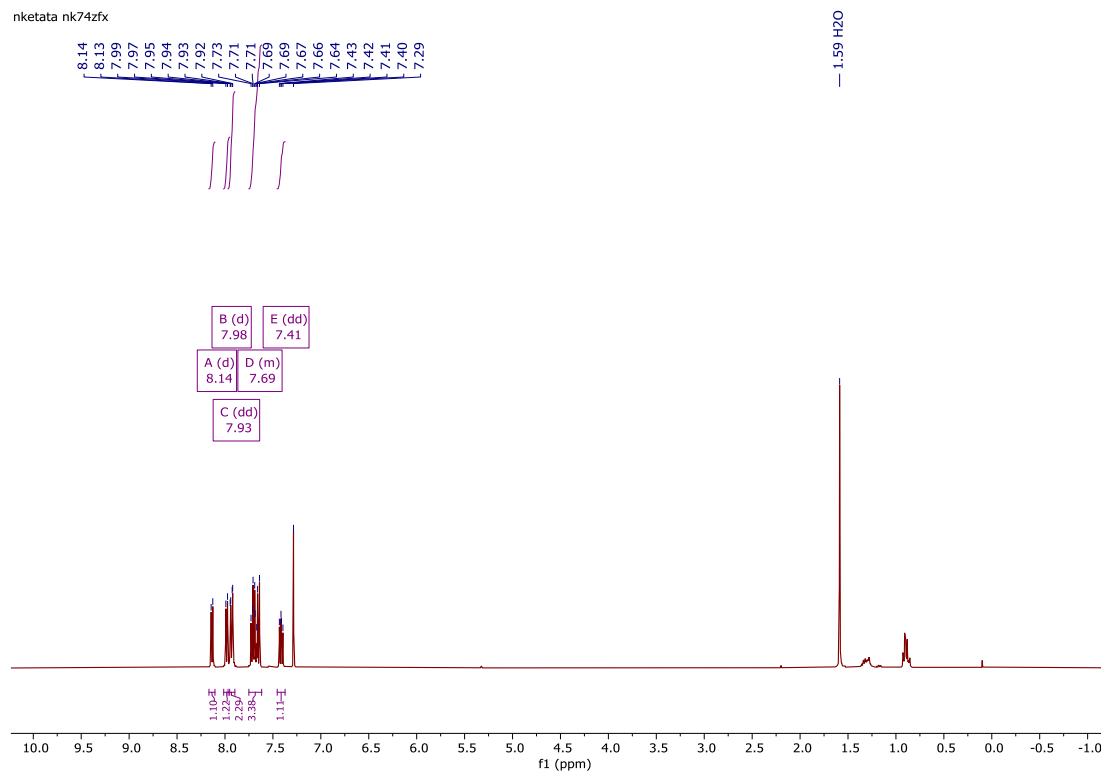


8-Chloro-7-fluorofluoranthene (7)



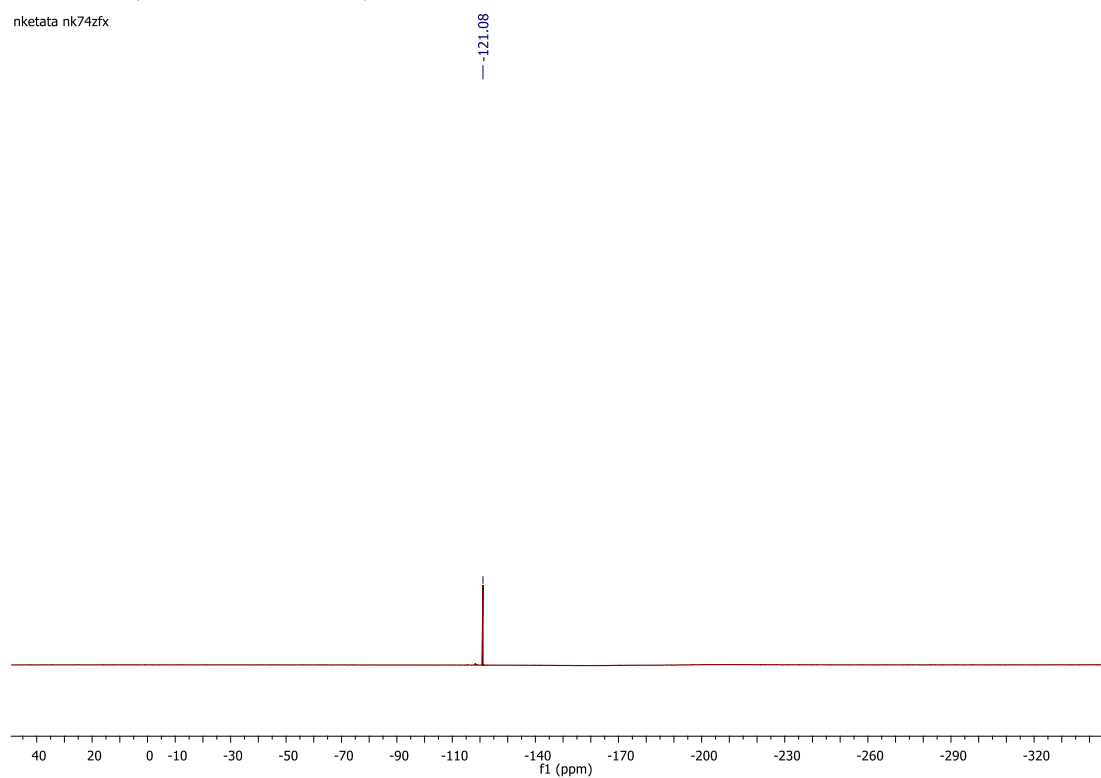
^1H NMR (400MHz, CDCl_3)

nketata nk74zfx



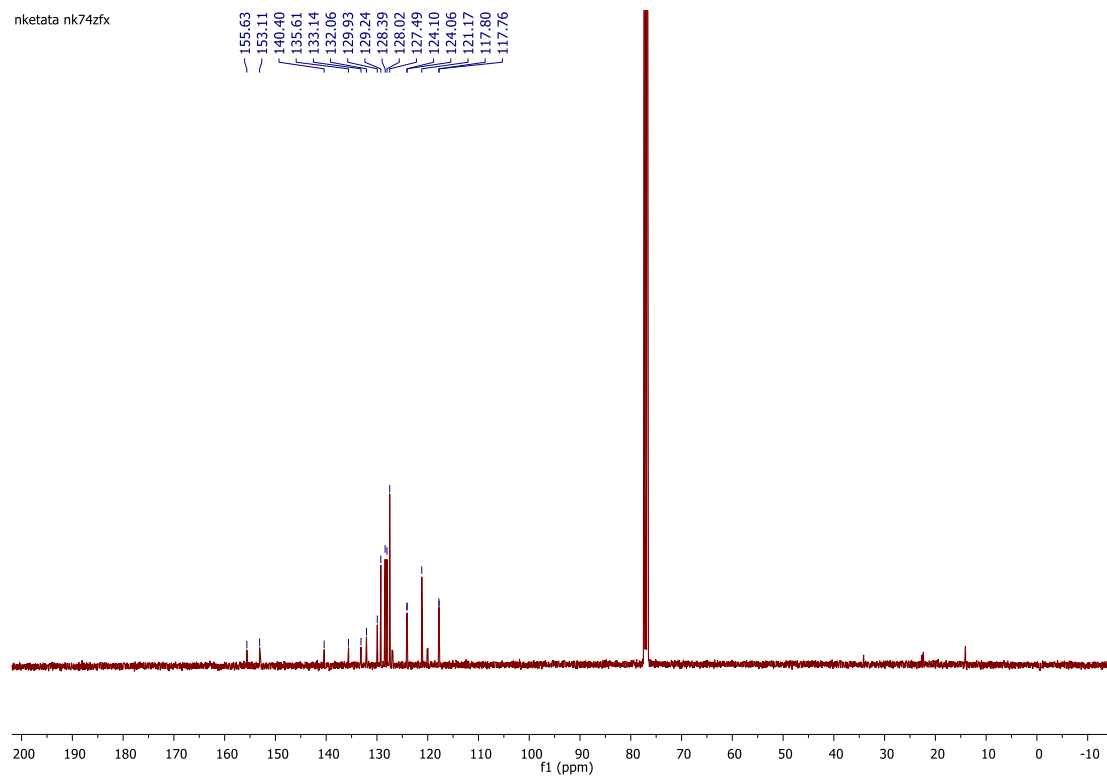
^{19}F NMR (376 MHz, CDCl_3)

nketata nk74zfx

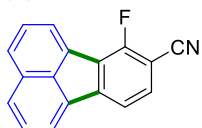


^{13}C NMR (100 MHz, CDCl_3)

nketata nk74zfx

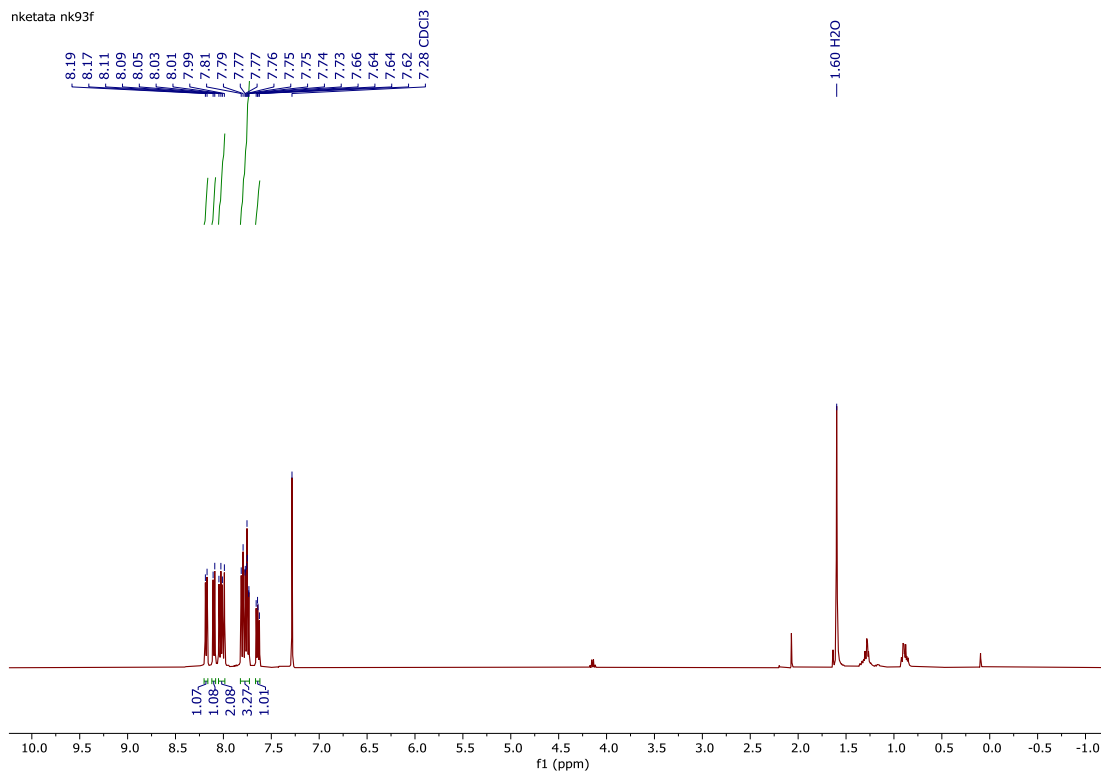


7-Fluorofluoranthene-8-carbonitrile (8)



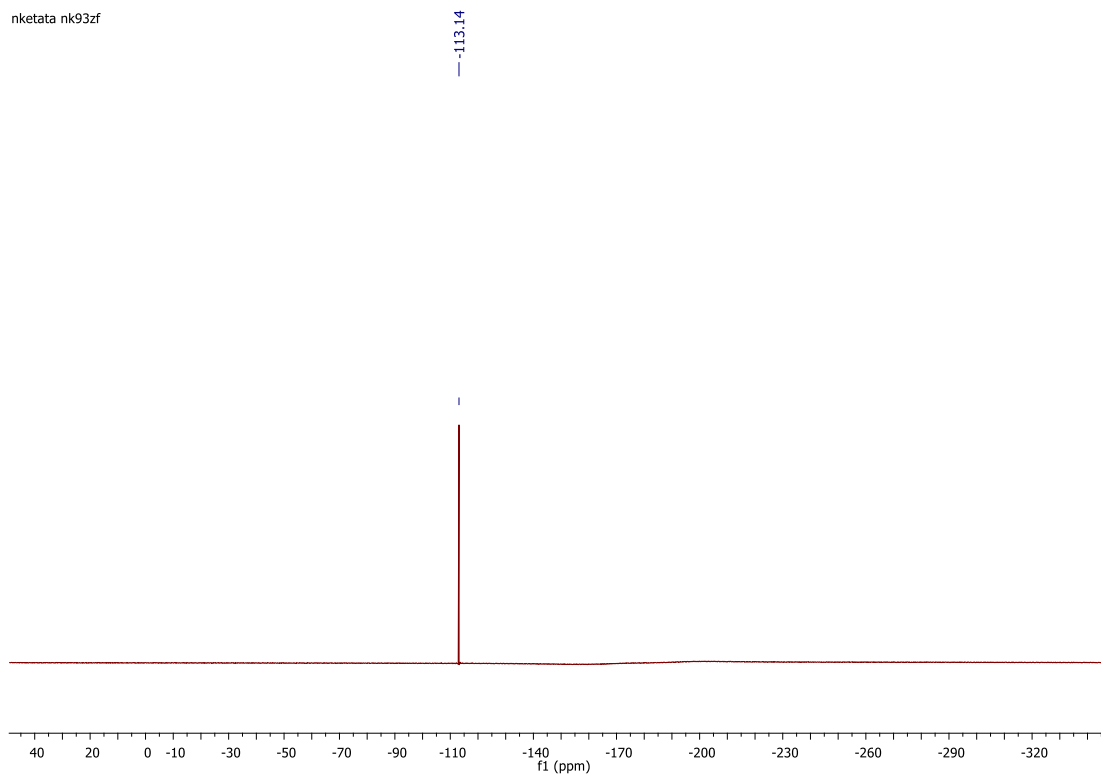
¹H NMR (400MHz, CDCl₃)

nketata nk93f



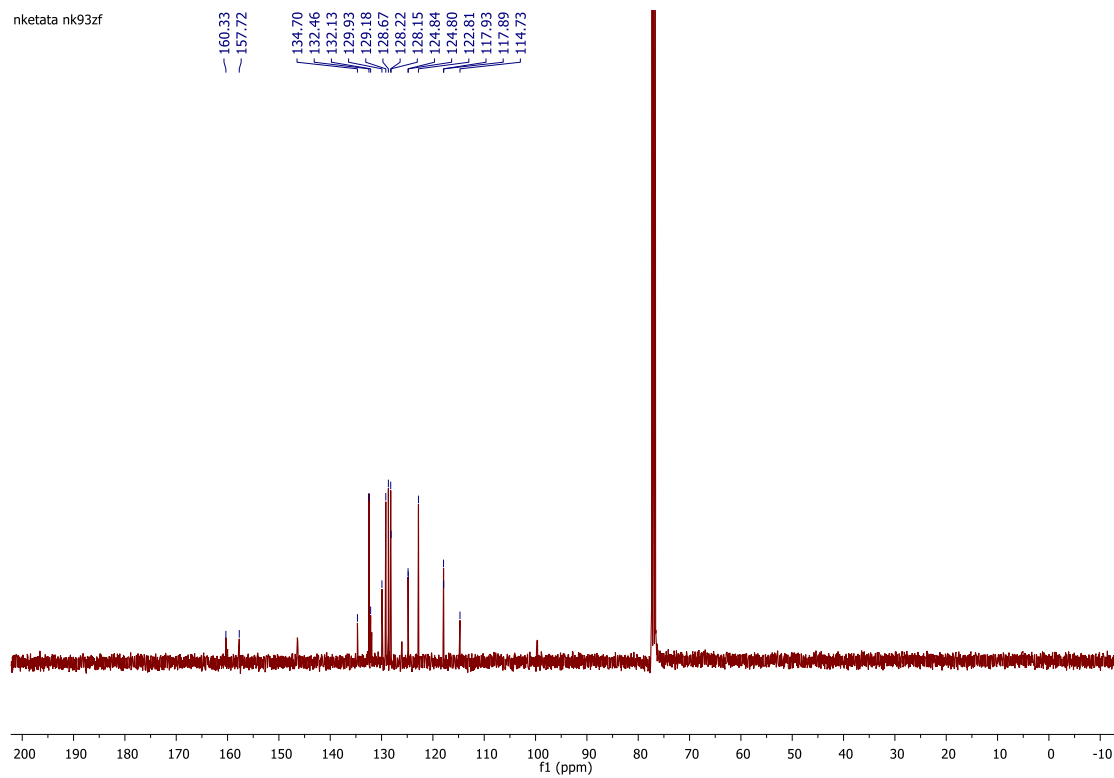
¹⁹F NMR (376 MHz, CDCl₃)

nketata nk93zf

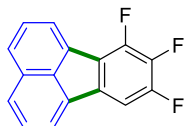


^{13}C NMR (100 MHz, CDCl_3)

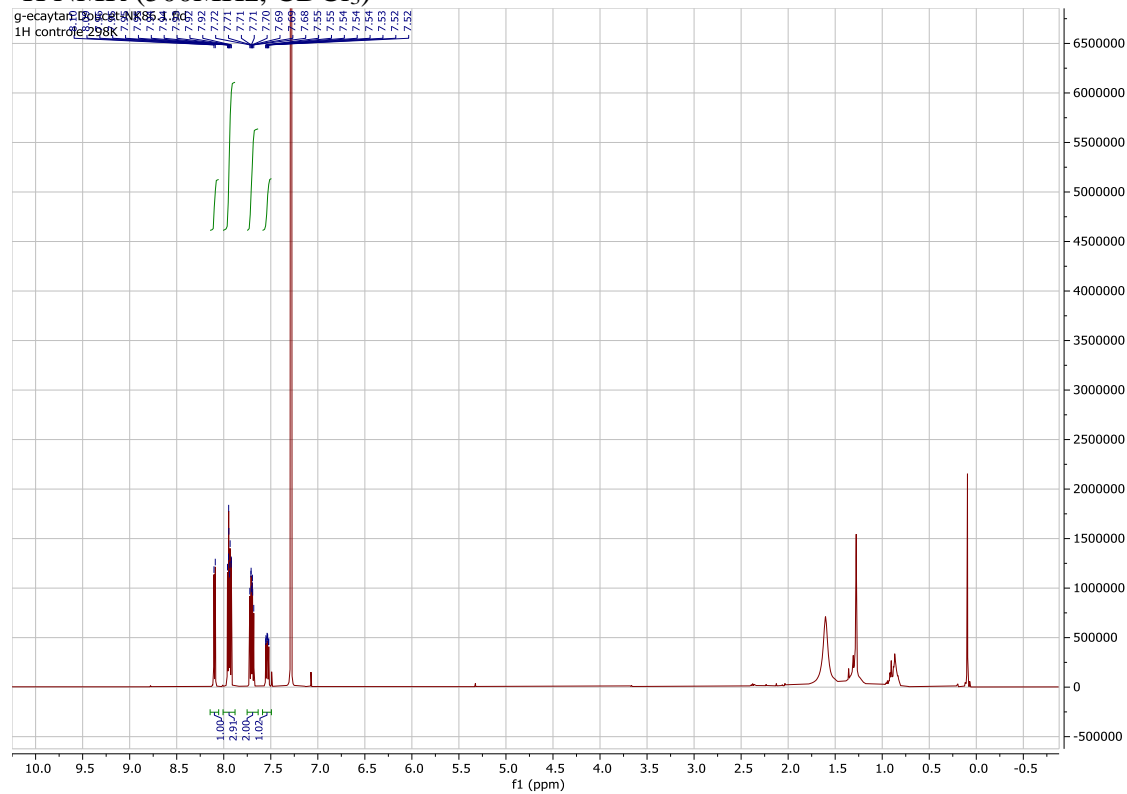
nketata nk93zf



7,8,9-Trifluorofluoranthene (9)



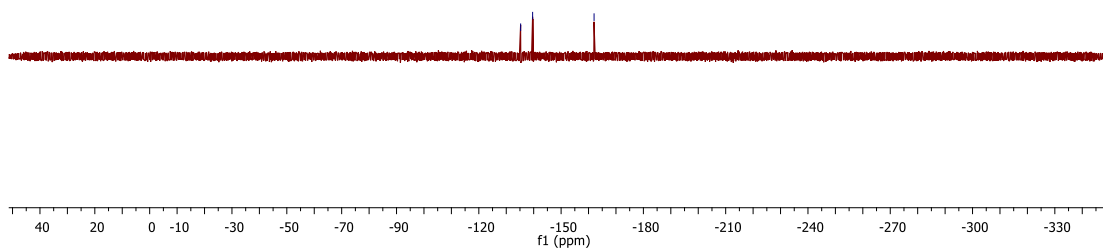
¹H NMR (500MHz, CDCl₃)



¹⁹F NMR (376 MHz, CDCl₃)

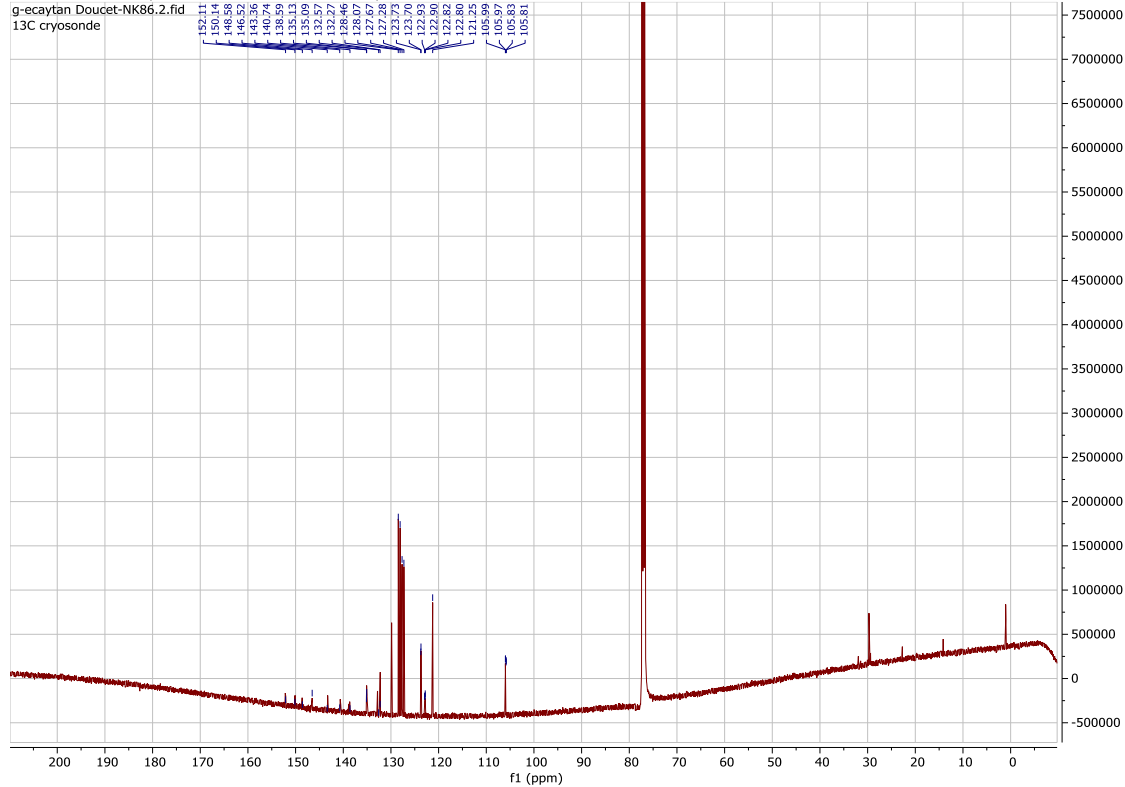
nketata nk86t9f

-135.25
-139.61
-162.02

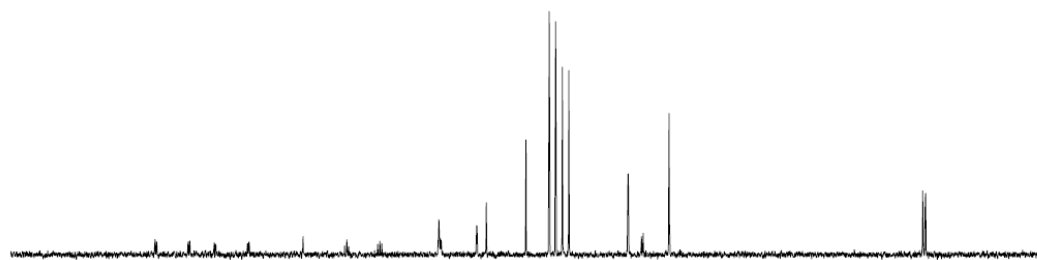


¹³C NMR (125 MHz, CDCl₃)

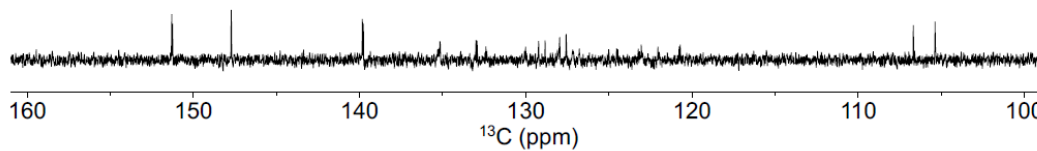
g-ecaytan Doucet-NK86.2.fid
13C cryosonde



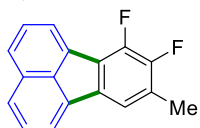
¹³C{¹H}



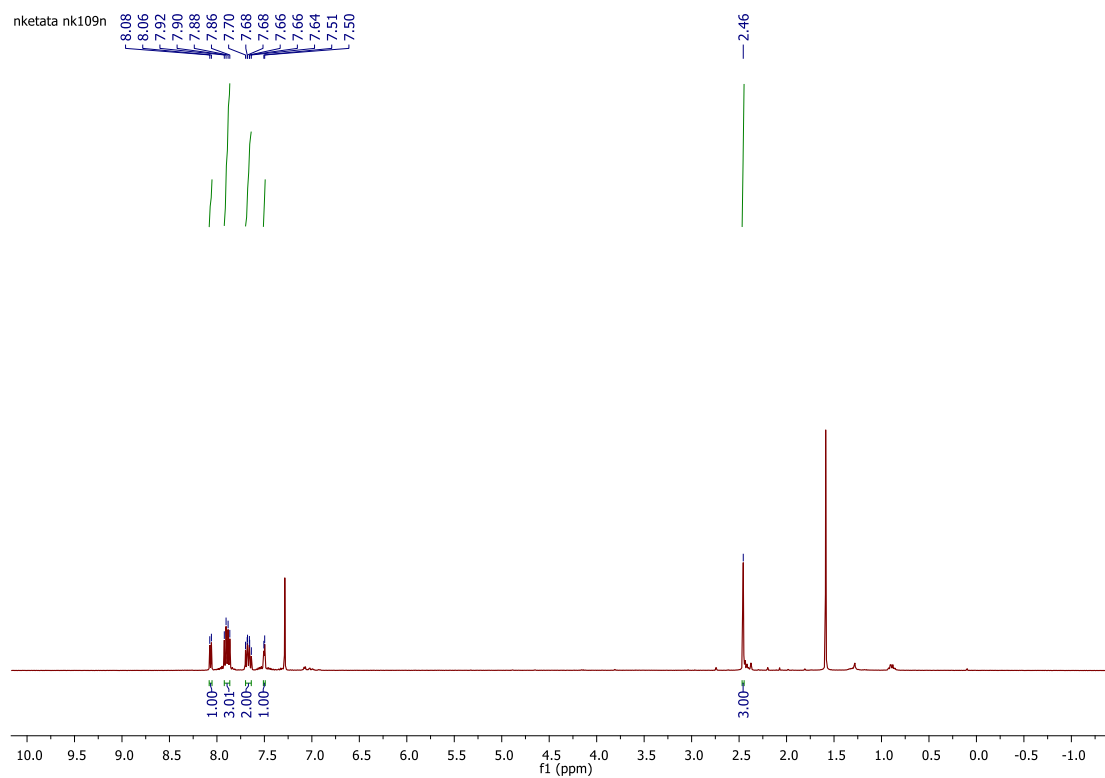
¹³C {¹⁹F}



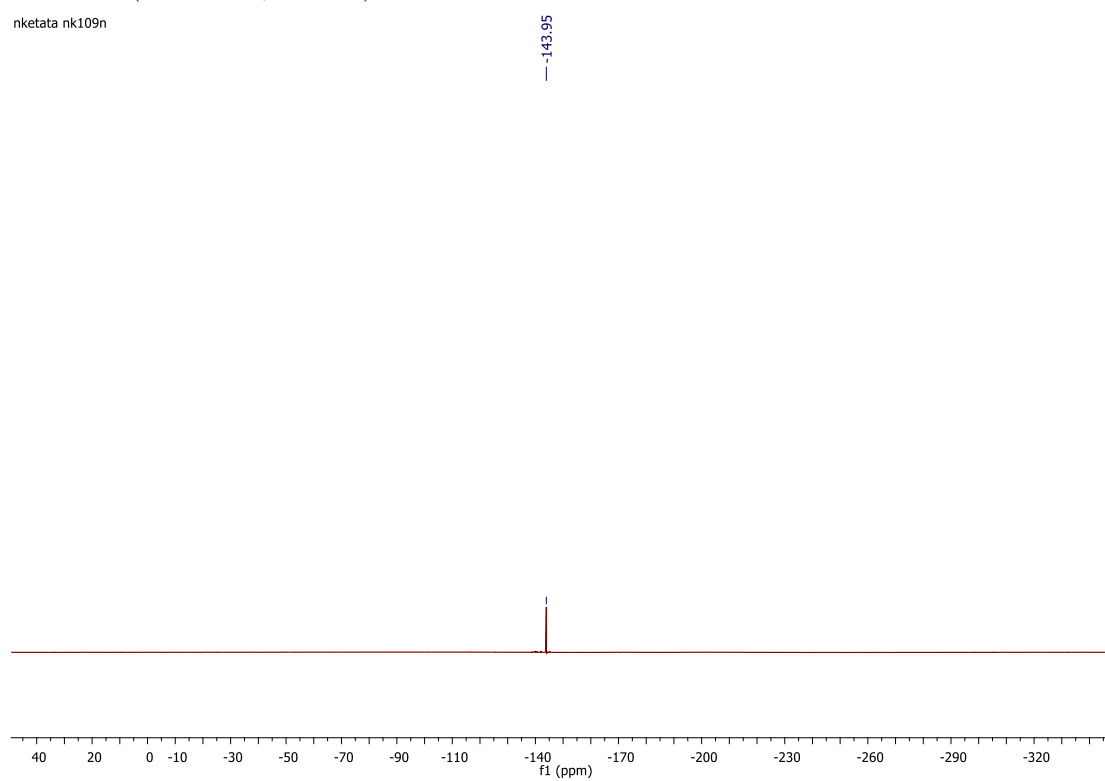
7,8-Difluoro-9-methylfluoranthene (10)



^1H NMR (400MHz, CDCl_3)

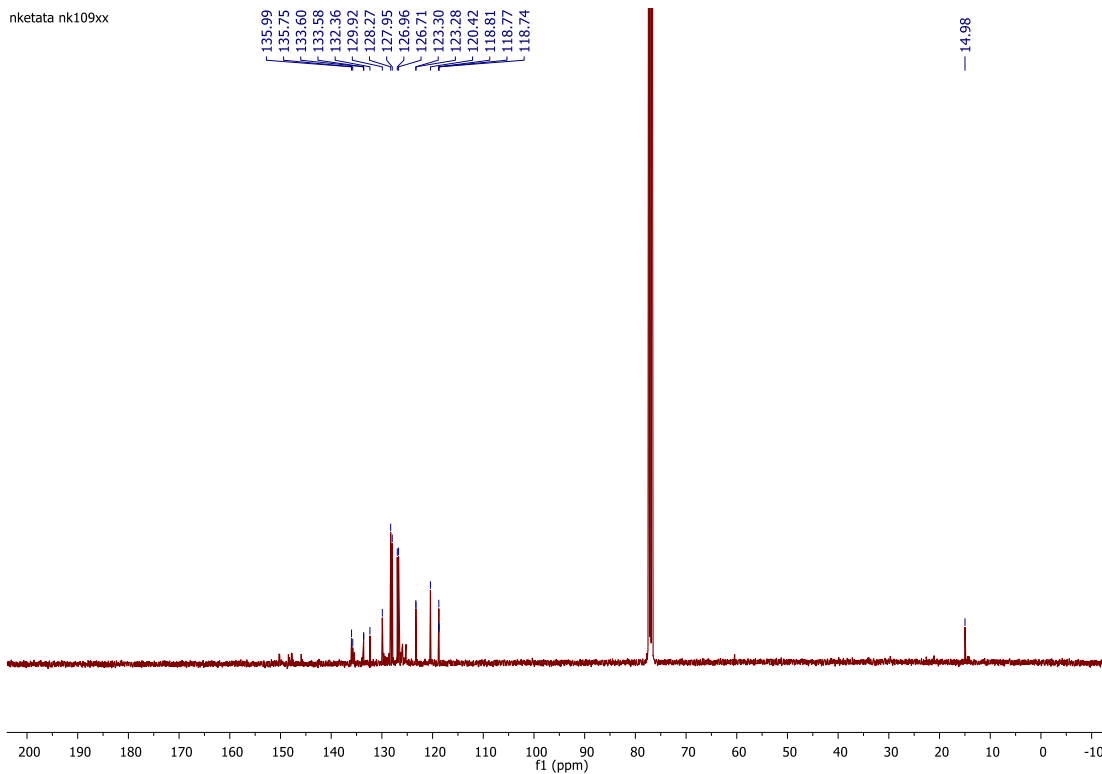


^{19}F NMR (376 MHz, CDCl_3)

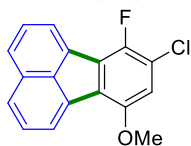


¹³C NMR (100 MHz, CDCl₃)

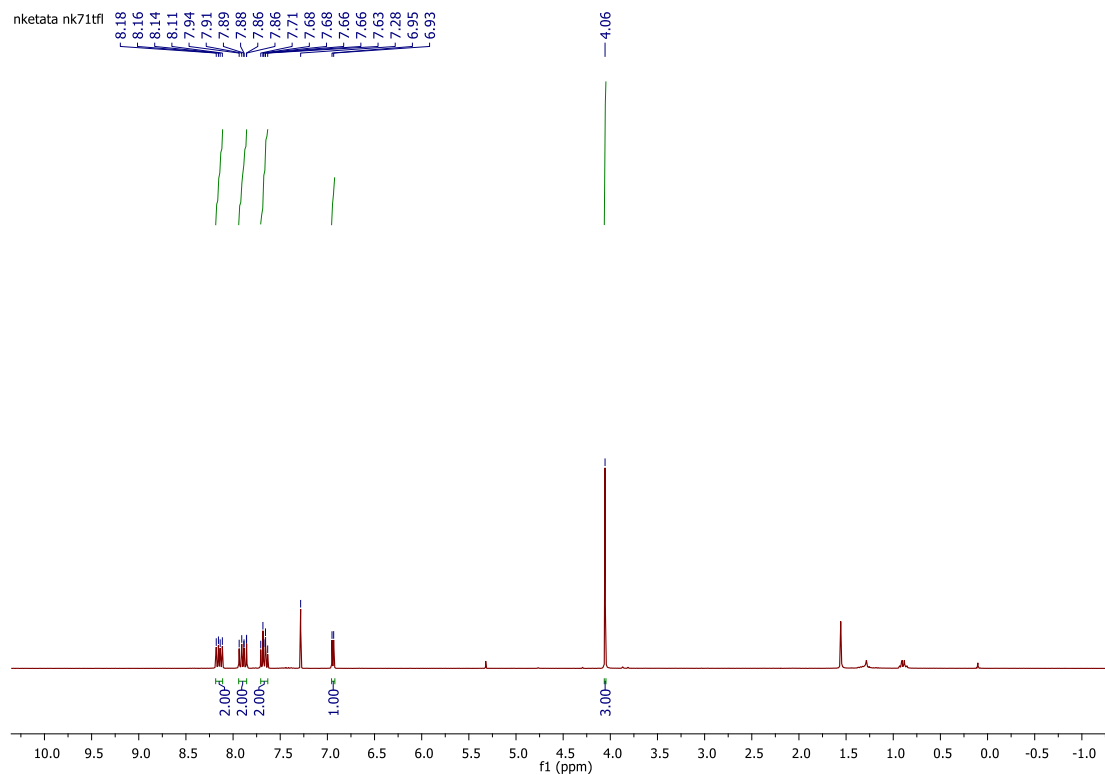
nketata nk109xx



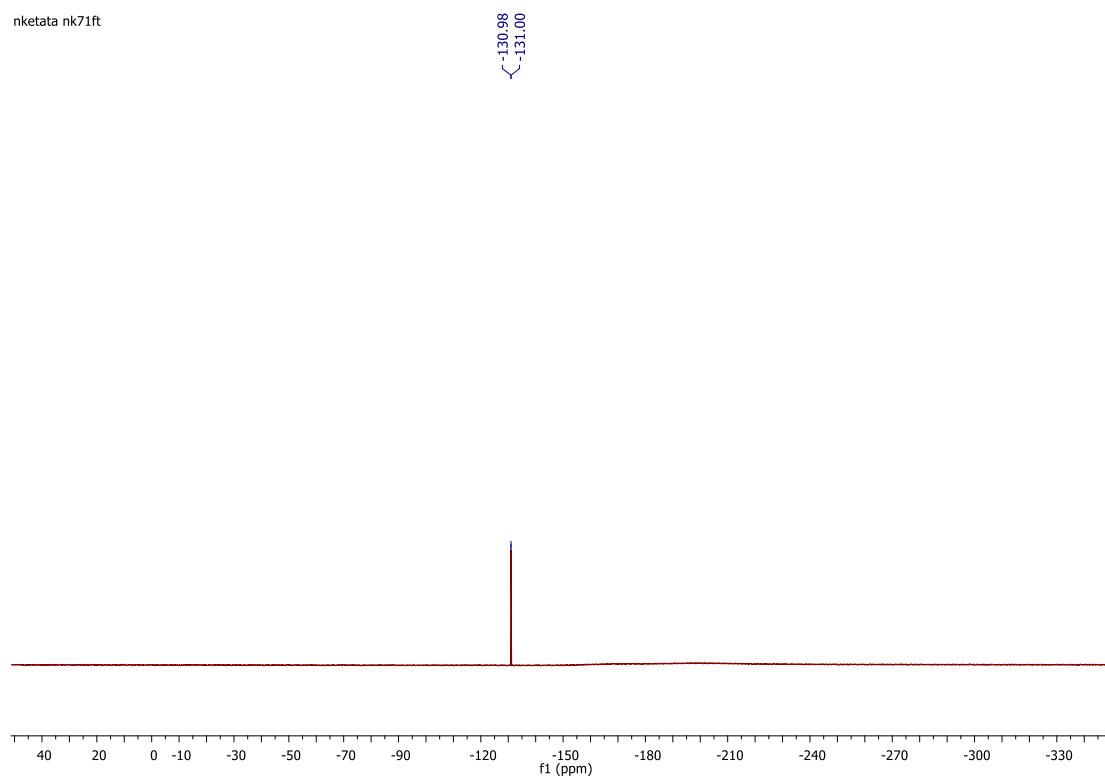
8-Chloro-7-fluoro-10-methoxyfluoranthene (11)



¹H NMR (400MHz, CDCl₃)

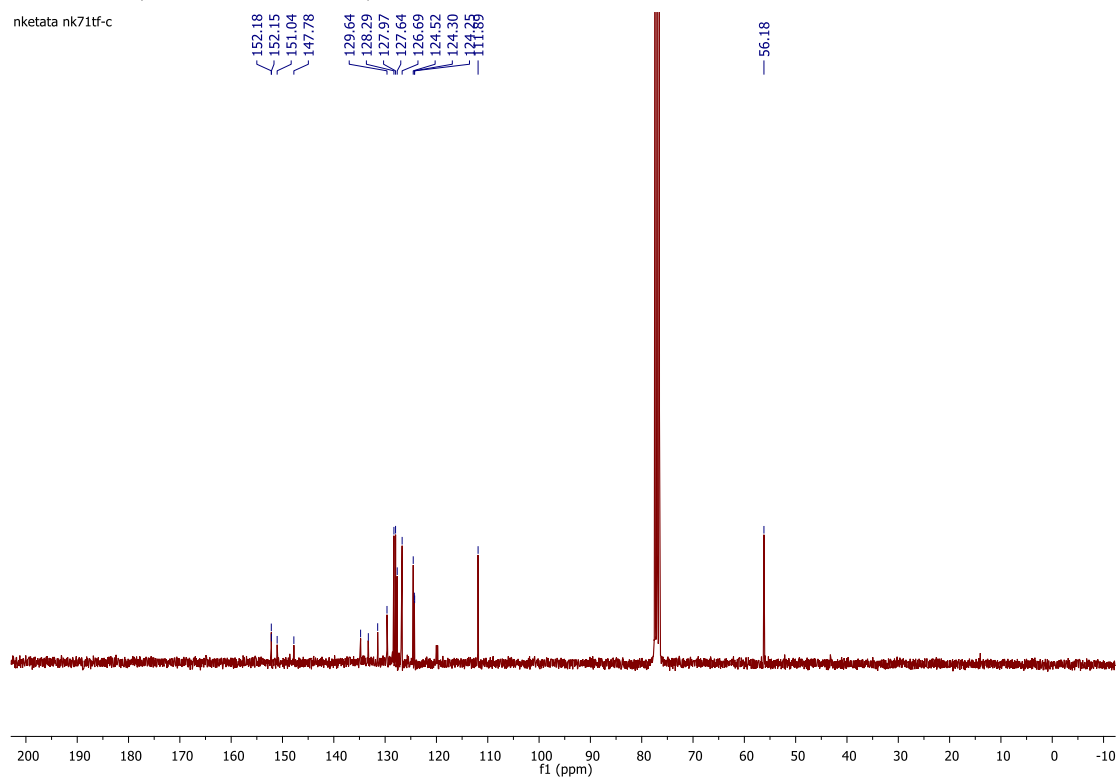


¹⁹F NMR (376 MHz, CDCl₃)

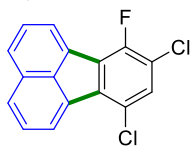


¹³C NMR (100 MHz, CDCl₃)

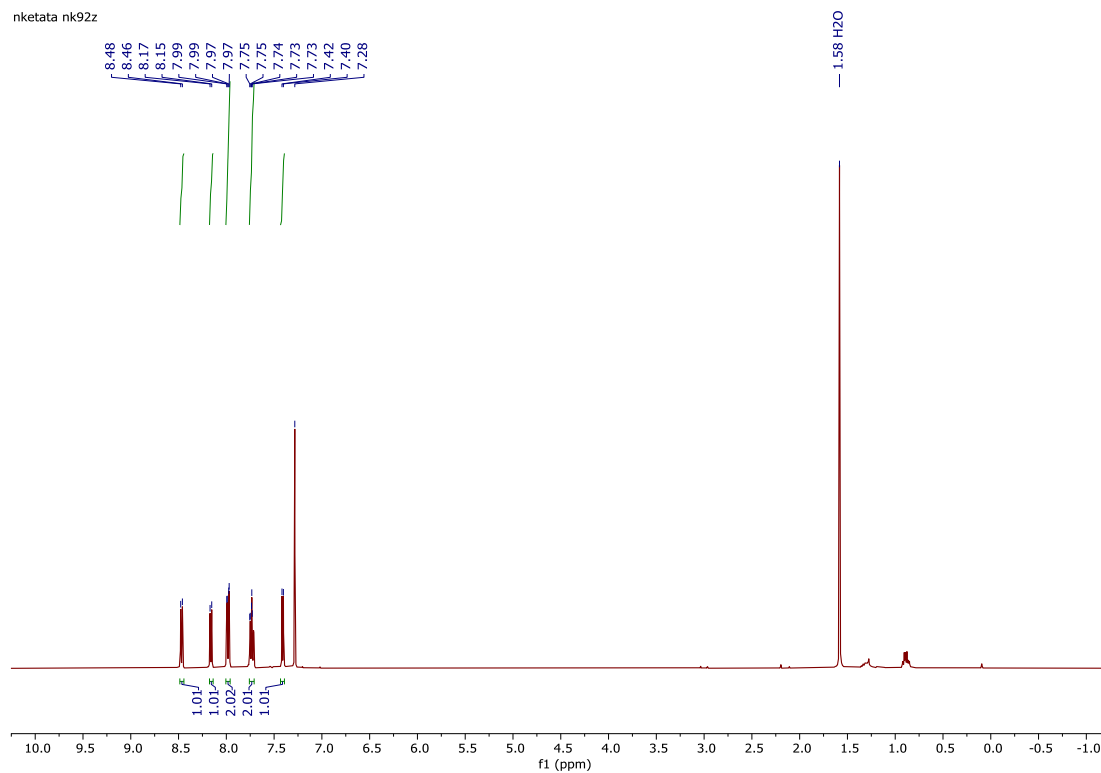
nketata nk71tf-c



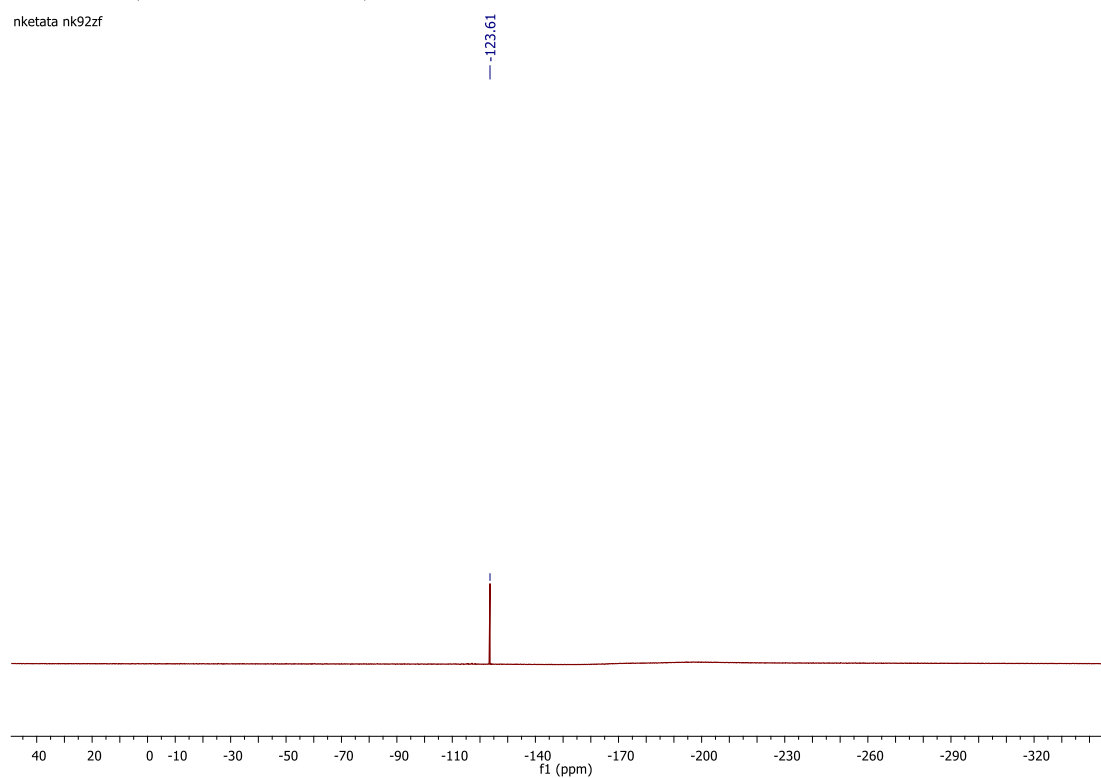
8,10-Dichloro-7-fluorofluoranthene (12)



^1H NMR (400MHz, CDCl_3)

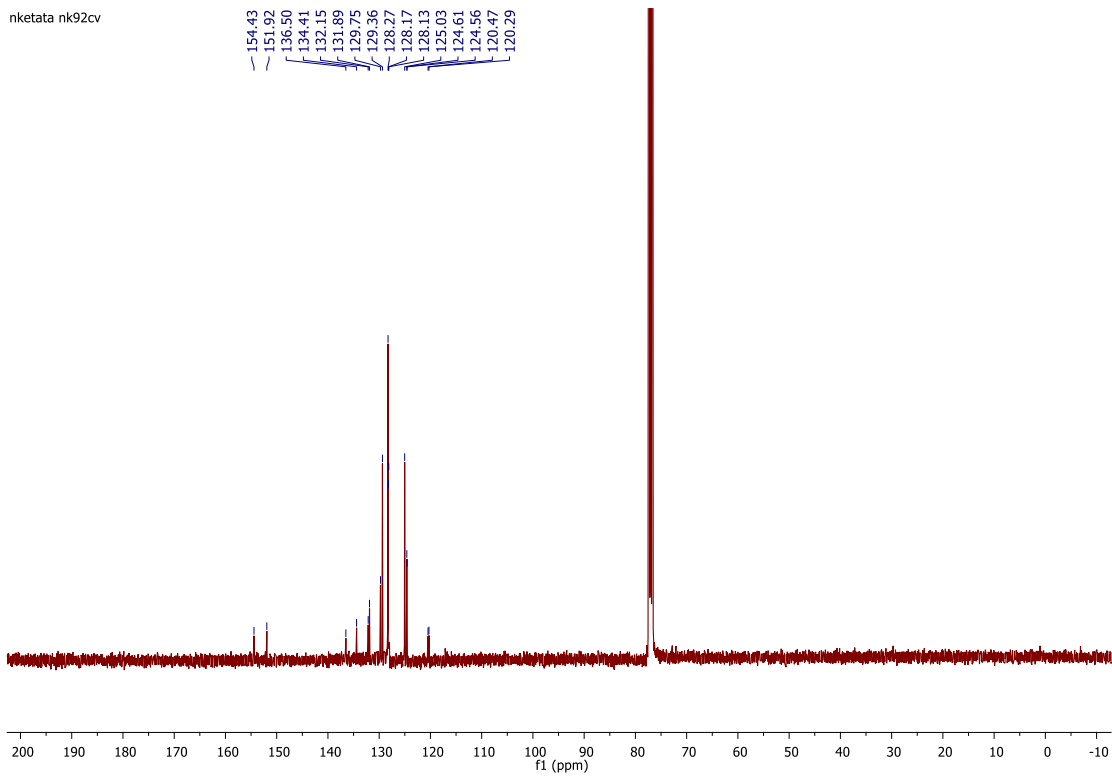


^{19}F NMR (376 MHz, CDCl_3)

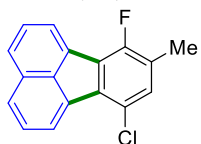


^{13}C NMR (100 MHz, CDCl_3)

nketata nk92cv

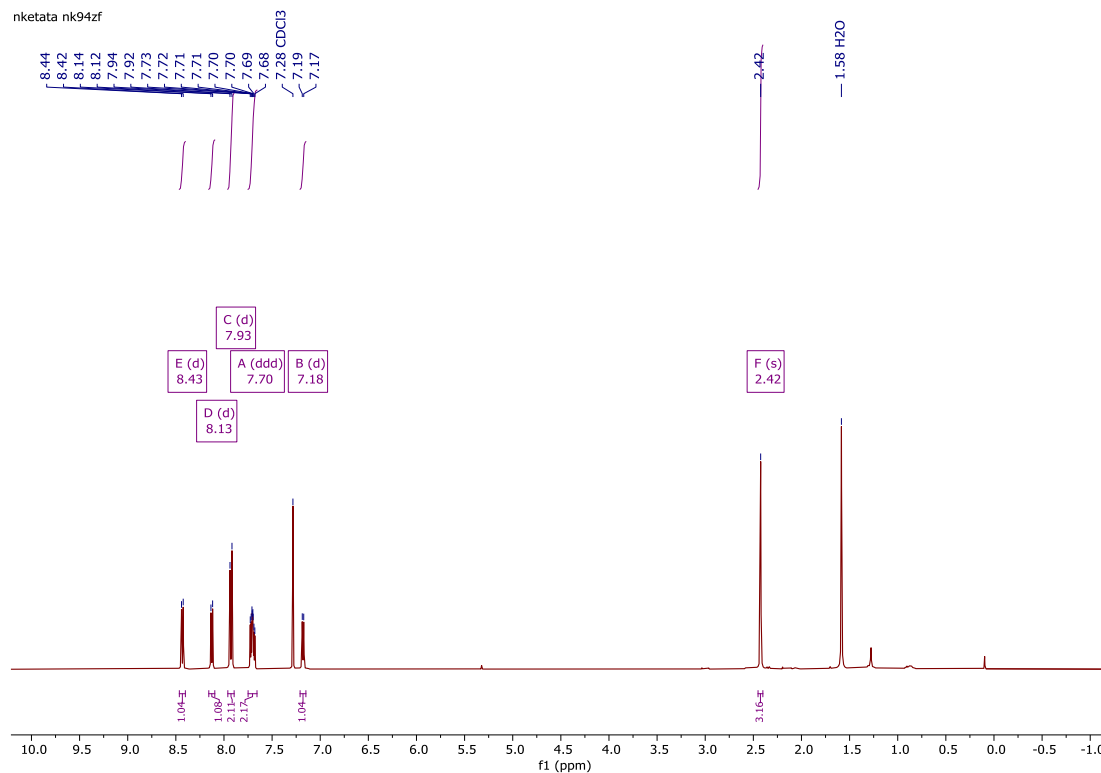


10-Chloro-7-fluoro-8-methylfluoranthene (13)



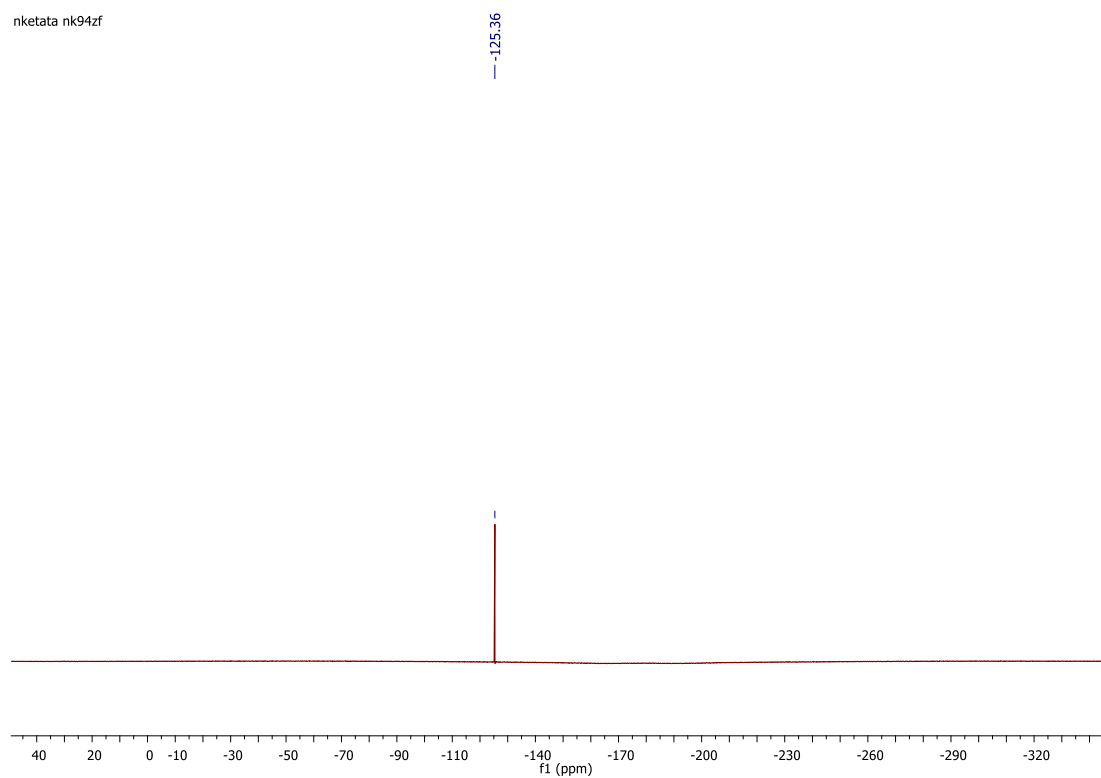
¹H NMR (400MHz, CDCl₃)

nketata nk94zf



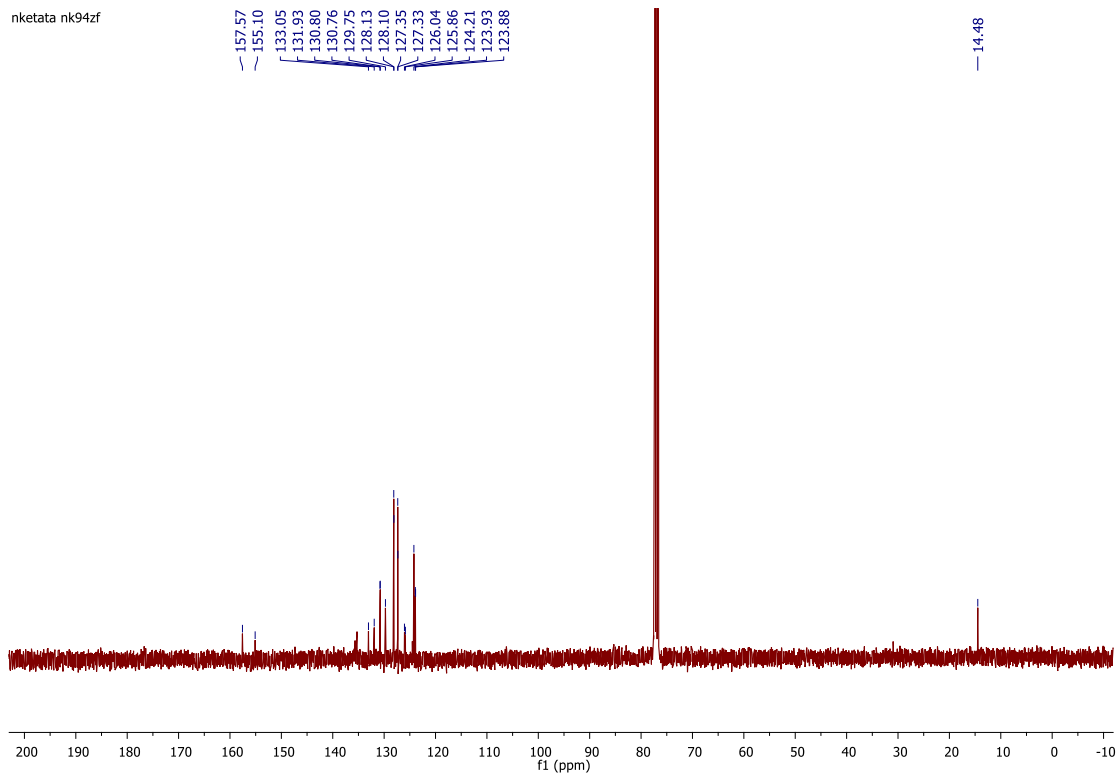
¹⁹F NMR (376 MHz, CDCl₃)

nketata nk94zf

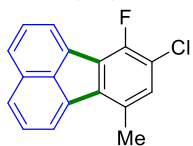


¹³C NMR (100 MHz, CDCl₃)

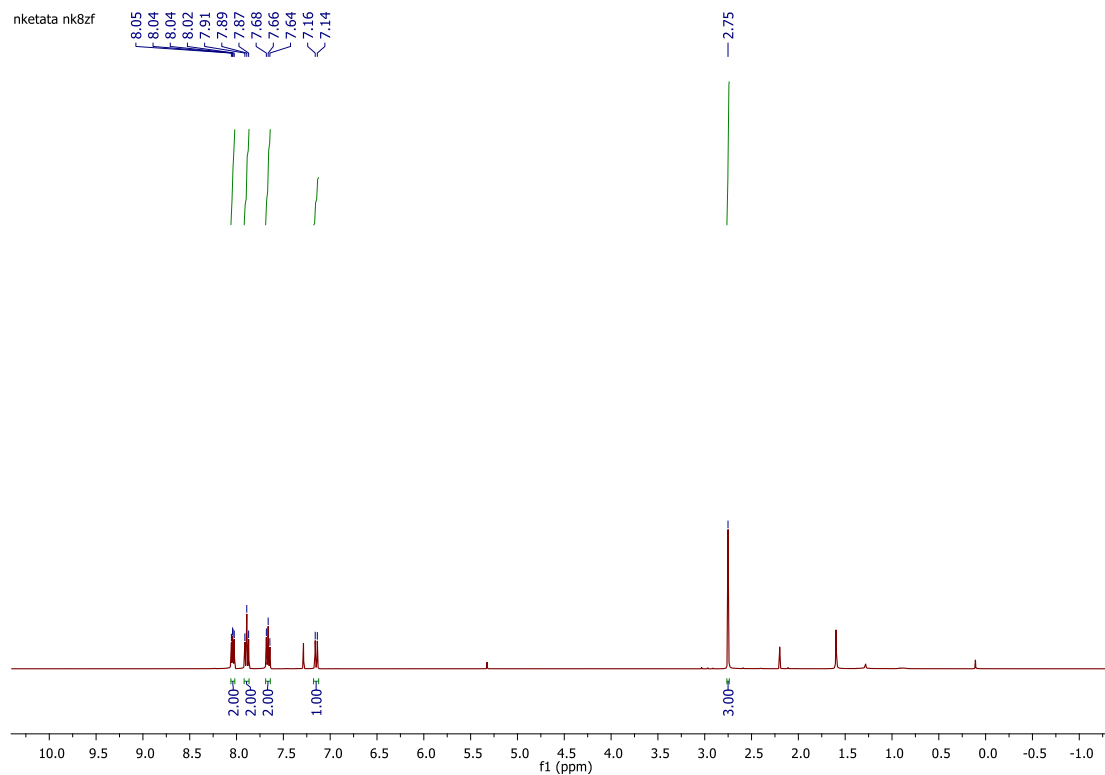
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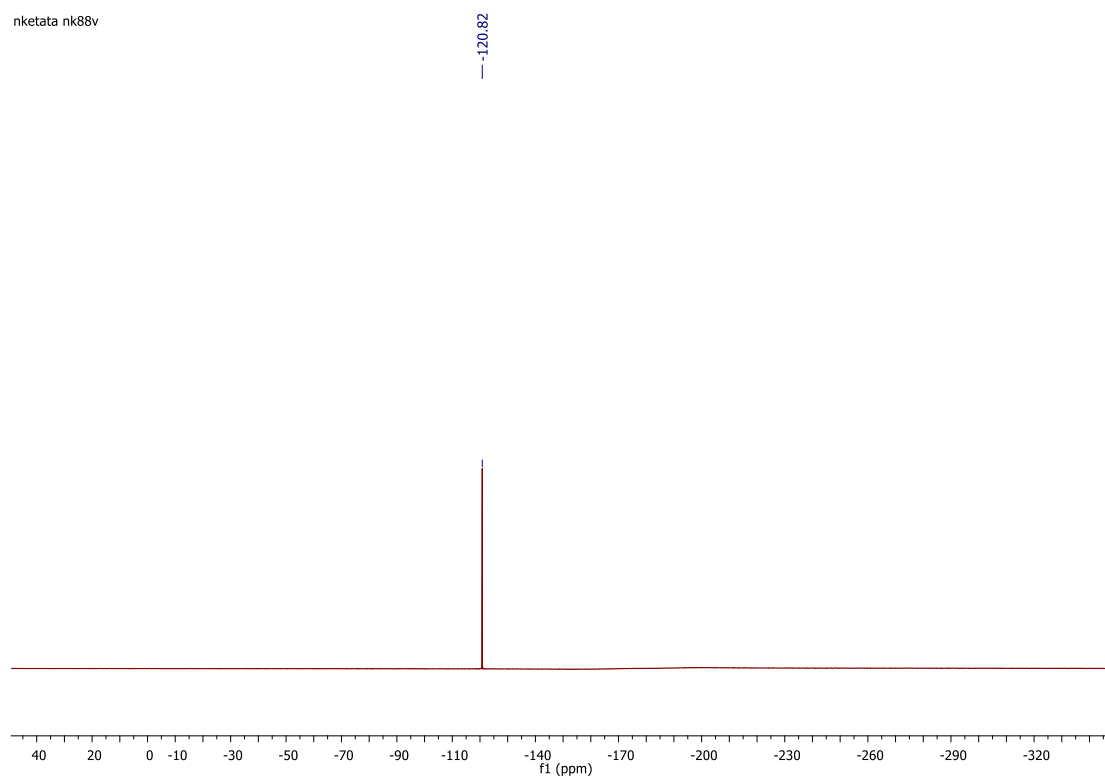
8-Chloro-10-fluoro-7-methylfluoranthene (14)



^1H NMR (400MHz, CDCl_3)

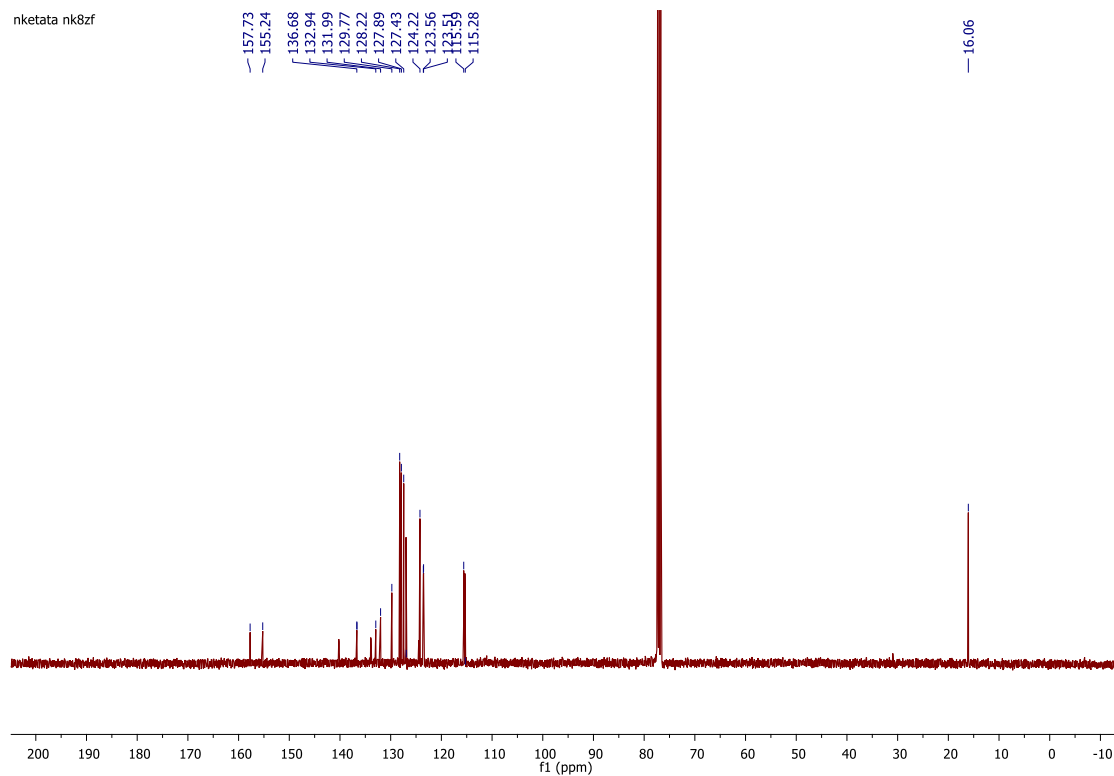


^{19}F NMR (376 MHz, CDCl_3)

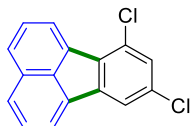


¹³C NMR (100 MHz, CDCl₃)

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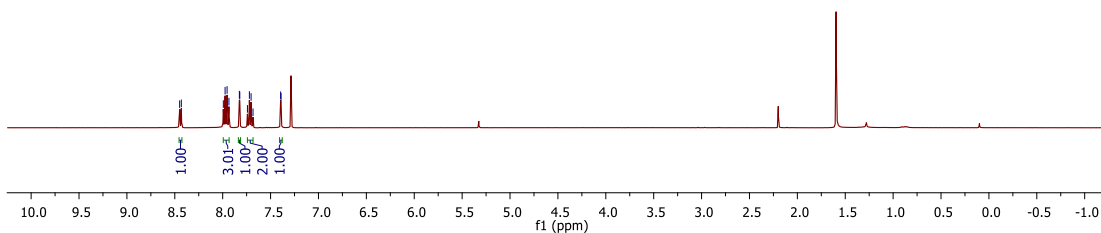
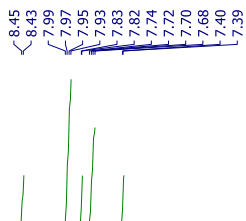


7,9-Dichlorofluoranthene (15)



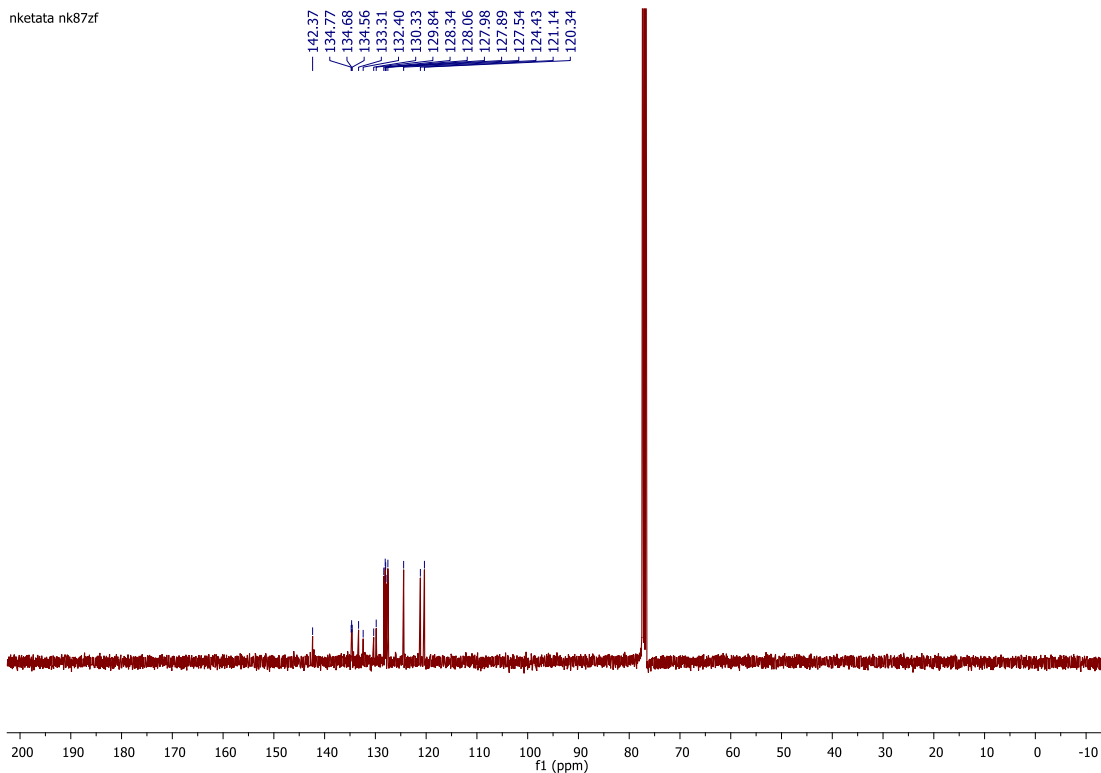
¹H NMR (400MHz, CDCl₃)

nketata nk87zf

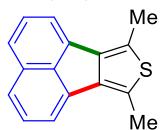


¹³C NMR (100 MHz, CDCl₃)

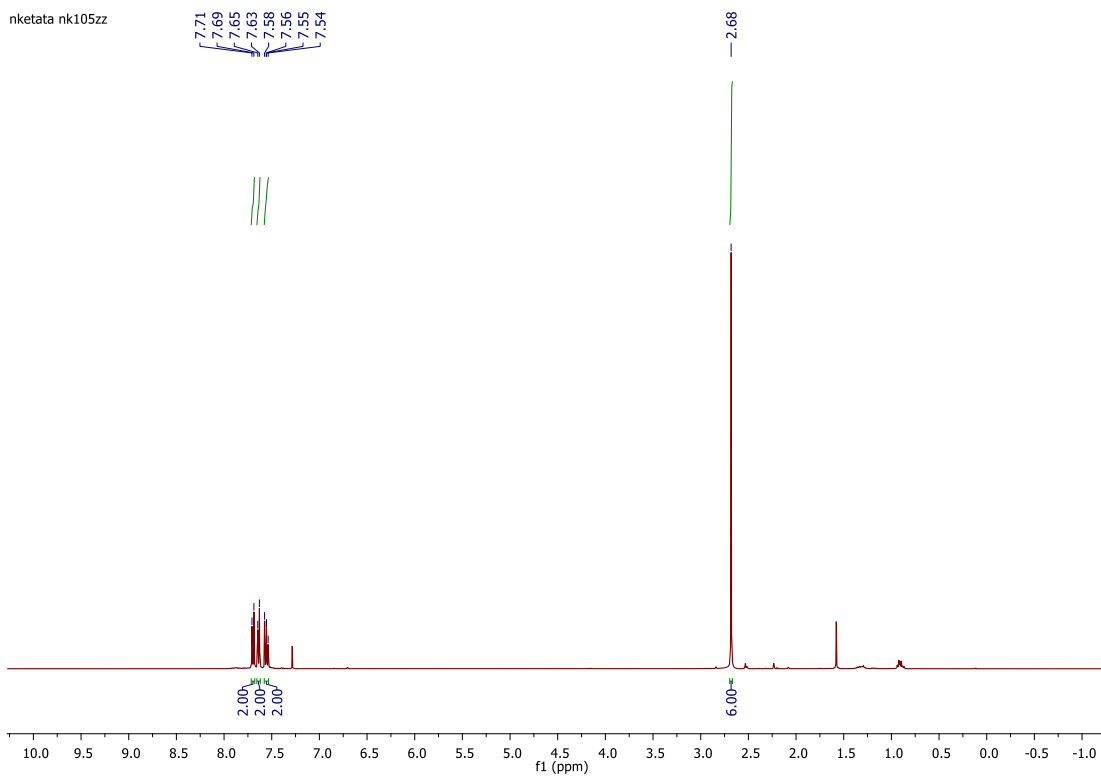
nketata nk87zf



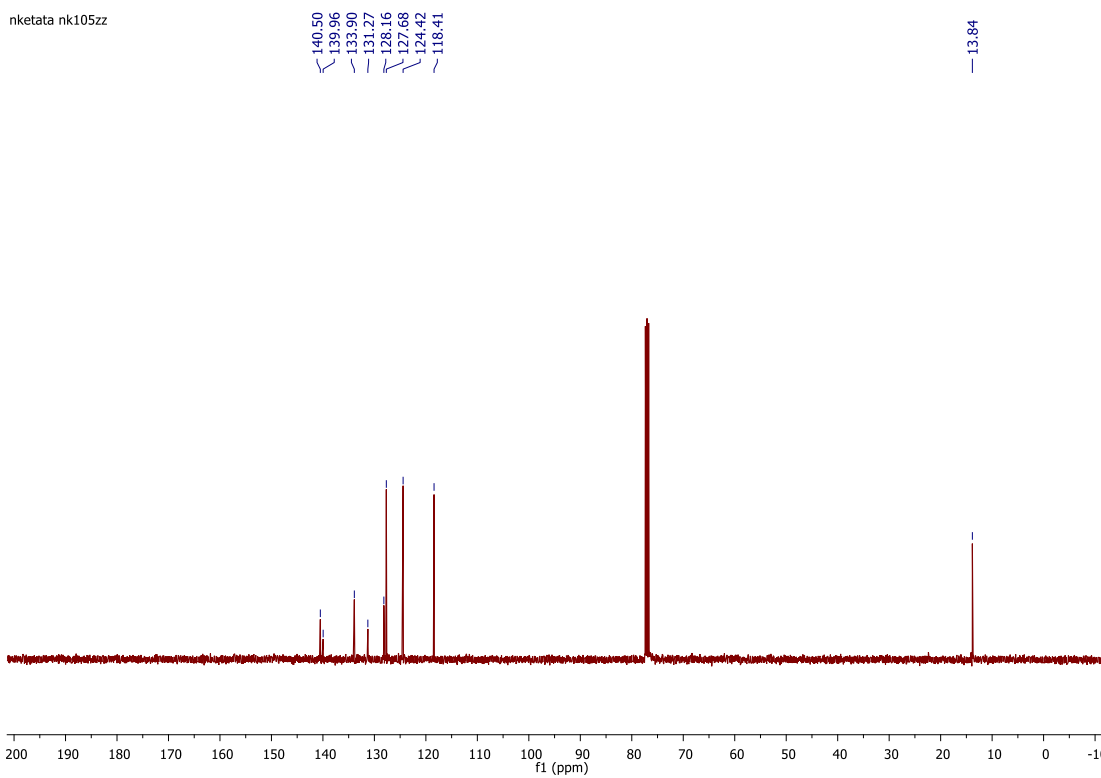
7,9-Dimethylacenaphtho[1,2-c]thiophene (16)



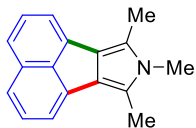
¹H NMR (400MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)

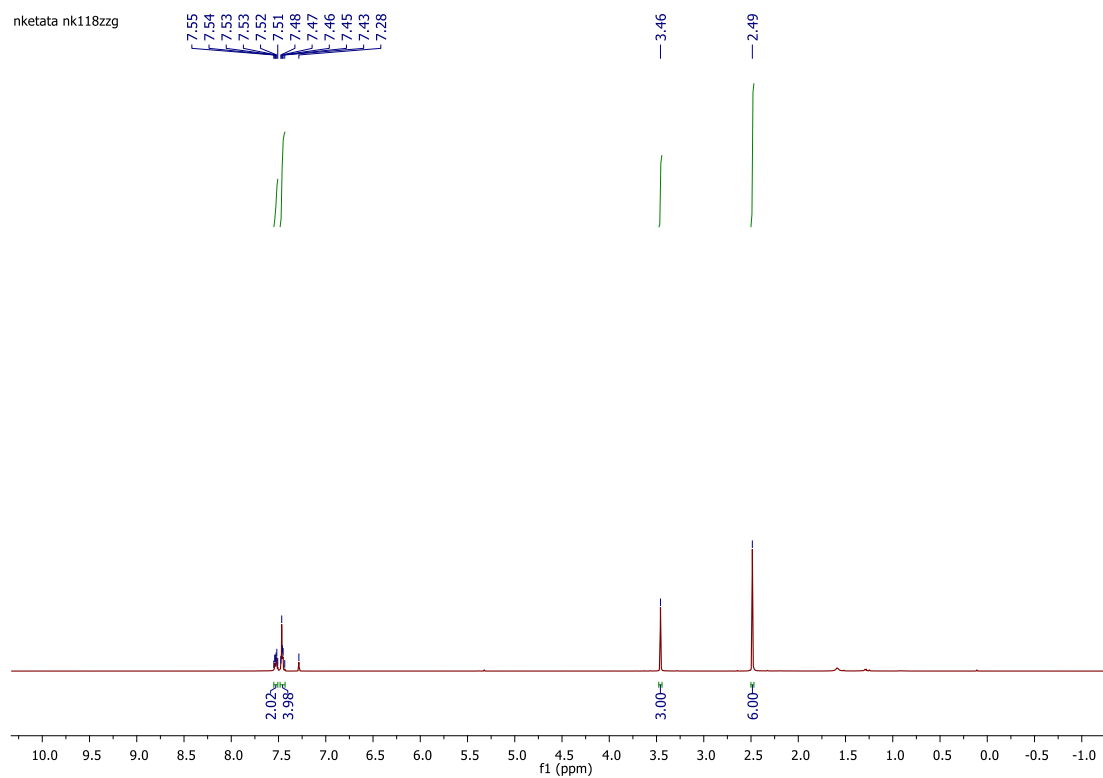


7,8,9-Trimethyl-8H-acenaphtho[1,2-c]pyrrole (17)



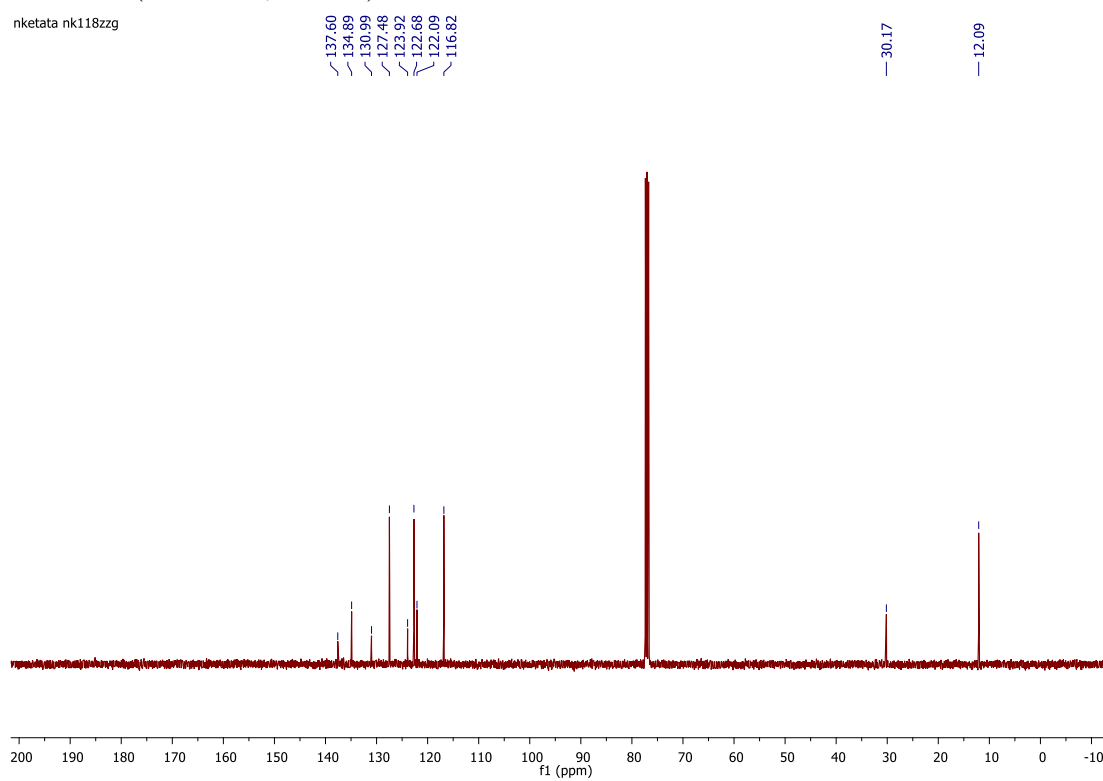
¹H NMR (400MHz, CDCl₃)

nketata nk118zzg

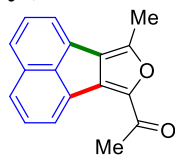


¹³C NMR (100 MHz, CDCl₃)

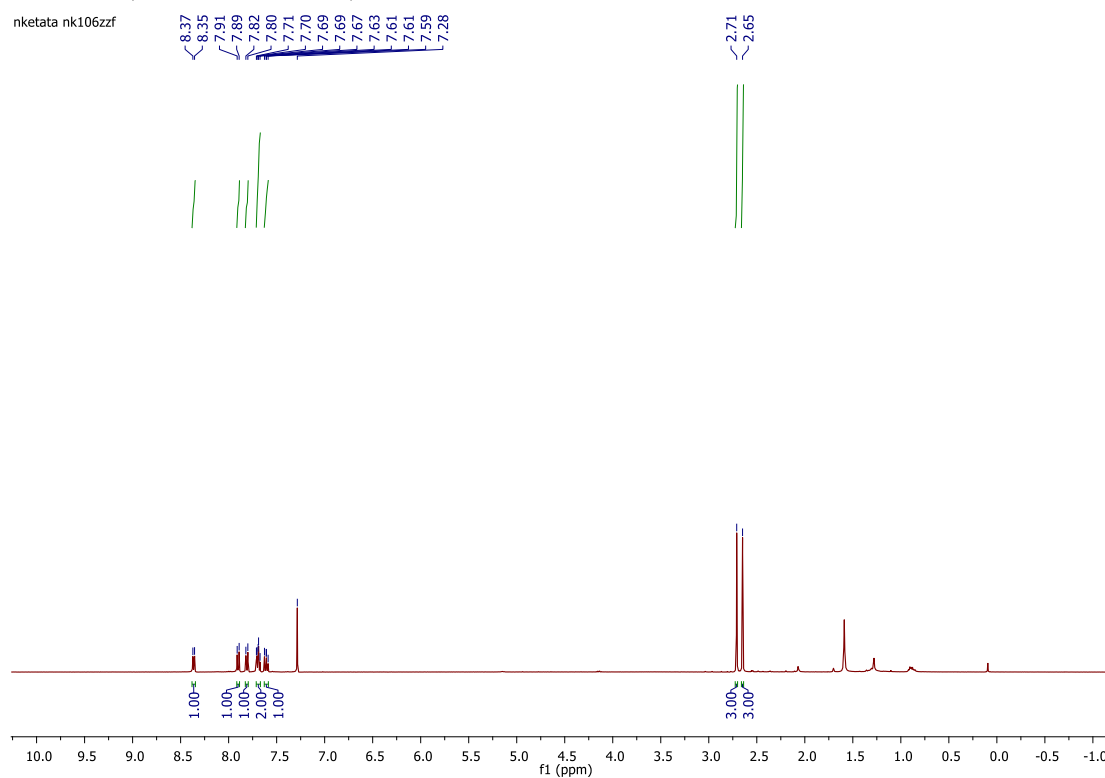
nketata nk118zzg



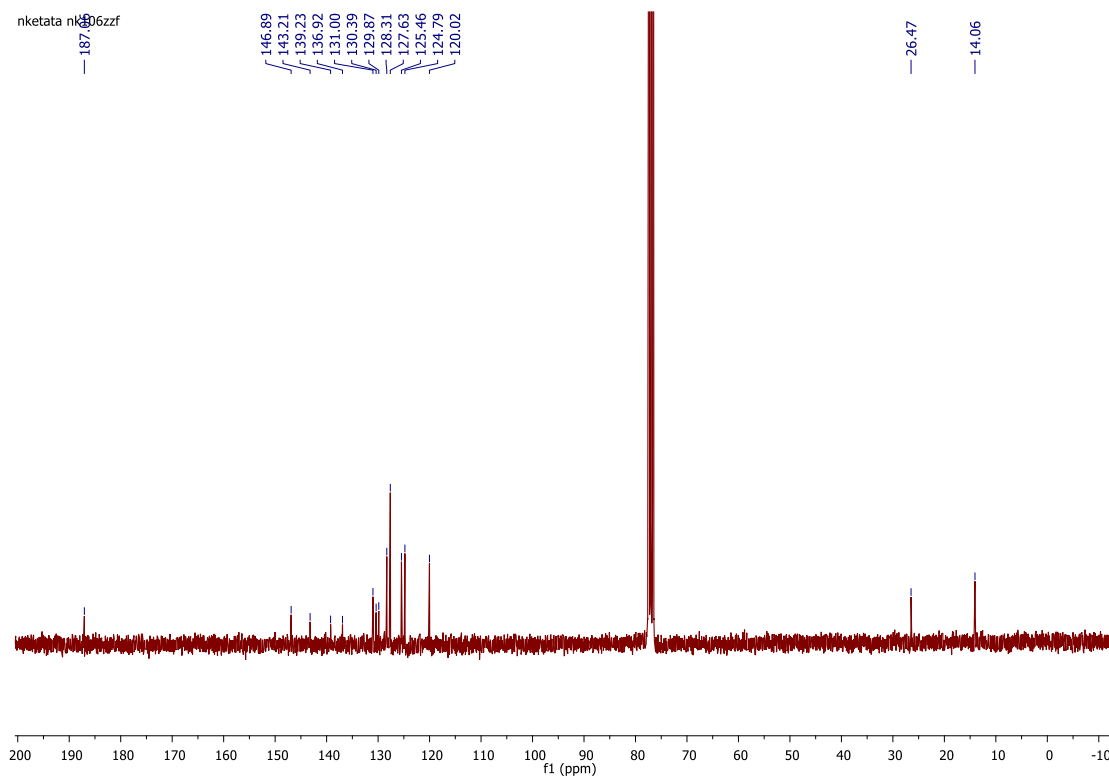
1-(9-Methylacnaphtho[1,2-c]furan-7-yl)ethan-1-one (18)



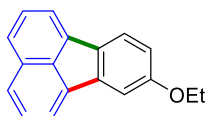
¹H NMR (400MHz, CDCl₃)



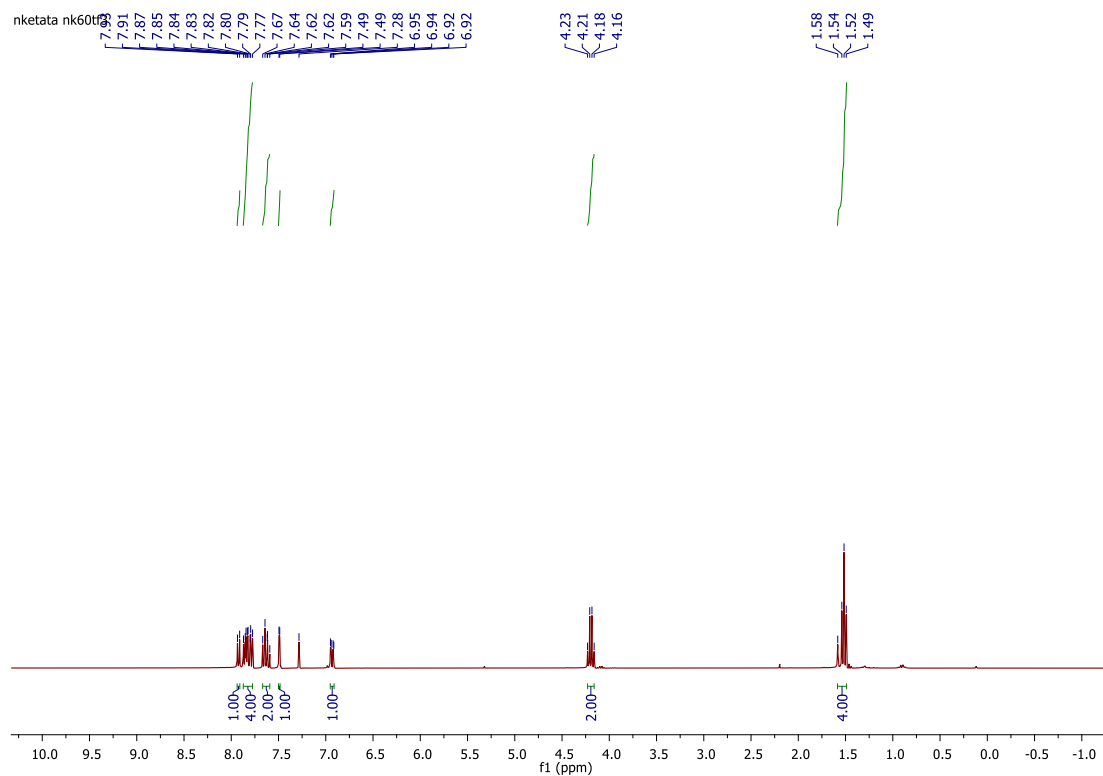
¹³C NMR (100 MHz, CDCl₃)



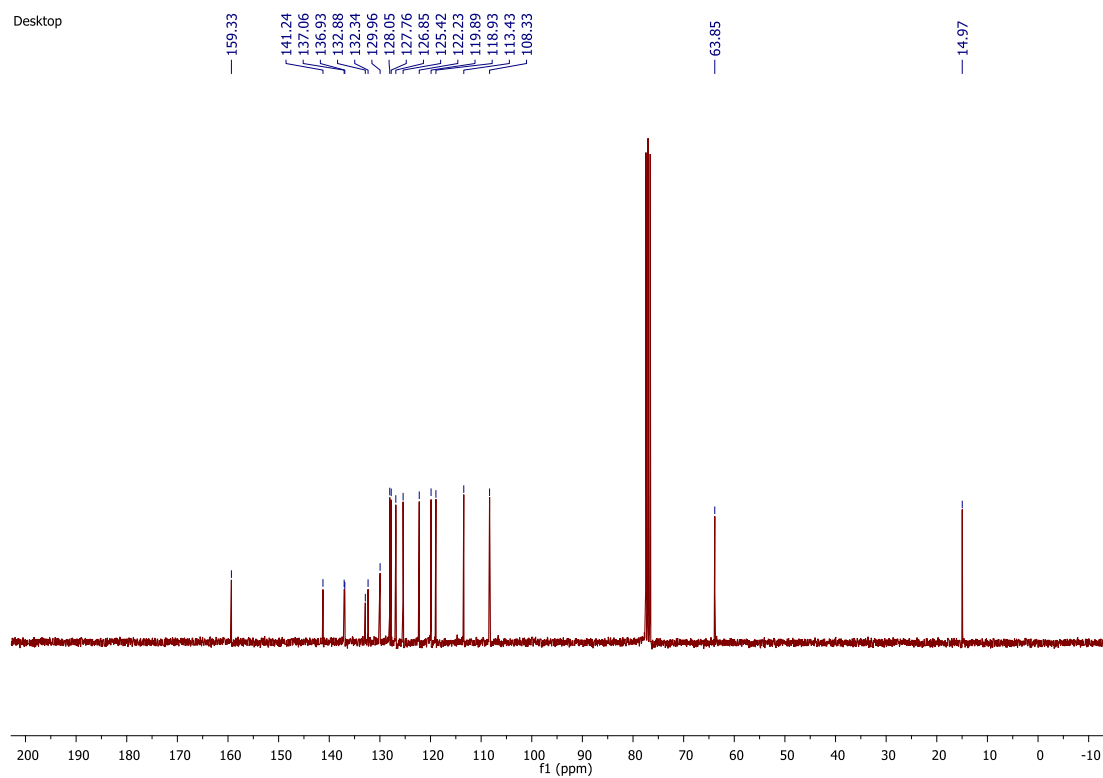
7-Ethoxyfluoranthene (19)



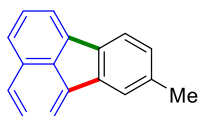
^1H NMR (400MHz, CDCl_3)



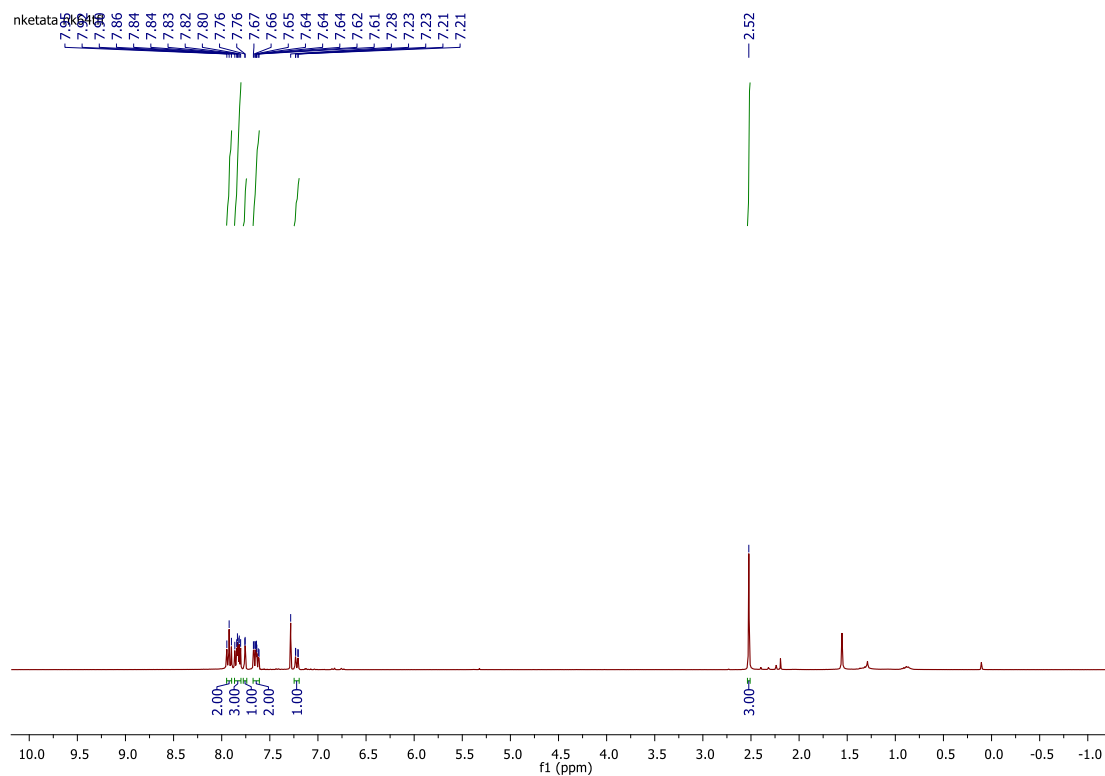
^{13}C NMR (100 MHz, CDCl_3)



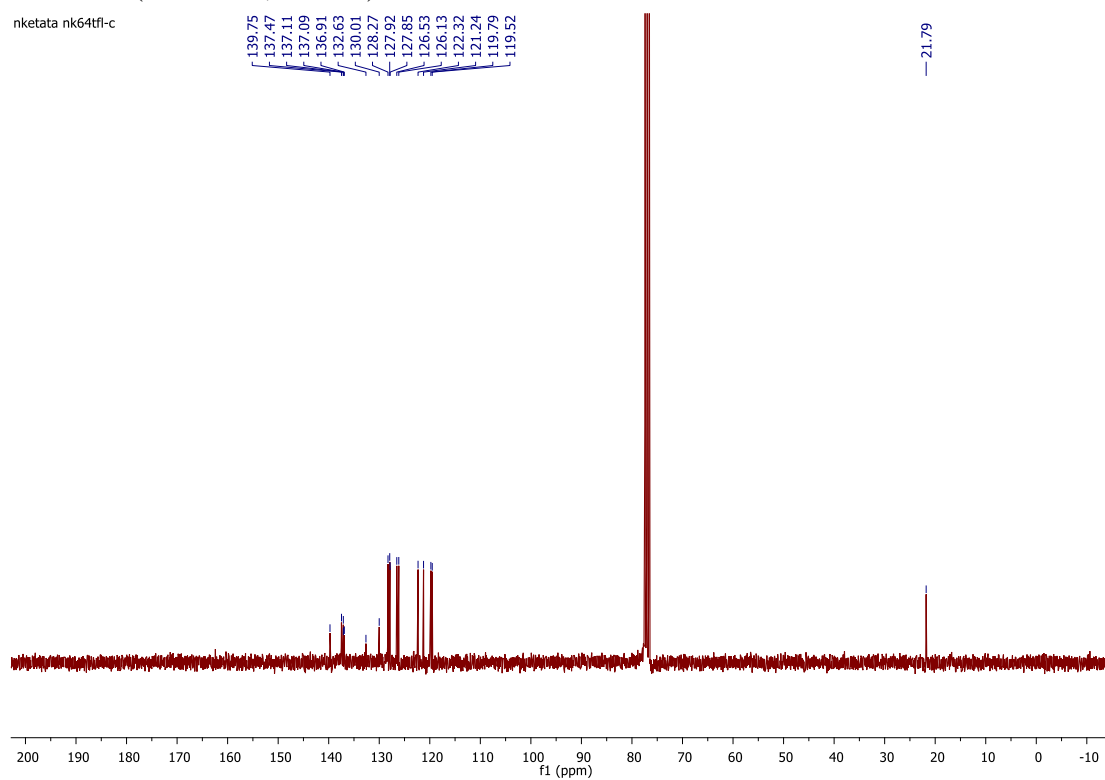
8-Methylfluoranthene (20)



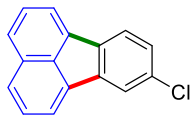
^1H NMR (400MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3)

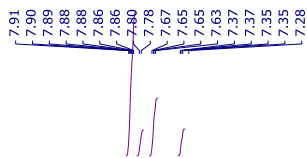


8-Chlorofluoranthene (21)

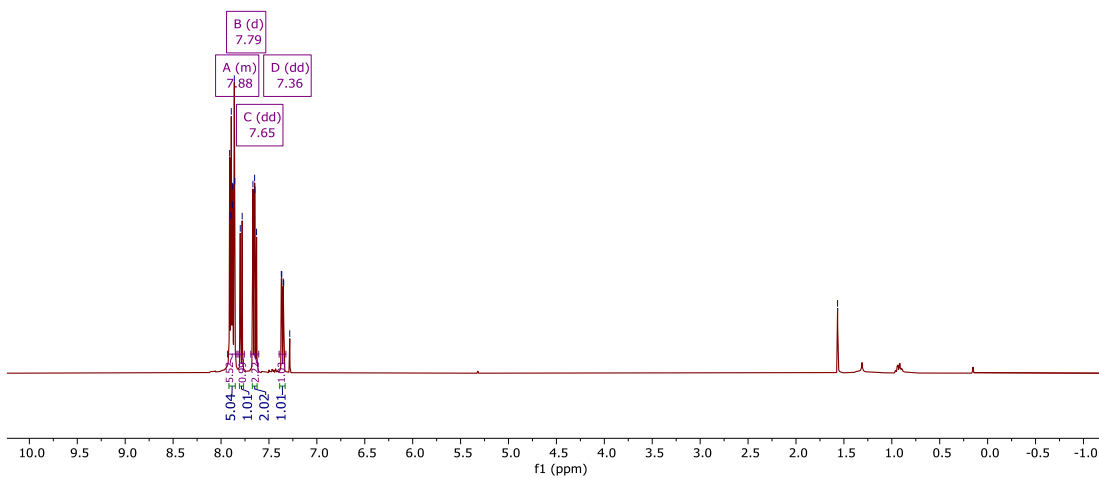


¹H NMR (400MHz, CDCl₃)

nketata nk53tf



— 1.57 H₂O

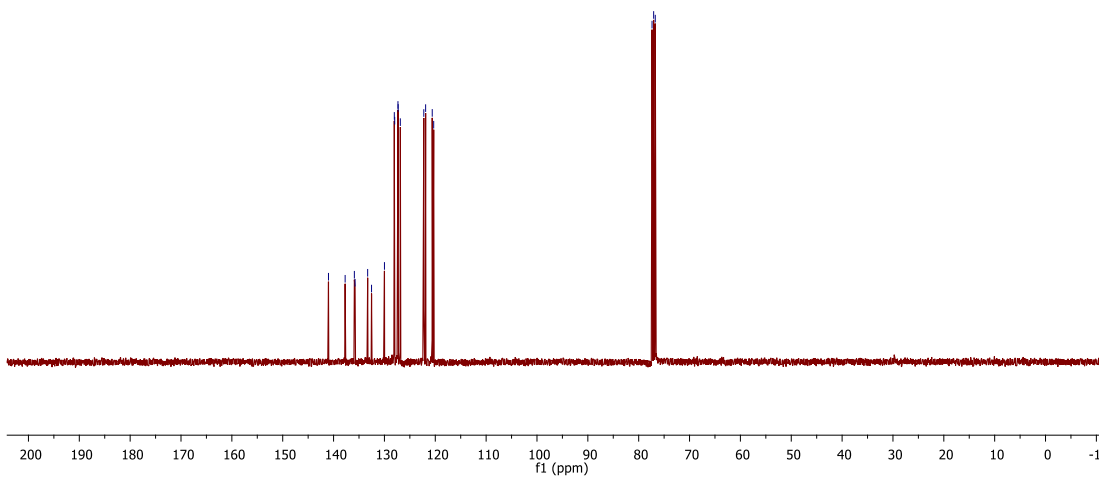


¹³C NMR (100 MHz, CDCl₃)

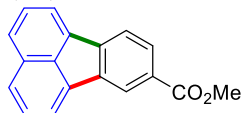
nketata nk53tf



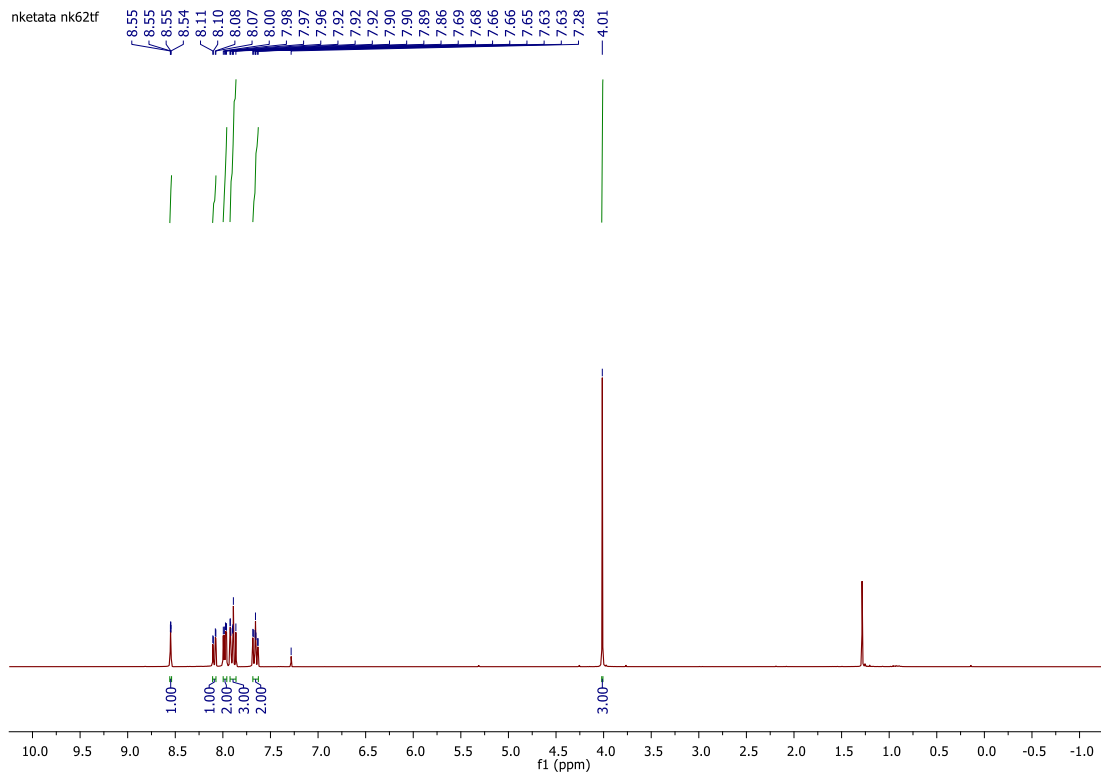
77.38
77.06
76.74



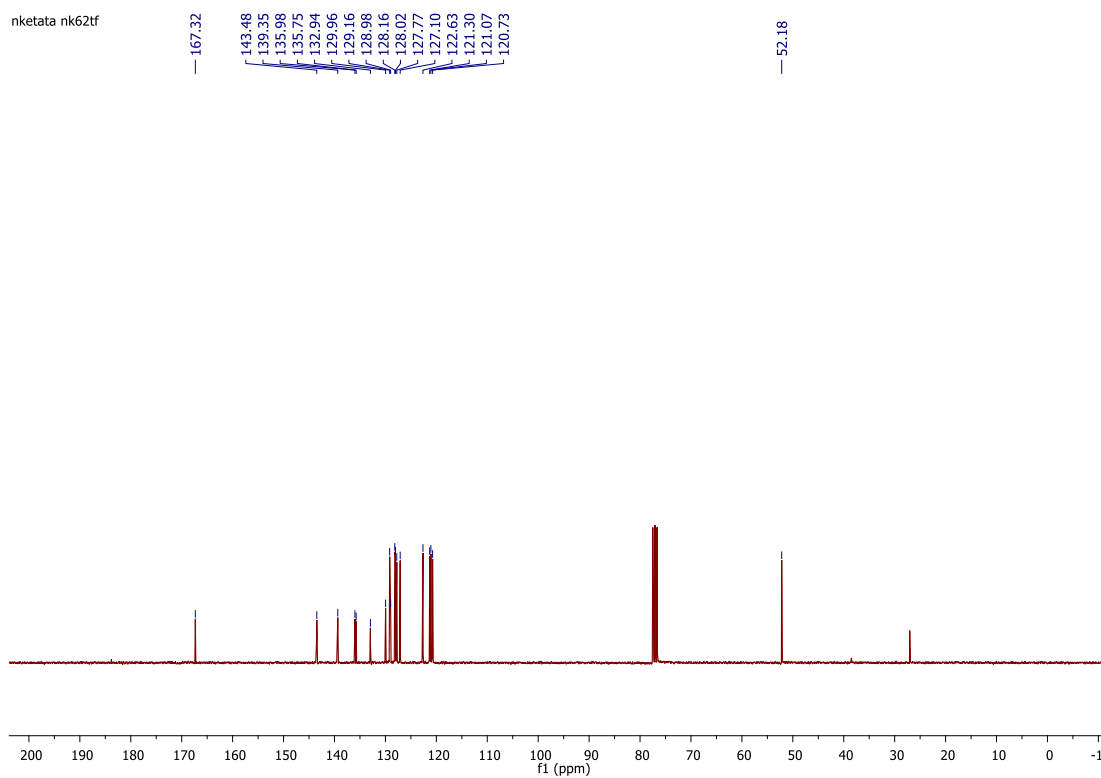
Methyl fluoranthene-8-carboxylate (22)



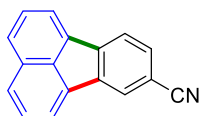
¹H NMR (400MHz, CDCl₃)



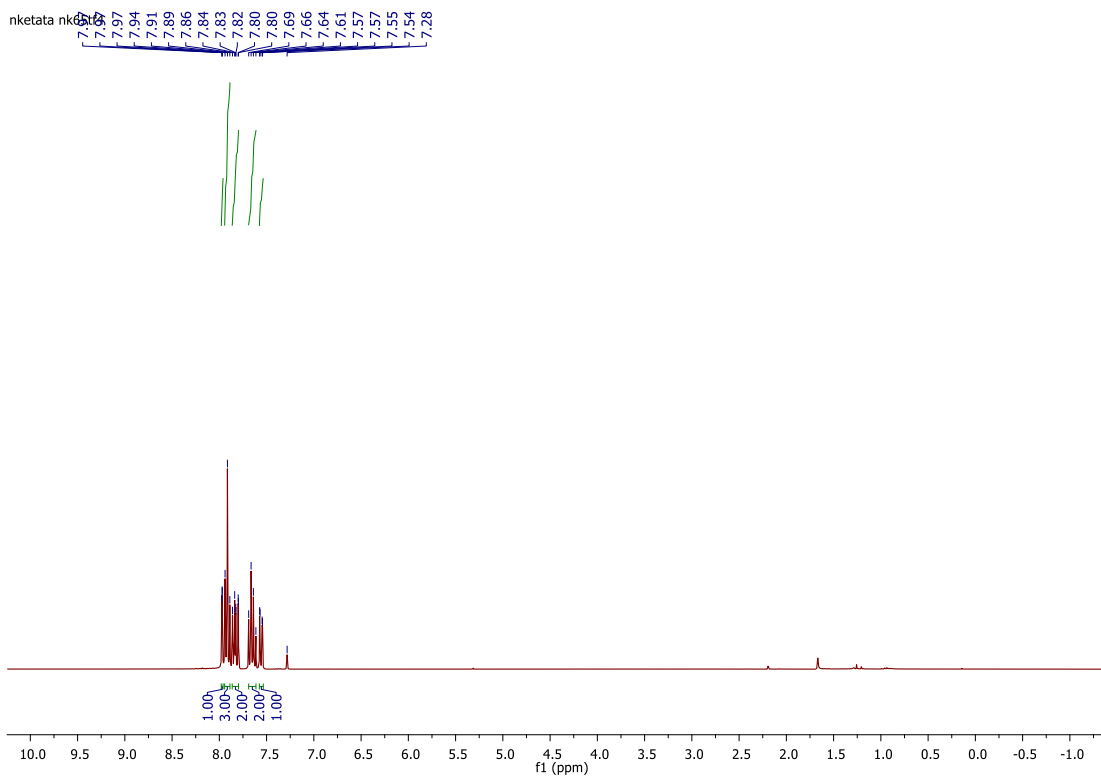
¹³C NMR (100 MHz, CDCl₃)



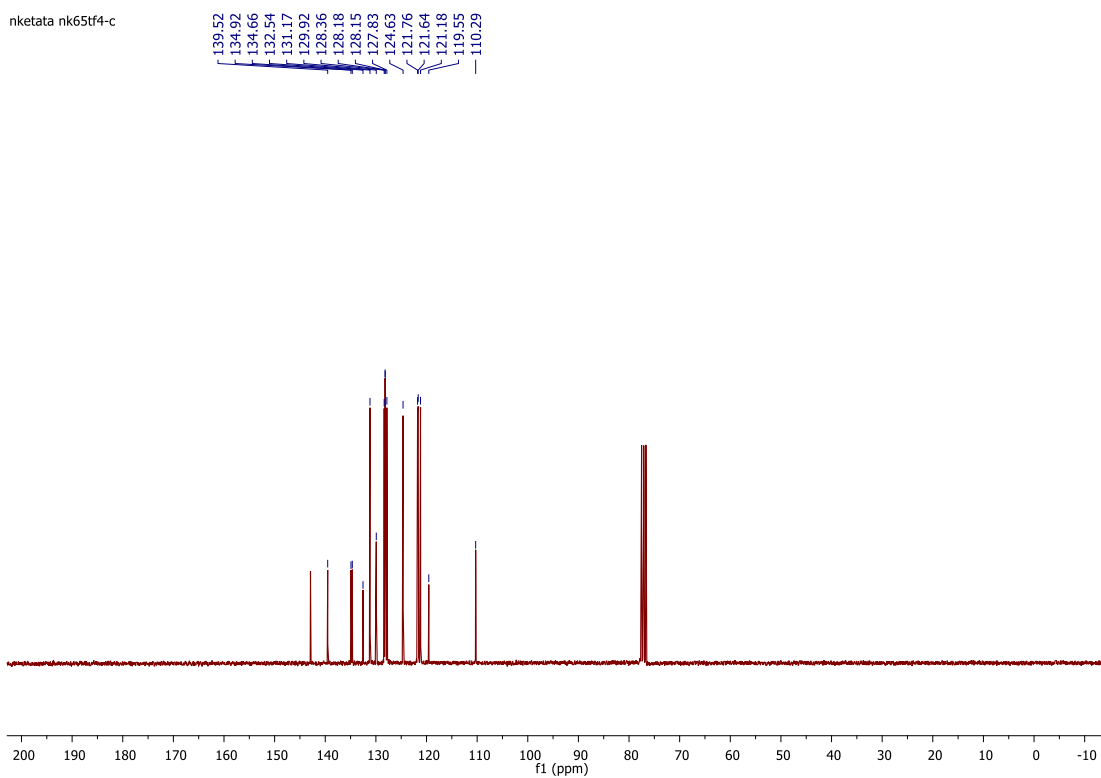
Fluoranthene-8-carbonitrile (23)



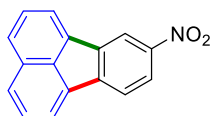
¹H NMR (400MHz, CDCl₃)



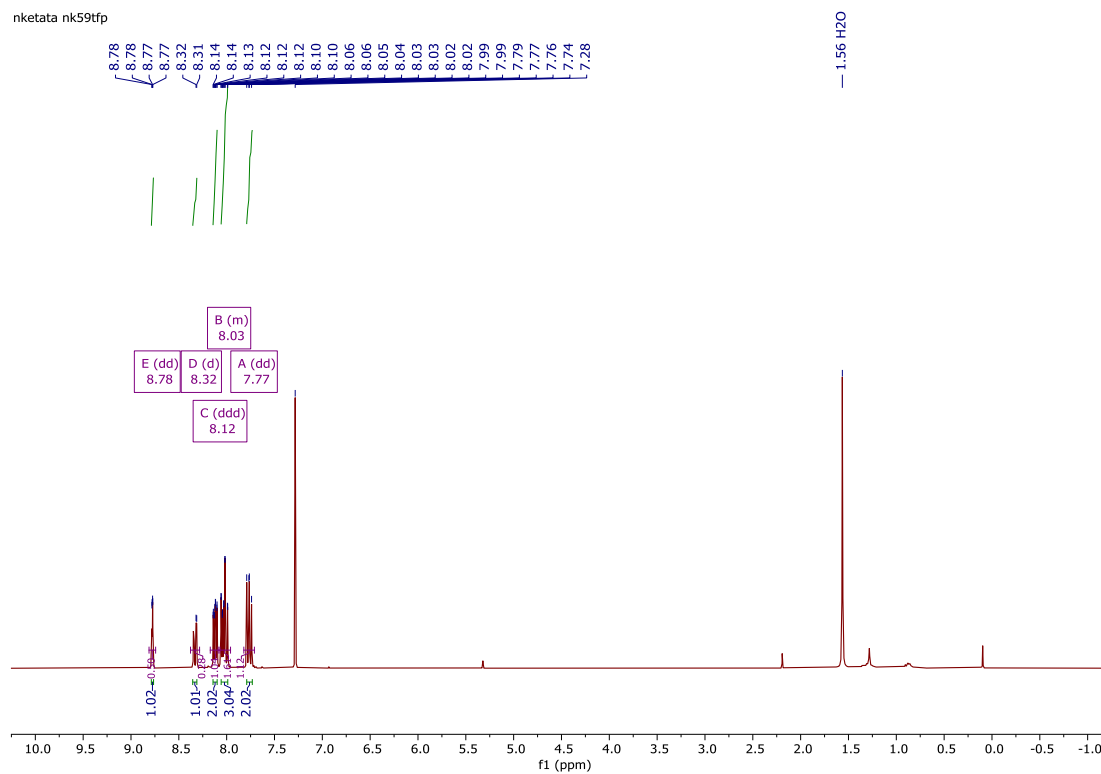
¹³C NMR (100 MHz, CDCl₃)



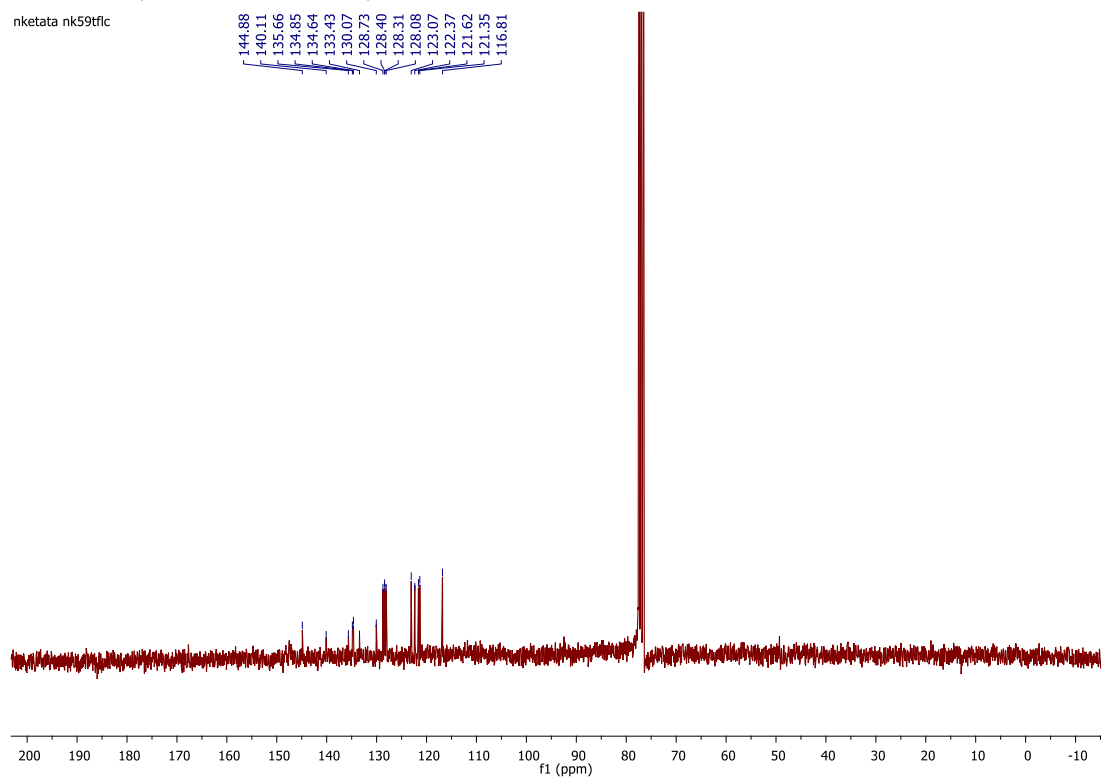
8-Nitrofluoranthene (24)



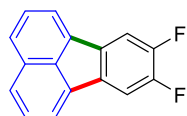
¹H NMR (400MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)

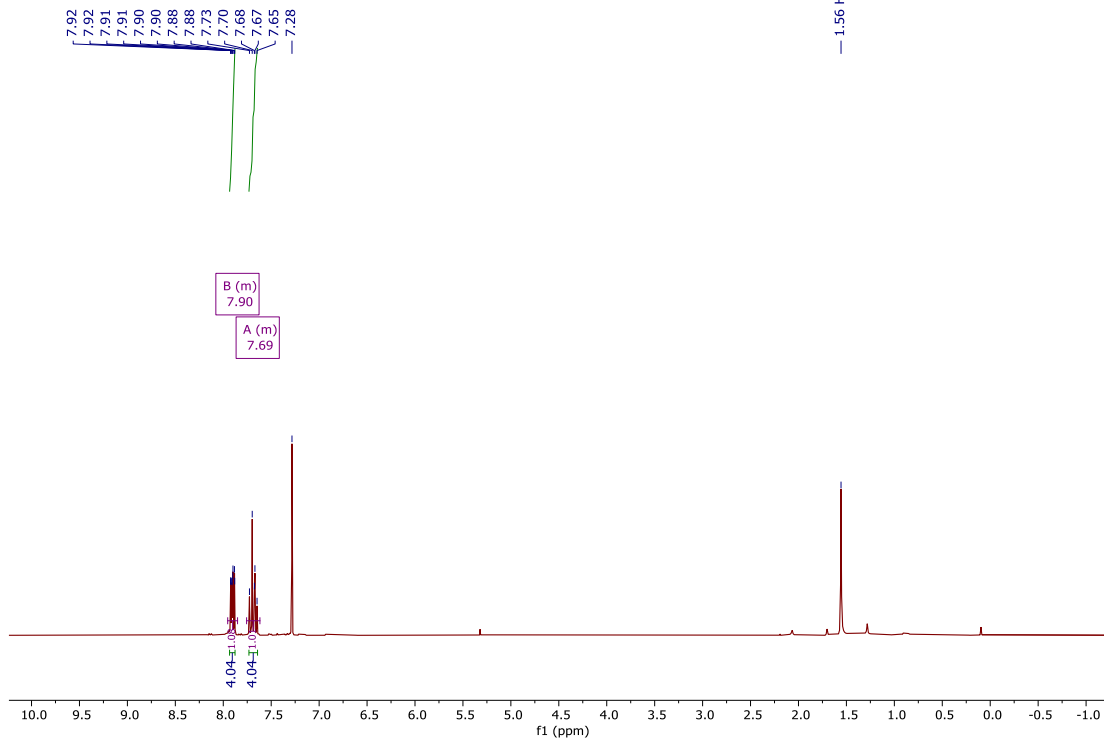


8,9-Difluorofluoranthene (25)



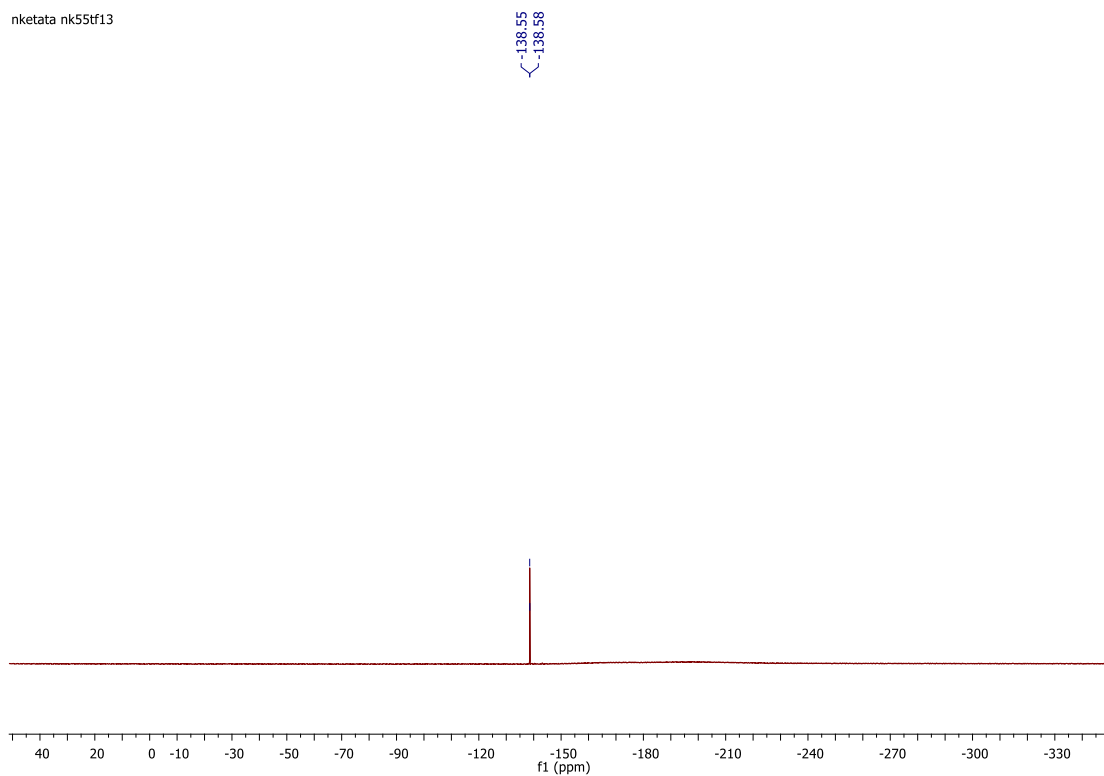
¹H NMR (400MHz, CDCl₃)

nketata nk55tf13



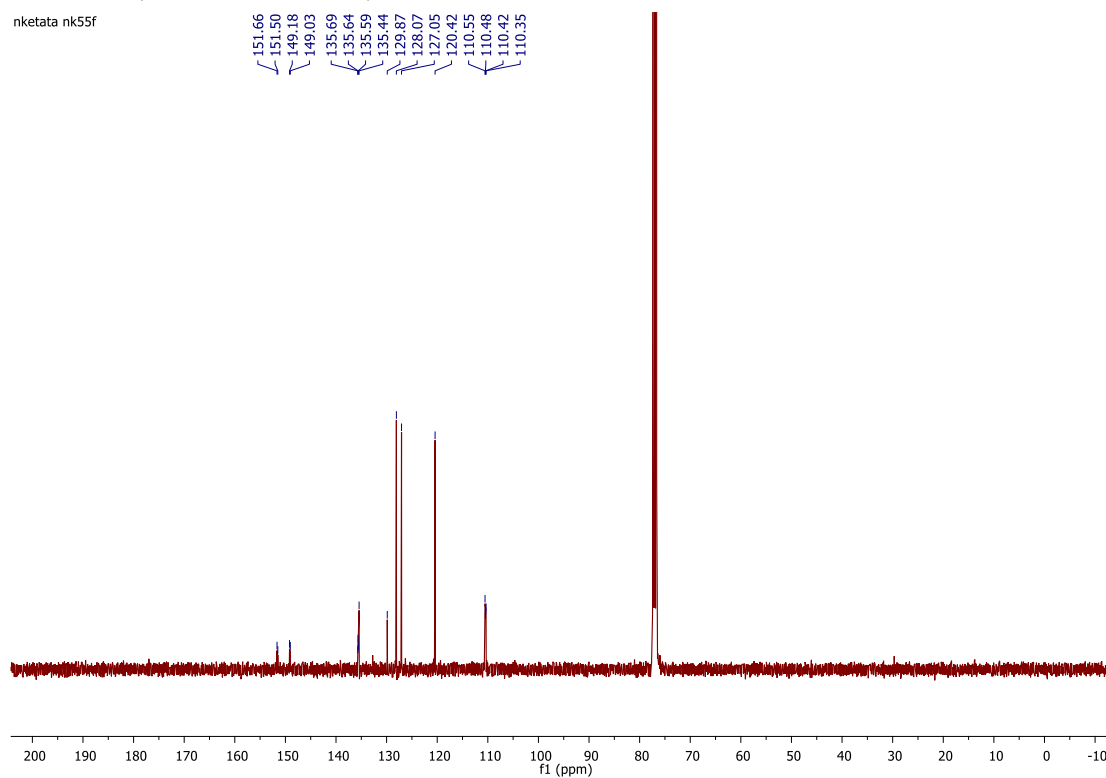
¹⁹F NMR (376 MHz, CDCl₃)

nketata nk55tf13

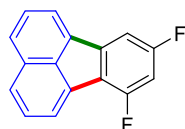


^{13}C NMR (100 MHz, CDCl_3)

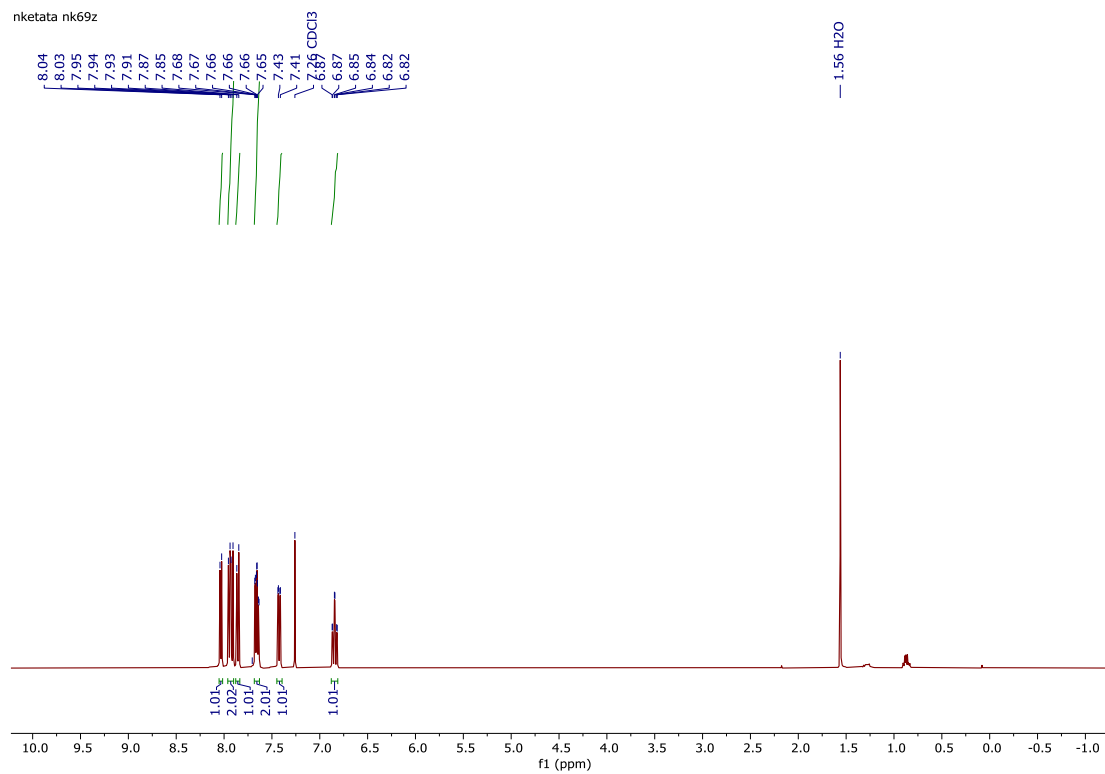
nketata nk55f



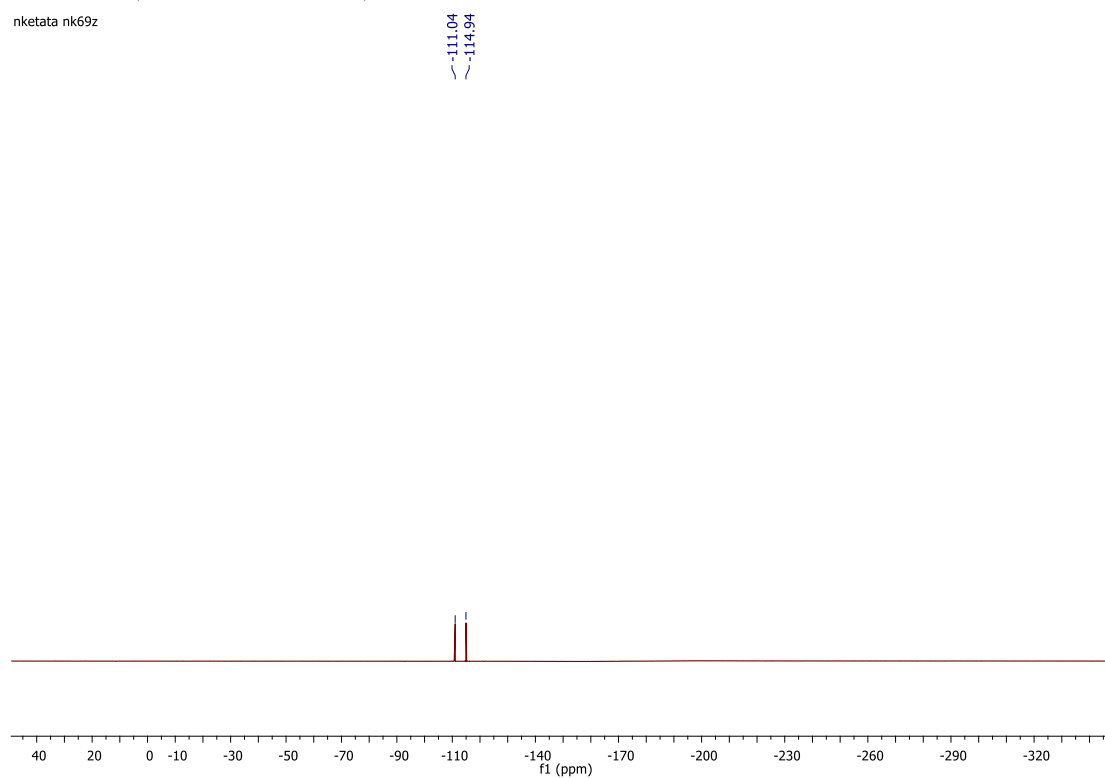
7,9-Difluorofluoranthene (26)



^1H NMR (400MHz, CDCl_3)

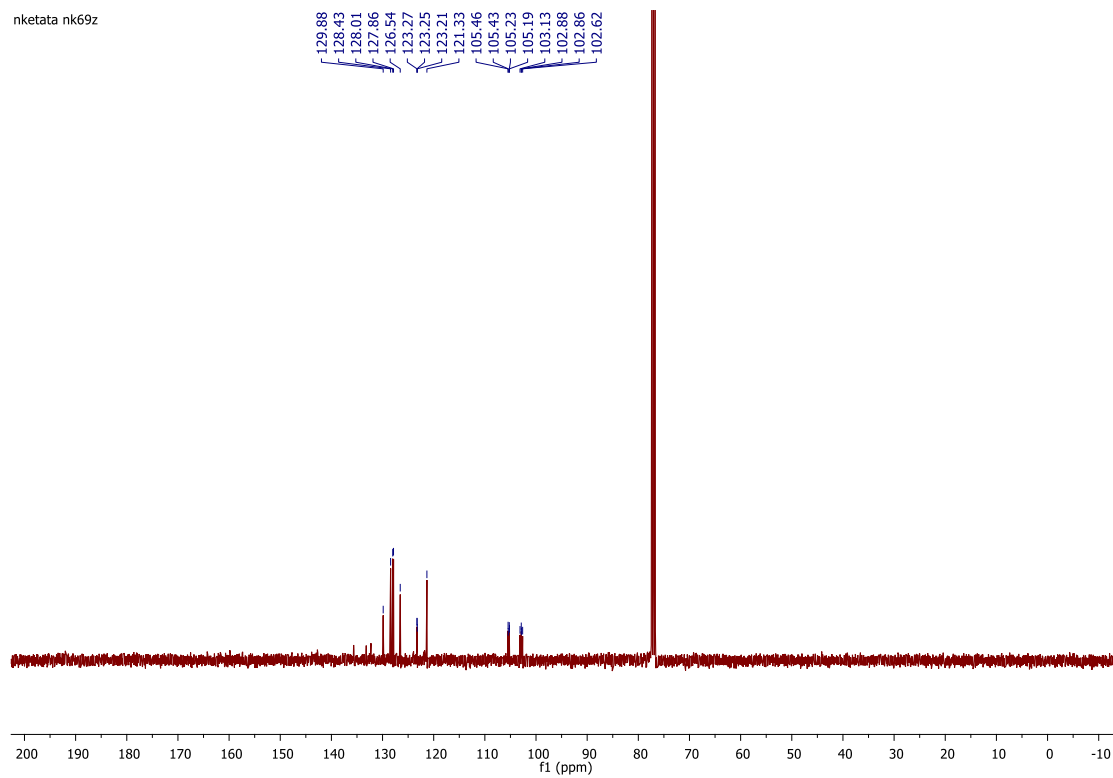


^{19}F NMR (376 MHz, CDCl_3)

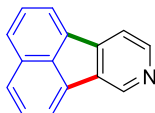


^{13}C NMR (100 MHz, CDCl_3)

nketata nk69z



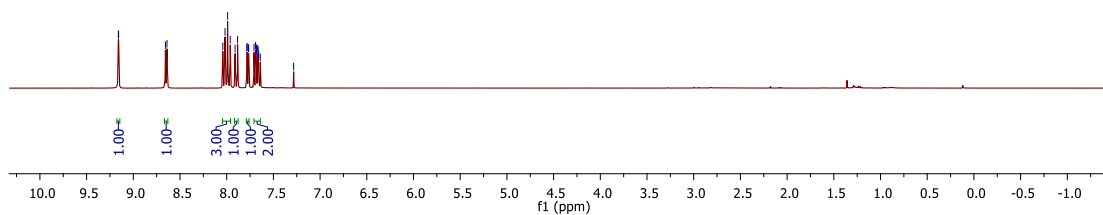
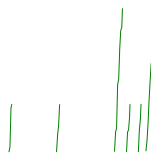
Acenaphtho[1,2-c]pyridine (27)



¹H NMR (400MHz, CDCl₃)

nketata nk61tf

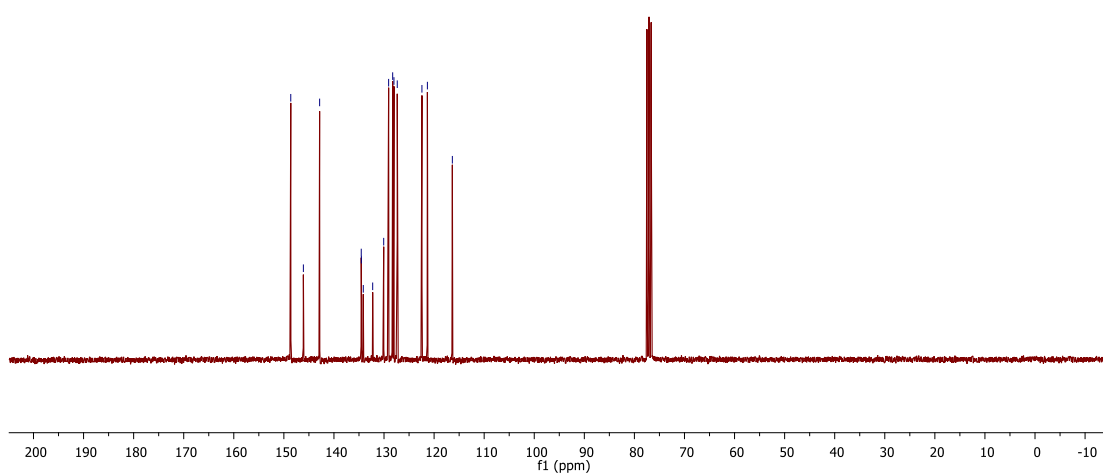
9.16	9.16	8.66	8.64	8.04	8.02	7.99	7.96	7.91	7.88	7.78	7.77	7.76	7.71	7.69	7.68	7.67	7.66	7.64	7.28
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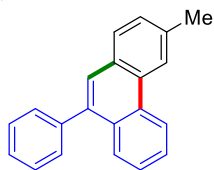
¹³C NMR (100 MHz, CDCl₃)

nketata nk61tf

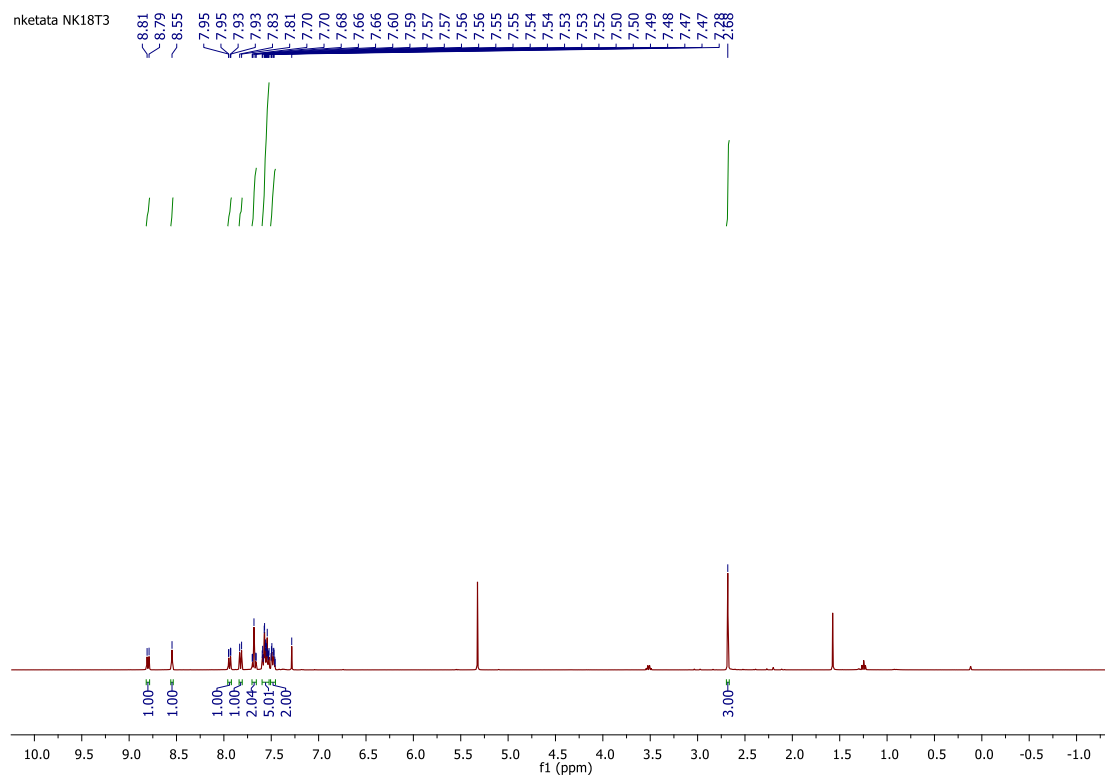
148.62	146.10	142.86	134.55	134.53	134.14	132.26	130.06	129.08	128.27	128.02	127.36	122.43	121.34	116.36
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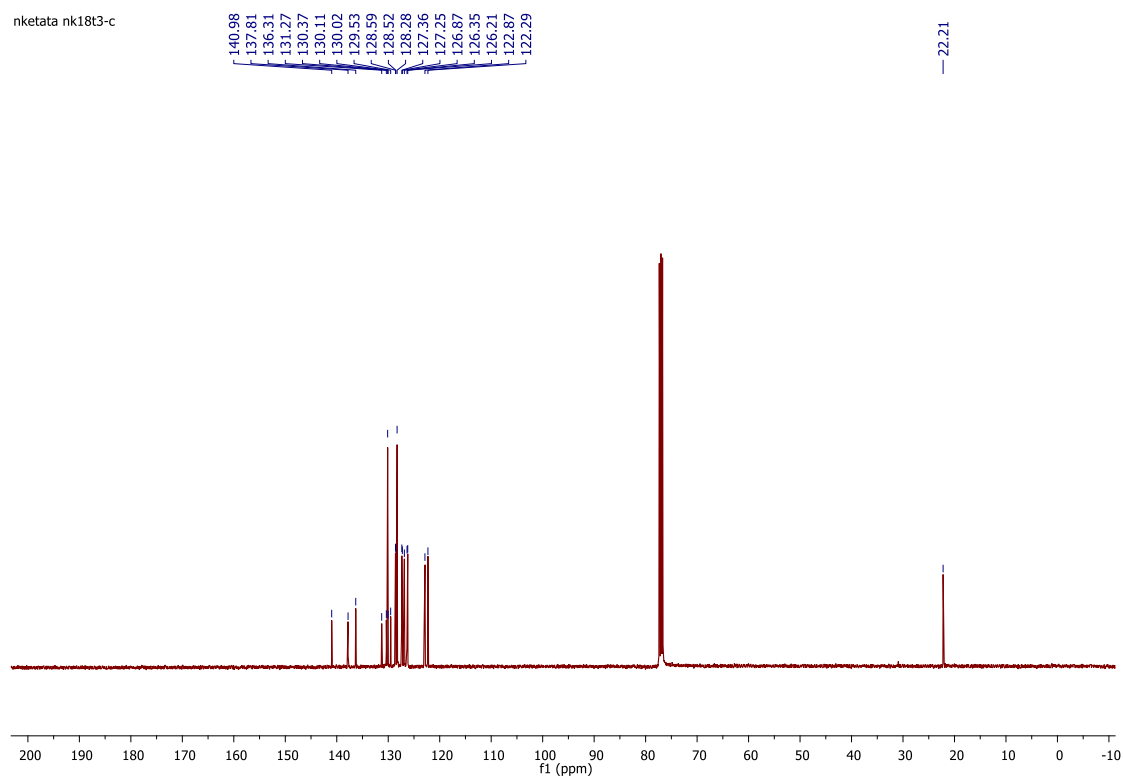
3-Methyl-9-phenylphenanthrene (28)



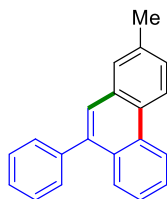
$^1\text{H NMR}$ (400MHz, CDCl_3)



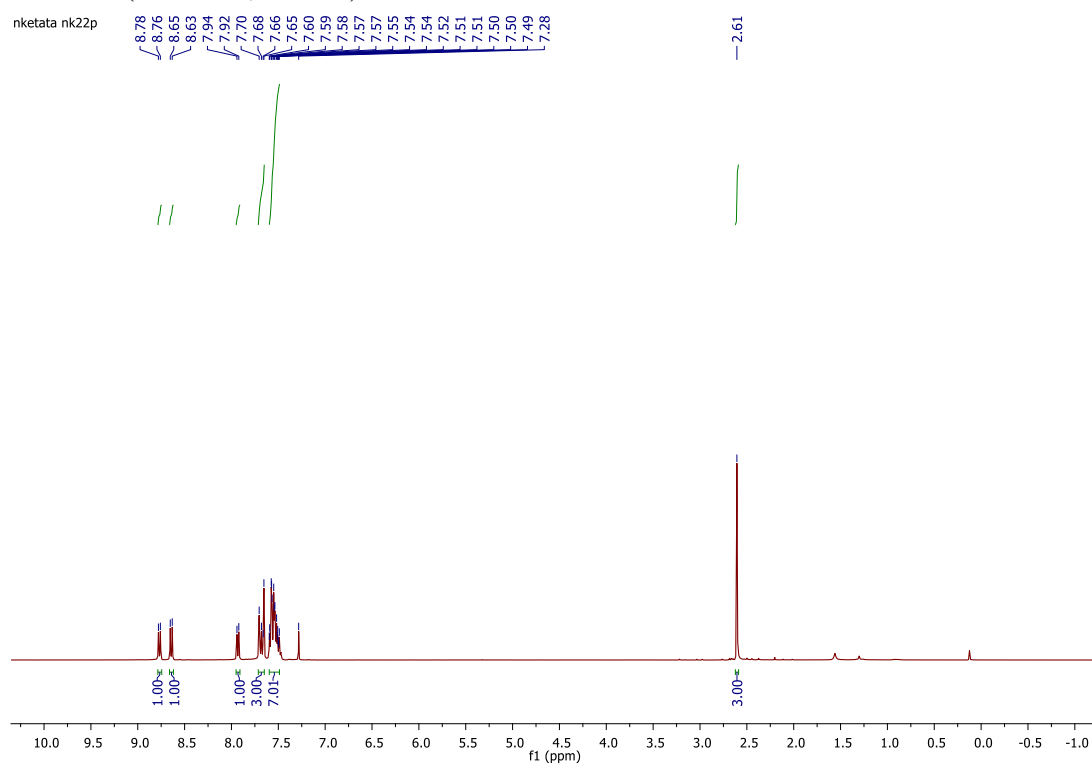
$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



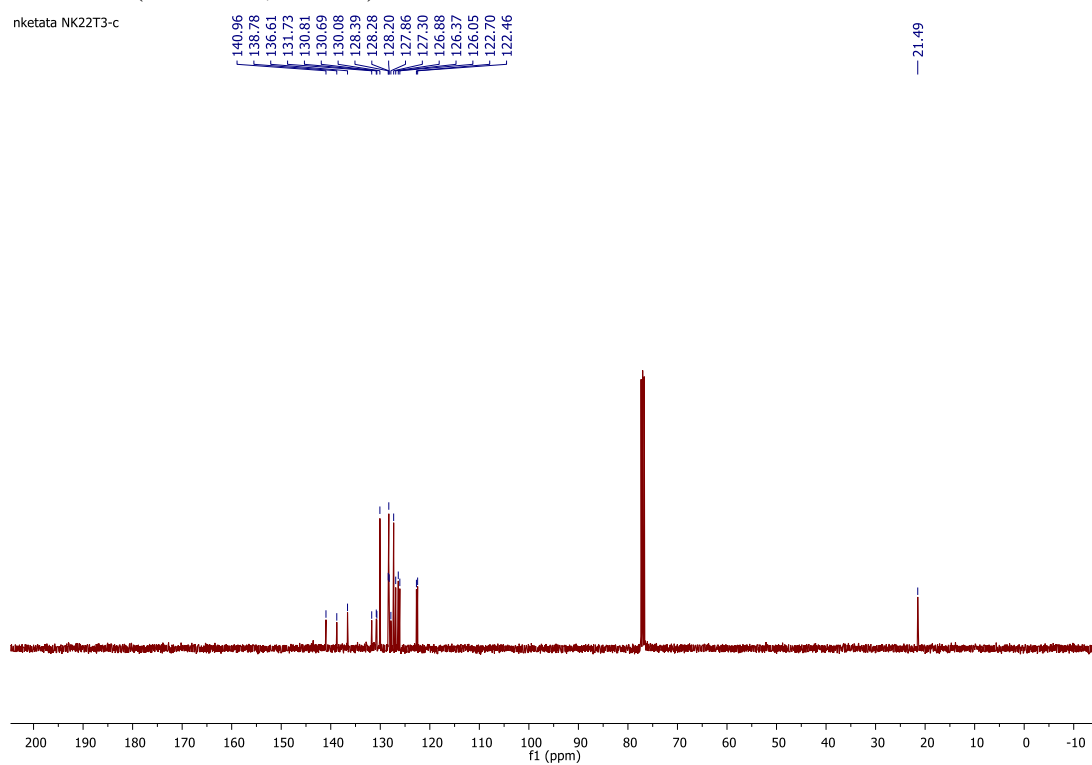
2-Methyl-9-phenylphenanthrene (29)



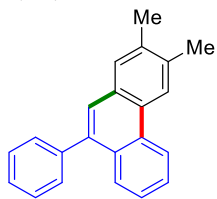
$^1\text{H NMR}$ (400MHz, CDCl_3)



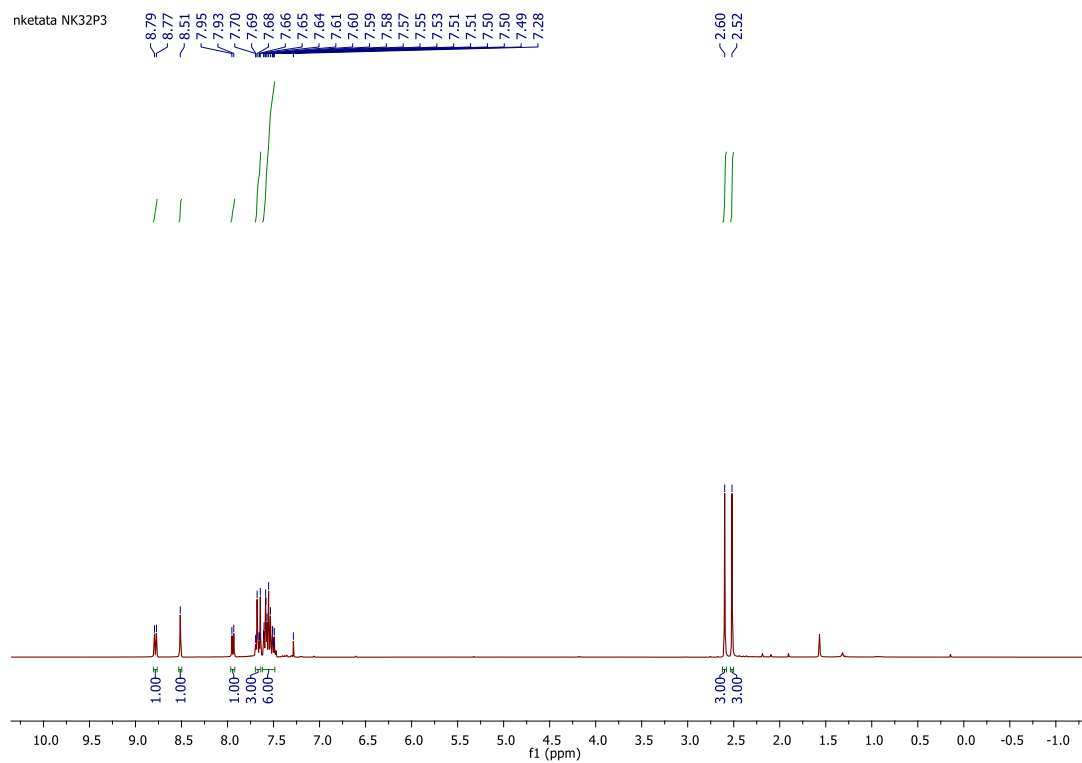
$^{13}\text{C NMR}$ (100 MHz, CDCl_3)



2,3-Dimethyl-9-phenylphenanthrene (30)



^1H NMR (400MHz, CDCl_3)



^{13}C NMR (100 MHz, CDCl_3)

