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

Supporting Information

High contrast stimuli-responsive luminescence switching of pyrene-1-carboxylic esters triggered by a crystal-to-crystal transition

Qunshou Kong,‡ Weihua Zhuang,‡ Gaocan Li,* Yangyang Xu, Qing Jiang and Yunbing Wang*

National Engineering Research Center for Biomaterials, Sichuan University, 29 Wangjiang Road, Chengdu 610064, China

*E-mail: gaocanli@scu.edu.cn; yunbing.wang@scu.edu.cn

‡These authors contribute equally to this work.

I. Photophysical Properties of pyrene-1-carboxylic esters and pyren-1-yl acetate

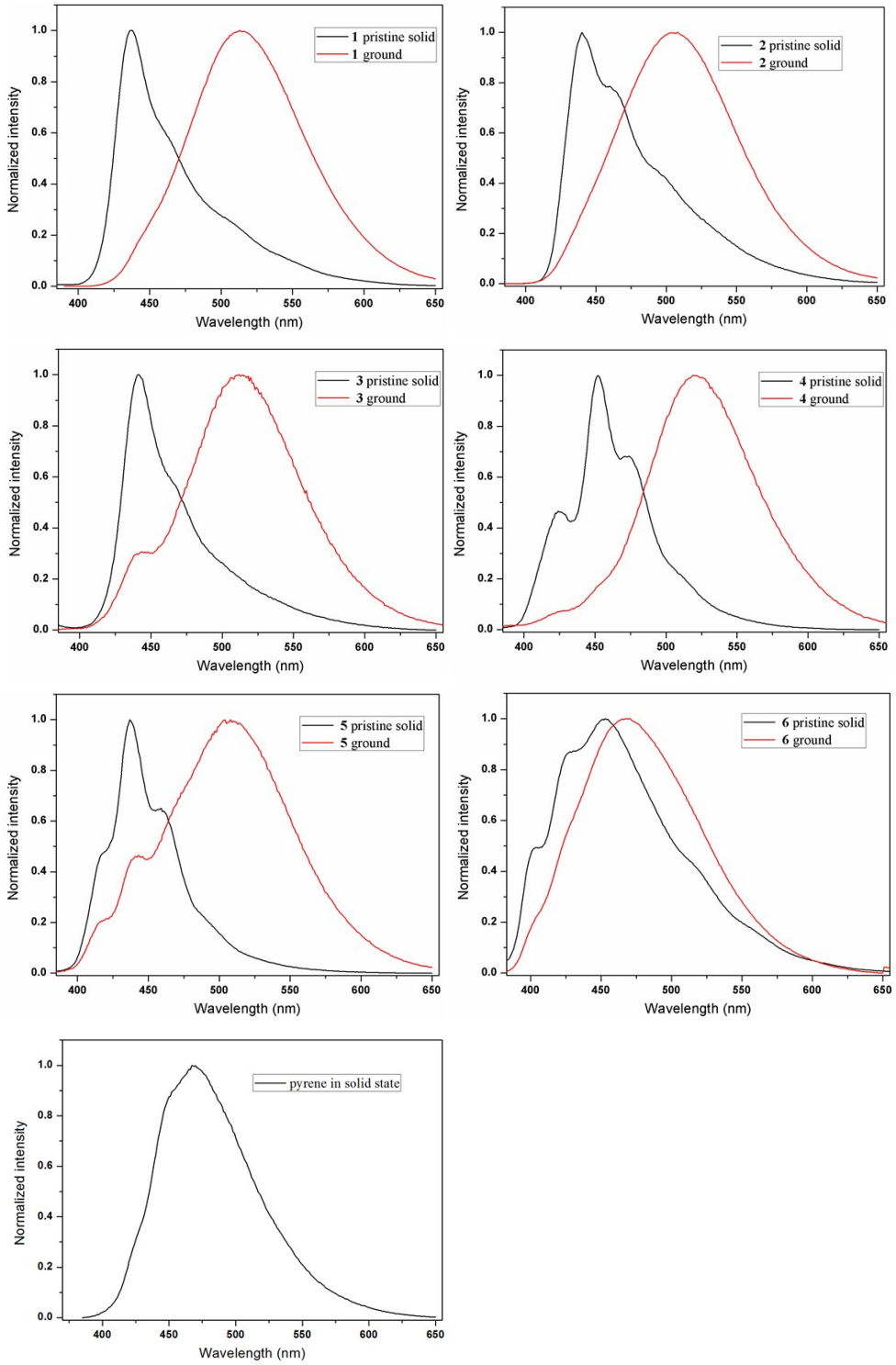


Figure S1. Fluorescence emission spectra of pyrene-1-carboxylic esters in different states (excited at the corresponding maximum excitation wavelength).

II. X-Ray structure determination

Green-emitting block crystals of benzyl pyrene-1-carboxylate (**1**) were obtained by slow evaporation of a MeOH solution in refrigerator. Block crystals of Pyren-1-yl acetate (**6**) were obtained by slow evaporation of its hexane solution at room temperature. X-Ray single-crystal diffraction data were collected on a Oxford Xcalibur E CCD area-detector diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) with ω scan mode. The crystal parameters, data collection and refinement results for these compounds are summarized in Table S1.

Table S1. Crystallographic Data for benzyl pyrene-1-carboxylate (**1**).

	1	**6**
empirical formula	$C_{24}H_{16}O_2$	$C_{18}H_{12}O_2$
formula weight (M)	336.37	260.28
temperature (K)	295	293
wavelength (Å)	0.71073	0.71073
crystal system	monoclinic	orthorhombic
space group	*P*-1	*P*-21
a (Å)	10.9965(6)	5.4969(3)
b (Å)	11.8076(8)	10.7350(7)
c (Å)	13.2007(7)	22.1474(12)
α (deg)	90	90
β (deg)	92.894(5)	90
γ (deg)	90	90
V (Å^3)	1711.82(17)	1306.90(14)
Z	4	4
D_{calc} (g cm^{-3})	1.305	1.323
μ (mm^{-1})	0.649	0.086
F(000)	704.0	544.0
crystal size (mm)	0.80×0.70×0.60	0.40×0.40×0.35
reflns collected	9414	3432
unique reflns	3346	2353
R_{int}	0.0310	0.0450
goodness-of-fit on F^2	1.028	1.084
R_1, wR_2 [I >2σ(I)]	0.0556, 0.1730	0.0450, 0.1018

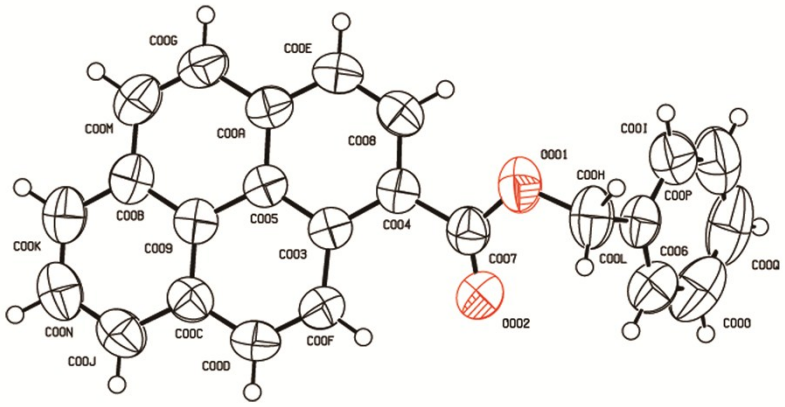


Figure S2. ORTEP drawing of the green-emitting single crystal of **1** with 50% probability thermal ellipsoids.

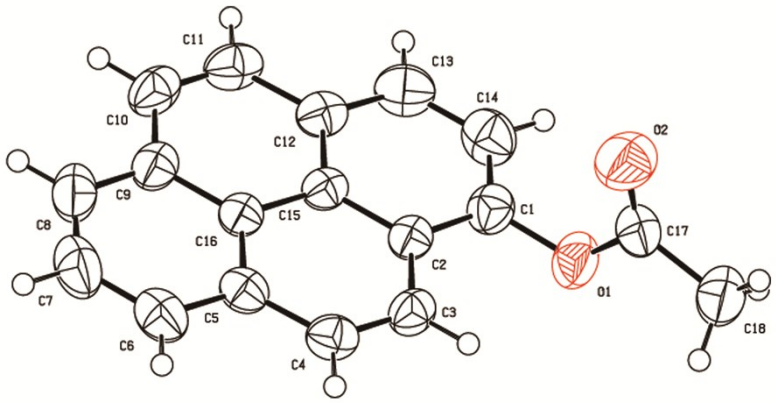


Figure S3. ORTEP drawing of the single crystal of **6** with 50% probability thermal ellipsoids.

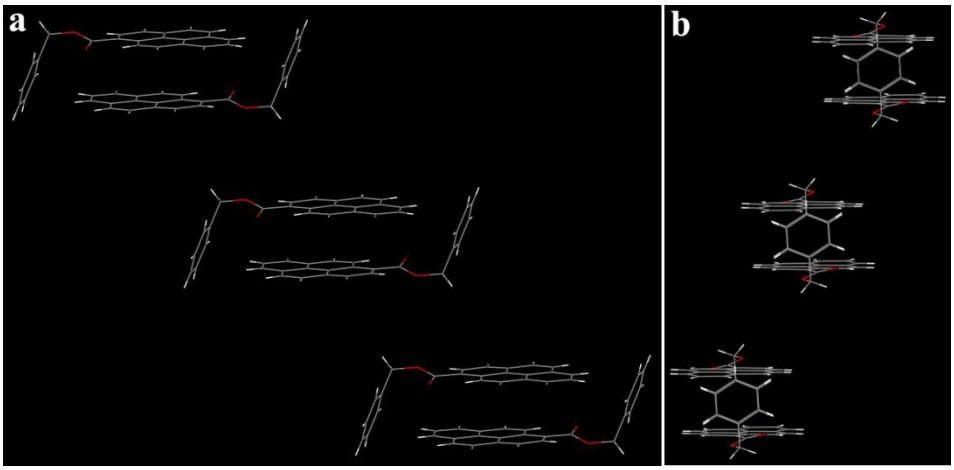


Figure S4. Molecular stacking of the the green-emitting single crystal of **1**: side view (a) and front view (b).

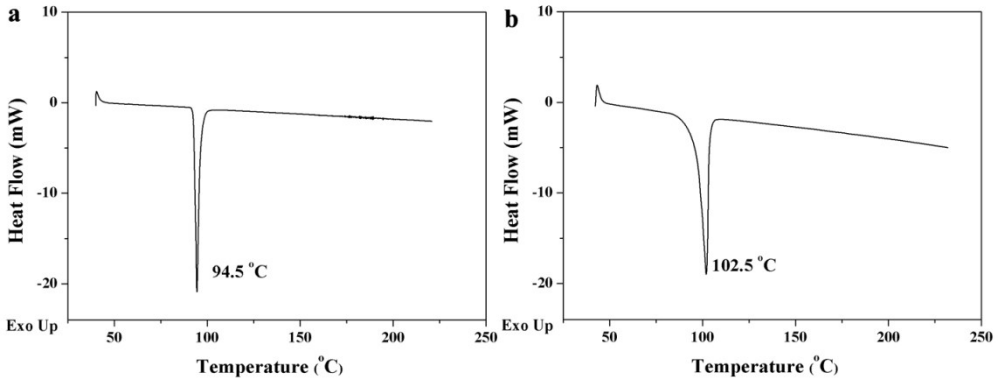
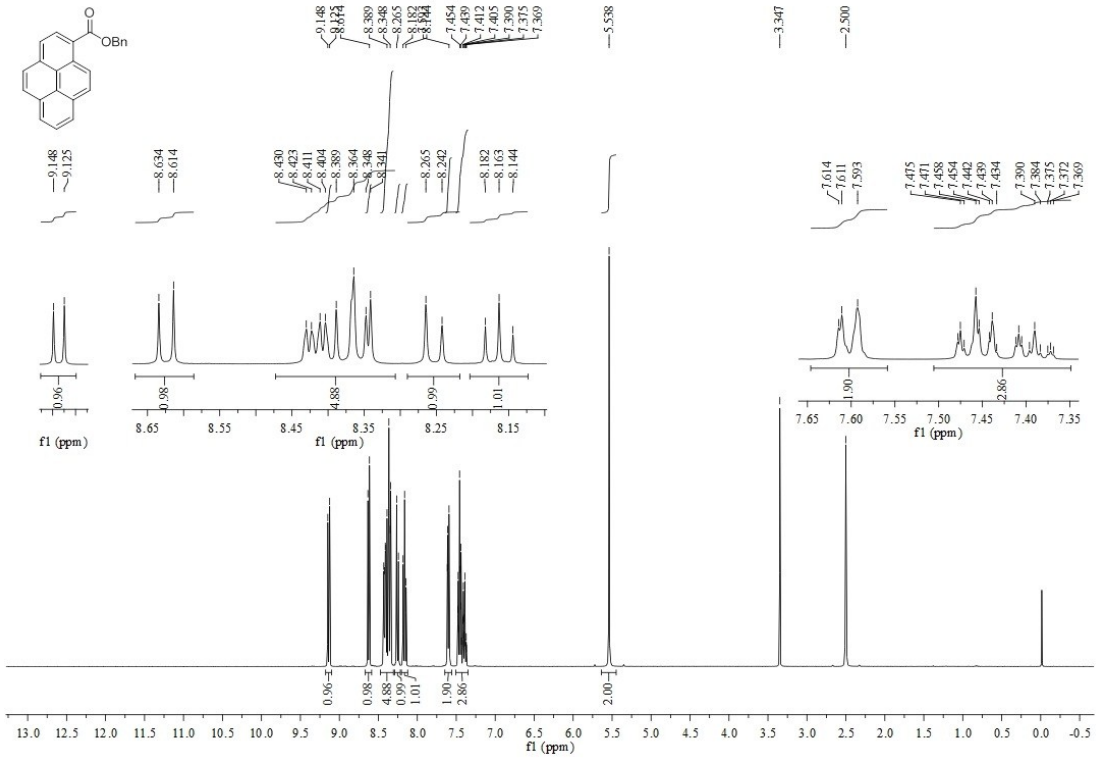
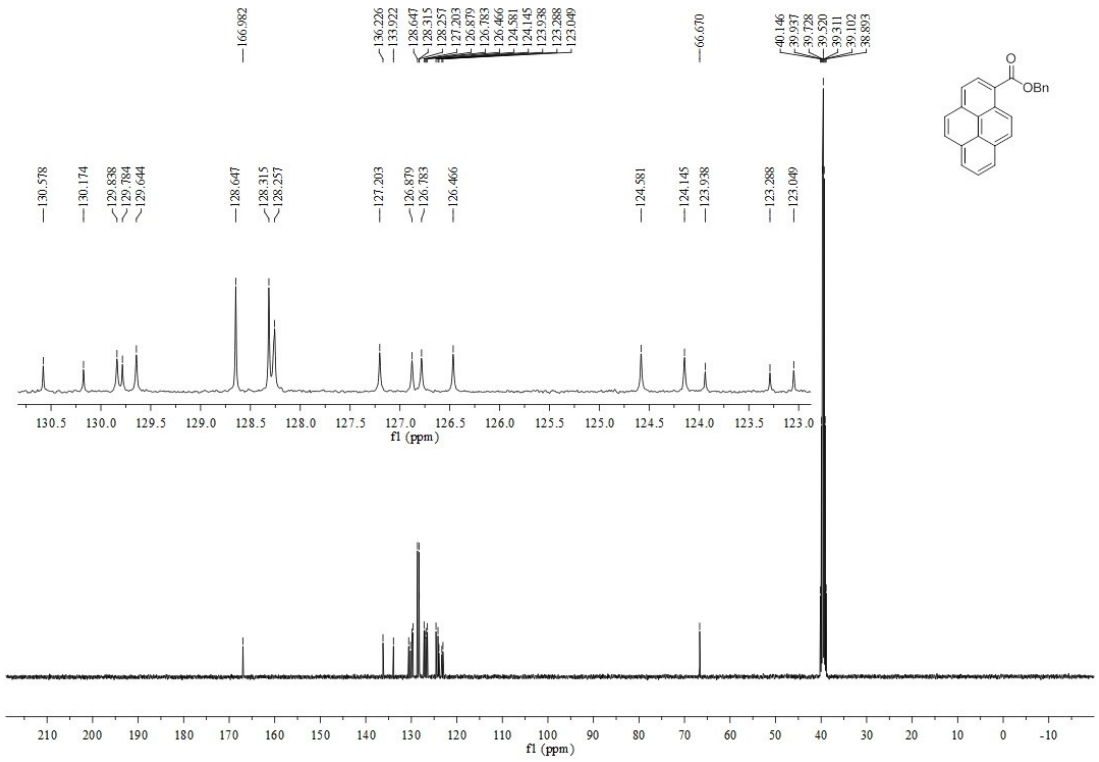
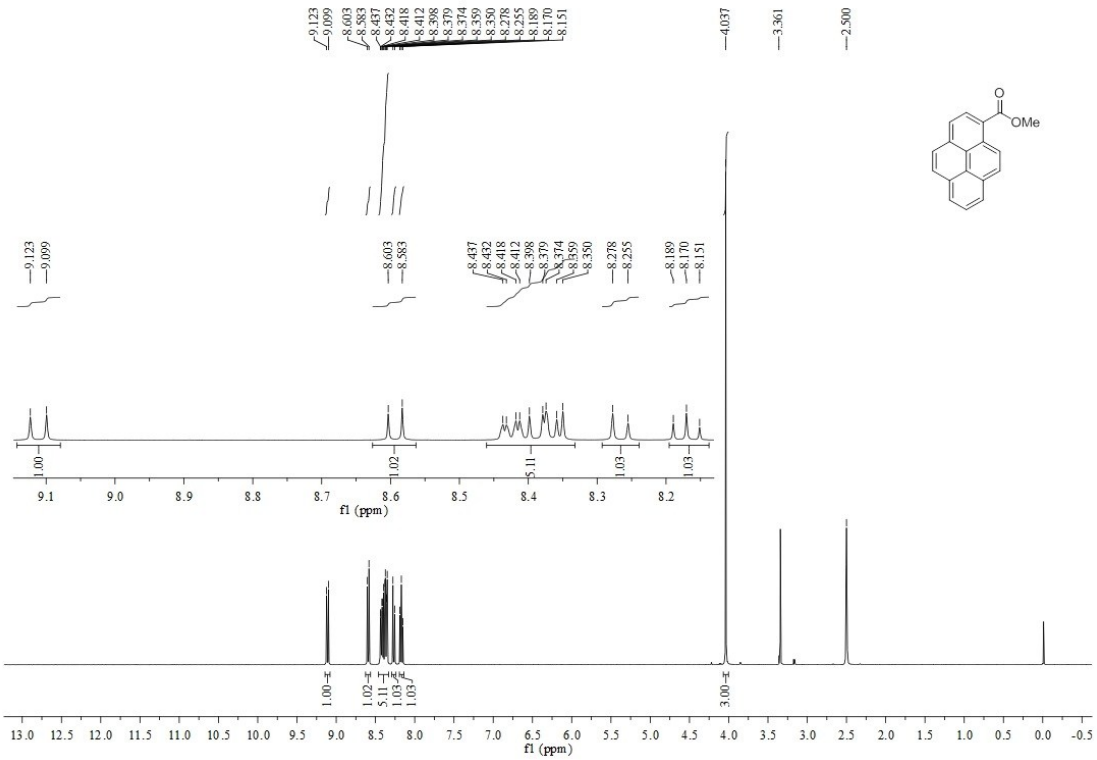


Figure S5. DSC curves (first heating) of crystals of **1**: (a) the blue-emitting crystals; and (b) the green-emitting crystals.

III. Copies of ^{1}H and ^{13}C spectra



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9.099
8.603
8.583
8.437
8.432
8.418
8.412
8.398
8.379
8.374
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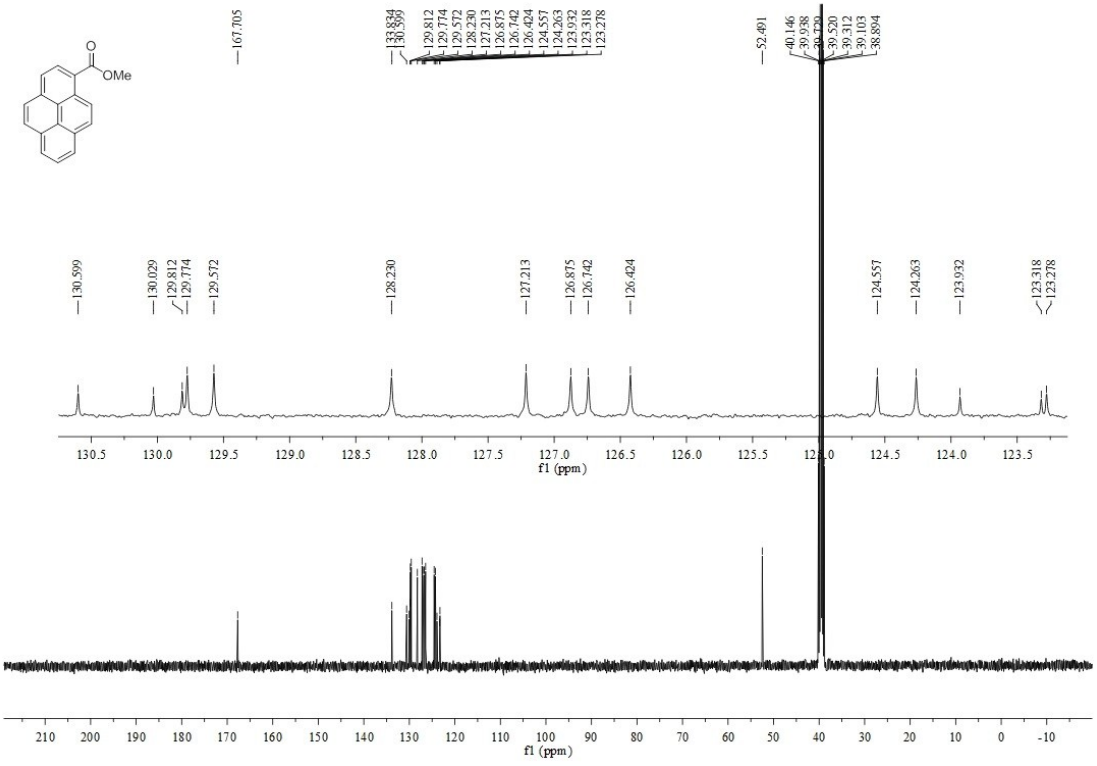
4.037
3.361
2.500
OMe
f1 (ppm)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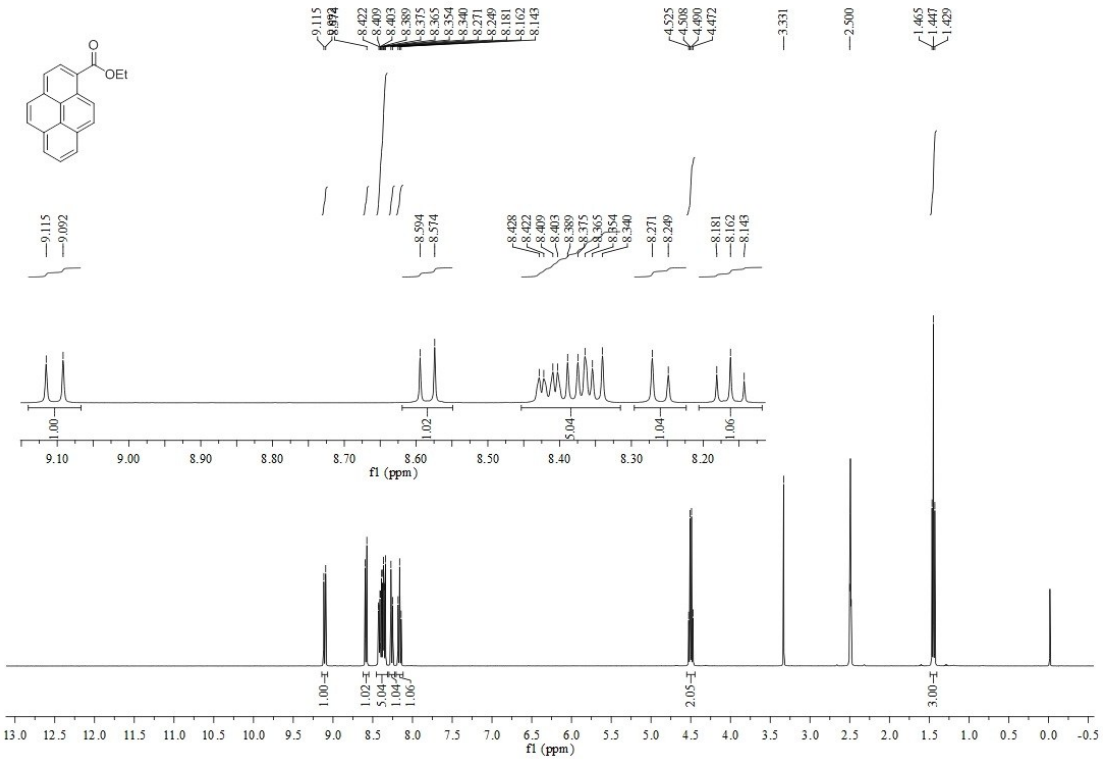
130.599
129.812
129.774
129.572
128.230
127.213
126.875
126.742
126.424
124.557
124.263
123.932
123.318
123.278
52.491
40.146
39.938
39.520
39.312
39.103
38.894
OMe
f1 (ppm)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8.574
8.428
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8.403
8.389
8.375
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8.354
8.340
8.271
8.249
8.181
8.162
8.143
4.525
4.508
4.490
4.472
3.331
2.500
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1.429
1.00
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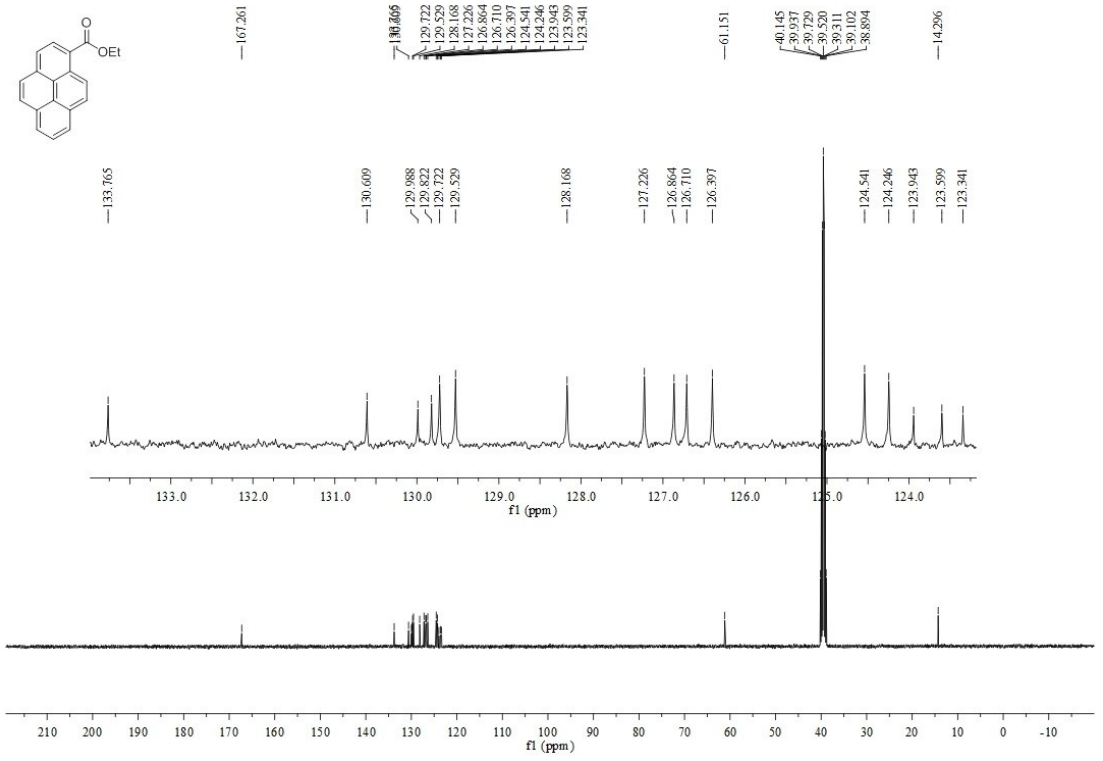
1.04
1.06
2.05
3.00
f1 (ppm)


OEt
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130.609
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127.226
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126.710
126.397
124.541
124.246
123.943
123.599
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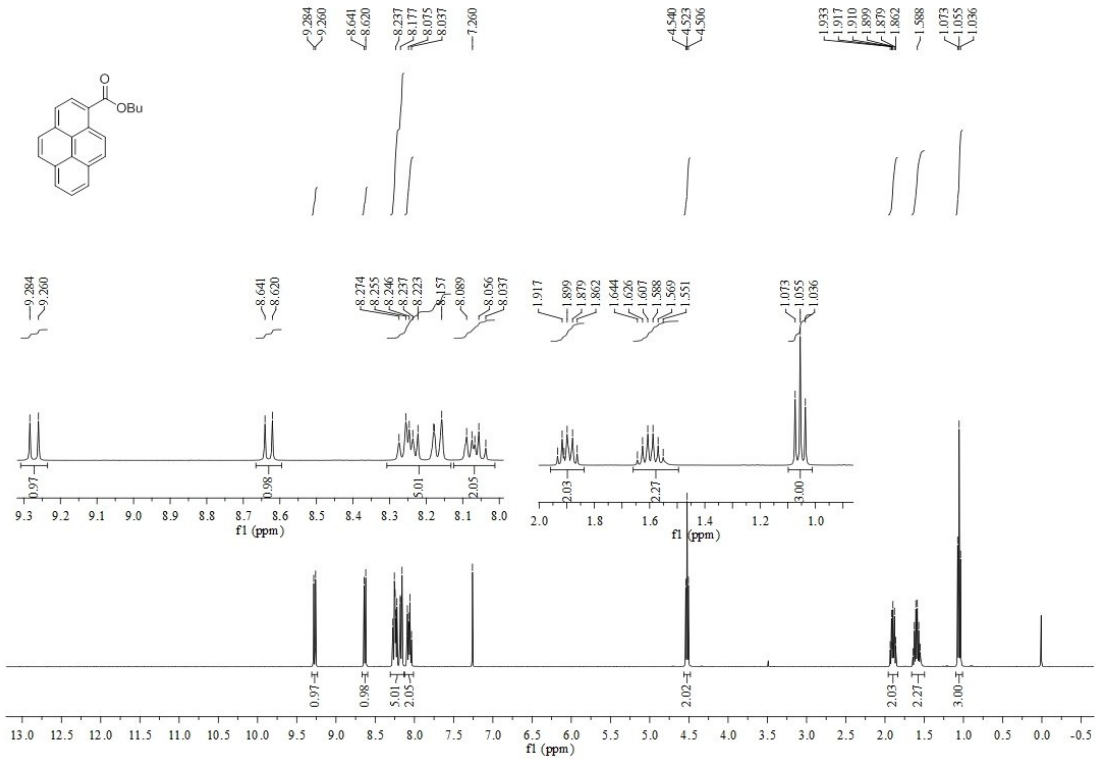
39.520
39.311
39.102
38.894
14.296
f1 (ppm)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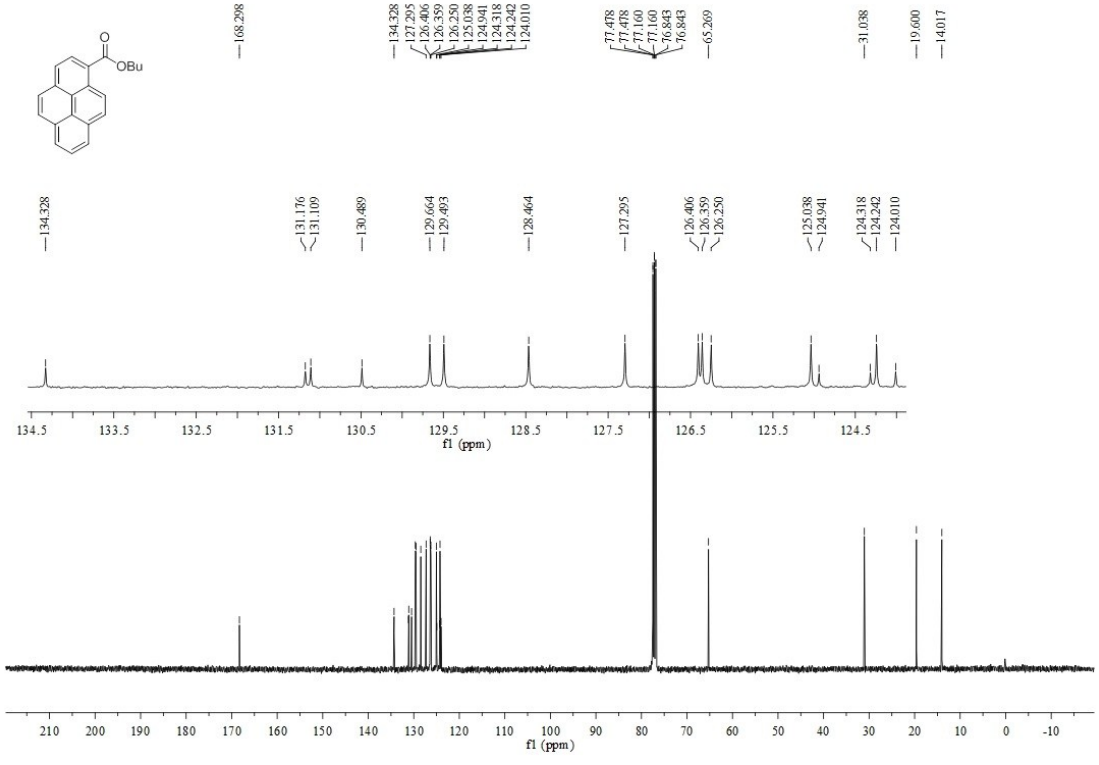
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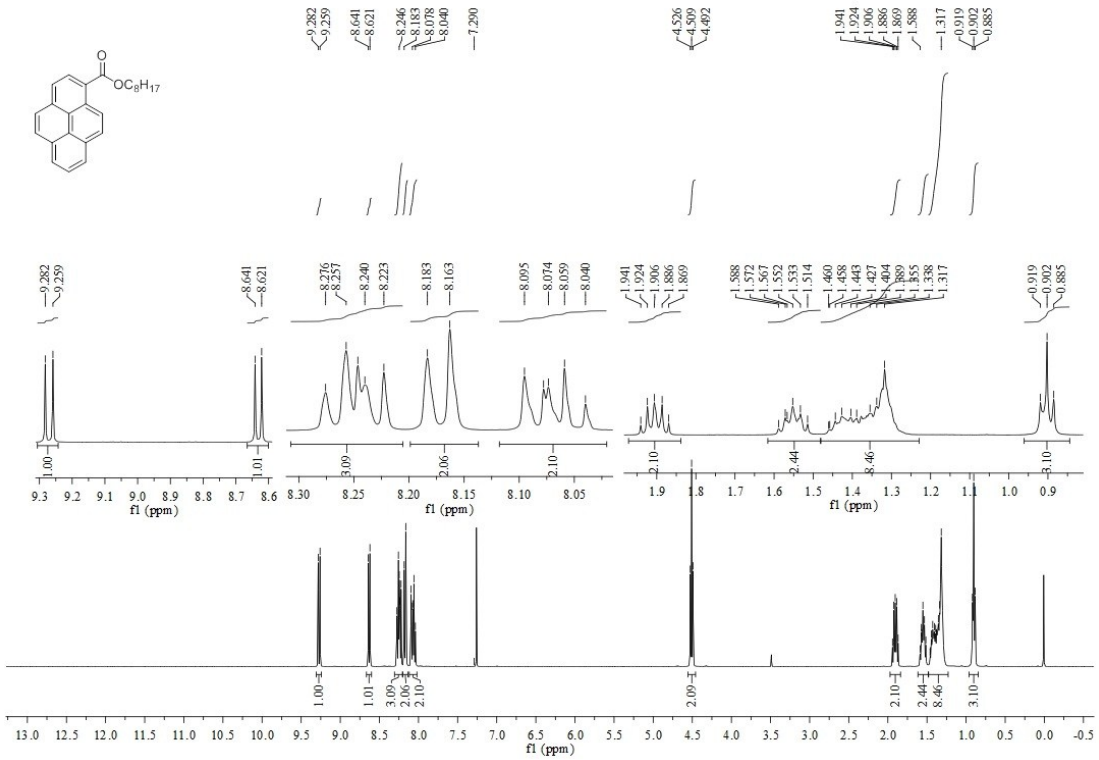
f1 (ppm)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8.621
8.246
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8.040
7.290
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4.509
4.492
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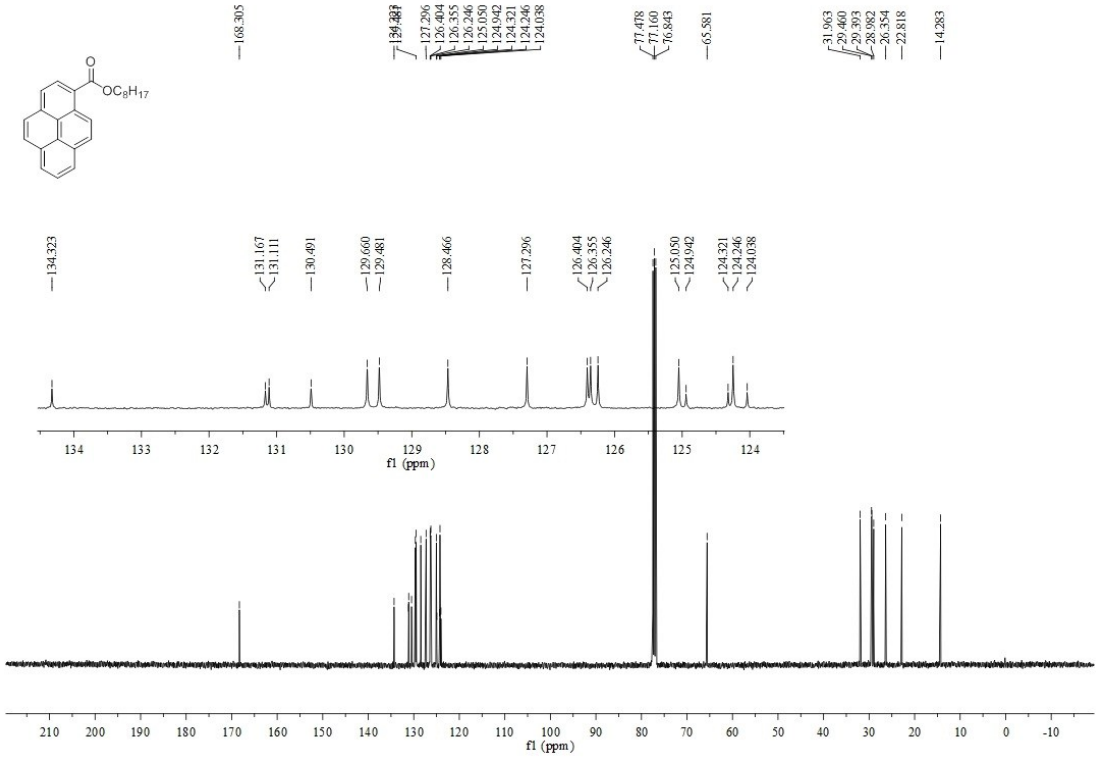
1.906
1.886
1.869
1.588
1.317
0.919
0.902
0.885
f1 (ppm)


OC8H17
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126.246
125.050
124.942
124.321
124.246
124.038
77.478
77.160
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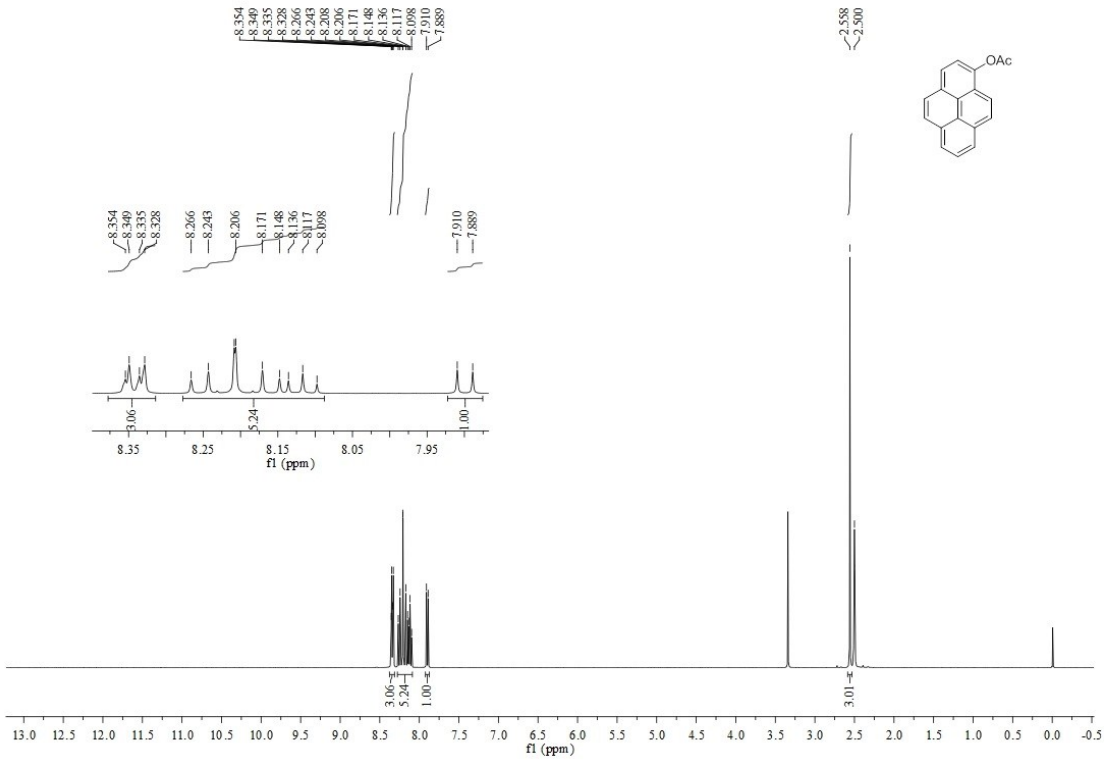
14.283
f1 (ppm)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2.500
OAc
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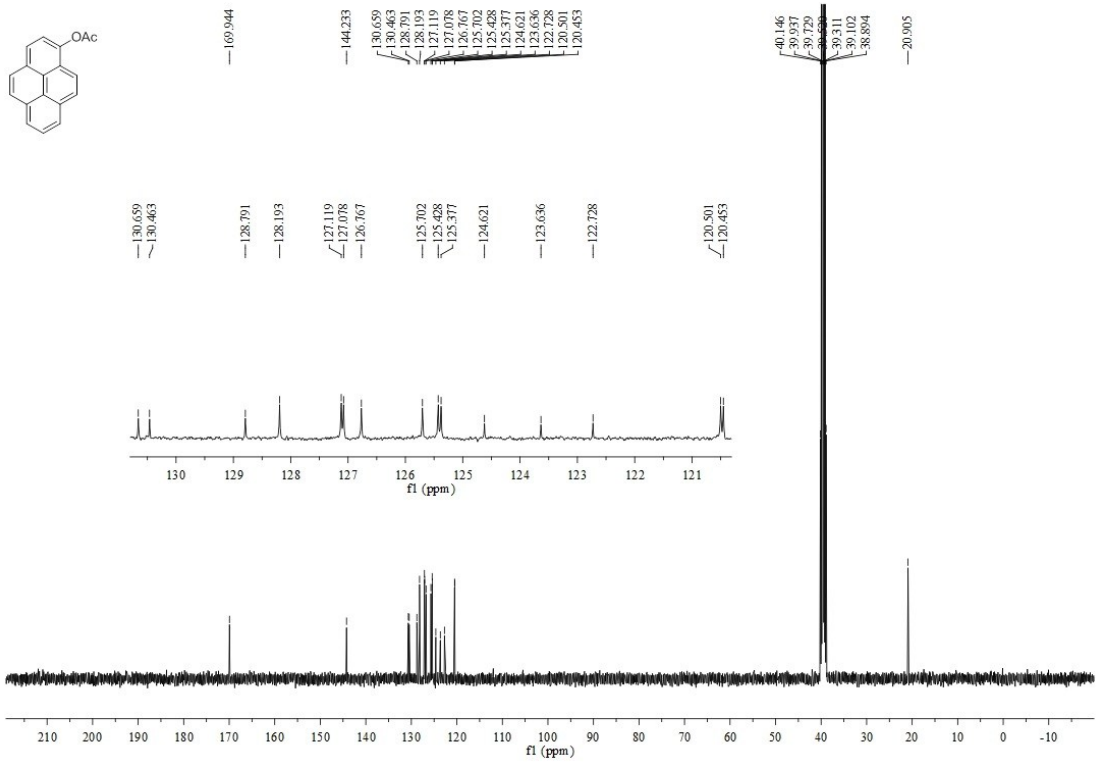
5.24
1.00
3.01
f1 (ppm)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125.377
124.621
123.636
122.728
120.501
120.453
40.146
39.937
39.729
39.311
39.102
38.894
20.905
f1 (ppm)