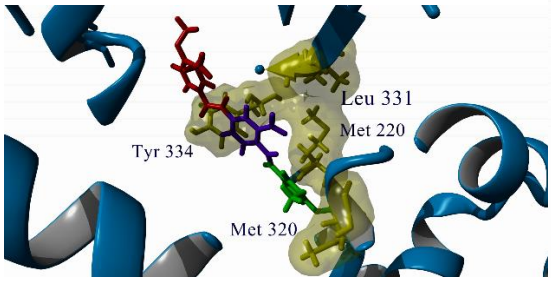
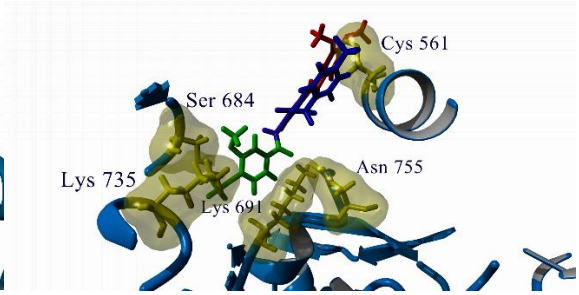
Supplementary material.

1. Predicted poses for compounds 2, 3 and 4 con the analyzed targets

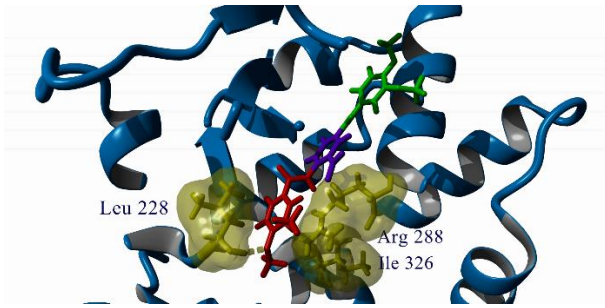
PPAR-alpha



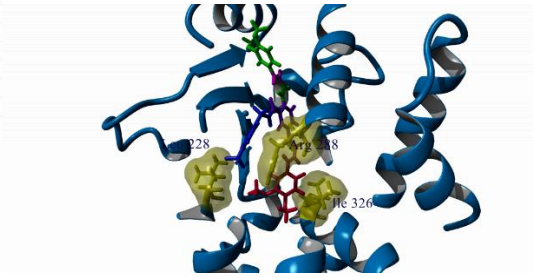
Compound **3**



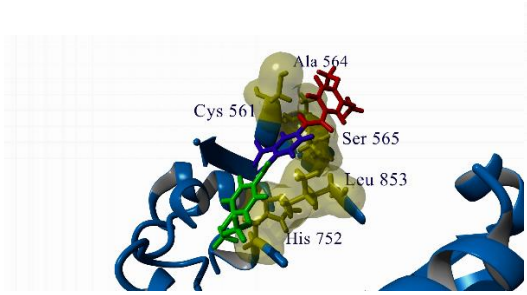
Compound **4**



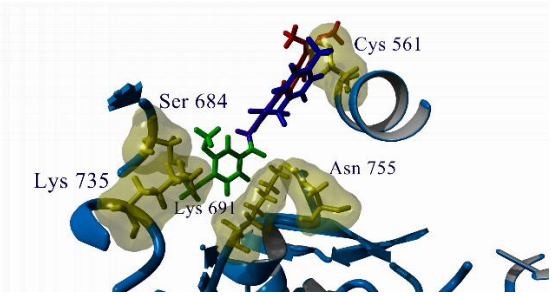
Compound **3**



Compound **4**

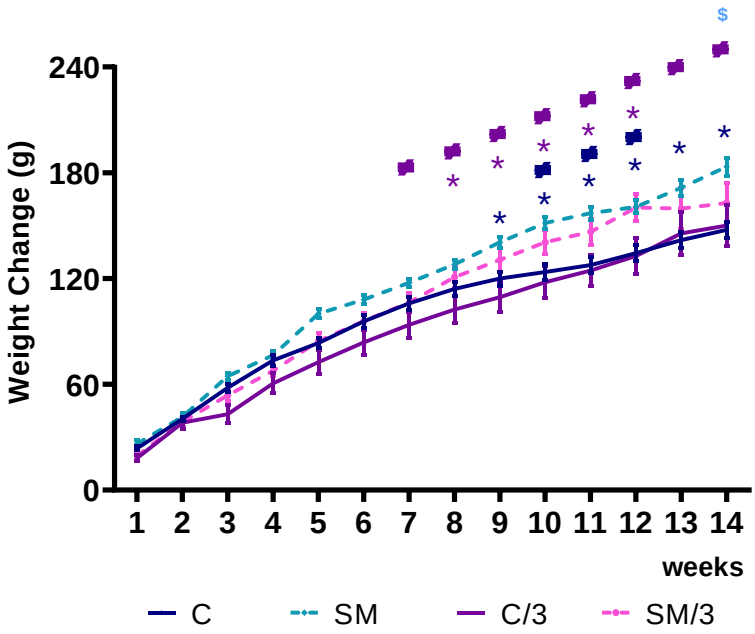


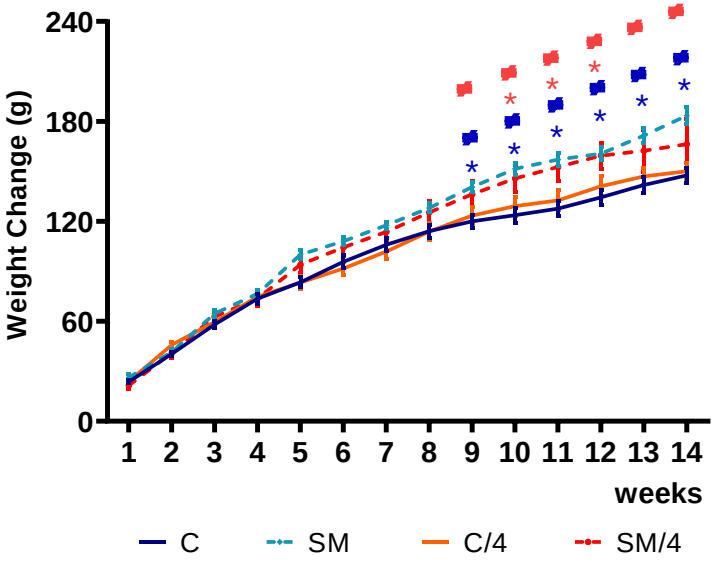
Compound **3**



Compound **4**

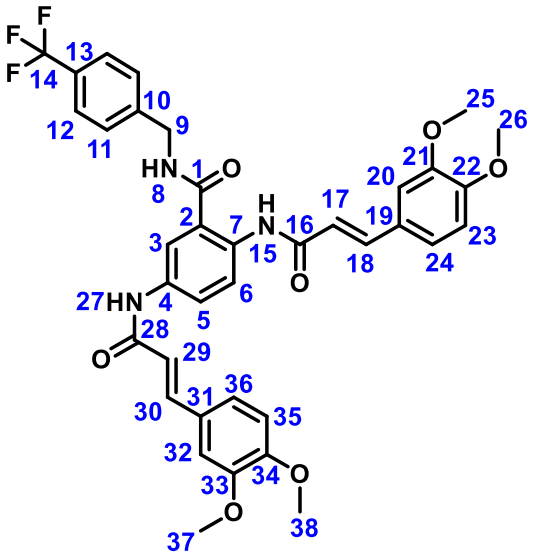
2. Weight variation during MetS induction and treatment with compounds **3** and **4** periods.





3. NMR spectra for compounds **3** and **4**

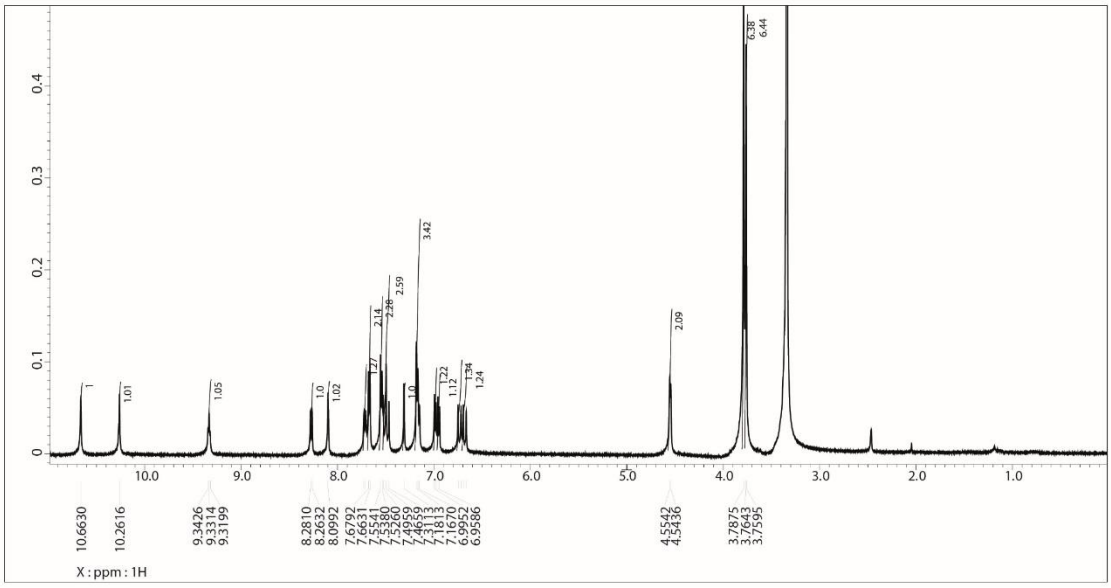
3.1 Compound **4**

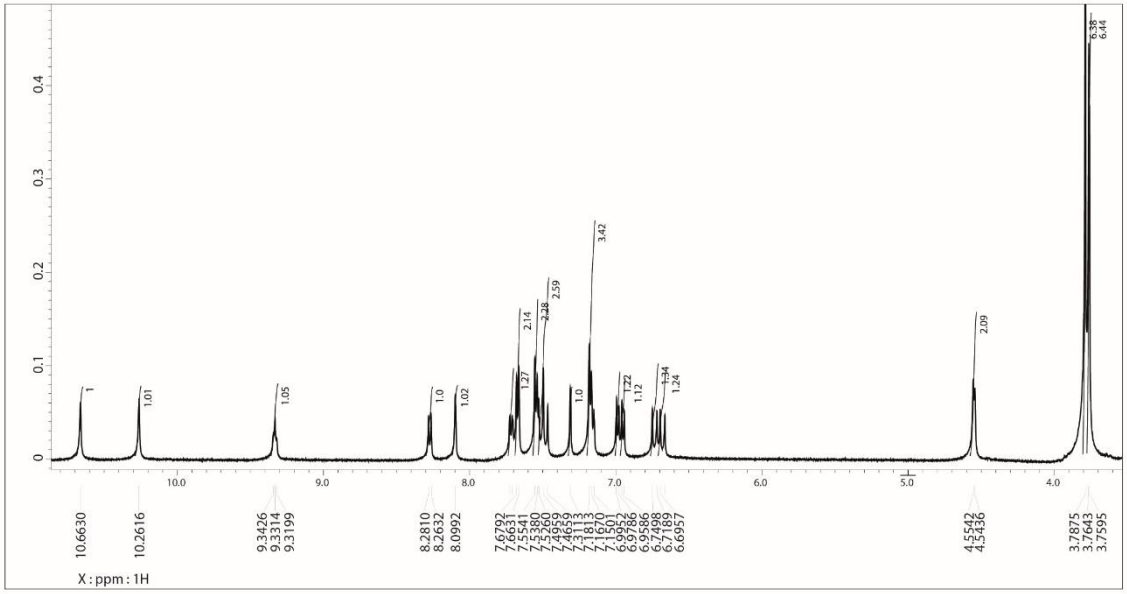


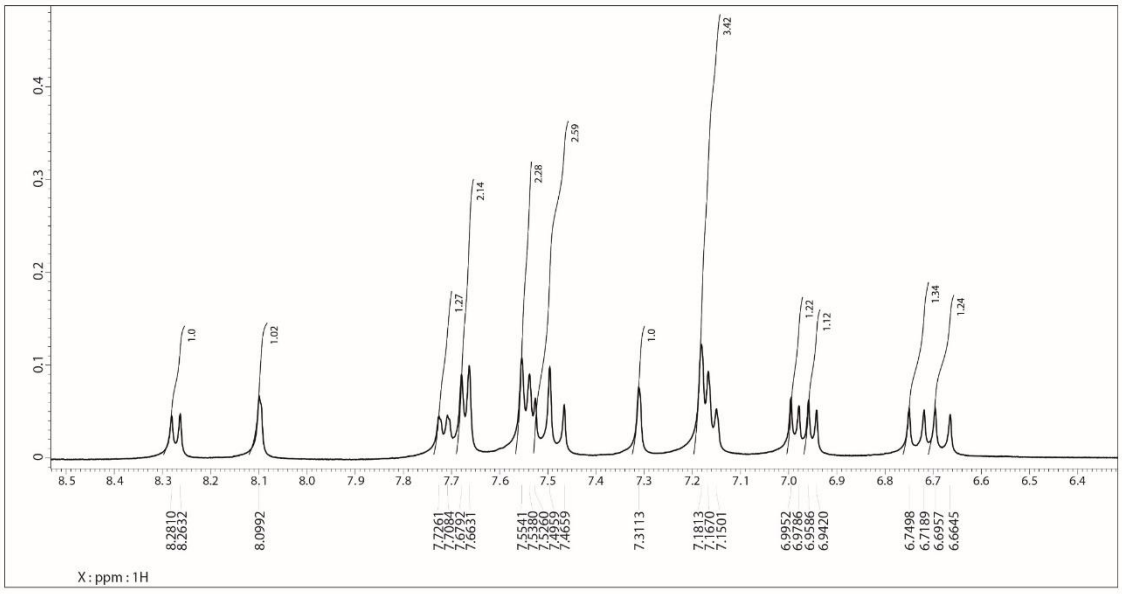
^{1}H NMR (DMSO-d$_6$, 500 MHz) δ: 10.66 (1H, s, **H15**), 10.26, (1H, s, **H27**), 9.33 (1H, t, J = 5.5 Hz, **H8**), 8.27 (1H, d, J = 8.9 Hz, **H6**), 8.09 (1H, $J_{H3,H5}$<2 Hz, **H3**), 7.71 (1H, d, J = 8.9 Hz, **H5**), 7.67 (2H, d, J = 8.0 Hz, **H12**) 7.54 (2H, d, J = 8.1 Hz, **H11**), 7.51 (1H, d, J = 15.0 Hz, **H30**), 7.48 (1H, d, J = 15.2 Hz, **H18**), 7.31 (1H, $J_{H3,H5}$<2 Hz, **H20**), 7.18 (1H, $J_{H3,H5}$<2 Hz, **H32**), 7.17 (1H, d, J = 8.4 Hz, **H24**), 7.15 (1H, d, J = 8.3 Hz, **H36**), 6.98 (1H, d, J = 8.3 Hz, **H35**), 6.95 (1H, d, J = 8.4 Hz, **H23**), 6.73 (1H, d, J = 15.2 Hz, **H17**), 6.68 (1H, d, J = 15.0 Hz, **H29**), 4.54 (2H, d, J = 5.5 Hz, **H9**), 3.79 (3H, s, **H37**), 3.79 (3H, s, **H38**), 3.76 (3H, s, **H25**), 3.75 (3H, s, **H26**).

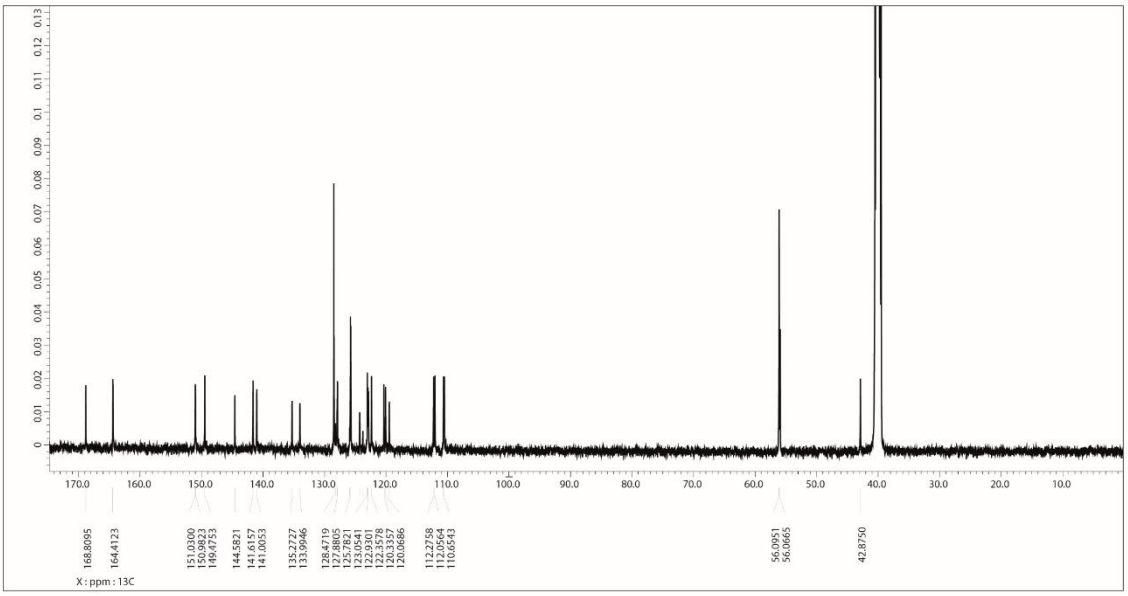
^{13}C {^{1}H} NMR (DMSO-d$_6$, 125 MHz) δ: 168.80 (**C1**), 164.41 (**C28**), 164. 37 (**C16**), 151.03 (**C33**), 150.98 (**C21**), 149.47 (**C22**), 149.44 (**C34**), 144.58 (**C10**), 141.61 (**C18**), 141.00 (**C30**), 135.22 (**C7**), 133.99 (**C4**), 128.47 (**C11**), 127.92 (**C19**), 127.77 (**C13**), 127.88 (**C31**), 125.78 (**C12**), 124.26 (**C2**) 123.76 (**C14**), 123.05 (**C24**), 122.93 (**C6**), 122.88 (**C5**), 122.35 (**C36**), 120.33 (**C17**), 120.06 (**C29**), 119.46 (**C3**), 112.27 (**C35**), 112.05 (**C23**), 110.65 (**C20**), 110.53 (**C32**), 56.09 (**C37, C38**), 56.06 (**C26**), 55.93 (**C25**), 42.87 (**C9**).

^{19}F {^{1}H} NMR (DMSO-d$_6$, 470 MHz) δ: 4.32 (**F**).

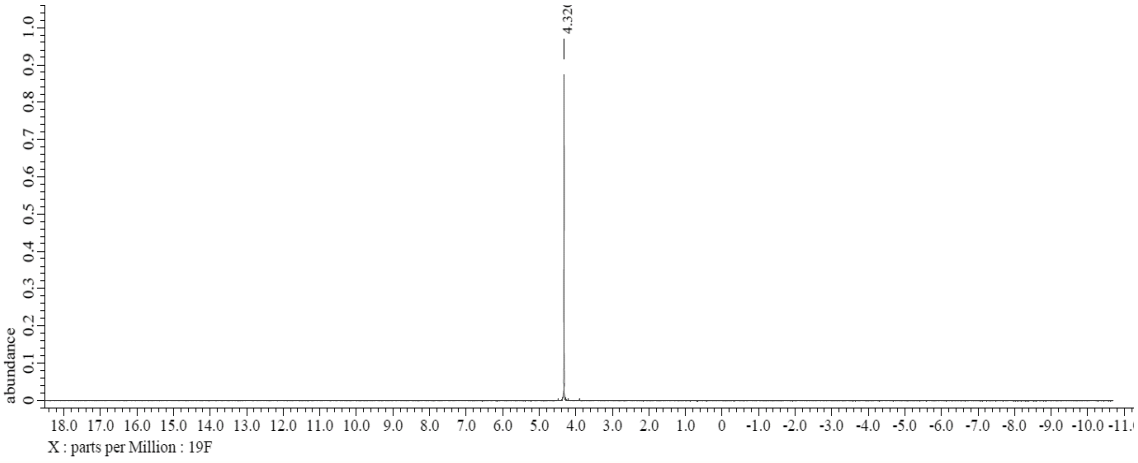

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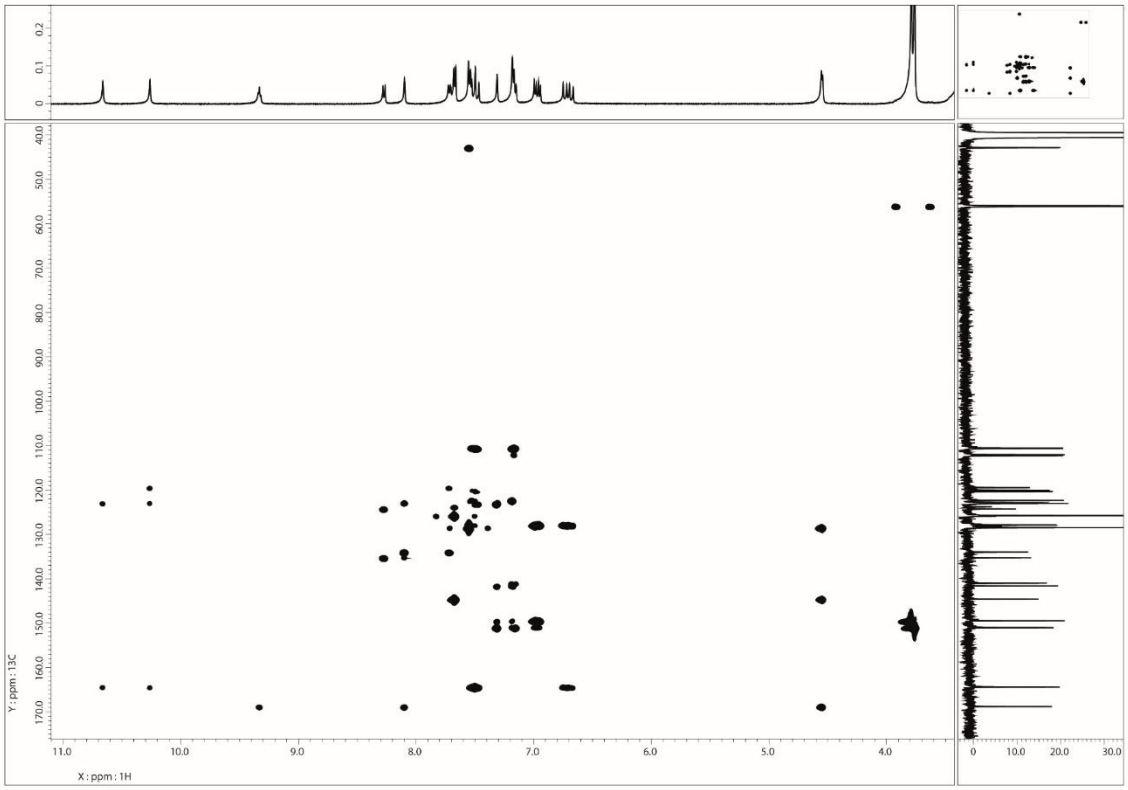

X : ppm : 1H


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2.28
2.59
1.0
3.42
1.22
1.12
1.34
1.24
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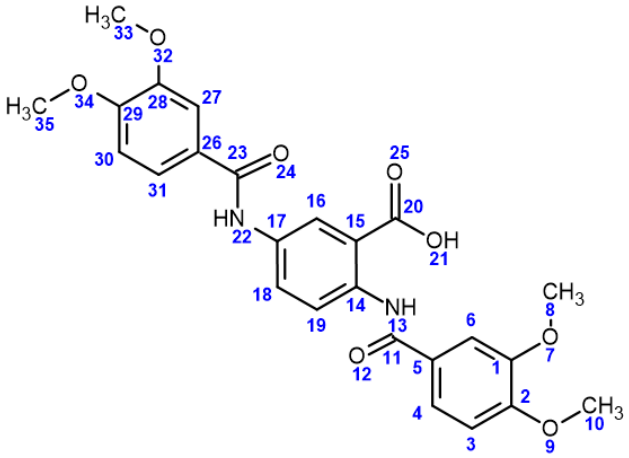

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150.9823
149.4753
144.5821
141.6157
141.0053
135.2727
133.9946
128.4719
127.9805
125.7821
123.0541
122.9301
121.3578
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1.

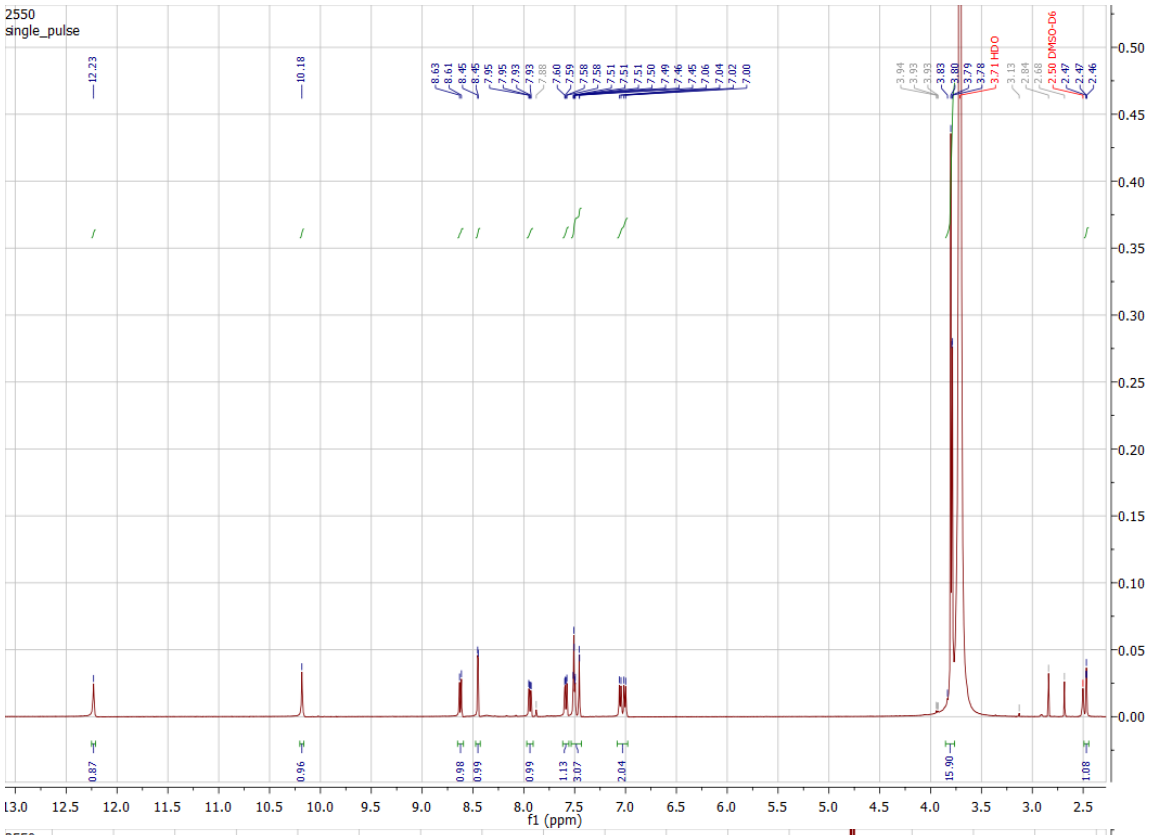


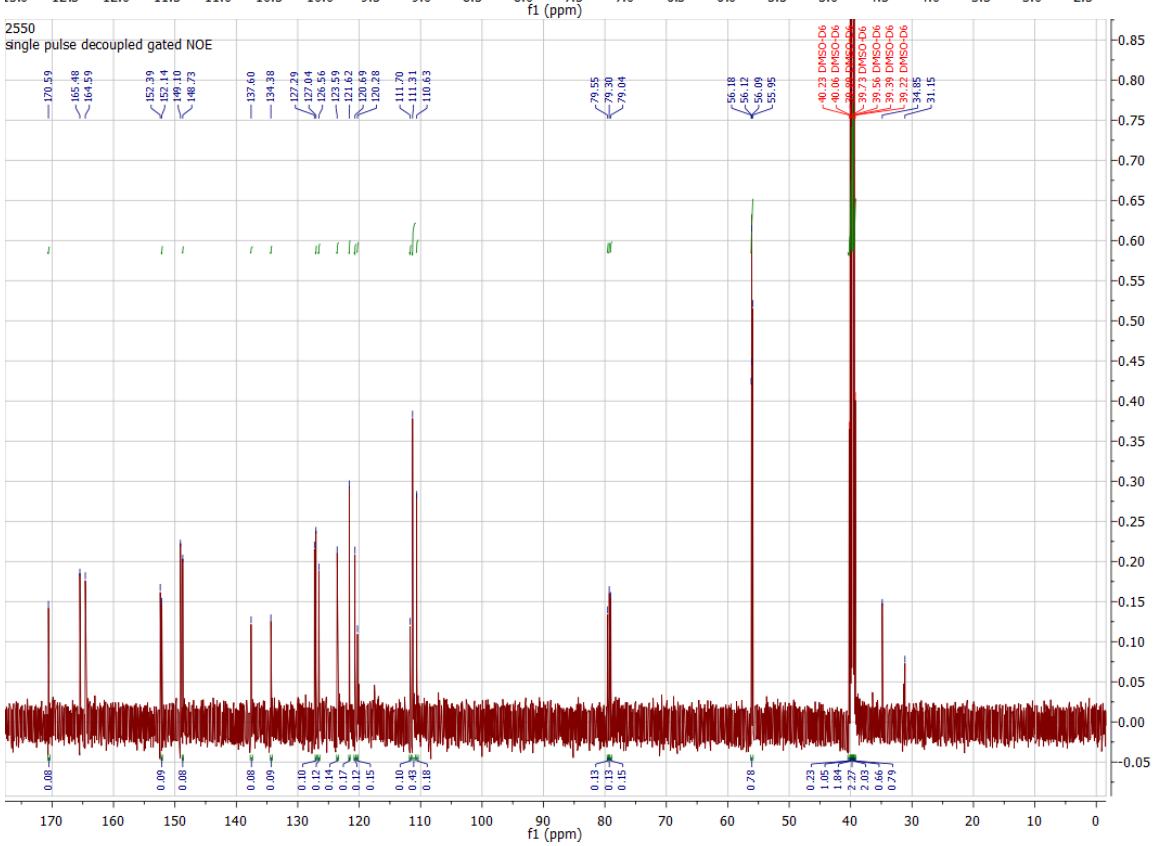


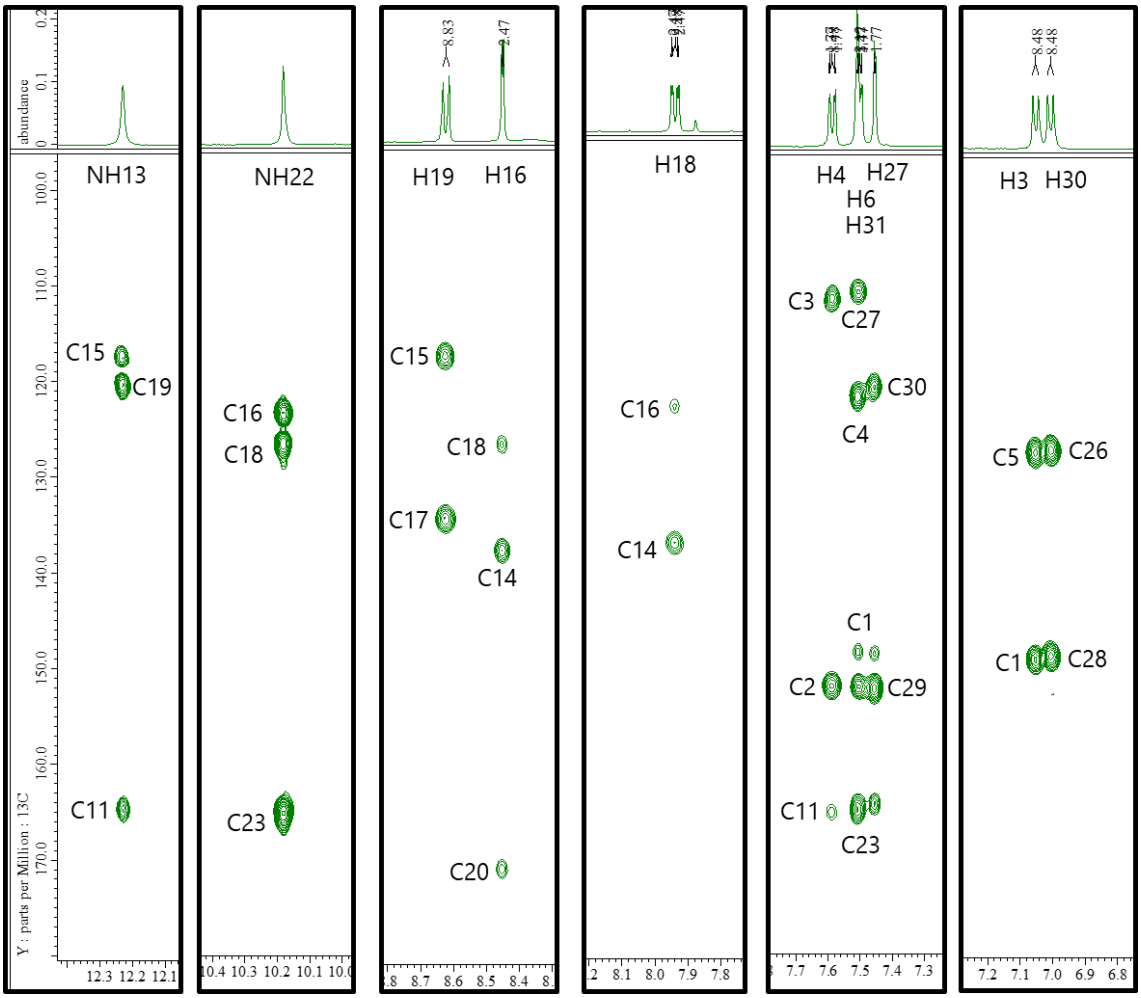
3.2 Compound **3**

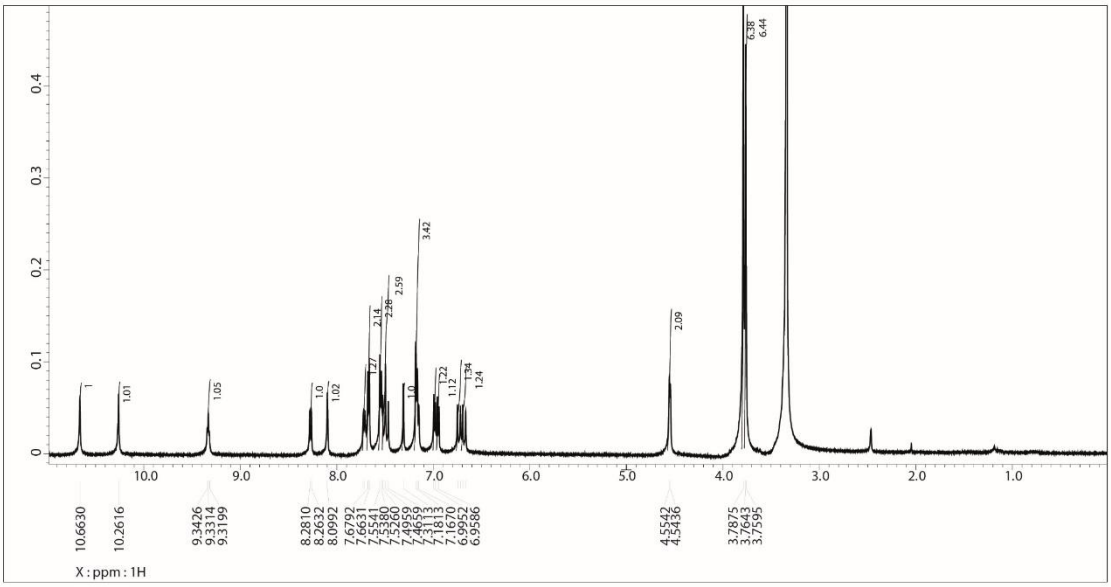


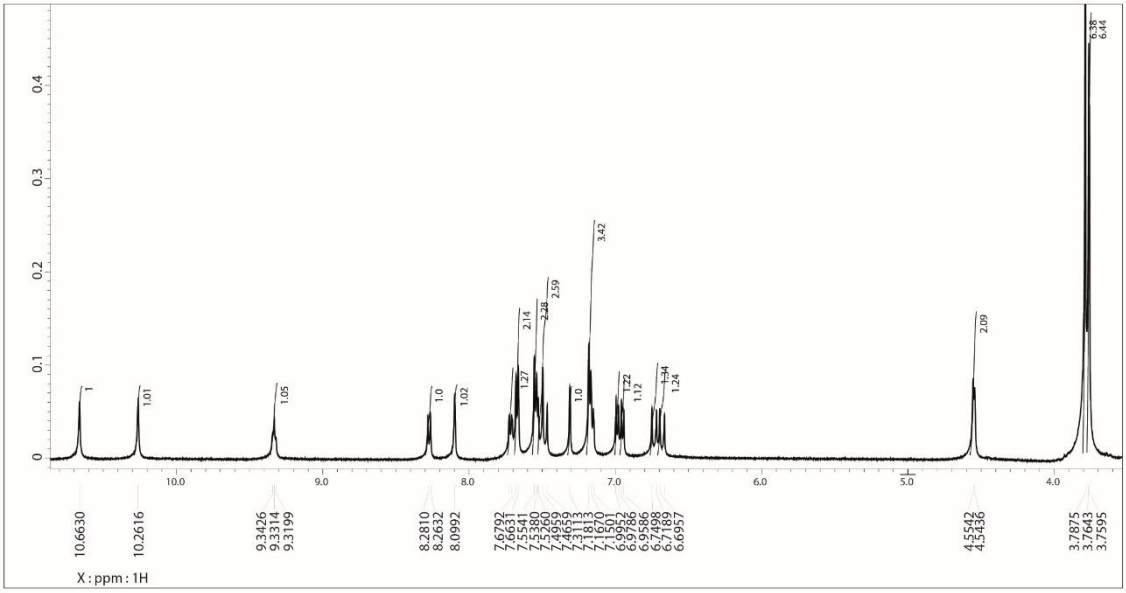
^{1}H NMR (DMSO-d_6, 500 MHz): δ = 12.23 (1H, s, H13), 10.18 (1H, s, H22), 8.62 (1H, d, J = 8.8 Hz, H19), 8.45 (1H, d, J = 2.5 Hz, H16), 7.94 (1H, dd, J = 8.8, 2.5 Hz, H18), 7.58 (1H, dd, J = 8.5, 1.8 Hz, H4), 7.51 (1H, d, J = 1.8 Hz, H6) 7.50 (1H, dd, J = 8.5, 1.8 Hz, H31), 7.45 (1H, d, J = 1.8 Hz, H27), 7.05 (1H, d, J = 8.5 Hz, H3), 7.01 (1H, d, J = 8.5 Hz, H30), 3.80 (6H, s, H10, H35), 3.79 (3H, s, H8*), 3.76 (3H, s, H32*), the assignment could be change. ^{13}C{^{1}H} NMR (DMSO-d_6, 125 MHz) δ: 170.60 C20), 165.49 (C23), 164.59 (C11), 152.39 (C2), 152.14 (C29), 149.10 (C1), 148.73 (C28), 137.60 (C14), 134.38 (C17), 127.29 (C5), 127.04 (C26), 126.57 (C18), 123.59 (C16), 121.62 (C4), 120.69 (C31), 120.30 (C19), 117.53 (C15), 111.70 (C3), 111.31 (C6, C30), 110.63 (C27), 56.18 (C10), 56.12 (C35), 56.09 (C8), 55.95 (C32).

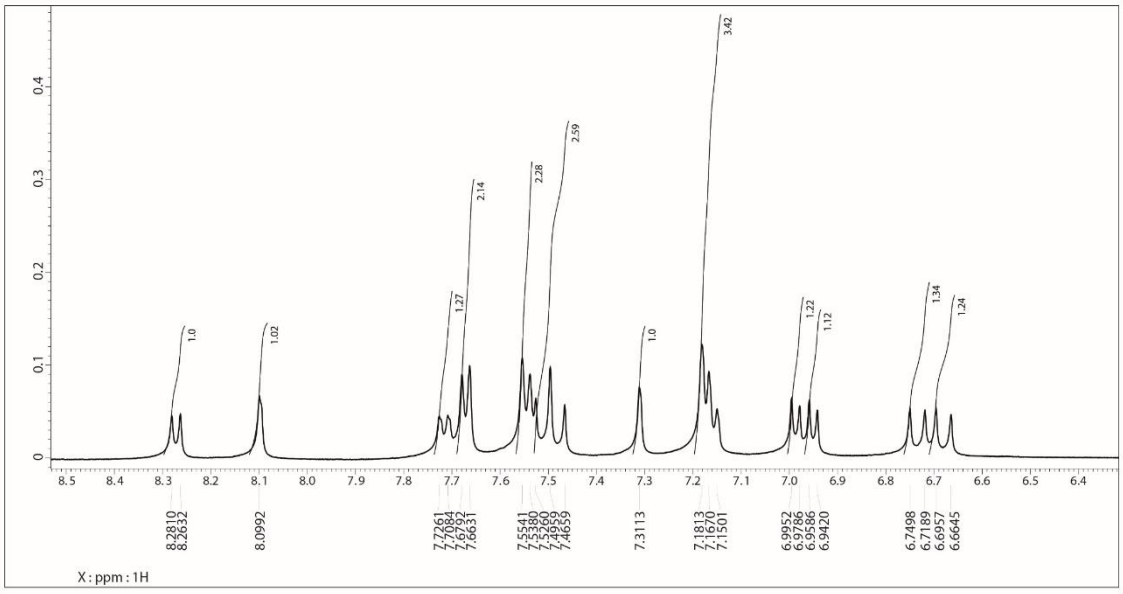

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single_pulse
f1 (ppm)

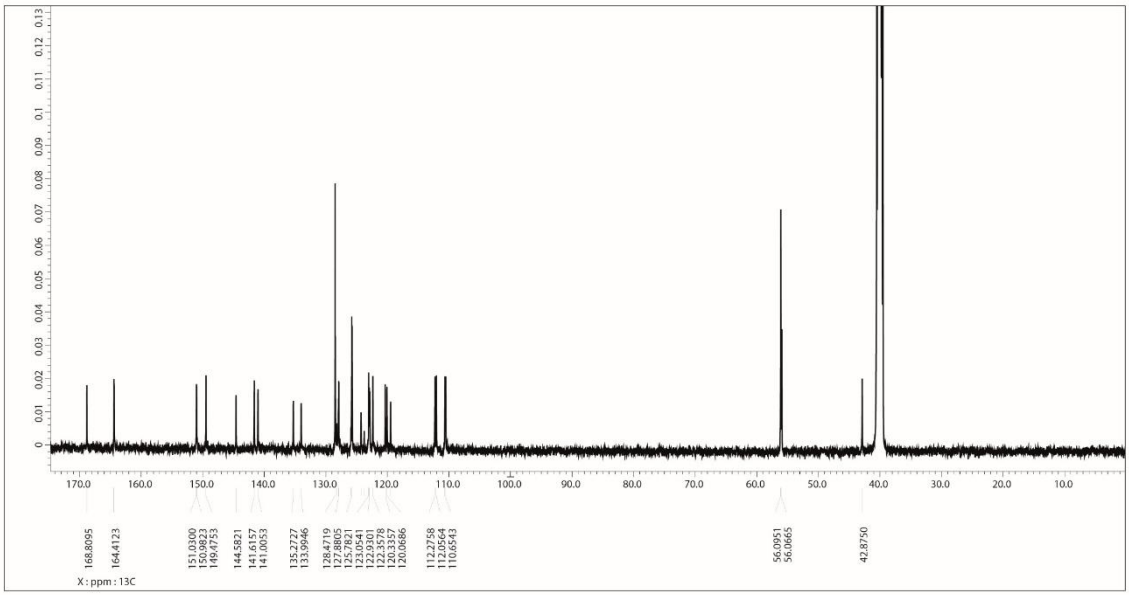

2550
single pulse decoupled gated NOE
f1 (ppm)

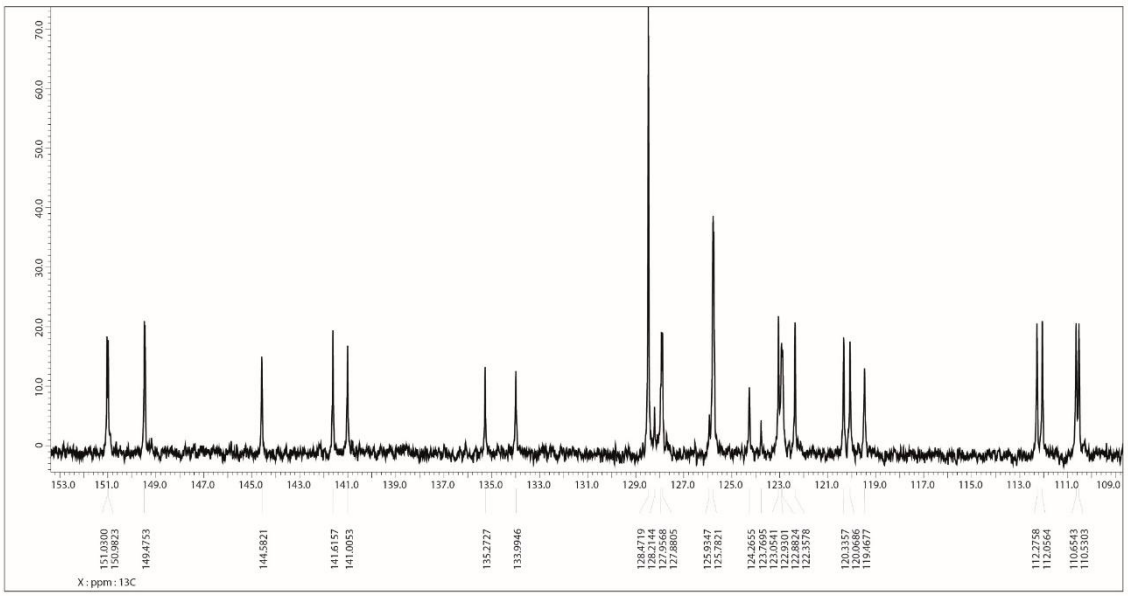

abundance
NH13
NH22
H19
H16
H18
H4
H27
H6
H31
H3
H30
Y : parts per Million : 13C
C15
C19
C16
C18
C15
C18
C17
C14
C16
C14
C3
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C23
C11
C23
C20

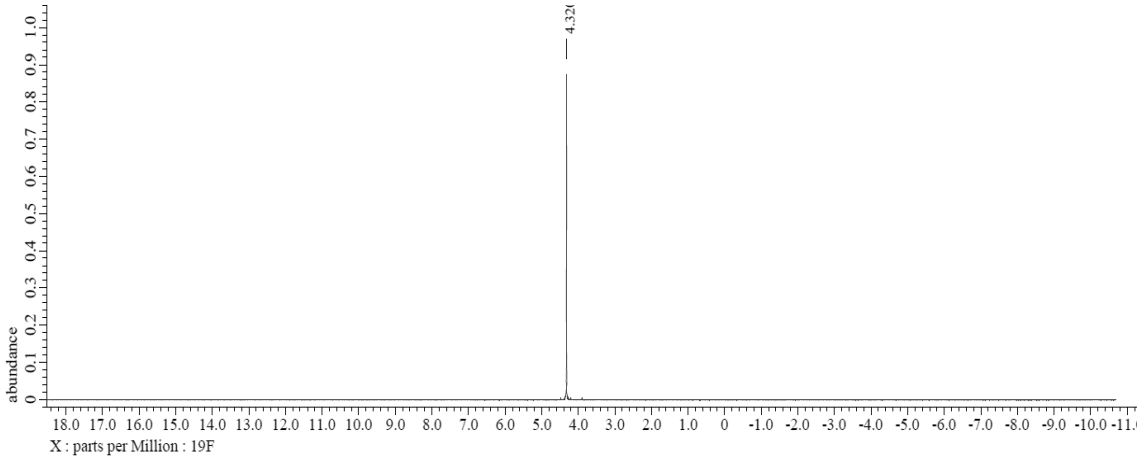

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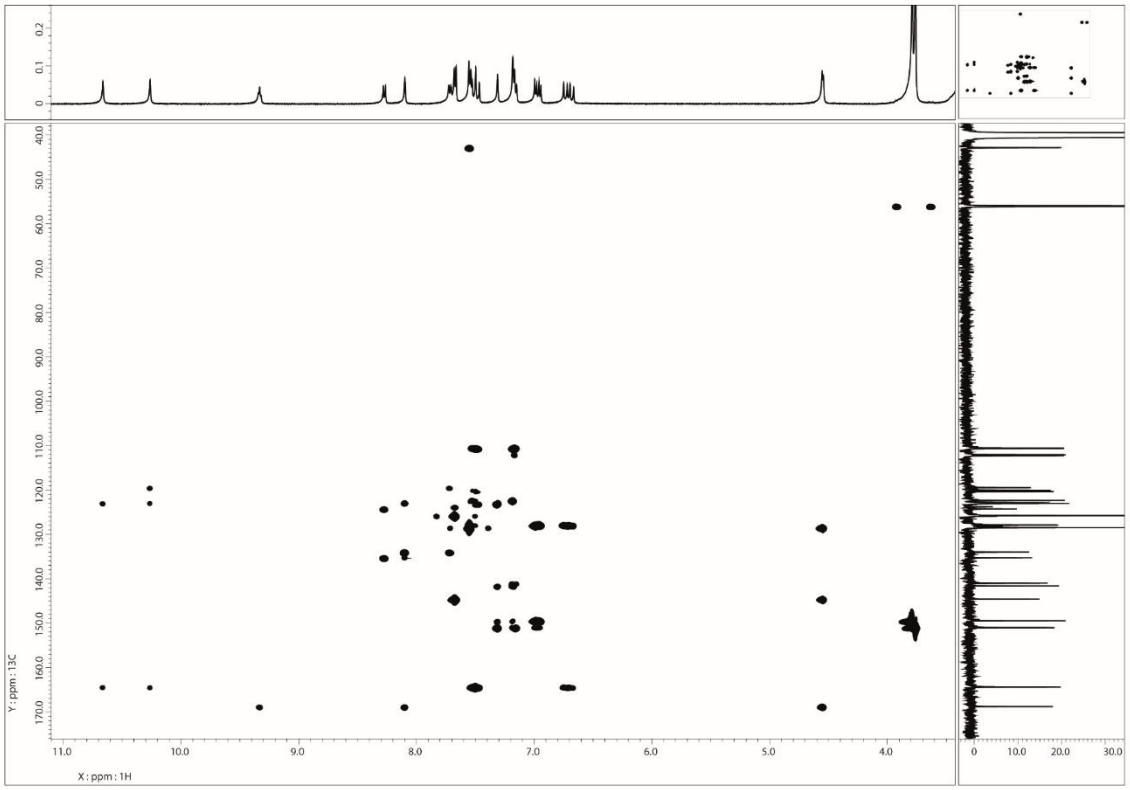

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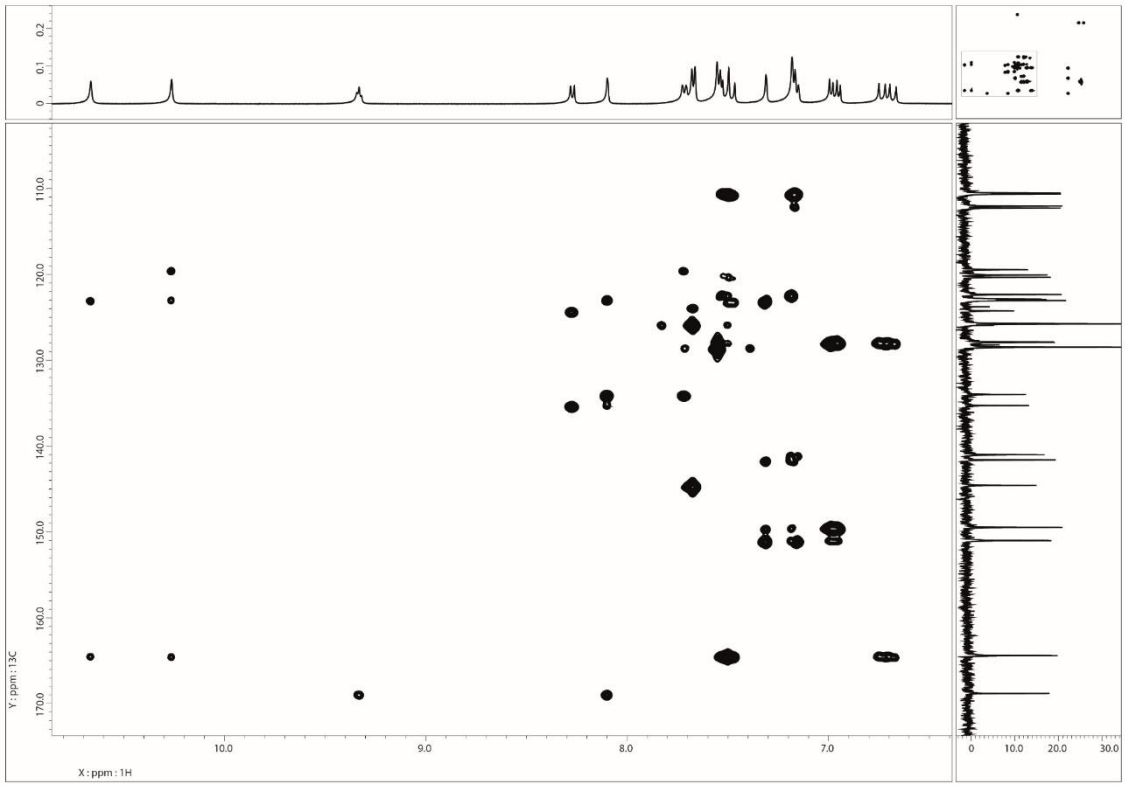

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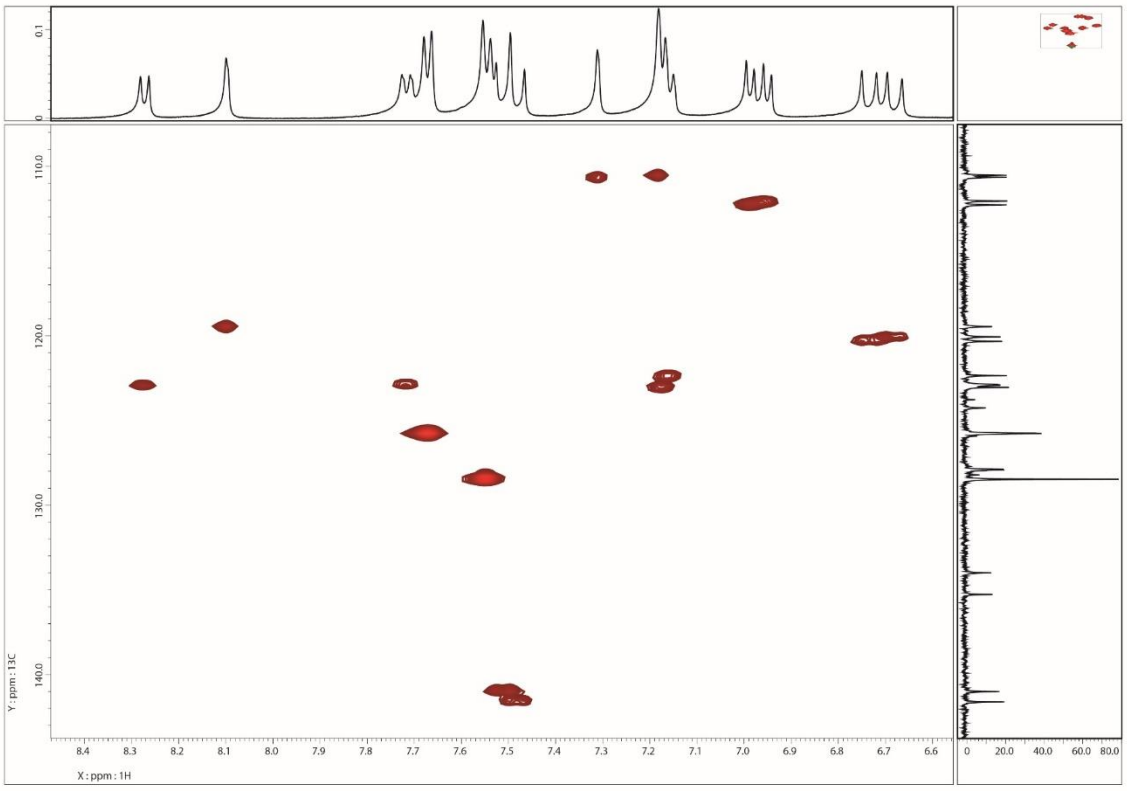

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X : ppm : 13C


abundance
X : parts per Million : 19F


Y: ppm : 13C
X : ppm : 1H


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X : ppm : 1H
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20.0
30.0


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7.7
7.6
7.5
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