

## Supplementary data

# Anticancer Potential of Novel Symmetrical and Asymmetrical Dihydropyridines Against Breast Cancer *via* EGFR Inhibition: Molecular Design, Synthesis, Analysis and Screening

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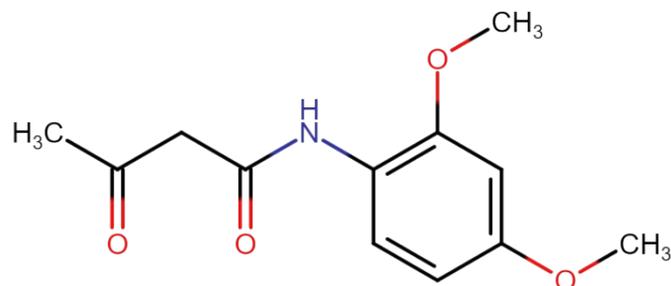
<sup>b</sup> Department of Pharmaceutical Chemistry, RAK Medical & Health Sciences University, Ras Al Khaimah, UAE.

<sup>c</sup> Department of Pharmaceutics, College of Pharmacy, King Khalid University, Abha, Saudi Arabia.

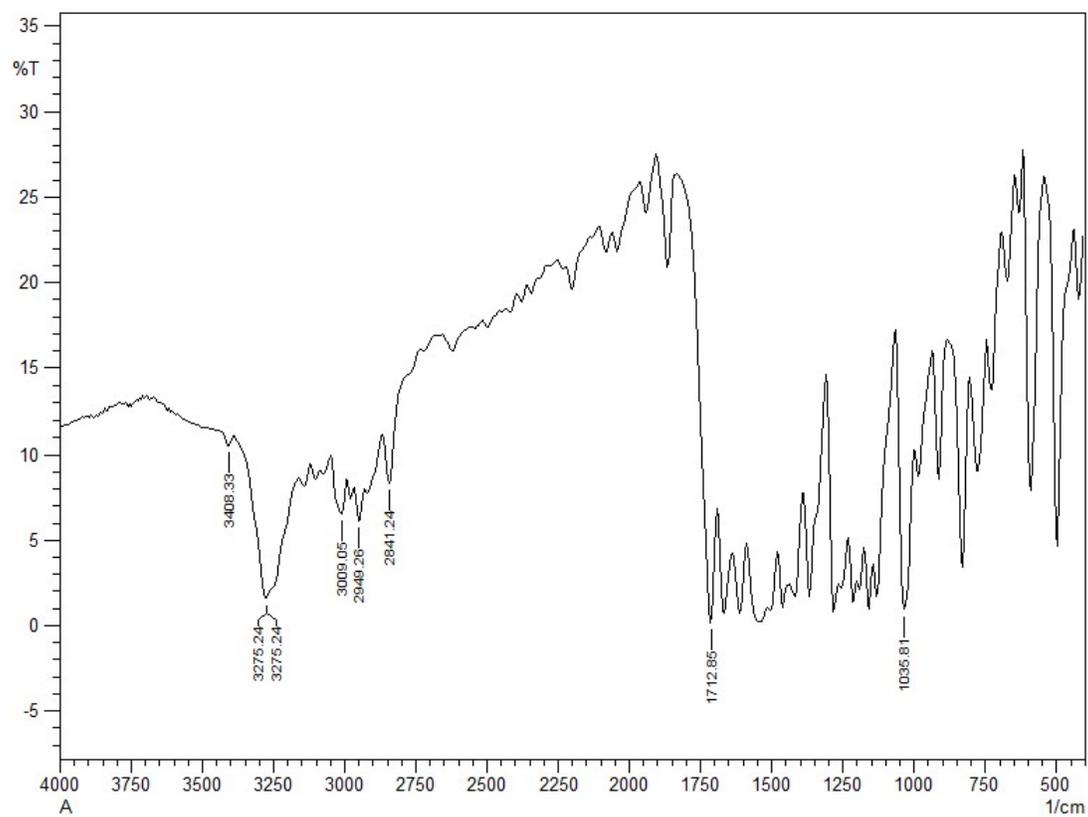
<sup>d</sup> Department of Pathology, College of Medicine, King Khalid University, Abha, Saudi Arabia.

# ANALYTICAL SPECTRA

A1:

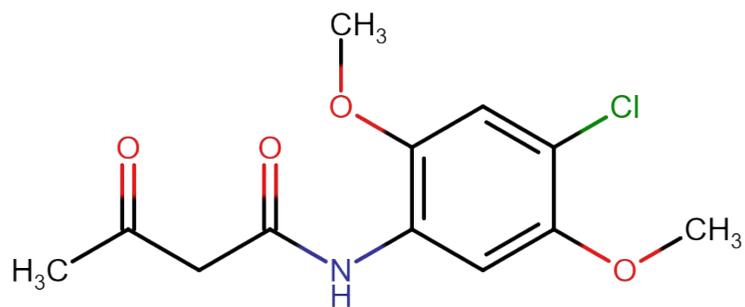


**Figure S1:** Chemical structure of compound A1

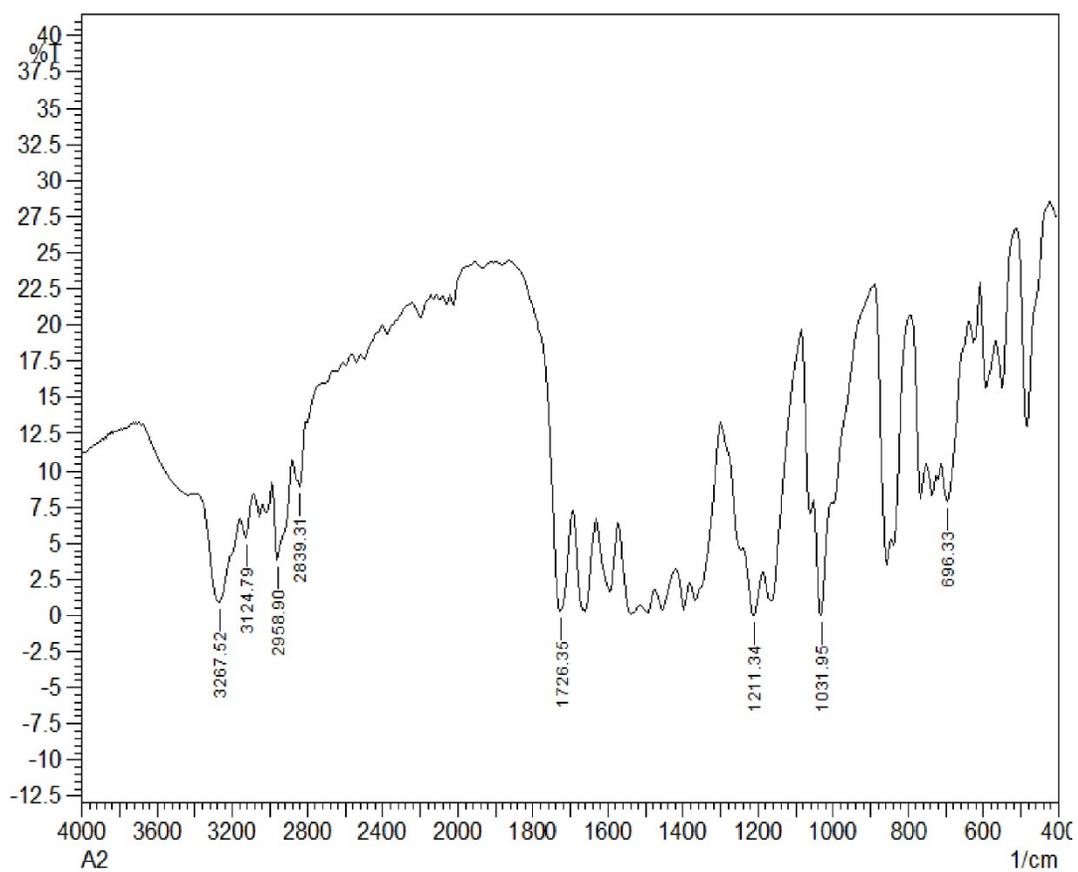


**Figure S2:** IR spectrum of compound A1

**A2:**

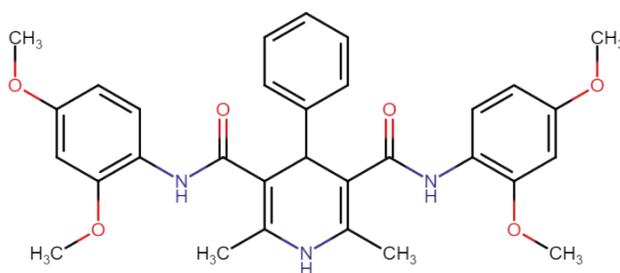


**Figure S3:** Chemical structure of compound A2

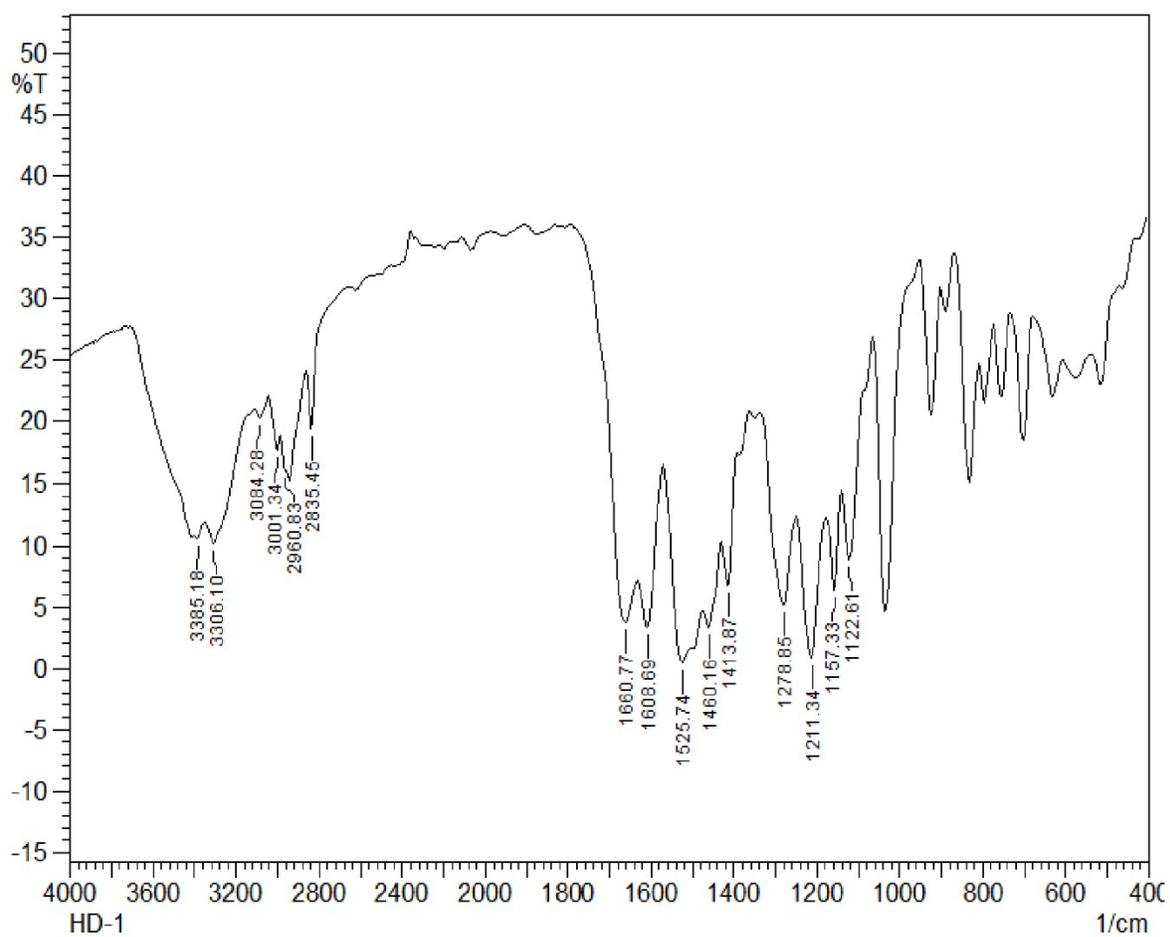


**Figure S4:** IR spectrum of compound A2

**HD-1:**



**Figure S5:** Chemical structure of compound HD-1



**Figure S6:** IR spectrum of compound HD-1

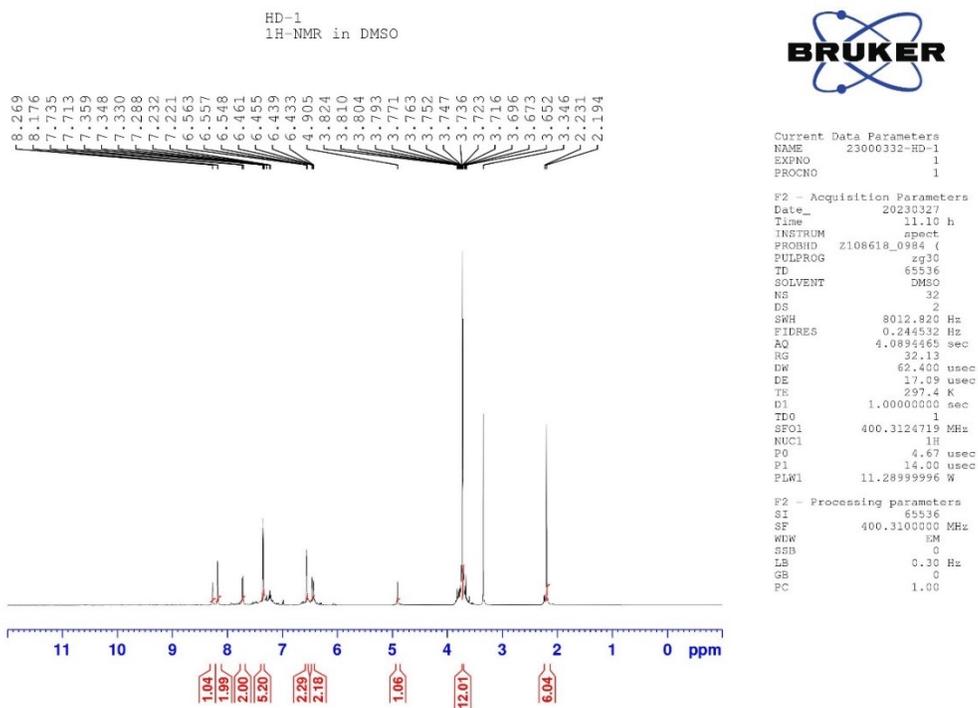


Figure S7: <sup>1</sup>H-NMR spectrum of compound HD-1

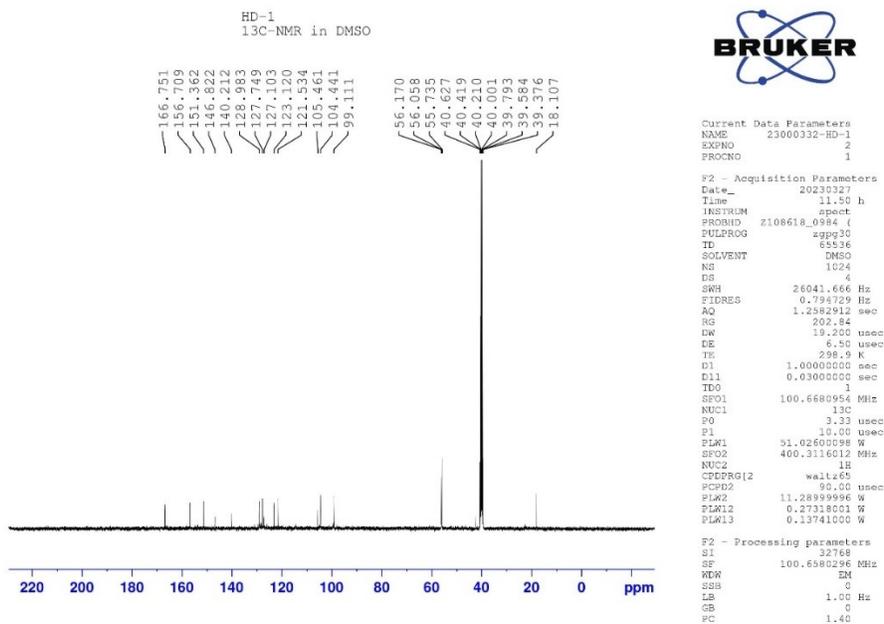
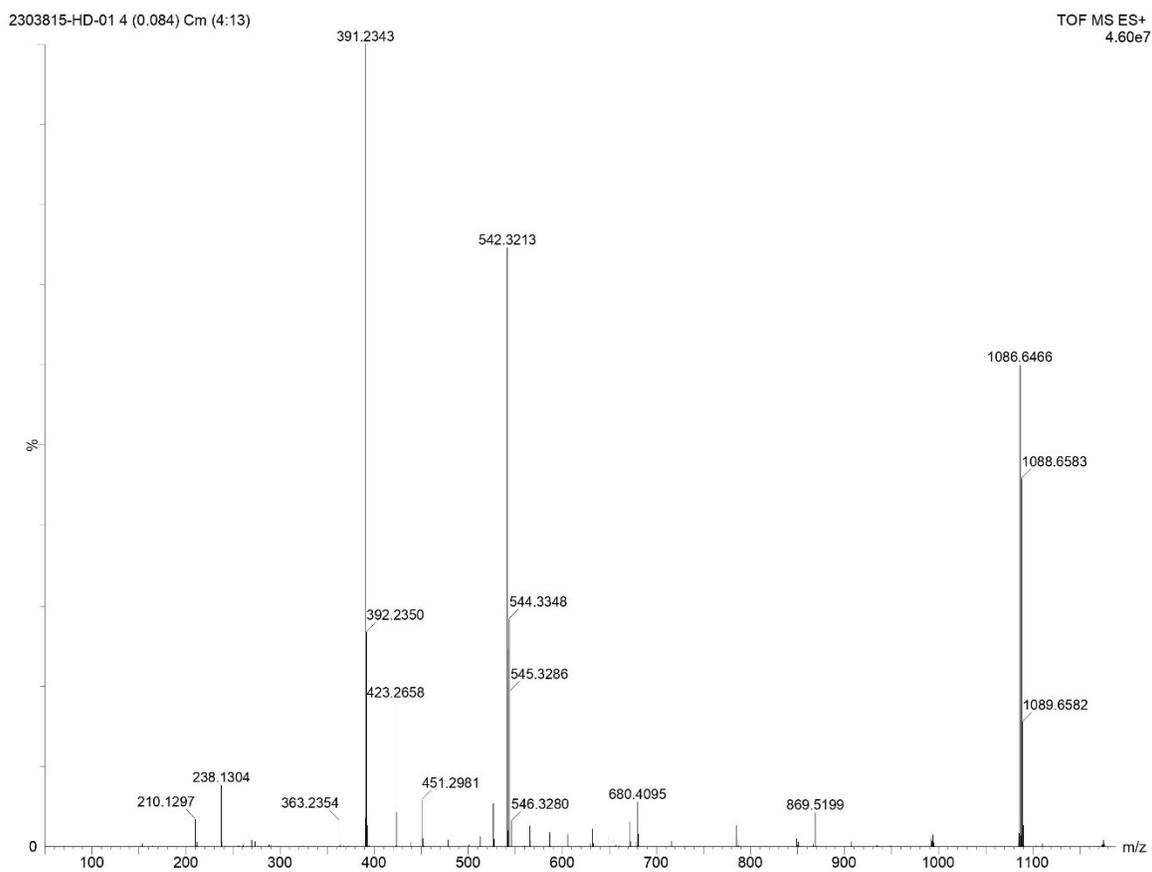
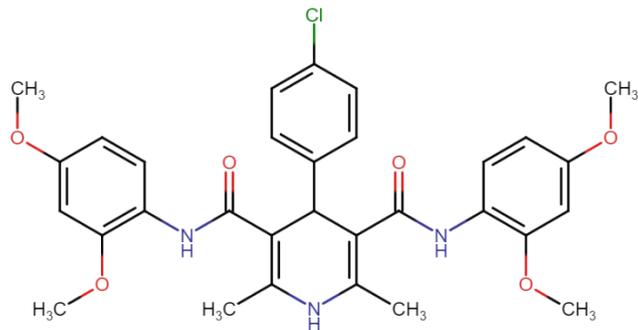


Figure S8: <sup>13</sup>C-NMR spectrum of compound HD-1

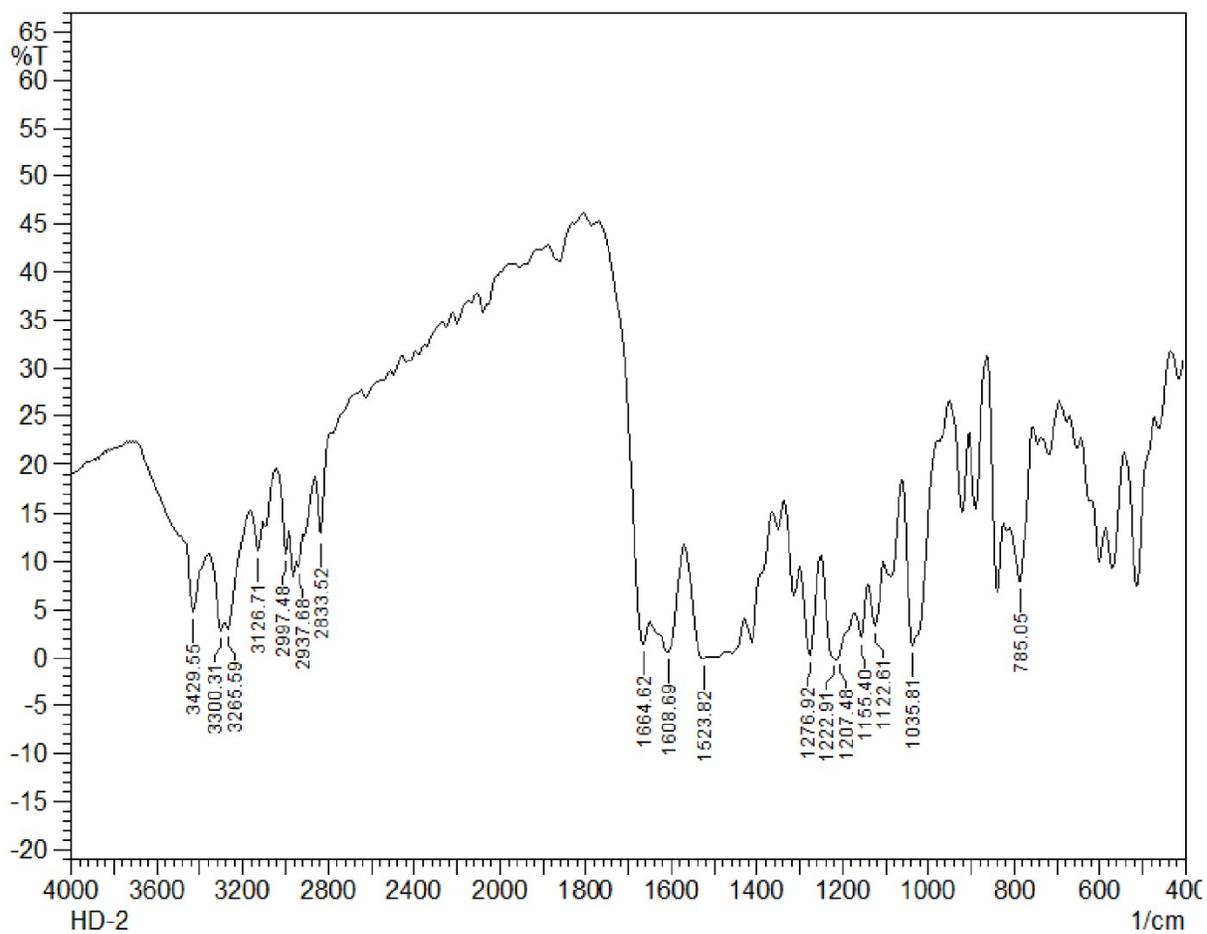


**Figure S9:** Mass spectrum of compound **HD-1**

**HD-2:**



**Figure S10:** Chemical structure of compound HD-2



**Figure S11:** IR spectrum of compound HD-2

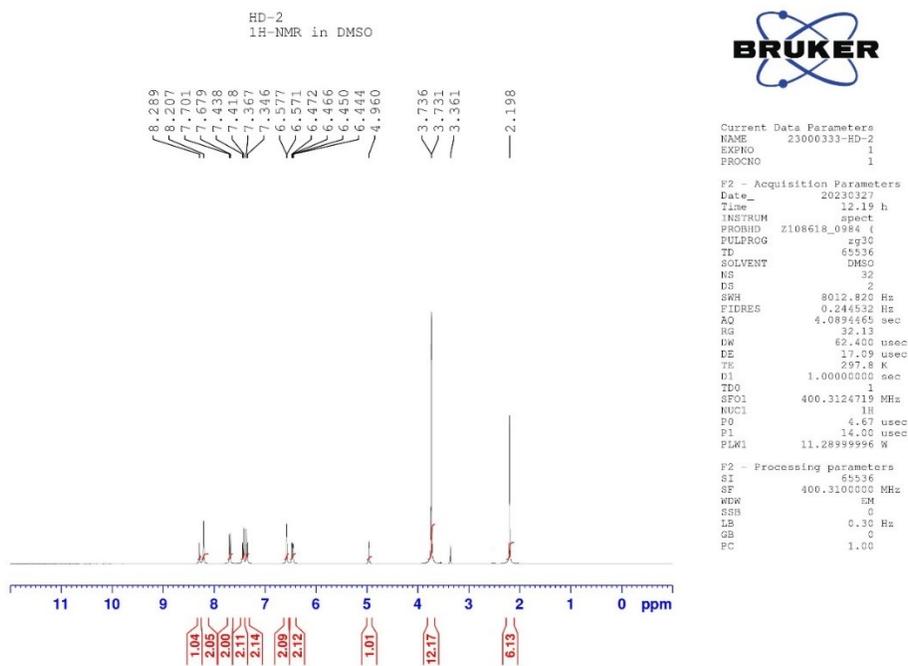


Figure S12: <sup>1</sup>H-NMR spectrum of compound HD-2

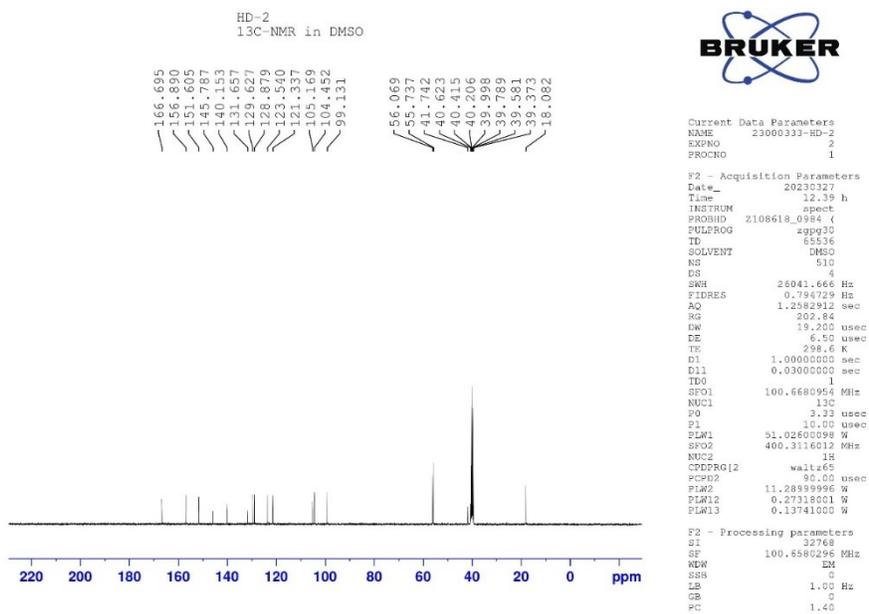
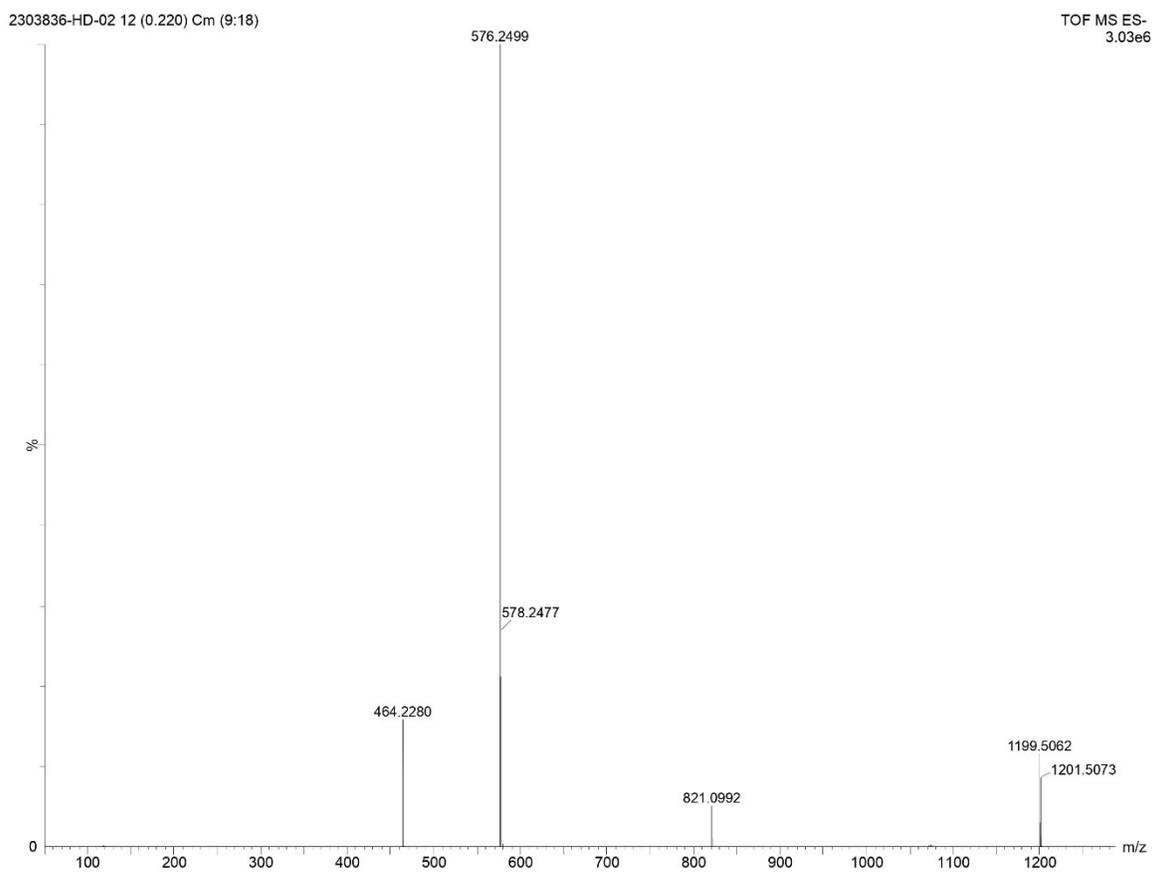
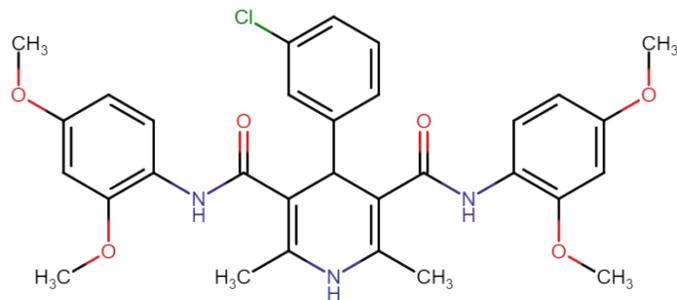


Figure S13: <sup>13</sup>C-NMR spectrum of compound HD-2

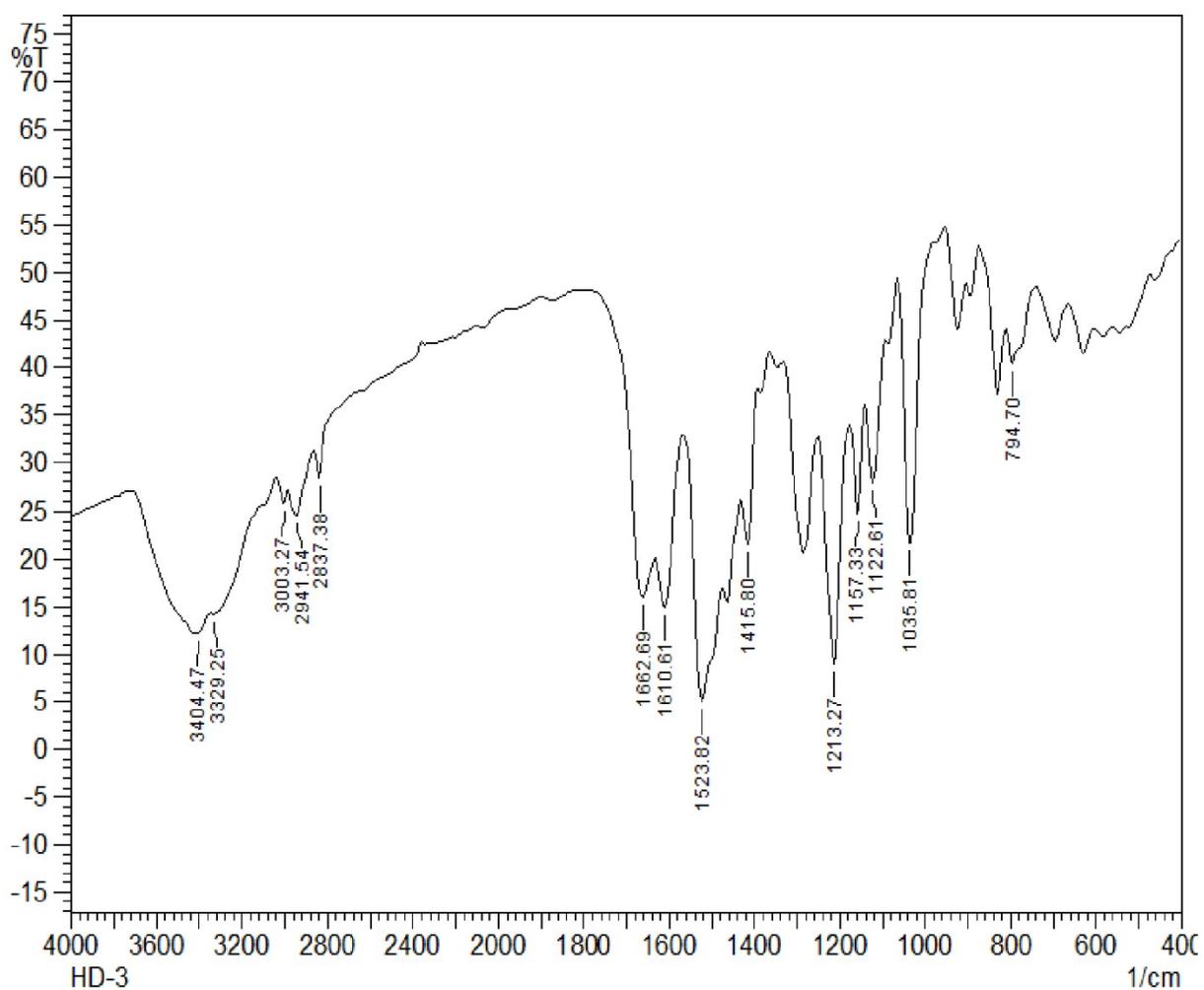


**Figure S14:** Mass spectrum of compound **HD-2**

**HD-3:**



**Figure S15:** Chemical structure of compound HD-3



**Figure S16:** IR spectrum of compound HD-3

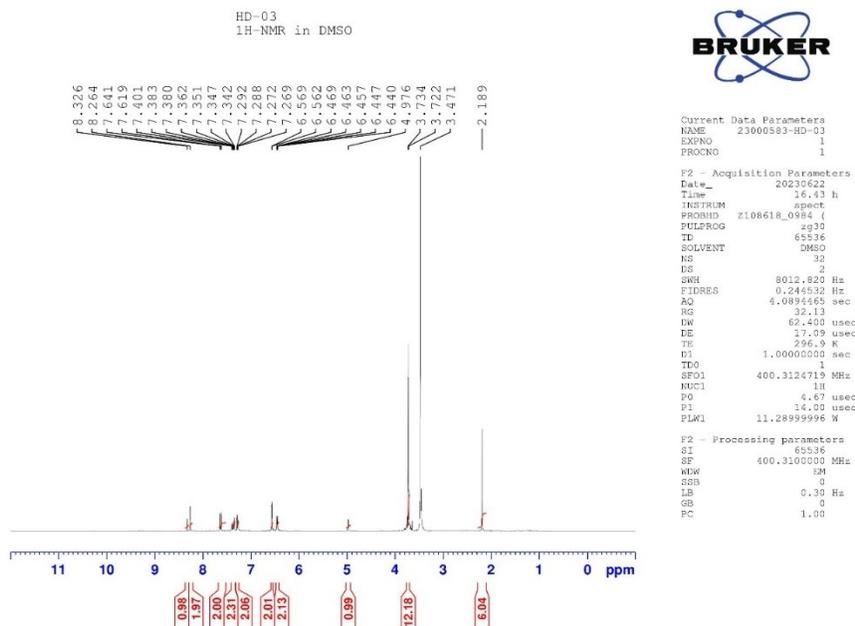


Figure S17: <sup>1</sup>H-NMR spectrum of compound HD-3

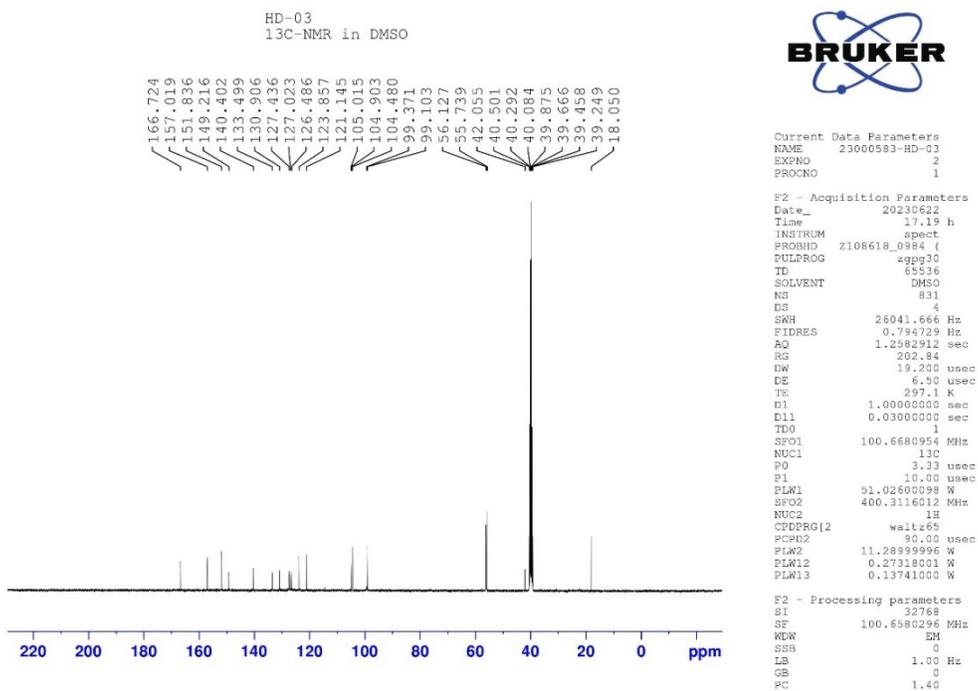
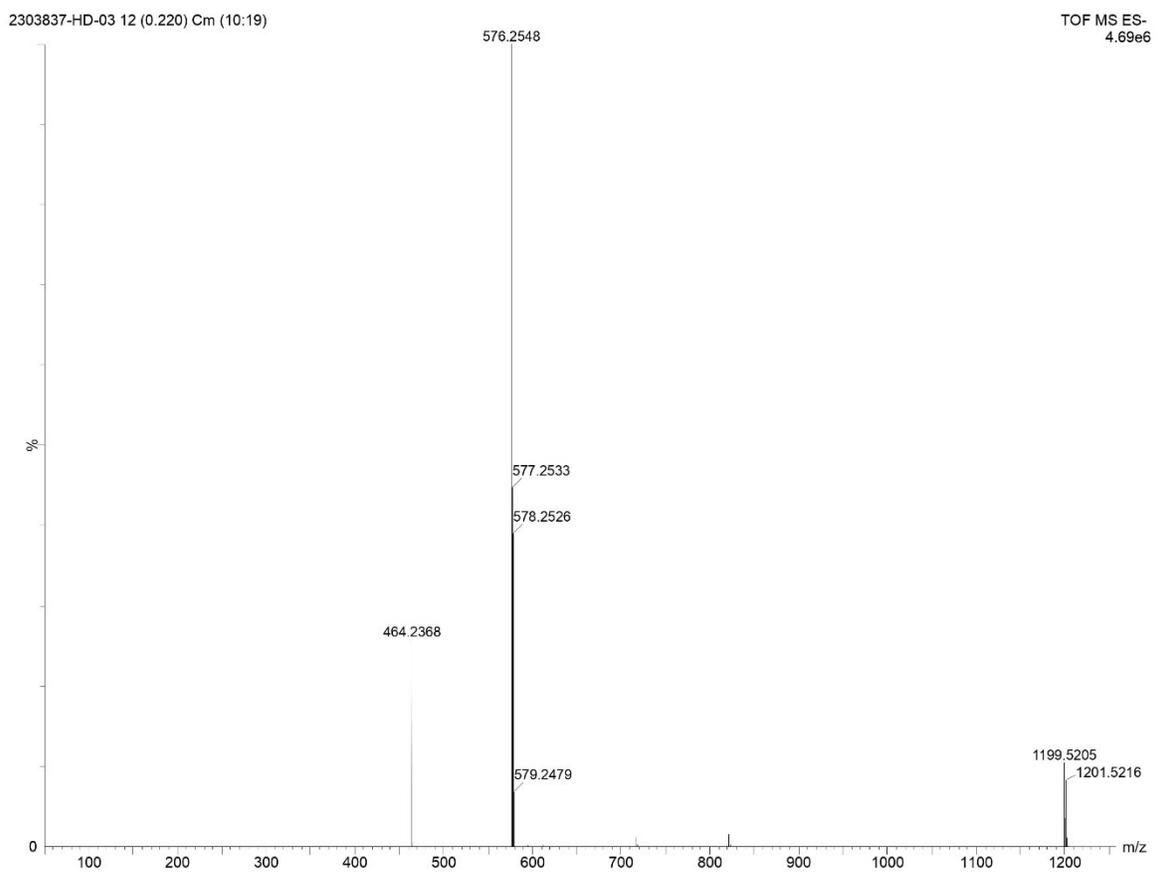
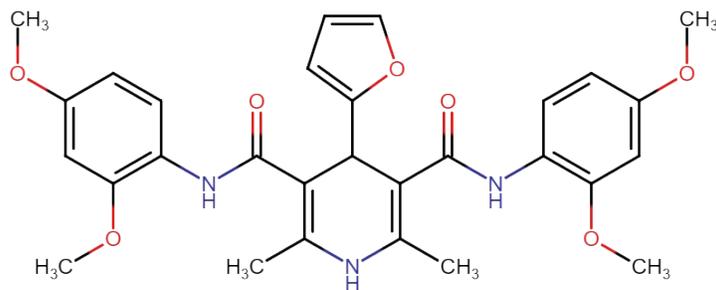


Figure S18: <sup>13</sup>C-NMR spectrum of compound HD-3

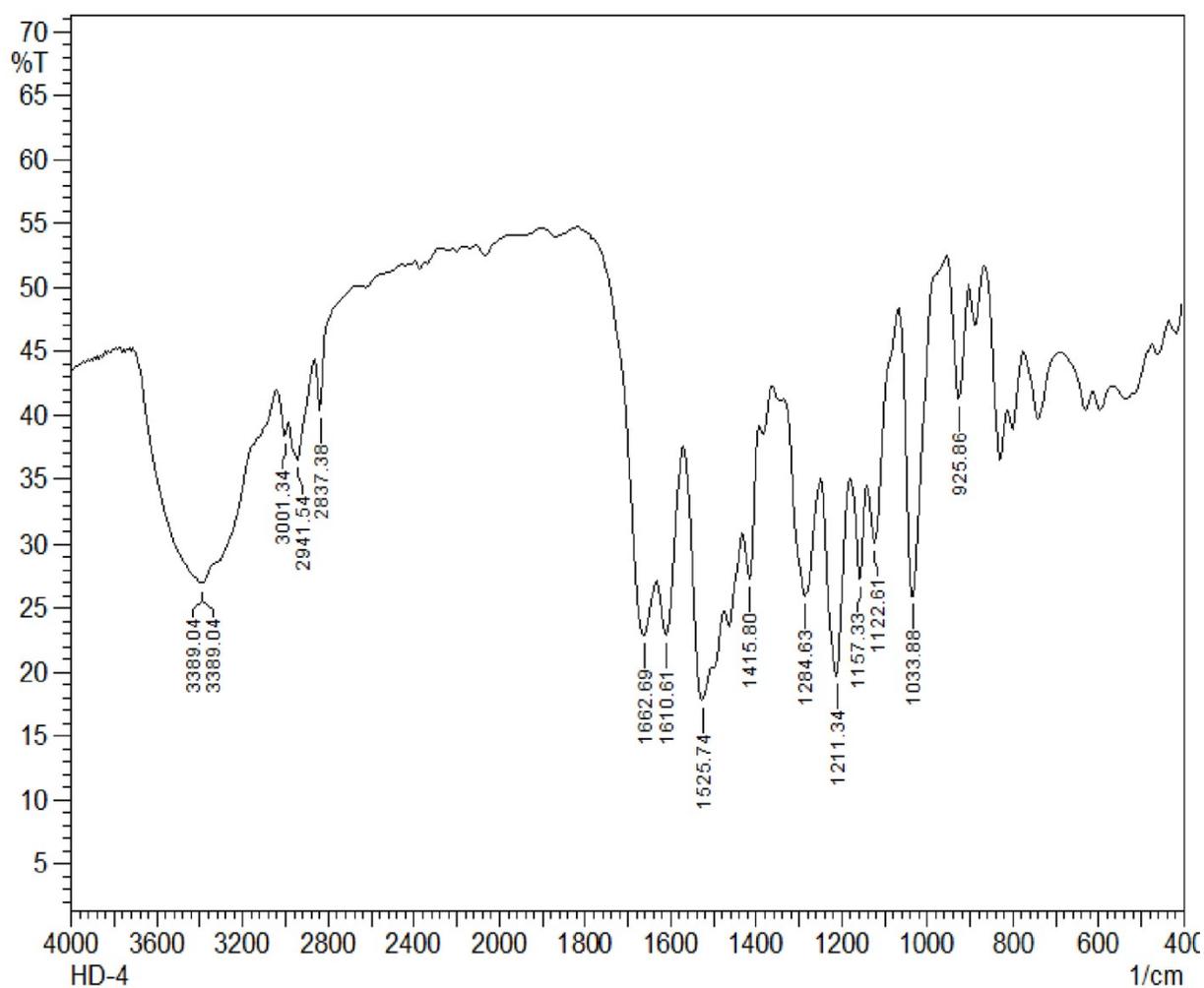


**Figure S19:** Mass spectrum of compound **HD-3**

**HD-4:**



**Figure S20:** Chemical structure of compound HD-4



**Figure S21:** IR spectrum of compound HD-4

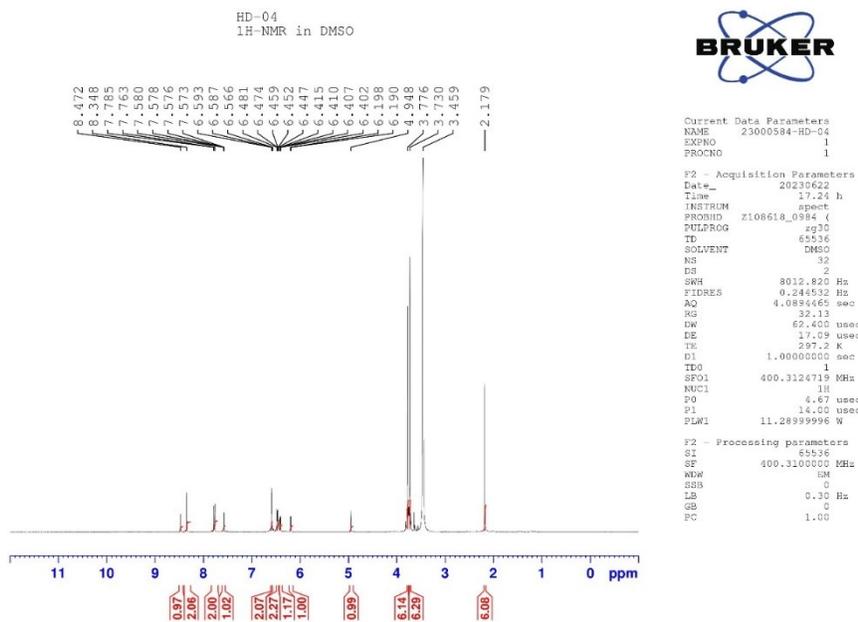


Figure S22: <sup>1</sup>H-NMR spectrum of compound HD-4

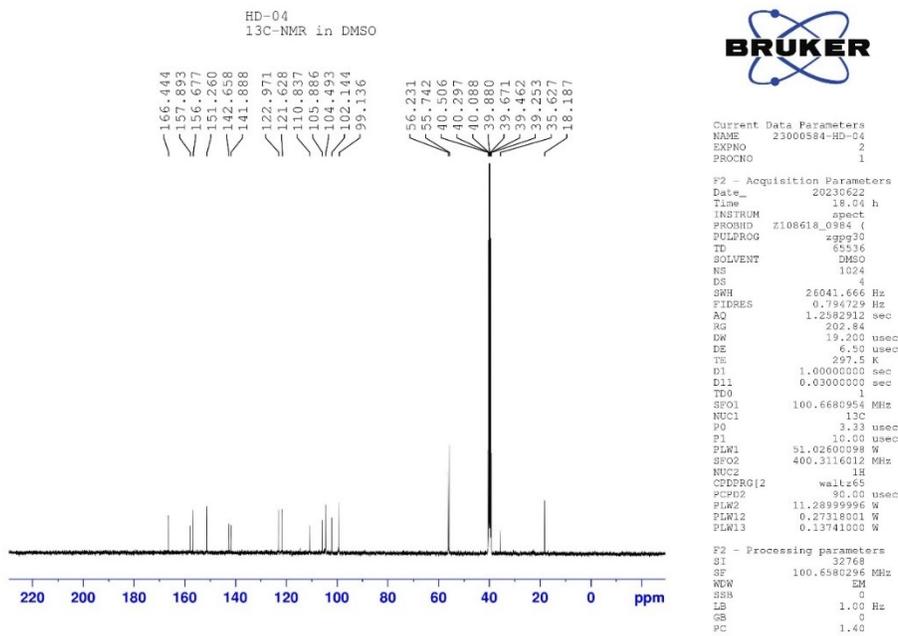
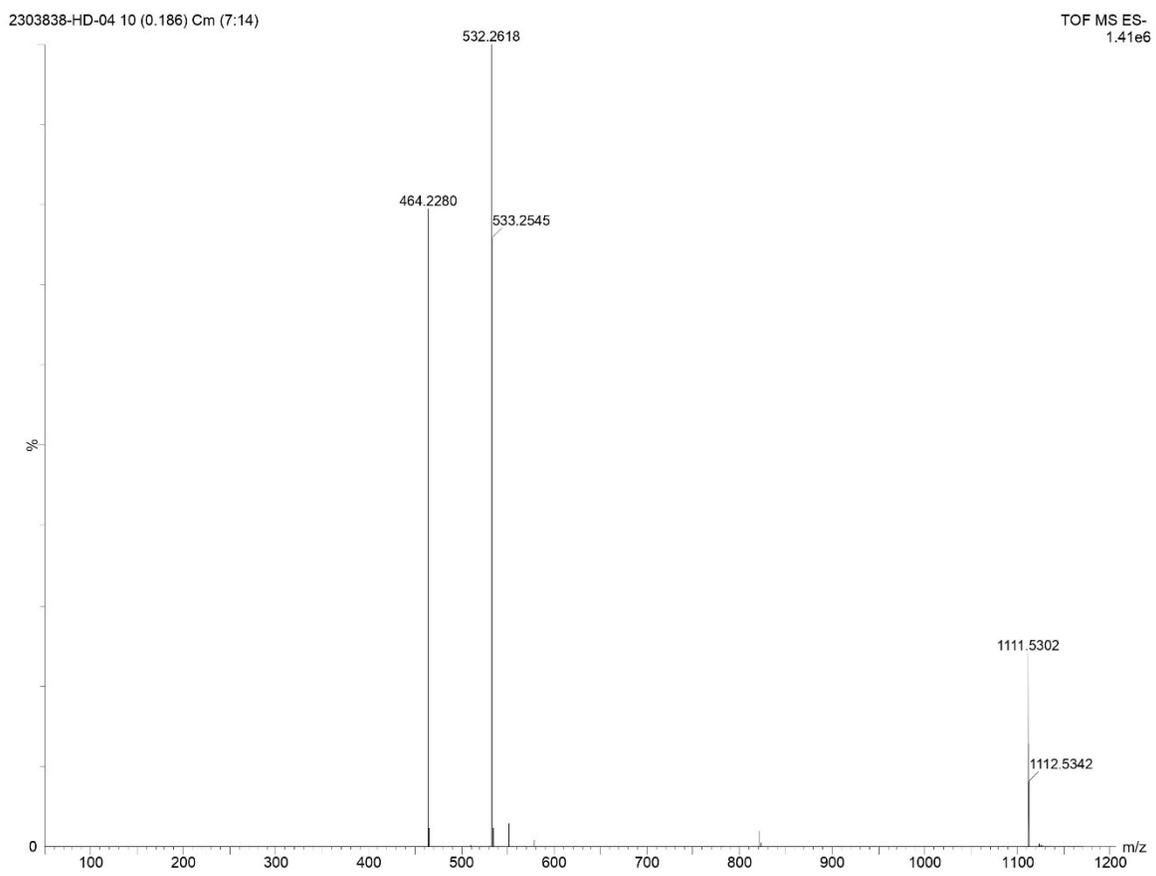
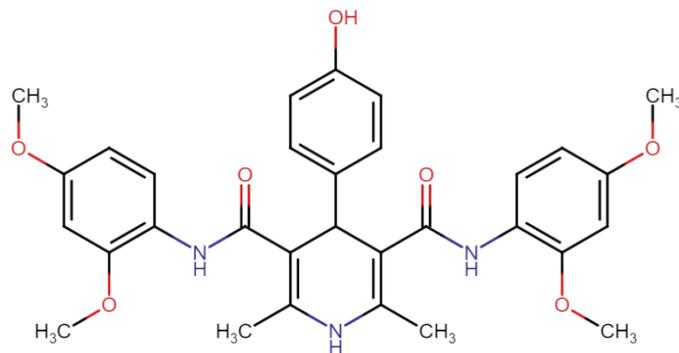


Figure S23: <sup>13</sup>C-NMR spectrum of compound HD-4

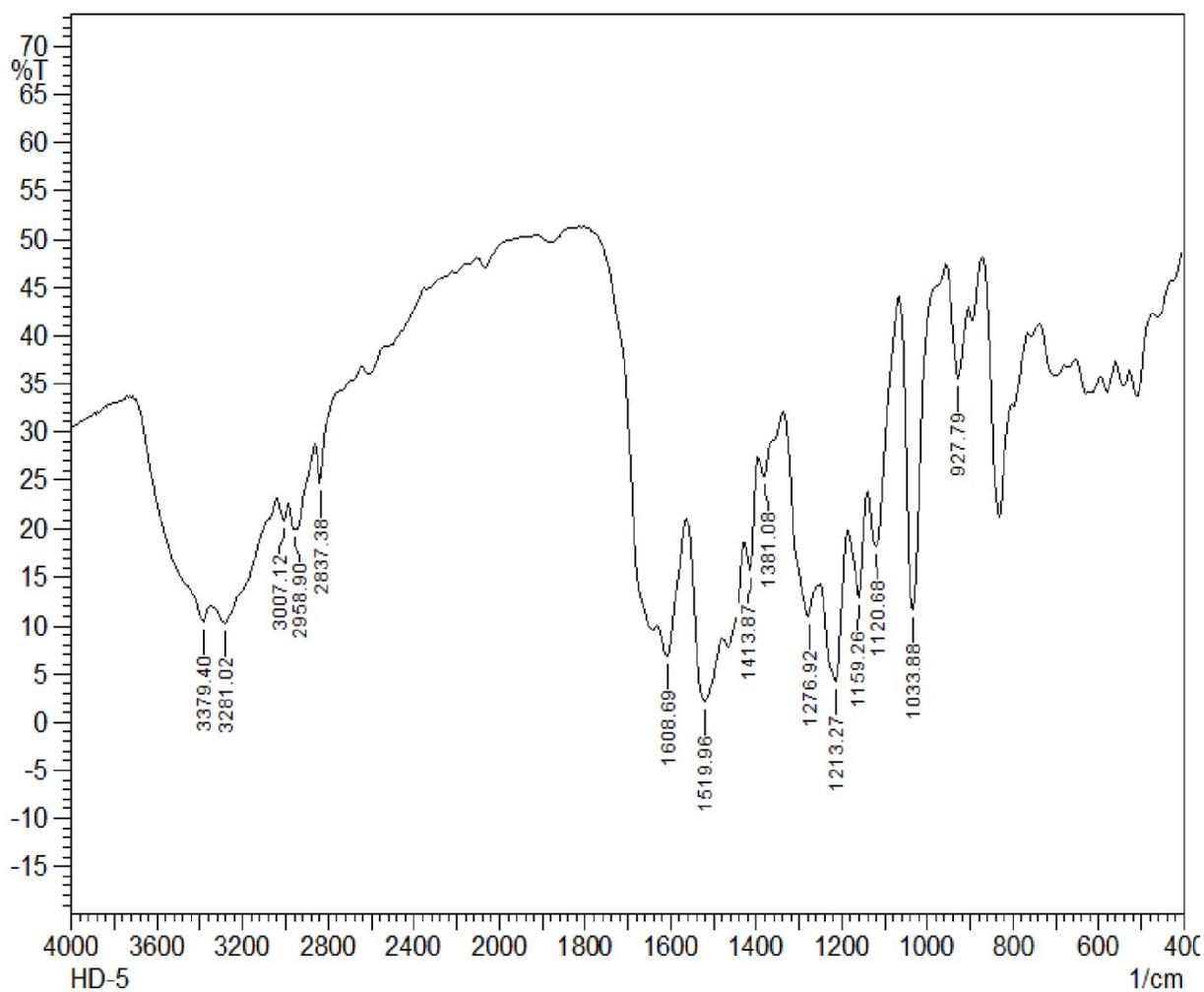


**Figure S24:** Mass spectrum of compound **HD-4**

**HD-5:**



**Figure S25:** Chemical structure of compound HD-5



**Figure S26:** IR spectrum of compound HD-5

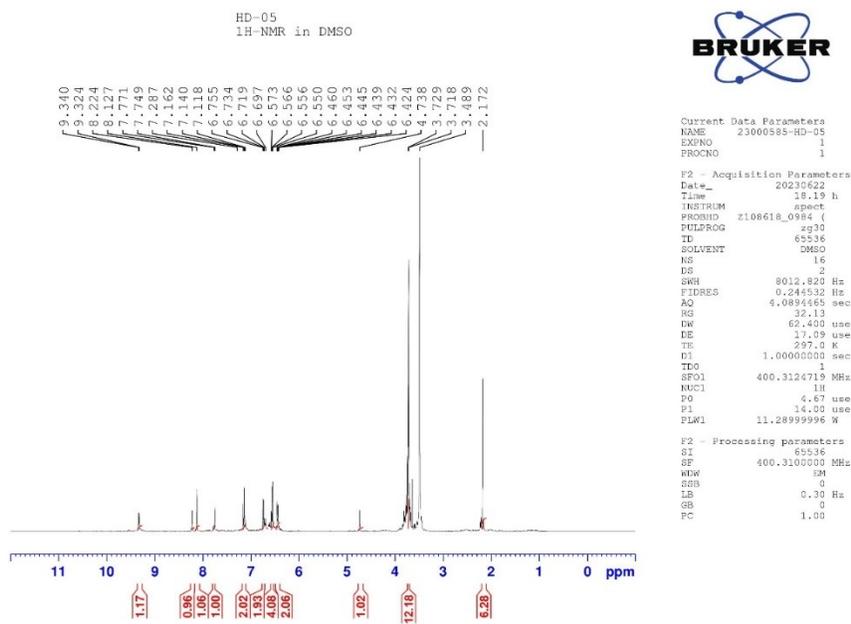


Figure S27: <sup>1</sup>H-NMR spectrum of compound HD-5

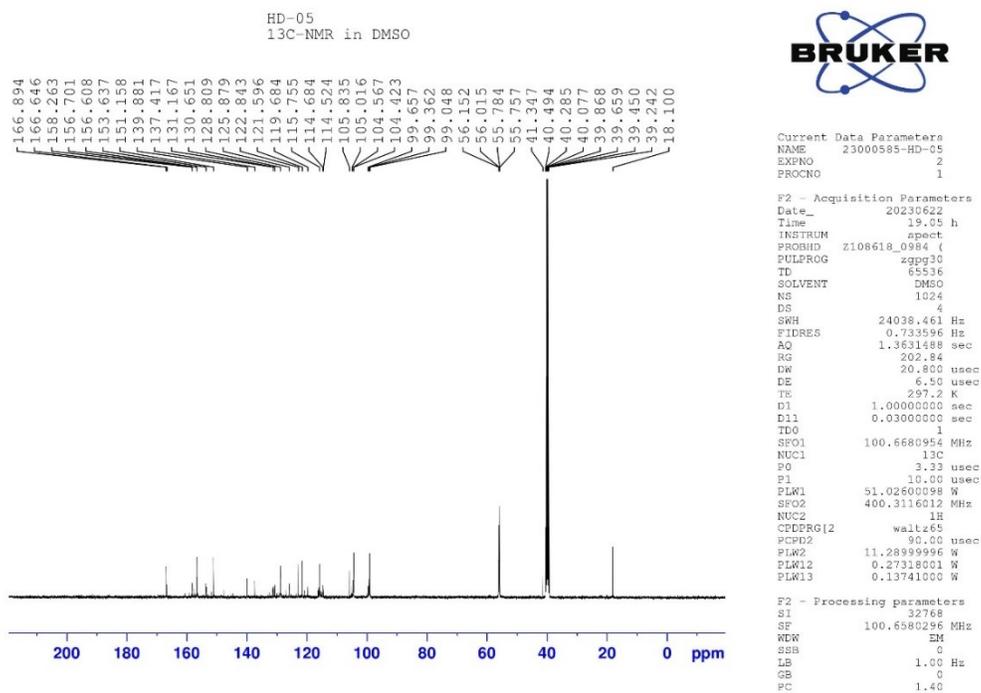
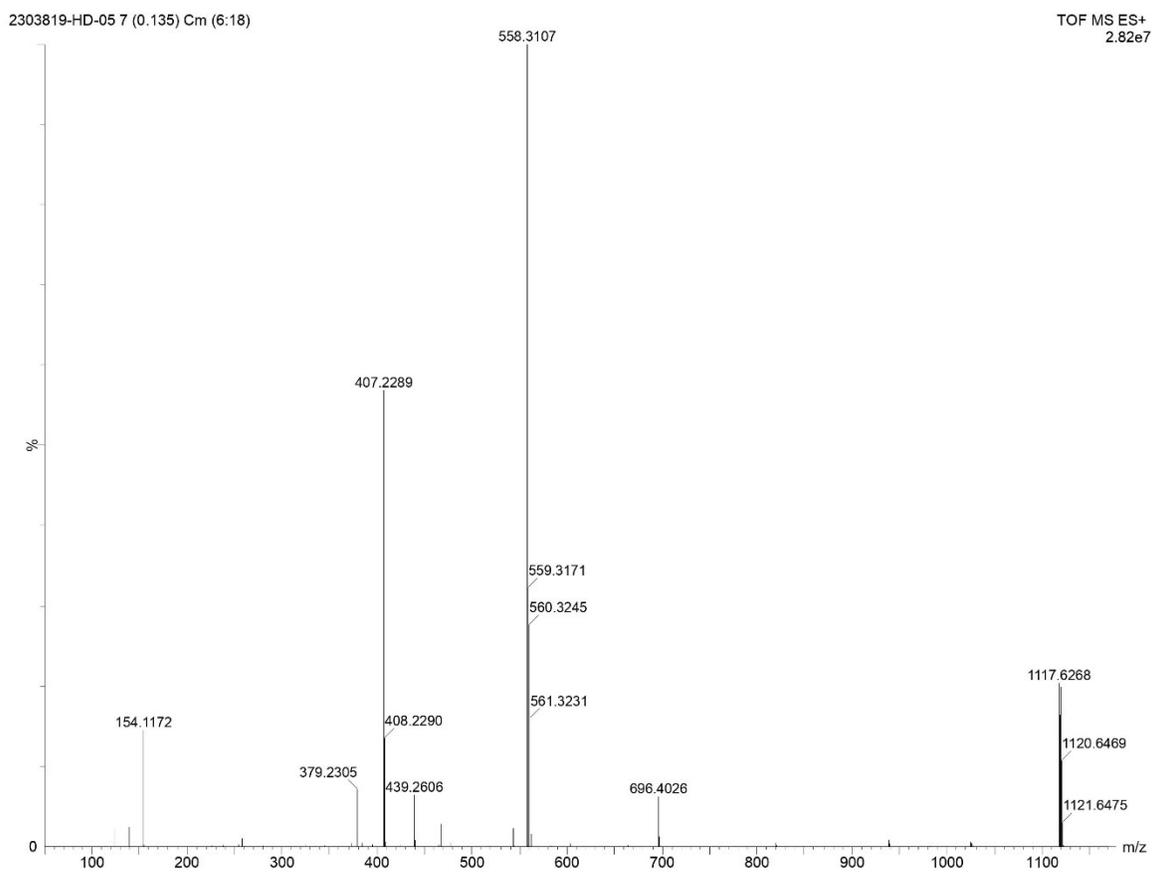
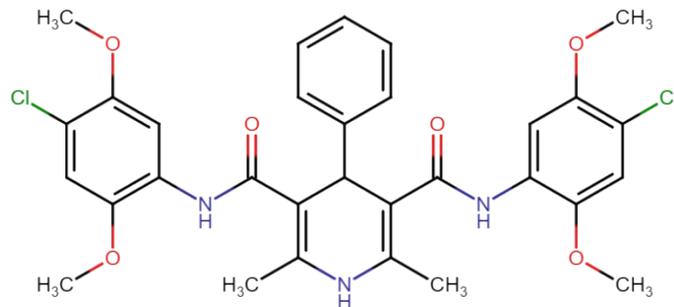


Figure S28: <sup>13</sup>C-NMR spectrum of compound HD-5

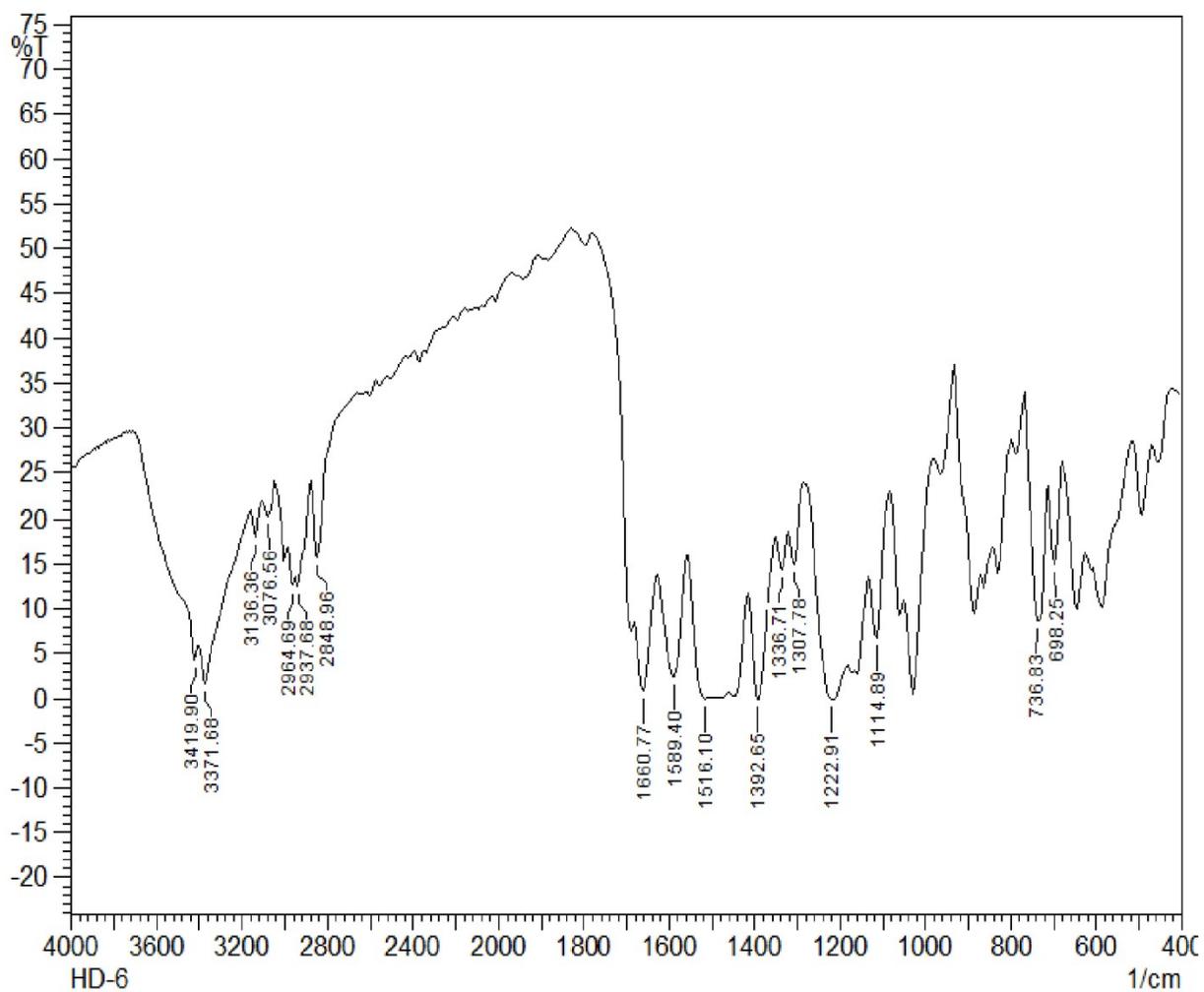


**Figure S29:** Mass spectrum of compound **HD-5**

**HD-6:**



**Figure S30:** Chemical structure of compound HD-6



**Figure S31:** IR spectrum of compound HD-6

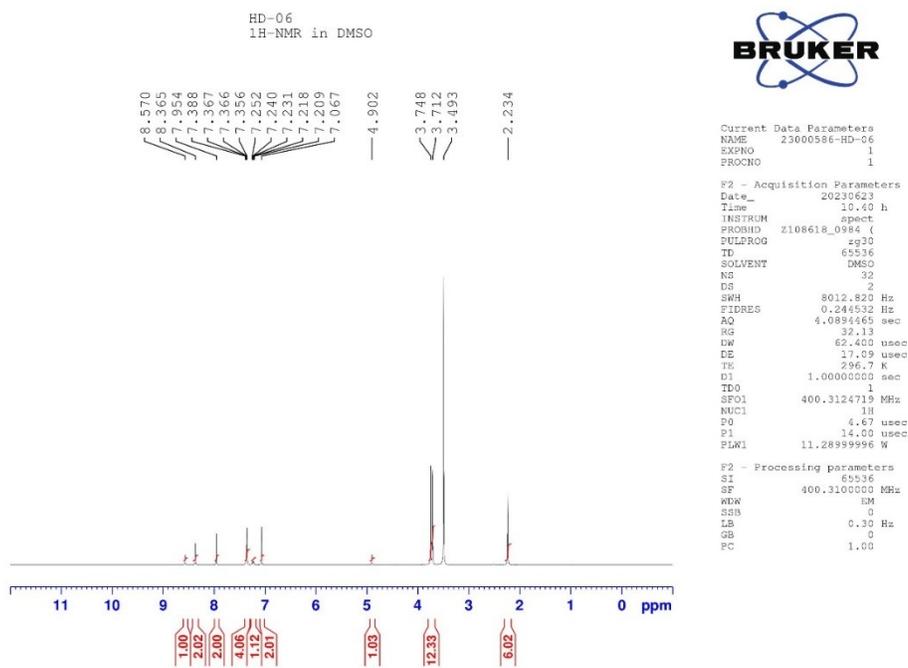


Figure S32:  $^1\text{H}$ -NMR spectrum of compound HD-6

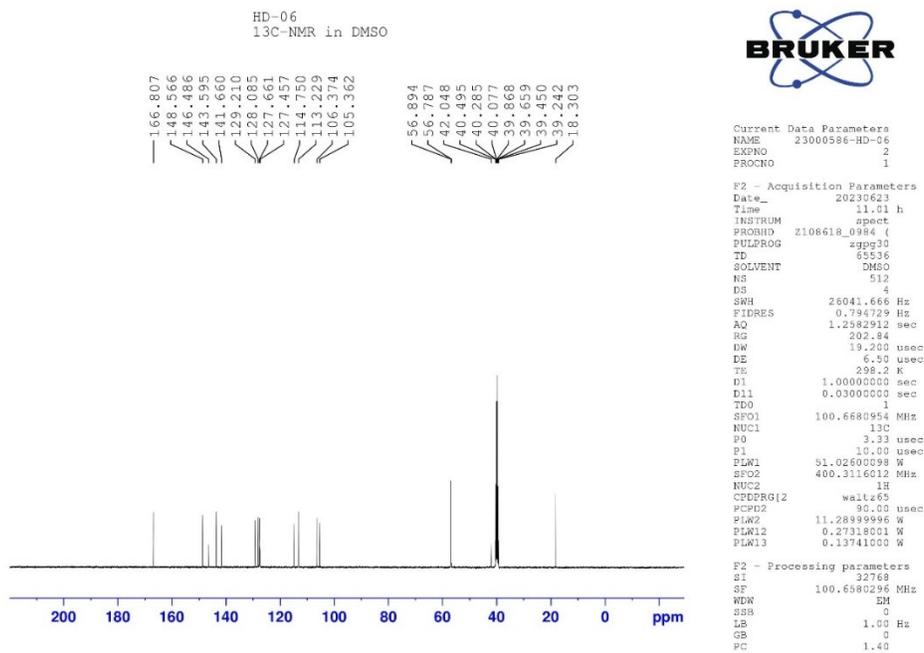
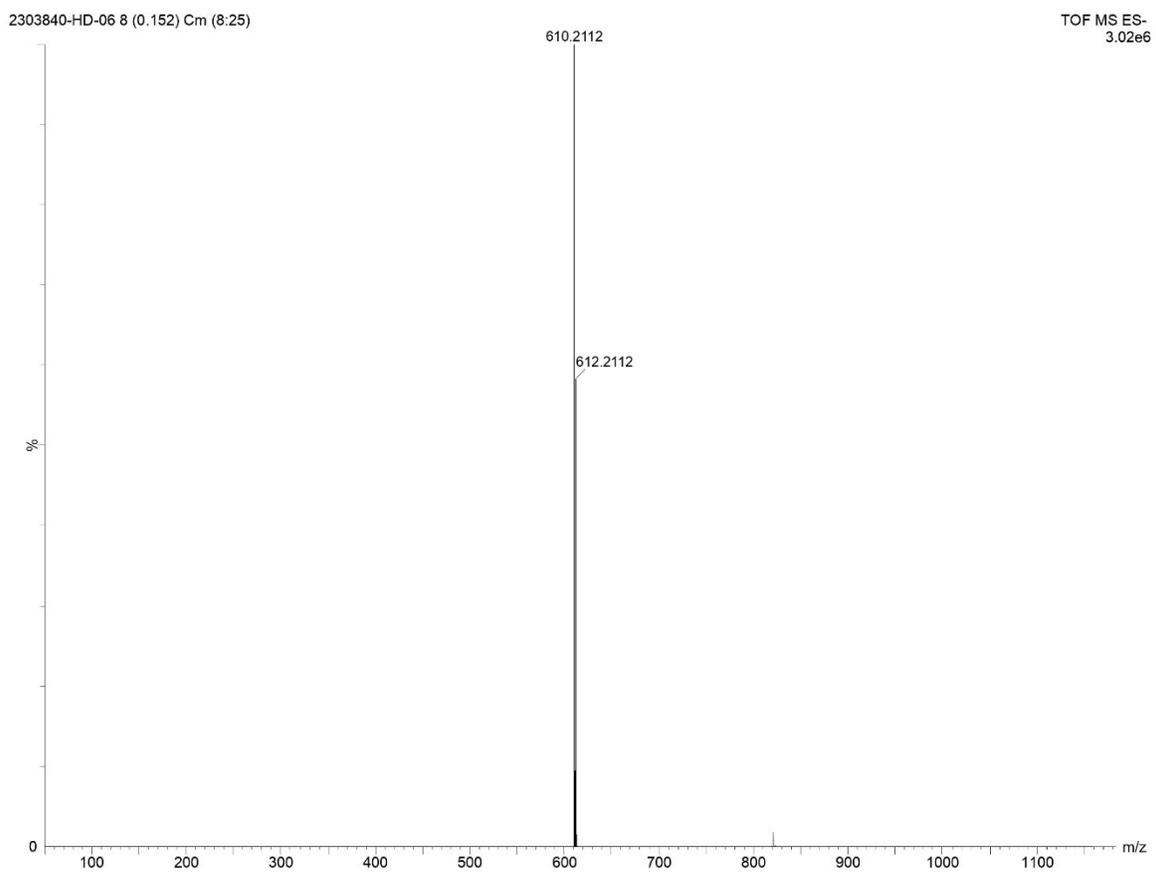
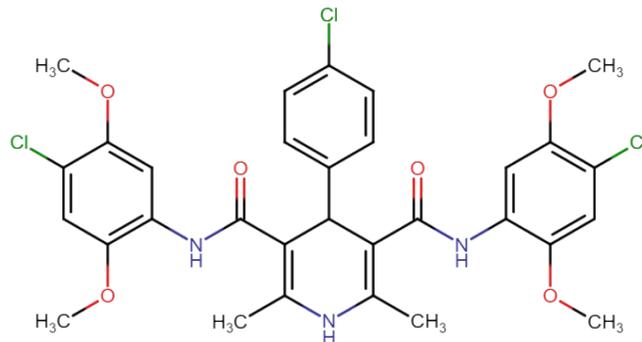


Figure S33:  $^{13}\text{C}$ -NMR spectrum of compound HD-6

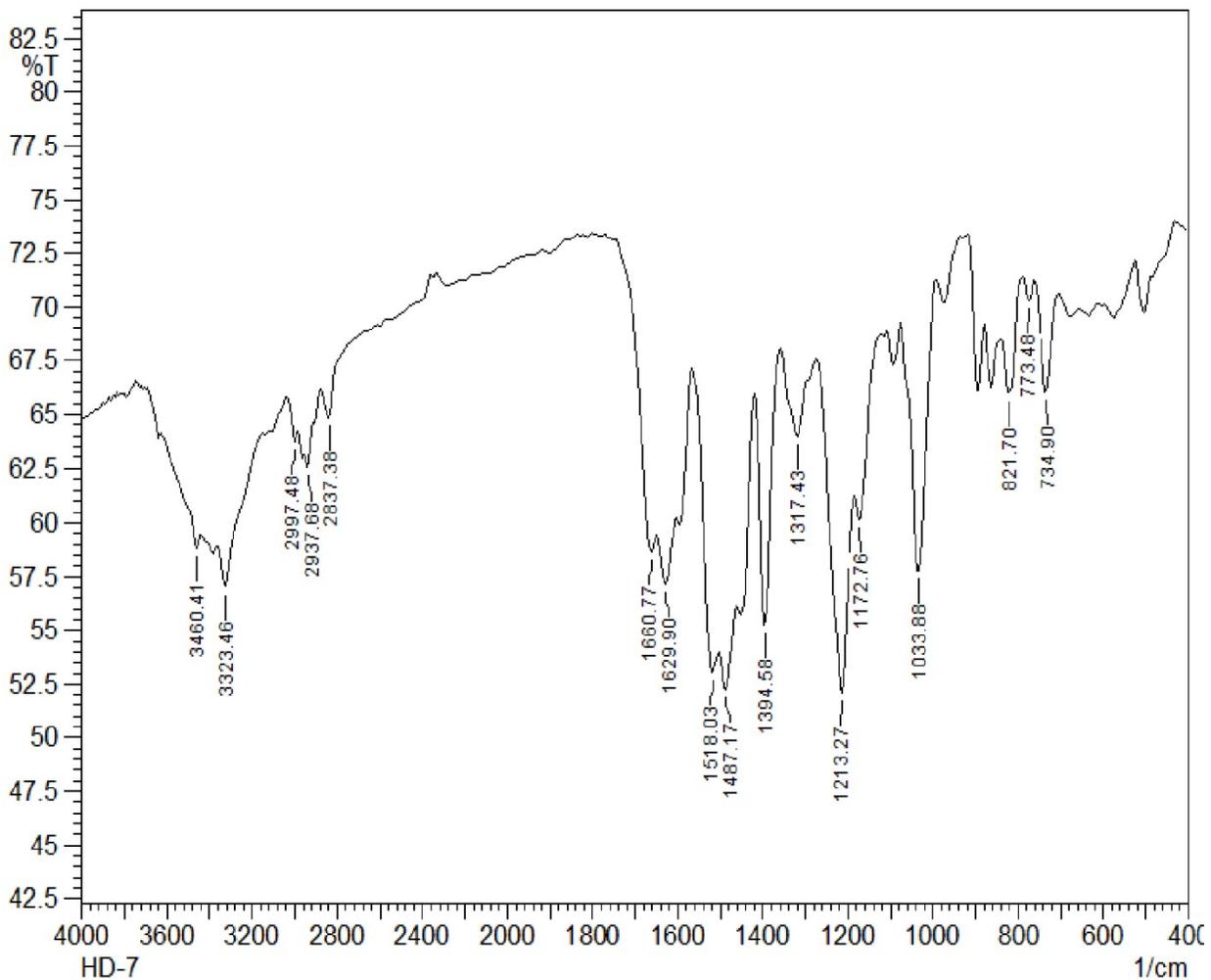


**Figure S34:** Mass spectrum of compound **HD-6**

**HD-7:**



**Figure S35:** Chemical structure of compound HD-7



**Figure S36:** IR spectrum of compound HD-7

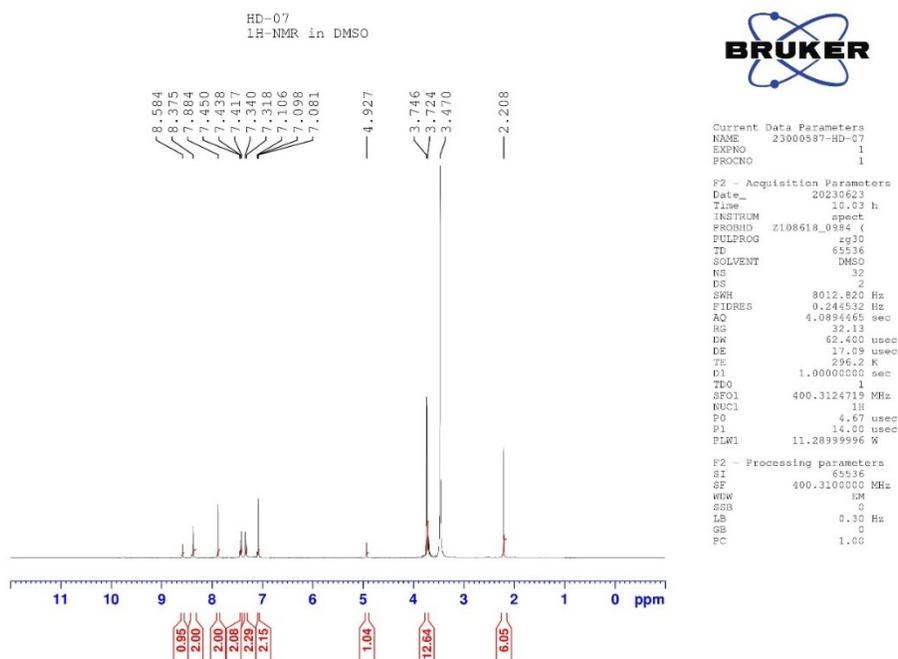


Figure S37: <sup>1</sup>H-NMR spectrum of compound HD-7

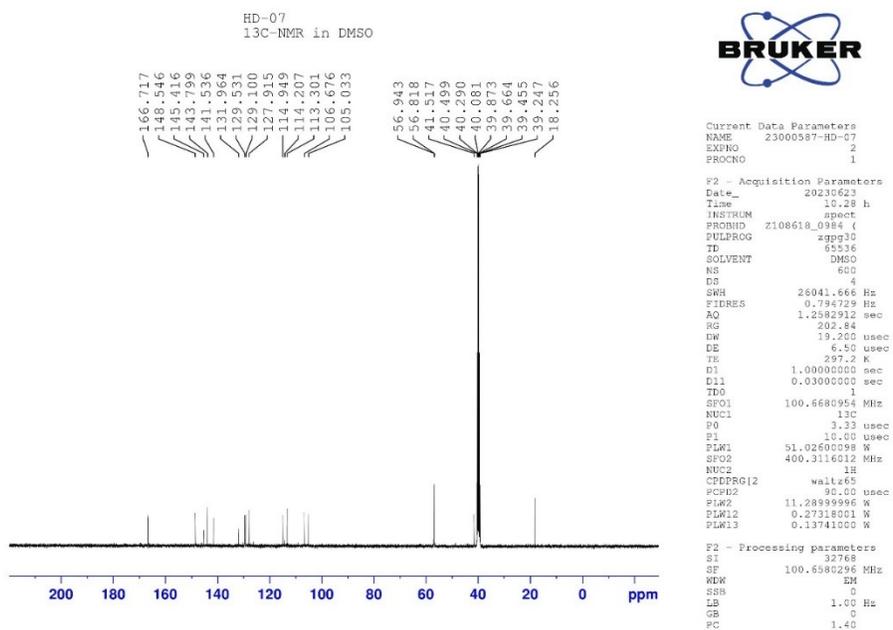
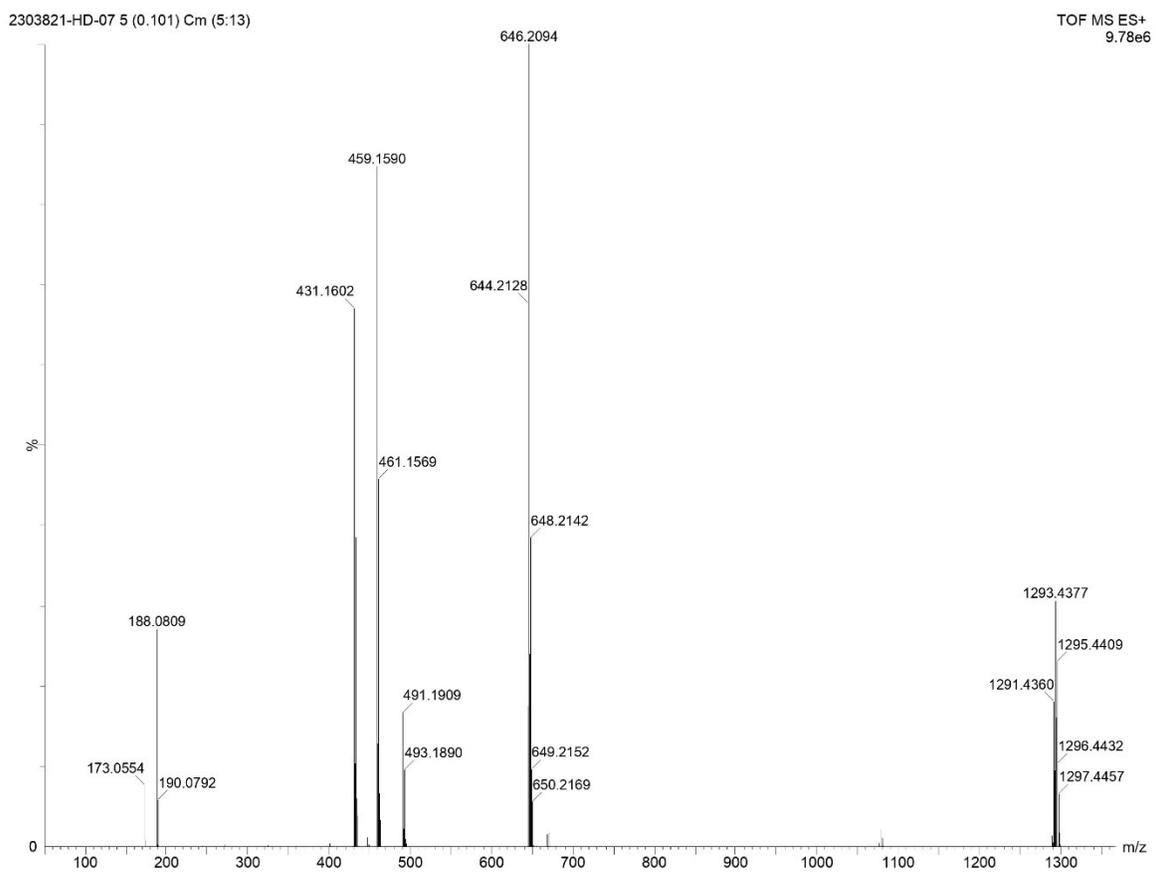
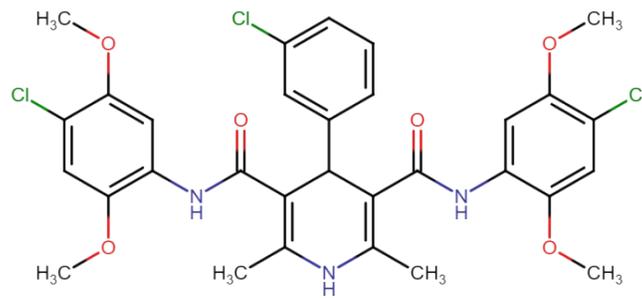


Figure S38: <sup>13</sup>C-NMR spectrum of compound HD-7

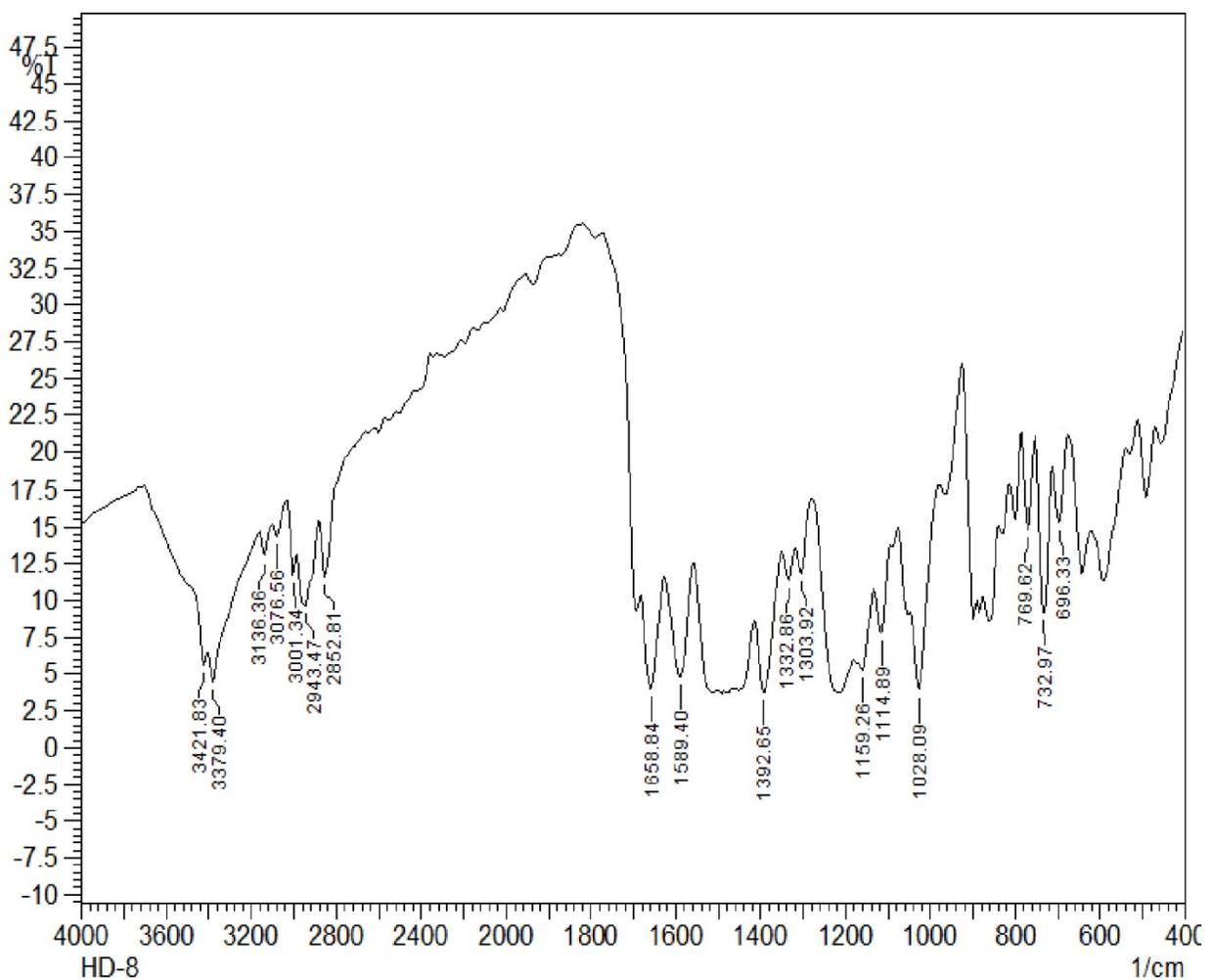


**Figure S39:** Mass spectrum of compound **HD-7**

**HD-8:**



**Figure S40:** Chemical structure of compound HD-8



**Figure S41:** IR spectrum of compound HD-8

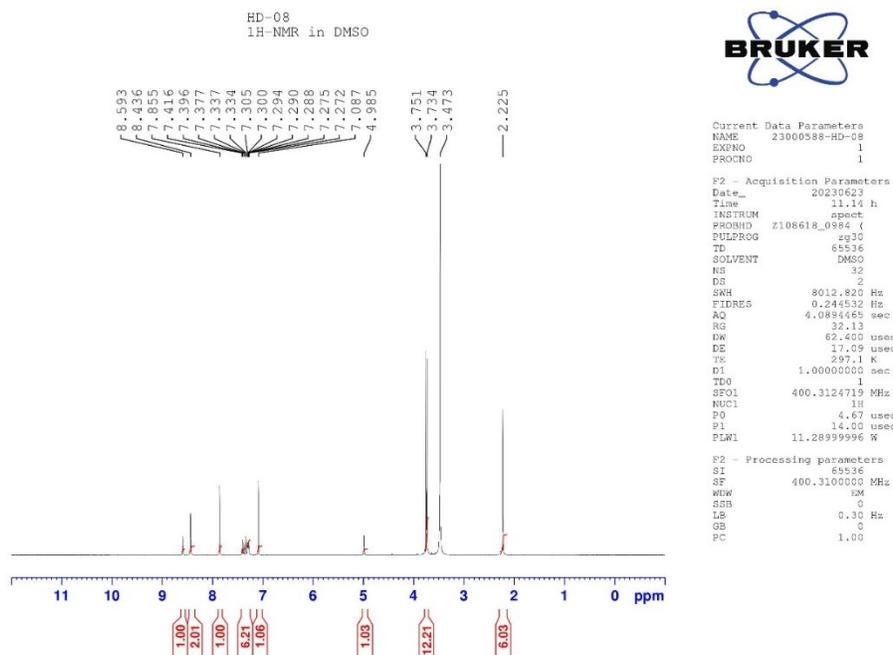


Figure S42: <sup>1</sup>H-NMR spectrum of compound HD-8

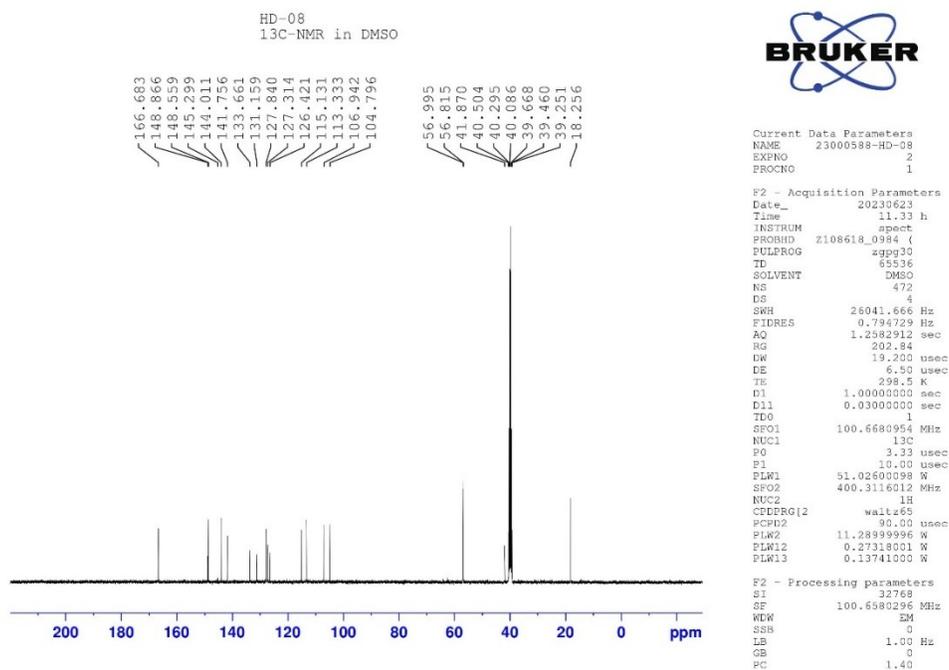
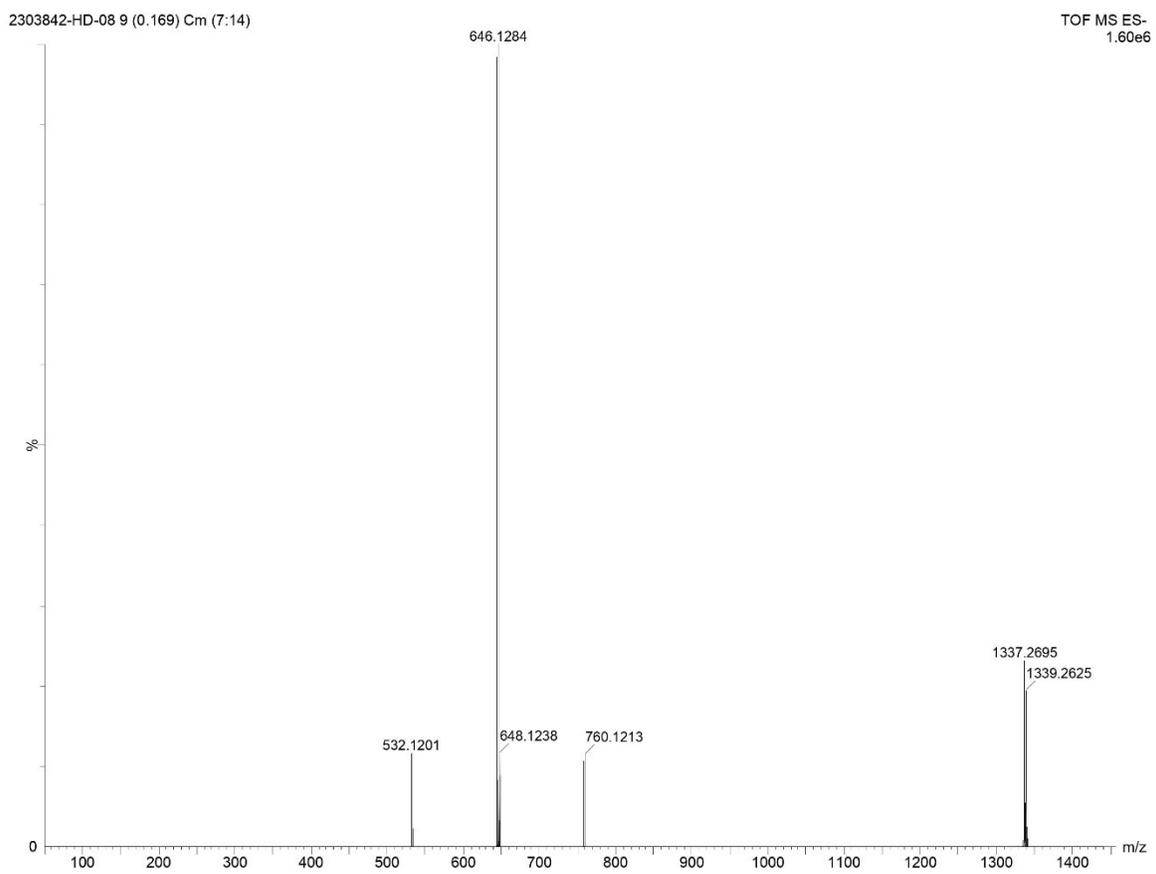
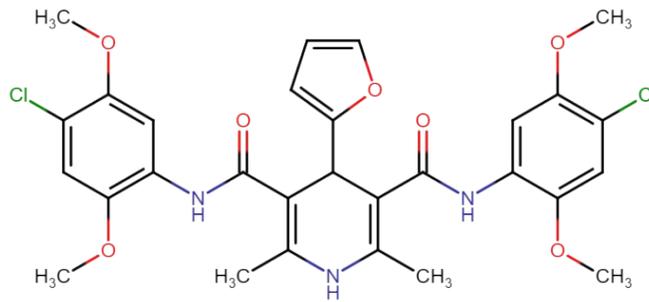


Figure S43: <sup>13</sup>C-NMR spectrum of compound HD-8

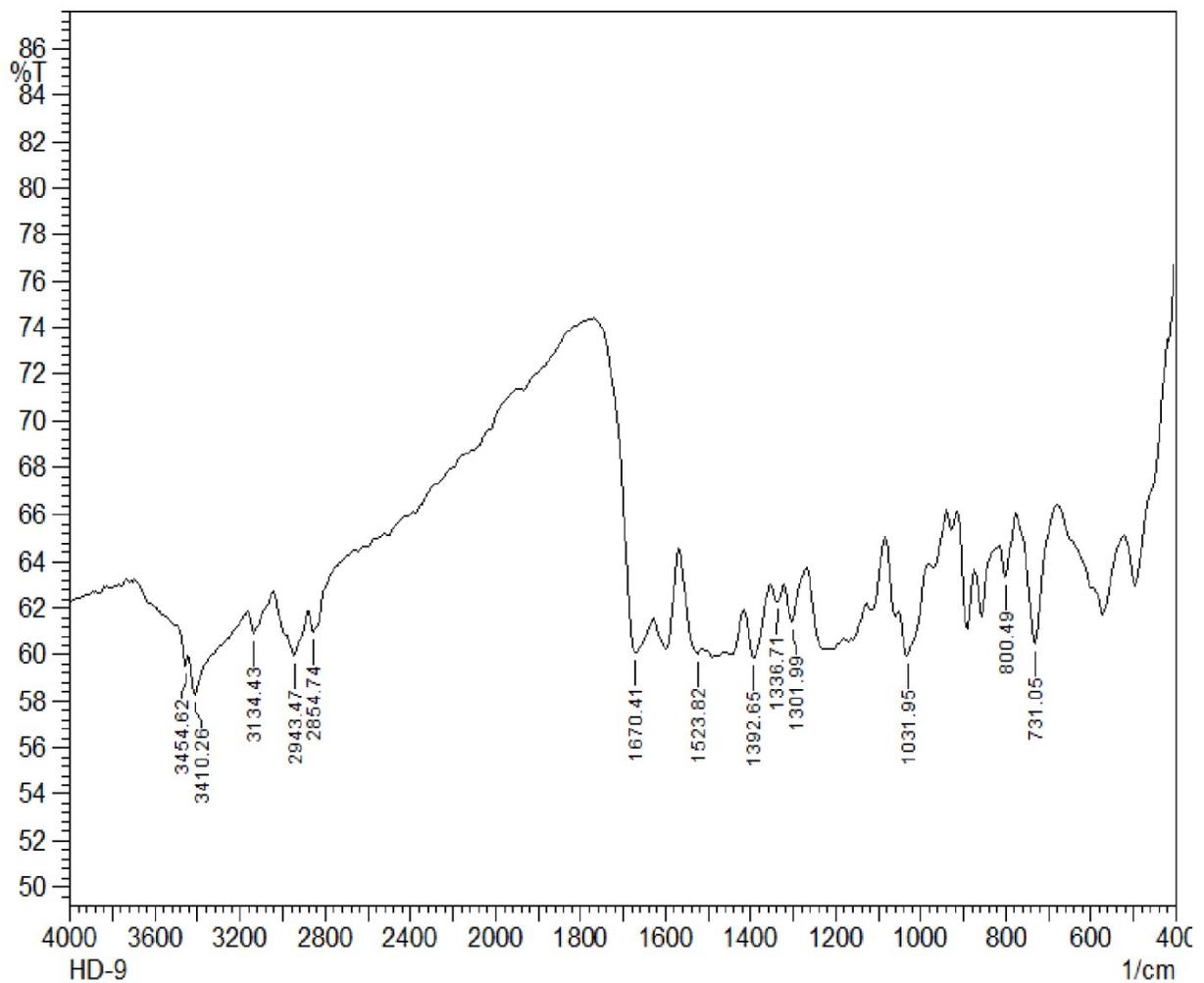


**Figure S44:** Mass spectrum of compound **HD-8**

**HD-9:**



**Figure S45:** Chemical structure of compound HD-9



**Figure S46:** IR spectrum of compound HD-9

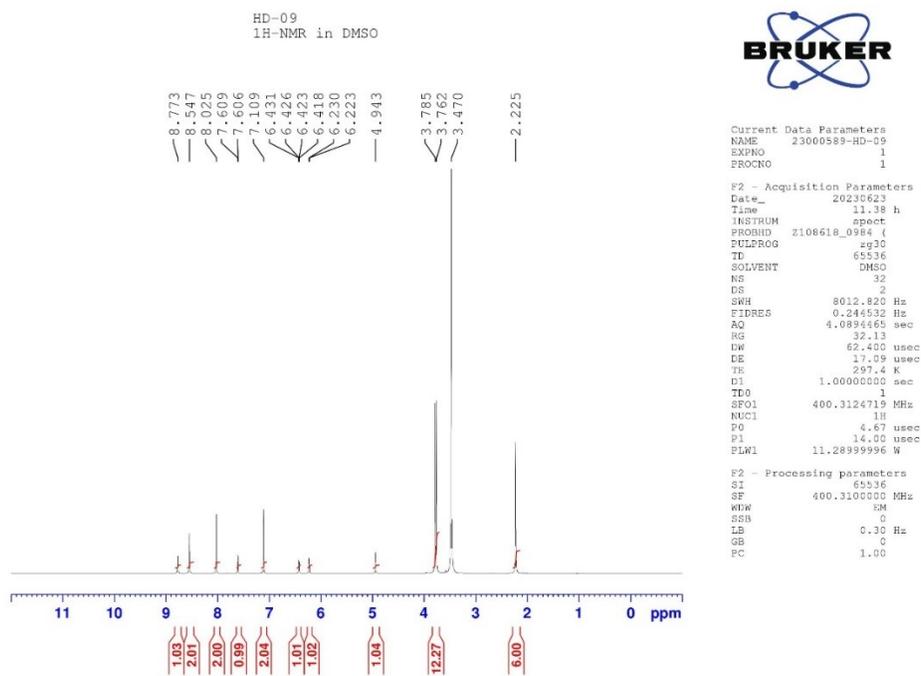


Figure S47: <sup>1</sup>H-NMR spectrum of compound HD-9

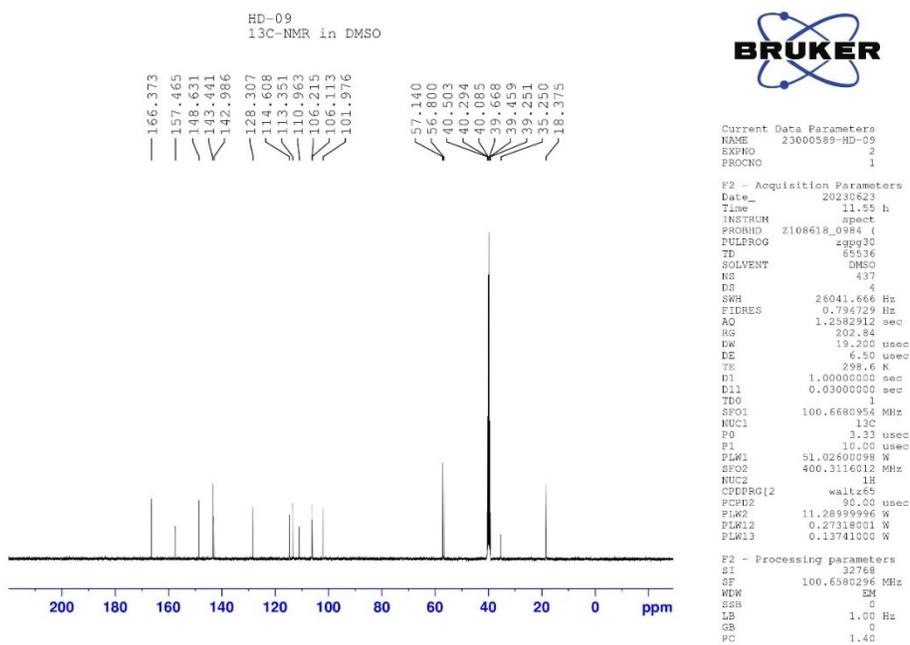
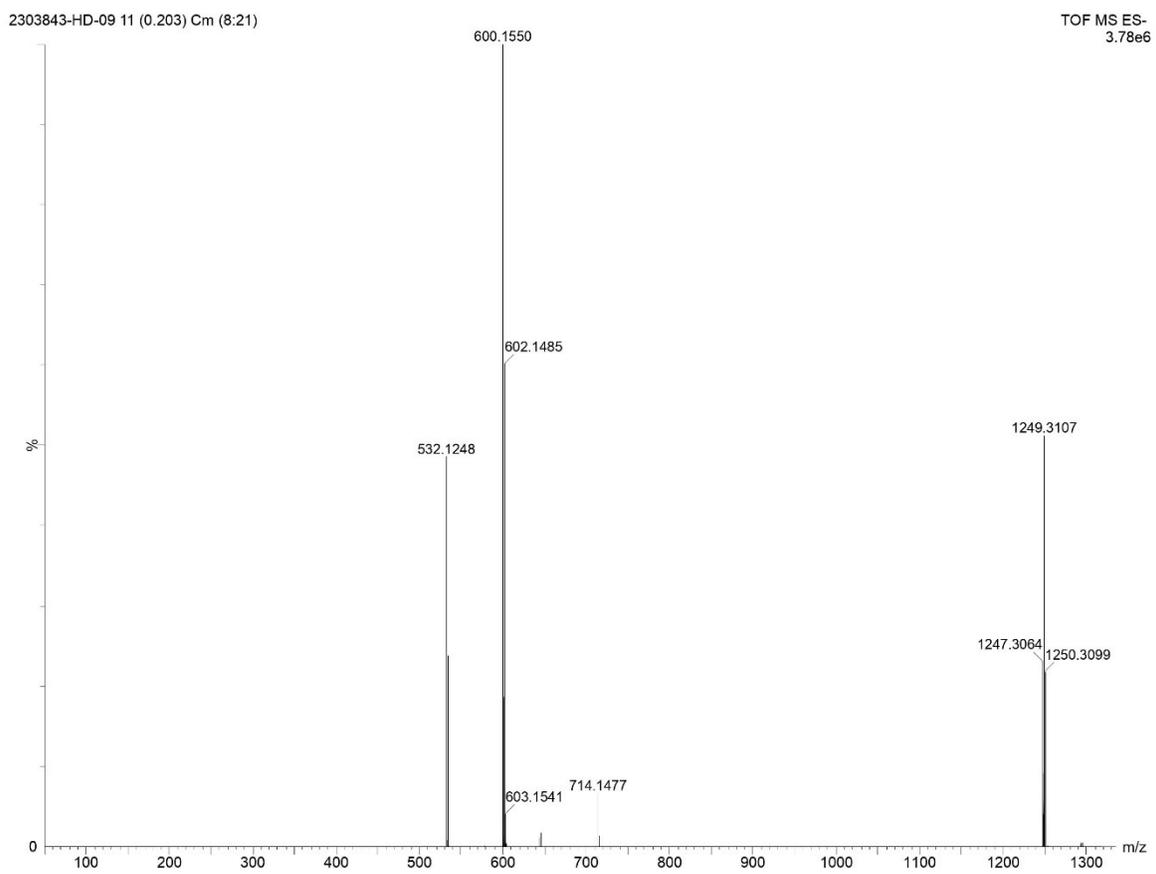
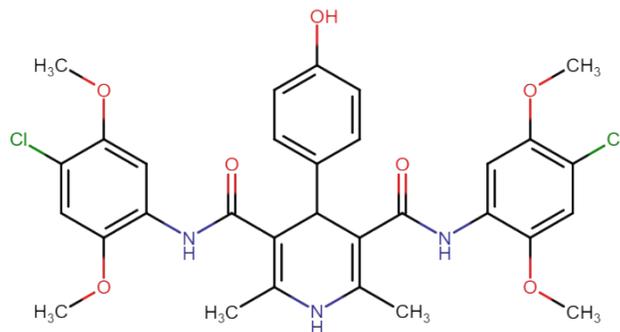


Figure S48: <sup>13</sup>C-NMR spectrum of compound HD-9

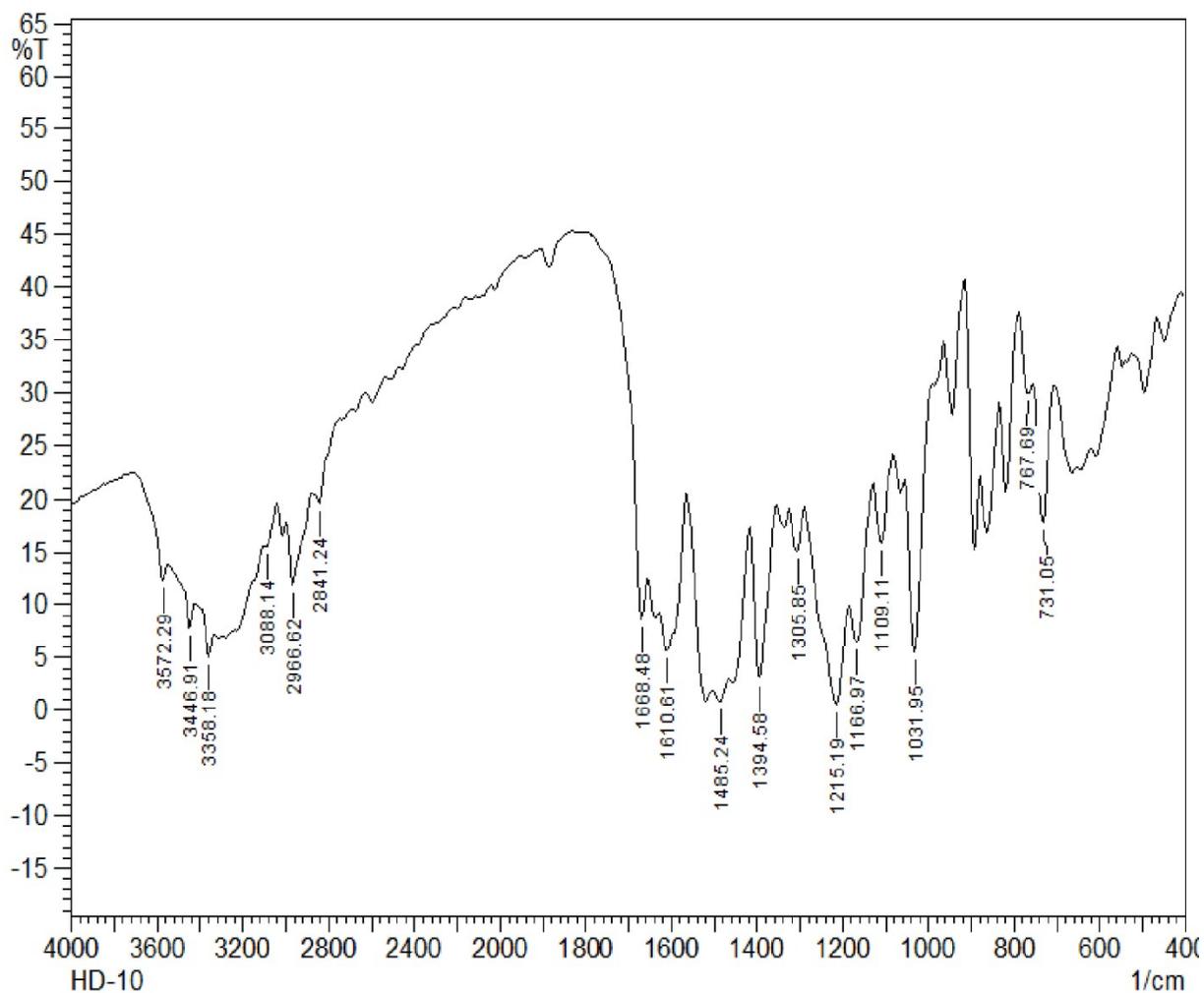


**Figure S49:** Mass spectrum of compound **HD-9**

**HD-10:**



**Figure S50:** Chemical structure of compound **HD-10**



**Figure S51:** IR spectrum of compound **HD-10**

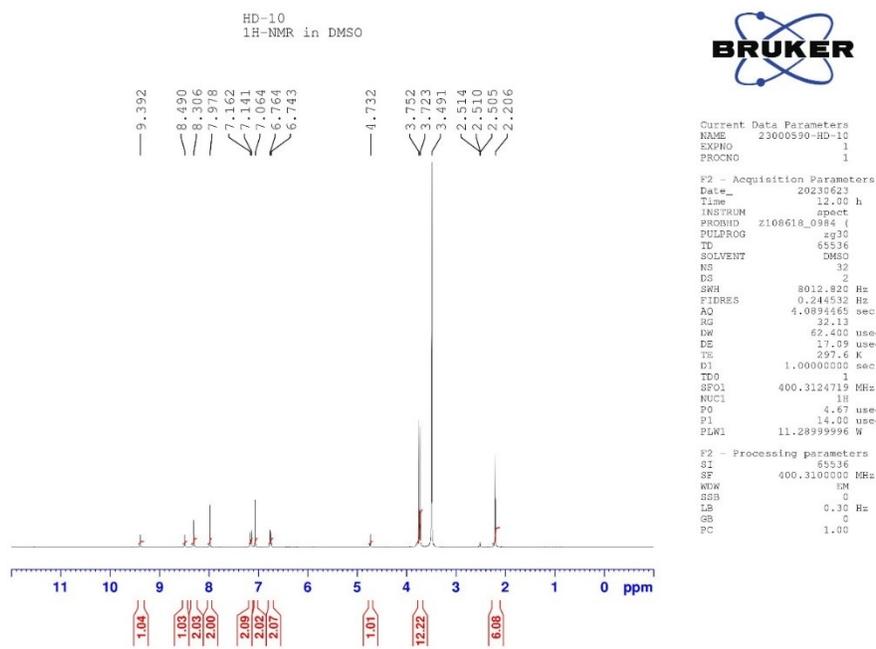


Figure S52: <sup>1</sup>H-NMR spectrum of compound HD-10

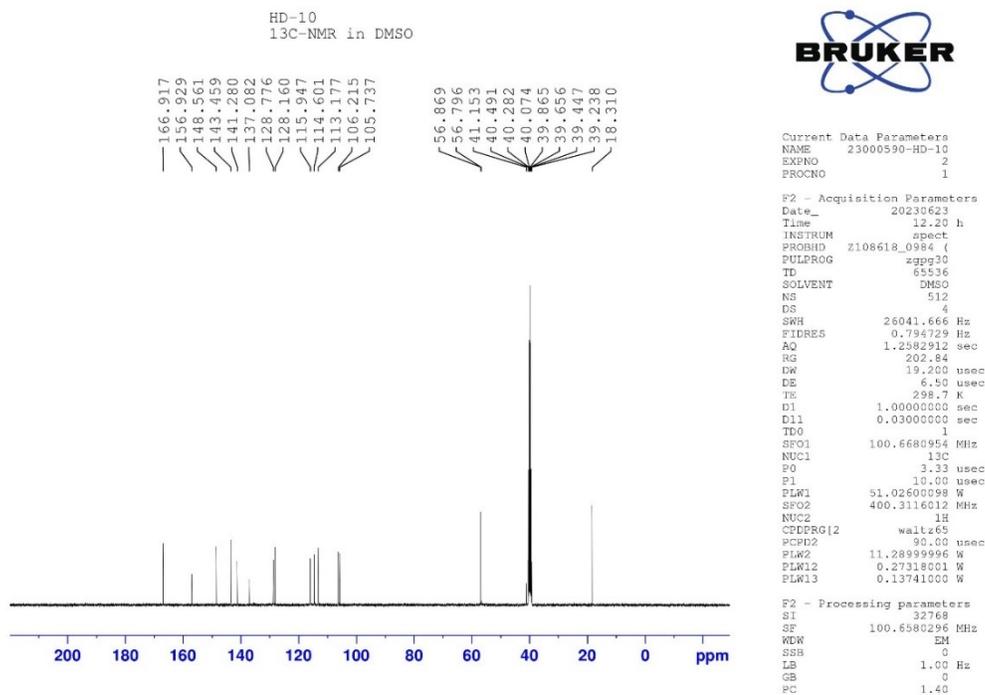
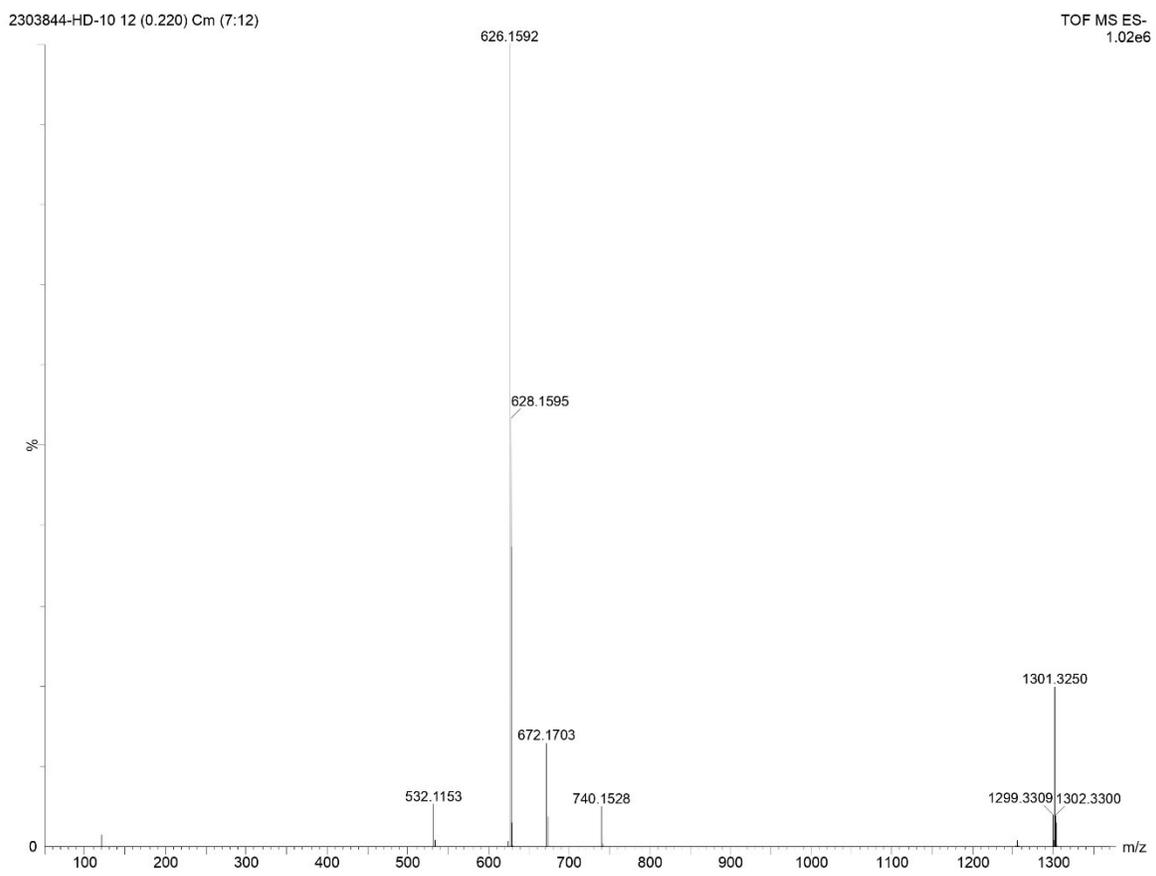
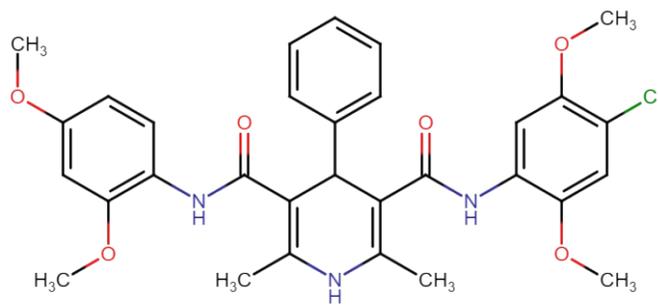


Figure S53: <sup>13</sup>C-NMR spectrum of compound HD-10

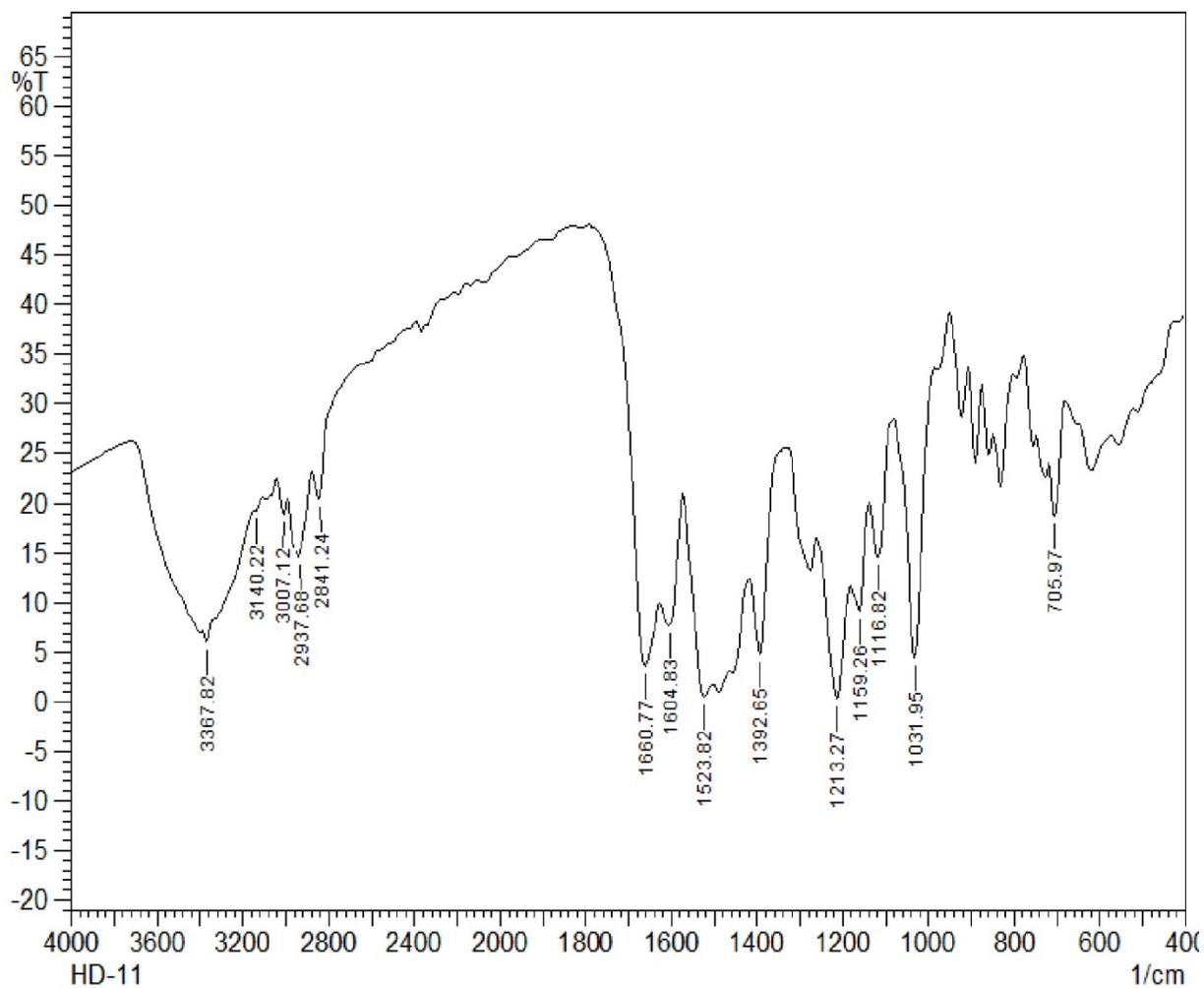


**Figure S54:** Mass spectrum of compound **HD-10**

**HD-11:**



**Figure S55:** Chemical structure of compound **HD-11**



**Figure S56:** IR spectrum of compound **HD-11**

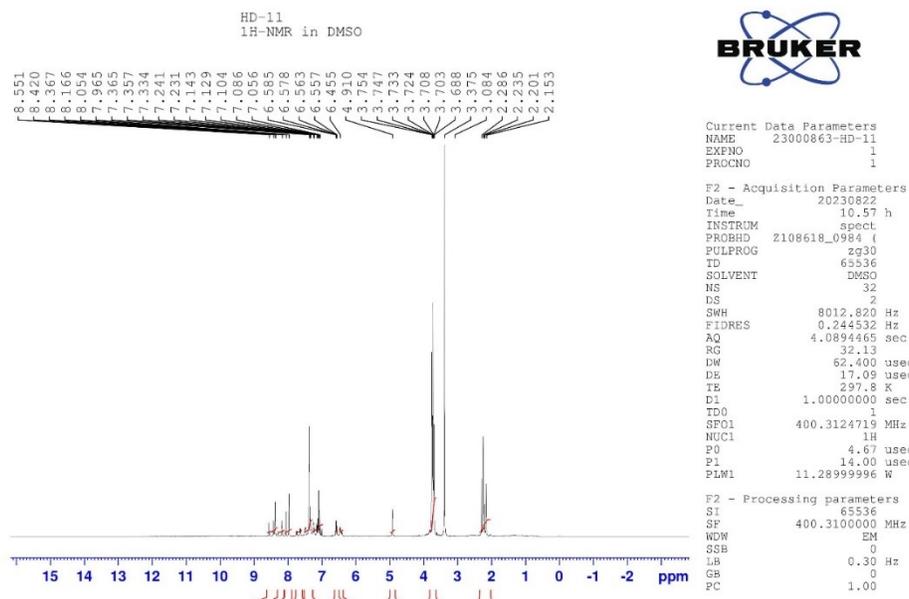


Figure S57: <sup>1</sup>H-NMR spectrum of compound HD-11

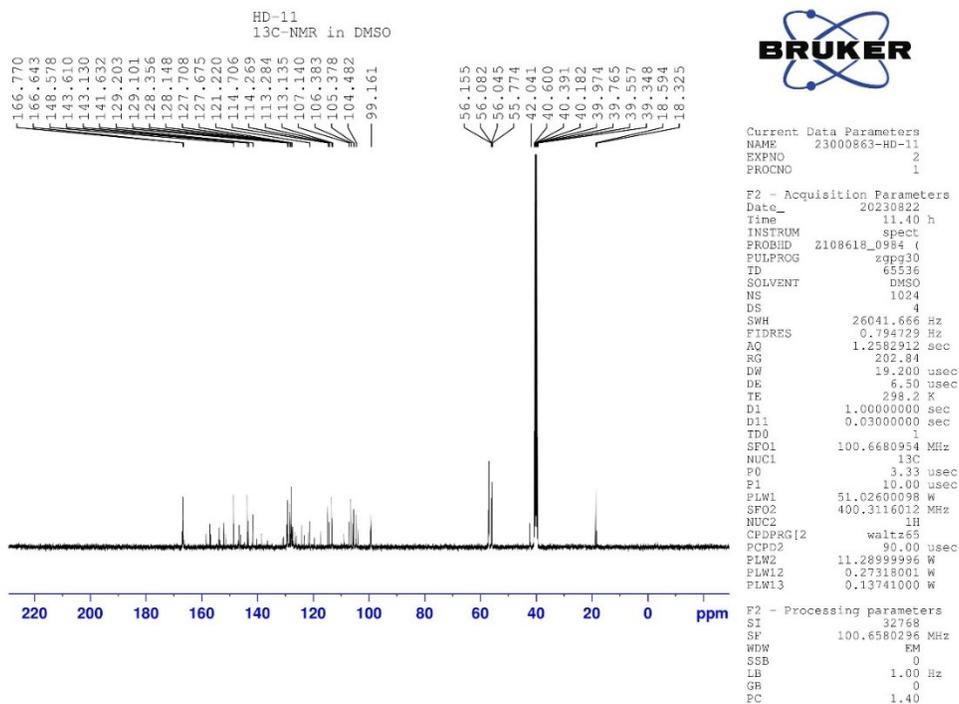
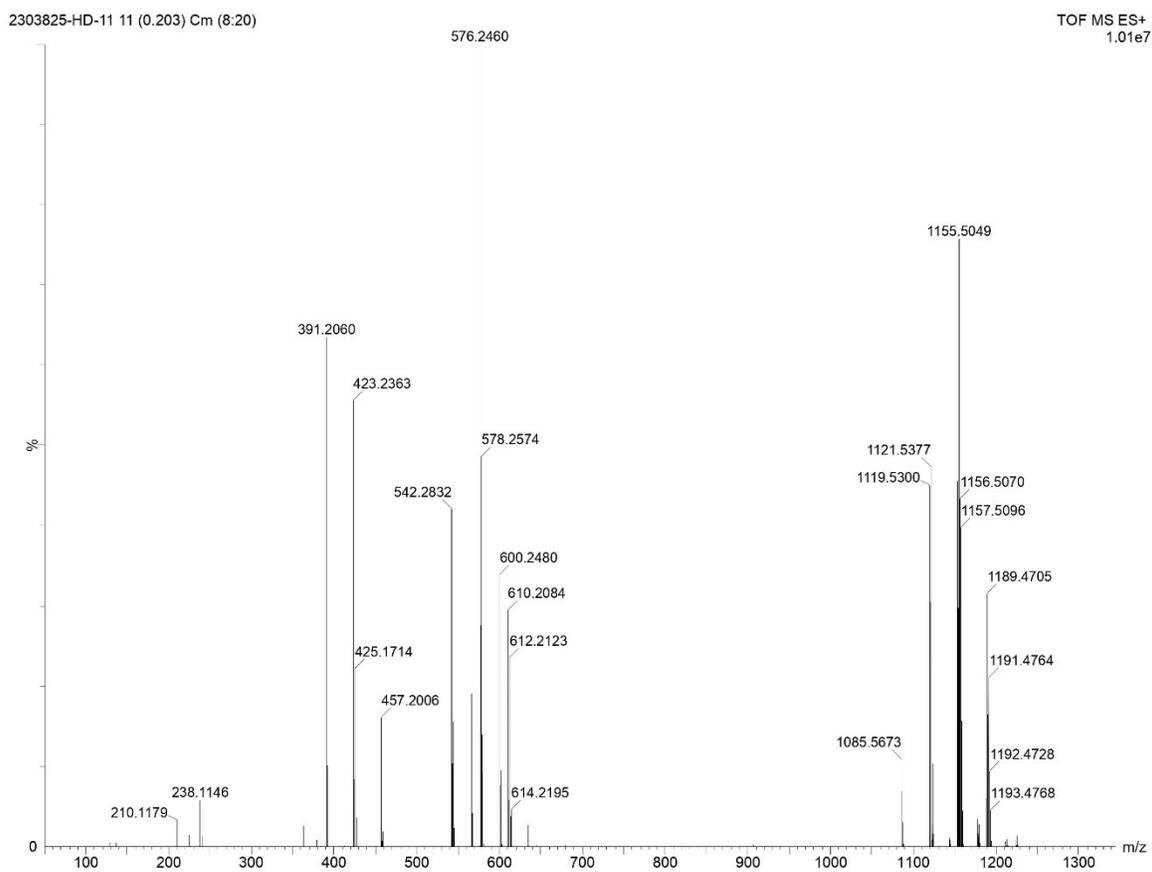
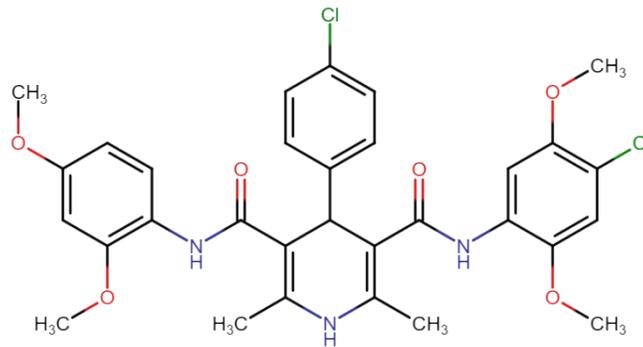


Figure S58: <sup>13</sup>C-NMR spectrum of compound HD-11

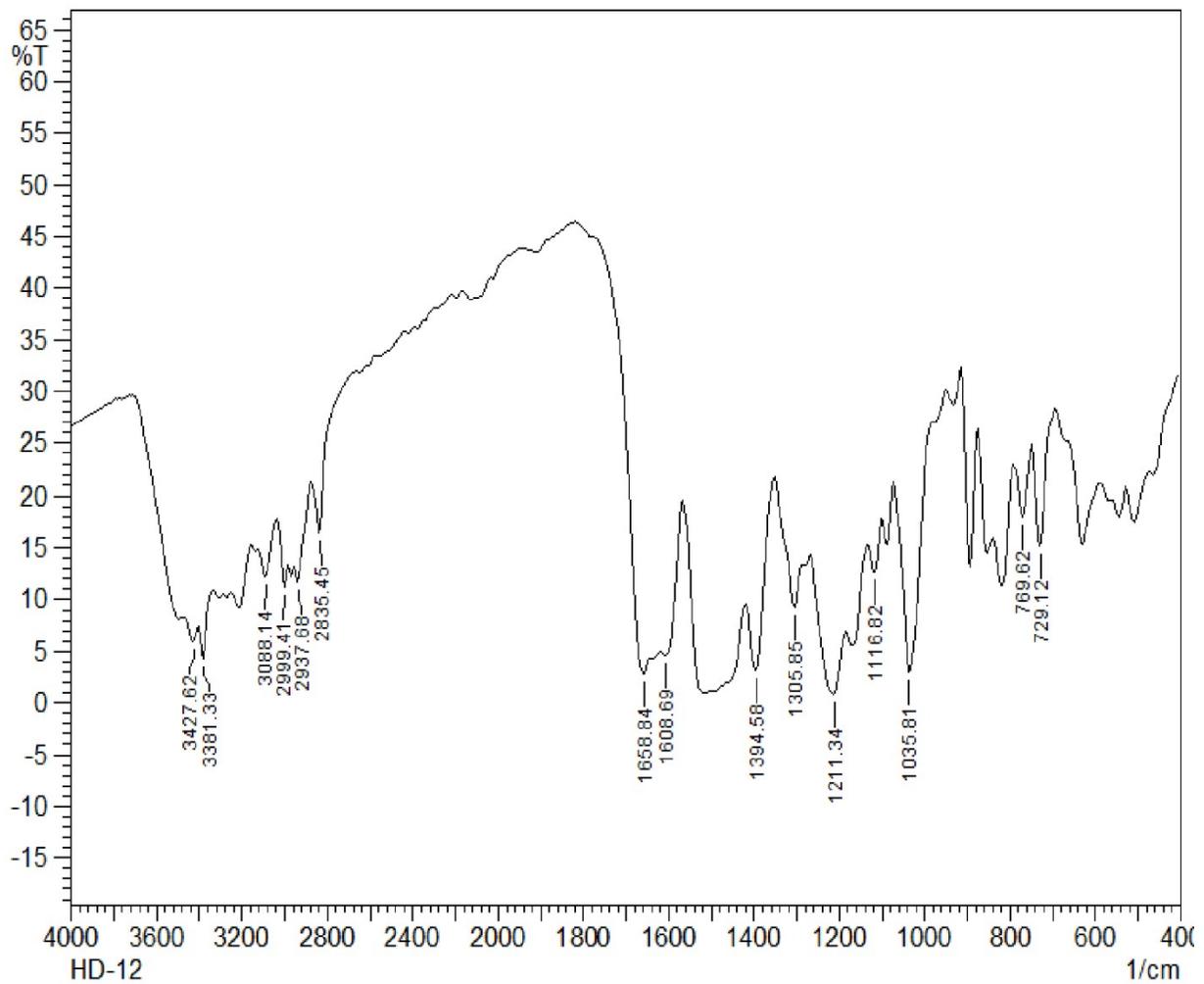


**Figure S59:** Mass spectrum of compound **HD-11**

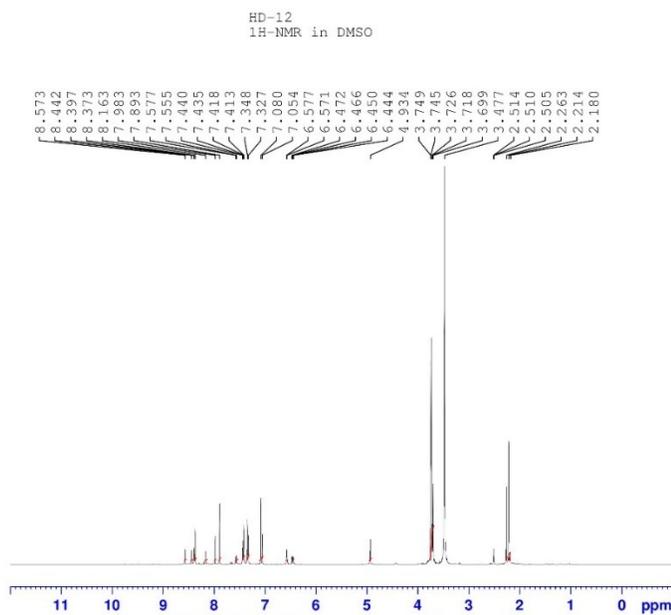
**HD-12:**



**Figure S60:** Chemical structure of compound HD-12



**Figure S61:** IR spectrum of compound HD-12



**BRUKER**

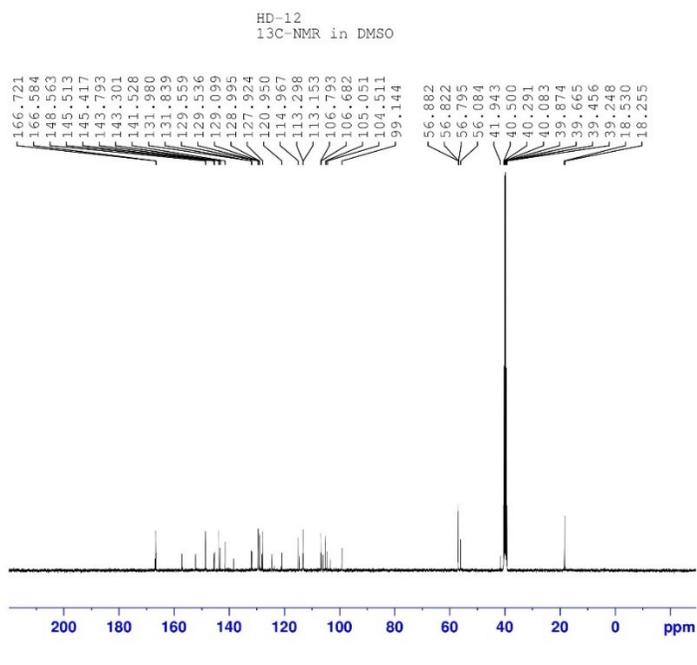
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DS        2
SWH       8012.826 Hz
FIDRES    0.244532 Hz
AQ        4.0894465 sec
RG         32.13
DE        62.400 usec
TE        17.09 usec
P1        297.6 K
D1        1.00000000 sec
TDO       1
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P0        4.67 usec
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PLW1     11.28999996 W

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Figure S62: <sup>1</sup>H-NMR spectrum of compound HD-12



**BRUKER**

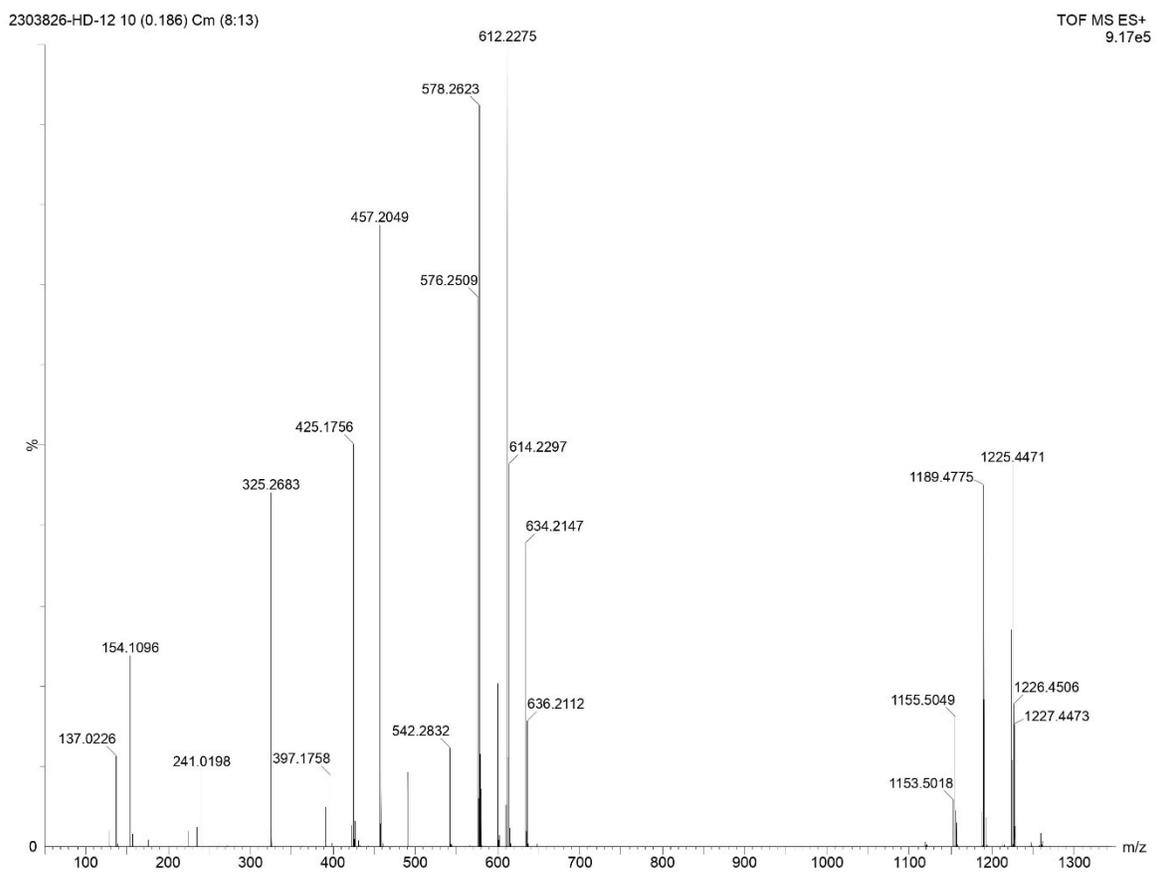
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TE        6.50 usec
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D11       0.03000000 sec
TDO       1
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NUC1      13C
P0        3.33 usec
P1        10.00 usec
PLW1     51.02600098 W
SFO2     400.3116012 MHz
NUC2      1H
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PCPD2    90.00 usec
PLW2     11.28999996 W
PLW12    0.27318001 W
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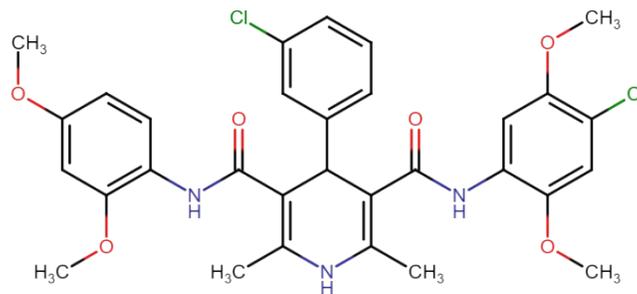
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Figure S63: <sup>13</sup>C-NMR spectrum of compound HD-12

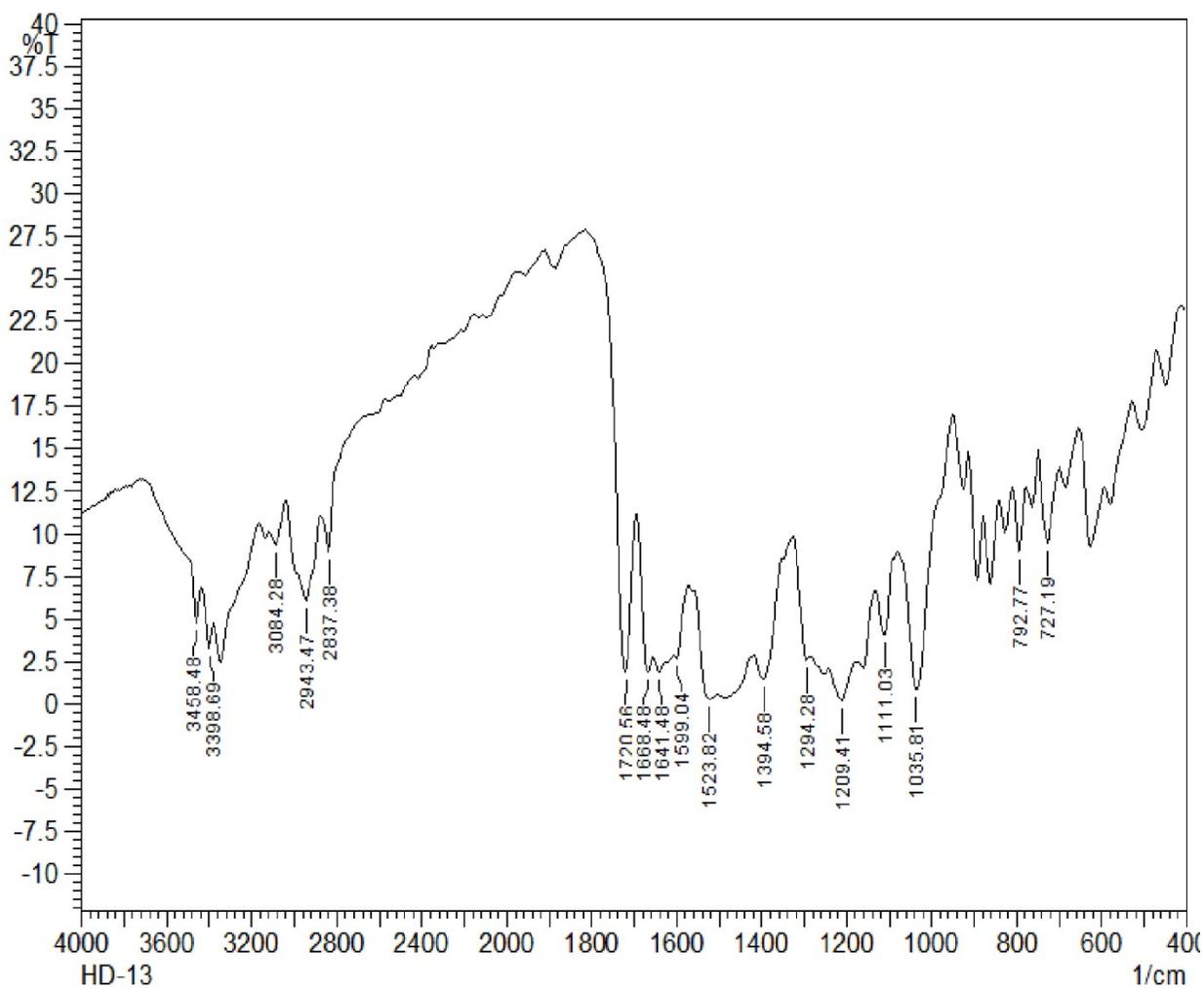


**Figure S64:** Mass spectrum of compound **HD-12**

**HD-13:**



**Figure S65:** Chemical structure of compound HD-13



**Figure S66:** IR spectrum of compound HD-13

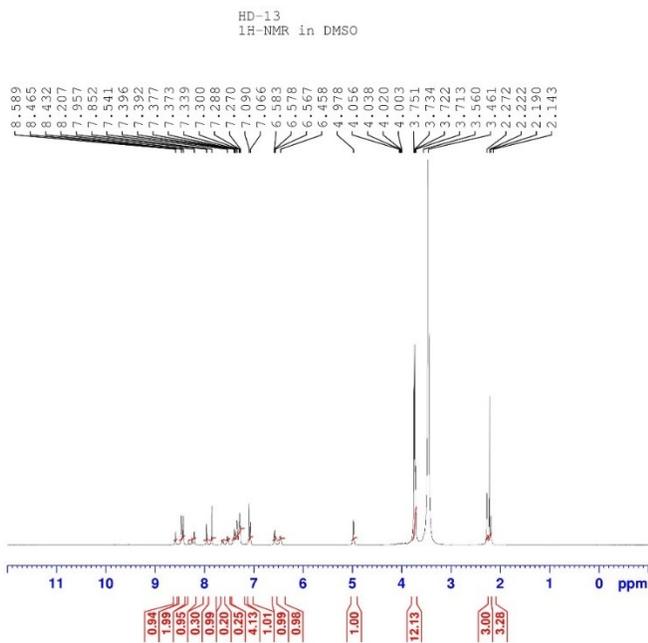


Figure S67: <sup>1</sup>H-NMR spectrum of compound HD-13

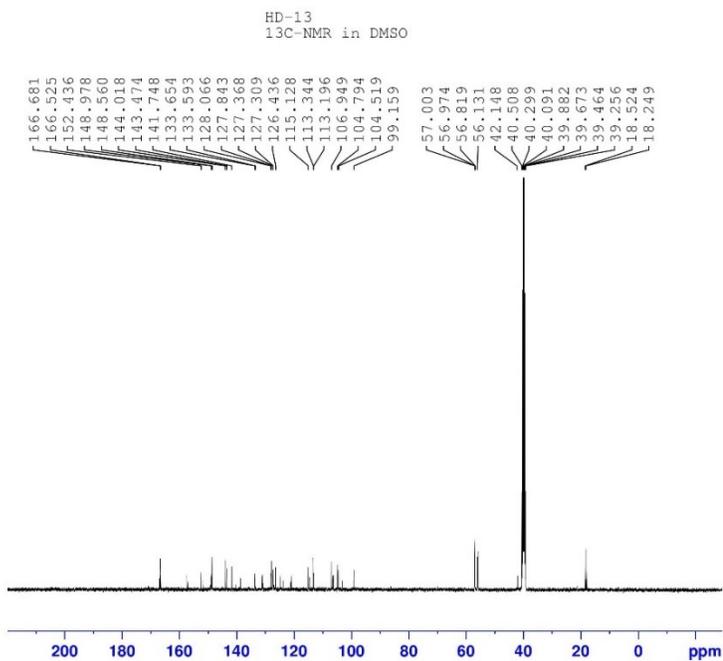
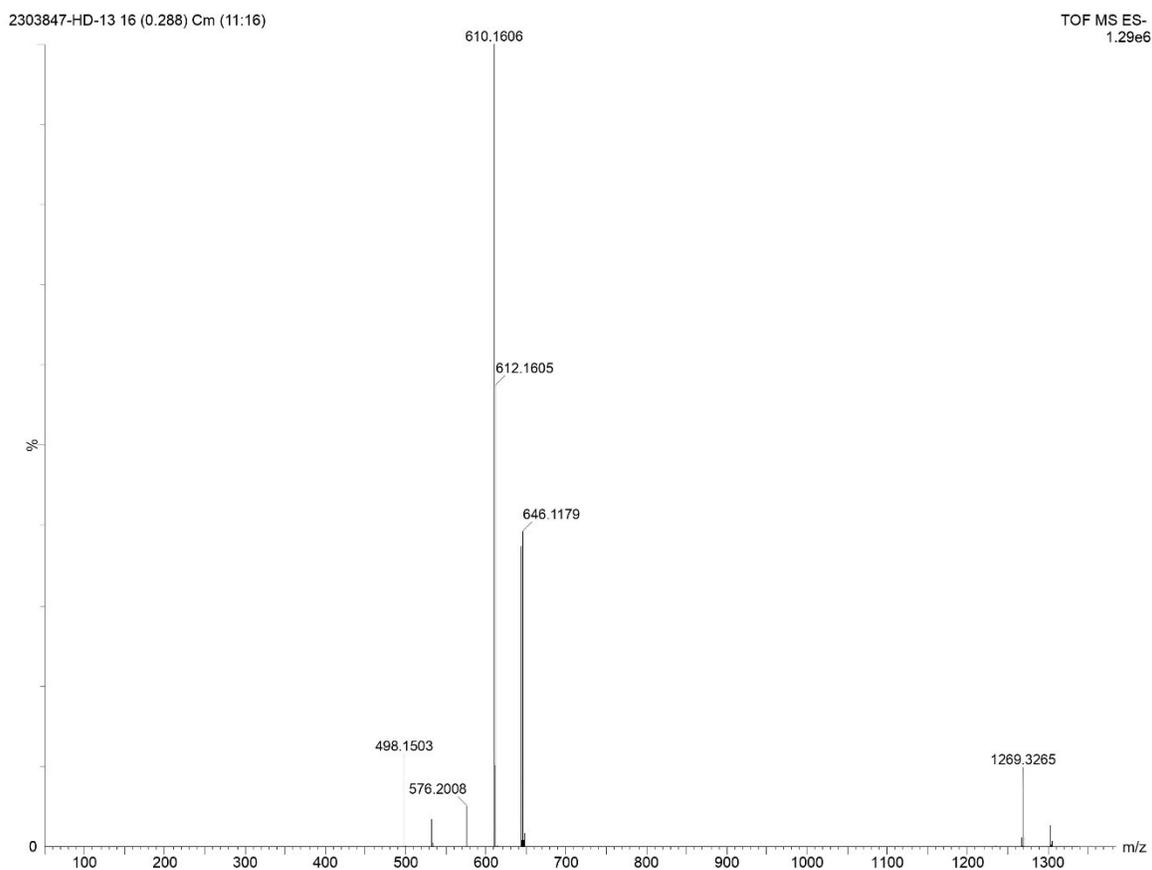
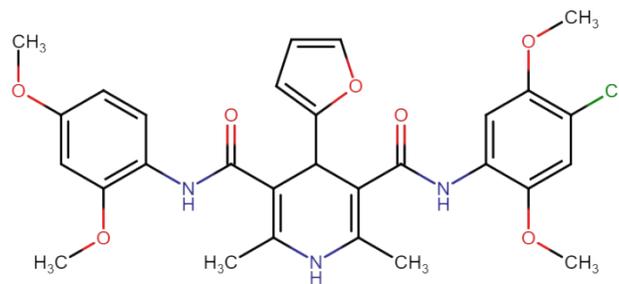


Figure S68: <sup>13</sup>C-NMR spectrum of compound HD-13

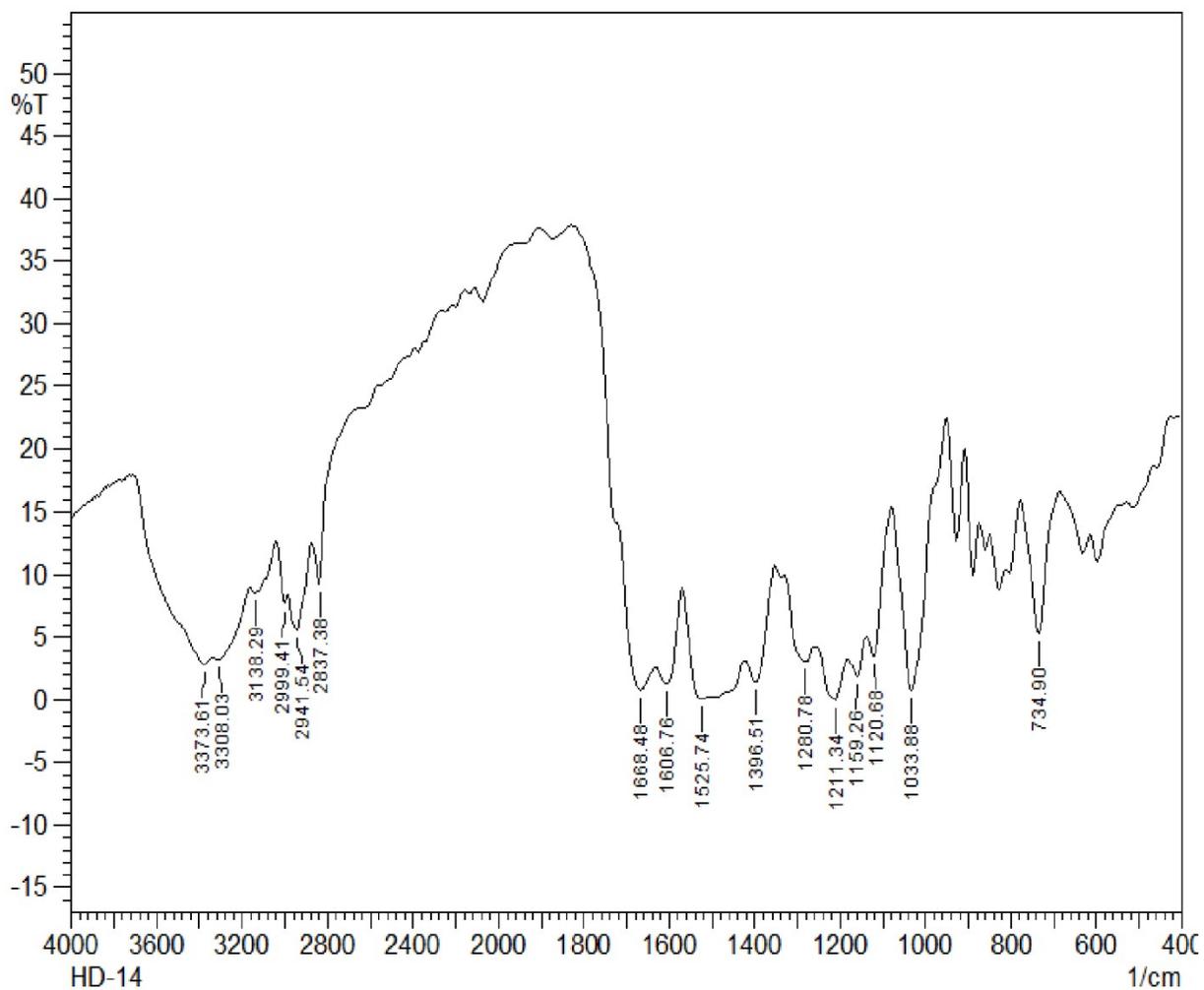


**Figure S69:** Mass spectrum of compound **HD-13**

**HD-14:**



**Figure S70:** Chemical structure of compound HD-14



**Figure S71:** IR spectrum of compound HD-14

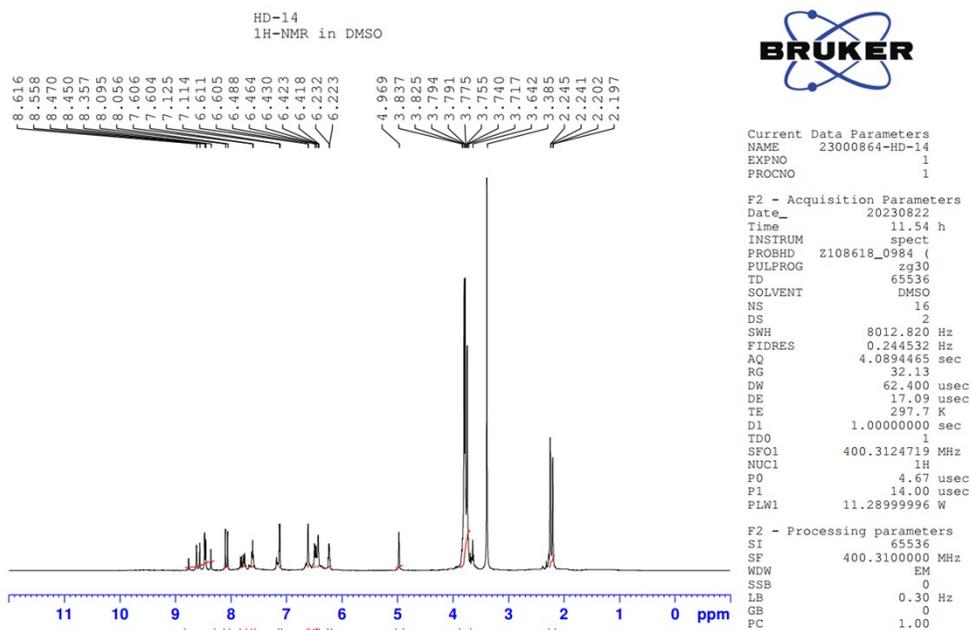


Figure S72: <sup>1</sup>H-NMR spectrum of compound HD-14

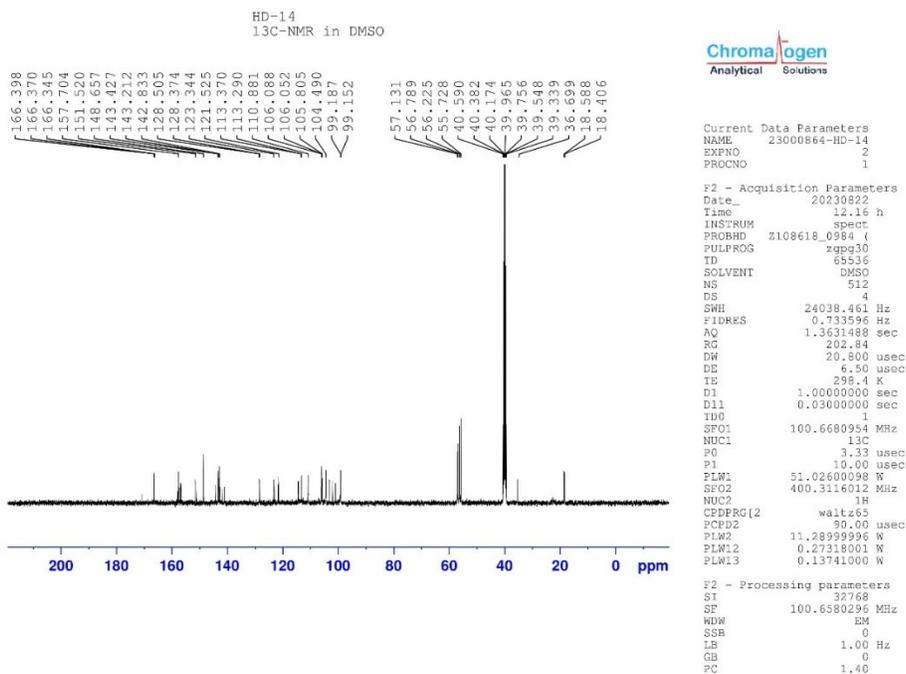
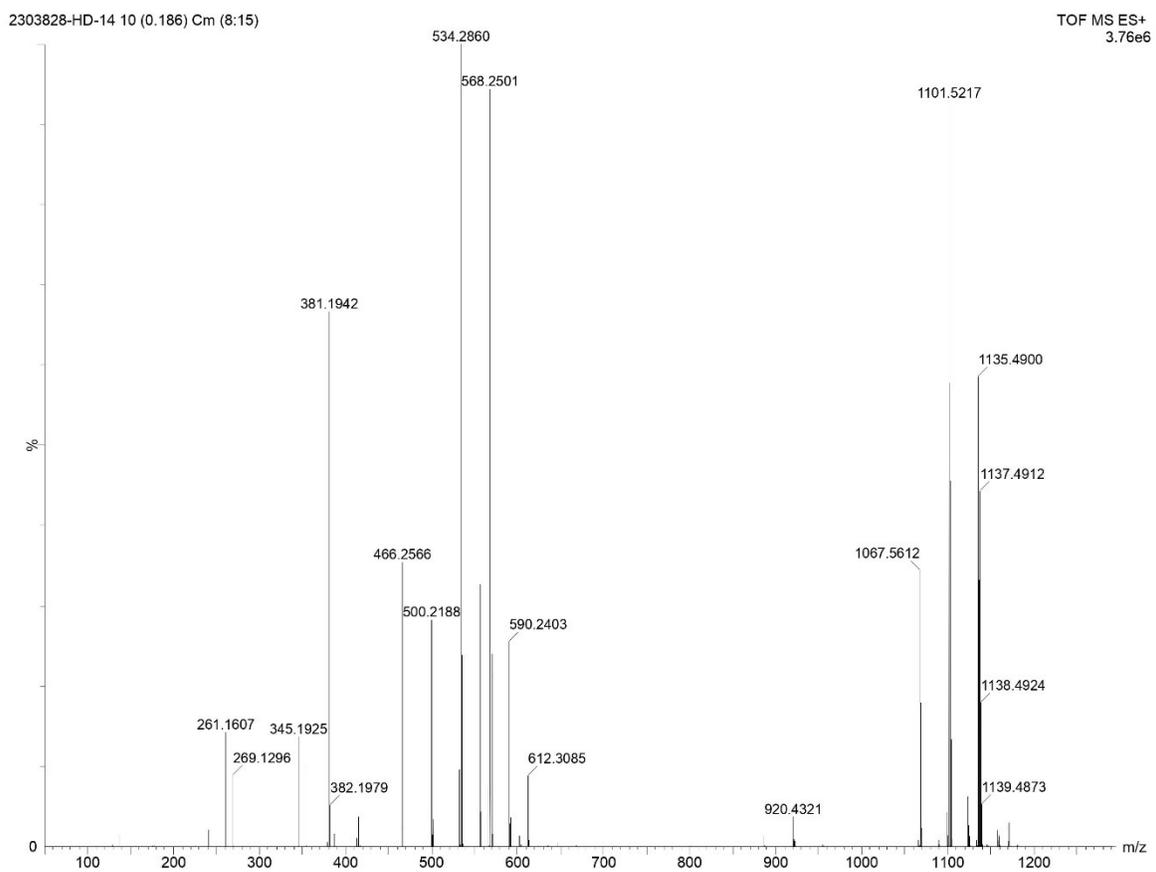
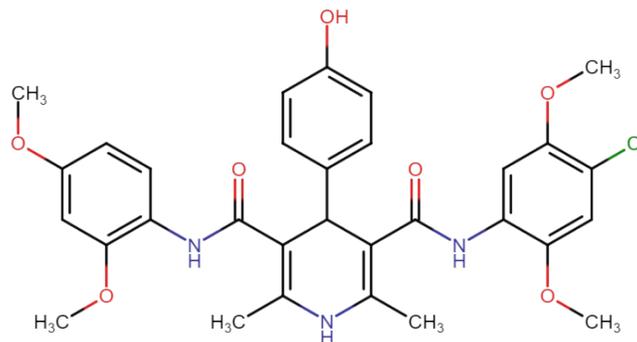


Figure S73: <sup>13</sup>C-NMR spectrum of compound HD-14

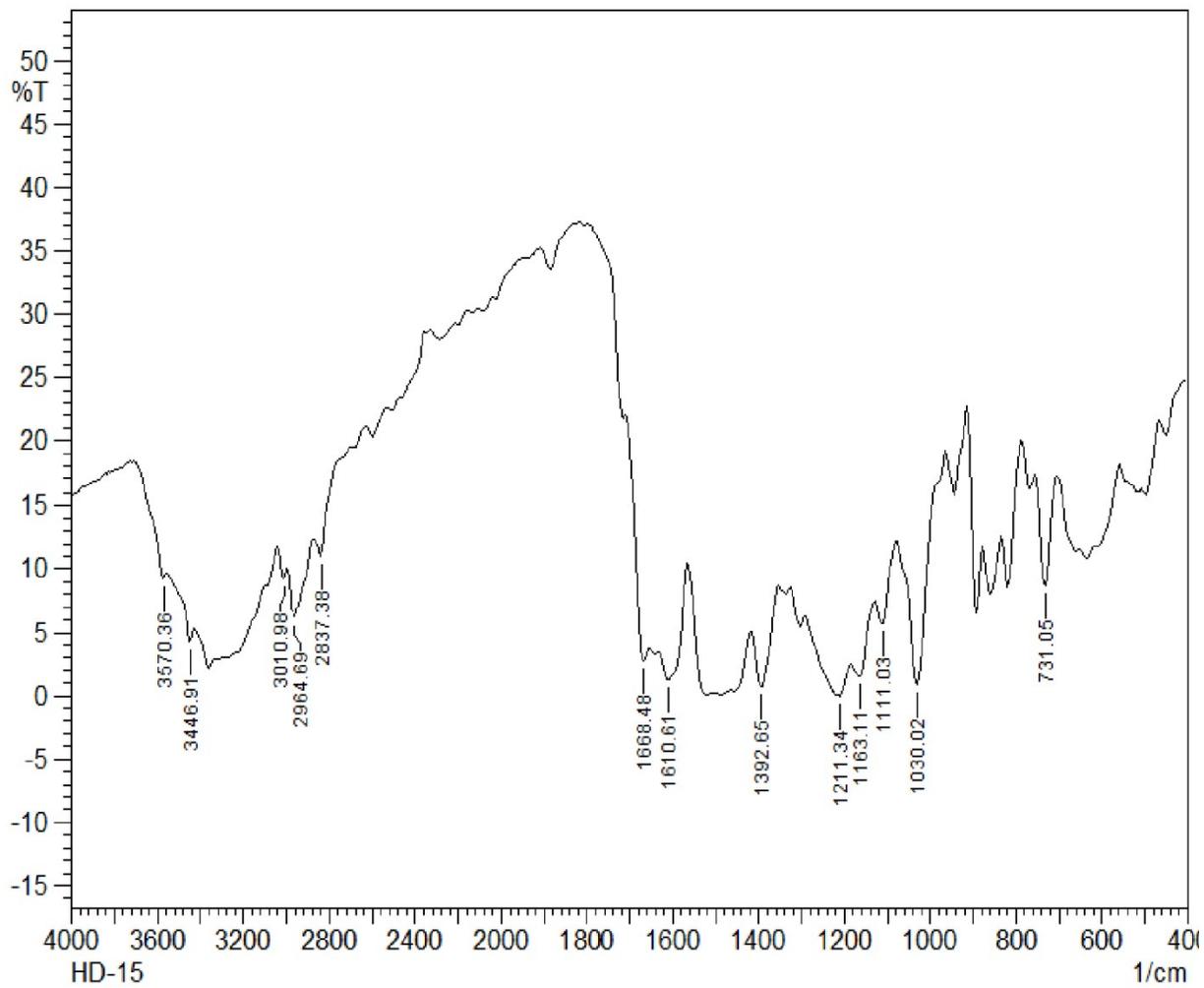


**Figure S74:** Mass spectrum of compound **HD-14**

**HD-15:**



**Figure S75:** Chemical structure of compound **HD-15**



**Figure S76:** IR spectrum of compound **HD-15**

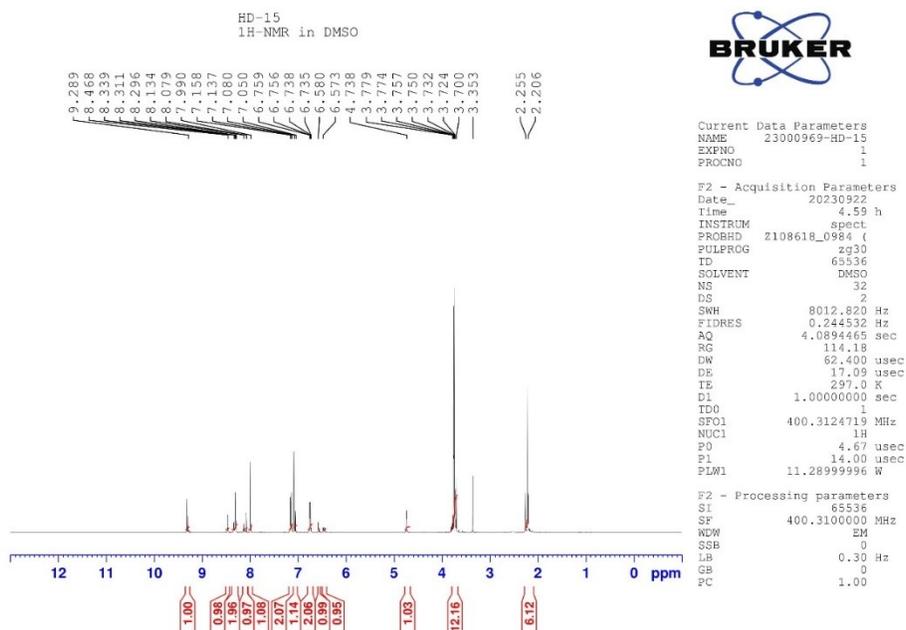


Figure S77: <sup>1</sup>H-NMR spectrum of compound HD-15

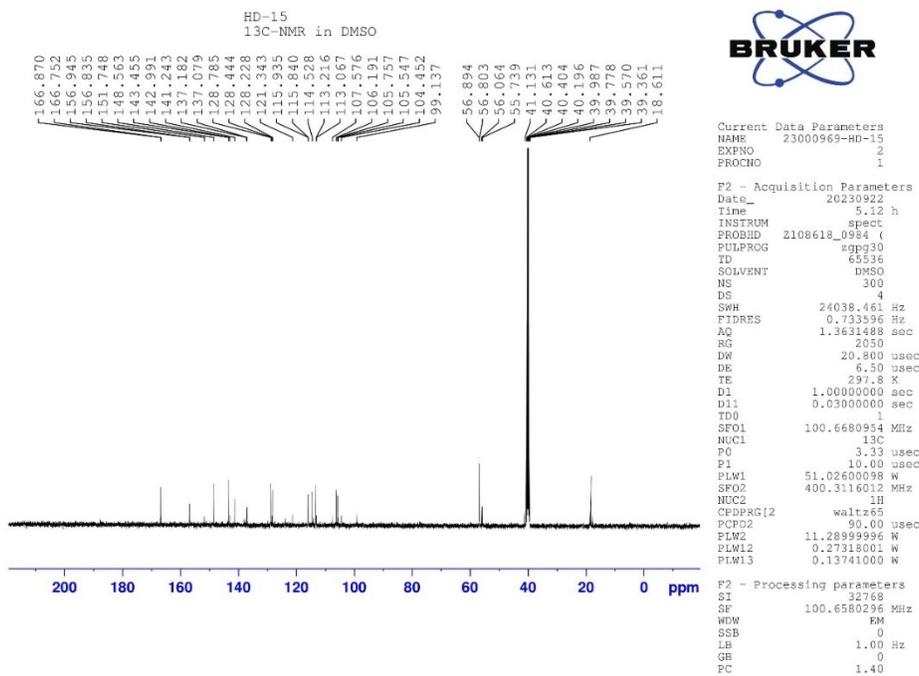
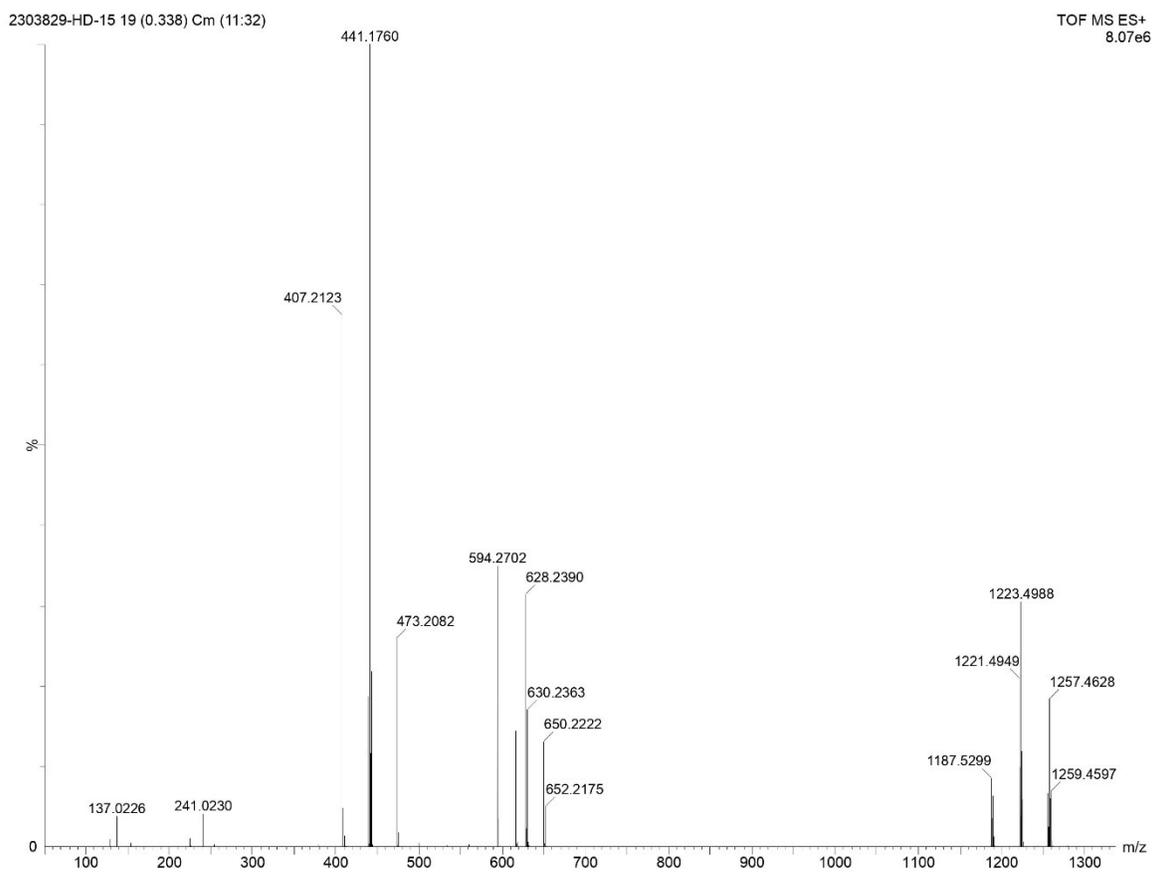


Figure S78: <sup>13</sup>C-NMR spectrum of compound HD-15



**Figure S79:** Mass spectrum of compound **HD-15**