# A New Method to Predict the Thermal Degradation Behaviour of Polybenzoxazines from Empirical Data Using Structure Property Relationships

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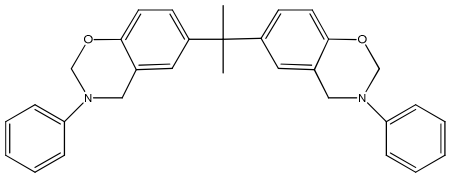
## SUPPLEMENTARY CHARACTERISATION MATERIAL

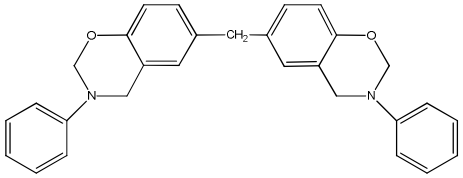
# Materials Overview

## MT 35600 Monomer- Bisphenol A based *bis*-benzoxazine BA-a



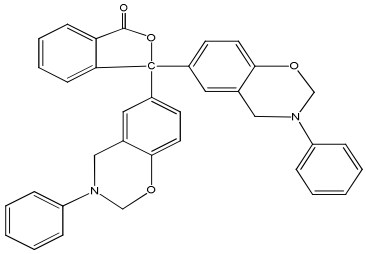
Chemical Formula: $C_{31}H_{30}N_2O_2$
Molecular Weight: 462.58
Elemental Analysis: C, 80.49; H, 6.54; N, 6.06; O, 6.92

## MT 35700 Monomer- Bisphenol F based *bis*-benzoxazine BF-a



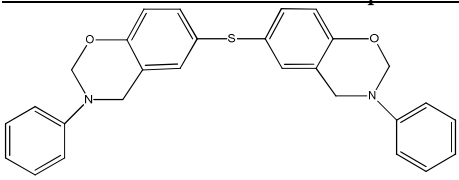
Chemical Formula: $C_{29}H_{26}N_2O_2$
Molecular Weight: 434.53
Elemental Analysis: C, 80.16; H, 6.03; N, 6.45; O, 7.36

## MT 35800 Monomer- Phenolphthalein based *bis*-benzoxazine BP-a



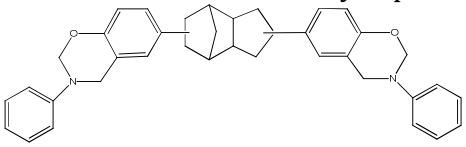
Chemical Formula: $C_{36}H_{28}N_2O_4$
Molecular Weight: 552.62
Elemental Analysis: C, 78.24; H, 5.11; N, 5.07; O, 11.58

## MT 35900 Monomer- Thiodiphenol based *bis*-benzoxazine BT-a

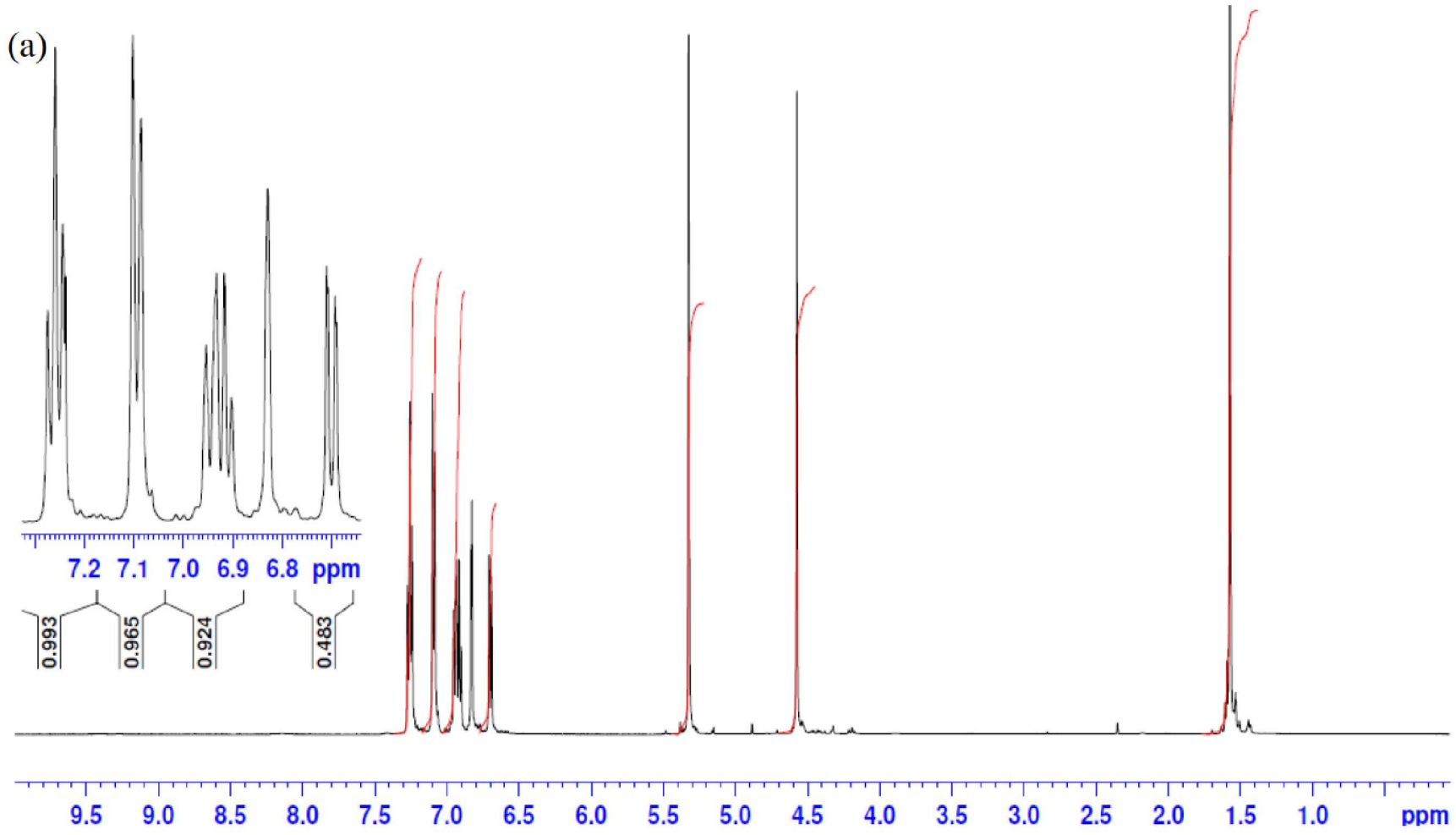


Chemical Formula: $C_{28}H_{24}N_2O_2S$
Molecular Weight: 452.57
Elemental Analysis: C, 74.31; H, 5.35; N, 6.19; O, 7.07; S, 7.09

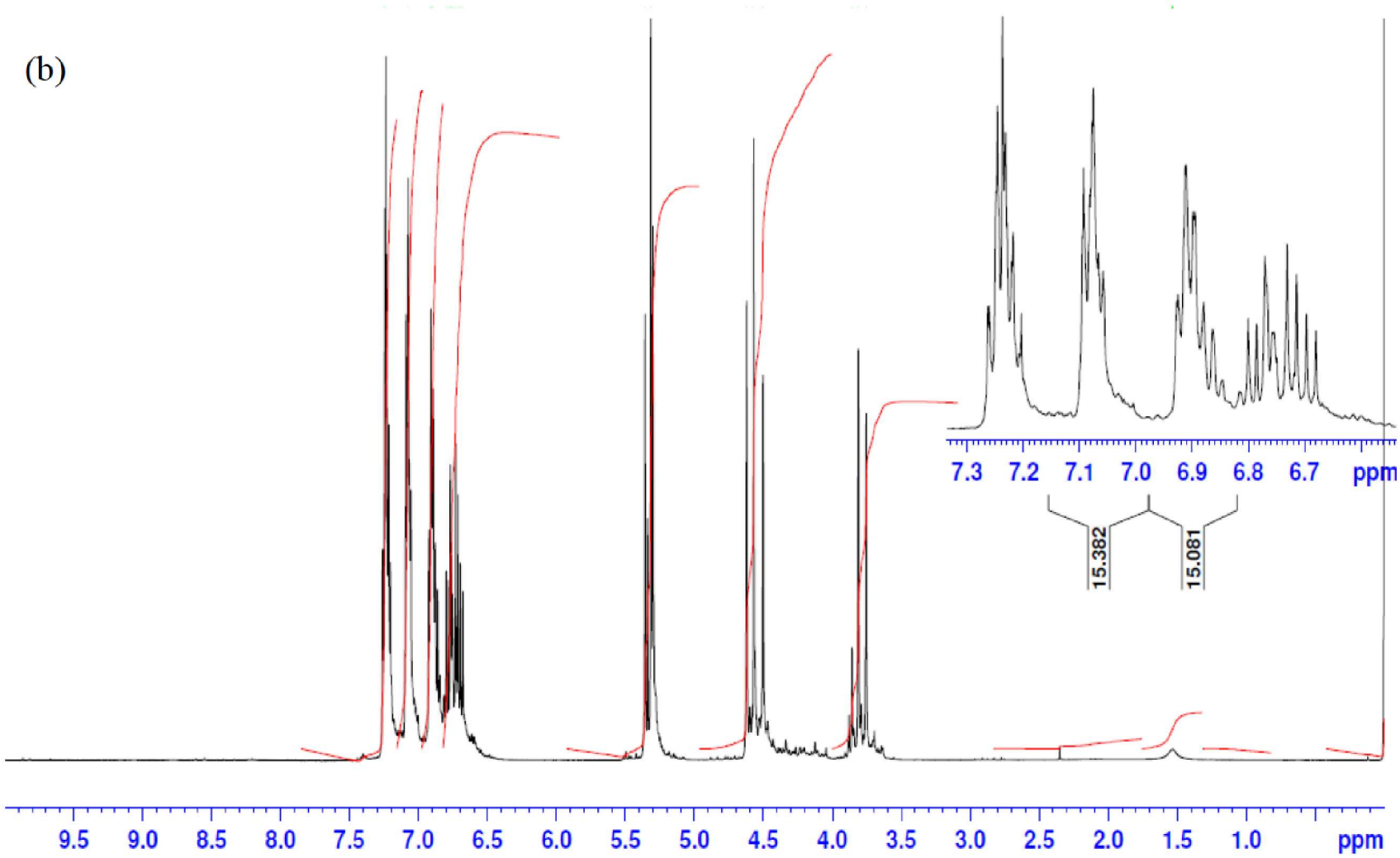
## LME 10140 Monomer- Dicyclopentadiene based *bis*-benzoxazine BD-a



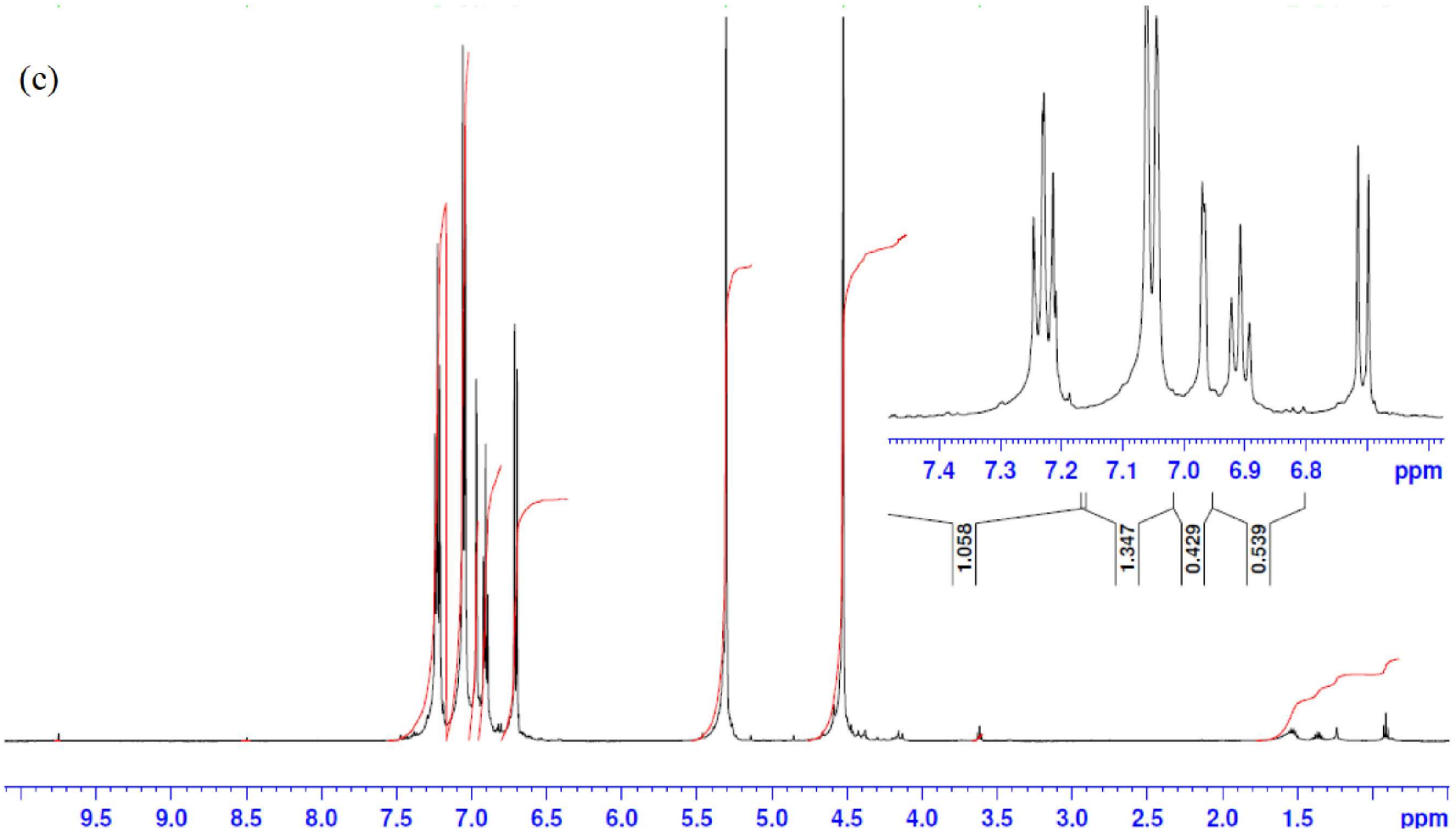
Chemical Formula: $C_{39}H_{42}N_2O_2$
Molecular Weight: 570.76
Elemental Analysis: C, 82.07; H, 7.42; N, 4.91; O, 5.61




$^{1}$H NMR Spectrum (500 MHz, $CDCl_3$, 298 K) of BA-a (expansion showing aromatic region)

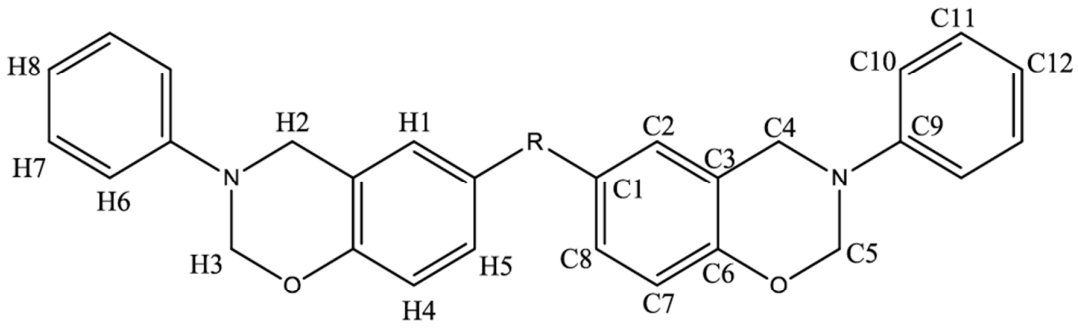


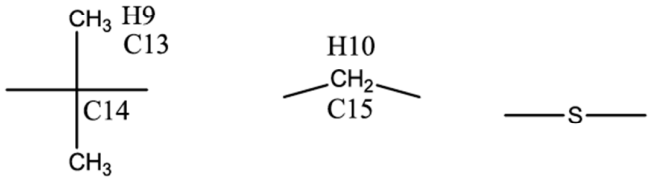

$^{1}$H NMR Spectrum (500 MHz, $CDCl_3$, 298 K) of BF-a (expansion showing aromatic region)




$^{1}$H NMR Spectrum (500 MHz, $CDCl_3$, 298 K) of BT-a (expansion showing aromatic region)

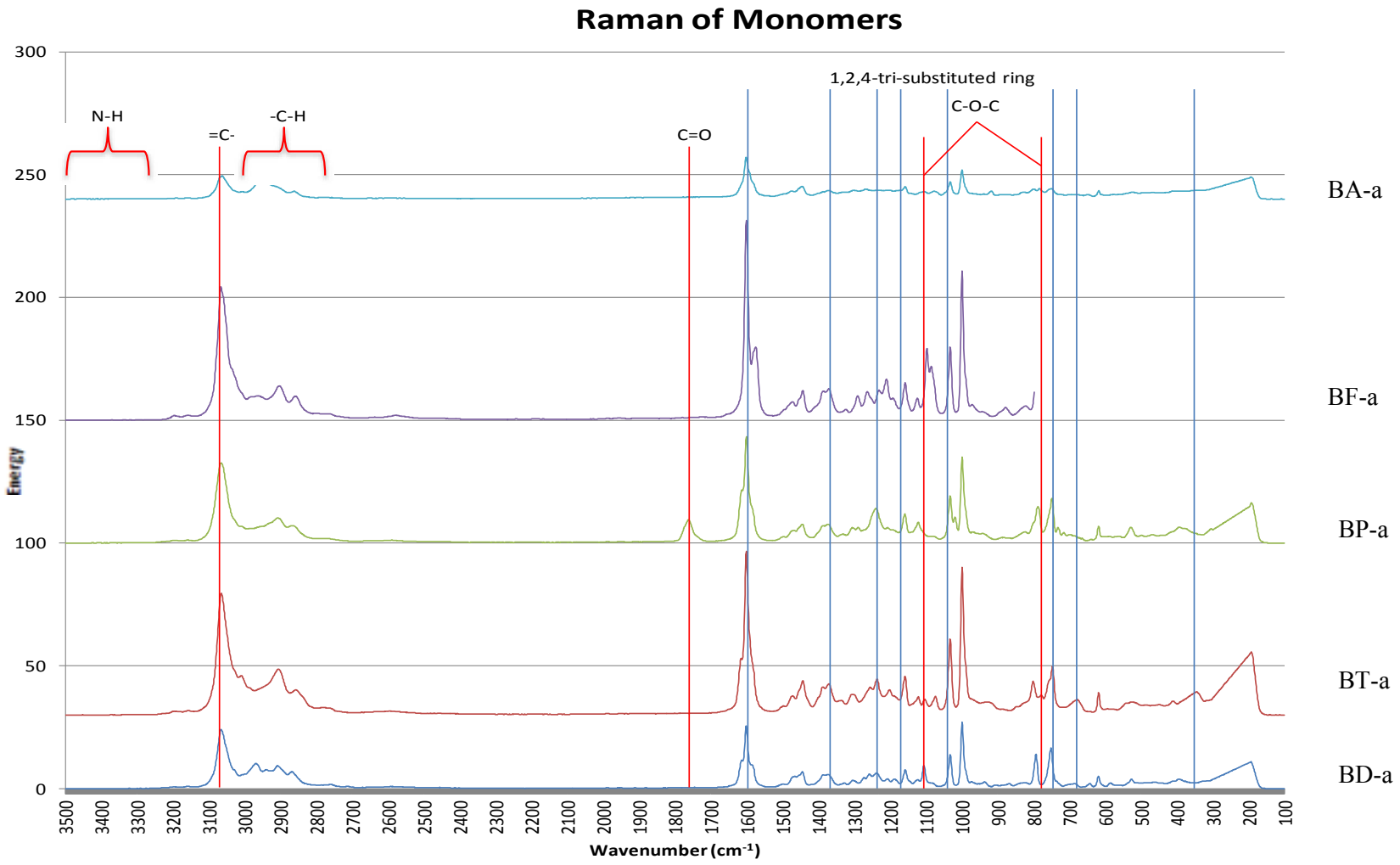
**NMR spectral assignments for BA-a, BF-a and BT-a. Only peaks that could be assigned have been included, some not possible to assign due to interferenceFrom unknowncontaminants.**




| ***Proton*** | **H1** | **H2** | **H3** | **H4** | **H5** | **H6** | **H7** | **H8** | **H9** | **H10** |
|---|---|---|---|---|---|---|---|---|---|---|
| *BA-a* | 6.83 (s) | 5.32 (s) | 4.57 (s) | 6.71 (d) | 6.95 (d) | 6.95 (d) | 7.24 (t) | 7.08 (t) | 1.61 (s) | - |
| *BF-a* | 6.8-6.93 | 5.33 (s) | 4.57 (s) | 6.68-6.79 | 6.8-6.93 | 6.8-6.93 | 7.20-7.22 | 7.06-7.10 | - | 3.76 (s) |
| *BT-a* | 6.85 | 5.23 (s) | 4.54 (s) | 6.71 (d) | 6.949 | 6.925 (d) | 7.22 (t) | 7.07 | - | - |

| ***Carbon*** | **C1** | **C2** | **C3** | **C4** | **C5** | **C6** | **C7** | **C8** | **C9** | **C10** | **C11** | **C12** | **C13** | **C14** | **C15** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *BA-a* | 143.24 | 126.40 | 124.77 | 79.13 | 50.70 | 152.21 | 116.39 | 121.21 | 148.52 | 120.09 | 129.27 | 118.03 | 41.80 | 31.08 | - |
| *BF-a* | 135.17? | 125.06 | 124.78 | 79.50 | 51.00 | 152.25 | 116.85 | 121.50 | 148.49 | 120.66 | 129.49 | 118.50 | - | - | 34.74 |
| *BT-a* | 131.21? | | 127.37 | 79.59 | 50.04 | 153.87 | 117.92 | 121.70 | 148.21 | | 129.74 | 118.34 | - | - | - |




**Raman Spectra of Monomers**

**Carbon, Hydrogen and Nitrogen Content of Monomers (duplicate measurements)**

| Measured | BA-a | BF-a | BP-a | BT-a | BD-a |
|---|---|---|---|---|---|
| **% C** | 80.25, 80.13 | 79.74, 79.91 | 77.57, 77.68 | 73.55, 73.96 | 75.38, 81.82 |
| **% H** | 6.46, 6.45 | 5.87, 5.88 | 5.30, 5.28 | 5.15, 5.33 | 5.51, 6.90 |
| **% N** | 5.79, 5.65 | 6.16, 6.14 | 4.55, 4.45 | 5.15, 5.33 | 5.22, 4.10 |

| Theoretical | BA-a | BF-a | BP-a | BT-a | BD-a |
|---|---|---|---|---|---|
| **% C** | 80.49 | 80.16 | 78.24 | 74.31 | 82.28 |
| **% H** | 6.54 | 6.03 | 5.11 | 5.35 | 6.92 |
| **% N** | 6.06 | 6.45 | 5.07 | 6.19 | 5.05 |