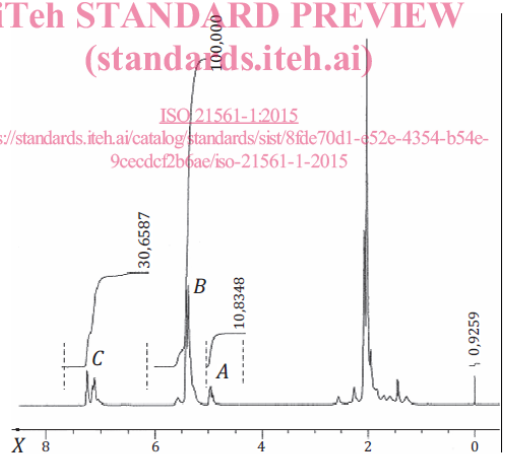
# Quality Control with BeautifulJason

# ISO 21561: Styrene-butadiene rubber (SBR) — Determination of the microstructure of solution-polymerized SBR

| Area | Signal integration range |
|---|---|
| $A$ | From 4,3 ppm to minimum intensity point around 5,0 ppm |
| $B$ | From minimum intensity point around 5,0 ppm to minimum intensity point around 6,1 ppm |
| $C$ | From minimum intensity point around 6,1 ppm to 7,7 ppm |
| $TMS_{blank}$ | Integrated signal intensity of TMS in $CDCl_3$ containing TMS |
| $CD_{blank}$ | From 6,1 ppm to 7,7 ppm in $CDCl_3$ containing TMS |
| $TMS$ | Integrated signal intensity of TMS in S-SBR sample solution |






$$C_{calib} = C - CD_{blank} \times \left(TMS / TMS_{blank}\right) \quad (1)$$

where

$C_{calib}$ is the integrated signal intensity of area $C$ compensated for the effect of $CHCl_3$ in $CDCl_3$.

**3.6.3** Calculate the content of each microstructure component (trans and cis, and vinyl) of the butadiene portion and the styrene content, using Formulae (2) to (4):

$$S_m = \frac{(C_{calib}/5) \times 104}{(C_{calib}/5) \times 104 + (B/2 + A/4) \times 54} \times 100 \quad (2)$$

$$V = \frac{A/2}{B/2 + A/4} \times 100 \quad (3)$$

$$TC = \frac{B/2 - A/4}{B/2 + A/4} \times 100 \quad (4)$$

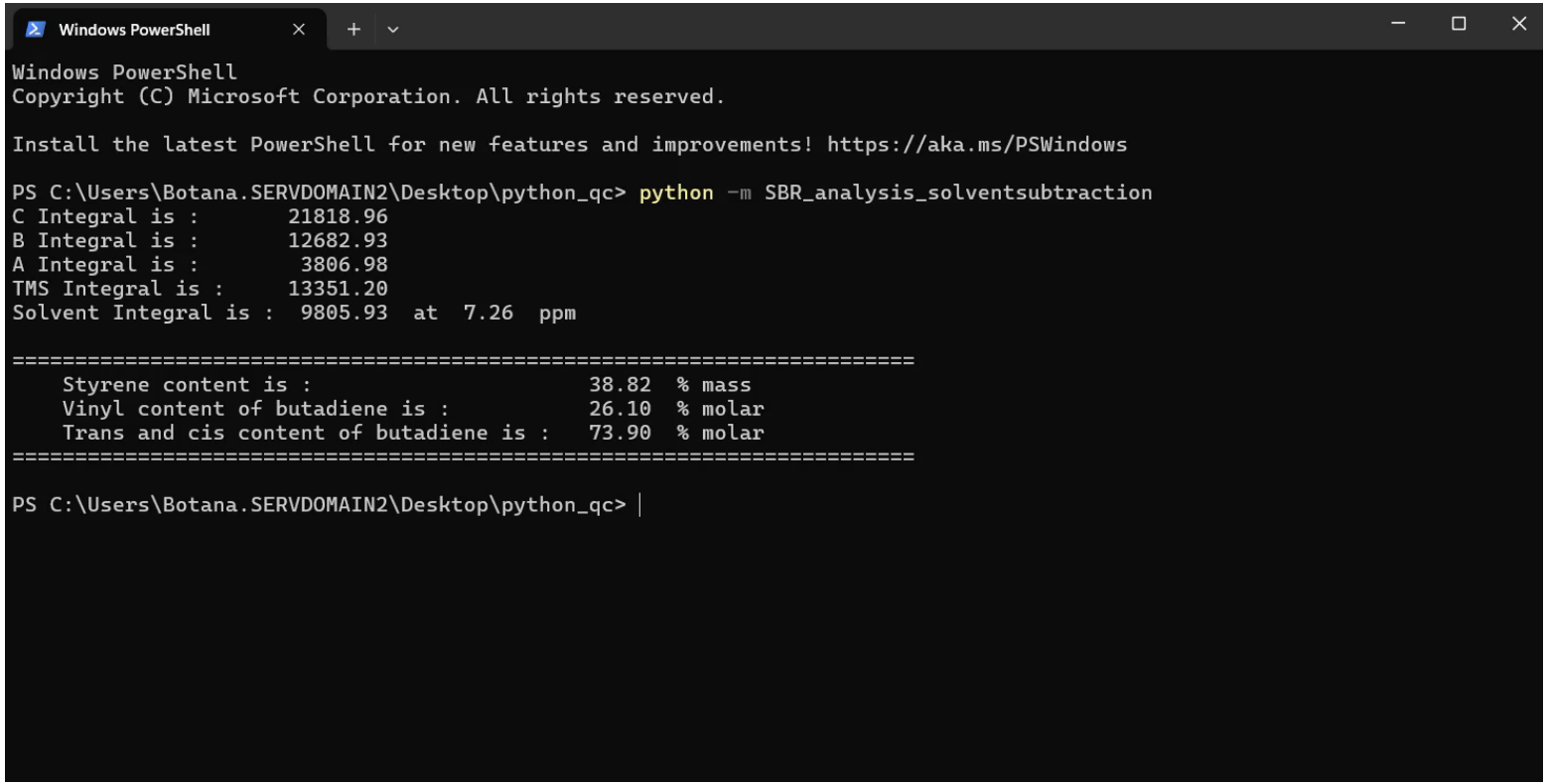
where

$S_m$ is the styrene content of the S-SBR, in mass %;

$V$ is the vinyl content of the butadiene portion of the S-SBR, in mol %;

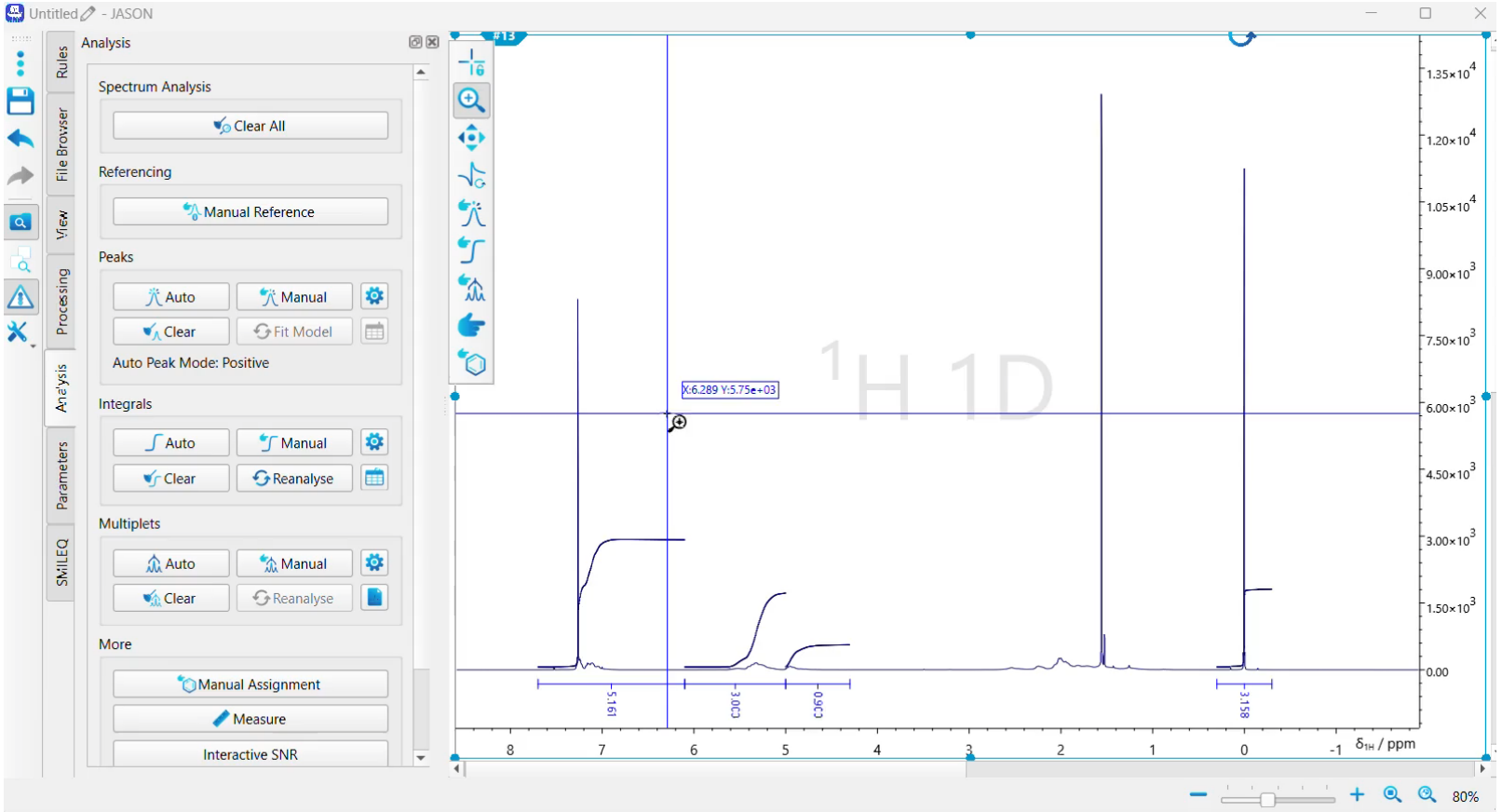
$TC$ is the trans and the cis content of the butadiene portion of the S-SBR, in mol %.

# How to do this?




Pirelli is gratefully acknowledged for providing a SBR sample

# Peak picking and creating rules




Jason 4.0 introduced rules with custom integration ranges

# Script creation (I)

```
import beautifuljason as bjason

# python -m SBR_analysis_solventsubstraction

# Initialize variables
file1 = 'C:/Users/Botana.SERVDOMAIN2/Desktop/python_qc/SBR_proton-1-1.jdf'
rules_name = 'ISO_SBR'


# Initialize JASON object
jason = bjason.JASON()

# Open the file and apply the rules
with jason.create_document(file1, rules=rules_name) as doc:
    spec = doc.nmr_data[0]
```

# Script creation (II)

```
# Extract the integrals and print the with 2 decimals
    multiplet1 = spec.multiplets[0]
    int_C_file1 = multiplet1.value_hz
    print('C Integral is :      ', "{:.2f}".format(int_C_file1))
    multiplet2 = spec.multiplets[1]
    int_B_file1 = multiplet2.value_hz
    print('B Integral is :      ', "{:.2f}".format(int_B_file1))
    multiplet3 = spec.multiplets[2]
    int_A_file1 = multiplet3.value_hz
    print('A Integral is :       ', "{:.2f}".format(int_A_file1))
    multiplet4 = spec.multiplets[3]
    int_TMS_file1 = multiplet4.value_hz
    print('TMS Integral is :    ', "{:.2f}".format(int_TMS_file1))
```

# Script creation (III)

```
# Find the solvent peak and extract its area (assuming it is only one peak, otherwise keep adding the areas of each solvent peak and/or impurities)
    solvent = None
    for peak in spec.peaks:
        if peak.classification == bjason.NMRPeak.PeakClassification.NMRSolvent:
            solvent = peak
            break
    int_solvent = solvent.area
    print('Solvent Integral is : ', "{:.2f}".format(solvent.area), ' at ', "{:.2f}".format(solvent.pos[0]), ' ppm')

    # Uncomment the below lines to save the document
    # doc.close()
    # doc.copy('C:/Users/Botana.SERVDOMAIN2/Desktop/python_qc/simple_integral_example.jjh5')
```

BeautifulJason 1.0.4 + Jason 4.1 introduced peak areas

# Script creation (IV)

```
# Subtract the solvent area from C integral
c_calib = int_C_file1 - int_solvent

# Calculate concentrations
s_m = c_calib*104/5*100/(c_calib*104/5+(int_B_file1/2+int_A_file1/4)*54)
v_ = int_A_file1/2*100/(int_B_file1/2+int_A_file1/4)
tc_ = (int_B_file1/2-int_A_file1/4)/(int_B_file1/2+int_A_file1/4)*100


print('')
print('================================================================================')
print('    Styrene content is :                    ', "{:.2f}".format(s_m), ' % mass')
print('    Vinyl content of butadiene is :         ', "{:.2f}".format(v_), ' % molar')
print('    Trans and cis content of butadiene is :  ', "{:.2f}".format(tc_), ' % molar')
print('================================================================================')
print('')
```