Supplementary Material

Serendipitous synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones in $ZnCl_2$/urea deep eutectic solvent

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Experimental

General. All chemicals were purchased from commercial sources (Acros, Spectrochem, Merck, and Aldrich). ^{1}H and ^{13}C NMR spectra were recorded on Bruker spectrometer using 600 MHz spectrometer. TLC was used of Merck Kieselgel-60 F-254 to monitor the reaction. Melting points were recorded using melting point apparatus.

Preparation of DES. The DES were prepared as per the reported method.[1] The $ZnCl_2$ and Urea (1:3.5) were taken in test tube and heated at 80^{o}C until solid phase converted into transparent liquid and used further any purification.

General procedure for the synthesis of DHQ. A mixture of isotonic anhydride (**1a**) and benzaldehyde (**2a**) were dissolved in $ZnCl_2$/urea deep eutectic solvent for 25min, reaction monitored on TLC, water added into the mixture after completion of reaction. The solid precipitates were filter-out and further purified by using recrystallization in ethanol.

The compound **3a**, **3c**, **3f**, **3g**, **3j**, and **3m** were characterized with NMR spectroscopy, remaining derivatives were confirmed with melting points, IR spectrum and LCMS.

2-Phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3a).[2] (CAS Registry Number: 954-91-6) IR (ATR): 1608, 1653, 3067, 3166, 3299 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 5.75 (s, 1H), 6.66-6.69 (t, *J* 15.03 Hz, *J* 7.42 Hz, 1H), 6.74-6.75 (d, *J* 8.02 Hz, 1H), 7.11 (s, 1H), 7.23-7.26 (dd, *J* 7.15 Hz, *J* 1.02 Hz, 1H), 7.33-7.40 (m, 3H), 7.49-7.50 (d, *J* 7.30 Hz, 2H), 7.61-7.62 (d, *J* 7.30 Hz, 1H), 8.29 (s, 1H); ^{13}C NMR (APT) (150 MHz, DMSO-d6): 67.03, 114.86, 115.43, 117.56, 127.30, 127.81, 128.77, 128.89, 133.75, 142.13, 148.31, and 164.03. MS *m/z* 224.09 (M+1); Anal. Calc. for $C_{14}H_{12}N_2O$: 224.09; found: 225.

2-(4-Chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3b).[2] (CAS Registry Number:13165-11-2) IR (ATR): 1609, 1651, 3058, 3190, 3311 cm^{-1}. MS *m/z* 258.05 (M+1); Anal. Calc. for $C_{14}H_{11}ClN_2O$: 258.05; found: 259.

2-(4-Fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3c).[2] (CAS Registry Number:359605-44-0) IR (ATR): 1603, 1648, 3040, 3175, 3302 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 5.78 (s, 1H), 6.67-6.70 (t, *J* 14.77 Hz, *J* 7.50 Hz, 1H), 6.74-6.75 (d, *J* 7.94 Hz, 1H), 7.10 (s, 1H), 7.21-7.26 (m, 3H), 7.53-7.55

(dd, *J* 14.11 Hz, *J* 3.39 Hz, 2H), 7.61-7.62 (d, *J* 7.80 Hz, 1H), 8.29 (s, 1H); ^{13}C NMR (APT) (150 MHz, DMSO-d6): 66.41, 114.91, 115.47, 115.61, 117.71, 127.82, 129.45, 129.50, 133.80, 138.30, 148.24, 161.77, 163.38, and 164.00. MS *m/z* 242.08 (M+1); Anal. Calc. for $C_{14}H_{11}FN_2O$: 242.08; found: 243.

2-(4-Nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3d).[2] (CAS Registry Number:26029-31-2) IR (ATR): 1604, 1640, 3030, 3162, 3290 cm^{-1}. MS *m/z* 269.08 (M+1); Anal. Calc. for $C_{14}H_{11}N_3O_3$: 269.08; found: 270.

2-(4-Bromophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3e).[2] (CAS Registry Number:358386-50-2) IR (ATR): 1603, 1644, 3012, 3191, 3290 cm^{-1}. MS *m/z* 302.00 (M+1); Anal. Calc. for $C_{14}H_{11}BrN_2O$: 302.00; found: 303.

2-(4-Methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3f).[2] (CAS Registry Number:61195-16-2) IR (ATR): 1611, 1648, 2991, 3177, 3304 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 3.75 (s, 3H), 5.71 (s, 1H), 6.66-6.69 (t, *J* 14.79 Hz, *J* 7.39 Hz, 1H), 6.73-6.75 (d, *J* 8.08 Hz, 1H), 6.94-6.95 (d, *J* 8.62 Hz, 2H), 7.01 (s, 1H), 7.23-7.25 (t, *J* 7.60 Hz, *J* 7.26 Hz, 1H), 7.41-7.43 (d, *J* 8.62 Hz, 2H), 7.60-7.62 (d, *J* 7.67 Hz, 1H), 8.19 (s, 1H); 13C NMR (APT) (150 MHz, DMSO-d6): 55.65, 66.77, 114.11, 114.89, 115.48, 11.54, 127.81, 128.68, 13420, 134.84, 148.46, 159.91, 164.14. MS *m/z* 254.10 (M+1); Anal. Calc. for $C_{15}H_{14}N_2O_2$: 254.10; found: 255.

2-(4-Isopropylphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3g).[2] (CAS Registry Number:83800-96-8) IR (ATR): 1607, 1654, 2948, 3196, 3298 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 1.18 (d, *J* 6.99 Hz, 6H), 2.85 (septet, 7H), 5.7 (s, 1H), 6.66-6.68 (t, *J* 15.02 Hz, *J* 7.36 Hz, 1H), 6.73-6.74 (d, *J* 7.66 Hz, 1H), 7.07 (s, 1H), 7.22-7.27 (m, 3H), 7.41-7.43 (d, *J* 7.95 Hz, 2H), 7.61-7.62 (d, *J* 7.82 Hz, 1H), 8.24 (s, 1H); ^{13}C NMR (APT) (150 MHz, DMSO-d6): 24.33, 33.69, 67.02, 114.83, 115.42, 117.51, 126.69, 127.41, 127.82, 133.71, 139.49, 148.42, 149.28, and 164.11. MS *m/z* 266.14 (M+1); Anal. Calc. for $C_{17}H_{18}N_2O$: 266.14; found: 267.

2-(p-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3h).[2] (CAS Registry Number:13324-79-3) IR (ATR): 1600, 1654, 3045, 3198, 3302 cm^{-1}. MS *m/z* 238.11 (M+1); Anal. Calc. for $C_{15}H_{14}N_2O$: 238.11; found: 239.

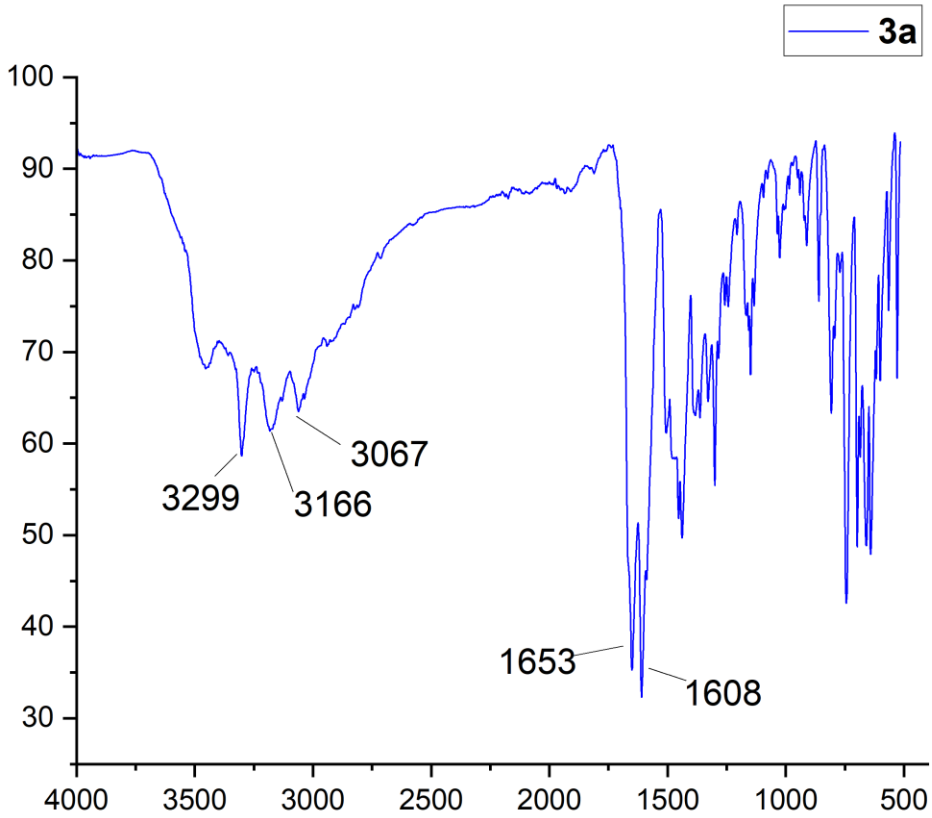
2-(3-Chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3i).[2] (CAS Registry Number:83800-92-4) IR (ATR): 1612, 1643, 3028, 3181, 3290 cm^{-1}. . MS *m/z* 242.08 (M+1); Anal. Calc. for $C_{14}H_{11}FN_2O$: 242.08; found: 243.

2-(3-Fluorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3j).[2] (CAS Registry Number:386242-54-2) IR (ATR): 1609, 1648, 3178, 3284, 3345 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 5.79 (s, 1H), 6.67-6.70 (t, *J* 14.85 Hz, *J* 7.68 Hz, 1H), 6.76-6.77 (d, *J* 8.30 Hz, 1H), 7.16-7.34 (m, 5H), 7.41-7.45 (dd, *J* 7.81 Hz, 1H), 7.60 (d, *J* 7.46 Hz, 1H), 8.42 (s, 1H); 13C NMR (APT) (150 MHz, DMSO-d6): 66.12, 113.94, 114.09, 11.95, 115.49, 115.62, 117.77, 123.21, 127.83, 130.79, 130.84, 133.86, 145.33, 147.99, 161.73, 163.34, and 163.88. MS *m/z* 242.08 (M+1); Anal. Calc. for $C_{14}H_{11}FN_2O$: 242.08; found: 243.

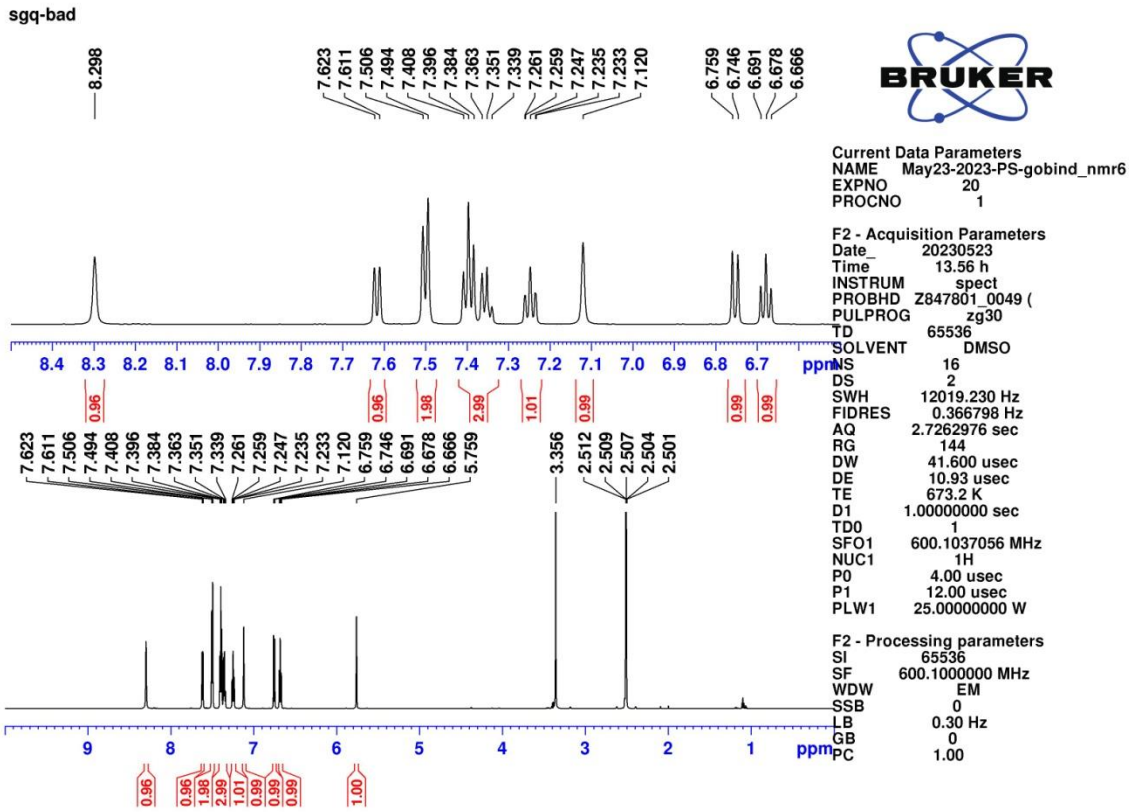
2-(3-Bromophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3k).[2] (CAS Registry Number:304451-29-4) IR (ATR): 1609, 1646, 3033, 3199, 3281 cm^{-1}. MS *m/z* 302.00 (M+1); Anal. Calc. for $C_{14}H_{11}BrN_2O$: 302.00; found: 303.

2-(3-Methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (3l).[2] (CAS Registry Number:198068-91-6) IR (ATR): 1606, 1643, 2911, 3060, 3200 cm^{-1} MS *m/z* 254.10 (M+1); Anal. Calc. for $C_{15}H_{14}N_2O_2$: 254.10; found: 255.

2-(m-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3m).[2] (CAS Registry Number:83800-93-5) IR (ATR): 1612, 1645, 3030, 3183, 3299 cm^{-1}. ^{1}HNMR (600 MHz, DMSO-d6): 2.31 (s, 3H), 5.71 (s, 1H), 6.66-6.68 (t, *J* 14.84 Hz, *J* 7.42 Hz, 1H), 6.73-6.75 (d, *J* 7.81 Hz, 1H), 7.07 (s, 1H), 7.16 (d, *J* 4.15 Hz, 1H), 7.22-7.28 (m, 3H), 7.60 (d, *J* 8.04 Hz, 1H), 8.24 (s, 1H); 13C NMR (APT) (150 MHz, DMSO-d6): 21.53, 67.09, 114.84, 117.53, 124.47, 127.80, 127.95, 128.69, 129.52, 133.73, 137.88, 141.99, 148.35, and 164.04. MS *m/z* 238.11 (M+1); Anal. Calc. for $C_{15}H_{14}N_2O$: 238.11; found: 239.



IR spectra of **3a**.



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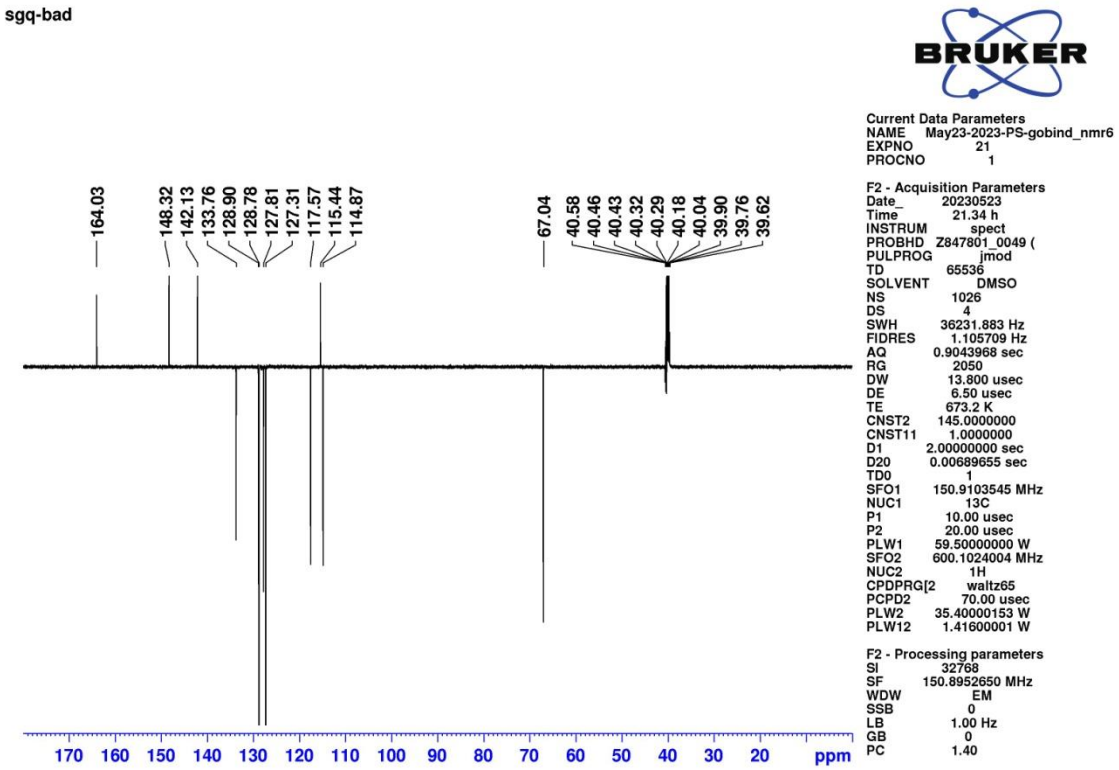

^{13}CNMR of **3a**.

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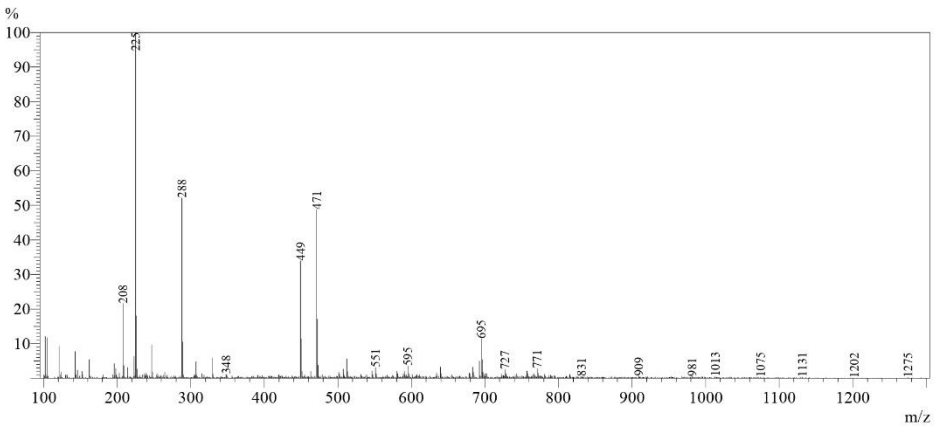

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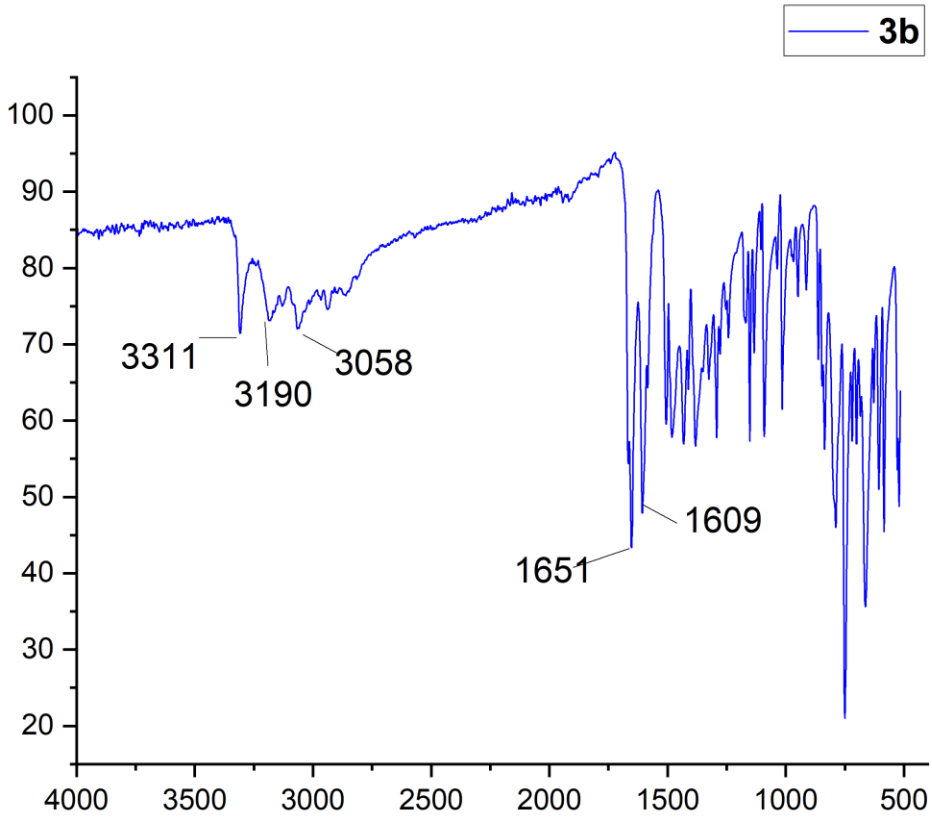

IR spectra of **3b**.

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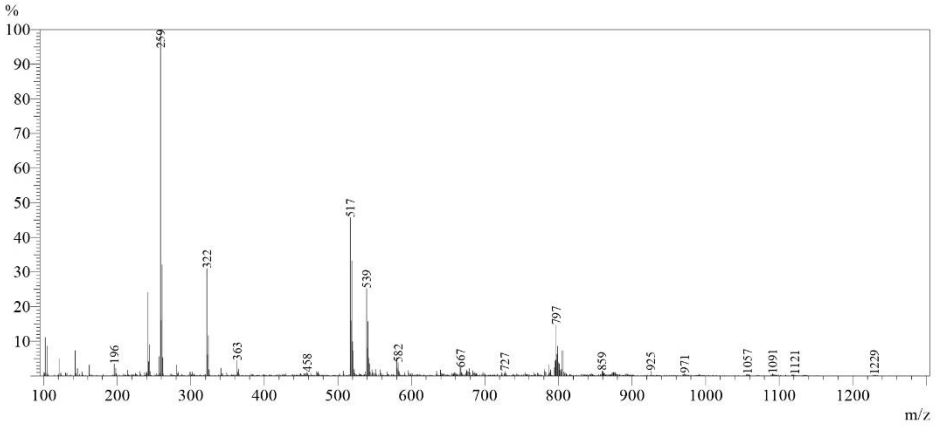
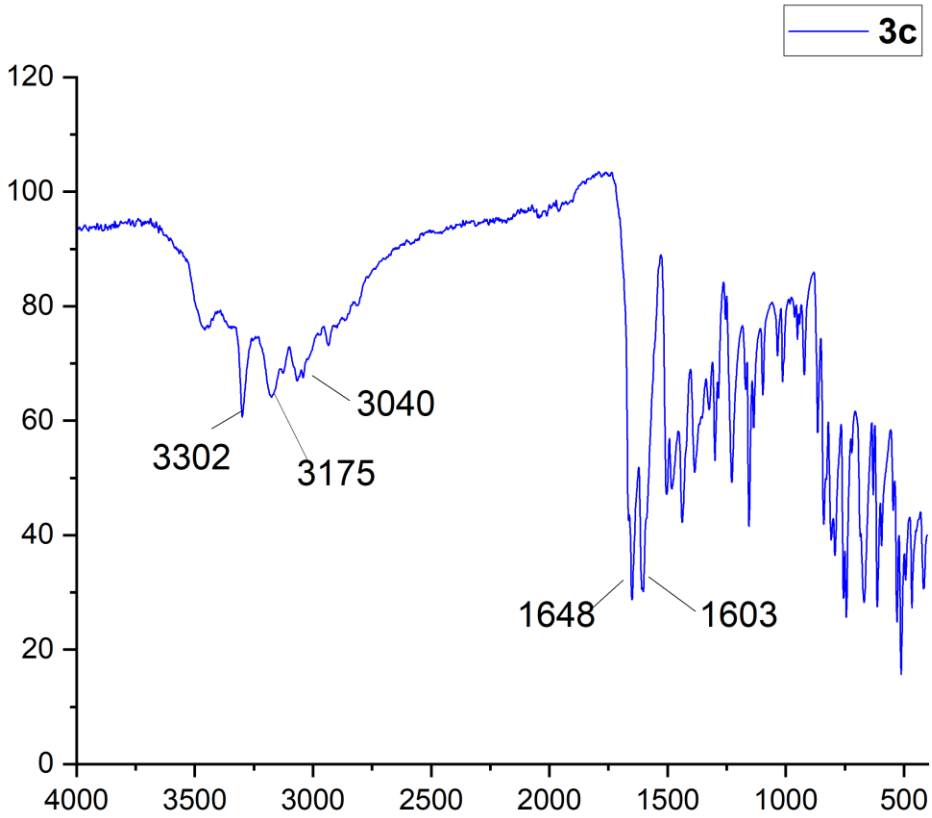
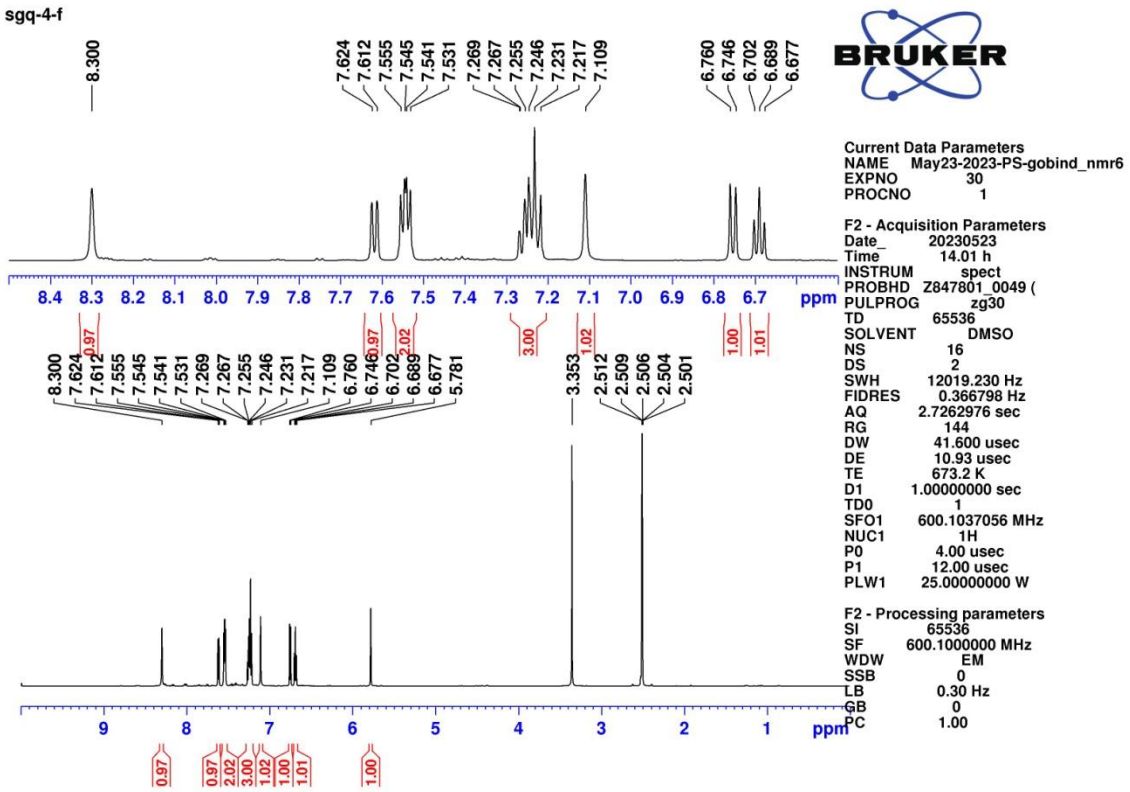


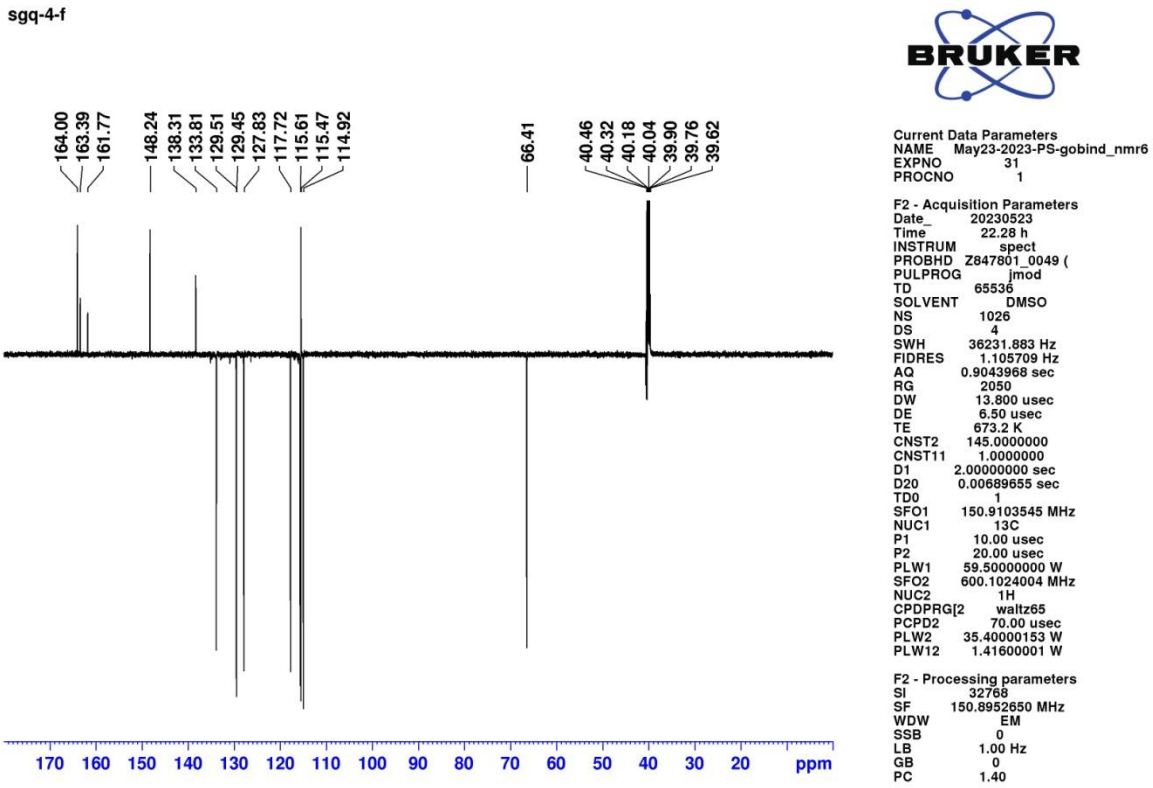
MS spectra of **3b**.



IR spectra of **3c**.



^{1}HNMR of **3c**.



^{13}CNMR of **3c**.

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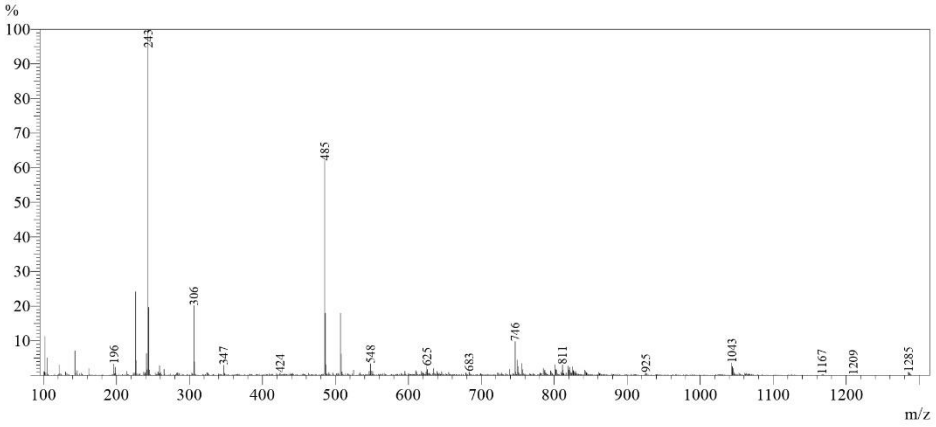
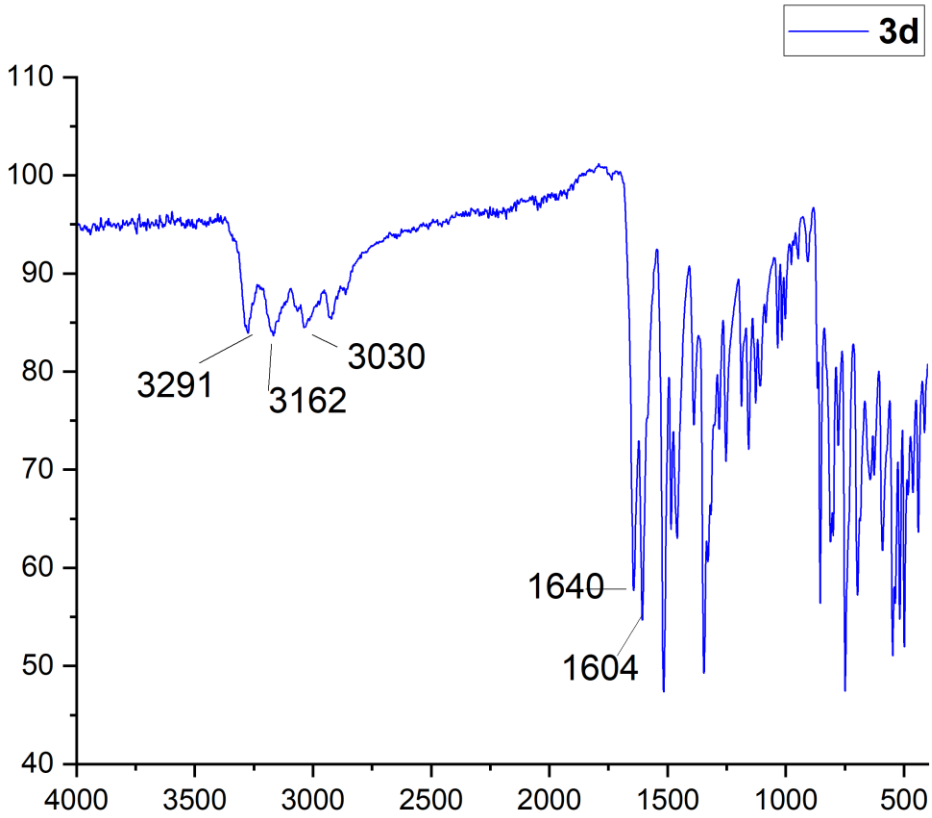


MS spectra of **3c**.



IR spectra of **3d**.

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MS Spectrum

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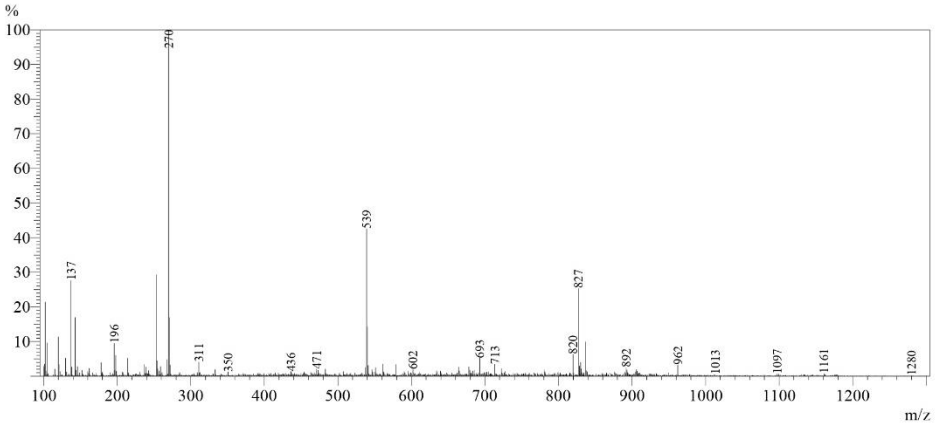
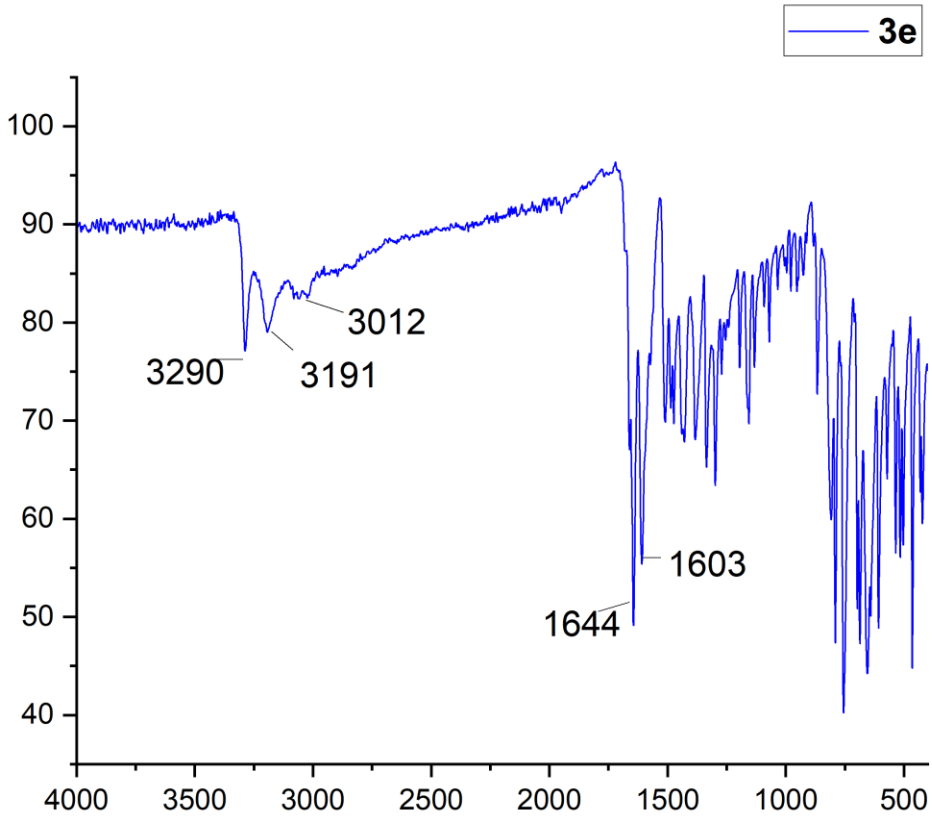


MS spectra of **3d**.



IR spectra of **3e**.

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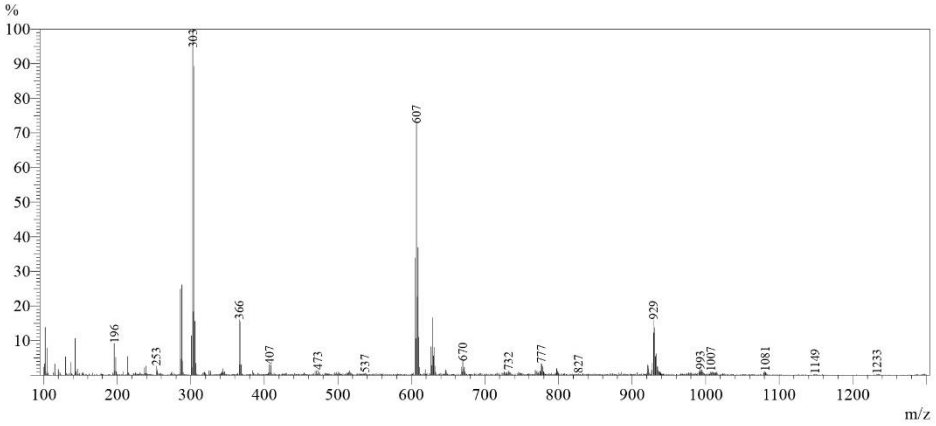
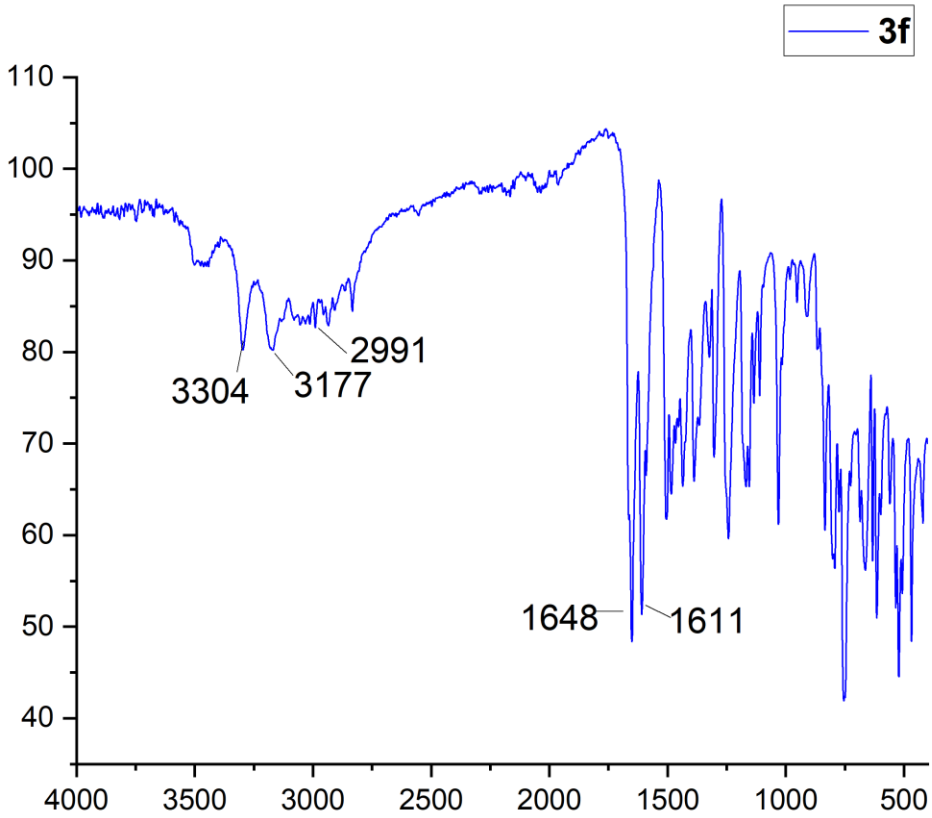
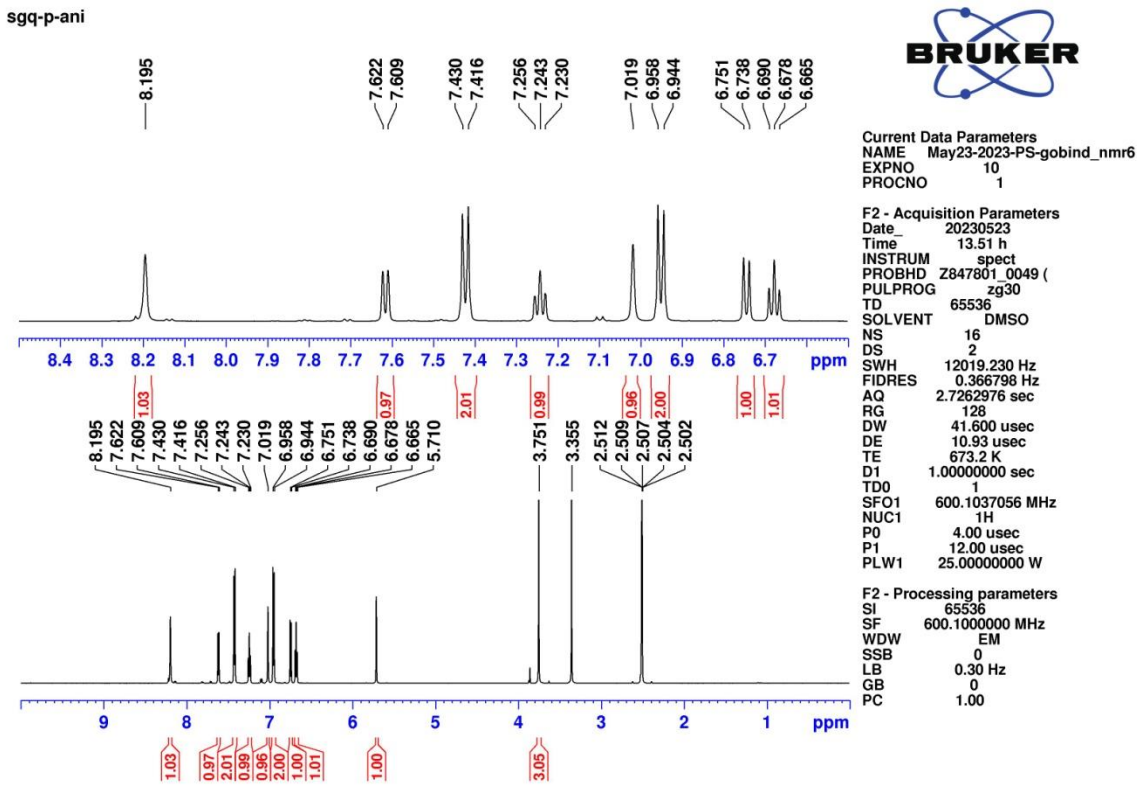


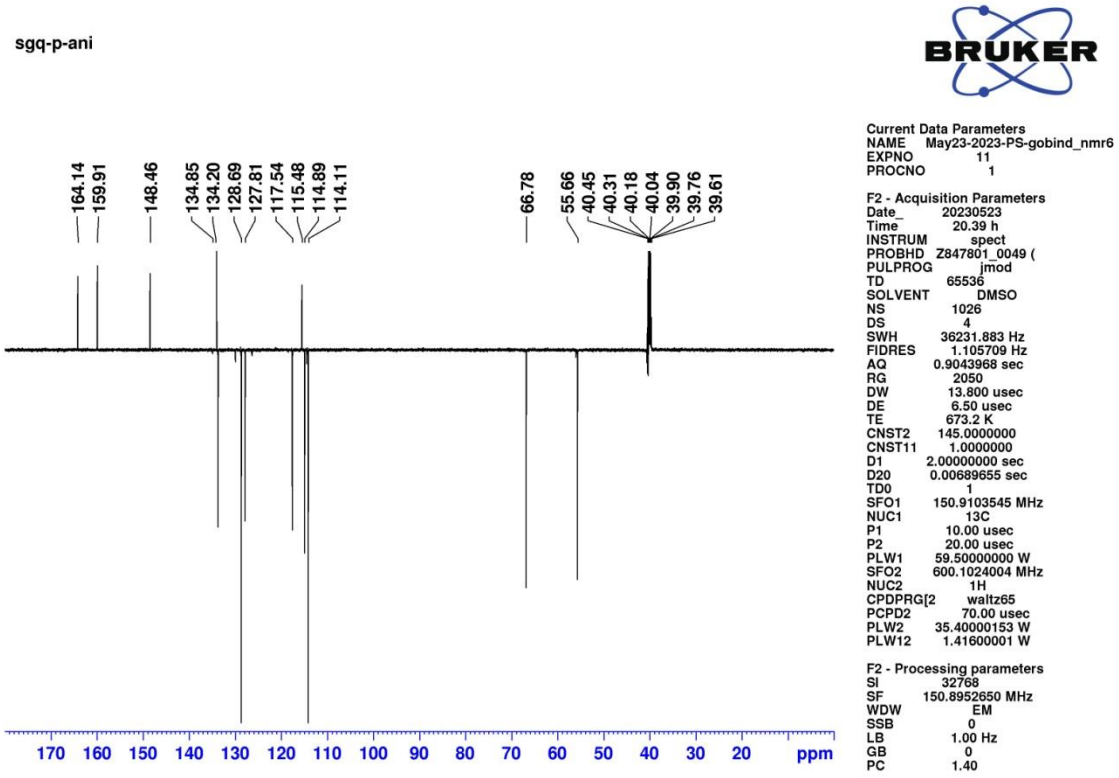
MS spectra of **3e**.



IR spectra of **3f**.



^{1}HNMR of **3f**.



^{13}CNMR of **3f**.

Sample Information

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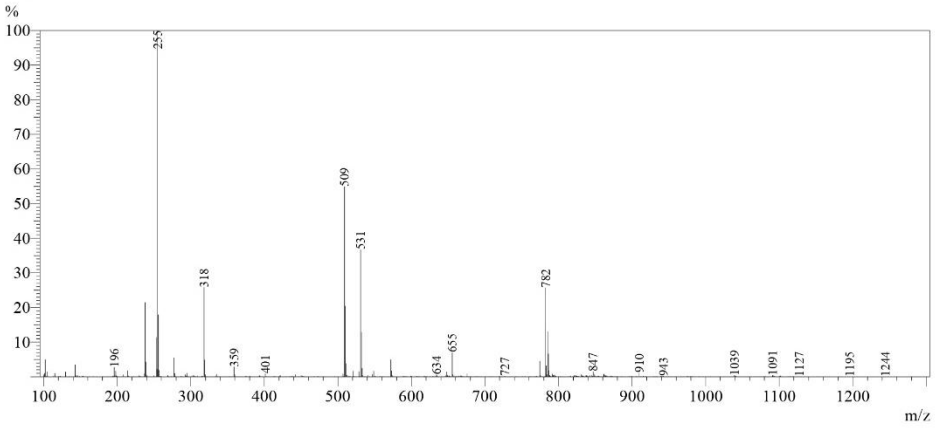
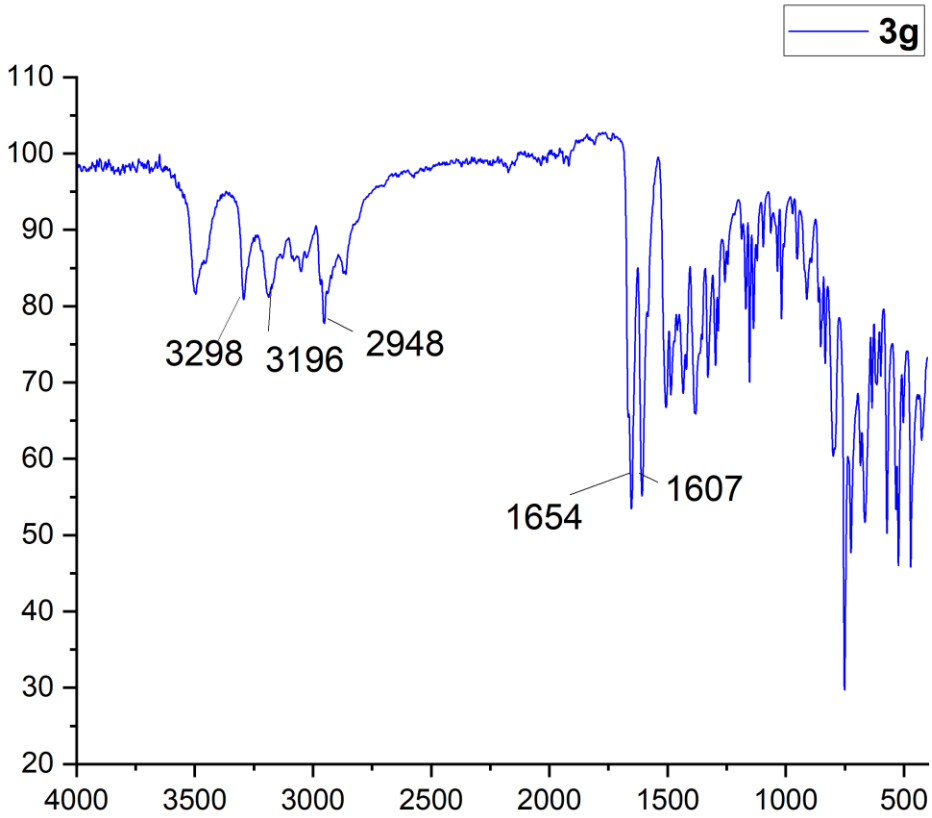
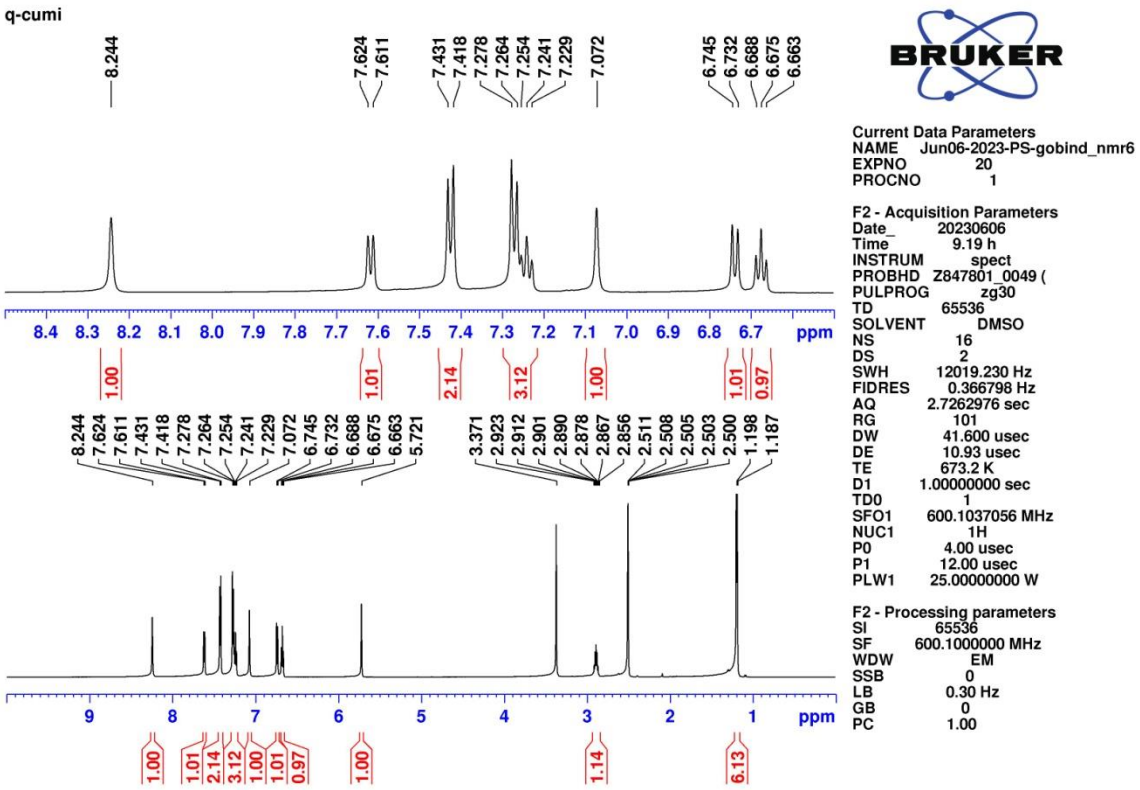


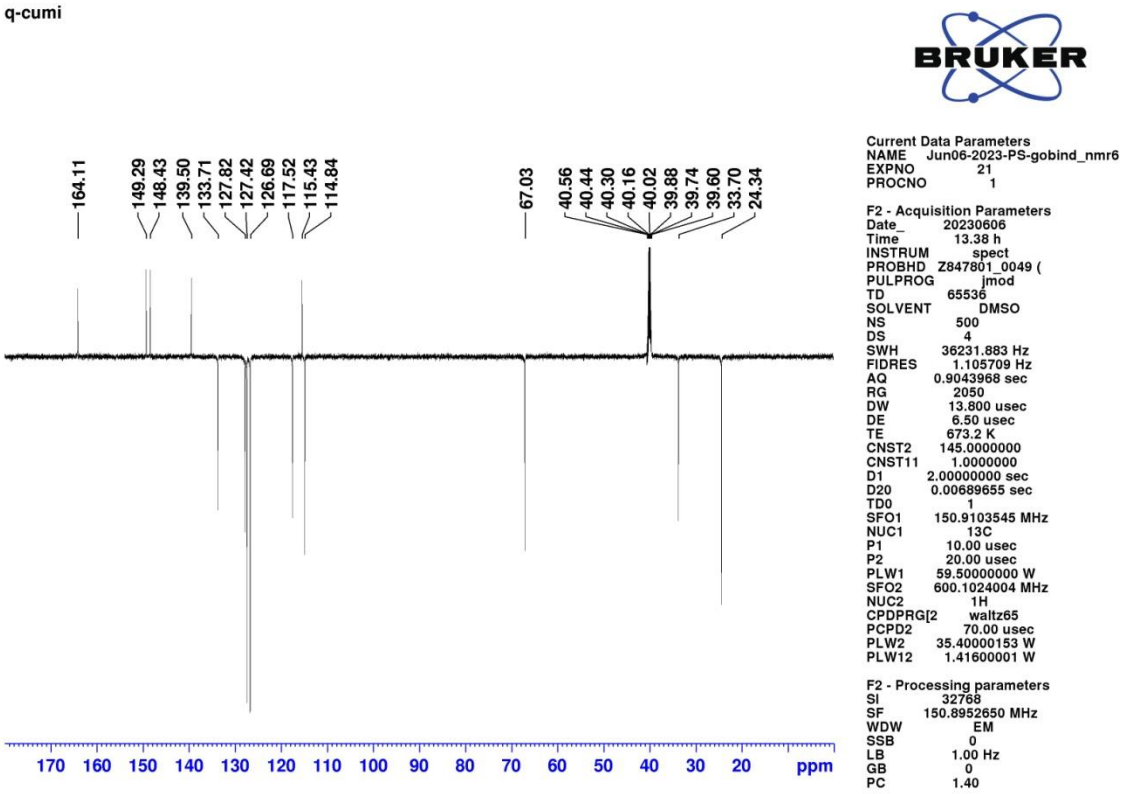
MS spectra of **3f**.



IR spectra of **3g**.



^{1}HNMR of **3g.**



^{13}CNMR of **3g**.

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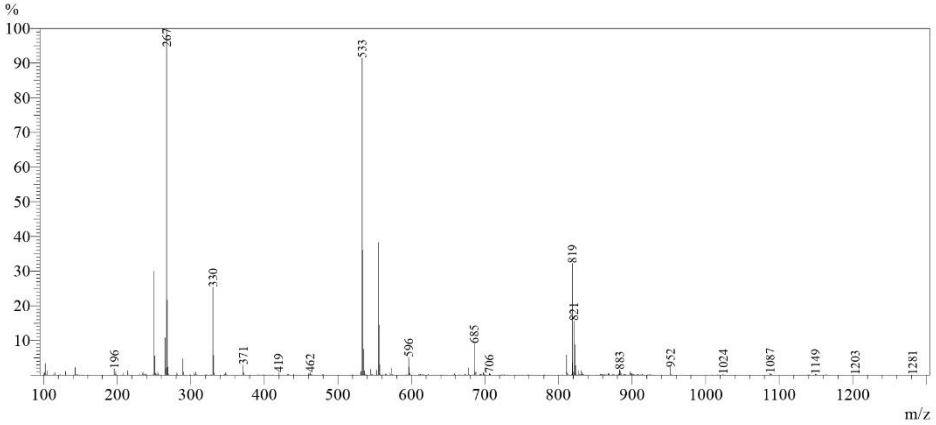
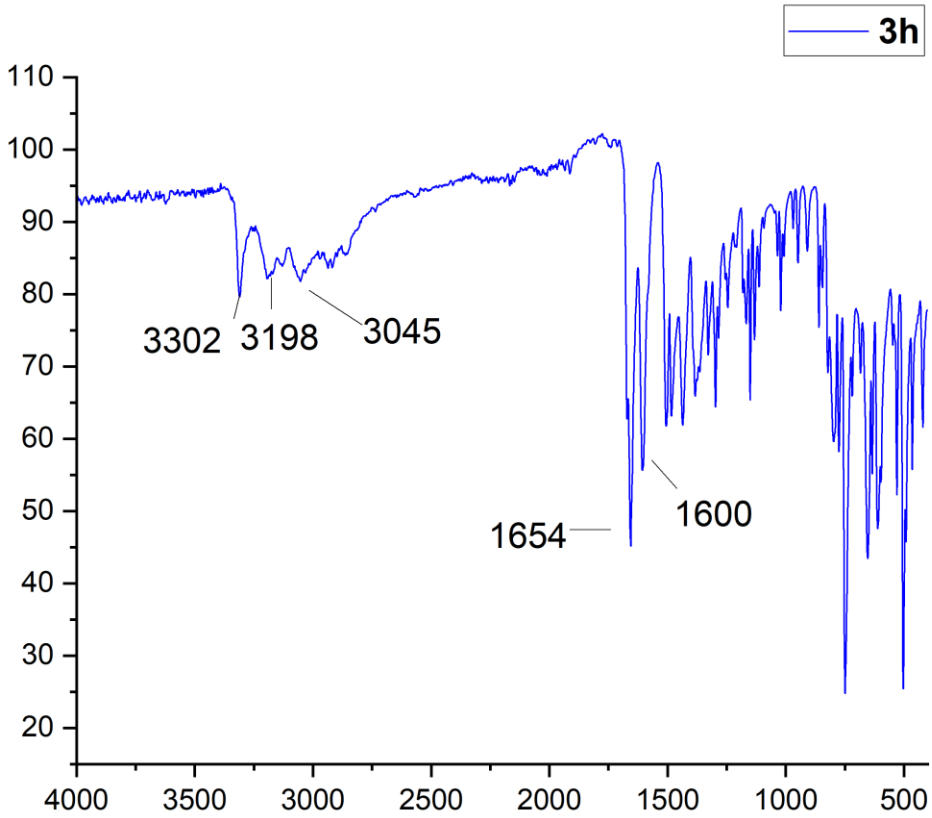


MS spectra of **3g**.



IR spectra of **3h**.

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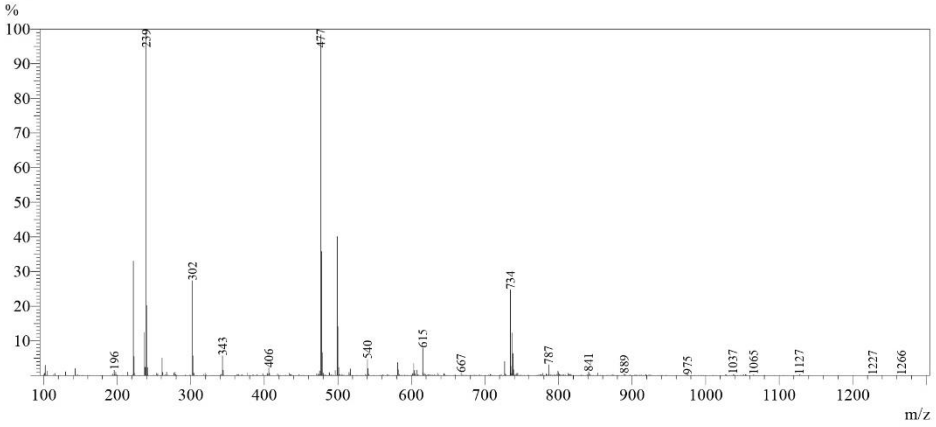
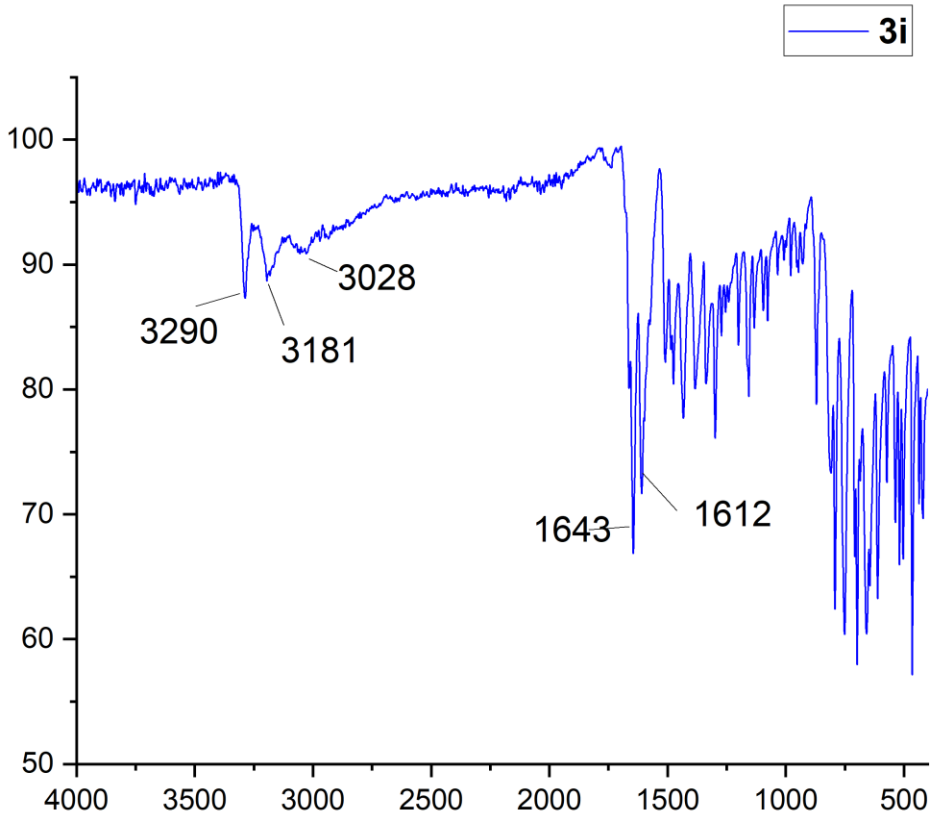


MS spectra of **3h**.



IR spectra of **3i**.

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MS Spectrum

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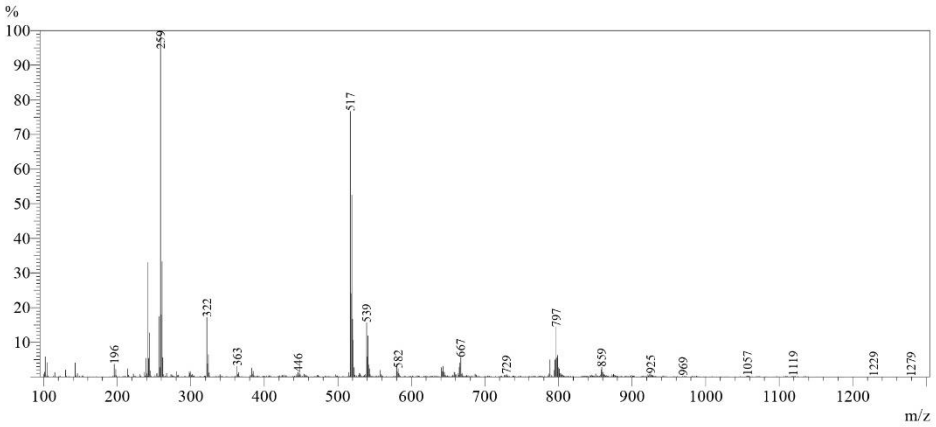
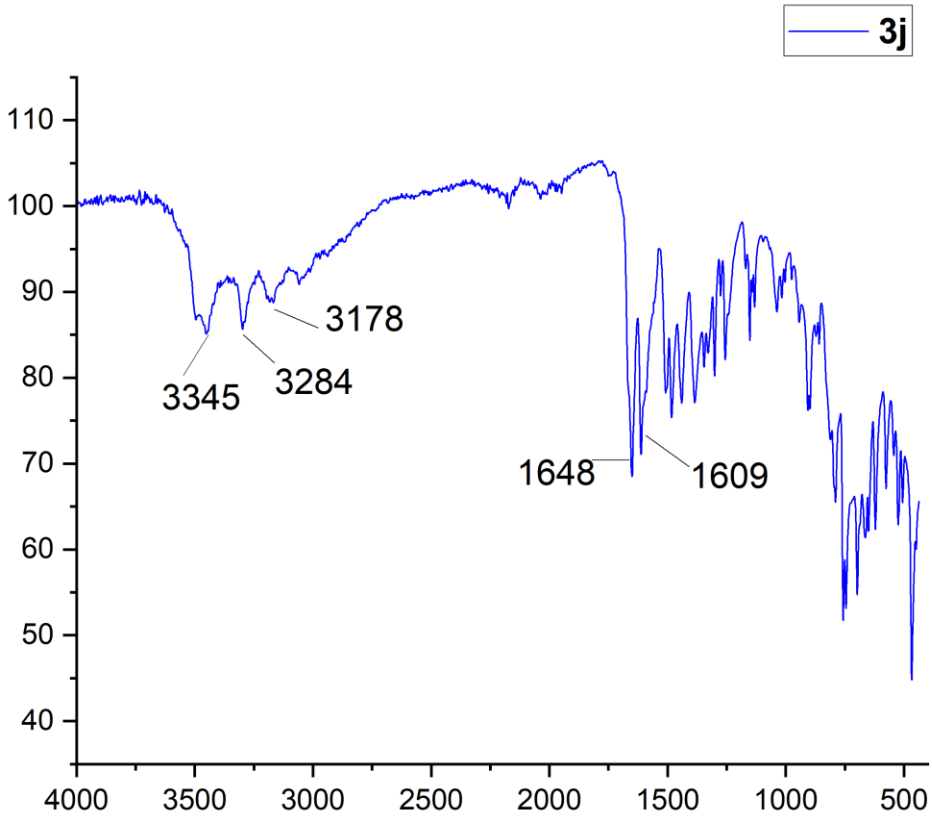
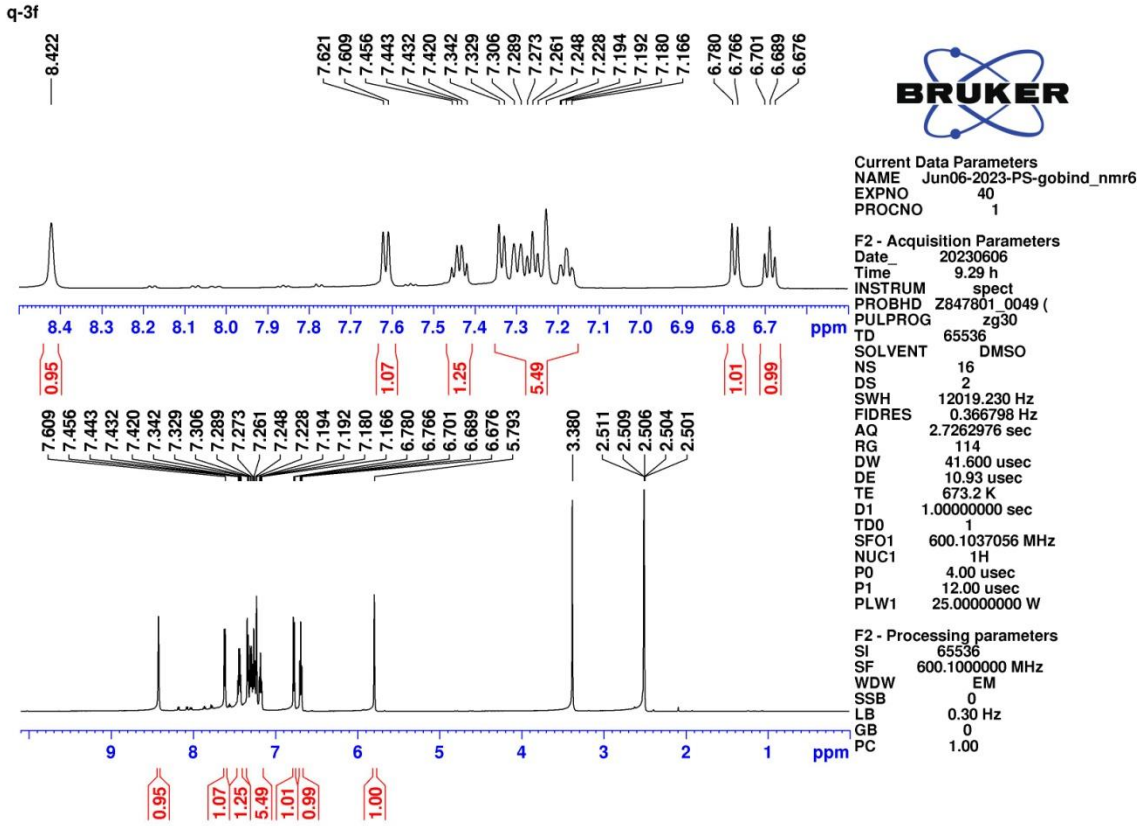
MassPeaks:1255
Segment 1 - Event 1



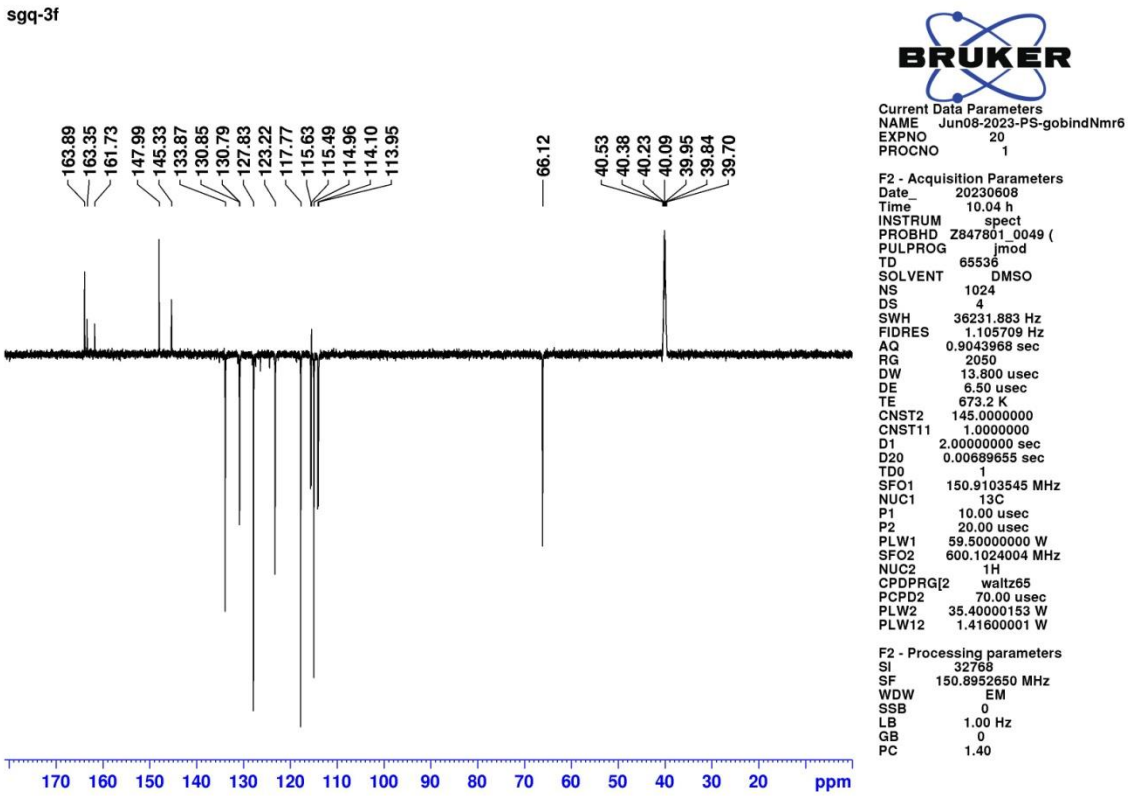
MS spectra of **3i**.



IR spectra of **3j**.



^{1}HNMR of **3j**.



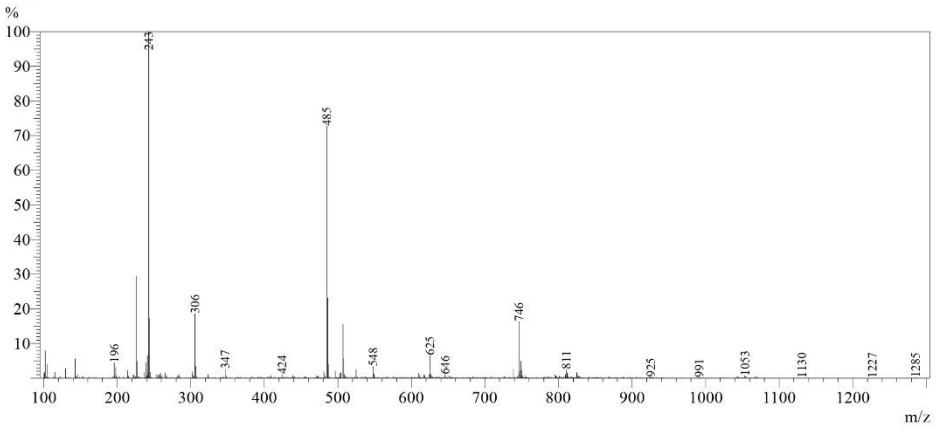
^{13}CNMR of **3j**.

Sample Information

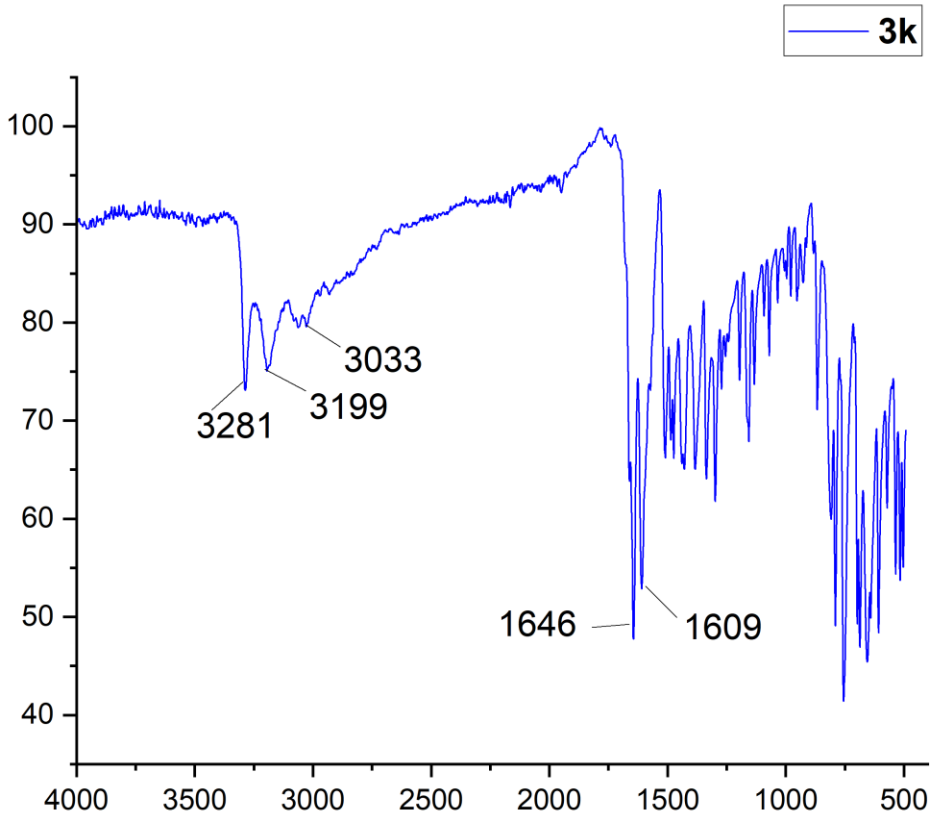
Date Acquired	: 2012/01/28 01:12:41 AM
Sample Type	: Unknown
Sample Name	: 3J
Sample ID	: 3J
Data File	: 3J.lcd
Method File	: no column run 2023.lcm
Report Format File	: DEFAULT.lsr
Tuning File	: 27092021.lct

MS Spectrum

R.Time:1.067(Scan#:65)
MassPeaks:1274
Segment 1 - Event 1



MS spectra of **3j**.



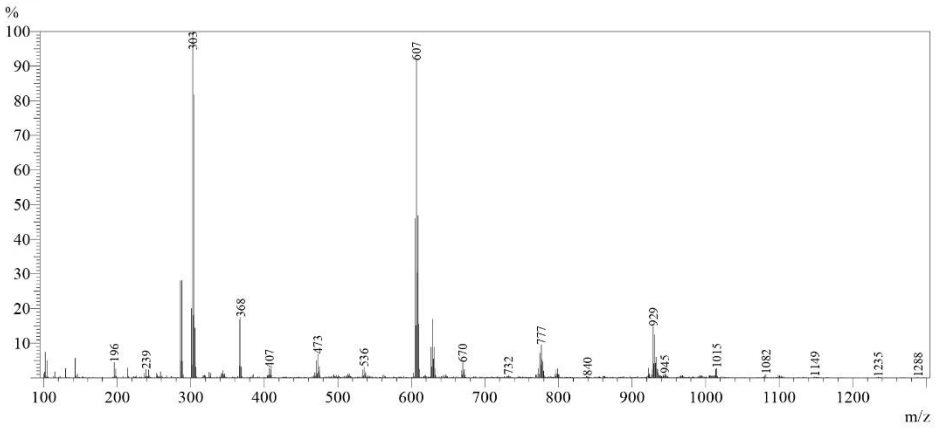
IR spectra of **3k**.

Sample Information

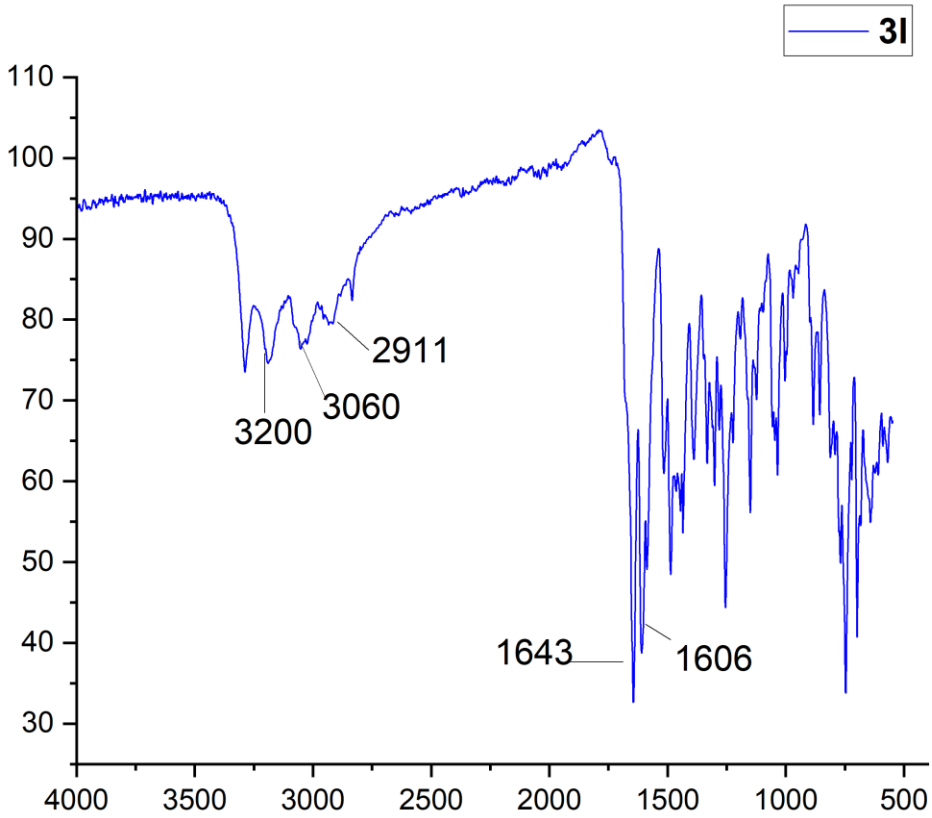
Date Acquired	: 2012/01/28 01:16:15 AM
Sample Type	: Unknown
Sample Name	: 3K
Sample ID	: 3K
Data File	: 3K.lcd
Method File	: no column run 2023.lcm
Report Format File	: DEFAULT.lsr
Tuning File	: 27092021.lct

MS Spectrum

R.Time:1.067(Scan#:65)
MassPeaks:1242
Segment 1 - Event 1



MS spectra of **3k**.



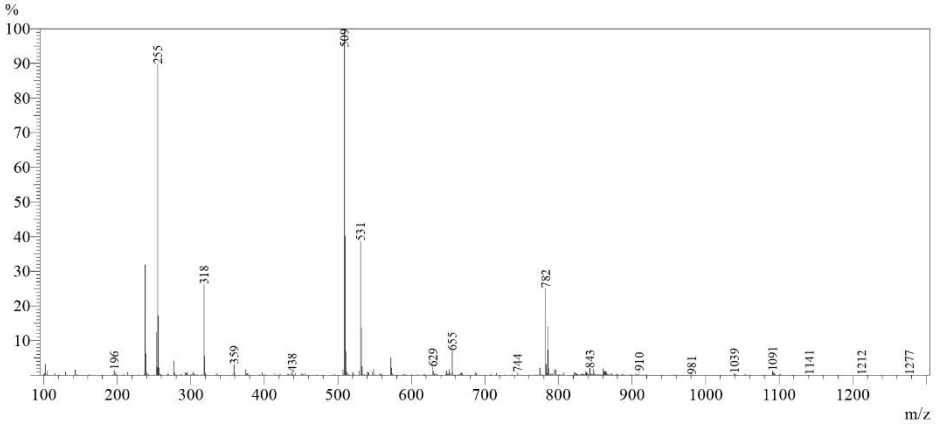
IR spectra of **3l**.

Sample Information

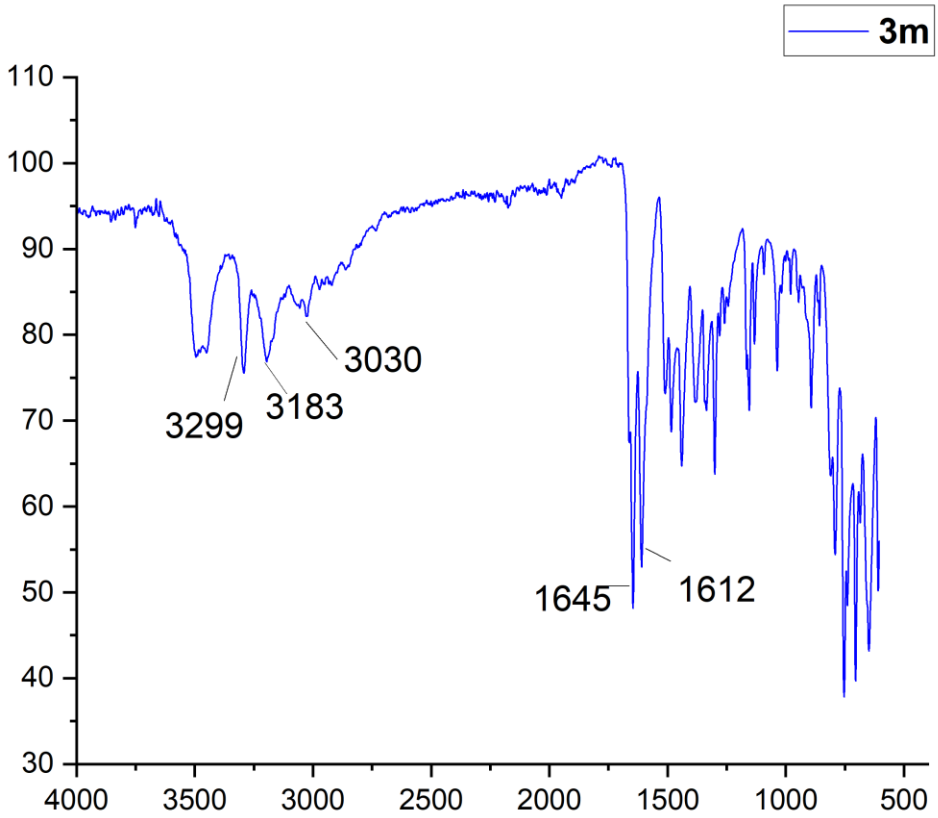
Date Acquired	: 2012/01/28 01:19:35 AM
Sample Type	: Unknown
Sample Name	: 3L
Sample ID	: 3L
Data File	: 3L.lcd
Method File	: no column run 2023.lcm
Report Format File	: DEFAULT.lsr
Tuning File	: 27092021.lct

MS Spectrum

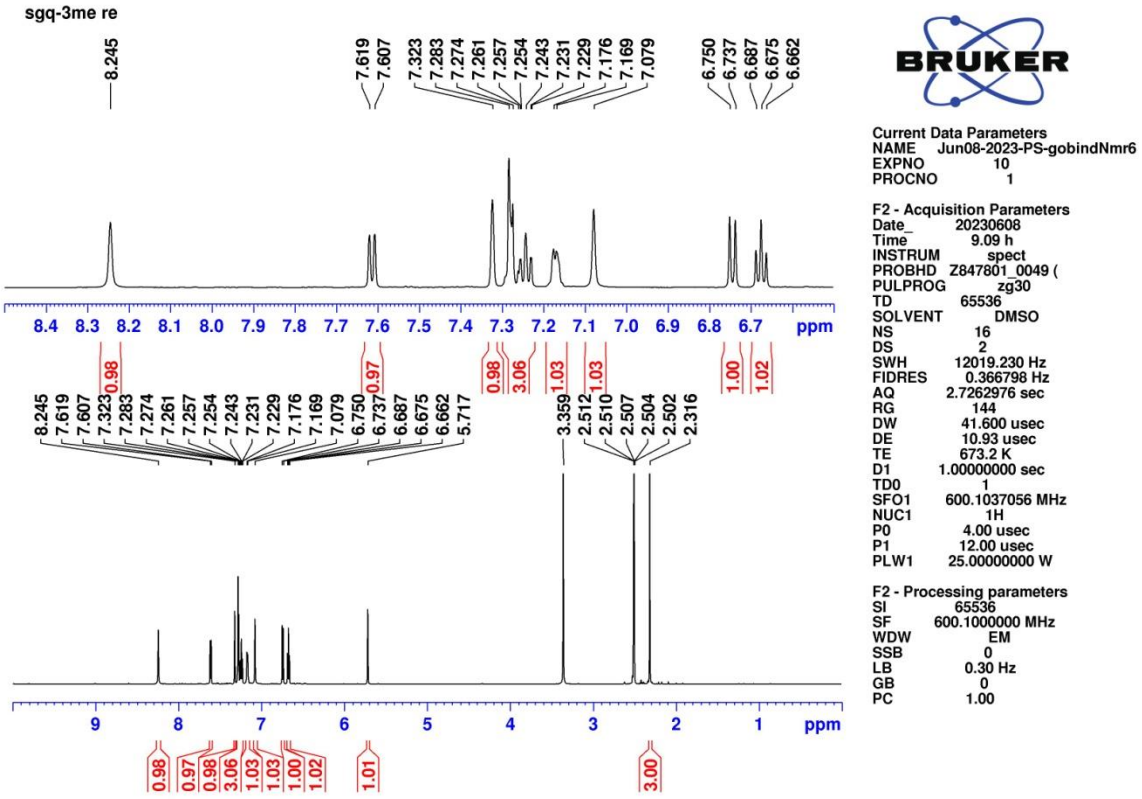
R.Time:1.067(Scan#:65)
MassPeaks:1231
Segment 1 - Event 1



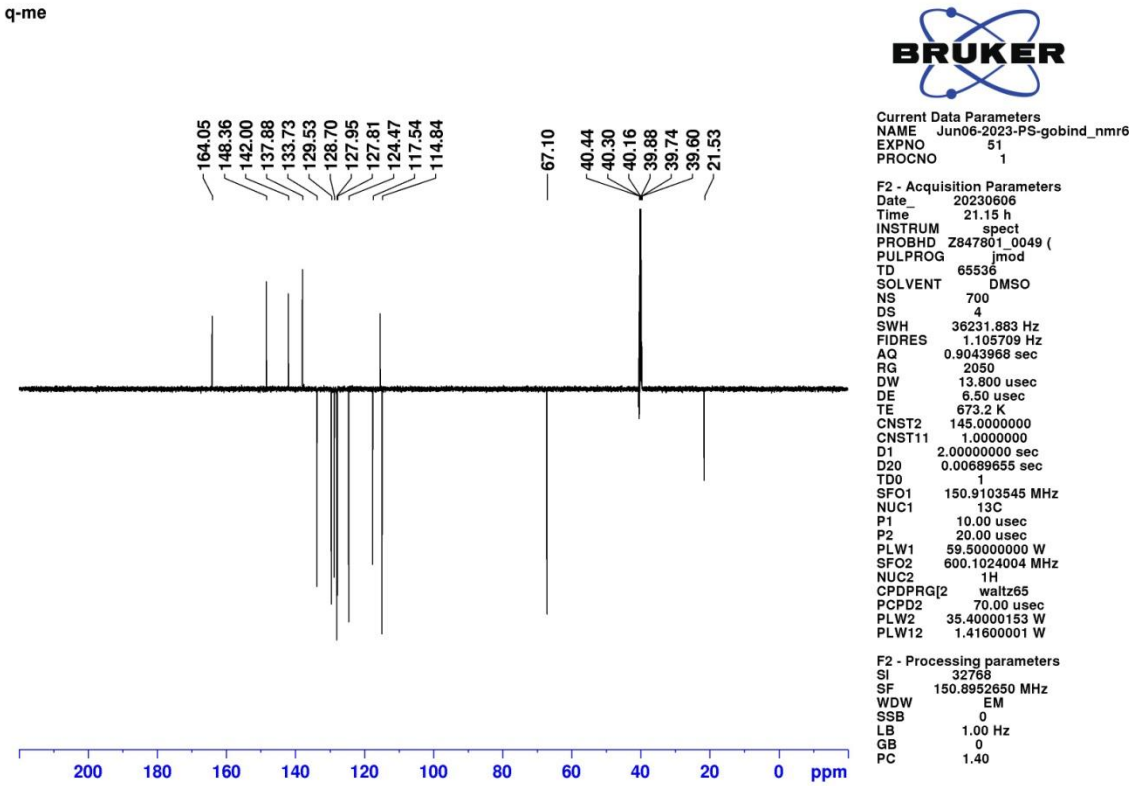
MS spectra of **3l**.



IR spectra of **3m**.



^{1}HNMR of **3m**.



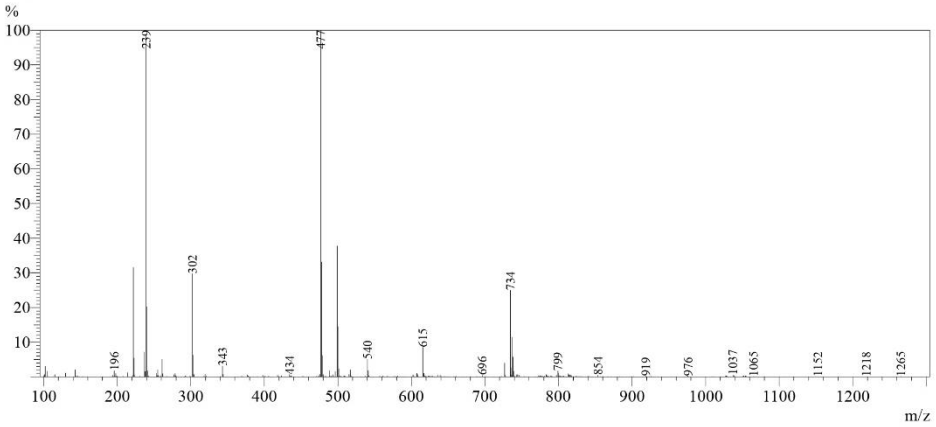
^{13}CNMR of **3m**.

Sample Information

Date Acquired	: 2012/01/28 01:23:24 AM
Sample Type	: Unknown
Sample Name	: 3M
Sample ID	: 3M
Data File	: 3M.lcd
Method File	: no column run 2023.lcm
Report Format File	: DEFAULT.lsr
Tuning File	: 27092021.lct

MS Spectrum

R.Time:1.067(Scan#:65)
MassPeaks:1273
Segment 1 - Event 1



MS spectra of **3m**.

Reference

1. Peña-Solórzano, D.; Guilombo, C. E. G.; Ochoa-Puentes, C., *Sus. Chem. Pharm.* **2019,** *14*, 100167.
2. Kumar, G.; Seboletswe, P.; Manhas, N.; Singh, P.; Bhargava, G.; Rajput, J. K.; Kumar, R. *J. Het. Chem.* **2023**.

