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Ka-Band Rotational Spectroscopy of N-Halosuccinimides

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20 June 2023

Introduction
cyclopentanediones

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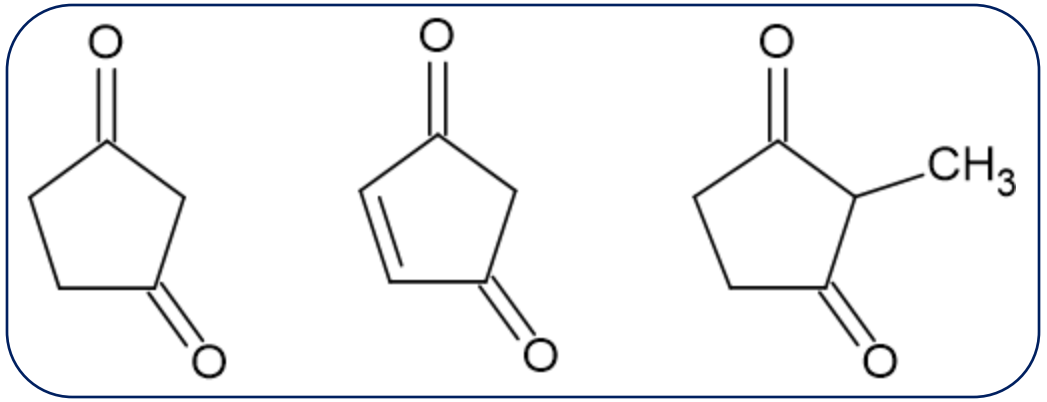

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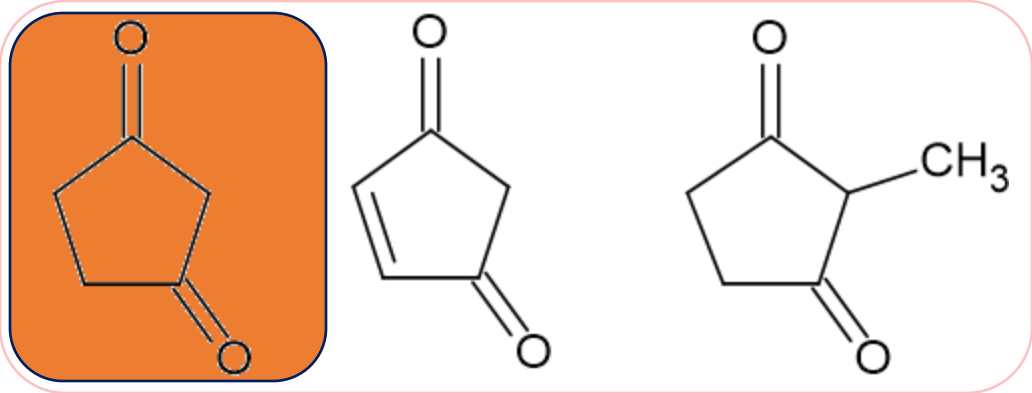

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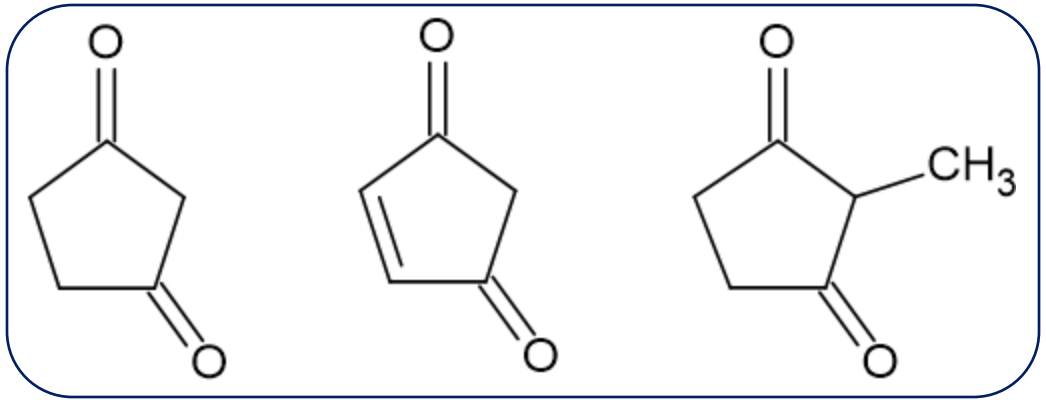
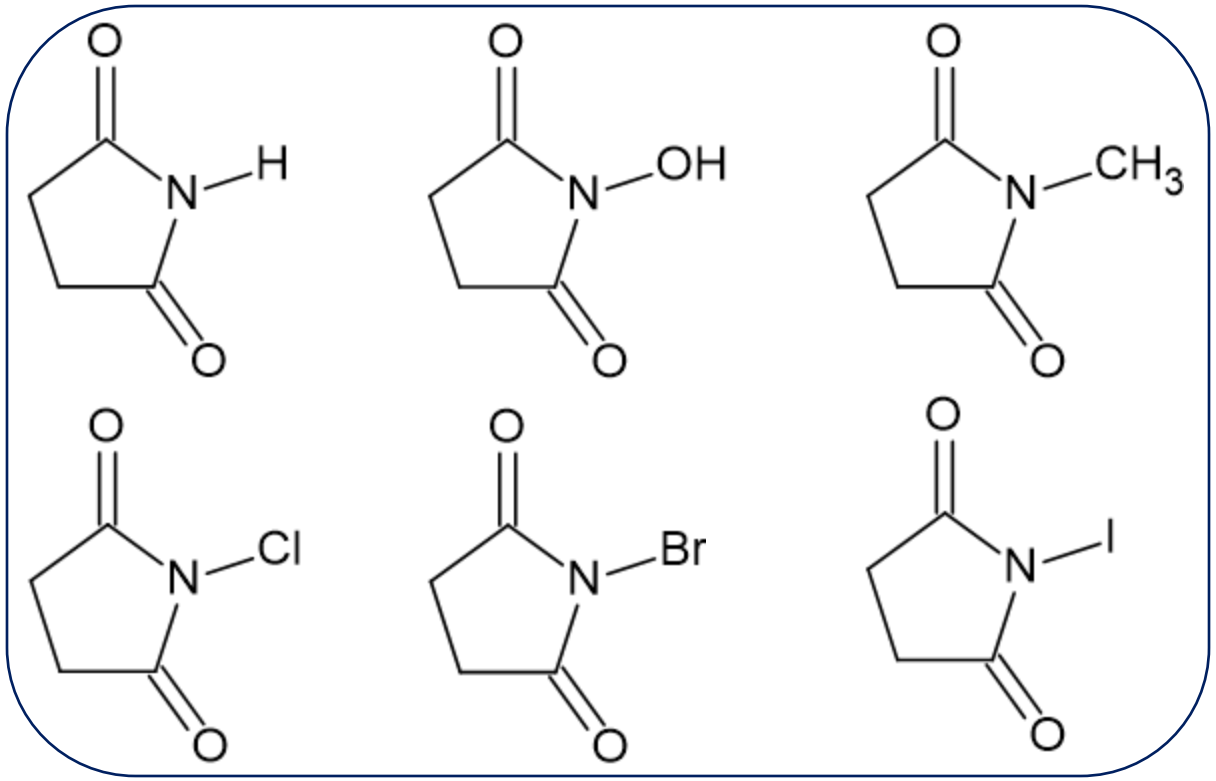
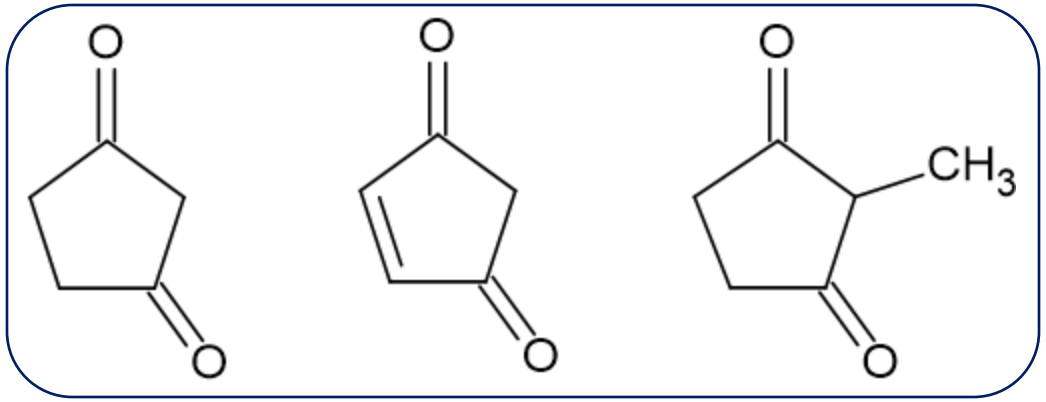
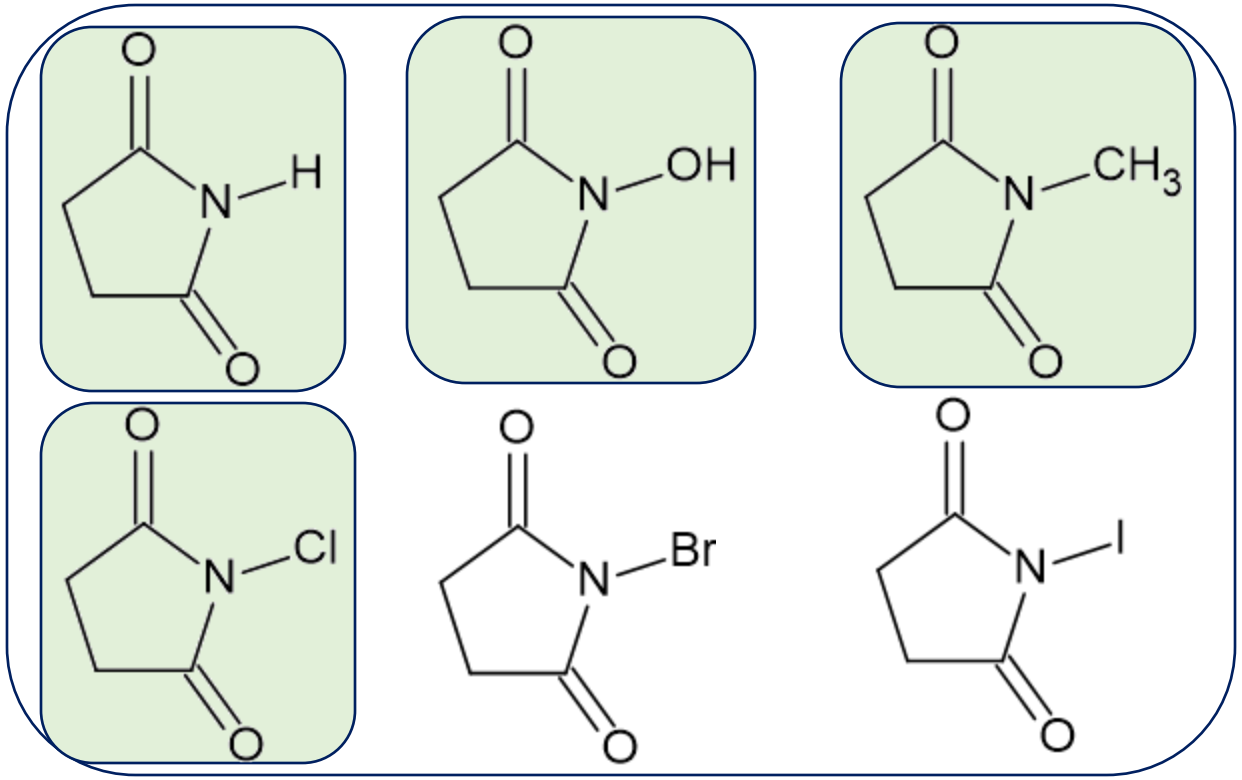
Introduction
cyclopentanediones, succinimdes





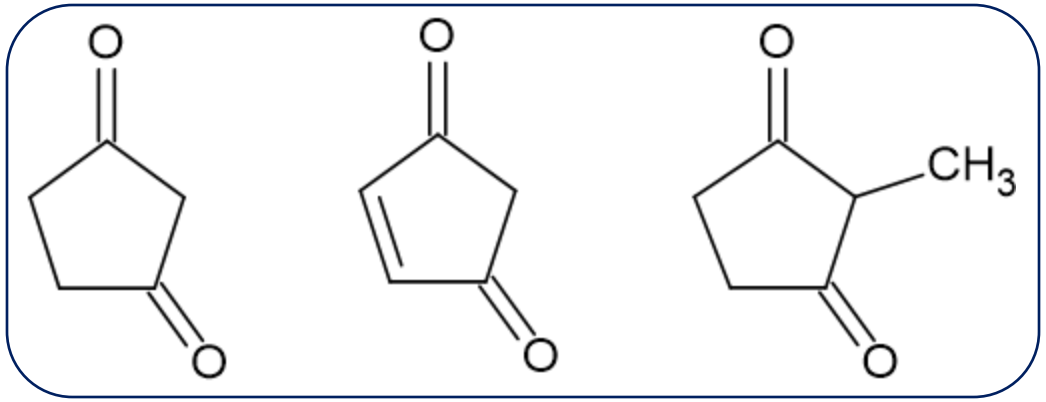
Introduction
cyclopentanediones, succinimdes

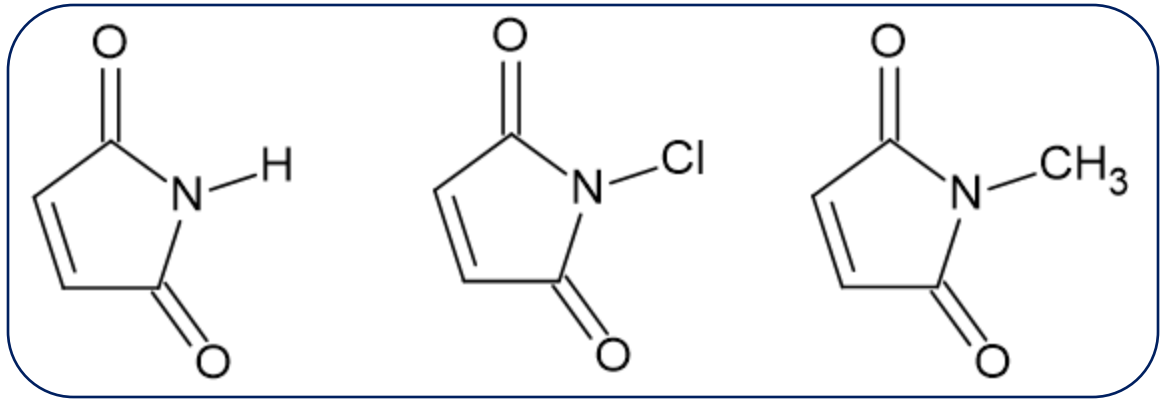


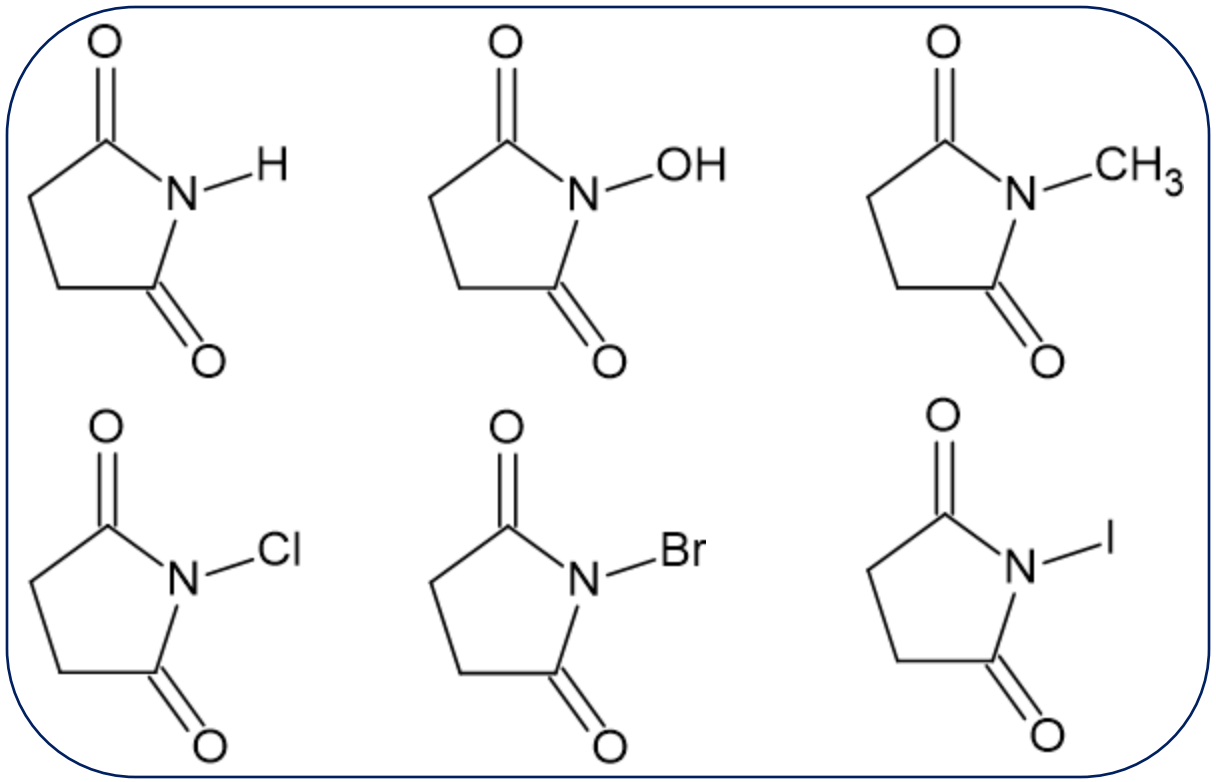


Introduction

cyclopentanediones, succinimdes, maleimides







Introduction

cyclopentanediones, succinimdes, maleimides, piperidinediones

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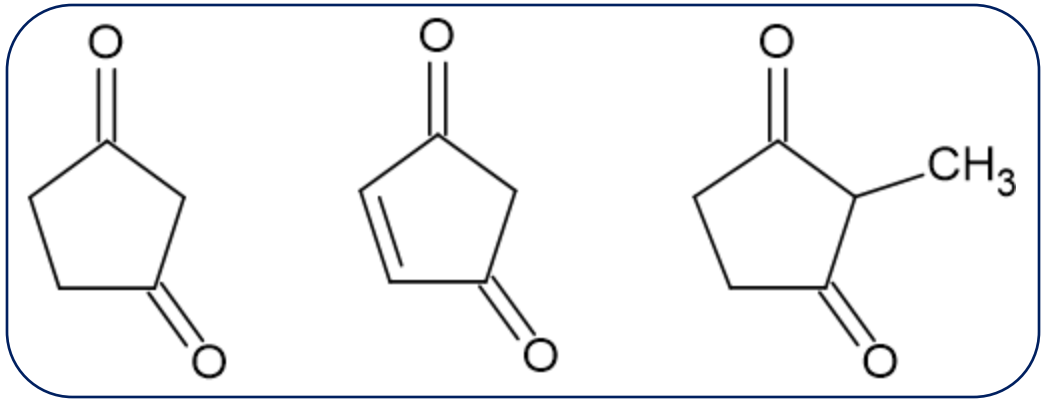

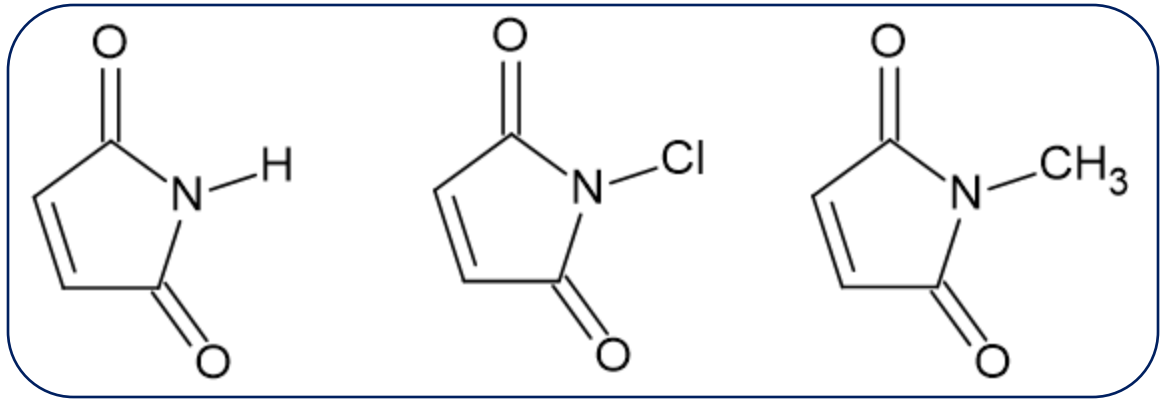

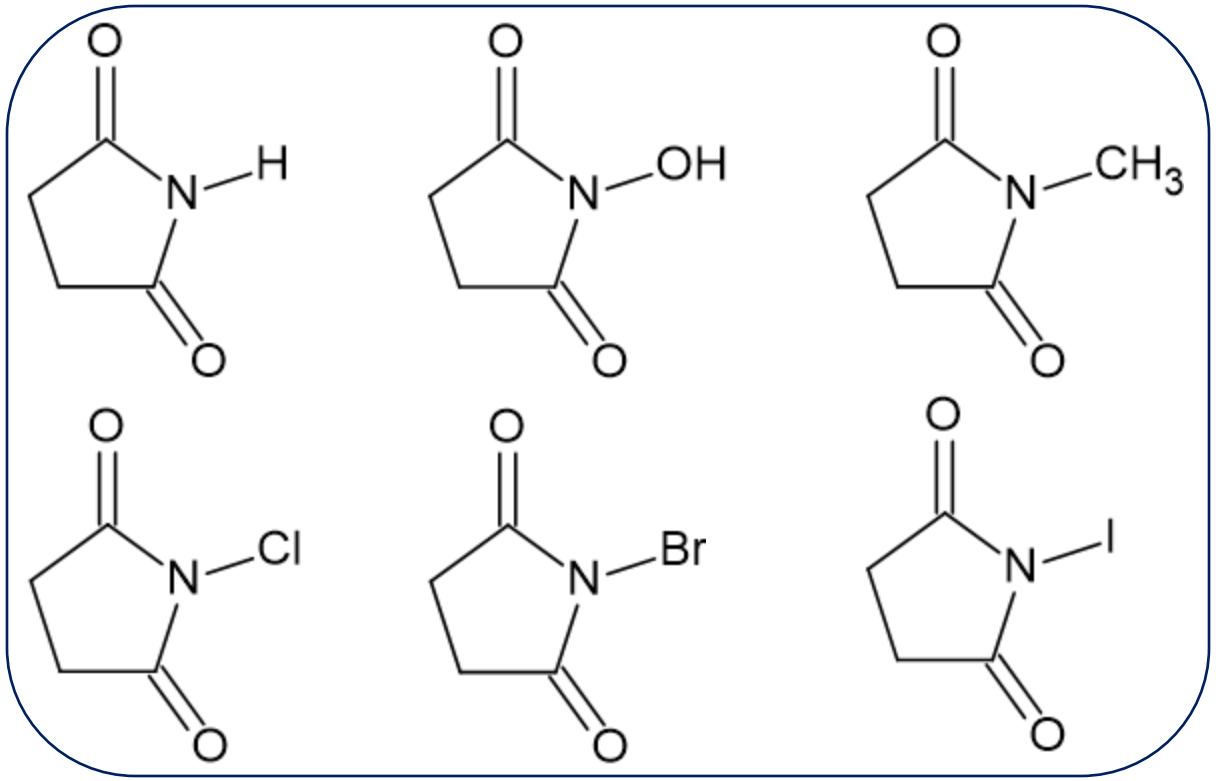

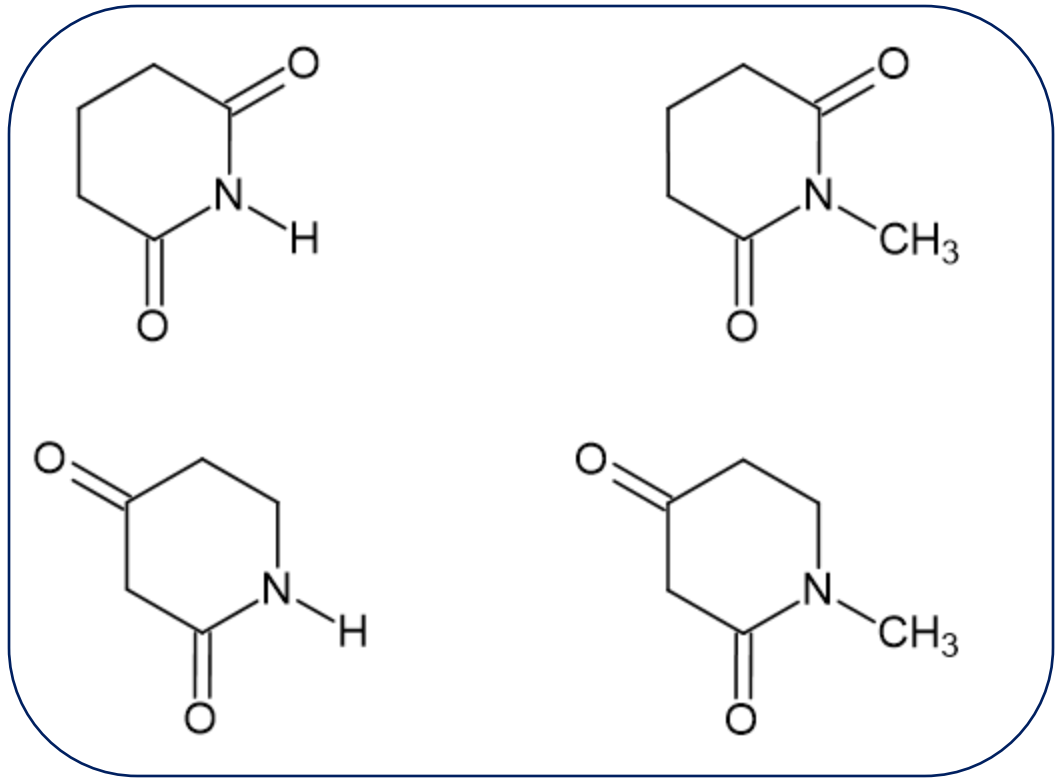

Introduction

cyclopentanediones, succinimdes, maleimides, piperidinediones

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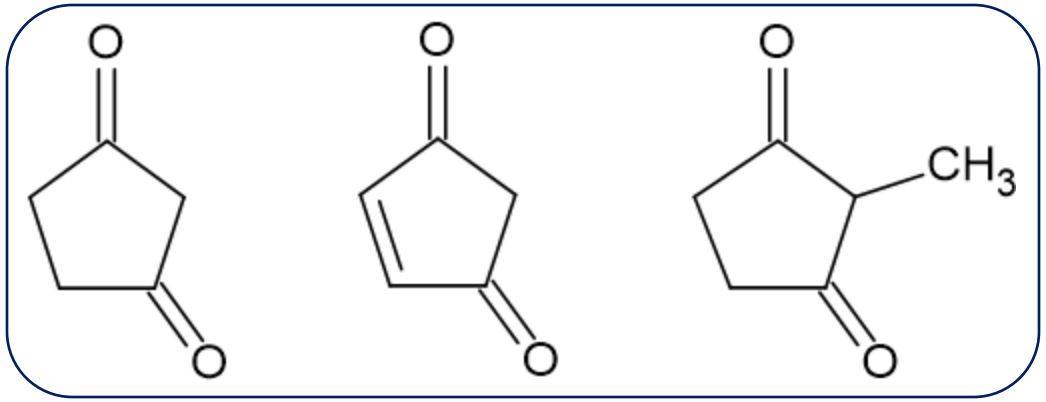

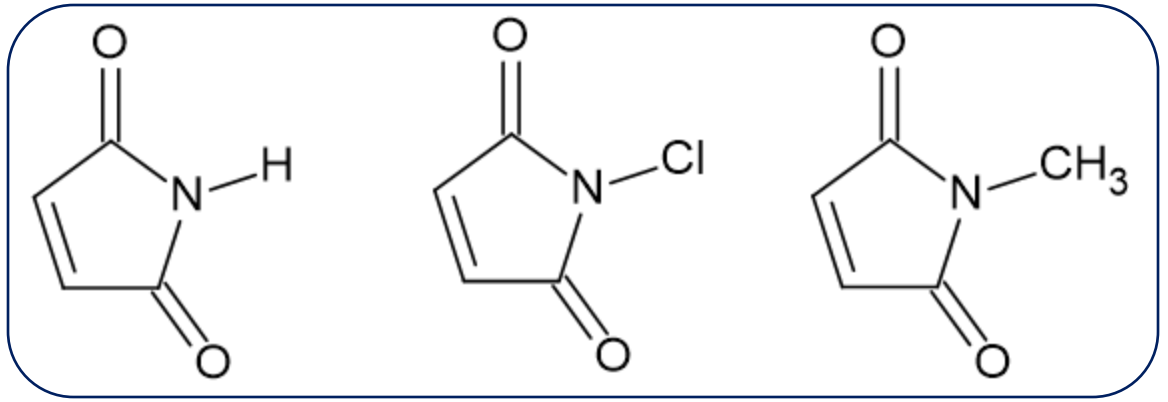

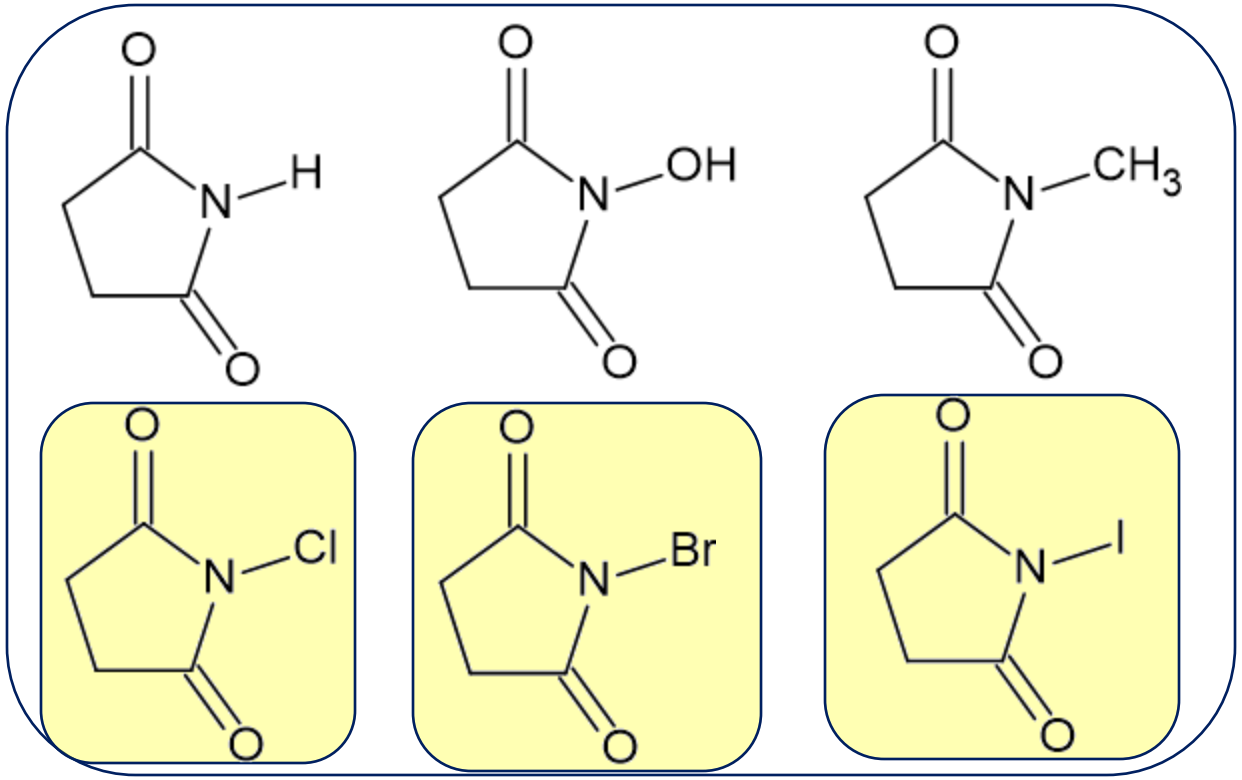

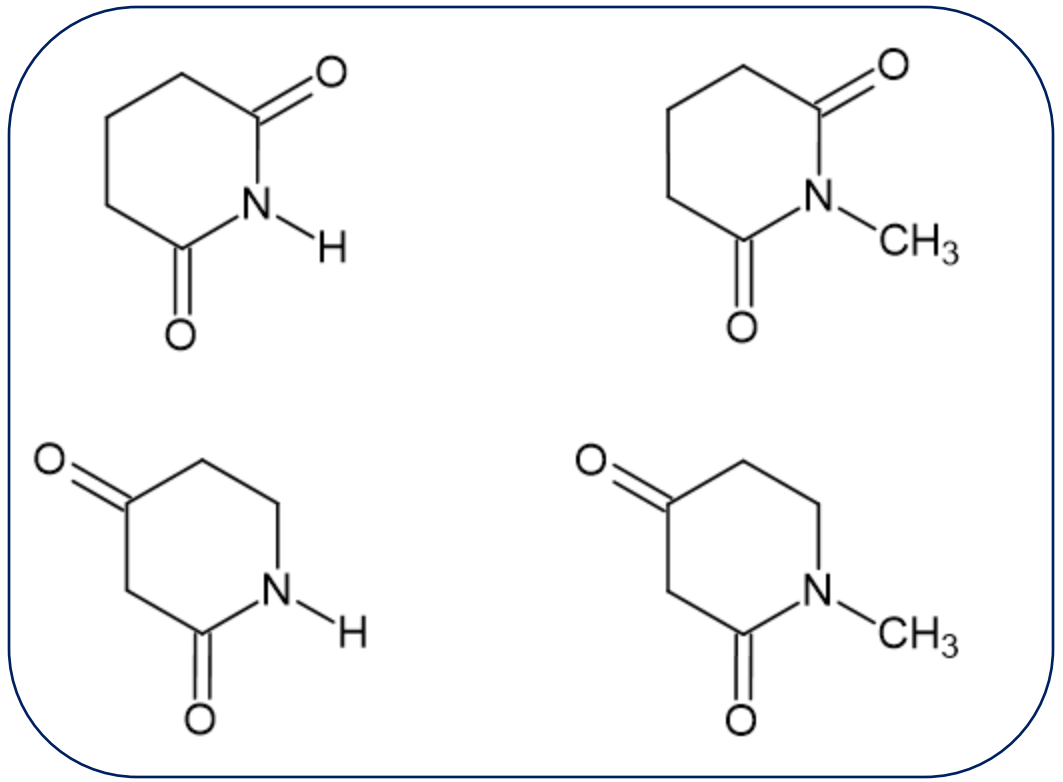

Ka-Band Rotational Spectrometer

spectra acquisition

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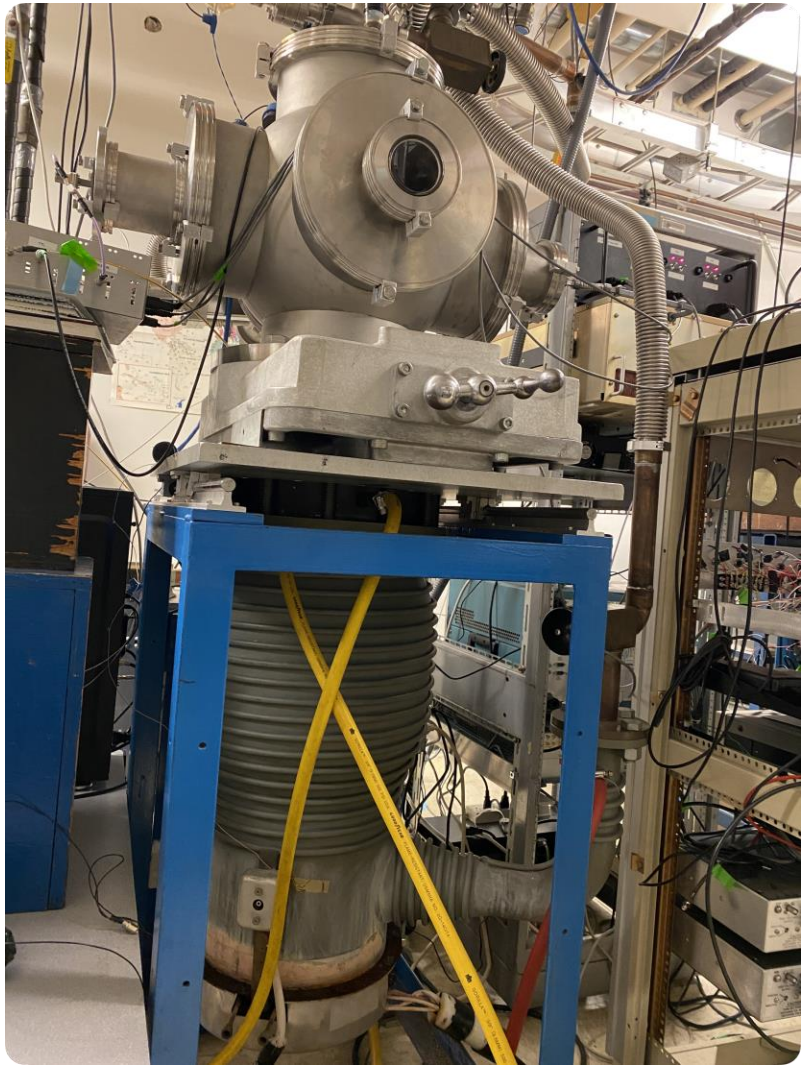
Vacuum chamber + diffusion pump



Ka-Band Rotational Spectrometer

spectra acquisition

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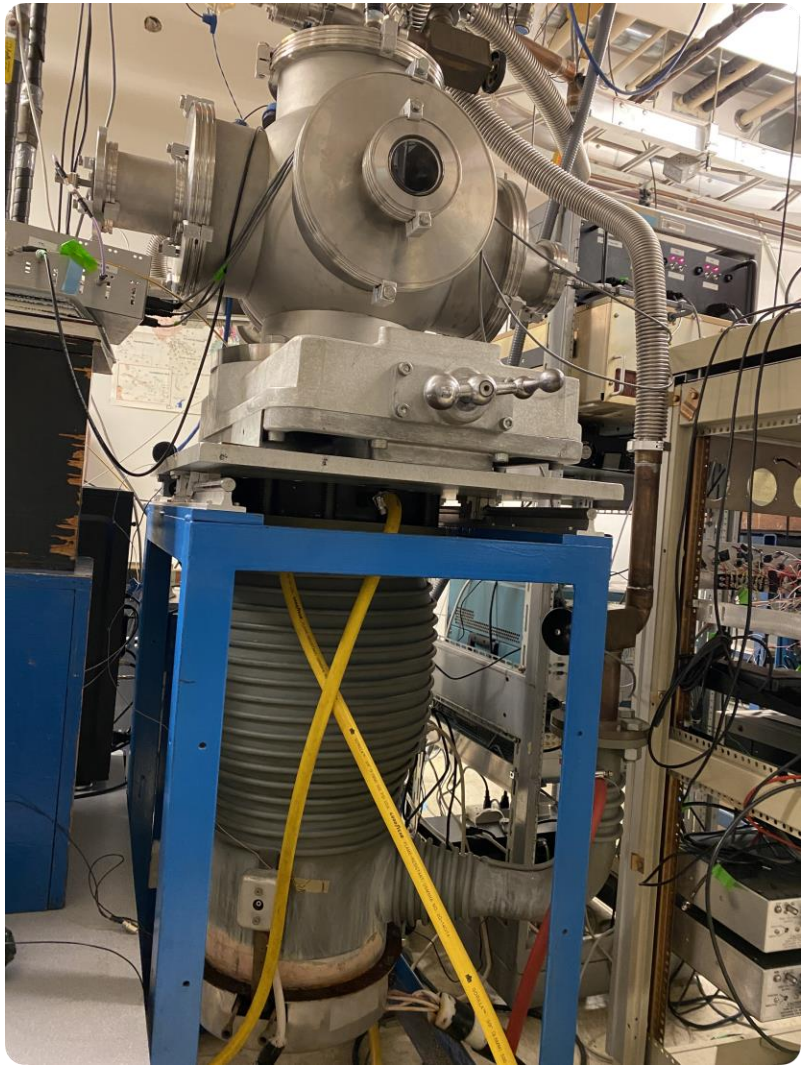
Vacuum chamber + diffusion pump



pulsed solenoid valve

Supersonic expansion

Ka-Band Rotational Spectrometer

spectra acquisition

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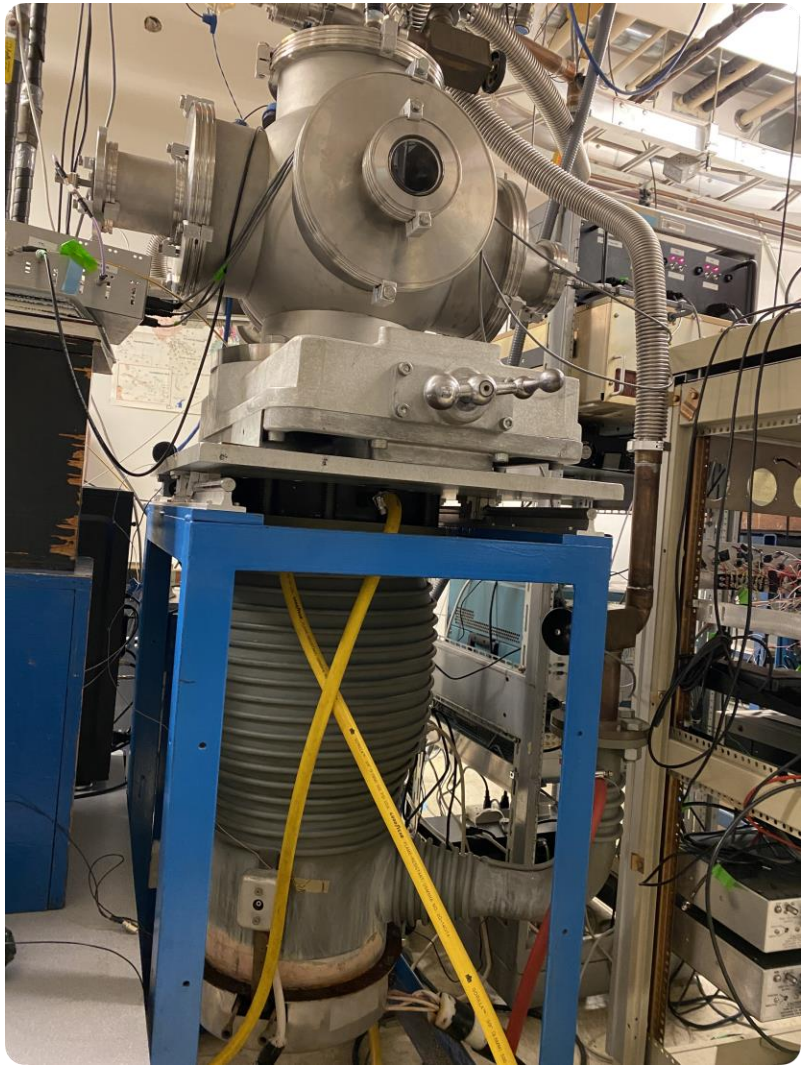
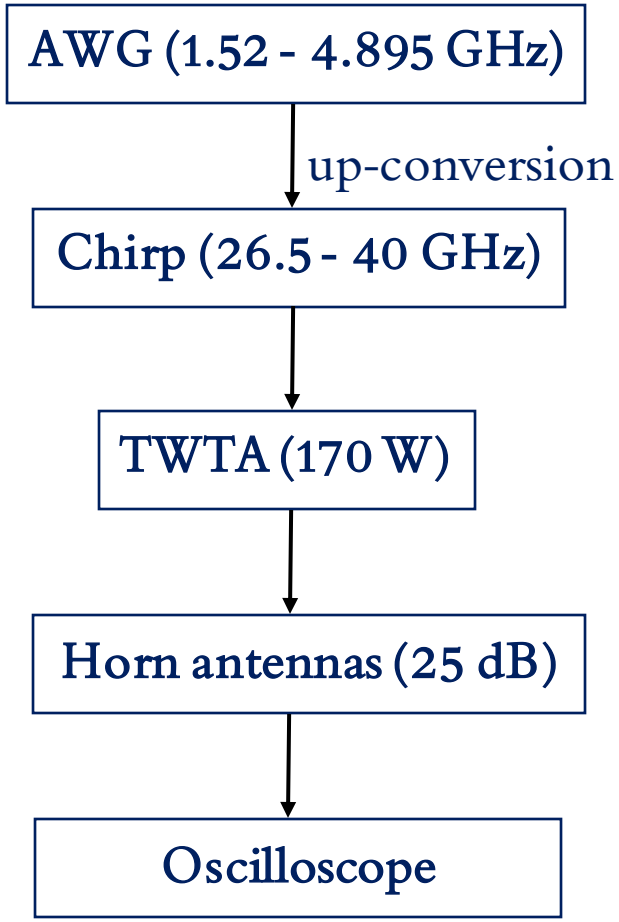
Vacuum chamber + diffusion pump



pulsed solenoid valve

Supersonic expansion



Heated Source Assembly

spectra acquisition

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Heated Source Assembly

spectra acquisition

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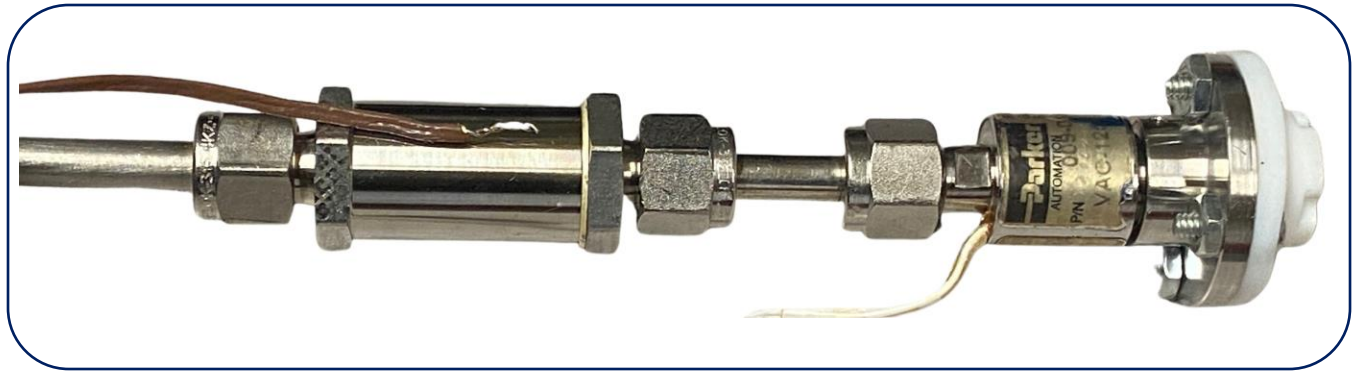

Heated Source Assembly

spectra acquisition

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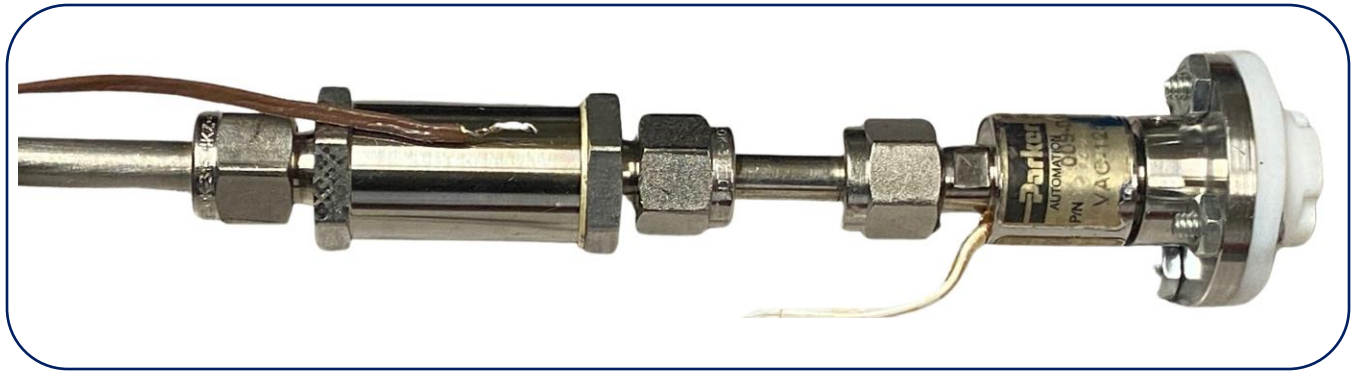

Heated Source Assembly

spectra acquisition

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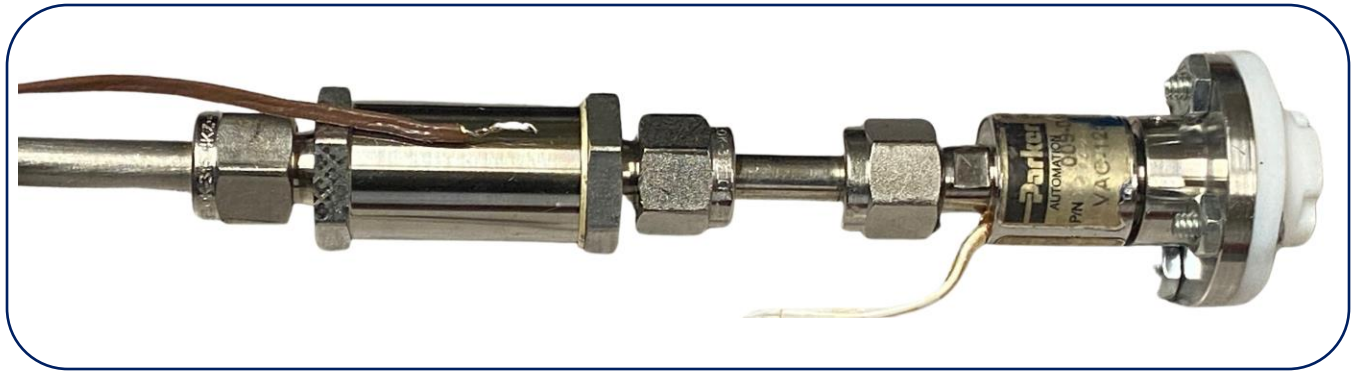

Heated Source Assembly
spectra acquisition

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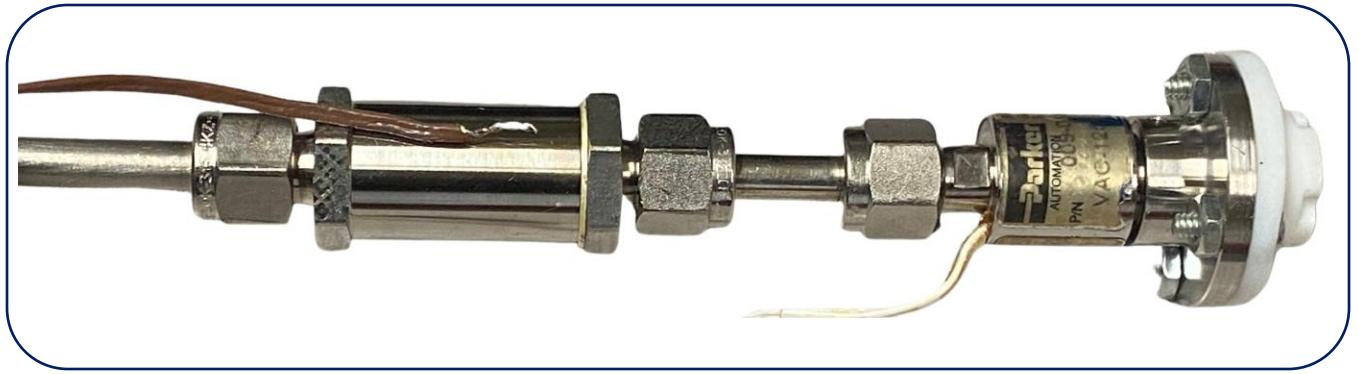

Theoretical
calculated rotational constants

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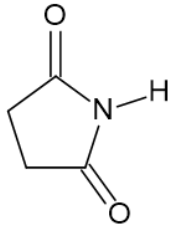
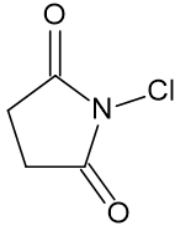
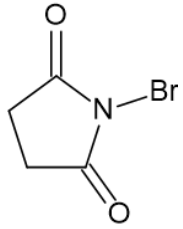
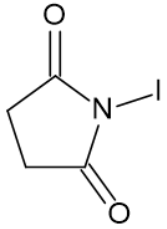
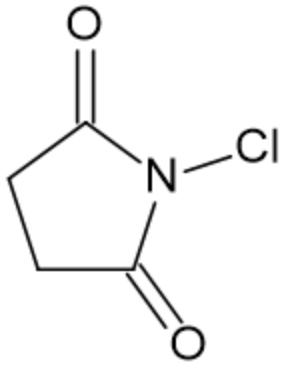
						
		^{35}Cl	^{37}Cl	^{79}Br	^{81}Br	
A (MHz)	5924.9	2232.3	2244.6	2233.9	2246.2	2253.9
B (MHz)	2257.7	1947.1	1911.4	1196.2	1194.1	884.8
C (MHz)	1668.3	1053.5	1045.6	786.6	787.2	640.4
K	-0.72	0.52	0.44	-0.43	-0.44	-0.70
μ_a (D)	0	3.44		2.97		2.23
μ_b (D)	-2.22	0	0	0	0	0
μ_c (D)	0	0	0	0	0	0
Level of Theory	B3LYP/6-311++g(d,p)	B3LYP/6-311++g(d,p)	B3LYP/def2tzvp	B3LYP/6-311++g(d,p)	B3LYP/def2tzvp	B3LYP/def2tzvp
%	100	75	25	50.7	49.3	100

N-chlorosuccinimide
experimental rotational spectrum



N-chlorosuccinimide
experimental rotational spectrum

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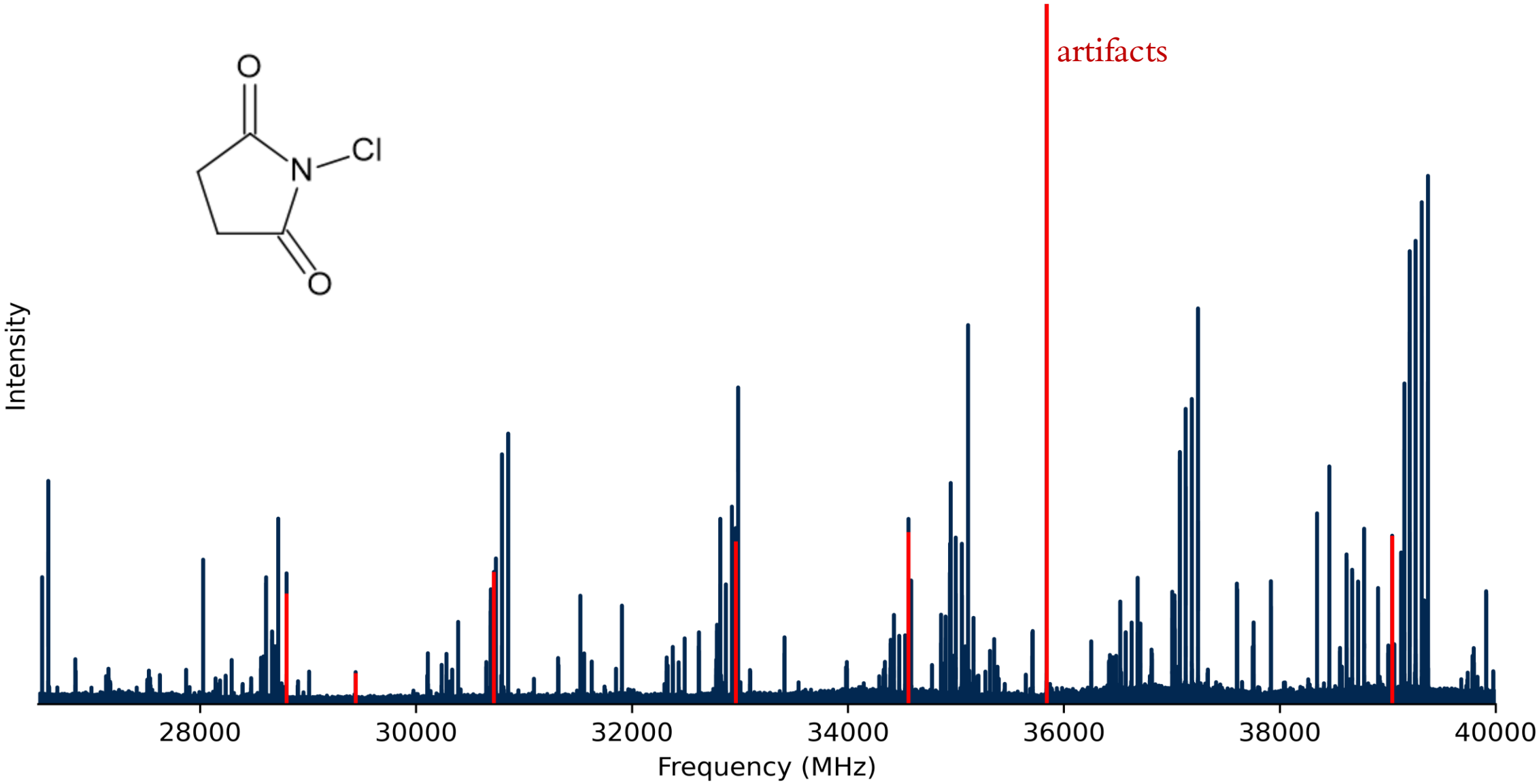

N-chlorosuccinimide

experimental and fitted rotational spectrum

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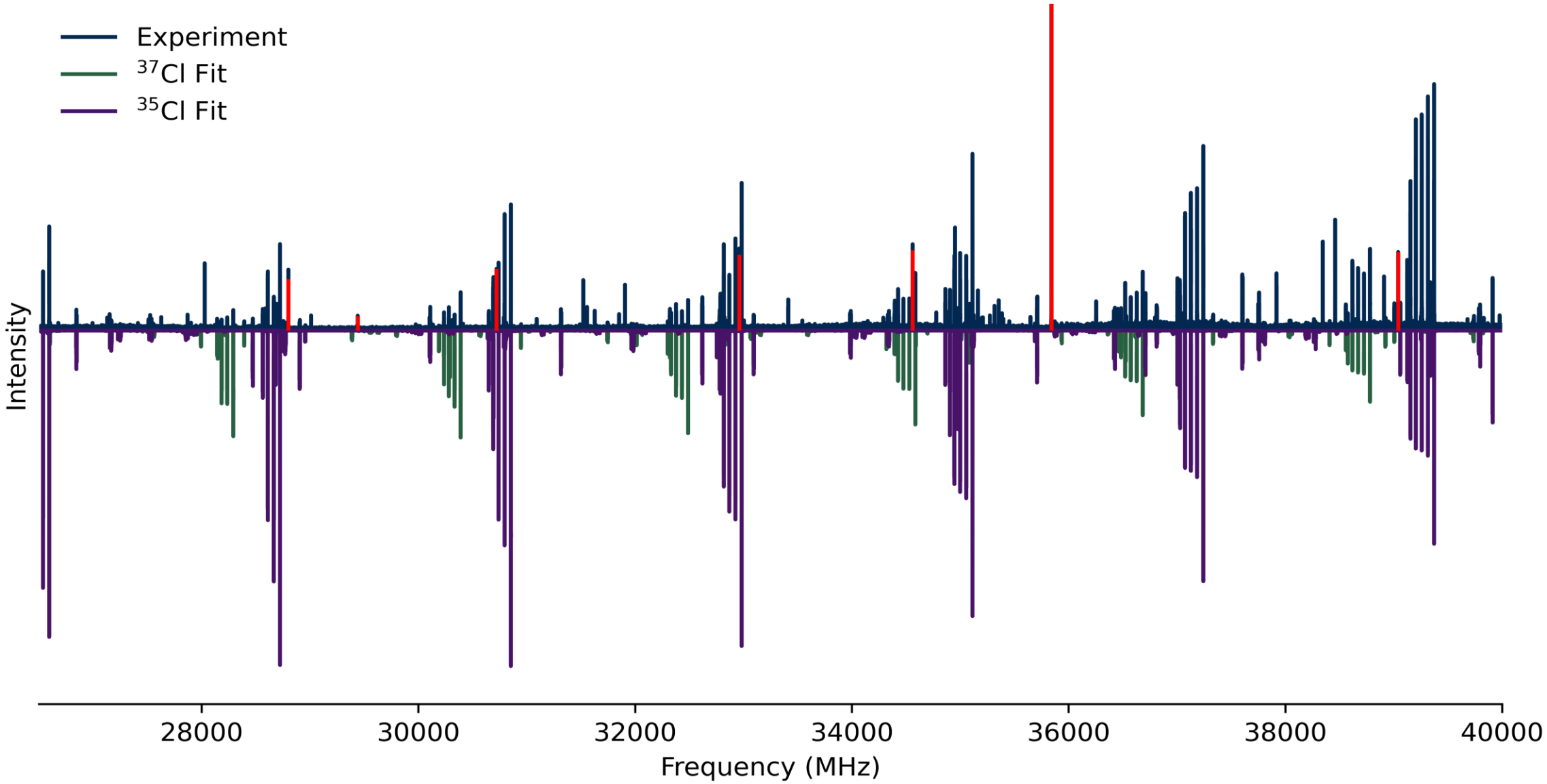

N-chlorosuccinimide

Quadrupolar nuclei hyperfine splitting

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chlorine hyperfine splitting

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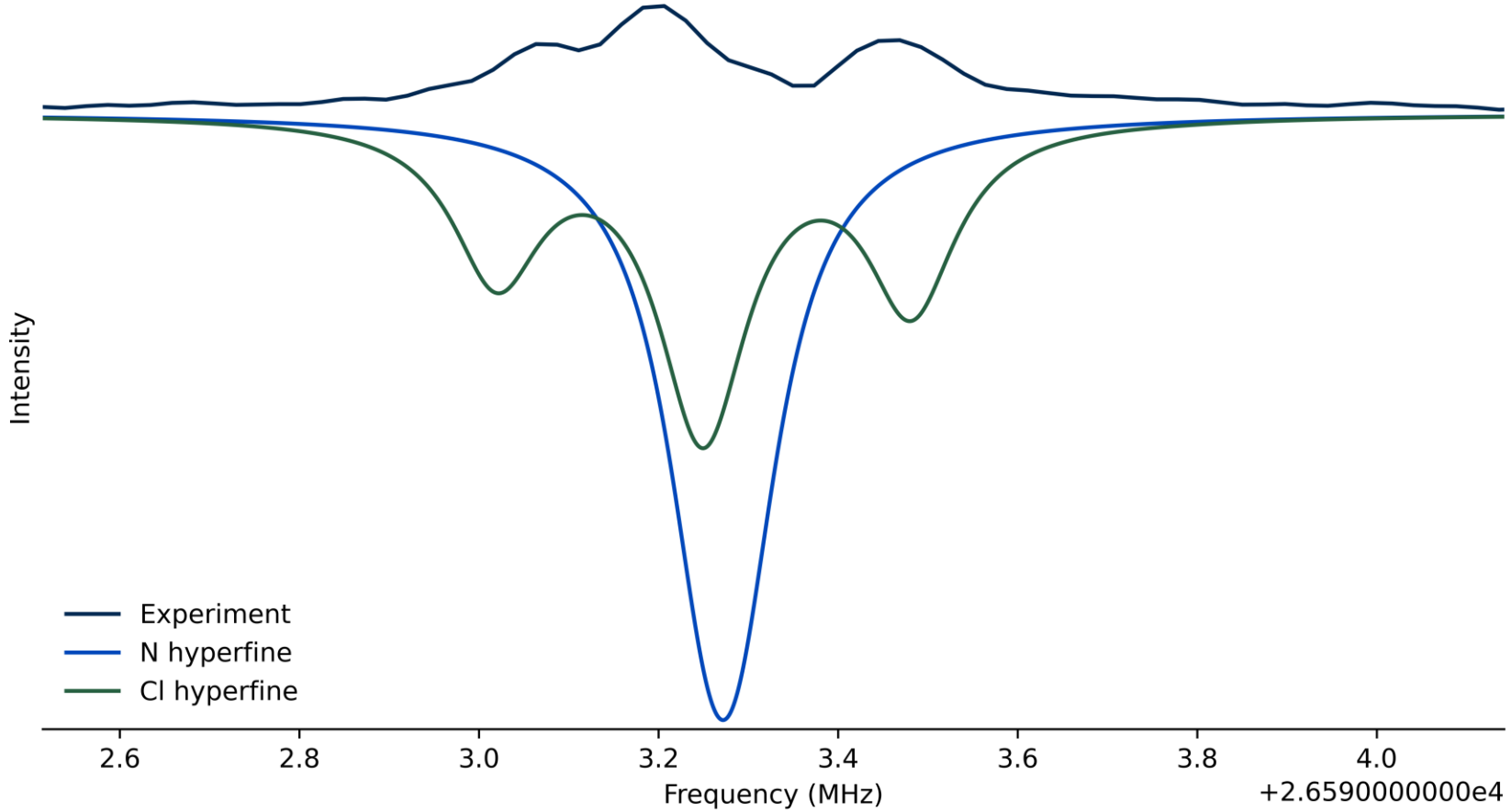

N-chlorosuccinimide

Quadrupolar nuclei hyperfine splitting

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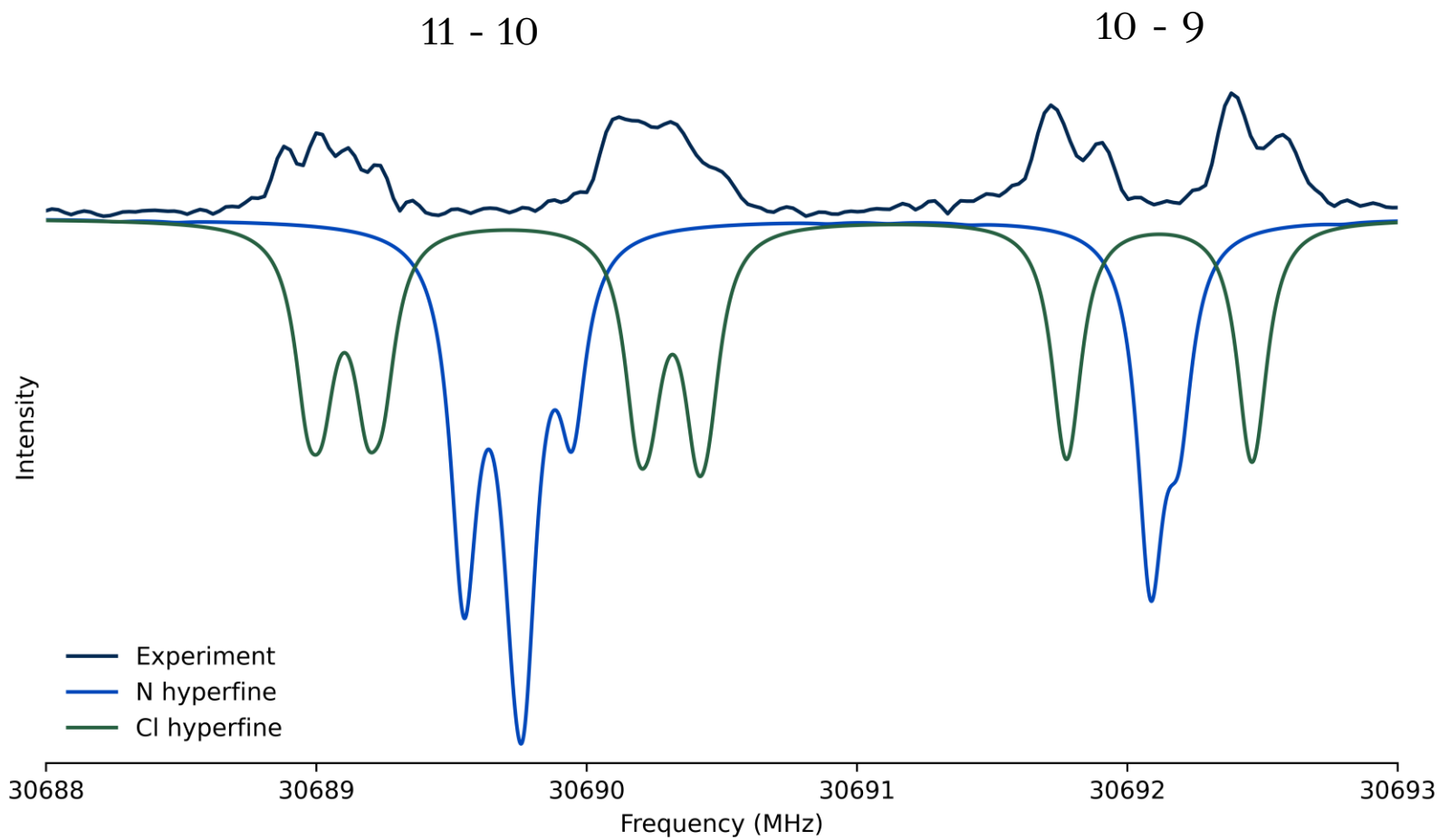
nitrogen hyperfine splitting



N-chlorosuccinimide
fitted rotational parameters

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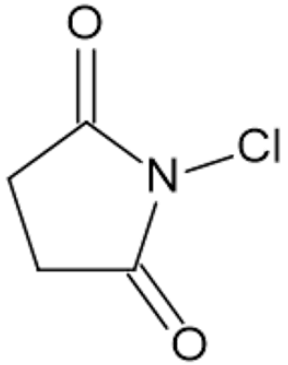
^{35}Cl	Fitted	Calculated
A (MHz)	2243.122(1)	2232.3
B (MHz)	1975.9659(7)	1947.1
C (MHz)	1064.8887(4)	1053.5
χ_{aa}(Cl)(MHz)	-109.5(4)	106.7
$\chi_{bb}-\chi_{cc}$(Cl)(MHz)	3.2(4)	2.64
χ_{aa}(N)(MHz)	10.8(4)	5.03
$\chi_{bb}-\chi_{cc}$(N)(MHz)	[5.12]	5.12
ΔJ (kHz)	0.2001(8)	-0.00014
ΔK (kHz)	-0.022(1)	0.00027
ΔJK (kHz)	-0.1558(10)	-0.00015
δN(kHz)	[0.0000029]	0.0000029
δK (kHz)	-0.64(2)	-0.00128



N-chlorosuccinimide
fitted rotational parameters

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χ_{aa}(N)(MHz)	10.8(4)	5.03
$\chi_{bb}-\chi_{cc}$(N)(MHz)	[5.12]	5.12
ΔJ (kHz)	0.2001(8)	-0.00014
ΔK (kHz)	-0.022(1)	0.00027
ΔJK (kHz)	-0.1558(10)	-0.00015
δN(kHz)	[0.0000029]	0.0000029
δK (kHz)	-0.64(2)	-0.00128

No. Of lines fitted	250
RMS (MHz)	0.104009

N-chlorosuccinimide
fitted rotational parameters

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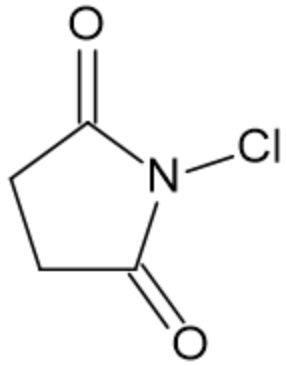

^{37}Cl	Fitted	Calculated
A (MHz)	2243.07(3)	2232.3
B (MHz)	1975.9659(7)	1947.1
C (MHz)	1048.892(3)	1053.5
χ_{aa} (MHz)	-85.3(2)	-91.33
$\chi_{bb}-\chi_{cc}$ (MHz)	4.4(20)	2.59
χ_{aa} (MHz)	[4.72]	4.72
$\chi_{bb}-\chi_{cc}$ (MHz)	[4.60]	4.60
ΔJ (kHz)	-1.4(2)	-0.00014
ΔK (kHz)	-4.7(8)	0.00028
ΔJK (kHz)	6.(1)	-0.00015
δN (kHz)	1.6(2)	0.0000011
δK (kHz)	-12.(2)	-0.0011

N-chlorosuccinimide
fitted rotational parameters

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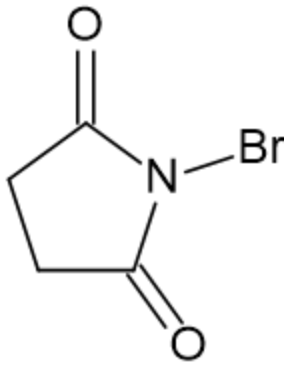
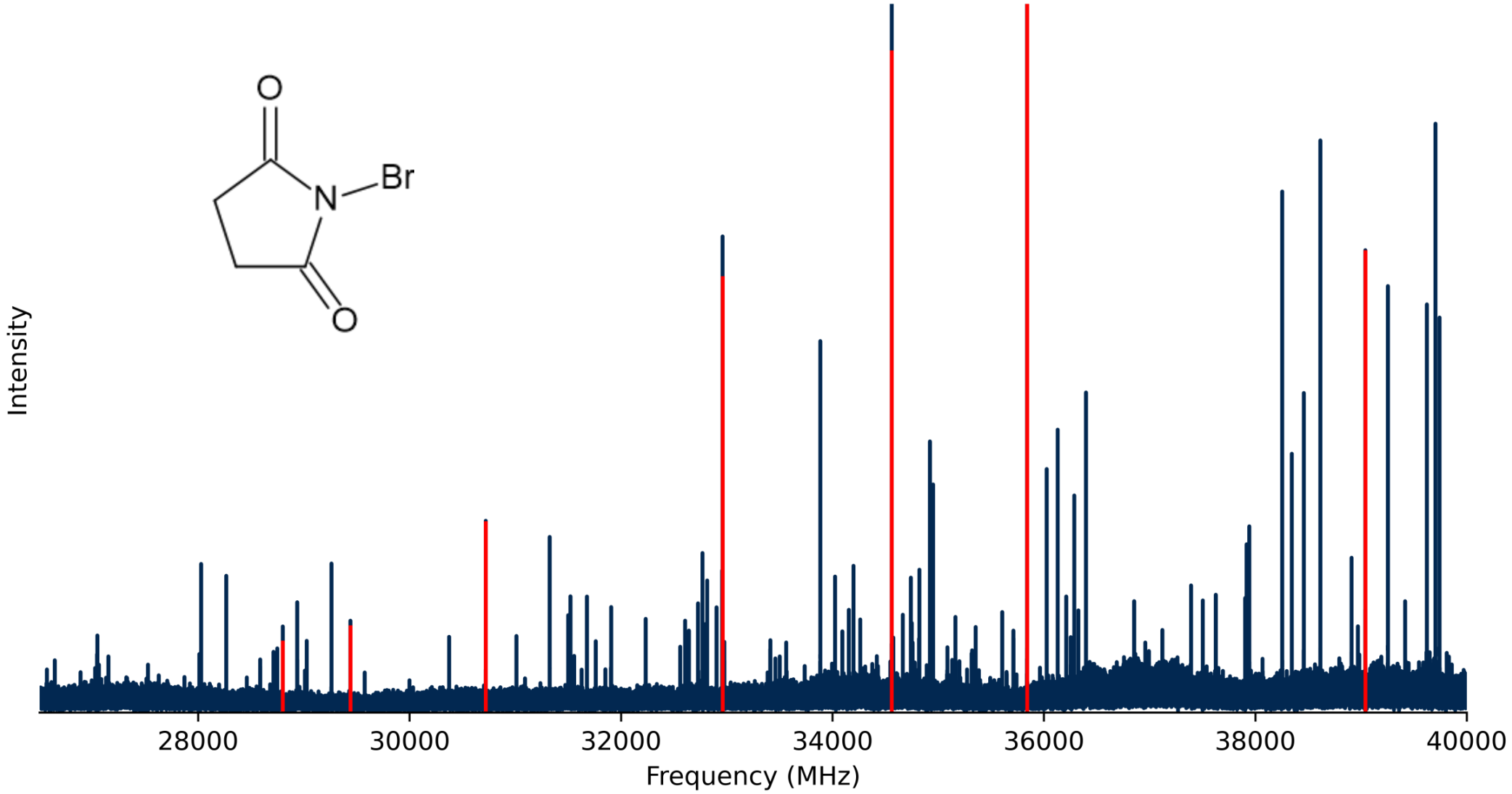
No. Of lines fitted	366
RMS (MHz)	0.076413

^{37}Cl	Fitted	Calculated
A (MHz)	2243.07(3)	2232.3
B (MHz)	1975.9659(7)	1947.1
C (MHz)	1048.892(3)	1053.5
χ_{aa} (MHz)	-85.3(2)	-91.33
χ_{bb}-χ_{cc} (MHz)	4.4(20)	2.59
χ_{aa} (MHz)	[4.72]	4.72
χ_{bb}-χ_{cc} (MHz)	[4.60]	4.60
ΔJ (kHz)	-1.4(2)	-0.00014
ΔK (kHz)	-4.7(8)	0.00028
ΔJK (kHz)	6.(1)	-0.00015
δN (kHz)	1.6(2)	0.0000011
δK (kHz)	-12.(2)	-0.0011

N-Bromosuccinimide



N-Bromosuccinimide



N-Bromosuccinimide

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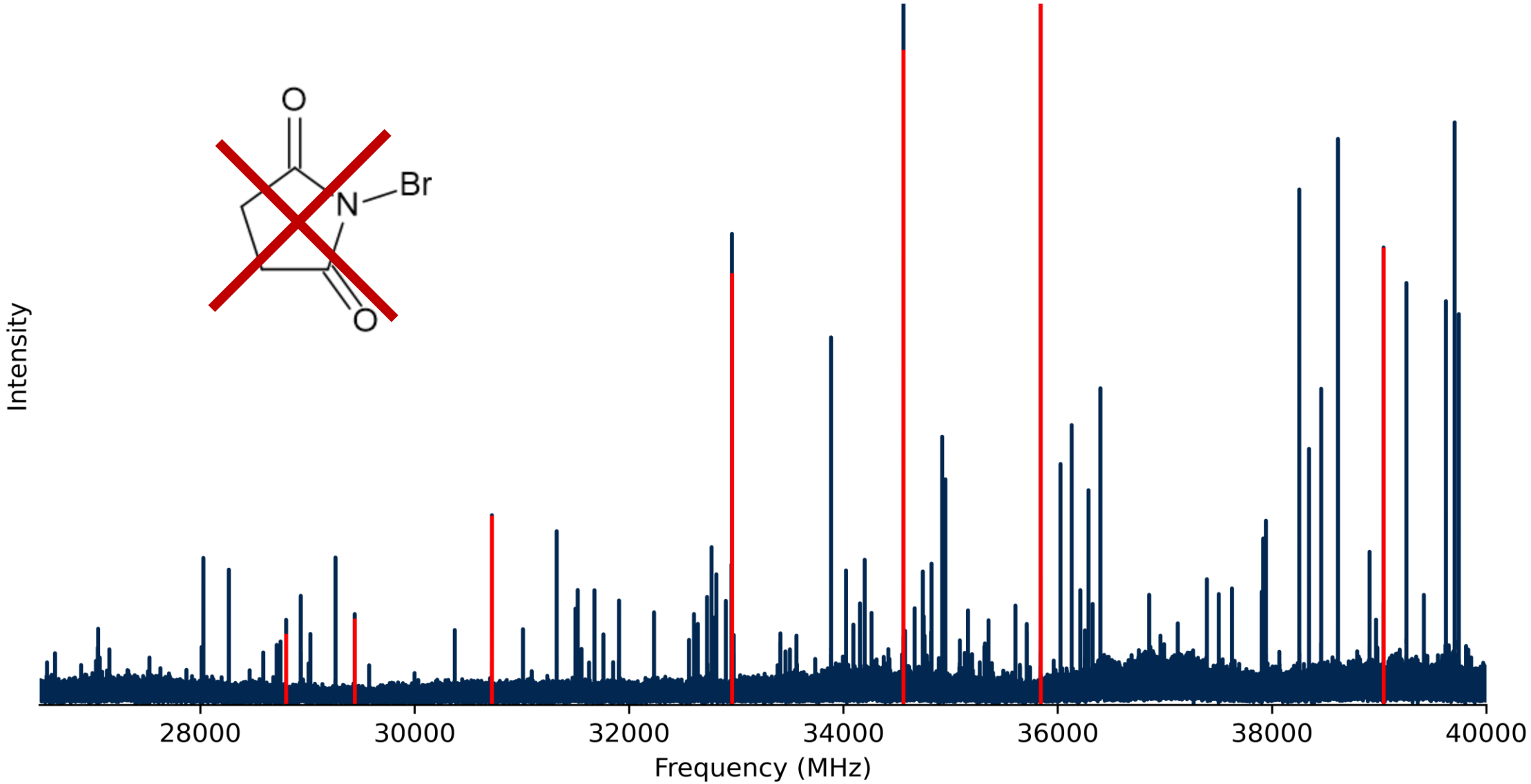

N-Bromosuccinimide

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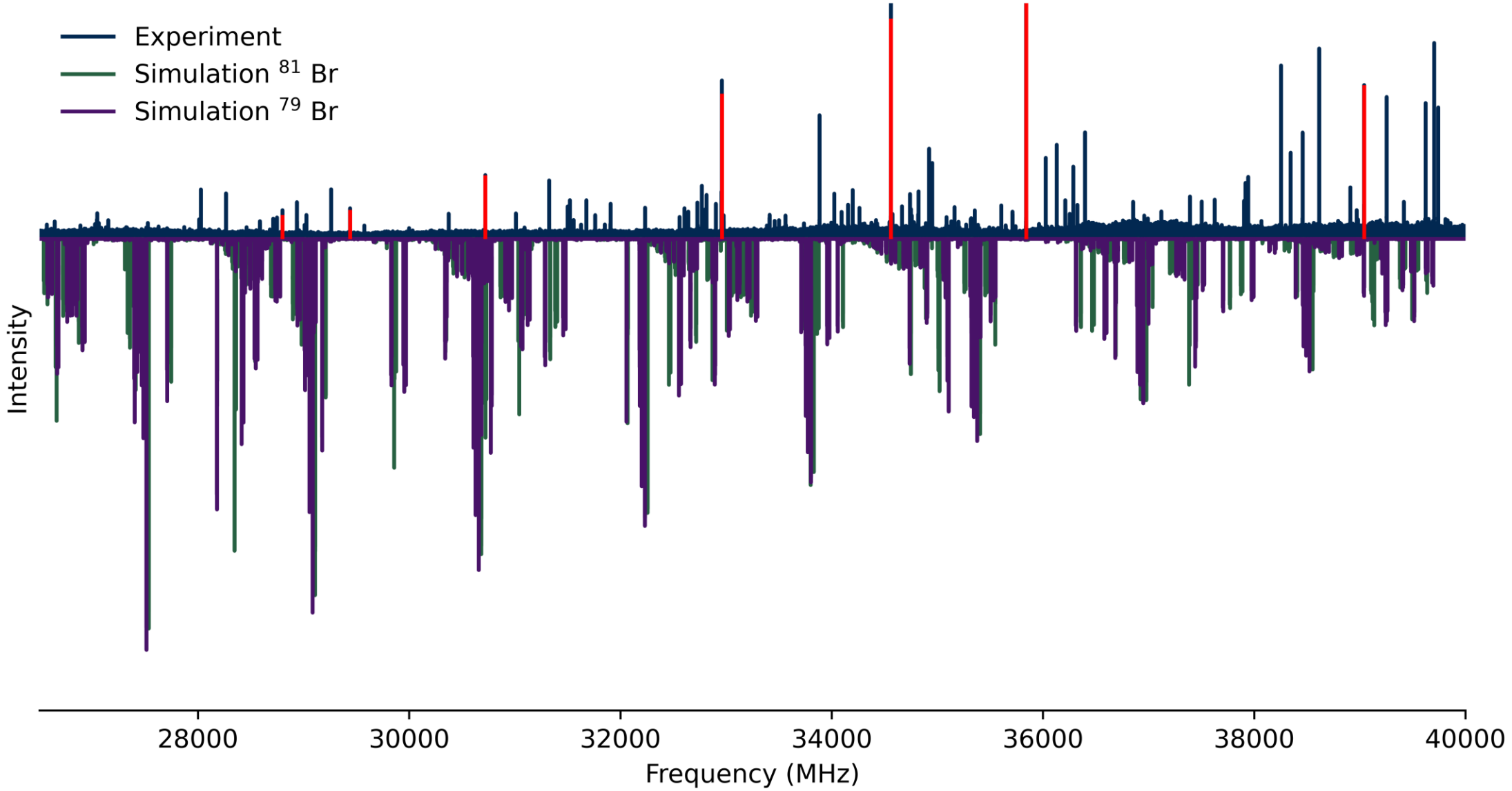

N-Bromosuccinimide

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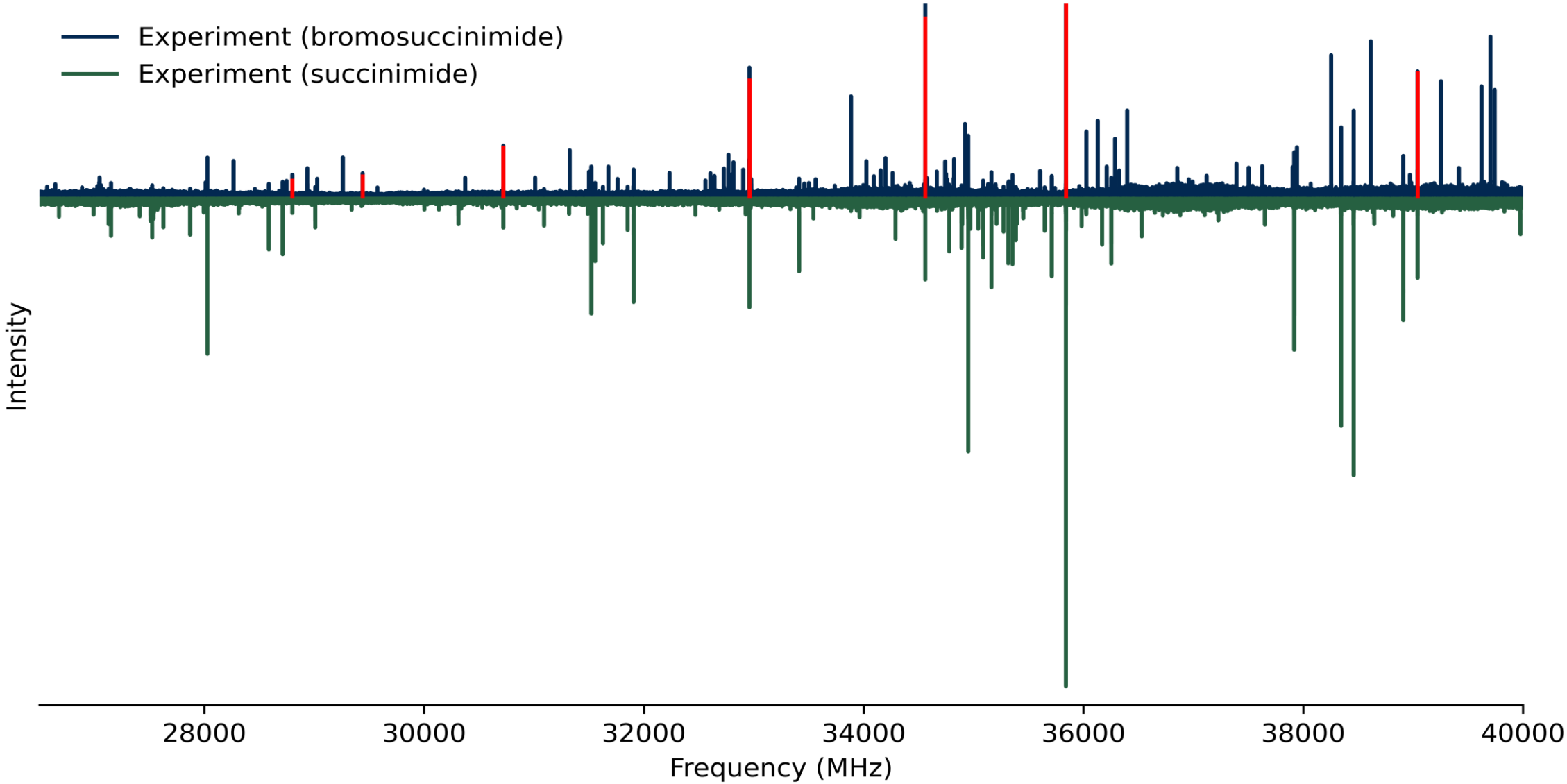

N-Iodosuccinimide

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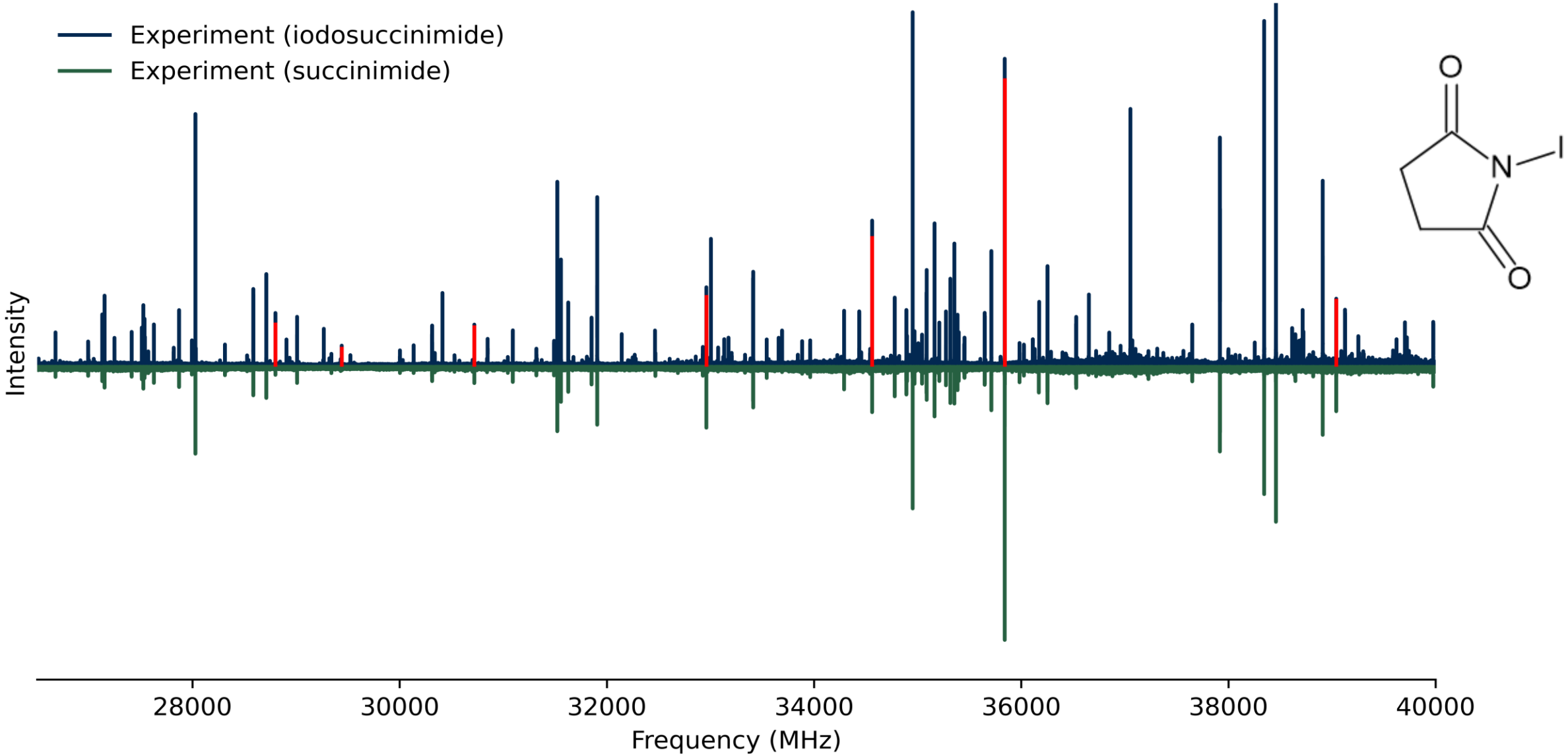

N-Iodosuccinimide

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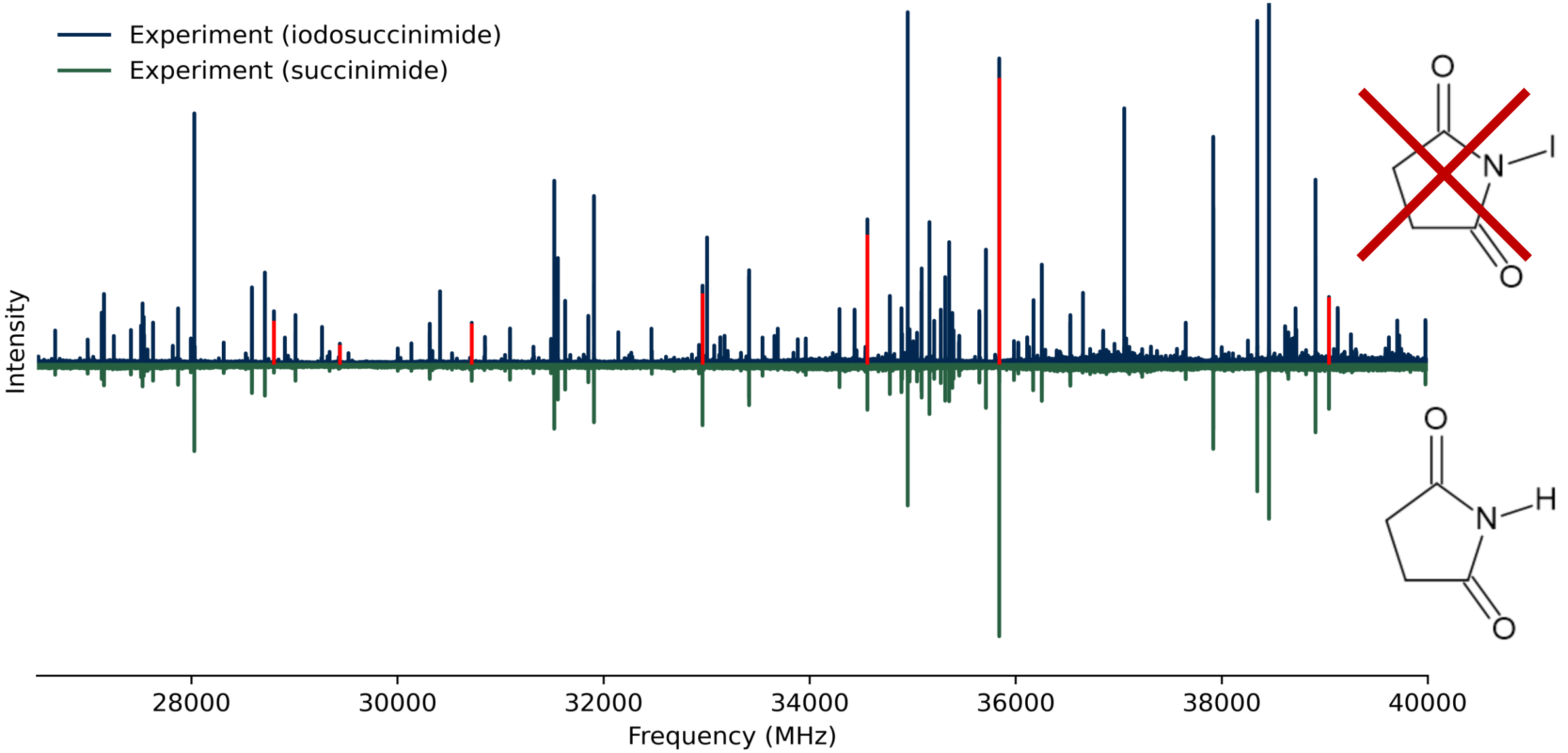
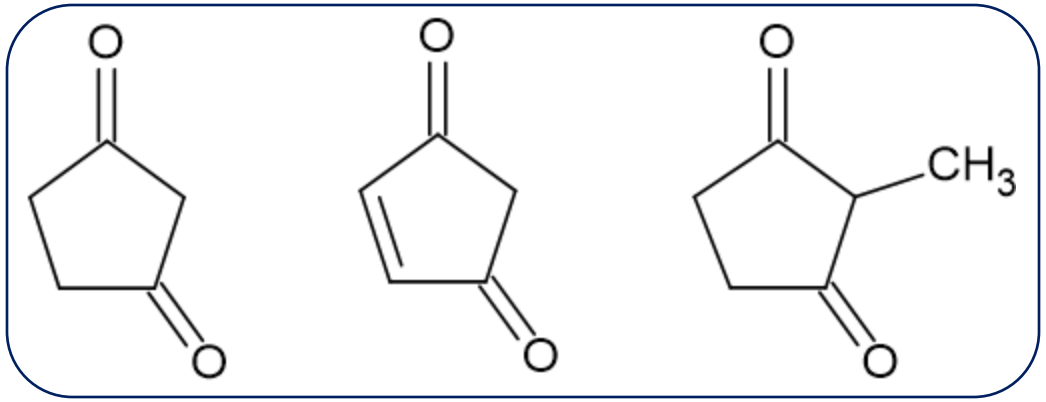
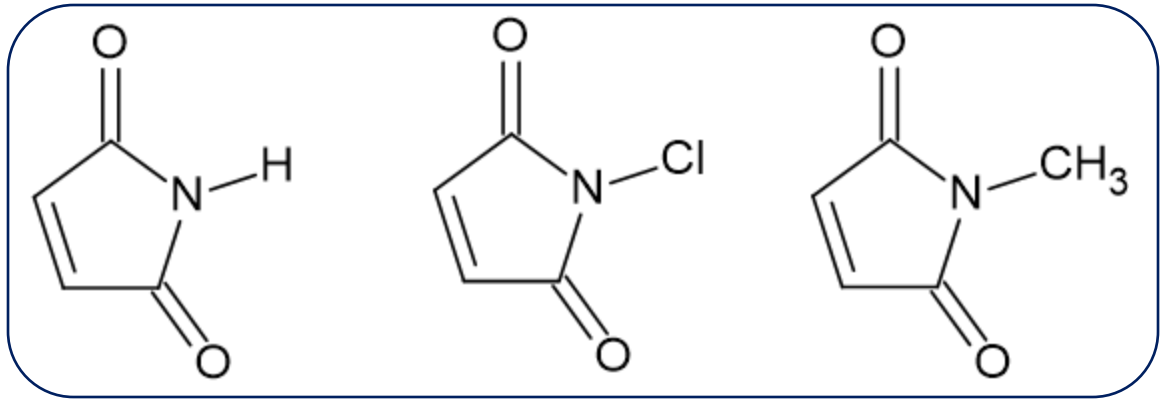
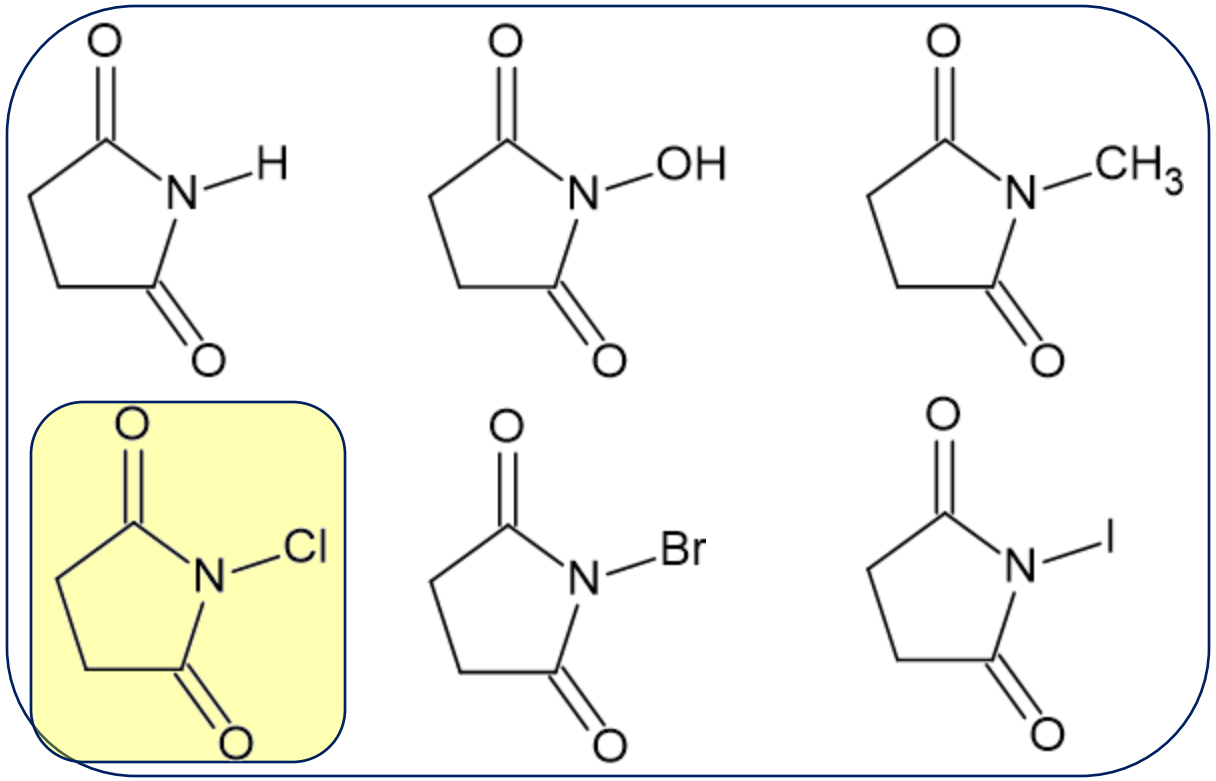
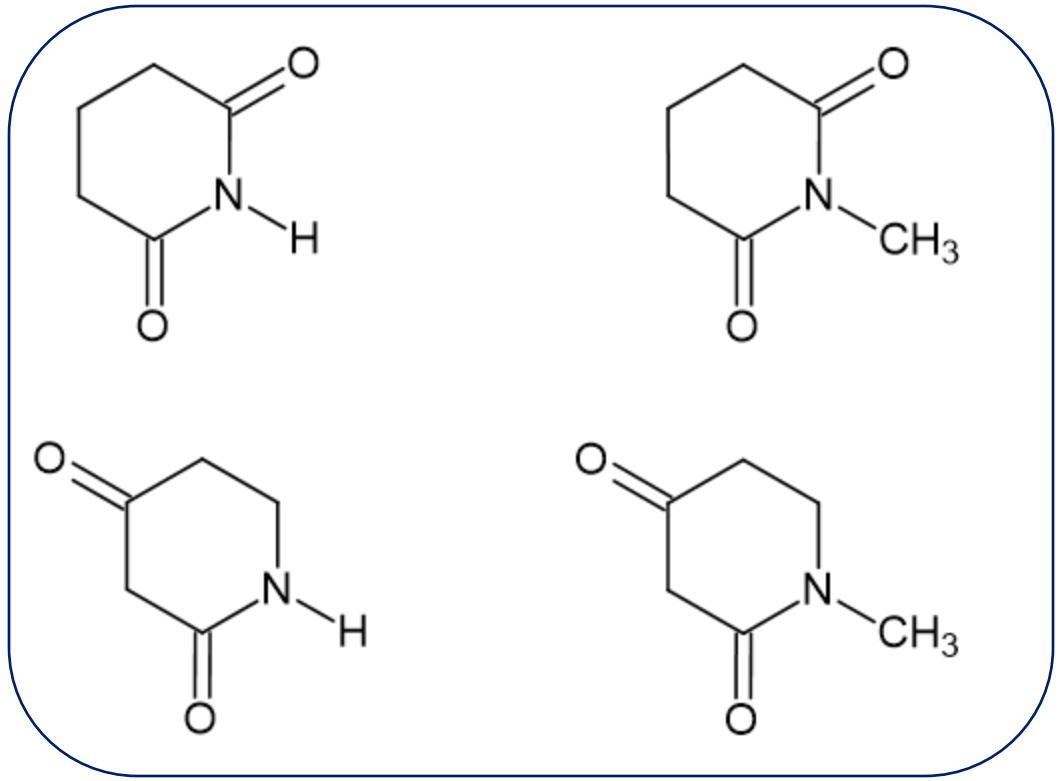


2,6-Piperidinedione









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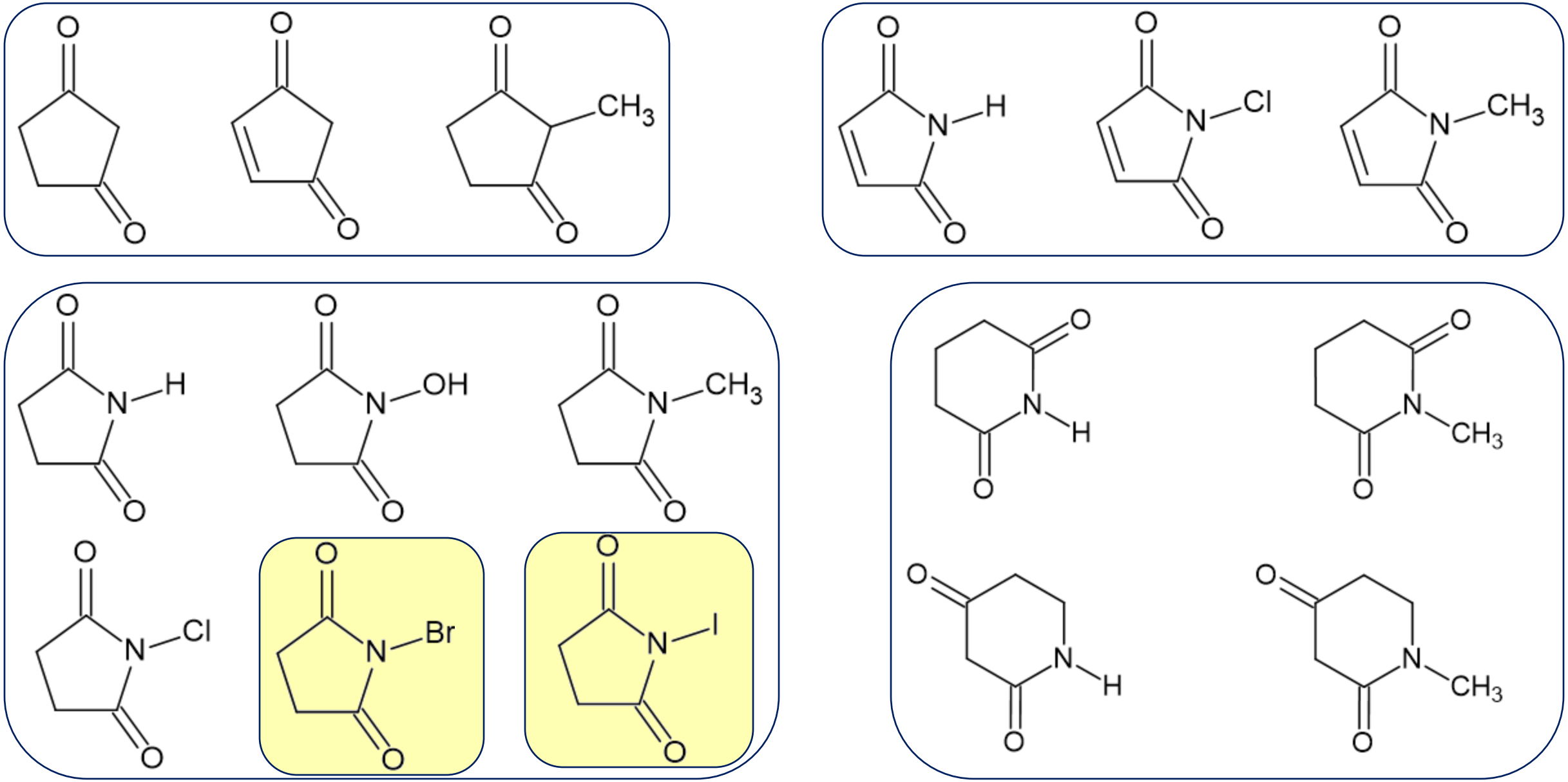

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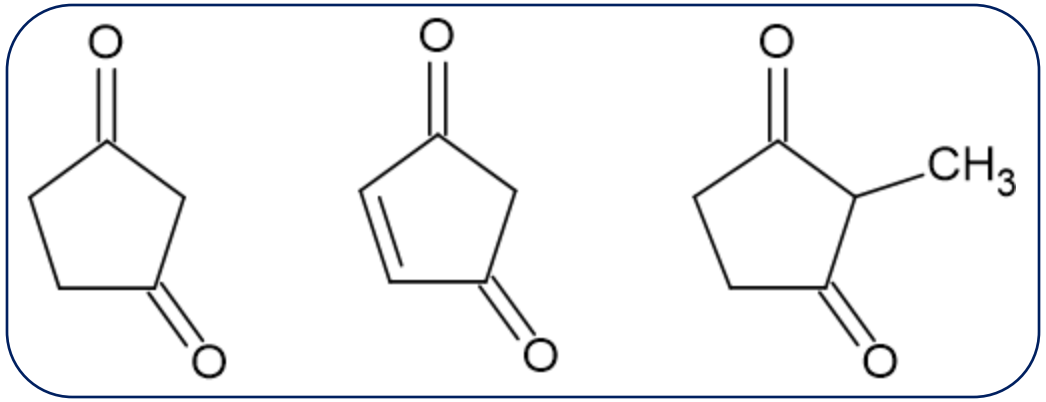

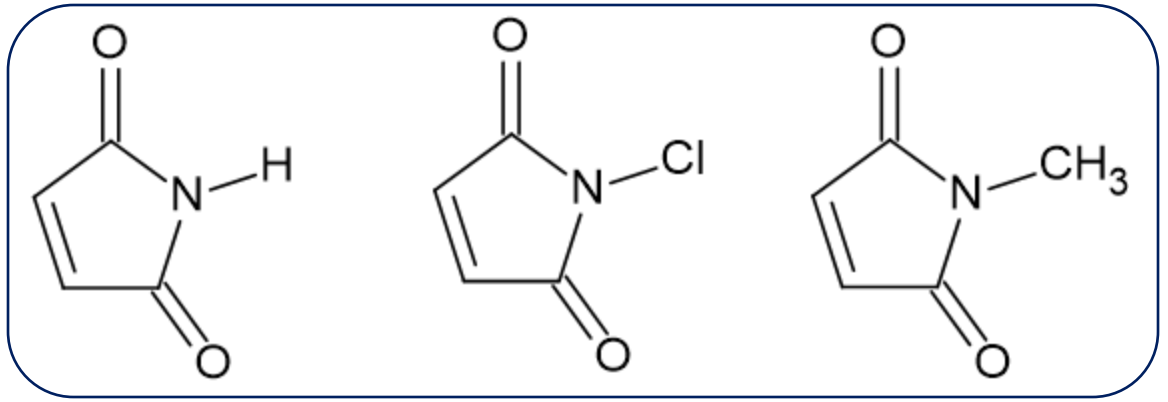

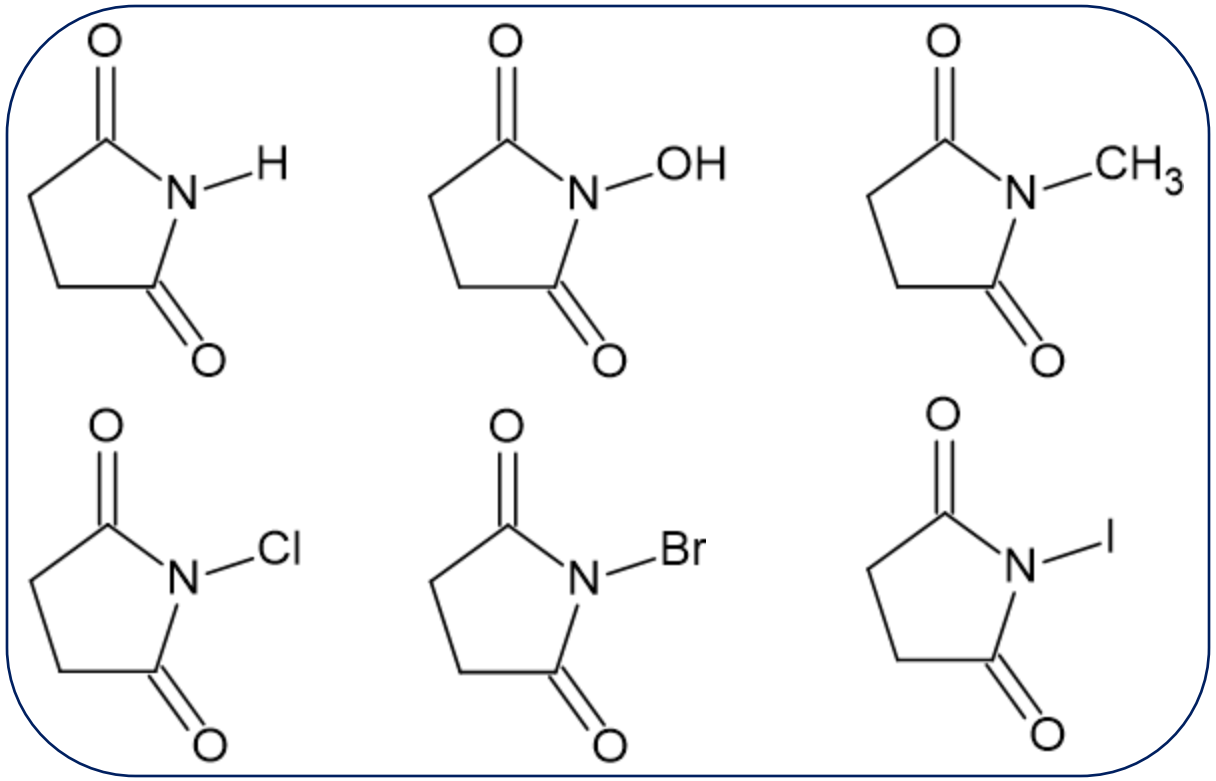

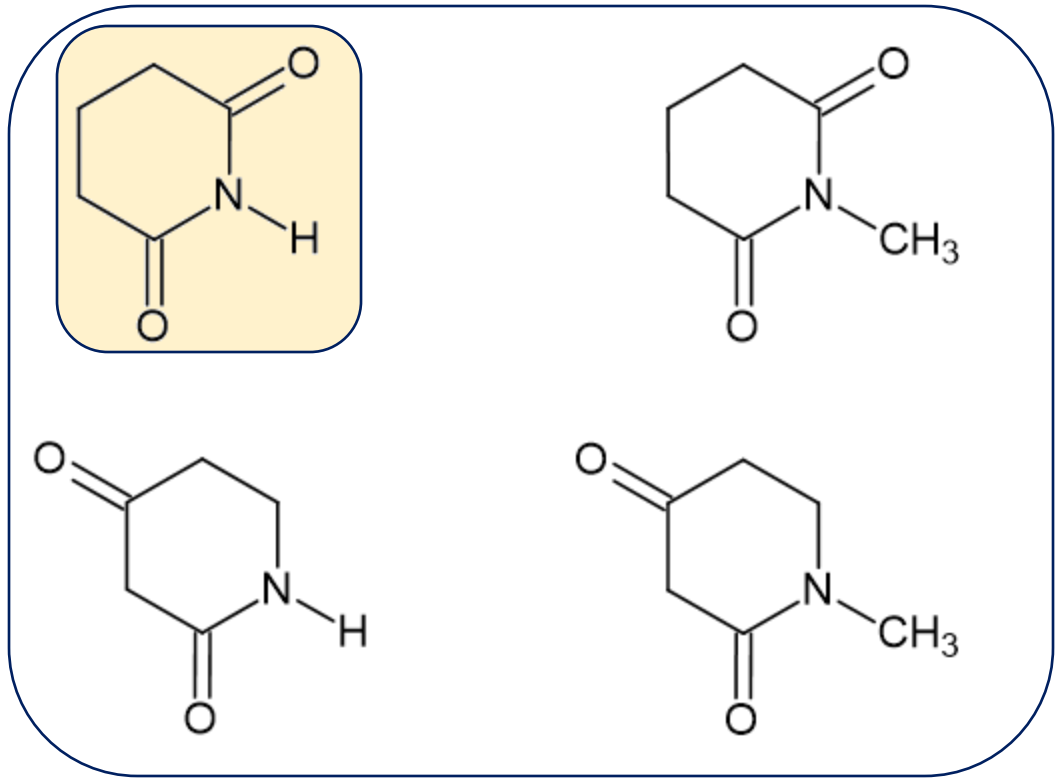

2,6-Piperidinedione

calculated rotational constants

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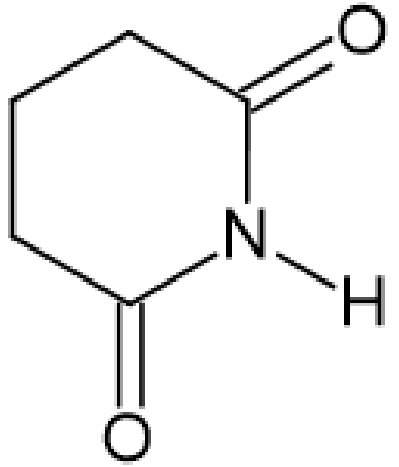
A (MHz)	3354.8
B (MHz)	1941.9
C (MHz)	1283.7
K	-0.36
μ_a (D)	0
μ_b (D)	-3.14
μ_c (D)	0.32
Level of Theory	MP2/cc-pVTZ



2,6-Piperidinedione

experimental rotational spectrum

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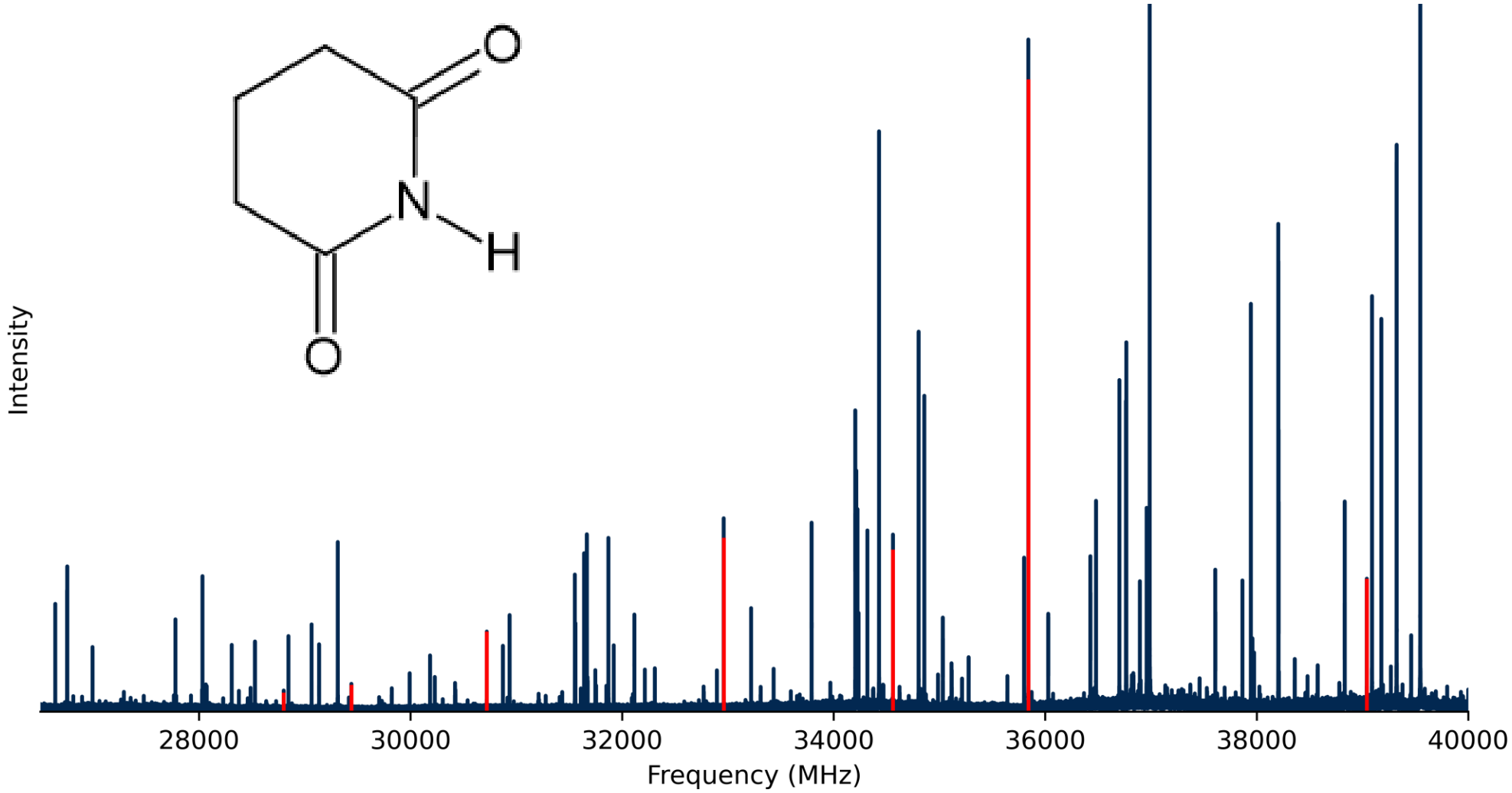

2,6-Piperidinedione

experimental and fitted rotational spectrum

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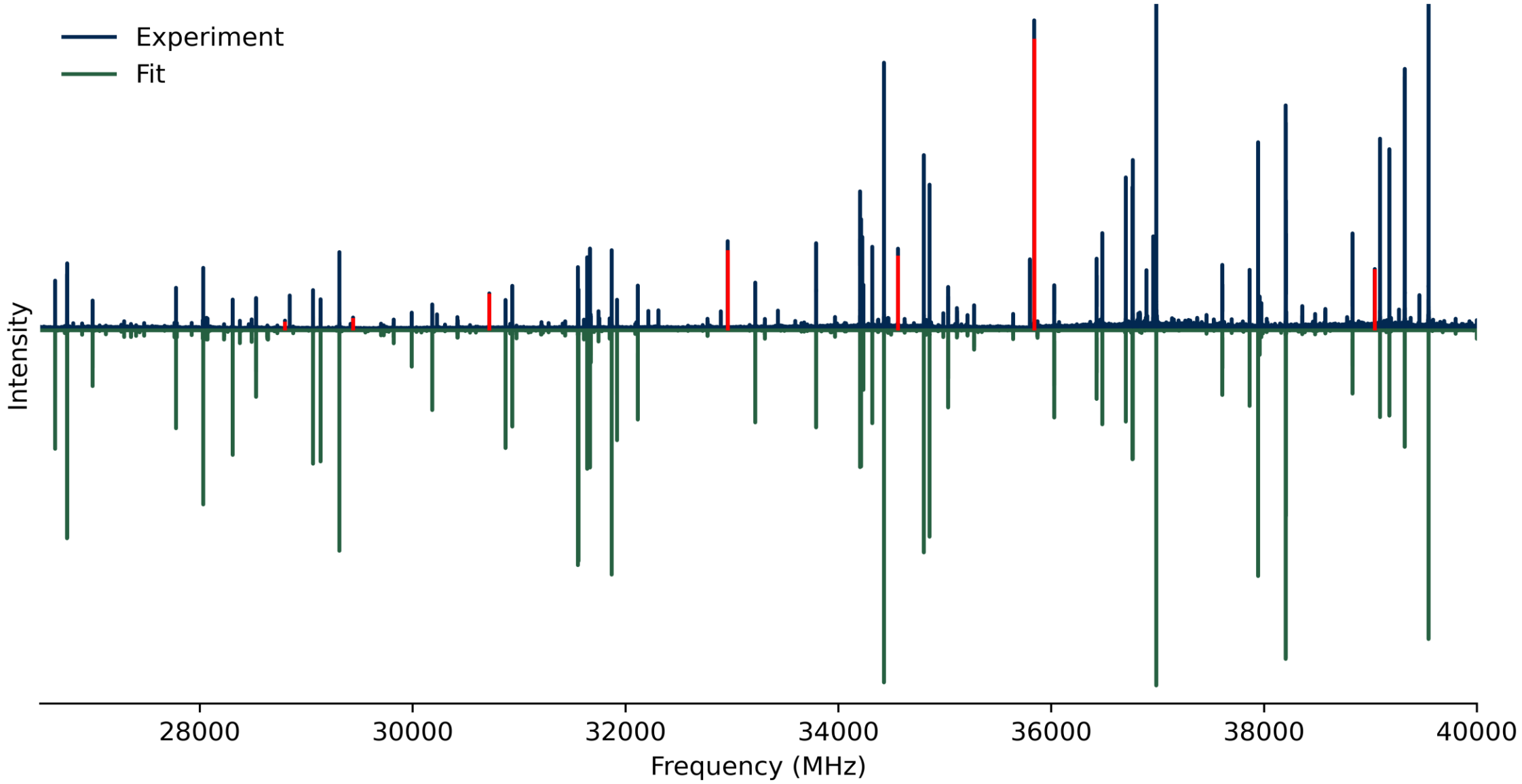

2,6-Piperidinedione

fitted rotational parameters

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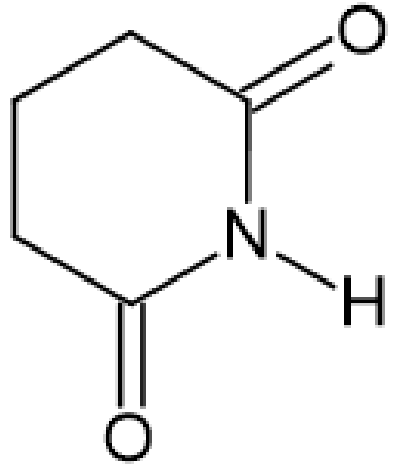
	Fitted	Calculated
A (MHz)	3323.7799(5)	3354.8
B (MHz)	1942.0857(3)	1941.9
C (MHz)	1279.3759(4)	1283.7
χ_{aa} (MHz)	1.73(4)	1.57
$\chi_{bb} - \chi_{cc}$ (MHz)	4.676(32)	4.48
ΔJ (kHz)	0.071(1)	-
ΔK (kHz)	0.317(2)	-
ΔJK (kHz)	0.161(3)	-
δN (kHz)	0.0212(3)	-
δK (kHz)	0.127(2)	-
No. of lines fitted	303	-
RMS (MHz)	0.018154	-



Summary and Conclusion

cyclopentanediones, succinimdes, maleimides, piperidinediones

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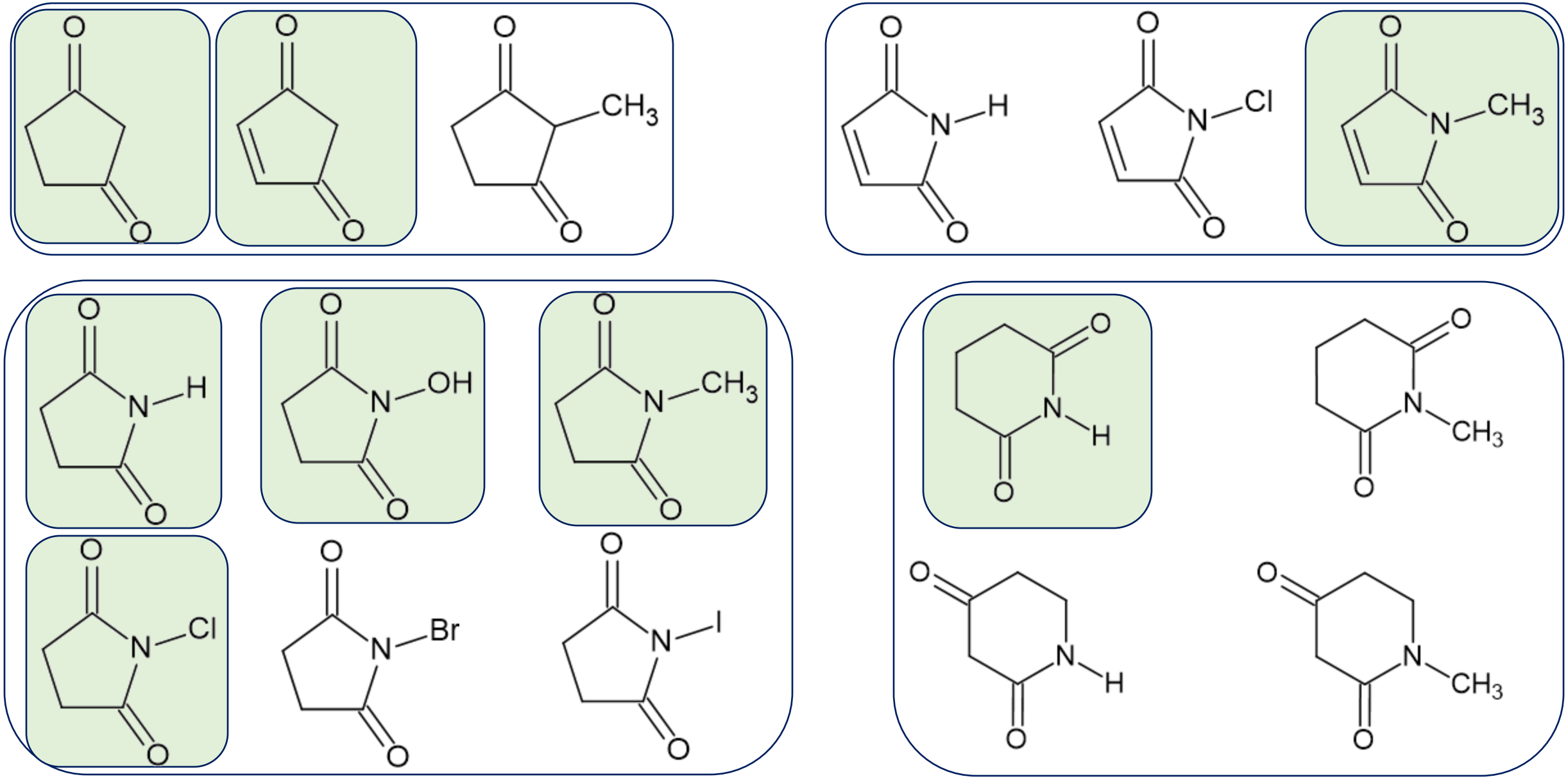

Summary and Conclusion

cyclopentanediones, succinimdes, maleimides, piperidinediones

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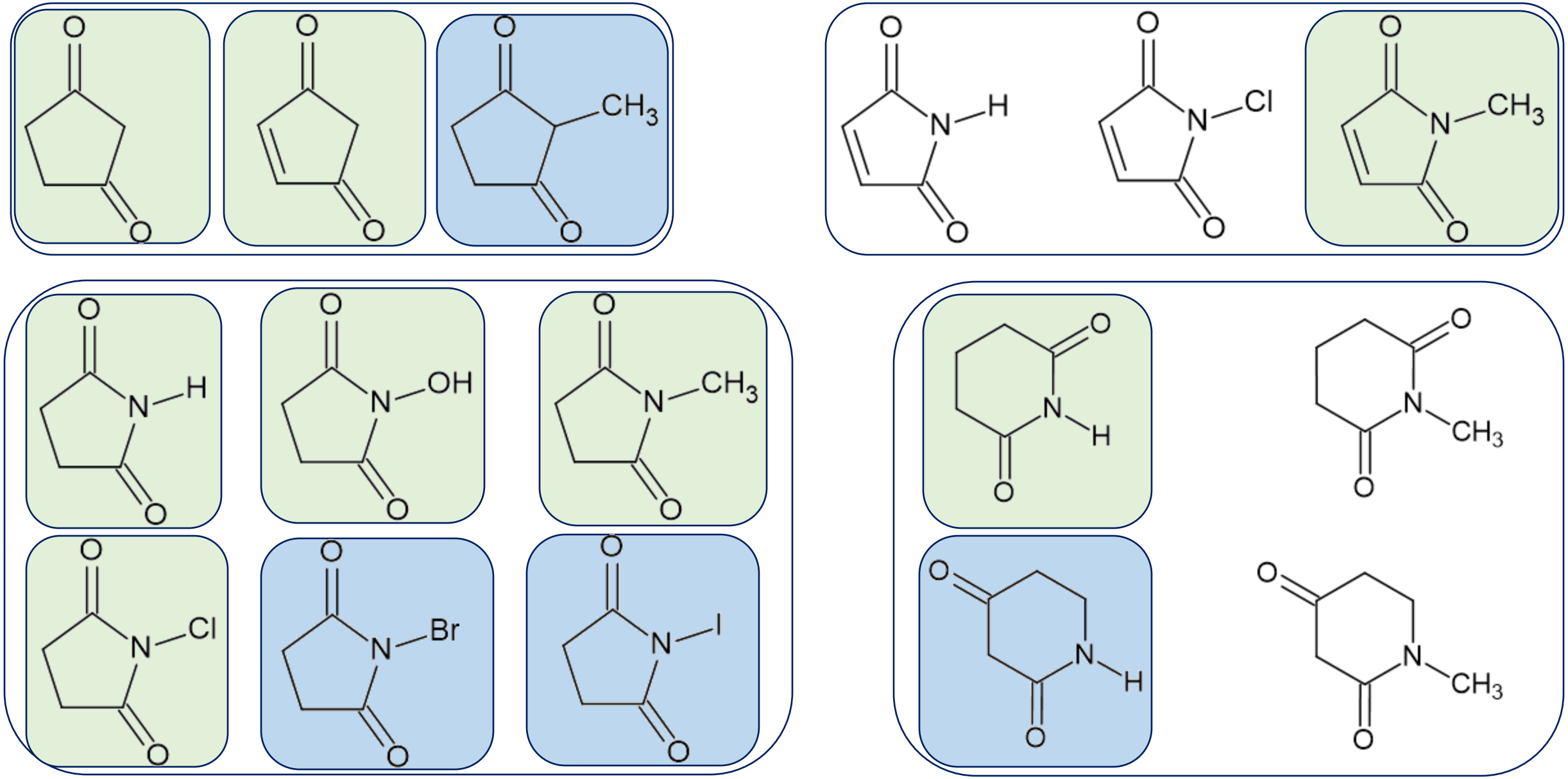

Summary and Conclusion

cyclopentanediones, succinimdes, maleimides, piperidinediones

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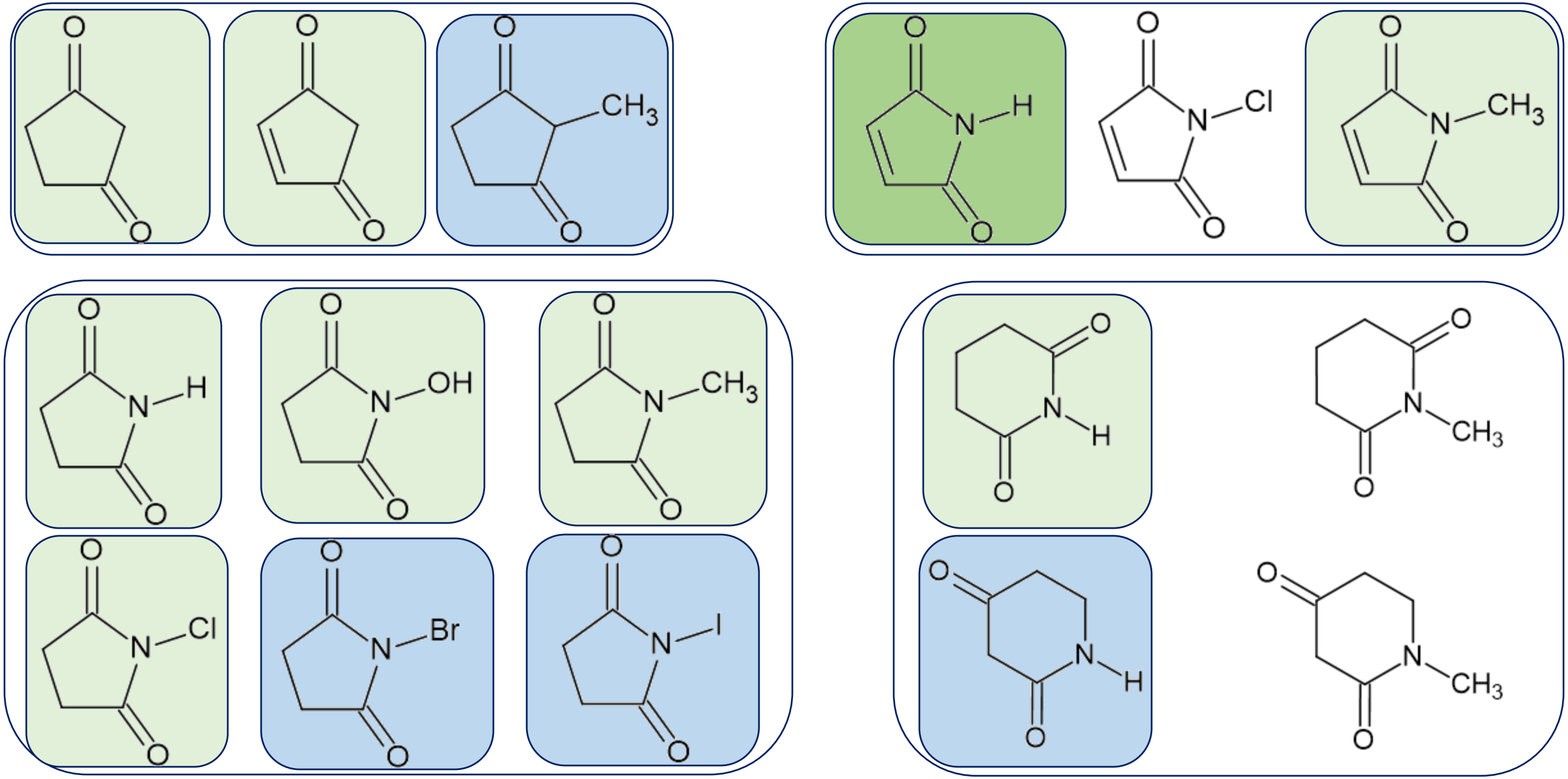

Summary and Conclusion

cyclopentanediones, succinimdes, maleimides, piperidinediones

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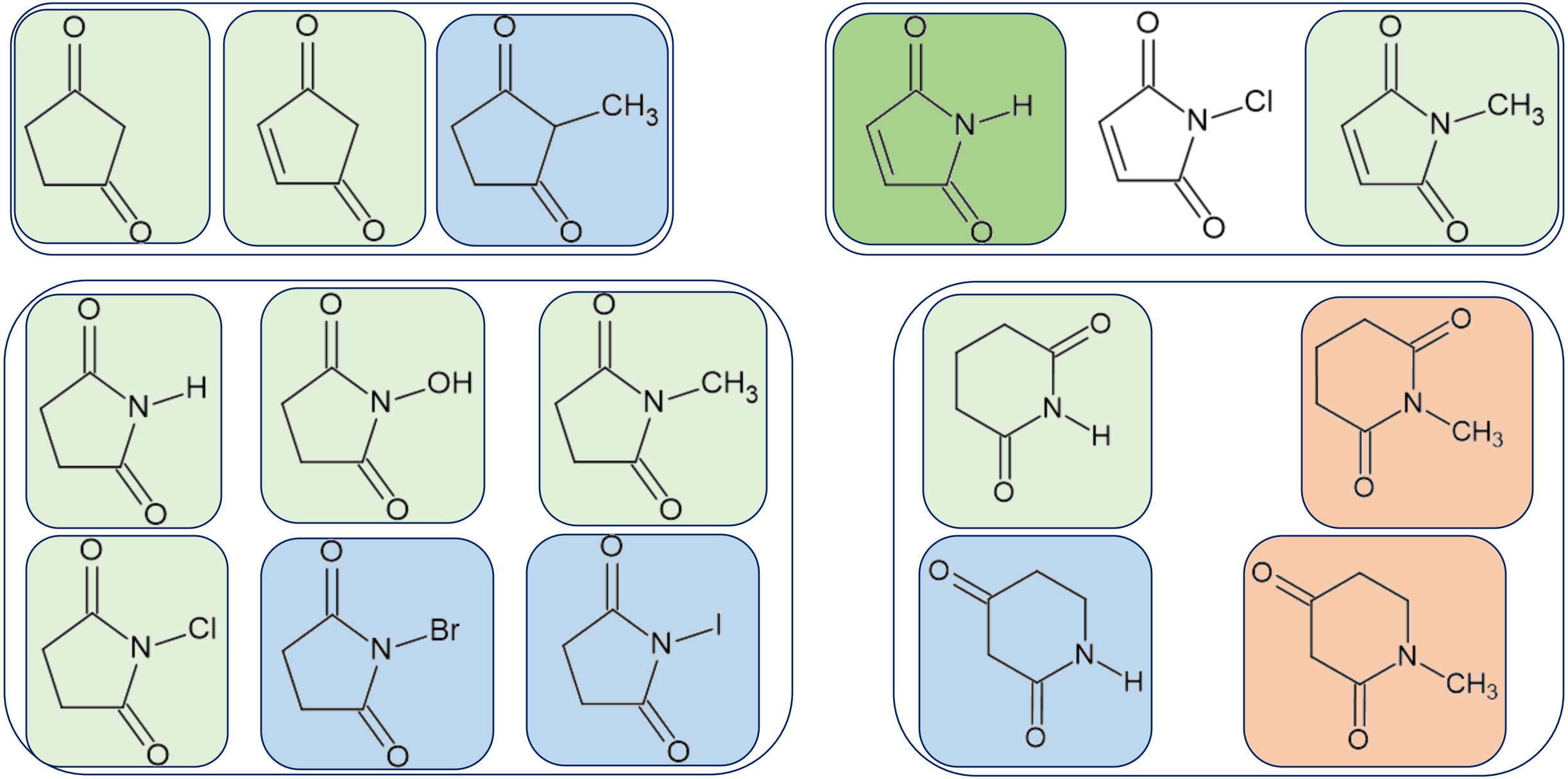

Summary and Conclusion

cyclopentanediones, succinimdes, maleimides, piperidinediones

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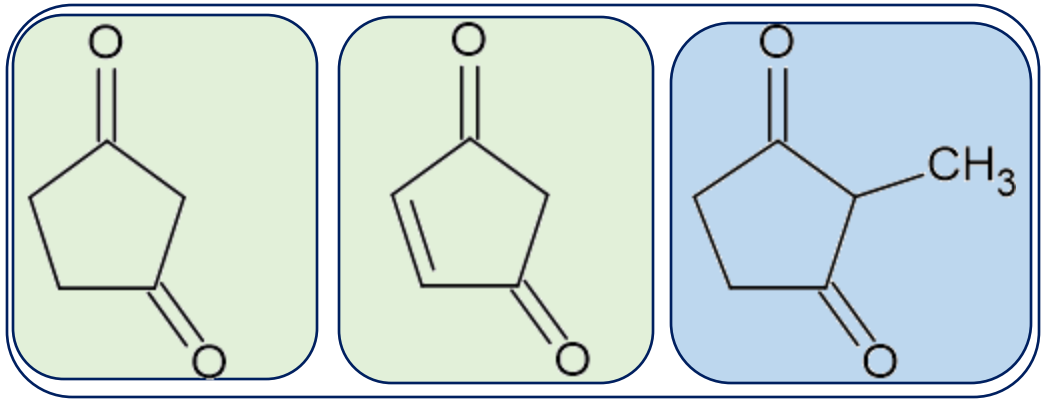

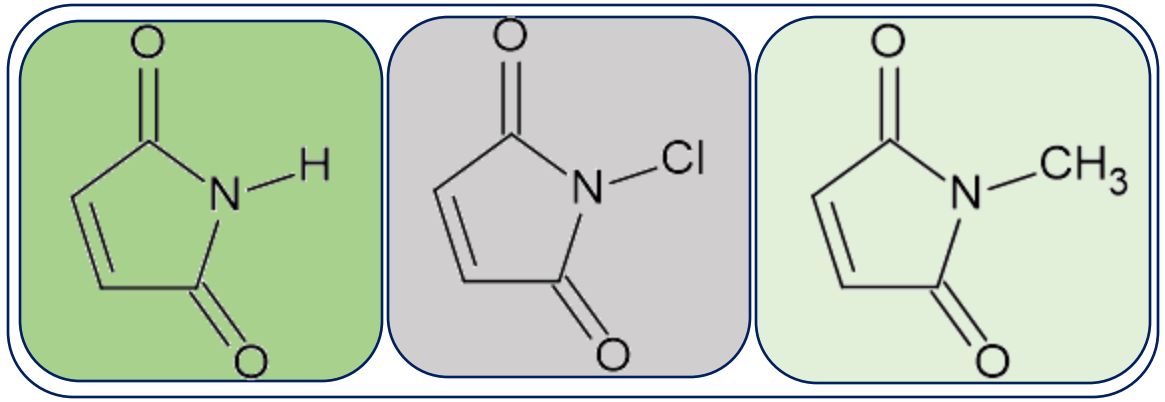

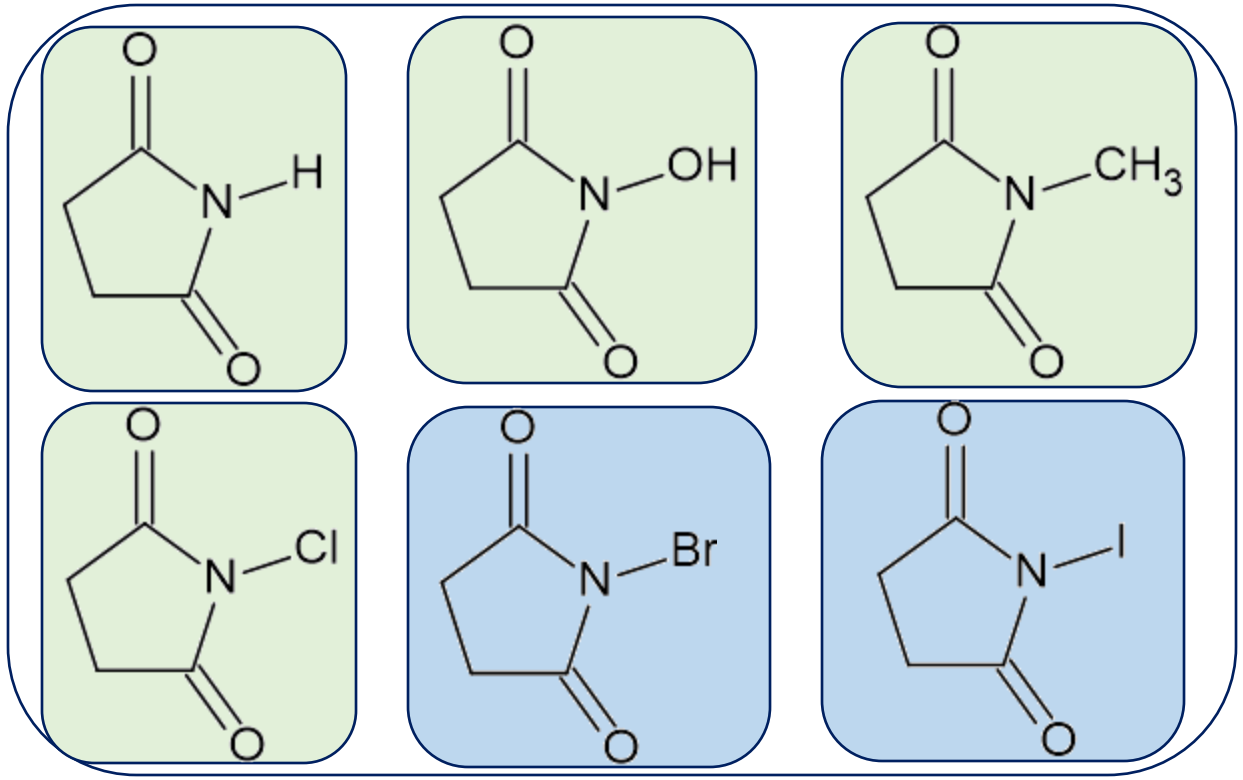

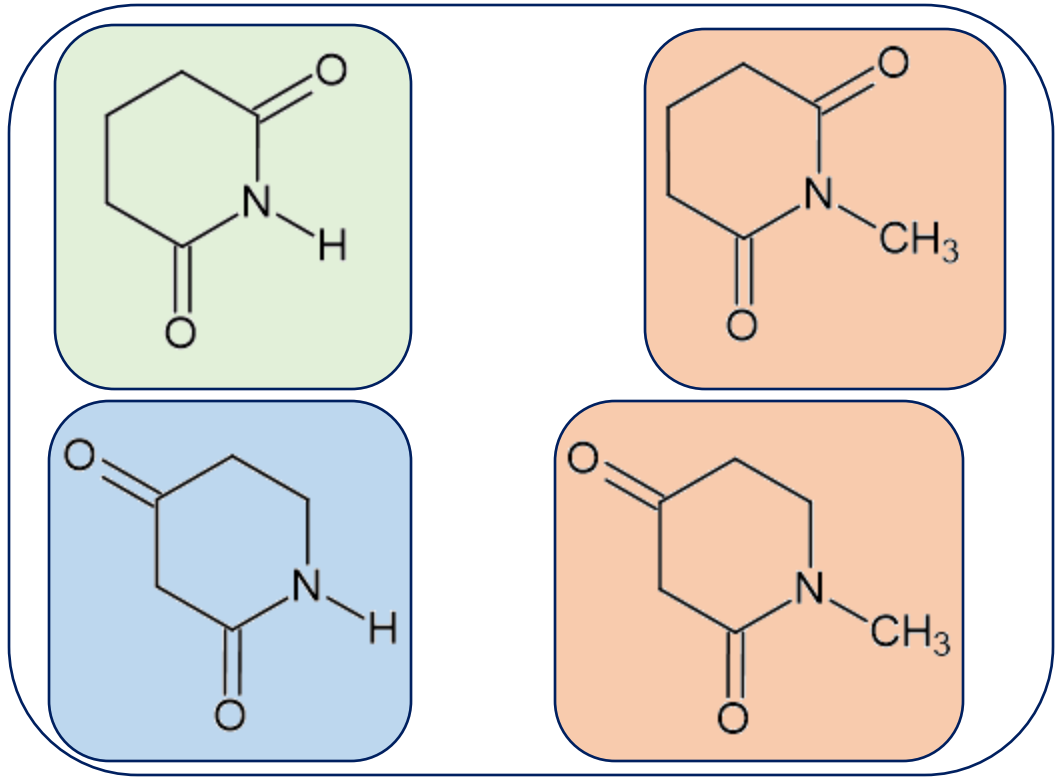

Acknowledgements

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