Supporting Information

For

Synthesis of pentacycloundecane (PCUD) based spiro-pyrano-cage framework via ring-closing metathesis

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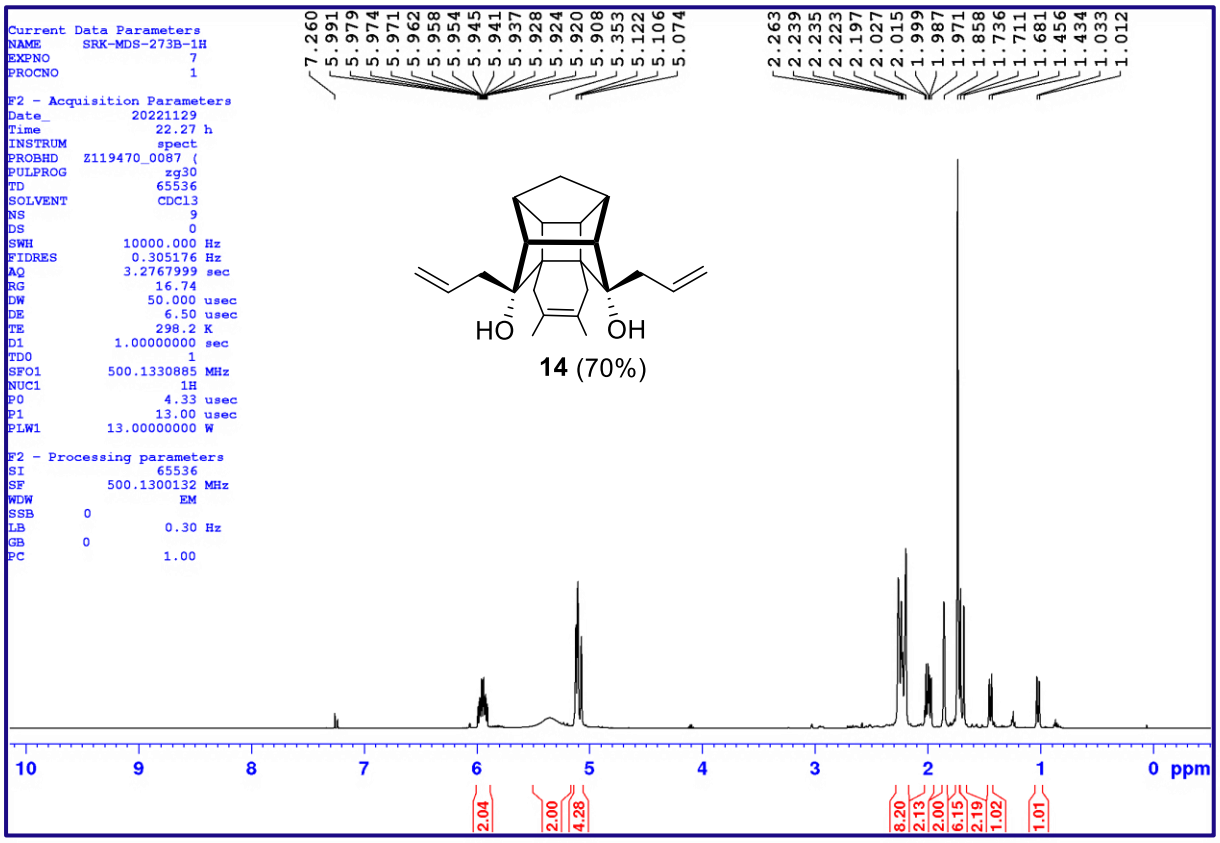
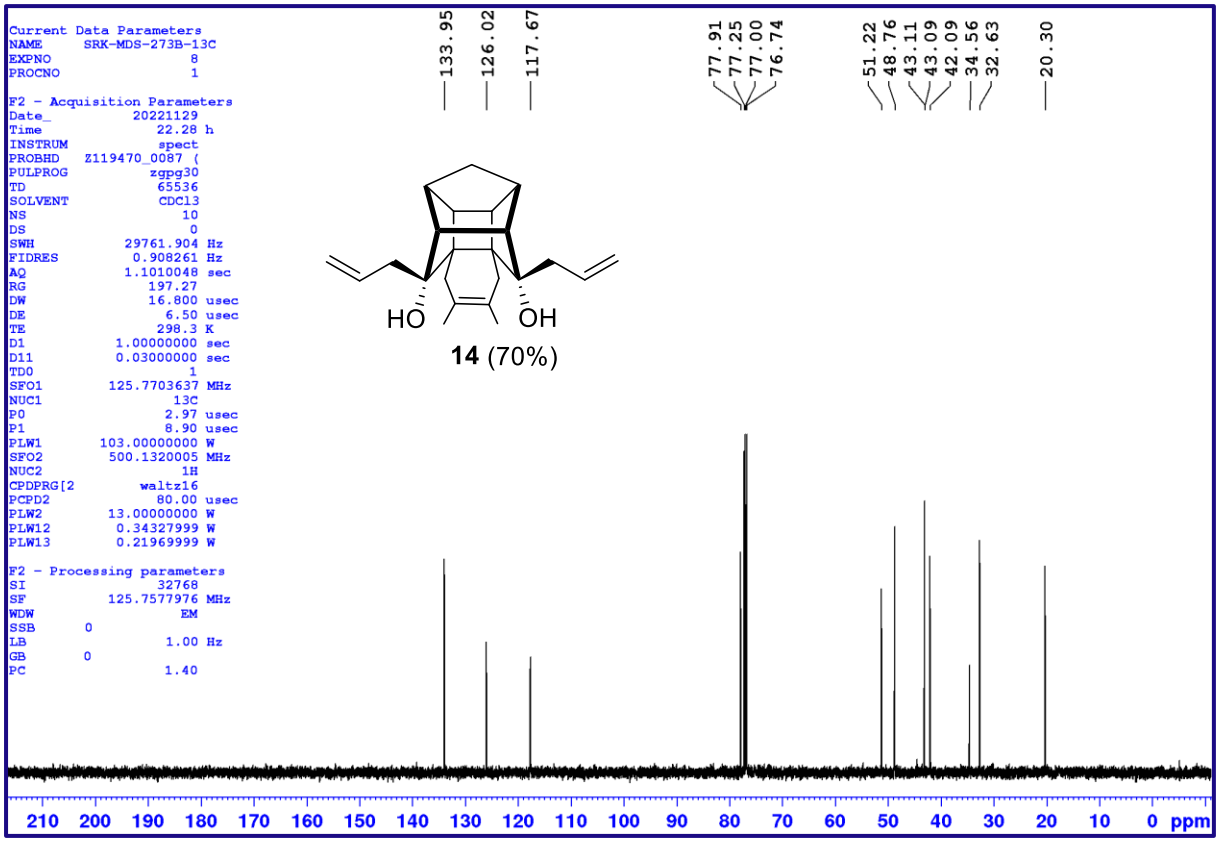
Table of Contents

^{1}H NMR of Compound 14 (500 MHz, $CDCl_3$)



^{13}C NMR of Compound 14 (125 MHz, $CDCl_3$)



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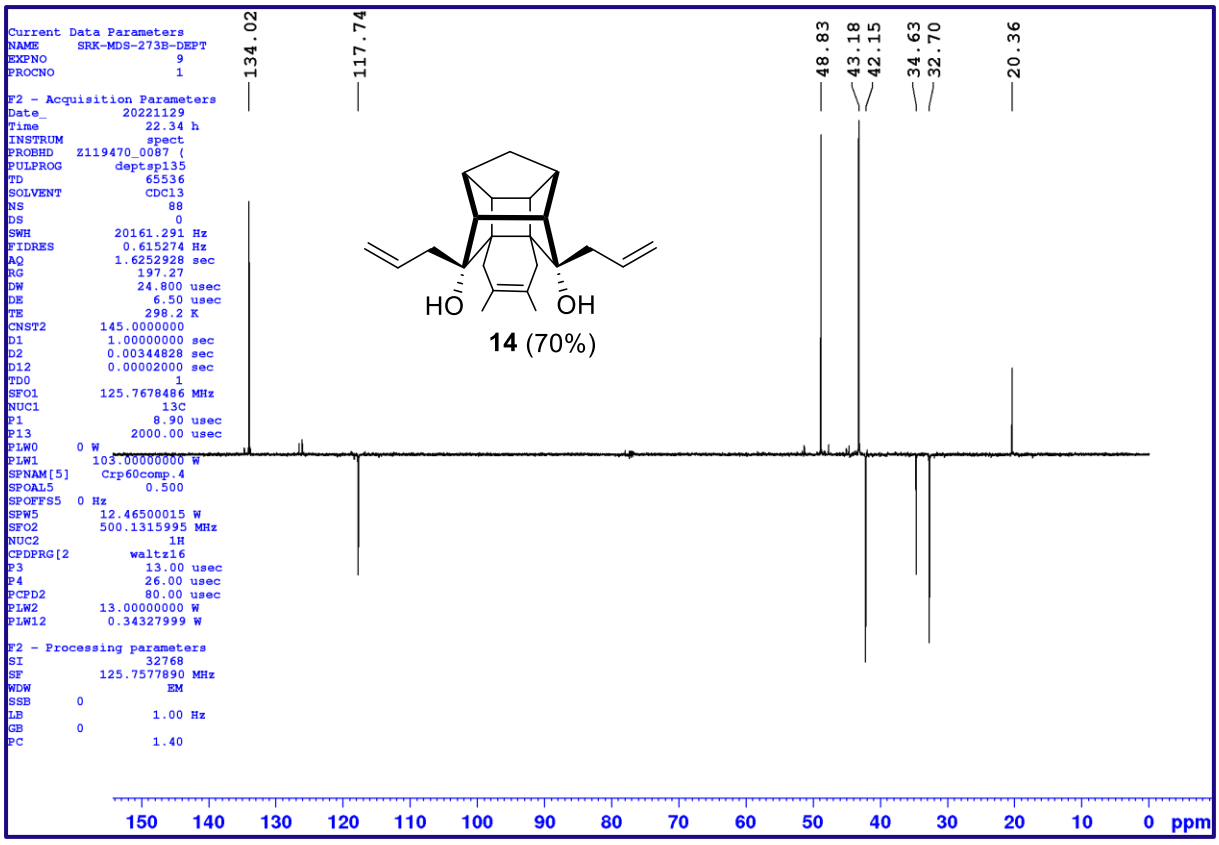

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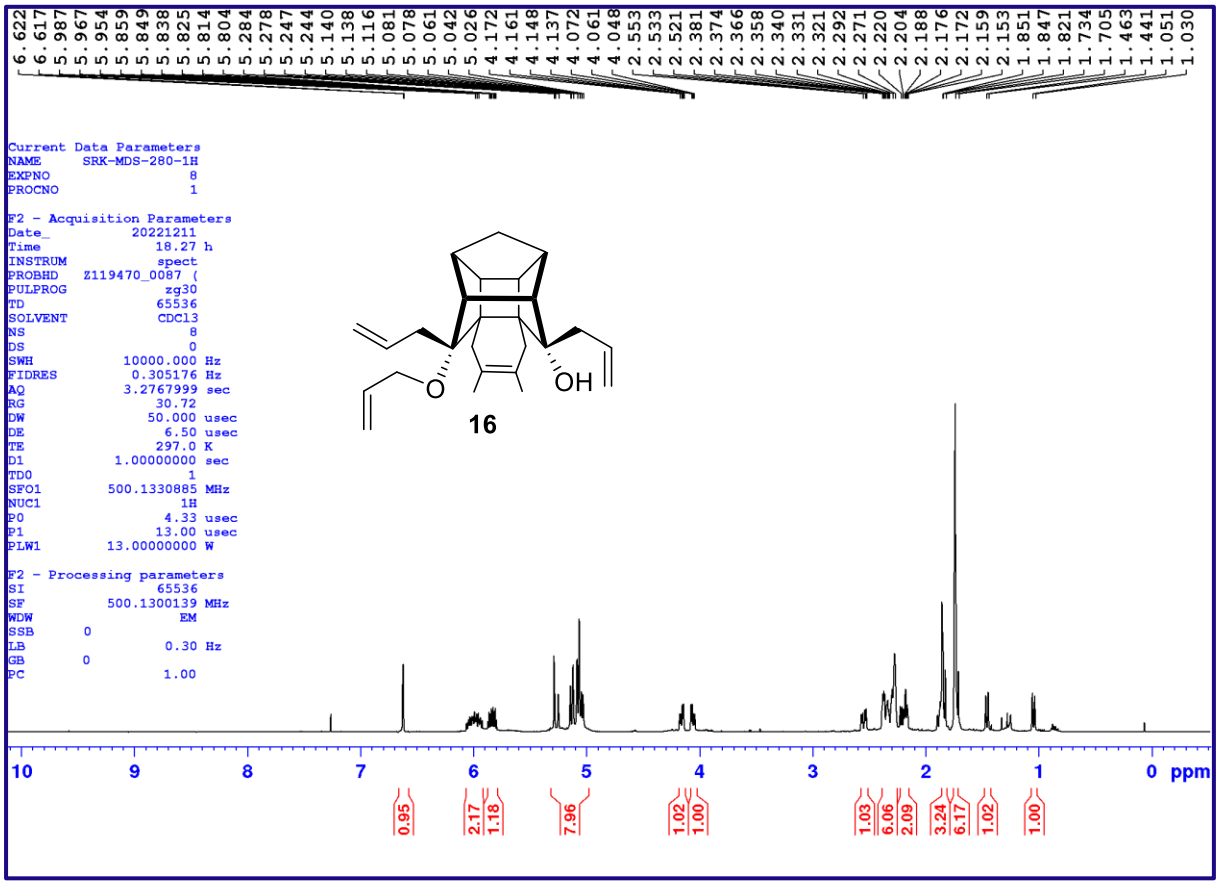

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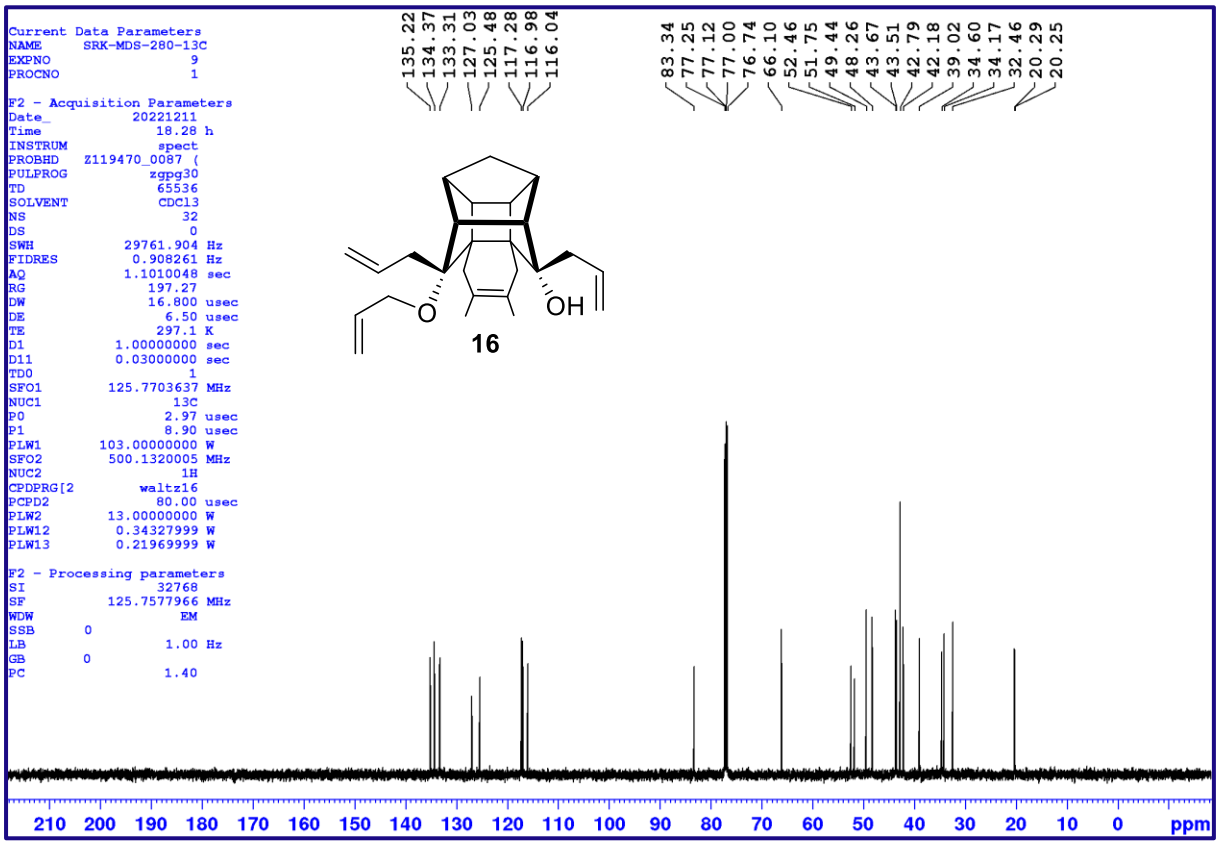

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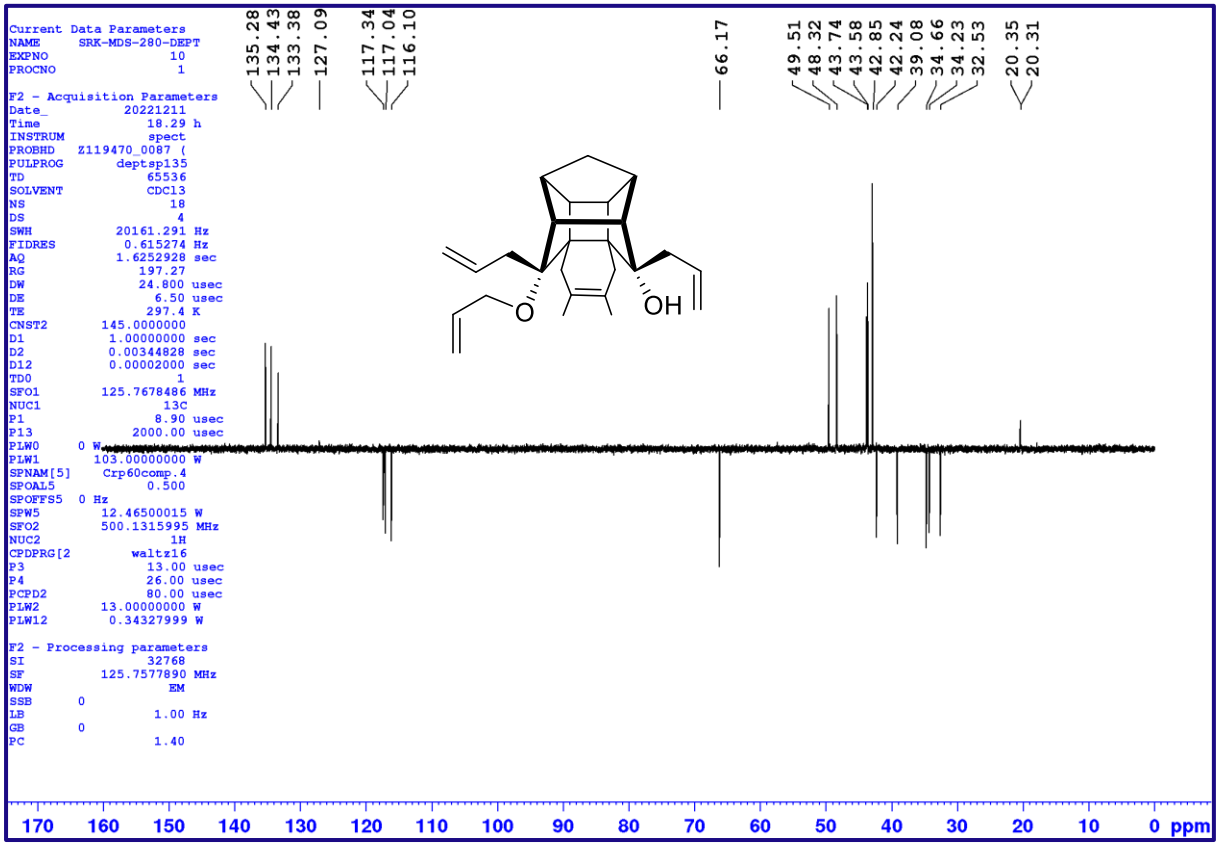

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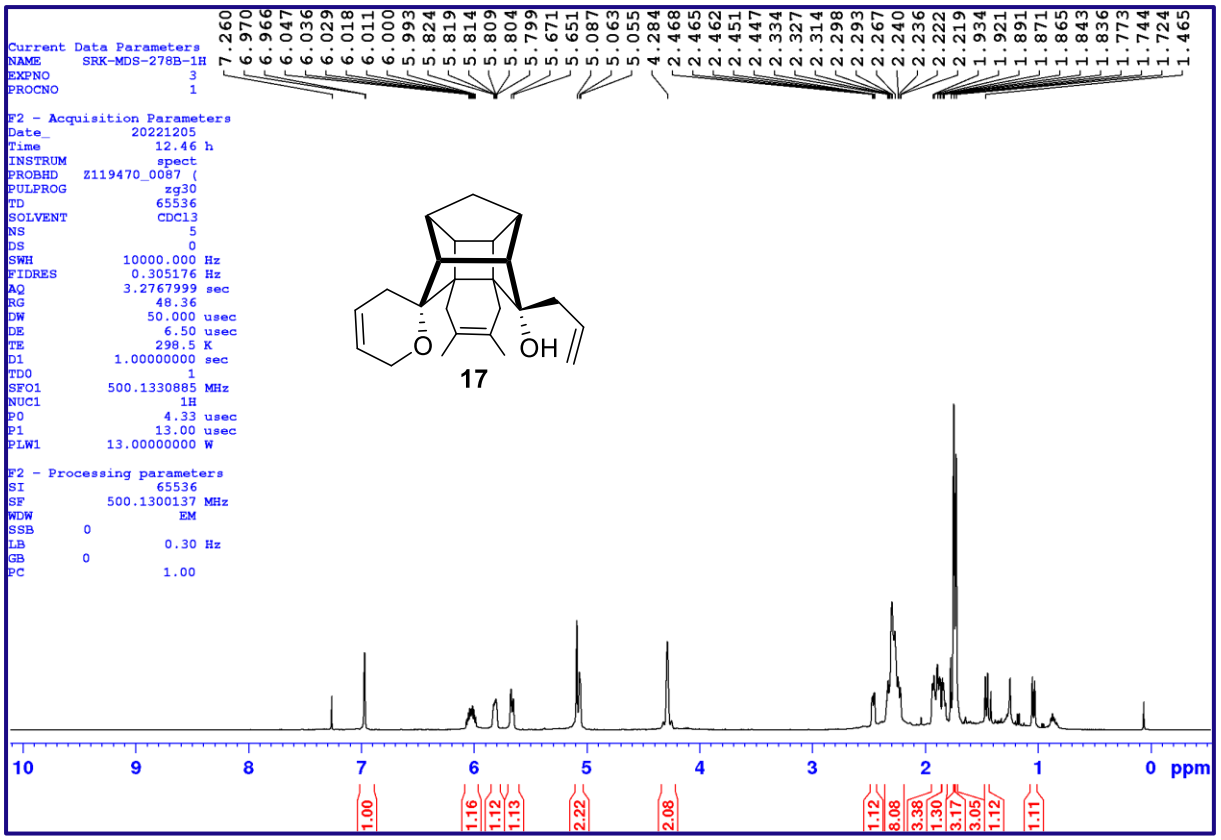

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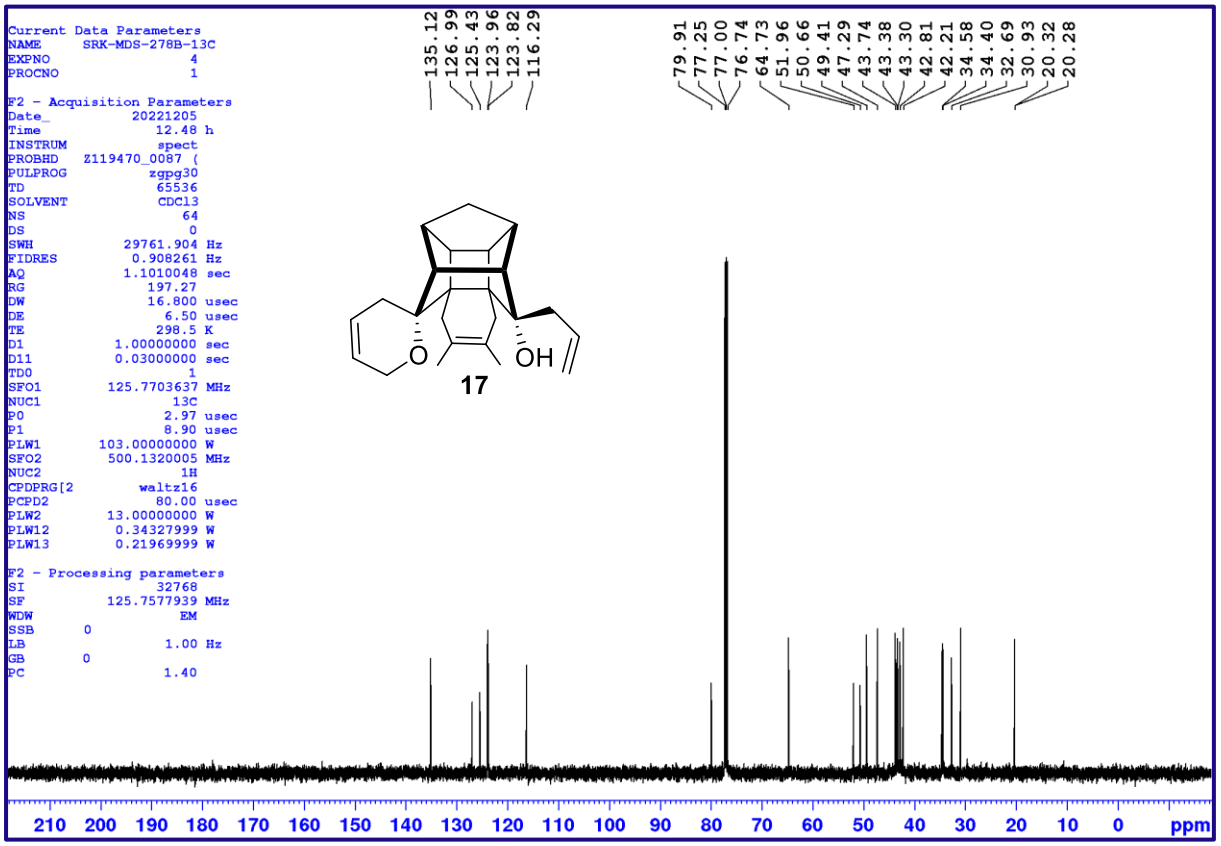

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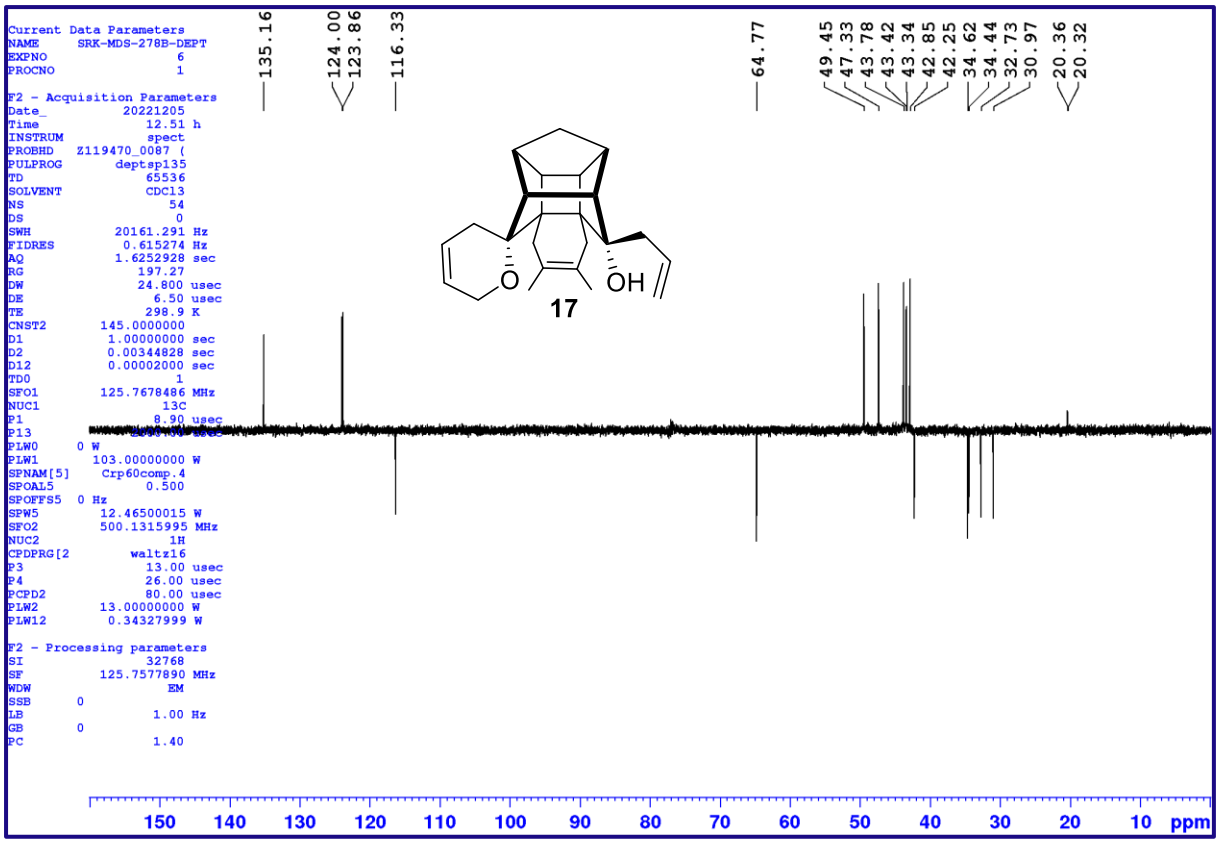

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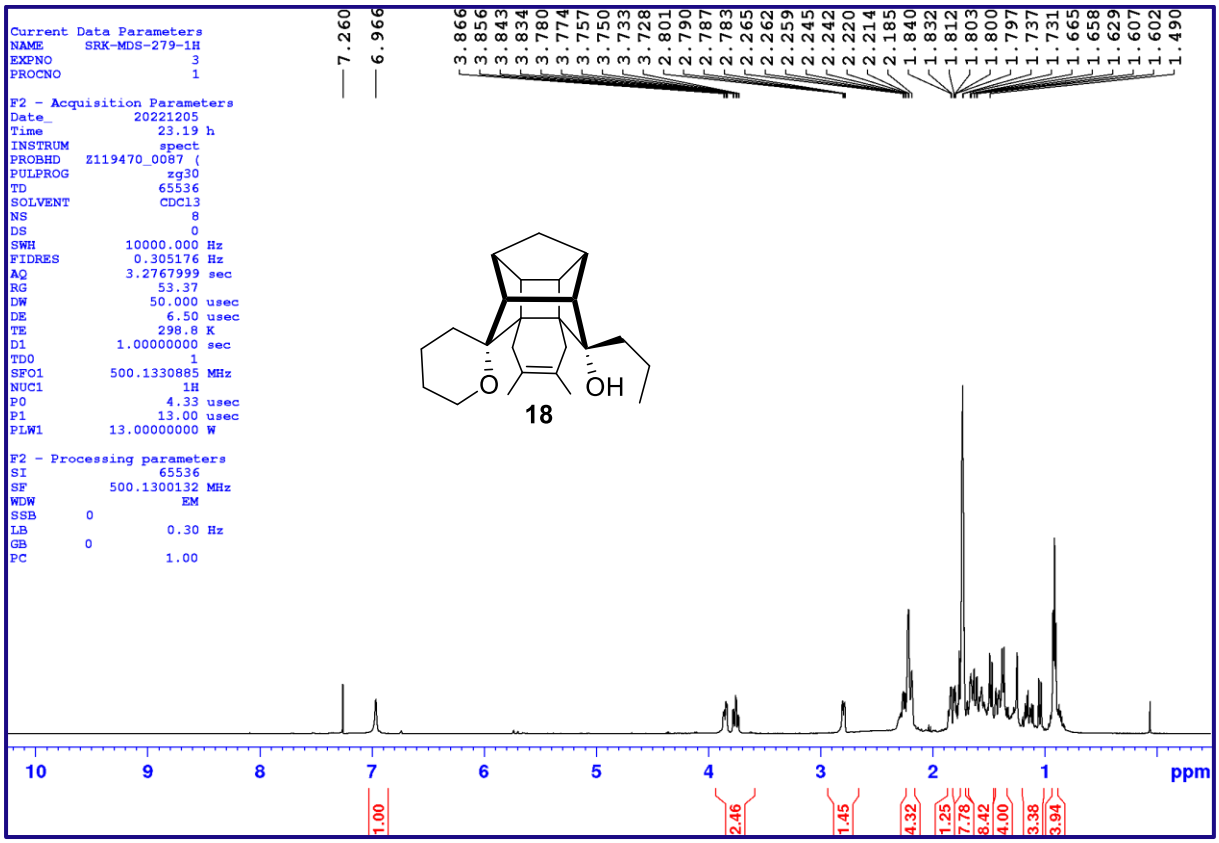

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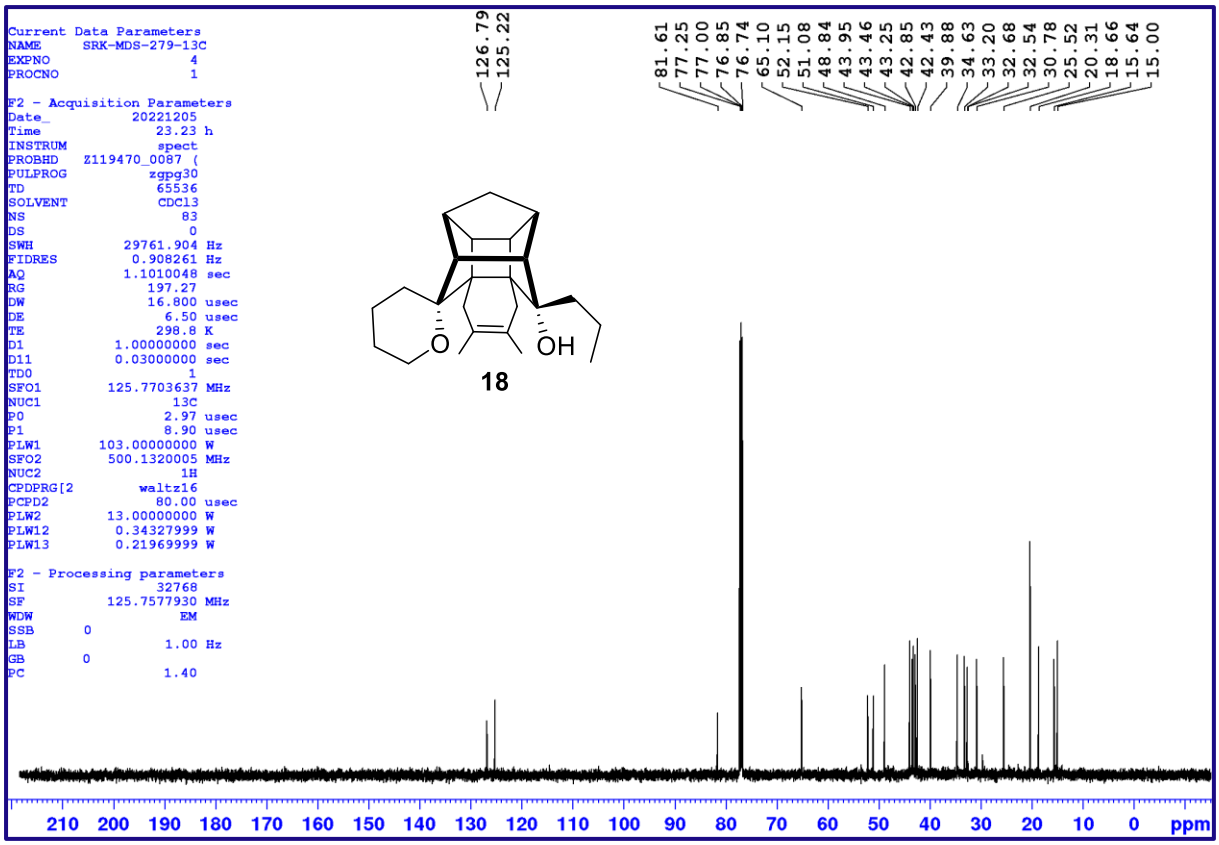

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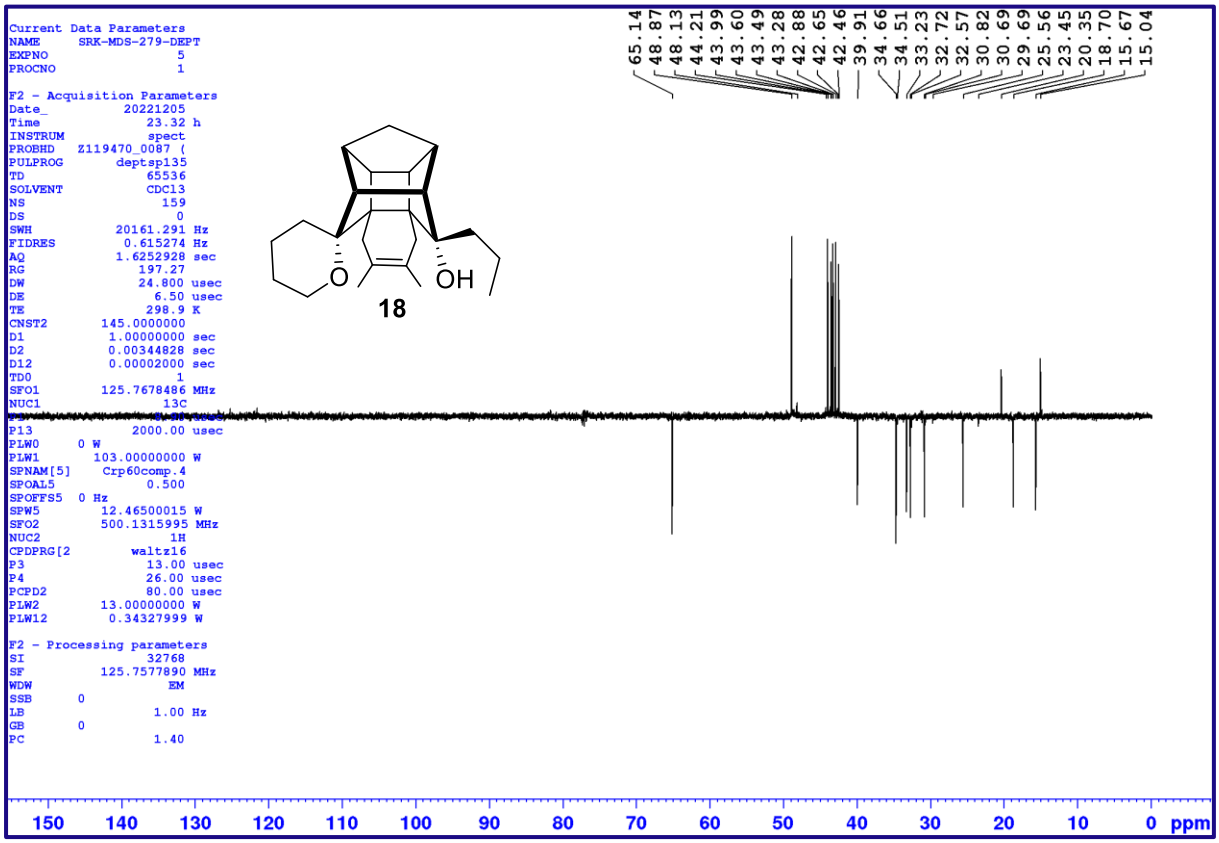

HRMS of Compound 14

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

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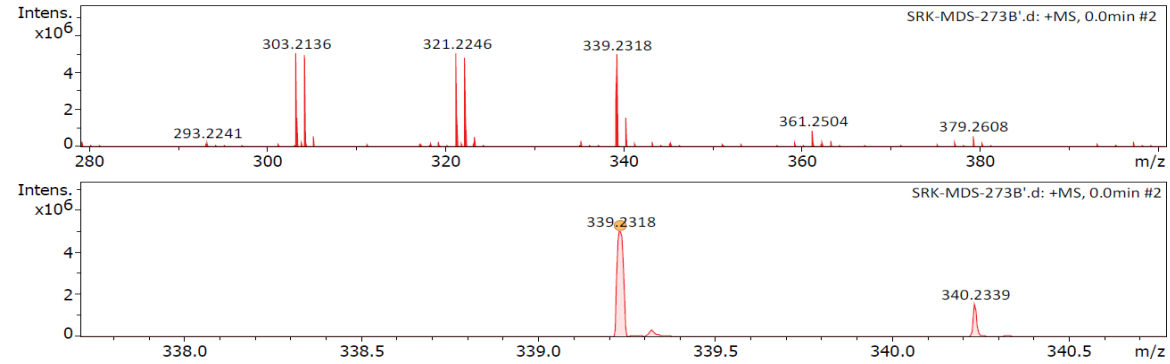
Method	Naformat_pos_50-600.m	Operator	SRK-IN
Sample Name	SRK-MDS-273B'	Instrument	maXis impact 282001.00081
Comment	C23H30O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	650 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
339.2318	1	C23H31O2	339.2319	0.2	33.5	1	100.00	9.0	even	ok

HRMS of Compound 15

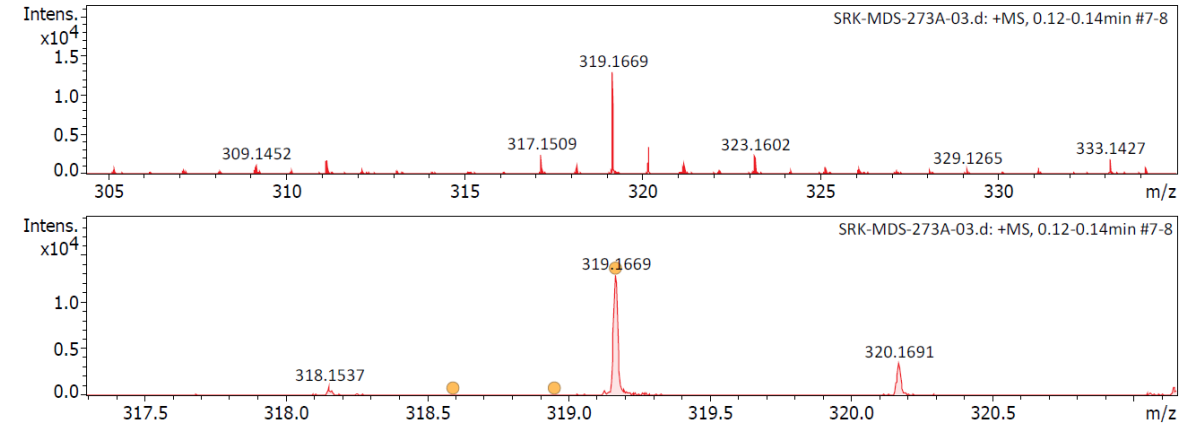
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\DEC-2022\SRK-MDS-273A-03.d	Acquisition Date	12/23/2022 8:54:16 PM
Method	Naformat_pos_50-600.m	Operator	PPI
Sample Name	SRK-MDS-273A-03	Instrument	maXis impact 282001.00081
Comment	C20H27O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	650 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
319.1669	1	C20H24NaO2	319.1669	-0.0	48.1	1	100.00	9.0	even	ok

HRMS of Compound 16

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\DEC-2022\SRK-MDS-280'.d	Acquisition Date	12/16/2022 1:30:30 PM
Method	Naformat_pos_50-600.m	Operator	SRK-IN
Sample Name	SRK-MDS-280'	Instrument	maXis impact 282001.00081
Comment	C26H34O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
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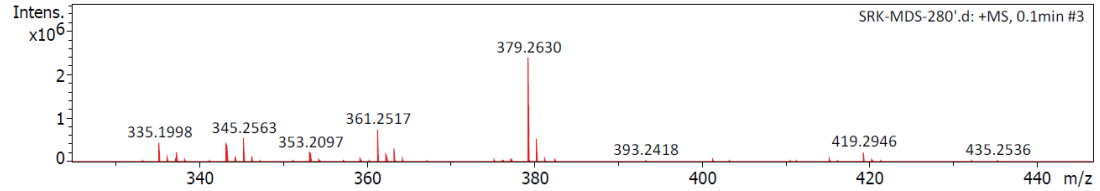
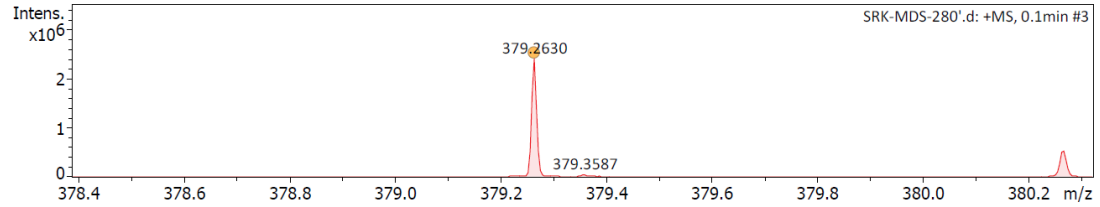
Scan End	650 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
379.2630	1	C26H35O2	379.2632	0.4	38.5	1	100.00	10.0	even	ok

HRMS of Compound 17

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\DEC-2022\SRK-MDS-278'.d	Acquisition Date	12/20/2022 12:54:10 PM
Method	Naformat_pos_50-600.m	Operator	SRK-IN
Sample Name	SRK-MDS-278'	Instrument	maXis impact 282001.00081
Comment	C24H30O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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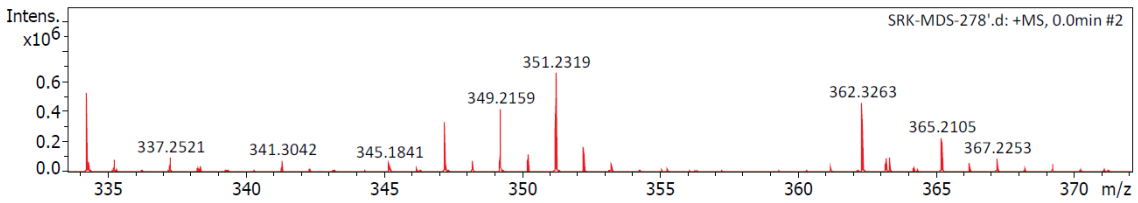
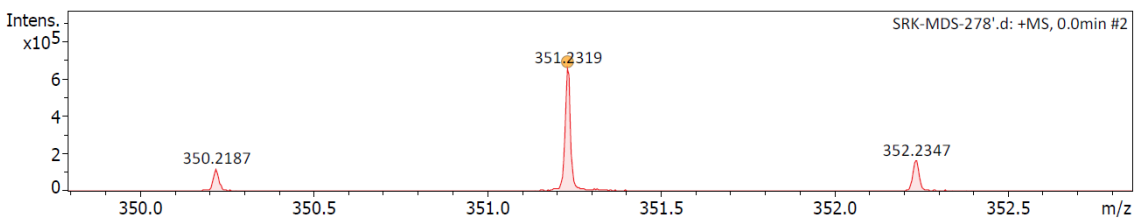
Scan End	650 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
351.2319	1	C24H31O2	351.2319	-0.1	24.0	1	100.00	10.0	even	ok

HRMS of Compound 18

DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

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Method	Naformat_pos_50-600.m	Operator	SRK-IN
Sample Name	SRK-MDS-279	Instrument	maXis impact 282001.00081
Comment	C24H34O2		

Acquisition Parameter

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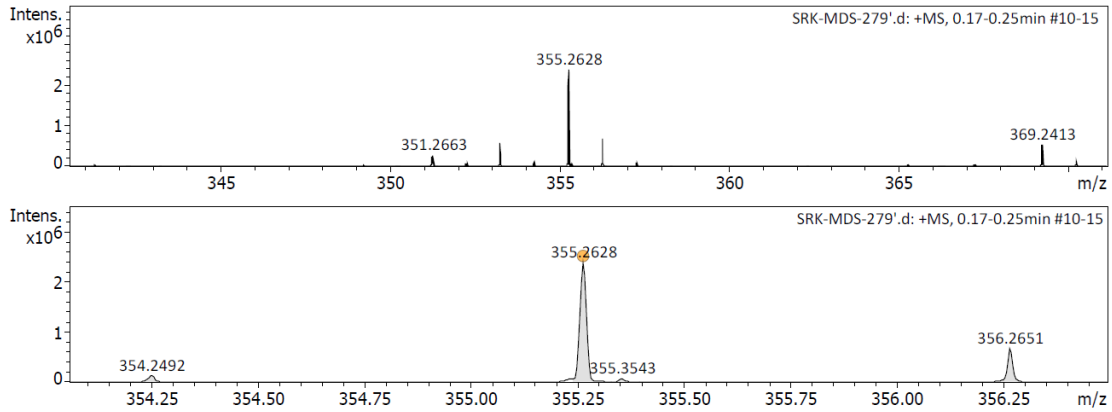
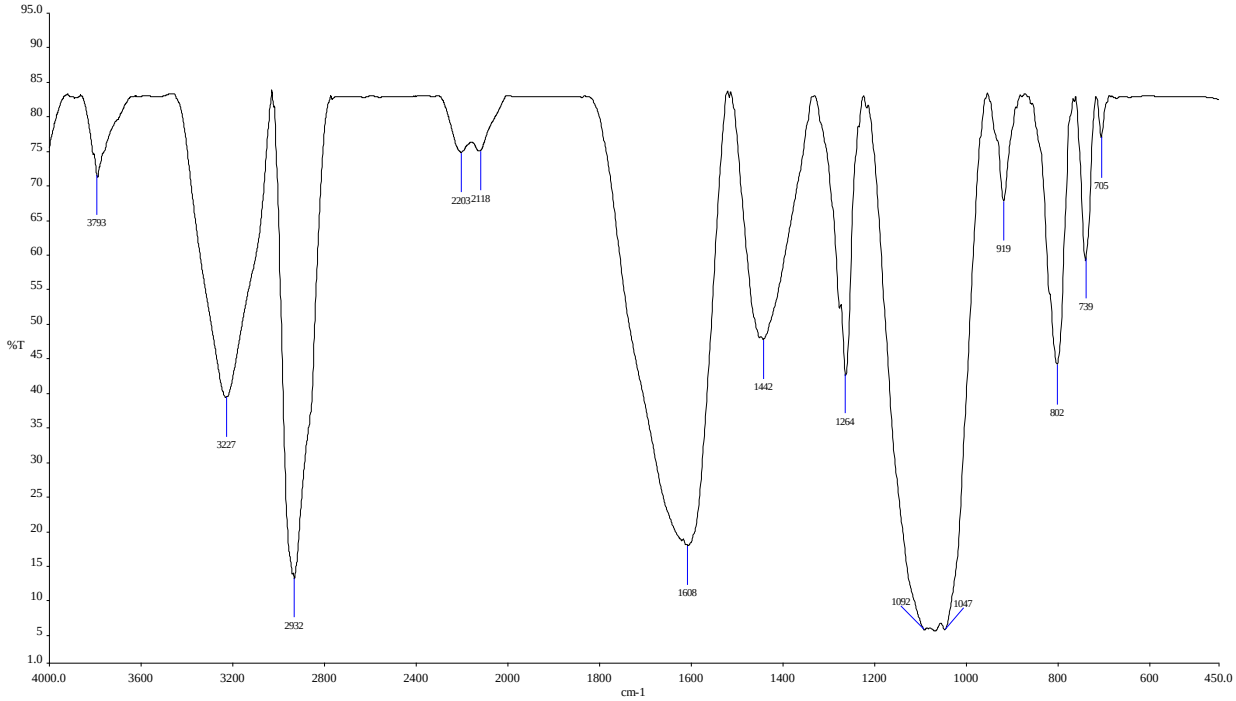
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	650 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

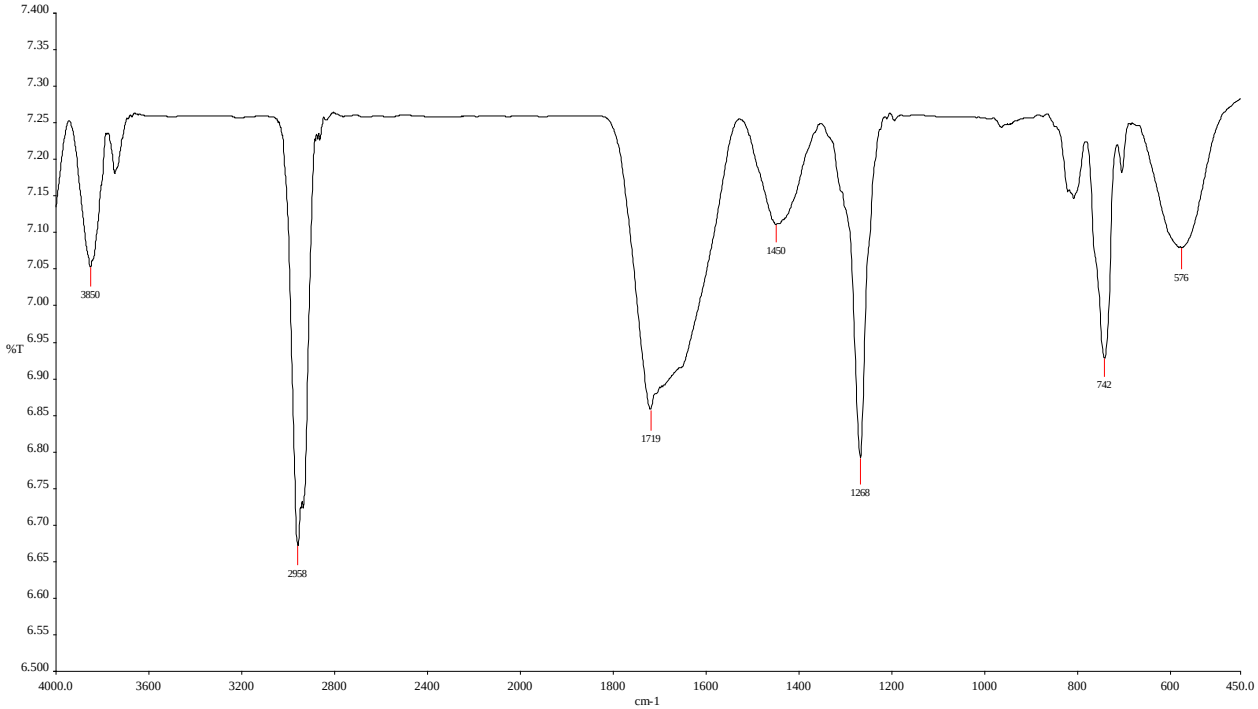


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
355.2628	1	C24H35O2	355.2632	1.0	9.6	1	100.00	8.0	even	ok

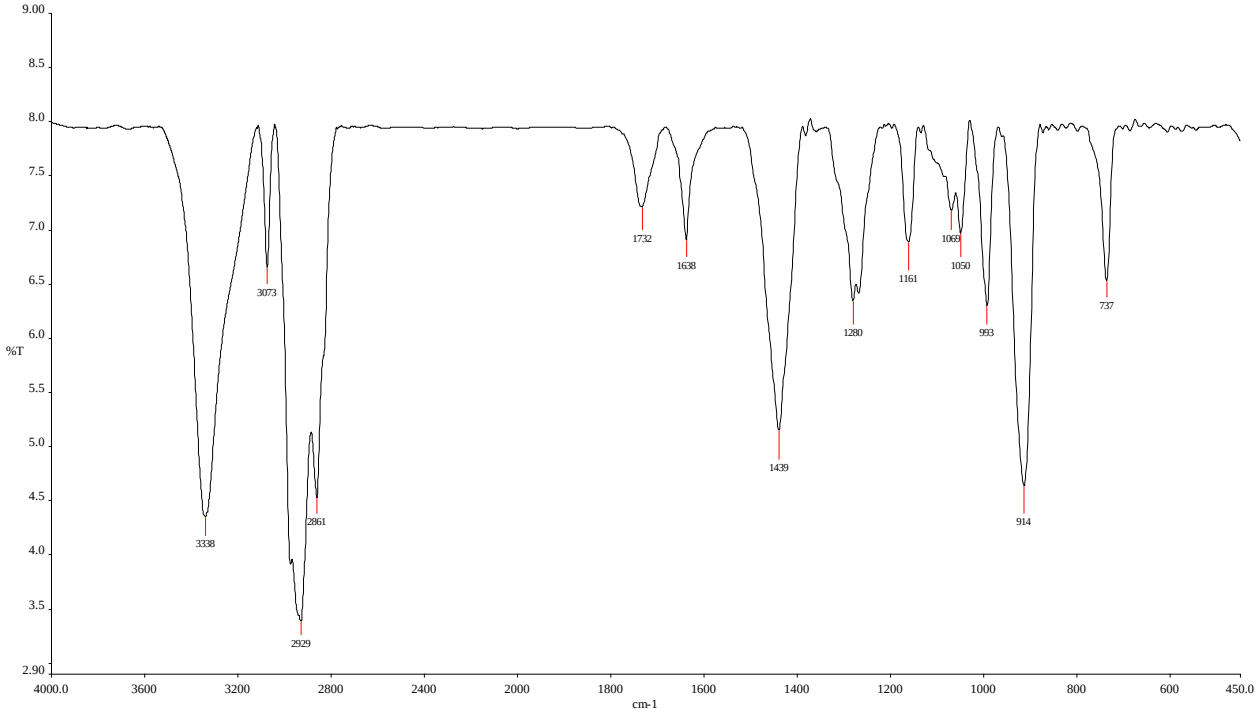
IR spectra of compound 14



IR spectra of compound 15



IR spectra of compound 16



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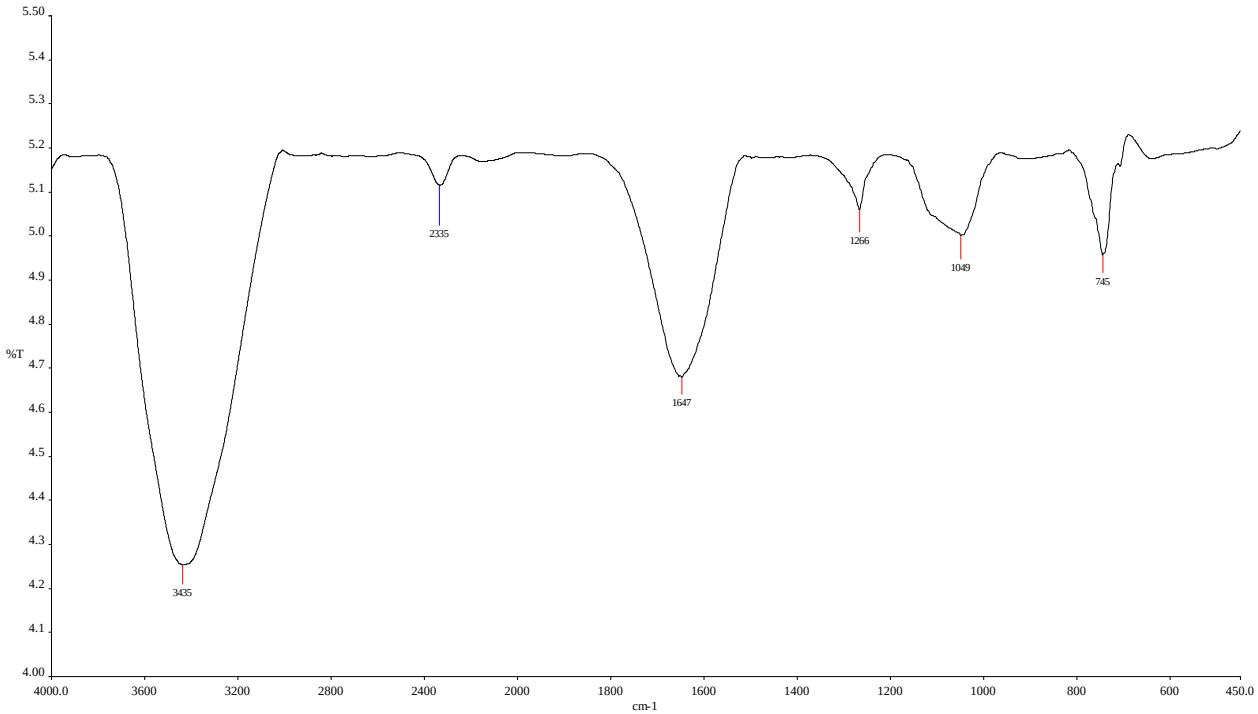

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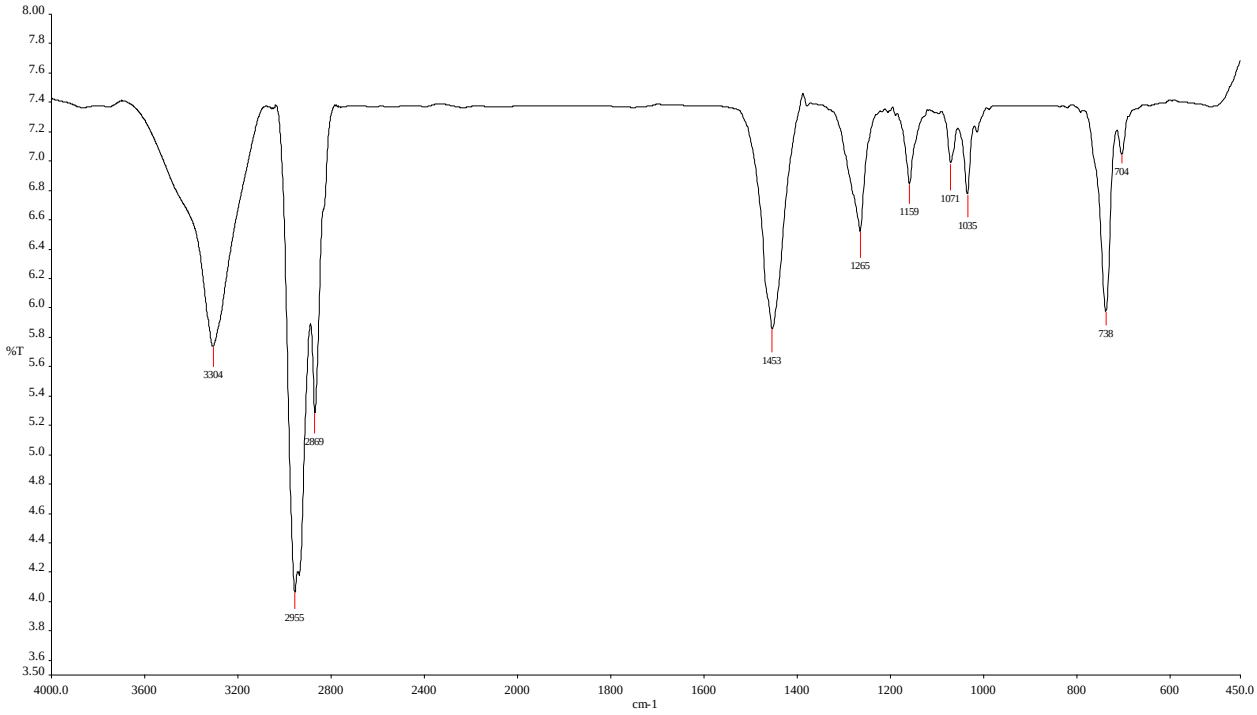
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