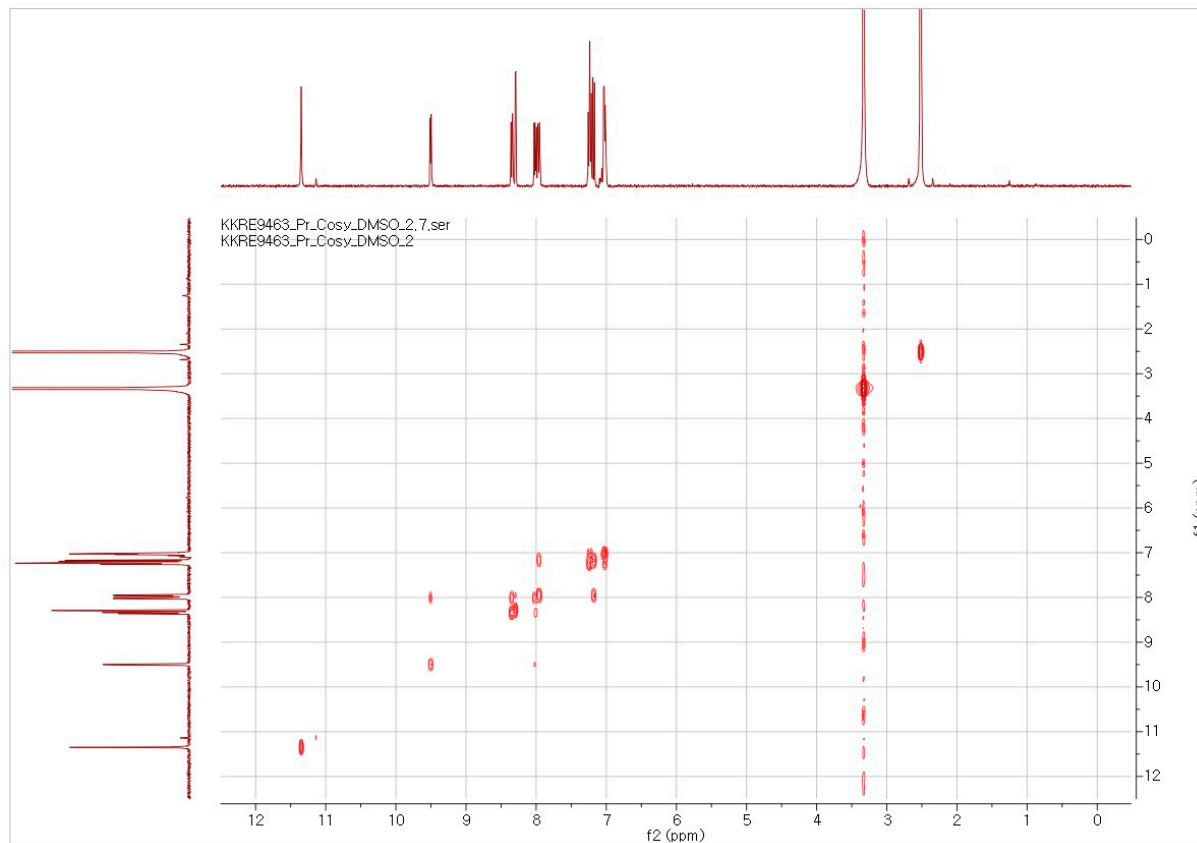


Supplementary Material

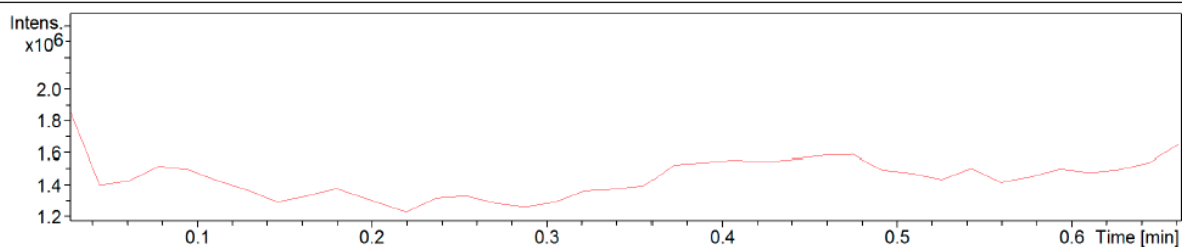
2D-NMR representative spectrum of compound **4a**



HRMS chat of compound **4a**

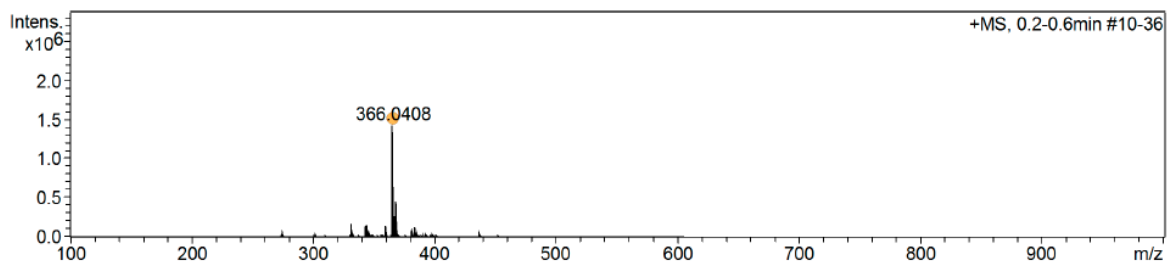
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	366.0408	n.a.

+MS, 0.2-0.6min #10-36

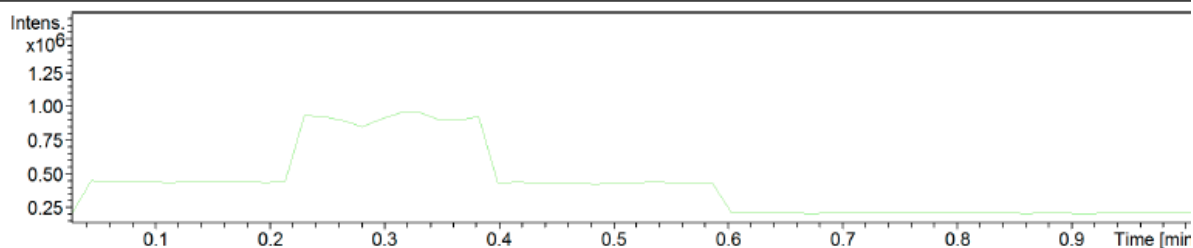


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
366.0408	1	C17H11ClFN3NaO2	366.0416	-2.1	8.4	1	100.00	12.5	even	ok
	2	C15H10ClF4N3Na	366.0392	4.6	9.2	2	57.18	9.5	even	ok

HRMS chat of compound **4b**

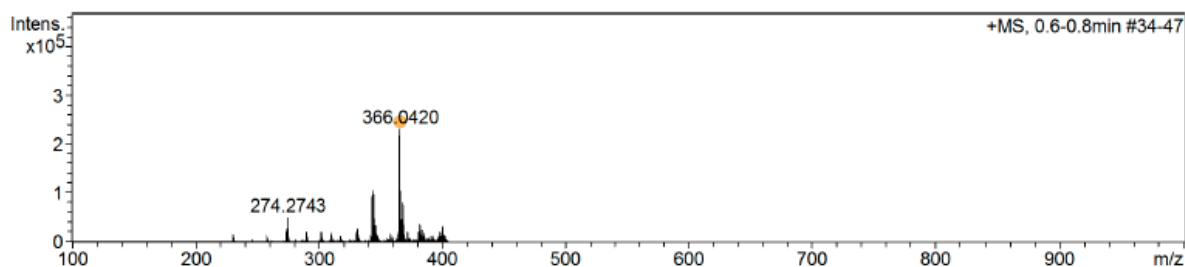
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	425 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.7	n.a.	Average spectrum	n.a.	n.a.	n.a.	366.0420	n.a.

+MS, 0.6-0.8min #34-47



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
366.0420	1	C15H6ClF9	366.0413	-1.7	5.6	1	89.02	16.5	even	ok
	2	C17H9ClF4N3	366.0416	1.1	5.6	2	100.00	12.5	even	ok
	3	C19H10ClF3N3O2	366.0440	-5.6	7.5	3	34.87	15.5	even	ok
	4	C16H11ClF2N3O3	366.0452	8.7	8.0	4	12.48	11.5	even	ok
	5	C14H10ClF5N3O4	366.0400	-5.4	14.5	5	32.58	11.5	even	ok
	6	C14H10ClF5N3O	366.0427	2.1	19.3	6	64.23	8.5	even	ok
	7	C12H7ClF2N9O	366.0425	-1.4	19.3	7	72.51	12.5	even	ok
	8	C13H14ClFNO8	366.0386	-9.0	25.2	8	7.84	6.5	even	ok
	9	C13H15Cl2F5NO	366.0445	7.1	133.7	9	0.19	3.5	even	ok
	10	C14H13Cl2F3N3O	366.0382	10.2	134.4	10	0.06	7.5	even	ok
	11	C16H14Cl2F4N	366.0434	3.9	134.5	11	0.44	7.5	even	ok
	12	C14H11Cl2FN7	366.0432	-3.3	134.5	12	0.51	11.5	even	ok
	13	C13H15Cl2FN3O4	366.0418	0.4	136.9	13	0.76	6.5	even	ok
	14	C18H15Cl2FNO2	366.0458	10.6	139.1	14	0.04	10.5	even	ok
	15	C13H18Cl3F3NO	366.0401	-5.2	249.4	15	0.00	2.5	even	ok
	16	C13H16Cl3FN5	366.0450	-8.3	249.8	16	0.00	6.5	even	ok
	17	C12H20Cl3FNO4	366.0436	-4.6	251.7	17	0.00	1.5	even	ok
	18	C16H17Cl3F2N	366.0389	8.3	251.8	18	0.00	6.5	even	ok
	1	C17H11ClF3NaO2	366.0416	-1.0	3.7	1	100.00	12.5	even	ok

HRMS chat of compound 4c

Analysis Info

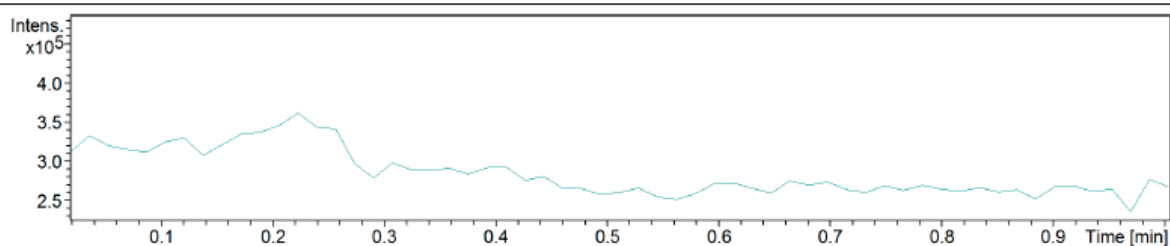
Analysis Name D:\Data\Data\2022\KIST\NEJ\KSJ07\KSJ006.d
 Method Tune_pos_Standard_50_600_20210713.d.m
 Sample Name 6KKRE9468
 Comment

Acquisition Date 7/12/2022 5:19:41 PM

Operator lee
 Instrument compact 8255754.10024

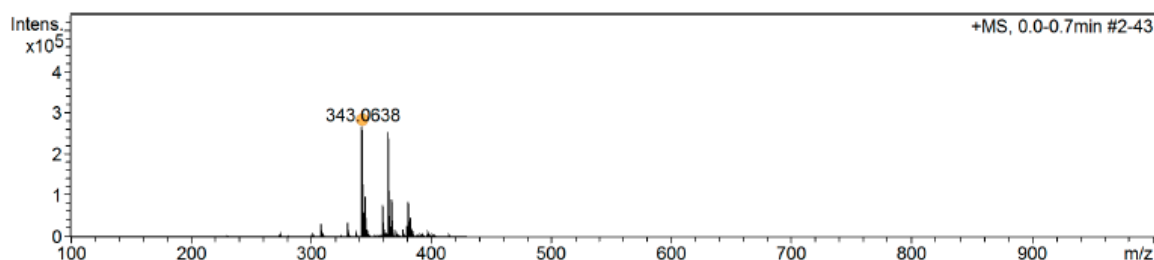
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	400 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	343.0638	n.a.

+MS, 0.0-0.7min #2-43

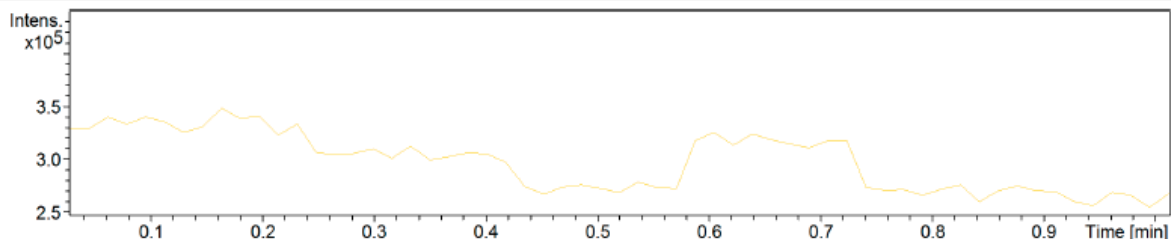


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
343.0638	1	C18H13ClFN2O2	343.0644	-1.7	26.5	1	100.00	12.5	even	ok
	2	C14H9ClFN8	343.0617	6.1	33.6	2	32.41	13.5	even	ok
	3	C16H12ClF4N2	343.0620	-5.4	33.6	3	38.88	9.5	even	ok
	4	C15H14ClF2N2O3	343.0656	-5.1	34.9	4	40.82	8.5	even	ok
	5	C15H17Cl2F4	343.0638	-0.1	121.2	5	4.00	4.5	even	ok
	6	C14H19Cl2F2O3	343.0674	10.4	123.8	6	0.26	3.5	even	ok
	7	C17H18Cl2FO2	343.0662	7.1	124.2	7	0.77	7.5	even	ok
	1	C21H14ClFNa	343.0660	-6.4	25.3	1	86.56	13.5	even	ok
	2	C18H15ClF2NaO	343.0672	9.8	28.8	2	27.76	9.5	even	ok
	3	C16H14ClFN2NaO2	343.0620	-5.3	32.1	3	100.00	9.5	even	ok
	4	C15H19Cl2FNaO2	343.0638	-0.1	123.0	4	8.68	4.5	even	ok

HRMS chat of compound **4d**

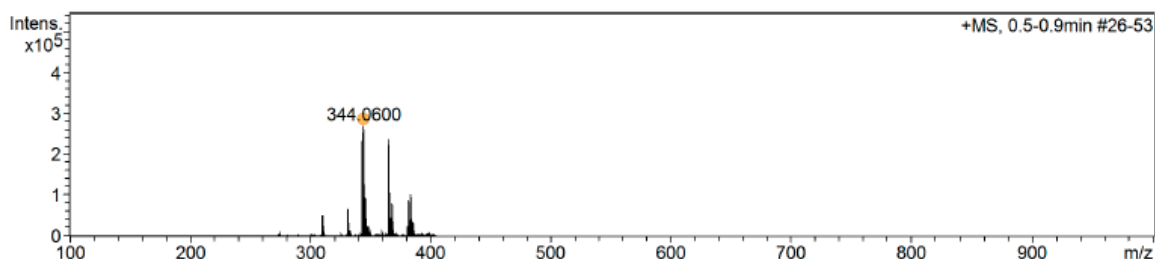
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	400 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.7	n.a.	Average spectrum	n.a.	n.a.	n.a.	344.0600	n.a.

+MS, 0.5-0.9min #26-53

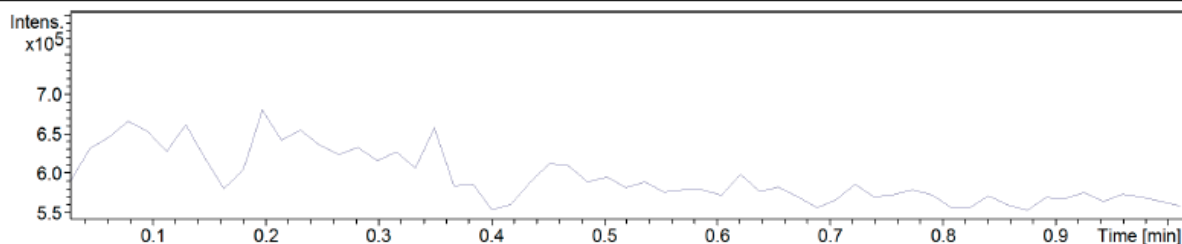


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
344.0600	1	C17H12ClFN3O2	344.0597	-1.0	37.1	1	100.00	12.5	even		ok
	2	C22H12ClFN	344.0637	10.7	38.6	2	7.46	16.5	even		ok
	3	C13H8ClFN9	344.0570	8.8	42.0	3	13.06	13.5	even		ok
	4	C15H11ClF4N3	344.0572	-8.1	42.0	4	16.43	9.5	even		ok
	5	C14H13ClF2N3O3	344.0608	2.3	43.0	5	68.66	8.5	even		ok
	6	C14H13ClF6N	344.0635	-10.2	46.7	6	7.06	5.5	even		ok
	7	C14H16Cl2F4N	344.0590	-2.8	124.3	7	2.47	4.5	even		ok
	8	C13H18Cl2F2NO3	344.0626	7.6	126.9	8	0.65	3.5	even		ok
	9	C16H17Cl2FNO2	344.0615	-4.3	127.1	9	1.55	7.5	even		ok
	1	C20H13ClFNNa	344.0613	3.7	36.7	1	100.00	13.5	even		ok
	2	C17H14ClF2NNaO	344.0624	7.0	38.6	2	41.30	9.5	even		ok
	3	C15H13ClFN3NaO2	344.0573	-8.0	40.9	3	28.35	9.5	even		ok
	4	C14H15ClF3NNaO2	344.0636	-10.3	45.5	4	11.29	5.5	even		ok
	5	C14H18Cl2FNNaO2	344.0591	-2.7	126.1	5	3.68	4.5	even		ok

HRMS chat of compound 4e

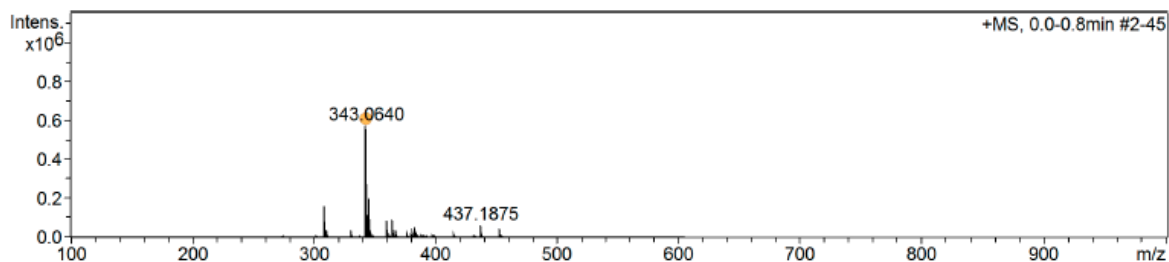
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	400 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	343.0640	n.a.

+MS, 0.0-0.8min #2-45

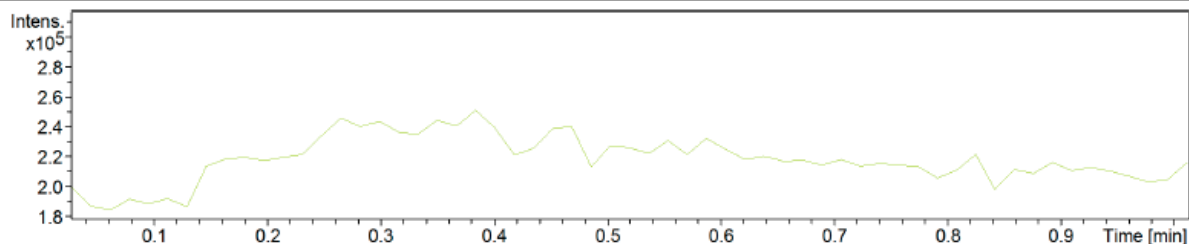


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
343.0640	1	C18H13ClFN2O2	343.0644	-1.2	10.8	1	100.00	12.5	even	ok
	2	C14H9ClFN8	343.0617	6.7	17.9	2	26.02	13.5	even	ok
	3	C16H12ClF4N2	343.0620	-6.0	18.0	3	31.52	9.5	even	ok
	4	C15H14ClF2N2O3	343.0656	-4.5	20.0	4	43.56	8.5	even	ok
	5	C13H13ClFN4O4	343.0604	-10.6	25.6	5	6.09	8.5	even	ok
	6	C13H13ClF5N2O	343.0631	2.6	30.5	6	50.48	5.5	even	ok
	7	C15H17Cl2F4	343.0638	0.6	128.9	7	1.56	4.5	even	ok
	8	C13H14Cl2FN6	343.0636	-1.3	129.0	8	1.39	8.5	even	ok
	9	C14H19Cl2F2O3	343.0674	9.8	131.4	9	0.14	3.5	even	ok
	10	C17H18Cl2FO2	343.0662	-6.5	132.6	10	0.37	7.5	even	ok
	1	C18H15ClF2NaO	343.0672	9.2	12.7	1	24.63	9.5	even	ok
	2	C21H14ClFNa	343.0660	-5.9	14.9	2	64.80	13.5	even	ok
	3	C16H14ClFN2NaO2	343.0620	-5.9	16.4	3	63.07	9.5	even	ok
	4	C13H15ClF2N2NaO3	343.0631	2.5	29.3	4	100.00	5.5	even	ok
	5	C13H15ClF6Na	343.0659	5.4	35.8	5	36.10	2.5	even	ok
	6	C13H18Cl2F4Na	343.0614	-7.6	128.4	6	0.63	1.5	even	ok
	7	C15H19Cl2FNaO2	343.0638	0.5	130.9	7	2.66	4.5	even	ok

HRMS chat of compound **4g**

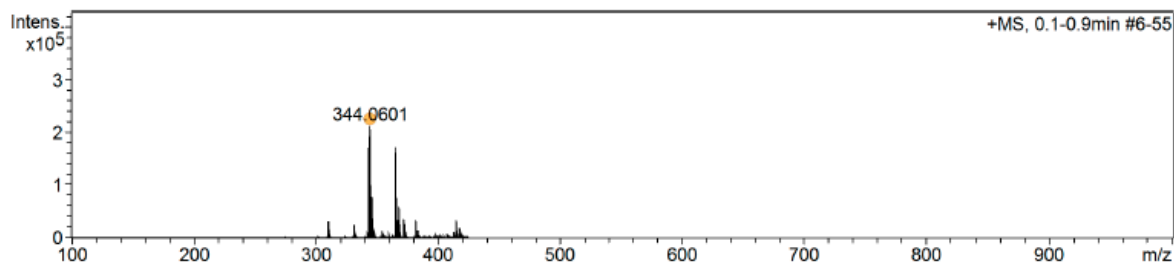
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	420 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.5	n.a.	Average spectrum	n.a.	n.a.	n.a.	344.0601	n.a.

+MS, 0.1-0.9min #6-55

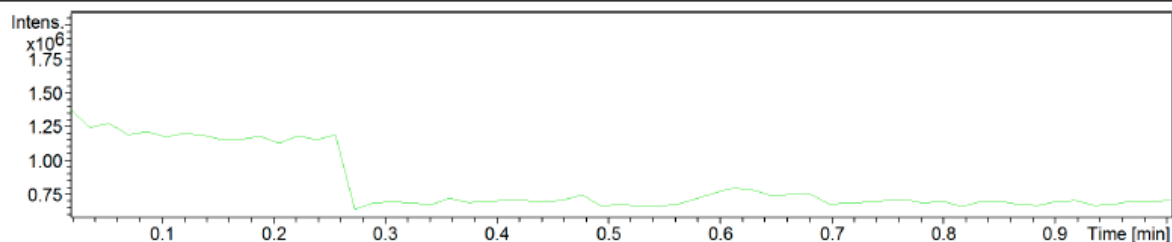


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
344.0601	1	C17H12ClFN3O2	344.0597	-1.2	19.8	1	100.00	12.5	even	ok
	2	C22H12ClFN	344.0637	10.5	20.6	2	8.17	16.5	even	ok
	3	C13H8ClFN9	344.0570	-9.0	28.7	3	11.97	13.5	even	ok
	4	C15H11ClF4N3	344.0572	8.3	28.7	4	15.08	9.5	even	ok
	5	C14H13ClF2N3O3	344.0608	-2.2	30.4	5	66.13	8.5	even	ok
	6	C14H13ClF6N	344.0635	-10.1	35.6	6	6.79	5.5	even	ok
	7	C14H16Cl2F4N	344.0590	2.9	122.0	7	1.86	4.5	even	ok
	8	C13H18Cl2F2NO3	344.0626	-7.5	124.7	8	0.51	3.5	even	ok
	9	C16H17Cl2FNO2	344.0615	-4.2	124.9	9	1.22	7.5	even	ok
	1	C20H13ClFNNa	344.0613	3.5	17.9	1	100.00	13.5	even	ok
	2	C17H14ClF2NNaO	344.0624	-6.9	22.8	2	39.47	9.5	even	ok
	3	C15H13ClFN3NaO2	344.0573	8.1	26.9	3	24.32	9.5	even	ok
	4	C14H15ClF3NNaO2	344.0636	-10.2	34.1	4	10.12	5.5	even	ok
	5	C14H18Cl2FNNaO2	344.0591	2.8	123.9	5	2.55	4.5	even	ok

HRMS chat of compound **4i**

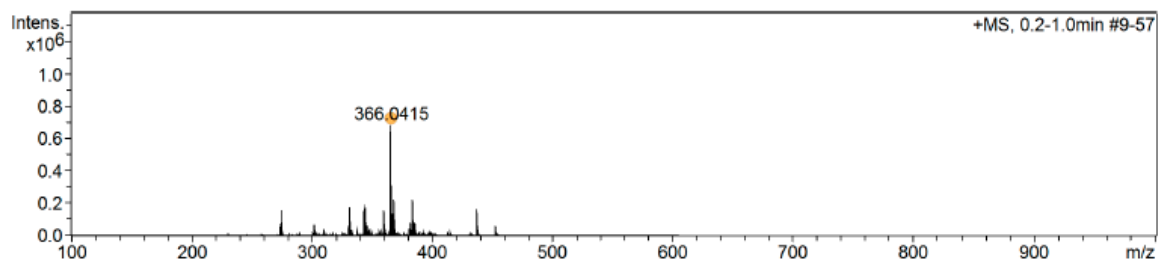
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.6	n.a.	Average spectrum	n.a.	n.a.	n.a.	366.0415	n.a.

+MS, 0.2-1.0min #9-57

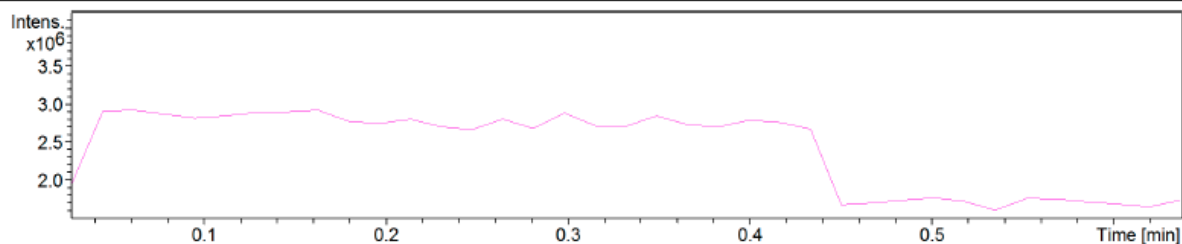


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
366.0415	1	C17H11ClFN3NaO2	366.0416	0.2	4.9	1	100.00	12.5	even	ok
	2	C15H10ClF4N3Na	366.0392	-6.4	11.9	2	21.86	9.5	even	ok
	3	C13H7ClFN9Na	366.0389	-7.1	11.9	3	17.77	13.5	even	ok
	4	C14H12ClF2N3NaO3	366.0427	3.4	16.3	4	45.02	8.5	even	ok
	5	C14H12ClF6NNa	366.0455	-10.8	20.2	5	3.71	5.5	even	ok
	6	C12H9ClF3N7Na	366.0452	10.1	20.2	6	4.89	9.5	even	ok
	7	C12H11ClFN5NaO4	366.0376	-10.7	22.8	7	3.60	8.5	even	ok
	8	C12H11ClF5N3NaO	366.0403	-3.3	26.7	8	36.32	5.5	even	ok
	9	C14H15Cl2F4NNa	366.0410	1.4	138.7	9	0.49	4.5	even	ok
	10	C12H12Cl2FN7Na	366.0407	-2.1	138.8	10	0.44	8.5	even	ok
	11	C13H17Cl2F2NNaO3	366.0446	-8.4	141.3	11	0.07	3.5	even	ok
	12	C16H16Cl2FNNaO2	366.0434	5.2	142.4	12	0.17	7.5	even	ok

HRMS chat of compound 4j

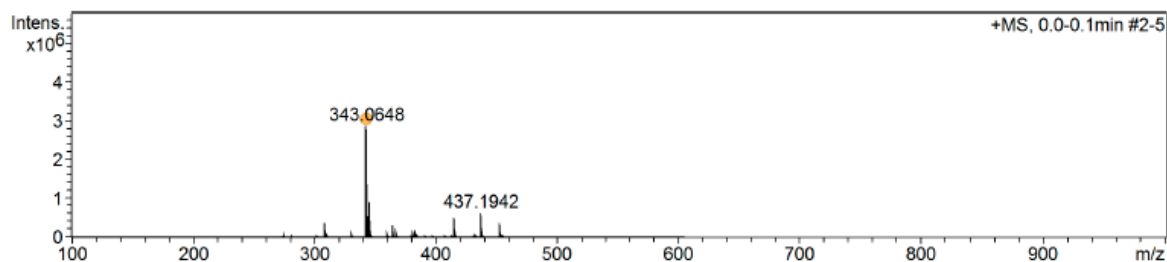
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.1	n.a.	Average spectrum	n.a.	n.a.	n.a.	343.0648	n.a.

+MS, 0.0-0.1min #2-5

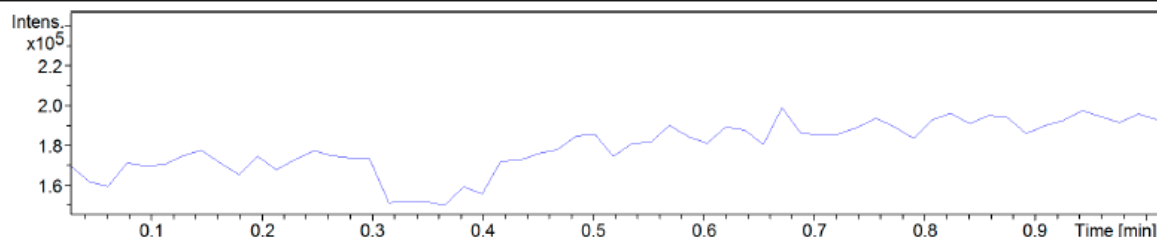


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
343.0648	1	C16H12ClF4N2	343.0620	-8.2	9.7	1	20.58	9.5	even	ok
	2	C14H9ClF8	343.0617	8.9	9.7	2	16.33	13.5	even	ok
	3	C15H14ClF2N2O3	343.0656	-2.2	12.8	3	86.95	8.5	even	ok
	4	C15H14ClF6	343.0683	10.1	13.6	4	9.93	5.5	even	ok
	5	C13H11ClF3N6	343.0680	9.4	13.7	5	12.77	9.5	even	ok
	6	C18H13ClF2N2O2	343.0644	-1.1	15.1	6	100.00	12.5	even	ok
	7	C13H13ClF5N2O	343.0631	4.9	19.2	7	43.28	5.5	even	ok
	8	C11H10ClF2N8O	343.0629	-5.6	19.2	8	36.34	9.5	even	ok
	9	C12H15ClF3N2O4	343.0667	5.5	23.7	9	33.53	4.5	even	ok
	10	C23H13ClF	343.0684	-10.6	33.7	10	5.33	16.5	even	ok
	11	C12H18Cl2F5O	343.0649	-0.4	143.2	11	0.73	0.5	even	ok
	12	C15H17Cl2F4	343.0638	2.9	143.8	12	0.46	4.5	even	ok
	13	C13H14Cl2FN6	343.0636	-3.6	143.9	13	0.40	8.5	even	ok
	14	C11H20Cl2F3O4	343.0685	-10.9	146.0	14	0.04	-0.5	even	ok
	15	C14H19Cl2F2O3	343.0674	7.5	146.0	15	0.13	3.5	even	ok
	16	C12H18Cl2FN2O4	343.0622	-7.5	146.3	16	0.13	3.5	even	ok
	17	C17H18Cl2FO2	343.0662	4.2	148.2	17	0.26	7.5	even	ok
	18	C12H19Cl3FN4	343.0654	-1.7	256.8	18	0.00	3.5	even	ok
	1	C16H14ClF2N2NaO2	343.0620	-8.1	11.0	1	39.38	9.5	even	ok

HRMS chat of compound **4k**

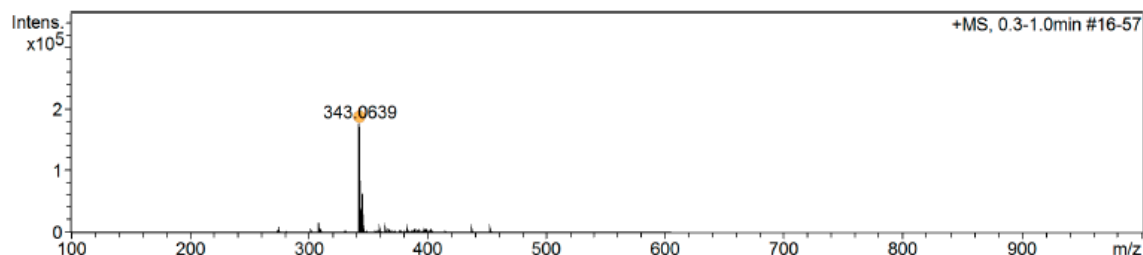
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.6	n.a.	Average spectrum	n.a.	n.a.	n.a.	343.0639	n.a.

+MS, 0.3-1.0min #16-57

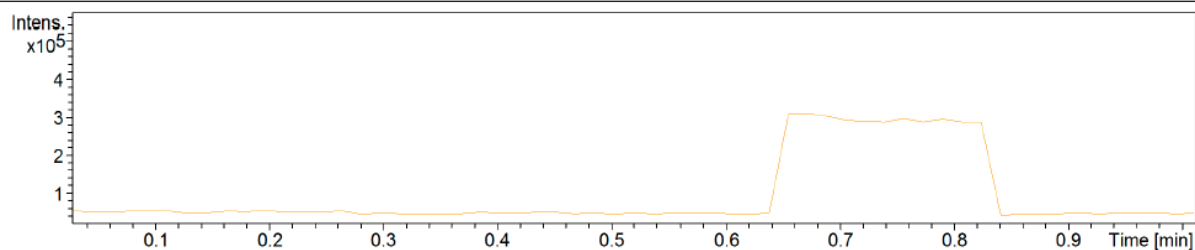


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
343.0639	1	C18H13ClFN2O2	343.0644	1.6	8.2	1	100.00	12.5	even	ok
	2	C16H12ClF4N2	343.0620	5.5	18.6	2	35.85	9.5	even	ok
	3	C14H9ClFN8	343.0617	6.2	18.6	3	29.82	13.5	even	ok
	4	C15H14ClF2N2O3	343.0656	-4.9	21.2	4	39.11	8.5	even	ok
	5	C13H13ClFN4O4	343.0604	-10.1	27.4	5	7.08	8.5	even	ok
	6	C13H13ClF5N2O	343.0631	-2.2	32.5	6	53.58	5.5	even	ok
	7	C15H17Cl2F4	343.0638	-0.2	128.9	7	1.70	4.5	even	ok
	8	C13H14Cl2FN6	343.0636	-0.9	129.0	8	1.53	8.5	even	ok
	9	C14H19Cl2F2O3	343.0674	10.3	131.6	9	0.12	3.5	even	ok
	10	C17H18Cl2FO2	343.0662	6.9	132.4	10	0.33	7.5	even	ok
	1	C21H14ClFNa	343.0660	-6.3	9.7	1	61.38	13.5	even	ok
	2	C18H15ClF2NaO	343.0672	9.7	11.7	2	20.75	9.5	even	ok
	3	C16H14ClFN2NaO2	343.0620	5.4	17.0	3	67.66	9.5	even	ok
	4	C13H15ClF2N2NaO3	343.0631	-2.1	31.3	4	100.00	5.5	even	ok
	5	C13H15ClF6Na	343.0659	5.9	40.4	5	27.53	2.5	even	ok
	6	C13H18Cl2F4Na	343.0614	-7.2	128.6	6	0.68	1.5	even	ok
	7	C15H19Cl2FNaO2	343.0638	0.1	130.9	7	2.73	4.5	even	ok

HRMS chat of compound **4l**

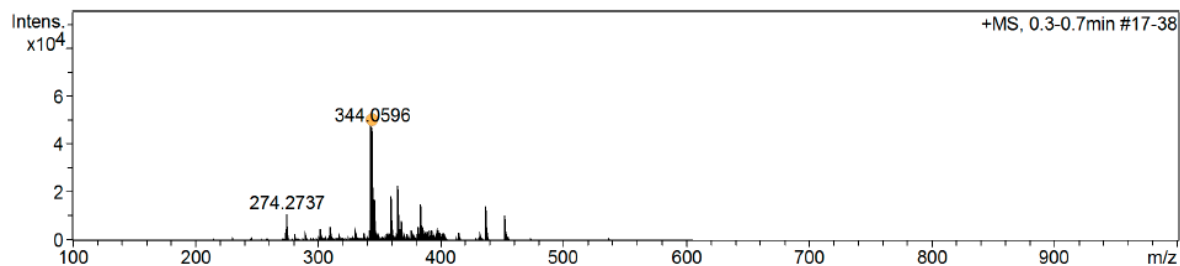
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	400 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.5	n.a.	Average spectrum	n.a.	n.a.	n.a.	344.0596	n.a.

+MS, 0.3-0.7min #17-38

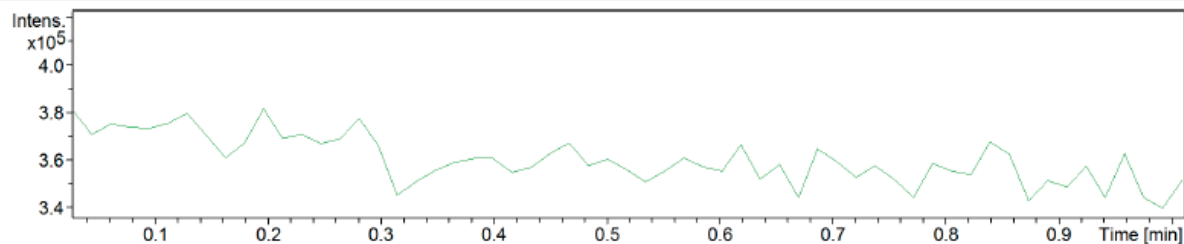


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
344.0596	1	C17H12ClFN3O2	344.0597	0.0	24.3	1	100.00	12.5	even	ok
	2	C15H11ClF4N3	344.0572	7.1	34.6	2	17.53	9.5	even	ok
	3	C16H17Cl2FNO2	344.0615	5.4	127.9	3	0.72	7.5	even	ok
	1	C20H13ClFNNa	344.0613	-4.7	17.6	1	100.00	13.5	even	ok
	2	C17H14ClF2NNaO	344.0624	8.1	27.8	2	31.80	9.5	even	ok
	3	C15H13ClFN3NaO2	344.0573	-7.0	33.2	3	38.93	9.5	even	ok

HRMS chat of compound 4m

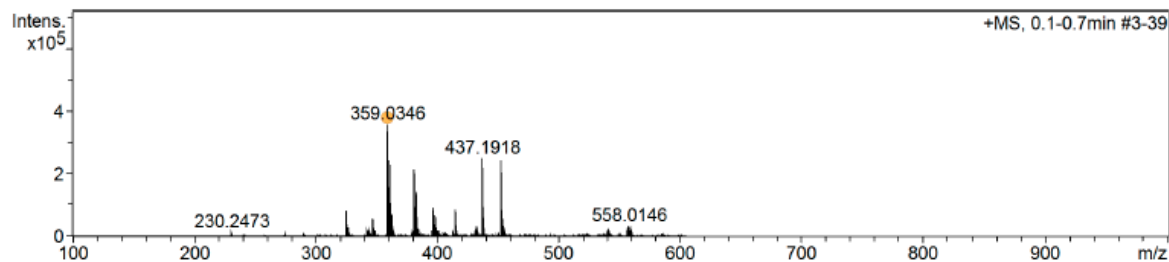
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.4	n.a.	Average spectrum	n.a.	n.a.	n.a.	359.0346	n.a.

+MS, 0.1-0.7min #3-39

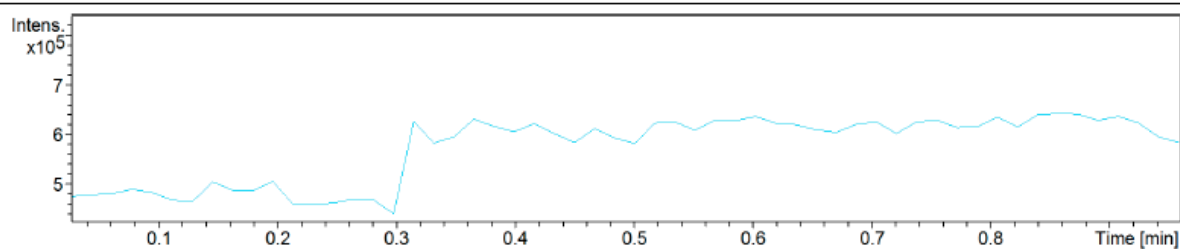


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
359.0346	1	C18H13Cl2N2O2	359.0349	-0.6	36.1	1	100.00	12.5	even	ok
	2	C14H9Cl2N8	359.0322	-6.9	42.1	2	20.19	13.5	even	ok
	3	C13H13Cl2N4O4	359.0308	10.6	46.4	3	4.69	8.5	even	ok
	4	C13H14Cl3N6	359.0340	-1.8	113.2	4	5.49	8.5	even	ok
	5	C17H18Cl3O2	359.0367	-5.7	116.6	5	1.88	7.5	even	ok
	6	C24H8ClN2	359.0371	6.7	172.1	6	0.03	21.5	even	ok
	7	C18H12ClO6	359.0317	8.2	173.5	7	0.01	12.5	even	ok
	8	C19H8ClN4O2	359.0330	-4.5	174.5	8	0.04	17.5	even	ok
	1	C21H14Cl2Na	359.0365	5.1	36.0	1	100.00	13.5	even	ok
	2	C16H14Cl2N2NaO2	359.0325	6.1	40.4	2	67.62	9.5	even	ok
	3	C15H19Cl3NaO2	359.0343	1.0	115.0	3	14.43	4.5	even	ok
	4	C22H9ClN2Na	359.0346	-0.0	173.9	4	0.25	18.5	even	ok

HRMS chat of compound **4n**

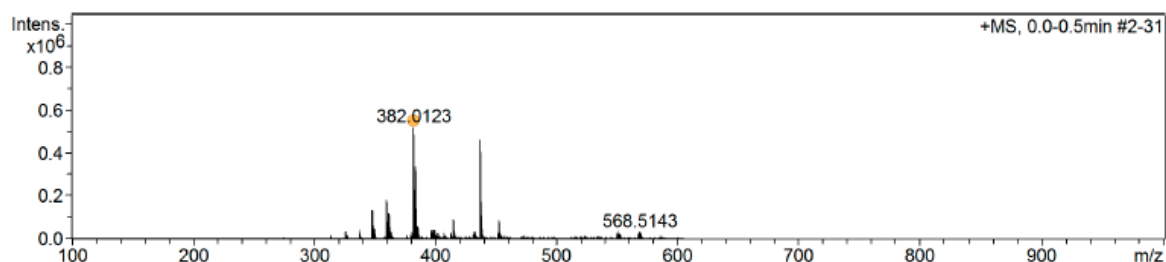
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.3	n.a.	Average spectrum	n.a.	n.a.	n.a.	382.0123	n.a.

+MS, 0.0-0.5min #2-31

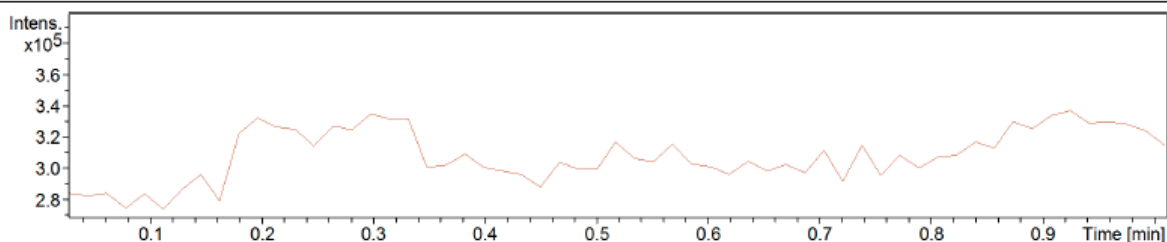


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
382.0123	1	C15H6Cl2N9	382.0118	1.3	6.3	1	100.00	16.5	even	ok
	2	C19H10Cl2N3O2	382.0145	5.7	9.8	2	32.45	15.5	even	ok
	3	C14H10Cl2N5O4	382.0104	-4.8	17.0	3	36.35	11.5	even	ok
	4	C13H14Cl2NO8	382.0091	8.3	28.3	4	8.86	6.5	even	ok
	5	C14H11Cl3N7	382.0136	-3.5	138.2	5	0.54	11.5	even	ok
	6	C13H15Cl3N3O4	382.0123	-0.0	140.4	6	0.92	6.5	even	ok
	7	C19H9ClNO6	382.0113	2.6	142.8	7	0.31	15.5	even	ok
	8	C20H5ClN5O2	382.0126	-0.9	144.3	8	0.39	20.5	even	ok
	9	C15H5ClN7O4	382.0086	-9.6	147.7	9	0.02	16.5	even	ok
	10	C16HCIN11	382.0099	-6.1	148.6	10	0.08	21.5	even	ok
	11	C13H16Cl4N5	382.0154	8.3	192.4	11	0.00	6.5	even	ok
	1	C17H11Cl2N3NaO2	382.0121	0.6	7.0	1	100.00	12.5	even	ok
	2	C13H7Cl2N9Na	382.0094	-7.6	15.8	2	13.51	13.5	even	ok
	3	C22H11Cl2NNa	382.0161	9.9	19.9	3	4.94	16.5	even	ok
	4	C16H16Cl3NNaO2	382.0139	4.2	140.3	4	0.35	7.5	even	ok
	5	C23H6ClN3Na	382.0142	5.1	144.3	5	0.13	21.5	even	ok
	6	C17H10ClNNaO6	382.0089	8.9	145.6	6	0.03	12.5	even	ok
	7	C18H6ClN5NaO2	382.0102	5.4	146.5	7	0.11	17.5	even	ok

HRMS chat of compound **4o**

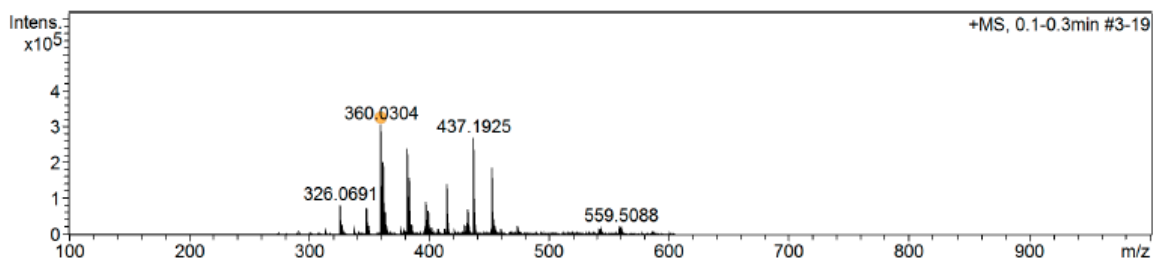
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.2	n.a.	Average spectrum	n.a.	n.a.	n.a.	360.0304	n.a.

+MS, 0.1-0.3min #3-19

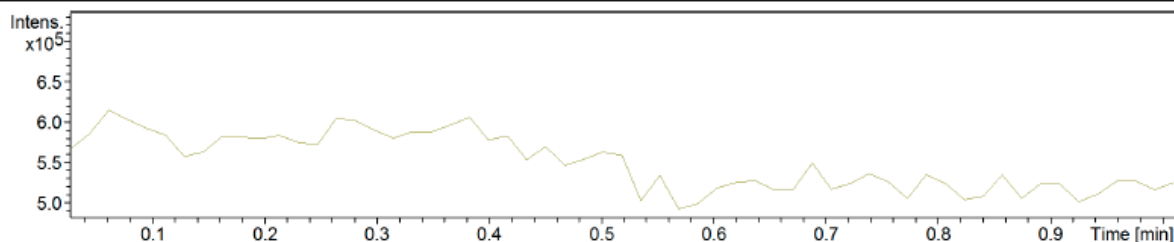


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
360.0304	1	C17H12Cl2N3O2	360.0301	-0.8	40.1	1	100.00	12.5	even	ok
	2	C22H12Cl2N	360.0341	-10.4	43.1	2	6.43	16.5	even	ok
	3	C13H8Cl2N9	360.0274	8.3	44.6	3	13.63	13.5	even	ok
	4	C12H13Cl3N7	360.0293	-3.2	117.6	4	3.77	8.5	even	ok
	5	C16H17Cl3NO2	360.0319	-4.3	121.0	5	2.44	7.5	even	ok
	6	C23H7ClN3	360.0323	-5.3	168.0	6	0.06	21.5	even	ok
	7	C17H11ClNO6	360.0269	-9.6	168.6	7	0.01	12.5	even	ok
	8	C18H7ClN5O2	360.0283	-5.9	169.8	8	0.04	17.5	even	ok
	1	C20H13Cl2NNa	360.0317	3.7	40.7	1	100.00	13.5	even	ok
	2	C15H13Cl2N3NaO2	360.0277	-7.5	43.2	2	32.70	9.5	even	ok
	3	C14H18Cl3NNaO2	360.0295	2.4	119.5	3	7.11	4.5	even	ok
	4	C21H8ClN3Na	360.0299	1.4	169.5	4	0.22	18.5	even	ok

HRMS chat of compound **4p**

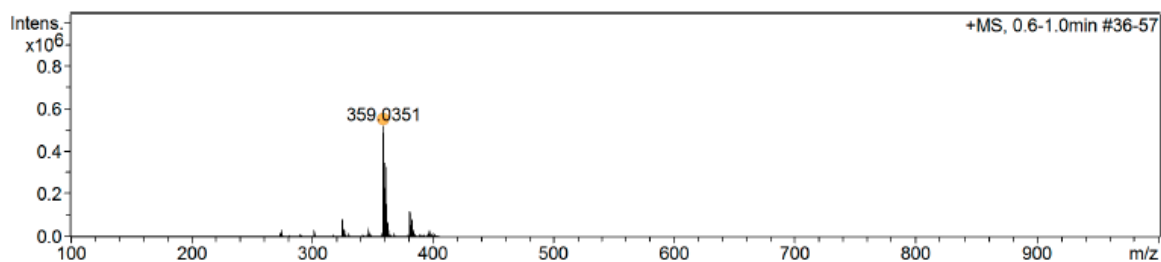
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.8	n.a.	Average spectrum	n.a.	n.a.	n.a.	359.0351	n.a.

+MS, 0.6-1.0min #36-57

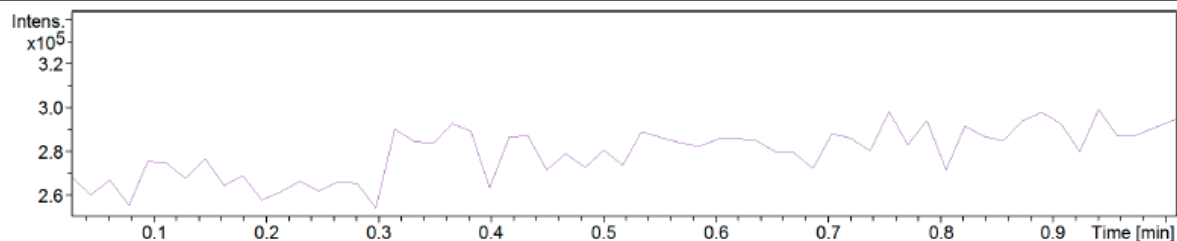


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
359.0351	1	C18H13Cl2N2O2	359.0349	0.7	7.3	1	100.00	12.5	even	ok
	2	C14H9Cl2N8	359.0322	8.1	18.1	2	12.90	13.5	even	ok
	3	C23H13Cl2	359.0389	-10.5	18.7	3	5.16	16.5	even	ok
	4	C13H14Cl3N6	359.0340	3.0	128.8	4	0.97	8.5	even	ok
	5	C17H18Cl3O2	359.0367	4.4	132.7	5	0.56	7.5	even	ok
	6	C24H8ClN2	359.0371	-5.4	154.1	6	0.07	21.5	even	ok
	7	C18H12ClO6	359.0317	-9.5	155.4	7	0.02	12.5	even	ok
	8	C19H8ClN4O2	359.0330	5.8	156.4	8	0.06	17.5	even	ok
	1	C21H14Cl2Na	359.0365	-3.8	9.4	1	100.00	13.5	even	ok
	2	C16H14Cl2N2NaO2	359.0325	7.4	16.6	2	33.08	9.5	even	ok
	3	C15H19Cl3NaO2	359.0343	2.3	130.9	3	1.94	4.5	even	ok
	4	C22H9ClN2Na	359.0346	1.3	155.8	4	0.30	18.5	even	ok

HRMS chat of compound **4r**

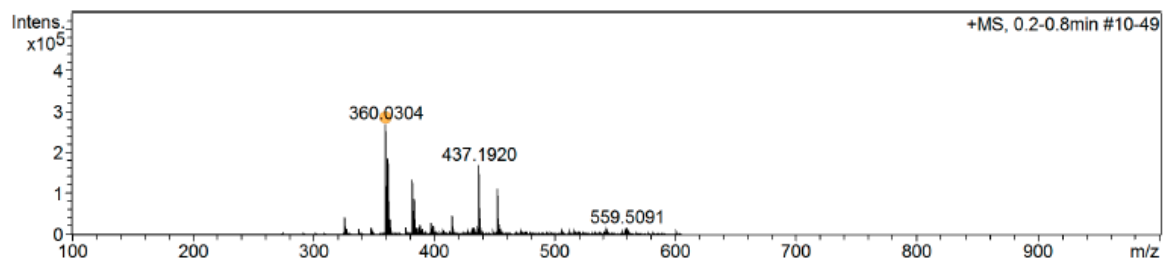
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	0.5	n.a.	Average spectrum	n.a.	n.a.	n.a.	360.0304	n.a.

+MS, 0.2-0.8min #10-49



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
360.0304	1	C17H12Cl2N3O2	360.0301	0.9	16.9	1	100.00	12.5	even	ok
	2	C22H12Cl2N	360.0341	10.3	21.2	2	6.79	16.5	even	ok
	3	C13H8Cl2N9	360.0274	-8.4	26.1	3	12.41	13.5	even	ok
	4	C12H13Cl3N7	360.0293	3.3	119.3	4	1.97	8.5	even	ok
	5	C16H17Cl3NO2	360.0319	4.2	122.9	5	1.32	7.5	even	ok
	6	C23H7ClN3	360.0323	-5.2	165.5	6	0.04	21.5	even	ok
	7	C17H11ClNO6	360.0269	9.7	166.7	7	0.01	12.5	even	ok
	8	C18H7ClN5O2	360.0283	-6.0	167.8	8	0.03	17.5	even	ok
	1	C20H13Cl2NNa	360.0317	-3.6	16.7	1	100.00	13.5	even	ok
	2	C15H13Cl2N3NaO2	360.0277	-7.6	24.2	2	28.14	9.5	even	ok
	3	C14H18Cl3NNaO2	360.0295	2.5	121.3	3	3.45	4.5	even	ok
	4	C21H8ClN3Na	360.0299	1.5	167.3	4	0.14	18.5	even	ok