

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074542.D
 Acq On : 17 Sep 2022 04:57
 Operator : JC\MD
 Sample : N4549-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-58

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	48	53	60	rBV	238842	452237	23.62%	2.945%
2	2.693	131	137	141	rBV3	66318	153574	8.02%	1.000%
3	4.457	431	437	442	rBV3	11169	26751	1.40%	0.174%
4	5.528	606	619	632	rBV3	55599	195631	10.22%	1.274%
5	7.063	870	880	887	rBV5	18300	50089	2.62%	0.326%
6	7.769	995	1000	1009	rVB7	10148	25033	1.31%	0.163%
7	7.951	1018	1031	1036	rBV2	268760	641480	33.50%	4.178%
8	8.016	1036	1042	1051	rVB	404611	916658	47.87%	5.970%
9	8.369	1092	1102	1114	rBV	310392	733764	38.32%	4.779%
10	8.904	1184	1193	1207	rBV	679021	1412737	73.78%	9.201%
11	9.180	1236	1240	1247	rVB6	11214	22406	1.17%	0.146%
12	9.357	1263	1270	1274	rBV6	18707	44442	2.32%	0.289%
13	9.392	1274	1276	1283	rVB5	16837	27345	1.43%	0.178%
14	9.910	1358	1364	1369	rBV4	23121	44076	2.30%	0.287%
15	10.139	1397	1403	1407	rBV7	11398	23808	1.24%	0.155%
16	10.263	1417	1424	1430	rBV3	22611	43729	2.28%	0.285%
17	10.380	1436	1444	1453	rBV	1031082	1914803	100.00%	12.471%
18	10.580	1472	1478	1485	rVB3	69863	127716	6.67%	0.832%
19	10.657	1485	1491	1498	rVB2	72615	123986	6.48%	0.808%
20	10.798	1509	1515	1525	rVB5	26882	61585	3.22%	0.401%
21	11.686	1657	1666	1674	rBV	1066181	1845750	96.39%	12.021%
22	11.780	1678	1682	1691	rVB6	16082	39123	2.04%	0.255%
23	11.892	1691	1701	1705	rBV5	17756	40517	2.12%	0.264%
24	12.521	1801	1808	1815	rVB2	45628	75144	3.92%	0.489%
25	12.674	1826	1834	1843	rBV	828214	1418997	74.11%	9.242%
26	12.862	1861	1866	1873	rVB	32658	49484	2.58%	0.322%
27	13.051	1893	1898	1903	rBV	13656	22219	1.16%	0.145%
28	13.162	1912	1917	1924	rBV3	29209	43086	2.25%	0.281%
29	13.433	1956	1963	1970	rVB4	26631	60692	3.17%	0.395%
30	13.615	1987	1994	2006	rBV	1000290	1747969	91.29%	11.384%
31	13.709	2006	2010	2015	rVV3	26528	42766	2.23%	0.279%
32	13.780	2015	2022	2024	rVV3	77760	113837	5.95%	0.741%
33	13.815	2024	2028	2033	rVV	222581	377497	19.71%	2.459%
34	13.857	2033	2035	2042	rVV2	44937	73895	3.86%	0.481%
35	13.951	2045	2051	2055	rVB3	42263	70469	3.68%	0.459%
36	14.092	2068	2075	2081	rBV2	90803	161595	8.44%	1.052%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074542.D
 Acq On : 17 Sep 2022 04:57
 Operator : JC\MD
 Sample : N4549-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-58

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

37	14.157	2081	2086	2092	rVV	70188	111086	5.80%	0.723%
38	14.227	2092	2098	2100	rVV3	21731	36524	1.91%	0.238%
39	14.274	2100	2106	2111	rVV	254339	437684	22.86%	2.851%
40	14.345	2111	2118	2123	rVB8	15217	33150	1.73%	0.216%
41	14.404	2123	2128	2133	rBV3	29583	46278	2.42%	0.301%
42	14.480	2133	2141	2148	rVV2	182529	292584	15.28%	1.906%
43	14.598	2157	2161	2165	rBV4	14397	20207	1.06%	0.132%
44	14.704	2173	2179	2183	rBV5	30153	47527	2.48%	0.310%
45	14.756	2183	2188	2200	rVB6	48459	101353	5.29%	0.660%
46	14.874	2200	2208	2213	rBV4	86622	176072	9.20%	1.147%
47	14.933	2213	2218	2224	rVB7	29179	53573	2.80%	0.349%
48	15.133	2246	2252	2257	rBV5	52071	97612	5.10%	0.636%
49	15.239	2262	2270	2278	rVB7	32373	98123	5.12%	0.639%
50	15.498	2307	2314	2319	rBV3	47603	97068	5.07%	0.632%
51	15.568	2319	2326	2338	rVB5	58459	153883	8.04%	1.002%
52	15.727	2349	2353	2358	rVB4	10818	19298	1.01%	0.126%
53	15.815	2358	2368	2373	rBV10	14669	37239	1.94%	0.243%
54	15.933	2382	2388	2390	rBV6	12318	23870	1.25%	0.155%
55	16.039	2400	2406	2412	rBV5	14692	33034	1.73%	0.215%
56	16.268	2438	2445	2453	rVB9	16518	33677	1.76%	0.219%
57	16.474	2474	2480	2485	rVB5	21303	41076	2.15%	0.268%
58	16.745	2517	2526	2532	rBV3	59537	138344	7.22%	0.901%

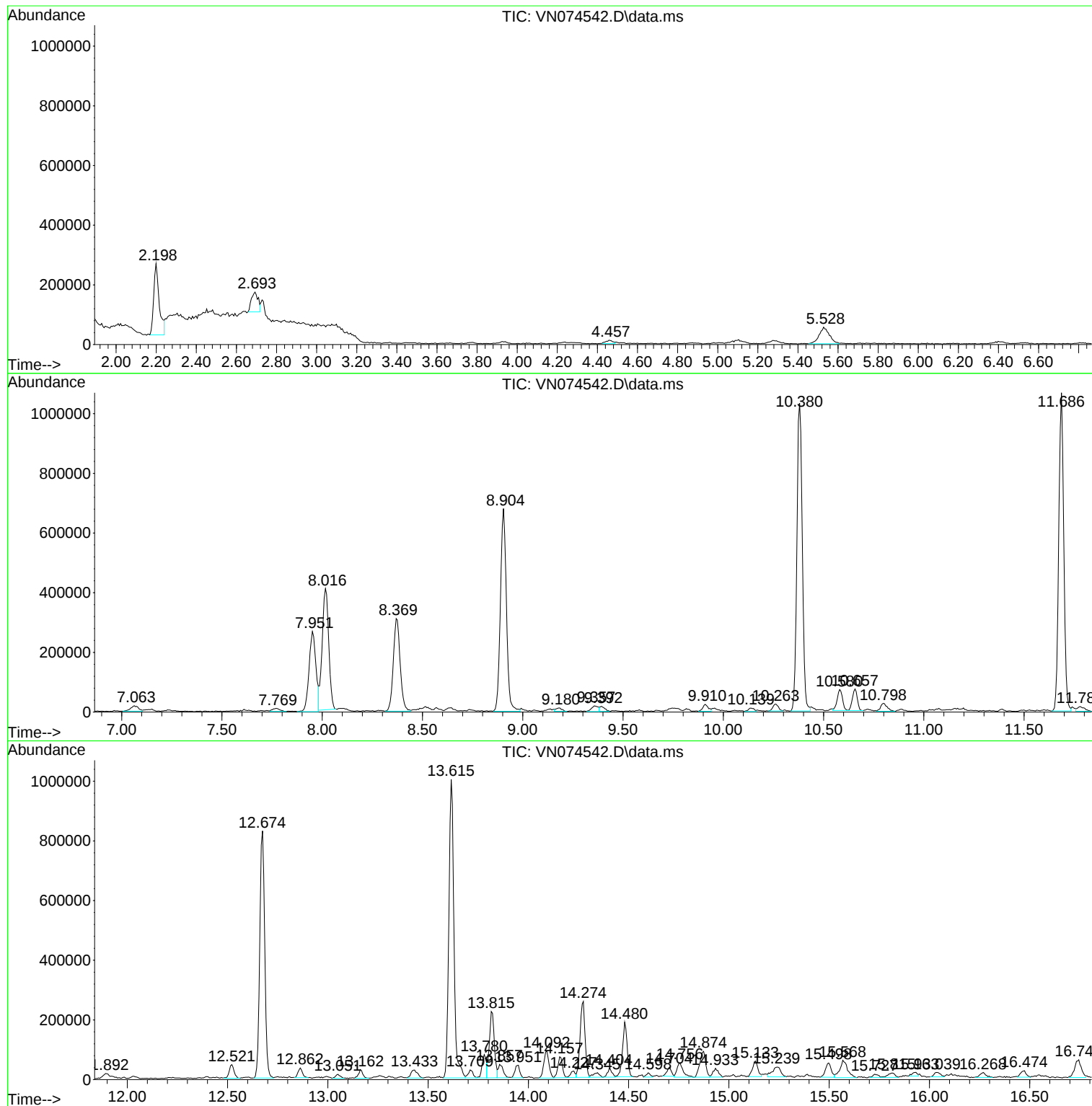
Sum of corrected areas: 15354152

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

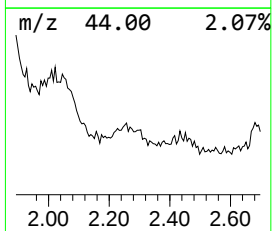
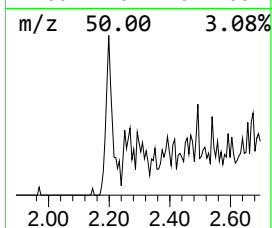
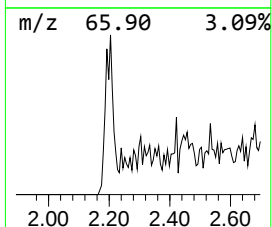
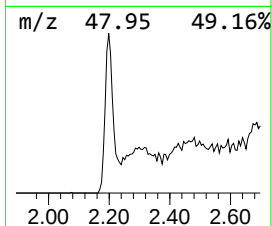
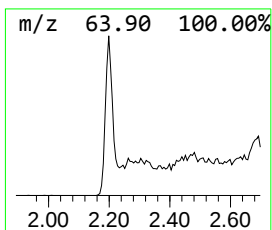
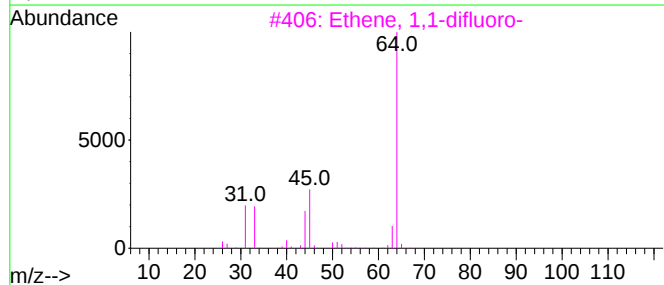
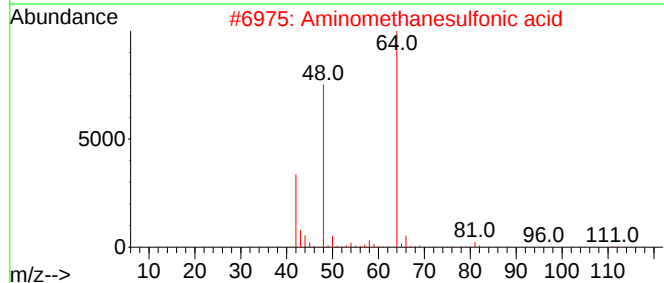
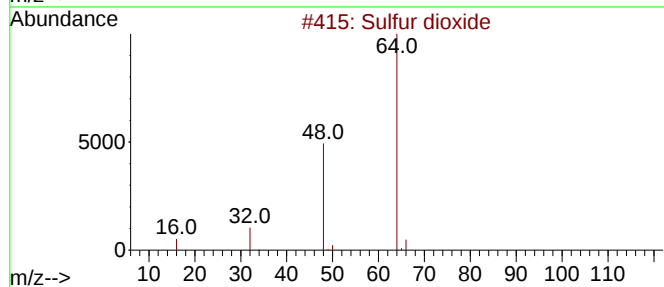
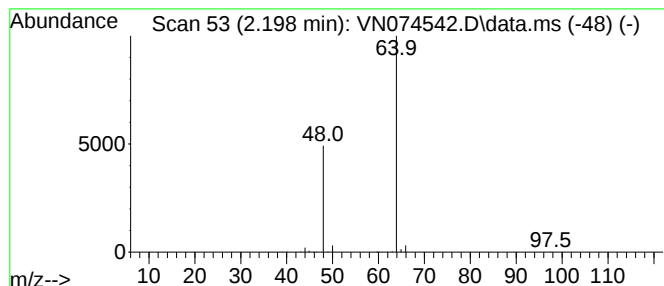
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.198	24.67 ug/l	452237	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

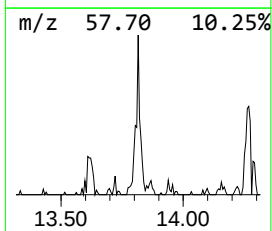
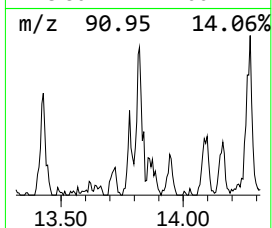
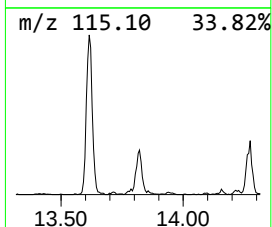
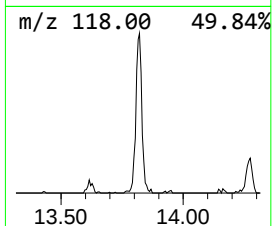
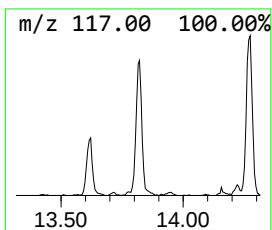
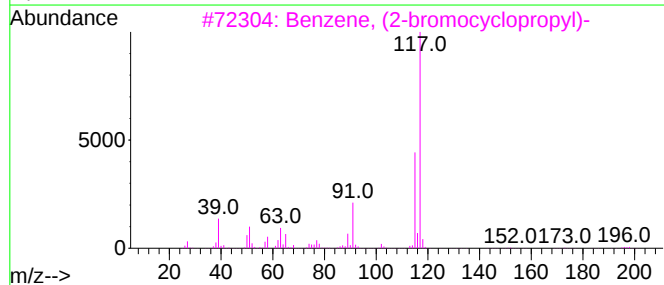
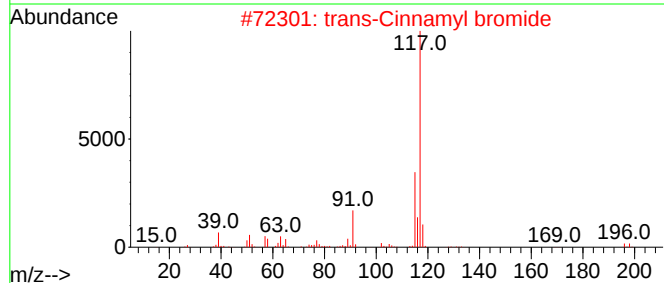
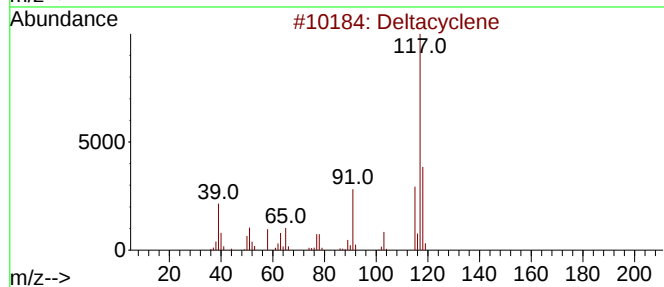
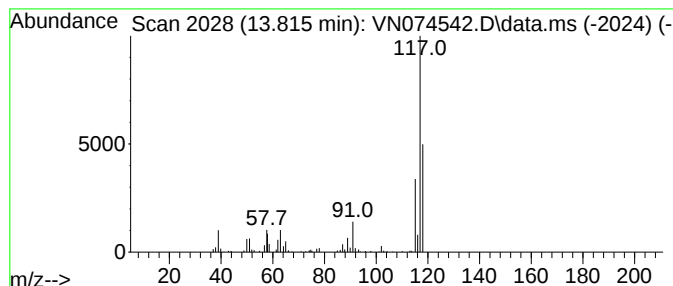
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-Cinnamyl bromide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	10.80 ug/l	377497	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Deltacyclene	118	C9H10	007785-10-6	53
2			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	50
3			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	47
4			2,4-Dicyanopyrrole	117	C6H3N3	074023-87-3	43
5			Indole	117	C8H7N	000120-72-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

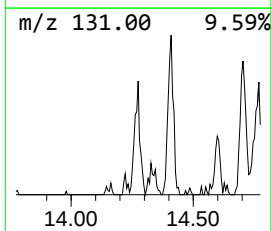
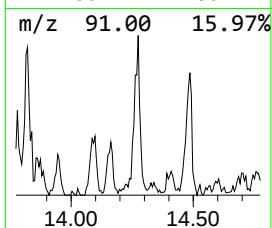
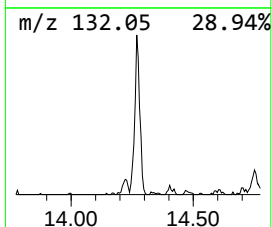
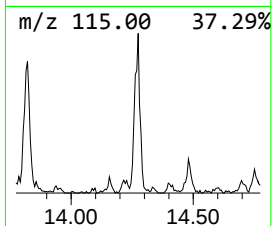
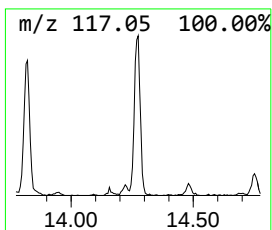
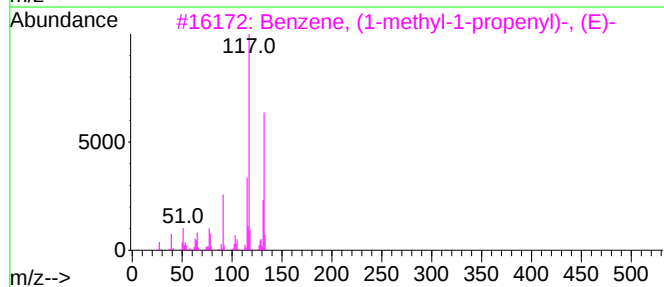
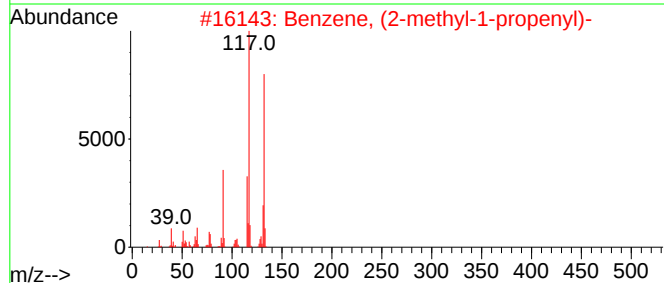
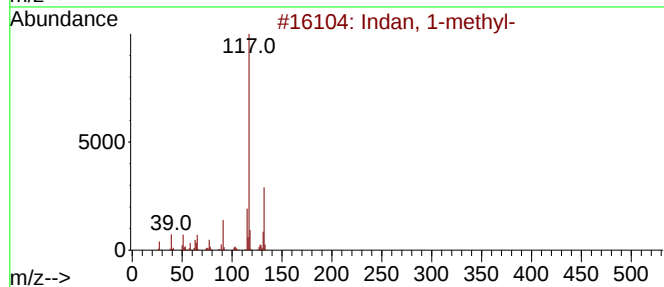
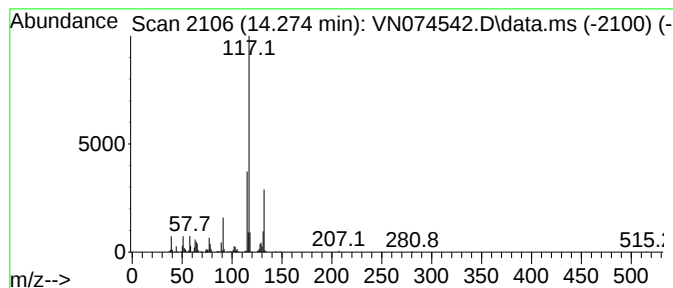
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indan, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.274	12.52 ug/l	437684	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	90
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	80
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

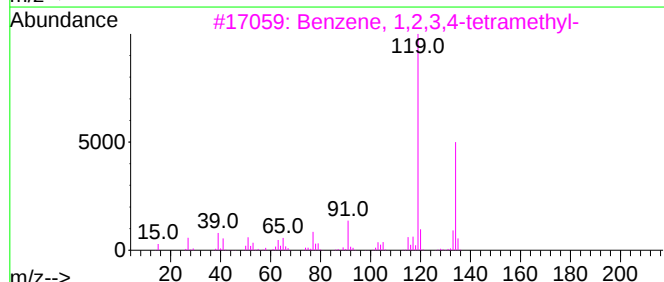
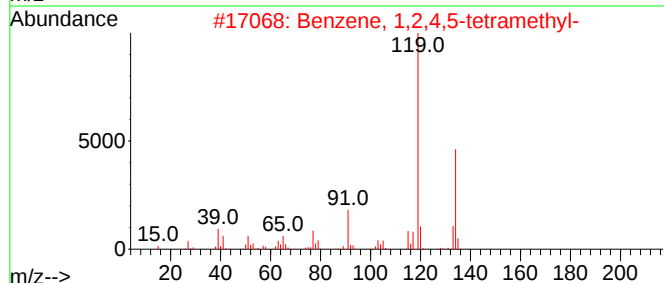
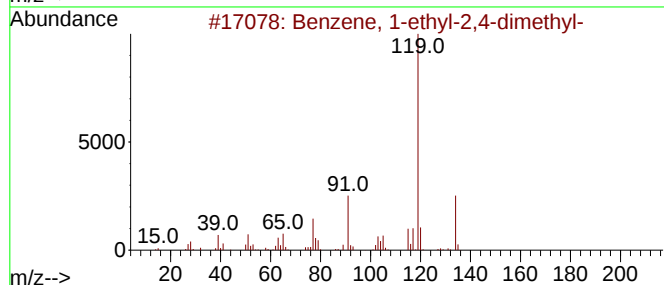
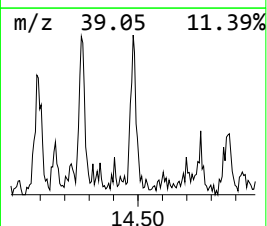
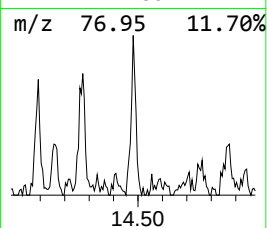
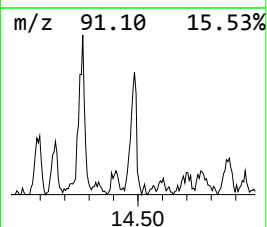
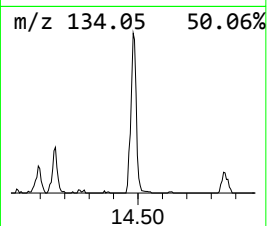
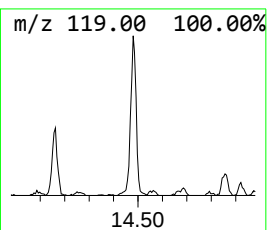
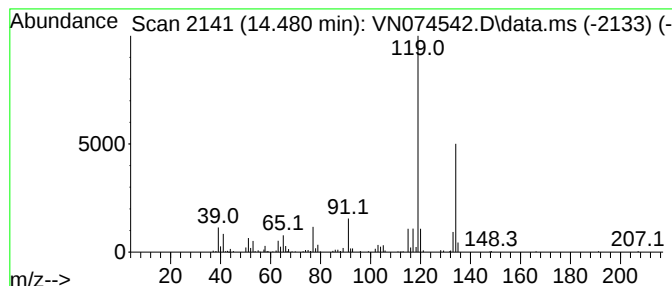
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	8.37 ug/l	292584	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5			o-Cymene	134	C10H14	000527-84-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

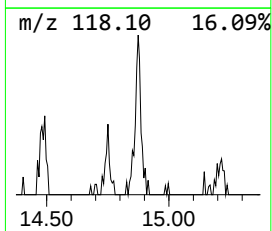
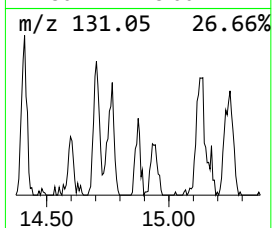
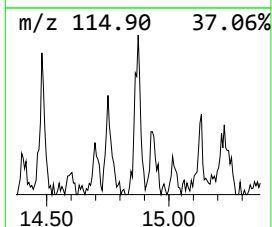
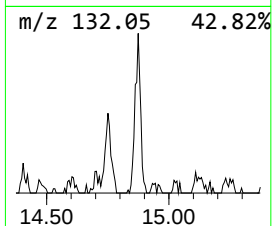
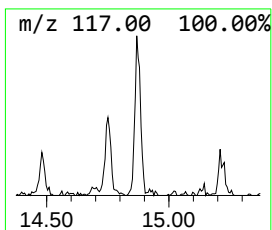
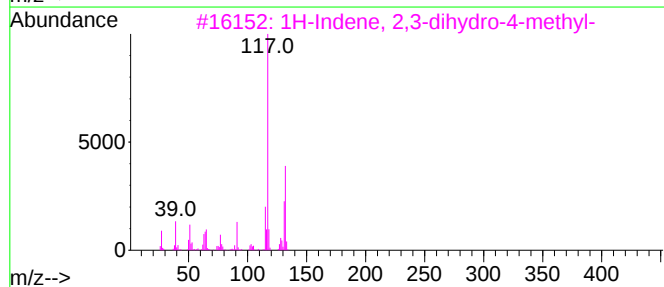
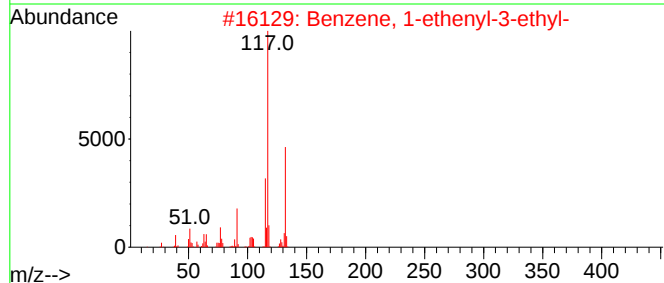
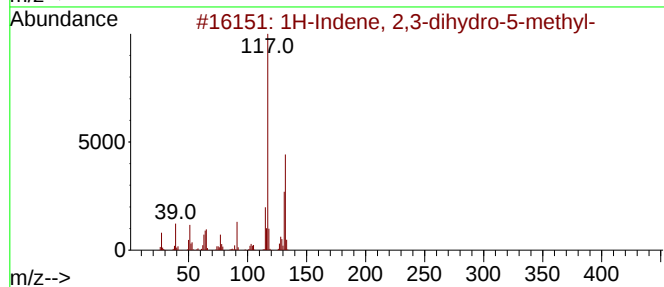
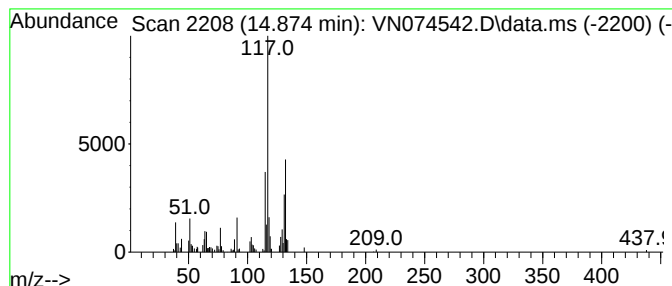
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	5.04 ug/l	176072	1,4-Dichlorobenzene-d4	13.615

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	97
2		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074542.D
Acq On : 17 Sep 2022 04:57
Operator : JC\MD
Sample : N4549-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.198	24.7	ug/l	452237	1	8.016	916658	50.0
unknown2.693	2.693	8.4	ug/l	153574	1	8.016	916658	50.0
trans-Cinnamyl ...	13.815	10.8	ug/l	377497	4	13.615	1747970	50.0
Indan, 1-methyl-	14.274	12.5	ug/l	437684	4	13.615	1747970	50.0
Benzene, 1-ethy...	14.480	8.4	ug/l	292584	4	13.615	1747970	50.0
1H-Indene, 2,3-...	14.874	5.0	ug/l	176072	4	13.615	1747970	50.0