LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

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\82N111623W.M
Title : SW846 8260

Signal : TIC: VN080371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.512	88	95	101	rVB	48341	85916	1.52%	0.222%
2	3.248	211	220	230	rVB2	98119	225771	3.99%	0.584%
3	3.653	278	289	301	rBV5	28379	96816	1.71%	0.250%
4	4.147	363	373	386	rBV3	53225	143855	2.54%	0.372%
5	5.277	555	565	568	rBV5	20543	56729	1.00%	0.147%
6	5.353	570	578	579	rBV3	34471	65425	1.16%	0.169%
7	5.806	641	655	670	rVB3	101727	386948	6.84%	1.001%
8	6.665	791	801	810	rVB2	20432	59751	1.06%	0.155%
9	7.330	904	914	922	rBV4	65121	190976	3.38%	0.494%
10	8.006	1022	1029	1036	rVB3	38762	93758	1.66%	0.242%
11	8.171	1047	1057	1061	rBV	177500	425191	7.52%	1.100%
12	8.224	1061	1066	1078	rVV	299063	746812	13.21%	1.931%
13	8.330	1078	1084	1091	rVV6	46997	115076	2.04%	0.298%
14	8.447	1099	1104	1112	rVB4	48985	105902	1.87%	0.274%
15	8.606	1118	1131	1144	rBV	2421875	5654675	100.00%	14.623%
16	8.777	1144	1160	1169	rVV	1283967	3177338	56.19%	8.217%
17	8.859	1169	1174	1180	rVB7	29300	65209	1.15%	0.169%
18	9.106	1206	1216	1224	rBV	437559	953745	16.87%	2.466%
19	9.600	1286	1300	1306	rBV5	78681	268518	4.75%	0.694%
20	10.018	1365	1371	1378	rVB5	56331	122350	2.16%	0.316%
21	10.147	1389	1393	1399	rVB4	66235	122255	2.16%	0.316%
22	10.347	1418	1427	1429	rBV5	33250	80439	1.42%	0.208%
23	10.412	1429	1438	1442	rVB	107987	225198	3.98%	0.582%
24	10.565	1457	1464	1470	rBV	686908	1297615	22.95%	3.356%
25	10.629	1470	1475	1484	rVV	545473	1036745	18.33%	2.681%
26	10.729	1486	1492	1504	rVB	93635	244416	4.32%	0.632%
27	10.988	1529	1536	1545	rBV5	64065	173898	3.08%	0.450%
28	11.247	1574	1580	1588	rBV5	42355	99858	1.77%	0.258%
29	11.347	1592	1597	1602	rBV6	42460	82442	1.46%	0.213%
30	11.865	1676	1685	1694	rBV	615957	1140378	20.17%	2.949%
31	11.965	1695	1702	1711	rVV	1586080	2678348	47.37%	6.926%
32	12.071	1711	1720	1731	rVB	2109159	4126738	72.98%	10.672%
33	12.212	1738	1744	1750	rVB4	37935	67604	1.20%	0.175%
34	12.400	1764	1776	1785	rBV	671115	1150909	20.35%	2.976%
35	12.694	1821	1826	1832	rVB	116712	200485	3.55%	0.518%
36	12.853	1846	1853	1863	rVB	529395	929265	16.43%	2.403%

LSC Area Percent Report

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Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

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\82N111623W.M
Title : SW846 8260

37	13.035	1879	1884	1889	rBV	110028	184717	3.27%	0.478%
38	13.100	1889	1895	1897	rVV	207815	336558	5.95%	0.870%
39	13.135	1897	1901	1904	rVV	235444	407573	7.21%	1.054%
40	13.176	1904	1908	1914	rVB	241709	386397	6.83%	0.999%
41	13.335	1928	1935	1944	rBV	589077	984290	17.41%	2.545%
42	13.482	1953	1960	1966	rBV	1175299	1911318	33.80%	4.943%
43	13.794	2006	2013	2016	rBV	650883	1190783	21.06%	3.079%
44	13.953	2034	2040	2043	rBV	160053	272951	4.83%	0.706%
45	13.994	2043	2047	2063	rVB3	659595	1456811	25.76%	3.767%
46	14.123	2063	2069	2073	rBV4	36264	67507	1.19%	0.175%
47	14.182	2073	2079	2085	rBV3	125250	219883	3.89%	0.569%
48	14.247	2085	2090	2092	rBV	138522	210666	3.73%	0.545%
49	14.276	2092	2095	2099	rVV2	110381	171999	3.04%	0.445%
50	14.329	2099	2104	2110	rVB	236355	374944	6.63%	0.970%
51	14.400	2110	2116	2119	rBV3	53802	94558	1.67%	0.245%
52	14.447	2119	2124	2132	rVB2	301928	514924	9.11%	1.332%
53	14.576	2142	2146	2152	rVB3	51487	87525	1.55%	0.226%
54	14.659	2152	2160	2163	rBV	261344	462890	8.19%	1.197%
55	14.694	2163	2166	2171	rVV	312914	485359	8.58%	1.255%
56	14.929	2201	2206	2211	rVV2	185079	325649	5.76%	0.842%
57	15.053	2217	2227	2232	rBV4	189947	509323	9.01%	1.317%
58	15.117	2232	2238	2245	rVB5	55540	136251	2.41%	0.352%
59	15.206	2248	2253	2262	rBV6	41157	98386	1.74%	0.254%
60	15.317	2262	2272	2284	rVV5	129616	405038	7.16%	1.047%
61	15.441	2286	2293	2301	rVB4	92475	234032	4.14%	0.605%
62	15.641	2321	2327	2335	rVB	146838	274881	4.86%	0.711%
63	15.747	2341	2345	2351	rBV4	34572	66096	1.17%	0.171%
64	15.947	2371	2379	2386	rBV3	45778	100574	1.78%	0.260%

Sum of corrected areas: 38669237

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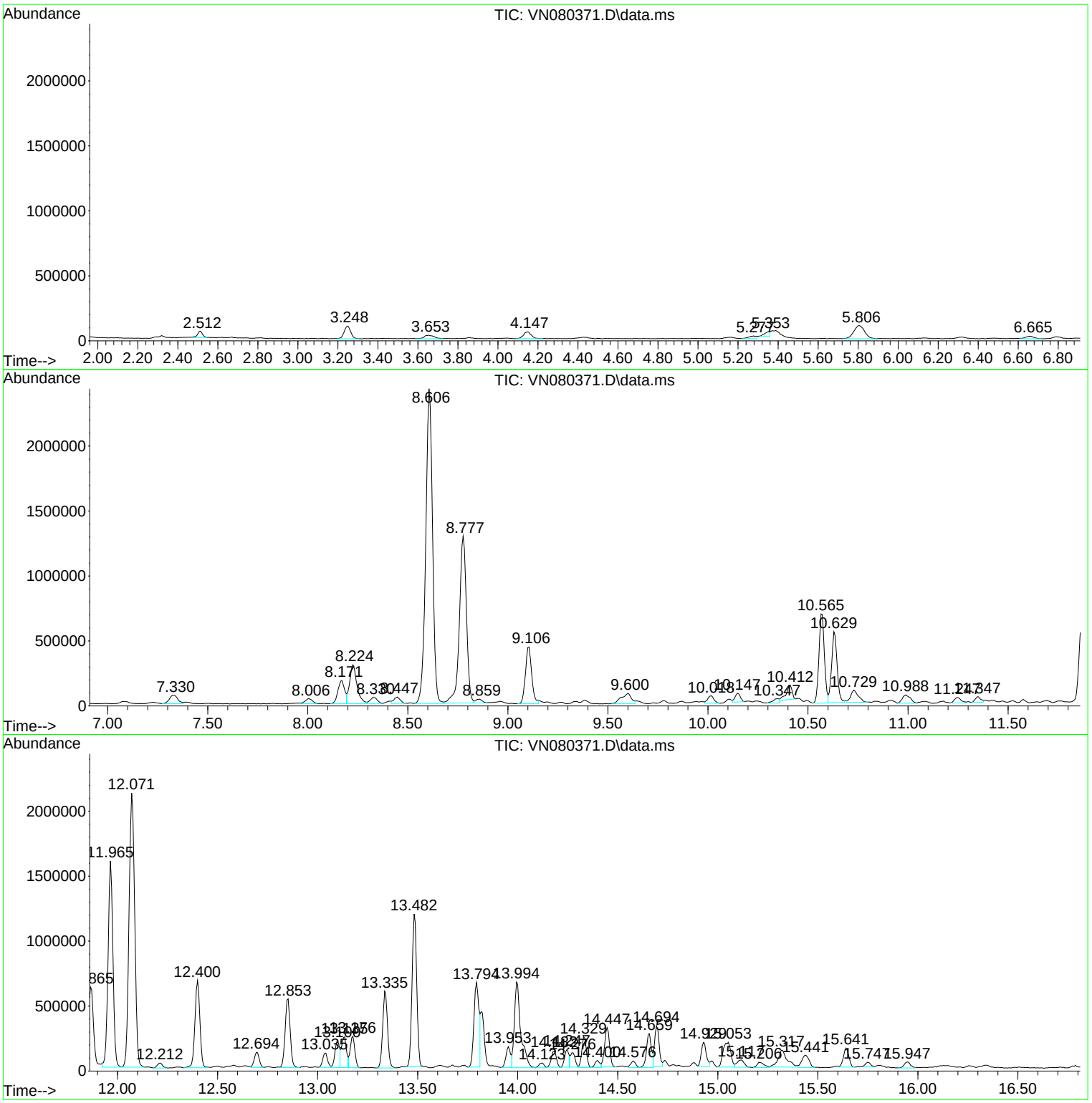
Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
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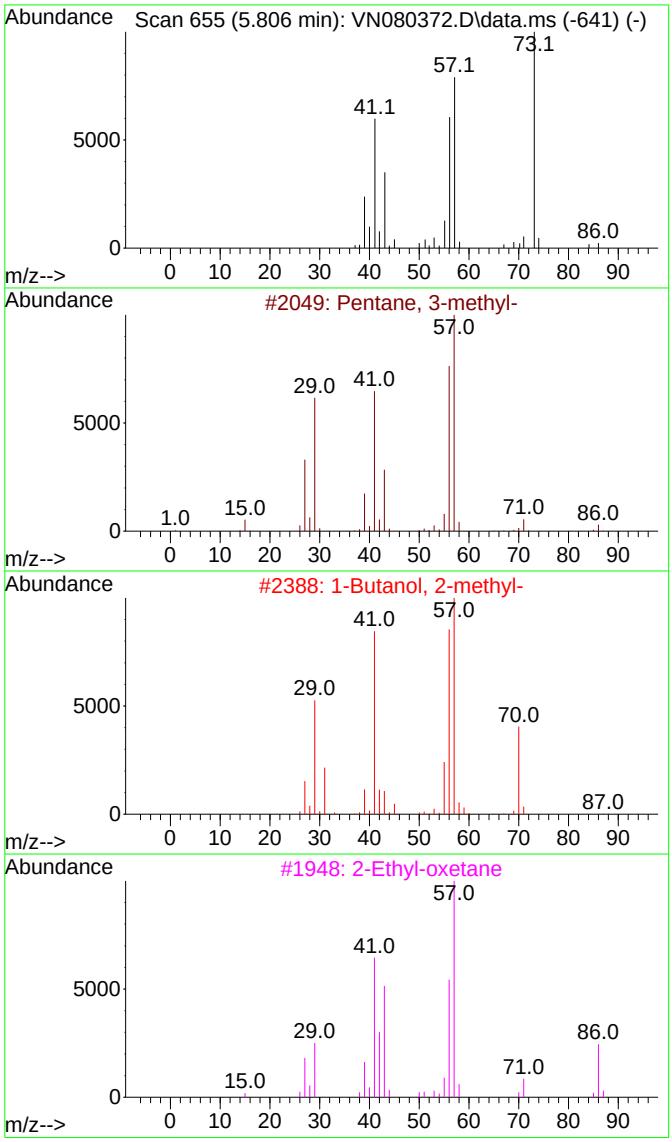
Quant Title : SW846 8260

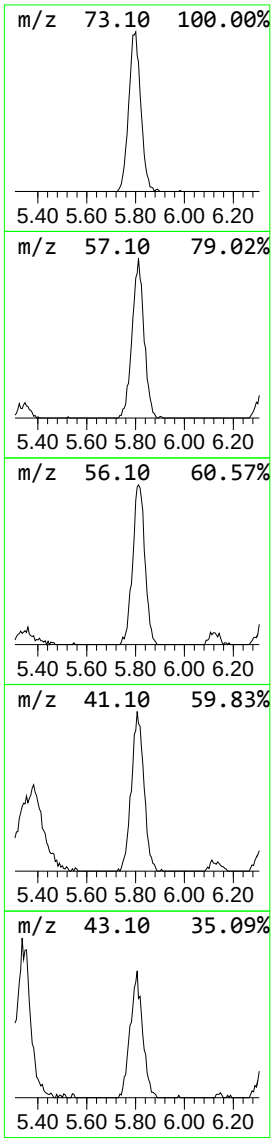
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown5.806 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.806	25.91 ug/l	386948	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	49
2	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	47
3	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	40
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

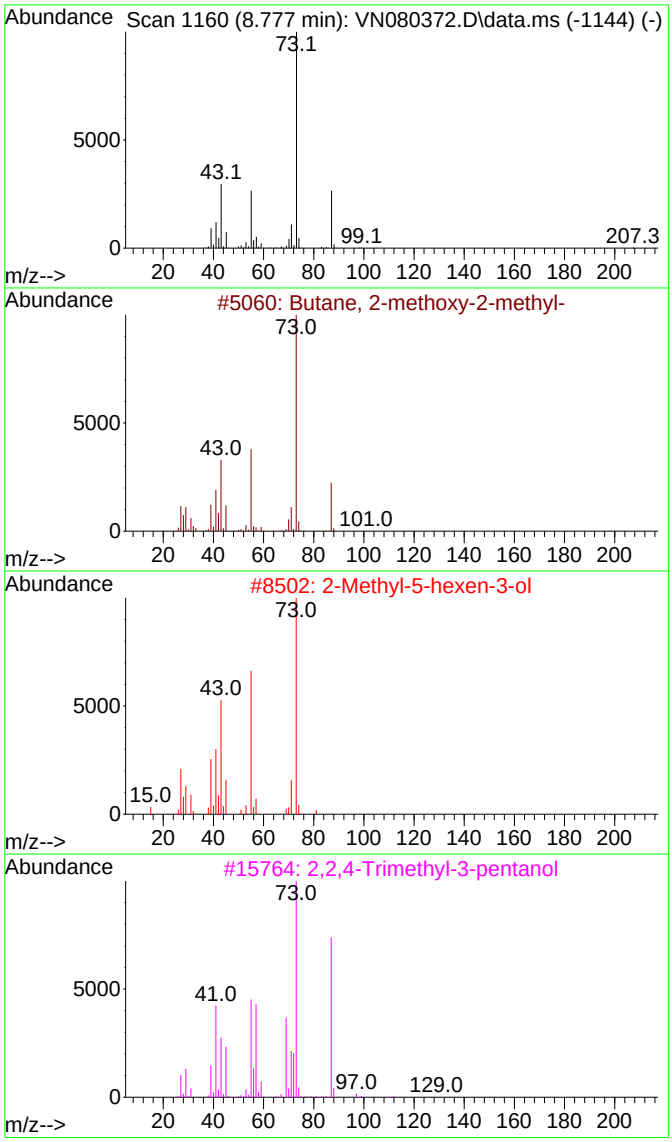
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

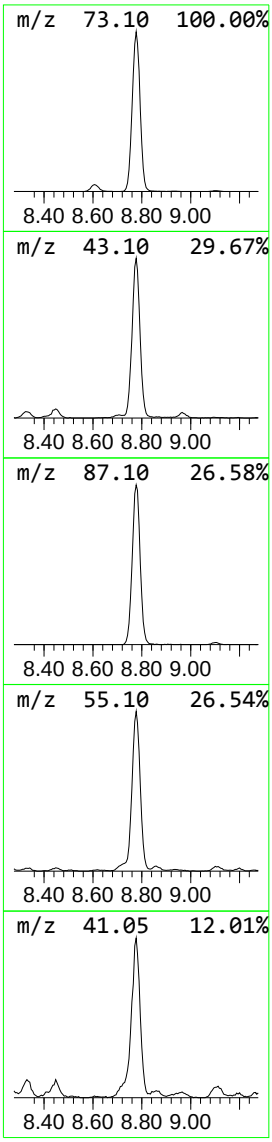
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.777	166.57 ug/l	3177340	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	25
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	10





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

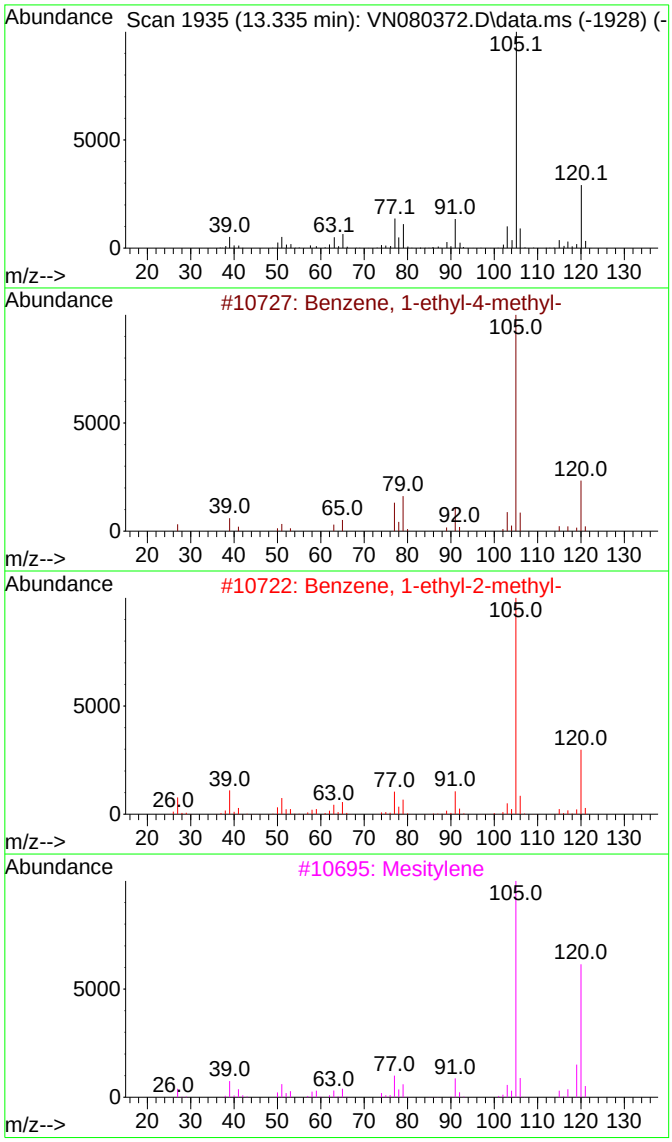
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

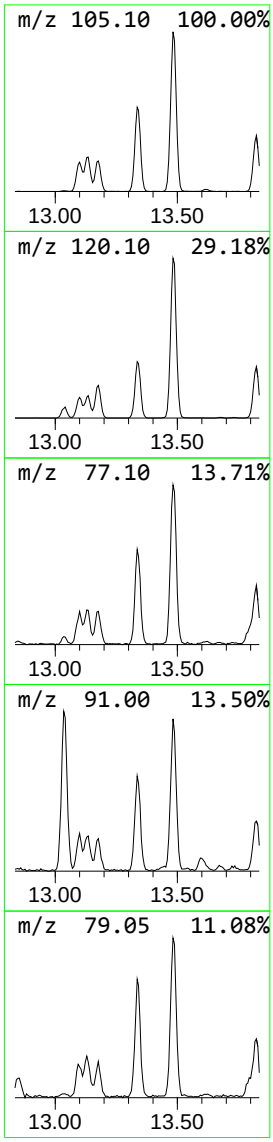
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	41.33 ug/l	984290	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

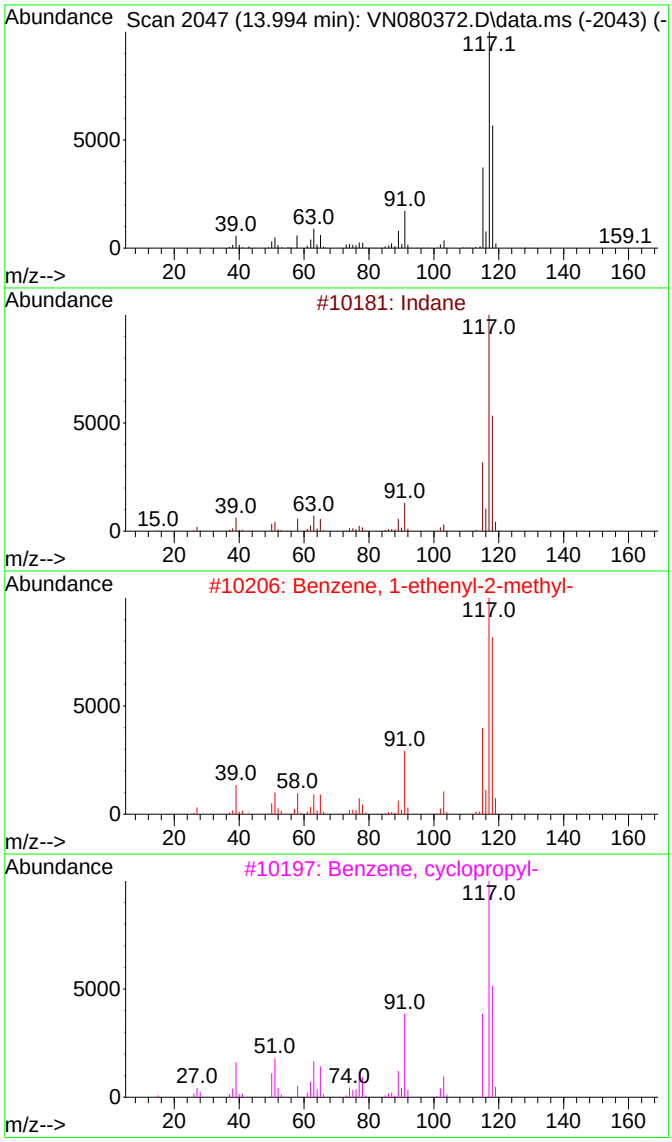
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

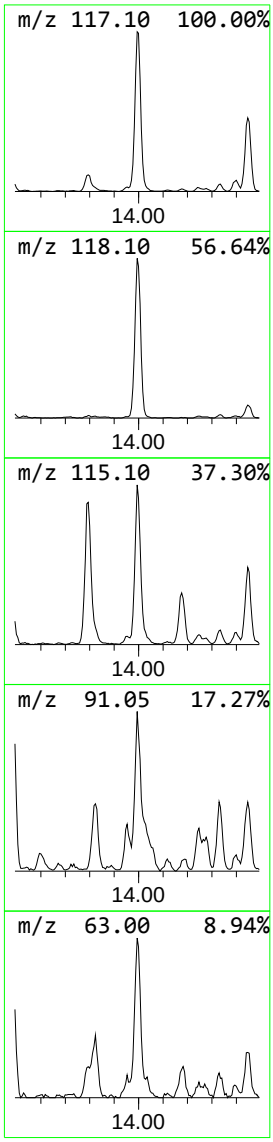
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	61.17 ug/l	1456810	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59





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Operator : JC\MD
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

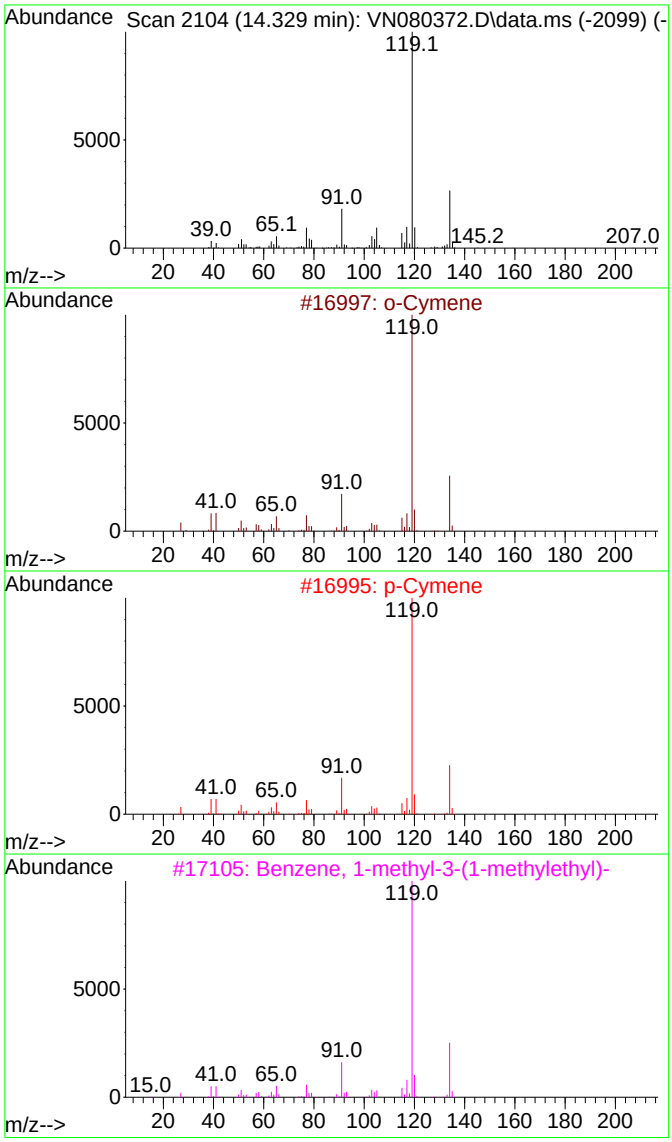
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

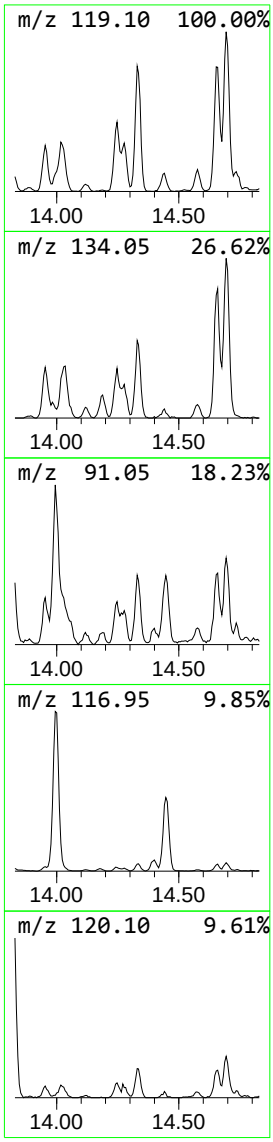
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	15.74 ug/l	374944	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	p-Cymene	134	C10H14	000099-87-6	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

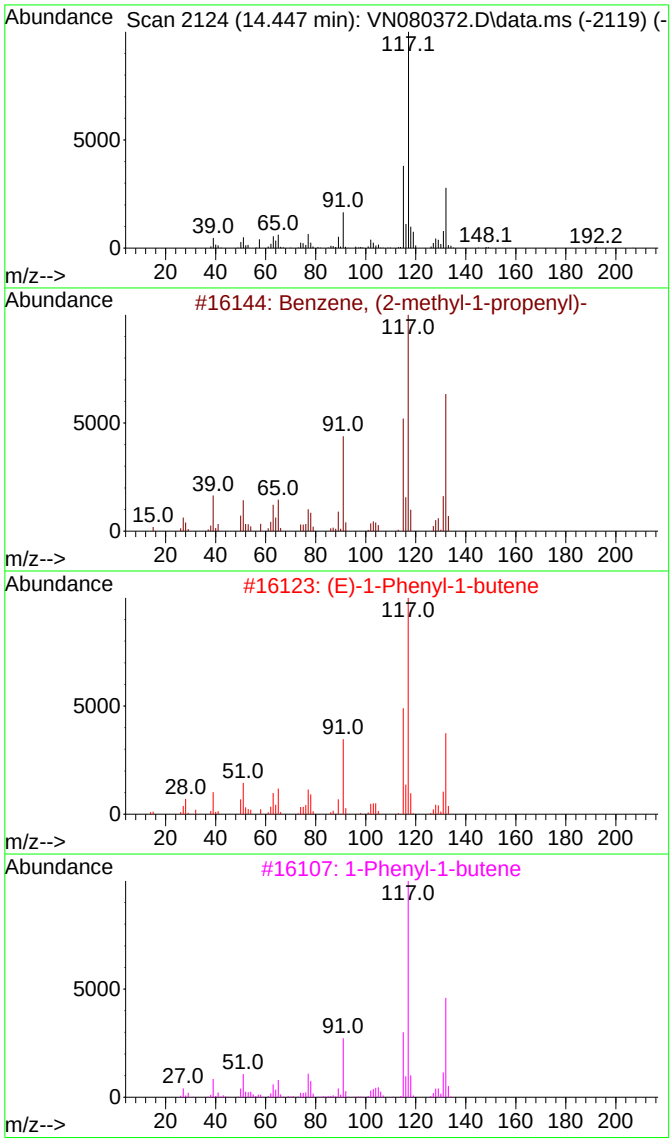
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

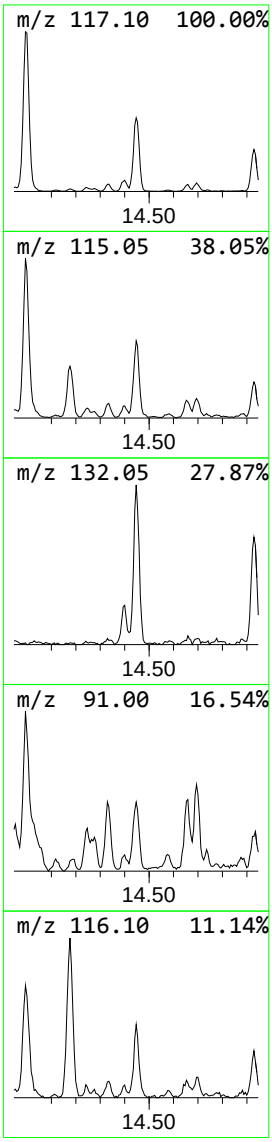
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (2-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	21.62 ug/l	514924	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
2	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	91
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	86
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

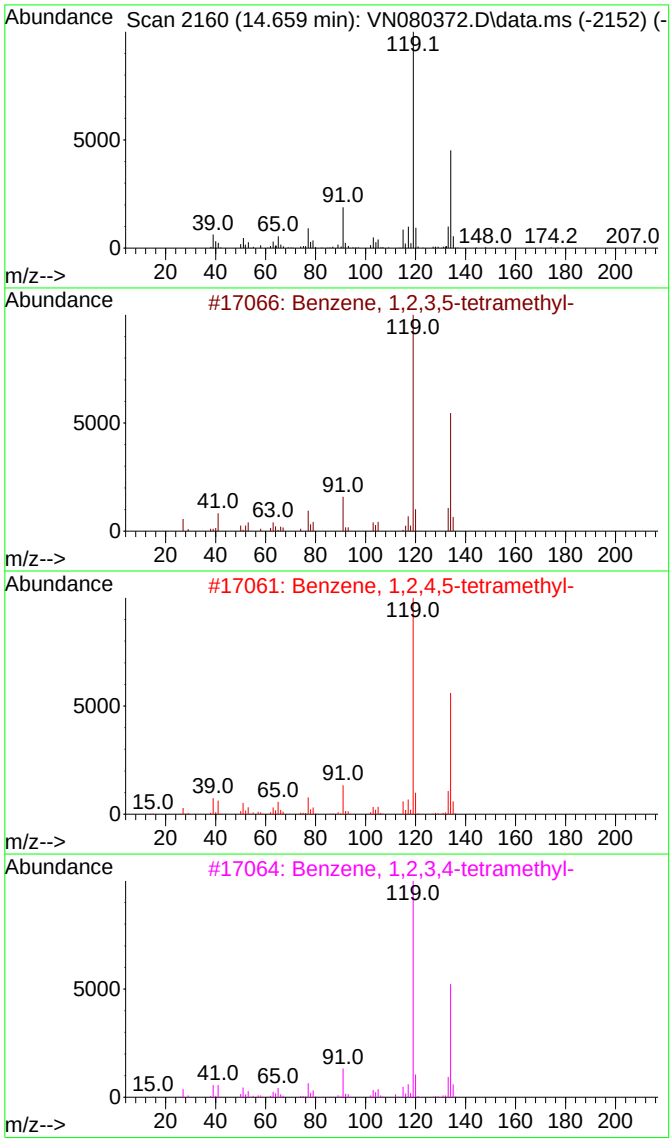
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

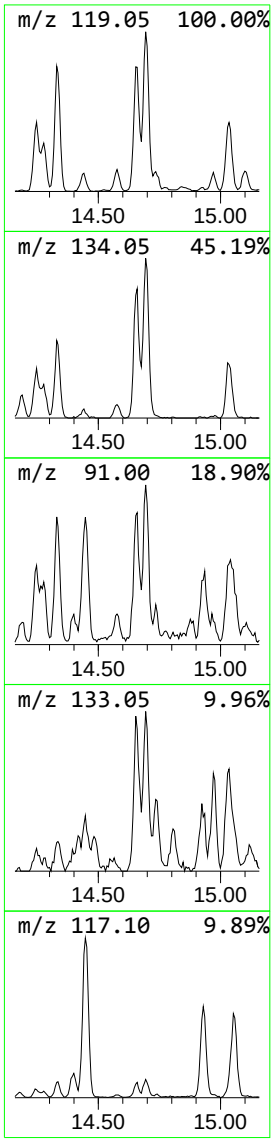
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.659	19.44 ug/l	462890	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
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	95
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	95
5	o-Cymene	134	C10H14	000527-84-4	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

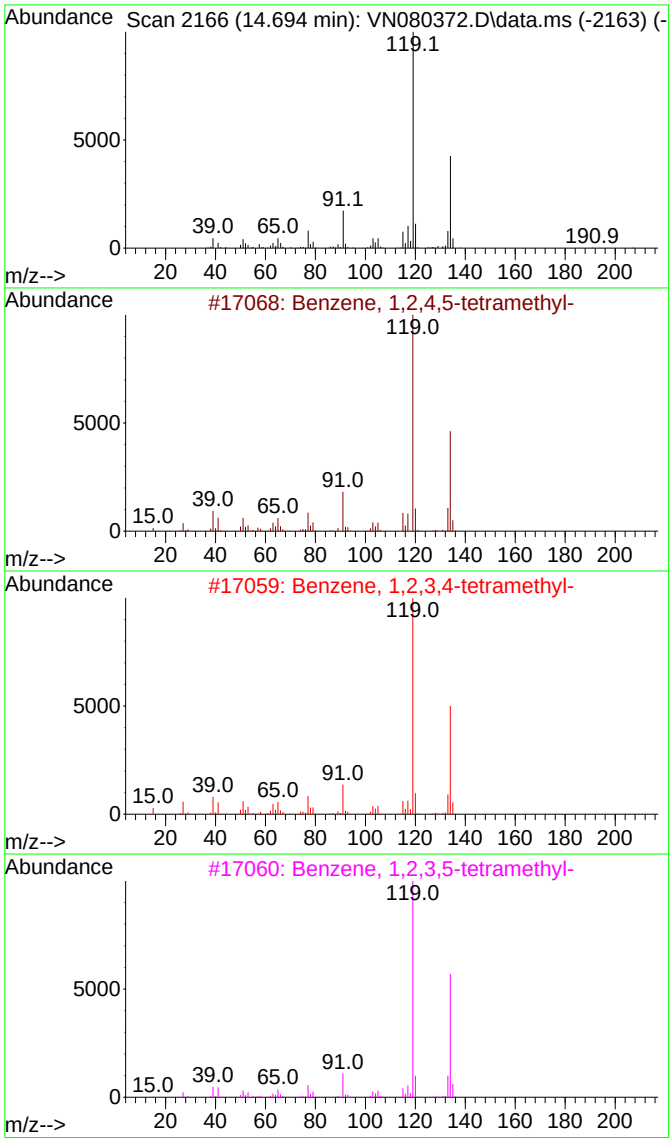
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

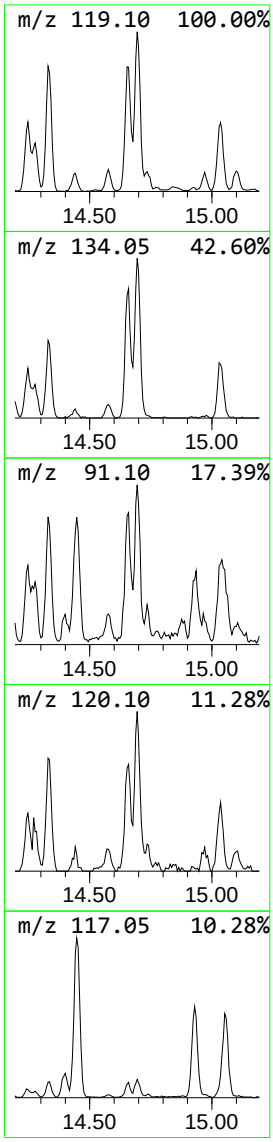
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.694	20.38 ug/l	485359	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

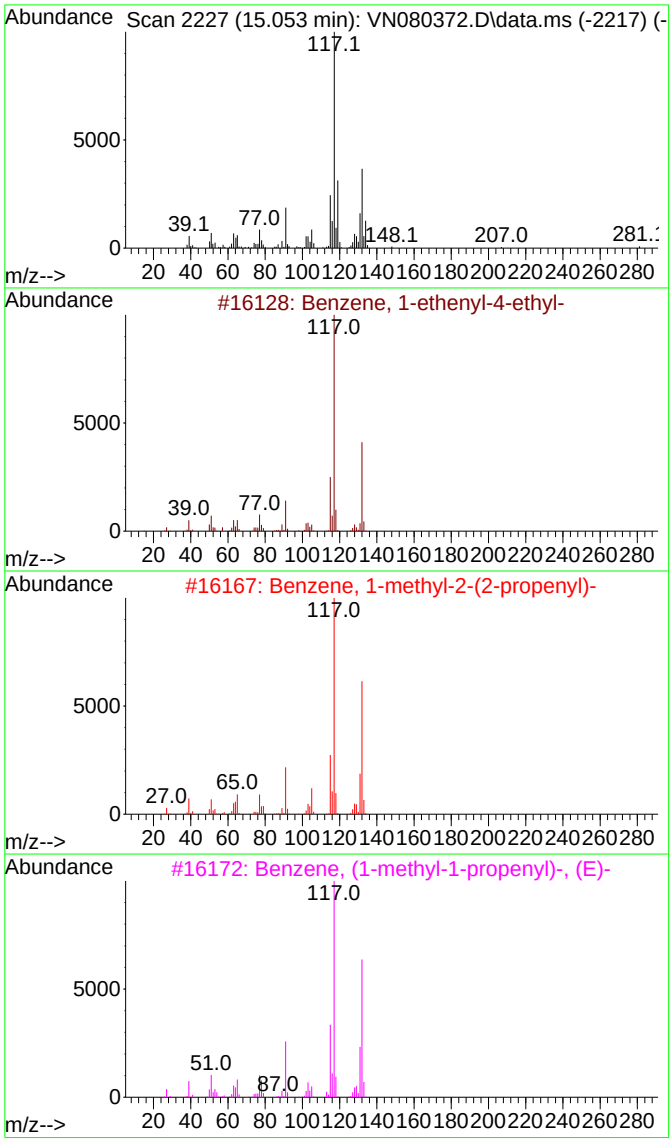
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

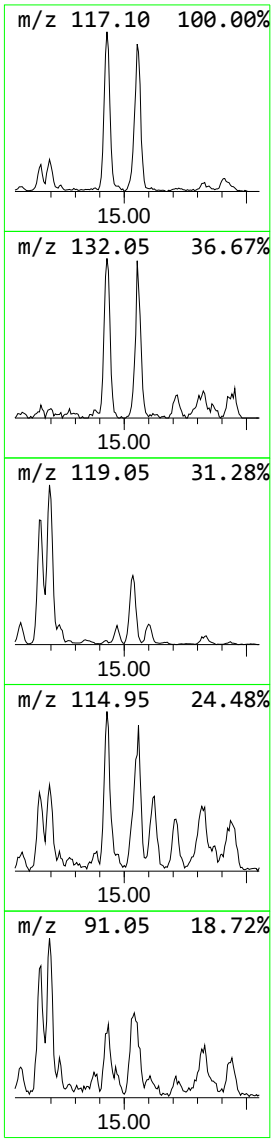
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	21.39 ug/l	509323	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

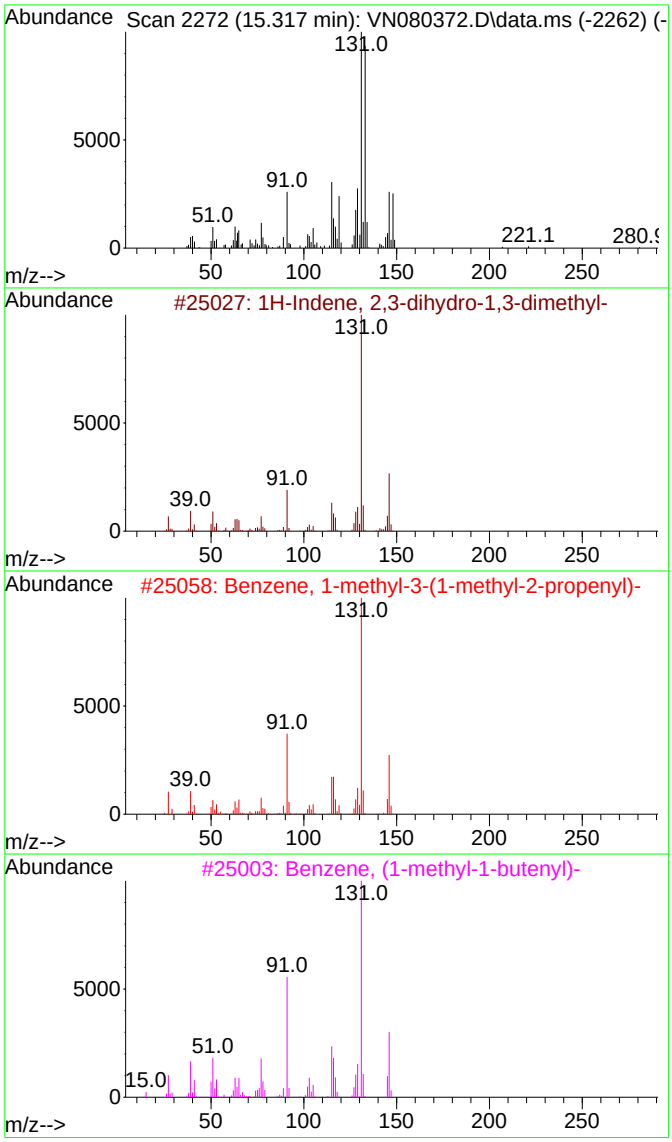
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

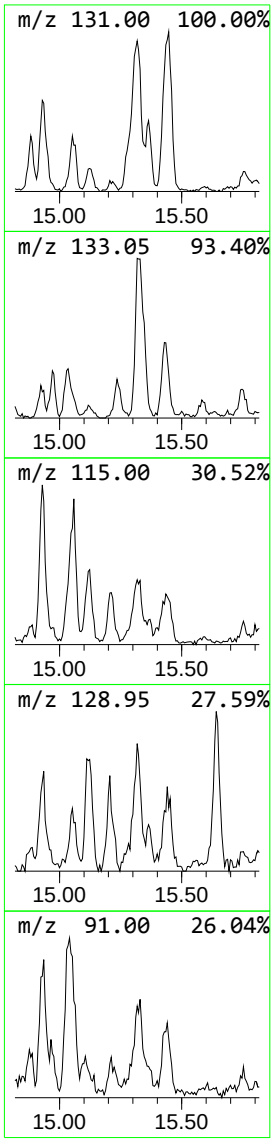
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-1,3-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	17.01 ug/l	405038	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	50
2	Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	50
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	50
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120523\
Data File : VN080372.D
Acq On : 05 Dec 2023 17:44
Operator : JC\MD
Sample : 05622-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.806	5.806	25.9	ug/l	386948	1	8.230	746812	50.0
Butane, 2-metho...	8.777	166.6	ug/l	3177340	2	9.106	953745	50.0
Benzene, 1-ethy...	13.335	41.3	ug/l	984290	4	13.794	1190780	50.0
Indane	13.994	61.2	ug/l	1456810	4	13.794	1190780	50.0
o-Cymene	14.329	15.7	ug/l	374944	4	13.794	1190780	50.0
Benzene, (2-met...	14.447	21.6	ug/l	514924	4	13.794	1190780	50.0
Benzene, 1,2,3,...	14.659	19.4	ug/l	462890	4	13.794	1190780	50.0
Benzene, 1,2,4,...	14.694	20.4	ug/l	485359	4	13.794	1190780	50.0
Benzene, 1-ethe...	15.053	21.4	ug/l	509323	4	13.794	1190780	50.0
1H-Indene, 2,3-...	15.317	17.0	ug/l	405038	4	13.794	1190780	50.0