LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

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\82N112224W.M
Title : SW846 8260

Signal : TIC: VN085235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.318	50	62	77	rBV2	49784	177002	2.74%	0.460%
2	2.506	86	94	103	rVB	73219	122460	1.90%	0.318%
3	3.247	210	220	231	rVB	219831	504779	7.82%	1.311%
4	3.647	277	288	301	rBV3	55232	175713	2.72%	0.456%
5	4.142	361	372	386	rVB	82565	220927	3.42%	0.574%
6	5.147	532	543	555	rBV2	22863	78568	1.22%	0.204%
7	5.277	555	565	568	rVV4	28025	86976	1.35%	0.226%
8	5.353	568	578	608	rVB6	83496	512323	7.94%	1.331%
9	5.806	642	655	671	rVB4	102102	356169	5.52%	0.925%
10	6.312	730	741	751	rBV2	23906	72291	1.12%	0.188%
11	6.653	789	799	811	rVB2	31814	91791	1.42%	0.238%
12	7.082	863	872	882	rBV4	27526	76263	1.18%	0.198%
13	7.324	904	913	922	rBV	109927	315980	4.90%	0.821%
14	8.006	1021	1029	1037	rVB2	55948	138948	2.15%	0.361%
15	8.165	1047	1056	1060	rBV	120398	281021	4.35%	0.730%
16	8.224	1060	1066	1078	rVV2	271858	763234	11.83%	1.983%
17	8.324	1078	1083	1092	rVV3	51802	129123	2.00%	0.335%
18	8.441	1092	1103	1110	rVV3	57531	139276	2.16%	0.362%
19	8.606	1118	1131	1143	rBV	2355663	5587788	86.59%	14.516%
20	8.777	1143	1160	1168	rVV2	518266	1500344	23.25%	3.898%
21	8.853	1168	1173	1180	rVV4	40698	96159	1.49%	0.250%
22	9.100	1206	1215	1228	rBV	363100	832336	12.90%	2.162%
23	9.382	1258	1263	1272	rVB2	31178	65709	1.02%	0.171%
24	9.600	1283	1300	1316	rBV4	147931	475719	7.37%	1.236%
25	10.012	1365	1370	1379	rVB	62856	128299	1.99%	0.333%
26	10.100	1379	1385	1389	rBV	80447	160733	2.49%	0.418%
27	10.147	1389	1393	1399	rVB2	81467	146839	2.28%	0.381%
28	10.341	1415	1426	1429	rBV6	32028	84332	1.31%	0.219%
29	10.406	1429	1437	1441	rVV	98282	239163	3.71%	0.621%
30	10.447	1441	1444	1449	rVV	63613	115403	1.79%	0.300%
31	10.565	1457	1464	1469	rBV	519016	963533	14.93%	2.503%
32	10.629	1469	1475	1483	rVV	749606	1382069	21.42%	3.590%
33	10.729	1483	1492	1503	rVB3	75629	215786	3.34%	0.561%
34	10.982	1529	1535	1545	rVB4	59551	162171	2.51%	0.421%
35	11.865	1675	1685	1691	rBV	419724	776459	12.03%	2.017%
36	11.965	1695	1702	1711	rVV	1489988	2617129	40.55%	6.799%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

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\82N112224W.M
Title : SW846 8260

37	12.065	1711	1719	1732	rVB	3276323	6453473	100.00%	16.765%
38	12.206	1738	1743	1750	rVB3	39411	70524	1.09%	0.183%
39	12.394	1764	1775	1784	rBV	1207073	2070479	32.08%	5.379%
40	12.694	1820	1826	1833	rVB	80042	132409	2.05%	0.344%
41	12.847	1843	1852	1861	rBV	358093	613215	9.50%	1.593%
42	13.035	1878	1884	1889	rBV	95914	157325	2.44%	0.409%
43	13.094	1889	1894	1897	rVV	222068	365137	5.66%	0.949%
44	13.129	1897	1900	1903	rVV	203826	301050	4.66%	0.782%
45	13.170	1903	1907	1914	rVB	206459	333095	5.16%	0.865%
46	13.335	1927	1935	1944	rBV	496110	814254	12.62%	2.115%
47	13.482	1952	1960	1967	rBV	1218124	1976735	30.63%	5.135%
48	13.788	2005	2012	2015	rBV	409914	771695	11.96%	2.005%
49	13.817	2015	2017	2025	rVB	438351	568596	8.81%	1.477%
50	13.947	2033	2039	2041	rBV	88380	128011	1.98%	0.333%
51	13.994	2041	2047	2060	rVV3	457759	1096448	16.99%	2.848%
52	14.176	2072	2078	2084	rVV3	112895	190544	2.95%	0.495%
53	14.241	2084	2089	2092	rVV	114062	194418	3.01%	0.505%
54	14.270	2092	2094	2099	rVV	104002	138315	2.14%	0.359%
55	14.329	2099	2104	2110	rVB	193334	291161	4.51%	0.756%
56	14.441	2118	2123	2131	rVB2	153538	268447	4.16%	0.697%
57	14.570	2140	2145	2151	rVB2	43832	75162	1.16%	0.195%
58	14.653	2151	2159	2162	rBV	129993	218293	3.38%	0.567%
59	14.688	2162	2165	2170	rVV	174786	270412	4.19%	0.702%
60	14.923	2200	2205	2210	rBV	94260	162398	2.52%	0.422%
61	15.047	2217	2226	2232	rBV3	144871	356754	5.53%	0.927%
62	15.317	2262	2272	2277	rBV4	61025	163052	2.53%	0.424%
63	15.435	2285	2292	2300	rVB3	46565	120506	1.87%	0.313%
64	15.641	2319	2327	2335	rVB	203222	399254	6.19%	1.037%

Sum of corrected areas: 38493977

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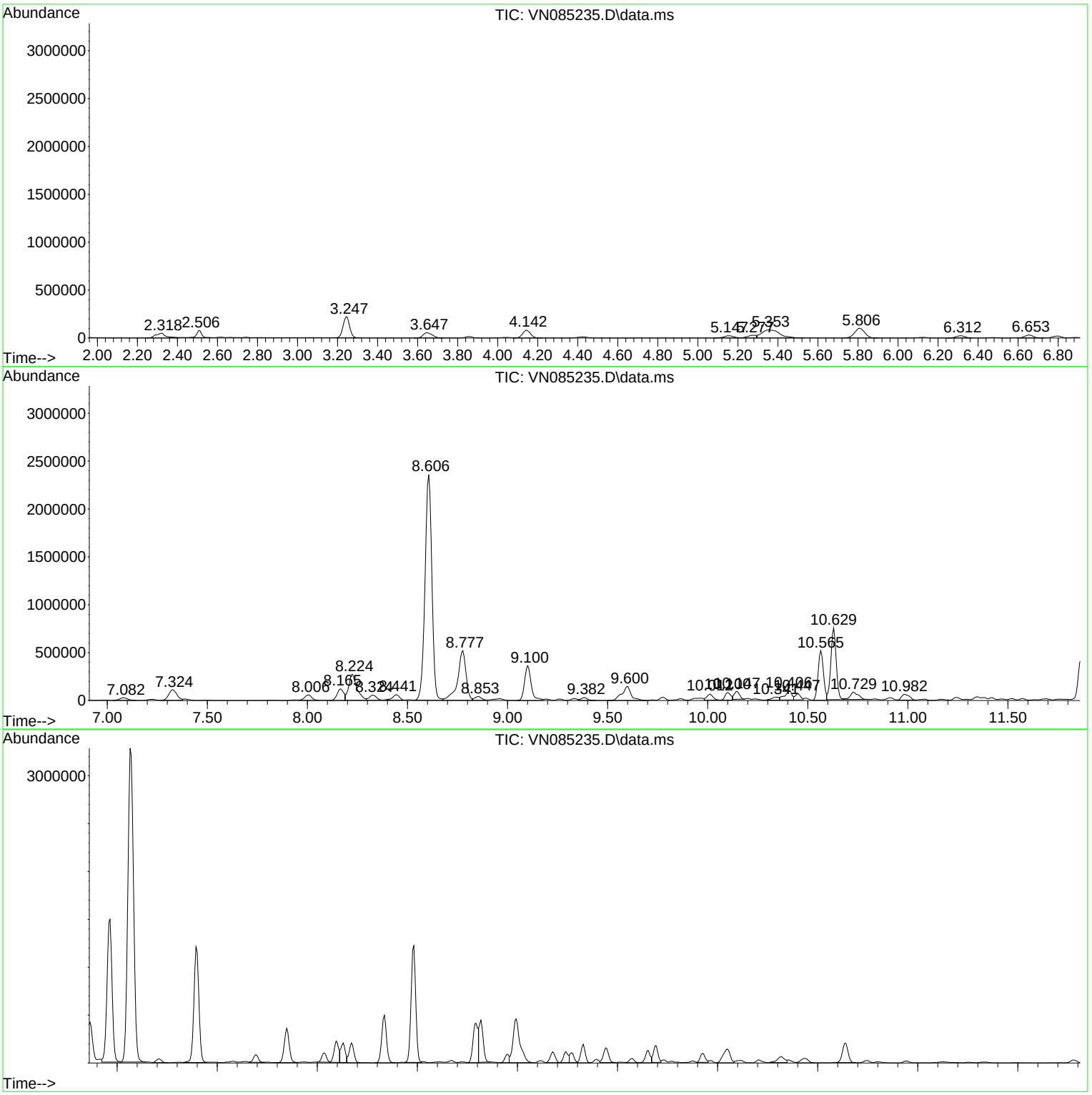
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
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Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

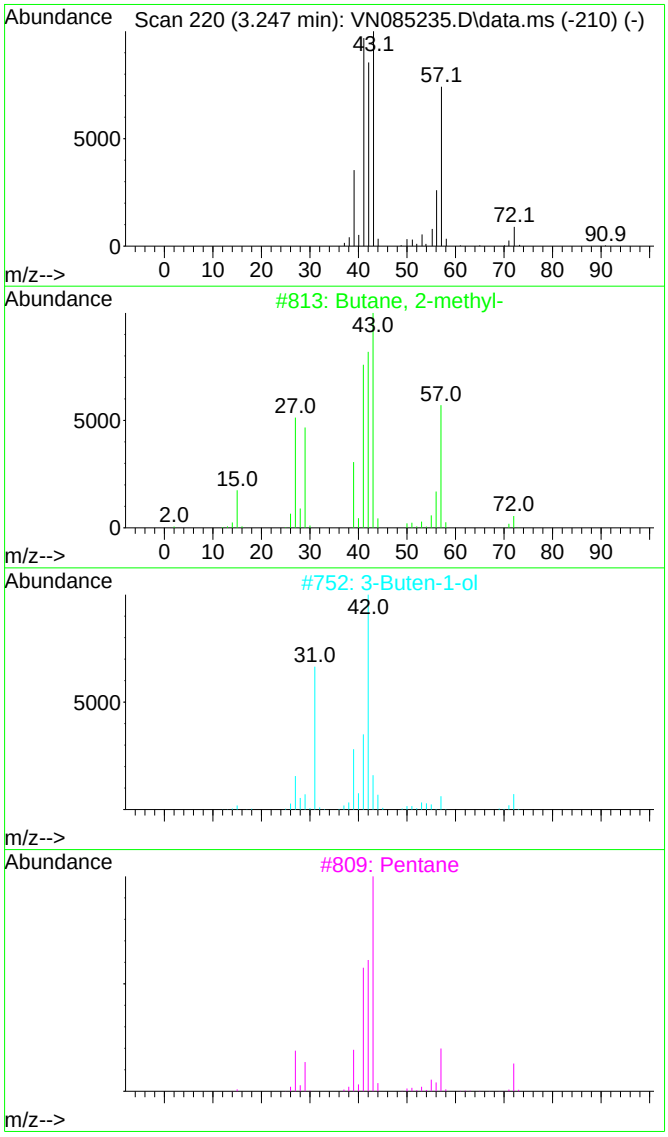
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

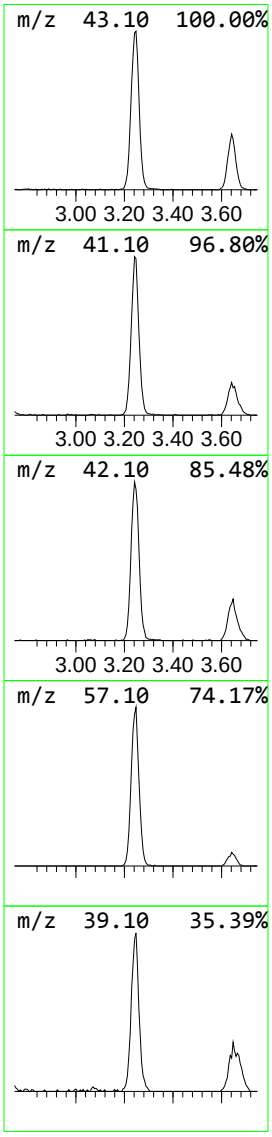
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.247	33.07 ug/l	504779	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Pentane	72	C5H12	000109-66-0	33
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

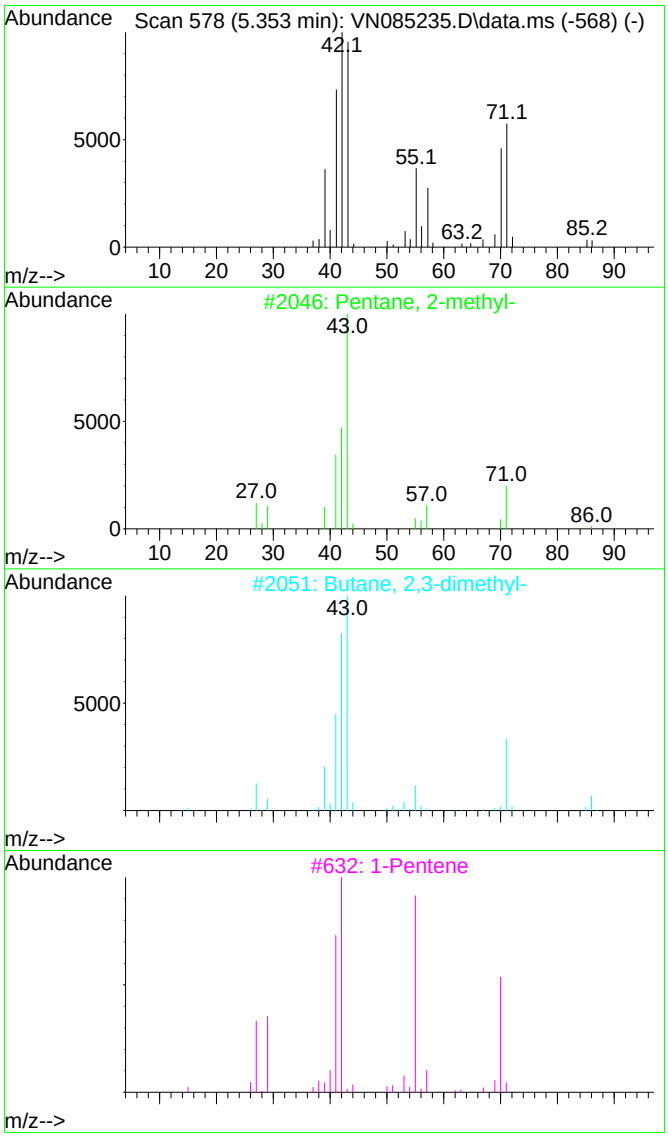
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

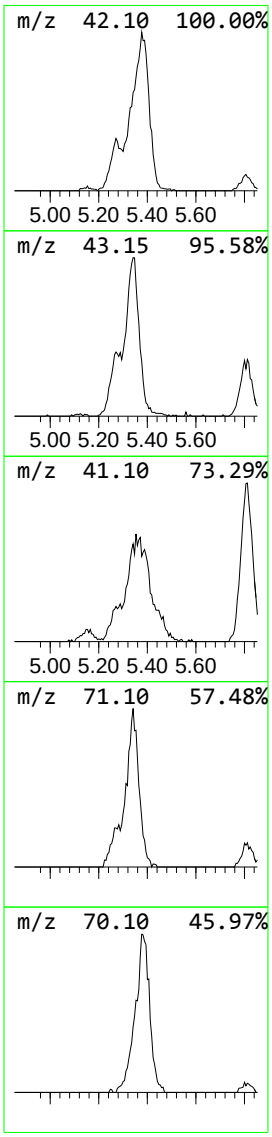
****

Peak Number 2 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.353	33.56 ug/l	512323	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53
3	1-Pentene	70	C5H10	000109-67-1	52
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

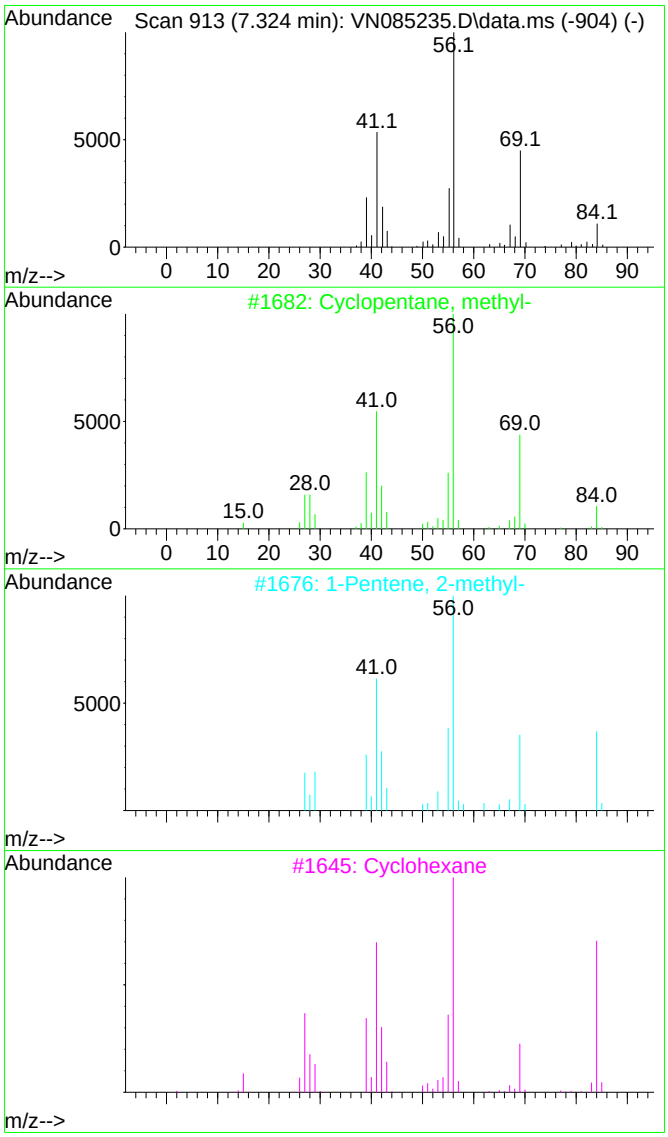
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

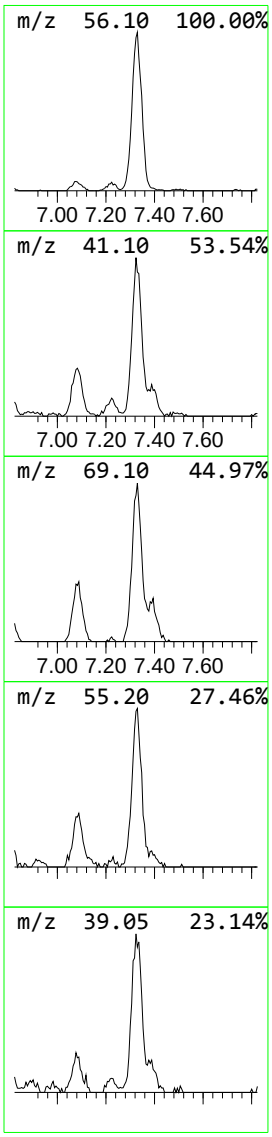
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.324	20.70 ug/l	315980	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	Cyclohexane	84	C6H12	000110-82-7	80
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

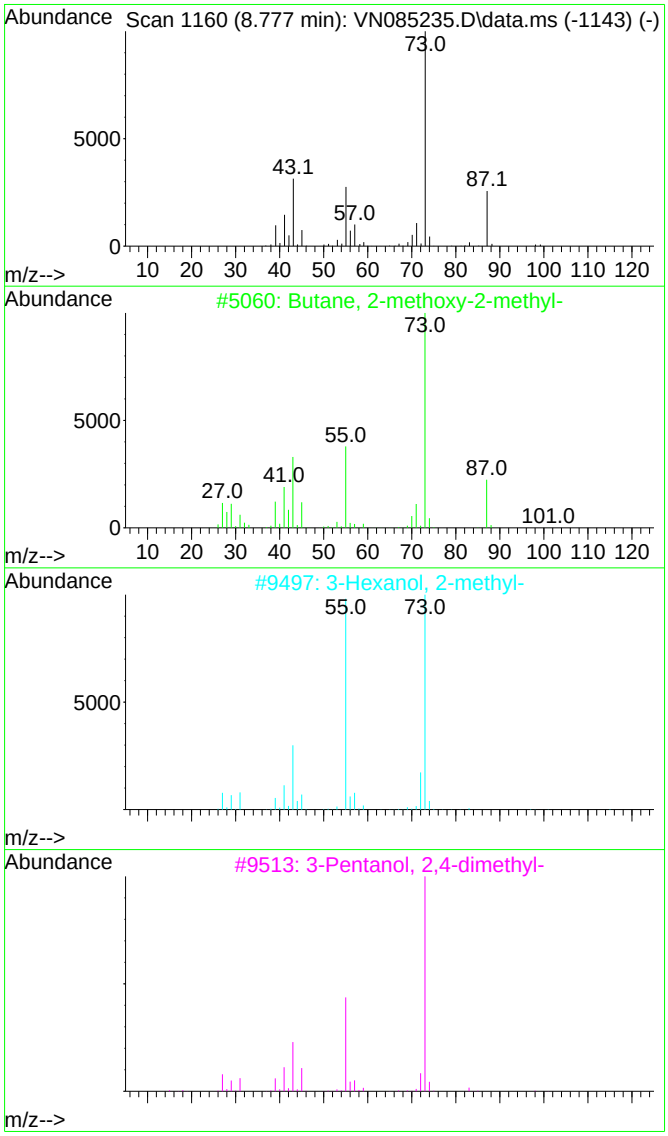
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

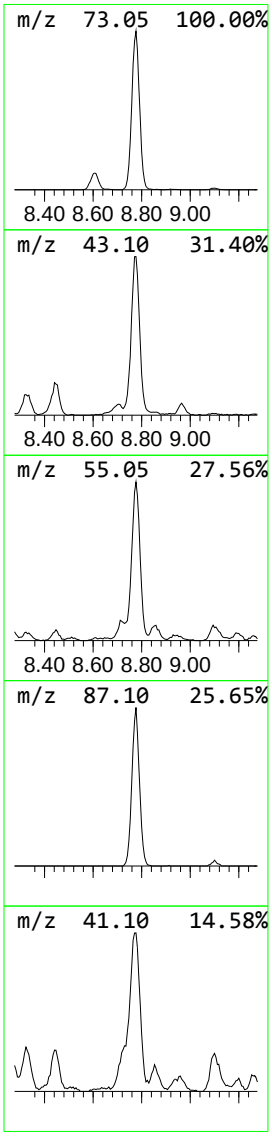
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.777	90.13 ug/l	1500340	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	meso-2,5-Dimethyl-3,4-hexanediol	146	C8H18O2	022520-38-3	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

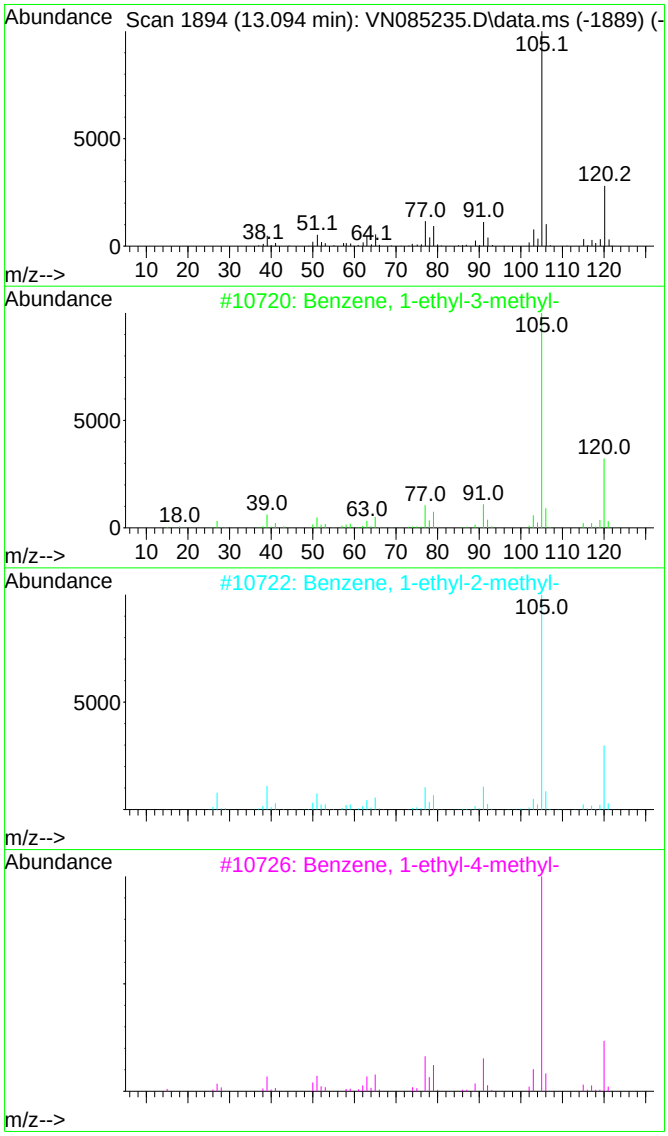
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

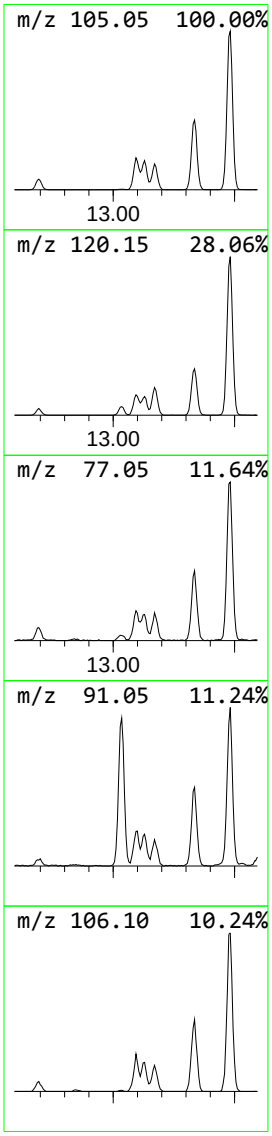
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	23.66 ug/l	365137	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

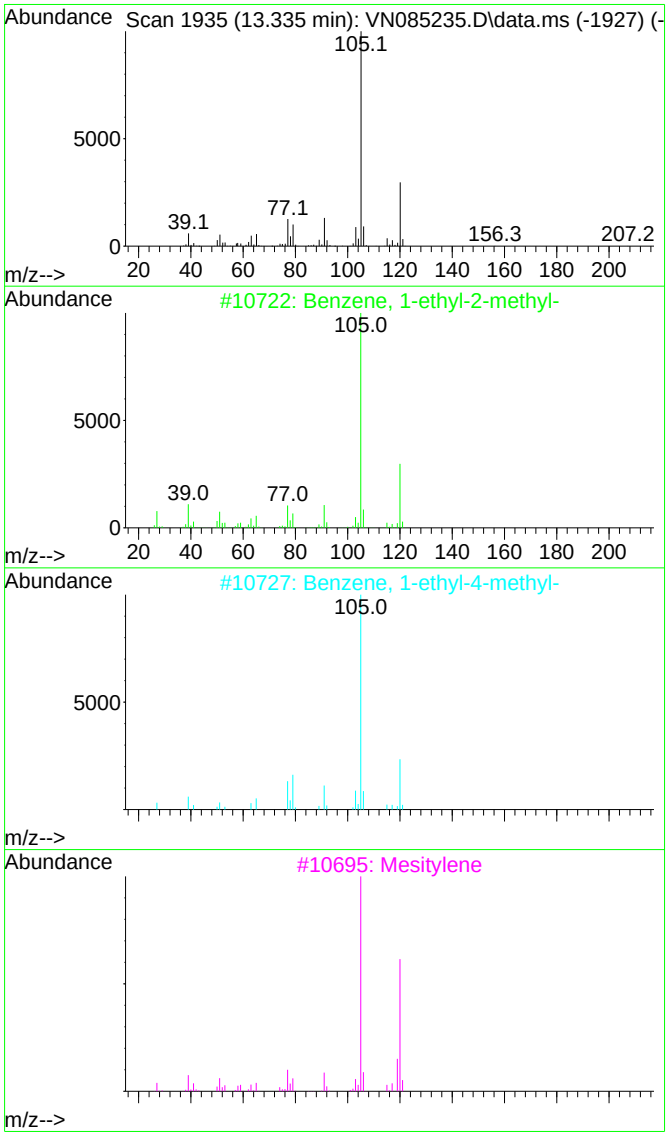
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

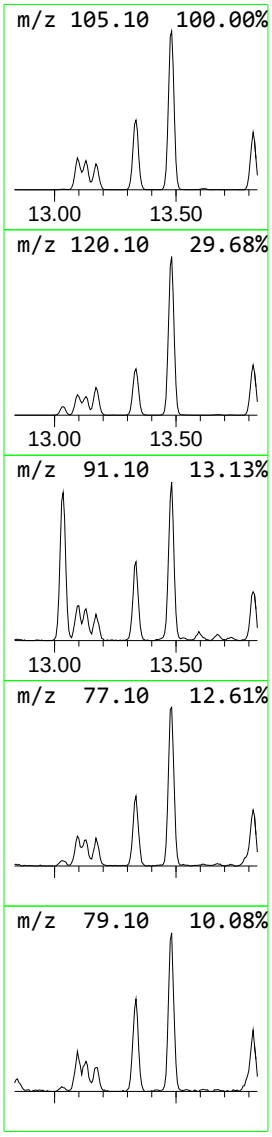
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	52.76 ug/l	814254	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

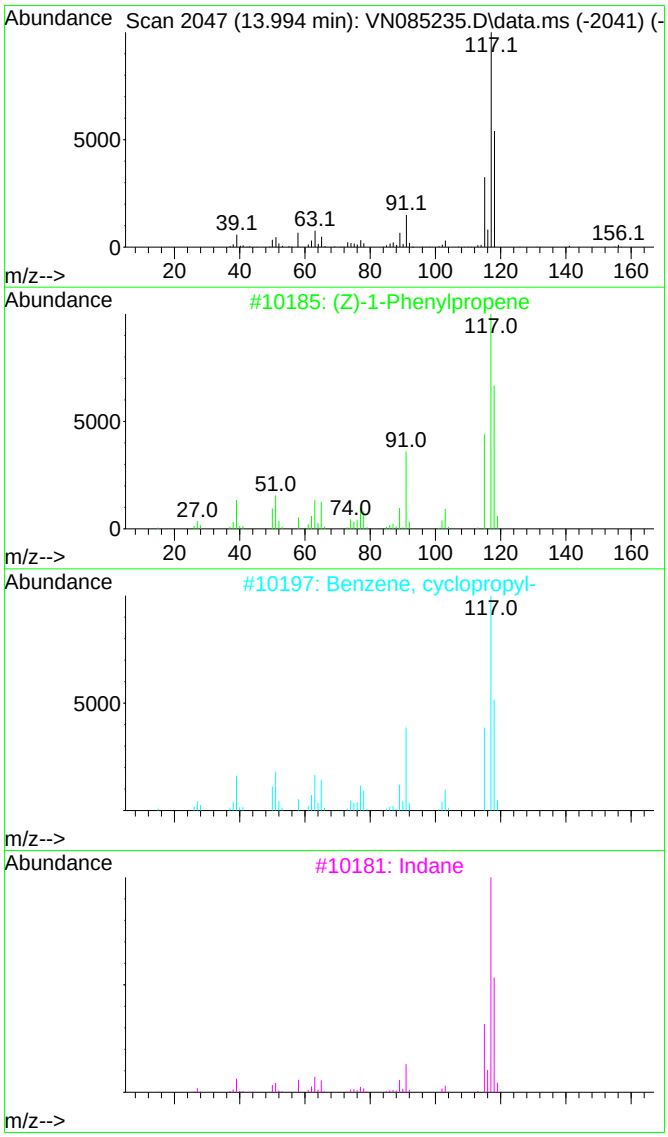
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

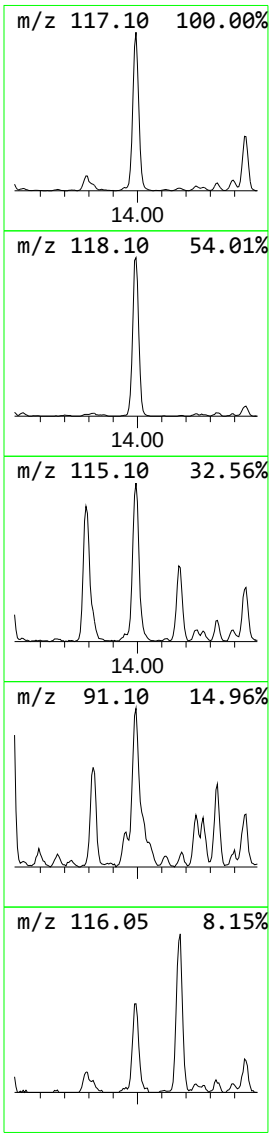
****

Peak Number 7 (Z)-1-Phenylpropene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	71.04 ug/l	1096450	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	74
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3	Indane	118	C9H10	000496-11-7	72
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	59





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Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

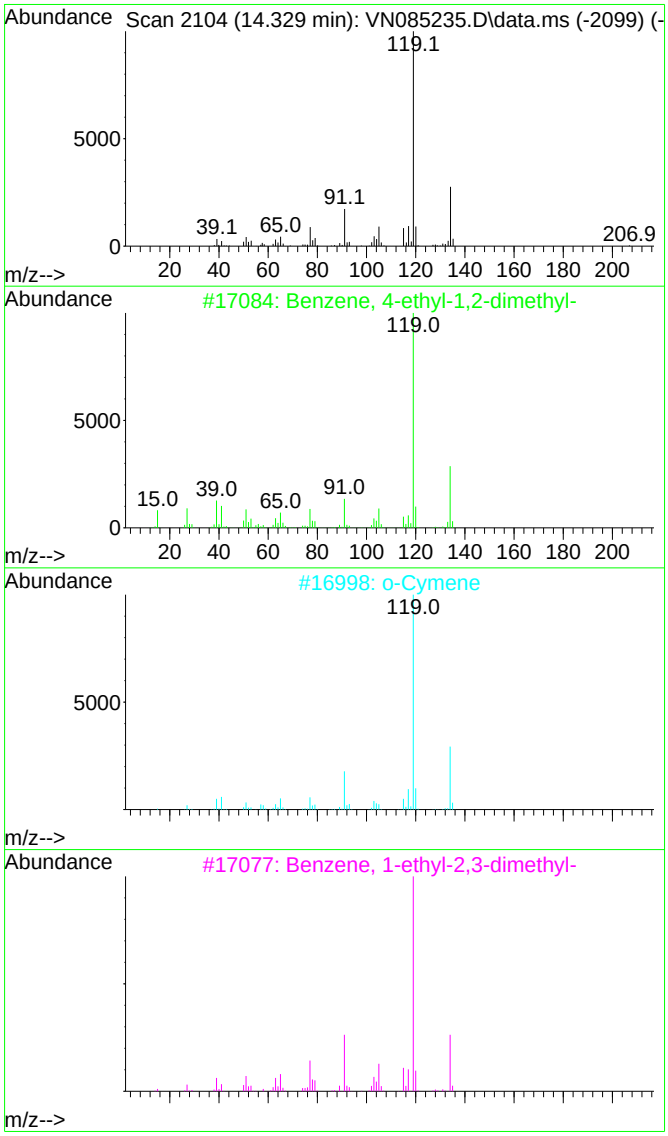
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

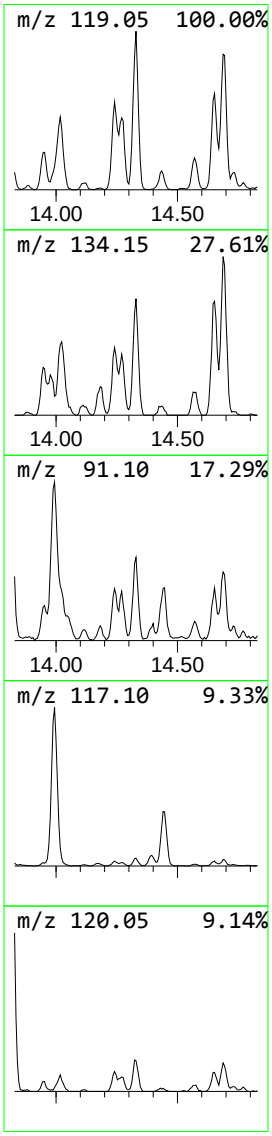
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	18.86 ug/l	291161	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

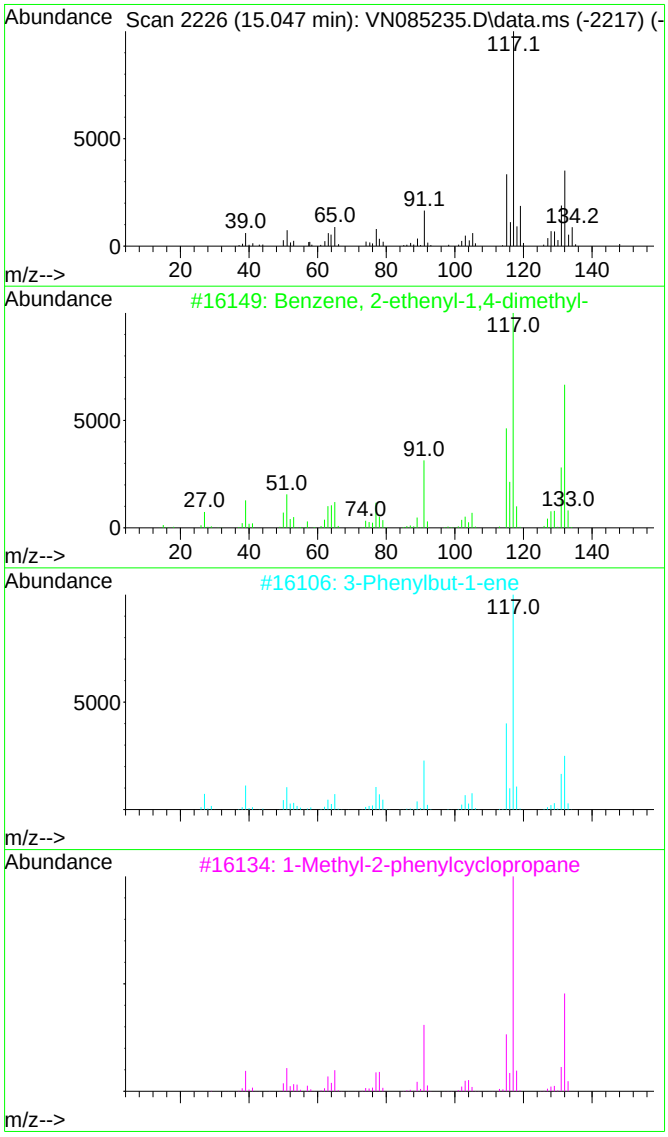
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

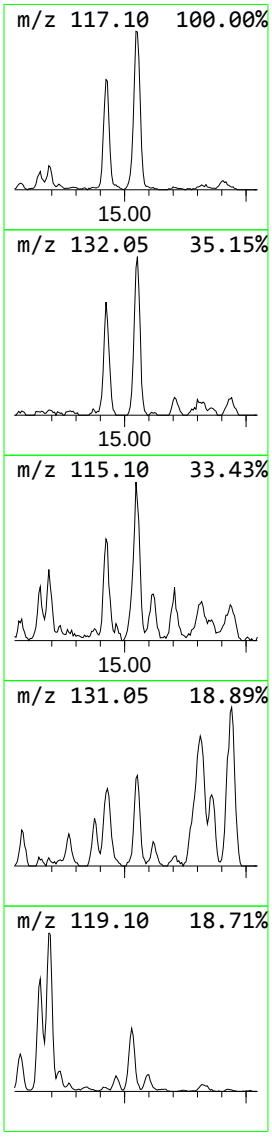
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	23.11 ug/l	356754	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	93
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085235.D
Acq On : 17 Dec 2024 19:34
Operator : JC\MD
Sample : P5291-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213-A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.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
Butane, 2-methyl-	3.247	33.1	ug/l	504779	1	8.224	763234	50.0
Pentane, 2-methyl-	5.353	33.6	ug/l	512323	1	8.224	763234	50.0
Cyclopentane, m...	7.324	20.7	ug/l	315980	1	8.224	763234	50.0
Butane, 2-metho...	8.777	90.1	ug/l	1500340	2	9.100	832336	50.0
Benzene, 1-ethy...	13.094	23.7	ug/l	365137	4	13.788	771695	50.0
Benzene, 1-ethy...	13.335	52.8	ug/l	814254	4	13.788	771695	50.0
(Z)-1-Phenylpro...	13.994	71.0	ug/l	1096450	4	13.788	771695	50.0
Benzene, 4-ethy...	14.329	18.9	ug/l	291161	4	13.788	771695	50.0
Benzene, 2-ethe...	15.047	23.1	ug/l	356754	4	13.788	771695	50.0