LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

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: VN085239.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	75	rBV3	47760	160201	2.61%	0.437%
2	2.506	84	94	101	rVB	73586	117728	1.92%	0.321%
3	3.242	210	219	233	rVB2	202400	461643	7.53%	1.258%
4	3.648	278	288	299	rBV5	47605	157143	2.56%	0.428%
5	4.148	362	373	386	rBV	74353	201989	3.29%	0.550%
6	5.159	530	545	554	rBV3	22947	75717	1.23%	0.206%
7	5.347	569	577	579	rBV3	50575	120115	1.96%	0.327%
8	5.806	640	655	672	rVB3	97731	340876	5.56%	0.929%
9	6.318	729	742	757	rBV5	21402	66621	1.09%	0.182%
10	6.653	787	799	813	rVB2	29218	86321	1.41%	0.235%
11	7.083	863	872	884	rVB3	26157	71145	1.16%	0.194%
12	7.330	903	914	924	rBV3	99869	307846	5.02%	0.839%
13	8.000	1020	1028	1038	rVB2	49968	122674	2.00%	0.334%
14	8.165	1046	1056	1060	rBV2	124176	283330	4.62%	0.772%
15	8.224	1060	1066	1078	rVV3	263340	743311	12.12%	2.025%
16	8.330	1078	1084	1091	rVV2	52785	126313	2.06%	0.344%
17	8.447	1091	1104	1111	rVV3	54979	136460	2.23%	0.372%
18	8.606	1118	1131	1143	rBV	2325302	5386687	87.85%	14.677%
19	8.777	1143	1160	1168	rVV2	514681	1489514	24.29%	4.059%
20	8.853	1168	1173	1181	rVV3	41035	98611	1.61%	0.269%
21	9.100	1206	1215	1227	rBV	364078	811137	13.23%	2.210%
22	9.600	1282	1300	1316	rBV3	143186	462983	7.55%	1.262%
23	10.012	1365	1370	1379	rVB	58939	126026	2.06%	0.343%
24	10.100	1379	1385	1389	rBV2	78383	160308	2.61%	0.437%
25	10.147	1389	1393	1399	rVB3	77714	138274	2.26%	0.377%
26	10.341	1415	1426	1428	rBV6	36680	80318	1.31%	0.219%
27	10.406	1432	1437	1441	rVV	95478	196243	3.20%	0.535%
28	10.453	1441	1445	1449	rVV	66017	117799	1.92%	0.321%
29	10.565	1457	1464	1469	rBV	521360	962132	15.69%	2.622%
30	10.629	1469	1475	1485	rVV	702232	1318204	21.50%	3.592%
31	10.729	1485	1492	1502	rVB4	71772	201101	3.28%	0.548%
32	10.982	1528	1535	1545	rVB5	59454	161718	2.64%	0.441%
33	11.865	1676	1685	1691	rBV	430367	787171	12.84%	2.145%
34	11.965	1695	1702	1711	rVV	1463522	2501545	40.80%	6.816%
35	12.065	1711	1719	1731	rVV	3083247	6131356	100.00%	16.706%
36	12.206	1738	1743	1750	rVB3	36894	68301	1.11%	0.186%

LSC Area Percent Report

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Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW6-20241213

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	12.394	1763	1775	1783	rBV	1197152	2037696	33.23%	5.552%
38	12.694	1821	1826	1831	rVB	77233	127652	2.08%	0.348%
39	12.847	1844	1852	1862	rBV	358167	632942	10.32%	1.725%
40	13.035	1878	1884	1889	rBV	91057	146604	2.39%	0.399%
41	13.094	1889	1894	1897	rVV	200804	337779	5.51%	0.920%
42	13.129	1897	1900	1903	rVV	194196	295011	4.81%	0.804%
43	13.170	1903	1907	1914	rVB	198721	323268	5.27%	0.881%
44	13.335	1926	1935	1944	rBV	496472	822719	13.42%	2.242%
45	13.482	1953	1960	1966	rBV	1192096	1907269	31.11%	5.197%
46	13.794	2006	2013	2015	rBV	419180	785592	12.81%	2.141%
47	13.817	2015	2017	2033	rVB	434806	605837	9.88%	1.651%
48	13.947	2033	2039	2042	rBV	85882	150043	2.45%	0.409%
49	13.994	2042	2047	2062	rVB3	448596	1034870	16.88%	2.820%
50	14.176	2072	2078	2084	rVV2	103485	181050	2.95%	0.493%
51	14.241	2084	2089	2092	rVV	106961	186266	3.04%	0.508%
52	14.270	2092	2094	2099	rVV	102040	134350	2.19%	0.366%
53	14.329	2099	2104	2110	rVB	178394	279277	4.55%	0.761%
54	14.441	2118	2123	2131	rVB2	153624	268659	4.38%	0.732%
55	14.570	2140	2145	2151	rVB3	44666	71205	1.16%	0.194%
56	14.653	2151	2159	2162	rBV	123554	207007	3.38%	0.564%
57	14.688	2162	2165	2170	rVV	162978	258701	4.22%	0.705%
58	14.923	2200	2205	2210	rBV	89648	147129	2.40%	0.401%
59	15.047	2217	2226	2232	rBV3	135236	335560	5.47%	0.914%
60	15.111	2232	2237	2246	rVB4	26284	62617	1.02%	0.171%
61	15.317	2261	2272	2277	rBV3	59521	150521	2.45%	0.410%
62	15.441	2284	2293	2300	rVB4	43276	110864	1.81%	0.302%
63	15.635	2319	2326	2335	rVB	165678	321132	5.24%	0.875%

Sum of corrected areas: 36700481

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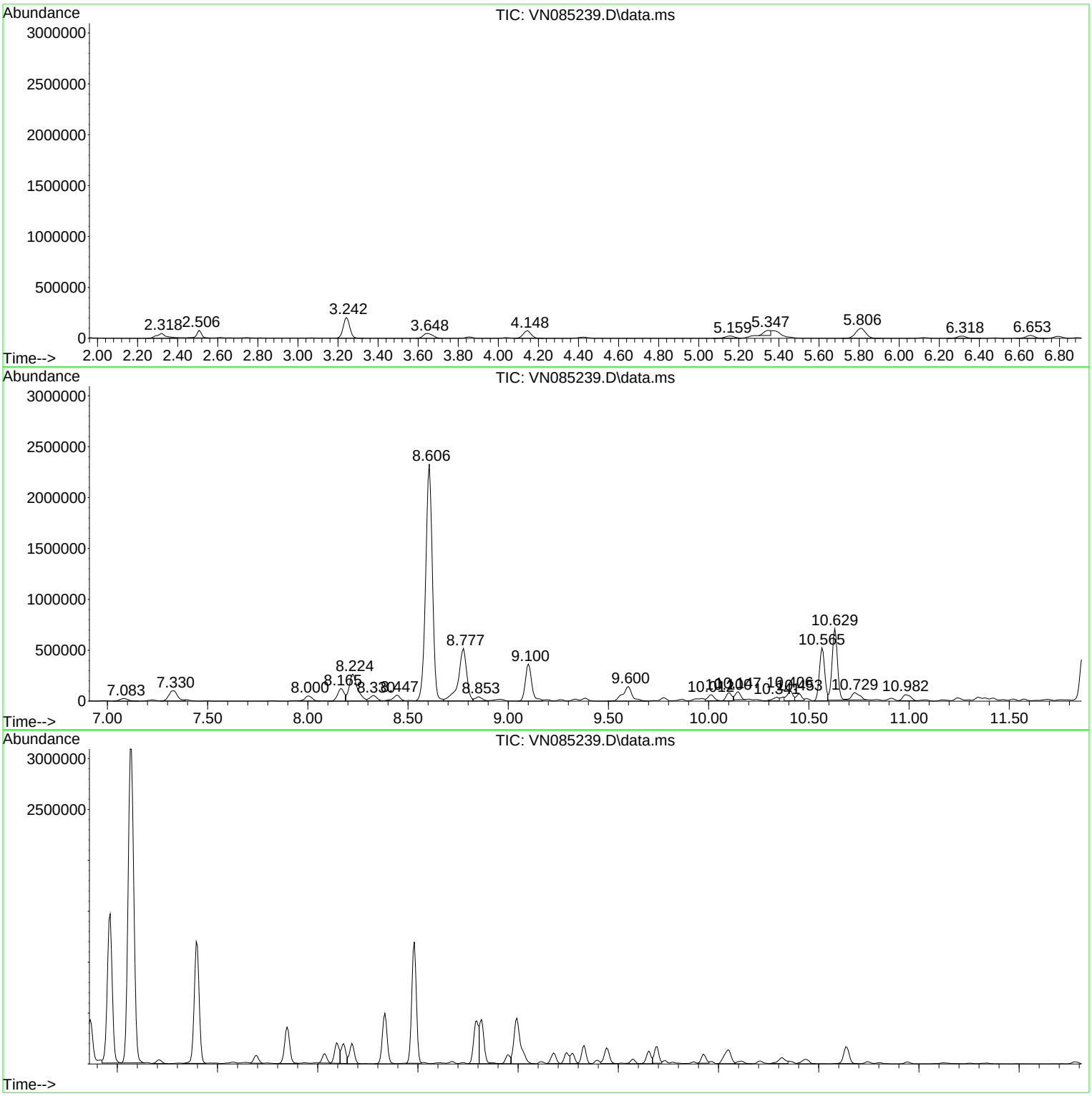
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

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 : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
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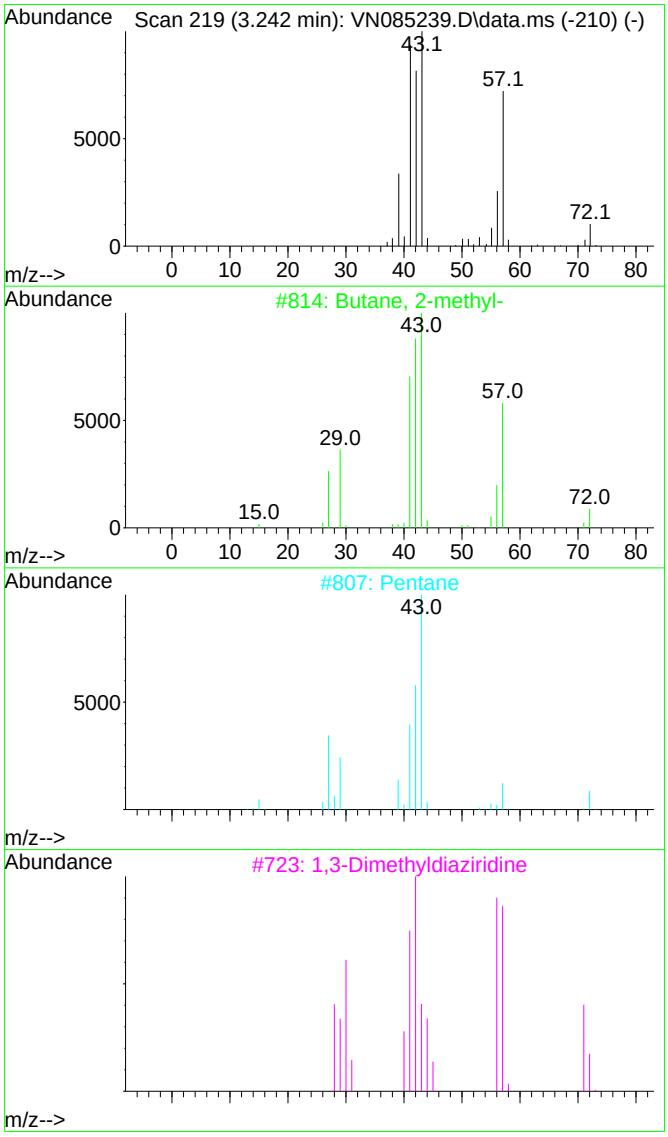
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

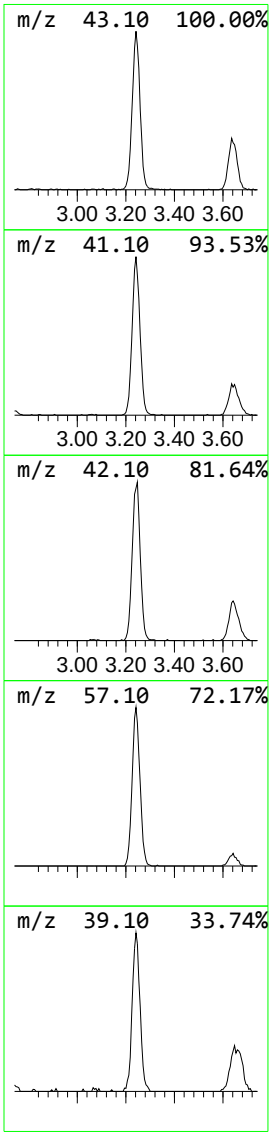
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.242	31.05 ug/l	461643	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Pentane	72	C5H12	000109-66-0	45
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

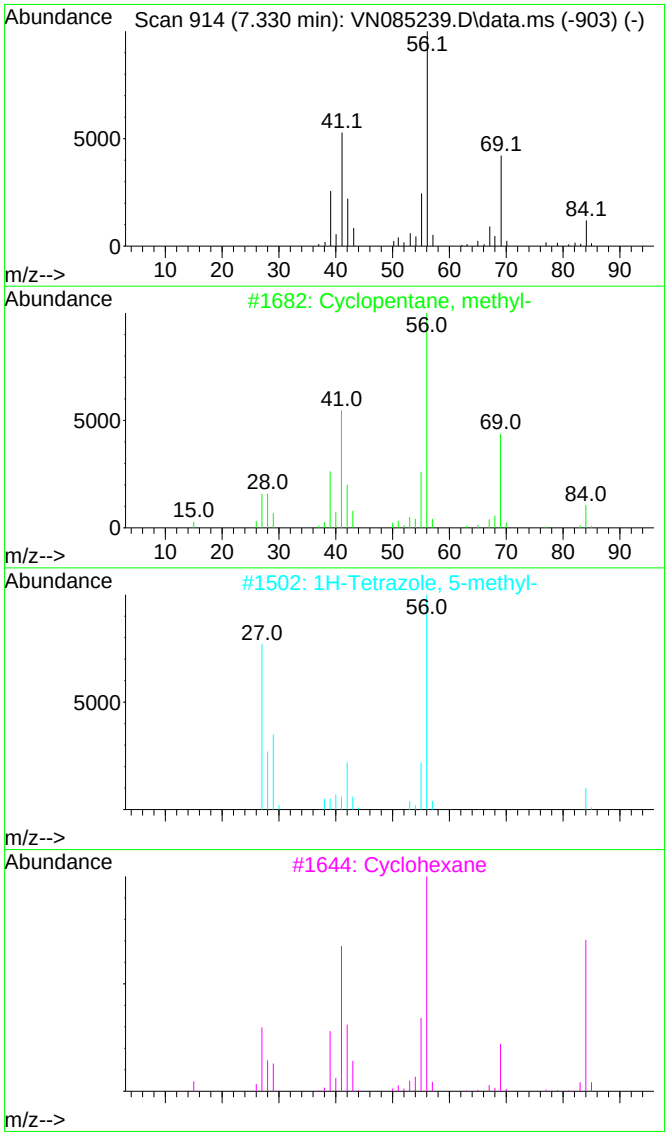
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

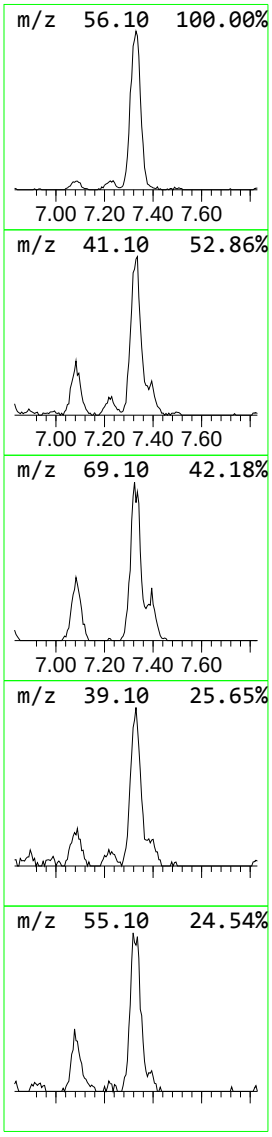
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.330	20.71 ug/l	307846	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclohexane	84	C6H12	000110-82-7	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclobutane	56	C4H8	000287-23-0	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
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Acq On : 17 Dec 2024 21:11
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

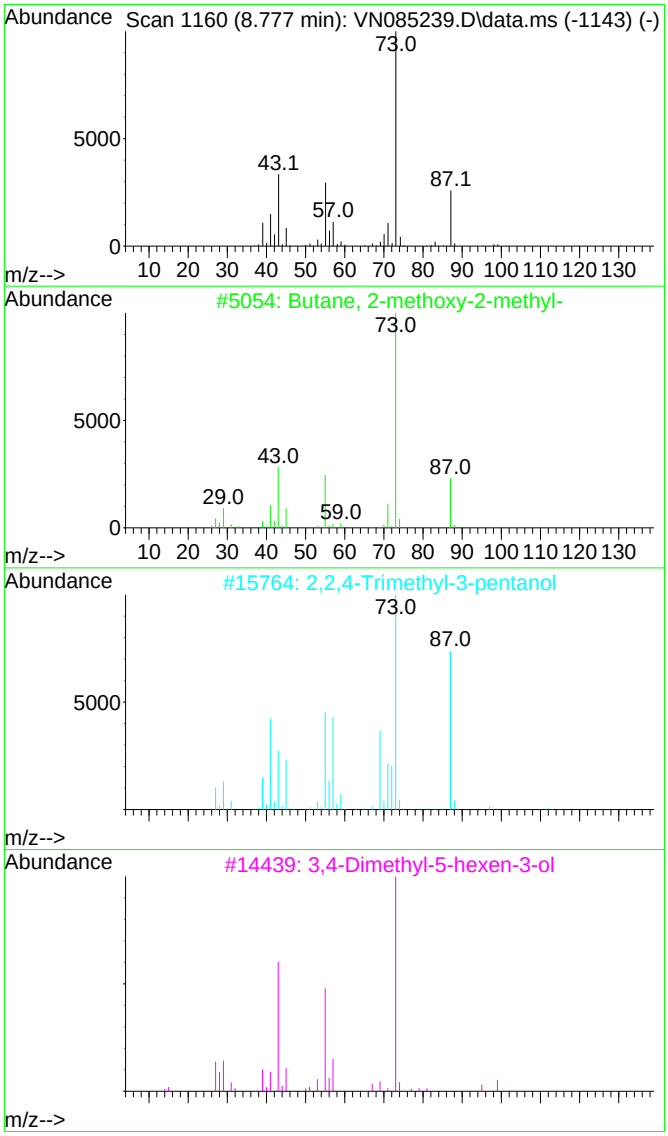
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

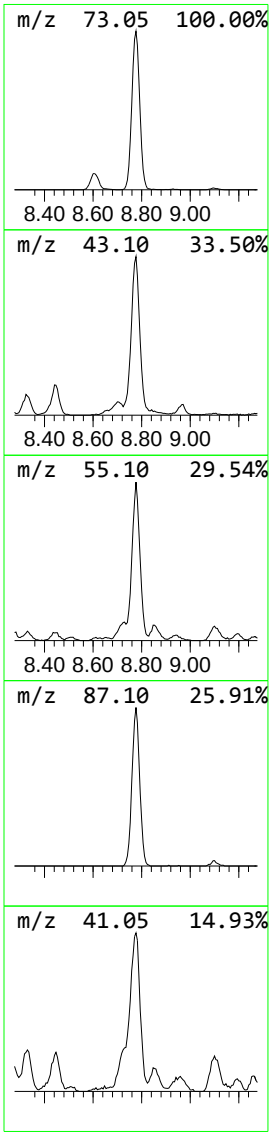
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.777	91.82 ug/l	1489510	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	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	3,4-Dimethyl-5-hexen-3-ol	128	C8H16O	001569-45-5	35
4	meso-2,5-Dimethyl-3,4-hexanediol	146	C8H18O2	022520-38-3	25
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
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Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

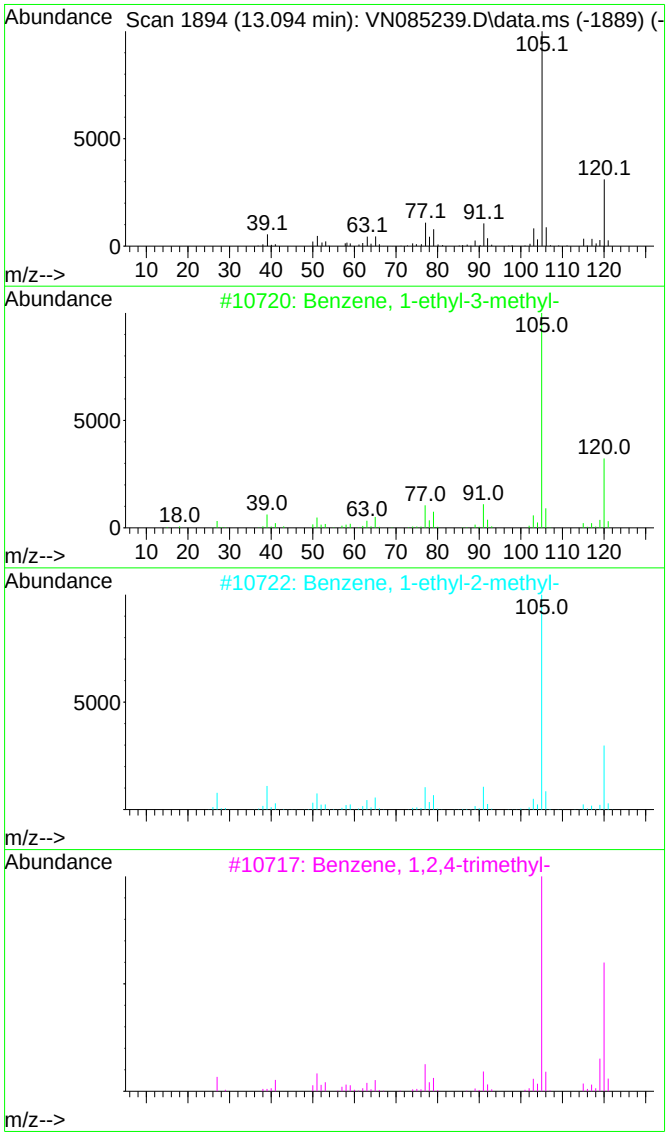
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

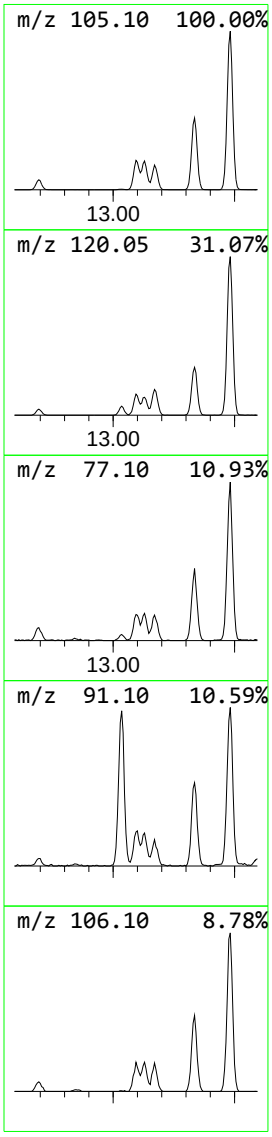
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	21.50 ug/l	337779	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	94
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5	Mesitylene	120	C9H12	000108-67-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

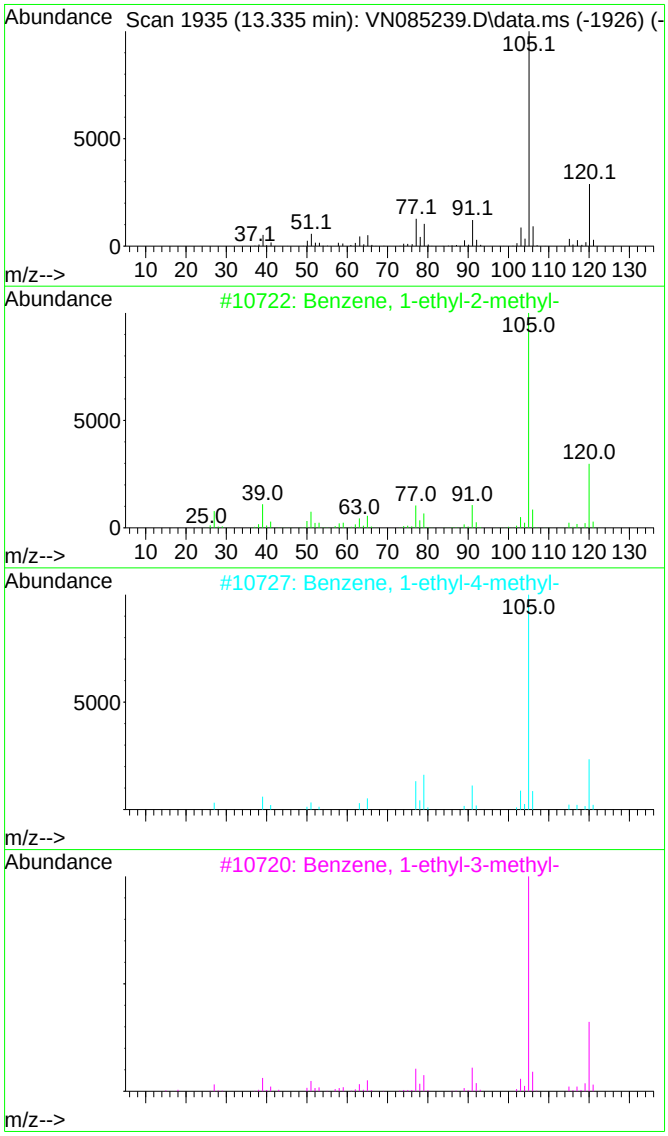
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

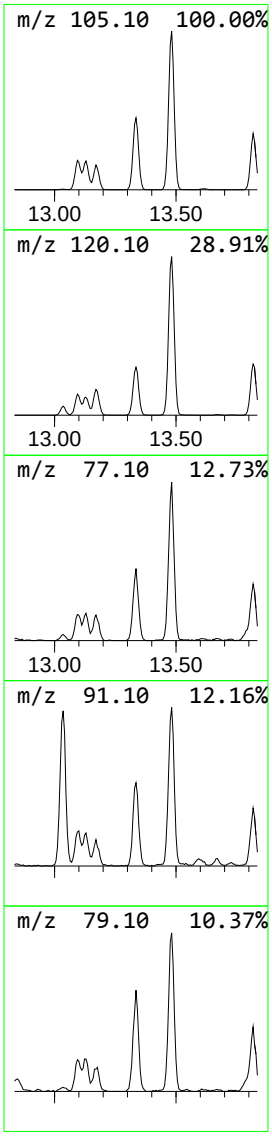
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	52.36 ug/l	822719	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	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

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

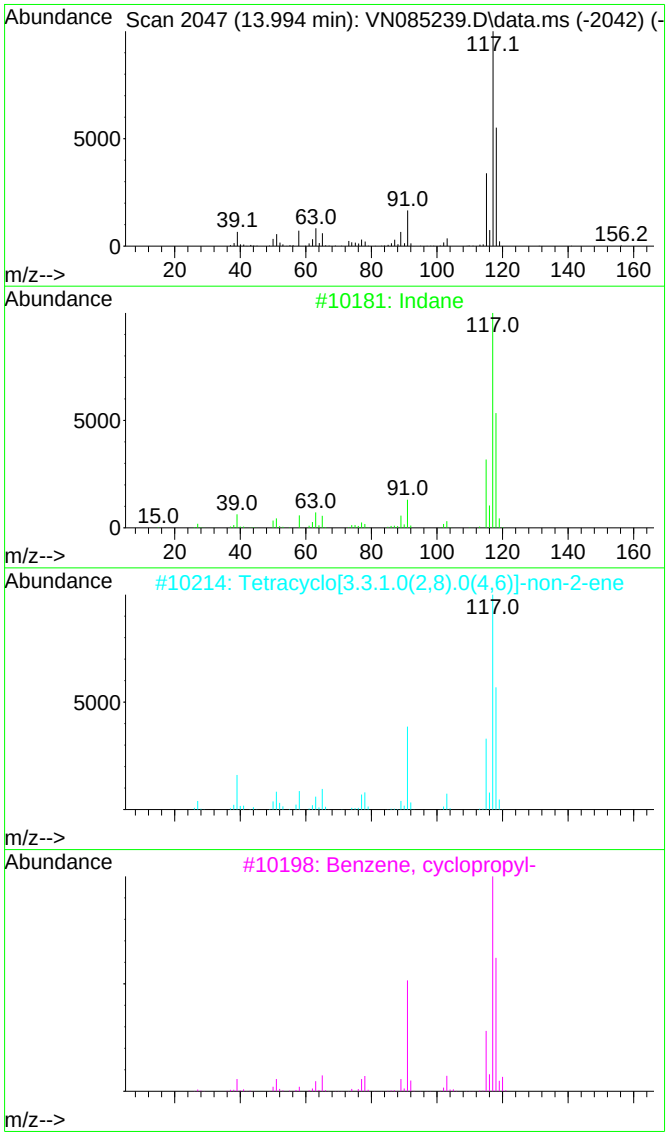
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

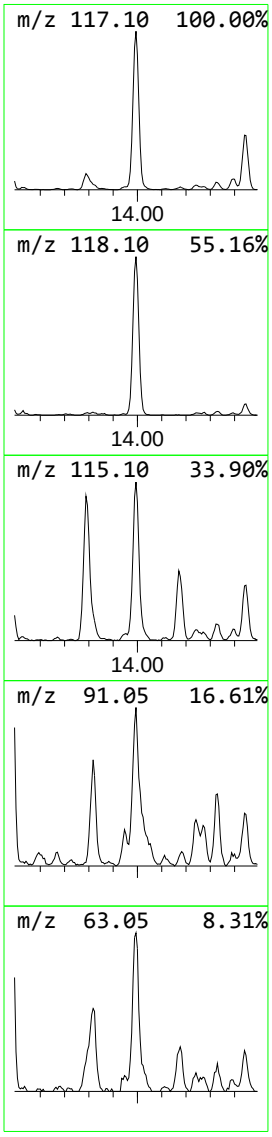
****

Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	65.87 ug/l	1034870	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	81
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

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

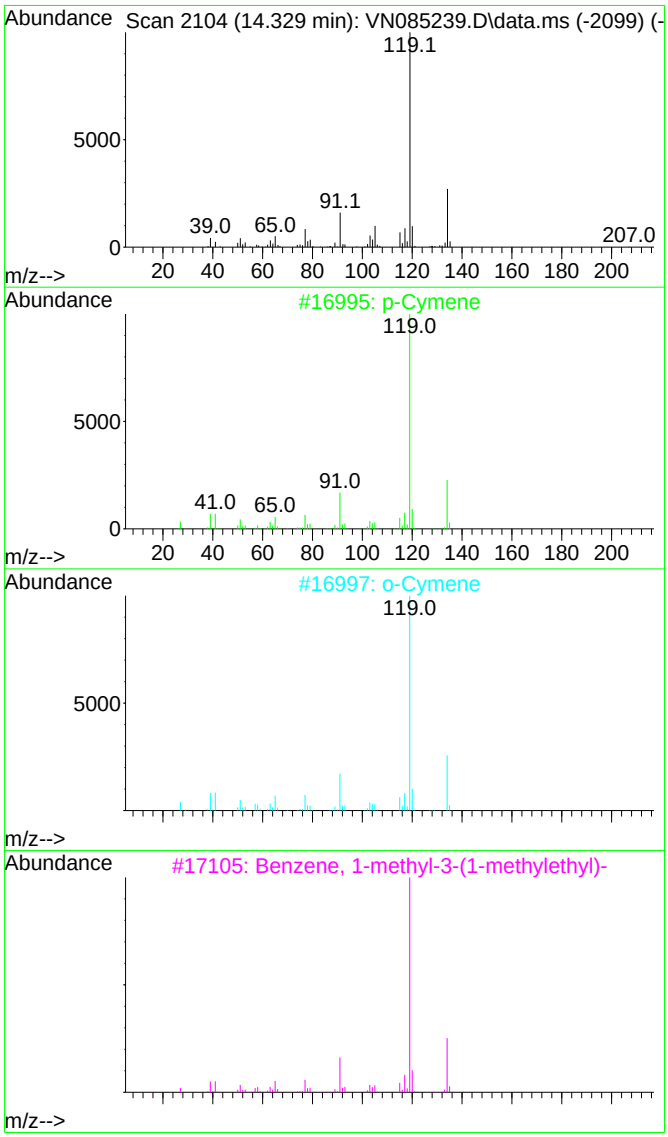
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

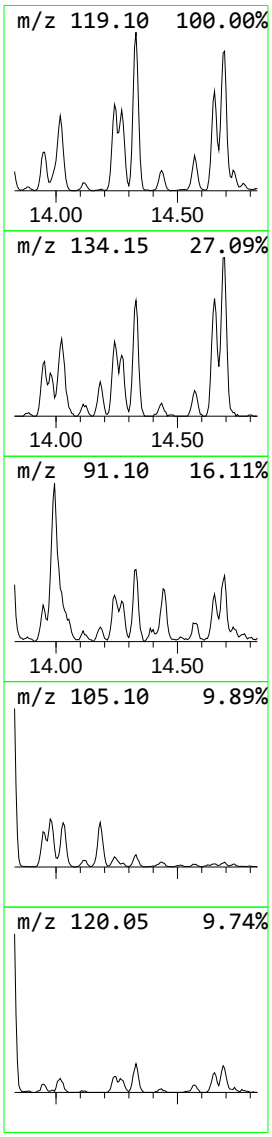
****

Peak Number 7 p-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	17.77 ug/l	279277	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	94
2	o-Cymene	134	C10H14	000527-84-4	94
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

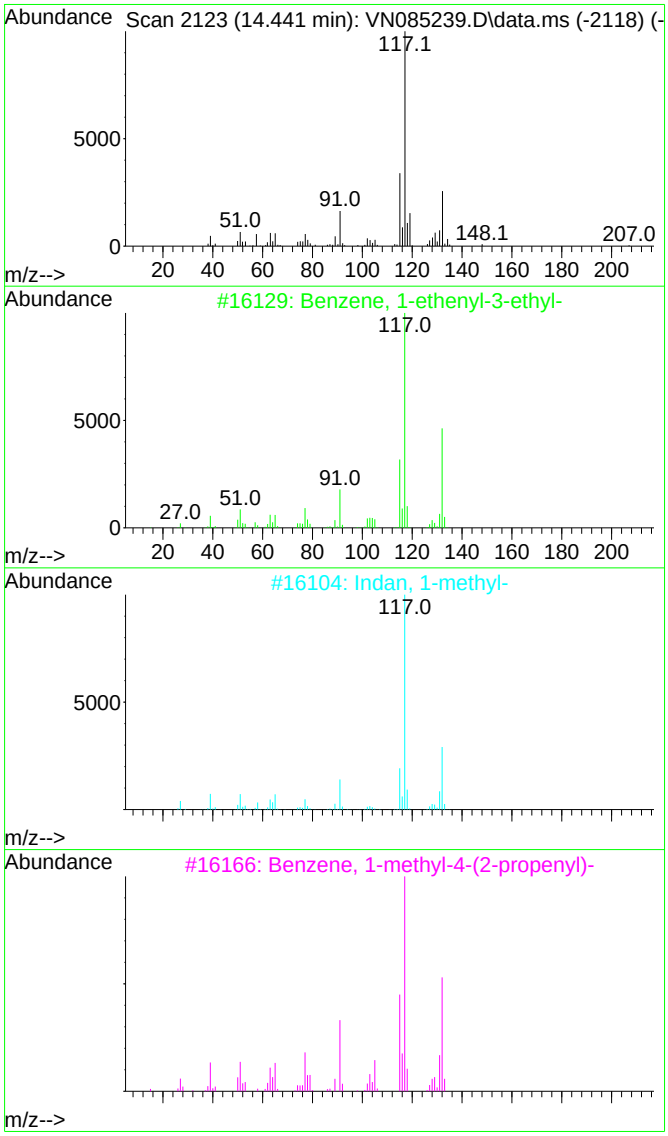
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

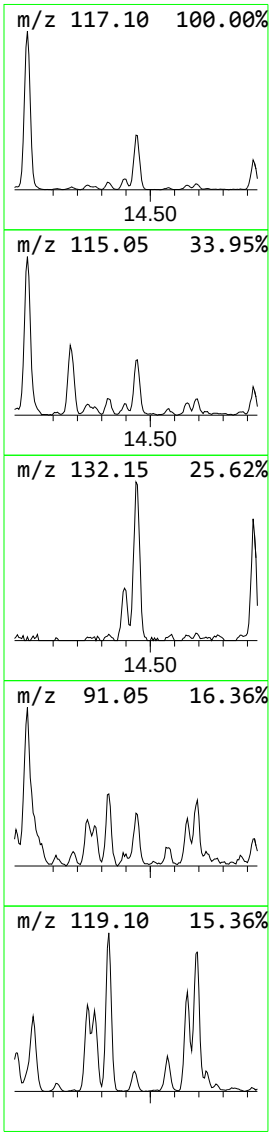
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.441	17.10 ug/l	268659	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
2	Indan, 1-methyl-	132	C10H12	000767-58-8	81
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	80
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

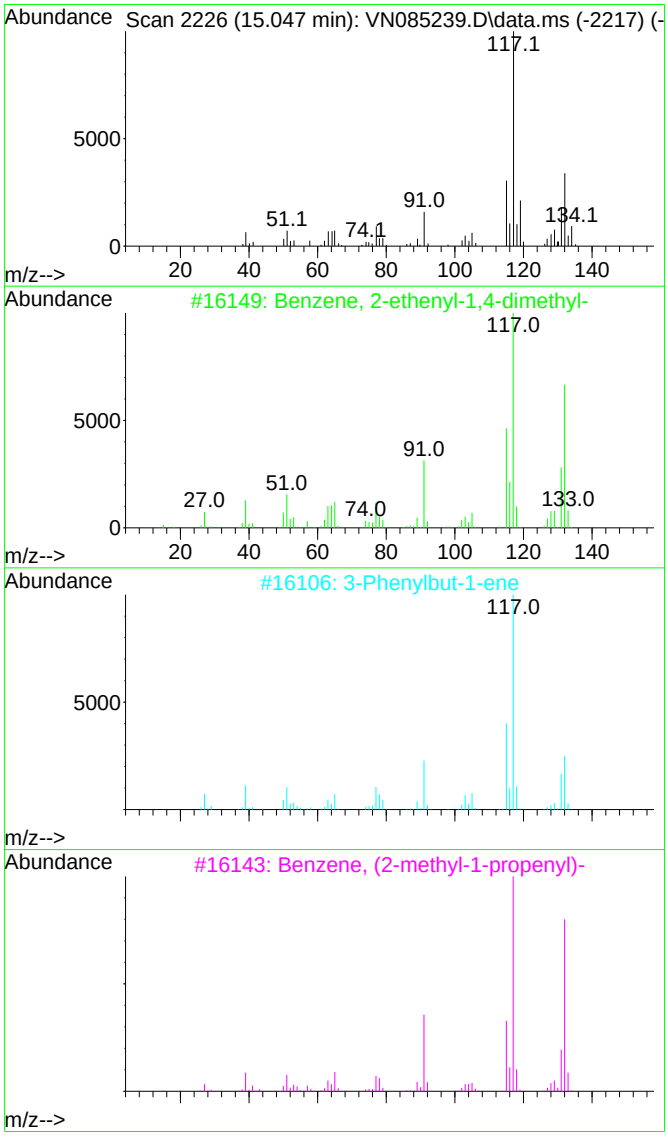
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

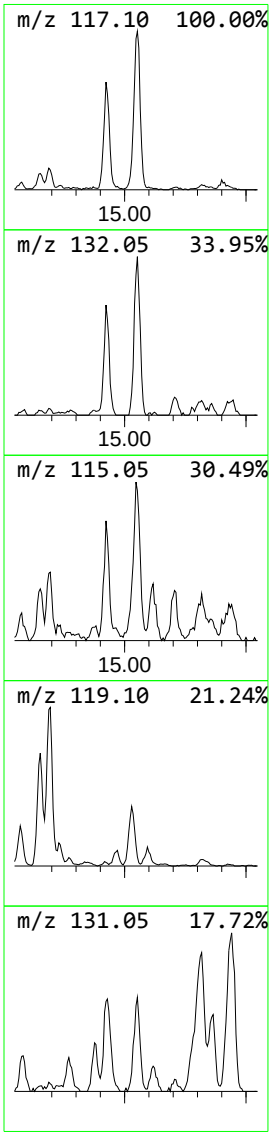
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	21.36 ug/l	335560	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	90
2	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
4	2,4-Dimethylstyrene	132	C10H12	002234-20-0	78
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085239.D
Acq On : 17 Dec 2024 21:11
Operator : JC\MD
Sample : P5291-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW6-20241213

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-	3.242	31.1	ug/l	461643	1	8.224	743311	50.0
Cyclopentane, m...	7.330	20.7	ug/l	307846	1	8.224	743311	50.0
Butane, 2-metho...	8.777	91.8	ug/l	1489510	2	9.100	811137	50.0
Benzene, 1-ethy...	13.094	21.5	ug/l	337779	4	13.788	785592	50.0
Benzene, 1-ethy...	13.335	52.4	ug/l	822719	4	13.788	785592	50.0
Indane	13.994	65.9	ug/l	1034870	4	13.788	785592	50.0
p-Cymene	14.329	17.8	ug/l	279277	4	13.788	785592	50.0
Benzene, 1-ethe...	14.441	17.1	ug/l	268659	4	13.788	785592	50.0
Benzene, 2-ethe...	15.047	21.4	ug/l	335560	4	13.788	785592	50.0