LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050925\
Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

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\82N041525W.M
Title : SW846 8260

Signal : TIC: VN086559.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.212	1045	1064	1074	rBV2	1945732	4828256	4.84%	1.785%
2	8.318	1074	1082	1091	rVB	541919	1296847	1.30%	0.480%
3	8.435	1092	1102	1111	rBV	2553757	5690164	5.70%	2.104%
4	8.959	1181	1191	1206	rBV	2634730	5093192	5.10%	1.883%
5	9.594	1284	1299	1316	rBV	702143	1639121	1.64%	0.606%
6	10.565	1456	1464	1467	rBV	859534	1593036	1.60%	0.589%
7	10.629	1467	1475	1488	rVV2	47890042	99852510	100.00%	36.920%
8	10.741	1488	1494	1505	rVB	853350	1566484	1.57%	0.579%
9	11.100	1547	1555	1561	rVB2	516157	1034625	1.04%	0.383%
10	11.641	1639	1647	1659	rVV3	990067	2685541	2.69%	0.993%
11	11.741	1659	1664	1670	rVB	999308	1543692	1.55%	0.571%
12	11.959	1694	1701	1710	rVV	5511522	9848982	9.86%	3.642%
13	12.065	1710	1719	1730	rVV	24517587	47857820	47.93%	17.695%
14	12.147	1730	1733	1739	rVB2	690891	1164176	1.17%	0.430%
15	12.394	1762	1775	1783	rBV	7337911	15235086	15.26%	5.633%
16	12.476	1784	1789	1794	rVB	1346421	2223384	2.23%	0.822%
17	12.594	1794	1809	1811	rBV4	1266222	4055631	4.06%	1.500%
18	12.688	1821	1825	1829	rBV2	554607	1052557	1.05%	0.389%
19	12.741	1829	1834	1835	rVV3	645495	1131909	1.13%	0.419%
20	12.765	1835	1838	1841	rVV	1234894	2086561	2.09%	0.771%
21	12.794	1841	1843	1847	rVB	1231898	1386986	1.39%	0.513%
22	12.847	1847	1852	1854	rBV	655706	1029955	1.03%	0.381%
23	12.876	1854	1857	1861	rVB	925624	1225834	1.23%	0.453%
24	13.029	1876	1883	1888	rVB2	1279991	2409541	2.41%	0.891%
25	13.094	1888	1894	1897	rBV	2962967	4888172	4.90%	1.807%
26	13.159	1897	1905	1912	rVV3	6486285	14357139	14.38%	5.308%
27	13.223	1912	1916	1921	rVB2	794965	1291239	1.29%	0.477%
28	13.335	1922	1935	1940	rBV2	1365760	3885612	3.89%	1.437%
29	13.388	1940	1944	1953	rVV2	1041160	2309950	2.31%	0.854%
30	13.476	1953	1959	1970	rVB	3679673	6535553	6.55%	2.416%
31	13.670	1986	1992	1997	rBV3	1431581	2886575	2.89%	1.067%
32	13.782	2007	2011	2014	rBV2	714598	1192289	1.19%	0.441%
33	13.817	2014	2017	2021	rVB	1009040	1327445	1.33%	0.491%
34	13.941	2030	2038	2040	rBV5	497509	1068575	1.07%	0.395%
35	13.982	2040	2045	2049	rBV2	1288055	2249725	2.25%	0.832%
36	14.100	2061	2065	2075	rBV3	2051749	4117783	4.12%	1.523%

LSC Area Percent Report

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
3848

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\82N041525W.M
Title : SW846 8260

37	14.323	2099	2103	2108	rVB	774605	1197141	1.20%	0.443%
38	14.435	2117	2122	2128	rVB3	921905	1624499	1.63%	0.601%
39	14.623	2149	2154	2157	rBV	661500	1025268	1.03%	0.379%
40	15.047	2217	2226	2232	rBV3	688204	1777853	1.78%	0.657%
41	16.776	2512	2520	2522	rBV	644708	1190487	1.19%	0.440%

Sum of corrected areas: 270457195

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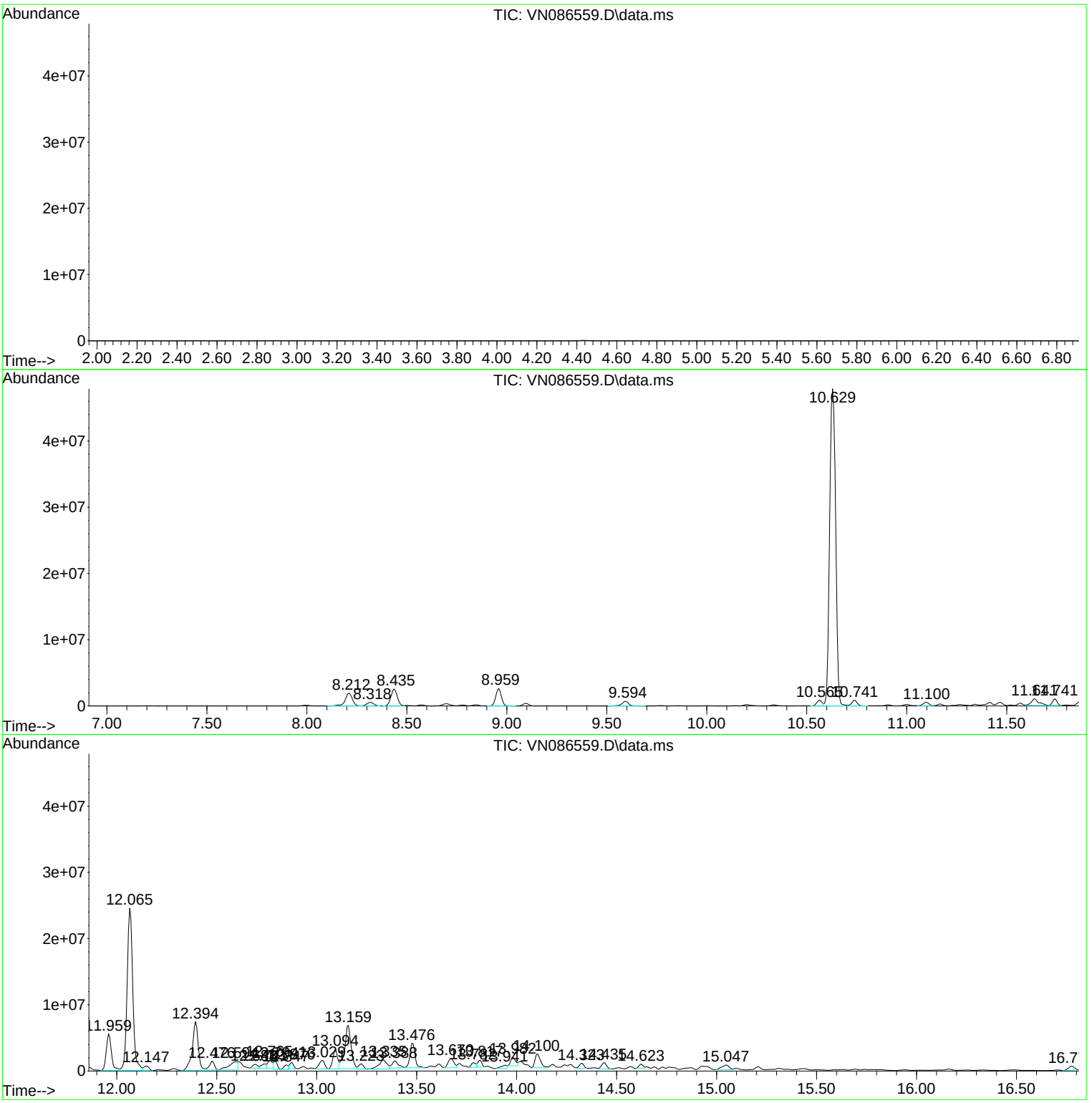
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



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Data File : VN086559.D
Acq On : 09 May 2025 13:55
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

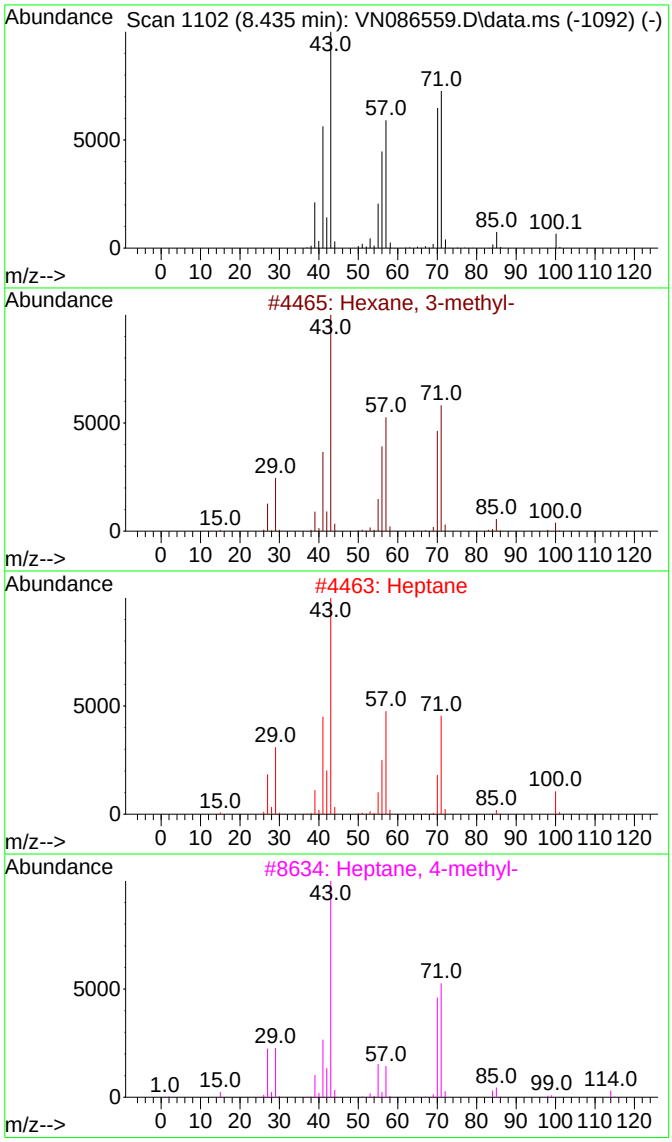
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

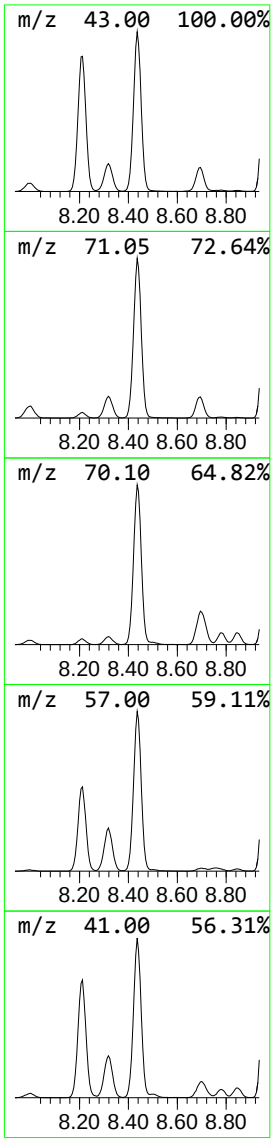
****

Peak Number 1 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.435	58.93 ug/l	5690160	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	64
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53





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Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

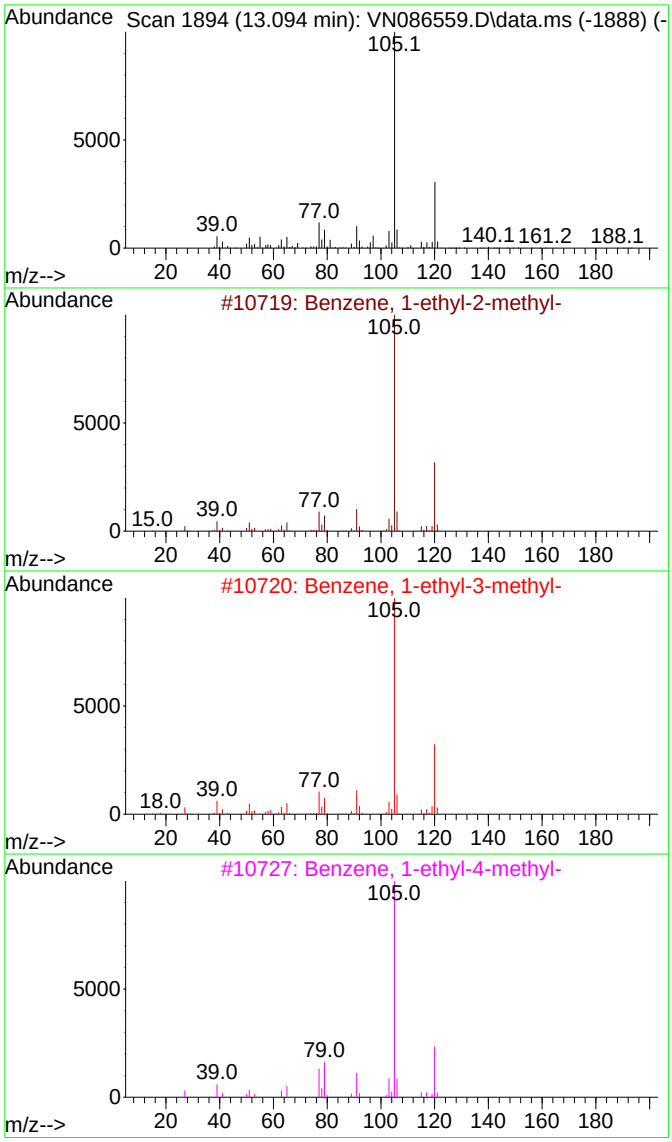
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

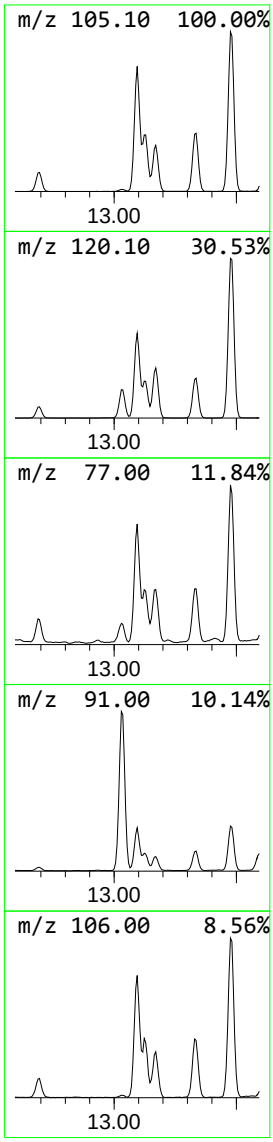
****

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	204.99 ug/l	4888170	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-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





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Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

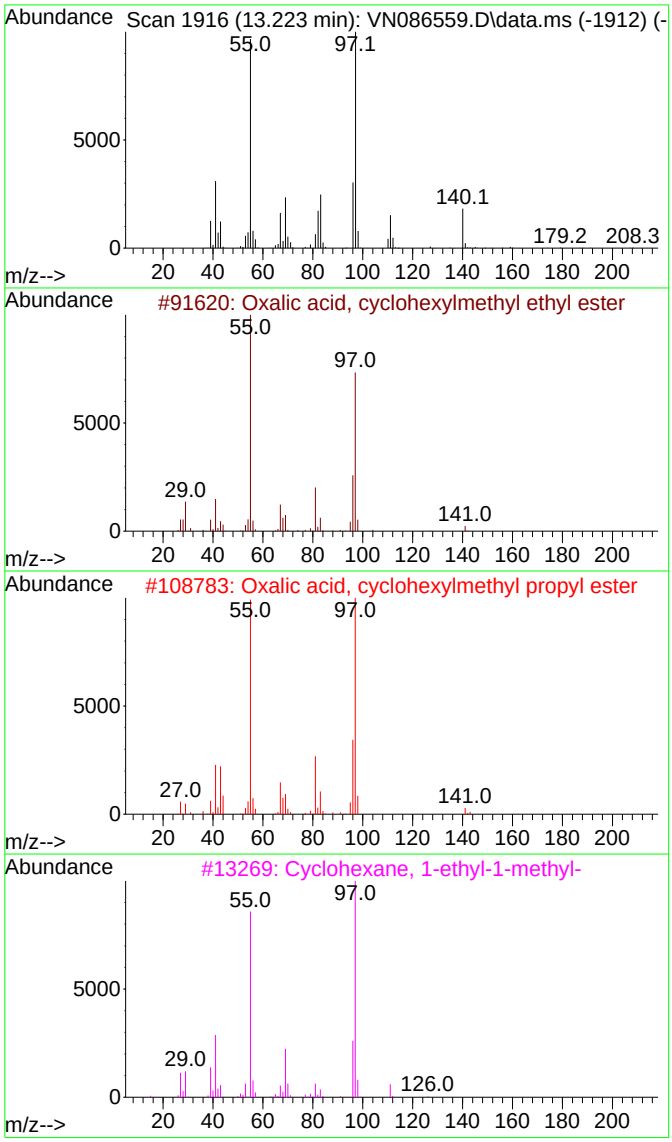
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

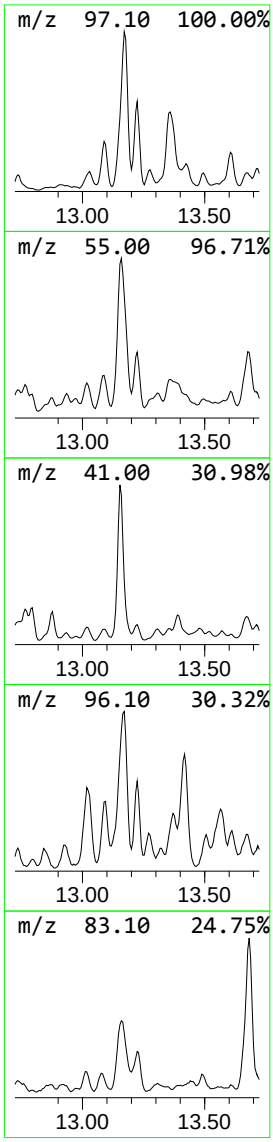
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Oxalic acid, cyclohexylmeth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.223	54.15 ug/l	1291240	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	53
2	Oxalic acid, cyclohexylmethyl pr...	228	C12H20O4	1010309-68-1	53
3	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	53
4	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	52
5	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050925\
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Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

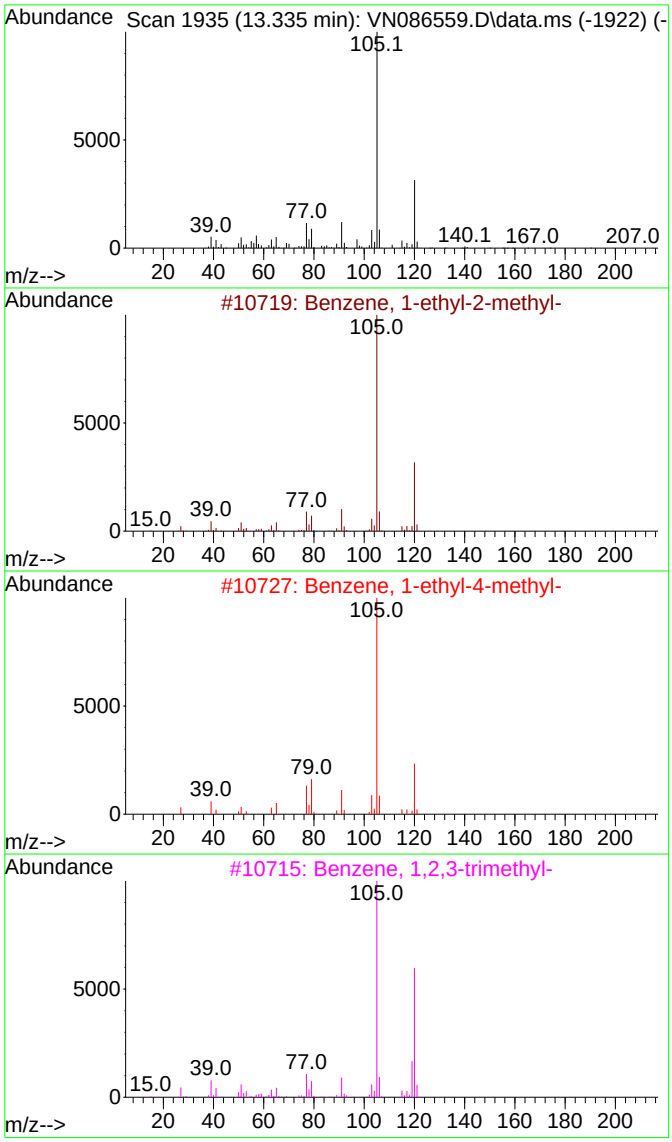
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

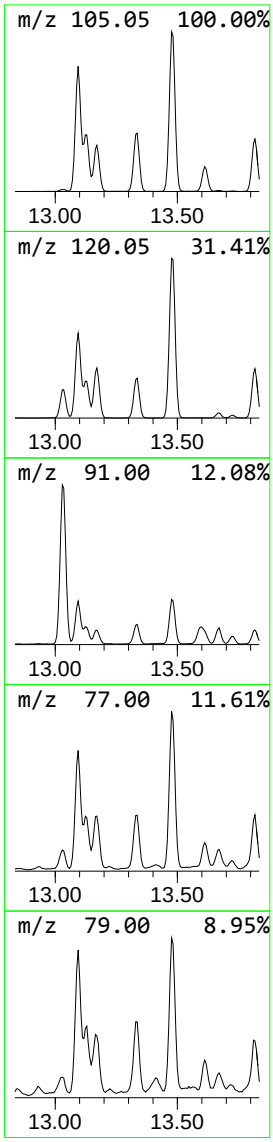
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	162.95 ug/l	3885610	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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4	Mesitylene	120	C9H12	000108-67-8	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





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Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

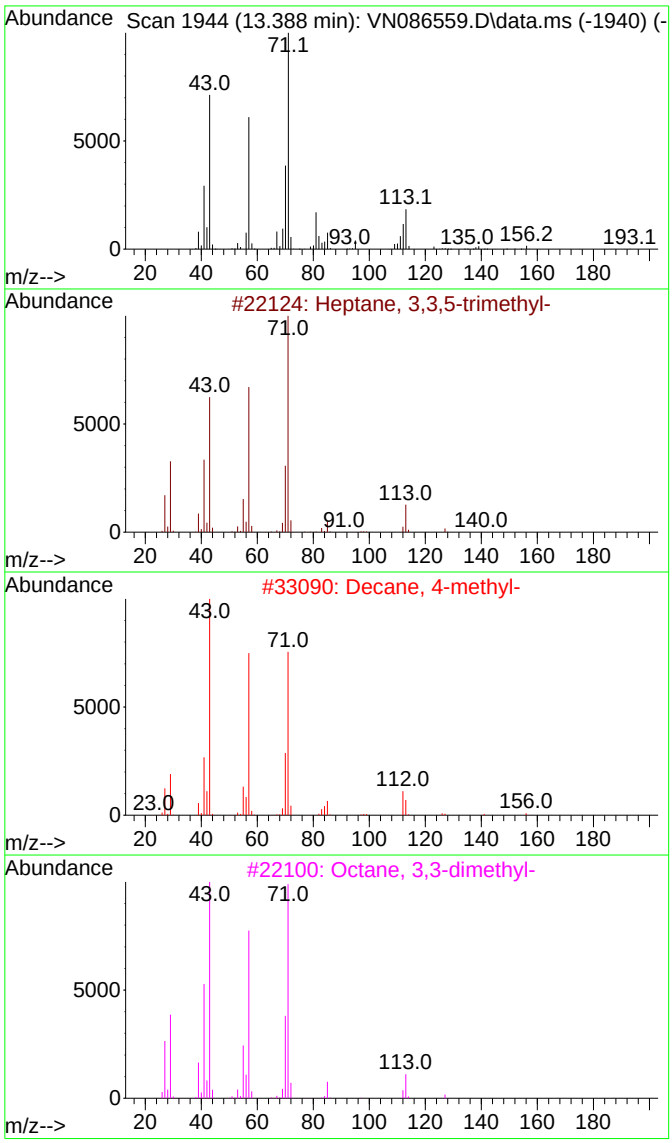
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

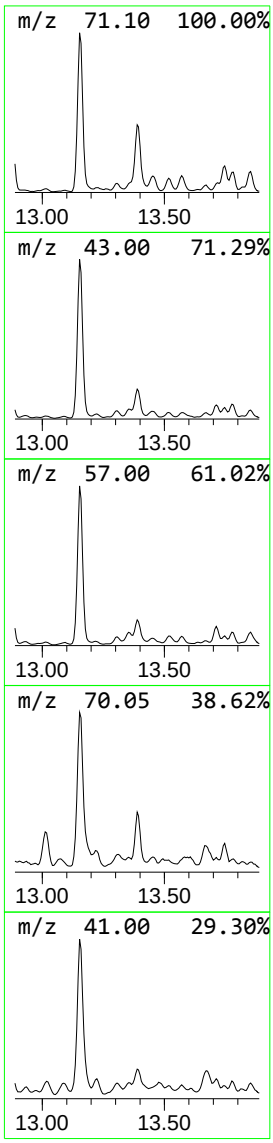
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptane, 3,3,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.388	96.87 ug/l	2309950	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	80
2	Decane, 4-methyl-	156	C11H24	002847-72-5	72
3	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
4	Decane, 3,3,8-trimethyl-	184	C13H28	062338-16-3	59
5	1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	53





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Instrument :
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Quant Title : SW846 8260

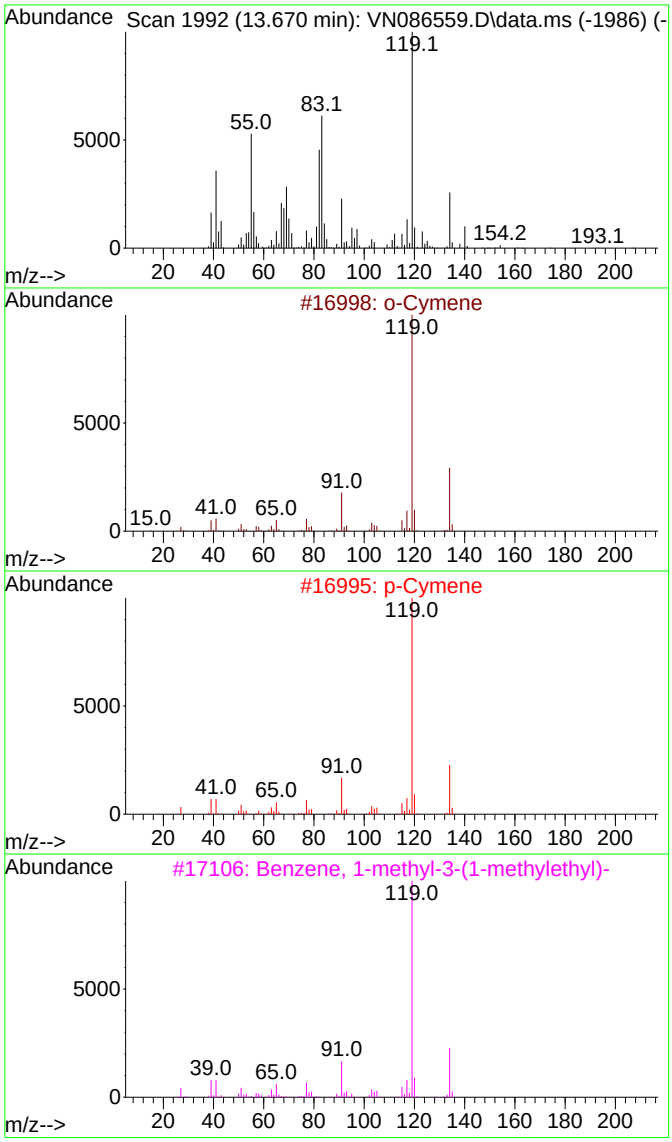
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

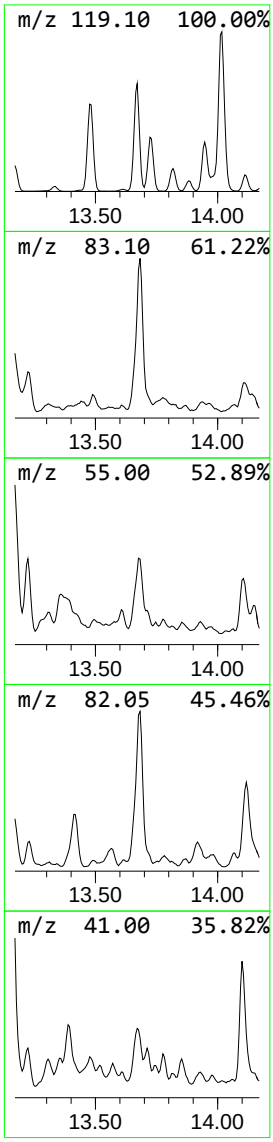
****

Peak Number 6 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	121.05 ug/l	2886580	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	89
2	p-Cymene	134	C10H14	000099-87-6	89
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	83
4	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	83
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	46





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Quant Title : SW846 8260

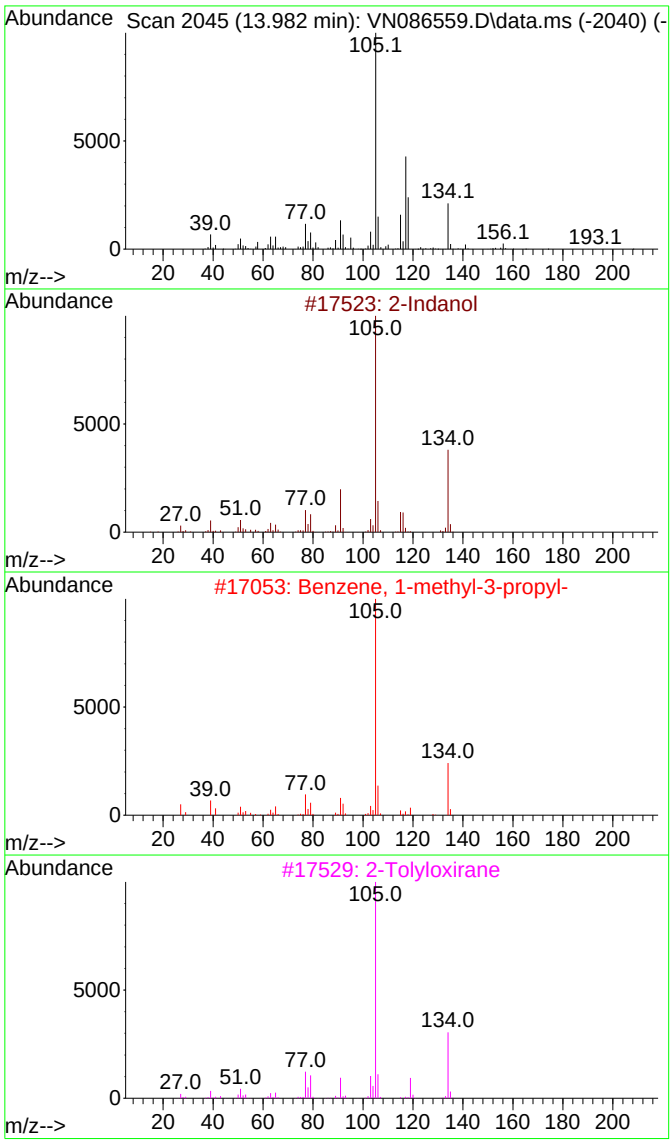
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

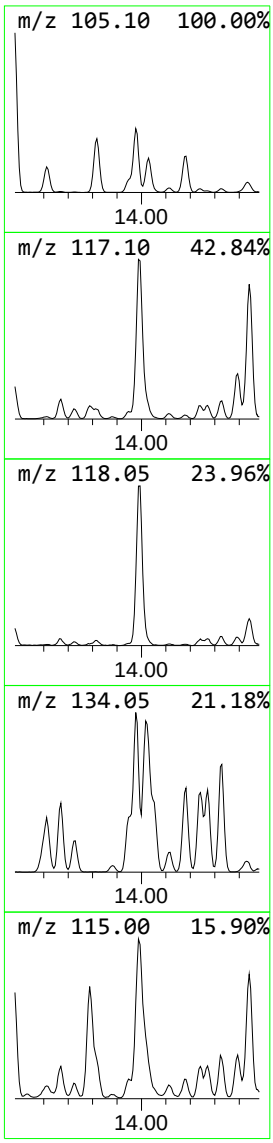
****

Peak Number 7 unknown13.982 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.982	94.34 ug/l	2249730	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Indanol	134	C9H10O	004254-29-9	43
2	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	42
3	2-Tolyloxirane	134	C9H10O	002783-26-8	42
4	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	38
5	Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	38





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Data File : VN086559.D
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Operator : JC\MD
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Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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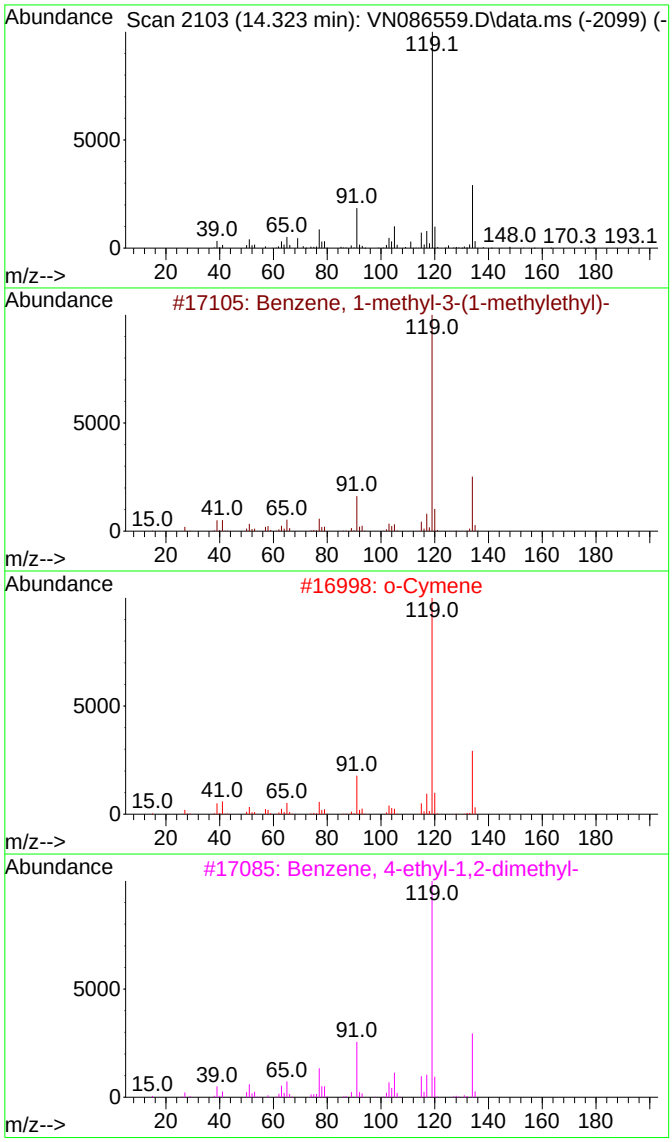
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

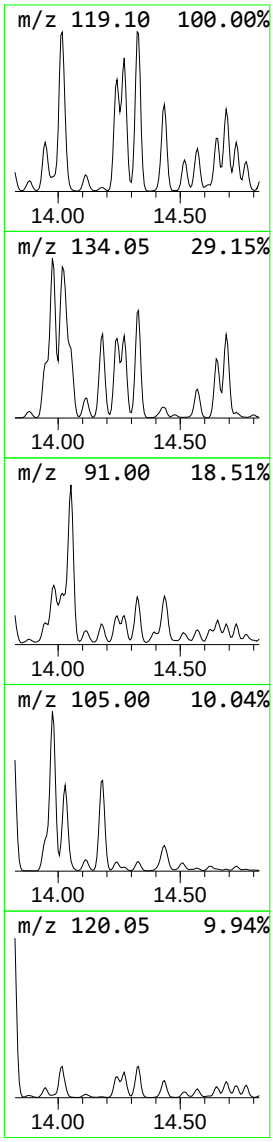
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.323	50.20 ug/l	1197140	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94





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Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

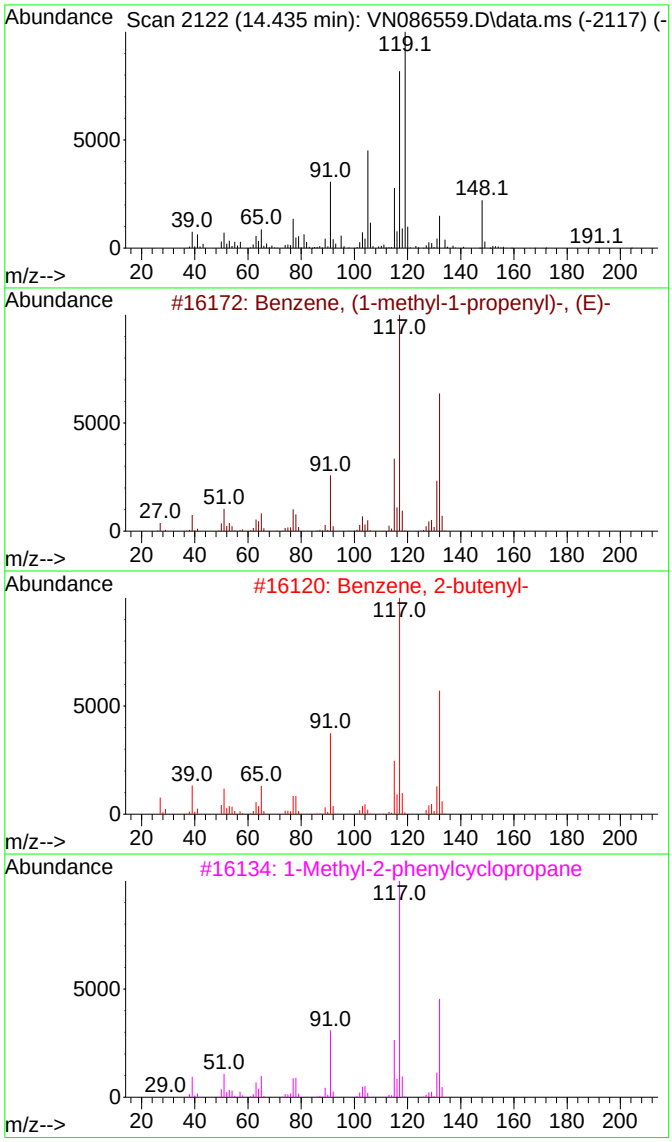
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

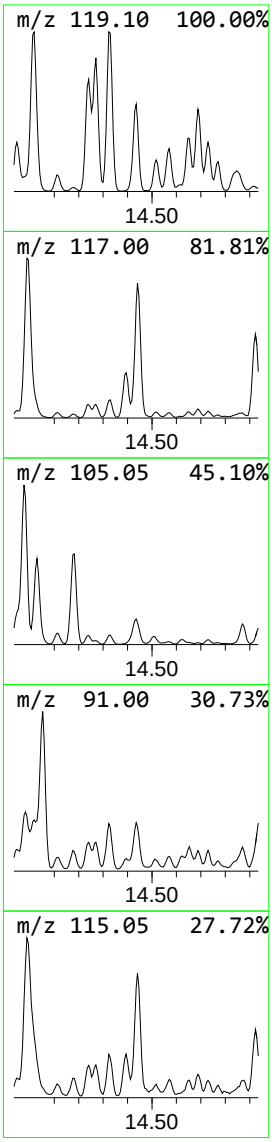
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-propen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.435	68.13 ug/l	1624500	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	50
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	46
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	46
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	46
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050925\
Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

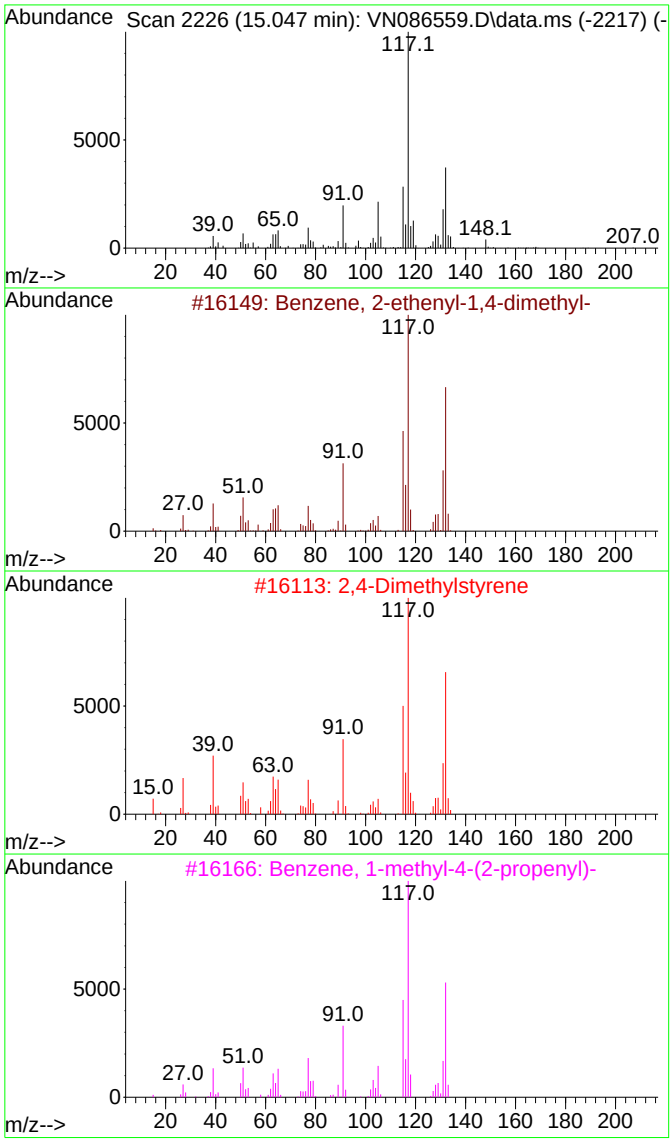
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

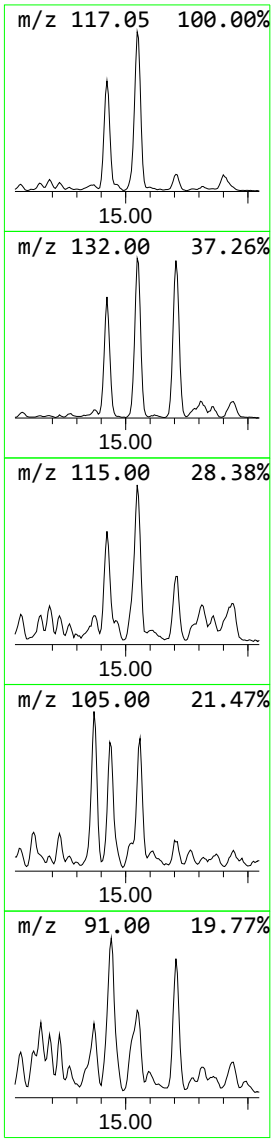
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	74.56 ug/l	1777850	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	95
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5	Indan, 1-methyl-	132	C10H12	000767-58-8	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN050925\
Data File : VN086559.D
Acq On : 09 May 2025 13:55
Operator : JC\MD
Sample : Q1980-04
Misc : 1.22g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
Hexane, 3-methyl-	8.435	58.9	ug/l	5690160	1	8.218	4828260	50.0
Benzene, 1-ethy...	13.094	205.0	ug/l	4888170	4	13.788	1192290	50.0
Oxalic acid, cy...	13.223	54.1	ug/l	1291240	4	13.788	1192290	50.0
Benzene, 1-ethy...	13.335	162.9	ug/l	3885610	4	13.788	1192290	50.0
Heptane, 3,3,5-...	13.388	96.9	ug/l	2309950	4	13.788	1192290	50.0
o-Cymene	13.670	121.1	ug/l	2886580	4	13.788	1192290	50.0
unknown13.982	13.982	94.3	ug/l	2249730	4	13.788	1192290	50.0
Benzene, 1-meth...	14.323	50.2	ug/l	1197140	4	13.788	1192290	50.0
Benzene, (1-met...	14.435	68.1	ug/l	1624500	4	13.788	1192290	50.0
Benzene, 2-ethe...	15.047	74.6	ug/l	1777850	4	13.788	1192290	50.0