LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062422\
Data File : VX029772.D
Acq On : 24 Jun 2022 13:59
Operator : JC/MD
Sample : N3366-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

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_X\Method\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029772.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	41	rVB	14080	29642	2.34%	0.300%
2	2.337	200	205	211	rBV2	6570	13857	1.09%	0.140%
3	2.782	269	278	288	rBV3	9428	23000	1.82%	0.233%
4	2.959	300	307	317	rBV	20571	46653	3.69%	0.472%
5	3.105	322	331	341	rVB4	15144	39825	3.15%	0.403%
6	3.757	430	438	452	rBV2	11461	30977	2.45%	0.313%
7	5.391	694	706	720	rBV3	137585	404460	31.96%	4.092%
8	5.556	721	733	758	rVB	267439	792289	62.60%	8.015%
9	5.964	790	800	809	rBV	150022	398959	31.52%	4.036%
10	6.159	826	832	838	rBV4	5873	15845	1.25%	0.160%
11	6.251	838	847	857	rVB3	38057	119637	9.45%	1.210%
12	6.763	920	931	945	rBV	393682	940731	74.33%	9.517%
13	7.360	1019	1029	1036	rBV4	5112	13192	1.04%	0.133%
14	7.988	1122	1132	1139	rVB2	26377	56922	4.50%	0.576%
15	8.110	1144	1152	1160	rBV	48949	100687	7.96%	1.019%
16	8.653	1226	1241	1250	rBV	795839	1265674	100.00%	12.805%
17	9.104	1311	1315	1320	rVB	11471	18200	1.44%	0.184%
18	9.165	1320	1325	1336	rBV	32082	54739	4.32%	0.554%
19	9.513	1377	1382	1387	rVB5	7420	13914	1.10%	0.141%
20	9.762	1419	1423	1428	rBV5	8981	14834	1.17%	0.150%
21	10.055	1466	1471	1477	rBV	773288	1033465	81.65%	10.455%
22	10.195	1489	1494	1503	rVB	207719	258910	20.46%	2.619%
23	10.963	1615	1620	1626	rBV	78316	102080	8.07%	1.033%
24	11.085	1632	1640	1645	rBV	591276	766546	60.56%	7.755%
25	11.305	1672	1676	1684	rVB	27680	37624	2.97%	0.381%
26	11.616	1720	1727	1735	rBV	12833	21181	1.67%	0.214%
27	11.890	1769	1772	1778	rVB	10565	14433	1.14%	0.146%
28	12.024	1788	1794	1799	rBV	778832	960635	75.90%	9.719%
29	12.177	1815	1819	1824	rVB	11857	16703	1.32%	0.169%
30	12.244	1825	1830	1837	rVV2	423431	563622	44.53%	5.702%
31	12.317	1837	1842	1851	rVB	51866	69253	5.47%	0.701%
32	12.414	1851	1858	1863	rBV2	29539	41805	3.30%	0.423%
33	12.475	1863	1868	1872	rVB2	14237	19000	1.50%	0.192%
34	12.646	1892	1896	1900	rBV	66938	77875	6.15%	0.788%
35	12.701	1900	1905	1912	rVV	482328	594386	46.96%	6.013%
36	12.841	1920	1928	1934	rBV2	12423	19151	1.51%	0.194%

LSC Area Percent Report

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
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MW-25

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
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Title : SW846 8260

37	13.030	1953	1959	1967	rVB3	17620	28290	2.24%	0.286%
38	13.140	1969	1977	1979	rBV2	18608	32132	2.54%	0.325%
39	13.170	1979	1982	1990	rVB	44294	62541	4.94%	0.633%
40	13.292	1997	2002	2007	rBV	273357	339101	26.79%	3.431%
41	13.347	2007	2011	2015	rVB2	43803	55244	4.36%	0.559%
42	13.426	2020	2024	2030	rVB2	57266	74926	5.92%	0.758%
43	13.542	2039	2043	2047	rBV	32141	41934	3.31%	0.424%
44	13.585	2047	2050	2054	rVV	14924	19486	1.54%	0.197%
45	13.640	2054	2059	2060	rVV2	23966	33197	2.62%	0.336%
46	13.664	2060	2063	2068	rVB	48892	62923	4.97%	0.637%
47	13.865	2090	2096	2101	rBV2	10603	21539	1.70%	0.218%
48	13.926	2101	2106	2110	rVV3	15117	21314	1.68%	0.216%
49	14.219	2149	2154	2158	rBV3	8109	14634	1.16%	0.148%
50	14.323	2167	2171	2175	rBV2	10309	14340	1.13%	0.145%
51	14.378	2175	2180	2183	rVB2	9516	13057	1.03%	0.132%
52	14.603	2210	2217	2225	rBV	18833	36900	2.92%	0.373%
53	14.792	2241	2248	2255	rBV3	13048	22336	1.76%	0.226%

Sum of corrected areas: 9884600

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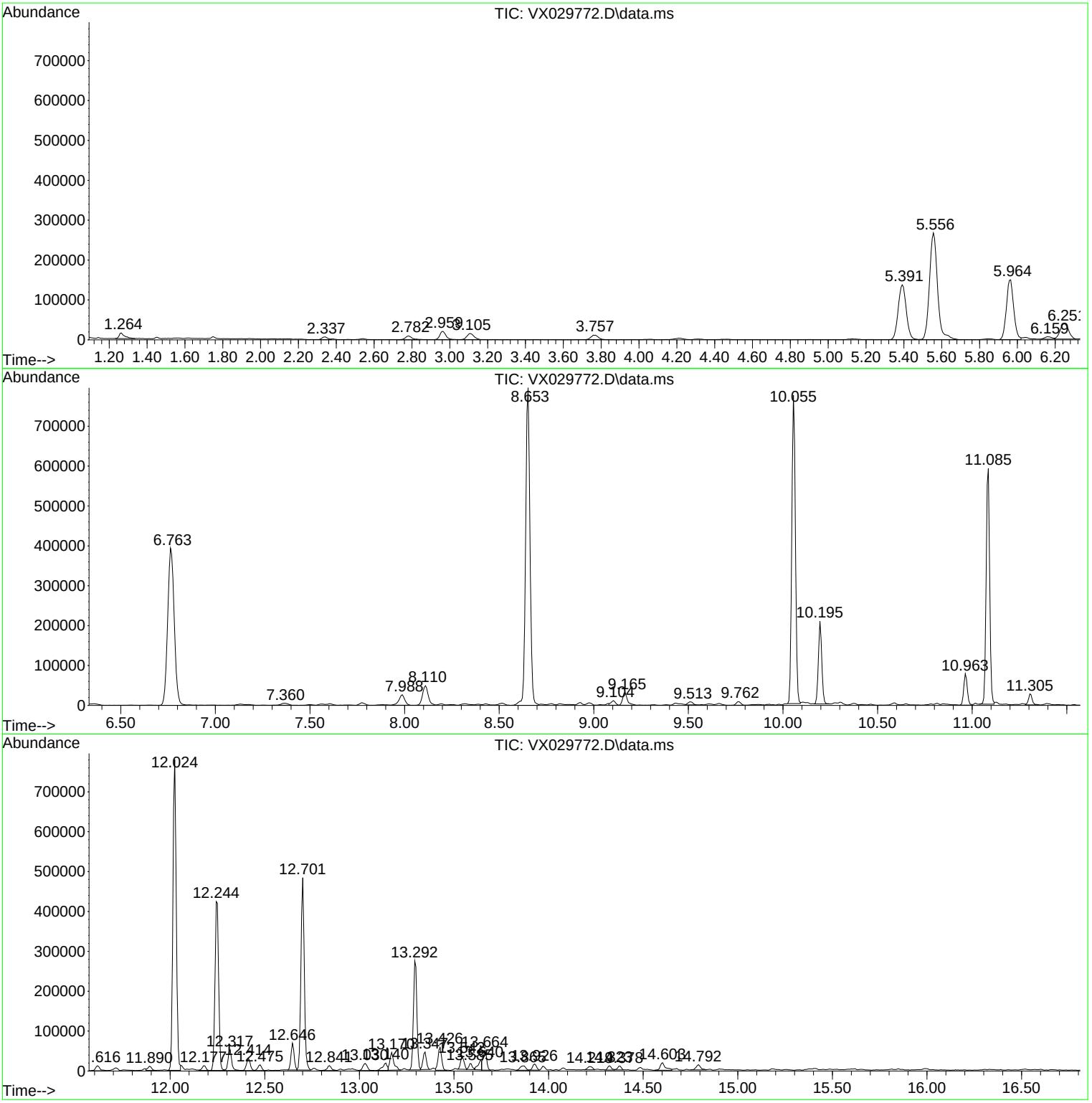
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062422\
Data File : VX029772.D
Acq On : 24 Jun 2022 13:59
Operator : JC/MD
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

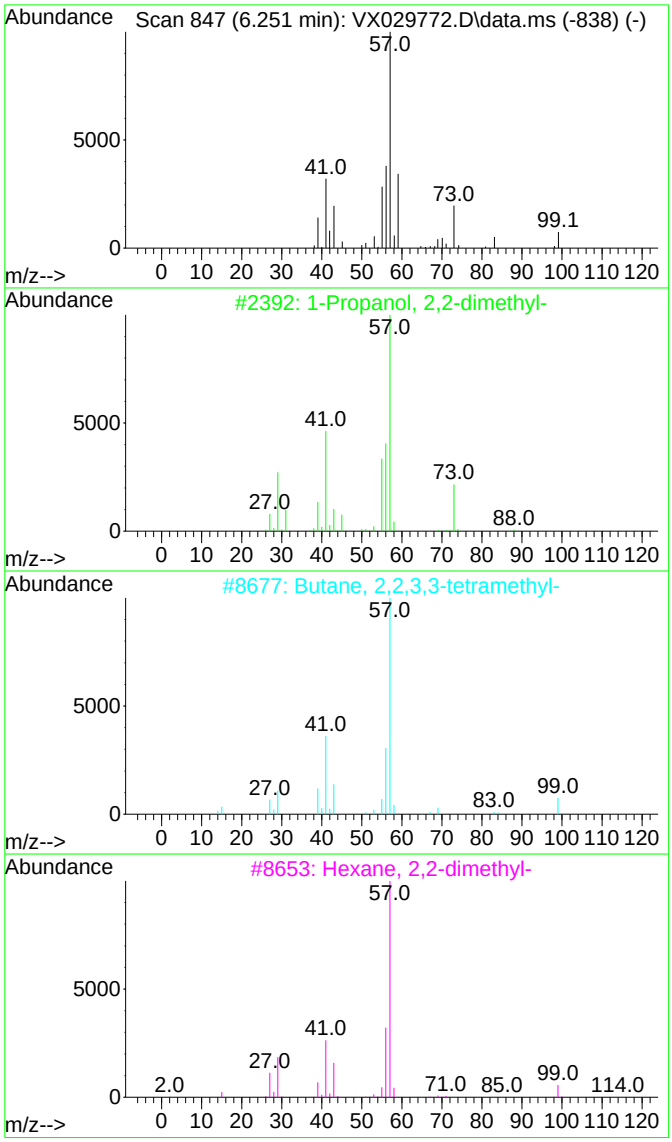
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

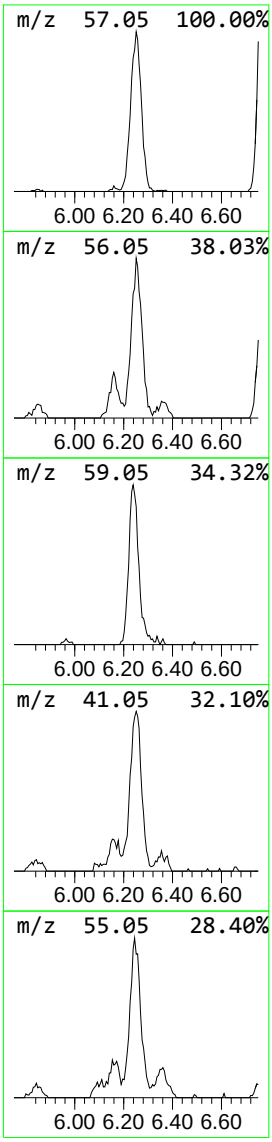
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown6.251 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	6.36 ug/l	119637	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	47
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	37
3	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	32
4	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	28
5	Heptane, 2-bromo-	178	C7H15Br	001974-04-5	27





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

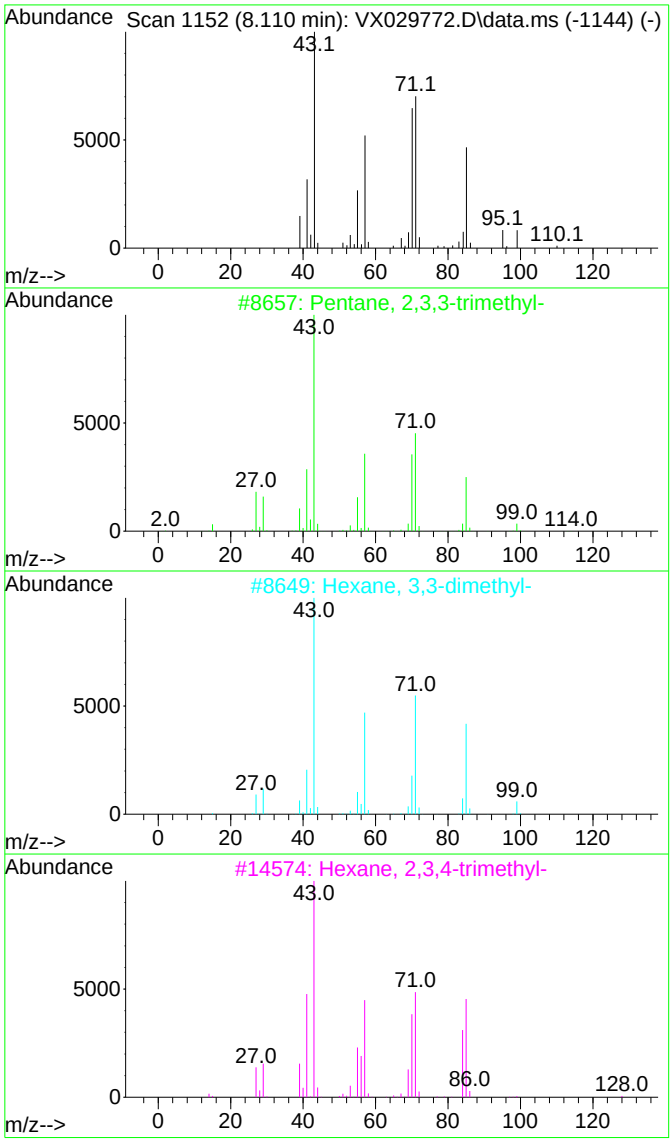
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

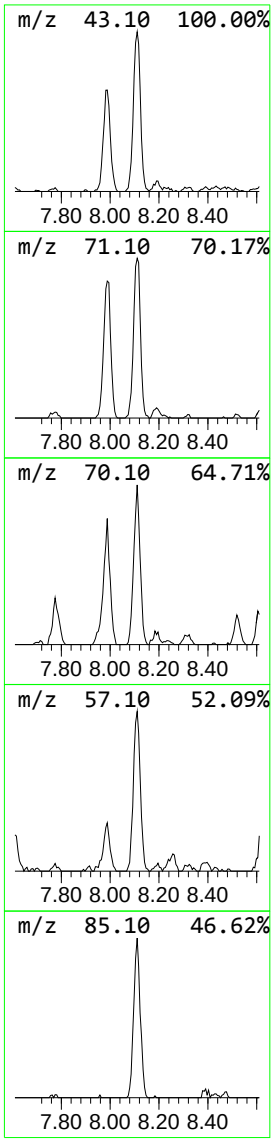
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	5.35 ug/l	100687	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	47
5	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	43





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Instrument :
MSVOA_X
ClientSampleId :
MW-25

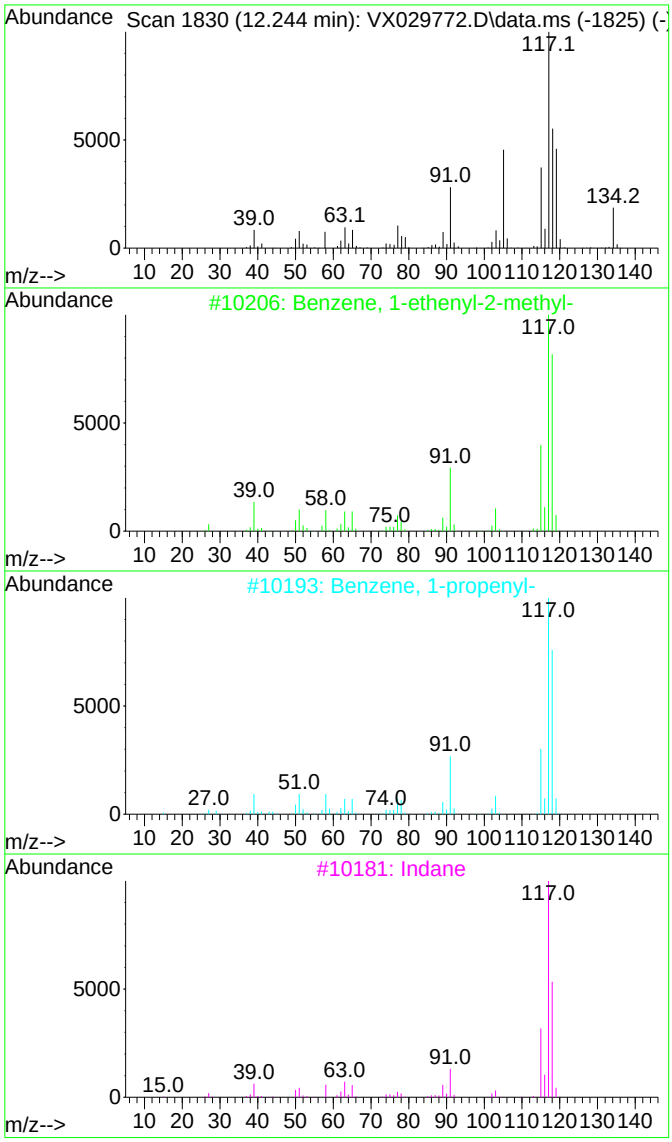
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

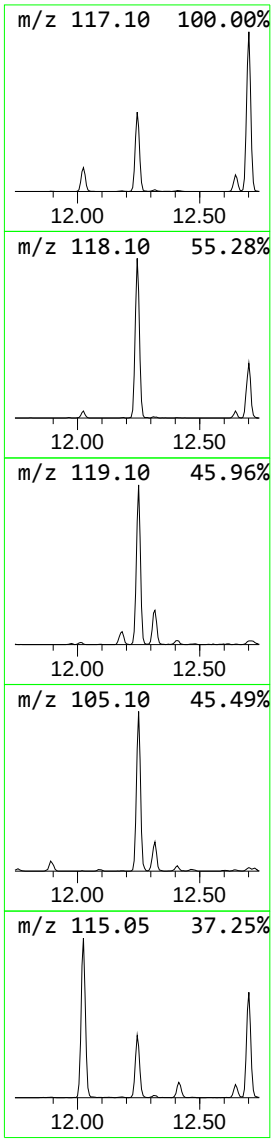
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	29.34 ug/l	563622	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	92
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	91
3	Indane	118	C9H10	000496-11-7	60
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

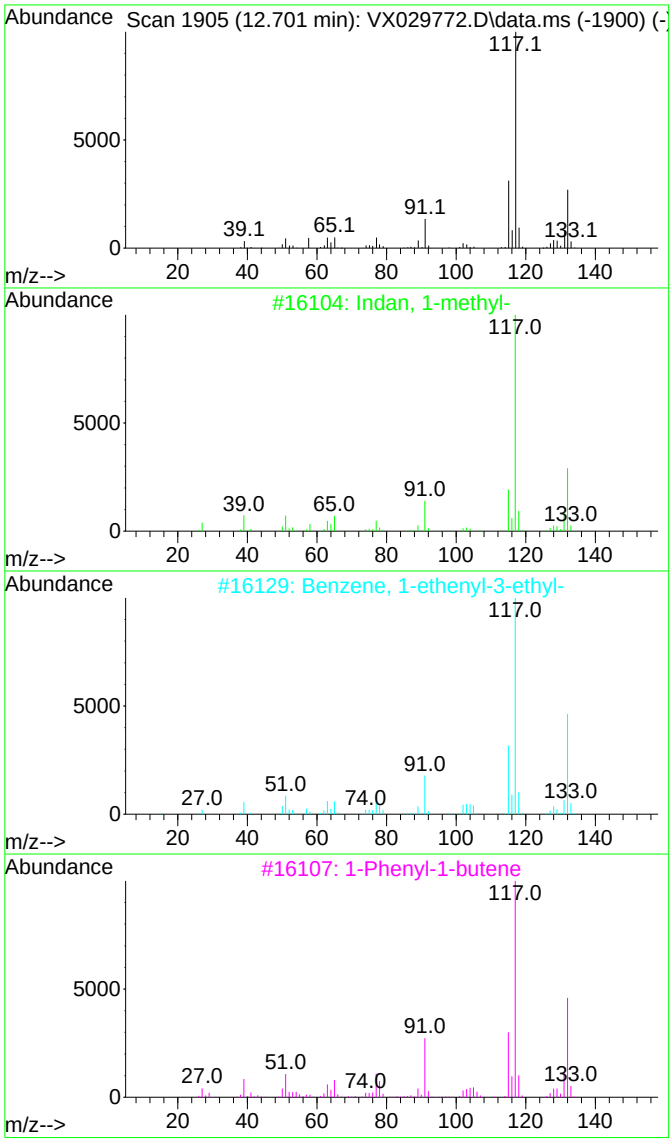
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

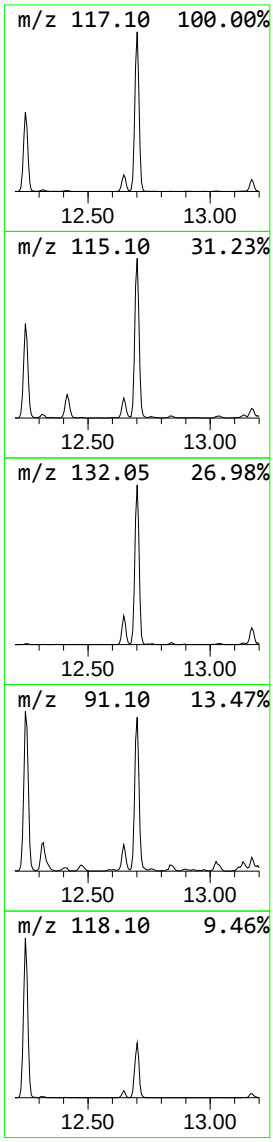
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	30.94 ug/l	594386	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-25

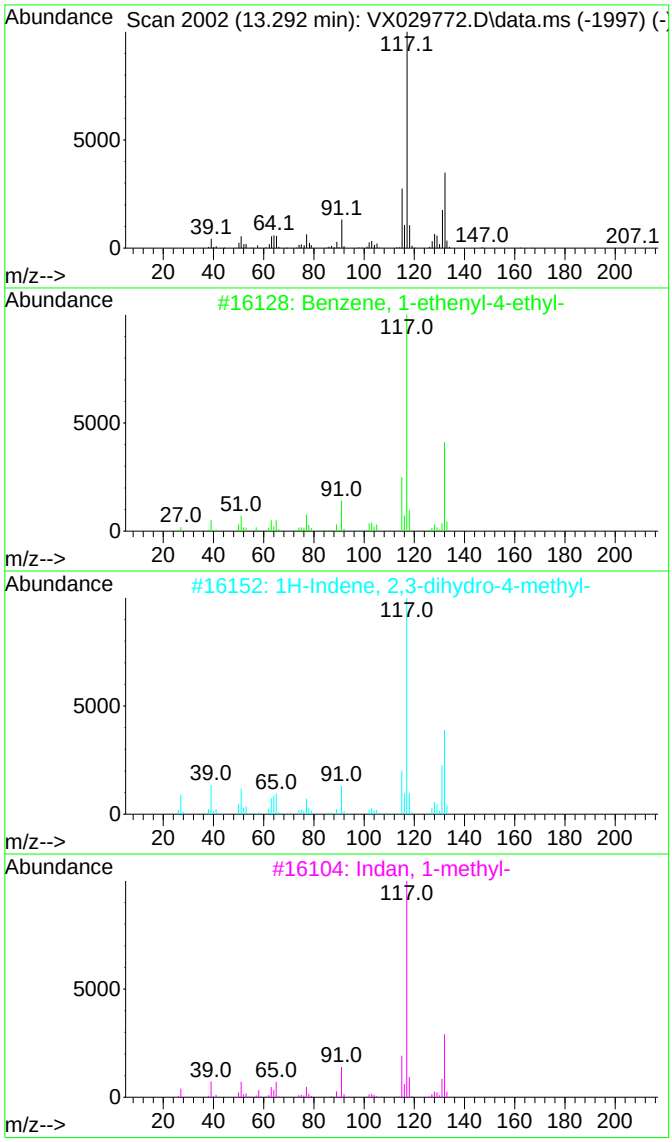
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

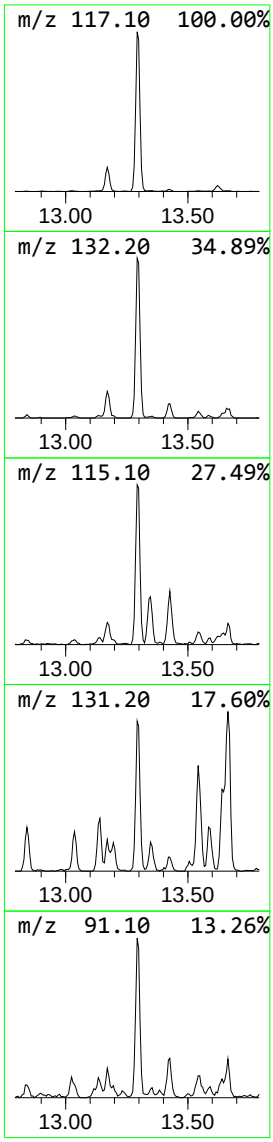
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	17.65 ug/l	339101	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3	Indan, 1-methyl-	132	C10H12	000767-58-8	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87





Tentatively Identified Compound (LSC) summary

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MSVOA_X
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MW-25

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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
unknown6.251	6.251	6.4	ug/l	119637	2	6.763	940731	50.0
Pentane, 2,3,3-...	8.110	5.3	ug/l	100687	2	6.763	940731	50.0
Benzene, 1-ethe...	12.244	29.3	ug/l	563622	4	12.024	960635	50.0
Indan, 1-methyl-	12.701	30.9	ug/l	594386	4	12.024	960635	50.0
Benzene, 1-ethe...	13.292	17.6	ug/l	339101	4	12.024	960635	50.0