LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040822\
Data File : VX028022.D
Acq On : 08 Apr 2022 13:14
Operator : JC/MD
Sample : N2333-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X040722W.M
Title : SW846 8260

Signal : TIC: VX028022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.752	101	109	117	rBV	46323	65652	13.49%	2.031%
2	1.953	137	142	147	rBV2	3343	5044	1.04%	0.156%
3	2.215	180	185	192	rVB3	3449	5471	1.12%	0.169%
4	2.337	200	205	210	rBV	6538	13189	2.71%	0.408%
5	2.532	230	237	245	rBV3	2534	5071	1.04%	0.157%
6	2.782	269	278	283	rBV	25459	57219	11.76%	1.770%
7	3.099	321	330	342	rBV4	15837	37121	7.63%	1.148%
8	4.215	506	513	519	rBV4	1936	5068	1.04%	0.157%
9	4.306	519	528	539	rVB3	7978	22721	4.67%	0.703%
10	4.434	539	549	559	rBV6	1533	5200	1.07%	0.161%
11	5.391	695	706	714	rBV	60469	175995	36.18%	5.445%
12	5.471	715	719	724	rVV3	8857	23137	4.76%	0.716%
13	5.556	724	733	753	rVB	99199	289778	59.56%	8.965%
14	5.849	773	781	789	rBV4	1934	5378	1.11%	0.166%
15	5.958	789	799	809	rBV	69520	180885	37.18%	5.596%
16	6.044	809	813	821	rVB4	2517	5778	1.19%	0.179%
17	6.159	825	832	837	rBV4	1994	5220	1.07%	0.161%
18	6.251	843	847	857	rVB4	2867	7815	1.61%	0.242%
19	6.355	857	864	872	rBV5	2992	8294	1.70%	0.257%
20	6.763	922	931	943	rBV	156714	370956	76.25%	11.476%
21	7.367	1021	1030	1039	rBV4	4269	11524	2.37%	0.357%
22	8.653	1233	1241	1250	rBV	310416	486508	100.00%	15.051%
23	8.958	1279	1291	1301	rVB4	6401	13624	2.80%	0.421%
24	9.049	1301	1306	1311	rBV2	6213	9649	1.98%	0.299%
25	10.055	1465	1471	1478	rBV	338212	450456	92.59%	13.936%
26	10.305	1505	1512	1517	rBV	6300	9035	1.86%	0.280%
27	10.963	1615	1620	1627	rVB	18938	23491	4.83%	0.727%
28	11.085	1634	1640	1650	rVB	270371	354788	72.93%	10.976%
29	11.305	1671	1676	1685	rBV	35558	43859	9.02%	1.357%
30	12.024	1789	1794	1803	rBV	338580	423400	87.03%	13.099%
31	12.244	1824	1830	1837	rVB2	36069	48892	10.05%	1.513%
32	12.616	1885	1891	1895	rBV	10990	13283	2.73%	0.411%
33	12.701	1900	1905	1913	rVB	17534	21891	4.50%	0.677%
34	12.927	1937	1942	1950	rVB	17103	21451	4.41%	0.664%
35	13.292	1998	2002	2006	rBV2	4303	5540	1.14%	0.171%

LSC Area Percent Report

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Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X040722W.M
Title : SW846 8260

Sum of corrected areas: 3232383

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MSVOA_X
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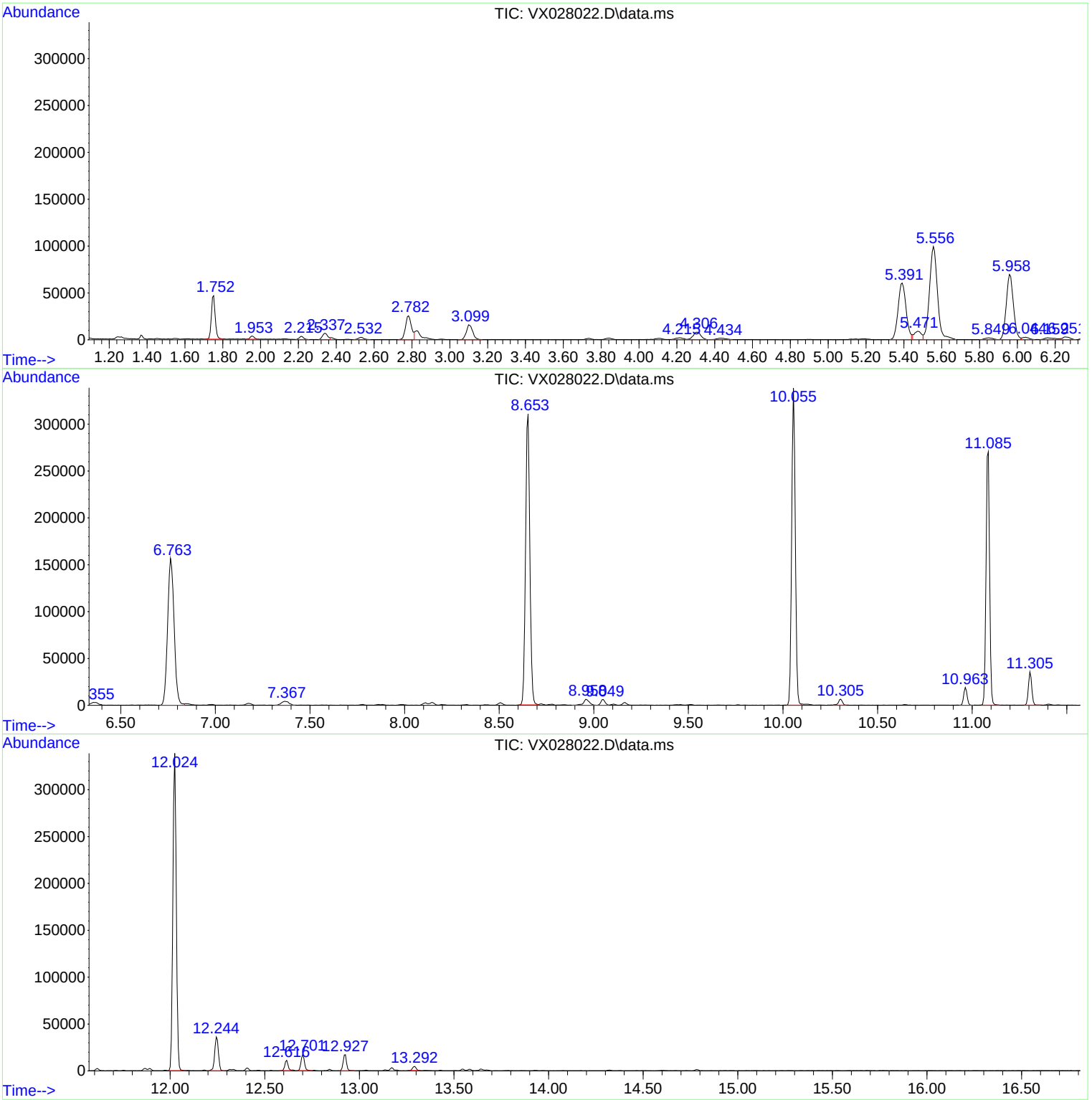
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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



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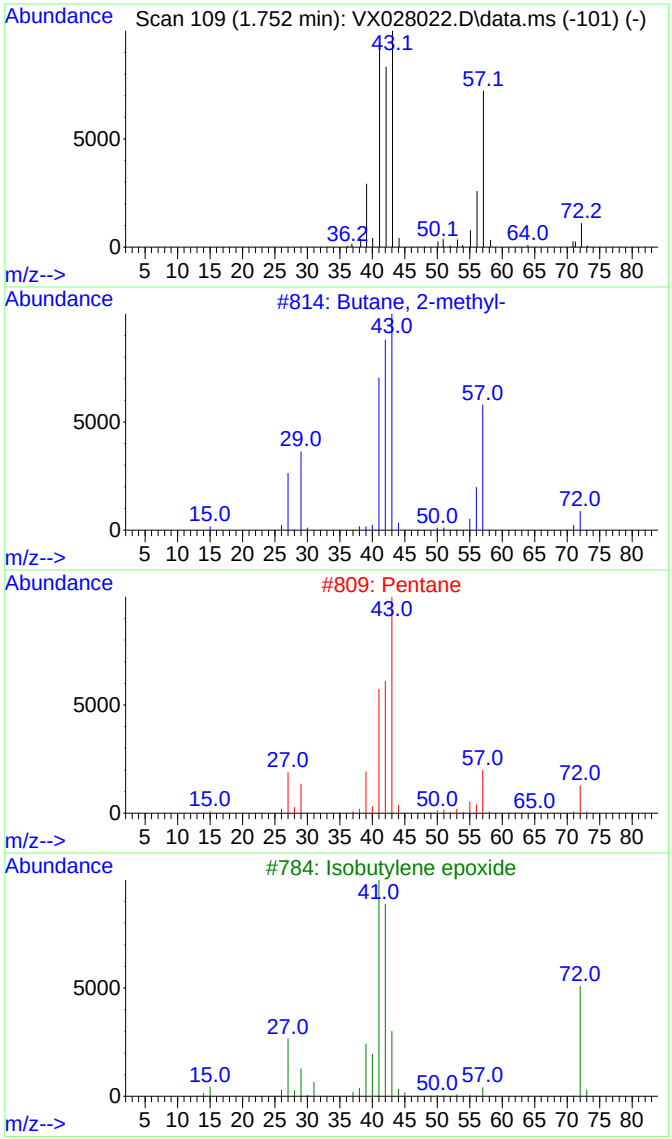
Quant Title : SW846 8260

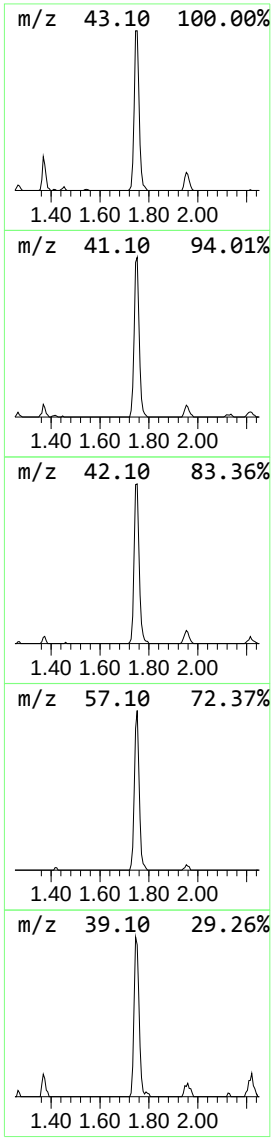
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	11.33 ug/l	65652	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	47
3	Isobutylene epoxide	72	C4H8O	000558-30-5	40
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	33
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33





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Instrument :
MSVOA_X
ClientSampleId :
MW-2

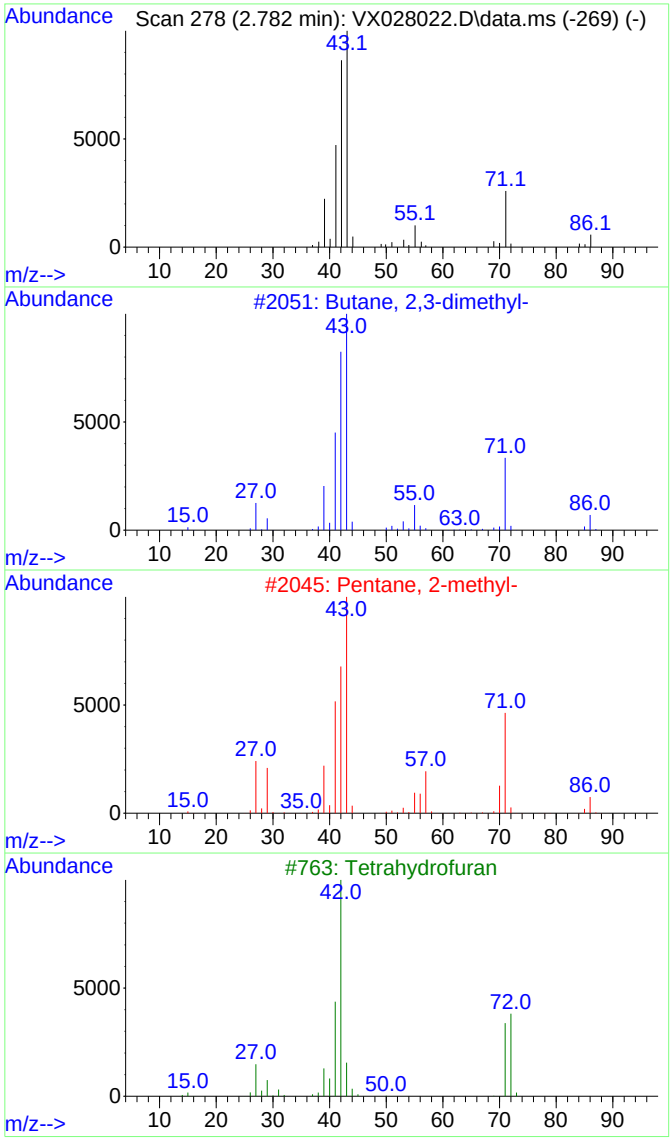
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

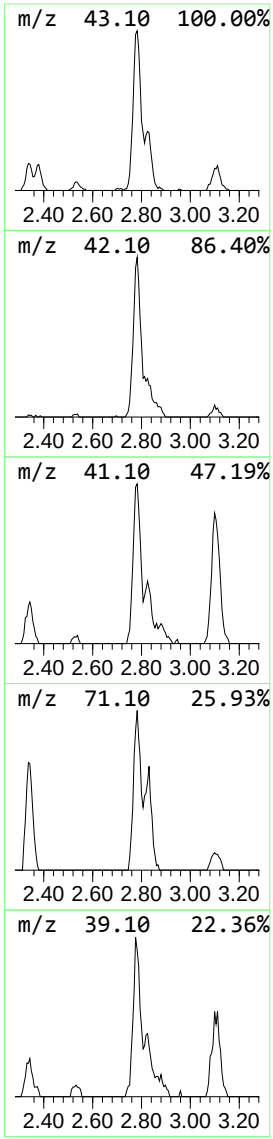
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	9.87 ug/l	57219	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Pentane	72	C5H12	000109-66-0	38
5	Pyrrolidine	71	C4H9N	000123-75-1	16





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

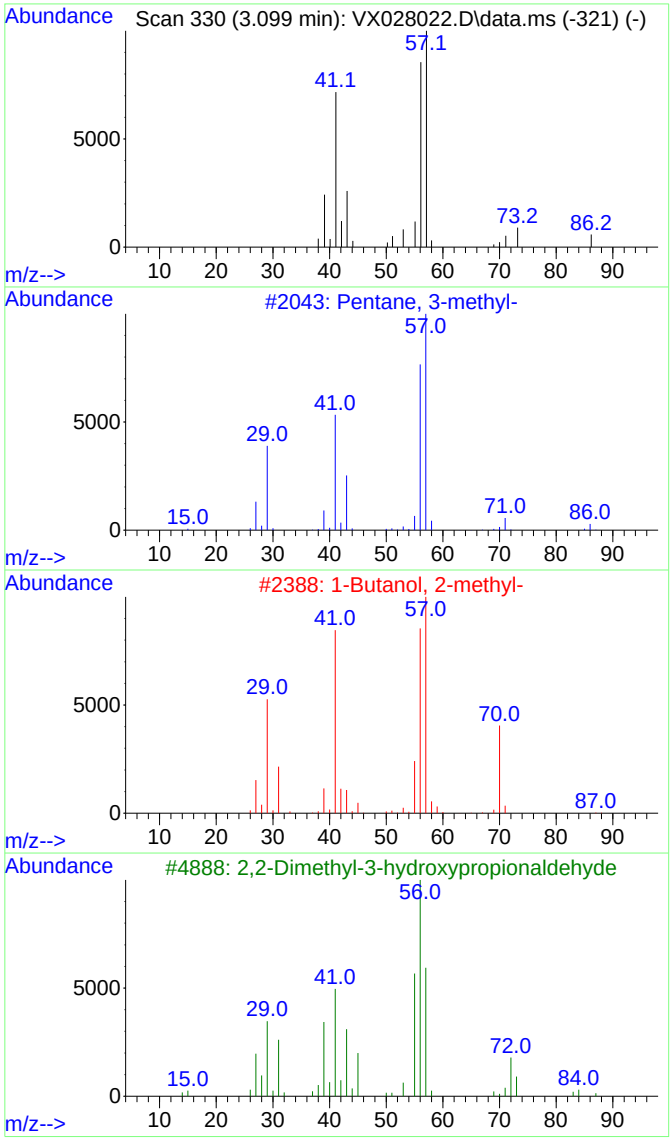
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

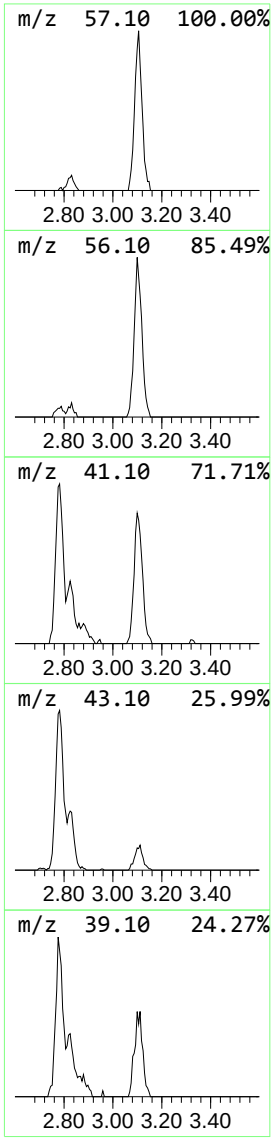
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.099	6.41 ug/l	37121	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	72
2	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	39
3	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	39
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

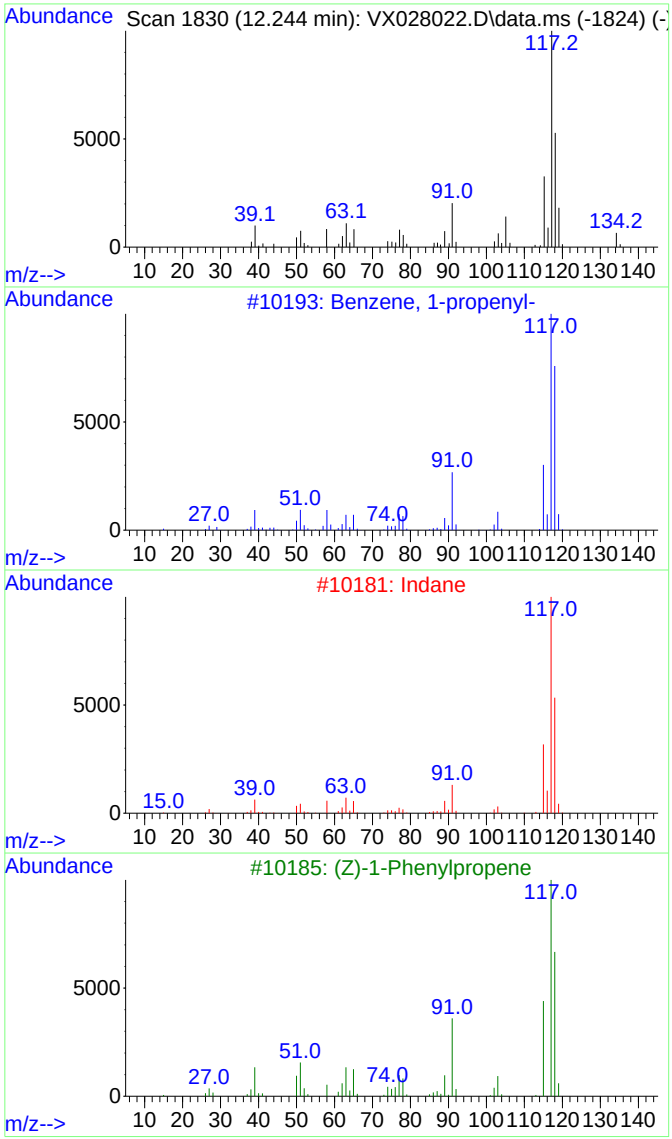
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

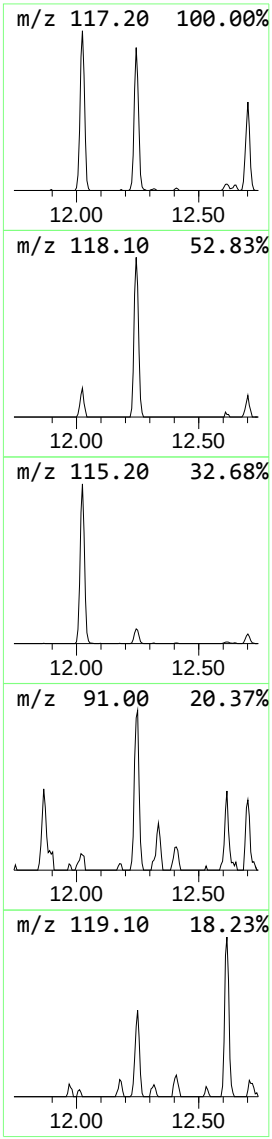
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-propenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	5.77 ug/l	48892	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
2	Indane	118	C9H10	000496-11-7	93
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	89
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	89
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87





Tentatively Identified Compound (LSC) summary

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.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-	1.752	11.3	ug/l	65652	1	5.556	289778	50.0
Butane, 2,3-dim...	2.782	9.9	ug/l	57219	1	5.556	289778	50.0
Pentane, 3-methyl-	3.099	6.4	ug/l	37121	1	5.556	289778	50.0
Benzene, 1-prop...	12.244	5.8	ug/l	48892	4	12.024	423400	50.0