LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092222\
Data File : VX031570.D
Acq On : 22 Sep 2022 15:11
Operator : JC/MD
Sample : N4642-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11R

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\82X091922W.M
Title : SW846 8260

Signal : TIC: VX031570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.611	79	86	96	rBV10	3301	10448	1.64%	0.309%
2	2.337	197	205	212	rBV2	9793	18654	2.93%	0.552%
3	2.782	271	278	287	rBV3	5574	12862	2.02%	0.381%
4	4.208	504	512	521	rVB6	2513	7146	1.12%	0.212%
5	5.391	695	706	723	rBV	73708	215636	33.87%	6.385%
6	5.556	723	733	742	rBV	72226	205867	32.33%	6.095%
7	5.958	788	799	809	rBV	80643	213322	33.50%	6.316%
8	6.031	809	811	820	rVB4	3242	7158	1.12%	0.212%
9	6.251	840	847	855	rVB4	5688	16596	2.61%	0.491%
10	6.763	921	931	941	rBV	114035	266212	41.81%	7.882%
11	7.982	1123	1131	1138	rVB4	3887	9558	1.50%	0.283%
12	8.110	1145	1152	1156	rBV2	8945	18612	2.92%	0.551%
13	8.653	1229	1241	1251	rBV	393213	636708	100.00%	18.852%
14	8.958	1281	1291	1299	rVV	61147	97910	15.38%	2.899%
15	9.049	1299	1306	1311	rVV	71941	104075	16.35%	3.081%
16	9.098	1311	1314	1319	rVV2	4100	6629	1.04%	0.196%
17	9.165	1319	1325	1333	rVV	7049	10671	1.68%	0.316%
18	9.457	1365	1373	1377	rBV5	3374	7113	1.12%	0.211%
19	10.055	1461	1471	1478	rBV	251929	336959	52.92%	9.977%
20	10.963	1616	1620	1625	rVB	16675	21773	3.42%	0.645%
21	11.079	1634	1639	1645	rBV	326378	416063	65.35%	12.319%
22	11.305	1672	1676	1681	rVB2	6598	8259	1.30%	0.245%
23	11.610	1722	1726	1731	rVB2	9988	12921	2.03%	0.383%
24	11.890	1770	1772	1779	rVB	6729	7370	1.16%	0.218%
25	12.024	1788	1794	1800	rBV	263296	318116	49.96%	9.419%
26	12.244	1825	1830	1838	rBV2	105718	136217	21.39%	4.033%
27	12.317	1838	1842	1848	rVB	11026	14914	2.34%	0.442%
28	12.646	1893	1896	1900	rVB	11561	13125	2.06%	0.389%
29	12.701	1900	1905	1912	rVB	63215	78782	12.37%	2.333%
30	13.170	1978	1982	1990	rVB	45746	56552	8.88%	1.674%
31	13.292	1998	2002	2008	rBV	15094	20106	3.16%	0.595%
32	13.347	2008	2011	2013	rVV3	5770	7114	1.12%	0.211%
33	13.426	2020	2024	2029	rVB	5632	6757	1.06%	0.200%
34	13.542	2040	2043	2047	rVV	14220	19301	3.03%	0.571%
35	13.591	2047	2051	2054	rVV5	3496	6753	1.06%	0.200%
36	13.664	2057	2063	2072	rVB2	16724	31197	4.90%	0.924%

LSC Area Percent Report

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Integration Parameters: RTEINT.P
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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\82X091922W.M
Title : SW846 8260

Sum of corrected areas: 3377456

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ClientSampleId :
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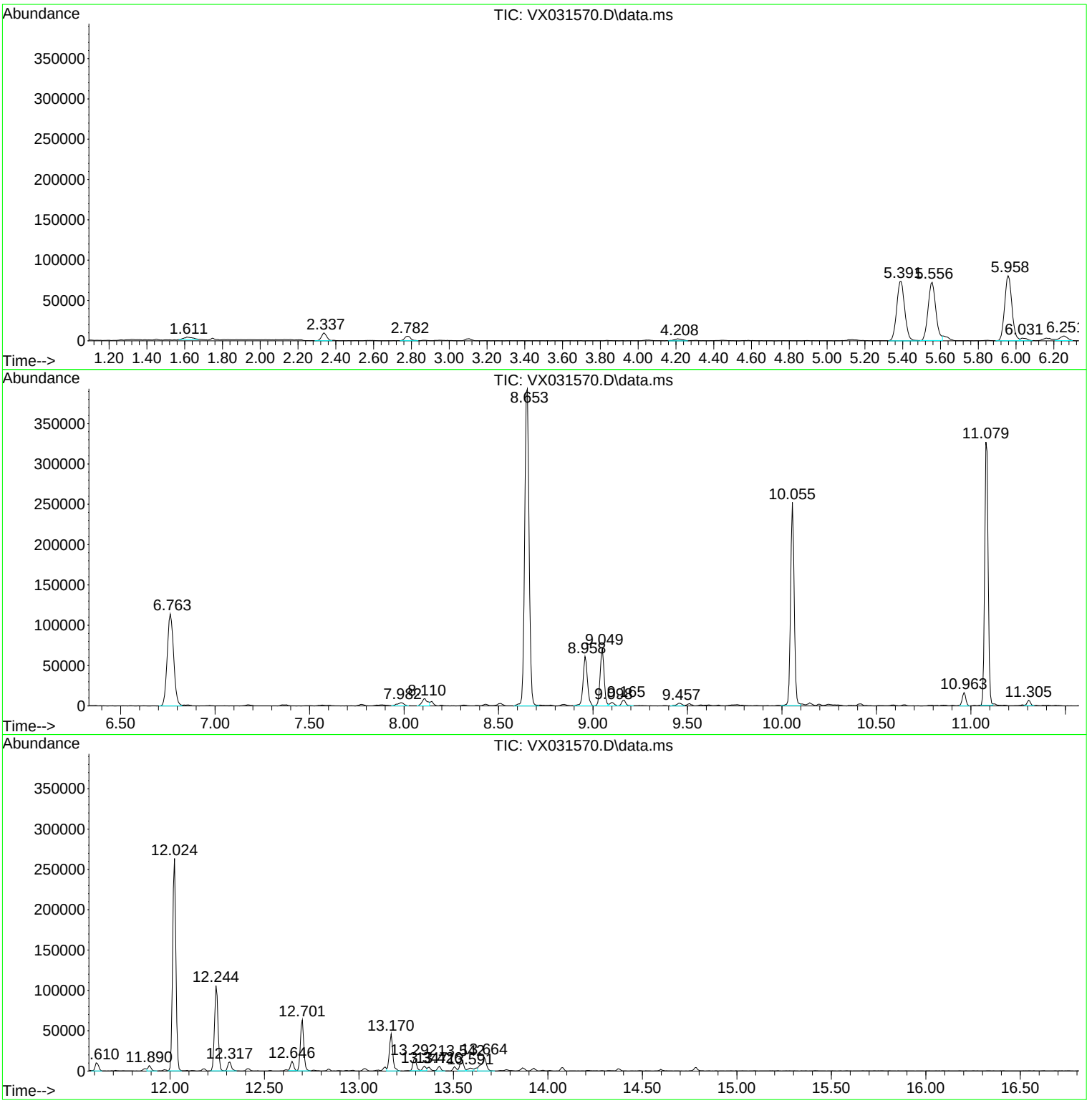
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

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



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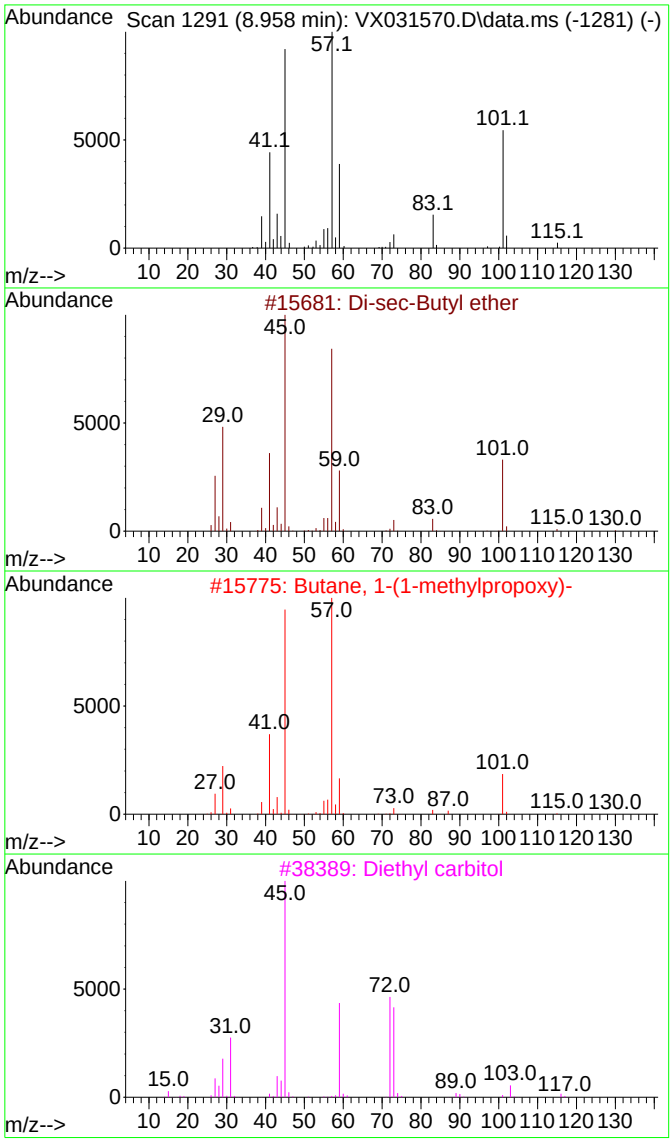
Quant Title : SW846 8260

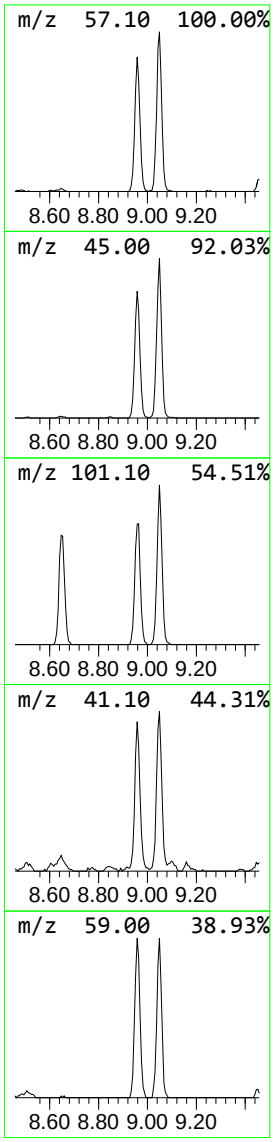
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Di-sec-Butyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	14.53 ug/l	97910	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3	Diethyl carbitol	162	C8H18O3	000112-36-7	47
4	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	42
5	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	42





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MSVOA_X
ClientSampleId :
MW-11R

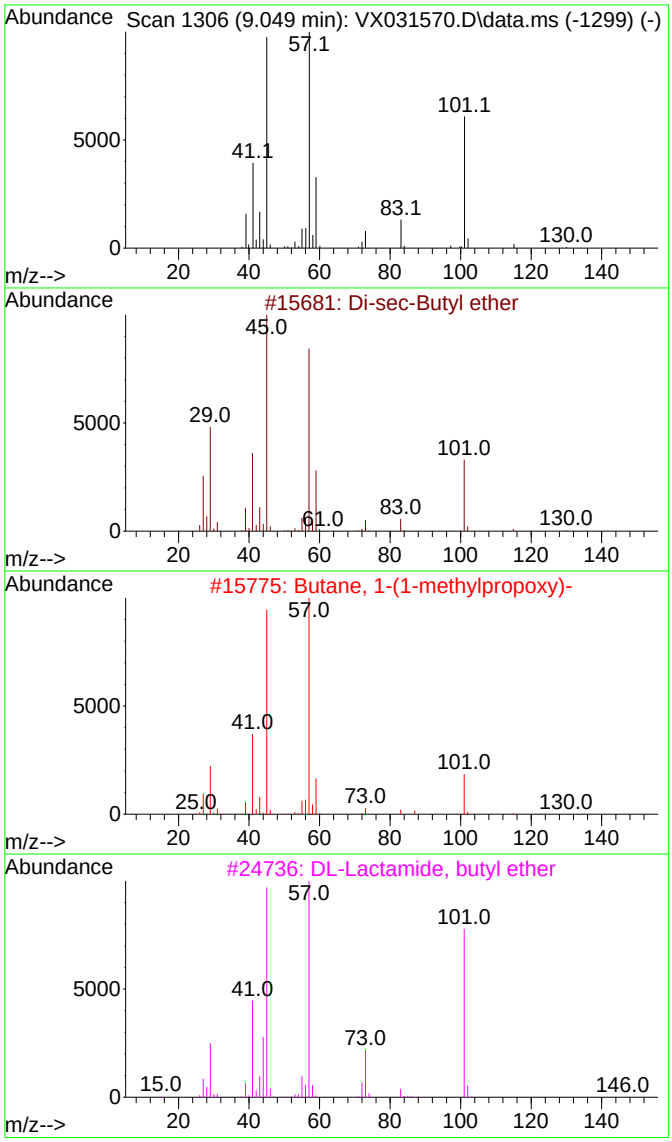
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

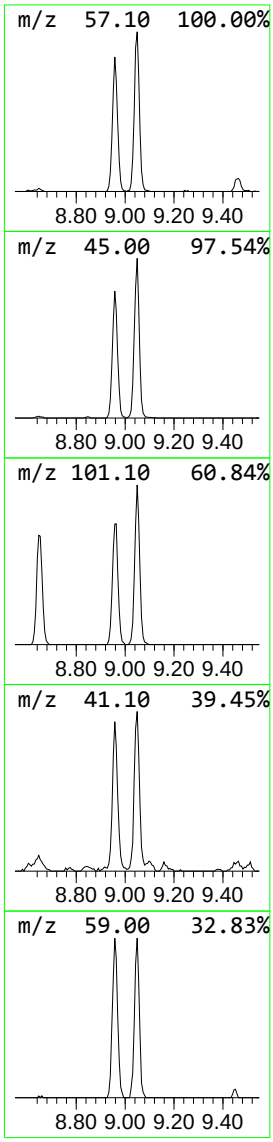
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 1-(1-methylpropoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	15.44 ug/l	104075	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	72
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
4	Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	50
5	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	42





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11R

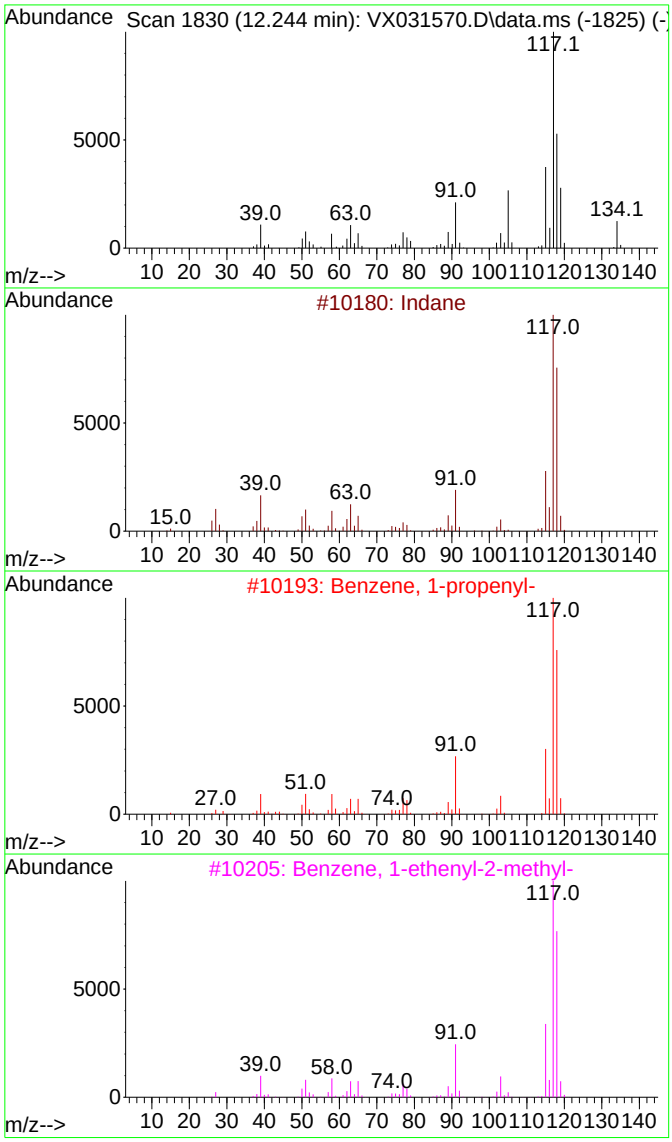
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

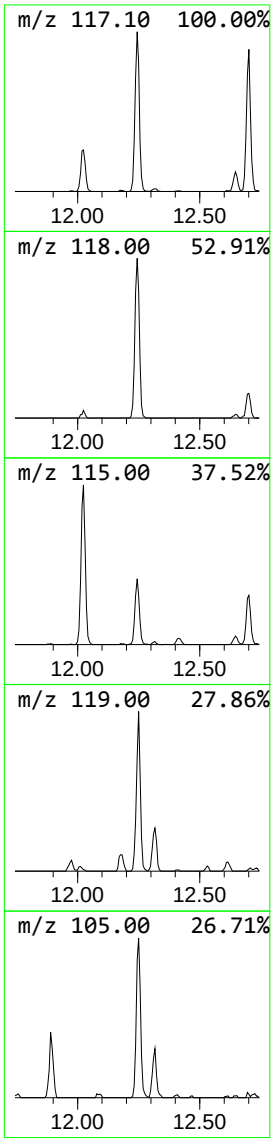
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	21.41 ug/l	136217	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	91
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	91
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64





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ClientSampleId :
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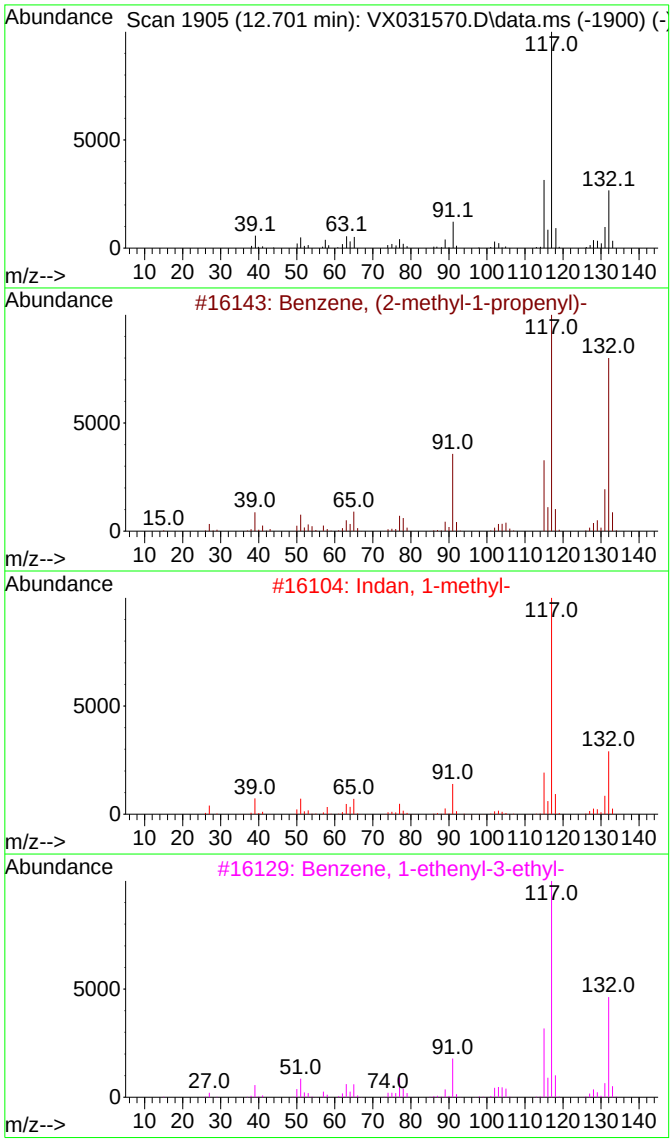
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

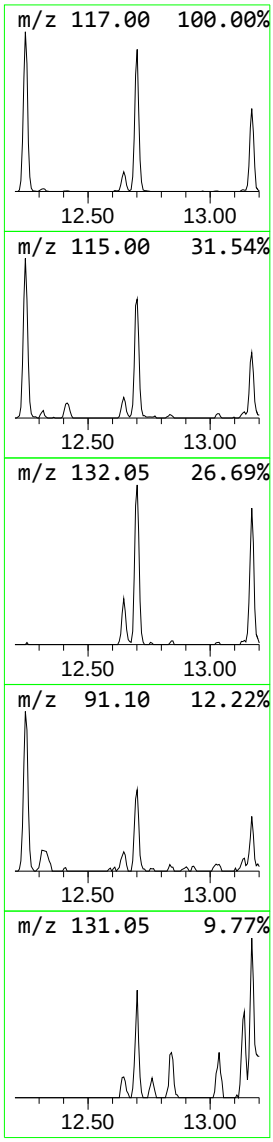
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	12.38 ug/l	78782	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	90
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	87





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-11R

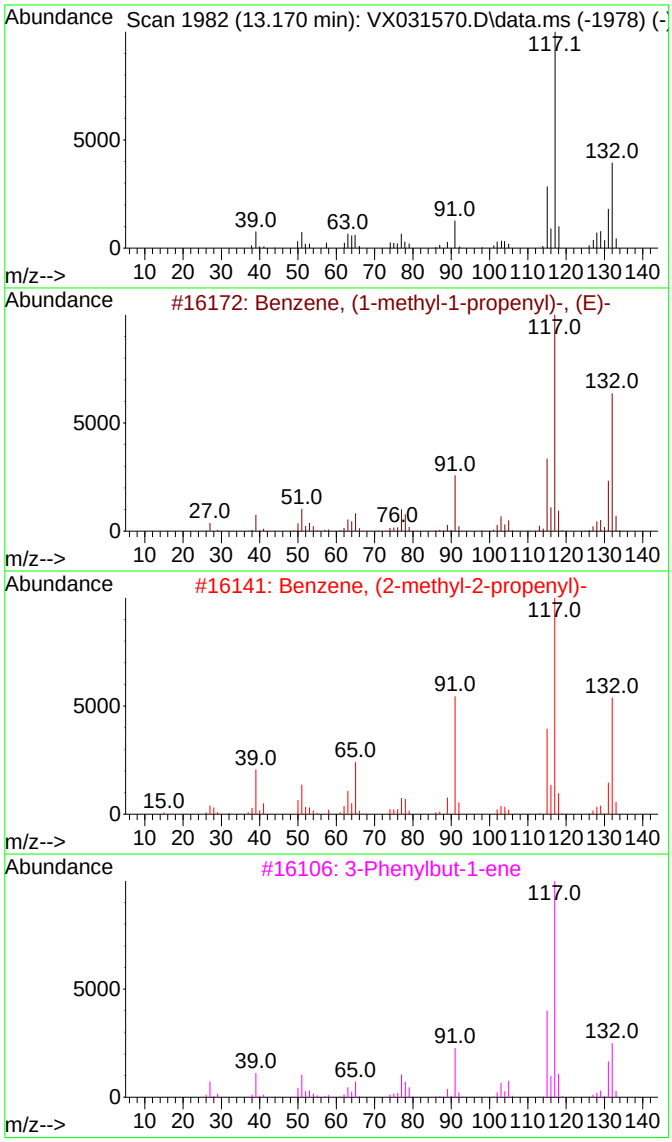
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

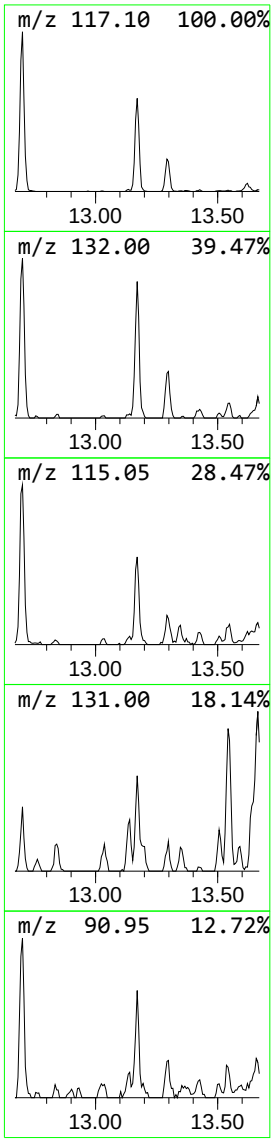
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (1-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	8.89 ug/l	56552	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
2	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	90
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	90





Tentatively Identified Compound (LSC) summary

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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
Di-sec-Butyl ether	8.958	14.5	ug/l	97910	3	10.055	336959	50.0
Butane, 1-(1-me...	9.049	15.4	ug/l	104075	3	10.055	336959	50.0
Indane	12.244	21.4	ug/l	136217	4	12.024	318116	50.0
Benzene, (2-met...	12.701	12.4	ug/l	78782	4	12.024	318116	50.0
Benzene, (1-met...	13.170	8.9	ug/l	56552	4	12.024	318116	50.0