LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033121\
Data File : VU042855.D
Acq On : 31 Mar 2021 14:22
Operator : SY/MD
Sample : M1836-15 10X
Misc : 8.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : B7-0-2

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_U\Method\82U032421W.M
Title : SW846 8260

Signal : TIC: VU042855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.880	162	168	174	rVB5	4218	6363	1.05%	0.145%
2	1.996	195	204	212	rVB2	5809	8416	1.39%	0.191%
3	2.208	261	270	285	rVB5	4209	7113	1.18%	0.162%
4	3.089	537	544	554	rVB4	4228	8633	1.43%	0.196%
5	3.369	620	631	643	rVB3	3456	6871	1.14%	0.156%
6	3.710	726	737	746	rVB5	3129	6229	1.03%	0.142%
7	4.539	985	995	1006	rVB3	3030	6785	1.12%	0.154%
8	5.298	1216	1231	1244	rBV2	96378	203535	33.65%	4.629%
9	5.382	1244	1257	1274	rVV	159119	329149	54.42%	7.486%
10	5.468	1274	1284	1302	rVB6	5103	11288	1.87%	0.257%
11	5.597	1313	1324	1336	rVB5	4268	8300	1.37%	0.189%
12	5.710	1342	1359	1373	rBV	108526	223405	36.94%	5.081%
13	5.783	1373	1382	1395	rVB3	12586	24866	4.11%	0.566%
14	5.909	1406	1421	1437	rVB2	26532	62734	10.37%	1.427%
15	6.140	1484	1493	1504	rVB4	4497	7556	1.25%	0.172%
16	6.259	1515	1530	1556	rBV	222665	427676	70.71%	9.726%
17	6.767	1676	1688	1696	rBV8	3737	8816	1.46%	0.200%
18	6.816	1696	1703	1711	rVV5	4630	7933	1.31%	0.180%
19	6.873	1711	1721	1731	rVB5	4676	7853	1.30%	0.179%
20	7.266	1830	1843	1855	rVB2	21898	41312	6.83%	0.940%
21	7.388	1869	1881	1891	rBV3	21087	43572	7.20%	0.991%
22	7.436	1891	1896	1906	rVB4	5433	8752	1.45%	0.199%
23	7.844	2012	2023	2029	rBV4	4833	8922	1.48%	0.203%
24	7.906	2029	2042	2060	rVB	356850	604796	100.00%	13.754%
25	9.423	2501	2514	2542	rBV	329796	545883	90.26%	12.415%
26	9.578	2549	2562	2576	rBV	36044	56124	9.28%	1.276%
27	9.700	2590	2600	2610	rBV2	6552	10017	1.66%	0.228%
28	10.491	2836	2846	2859	rBV3	6269	9434	1.56%	0.215%
29	10.642	2880	2893	2915	rVB	287925	464605	76.82%	10.566%
30	10.912	2957	2977	2989	rBV2	29191	52604	8.70%	1.196%
31	11.301	3089	3098	3106	rBV3	4331	6522	1.08%	0.148%
32	11.819	3246	3259	3273	rBV	378903	595966	98.54%	13.554%
33	12.102	3337	3347	3362	rVB2	43470	67347	11.14%	1.532%
34	12.192	3362	3375	3378	rBV9	7211	11027	1.82%	0.251%
35	12.385	3427	3435	3447	rVB	8884	13199	2.18%	0.300%
36	12.577	3486	3495	3504	rBV	41371	59575	9.85%	1.355%

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Instrument : MSVOA_U
ClientSampleId : B7-0-2

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

37	12.690	3520	3530	3549	rVB3	14999	28398	4.70%	0.646%
38	12.979	3604	3620	3634	rBV2	24936	39747	6.57%	0.904%
39	13.111	3653	3661	3677	rBV5	5637	9227	1.53%	0.210%
40	13.301	3712	3720	3731	rVB	17620	25469	4.21%	0.579%
41	13.462	3750	3770	3784	rBV3	38915	74468	12.31%	1.694%
42	13.565	3795	3802	3810	rBV2	5540	7058	1.17%	0.161%
43	13.632	3816	3823	3833	rBV9	4560	6707	1.11%	0.153%
44	13.793	3865	3873	3880	rVV3	6807	9957	1.65%	0.226%
45	13.844	3880	3889	3898	rVB5	11714	18113	2.99%	0.412%
46	14.095	3955	3967	3986	rVB	44237	72750	12.03%	1.654%
47	14.294	4020	4029	4040	rBV8	4045	7208	1.19%	0.164%
48	14.497	4082	4092	4100	rBV3	5783	8757	1.45%	0.199%
49	14.677	4138	4148	4160	rBV6	6783	13066	2.16%	0.297%
50	15.230	4306	4320	4332	rBV	31721	51337	8.49%	1.168%
51	15.420	4367	4379	4391	rVB	16411	25644	4.24%	0.583%
52	16.272	4635	4644	4654	rBV4	6658	12013	1.99%	0.273%
53	16.420	4680	4690	4697	rBV3	8588	14026	2.32%	0.319%

Sum of corrected areas: 4397123

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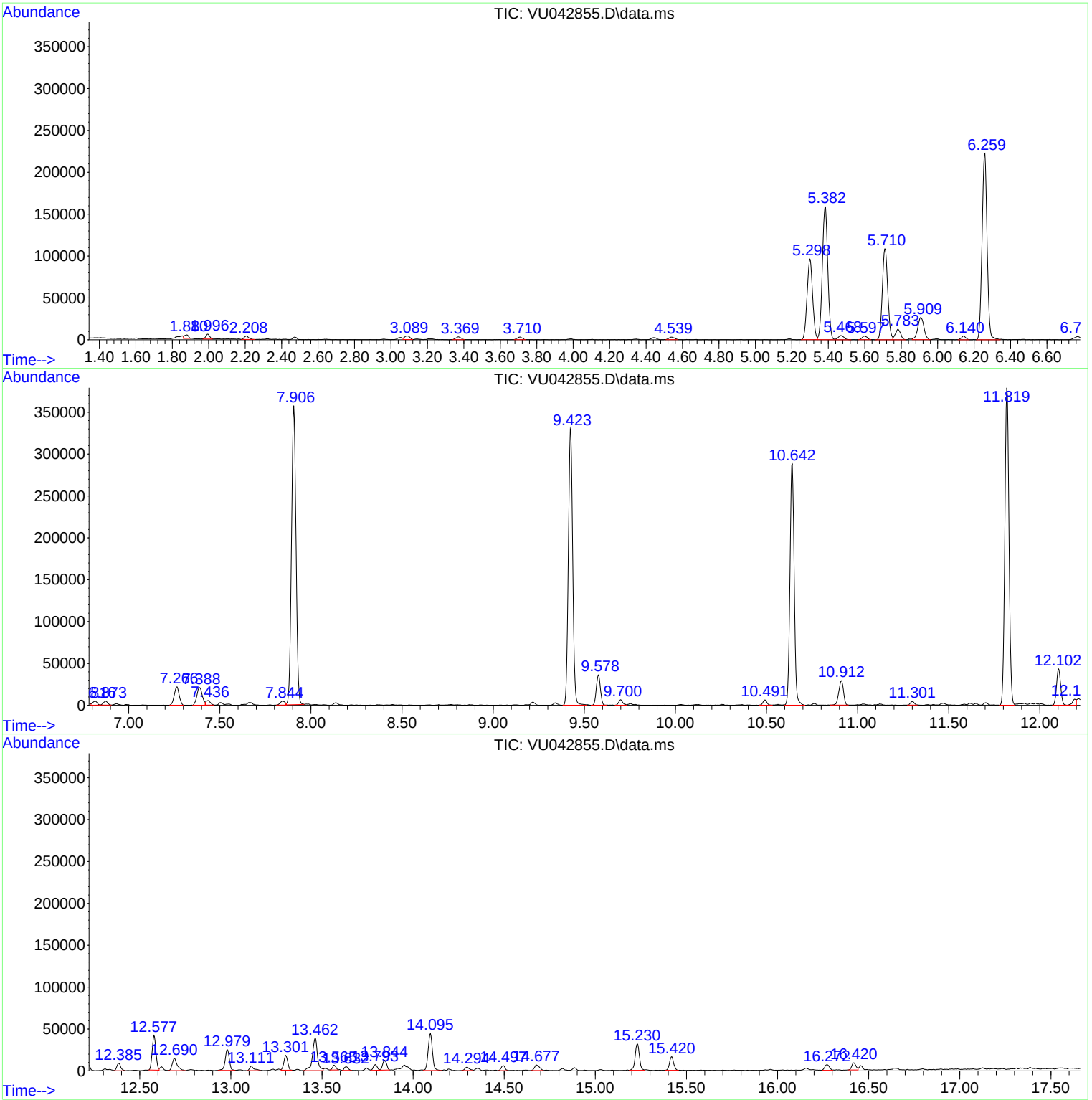
Instrument :
MSVOA_U
ClientSampleId :
B7-0-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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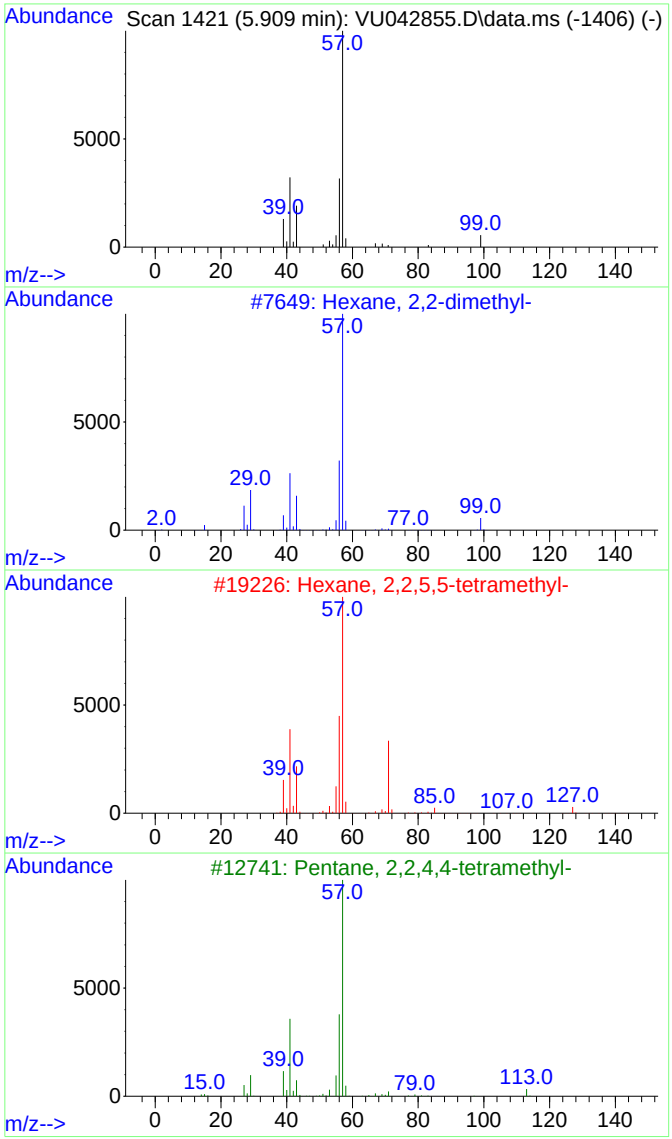
Quant Title : SW846 8260

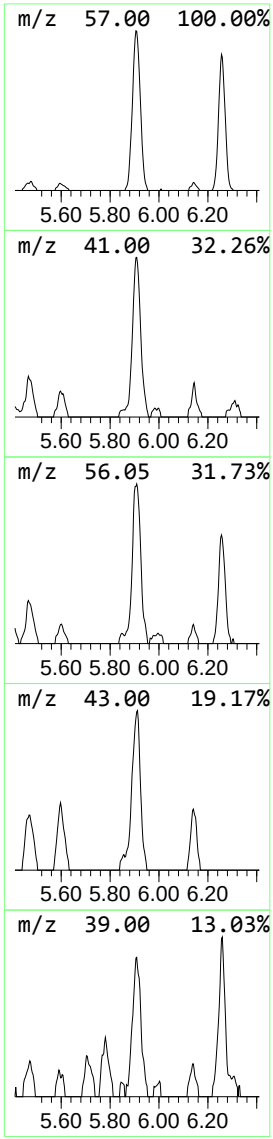
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.909	7.33 ug/l	62734	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
3	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
4	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	56
5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	56





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Instrument :
MSVOA_U
ClientSampleId :
B7-0-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

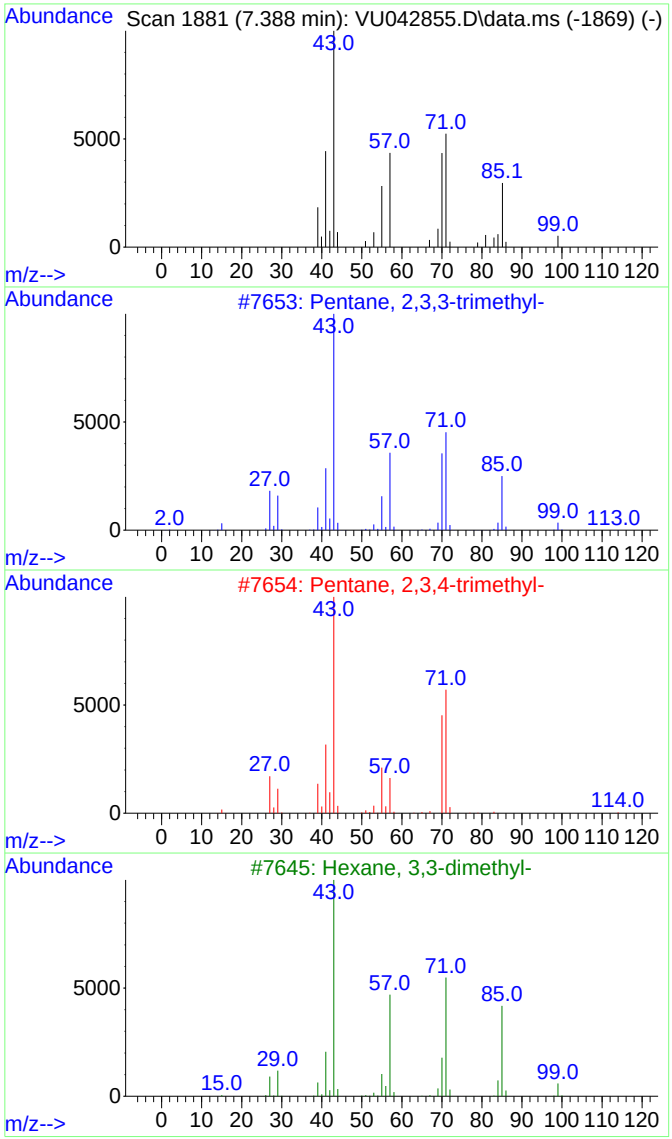
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

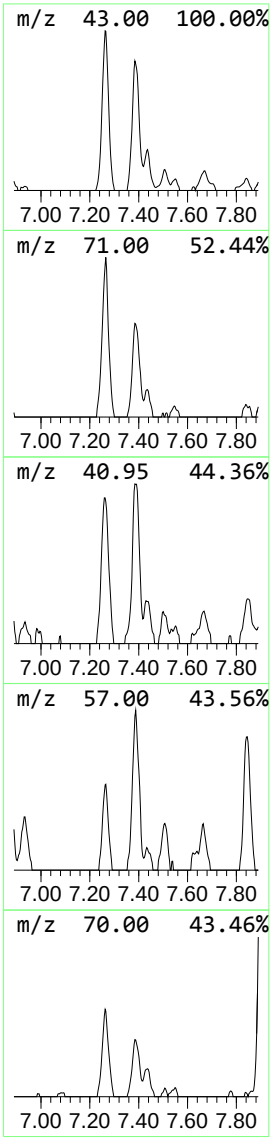
****

Peak Number 2 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.388	5.09 ug/l	43572	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50





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ClientSampleId :
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Quant Title : SW846 8260

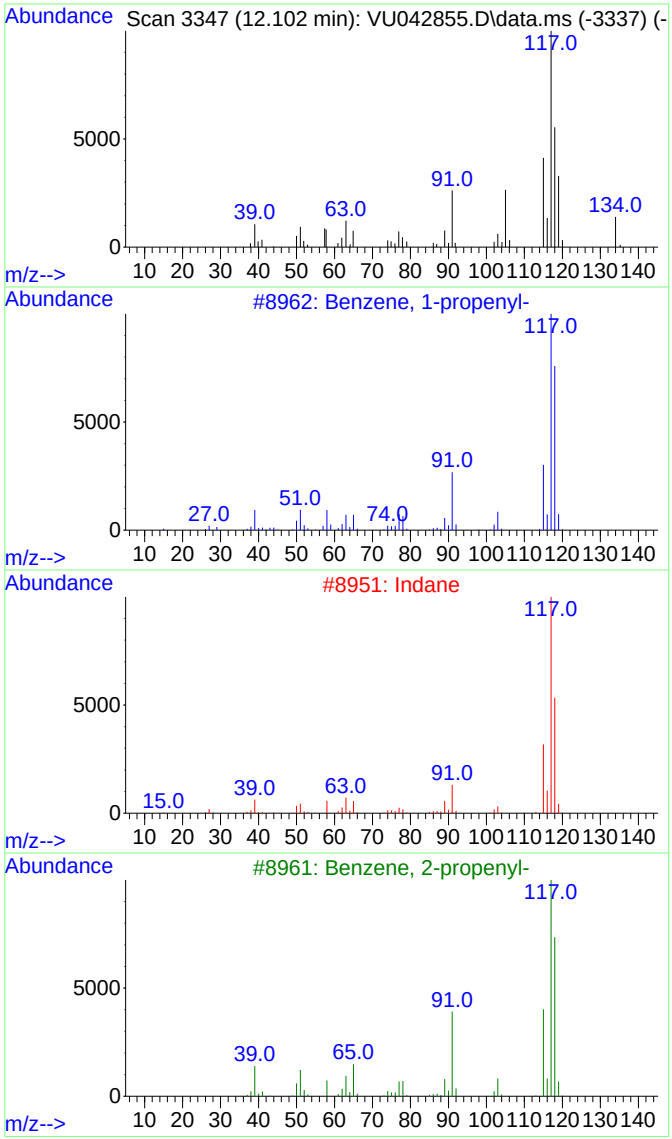
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

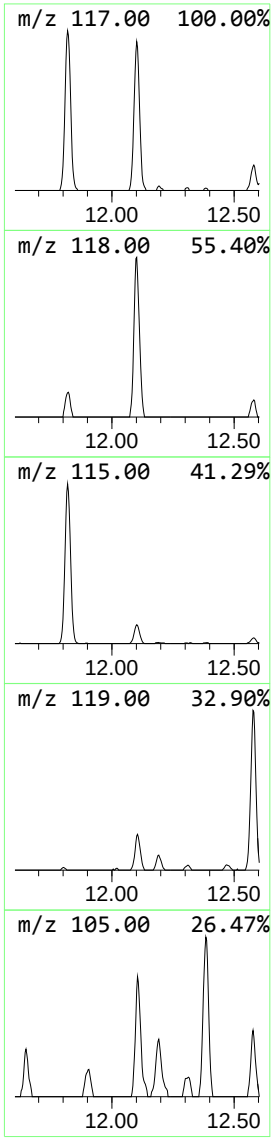
****

Peak Number 3 Benzene, 1-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	5.65 ug/l	67347	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	87
2	Indane	118	C9H10	000496-11-7	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	49
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	49





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
B7-0-2

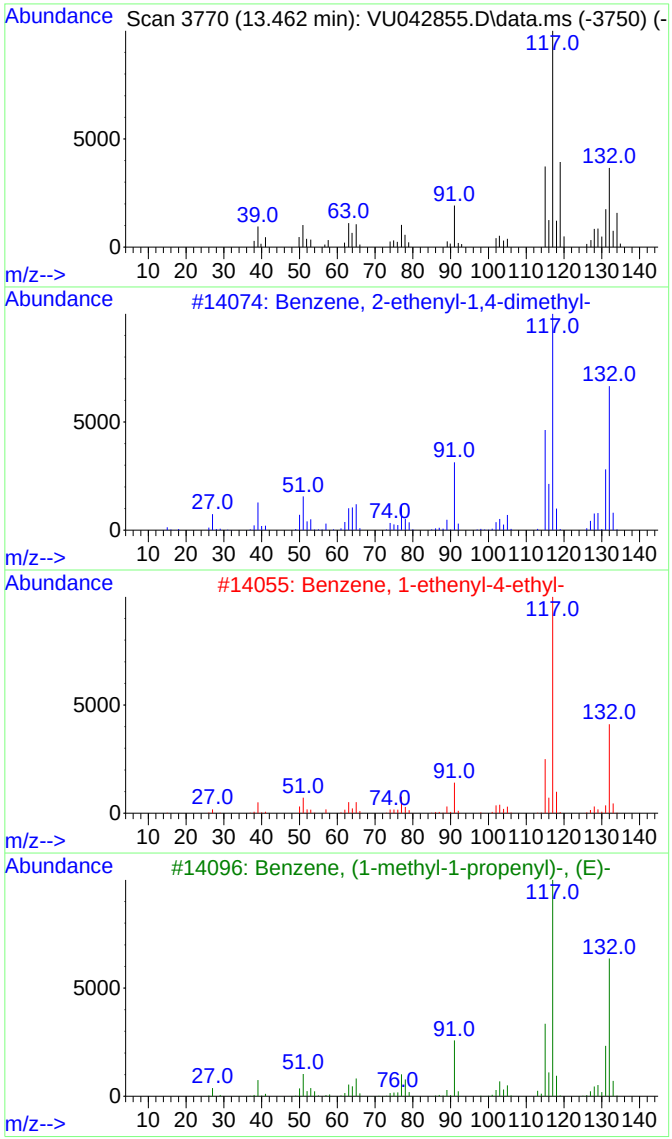
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

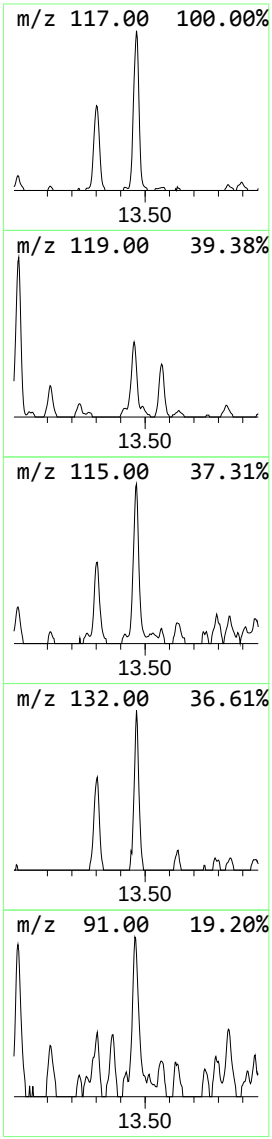
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.462	6.25 ug/l	74468	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	68
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	62





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 2,2-dim...	5.909	7.3	ug/l	62734	2	6.259	427676	50.0
Pentane, 2,3,3-...	7.388	5.1	ug/l	43572	2	6.259	427676	50.0
Benzene, 1-prop...	12.102	5.7	ug/l	67347	4	11.819	595966	50.0
Benzene, 2-ethe...	13.462	6.3	ug/l	74468	4	11.819	595966	50.0