LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070169.D
Acq On : 17 Dec 2021 17:27
Operator : JC/MD
Sample : M5039-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-22

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN070169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	417	428	444	rVB5	22190	49756	1.03%	0.122%
2	5.388	1236	1267	1322	rBV2	1141765	4191602	87.12%	10.261%
3	5.621	1326	1354	1396	rVB2	1111008	3964695	82.40%	9.706%
4	6.503	1661	1683	1706	rVB	62300	200232	4.16%	0.490%
5	8.024	2224	2250	2260	rBV2	624028	1470411	30.56%	3.600%
6	8.086	2261	2273	2298	rVB	1123833	2566428	53.34%	6.283%
7	8.440	2384	2405	2426	rBV	811722	1936955	40.26%	4.742%
8	8.539	2427	2442	2460	rBV2	448688	1023487	21.27%	2.506%
9	8.968	2581	2602	2636	rBV	1735718	3647163	75.80%	8.928%
10	9.199	2674	2688	2702	rBV5	27131	56509	1.17%	0.138%
11	9.883	2928	2943	2960	rVB3	66157	129893	2.70%	0.318%
12	10.017	2965	2993	3009	rBV3	127153	287297	5.97%	0.703%
13	10.202	3044	3062	3093	rBV2	283036	743160	15.45%	1.819%
14	10.443	3134	3152	3172	rBV	2574129	4811439	100.00%	11.779%
15	10.553	3180	3193	3218	rVB	382450	733984	15.25%	1.797%
16	11.092	3381	3394	3404	rBV3	52229	101739	2.11%	0.249%
17	11.215	3429	3440	3468	rVB8	47620	122077	2.54%	0.299%
18	11.634	3581	3596	3617	rVB4	47743	122869	2.55%	0.301%
19	11.747	3617	3638	3665	rBV	2448753	4557970	94.73%	11.158%
20	11.851	3665	3677	3698	rVV5	93127	234574	4.88%	0.574%
21	11.956	3702	3716	3743	rVB3	186281	442260	9.19%	1.083%
22	12.278	3825	3836	3855	rVB3	25460	56384	1.17%	0.138%
23	12.538	3921	3933	3940	rVV7	26856	52698	1.10%	0.129%
24	12.581	3941	3949	3961	rVV2	48232	87328	1.82%	0.214%
25	12.634	3964	3969	3988	rVB4	29203	55733	1.16%	0.136%
26	12.731	3988	4005	4030	rBV	1672006	3007801	62.51%	7.363%
27	13.015	4104	4111	4119	rVV4	35437	51212	1.06%	0.125%
28	13.058	4122	4127	4149	rVB4	45194	80052	1.66%	0.196%
29	13.222	4178	4188	4198	rBV	34541	55709	1.16%	0.136%
30	13.369	4234	4243	4260	rVB2	126147	217523	4.52%	0.533%
31	13.501	4281	4292	4306	rVB5	27854	55314	1.15%	0.135%
32	13.675	4341	4357	4382	rBV	1711362	3119772	64.84%	7.637%
33	13.774	4384	4394	4404	rVB3	43576	67421	1.40%	0.165%
34	13.838	4407	4418	4426	rBV	185384	294917	6.13%	0.722%
35	13.879	4426	4433	4442	rVB	127112	188246	3.91%	0.461%
36	14.217	4549	4559	4571	rVB2	34836	53874	1.12%	0.132%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

37	14.281	4571	4583	4590	rBV3	49847	90048	1.87%	0.220%
38	14.329	4590	4601	4615	rVV	277556	471974	9.81%	1.155%
39	14.466	4640	4652	4664	rBV	68239	115805	2.41%	0.283%
40	14.659	4713	4724	4738	rVB4	59089	96963	2.02%	0.237%
41	14.823	4771	4785	4797	rBV6	68276	137760	2.86%	0.337%
42	14.930	4810	4825	4839	rBV7	40151	84866	1.76%	0.208%
43	15.000	4841	4851	4862	rVB4	36631	60308	1.25%	0.148%
44	15.314	4950	4968	4984	rVB4	107563	293491	6.10%	0.718%
45	15.507	5015	5040	5061	rBV	210657	447940	9.31%	1.097%
46	16.622	5440	5456	5473	rVB2	88024	211208	4.39%	0.517%

Sum of corrected areas: 40848847

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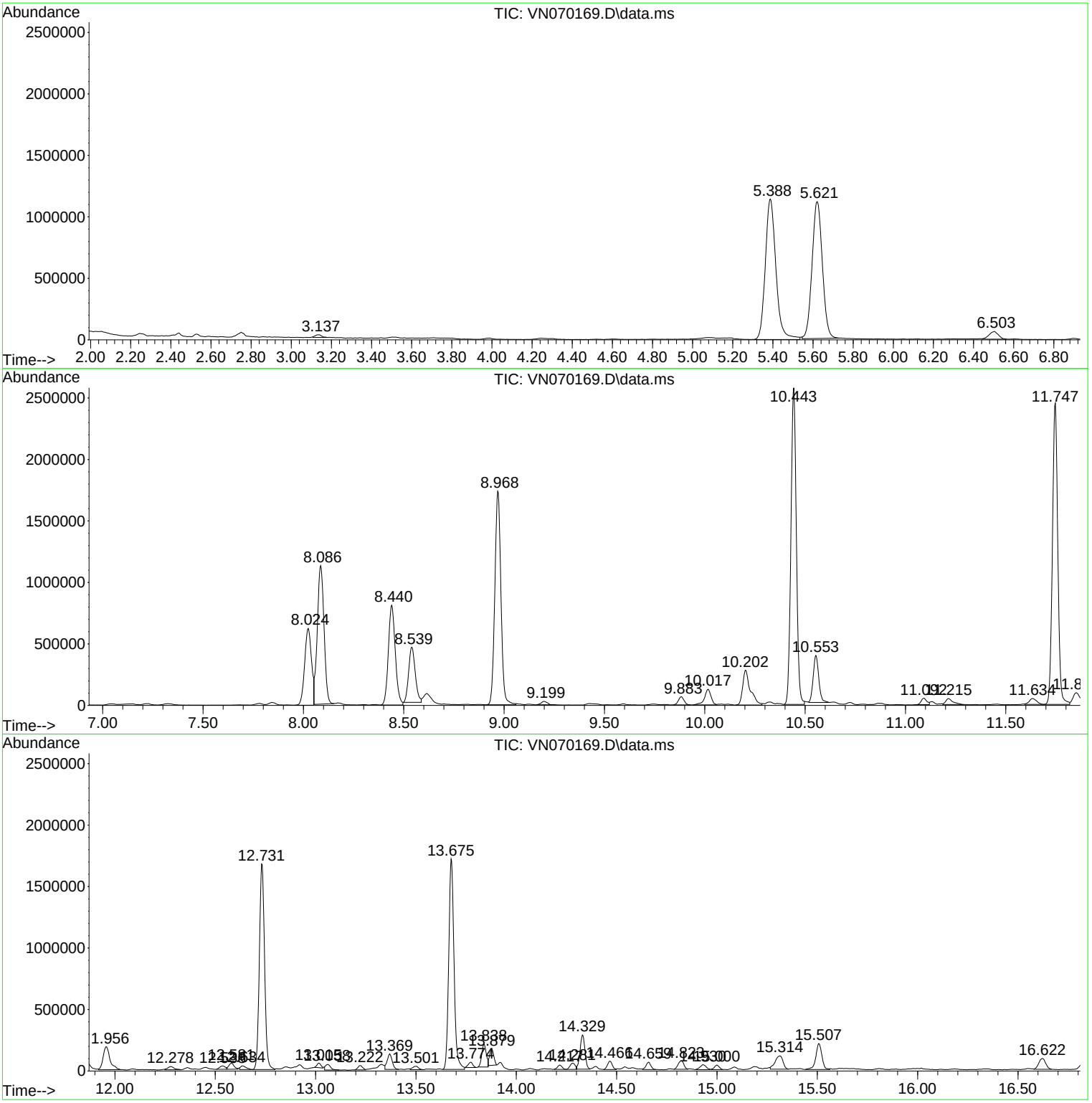
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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
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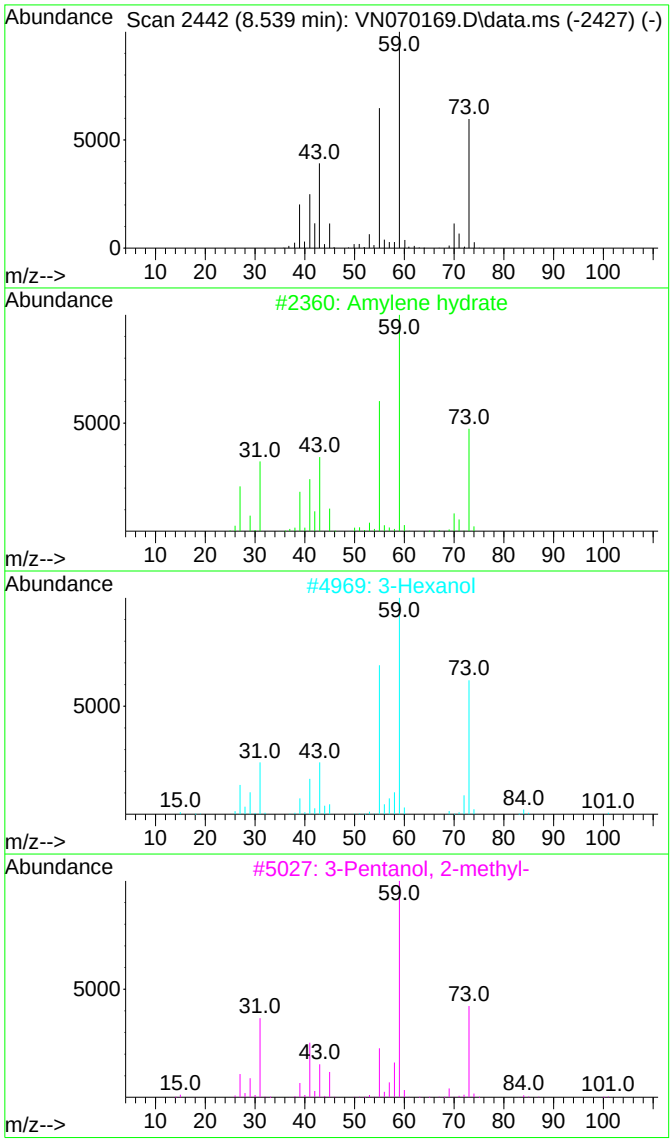
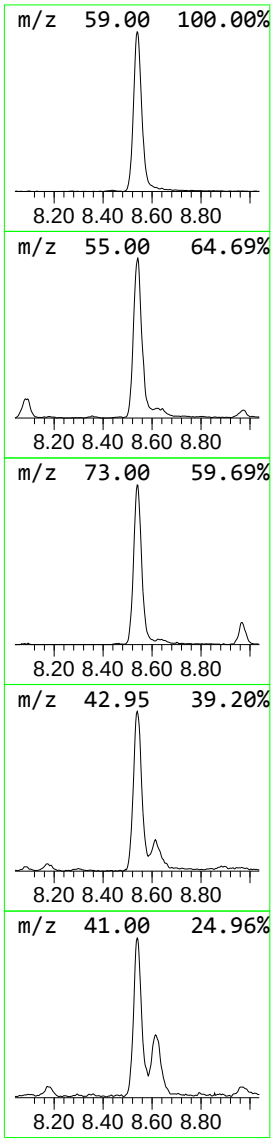
****
Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	14.03 ug/l	1023490	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	3-Hexanol	102	C6H14O	000623-37-0	38
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	36
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	10





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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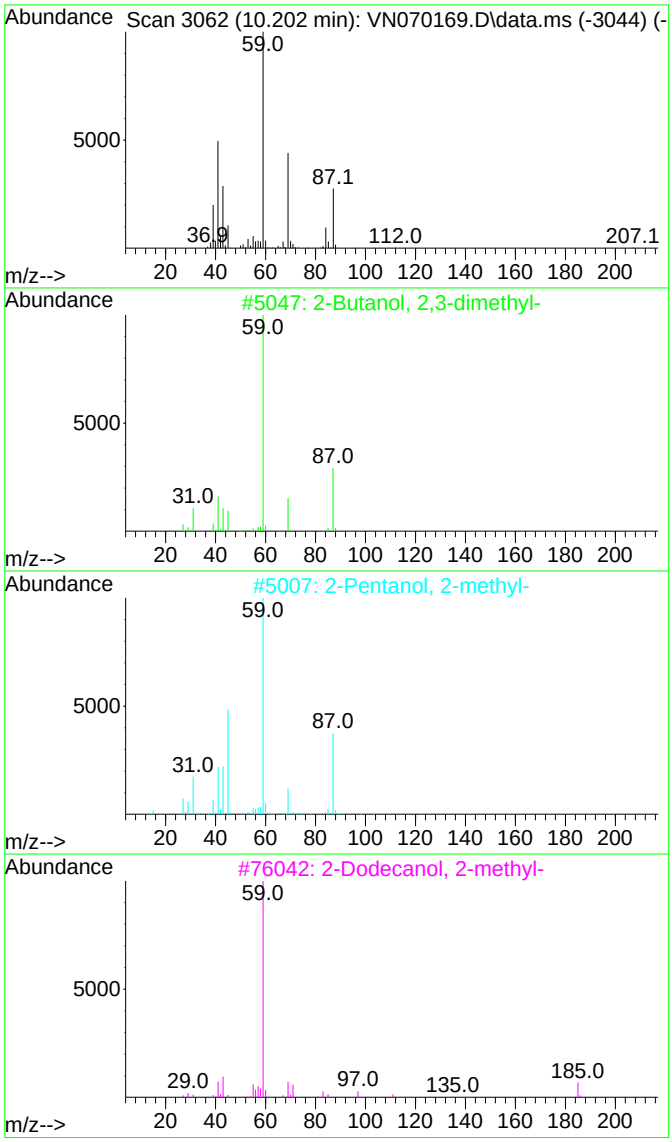
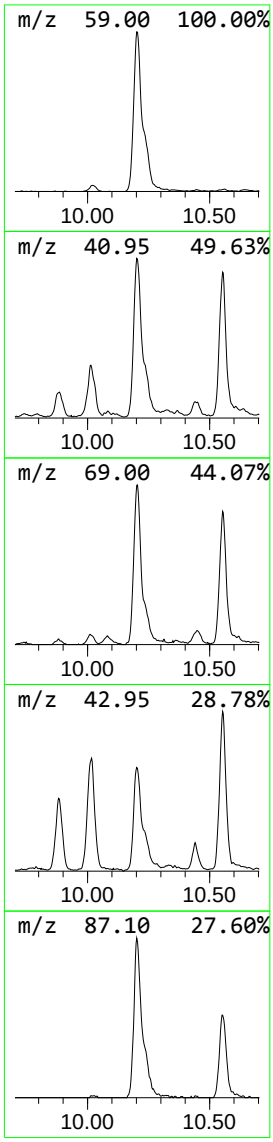
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.202	10.19 ug/l	743160	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	2-Dodecanol, 2-methyl-	200	C13H28O	001653-37-8	53
4	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	50
5	3-Heptanol	116	C7H16O	000589-82-2	50





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ClientSampleId :
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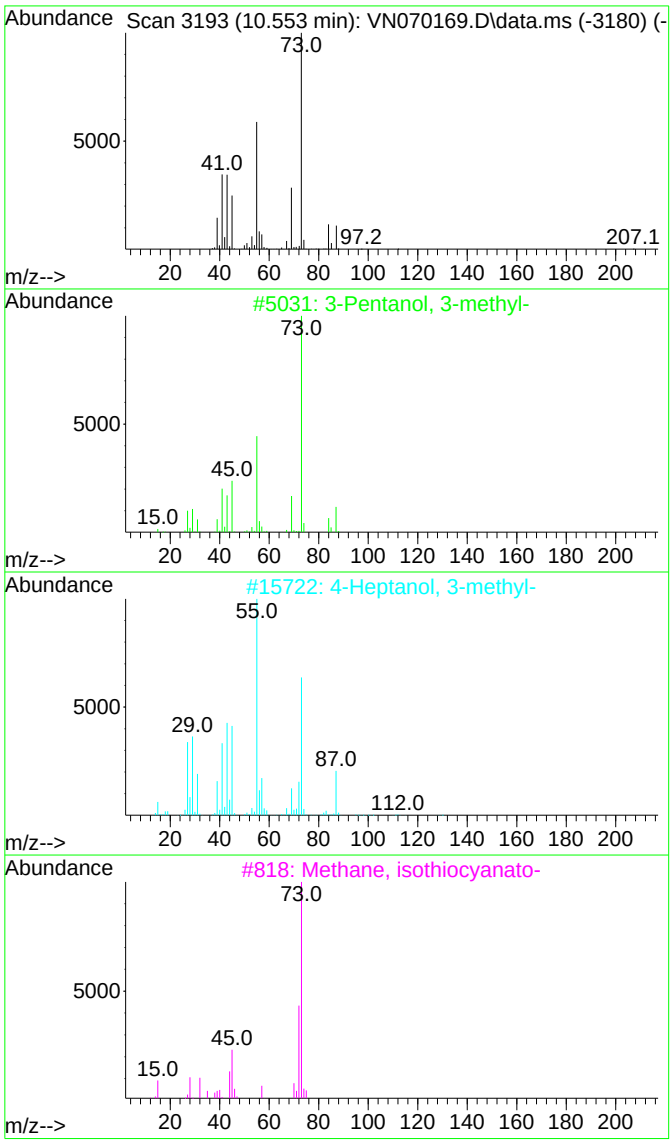
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

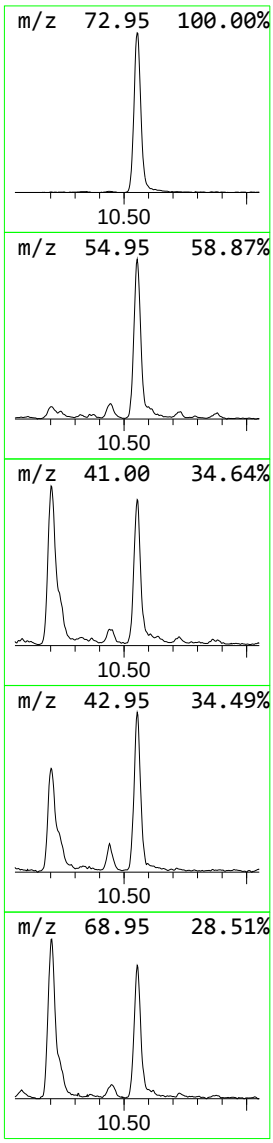
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.553	8.05 ug/l	733984	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	72
2	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	36
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	32
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	23
5	2,3-Epoxyhexanol	116	C6H12O2	090528-63-5	10





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Instrument :
MSVOA_N
ClientSampleId :
MW-22

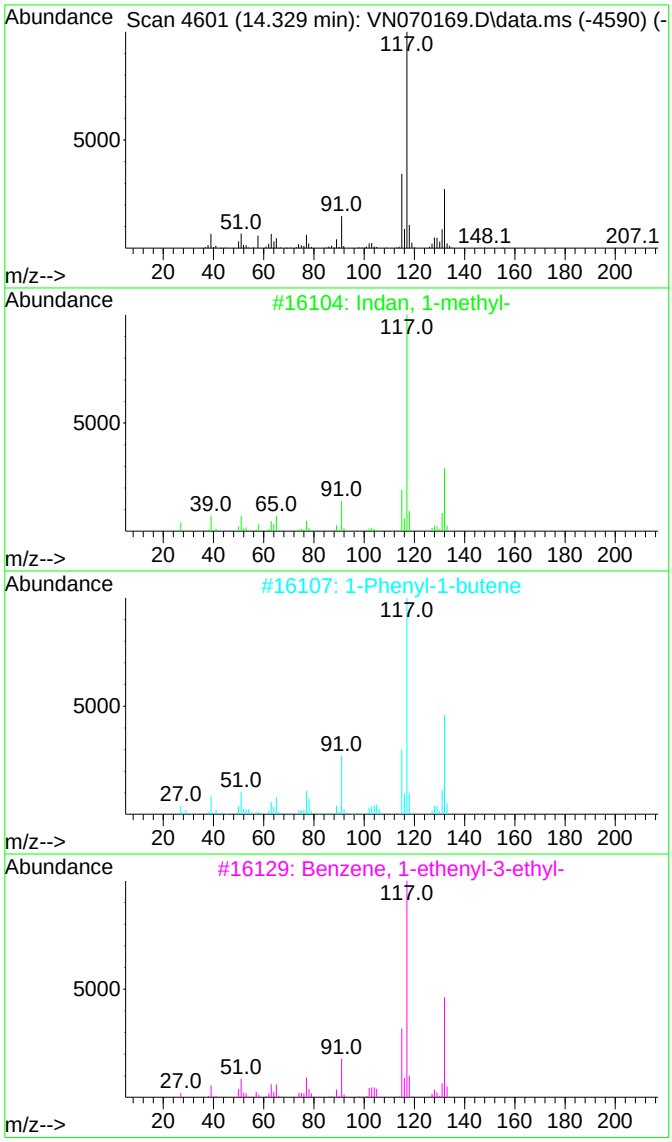
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

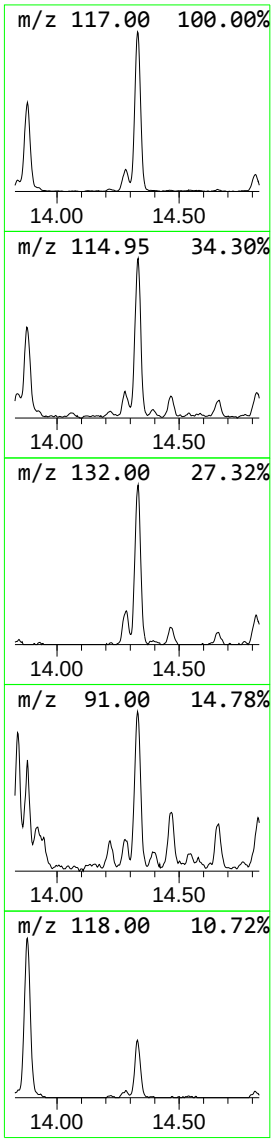
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	7.56 ug/l	471974	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	86
3	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Amylene hydrate	8.539	14.0	ug/l	1023490	2	8.971	3647160	50.0
2-Butanol, 2,3-...	10.202	10.2	ug/l	743160	2	8.971	3647160	50.0
3-Pentanol, 3-m...	10.553	8.1	ug/l	733984	3	11.746	4557970	50.0
Indan, 1-methyl-	14.329	7.6	ug/l	471974	4	13.675	3119770	50.0