

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062322\
 Data File : VX029757.D
 Acq On : 23 Jun 2022 20:20
 Operator : JC/MD
 Sample : N3366-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-16S

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: VX029757.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	21	28	32	rBV	12142	21630	1.68%	0.224%
2	2.337	197	205	210	rBV	36073	69313	5.38%	0.718%
3	2.776	271	277	289	rBV	5747	13763	1.07%	0.143%
4	2.959	298	307	322	rBV	231912	512937	39.79%	5.314%
5	3.117	324	333	344	rVB	80617	189402	14.69%	1.962%
6	3.764	425	439	458	rBV	61363	164332	12.75%	1.703%
7	4.318	522	530	539	rBV3	4559	13236	1.03%	0.137%
8	5.391	694	706	721	rBV	140374	408627	31.70%	4.233%
9	5.556	721	733	758	rVB	266920	762447	59.14%	7.899%
10	5.958	788	799	810	rBV2	145620	390816	30.32%	4.049%
11	6.038	810	812	828	rVB6	7734	21124	1.64%	0.219%
12	6.233	834	844	857	rBV3	175860	518719	40.24%	5.374%
13	6.324	857	859	876	rVB3	7949	25633	1.99%	0.266%
14	6.763	921	931	943	rBV	400349	954299	74.03%	9.887%
15	7.775	1091	1097	1104	rVB2	9713	19228	1.49%	0.199%
16	7.885	1104	1115	1121	rBV9	4938	16623	1.29%	0.172%
17	7.988	1122	1132	1140	rVB	35339	81536	6.32%	0.845%
18	8.110	1143	1152	1163	rBV2	62918	136346	10.58%	1.413%
19	8.427	1194	1204	1211	rVB	18125	32606	2.53%	0.338%
20	8.507	1211	1217	1227	rVB4	13127	24132	1.87%	0.250%
21	8.653	1227	1241	1252	rBV	789301	1289146	100.00%	13.356%
22	8.976	1289	1294	1299	rVB3	9074	16775	1.30%	0.174%
23	9.165	1319	1325	1335	rVB	28290	51901	4.03%	0.538%
24	9.445	1364	1371	1377	rBV2	17665	37158	2.88%	0.385%
25	9.506	1377	1381	1387	rVB3	7669	14176	1.10%	0.147%
26	9.763	1417	1423	1431	rBV7	10658	19052	1.48%	0.197%
27	10.012	1459	1464	1466	rBV	32874	42894	3.33%	0.444%
28	10.055	1466	1471	1477	rVV	813113	1065146	82.62%	11.035%
29	10.275	1504	1507	1517	rVB	6371	16750	1.30%	0.174%
30	10.378	1517	1524	1529	rBV	22550	35320	2.74%	0.366%
31	10.964	1615	1620	1625	rBV	53854	71954	5.58%	0.745%
32	11.018	1625	1629	1632	rVV2	16801	24771	1.92%	0.257%
33	11.085	1634	1640	1645	rVV	613268	810901	62.90%	8.401%
34	11.713	1735	1743	1747	rBV2	9785	15729	1.22%	0.163%
35	11.890	1763	1772	1778	rBV4	8562	15398	1.19%	0.160%
36	12.024	1788	1794	1802	rBV	799216	1003138	77.81%	10.393%

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37	12.110	1802	1808	1815	rVV10	5498	13215	1.03%	0.137%
38	12.177	1816	1819	1825	rVB	10876	14104	1.09%	0.146%
39	12.250	1825	1831	1836	rBV2	23688	36340	2.82%	0.376%
40	12.646	1893	1896	1900	rVB	13624	16176	1.25%	0.168%
41	12.701	1900	1905	1912	rVB	320292	379580	29.44%	3.933%
42	12.841	1920	1928	1933	rBV	12512	17405	1.35%	0.180%
43	13.030	1955	1959	1968	rVB2	9588	14890	1.16%	0.154%
44	13.140	1968	1977	1978	rBV	15768	24280	1.88%	0.252%
45	13.170	1978	1982	1990	rVV	59074	86052	6.68%	0.892%
46	13.292	1997	2002	2007	rBV2	31054	43114	3.34%	0.447%
47	13.347	2007	2011	2014	rBV3	10626	13862	1.08%	0.144%
48	13.426	2020	2024	2028	rVB2	11394	13409	1.04%	0.139%
49	13.542	2039	2043	2047	rBV	26848	34108	2.65%	0.353%
50	13.664	2061	2063	2071	rVB	23656	25745	2.00%	0.267%
51	13.780	2074	2082	2090	rBV2	5462	13137	1.02%	0.136%

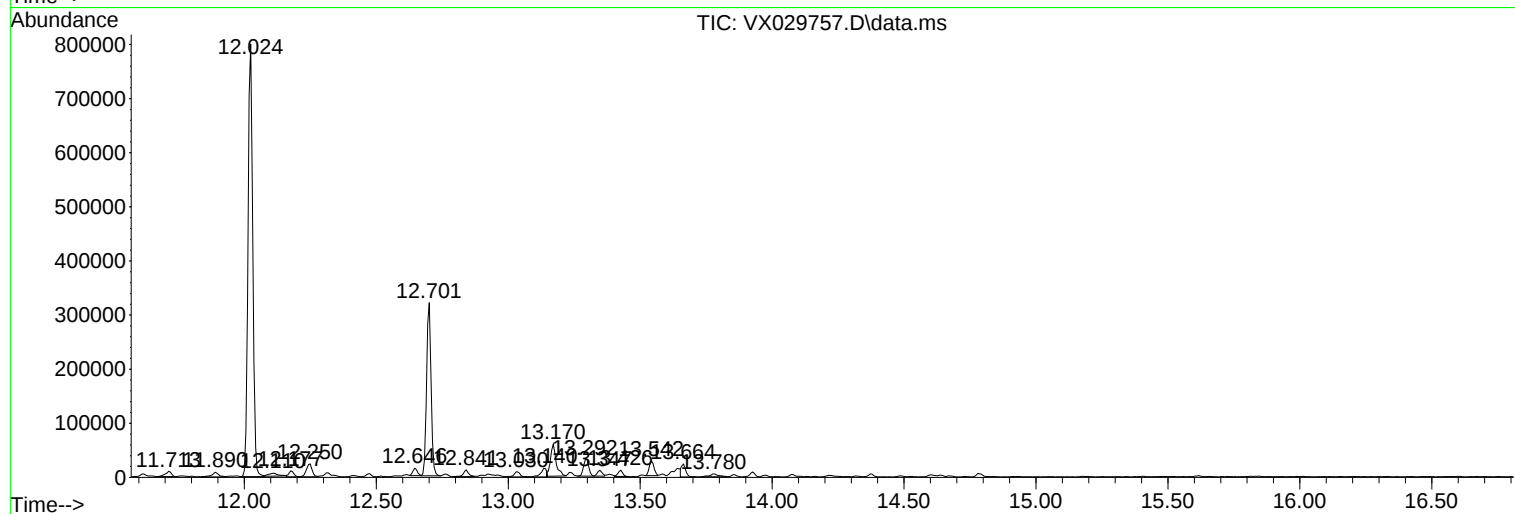
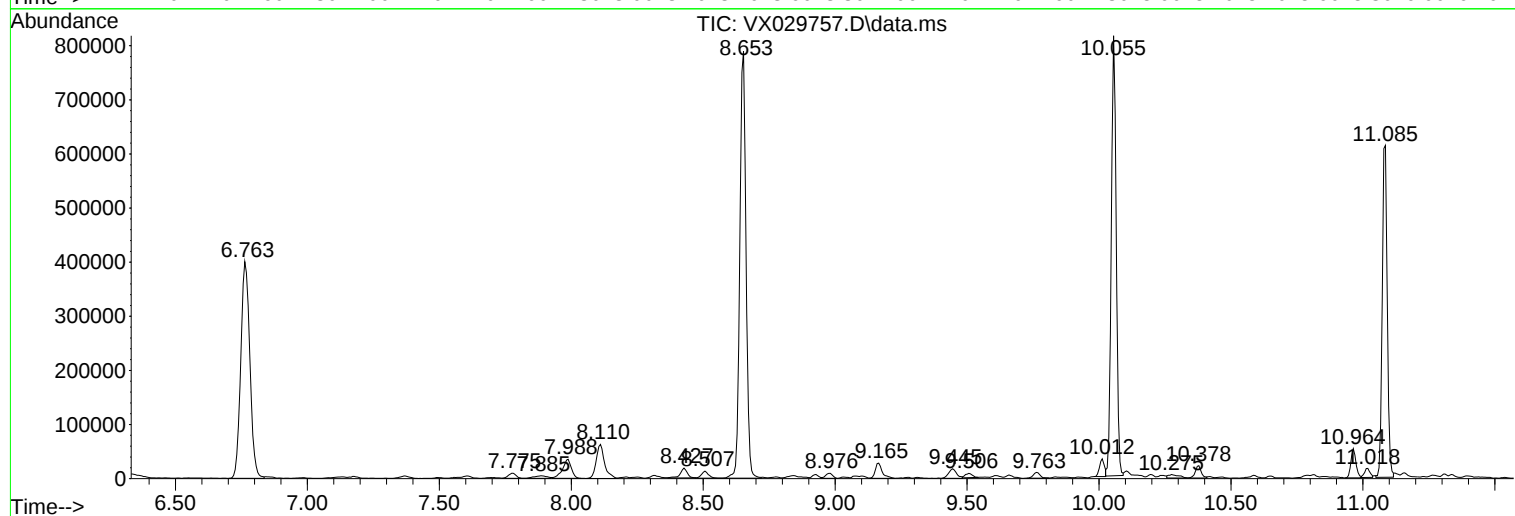
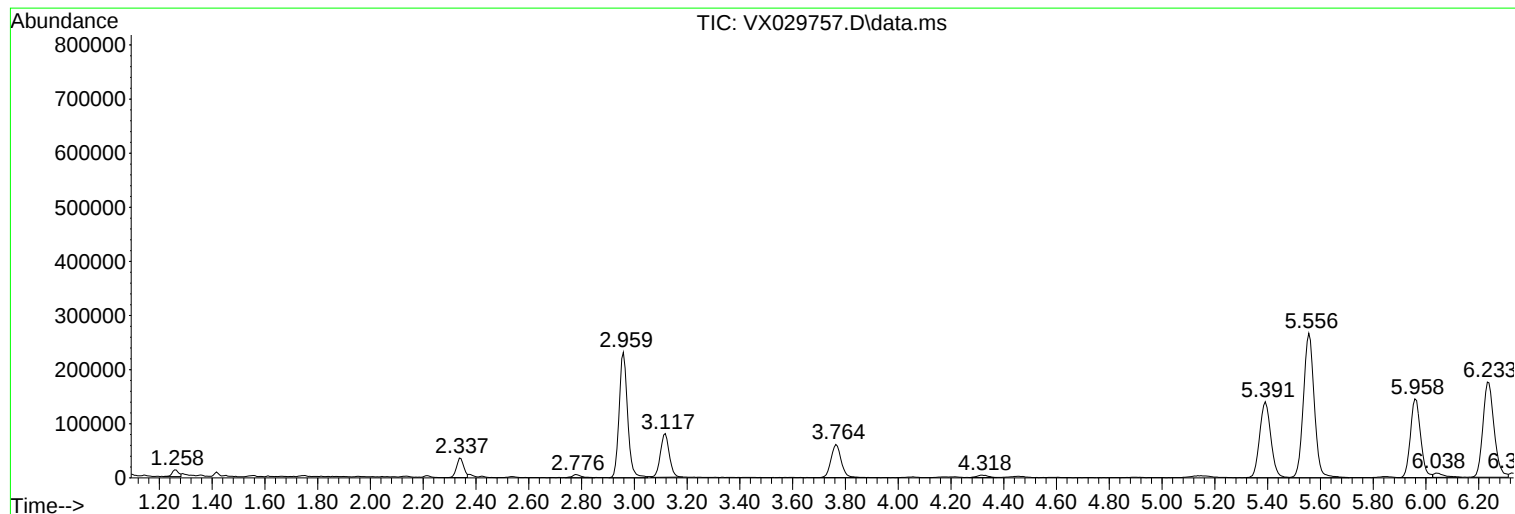
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ClientSampleId :
MW-16S

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



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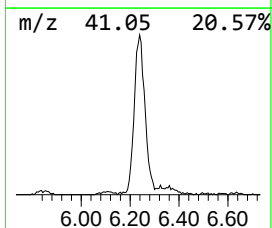
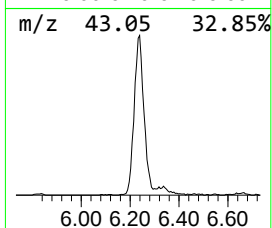
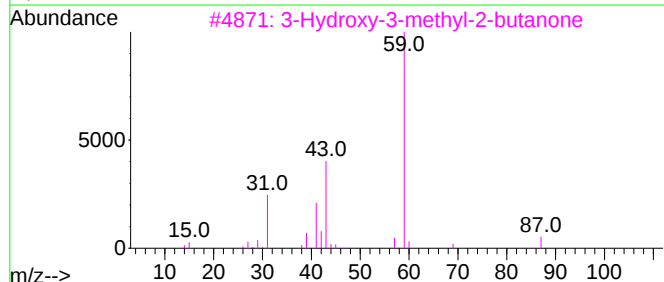
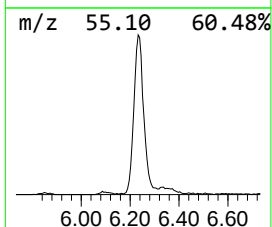
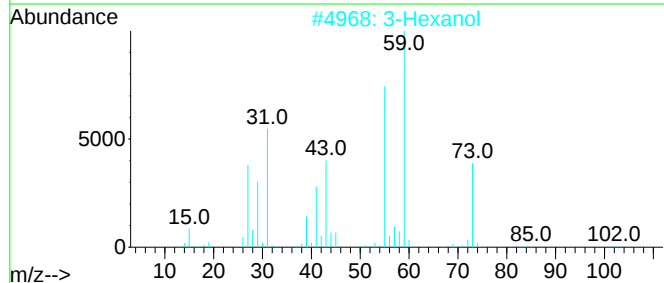
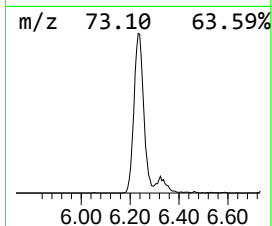
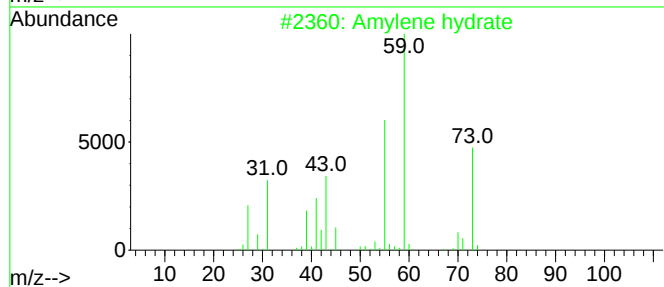
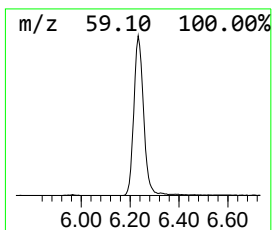
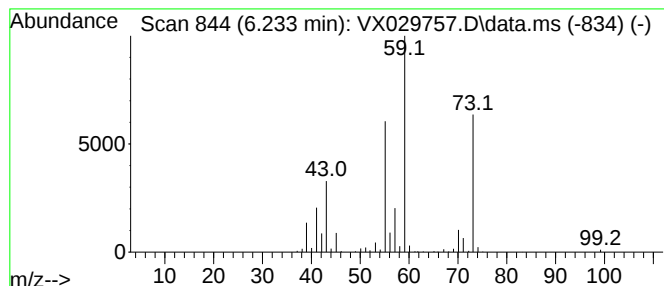
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	27.18 ug/l	518719	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	64
2			3-Hexanol	102	C6H14O	000623-37-0	64
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	25
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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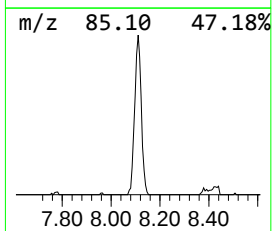
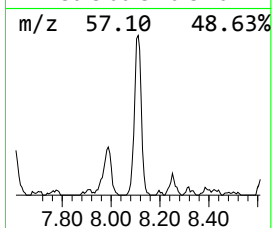
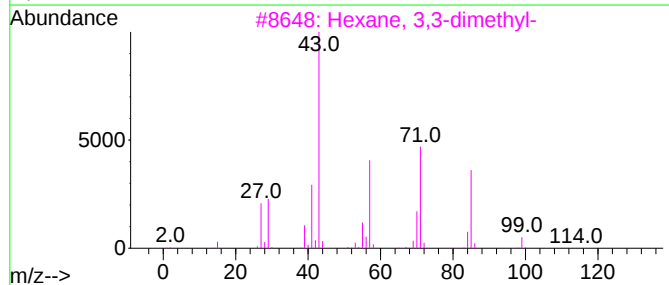
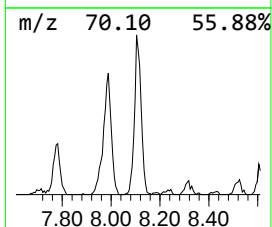
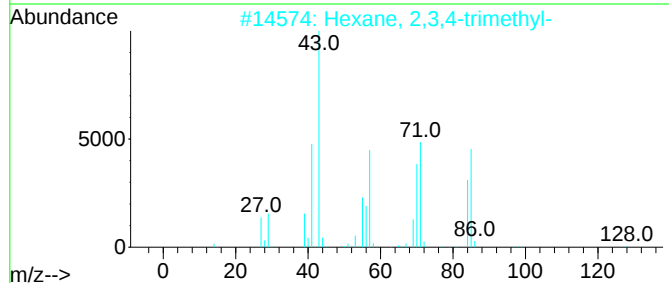
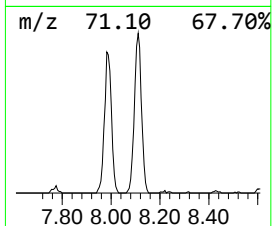
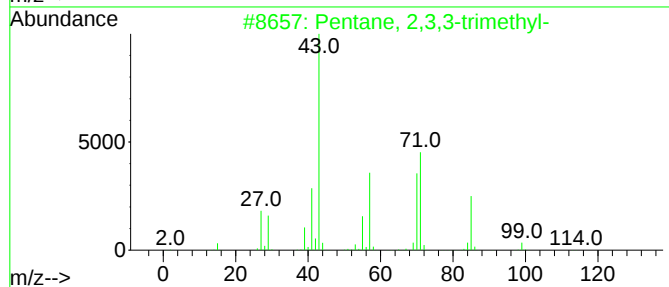
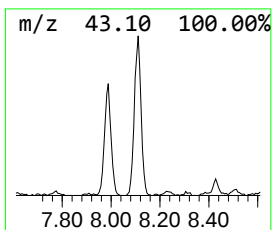
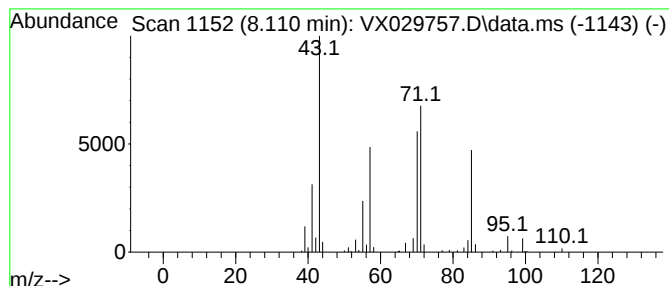
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	7.14 ug/l	136346	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, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4		Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	53



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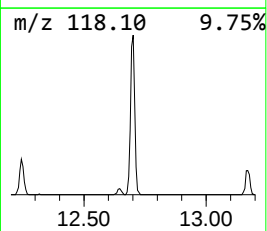
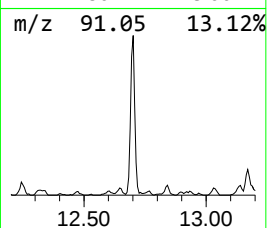
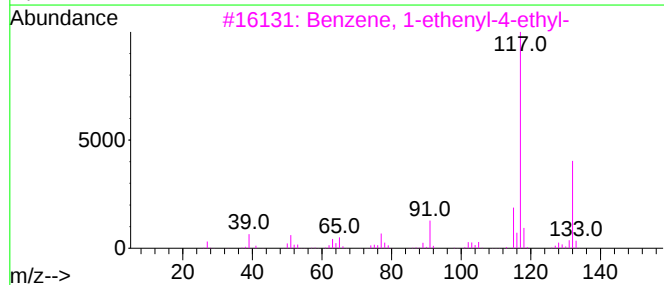
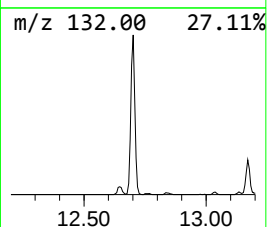
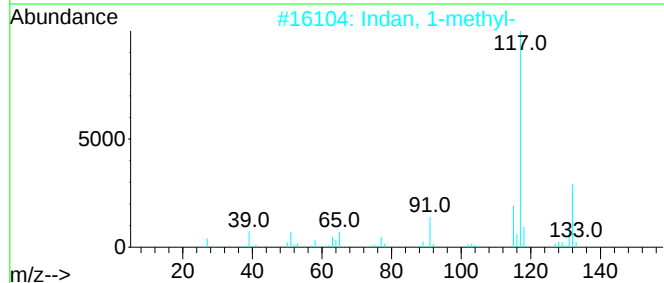
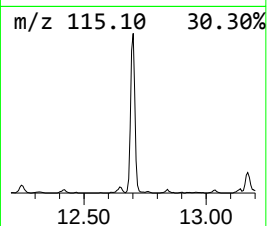
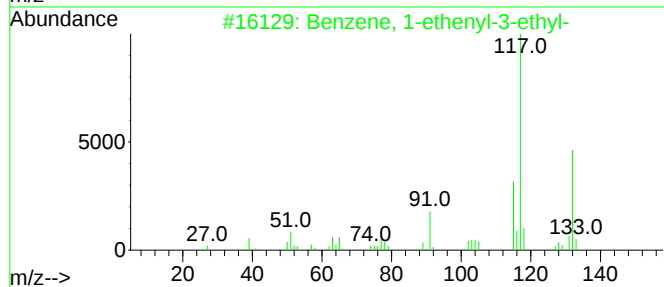
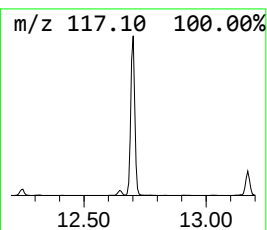
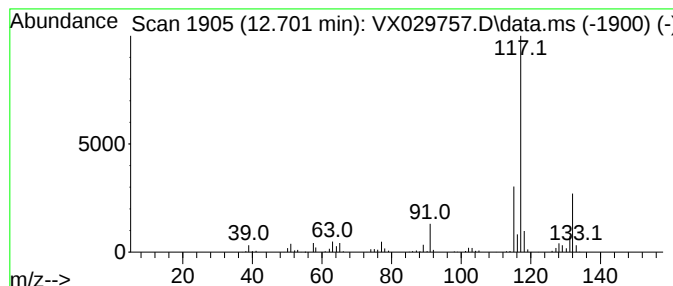
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	18.92 ug/l	379580	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	90
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.233	27.2	ug/l	518719	2	6.763	954299	50.0
Pentane, 2,3,3-...	8.110	7.1	ug/l	136346	2	6.763	954299	50.0
Benzene, 1-ethe...	12.701	18.9	ug/l	379580	4	12.024	1003140	50.0