

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120121\
 Data File : VX025408.D
 Acq On : 01 Dec 2021 13:15
 Operator : JC/MD
 Sample : M4866-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 16986

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	83439	74444	5.77%	1.445%
2	2.380	206	212	223	rBV	12339	20521	1.59%	0.398%
3	5.391	693	706	719	rBV2	67574	198417	15.39%	3.852%
4	5.556	722	733	750	rVB	114344	324039	25.14%	6.291%
5	5.958	788	799	809	rBV	70201	190741	14.80%	3.703%
6	6.763	921	931	944	rBV	177631	424494	32.93%	8.242%
7	8.653	1233	1241	1248	rBV	362648	579438	44.95%	11.250%
8	8.720	1248	1252	1259	rVB	21583	33280	2.58%	0.646%
9	10.055	1465	1471	1483	rBV	379997	506963	39.33%	9.843%
10	10.153	1483	1487	1491	rVV	22757	32765	2.54%	0.636%
11	10.195	1491	1494	1501	rVV	7698	14583	1.13%	0.283%
12	10.268	1501	1506	1509	rVV	13840	22326	1.73%	0.433%
13	10.305	1509	1512	1520	rVB	21528	29881	2.32%	0.580%
14	10.646	1563	1568	1572	rBV	38812	58741	4.56%	1.140%
15	10.756	1581	1586	1592	rBV	43923	61041	4.74%	1.185%
16	11.079	1634	1639	1645	rBV	289244	385267	29.89%	7.480%
17	11.573	1715	1720	1723	rBV	18025	24494	1.90%	0.476%
18	11.610	1723	1726	1737	rVB3	18472	33490	2.60%	0.650%
19	11.835	1754	1763	1765	rBV4	7417	14095	1.09%	0.274%
20	11.872	1765	1769	1779	rVV2	25481	45949	3.56%	0.892%
21	11.957	1779	1783	1789	rVV4	10772	18933	1.47%	0.368%
22	12.024	1789	1794	1801	rVV	382076	483362	37.50%	9.385%
23	12.085	1801	1804	1809	rVB	11887	14856	1.15%	0.288%
24	12.219	1821	1826	1837	rBV	1088242	1289125	100.00%	25.029%
25	12.311	1837	1841	1853	rVV7	15763	36369	2.82%	0.706%
26	12.414	1853	1858	1862	rVV	45070	56492	4.38%	1.097%
27	12.805	1917	1922	1927	rBV	11918	16844	1.31%	0.327%
28	13.774	2076	2081	2088	rVB	124165	159622	12.38%	3.099%

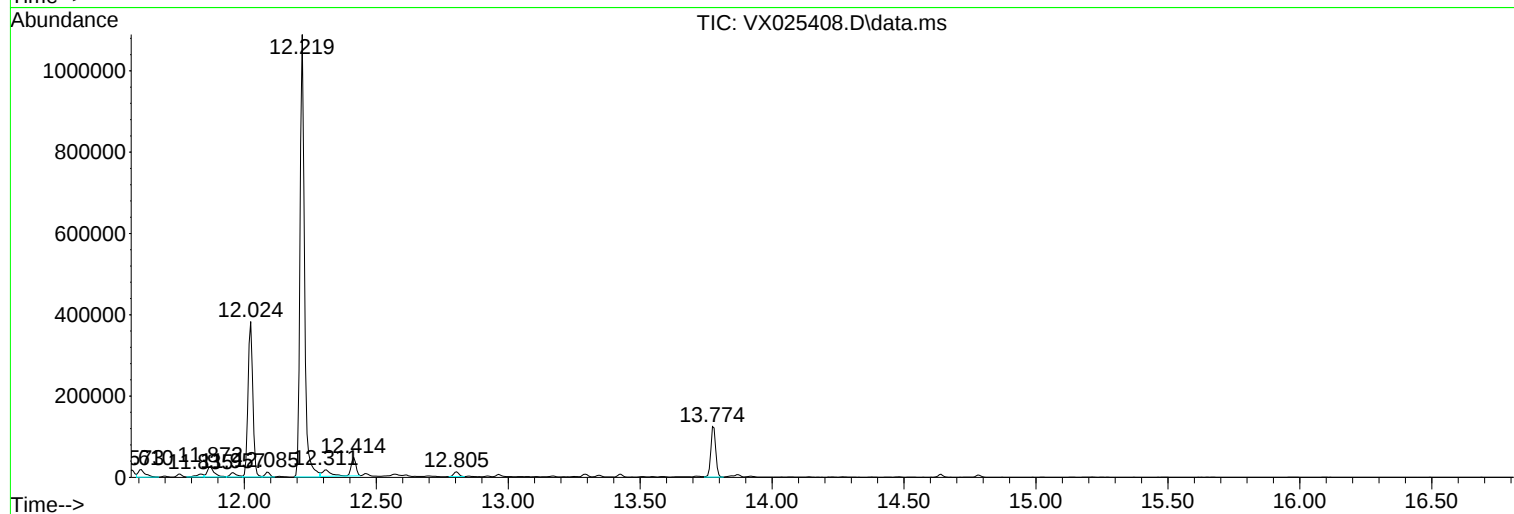
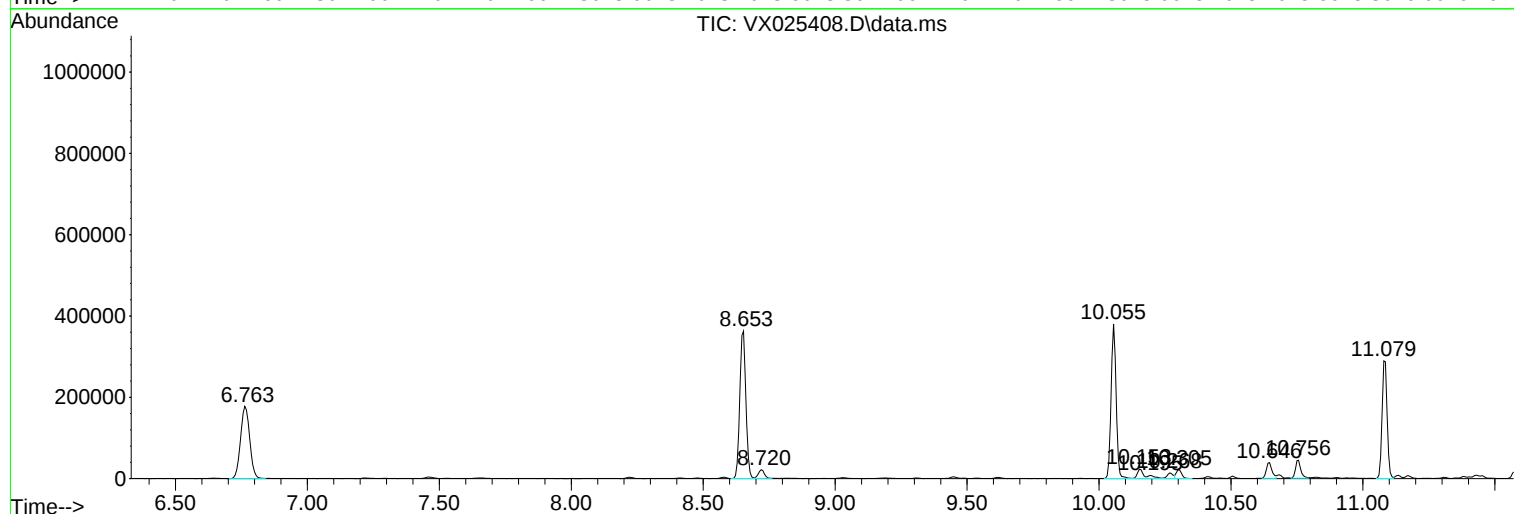
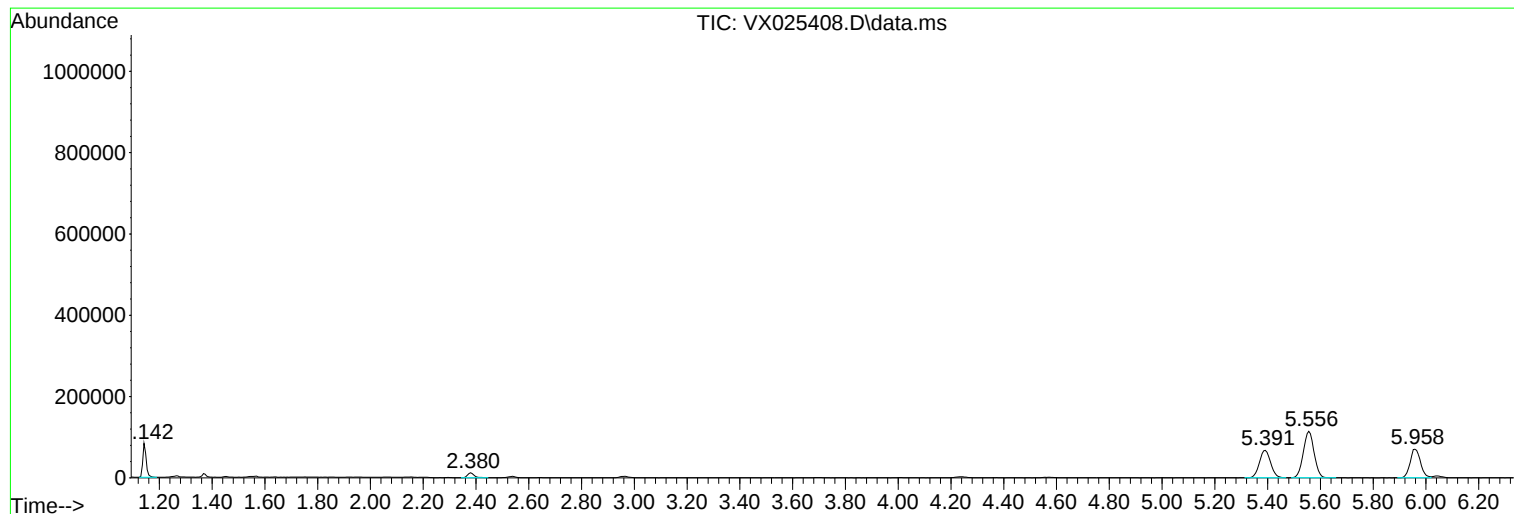
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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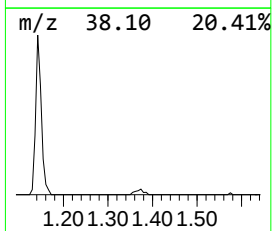
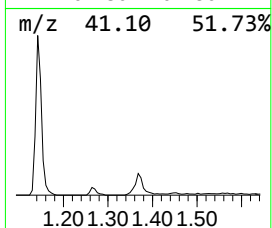
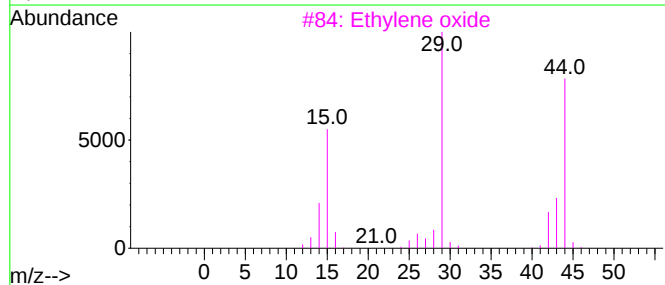
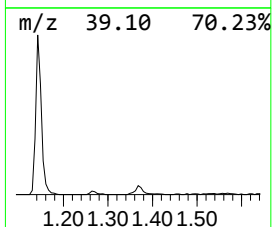
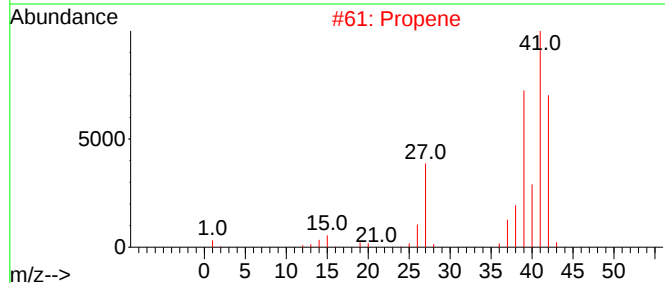
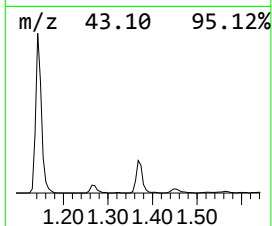
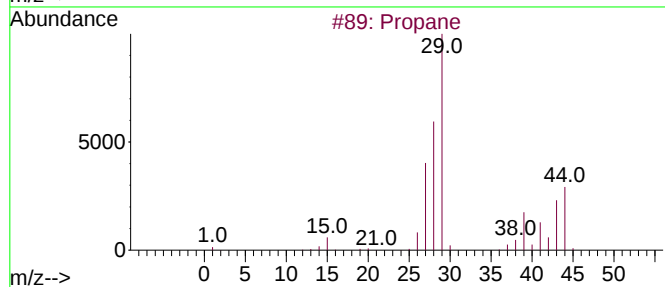
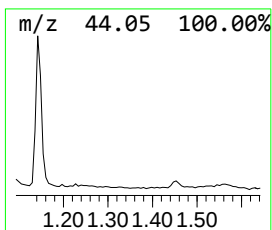
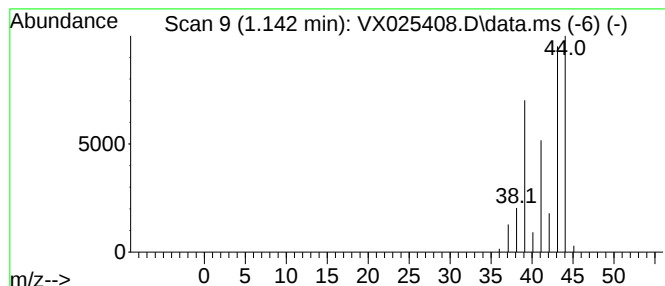
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	11.49 ug/l	74444	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Propene			42	C3H6	000115-07-1	9
3	Ethylene oxide			44	C2H4O	000075-21-8	5
4	Acetaldehyde			44	C2H4O	000075-07-0	5
5	Ethyne, fluoro-			44	C2HF	002713-09-9	3



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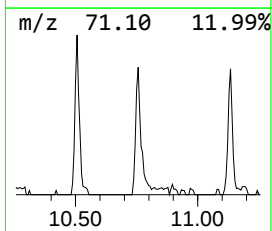
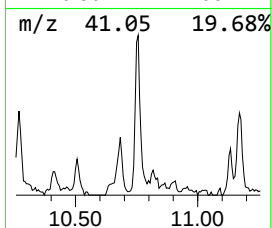
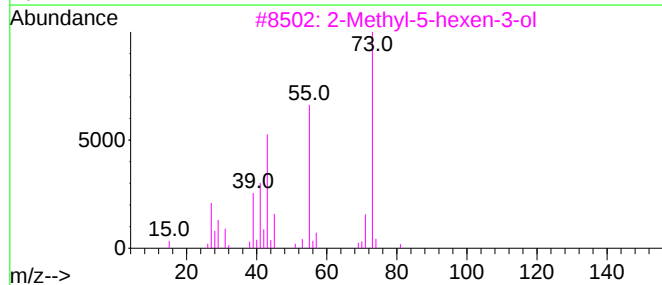
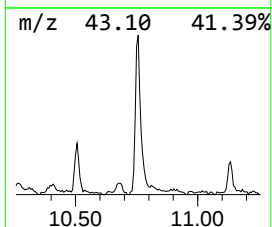
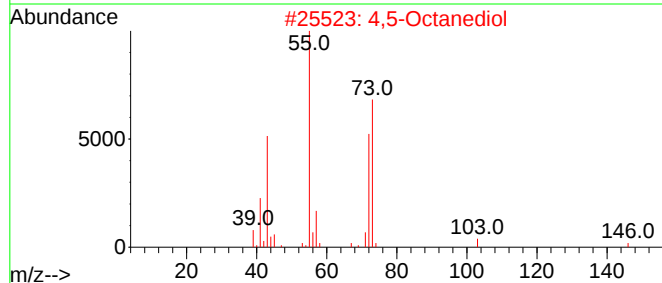
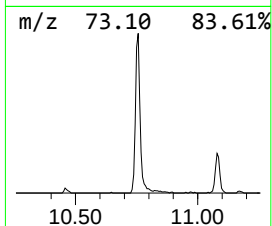
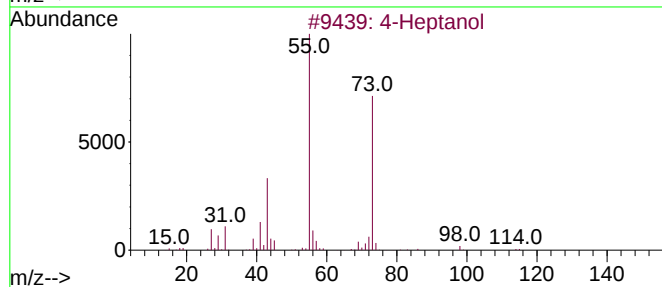
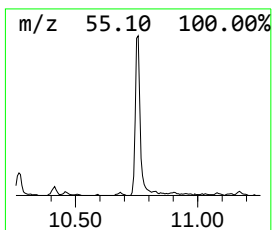
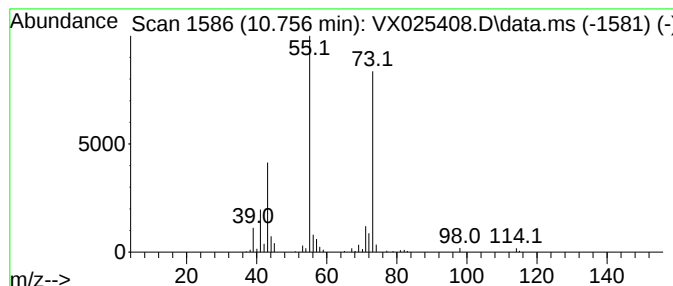
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Heptanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	6.02 ug/l	61041	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	64
2			4,5-Octanediol	146	C8H18O2	022607-10-9	45
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	42
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	40
5			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	36



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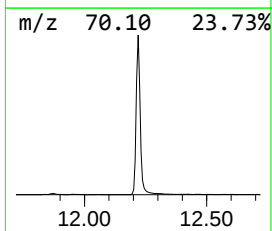
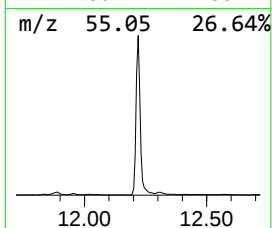
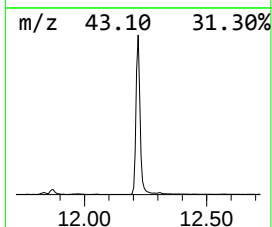
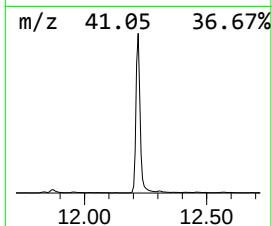
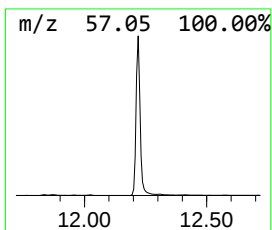
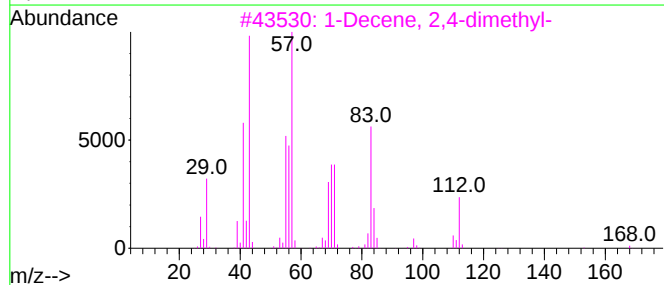
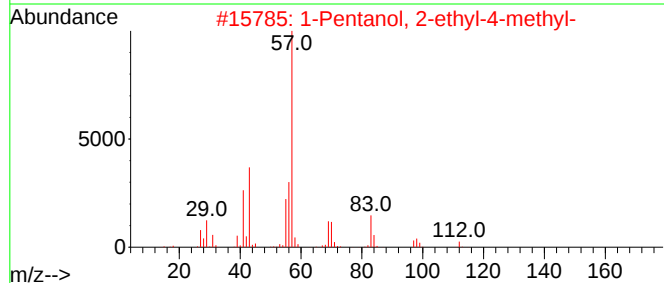
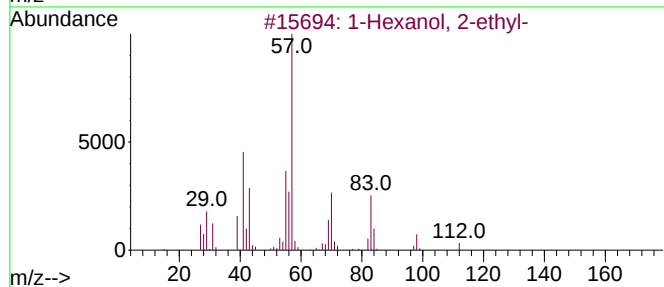
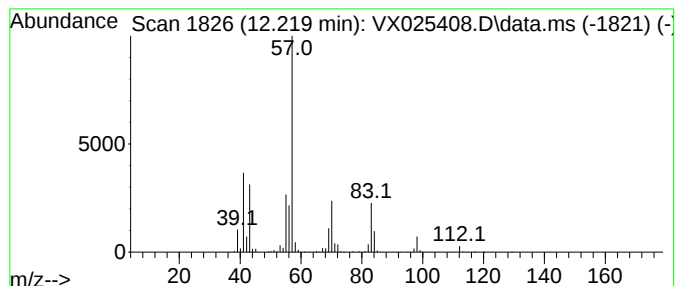
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	133.35 ug/l	1289130	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
4			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



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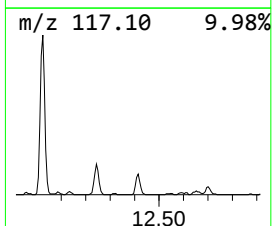
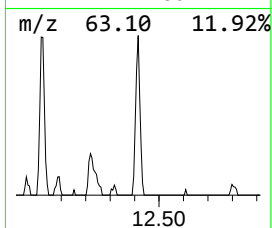
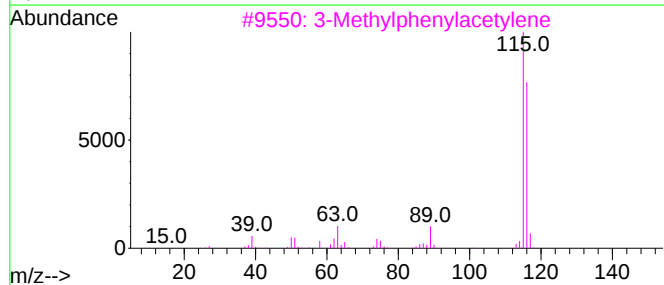
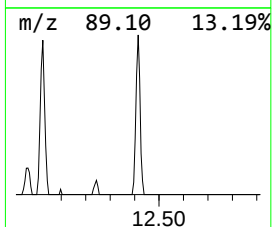
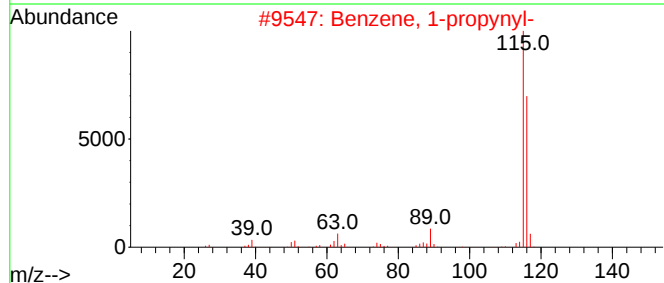
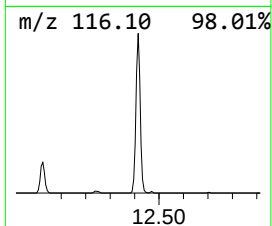
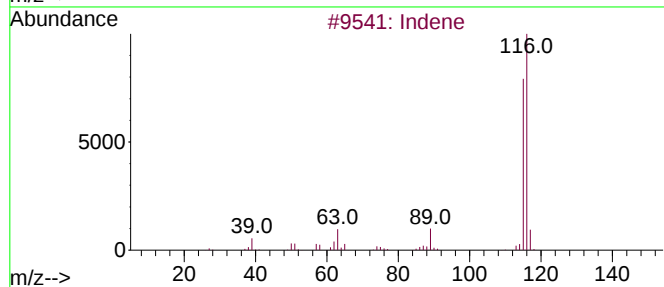
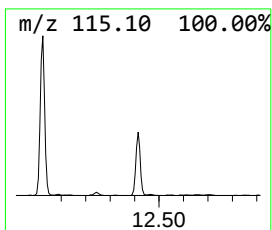
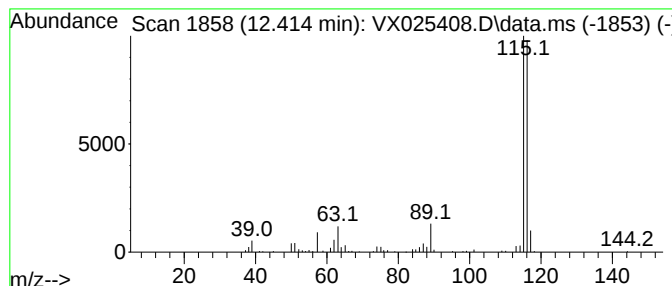
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Quant Title : SW846 8260

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

Peak Number 4 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	5.84 ug/l	56492	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	1.142	11.5	ug/l	74444	1	5.556	324039	50.0
4-Heptanol	10.756	6.0	ug/l	61041	3	10.055	506963	50.0
1-Hexanol, 2-et...	12.219	133.3	ug/l	1289130	4	12.024	483362	50.0
Indene	12.414	5.8	ug/l	56492	4	12.024	483362	50.0