

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
 Data File : VN080957.D
 Acq On : 08 Feb 2024 12:34
 Operator : JC\MD
 Sample : P1373-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1289

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\82N020624W.M
 Title : SW846 8260

Signal : TIC: VN080957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	31	rVB	46804	74439	3.08%	0.492%
2	2.818	140	147	153	rVB5	40251	98911	4.09%	0.653%
3	4.424	412	420	432	rBV2	17617	52443	2.17%	0.346%
4	7.224	887	896	906	rBV4	43683	124120	5.13%	0.820%
5	8.171	1045	1057	1061	rBV2	287936	687786	28.42%	4.544%
6	8.224	1061	1066	1080	rVB	540466	1184228	48.94%	7.824%
7	8.577	1112	1126	1138	rBV	294474	698203	28.85%	4.613%
8	9.100	1207	1215	1231	rBV	804819	1653119	68.31%	10.921%
9	9.271	1236	1244	1255	rBV2	32097	79812	3.30%	0.527%
10	9.641	1298	1307	1316	rBV6	12056	31176	1.29%	0.206%
11	9.888	1341	1349	1356	rBV2	30901	56234	2.32%	0.372%
12	10.571	1456	1465	1473	rBV	967023	1828226	75.55%	12.078%
13	11.865	1670	1685	1698	rVB	1041522	1912985	79.05%	12.638%
14	12.212	1738	1744	1750	rBV	18014	29784	1.23%	0.197%
15	12.423	1775	1780	1788	rVB2	61992	103603	4.28%	0.684%
16	12.853	1844	1853	1864	rBV	665045	1244844	51.44%	8.224%
17	12.941	1864	1868	1880	rVB2	35727	65592	2.71%	0.433%
18	13.088	1887	1893	1897	rBV4	19788	37280	1.54%	0.246%
19	13.265	1912	1923	1929	rBV3	157726	323663	13.37%	2.138%
20	13.341	1929	1936	1946	rVB	1634201	2419966	100.00%	15.988%
21	13.506	1957	1964	1976	rVB7	18925	48047	1.99%	0.317%
22	13.688	1987	1995	2005	rBV2	113101	215313	8.90%	1.422%
23	13.794	2005	2013	2021	rVV	950953	1567496	64.77%	10.356%
24	13.876	2021	2027	2036	rVV	201631	371396	15.35%	2.454%
25	13.959	2036	2041	2047	rVB7	16640	32504	1.34%	0.215%
26	14.253	2084	2091	2097	rVB5	16667	30064	1.24%	0.199%
27	15.347	2266	2277	2281	rBV6	30877	64278	2.66%	0.425%
28	15.394	2281	2285	2291	rVB2	57781	101070	4.18%	0.668%

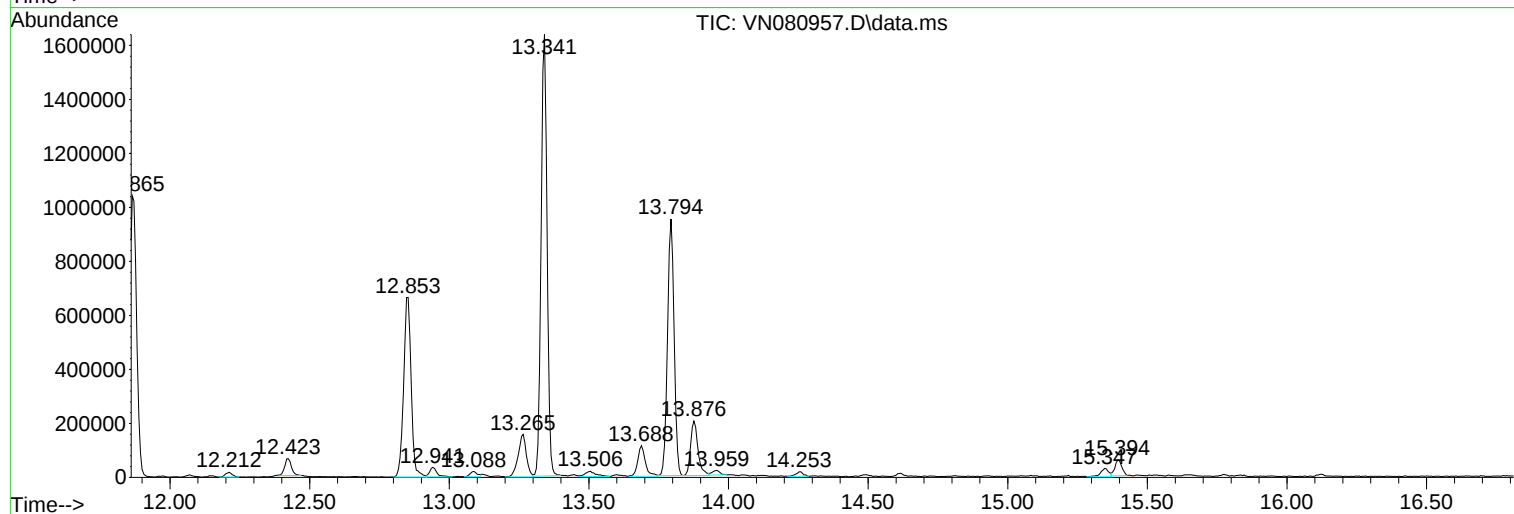
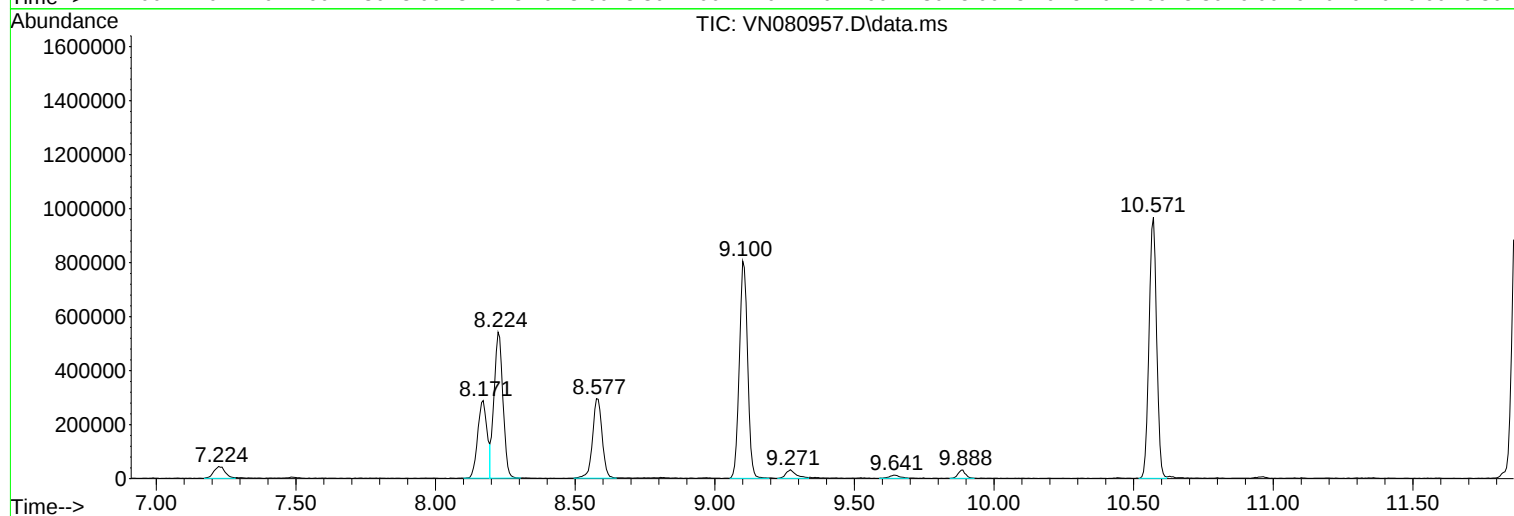
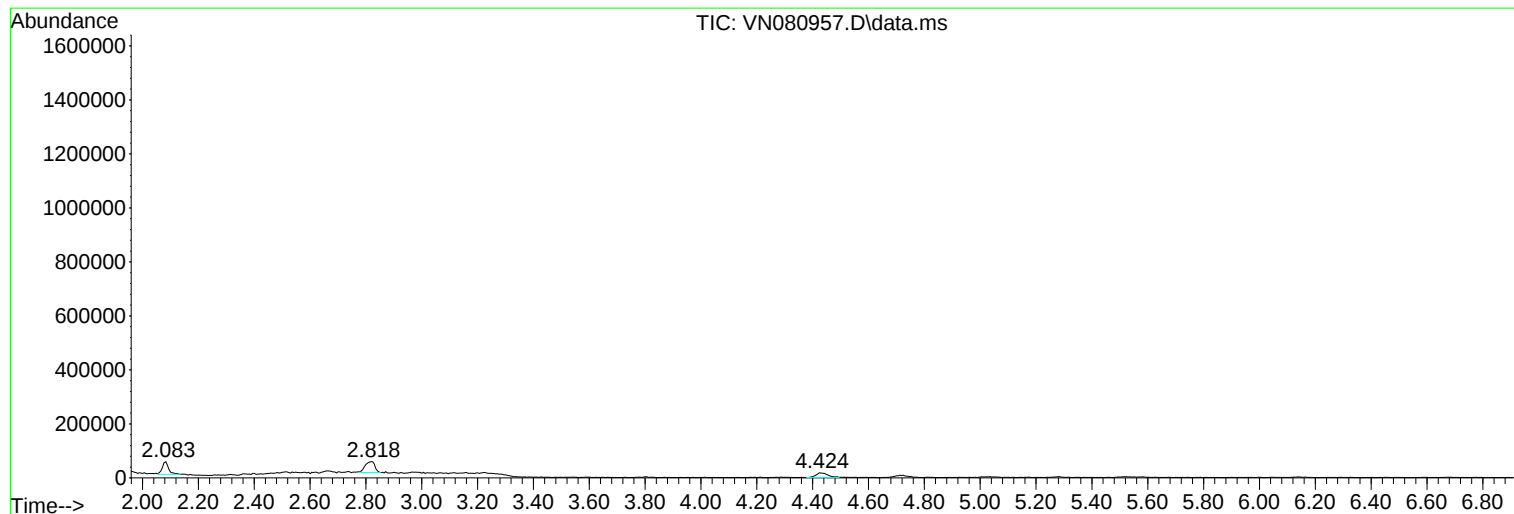
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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



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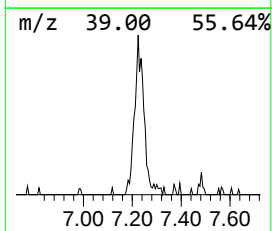
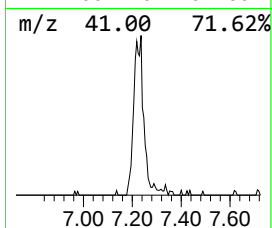
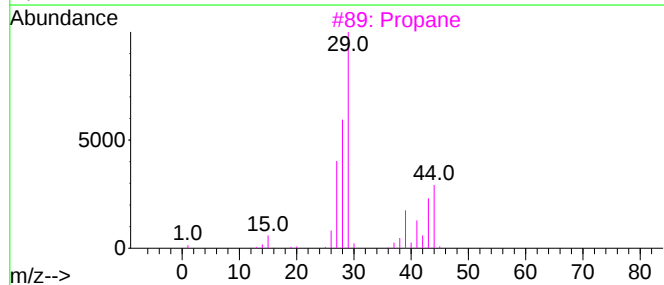
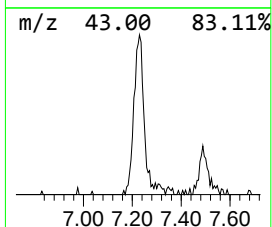
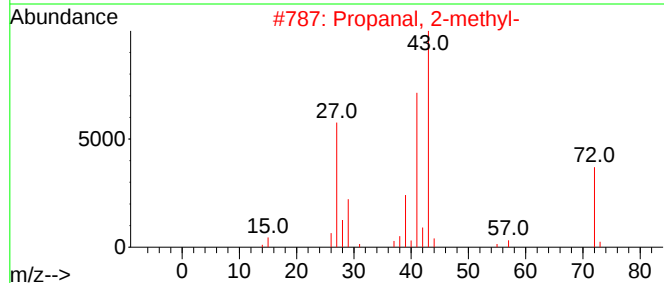
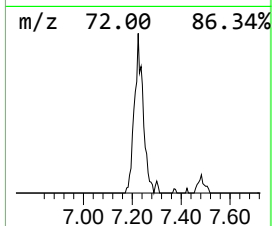
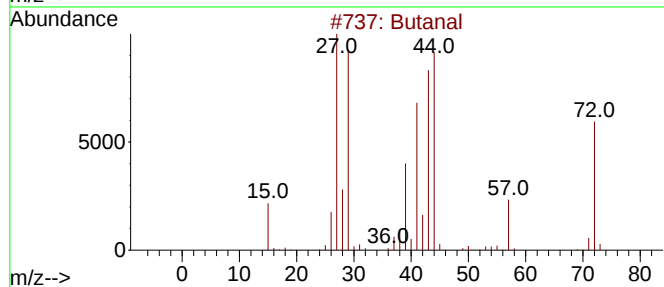
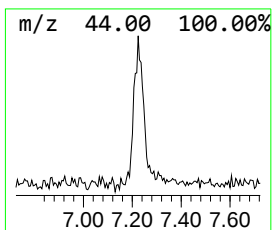
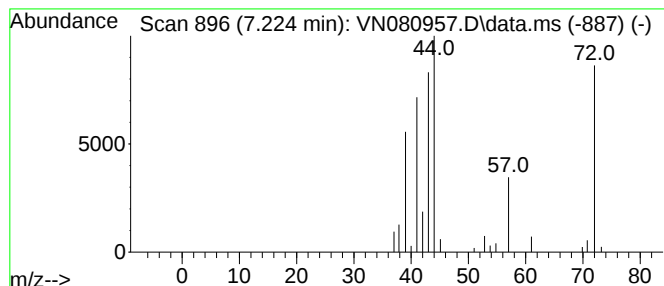
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	5.24 ug/l	124120	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	80
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
3		Propane	44	C3H8	000074-98-6	40
4		Methacrolein	70	C4H6O	000078-85-3	22
5		2-Butenal	70	C4H6O	004170-30-3	22



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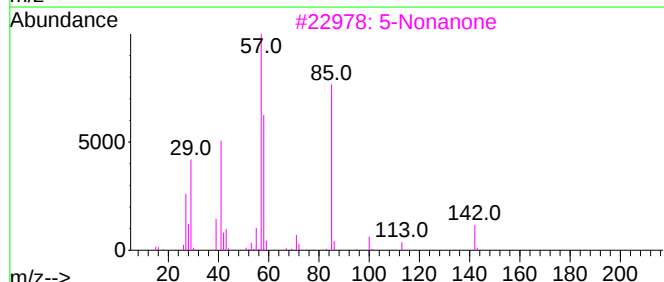
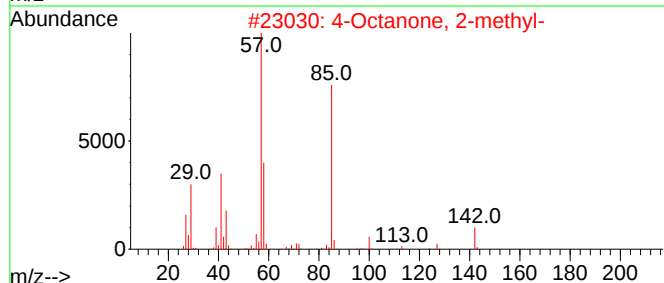
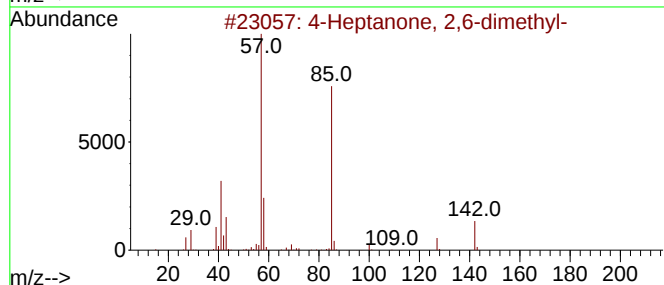
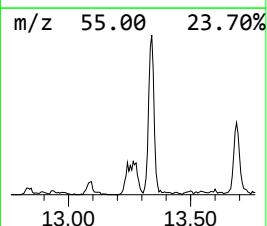
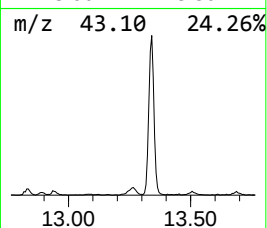
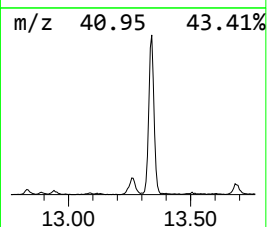
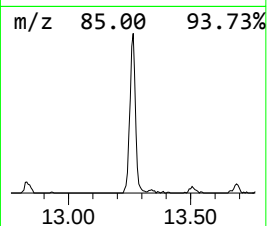
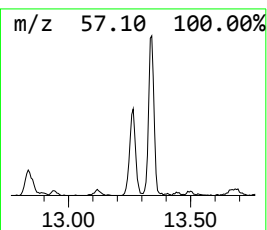
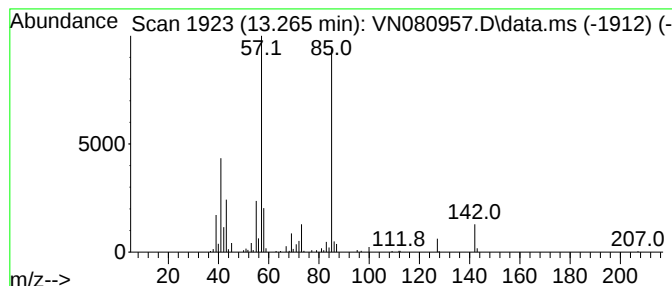
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Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	10.32 ug/l	323663	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	87
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	59
5			1,3-Propanediol, decyl ethyl ether	244	C15H32O2	1000406-35-0	59



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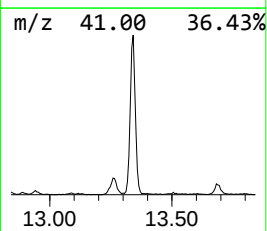
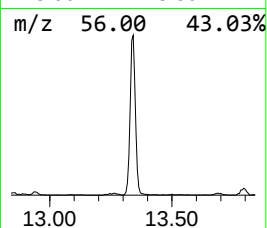
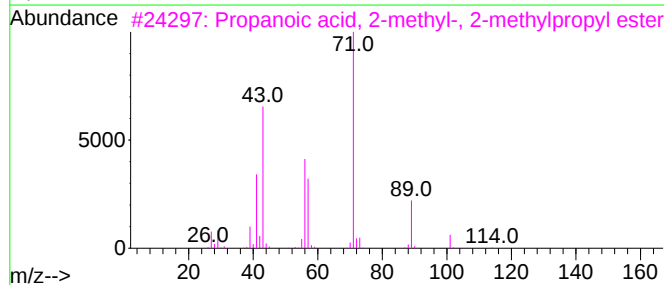
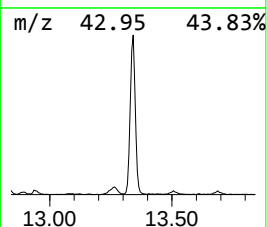
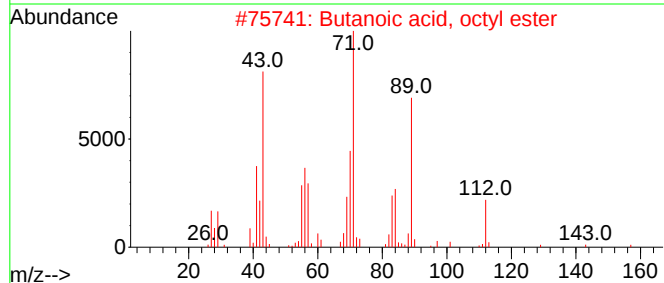
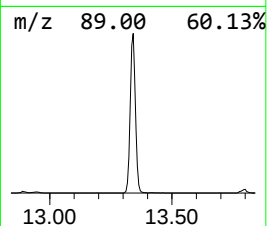
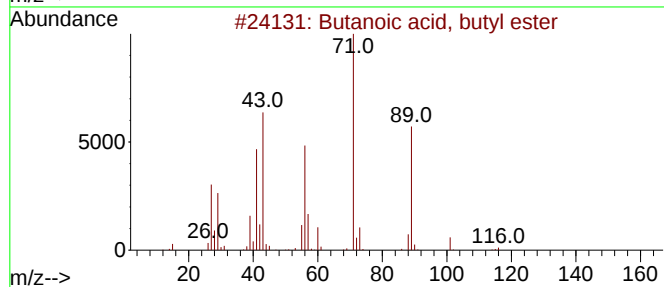
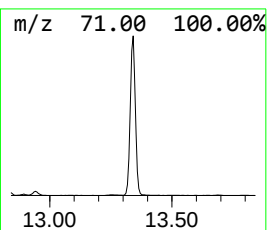
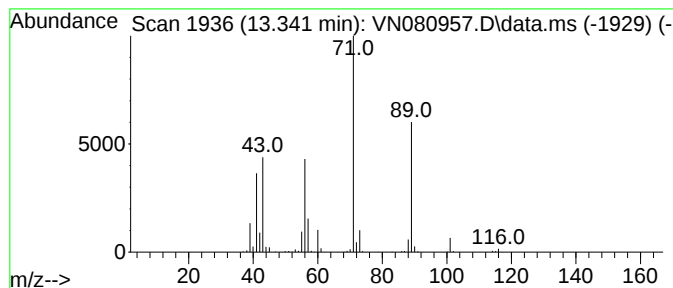
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Quant Title : SW846 8260

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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	77.19 ug/l	2419970	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
3			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	53
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50



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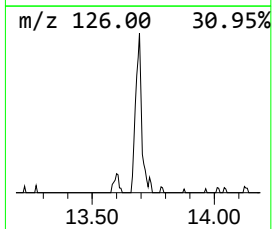
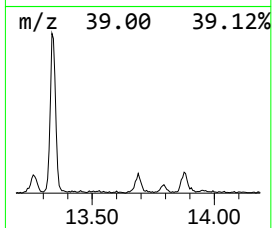
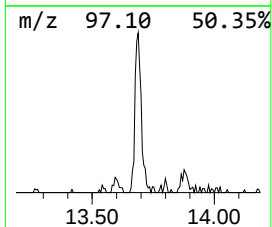
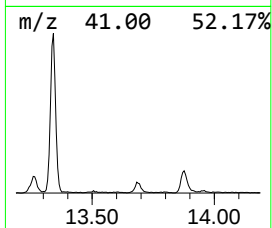
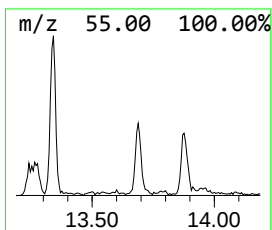
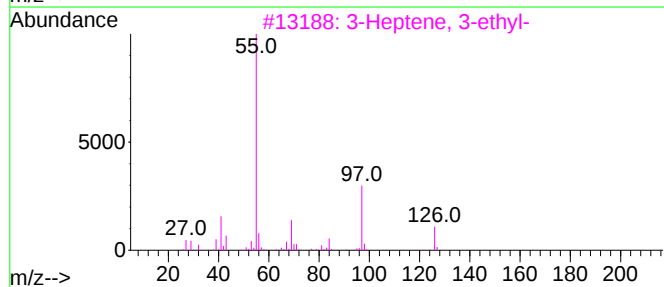
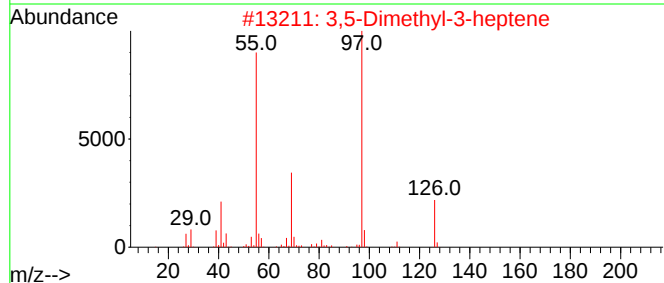
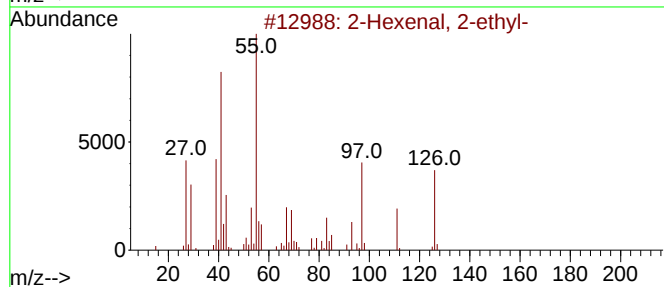
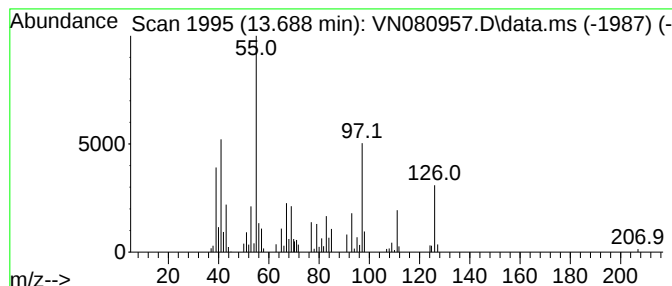
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Peak Number 4 2-Hexenal, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	6.87 ug/l	215313	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	96
2			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	38
3			3-Heptene, 3-ethyl-	126	C9H18	074764-46-8	38
4			2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	30
5			Cyclopropane, 1-bromo-2,2-diethyl-	176	C7H13Br	343926-55-6	27



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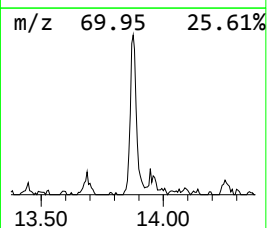
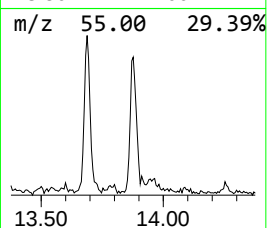
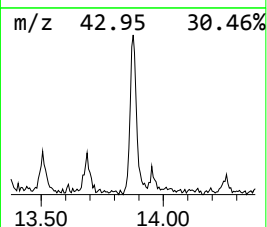
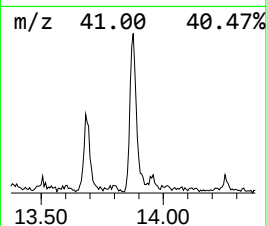
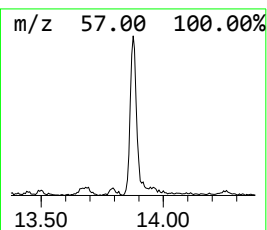
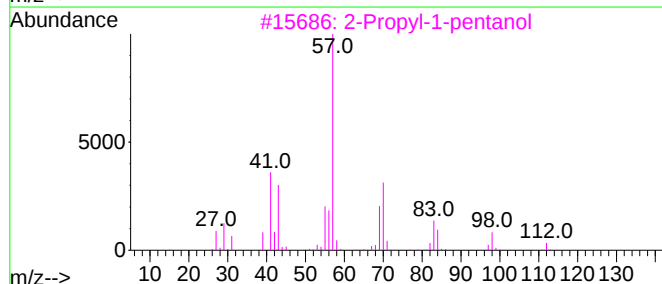
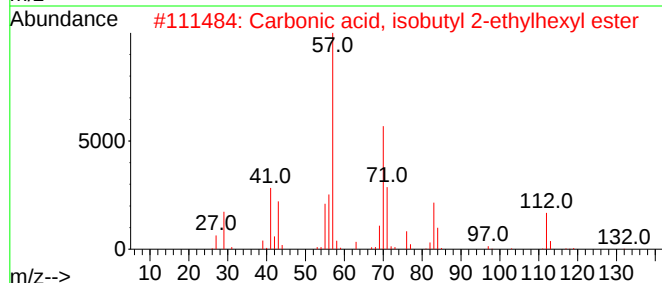
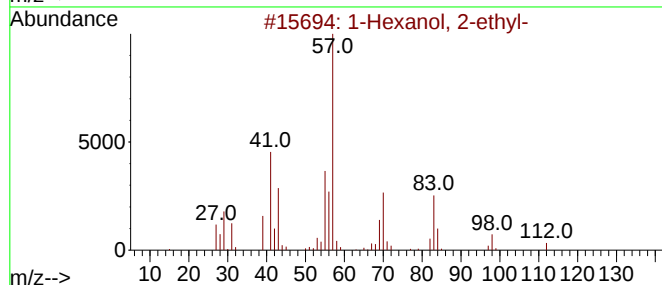
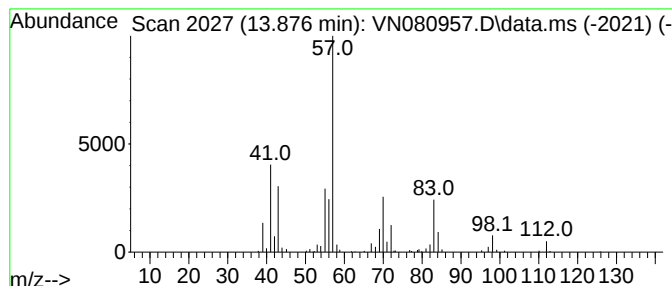
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	11.85 ug/l	371396	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.224	5.2	ug/l	124120	1	8.224	1184230	50.0
4-Heptanone, 2,...	13.265	10.3	ug/l	323663	4	13.794	1567500	50.0
Butanoic acid, ...	13.341	77.2	ug/l	2419970	4	13.794	1567500	50.0
2-Hexenal, 2-et...	13.688	6.9	ug/l	215313	4	13.794	1567500	50.0
1-Hexanol, 2-et...	13.876	11.9	ug/l	371396	4	13.794	1567500	50.0