

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091422\
 Data File : VX031324.D
 Acq On : 14 Sep 2022 22:35
 Operator : JC/MD
 Sample : N4580-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CO-1

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\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.630	79	89	90	rBV5	4064	8968	1.31%	0.245%
2	2.392	207	214	226	rBV	47711	86337	12.60%	2.361%
3	2.953	295	306	307	rBV	12527	26408	3.85%	0.722%
4	2.989	308	312	334	rVB	23498	74692	10.90%	2.043%
5	4.580	563	573	589	rBV2	10760	38213	5.58%	1.045%
6	5.391	695	706	718	rBV2	57859	165867	24.20%	4.536%
7	5.556	721	733	746	rVV2	70497	199211	29.07%	5.448%
8	5.958	788	799	812	rBV	71535	187624	27.37%	5.131%
9	6.763	922	931	943	rVB	117954	276438	40.33%	7.560%
10	7.244	1001	1010	1027	rBV3	16614	58688	8.56%	1.605%
11	7.397	1029	1035	1041	rVV3	4057	11369	1.66%	0.311%
12	7.464	1041	1046	1055	rVB	6708	15424	2.25%	0.422%
13	7.903	1111	1118	1130	rVB	13377	27088	3.95%	0.741%
14	8.653	1234	1241	1248	rBV	335075	524984	76.60%	14.358%
15	9.055	1302	1307	1311	rVB2	4586	7313	1.07%	0.200%
16	9.244	1331	1338	1343	rBV2	9319	16152	2.36%	0.442%
17	9.305	1343	1348	1355	rVB3	3268	7855	1.15%	0.215%
18	9.439	1365	1370	1378	rBV2	8813	16303	2.38%	0.446%
19	9.592	1389	1395	1399	rBV	7069	10091	1.47%	0.276%
20	10.055	1465	1471	1479	rBV	249292	329925	48.14%	9.023%
21	10.378	1517	1524	1537	rBV	51784	75407	11.00%	2.062%
22	10.597	1554	1560	1567	rBV4	6652	13031	1.90%	0.356%
23	10.683	1570	1574	1581	rVB	11231	14230	2.08%	0.389%
24	10.768	1584	1588	1594	rVV	9980	11622	1.70%	0.318%
25	11.079	1634	1639	1650	rVB	255166	324162	47.30%	8.865%
26	11.481	1700	1705	1713	rVB	6705	10680	1.56%	0.292%
27	11.567	1715	1719	1722	rBV2	6072	8326	1.21%	0.228%
28	11.658	1730	1734	1739	rBV2	4653	8012	1.17%	0.219%
29	11.896	1768	1773	1781	rVB4	3674	7608	1.11%	0.208%
30	12.024	1788	1794	1801	rVB	229188	282352	41.20%	7.722%
31	12.219	1821	1826	1835	rBV	540657	685391	100.00%	18.744%
32	12.585	1881	1886	1897	rBV3	10713	20849	3.04%	0.570%
33	12.865	1928	1932	1941	rVB4	5081	8931	1.30%	0.244%
34	13.134	1968	1976	1987	rBV5	14758	50058	7.30%	1.369%
35	13.219	1987	1990	1996	rVV2	8061	13121	1.91%	0.359%
36	14.463	2189	2194	2197	rBV	15506	20380	2.97%	0.557%

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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\82X091422W.M
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37	14.566	2205	2211	2215	rBV	10015	13404	1.96%	0.367%
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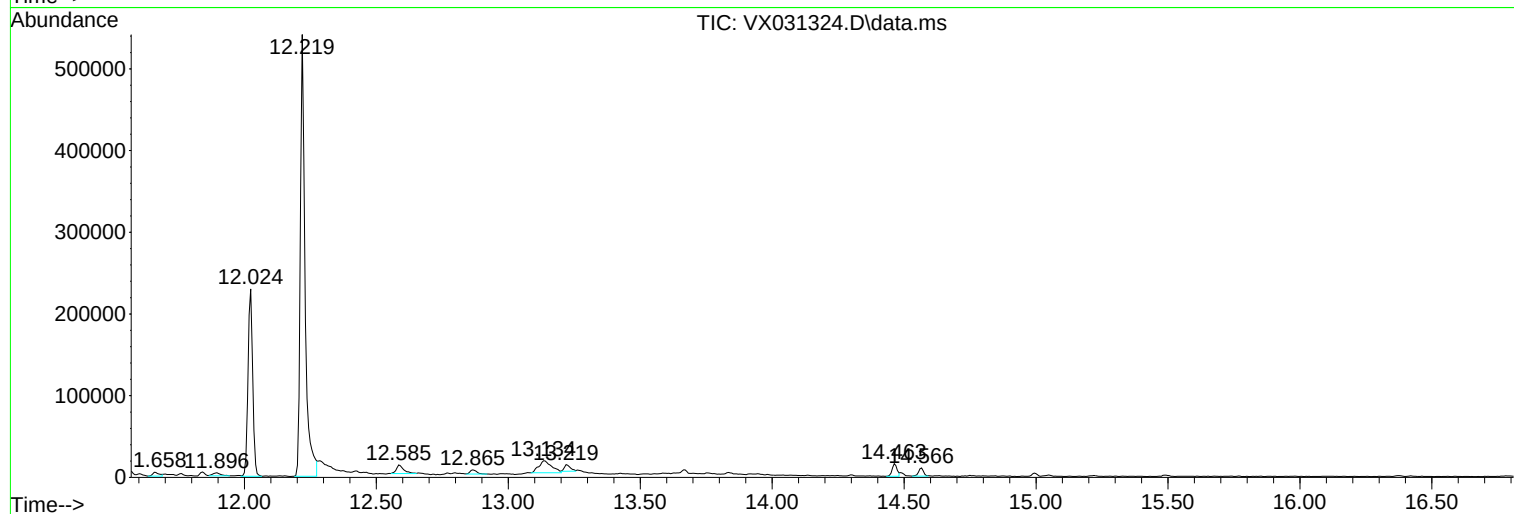
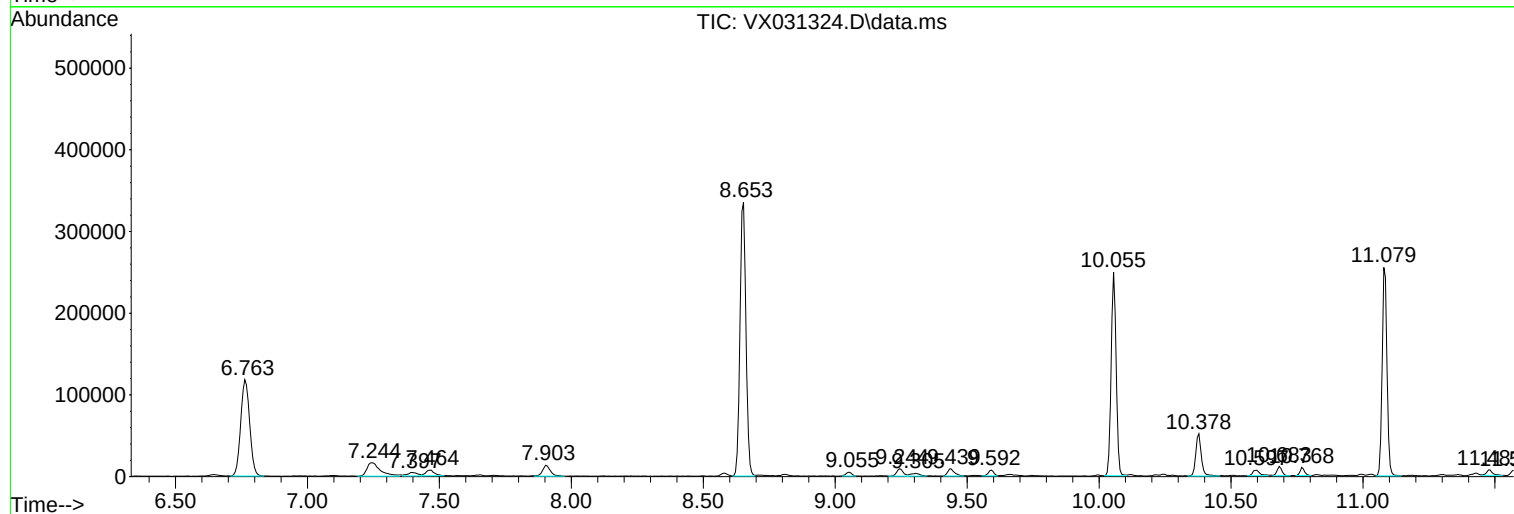
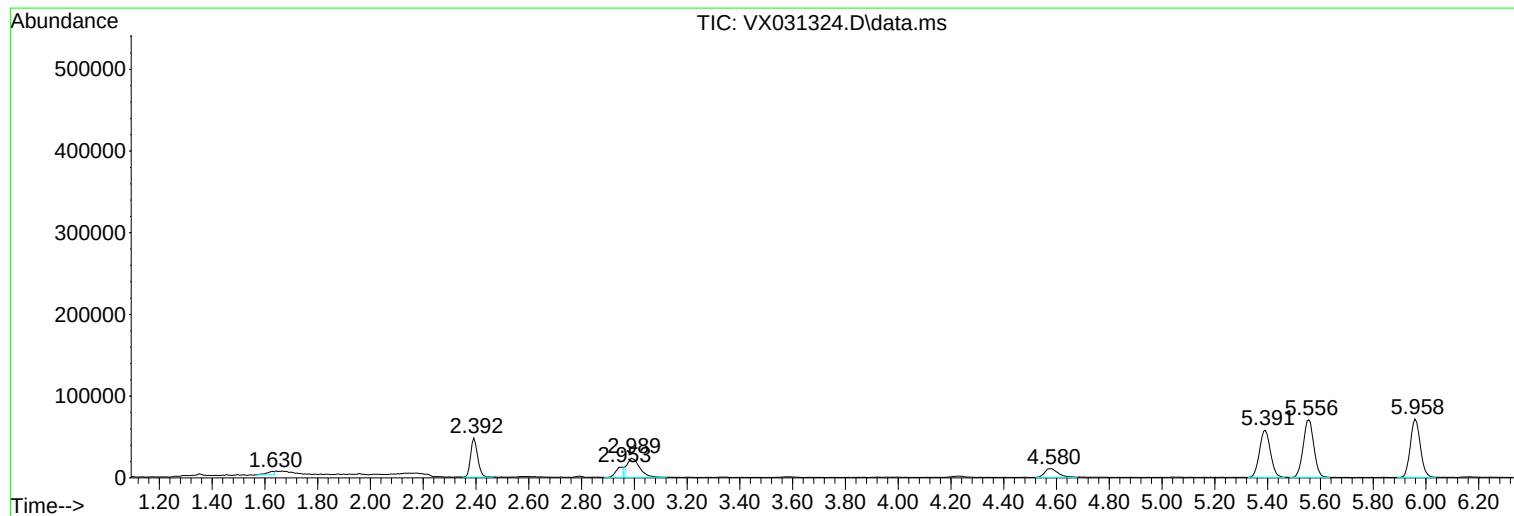
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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



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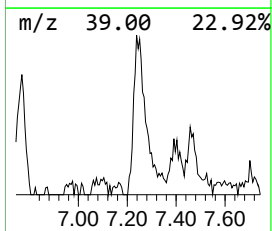
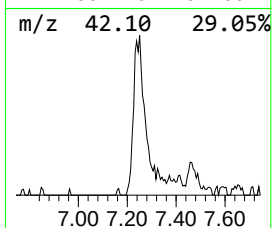
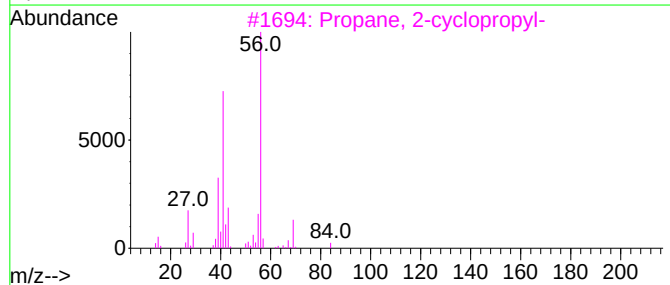
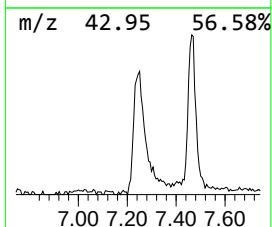
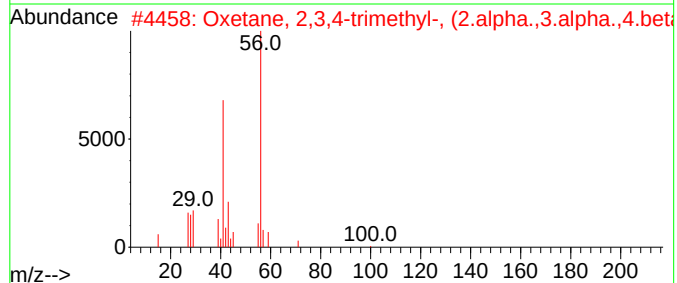
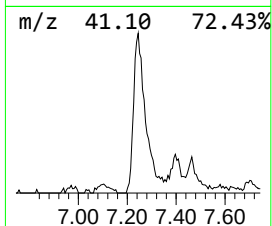
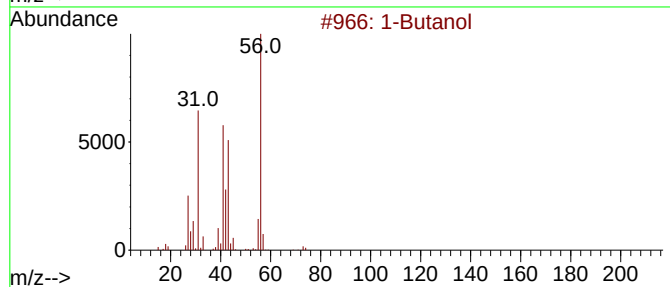
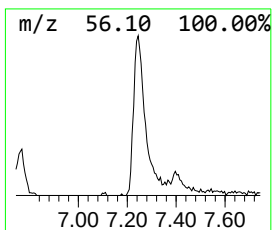
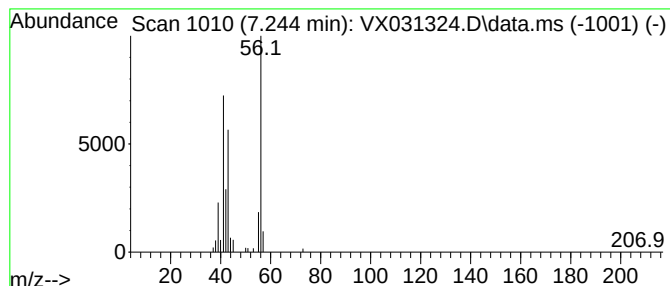
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.244	10.62 ug/l	58688	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	83
2			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	9



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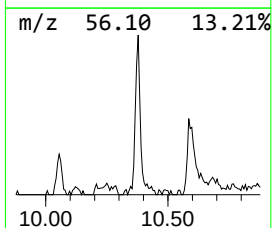
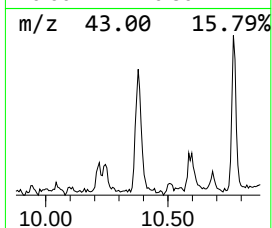
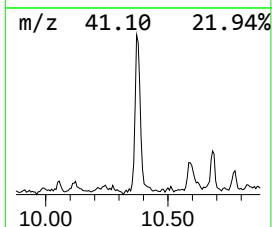
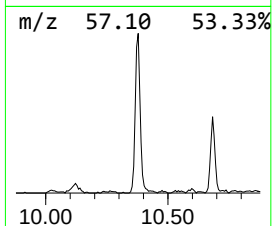
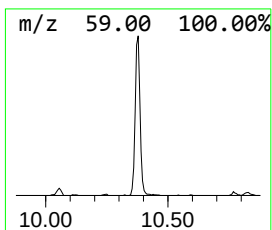
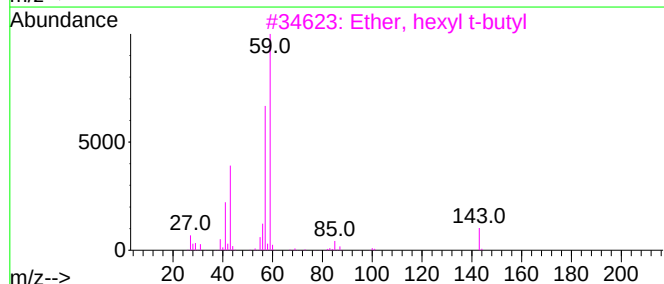
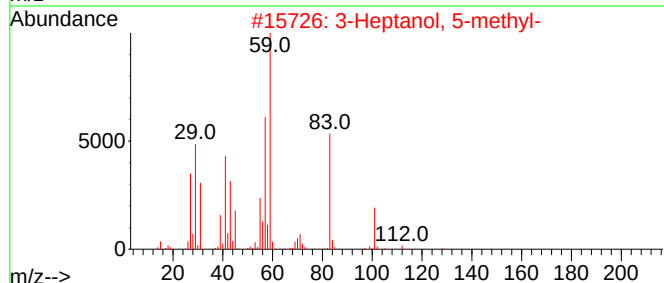
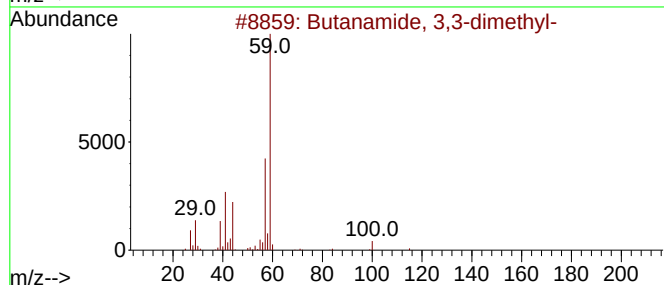
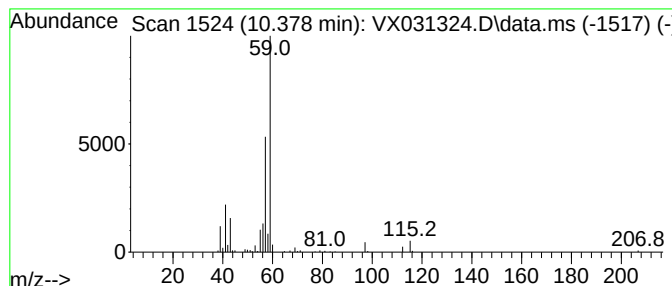
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Peak Number 2 Butanamide, 3,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.378	11.43 ug/l	75407	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	50
2			3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	40
3			Ether, hexyl t-butyl	158	C10H22O	069775-79-7	40
4			1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	39
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	39



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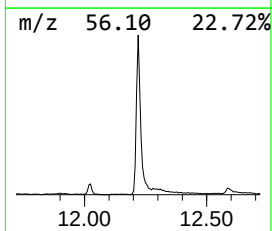
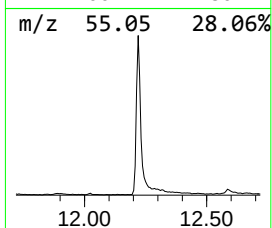
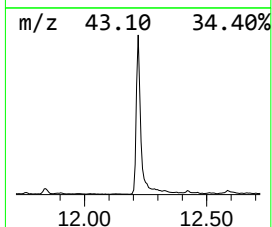
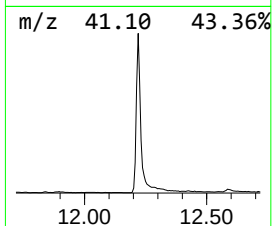
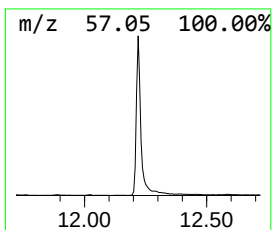
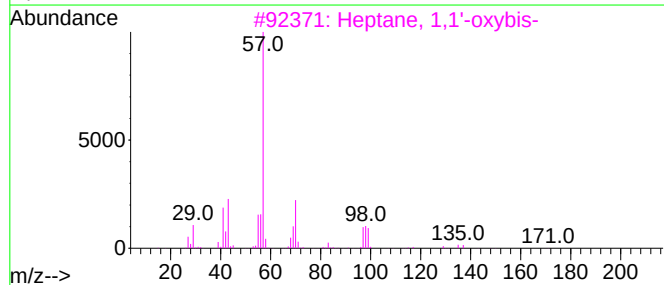
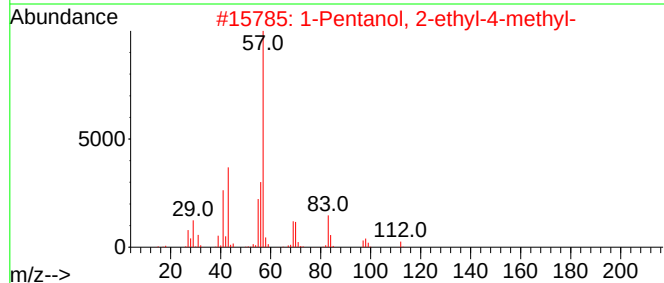
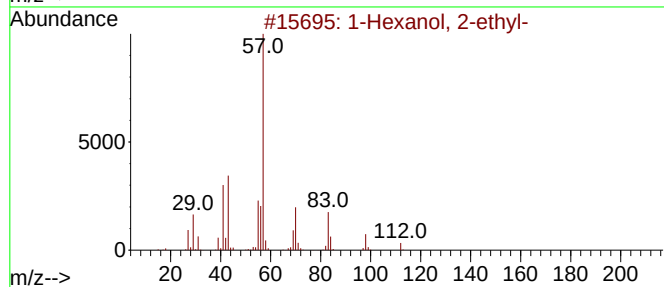
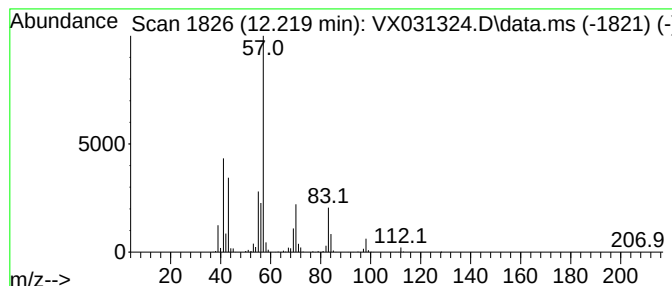
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	121.37 ug/l	685391	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	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43



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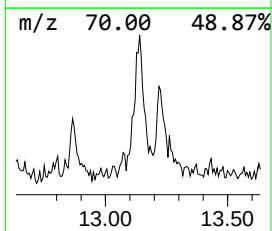
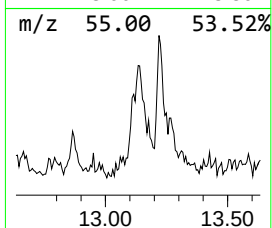
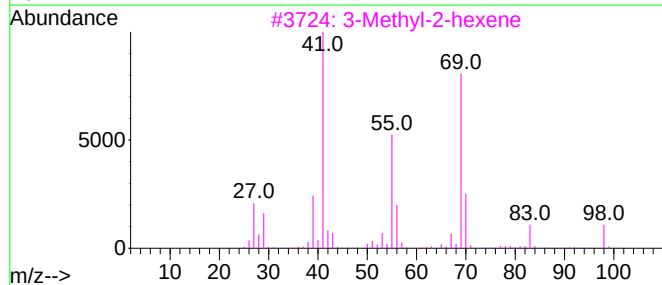
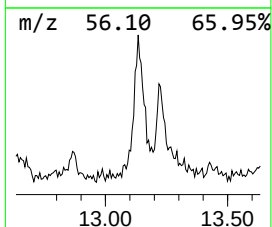
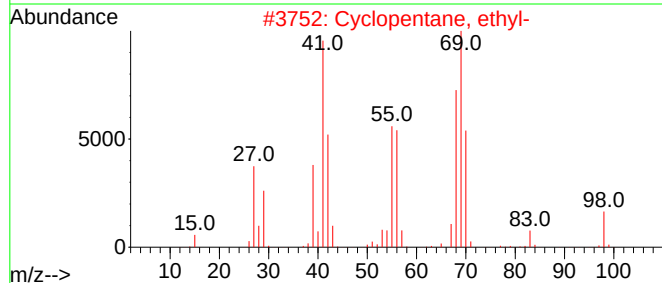
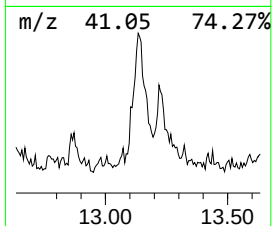
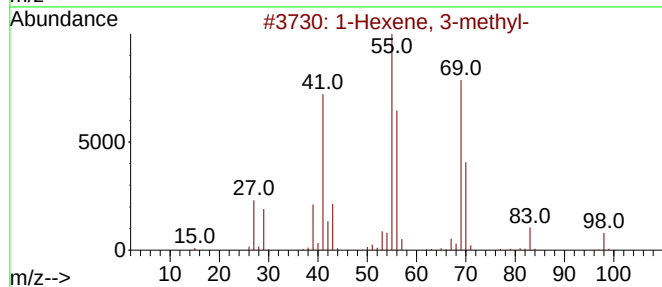
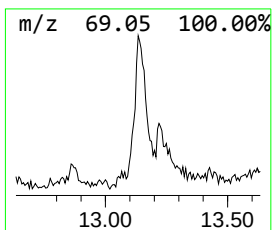
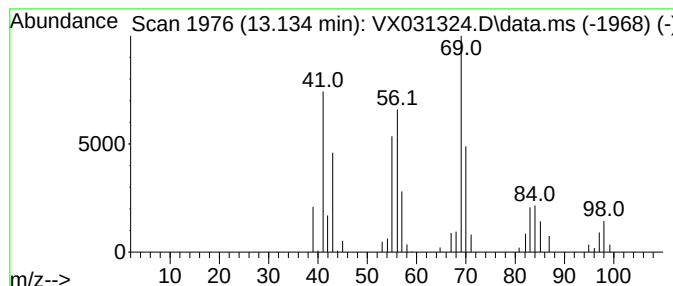
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexene, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.134	8.86 ug/l	50058	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexene, 3-methyl-	98	C7H14	003404-61-3	64
2		Cyclopentane, ethyl-	98	C7H14	001640-89-7	58
3		3-Methyl-2-hexene	98	C7H14	017618-77-8	46
4		3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	38
5		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	38



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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
1-Butanol	7.244	10.6	ug/l	58688	2	6.763	276438	50.0
Butanamide, 3,3...	10.378	11.4	ug/l	75407	3	10.055	329925	50.0
1-Hexanol, 2-et...	12.219	121.4	ug/l	685391	4	12.024	282352	50.0
1-Hexene, 3-met...	13.134	8.9	ug/l	50058	4	12.024	282352	50.0