

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY040224\
 Data File : VY017816.D
 Acq On : 02 Apr 2024 11:01
 Operator : SY/MD
 Sample : P1945-01
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SEW-10

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_Y\methods\82Y032924S.M
 Title : SW846 8260

Signal : TIC: VY017816.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	3	8	14	rVB4	3580	6348	1.15%	0.190%
2	2.119	37	49	53	rBV4	3752	10463	1.90%	0.313%
3	2.223	61	66	74	rBV2	11323	20541	3.72%	0.614%
4	2.387	88	93	101	rBV	11283	20535	3.72%	0.614%
5	3.838	321	331	339	rVB2	3159	8781	1.59%	0.262%
6	3.960	342	351	361	rVB3	3877	11126	2.02%	0.333%
7	4.204	384	391	401	rBV7	3539	10871	1.97%	0.325%
8	4.716	467	475	491	rVB3	5341	16542	3.00%	0.494%
9	5.759	638	646	655	rVB3	3399	9586	1.74%	0.287%
10	6.716	792	803	814	rBV5	5221	16448	2.98%	0.492%
11	6.984	837	847	863	rBV2	7089	22983	4.16%	0.687%
12	7.722	959	968	974	rBV	86859	205945	37.31%	6.155%
13	7.795	974	980	993	rVB	138082	310857	56.32%	9.291%
14	8.149	1027	1038	1050	rBV	81503	180757	32.75%	5.403%
15	8.697	1120	1128	1137	rBV	218359	423940	76.81%	12.671%
16	9.270	1215	1222	1236	rBV	18024	37571	6.81%	1.123%
17	10.075	1350	1354	1359	rBV4	2883	5553	1.01%	0.166%
18	10.191	1366	1373	1380	rBV	321810	551944	100.00%	16.497%
19	10.587	1433	1438	1445	rBV2	3682	7120	1.29%	0.213%
20	10.941	1489	1496	1510	rBV2	60275	111544	20.21%	3.334%
21	11.502	1580	1588	1601	rBV	280616	476916	86.41%	14.254%
22	11.709	1613	1622	1627	rBV5	5234	12338	2.24%	0.369%
23	12.038	1669	1676	1683	rVB4	6242	12338	2.24%	0.369%
24	12.215	1699	1705	1715	rBV	24584	40065	7.26%	1.197%
25	12.489	1743	1750	1762	rVB	177631	288604	52.29%	8.626%
26	12.654	1772	1777	1785	rVB7	2618	7387	1.34%	0.221%
27	12.818	1800	1804	1808	rBV3	8929	12910	2.34%	0.386%
28	12.916	1815	1820	1825	rBV	21620	32160	5.83%	0.961%
29	13.129	1850	1855	1858	rBV2	6745	10483	1.90%	0.313%
30	13.166	1858	1861	1869	rVB7	5184	11389	2.06%	0.340%
31	13.282	1873	1880	1886	rBV3	24252	43566	7.89%	1.302%
32	13.349	1886	1891	1894	rVV4	9518	15943	2.89%	0.477%
33	13.434	1898	1905	1915	rVV	196866	320253	58.02%	9.572%
34	13.757	1953	1958	1963	rBV6	4365	7428	1.35%	0.222%
35	13.977	1989	1994	1998	rVB3	3734	6125	1.11%	0.183%
36	14.215	2027	2033	2039	rBV	34145	51024	9.24%	1.525%

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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

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37	15.324	2210	2215	2221	rVB2	4296	7353	1.33%	0.220%
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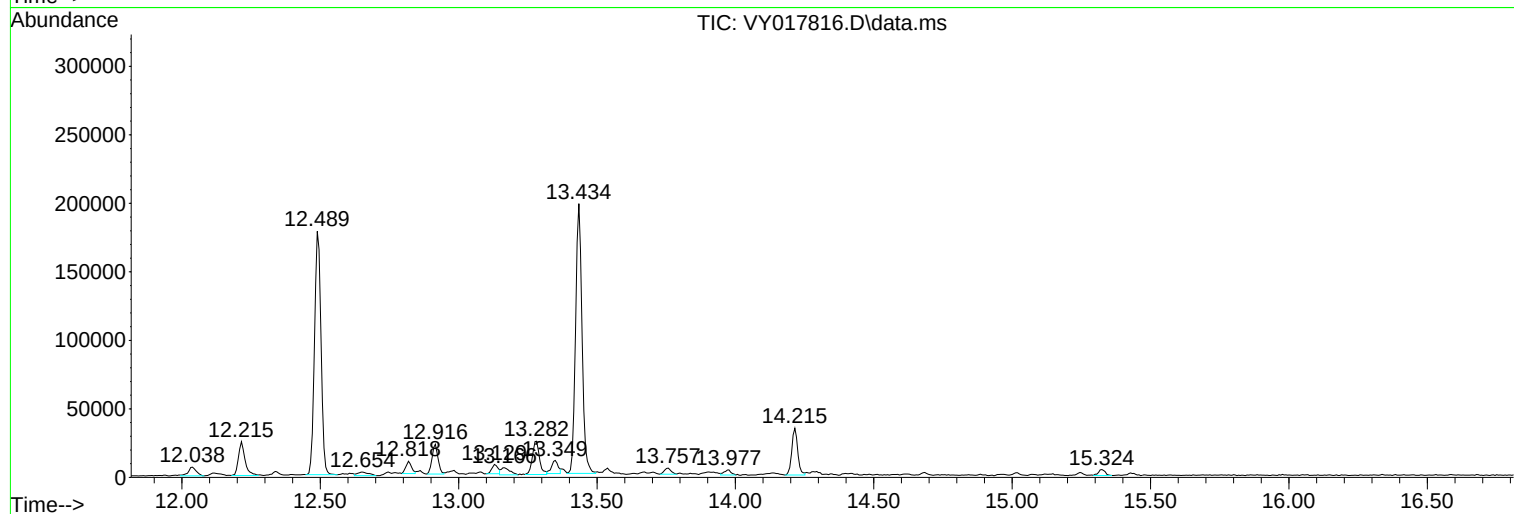
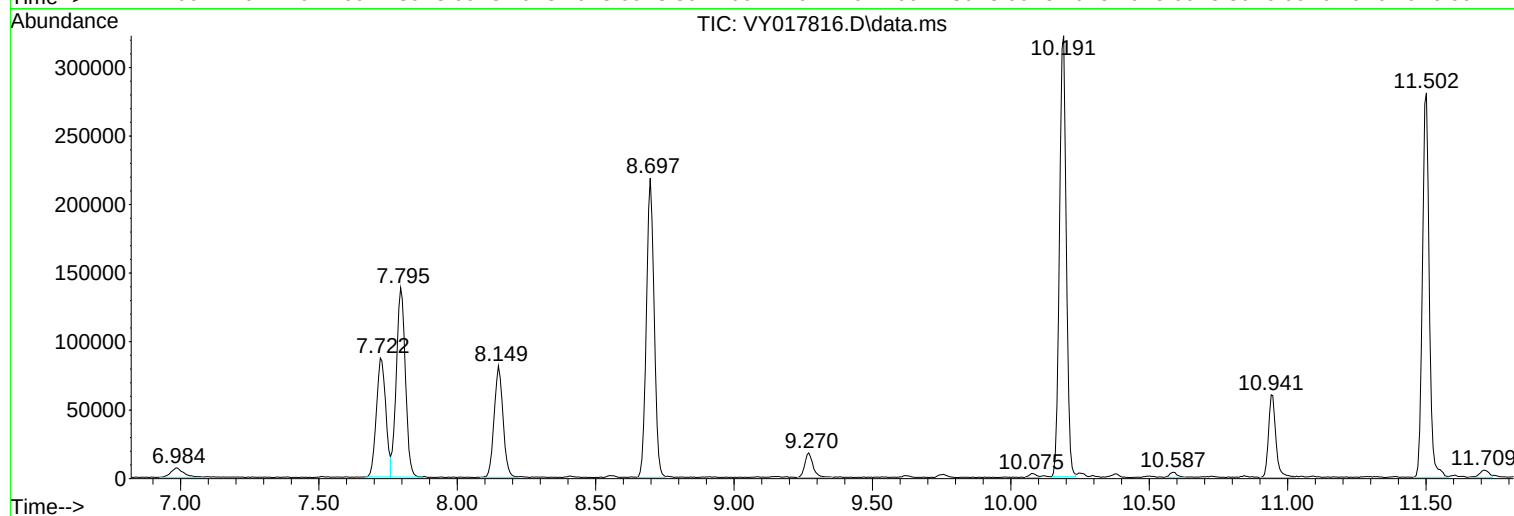
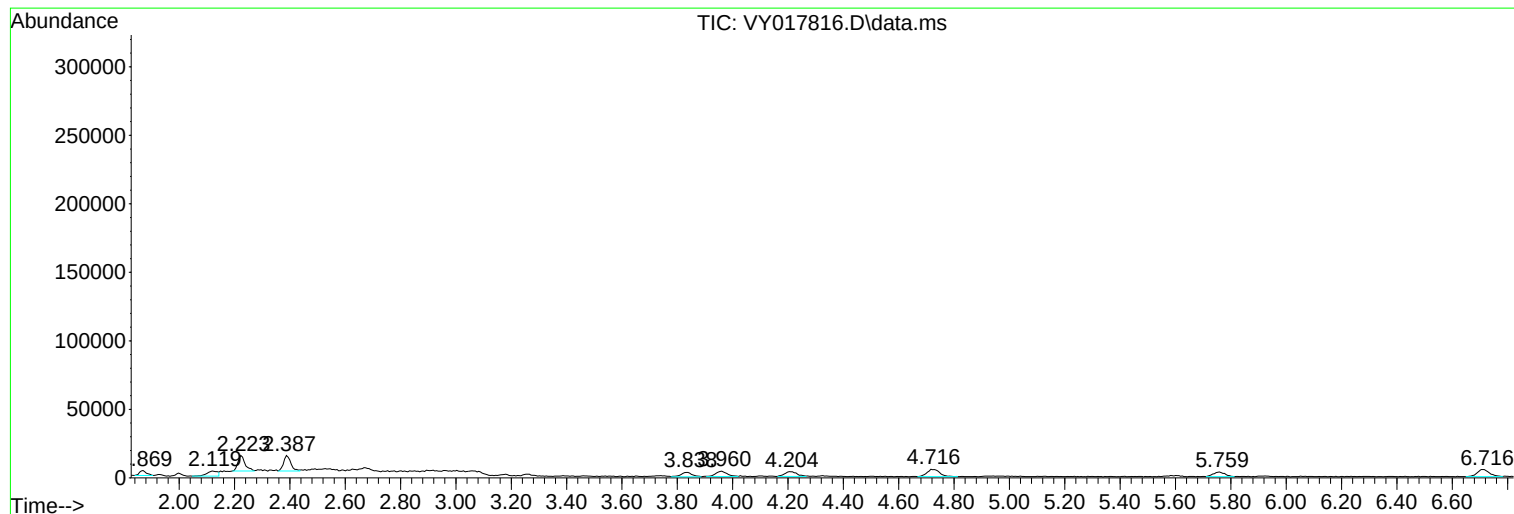
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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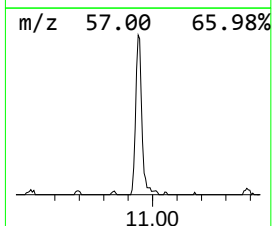
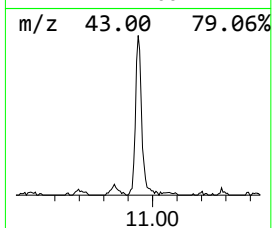
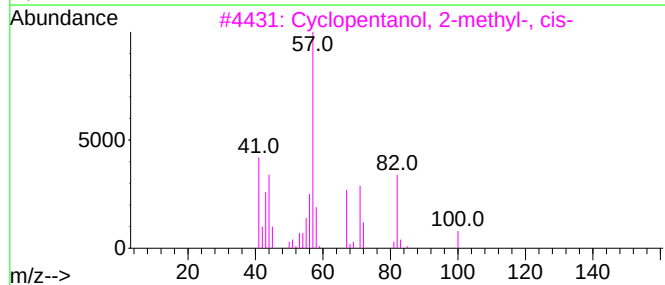
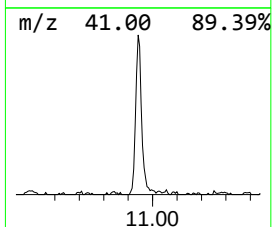
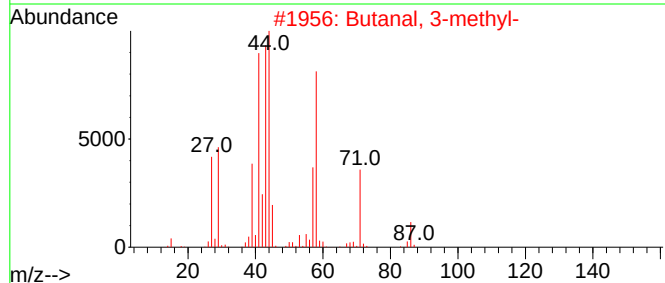
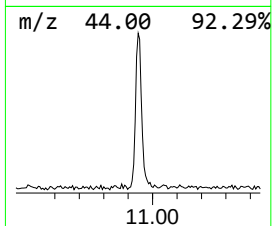
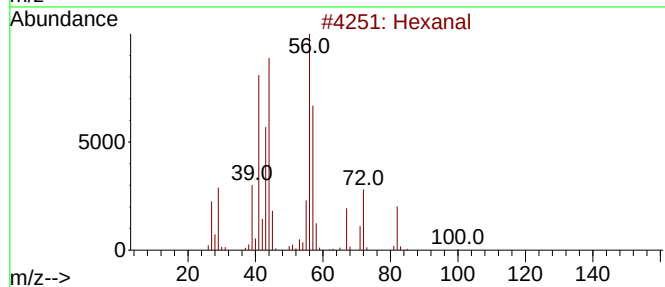
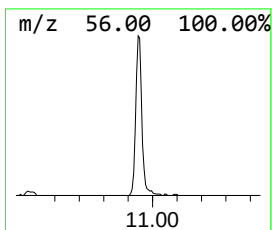
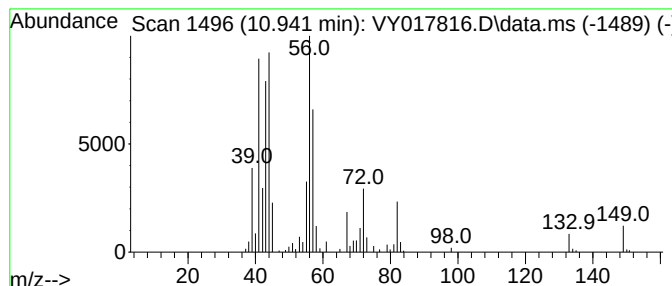
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y032924S.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.941	11.69 ug/l	111544	Chlorobenzene-d5	11.502

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	64
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	38
3			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	38
4			4-Piperidinecarboxamide	128	C6H12N2O	039546-32-2	37
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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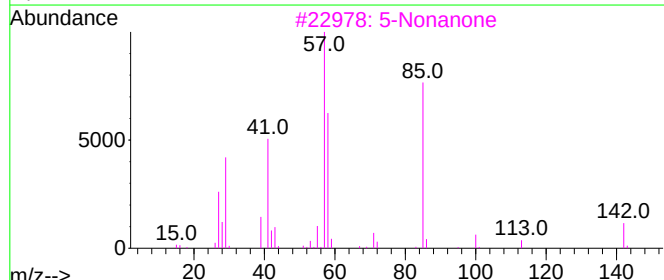
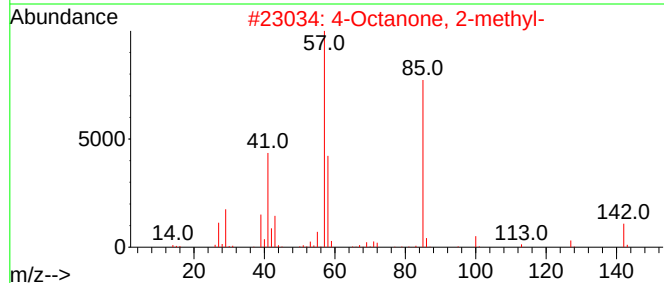
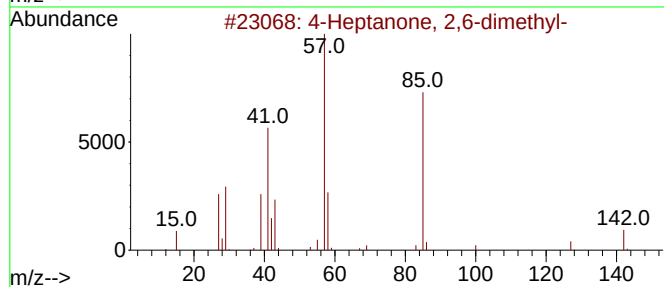
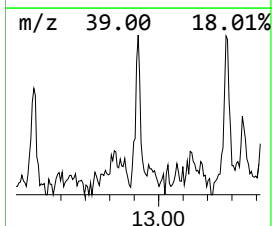
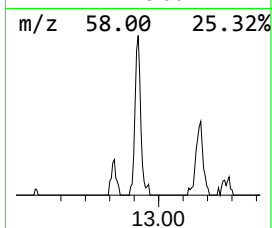
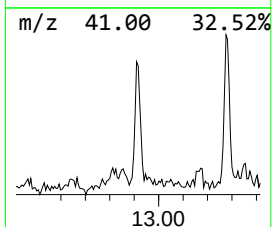
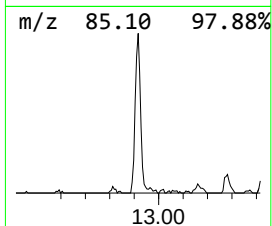
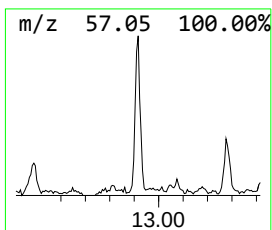
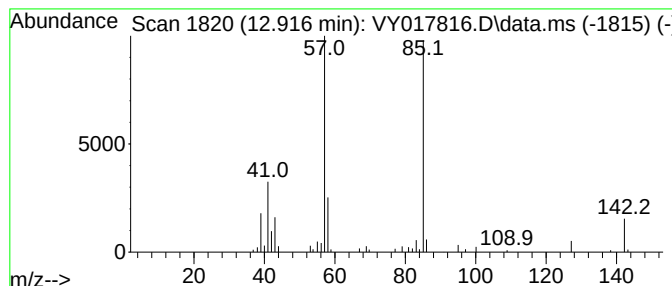
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Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.916	5.02 ug/l	32160	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
3			5-Nonanone	142	C9H18O	000502-56-7	64
4			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50
5			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50



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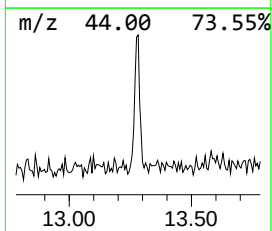
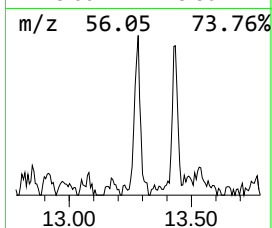
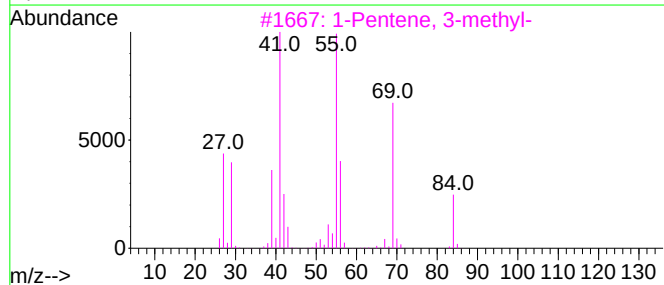
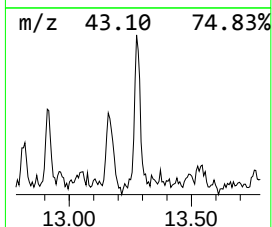
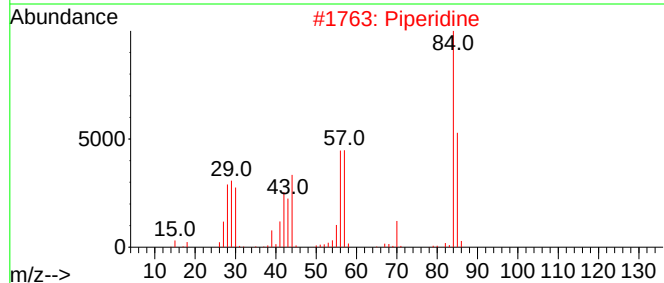
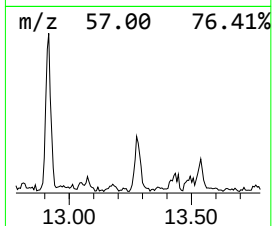
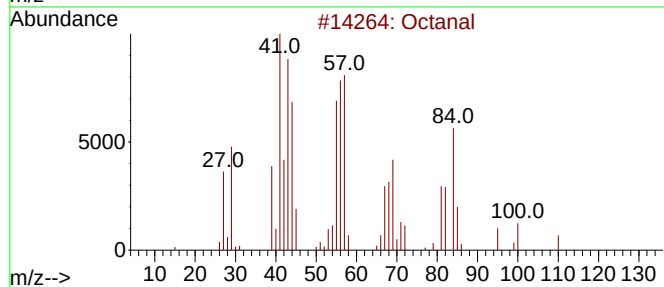
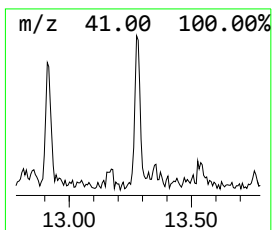
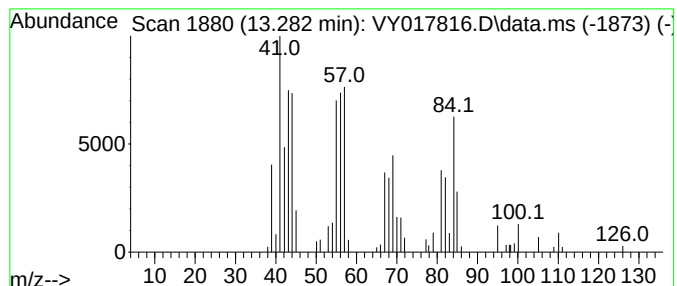
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	6.80 ug/l	43566	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	91
2	Piperidine			85	C5H11N	000110-89-4	47
3	1-Pentene, 3-methyl-			84	C6H12	000760-20-3	38
4	Butane, 1-(ethenyl)-			100	C6H12O	000111-34-2	30
5	Bromoacetic acid, 10-undecenyl e...			290	C13H23BrO2	195373-65-0	22



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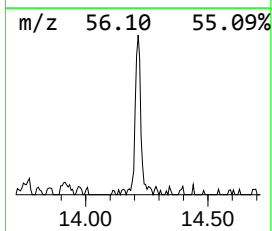
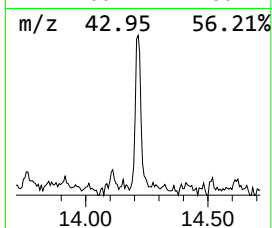
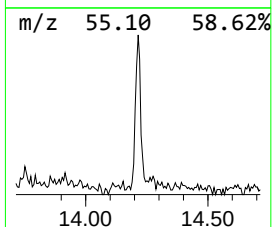
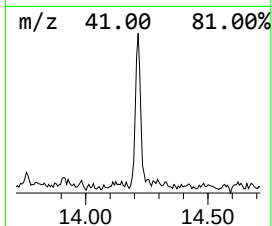
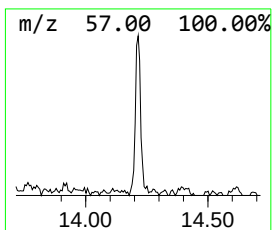
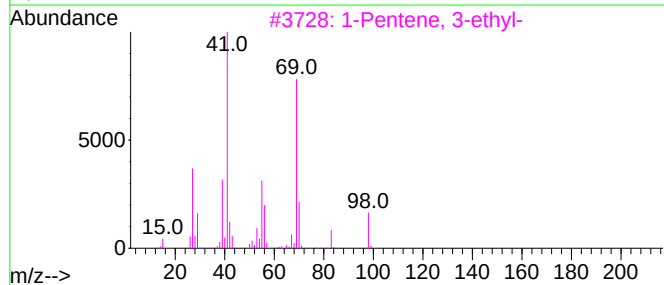
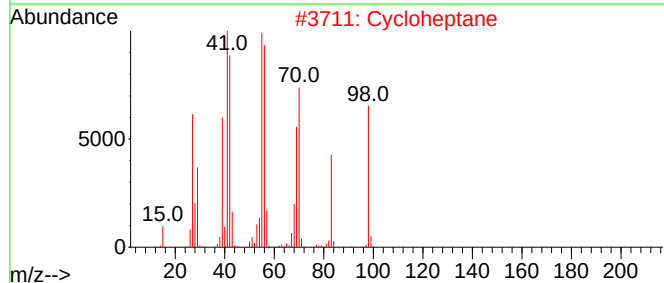
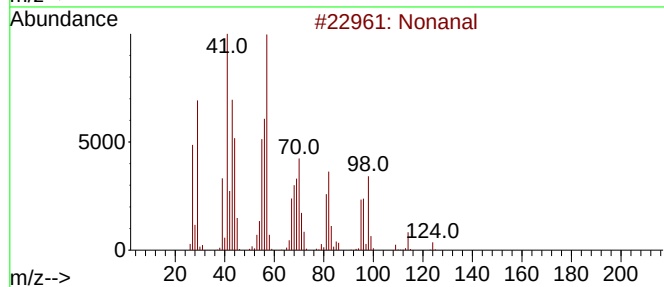
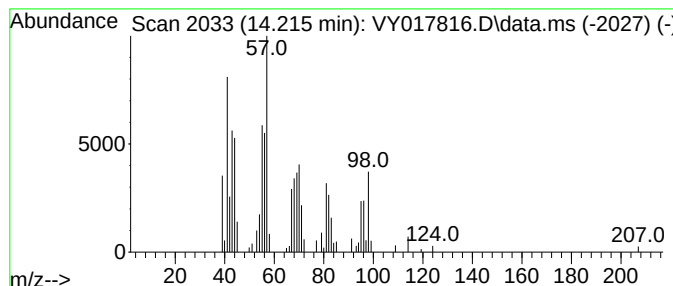
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	7.97 ug/l	51024	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	87
2			Cycloheptane	98	C7H14	000291-64-5	41
3			1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	27
4			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	25
5			Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	25



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	10.941	11.7	ug/l	111544	3	11.502	476916	50.0
4-Heptanone, 2,...	12.916	5.0	ug/l	32160	4	13.434	320253	50.0
Octanal	13.282	6.8	ug/l	43566	4	13.434	320253	50.0
Nonanal	14.214	8.0	ug/l	51024	4	13.434	320253	50.0