

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU031120\
 Data File : VU037181.D
 Acq On : 11 Mar 2020 21:14
 Operator : JC/MD
 Sample : L1891-05
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBER5

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR031120WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.658	92	99	103	rBV	61490	79706	2.76%	1.059%
2	2.642	394	405	419	rVB2	80337	147254	5.09%	1.956%
3	3.443	639	654	675	rVB	183840	365682	12.64%	4.858%
4	3.964	799	816	835	rBV6	36766	112362	3.88%	1.493%
5	4.751	1044	1061	1094	rBV	1286375	2892908	100.00%	38.432%
6	5.150	1164	1185	1227	rBV3	284696	1008228	34.85%	13.394%
7	5.832	1378	1397	1428	rBV3	141820	354802	12.26%	4.713%
8	6.102	1464	1481	1510	rBV4	21797	73922	2.56%	0.982%
9	6.346	1545	1557	1572	rVB2	119540	220671	7.63%	2.932%
10	6.552	1608	1621	1641	rBV	25542	63574	2.20%	0.845%
11	6.780	1678	1692	1708	rBV2	84993	161258	5.57%	2.142%
12	6.960	1735	1748	1770	rVB3	15490	39495	1.37%	0.525%
13	7.632	1943	1957	1971	rBV2	38762	66638	2.30%	0.885%
14	7.957	2045	2058	2073	rBV	145484	251887	8.71%	3.346%
15	8.066	2076	2092	2108	rVB	34553	73787	2.55%	0.980%
16	8.234	2133	2144	2160	rBV2	23410	39085	1.35%	0.519%
17	8.690	2274	2286	2297	rVV	85224	151970	5.25%	2.019%
18	8.764	2297	2309	2327	rVB	102903	222111	7.68%	2.951%
19	9.455	2511	2524	2533	rBV	161775	277409	9.59%	3.685%
20	9.507	2533	2540	2554	rVB2	52971	96397	3.33%	1.281%
21	10.787	2925	2938	2956	rVB2	44553	117803	4.07%	1.565%
22	11.832	3251	3263	3281	rBV	193705	348763	12.06%	4.633%
23	12.214	3370	3382	3396	rVB	177776	314256	10.86%	4.175%
24	13.925	3902	3914	3924	rBV3	29767	47428	1.64%	0.630%

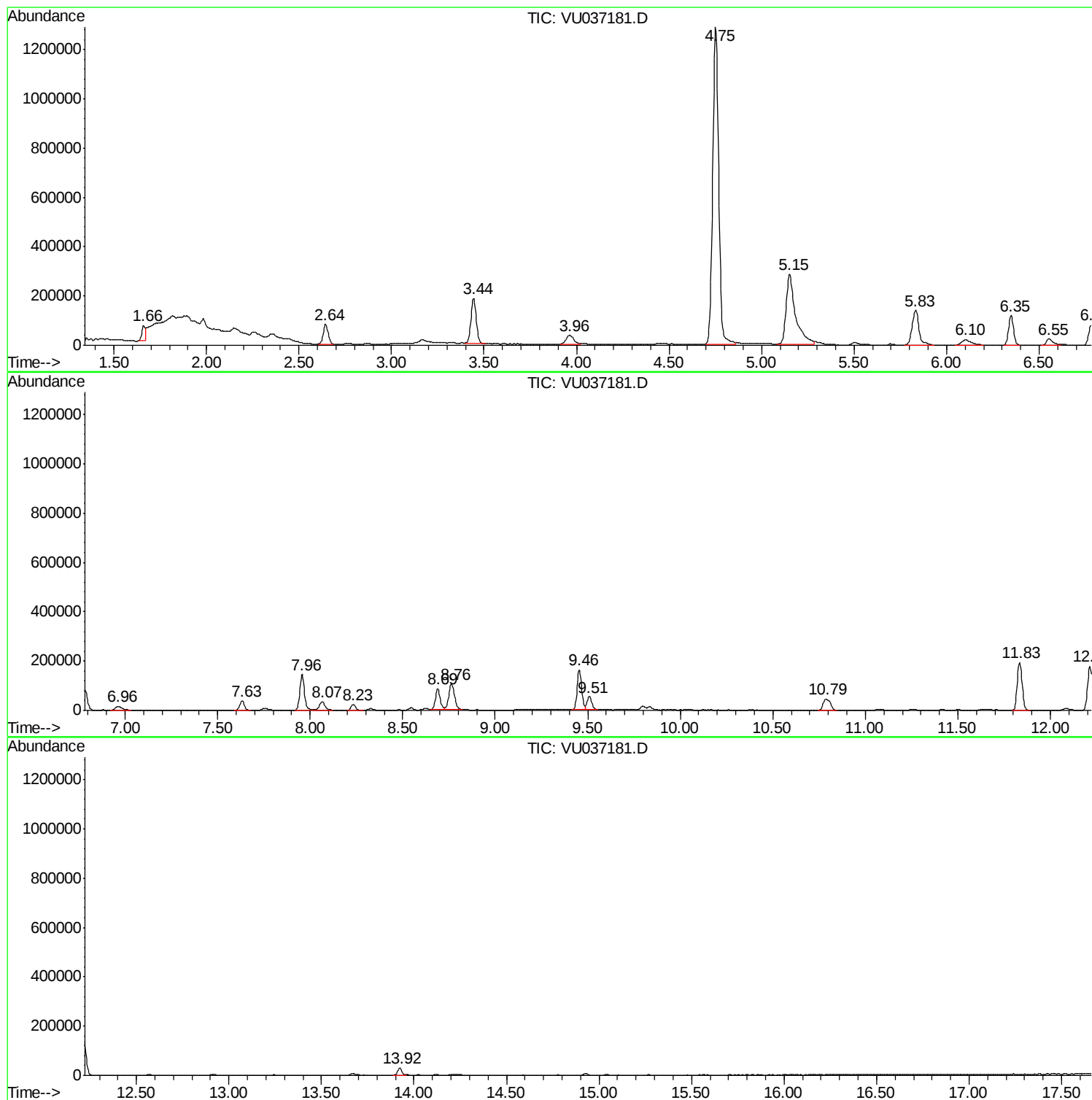
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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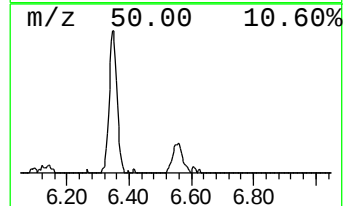
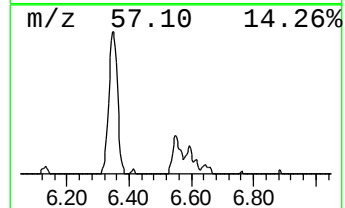
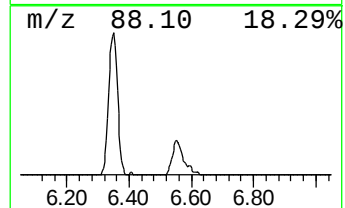
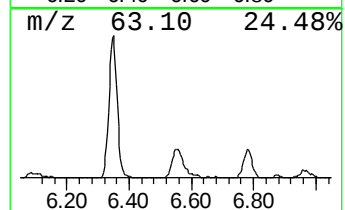
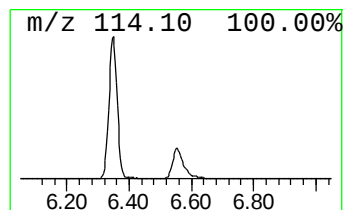
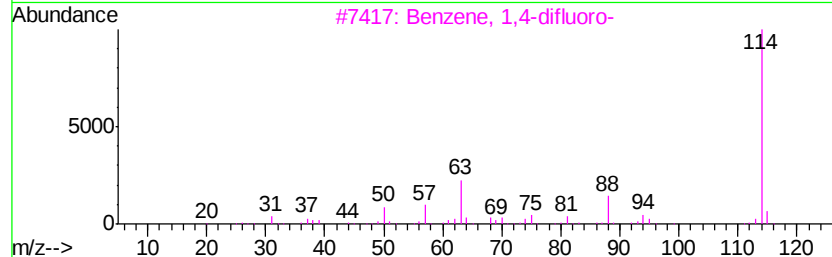
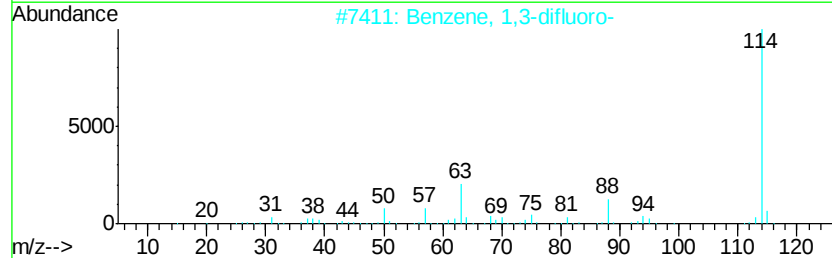
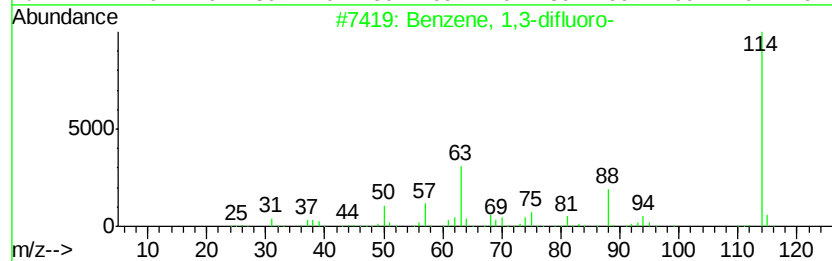
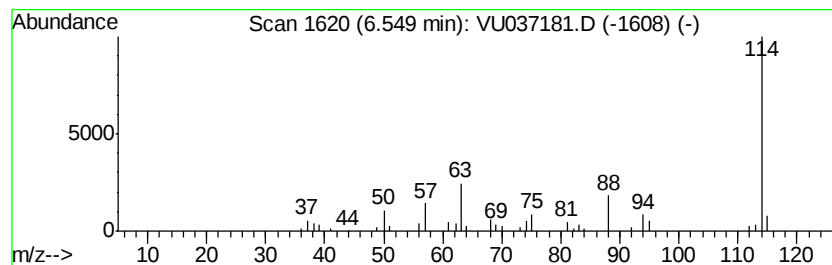
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR031120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,3-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	1.44 ug/L	63574	1,4-Difluorobenzene	6.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-difluoro-	114	C6H4F2	000372-18-9	97
2		Benzene, 1,3-difluoro-	114	C6H4F2	000372-18-9	95
3		Benzene, 1,4-difluoro-	114	C6H4F2	000540-36-3	95
4		Benzene, 1,2-difluoro-	114	C6H4F2	000367-11-3	95
5		Benzene, 1,4-difluoro-	114	C6H4F2	000540-36-3	95



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Instrument :
MSVOA_U
ClientSampled :
DBER5

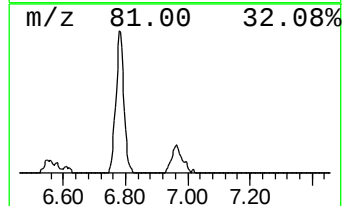
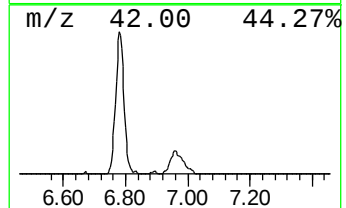
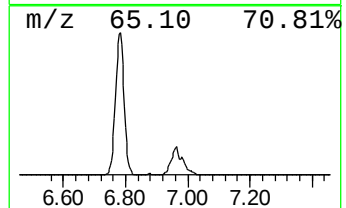
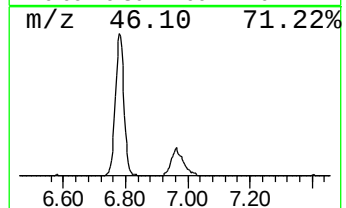
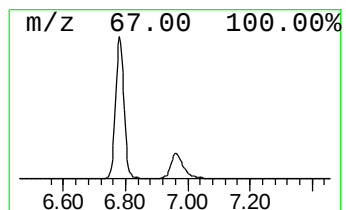
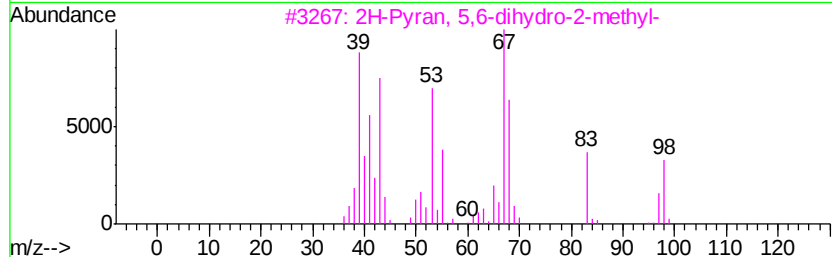
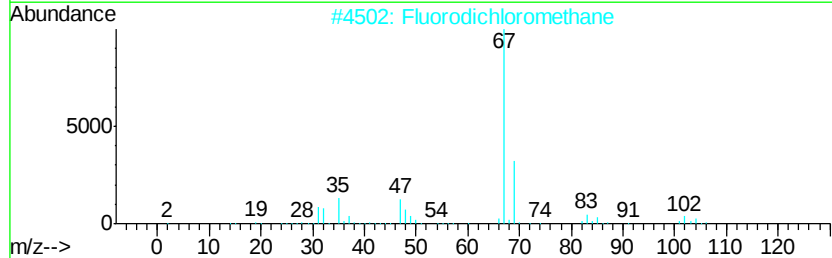
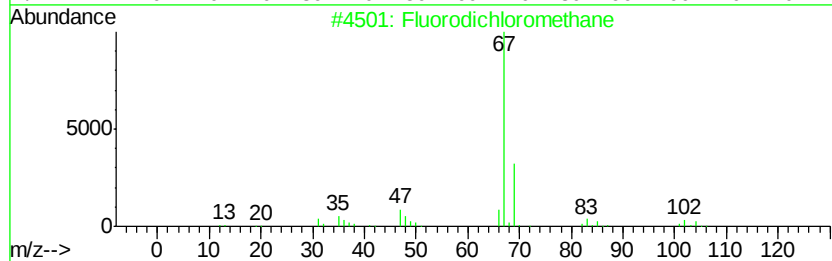
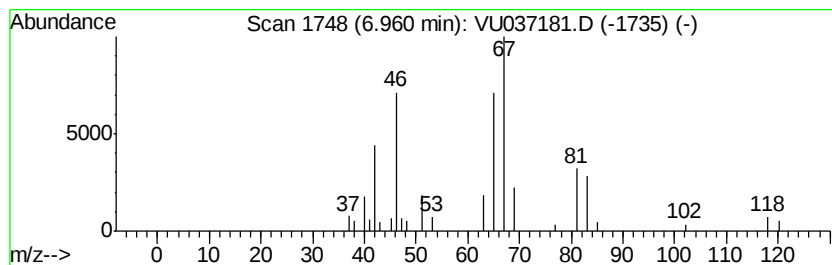
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR031120WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	0.89 ug/L	39495	1,4-Difluorobenzene	6.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluorodichloromethane	102	CHCl2F	000075-43-4	10
2			Fluorodichloromethane	102	CHCl2F	000075-43-4	9
3			2H-Pyran, 5,6-dihydro-2-methyl-	98	C6H10O	055230-25-6	9
4			Ethyl 2-butyrate	112	C6H12O2	004341-76-8	9
5			Thiazolidin-4-one, 2-hydroxymeth...	146	C4H6N2O2S	104959-22-0	7



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Instrument :
MSVOA_U
ClientSampleId :
DBER5

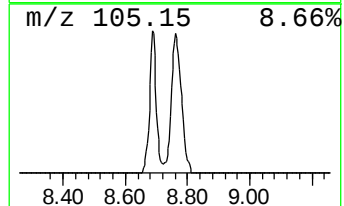
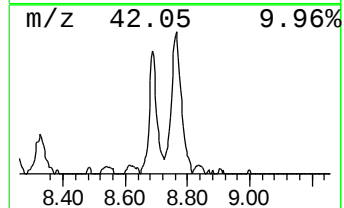
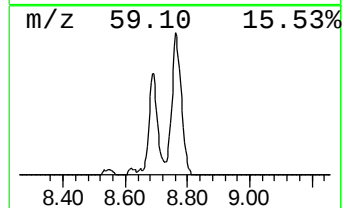
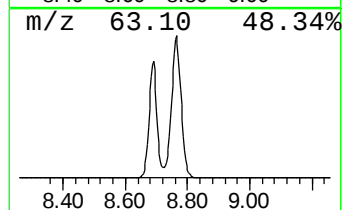
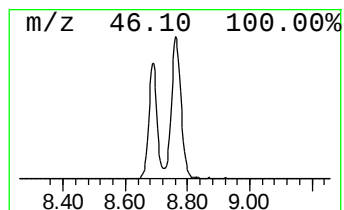
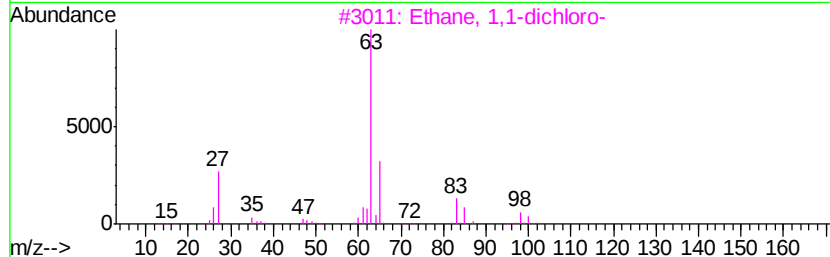
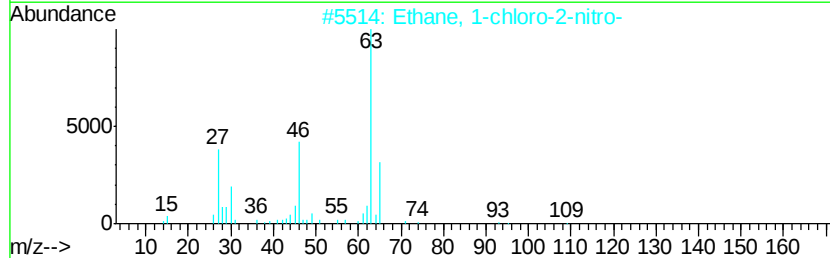
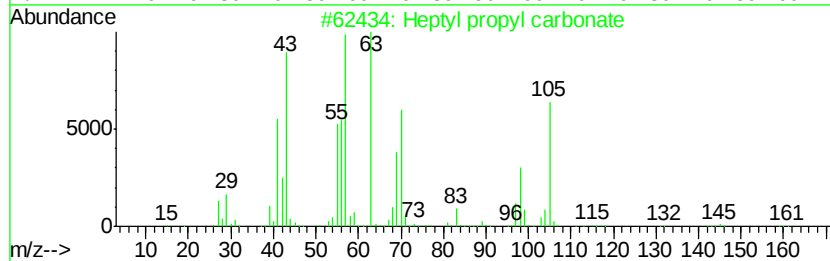
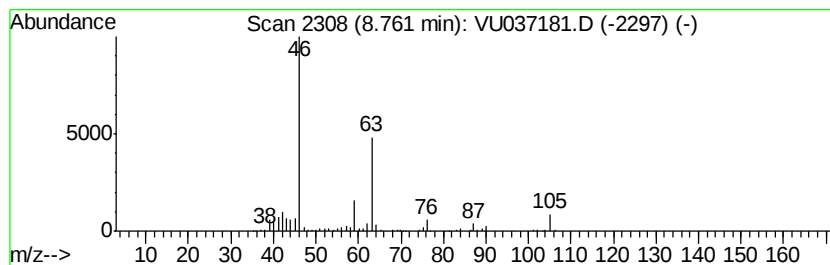
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	4.00 ug/L	222111	Chlorobenzene-d5	9.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptyl propyl carbonate	202	C11H22O3	959272-47-0	38
2		Ethane, 1-chloro-2-nitro-	109	C2H4ClNO2	000625-47-8	33
3		Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	28
4		Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	28
5		1,4-Butanediol, dinitrate	180	C4H8N2O6	003457-91-8	14



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ClientSampleId :
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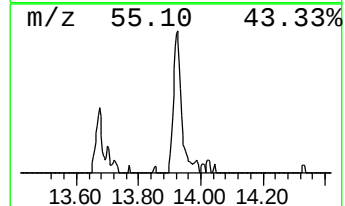
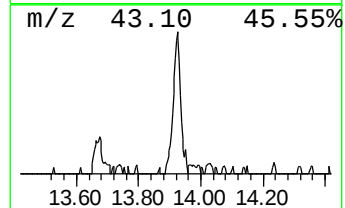
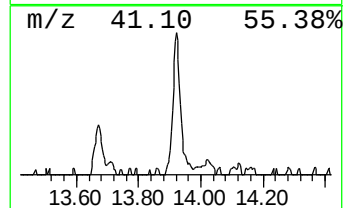
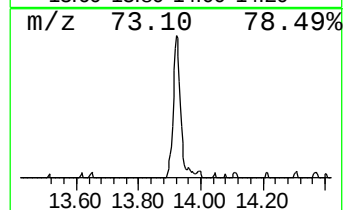
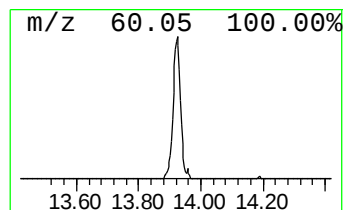
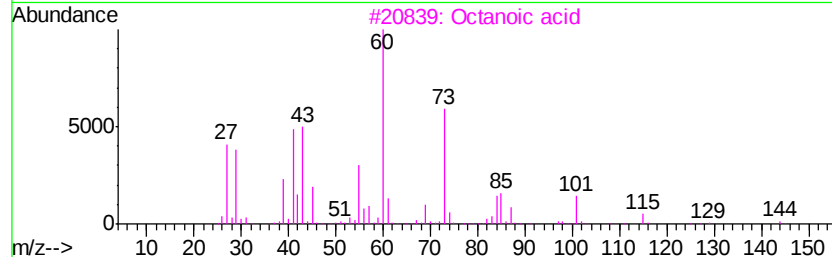
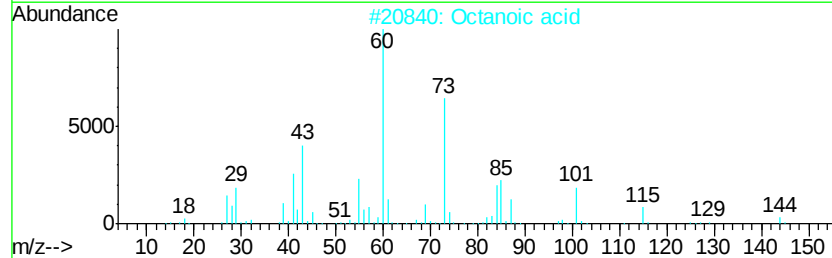
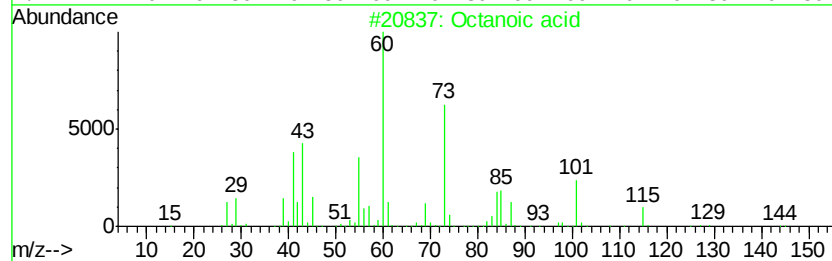
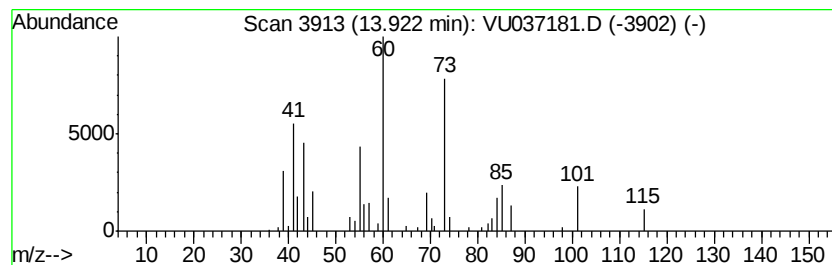
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	0.68 ug/L	47428	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid		144	C8H16O2	000124-07-2	90
2	Octanoic acid		144	C8H16O2	000124-07-2	78
3	Octanoic acid		144	C8H16O2	000124-07-2	72
4	Hexanoic acid		116	C6H12O2	000142-62-1	47
5	Hexanoic acid		116	C6H12O2	000142-62-1	47



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3-difl...	6.55	1.4	ug/L	63574	1	6.35	220671	5.0
unknown-01	6.96	0.9	ug/L	39495	1	6.35	220671	5.0
unknown-02	8.76	4.0	ug/L	222111	2	9.46	277409	5.0
Octanoic acid	13.92	0.7	ug/L	47428	3	11.83	348763	5.0