

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081518\
 Data File : VX004107.D
 Acq On : 16 Aug 2018 07:33
 Operator : JC/MD
 Sample : J4495-10
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS050MW513-180814

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 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_X\METHOD\82X081418W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	75	80	94	rBV	2509436	3212949	100.00%	24.709%
2	1.368	120	128	130	rBV	12582	33836	1.05%	0.260%
3	1.404	131	134	139	rVB	28650	37258	1.16%	0.287%
4	2.270	271	276	285	rBV	24119	42610	1.33%	0.328%
5	2.636	332	336	364	rVB	20071	117992	3.67%	0.907%
6	4.599	647	658	668	rBV2	39087	109515	3.41%	0.842%
7	4.727	668	679	690	rVV3	9116	37612	1.17%	0.289%
8	5.507	795	807	820	rBV	191362	539788	16.80%	4.151%
9	5.666	822	833	855	rVB	259691	727382	22.64%	5.594%
10	6.068	887	899	917	rBV	215168	566985	17.65%	4.360%
11	6.867	1019	1030	1044	rBV	398249	943132	29.35%	7.253%
12	7.556	1136	1143	1150	rBV	32347	64285	2.00%	0.494%
13	7.732	1166	1172	1188	rVB	83175	152228	4.74%	1.171%
14	7.995	1204	1215	1227	rBV4	19540	51227	1.59%	0.394%
15	8.720	1327	1334	1341	rBV	997673	1570344	48.88%	12.077%
16	9.500	1454	1462	1470	rBV	26332	40082	1.25%	0.308%
17	9.586	1470	1476	1481	rBV	29285	44570	1.39%	0.343%
18	10.116	1550	1563	1577	rBV	873189	1180075	36.73%	9.075%
19	10.738	1661	1665	1674	rVB	29358	38390	1.19%	0.295%
20	10.829	1674	1680	1685	rBV	56325	75670	2.36%	0.582%
21	10.933	1691	1697	1707	rVB	22620	38955	1.21%	0.300%
22	11.140	1726	1731	1738	rVB	871649	1086377	33.81%	8.355%
23	11.628	1806	1811	1816	rBV2	57163	83151	2.59%	0.639%
24	11.817	1837	1842	1850	rBV	216021	277388	8.63%	2.133%
25	11.902	1850	1856	1861	rVV2	140066	234382	7.29%	1.802%
26	11.957	1861	1865	1874	rVB	45666	71553	2.23%	0.550%
27	12.079	1879	1885	1893	rBV	1184597	1402666	43.66%	10.787%
28	12.201	1901	1905	1913	rVB	27316	36663	1.14%	0.282%
29	12.750	1990	1995	2002	rBV	24480	37001	1.15%	0.285%
30	12.823	2002	2007	2010	rBV	73962	98856	3.08%	0.760%
31	12.853	2010	2012	2018	rVB	45642	50303	1.57%	0.387%

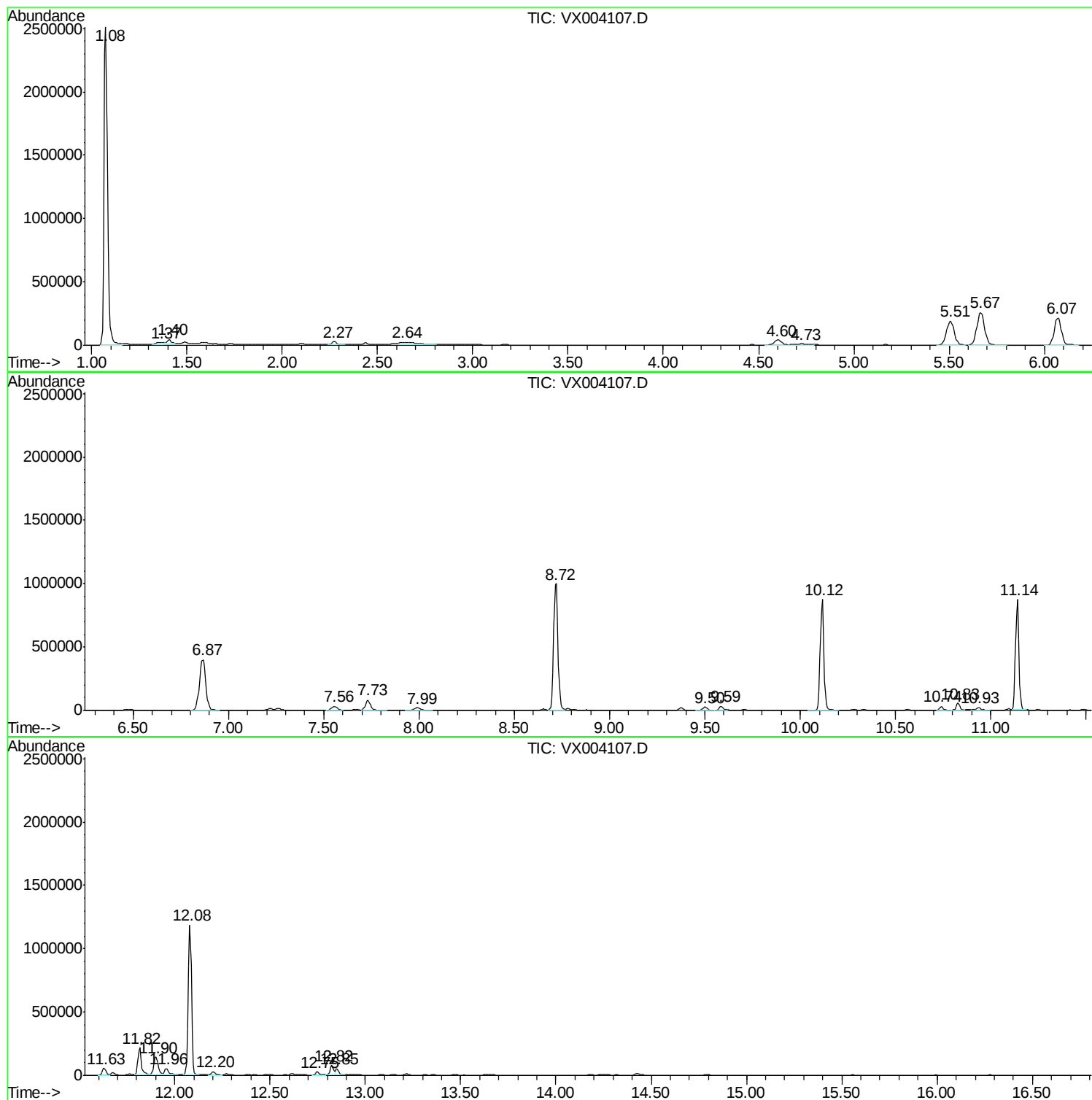
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ClientSampleId :
SS050MW513-180814

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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



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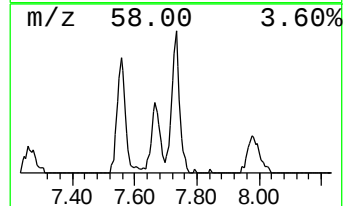
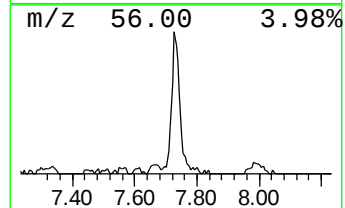
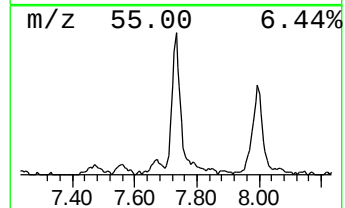
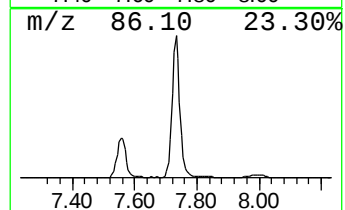
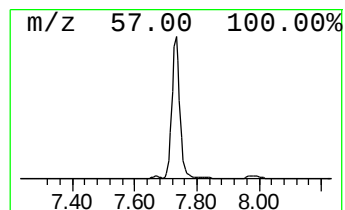
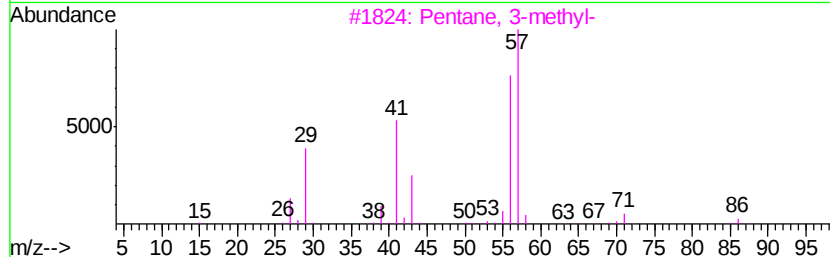
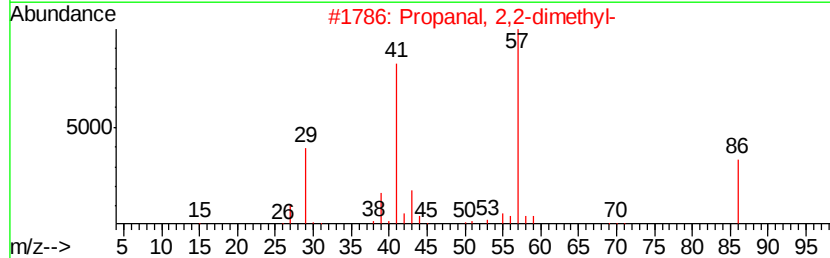
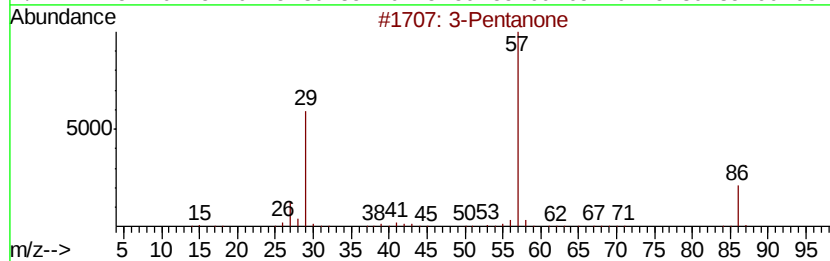
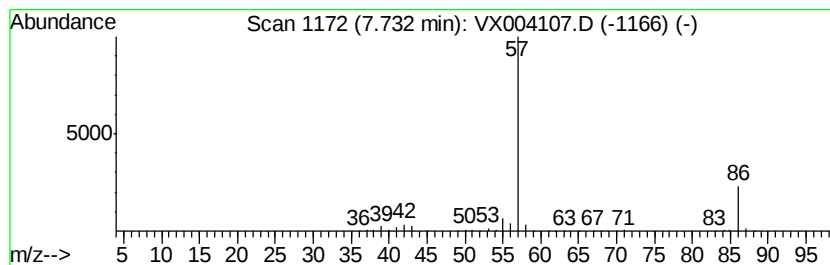
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081418W.M
Quant Title : SW846 8260

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

Peak Number 3 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	8.07 ug/l	152228	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone	86	C5H10O	000096-22-0	86
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	9
4		Neopentane	72	C5H12	000463-82-1	9
5		Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9



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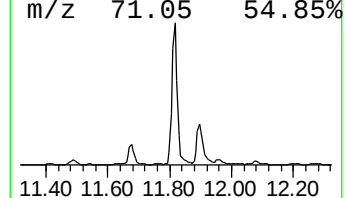
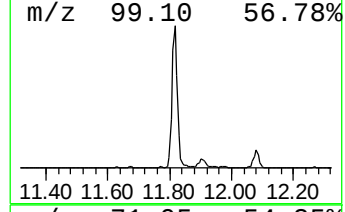
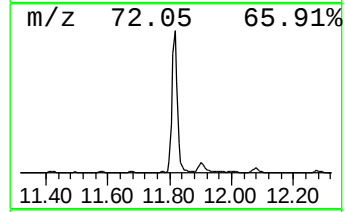
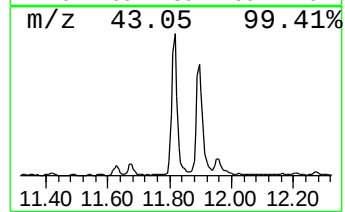
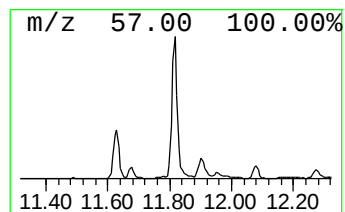
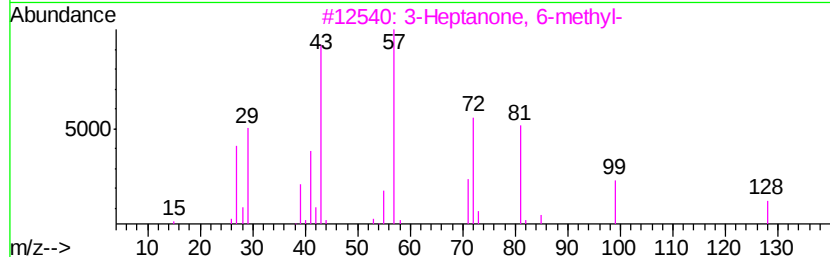
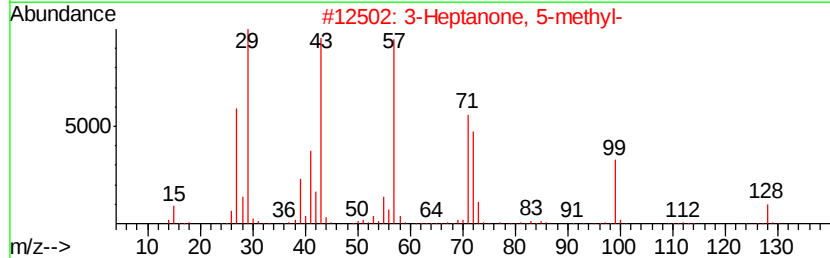
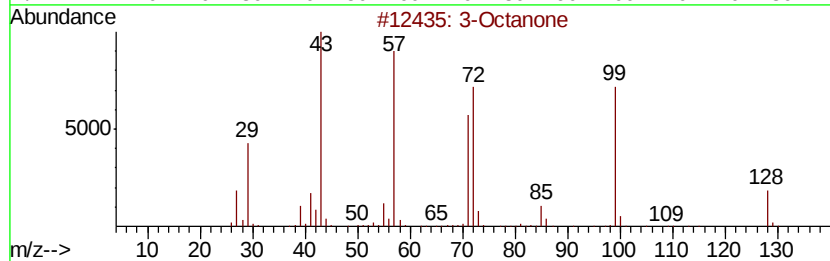
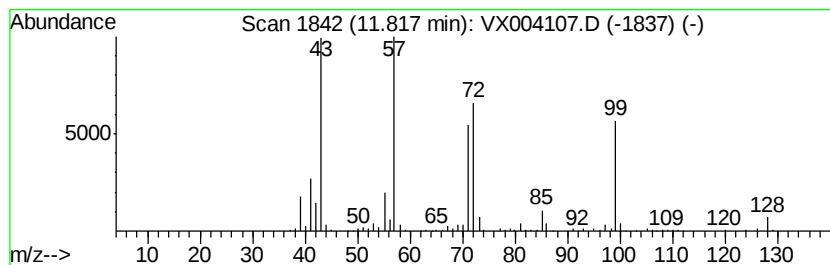
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Peak Number 4 3-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	9.89 ug/l	277388	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Octanone	128 C8H16O	000106-68-3	94
2	3-Heptanone, 5-methyl-	128 C8H16O	000541-85-5	59
3	3-Heptanone, 6-methyl-	128 C8H16O	000624-42-0	47
4	4-Methylthiazole	99 C4H5NS	000693-95-8	46
5	1-Pyrrolidinecarboxaldehyde	99 C5H9NO	003760-54-1	43



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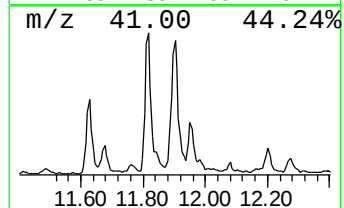
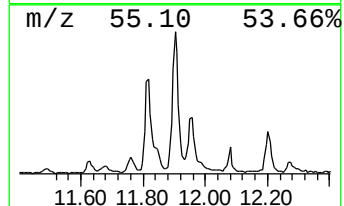
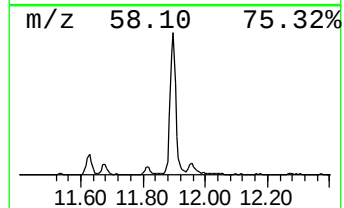
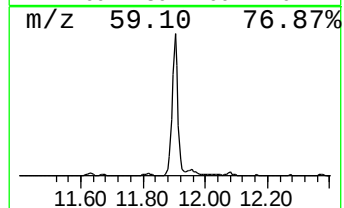
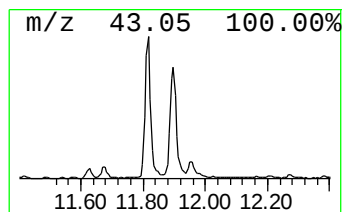
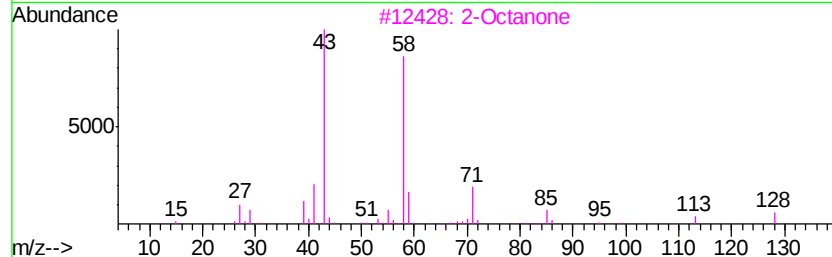
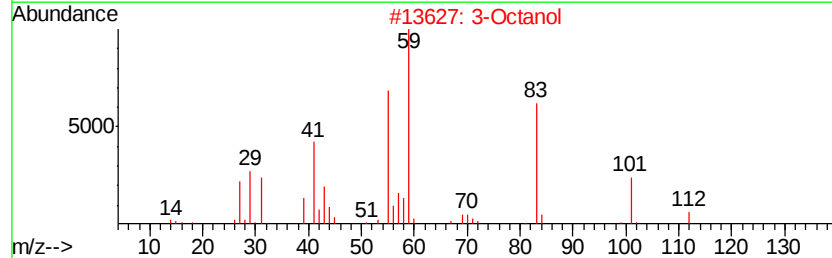
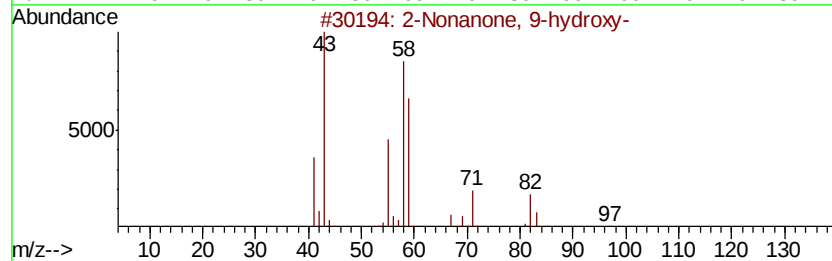
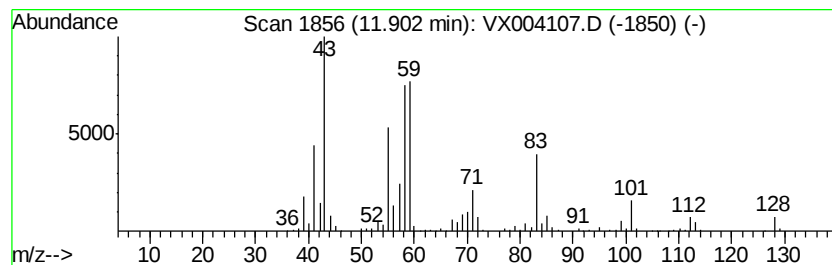
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Peak Number 5 2-Nonanone, 9-hydroxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	8.35 ug/l	234382	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	53
2		3-Octanol	130	C8H18O	000589-98-0	43
3		2-Octanone	128	C8H16O	000111-13-7	43
4		3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	38
5		3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone	7.73	8.1	ug/l	152228	2	6.87	943132	50.0
3-Octanone	11.82	9.9	ug/l	277388	4	12.08	1402670	50.0
2-Nonanone, 9-hyd...	11.90	8.3	ug/l	234382	4	12.08	1402670	50.0