

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX070218\
 Data File : VX003130.D
 Acq On : 02 Jul 2018 16:37
 Operator : JC/MD
 Sample : J3787-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SP18-CHY07

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\82X062518W.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	76	80	93	rBV	1069863	1415952	100.00%	14.943%
2	1.276	108	113	123	rBV	44133	100255	7.08%	1.058%
3	1.398	128	133	142	rVB3	15774	31499	2.22%	0.332%
4	2.001	227	232	239	rVB	30997	47384	3.35%	0.500%
5	2.453	300	306	310	rBV	15646	28414	2.01%	0.300%
6	2.623	328	334	341	rVB	34219	61594	4.35%	0.650%
7	4.605	648	659	669	rBV2	14528	46674	3.30%	0.493%
8	5.507	793	807	821	rBV	174110	497882	35.16%	5.254%
9	5.665	822	833	848	rVB	258609	736135	51.99%	7.769%
10	6.074	886	900	918	rBV	182579	476082	33.62%	5.024%
11	6.866	1020	1030	1043	rBV	369526	860940	60.80%	9.086%
12	7.220	1081	1088	1094	rBV	15233	34790	2.46%	0.367%
13	8.720	1326	1334	1344	rBV	883694	1362069	96.19%	14.375%
14	9.585	1470	1476	1488	rBV	19712	30421	2.15%	0.321%
15	10.116	1554	1563	1574	rBV	777991	1028351	72.63%	10.853%
16	10.829	1675	1680	1686	rBV	20445	26336	1.86%	0.278%
17	10.939	1696	1698	1707	rVB	14048	18825	1.33%	0.199%
18	11.140	1724	1731	1741	rBV	783081	984287	69.51%	10.388%
19	11.817	1838	1842	1847	rBV2	18517	23902	1.69%	0.252%
20	11.896	1850	1855	1861	rBV	143565	191729	13.54%	2.023%
21	11.957	1861	1865	1875	rVB	167910	208387	14.72%	2.199%
22	12.079	1880	1885	1895	rVB	905550	1184078	83.62%	12.496%
23	12.829	2001	2008	2010	rBV	17975	27177	1.92%	0.287%
24	12.853	2010	2012	2020	rVB2	29818	37630	2.66%	0.397%
25	13.664	2140	2145	2153	rVB3	8997	14671	1.04%	0.155%

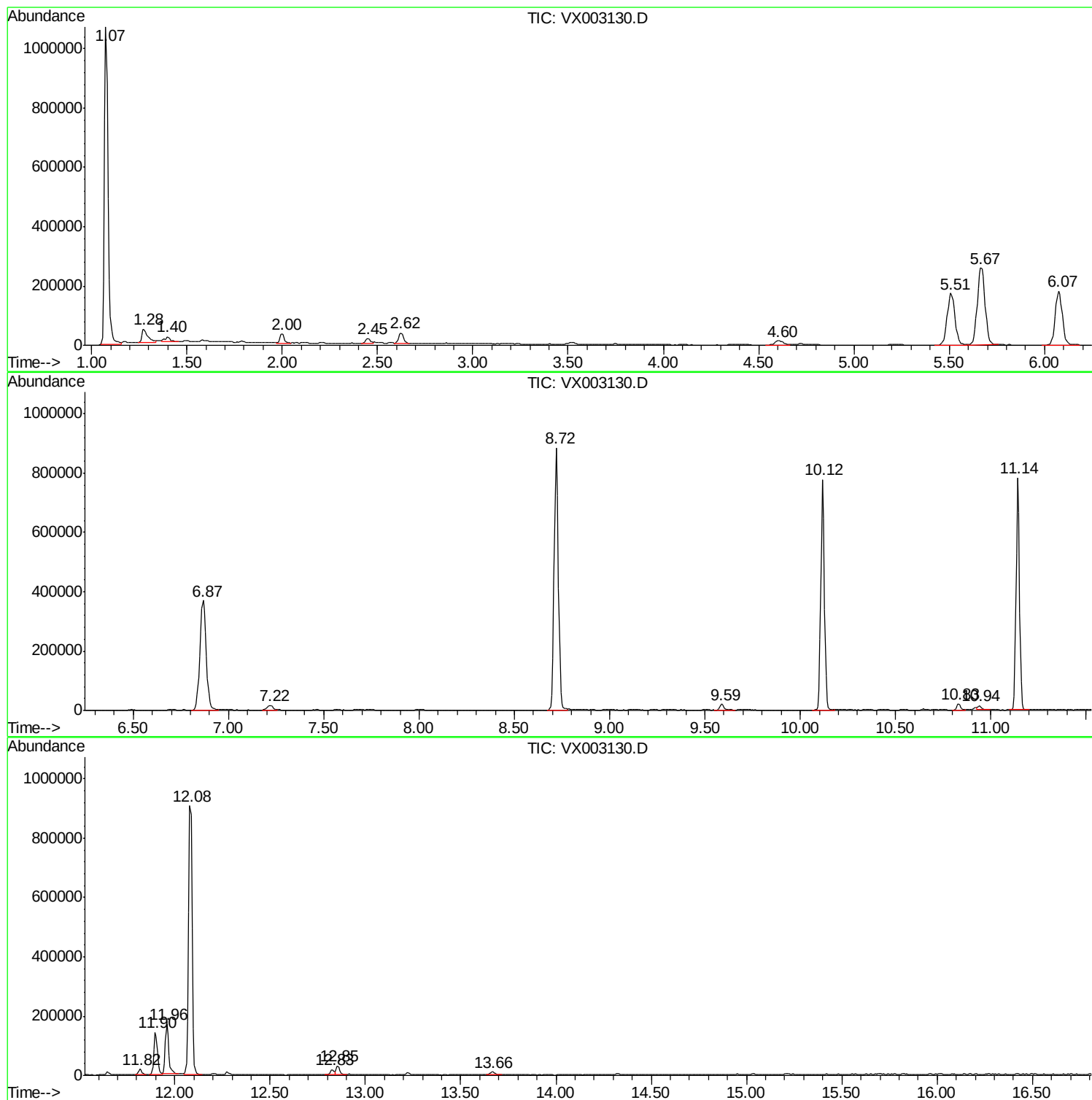
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Quant Title : SW846 8260

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



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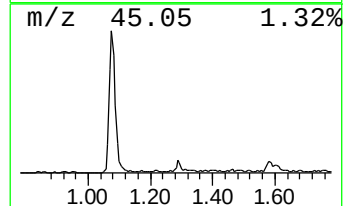
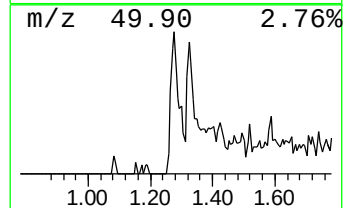
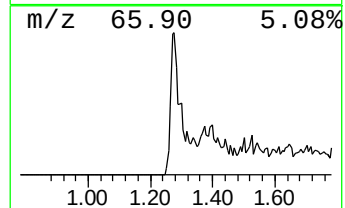
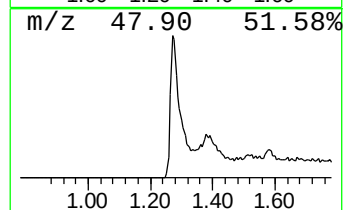
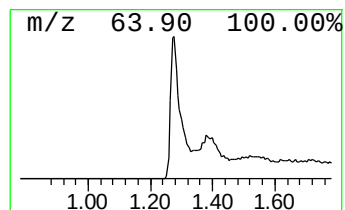
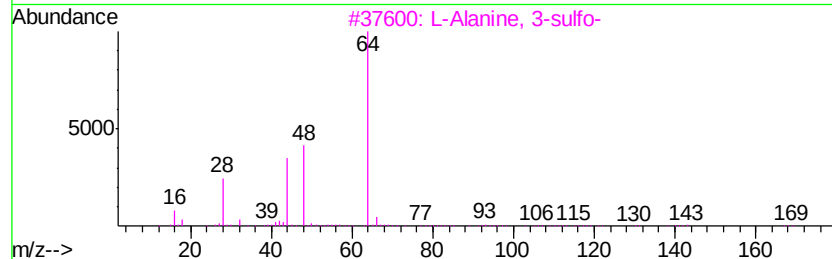
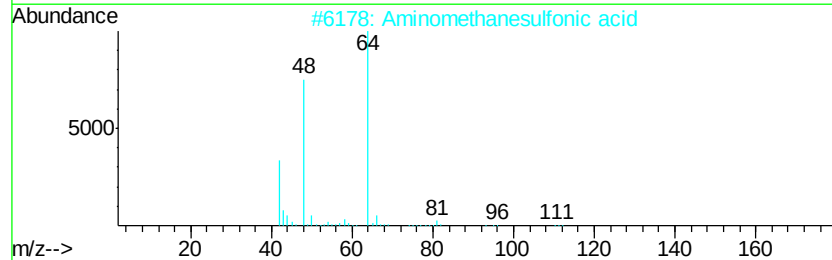
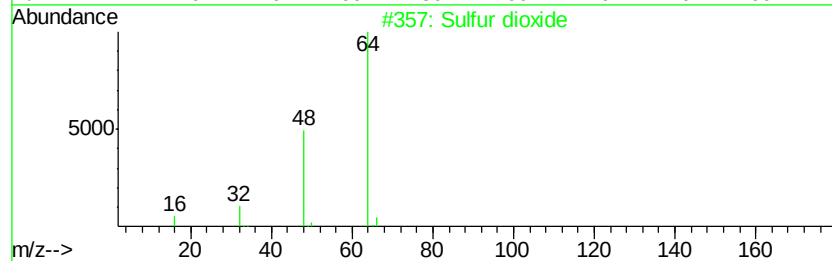
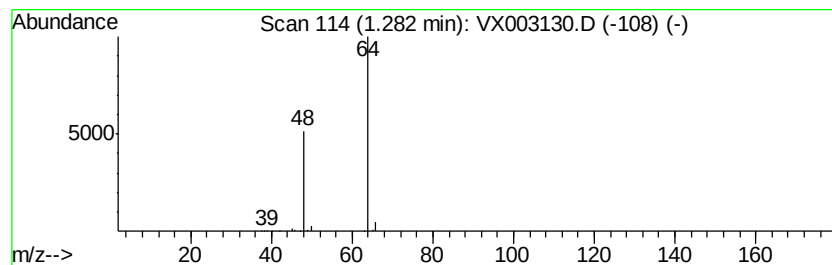
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	6.81 ug/l	100255	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-		64	C2H2F2	000075-38-7	4
5	Ethyl Chloride		64	C2H5Cl	000075-00-3	3



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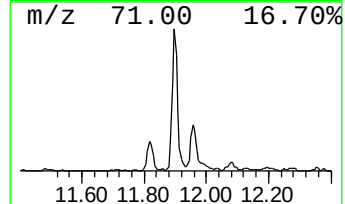
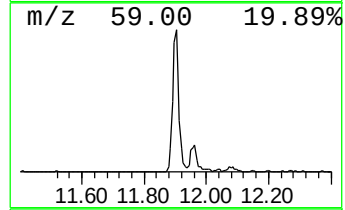
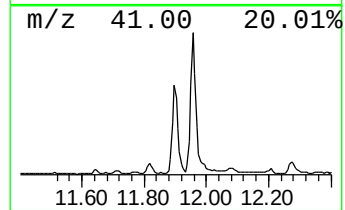
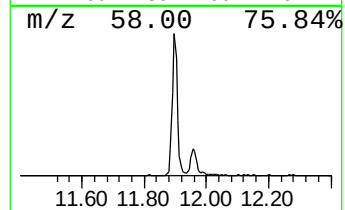
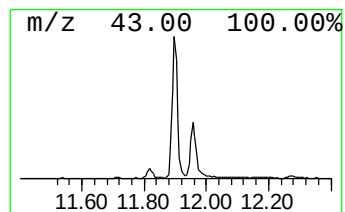
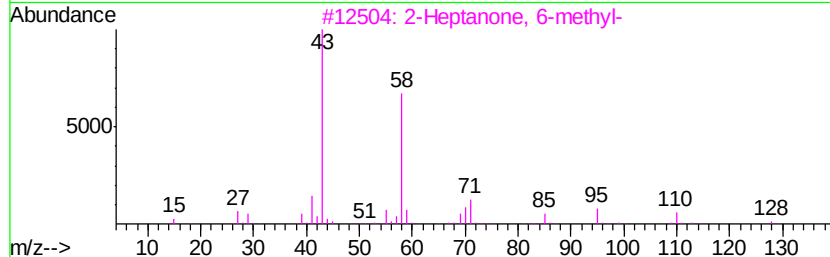
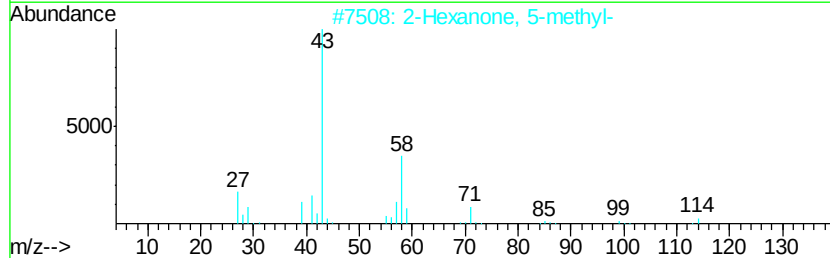
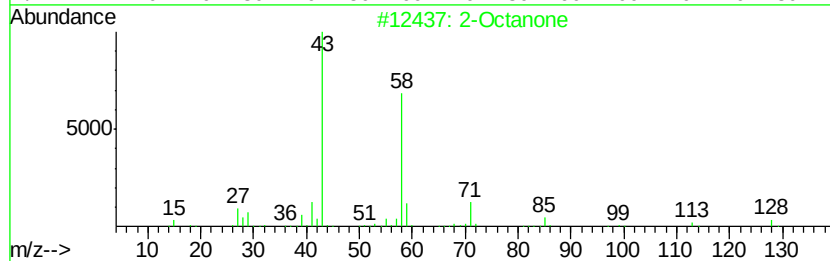
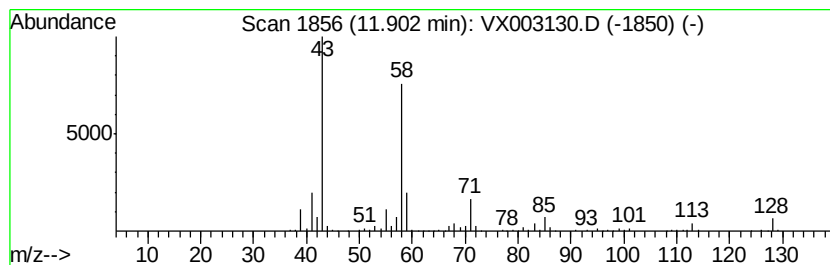
Instrument :
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ClientSampled :
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Peak Number 3 2-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	8.10 ug/l	191729	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Octanone	128 C8H16O	000111-13-7	91
2	2-Hexanone, 5-methyl-	114 C7H14O	000110-12-3	78
3	2-Heptanone, 6-methyl-	128 C8H16O	000928-68-7	56
4	2-Heptanone	114 C7H14O	000110-43-0	56
5	2-Nonanone	142 C9H18O	000821-55-6	56



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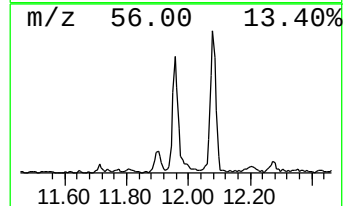
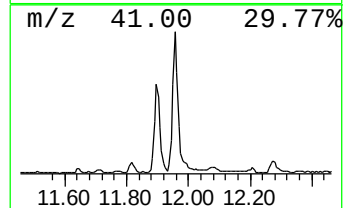
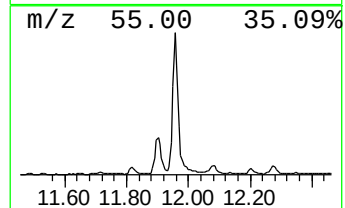
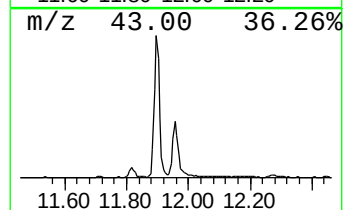
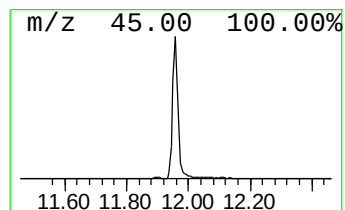
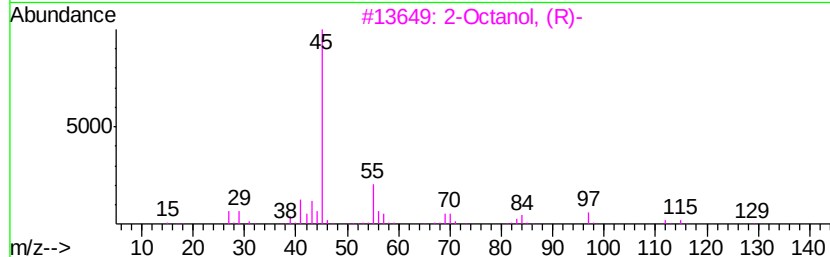
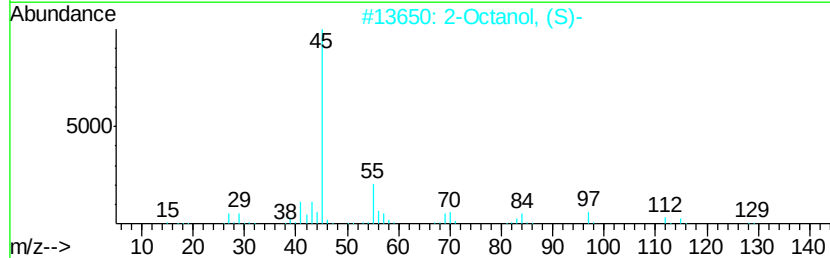
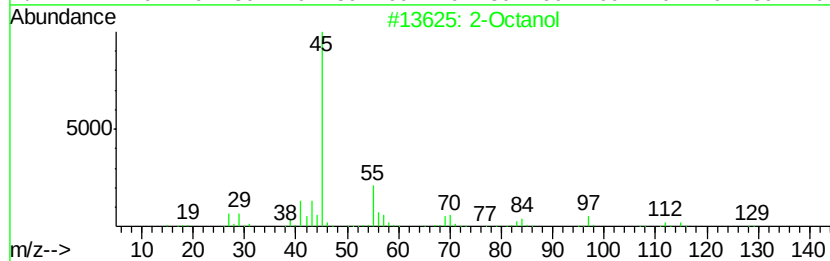
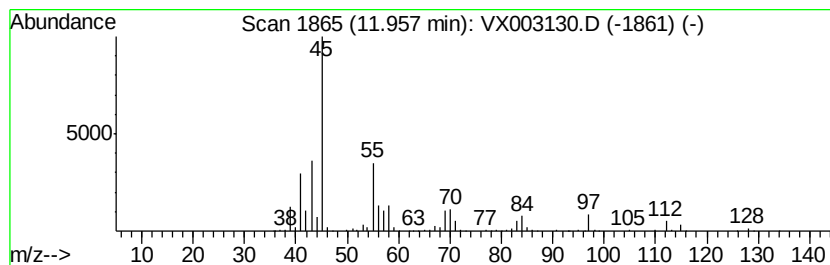
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Peak Number 4 2-Octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	8.80 ug/l	208387	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanol	130	C8H18O	000123-96-6	86
2		2-Octanol, (S)-	130	C8H18O	006169-06-8	78
3		2-Octanol, (R)-	130	C8H18O	005978-70-1	78
4		2-Decanol	158	C10H22O	001120-06-5	64
5		2-Nonanol	144	C9H20O	000628-99-9	64



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.28	6.8	ug/l	100255	1	5.67	736135	50.0
2-Octanone	11.90	8.1	ug/l	191729	4	12.09	1184080	50.0
2-Octanol	11.96	8.8	ug/l	208387	4	12.09	1184080	50.0