

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062522\
 Data File : VN073132.D
 Acq On : 26 Jun 2022 02:05
 Operator : JC\MD
 Sample : N3494-06
 Misc : 4.99g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SP-EXC-1-4

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_N\methods\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN073132.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.405	79	88	97	rBV2	10978	22098	1.07%	0.169%
2	3.328	239	245	256	rVB4	19652	51538	2.50%	0.393%
3	4.769	479	490	507	rBV	120442	393259	19.05%	2.999%
4	5.222	552	567	578	rBV3	20567	90780	4.40%	0.692%
5	5.993	687	698	708	rVB6	12495	42607	2.06%	0.325%
6	7.287	911	918	926	rBV3	16545	48009	2.33%	0.366%
7	7.945	1019	1030	1035	rBV	210637	531279	25.74%	4.052%
8	8.010	1035	1041	1050	rVB	416762	958902	46.46%	7.313%
9	8.363	1092	1101	1115	rBV2	235796	563238	27.29%	4.295%
10	8.745	1160	1166	1172	rBV5	18807	40836	1.98%	0.311%
11	8.898	1183	1192	1200	rBV	582034	1202318	58.25%	9.169%
12	9.381	1266	1274	1281	rBV6	20445	53421	2.59%	0.407%
13	10.375	1433	1443	1450	rBV	810293	1512655	73.29%	11.536%
14	10.439	1450	1454	1460	rVB	36654	63173	3.06%	0.482%
15	10.586	1476	1479	1487	rVB2	43092	76770	3.72%	0.585%
16	10.716	1497	1501	1506	rBV7	13787	22203	1.08%	0.169%
17	11.680	1659	1665	1677	rVB2	906748	2063905	100.00%	15.740%
18	11.780	1679	1682	1686	rVV	23023	33057	1.60%	0.252%
19	11.892	1695	1701	1707	rBV2	121375	281406	13.63%	2.146%
20	12.669	1827	1833	1839	rBV	830153	1405782	68.11%	10.721%
21	12.833	1859	1861	1862	rBV2	43949	39358	1.91%	0.300%
22	13.221	1924	1927	1931	rBV3	51082	71627	3.47%	0.546%
23	13.610	1987	1993	2002	rBV	1042120	1795752	87.01%	13.695%
24	13.927	2044	2047	2055	rVB4	217258	368521	17.86%	2.810%
25	14.445	2131	2135	2139	rBV5	91807	132797	6.43%	1.013%
26	14.610	2159	2163	2166	rBV5	60320	93621	4.54%	0.714%
27	14.904	2209	2213	2220	rVB2	161558	310556	15.05%	2.368%
28	15.398	2293	2297	2307	rBV3	153130	338063	16.38%	2.578%
29	15.810	2363	2367	2374	rVB5	134511	250509	12.14%	1.910%
30	16.374	2459	2463	2472	rVB2	125627	254777	12.34%	1.943%

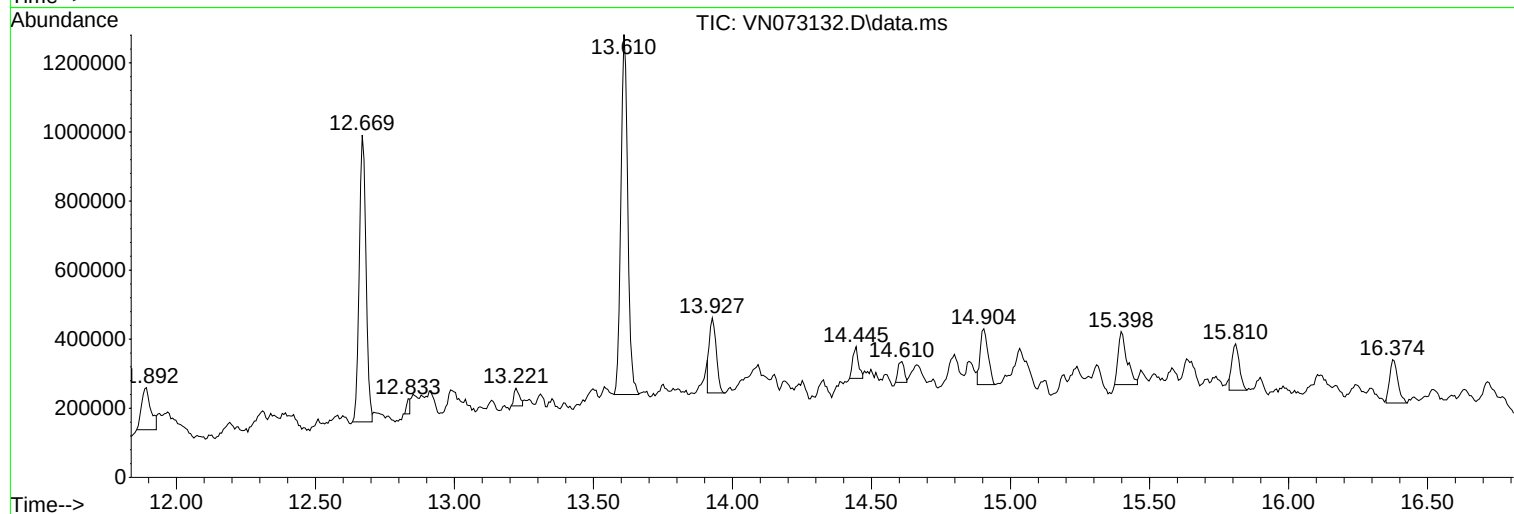
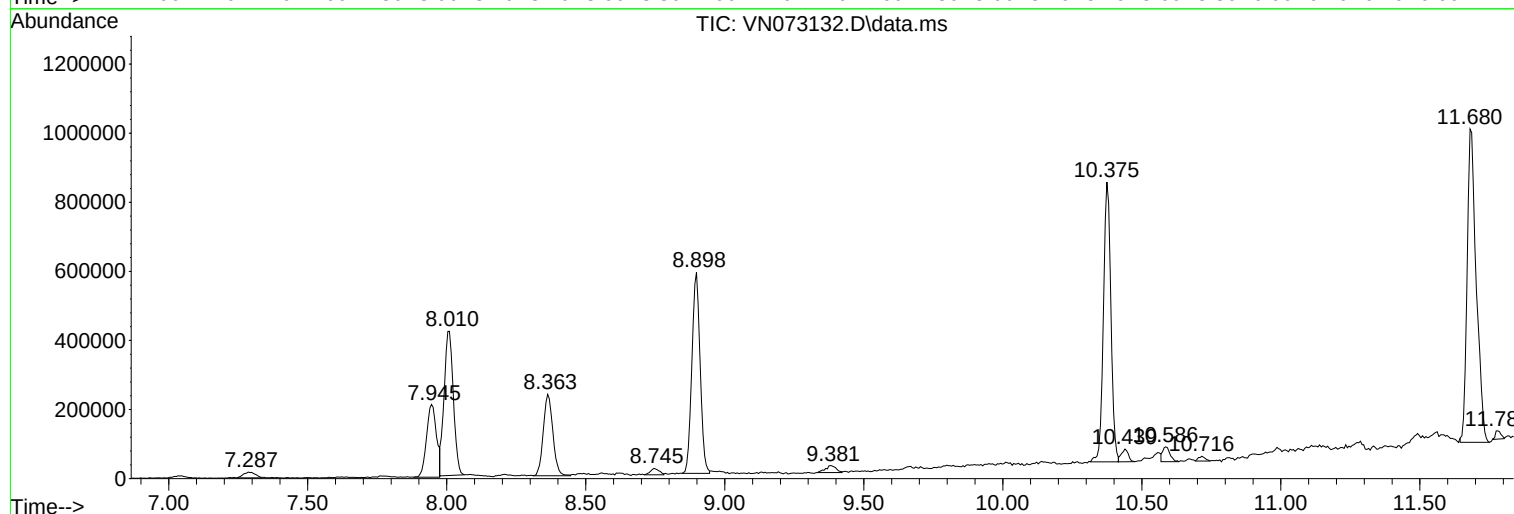
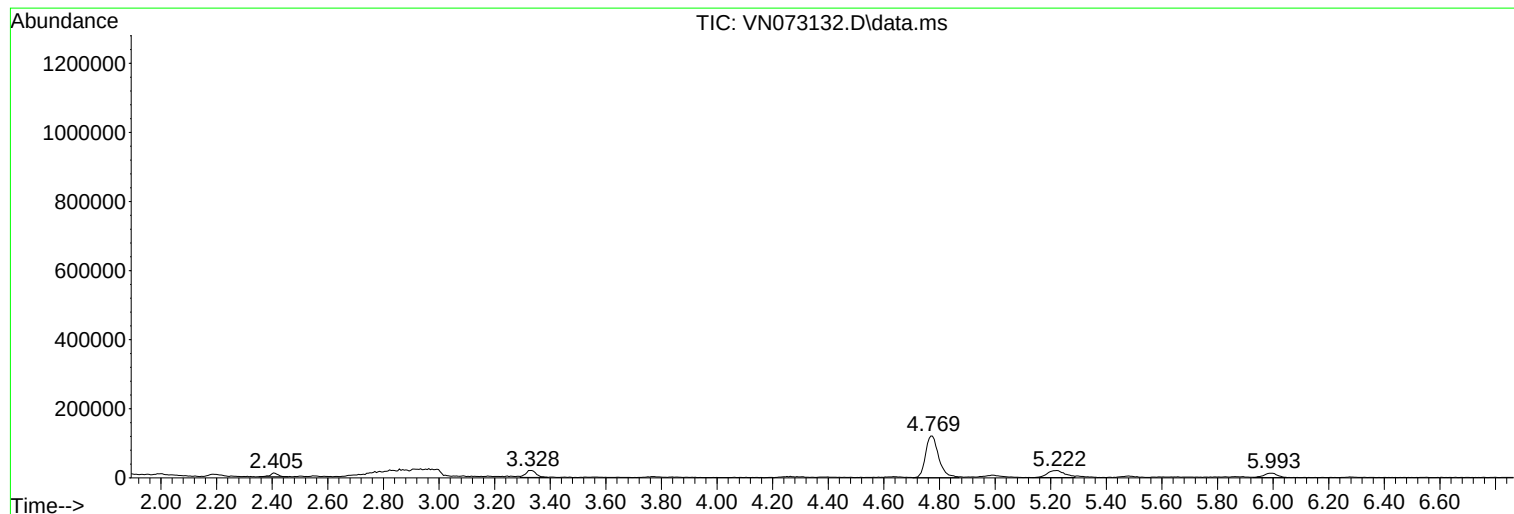
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Instrument :
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ClientSampleId :
SP-EXC-1-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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



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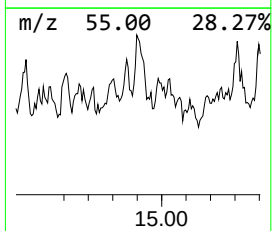
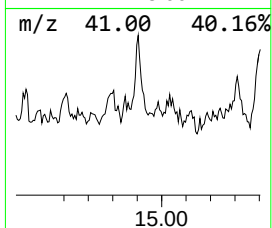
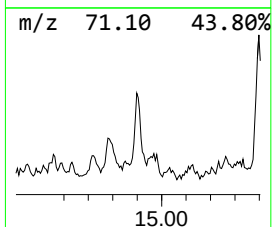
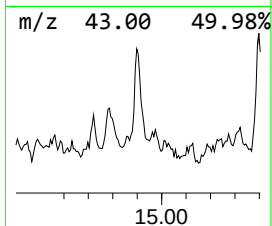
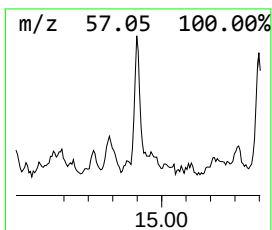
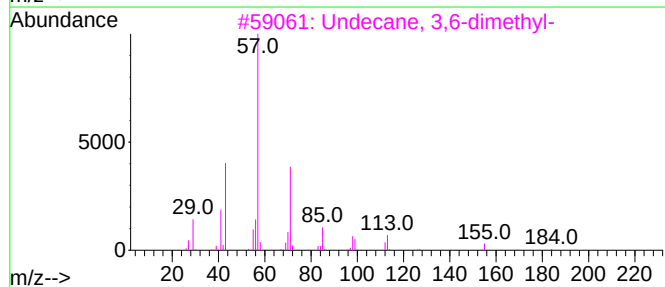
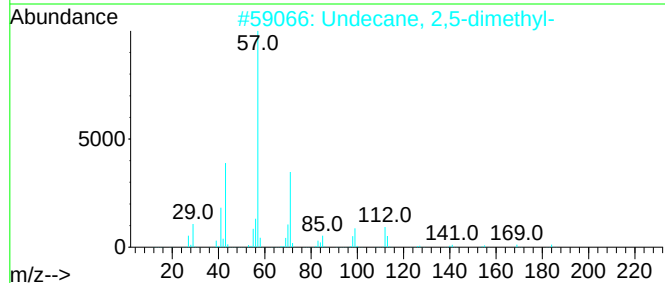
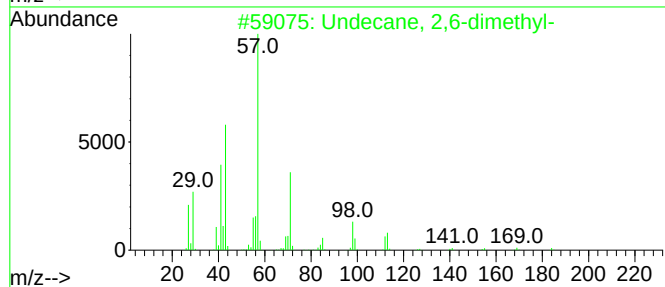
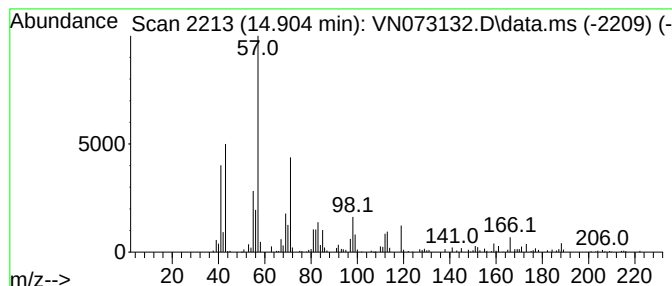
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	8.65 ug/l	310556	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	87
2			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	76
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
4			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	59
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	47



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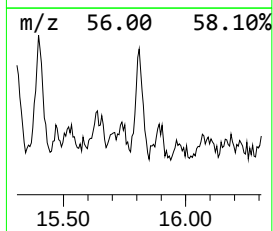
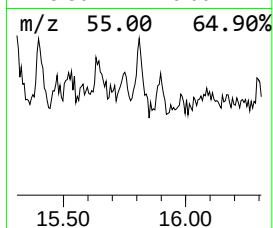
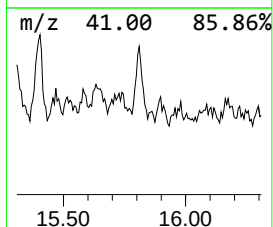
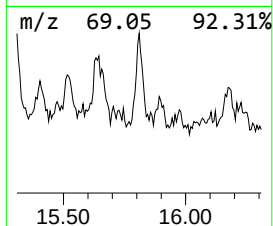
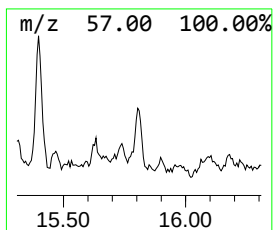
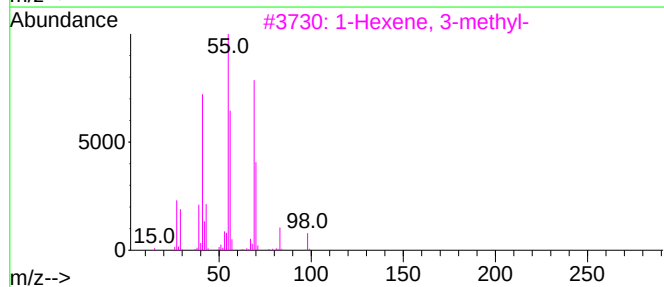
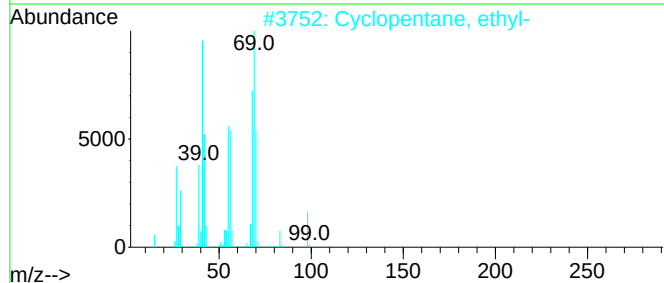
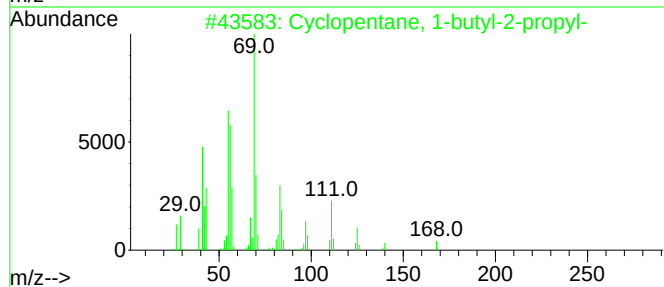
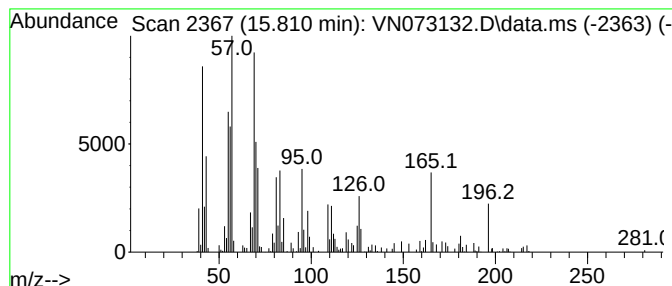
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown15.810 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.810	6.98 ug/l	250509	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	42
2			Cyclopentane, ethyl-	98	C7H14	001640-89-7	38
3			1-Hexene, 3-methyl-	98	C7H14	003404-61-3	35
4			Cyclohexanone, 3,5-dimethyl-	126	C8H14O	002320-30-1	30
5			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	27



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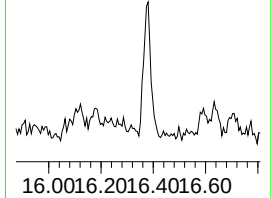
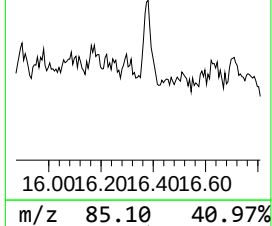
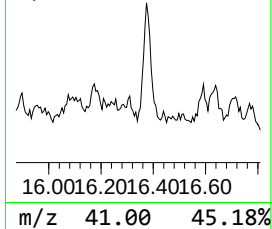
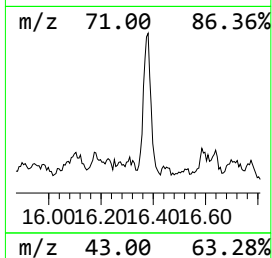
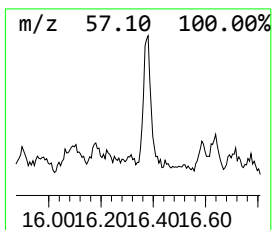
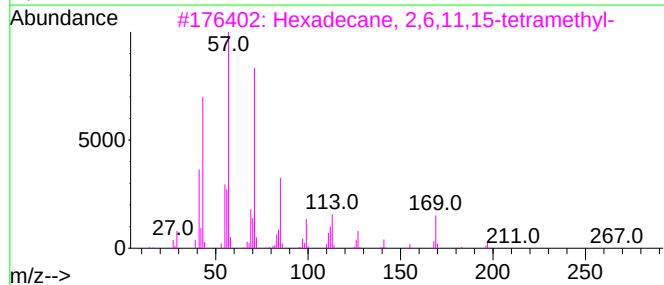
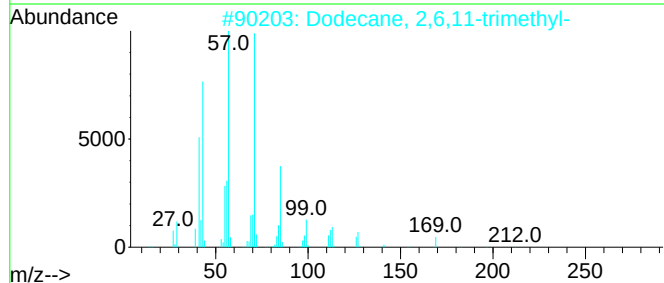
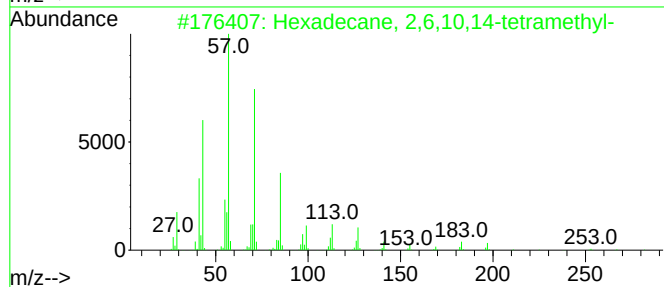
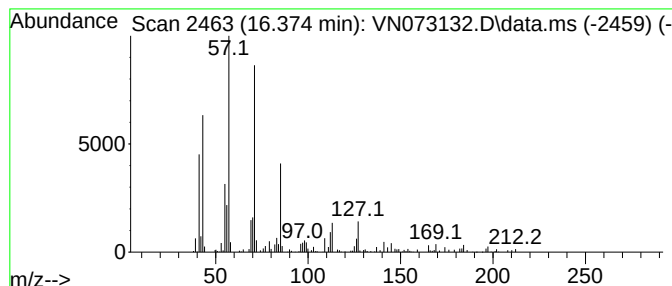
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Quant Title : SW846 8260

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

Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.374	7.09 ug/l	254777	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	87
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	80
4			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	80
5			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	80



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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
Undecane, 2,6-d...	14.904	8.7	ug/l	310556	4	13.610	1795750	50.0
unknown15.810	15.810	7.0	ug/l	250509	4	13.610	1795750	50.0
Hexadecane, 2,6...	16.374	7.1	ug/l	254777	4	13.610	1795750	50.0