

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011224\
 Data File : VN080700.D
 Acq On : 12 Jan 2024 19:17
 Operator : JC\MD
 Sample : P1111-06
 Misc : 2.75g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRYER-6

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\82N011024W.M

Title : SW846 8260

Signal : TIC: VN080700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.842	139	151	152	rBV7	27942	69810	6.12%	0.982%
2	2.865	152	155	156	rVV3	11148	12714	1.11%	0.179%
3	6.294	727	738	753	rBV2	179617	550855	48.31%	7.746%
4	8.165	1047	1056	1060	rBV2	123711	298008	26.13%	4.190%
5	8.218	1060	1065	1077	rVB2	230360	524407	45.99%	7.374%
6	8.577	1116	1126	1138	rBV2	142733	321058	28.16%	4.515%
7	9.100	1206	1215	1224	rBV	413790	850264	74.57%	11.956%
8	10.565	1455	1464	1473	rBV	544911	1031679	90.48%	14.507%
9	11.282	1580	1586	1592	rBV3	7156	14412	1.26%	0.203%
10	11.865	1675	1685	1694	rBV	630103	1140291	100.00%	16.034%
11	12.853	1845	1853	1863	rVB	400782	700045	61.39%	9.844%
12	13.335	1928	1935	1942	rBV2	13231	26444	2.32%	0.372%
13	13.688	1988	1995	1998	rBV5	7502	13538	1.19%	0.190%
14	13.794	2005	2013	2023	rBV	607353	1011379	88.69%	14.222%
15	14.176	2073	2078	2083	rVV3	11466	18532	1.63%	0.261%
16	14.612	2146	2152	2158	rBV3	12805	24235	2.13%	0.341%
17	14.965	2206	2212	2219	rBV2	26066	42139	3.70%	0.593%
18	15.076	2229	2231	2240	rVB10	9797	15136	1.33%	0.213%
19	15.406	2280	2287	2288	rBV5	8205	14716	1.29%	0.207%
20	15.517	2301	2306	2312	rVB7	13469	27414	2.40%	0.385%
21	15.594	2313	2319	2327	rBV2	25175	46840	4.11%	0.659%
22	15.835	2353	2360	2366	rVB2	86796	150941	13.24%	2.122%
23	15.959	2373	2381	2382	rBV7	7479	18539	1.63%	0.261%
24	16.176	2412	2418	2421	rBV6	15628	28042	2.46%	0.394%
25	16.317	2435	2442	2444	rBV8	9265	20461	1.79%	0.288%
26	16.476	2462	2469	2476	rBV3	37651	92573	8.12%	1.302%
27	16.541	2478	2480	2486	rVV7	12330	21008	1.84%	0.295%
28	16.617	2489	2493	2500	rVB8	13543	26104	2.29%	0.367%

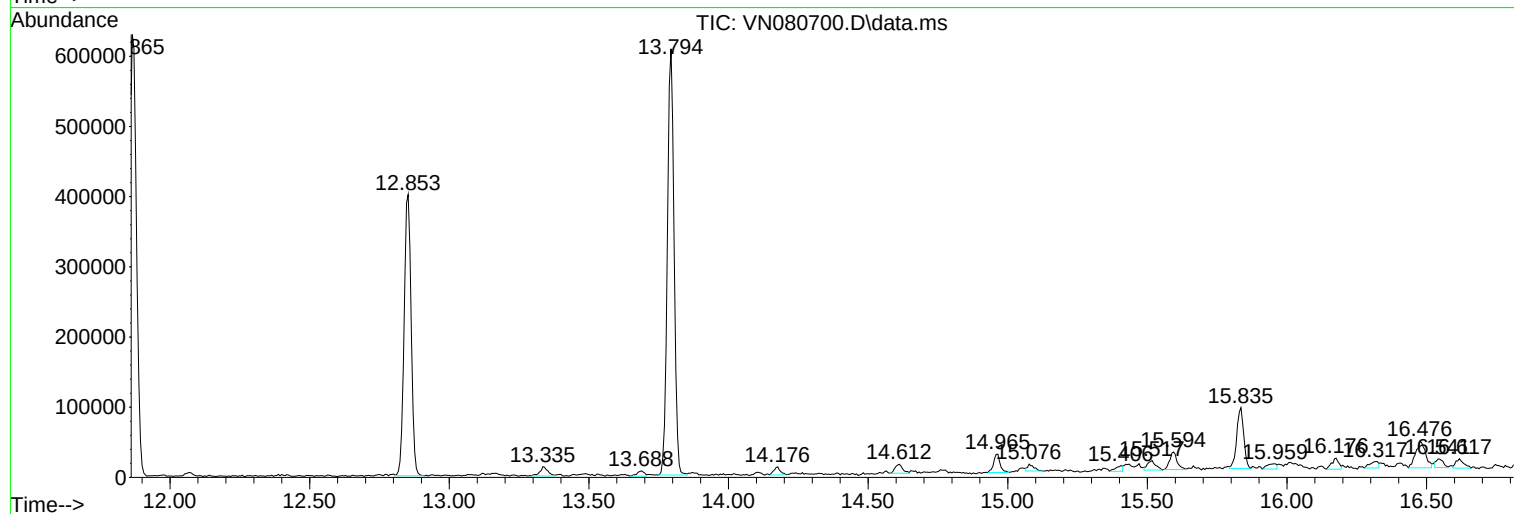
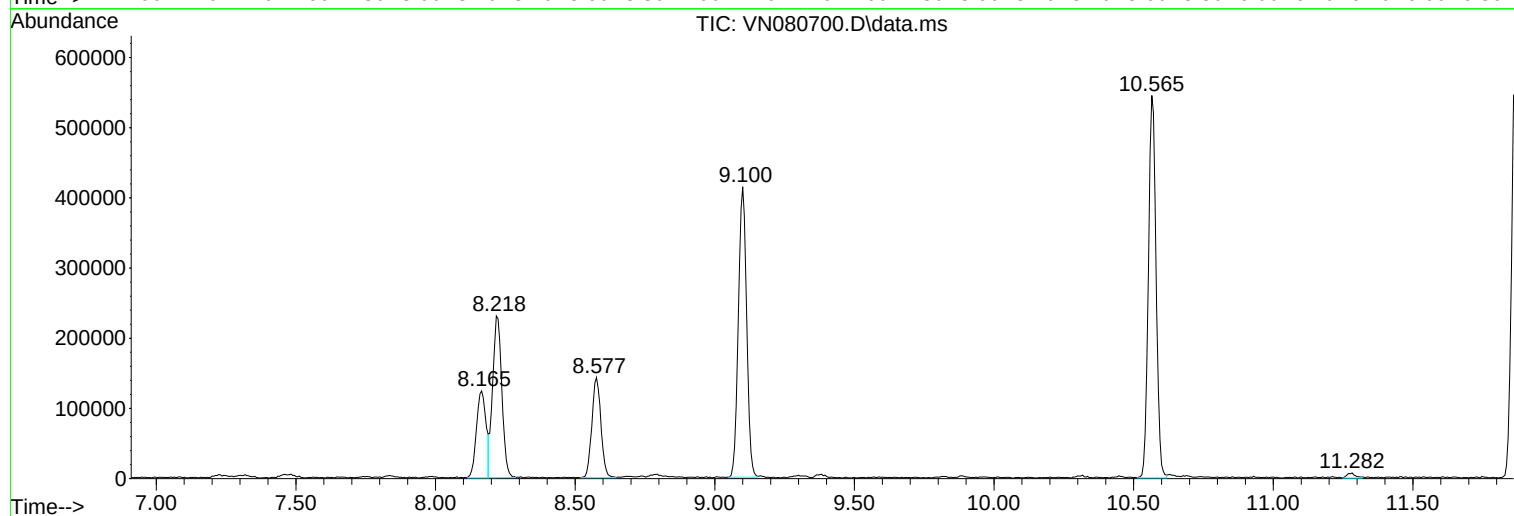
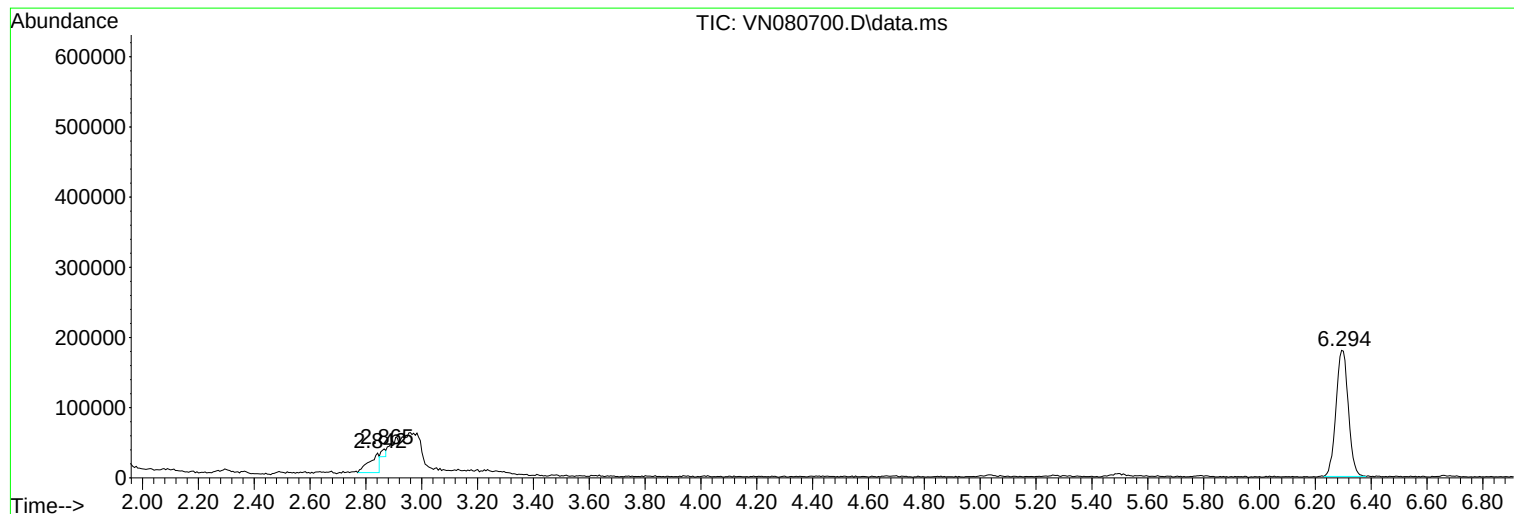
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Instrument :
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ClientSampleId :
DRYER-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011024W.M
Quant Title : SW846 8260

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



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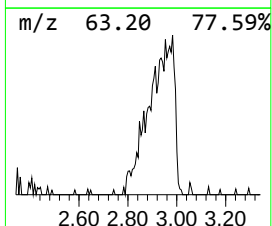
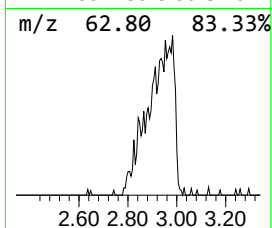
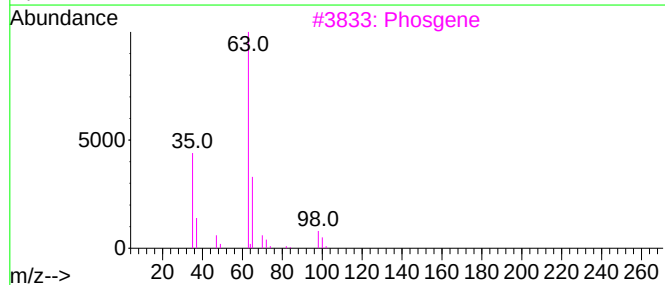
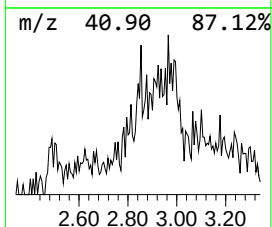
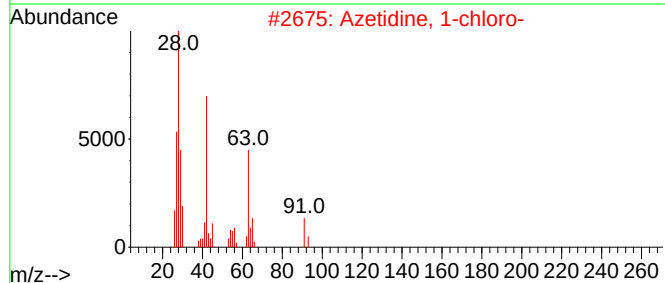
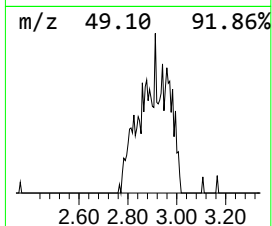
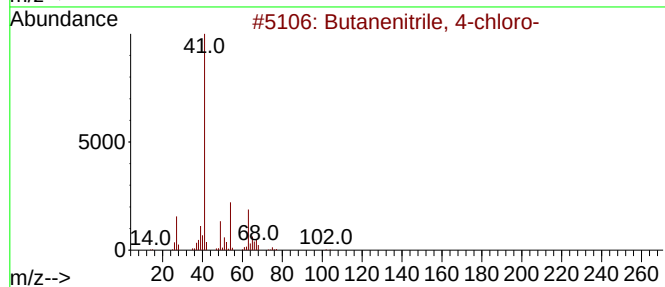
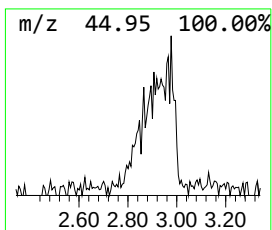
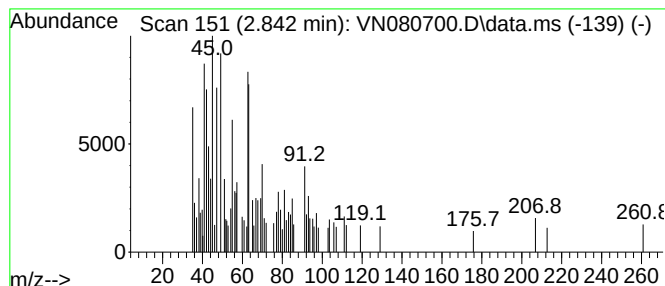
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011024W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.842 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.842	6.66 ug/l	69810	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanenitrile, 4-chloro-	103	C4H6ClN	000628-20-6	40
2			Azetidine, 1-chloro-	91	C3H6ClN	032115-53-0	22
3			Phosgene	98	CCl2O	000075-44-5	16
4			Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	14
5			2,3-Dichloropropionitrile	123	C3H3Cl2N	002601-89-0	12



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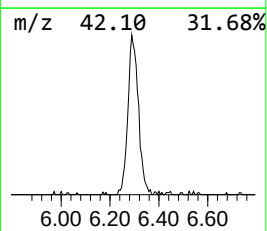
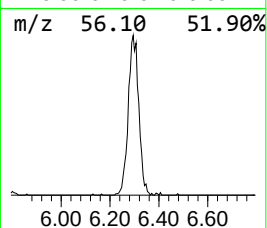
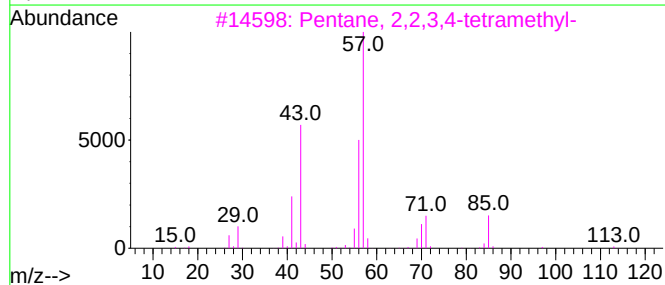
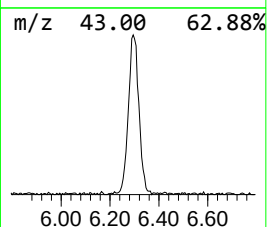
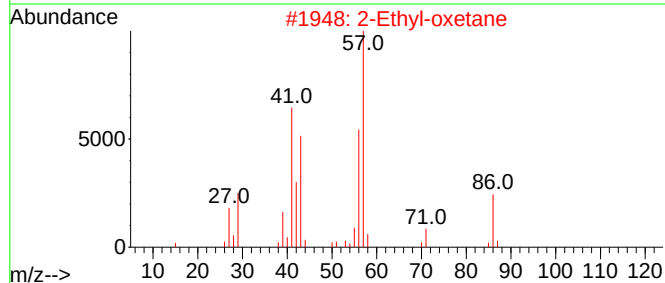
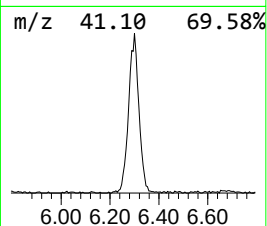
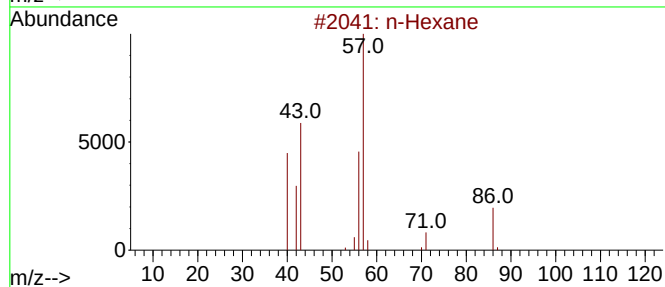
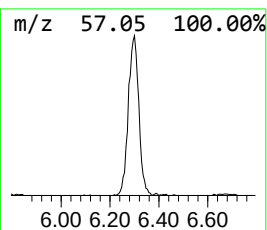
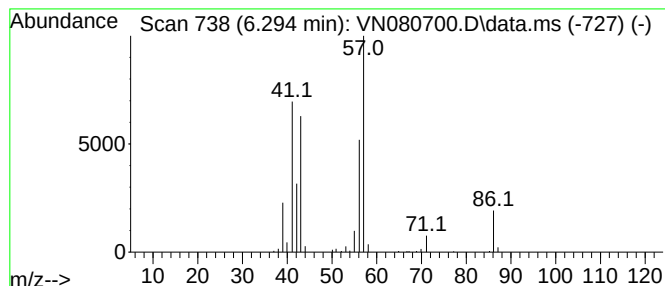
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011024W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Hexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.294	52.52 ug/l	550855	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	87
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	74
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	47
4			Pentane, 3-methyl-	86	C6H14	000096-14-0	40
5			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	38



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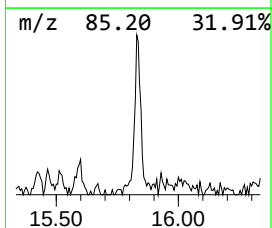
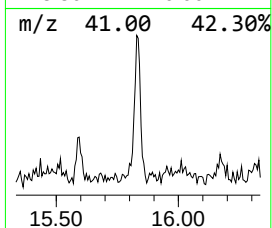
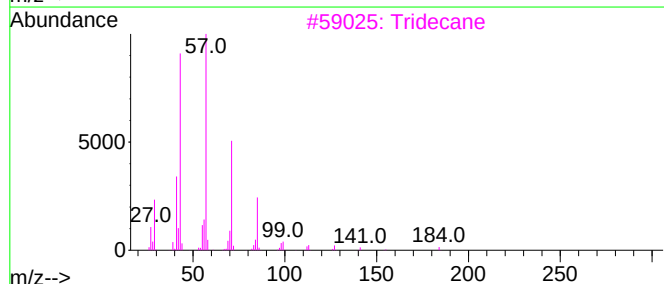
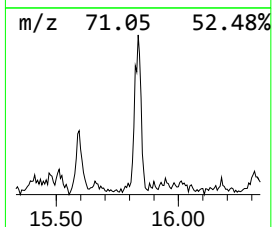
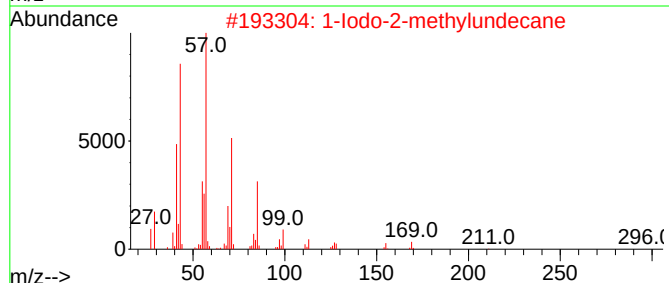
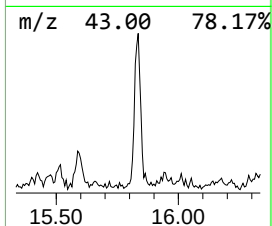
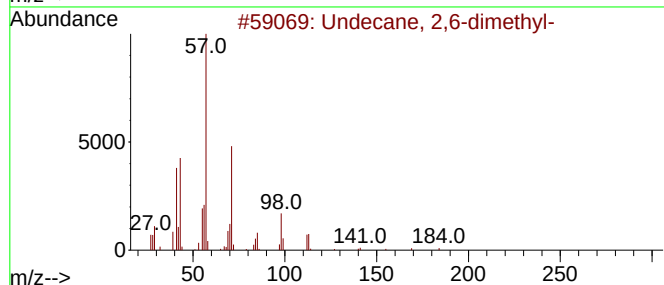
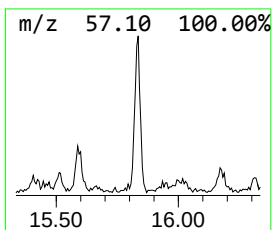
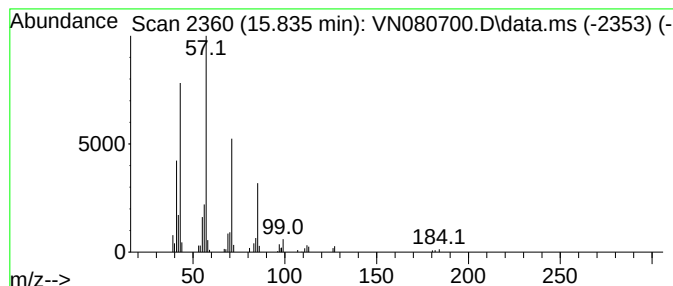
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Undecane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	7.46 ug/l	150941	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	87
2			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
3			Tridecane	184	C13H28	000629-50-5	81
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
5			Hexadecane	226	C16H34	000544-76-3	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
unknown2.842	2.842	6.7	ug/l	69810	1	8.224	524407	50.0
n-Hexane	6.294	52.5	ug/l	550855	1	8.224	524407	50.0
Undecane, 2,6-d...	15.835	7.5	ug/l	150941	4	13.794	1011380	50.0