

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070047.D
 Acq On : 13 Dec 2021 22:51
 Operator : JC/MD
 Sample : M5007-01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-02

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.740	270	280	298	rBV5	40564	90063	1.26%	0.177%
2	3.140	418	429	451	rVB5	125898	277345	3.87%	0.544%
3	3.513	557	568	590	rVB2	44872	110648	1.55%	0.217%
4	4.586	949	968	995	rVB2	53768	166357	2.32%	0.326%
5	5.087	1122	1155	1156	rBV3	87987	220653	3.08%	0.433%
6	5.618	1323	1353	1391	rBV3	458632	1614963	22.55%	3.168%
7	6.120	1514	1540	1563	rBV4	77467	241441	3.37%	0.474%
8	7.147	1895	1923	1964	rVB	1432729	4255808	59.44%	8.349%
9	8.021	2227	2249	2260	rBV2	779620	1881643	26.28%	3.691%
10	8.088	2261	2274	2297	rVB2	1799120	4370291	61.04%	8.573%
11	8.295	2335	2351	2363	rBV6	31344	74669	1.04%	0.146%
12	8.440	2386	2405	2434	rBV	920567	2244514	31.35%	4.403%
13	8.574	2440	2455	2460	rBV9	42736	87976	1.23%	0.173%
14	8.705	2493	2504	2521	rVB7	58487	134103	1.87%	0.263%
15	8.968	2582	2602	2646	rBV	2221312	4736587	66.15%	9.292%
16	9.201	2671	2689	2724	rVB	202069	532164	7.43%	1.044%
17	9.456	2755	2784	2801	rBV6	257487	713558	9.97%	1.400%
18	9.880	2931	2942	2958	rVB6	44851	90855	1.27%	0.178%
19	10.017	2985	2993	3008	rVB4	71768	139345	1.95%	0.273%
20	10.202	3045	3062	3078	rBV4	29961	74580	1.04%	0.146%
21	10.443	3134	3152	3187	rBV	3797992	7160214	100.00%	14.047%
22	10.607	3203	3213	3219	rBV3	63473	110676	1.55%	0.217%
23	10.717	3241	3254	3265	rBV4	56023	100975	1.41%	0.198%
24	10.781	3266	3278	3293	rVB3	124738	235730	3.29%	0.462%
25	10.875	3293	3313	3329	rBV7	77093	181172	2.53%	0.355%
26	11.293	3462	3469	3481	rVB2	91658	146401	2.04%	0.287%
27	11.744	3619	3637	3663	rBV	3881147	7031749	98.21%	13.795%
28	11.838	3666	3672	3685	rVB4	55944	93463	1.31%	0.183%
29	11.991	3723	3729	3748	rVB4	56840	107761	1.50%	0.211%
30	12.578	3936	3948	3962	rVB2	125306	215282	3.01%	0.422%
31	12.731	3989	4005	4027	rBV	3033814	5327699	74.41%	10.452%
32	12.921	4066	4076	4088	rVB2	66668	123806	1.73%	0.243%
33	13.219	4175	4187	4203	rVB2	94911	172027	2.40%	0.337%
34	13.321	4203	4225	4234	rBV7	31656	85463	1.19%	0.168%
35	13.495	4275	4290	4305	rBV2	84318	204426	2.86%	0.401%
36	13.675	4342	4357	4381	rVV	3356541	5874633	82.05%	11.525%

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Max Peaks: 100

Peak Location: TOP

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37	13.838	4407	4418	4423	rVV3	44621	72538	1.01%	0.142%
38	13.876	4423	4432	4446	rVV	157792	271938	3.80%	0.533%
39	13.943	4446	4457	4466	rVV	47154	78261	1.09%	0.154%
40	13.997	4466	4477	4491	rVB9	72686	142669	1.99%	0.280%
41	14.217	4549	4559	4570	rBV2	88785	142843	1.99%	0.280%
42	14.327	4590	4600	4612	rVB3	141958	239483	3.34%	0.470%
43	14.466	4639	4652	4660	rBV2	45798	79389	1.11%	0.156%
44	14.541	4662	4680	4691	rVB3	96602	172230	2.41%	0.338%
45	14.815	4771	4782	4793	rVV6	44376	82264	1.15%	0.161%
46	14.922	4808	4822	4840	rBV3	117174	274295	3.83%	0.538%
47	15.507	5029	5040	5054	rVB2	54870	102322	1.43%	0.201%
48	15.697	5102	5111	5126	rVB3	41924	87477	1.22%	0.172%

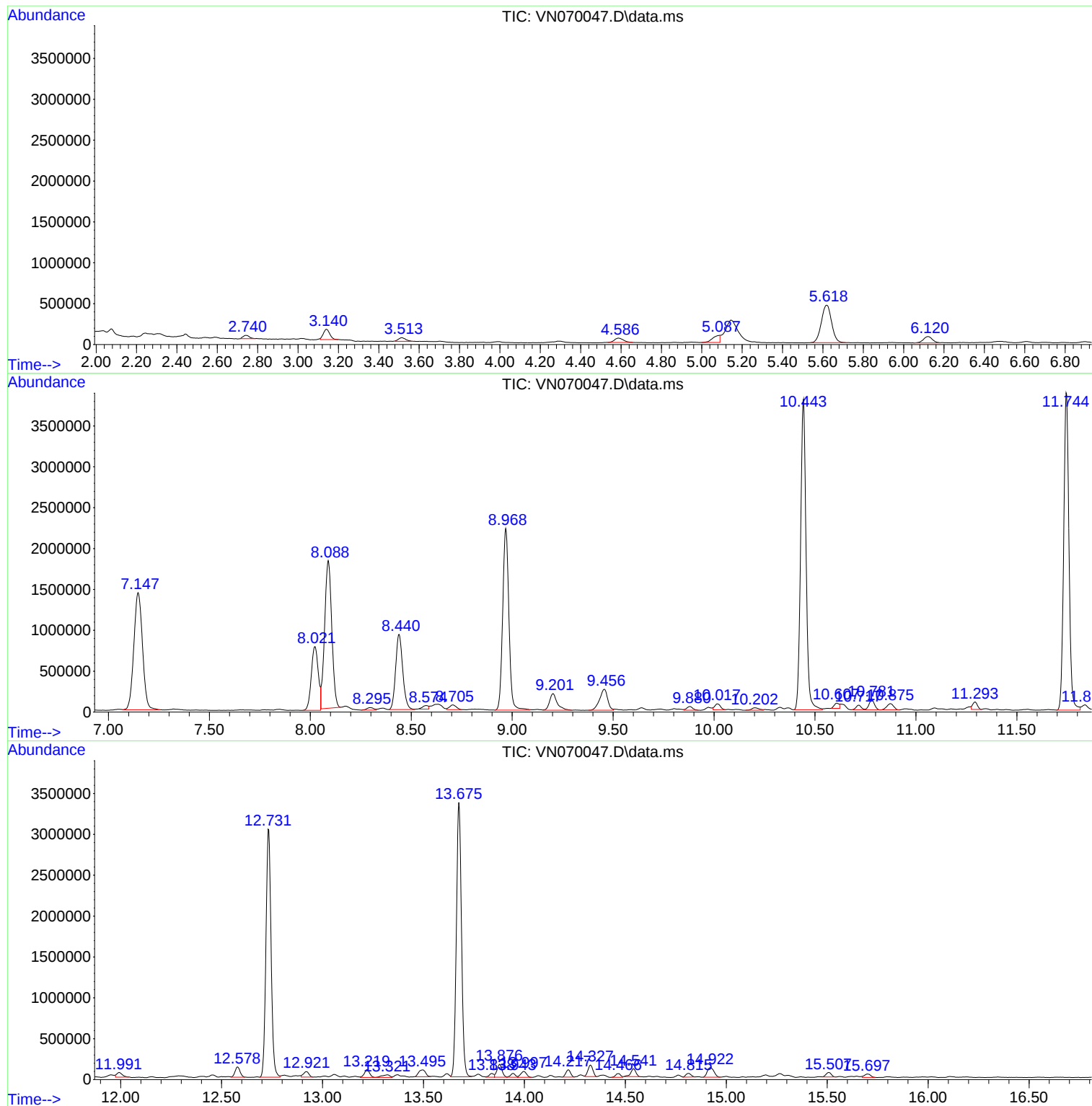
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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TOLL-MW-02

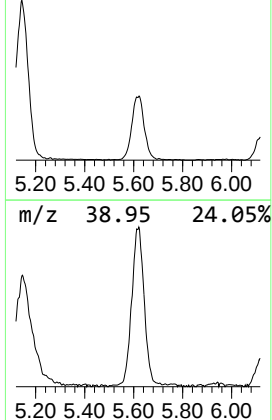
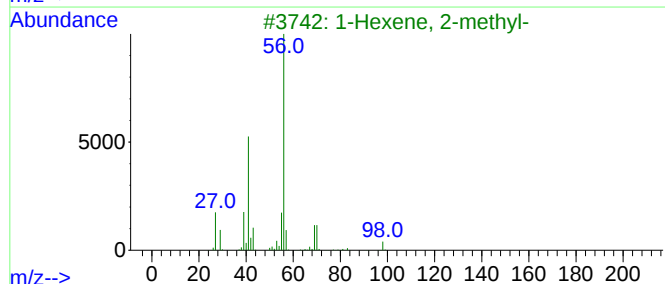
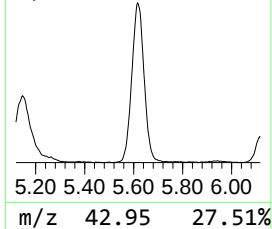
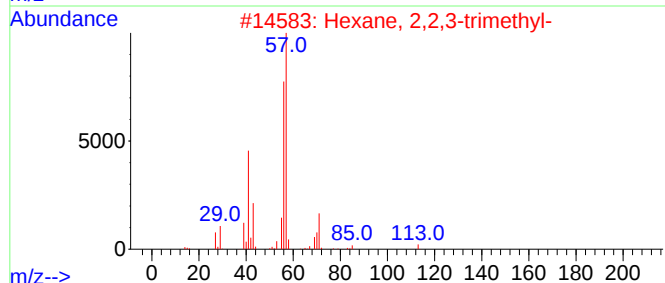
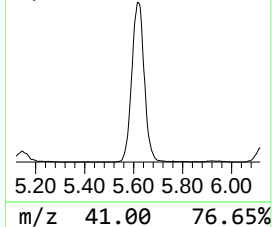
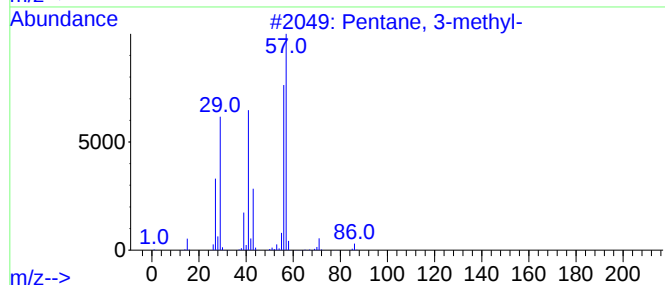
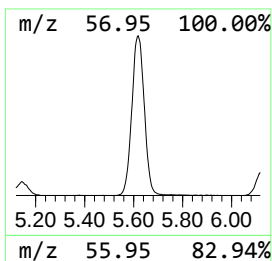
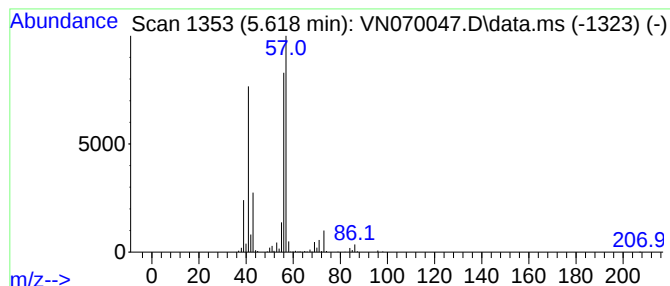
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.618	18.48 ug/l	1614960	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
3			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	53
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TOLL-MW-02

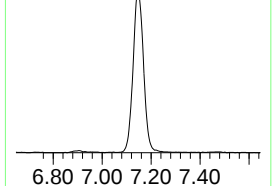
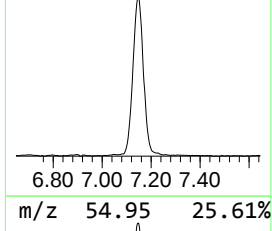
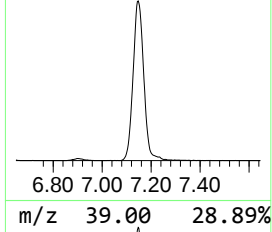
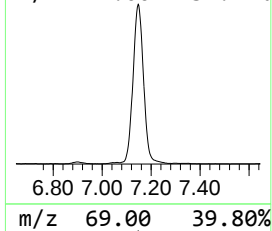
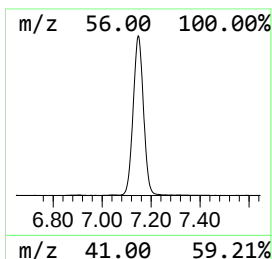
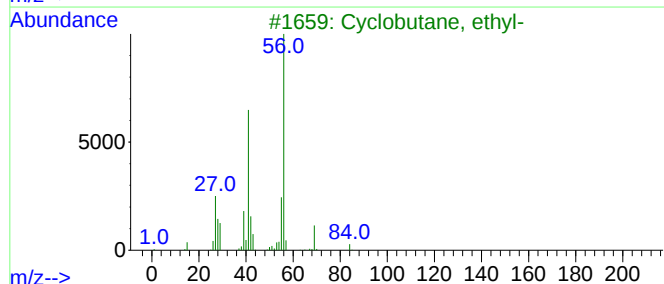
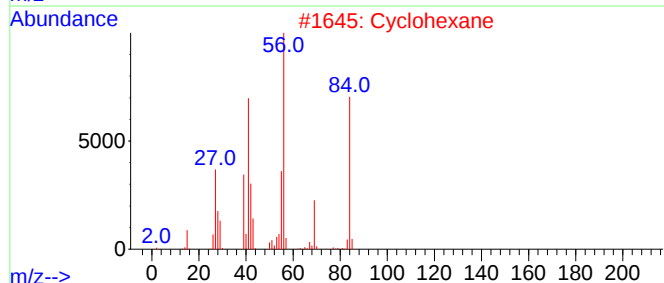
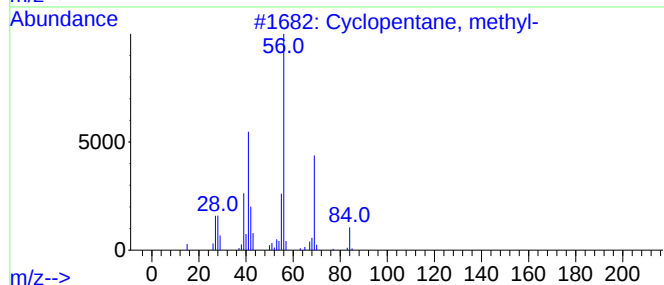
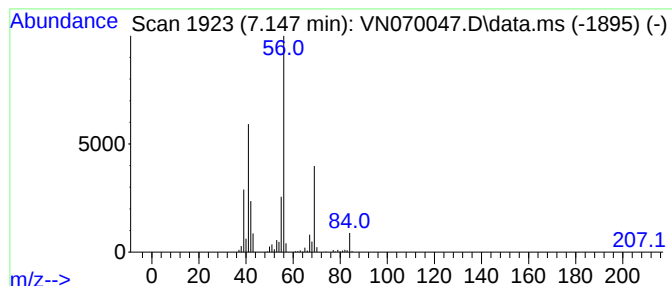
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	48.69 ug/l	4255810	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	86
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56



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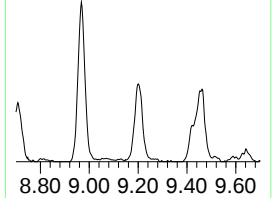
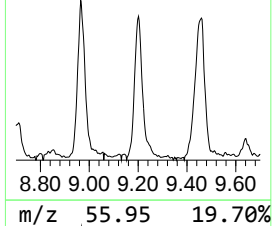
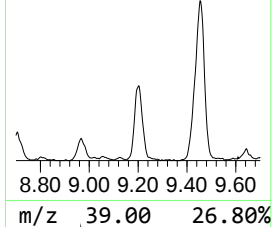
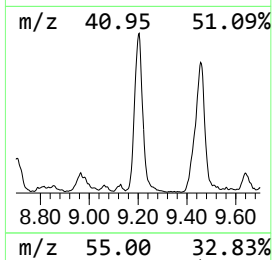
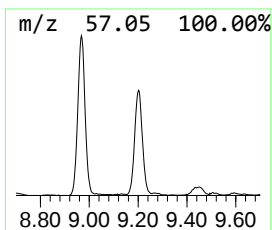
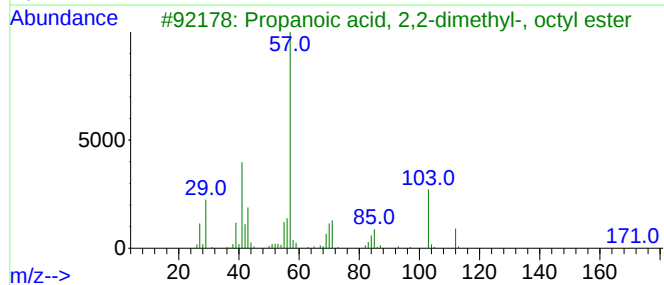
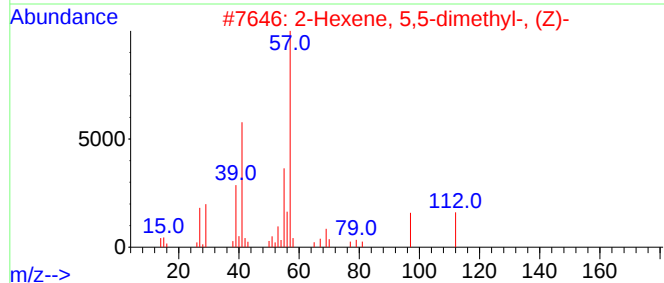
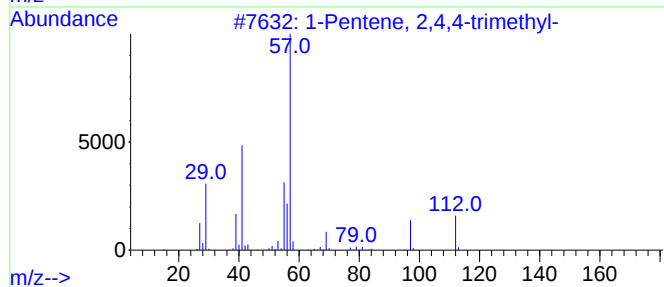
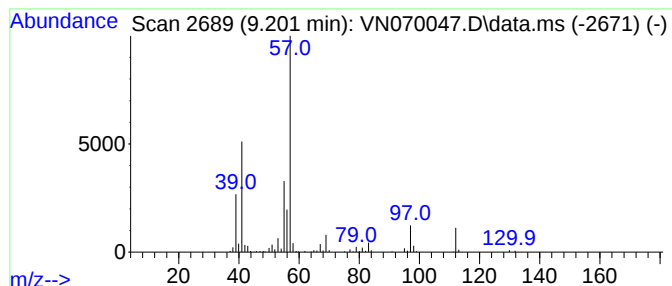
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TIC Library : C:\Database\NIST0.L
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Peak Number 3 1-Pentene, 2,4,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.201	5.62 ug/l	532164	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	87
2			2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	64
3			Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	45
4			Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	40
5			2,4,4-Trimethyl-1-pentanol	130	C8H18O	016325-63-6	37



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 3-methyl-	5.618	18.5	ug/l	1614960	1	8.088	4370290	50.0
Cyclopentane, m...	7.147	48.7	ug/l	4255810	1	8.088	4370290	50.0
1-Pentene, 2,4,...	9.201	5.6	ug/l	532164	2	8.968	4736590	50.0