LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122921\
Data File : VN070374.D
Acq On : 30 Dec 2021 3:45
Operator : JC/MD
Sample : M5007-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-02RE

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	417	428	449	rVB4	123429	281506	5.26%	0.729%
2	3.513	557	568	588	rVB5	37495	93103	1.74%	0.241%
3	5.082	1127	1153	1156	rBV2	76929	192137	3.59%	0.497%
4	5.618	1316	1353	1381	rBV3	418019	1477385	27.61%	3.825%
5	6.120	1519	1540	1541	rBV2	56136	94684	1.77%	0.245%
6	7.147	1894	1923	1969	rBV	1377566	4112575	76.85%	10.647%
7	8.024	2227	2250	2260	rBV	649573	1539759	28.77%	3.986%
8	8.088	2261	2274	2297	rVB2	1637736	3993084	74.62%	10.337%
9	8.440	2386	2405	2436	rVB2	828785	2001088	37.39%	5.180%
10	8.579	2439	2457	2461	rBV6	61488	129984	2.43%	0.337%
11	8.968	2583	2602	2633	rBV	1880244	3935842	73.55%	10.189%
12	9.201	2673	2689	2727	rVB2	218794	594569	11.11%	1.539%
13	9.456	2756	2784	2802	rBV7	245850	695523	13.00%	1.801%
14	9.633	2838	2850	2867	rVB7	43965	96648	1.81%	0.250%
15	9.882	2931	2943	2955	rVB7	35626	73058	1.37%	0.189%
16	9.971	2964	2976	2984	rBV3	42115	80041	1.50%	0.207%
17	10.019	2985	2994	3008	rVB6	72985	142978	2.67%	0.370%
18	10.202	3048	3062	3072	rBV9	23534	53749	1.00%	0.139%
19	10.322	3095	3107	3116	rBV7	32613	62624	1.17%	0.162%
20	10.443	3134	3152	3184	rBV	2784893	5351364	100.00%	13.854%
21	10.609	3203	3214	3219	rBV3	56856	98493	1.84%	0.255%
22	10.717	3241	3254	3265	rBV3	57284	103843	1.94%	0.269%
23	10.781	3266	3278	3292	rVV3	106600	196667	3.68%	0.509%
24	10.875	3296	3313	3329	rVV7	70257	174216	3.26%	0.451%
25	10.950	3330	3341	3359	rVB5	28981	69454	1.30%	0.180%
26	11.092	3382	3394	3416	rBV3	71307	157452	2.94%	0.408%
27	11.293	3462	3469	3481	rVB2	75214	121861	2.28%	0.315%
28	11.744	3620	3637	3659	rBV	2388919	4396203	82.15%	11.381%
29	11.835	3664	3671	3687	rVB4	49431	91289	1.71%	0.236%
30	12.578	3937	3948	3965	rVB2	73663	131351	2.45%	0.340%
31	12.731	3989	4005	4026	rBV	1860043	3293755	61.55%	8.527%
32	12.918	4063	4075	4086	rVB2	27505	54577	1.02%	0.141%
33	13.222	4175	4188	4200	rVB	88164	147677	2.76%	0.382%
34	13.492	4278	4289	4302	rVB5	33635	74038	1.38%	0.192%
35	13.675	4342	4357	4376	rBV	1773222	3138589	58.65%	8.125%
36	13.838	4409	4418	4423	rBV3	36526	55737	1.04%	0.144%

LSC Area Percent Report

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Title : SW846 8260

37	13.876	4423	4432	4446	rVB	147237	247279	4.62%	0.640%
38	13.999	4465	4478	4491	rVB7	54321	102326	1.91%	0.265%
39	14.217	4548	4559	4570	rBV2	83141	132530	2.48%	0.343%
40	14.327	4589	4600	4612	rVV2	138618	241775	4.52%	0.626%
41	14.383	4615	4621	4637	rVB2	27536	53660	1.00%	0.139%
42	14.466	4639	4652	4661	rBV2	45403	78090	1.46%	0.202%
43	14.538	4670	4679	4694	rVB3	91367	154034	2.88%	0.399%
44	14.812	4771	4781	4793	rVV3	42641	73850	1.38%	0.191%
45	14.922	4808	4822	4840	rBV5	98992	237643	4.44%	0.615%

Sum of corrected areas: 38628090

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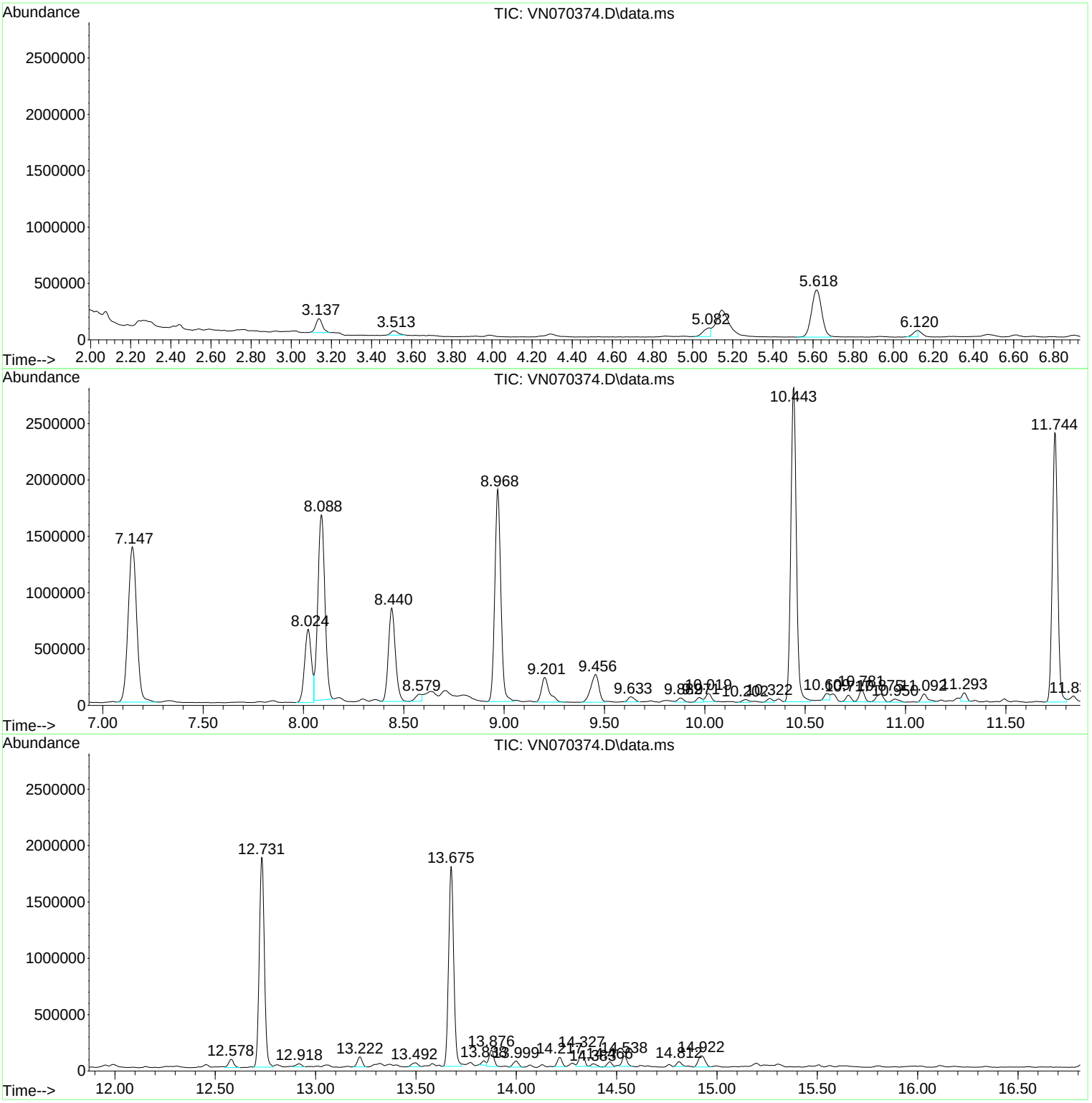
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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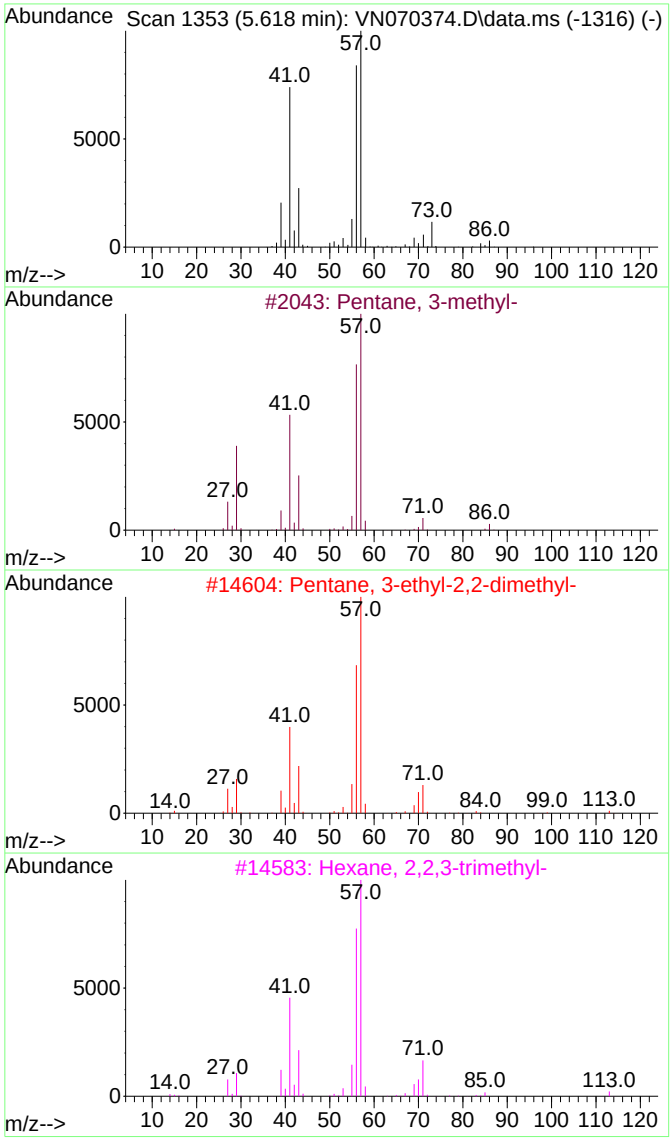
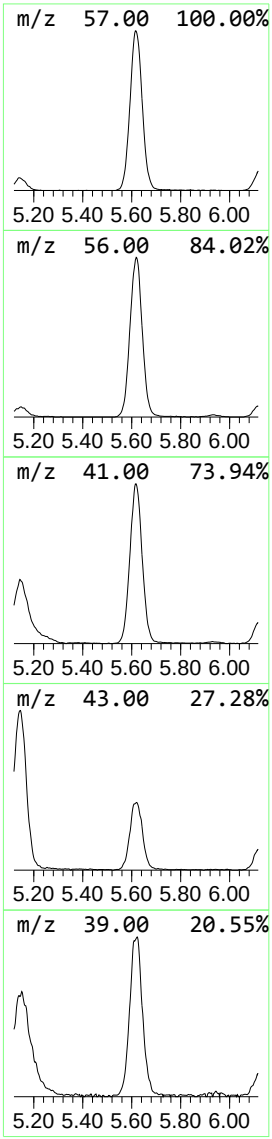
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.618	18.50 ug/l	1477390	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	40





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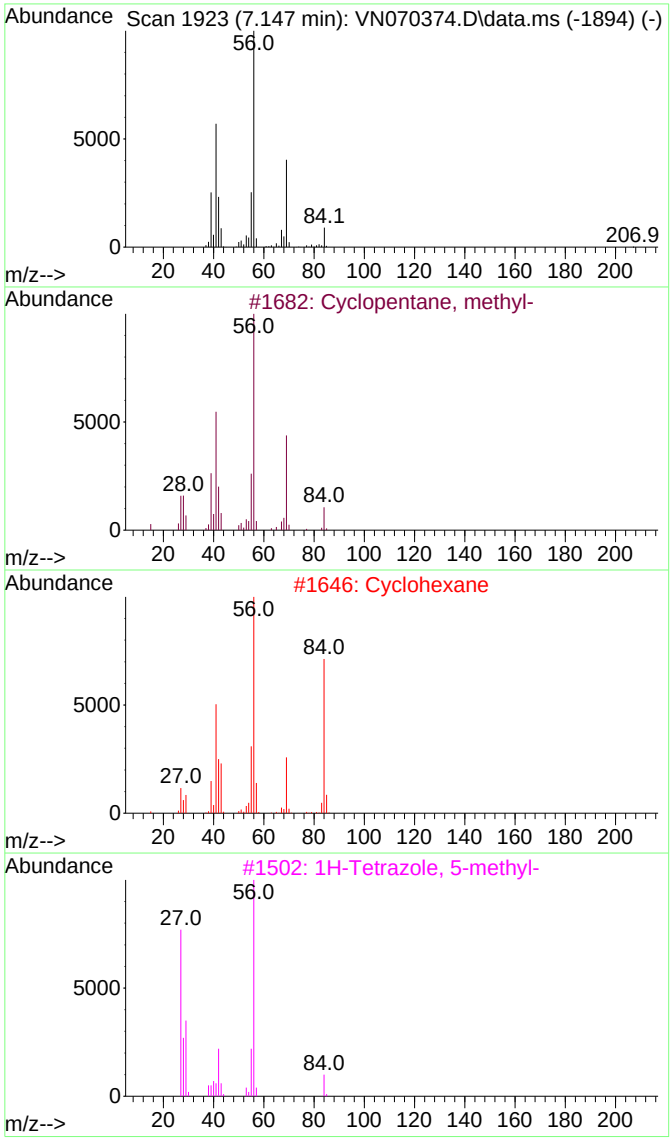
Quant Title : SW846 8260

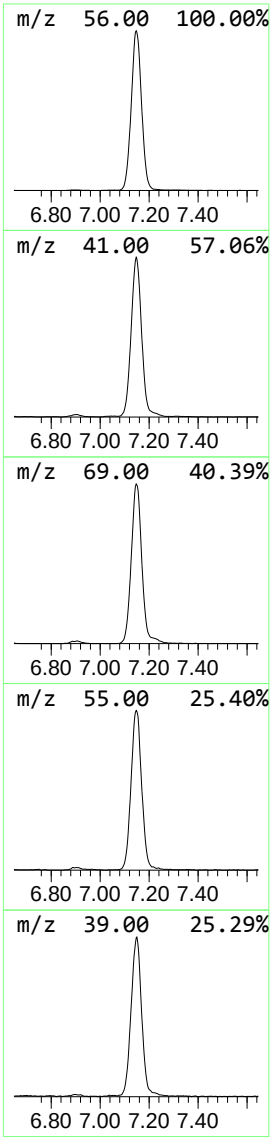
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	51.50 ug/l	4112580	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	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	56





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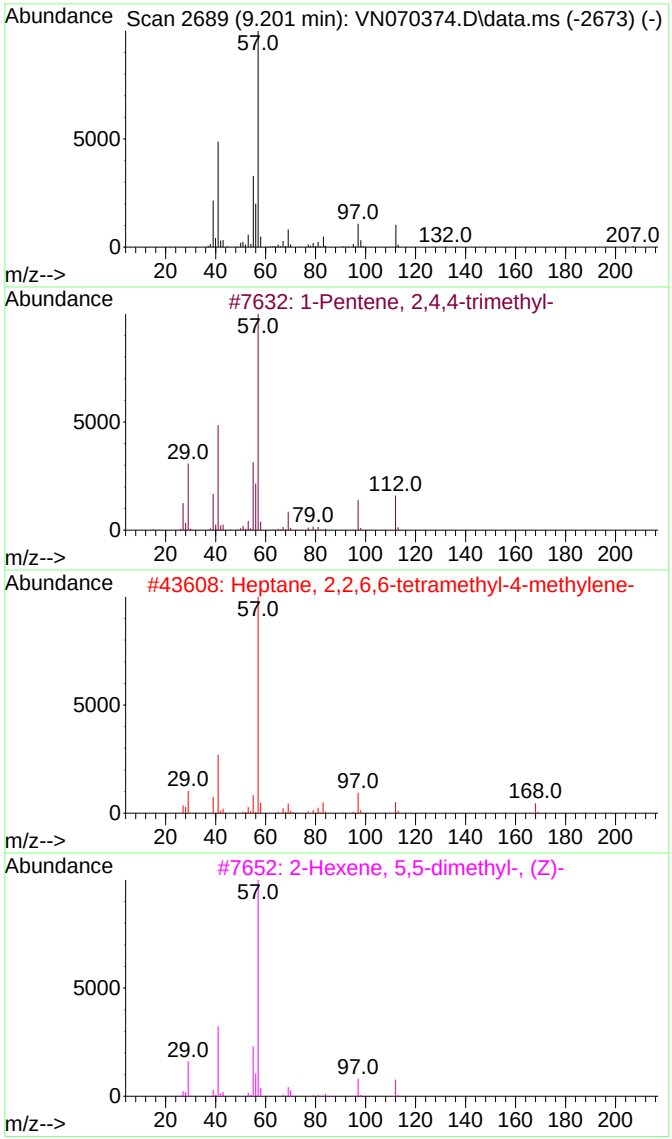
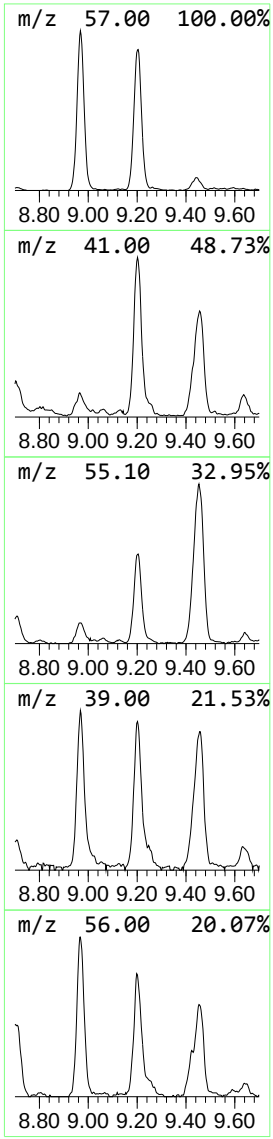
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Pentene, 2,4,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.201	7.55 ug/l	594569	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	Heptane, 2,2,6,6-tetramethyl-4-m...	168	C12H24	000141-70-8	53
3	2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	47
4	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	38
5	Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	37





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 3-methyl-	5.618	18.5	ug/l	1477390	1	8.088	3993080	50.0
Cyclopentane, m...	7.147	51.5	ug/l	4112580	1	8.088	3993080	50.0
1-Pentene, 2,4,...	9.201	7.5	ug/l	594569	2	8.968	3935840	50.0