

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091820\
 Data File : VX018499.D
 Acq On : 18 Sep 2020 17:48
 Operator : JC/SP
 Sample : L4058-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2R

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\82X091720W.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	2.581	237	245	254	rVB	21321	43198	1.43%	0.195%
2	3.008	307	315	324	rBV	61472	135825	4.49%	0.615%
3	3.166	330	341	351	rBV	156880	370785	12.26%	1.678%
4	4.526	556	564	575	rVB6	11556	41748	1.38%	0.189%
5	4.641	575	583	592	rBV	13574	39961	1.32%	0.181%
6	5.471	705	719	731	rBV2	346543	1010200	33.41%	4.571%
7	5.635	733	746	759	rVV2	596741	1695355	56.07%	7.671%
8	6.037	799	812	827	rBV	380583	1010491	33.42%	4.572%
9	6.324	846	859	881	rVB	864306	2604449	86.13%	11.784%
10	6.830	932	942	954	rBV	903322	2169406	71.75%	9.816%
11	7.659	1070	1078	1084	rBV	71001	155325	5.14%	0.703%
12	8.037	1129	1140	1151	rBV	931489	1761357	58.25%	7.969%
13	8.159	1151	1160	1171	rVB	368941	710464	23.50%	3.215%
14	8.696	1237	1248	1261	rBV	1920493	3023715	100.00%	13.681%
15	10.098	1472	1478	1490	rVB	1905120	2572680	85.08%	11.640%
16	11.122	1639	1646	1656	rBV	1683849	2072728	68.55%	9.378%
17	11.927	1776	1778	1783	rVB	31833	37624	1.24%	0.170%
18	12.061	1795	1800	1809	rBV	2127320	2609099	86.29%	11.805%
19	12.353	1840	1848	1857	rVB	15464	37320	1.23%	0.169%

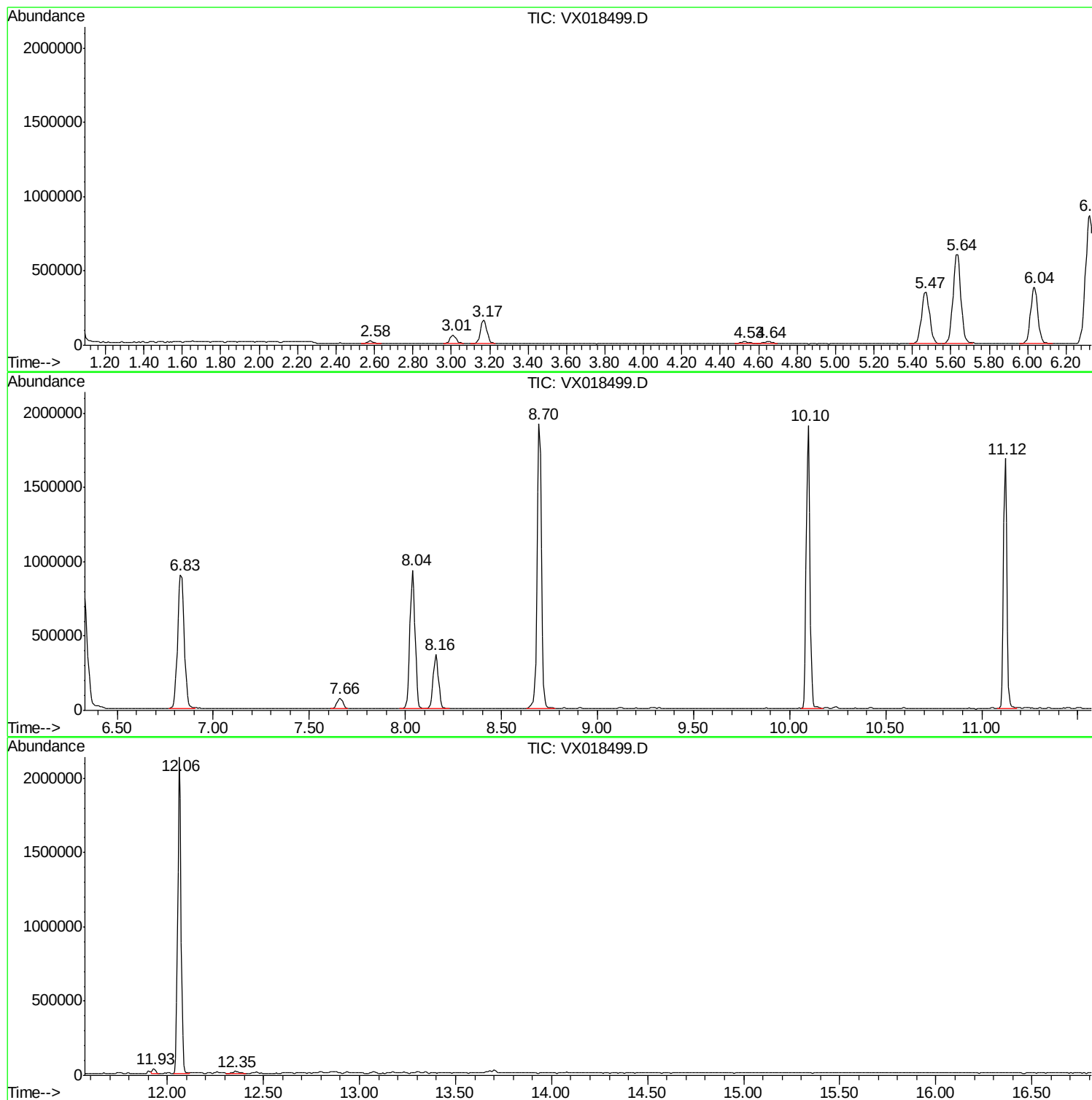
Sum of corrected areas: 22101730

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091720W.M
Quant Title : SW846 8260

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



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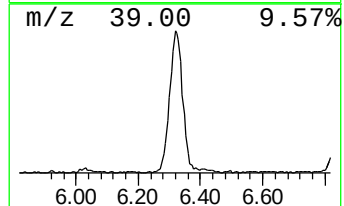
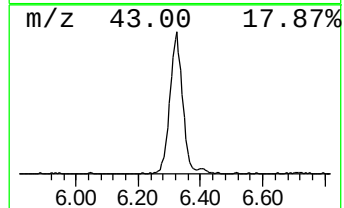
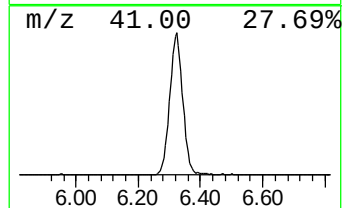
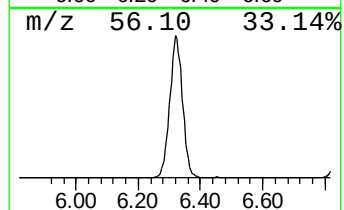
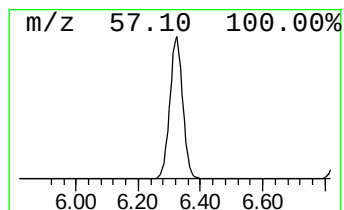
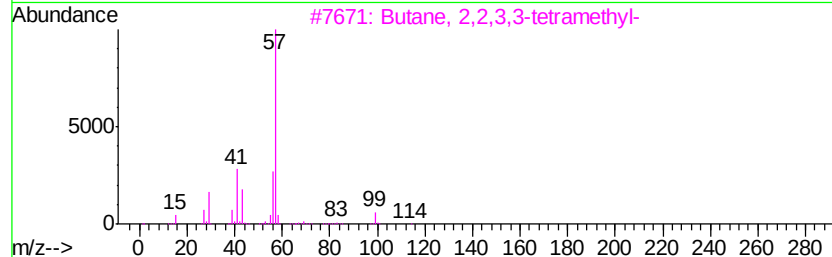
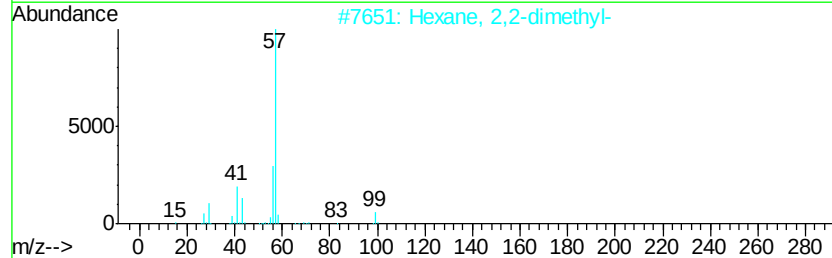
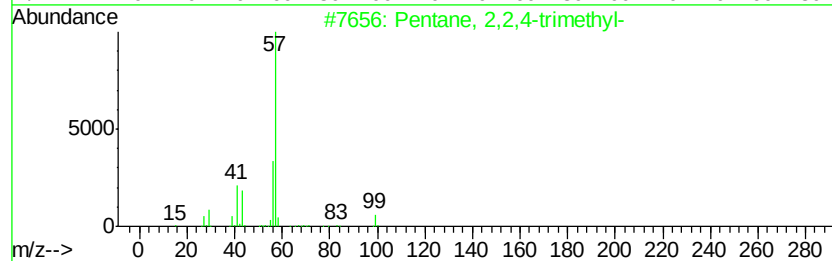
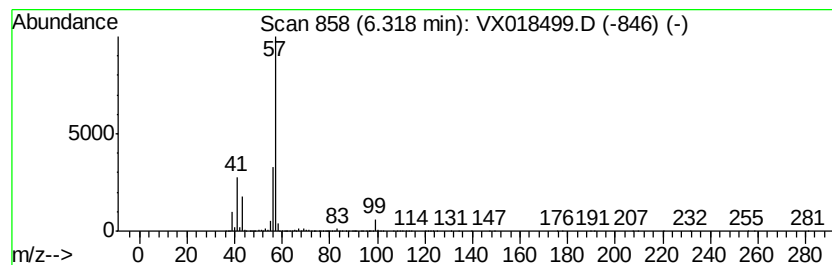
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091720W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	60.03 ug/l	2604450	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45



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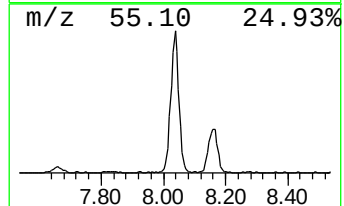
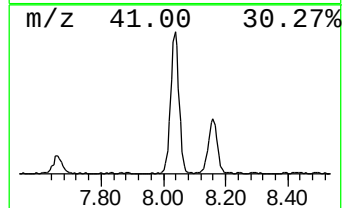
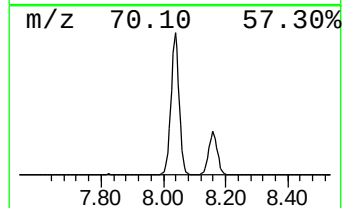
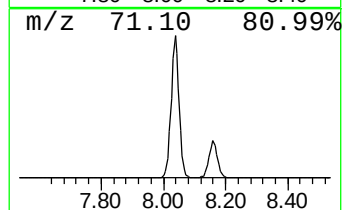
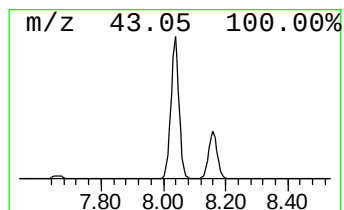
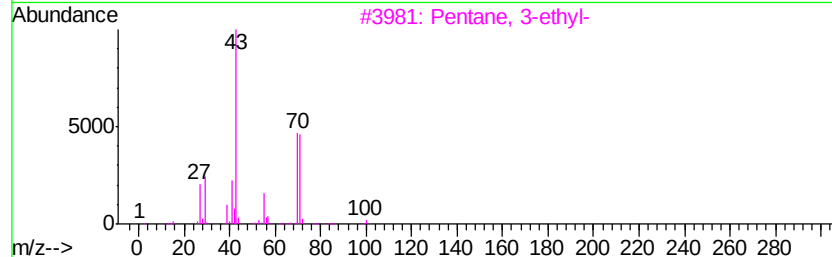
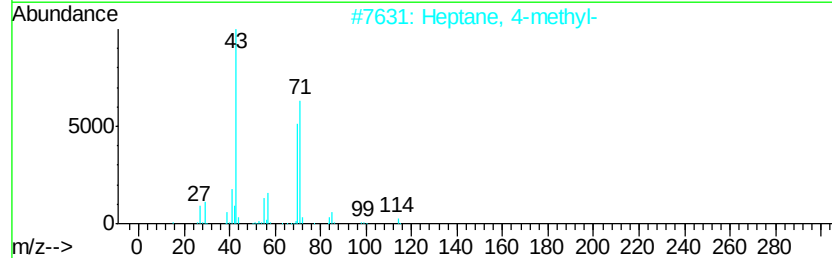
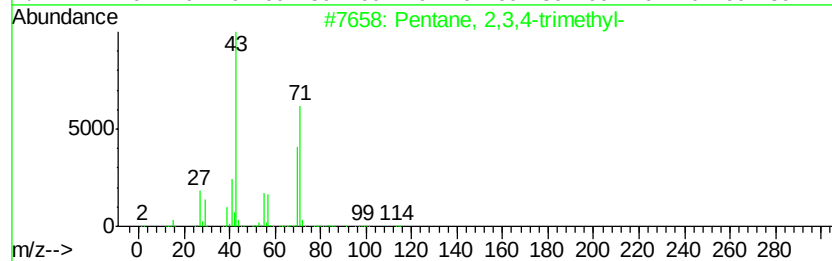
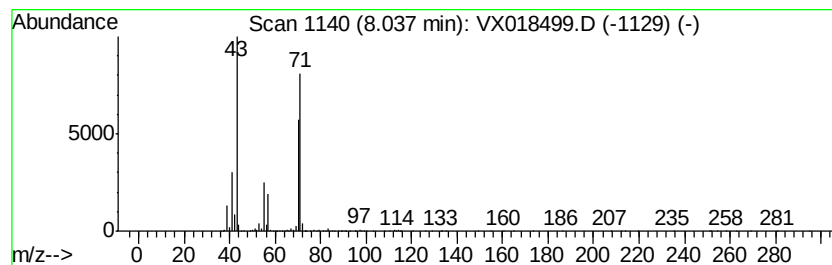
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 Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	40.60 ug/l	1761360	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	64



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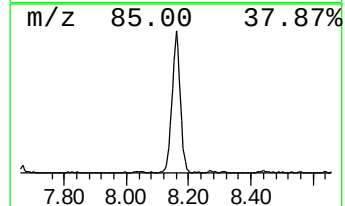
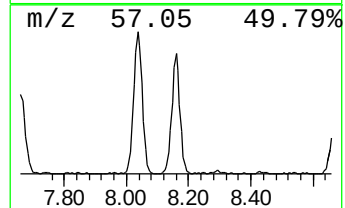
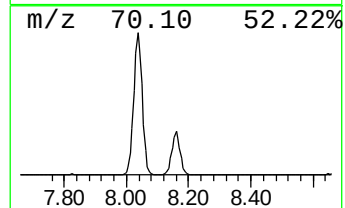
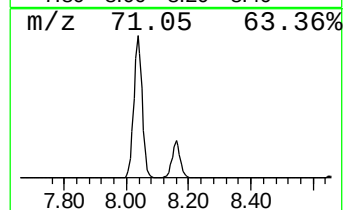
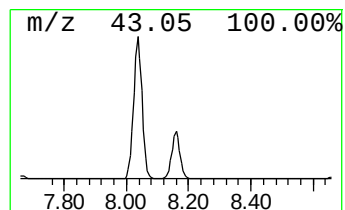
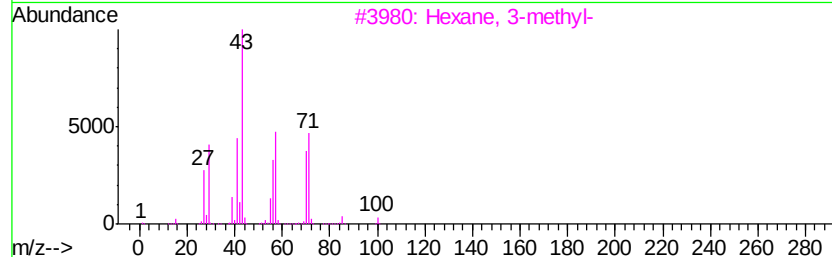
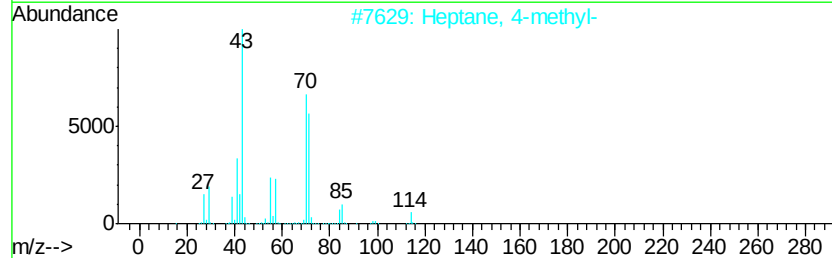
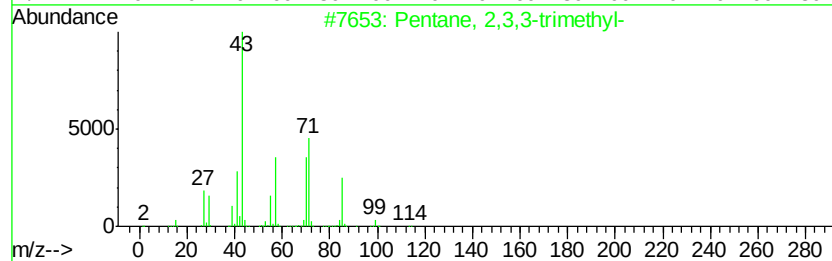
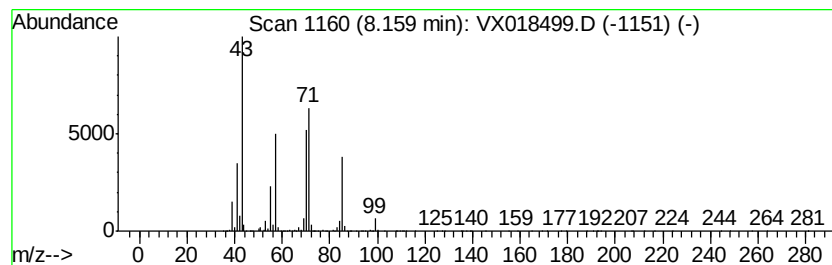
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Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	16.37 ug/l	710464	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	64
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,4-tr...	6.32	60.0	ug/l	2604450	2	6.83	2169410	50.0
Pentane, 2,3,4-tr...	8.04	40.6	ug/l	1761360	2	6.83	2169410	50.0
Pentane, 2,3,3-tr...	8.16	16.4	ug/l	710464	2	6.83	2169410	50.0