

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040622\
 Data File : VX027991.D
 Acq On : 06 Apr 2022 12:31
 Operator : JC/MD
 Sample : N2253-01
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 101221

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_X\Method\82X040522W.M
 Title : SW846 8260

Signal : TIC: VX027991.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	693	706	714	rBV	57288	176883	10.92%	3.040%
2	5.495	714	723	726	rVV3	44651	134867	8.33%	2.318%
3	5.550	726	732	753	rVB	107336	358194	22.12%	6.156%
4	5.812	764	775	787	rBV2	64383	187291	11.57%	3.219%
5	5.958	787	799	813	rBV	64342	181049	11.18%	3.111%
6	6.159	820	832	833	rBV4	7808	17618	1.09%	0.303%
7	6.245	839	846	856	rVB6	12278	36026	2.22%	0.619%
8	6.348	856	863	879	rVB4	8579	27590	1.70%	0.474%
9	6.598	891	904	915	rBV2	41911	102147	6.31%	1.755%
10	6.763	920	931	952	rBV	163385	399064	24.64%	6.858%
11	7.373	1020	1031	1041	rBV2	37747	85451	5.28%	1.469%
12	7.976	1120	1130	1137	rBV4	8742	19711	1.22%	0.339%
13	8.104	1141	1151	1155	rBV3	7422	16786	1.04%	0.288%
14	8.647	1227	1240	1246	rBV	319924	539899	33.34%	9.278%
15	8.720	1246	1252	1265	rVB	1051806	1619309	100.00%	27.829%
16	8.909	1278	1283	1290	rBV2	11288	18326	1.13%	0.315%
17	10.055	1466	1471	1485	rVB	317456	467379	28.86%	8.032%
18	10.195	1488	1494	1501	rBV	36755	53062	3.28%	0.912%
19	10.305	1503	1512	1518	rVV	128134	185642	11.46%	3.190%
20	10.360	1518	1521	1526	rVB	20182	24187	1.49%	0.416%
21	10.646	1563	1568	1576	rBV	44665	64095	3.96%	1.102%
22	11.085	1634	1640	1650	rVB	272601	386934	23.90%	6.650%
23	11.384	1684	1689	1695	rBV	21807	39169	2.42%	0.673%
24	11.476	1701	1704	1709	rVB	41478	50877	3.14%	0.874%
25	11.756	1746	1750	1759	rVB	31261	41146	2.54%	0.707%
26	12.024	1789	1794	1800	rBV	362717	458322	28.30%	7.876%
27	12.097	1800	1806	1810	rVB3	8021	18003	1.11%	0.309%
28	12.427	1855	1860	1864	rBV	36306	41275	2.55%	0.709%
29	15.194	2307	2314	2325	rBV2	21609	41999	2.59%	0.722%
30	15.670	2387	2392	2399	rBV4	15615	26577	1.64%	0.457%

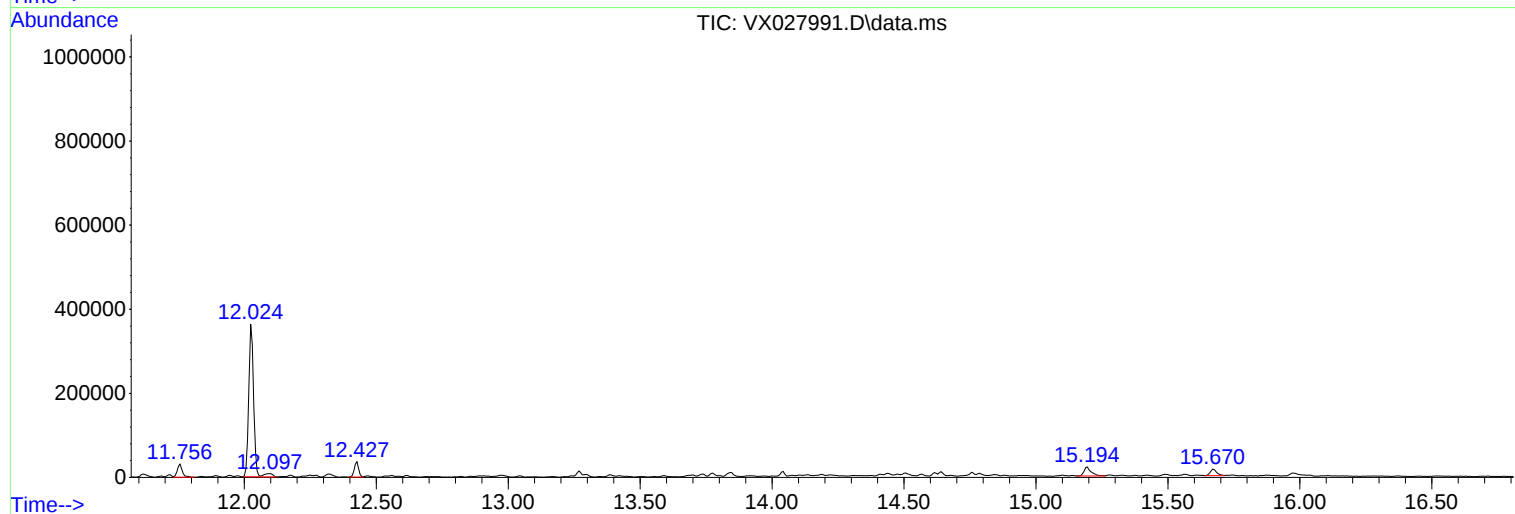
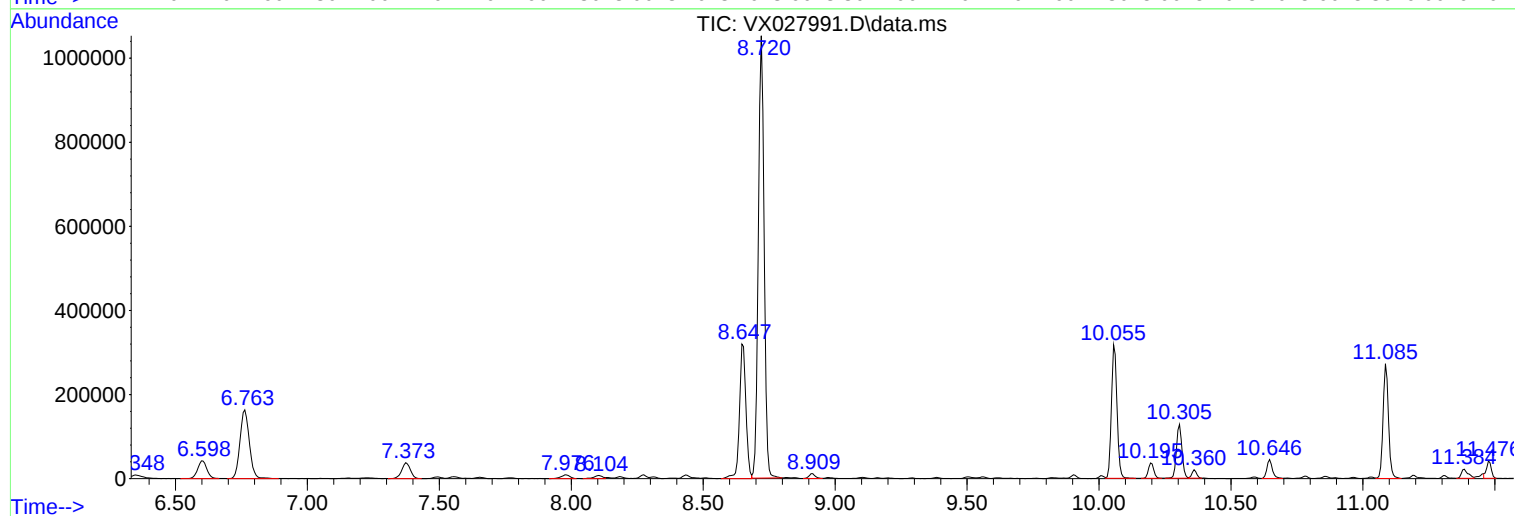
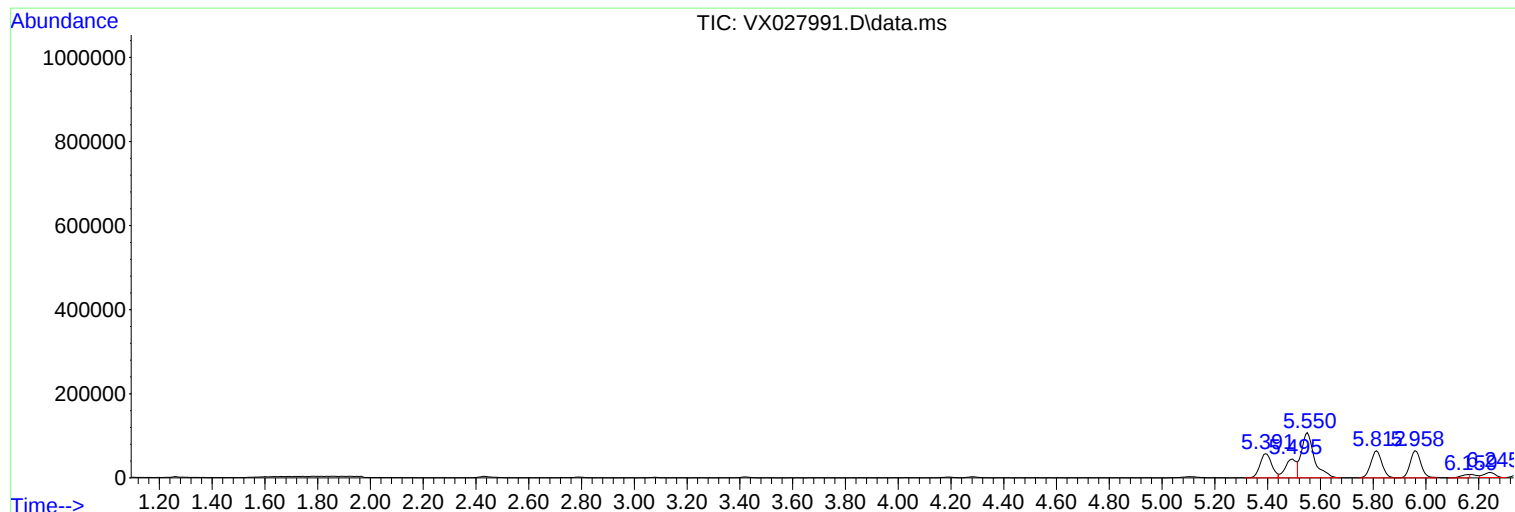
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
Quant Title : SW846 8260

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



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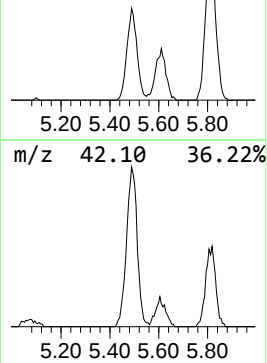
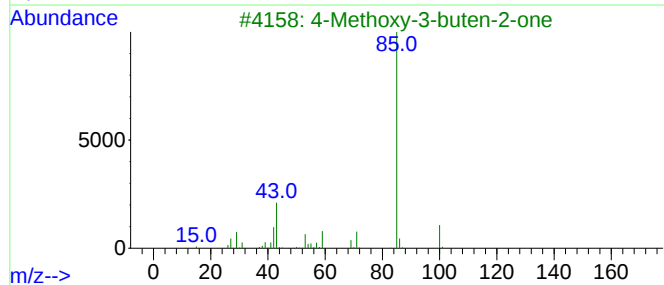
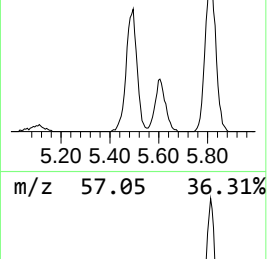
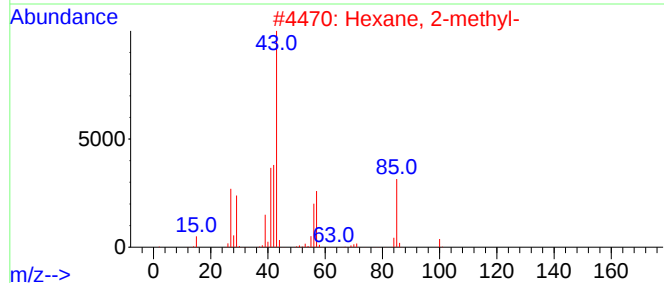
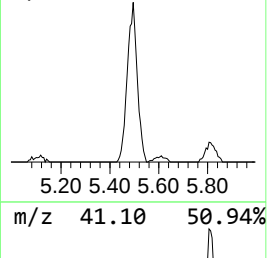
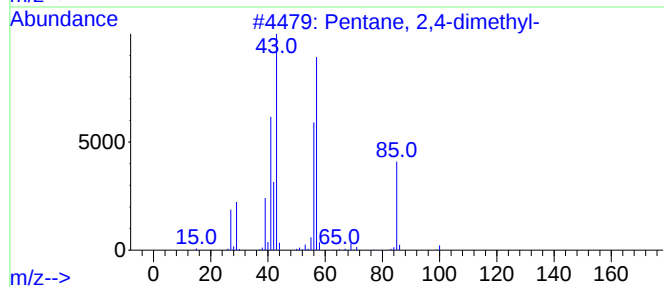
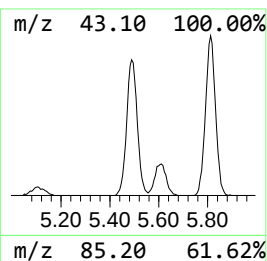
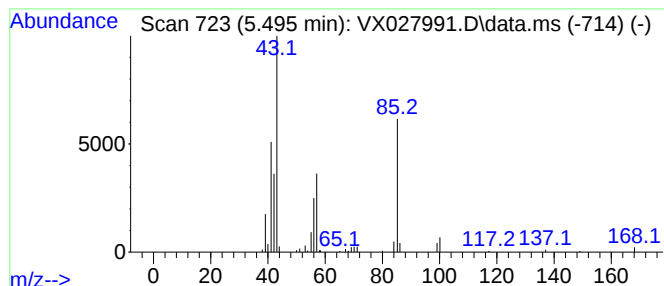
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040522W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.495	18.83 ug/l	134867	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	64
2			Hexane, 2-methyl-	100	C7H16	000591-76-4	62
3			4-Methoxy-3-buten-2-one	100	C5H8O2	004652-27-1	53
4			2-Pyrrolidinone	85	C4H7NO	000616-45-5	50
5			2,2-Dimethylpropanimidamide	100	C5H12N2	1000484-56-1	47



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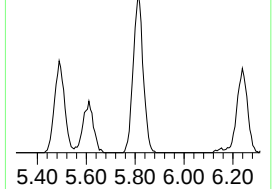
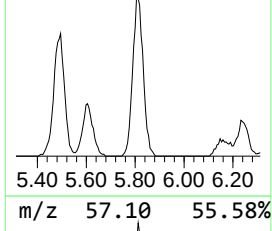
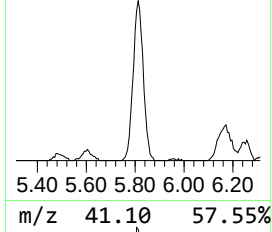
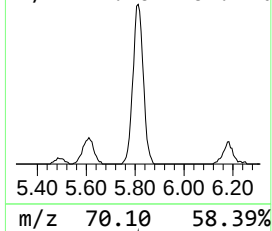
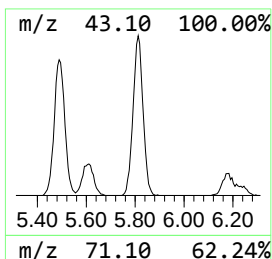
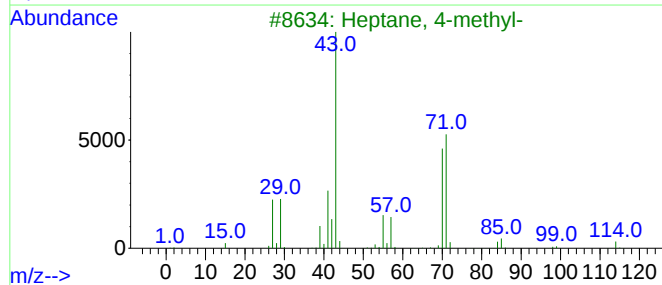
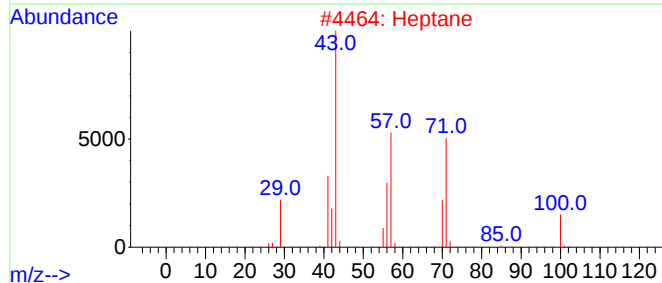
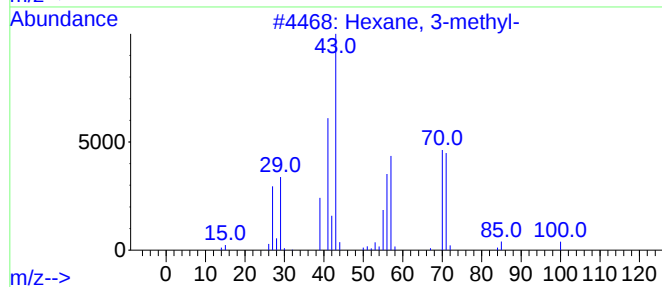
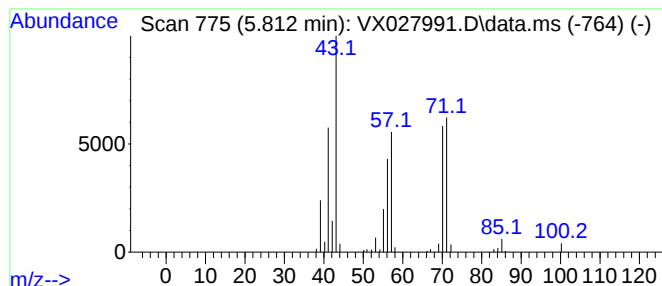
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	26.14 ug/l	187291	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	58
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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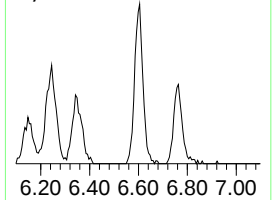
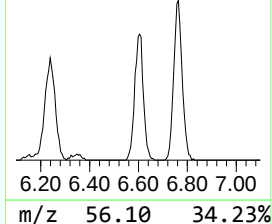
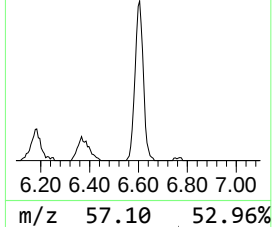
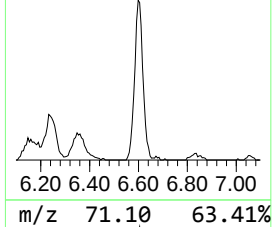
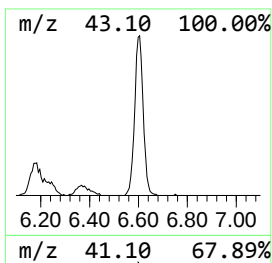
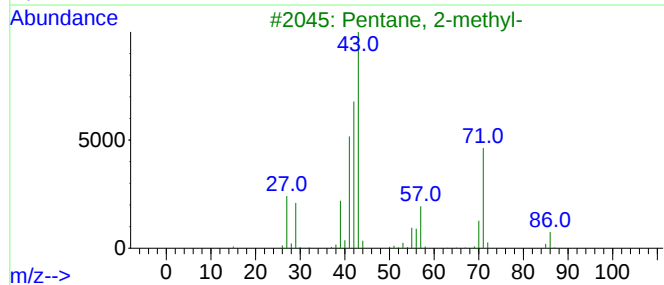
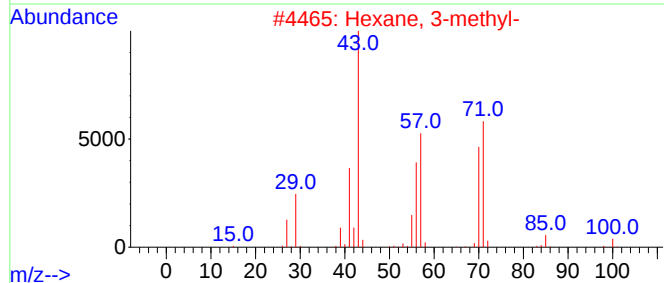
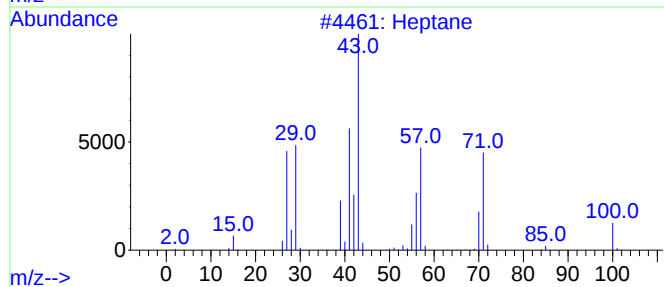
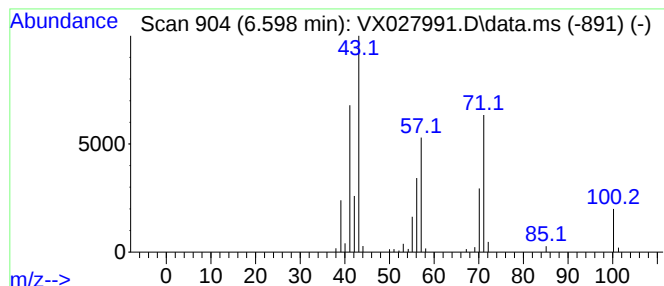
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	12.80 ug/l	102147	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	78
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	47
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37
5			3-Hexanone	100	C6H12O	000589-38-8	35



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,4-di...	5.495	18.8	ug/l	134867	1	5.550	358194	50.0
Hexane, 3-methyl-	5.812	26.1	ug/l	187291	1	5.550	358194	50.0
Heptane	6.598	12.8	ug/l	102147	2	6.763	399064	50.0