

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121222\
 Data File : VN075720.D
 Acq On : 12 Dec 2022 18:05
 Operator : JC\MD
 Sample : N5978-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-04

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\82N120922W.M
 Title : SW846 8260

Signal : TIC: VN075720.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.300	34	42	45	rBV	20643	46832	4.24%	0.619%
2	2.342	45	49	57	rVB2	33318	61210	5.54%	0.810%
3	2.530	75	81	89	rVB2	32551	54193	4.90%	0.717%
4	2.836	131	133	142	rVB2	11111	15224	1.38%	0.201%
5	3.253	198	204	215	rVB5	8913	23196	2.10%	0.307%
6	5.806	627	638	639	rBV	15252	26857	2.43%	0.355%
7	7.235	869	881	891	rBV3	13279	38600	3.49%	0.511%
8	7.500	916	926	935	rBV2	21130	56824	5.14%	0.752%
9	8.171	1030	1040	1045	rBV	152538	362700	32.80%	4.797%
10	8.230	1045	1050	1060	rVV	295426	652988	59.06%	8.637%
11	8.335	1060	1068	1078	rVB	80650	191071	17.28%	2.527%
12	8.588	1102	1111	1123	rVV	146405	335288	30.32%	4.435%
13	8.765	1126	1141	1152	rVV	144517	353915	32.01%	4.681%
14	9.106	1190	1199	1212	rBV	398462	804070	72.72%	10.635%
15	9.588	1270	1281	1287	rBV7	19473	50290	4.55%	0.665%
16	9.647	1287	1291	1298	rVB3	13273	25063	2.27%	0.332%
17	9.735	1298	1306	1312	rBV2	15574	32299	2.92%	0.427%
18	9.865	1322	1328	1335	rVB5	4580	11773	1.06%	0.156%
19	10.018	1346	1354	1363	rBV	148896	297458	26.90%	3.934%
20	10.147	1368	1376	1389	rBV	216994	441661	39.94%	5.842%
21	10.329	1400	1407	1413	rBV3	8965	18329	1.66%	0.242%
22	10.494	1429	1435	1441	rBV	33847	60904	5.51%	0.806%
23	10.571	1441	1448	1464	rVB	610877	1105719	100.00%	14.625%
24	10.765	1472	1481	1487	rVB4	17170	35936	3.25%	0.475%
25	10.835	1487	1493	1499	rVV4	13185	23746	2.15%	0.314%
26	11.012	1514	1523	1529	rVB6	13086	37578	3.40%	0.497%
27	11.870	1659	1669	1677	rBV	508749	929751	84.09%	12.298%
28	12.853	1827	1836	1846	rBV	397389	671261	60.71%	8.879%
29	13.794	1988	1996	2005	rBV	483155	795725	71.96%	10.525%

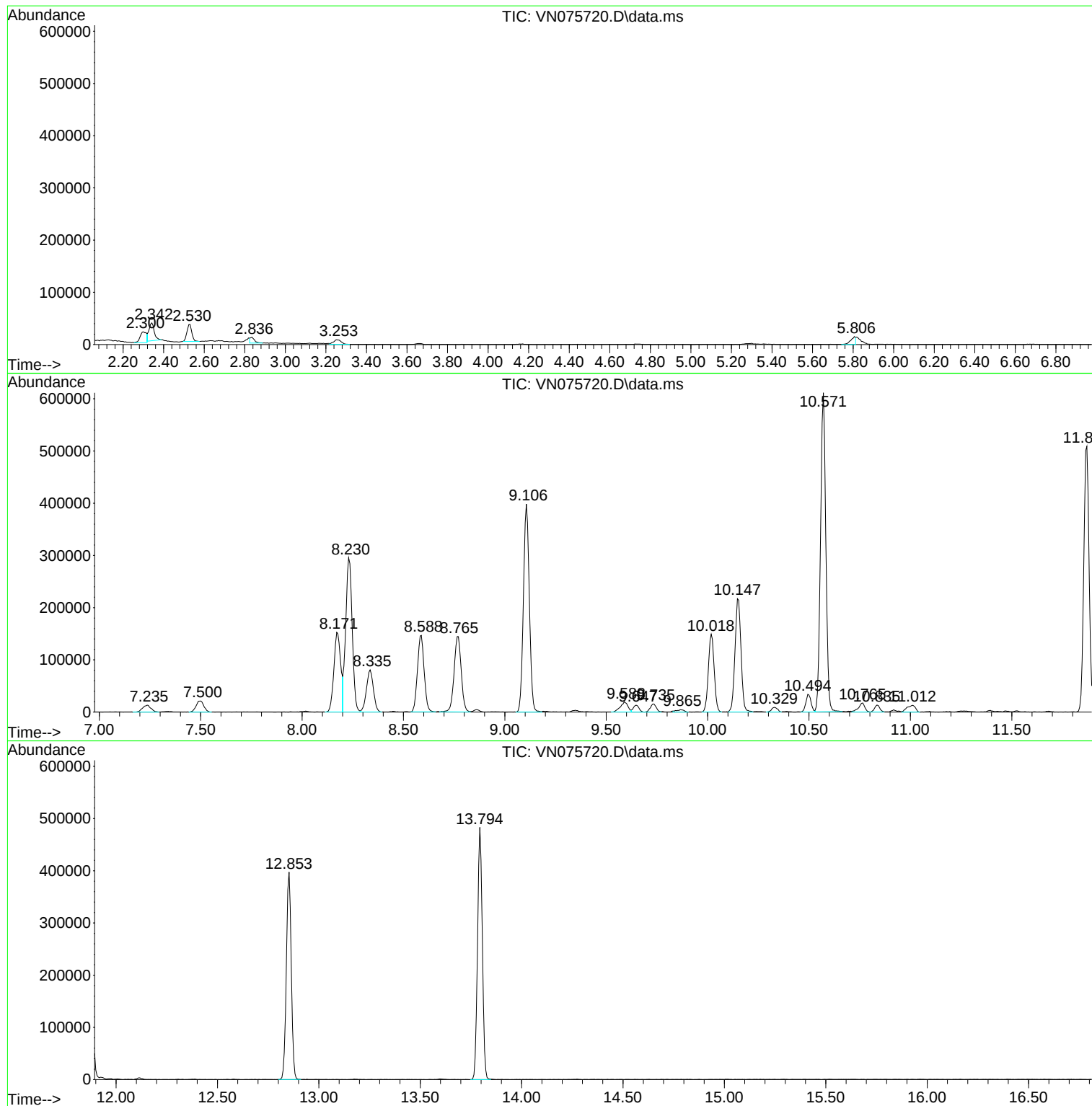
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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



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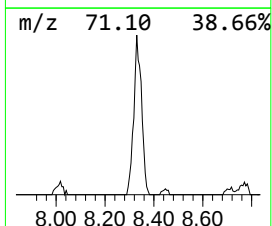
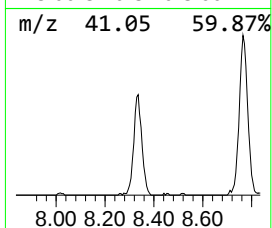
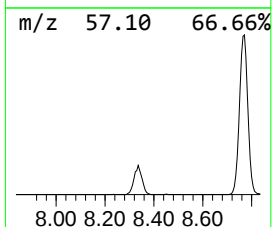
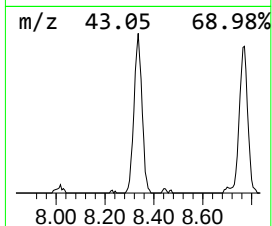
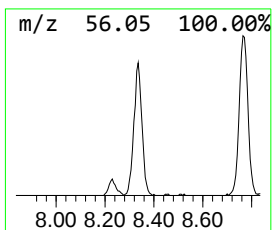
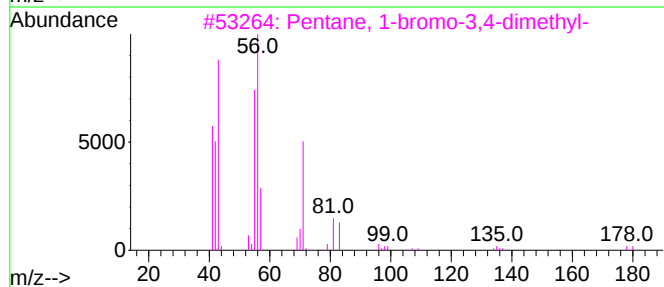
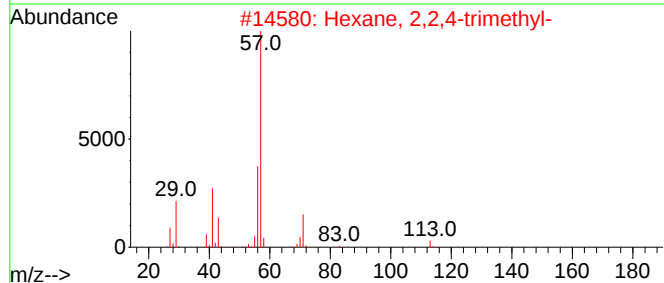
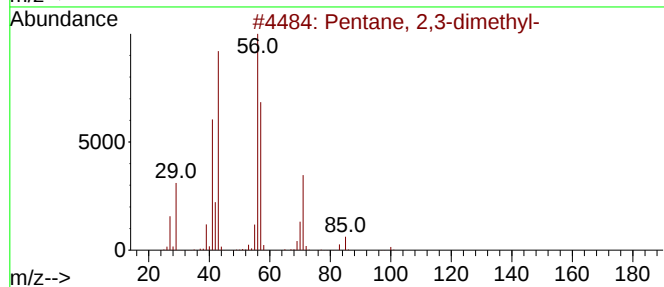
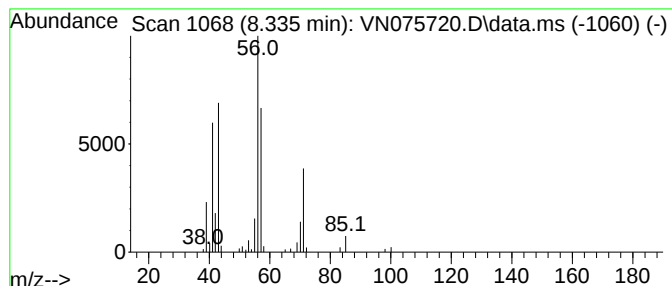
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.335	14.63 ug/l	191071	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	72
3			Pentane, 1-bromo-3,4-dimethyl-	178	C7H15Br	006570-92-9	50
4			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
5			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47



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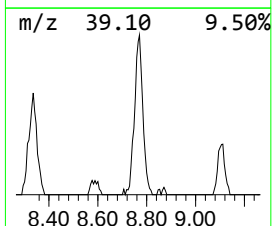
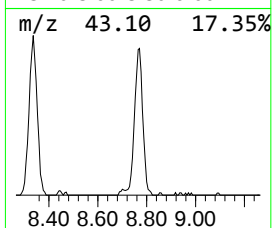
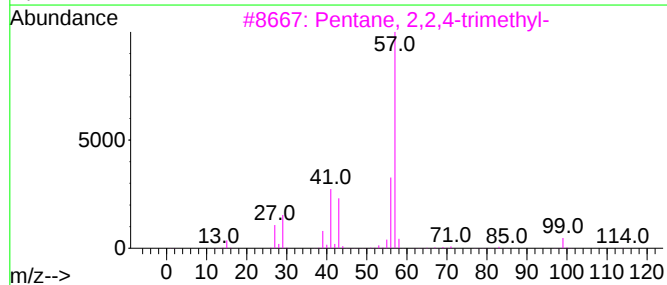
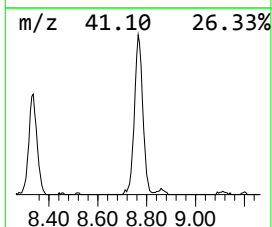
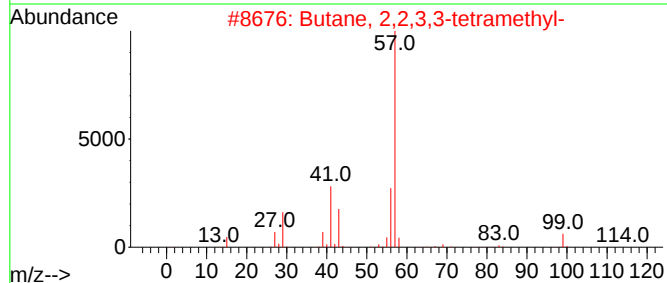
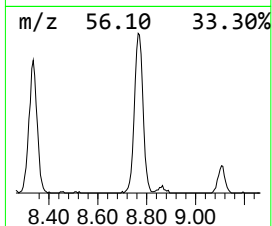
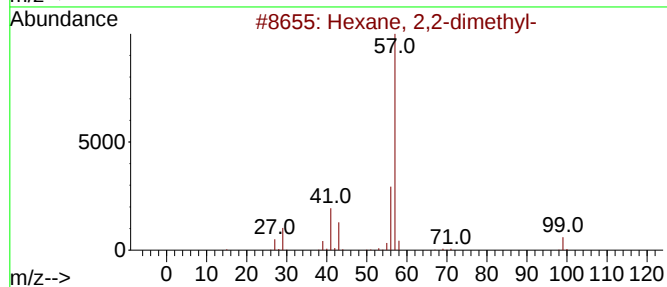
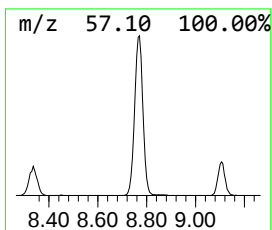
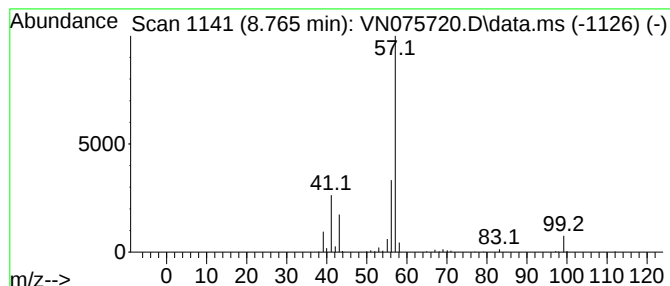
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120922W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	22.01 ug/l	353915	1,4-Difluorobenzene	9.106

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



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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
TOLL-MW-04

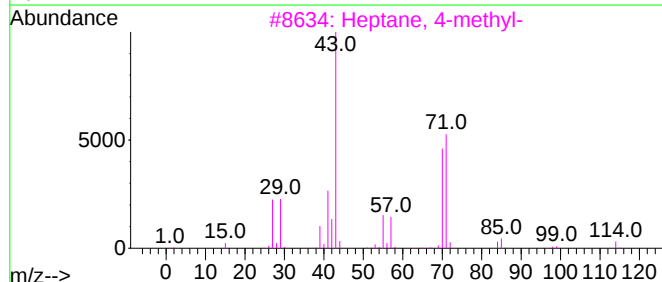
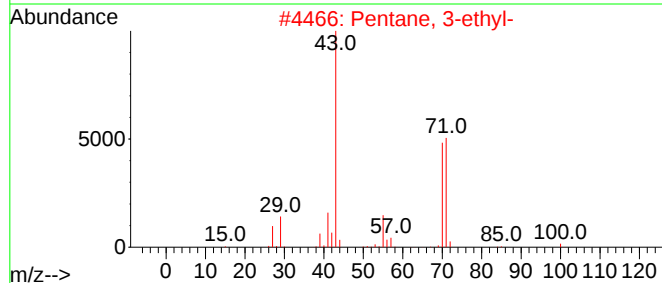
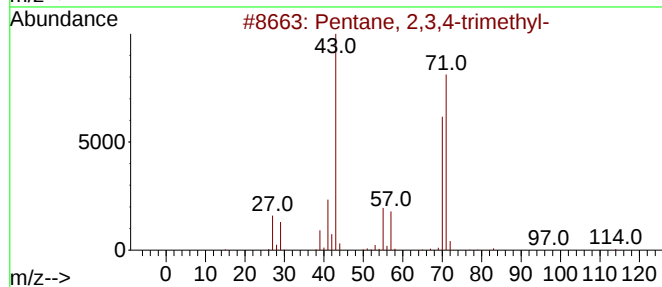
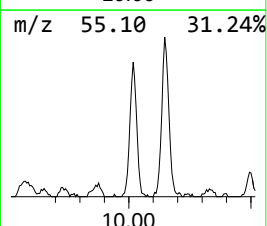
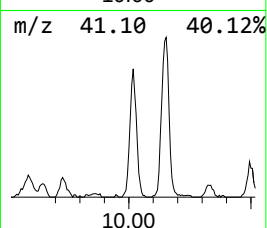
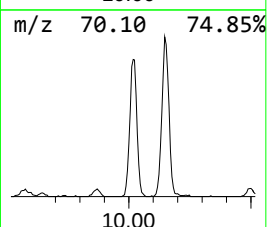
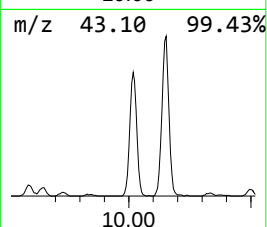
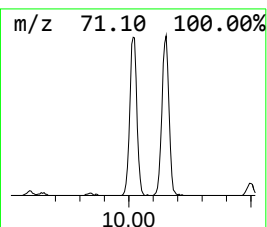
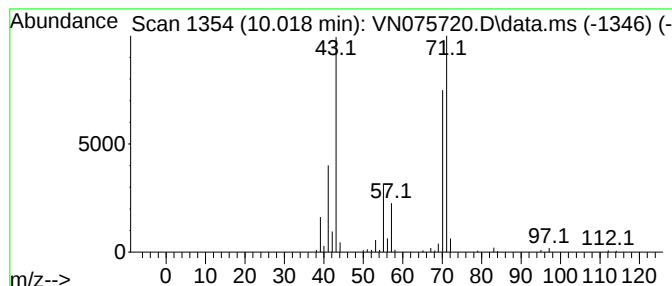
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.018	18.50 ug/l	297458	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	83
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



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Instrument :
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ClientSampleId :
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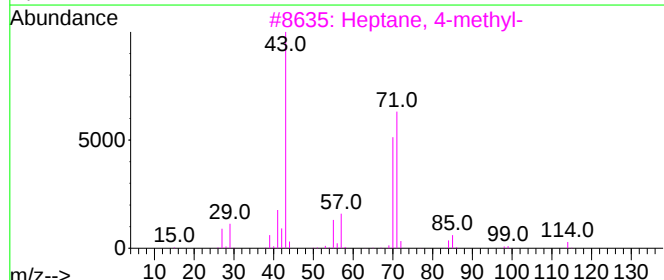
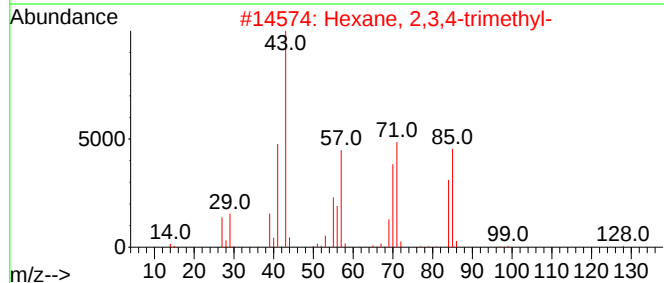
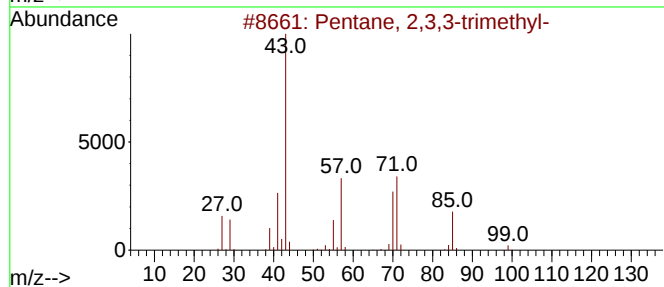
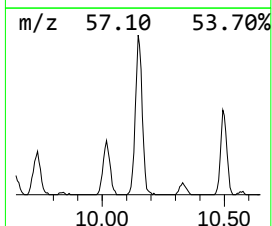
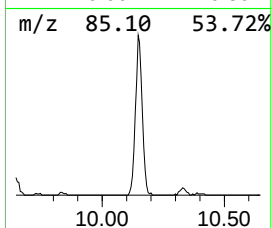
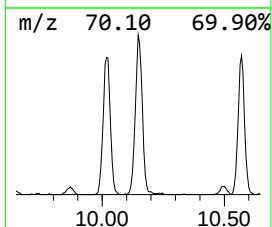
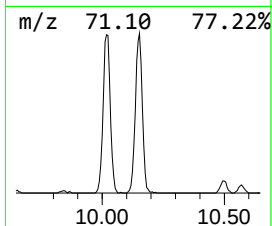
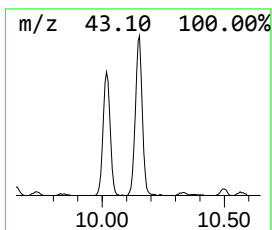
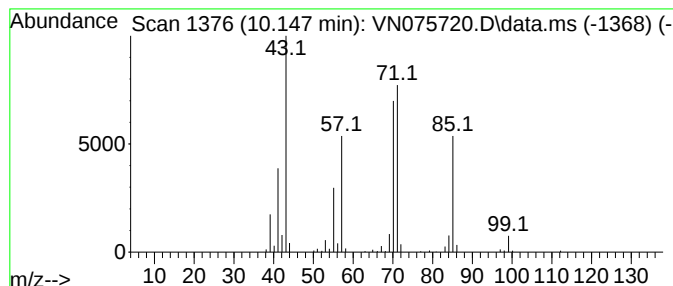
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.147	27.46 ug/l	441661	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
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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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, 2,3-di...	8.335	14.6	ug/l	191071	1	8.230	652988	50.0
Hexane, 2,2-dim...	8.765	22.0	ug/l	353915	2	9.106	804070	50.0
Pentane, 2,3,4-...	10.018	18.5	ug/l	297458	2	9.106	804070	50.0
Pentane, 2,3,3-...	10.147	27.5	ug/l	441661	2	9.106	804070	50.0