

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074666.D
 Acq On : 30 Sep 2022 14:52
 Operator : JC\MD
 Sample : N4863-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2R

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\82N092922W.M
 Title : SW846 8260

Signal : TIC: VN074666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	39	45	51	rBV	342537	632030	9.88%	2.004%
2	5.422	589	601	611	rBV3	62562	219615	3.43%	0.696%
3	7.869	1008	1017	1023	rBV	858400	2075254	32.44%	6.579%
4	7.934	1023	1028	1037	rVB	812147	1760648	27.52%	5.582%
5	8.292	1080	1089	1099	rBV	962268	2207709	34.51%	6.999%
6	8.469	1109	1119	1130	rBV2	727024	1776698	27.78%	5.633%
7	8.828	1171	1180	1192	rBV	1308806	2735342	42.76%	8.672%
8	9.457	1279	1287	1292	rBV3	49956	112831	1.76%	0.358%
9	9.751	1327	1337	1349	rBV	556521	1115849	17.44%	3.538%
10	9.881	1351	1359	1367	rVV2	190703	387766	6.06%	1.229%
11	10.310	1424	1432	1448	rBV	3553867	6396707	100.00%	20.280%
12	11.622	1646	1655	1666	rBV	2219727	3899084	60.95%	12.362%
13	12.604	1810	1822	1834	rBV	2645624	4419142	69.08%	14.011%
14	13.551	1975	1983	1995	rBV	2234427	3802660	59.45%	12.056%

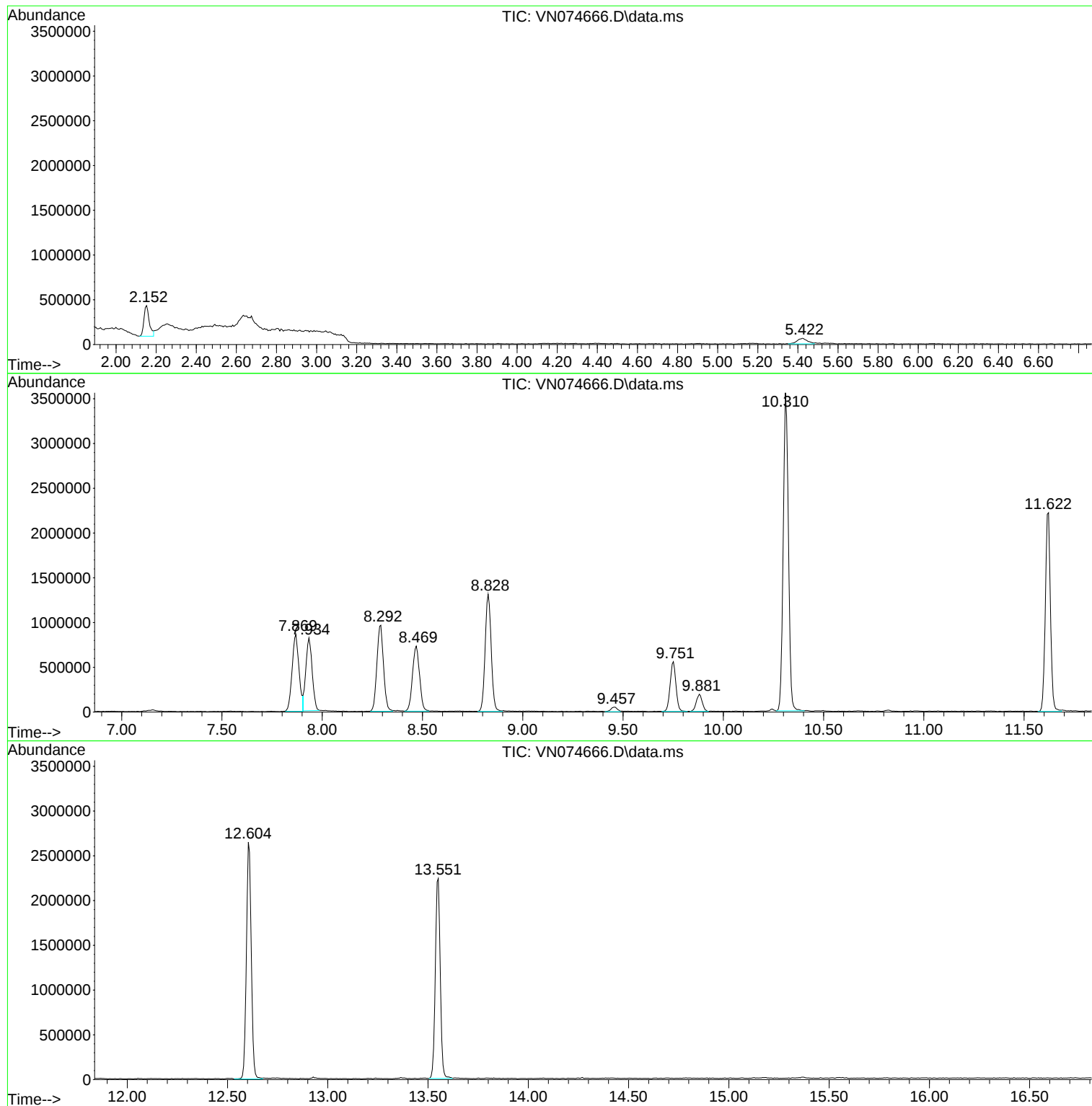
Sum of corrected areas: 31541335

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Quant Title : SW846 8260

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



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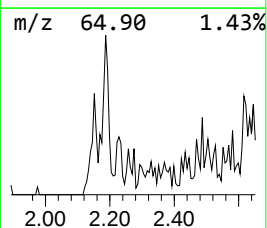
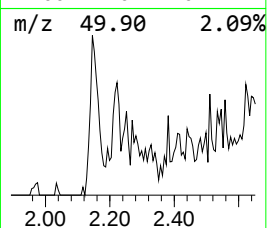
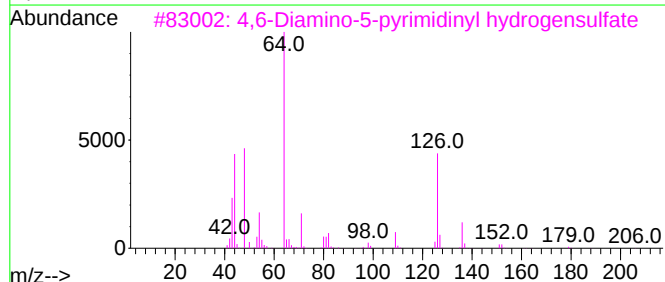
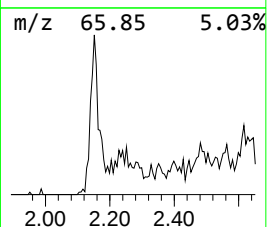
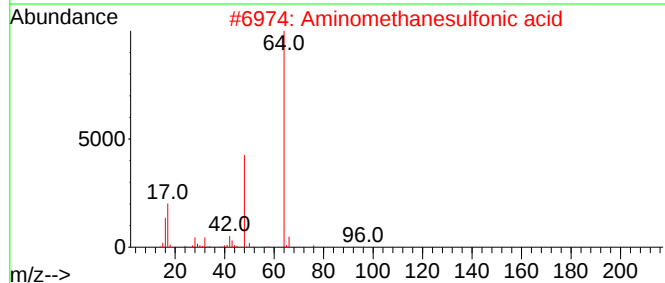
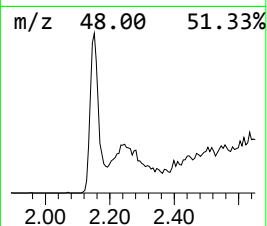
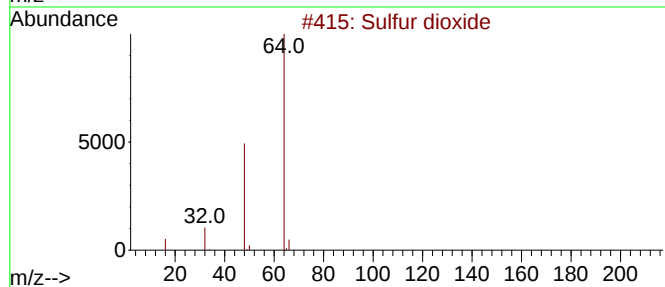
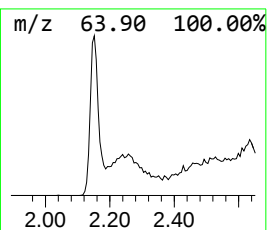
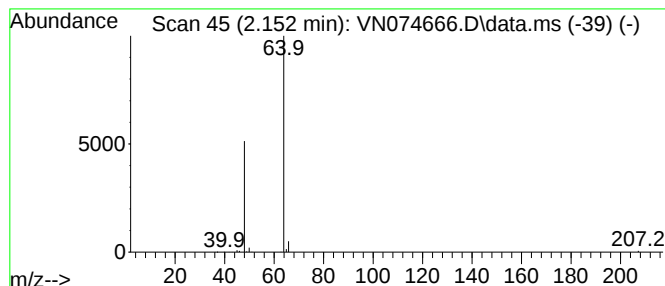
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	17.95 ug/l	632030	Pentafluorobenzene	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9
4			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	9
5			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9



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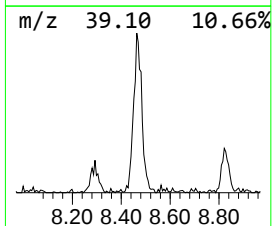
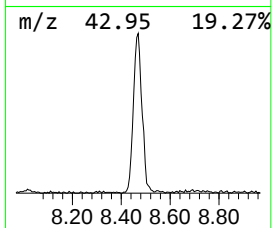
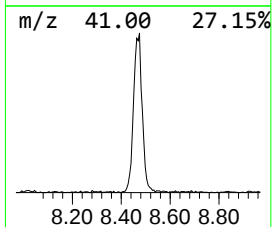
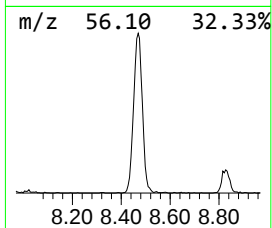
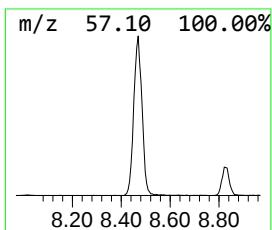
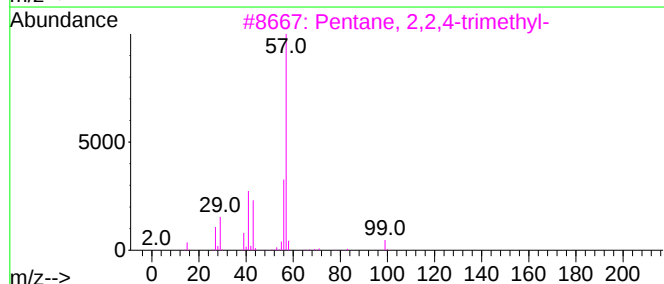
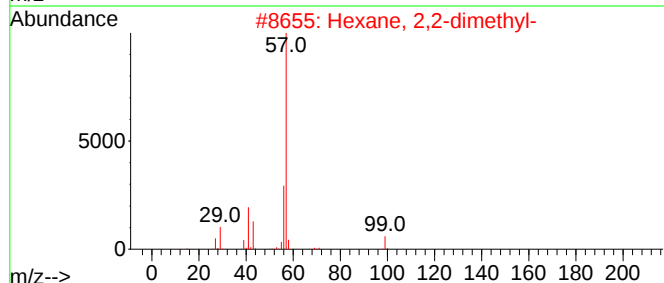
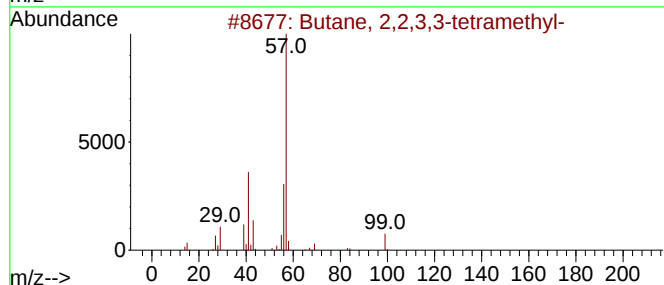
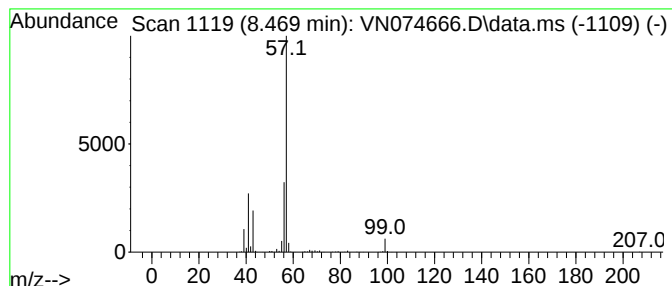
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	32.48 ug/l	1776700	1,4-Difluorobenzene	8.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	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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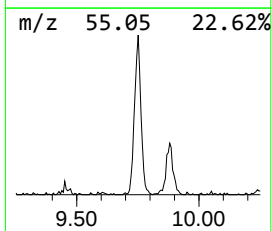
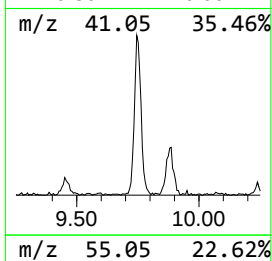
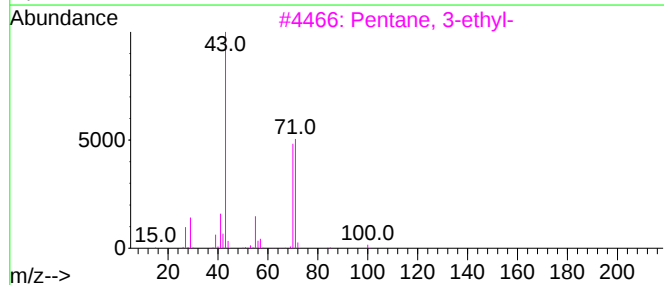
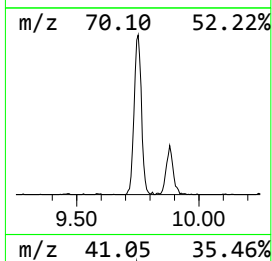
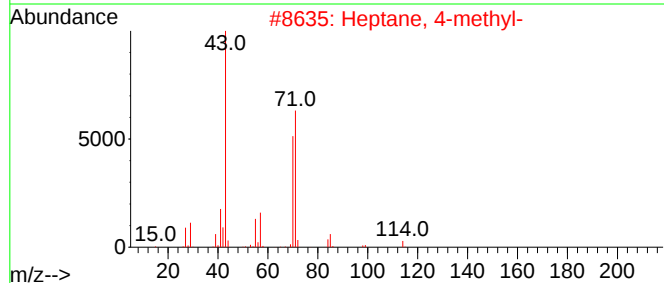
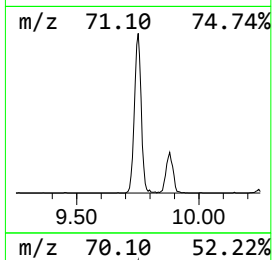
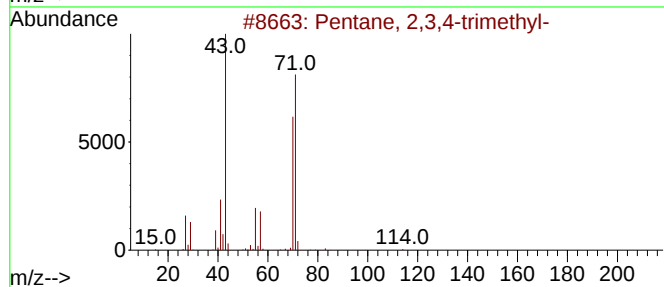
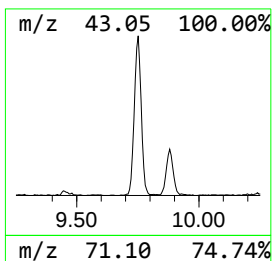
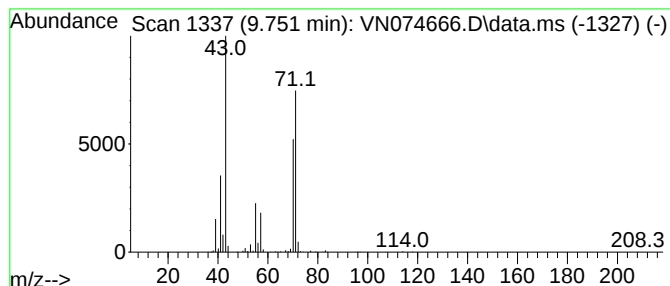
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Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	20.40 ug/l	1115850	1,4-Difluorobenzene	8.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	72



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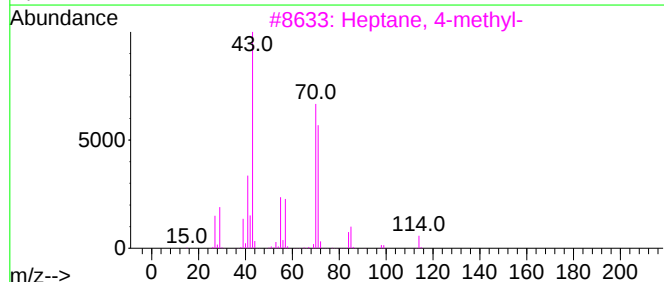
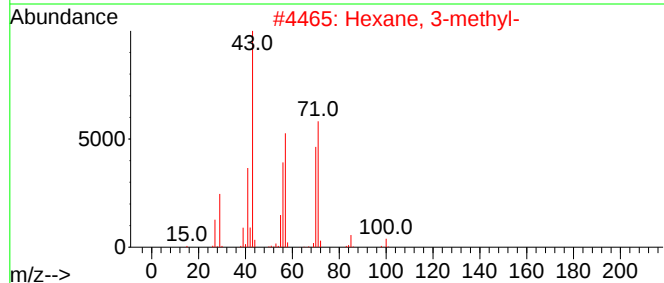
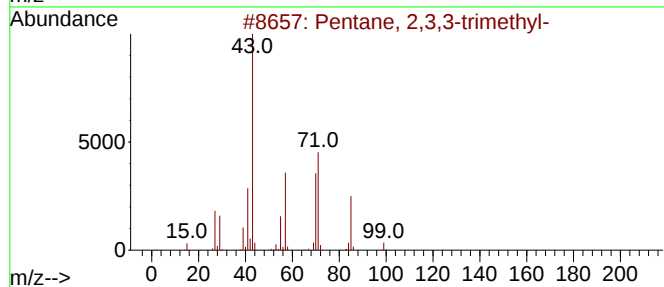
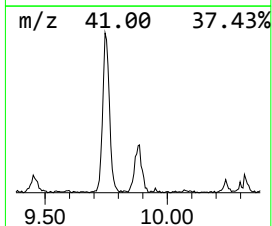
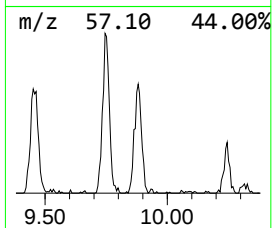
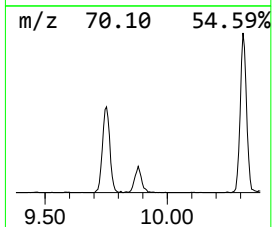
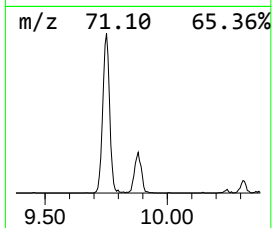
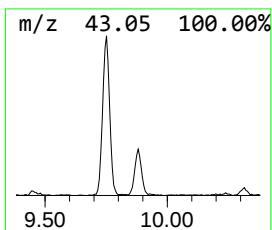
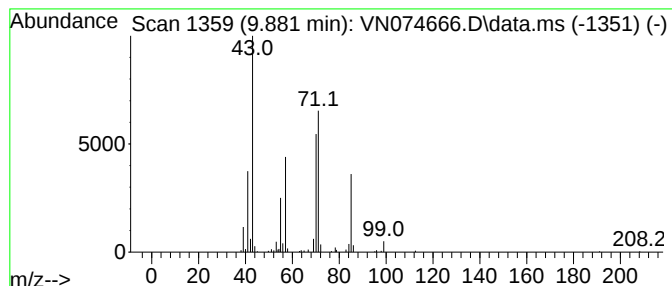
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.881	7.09 ug/l	387766	1,4-Difluorobenzene	8.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.152	17.9	ug/l	632030	1	7.934	1760650	50.0
Butane, 2,2,3,3...	8.469	32.5	ug/l	1776700	2	8.828	2735340	50.0
Pentane, 2,3,4-...	9.751	20.4	ug/l	1115850	2	8.828	2735340	50.0
Pentane, 2,3,3-...	9.881	7.1	ug/l	387766	2	8.828	2735340	50.0