LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027954.D
Acq On : 04 Apr 2022 13:52
Operator : JC/MD
Sample : N2249-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027954.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	38	rVB	40427	42979	9.07%	1.340%
2	1.373	42	47	52	rVV	34219	34538	7.29%	1.077%
3	1.751	104	109	116	rVB	31915	44515	9.40%	1.388%
4	1.971	138	145	152	rVB3	7267	11422	2.41%	0.356%
5	2.129	165	171	176	rBV5	2518	5220	1.10%	0.163%
6	2.215	179	185	192	rVB	8809	13555	2.86%	0.423%
7	2.337	200	205	215	rVB5	5815	12067	2.55%	0.376%
8	2.782	263	278	286	rBV2	19858	50467	10.65%	1.574%
9	2.873	286	293	301	rVV2	12366	29696	6.27%	0.926%
10	2.946	301	305	314	rVB3	2926	6431	1.36%	0.201%
11	3.105	321	331	343	rVB2	27401	63911	13.49%	1.993%
12	3.733	425	434	444	rBV4	2802	8235	1.74%	0.257%
13	3.836	444	451	459	rBV2	4465	10608	2.24%	0.331%
14	4.105	487	495	502	rBV3	2611	6538	1.38%	0.204%
15	4.300	521	527	538	rVB3	3577	9553	2.02%	0.298%
16	4.428	538	548	555	rBV6	2149	6695	1.41%	0.209%
17	5.385	693	705	716	rBV2	57303	165745	34.99%	5.169%
18	5.550	722	732	758	rVB	104568	310902	65.63%	9.695%
19	5.952	788	798	806	rBV	52692	138466	29.23%	4.318%
20	6.037	806	812	821	rVB2	16169	42421	8.95%	1.323%
21	6.232	832	844	858	rVB6	21470	75107	15.85%	2.342%
22	6.763	921	931	940	rBV	145199	350642	74.02%	10.934%
23	7.129	984	991	995	rBV2	4542	9454	2.00%	0.295%
24	7.177	995	999	1009	rVB4	2772	5789	1.22%	0.181%
25	7.982	1122	1131	1138	rVB2	4820	10023	2.12%	0.313%
26	8.110	1146	1152	1157	rVB3	5270	10293	2.17%	0.321%
27	8.427	1198	1204	1210	rVB3	3797	6850	1.45%	0.214%
28	8.500	1210	1216	1224	rBV2	7853	12535	2.65%	0.391%
29	8.647	1233	1240	1249	rBV	301428	473732	100.00%	14.773%
30	8.836	1261	1271	1279	rVB	10444	16799	3.55%	0.524%
31	10.055	1459	1471	1477	rBV	318226	424074	89.52%	13.224%
32	10.195	1490	1494	1499	rBV2	4006	4904	1.04%	0.153%
33	10.299	1507	1511	1517	rVB	5472	7346	1.55%	0.229%
34	11.079	1634	1639	1648	rBV	276989	359143	75.81%	11.199%
35	12.024	1789	1794	1801	rBV	314126	384537	81.17%	11.991%
36	12.243	1825	1830	1835	rVB	32631	41619	8.79%	1.298%

LSC Area Percent Report

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Data File : VX027954.D
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Operator : JC/MD
Sample : N2249-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Sum of corrected areas: 3206811

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027954.D
Acq On : 04 Apr 2022 13:52
Operator : JC/MD
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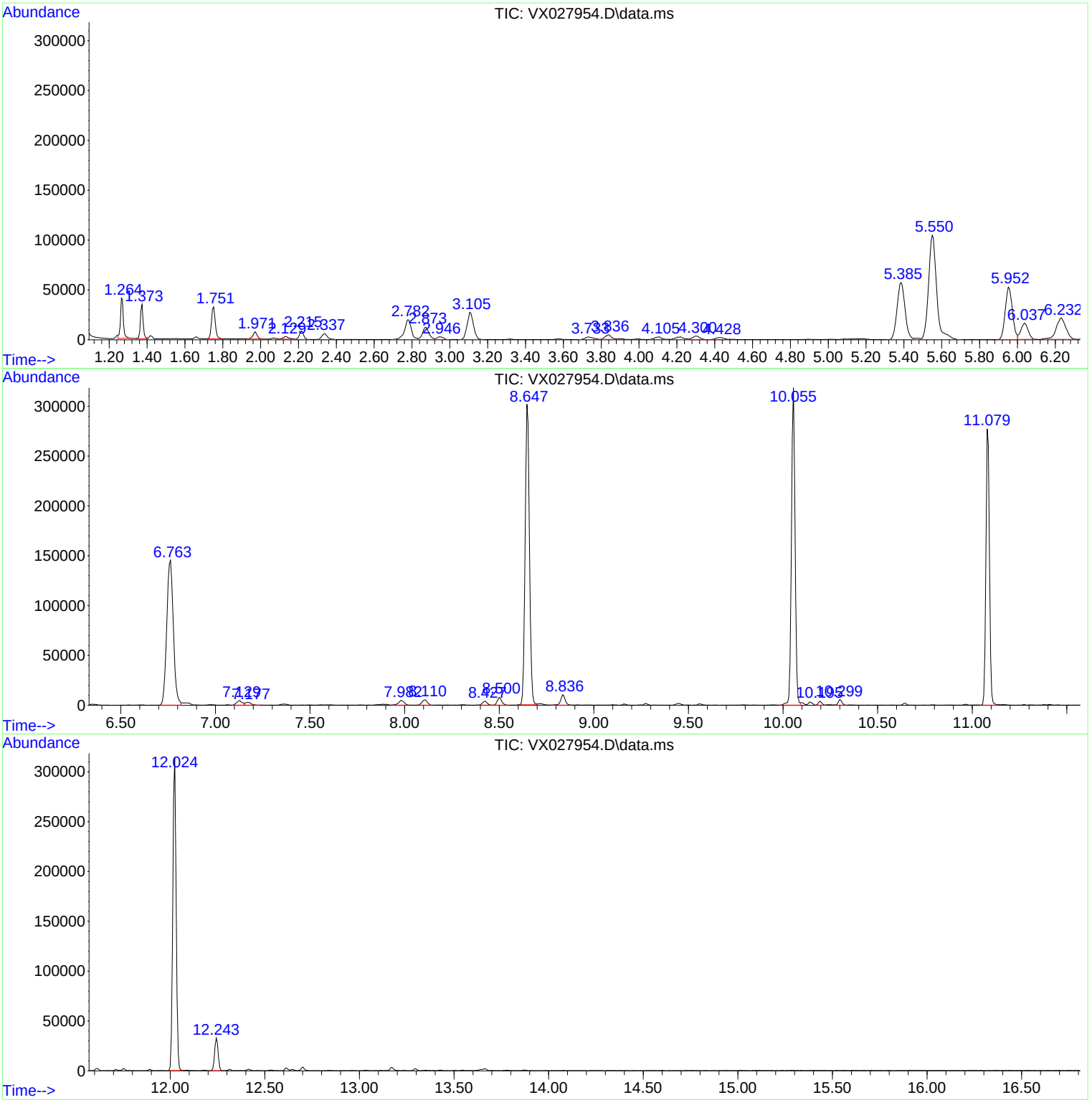
Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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Data File : VX027954.D
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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

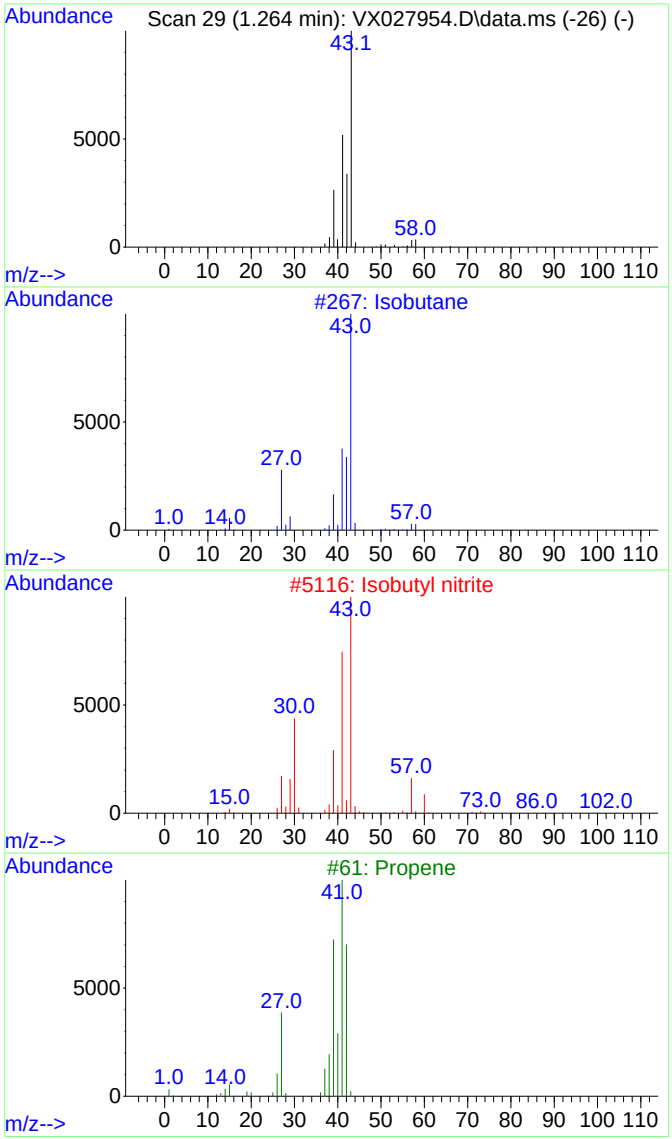
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

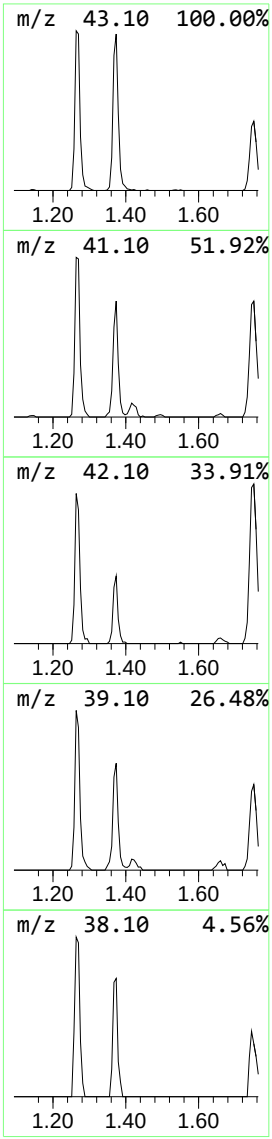
****

Peak Number 1 Isobutane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.91 ug/l	42979	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
3	Propene	42	C3H6	000115-07-1	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	4
5	Borane, trimethyl-	56	C3H9B	000593-90-8	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027954.D
Acq On : 04 Apr 2022 13:52
Operator : JC/MD
Sample : N2249-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

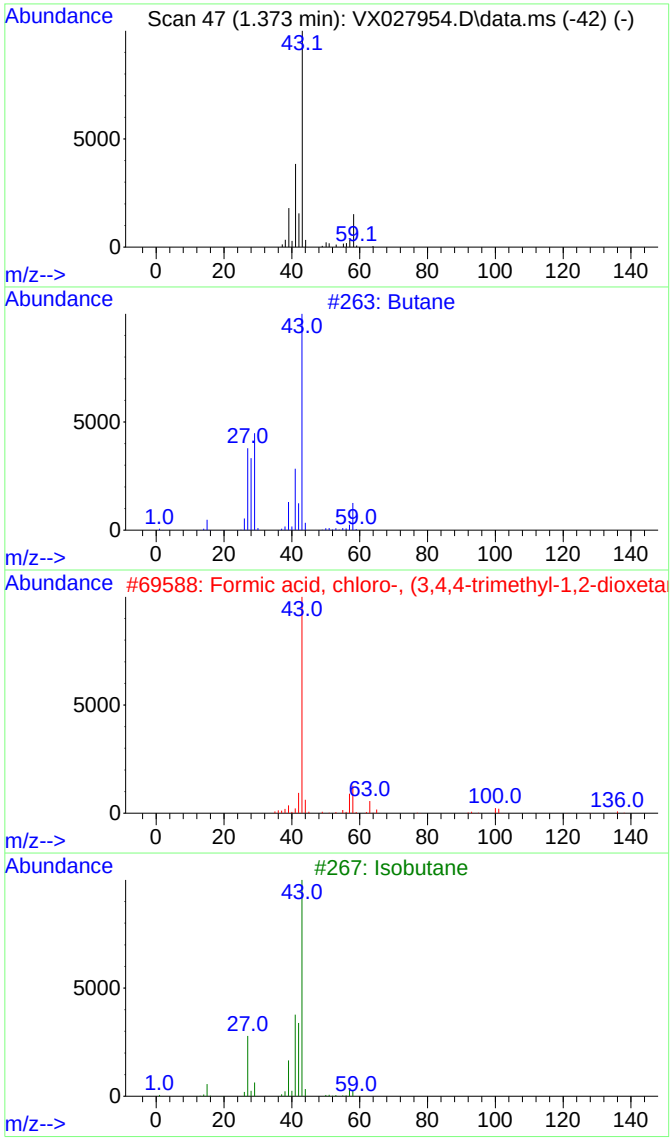
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

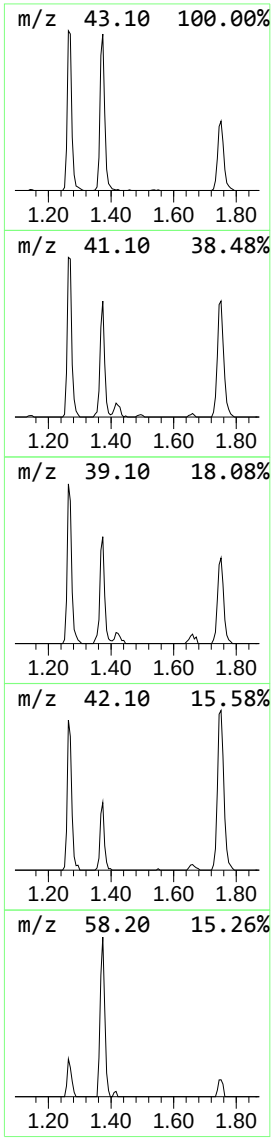
****

Peak Number 2 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.373	5.55 ug/l	34538	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	38
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





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Data File : VX027954.D
Acq On : 04 Apr 2022 13:52
Operator : JC/MD
Sample : N2249-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

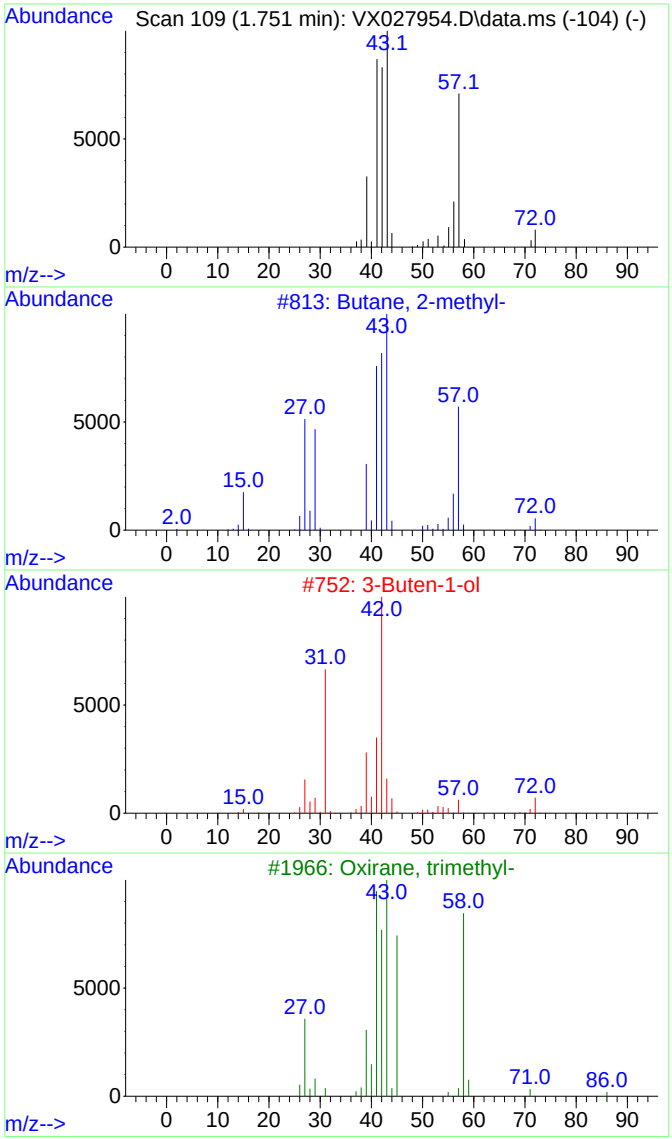
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

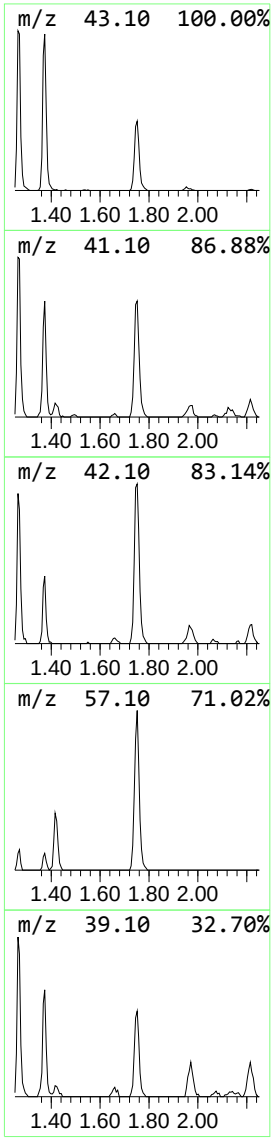
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.751	7.16 ug/l	44515	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
4	Pentane	72	C5H12	000109-66-0	33
5	Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	28





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

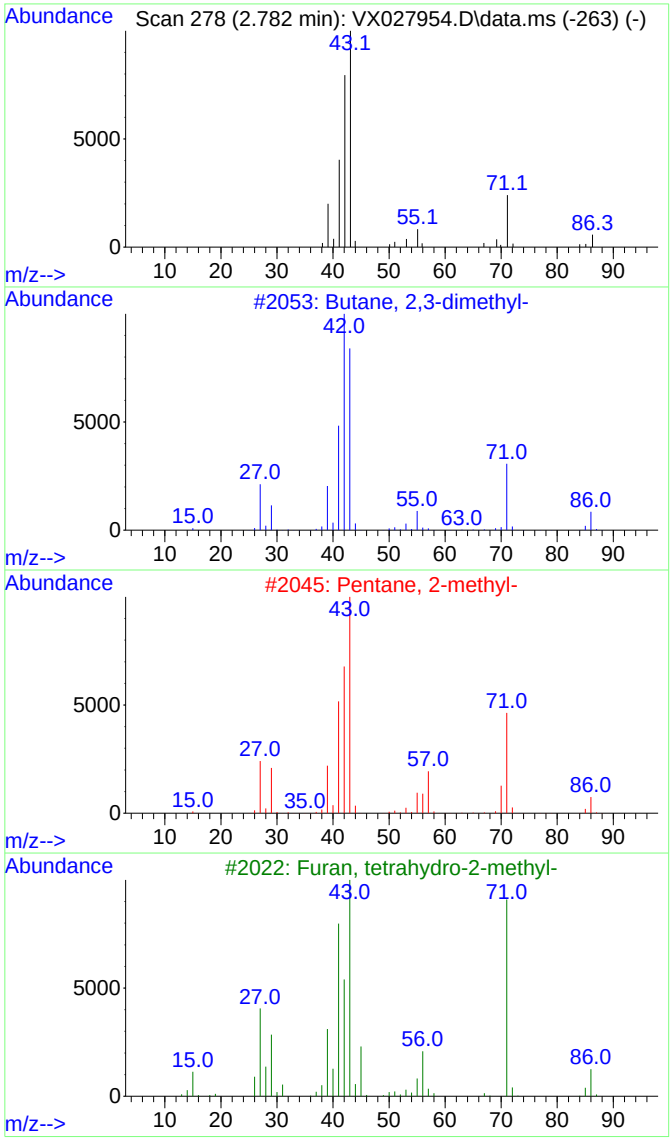
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

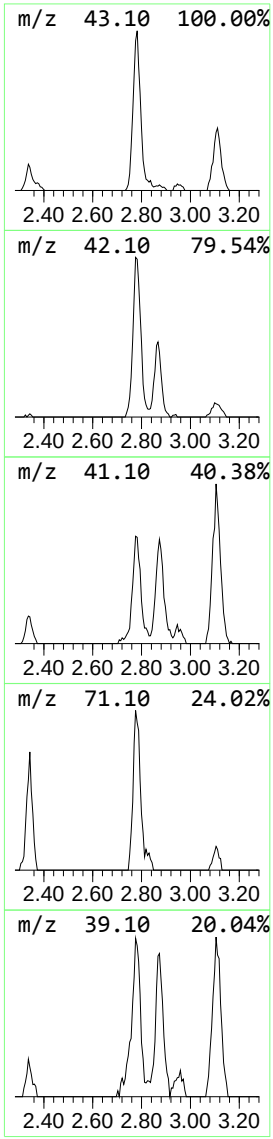
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	8.12 ug/l	50467	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	10
4	Pyrrolidine	71	C4H9N	000123-75-1	9
5	Octane, 2-methyl-	128	C9H20	003221-61-2	9





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

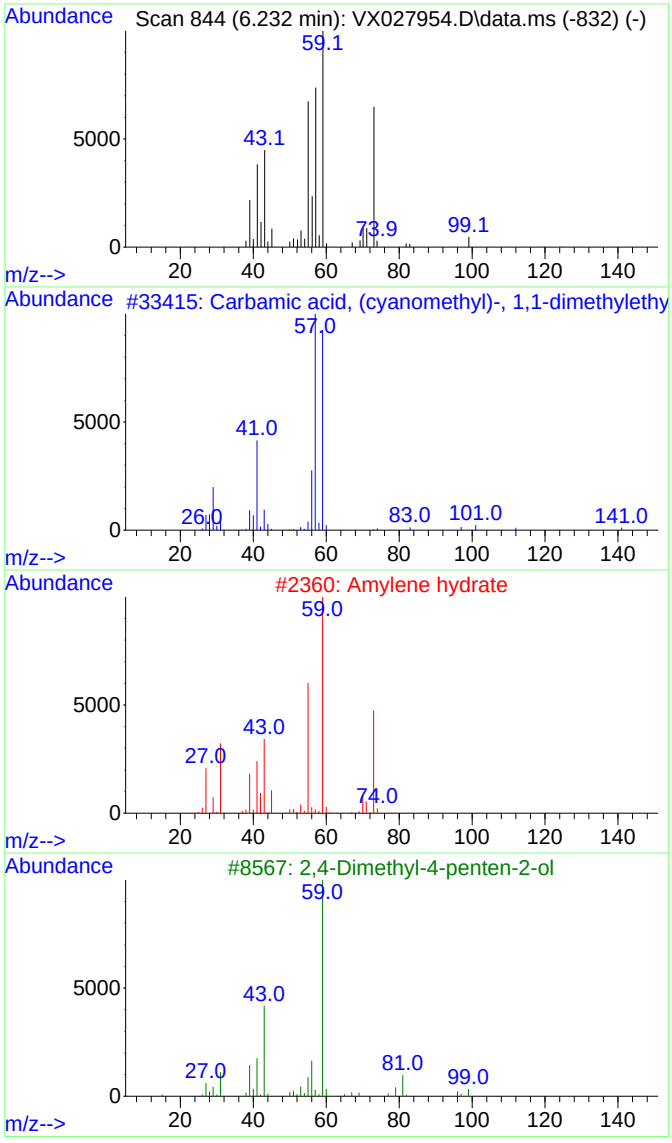
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

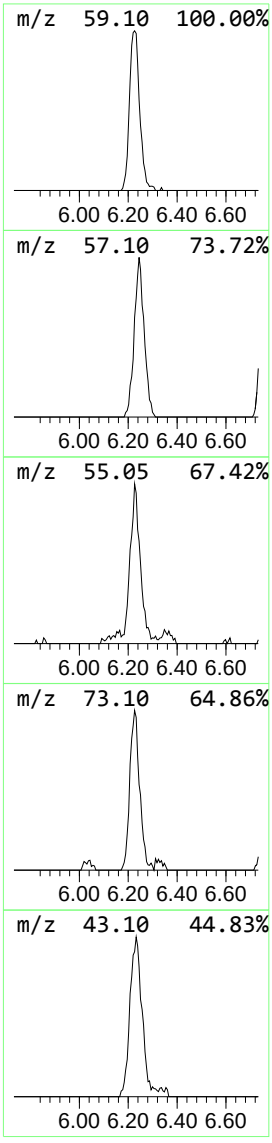
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Carbamic acid, (cyanomethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.232	10.71 ug/l	75107	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, (cyanomethyl)-, 1...	156	C7H12N2O2	085363-04-8	59
2	Amylene hydrate	88	C5H12O	000075-85-4	42
3	2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	33
4	Butanamide	87	C4H9NO	000541-35-5	25
5	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	22





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Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

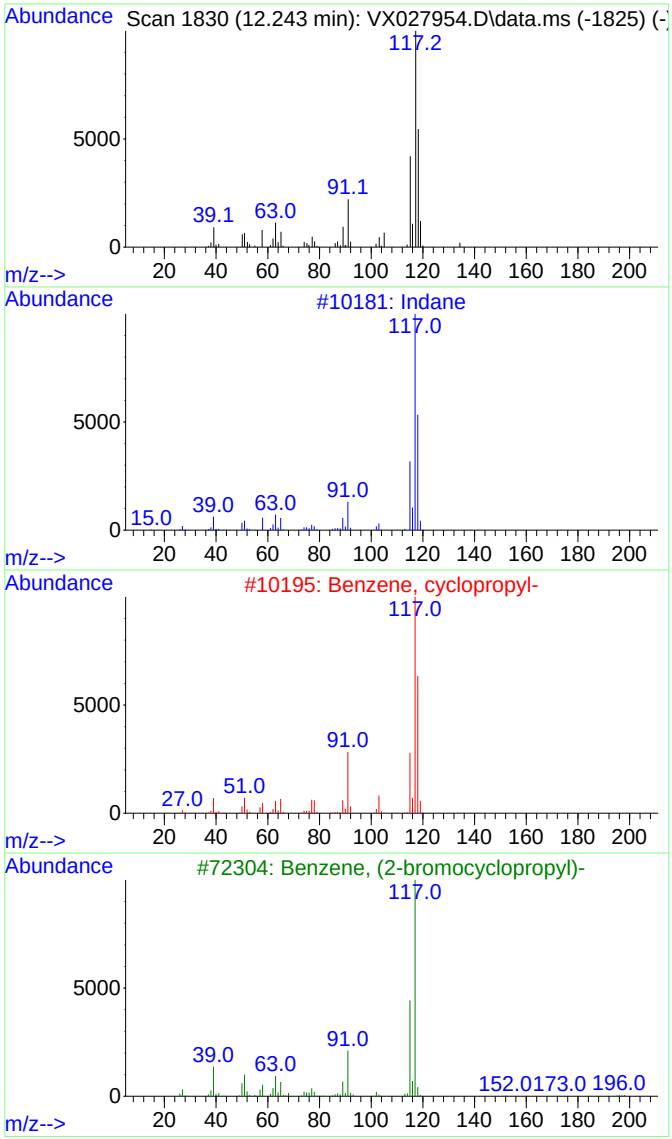
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

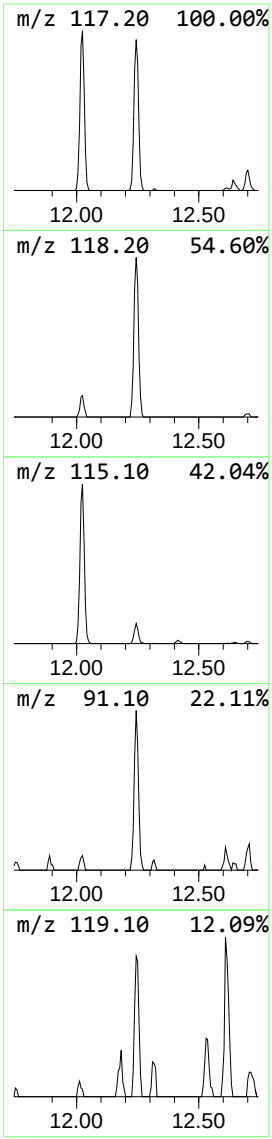
****

Peak Number 6 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	5.41 ug/l	41619	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	59
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58





Tentatively Identified Compound (LSC) summary

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isobutane	1.264	6.9	ug/l	42979	1	5.556	310902	50.0
Butane	1.373	5.6	ug/l	34538	1	5.556	310902	50.0
Butane, 2-methyl-	1.751	7.2	ug/l	44515	1	5.556	310902	50.0
Butane, 2,3-dim...	2.782	8.1	ug/l	50467	1	5.556	310902	50.0
Carbamic acid, ...	6.232	10.7	ug/l	75107	2	6.763	350642	50.0
Indane	12.243	5.4	ug/l	41619	4	12.024	384537	50.0