LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072922\
Data File : VX030306.D
Acq On : 29 Jul 2022 16:32
Operator : JC/MD
Sample : N3861-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-17

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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030306.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.227	20	23	27	rBV	11843	16914	1.39%	0.258%
2	1.368	41	46	50	rBV	20218	25242	2.08%	0.386%
3	1.746	104	108	122	rVB	82594	115212	9.49%	1.760%
4	1.953	137	142	147	rVB2	11330	17335	1.43%	0.265%
5	2.209	180	184	191	rVB	10261	16733	1.38%	0.256%
6	2.386	209	213	217	rVB	7539	12355	1.02%	0.189%
7	2.544	229	239	246	rBV2	6919	16517	1.36%	0.252%
8	2.782	268	278	283	rBV2	21644	53000	4.36%	0.810%
9	2.867	286	292	303	rVB2	38744	85610	7.05%	1.308%
10	3.105	323	331	339	rVB3	11084	26642	2.19%	0.407%
11	3.733	427	434	442	rBV2	7694	18135	1.49%	0.277%
12	3.837	442	451	459	rBV4	6076	14837	1.22%	0.227%
13	4.105	485	495	502	rBV5	5970	16856	1.39%	0.258%
14	4.306	518	528	540	rVB	63823	181129	14.92%	2.768%
15	4.434	540	549	558	rVB3	7352	20544	1.69%	0.314%
16	5.196	666	674	685	rVB5	5511	15888	1.31%	0.243%
17	5.391	695	706	714	rBV	137543	395280	32.55%	6.040%
18	5.471	714	719	725	rVV3	31489	91926	7.57%	1.405%
19	5.556	725	733	758	rVB	149975	457349	37.66%	6.988%
20	5.958	789	799	808	rBV	164540	438345	36.10%	6.698%
21	6.044	808	813	821	rVB2	18638	51711	4.26%	0.790%
22	6.172	826	834	839	rVV8	4023	13361	1.10%	0.204%
23	6.257	842	848	856	rVV4	6669	19407	1.60%	0.297%
24	6.361	859	865	873	rVB6	8553	21525	1.77%	0.329%
25	6.769	922	932	944	rBV	237160	592125	48.76%	9.048%
26	6.854	944	946	954	rVB6	7678	14717	1.21%	0.225%
27	7.178	992	999	1006	rVB6	8122	18375	1.51%	0.281%
28	7.385	1020	1033	1042	rBV6	21425	65835	5.42%	1.006%
29	7.988	1124	1132	1138	rVB3	5997	12542	1.03%	0.192%
30	8.110	1145	1152	1155	rBV2	15571	32449	2.67%	0.496%
31	8.141	1155	1157	1163	rVB2	17458	26702	2.20%	0.408%
32	8.513	1211	1218	1224	rVB6	9120	16516	1.36%	0.252%
33	8.653	1234	1241	1252	rVB	789052	1214308	100.00%	18.555%
34	9.165	1320	1325	1332	rBV	9964	15811	1.30%	0.242%
35	10.055	1466	1471	1479	rBV	565220	748489	61.64%	11.437%
36	11.085	1633	1640	1650	rBV	594612	754273	62.12%	11.525%

LSC Area Percent Report

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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

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Peak separation: 5

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Title : SW846 8260

37	12.024	1788	1794	1804	rBV	721072	878171	72.32%	13.419%
38	12.250	1823	1831	1836	rBV5	5738	12251	1.01%	0.187%

Sum of corrected areas: 6544417

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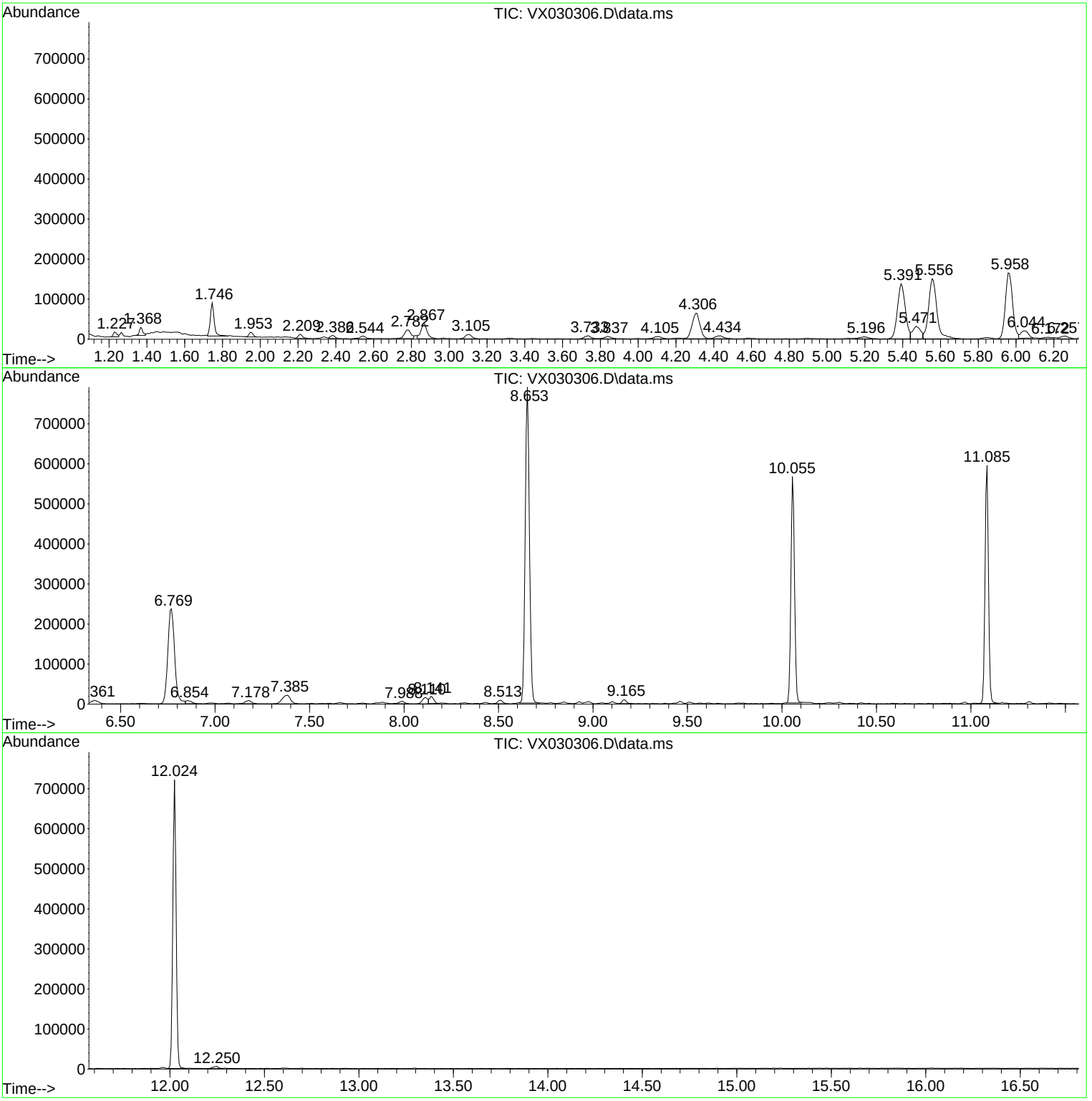
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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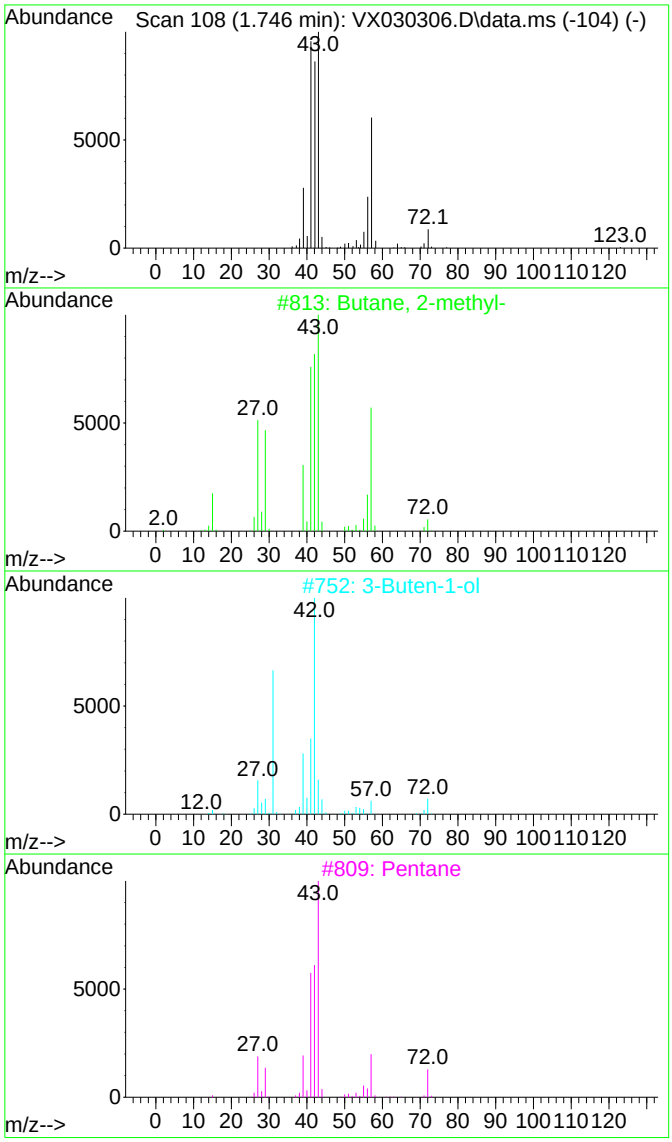
Quant Title : SW846 8260

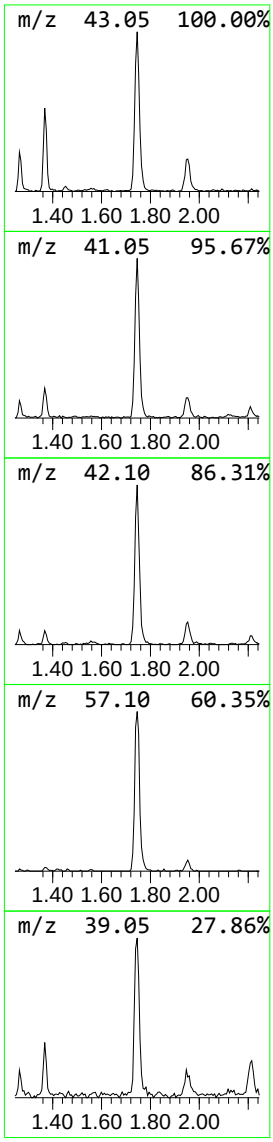
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	12.60 ug/l	115212	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	49
3	Pentane	72	C5H12	000109-66-0	40
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14
5	Butane, 1-isocyano-	83	C5H9N	002769-64-4	12





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MSVOA_X
ClientSampleId :
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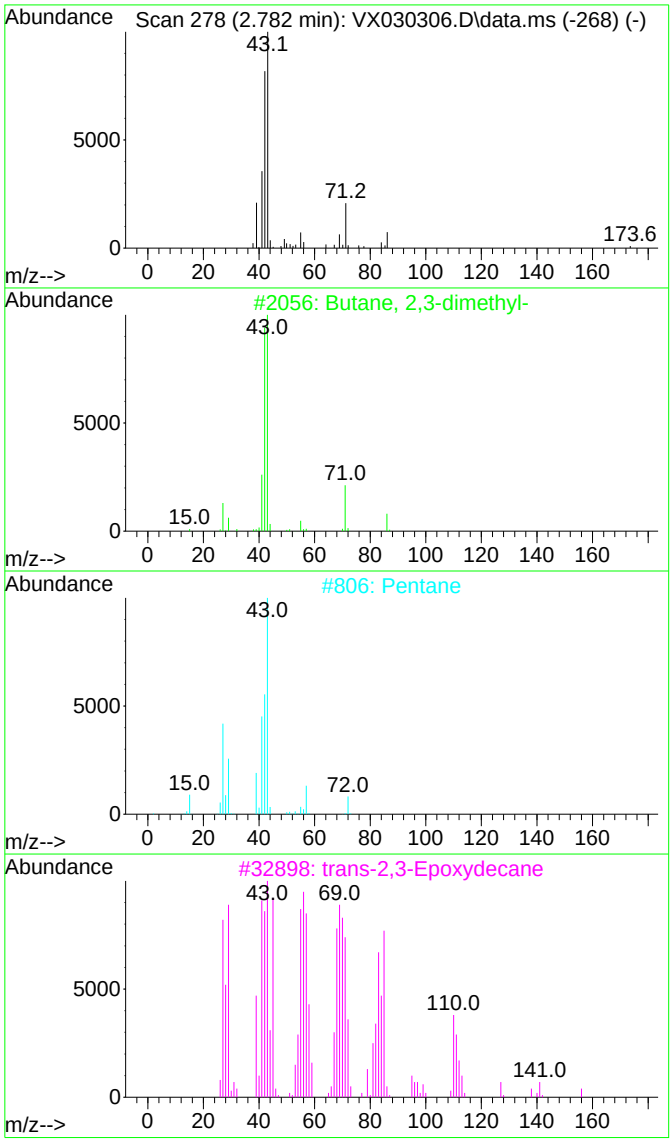
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

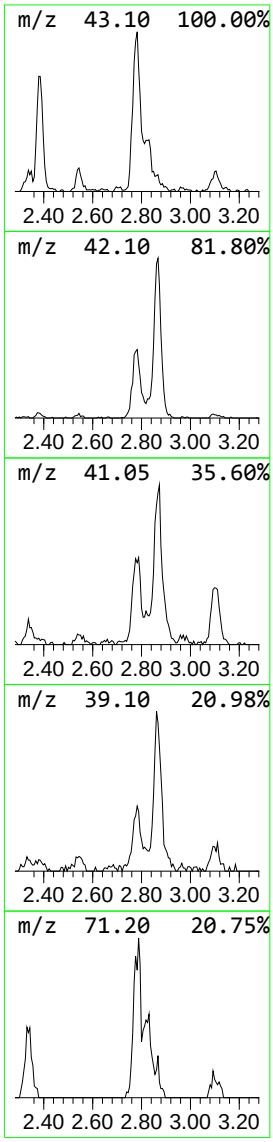
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	5.79 ug/l	53000	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane	72	C5H12	000109-66-0	36
3	trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	36
4	1-Pentene	70	C5H10	000109-67-1	28
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	28





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Instrument :
MSVOA_X
ClientSampleId :
MW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

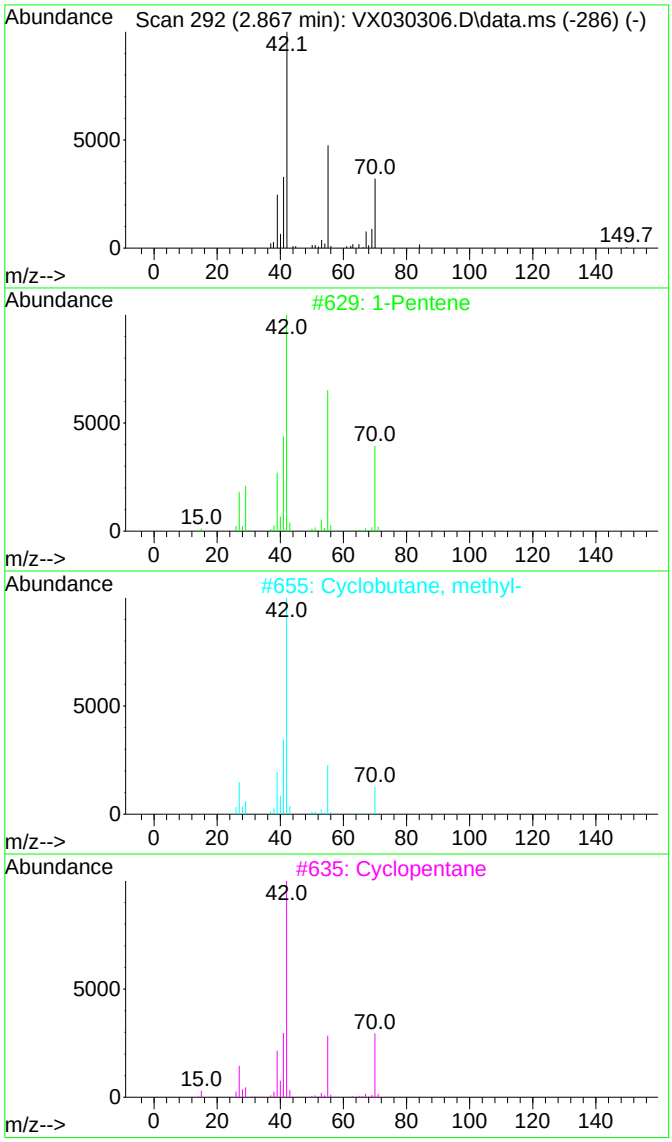
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

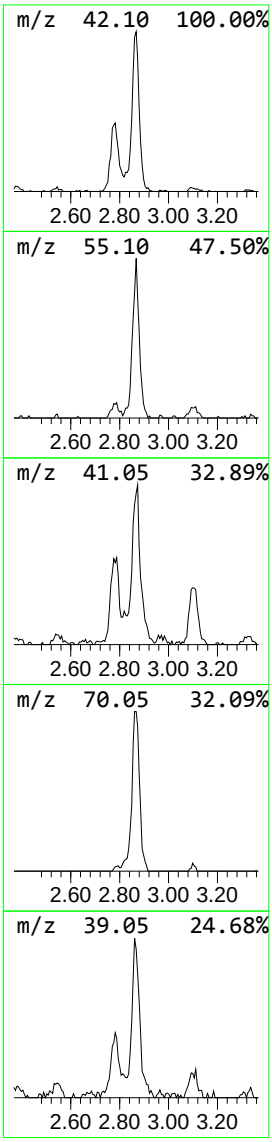
****

Peak Number 3 1-Pentene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	9.36 ug/l	85610	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	Cyclopentane	70	C5H10	000287-92-3	64
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
5	3-Buten-1-ol	72	C4H8O	000627-27-0	40





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MSVOA_X
ClientSampleId :
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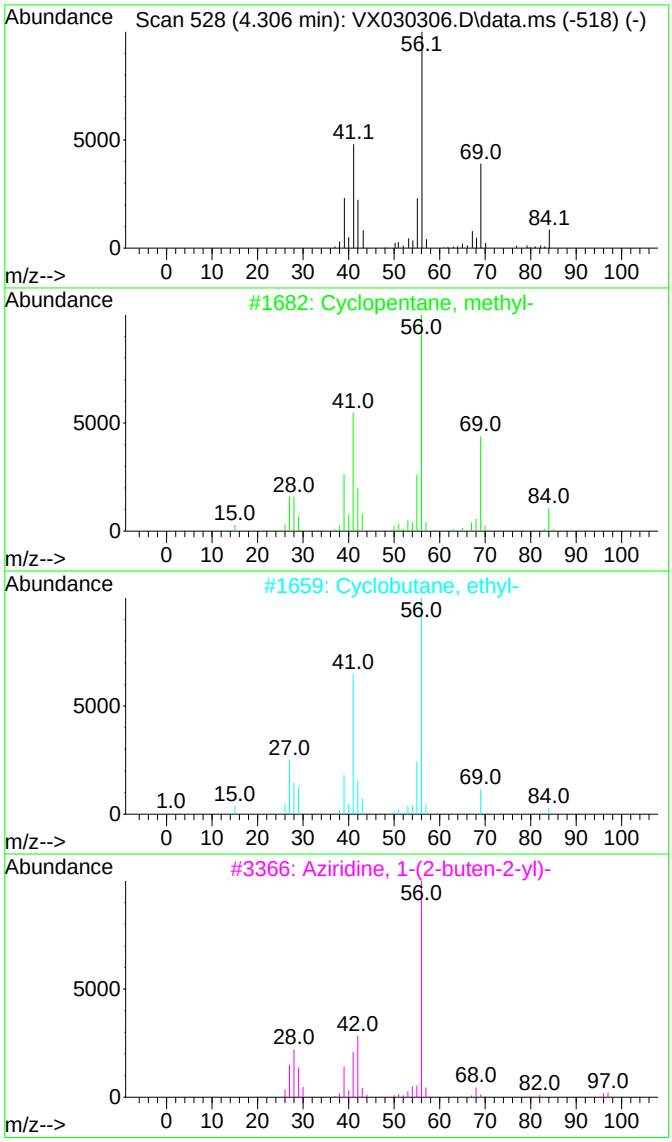
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

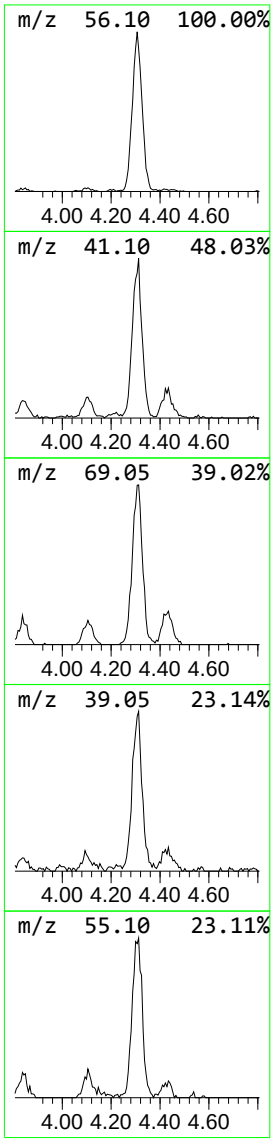
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	19.80 ug/l	181129	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3	Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	39
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	39
5	Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	36





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
Butane, 2-methyl-	1.746	12.6	ug/l	115212	1	5.556	457349	50.0
Butane, 2,3-dim...	2.782	5.8	ug/l	53000	1	5.556	457349	50.0
1-Pentene	2.867	9.4	ug/l	85610	1	5.556	457349	50.0
Cyclopentane, m...	4.306	19.8	ug/l	181129	1	5.556	457349	50.0