

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121619\
 Data File : VU036243.D
 Acq On : 16 Dec 2019 18:56
 Operator : JC/MD
 Sample : K6275-09
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDS5

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.369	3	9	29	rVB	1940378	1911322	100.00%	16.014%
2	1.456	30	36	45	rBV	35120	37315	1.95%	0.313%
3	1.507	45	52	59	rBV	73087	78306	4.10%	0.656%
4	1.607	74	83	94	rBV3	761548	1199360	62.75%	10.049%
5	1.678	100	105	109	rBV	39469	38548	2.02%	0.323%
6	1.703	109	113	119	rVB	32395	31697	1.66%	0.266%
7	1.748	121	127	138	rBV3	113550	139121	7.28%	1.166%
8	1.928	175	183	199	rVB2	146856	223195	11.68%	1.870%
9	2.015	203	210	222	rVB	74951	102933	5.39%	0.862%
10	2.176	251	260	268	rBV	161071	217816	11.40%	1.825%
11	2.227	268	276	287	rBV3	83679	152457	7.98%	1.277%
12	2.340	304	311	318	rBV	24578	38771	2.03%	0.325%
13	2.385	318	325	332	rVV3	34692	52896	2.77%	0.443%
14	2.440	334	342	351	rVB2	52045	83641	4.38%	0.701%
15	2.594	374	390	403	rBV	150740	258305	13.51%	2.164%
16	2.662	403	411	422	rVB	20417	33944	1.78%	0.284%
17	2.825	448	462	476	rBV	55477	106251	5.56%	0.890%
18	3.015	505	521	526	rBV6	17548	41024	2.15%	0.344%
19	3.411	627	644	661	rBV2	87232	219561	11.49%	1.840%
20	3.626	697	711	730	rVB5	22708	57334	3.00%	0.480%
21	4.237	884	901	913	rBV5	6632	20190	1.06%	0.169%
22	4.684	1026	1040	1089	rBV2	124620	449871	23.54%	3.769%
23	5.112	1157	1173	1196	rBV2	157994	359716	18.82%	3.014%
24	5.771	1357	1378	1406	rBV2	285023	806853	42.21%	6.760%
25	6.060	1461	1468	1481	rVB5	10221	20405	1.07%	0.171%
26	6.292	1525	1540	1563	rBV	289683	581597	30.43%	4.873%
27	6.581	1616	1630	1652	rBV	183641	359947	18.83%	3.016%
28	6.732	1663	1677	1694	rBV	186378	378199	19.79%	3.169%
29	7.603	1933	1948	1969	rBV	86096	165865	8.68%	1.390%
30	7.931	2038	2050	2064	rBV	307283	549470	28.75%	4.604%
31	8.002	2065	2072	2082	rVB2	17406	32167	1.68%	0.270%
32	8.214	2125	2138	2149	rBV	54800	103617	5.42%	0.868%
33	8.684	2269	2284	2321	rBV	317147	868402	45.43%	7.276%
34	8.832	2322	2330	2341	rVB	9199	20863	1.09%	0.175%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR121319WMA.M
Title : TRACE VOA SOM01.0

35	9.446	2508	2521	2542	rBV	412971	772294	40.41%	6.470%
36	10.783	2924	2937	2958	rBV2	165723	286583	14.99%	2.401%
37	11.838	3253	3265	3282	rVB	310347	538436	28.17%	4.511%
38	12.217	3368	3383	3402	rBV	278311	477846	25.00%	4.004%
39	13.468	3764	3772	3786	rBV4	20722	31610	1.65%	0.265%
40	13.963	3919	3926	3938	rVB9	9433	19664	1.03%	0.165%
41	14.304	4021	4032	4044	rBV8	11412	23199	1.21%	0.194%
42	14.696	4139	4154	4166	rBV8	10396	25513	1.33%	0.214%
43	15.037	4251	4260	4268	rBV10	10536	19567	1.02%	0.164%

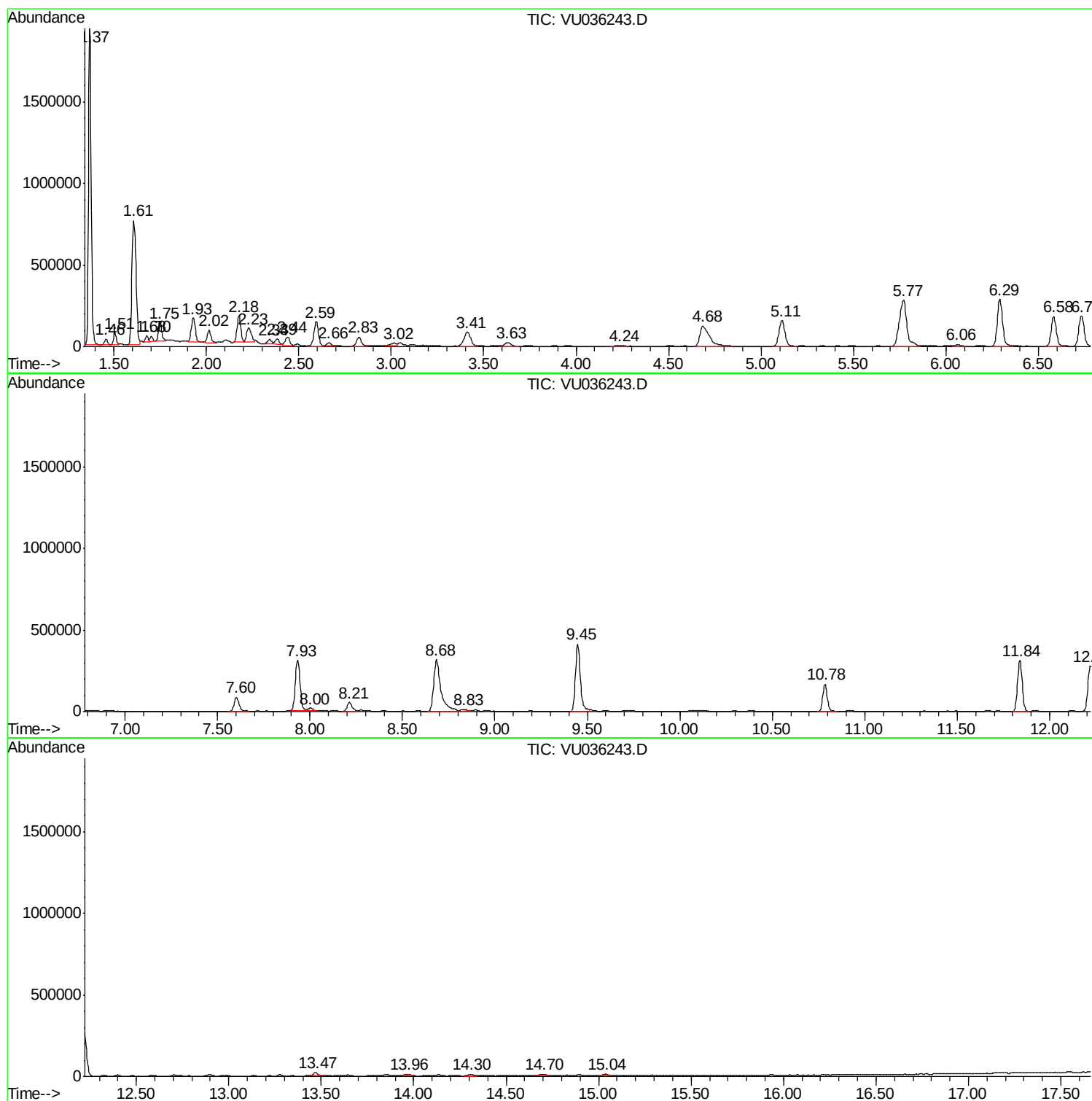
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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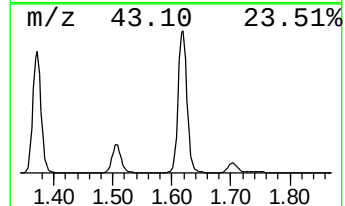
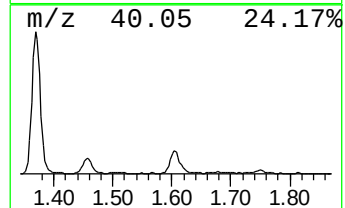
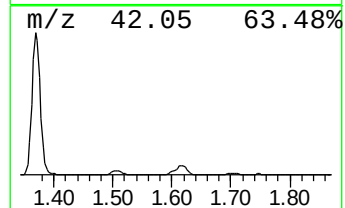
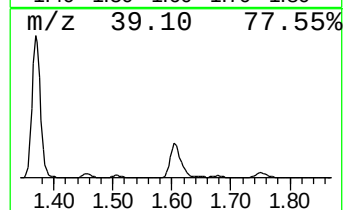
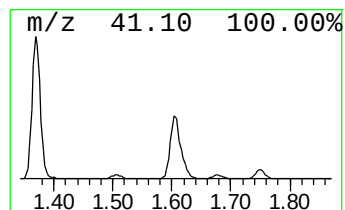
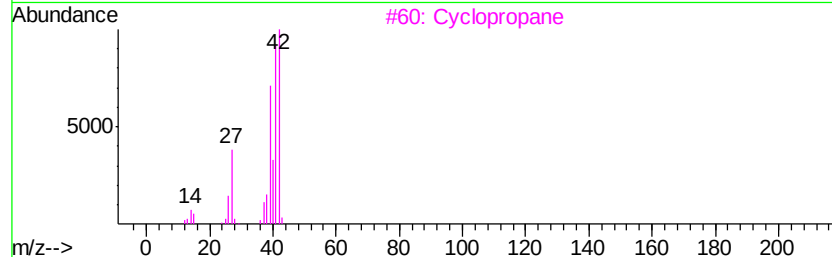
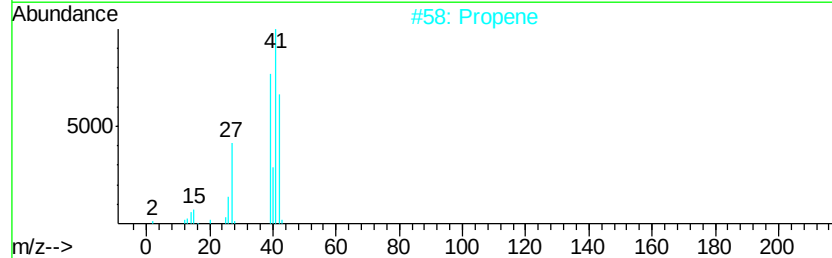
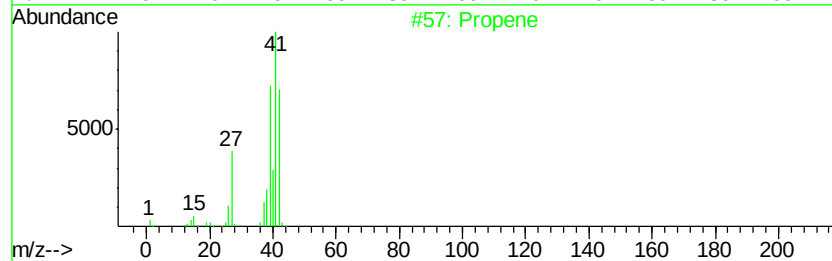
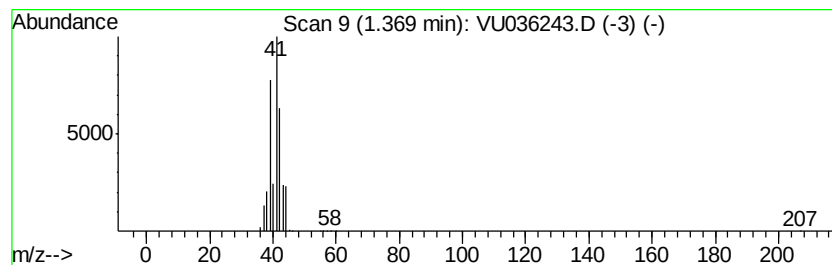
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Cyclic1.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	16.43 ug/L	1911320	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Propene	42	C3H6	000115-07-1	42
3		Cyclopropane	42	C3H6	000075-19-4	9
4		Cyclopropene	40	C3H4	002781-85-3	9
5		Cyclopropane	42	C3H6	000075-19-4	7



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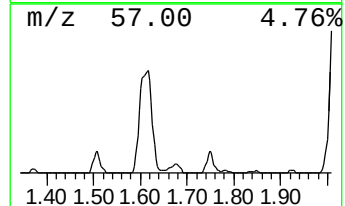
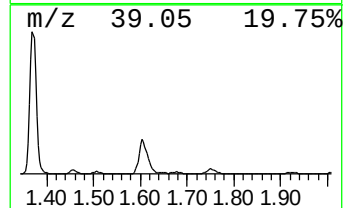
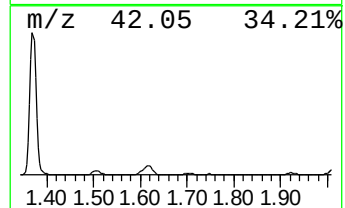
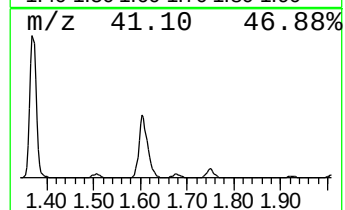
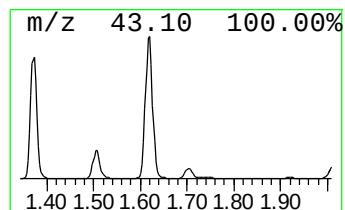
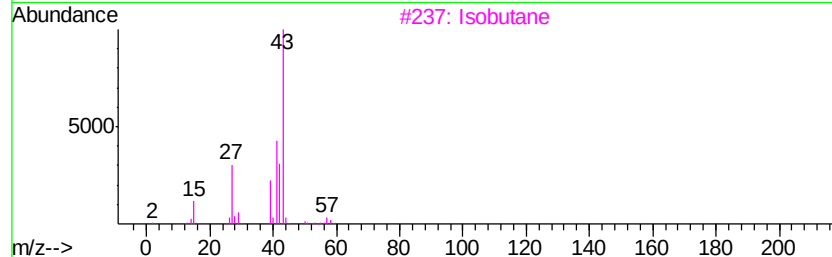
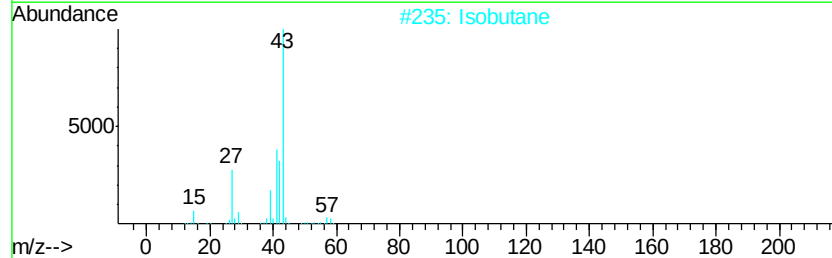
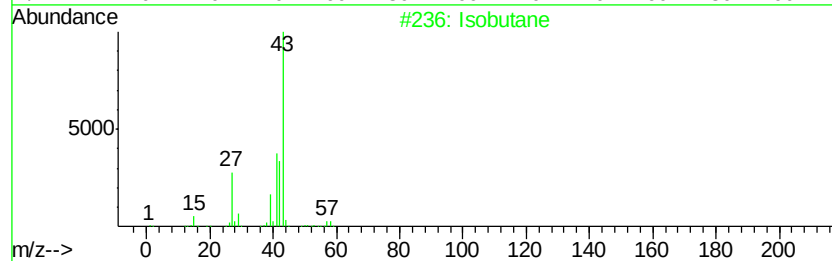
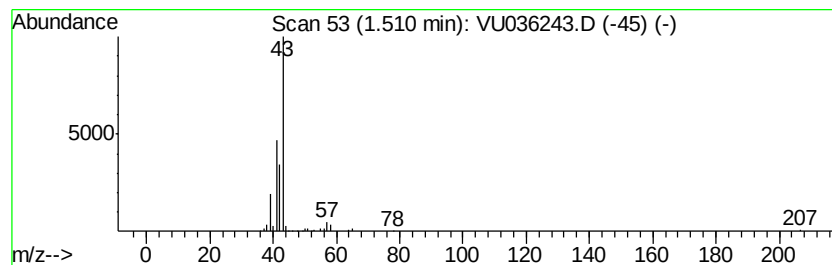
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.51	0.67 ug/L	78306	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	45
5		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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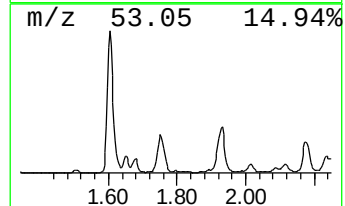
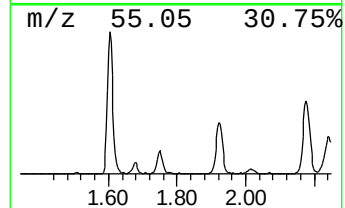
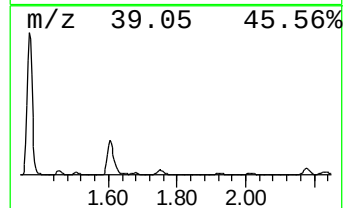
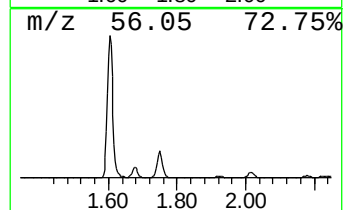
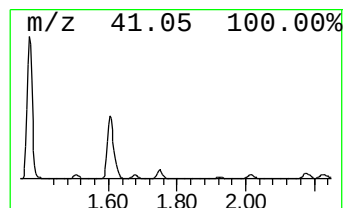
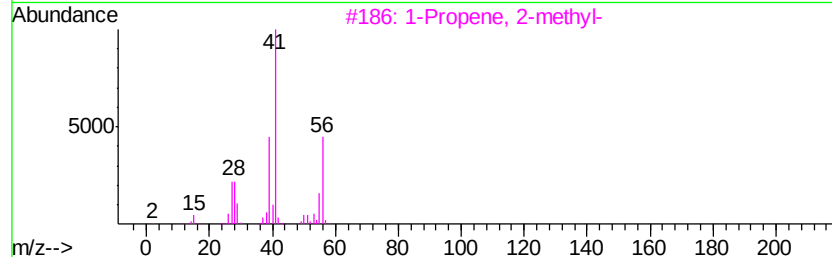
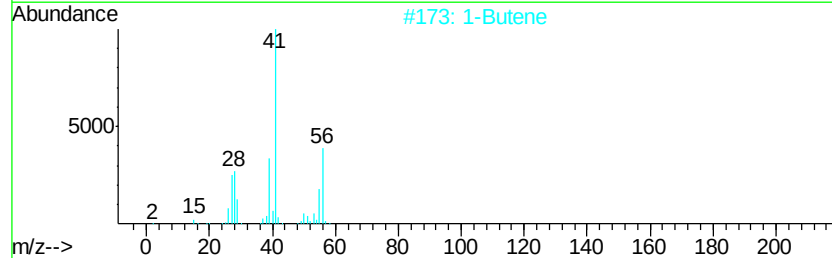
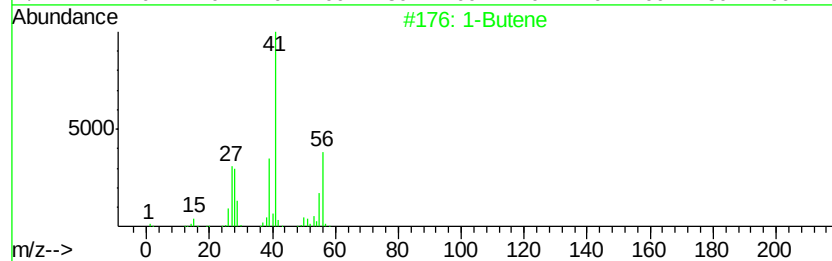
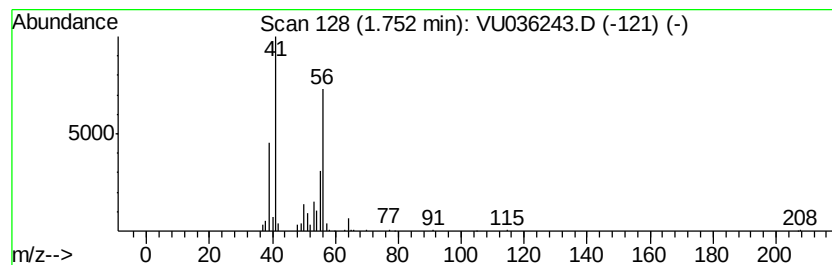
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic1.75 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	1.20 ug/L	139121	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butene	56	C4H8	000106-98-9	83
2		1-Butene	56	C4H8	000106-98-9	83
3		1-Propene, 2-methyl-	56	C4H8	000115-11-7	83
4		1-Butene	56	C4H8	000106-98-9	83
5		2-Butene, (Z)-	56	C4H8	000590-18-1	80



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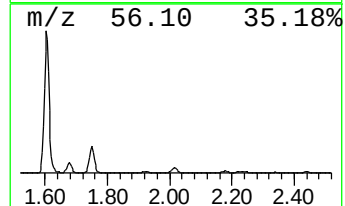
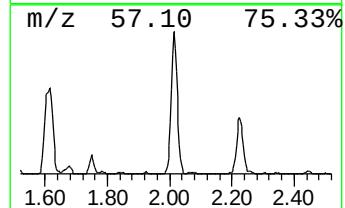
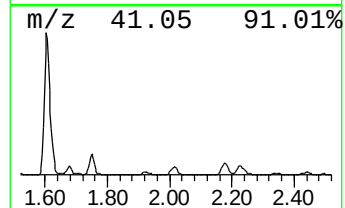
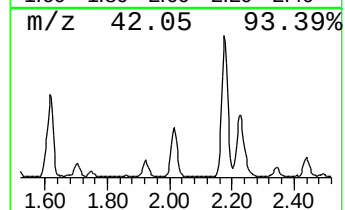
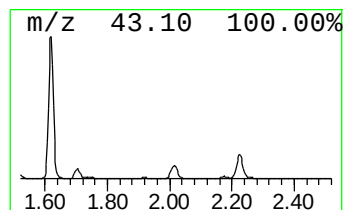
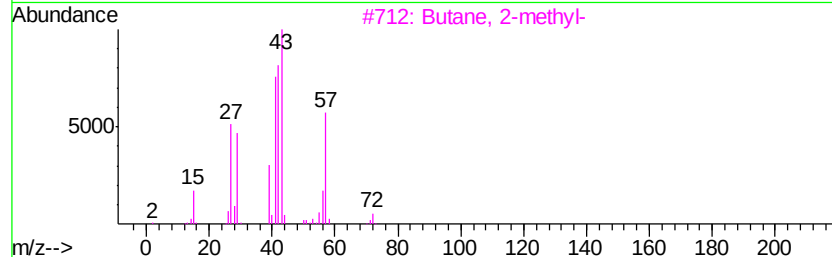
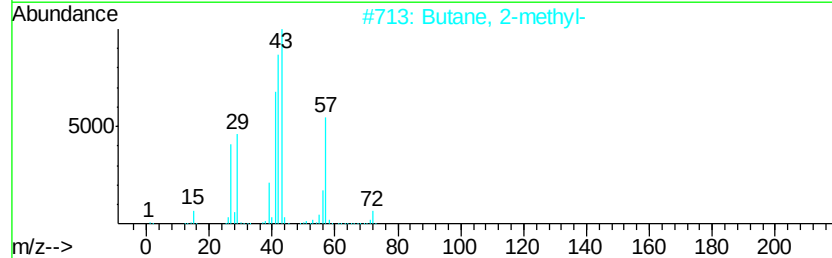
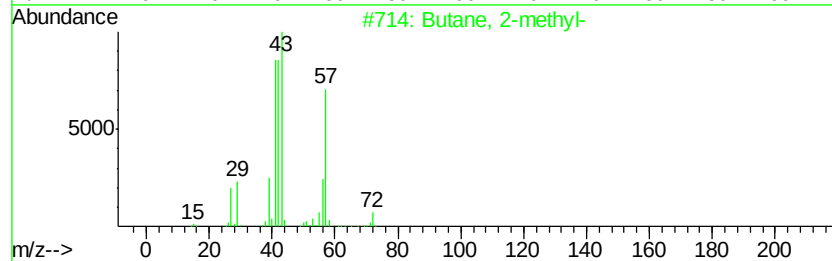
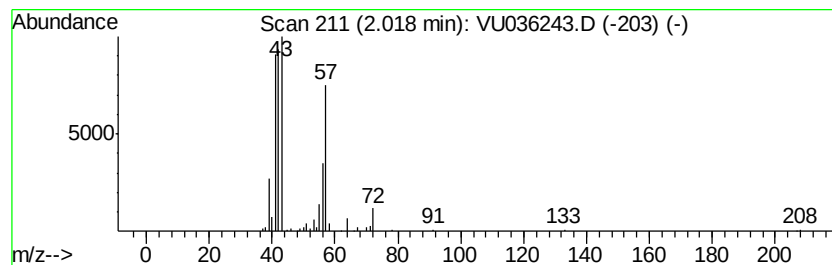
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	0.88 ug/L	102933	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2		Butane, 2-methyl-	72	C5H12	000078-78-4	86
3		Butane, 2-methyl-	72	C5H12	000078-78-4	78
4		Taurultam	136	C3H8N2O2S	038668-01-8	33
5		1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33



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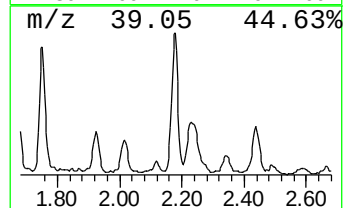
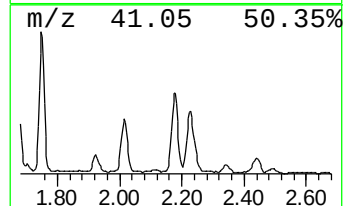
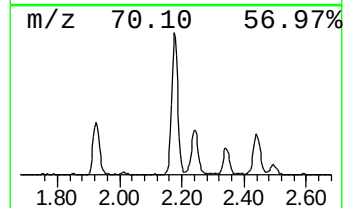
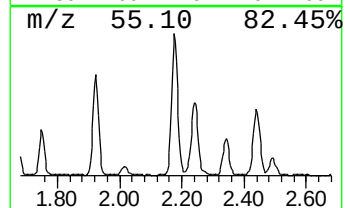
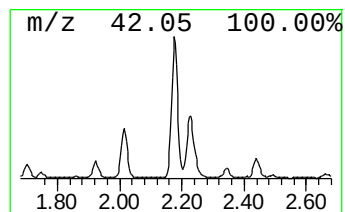
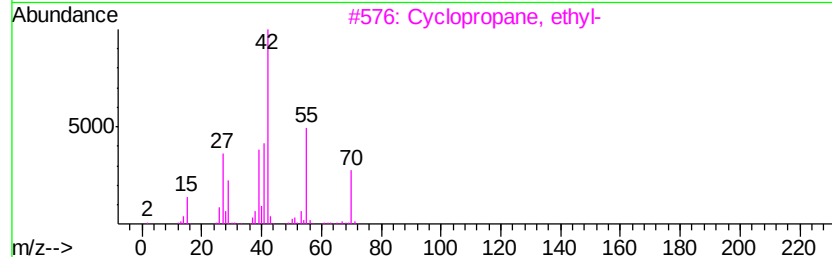
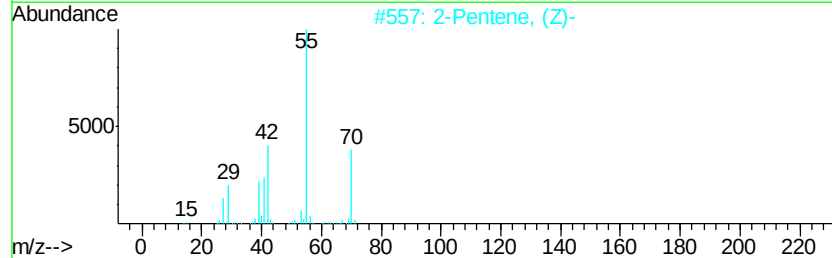
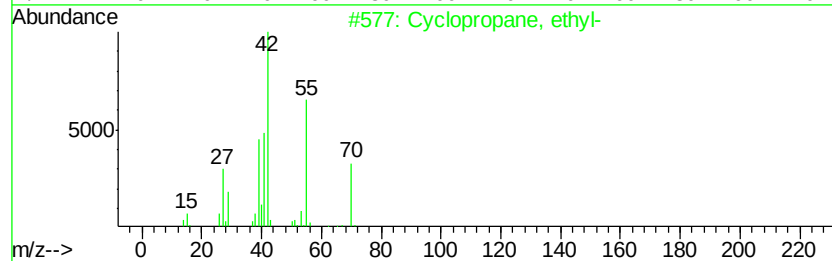
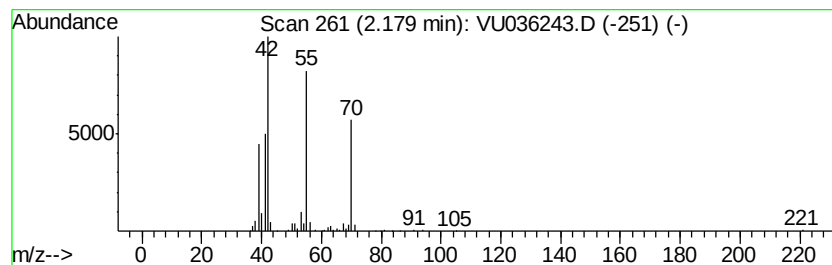
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Cyclic2.18 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	1.87 ug/L	217816	1,4-Difluorobenzene	6.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, ethyl-	70	C5H10	001191-96-4	86
2		2-Pentene, (Z)-	70	C5H10	000627-20-3	83
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
4		1-Pentene	70	C5H10	000109-67-1	74
5		Cyclopropane, ethyl-	70	C5H10	001191-96-4	68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU121619\
Data File : VU036243.D
Acq On : 16 Dec 2019 18:56
Operator : JC/MD
Sample : K6275-09
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDS5

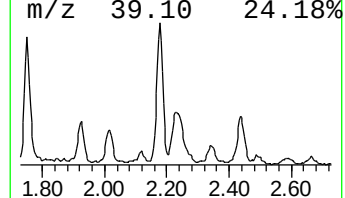
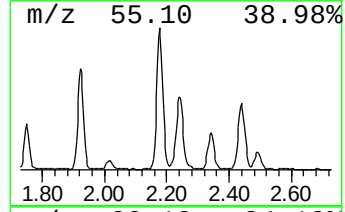
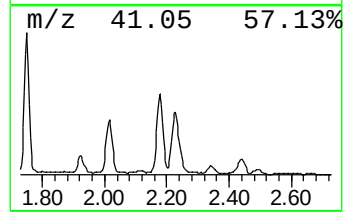
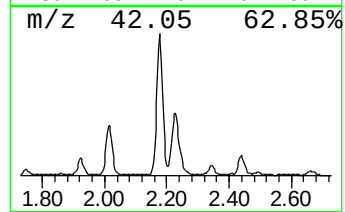
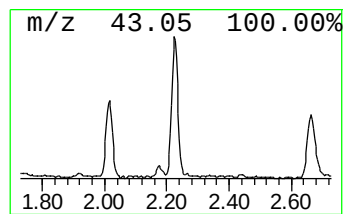
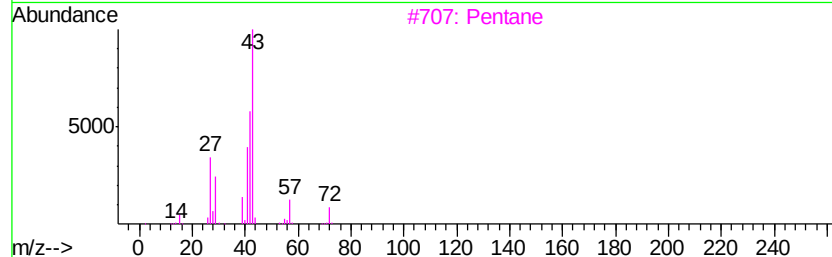
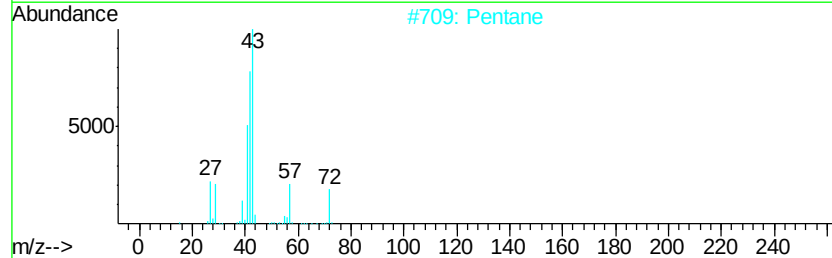
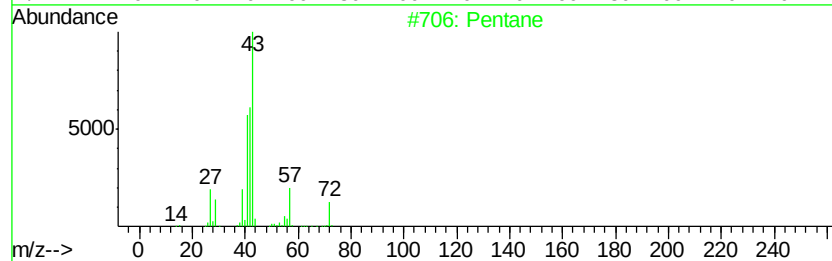
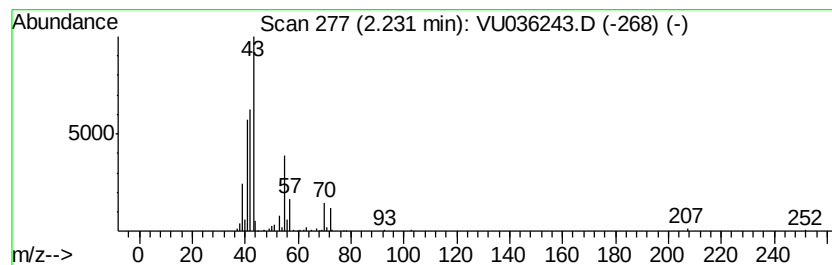
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	1.31 ug/L	152457	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	83
2		Pentane	72	C5H12	000109-66-0	72
3		Pentane	72	C5H12	000109-66-0	72
4		Pentane	72	C5H12	000109-66-0	64
5		3-Methyl-3-isopropyldiaziridine	100	C5H12N2	024476-95-7	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU121619\
Data File : VU036243.D
Acq On : 16 Dec 2019 18:56
Operator : JC/MD
Sample : K6275-09
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDS5

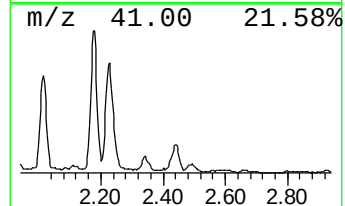
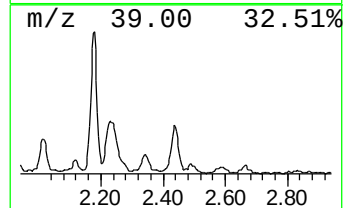
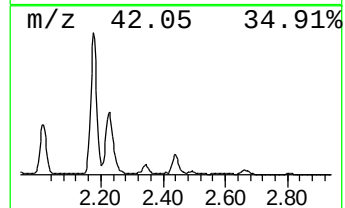
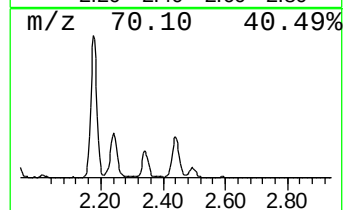
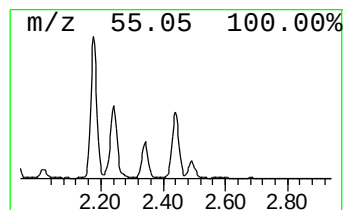
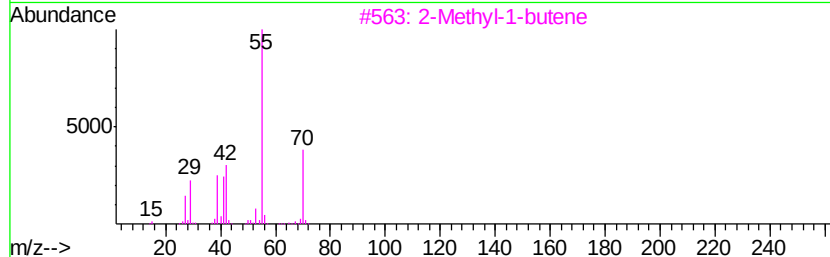
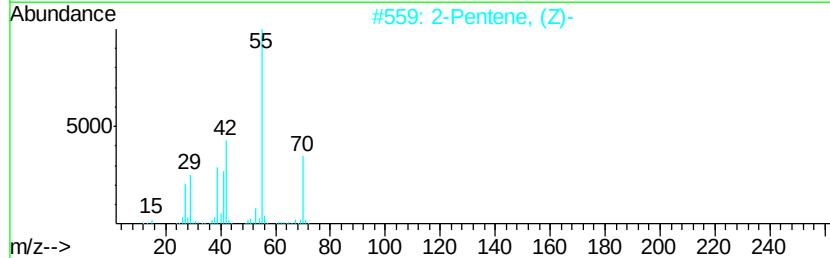
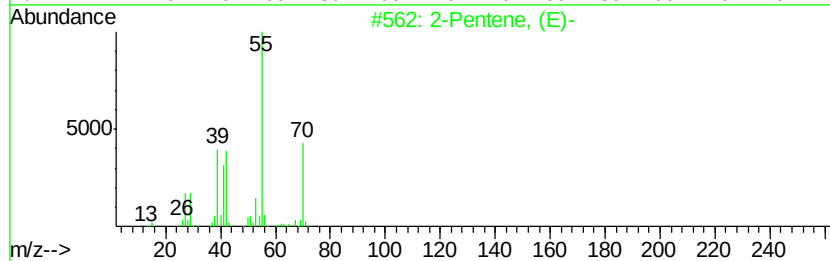
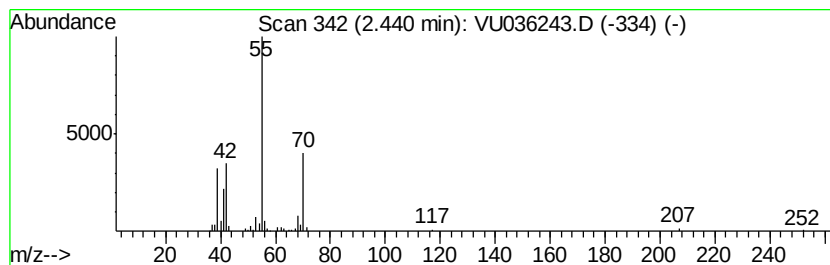
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Cyclic2.44 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	0.72 ug/L	83641	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, (E)-	70	C5H10	000646-04-8	83
2		2-Pentene, (Z)-	70	C5H10	000627-20-3	81
3		2-Methyl-1-butene	70	C5H10	000563-46-2	76
4		2-Pentene	70	C5H10	000109-68-2	72
5		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121619\
Data File : VU036243.D
Acq On : 16 Dec 2019 18:56
Operator : JC/MD
Sample : K6275-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDS5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.37	16.4	ug/L	1911320	1	6.29	581597	5.0
(DEL) Alkane: Str...	1.51	0.7	ug/L	78306	1	6.29	581597	5.0
(DEL) Alkane: Cyc...	1.75	1.2	ug/L	139121	1	6.29	581597	5.0
(DEL) Alkane: Str...	2.02	0.9	ug/L	102933	1	6.29	581597	5.0
(DEL) Alkane: Cyc...	2.18	1.9	ug/L	217816	1	6.29	581597	5.0
(DEL) Alkane: Str...	2.23	1.3	ug/L	152457	1	6.29	581597	5.0
(DEL) Alkane: Cyc...	2.44	0.7	ug/L	83641	1	6.29	581597	5.0