

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060523\
 Data File : VV031349.D
 Acq On : 05 Jun 2023 16:02
 Operator : SY/MD
 Sample : 03000-05DL 50X
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F6C29DL

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_V\Method\SFAMVTR060123WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV031349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.188	41	46	51	rBV	12864	11807	1.36%	0.114%
2	1.278	67	74	96	rVB	120629	136606	15.78%	1.322%
3	1.532	145	153	164	rBV	73246	85599	9.89%	0.829%
4	1.597	164	173	187	rVV	190386	238768	27.57%	2.311%
5	1.764	216	225	237	rBV	138517	179004	20.67%	1.733%
6	2.060	306	317	337	rBV	162247	264213	30.51%	2.557%
7	2.468	421	444	452	rBV3	62851	185922	21.47%	1.800%
8	2.516	452	459	477	rVB2	67995	125046	14.44%	1.210%
9	2.696	501	515	536	rVB3	46989	97876	11.30%	0.947%
10	2.970	583	600	620	rBV2	29520	61434	7.09%	0.595%
11	3.674	802	819	842	rBV2	162988	412796	47.67%	3.996%
12	3.825	851	866	904	rBV3	170205	532203	61.46%	5.151%
13	4.256	984	1000	1024	rBV2	97770	259624	29.98%	2.513%
14	4.590	1083	1104	1124	rBV2	336503	865898	100.00%	8.381%
15	4.966	1205	1221	1228	rBV2	239841	561639	64.86%	5.436%
16	5.014	1229	1236	1254	rVB	285026	624246	72.09%	6.042%
17	5.166	1277	1283	1296	rVB10	11912	25239	2.91%	0.244%
18	5.243	1296	1307	1323	rVB6	19334	44213	5.11%	0.428%
19	5.416	1351	1361	1378	rVB9	4637	10814	1.25%	0.105%
20	5.542	1386	1400	1425	rBV	164456	351016	40.54%	3.398%
21	5.838	1477	1492	1517	rBV	372477	762032	88.00%	7.376%
22	5.998	1529	1542	1550	rBV2	133789	274523	31.70%	2.657%
23	6.056	1550	1560	1580	rVB2	224617	484137	55.91%	4.686%
24	6.294	1625	1634	1646	rVB10	7098	13534	1.56%	0.131%
25	6.921	1817	1829	1850	rBV	55016	111993	12.93%	1.084%
26	7.198	1903	1915	1920	rBV7	9318	17184	1.98%	0.166%
27	7.249	1920	1931	1950	rVV	240122	427754	49.40%	4.140%
28	7.564	2020	2029	2052	rBV3	33522	81510	9.41%	0.789%
29	7.911	2119	2137	2159	rBV	116307	206460	23.84%	1.998%
30	8.040	2166	2177	2211	rBV	205723	492209	56.84%	4.764%
31	8.227	2228	2235	2245	rVB6	8404	13453	1.55%	0.130%
32	8.792	2399	2411	2431	rBV	239549	412149	47.60%	3.989%
33	8.953	2450	2461	2479	rBV	90611	154250	17.81%	1.493%
34	9.079	2485	2500	2522	rBV	276990	475460	54.91%	4.602%
35	9.487	2615	2627	2646	rBV	42728	72142	8.33%	0.698%
36	9.876	2738	2748	2758	rBV2	16538	26272	3.03%	0.254%

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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_V\Method\SFAMVTR060123WMA.M
Title : TRACE VOA SFAM1.0

37	10.162	2825	2837	2856	rBV	92244	154938	17.89%	1.500%
38	10.297	2869	2879	2886	rBV	10299	16289	1.88%	0.158%
39	10.390	2899	2908	2926	rBV	34599	75319	8.70%	0.729%
40	10.484	2928	2937	2949	rVB2	25586	40410	4.67%	0.391%
41	10.680	2989	2998	3011	rBV2	13003	20896	2.41%	0.202%
42	10.860	3043	3054	3072	rBV	59163	92813	10.72%	0.898%
43	11.191	3147	3157	3175	rVV	245117	391169	45.17%	3.786%
44	11.281	3175	3185	3199	rVB	33344	55067	6.36%	0.533%
45	11.567	3263	3274	3289	rBV	239205	385237	44.49%	3.729%

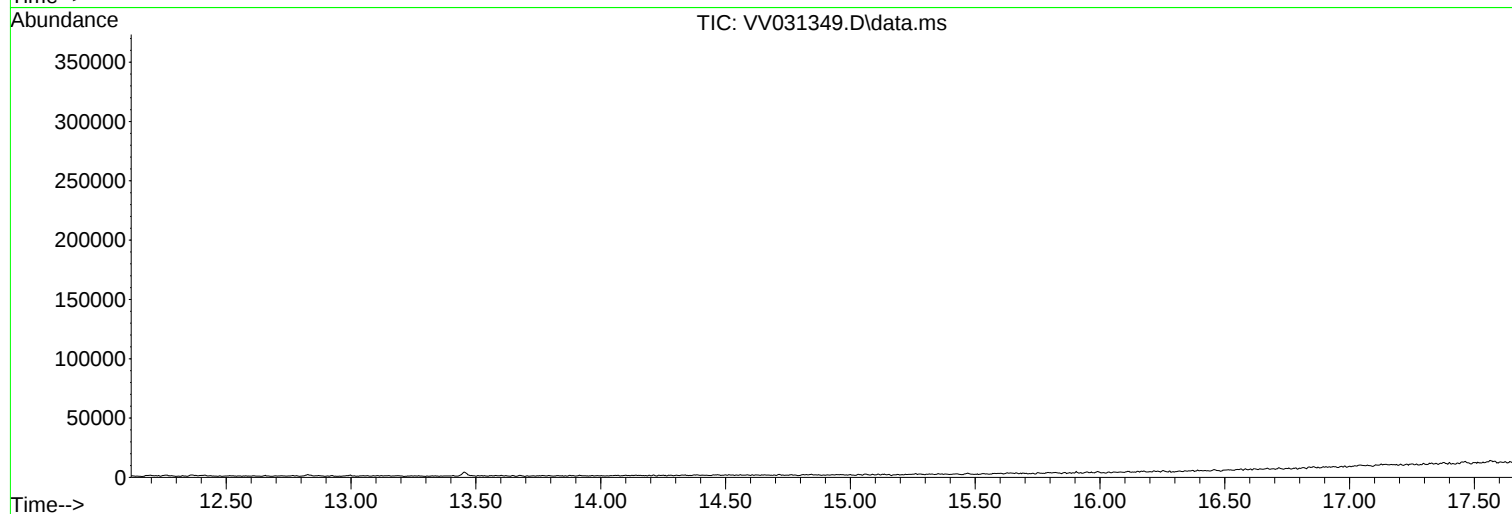
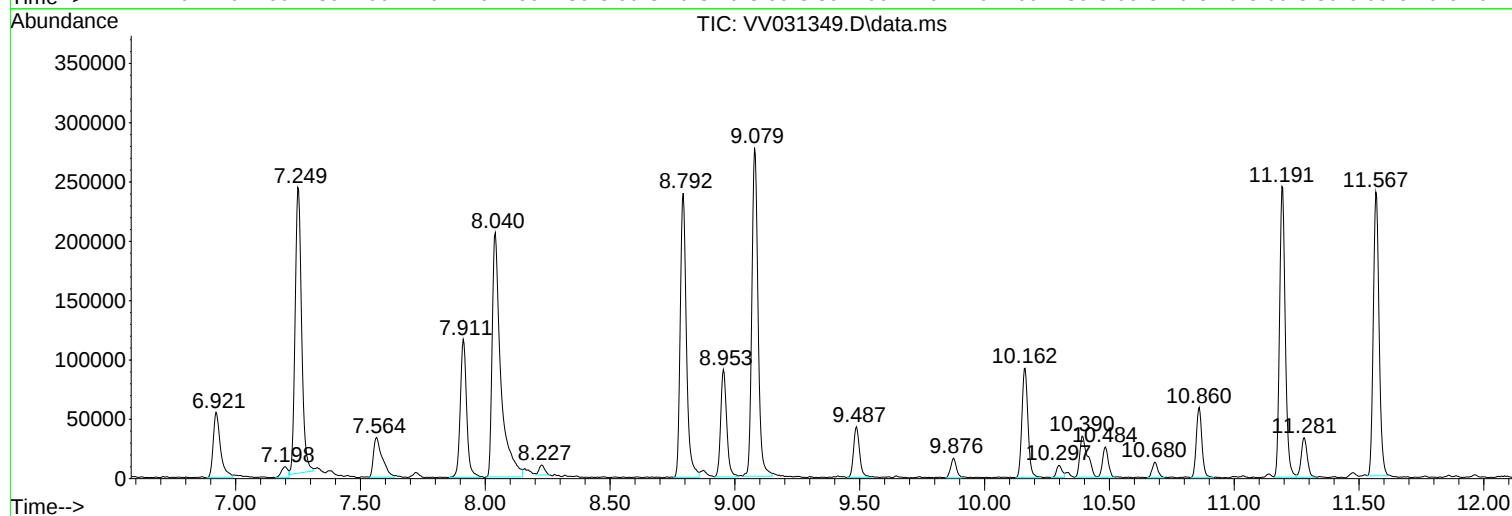
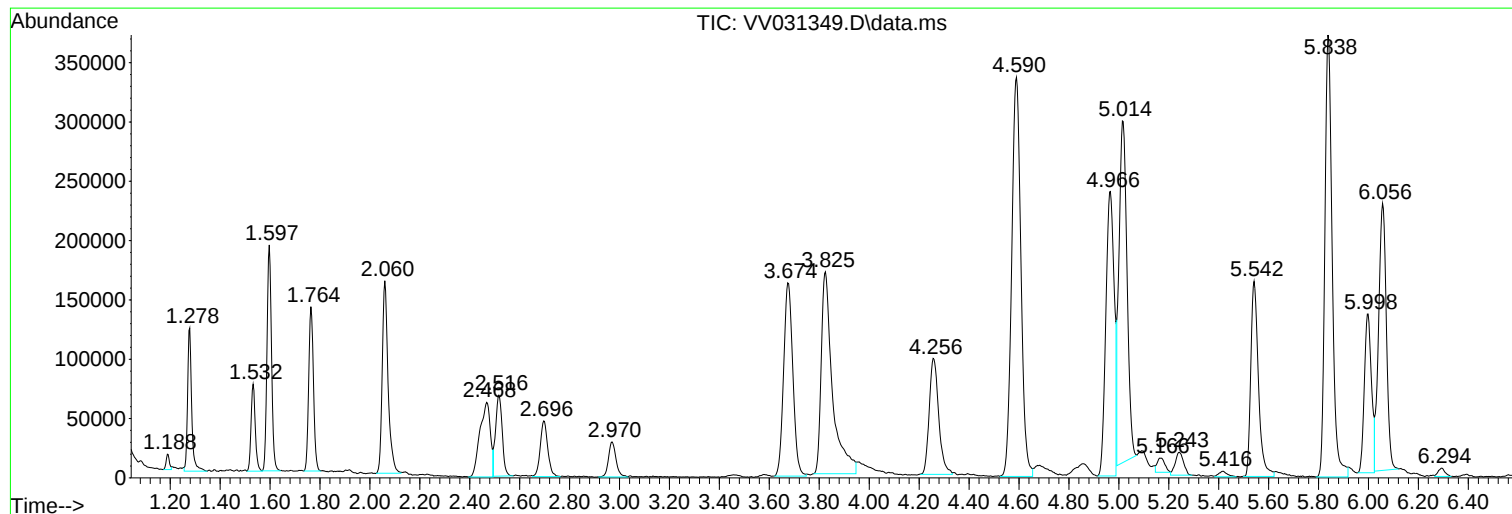
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR060123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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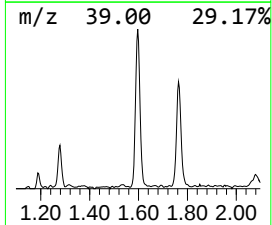
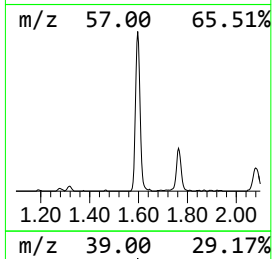
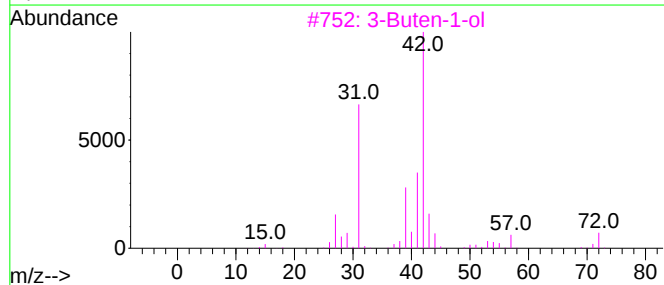
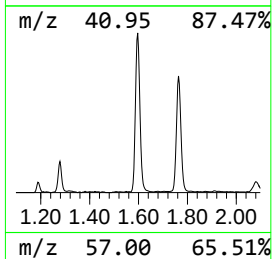
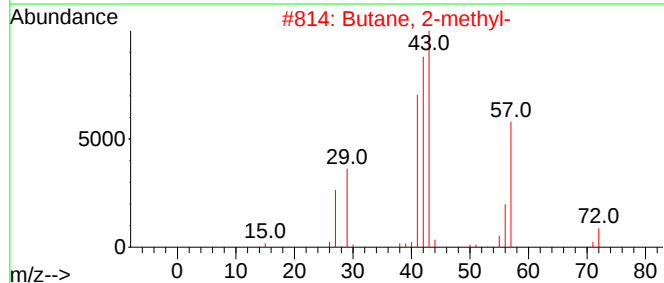
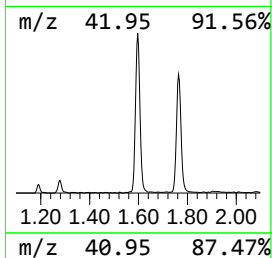
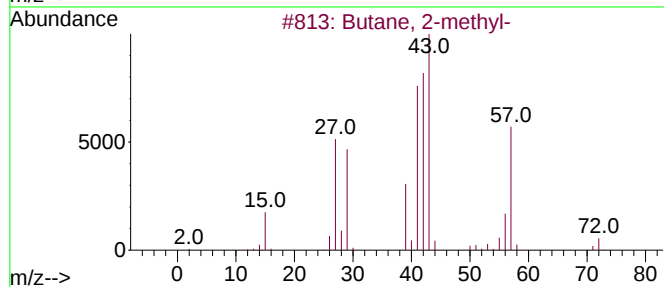
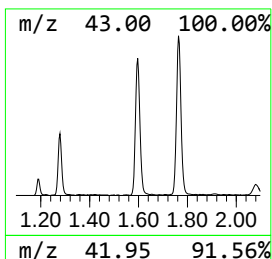
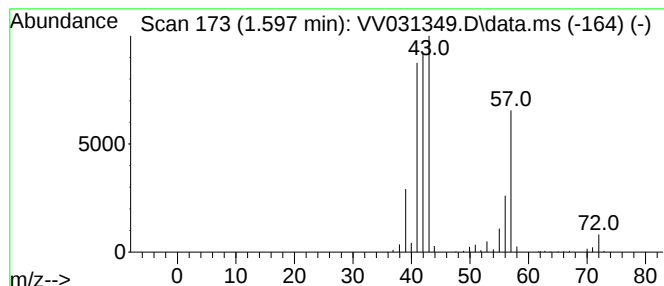
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.597	3.40 ug/L	238768	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	80
2	Butane, 2-methyl-			72	C5H12	000078-78-4	64
3	3-Buten-1-ol			72	C4H8O	000627-27-0	47
4	Pentane			72	C5H12	000109-66-0	42
5	1-Butene			56	C4H8	000106-98-9	10



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Instrument :
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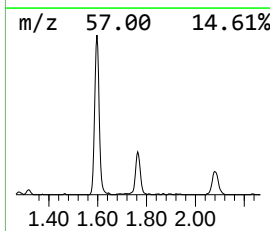
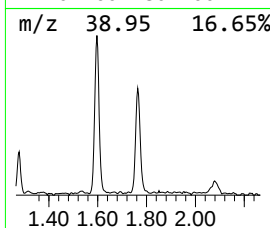
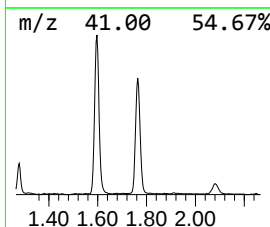
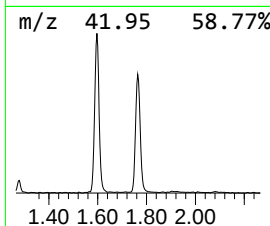
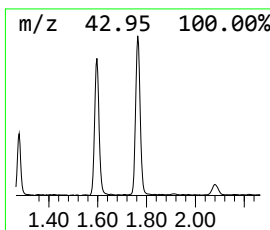
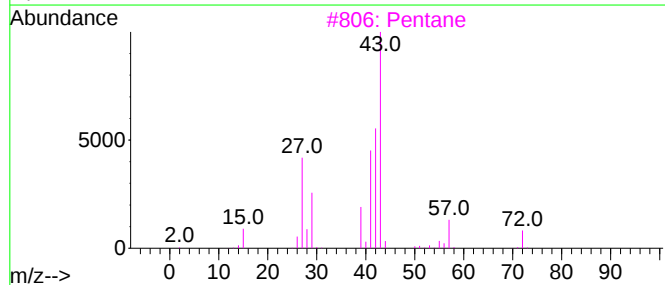
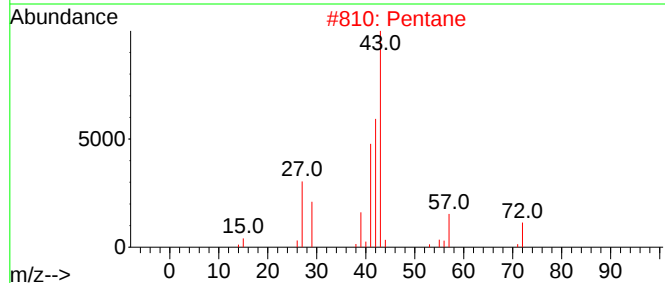
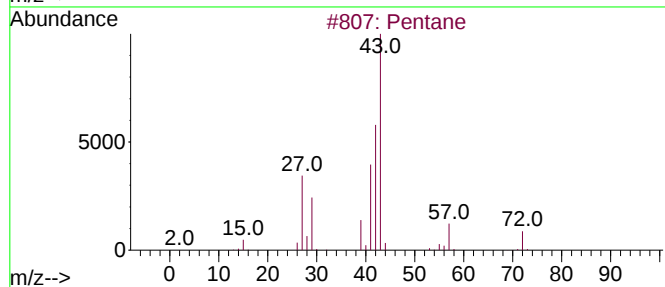
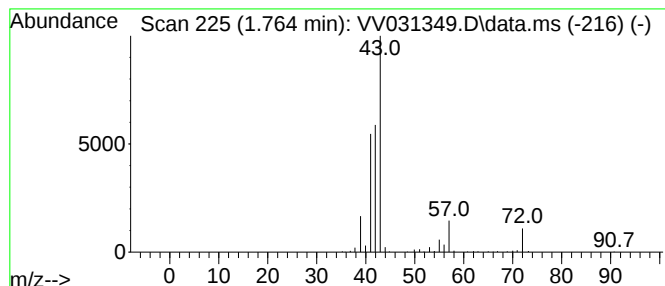
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR060123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.764	2.55 ug/L	179004	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	86
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	80
4	Pentane			72	C5H12	000109-66-0	72
5	Pentane			72	C5H12	000109-66-0	64



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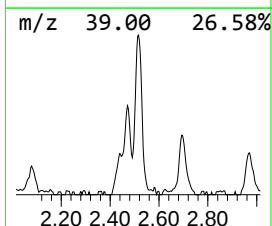
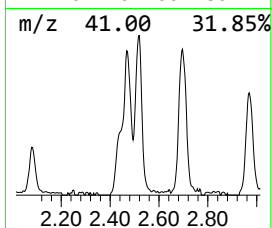
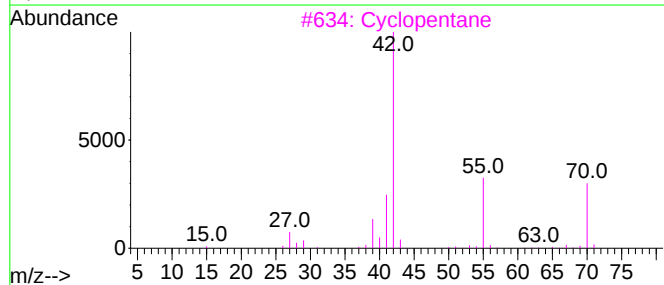
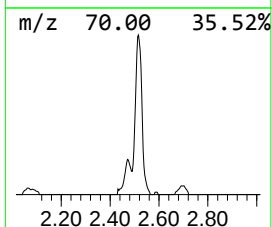
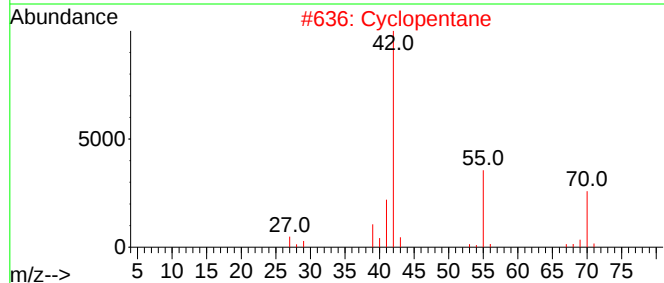
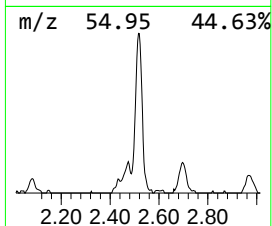
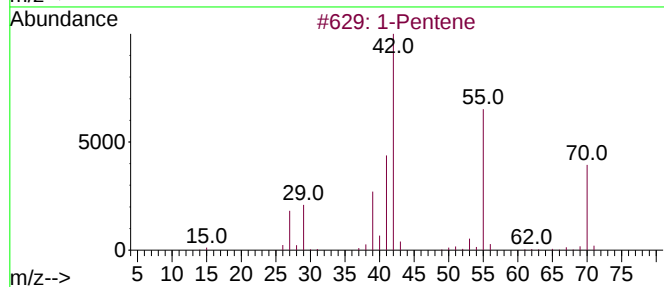
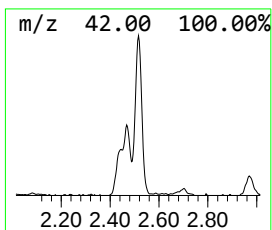
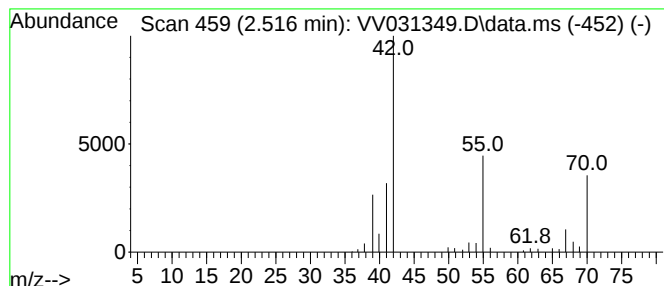
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR060123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.516	1.78 ug/L	125046	1,4-Difluorobenzene	5.542

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	80
2		Cyclopentane	70	C5H10	000287-92-3	72
3		Cyclopentane	70	C5H10	000287-92-3	72
4		Cyclobutane, methyl-	70	C5H10	000598-61-8	64
5		Cyclopentane	70	C5H10	000287-92-3	64



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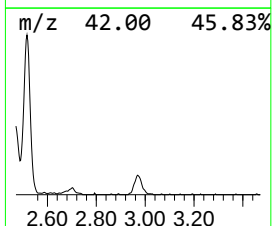
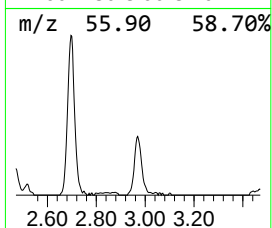
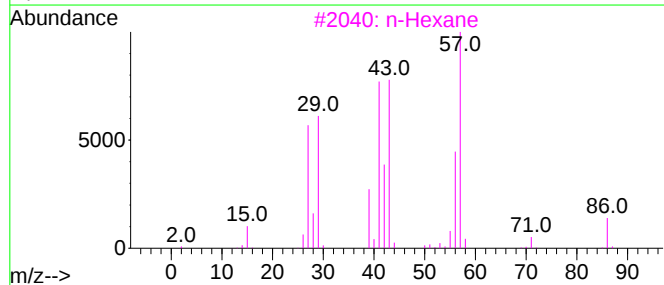
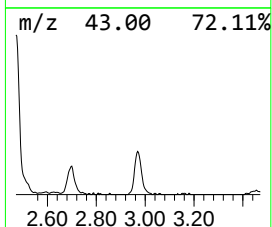
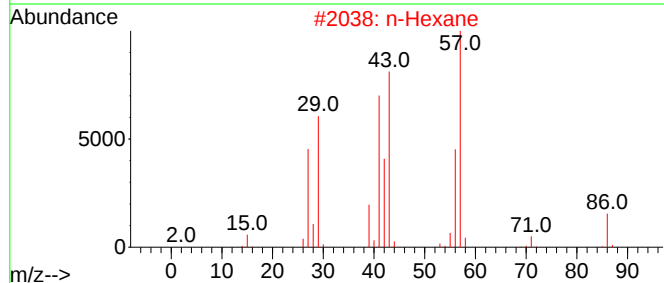
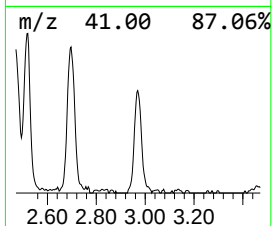
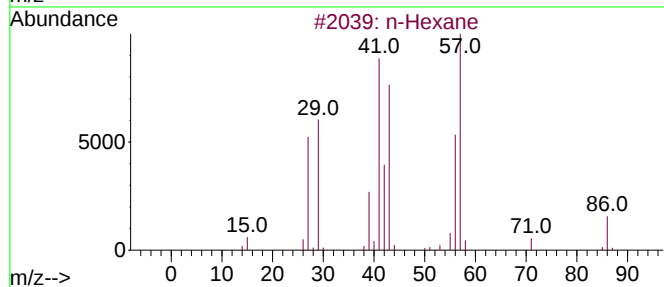
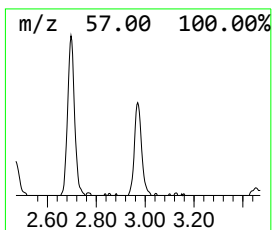
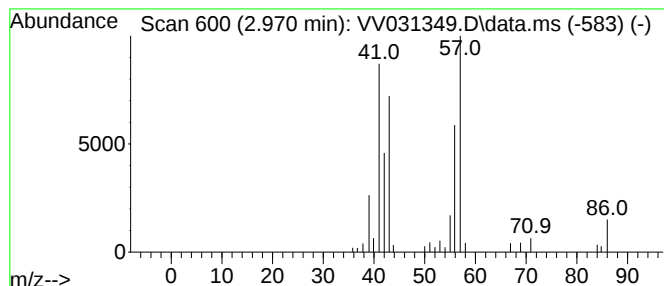
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.970	0.88 ug/L	61434	1,4-Difluorobenzene	5.542

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexane	86	C6H14	000110-54-3	87
2		n-Hexane	86	C6H14	000110-54-3	80
3		n-Hexane	86	C6H14	000110-54-3	80
4		2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
5		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	42



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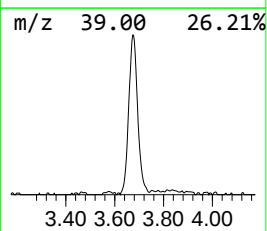
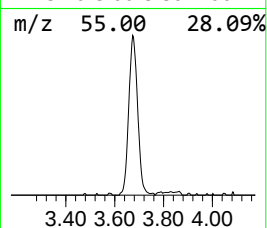
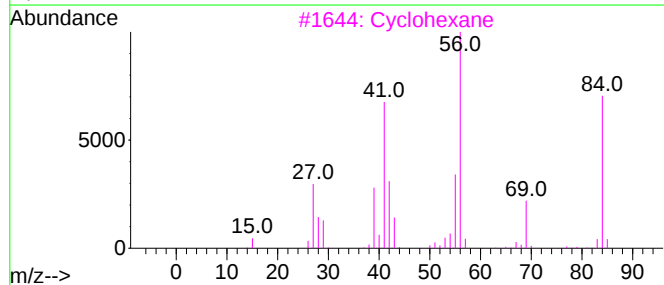
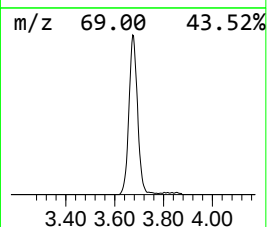
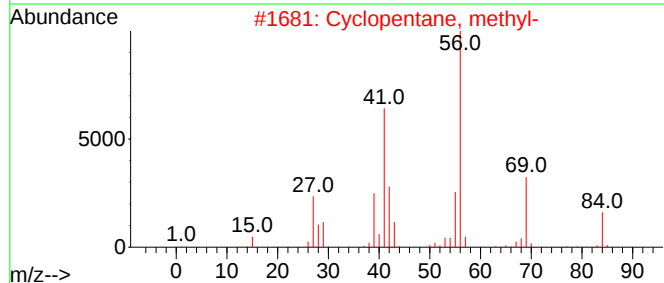
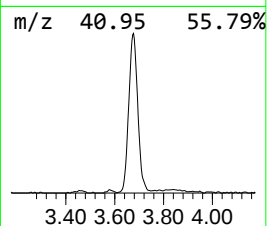
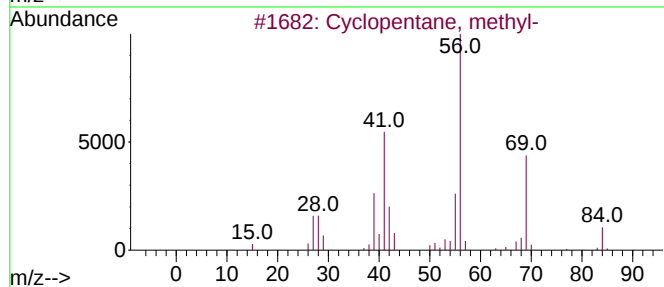
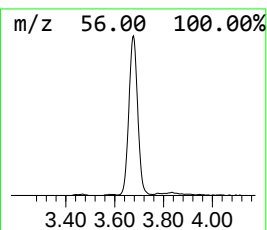
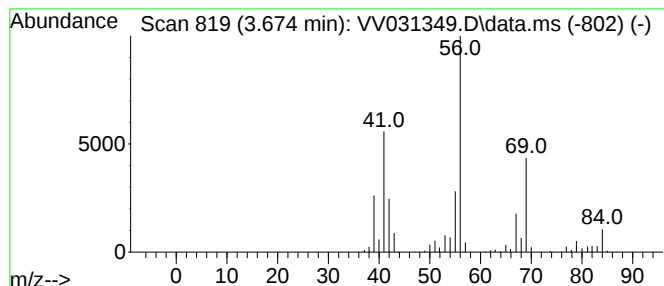
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic3.674 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.674	5.88 ug/L	412796	1,4-Difluorobenzene	5.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3			Cyclohexane	84	C6H12	000110-82-7	80
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060523\
Data File : VV031349.D
Acq On : 05 Jun 2023 16:02
Operator : SY/MD
Sample : 03000-05DL 50X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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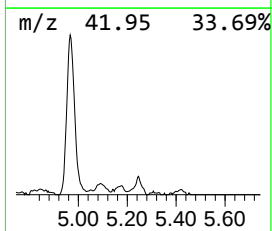
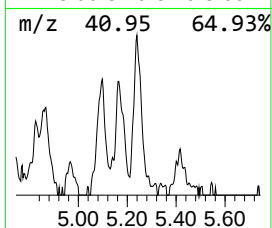
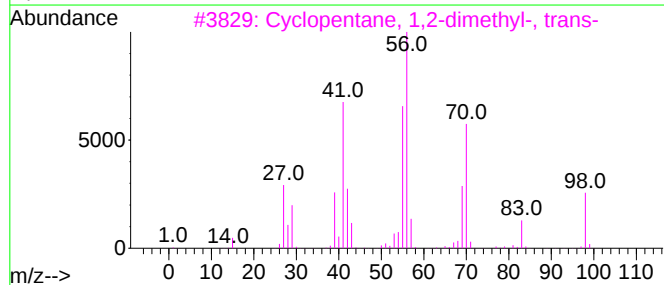
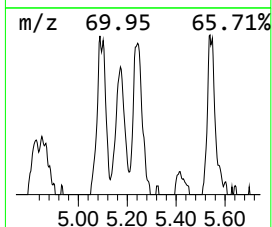
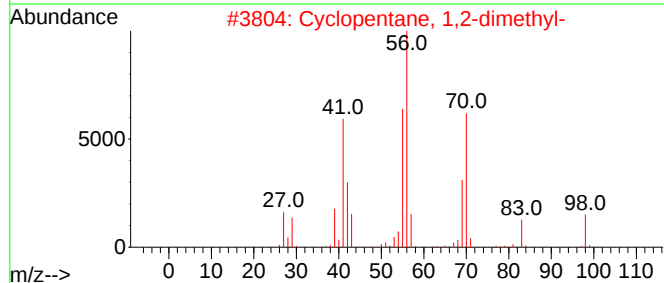
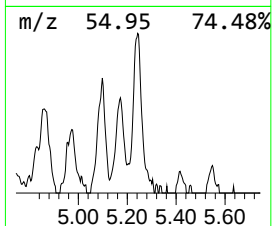
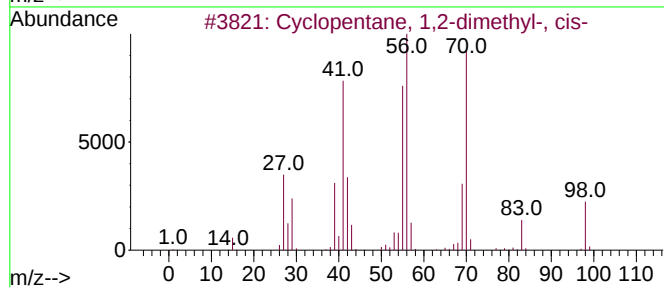
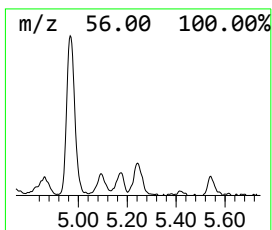
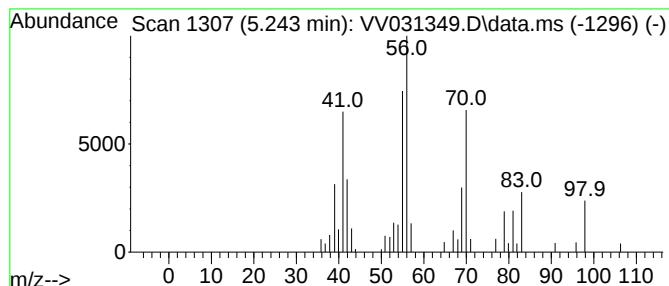
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Cyclic5.243 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.243	0.63 ug/L	44213	1,4-Difluorobenzene	5.542

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	87
2		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87
3		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	87
4		Isopropylcyclobutane	98	C7H14	000872-56-0	87
5		1-Heptene	98	C7H14	000592-76-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060523\
Data File : VV031349.D
Acq On : 05 Jun 2023 16:02
Operator : SY/MD
Sample : 03000-05DL 50X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F6C29DL

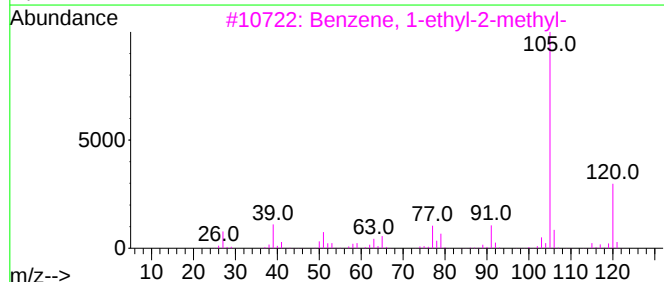
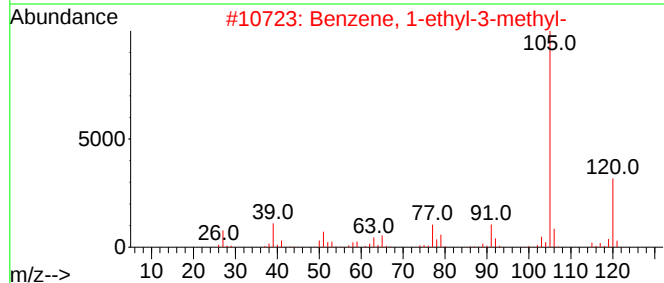
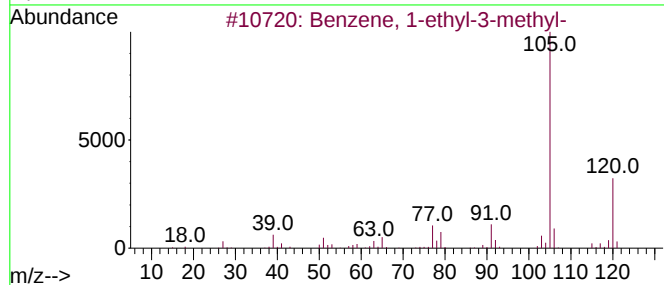
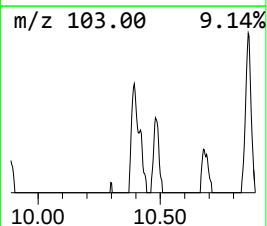
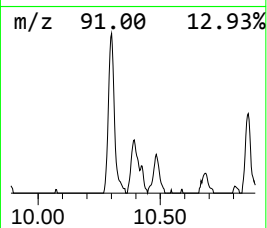
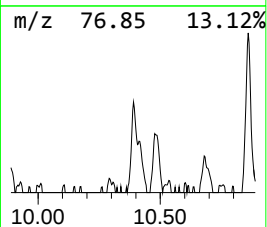
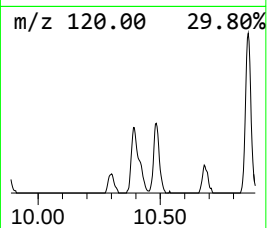
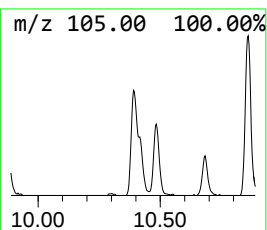
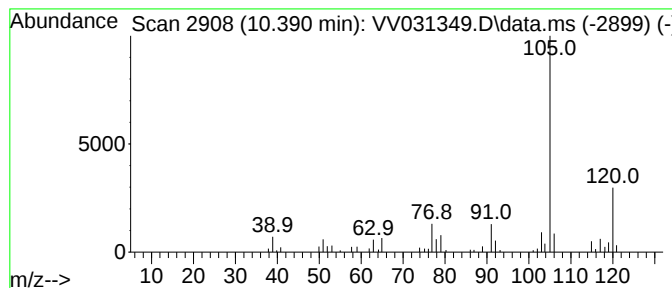
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.390	0.96 ug/L	75319	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060523\
Data File : VV031349.D
Acq On : 05 Jun 2023 16:02
Operator : SY/MD
Sample : 03000-05DL 50X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F6C29DL

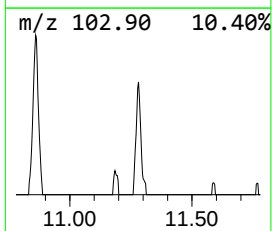
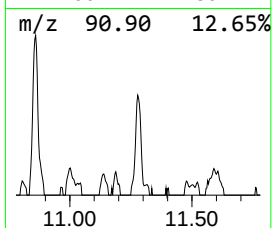
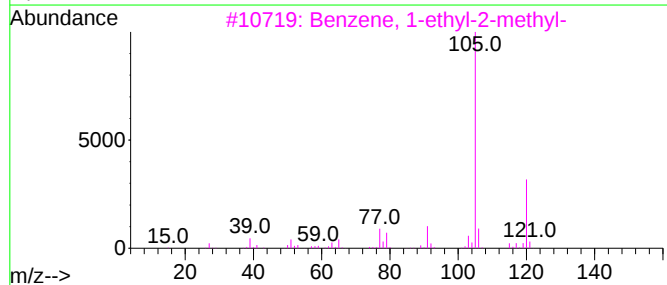
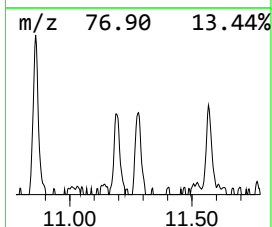
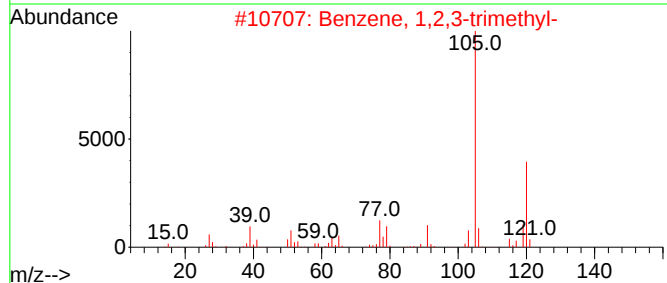
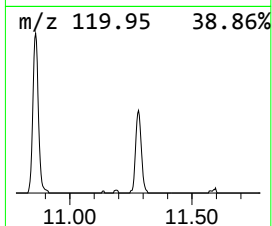
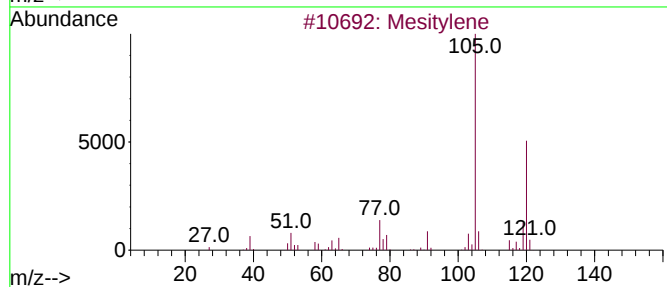
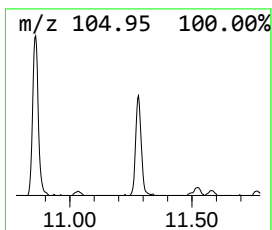
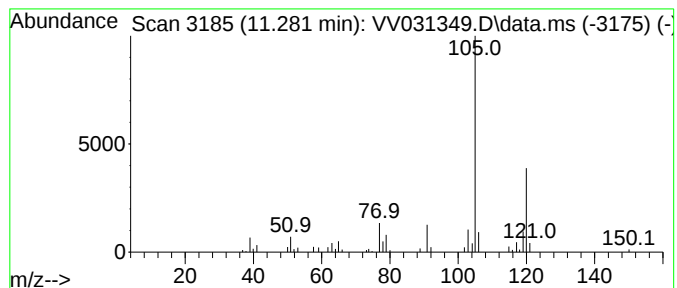
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.281	0.70 ug/L	55067	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	95
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060523\
 Data File : VV031349.D
 Acq On : 05 Jun 2023 16:02
 Operator : SY/MD
 Sample : 03000-05DL 50X
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F6C29DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR060123WMA.M
 Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.597	3.4	ug/L	238768	1	5.542	351016	5.0
(DEL) Alkane: S...	1.764	2.5	ug/L	179004	1	5.542	351016	5.0
(DEL) Alkane: S...	2.516	1.8	ug/L	125046	1	5.542	351016	5.0
(DEL) Alkane: S...	2.970	0.9	ug/L	61434	1	5.542	351016	5.0
(DEL) Alkane: C...	3.674	5.9	ug/L	412796	1	5.542	351016	5.0
(DEL) Alkane: C...	5.243	0.6	ug/L	44213	1	5.542	351016	5.0
Benzene, 1-ethy...	10.390	1.0	ug/L	75319	3	11.194	391169	5.0
Benzene, 1,2,3-...	11.281	0.7	ug/L	55067	3	11.194	391169	5.0