

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
 Data File : VU056514.D
 Acq On : 19 Nov 2023 05:45
 Operator : MD/SY
 Sample : 05455-06
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E05M0

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\SFAMUTR111323WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056514.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	14	21	35	rVB2	102593	110149	10.41%	1.174%
2	1.486	50	61	85	rBV2	212026	535630	50.62%	5.708%
3	1.596	89	95	106	rVB2	159714	198089	18.72%	2.111%
4	1.911	186	193	207	rVB	81394	109169	10.32%	1.163%
5	1.994	211	219	230	rVB	65116	89970	8.50%	0.959%
6	2.200	276	283	292	rVB	45044	60366	5.71%	0.643%
7	2.563	380	396	414	rBV	146816	246194	23.27%	2.623%
8	3.039	531	544	550	rBV4	12317	25387	2.40%	0.271%
9	3.081	550	557	566	rVB3	13945	25456	2.41%	0.271%
10	3.354	629	642	657	rVB3	10020	21494	2.03%	0.229%
11	3.695	735	748	760	rBV5	16510	41197	3.89%	0.439%
12	4.525	994	1006	1023	rVB5	10345	26218	2.48%	0.279%
13	4.634	1028	1040	1089	rBV2	103475	398565	37.67%	4.247%
14	5.055	1155	1171	1191	rBV	173736	387429	36.62%	4.128%
15	5.380	1256	1272	1283	rBV7	12683	33806	3.20%	0.360%
16	5.586	1324	1336	1349	rBV4	6630	14638	1.38%	0.156%
17	5.721	1357	1378	1408	rBV2	332063	908421	85.86%	9.680%
18	5.981	1450	1459	1470	rVB10	6085	12088	1.14%	0.129%
19	6.132	1495	1506	1524	rBV4	11549	25583	2.42%	0.273%
20	6.245	1527	1541	1565	rBV	343151	667064	63.05%	7.108%
21	6.685	1663	1678	1692	rBV2	215292	428999	40.55%	4.571%
22	6.756	1692	1700	1718	rVB6	26280	53899	5.09%	0.574%
23	7.560	1939	1950	1966	rBV2	90587	167178	15.80%	1.781%
24	7.894	2042	2054	2068	rVV	355866	646400	61.09%	6.888%
25	7.965	2068	2076	2089	rVB	46899	88462	8.36%	0.943%
26	8.177	2132	2142	2153	rVV2	53862	93129	8.80%	0.992%
27	8.238	2155	2161	2175	rVB2	6235	14272	1.35%	0.152%
28	8.631	2269	2283	2318	rBV2	516210	1058067	100.00%	11.274%
29	8.788	2324	2332	2345	rVV5	15181	28607	2.70%	0.305%
30	8.856	2346	2353	2365	rVB6	7239	13128	1.24%	0.140%
31	9.412	2513	2526	2547	rBV	494377	852769	80.60%	9.087%
32	9.570	2563	2575	2583	rBV2	16939	30186	2.85%	0.322%
33	9.692	2600	2613	2624	rBV2	30634	59558	5.63%	0.635%
34	10.100	2728	2740	2748	rBV3	15393	26067	2.46%	0.278%
35	10.348	2806	2817	2828	rBV8	13442	25912	2.45%	0.276%
36	10.750	2930	2942	2960	rBV	174750	288331	27.25%	3.072%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
 Data File : VU056514.D
 Acq On : 19 Nov 2023 05:45
 Operator : MD/SY
 Sample : 05455-06
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E05M0

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\SFAMUTR111323WMA.M

Title : TRACE VOA SFAM1.0

37	10.997	3009	3019	3024	rBV2	7203	11214	1.06%	0.119%
38	11.042	3027	3033	3040	rVB5	10509	15919	1.50%	0.170%
39	11.463	3156	3164	3181	rVB2	18570	29795	2.82%	0.317%
40	11.688	3222	3234	3248	rBV8	14129	26720	2.53%	0.285%
41	11.807	3259	3271	3289	rBV	432773	719498	68.00%	7.667%
42	12.061	3337	3350	3368	rBV3	34019	85067	8.04%	0.906%
43	12.187	3377	3389	3409	rVB	376902	627730	59.33%	6.689%
44	12.885	3593	3606	3621	rBV5	23663	43550	4.12%	0.464%
45	14.090	3969	3981	3990	rBV3	7469	13282	1.26%	0.142%

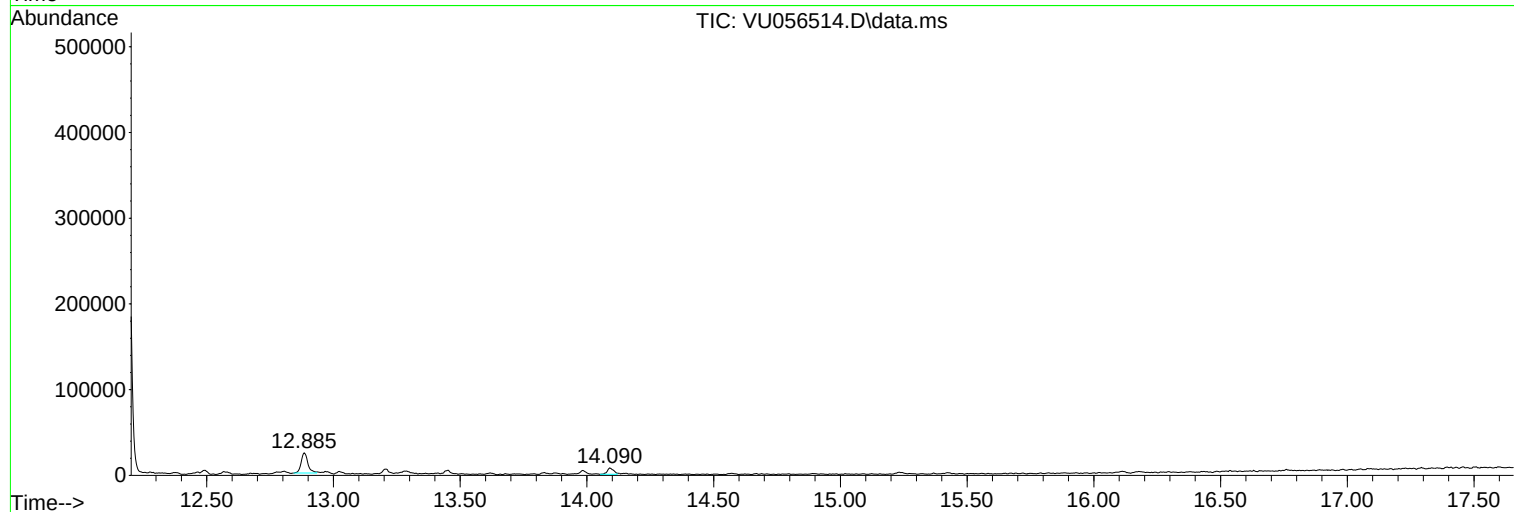
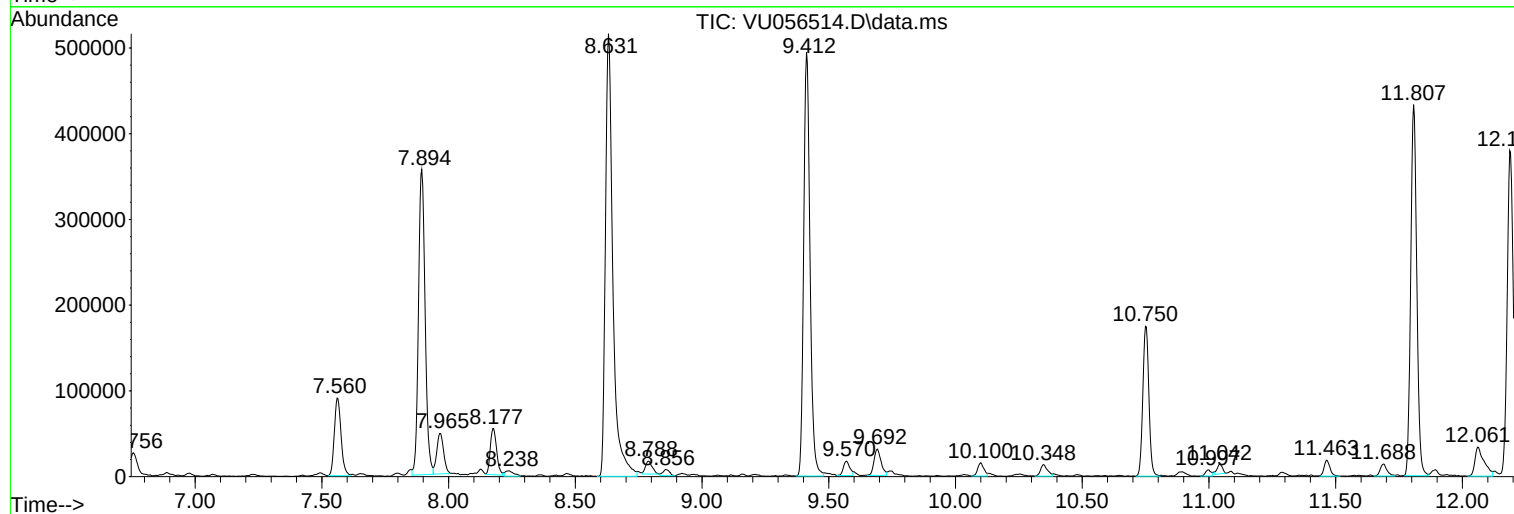
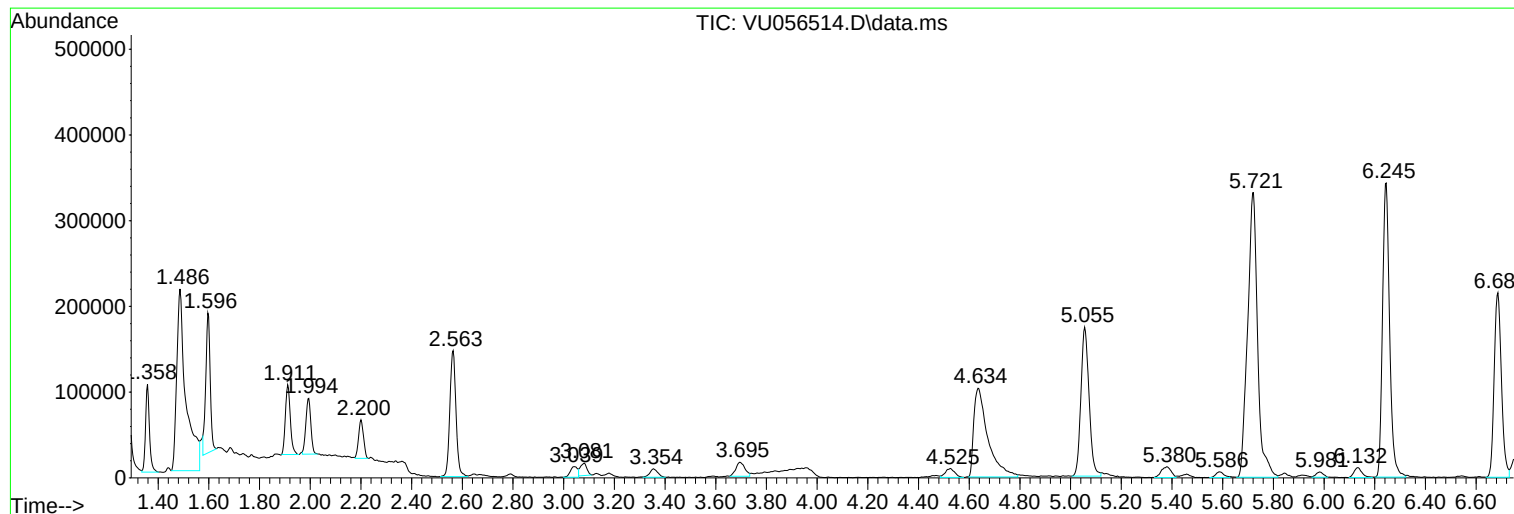
Sum of corrected areas: 9384652

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

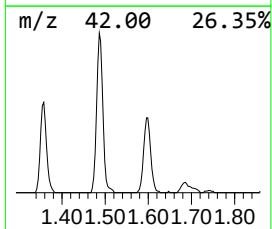
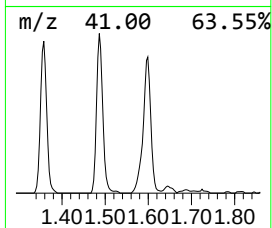
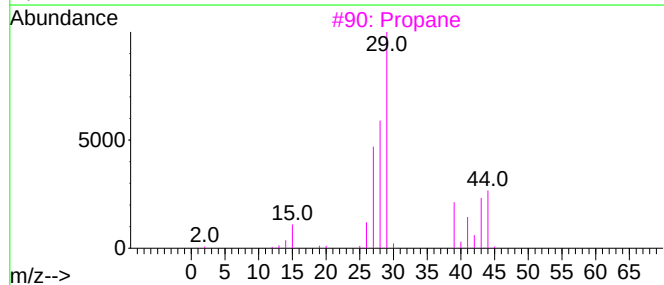
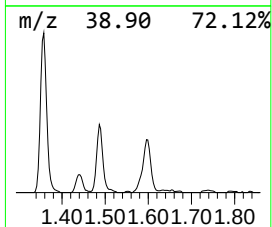
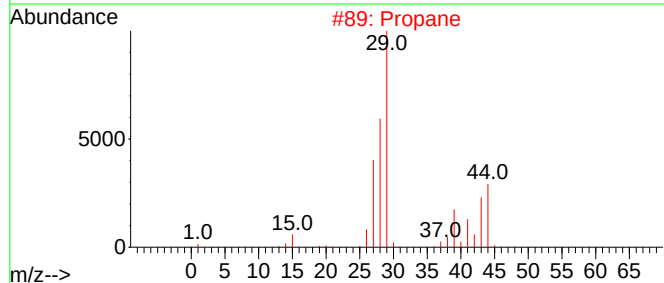
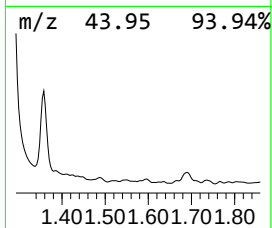
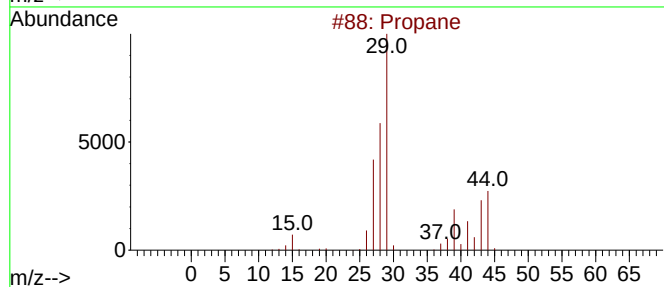
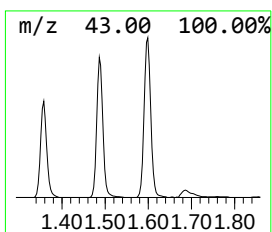
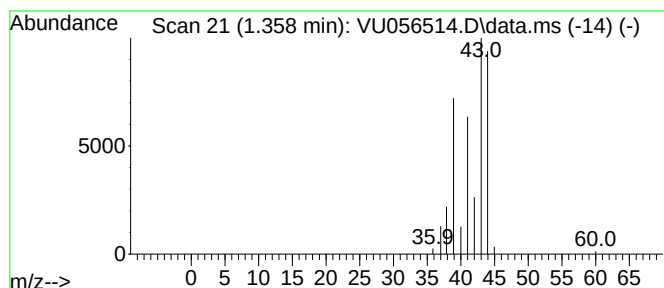
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	0.83 ug/L	110149	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propane	44	C3H8	000074-98-6	83
3			Propane	44	C3H8	000074-98-6	9
4			Propene	42	C3H6	000115-07-1	9
5			Ethylene oxide	44	C2H4O	000075-21-8	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

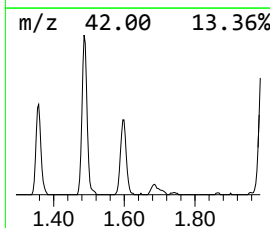
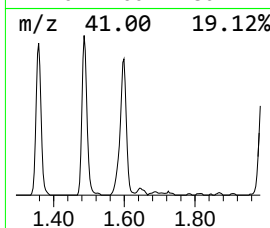
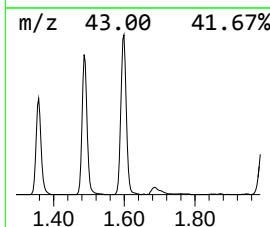
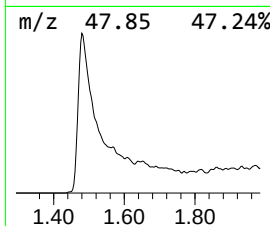
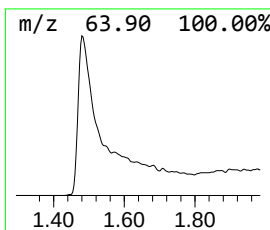
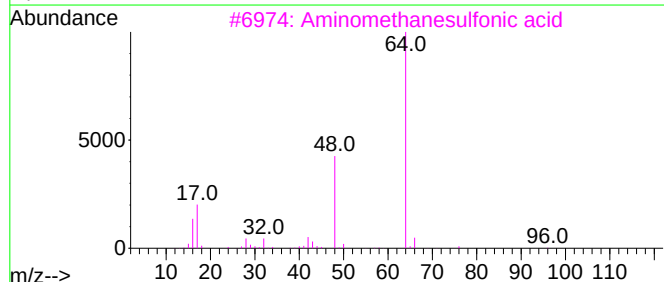
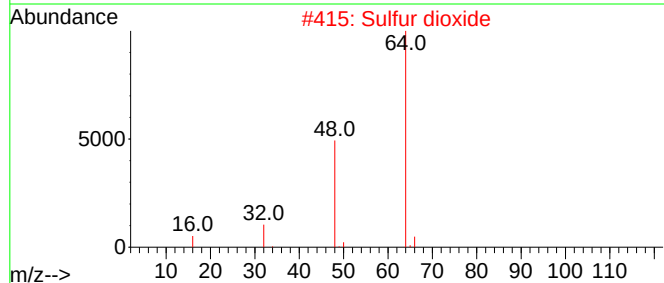
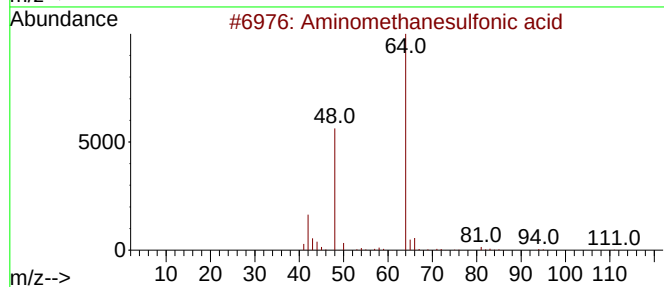
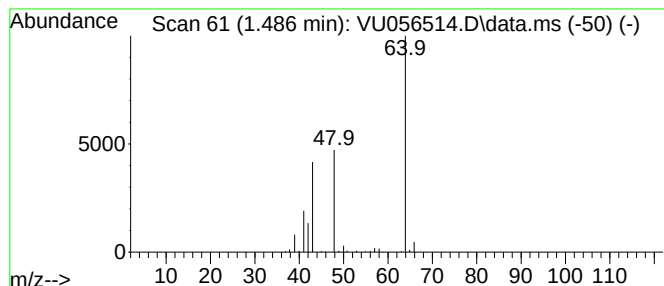
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.486	4.01 ug/L	535630	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	78
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

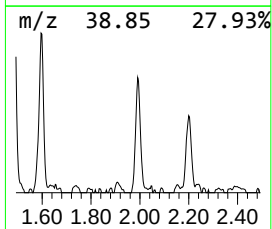
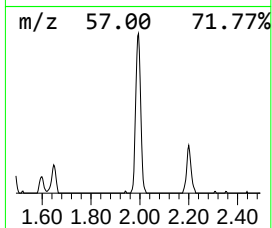
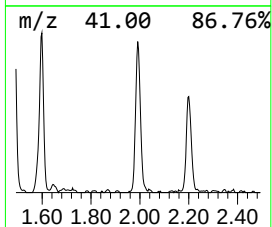
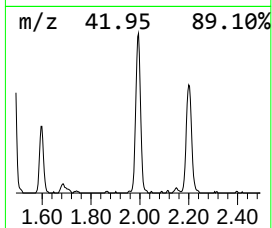
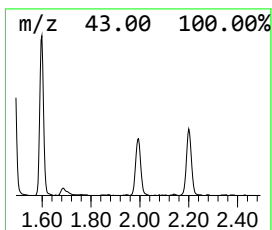
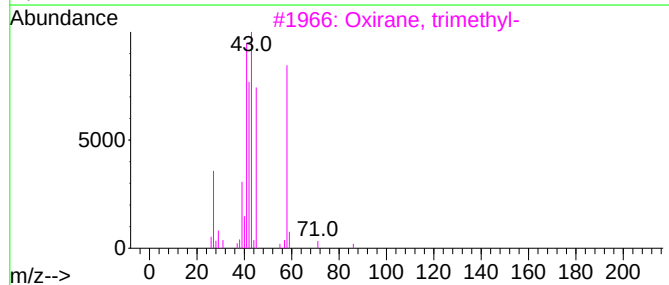
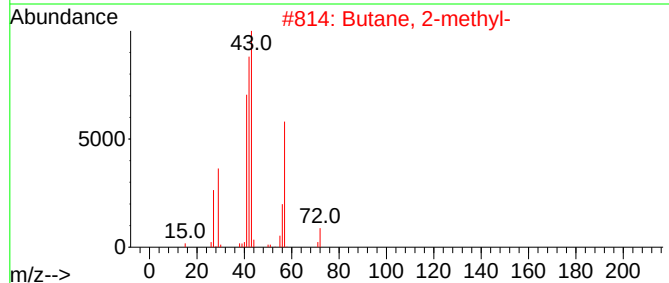
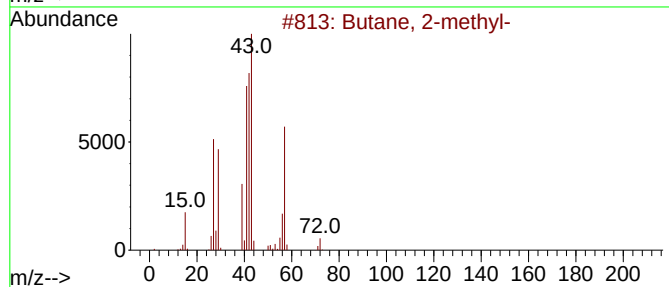
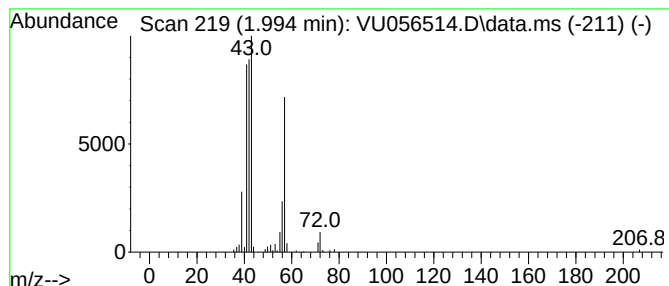
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.994	0.67 ug/L	89970	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	Oxirane, trimethyl-			86	C5H10O	005076-19-7	36
4	Isobutylene epoxide			72	C4H8O	000558-30-5	33
5	Pentane			72	C5H12	000109-66-0	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

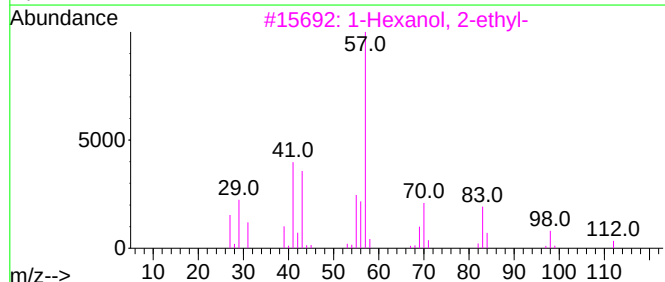
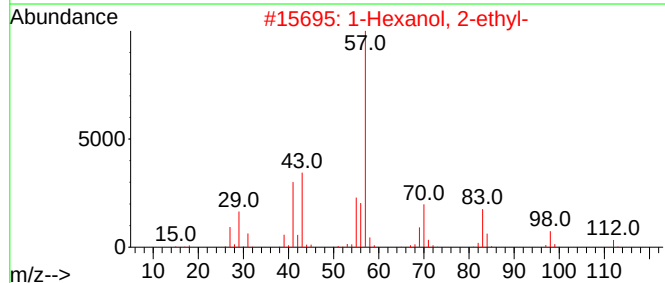
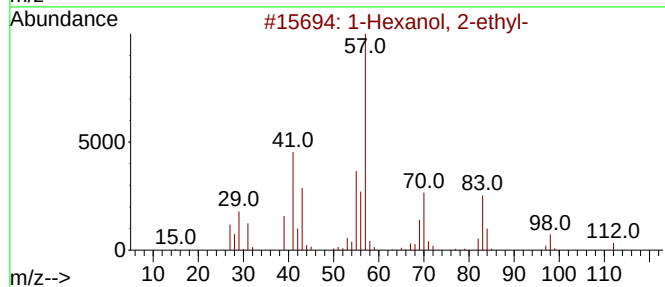
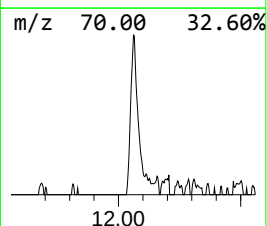
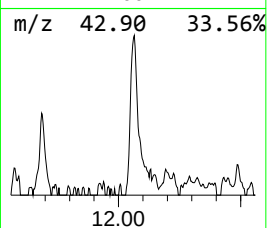
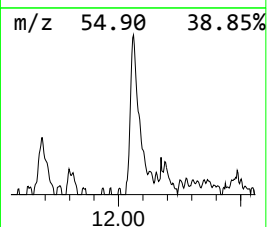
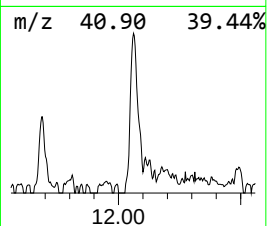
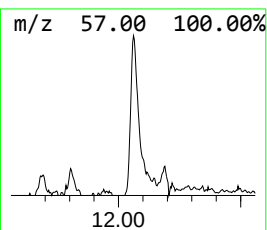
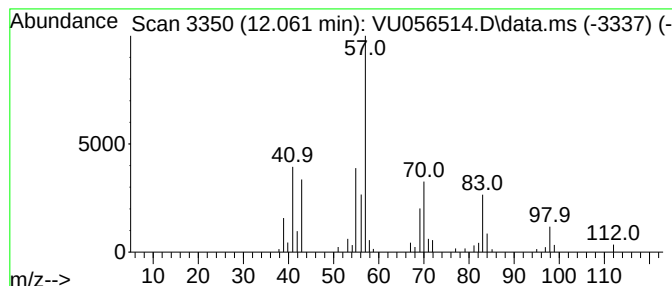
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.59 ug/L	85067	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111823\
Data File : VU056514.D
Acq On : 19 Nov 2023 05:45
Operator : MD/SY
Sample : 05455-06
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E05M0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.358	0.8	ug/L	110149	1	6.245	667064	5.0
Aminomethanesul...	1.486	4.0	ug/L	535630	1	6.245	667064	5.0
(DEL) Alkane: S...	1.994	0.7	ug/L	89970	1	6.245	667064	5.0
1-Hexanol, 2-et...	12.061	0.6	ug/L	85067	3	11.807	719498	5.0