

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
 Data File : VU055345.D
 Acq On : 15 Sep 2023 17:48
 Operator : MD/SY
 Sample : 04380-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4F3

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\SFAMUTR091523WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU055345.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	16	21	27	rBV	27249	30089	5.08%	0.504%
2	1.596	88	95	105	rVB2	51641	62513	10.55%	1.046%
3	1.911	185	193	206	rBV	55284	73901	12.47%	1.237%
4	2.560	385	395	408	rBV	73416	120952	20.40%	2.024%
5	3.042	531	545	561	rVB	10401	20101	3.39%	0.336%
6	3.132	561	573	581	rBV3	5339	9973	1.68%	0.167%
7	4.640	1030	1042	1066	rBV3	56540	207986	35.08%	3.481%
8	5.058	1158	1172	1192	rBV2	102865	228088	38.48%	3.817%
9	5.383	1260	1273	1282	rBV5	5434	10645	1.80%	0.178%
10	5.721	1358	1378	1405	rBV2	178800	484738	81.77%	8.112%
11	6.245	1528	1541	1566	rBV	206103	405547	68.41%	6.787%
12	6.537	1620	1632	1645	rBV	6212	12298	2.07%	0.206%
13	6.689	1663	1679	1697	rBV2	127990	262023	44.20%	4.385%
14	7.190	1826	1835	1846	rVB9	5132	9915	1.67%	0.166%
15	7.566	1940	1952	1968	rBV2	34446	66731	11.26%	1.117%
16	7.894	2042	2054	2073	rBV	196373	348520	58.79%	5.832%
17	8.180	2131	2143	2152	rBV2	21745	36823	6.21%	0.616%
18	8.242	2156	2162	2173	rVB9	4273	6789	1.15%	0.114%
19	8.409	2206	2214	2224	rVB4	5984	9809	1.65%	0.164%
20	8.634	2273	2284	2325	rBV4	200598	592818	100.00%	9.921%
21	9.415	2515	2527	2550	rBV	314557	551695	93.06%	9.233%
22	9.508	2551	2556	2566	rVB10	5365	8841	1.49%	0.148%
23	9.685	2602	2611	2623	rVB10	8079	17133	2.89%	0.287%
24	10.274	2787	2794	2802	rVB7	5729	8368	1.41%	0.140%
25	10.367	2815	2823	2838	rVB7	7606	16215	2.74%	0.271%
26	10.698	2917	2926	2931	rVV10	5541	10146	1.71%	0.170%
27	10.753	2932	2943	2962	rVB	102602	188726	31.84%	3.158%
28	10.894	2974	2987	2990	rBV10	4361	7027	1.19%	0.118%
29	10.926	2992	2997	3012	rVB10	4397	8722	1.47%	0.146%
30	11.013	3012	3024	3027	rBV7	4918	7060	1.19%	0.118%
31	11.322	3108	3120	3130	rVB8	15684	31588	5.33%	0.529%
32	11.399	3130	3144	3155	rBV8	13138	29706	5.01%	0.497%
33	11.643	3213	3220	3230	rVB7	12935	20641	3.48%	0.345%
34	11.740	3241	3250	3257	rVB7	5670	9365	1.58%	0.157%
35	11.811	3257	3272	3295	rVB	338522	566465	95.55%	9.480%
36	12.003	3327	3332	3343	rBV10	4849	6991	1.18%	0.117%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
 Data File : VU055345.D
 Acq On : 15 Sep 2023 17:48
 Operator : MD/SY
 Sample : 04380-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4F3

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\SFAMUTR091523WMA.M
 Title : TRACE VOA SFAM1.0

37	12.190	3375	3390	3408	rVB	224869	403183	68.01%	6.747%
38	12.412	3451	3459	3460	rBV6	7132	7728	1.30%	0.129%
39	12.528	3488	3495	3496	rBV5	5914	6399	1.08%	0.107%
40	12.630	3513	3527	3537	rBV9	16392	36566	6.17%	0.612%
41	12.759	3561	3567	3577	rVB7	8332	12635	2.13%	0.211%
42	12.830	3577	3589	3594	rBV7	11078	21504	3.63%	0.360%
43	12.946	3615	3625	3629	rBV7	11563	19728	3.33%	0.330%
44	13.113	3664	3677	3688	rBV3	30660	49369	8.33%	0.826%
45	13.248	3706	3719	3728	rBV	21554	38781	6.54%	0.649%
46	13.325	3734	3743	3755	rBV2	48794	77969	13.15%	1.305%
47	13.531	3799	3807	3816	rVB3	9627	14559	2.46%	0.244%
48	13.601	3821	3829	3839	rVB3	6721	14442	2.44%	0.242%
49	13.836	3893	3902	3908	rBV3	8516	16631	2.81%	0.278%
50	13.881	3908	3916	3929	rVV3	30924	56500	9.53%	0.946%
51	13.958	3931	3940	3956	rVB2	55807	103715	17.50%	1.736%
52	14.064	3968	3973	3976	rBV6	7286	8091	1.36%	0.135%
53	14.116	3983	3989	3991	rBV6	7897	9530	1.61%	0.159%
54	14.251	4023	4031	4035	rBV5	16458	22823	3.85%	0.382%
55	14.283	4037	4041	4050	rVV7	16807	28246	4.76%	0.473%
56	14.341	4051	4059	4071	rVV3	25424	44763	7.55%	0.749%
57	14.470	4093	4099	4106	rVB9	12102	17520	2.96%	0.293%
58	14.518	4106	4114	4122	rVB8	10995	15334	2.59%	0.257%
59	14.663	4153	4159	4174	rVB8	14033	28978	4.89%	0.485%
60	14.775	4187	4194	4196	rBV7	8210	10469	1.77%	0.175%
61	14.804	4197	4203	4212	rVB2	26393	38632	6.52%	0.647%
62	14.878	4219	4226	4237	rVB7	32663	63882	10.78%	1.069%
63	14.942	4242	4246	4261	rVB7	7937	16551	2.79%	0.277%
64	15.026	4262	4272	4280	rBV3	31690	55074	9.29%	0.922%
65	15.154	4304	4312	4321	rVB8	10952	18992	3.20%	0.318%
66	15.267	4339	4347	4353	rBV7	14818	24500	4.13%	0.410%
67	15.425	4388	4396	4406	rVB3	28985	54183	9.14%	0.907%
68	15.598	4443	4450	4458	rBV8	13077	20789	3.51%	0.348%
69	15.762	4496	4501	4508	rVB10	7877	10239	1.73%	0.171%
70	15.923	4538	4551	4563	rVB4	23842	53602	9.04%	0.897%
71	16.148	4616	4621	4625	rBV7	8144	8811	1.49%	0.147%
72	16.183	4628	4632	4639	rVB7	10819	12872	2.17%	0.215%
73	16.228	4639	4646	4652	rVB4	6796	8377	1.41%	0.140%
74	16.521	4730	4737	4743	rBV2	10802	18624	3.14%	0.312%
75	16.884	4842	4850	4859	rBV2	9467	16001	2.70%	0.268%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

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\SFAMUTR091523WMA.M
Title : TRACE VOA SFAM1.0

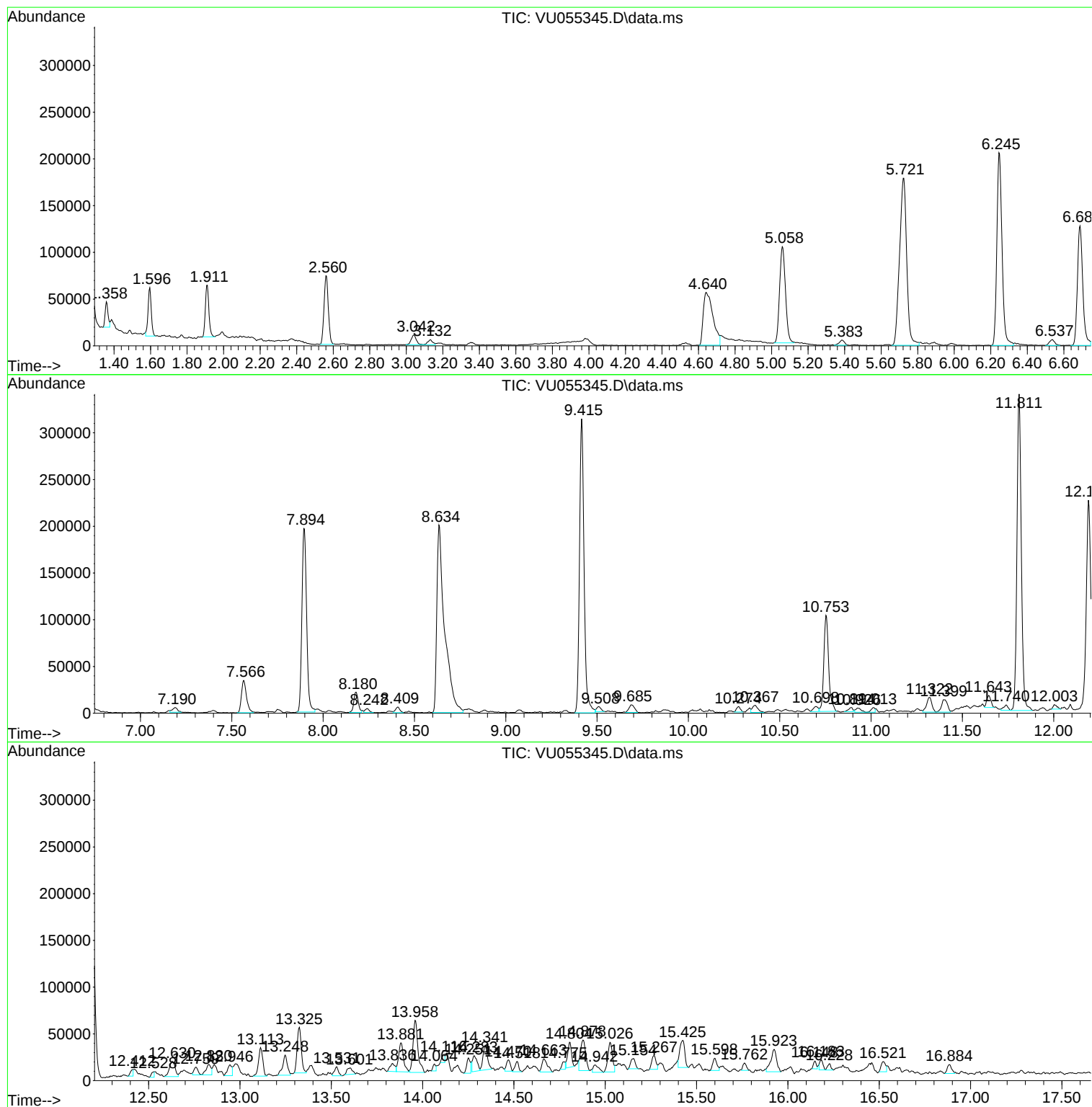
Sum of corrected areas: 5975540

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091523WMA.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\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

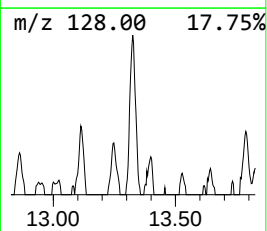
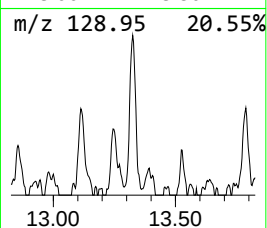
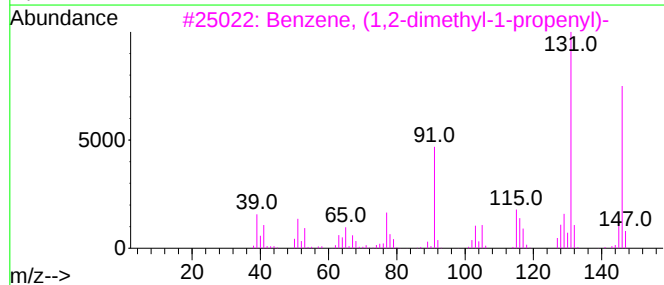
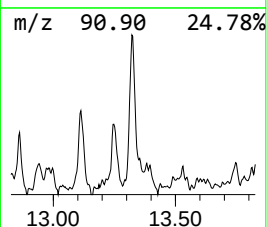
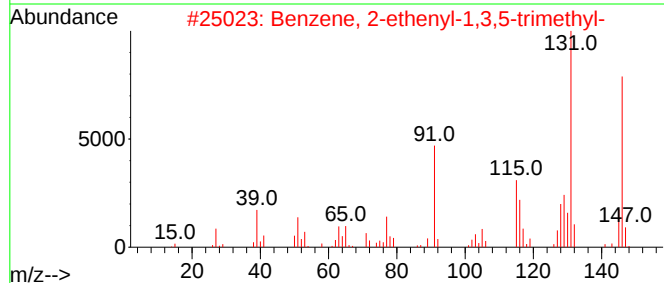
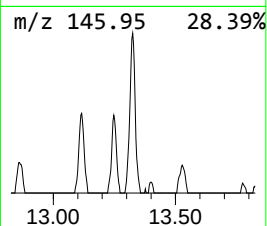
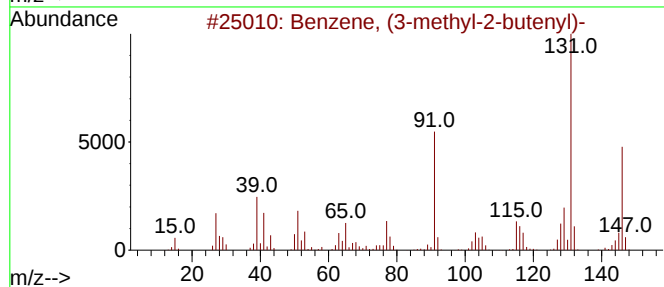
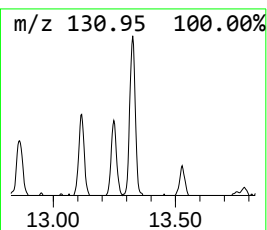
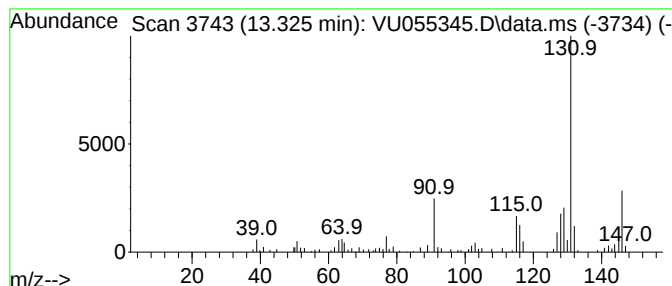
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091523WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzene, (3-methyl-2-butenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.325	0.69 ug/L	77969	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	91
2			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	90
3			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	90
4			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	87
5			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

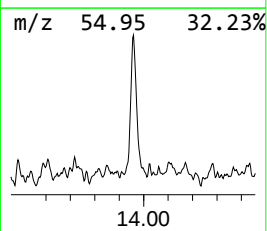
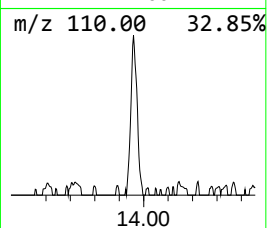
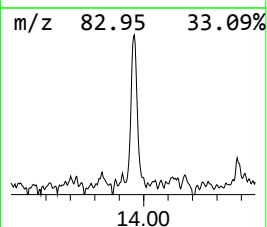
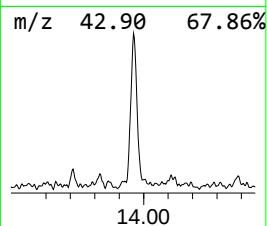
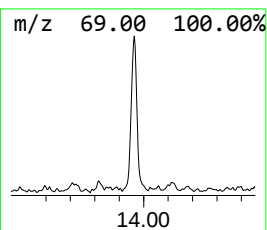
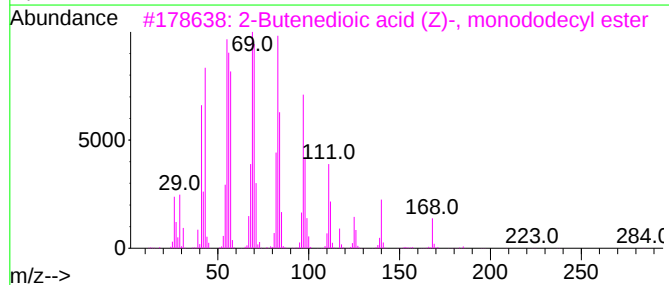
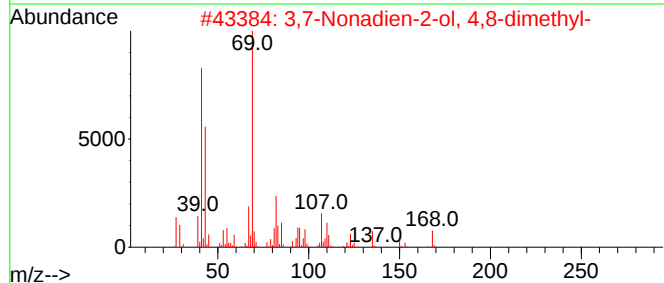
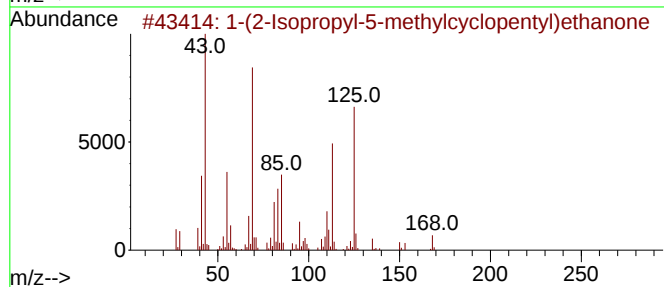
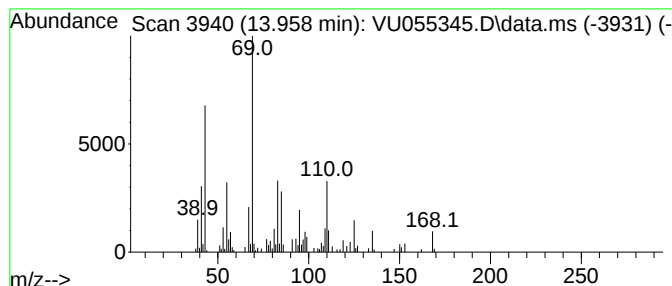
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091523WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-(2-Isopropyl-5-methylcyclopentyl)ethanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.958	0.92 ug/L	103715	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Isopropyl-5-methylcyclopentyl)ethanone	168	C11H20O	1000191-21-0	50		
2	3,7-Nonadien-2-ol, 4,8-dimethyl-	168	C11H20O	067845-50-5	45		
3	2-Butenedioic acid (Z)-, monododecyl ester	284	C16H28O4	002424-61-5	43		
4	7-Nonen-2-one, 4,8-dimethyl-	168	C11H20O	003664-64-0	42		
5	4,4,8-Trimethyl-non-5-enal	182	C12H22O	066822-00-2	40		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

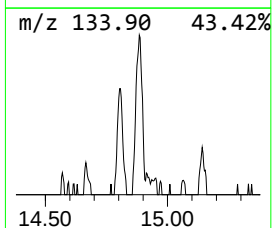
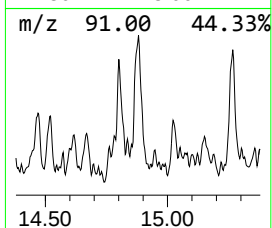
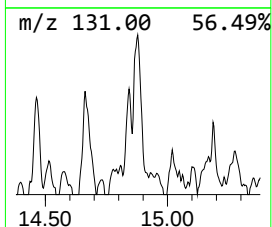
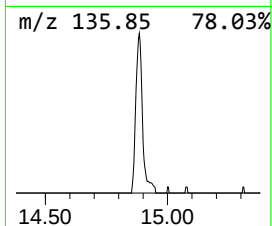
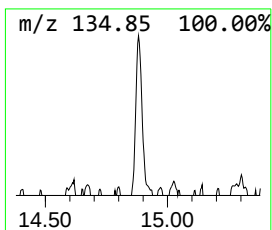
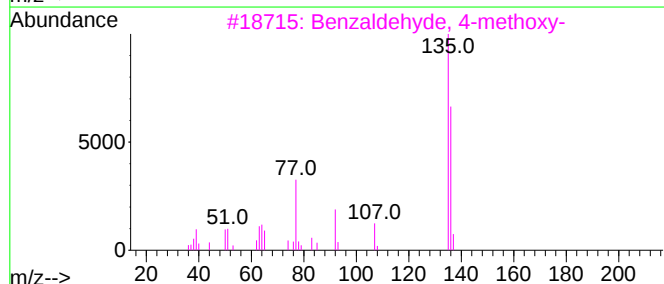
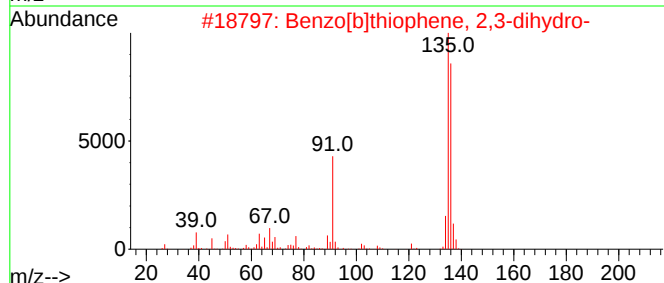
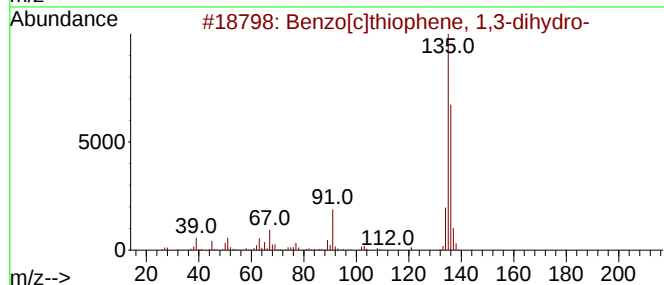
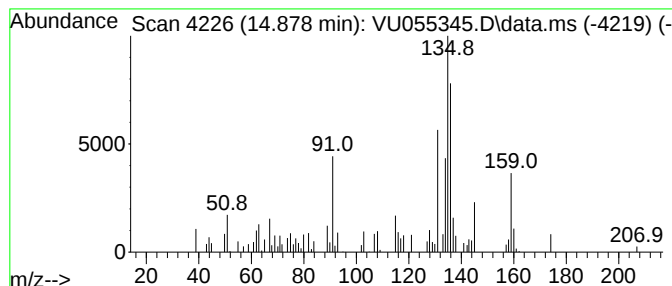
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091523WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.878	0.56 ug/L	63882	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	46
2			Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	43
3			Benzaldehyde, 4-methoxy-	136	C8H8O2	000123-11-5	38
4			N-Methyl-4-pyridinecarboxamide	136	C7H8N2O	006843-37-4	38
5			Benzaldehyde, 2-hydroxy-4-methyl-	136	C8H8O2	000698-27-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091523\
Data File : VU055345.D
Acq On : 15 Sep 2023 17:48
Operator : MD/SY
Sample : 04380-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091523WMA.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
Benzene, (3-met...	13.325	0.7	ug/L	77969	3	11.810	566465	5.0
1-(2-Isopropyl-...	13.958	0.9	ug/L	103715	3	11.810	566465	5.0
unknown-01	14.878	0.6	ug/L	63882	3	11.810	566465	5.0