

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083022\
 Data File : VV027594.D
 Acq On : 30 Aug 2022 18:30
 Operator : SY/MD
 Sample : N4400-19
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBVC3

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\SFAMVTR081922WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV027594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	14	20	35	rVB	20311	33252	6.85%	0.643%
2	1.304	74	82	101	rVB	72250	85998	17.71%	1.662%
3	1.565	155	163	174	rBV	64283	76417	15.74%	1.477%
4	2.105	321	331	344	rVB	131913	192961	39.74%	3.728%
5	2.192	352	358	376	rVB6	6798	16437	3.38%	0.318%
6	3.761	832	846	860	rBV6	4969	11893	2.45%	0.230%
7	3.905	880	891	912	rBV3	35175	122955	25.32%	2.376%
8	4.346	1008	1028	1049	rBV2	117240	310729	63.99%	6.004%
9	5.044	1231	1245	1262	rBV3	194535	485586	100.00%	9.383%
10	5.616	1411	1423	1442	rBV	158870	339185	69.85%	6.554%
11	5.925	1507	1519	1522	rBV9	7535	13146	2.71%	0.254%
12	6.069	1549	1564	1595	rBV	118830	267873	55.16%	5.176%
13	6.989	1840	1850	1862	rBV2	37970	72954	15.02%	1.410%
14	7.314	1941	1951	1969	rBV	189223	350398	72.16%	6.771%
15	7.629	2040	2049	2063	rBV2	20717	40187	8.28%	0.777%
16	8.092	2182	2193	2212	rBV	161967	380761	78.41%	7.357%
17	8.185	2213	2222	2236	rVV	157542	300786	61.94%	5.812%
18	8.252	2238	2243	2251	rVV8	10810	21843	4.50%	0.422%
19	8.317	2252	2263	2289	rVB	159614	311542	64.16%	6.020%
20	8.850	2417	2429	2450	rBV	263135	454245	93.55%	8.777%
21	9.018	2472	2481	2489	rBV9	4348	7960	1.64%	0.154%
22	9.140	2507	2519	2536	rBV	62686	106792	21.99%	2.063%
23	9.262	2547	2557	2569	rVB4	13047	24170	4.98%	0.467%
24	9.551	2636	2647	2655	rBV7	5265	8530	1.76%	0.165%
25	9.706	2687	2695	2700	rBV7	3282	4976	1.02%	0.096%
26	10.217	2843	2854	2868	rBV	83075	136688	28.15%	2.641%
27	10.455	2919	2928	2939	rVB7	4505	8136	1.68%	0.157%
28	10.722	3003	3011	3026	rVB2	8956	13645	2.81%	0.264%
29	11.249	3163	3175	3183	rBV	226329	375174	77.26%	7.249%
30	11.419	3219	3228	3241	rVB	4327	9224	1.90%	0.178%
31	11.529	3252	3262	3281	rBV2	86343	165664	34.12%	3.201%
32	11.622	3281	3291	3305	rVB	204018	326220	67.18%	6.303%
33	12.349	3509	3517	3529	rVB7	6606	10599	2.18%	0.205%
34	12.580	3577	3589	3606	rVB4	27277	62324	12.83%	1.204%
35	12.998	3711	3719	3729	rBV5	8493	14138	2.91%	0.273%
36	13.442	3850	3857	3869	rVB5	3060	5888	1.21%	0.114%

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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

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Title : TRACE VOA SFAM1.0

37	15.078	4359	4366	4374	rBV7	4377	6034	1.24%	0.117%
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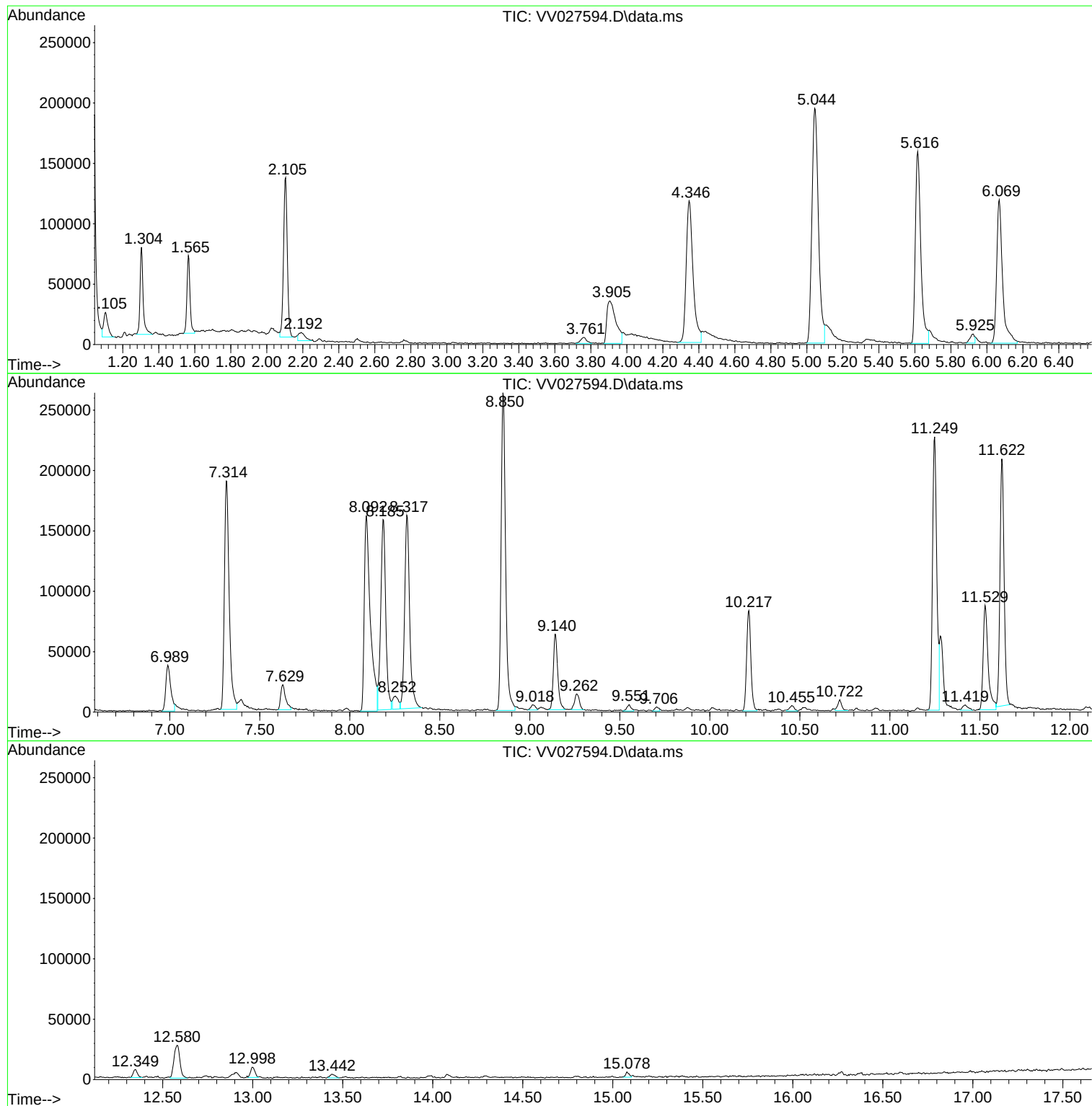
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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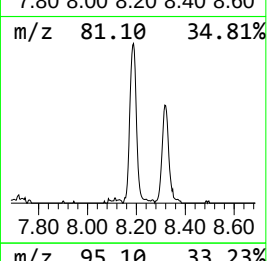
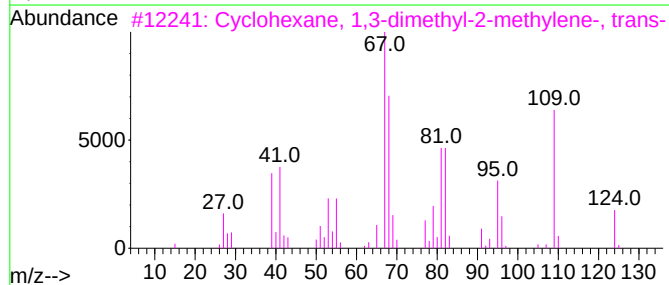
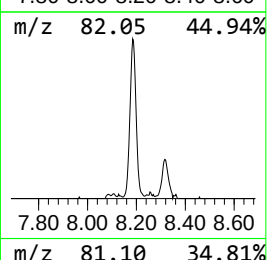
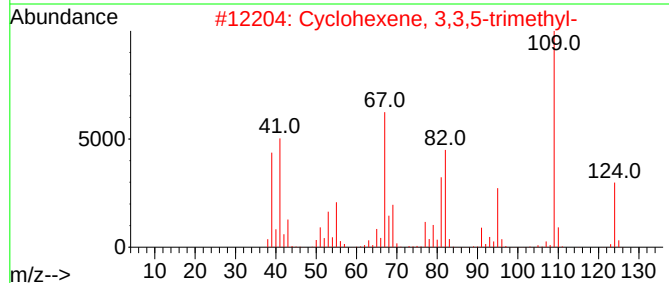
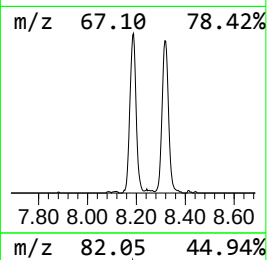
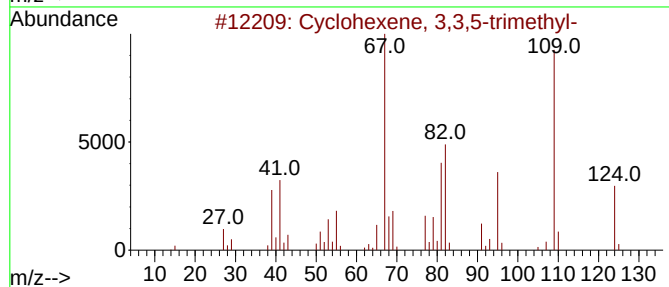
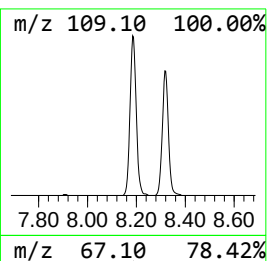
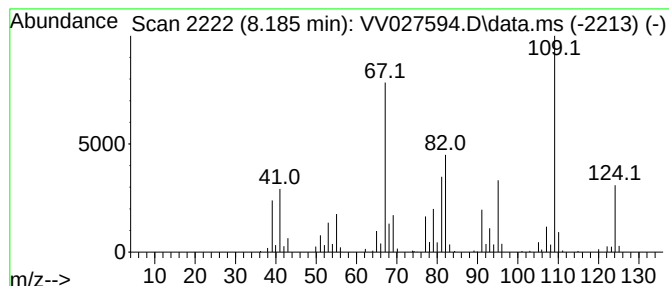
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Cyclohexene, 3,3,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	3.31 ug/L	300786	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	95
2			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	89
3			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	020348-74-7	87
4			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	019781-47-6	87
5			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	86



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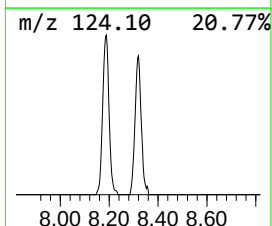
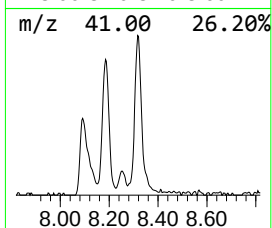
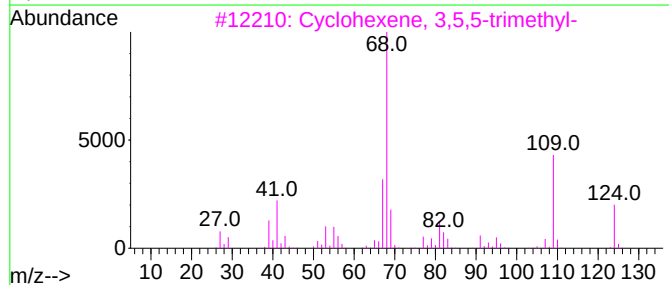
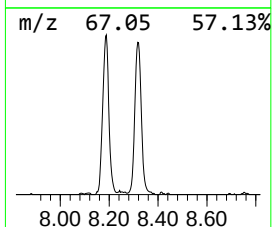
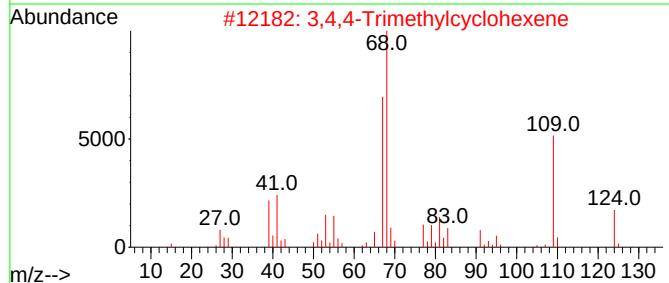
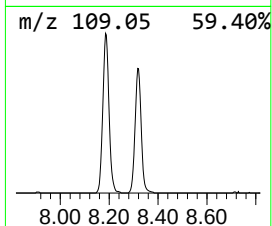
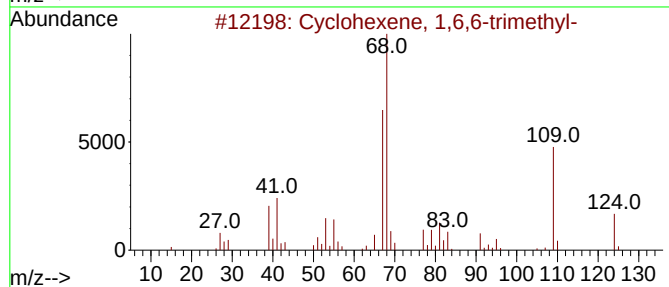
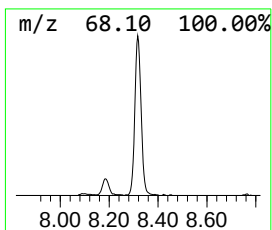
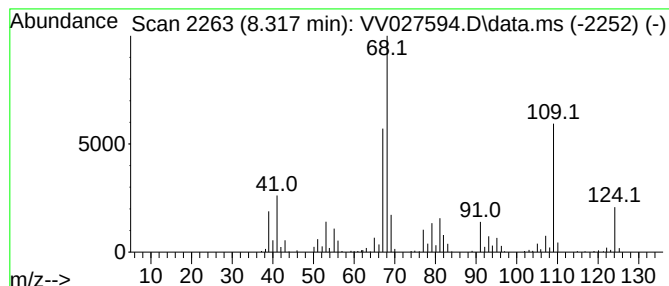
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Cyclohexene, 1,6,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.317	3.43 ug/L	311542	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1,6,6-trimethyl-	124	C9H16	069745-49-9	94
2			3,4,4-Trimethylcyclohexene	124	C9H16	1000113-50-1	90
3			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	76
4			6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	53
5			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	52



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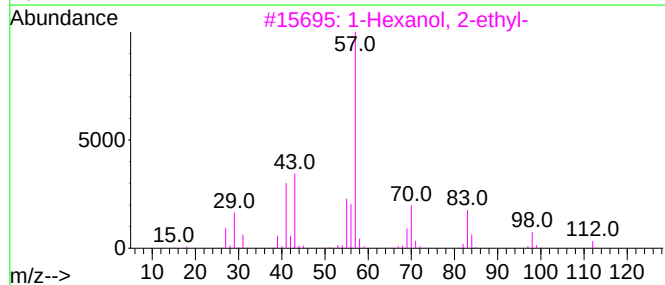
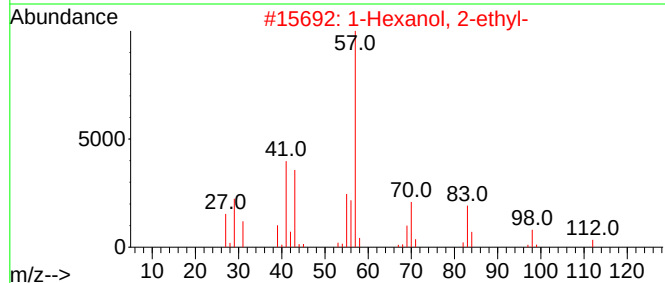
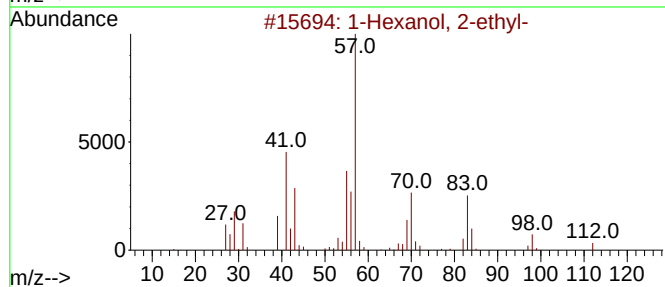
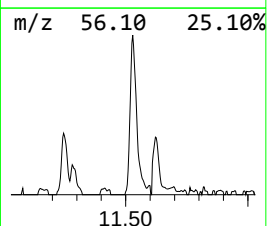
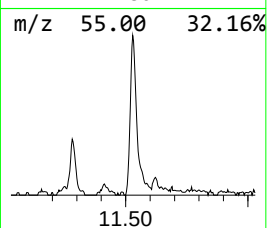
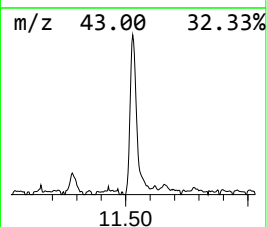
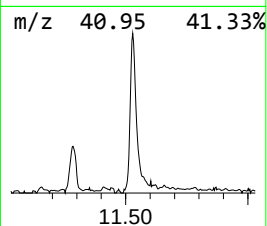
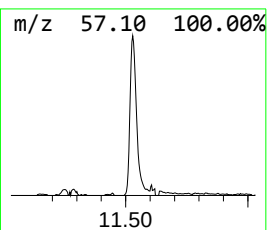
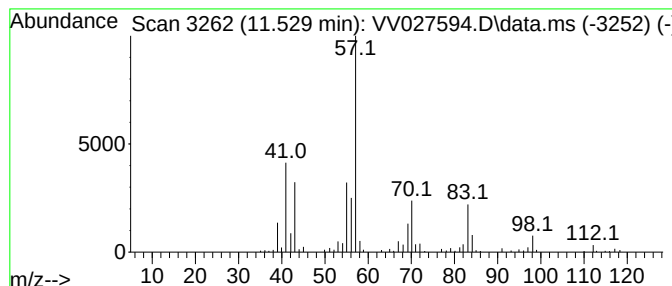
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	2.21 ug/L	165664	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53



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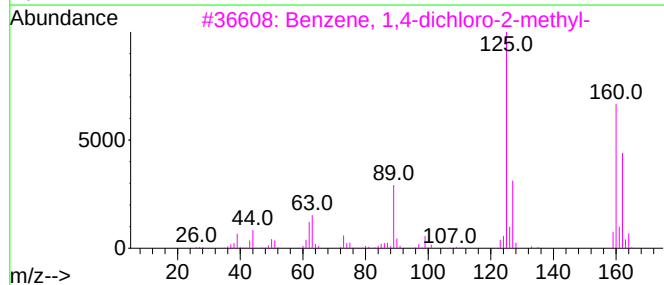
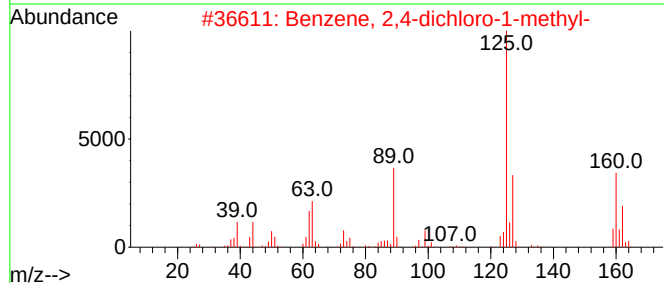
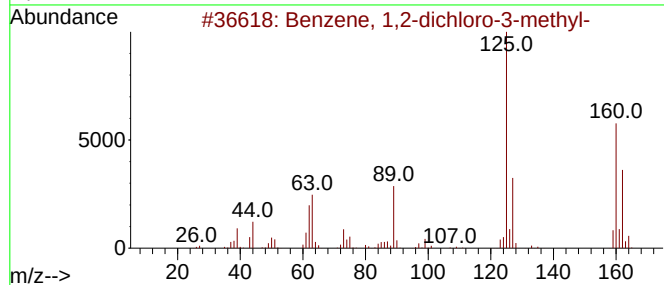
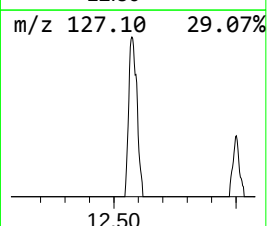
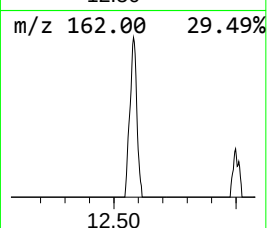
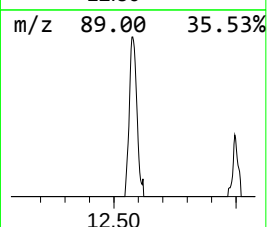
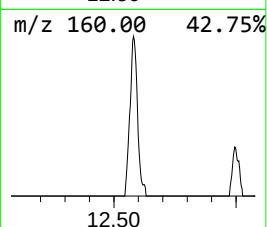
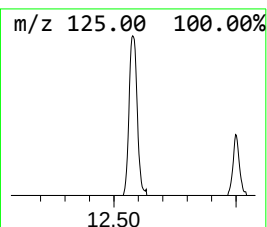
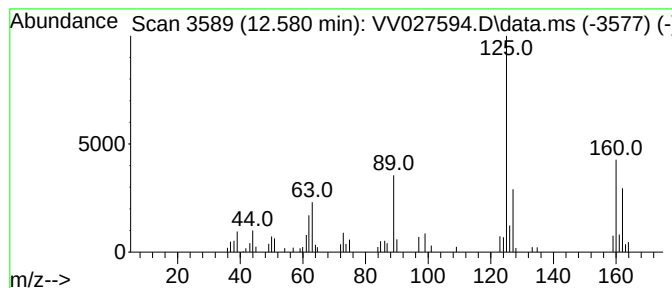
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Benzene, 1,2-dichloro-3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.580	0.83 ug/L	62324	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	97
2			Benzene, 2,4-dichloro-1-methyl-	160	C7H6Cl2	000095-73-8	97
3			Benzene, 1,4-dichloro-2-methyl-	160	C7H6Cl2	019398-61-9	96
4			Benzene, 1-chloro-4-(chloromethyl)-	160	C7H6Cl2	000104-83-6	96
5			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	96



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexene, 3,...	8.185	3.3	ug/L	300786	2	8.850	454245	5.0
Cyclohexene, 1,...	8.317	3.4	ug/L	311542	2	8.850	454245	5.0
1-Hexanol, 2-et...	11.529	2.2	ug/L	165664	3	11.249	375174	5.0
Benzene, 1,2-di...	12.580	0.8	ug/L	62324	3	11.249	375174	5.0