

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
 Data File : VU051519.D
 Acq On : 26 Oct 2022 22:43
 Operator : JC/MD
 Sample : N5300-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAE6

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\SFAMUTR100722WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	35	45	52	rBV2	10688	21469	1.88%	0.215%
2	1.597	73	80	88	rBV	142642	171142	14.98%	1.715%
3	1.909	169	177	196	rVB	114299	161677	14.15%	1.620%
4	2.565	369	381	392	rBV	203700	326542	28.57%	3.272%
5	2.623	392	399	414	rVB	18750	33276	2.91%	0.333%
6	2.755	427	440	459	rBV	18869	40272	3.52%	0.403%
7	3.182	559	573	598	rBV2	21567	52805	4.62%	0.529%
8	3.578	677	696	716	rBV5	15497	45176	3.95%	0.453%
9	3.867	758	786	787	rBV	14633	44184	3.87%	0.443%
10	4.620	1004	1020	1051	rBV	204713	520426	45.54%	5.214%
11	5.063	1141	1158	1182	rBV2	208595	582177	50.94%	5.833%
12	5.723	1340	1363	1374	rBV2	390311	1024215	89.62%	10.262%
13	6.157	1488	1498	1512	rVB3	5974	12460	1.09%	0.125%
14	6.247	1513	1526	1549	rBV	344160	658909	57.66%	6.602%
15	6.690	1650	1664	1682	rBV	247822	491582	43.02%	4.925%
16	7.160	1795	1810	1834	rBV4	45095	98881	8.65%	0.991%
17	7.565	1923	1936	1950	rBV2	97865	174334	15.25%	1.747%
18	7.713	1969	1982	2001	rBV2	41360	79695	6.97%	0.798%
19	7.896	2026	2039	2055	rBV	426085	750885	65.70%	7.523%
20	7.967	2056	2061	2079	rVB2	12725	23688	2.07%	0.237%
21	8.179	2115	2127	2139	rBV	60804	103012	9.01%	1.032%
22	8.632	2255	2268	2300	rBV2	591484	1142813	100.00%	11.450%
23	8.787	2308	2316	2329	rVB5	16236	28740	2.51%	0.288%
24	9.417	2497	2512	2533	rBV	506131	860931	75.33%	8.626%
25	9.571	2551	2560	2576	rVB	13766	24907	2.18%	0.250%
26	9.687	2582	2596	2608	rBV6	16719	33974	2.97%	0.340%
27	10.115	2715	2729	2742	rBV8	6396	13404	1.17%	0.134%
28	10.755	2914	2928	2948	rBV	209938	335106	29.32%	3.357%
29	11.468	3140	3150	3167	rVB3	17389	29369	2.57%	0.294%
30	11.809	3243	3256	3274	rBV	433429	717580	62.79%	7.189%
31	12.063	3322	3335	3338	rBV4	15676	24236	2.12%	0.243%
32	12.092	3338	3344	3356	rVB3	31014	49502	4.33%	0.496%
33	12.192	3362	3375	3390	rBV	381690	627742	54.93%	6.289%
34	12.517	3471	3476	3487	rVB7	7737	12785	1.12%	0.128%
35	12.889	3583	3592	3601	rBV3	18119	28518	2.50%	0.286%
36	13.851	3883	3891	3905	rVB7	16068	26937	2.36%	0.270%

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37	13.944	3910	3920	3928	rBV8	8400	15561	1.36%	0.156%
38	13.992	3928	3935	3946	rVB10	7176	13393	1.17%	0.134%
39	14.086	3951	3964	3979	rBV	118821	206812	18.10%	2.072%
40	14.899	4207	4217	4225	rBV4	36418	60967	5.33%	0.611%
41	14.941	4226	4230	4236	rVB6	9056	11634	1.02%	0.117%
42	15.073	4263	4271	4279	rVB6	18590	26792	2.34%	0.268%
43	15.224	4306	4318	4327	rBV	53456	95226	8.33%	0.954%
44	15.410	4364	4376	4389	rBV2	49659	89892	7.87%	0.901%
45	16.404	4674	4685	4692	rBV7	11179	23796	2.08%	0.238%
46	16.883	4828	4834	4843	rVB8	9771	14061	1.23%	0.141%
47	17.095	4891	4900	4910	rBV3	29067	49606	4.34%	0.497%

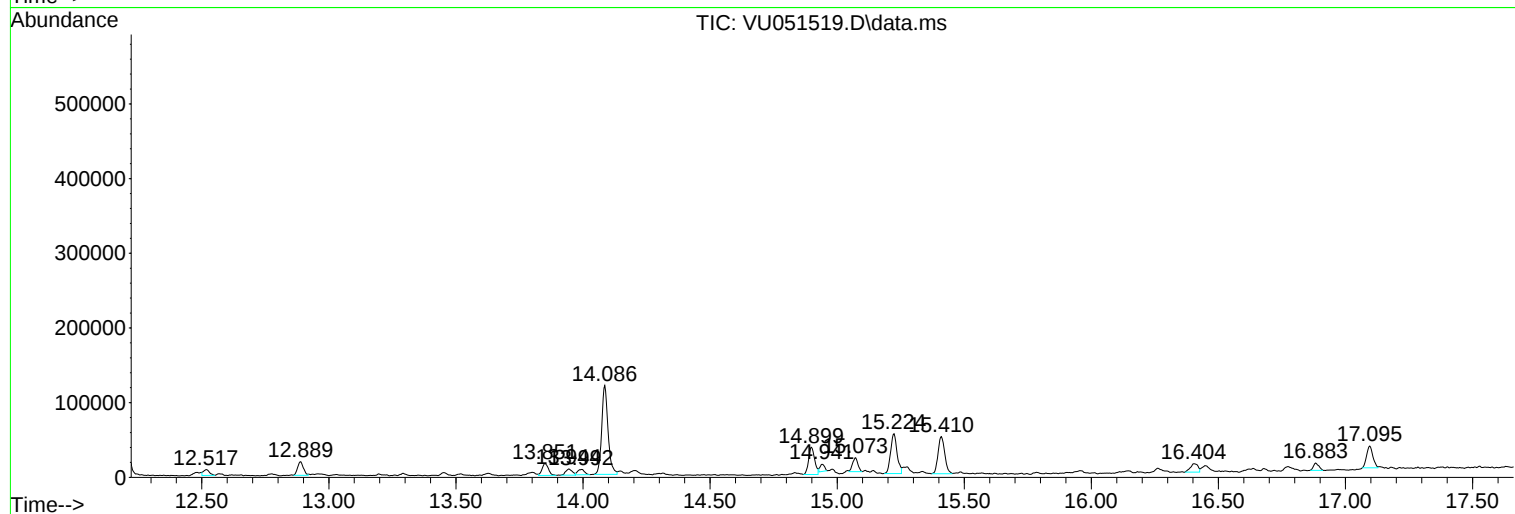
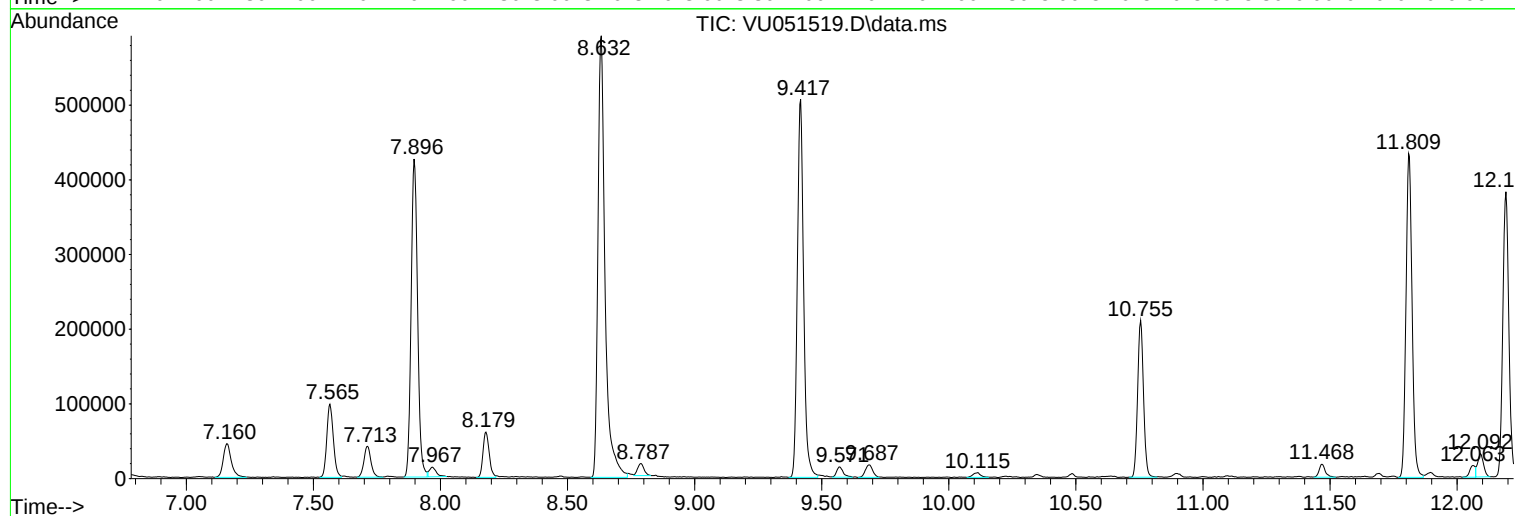
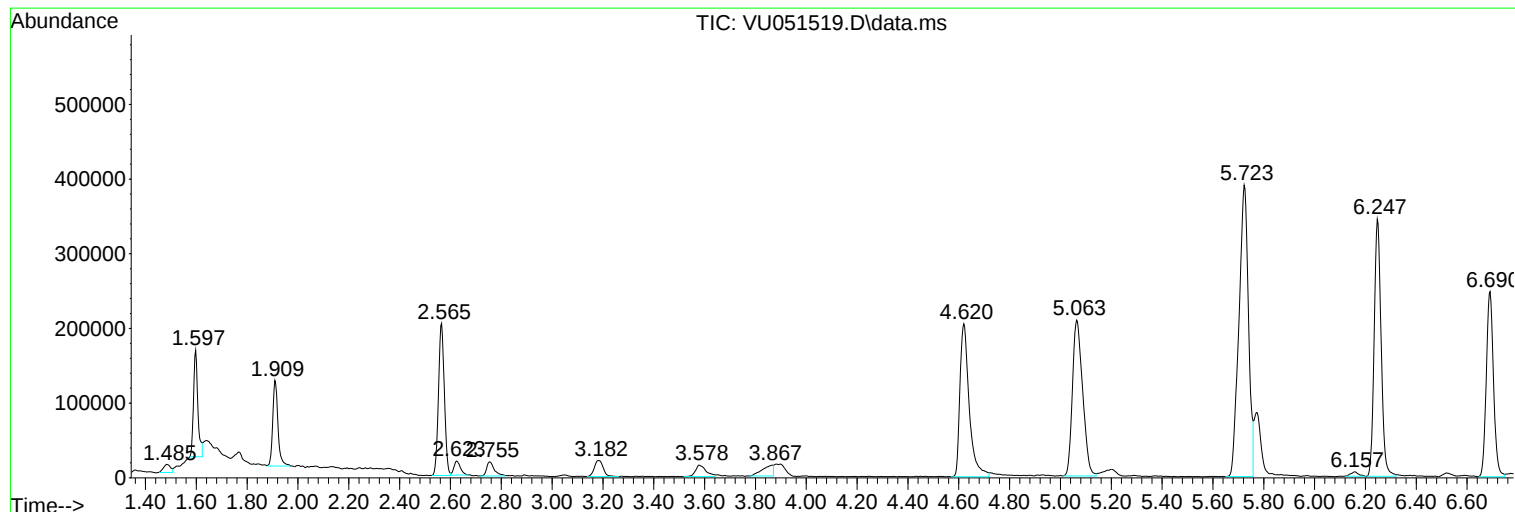
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MSVOA_U
ClientSampleId :
BHA66

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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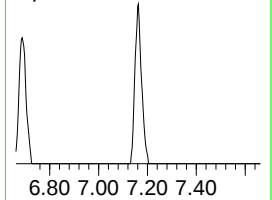
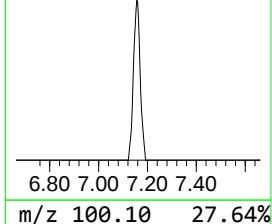
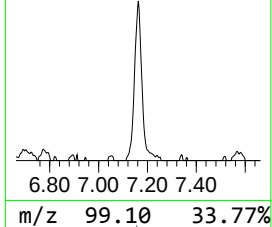
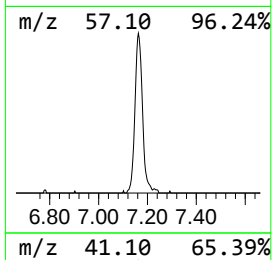
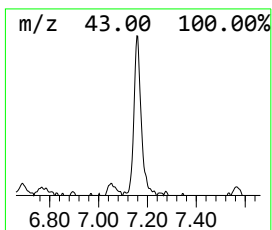
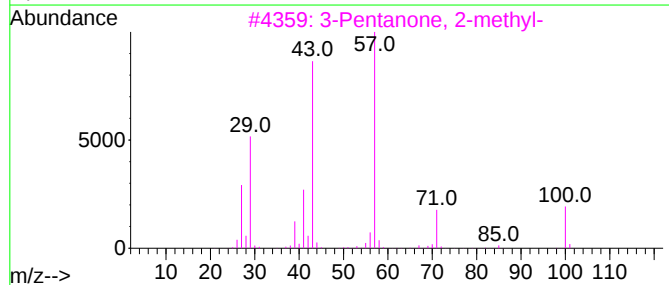
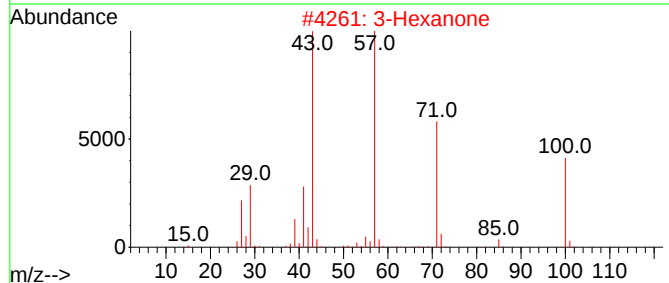
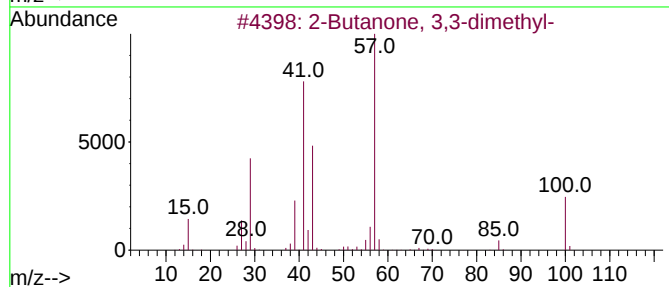
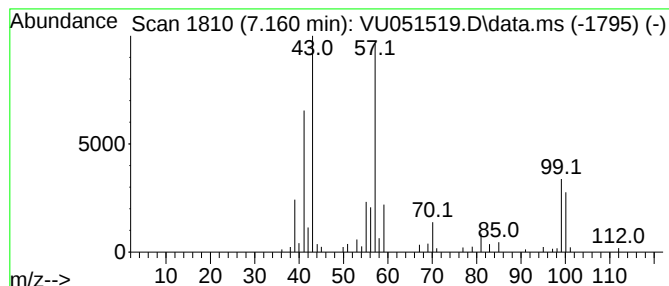
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.160	0.75 ug/L	98881	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	43
2	3-Hexanone			100	C6H12O	000589-38-8	43
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	43
4	Carbonic acid, prop-1-en-2-yl un...			256	C15H28O3	1000382-90-6	40
5	3-Hexanone			100	C6H12O	000589-38-8	38



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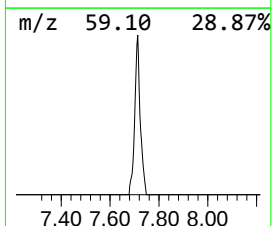
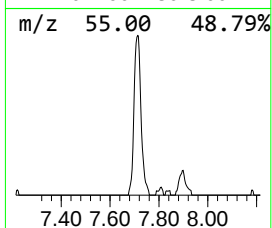
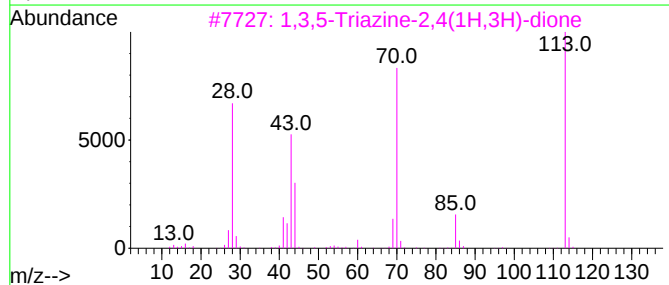
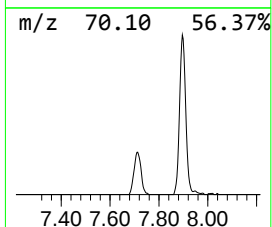
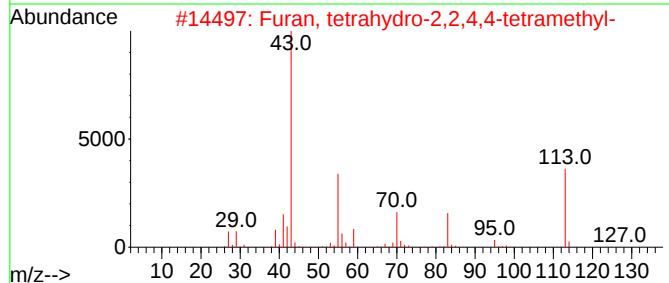
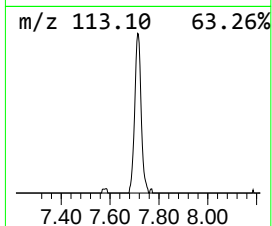
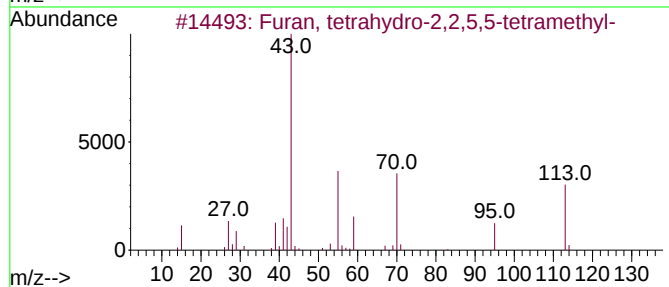
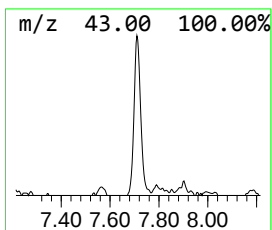
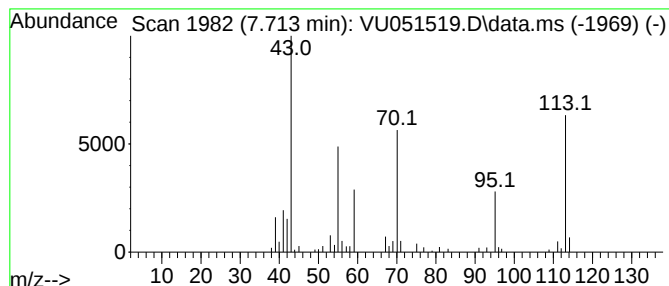
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.713	0.60 ug/L	79695	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3			1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	50
4			Pyrrolidine, 1-acetyl-	113	C6H11NO	004030-18-6	50
5			4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	47



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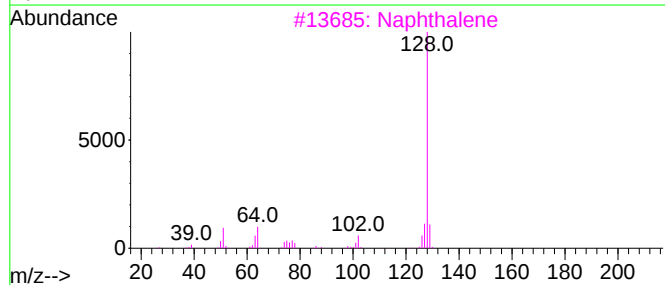
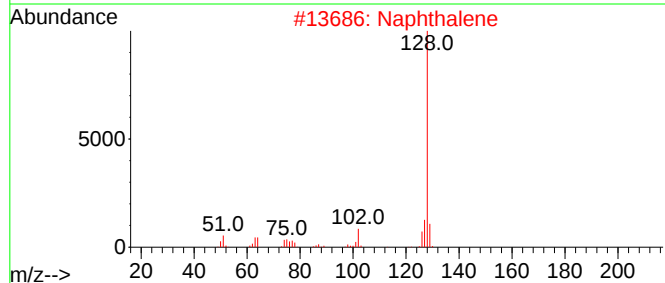
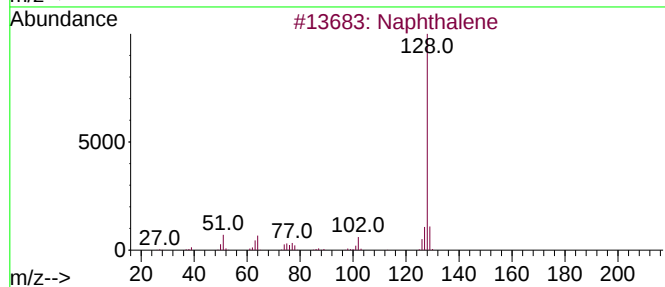
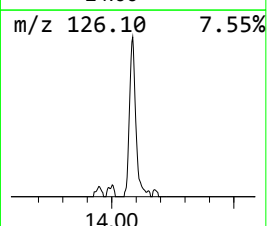
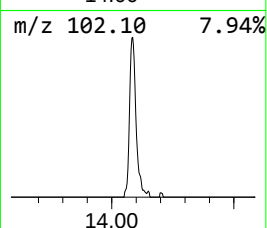
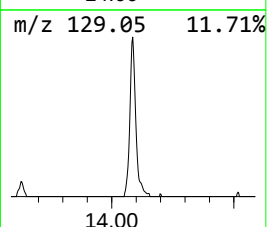
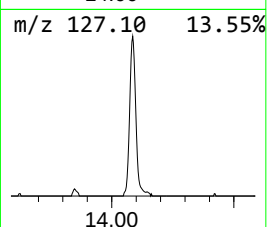
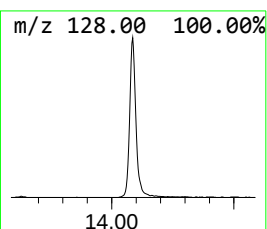
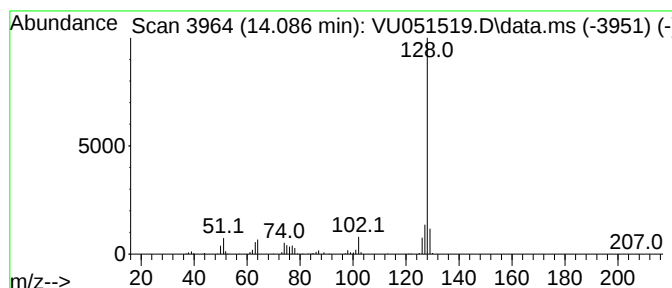
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	1.44 ug/L	206812	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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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
unknown-01	7.160	0.8	ug/L	98881	1	6.247	658909	5.0
Furan, tetrahyd...	7.713	0.6	ug/L	79695	1	6.247	658909	5.0
Azulene	14.086	1.4	ug/L	206812	3	11.812	717580	5.0