

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010522\
 Data File : VD071612.D
 Acq On : 05 Jan 2022 14:19
 Operator : VA/SY
 Sample : N1007-01
 Misc : 2.86G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BARNUM-ST-SP

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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_D\Method\82D122221S.M
 Title : SW846 8260

Signal : TIC: VD071612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.415	416	424	435	rVB2	25648	75619	2.91%	0.389%
2	4.967	506	518	534	rBV2	71271	224927	8.65%	1.156%
3	5.997	683	693	703	rVB6	11135	35040	1.35%	0.180%
4	7.914	1009	1019	1024	rBV2	257941	620423	23.86%	3.189%
5	7.979	1024	1030	1040	rVB	596956	1344971	51.73%	6.913%
6	8.332	1080	1090	1100	rBV	322482	736435	28.33%	3.785%
7	8.861	1168	1180	1191	rBV	905961	1856865	71.42%	9.545%
8	9.426	1270	1276	1281	rBV2	29499	62219	2.39%	0.320%
9	10.338	1423	1431	1440	rBV	1437487	2599781	100.00%	13.363%
10	11.079	1551	1557	1566	rBV	495097	840336	32.32%	4.320%
11	11.638	1645	1652	1661	rBV	1257622	2249307	86.52%	11.562%
12	12.349	1769	1773	1776	rBV6	29096	50273	1.93%	0.258%
13	12.626	1813	1820	1826	rBV	1238904	2103850	80.92%	10.814%
14	12.738	1828	1839	1858	rVB8	194916	1049878	40.38%	5.397%
15	12.873	1858	1862	1865	rBV	50717	76620	2.95%	0.394%
16	12.944	1871	1874	1882	rVB5	62145	103978	4.00%	0.534%
17	13.255	1923	1927	1932	rBV	102688	154426	5.94%	0.794%
18	13.567	1973	1980	1990	rBV	1179215	2180214	83.86%	11.207%
19	13.802	2009	2020	2030	rVV9	183158	717307	27.59%	3.687%
20	13.879	2030	2033	2038	rVB3	55366	76767	2.95%	0.395%
21	13.961	2043	2047	2052	rBV5	37999	76106	2.93%	0.391%
22	14.102	2065	2071	2077	rBV4	84663	180636	6.95%	0.929%
23	14.214	2086	2090	2095	rVB2	52957	88860	3.42%	0.457%
24	14.338	2106	2111	2116	rBV5	87869	166053	6.39%	0.854%
25	14.467	2130	2133	2137	rVB	57032	77448	2.98%	0.398%
26	14.508	2137	2140	2143	rBV5	29472	38930	1.50%	0.200%
27	14.555	2145	2148	2154	rVB8	31371	43464	1.67%	0.223%
28	14.702	2168	2173	2175	rBV2	54264	95417	3.67%	0.490%
29	14.738	2177	2179	2184	rVB3	76207	98231	3.78%	0.505%
30	14.820	2185	2193	2197	rBV3	132885	310582	11.95%	1.596%
31	14.967	2213	2218	2224	rVB	121127	216954	8.35%	1.115%
32	15.079	2234	2237	2240	rBV5	22670	33500	1.29%	0.172%
33	15.349	2279	2283	2287	rBV7	26894	44576	1.71%	0.229%
34	15.443	2294	2299	2302	rBV2	38605	61005	2.35%	0.314%
35	15.496	2304	2308	2317	rVV8	36888	109445	4.21%	0.563%
36	15.579	2319	2322	2332	rVB9	44501	87014	3.35%	0.447%

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Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122221S.M

Title : SW846 8260

37	15.679	2334	2339	2345	rVB4	37494	77604	2.99%	0.399%
38	15.890	2370	2375	2384	rVB3	108915	209816	8.07%	1.078%
39	16.208	2422	2429	2436	rBV5	53679	125425	4.82%	0.645%
40	16.414	2457	2464	2470	rVB6	40618	90576	3.48%	0.466%
41	16.473	2470	2474	2480	rBV8	16548	33140	1.27%	0.170%
42	16.679	2503	2509	2510	rBV6	18010	30439	1.17%	0.156%

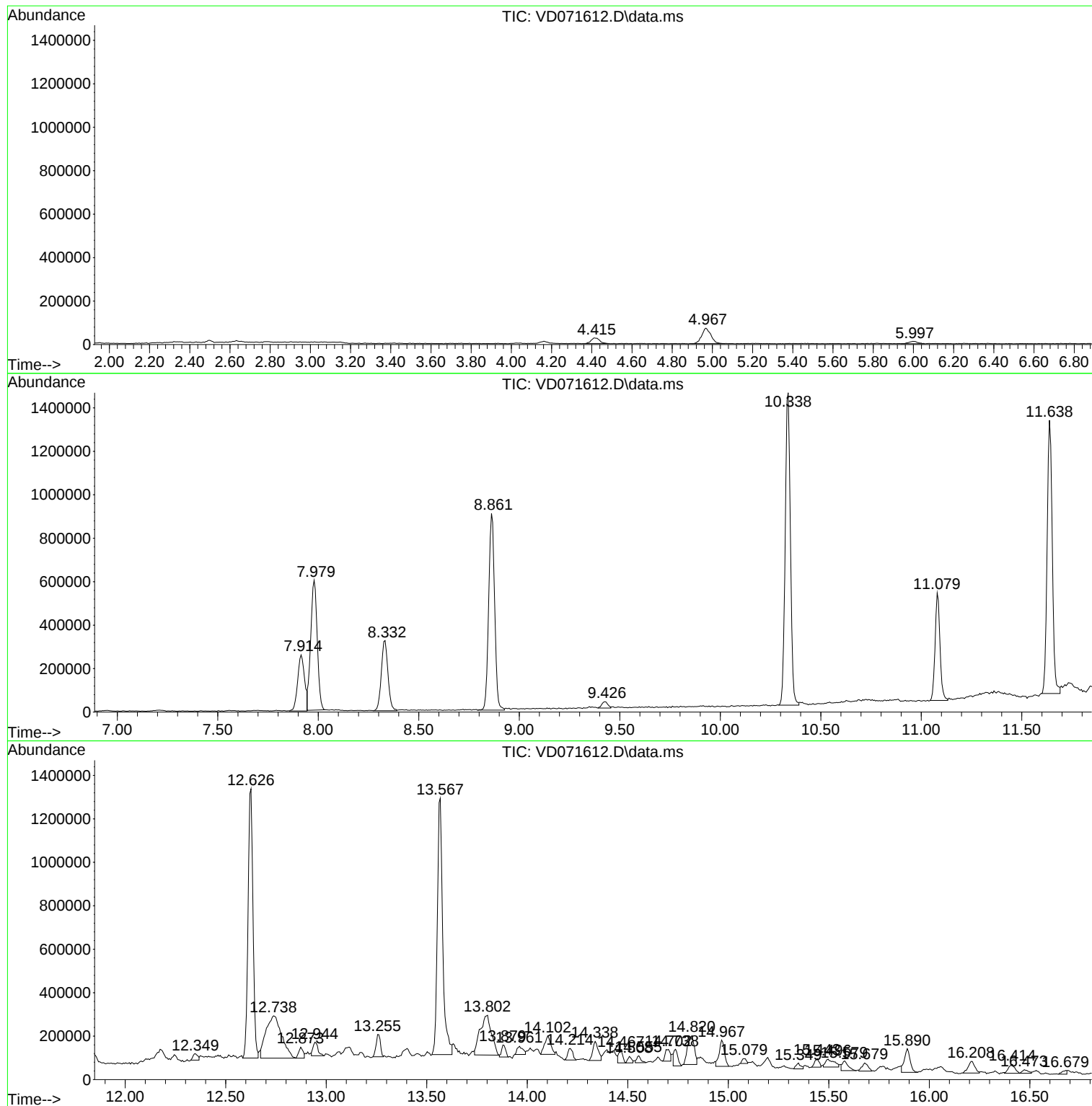
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122221S.M
Quant Title : SW846 8260

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



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BARNUM-ST-SP

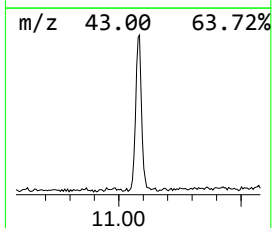
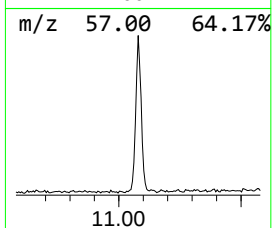
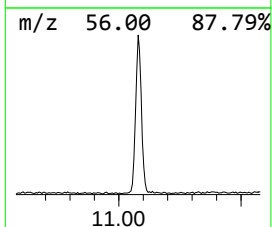
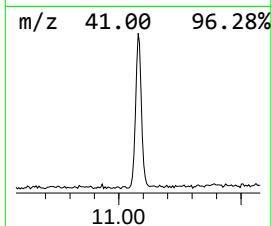
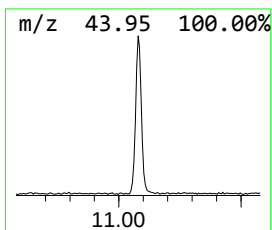
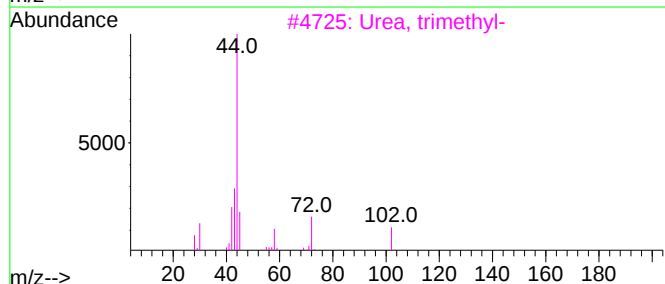
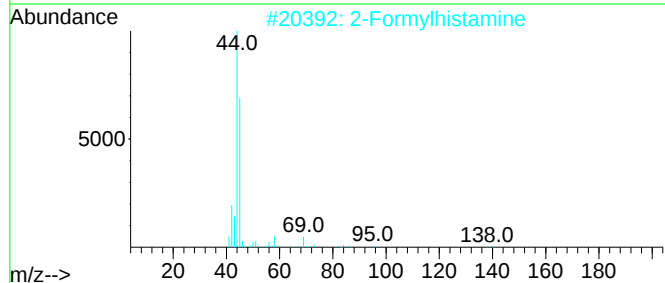
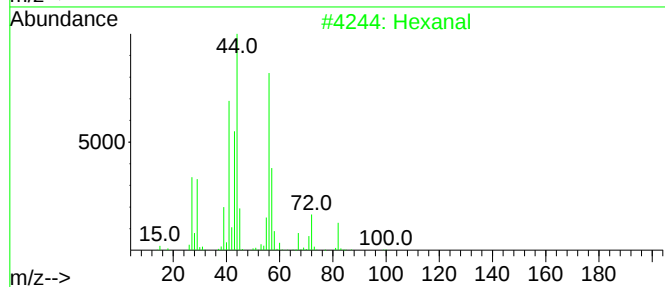
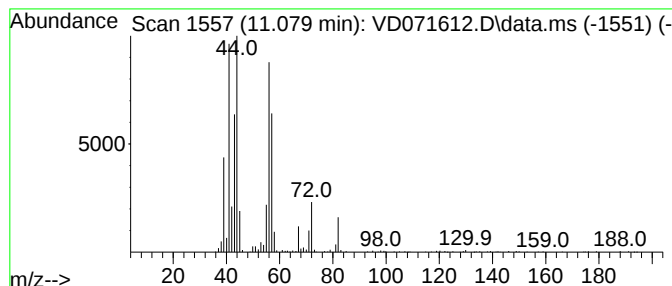
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122221S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.079	18.68 ug/l	840336	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	72
2			2-Formylhistamine	139	C6H9N3O	1000132-95-8	27
3			Urea, trimethyl-	102	C4H10N2O	000632-14-4	25
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	22
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	16



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
BARNUM-ST-SP

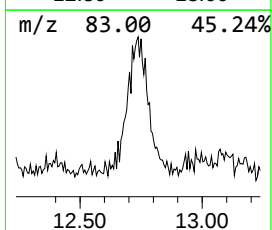
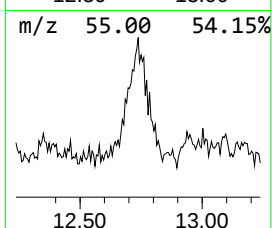
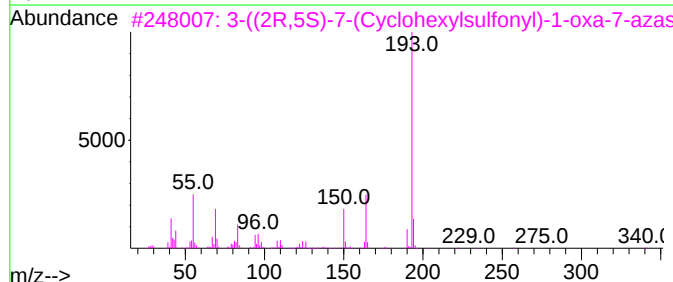
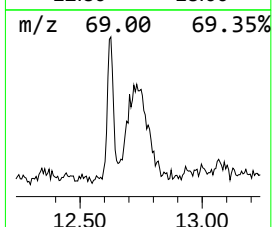
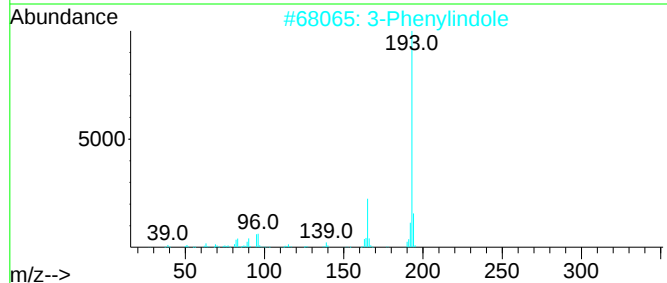
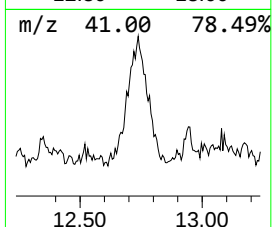
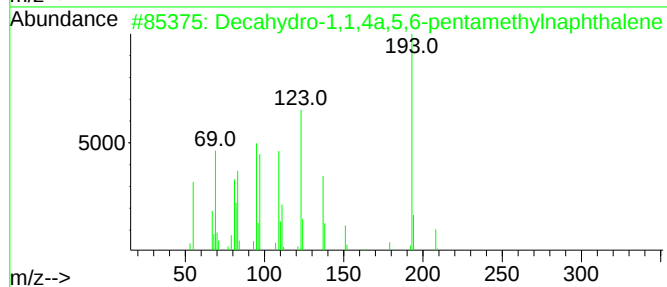
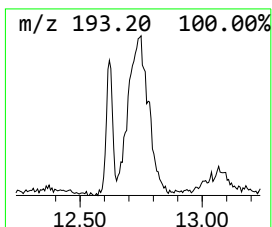
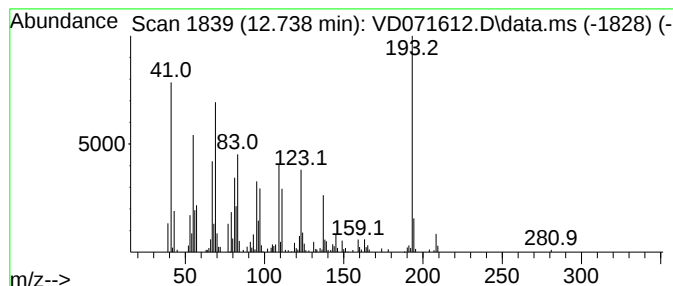
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122221S.M
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Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.738	24.08 ug/l	1049880	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	53
2			3-Phenylindole	193	C14H11N	001504-16-1	27
3			3-((2R,5S)-7-(Cyclohexylsulfonyl)...	340	C17H28N2O3S	1000483-82-6	27
4			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	22
5			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	18



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ALS Vial : 1 Sample Multiplier: 1

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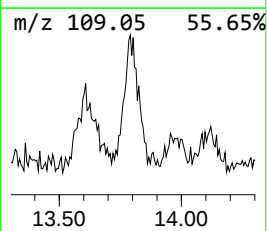
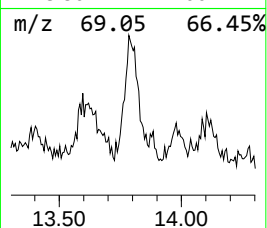
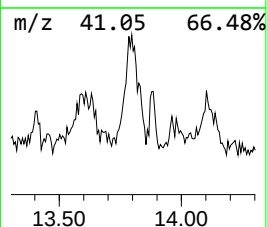
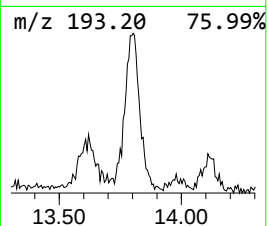
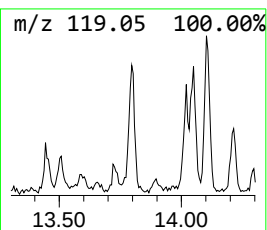
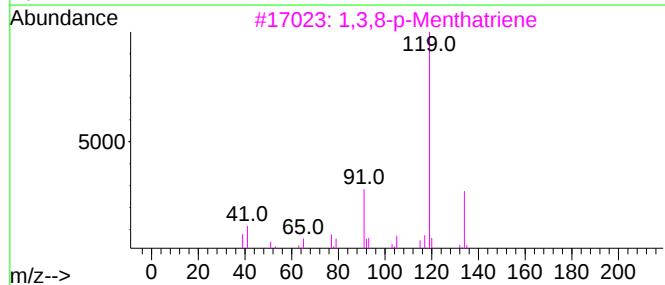
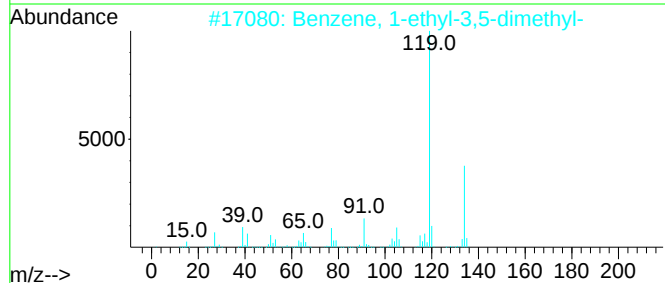
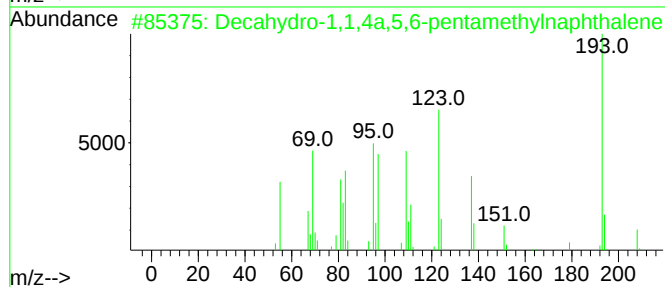
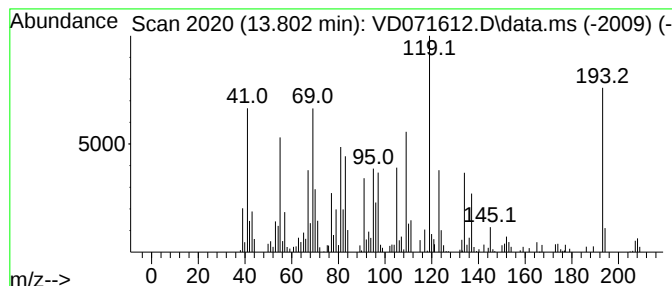
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D12221S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.802 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.802	16.45 ug/l	717307	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	78
2			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	25
3			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	25
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	25
5			o-Cymene	134	C10H14	000527-84-4	25



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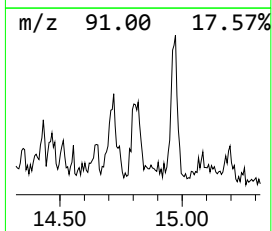
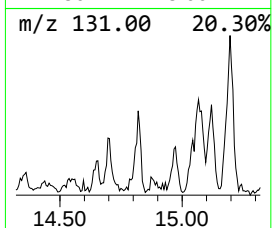
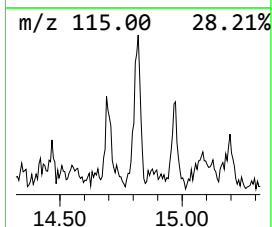
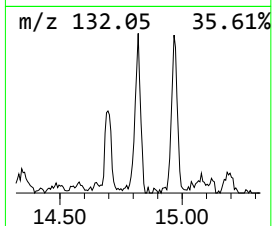
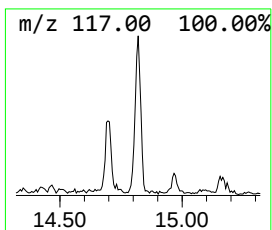
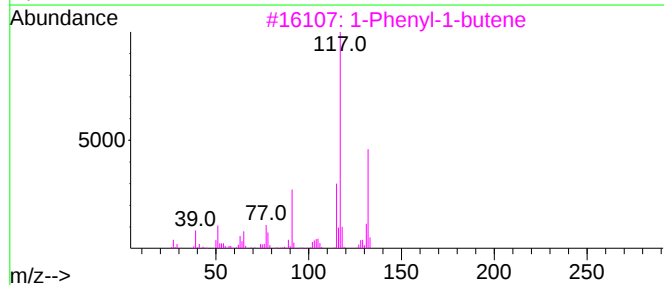
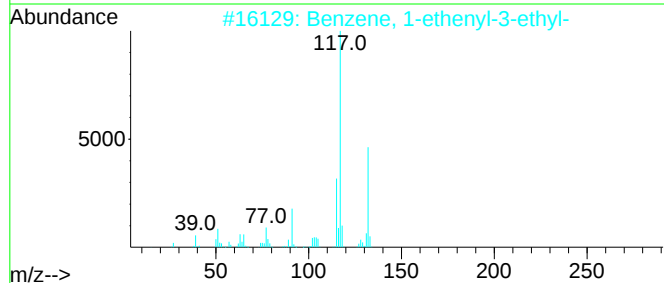
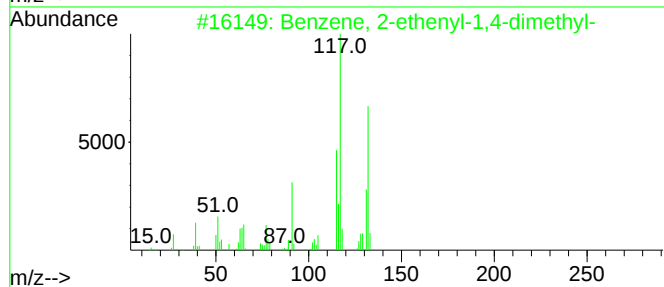
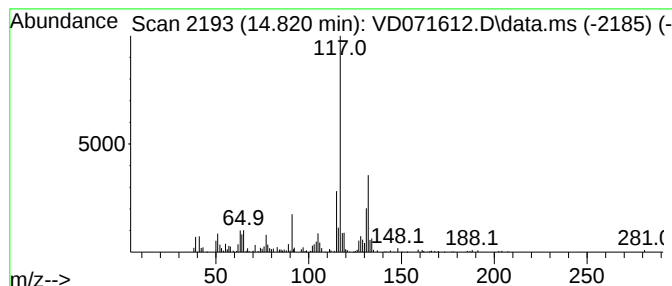
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.820	7.12 ug/l	310582	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4			2,4-Dimethylstyrene	132	C10H12	002234-20-0	91
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



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MSVOA_D
ClientSampleId :
BARNUM-ST-SP

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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	11.079	18.7	ug/l	840336	3	11.638	2249310	50.0
Decahydro-1,1,4...	12.738	24.1	ug/l	1049880	4	13.567	2180210	50.0
unknown13.802	13.802	16.4	ug/l	717307	4	13.567	2180210	50.0
Benzene, 2-ethe...	14.820	7.1	ug/l	310582	4	13.567	2180210	50.0