

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042924\
 Data File : VX041284.D
 Acq On : 29 Apr 2024 18:37
 Operator : JC/MD
 Sample : P2183-05 20X
 Misc : 1.41g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1230

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_X\Method\82X042224W.M
 Title : SW846 8260

Signal : TIC: VX041284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	207	214	240	rBV	1535548	2951914	96.40%	27.452%
2	5.385	693	705	715	rBV	72357	214337	7.00%	1.993%
3	5.550	715	732	740	rBV3	127368	513046	16.75%	4.771%
4	5.818	765	776	790	rBV2	91366	271093	8.85%	2.521%
5	5.952	790	798	816	rVB	74564	199464	6.51%	1.855%
6	6.178	822	835	843	rBV4	11996	44557	1.46%	0.414%
7	6.604	895	905	921	rBV	102196	245045	8.00%	2.279%
8	6.763	922	931	949	rVV	183885	448562	14.65%	4.171%
9	7.373	1020	1031	1042	rVB3	16940	44668	1.46%	0.415%
10	8.647	1234	1240	1246	rBV	388034	610709	19.94%	5.679%
11	8.720	1246	1252	1276	rVB	1965383	3062225	100.00%	28.477%
12	10.055	1465	1471	1487	rBV	398343	548498	17.91%	5.101%
13	11.079	1634	1639	1652	rBV	353487	457074	14.93%	4.251%
14	11.573	1711	1720	1724	rBV	22777	31299	1.02%	0.291%
15	11.750	1745	1749	1758	rVB	28201	37704	1.23%	0.351%
16	12.018	1788	1793	1800	rBV	422015	555013	18.12%	5.161%
17	12.317	1837	1842	1849	rVB3	24137	39411	1.29%	0.367%
18	12.420	1855	1859	1863	rBV	27154	31793	1.04%	0.296%
19	12.920	1933	1941	1944	rBV	24716	38994	1.27%	0.363%
20	12.963	1944	1948	1955	rVB	42652	62972	2.06%	0.586%
21	13.164	1975	1981	1986	rBV3	21746	30918	1.01%	0.288%
22	13.262	1992	1997	1999	rBV3	27739	39429	1.29%	0.367%
23	13.292	1999	2002	2007	rVB2	49461	68174	2.23%	0.634%
24	13.579	2046	2049	2056	rVB3	17878	30689	1.00%	0.285%
25	13.774	2077	2081	2087	rVB	35199	49234	1.61%	0.458%
26	14.633	2215	2222	2227	rBV	56288	86470	2.82%	0.804%
27	14.780	2243	2246	2252	rVB	30066	39848	1.30%	0.371%

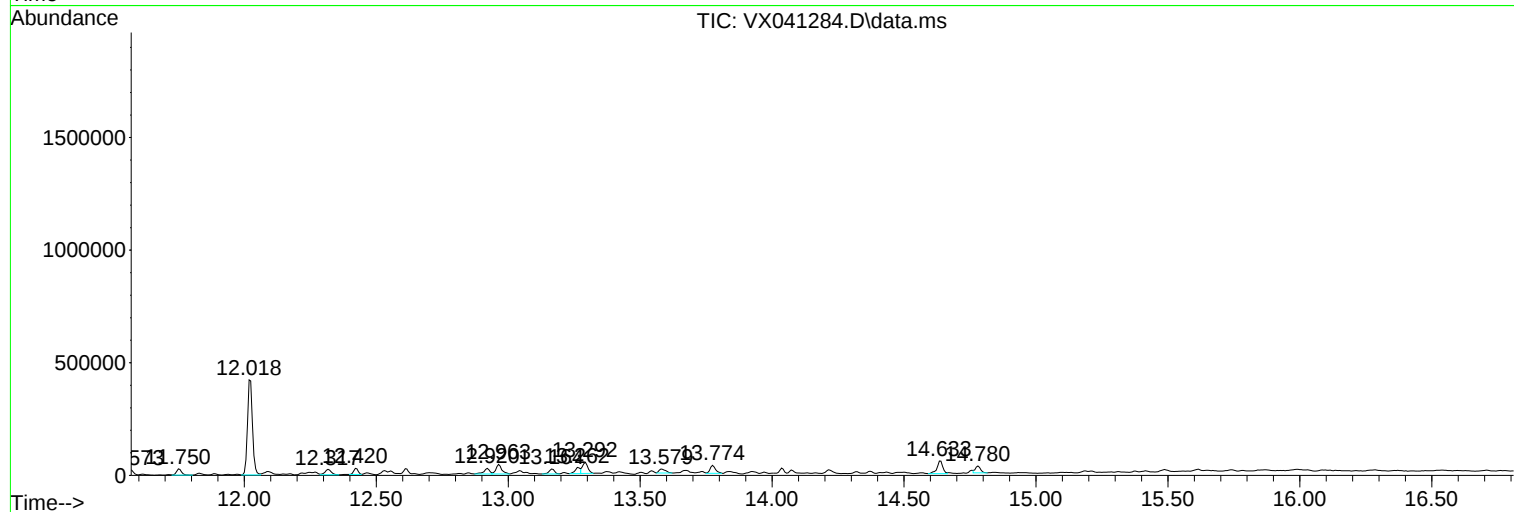
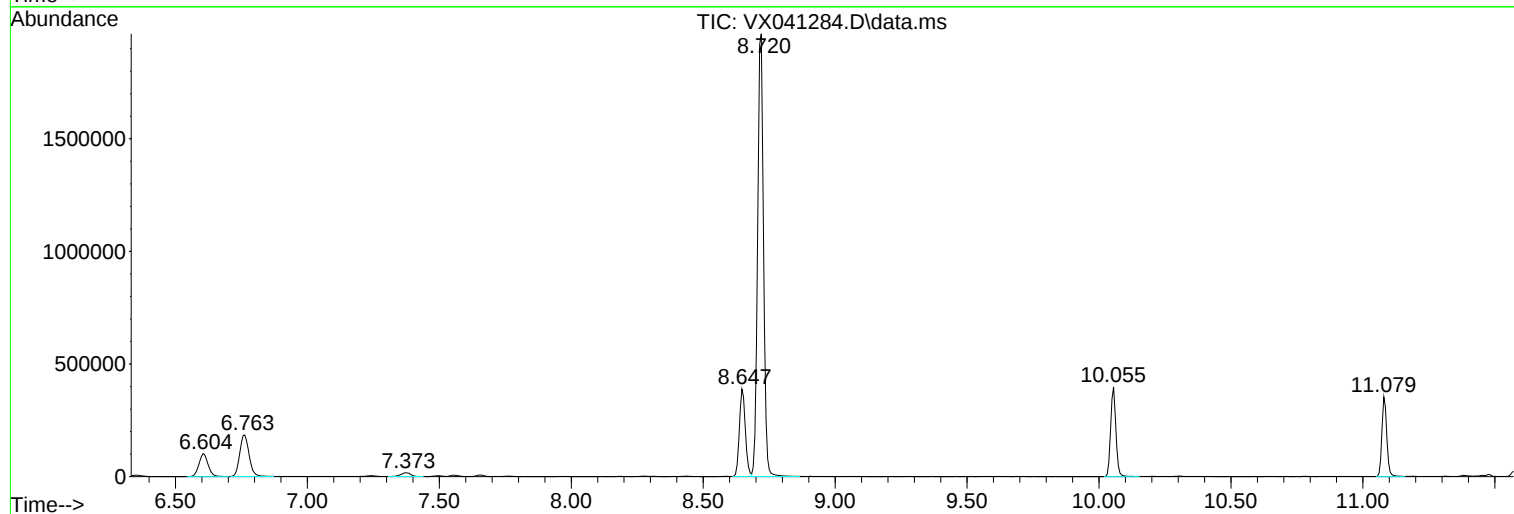
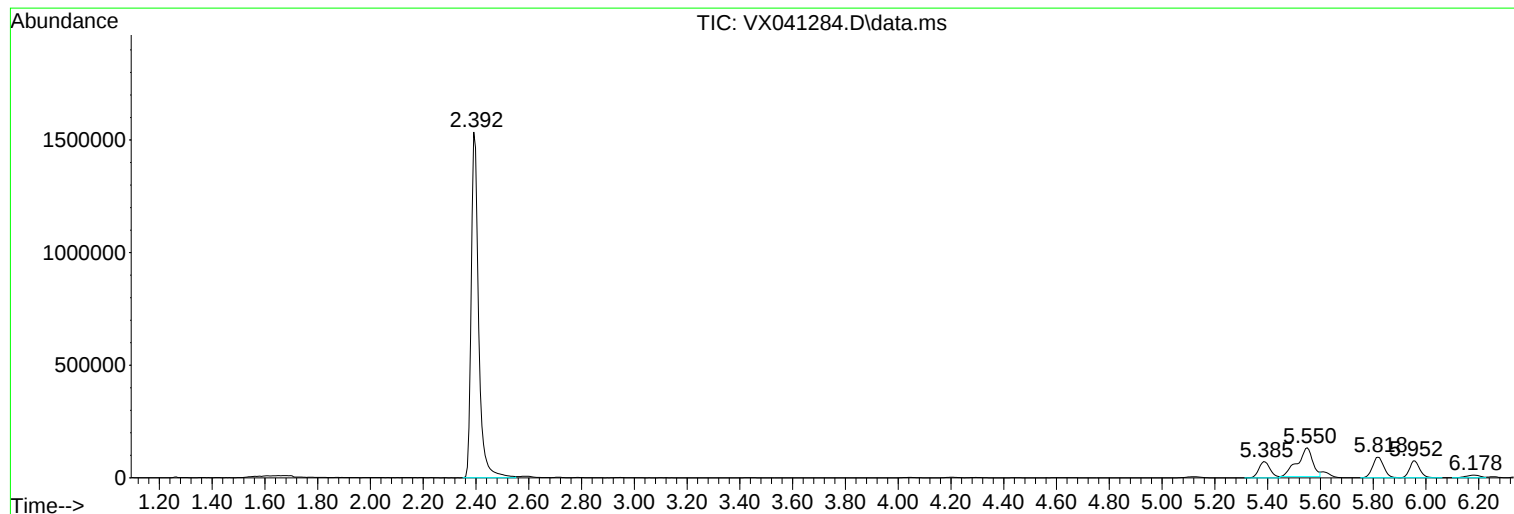
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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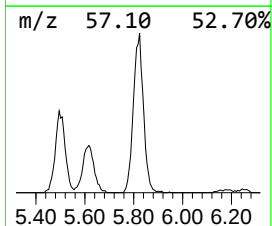
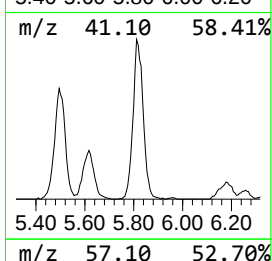
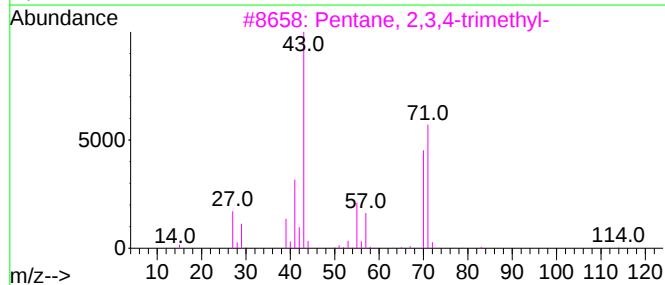
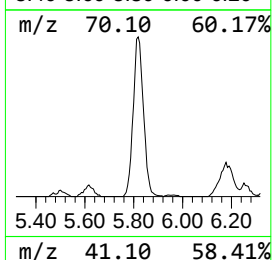
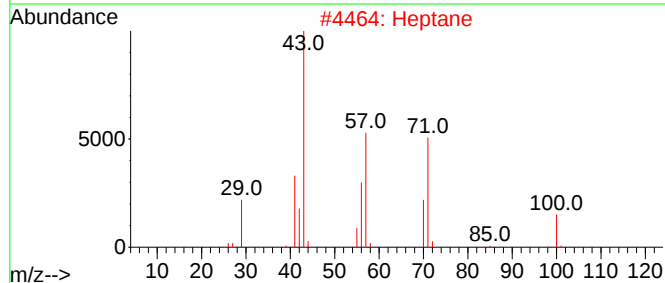
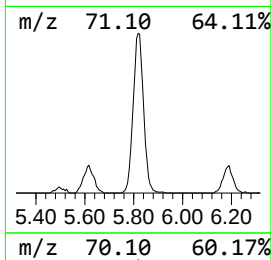
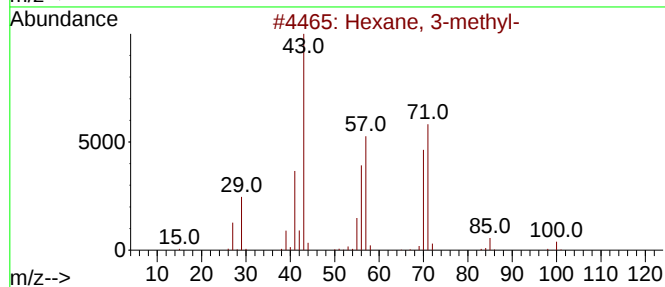
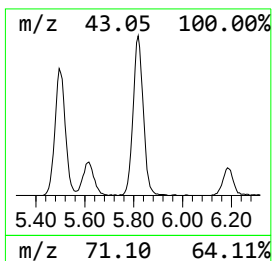
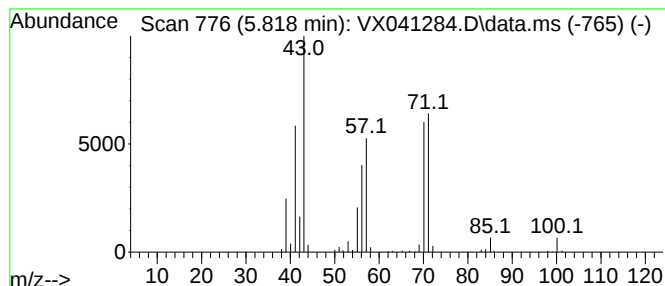
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	26.42 ug/l	271093	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	80
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5			Diisooamyl ether	158	C10H22O	000544-01-4	50



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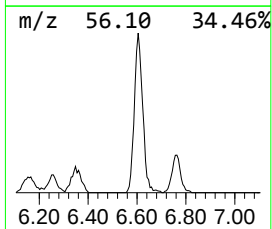
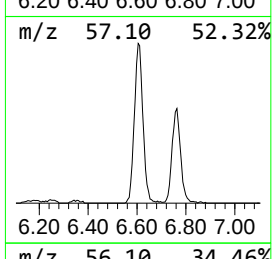
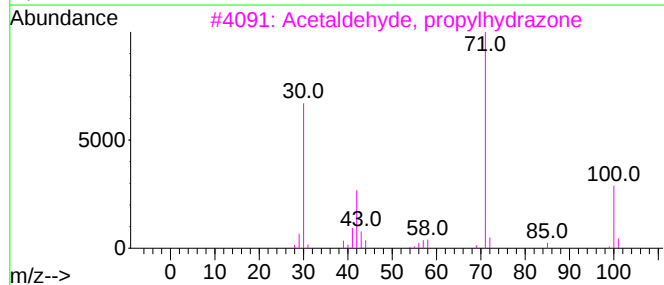
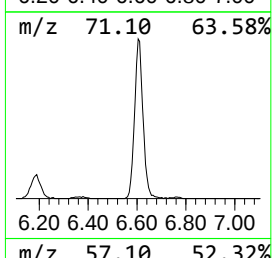
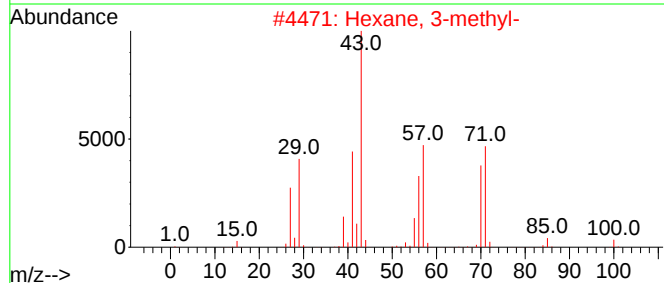
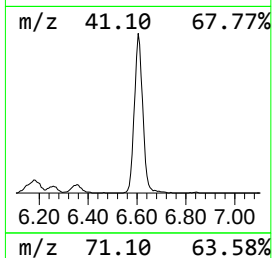
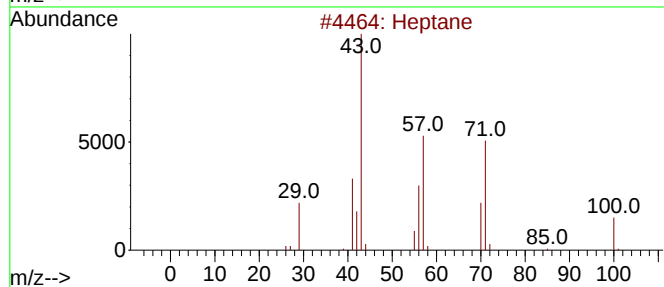
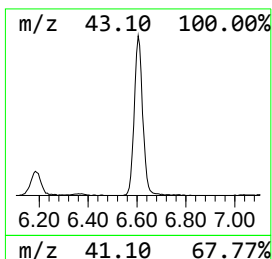
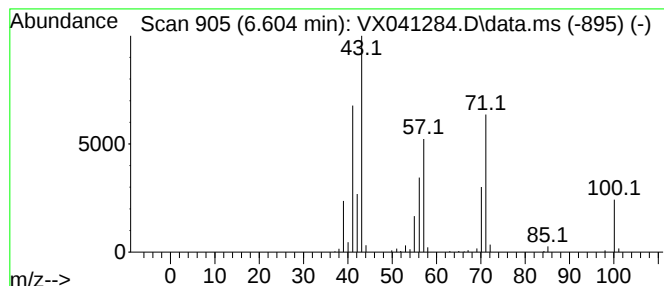
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	27.31 ug/l	245045	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	86
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	43
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40



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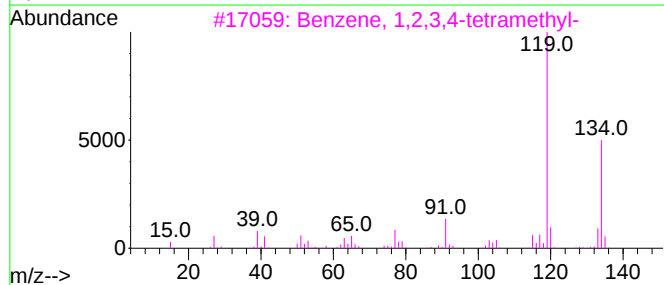
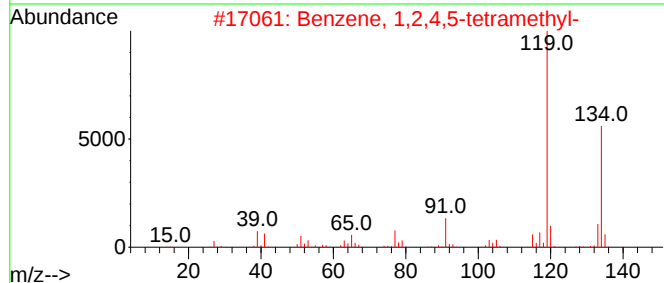
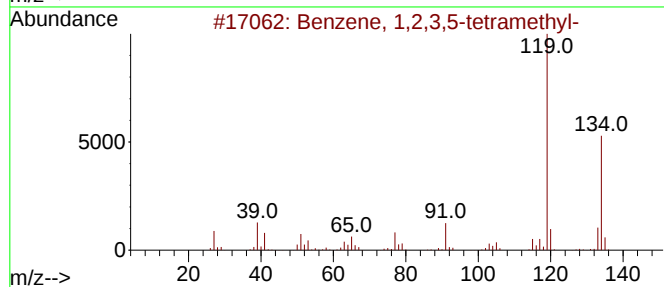
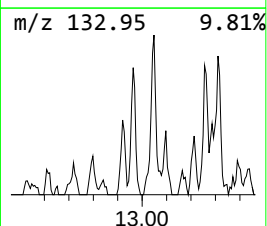
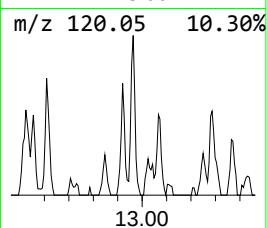
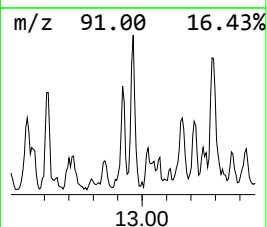
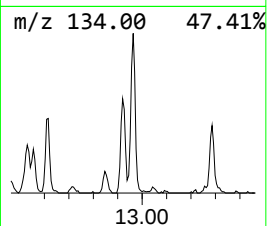
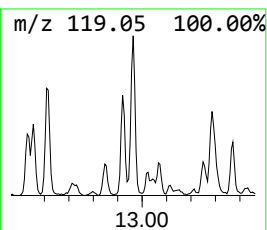
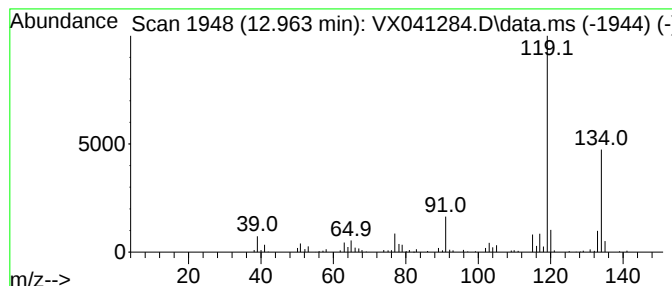
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	5.67 ug/l	62972	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	93
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



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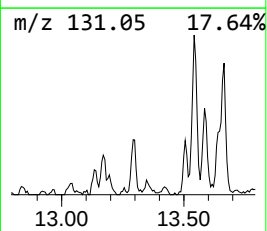
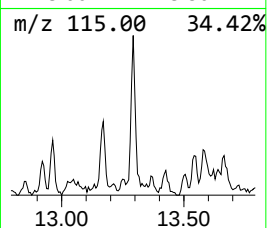
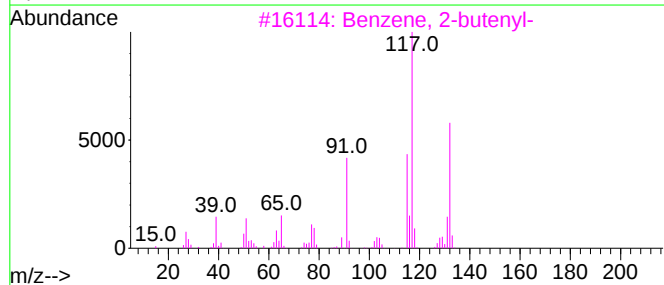
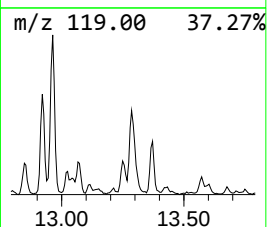
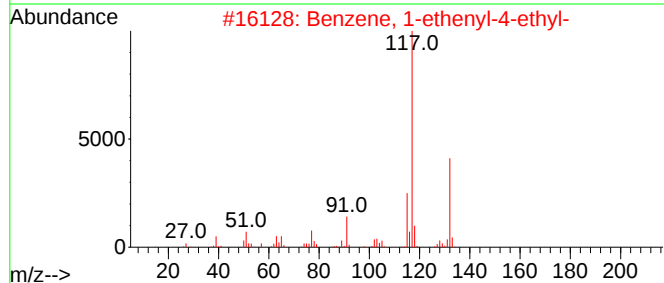
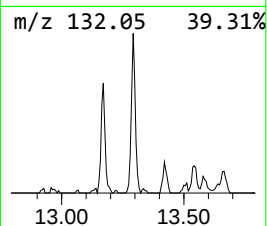
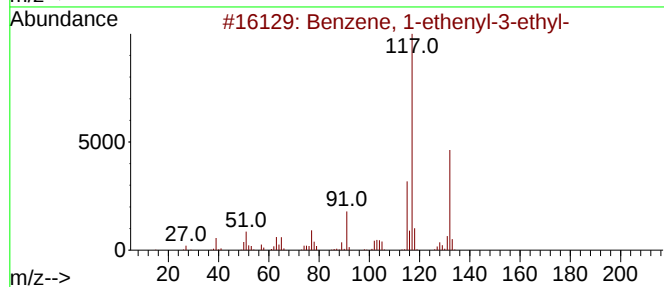
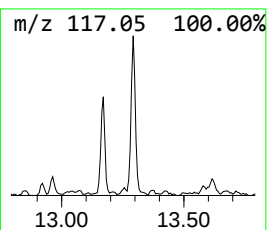
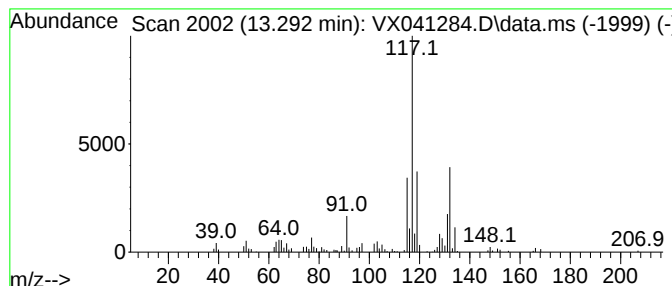
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.14 ug/l	68174	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	74
4			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	72
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	72



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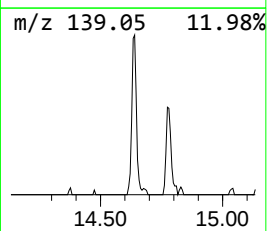
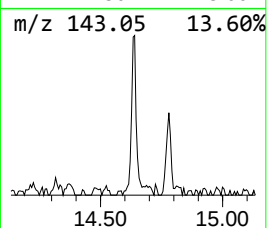
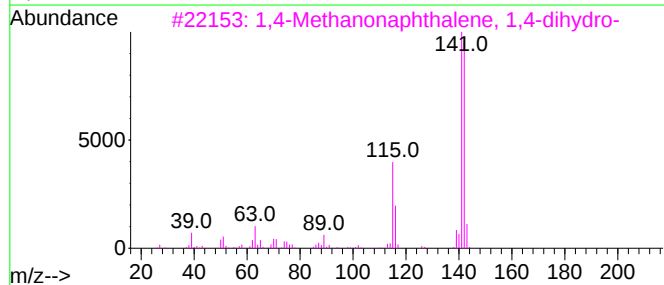
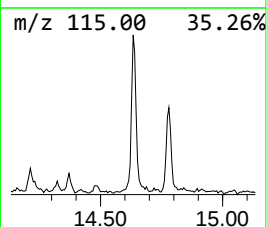
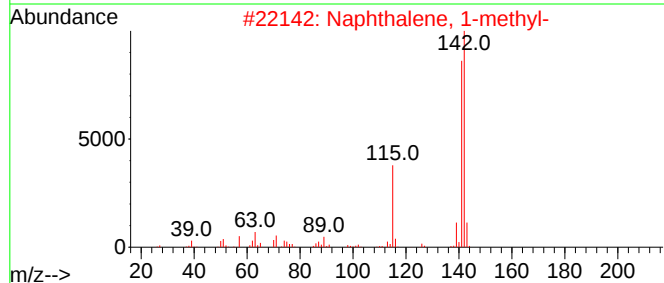
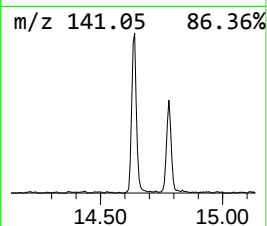
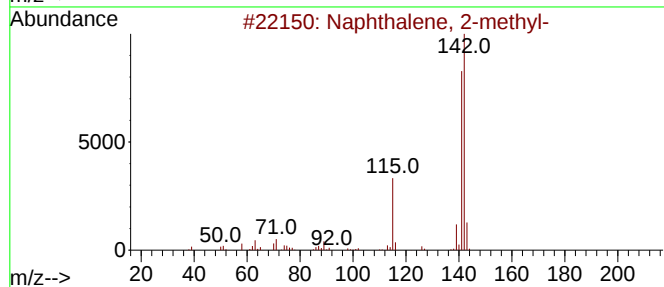
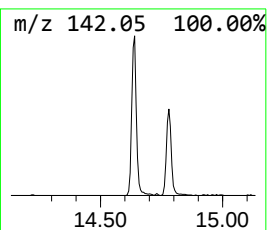
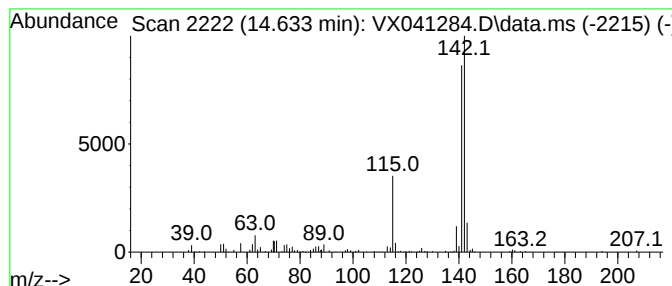
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	7.79 ug/l	86470	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	5.818	26.4	ug/l	271093	1	5.550	513046	50.0
Heptane	6.604	27.3	ug/l	245045	2	6.763	448562	50.0
Benzene, 1,2,3,...	12.963	5.7	ug/l	62972	4	12.024	555013	50.0
Benzene, 1-ethe...	13.292	6.1	ug/l	68174	4	12.024	555013	50.0
Naphthalene, 2-...	14.634	7.8	ug/l	86470	4	12.024	555013	50.0