

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
 Data File : VX001976.D
 Acq On : 25 May 2018 14:50
 Operator : JC/MD
 Sample : J3125-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 72-12013

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	94	rBV	2514588	2969737	100.00%	12.845%
2	2.623	329	334	340	rVB	26797	47734	1.61%	0.206%
3	5.513	793	808	821	rBV	264639	762444	25.67%	3.298%
4	5.672	823	834	848	rVB	306697	858497	28.91%	3.713%
5	6.074	887	900	911	rBV	296292	771662	25.98%	3.338%
6	6.866	1020	1030	1043	rBV	462858	1094935	36.87%	4.736%
7	8.720	1327	1334	1349	rBV	1367474	2136266	71.93%	9.240%
8	10.116	1557	1563	1573	rBV	941803	1299378	43.75%	5.620%
9	10.360	1596	1603	1610	rBV	19546	30785	1.04%	0.133%
10	10.701	1655	1659	1667	rVB	24586	33195	1.12%	0.144%
11	11.140	1726	1731	1745	rBV	1203459	1510238	50.85%	6.532%
12	11.439	1775	1780	1788	rBV	75436	139426	4.69%	0.603%
13	11.512	1788	1792	1801	rVB	66182	91609	3.08%	0.396%
14	11.670	1812	1818	1825	rBV	49928	69462	2.34%	0.300%
15	11.811	1836	1841	1848	rVB	259506	311805	10.50%	1.349%
16	12.030	1869	1877	1880	rBV	25123	32139	1.08%	0.139%
17	12.085	1880	1886	1892	rVV	1107145	1394104	46.94%	6.030%
18	12.146	1892	1896	1901	rVB	116920	140827	4.74%	0.609%
19	12.304	1918	1922	1924	rBV	79151	97758	3.29%	0.423%
20	12.329	1924	1926	1929	rVB	72061	71791	2.42%	0.311%
21	12.378	1929	1934	1942	rVB3	138512	205379	6.92%	0.888%
22	12.524	1954	1958	1964	rVB	40614	50448	1.70%	0.218%
23	12.591	1964	1969	1971	rBV	87284	112410	3.79%	0.486%
24	12.615	1971	1973	1977	rVB	84578	86319	2.91%	0.373%
25	12.670	1977	1982	1986	rBV	130650	161801	5.45%	0.700%
26	12.707	1986	1988	1992	rVB	32025	33019	1.11%	0.143%
27	12.762	1992	1997	2005	rBV3	103114	182149	6.13%	0.788%
28	12.908	2016	2021	2026	rVB2	54257	73475	2.47%	0.318%
29	12.981	2026	2033	2036	rBV	99404	130873	4.41%	0.566%
30	13.024	2036	2040	2046	rVB	160012	188883	6.36%	0.817%
31	13.085	2046	2050	2052	rBV	33308	47879	1.61%	0.207%
32	13.231	2070	2074	2078	rVV2	121373	156817	5.28%	0.678%
33	13.274	2078	2081	2084	rVB	27612	32011	1.08%	0.138%
34	13.317	2084	2088	2090	rBV2	42670	60812	2.05%	0.263%

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35	13.353	2090	2094	2099	rVB2	295717	389058	13.10%	1.683%
36	13.432	2104	2107	2111	rVB	27970	31920	1.07%	0.138%
37	13.487	2111	2116	2123	rVB	87079	123133	4.15%	0.533%
38	13.566	2124	2129	2132	rBV2	48938	66827	2.25%	0.289%
39	13.603	2132	2135	2138	rVV	94824	131552	4.43%	0.569%
40	13.646	2138	2142	2147	rVV4	108816	208613	7.02%	0.902%
41	13.707	2148	2152	2153	rVV	47999	72558	2.44%	0.314%
42	13.725	2153	2155	2161	rVB2	109030	150313	5.06%	0.650%
43	13.841	2167	2174	2182	rBV	205411	289875	9.76%	1.254%
44	13.920	2182	2187	2191	rVB2	43972	67189	2.26%	0.291%
45	13.987	2191	2198	2202	rBV2	92908	141550	4.77%	0.612%
46	14.036	2202	2206	2209	rVB	49360	57344	1.93%	0.248%
47	14.140	2218	2223	2227	rBV	127454	153337	5.16%	0.663%
48	14.280	2240	2246	2255	rBV3	151124	318857	10.74%	1.379%
49	14.383	2259	2263	2268	rVV	72281	98491	3.32%	0.426%
50	14.438	2268	2272	2276	rVB	130303	159699	5.38%	0.691%
51	14.481	2276	2279	2284	rVB3	24670	31120	1.05%	0.135%
52	14.548	2284	2290	2294	rBV2	90759	135138	4.55%	0.585%
53	14.700	2302	2315	2319	rBV	874841	1156743	38.95%	5.003%
54	14.737	2319	2321	2325	rVB	54289	60505	2.04%	0.262%
55	14.792	2325	2330	2333	rBV	37186	49988	1.68%	0.216%
56	14.847	2334	2339	2343	rBV	528084	690834	23.26%	2.988%
57	14.969	2355	2359	2365	rBV3	15225	31828	1.07%	0.138%
58	15.255	2401	2406	2414	rBV2	68788	146222	4.92%	0.632%
59	15.328	2414	2418	2425	rVB3	22905	41121	1.38%	0.178%
60	15.450	2433	2438	2441	rBV	157806	225053	7.58%	0.973%
61	15.487	2441	2444	2448	rVB	58081	78872	2.66%	0.341%
62	15.554	2448	2455	2461	rBV	347555	576698	19.42%	2.494%
63	15.694	2472	2478	2482	rBV	462425	725137	24.42%	3.136%
64	15.731	2482	2484	2492	rVB	260040	353597	11.91%	1.529%
65	15.926	2505	2516	2533	rVB	114266	317184	10.68%	1.372%
66	16.078	2536	2541	2553	rVB	74507	132666	4.47%	0.574%
67	16.176	2553	2557	2565	rBV	27222	49701	1.67%	0.215%
68	16.292	2566	2576	2582	rVB3	22455	59261	2.00%	0.256%
69	16.432	2590	2599	2610	rBV3	57674	180978	6.09%	0.783%
70	16.572	2618	2622	2628	rVB	17826	31850	1.07%	0.138%
71	16.663	2628	2637	2638	rBV5	22758	49651	1.67%	0.215%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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72	16.700	2639	2643	2648	rVB	45896	76941	2.59%	0.333%
73	16.761	2648	2653	2657	rBV	39768	71983	2.42%	0.311%

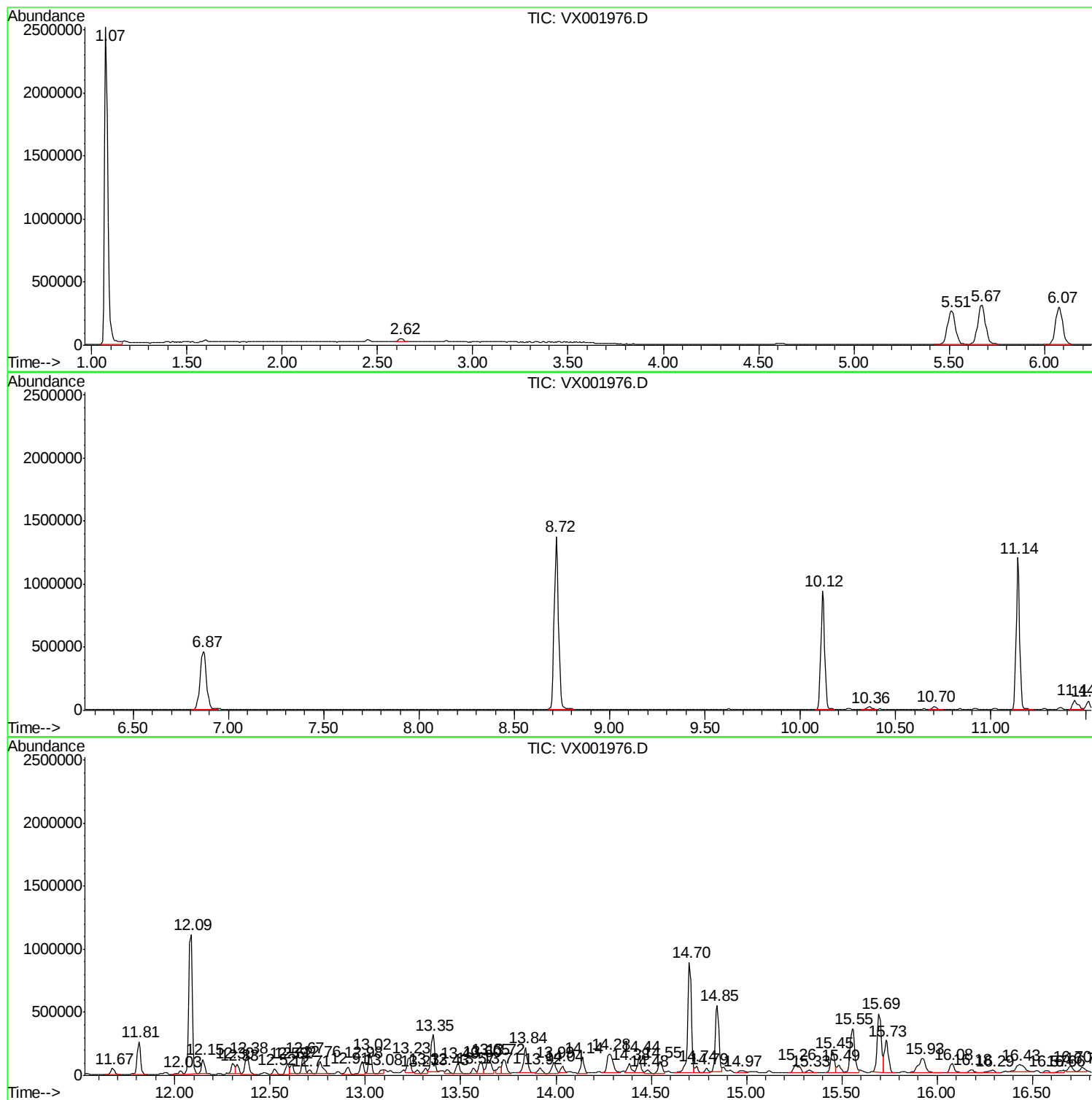
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Instrument :
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ClientSampleId :
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
72-12013

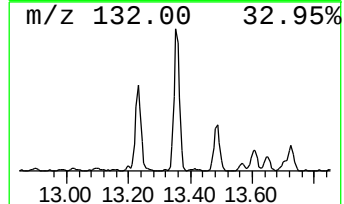
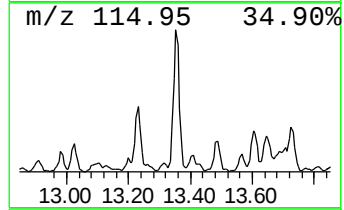
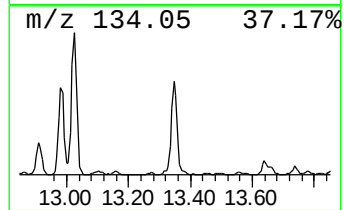
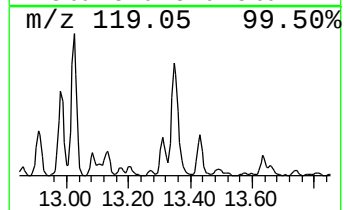
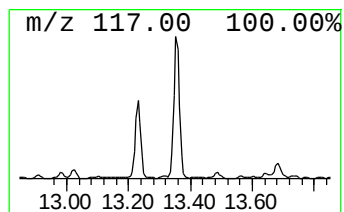
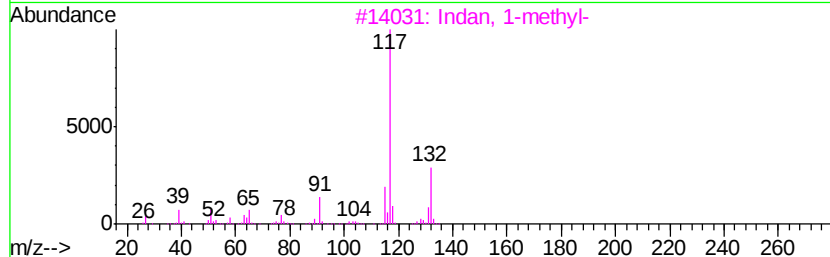
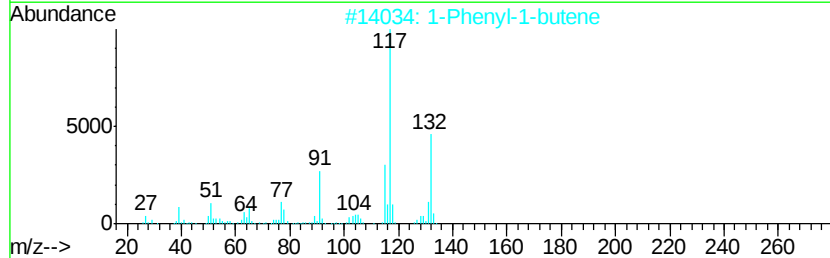
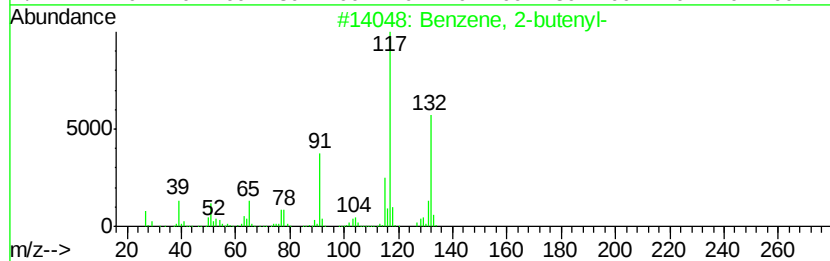
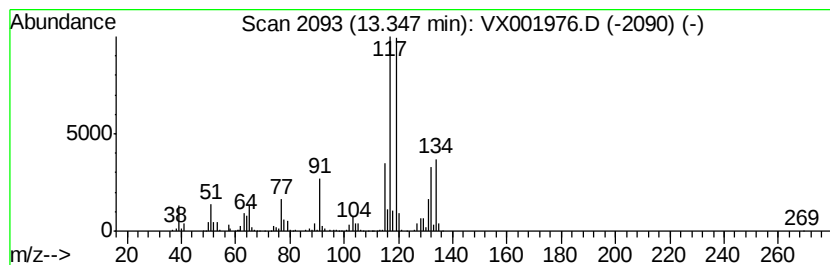
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 2-butenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	13.95 ug/l	389058	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3		Indan, 1-methyl-	132	C10H12	000767-58-8	70
4		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70



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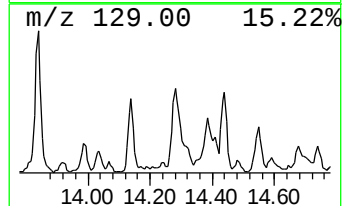
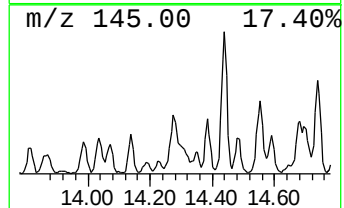
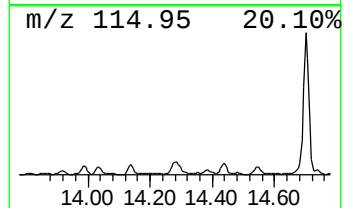
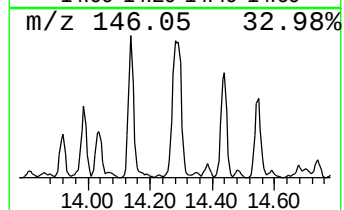
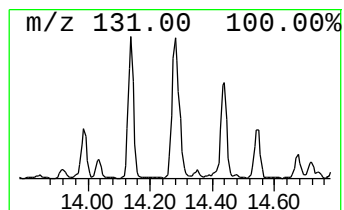
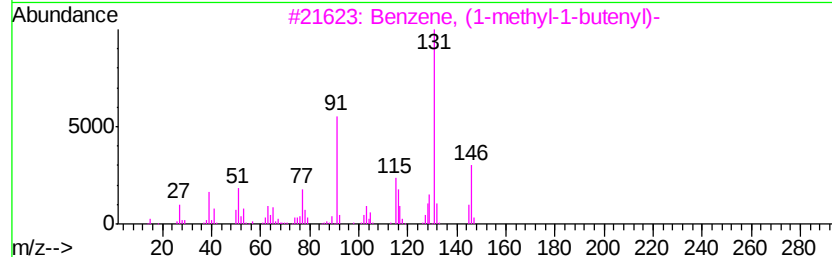
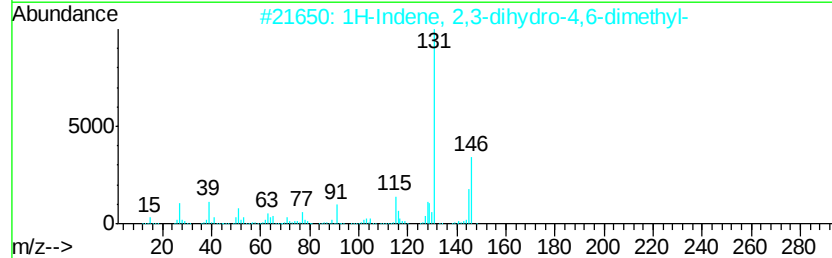
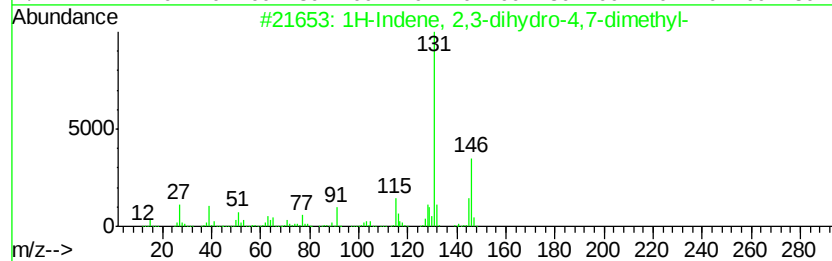
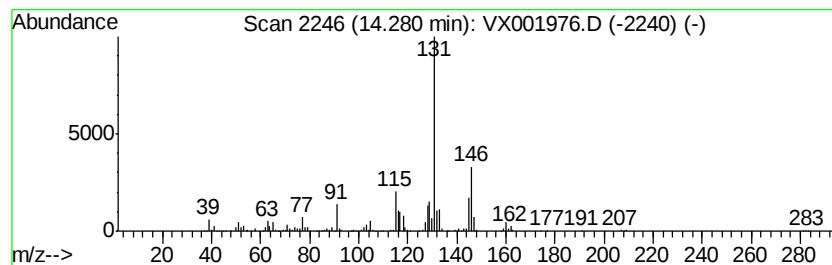
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	11.44 ug/l	318857	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	94
2		1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	93
3		Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	93
4		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	93
5		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	90



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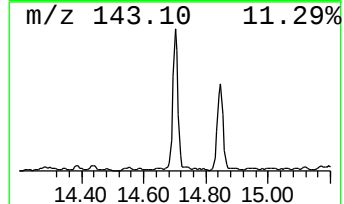
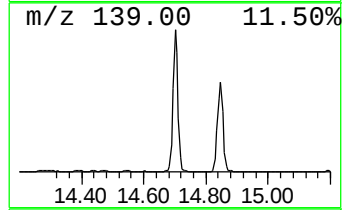
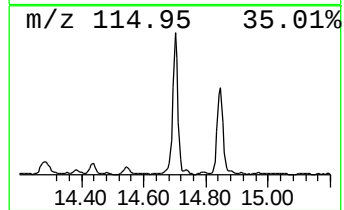
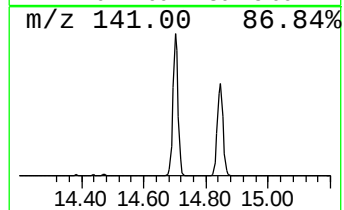
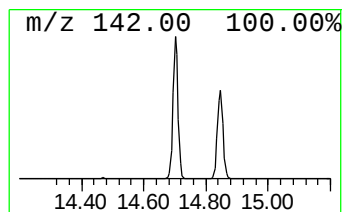
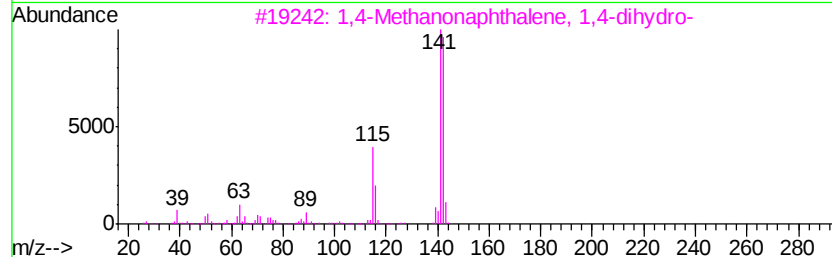
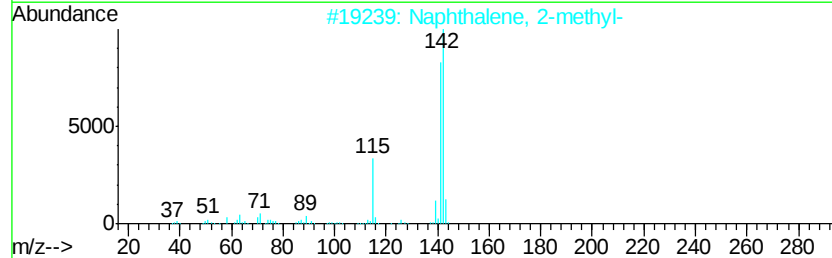
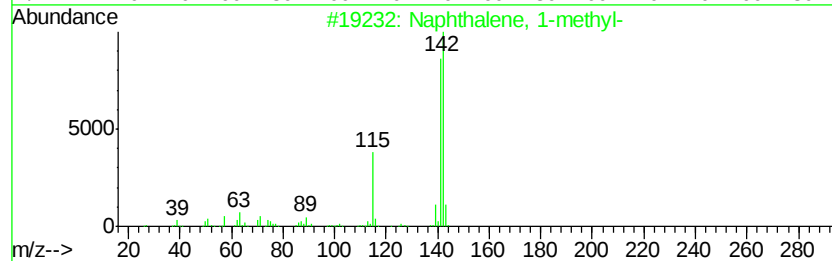
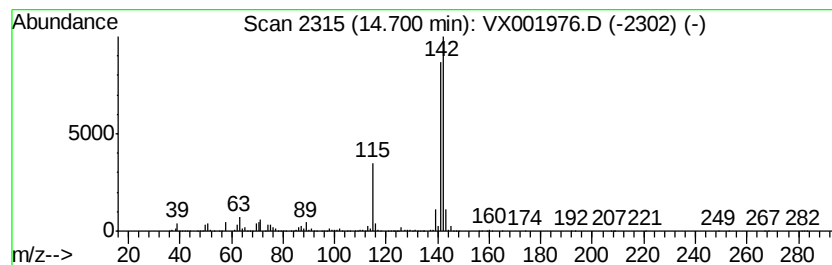
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	41.49 ug/l	1156740	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



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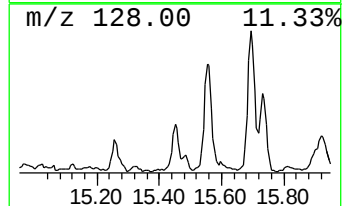
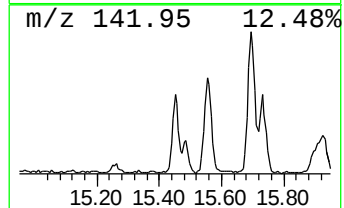
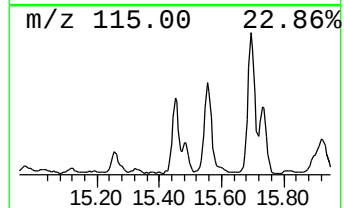
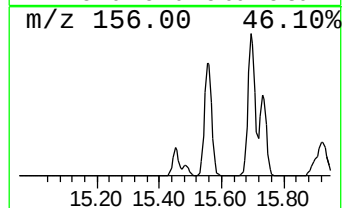
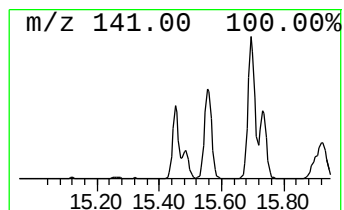
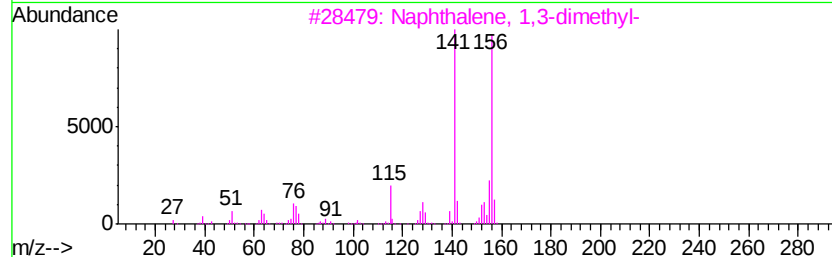
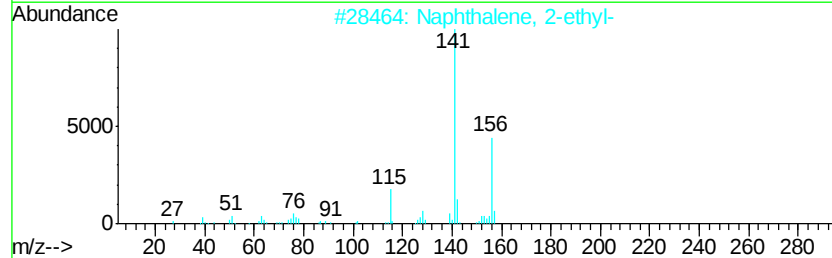
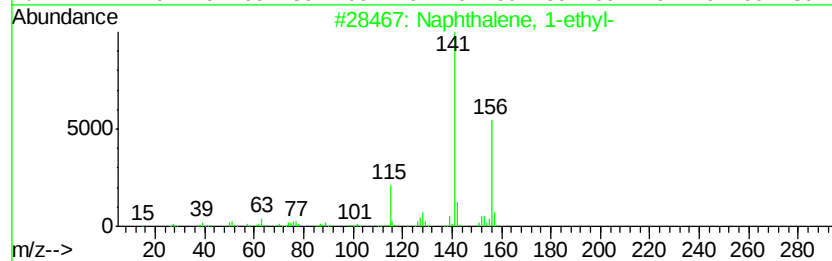
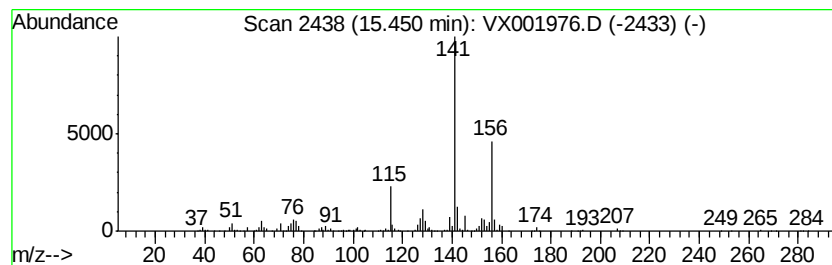
Instrument :
MSVOA_X
ClientSampleId :
72-12013

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	8.07 ug/l	225053	1,4-Dichlorobenzene-d4	12.09
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1-ethyl-	156 C12H12	001127-76-0 97
2		Naphthalene, 2-ethyl-	156 C12H12	000939-27-5 95
3		Naphthalene, 1,3-dimethyl-	156 C12H12	000575-41-7 93
4		2-Thiophenecarboxylic acid, 5-et...	156 C7H8O2S	023229-72-3 64
5		Butethal	212 C10H16N2O3	000077-28-1 59



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001976.D
Acq On : 25 May 2018 14:50
Operator : JC/MD
Sample : J3125-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-12013

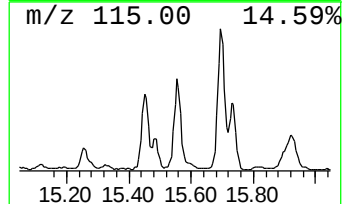
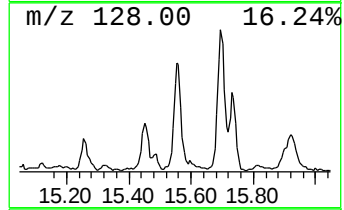
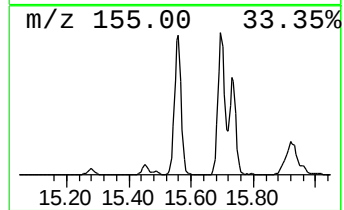
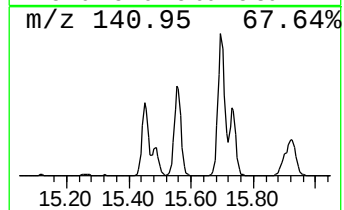
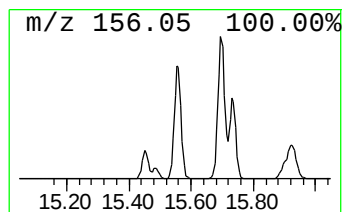
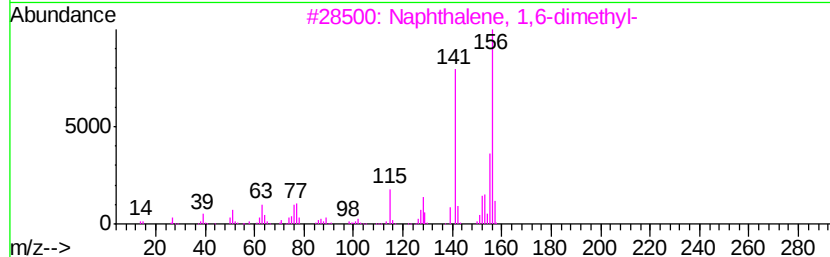
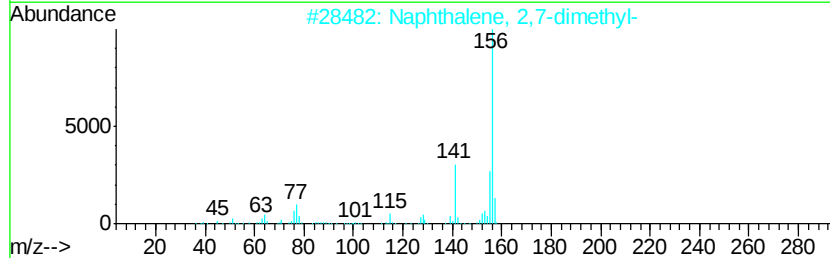
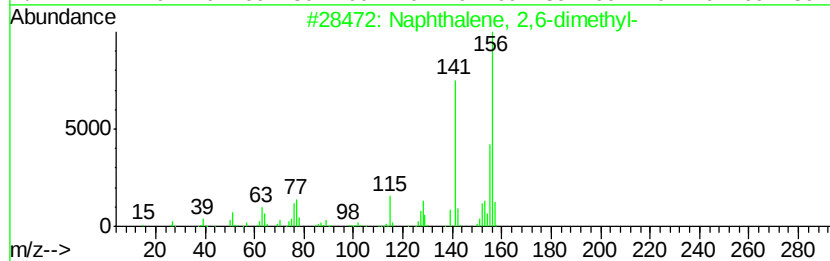
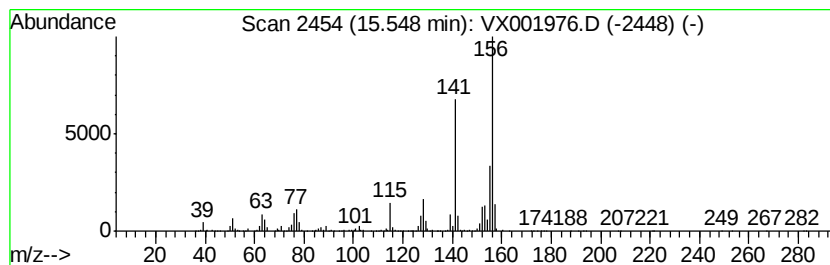
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.55	20.68 ug/l	576698	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3		Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
5		Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001976.D
Acq On : 25 May 2018 14:50
Operator : JC/MD
Sample : J3125-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-12013

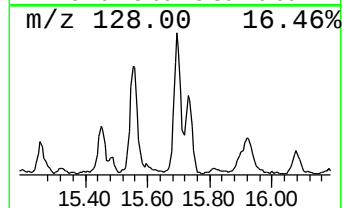
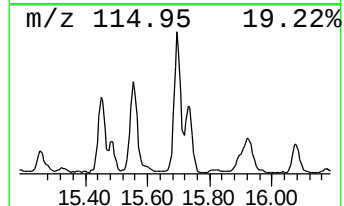
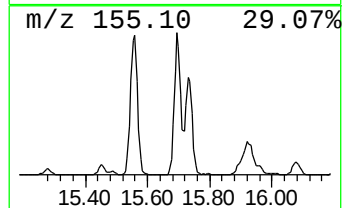
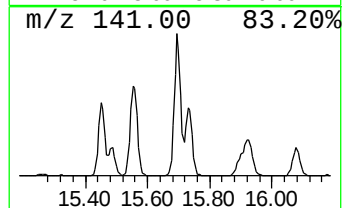
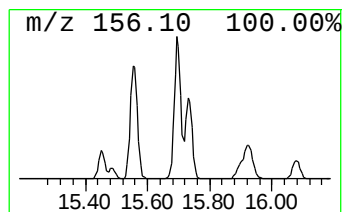
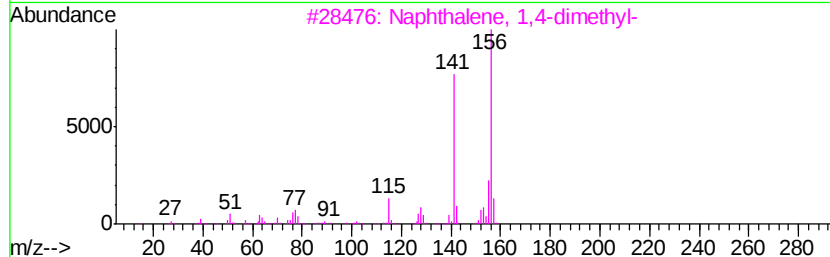
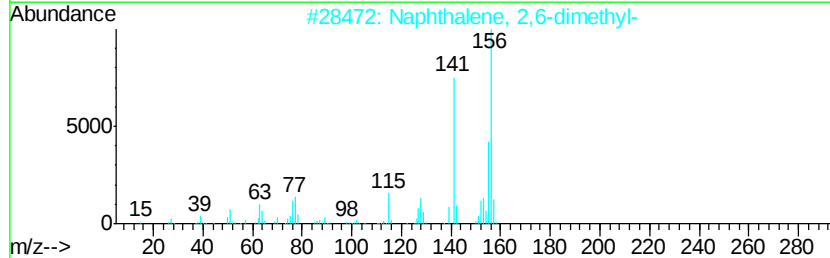
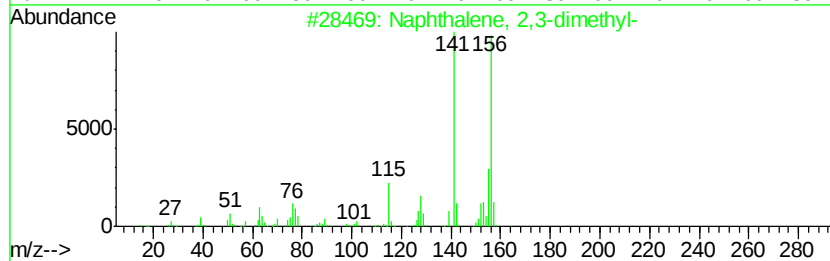
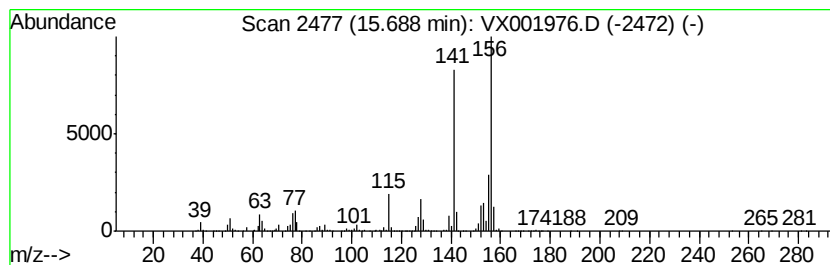
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	26.01 ug/l	725137	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2		Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3		Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4		Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5		Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001976.D
Acq On : 25 May 2018 14:50
Operator : JC/MD
Sample : J3125-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-12013

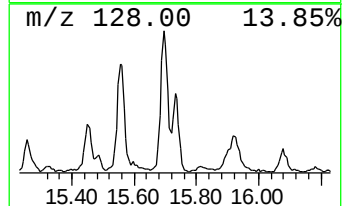
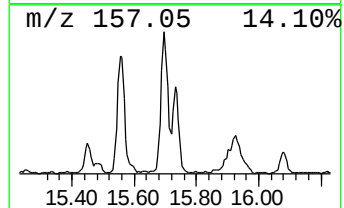
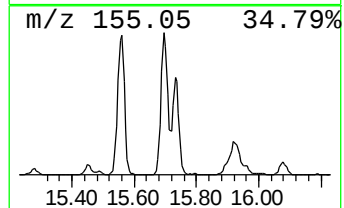
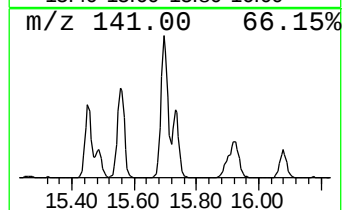
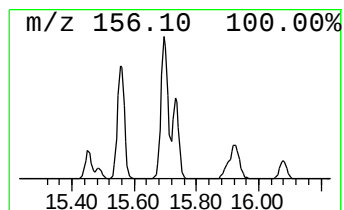
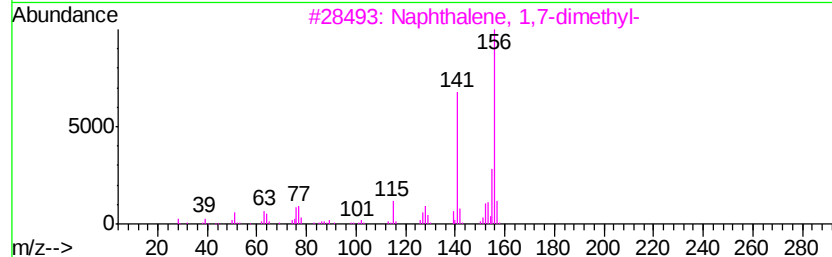
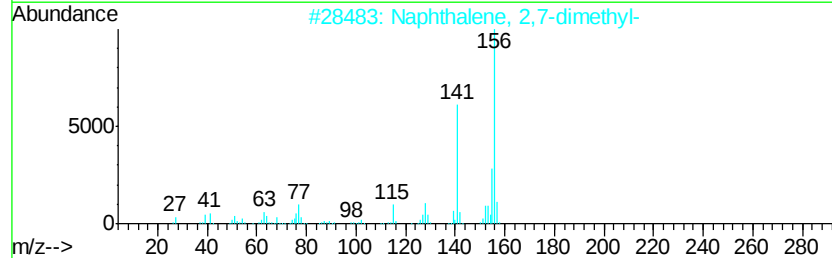
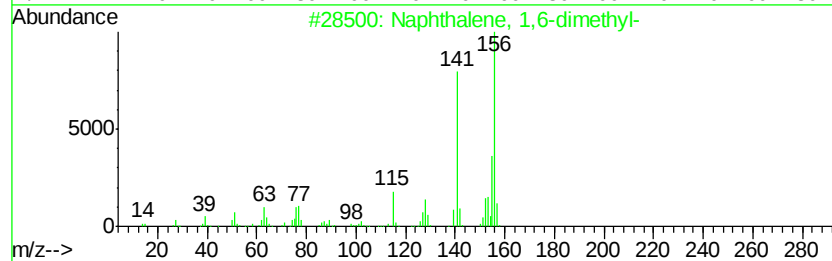
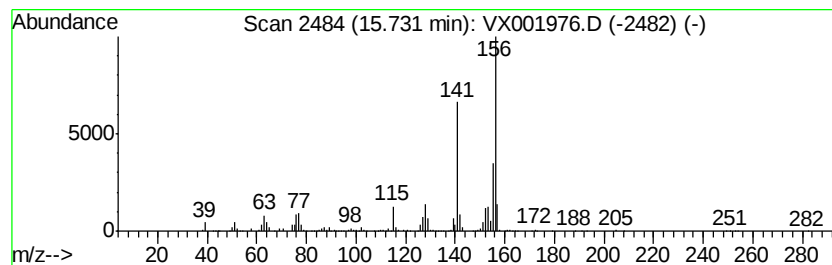
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	12.68 ug/l	353597	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3		Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4		Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5		Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001976.D
Acq On : 25 May 2018 14:50
Operator : JC/MD
Sample : J3125-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
72-12013

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 2-butenyl-	13.35	13.9	ug/l	389058	4	12.09	1394100	50.0
1H-Indene, 2,3-di...	14.28	11.4	ug/l	318857	4	12.09	1394100	50.0
Naphthalene, 1-me...	14.70	41.5	ug/l	1156740	4	12.09	1394100	50.0
Naphthalene, 1-et...	15.45	8.1	ug/l	225053	4	12.09	1394100	50.0
Naphthalene, 2,6-...	15.55	20.7	ug/l	576698	4	12.09	1394100	50.0
Naphthalene, 2,3-...	15.69	26.0	ug/l	725137	4	12.09	1394100	50.0
Naphthalene, 1,6-...	15.73	12.7	ug/l	353597	4	12.09	1394100	50.0