

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
 Data File : VX022251.D
 Acq On : 28 May 2021 14:09
 Operator : JC/MD
 Sample : M2520-02 10X
 Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WC-02-2021-05-24

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\82X051921W.M
 Title : SW846 8260

Signal : TIC: VX022251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	694	706	720	rBV2	50362	145151	1.26%	0.349%
2	5.556	723	733	747	rVB2	79070	221367	1.92%	0.532%
3	5.958	790	799	814	rVB	64387	165742	1.44%	0.398%
4	6.763	921	931	945	rBV	141990	343364	2.98%	0.825%
5	8.653	1233	1241	1249	rBV	306244	482562	4.19%	1.159%
6	10.055	1465	1471	1478	rBV	304286	408150	3.54%	0.980%
7	10.195	1488	1494	1505	rBV	548110	706875	6.14%	1.698%
8	10.963	1614	1620	1628	rBV	103639	134092	1.16%	0.322%
9	11.085	1634	1640	1651	rVB	240414	308490	2.68%	0.741%
10	11.616	1722	1727	1734	rBV	159272	198899	1.73%	0.478%
11	11.756	1741	1750	1755	rBV	513355	662277	5.75%	1.590%
12	12.024	1789	1794	1800	rVB2	330838	443880	3.86%	1.066%
13	12.091	1800	1805	1810	rBV	217424	265442	2.31%	0.637%
14	12.244	1825	1830	1838	rBV	2396784	3050434	26.49%	7.325%
15	12.317	1838	1842	1848	rBV	119432	161925	1.41%	0.389%
16	12.414	1854	1858	1864	rBV	86972	115387	1.00%	0.277%
17	12.616	1886	1891	1895	rBV	273702	330432	2.87%	0.794%
18	12.701	1901	1905	1911	rBV	137064	213031	1.85%	0.512%
19	12.969	1945	1949	1954	rBV	142982	187861	1.63%	0.451%
20	13.170	1978	1982	1987	rVB	360936	421272	3.66%	1.012%
21	13.292	1998	2002	2007	rBV2	221702	291972	2.54%	0.701%
22	13.347	2007	2011	2017	rVV	515015	608777	5.29%	1.462%
23	13.426	2019	2024	2029	rVB	864980	1099782	9.55%	2.641%
24	13.548	2040	2044	2048	rBV	109031	136801	1.19%	0.329%
25	13.786	2074	2083	2089	rBV	8419632	11514323	100.00%	27.651%
26	13.871	2090	2097	2102	rVV	300912	424277	3.68%	1.019%
27	13.926	2102	2106	2111	rVB2	92874	125759	1.09%	0.302%
28	14.103	2132	2135	2137	rVV	134079	155776	1.35%	0.374%
29	14.134	2137	2140	2146	rVV2	75078	139878	1.21%	0.336%
30	14.225	2150	2155	2158	rBV	186954	267325	2.32%	0.642%
31	14.323	2164	2171	2177	rBV	177530	297175	2.58%	0.714%
32	14.524	2200	2204	2211	rVB2	82823	122984	1.07%	0.295%
33	14.603	2212	2217	2219	rVV	125176	168845	1.47%	0.405%
34	14.640	2219	2223	2233	rVB2	578365	828170	7.19%	1.989%
35	14.786	2241	2247	2257	rBV	4236477	5414162	47.02%	13.002%
36	15.213	2309	2317	2321	rBV	513330	701566	6.09%	1.685%

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	15.377	2332	2344	2347	rBV2	410718	716202	6.22%	1.720%
38	15.414	2347	2350	2354	rVB	189704	251709	2.19%	0.604%
39	15.481	2355	2361	2366	rBV	1120572	1753022	15.22%	4.210%
40	15.621	2372	2384	2387	rBV	1296005	2171293	18.86%	5.214%
41	15.658	2387	2390	2395	rVB	446033	623985	5.42%	1.498%
42	15.841	2410	2420	2432	rVB	404386	1118069	9.71%	2.685%
43	15.993	2438	2445	2455	rVB	272419	465872	4.05%	1.119%
44	16.091	2455	2461	2468	rBV	185208	301726	2.62%	0.725%
45	16.200	2469	2479	2485	rVB2	90497	173723	1.51%	0.417%
46	16.334	2492	2501	2510	rBV2	975935	2074399	18.02%	4.982%
47	16.566	2530	2539	2541	rBV3	85839	179654	1.56%	0.431%
48	16.603	2541	2545	2550	rVV	121449	237352	2.06%	0.570%
49	16.664	2550	2555	2569	rVB2	118453	310648	2.70%	0.746%

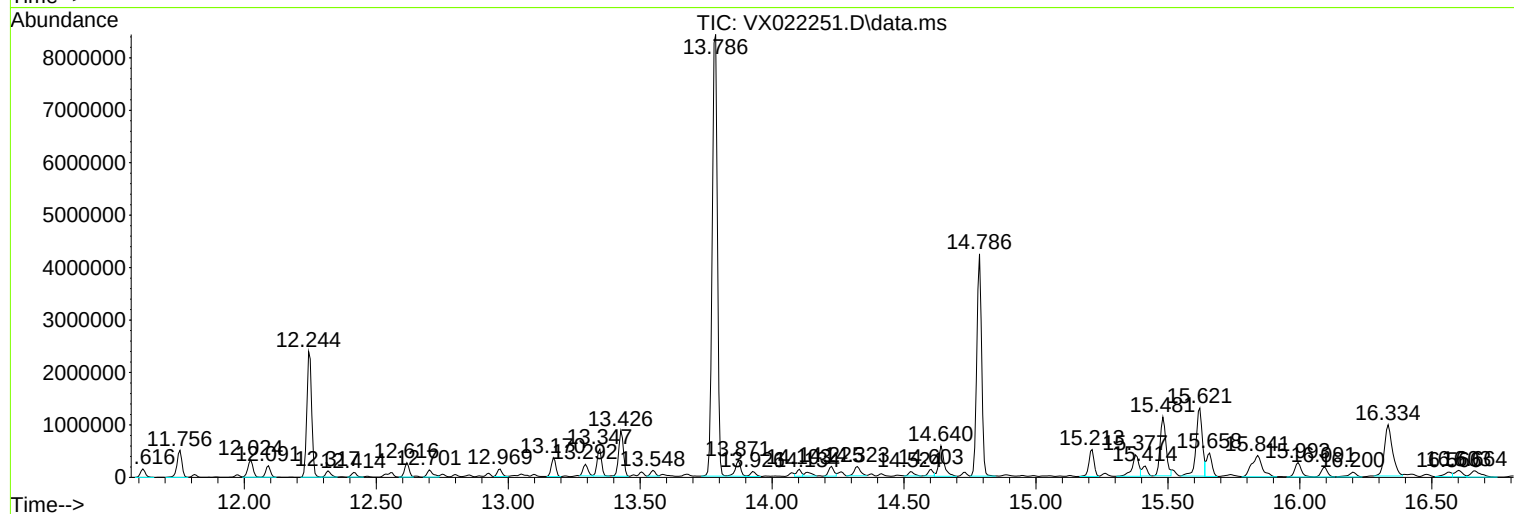
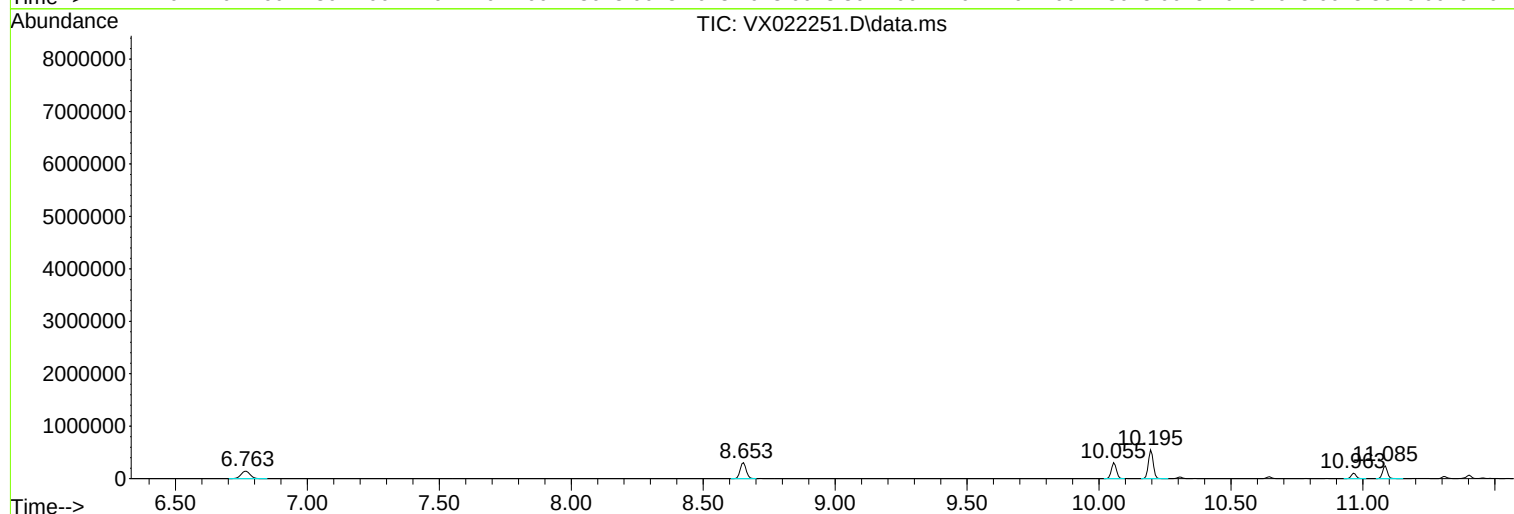
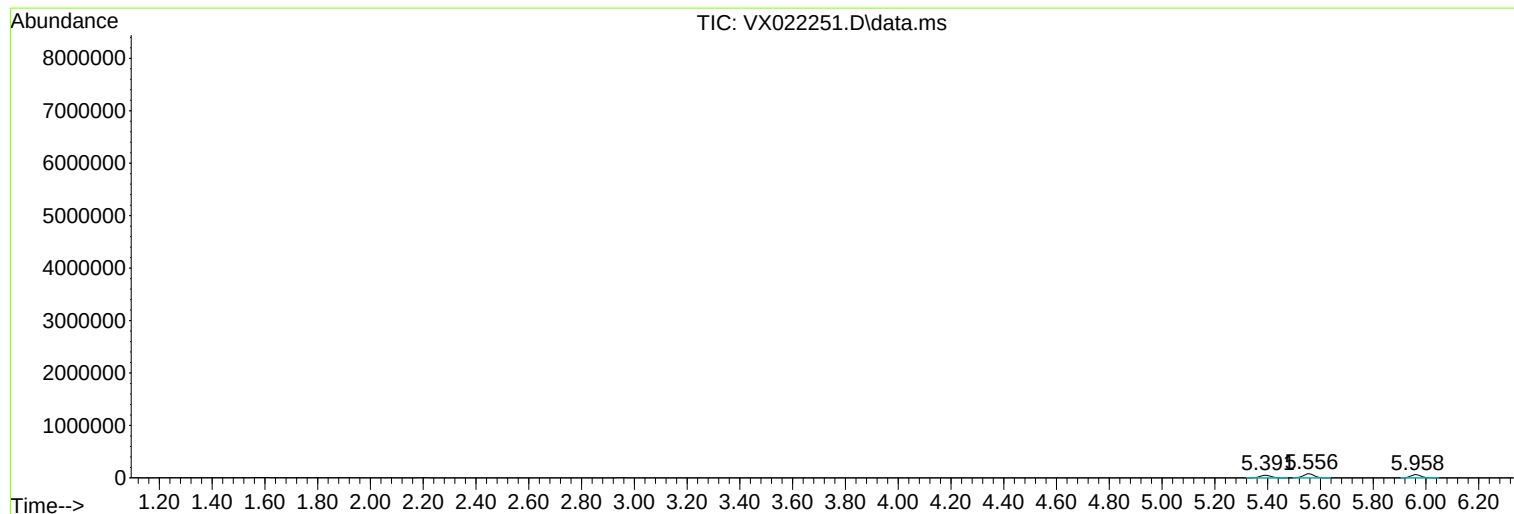
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Quant Title : SW846 8260

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



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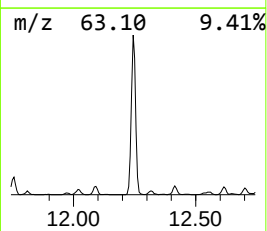
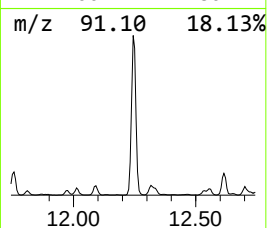
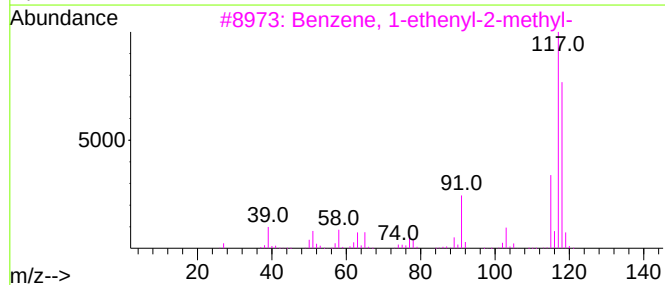
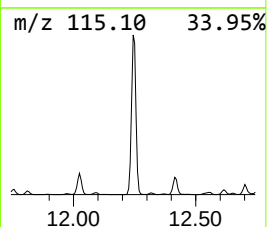
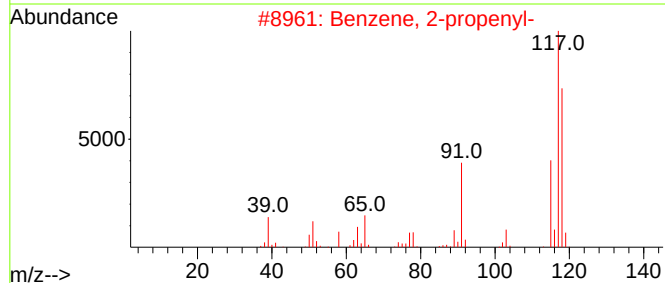
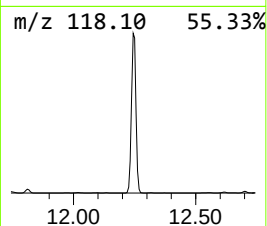
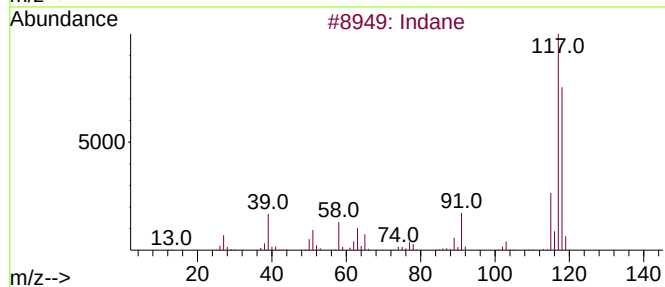
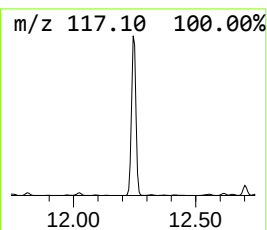
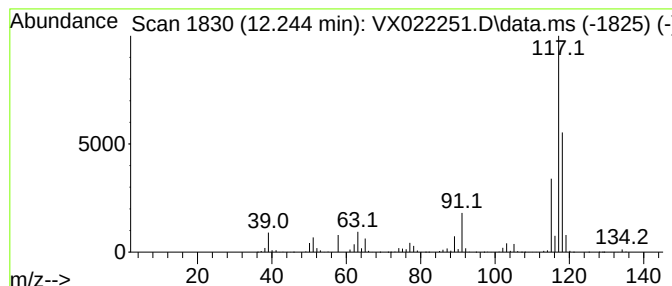
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 1 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	343.61 ug/l	3050430	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
5			Deltacyclene	118	C9H10	007785-10-6	64



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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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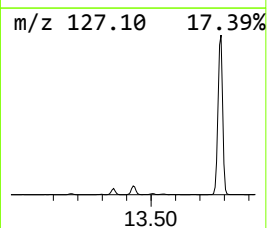
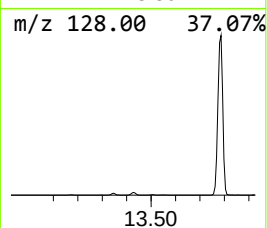
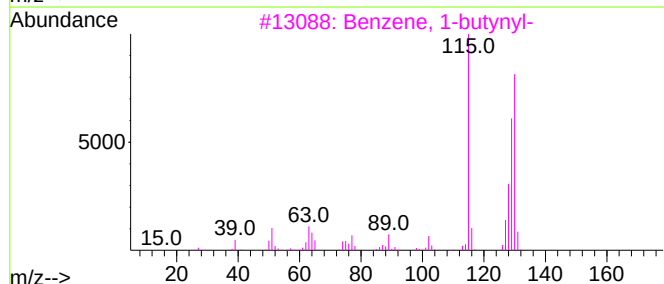
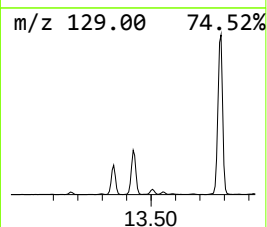
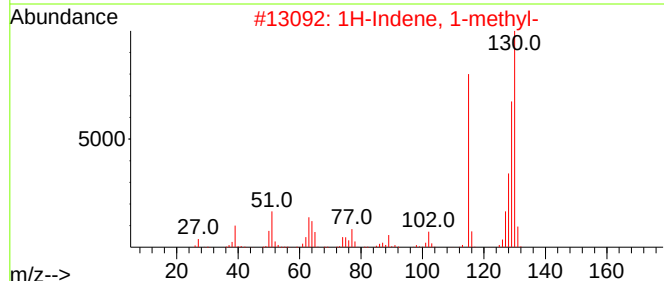
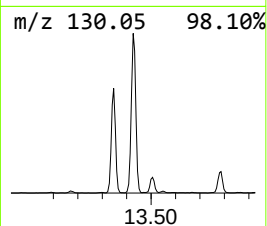
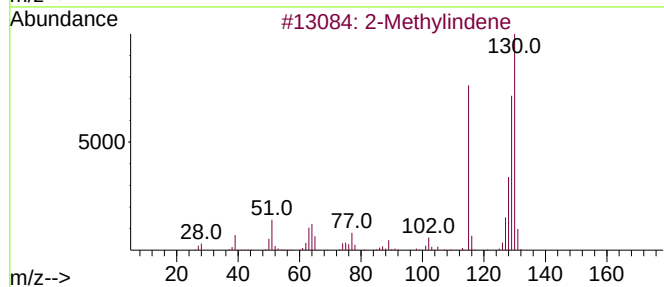
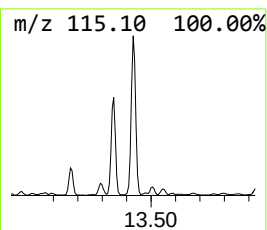
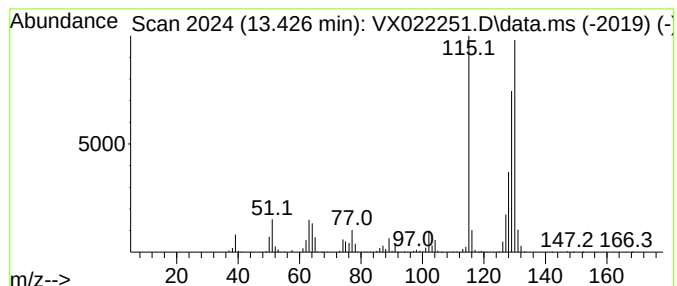
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Methylindene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	123.88 ug/l	1099780	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindene	130	C10H10	002177-47-1	97
2			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
3			Benzene, 1-butynyl-	130	C10H10	000622-76-4	96
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	96
5			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
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Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

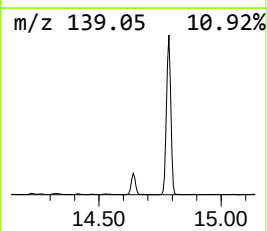
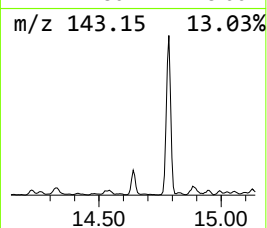
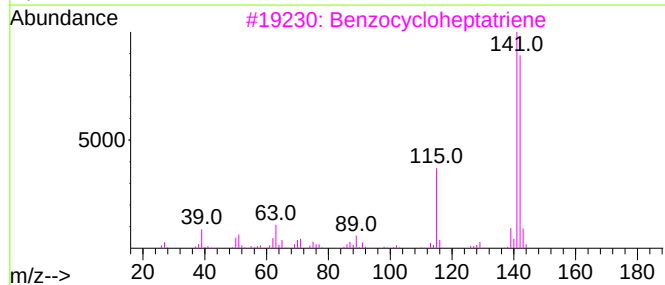
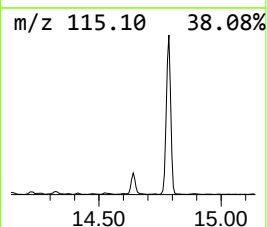
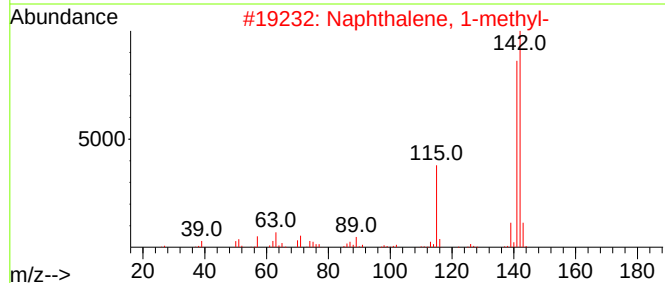
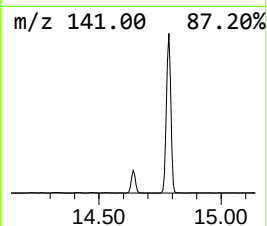
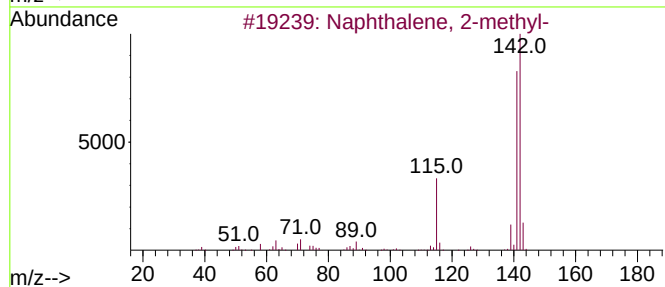
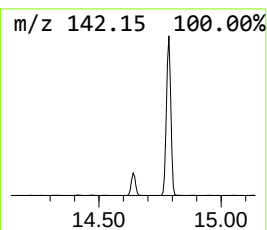
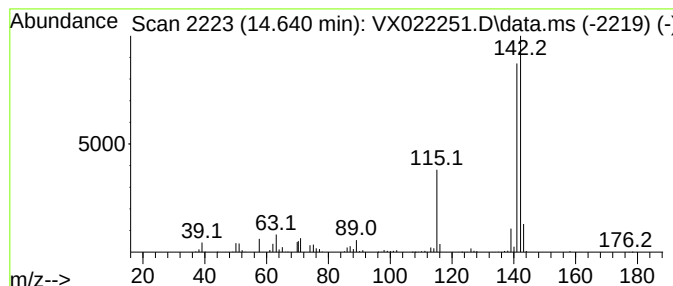
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Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	93.29 ug/l	828170	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	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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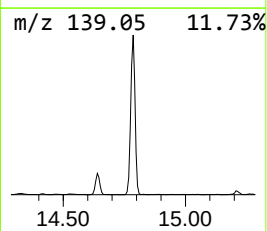
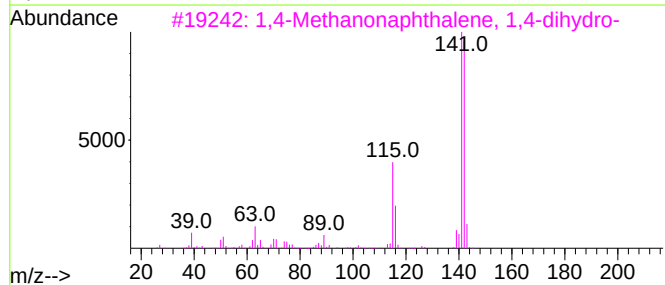
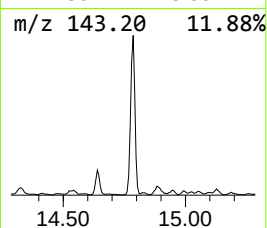
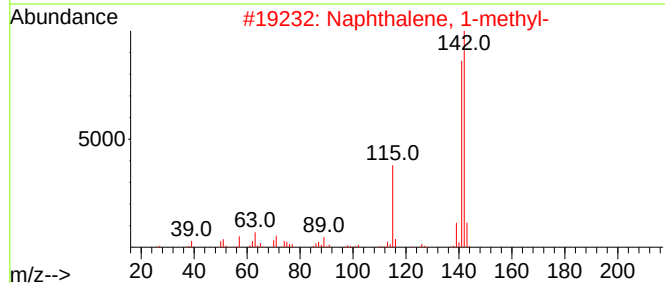
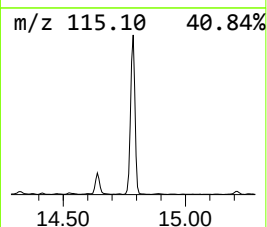
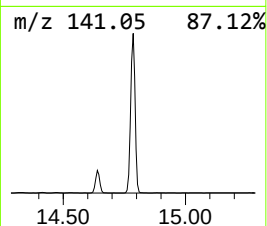
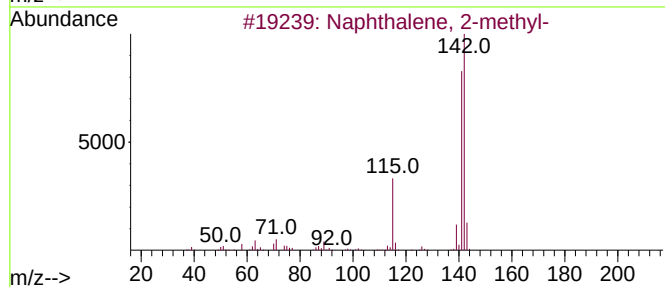
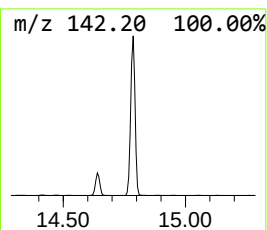
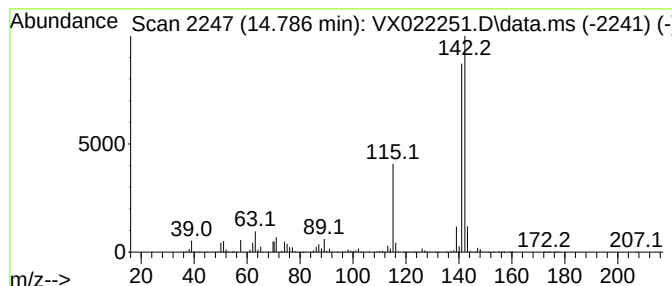
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.786	609.87 ug/l	5414160	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	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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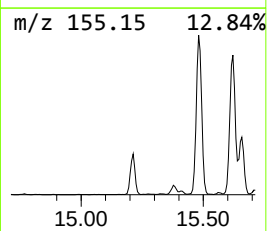
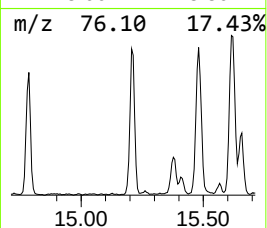
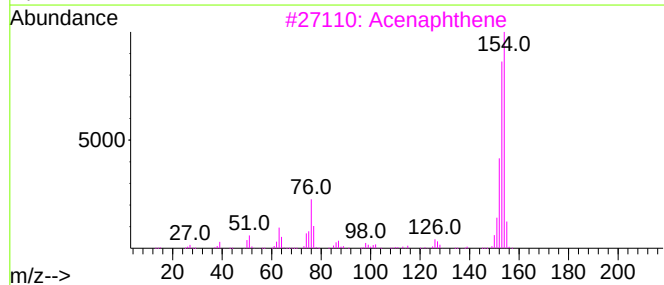
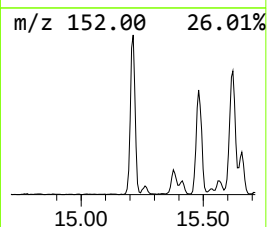
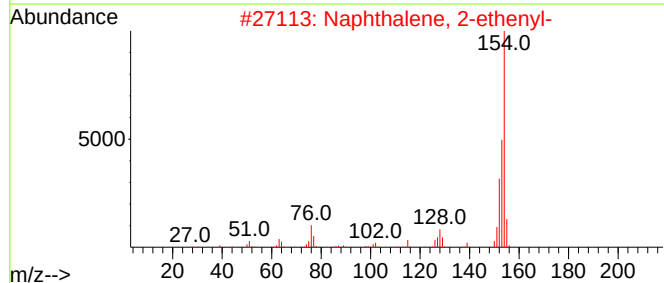
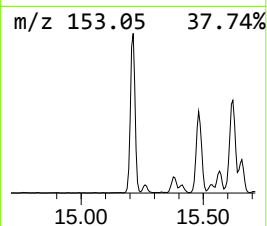
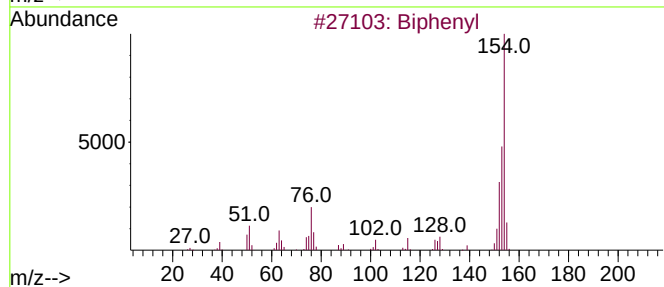
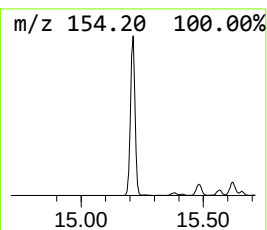
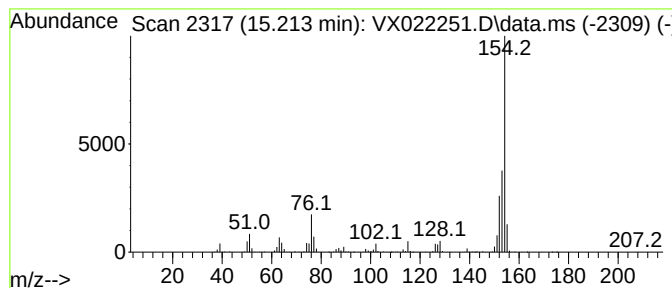
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Quant Title : SW846 8260

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

Peak Number 5 Biphenyl Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.213	79.03 ug/l	701566	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	96
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3			Acenaphthene	154	C12H10	000083-32-9	53
4			6-Cyanoquinoline	154	C10H6N2	023395-72-4	50
5			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022251.D
Acq On : 28 May 2021 14:09
Operator : JC/MD
Sample : M2520-02 10X
Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

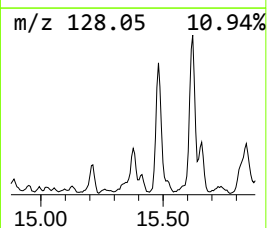
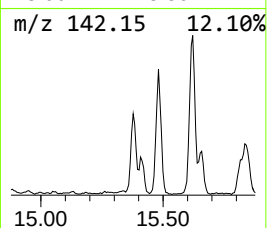
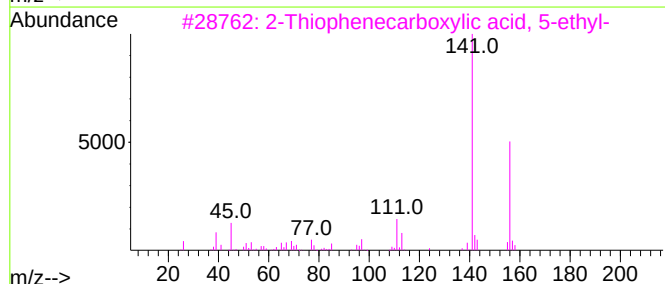
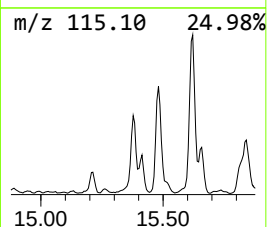
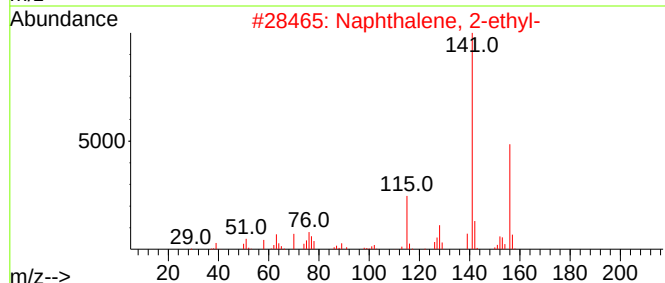
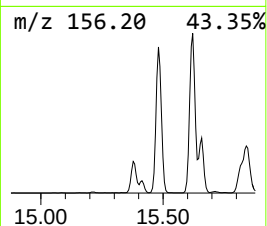
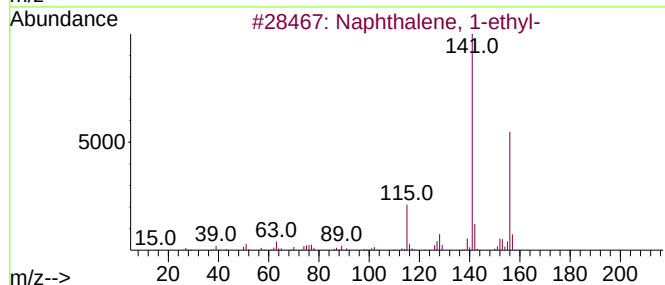
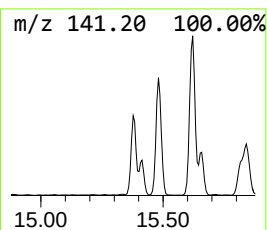
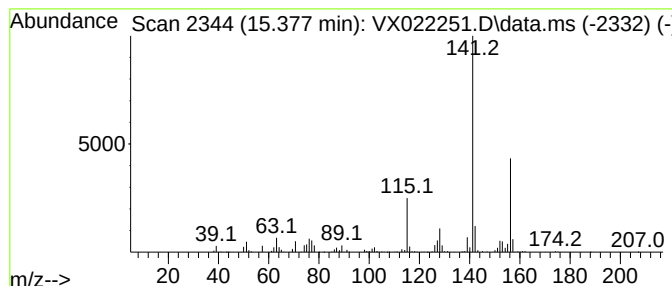
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.377	80.68 ug/l	716202	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-ethyl-	156	C12H12	001127-76-0	96
2			Naphthalene, 2-ethyl-	156	C12H12	000939-27-5	96
3			2-Thiophenecarboxylic acid, 5-et...	156	C7H8O2S	023229-72-3	64
4			Naphthalene, 1-propyl-	170	C13H14	002765-18-6	59
5			Benzaldehyde, 3-methoxy-4-(1-nap...	292	C19H16O3	1000338-37-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022251.D
Acq On : 28 May 2021 14:09
Operator : JC/MD
Sample : M2520-02 10X
Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

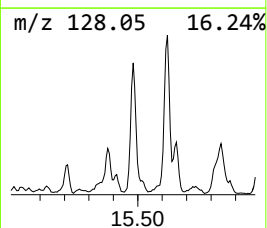
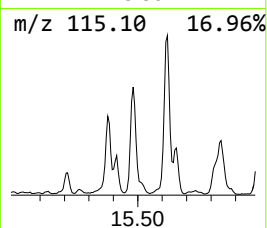
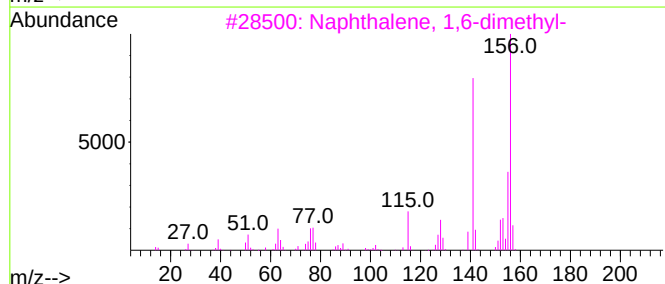
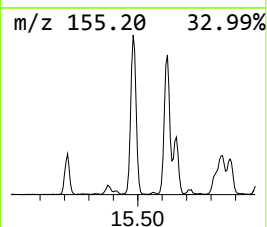
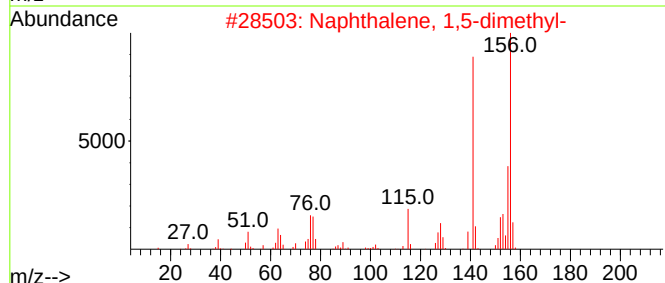
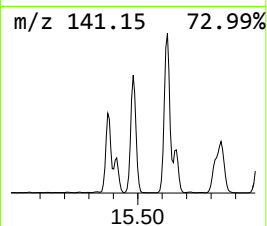
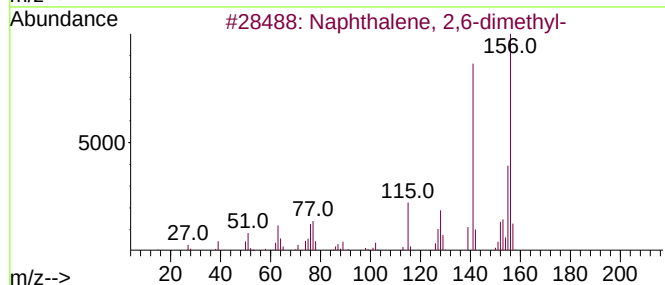
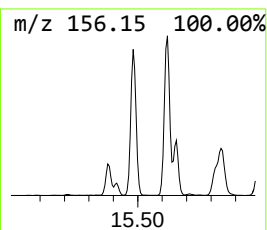
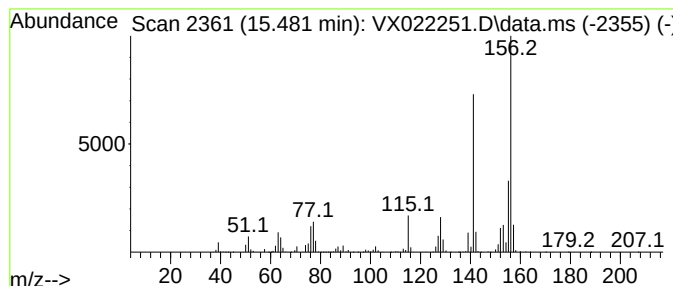
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Quant Title : SW846 8260

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.
15.481	197.47 ug/l	1753020	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	98
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022251.D
Acq On : 28 May 2021 14:09
Operator : JC/MD
Sample : M2520-02 10X
Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

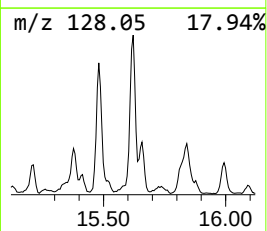
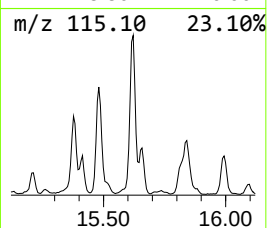
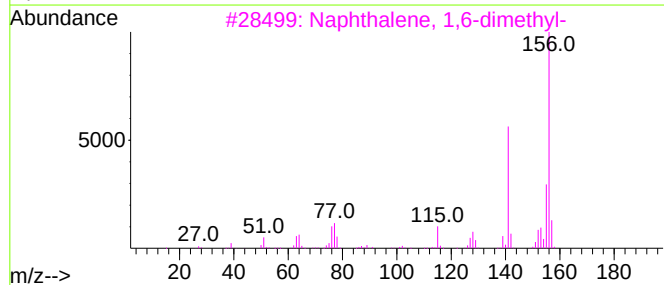
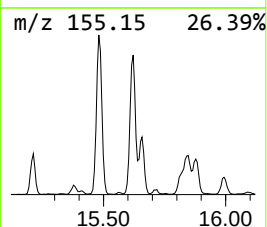
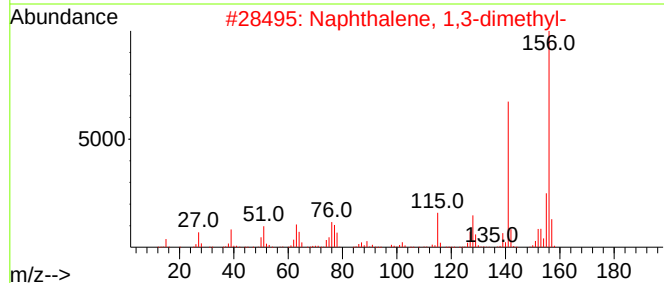
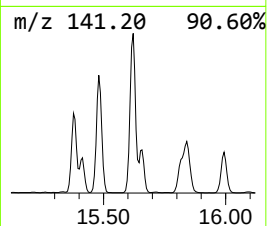
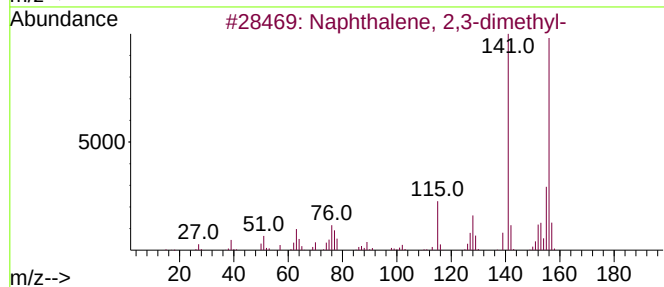
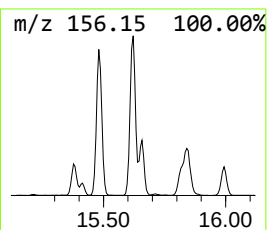
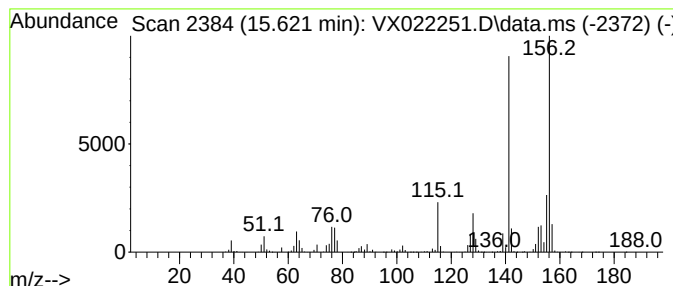
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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.
15.621	244.58 ug/l	2171290	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022251.D
Acq On : 28 May 2021 14:09
Operator : JC/MD
Sample : M2520-02 10X
Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

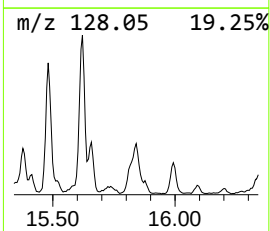
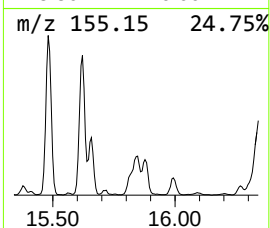
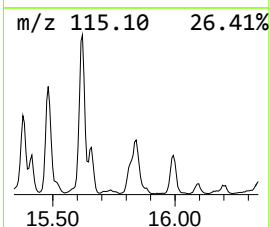
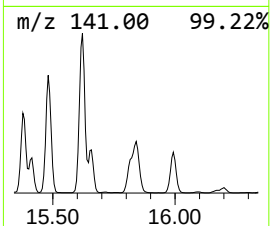
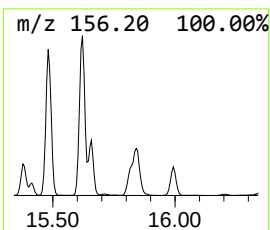
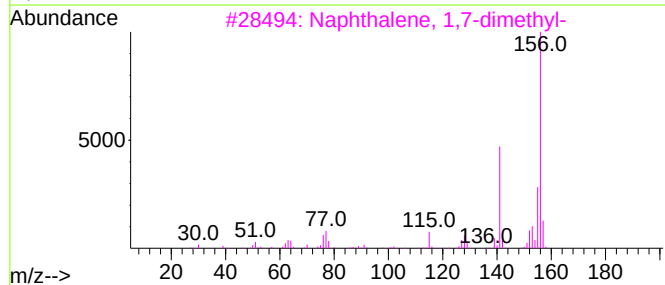
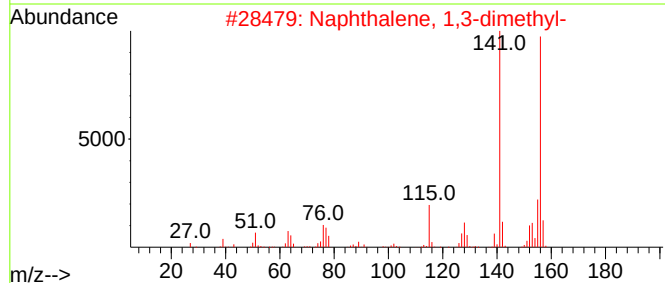
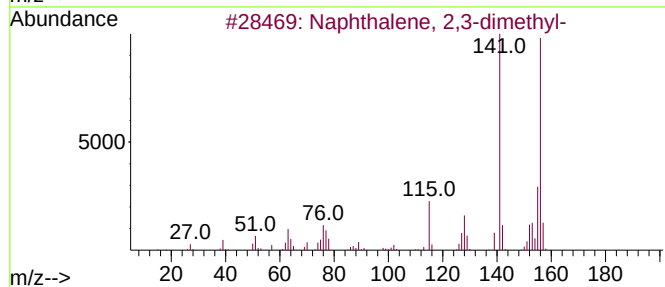
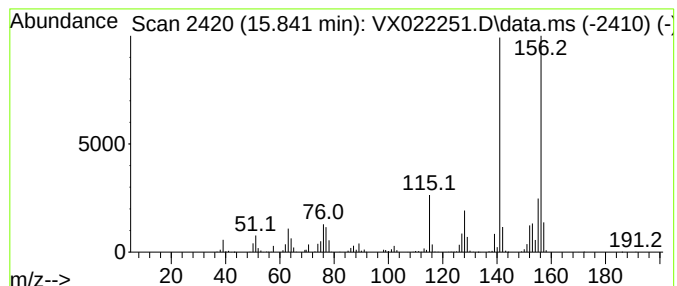
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	125.94 ug/l	1118070	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022251.D
Acq On : 28 May 2021 14:09
Operator : JC/MD
Sample : M2520-02 10X
Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-02-2021-05-24

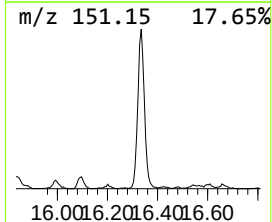
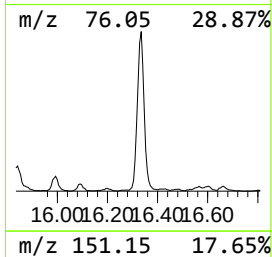
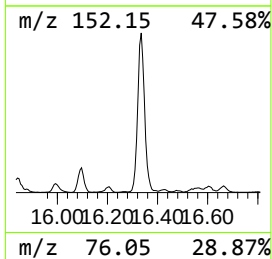
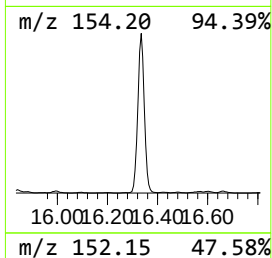
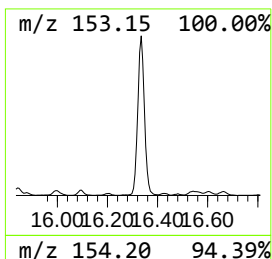
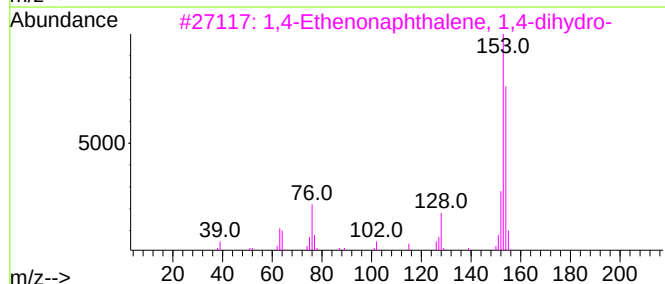
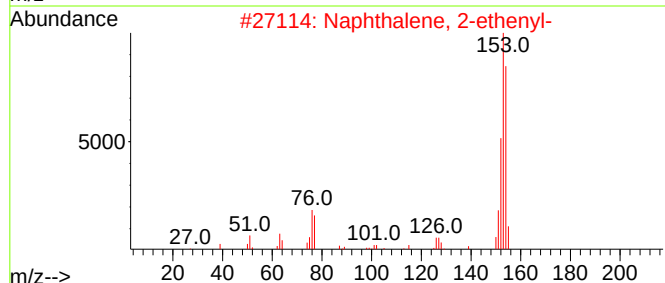
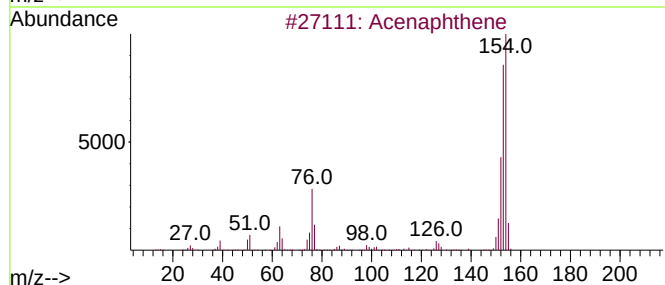
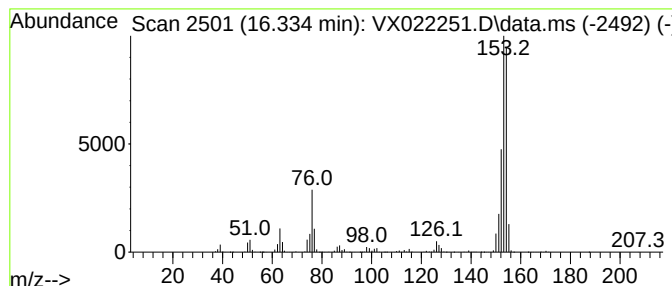
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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

Peak Number 10 Acenaphthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.334	233.67 ug/l	2074400	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	96
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	76
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	64
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
5			Biphenyl	154	C12H10	000092-52-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
 Data File : VX022251.D
 Acq On : 28 May 2021 14:09
 Operator : JC/MD
 Sample : M2520-02 10X
 Misc : 15.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WC-02-2021-05-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.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
Indane	12.244	343.6	ug/l	3050430	4	12.024	443880	50.0
2-Methylindene	13.426	123.9	ug/l	1099780	4	12.024	443880	50.0
Naphthalene, 1-...	14.640	93.3	ug/l	828170	4	12.024	443880	50.0
1,4-Methanonaph...	14.786	609.9	ug/l	5414160	4	12.024	443880	50.0
Biphenyl	15.213	79.0	ug/l	701566	4	12.024	443880	50.0
Naphthalene, 1-...	15.377	80.7	ug/l	716202	4	12.024	443880	50.0
Naphthalene, 2,...	15.481	197.5	ug/l	1753020	4	12.024	443880	50.0
Naphthalene, 2,...	15.621	244.6	ug/l	2171290	4	12.024	443880	50.0
Naphthalene, 1,...	15.841	125.9	ug/l	1118070	4	12.024	443880	50.0
Acenaphthene	16.334	233.7	ug/l	2074400	4	12.024	443880	50.0