

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
 Data File : VX041706.D
 Acq On : 03 Jun 2024 15:53
 Operator : JC/MD
 Sample : P2660-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-06

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\82X052924W.M
 Title : SW846 8260

Signal : TIC: VX041706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	31	rBV2	16920	28151	4.04%	0.407%
2	1.563	70	78	79	rBV4	18965	42680	6.13%	0.616%
3	2.776	269	277	281	rBV3	8959	21389	3.07%	0.309%
4	2.947	296	305	316	rVB	6288	16381	2.35%	0.237%
5	3.099	319	330	341	rBV4	6810	21239	3.05%	0.307%
6	4.209	499	512	519	rBV3	8532	26160	3.76%	0.378%
7	4.294	519	526	537	rVB3	8834	25903	3.72%	0.374%
8	5.385	692	705	718	rBV	80427	245418	35.26%	3.544%
9	5.550	723	732	740	rBV	138556	402889	57.88%	5.819%
10	5.824	768	777	789	rVB6	2888	9683	1.39%	0.140%
11	5.958	789	799	808	rBV	83413	224952	32.32%	3.249%
12	6.044	808	813	825	rVV	10873	31934	4.59%	0.461%
13	6.245	825	846	858	rVV2	44975	154753	22.23%	2.235%
14	6.349	858	863	876	rVB6	3557	10328	1.48%	0.149%
15	6.763	921	931	951	rBV	208511	513946	73.83%	7.423%
16	7.367	1020	1030	1043	rVB6	9004	26895	3.86%	0.388%
17	7.556	1057	1061	1065	rBV3	3597	7302	1.05%	0.105%
18	7.982	1122	1131	1140	rBV	36305	73599	10.57%	1.063%
19	8.104	1143	1151	1161	rBV	62844	127463	18.31%	1.841%
20	8.647	1234	1240	1251	rVB	443249	696081	100.00%	10.053%
21	8.976	1288	1294	1300	rVB5	3430	7316	1.05%	0.106%
22	9.098	1309	1314	1319	rVB3	3718	7257	1.04%	0.105%
23	9.159	1319	1324	1329	rBV	4551	8205	1.18%	0.118%
24	10.055	1461	1471	1479	rBV	475548	652905	93.80%	9.429%
25	10.305	1503	1512	1517	rVB2	8242	13946	2.00%	0.201%
26	10.964	1612	1620	1625	rBV	111443	144775	20.80%	2.091%
27	11.079	1634	1639	1651	rBV	420278	548485	78.80%	7.921%
28	11.305	1667	1676	1684	rBV	157960	204117	29.32%	2.948%
29	11.616	1723	1727	1731	rBV2	5475	9766	1.40%	0.141%
30	11.866	1763	1768	1770	rBV	21864	29732	4.27%	0.429%
31	11.890	1770	1772	1777	rVB	18850	21544	3.10%	0.311%
32	12.024	1788	1794	1802	rBV	493010	643682	92.47%	9.296%
33	12.177	1816	1819	1823	rVB	6486	7085	1.02%	0.102%
34	12.244	1824	1830	1837	rBV2	308002	395456	56.81%	5.711%
35	12.311	1837	1841	1848	rVV2	36038	58622	8.42%	0.847%
36	12.402	1852	1856	1862	rVV2	23814	41045	5.90%	0.593%

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Integrator: RTE

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

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37	12.469	1863	1867	1872	rVB2	10082	16220	2.33%	0.234%
38	12.616	1886	1891	1894	rBV	82610	108120	15.53%	1.562%
39	12.646	1894	1896	1900	rVV	14028	16028	2.30%	0.231%
40	12.701	1900	1905	1913	rVB2	94143	138900	19.95%	2.006%
41	12.920	1933	1941	1947	rBV	76970	100913	14.50%	1.457%
42	13.030	1955	1959	1964	rBV4	7707	15003	2.16%	0.217%
43	13.170	1979	1982	1985	rBV	13536	14253	2.05%	0.206%
44	13.268	1994	1998	1999	rBV2	9764	12140	1.74%	0.175%
45	13.292	1999	2002	2008	rVB2	30838	40719	5.85%	0.588%
46	13.420	2020	2023	2030	rBV5	16165	24634	3.54%	0.356%
47	13.542	2040	2043	2046	rBV2	6255	8414	1.21%	0.122%
48	13.579	2046	2049	2054	rVB2	8957	10561	1.52%	0.153%
49	13.750	2072	2077	2079	rBV	35651	50575	7.27%	0.730%
50	13.774	2079	2081	2088	rVB	58212	72241	10.38%	1.043%
51	14.036	2121	2124	2128	rBV	14117	16790	2.41%	0.242%
52	14.073	2128	2130	2134	rVB5	6320	7511	1.08%	0.108%
53	14.195	2146	2150	2162	rVB2	40525	74033	10.64%	1.069%
54	14.317	2167	2170	2175	rVB	10273	12958	1.86%	0.187%
55	14.573	2207	2212	2214	rBV5	6821	11105	1.60%	0.160%
56	14.609	2214	2218	2228	rVB6	10079	28035	4.03%	0.405%
57	14.756	2238	2242	2244	rBV	22188	25899	3.72%	0.374%
58	14.780	2244	2246	2251	rVV2	28399	43132	6.20%	0.623%
59	14.823	2251	2253	2263	rVV10	7502	15801	2.27%	0.228%
60	14.914	2263	2268	2285	rVV	73539	134318	19.30%	1.940%
61	15.182	2309	2312	2314	rBV3	7654	9672	1.39%	0.140%
62	15.213	2314	2317	2319	rVV	9542	12132	1.74%	0.175%
63	15.249	2319	2323	2332	rVB	45878	74981	10.77%	1.083%
64	15.487	2357	2362	2368	rBV2	32584	50815	7.30%	0.734%
65	15.542	2368	2371	2374	rBV4	5196	7474	1.07%	0.108%
66	15.664	2387	2391	2403	rVB2	52481	102398	14.71%	1.479%
67	15.883	2424	2427	2433	rVB7	4442	7508	1.08%	0.108%
68	16.030	2448	2451	2456	rVB5	7796	10383	1.49%	0.150%
69	16.097	2456	2462	2468	rBV7	7272	22143	3.18%	0.320%
70	16.328	2494	2500	2503	rBV2	20523	38887	5.59%	0.562%
71	16.377	2503	2508	2515	rVB	52801	88320	12.69%	1.276%

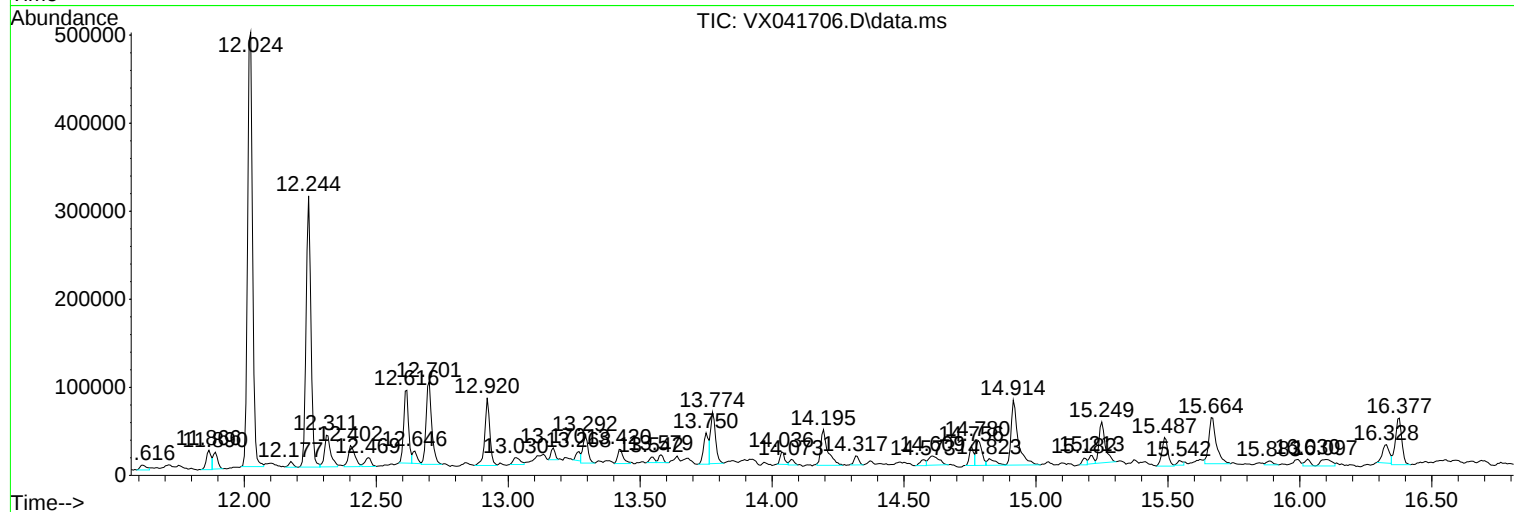
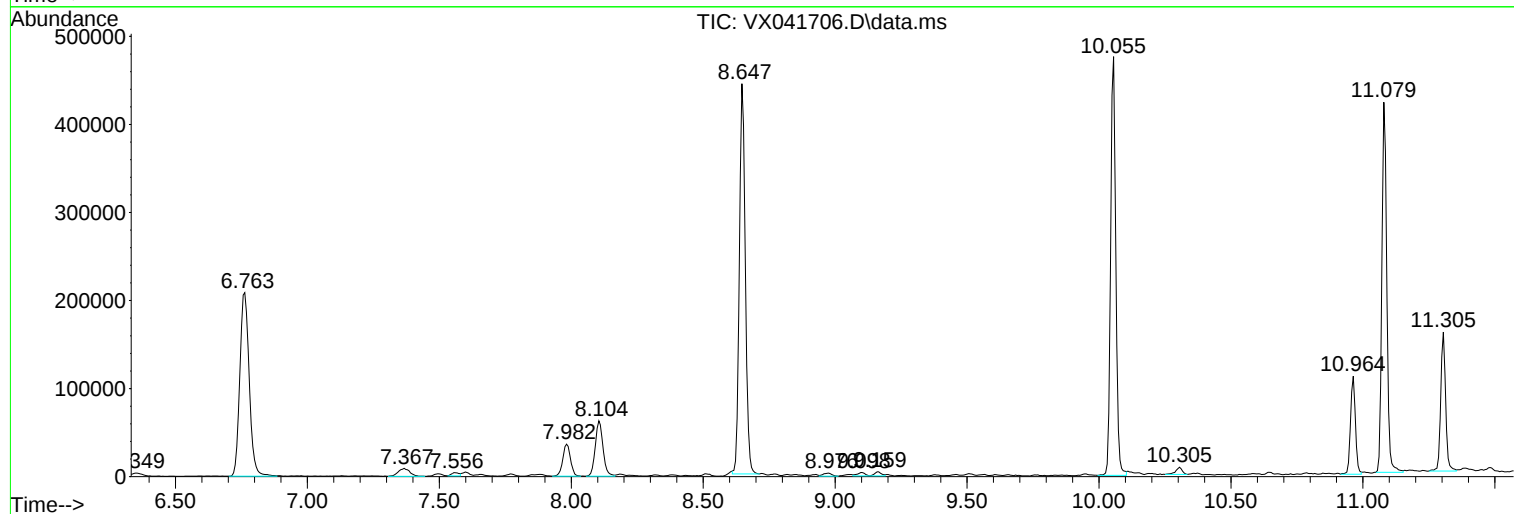
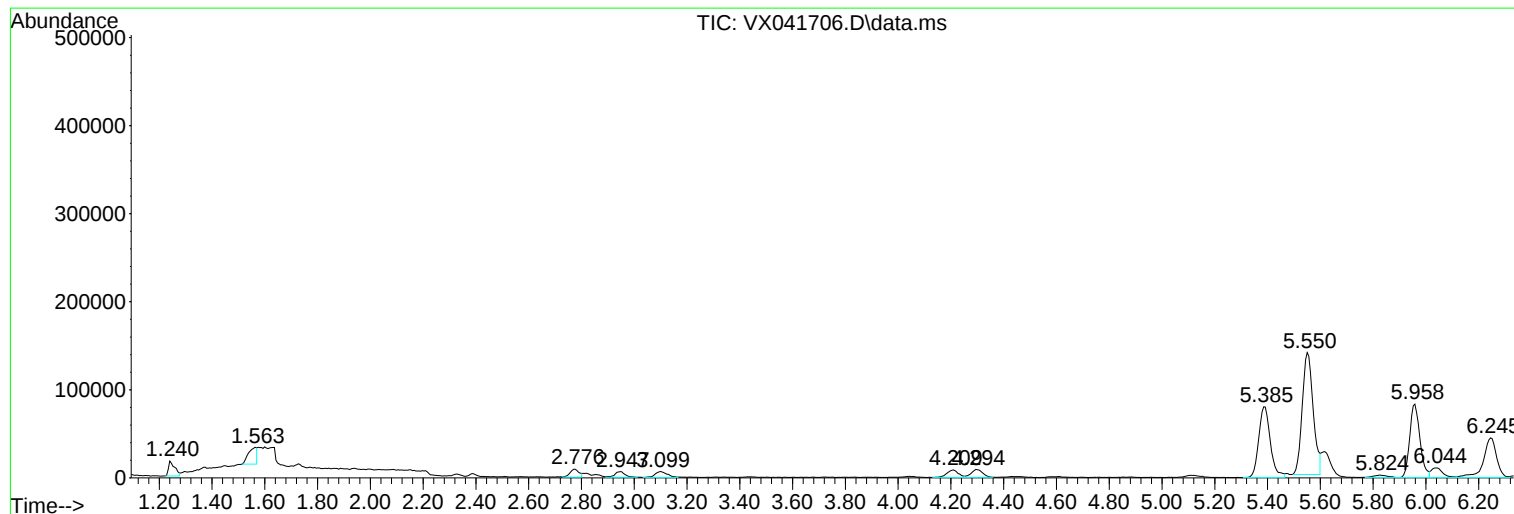
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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



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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

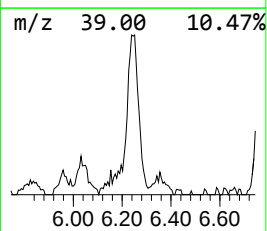
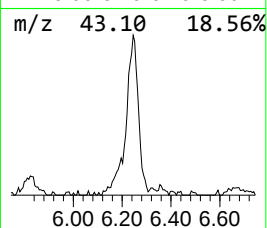
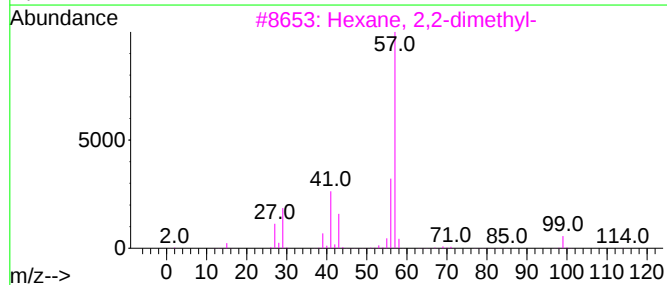
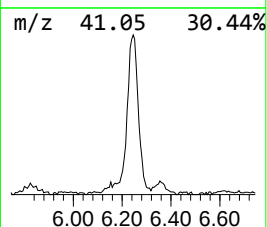
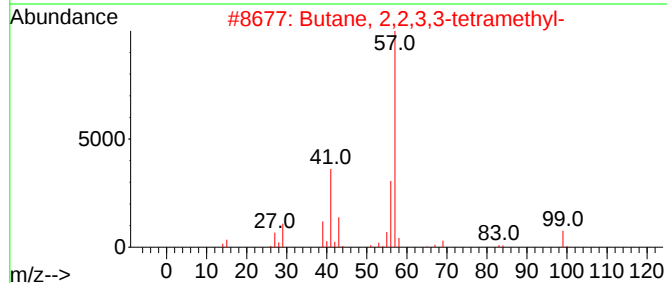
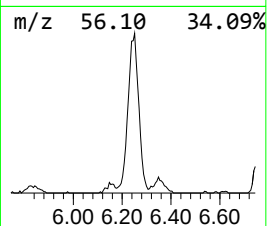
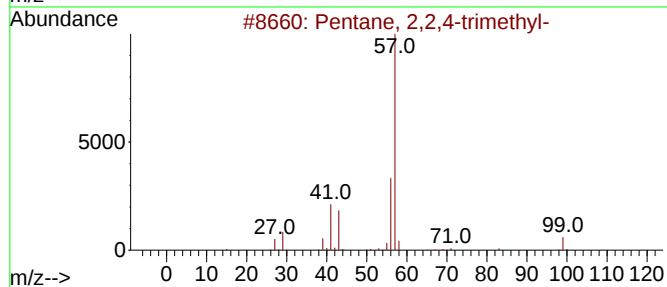
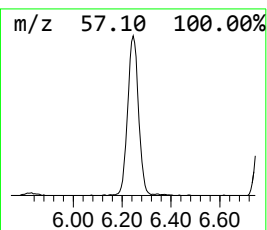
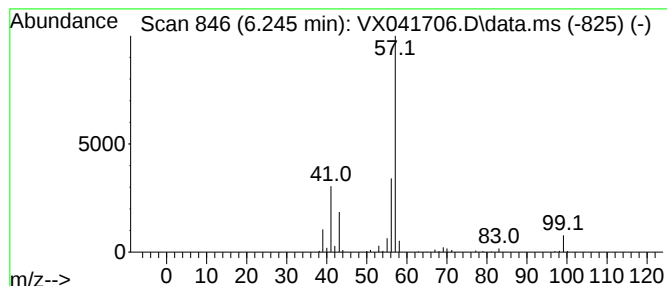
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	15.06 ug/l	154753	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
5			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	50



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Instrument :
MSVOA_X
ClientSampleId :
MW-06

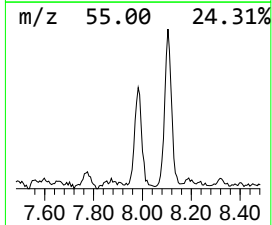
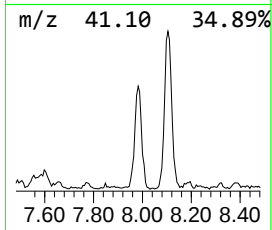
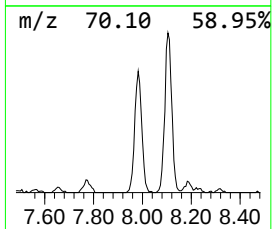
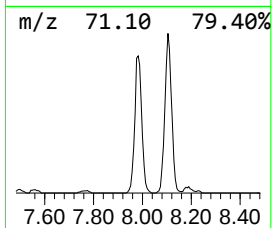
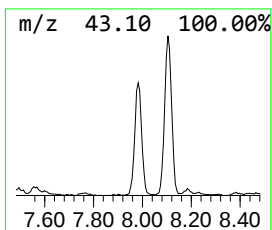
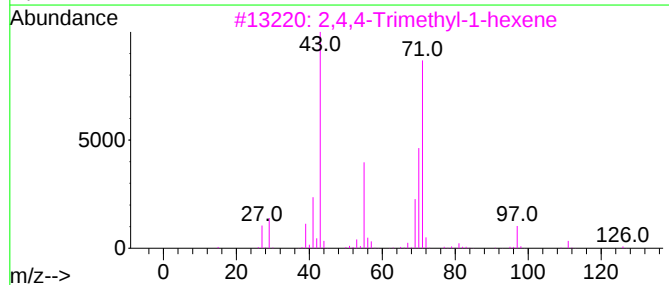
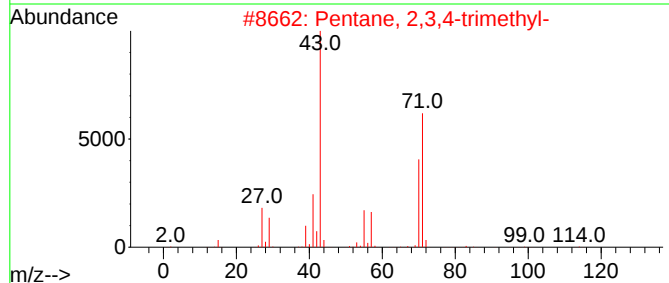
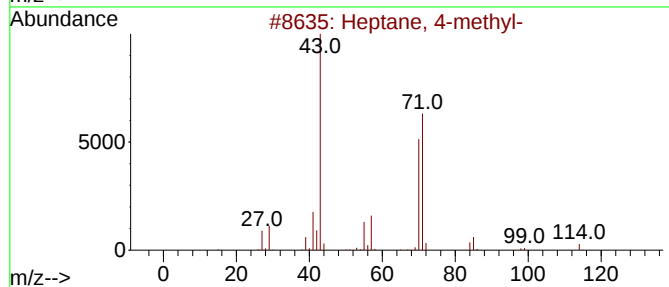
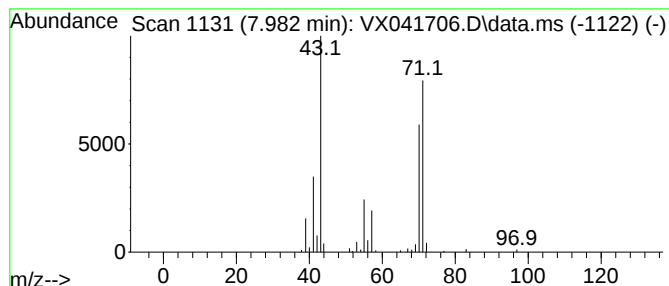
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.982	7.16 ug/l	73599	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
2		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
3		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4		Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
5		Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53



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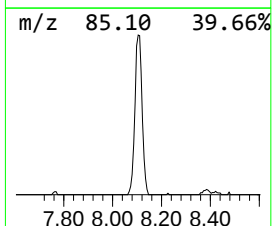
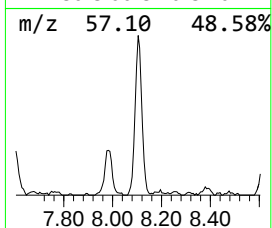
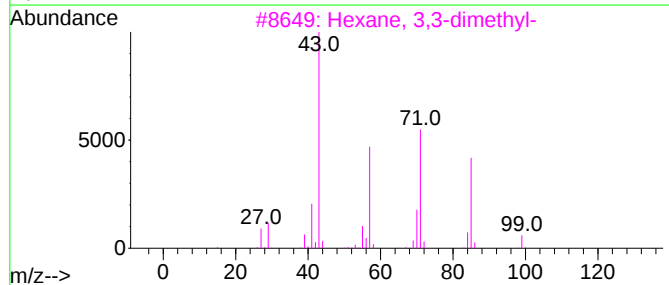
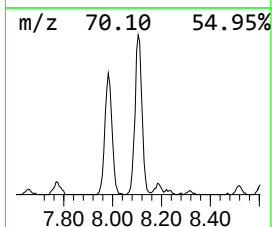
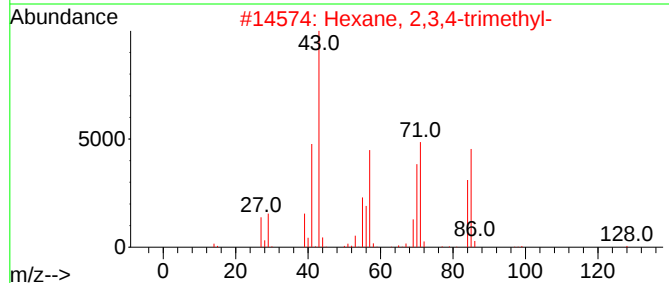
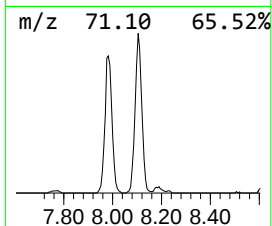
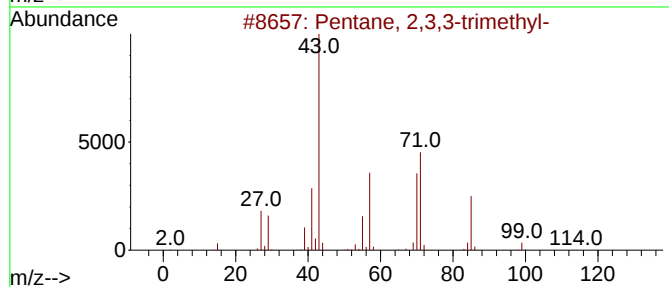
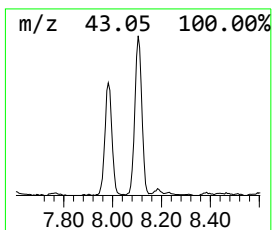
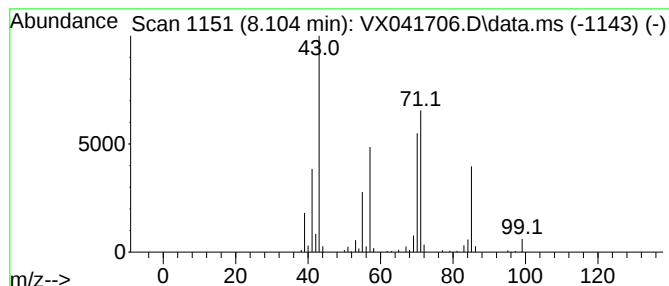
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	12.40 ug/l	127463	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	53



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

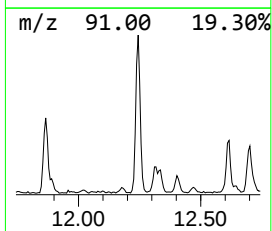
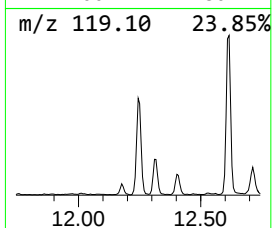
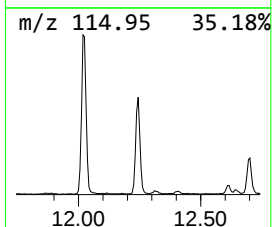
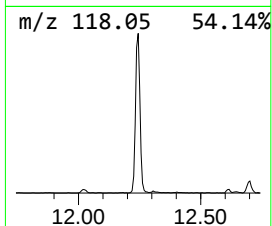
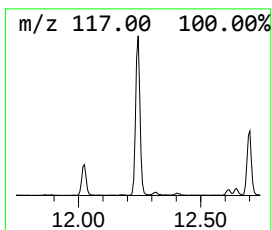
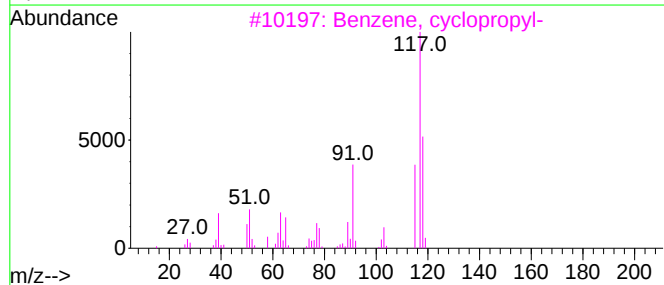
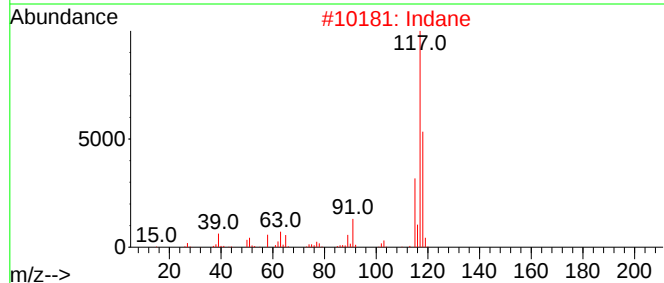
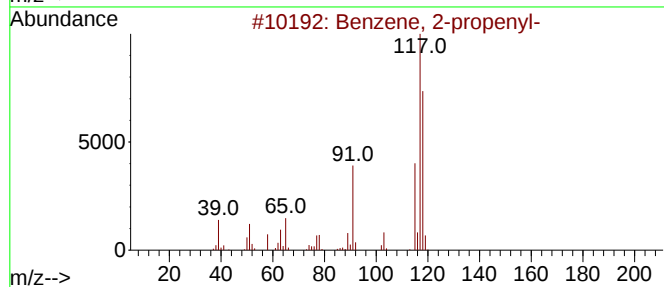
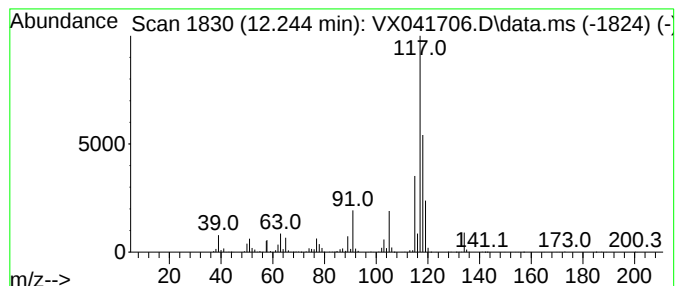
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 2-propenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	30.72 ug/l	395456	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
2			Indane	118	C9H10	000496-11-7	64
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

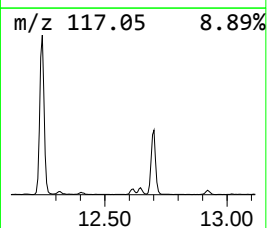
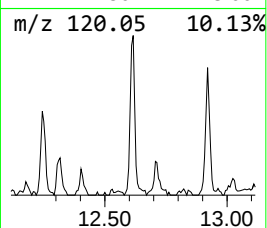
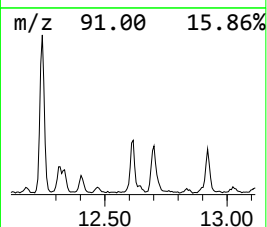
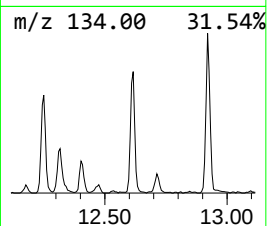
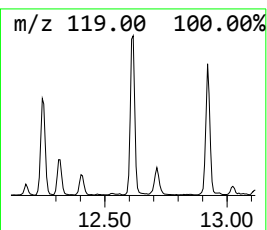
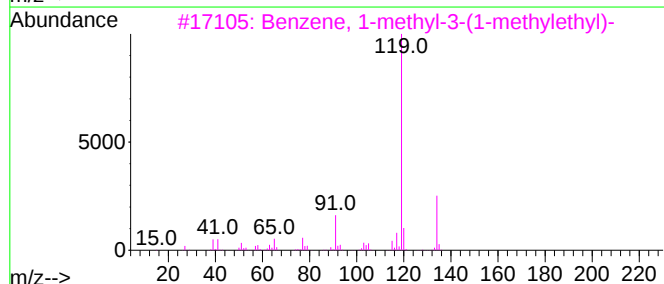
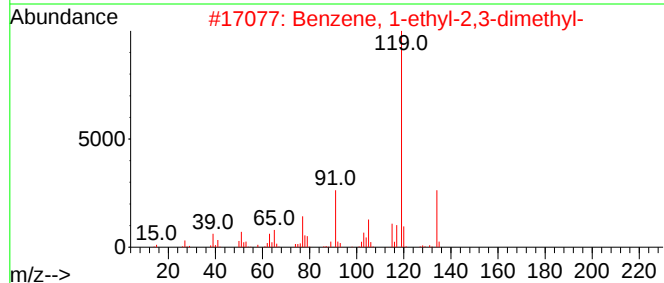
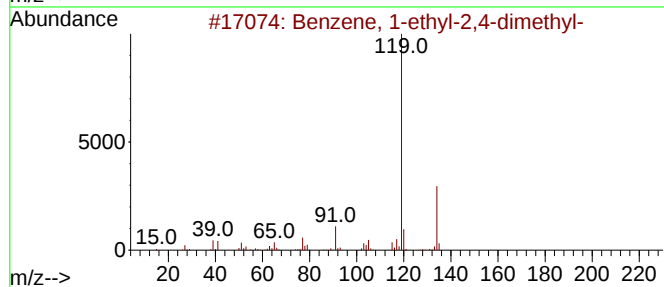
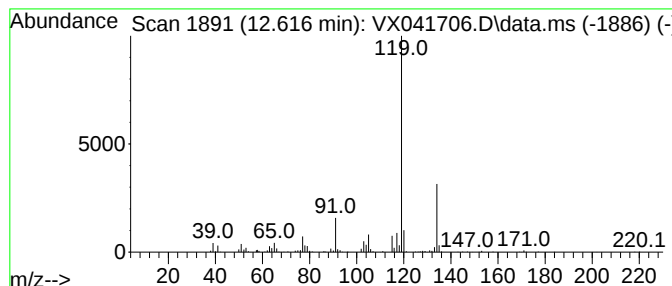
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	8.40 ug/l	108120	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

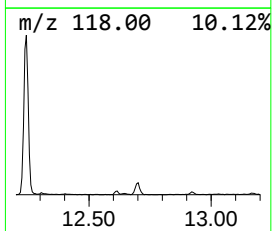
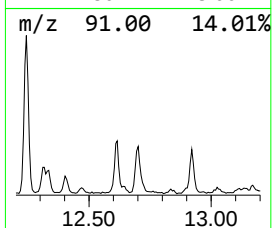
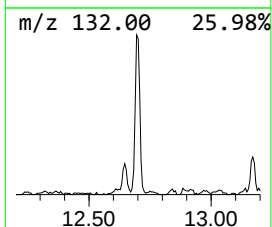
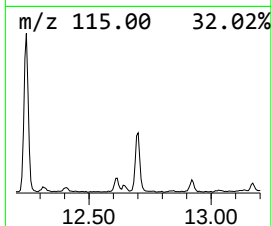
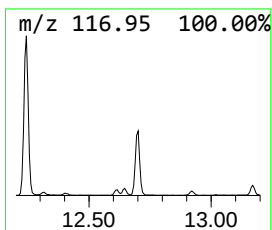
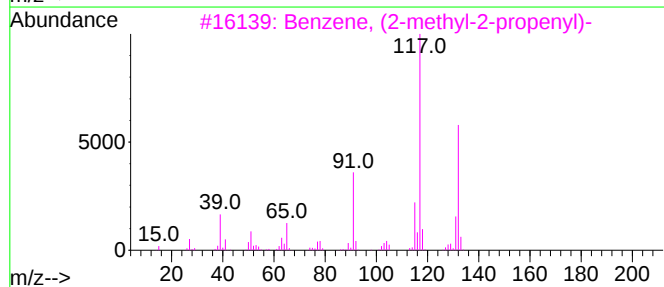
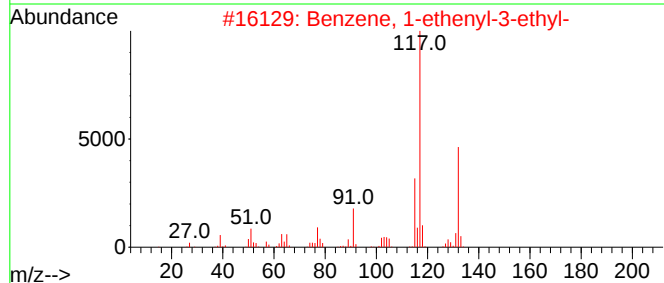
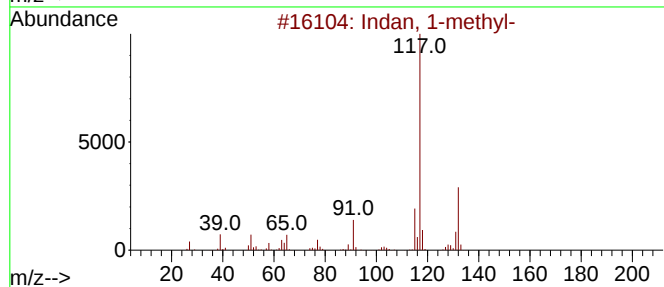
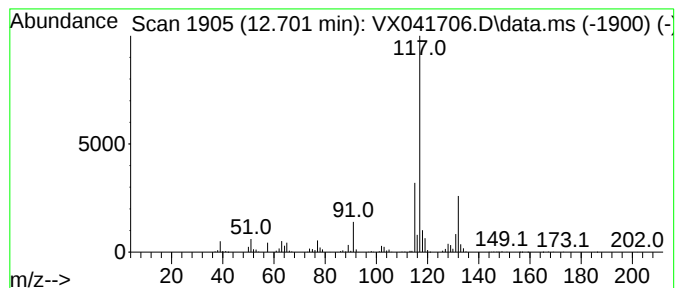
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Quant Title : SW846 8260

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

Peak Number 6 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	10.79 ug/l	138900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	87
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

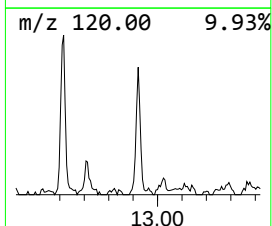
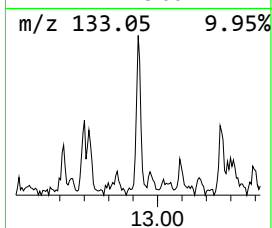
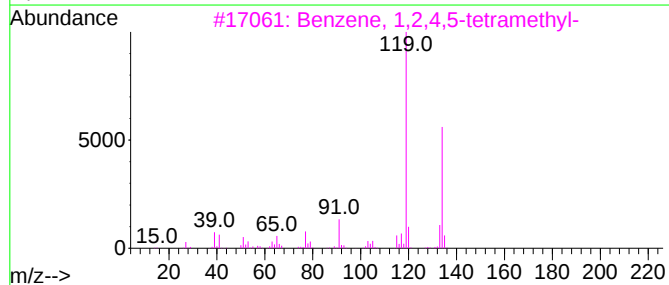
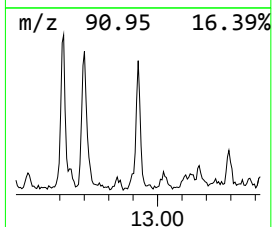
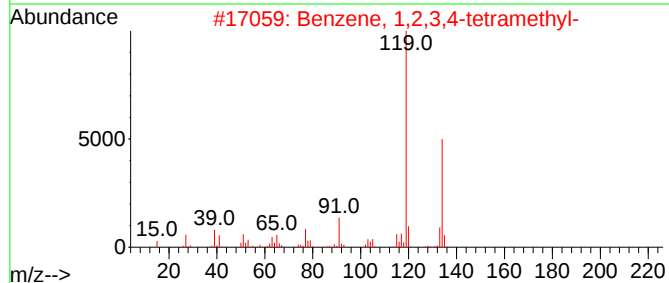
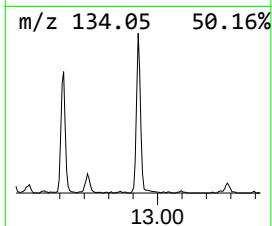
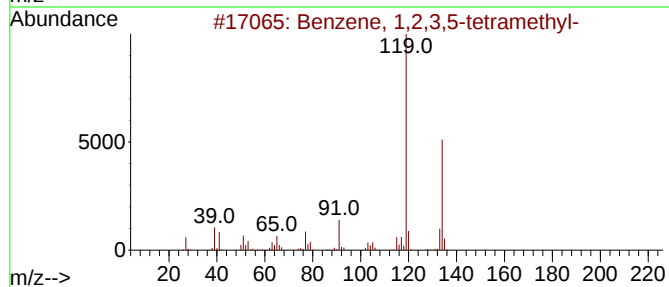
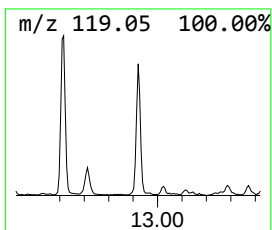
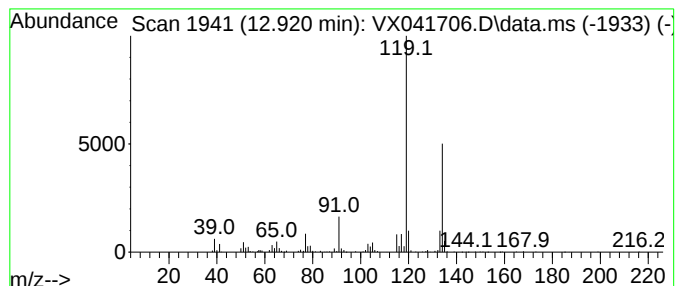
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	7.84 ug/l	100913	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	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

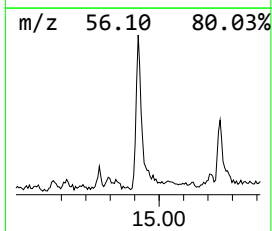
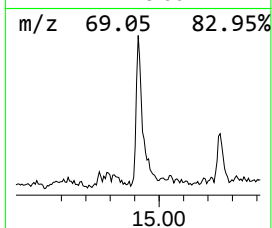
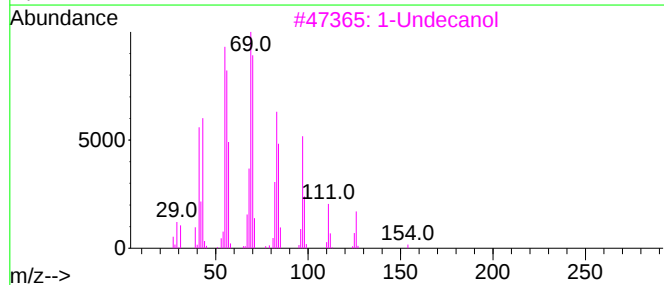
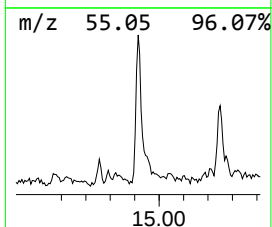
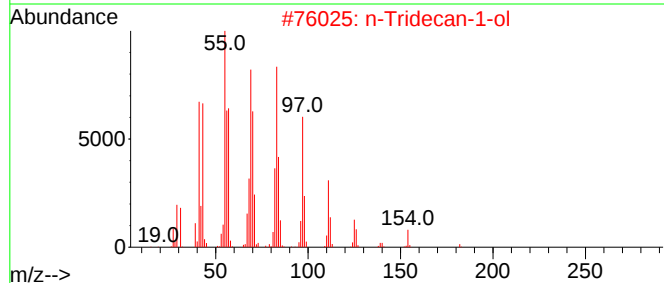
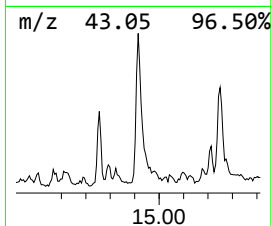
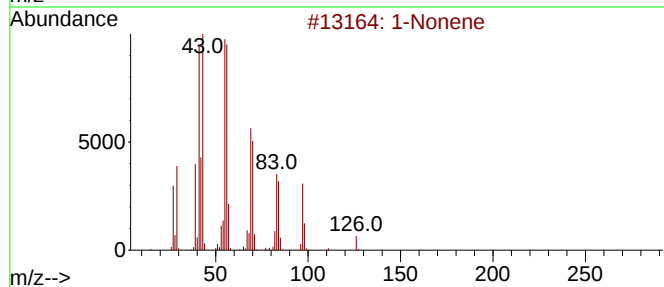
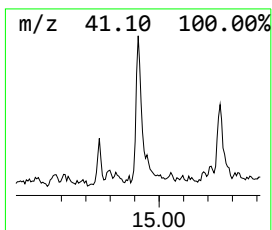
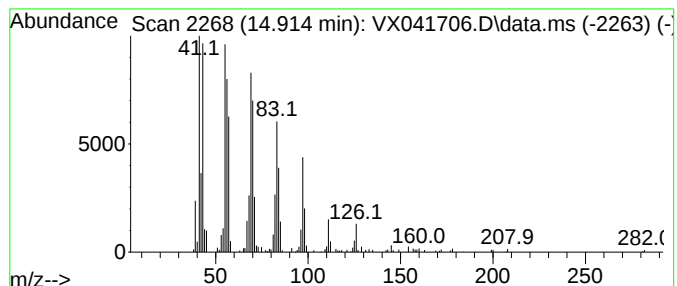
Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Nonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.914	10.43 ug/l	134318	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene	126	C9H18	000124-11-8	94
2	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
3	1-Undecanol	172	C11H24O	000112-42-5	91
4	Cyclopropane, octyl-	154	C11H22	001472-09-9	91
5	1-Dodecanol	186	C12H26O	000112-53-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

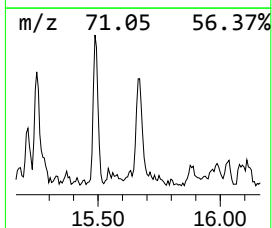
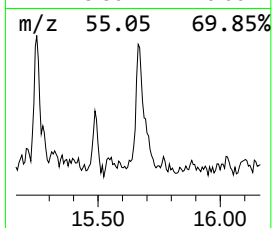
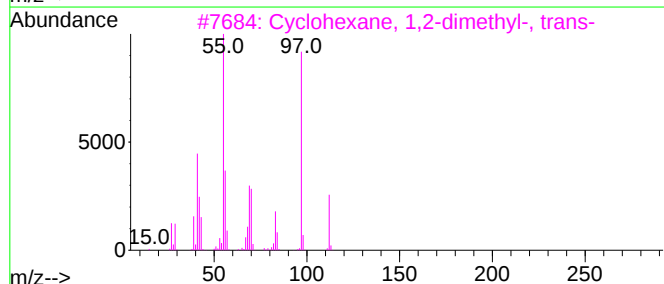
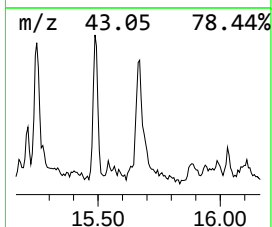
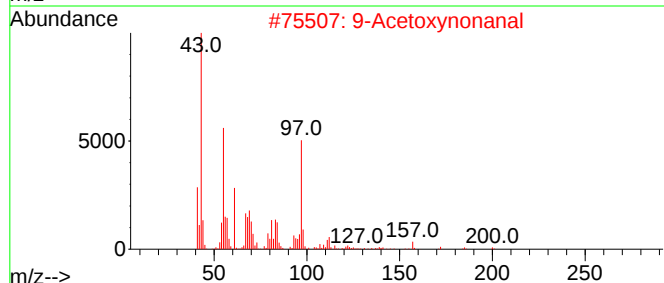
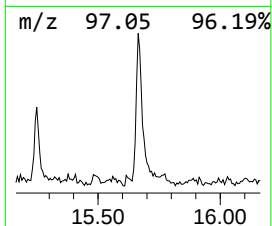
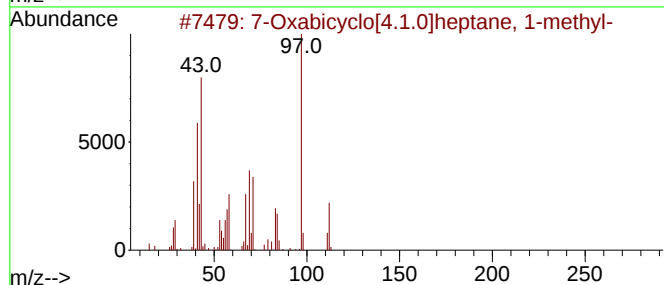
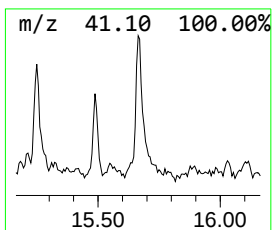
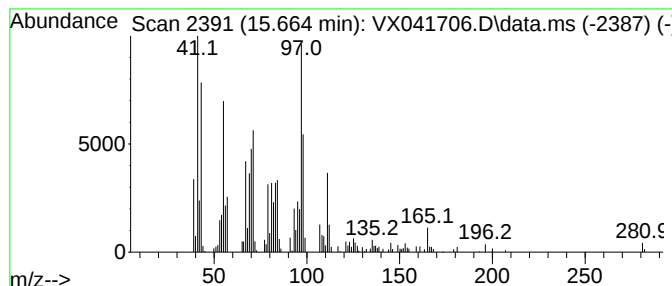
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Quant Title : SW846 8260

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

Peak Number 9 7-Oxabicyclo[4.1.0]heptane,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.664	7.95 ug/l	102398	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	55
2			9-Acetoxynonanal	200	C11H20O3	029541-97-7	41
3			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	38
4			2-n-Butylacrolein	112	C7H12O	001070-66-2	38
5			Cyclooctanone	126	C8H14O	000502-49-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

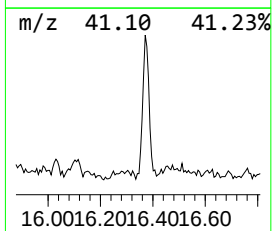
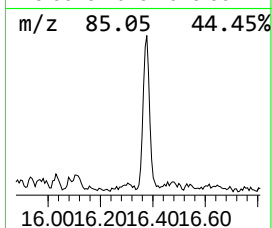
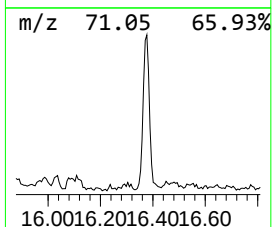
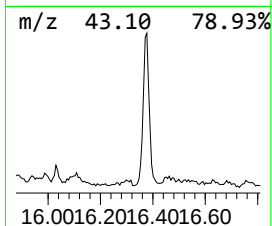
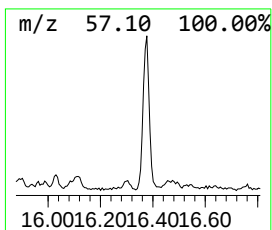
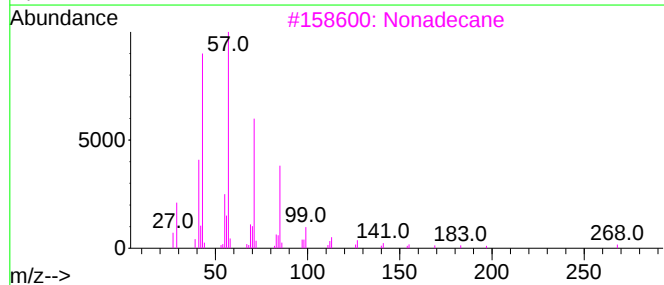
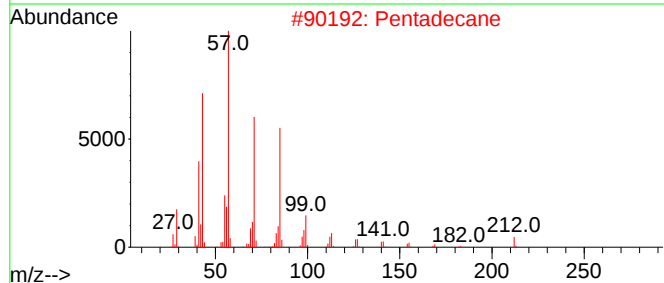
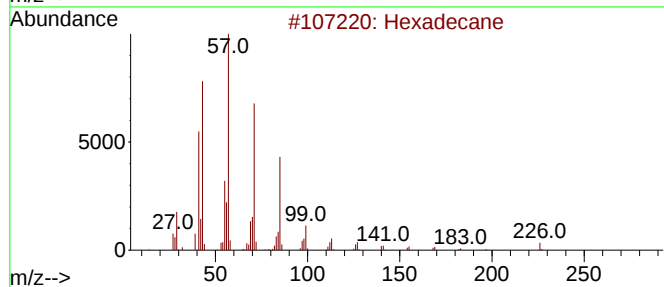
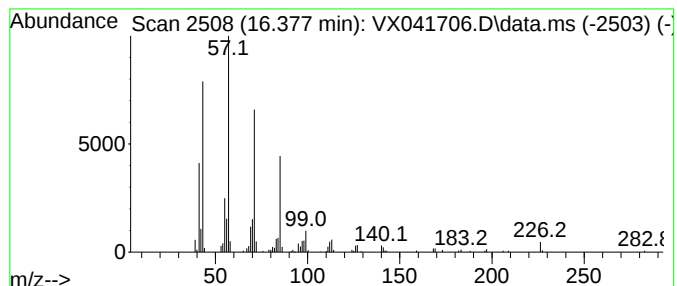
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Quant Title : SW846 8260

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

Peak Number 10 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.377	6.86 ug/l	88320	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	99
2		Pentadecane	212	C15H32	000629-62-9	91
3		Nonadecane	268	C19H40	000629-92-5	90
4		Tetradecane	198	C14H30	000629-59-4	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060324\
Data File : VX041706.D
Acq On : 03 Jun 2024 15:53
Operator : JC/MD
Sample : P2660-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-06

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X052924W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Heptane, 4-methyl-	7.982	7.2	ug/l	73599	2	6.763	513946	50.0
Pentane, 2,3,3-...	8.104	12.4	ug/l	127463	2	6.763	513946	50.0
Benzene, 2-prop...	12.244	30.7	ug/l	395456	4	12.024	643682	50.0
Benzene, 1-ethy...	12.616	8.4	ug/l	108120	4	12.024	643682	50.0
Indan, 1-methyl-	12.701	10.8	ug/l	138900	4	12.024	643682	50.0
Benzene, 1,2,3,...	12.921	7.8	ug/l	100913	4	12.024	643682	50.0
1-Nonene	14.914	10.4	ug/l	134318	4	12.024	643682	50.0
7-Oxabicyclo[4....	15.664	8.0	ug/l	102398	4	12.024	643682	50.0
Hexadecane	16.377	6.9	ug/l	88320	4	12.024	643682	50.0