

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NP-WS-001

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 : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Title : SW846 8260

Signal : TIC: VX044208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.727	99	105	114	rBV	51606	71225	1.07%	0.187%
2	2.770	258	276	279	rBV2	37689	87734	1.31%	0.230%
3	2.812	279	283	288	rVV	104767	228144	3.42%	0.598%
4	2.855	288	290	302	rVV2	52795	111402	1.67%	0.292%
5	2.983	303	311	320	rVV	38083	90414	1.35%	0.237%
6	3.093	320	329	343	rVB2	104809	247970	3.71%	0.650%
7	3.721	424	432	442	rBV2	38094	98135	1.47%	0.257%
8	4.294	517	526	542	rVB	204917	600506	8.99%	1.575%
9	5.385	689	705	711	rBV2	81651	247953	3.71%	0.650%
10	5.464	711	718	726	rVV2	95415	292108	4.37%	0.766%
11	5.550	726	732	738	rVB	82254	195152	2.92%	0.512%
12	5.818	767	776	790	rVB3	62324	193689	2.90%	0.508%
13	5.958	790	799	805	rBV	90985	243794	3.65%	0.639%
14	6.037	805	812	822	rVB2	69739	183575	2.75%	0.481%
15	6.159	822	832	835	rBV3	40432	114839	1.72%	0.301%
16	6.245	842	846	856	rVB3	59515	158361	2.37%	0.415%
17	6.354	856	864	875	rVB3	47147	135609	2.03%	0.356%
18	6.757	921	930	940	rBV	199588	573207	8.58%	1.503%
19	6.848	941	945	958	rVB5	59721	146868	2.20%	0.385%
20	7.372	1019	1031	1044	rBV4	214419	574085	8.60%	1.505%
21	7.653	1071	1077	1088	rVB2	46170	91979	1.38%	0.241%
22	7.982	1122	1131	1142	rVB4	30111	91198	1.37%	0.239%
23	8.104	1144	1151	1155	rBV3	52829	113728	1.70%	0.298%
24	8.500	1210	1216	1226	rVB	79814	154908	2.32%	0.406%
25	8.647	1235	1240	1249	rVB	411274	661745	9.91%	1.735%
26	10.055	1466	1471	1476	rBV	403135	557234	8.34%	1.461%
27	10.195	1489	1494	1501	rBV	155559	210445	3.15%	0.552%
28	10.299	1501	1511	1518	rVB	79079	135524	2.03%	0.355%
29	10.963	1614	1620	1628	rBV	455450	586962	8.79%	1.539%
30	11.079	1634	1639	1645	rBV	336546	431248	6.46%	1.131%
31	11.305	1671	1676	1683	rBV	494460	615514	9.22%	1.614%
32	11.396	1685	1691	1695	rVV	113038	157128	2.35%	0.412%
33	11.451	1695	1700	1711	rVB	360628	449010	6.72%	1.177%
34	11.609	1721	1726	1735	rBV	299562	377684	5.66%	0.990%
35	11.750	1745	1749	1759	rVB	486090	593373	8.89%	1.556%
36	12.018	1788	1793	1797	rBV	391640	520925	7.80%	1.366%

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37	12.085	1801	1804	1809	rVB	240399	286189	4.29%	0.750%
38	12.243	1824	1830	1837	rBV	5465929	6678147	100.00%	17.512%
39	12.311	1837	1841	1849	rVB	424484	597685	8.95%	1.567%
40	12.402	1851	1856	1862	rBV3	200555	264163	3.96%	0.693%
41	12.463	1862	1866	1872	rVB2	50902	75447	1.13%	0.198%
42	12.530	1872	1877	1885	rBV	173223	246813	3.70%	0.647%
43	12.615	1885	1891	1894	rBV	2094534	2703512	40.48%	7.089%
44	12.646	1894	1896	1900	rVB	347598	346179	5.18%	0.908%
45	12.701	1900	1905	1913	rBV2	1181172	1758895	26.34%	4.612%
46	12.841	1923	1928	1933	rVB3	58823	89869	1.35%	0.236%
47	12.920	1933	1941	1945	rBV	1239664	1483059	22.21%	3.889%
48	12.963	1945	1948	1954	rVB	190901	239006	3.58%	0.627%
49	13.024	1954	1958	1966	rBV4	97382	156774	2.35%	0.411%
50	13.170	1978	1982	1991	rVB	1137335	1453875	21.77%	3.812%
51	13.292	1997	2002	2008	rVB2	2621339	3494823	52.33%	9.164%
52	13.371	2012	2015	2019	rVB	75479	86132	1.29%	0.226%
53	13.420	2019	2023	2031	rVB	258248	353032	5.29%	0.926%
54	13.505	2031	2037	2040	rBV2	97068	141574	2.12%	0.371%
55	13.542	2040	2043	2046	rVV	219856	275737	4.13%	0.723%
56	13.579	2046	2049	2054	rVV3	260778	399246	5.98%	1.047%
57	13.640	2054	2059	2060	rVV2	121160	158280	2.37%	0.415%
58	13.664	2060	2063	2072	rVB2	255993	408765	6.12%	1.072%
59	13.774	2073	2081	2090	rBV	531138	724788	10.85%	1.901%
60	13.853	2090	2094	2100	rVB2	68697	101828	1.52%	0.267%
61	13.926	2100	2106	2110	rBV2	166675	235303	3.52%	0.617%
62	13.969	2110	2113	2117	rVB2	109171	123596	1.85%	0.324%
63	14.072	2125	2130	2137	rBV	204413	275629	4.13%	0.723%
64	14.219	2148	2154	2163	rBV4	213299	451369	6.76%	1.184%
65	14.316	2166	2170	2175	rVV	97374	134022	2.01%	0.351%
66	14.371	2175	2179	2184	rVB	150954	189220	2.83%	0.496%
67	14.481	2192	2197	2201	rBV2	133600	184487	2.76%	0.484%
68	14.633	2218	2222	2233	rVB	874924	1140139	17.07%	2.990%
69	14.780	2240	2246	2251	rBV	1062692	1350525	20.22%	3.541%
70	15.182	2307	2312	2320	rBV2	39701	79902	1.20%	0.210%
71	15.377	2337	2344	2346	rBV2	46129	70717	1.06%	0.185%
72	15.475	2355	2360	2373	rVB	145987	265105	3.97%	0.695%
73	15.615	2373	2383	2386	rVV	223033	368284	5.51%	0.966%
74	15.645	2386	2388	2396	rVB	120557	174863	2.62%	0.459%
75	15.834	2408	2419	2428	rBV2	55254	154688	2.32%	0.406%
76	15.987	2437	2444	2456	rVB	36500	70264	1.05%	0.184%

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Title : SW846 8260

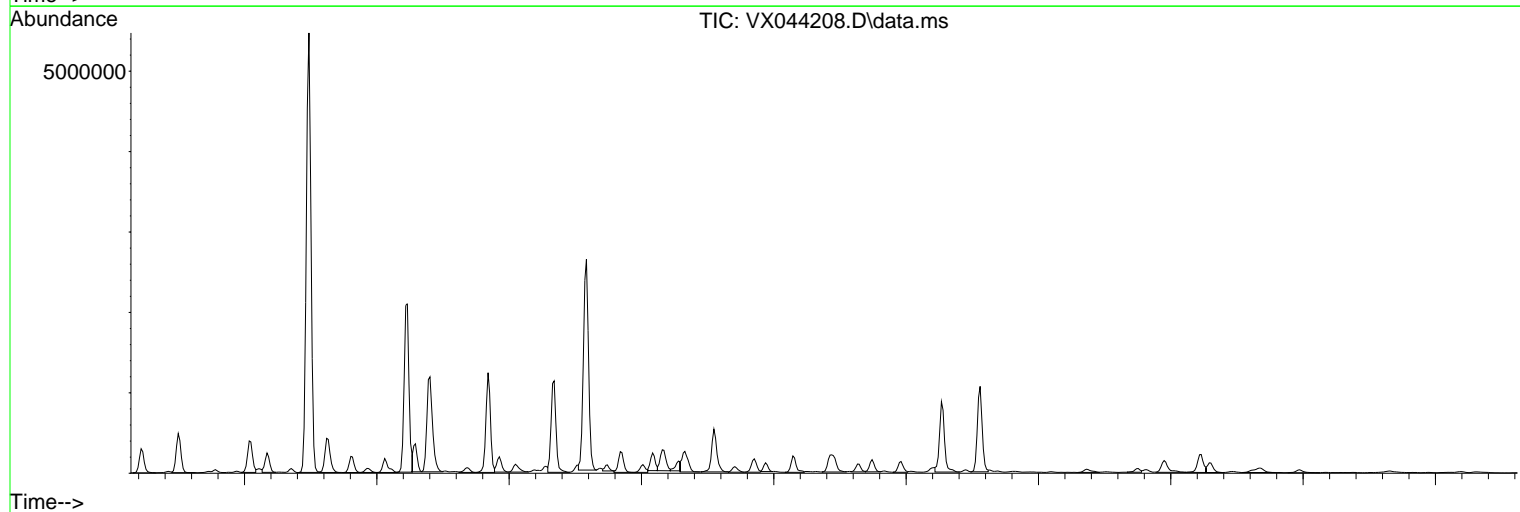
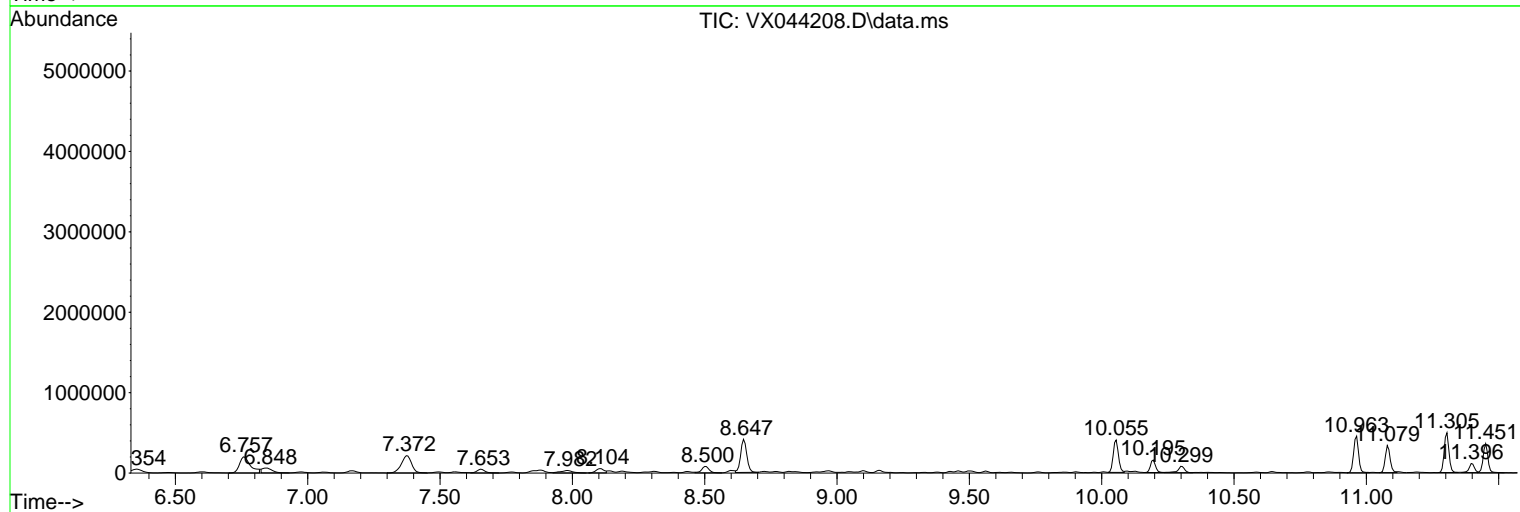
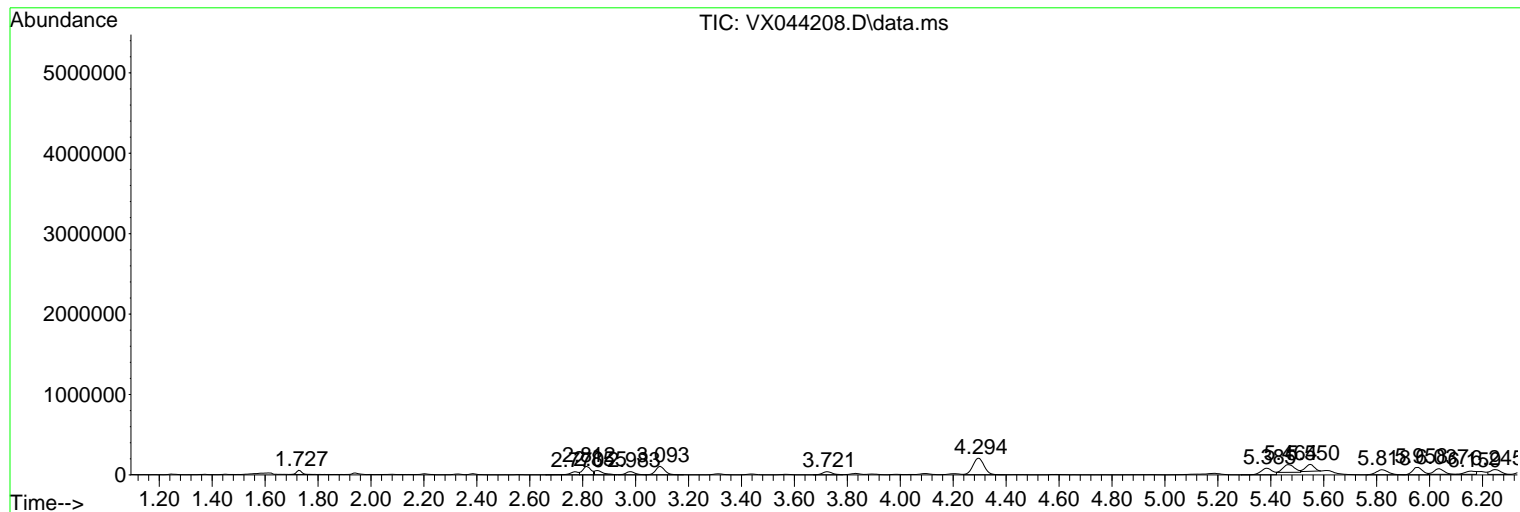
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Quant Title : SW846 8260

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



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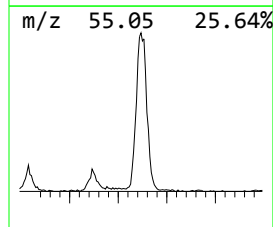
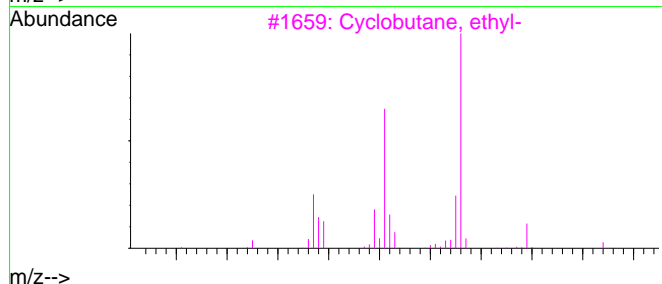
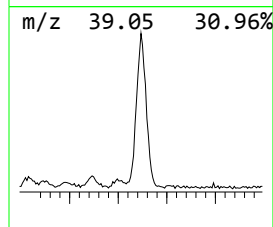
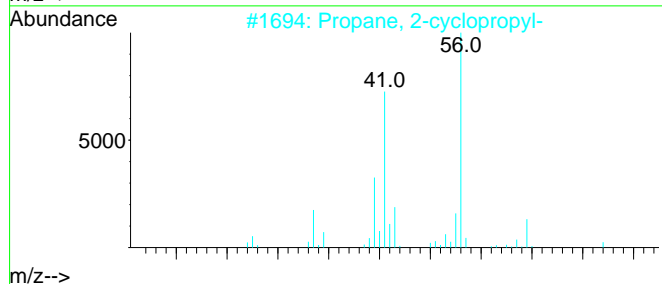
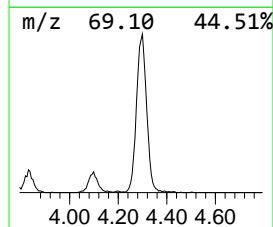
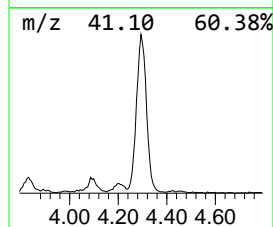
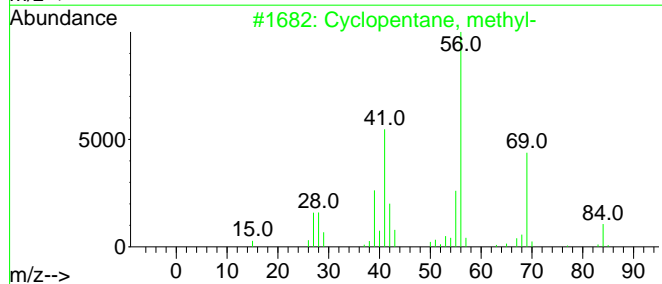
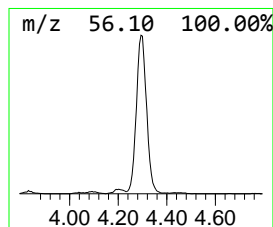
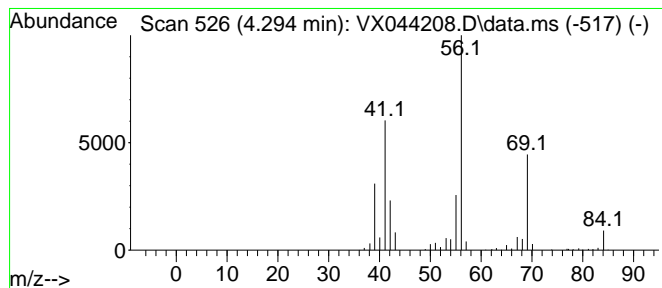
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Quant Title : SW846 8260

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

 Peak Number 1 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	153.86 ug/l	600506	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5	Cyclobutane	56	C4H8	000287-23-0	53



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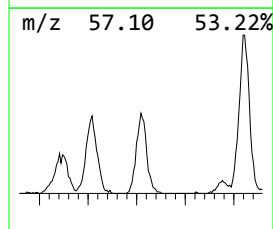
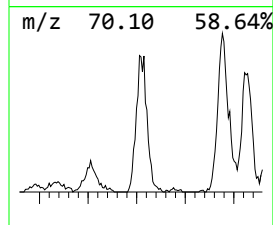
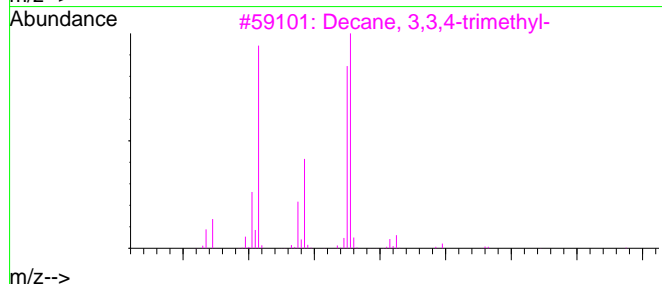
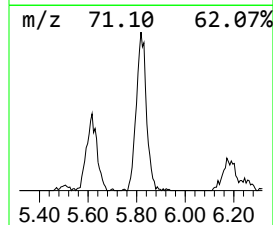
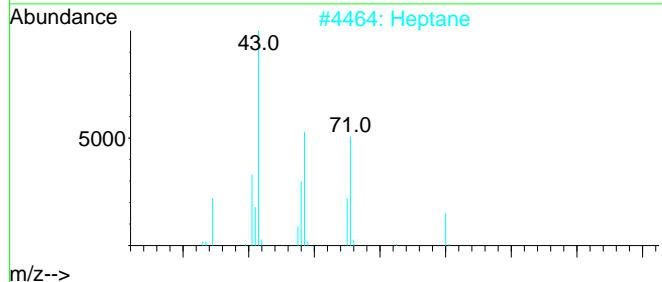
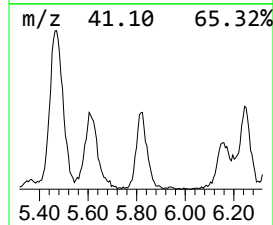
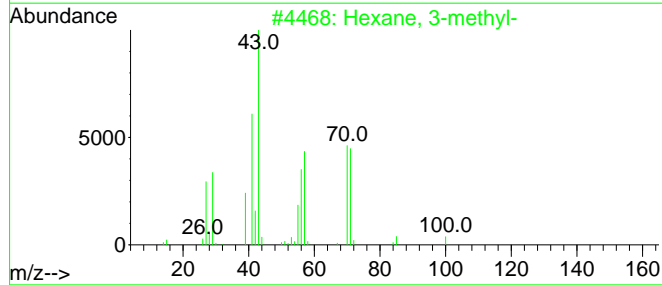
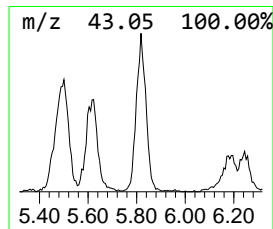
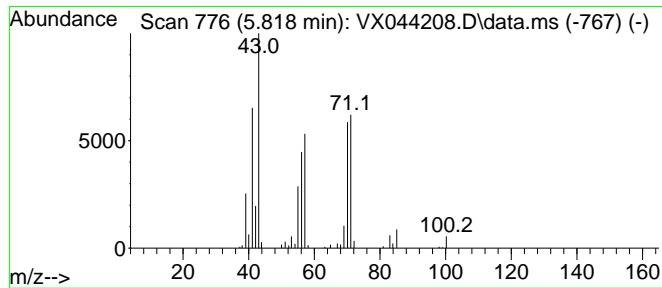
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 Hexane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.818	49.63 ug/l	193689	Pentafluorobenzene	5.550

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91	
2	Heptane	100	C7H16	000142-82-5	59	
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50	
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50	
5	1-Pentanol, 3,4-dimethyl-	116	C7H16O	006570-87-2	45	



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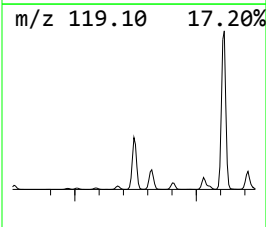
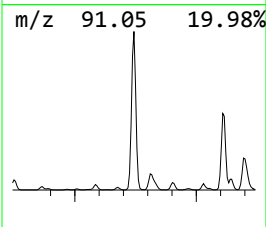
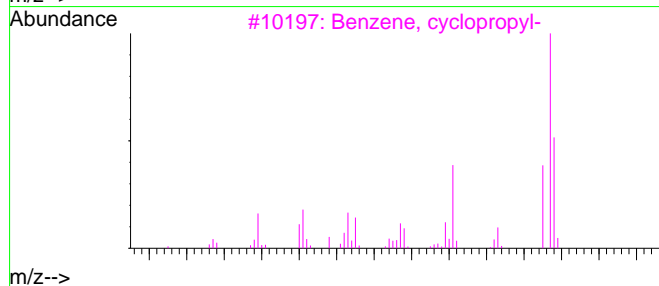
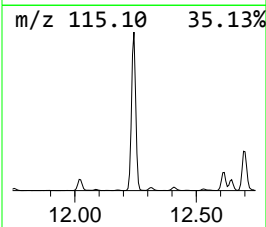
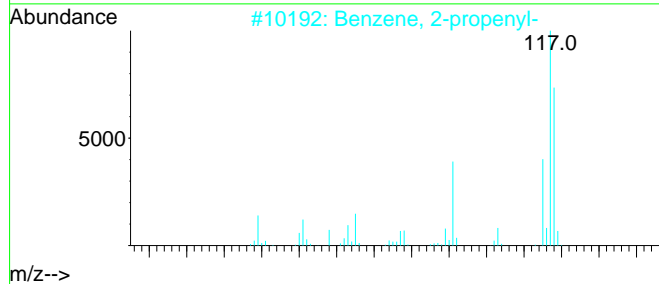
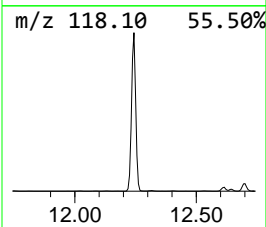
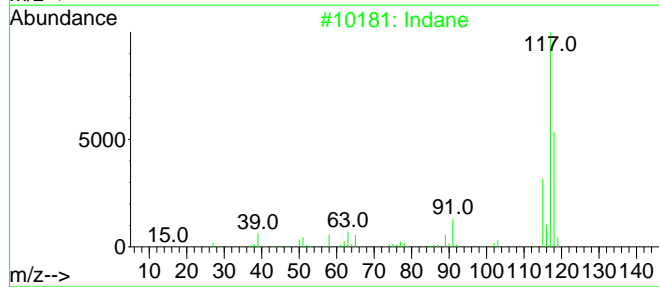
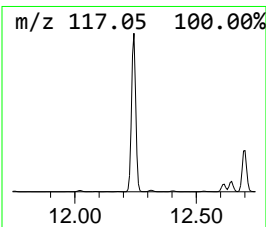
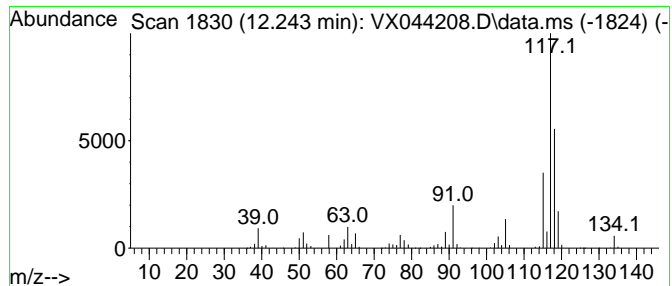
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	640.99 ug/l	6678150	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	70
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64



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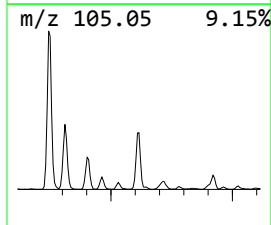
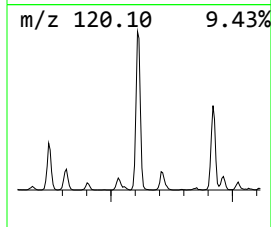
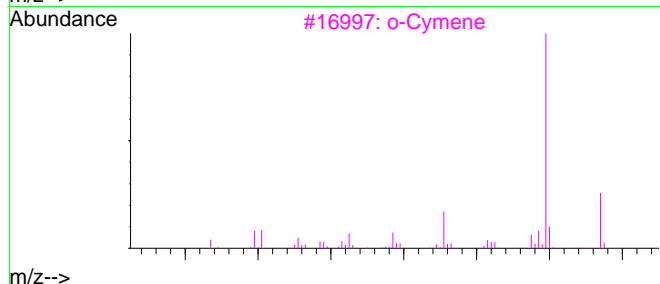
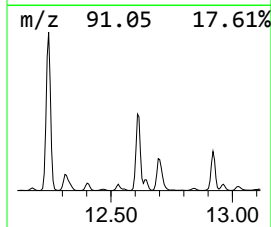
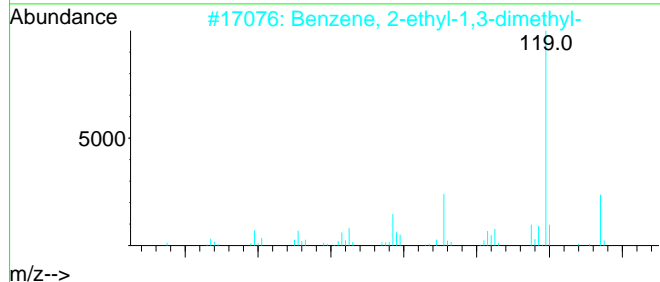
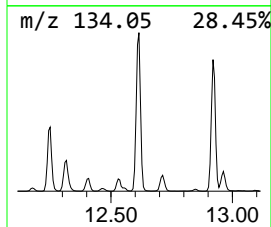
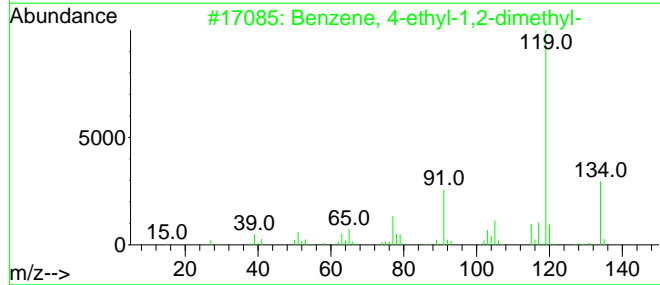
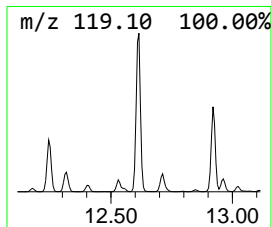
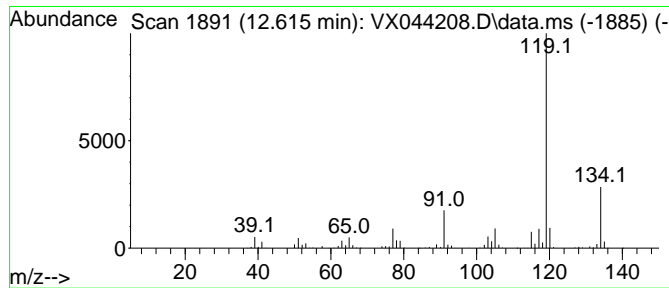
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 Quant Title : SW846 8260

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

 Peak Number 4 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.615	259.49 ug/l	2703510	1,4-Dichlorobenzene-d4	12.024

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3		o-Cymene	134	C10H14	000527-84-4	95
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NP-WS-001

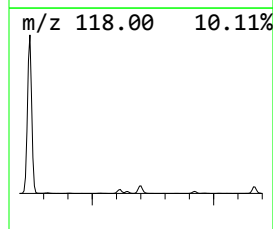
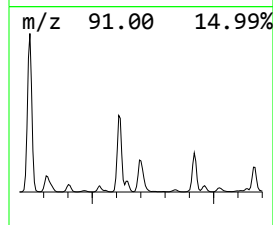
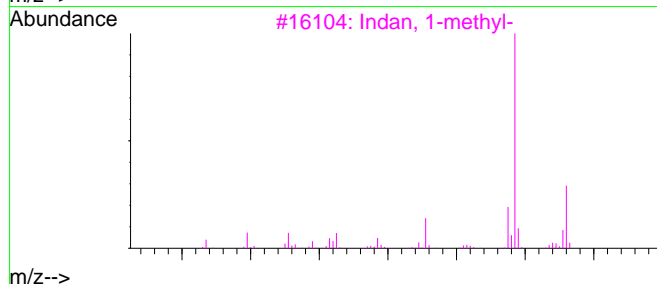
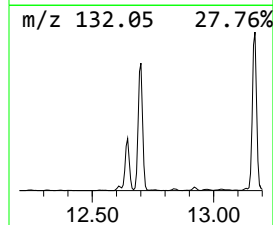
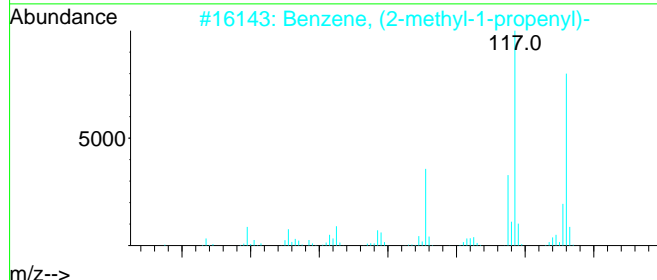
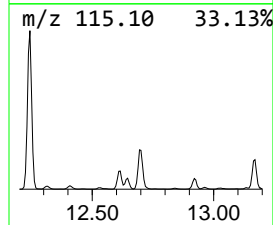
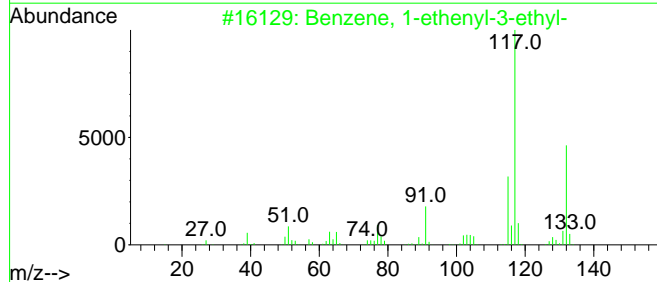
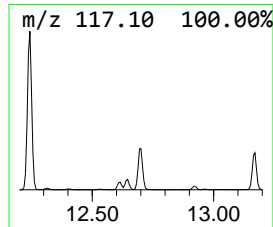
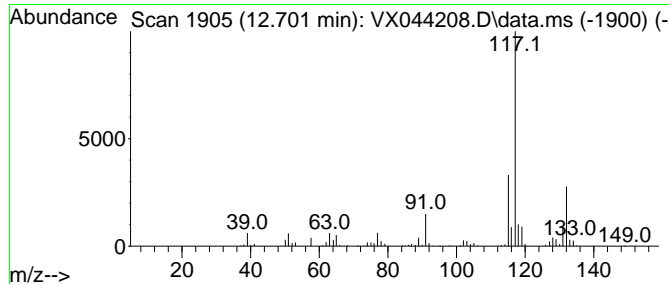
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 Quant Title : SW846 8260

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

 Peak Number 5 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	168.82 ug/l	1758900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
3		Indan, 1-methyl-	132	C10H12	000767-58-8	87
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NP-WS-001

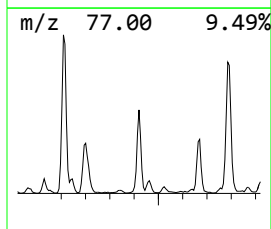
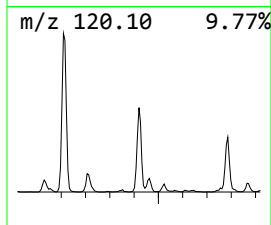
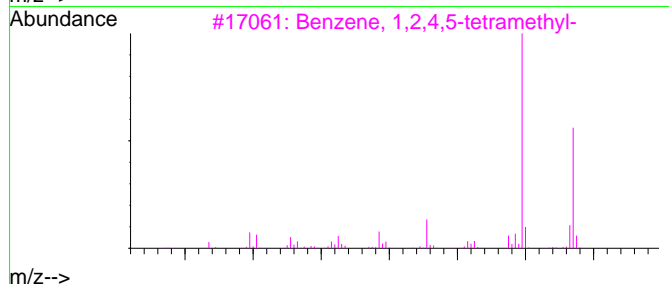
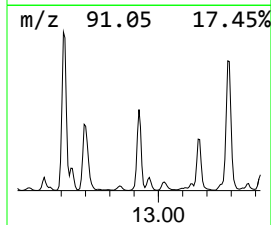
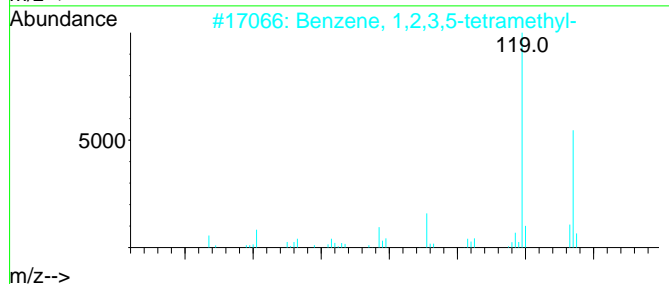
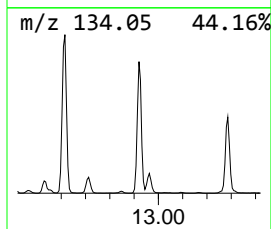
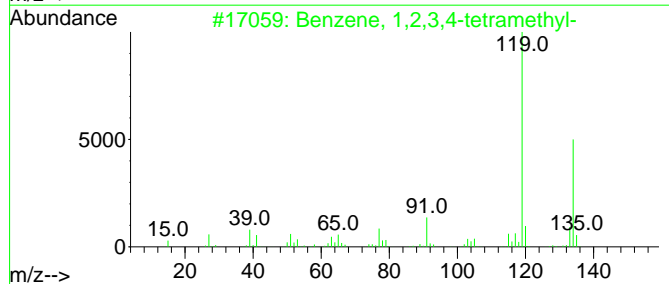
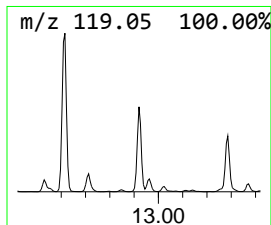
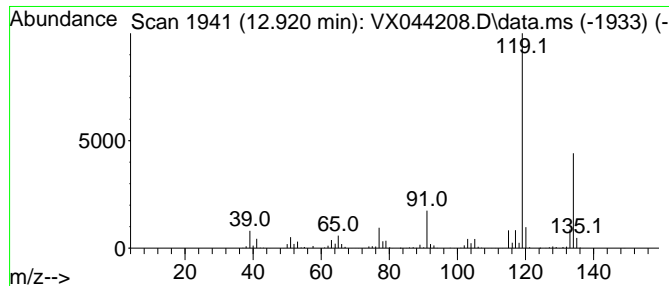
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 Quant Title : SW846 8260

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

 Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	142.35 ug/l	1483060	1,4-Dichlorobenzene-d4	12.024

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5		o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
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 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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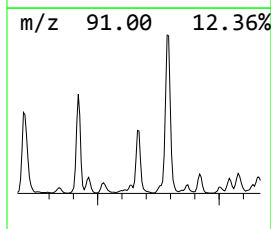
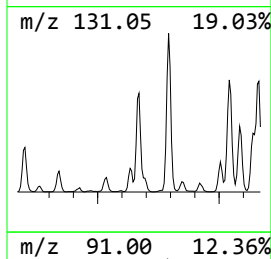
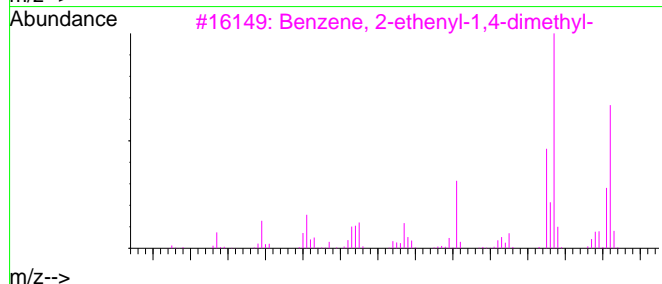
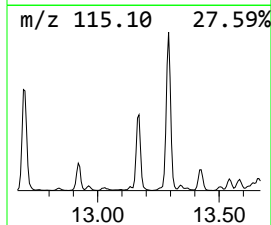
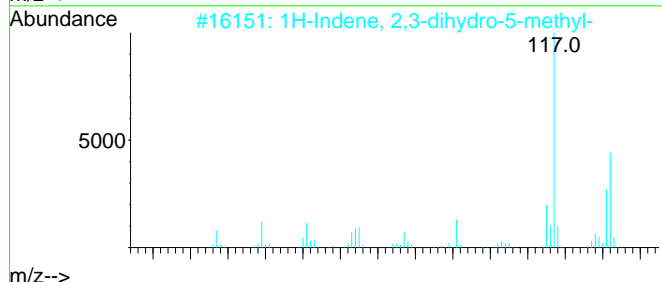
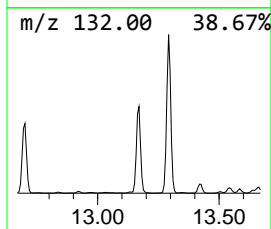
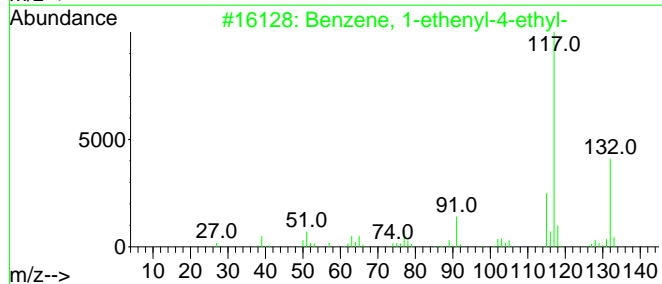
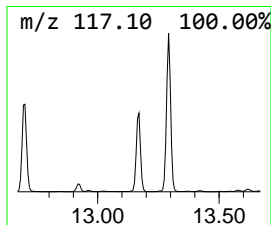
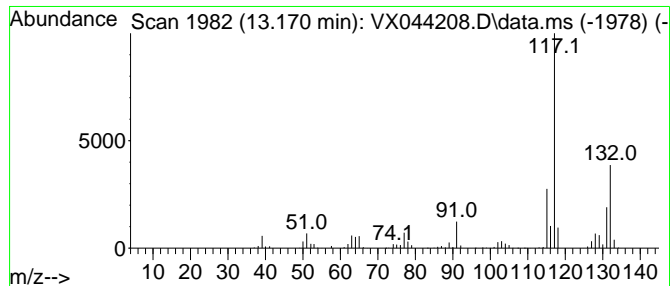
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 Quant Title : SW846 8260

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

 Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	139.55 ug/l	1453880	1,4-Dichlorobenzene-d4	12.024

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
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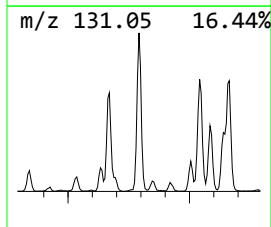
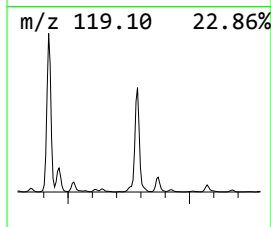
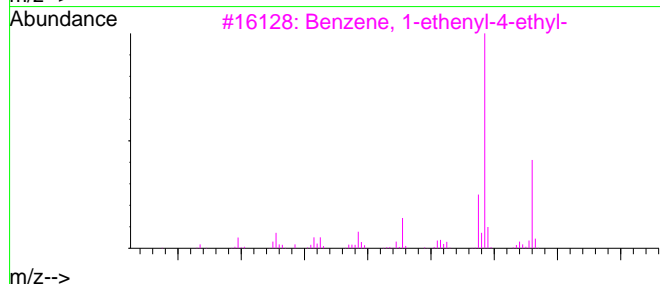
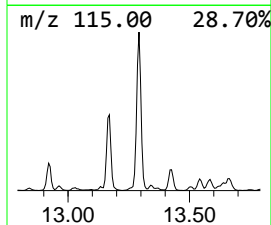
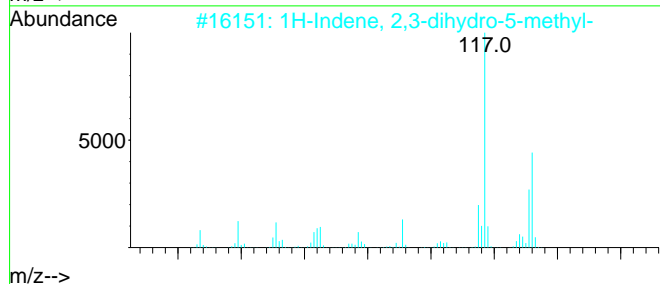
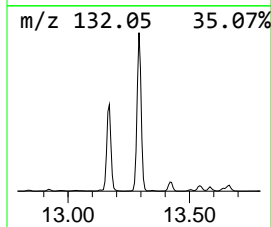
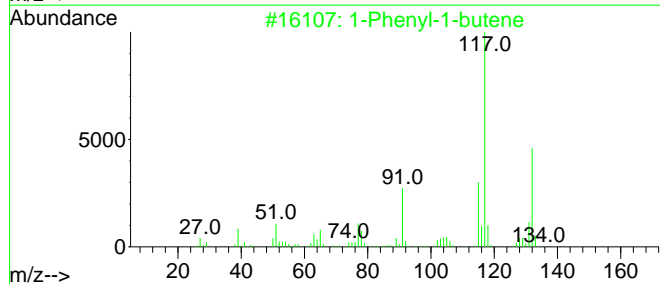
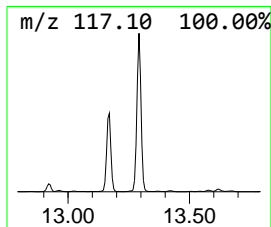
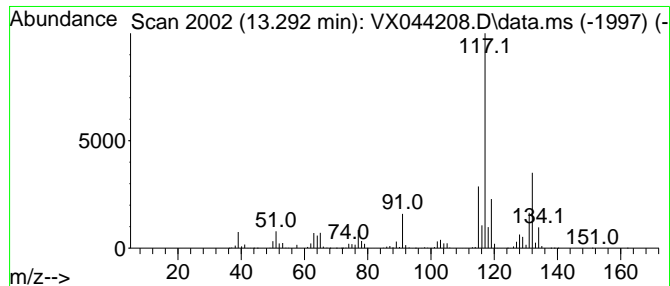
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 Quant Title : SW846 8260

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

 Peak Number 8 1-Phenyl-1-butene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	335.44 ug/l	3494820	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	89
3		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	89
4		Indan, 1-methyl-	132	C10H12	000767-58-8	76
5		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NP-WS-001

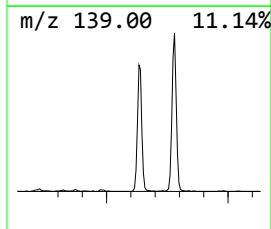
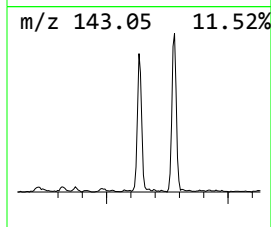
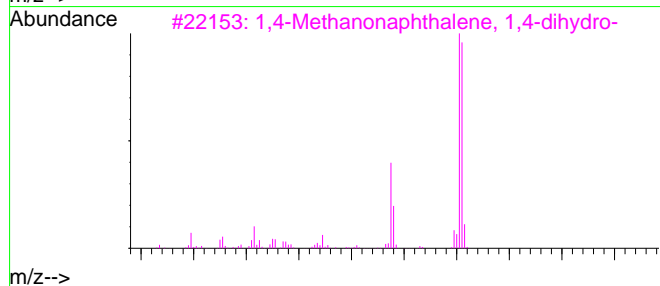
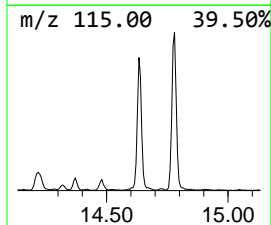
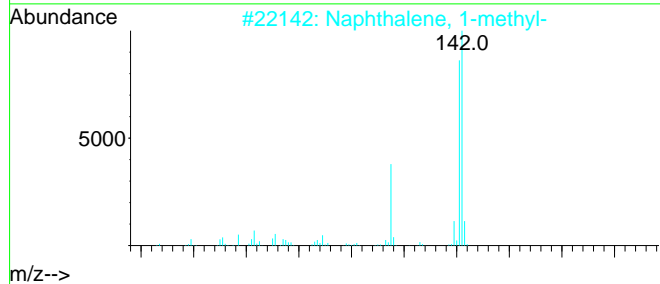
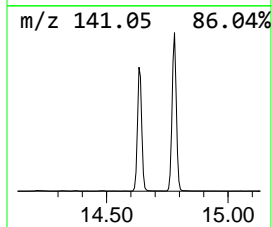
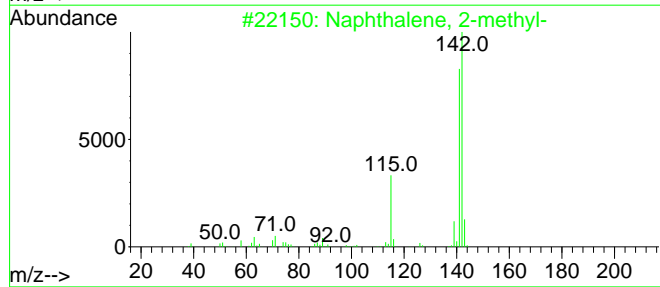
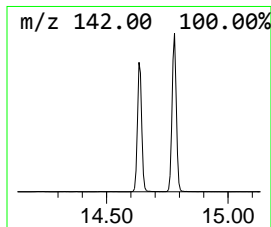
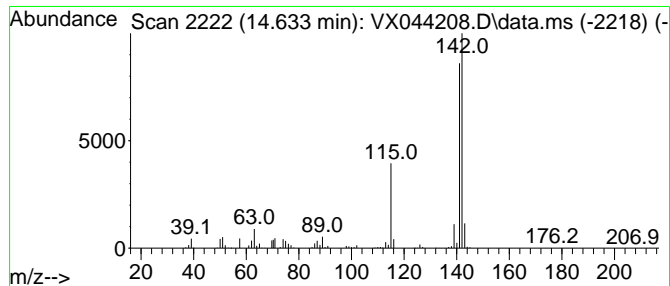
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 Quant Title : SW846 8260

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

 Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	109.43 ug/l	1140140	1,4-Dichlorobenzene-d4	12.024

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	94
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	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
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 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 NP-WS-001

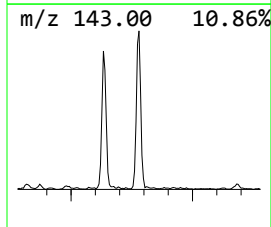
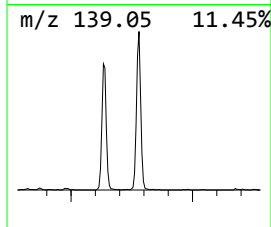
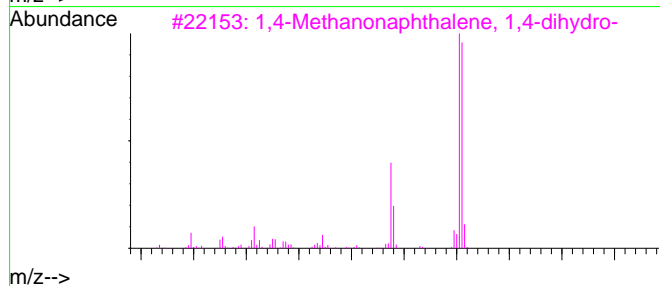
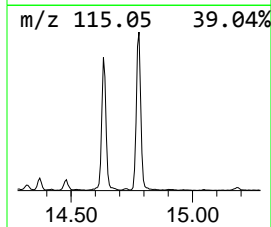
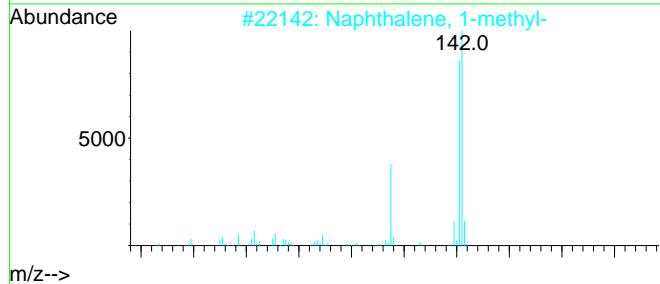
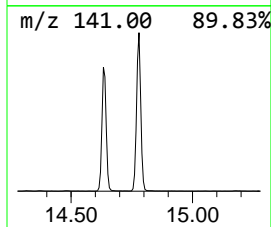
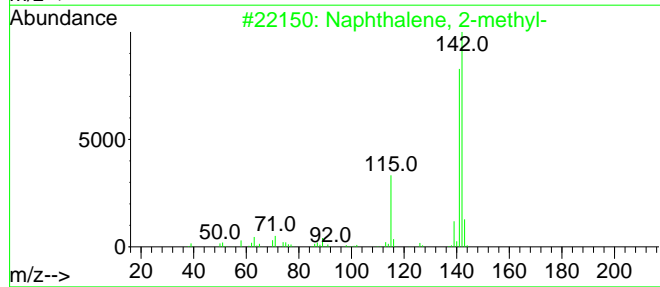
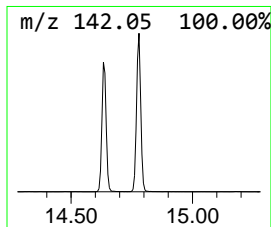
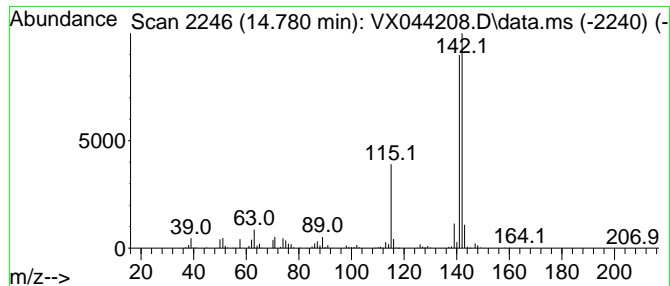
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 Quant Title : SW846 8260

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

 Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	129.63 ug/l	1350530	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	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121024\
 Data File : VX044208.D
 Acq On : 10 Dec 2024 15:13
 Operator : JC/MD
 Sample : P5224-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NP-WS-001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112124W.M
 Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, m...	4.294	153.9	ug/l	600506	1	5.550	195152	50.0
Hexane, 3-methyl-	5.818	49.6	ug/l	193689	1	5.550	195152	50.0
Indane	12.243	641.0	ug/l	6678150	4	12.024	520925	50.0
Benzene, 4-ethy...	12.615	259.5	ug/l	2703510	4	12.024	520925	50.0
Benzene, 1-ethe...	12.701	168.8	ug/l	1758900	4	12.024	520925	50.0
Benzene, 1,2,3,...	12.920	142.3	ug/l	1483060	4	12.024	520925	50.0
Benzene, 1-ethe...	13.170	139.6	ug/l	1453880	4	12.024	520925	50.0
1-Phenyl-1-butene	13.292	335.4	ug/l	3494820	4	12.024	520925	50.0
Naphthalene, 2-...	14.633	109.4	ug/l	1140140	4	12.024	520925	50.0
Naphthalene, 1-...	14.780	129.6	ug/l	1350530	4	12.024	520925	50.0