

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080840.D
 Acq On : 31 Jan 2024 15:08
 Operator : JC\MD
 Sample : P1279-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1255

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_N\methods\82N012924W.M
 Title : SW846 8260

Signal : TIC: VN080840.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.789	305	312	320	rBV3	7344	20087	2.54%	0.266%
2	4.712	459	469	470	rBV4	7652	16032	2.02%	0.212%
3	7.424	920	930	938	rBV2	13036	35632	4.50%	0.471%
4	7.783	983	991	998	rBV2	12383	28403	3.58%	0.375%
5	8.165	1045	1056	1061	rBV	79965	192399	24.28%	2.544%
6	8.224	1061	1066	1076	rVB2	132023	300129	37.88%	3.968%
7	8.577	1115	1126	1137	rBV2	93766	213069	26.89%	2.817%
8	9.100	1207	1215	1224	rBV	261424	523290	66.05%	6.918%
9	10.565	1456	1464	1471	rBV	349156	645576	81.48%	8.535%
10	10.630	1471	1475	1484	rVB	68529	128177	16.18%	1.695%
11	11.865	1678	1685	1697	rBV	416892	747251	94.32%	9.879%
12	12.071	1713	1720	1729	rBV2	45671	87207	11.01%	1.153%
13	12.400	1766	1776	1783	rBV	59389	96669	12.20%	1.278%
14	12.847	1845	1852	1860	rVB	259531	455939	57.55%	6.028%
15	13.100	1888	1895	1899	rVV	51034	95662	12.07%	1.265%
16	13.135	1899	1901	1904	rVV2	26126	28186	3.56%	0.373%
17	13.176	1904	1908	1913	rVB2	31829	49356	6.23%	0.652%
18	13.335	1928	1935	1944	rVB2	45775	78243	9.88%	1.034%
19	13.482	1954	1960	1966	rBV	65363	103047	13.01%	1.362%
20	13.670	1988	1992	1996	rVV5	10239	16463	2.08%	0.218%
21	13.794	2006	2013	2023	rVV2	384129	792286	100.00%	10.474%
22	13.876	2023	2027	2036	rVV2	61006	106823	13.48%	1.412%
23	13.953	2036	2040	2041	rVV4	13075	16675	2.10%	0.220%
24	13.994	2041	2047	2064	rVB4	69328	210198	26.53%	2.779%
25	14.123	2064	2069	2073	rBV5	6356	10990	1.39%	0.145%
26	14.182	2073	2079	2085	rVB2	21879	35240	4.45%	0.466%
27	14.247	2085	2090	2093	rBV3	40127	64012	8.08%	0.846%
28	14.276	2093	2095	2099	rVB2	27508	31533	3.98%	0.417%
29	14.329	2099	2104	2111	rVB2	44782	65816	8.31%	0.870%
30	14.400	2111	2116	2118	rBV3	15354	20918	2.64%	0.277%
31	14.447	2118	2124	2129	rVB2	58628	97587	12.32%	1.290%
32	14.576	2138	2146	2153	rVB4	24934	45094	5.69%	0.596%
33	14.653	2153	2159	2163	rBV2	35870	65424	8.26%	0.865%
34	14.694	2163	2166	2171	rVV2	52309	83706	10.57%	1.107%
35	14.735	2171	2173	2177	rVB4	10726	13330	1.68%	0.176%
36	14.882	2193	2198	2201	rBV5	7585	10278	1.30%	0.136%

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Peak Location: TOP

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

Peak separation: 5

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37	14.923	2201	2205	2211	rBV2	75195	130921	16.52%	1.731%
38	15.053	2218	2227	2234	rBV2	164579	363866	45.93%	4.810%
39	15.112	2234	2237	2243	rVB7	8810	16476	2.08%	0.218%
40	15.212	2247	2254	2261	rVV	161371	290920	36.72%	3.846%
41	15.317	2261	2272	2277	rVV6	37527	104629	13.21%	1.383%
42	15.364	2277	2280	2286	rVV5	29107	57653	7.28%	0.762%
43	15.441	2286	2293	2302	rVB4	42666	108423	13.68%	1.433%
44	15.641	2321	2327	2333	rVV	60958	126005	15.90%	1.666%
45	15.700	2333	2337	2342	rVV2	33076	64098	8.09%	0.847%
46	15.747	2342	2345	2346	rVV3	21692	24969	3.15%	0.330%
47	15.788	2349	2352	2367	rVB7	34929	95013	11.99%	1.256%
48	15.947	2372	2379	2388	rBV3	32096	63595	8.03%	0.841%
49	16.035	2388	2394	2398	rBV5	4057	8182	1.03%	0.108%
50	16.164	2401	2416	2426	rBV3	91414	258862	32.67%	3.422%
51	16.259	2428	2432	2435	rBV4	7330	12423	1.57%	0.164%
52	16.341	2439	2446	2447	rBV5	20140	32112	4.05%	0.425%
53	16.506	2464	2474	2484	rBV5	67810	154484	19.50%	2.042%
54	16.711	2507	2509	2515	rVB3	17729	23909	3.02%	0.316%
55	16.782	2515	2521	2522	rBV3	63020	96973	12.24%	1.282%

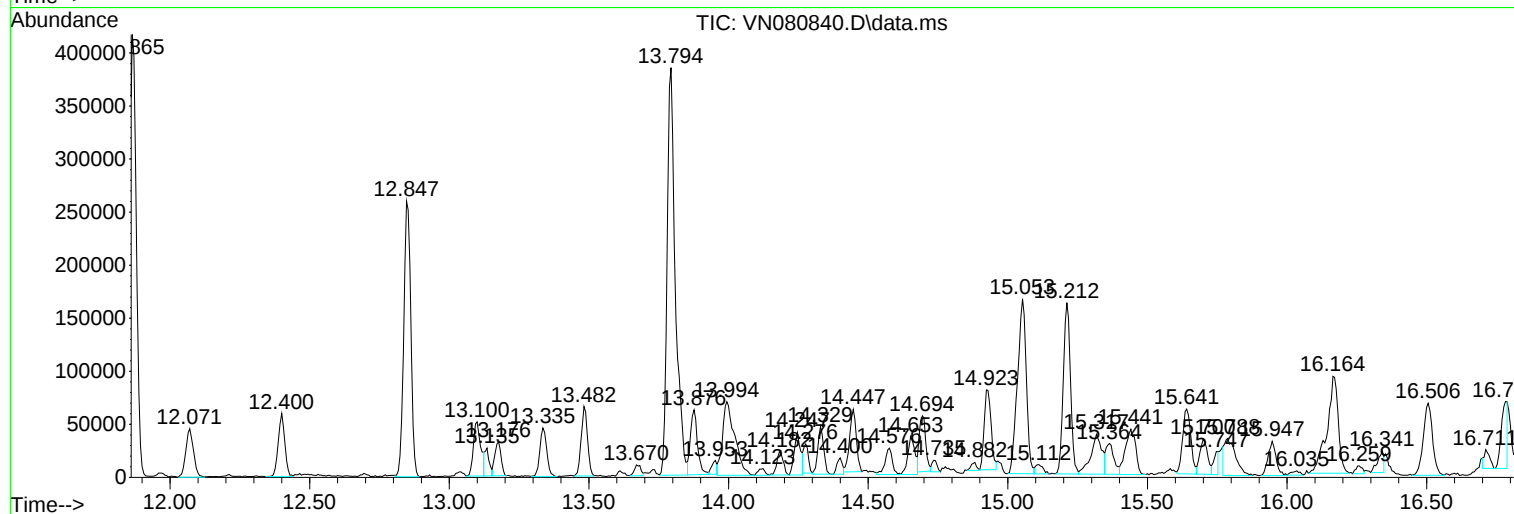
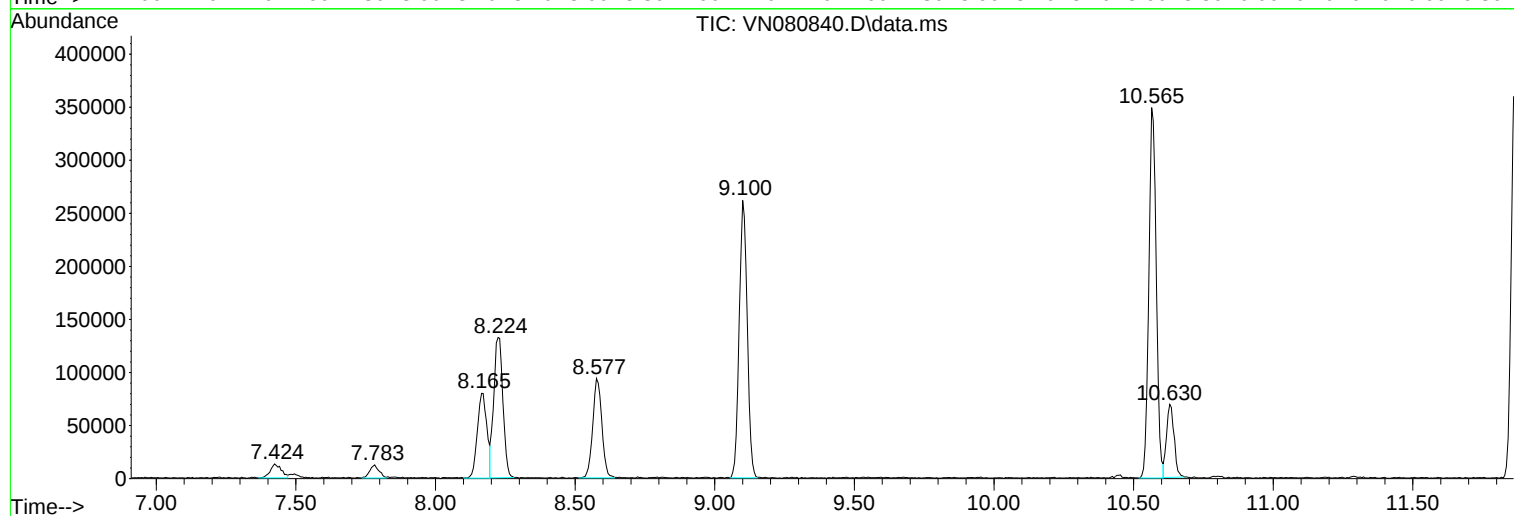
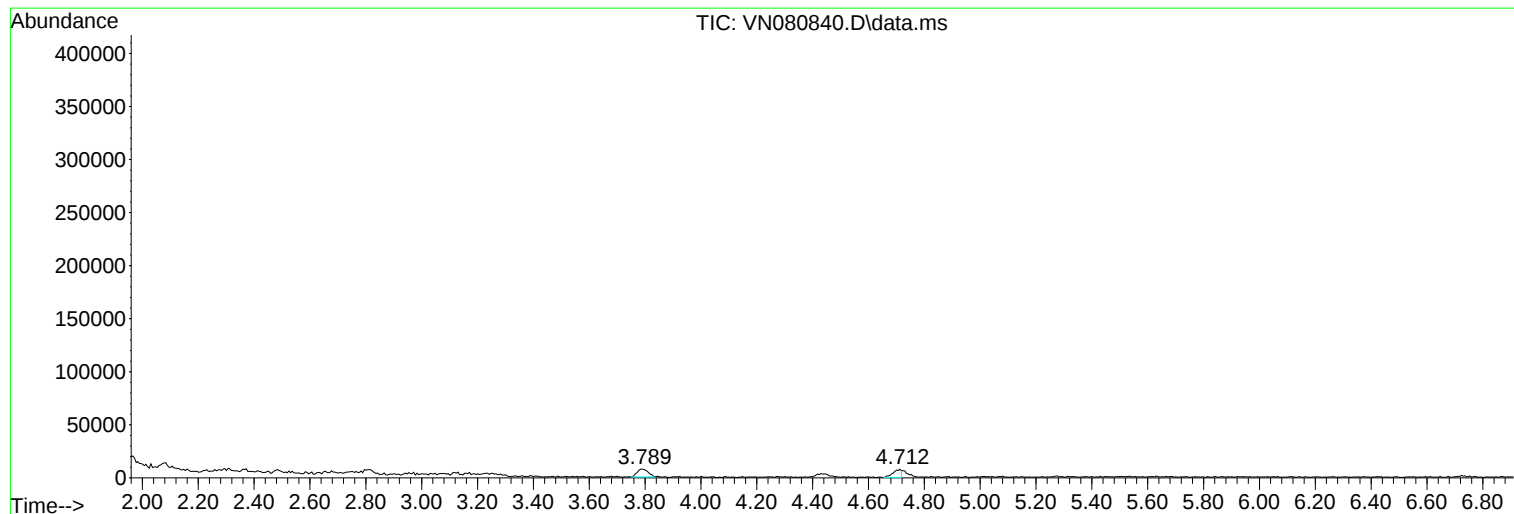
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Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
1255

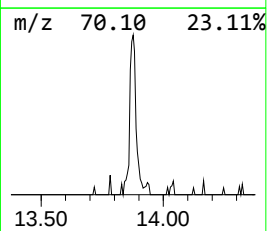
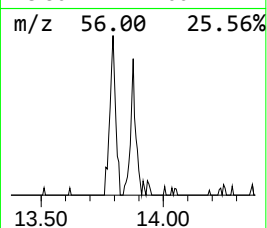
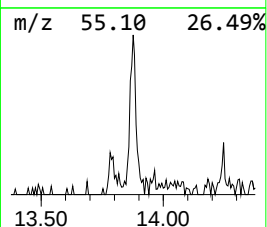
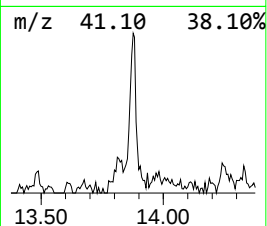
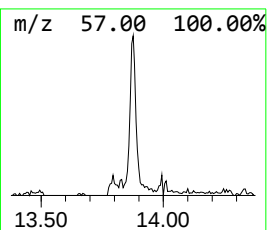
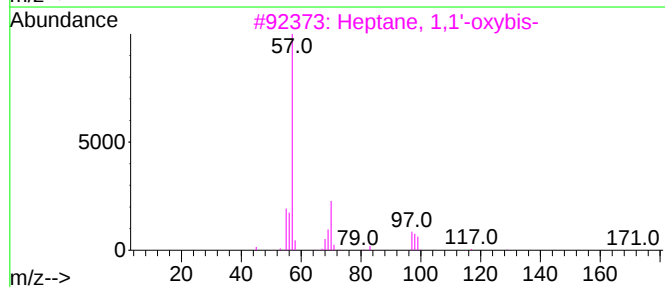
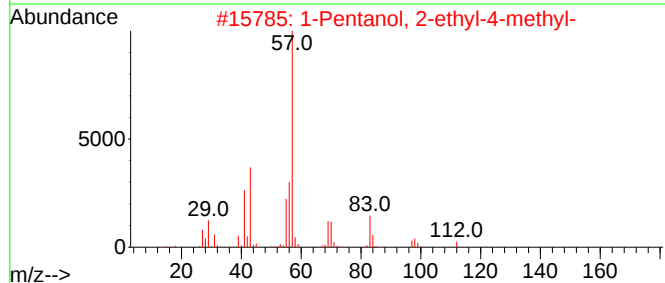
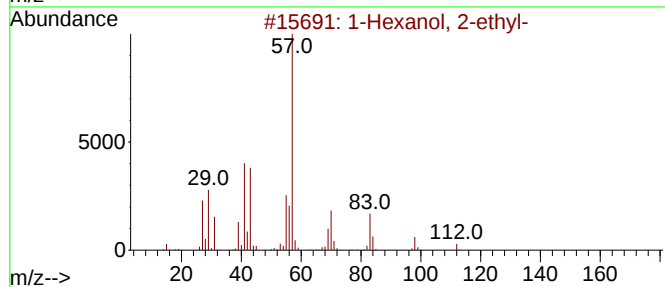
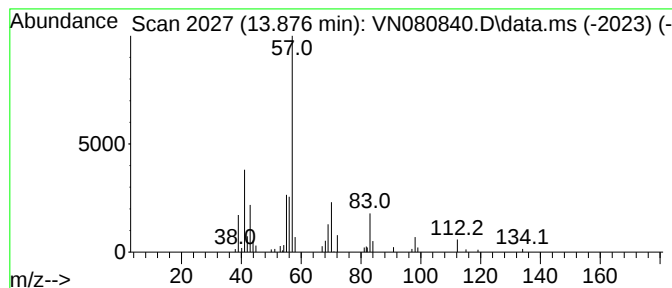
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	6.74 ug/l	106823	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4			2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	53
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	45



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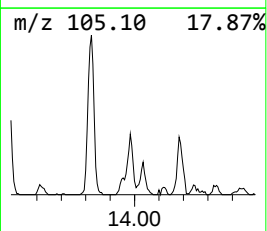
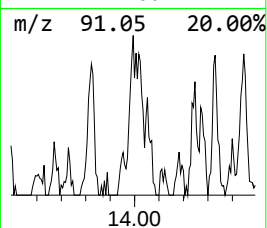
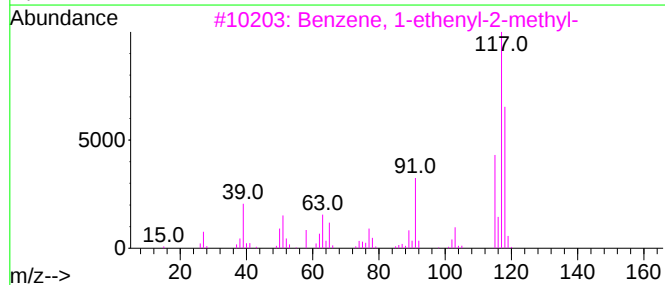
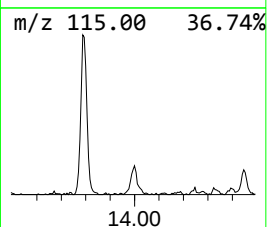
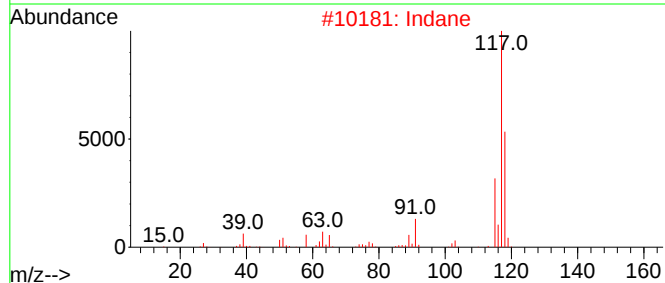
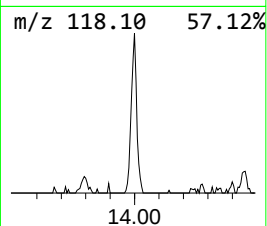
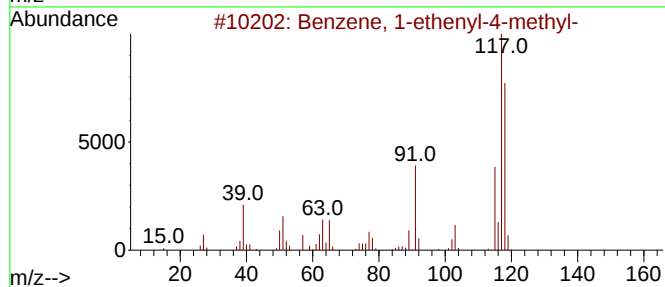
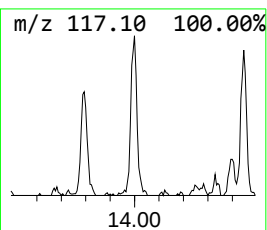
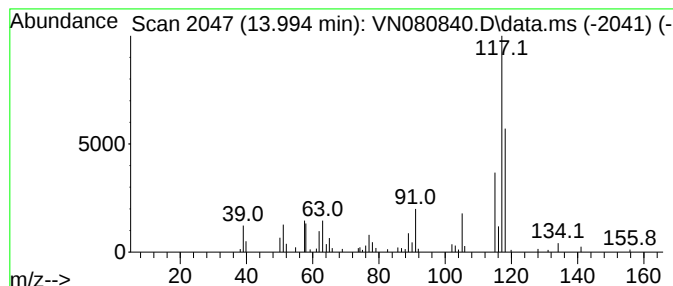
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethenyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	13.27 ug/l	210198	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	60
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

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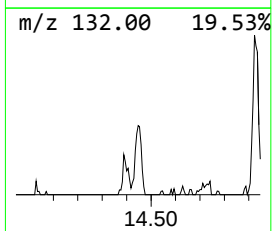
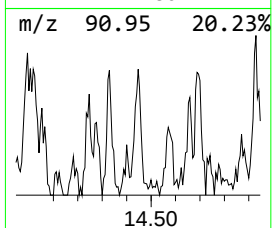
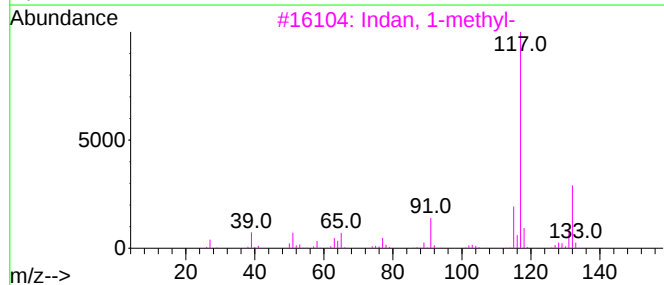
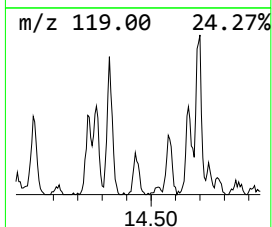
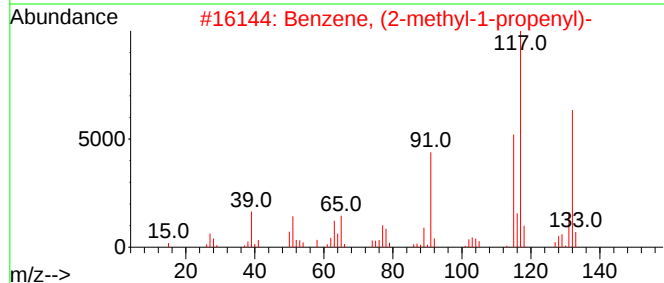
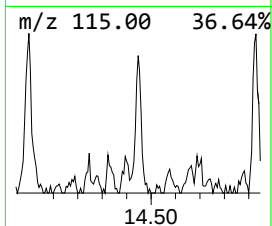
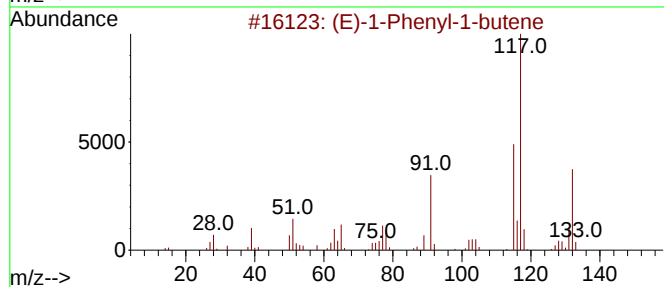
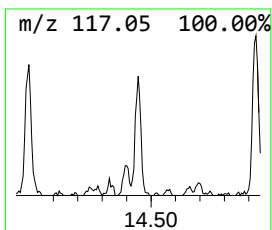
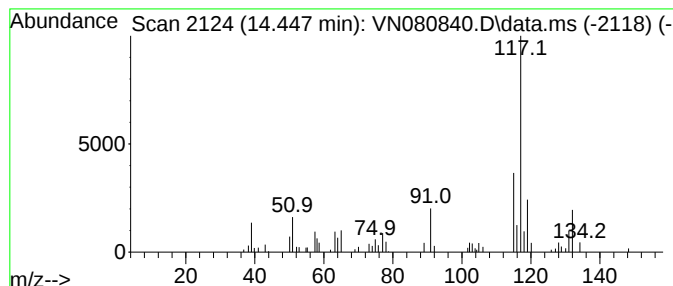
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (E)-1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	6.16 ug/l	97587	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	90
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81
3			Indan, 1-methyl-	132	C10H12	000767-58-8	81
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	74
5			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	74



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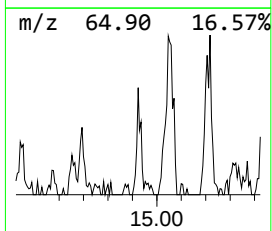
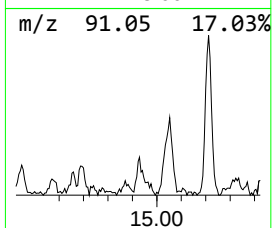
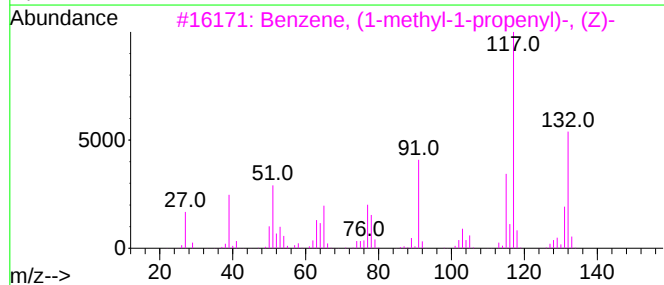
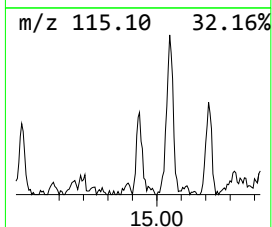
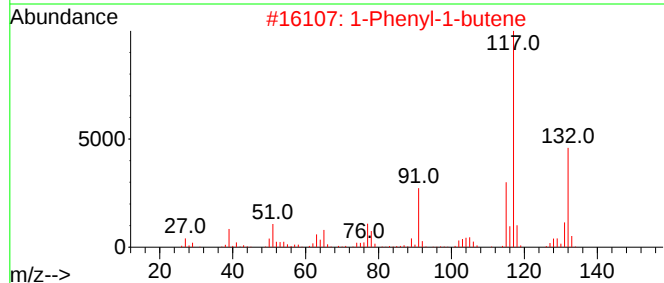
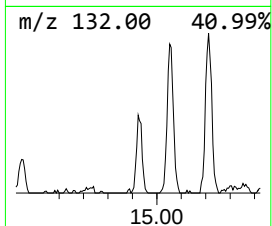
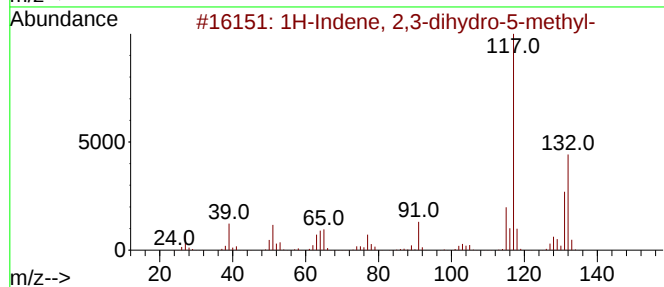
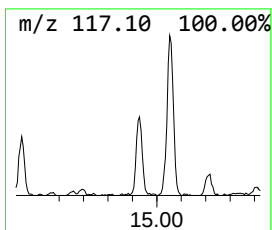
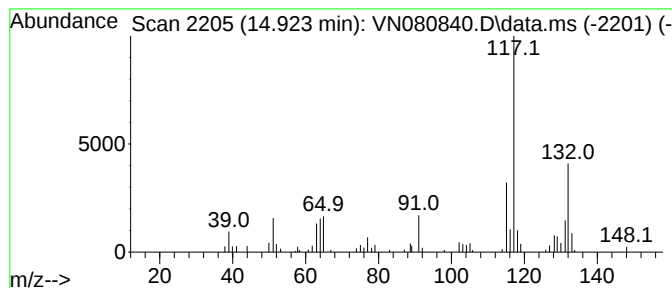
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.923	8.26 ug/l	130921	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	91
4		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91
5		(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	90



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1255

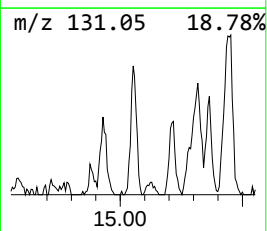
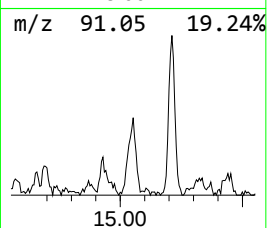
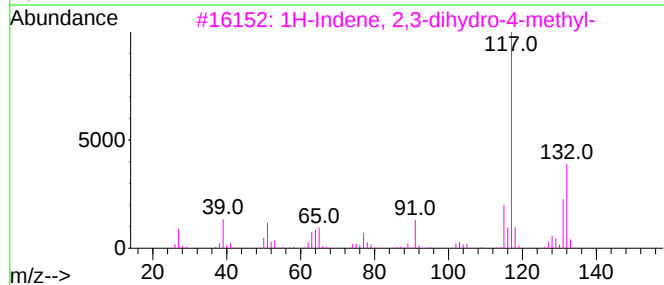
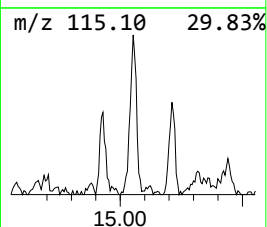
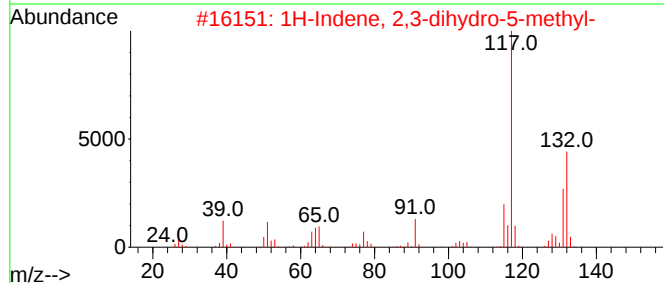
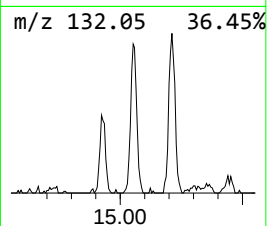
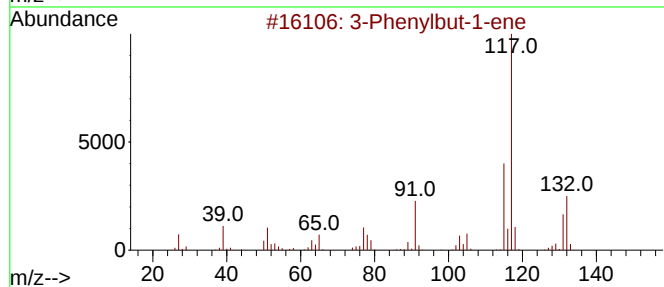
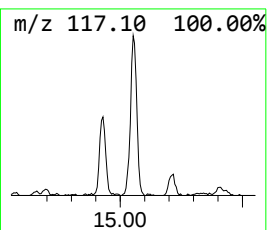
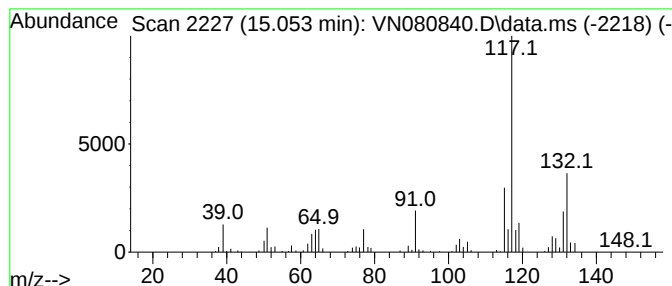
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Quant Title : SW846 8260

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

Peak Number 5 3-Phenylbut-1-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	22.96 ug/l	363866	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
5			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

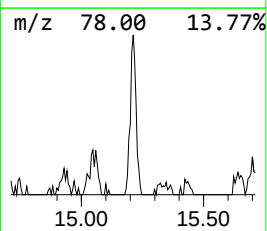
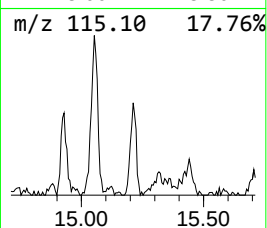
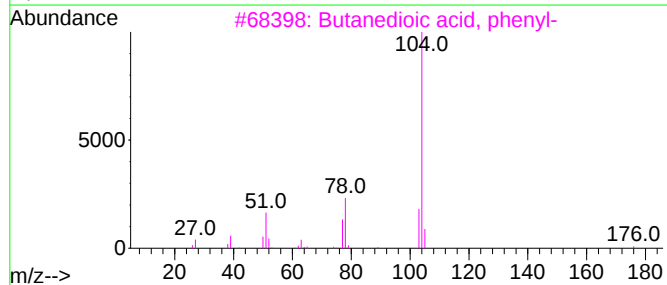
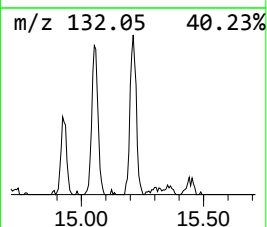
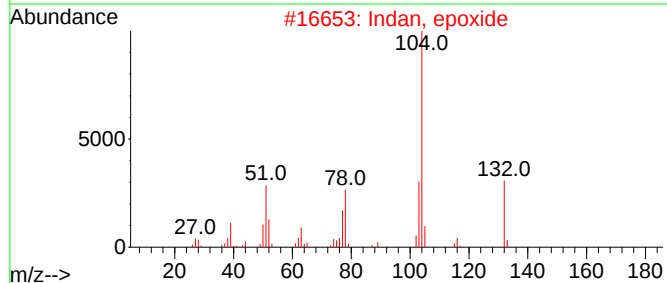
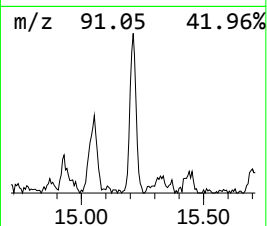
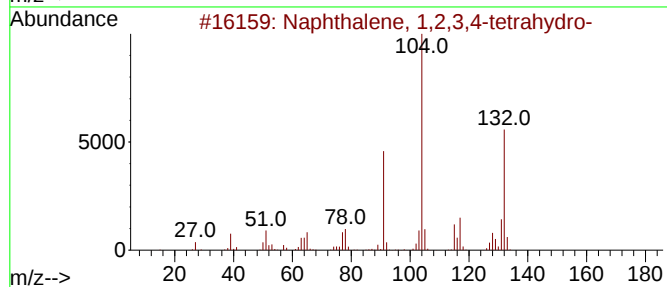
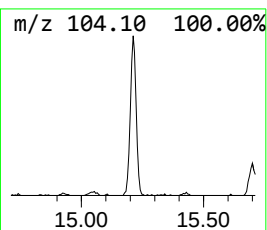
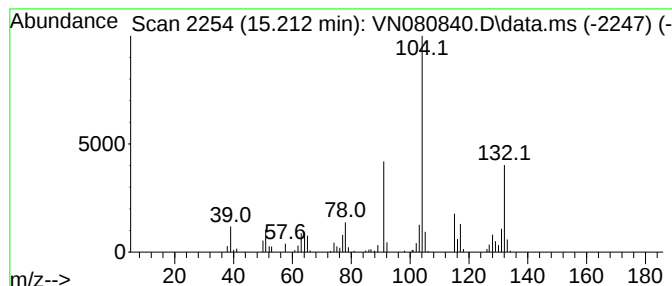
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	18.36 ug/l	290920	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			Indan, epoxide	132	C9H8O	000768-22-9	58
3			Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	38
4			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	38
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

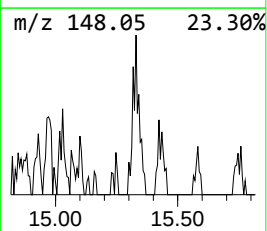
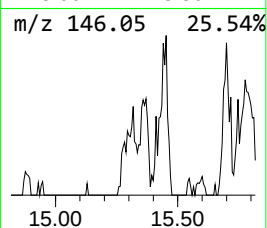
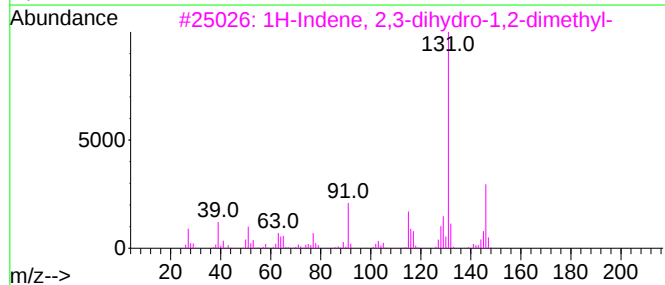
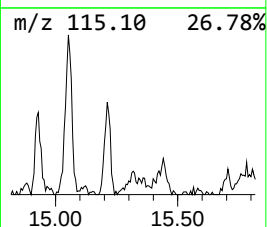
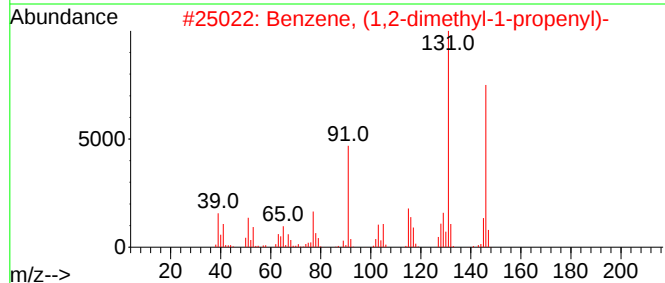
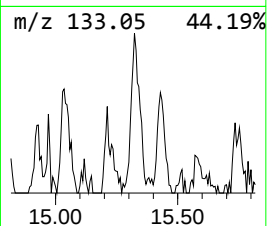
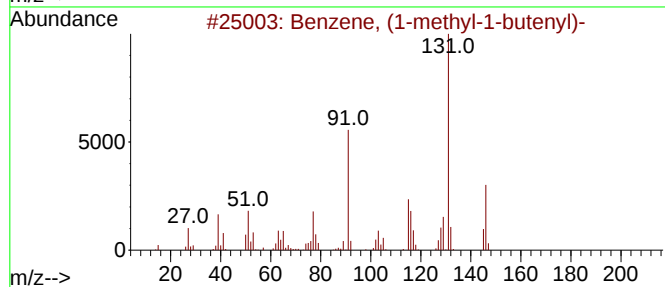
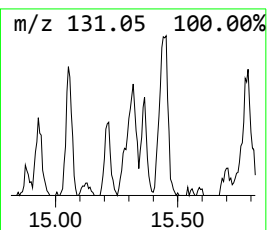
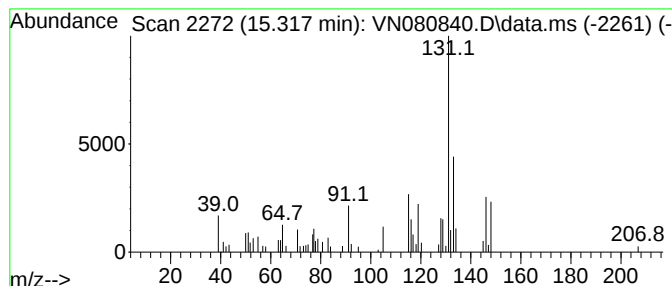
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, (1-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.317	6.60 ug/l	104629	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	60
2			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	60
3			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	60
4			Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	60
5			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

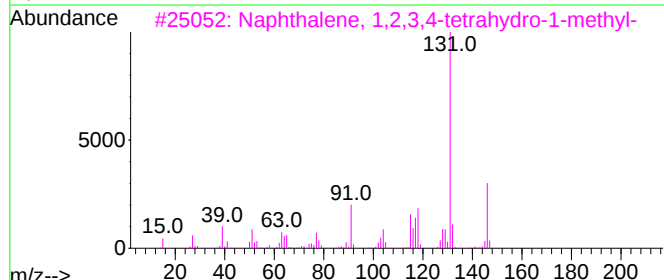
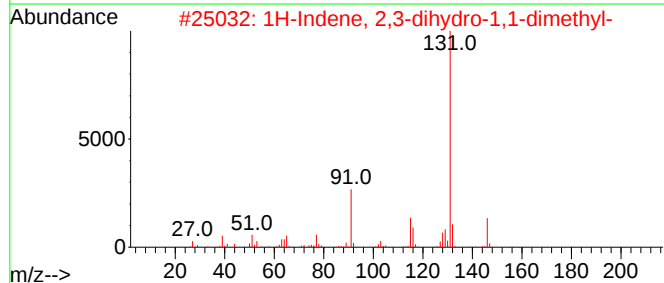
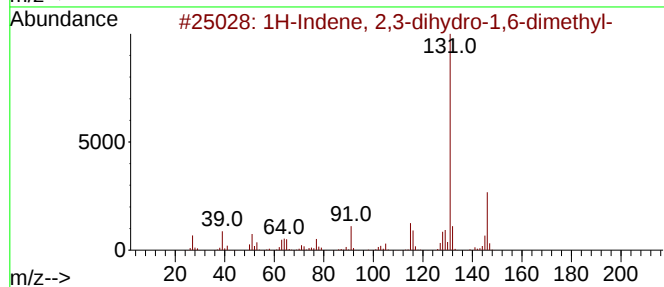
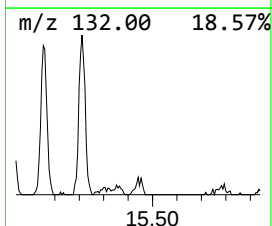
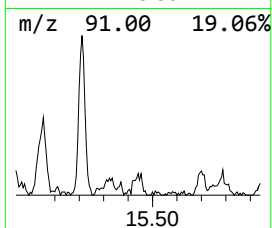
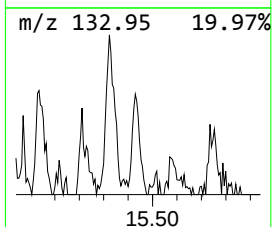
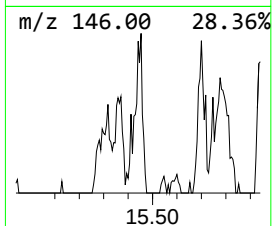
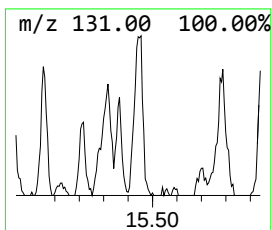
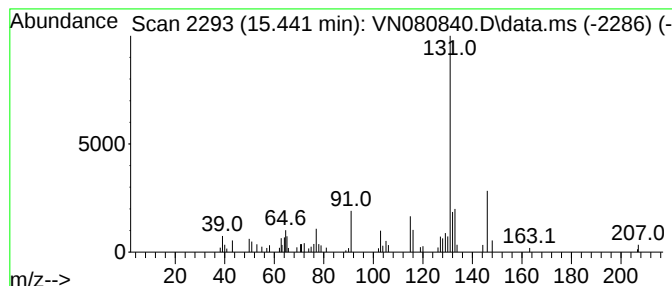
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	6.84 ug/l	108423	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	68
2			1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	64
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	64
4			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	59
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

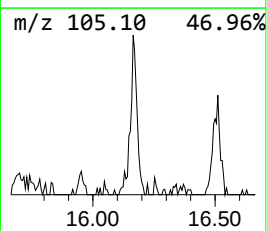
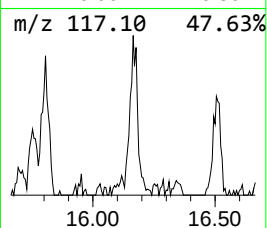
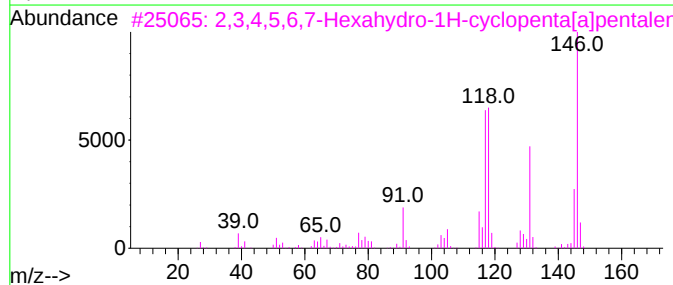
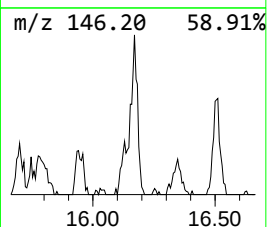
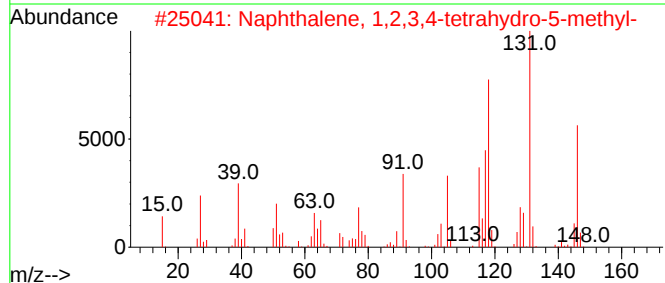
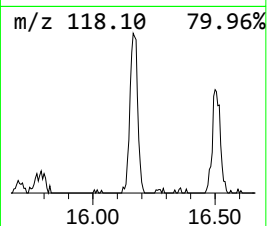
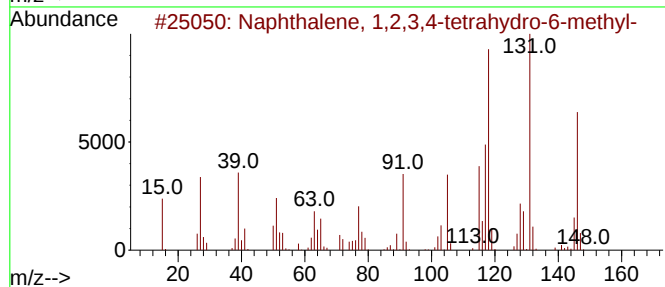
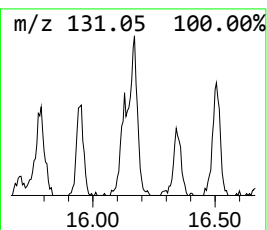
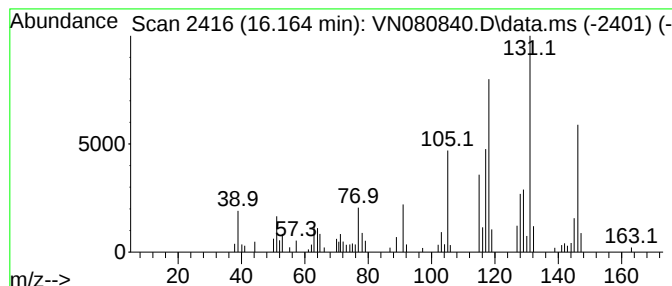
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	16.34 ug/l	258862	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	94
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	76
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

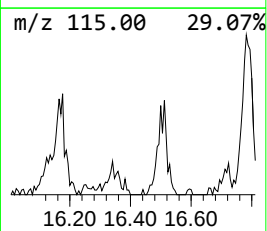
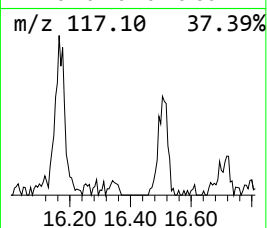
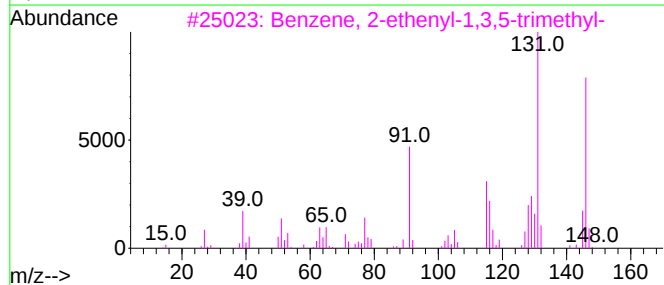
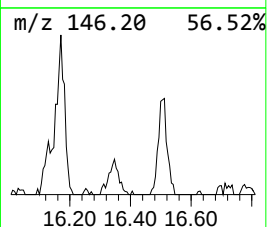
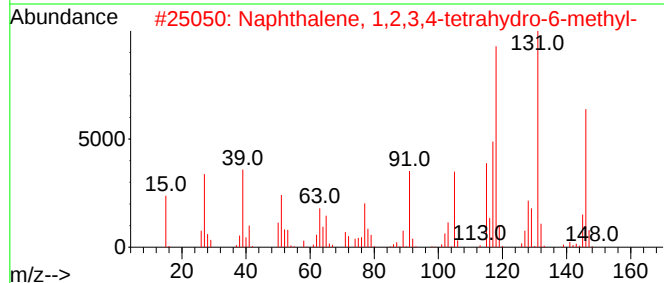
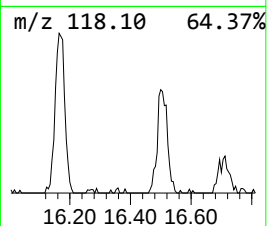
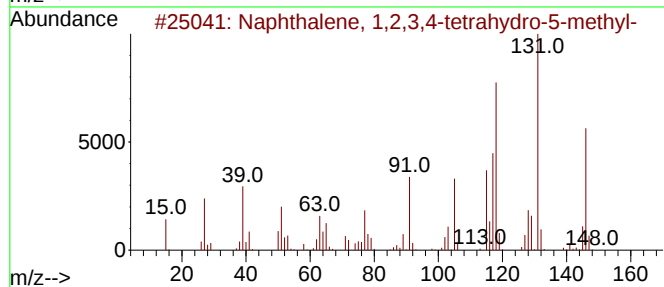
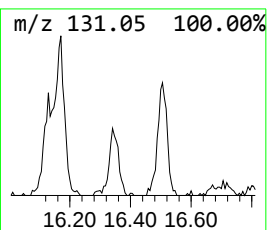
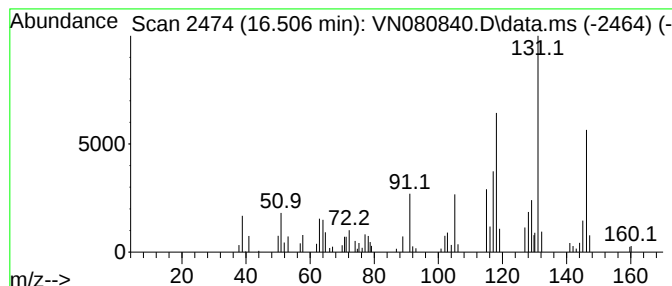
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.506	9.75 ug/l	154484	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	93
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	76
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	70
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080840.D
Acq On : 31 Jan 2024 15:08
Operator : JC\MD
Sample : P1279-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1255

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.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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Benzene, 1-ethe...	13.994	13.3	ug/l	210198	4	13.794	792286	50.0
(E)-1-Phenyl-1-...	14.447	6.2	ug/l	97587	4	13.794	792286	50.0
1H-Indene, 2,3-...	14.923	8.3	ug/l	130921	4	13.794	792286	50.0
3-Phenylbut-1-ene	15.053	23.0	ug/l	363866	4	13.794	792286	50.0
Naphthalene, 1,...	15.212	18.4	ug/l	290920	4	13.794	792286	50.0
Benzene, (1-met...	15.317	6.6	ug/l	104629	4	13.794	792286	50.0
1H-Indene, 2,3-...	15.441	6.8	ug/l	108423	4	13.794	792286	50.0
Naphthalene, 1,...	16.164	16.3	ug/l	258862	4	13.794	792286	50.0
Naphthalene, 1,...	16.506	9.8	ug/l	154484	4	13.794	792286	50.0