

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
 Data File : VN080500.D
 Acq On : 15 Dec 2023 14:00
 Operator : JC\MD
 Sample : 05829-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2

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\82N121223W.M
 Title : SW846 8260

Signal : TIC: VN080500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.247	211	220	236	rVB	228183	519781	3.82%	0.463%
2	3.647	277	288	299	rBV3	56975	151776	1.11%	0.135%
3	4.424	408	420	435	rBV3	65019	205831	1.51%	0.184%
4	5.277	552	565	568	rBV2	99933	295445	2.17%	0.263%
5	5.347	570	577	593	rVB3	163399	665616	4.89%	0.593%
6	5.812	638	656	671	rBV2	299475	1025769	7.53%	0.915%
7	6.653	784	799	811	rBV	108774	321049	2.36%	0.286%
8	6.794	811	823	836	rBV3	78022	251414	1.85%	0.224%
9	7.083	862	872	887	rBV3	94027	289349	2.12%	0.258%
10	7.330	903	914	923	rBV2	392328	1142149	8.39%	1.018%
11	8.006	1022	1029	1037	rVB	129188	324516	2.38%	0.289%
12	8.165	1047	1056	1061	rBV	181255	452917	3.33%	0.404%
13	8.229	1061	1067	1079	rVV3	405806	1337156	9.82%	1.192%
14	8.329	1079	1084	1094	rVB3	148475	375224	2.76%	0.335%
15	8.447	1096	1104	1111	rBV	119543	274257	2.01%	0.245%
16	8.606	1120	1131	1142	rVB2	511863	1419688	10.42%	1.266%
17	8.724	1142	1151	1156	rVV5	189980	555398	4.08%	0.495%
18	8.788	1156	1162	1168	rVV4	268436	710722	5.22%	0.634%
19	8.859	1168	1174	1182	rVV2	100447	237139	1.74%	0.211%
20	8.941	1182	1188	1200	rVB3	55417	148457	1.09%	0.132%
21	9.100	1206	1215	1222	rBV2	707344	1696572	12.46%	1.513%
22	9.335	1248	1255	1259	rBV2	109861	217264	1.60%	0.194%
23	9.382	1259	1263	1272	rVB	126966	253640	1.86%	0.226%
24	9.565	1283	1294	1295	rBV	181428	279960	2.06%	0.250%
25	9.600	1296	1300	1316	rVB	313206	709997	5.21%	0.633%
26	9.776	1323	1330	1337	rVB	89202	171504	1.26%	0.153%
27	9.941	1351	1358	1360	rBV2	72467	144846	1.06%	0.129%
28	10.012	1366	1370	1378	rVB4	84756	178508	1.31%	0.159%
29	10.100	1378	1385	1390	rBV	307100	594565	4.37%	0.530%
30	10.153	1390	1394	1405	rVB5	140799	302024	2.22%	0.269%
31	10.453	1439	1445	1450	rBV	194318	336054	2.47%	0.300%
32	10.571	1457	1465	1471	rBV	725188	1366428	10.03%	1.218%
33	10.759	1488	1497	1503	rVV4	97269	238946	1.75%	0.213%
34	10.982	1529	1535	1546	rVB3	220858	541548	3.98%	0.483%
35	11.865	1678	1685	1692	rBV	710537	1286881	9.45%	1.147%
36	11.965	1692	1702	1711	rVV	5375473	9033344	66.33%	8.054%

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

Peak separation: 5

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37	12.076	1711	1721	1734	rVB	6325528	11643938	85.50%	10.382%
38	12.400	1767	1776	1785	rBV	175076	319160	2.34%	0.285%
39	12.694	1817	1826	1833	rVB	538394	877868	6.45%	0.783%
40	12.847	1842	1852	1862	rVB	495618	887873	6.52%	0.792%
41	13.035	1878	1884	1889	rBV	938883	1508525	11.08%	1.345%
42	13.100	1889	1895	1897	rVV	1003664	1641320	12.05%	1.463%
43	13.129	1897	1900	1904	rVV	1772399	2916764	21.42%	2.601%
44	13.176	1904	1908	1916	rVB	2178571	3448256	25.32%	3.074%
45	13.335	1927	1935	1946	rBV	2509904	4142621	30.42%	3.694%
46	13.482	1946	1960	1967	rBV	8301173	13618947	100.00%	12.142%
47	13.612	1974	1982	1988	rVB3	74375	185951	1.37%	0.166%
48	13.676	1988	1993	1997	rBV	87464	137567	1.01%	0.123%
49	13.823	2006	2018	2027	rBV2	2823671	5884483	43.21%	5.247%
50	13.953	2033	2040	2042	rBV	702122	1049617	7.71%	0.936%
51	13.994	2042	2047	2063	rVB2	4374770	8946365	65.69%	7.976%
52	14.117	2063	2068	2073	rBV	148045	223305	1.64%	0.199%
53	14.182	2073	2079	2084	rBV2	456995	762400	5.60%	0.680%
54	14.247	2084	2090	2092	rVV	610186	961410	7.06%	0.857%
55	14.276	2092	2095	2099	rVV	523939	773834	5.68%	0.690%
56	14.329	2099	2104	2110	rVV	1623721	2530817	18.58%	2.256%
57	14.400	2110	2116	2119	rVV	339003	572704	4.21%	0.511%
58	14.447	2119	2124	2133	rVB2	1485276	2494150	18.31%	2.224%
59	14.576	2141	2146	2152	rVB2	303017	486233	3.57%	0.434%
60	14.653	2152	2159	2163	rBV	1046418	1781189	13.08%	1.588%
61	14.694	2163	2166	2171	rVV	1124609	1670211	12.26%	1.489%
62	14.929	2201	2206	2211	rBV	1061194	1677401	12.32%	1.496%
63	15.053	2218	2227	2233	rBV2	1908147	4053638	29.76%	3.614%
64	15.117	2233	2238	2247	rVB3	227640	452734	3.32%	0.404%
65	15.211	2247	2254	2261	rBV3	361632	686866	5.04%	0.612%
66	15.317	2261	2272	2278	rBV4	379381	1006178	7.39%	0.897%
67	15.441	2285	2293	2301	rVB3	321643	810028	5.95%	0.722%
68	15.641	2319	2327	2335	rVB	2119318	4037321	29.64%	3.600%
69	15.747	2339	2345	2351	rVV2	161049	326929	2.40%	0.291%
70	15.805	2351	2355	2367	rVB	92743	203345	1.49%	0.181%
71	15.947	2370	2379	2389	rBV	153629	313399	2.30%	0.279%
72	16.129	2399	2410	2419	rBV3	88600	292057	2.14%	0.260%
73	16.347	2438	2447	2454	rVB5	58612	165550	1.22%	0.148%
74	16.782	2514	2521	2522	rBV	410519	613027	4.50%	0.547%

Sum of corrected areas: 112159715

Instrument :

MSVOA_N

ClientSampleId :

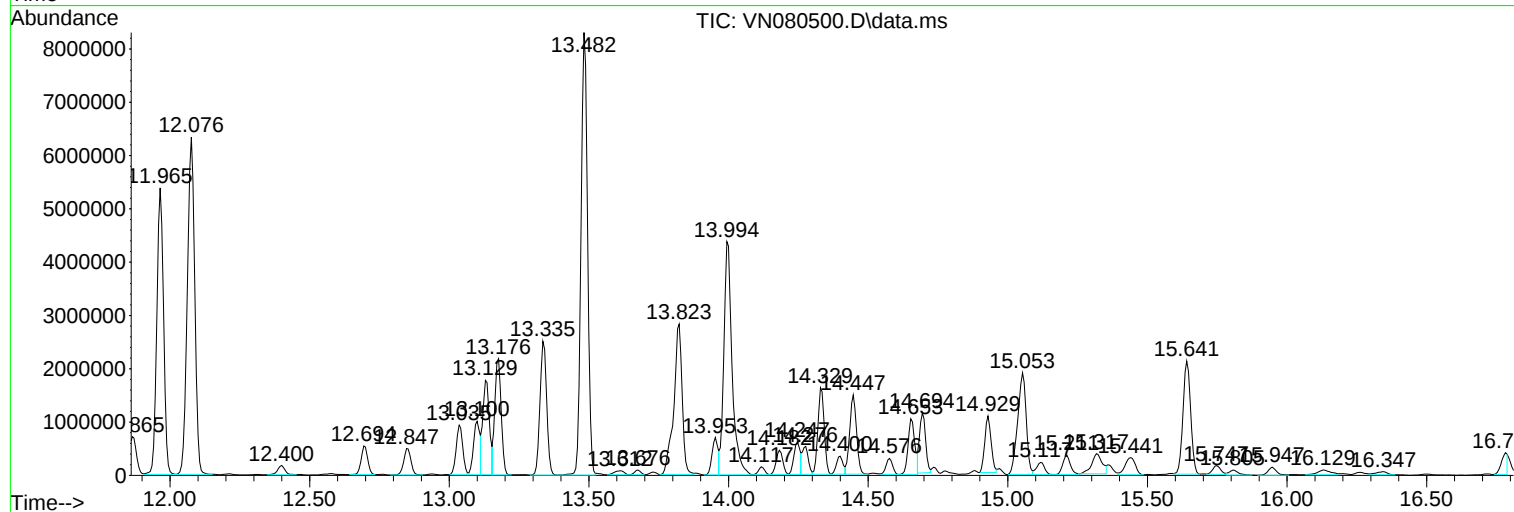
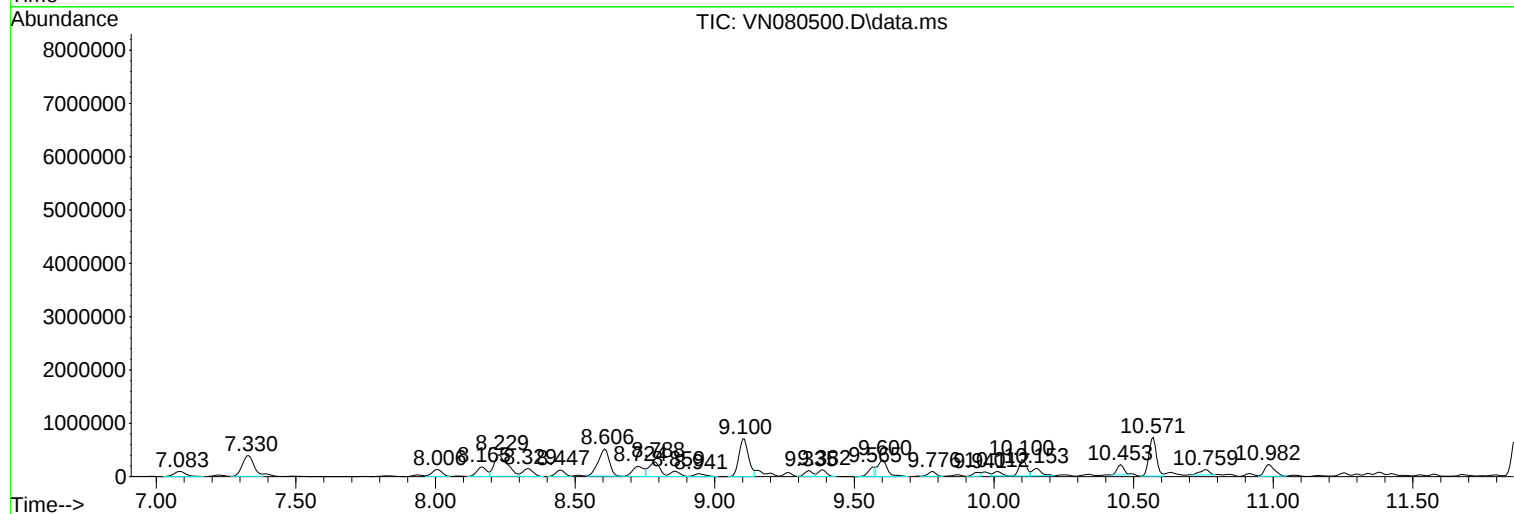
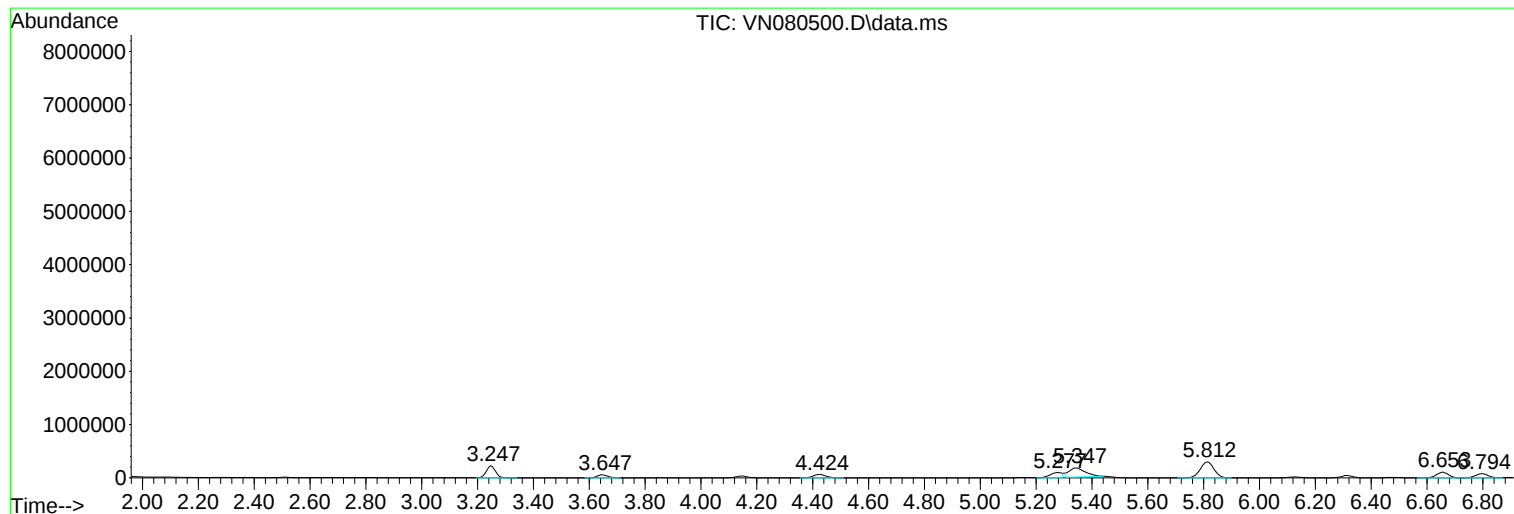
MW-2

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Instrument :
MSVOA_N
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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Data File : VN080500.D
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Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

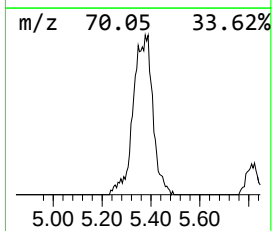
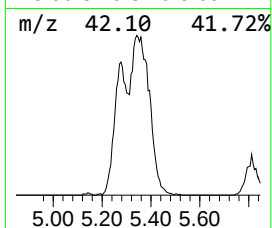
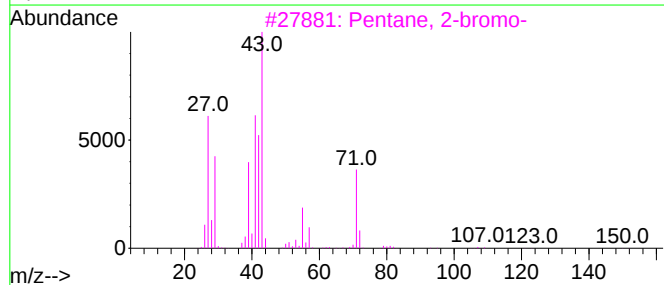
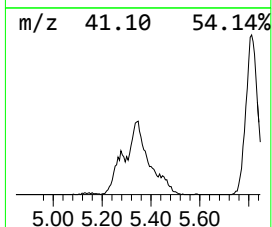
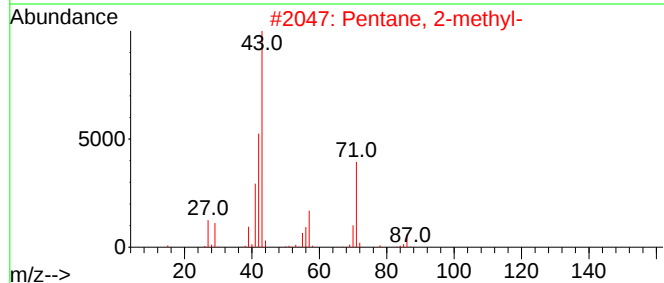
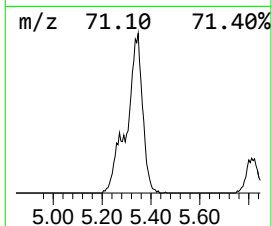
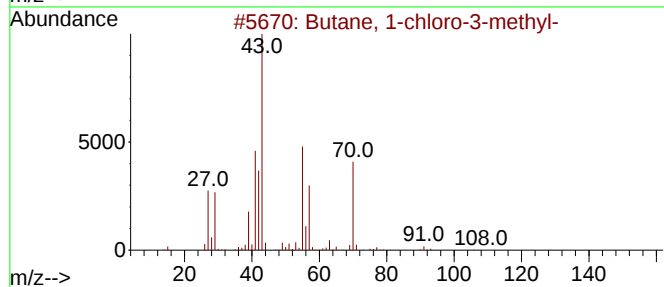
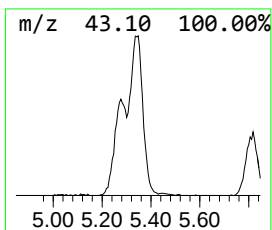
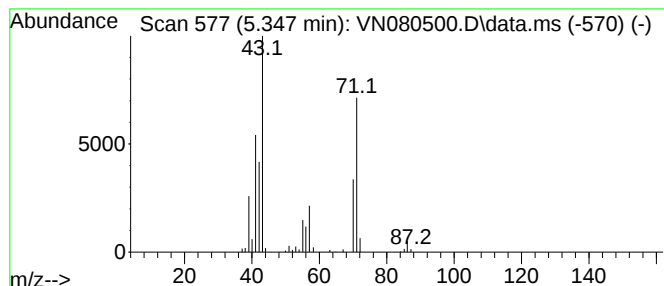
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown5.347 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.347	24.89 ug/l	665616	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	47
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	36
4			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	33
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	33



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Instrument :
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ClientSampleId :
MW-2

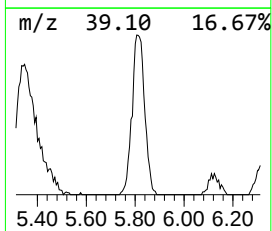
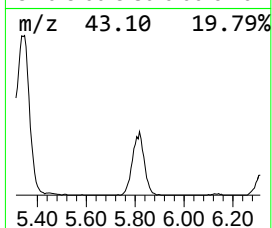
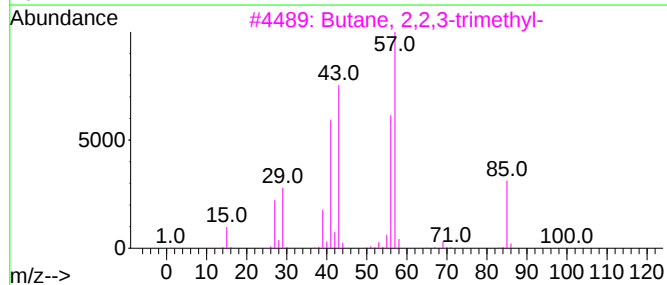
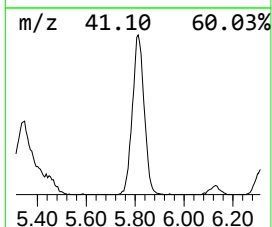
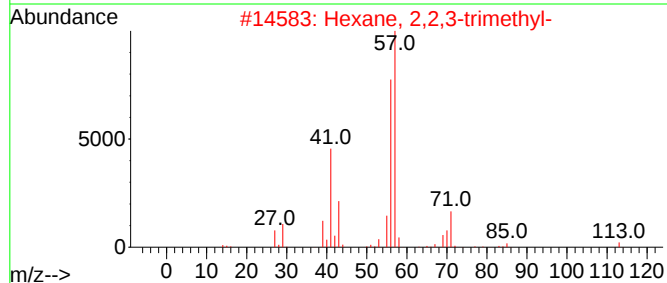
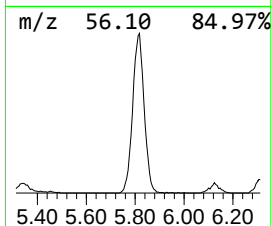
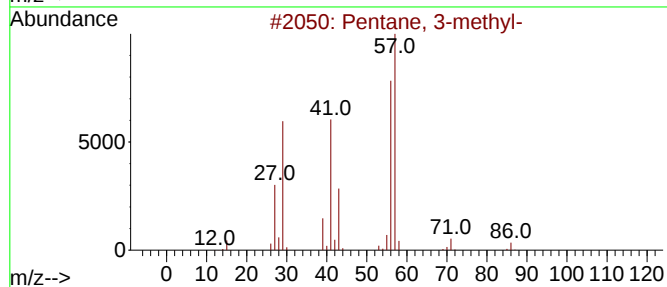
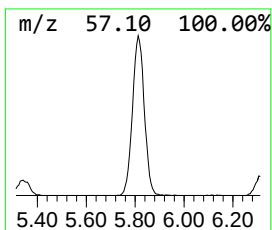
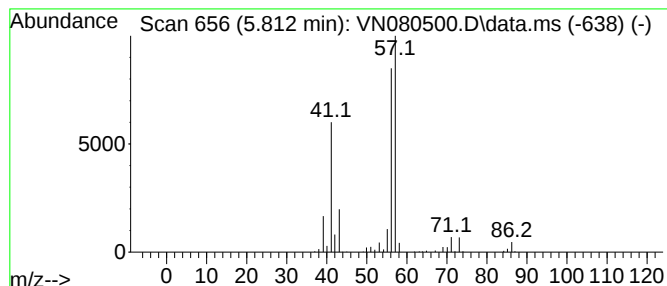
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	38.36 ug/l	1025770	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
4			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	40
5			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



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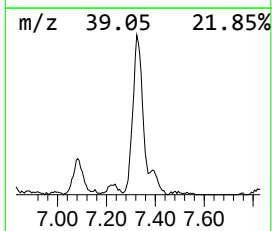
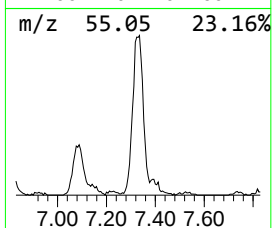
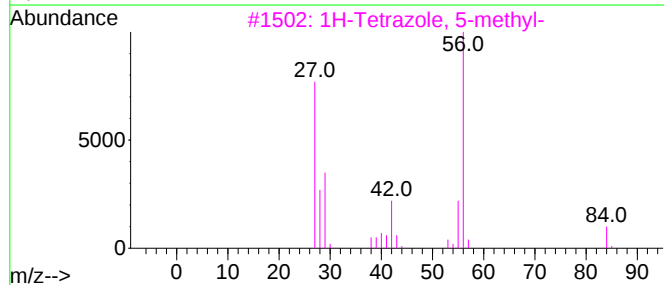
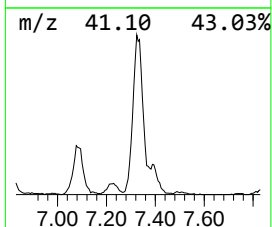
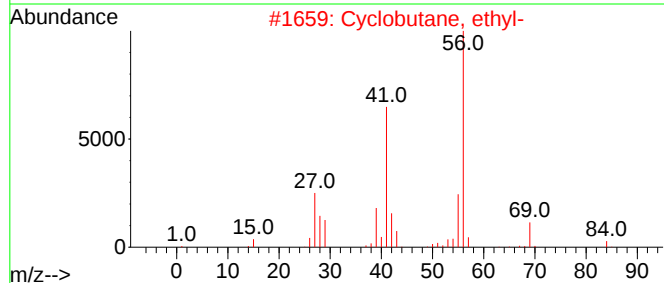
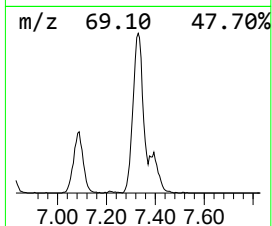
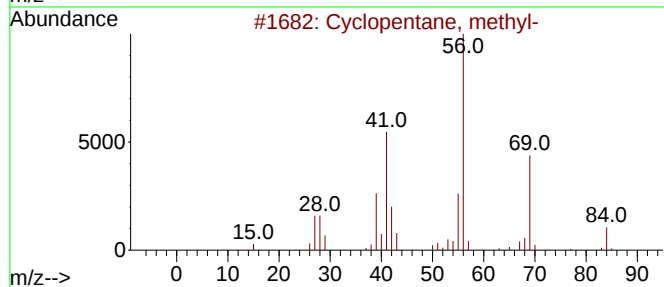
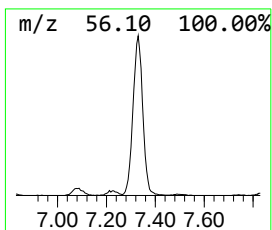
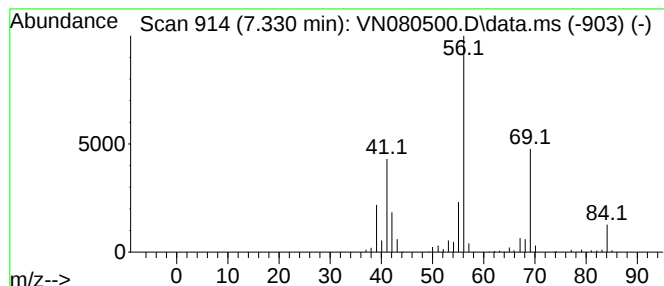
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.330	42.71 ug/l	1142150	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	86
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	59
5			Cyclohexane	84	C6H12	000110-82-7	52



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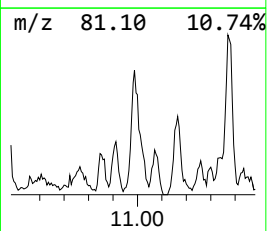
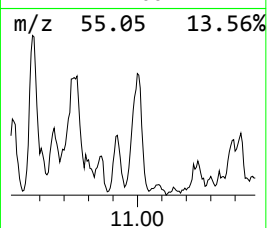
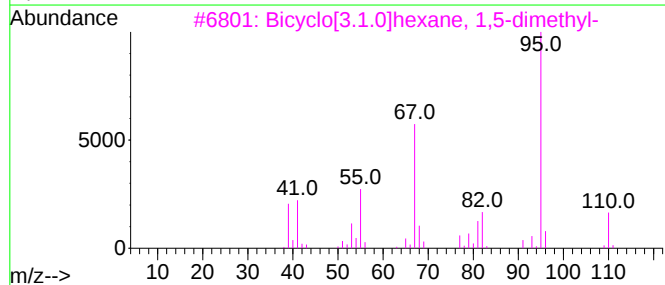
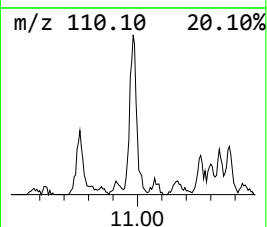
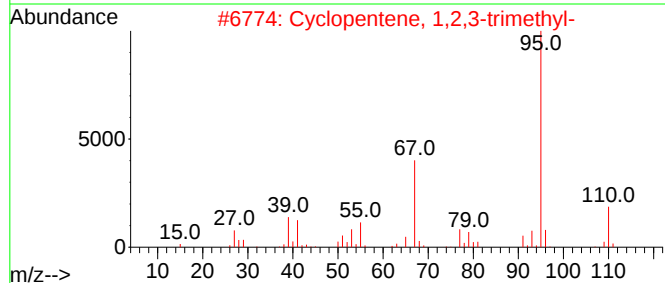
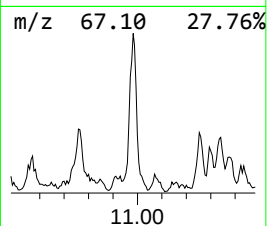
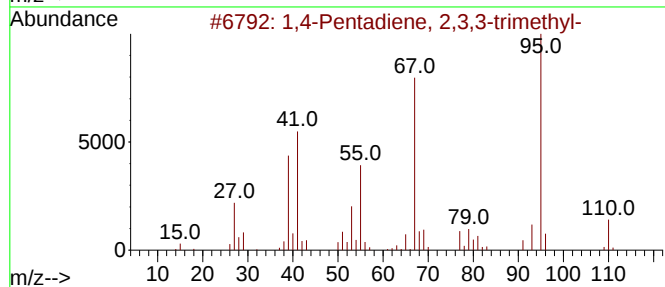
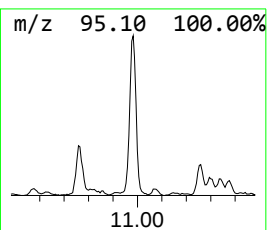
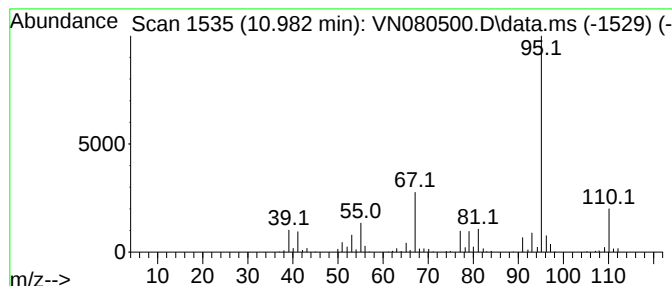
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Quant Title : SW846 8260

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

Peak Number 4 1,4-Pentadiene, 2,3,3-trime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.982	21.04 ug/l	541548	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	81
2			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	76
3			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	74
4			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	72
5			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

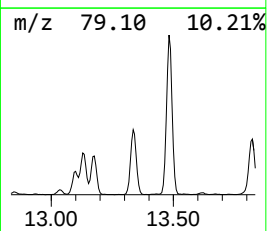
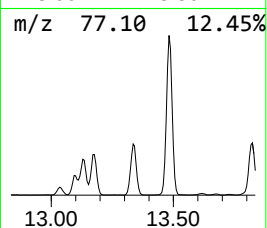
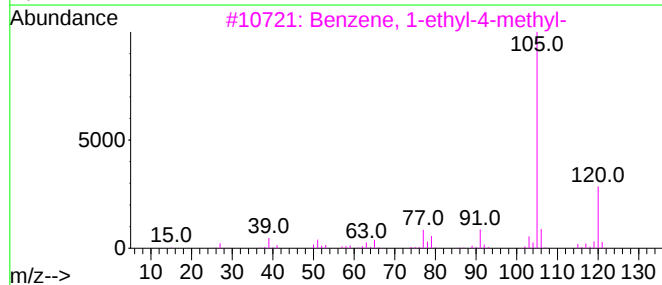
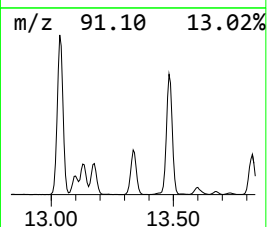
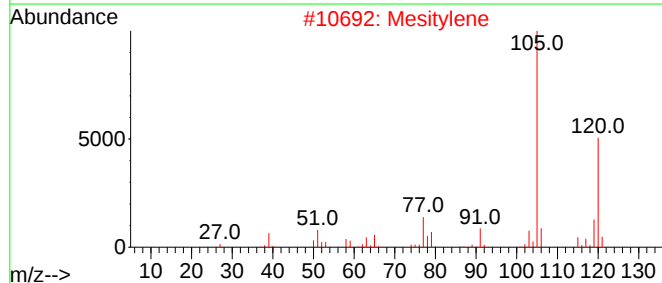
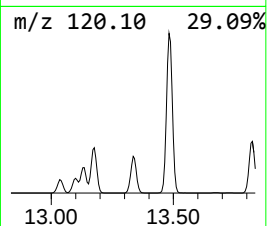
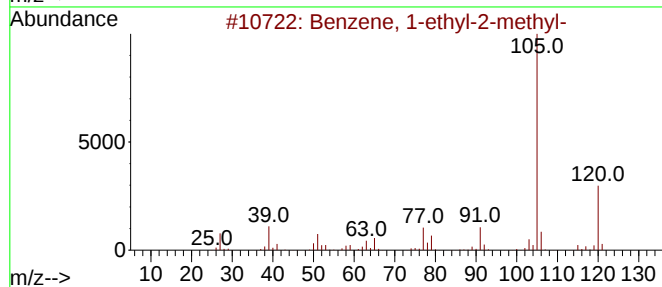
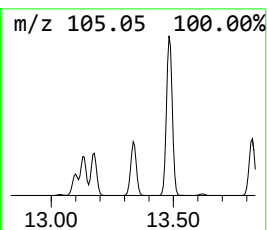
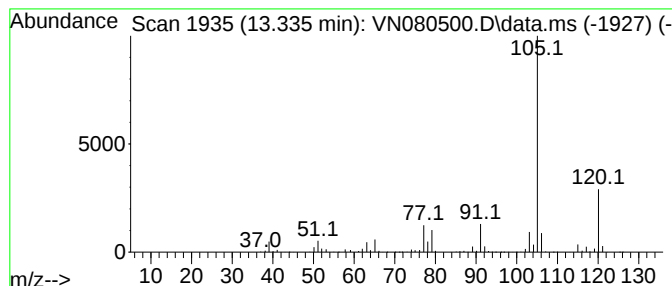
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	35.20 ug/l	4142620	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Mesitylene	120	C9H12	000108-67-8	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

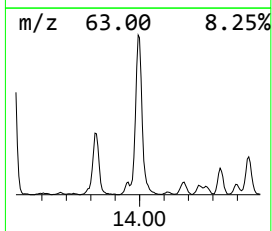
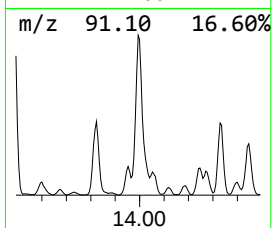
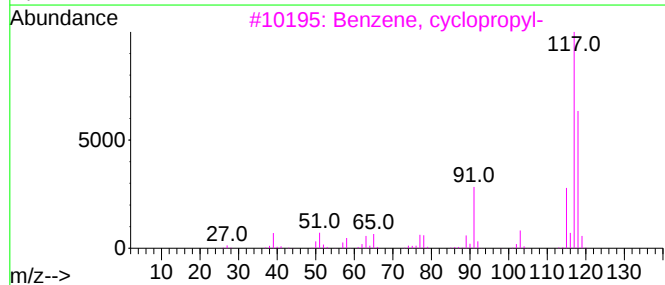
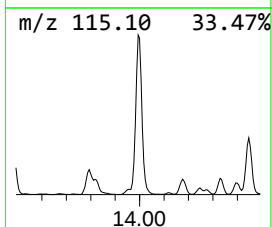
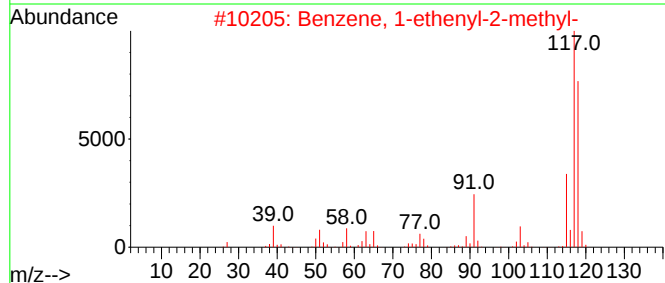
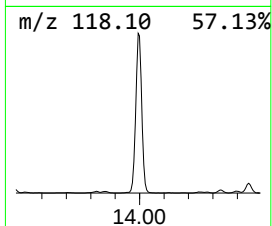
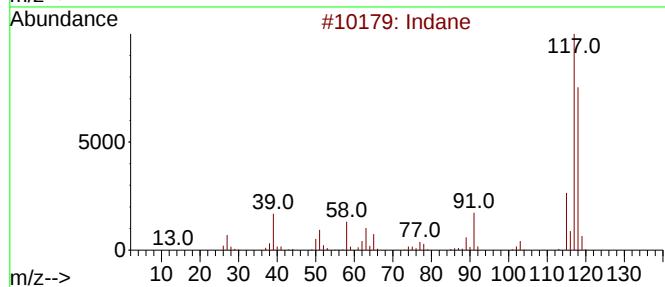
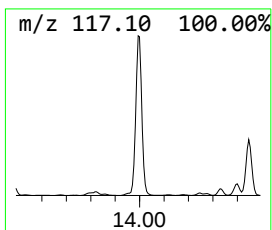
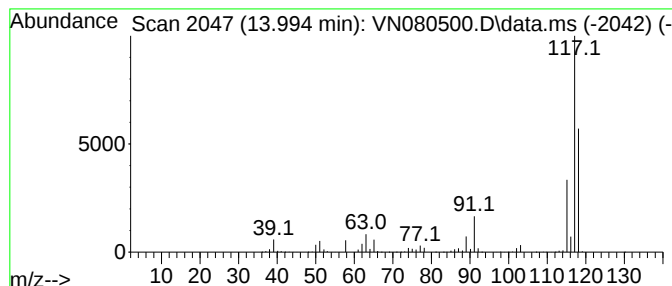
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	76.02 ug/l	8946370	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	59
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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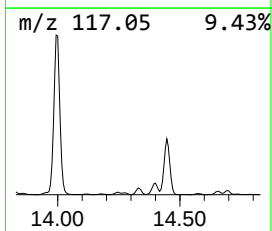
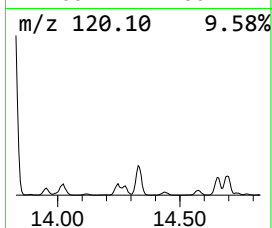
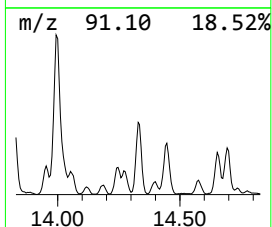
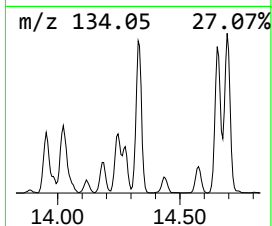
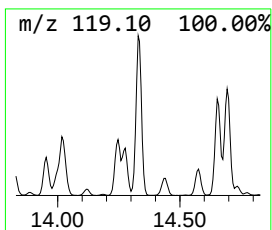
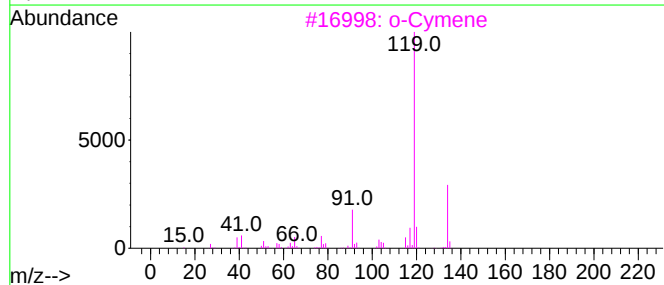
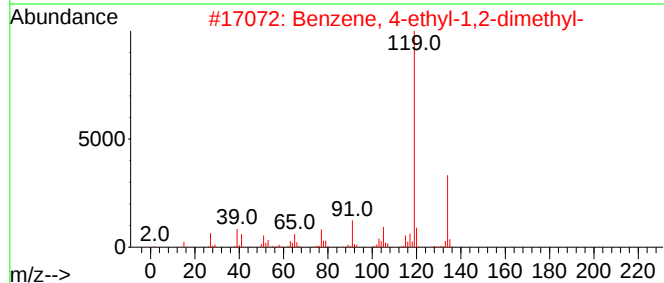
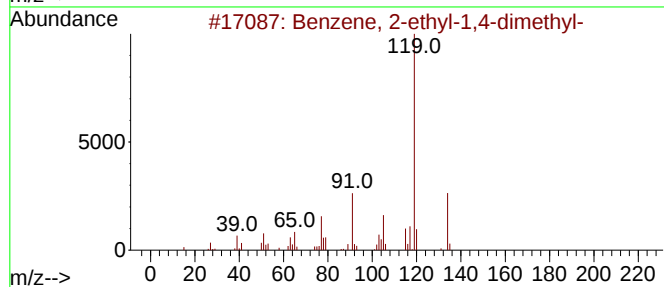
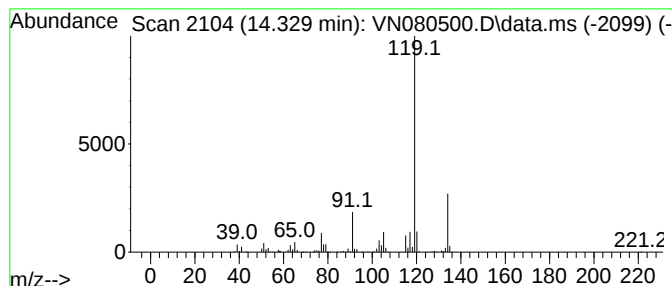
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	21.50 ug/l	2530820	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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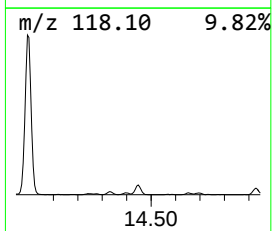
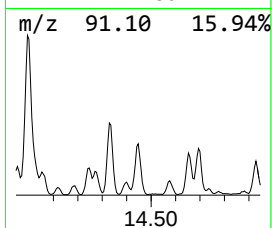
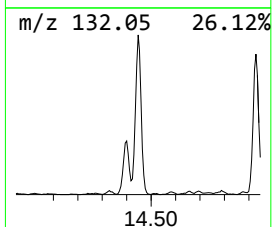
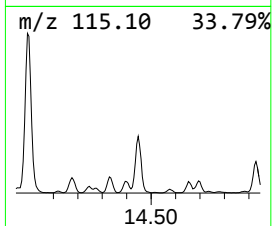
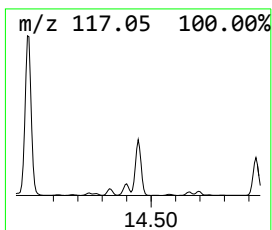
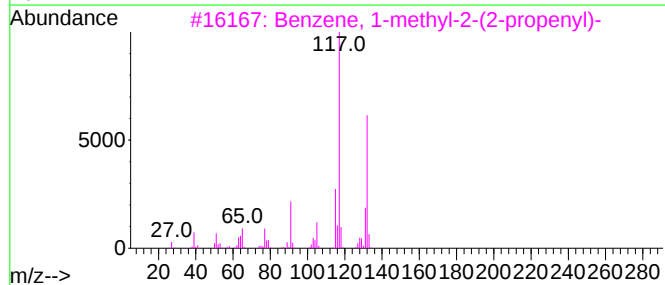
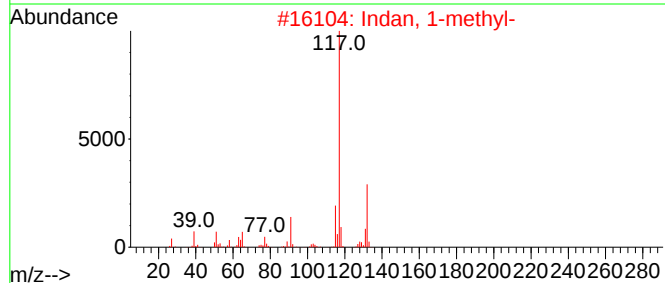
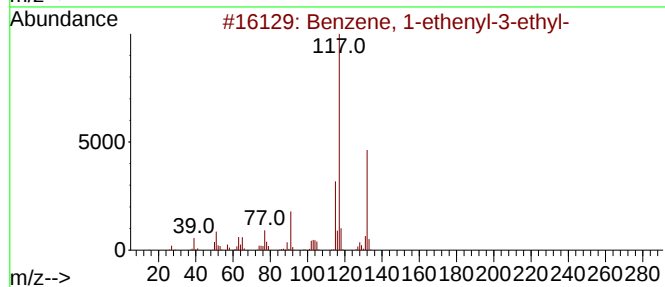
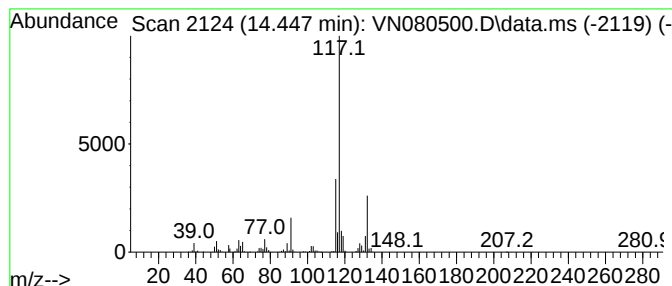
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	21.19 ug/l	2494150	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	91
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

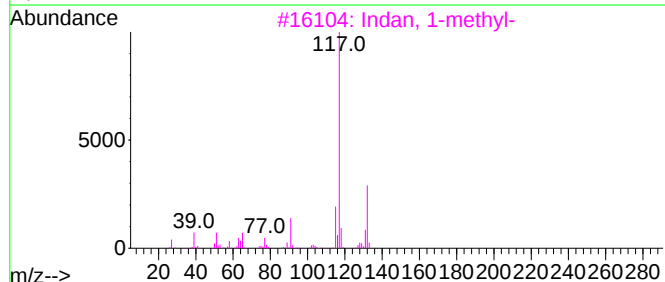
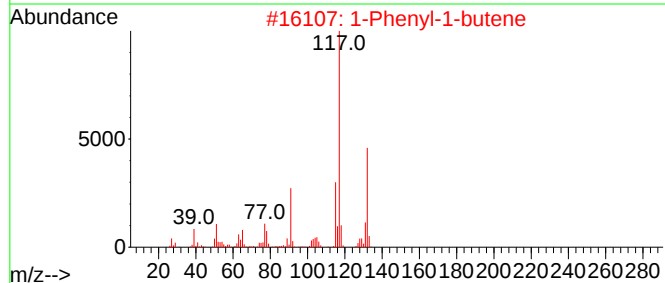
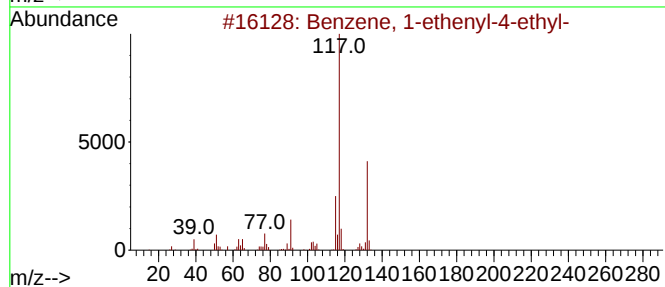
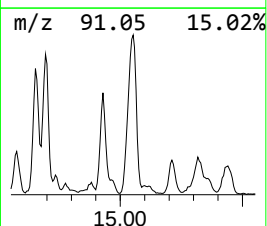
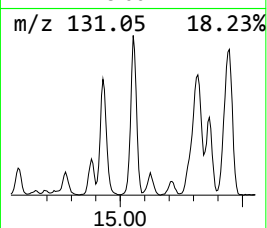
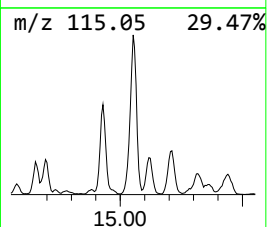
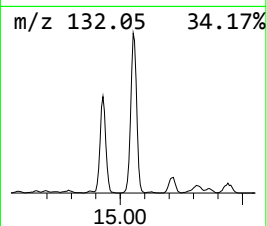
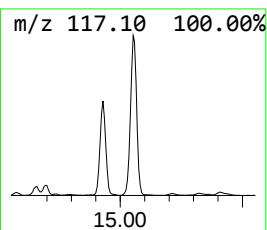
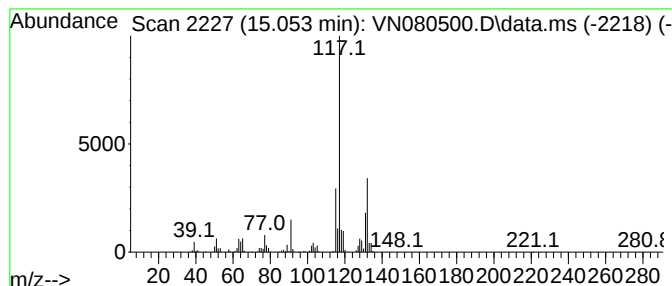
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	34.44 ug/l	4053640	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	90
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	90
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-2

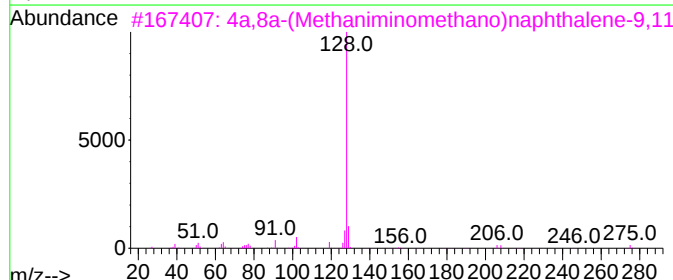
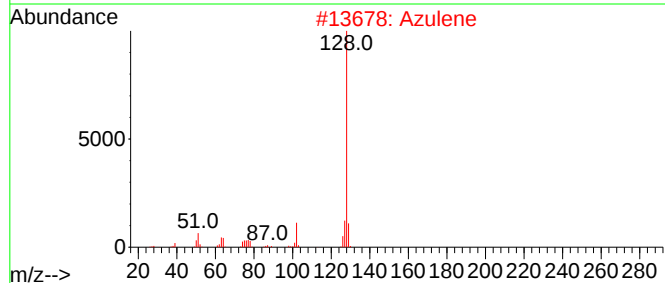
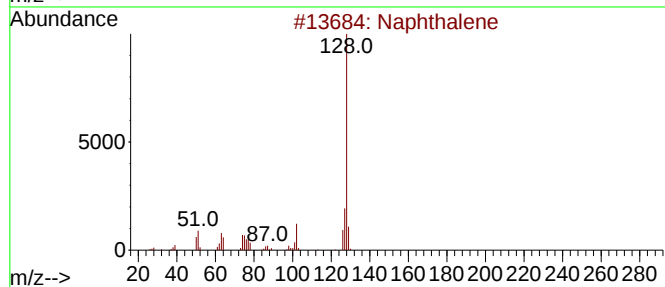
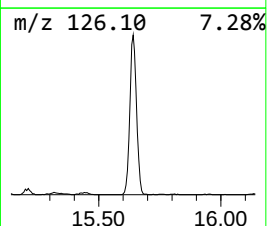
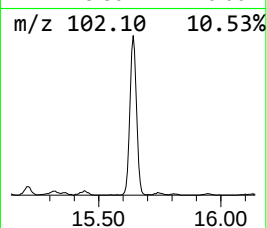
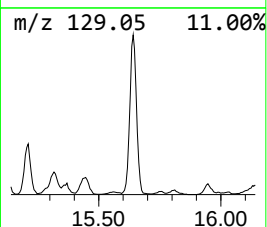
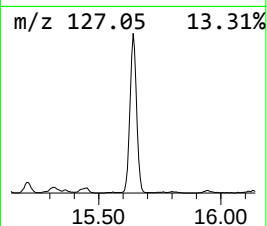
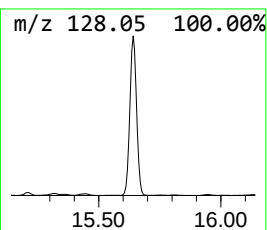
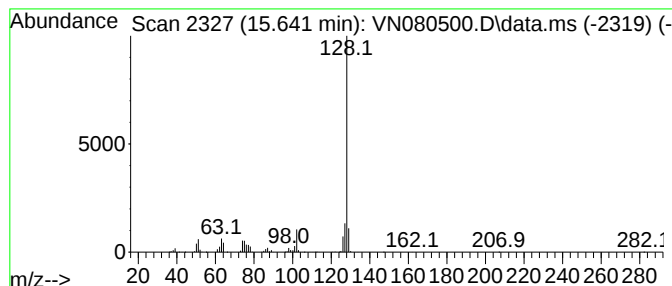
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	34.30 ug/l	4037320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Azulene	128	C10H8	000275-51-4	94
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	83
4			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121523\
Data File : VN080500.D
Acq On : 15 Dec 2023 14:00
Operator : JC\MD
Sample : 05829-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.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
unknown5.347	5.347	24.9	ug/l	665616	1	8.224	1337160	50.0
Pentane, 3-methyl-	5.812	38.4	ug/l	1025770	1	8.224	1337160	50.0
Cyclopentane, m...	7.330	42.7	ug/l	1142150	1	8.224	1337160	50.0
1,4-Pentadiene,...	10.982	21.0	ug/l	541548	3	11.865	1286880	50.0
Benzene, 1-ethy...	13.335	35.2	ug/l	4142620	4	13.794	5884480	50.0
Indane	13.994	76.0	ug/l	8946370	4	13.794	5884480	50.0
Benzene, 2-ethy...	14.329	21.5	ug/l	2530820	4	13.794	5884480	50.0
Benzene, 1-ethe...	14.447	21.2	ug/l	2494150	4	13.794	5884480	50.0
Benzene, 1-ethe...	15.053	34.4	ug/l	4053640	4	13.794	5884480	50.0
Azulene	15.641	34.3	ug/l	4037320	4	13.794	5884480	50.0