

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
 Data File : VN071763.D
 Acq On : 01 Apr 2022 19:20
 Operator : JC\MD
 Sample : N2090-14
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-58

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\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	37	43	44	rBV	44974	67982	2.06%	0.328%
2	4.581	431	441	449	rBV3	16015	54981	1.67%	0.265%
3	5.616	603	617	632	rBV5	28267	110019	3.33%	0.531%
4	7.145	866	877	885	rBV4	22644	65729	1.99%	0.317%
5	8.022	1013	1026	1031	rBV2	393574	951196	28.82%	4.590%
6	8.087	1031	1037	1046	rVB	739143	1681167	50.94%	8.113%
7	8.434	1087	1096	1109	rBV	415055	945698	28.65%	4.564%
8	8.581	1114	1121	1126	rBV9	14982	42950	1.30%	0.207%
9	8.698	1137	1141	1153	rVB5	17849	49605	1.50%	0.239%
10	8.963	1177	1186	1200	rBV	1107145	2299537	69.67%	11.097%
11	9.422	1257	1264	1266	rBV2	25713	46065	1.40%	0.222%
12	9.975	1351	1358	1362	rBV3	15726	33118	1.00%	0.160%
13	10.439	1428	1437	1455	rBV	1787952	3300475	100.00%	15.927%
14	10.639	1461	1471	1478	rVB2	69743	133273	4.04%	0.643%
15	10.716	1478	1484	1490	rBV	62900	109295	3.31%	0.527%
16	10.857	1502	1508	1517	rVB5	23432	54821	1.66%	0.265%
17	11.739	1651	1658	1669	rBV	1667544	3008233	91.15%	14.517%
18	11.945	1686	1693	1698	rBV	18539	36940	1.12%	0.178%
19	12.575	1795	1800	1807	rVB	51144	85405	2.59%	0.412%
20	12.727	1818	1826	1836	rBV	1198656	2072709	62.80%	10.002%
21	12.916	1853	1858	1866	rVB	29441	49038	1.49%	0.237%
22	13.222	1903	1910	1918	rVB	34727	59590	1.81%	0.288%
23	13.492	1948	1956	1962	rBV4	28178	68574	2.08%	0.331%
24	13.674	1979	1987	1999	rBV	1247443	2249649	68.16%	10.856%
25	13.769	1999	2003	2008	rVV2	23864	38463	1.17%	0.186%
26	13.833	2008	2014	2016	rVV	85395	123695	3.75%	0.597%
27	13.874	2016	2021	2026	rVV	370207	642141	19.46%	3.099%
28	13.916	2026	2028	2037	rVV4	49689	69175	2.10%	0.334%
29	14.004	2037	2043	2049	rVB2	49876	81427	2.47%	0.393%
30	14.145	2059	2067	2074	rBV	109689	201477	6.10%	0.972%
31	14.216	2074	2079	2084	rVV	96651	153138	4.64%	0.739%
32	14.274	2084	2089	2092	rVV	30539	54534	1.65%	0.263%
33	14.327	2092	2098	2104	rVV	338572	565119	17.12%	2.727%
34	14.398	2104	2110	2116	rVV7	17000	41620	1.26%	0.201%
35	14.463	2116	2121	2126	rVV2	27789	48015	1.45%	0.232%
36	14.539	2126	2134	2142	rVB	178331	296961	9.00%	1.433%

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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\82N033022W.M
Title : SW846 8260

37	14.757	2163	2171	2175	rBV3	29486	50694	1.54%	0.245%
38	14.810	2175	2180	2186	rVV3	53022	94369	2.86%	0.455%
39	14.927	2191	2200	2207	rBV3	152353	296395	8.98%	1.430%
40	15.192	2236	2245	2250	rBV2	45821	91854	2.78%	0.443%
41	15.304	2255	2264	2272	rVB4	35428	101547	3.08%	0.490%
42	15.557	2301	2307	2312	rBV2	37260	70470	2.14%	0.340%
43	15.639	2312	2321	2332	rVB2	45046	125032	3.79%	0.603%

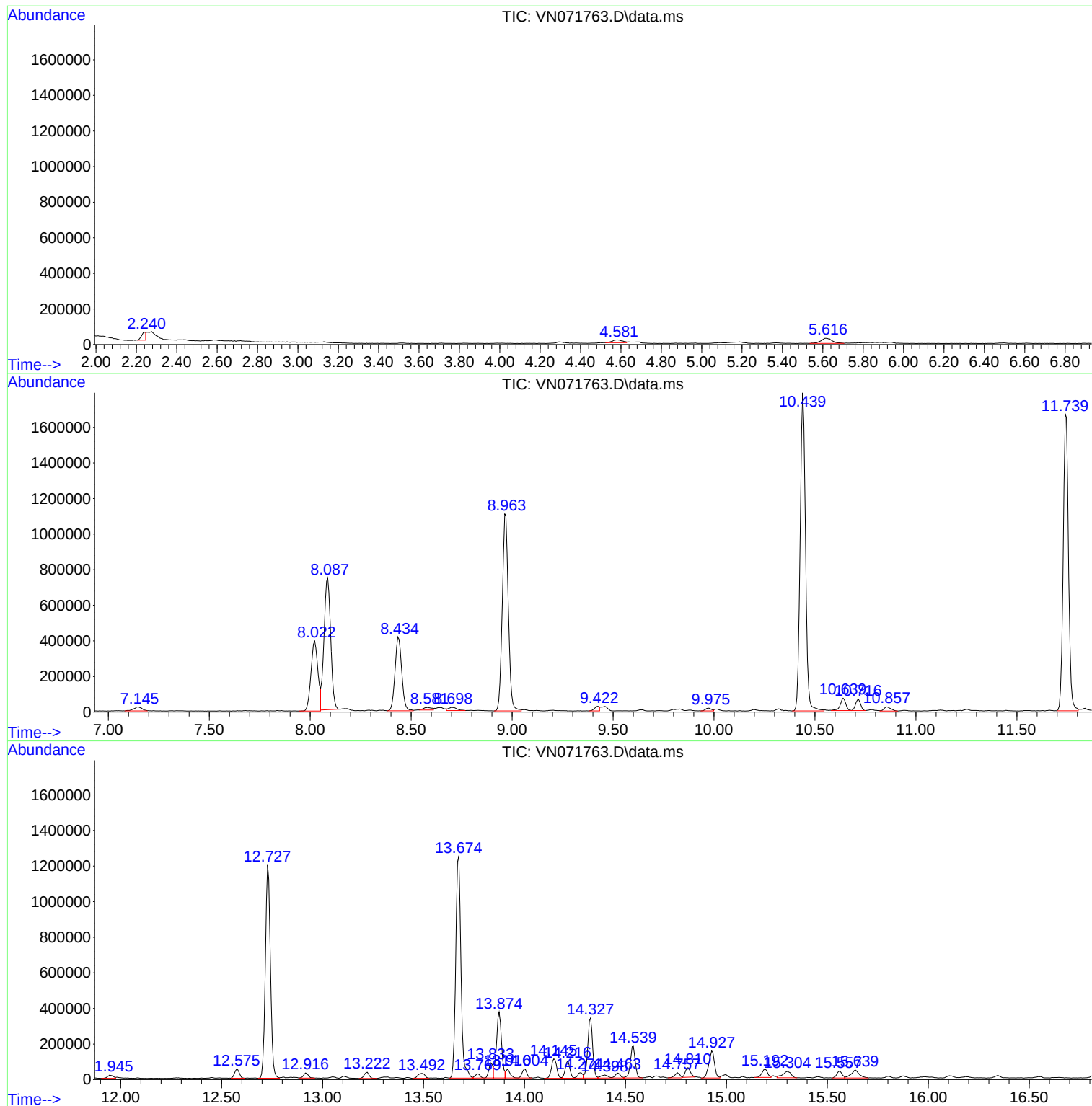
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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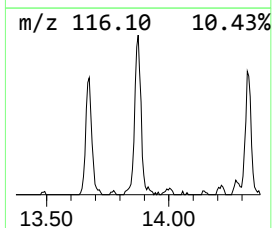
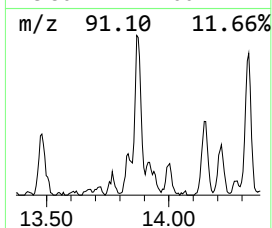
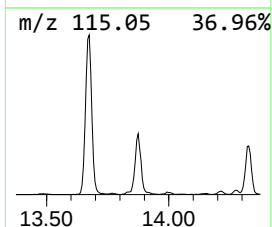
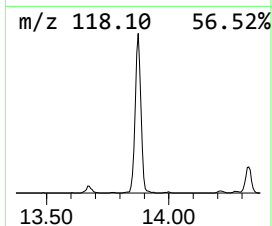
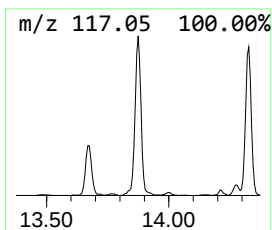
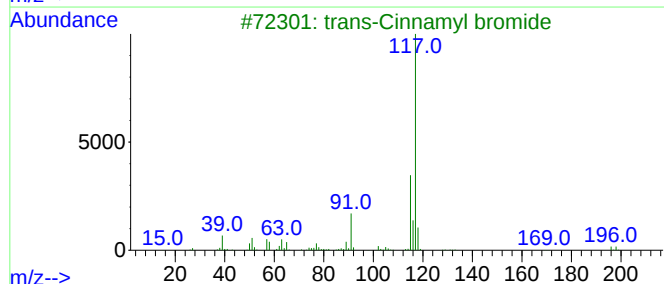
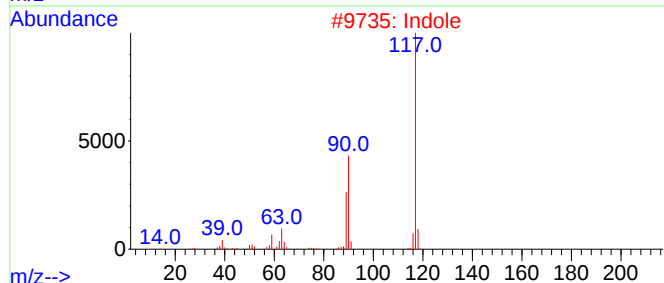
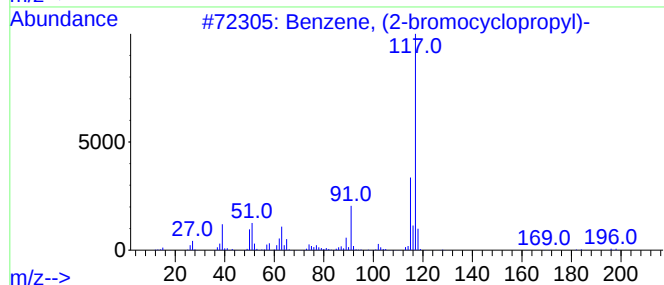
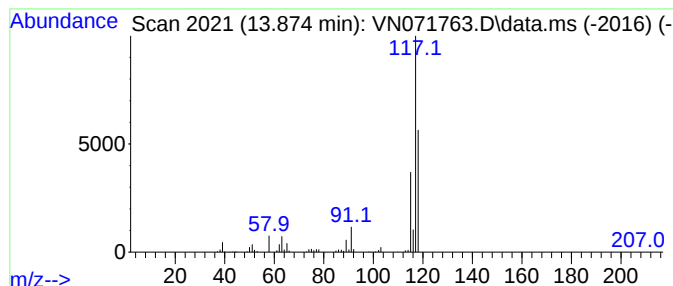
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	14.27 ug/l	642141	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	50
2			Indole	117	C8H7N	000120-72-9	43
3			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42
4			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	40
5			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	40



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Instrument :
MSVOA_N
ClientSampleId :
MW-58

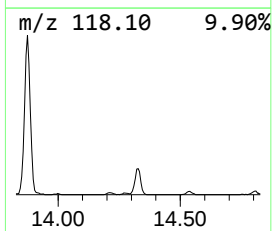
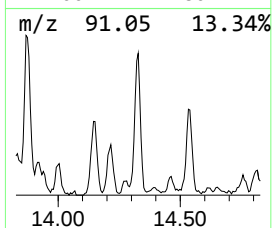
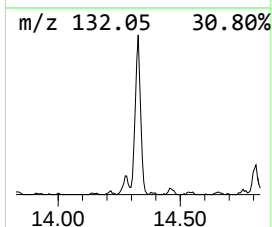
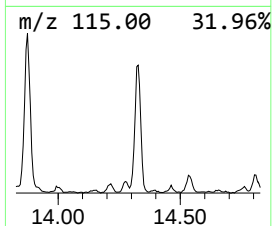
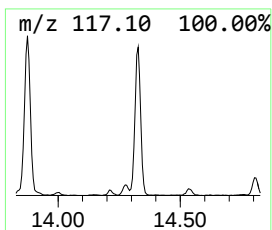
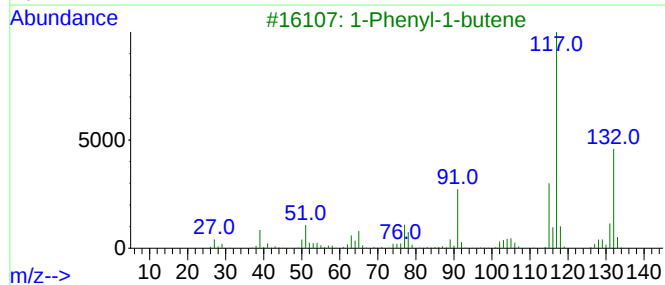
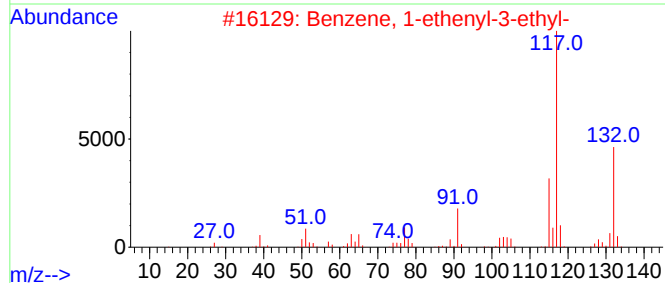
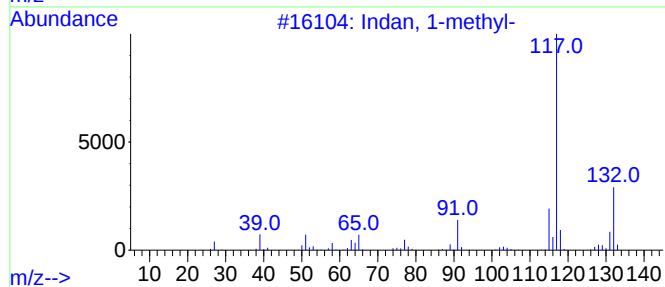
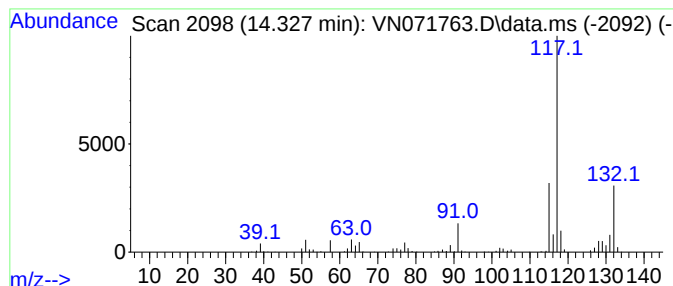
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 2 Indan, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	12.56 ug/l	565119	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	90
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	86
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	80
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	78



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-58

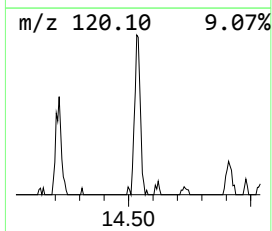
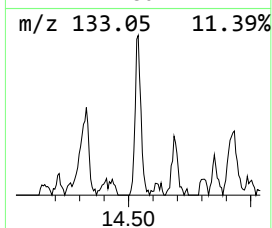
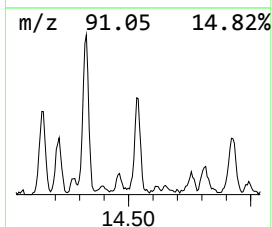
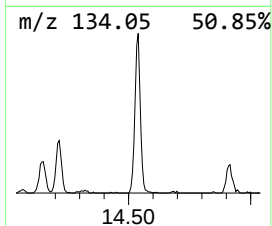
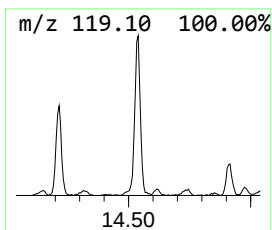
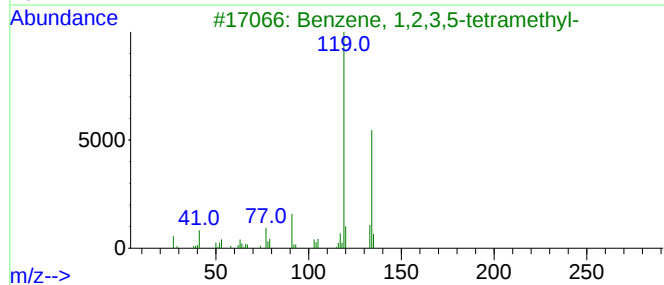
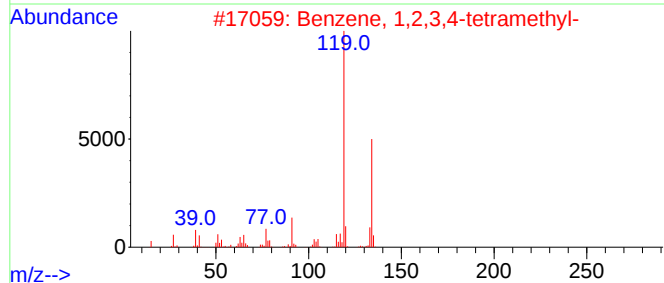
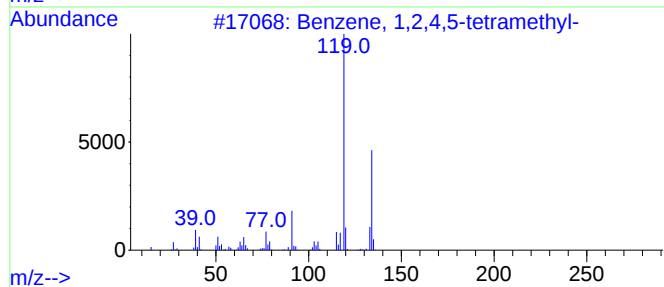
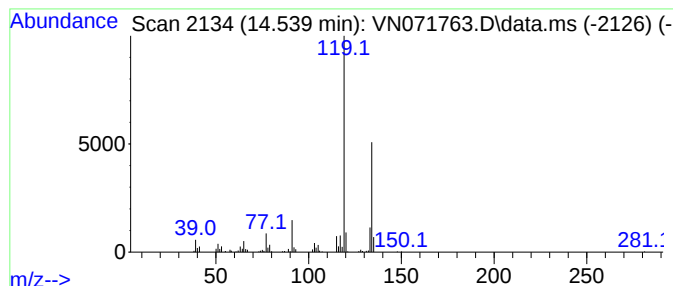
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	6.60 ug/l	296961	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



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Instrument :
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ClientSampleId :
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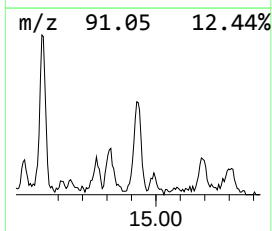
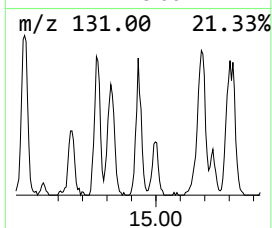
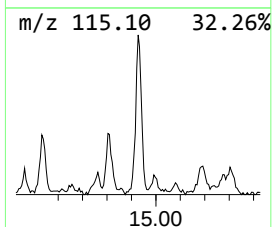
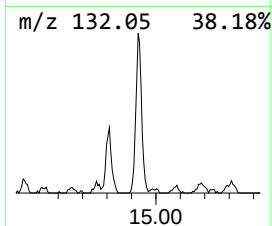
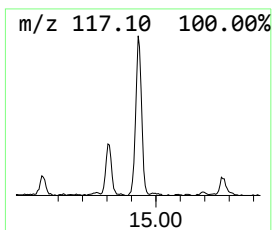
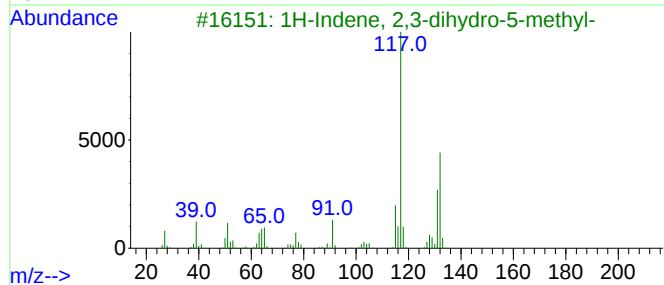
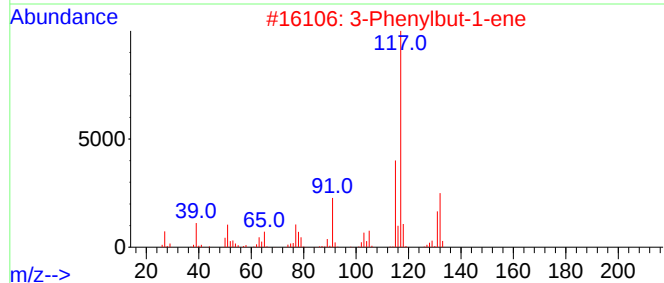
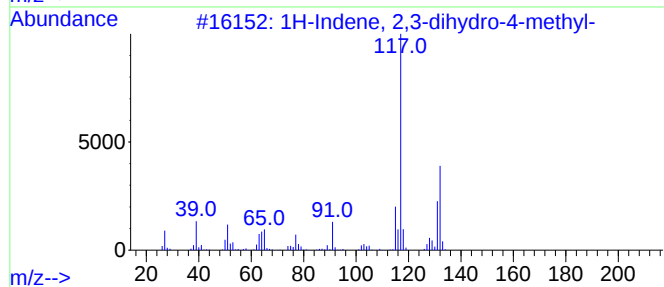
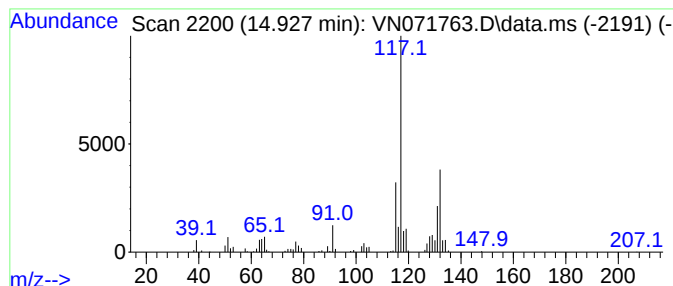
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	6.59 ug/l	296395	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
5		Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	83



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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
Benzene, (2-bro...	13.874	14.3	ug/l	642141	4	13.675	2249650	50.0
Indan, 1-methyl-	14.327	12.6	ug/l	565119	4	13.675	2249650	50.0
Benzene, 1,2,4,...	14.539	6.6	ug/l	296961	4	13.675	2249650	50.0
1H-Indene, 2,3-...	14.927	6.6	ug/l	296395	4	13.675	2249650	50.0