

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020224\
 Data File : VN080885.D
 Acq On : 02 Feb 2024 19:51
 Operator : JC\MD
 Sample : P1331-01 20X
 Misc : 5.02g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-1

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: VN080885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	143	148	155	rVB8	10421	28047	4.09%	0.657%
2	8.171	1046	1057	1061	rBV	76695	180842	26.34%	4.235%
3	8.229	1061	1067	1077	rVB	121537	273852	39.89%	6.413%
4	8.582	1118	1127	1137	rBV3	85720	195110	28.42%	4.569%
5	9.106	1207	1216	1224	rBV	234643	484015	70.50%	11.335%
6	10.571	1457	1465	1475	rBV	347276	644884	93.93%	15.103%
7	11.870	1677	1686	1695	rBV	377703	686560	100.00%	16.079%
8	12.853	1846	1853	1862	rVB	237787	409015	59.57%	9.579%
9	13.176	1902	1908	1913	rVV6	7540	15109	2.20%	0.354%
10	13.435	1942	1952	1957	rBV7	5112	12134	1.77%	0.284%
11	13.482	1957	1960	1967	rVB5	6964	11117	1.62%	0.260%
12	13.729	1998	2002	2006	rBV3	4985	7249	1.06%	0.170%
13	13.794	2006	2013	2026	rVV	348911	600597	87.48%	14.065%
14	14.117	2062	2068	2078	rBV9	13640	30420	4.43%	0.712%
15	14.447	2117	2124	2126	rBV6	8044	12890	1.88%	0.302%
16	14.511	2130	2135	2139	rVV5	8500	14522	2.12%	0.340%
17	14.576	2139	2146	2150	rVB7	6761	13887	2.02%	0.325%
18	14.629	2150	2155	2158	rBV4	13826	25928	3.78%	0.607%
19	14.664	2158	2161	2165	rVV3	13089	23367	3.40%	0.547%
20	14.788	2176	2182	2188	rVB10	11110	24136	3.52%	0.565%
21	14.847	2188	2192	2196	rBV6	8141	10532	1.53%	0.247%
22	15.035	2220	2224	2226	rBV4	9548	13345	1.94%	0.313%
23	15.106	2234	2236	2240	rVB4	11958	13808	2.01%	0.323%
24	15.217	2251	2255	2260	rVV7	14898	32194	4.69%	0.754%
25	15.270	2260	2264	2269	rVV8	17289	31146	4.54%	0.729%
26	15.323	2269	2273	2282	rVV8	11242	27397	3.99%	0.642%
27	15.394	2282	2285	2288	rVV4	7222	12417	1.81%	0.291%
28	15.435	2288	2292	2298	rVB9	12354	26374	3.84%	0.618%
29	15.500	2298	2303	2306	rBV7	5465	8786	1.28%	0.206%
30	15.606	2316	2321	2324	rBV6	7639	11008	1.60%	0.258%
31	15.700	2332	2337	2341	rBV6	22125	43787	6.38%	1.025%
32	15.782	2347	2351	2357	rVB8	14039	28432	4.14%	0.666%
33	15.923	2372	2375	2376	rBV3	6966	7065	1.03%	0.165%
34	16.029	2391	2393	2397	rVB5	6472	7222	1.05%	0.169%
35	16.170	2411	2417	2422	rBV8	28558	61520	8.96%	1.441%
36	16.270	2432	2434	2438	rVB5	12065	12798	1.86%	0.300%

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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

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Title : SW846 8260

37	16.505	2469	2474	2480	rVB9	21581	48494	7.06%	1.136%
38	16.717	2501	2510	2516	rBV3	75332	180029	26.22%	4.216%

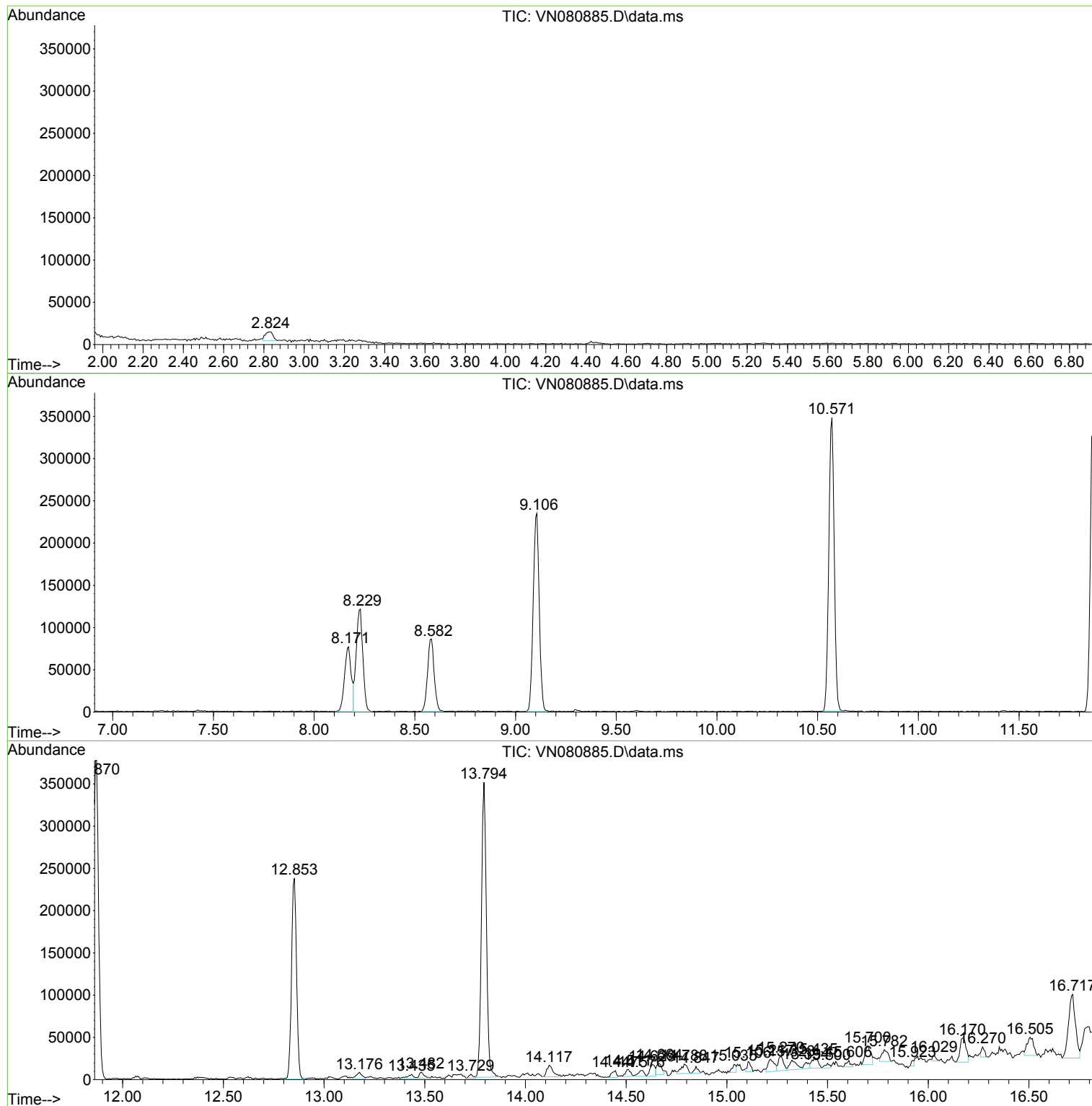
Sum of corrected areas: 4270035

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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



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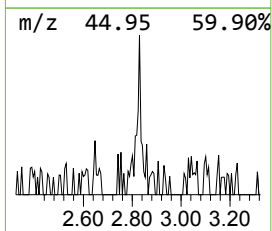
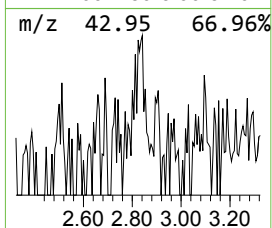
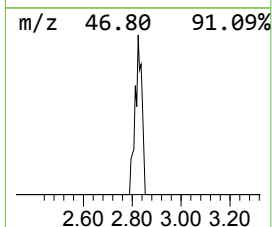
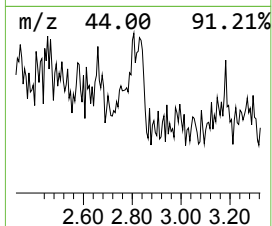
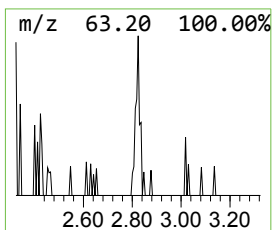
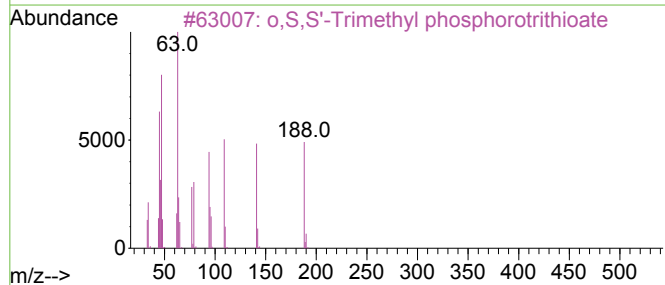
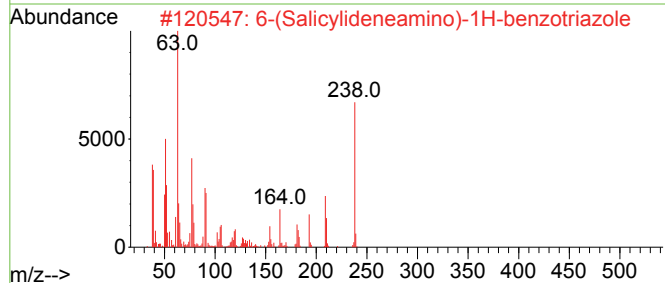
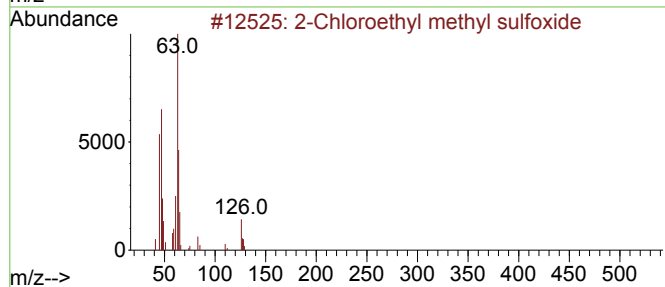
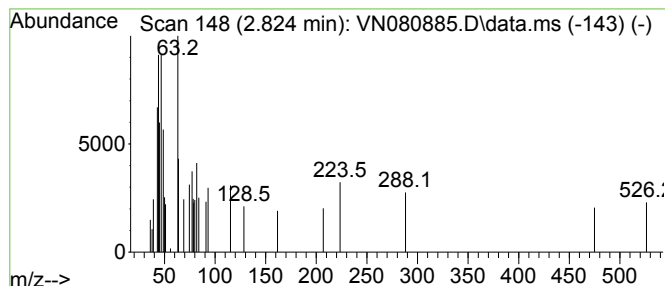
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.824 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	5.12 ug/l	28047	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	47
2			6-(Salicylideneamino)-1H-benzotr...	238	C13H10N4O	1000225-69-0	10
3			o,S,S'-Trimethyl phosphorotrithi...	188	C3H9OPS3	1000306-06-4	9
4			Carmustine	213	C5H9Cl2N3O2	000154-93-8	9
5			Pyrimidine-2,4,6(1H,3H,5H)-trion...	343	C15H9N3O5S	346612-55-3	9



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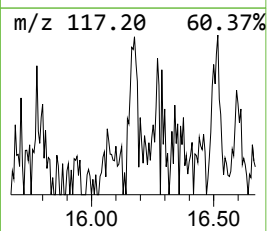
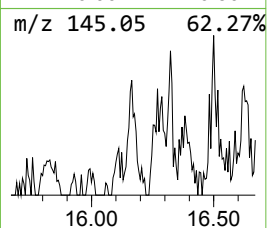
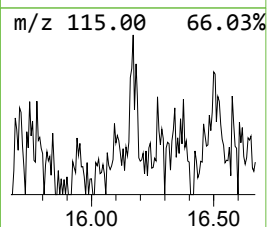
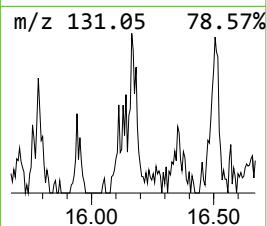
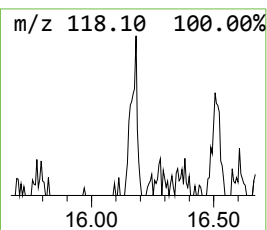
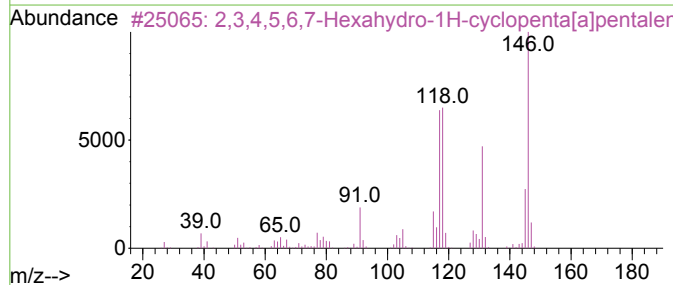
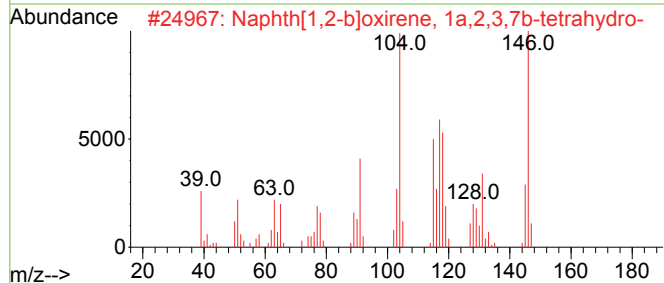
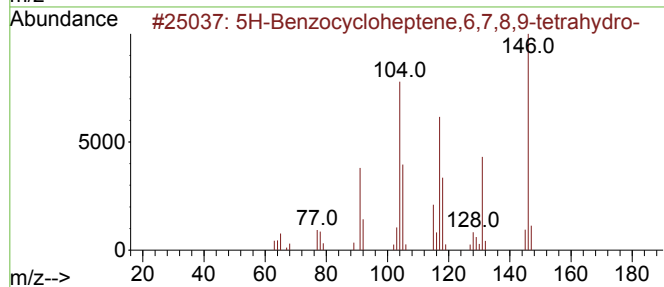
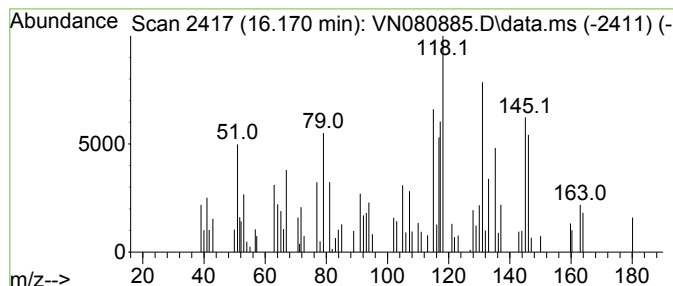
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown16.170 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	5.12 ug/l	61520	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Benzocycloheptene,6,7,8,9-tet...	146	C11H14	001075-16-7	49
2			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	49
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	49
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	46
5			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	46



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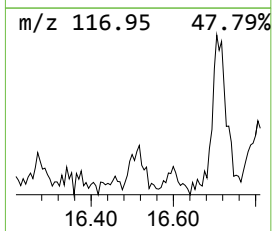
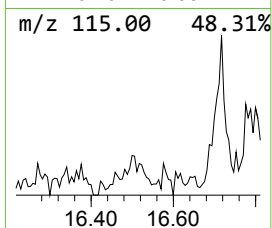
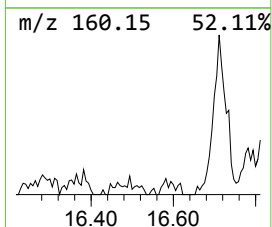
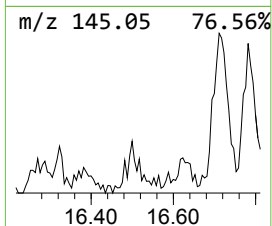
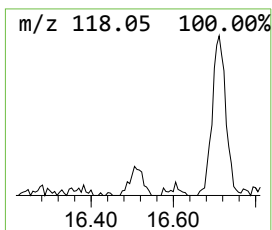
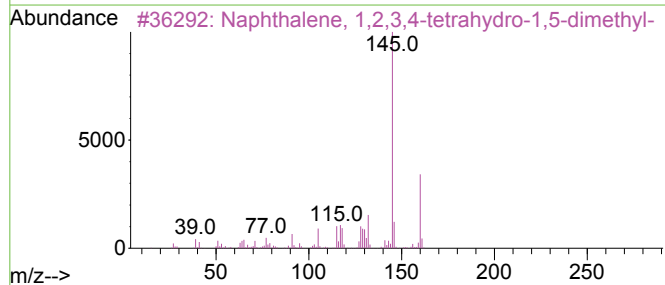
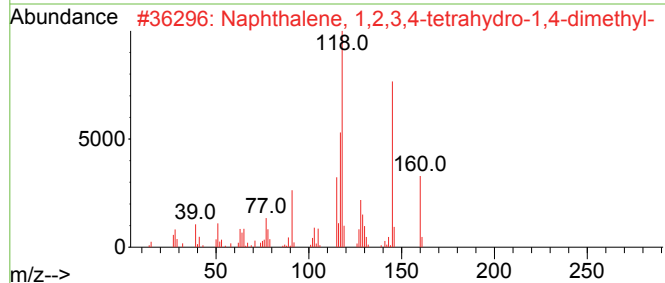
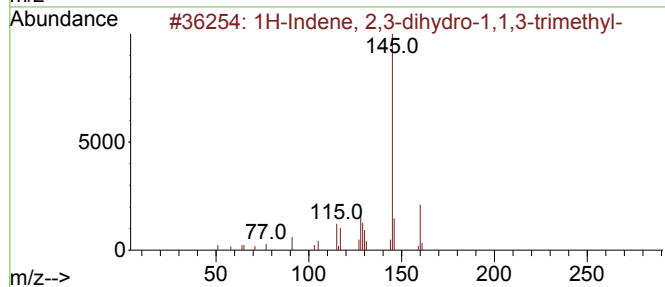
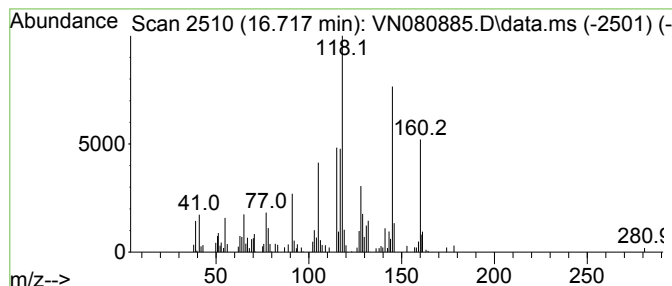
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.717	14.99 ug/l	180029	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	92		
2	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	87		
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	64		
4	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	62		
5	1H-Indene, 2,3-dihydro-1,5,7-tri...	160	C12H16	054340-88-4	55		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.824	2.824	5.1	ug/l	28047	1	8.229	273852	50.0
unknown16.170	16.170	5.1	ug/l	61520	4	13.794	600597	50.0
1H-Indene, 2,3-...	16.717	15.0	ug/l	180029	4	13.794	600597	50.0