

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
 Data File : VN073902.D
 Acq On : 15 Aug 2022 17:56
 Operator : JC\MD
 Sample : N4107-07
 Misc : 5.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 CONCRETE-STOCKPILE

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\82N081522W.M
 Title : SW846 8260

Signal : TIC: VN073902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.628	118	126	129	rBV	19306	40208	1.29%	0.206%
2	2.698	130	138	140	rBV6	17365	38768	1.24%	0.198%
3	4.781	481	492	494	rBV	26781	60397	1.93%	0.309%
4	5.204	553	564	578	rBV2	16378	74032	2.37%	0.378%
5	7.298	909	920	933	rBV	78217	224164	7.18%	1.146%
6	7.945	1019	1030	1035	rBV	375579	926466	29.67%	4.736%
7	8.004	1035	1040	1057	rVB	717396	1640661	52.55%	8.388%
8	8.363	1090	1101	1111	rBV	335964	771162	24.70%	3.942%
9	8.574	1126	1137	1145	rBV3	67035	244423	7.83%	1.250%
10	8.686	1146	1156	1176	rVB	215366	626772	20.08%	3.204%
11	8.898	1183	1192	1212	rVB	938167	1956605	62.67%	10.003%
12	10.380	1436	1444	1451	rBV	1309687	2425418	77.69%	12.400%
13	10.445	1451	1455	1461	rVB2	28733	56376	1.81%	0.288%
14	11.133	1565	1572	1579	rVB4	22458	49813	1.60%	0.255%
15	11.686	1657	1666	1674	rBV	1463316	2629686	84.23%	13.444%
16	12.380	1773	1784	1785	rBV2	49463	114645	3.67%	0.586%
17	12.674	1827	1834	1843	rVB	1385305	2307776	73.92%	11.798%
18	12.992	1881	1888	1889	rBV5	31808	57261	1.83%	0.293%
19	13.492	1964	1973	1986	rVB6	99068	432885	13.87%	2.213%
20	13.615	1987	1994	2004	rBV	1873654	3122050	100.00%	15.961%
21	13.803	2017	2026	2036	rBV9	103503	366811	11.75%	1.875%
22	14.315	2106	2113	2122	rVB4	83999	232181	7.44%	1.187%
23	15.080	2235	2243	2255	rVB2	124614	434492	13.92%	2.221%
24	15.203	2258	2264	2277	rVB4	71506	237570	7.61%	1.215%
25	15.774	2354	2361	2370	rBV5	46842	138434	4.43%	0.708%
26	16.127	2411	2421	2436	rVB4	53335	212955	6.82%	1.089%
27	16.297	2441	2450	2460	rVV4	39372	138400	4.43%	0.708%

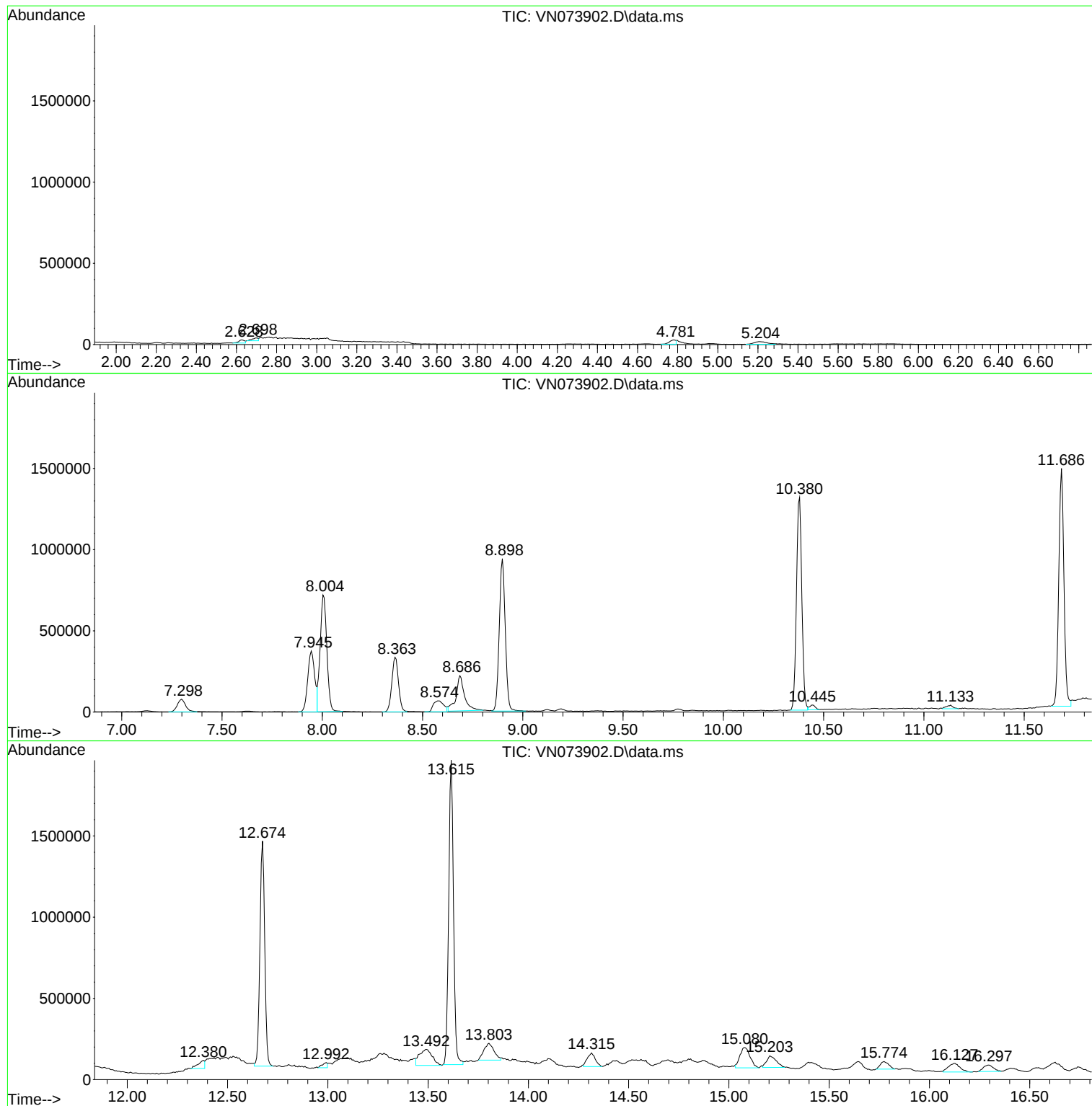
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CONCRETE-STOCKPILE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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



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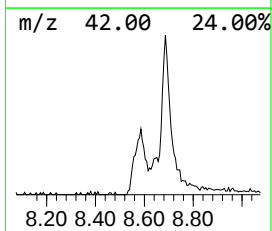
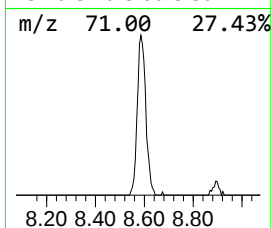
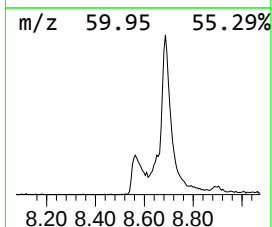
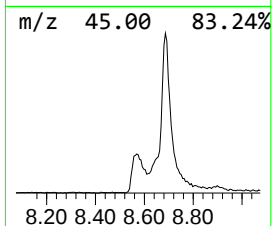
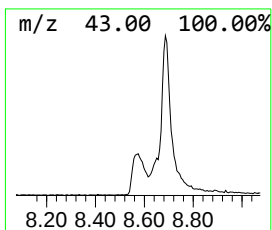
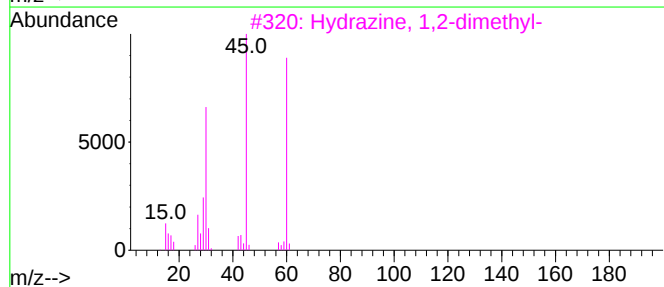
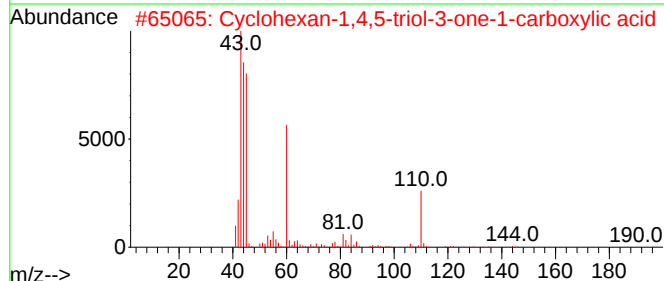
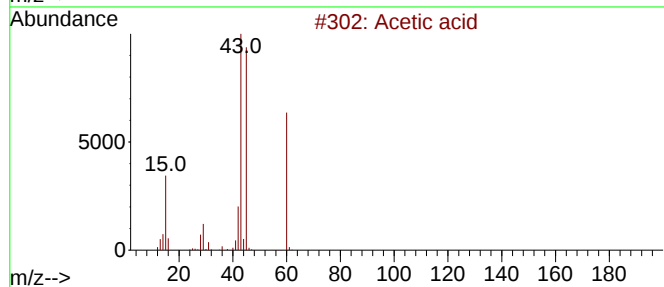
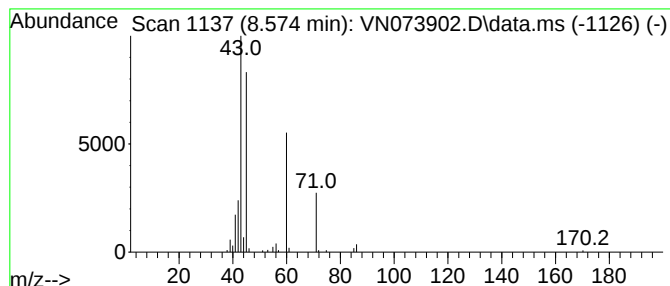
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	6.25 ug/l	244423	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	80
2			Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	56
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	40
4			Ammonium acetate	77	C2H7NO2	000631-61-8	38
5			N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	36



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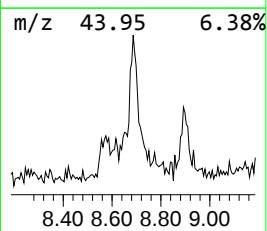
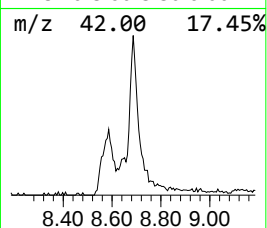
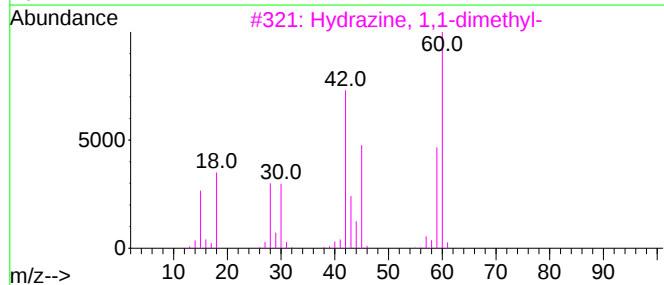
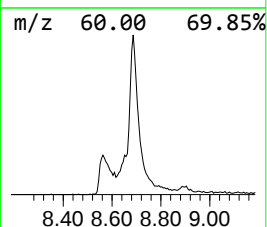
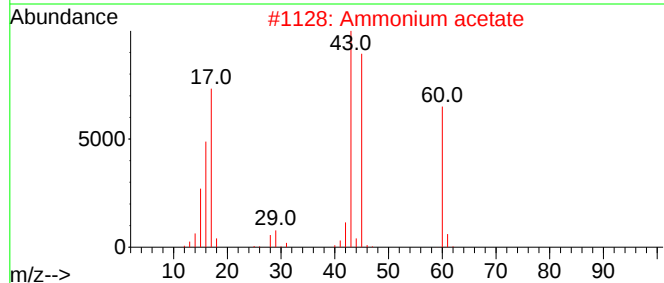
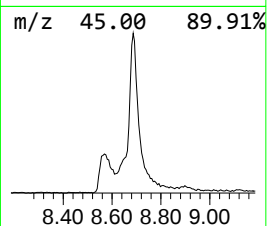
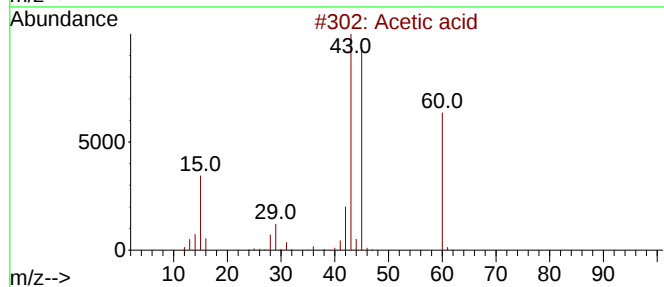
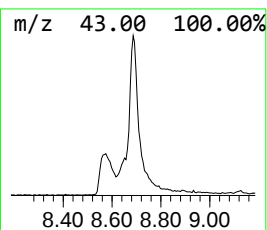
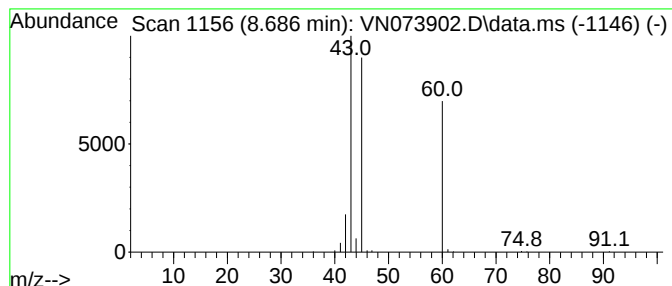
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Peak Number 3 Ammonium acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.686	16.02 ug/l	626772	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Ammonium acetate	77	C2H7NO2	000631-61-8	64
3			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5			Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	9



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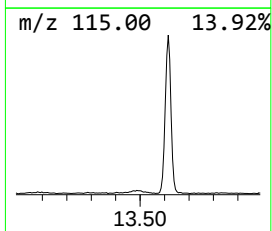
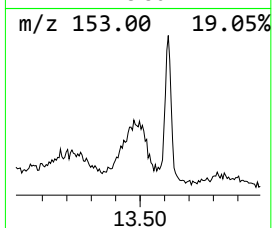
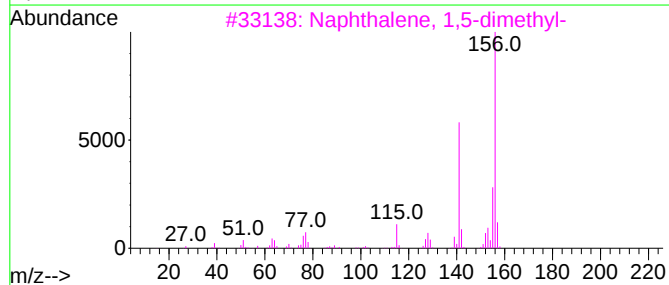
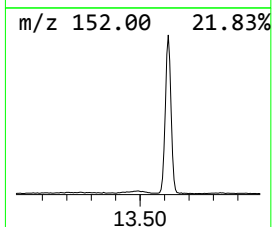
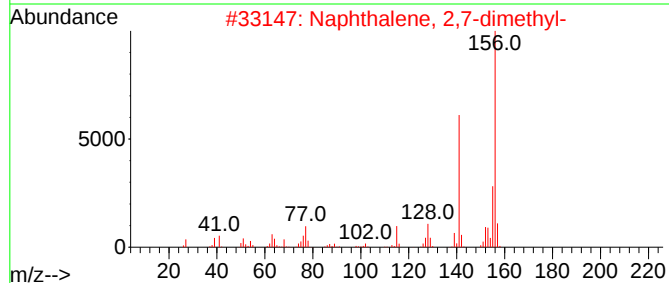
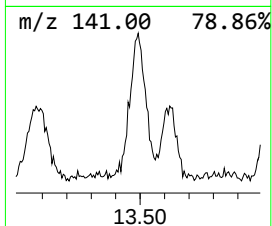
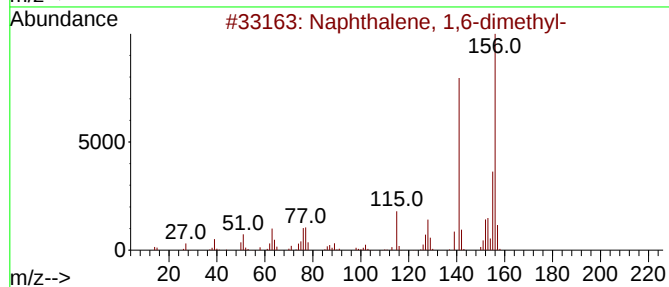
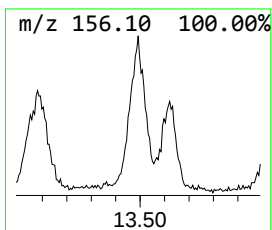
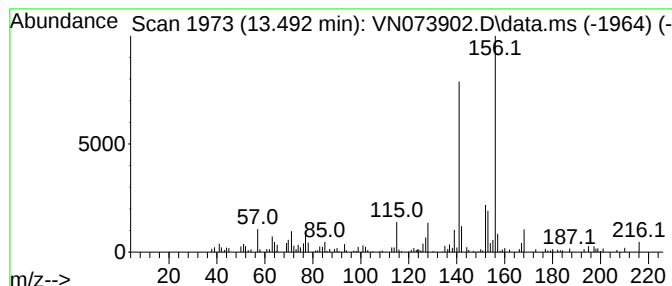
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.492	6.93 ug/l	432885	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	89
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	76
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	76
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	74
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	74



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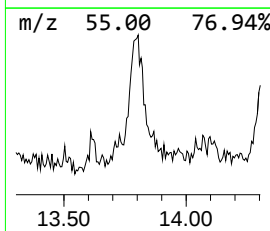
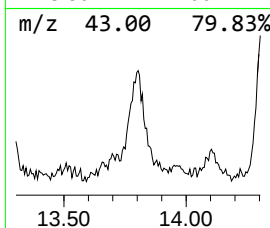
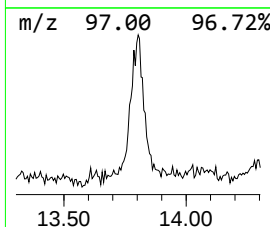
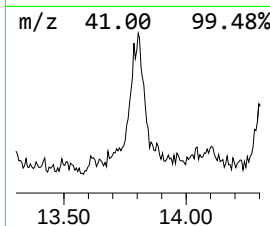
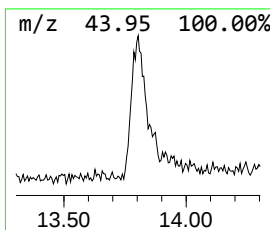
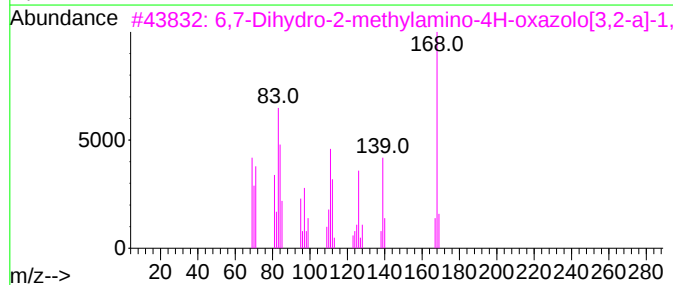
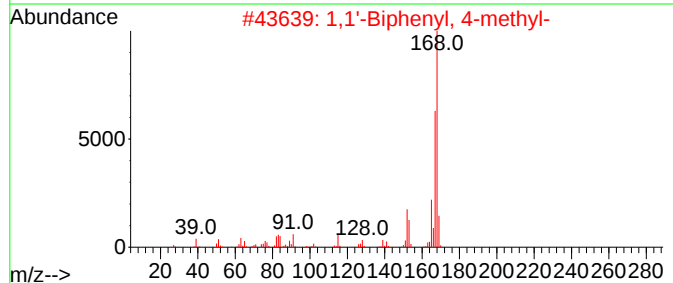
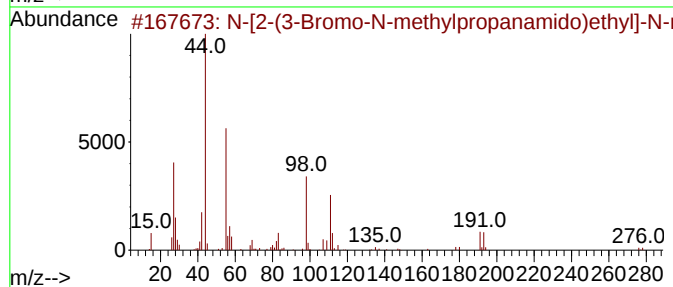
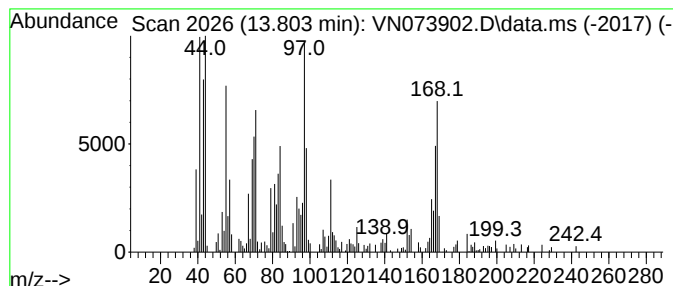
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.804 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	5.87 ug/l	366811	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-[2-(3-Bromo-N-methylpropanamid...	276	C10H17BrN2O2	1000436-87-8	22
2			1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	18
3			6,7-Dihydro-2-methylamino-4H-oxa...	168	C6H8N4O2	081287-23-2	18
4			1H-Imidazole-4-methanol	98	C4H6N2O	000822-55-9	14
5			1,3-Cyclohexanediamine	114	C6H14N2	003385-21-5	14



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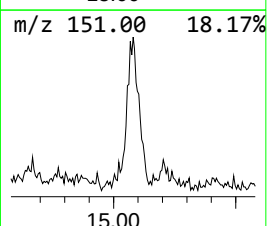
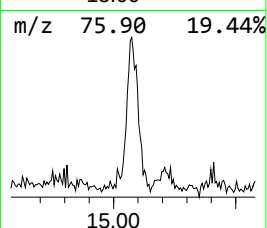
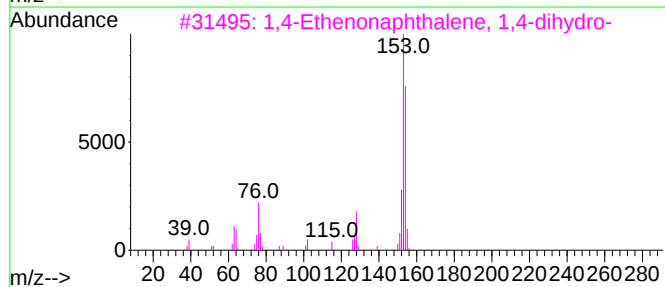
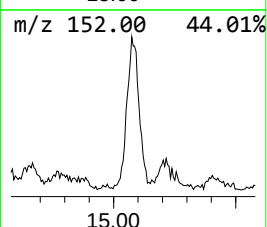
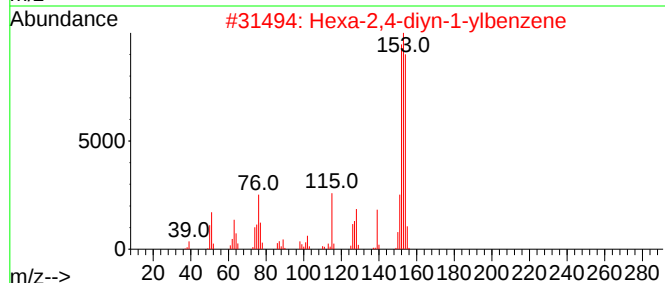
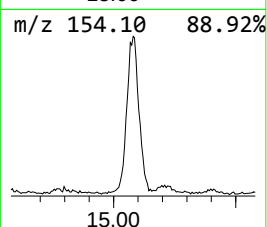
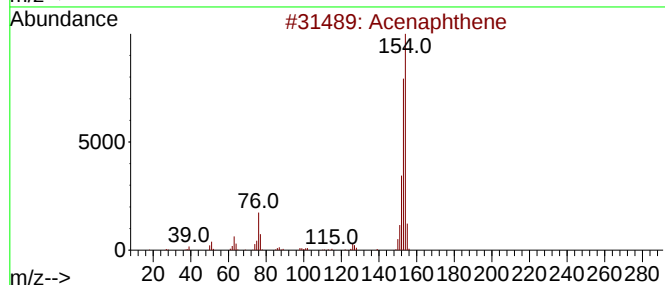
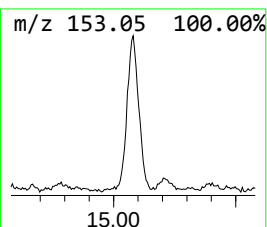
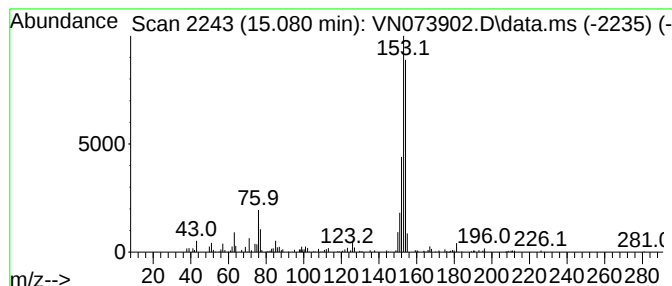
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Acenaphthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	6.96 ug/l	434492	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	81
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	59
3			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	59
4			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	52
5			2,3,4-Trihydroxybenzaldehyde	154	C7H6O4	002144-08-3	50



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	8.574	6.3	ug/l	244423	2	8.898	1956610	50.0
Ammonium acetate	8.686	16.0	ug/l	626772	2	8.898	1956610	50.0
Naphthalene, 1,...	13.492	6.9	ug/l	432885	4	13.615	3122050	50.0
unknown13.804	13.804	5.9	ug/l	366811	4	13.615	3122050	50.0
Acenaphthene	15.080	7.0	ug/l	434492	4	13.615	3122050	50.0