

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032219\
 Data File : VN054577.D
 Acq On : 23 Mar 2019 00:58
 Operator : JC/SP
 Sample : K2045-03
 Misc : 4.91g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WP022SB439-190318-(13-14)MSD

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\82N032019W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.503	207	227	228	rBV6	37889	78547	2.87%	0.485%
2	2.558	241	244	256	rVB3	83668	106515	3.90%	0.657%
3	7.587	1789	1808	1819	rBV	338467	833173	30.48%	5.142%
4	7.661	1819	1831	1859	rVB	602949	1486774	54.40%	9.176%
5	8.024	1927	1944	1967	rVB2	398030	924786	33.83%	5.707%
6	8.583	2103	2118	2160	rVB	921788	2031575	74.33%	12.538%
7	10.088	2573	2586	2633	rBV	1369735	2733239	100.00%	16.868%
8	11.406	2983	2996	3032	rBV	1199388	2229326	81.56%	13.759%
9	12.400	3293	3305	3332	rVB	937245	1626576	59.51%	10.039%
10	13.342	3586	3598	3616	rVB	1073780	1816385	66.46%	11.210%
11	15.127	4146	4153	4162	rVB4	21029	31417	1.15%	0.194%
12	15.593	4289	4298	4320	rVB3	31054	92585	3.39%	0.571%
13	15.693	4321	4329	4338	rBV2	24100	46950	1.72%	0.290%
14	15.779	4344	4356	4369	rBV3	107884	245742	8.99%	1.517%
15	16.201	4472	4487	4497	rBV4	198885	532917	19.50%	3.289%
16	16.496	4572	4579	4591	rVB2	125931	252355	9.23%	1.557%
17	16.606	4602	4613	4633	rVB2	511744	1134363	41.50%	7.001%

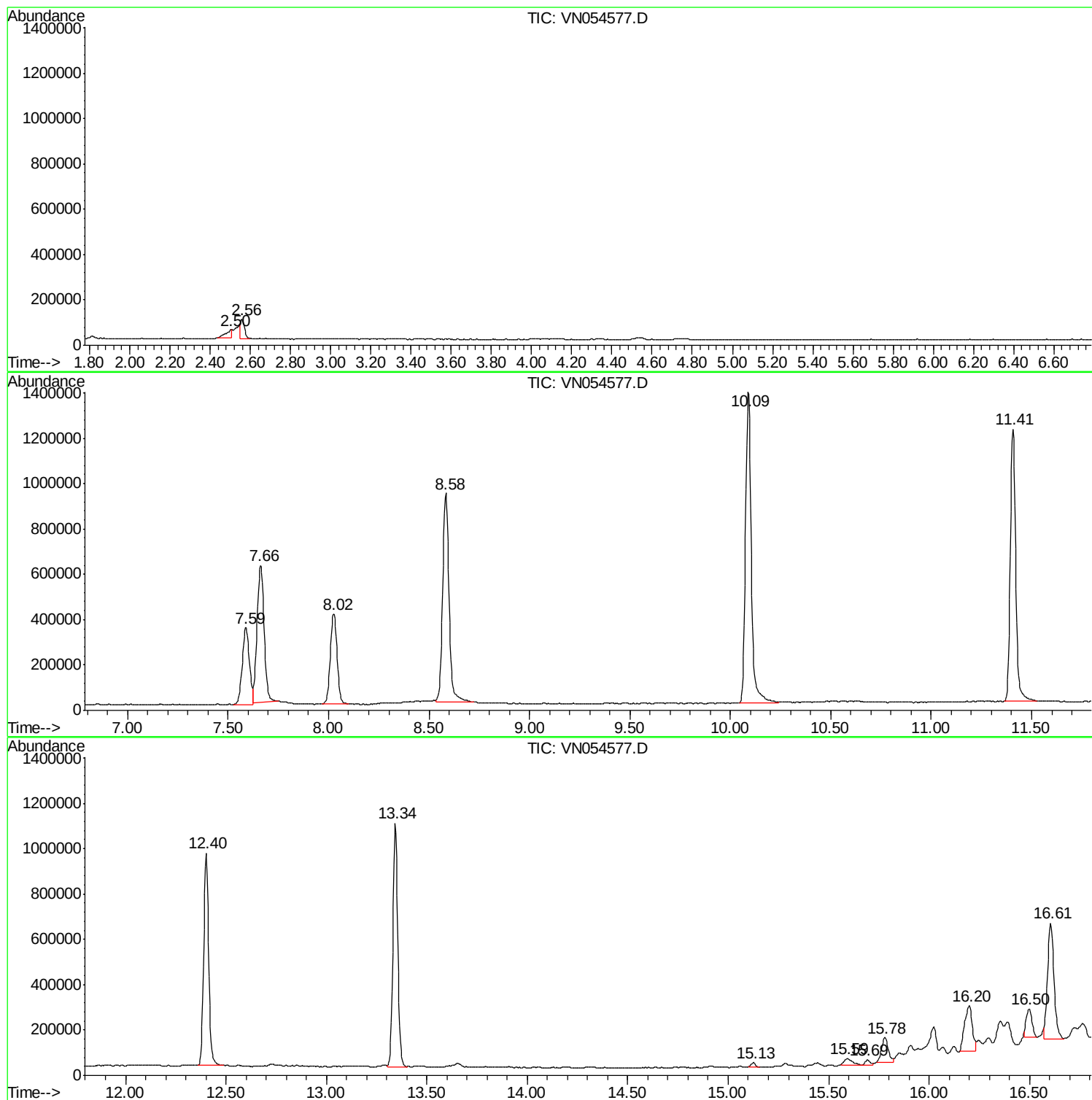
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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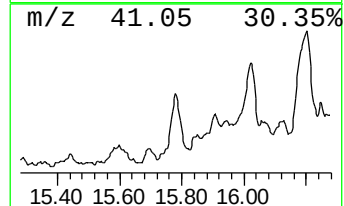
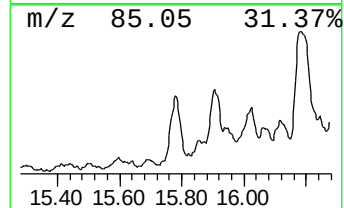
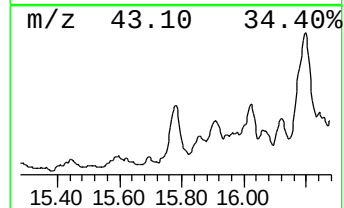
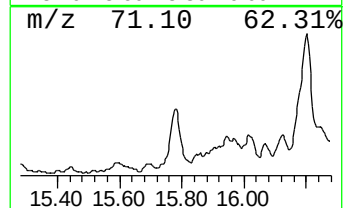
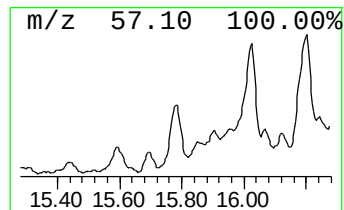
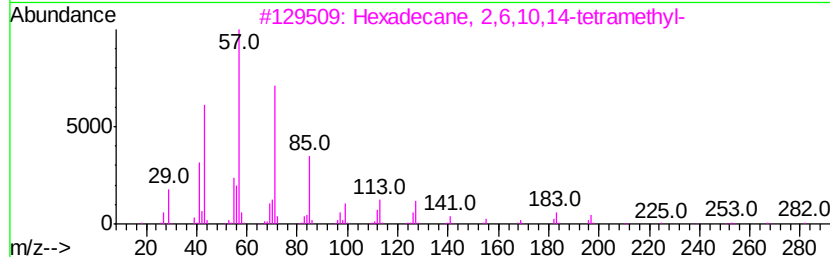
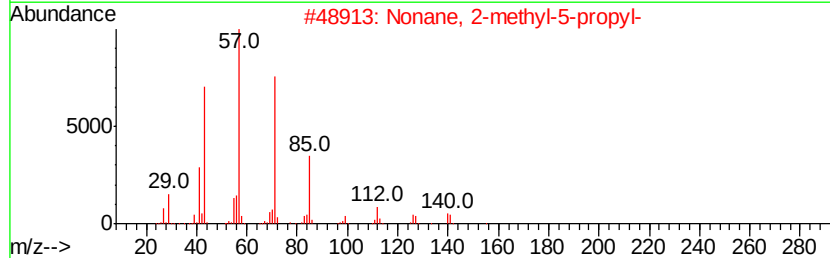
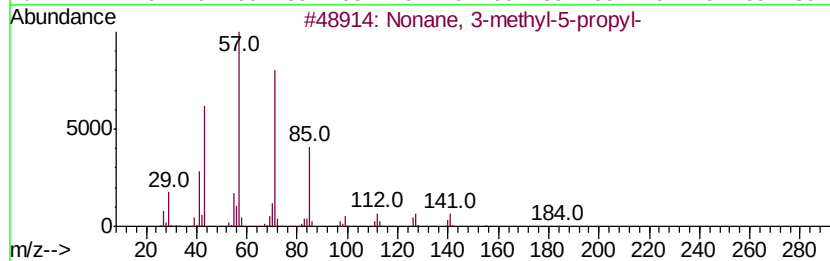
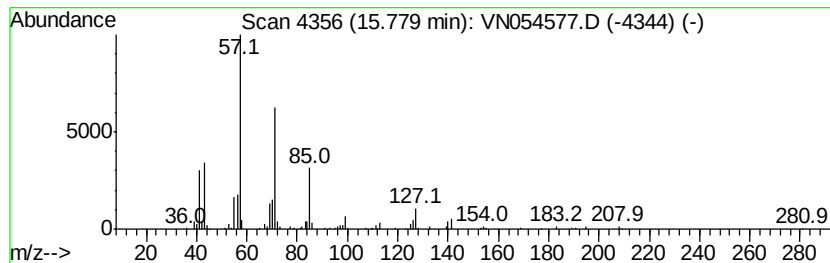
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Nonane, 3-methyl-5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	6.76 ug/l	245742	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	90
2		Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	86
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
4		Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
5		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59



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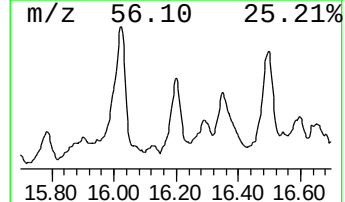
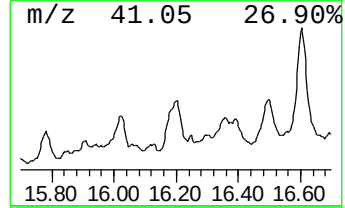
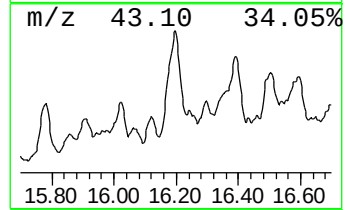
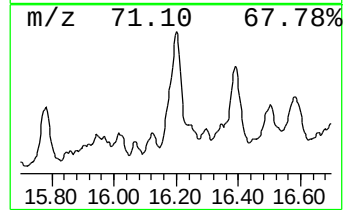
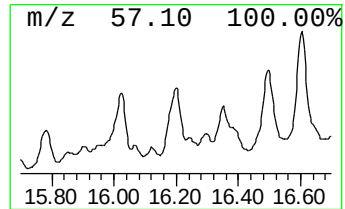
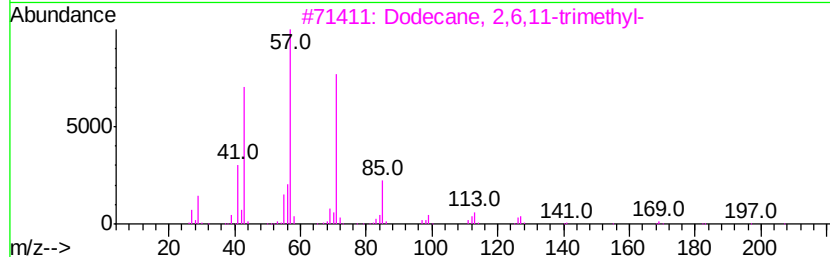
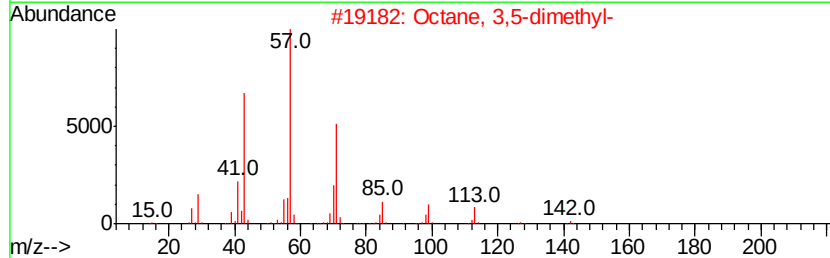
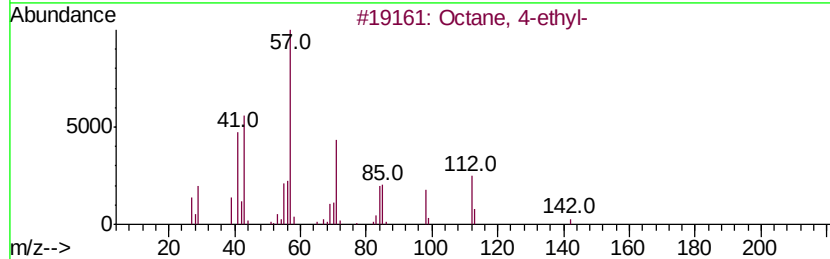
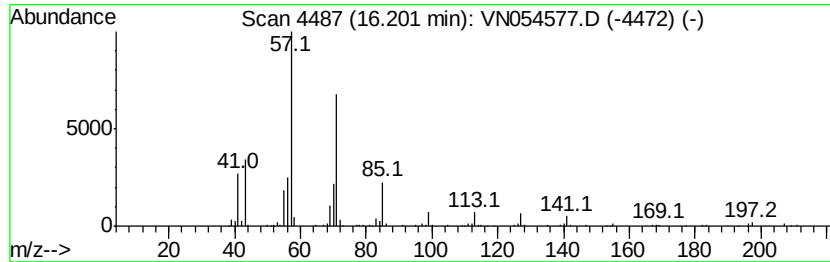
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 4-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	14.67 ug/l	532917	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octane, 4-ethyl-	142 C10H22	015869-86-0	59
2	Octane, 3,5-dimethyl-	142 C10H22	015869-93-9	59
3	Dodecane, 2,6,11-trimethyl-	212 C15H32	031295-56-4	59
4	Undecane, 3,8-dimethyl-	184 C13H28	017301-30-3	53
5	Octane, 3,6-dimethyl-	142 C10H22	015869-94-0	50



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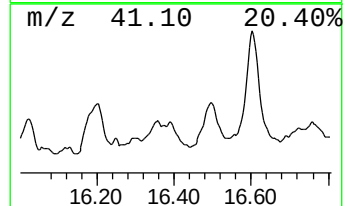
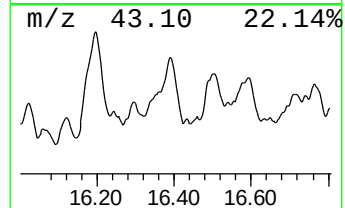
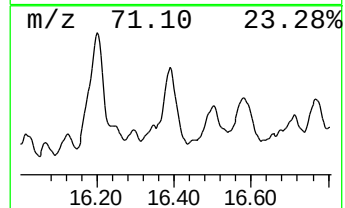
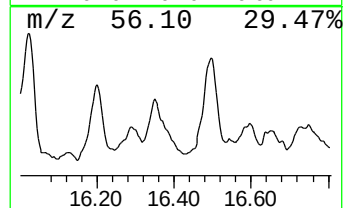
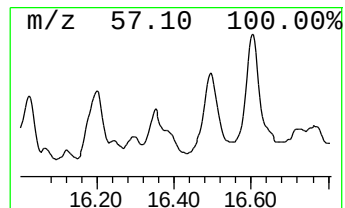
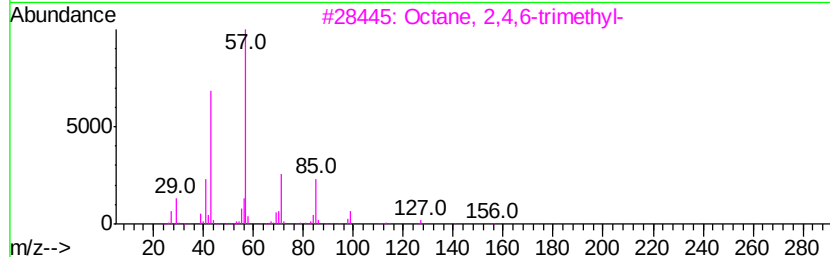
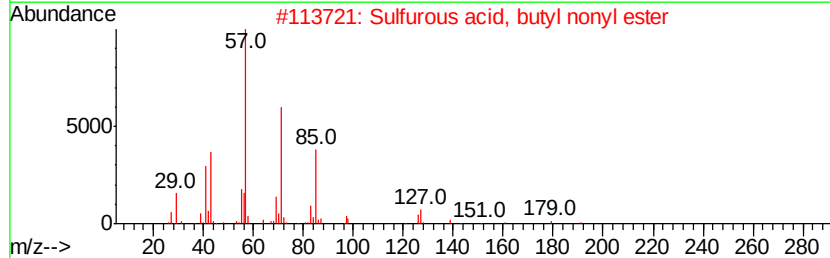
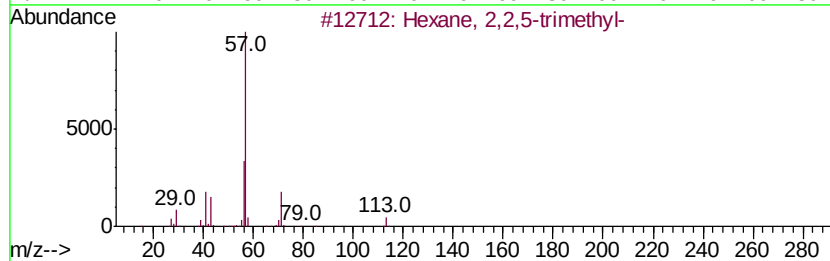
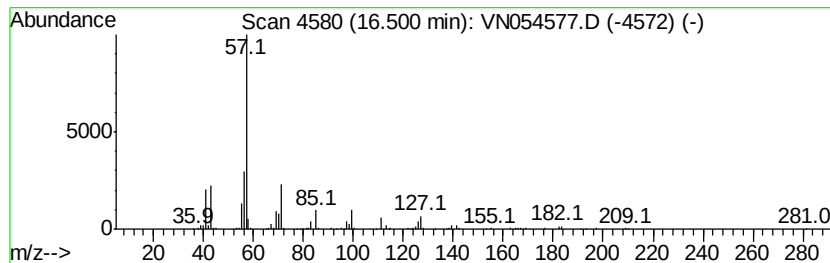
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Peak Number 3 Hexane, 2,2,5-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	6.95 ug/l	252355	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexane, 2,2,5-trimethyl-	128 C9H20	003522-94-9	50
2	Sulfurous acid, butyl nonyl ester	264 C13H28O3S	1000309-17-6	50
3	Octane, 2,4,6-trimethyl-	156 C11H24	062016-37-9	50
4	Hexane, 2,2,4-trimethyl-	128 C9H20	016747-26-5	50
5	Heptane, 4-ethyl-2,2,6,6-tetrame...	184 C13H28	062108-31-0	47



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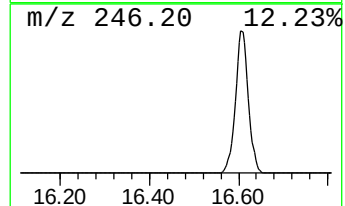
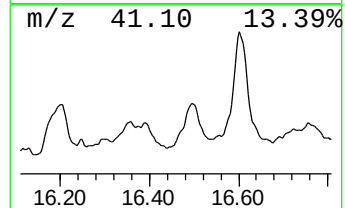
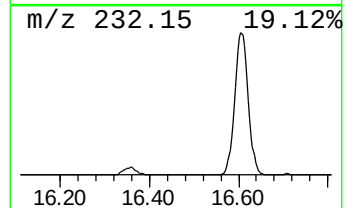
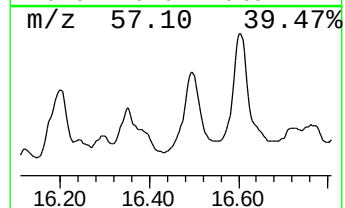
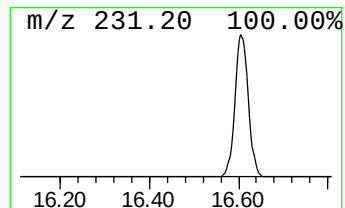
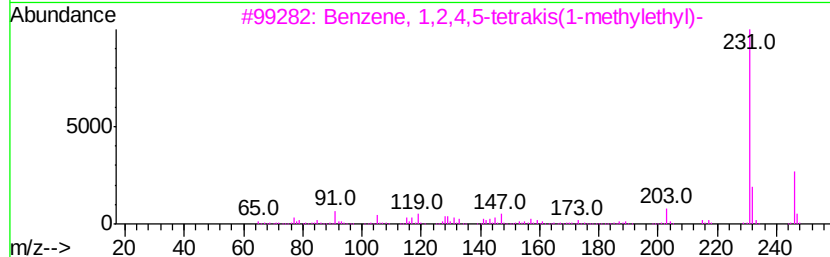
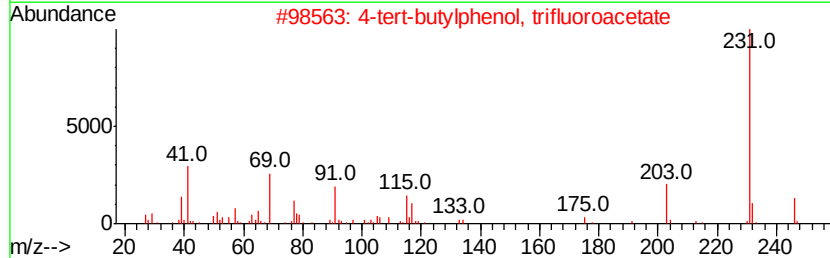
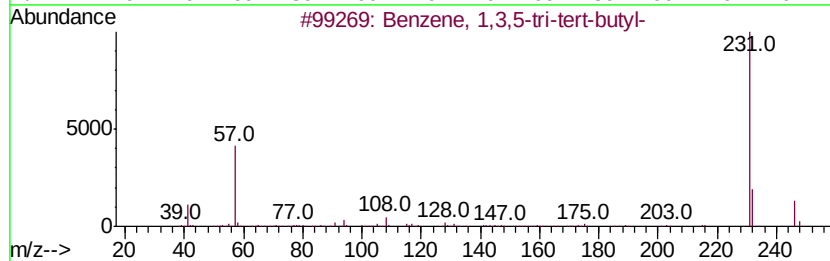
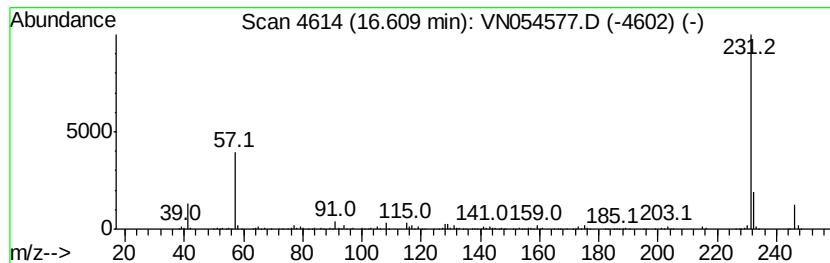
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Peak Number 4 Benzene, 1,3,5-tri-tert-butyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	31.23 ug/l	1134360	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	93
2		4-tert-butylphenol, trifluoroace...	246	C12H13F3O2	1000376-51-5	64
3		Benzene, 1,2,4,5-tetrakis(1-meth...	246	C18H30	000635-11-0	56
4		2-Cyano-3-phenylquinoxaline	231	C15H9N3	059393-45-2	53
5		Benzene, hexaethyl-	246	C18H30	000604-88-6	50



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Nonane, 3-methyl-...	15.78	6.8	ug/l	245742	4	13.34	1816390	50.0
Octane, 4-ethyl-	16.20	14.7	ug/l	532917	4	13.34	1816390	50.0
Hexane, 2,2,5-tri...	16.50	7.0	ug/l	252355	4	13.34	1816390	50.0
Benzene, 1,3,5-tr...	16.61	31.2	ug/l	1134360	4	13.34	1816390	50.0