

Data Path : Z:\VOASRV\HPCHEM1\MSVOA D\DATA\VD013020\
 Data File : VD065007.D
 Acq On : 30 Jan 2020 12:24
 Operator : VA/SY
 Sample : L1004-16
 Misc : 5.33G/5.00ml/MSVOA D/SOIL
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BU-01-012920

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_D\METHOD\82D012320S.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	2.320	58	68	72	rBV2	40544	81414	2.90%	0.439%
2	4.167	374	382	393	rBV2	37466	106427	3.79%	0.574%
3	4.967	507	518	529	rBV5	12793	44431	1.58%	0.240%
4	7.920	1009	1020	1025	rBV	384896	929083	33.07%	5.011%
5	7.985	1025	1031	1043	rVB	715079	1596922	56.85%	8.612%
6	8.338	1081	1091	1105	rBV	339707	776020	27.63%	4.185%
7	8.867	1172	1181	1191	rBV	1011971	2034967	72.44%	10.975%
8	10.344	1424	1432	1439	rBV	1585745	2809020	100.00%	15.149%
9	10.408	1439	1443	1450	rVV	75563	140256	4.99%	0.756%
10	10.726	1491	1497	1506	rBV2	23202	42303	1.51%	0.228%
11	11.649	1646	1654	1666	rBV	1463112	2537339	90.33%	13.684%
12	11.749	1666	1671	1677	rVB3	22980	39459	1.40%	0.213%
13	11.855	1683	1689	1699	rBV	84951	162853	5.80%	0.878%
14	12.191	1738	1746	1752	rBV2	31541	61500	2.19%	0.332%
15	12.643	1814	1823	1834	rVB	1163750	1935286	68.90%	10.437%
16	12.961	1873	1877	1883	rVB6	24019	40158	1.43%	0.217%
17	13.143	1899	1908	1914	rBV3	34399	58690	2.09%	0.317%
18	13.585	1976	1983	1992	rVB	1518287	2483958	88.43%	13.396%
19	13.685	1992	2000	2008	rVB5	18296	37305	1.33%	0.201%
20	13.908	2033	2038	2041	rBV4	25921	41671	1.48%	0.225%
21	13.967	2041	2048	2054	rVV	353206	562609	20.03%	3.034%
22	14.032	2054	2059	2063	rBV2	35343	63479	2.26%	0.342%
23	14.120	2069	2074	2079	rVB4	32021	61662	2.20%	0.333%
24	14.402	2111	2122	2129	rBV	176444	340699	12.13%	1.837%
25	14.561	2143	2149	2158	rVB	367042	587038	20.90%	3.166%
26	14.761	2179	2183	2190	rVB3	34390	51874	1.85%	0.280%
27	14.849	2190	2198	2202	rBV2	80956	153669	5.47%	0.829%
28	15.290	2267	2273	2280	rVB10	11147	29755	1.06%	0.160%
29	15.373	2283	2287	2291	rBV7	18437	37146	1.32%	0.200%
30	15.608	2320	2327	2334	rVB6	30542	56010	1.99%	0.302%
31	15.931	2375	2382	2388	rVB2	47580	91985	3.27%	0.496%
32	16.220	2424	2431	2440	rBV	181197	365124	13.00%	1.969%
33	16.514	2472	2481	2490	rVB5	32798	83520	2.97%	0.450%
34	16.720	2506	2516	2526	rBV3	37124	98489	3.51%	0.531%

LSC Area Percent Report

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ClientSampleId :
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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_D\METHOD\82D012320S.M
Title : SW846 8260

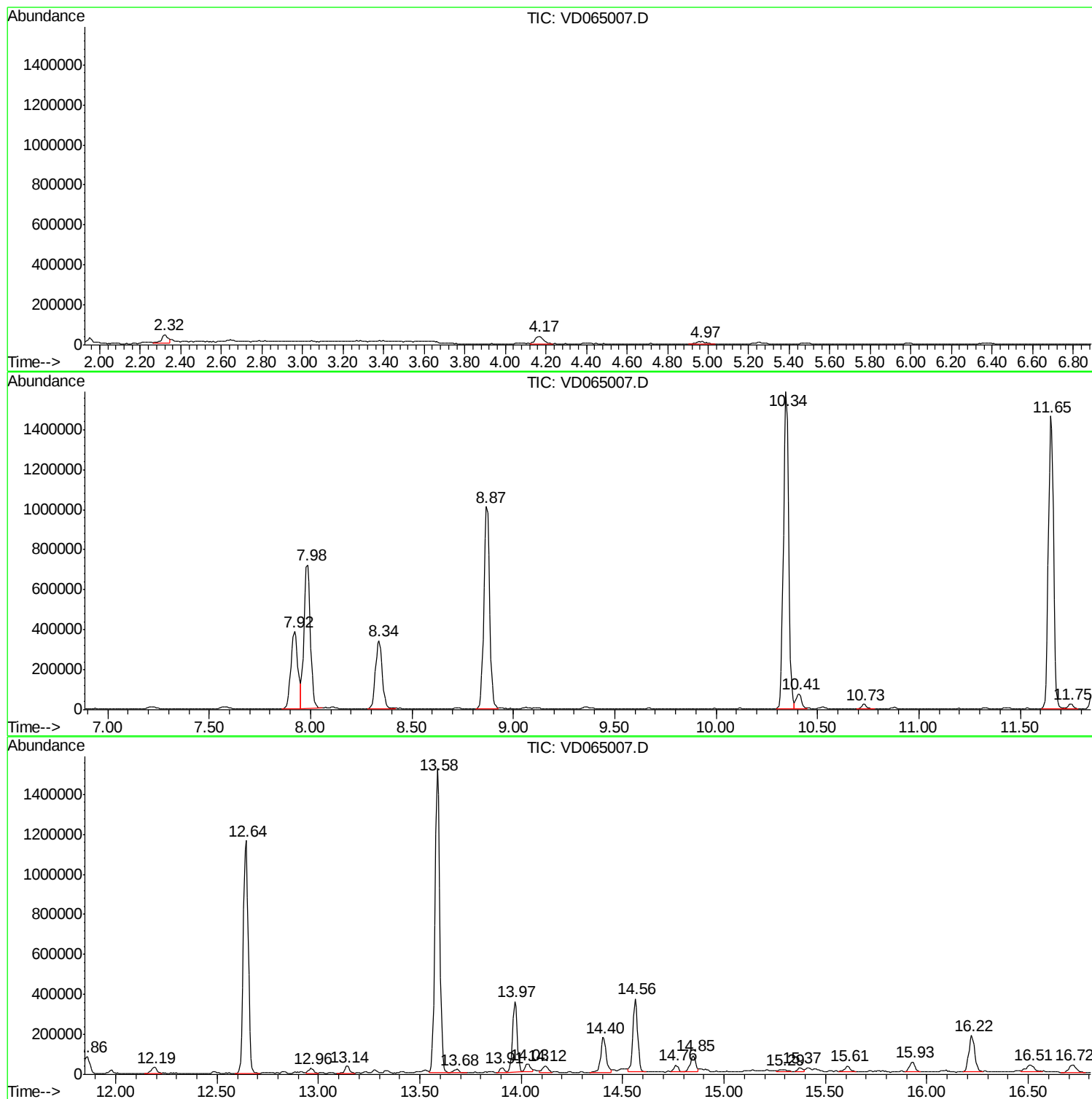
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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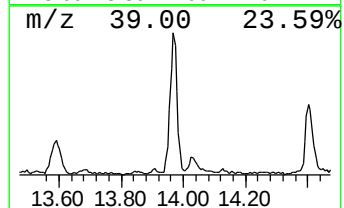
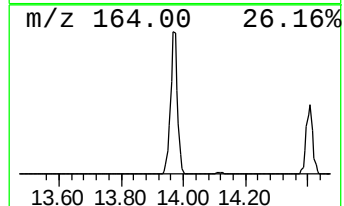
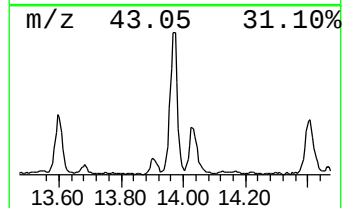
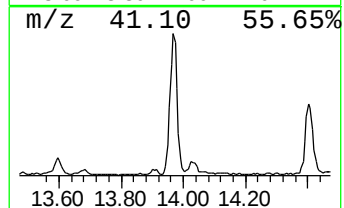
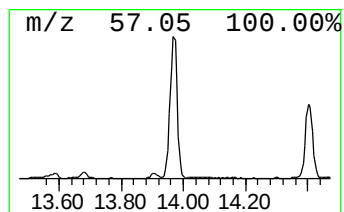
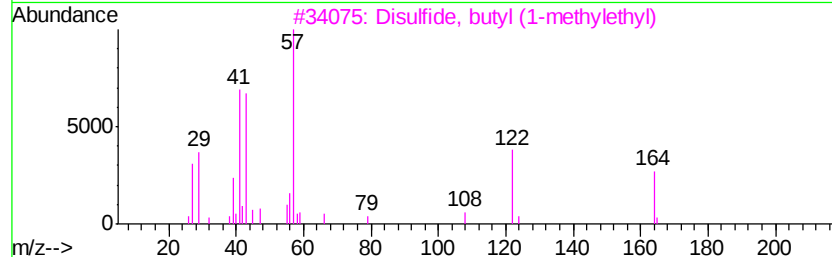
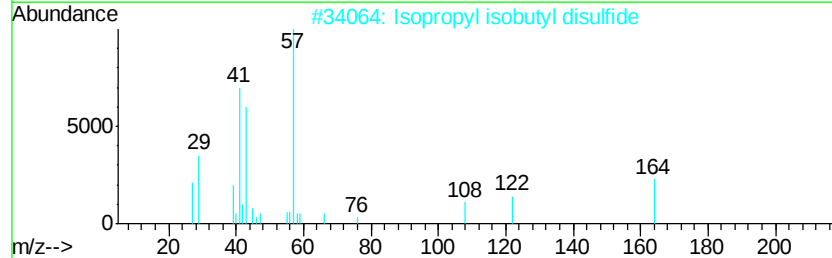
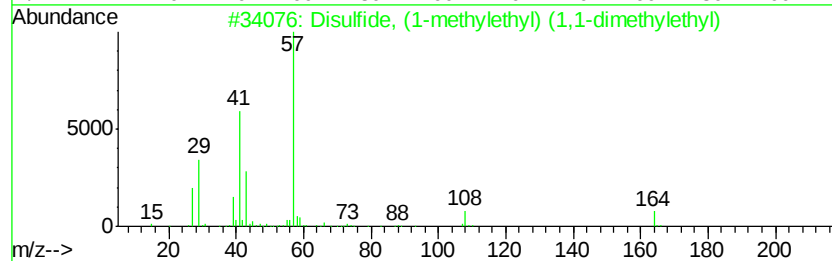
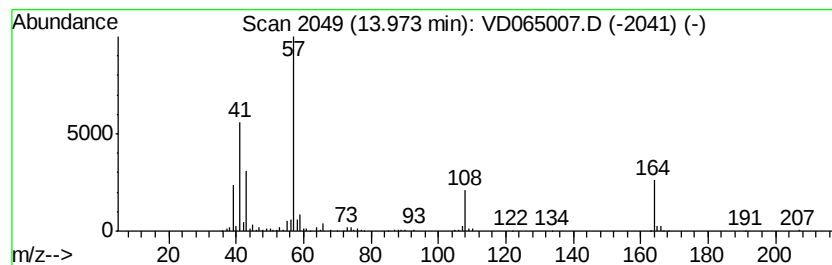
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_D\METHOD\82D012320S.M
Quant Title : SW846 8260

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

Peak Number 1 Disulfide, (1-methylethyl) ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.97	11.32 ug/l	562609	1,4-Dichlorobenzene-d4	13.58		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	87
2		Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	45
3		Disulfide, butyl (1-methylethyl)	164	C7H16S2	072437-53-7	40
4		t-Butylthiothioacetic acid, S-t-...	220	C10H20O2S2	1000189-14-7	36
5		Valeric acid, 3,4-dichlorophenyl...	246	C11H12Cl2O2	1000307-98-8	17



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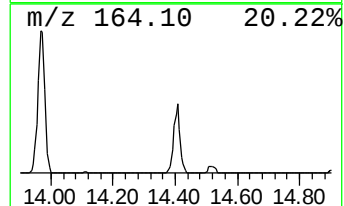
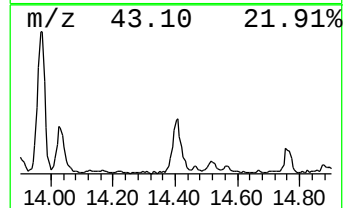
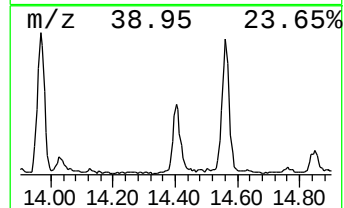
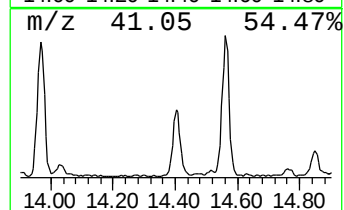
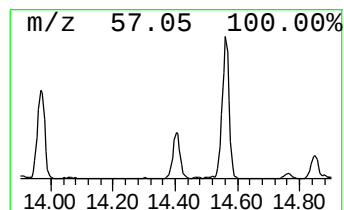
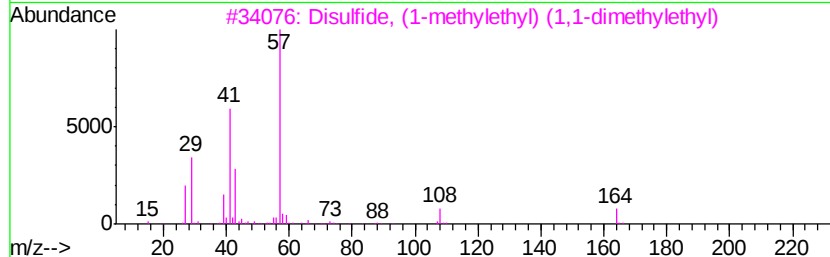
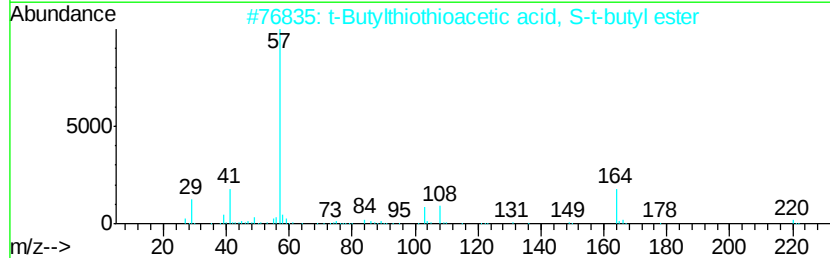
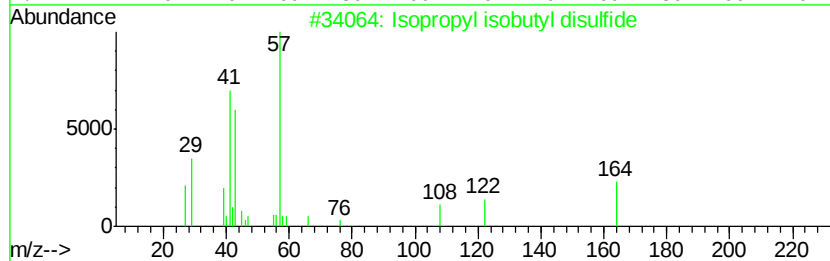
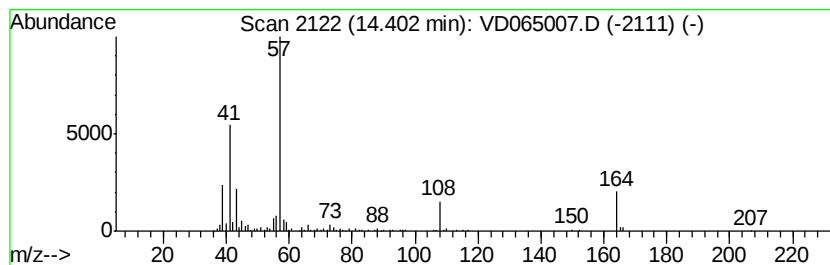
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Quant Title : SW846 8260

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

Peak Number 2 Isopropyl isobutyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.40	6.86 ug/l	340699	1,4-Dichlorobenzene-d4	13.58		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	83
2		t-Butylthiothioacetic acid, S-t-	220	C10H20O2S2	1000189-14-7	78
3		Disulfide, (1-methylethyl) (1,1-	164	C7H16S2	043022-60-2	64
4		Disulfide, butyl (1-methylethyl)	164	C7H16S2	072437-53-7	45
5		Acetic acid, [(1,1-dimethylethyl...	148	C6H12O2S	024310-22-3	16



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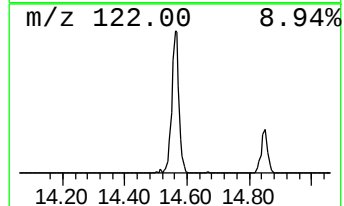
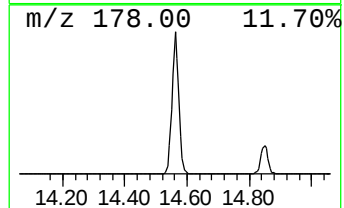
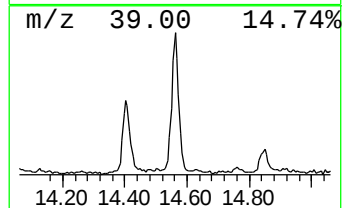
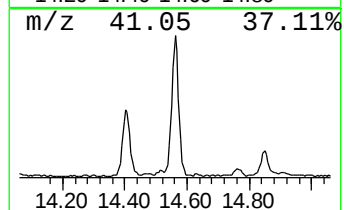
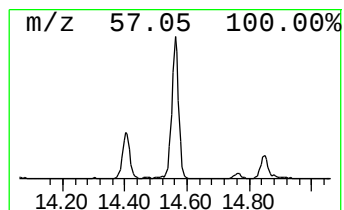
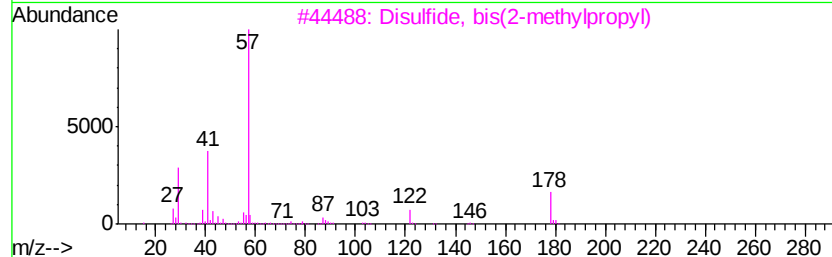
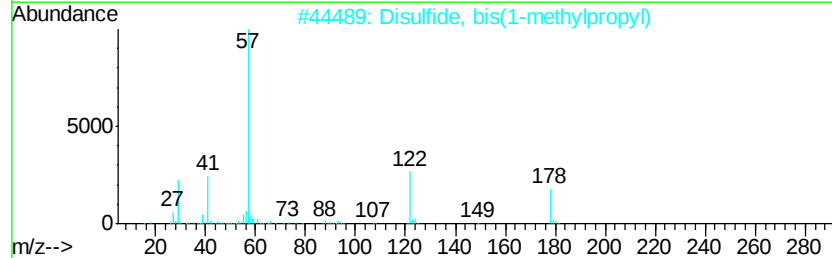
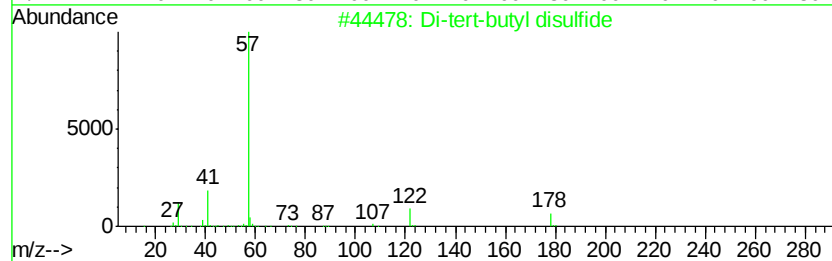
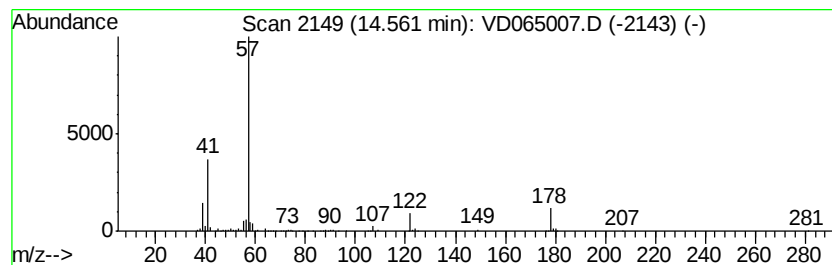
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Quant Title : SW846 8260

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

Peak Number 3 Di-tert-butyl disulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.56	11.82 ug/l	587038	1,4-Dichlorobenzene-d4		13.58	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	80
2		Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	72
3		Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	64
4		Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	40
5		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38



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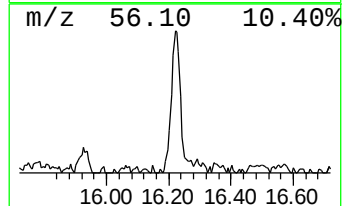
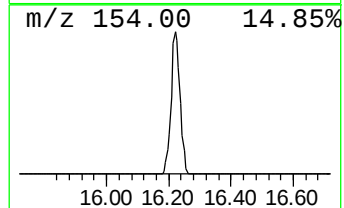
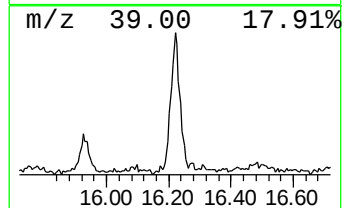
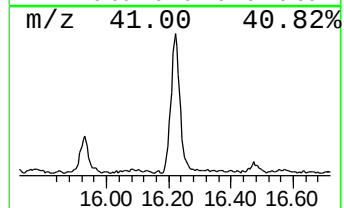
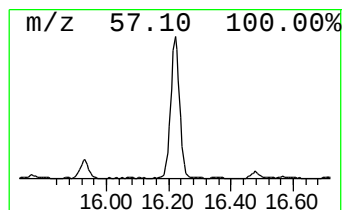
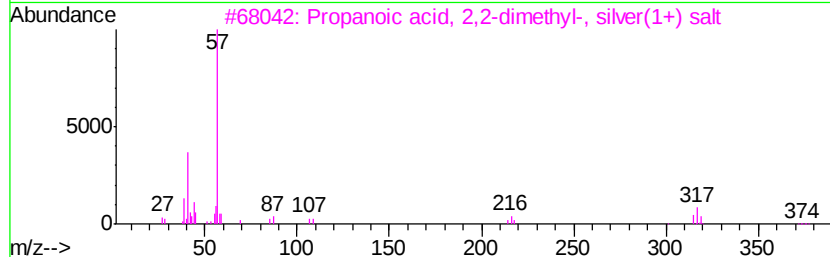
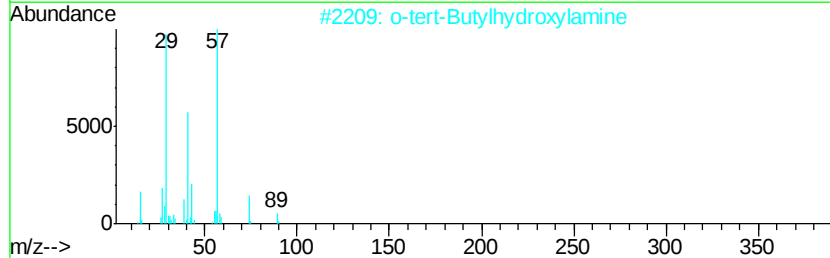
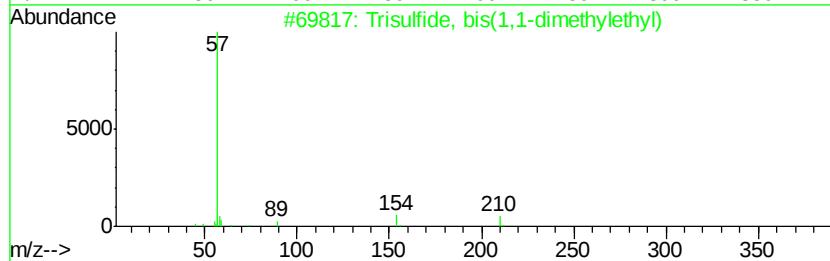
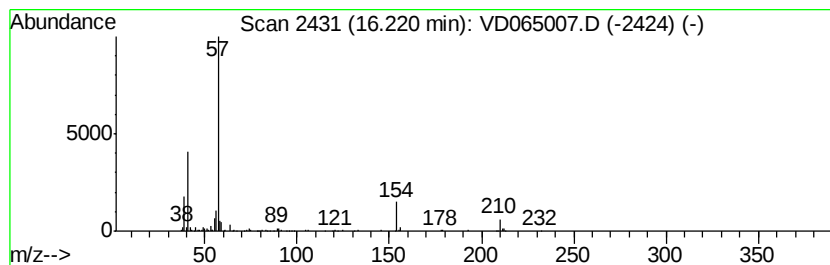
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	7.35 ug/l	365124	1,4-Dichlorobenzene-d4	13.58

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	58
2		o-tert-Butylhydroxylamine	89	C4H11NO	1000322-43-1	43
3		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AqO2	007324-58-5	43
4		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	25
5		Butane, 2-bromo-	136	C4H9Br	000078-76-2	25



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, (1-met...	13.97	11.3	ug/l	562609	4	13.58	2483960	50.0
Isopropyl isobuty...	14.40	6.9	ug/l	340699	4	13.58	2483960	50.0
Di-tert-butyl dis...	14.56	11.8	ug/l	587038	4	13.58	2483960	50.0
Trisulfide, bis(1...	16.22	7.3	ug/l	365124	4	13.58	2483960	50.0