LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA F\DATA\VF111918\
Data File : VF060793.D
Acq On : 19 Nov 2018 23:22
Operator : VA/AP
Sample : J5950-12
Misc : 5.50g/5mL/MSVOA-F/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : SSI-15

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_F\METHODS\82F111318S.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	1.090	43	47	55	rBV4	9451	30661	2.82%	0.368%
2	2.185	153	158	160	rBV2	9120	19656	1.81%	0.236%
3	2.234	160	163	168	rVB4	8878	25288	2.32%	0.304%
4	2.382	175	178	183	rBV3	8172	18439	1.69%	0.221%
5	3.872	320	329	333	rBV7	3586	13678	1.26%	0.164%
6	4.029	337	345	348	rBV2	7627	29092	2.67%	0.349%
7	4.128	348	355	366	rVB	127719	409582	37.62%	4.917%
8	4.434	378	386	390	rBV6	3388	11106	1.02%	0.133%
9	4.878	422	431	443	rBV2	230962	854851	78.52%	10.262%
10	5.608	498	505	519	rBV	292982	788943	72.47%	9.471%
11	6.269	567	572	577	rVB4	4797	14238	1.31%	0.171%
12	6.456	585	591	595	rBV5	4925	15579	1.43%	0.187%
13	7.146	655	661	665	rBV5	3908	13760	1.26%	0.165%
14	7.294	675	676	678	rBV	59325	37842	3.48%	0.454%
15	7.561	697	703	719	rBV	351936	865774	79.53%	10.393%
16	8.232	766	771	774	rBV3	5445	14019	1.29%	0.168%
17	9.780	923	928	937	rBV	386660	880628	80.89%	10.571%
18	11.280	1077	1080	1083	rVB4	6710	12331	1.13%	0.148%
19	11.418	1090	1094	1102	rBV	402281	700623	64.36%	8.411%
20	11.566	1106	1109	1116	rVV4	14893	33096	3.04%	0.397%
21	11.664	1116	1119	1122	rVV2	22267	30778	2.83%	0.369%
22	11.832	1133	1136	1140	rBV5	10384	18468	1.70%	0.222%
23	11.891	1140	1142	1145	rBV4	5011	11324	1.04%	0.136%
24	12.000	1150	1153	1158	rVB6	11038	27089	2.49%	0.325%
25	12.079	1158	1161	1164	rBV4	11180	21647	1.99%	0.260%
26	12.207	1172	1174	1178	rVB4	18431	30976	2.85%	0.372%
27	12.296	1180	1183	1186	rBV3	14461	27243	2.50%	0.327%
28	12.384	1190	1192	1194	rBV3	8553	12954	1.19%	0.156%
29	12.434	1194	1197	1198	rVV2	14202	25867	2.38%	0.311%
30	12.463	1198	1200	1202	rVV2	18165	27919	2.56%	0.335%
31	12.562	1206	1210	1218	rVB	623115	1088645	100.00%	13.069%
32	12.818	1233	1236	1243	rVB3	36434	73713	6.77%	0.885%
33	13.016	1253	1256	1259	rVB5	7160	13177	1.21%	0.158%
34	13.164	1269	1271	1274	rVB3	12170	19199	1.76%	0.230%

LSC Area Percent Report

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Misc : 5.50g/5mL/MSVOA-F/SOIL
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : SSI-15

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_F\METHODS\82F111318S.M
Title : SW846 8260

35	13.292	1279	1284	1287	rBV3	12849	30325	2.79%	0.364%
36	13.420	1296	1297	1301	rVB3	10174	18389	1.69%	0.221%
37	13.509	1303	1306	1308	rVV3	20252	35365	3.25%	0.425%
38	13.548	1308	1310	1315	rVB2	14407	24449	2.25%	0.293%
39	13.716	1322	1327	1332	rBV3	39747	75817	6.96%	0.910%
40	13.785	1332	1334	1337	rVV	43901	64343	5.91%	0.772%
41	13.854	1337	1341	1347	rVV2	73433	190081	17.46%	2.282%
42	13.933	1347	1349	1352	rVB3	12794	18069	1.66%	0.217%
43	14.091	1363	1365	1368	rVB	31941	42028	3.86%	0.505%
44	14.160	1368	1372	1374	rBV3	30939	62308	5.72%	0.748%
45	14.199	1374	1376	1379	rVV	37854	70694	6.49%	0.849%
46	14.249	1379	1381	1383	rVB	36810	46964	4.31%	0.564%
47	14.436	1397	1400	1401	rBV	39348	49969	4.59%	0.600%
48	14.466	1401	1403	1404	rVV	46284	60495	5.56%	0.726%
49	14.525	1404	1409	1411	rVV	91332	238517	21.91%	2.863%
50	14.574	1411	1414	1416	rVV2	49465	109374	10.05%	1.313%
51	14.614	1416	1418	1427	rVB	126610	223920	20.57%	2.688%
52	14.752	1427	1432	1434	rBV6	8403	18088	1.66%	0.217%
53	14.841	1435	1441	1443	rBV3	28487	69851	6.42%	0.839%
54	14.900	1446	1447	1451	rVB2	22952	34798	3.20%	0.418%
55	14.989	1451	1456	1457	rBV4	17288	39187	3.60%	0.470%
56	15.018	1457	1459	1461	rVB	27981	30891	2.84%	0.371%
57	15.127	1467	1470	1473	rBV	75175	92669	8.51%	1.112%
58	15.176	1473	1475	1477	rVV2	13681	19043	1.75%	0.229%
59	15.215	1477	1479	1482	rVV2	21317	34537	3.17%	0.415%
60	15.284	1484	1486	1489	rVB	34033	50538	4.64%	0.607%
61	15.413	1497	1499	1501	rBV	23683	34666	3.18%	0.416%
62	15.452	1501	1503	1508	rVB4	17867	35094	3.22%	0.421%
63	15.521	1508	1510	1511	rBV	13007	14953	1.37%	0.180%
64	15.571	1511	1515	1517	rVV	50487	88830	8.16%	1.066%
65	15.610	1517	1519	1522	rVB2	23231	36398	3.34%	0.437%
66	15.788	1534	1537	1543	rVV	62054	103668	9.52%	1.244%
67	15.886	1544	1547	1549	rVV4	8533	14897	1.37%	0.179%
68	15.926	1549	1551	1556	rVV5	6543	17000	1.56%	0.204%
69	16.005	1556	1559	1563	rVB6	8476	15877	1.46%	0.191%

Sum of corrected areas: 8330277

LSC Report - Integrated Chromatogram

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Operator : VA/AP
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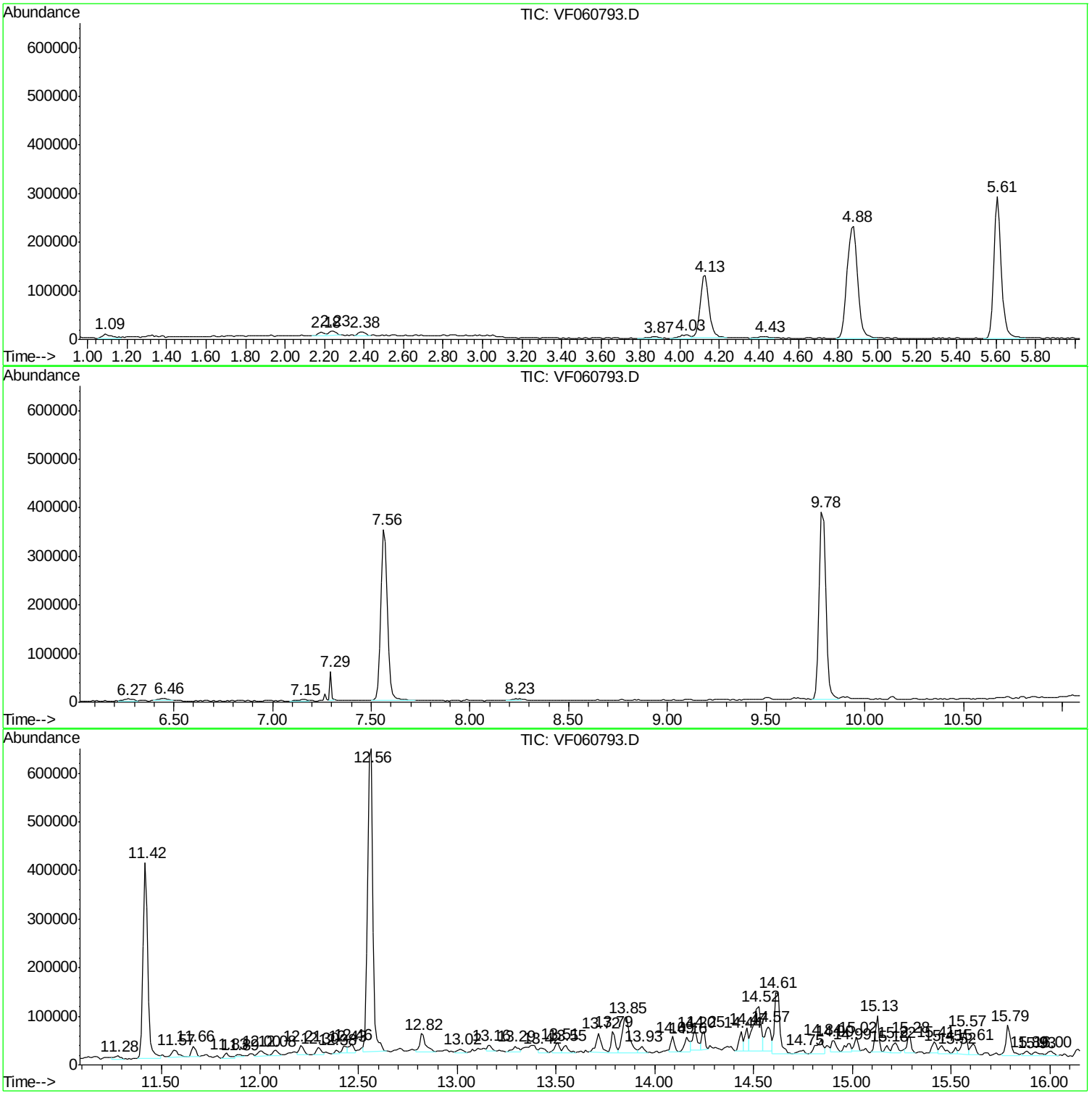
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_F
ClientSampleId :
SSI-15

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F111318S.M
Quant Title : SW846 8260

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



Library Search Compound Report

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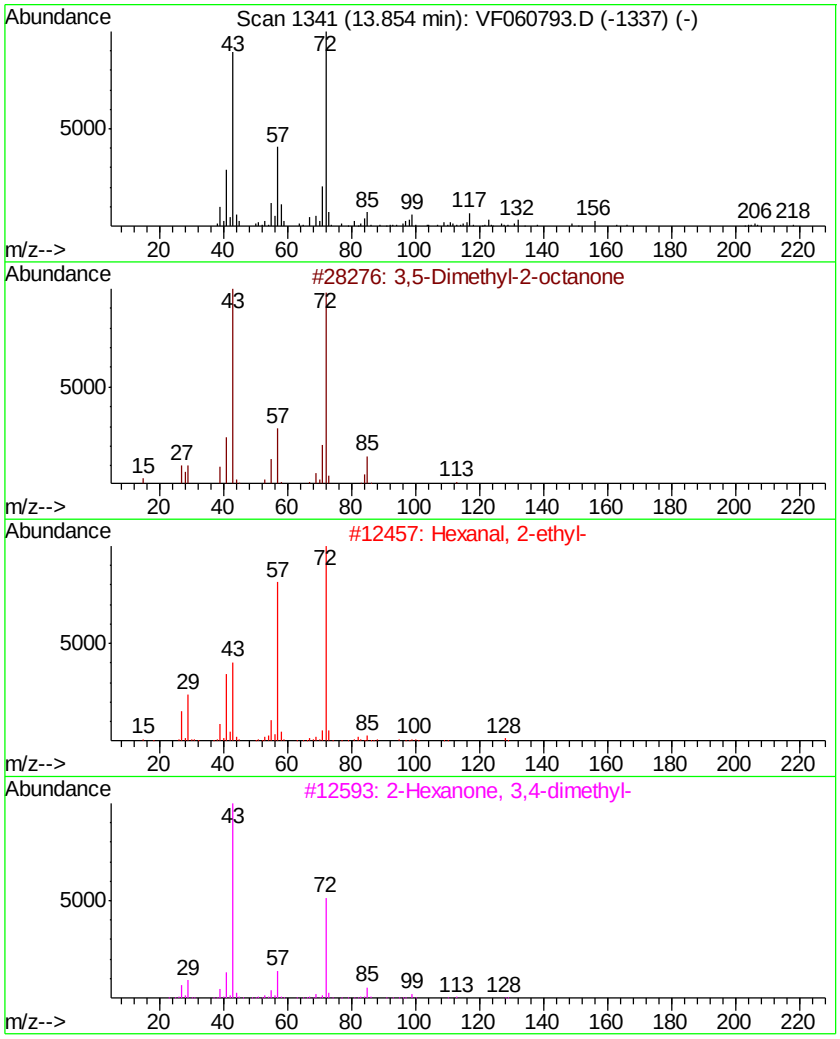
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

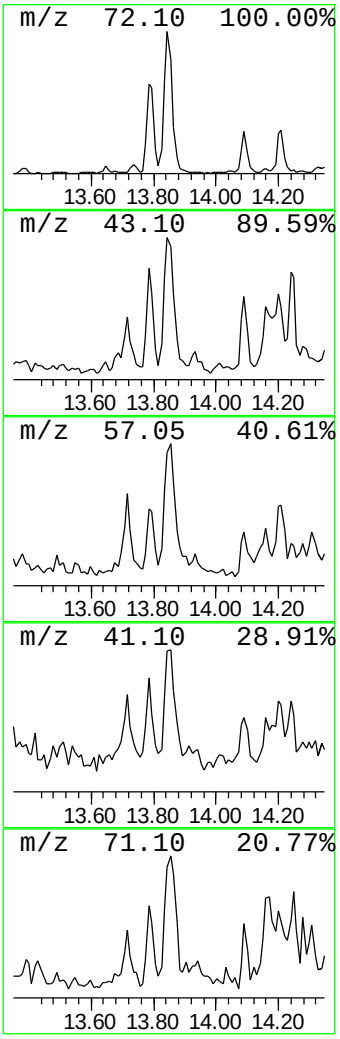
****

Peak Number 1 3,5-Dimethyl-2-octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	8.73 ug/l	190081	1,4-Dichlorobenzene-d4	12.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethyl-2-octanone	156	C10H20O	019781-14-7	64
2	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	53
3	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	50
4	Benzeneethanamine, N,N,.alpha.-t...	163	C11H17N	004075-96-1	50
5	L-2-Aminobutyric acid, N-methyl-...	131	C6H13NO2	1000332-98-7	47





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Sample : J5950-12
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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : SSI-15

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F111318S.M
Quant Title : SW846 8260

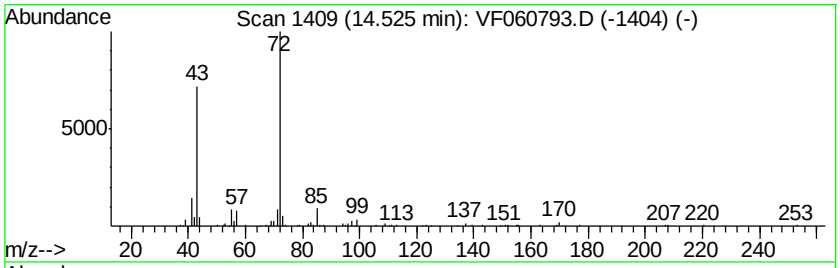
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

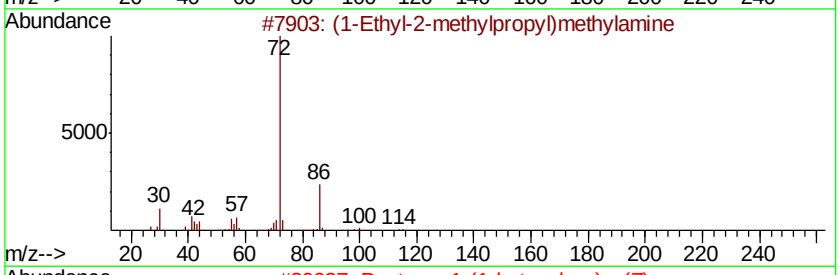
****

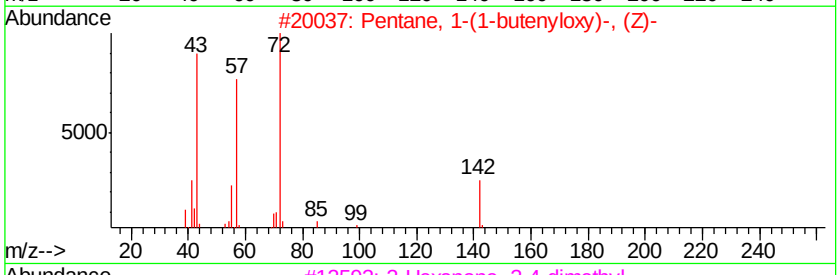
Peak Number 2 (1-Ethyl-2-methylpropyl)met... Concentration Rank 1

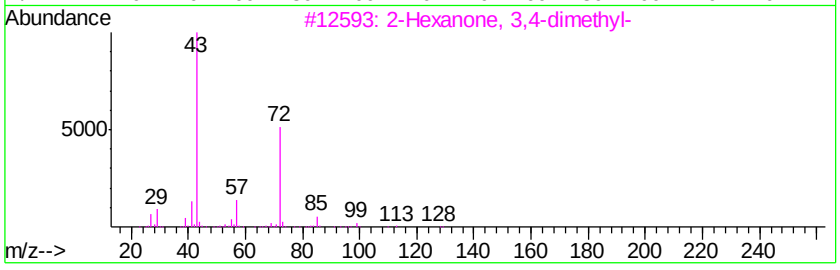
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	10.95 ug/l	238517	1,4-Dichlorobenzene-d4	12.56

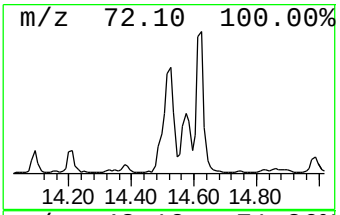
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Ethyl-2-methylpropyl)methylamine	115	C7H17N	1000195-05-6	59
2	Pentane, 1-(1-butenyloxy)-, (Z)-	142	C9H18O	056052-76-7	56
3	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	56
4	S-[4-Cyanophenyl]-N,N-dimethylth...	206	C10H10N2OS	019290-43-8	50
5	N,N Dimethyl-3,4-methylenedioxya...	207	C12H17NO2	074698-50-3	45

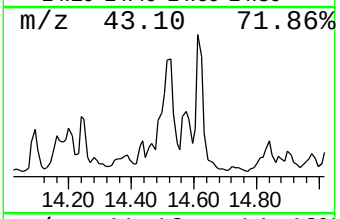


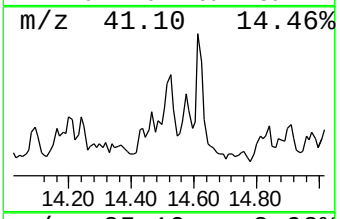


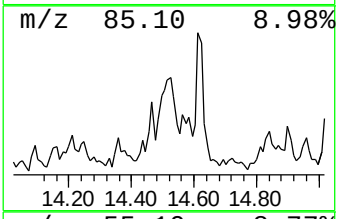


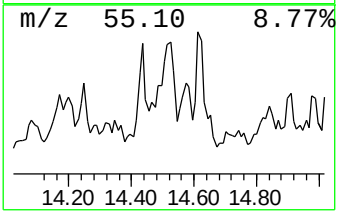












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Quant Title : SW846 8260

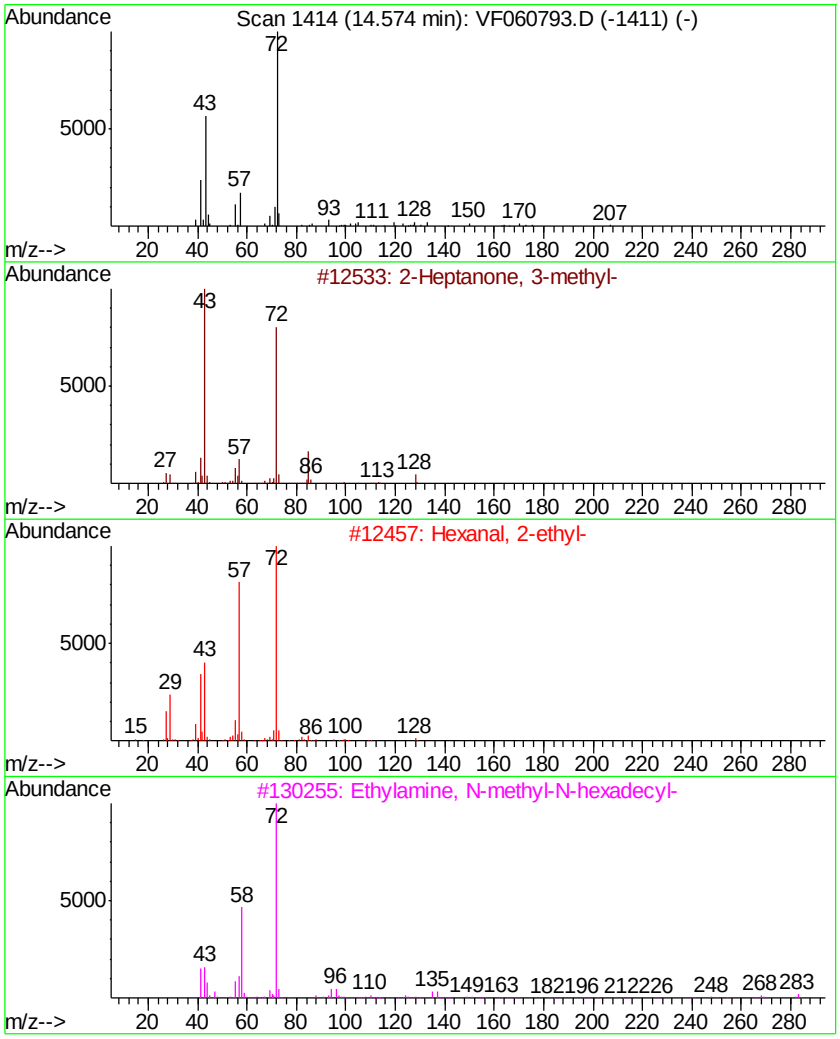
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

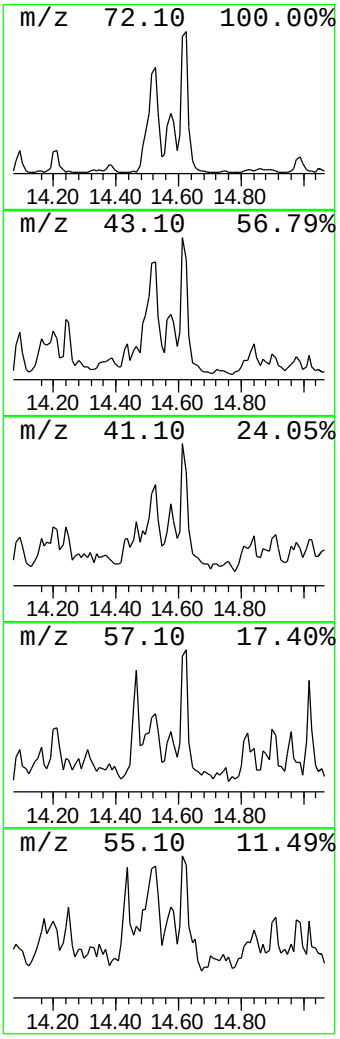
****

Peak Number 3 2-Heptanone, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	5.02 ug/l	109374	1,4-Dichlorobenzene-d4	12.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	64
2	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	64
3	Ethylamine, N-methyl-N-hexadecyl-	283	C19H41N	066997-40-8	39
4	Ether, 1-butylvinyl methyl	114	C7H14O	016519-66-7	38
5	L-Valine, N-(3-cyclopentylpropio...	297	C17H31NO3	1000346-65-5	38





Library Search Compound Report

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Quant Title : SW846 8260

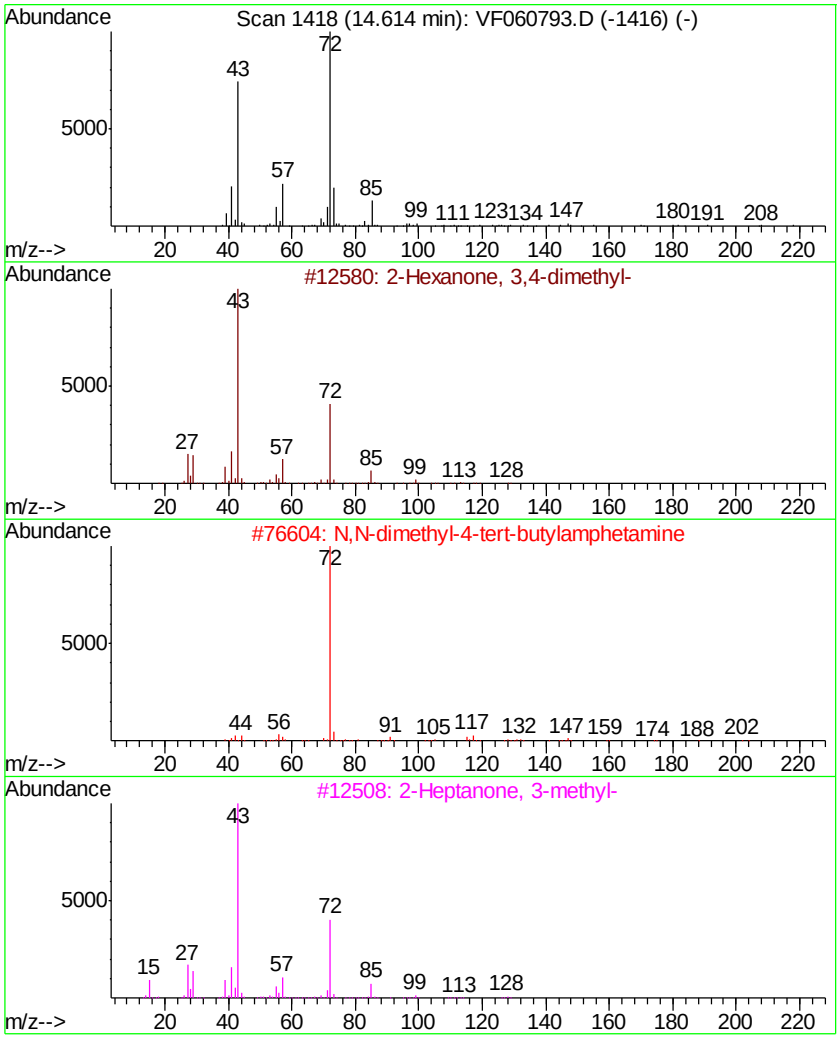
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

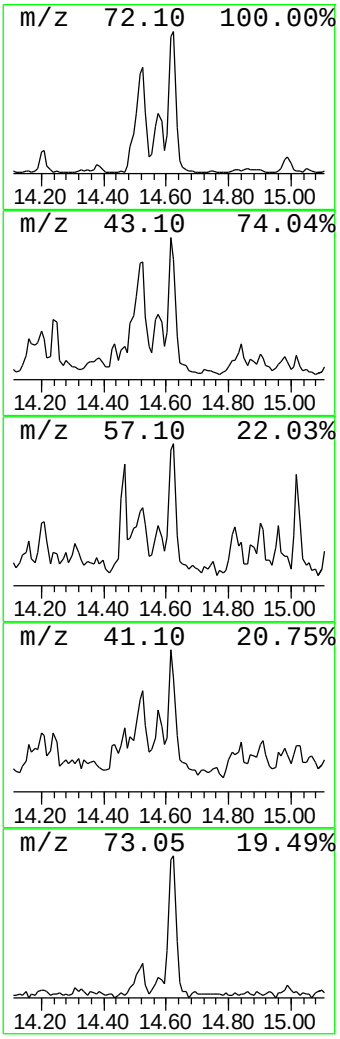
****

Peak Number 4 unknown14.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	10.28 ug/l	223920	1,4-Dichlorobenzene-d4	12.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	47
2	N,N-dimethyl-4-tert-butylampheta...	219	C15H25N	1000378-90-5	37
3	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	33
4	3,3-Dimethyl-3-silathietane	118	C4H10SSi	077205-52-8	33
5	2-Chloro-N,N-dimethyl-acrylamide	133	C5H8ClNO	071364-54-0	32





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F111318S.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3,5-Dimethyl-2-oc...	13.85	8.7	ug/l	190081	4	12.56	1088650	50.0
(1-Ethyl-2-methyl...	14.52	10.9	ug/l	238517	4	12.56	1088650	50.0
2-Heptanone, 3-me...	14.57	5.0	ug/l	109374	4	12.56	1088650	50.0
unknown14.61	14.61	10.3	ug/l	223920	4	12.56	1088650	50.0