LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM102717\
Data File : BM012516.D
Acq On : 28 Oct 2017 09:38
Operator : SJ/JU
Sample : I5786-06 5X
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.169	10	14	21	rVB	492164	572823	7.48%	0.927%
2	3.275	28	32	42	rVB	59356	94362	1.23%	0.153%
3	3.722	90	108	111	rBV	602319	1880677	24.56%	3.042%
4	4.069	148	167	170	rBV	756792	2573441	33.61%	4.163%
5	4.757	279	284	291	rVB	58622	90550	1.18%	0.146%
6	5.728	443	449	458	rBV	612656	832321	10.87%	1.346%
7	5.887	471	476	483	rBV2	62482	111633	1.46%	0.181%
8	6.393	551	562	565	rBV6	53982	119050	1.55%	0.193%
9	6.546	580	588	599	rVB3	51696	121528	1.59%	0.197%
10	6.928	638	653	657	rBV	468250	1192865	15.58%	1.930%
11	7.040	664	672	688	rVB2	511194	1091797	14.26%	1.766%
12	7.198	694	699	706	rVB	360605	561826	7.34%	0.909%
13	7.404	723	734	747	rVB	485741	873248	11.40%	1.413%
14	7.798	792	801	805	rBV6	46001	121955	1.59%	0.197%
15	7.869	805	813	820	rVB	2022919	3356246	43.83%	5.429%
16	8.057	841	845	850	rVB3	64424	107287	1.40%	0.174%
17	8.428	901	908	918	rVB7	55304	142735	1.86%	0.231%
18	8.575	925	933	940	rBV	495035	823160	10.75%	1.332%
19	8.975	991	1001	1004	rBV8	59866	150572	1.97%	0.244%
20	9.028	1004	1010	1016	rVB	393922	653449	8.53%	1.057%
21	9.745	1125	1132	1139	rBV	360668	615149	8.03%	0.995%
22	9.998	1168	1175	1183	rBV	365488	669727	8.75%	1.083%
23	10.286	1213	1224	1231	rBV	571688	970493	12.67%	1.570%
24	10.663	1278	1288	1298	rBV	2508927	4162286	54.35%	6.733%
25	10.798	1305	1311	1322	rVB2	231634	475532	6.21%	0.769%
26	11.980	1504	1512	1520	rVB2	64899	128002	1.67%	0.207%
27	13.910	1831	1840	1845	rBV	870053	1287048	16.81%	2.082%
28	14.192	1883	1888	1900	rVB	1021046	1536665	20.07%	2.486%
29	14.404	1920	1924	1930	rBV	74311	100567	1.31%	0.163%
30	14.504	1932	1941	1949	rBV2	3313082	5134610	67.05%	8.306%
31	14.698	1970	1974	1984	rBV	348030	584798	7.64%	0.946%
32	14.904	2004	2009	2015	rVB4	58145	102702	1.34%	0.166%
33	15.357	2082	2086	2090	rVB	86074	101610	1.33%	0.164%
34	15.492	2099	2109	2115	rBV	1339308	1948291	25.44%	3.152%

LSC Area Percent Report

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Data File : BM012516.D
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Operator : SJ/JU
Sample : I5786-06 5X
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Title : SVOA CALIBRATION

35	15.616	2125	2130	2135	rBV	185638	263994	3.45%	0.427%
36	15.757	2152	2154	2161	rVB2	61287	89561	1.17%	0.145%
37	15.857	2166	2171	2176	rVB	296004	404419	5.28%	0.654%
38	16.215	2228	2232	2234	rBV2	140732	193741	2.53%	0.313%
39	17.004	2363	2366	2371	rBV2	112464	158381	2.07%	0.256%
40	17.057	2372	2375	2383	rVB2	115698	205436	2.68%	0.332%
41	17.245	2401	2407	2412	rBV2	4087212	5972898	78.00%	9.662%
42	17.286	2412	2414	2418	rVV	246904	278163	3.63%	0.450%
43	17.339	2418	2423	2433	rVB	1385522	2116963	27.64%	3.425%
44	17.739	2488	2491	2495	rBV	109052	134706	1.76%	0.218%
45	18.133	2555	2558	2562	rBV2	228924	290491	3.79%	0.470%
46	19.292	2752	2755	2762	rVB	411702	596334	7.79%	0.965%
47	19.627	2808	2812	2817	rBV	1721221	2693429	35.17%	4.357%
48	21.415	3111	3116	3120	rBV	5902023	7470577	97.55%	12.085%
49	23.721	3503	3508	3516	rVB2	4078610	7657855	100.00%	12.388%

Sum of corrected areas: 61815953

LSC Report - Integrated Chromatogram

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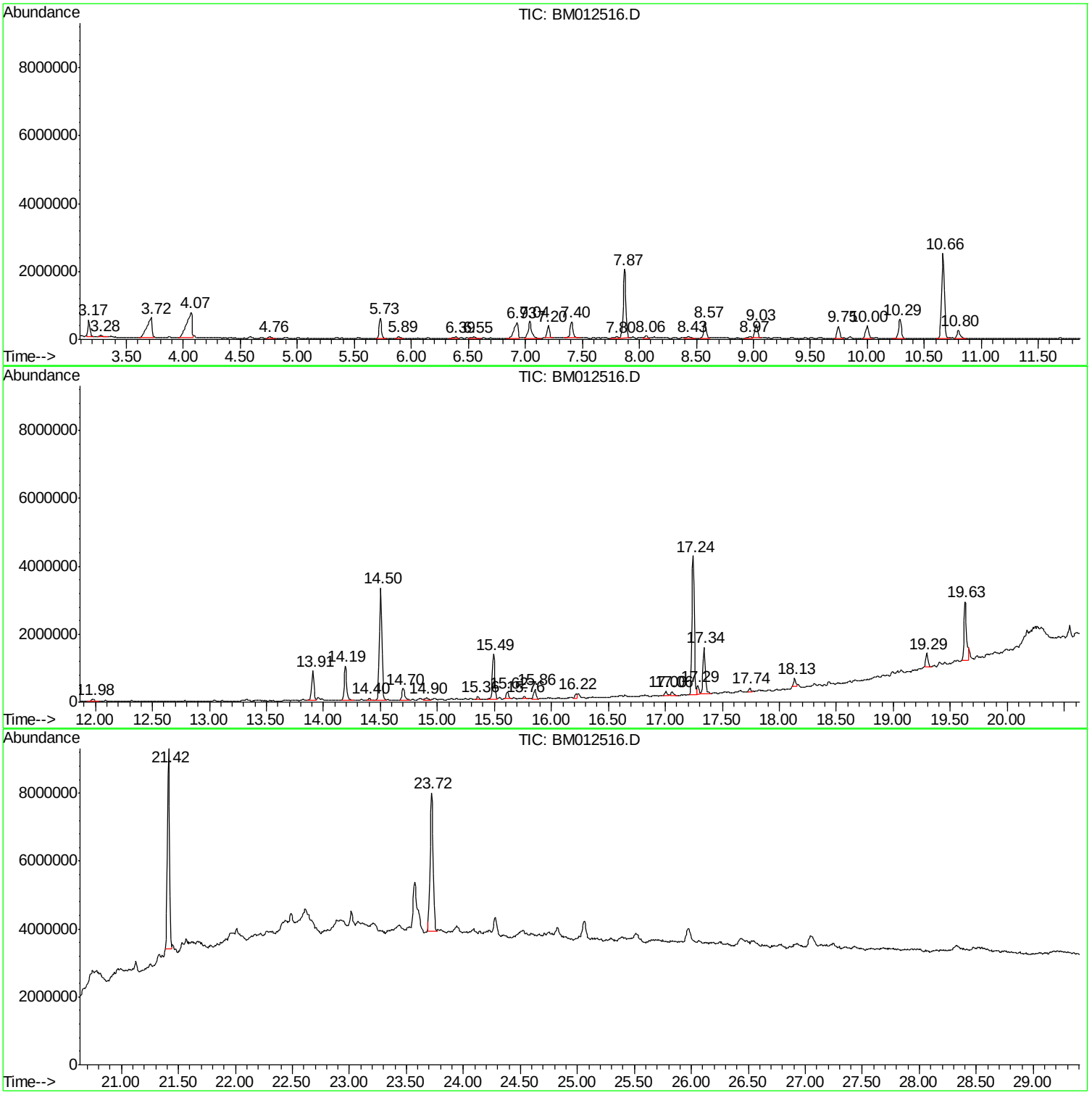
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM102717\
Data File : BM012516.D
Acq On : 28 Oct 2017 09:38
Operator : SJ/JU
Sample : I5786-06 5X
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

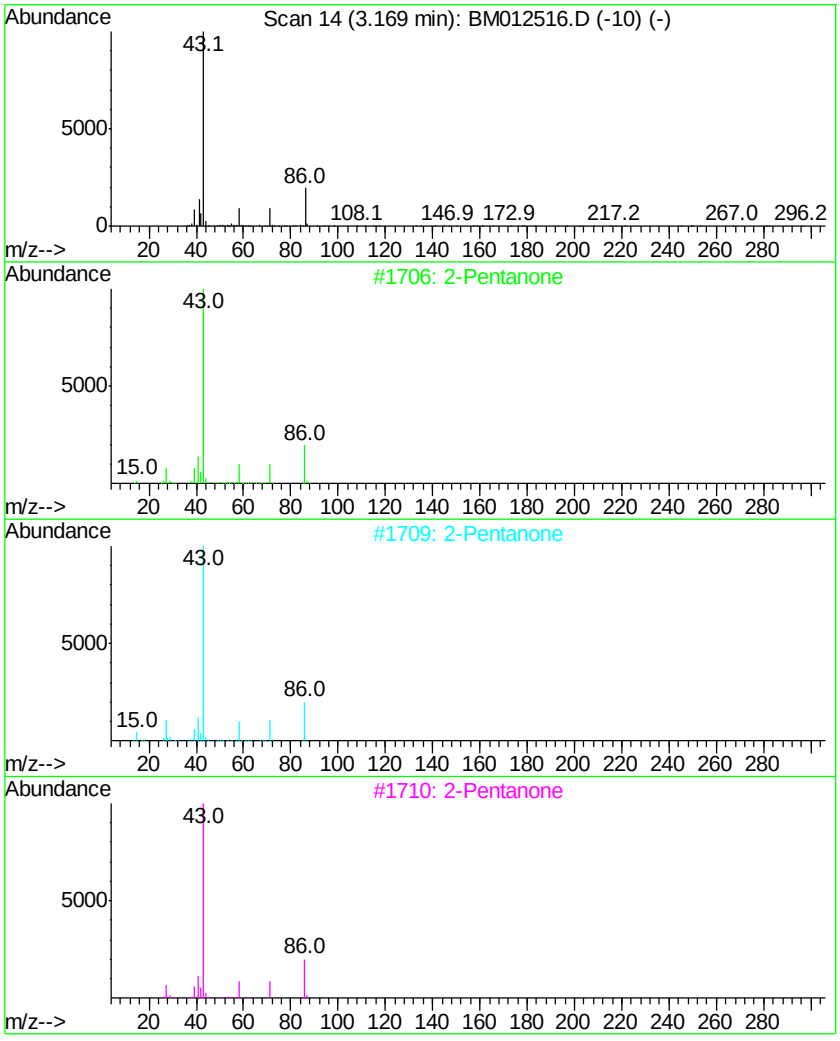
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

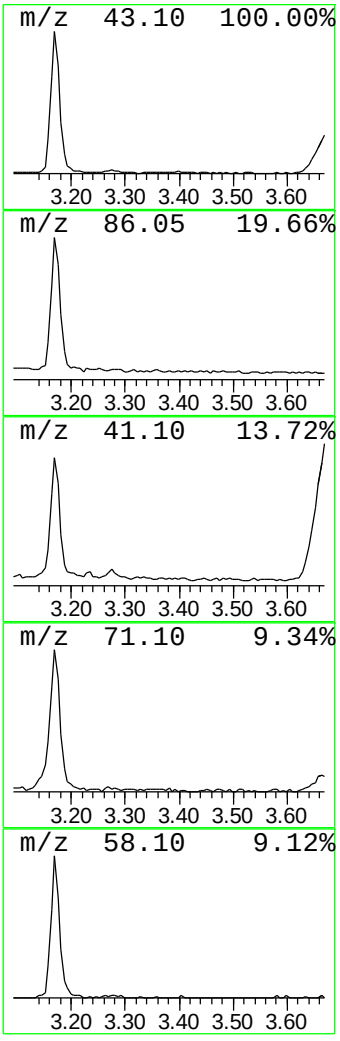
****

Peak Number 1 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	3.41 ng/ul	572823	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	87
2	2-Pentanone	86	C5H10O	000107-87-9	86
3	2-Pentanone	86	C5H10O	000107-87-9	83
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
5	2,3-Butanedione	86	C4H6O2	000431-03-8	49





Library Search Compound Report

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Misc :
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Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

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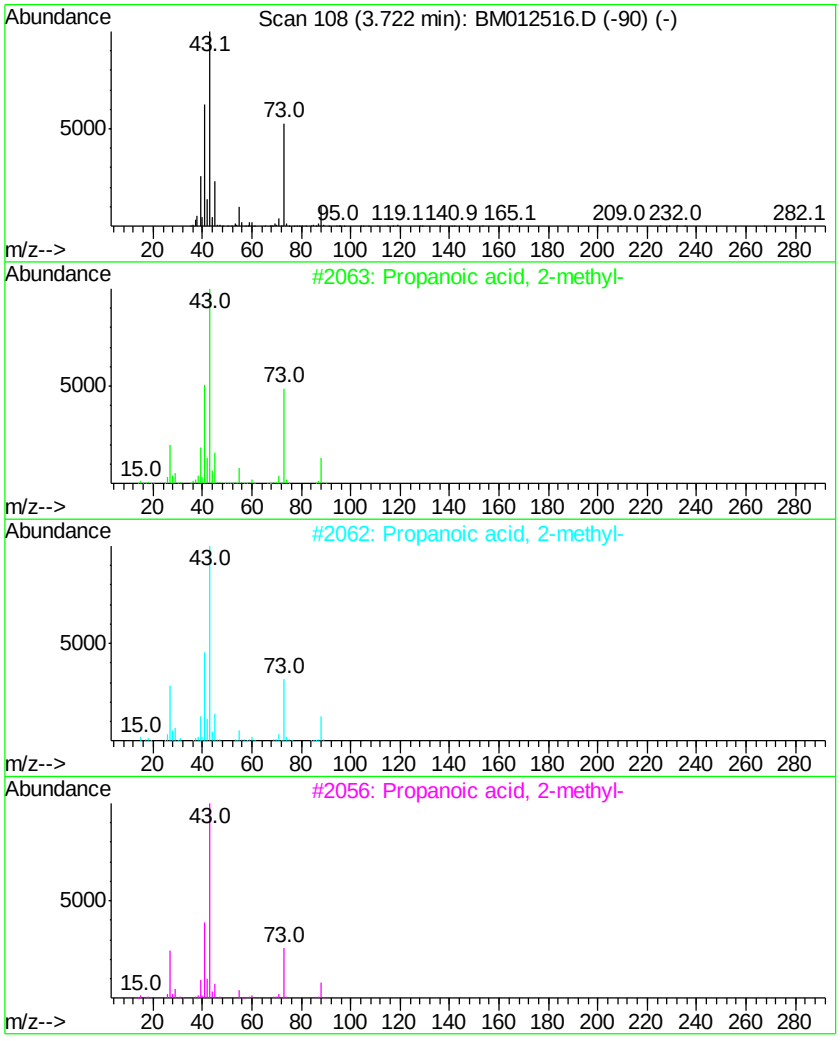
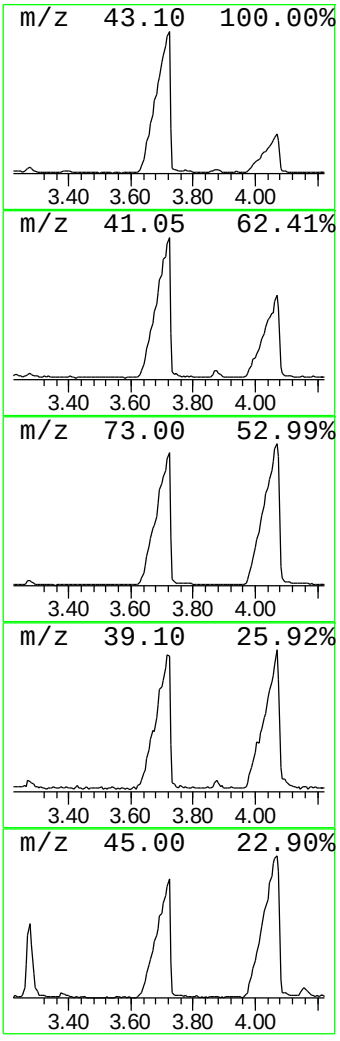
Peak Number 2 Propanoic acid, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	11.21 ng/ul	1880680	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	86
3	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	80
4	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	80
5	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	72





Library Search Compound Report

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Operator : SJ/JU
Sample : I5786-06 5X
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

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

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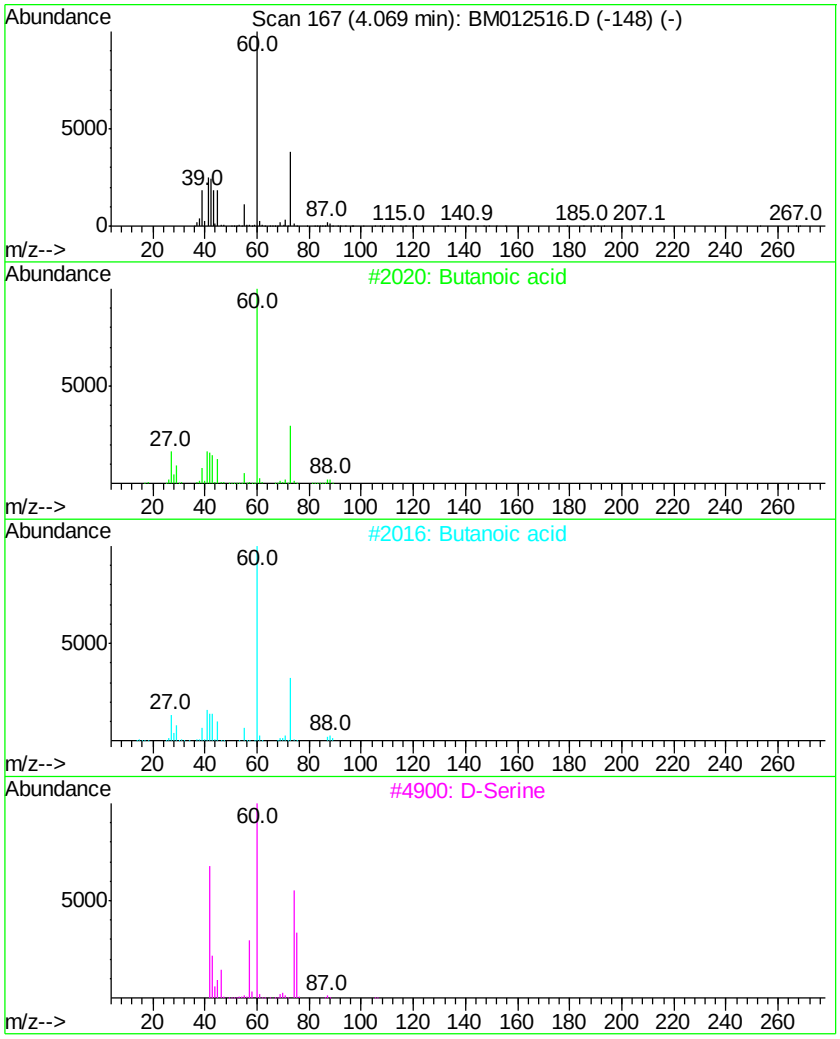
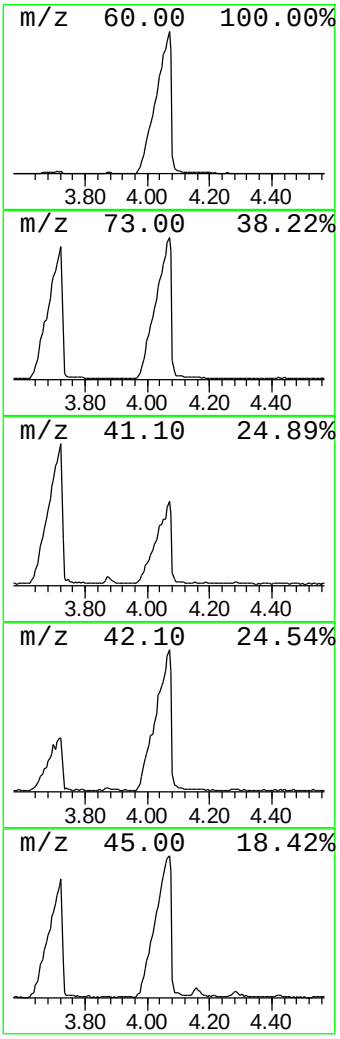
Peak Number 3 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	15.34 ng/ul	2573440	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	56
2	Butanoic acid	88	C4H8O2	000107-92-6	50
3	D-Serine	105	C3H7NO3	000312-84-5	36
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	9





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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

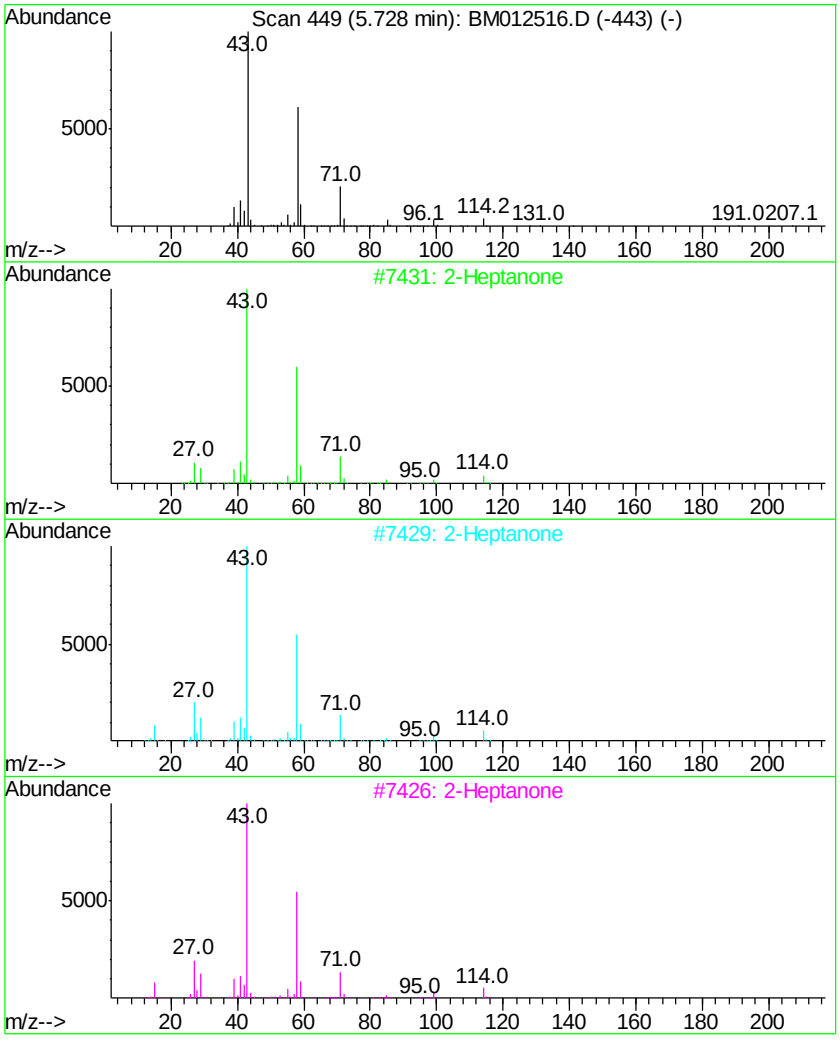
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

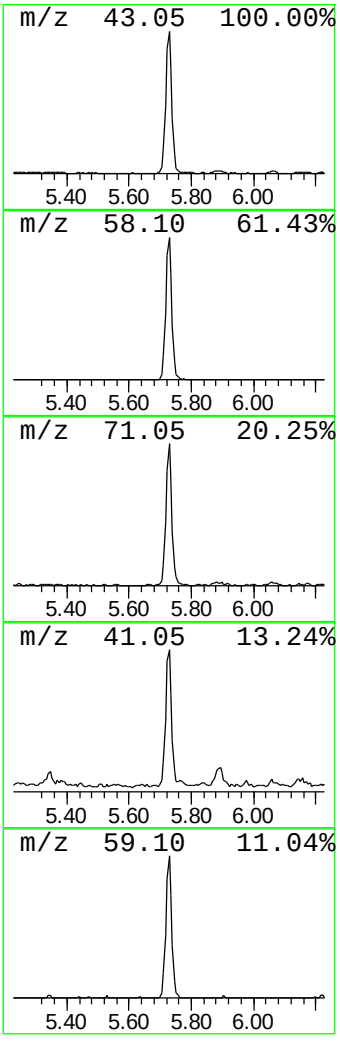
****

Peak Number 4 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	4.96 ng/ul	832321	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	87
2	2-Heptanone	114	C7H14O	000110-43-0	83
3	2-Heptanone	114	C7H14O	000110-43-0	80
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
5	2-Heptanone	114	C7H14O	000110-43-0	72





Library Search Compound Report

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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

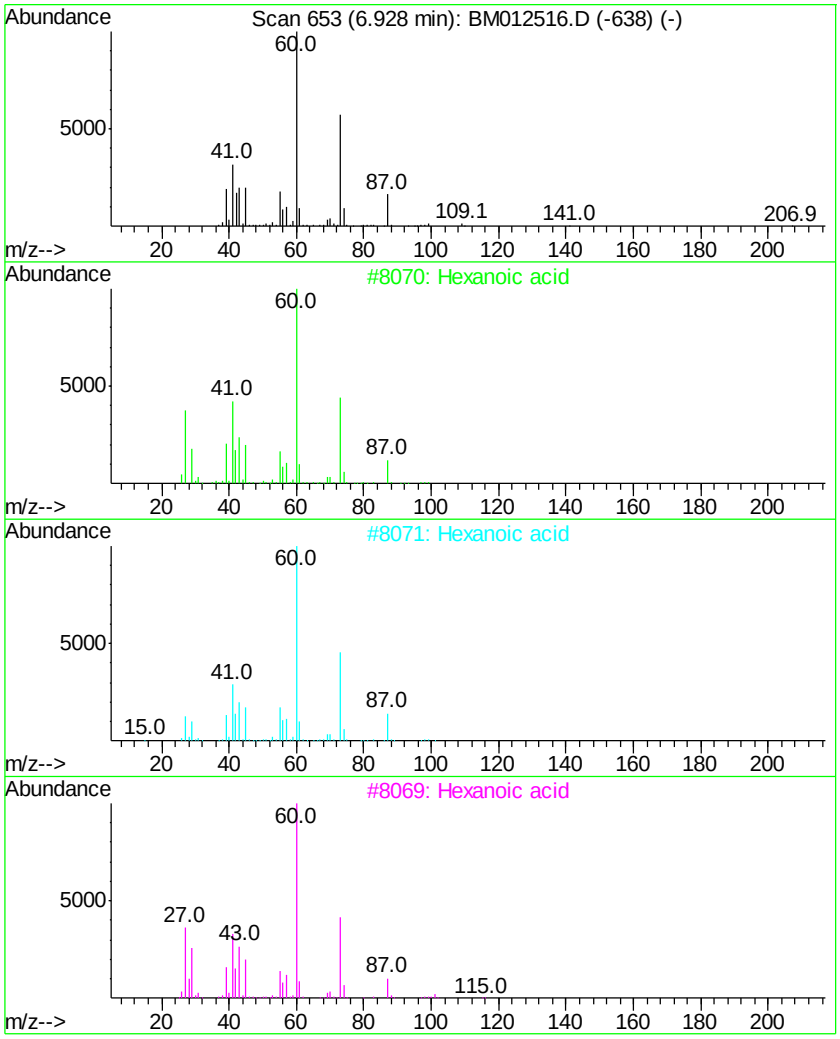
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

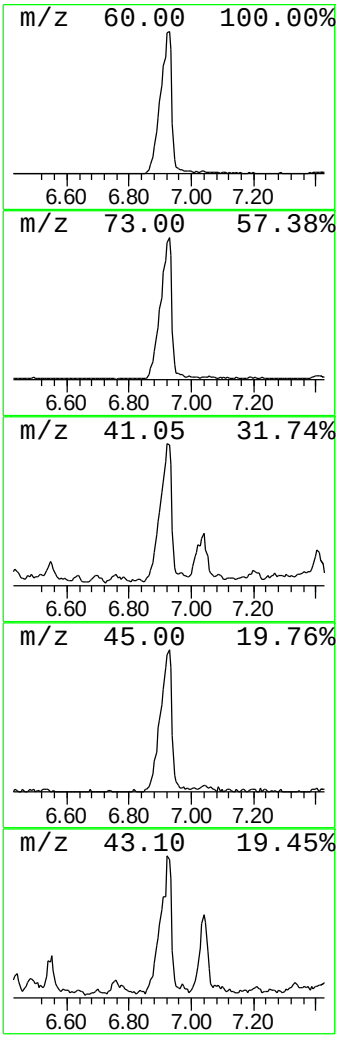
****

Peak Number 5 Hexanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	7.11 ng/ul	1192870	1,4-Dichlorobenzene-d4	7.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	83
3	Hexanoic acid	116	C6H12O2	000142-62-1	83
4	Hexanoic acid	116	C6H12O2	000142-62-1	72
5	Heptanoic acid	130	C7H14O2	000111-14-8	59





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ClientSampleId : B-8(5-6.25)_101017

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM102417.M
Quant Title : SVOA CALIBRATION

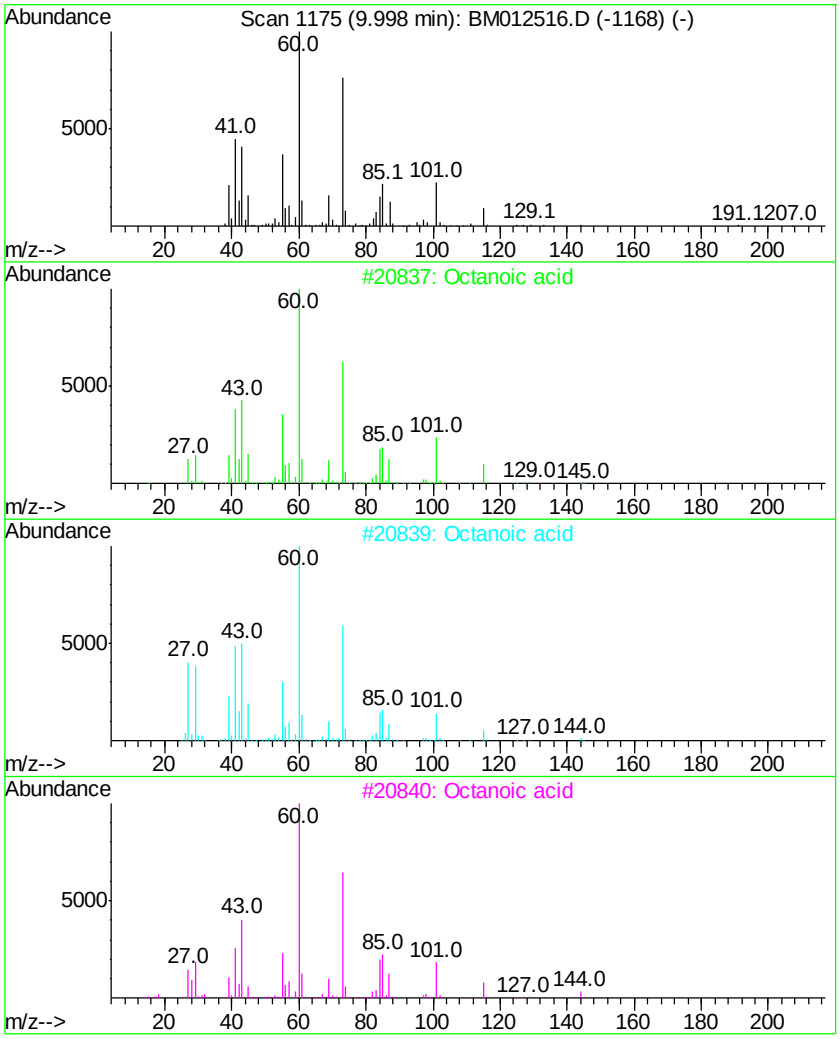
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

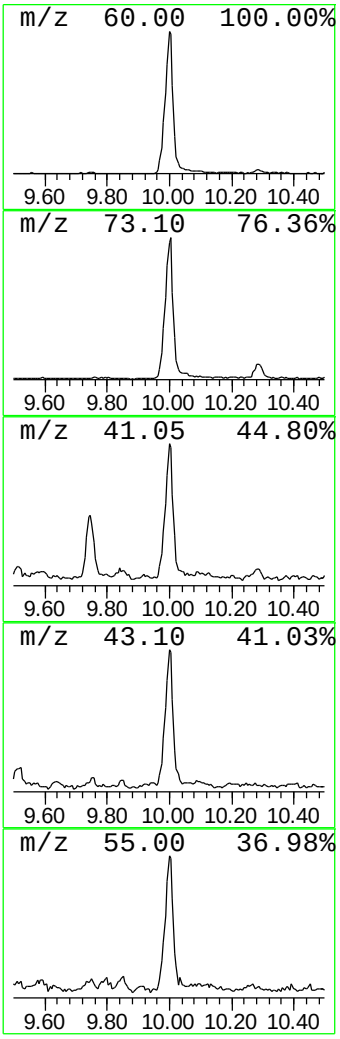
****

Peak Number 6 Octanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.00	3.22 ng/ul	669727	Naphthalene-d8	10.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	91
2	Octanoic acid	144	C8H16O2	000124-07-2	83
3	Octanoic acid	144	C8H16O2	000124-07-2	72
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	53





Tentatively Identified Compound (LSC) summary

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Quant Title : SVOA CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone	3.17	3.4	ng/ul	572823	1	7.87	3356250	20.0
Propanoic acid, 2...	3.72	11.2	ng/ul	1880680	1	7.87	3356250	20.0
Butanoic acid	4.07	15.3	ng/ul	2573440	1	7.87	3356250	20.0
2-Heptanone	5.73	5.0	ng/ul	832321	1	7.87	3356250	20.0
Hexanoic acid	6.93	7.1	ng/ul	1192870	1	7.87	3356250	20.0
Octanoic acid	10.00	3.2	ng/ul	669727	2	10.66	4162290	20.0