

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
 Data File : BM005543.D
 Acq On : 21 May 2016 06:11
 Operator : UM/SJ
 Sample : H2853-19RX
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 D9X11RX

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.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	2.652	9	11	26	rVB2	40071	86112	5.14%	0.471%
2	2.975	57	66	81	rVB2	49410	122305	7.29%	0.669%
3	3.605	163	173	183	rVB	60718	130390	7.78%	0.713%
4	3.922	218	227	233	rBV	40229	74515	4.44%	0.407%
5	4.757	349	369	376	rBV	142944	494625	29.50%	2.704%
6	4.910	379	395	400	rBV	123307	362429	21.61%	1.982%
7	5.299	454	461	470	rBV	37860	70224	4.19%	0.384%
8	6.804	712	717	725	rBV2	14363	23275	1.39%	0.127%
9	6.987	739	748	749	rBV	34026	48649	2.90%	0.266%
10	7.010	749	752	760	rVB	36089	56748	3.38%	0.310%
11	7.157	770	777	783	rBV	72062	108534	6.47%	0.593%
12	7.351	802	810	819	rBV	92839	149570	8.92%	0.818%
13	7.822	883	890	897	rBV	338467	541053	32.27%	2.958%
14	8.522	1002	1009	1013	rBV	80606	130567	7.79%	0.714%
15	8.581	1013	1019	1026	rVB	725082	1182405	70.52%	6.465%
16	8.975	1080	1086	1093	rBV	80343	129384	7.72%	0.707%
17	9.081	1096	1104	1108	rBV2	11403	18587	1.11%	0.102%
18	9.692	1202	1208	1214	rVB	63890	102220	6.10%	0.559%
19	9.916	1241	1246	1253	rBV	22859	36735	2.19%	0.201%
20	10.228	1293	1299	1306	rVB	115011	189007	11.27%	1.033%
21	10.610	1357	1364	1373	rVB	455277	756720	45.13%	4.137%
22	11.169	1445	1459	1476	rBV	293667	739748	44.12%	4.045%
23	12.104	1610	1618	1627	rVB	254516	410408	24.48%	2.244%
24	12.222	1632	1638	1647	rVV2	12302	22431	1.34%	0.123%
25	13.857	1910	1916	1920	rBV	187178	264957	15.80%	1.449%
26	13.910	1920	1925	1933	rVB	240781	340970	20.33%	1.864%
27	14.145	1959	1965	1971	rVB	196587	290017	17.30%	1.586%
28	14.251	1977	1983	1990	rBV	115396	178361	10.64%	0.975%
29	14.357	1995	2001	2007	rVV	17334	24982	1.49%	0.137%
30	14.451	2011	2017	2025	rVB2	641731	984209	58.70%	5.381%
31	14.639	2042	2049	2056	rBV	29926	46390	2.77%	0.254%
32	14.863	2082	2087	2093	rBV	35394	49365	2.94%	0.270%
33	15.304	2158	2162	2167	rVB	56100	68999	4.11%	0.377%
34	15.445	2180	2186	2192	rVB	280428	408908	24.39%	2.236%

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35	15.551	2200	2204	2211	rBV	57879	85859	5.12%	0.469%
36	15.716	2220	2232	2235	rBV5	15652	37918	2.26%	0.207%
37	16.163	2303	2308	2321	rBV	382624	514924	30.71%	2.815%
38	16.339	2333	2338	2342	rVB2	17021	21554	1.29%	0.118%
39	16.515	2361	2368	2374	rBV	38624	69905	4.17%	0.382%
40	16.598	2374	2382	2390	rVV	114725	170332	10.16%	0.931%
41	16.957	2438	2443	2447	rBV	61060	78198	4.66%	0.428%
42	17.004	2449	2451	2455	rVB3	14220	17869	1.07%	0.098%
43	17.086	2461	2465	2473	rVB4	20267	32133	1.92%	0.176%
44	17.192	2477	2483	2488	rVV	828909	1207438	72.01%	6.602%
45	17.239	2488	2491	2494	rVV2	51563	65433	3.90%	0.358%
46	17.286	2494	2499	2505	rVV	313458	461531	27.52%	2.523%
47	17.357	2509	2511	2518	rVV3	11464	16873	1.01%	0.092%
48	17.421	2518	2522	2530	rVB6	10864	17860	1.07%	0.098%
49	17.557	2542	2545	2557	rVB5	22668	44167	2.63%	0.241%
50	17.692	2563	2568	2573	rBV2	15663	22087	1.32%	0.121%
51	18.098	2628	2637	2655	rBV	1032467	1676804	100.00%	9.168%
52	18.515	2703	2708	2712	rBV3	11394	16908	1.01%	0.092%
53	18.951	2778	2782	2785	rBV3	16007	23771	1.42%	0.130%
54	19.280	2835	2838	2847	rVB3	31876	52334	3.12%	0.286%
55	19.362	2848	2852	2867	rBV	154978	233190	13.91%	1.275%
56	19.580	2883	2889	2895	rBV	374433	528078	31.49%	2.887%
57	20.127	2980	2982	2987	rVB4	18946	19414	1.16%	0.106%
58	20.609	3060	3064	3070	rBV7	16290	30064	1.79%	0.164%
59	21.080	3140	3144	3154	rBV	299073	397061	23.68%	2.171%
60	21.362	3187	3192	3199	rBV	1256784	1602179	95.55%	8.760%
61	23.491	3548	3554	3564	rVB2	284961	569235	33.95%	3.112%
62	23.639	3572	3579	3591	rVB2	827580	1632988	97.39%	8.928%

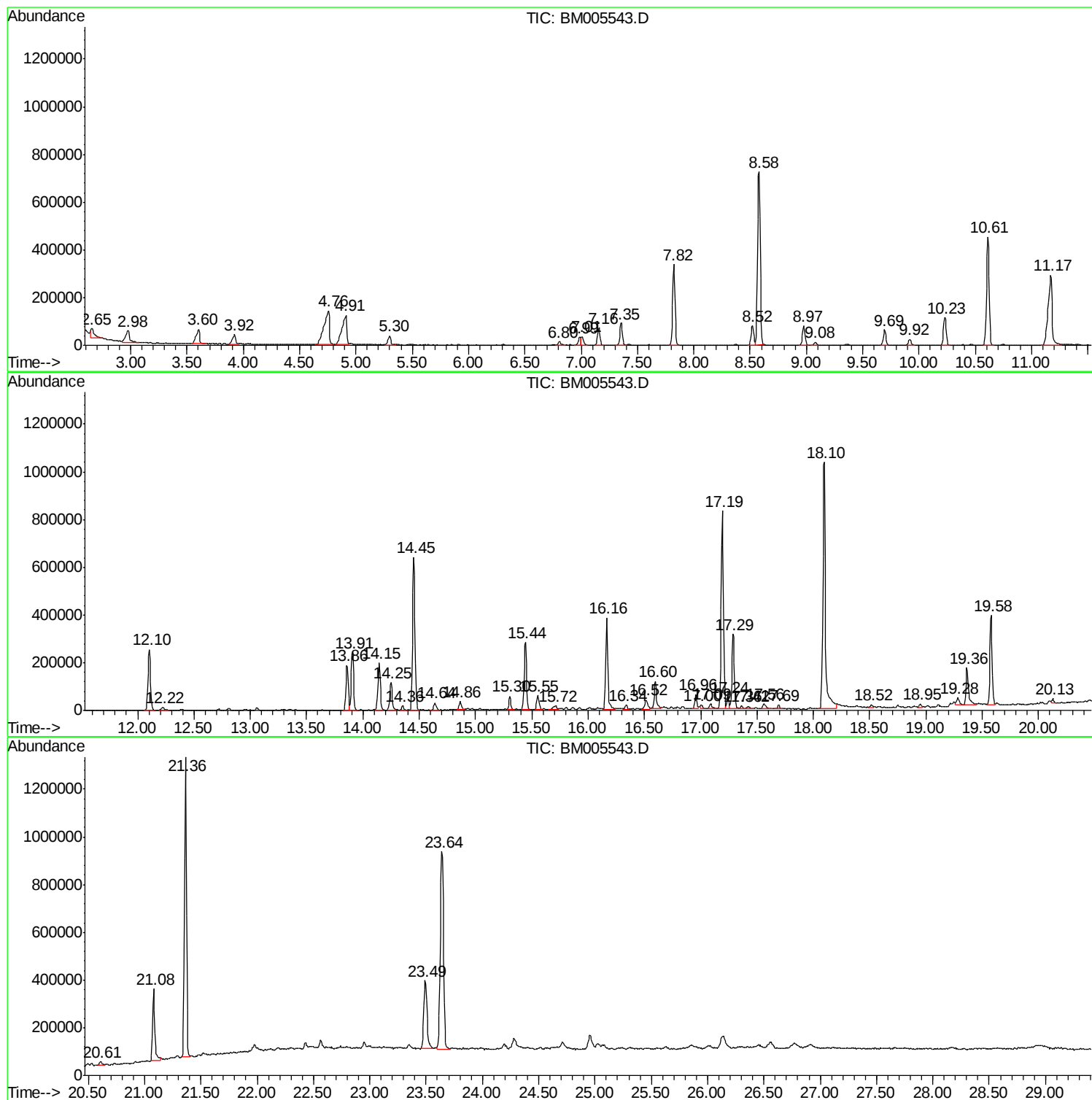
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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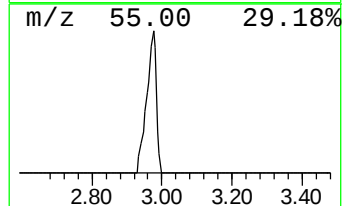
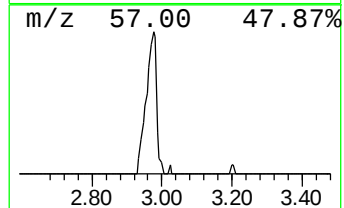
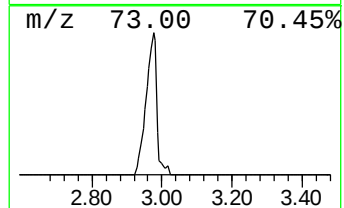
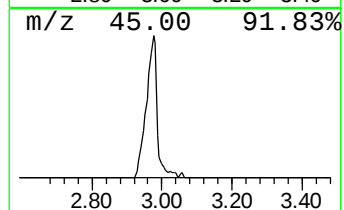
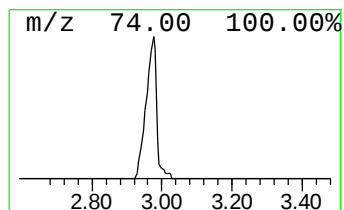
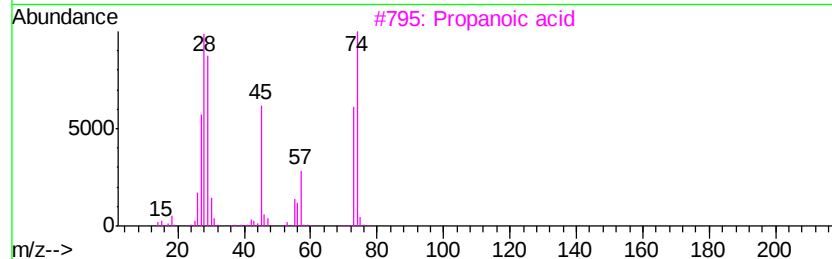
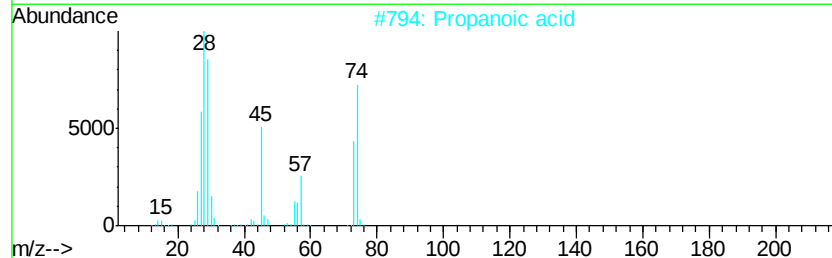
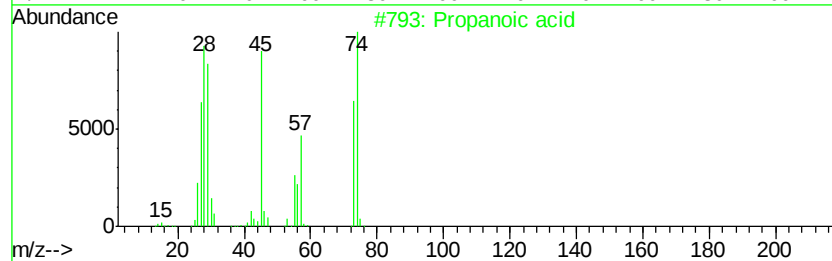
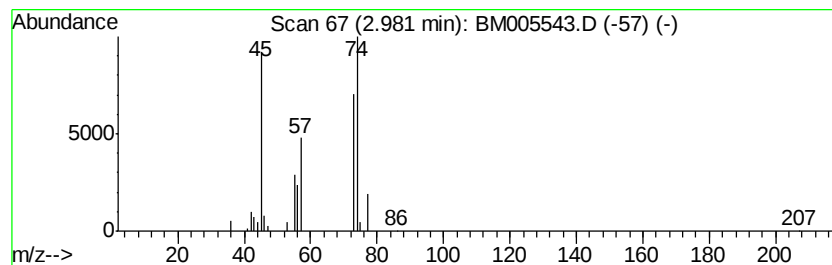
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM02.2-EPA-BM052016.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	4.52 ng/ul	122305	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid	74	C3H6O2	000079-09-4	91
2		Propanoic acid	74	C3H6O2	000079-09-4	86
3		Propanoic acid	74	C3H6O2	000079-09-4	80
4		Homoserine	119	C4H9NO3	000498-19-1	25
5		Homoserine	119	C4H9NO3	000498-19-1	25



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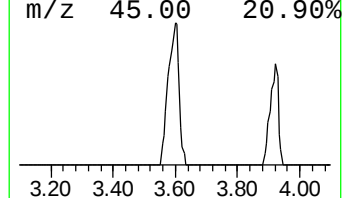
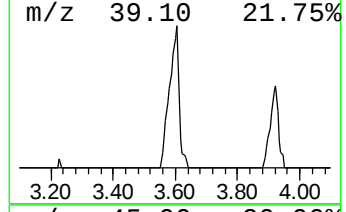
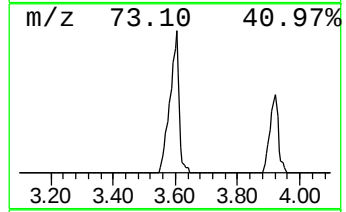
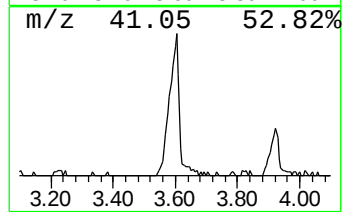
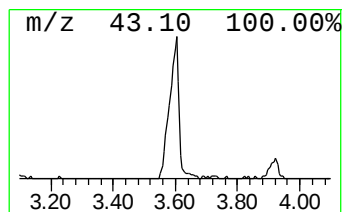
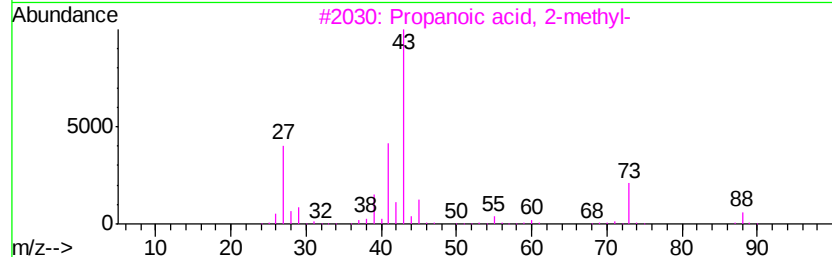
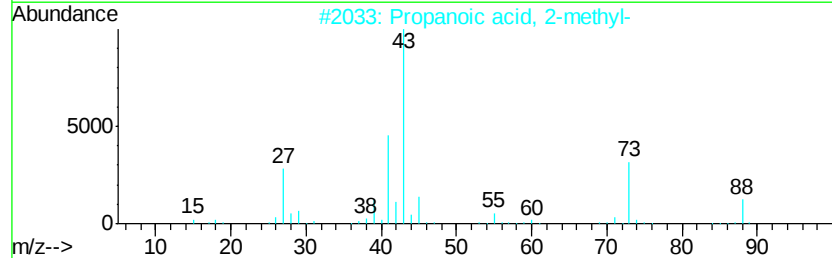
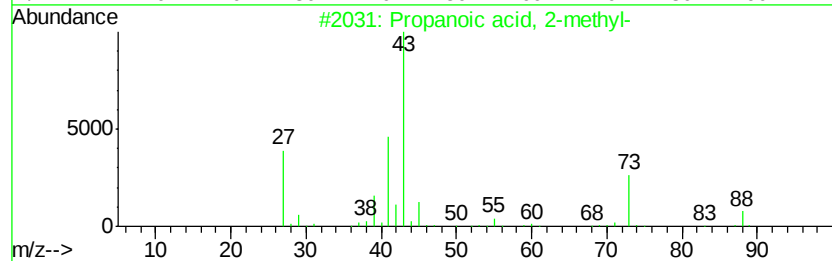
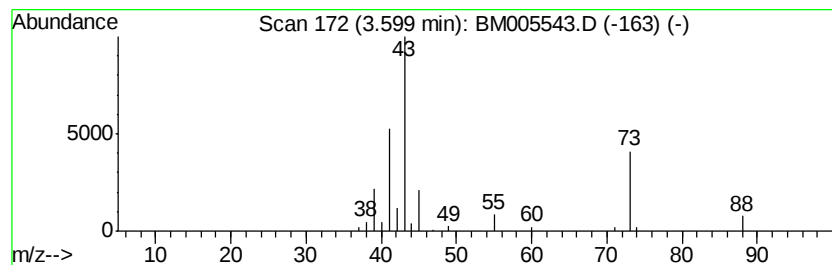
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	4.82 ng/ul	130390	1,4-Dichlorobenzene-d4	7.82

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	64
3			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	64
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	59
5			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	49



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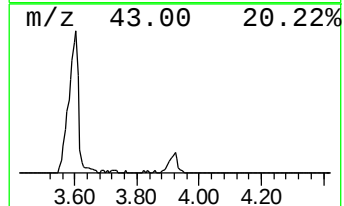
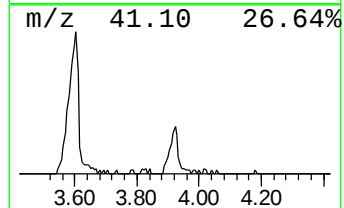
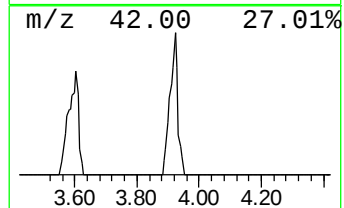
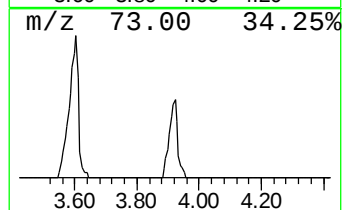
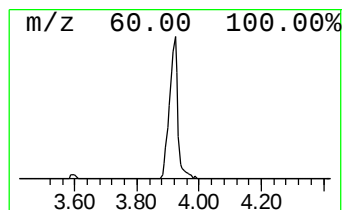
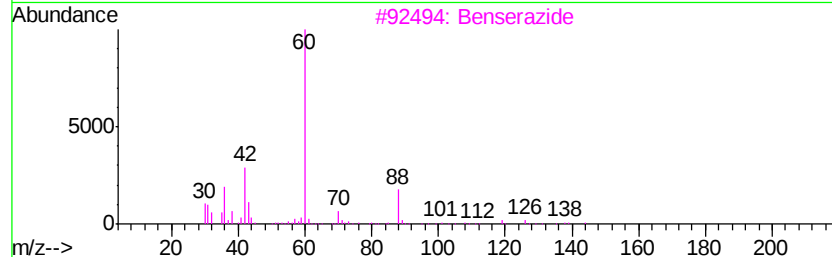
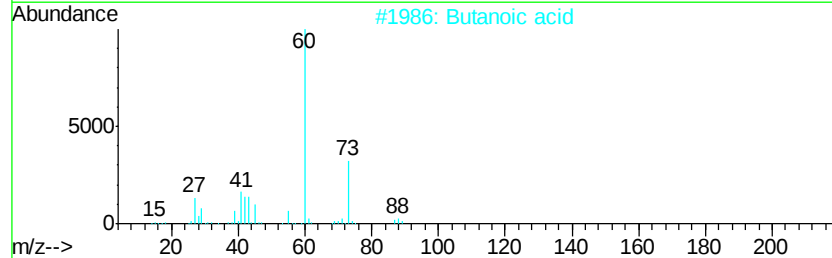
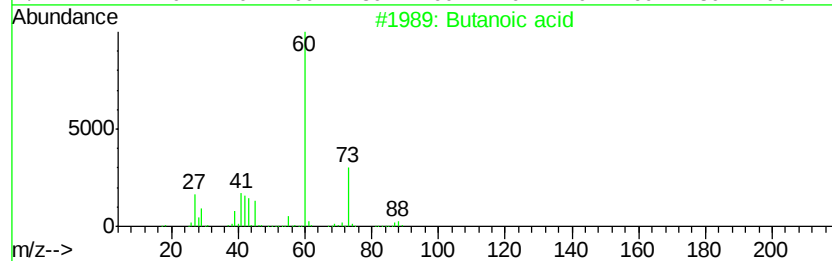
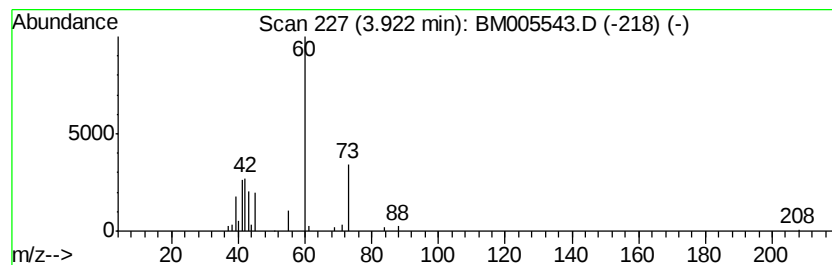
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Butanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	2.75 ng/ul	74515	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	64
2		Butanoic acid	88	C4H8O2	000107-92-6	64
3		Benserazide	257	C10H15N3O5	000322-35-0	9
4		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
5		5-Hexenoic acid	114	C6H10O2	001577-22-6	9



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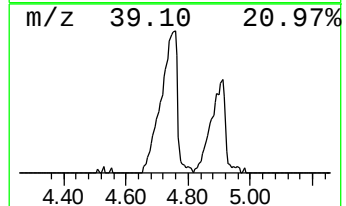
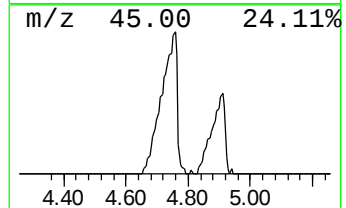
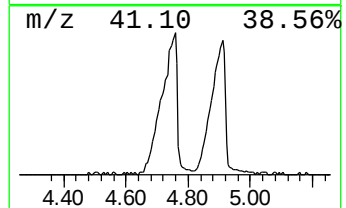
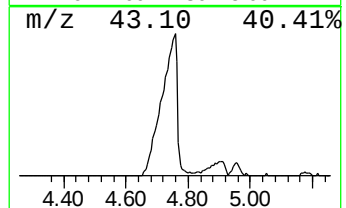
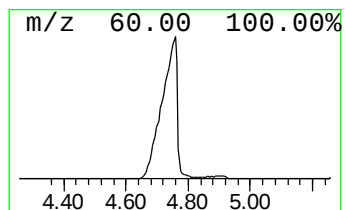
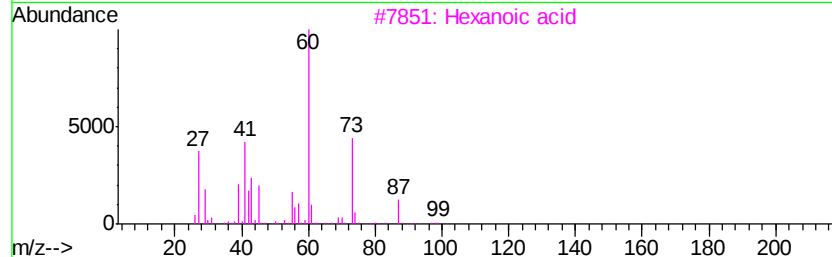
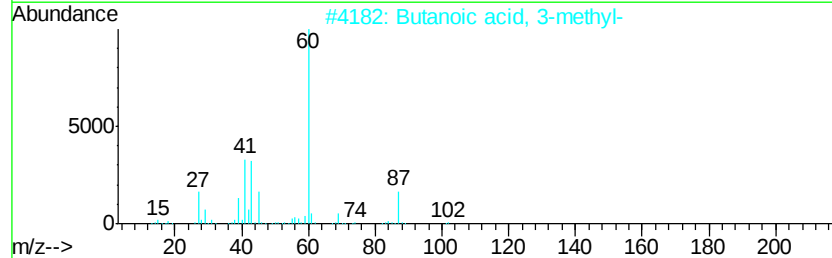
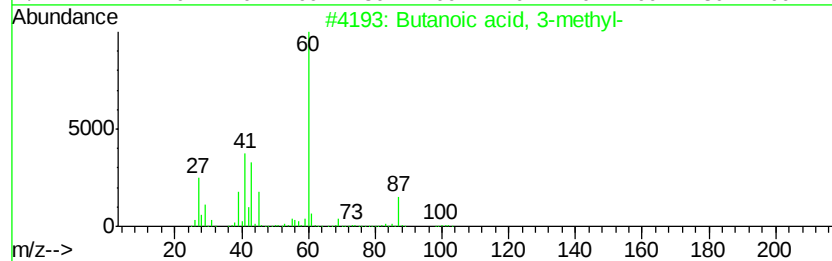
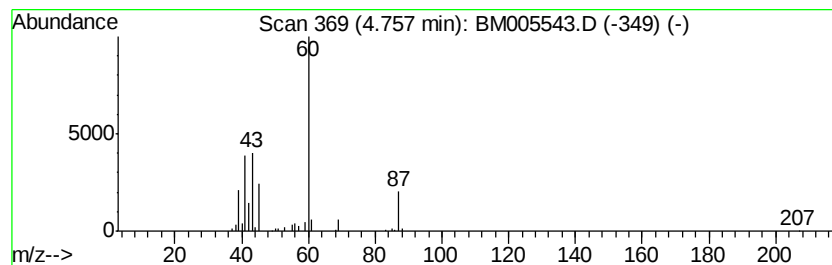
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanoic acid, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	18.28 ng/ul	494625	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
3		Hexanoic acid	116	C6H12O2	000142-62-1	39
4		1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	38
5		Pentanoic acid	102	C5H10O2	000109-52-4	36



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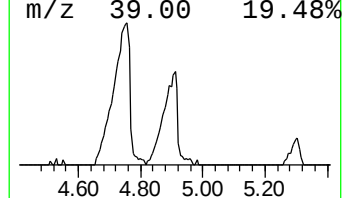
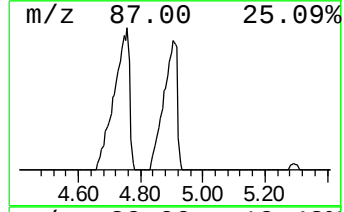
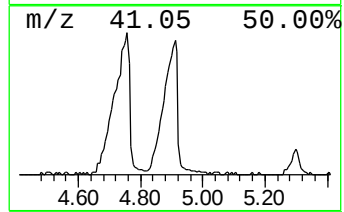
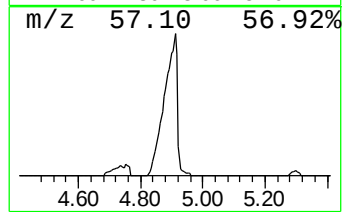
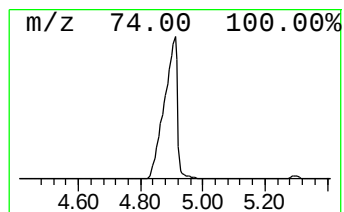
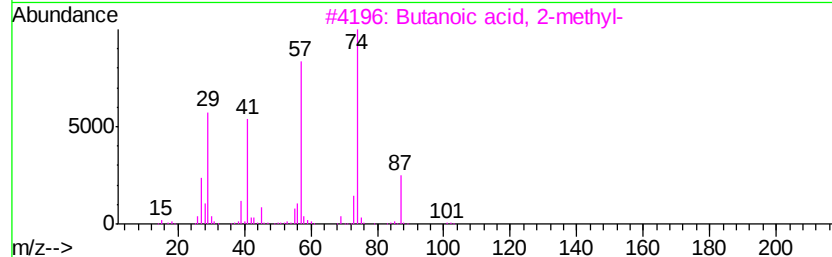
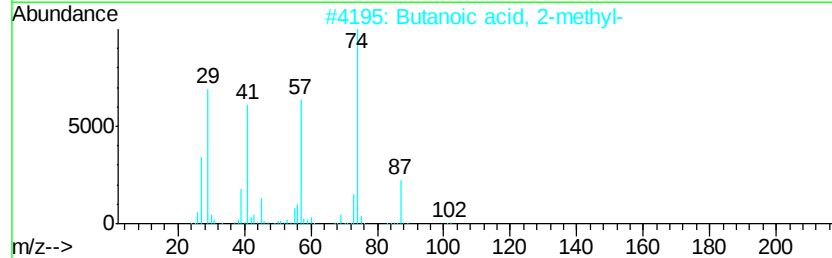
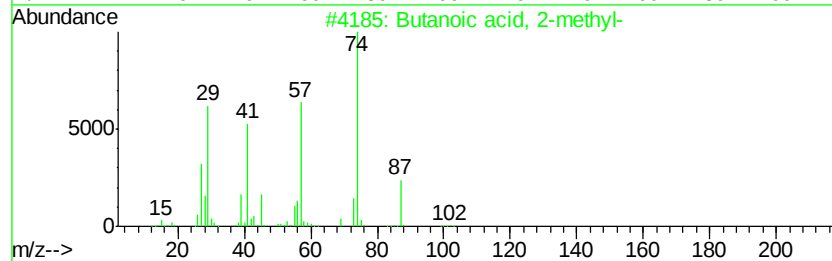
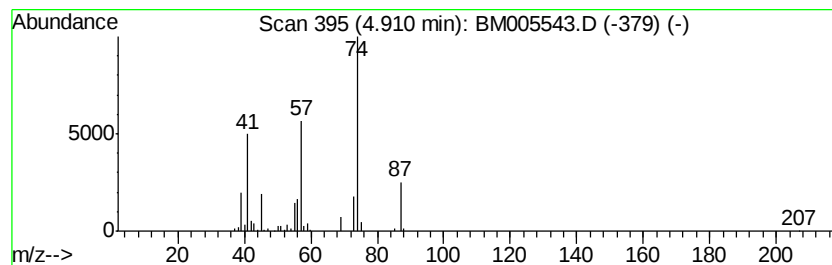
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanoic acid, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	13.40 ng/ul	362429	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
2		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	72
3		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	59
4		Methanamine, 1,1-bis(2,2-dimethy...	231	C13H29N02	004909-78-8	39
5		Methanamine, 1,1-bis(2,2-dimethy...	231	C13H29N02	004909-78-8	39



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
Data File : BM005543.D
Acq On : 21 May 2016 06:11
Operator : UM/SJ
Sample : H2853-19RX
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
D9X11RX

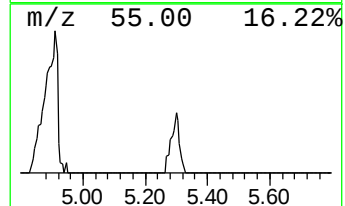
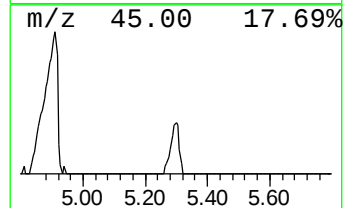
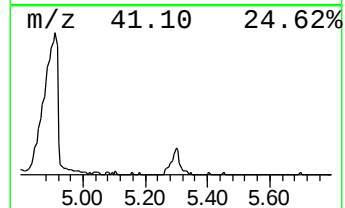
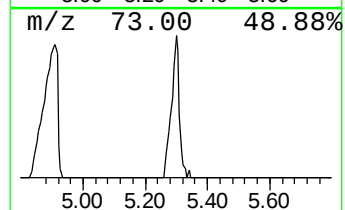
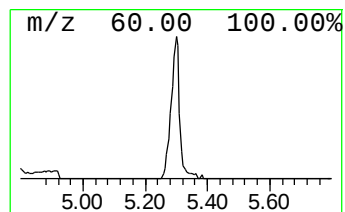
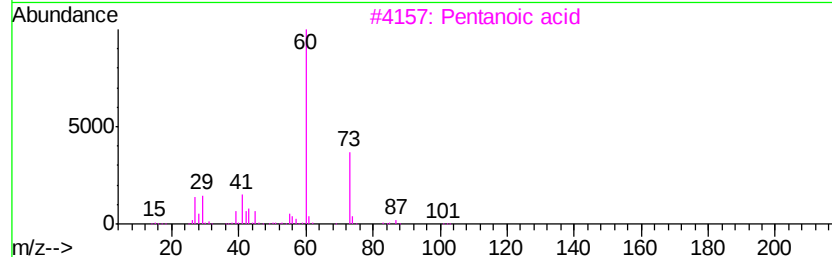
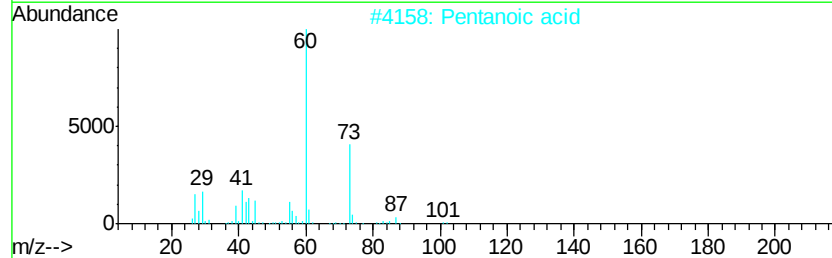
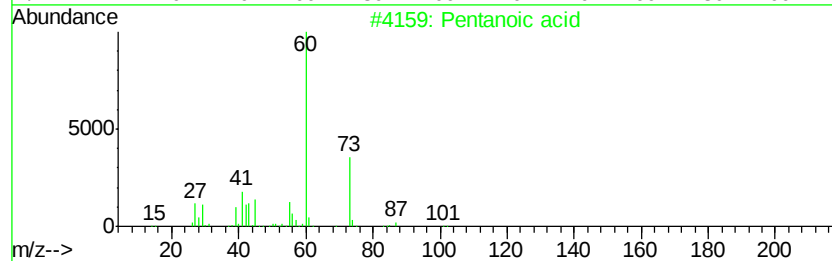
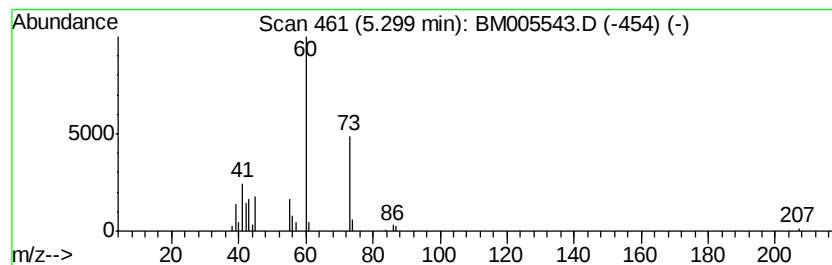
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Pentanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.30	2.60 ng/ul	70224	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid	102	C5H10O2	000109-52-4	83
2		Pentanoic acid	102	C5H10O2	000109-52-4	83
3		Pentanoic acid	102	C5H10O2	000109-52-4	78
4		Hexanoic acid	116	C6H12O2	000142-62-1	56
5		Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	42



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
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Misc :
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ClientSampleId :
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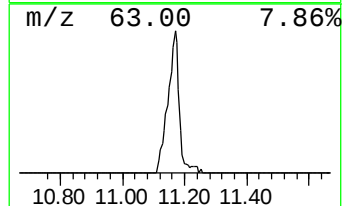
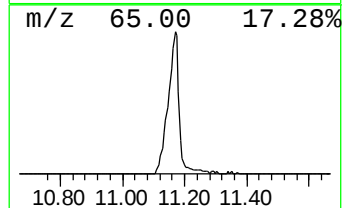
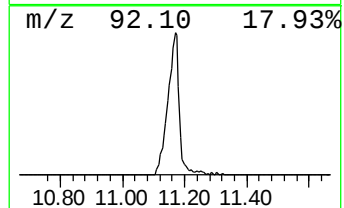
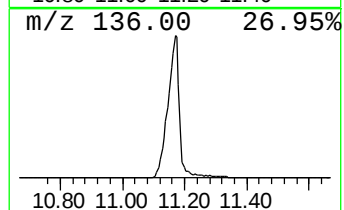
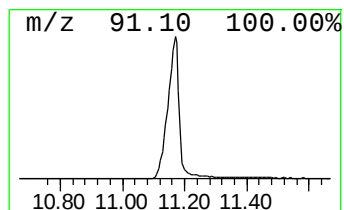
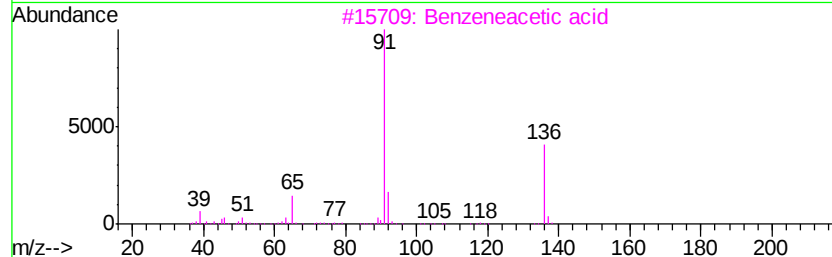
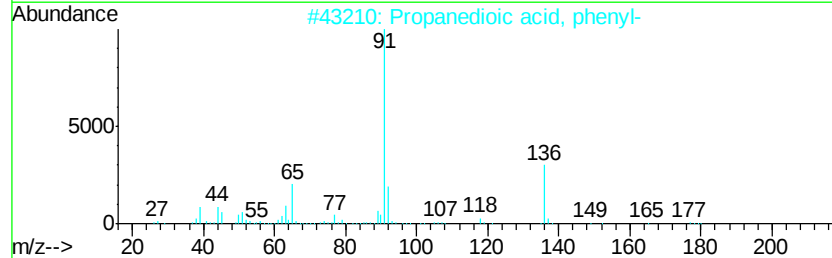
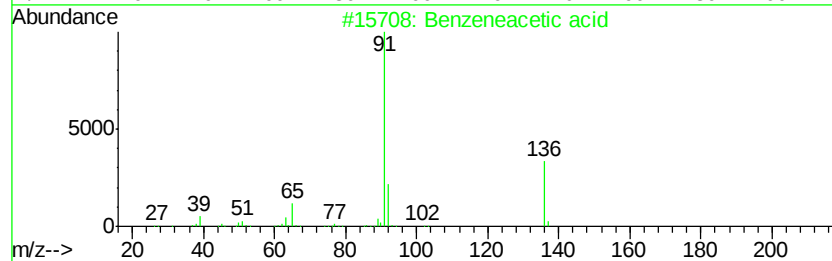
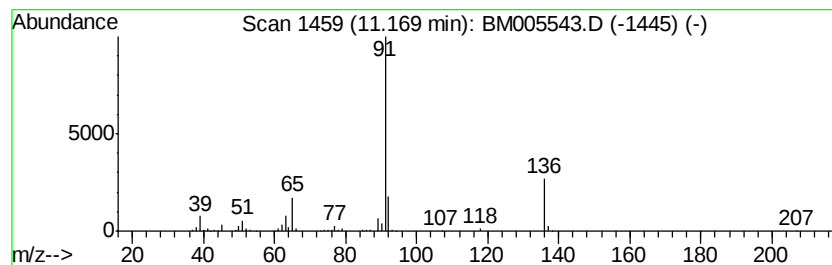
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzeneacetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	19.55 ng/ul	739748	Napthalene-d8	10.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetic acid	136	C8H8O2	000103-82-2	90
2		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	80
3		Benzeneacetic acid	136	C8H8O2	000103-82-2	80
4		Benzeneacetic acid	136	C8H8O2	000103-82-2	72
5		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	59



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
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Sample : H2853-19RX
Misc :
ALS Vial : 21 Sample Multiplier: 1

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ClientSampleId :
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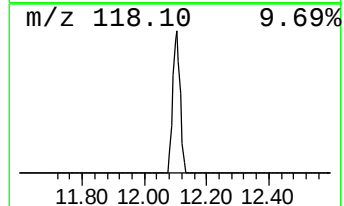
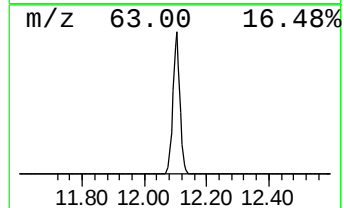
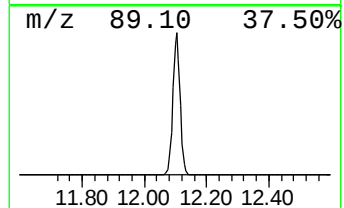
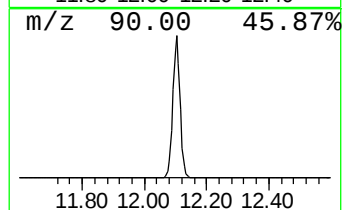
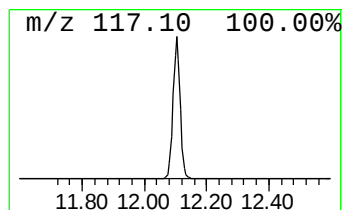
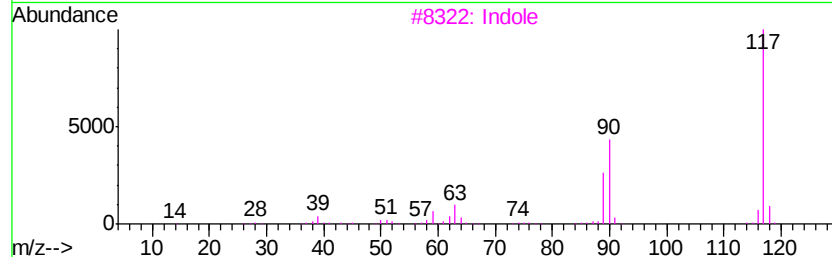
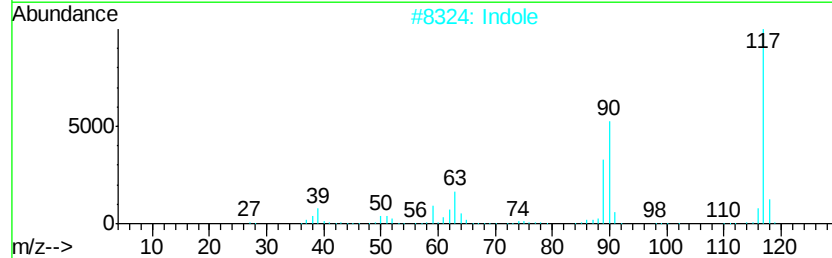
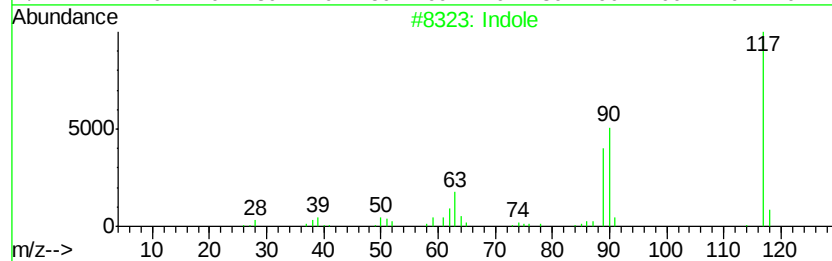
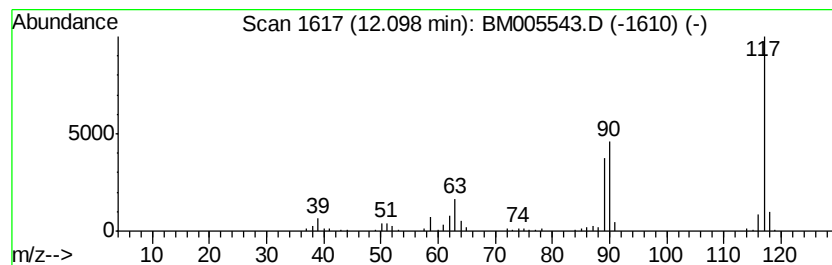
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	10.85 ng/ul	410408	Napthalene-d8	10.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole		117	C8H7N	000120-72-9	97
2	Indole		117	C8H7N	000120-72-9	97
3	Indole		117	C8H7N	000120-72-9	91
4	5H-1-Pyrindine		117	C8H7N	000270-91-7	91
5	Benzyl nitrile		117	C8H7N	000140-29-4	91



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
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Misc :
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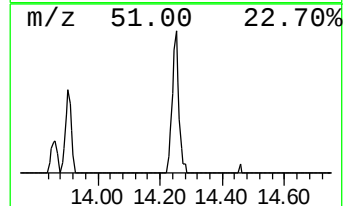
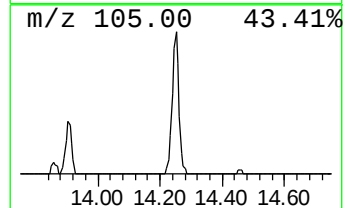
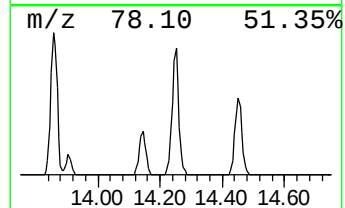
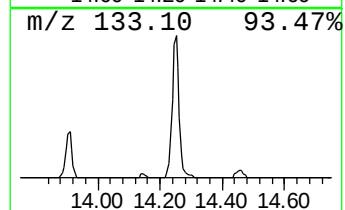
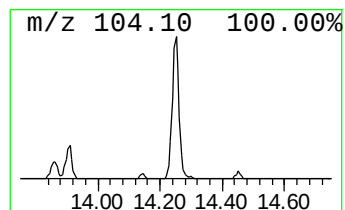
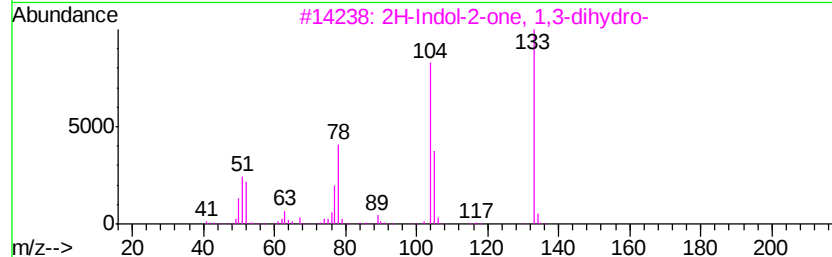
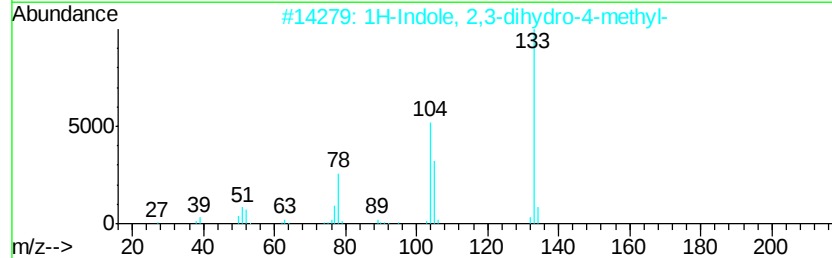
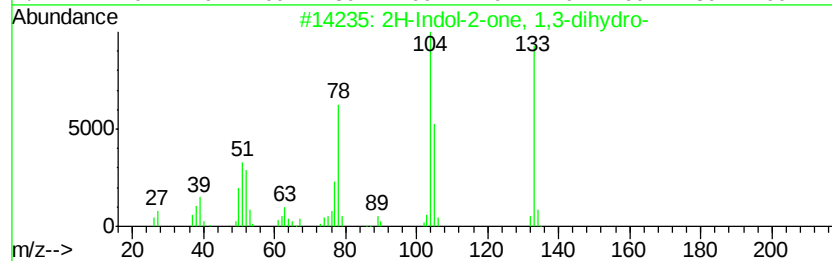
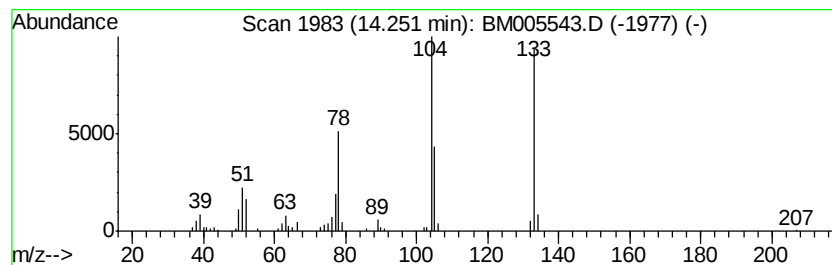
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2H-Indol-2-one, 1,3-dihydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	3.62 ng/ul	178361	Acenaphthene-d10	14.45

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	94
2			1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	94
3			2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	93
4			2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	91
5			1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	87



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
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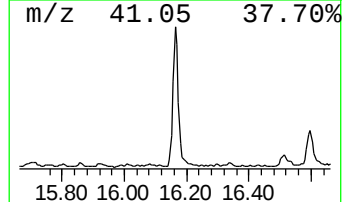
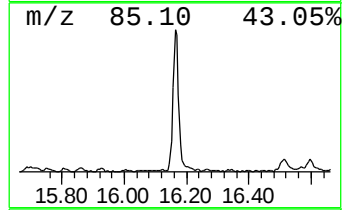
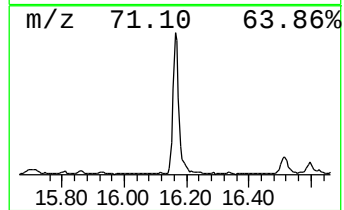
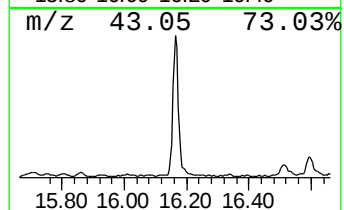
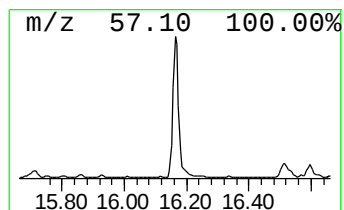
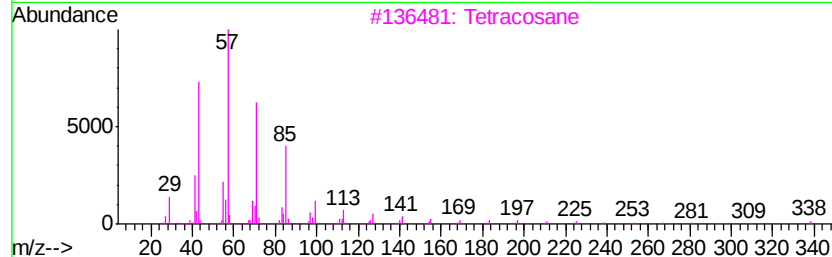
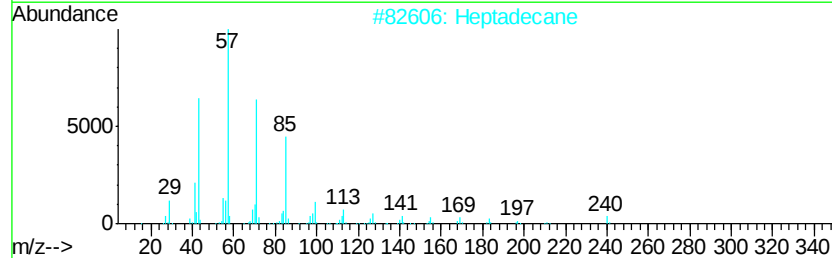
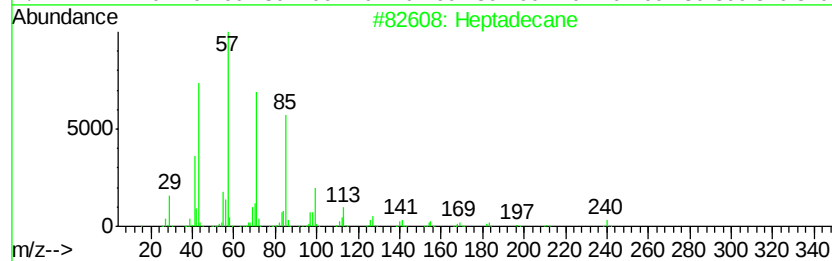
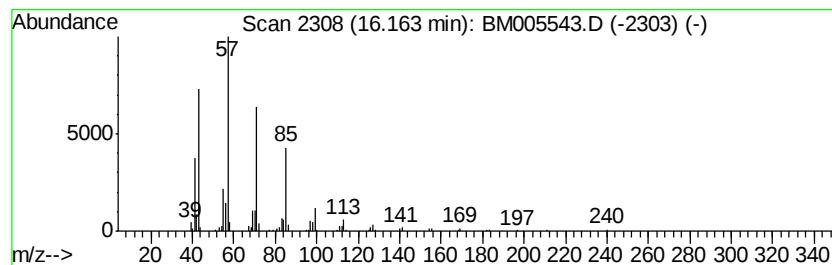
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	8.53 ng/ul	514924	Phenanthrene-d10	17.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	97
2			Heptadecane	240	C17H36	000629-78-7	95
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Hexadecane	226	C16H34	000544-76-3	90



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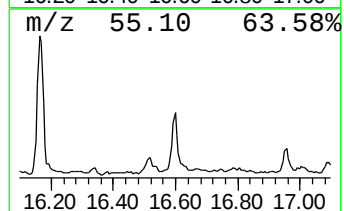
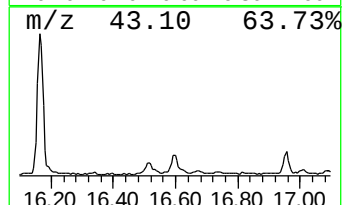
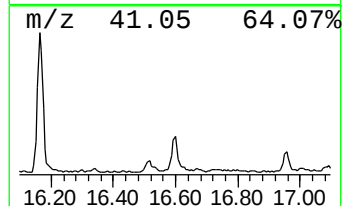
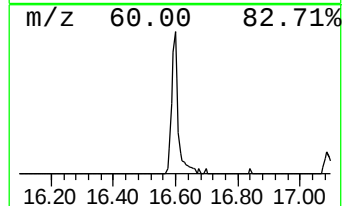
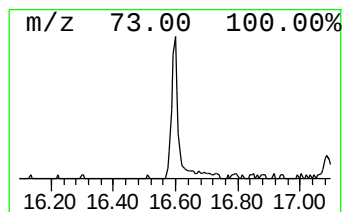
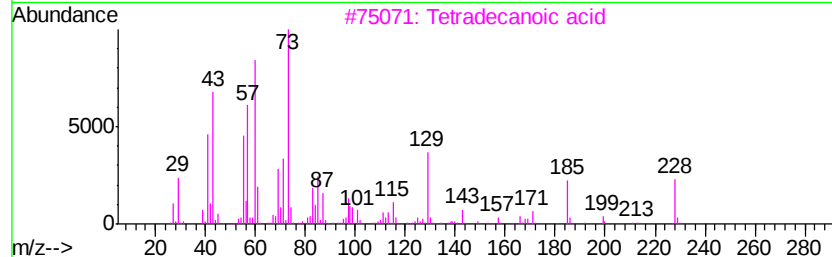
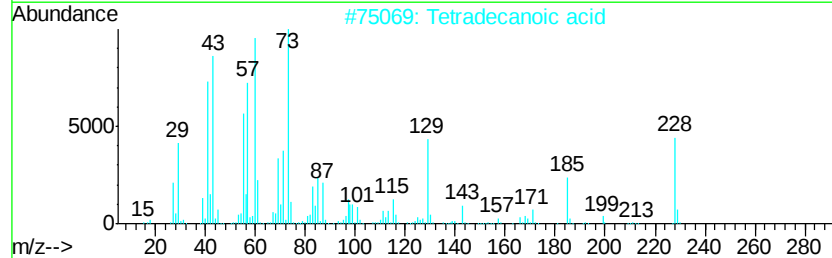
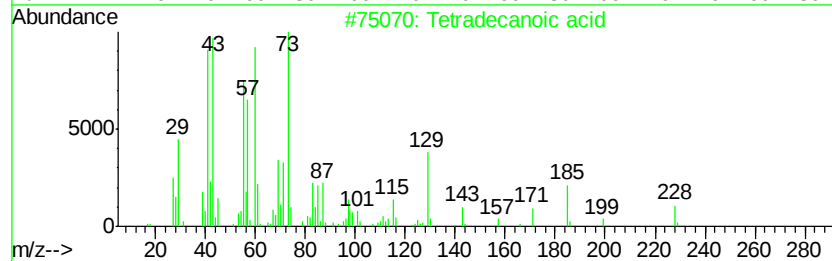
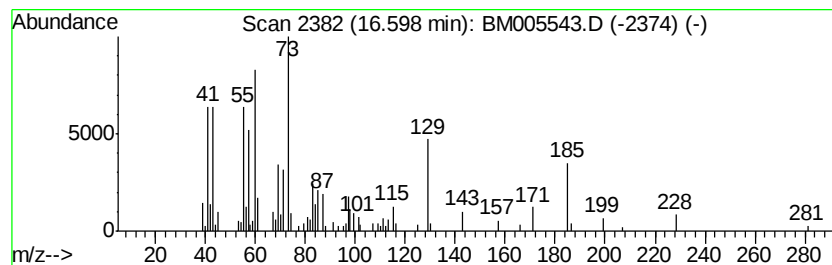
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetradecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	2.82 ng/ul	170332	Phenanthrene-d10	17.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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Sample : H2853-19RX
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D9X11RX

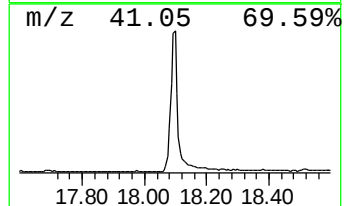
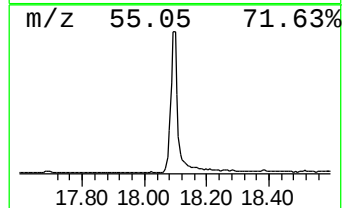
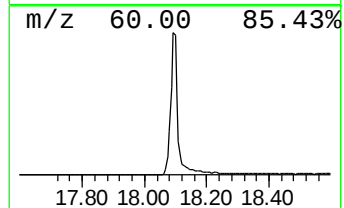
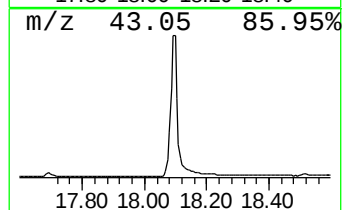
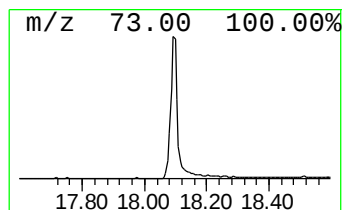
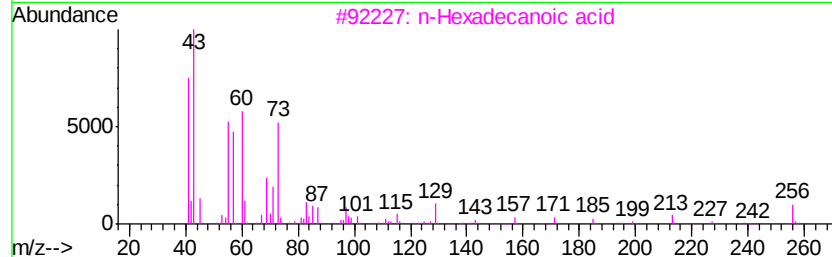
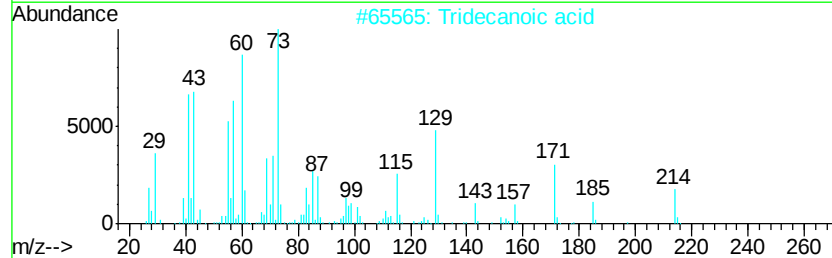
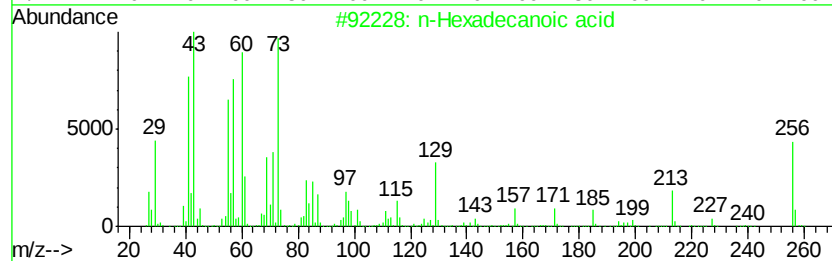
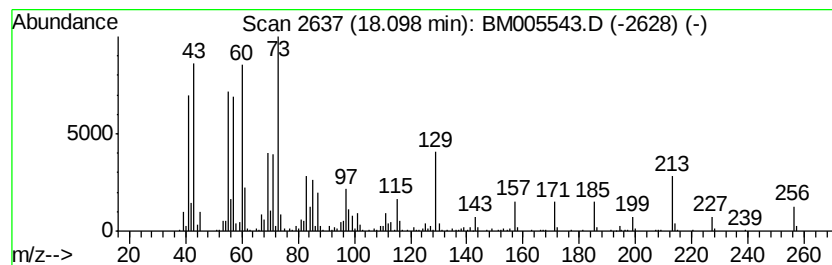
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	27.77 ng/ul	1676800	Phenanthrene-d10	17.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4		Tridecanoic acid	214	C13H26O2	000638-53-9	86
5		Undecanoic acid	186	C11H22O2	000112-37-8	83



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
Data File : BM005543.D
Acq On : 21 May 2016 06:11
Operator : UM/SJ
Sample : H2853-19RX
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D9X11RX

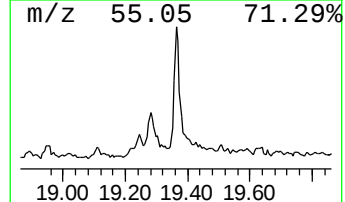
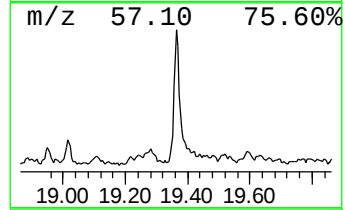
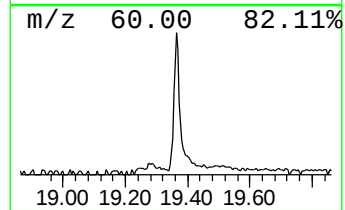
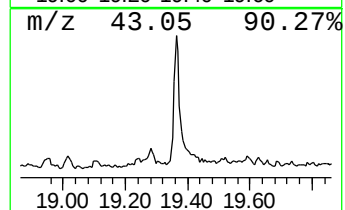
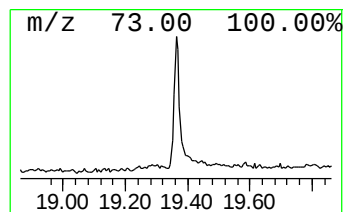
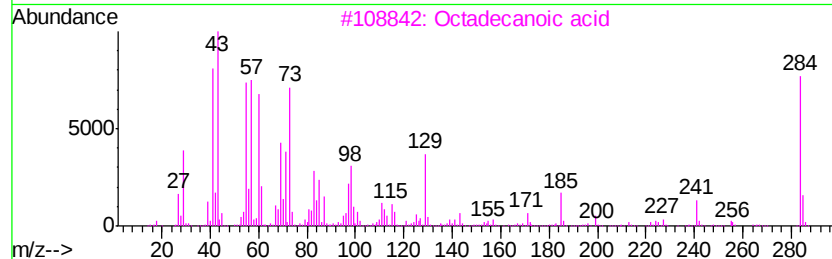
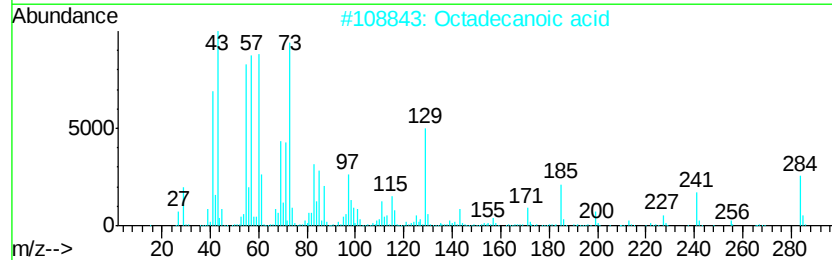
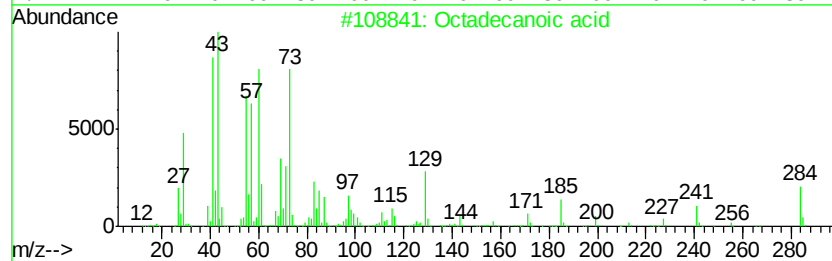
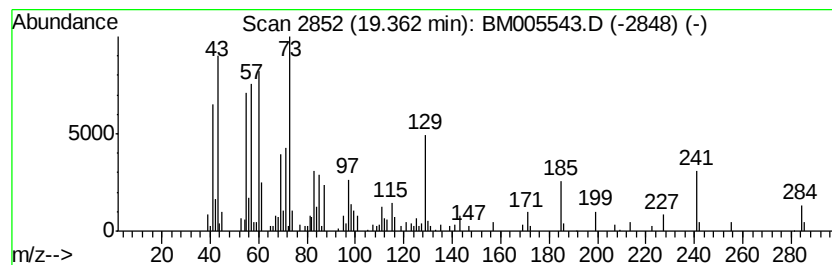
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.36	2.91 ng/ul	233190	Chrysene-d12	21.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	97
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052016\
Data File : BM005543.D
Acq On : 21 May 2016 06:11
Operator : UM/SJ
Sample : H2853-19RX
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D9X11RX

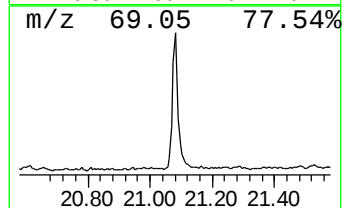
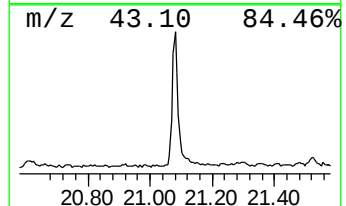
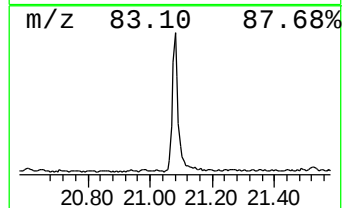
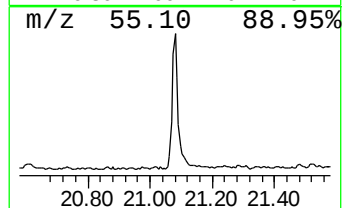
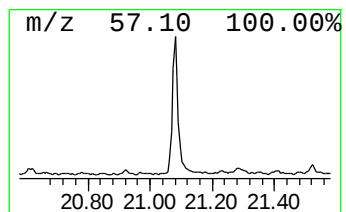
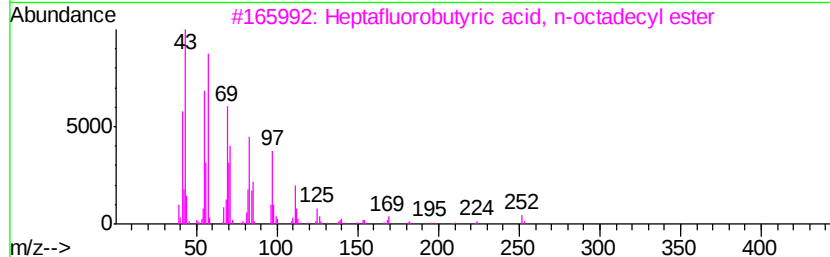
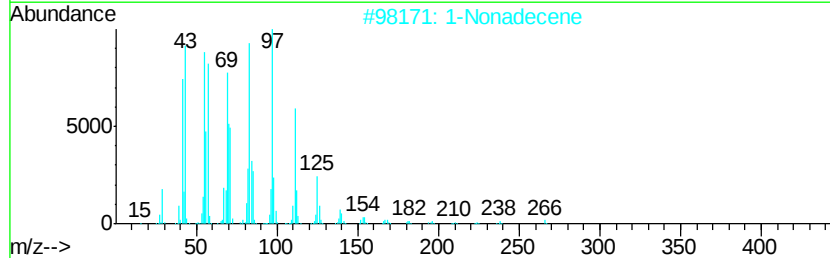
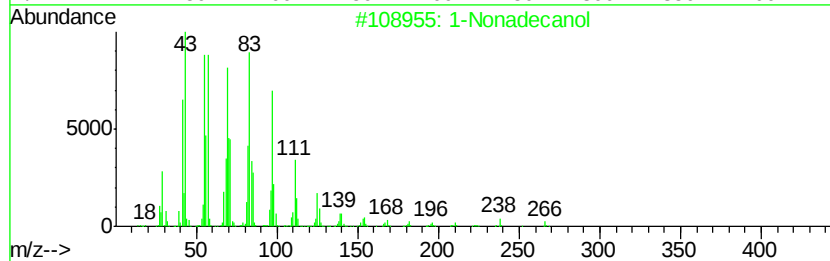
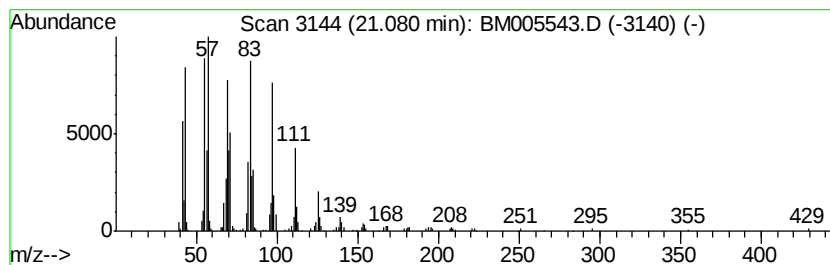
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1-Nonadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	4.96 ng/ul	397061	Chrysene-d12	21.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecanol	284	C19H40O	001454-84-8	93
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052016\
 Data File : BM005543.D
 Acq On : 21 May 2016 06:11
 Operator : UM/SJ
 Sample : H2853-19RX
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 D9X11RX

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid	2.98	4.5	ng/ul	122305	1	7.82	541053	20.0
Propanoic acid, 2...	3.60	4.8	ng/ul	130390	1	7.82	541053	20.0
Butanoic acid	3.92	2.8	ng/ul	74515	1	7.82	541053	20.0
Butanoic acid, 3-...	4.76	18.3	ng/ul	494625	1	7.82	541053	20.0
Butanoic acid, 2-...	4.91	13.4	ng/ul	362429	1	7.82	541053	20.0
Pentanoic acid	5.30	2.6	ng/ul	70224	1	7.82	541053	20.0
Benzeneacetic acid	11.17	19.6	ng/ul	739748	2	10.61	756720	20.0
Indole	12.10	10.9	ng/ul	410408	2	10.61	756720	20.0
2H-Indol-2-one, 1...	14.25	3.6	ng/ul	178361	3	14.45	984209	20.0
(DEL) Alkane: Str...	16.16	8.5	ng/ul	514924	4	17.19	1207440	20.0
Tetradecanoic acid	16.60	2.8	ng/ul	170332	4	17.19	1207440	20.0
n-Hexadecanoic acid	18.10	27.8	ng/ul	1676800	4	17.19	1207440	20.0
Octadecanoic acid	19.36	2.9	ng/ul	233190	5	21.36	1602180	20.0
1-Nonadecanol	21.08	5.0	ng/ul	397061	5	21.36	1602180	20.0