

Data Path : Z:\HPCHEM1\BNA M\DATA\BM120615\
 Data File : BM003385.D
 Acq On : 06 Dec 2015 12:45
 Operator : UM/IZ
 Sample : G4664-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E5E78

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 0.1 % 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-BM120115.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	3.187	14	17	21	rVB	4219	4944	0.25%	0.020%
2	6.887	641	646	654	rBB	75378	107777	5.42%	0.435%
3	7.058	669	675	685	rBB	275302	414216	20.82%	1.671%
4	7.252	702	708	717	rBB	283101	435080	21.87%	1.755%
5	7.722	782	788	795	rBB	266706	414960	20.86%	1.674%
6	8.422	901	907	918	rBB	223802	347472	17.47%	1.401%
7	8.881	978	985	994	rBB	307079	484846	24.37%	1.955%
8	9.599	1101	1107	1114	rBV	255270	397418	19.98%	1.603%
9	9.834	1143	1147	1154	rBB2	15369	21776	1.09%	0.088%
10	10.134	1191	1198	1209	rBV	412713	658677	33.11%	2.656%
11	10.516	1256	1263	1271	rVB	398442	659955	33.18%	2.662%
12	10.651	1283	1286	1291	rBB	1879	2998	0.15%	0.012%
13	10.998	1340	1345	1355	rBV	27448	44823	2.25%	0.181%
14	11.328	1398	1401	1405	rBB	2266	2550	0.13%	0.010%
15	12.110	1530	1534	1538	rBB	5388	7417	0.37%	0.030%
16	12.645	1620	1625	1632	rBB	22457	30513	1.53%	0.123%
17	13.781	1812	1818	1829	rBB	846321	1144750	57.55%	4.617%
18	14.063	1860	1866	1881	rBV	917134	1370416	68.89%	5.527%
19	14.375	1912	1919	1927	rBB2	625206	934910	47.00%	3.770%
20	14.569	1947	1952	1961	rBB	46897	67261	3.38%	0.271%
21	14.810	1986	1993	2008	rBV	276860	419163	21.07%	1.690%
22	15.192	2056	2058	2062	rVB	2015	2638	0.13%	0.011%
23	15.369	2081	2088	2095	rBV	1249013	1773762	89.17%	7.154%
24	15.486	2103	2108	2117	rBB	322707	419211	21.07%	1.691%
25	15.610	2125	2129	2133	rVB	10142	12897	0.65%	0.052%
26	15.933	2180	2184	2188	rBB	10586	12009	0.60%	0.048%
27	15.986	2188	2193	2197	rBB	26282	29403	1.48%	0.119%
28	16.269	2238	2241	2244	rVB2	1841	1995	0.10%	0.008%
29	16.522	2281	2284	2290	rBV	31835	40141	2.02%	0.162%
30	16.833	2335	2337	2341	rVB2	1860	2047	0.10%	0.008%
31	16.922	2346	2352	2359	rVB2	19947	29530	1.48%	0.119%
32	17.122	2380	2386	2392	rBV	757705	1079278	54.25%	4.353%
33	17.222	2396	2403	2422	rVV	1318890	1851177	93.06%	7.466%
34	17.410	2429	2435	2439	rBV	677530	823656	41.40%	3.322%

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35	17.457	2439	2443	2448	rVB	1344546	1593479	80.10%	6.426%
36	18.016	2533	2538	2541	rBV	3479	3439	0.17%	0.014%
37	18.351	2588	2595	2599	rVB	12437	15005	0.75%	0.061%
38	18.727	2655	2659	2663	rBV	113651	126495	6.36%	0.510%
39	18.769	2663	2666	2671	rVB	234599	277787	13.96%	1.120%
40	19.151	2727	2731	2737	rBV	10281	13827	0.70%	0.056%
41	19.410	2770	2775	2780	rBV	9111	11466	0.58%	0.046%
42	19.521	2788	2794	2800	rBV	1534973	1989291	100.00%	8.023%
43	19.580	2800	2804	2811	rVV	35519	45164	2.27%	0.182%
44	19.863	2847	2852	2855	rBV	641969	691810	34.78%	2.790%
45	19.898	2855	2858	2865	rVB	1236761	1292479	64.97%	5.213%
46	20.039	2875	2882	2883	rBV4	906	2135	0.11%	0.009%
47	20.598	2973	2977	2979	rBV	4425	5889	0.30%	0.024%
48	20.621	2979	2981	2984	rVB2	5154	4451	0.22%	0.018%
49	20.839	3014	3018	3021	rBV	196549	209120	10.51%	0.843%
50	20.874	3021	3024	3029	rVB	392664	414451	20.83%	1.671%
51	21.233	3082	3085	3089	rVB	34036	37753	1.90%	0.152%
52	21.315	3094	3099	3108	rVV	823014	1062257	53.40%	4.284%
53	21.462	3121	3124	3126	rBV3	3767	4554	0.23%	0.018%
54	21.715	3163	3167	3169	rBV	66813	76610	3.85%	0.309%
55	21.745	3169	3172	3177	rVB	164879	172308	8.66%	0.695%
56	22.333	3268	3272	3276	rBV	17638	20288	1.02%	0.082%
57	22.421	3284	3287	3292	rBV4	7734	9582	0.48%	0.039%
58	22.645	3321	3325	3328	rBV	40808	54854	2.76%	0.221%
59	22.686	3328	3332	3339	rVB	95373	131391	6.60%	0.530%
60	22.886	3362	3366	3371	rBV5	6398	9945	0.50%	0.040%
61	23.433	3451	3459	3469	rBV	839028	1527456	76.78%	6.160%
62	23.574	3476	3483	3498	rVB	502287	942556	47.38%	3.801%

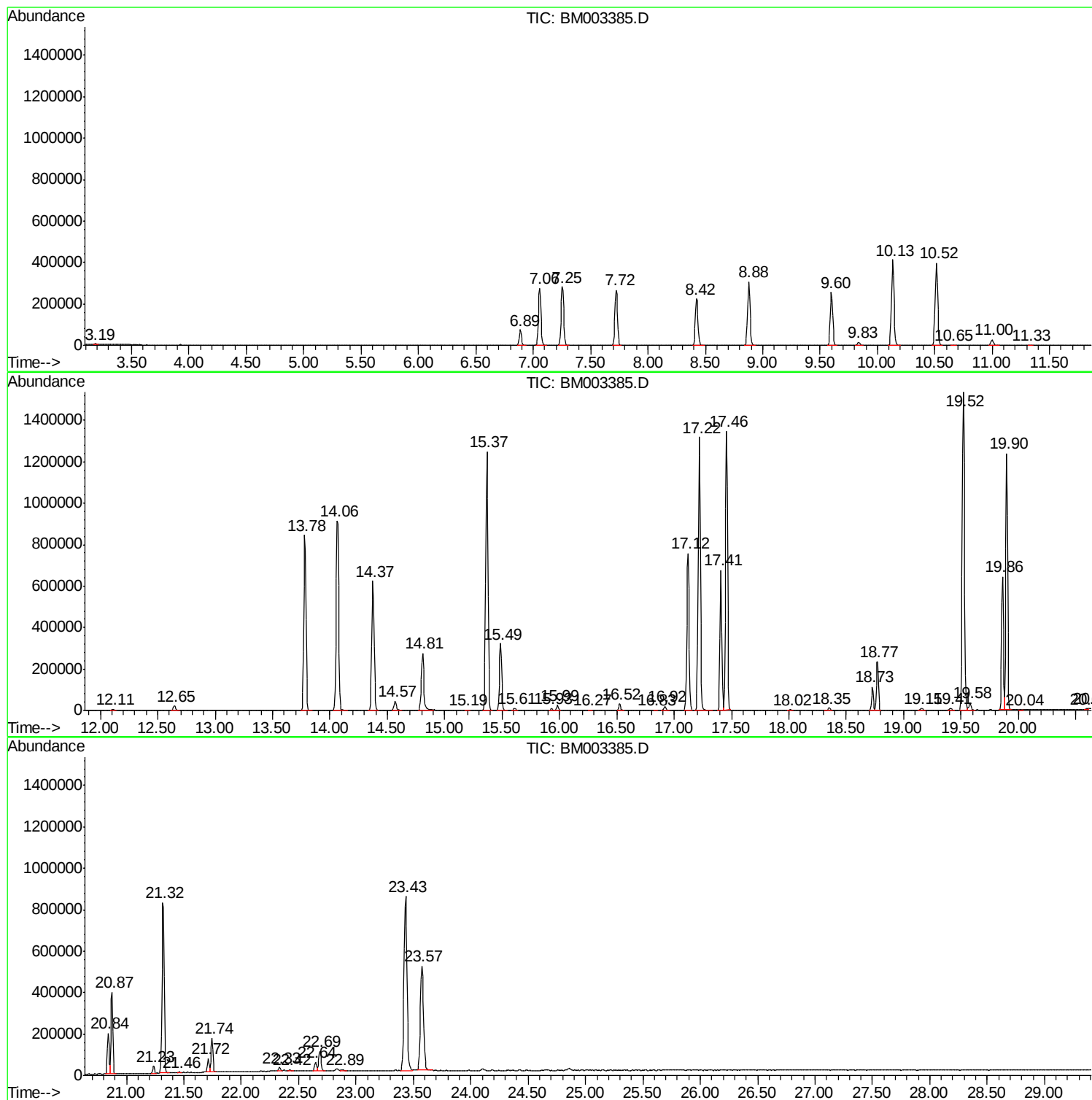
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TIC Library : C:\DATABASE\NIST02.L
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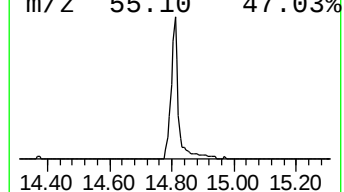
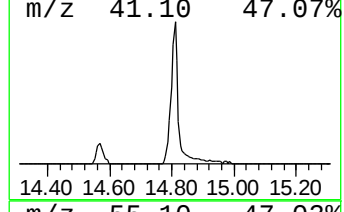
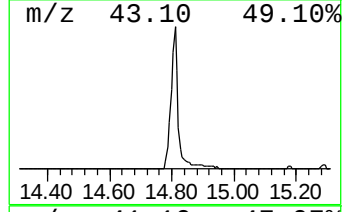
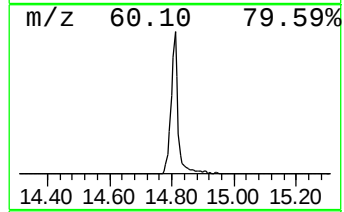
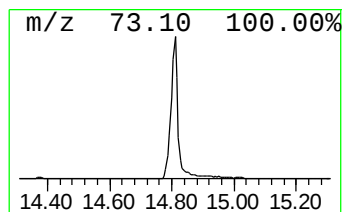
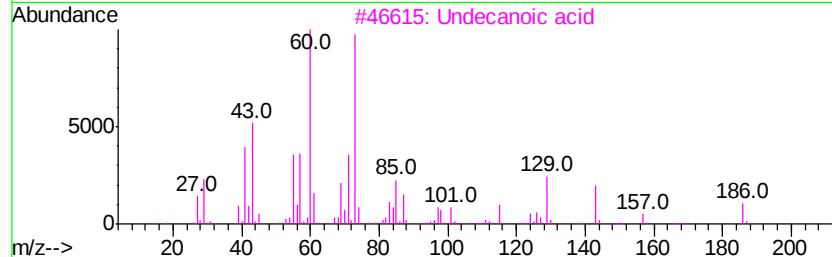
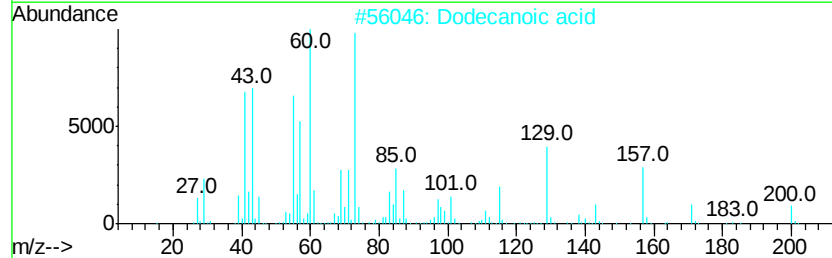
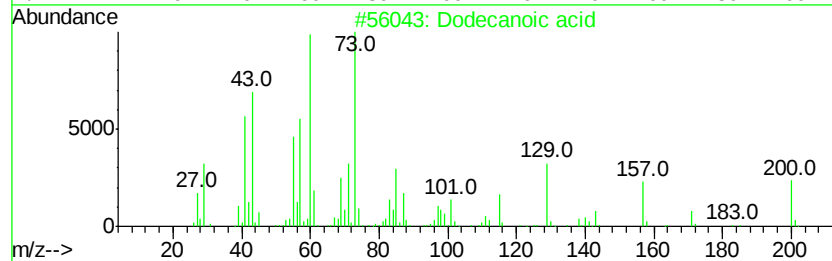
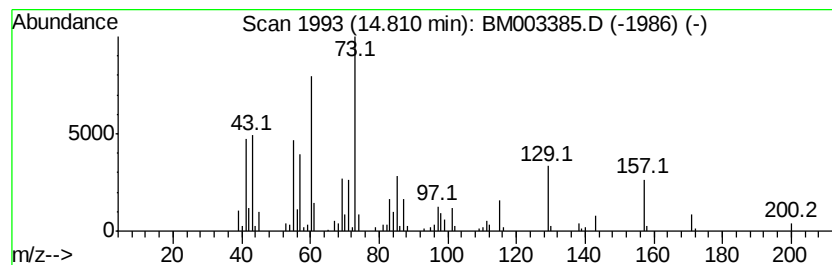
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	8.97 ng/ul	419163	Acenaphthene-d10	14.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	93
2		Dodecanoic acid	200	C12H24O2	000143-07-7	91
3		Undecanoic acid	186	C11H22O2	000112-37-8	72
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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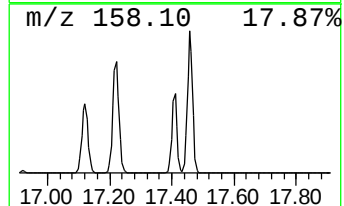
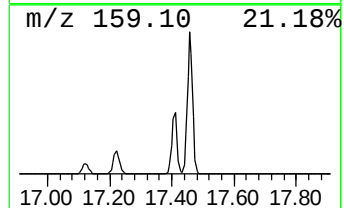
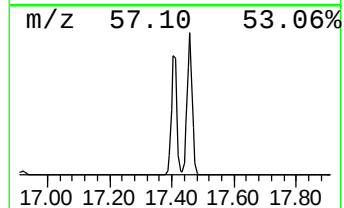
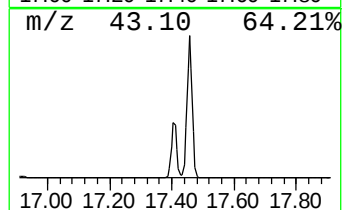
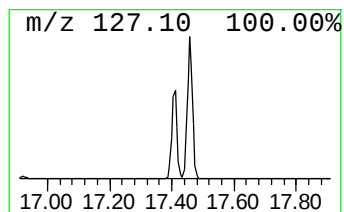
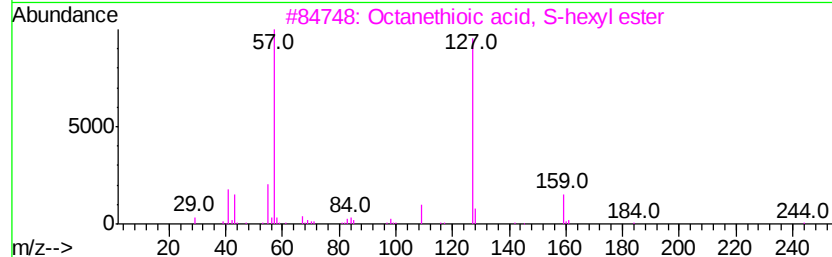
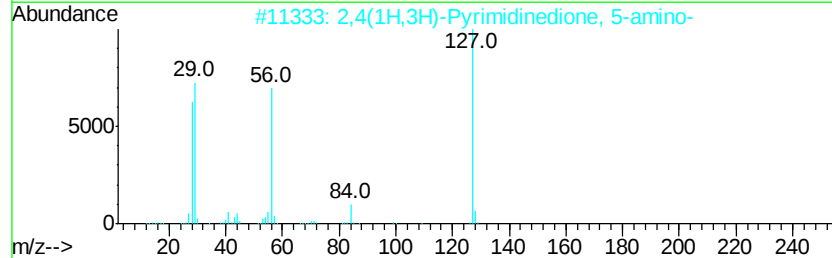
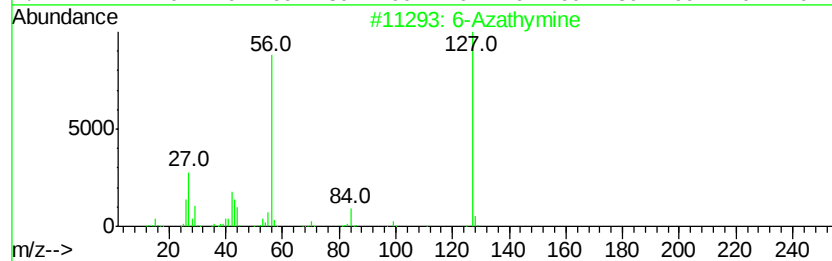
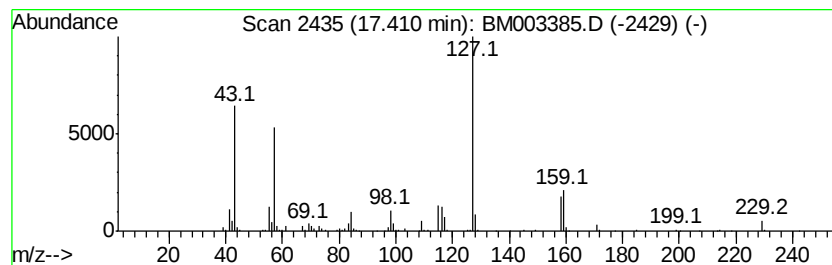
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	15.26 ng/ul	823656	Phenanthrene-d10	17.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Azathymine	127	C4H5N3O2	000932-53-6	43
2		2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	43
3		Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	40
4		Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	38
5		1,3,5-Triazin-2(1H)-one, 4,6-dia...	127	C3H5N5O	000645-92-1	37



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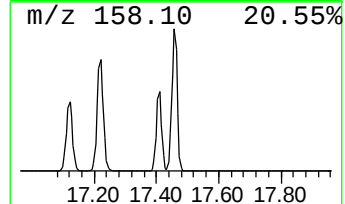
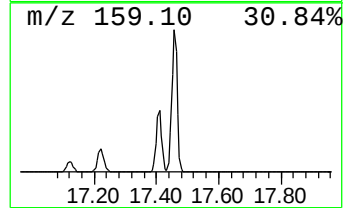
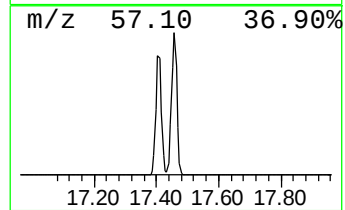
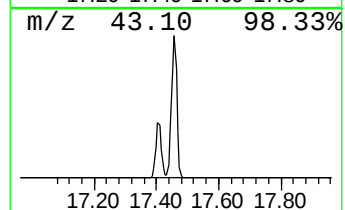
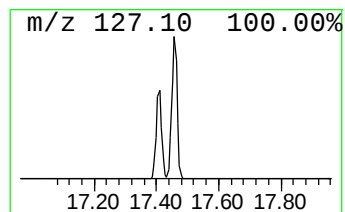
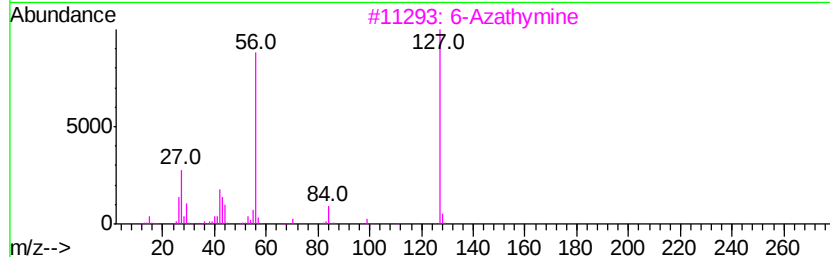
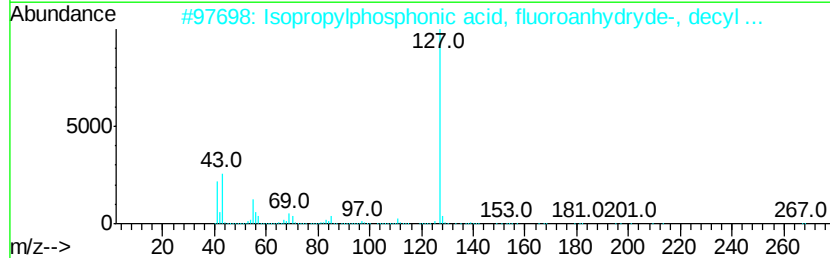
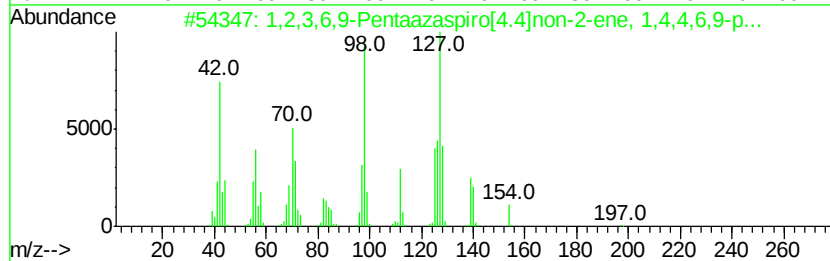
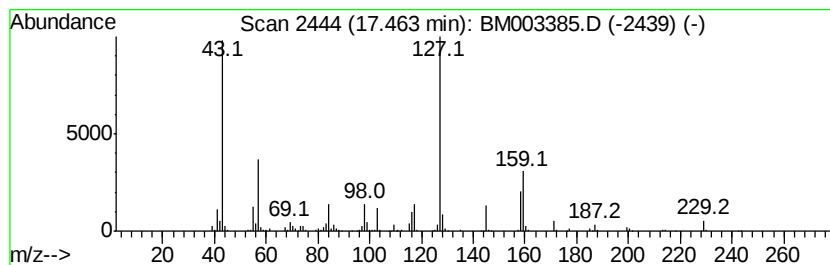
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	29.53 ng/ul	1593480	Phenanthrene-d10	17.12
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1,2,3,6,9-Pentaazaspiro[4.4]non-...	197 C9H19N5	1000221-38-7 43
2		Isopropylphosphonic acid, fluoro...	266 C13H28F02P	333416-36-7 35
3		6-Azathymine	127 C4H5N3O2	000932-53-6 32
4		Propylphosphonic acid, fluoroanh...	238 C11H24F02P	333416-20-9 32
5		Triazene, 1,3-bis(4-methoxyfuraz...	283 C9H13N7O4	349564-78-9 25



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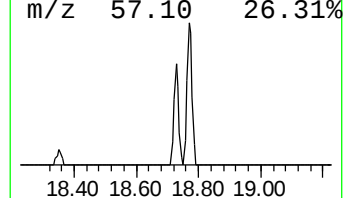
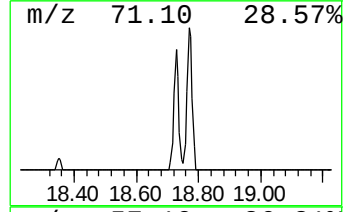
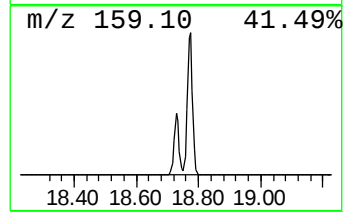
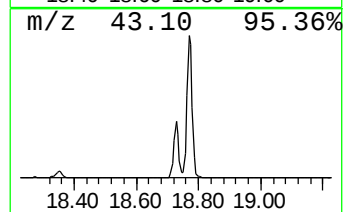
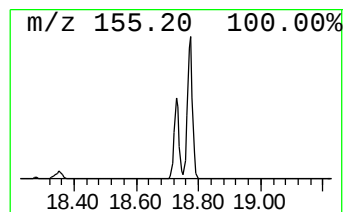
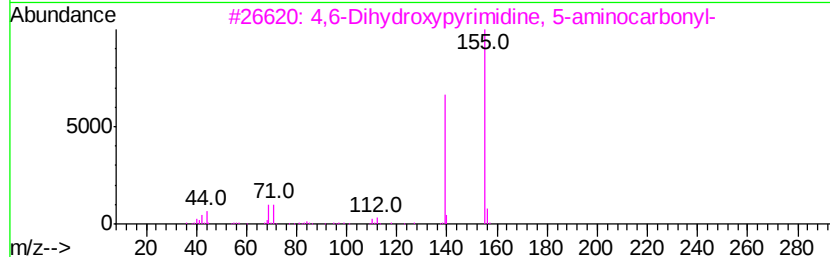
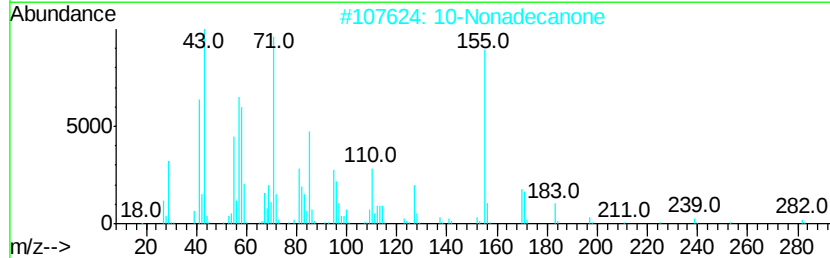
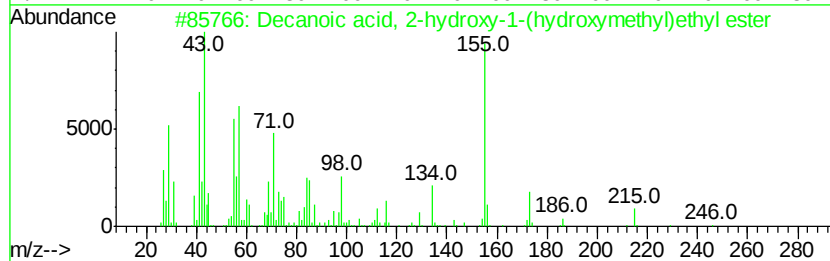
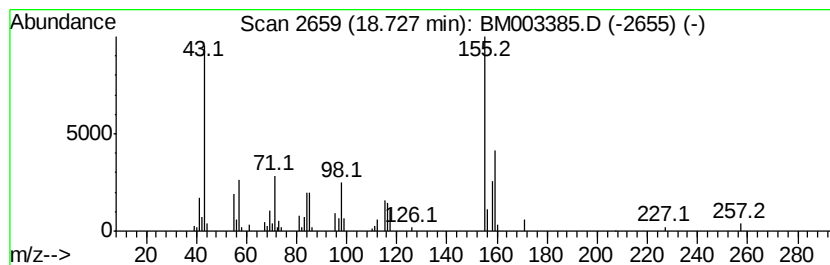
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	2.34 ng/ul	126495	Phenanthrene-d10	17.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decanoic acid, 2-hydroxy-1-(hydr...	246	C13H26O4	003376-48-5	40
2		10-Nonadecanone	282	C19H38O	000504-57-4	25
3		4,6-Dihydroxypyrimidine, 5-amino...	155	C5H5N3O3	001074-97-1	22
4		Xylitol, 1-O-decanoyl-	306	C15H30O6	1000155-78-0	17
5		[1,1'-Bicyclohexyl]-1,1'-diol, 3...	310	C20H38O2	068525-22-4	16



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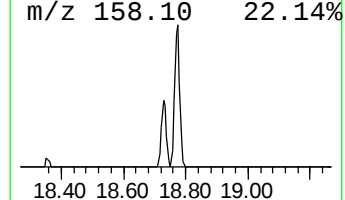
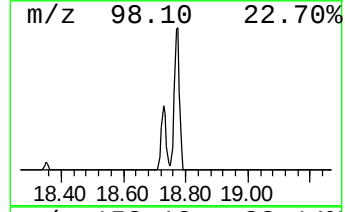
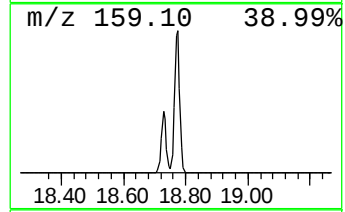
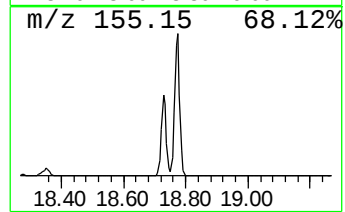
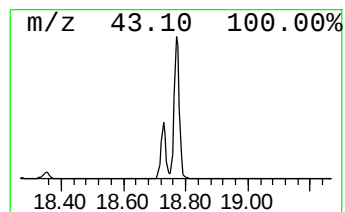
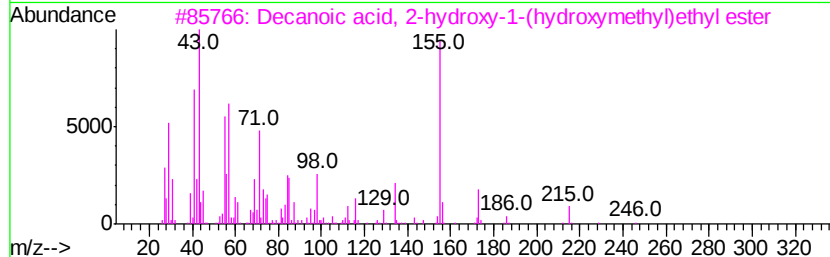
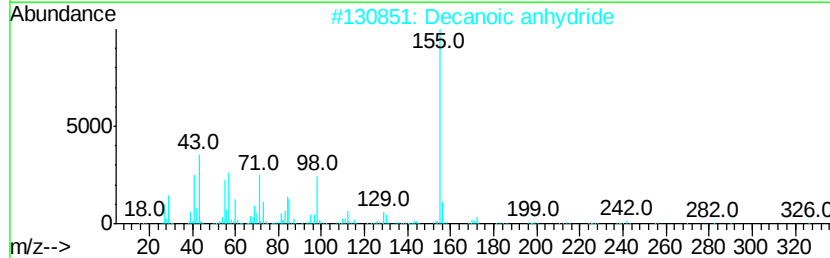
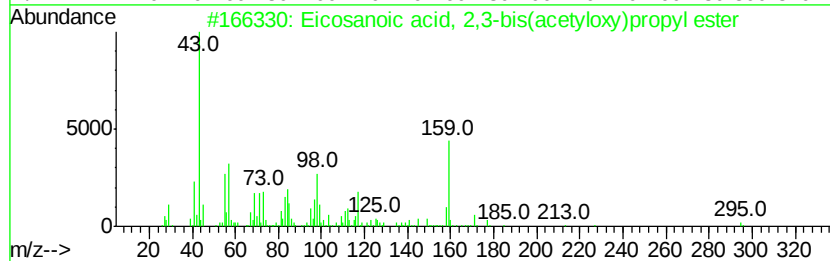
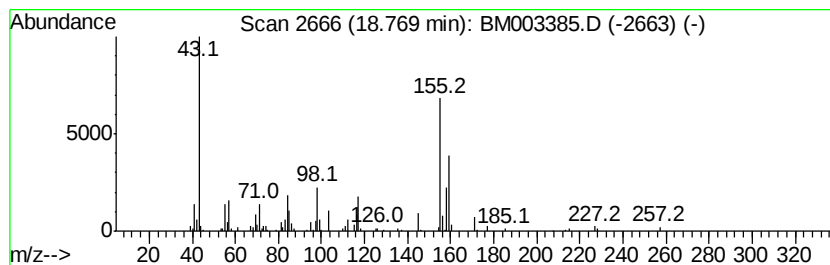
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	5.15 ng/ul	277787	Phenanthrene-d10	17.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	25
2		Decanoic anhydride	326	C20H38O3	002082-76-0	16
3		Decanoic acid, 2-hydroxy-1-(hydr...	246	C13H26O4	003376-48-5	16
4		3-Pyrrolidinecarboxamide, 2,2,5,...	170	C9H18N2O	000702-96-5	10
5		Pyridine, 2-phenyl-	155	C11H9N	001008-89-5	9



Data Path : Z:\HPCHEM1\BNA M\DATA\BM120615\
Data File : BM003385.D
Acq On : 06 Dec 2015 12:45
Operator : UM/IZ
Sample : G4664-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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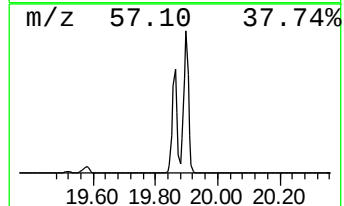
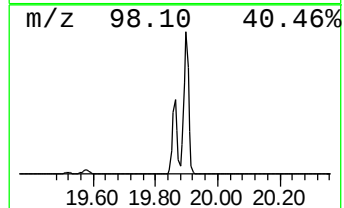
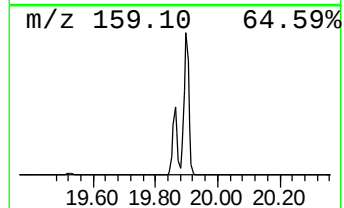
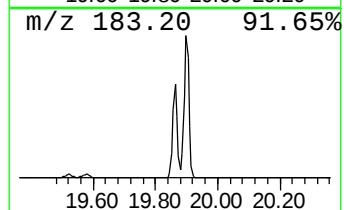
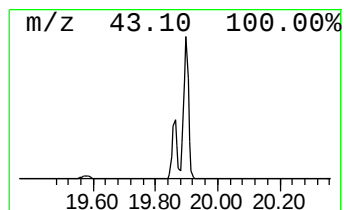
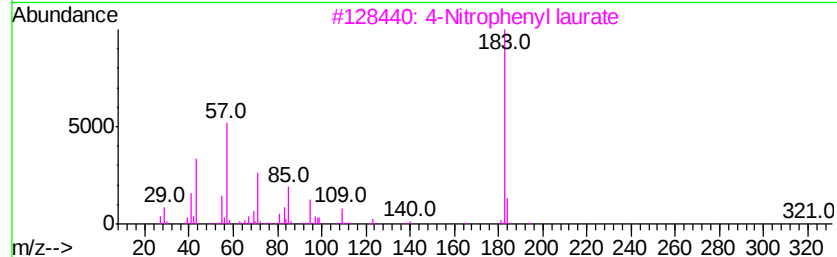
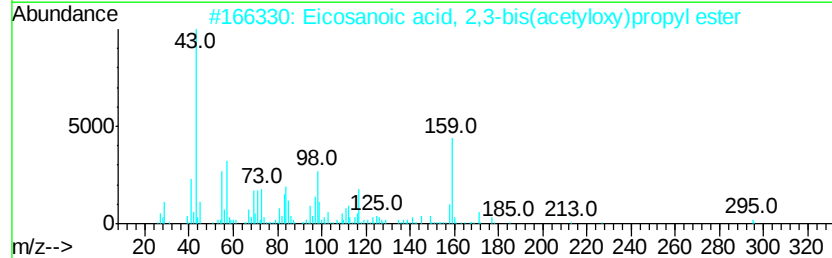
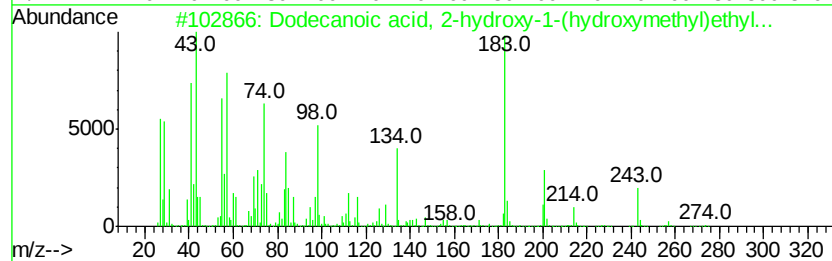
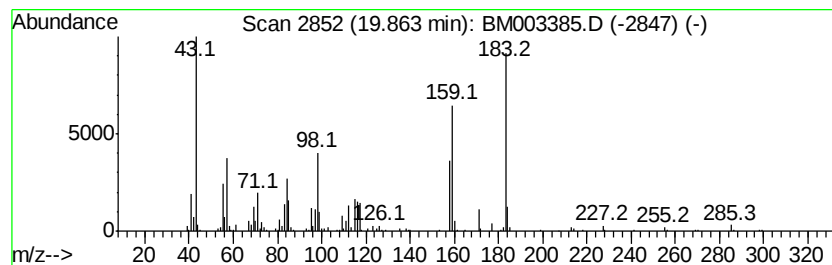
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Dodecanoic acid, 2-hydroxy-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	13.03 ng/ul	691810	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl...	274	C15H30O4	001678-45-1	50
2		Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470	C27H50O6	055429-67-9	25
3		4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	25
4		Lauric anhydride	382	C24H46O3	000645-66-9	25
5		Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	25



Data Path : Z:\HPCHEM1\BNA M\DATA\BM120615\
Data File : BM003385.D
Acq On : 06 Dec 2015 12:45
Operator : UM/IZ
Sample : G4664-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E5E78

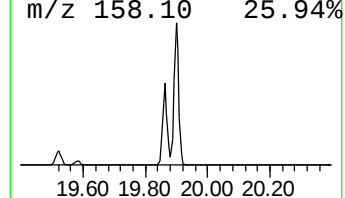
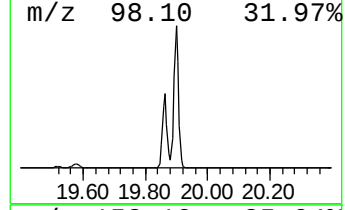
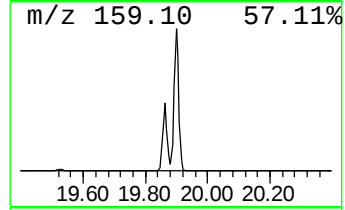
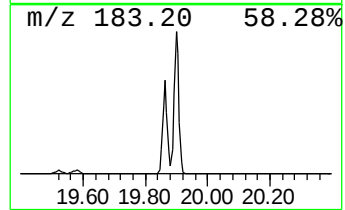
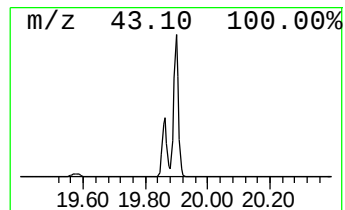
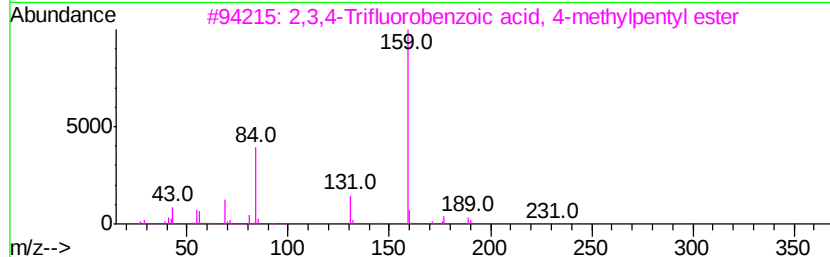
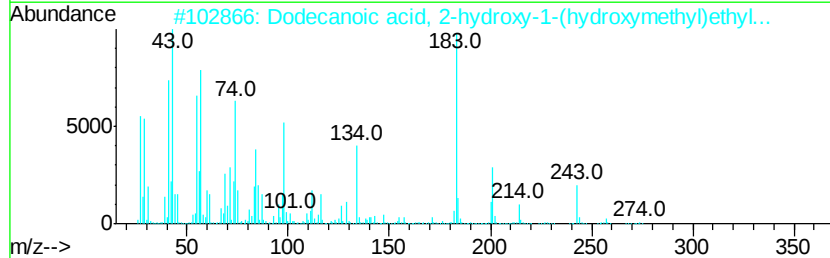
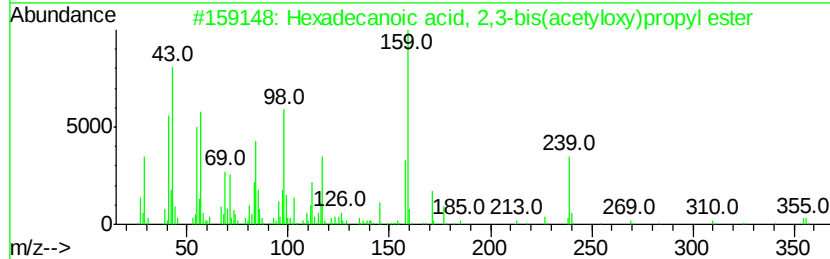
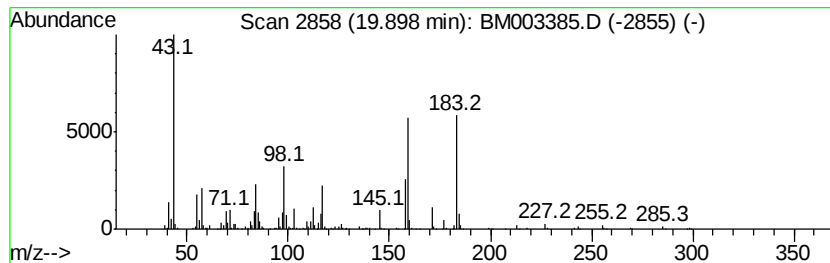
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-05 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	24.33 ng/ul	1292480	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	43
2		Dodecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	274	C15H30O4	001678-45-1	35
3		2,3,4-Trifluorobenzoic acid, 4-methylpentyl ester	260	C13H15F3O2	1000282-29-8	14
4		Dodecanoyl chloride	218	C12H23ClO	000112-16-3	12
5		1,2-Dicarbadodecaborane(12), 1-hydroxy-2-methylpentyl ester	230	C8H24B10	020740-05-0	11



Data Path : Z:\HPCHEM1\BNA M\DATA\BM120615\
Data File : BM003385.D
Acq On : 06 Dec 2015 12:45
Operator : UM/IZ
Sample : G4664-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E5E78

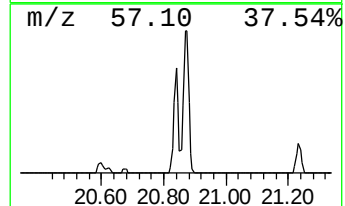
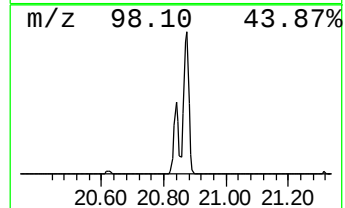
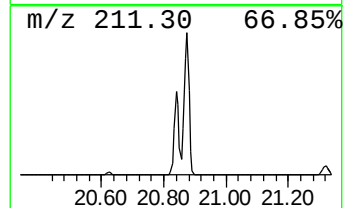
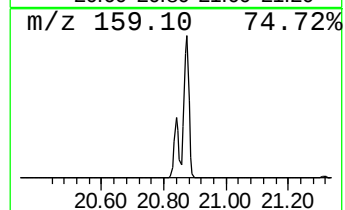
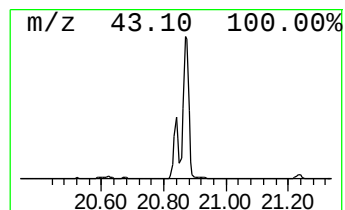
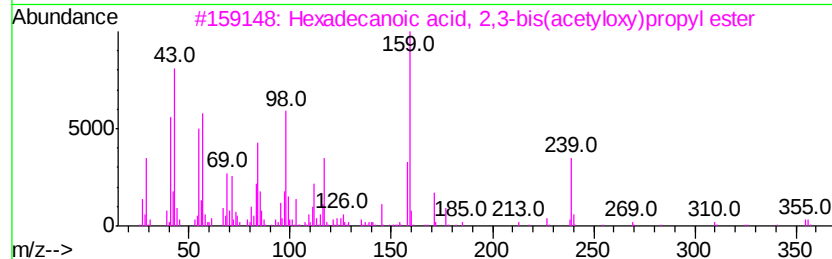
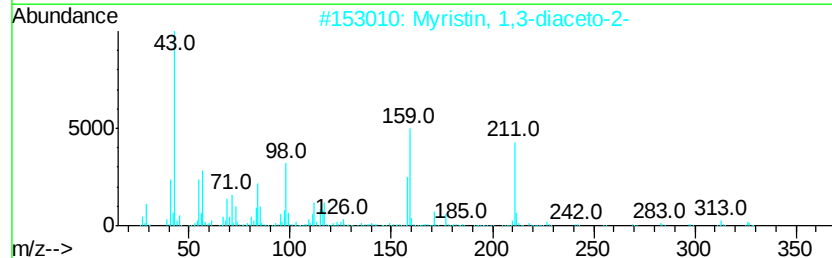
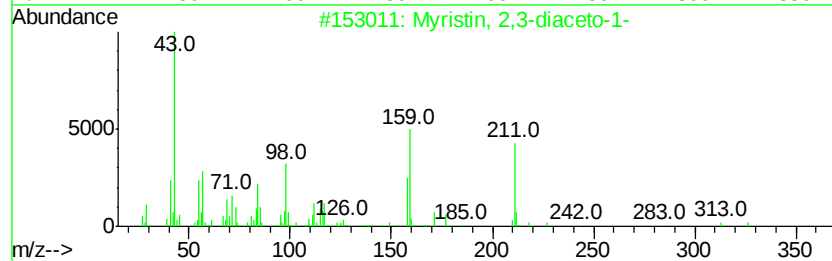
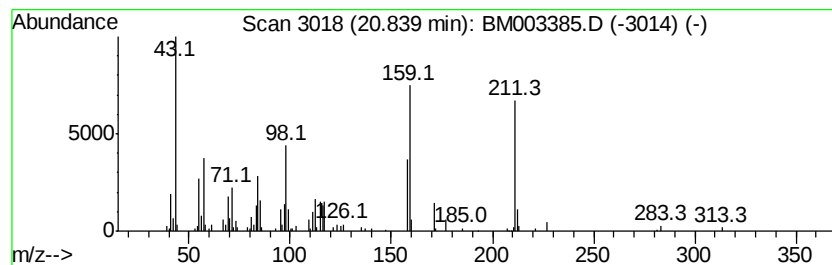
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Myristin, 2,3-diaceto-1- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	3.94 ng/ul	209120	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	91
2		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	91
3		Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414	C23H42O6	055268-70-7	64
4		2,3,4-Trifluorobenzoic acid, 4-methyl-	260	C13H15F3O2	1000282-29-8	27
5		1-Propene-1-amine, N-benzylidene-	159	C11H13N	039575-55-8	27



Data Path : Z:\HPCHEM1\BNA M\DATA\BM120615\
Data File : BM003385.D
Acq On : 06 Dec 2015 12:45
Operator : UM/IZ
Sample : G4664-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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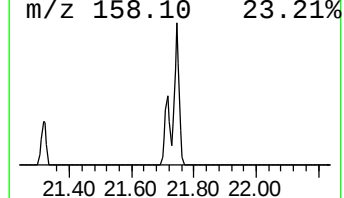
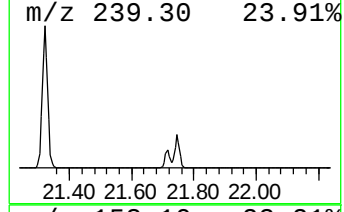
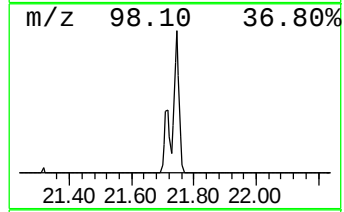
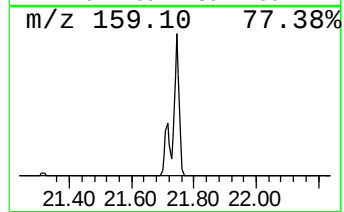
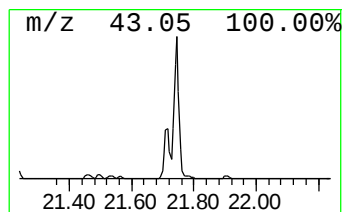
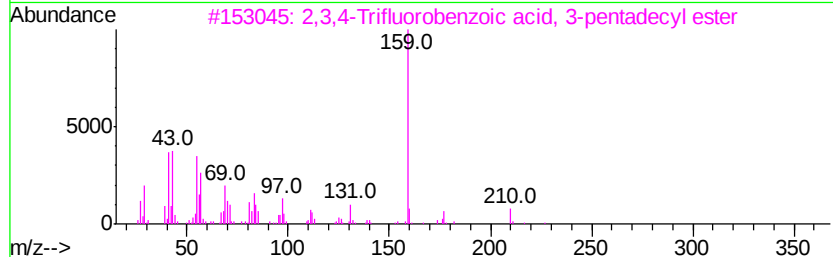
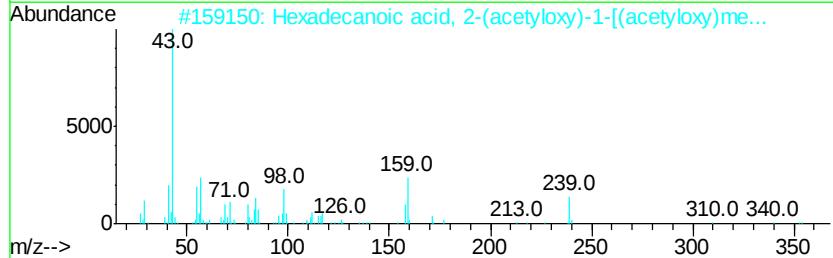
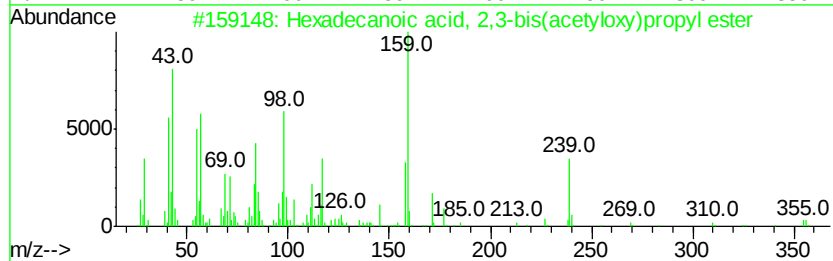
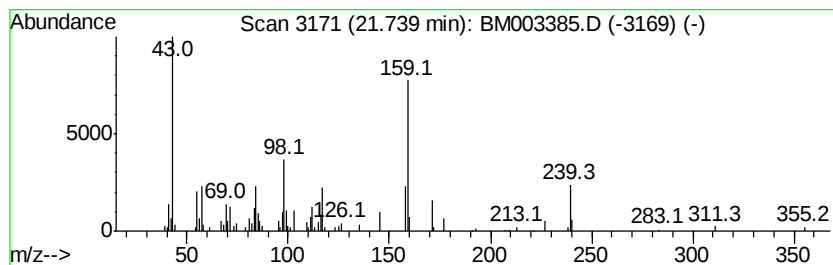
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM02.2-EPA-BM120115.M
Quant Title : SVOA CALIBRATION

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

Peak Number 10 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.74	3.24 ng/ul	172308	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	91
2		Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	58
3		2,3,4-Trifluorobenzoic acid, 3-p...	386	C22H33F3O2	1000280-62-2	25
4		2,6-Difluorobenzoic acid, octade...	410	C25H40F2O2	1000292-39-7	22
5		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	22



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM120615\
Data File : BM003385.D
Acq On : 06 Dec 2015 12:45
Operator : UM/IZ
Sample : G4664-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM120115.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
Dodecanoic acid	14.81	9.0	ng/ul	419163	3	14.37	934910	20.0
unknown-01	17.41	15.3	ng/ul	823656	4	17.12	1079280	20.0
unknown-02	17.46	29.5	ng/ul	1593480	4	17.12	1079280	20.0
unknown-03	18.73	2.3	ng/ul	126495	4	17.12	1079280	20.0
unknown-04	18.77	5.2	ng/ul	277787	4	17.12	1079280	20.0
Dodecanoic acid, ...	19.86	13.0	ng/ul	691810	5	21.32	1062260	20.0
unknown-05	19.90	24.3	ng/ul	1292480	5	21.32	1062260	20.0
Myristin, 2,3-dia...	20.84	3.9	ng/ul	209120	5	21.32	1062260	20.0
Hexadecanoic acid...	21.74	3.2	ng/ul	172308	5	21.32	1062260	20.0