

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081316\
 Data File : BM007063.D
 Acq On : 13 Aug 2016 11:20
 Operator : UM/SJ
 Sample : H4389-12
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PR002-SS006-0612-01

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-BM081116.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	2.669	12	14	28	rVB8	31784	75802	1.06%	0.090%
2	3.328	121	126	134	rVB	54044	83025	1.16%	0.099%
3	6.975	739	746	759	rVB	1052493	1717135	24.06%	2.045%
4	7.145	766	775	784	rBV	803228	1241407	17.40%	1.479%
5	7.345	802	809	819	rVB	1103340	1771458	24.82%	2.110%
6	7.810	880	888	897	rBV	1011184	1653648	23.17%	1.970%
7	8.504	998	1006	1015	rBV	1215788	1993445	27.93%	2.374%
8	8.963	1077	1084	1092	rBV	1008864	1661219	23.28%	1.979%
9	9.681	1198	1206	1215	rBV	835385	1412026	19.79%	1.682%
10	10.216	1289	1297	1308	rBV	1307136	2229891	31.25%	2.656%
11	10.598	1353	1362	1369	rBV	1319679	2234216	31.31%	2.661%
12	10.728	1376	1384	1401	rBV	940227	1718193	24.08%	2.047%
13	13.851	1908	1915	1919	rBV	2273096	3139095	43.99%	3.739%
14	13.898	1919	1923	1933	rVB	1784567	2455290	34.41%	2.925%
15	14.133	1953	1963	1975	rBV	2533249	3814518	53.45%	4.544%
16	14.439	2008	2015	2024	rBV2	1846295	2859589	40.07%	3.406%
17	14.627	2040	2047	2060	rBV	977013	1433160	20.08%	1.707%
18	15.298	2157	2161	2167	rVB2	62471	82092	1.15%	0.098%
19	15.433	2177	2184	2191	rBV	3213761	4660119	65.30%	5.551%
20	15.545	2197	2203	2213	rBV	904859	1292842	18.12%	1.540%
21	15.674	2220	2225	2229	rBV3	41343	75899	1.06%	0.090%
22	16.162	2303	2308	2324	rBV	105720	217698	3.05%	0.259%
23	16.951	2438	2442	2448	rBV2	79760	116096	1.63%	0.138%
24	17.186	2473	2482	2486	rBV2	2338743	3521844	49.35%	4.195%
25	17.221	2486	2488	2493	rVV	217498	300970	4.22%	0.358%
26	17.280	2493	2498	2508	rVB2	3408487	5102374	71.50%	6.078%
27	17.574	2537	2548	2559	rBV9	30617	91896	1.29%	0.109%
28	18.080	2621	2634	2643	rBV2	377177	772809	10.83%	0.921%
29	18.245	2657	2662	2666	rBV2	80963	146643	2.05%	0.175%
30	18.286	2666	2669	2675	rVB2	58135	84910	1.19%	0.101%
31	18.598	2719	2722	2727	rVB4	51392	75138	1.05%	0.090%
32	18.974	2782	2786	2791	rBV	81969	118258	1.66%	0.141%
33	19.115	2805	2810	2817	rBV4	40713	84926	1.19%	0.101%
34	19.239	2822	2831	2839	rVV	524843	810033	11.35%	0.965%

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Integration Parameters: LSCINT.P

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	19.362	2847	2852	2860	rBV3	165179	260190	3.65%	0.310%
36	19.574	2882	2888	2900	rBV	4584072	7136325	100.00%	8.500%
37	19.680	2902	2906	2911	rBV3	48204	84806	1.19%	0.101%
38	19.933	2944	2949	2955	rBV5	37637	81710	1.14%	0.097%
39	20.097	2973	2977	2986	rVB3	107380	246457	3.45%	0.294%
40	20.256	3000	3004	3008	rVB2	79151	115857	1.62%	0.138%
41	20.562	3053	3056	3060	rVB5	61302	79616	1.12%	0.095%
42	20.845	3101	3104	3110	rVB	60830	84911	1.19%	0.101%
43	21.080	3140	3144	3151	rBV2	724481	921570	12.91%	1.098%
44	21.286	3176	3179	3183	rBV	134403	158124	2.22%	0.188%
45	21.362	3185	3192	3197	rVV	3893668	5331335	74.71%	6.350%
46	21.397	3197	3198	3205	rVB	297945	307284	4.31%	0.366%
47	21.527	3217	3220	3223	rBV3	80826	93331	1.31%	0.111%
48	21.980	3292	3297	3305	rBV2	614551	1039756	14.57%	1.238%
49	22.433	3370	3374	3380	rBV3	300668	524476	7.35%	0.625%
50	22.674	3412	3415	3419	rVB4	76868	96946	1.36%	0.115%
51	22.956	3458	3463	3467	rBV2	759934	1329317	18.63%	1.583%
52	22.997	3467	3470	3484	rVB3	390212	713112	9.99%	0.849%
53	23.444	3542	3546	3548	rBV	109345	167938	2.35%	0.200%
54	23.491	3548	3554	3560	rBV2	3469395	6460262	90.53%	7.695%
55	23.638	3571	3579	3594	rVB	2498857	5127461	71.85%	6.108%
56	24.203	3669	3675	3682	rBV	660835	1317095	18.46%	1.569%
57	24.285	3684	3689	3698	rVB4	206792	469567	6.58%	0.559%
58	24.968	3800	3805	3813	rVB	272087	627865	8.80%	0.748%
59	25.868	3952	3958	3967	rBV2	243608	685231	9.60%	0.816%
60	26.768	4105	4111	4120	rVB6	259882	713087	9.99%	0.849%
61	27.450	4220	4227	4240	rVB6	222189	731597	10.25%	0.871%

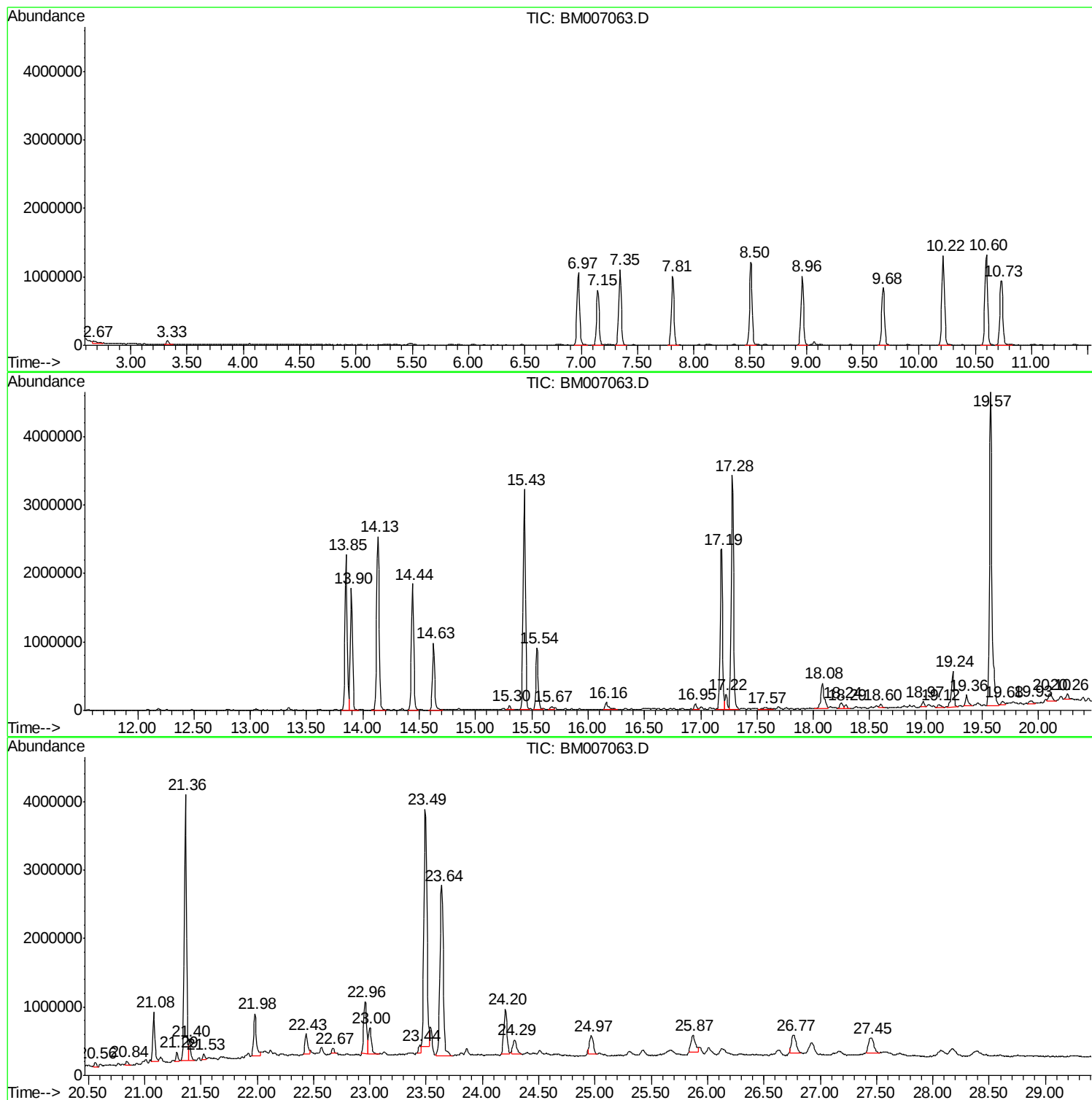
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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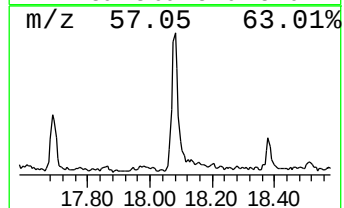
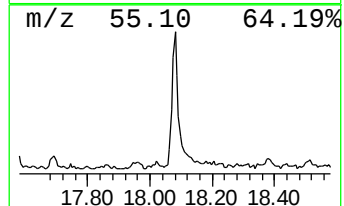
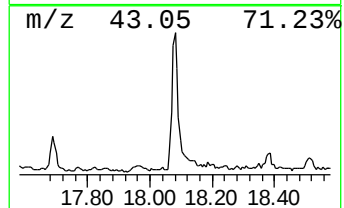
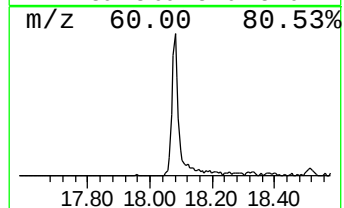
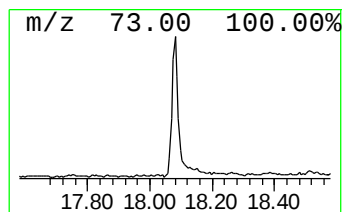
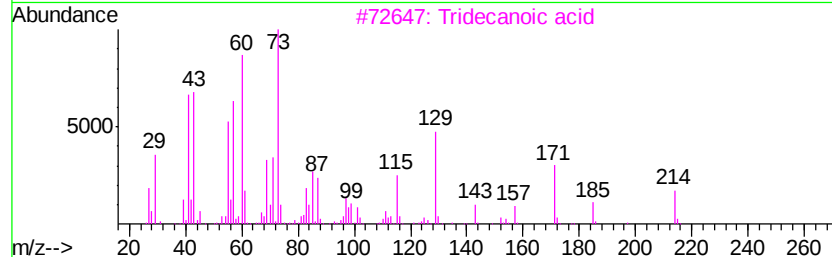
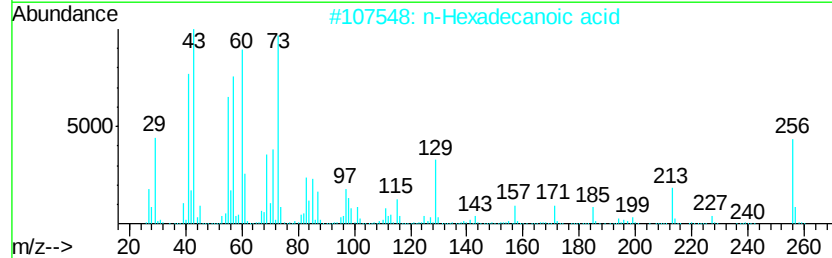
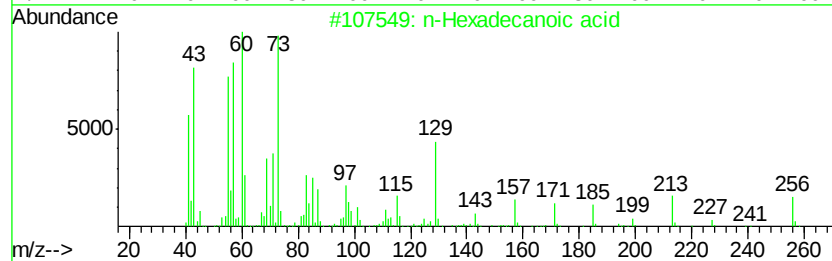
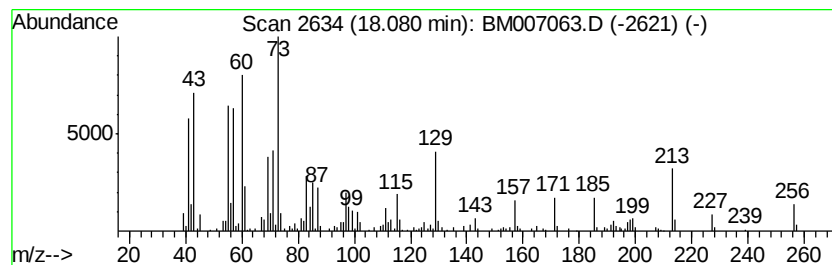
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM081116.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.08	4.39 ng/ul	772809	Phenanthrene-d10		17.19	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95	
3	Tridecanoic acid	214	C13H26O2	000638-53-9	94	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91	
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90	



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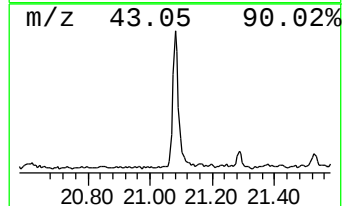
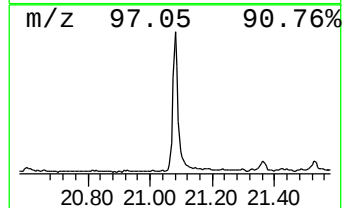
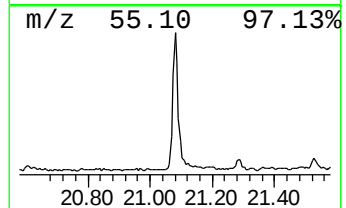
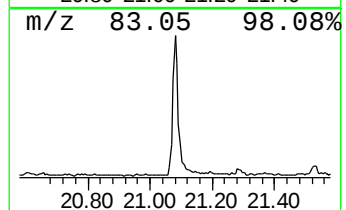
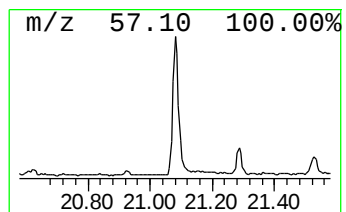
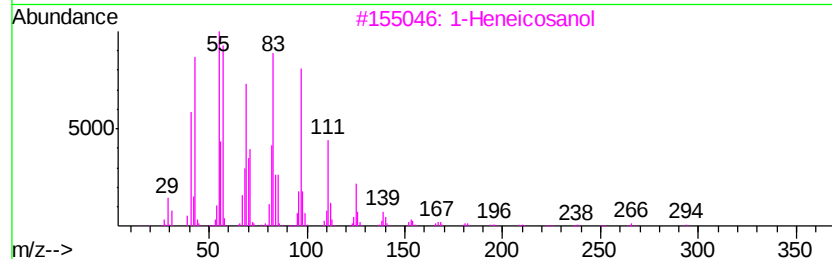
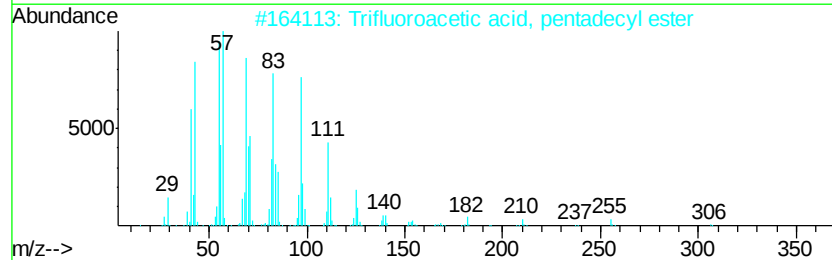
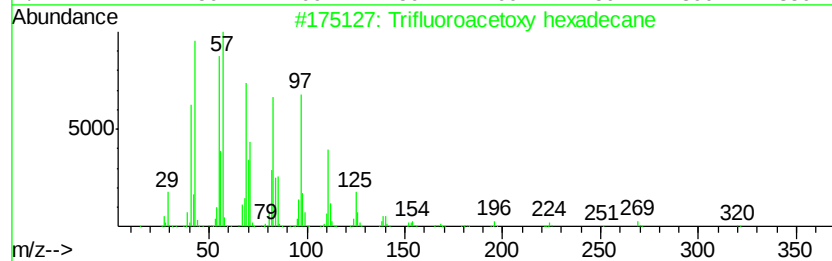
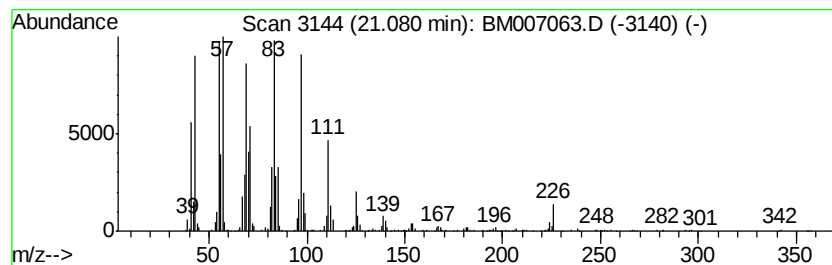
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	3.46 ng/ul	921570	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		1-Nonadecene	266	C19H38	018435-45-5	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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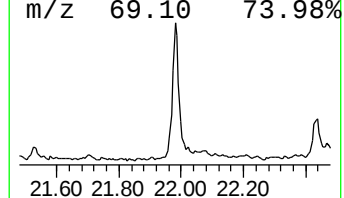
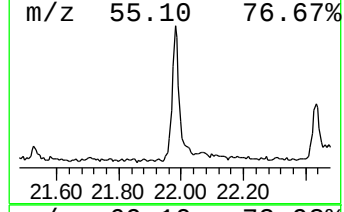
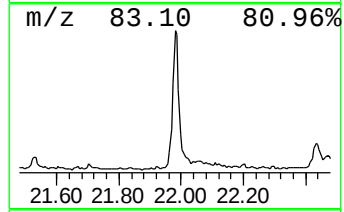
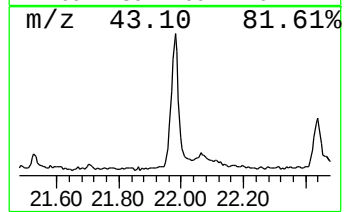
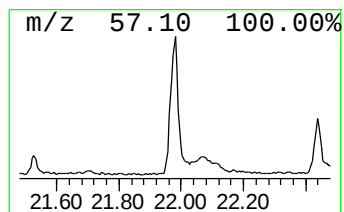
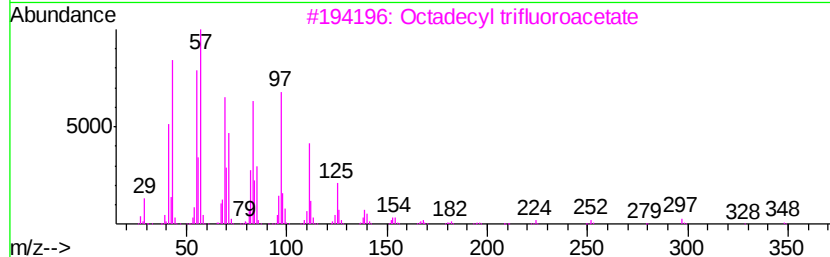
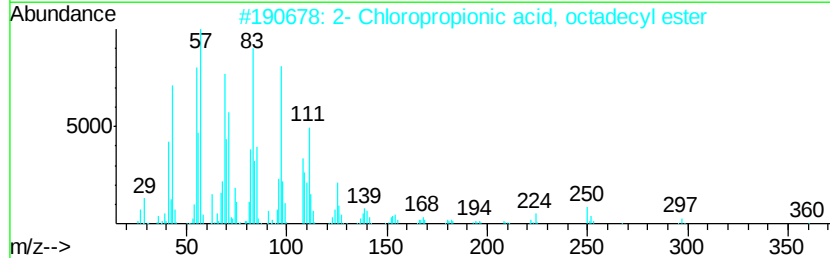
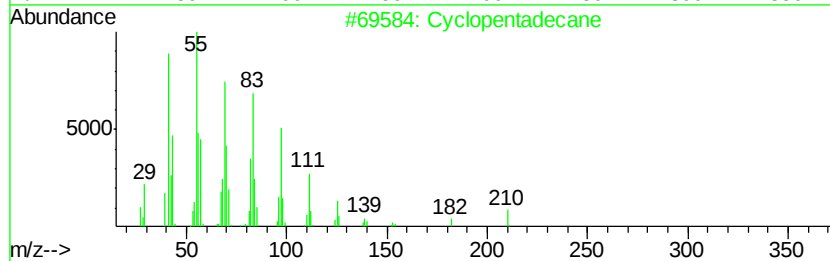
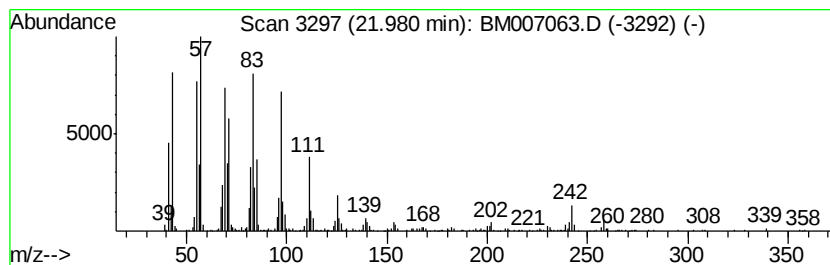
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic21.98 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.98	3.90 ng/ul	1039760	Chrysene-d12	21.36		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	97
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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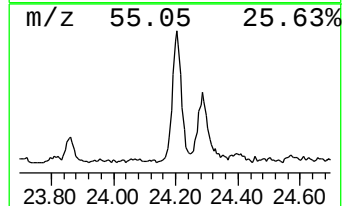
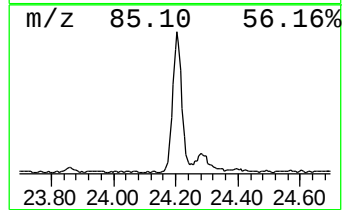
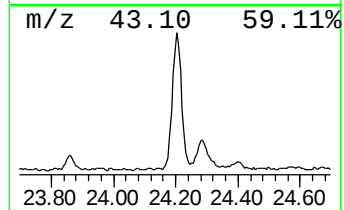
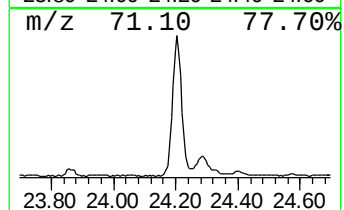
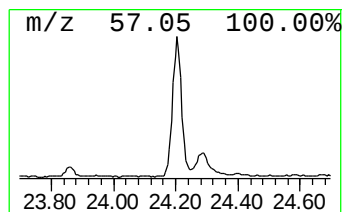
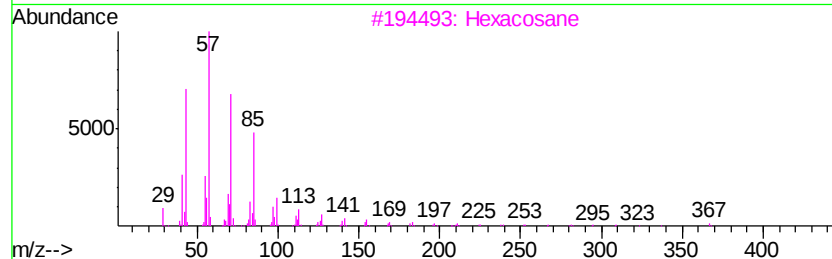
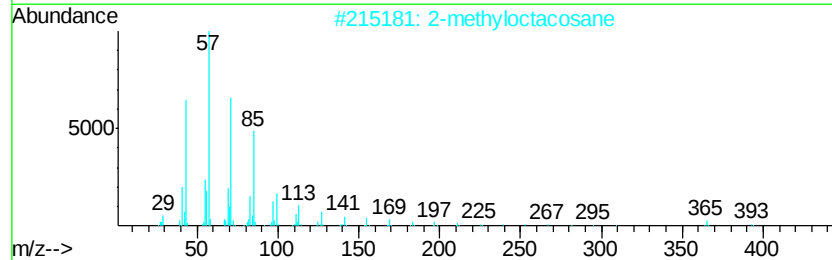
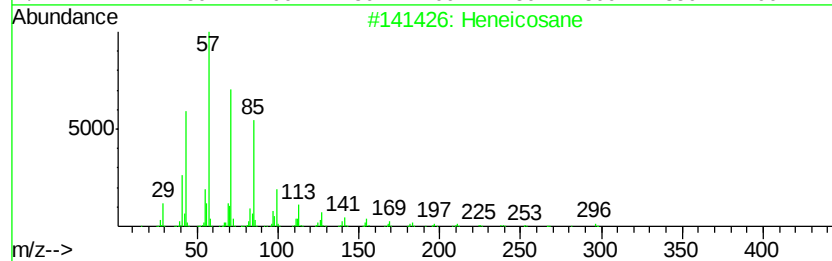
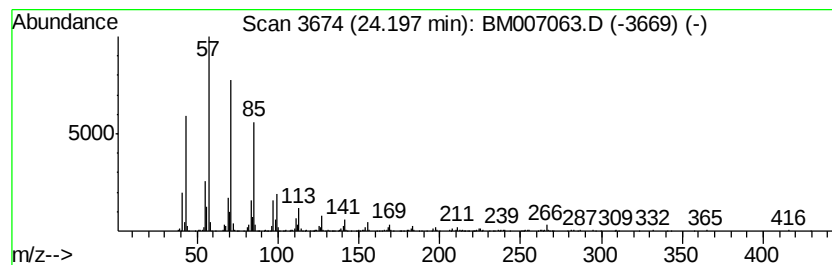
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.20	5.14 ng/ul	1317100	Perylene-d12	23.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Octacosane	394	C28H58	000630-02-4	91



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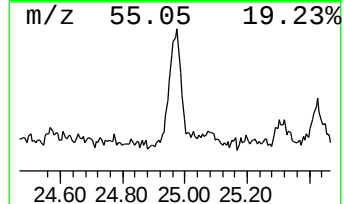
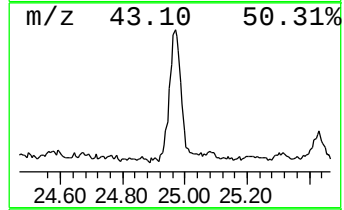
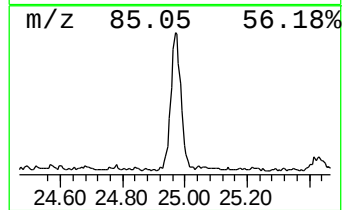
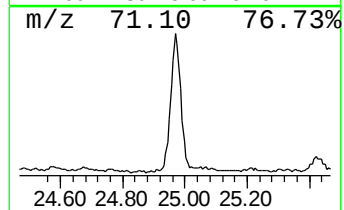
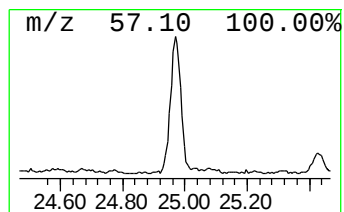
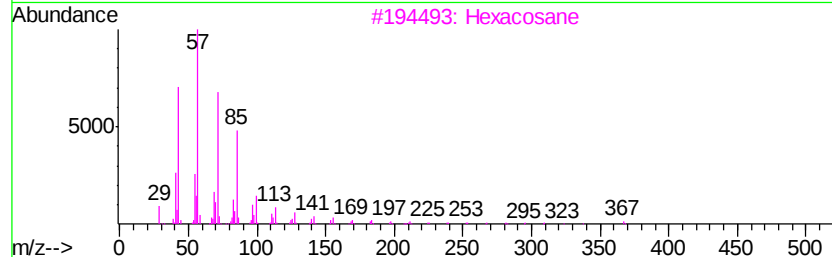
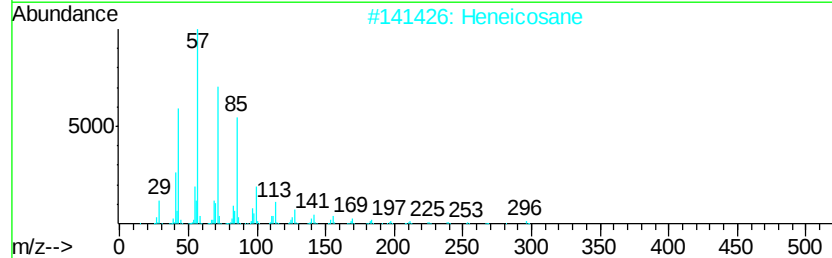
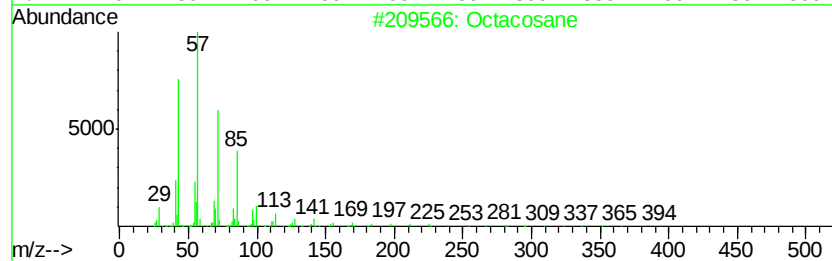
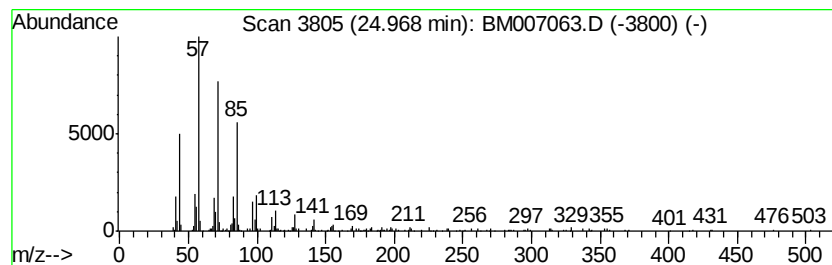
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	2.45 ng/ul	627865	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		5,5,7,7-Tetraethylundecane	268	C19H40	1000360-42-0	90



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081316\
Data File : BM007063.D
Acq On : 13 Aug 2016 11:20
Operator : UM/SJ
Sample : H4389-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PR002-SS006-0612-01

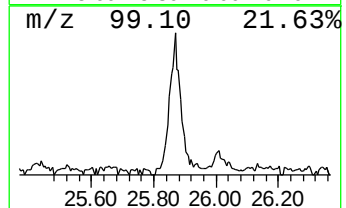
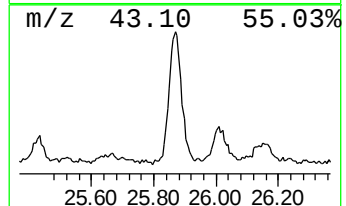
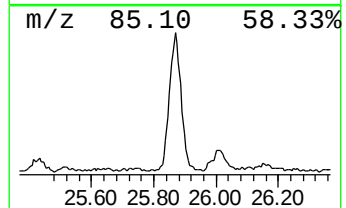
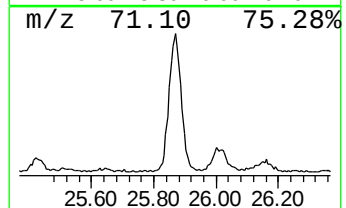
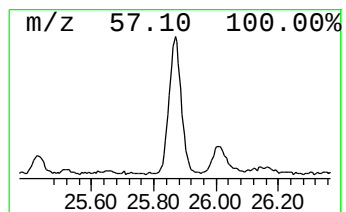
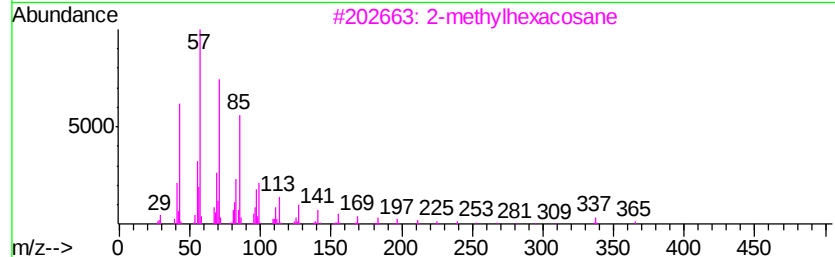
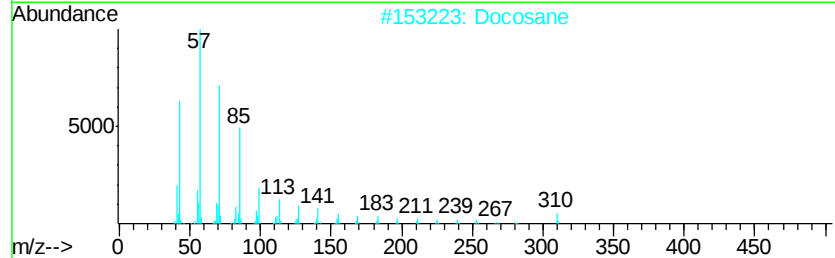
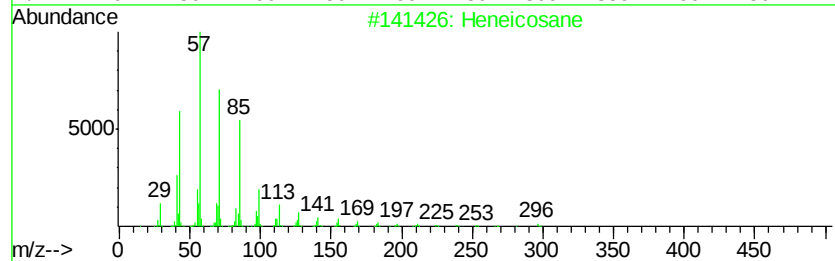
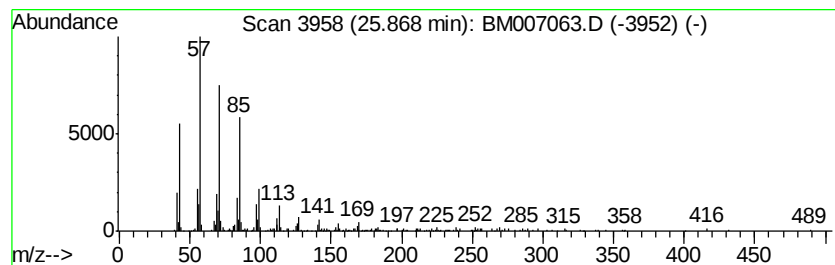
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.87	2.67 ng/ul	685231	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Docosane	310	C22H46	000629-97-0	94
3		2-methylhexacosane	380	C27H56	1000376-72-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081316\
Data File : BM007063.D
Acq On : 13 Aug 2016 11:20
Operator : UM/SJ
Sample : H4389-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

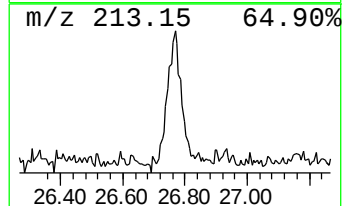
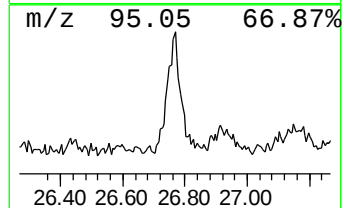
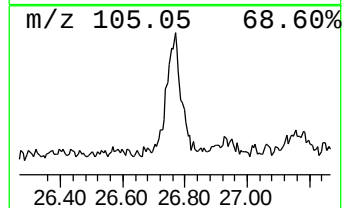
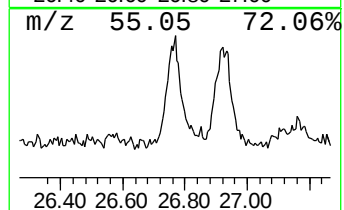
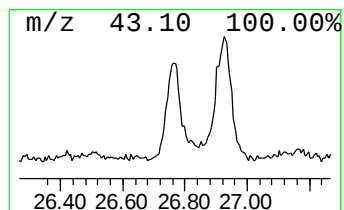
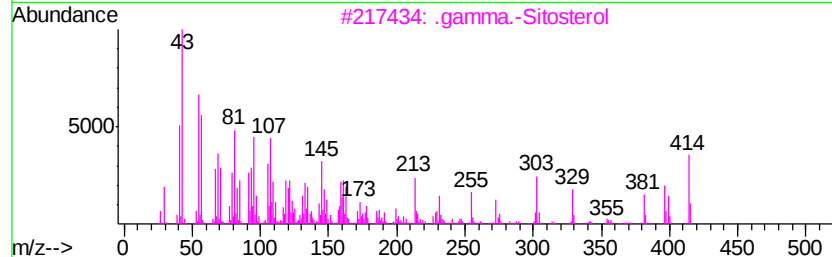
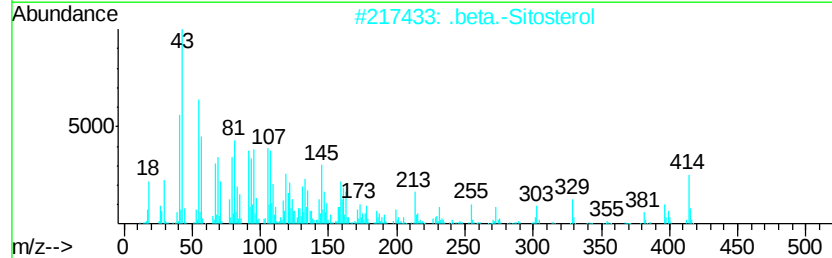
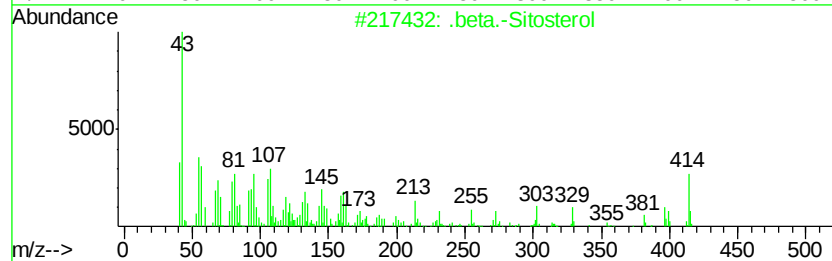
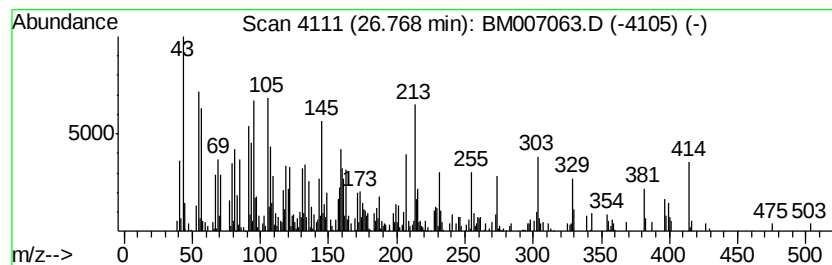
Instrument :
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ClientSampleId :
PR002-SS006-0612-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM081116.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 .beta.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.77	2.78 ng/ul	713087	Perylene-d12	23.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 90
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 87
3		.gamma.-Sitosterol	414 C29H50O	000083-47-6 87
4		.gamma.-Sitosterol	414 C29H50O	000083-47-6 47
5		Cyclopentanecarboxylic acid, 1-p...	273 C14H15N3OS	1000311-03-5 15



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081316\
Data File : BM007063.D
Acq On : 13 Aug 2016 11:20
Operator : UM/SJ
Sample : H4389-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PR002-SS006-0612-01

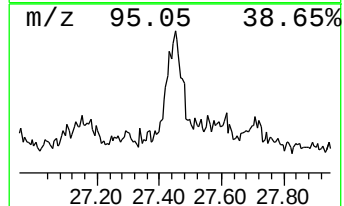
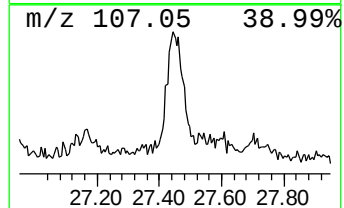
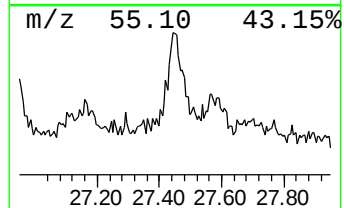
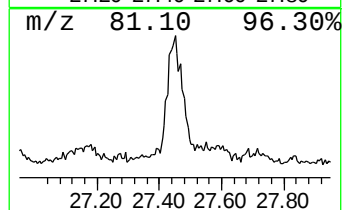
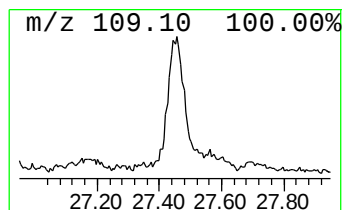
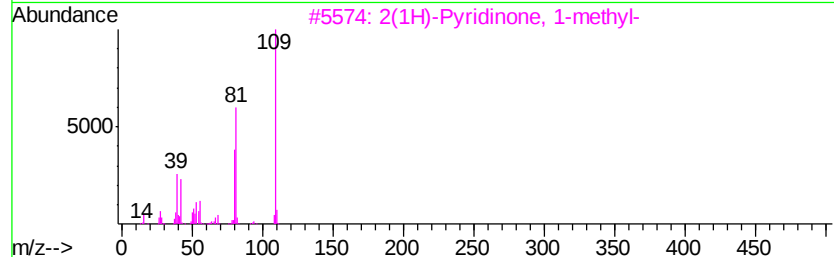
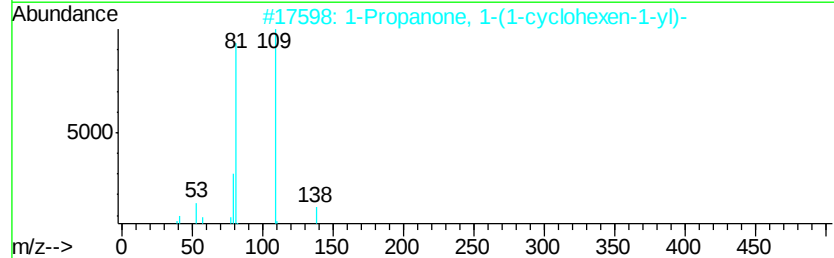
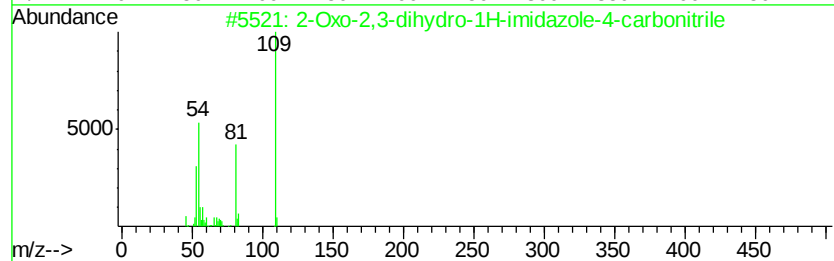
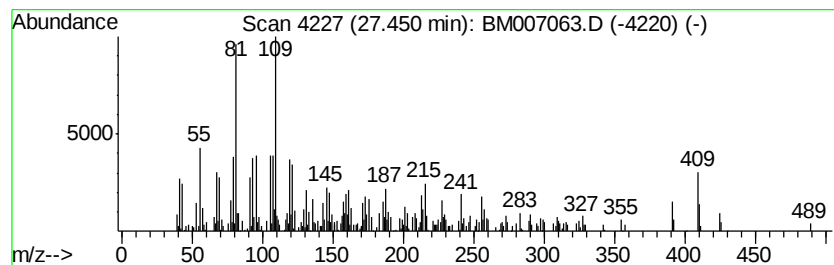
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.45	2.85 ng/ul	731597	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Oxo-2,3-dihydro-1H-imidazole-4...	109	C4H3N3O	1000294-08-6	38
2		1-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	001655-03-4	38
3		2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	000694-85-9	38
4		4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	35
5		Tris(2,7-dimethyl-2,7-octadien-1...	425	C30H51N	088399-36-4	35



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM081316\
Data File : BM007063.D
Acq On : 13 Aug 2016 11:20
Operator : UM/SJ
Sample : H4389-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PR002-SS006-0612-01

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM081116.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	18.08	4.4	ng/ul	772809	4	17.19	3521840	20.0
Trifluoroacetoxy ...	21.08	3.5	ng/ul	921570	5	21.36	5331340	20.0
(DEL) Alkane: Cyc...	21.98	3.9	ng/ul	1039760	5	21.36	5331340	20.0
(DEL) Alkane: Str...	24.20	5.1	ng/ul	1317100	6	23.64	5127460	20.0
(DEL) Alkane: Str...	24.97	2.5	ng/ul	627865	6	23.64	5127460	20.0
(DEL) Alkane: Str...	25.87	2.7	ng/ul	685231	6	23.64	5127460	20.0
.beta.-Sitosterol	26.77	2.8	ng/ul	713087	6	23.64	5127460	20.0
unknown-01	27.45	2.9	ng/ul	731597	6	23.64	5127460	20.0