

Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
 Data File : BM014530.D
 Acq On : 12 Mar 2018 22:47
 Operator : SJ/JU
 Sample : J1813-16
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F6F34

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\SOM-EPA-BM021418.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	4.628	290	296	299	rBV2	29523	40707	2.35%	0.224%
2	6.693	642	647	659	rBV2	101351	272089	15.74%	1.496%
3	6.834	665	671	682	rBV	93725	174629	10.10%	0.960%
4	7.022	698	703	721	rVB2	150856	300263	17.36%	1.651%
5	7.475	774	780	794	rBV2	253722	467306	27.03%	2.570%
6	8.222	901	907	923	rBV2	144647	354090	20.48%	1.947%
7	8.645	973	979	989	rBV	149705	290079	16.78%	1.595%
8	9.363	1095	1101	1117	rBV2	128831	280626	16.23%	1.543%
9	9.922	1190	1196	1214	rBV4	110023	346496	20.04%	1.906%
10	10.245	1243	1251	1265	rBV	360403	648542	37.51%	3.567%
11	10.445	1276	1285	1294	rBV5	50978	149450	8.64%	0.822%
12	11.810	1511	1517	1525	rBV4	62666	139183	8.05%	0.766%
13	13.569	1810	1816	1821	rBV	387235	621469	35.94%	3.418%
14	13.616	1821	1824	1835	rVB2	67666	137002	7.92%	0.754%
15	13.833	1854	1861	1869	rBV	454057	688662	39.83%	3.788%
16	14.039	1892	1896	1902	rBV	16481	26295	1.52%	0.145%
17	14.139	1908	1913	1923	rVB2	555500	877088	50.72%	4.824%
18	14.463	1963	1968	1979	rBV8	55463	203793	11.79%	1.121%
19	15.004	2056	2060	2066	rVB4	22596	32561	1.88%	0.179%
20	15.151	2078	2085	2096	rBV	510243	846546	48.96%	4.656%
21	15.333	2112	2116	2125	rBV3	121436	251946	14.57%	1.386%
22	15.404	2125	2128	2133	rVB6	18562	32343	1.87%	0.178%
23	15.874	2203	2208	2210	rBV3	17486	26138	1.51%	0.144%
24	16.904	2377	2383	2389	rBV	796075	1147127	66.34%	6.309%
25	17.010	2395	2401	2415	rVB2	573863	965869	55.86%	5.312%
26	17.568	2490	2496	2501	rBV6	12925	24868	1.44%	0.137%
27	17.692	2512	2517	2523	rBV7	12592	20355	1.18%	0.112%
28	17.815	2531	2538	2546	rBV	273353	408564	23.63%	2.247%
29	18.962	2728	2733	2734	rBV4	26282	39622	2.29%	0.218%
30	18.986	2734	2737	2745	rVB3	67520	114428	6.62%	0.629%
31	19.104	2751	2757	2768	rBV3	126389	236080	13.65%	1.298%
32	19.251	2778	2782	2787	rBV	165502	171134	9.90%	0.941%
33	19.321	2788	2794	2806	rVB	753586	1219263	70.51%	6.706%
34	19.845	2878	2883	2885	rBV6	27325	45717	2.64%	0.251%

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35	20.198	2940	2943	2947	rVB6	27017	29945	1.73%	0.165%
36	20.304	2957	2961	2965	rVB	173114	192063	11.11%	1.056%
37	20.833	3047	3051	3056	rVB	284126	318978	18.45%	1.754%
38	21.039	3084	3086	3087	rBV2	27364	17900	1.04%	0.098%
39	21.127	3095	3101	3113	rBV	1167390	1729160	100.00%	9.510%
40	21.692	3194	3197	3198	rBV3	76598	79870	4.62%	0.439%
41	22.133	3270	3272	3276	rVB5	53385	53533	3.10%	0.294%
42	22.609	3350	3353	3358	rVB	229053	319396	18.47%	1.757%
43	22.662	3358	3362	3367	rBV7	118001	201835	11.67%	1.110%
44	23.156	3440	3446	3459	rVB2	733239	1418240	82.02%	7.800%
45	23.292	3463	3469	3478	rVB	774211	1401249	81.04%	7.707%
46	23.750	3543	3547	3552	rVB	181811	304002	17.58%	1.672%
47	26.109	3943	3948	3958	rVB10	189934	515411	29.81%	2.835%

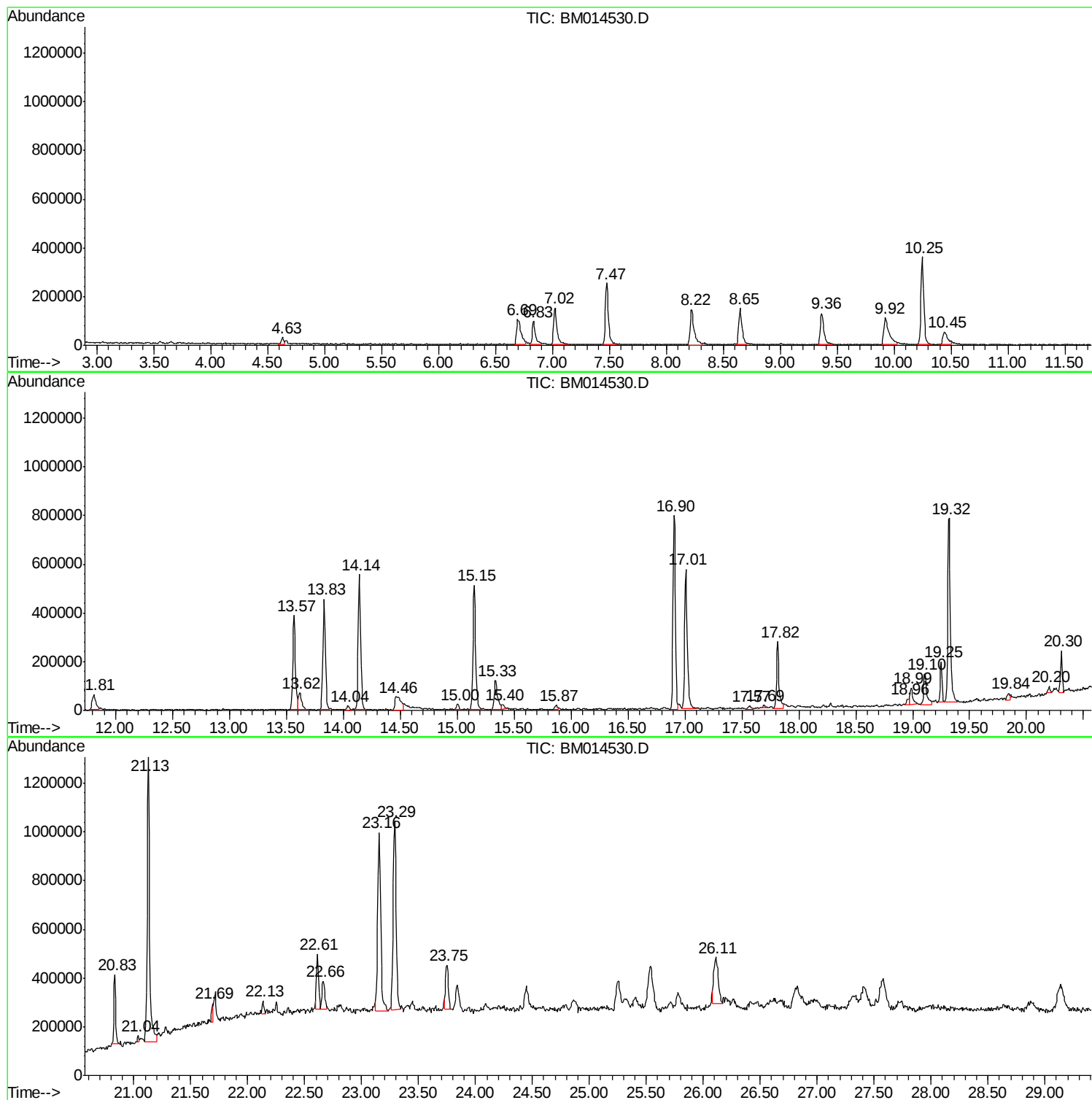
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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



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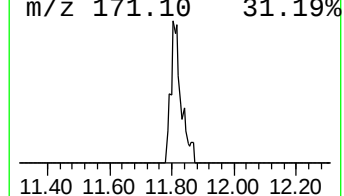
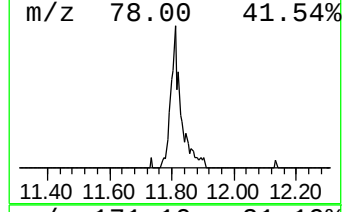
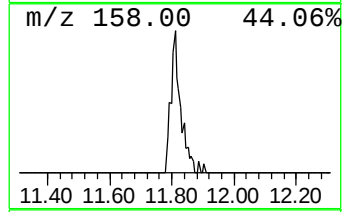
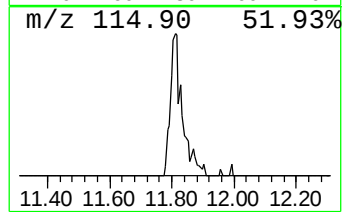
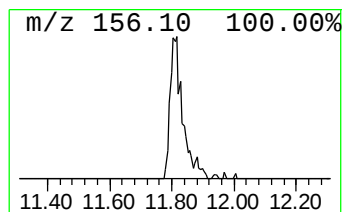
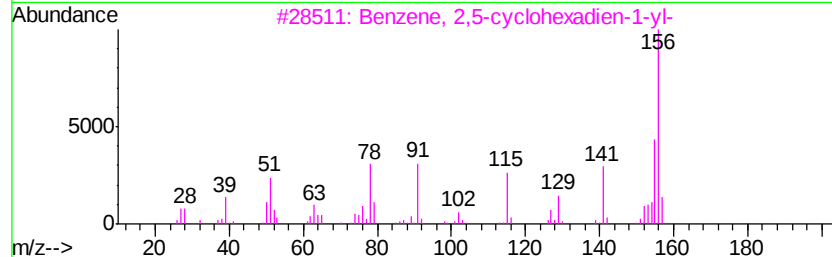
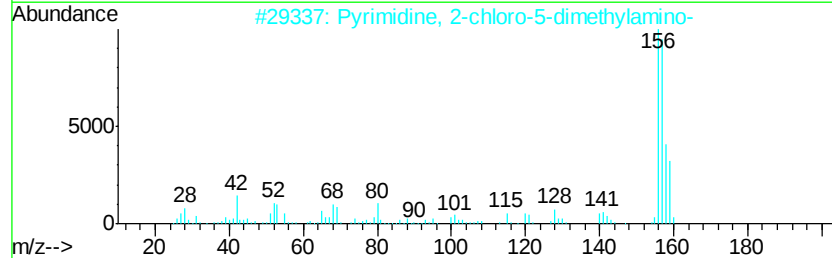
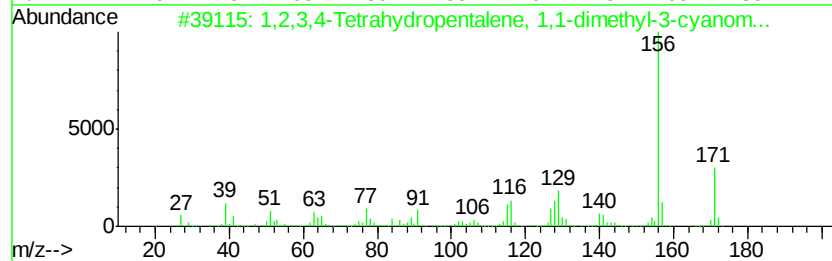
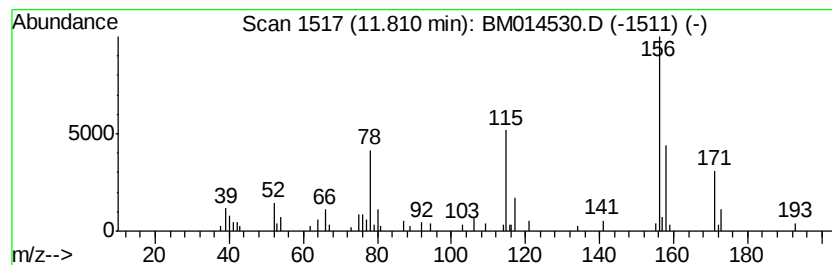
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	4.29 ng/ul	139183	Naphthalene-d8	10.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,3,4-Tetrahydropentalene, 1,1...	171	C12H13N	1000217-18-6	25
2		Pyrimidine, 2-chloro-5-dimethyla...	157	C6H8ClN3	062802-43-1	23
3		Benzene, 2,5-cvclohexadien-1-yl-	156	C12H12	004794-05-2	23
4		Tebuthiuron	228	C9H16N4OS	034014-18-1	12
5		1,3-Diaza-5,6-dedihydrocyclohexa...	171	C6H9N3OS	021263-85-4	12



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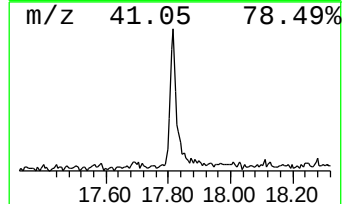
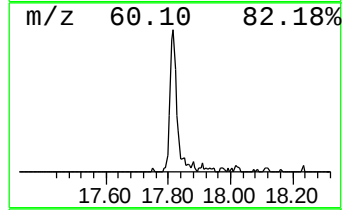
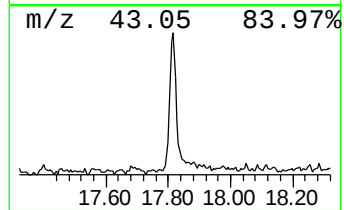
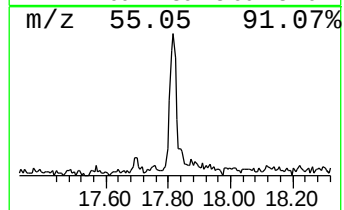
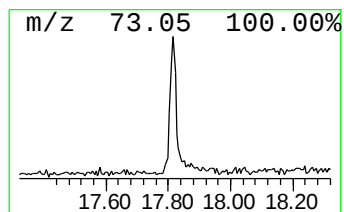
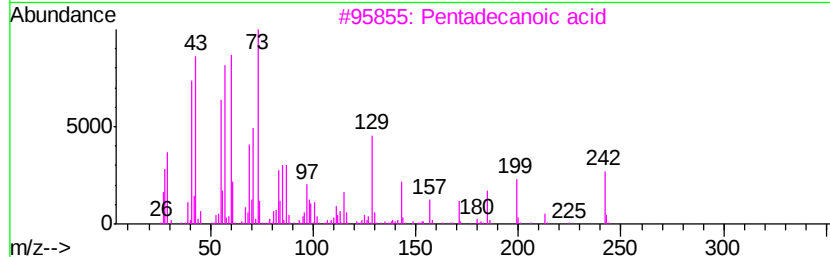
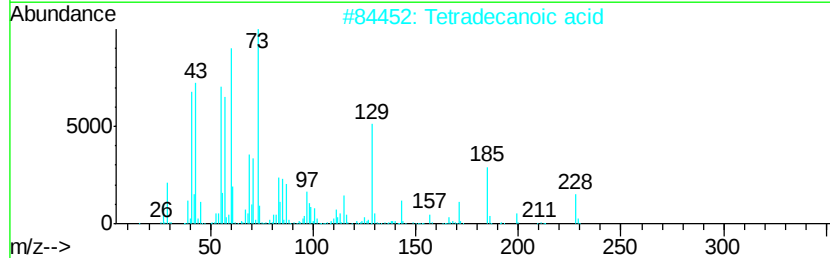
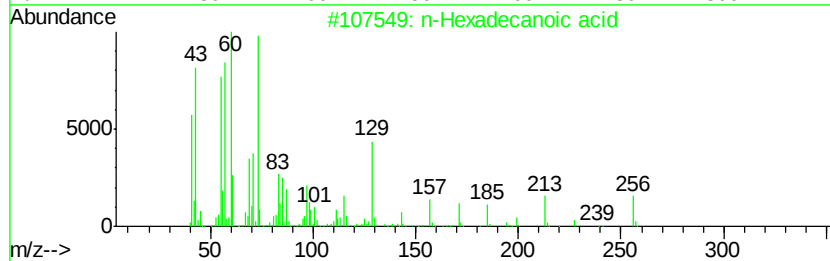
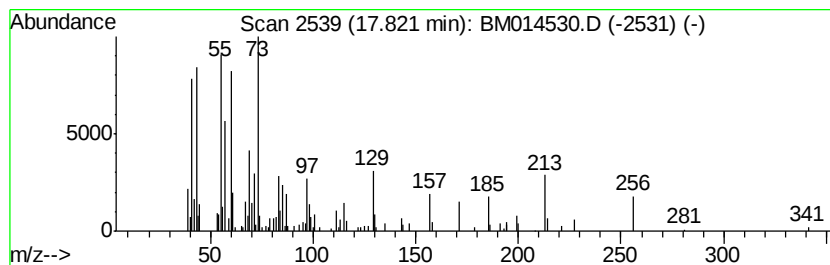
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	7.12 ng/ul	408564	Phenanthrene-d10	16.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5		Tridecanoic acid	214	C13H26O2	000638-53-9	70



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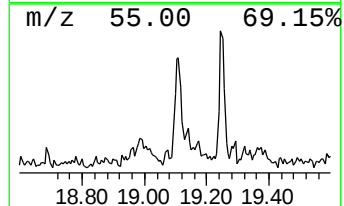
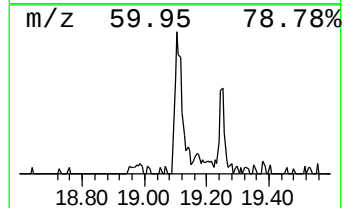
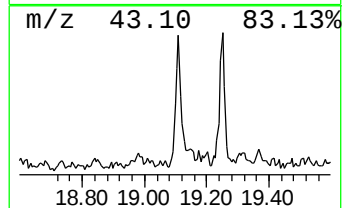
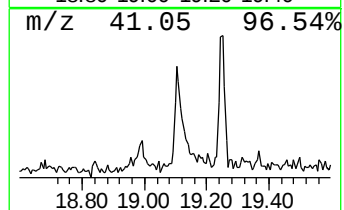
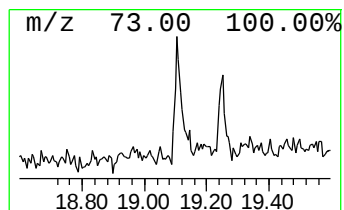
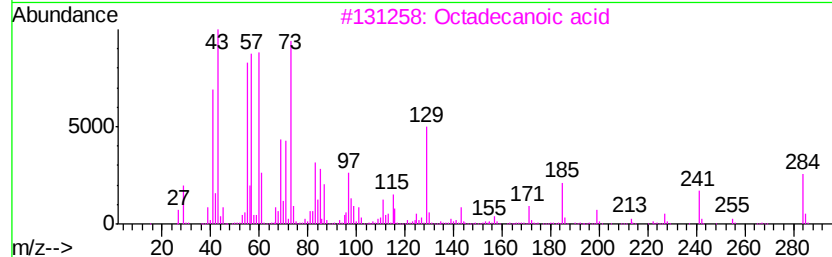
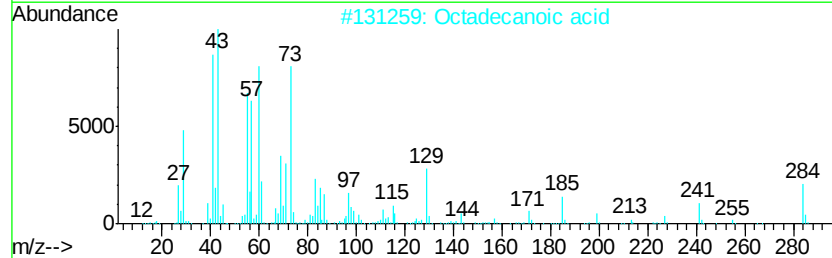
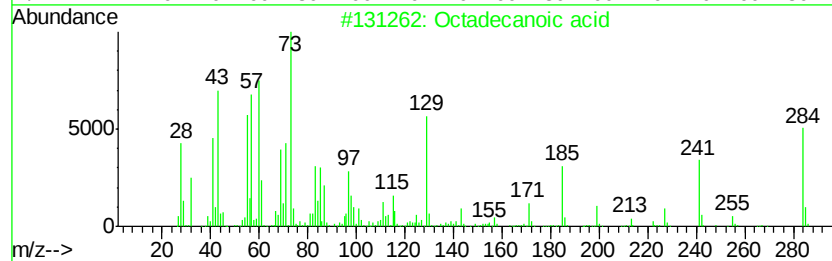
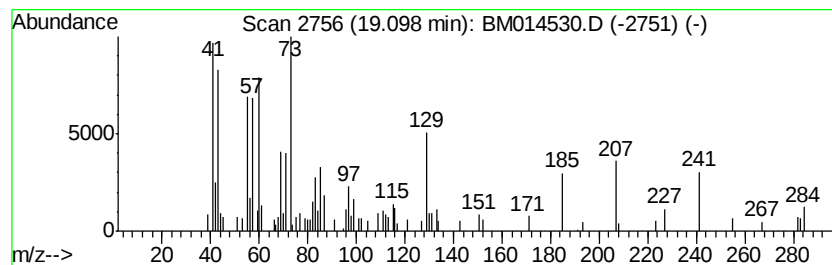
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.10	2.73 ng/ul	236080	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid	284	C18H36O2	000057-11-4	98
3		Octadecanoic acid	284	C18H36O2	000057-11-4	98
4		Octadecanoic acid	284	C18H36O2	000057-11-4	97
5		Octadecanoic acid	284	C18H36O2	000057-11-4	94



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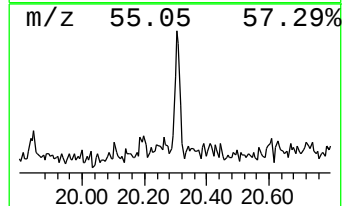
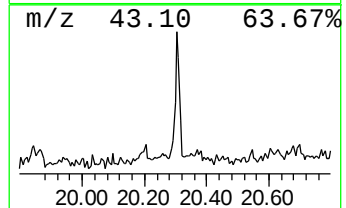
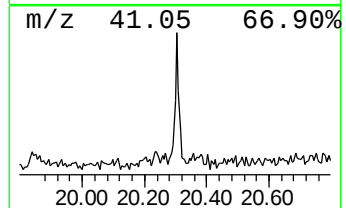
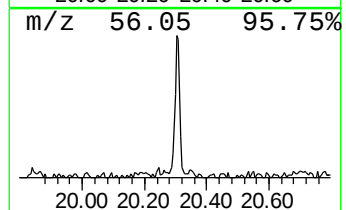
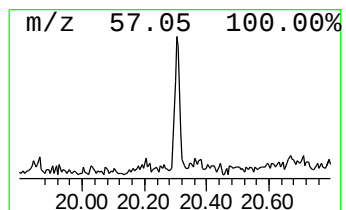
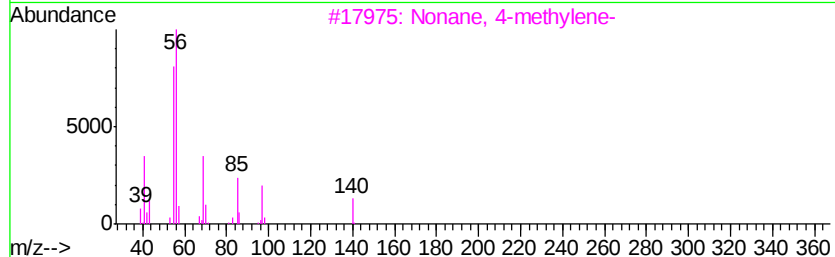
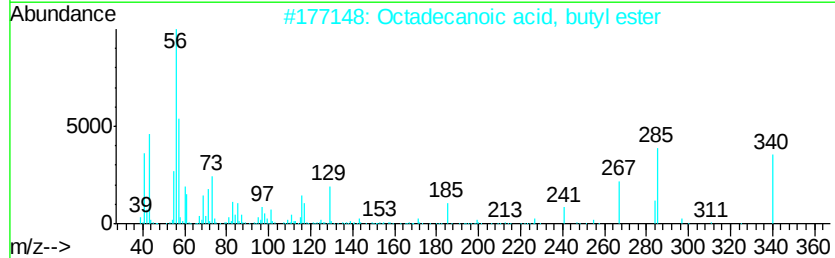
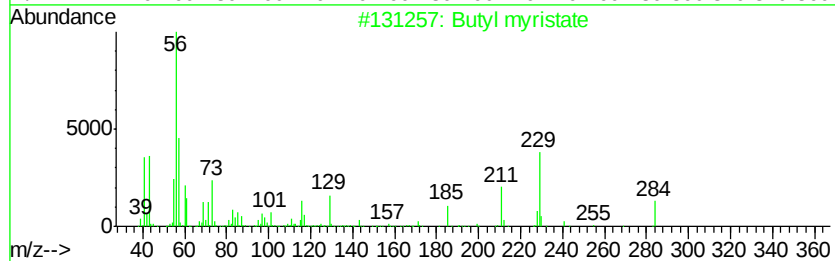
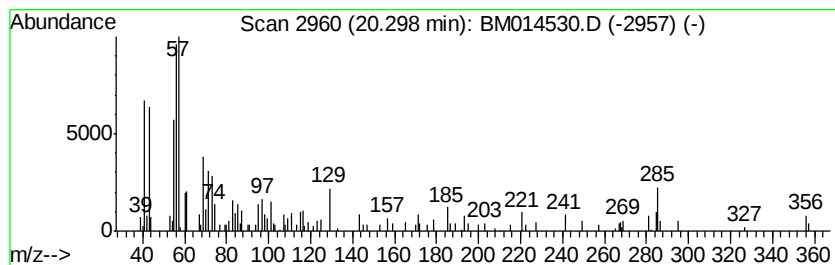
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.30	2.22 ng/ul	192063	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl myristate	284	C18H36O2	000110-36-1	47
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	46
3		Nonane, 4-methylene-	140	C10H20	033717-91-8	43
4		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	41
5		n-Butane, 2-cyclohexyl-1-[1-cycl...	181	C12H23N	038914-51-1	38



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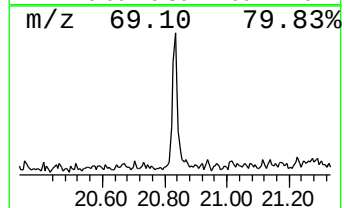
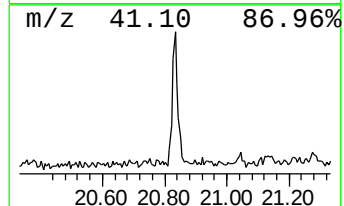
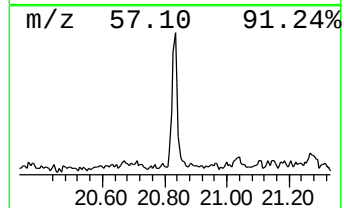
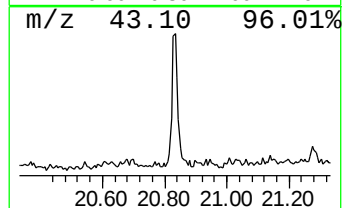
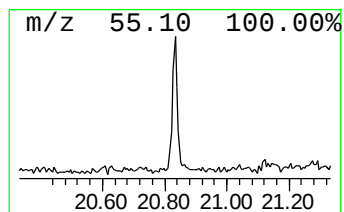
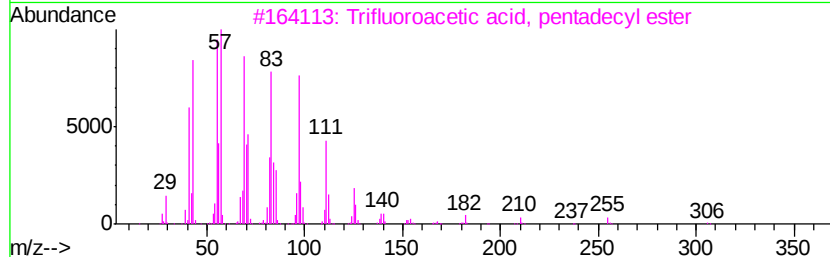
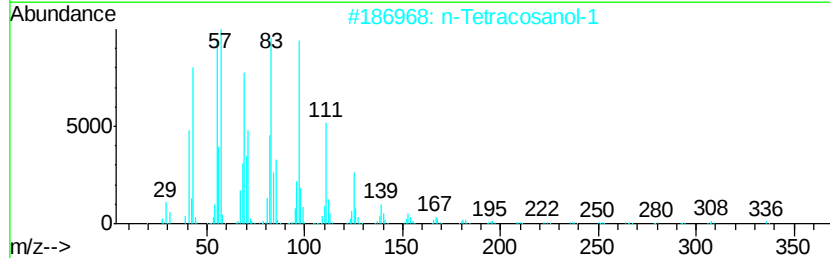
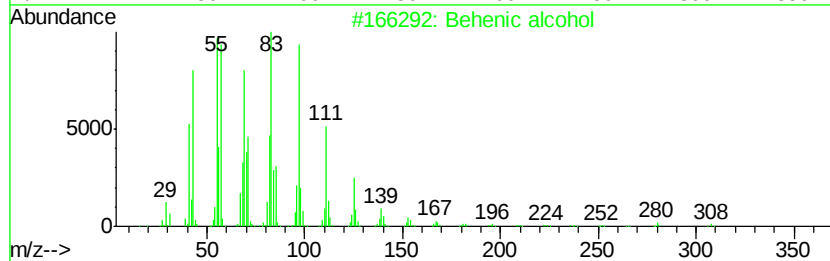
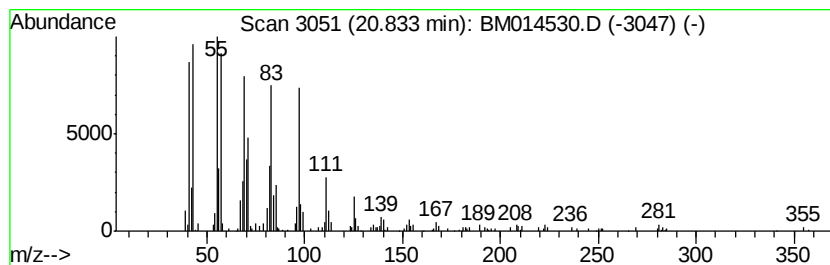
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.83	3.69 ng/ul	318978	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	91
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
4		1-Tridecene	182	C13H26	002437-56-1	87
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
Data File : BM014530.D
Acq On : 12 Mar 2018 22:47
Operator : SJ/JU
Sample : J1813-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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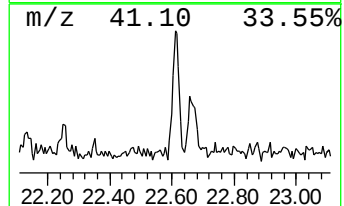
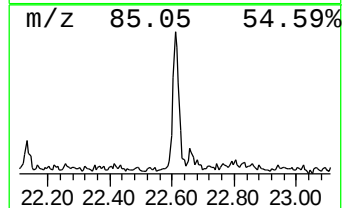
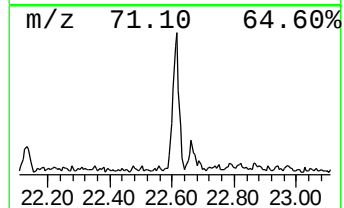
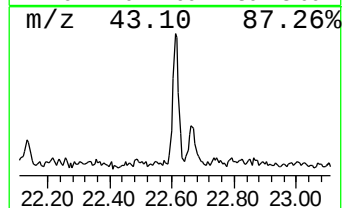
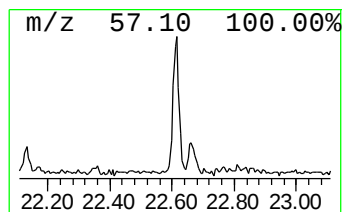
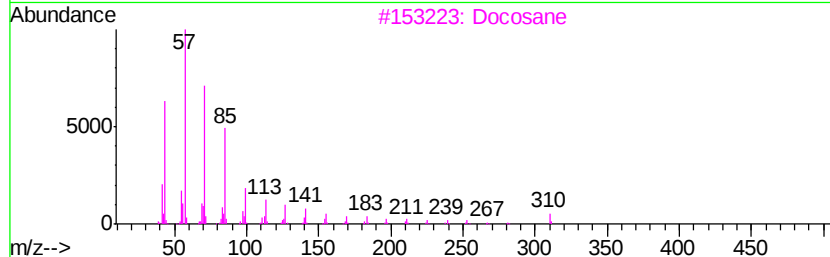
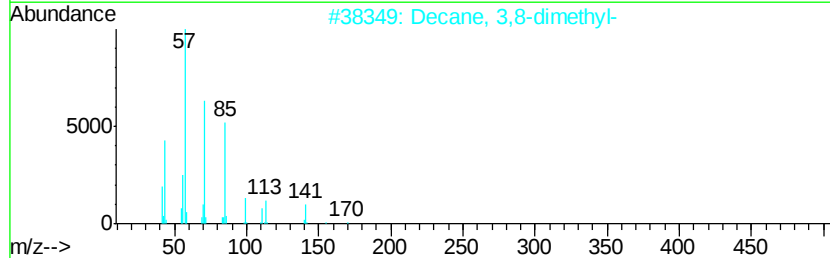
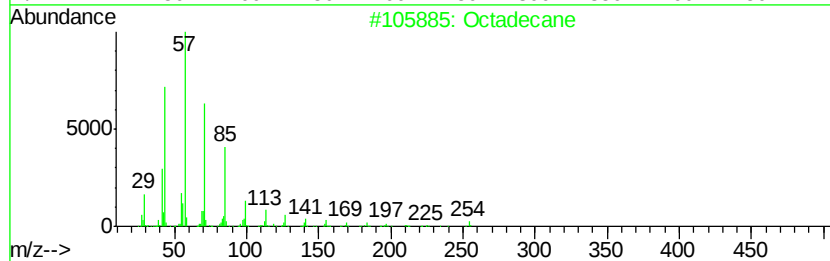
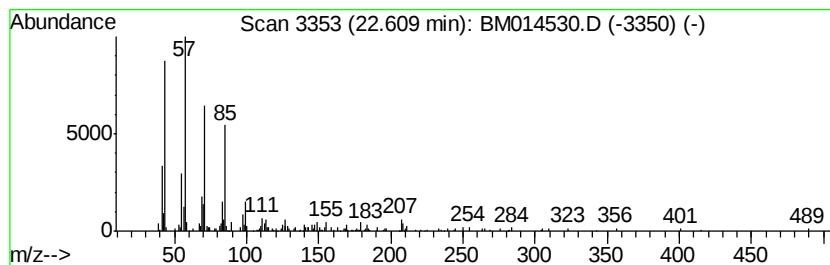
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.61	4.56 ng/ul	319396	Perylene-d12	23.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	86
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83
3			Docosane	310	C22H46	000629-97-0	83
4			Docosane	310	C22H46	000629-97-0	83
5			Heptadecane	240	C17H36	000629-78-7	80



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
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ClientSampleId :
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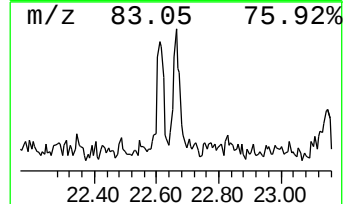
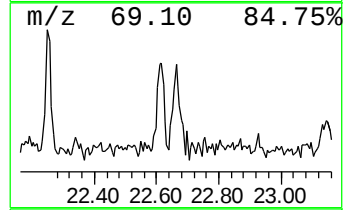
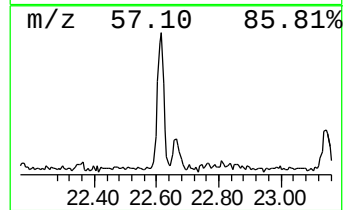
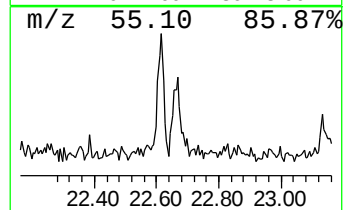
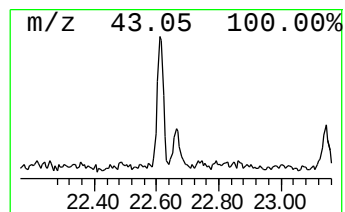
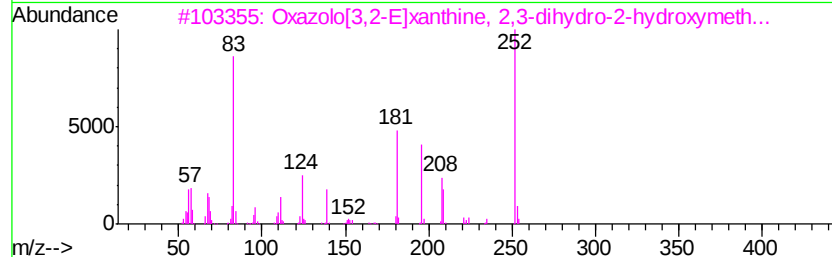
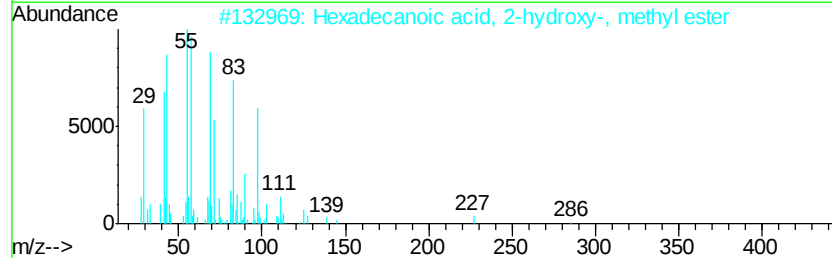
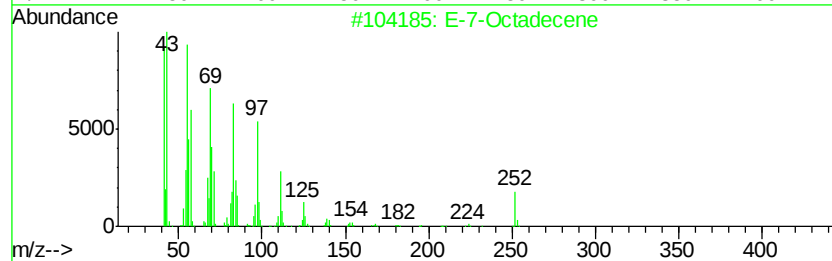
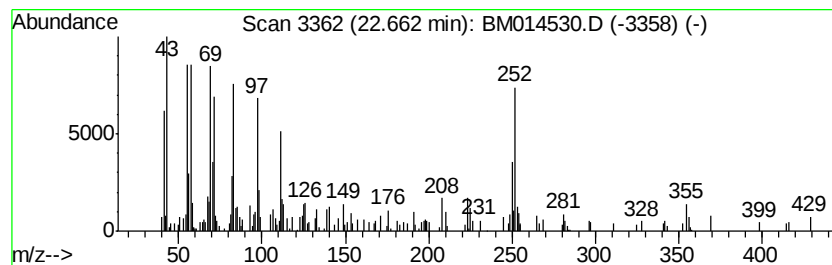
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Cyclic22.66 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	2.88 ng/ul	201835	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-7-Octadecene	252	C18H36	1000130-92-0	64
2		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	43
3		Oxazolo[3,2-E]xanthine, 2,3-dihy...	252	C10H12N4O4	1000285-58-3	38
4		2-Cyclopenten-1-one, 3,4-dihydro...	252	C14H20O4	038602-14-1	35
5		Phosphonic difluoride, (pentaflu...	252	C6F7OP	022474-68-6	27



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
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Acq On : 12 Mar 2018 22:47
Operator : SJ/JU
Sample : J1813-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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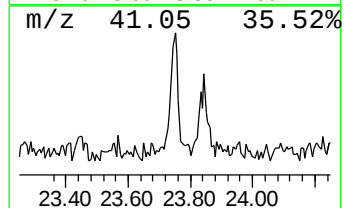
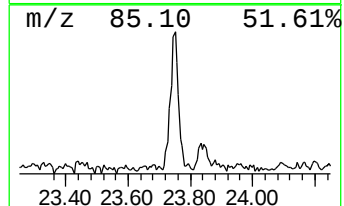
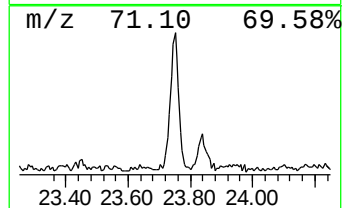
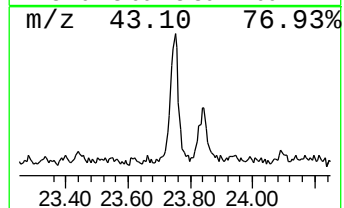
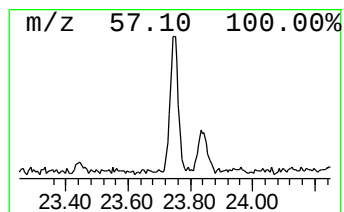
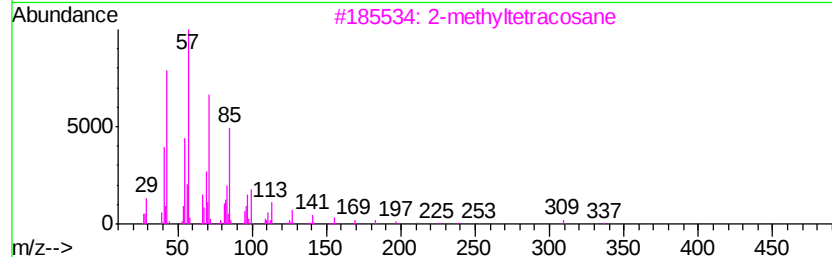
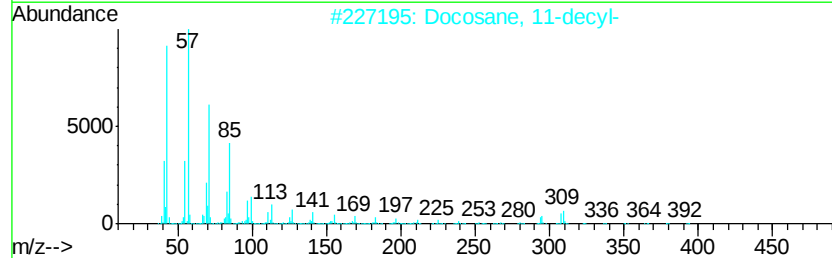
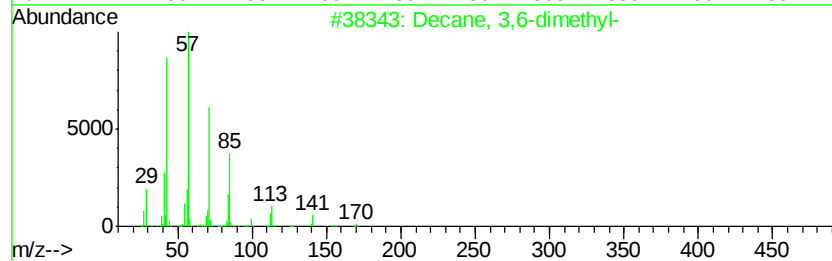
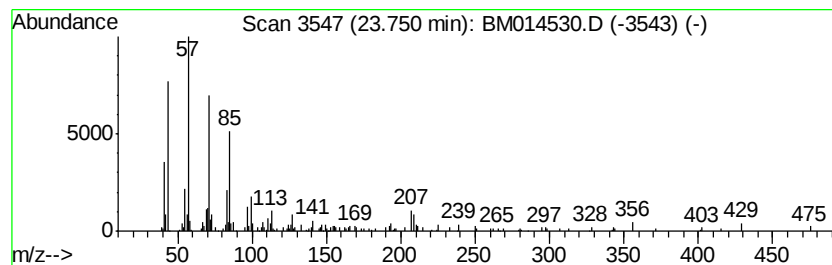
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.75	4.34 ng/ul	304002	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	68
2		Docosane, 11-decyl-	451	C32H66	055401-55-3	64
3		2-methyltetracosane	352	C25H52	1000376-72-6	64
4		2-methyloctacosane	408	C29H60	1000376-72-8	64
5		Tetracosane	338	C24H50	000646-31-1	64



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
Data File : BM014530.D
Acq On : 12 Mar 2018 22:47
Operator : SJ/JU
Sample : J1813-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

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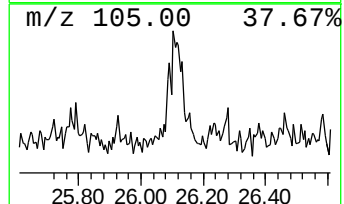
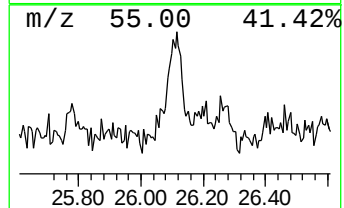
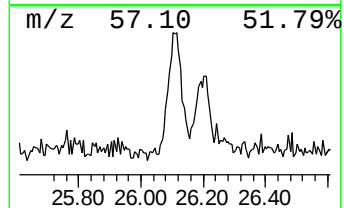
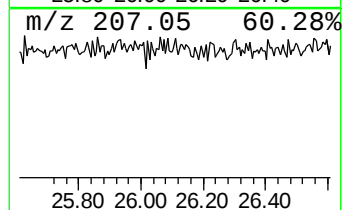
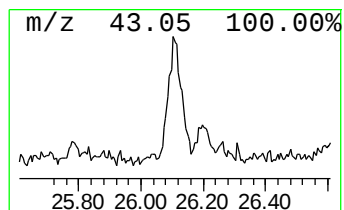
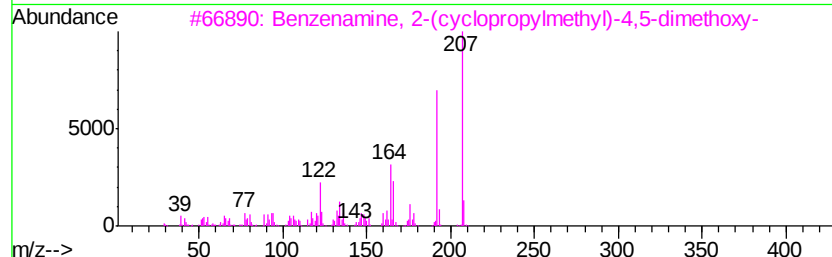
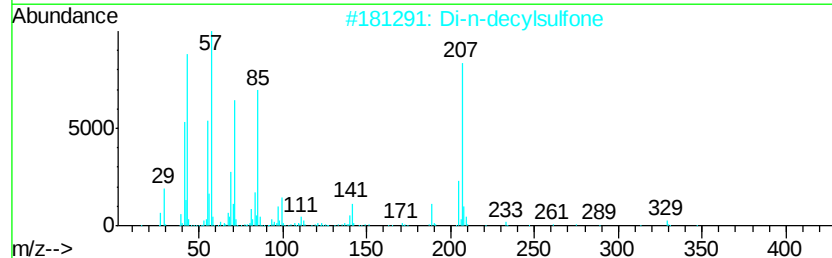
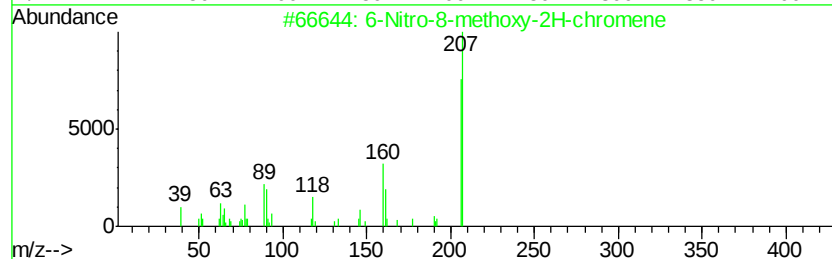
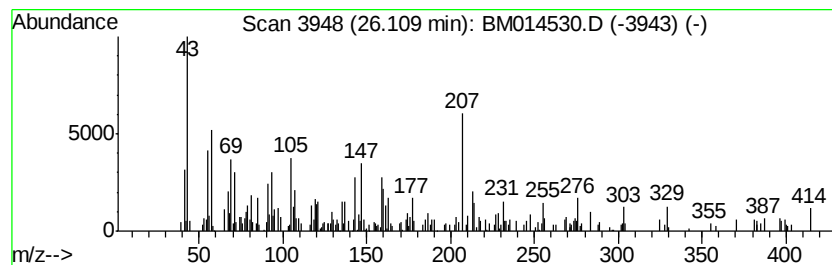
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.11	7.36 ng/ul	515411	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	30
2		Di-n-decylsulfone	346	C20H42O2S	111530-37-1	22
3		Benzenamine, 2-(cyclopropylmethyl)-	207	C12H17NO2	1000327-32-3	14
4		2-Amino-4-hydroxy-6,8-dimethyl-7...	207	C8H9N5O2	025477-64-9	11
5		1,2,4-Triazol-3-amine, 5-(1,3,5-...	207	C8H13N7	1000264-16-7	11



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM031218\
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Acq On : 12 Mar 2018 22:47
Operator : SJ/JU
Sample : J1813-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM021418.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
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n-Hexadecanoic acid	17.82	7.1	ng/ul	408564	4	16.90	1147130	20.0
Octadecanoic acid	19.10	2.7	ng/ul	236080	5	21.13	1729160	20.0
unknown-02	20.30	2.2	ng/ul	192063	5	21.13	1729160	20.0
Behenic alcohol	20.83	3.7	ng/ul	318978	5	21.13	1729160	20.0
(DEL) Alkane: Str...	22.61	4.6	ng/ul	319396	6	23.29	1401250	20.0
(DEL) Alkane: Cyc...	22.66	2.9	ng/ul	201835	6	23.29	1401250	20.0
(DEL) Alkane: Str...	23.75	4.3	ng/ul	304002	6	23.29	1401250	20.0
unknown-03	26.11	7.4	ng/ul	515411	6	23.29	1401250	20.0