

Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
 Data File : BM014529.D
 Acq On : 12 Mar 2018 22:11
 Operator : SJ/JU
 Sample : J1813-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F6F16

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	4.634	292	297	299	rBV2	16847	24488	1.73%	0.144%
2	6.693	638	647	662	rBV2	108667	290637	20.55%	1.706%
3	6.834	664	671	681	rVV	92329	165436	11.70%	0.971%
4	7.022	694	703	715	rBV	154980	292624	20.69%	1.718%
5	7.475	773	780	794	rBV	235983	439490	31.08%	2.580%
6	8.216	900	906	921	rBV3	131704	319565	22.60%	1.876%
7	8.328	921	925	932	rVB4	17503	33020	2.33%	0.194%
8	8.645	973	979	988	rBV	141309	291449	20.61%	1.711%
9	9.363	1095	1101	1113	rBV	133447	277854	19.65%	1.631%
10	9.916	1189	1195	1212	rBV4	111885	347376	24.56%	2.039%
11	10.245	1245	1251	1261	rBV	349638	600664	42.48%	3.526%
12	10.439	1277	1284	1297	rBV3	67664	204884	14.49%	1.203%
13	11.822	1512	1519	1527	rBV4	20121	47648	3.37%	0.280%
14	13.375	1777	1783	1788	rBV6	46653	68391	4.84%	0.401%
15	13.433	1788	1793	1797	rVB5	11150	17794	1.26%	0.104%
16	13.569	1809	1816	1822	rBV	366551	616637	43.60%	3.620%
17	13.616	1822	1824	1836	rVB	62862	101259	7.16%	0.594%
18	13.833	1854	1861	1872	rVB	436813	684463	48.40%	4.018%
19	14.039	1891	1896	1900	rBV4	21015	29798	2.11%	0.175%
20	14.139	1907	1913	1922	rBV2	505081	811604	57.39%	4.764%
21	14.469	1962	1969	1974	rBV4	63971	158341	11.20%	0.930%
22	14.663	2000	2002	2010	rVB8	10707	17459	1.23%	0.102%
23	15.004	2055	2060	2063	rBV3	22765	30327	2.14%	0.178%
24	15.151	2078	2085	2095	rBV	489484	819737	57.97%	4.812%
25	15.233	2095	2099	2106	rVB5	11761	21787	1.54%	0.128%
26	15.333	2111	2116	2125	rBV3	120671	244963	17.32%	1.438%
27	15.427	2125	2132	2137	rVB6	33472	70735	5.00%	0.415%
28	15.627	2160	2166	2170	rVB5	8410	14687	1.04%	0.086%
29	15.869	2202	2207	2215	rVB4	17756	27707	1.96%	0.163%
30	16.904	2377	2383	2394	rBV2	746532	1079862	76.36%	6.339%
31	17.010	2394	2401	2414	rVV	557290	925864	65.47%	5.435%
32	17.757	2524	2528	2533	rBV6	19549	27833	1.97%	0.163%
33	17.810	2533	2537	2546	rBV2	147021	241841	17.10%	1.420%
34	18.768	2696	2700	2704	rBV5	13284	19856	1.40%	0.117%

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35	18.957	2729	2732	2735	rBV4	26102	33274	2.35%	0.195%
36	18.986	2735	2737	2741	rVB5	18080	21720	1.54%	0.128%
37	19.109	2753	2758	2766	rBV2	74415	131902	9.33%	0.774%
38	19.251	2777	2782	2785	rBV	259052	288574	20.41%	1.694%
39	19.321	2788	2794	2800	rVV	740255	1133489	80.15%	6.654%
40	19.368	2800	2802	2806	rVB5	30865	29961	2.12%	0.176%
41	20.027	2910	2914	2916	rBV5	14147	22251	1.57%	0.131%
42	20.198	2938	2943	2948	rBV2	194775	240866	17.03%	1.414%
43	20.256	2948	2953	2958	rVV4	126172	223080	15.77%	1.310%
44	20.304	2958	2961	2967	rVB	210119	230857	16.32%	1.355%
45	20.368	2967	2972	2976	rBV6	32807	53338	3.77%	0.313%
46	20.404	2976	2978	2981	rVB3	18207	16452	1.16%	0.097%
47	20.833	3047	3051	3057	rVB4	105259	134234	9.49%	0.788%
48	21.127	3096	3101	3107	rBV2	985912	1414144	100.00%	8.302%
49	21.692	3194	3197	3199	rBV4	38547	58383	4.13%	0.343%
50	23.156	3439	3446	3455	rVB	717124	1310690	92.68%	7.694%
51	23.292	3462	3469	3477	rBV2	674270	1328352	93.93%	7.798%
52	23.750	3542	3547	3553	rVB	174217	314376	22.23%	1.846%
53	25.544	3843	3852	3859	rBV	231271	682524	48.26%	4.007%

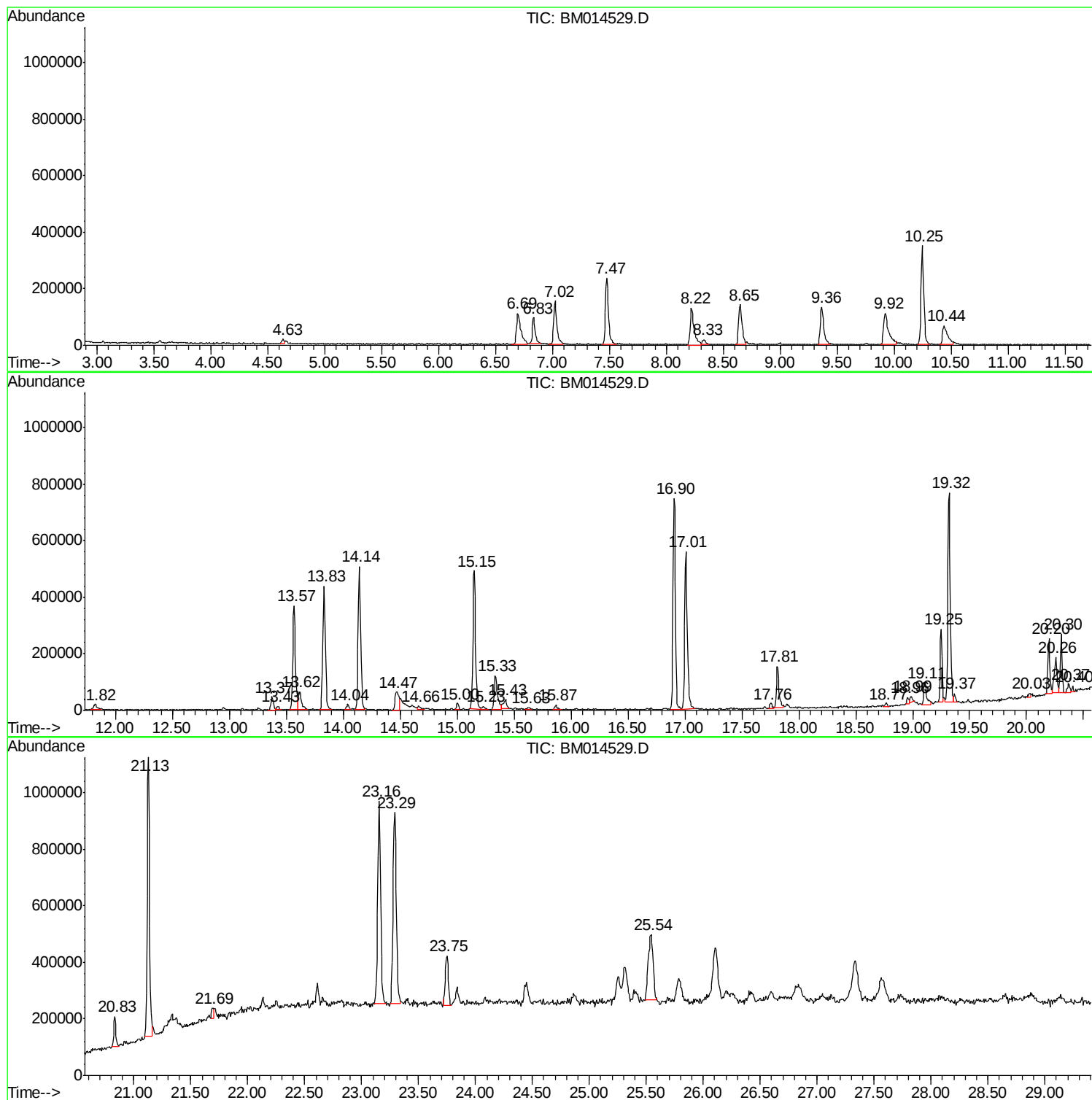
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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



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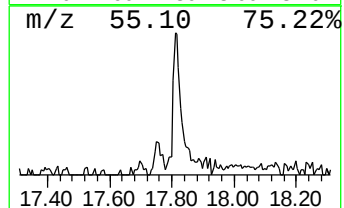
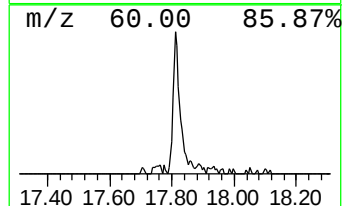
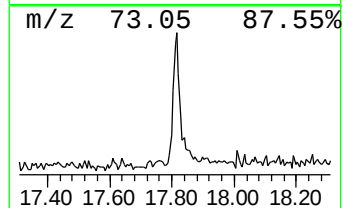
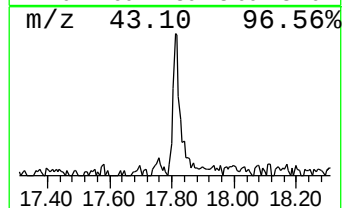
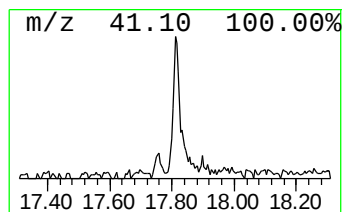
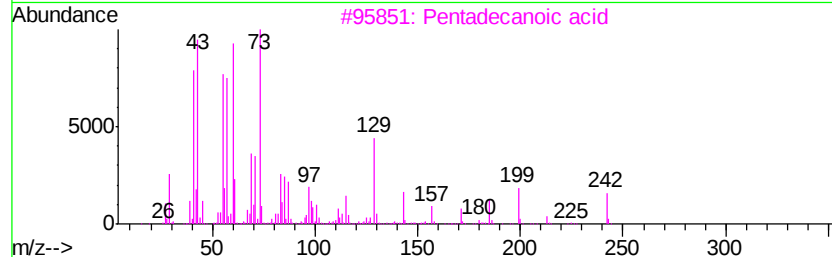
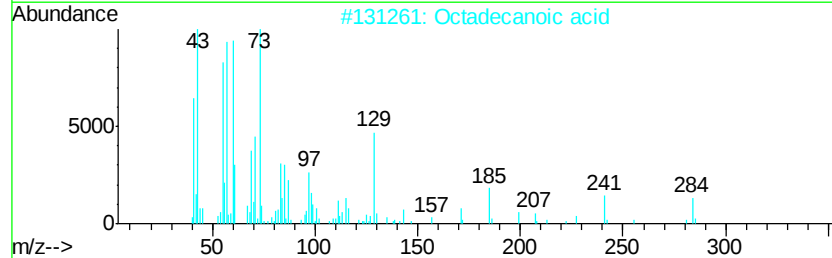
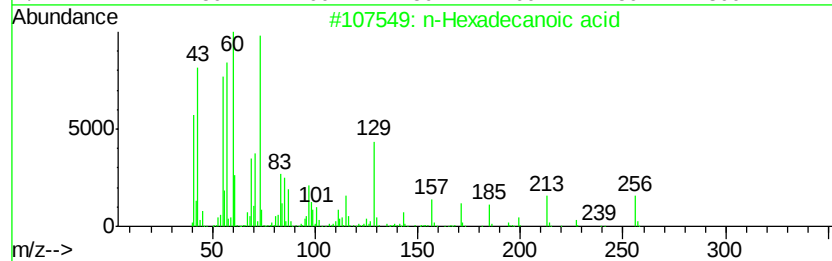
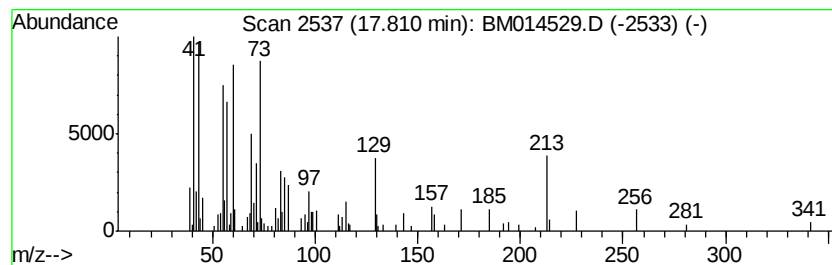
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.81	4.48 ng/ul	241841	Phenanthrene-d10	16.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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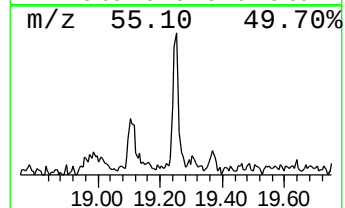
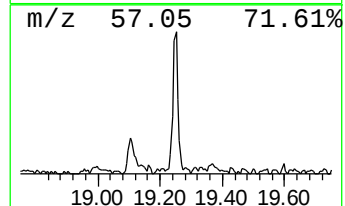
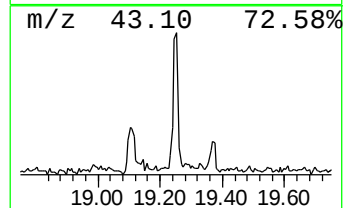
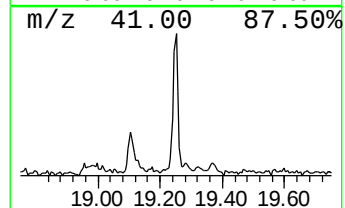
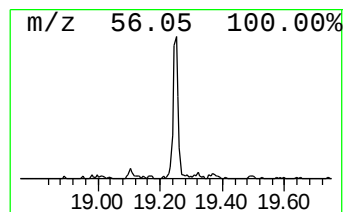
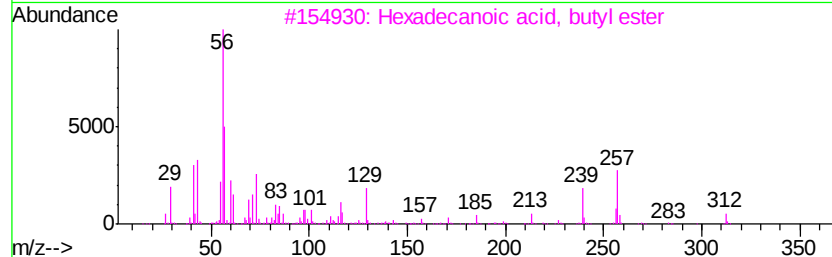
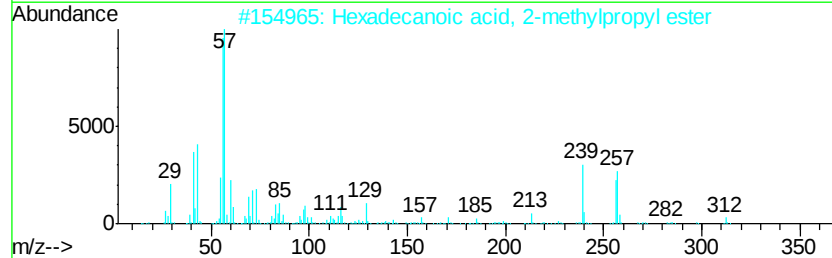
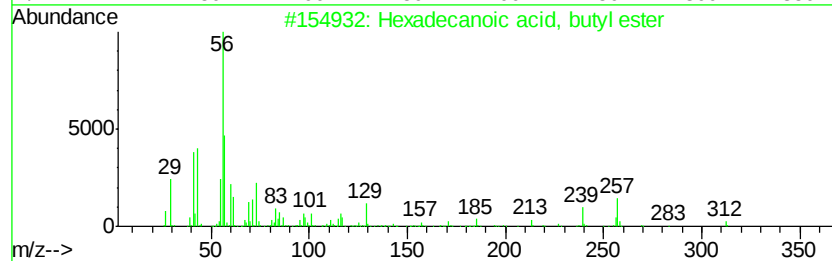
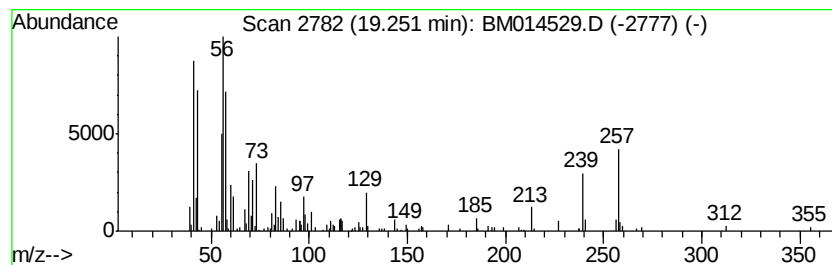
Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM021418.M
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.25	4.08 ng/ul	288574	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95	
2	Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	93	
3	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87	
4	Hexadecanoic acid, 1,1-dimethylester	312	C20H40O2	031158-91-5	64	
5	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	47	



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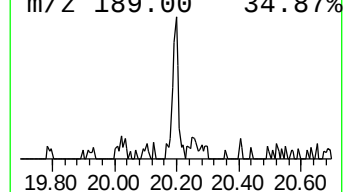
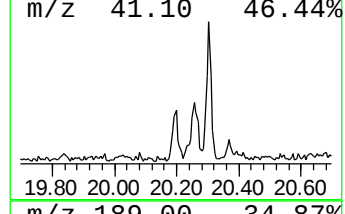
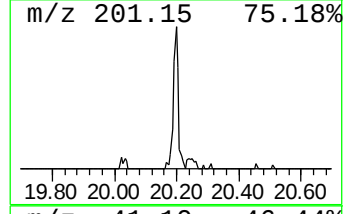
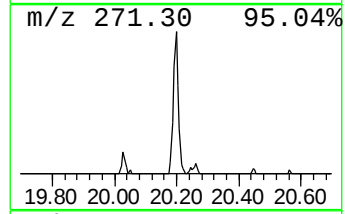
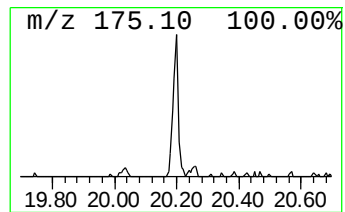
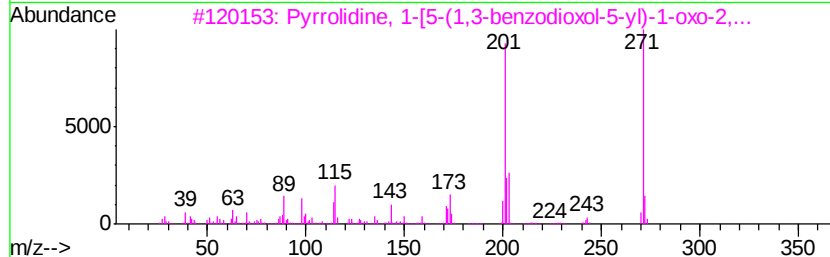
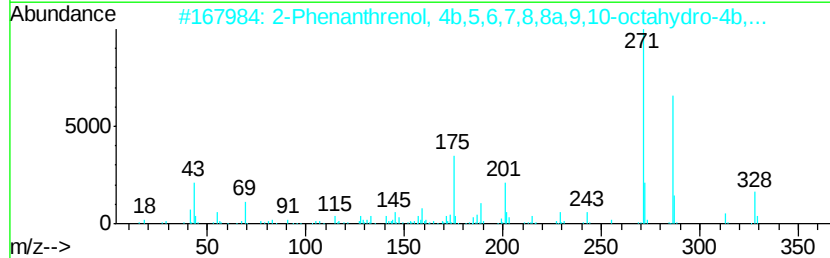
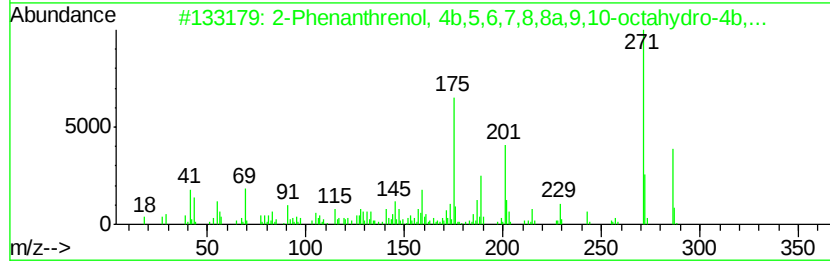
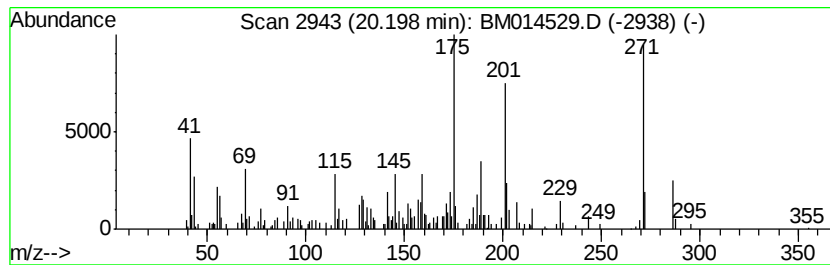
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.20	3.41 ng/ul	240866	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	98
2		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	72
3		Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	49
4		Silane, diethyl(cis-4-methylcyclo...	300	C17H36O2Si	1000363-55-2	35
5		13-Isopropylpodocarpene-12-ol-20-al	300	C20H28O2	024035-37-8	27



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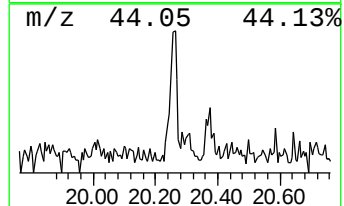
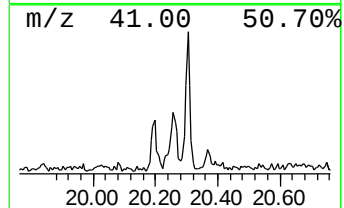
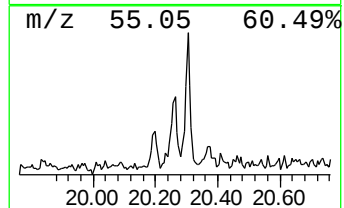
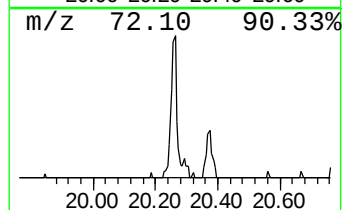
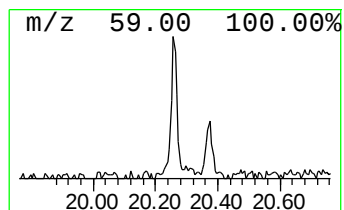
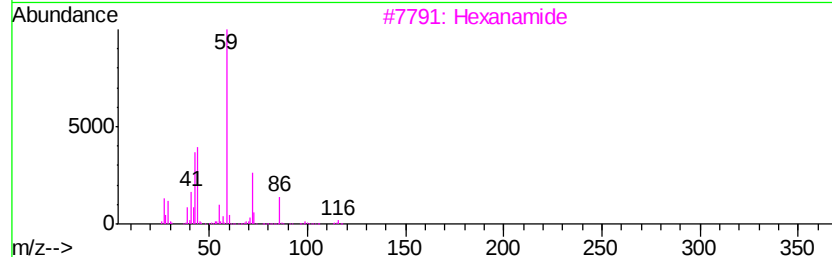
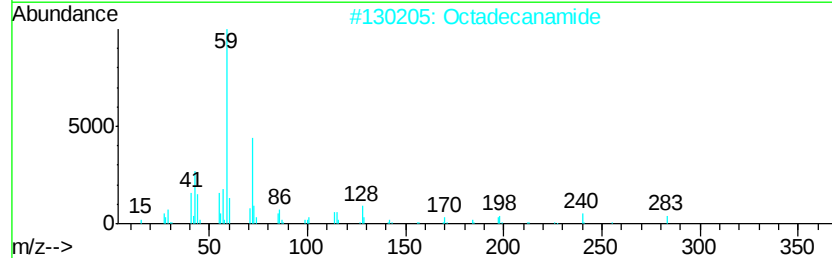
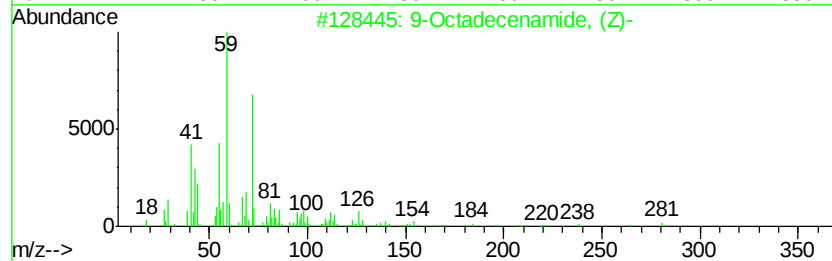
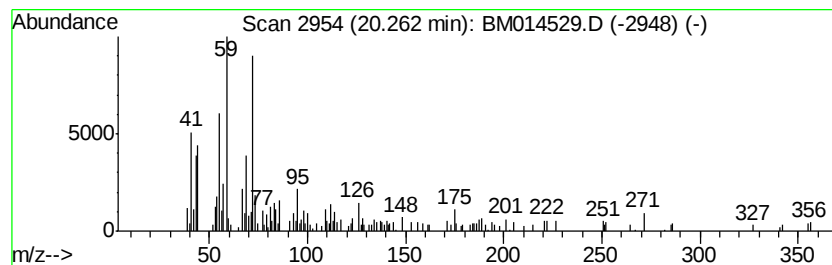
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.26	3.15 ng/ul	223080	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2		Octadecanamide	283	C18H37NO	000124-26-5	43
3		Hexanamide	115	C6H13NO	000628-02-4	38
4		Tetradecanamide	227	C14H29NO	000638-58-4	38
5		Hexanamide	115	C6H13NO	000628-02-4	38



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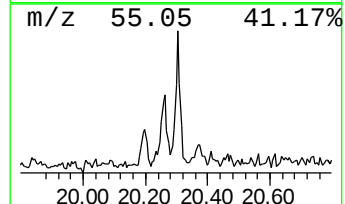
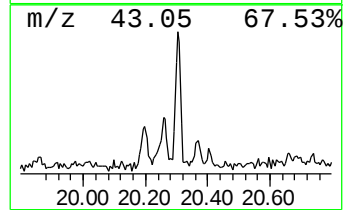
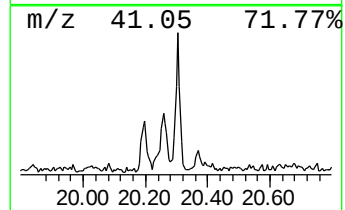
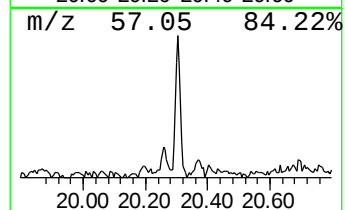
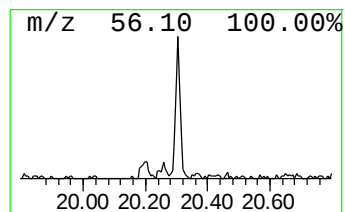
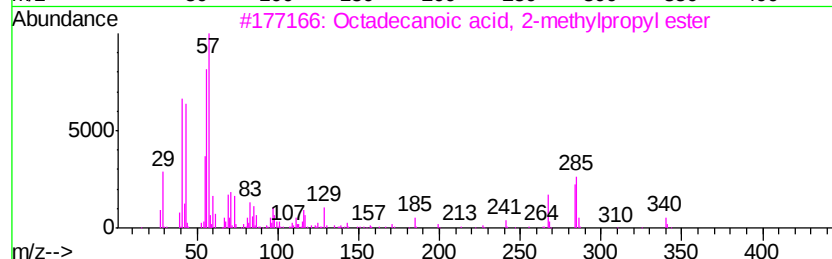
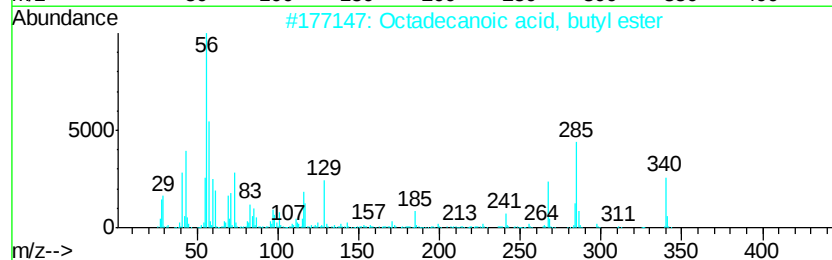
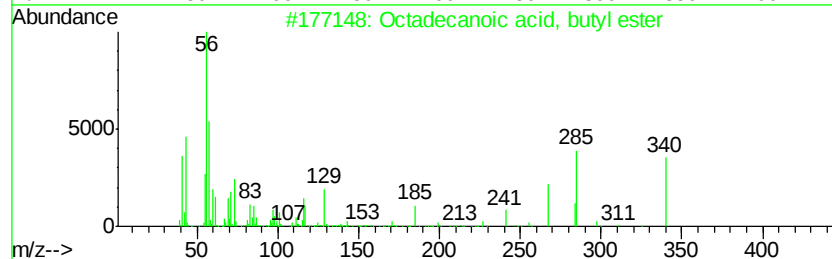
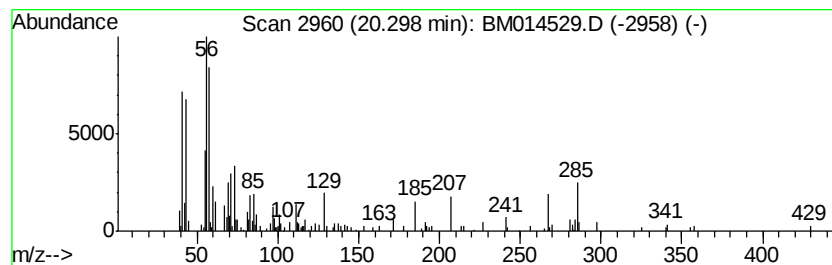
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.30	3.26 ng/ul	230857	Chrysene-d12	21.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	86
3		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	72
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Butyl myristate	284	C18H36O2	000110-36-1	40



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
Data File : BM014529.D
Acq On : 12 Mar 2018 22:11
Operator : SJ/JU
Sample : J1813-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

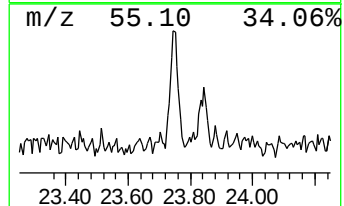
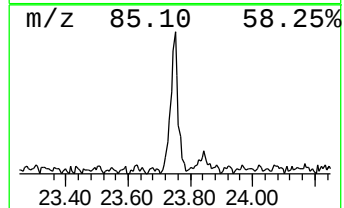
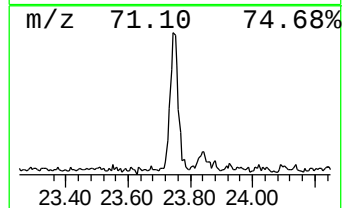
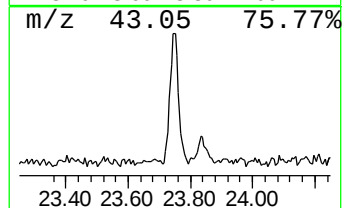
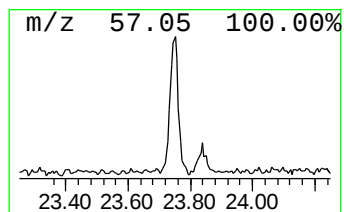
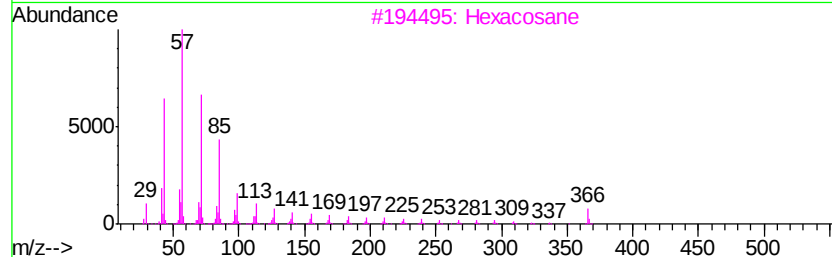
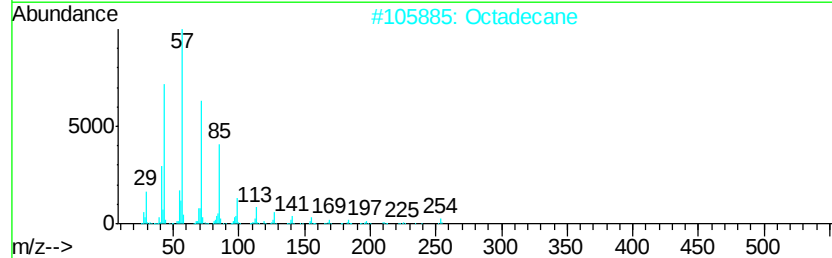
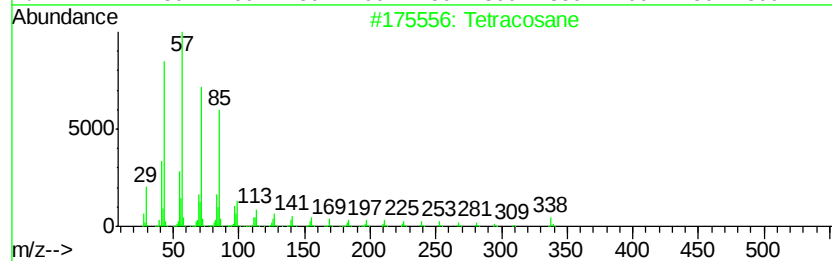
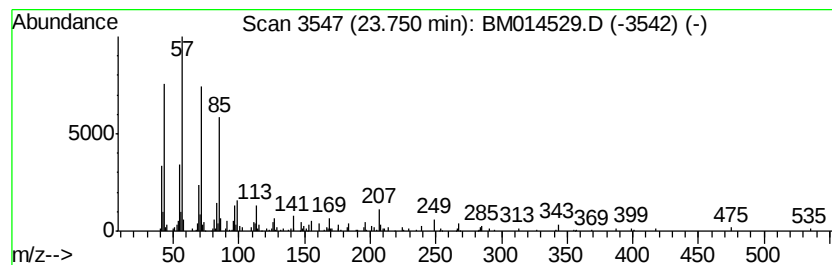
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\SOM-EPA-BM021418.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.75	4.73 ng/ul	314376	Perylene-d12	23.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	83
2	Octadecane	254	C18H38	000593-45-3	81
3	Hexacosane	366	C26H54	000630-01-3	80
4	Docosane	310	C22H46	000629-97-0	74
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74



Data Path : Z:\HPCHEM1\BNA M\DATA\BM031218\
Data File : BM014529.D
Acq On : 12 Mar 2018 22:11
Operator : SJ/JU
Sample : J1813-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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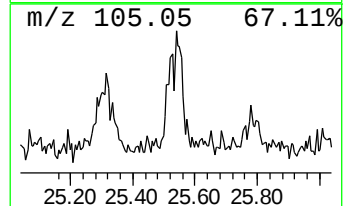
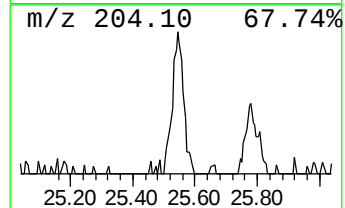
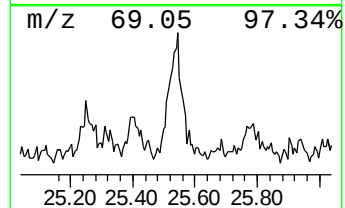
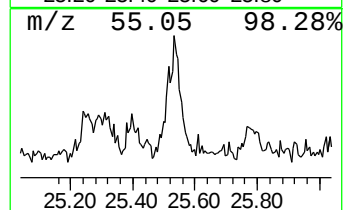
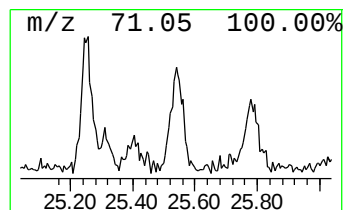
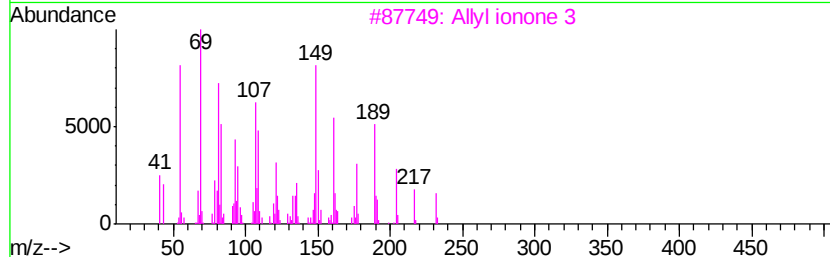
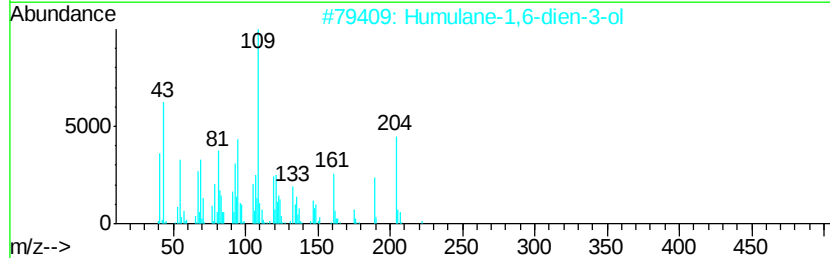
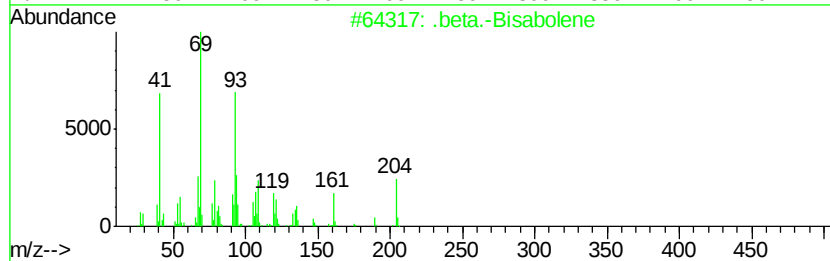
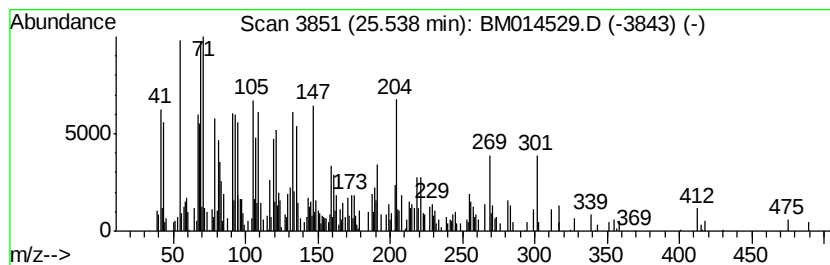
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.54	10.28 ng/ul	682524	Perylene-d12	23.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Bisabolene	204	C15H24	000495-61-4	47
2		Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	47
3		Allyl ionone 3	232	C16H24O	1000284-92-9	30
4		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	27
5		3-(3,7-Dimethyl-octa-2,6-dienyl)...	258	C17H22O2	1000192-28-0	25



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM031218\
Data File : BM014529.D
Acq On : 12 Mar 2018 22:11
Operator : SJ/JU
Sample : J1813-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F6F16

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
n-Hexadecanoic acid	17.81	4.5	ng/ul	241841	4	16.90	1079860	20.0
Hexadecanoic acid...	19.25	4.1	ng/ul	288574	5	21.13	1414140	20.0
2-Phenanthrenol, ...	20.20	3.4	ng/ul	240866	5	21.13	1414140	20.0
9-Octadecenamide, ...	20.26	3.1	ng/ul	223080	5	21.13	1414140	20.0
Octadecanoic acid...	20.30	3.3	ng/ul	230857	5	21.13	1414140	20.0
(DEL) Alkane: Str...	23.75	4.7	ng/ul	314376	6	23.29	1328350	20.0
unknown-01	25.54	10.3	ng/ul	682524	6	23.29	1328350	20.0