

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM062518\
 Data File : BM015745.D
 Acq On : 25 Jun 2018 12:11
 Operator : SJ/JU
 Sample : J3569-25 5X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DAXP3

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060818MA.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	7.481	707	713	722	rBV	30198	62025	1.48%	0.230%
2	7.639	735	740	751	rBV	23527	45715	1.09%	0.170%
3	7.851	770	776	785	rBV	35102	64977	1.56%	0.241%
4	8.316	849	855	870	rVB	376247	639930	15.32%	2.378%
5	9.039	973	978	991	rBV2	41396	79895	1.91%	0.297%
6	9.516	1054	1059	1069	rBV	28734	58269	1.39%	0.217%
7	10.780	1268	1274	1285	rBV2	40919	87191	2.09%	0.324%
8	11.145	1329	1336	1350	rBV	536493	907943	21.73%	3.374%
9	14.339	1873	1879	1883	rBV	126146	181405	4.34%	0.674%
10	14.639	1924	1930	1939	rBV	104063	158250	3.79%	0.588%
11	14.933	1974	1980	1992	rVB2	712671	1126841	26.97%	4.187%
12	15.921	2139	2148	2155	rBV	177061	263798	6.31%	0.980%
13	16.580	2256	2260	2268	rBV2	37939	46736	1.12%	0.174%
14	17.021	2330	2335	2342	rBV2	50910	62180	1.49%	0.231%
15	17.662	2437	2444	2449	rBV2	936970	1385986	33.18%	5.150%
16	17.762	2455	2461	2468	rVV	199958	291785	6.98%	1.084%
17	18.503	2581	2587	2600	rBV	588571	817207	19.56%	3.037%
18	19.633	2775	2779	2780	rBV2	41781	47155	1.13%	0.175%
19	19.656	2780	2783	2791	rVV5	62959	116696	2.79%	0.434%
20	19.744	2794	2798	2809	rVV	191570	261234	6.25%	0.971%
21	20.015	2839	2844	2851	rBV	262652	369964	8.86%	1.375%
22	20.827	2977	2982	2991	rVB	235980	324850	7.78%	1.207%
23	21.433	3081	3085	3092	rBV2	66025	95177	2.28%	0.354%
24	21.768	3137	3142	3148	rBV	1246905	1564696	37.45%	5.814%
25	22.315	3231	3235	3240	rVB2	269906	352543	8.44%	1.310%
26	22.433	3247	3255	3260	rBV	2025147	3342939	80.02%	12.422%
27	22.533	3268	3272	3282	rVB	822585	1097531	26.27%	4.078%
28	22.656	3288	3293	3298	rBV	1368870	1801566	43.12%	6.694%
29	22.903	3331	3335	3337	rBV2	211490	298649	7.15%	1.110%
30	22.927	3337	3339	3349	rVB3	295234	457675	10.96%	1.701%
31	23.156	3373	3378	3388	rVB	795798	1218861	29.18%	4.529%
32	23.327	3402	3407	3418	rVB3	321030	700729	16.77%	2.604%
33	23.432	3418	3425	3433	rBV	2678816	4177729	100.00%	15.524%
34	23.621	3450	3457	3470	rVB2	925249	1926151	46.11%	7.157%

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Integration Parameters: LSCINT.P

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Max Peaks: 100
Peak Location: TOP

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35	23.962	3512	3515	3520	rVV2	104400	137086	3.28%	0.509%
36	24.021	3521	3525	3529	rVV	183285	347923	8.33%	1.293%
37	24.062	3529	3532	3540	rVB3	225751	408884	9.79%	1.519%
38	24.174	3545	3551	3560	rVB	798832	1583903	37.91%	5.885%

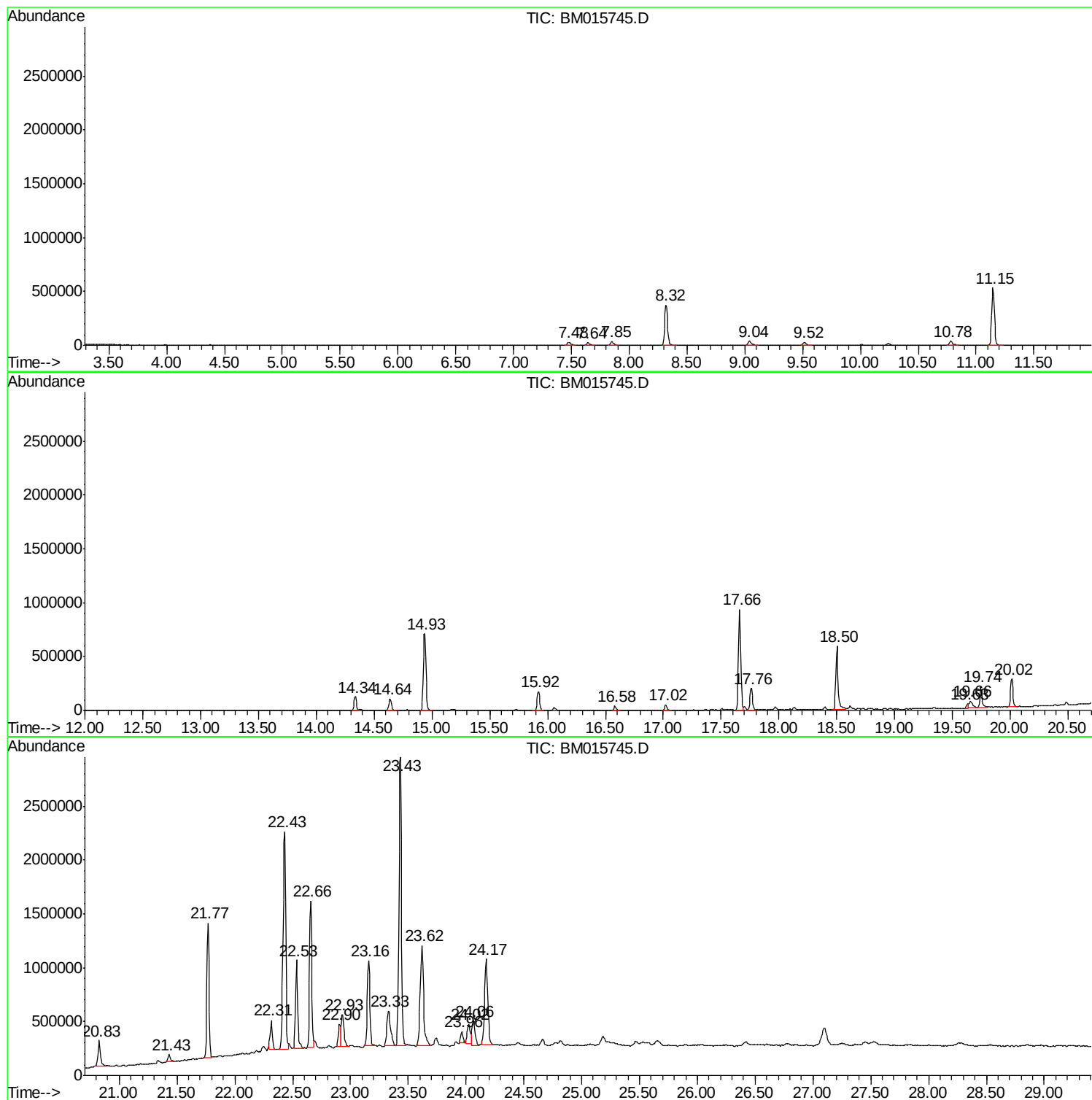
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Quant Title : SVOA CALIBRATION

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



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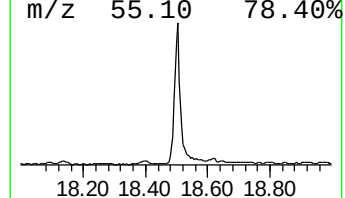
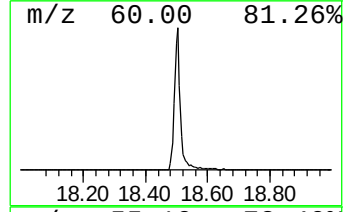
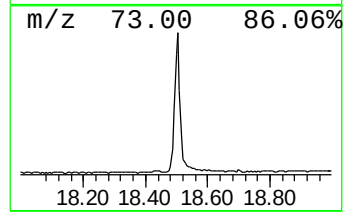
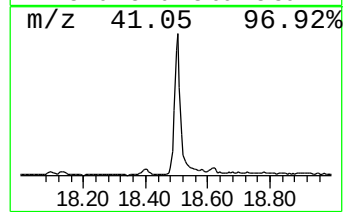
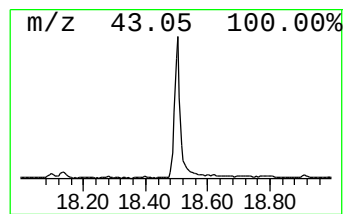
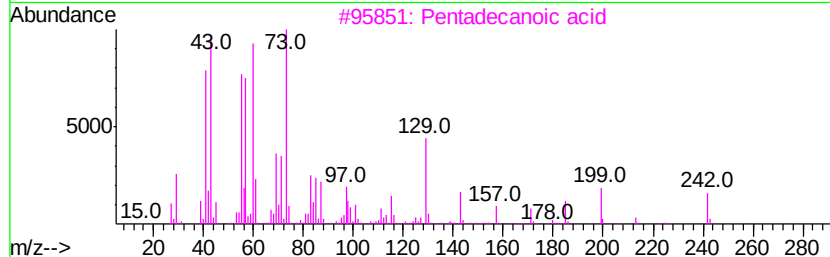
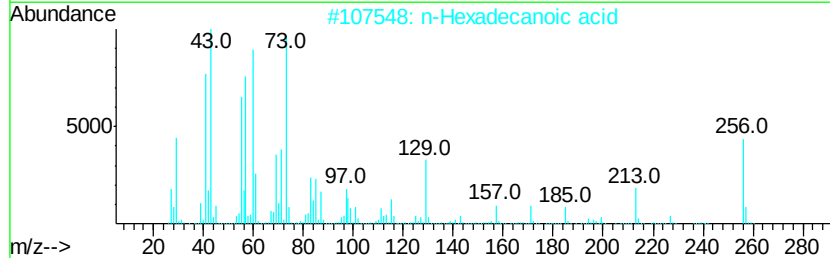
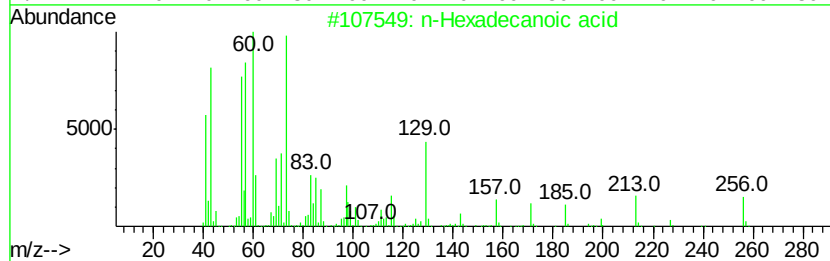
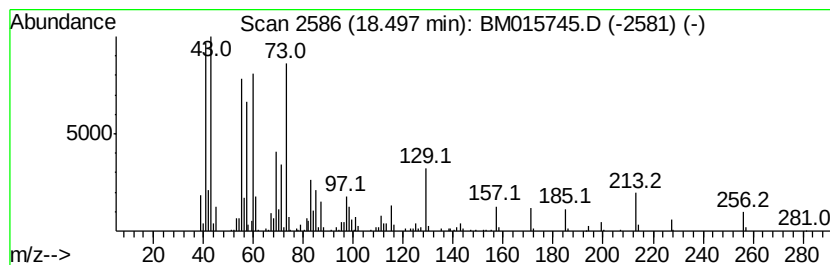
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TIC Library : C:\Database\NIST11.L
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Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	11.79 ng/ul	817207	Phenanthrene-d10	17.66
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	Pentadecanoic acid	242 C15H30O2	001002-84-2	81
4	Tridecanoic acid	214 C13H26O2	000638-53-9	76
5	Tridecanoic acid	214 C13H26O2	000638-53-9	76



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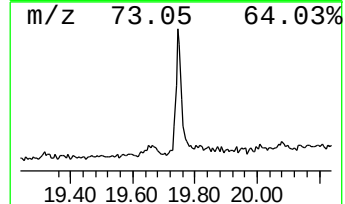
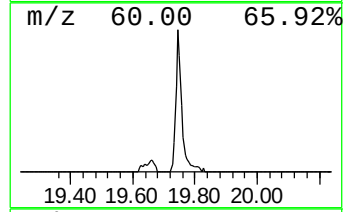
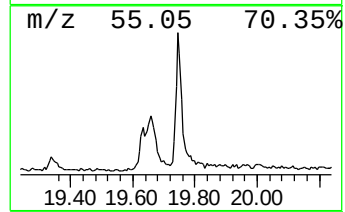
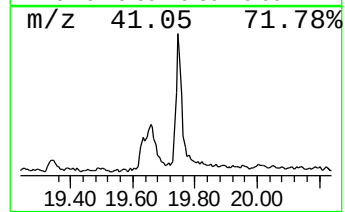
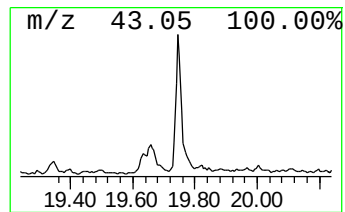
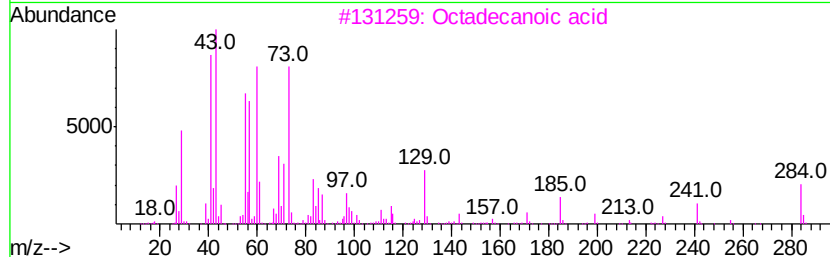
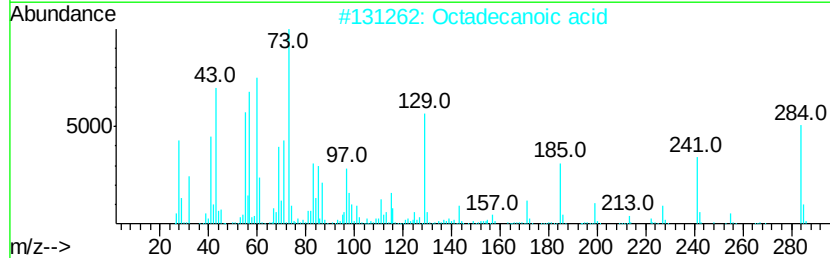
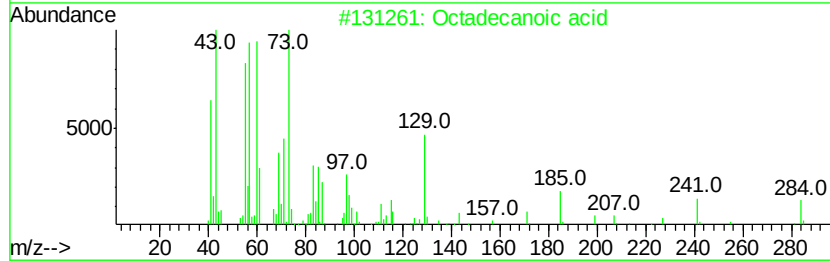
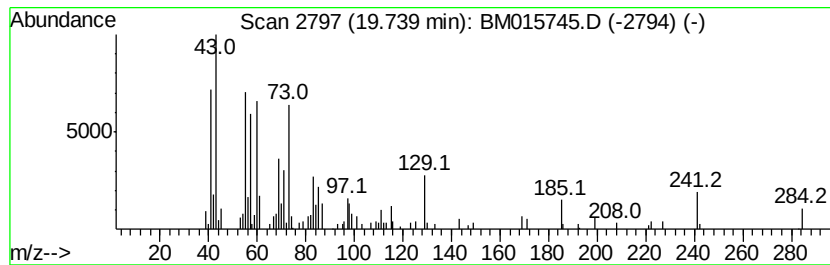
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.74	3.34 ng/ul	261234	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	99
3		Octadecanoic acid	284	C18H36O2	000057-11-4	98
4		Octadecanoic acid	284	C18H36O2	000057-11-4	96
5		Octadecanoic acid	284	C18H36O2	000057-11-4	91



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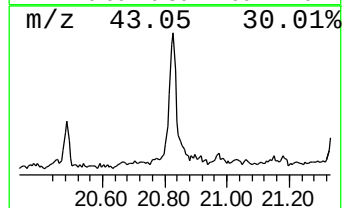
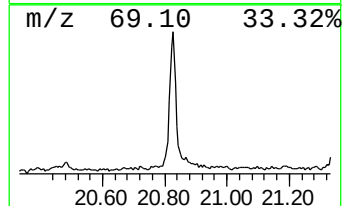
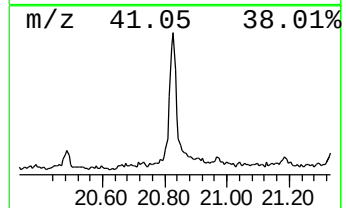
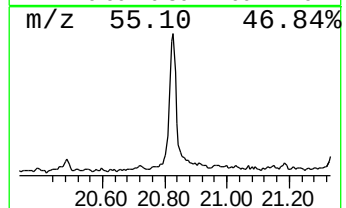
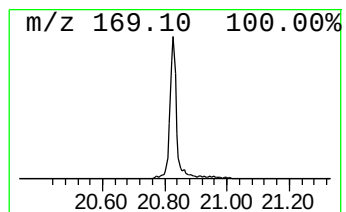
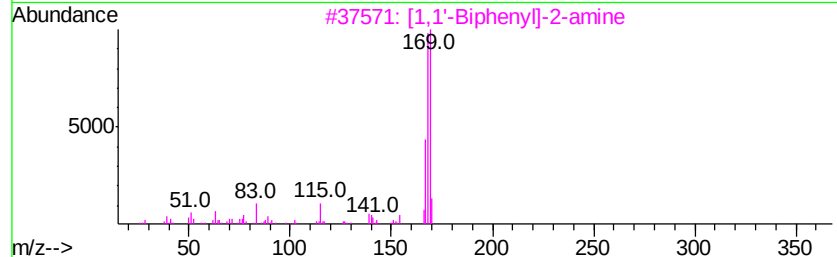
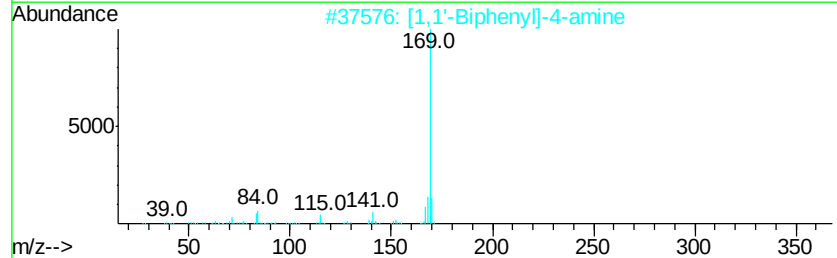
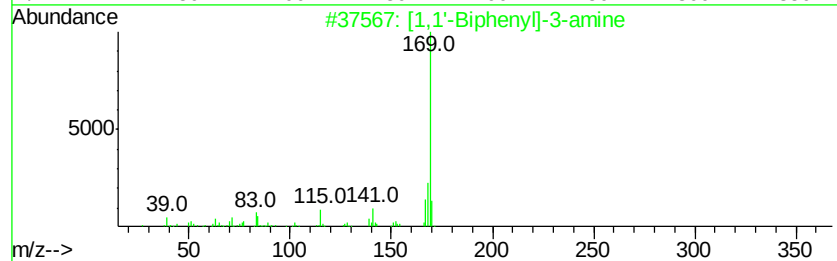
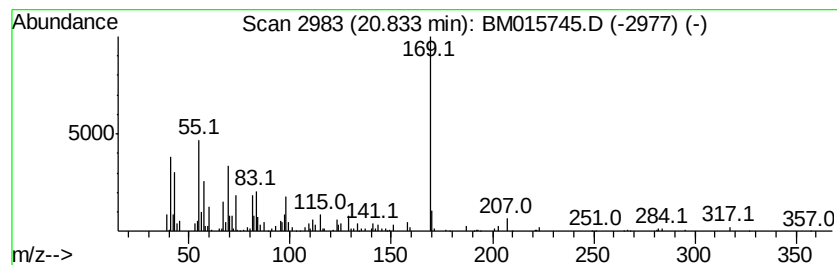
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060818MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.83	4.15 ng/ul	324850	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	[1,1'-Biphenyl]-3-amine	169	C12H11N	002243-47-2	43
2		[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	43
3		[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	38
4		[1,1'-Biphenyl]-2-amine	169	C12H11N	000090-41-5	38
5		5-Isopropyl-5-(2-hydroxy-2-prope...	226	C10H14N2O4	131147-52-9	38



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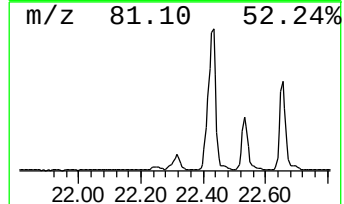
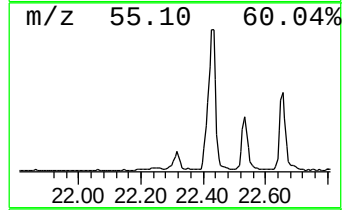
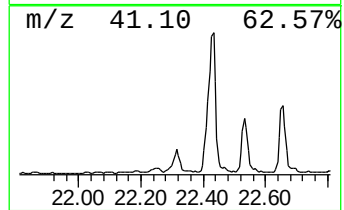
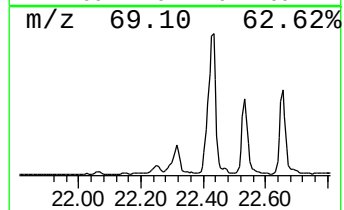
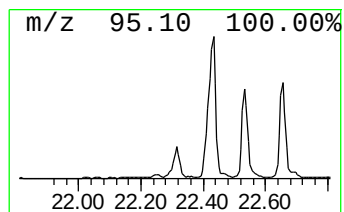
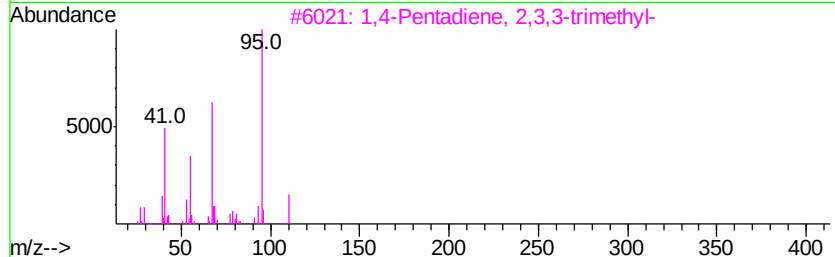
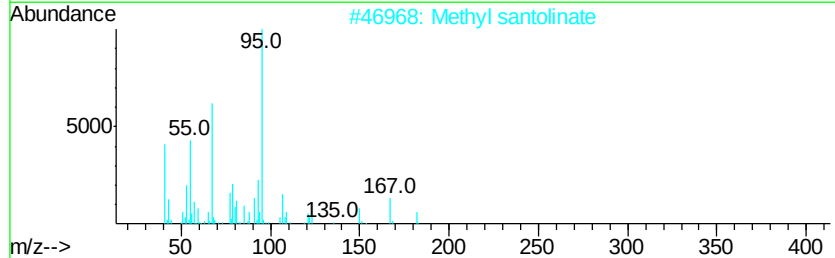
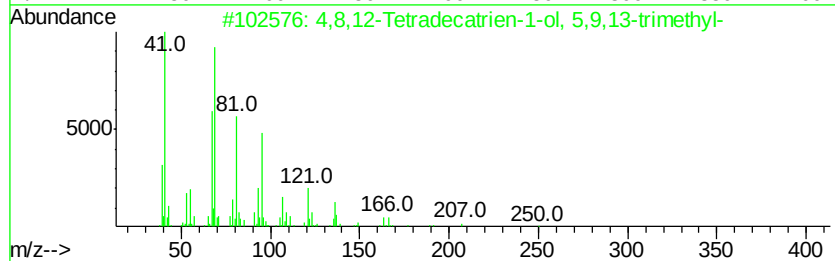
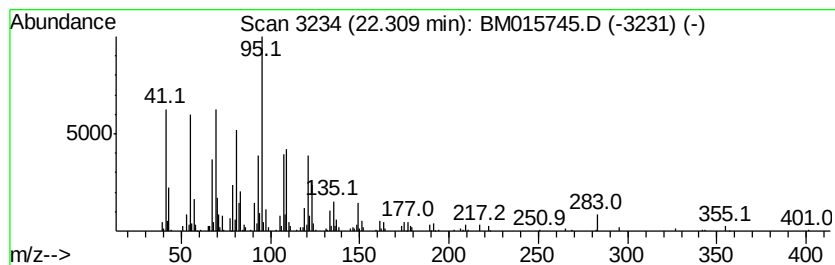
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown-02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.31	4.51 ng/ul	352543	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,8,12-Tetradecatrien-1-ol, 5,9,...	250	C17H30O	1000141-99-9	47
2		Methyl santolinate	182	C11H18O2	053163-37-4	43
3		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38
4		1,4-Cyclohexanedimethanol, trans-	144	C8H16O2	003236-48-4	38
5		Toluene-D3	95	C7H5D3	001124-18-1	35



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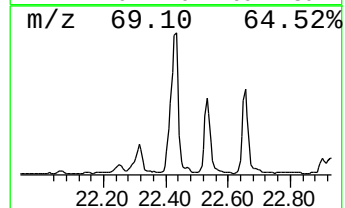
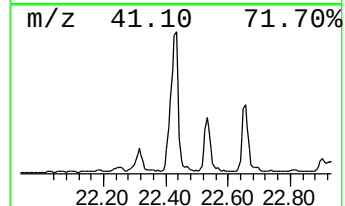
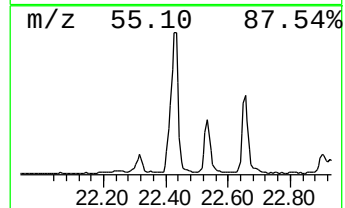
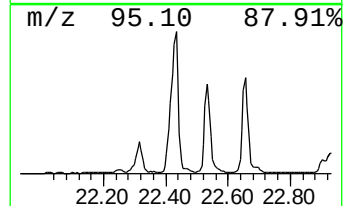
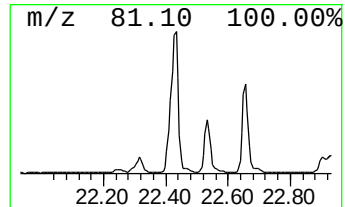
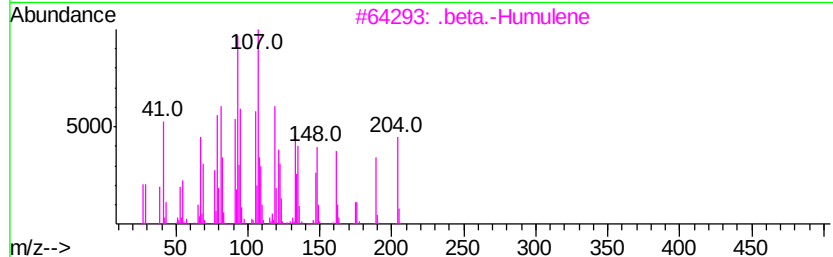
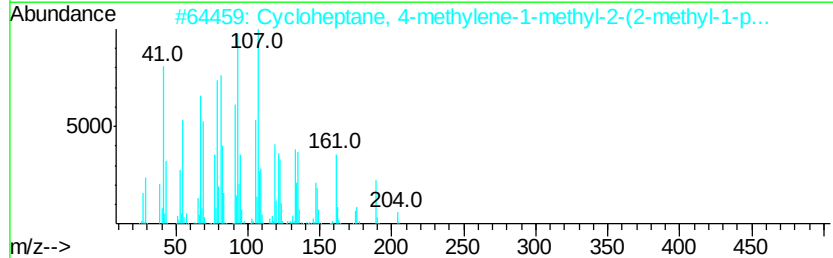
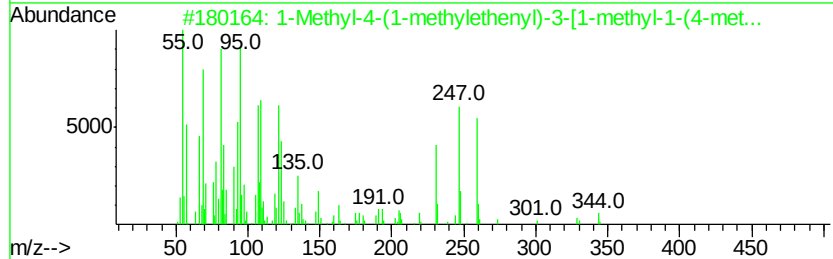
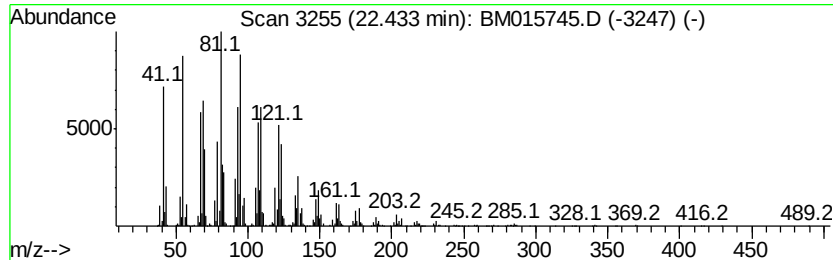
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Peak Number 5 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.43	42.73 ng/ul	3342940	Chrysene-d12	21.77	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-4-(1-methylethenyl)-3-[...]	344	C25H44	1000370-41-3	46
2	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	42
3	.beta.-Humulene	204	C15H24	000116-04-1	42
4	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	38
5	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	35



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Acq On : 25 Jun 2018 12:11
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Sample : J3569-25 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DAXP3

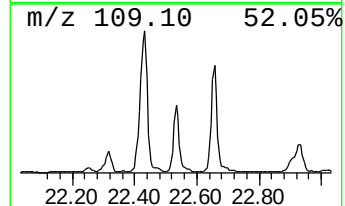
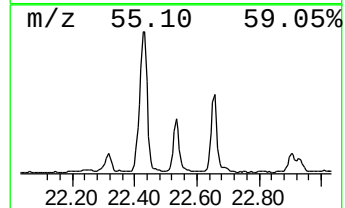
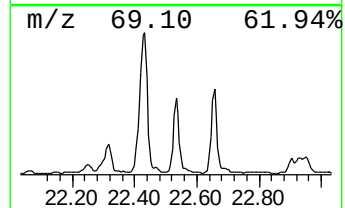
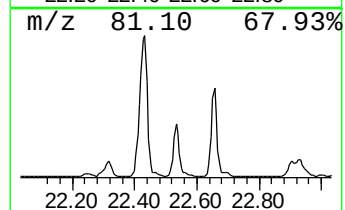
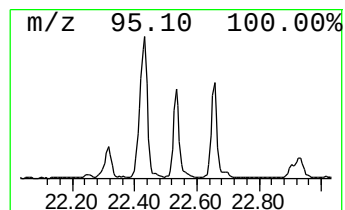
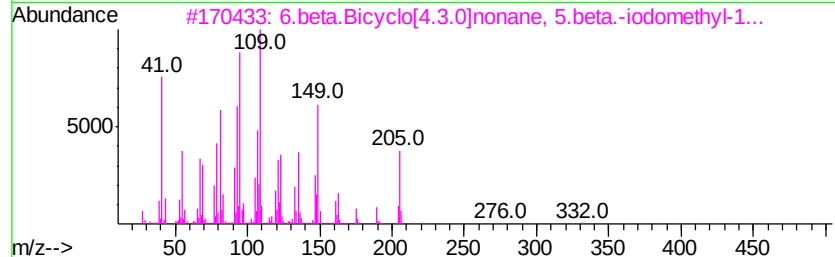
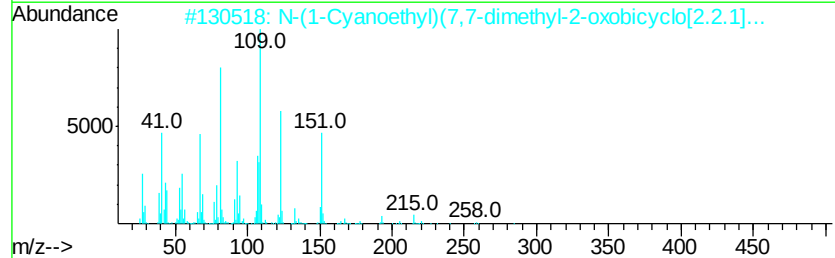
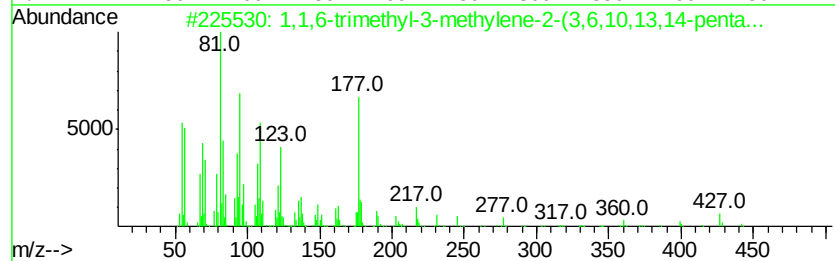
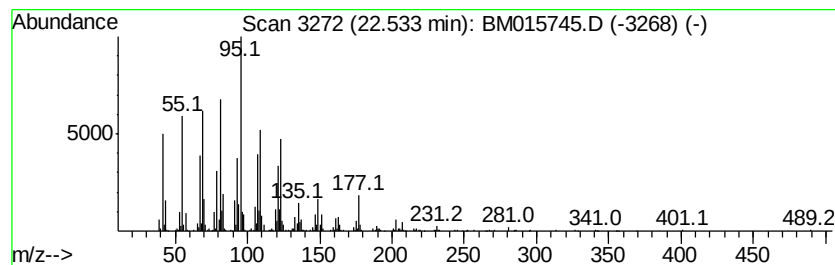
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	14.03 ng/ul	1097530	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,6-trimethyl-3-methylene-2-(3...	442	C32H58	1000373-94-0	47
2		N-(1-Cyanoethyl)(7,7-dimethyl-2-...	284	C13H20N2O3S	1000194-50-3	41
3		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	38
4		Cyclopentene, 1-isopropyl-2,3-di...	138	C10H18	007712-73-4	35
5		Cyclopentene, 1,4-dimethyl-5-(1-...	138	C10H18	061142-33-4	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM062518\
Data File : BM015745.D
Acq On : 25 Jun 2018 12:11
Operator : SJ/JU
Sample : J3569-25 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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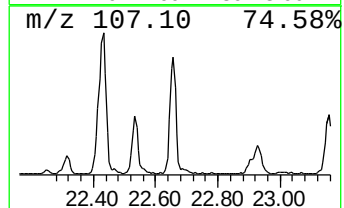
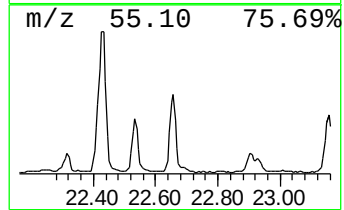
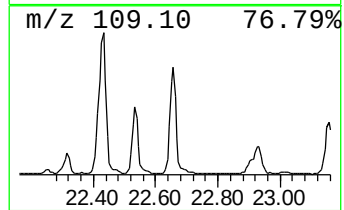
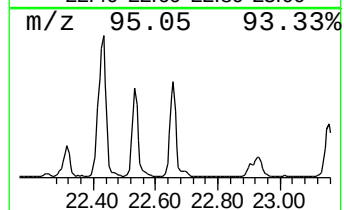
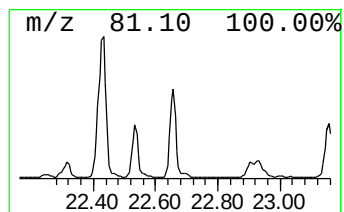
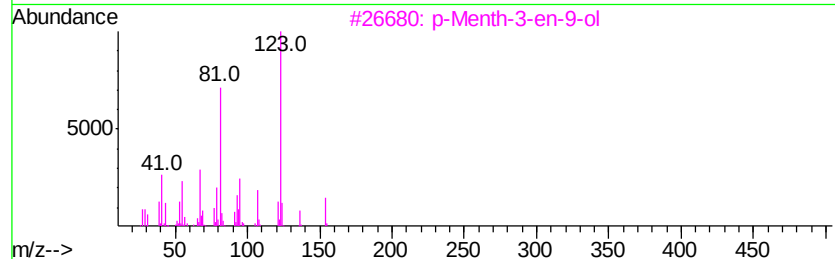
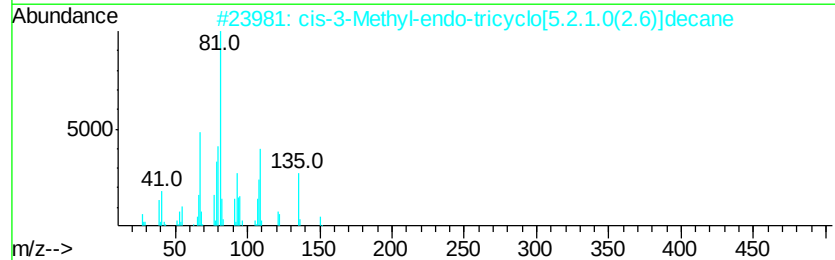
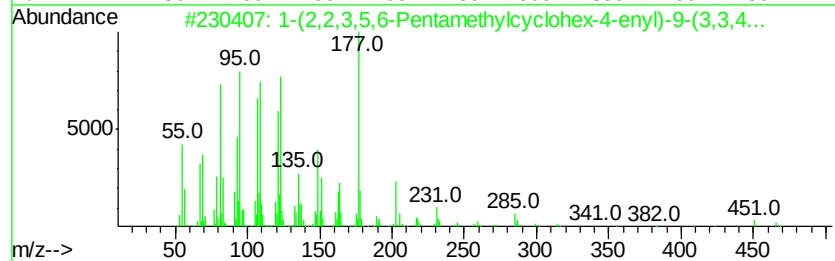
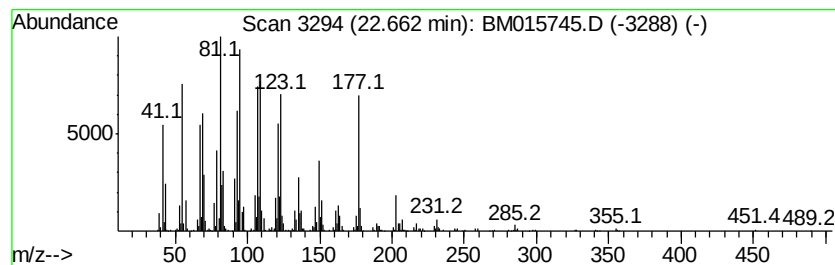
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-(2,2,3,5,6-Pentamethylcyc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.66	23.03 ng/ul	1801570	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(2,2,3,5,6-Pentamethylcyclohex...	466	C34H58	1000373-94-7	90
2		cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	27
3		p-Menth-3-en-9-ol	154	C10H18O	015714-10-0	27
4		Methyl Camphorsulfonates	246	C11H18O4S	046471-67-4	22
5		Verbenol	152	C10H16O	000473-67-6	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM062518\
Data File : BM015745.D
Acq On : 25 Jun 2018 12:11
Operator : SJ/JU
Sample : J3569-25 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

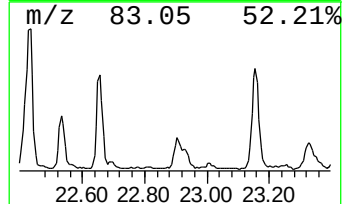
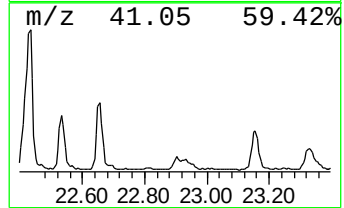
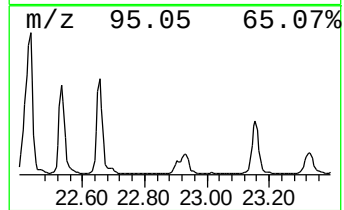
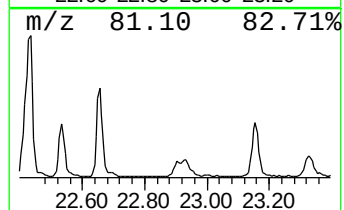
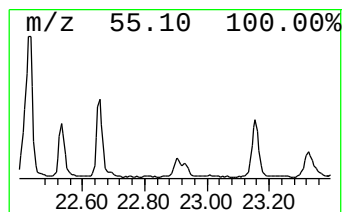
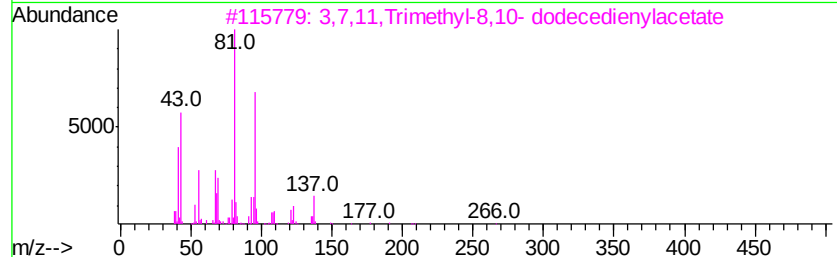
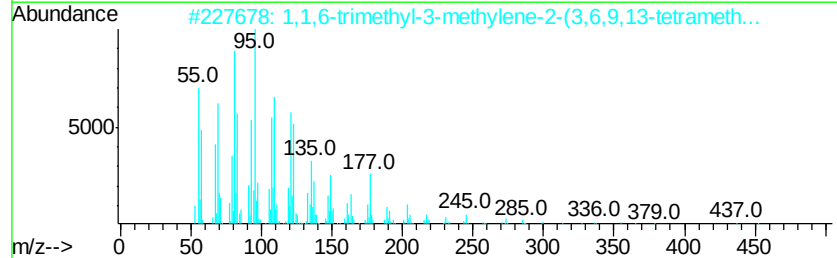
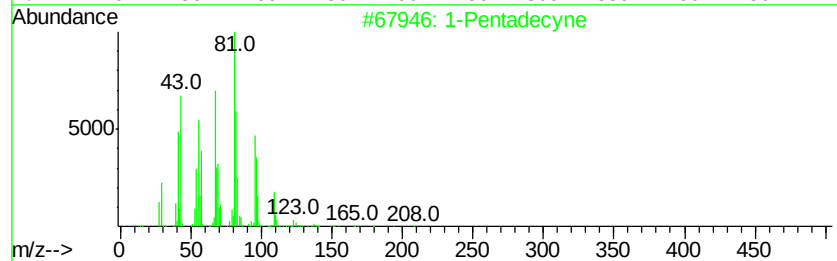
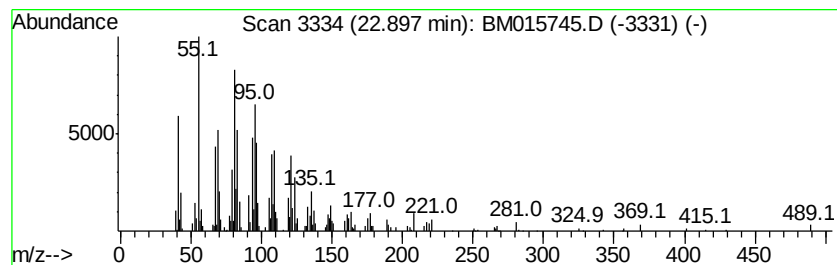
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060818MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 1-Pentadecyne Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	3.82 ng/ul	298649	Chrysene-d12	21.77
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Pentadecyne		208 C15H28	000765-13-9 50
2	1,1,6-trimethyl-3-methylene-2-(3...		452 C33H56	1000373-94-5 49
3	3,7,11-Trimethyl-8,10- dodecedie...		266 C17H30O2	1000374-10-3 38
4	Isoaromadendrene epoxide		220 C15H24O	1000159-36-6 38
5	trans-Geranylgeraniol		290 C20H34O	024034-73-9 30



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM062518\
Data File : BM015745.D
Acq On : 25 Jun 2018 12:11
Operator : SJ/JU
Sample : J3569-25 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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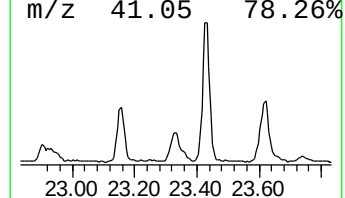
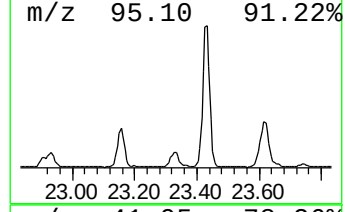
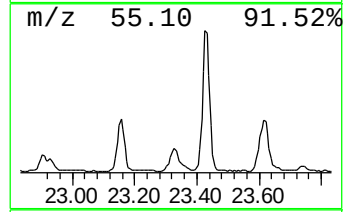
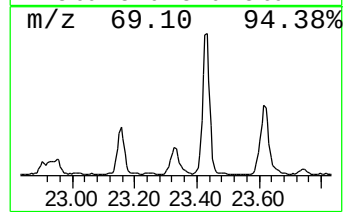
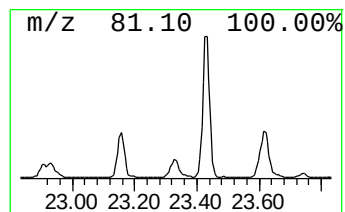
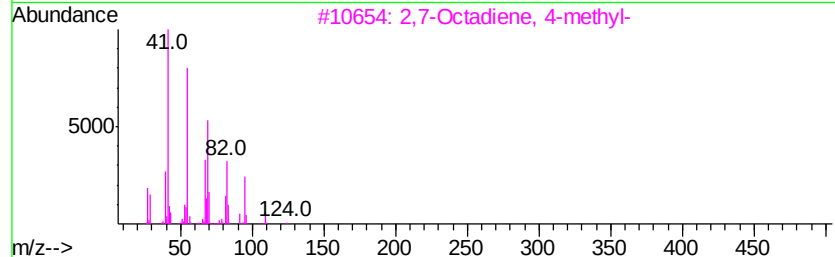
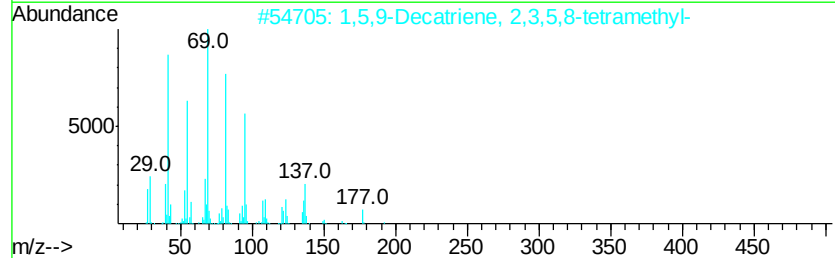
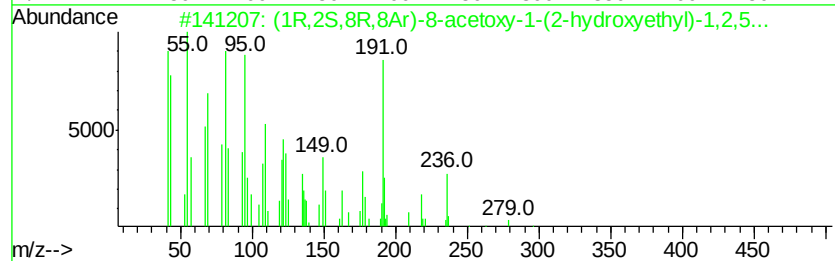
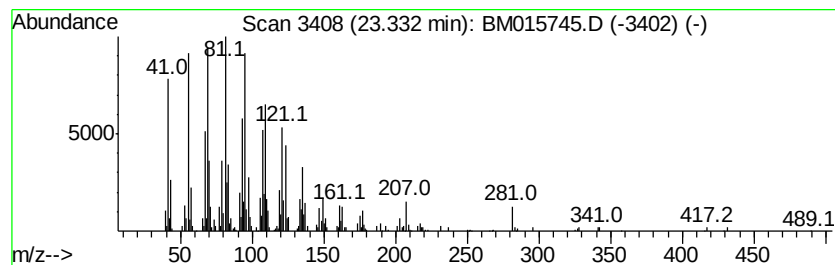
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 unknown-05 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	8.85 ng/ul	700729	Perylene-d12	24.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R,2S,8R,8Ar)-8-acetoxv-1-(2-hv...	296	C18H32O3	1000298-98-4	49
2		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	38
3		2,7-Octadiene, 4-methyl-	124	C9H16	1000061-78-0	38
4		cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	30
5		5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM062518\
Data File : BM015745.D
Acq On : 25 Jun 2018 12:11
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Sample : J3569-25 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DAXP3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM060818MA.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	18.50	11.8	ng/ul	817207	4	17.66	1385990	20.0
Octadecanoic acid	19.74	3.3	ng/ul	261234	5	21.77	1564700	20.0
unknown-01	20.83	4.2	ng/ul	324850	5	21.77	1564700	20.0
unknown-02	22.31	4.5	ng/ul	352543	5	21.77	1564700	20.0
unknown-03	22.43	42.7	ng/ul	3342940	5	21.77	1564700	20.0
unknown-04	22.53	14.0	ng/ul	1097530	5	21.77	1564700	20.0
1-(2,2,3,5,6-Pent...	22.66	23.0	ng/ul	1801570	5	21.77	1564700	20.0
1-Pentadecyne	22.90	3.8	ng/ul	298649	5	21.77	1564700	20.0
1,1,6-trimethyl-3...	23.16	15.4	ng/ul	1218860	6	24.17	1583900	20.0
unknown-05	23.33	8.8	ng/ul	700729	6	24.17	1583900	20.0