

Data Path : Z:\HPCHEM1\BNA M\DATA\BM012218\
 Data File : BM013694.D
 Acq On : 22 Jan 2018 15:13
 Operator : SJ/JU
 Sample : J1221-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F6A64

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-BM011018.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.163	26	30	38	rVB2	38075	52676	1.31%	0.117%
2	6.793	641	647	658	rBV2	644638	1178933	29.23%	2.627%
3	6.957	669	675	682	rBV	479085	715781	17.74%	1.595%
4	7.146	700	707	715	rBV	667149	1067306	26.46%	2.378%
5	7.610	779	786	795	rBV	503290	771767	19.13%	1.720%
6	8.322	900	907	918	rBV	792216	1323934	32.82%	2.950%
7	8.769	974	983	991	rBV	649129	1091670	27.06%	2.432%
8	9.481	1098	1104	1113	rBV	537680	928418	23.02%	2.069%
9	10.016	1188	1195	1211	rBV	789544	1410455	34.96%	3.143%
10	10.387	1251	1258	1266	rBV	647617	1049893	26.03%	2.339%
11	10.534	1275	1283	1292	rBV	719038	1280788	31.75%	2.854%
12	11.716	1477	1484	1499	rBV	201431	347919	8.62%	0.775%
13	12.604	1627	1635	1642	rBV3	88664	131305	3.25%	0.293%
14	13.128	1719	1724	1736	rVB2	95577	143734	3.56%	0.320%
15	13.575	1789	1800	1808	rBV2	347642	519942	12.89%	1.158%
16	13.680	1811	1818	1822	rVV	1433263	1954559	48.45%	4.355%
17	13.727	1822	1826	1834	rVB	688311	944973	23.43%	2.105%
18	13.951	1857	1864	1874	rBV	1617523	2405089	59.62%	5.359%
19	14.104	1884	1890	1893	rVB4	28191	42008	1.04%	0.094%
20	14.263	1911	1917	1924	rVV2	864050	1312725	32.54%	2.925%
21	14.333	1924	1929	1938	rVB3	64137	88918	2.20%	0.198%
22	14.486	1949	1955	1968	rBV	513054	1005577	24.93%	2.240%
23	14.586	1968	1972	1980	rVB3	75553	131791	3.27%	0.294%
24	14.798	2002	2008	2014	rVB3	26476	45580	1.13%	0.102%
25	15.263	2079	2087	2098	rVB	2276240	3191845	79.12%	7.111%
26	15.398	2105	2110	2116	rBV	589880	854492	21.18%	1.904%
27	15.504	2124	2128	2131	rBV4	36200	50603	1.25%	0.113%
28	15.633	2142	2150	2159	rBV	1799607	2417140	59.92%	5.385%
29	15.739	2163	2168	2174	rVB8	28604	54280	1.35%	0.121%
30	15.851	2180	2187	2193	rBV8	27155	62378	1.55%	0.139%
31	15.980	2204	2209	2217	rVV10	54178	127470	3.16%	0.284%
32	16.686	2324	2329	2332	rBV7	24302	44270	1.10%	0.099%
33	17.015	2375	2385	2391	rBV	1191884	1690548	41.91%	3.767%
34	17.116	2394	2402	2410	rBV	2220608	3132273	77.65%	6.979%

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Integration Parameters: LSCINT.P

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35	17.739	2503	2508	2513	rBV5	29764	48452	1.20%	0.108%
36	17.921	2535	2539	2549	rVV2	290550	417068	10.34%	0.929%
37	19.057	2726	2732	2734	rBV3	39711	60597	1.50%	0.135%
38	19.209	2754	2758	2765	rBV5	95740	147587	3.66%	0.329%
39	19.415	2787	2793	2801	rBV	2883041	3696382	91.63%	8.236%
40	20.933	3047	3051	3058	rBV	470753	662759	16.43%	1.477%
41	21.215	3093	3099	3104	rBV	1563485	2101652	52.10%	4.682%
42	21.821	3199	3202	3208	rVB6	117874	168789	4.18%	0.376%
43	23.274	3442	3449	3458	rBV2	2224426	4033964	100.00%	8.988%
44	23.415	3466	3473	3480	rVB	1071646	1974851	48.96%	4.400%

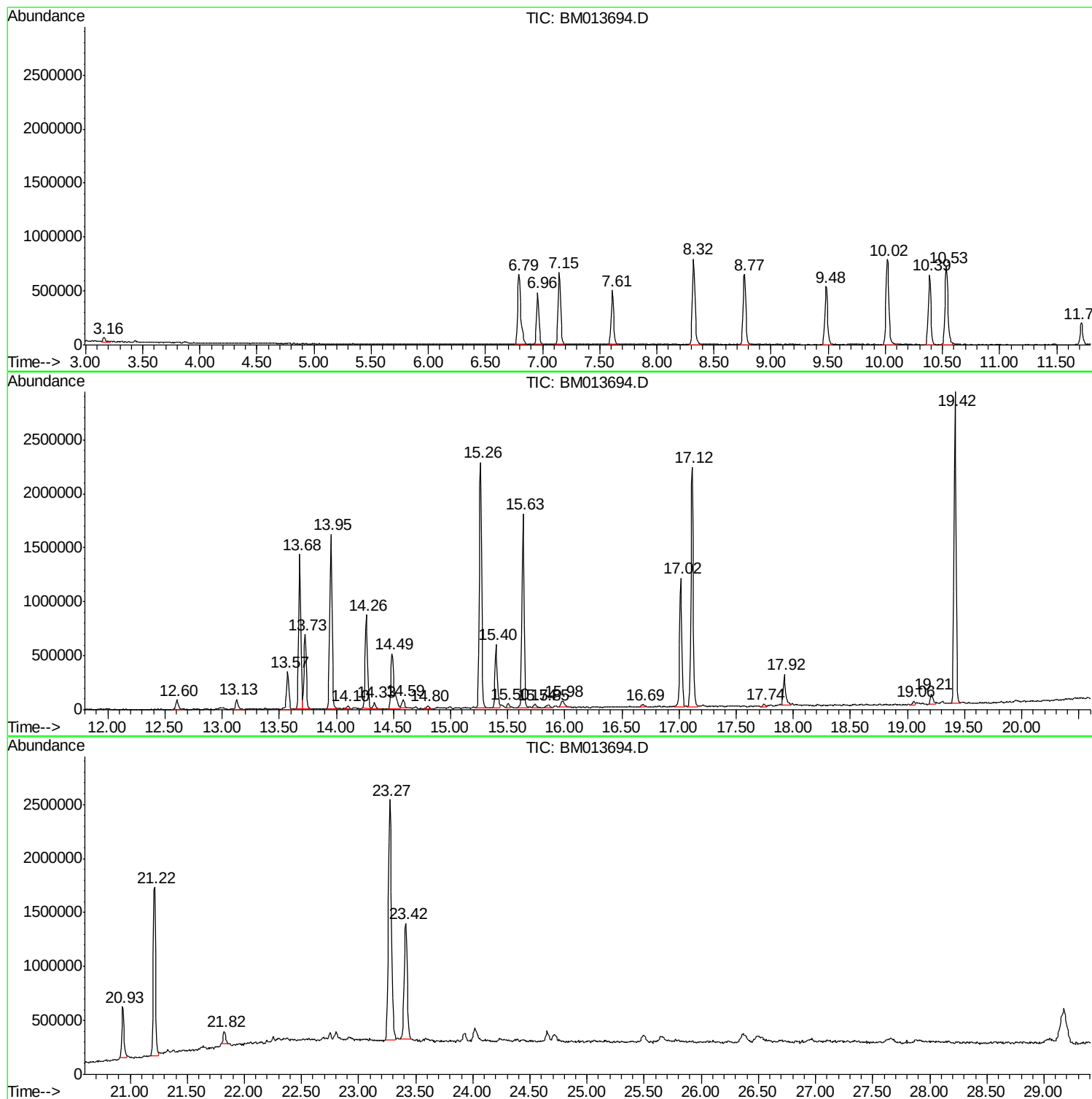
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Quant Method : Z:\HPCHEM1\BNA M\Methods\SOM-EPA-BM011018.M
Quant Title : SVOA CALIBRATION

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



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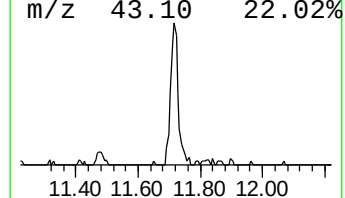
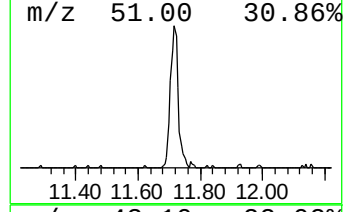
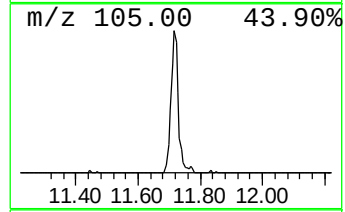
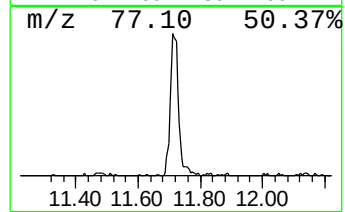
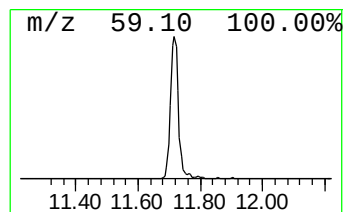
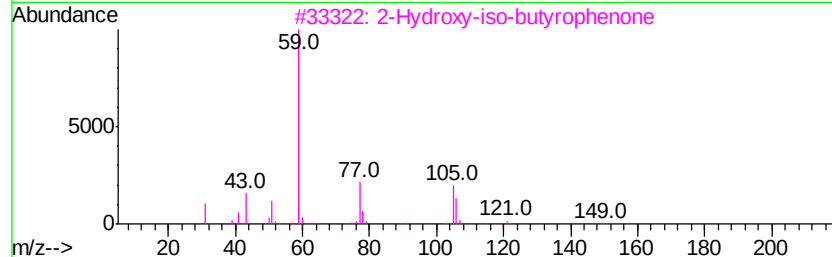
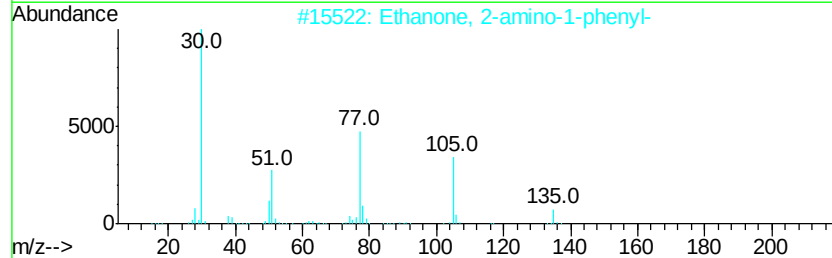
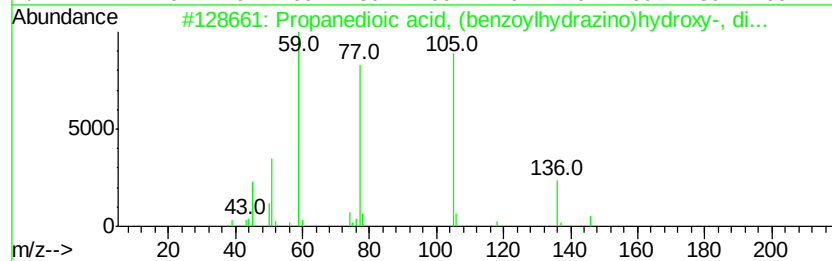
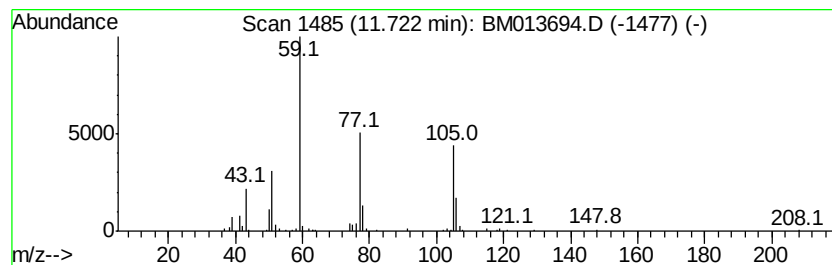
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Propanedioic acid, (benzoyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.72	6.63 ng/ul	347919	Napthalene-d8	10.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, (benzoylhvdra...	282	C12H14N2O6	1000142-99-9	50
2	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	43
3	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	32
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	9



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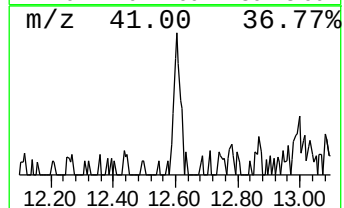
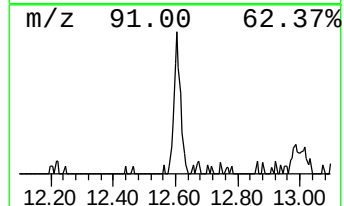
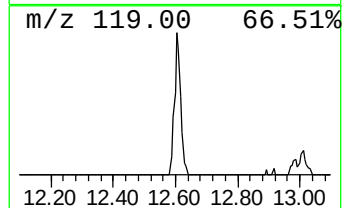
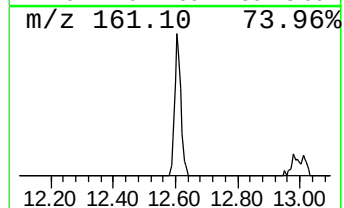
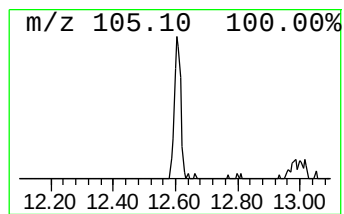
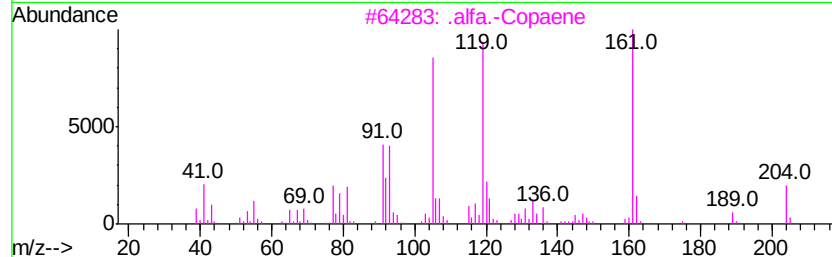
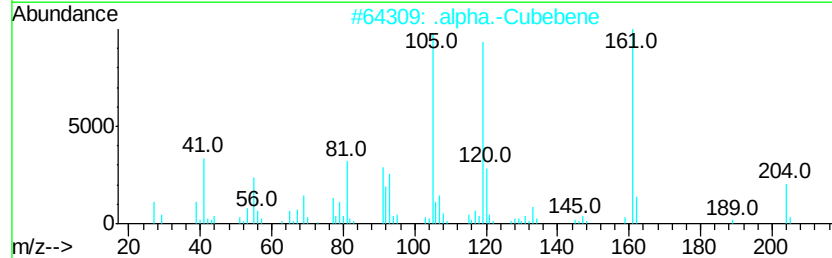
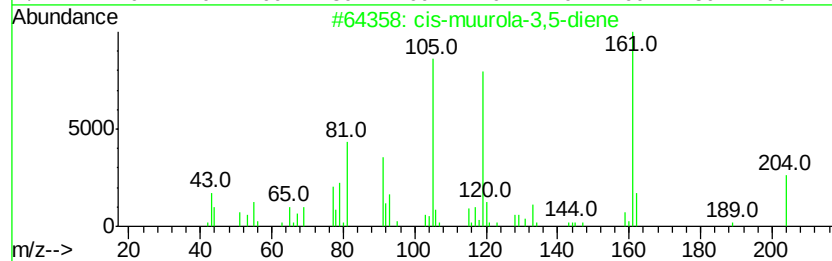
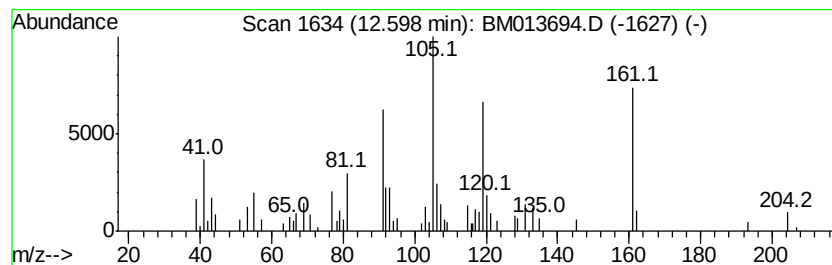
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Peak Number 2 cis-muurola-3,5-diene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	2.00 ng/ul	131305	Acenaphthene-d10	14.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		cis-muurola-3,5-diene	204 C15H24	1000365-95-4 96
2		.alpha.-Cubebene	204 C15H24	017699-14-8 93
3		.alfa.-Copaene	204 C15H24	1000360-33-0 92
4		.alpha.-Cubebene	204 C15H24	017699-14-8 87
5		.alpha.-Cubebene	204 C15H24	017699-14-8 80



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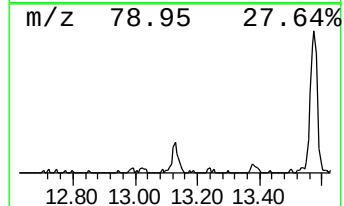
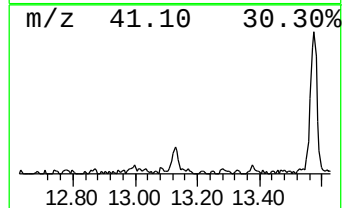
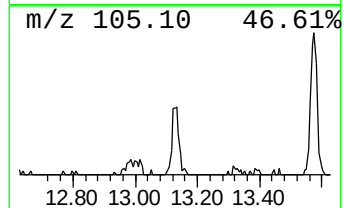
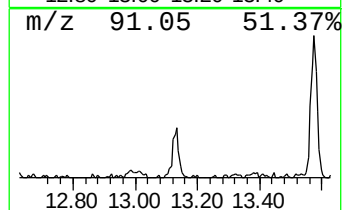
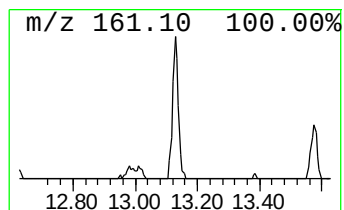
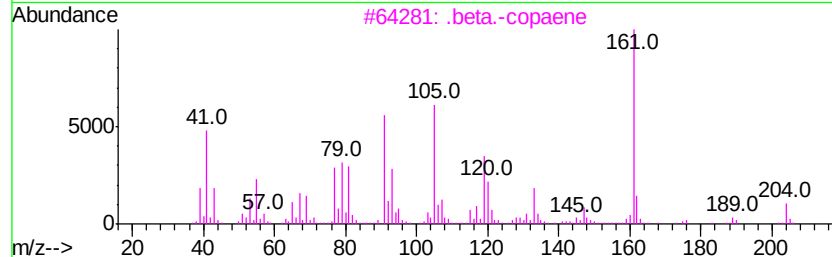
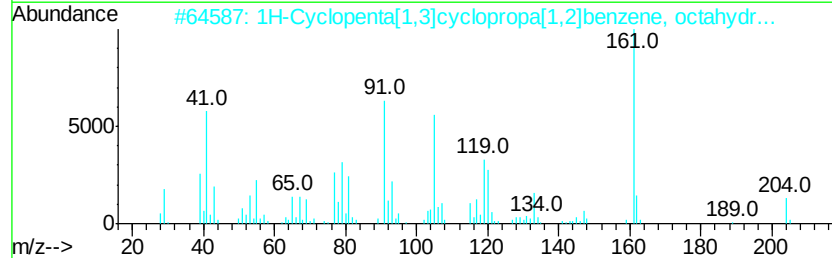
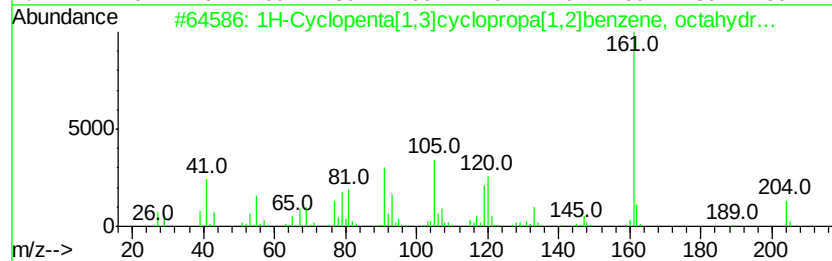
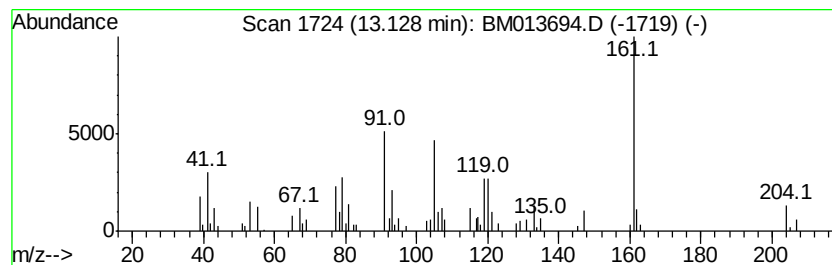
Quant Method : Z:\HPCHEM1\BNA M\Methods\SOM-EPA-BM011018.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1H-Cyclopenta[1,3]cycloprop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	2.19 ng/ul	143734	Acenaphthene-d10	14.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Cyclopenta[1,3]cyclopropa[1,2]...	204	C15H24	013744-15-5	96
2		1H-Cyclopenta[1,3]cyclopropa[1,2]...	204	C15H24	013744-15-5	94
3		.beta.-copaene	204	C15H24	1000374-18-9	93
4		Bicyclo[4.4.0]dec-1-ene, 2-isopr...	204	C15H24	150320-52-8	90
5		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	81



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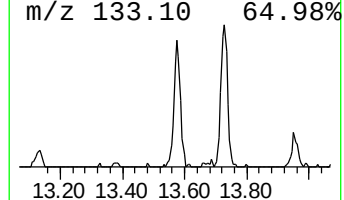
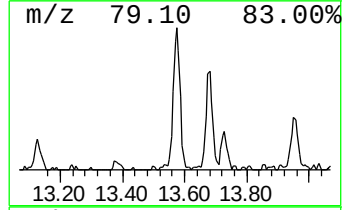
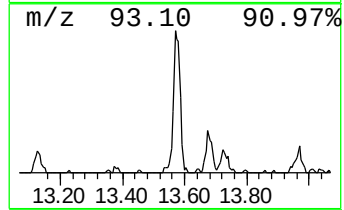
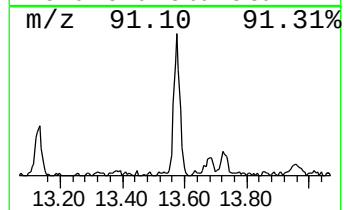
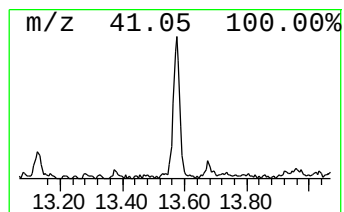
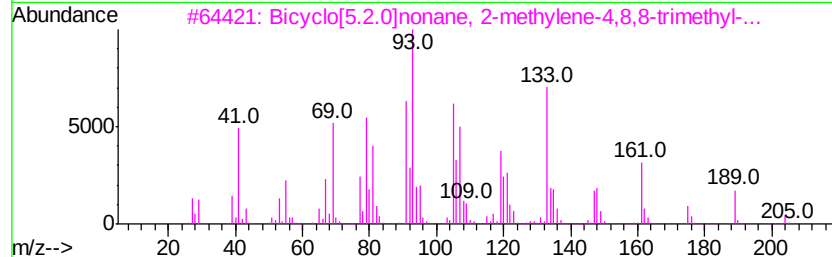
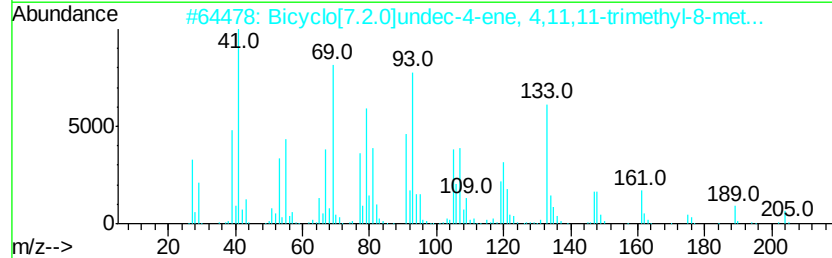
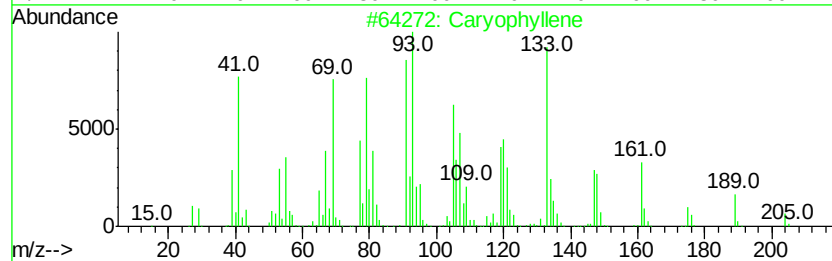
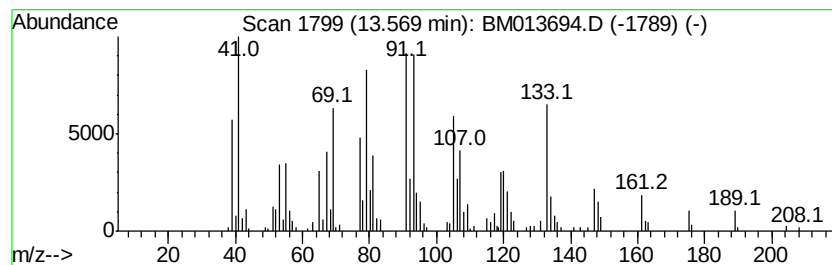
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Peak Number 4 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	7.92 ng/ul	519942	Acenaphthene-d10	14.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Caryophyllene	204 C15H24	000087-44-5 99
2		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	000118-65-0 83
3		Bicyclo[5.2.0]nonane, 2-methylen...	204 C15H24	242794-76-9 81
4		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	013877-93-5 76
5		Caryophyllene	204 C15H24	000087-44-5 70



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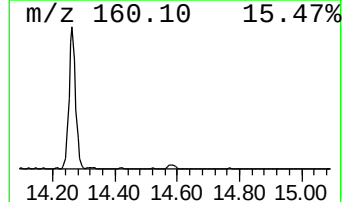
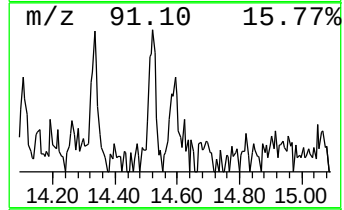
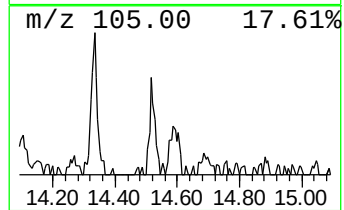
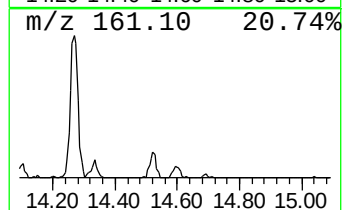
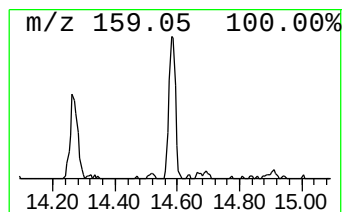
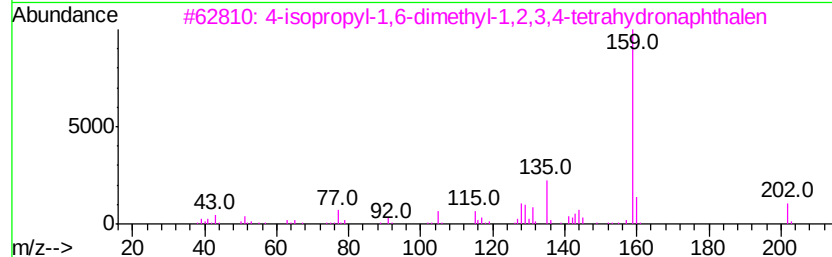
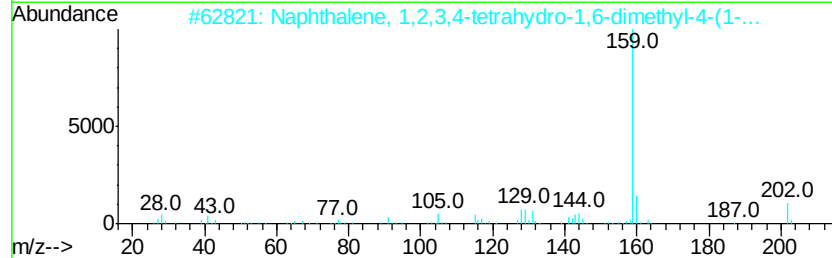
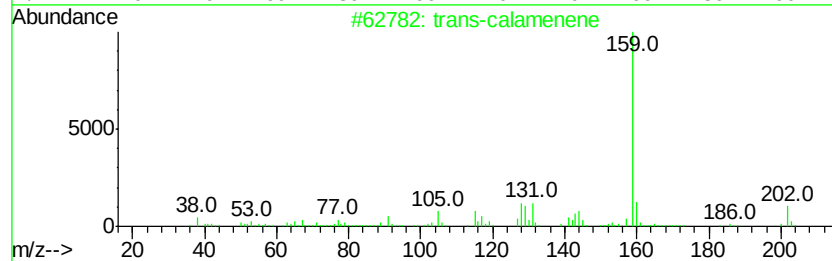
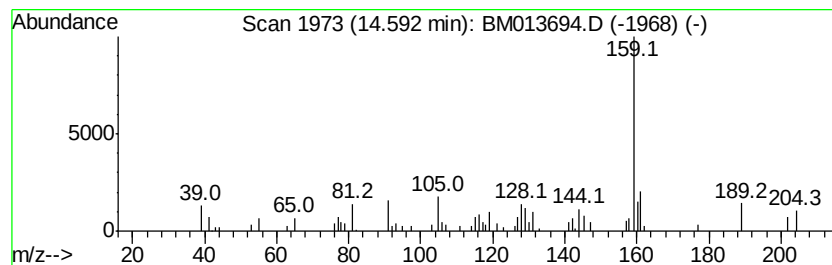
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TIC Integration Parameters: LSCINT.P

Peak Number 5 trans-calamenene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.01 ng/ul	131791	Acenaphthene-d10	14.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-calamenene	202	C15H22	1000374-17-3	87
2		Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	81
3		4-isopropyl-1,6-dimethyl-1,2,3,4...	202	C15H22	1000378-99-6	74
4		Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	72
5		Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	72



Data Path : Z:\HPCHEM1\BNA M\DATA\BM012218\
Data File : BM013694.D
Acq On : 22 Jan 2018 15:13
Operator : SJ/JU
Sample : J1221-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F6A64

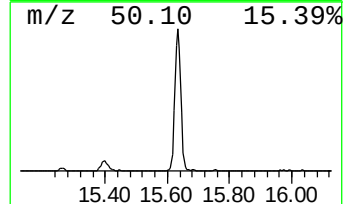
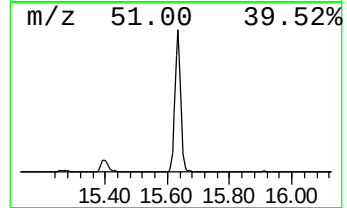
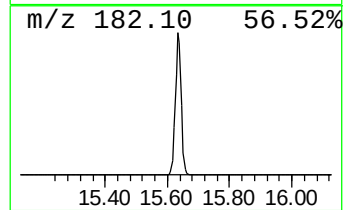
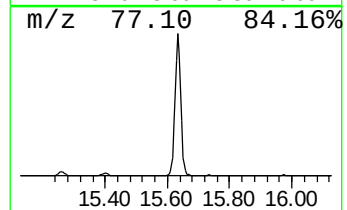
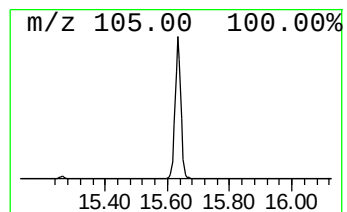
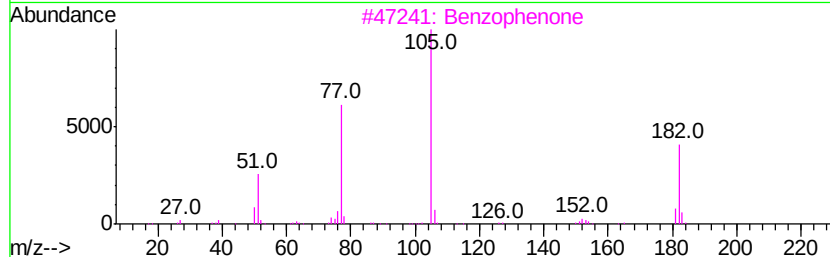
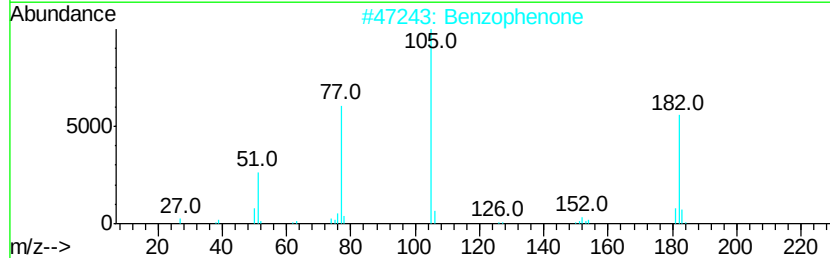
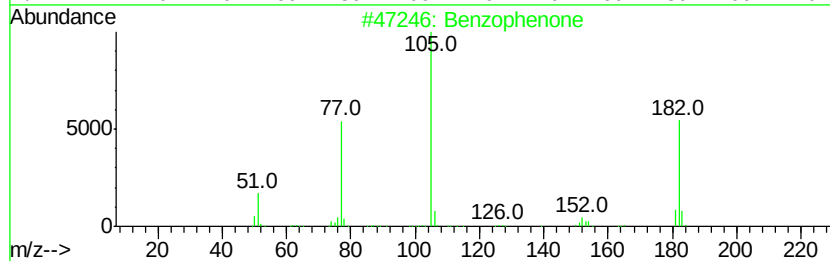
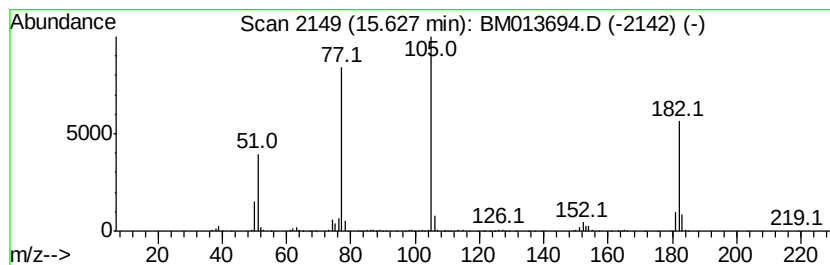
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	36.83 ng/ul	2417140	Acenaphthene-d10	14.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	97
2		Benzophenone	182	C13H10O	000119-61-9	96
3		Benzophenone	182	C13H10O	000119-61-9	94
4		Benzophenone	182	C13H10O	000119-61-9	93
5		Benzophenone	182	C13H10O	000119-61-9	91



Data Path : Z:\HPCHEM1\BNA M\DATA\BM012218\
Data File : BM013694.D
Acq On : 22 Jan 2018 15:13
Operator : SJ/JU
Sample : J1221-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F6A64

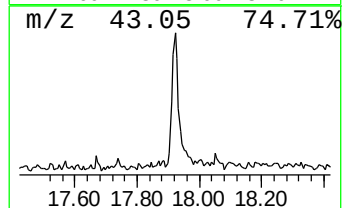
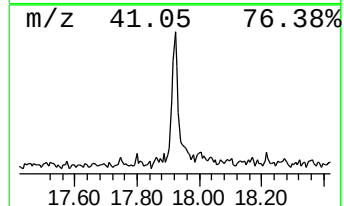
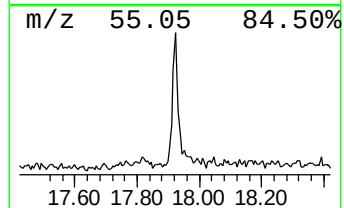
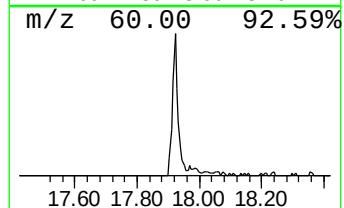
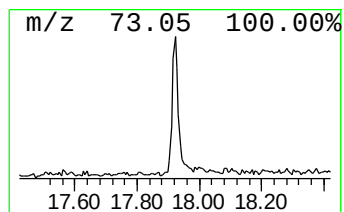
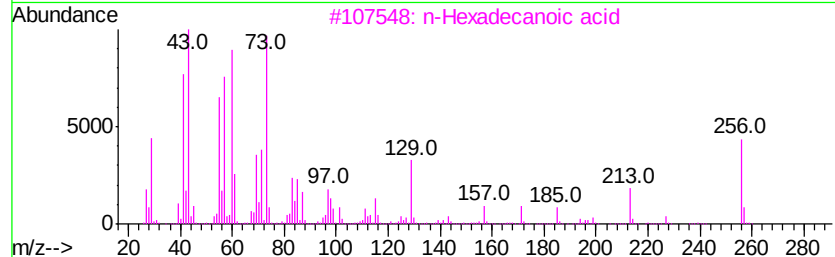
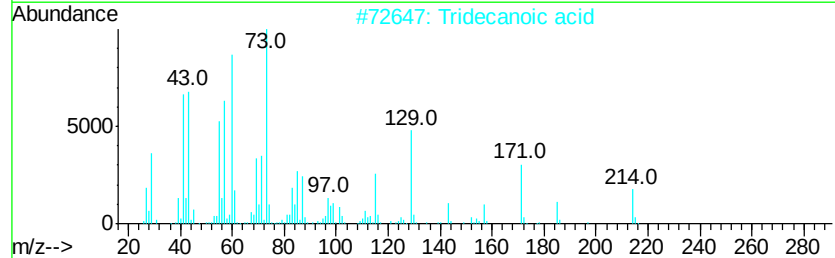
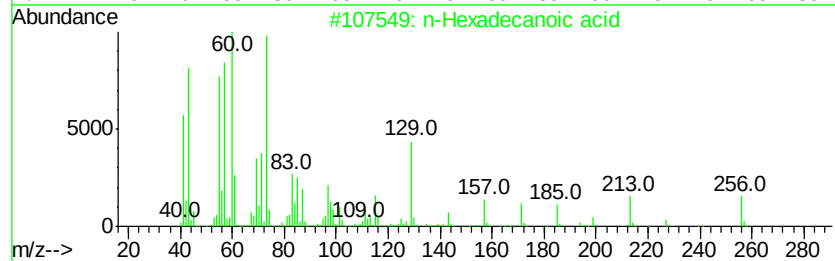
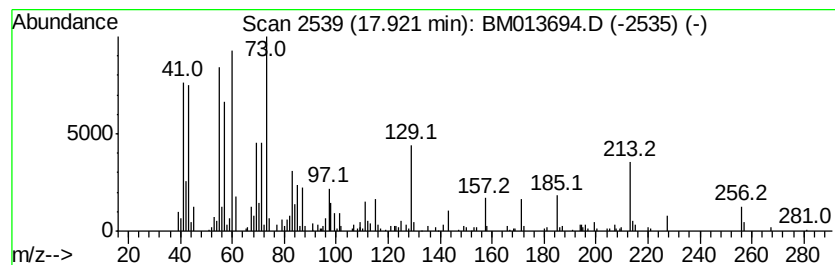
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	4.93 ng/ul	417068	Phenanthrene-d10	17.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	89
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	81



Data Path : Z:\HPCHEM1\BNA M\DATA\BM012218\
Data File : BM013694.D
Acq On : 22 Jan 2018 15:13
Operator : SJ/JU
Sample : J1221-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

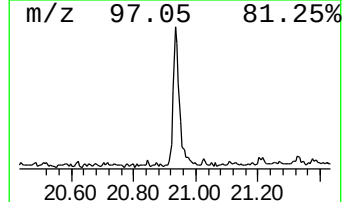
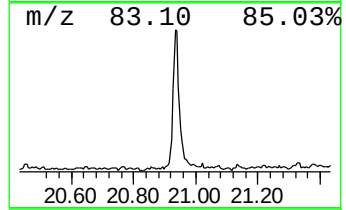
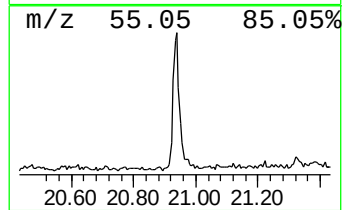
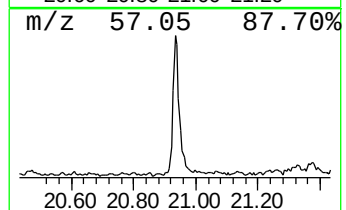
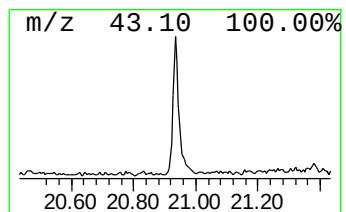
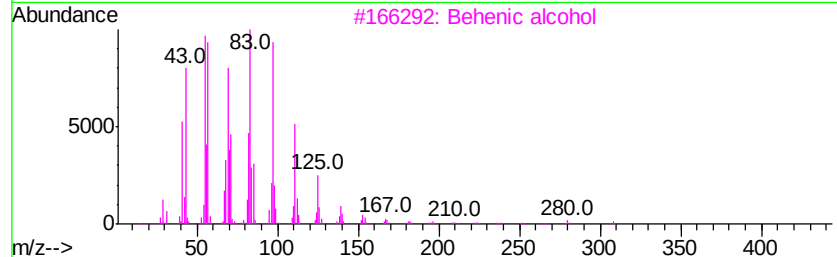
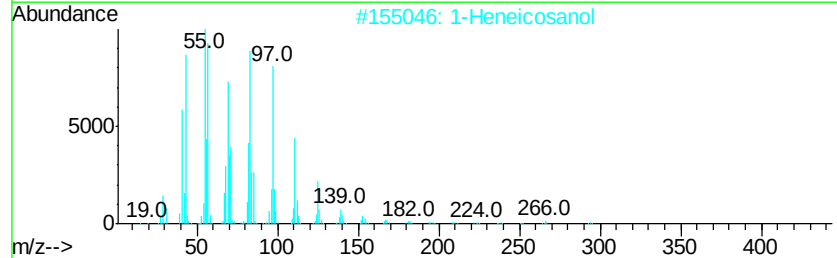
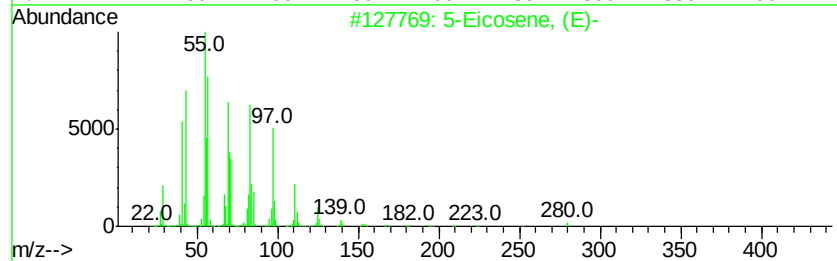
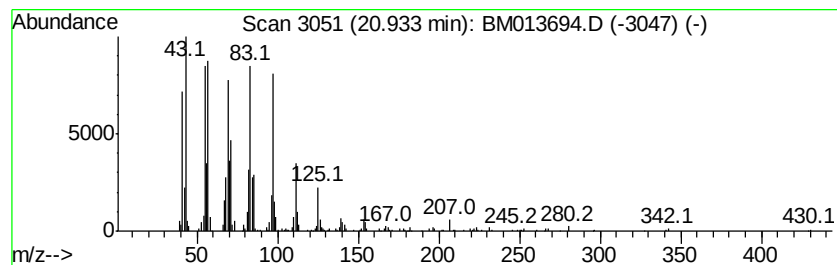
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA M\Methods\SOM-EPA-BM011018.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Cyclic20.93 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.93	6.31 ng/ul	662759	Chrysene-d12	21.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	93



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM012218\
Data File : BM013694.D
Acq On : 22 Jan 2018 15:13
Operator : SJ/JU
Sample : J1221-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F6A64

Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM011018.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
Propanedioic acid...	11.72	6.6	ng/ul	347919	2	10.39	1049890	20.0
cis-muurolo-3,5-d...	12.60	2.0	ng/ul	131305	3	14.26	1312730	20.0
1H-Cyclopenta[1,3...	13.13	2.2	ng/ul	143734	3	14.26	1312730	20.0
Caryophyllene	13.57	7.9	ng/ul	519942	3	14.26	1312730	20.0
trans-calamenene	14.59	2.0	ng/ul	131791	3	14.26	1312730	20.0
Benzophenone	15.63	36.8	ng/ul	2417140	3	14.26	1312730	20.0
n-Hexadecanoic acid	17.92	4.9	ng/ul	417068	4	17.02	1690550	20.0
(DEL) Alkane: Cyc...	20.93	6.3	ng/ul	662759	5	21.22	2101650	20.0