

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
 Data File : BM010461.D
 Acq On : 09 Jun 2017 19:40
 Operator : SJ/MA
 Sample : I3520-09
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 F5A41

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-BM052717.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	6.545	581	588	596	rVB	552153	847680	7.26%	1.183%
2	7.086	672	680	692	rBV2	576774	1246090	10.68%	1.738%
3	7.245	701	707	713	rBV	388312	595107	5.10%	0.830%
4	7.439	733	740	751	rBV	617509	1017486	8.72%	1.419%
5	7.904	812	819	828	rVB	1087004	1747999	14.98%	2.439%
6	8.622	934	941	952	rBV2	486532	837522	7.18%	1.168%
7	9.086	1014	1020	1029	rBV	543120	910985	7.81%	1.271%
8	9.798	1134	1141	1150	rBV	521744	878363	7.53%	1.225%
9	10.333	1224	1232	1241	rBV	827699	1438586	12.33%	2.007%
10	10.704	1285	1295	1305	rBV	1349868	2327067	19.94%	3.246%
11	10.874	1314	1324	1334	rBV	523661	989932	8.48%	1.381%
12	12.451	1586	1592	1600	rBV5	145541	311217	2.67%	0.434%
13	13.368	1740	1748	1759	rBV2	376227	584065	5.01%	0.815%
14	13.904	1833	1839	1842	rBV2	149277	212297	1.82%	0.296%
15	13.951	1842	1847	1852	rVV	1674147	2310524	19.80%	3.223%
16	13.998	1852	1855	1861	rVB	532439	716398	6.14%	0.999%
17	14.239	1885	1896	1904	rBV	1700230	2801691	24.01%	3.909%
18	14.462	1925	1934	1940	rVB	1423416	1965772	16.85%	2.742%
19	14.539	1940	1947	1963	rBV2	2241314	3853791	33.03%	5.376%
20	14.751	1977	1983	1984	rBV3	142528	173806	1.49%	0.242%
21	14.780	1984	1988	1994	rVB2	622542	931491	7.98%	1.300%
22	15.533	2107	2116	2123	rBV	2304931	3384805	29.01%	4.722%
23	15.656	2132	2137	2142	rBV	657016	899735	7.71%	1.255%
24	15.839	2164	2168	2173	rVB5	147555	201069	1.72%	0.281%
25	15.986	2188	2193	2199	rVB	443985	614507	5.27%	0.857%
26	17.286	2407	2414	2424	rBV	3224259	4450057	38.14%	6.208%
27	17.386	2425	2431	2440	rVV	2646969	3612138	30.96%	5.039%
28	18.021	2531	2539	2542	rBV10	53510	120321	1.03%	0.168%
29	18.133	2553	2558	2567	rBV2	494015	713233	6.11%	0.995%
30	19.403	2770	2774	2781	rBV4	290691	416465	3.57%	0.581%
31	19.674	2814	2820	2826	rBV	3270614	4294894	36.81%	5.992%
32	20.015	2874	2878	2879	rBV2	224532	245566	2.10%	0.343%
33	20.039	2879	2882	2886	rVB	491126	567955	4.87%	0.792%
34	20.186	2903	2907	2913	rBV2	388187	609535	5.22%	0.850%

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35	20.827	3012	3016	3021	rBV	427192	519082	4.45%	0.724%
36	20.997	3040	3045	3050	rVB	10305383	11668915	100.00%	16.279%
37	21.450	3117	3122	3128	rBV	3907881	4910896	42.09%	6.851%
38	23.638	3489	3494	3505	rVB2	1875569	3563815	30.54%	4.972%
39	23.791	3515	3520	3529	rVB	2164908	4189124	35.90%	5.844%

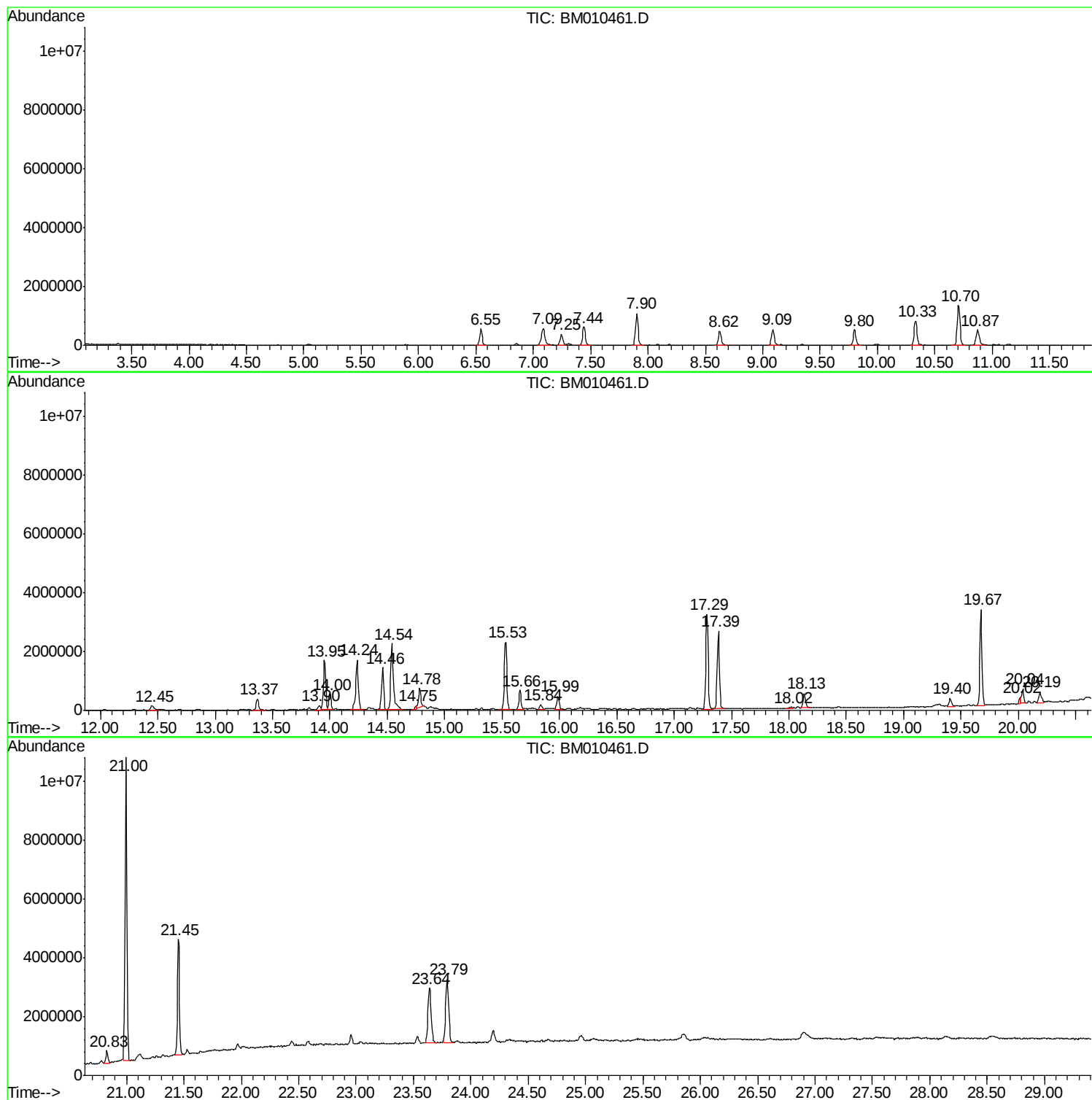
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Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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



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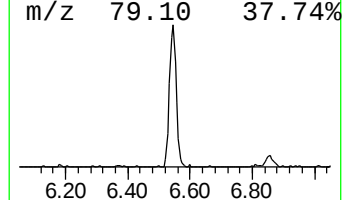
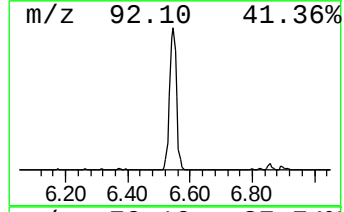
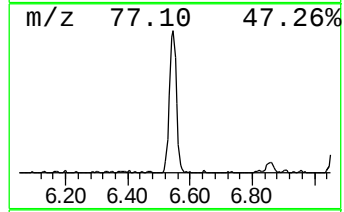
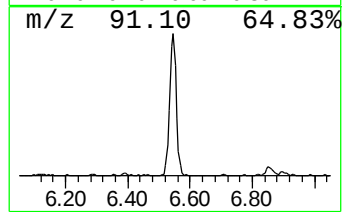
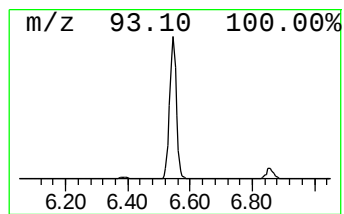
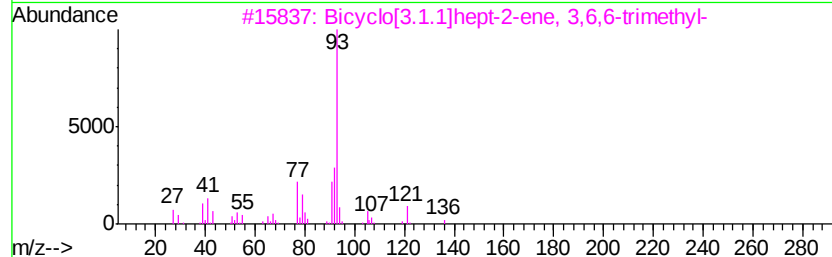
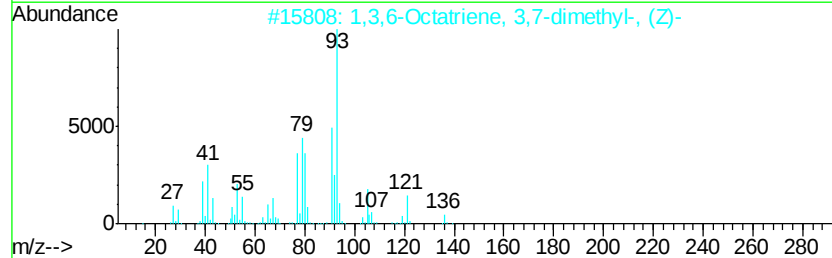
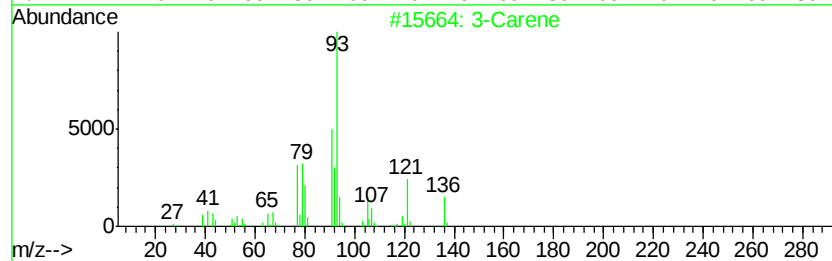
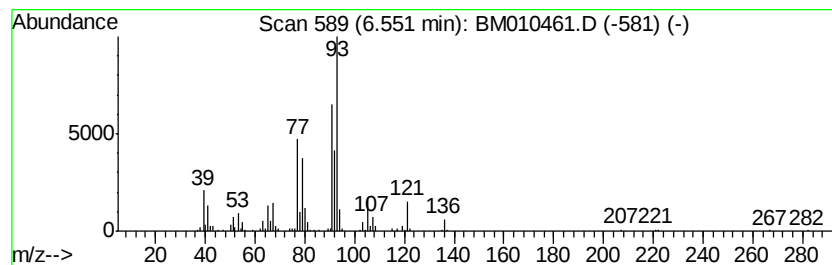
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Carene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	9.70 ng/ul	847680	1,4-Dichlorobenzene-d4	7.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	90
2			1,3,6-Octatriene, 3,7-dimethyl-, ...	136	C10H16	003338-55-4	87
3			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	87
4			trans-.beta.-Ocimene	136	C10H16	003779-61-1	83
5			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	81



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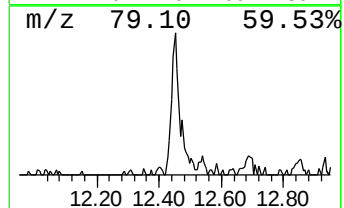
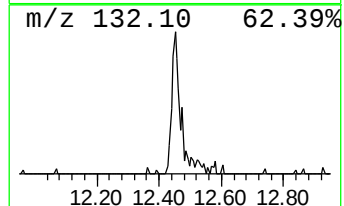
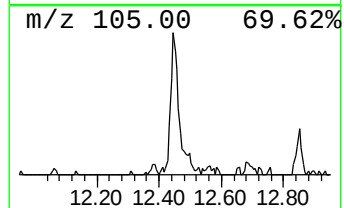
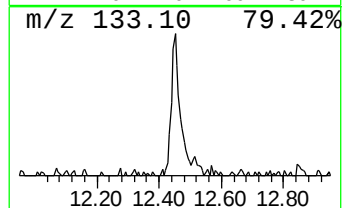
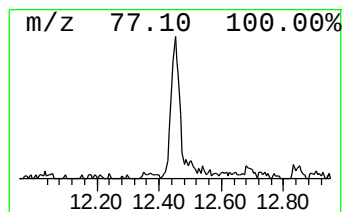
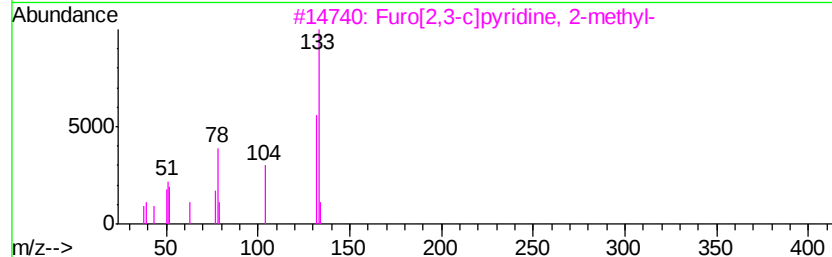
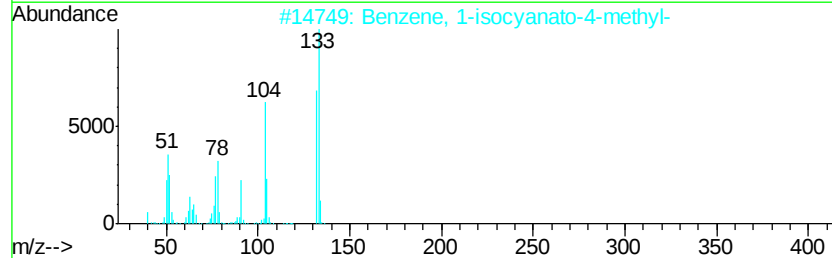
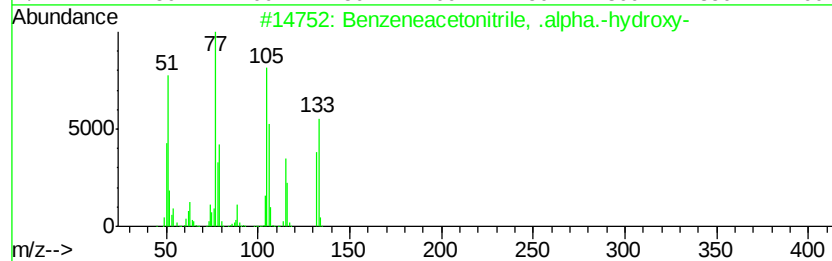
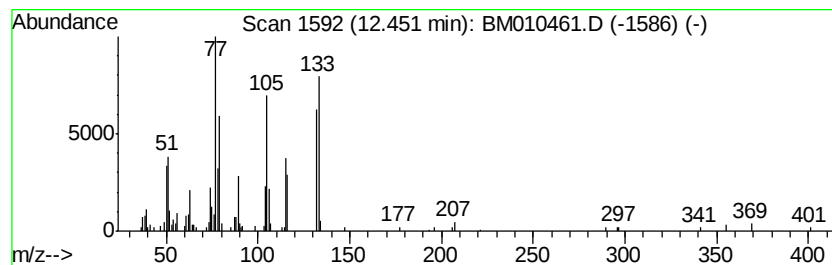
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Peak Number 2 Benzeneacetonitrile, .alpha... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	2.67 ng/ul	311217	Napthalene-d8	10.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetonitrile, .alpha.-hyd...	133	C8H7NO	000532-28-5	64
2		Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	38
3		Furo[2,3-c]pyridine, 2-methyl-	133	C8H7NO	069022-76-0	35
4		Benzyl isocyanate	133	C8H7NO	003173-56-6	25
5		1H-Indazol-3-amine	133	C7H7N3	000874-05-5	25



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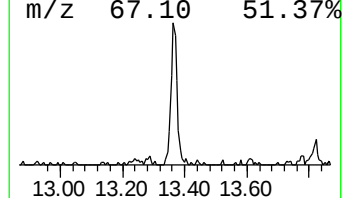
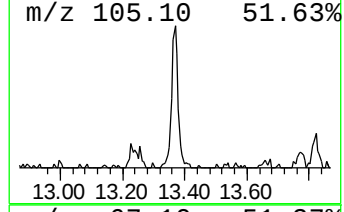
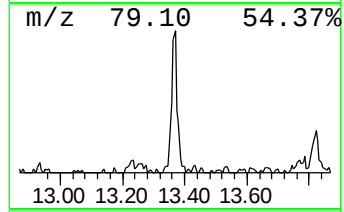
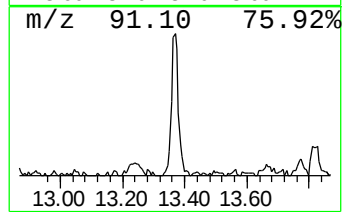
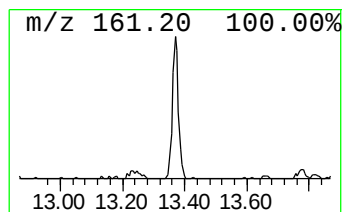
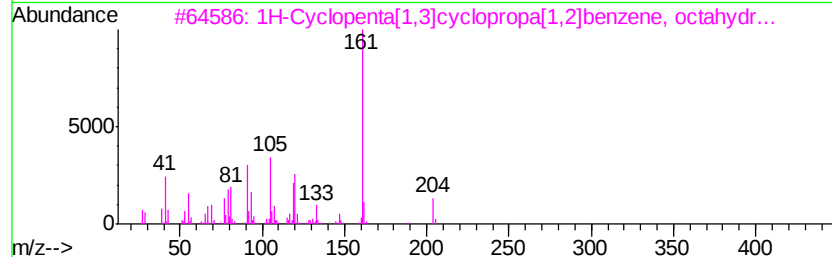
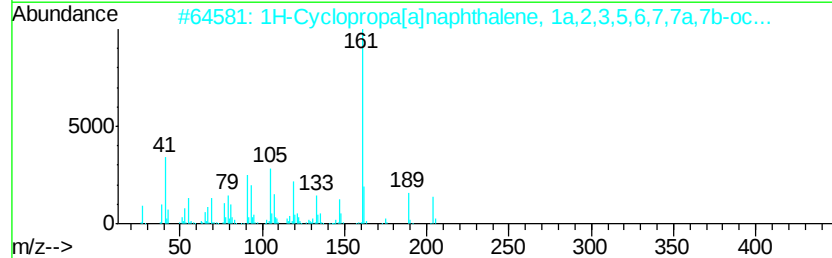
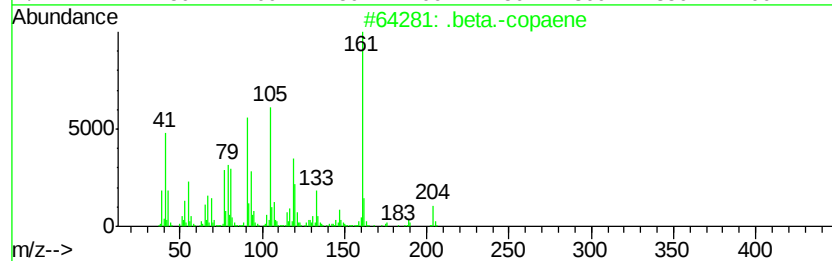
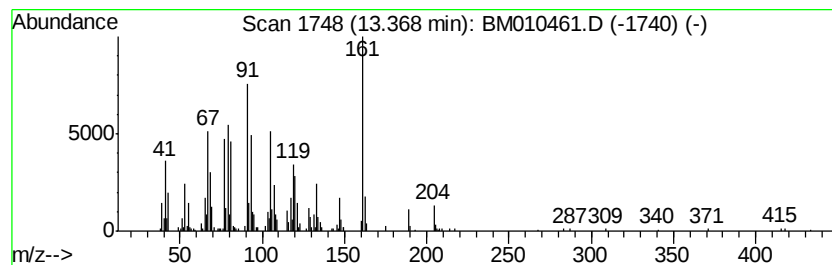
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 .beta.-copaene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	3.03 ng/ul	584065	Acenaphthene-d10	14.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-copaene	204 C15H24	1000374-18-9 93
2		1H-Cyclopropa[a]naphthalene, 1a,...	204 C15H24	017334-55-3 70
3		1H-Cyclopenta[1,3]cyclopropa[1,2]...	204 C15H24	013744-15-5 64
4		1H-Cyclopenta[1,3]cyclopropa[1,2]...	204 C15H24	013744-15-5 60
5		Alloaromadendrene	204 C15H24	025246-27-9 52



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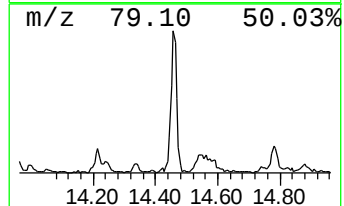
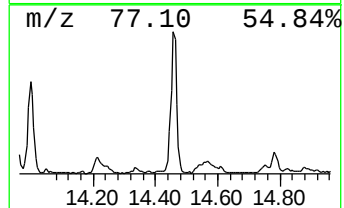
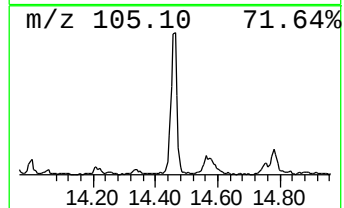
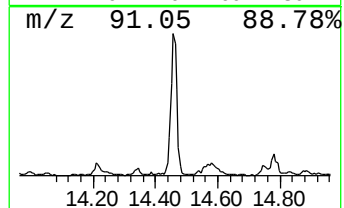
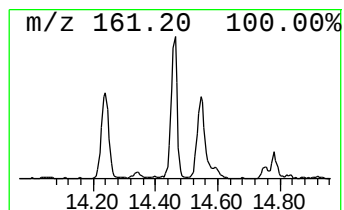
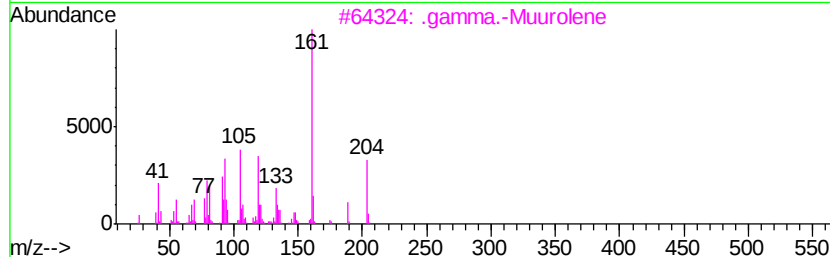
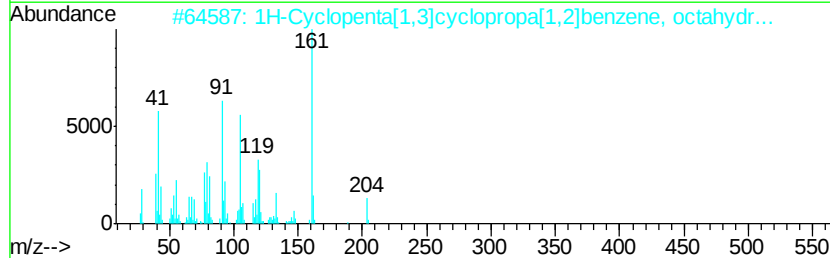
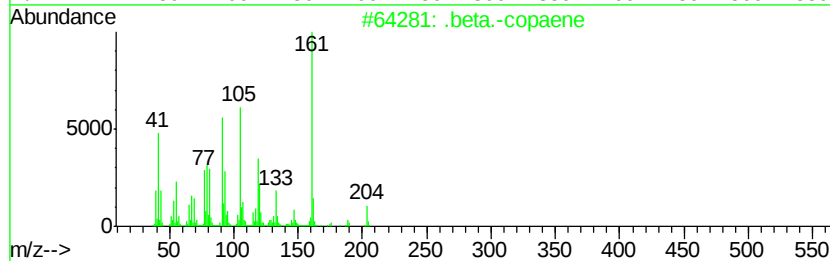
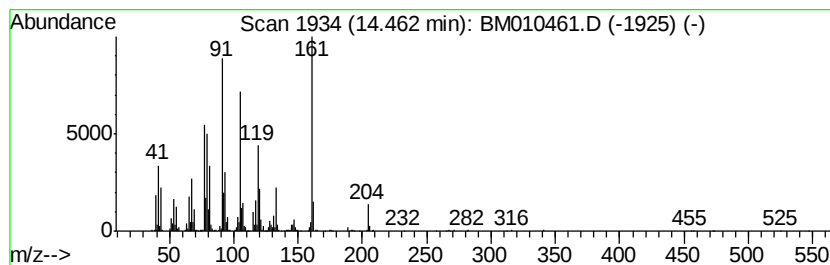
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Peak Number 4 1H-Cyclopenta[1,3]cycloprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	10.20 ng/ul	1965770	Acenaphthene-d10	14.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-copaene	204	C15H24	1000374-18-9	94
2		1H-Cyclopenta[1,3]cyclopropa[1,2]...	204	C15H24	013744-15-5	70
3		.gamma.-Muurolene	204	C15H24	030021-74-0	58
4		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	58
5		(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	55



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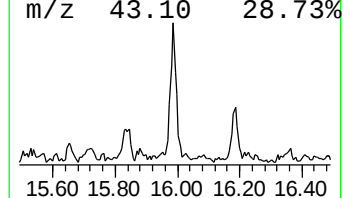
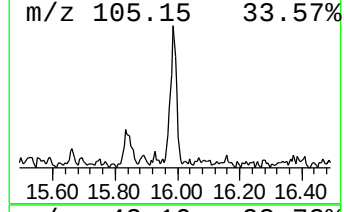
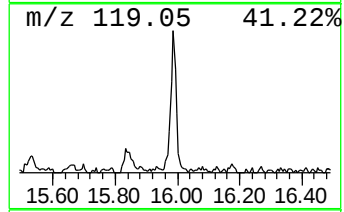
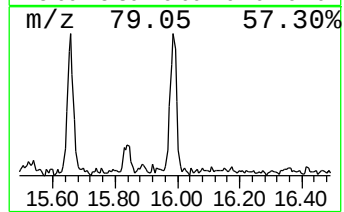
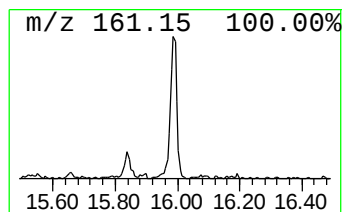
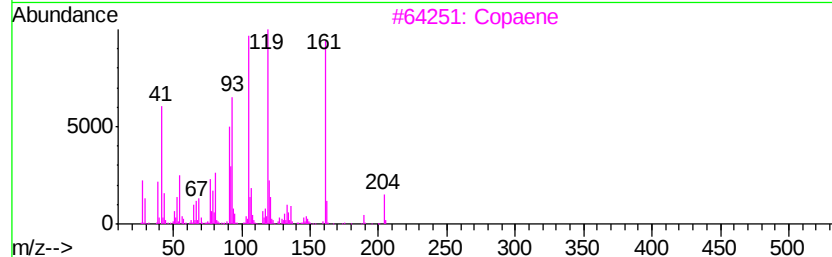
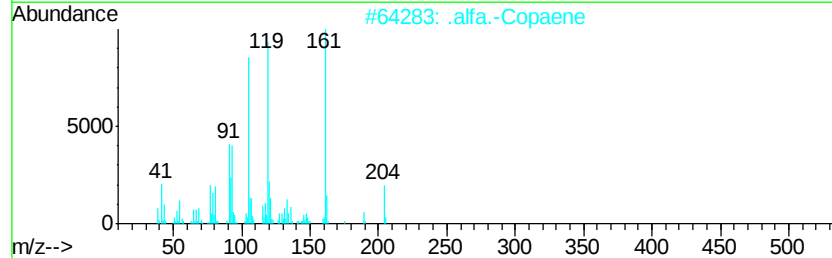
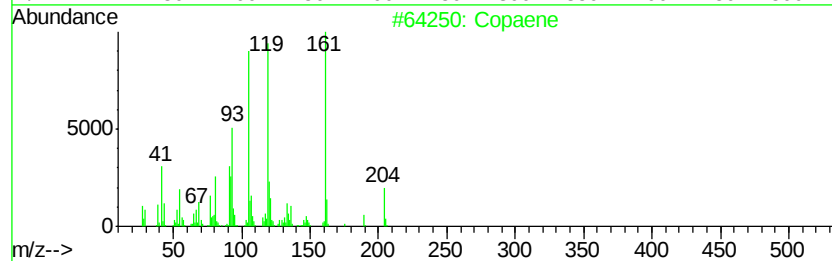
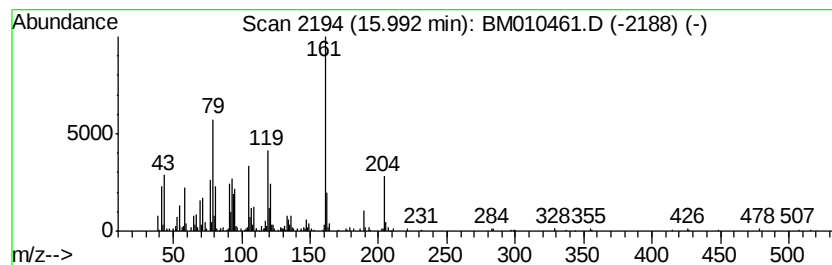
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Peak Number 5 Copaene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.76 ng/ul	614507	Phenanthrene-d10	17.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Copaene		204	C15H24	003856-25-5	91
2	.alfa.-Copaene		204	C15H24	1000360-33-0	91
3	Copaene		204	C15H24	003856-25-5	90
4	.alpha.-Cubebene		204	C15H24	017699-14-8	78
5	Isoledene		204	C15H24	1000156-10-8	64



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010461.D
Acq On : 09 Jun 2017 19:40
Operator : SJ/MA
Sample : I3520-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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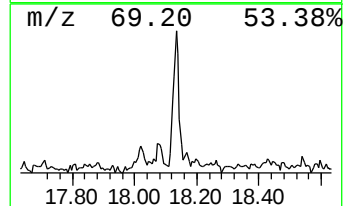
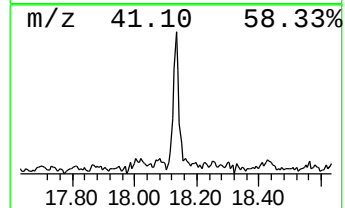
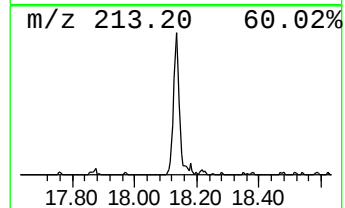
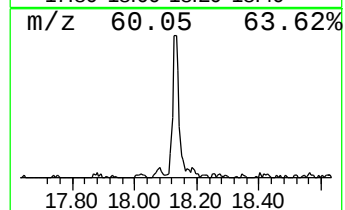
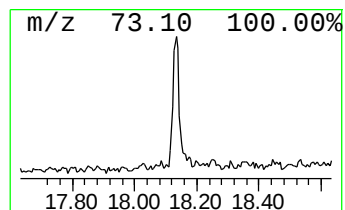
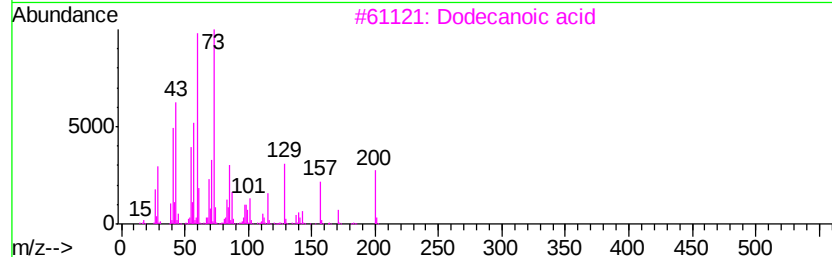
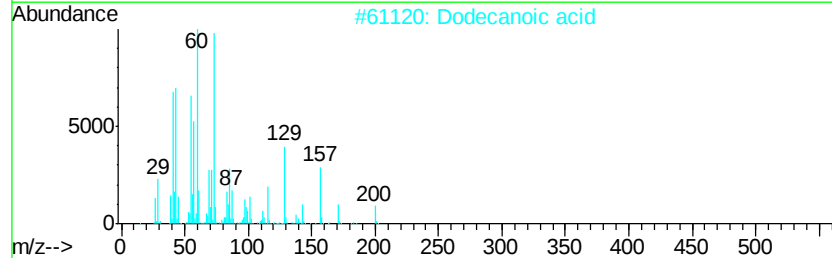
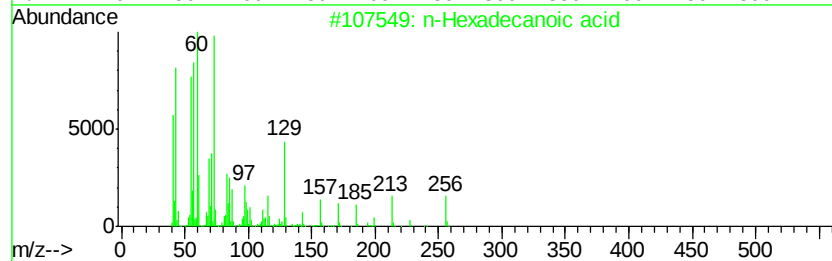
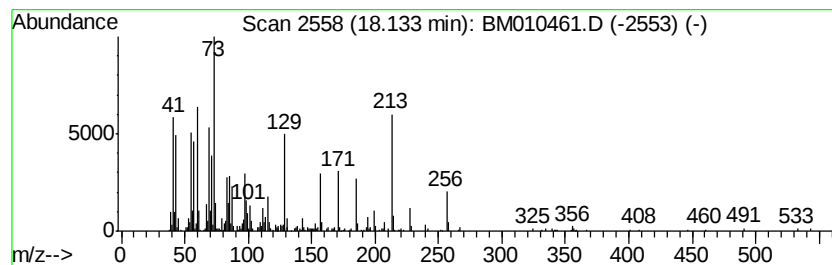
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	3.21 ng/ul	713233	Phenanthrene-d10	17.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2			Dodecanoic acid	200	C12H24O2	000143-07-7	50
3			Dodecanoic acid	200	C12H24O2	000143-07-7	43
4			Tridecanoic acid	214	C13H26O2	000638-53-9	43
5			Octadecanoic acid	284	C18H36O2	000057-11-4	41



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010461.D
Acq On : 09 Jun 2017 19:40
Operator : SJ/MA
Sample : I3520-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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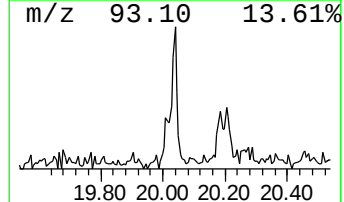
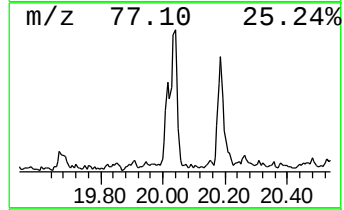
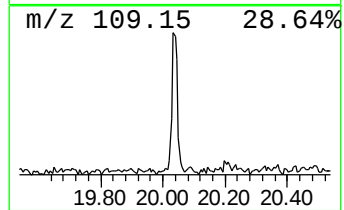
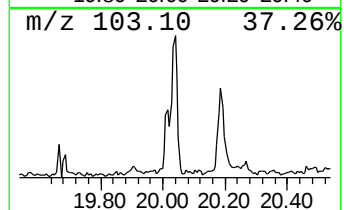
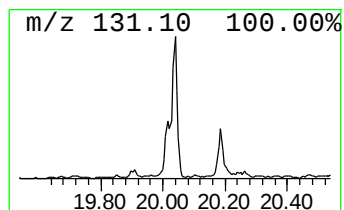
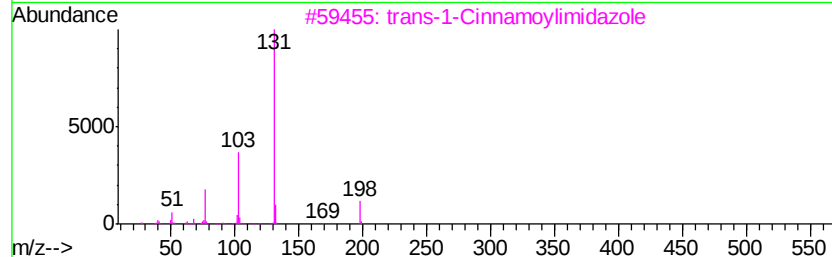
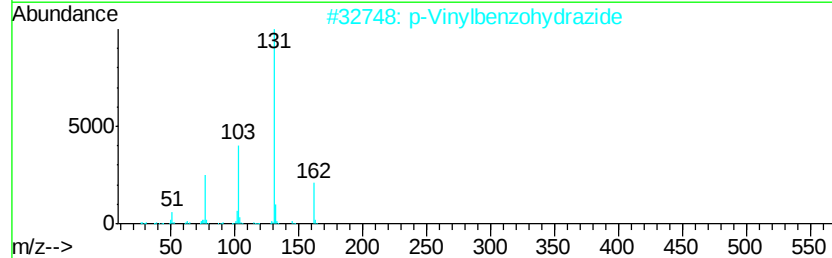
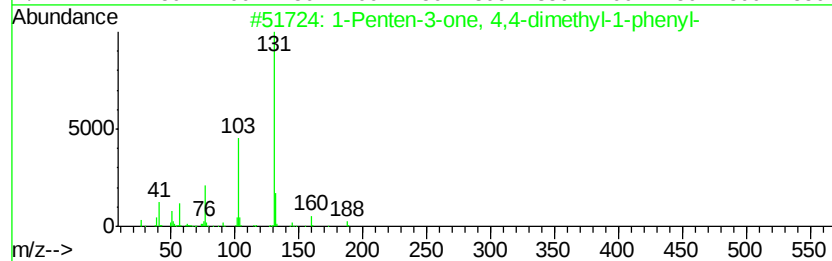
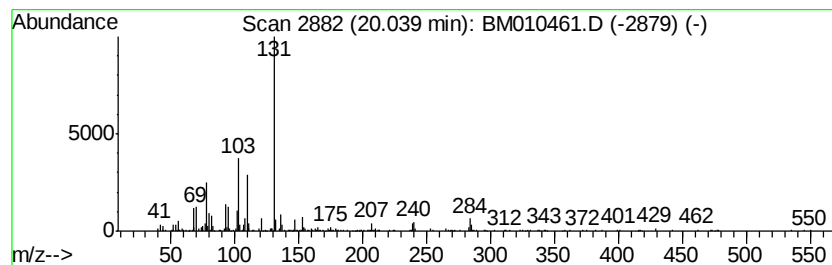
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Penten-3-one, 4,4-dimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.04	2.31 ng/ul	567955	Chrysene-d12	21.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	53
2		p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	53
3		trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	53
4		4-Chloro-3-cinnamylideneaminoben...	285	C16H12ClN02	1000254-94-5	47
5		Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	42



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010461.D
Acq On : 09 Jun 2017 19:40
Operator : SJ/MA
Sample : I3520-09
Misc :
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ClientSampleId :
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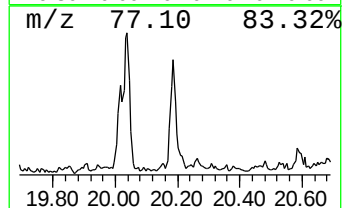
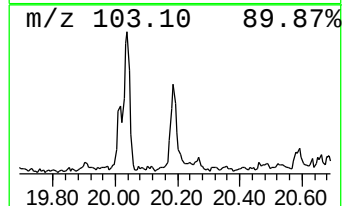
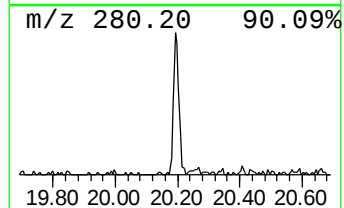
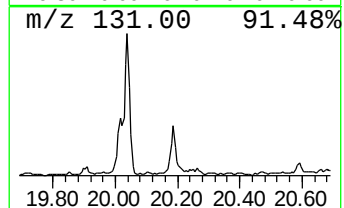
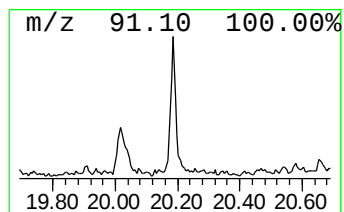
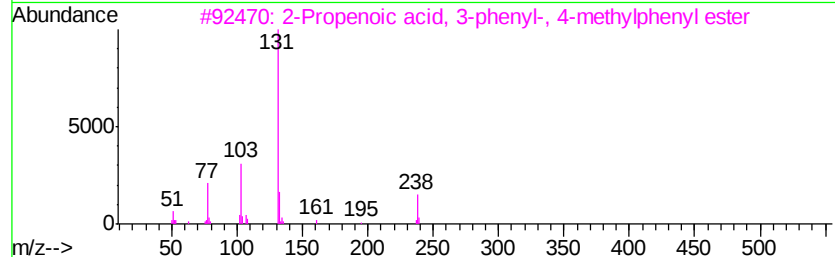
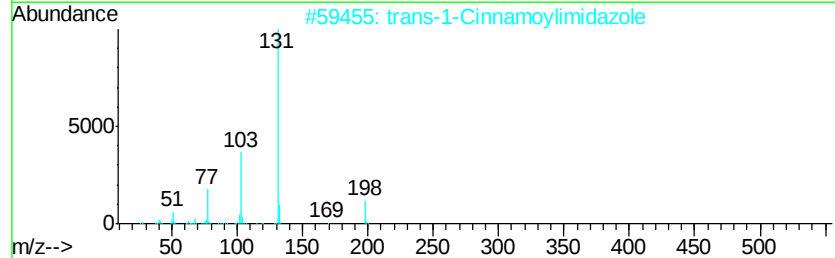
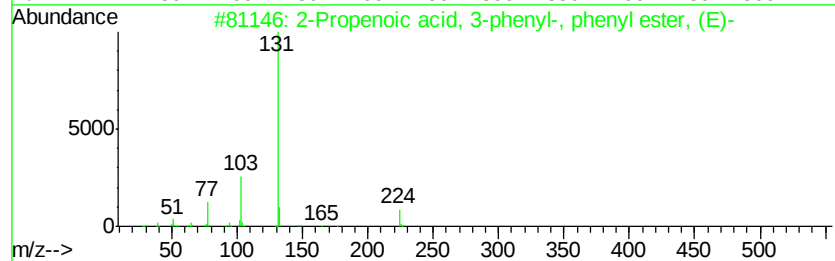
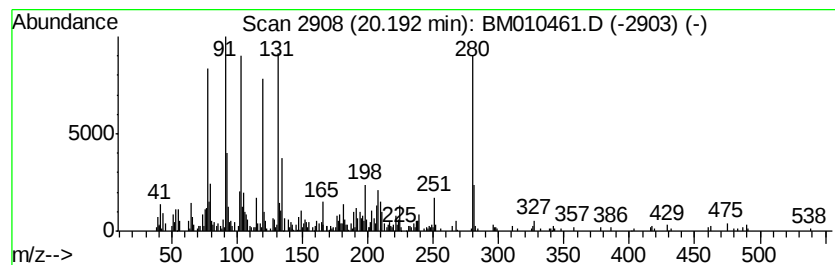
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 2-Propenoic acid, 3-phenyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.19	2.48 ng/ul	609535	Chrysene-d12	21.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	60
2		trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	58
3		2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	47
4		Oxalic acid, monoamide monohydra...	323	C18H17N3O3	1000294-01-4	38
5		1-Penten-3-one, 1-phenyl-	160	C11H12O	003152-68-9	32



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010461.D
Acq On : 09 Jun 2017 19:40
Operator : SJ/MA
Sample : I3520-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

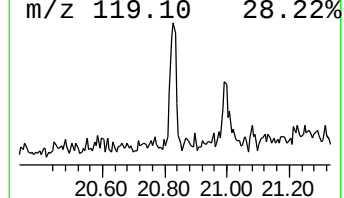
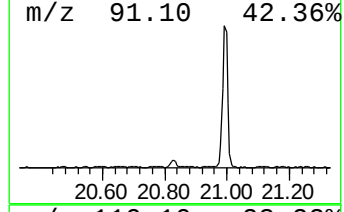
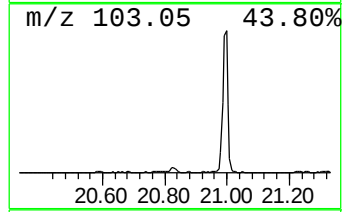
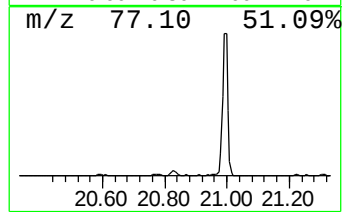
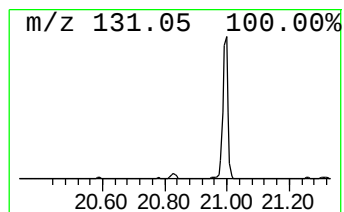
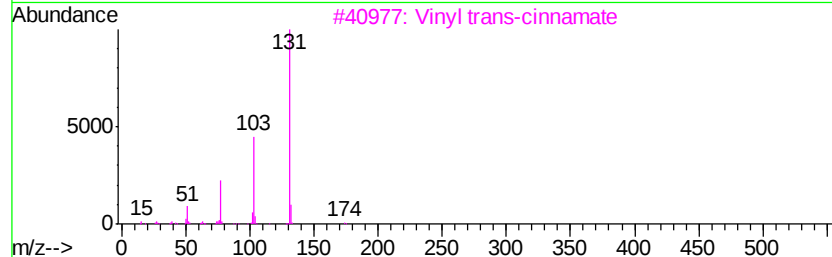
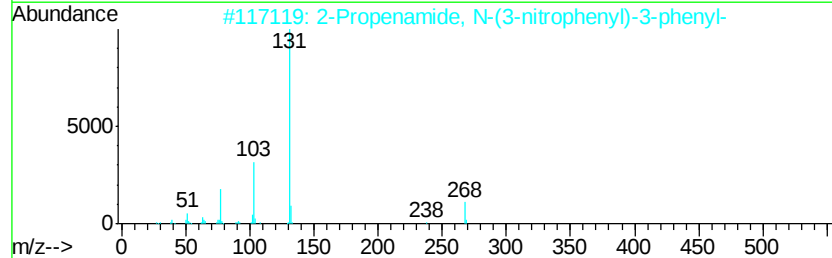
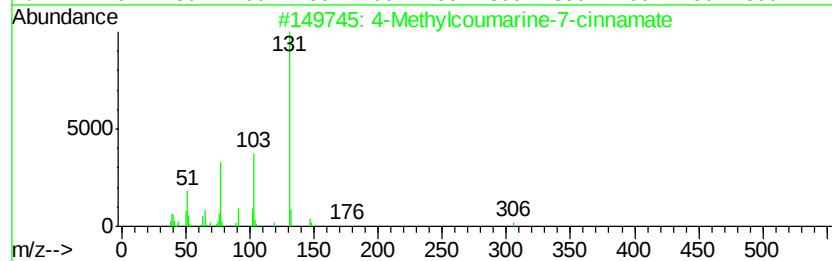
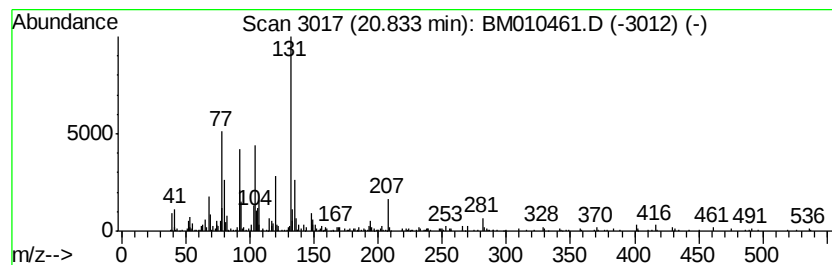
Instrument :
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Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 4-Methylcoumarine-7-cinnamate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.83	2.11 ng/ul	519082	Chrysene-d12	21.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	4-Methylcoumarine-7-cinnamate	306 C19H14O4	300829-05-4	53
2	2-Propenamide, N-(3-nitrophenyl)...	268 C15H12N2O3	055000-38-9	50
3	Vinyl trans-cinnamate	174 C11H10O2	017719-70-9	50
4	1-Penten-3-one, 4-methyl-1-phenyl-	174 C12H14O	003160-32-5	50
5	1,3-Phenylene, bis(3-phenylprope...	370 C24H18O4	1000259-62-4	50



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
Data File : BM010461.D
Acq On : 09 Jun 2017 19:40
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Sample : I3520-09
Misc :
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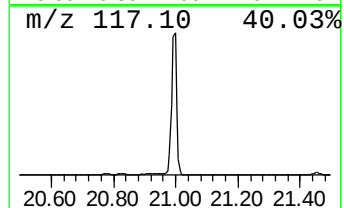
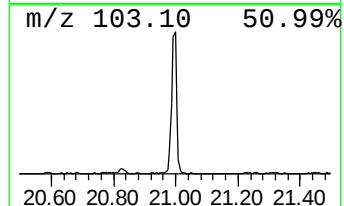
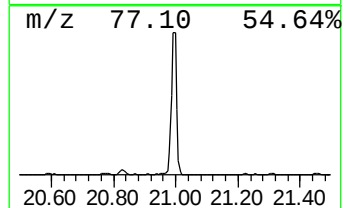
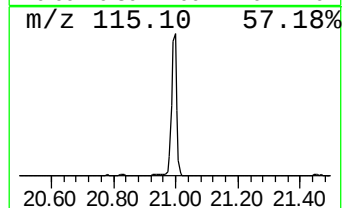
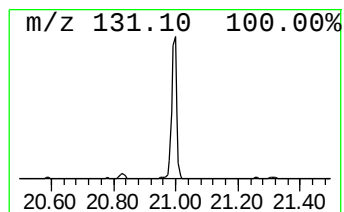
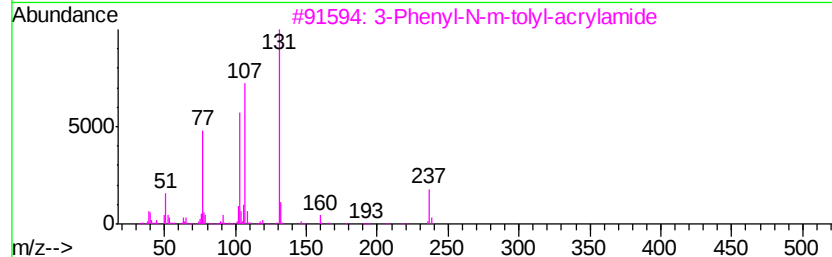
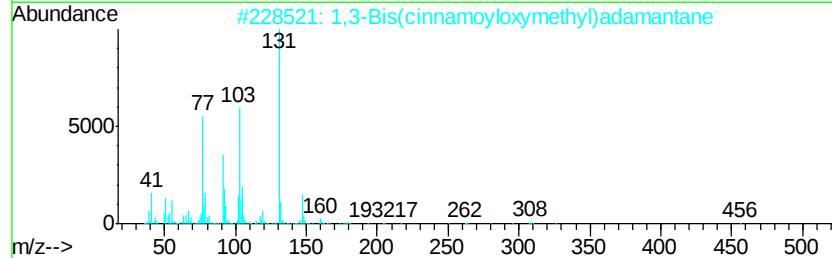
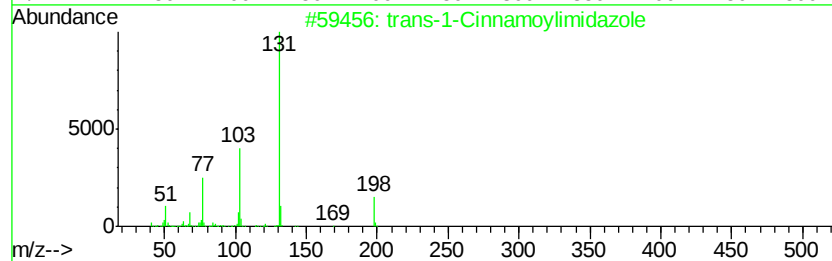
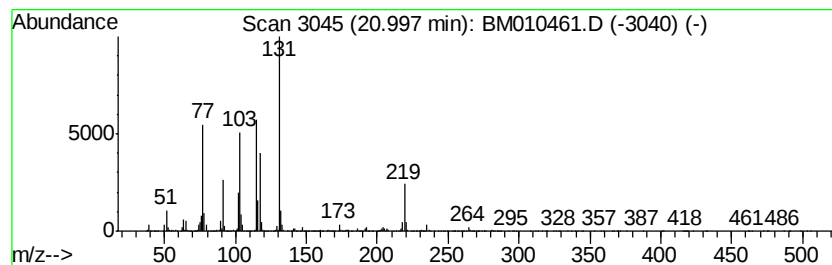
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	47.52 ng/ul	11668900	Chrysene-d12	21.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
2		1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	47
3		3-Phenyl-N-m-tolyl-acrylamide	237	C16H15NO	1000296-12-9	43
4		p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	43
5		1-Penten-3-one, 4-methyl-1-phenyl-	174	C12H14O	003160-32-5	38



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM060917\
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\Methods\SOM-EPA-BM052717.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
3-Carene	6.55	9.7	ng/ul	847680	1	7.90	1748000	20.0
Benzeneacetone...	12.45	2.7	ng/ul	311217	2	10.71	2327070	20.0
.beta.-copaene	13.37	3.0	ng/ul	584065	3	14.54	3853790	20.0
1H-Cyclopenta[1,3...	14.46	10.2	ng/ul	1965770	3	14.54	3853790	20.0
Copaene	15.99	2.8	ng/ul	614507	4	17.29	4450060	20.0
n-Hexadecanoic acid	18.13	3.2	ng/ul	713233	4	17.29	4450060	20.0
1-Penten-3-one, 4...	20.04	2.3	ng/ul	567955	5	21.45	4910900	20.0
2-Propenoic acid, ...	20.19	2.5	ng/ul	609535	5	21.45	4910900	20.0
4-Methylcoumarine...	20.83	2.1	ng/ul	519082	5	21.45	4910900	20.0
unknown-01	21.00	47.5	ng/ul	11668900	5	21.45	4910900	20.0