

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
 Data File : BF097013.D
 Acq On : 25 Jul 2017 4:12
 Operator : SJ/JU
 Sample : I4360-03
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CEMETERY-12-(0-2)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % 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_F\METHODS\8270-BF071317.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.663	468	472	482	rBV	208851	306613	10.80%	1.263%
2	5.122	545	550	563	rBV	2533940	2743200	96.58%	11.297%
3	6.181	725	730	744	rBV	2623172	2840276	100.00%	11.696%
4	6.293	744	749	752	rBV	2744922	2634783	92.77%	10.850%
5	6.516	783	787	791	rBV	944271	810230	28.53%	3.337%
6	6.669	809	813	817	rBV	2024728	2019913	71.12%	8.318%
7	7.081	878	883	886	rBV	1754378	1720787	60.59%	7.086%
8	7.798	1001	1005	1008	rBV	1266420	1040795	36.64%	4.286%
9	8.875	1183	1188	1192	rBV	2645988	2532091	89.15%	10.427%
10	9.269	1252	1255	1259	rBV	211653	186882	6.58%	0.770%
11	9.545	1297	1302	1305	rBV	904321	876601	30.86%	3.610%
12	9.998	1376	1379	1382	rVB	58347	48129	1.69%	0.198%
13	10.216	1412	1416	1419	rBV2	23800	29741	1.05%	0.122%
14	10.328	1431	1435	1439	rBV	1218057	1117698	39.35%	4.603%
15	10.469	1456	1459	1465	rBV	78181	89159	3.14%	0.367%
16	10.916	1526	1535	1537	rBV3	40683	51192	1.80%	0.211%
17	11.016	1546	1552	1555	rBV	827635	696488	24.52%	2.868%
18	11.533	1637	1640	1644	rBV	71906	72660	2.56%	0.299%
19	11.575	1644	1647	1654	rVV2	226385	216258	7.61%	0.891%
20	12.222	1754	1757	1762	rBV	68733	66681	2.35%	0.275%
21	12.357	1777	1780	1786	rBV6	34770	49401	1.74%	0.203%
22	12.445	1791	1795	1801	rVV	114296	114456	4.03%	0.471%
23	12.604	1817	1822	1825	rBV	1721374	1663893	58.58%	6.852%
24	12.780	1849	1852	1856	rBV5	25423	34663	1.22%	0.143%
25	13.063	1898	1900	1906	rVB2	48594	79083	2.78%	0.326%
26	13.151	1912	1915	1917	rBV	29715	30507	1.07%	0.126%
27	13.516	1974	1977	1984	rVB	167392	205837	7.25%	0.848%
28	13.639	1994	1998	2002	rBV	710529	737252	25.96%	3.036%
29	14.145	2081	2084	2091	rBV	131487	205959	7.25%	0.848%
30	14.433	2131	2133	2136	rBV2	70355	75275	2.65%	0.310%
31	14.727	2180	2183	2185	rBV	151130	165564	5.83%	0.682%
32	14.998	2225	2229	2235	rBV	481256	587167	20.67%	2.418%
33	15.415	2297	2300	2304	rBV	196951	233912	8.24%	0.963%

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ALS Vial : 23 Sample Multiplier: 1

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BNA_F
ClientSampleId :
CEMETERY-12-(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

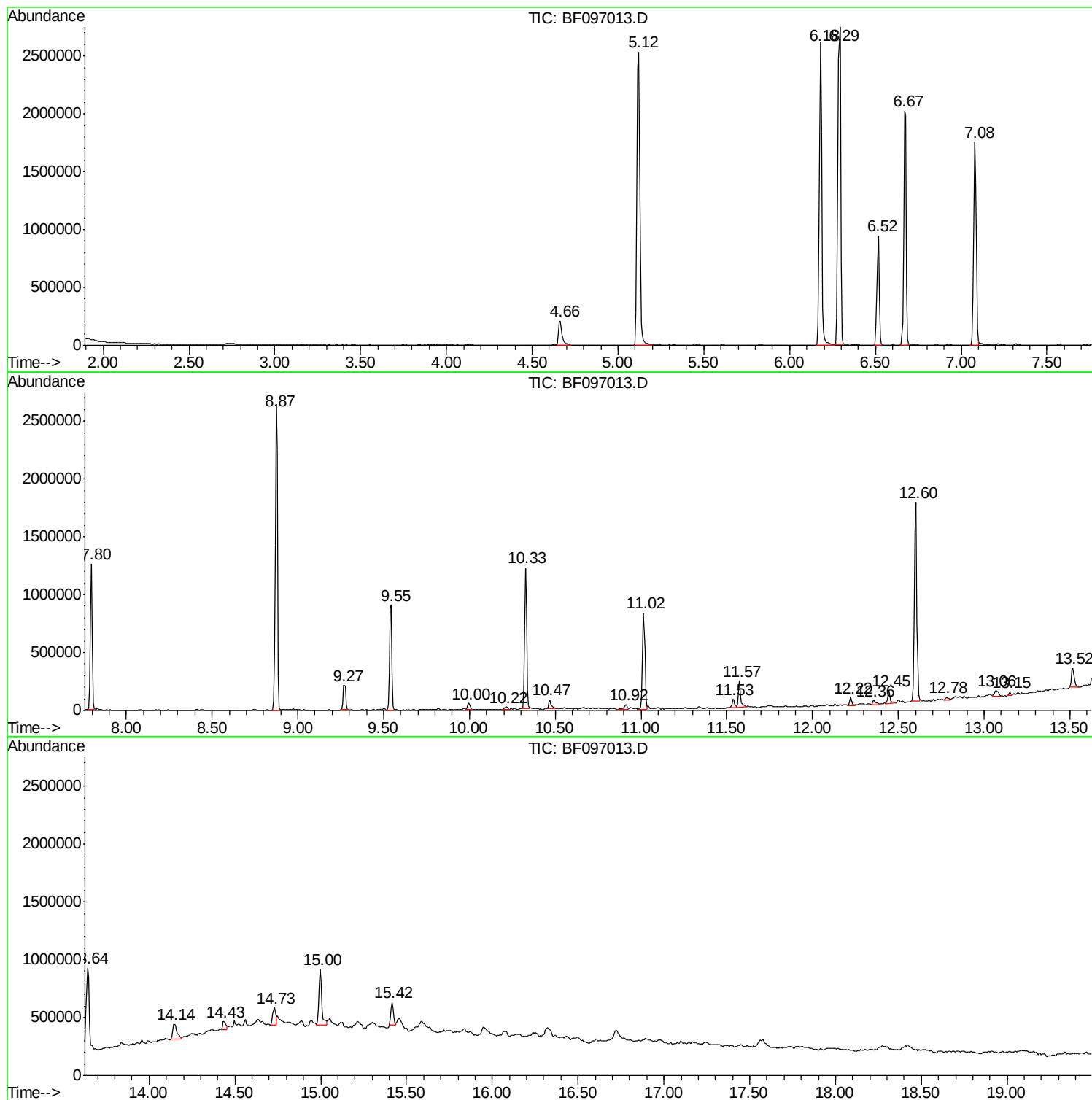
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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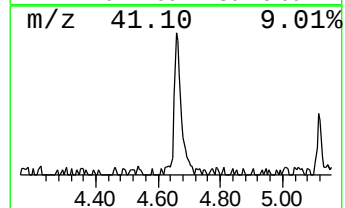
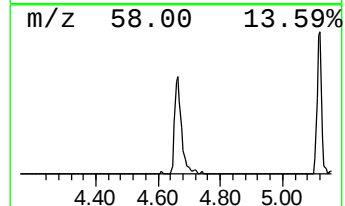
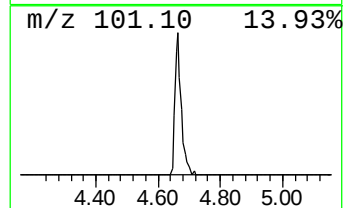
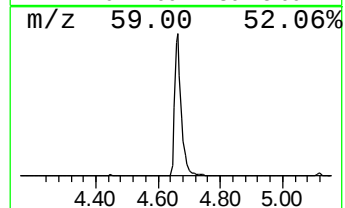
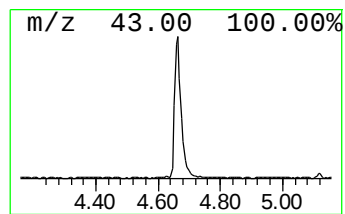
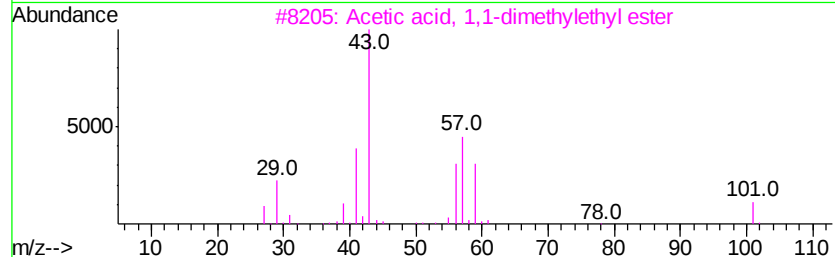
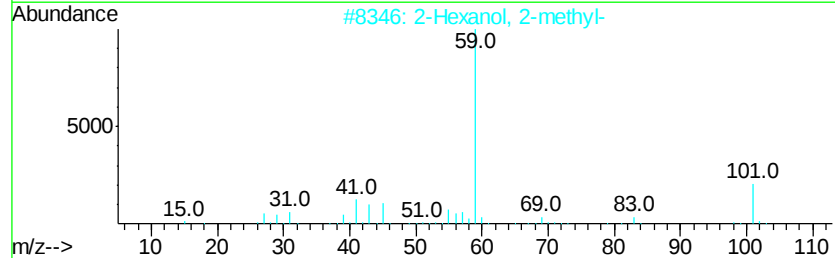
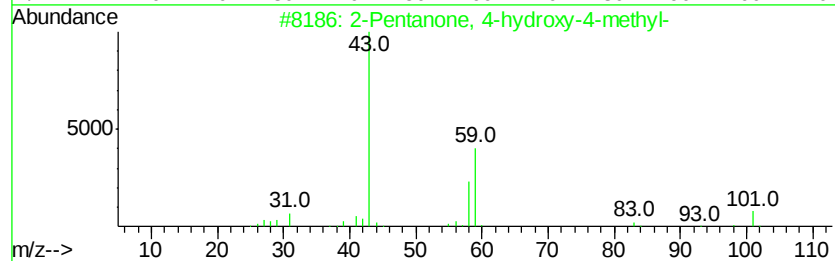
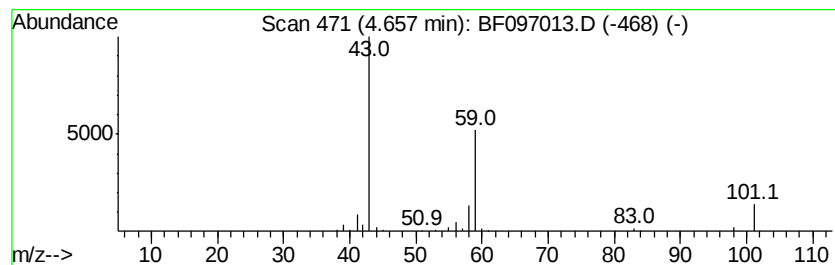
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	7.57 ng	306613	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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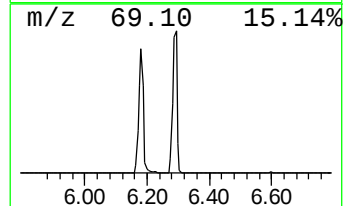
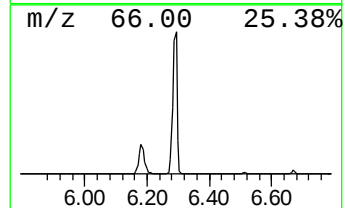
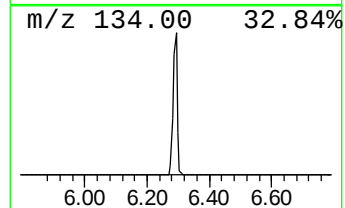
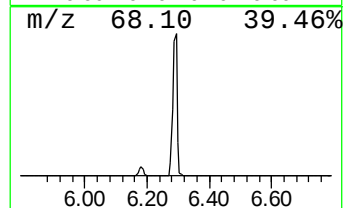
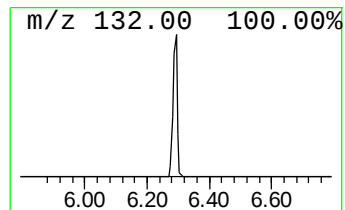
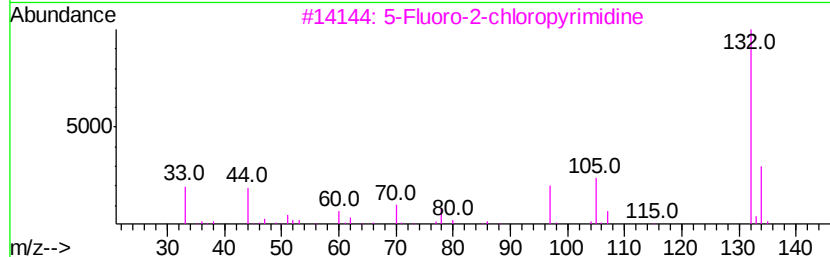
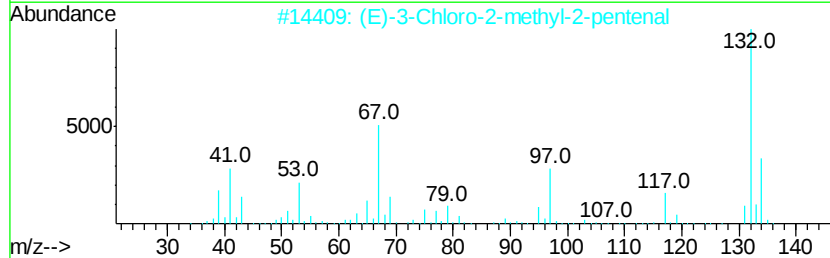
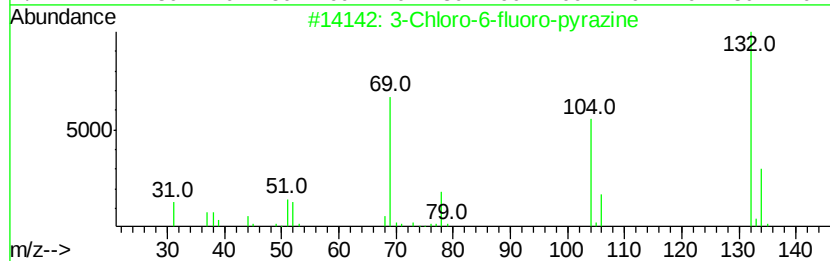
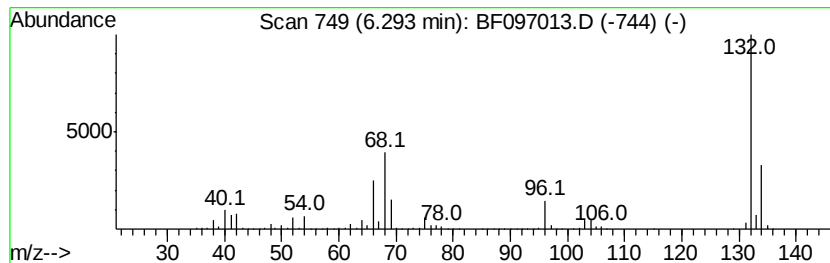
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	65.04 ng	2634780	1,4-Dichlorobenzene-d4	6.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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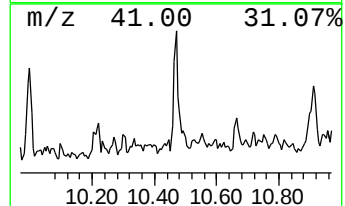
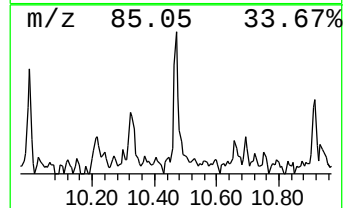
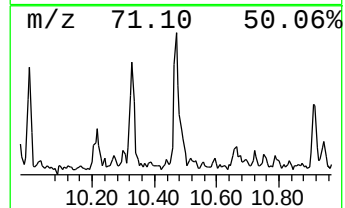
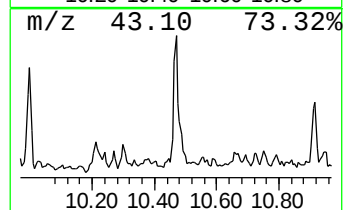
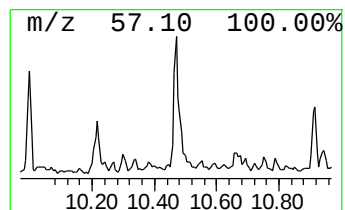
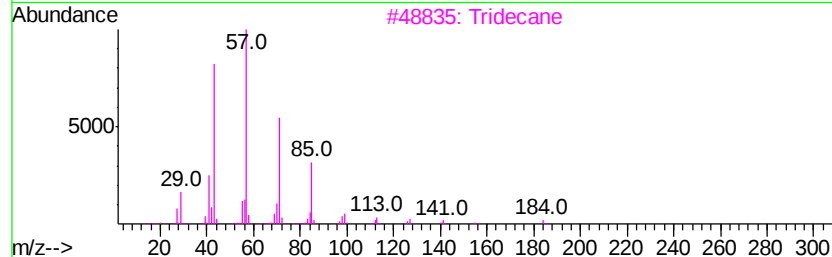
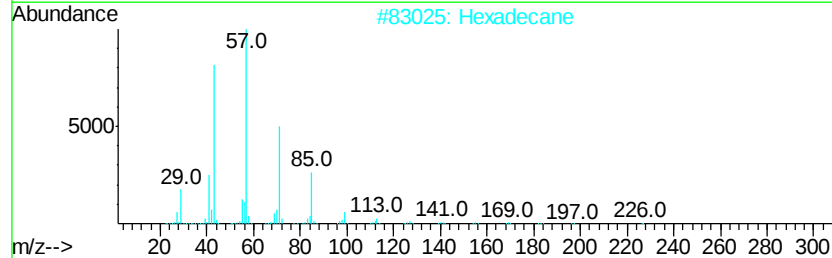
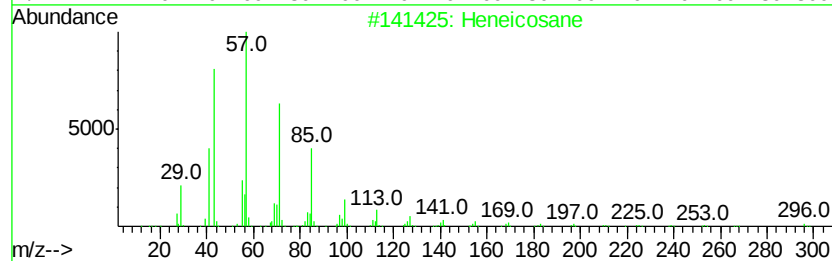
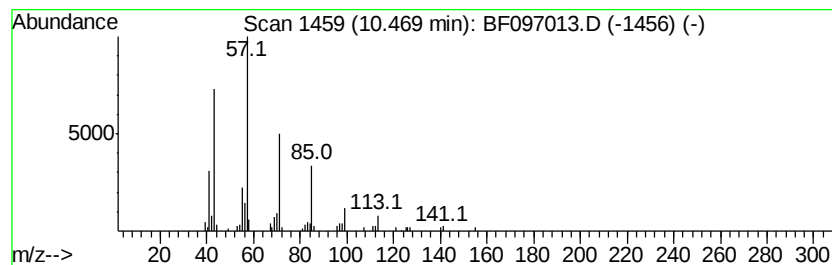
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.47	2.56 ng	89159	Phenanthrene-d10		11.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tridecane	184	C13H28	000629-50-5	64
4	Eicosane	282	C20H42	000112-95-8	64
5	Heptacosane	380	C27H56	000593-49-7	59



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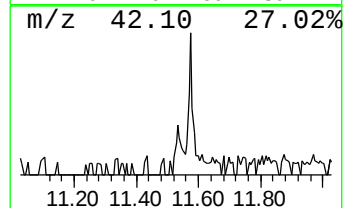
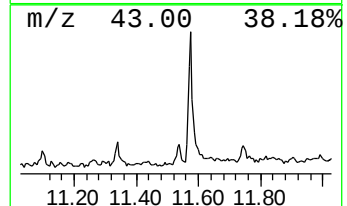
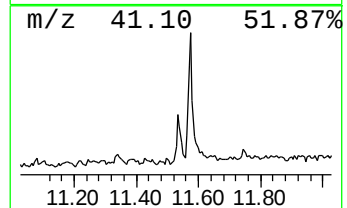
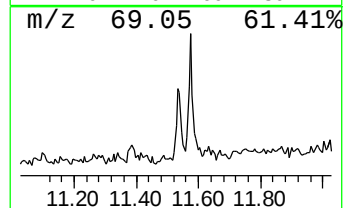
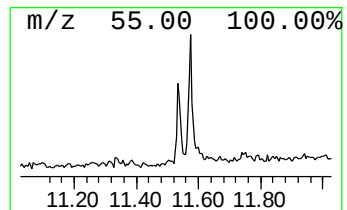
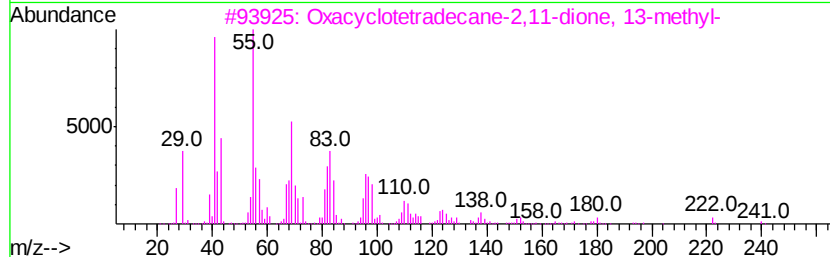
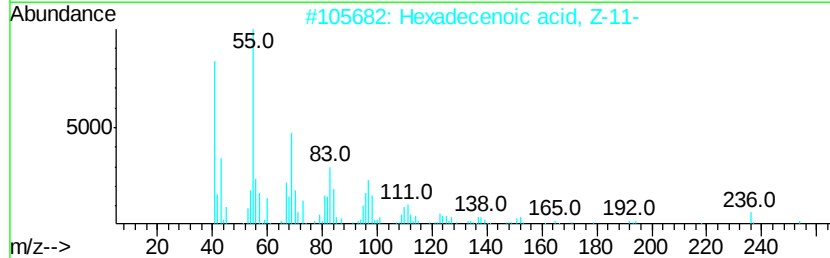
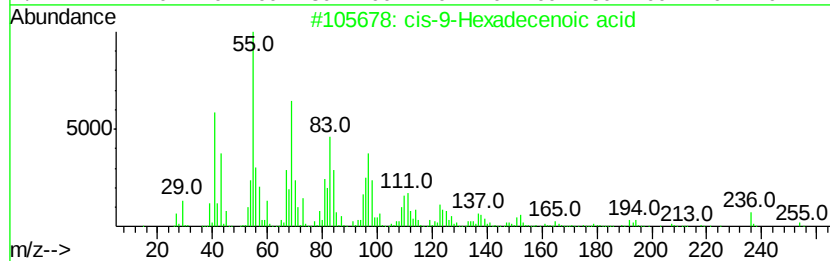
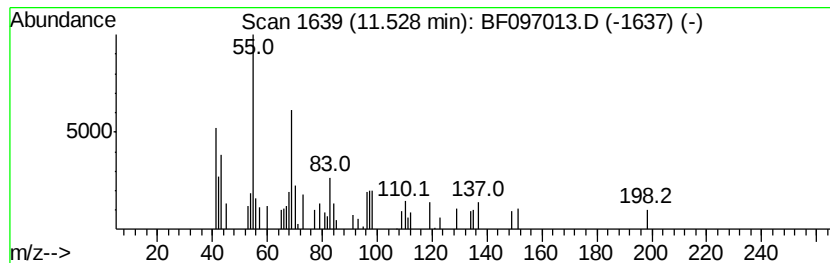
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 cis-9-Hexadecenoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.09 ng	72660	Phenanthrene-d10	11.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	87
2		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
3		Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	87
4		Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	80
5		Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	80



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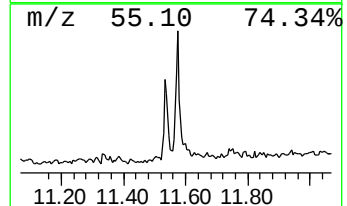
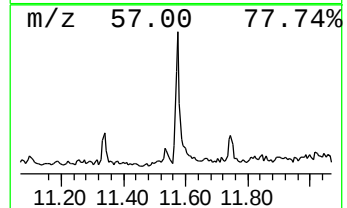
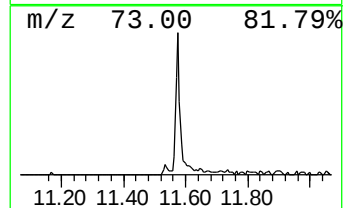
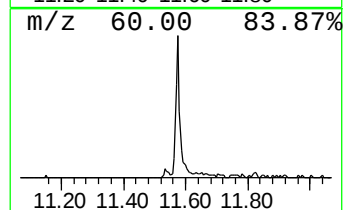
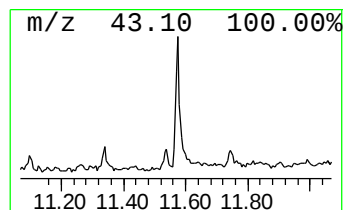
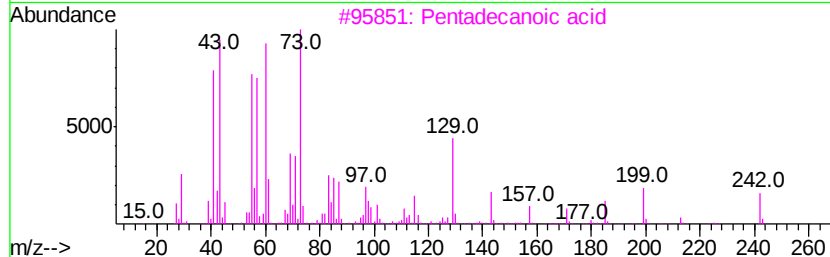
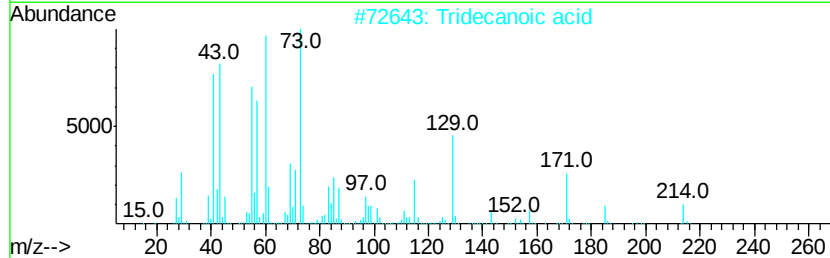
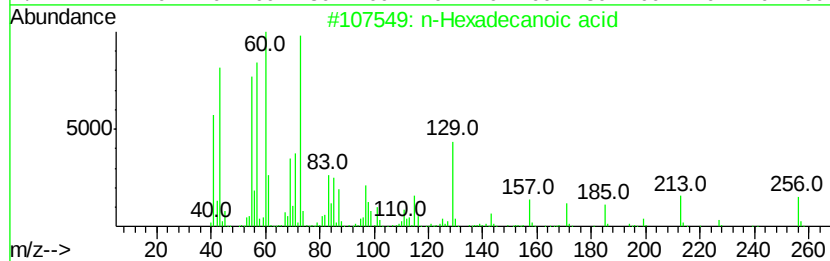
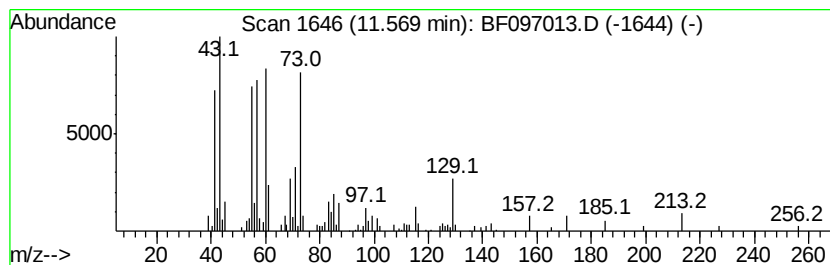
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	6.21 ng	216258	Phenanthrene-d10	11.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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CEMETERY-12-(0-2)

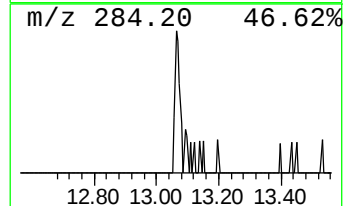
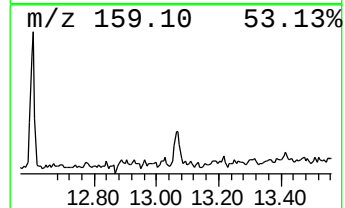
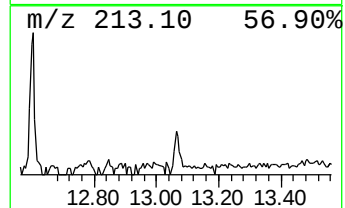
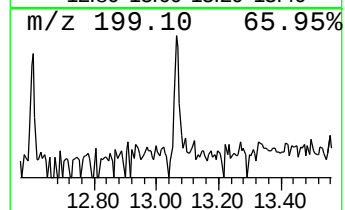
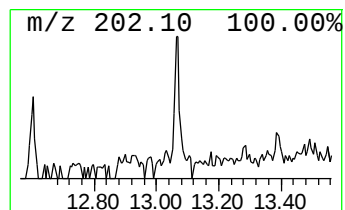
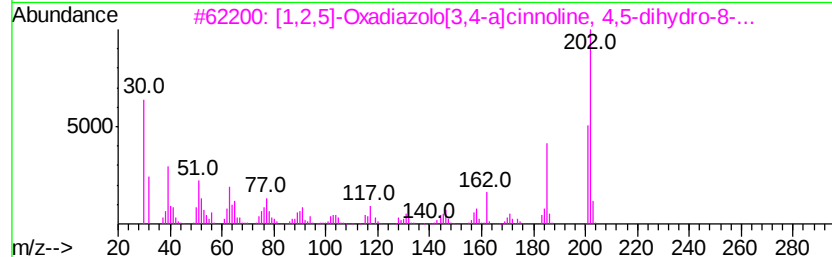
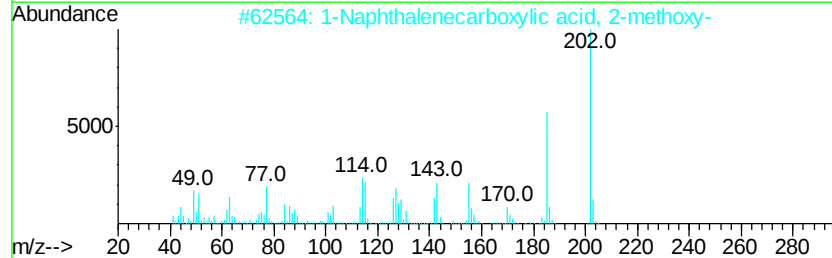
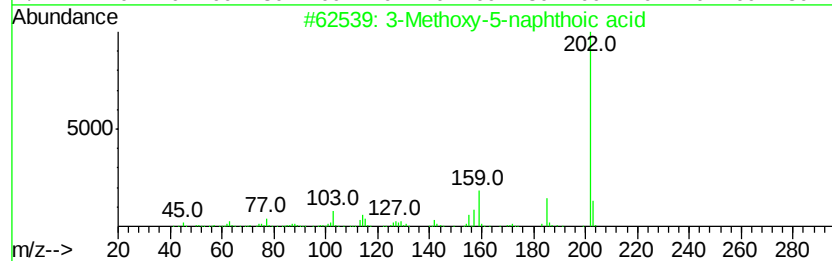
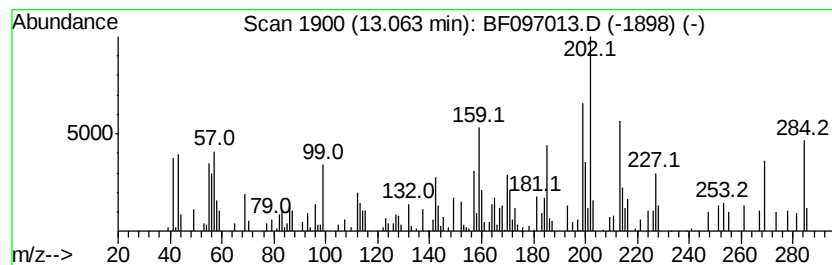
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.06 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	2.15 ng	79083	Chrysene-d12	13.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	41
2		1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	38
3		[1,2,5]-Oxadiazolo[3,4-a]cinnoli...	202	C10H10N4O	1000260-59-4	22
4		4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	14
5		5H-[1]Pyridine-4-carboxylic aci...	247	C12H13N3O3	1000302-65-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF097013.D
Acq On : 25 Jul 2017 4:12
Operator : SJ/JU
Sample : I4360-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

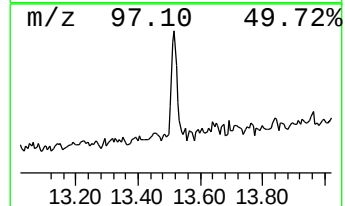
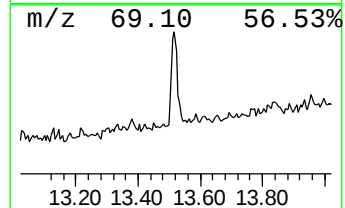
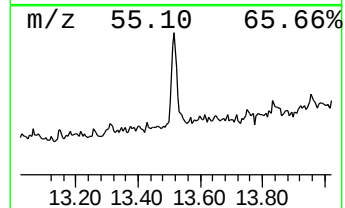
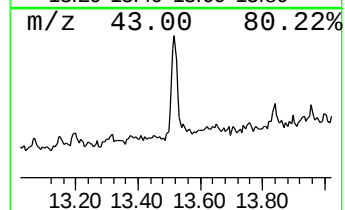
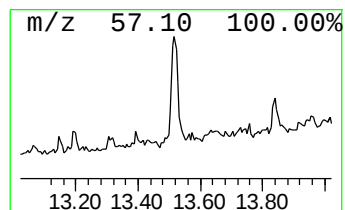
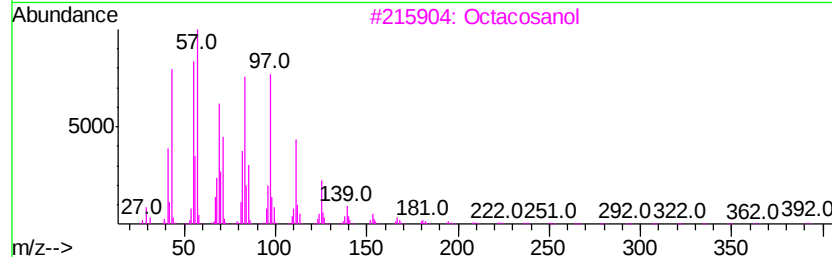
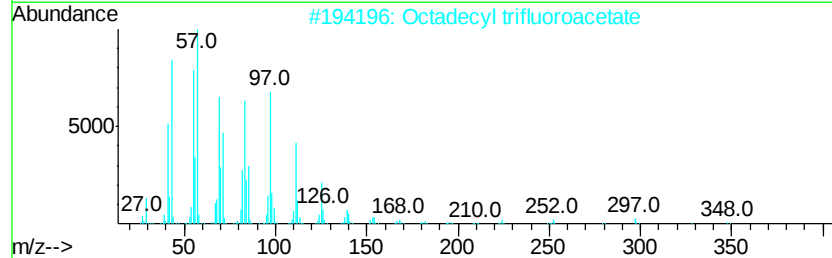
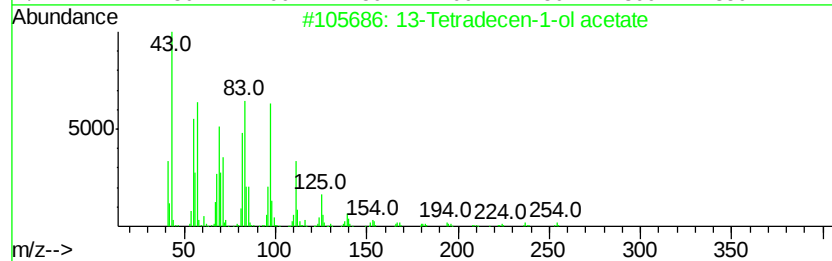
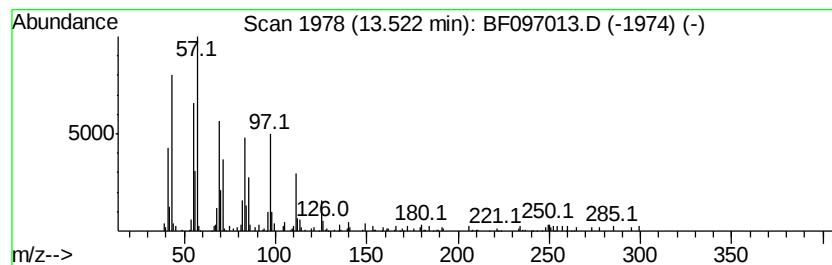
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Tetradecen-1-ol acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.52	5.58 ng	205837	Chrysene-d12		13.64
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Octacosanol	410	C28H58O	000557-61-9	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF097013.D
Acq On : 25 Jul 2017 4:12
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Instrument :
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ClientSampleId :
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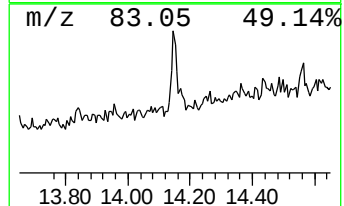
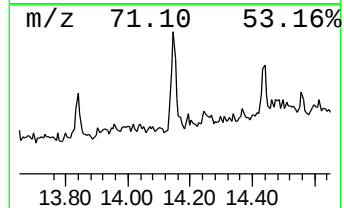
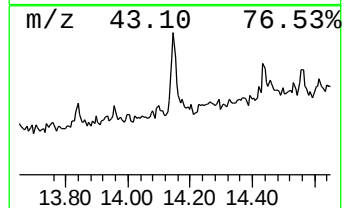
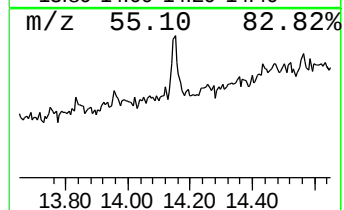
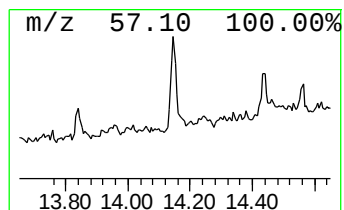
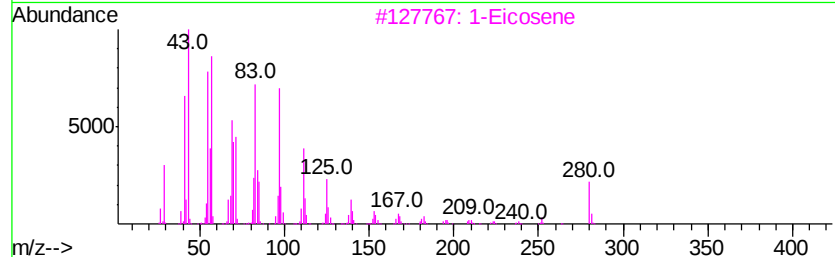
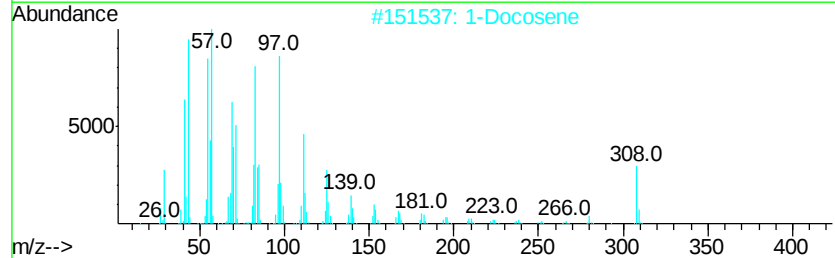
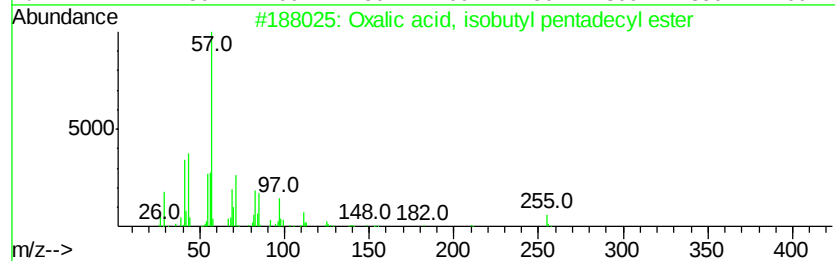
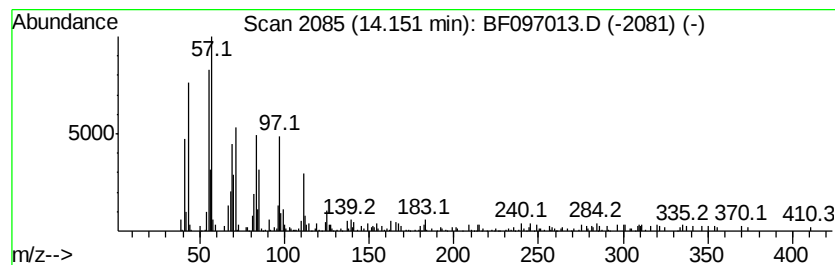
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, isobutyl penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	5.59 ng	205959	Chrysene-d12	13.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
2			1-Docosene	308	C22H44	001599-67-3	89
3			1-Eicosene	280	C20H40	003452-07-1	89
4			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	89
5			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF097013.D
Acq On : 25 Jul 2017 4:12
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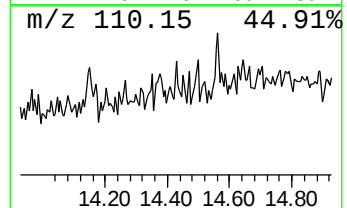
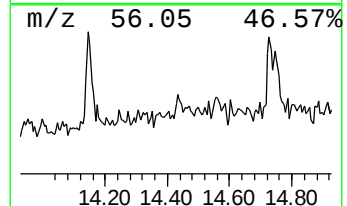
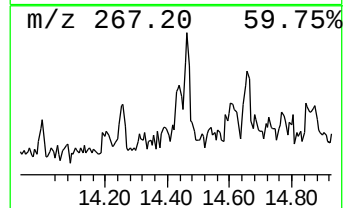
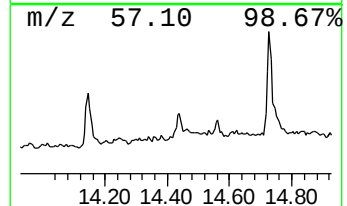
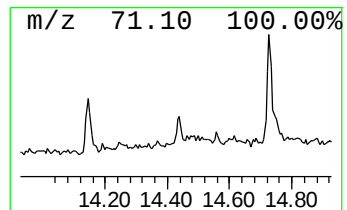
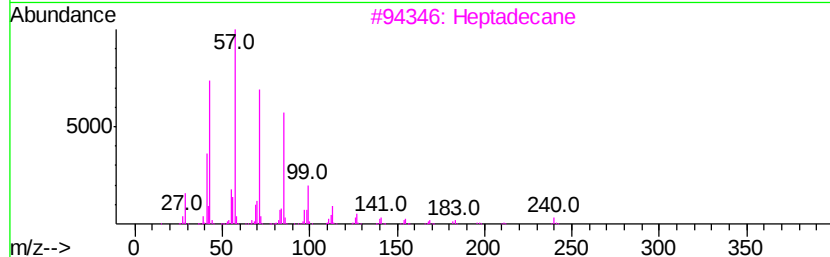
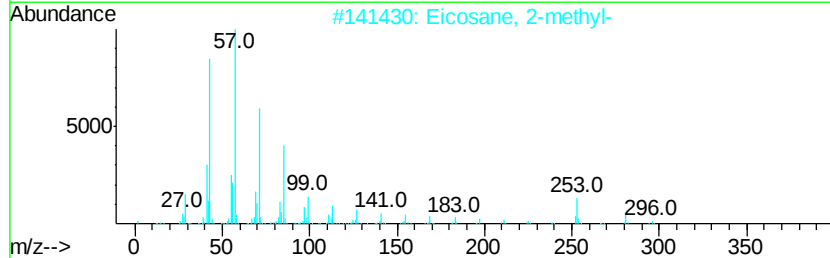
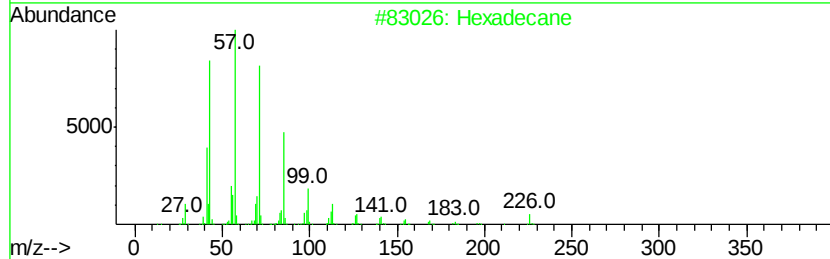
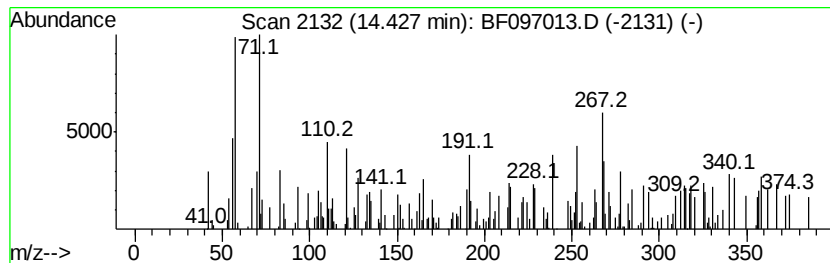
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.56 ng	75275	Perylene-d12	15.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	70
2	Eicosane, 2-methyl-	296 C21H44	001560-84-5	60
3	Heptadecane	240 C17H36	000629-78-7	49
4	Heneicosane	296 C21H44	000629-94-7	49
5	Dodecane, 2-methyl-	184 C13H28	001560-97-0	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF097013.D
Acq On : 25 Jul 2017 4:12
Operator : SJ/JU
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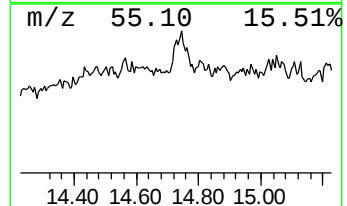
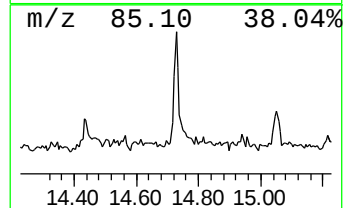
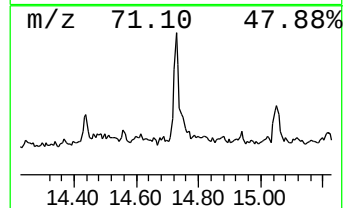
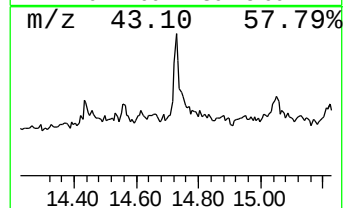
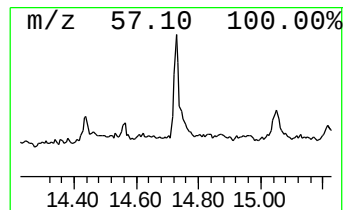
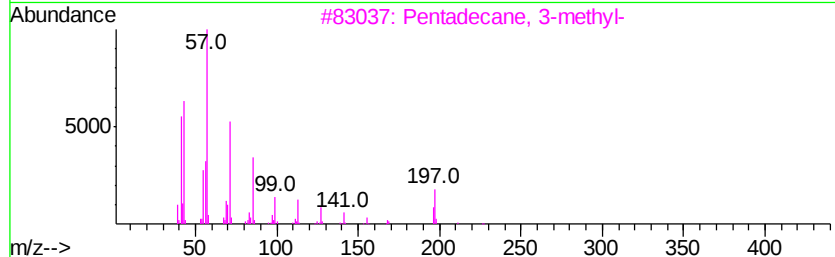
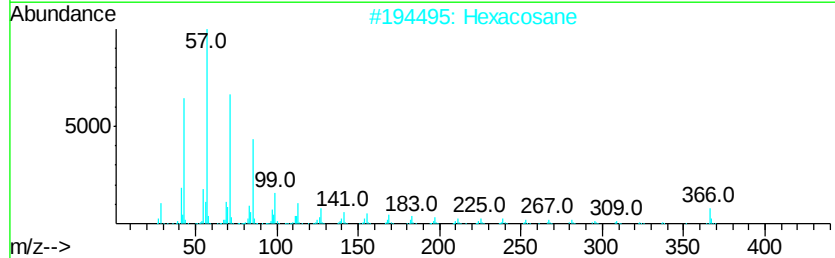
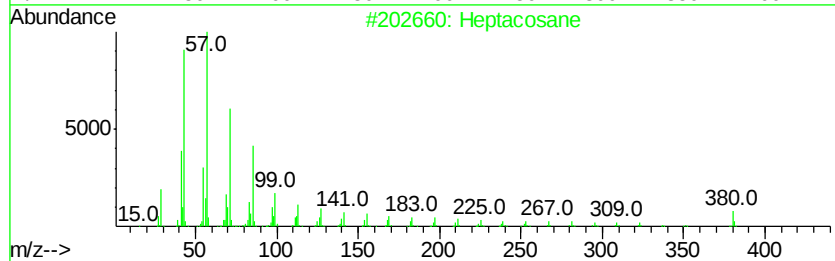
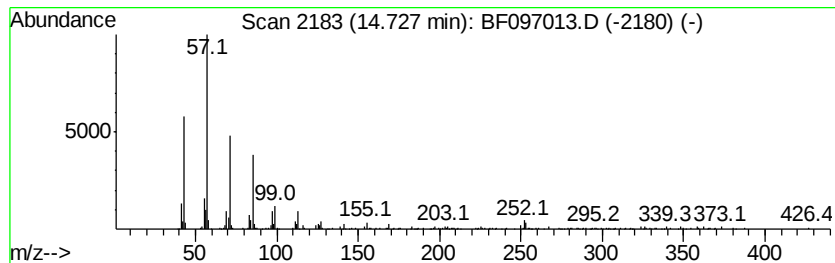
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	5.64 ng	165564	Perylene-d12	15.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Hexacosane	366	C26H54	000630-01-3	89
3			Pentadecane, 3-methyl-	226	C16H34	002882-96-4	83
4			Eicosane	282	C20H42	000112-95-8	83
5			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF097013.D
Acq On : 25 Jul 2017 4:12
Operator : SJ/JU
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ClientSampleId :
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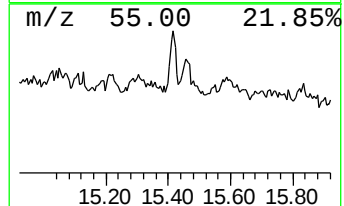
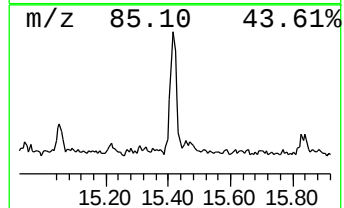
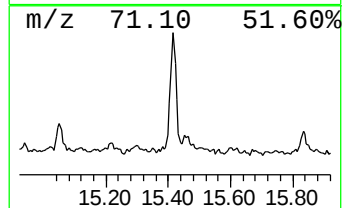
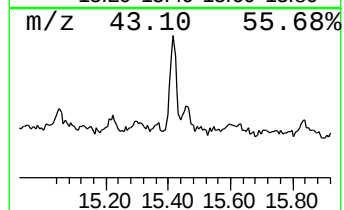
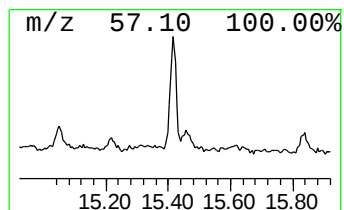
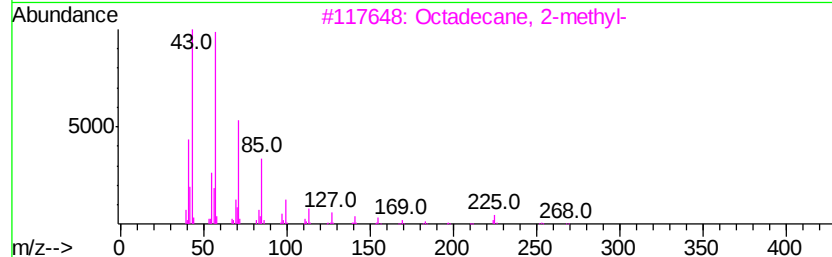
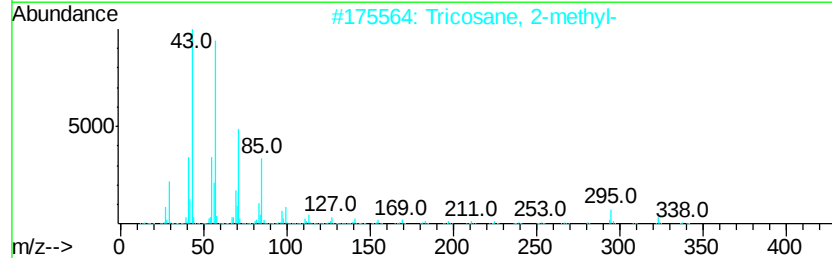
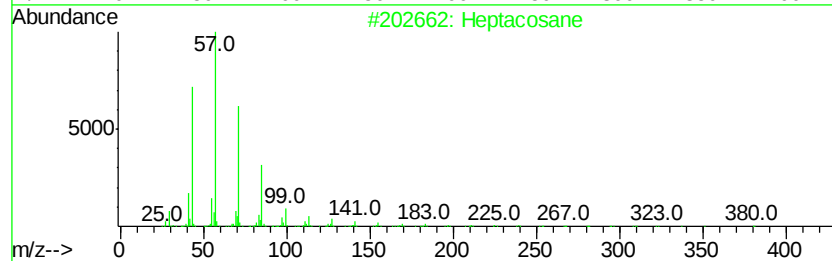
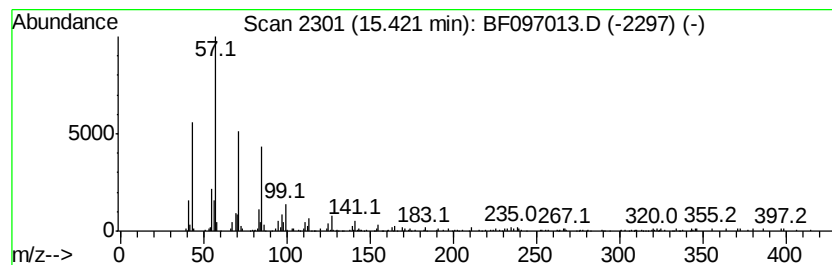
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tricosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	7.97 ng	233912	Perylene-d12	15.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	87
2		Tricosane, 2-methyl-	338	C24H50	001928-30-9	83
3		Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
4		Hexadecane	226	C16H34	000544-76-3	80
5		Heneicosane	296	C21H44	000629-94-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
 Data File : BF097013.D
 Acq On : 25 Jul 2017 4:12
 Operator : SJ/JU
 Sample : I4360-03
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.29	6.29	65.0	ng	2634780	1	6.52	810230	20.0
Heneicosane	10.47	2.6	ng	89159	4	11.02	696488	20.0
cis-9-Hexadeceno...	11.53	2.1	ng	72660	4	11.02	696488	20.0
n-Hexadecanoic acid	11.57	6.2	ng	216258	4	11.02	696488	20.0
unknown13.06	13.06	2.1	ng	79083	5	13.64	737252	20.0
13-Tetradecen-1-o...	13.52	5.6	ng	205837	5	13.64	737252	20.0
Oxalic acid, isob...	14.15	5.6	ng	205959	5	13.64	737252	20.0
Hexadecane	14.43	2.6	ng	75275	6	15.00	587167	20.0
Heptacosane	14.73	5.6	ng	165564	6	15.00	587167	20.0
Tricosane, 2-methyl-	15.42	8.0	ng	233912	6	15.00	587167	20.0