

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
 Data File : BF098794.D
 Acq On : 25 Sep 2017 20:36
 Operator : SJ/JU
 Sample : I5394-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-3992

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-BF092317.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	2.228	20	24	38	rVB	104082	178037	3.93%	0.447%
2	2.328	38	41	58	rVB	82149	143921	3.18%	0.361%
3	2.575	78	83	92	rVB2	34962	66278	1.46%	0.166%
4	5.145	516	520	534	rVB	556687	775886	17.13%	1.948%
5	5.539	581	587	590	rBV	3365667	3817683	84.31%	9.585%
6	6.539	750	757	760	rBV	3486126	3960737	87.47%	9.944%
7	6.686	776	782	785	rBV	3638682	3917449	86.51%	9.835%
8	6.910	817	820	824	rBV	922253	821906	18.15%	2.063%
9	7.069	843	847	851	rBV	3211404	3004858	66.36%	7.544%
10	7.475	910	916	919	rBV	2359913	2524128	55.74%	6.337%
11	8.192	1034	1038	1042	rBV	1228828	1134598	25.06%	2.848%
12	9.269	1215	1221	1225	rBV	4158059	4528105	100.00%	11.368%
13	9.657	1282	1287	1290	rBV	611587	495256	10.94%	1.243%
14	9.951	1332	1337	1341	rBV	1445920	1269083	28.03%	3.186%
15	10.374	1401	1409	1412	rBV2	75108	78406	1.73%	0.197%
16	10.739	1464	1471	1474	rBV	2529351	2670707	58.98%	6.705%
17	10.845	1486	1489	1498	rBV	94792	100525	2.22%	0.252%
18	11.439	1585	1590	1592	rBV	1538776	1345572	29.72%	3.378%
19	11.951	1672	1677	1682	rBV2	196059	197791	4.37%	0.497%
20	12.645	1792	1795	1799	rBV	131051	110397	2.44%	0.277%
21	12.739	1808	1811	1814	rBV2	52719	54472	1.20%	0.137%
22	12.874	1829	1834	1838	rBV	112776	112679	2.49%	0.283%
23	13.027	1854	1860	1863	rBV	4251957	4419233	97.60%	11.095%
24	13.904	2006	2009	2017	rBV	555834	512515	11.32%	1.287%
25	14.045	2030	2033	2034	rBV	56581	45909	1.01%	0.115%
26	14.074	2034	2038	2041	rVV	1352467	1252822	27.67%	3.145%
27	14.539	2112	2117	2123	rBV2	109433	148625	3.28%	0.373%
28	15.121	2212	2216	2223	rVB2	35888	72860	1.61%	0.183%
29	15.192	2224	2228	2231	rBV	75676	91098	2.01%	0.229%
30	15.562	2286	2291	2303	rVB	695513	956671	21.13%	2.402%
31	16.027	2367	2370	2375	rVB	60053	81424	1.80%	0.204%
32	16.080	2375	2379	2385	rBV2	75188	120509	2.66%	0.303%
33	16.545	2455	2458	2467	rVB2	42393	73972	1.63%	0.186%
34	16.668	2474	2479	2485	rBV	40423	75476	1.67%	0.189%

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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

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35	17.162	2560	2563	2571	rVB5	33817	61805	1.36%	0.155%
36	17.245	2573	2577	2585	rVV6	24040	53827	1.19%	0.135%
37	17.409	2601	2605	2612	rVB9	24463	47796	1.06%	0.120%
38	17.639	2638	2644	2653	rBV9	45526	139050	3.07%	0.349%
39	17.762	2660	2665	2673	rVB10	31364	74204	1.64%	0.186%
40	17.886	2682	2686	2694	rVB8	29789	70334	1.55%	0.177%
41	18.021	2703	2709	2714	rVB9	24760	54898	1.21%	0.138%
42	18.509	2784	2792	2807	rBV9	50953	170135	3.76%	0.427%

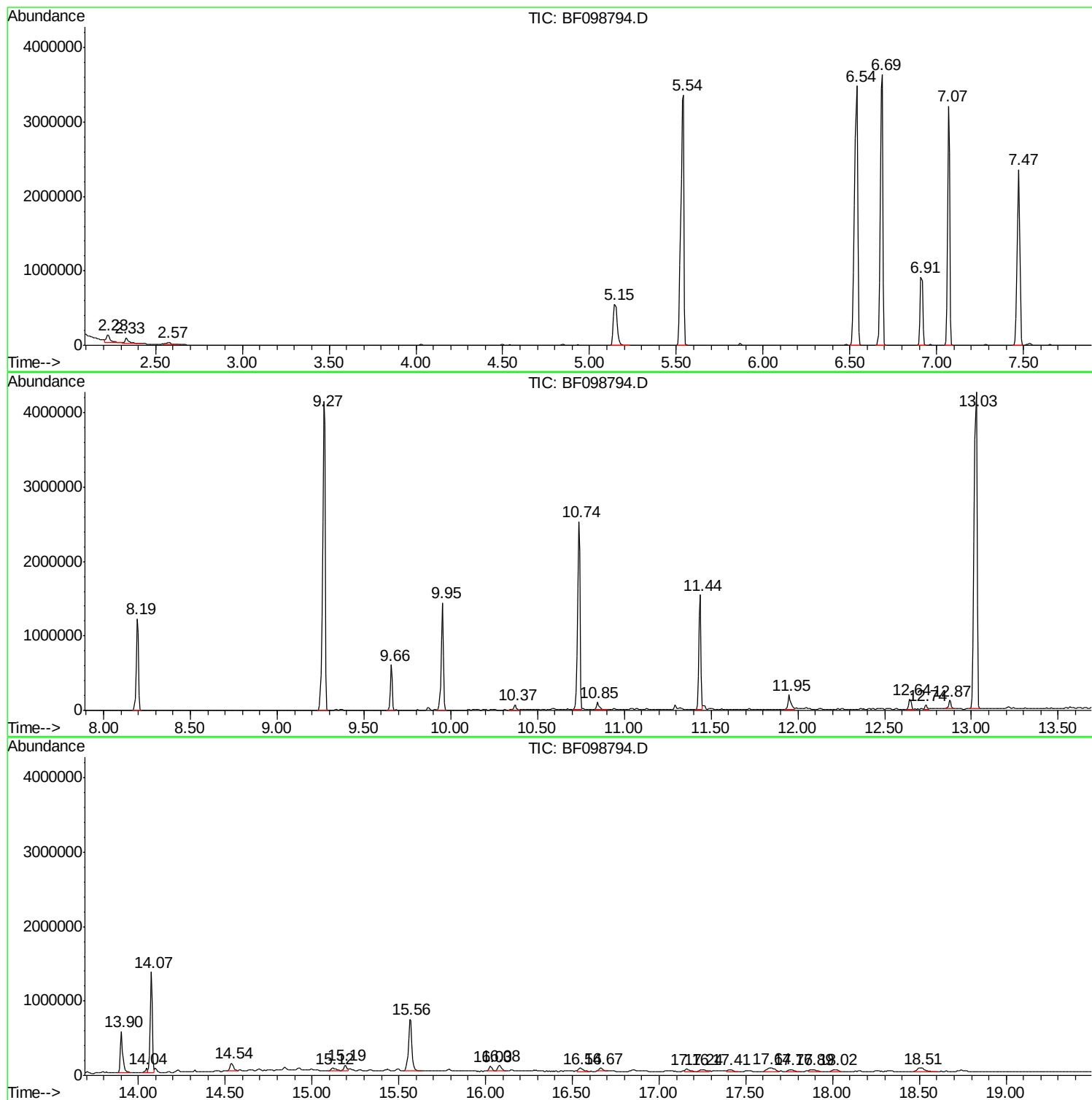
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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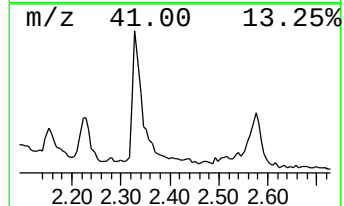
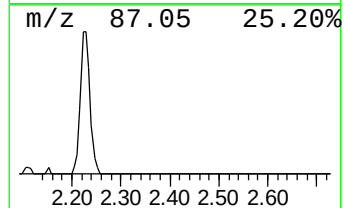
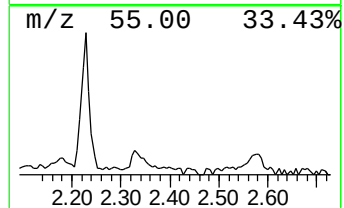
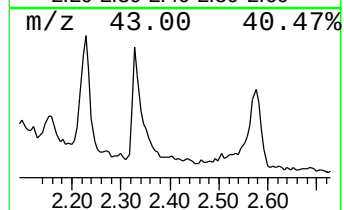
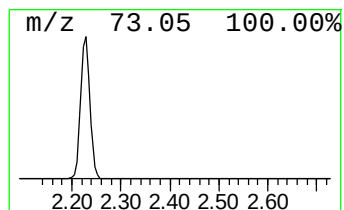
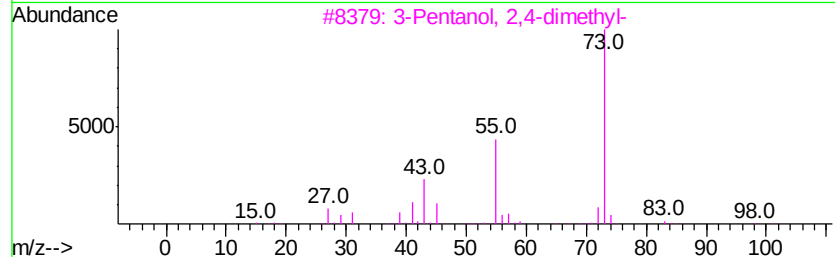
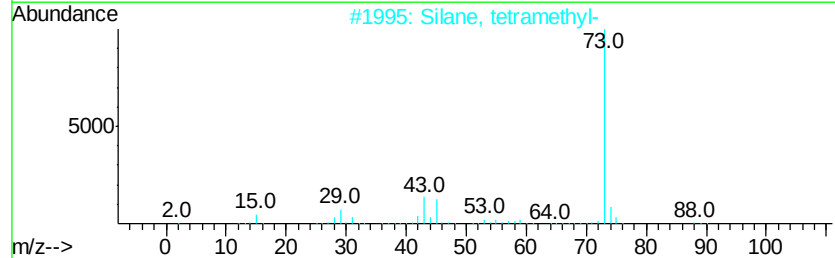
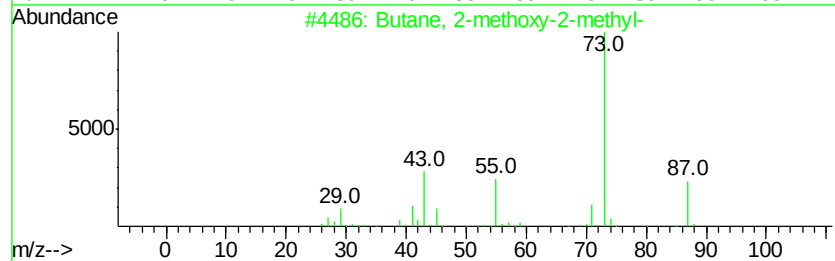
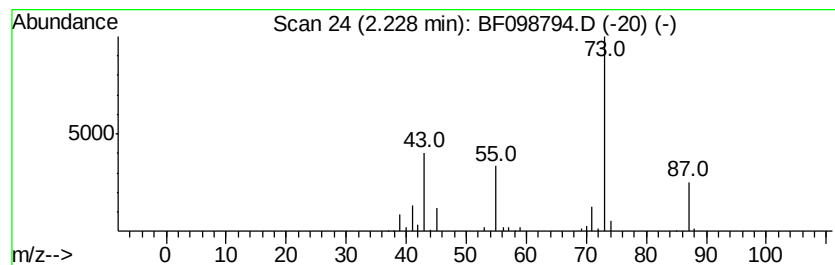
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.23	4.33 ng	178037	1,4-Dichlorobenzene-d4	6.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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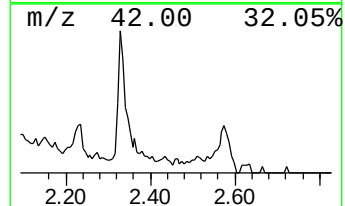
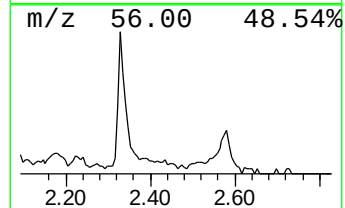
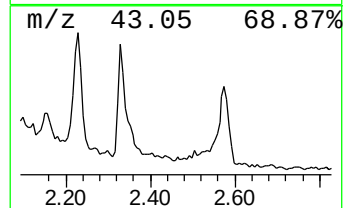
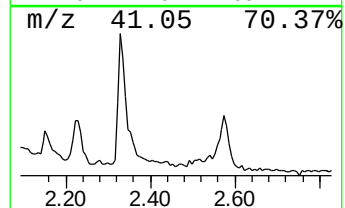
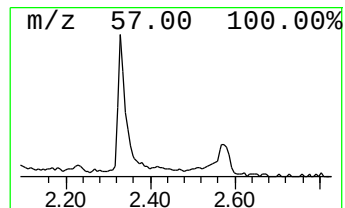
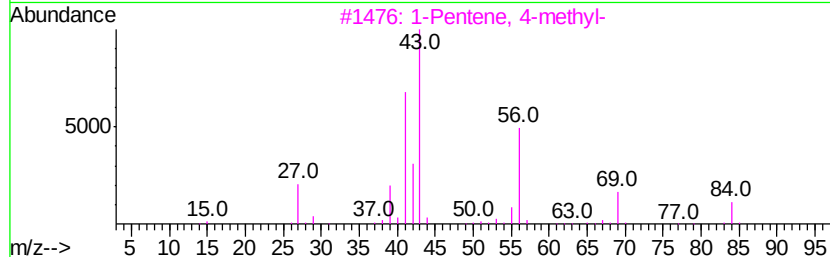
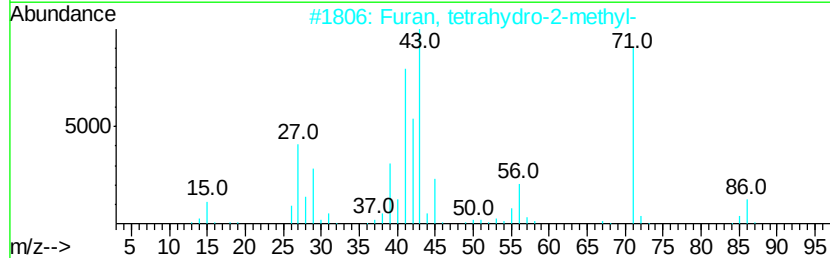
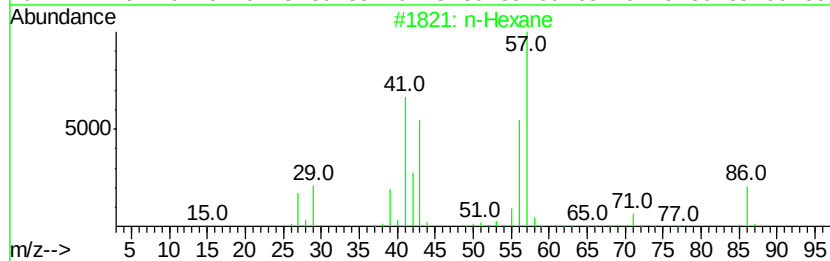
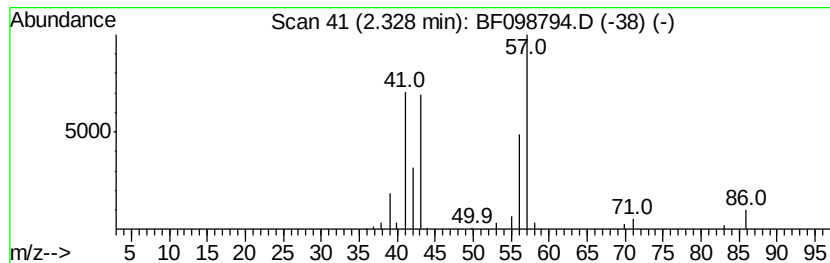
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	3.50 ng	143921	1,4-Dichlorobenzene-d4	6.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane		86	C6H14	000110-54-3	78
2	Furan, tetrahydro-2-methyl-		86	C5H10O	000096-47-9	43
3	1-Pentene, 4-methyl-		84	C6H12	000691-37-2	42
4	Butane, 1-chloro-2-methyl-		106	C5H11Cl	000616-13-7	36
5	Butanal, 2-methyl-		86	C5H10O	000096-17-3	25



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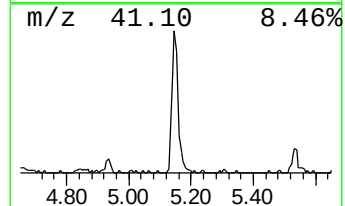
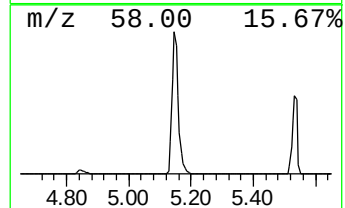
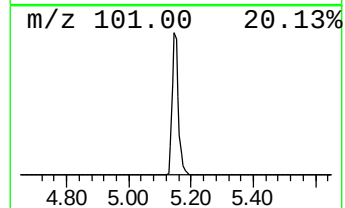
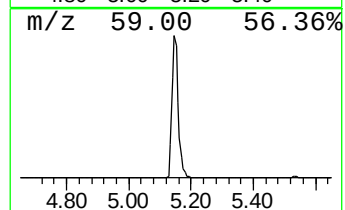
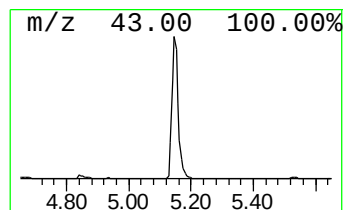
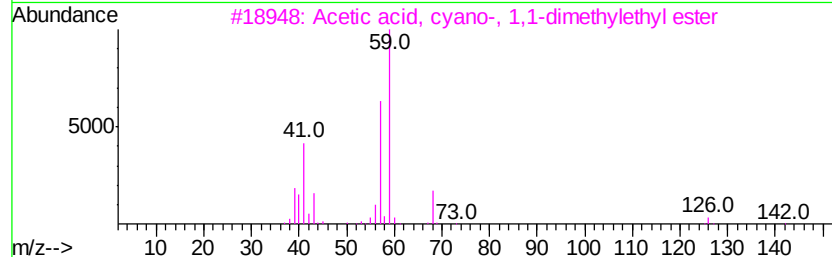
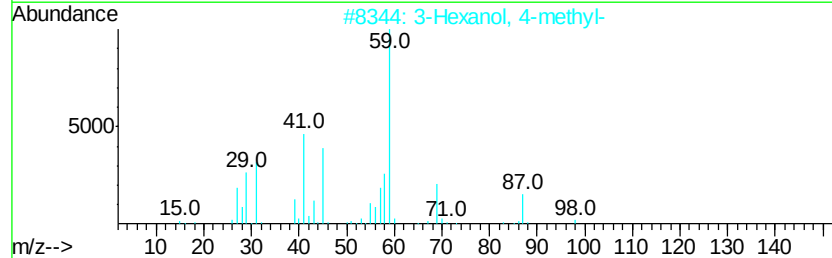
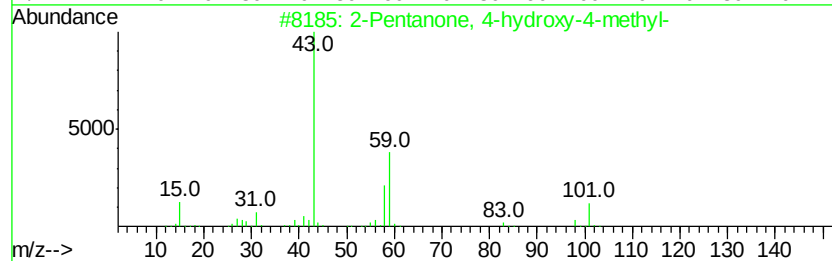
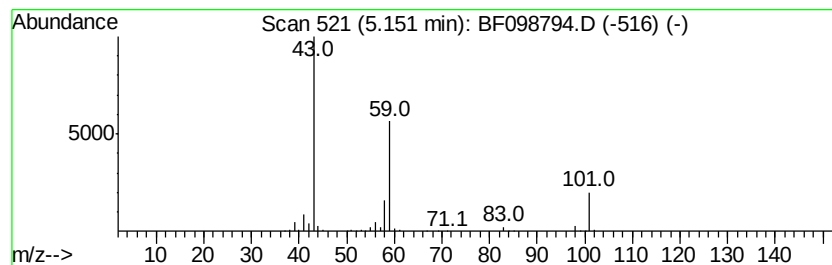
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	18.88 ng	775886	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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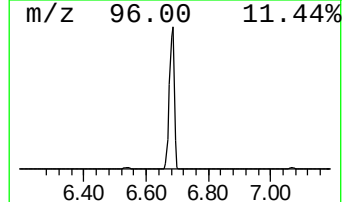
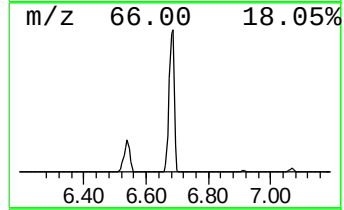
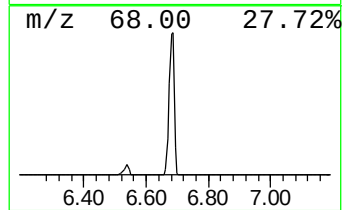
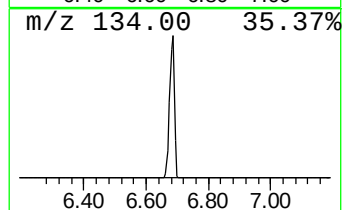
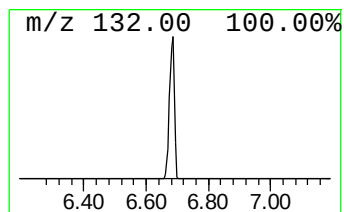
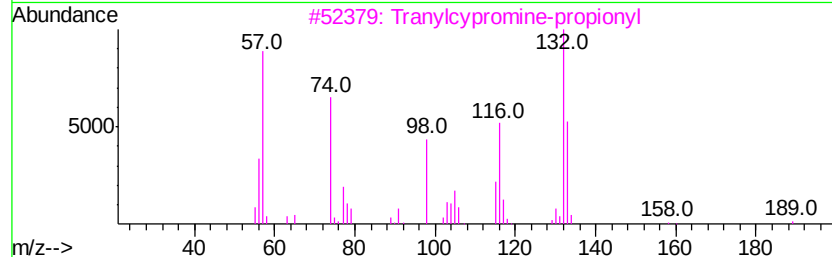
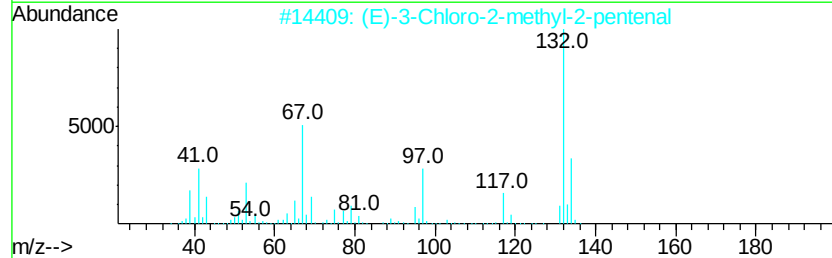
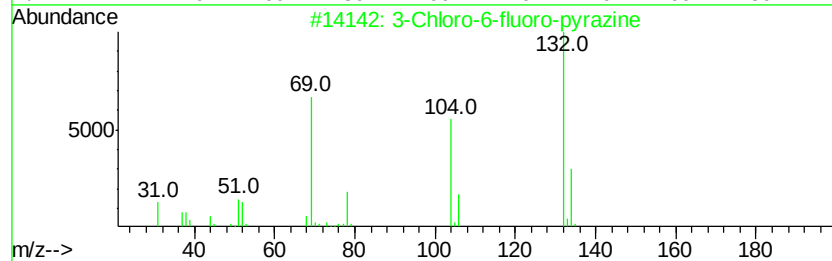
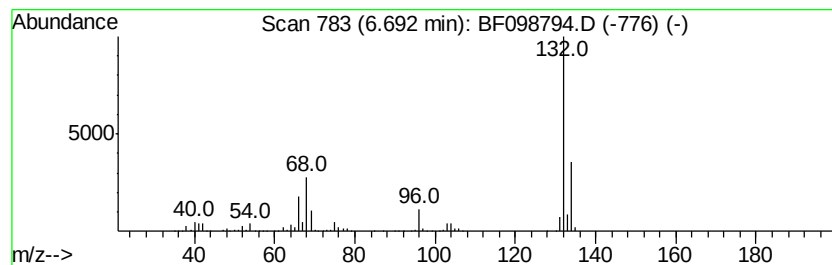
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	95.33 ng	3917450	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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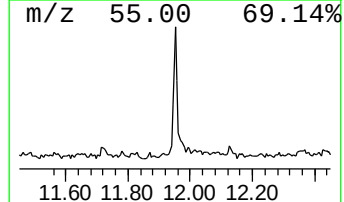
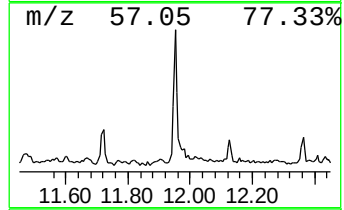
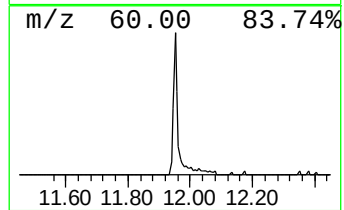
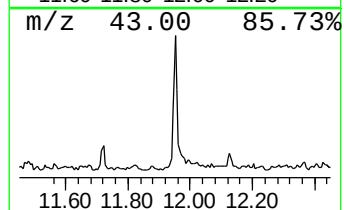
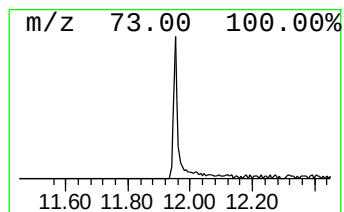
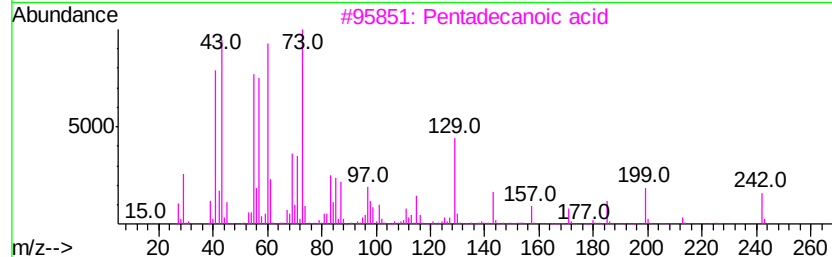
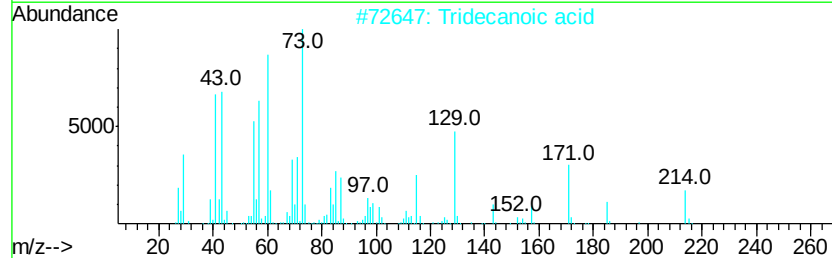
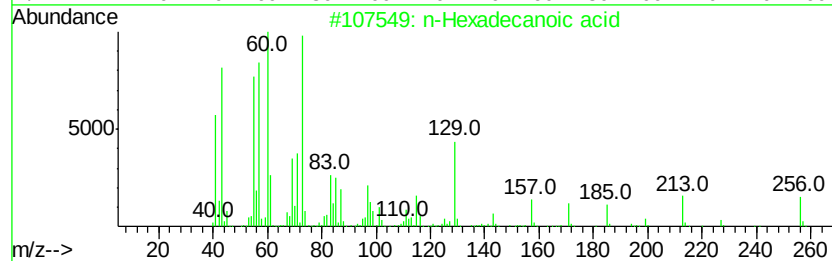
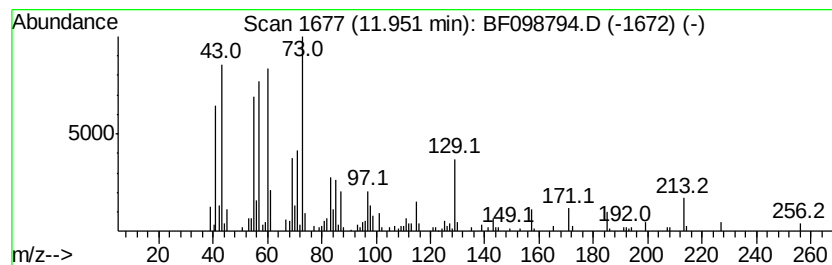
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.95	2.94 ng	197791	Phenanthrene-d10		11.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098794.D
Acq On : 25 Sep 2017 20:36
Operator : SJ/JU
Sample : I5394-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

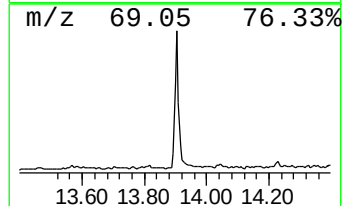
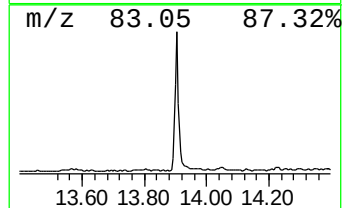
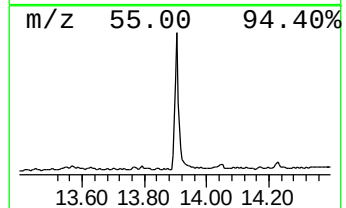
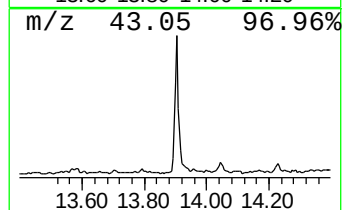
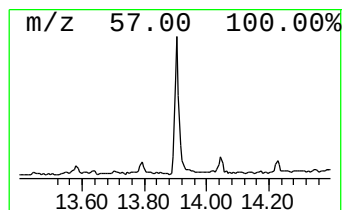
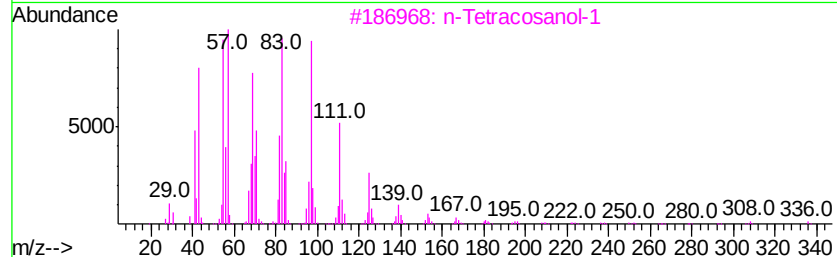
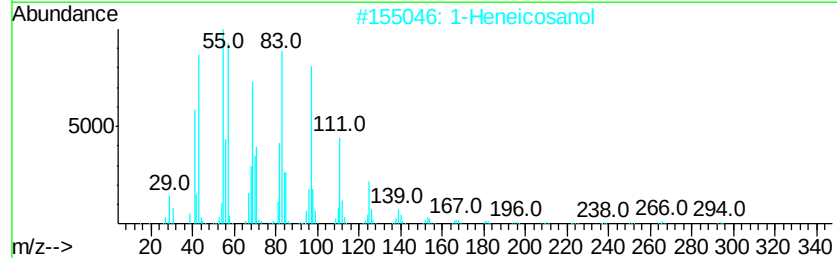
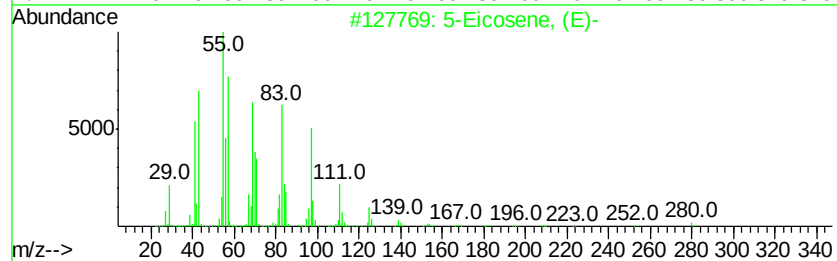
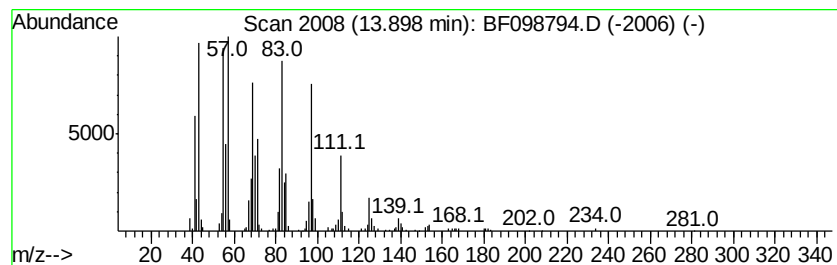
Instrument :
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ClientSampleId :
RT-3992

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	8.18 ng	512515	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098794.D
Acq On : 25 Sep 2017 20:36
Operator : SJ/JU
Sample : I5394-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

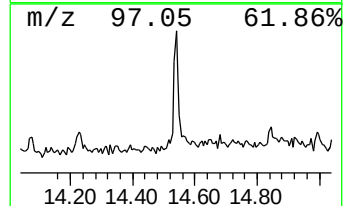
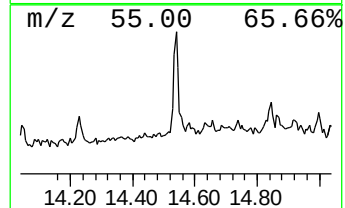
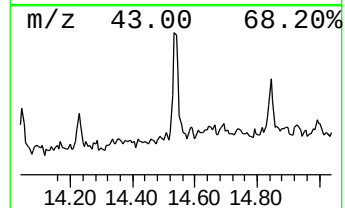
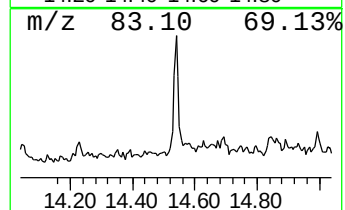
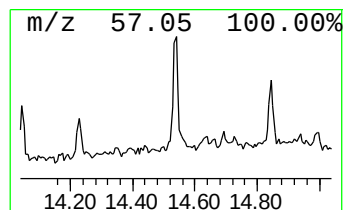
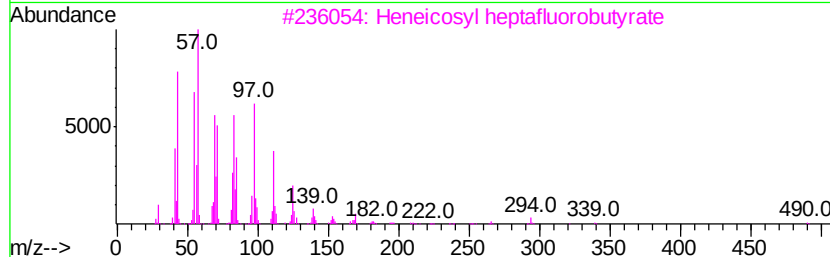
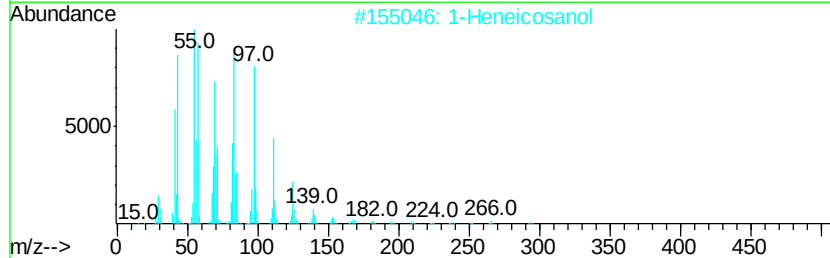
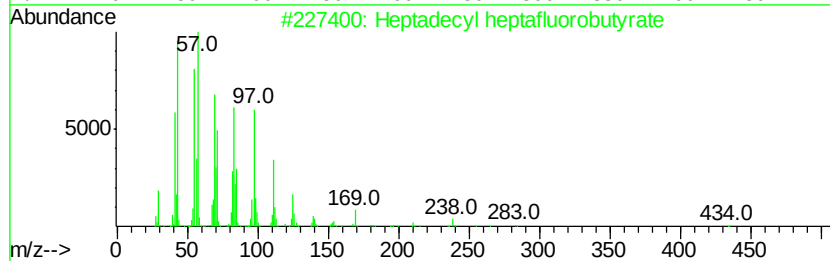
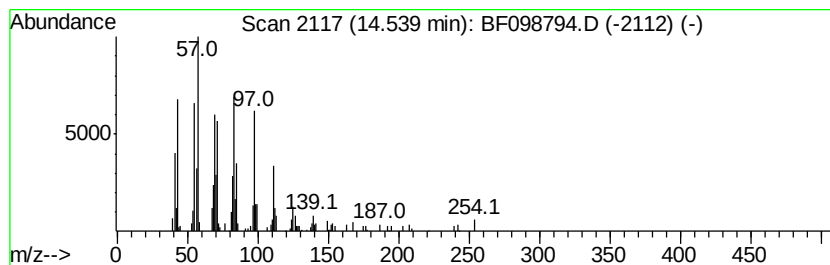
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.54	2.37 ng	148625	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Acq On : 25 Sep 2017 20:36
Operator : SJ/JU
Sample : I5394-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

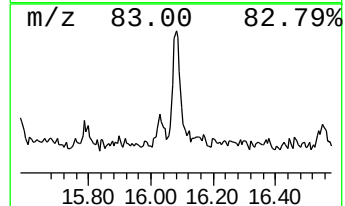
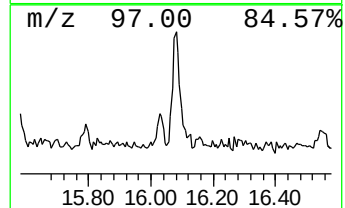
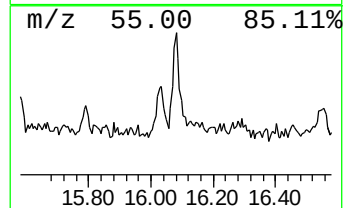
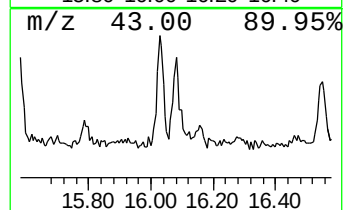
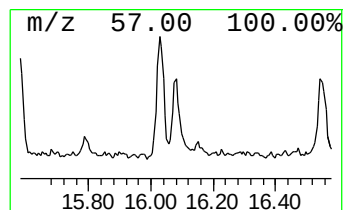
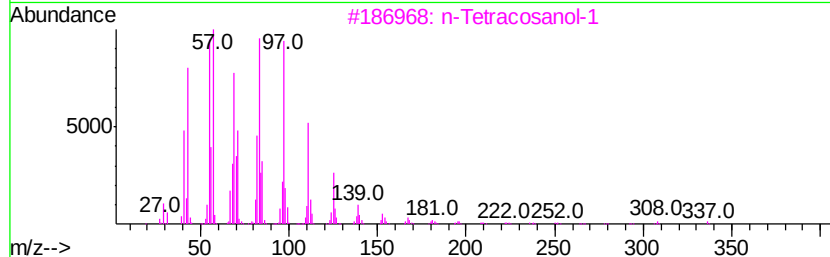
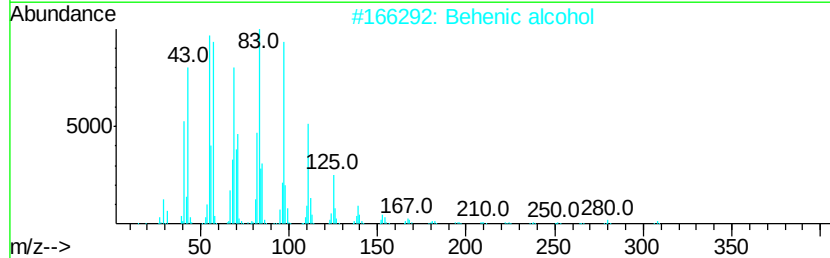
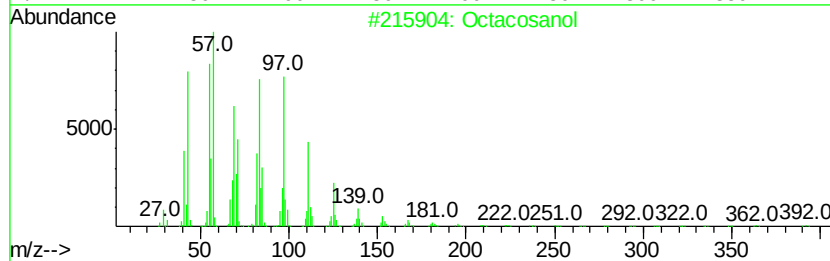
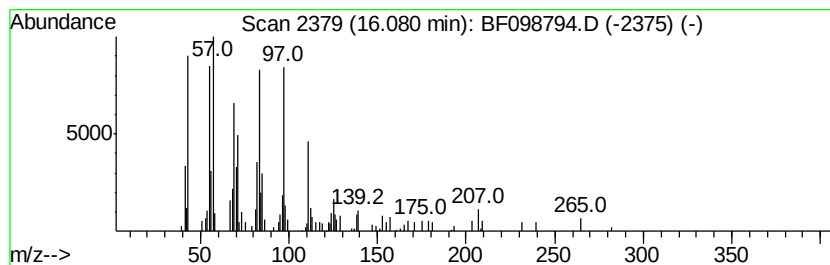
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	2.52 ng	120509	Perylene-d12	15.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosanol	410 C28H58O	000557-61-9	94
2	Behenic alcohol	326 C22H46O	000661-19-8	93
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	93
4	Heptacosyl acetate	438 C29H58O2	1000351-78-2	91
5	1-Heptacosanol	396 C27H56O	002004-39-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098794.D
Acq On : 25 Sep 2017 20:36
Operator : SJ/JU
Sample : I5394-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3992

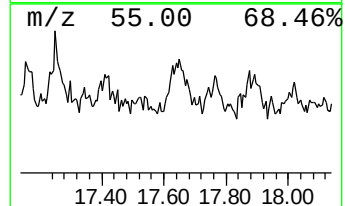
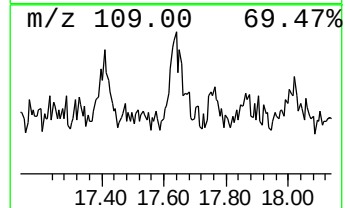
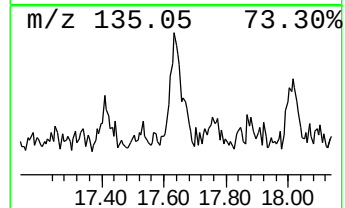
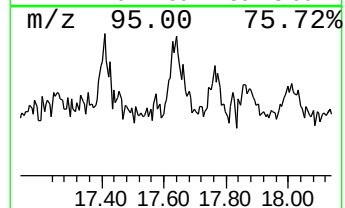
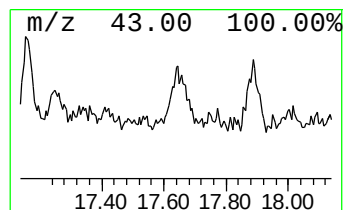
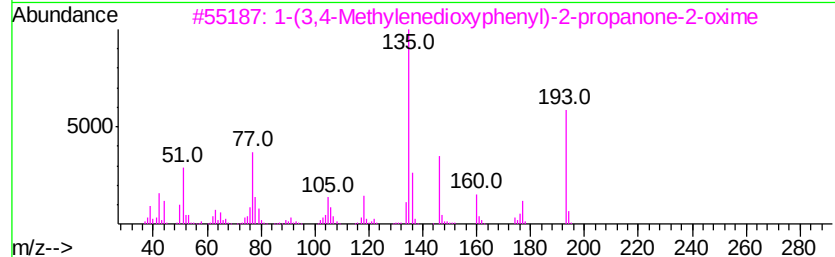
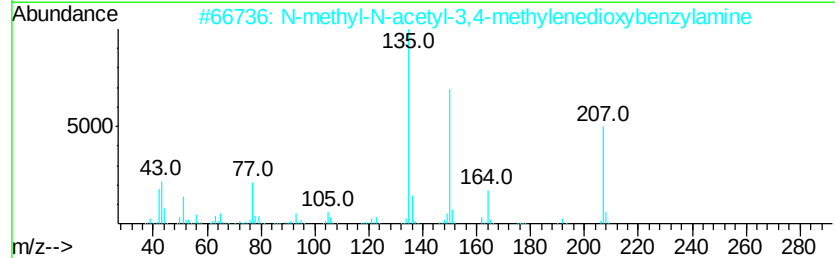
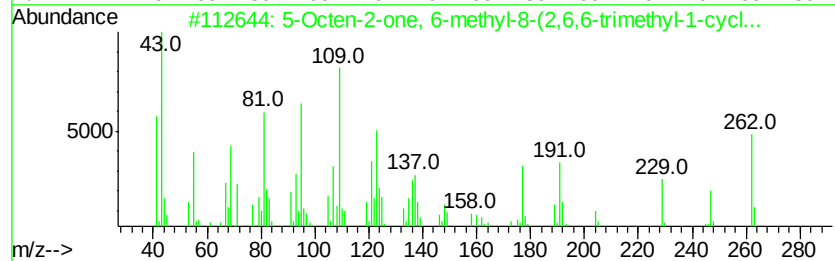
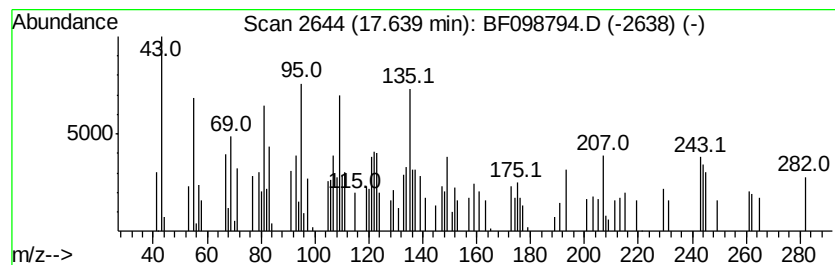
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Octen-2-one, 6-methyl-8-(... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	2.91 ng	139050	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Octen-2-one, 6-methyl-8-(2,6,6...	262	C18H30O	055638-41-0	20
2		N-methyl-N-acetyl-3,4-methylened...	207	C11H13NO3	1000378-88-3	14
3		1-(3,4-Methylenedioxyphenyl)-2-p...	193	C10H11NO3	052271-42-8	11
4		Ethanamine, 1-(2,4-cyclopentadie...	135	C9H13N	014469-77-3	11
5		N-Benzylformamide	135	C8H9NO	006343-54-0	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
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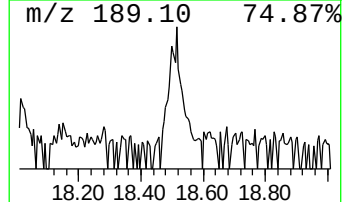
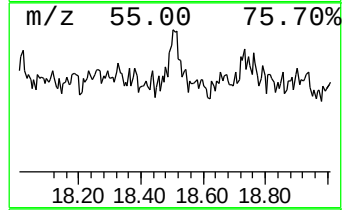
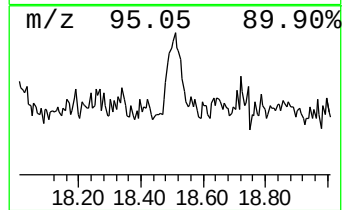
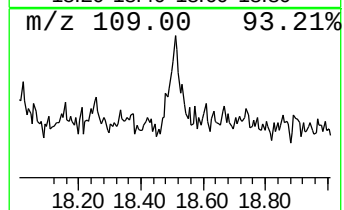
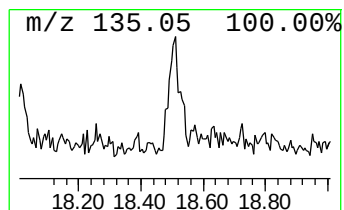
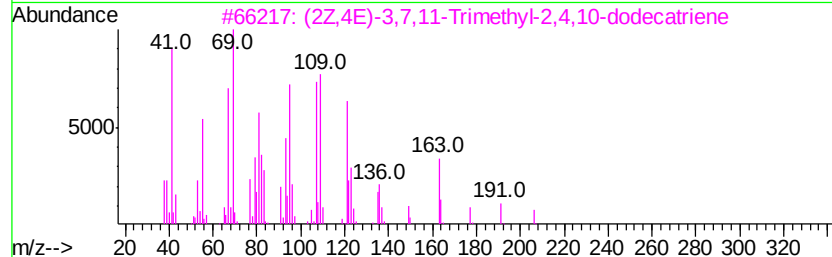
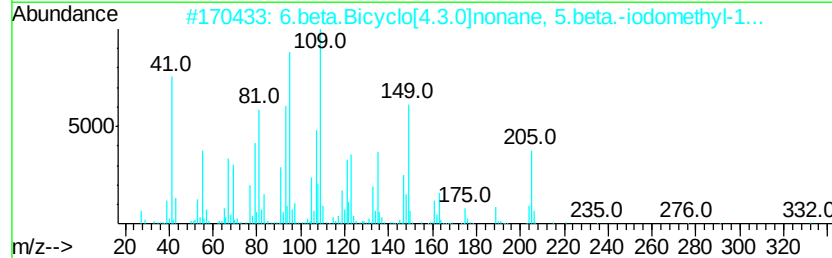
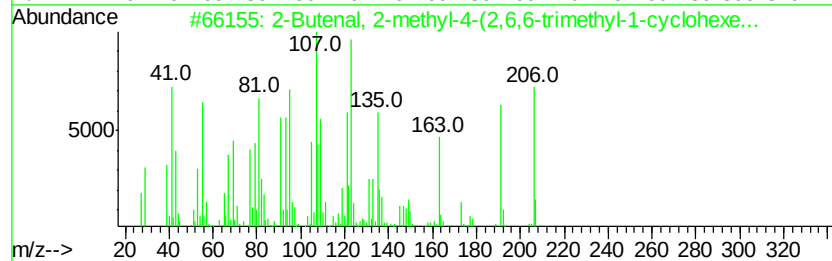
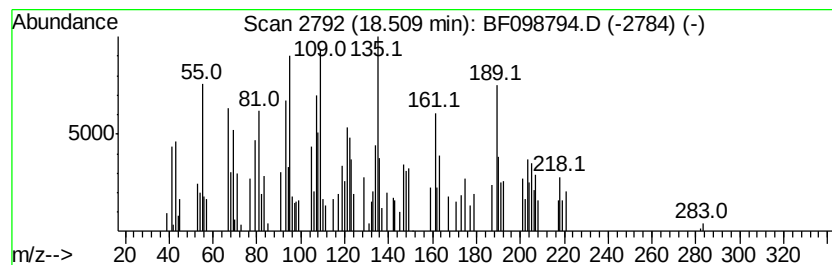
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown3.36 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.51	3.56 ng	170135	Perylene-d12	15.56	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	42
2	6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	27
3	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	27
4	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	25
5	2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
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Acq On : 25 Sep 2017 20:36
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Sample : I5394-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-3992

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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
Butane, 2-methoxy...	2.23	4.3	ng	178037	1	6.92	821906	20.0
n-Hexane	2.33	3.5	ng	143921	1	6.92	821906	20.0
2-Pentanone, 4-hy...	5.15	18.9	ng	775886	1	6.92	821906	20.0
unknown6.69	6.69	95.3	ng	3917450	1	6.92	821906	20.0
n-Hexadecanoic acid	11.95	2.9	ng	197791	4	11.44	1345570	20.0
5-Eicosene, (E)-	13.90	8.2	ng	512515	5	14.07	1252820	20.0
Heptadecyl heptaf...	14.54	2.4	ng	148625	5	14.07	1252820	20.0
Octacosanol	16.08	2.5	ng	120509	6	15.56	956671	20.0
5-Octen-2-one, 6-...	17.64	2.9	ng	139050	6	15.56	956671	20.0
unknown3.36	18.51	3.6	ng	170135	6	15.56	956671	20.0