

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
 Data File : BF098862.D
 Acq On : 27 Sep 2017 14:45
 Operator : SJ/JU
 Sample : I5434-14
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400535

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	2.210	17	21	27	rVB	73669	94555	3.01%	0.328%
2	5.139	515	519	532	rVB	522105	641809	20.45%	2.227%
3	5.534	581	586	589	rBV	3003605	2975694	94.84%	10.324%
4	6.539	751	757	761	rBV	2863109	3137726	100.00%	10.886%
5	6.681	777	781	785	rBV	3061260	3121885	99.50%	10.831%
6	6.916	817	821	824	rBV	884525	765241	24.39%	2.655%
7	7.069	843	847	850	rBV	2367636	1980584	63.12%	6.871%
8	7.475	911	916	919	rBV	2040472	1900150	60.56%	6.592%
9	8.192	1034	1038	1042	rBV	1172237	1038884	33.11%	3.604%
10	9.269	1216	1221	1224	rBV	3585524	3059137	97.50%	10.613%
11	9.657	1283	1287	1290	rBV	591409	463974	14.79%	1.610%
12	9.951	1333	1337	1341	rBV	1312537	1124355	35.83%	3.901%
13	10.369	1406	1408	1411	rVB	62943	51106	1.63%	0.177%
14	10.739	1466	1471	1474	rBV	1990127	1769749	56.40%	6.140%
15	10.845	1486	1489	1498	rBV	76640	80250	2.56%	0.278%
16	11.439	1586	1590	1593	rBV	1157557	1059839	33.78%	3.677%
17	11.951	1674	1677	1686	rBV2	54703	48765	1.55%	0.169%
18	13.021	1854	1859	1862	rBV	2984485	2776603	88.49%	9.633%
19	13.904	2005	2009	2021	rBV	300126	290535	9.26%	1.008%
20	14.074	2034	2038	2042	rBV	872986	734496	23.41%	2.548%
21	14.539	2112	2117	2123	rBV	81101	112720	3.59%	0.391%
22	14.827	2162	2166	2176	rBV	167806	205287	6.54%	0.712%
23	14.992	2191	2194	2200	rVB3	40616	41128	1.31%	0.143%
24	15.192	2224	2228	2230	rBV	77520	94385	3.01%	0.327%
25	15.215	2230	2232	2239	rVB2	44056	55966	1.78%	0.194%
26	15.562	2286	2291	2297	rBV	532076	690039	21.99%	2.394%
27	15.786	2325	2329	2333	rBV3	35604	49945	1.59%	0.173%
28	16.027	2365	2370	2375	rBV	63107	90416	2.88%	0.314%
29	16.080	2375	2379	2386	rVV4	35890	66421	2.12%	0.230%
30	16.850	2505	2510	2516	rVB5	26282	49419	1.57%	0.171%
31	17.156	2558	2562	2571	rVB4	20316	42765	1.36%	0.148%
32	17.662	2642	2648	2658	rVB9	50481	126849	4.04%	0.440%
33	18.509	2784	2792	2795	rBV9	13595	36089	1.15%	0.125%
34	19.203	2903	2910	2919	rBV9	17981	47592	1.52%	0.165%

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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

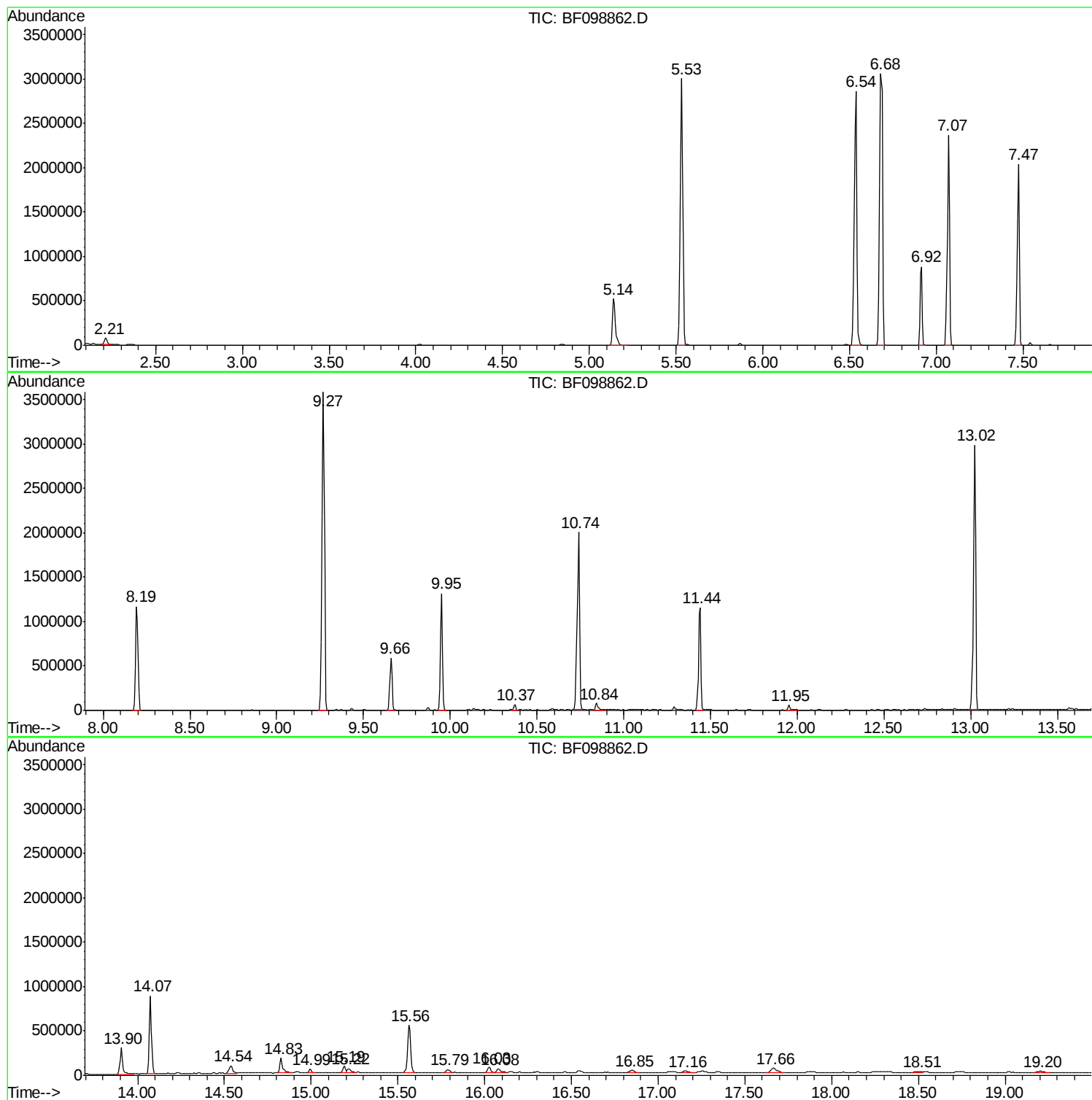
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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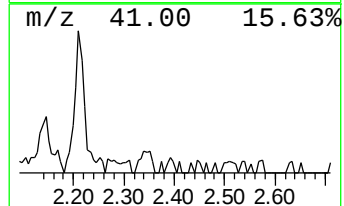
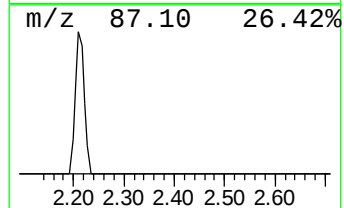
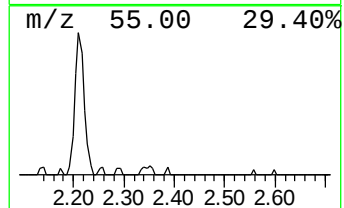
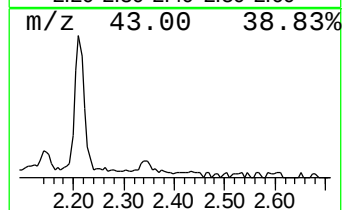
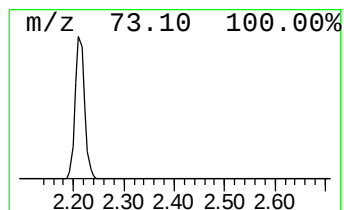
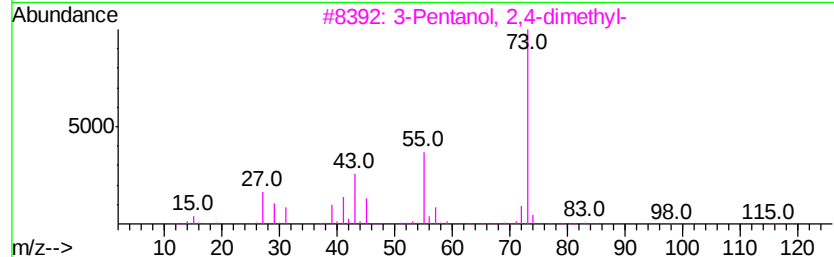
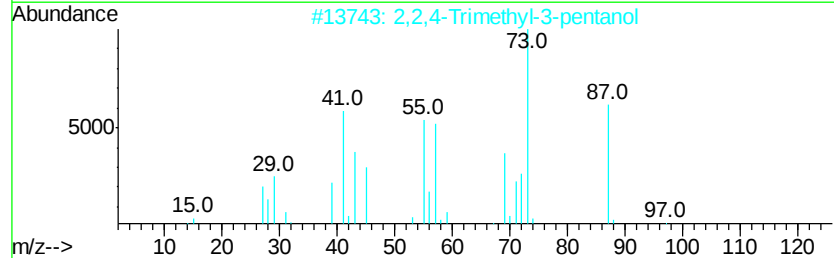
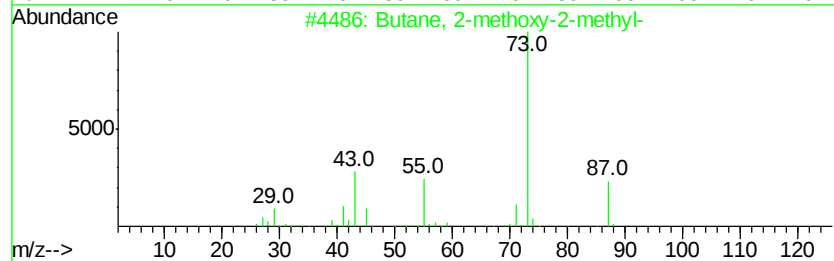
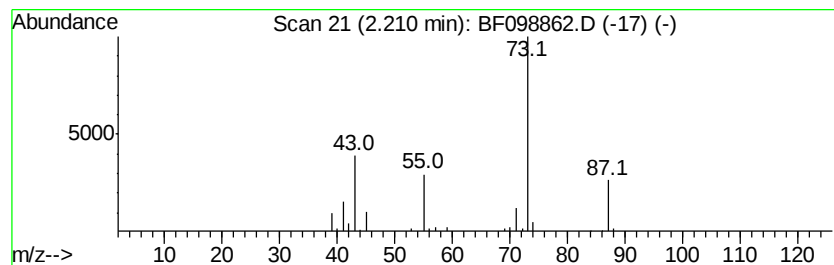
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	2.47 ng	94555	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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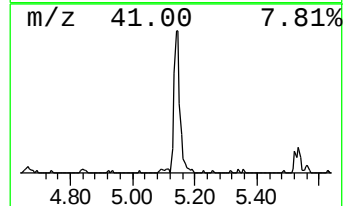
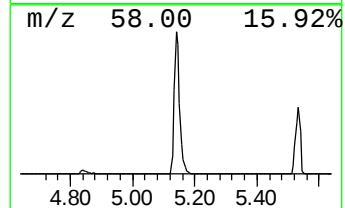
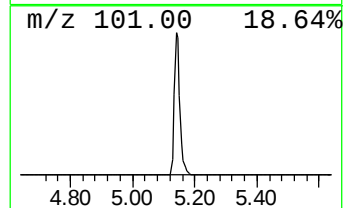
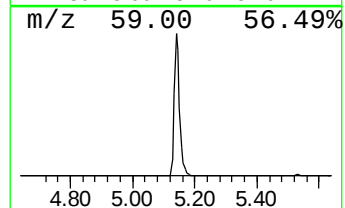
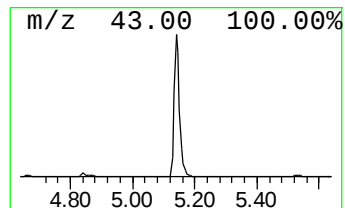
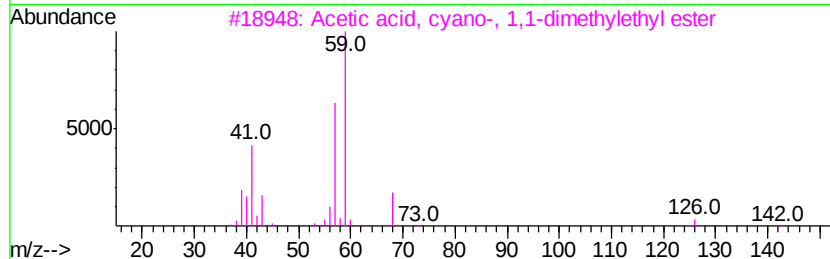
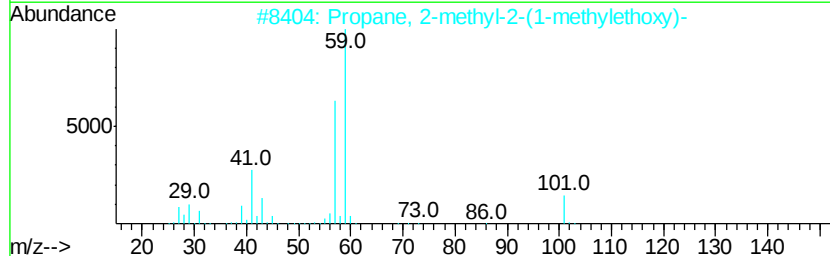
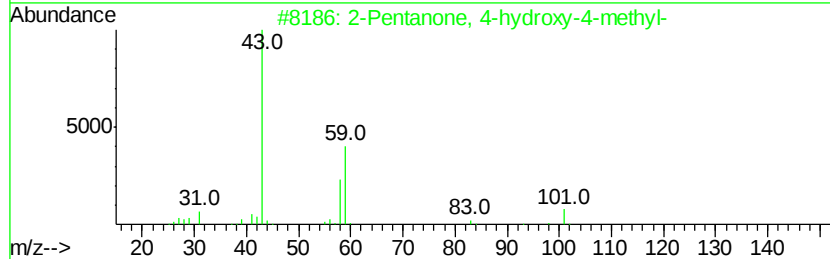
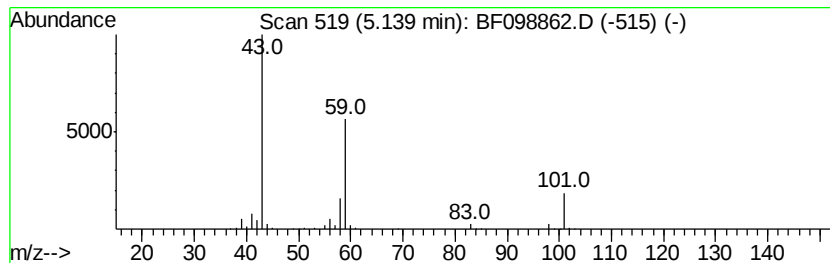
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.14 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	16.77 ng	641809	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	45
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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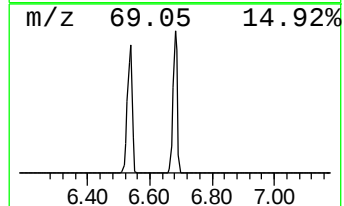
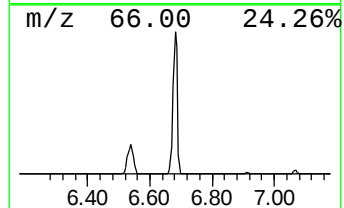
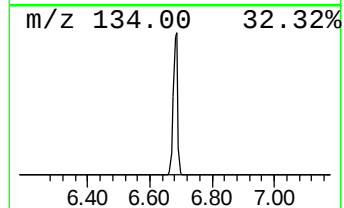
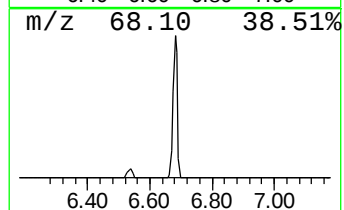
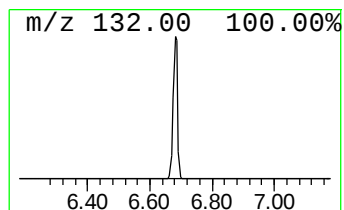
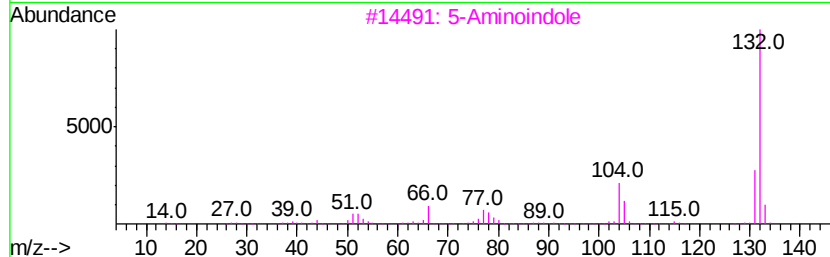
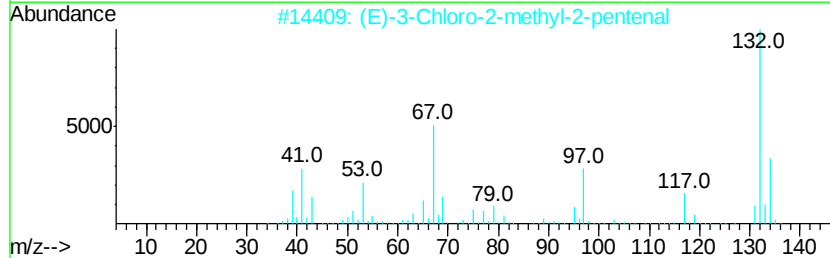
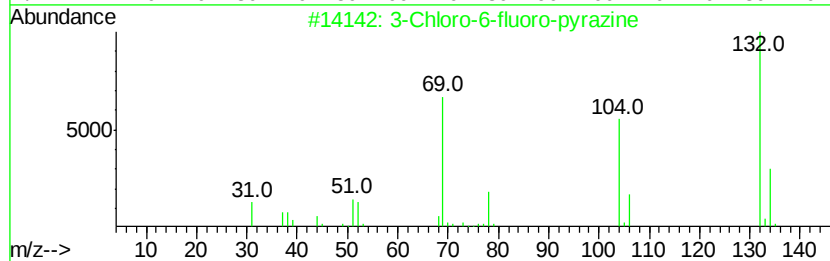
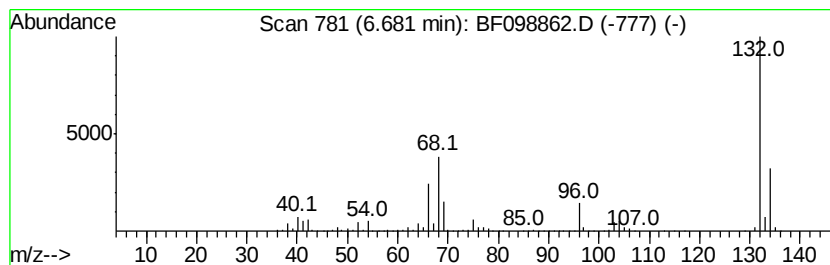
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	81.59 ng	3121890	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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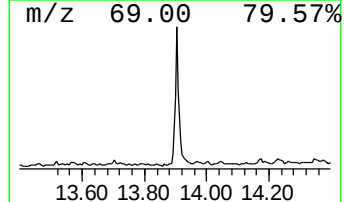
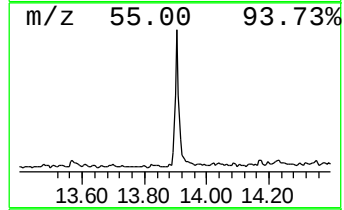
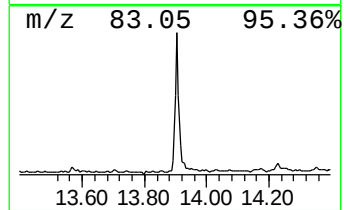
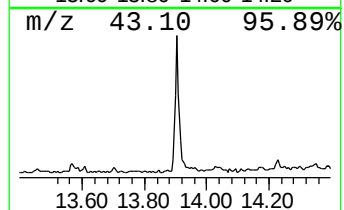
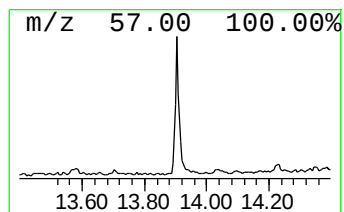
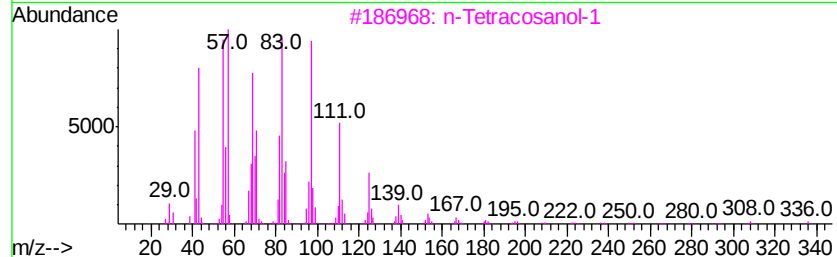
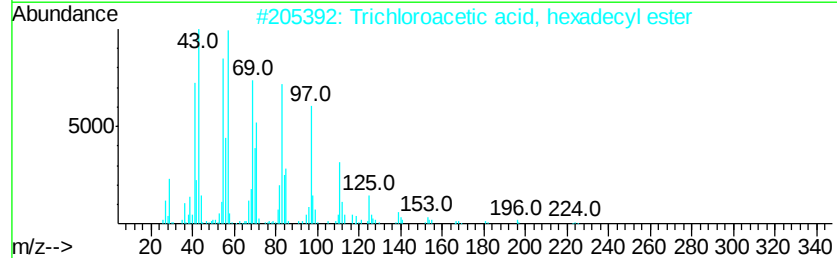
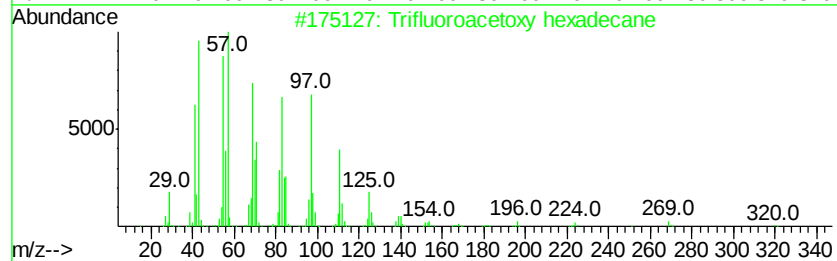
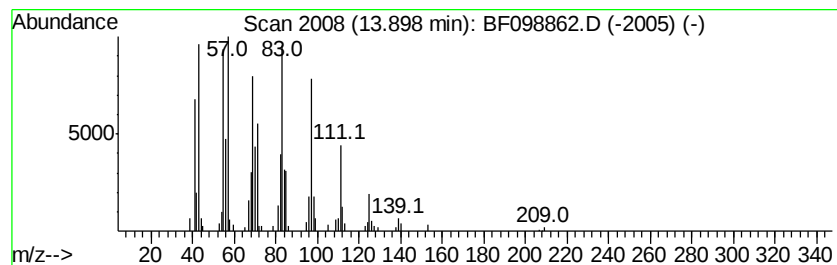
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	7.91 ng	290535	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Cyclopentadecane	210	C15H30	000295-48-7	93



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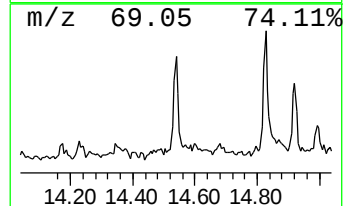
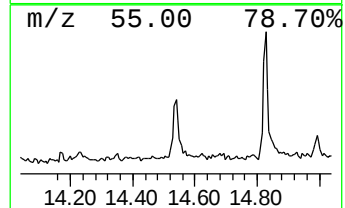
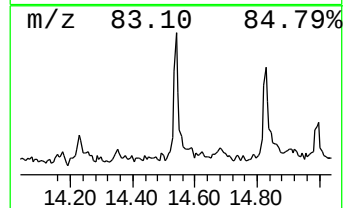
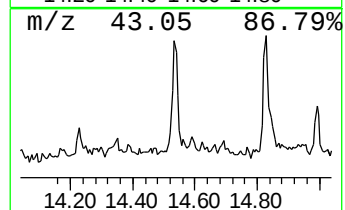
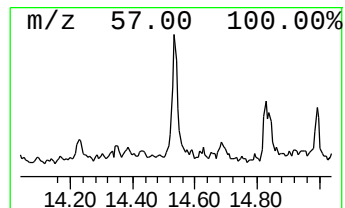
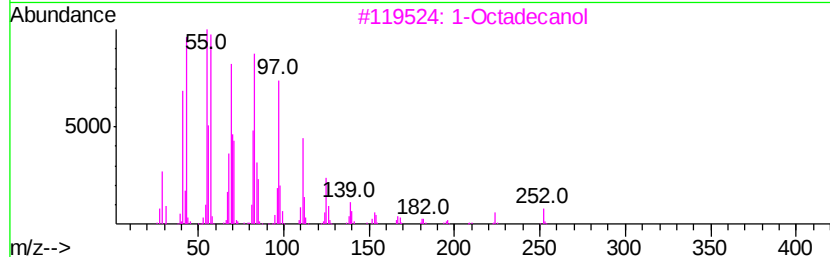
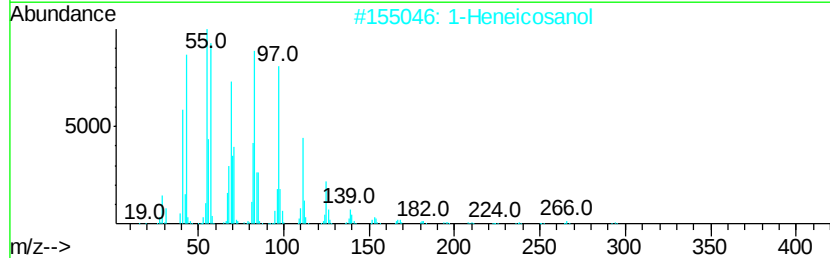
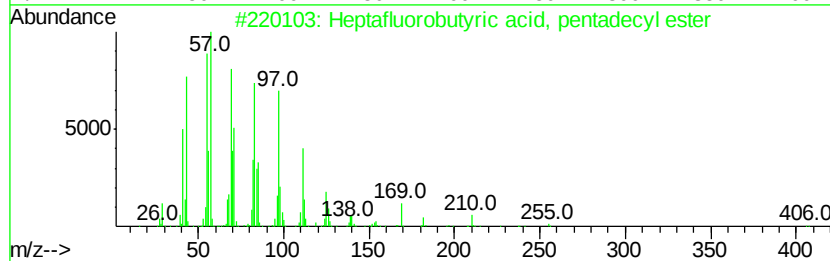
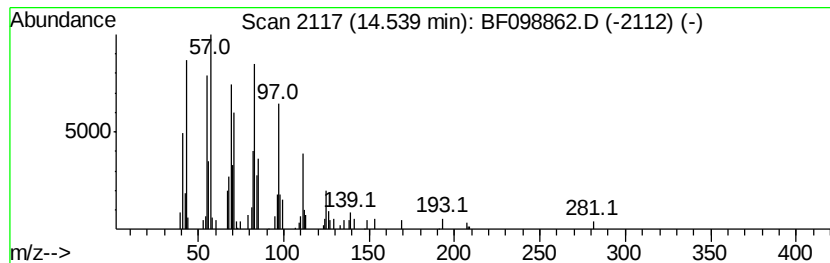
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.07 ng	112720	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		1-Octadecanol	270	C18H38O	000112-92-5	93
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		1-Heptacosanol	396	C27H56O	002004-39-9	90



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ClientSampleId :
UT5400535

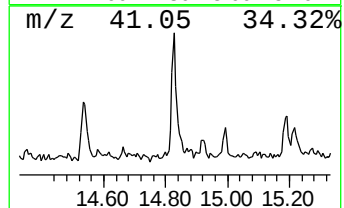
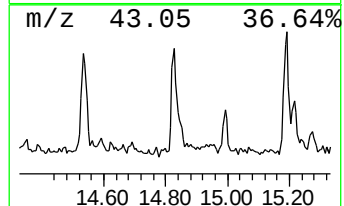
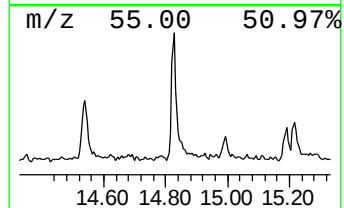
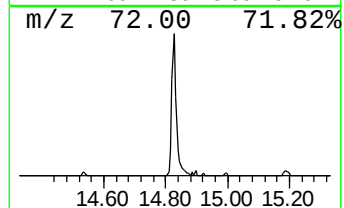
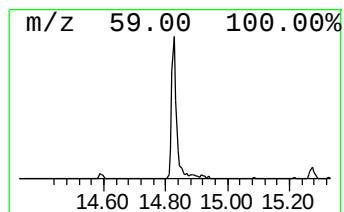
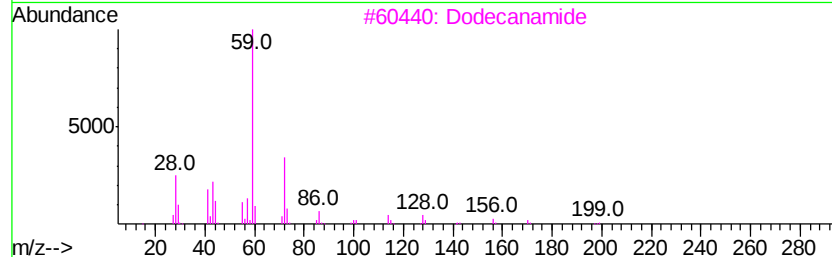
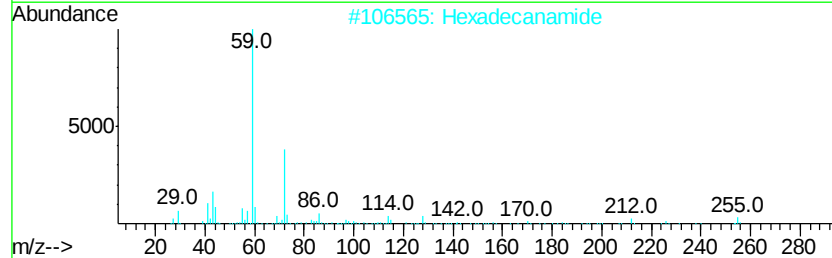
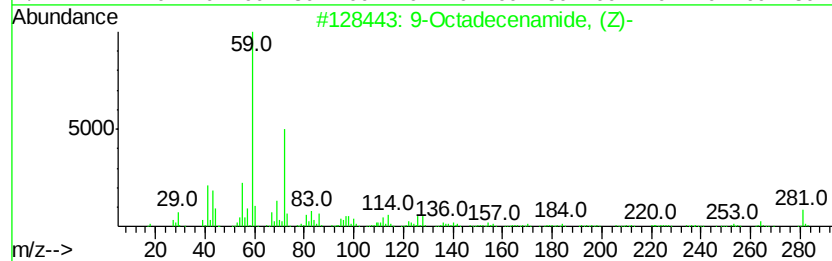
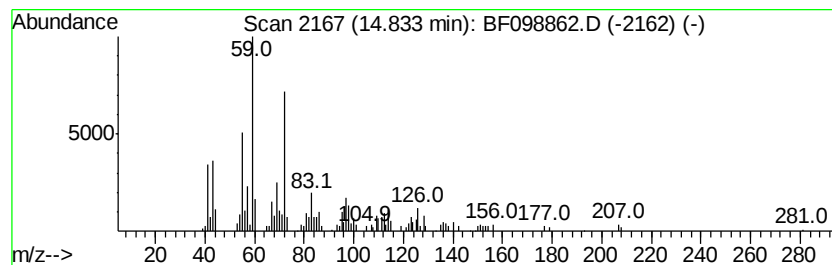
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	5.95 ng	205287	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Hexadecanamide	255	C16H33NO	000629-54-9	64
3		Dodecanamide	199	C12H25NO	001120-16-7	52
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50
5		3-Tetradecanol	214	C14H30O	001653-32-3	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098862.D
Acq On : 27 Sep 2017 14:45
Operator : SJ/JU
Sample : I5434-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

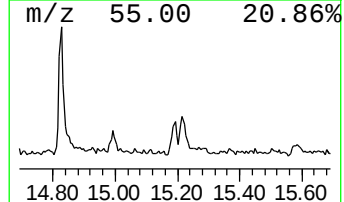
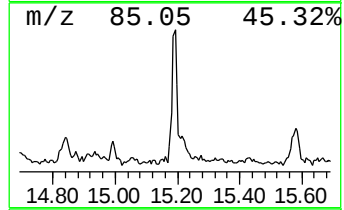
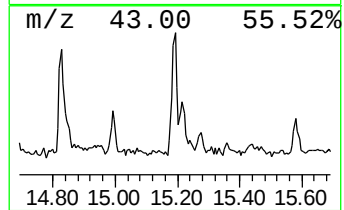
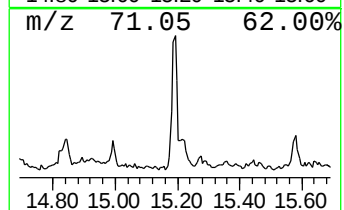
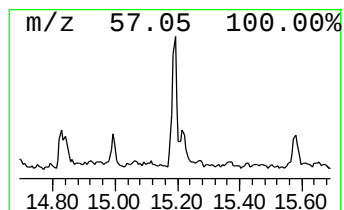
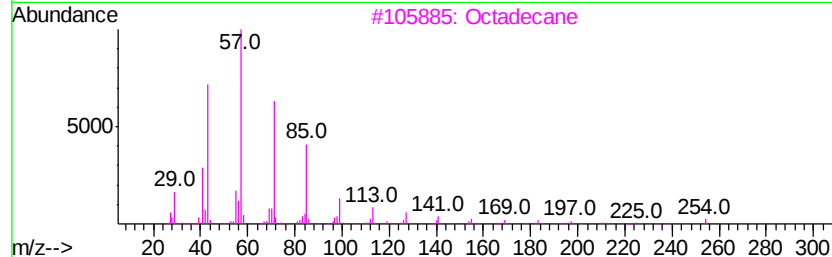
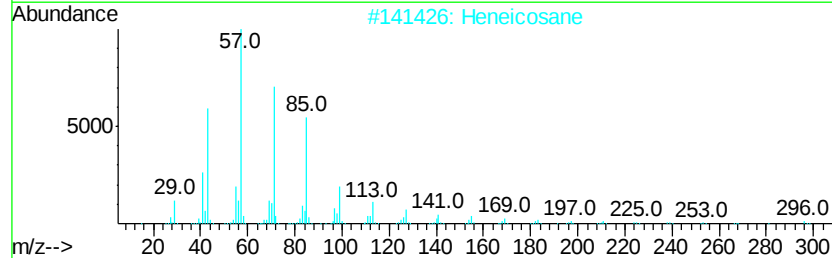
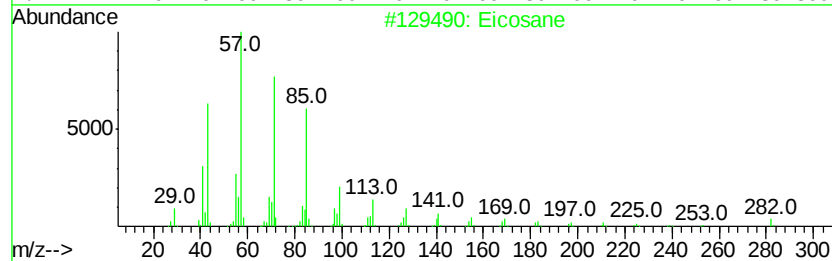
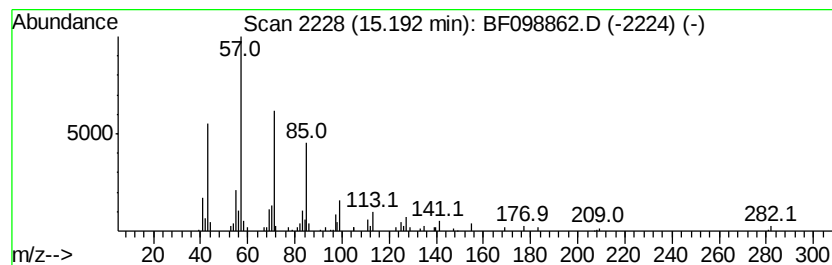
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.74 ng	94385	Perylene-d12	15.56
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	97
2	Heneicosane	296 C21H44	000629-94-7	91
3	Octadecane	254 C18H38	000593-45-3	91
4	Heptadecane	240 C17H36	000629-78-7	91
5	Octacosane	394 C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098862.D
Acq On : 27 Sep 2017 14:45
Operator : SJ/JU
Sample : I5434-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400535

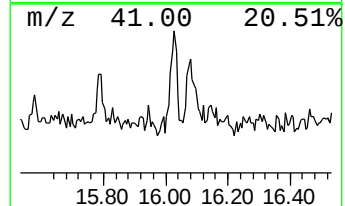
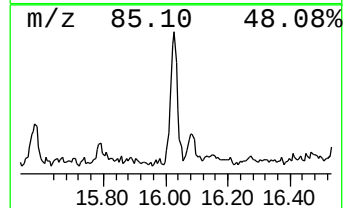
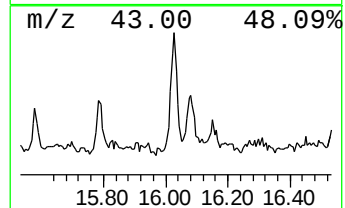
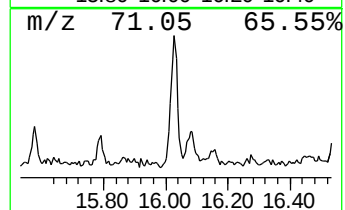
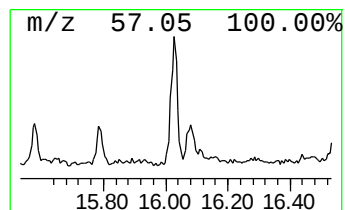
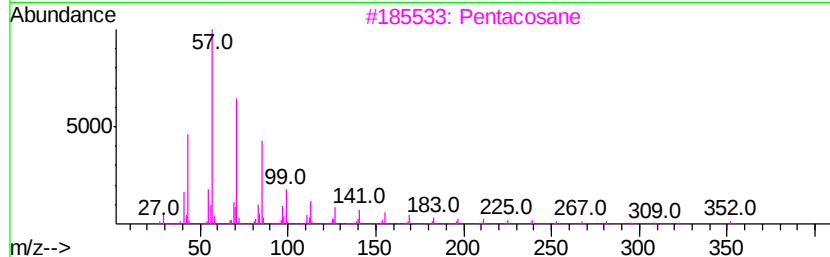
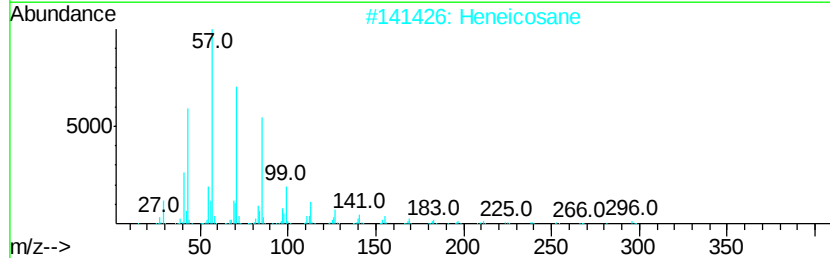
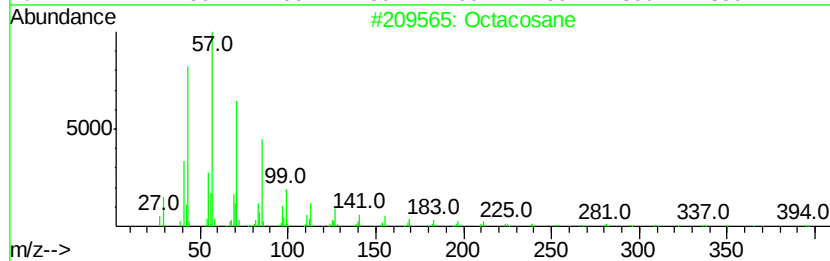
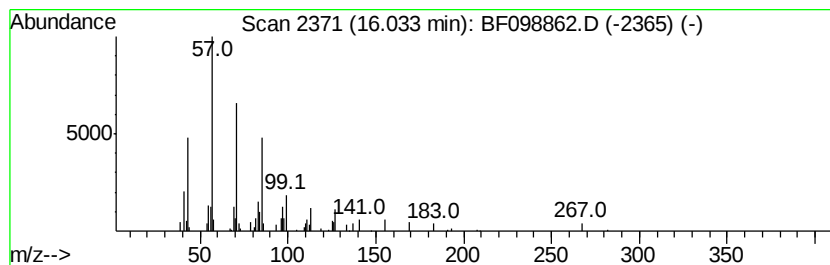
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.62 ng	90416	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098862.D
Acq On : 27 Sep 2017 14:45
Operator : SJ/JU
Sample : I5434-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UT5400535

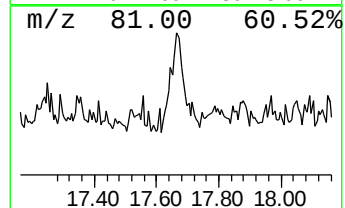
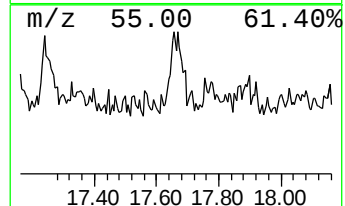
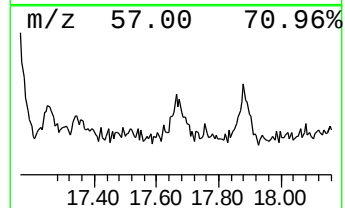
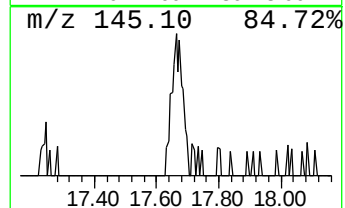
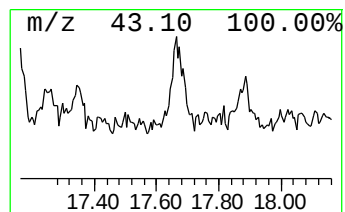
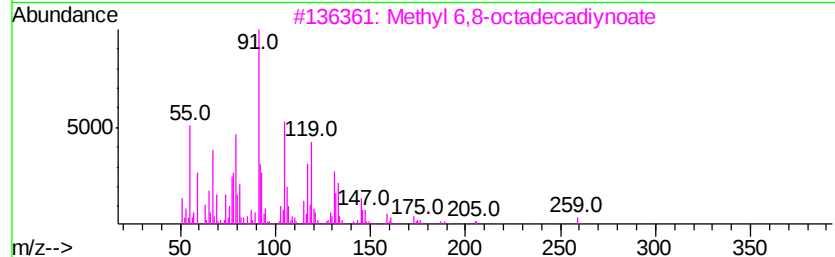
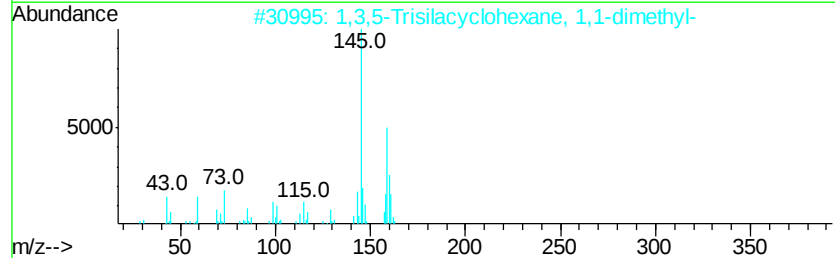
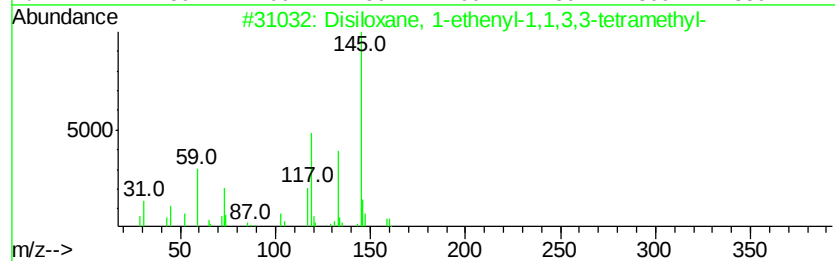
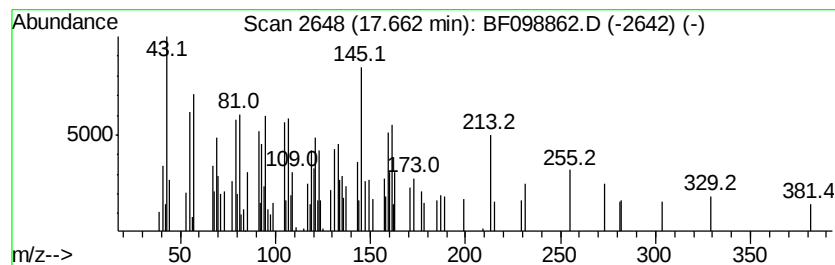
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.66 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	3.68 ng	126849	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disiloxane, 1-ethenyl-1,1,3,3-tetra-	160	C6H16OSi2	055967-52-7	27
2		1,3,5-Trisilacyclohexane, 1,1-dimethyl-	160	C5H16Si3	054424-15-6	18
3		Methyl 6,8-octadecadienoate	290	C19H30O2	1000336-47-6	14
4		Tricyclo[4.1.0.0(2,4)]heptane, 3,3-dimethyl-	204	C15H24	056348-21-1	14
5		2H-2,4a-Methanonaphthalene, 1,3,4,4a-tetra-	204	C15H24	001135-66-6	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098862.D
Acq On : 27 Sep 2017 14:45
Operator : SJ/JU
Sample : I5434-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown5.14	5.14	16.8	ng	641809	1	6.92	765241	20.0
unknown6.68	6.68	81.6	ng	3121890	1	6.92	765241	20.0
Trifluoroacetoxy ...	13.90	7.9	ng	290535	5	14.07	734496	20.0
Heptafluorobutyri...	14.54	3.1	ng	112720	5	14.07	734496	20.0
9-Octadecenamide,...	14.83	6.0	ng	205287	6	15.56	690039	20.0
Eicosane	15.19	2.7	ng	94385	6	15.56	690039	20.0
Octacosane	16.03	2.6	ng	90416	6	15.56	690039	20.0
unknown17.66	17.66	3.7	ng	126849	6	15.56	690039	20.0