

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
 Data File : BF096177.D
 Acq On : 24 Jun 2017 00:46
 Operator : SJ/MA
 Sample : I3784-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P.56-C-COMP

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-BF060517.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	1.540	7	9	29	rBV	325681	603444	38.34%	4.147%
2	4.428	496	500	517	rBV	43956	129553	8.23%	0.890%
3	5.151	620	623	649	rBV	350960	959751	60.98%	6.596%
4	6.839	907	910	920	rBV	387868	808789	51.39%	5.558%
5	6.922	920	924	946	rVB	657746	1324535	84.15%	9.103%
6	7.257	978	981	1002	rVB	256764	364393	23.15%	2.504%
7	7.492	1017	1021	1043	rBV	543572	793177	50.39%	5.451%
8	8.181	1135	1138	1156	rBV	309427	564407	35.86%	3.879%
9	9.292	1323	1327	1350	rBV	320429	479100	30.44%	3.292%
10	11.074	1625	1630	1650	rBV	932499	1184487	75.25%	8.140%
11	11.774	1745	1749	1761	rBV	68058	96821	6.15%	0.665%
12	12.116	1802	1807	1813	rBV2	366192	472510	30.02%	3.247%
13	13.416	2024	2028	2045	rBV	309457	489116	31.08%	3.361%
14	14.510	2210	2214	2220	rBV	289274	392151	24.91%	2.695%
15	16.351	2524	2527	2537	rVB	30212	38370	2.44%	0.264%
16	16.651	2575	2578	2586	rBV2	30344	44464	2.82%	0.306%
17	16.898	2615	2620	2629	rVB	750927	839752	53.35%	5.771%
18	17.268	2679	2683	2686	rBV2	18775	25182	1.60%	0.173%
19	17.303	2686	2689	2695	rVB2	16975	20201	1.28%	0.139%
20	17.892	2784	2789	2794	rBV	136035	144798	9.20%	0.995%
21	18.156	2829	2834	2843	rBV	840614	1063481	67.57%	7.308%
22	18.250	2843	2850	2859	rVV	332419	515784	32.77%	3.545%
23	18.315	2859	2861	2865	rVB3	15194	18556	1.18%	0.128%
24	18.515	2890	2895	2899	rBV4	25741	40746	2.59%	0.280%
25	18.568	2900	2904	2913	rVV2	72438	112691	7.16%	0.774%
26	18.645	2913	2917	2923	rVV4	9063	18750	1.19%	0.129%
27	18.721	2926	2930	2935	rVB	58904	65025	4.13%	0.447%
28	18.962	2966	2971	2978	rVV	1240515	1573968	100.00%	10.817%
29	19.021	2978	2981	2988	rVB	94253	124080	7.88%	0.853%
30	19.180	3004	3008	3013	rBV6	12202	17719	1.13%	0.122%
31	19.233	3013	3017	3020	rBV5	10759	16513	1.05%	0.113%
32	19.297	3023	3028	3030	rBV4	15706	19882	1.26%	0.137%
33	19.339	3030	3035	3041	rBV3	49149	78275	4.97%	0.538%
34	19.533	3065	3068	3071	rBV2	15487	18513	1.18%	0.127%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.697	3090	3096	3103	rBV2	142879	256715	16.31%	1.764%
36	19.750	3103	3105	3110	rVB3	31473	39609	2.52%	0.272%
37	19.886	3124	3128	3130	rBV	17854	25368	1.61%	0.174%
38	19.921	3130	3134	3145	rVB2	263734	363354	23.09%	2.497%
39	20.356	3205	3208	3210	rBV2	20095	19541	1.24%	0.134%
40	20.392	3211	3214	3218	rBV5	24338	37696	2.39%	0.259%
41	21.439	3387	3392	3396	rBV7	23356	46100	2.93%	0.317%
42	22.815	3618	3626	3633	rVB4	127602	303941	19.31%	2.089%

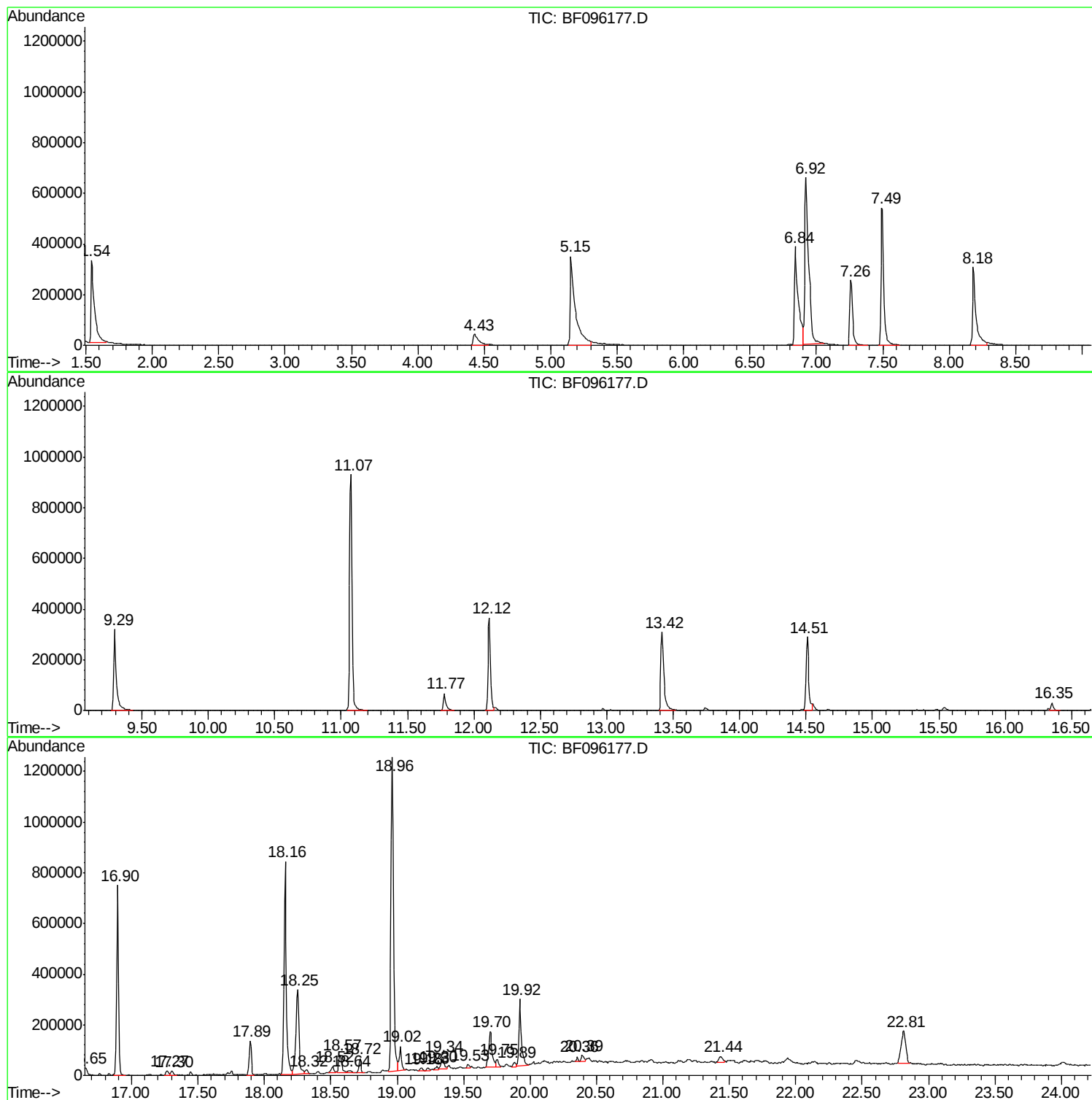
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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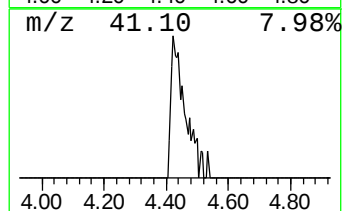
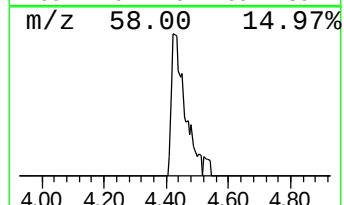
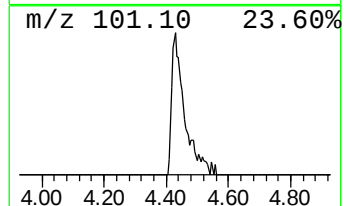
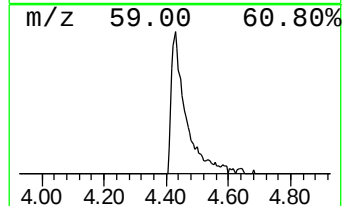
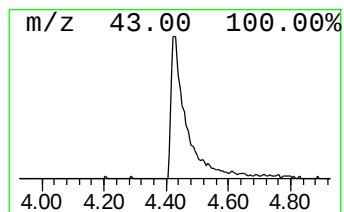
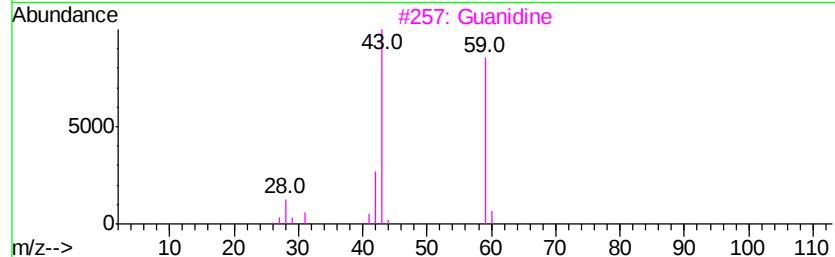
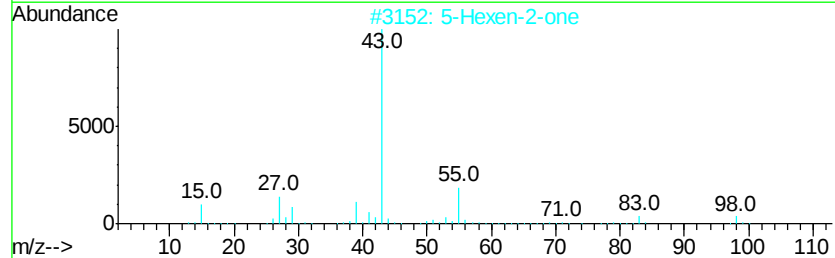
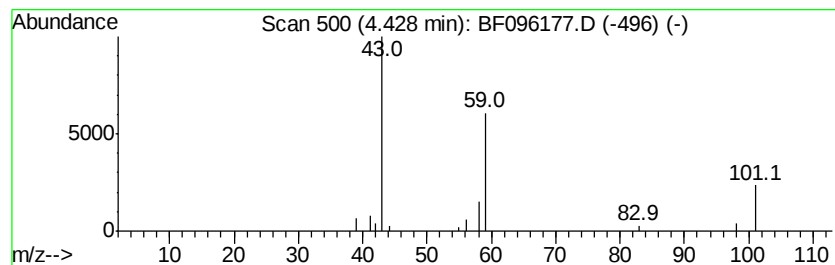
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	7.11 ng	129553	1,4-Dichlorobenzene-d4	7.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			Guanidine	59	CH5N3	000113-00-8	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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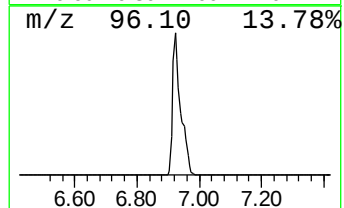
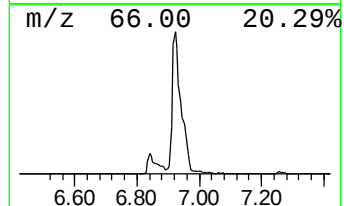
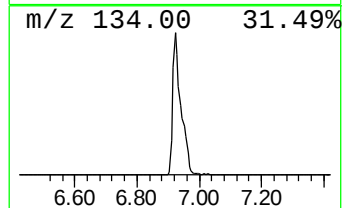
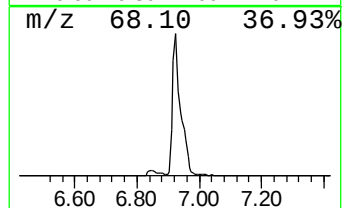
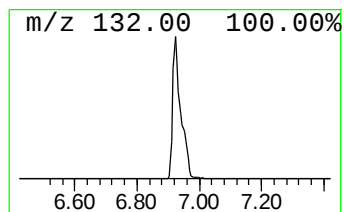
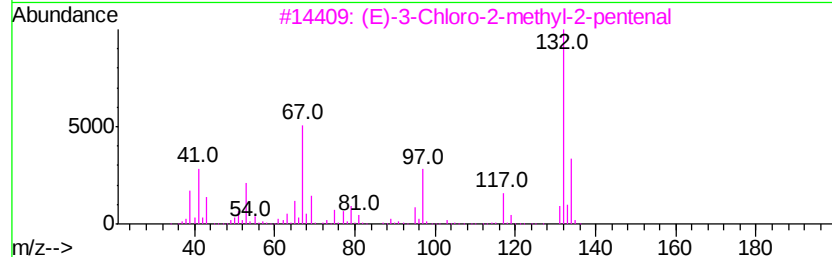
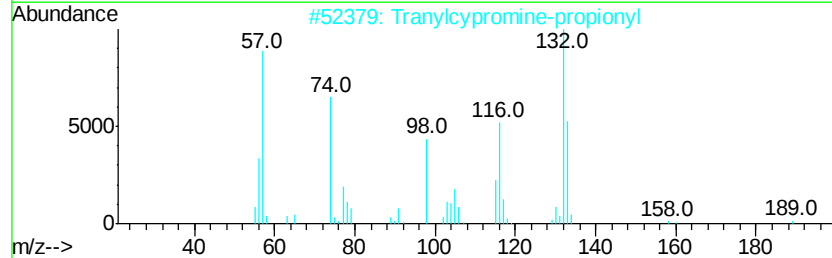
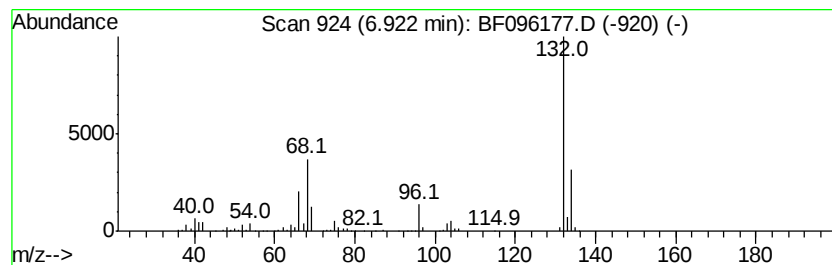
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	72.70 ng	1324540	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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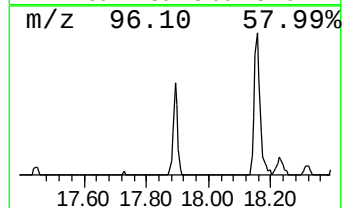
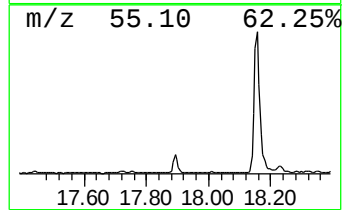
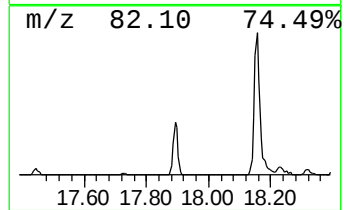
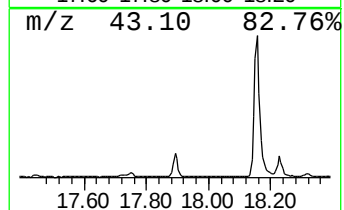
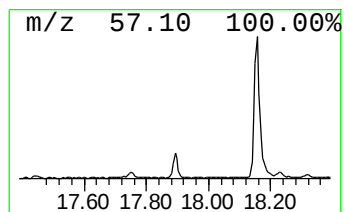
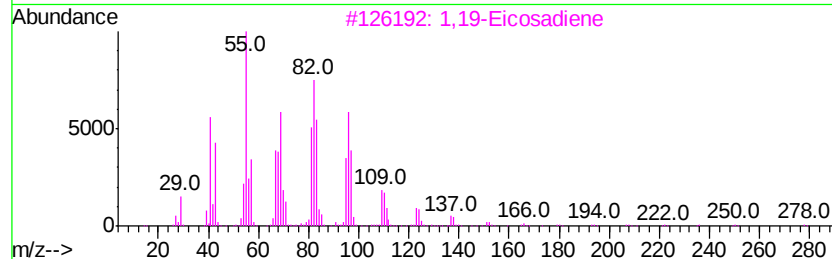
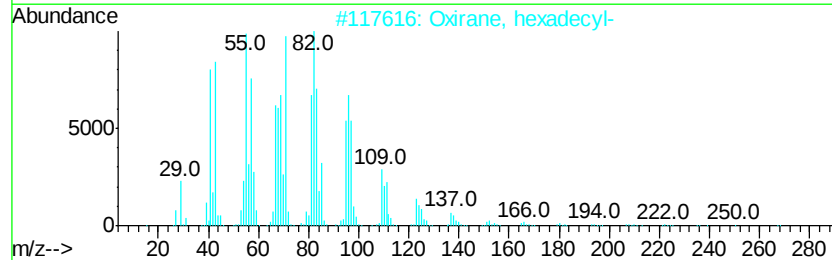
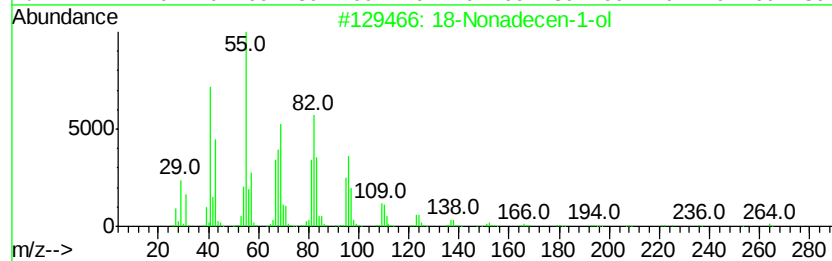
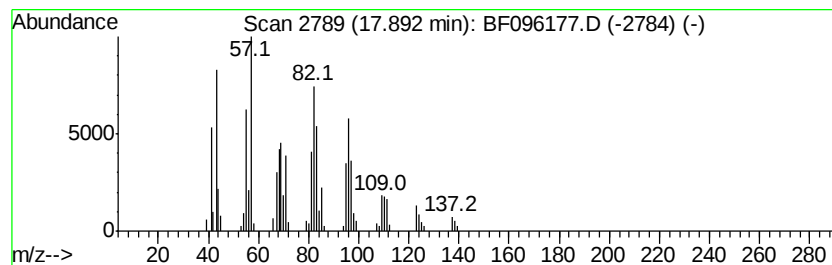
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 18-Nonadecen-1-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.89	5.61 ng	144798	Chrysene-d12		18.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	83
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
3	1,19-Eicosadiene	278	C20H38	014811-95-1	74
4	Pentadecanal-	226	C15H30O	002765-11-9	72
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	59



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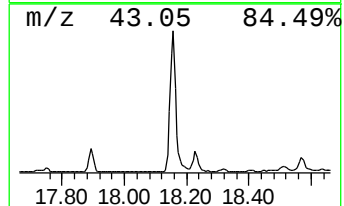
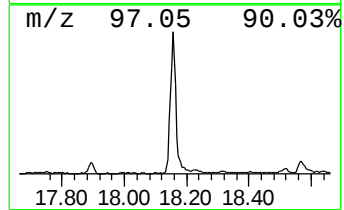
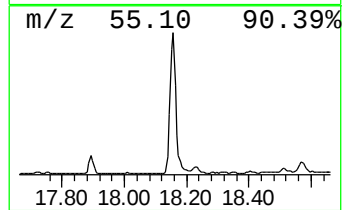
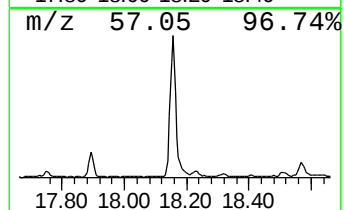
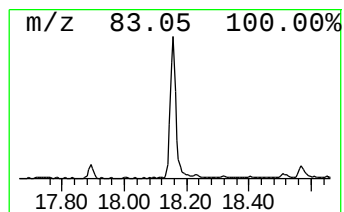
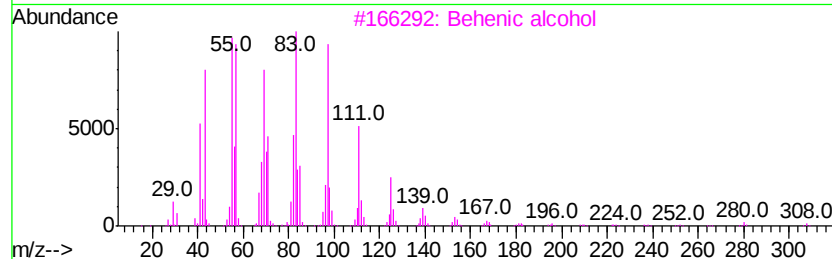
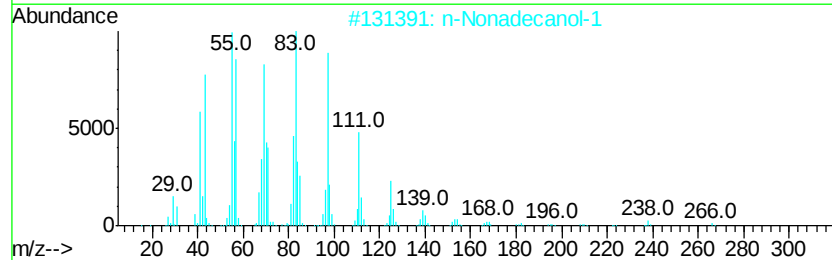
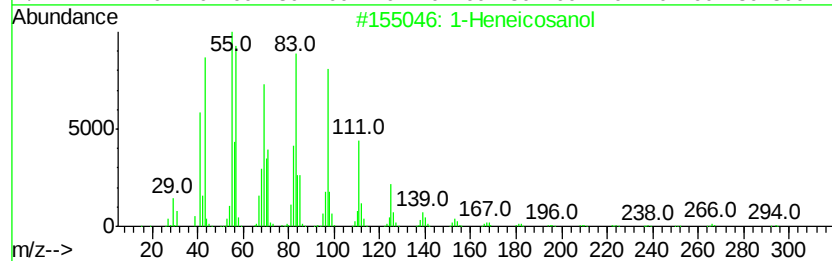
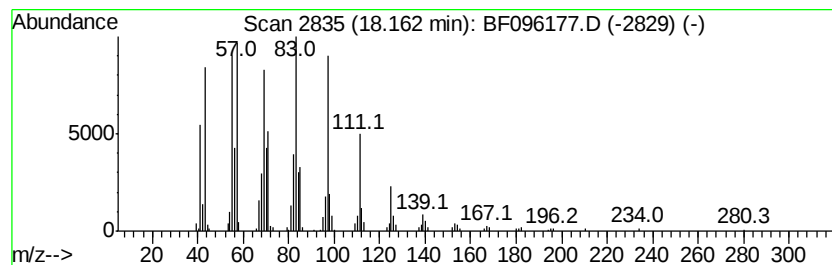
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.16	41.24 ng	1063480	Chrysene-d12		18.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			Behenic alcohol	326	C22H46O	000661-19-8	93
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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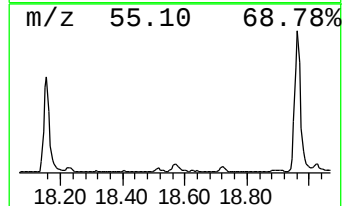
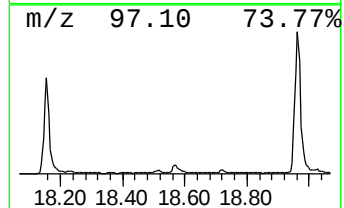
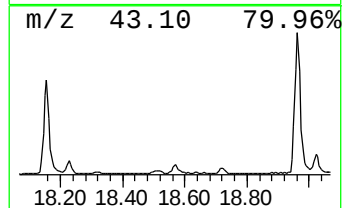
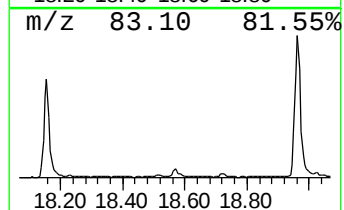
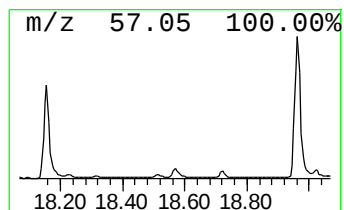
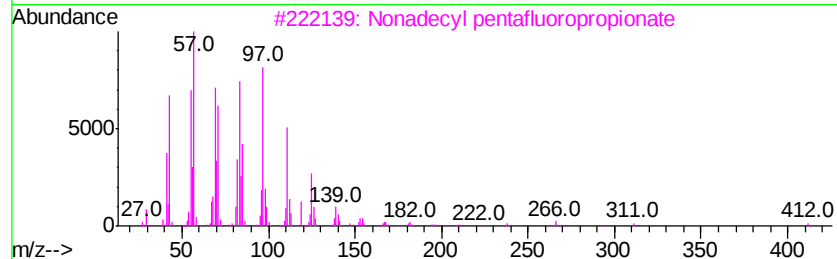
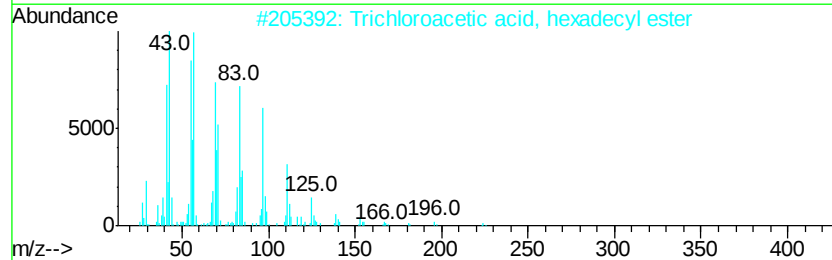
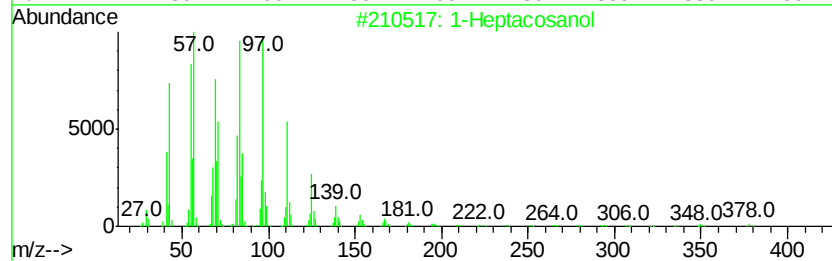
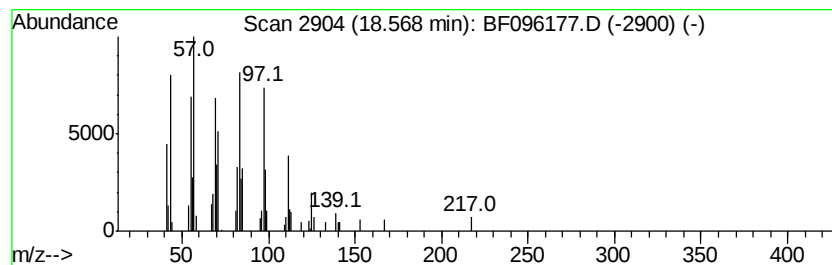
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heptacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	4.37 ng	112691	Chrysene-d12	18.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol		396 C27H56O	002004-39-9 93
2	Trichloroacetic acid, hexadecyl ...		386 C18H33Cl3O2	074339-54-1 91
3	Nonadecyl pentafluoropropionate		430 C22H39F5O2	1000351-88-8 91
4	Octacosyl acetate		452 C30H60O2	018206-97-8 90
5	Heptacosyl acetate		438 C29H58O2	1000351-78-2 90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096177.D
Acq On : 24 Jun 2017 00:46
Operator : SJ/MA
Sample : I3784-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P.56-C-COMP

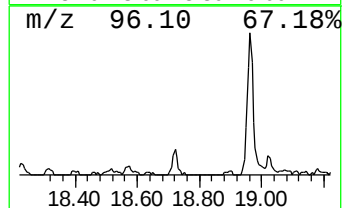
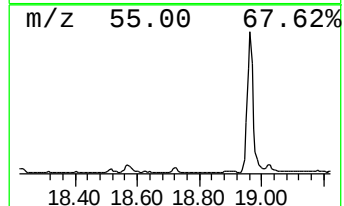
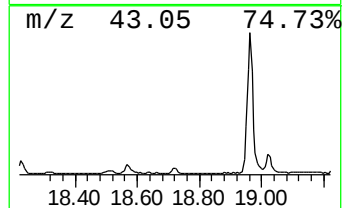
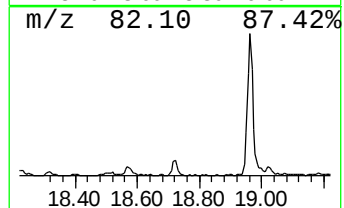
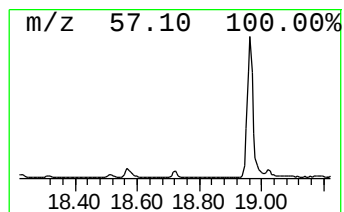
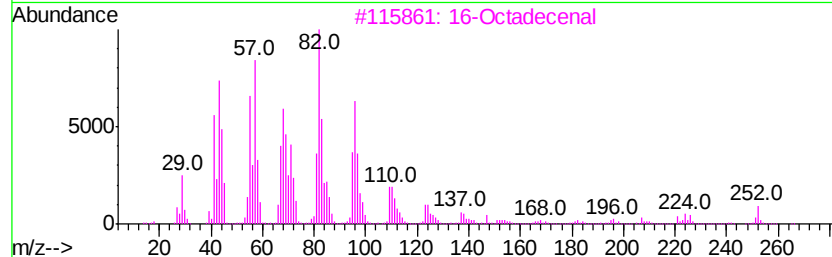
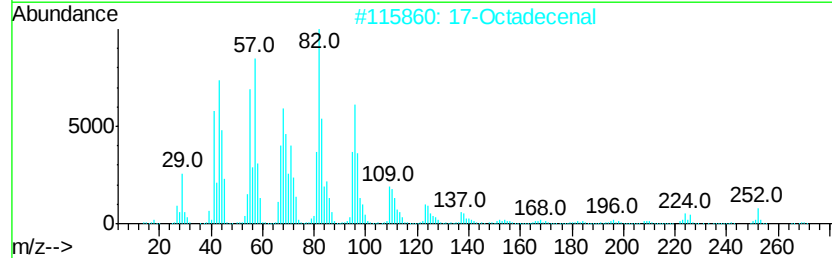
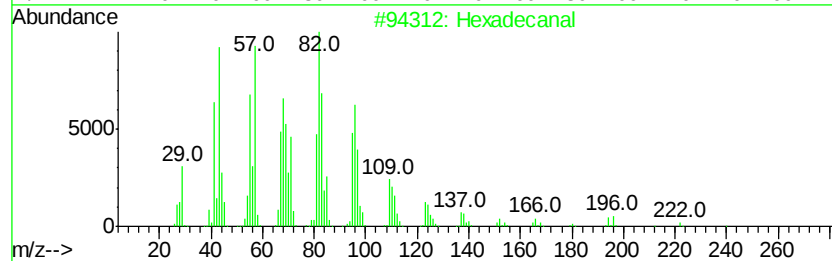
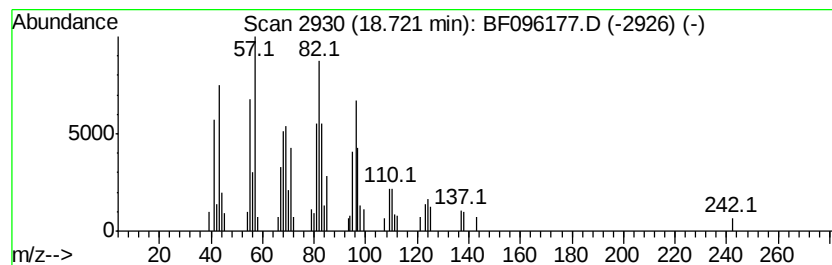
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanal Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.72	2.52 ng	65025	Chrysene-d12		18.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanal	240	C16H32O	000629-80-1	91
2			17-Octadecenal	266	C18H34O	056554-86-0	91
3			16-Octadecenal	266	C18H34O	056554-87-1	90
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5			1,16-Hexadecanediol	258	C16H34O2	007735-42-4	83



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Sample : I3784-05
Misc :
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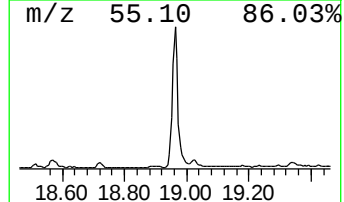
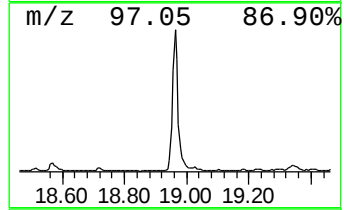
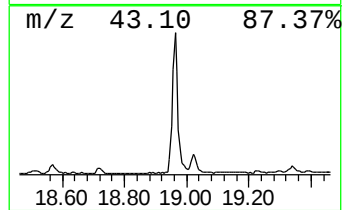
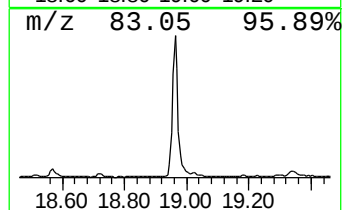
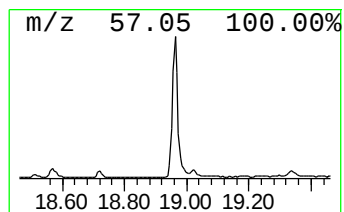
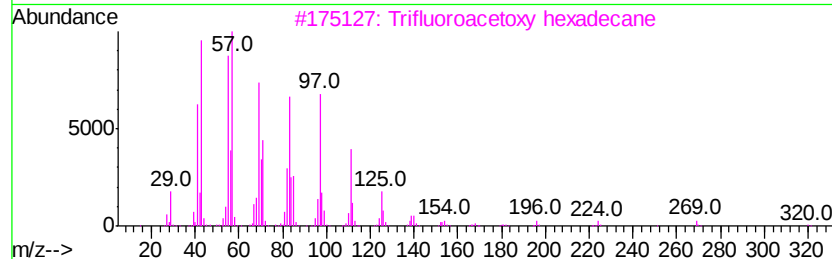
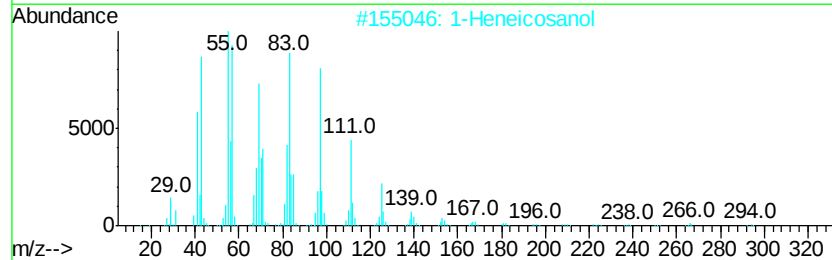
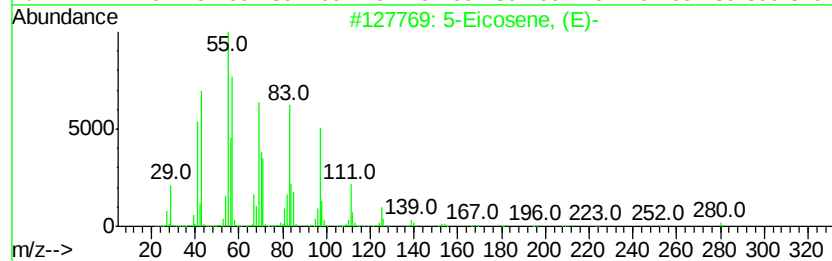
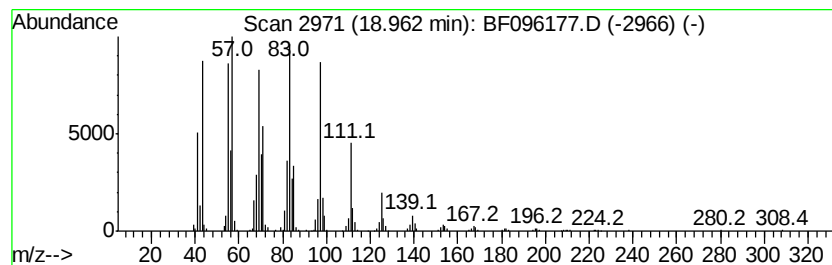
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.96	61.03 ng	1573970	Chrysene-d12		18.25	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
5	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94



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BNA_F
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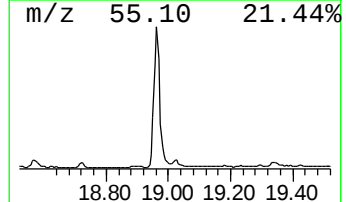
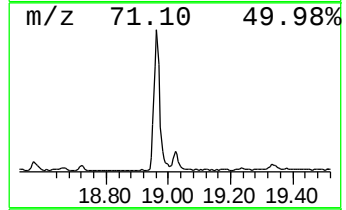
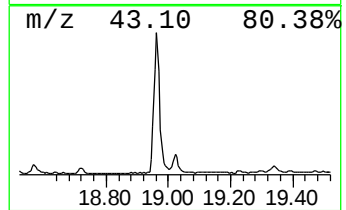
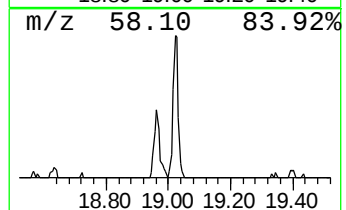
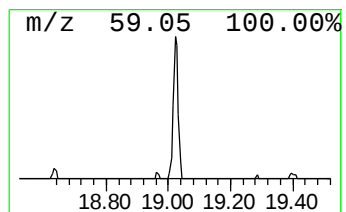
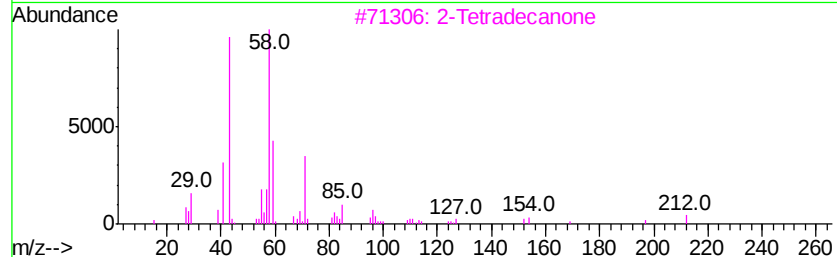
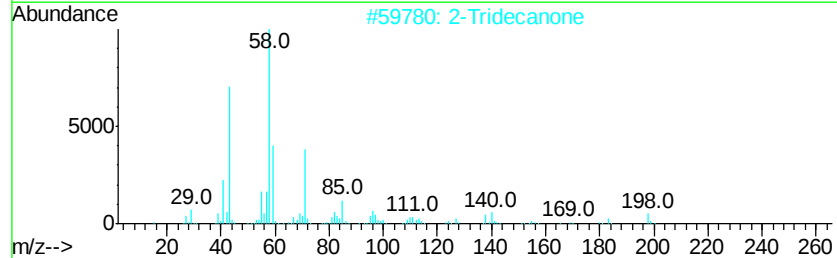
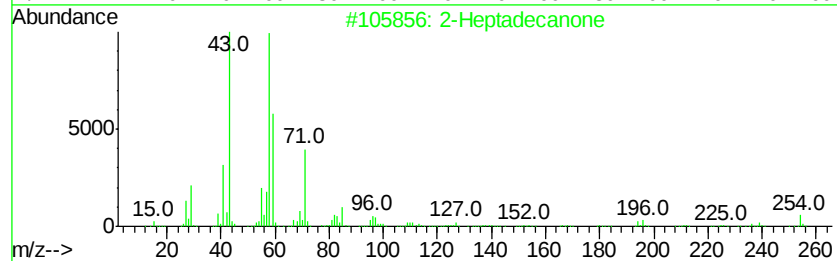
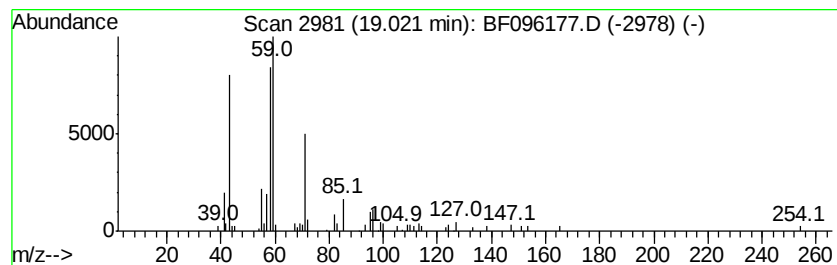
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Heptadecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	4.81 ng	124080	Chrysene-d12	18.25

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptadecanone	254	C17H34O	002922-51-2	59
2			2-Tridecanone	198	C13H26O	000593-08-8	53
3			2-Tetradecanone	212	C14H28O	002345-27-9	53
4			N-Methyl-N-methoxycarbonylcarbam...	175	C6H9NO5	073830-21-4	50
5			2-Nonadecanone	282	C19H38O	000629-66-3	50



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Misc :
ALS Vial : 22 Sample Multiplier: 1

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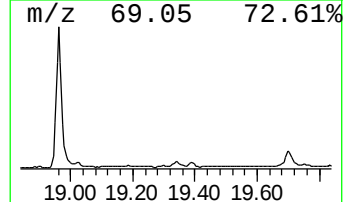
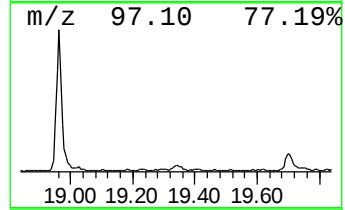
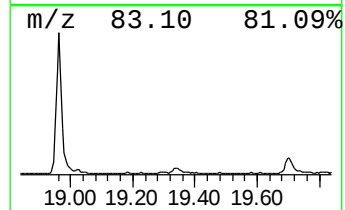
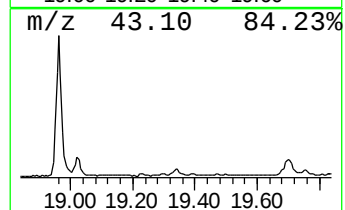
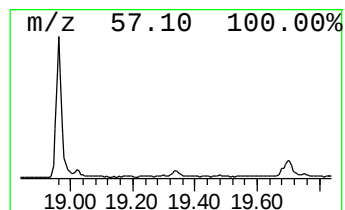
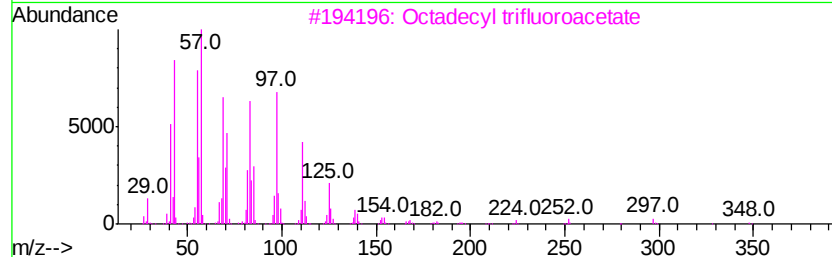
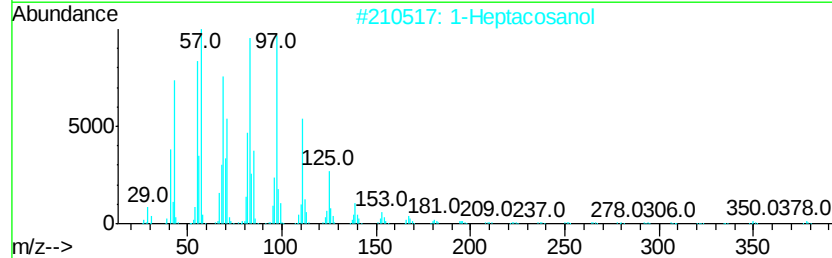
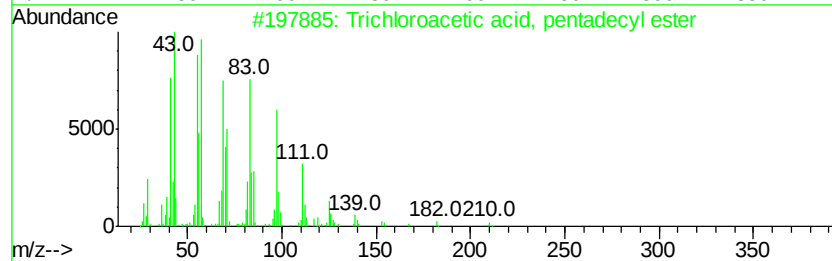
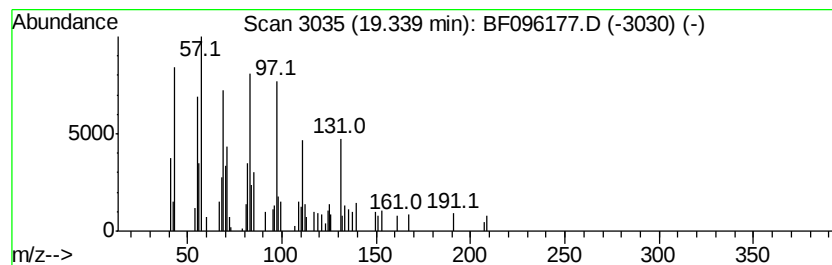
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Trichloroacetic acid, penta... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	4.31 ng	78275	Perylene-d12	19.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
2		1-Heptacosanol	396	C27H56O	002004-39-9	81
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
4		1-Nonadecene	266	C19H38	018435-45-5	76
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
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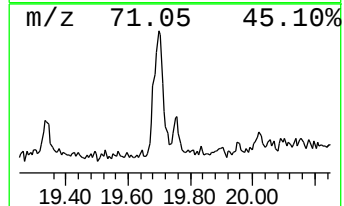
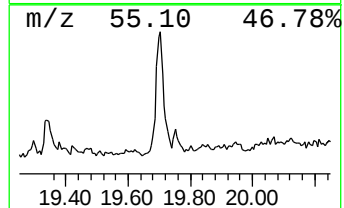
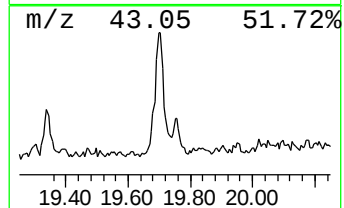
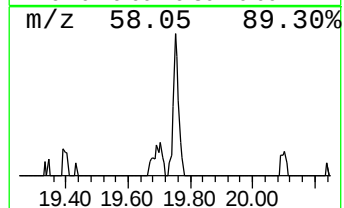
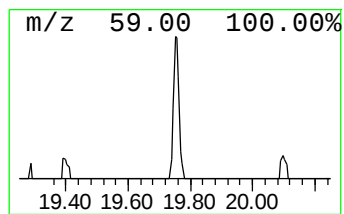
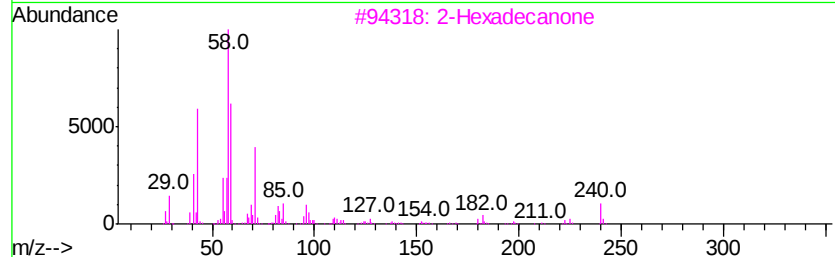
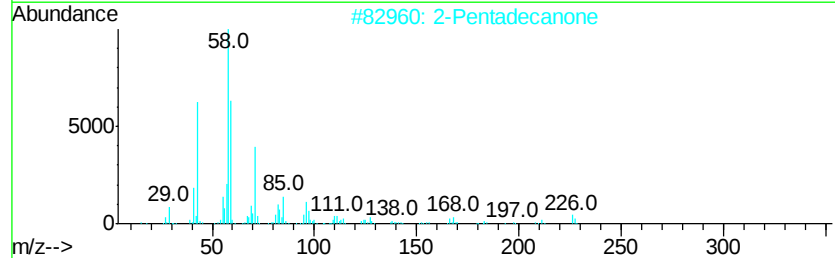
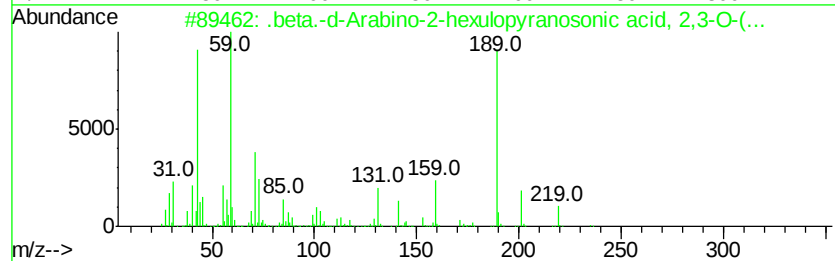
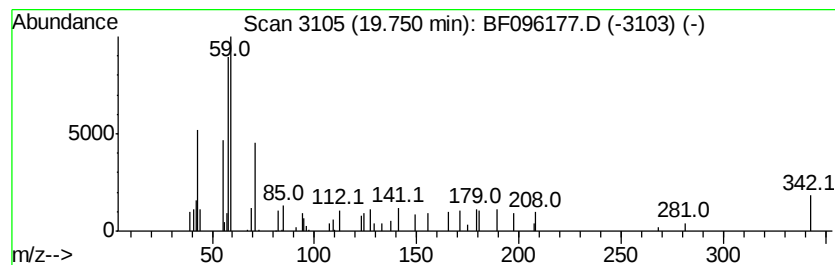
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown19.75 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	2.18 ng	39609	Perylene-d12	19.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-d-Arabino-2-hexulopvranos...	234	C9H14O7	058238-50-9	32	
2	2-Pentadecanone		226	C15H30O	002345-28-0	28	
3	2-Hexadecanone		240	C16H32O	018787-63-8	25	
4	Guanidine, N-[3-[(2-bromophenyl)]...		268	C10H13BrN4	1000349-85-6	25	
5	2-Pentadecanone, 6,10,14-trimethyl-		268	C18H36O	000502-69-2	23	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
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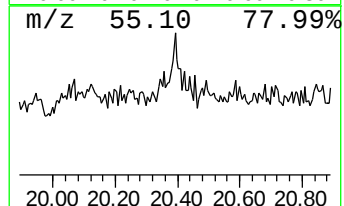
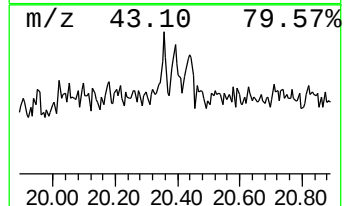
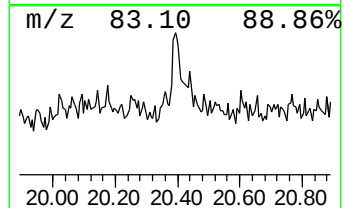
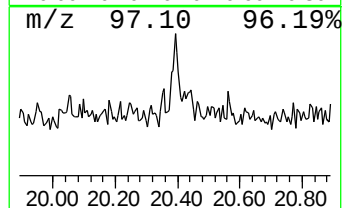
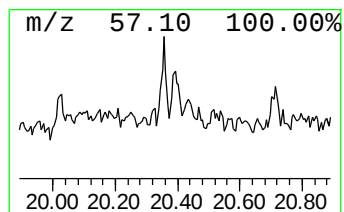
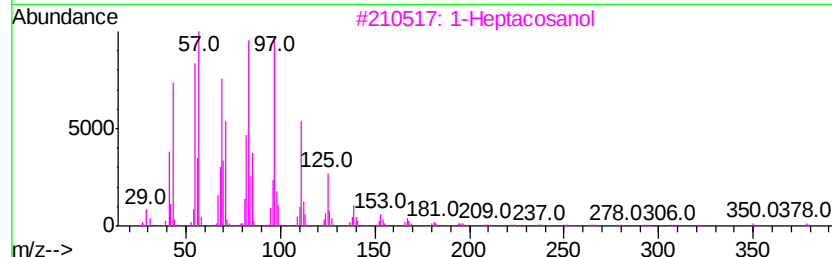
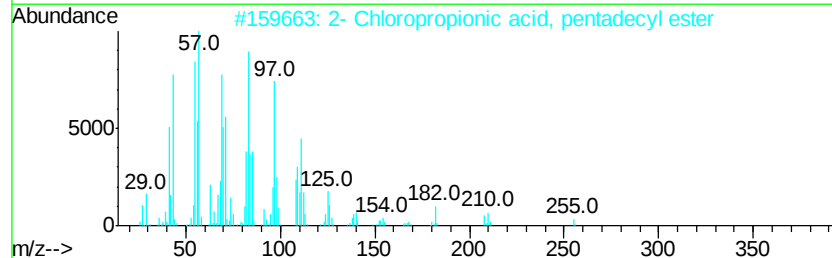
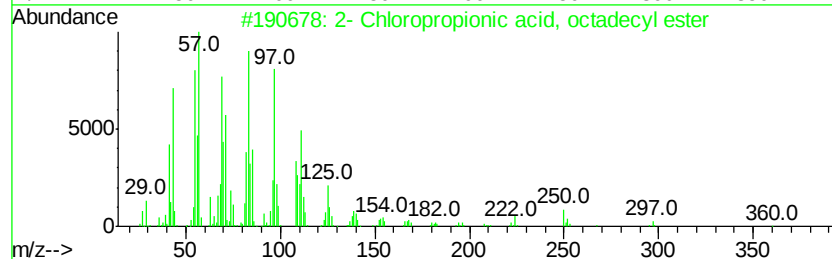
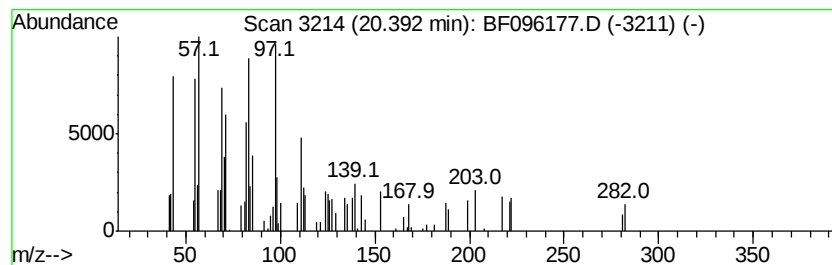
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 2- Chloropropionic acid, oc... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.39	2.07 ng	37696	Perylene-d12	19.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	74
2	2-	Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	72
3	1-	Heptacosanol	396	C27H56O	002004-39-9	64
4		Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	64
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	53



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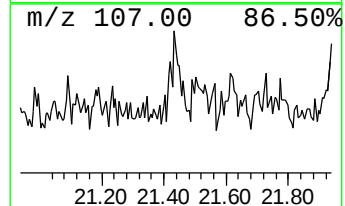
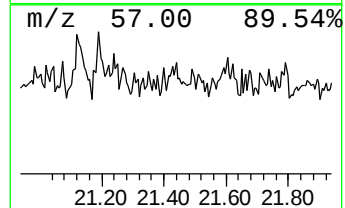
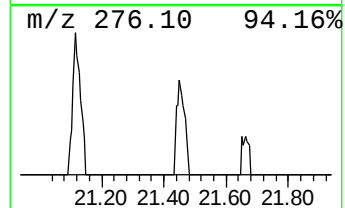
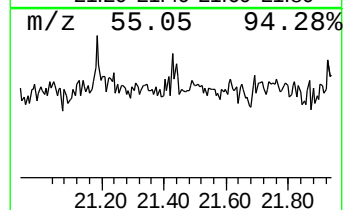
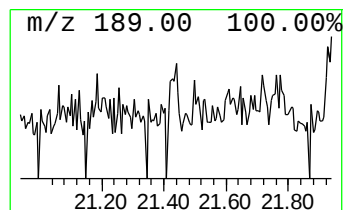
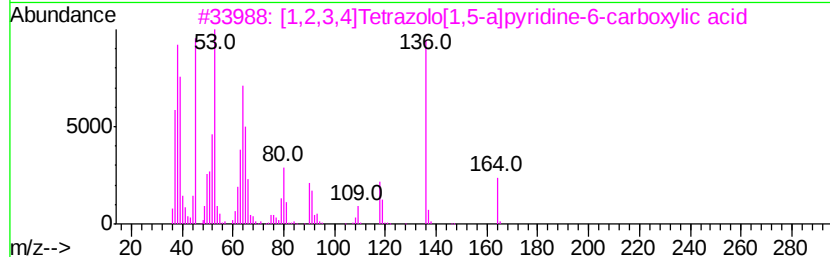
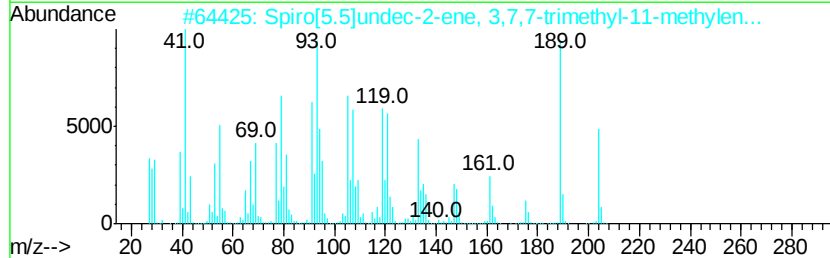
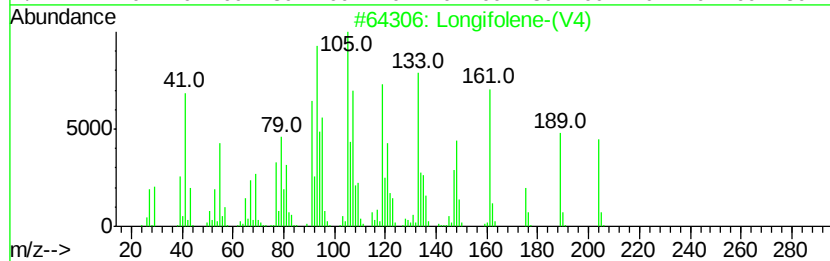
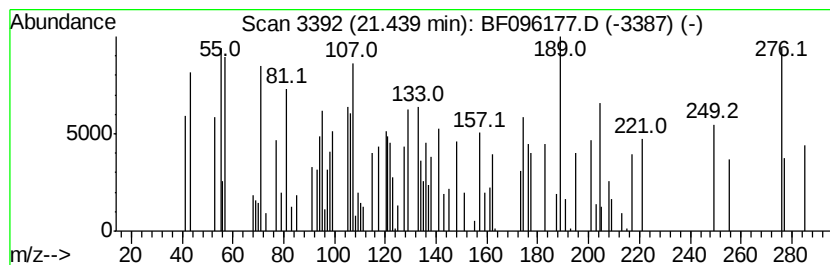
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown21.44 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	2.54 ng	46100	Perylene-d12	19.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Longifolene-(V4)	204 C15H24	061262-67-7 25
2		Spiro[5.5]undec-2-ene, 3,7,7-tri...	204 C15H24	018431-82-8 11
3		[1,2,3,4]Tetrazolo[1,5-a]pyridin...	164 C6H4N4O2	1000362-60-7 11
4		2,6,10,10-Tetramethylbicyclo[7.2...	204 C15H24	136296-37-2 11
5		Androstan-17-ol, (5.beta.,17.bet...	276 C19H32O	010328-72-0 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096177.D
Acq On : 24 Jun 2017 00:46
Operator : SJ/MA
Sample : I3784-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P.56-C-COMP

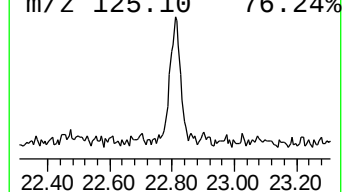
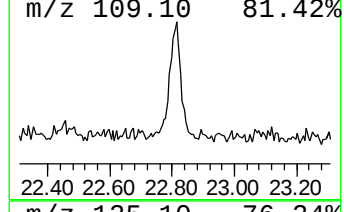
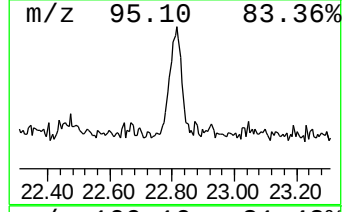
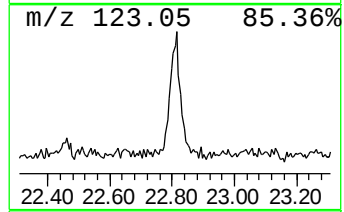
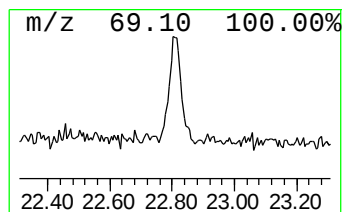
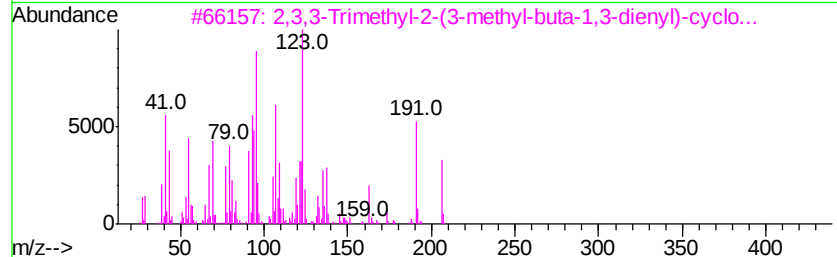
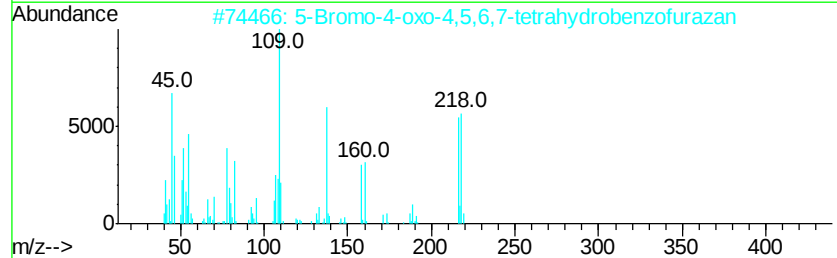
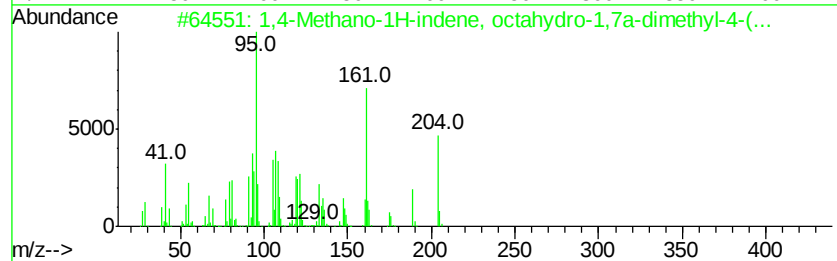
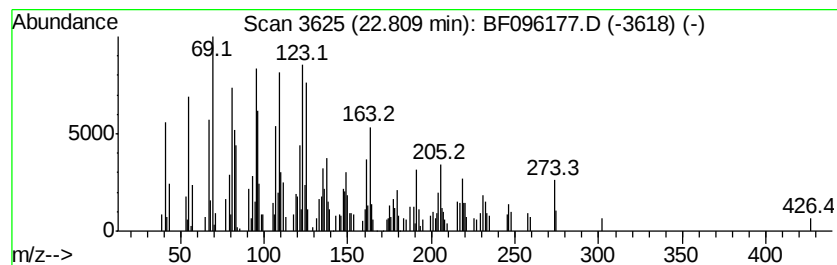
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1,4-Methano-1H-indene, octa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.81	16.73 ng	303941	Perylene-d12	19.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	62
2			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
3			2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	52
4			Caparratriene	206	C15H26	1000374-08-7	50
5			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
 Data File : BF096177.D
 Acq On : 24 Jun 2017 00:46
 Operator : SJ/MA
 Sample : I3784-05
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P.56-C-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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
2-Pentanone, 4-hy...	4.43	7.1 ng		129553	1	7.26	364393	20.0
unknown6.92	6.92	72.7 ng		1324540	1	7.26	364393	20.0
18-Nonadecen-1-ol	17.89	5.6 ng		144798	5	18.25	515784	20.0
1-Heneicosanol	18.16	41.2 ng		1063480	5	18.25	515784	20.0
1-Heptacosanol	18.57	4.4 ng		112691	5	18.25	515784	20.0
Hexadecanal	18.72	2.5 ng		65025	5	18.25	515784	20.0
5-Eicosene, (E)-	18.96	61.0 ng		1573970	5	18.25	515784	20.0
2-Heptadecanone	19.02	4.8 ng		124080	5	18.25	515784	20.0
Trichloroacetic a...	19.34	4.3 ng		78275	6	19.92	363354	20.0
unknown19.75	19.75	2.2 ng		39609	6	19.92	363354	20.0
2-Chloropropioni...	20.39	2.1 ng		37696	6	19.92	363354	20.0
unknown21.44	21.44	2.5 ng		46100	6	19.92	363354	20.0
1,4-Methano-1H-in...	22.81	16.7 ng		303941	6	19.92	363354	20.0