

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
 Data File : BF096618.D
 Acq On : 10 Jul 2017 23:11
 Operator : SJ/JU
 Sample : I4095-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-011

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-BF070117.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	4.869	468	473	484	rBV	429056	535938	20.86%	2.207%
2	5.298	541	546	549	rBV	2351763	2465134	95.96%	10.154%
3	6.322	715	720	731	rBV	2404984	2568821	100.00%	10.581%
4	6.451	738	742	746	rBV	2557194	2482896	96.66%	10.227%
5	6.681	778	781	785	rBV	953788	811575	31.59%	3.343%
6	6.840	804	808	811	rBV	2104080	1857932	72.33%	7.653%
7	7.245	871	877	880	rBV	1645538	1590513	61.92%	6.551%
8	7.963	995	999	1003	rBV	1227073	1085868	42.27%	4.473%
9	9.045	1177	1183	1186	rBV	2364624	2440290	95.00%	10.051%
10	9.434	1245	1249	1252	rBV	311072	241232	9.39%	0.994%
11	9.716	1292	1297	1301	rBV	1098993	1017278	39.60%	4.190%
12	10.163	1369	1373	1376	rVB	41708	35790	1.39%	0.147%
13	10.381	1402	1410	1413	rBV2	16741	27143	1.06%	0.112%
14	10.498	1425	1430	1441	rVB	1293766	1228045	47.81%	5.058%
15	10.633	1450	1453	1461	rBV	60141	66772	2.60%	0.275%
16	11.080	1525	1529	1531	rBV2	47924	40959	1.59%	0.169%
17	11.192	1543	1548	1551	rBV	968285	826234	32.16%	3.403%
18	12.774	1813	1817	1821	rBV	1652824	1534729	59.74%	6.321%
19	13.680	1967	1971	1978	rBV	176598	198331	7.72%	0.817%
20	13.821	1991	1995	1998	rBV	758078	742060	28.89%	3.056%
21	14.004	2021	2026	2030	rBV4	21305	32269	1.26%	0.133%
22	14.316	2075	2079	2085	rBV2	57418	77552	3.02%	0.319%
23	14.604	2125	2128	2134	rBV2	23512	38158	1.49%	0.157%
24	14.668	2137	2139	2144	rVB2	26279	32106	1.25%	0.132%
25	14.916	2178	2181	2184	rBV	38274	45590	1.77%	0.188%
26	15.215	2227	2232	2238	rBV2	594101	754894	29.39%	3.109%
27	15.268	2238	2241	2247	rVB	36386	48444	1.89%	0.200%
28	15.663	2305	2308	2313	rBV2	31627	40136	1.56%	0.165%
29	15.710	2313	2316	2324	rVB7	23496	46180	1.80%	0.190%
30	16.127	2383	2387	2391	rVB2	28548	42761	1.66%	0.176%
31	17.104	2547	2553	2567	rVB2	65360	208010	8.10%	0.857%
32	17.292	2583	2585	2593	rVB9	31350	59818	2.33%	0.246%
33	18.039	2706	2712	2716	rVB8	21443	41510	1.62%	0.171%
34	18.803	2837	2842	2843	rBV4	43582	57611	2.24%	0.237%

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-011

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.980	2861	2872	2886	rVB3	294365	956045	37.22%	3.938%
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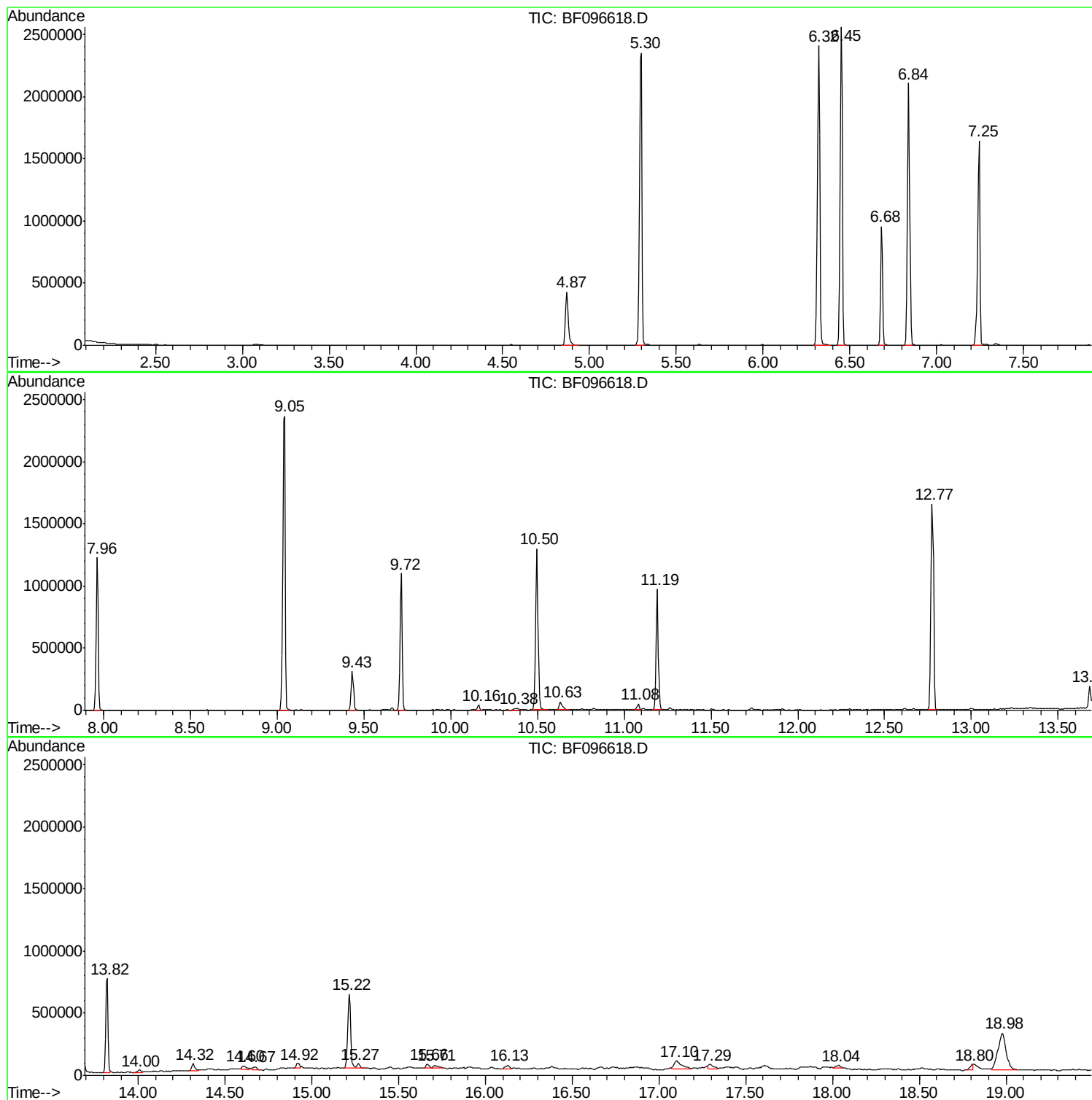
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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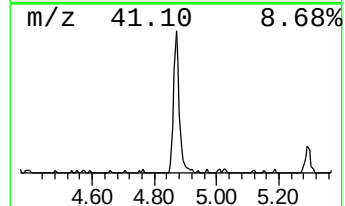
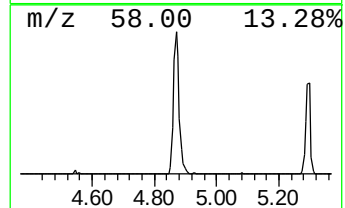
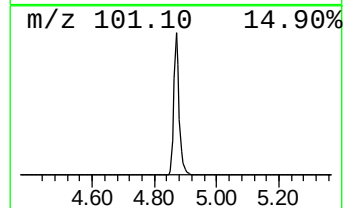
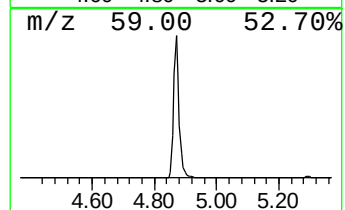
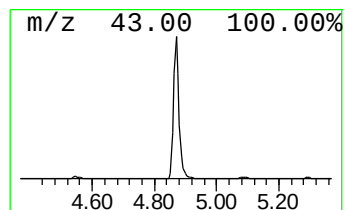
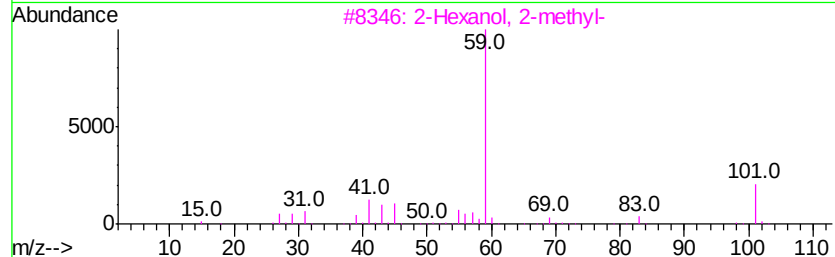
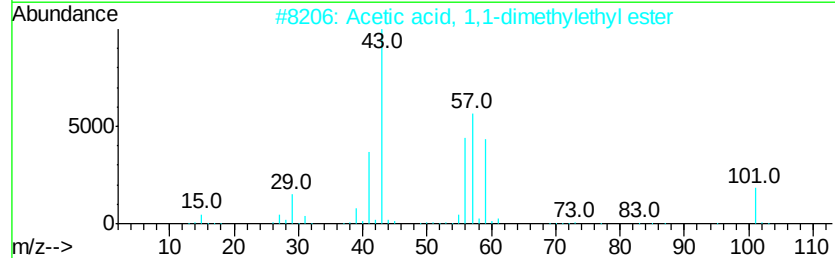
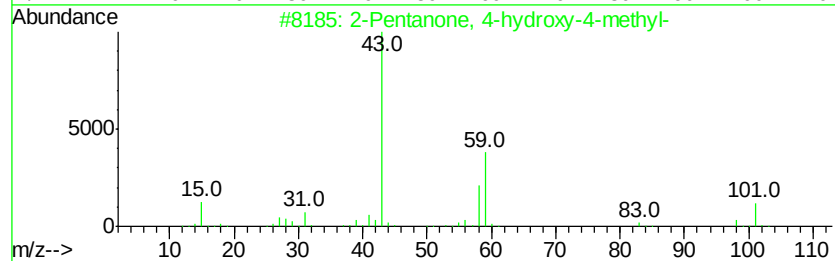
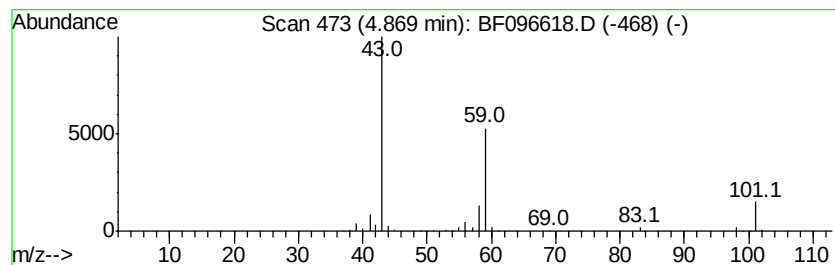
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	13.21 ng	535938	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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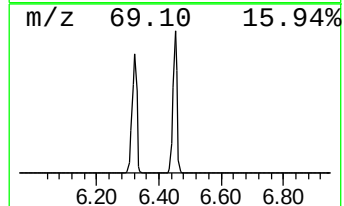
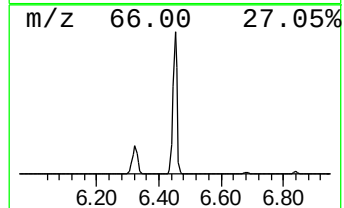
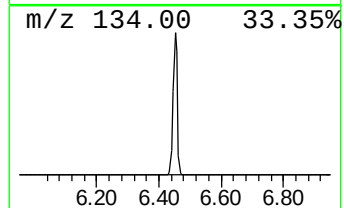
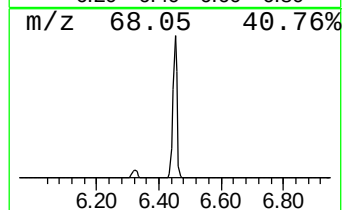
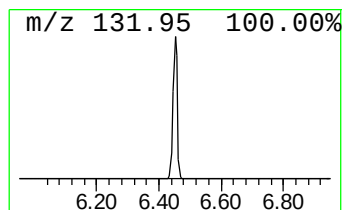
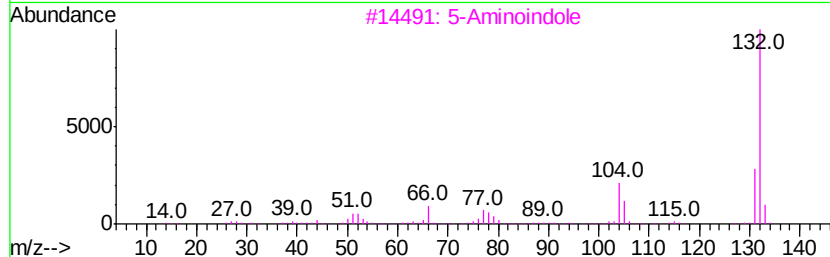
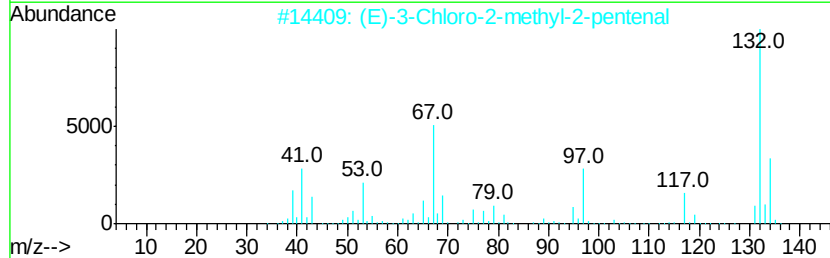
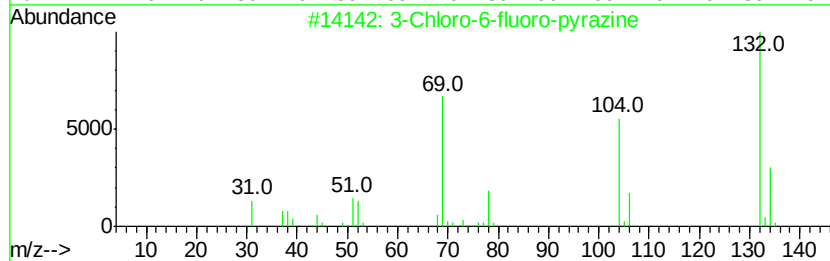
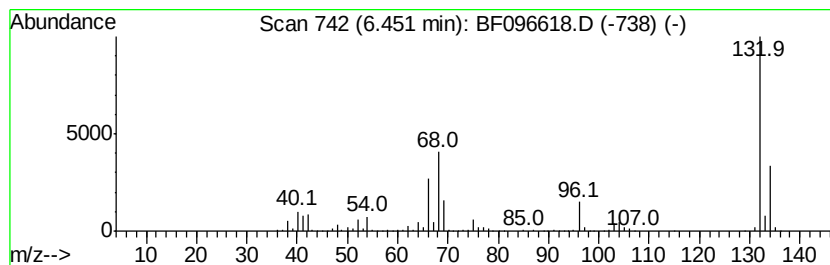
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	61.19 ng	2482900	1,4-Dichlorobenzene-d4	6.68

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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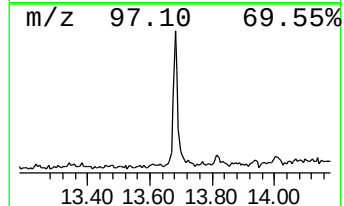
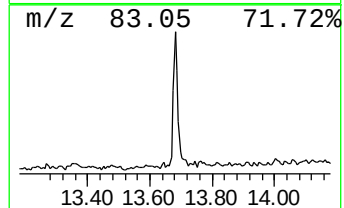
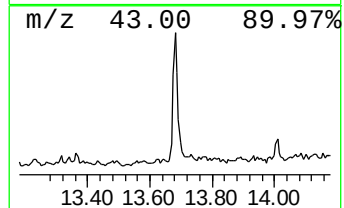
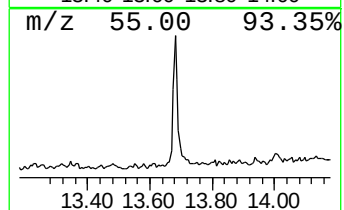
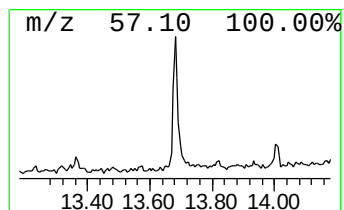
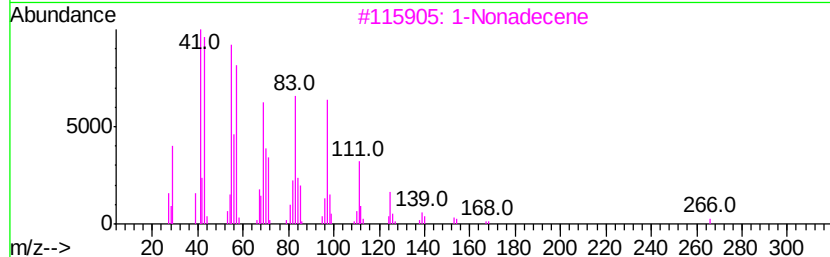
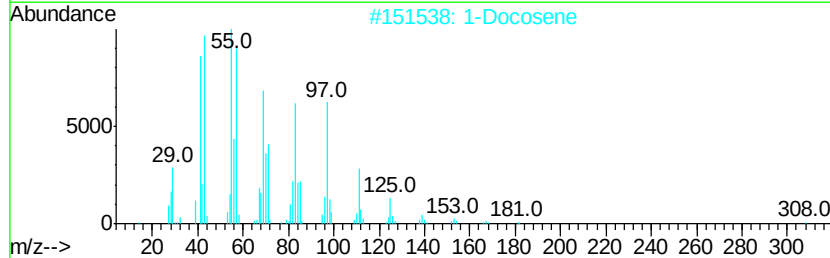
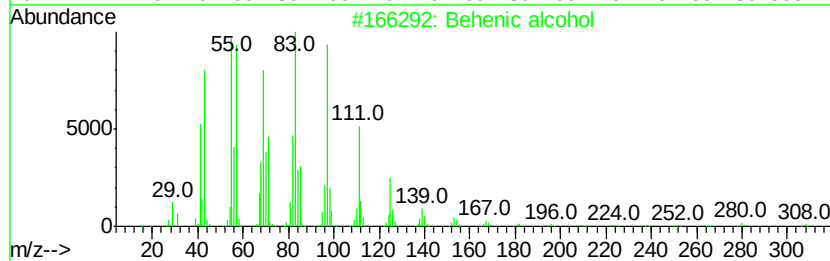
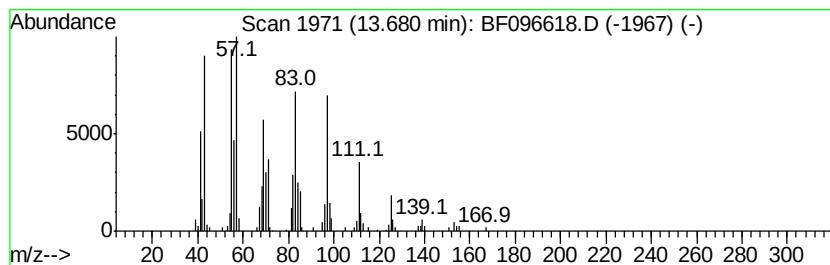
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	5.35 ng	198331	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	93
2		1-Docosene	308	C22H44	001599-67-3	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5		1-Octadecanol	270	C18H38O	000112-92-5	91



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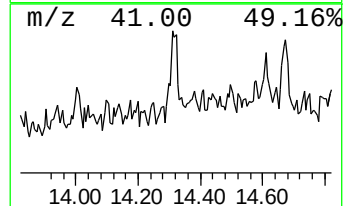
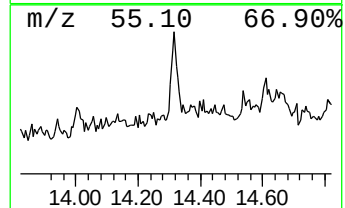
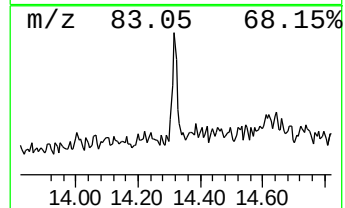
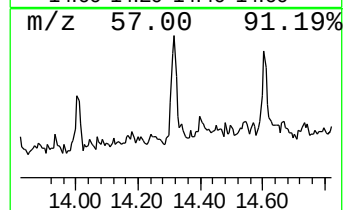
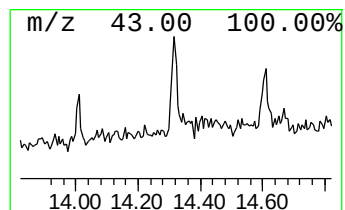
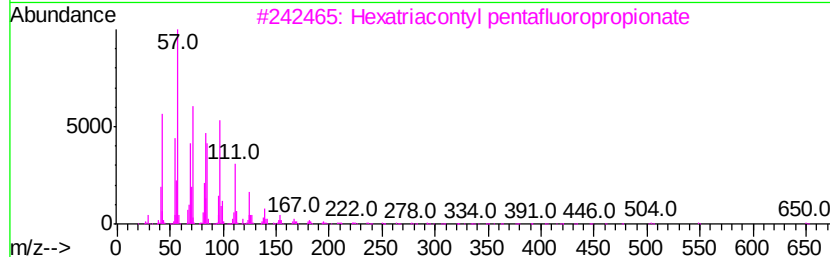
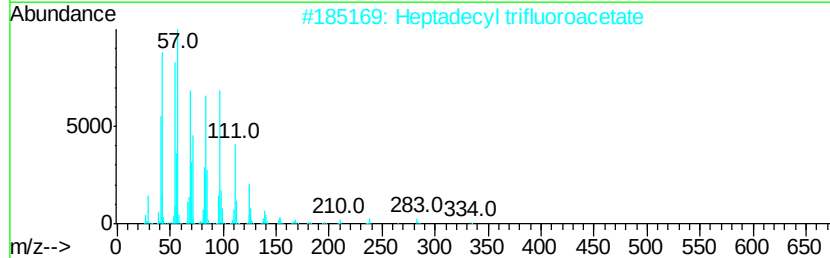
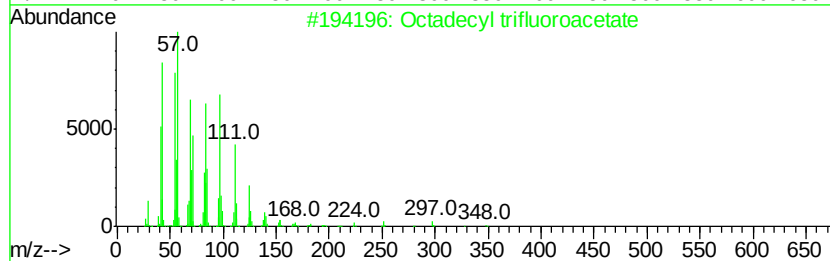
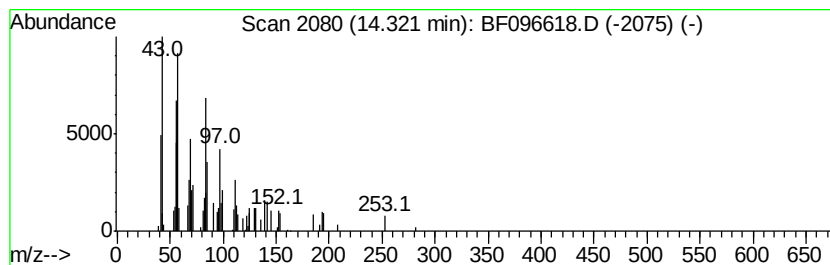
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.09 ng	77552	Chrysene-d12	13.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76
3		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	74
4		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	74
5		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	72



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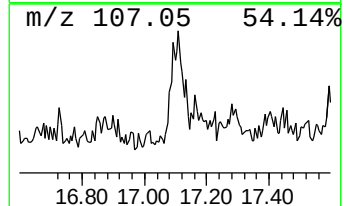
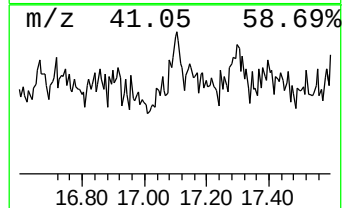
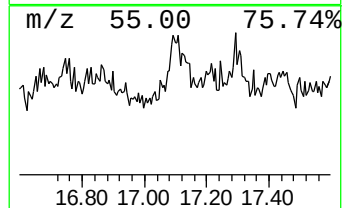
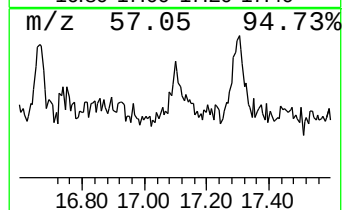
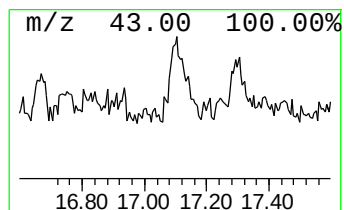
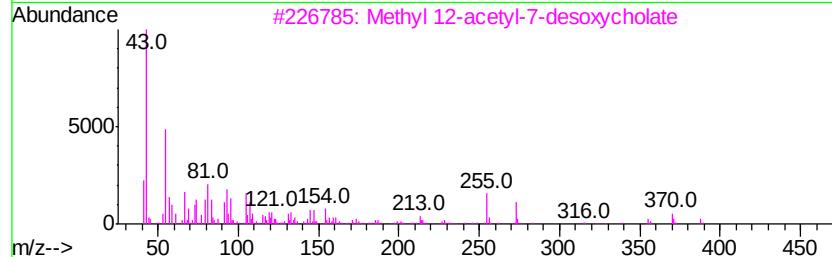
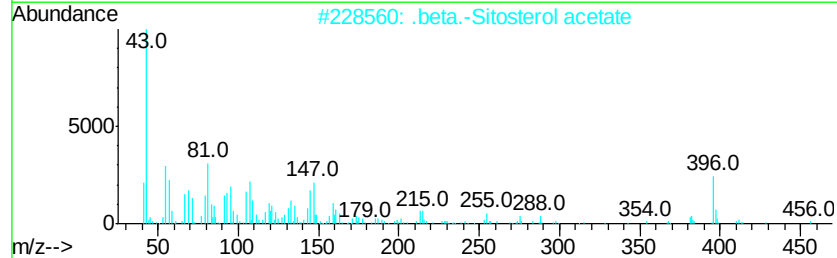
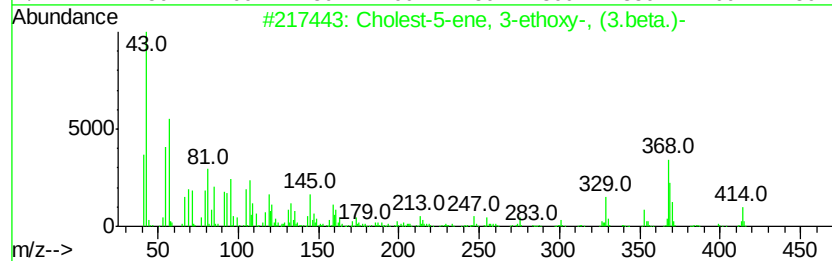
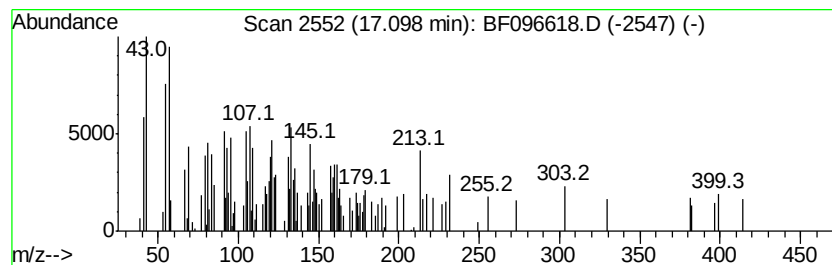
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown17.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.10	5.51 ng	208010	Perylene-d12	15.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	37
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	32
3	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	32
4	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	25
5	1,10,25,26-Tetraaza-4,7-dioxatet...	354	C20H26N4O2	286013-88-5	25



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ClientSampleId :
FK-PS-01-011

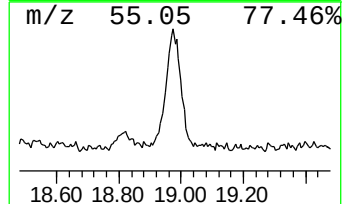
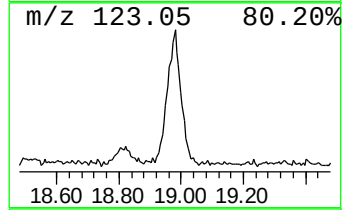
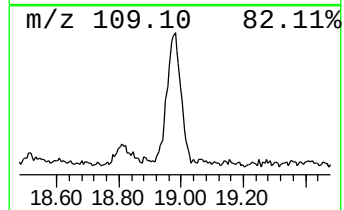
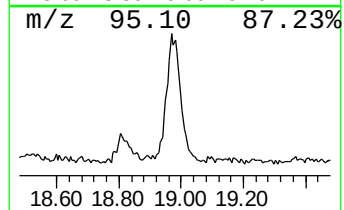
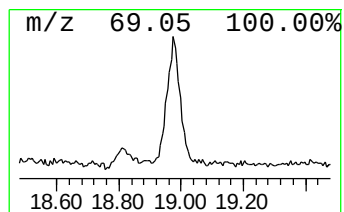
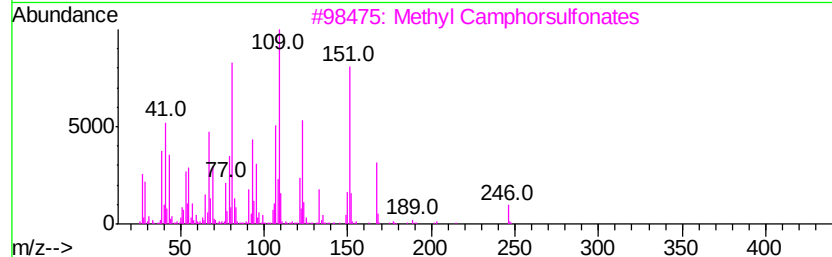
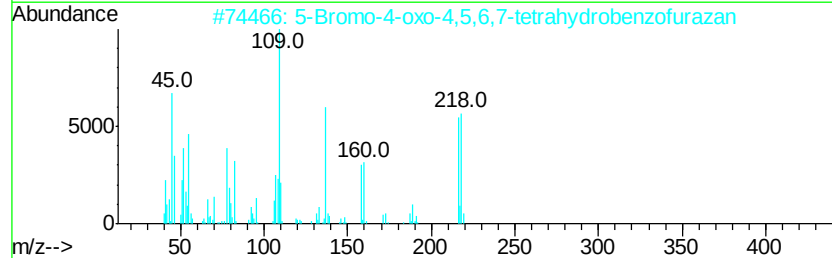
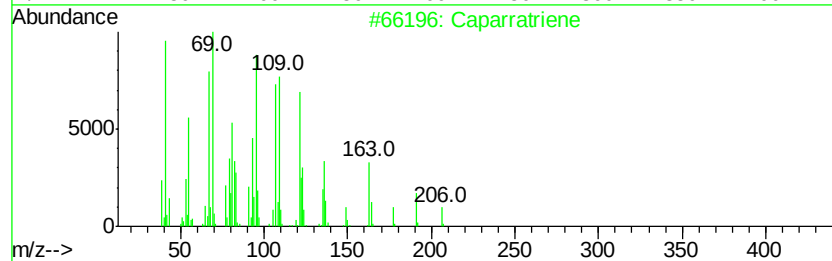
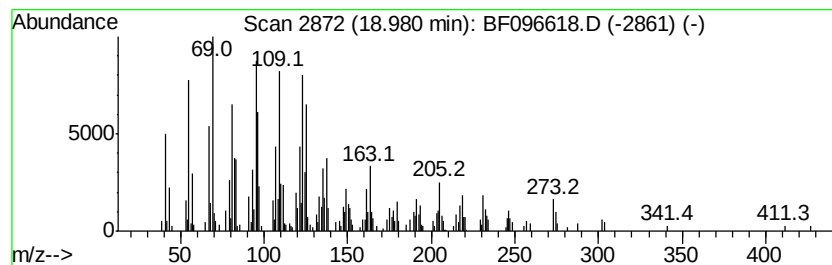
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Caparratriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.98	25.33 ng	956045	Perylene-d12	15.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	60
2		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60
3		Methyl Camphorsulfonates	246	C11H18O4S	046471-67-4	52
4		7-Tetradecyne	194	C14H26	035216-11-6	46
5		2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096618.D
Acq On : 10 Jul 2017 23:11
Operator : SJ/JU
Sample : I4095-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.87	13.2	ng	535938	1	6.68	811575	20.0
unknown6.45	6.45	61.2	ng	2482900	1	6.68	811575	20.0
Behenic alcohol	13.68	5.3	ng	198331	5	13.82	742060	20.0
Octadecyl trifluo...	14.32	2.1	ng	77552	5	13.82	742060	20.0
unknown17.10	17.10	5.5	ng	208010	6	15.22	754894	20.0
Caparratriene	18.98	25.3	ng	956045	6	15.22	754894	20.0