

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
 Data File : BF100837.D
 Acq On : 22 Nov 2017 21:41
 Operator : SJ/JU
 Sample : I6043-18
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N-T0A-BAJA-S001-0001-02

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-BF110817.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	5.087	505	510	520	rVB	196753	257707	12.95%	1.412%
2	5.481	572	577	580	rBV	1718362	1664820	83.64%	9.119%
3	6.492	743	749	753	rBV	1545537	1795860	90.22%	9.837%
4	6.628	767	772	775	rBV	1840187	1796058	90.23%	9.838%
5	6.857	807	811	815	rBB	595164	489480	24.59%	2.681%
6	7.016	834	838	841	rVB	1605345	1360029	68.33%	7.450%
7	7.422	902	907	910	rVB	1152147	1128530	56.70%	6.182%
8	8.139	1025	1029	1032	rBV	799864	660012	33.16%	3.615%
9	8.692	1119	1123	1126	rBV	160181	124162	6.24%	0.680%
10	9.216	1207	1212	1215	rBV	2268384	1990477	100.00%	10.903%
11	9.604	1275	1278	1282	rVB	127853	96299	4.84%	0.528%
12	9.898	1324	1328	1331	rBV	883819	739709	37.16%	4.052%
13	10.298	1392	1396	1402	rBV3	21634	38265	1.92%	0.210%
14	10.610	1445	1449	1452	rBV	680245	543217	27.29%	2.976%
15	10.686	1458	1462	1465	rBV	1330717	1256934	63.15%	6.885%
16	11.321	1567	1570	1574	rBV2	21431	26946	1.35%	0.148%
17	11.386	1577	1581	1584	rVB	790239	732781	36.81%	4.014%
18	11.898	1665	1668	1672	rBV	92646	85039	4.27%	0.466%
19	12.615	1783	1790	1798	rBV8	9002	22699	1.14%	0.124%
20	12.686	1798	1802	1806	rBV2	30986	34226	1.72%	0.187%
21	12.968	1845	1850	1853	rBV	1814503	1589715	79.87%	8.708%
22	13.851	1997	2000	2003	rBV	97446	93140	4.68%	0.510%
23	13.886	2003	2006	2010	rVB	29413	30248	1.52%	0.166%
24	14.021	2026	2029	2032	rVB	532079	436948	21.95%	2.393%
25	14.857	2169	2171	2178	rVB	28981	38454	1.93%	0.211%
26	15.492	2274	2279	2286	rBV	388184	472666	23.75%	2.589%
27	15.939	2350	2355	2359	rBV3	25069	33239	1.67%	0.182%
28	15.986	2359	2363	2369	rBV6	19671	31152	1.57%	0.171%
29	16.362	2422	2427	2435	rVB5	54733	94667	4.76%	0.519%
30	16.445	2435	2441	2447	rBV7	14005	31354	1.58%	0.172%
31	16.733	2486	2490	2496	rVB6	15105	26527	1.33%	0.145%
32	16.968	2524	2530	2536	rBV5	24646	47720	2.40%	0.261%
33	17.039	2536	2542	2547	rVB4	19544	38163	1.92%	0.209%
34	17.121	2550	2556	2565	rBV7	27445	62055	3.12%	0.340%

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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

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	17.533	2620	2626	2635	rBV6	33892	73312	3.68%	0.402%
36	18.103	2716	2723	2730	rVV5	60532	131218	6.59%	0.719%
37	18.174	2730	2735	2742	rVB6	21374	49901	2.51%	0.273%
38	18.392	2766	2772	2781	rVB7	36562	88351	4.44%	0.484%
39	18.568	2796	2802	2810	rVB8	17667	43562	2.19%	0.239%

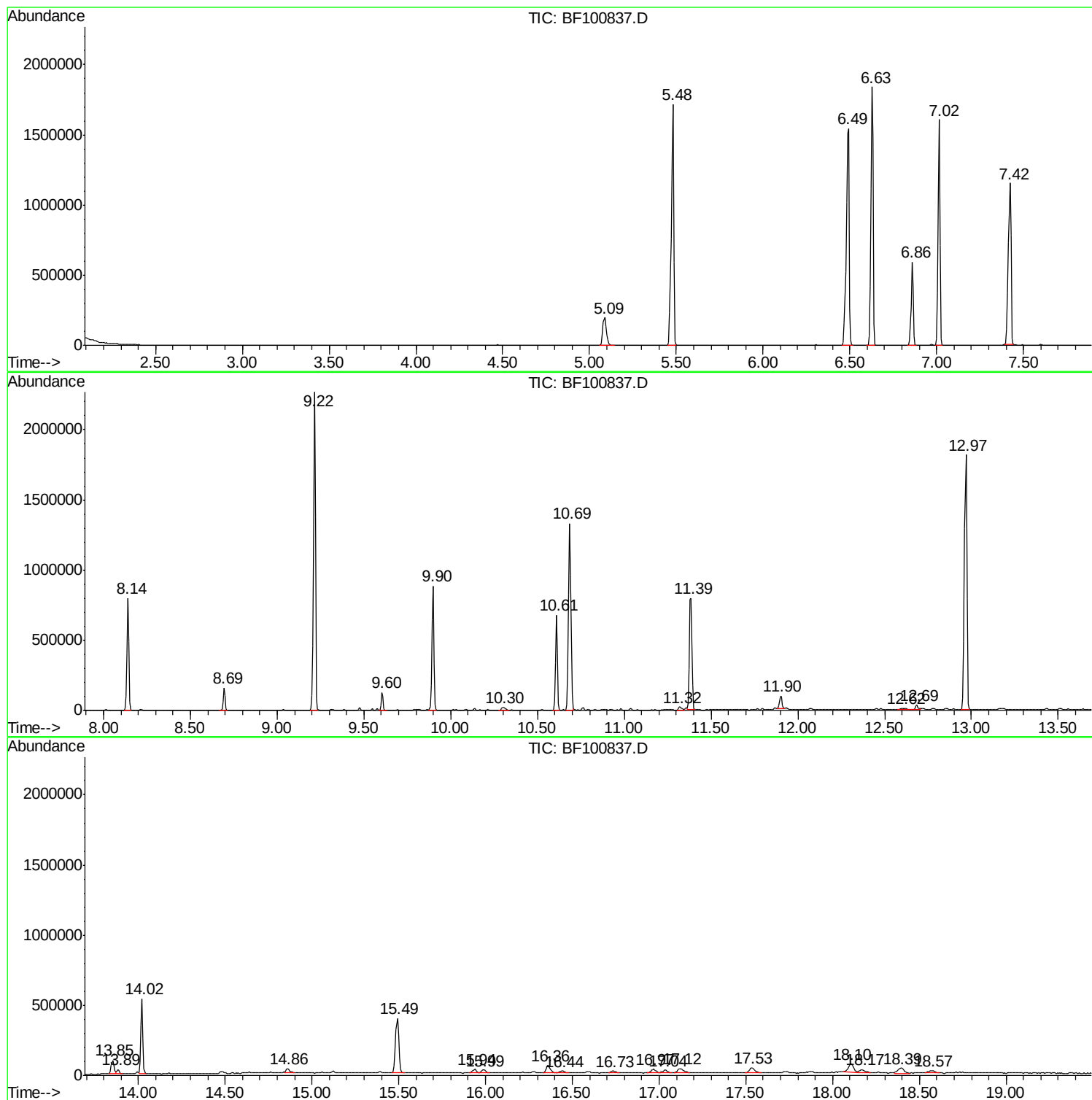
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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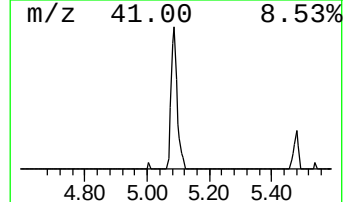
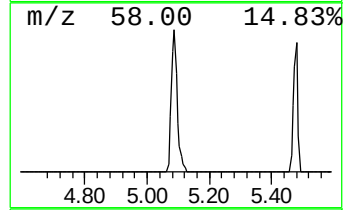
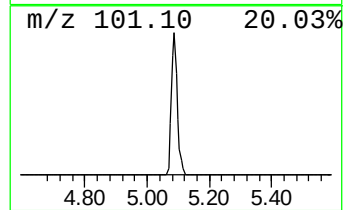
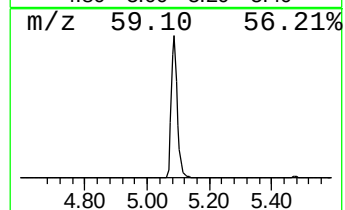
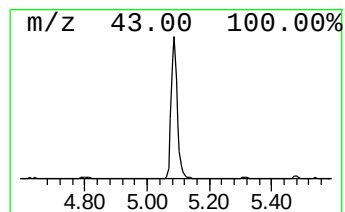
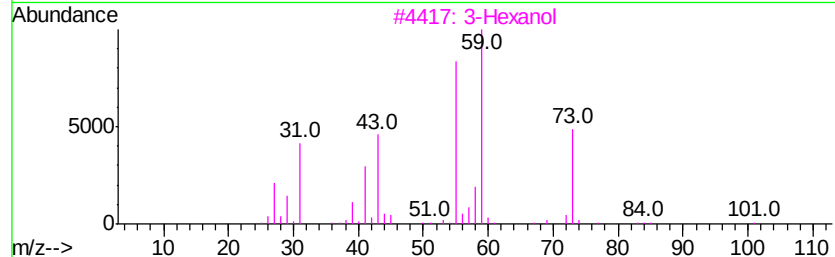
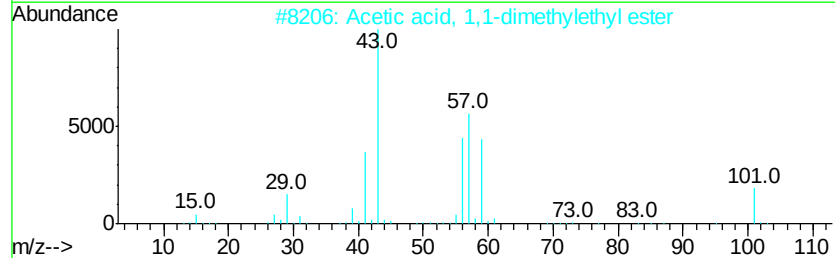
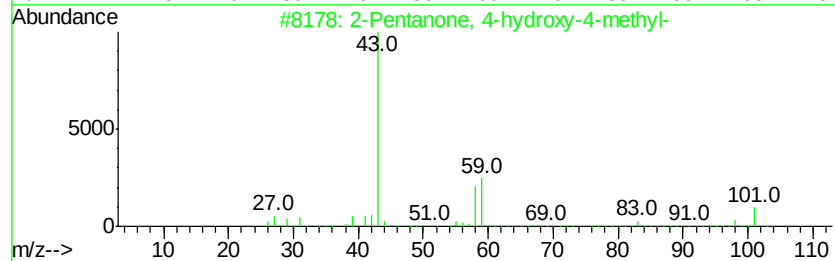
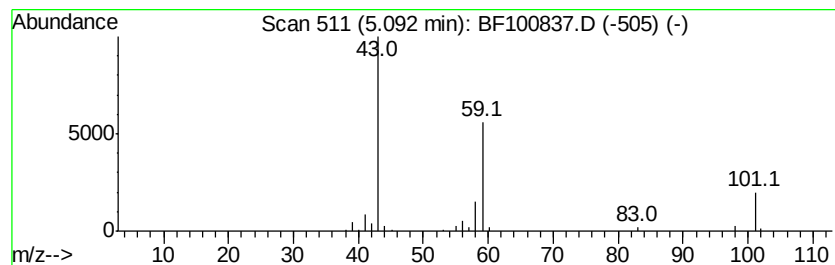
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	10.53 ng	257707	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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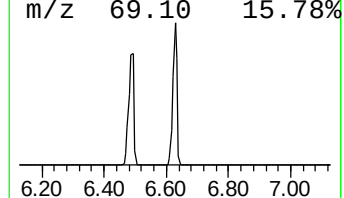
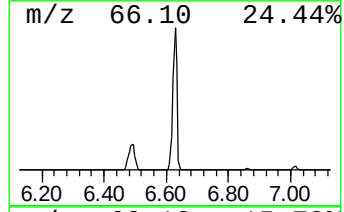
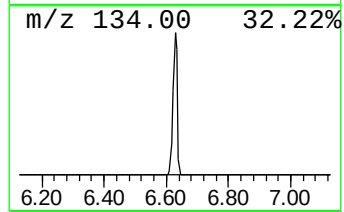
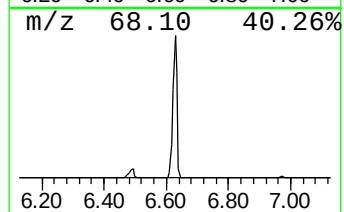
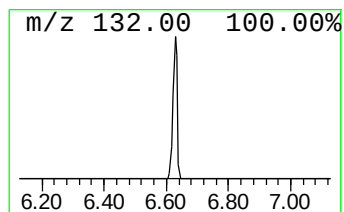
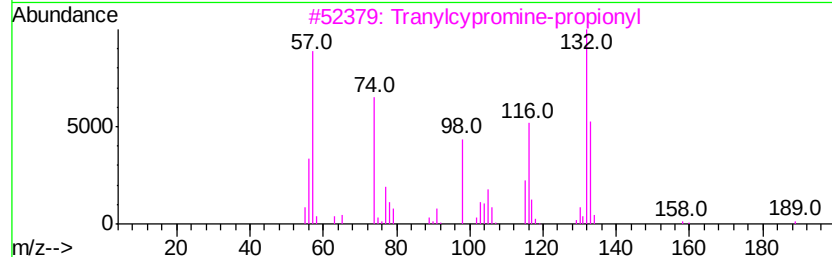
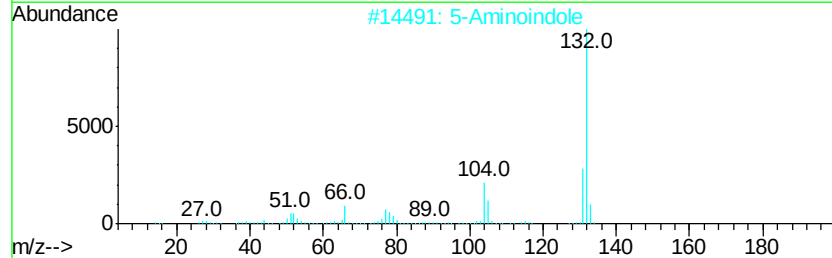
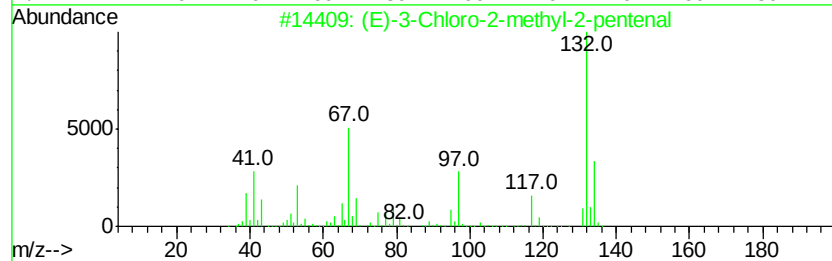
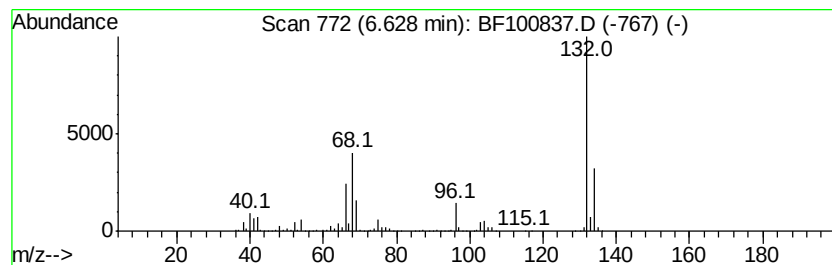
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	73.39 ng	1796060	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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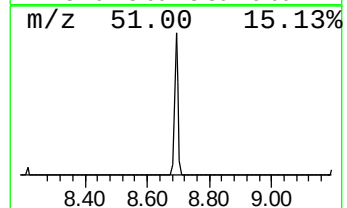
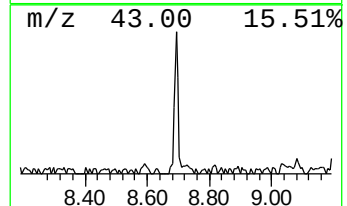
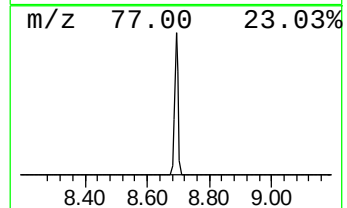
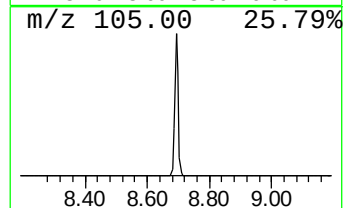
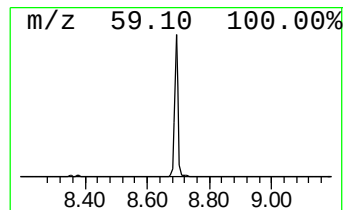
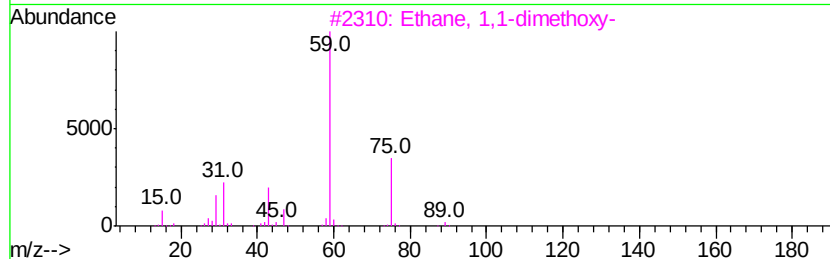
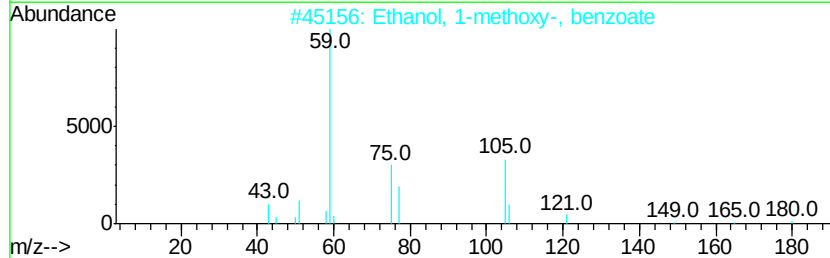
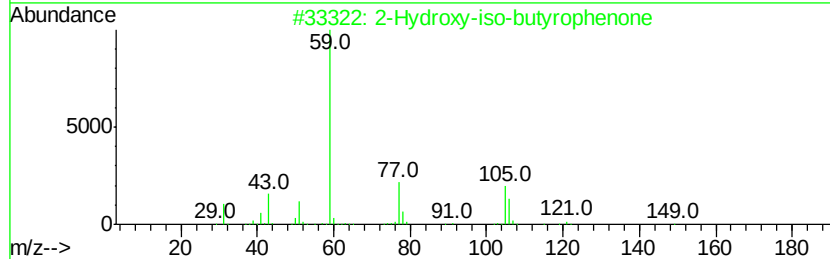
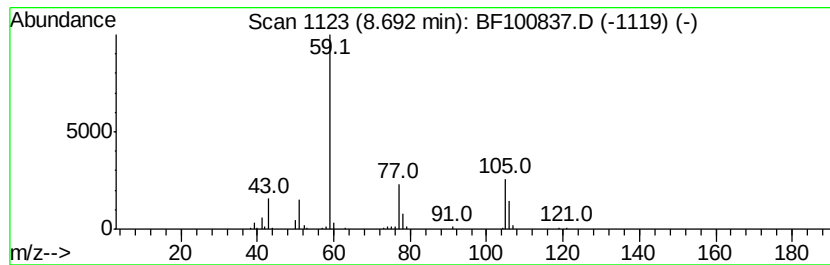
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
8.69	3.76 ng	124162	Naphthalene-d8		8.14		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-	iso-butyl-	phenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-,	benzoate		180	C10H12O3	051835-44-0	56
3	Ethane, 1,1-dimethoxy-			90	C4H10O2	000534-15-6	9
4	Formamide, N-methyl-			59	C2H5NO	000123-39-7	7
5	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	7



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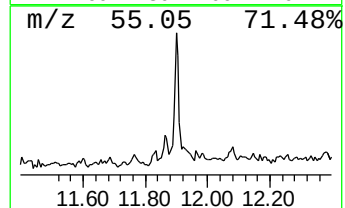
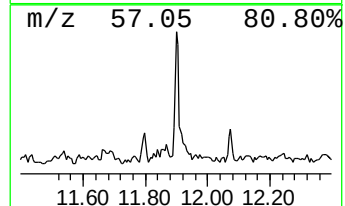
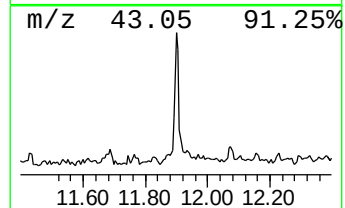
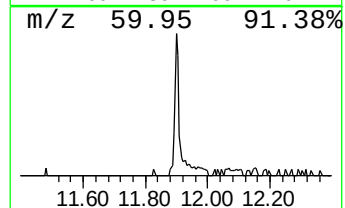
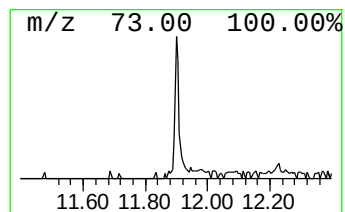
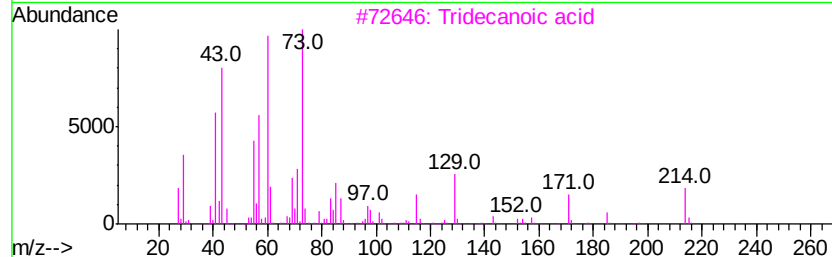
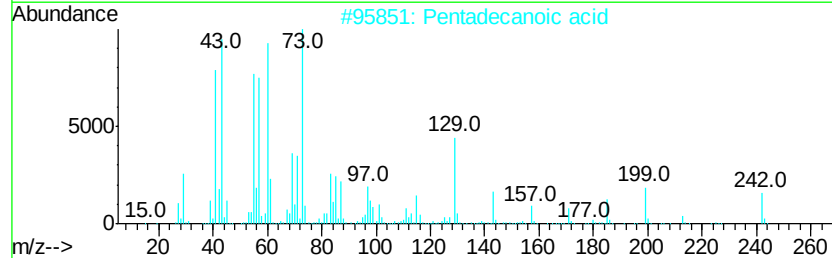
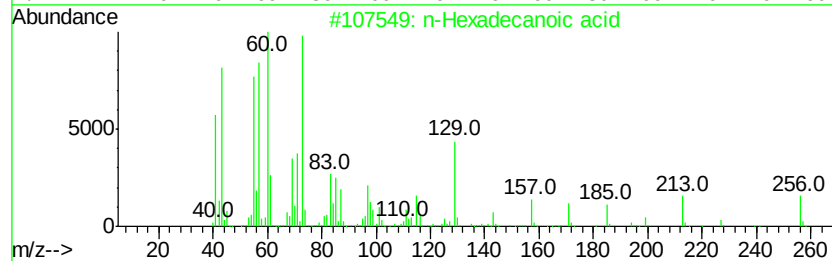
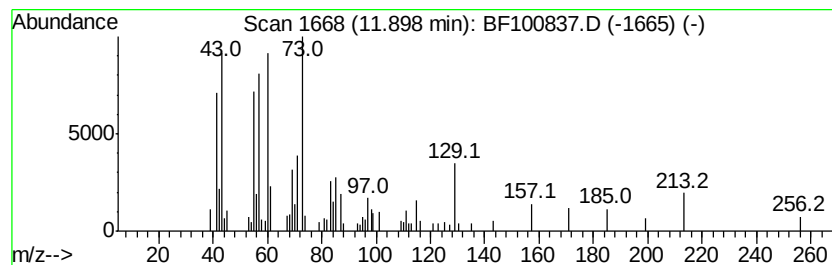
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.32 ng	85039	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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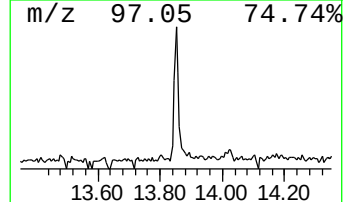
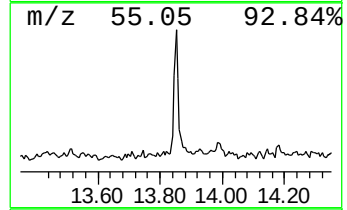
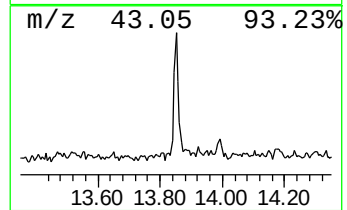
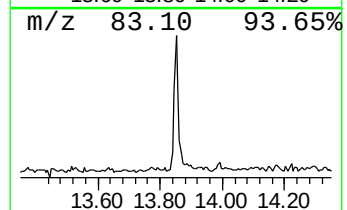
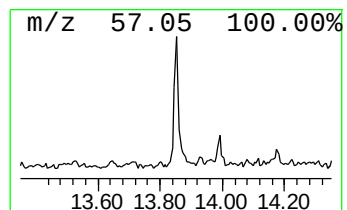
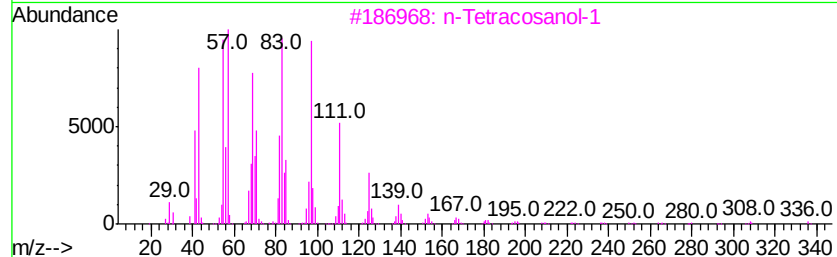
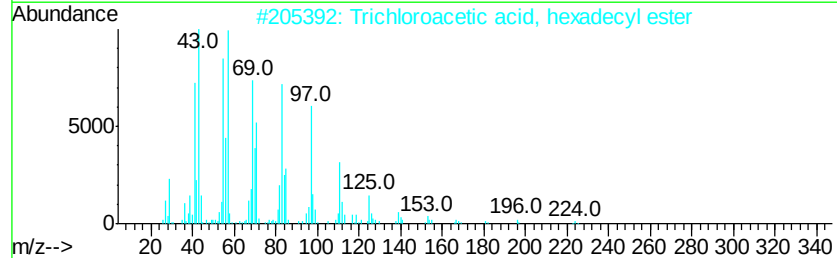
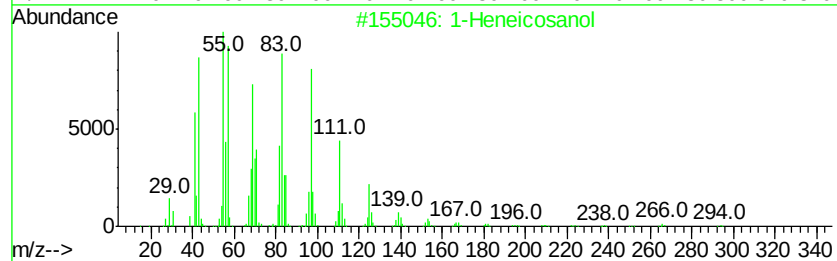
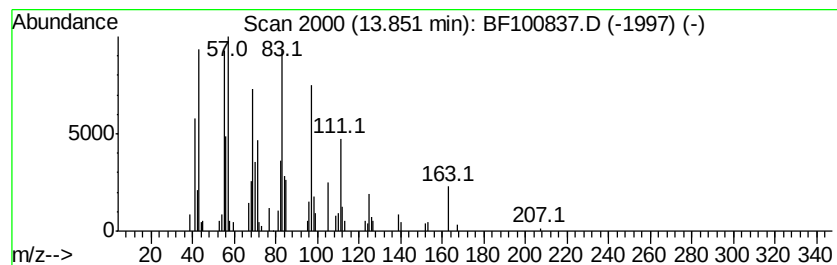
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.26 ng	93140	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
Operator : SJ/JU
Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-T0A-BAJA-S001-0001-02

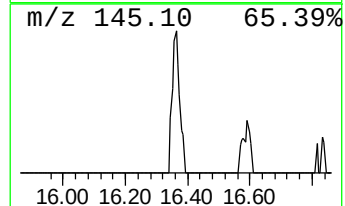
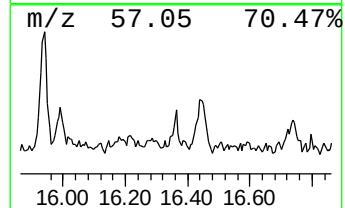
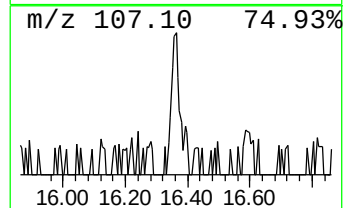
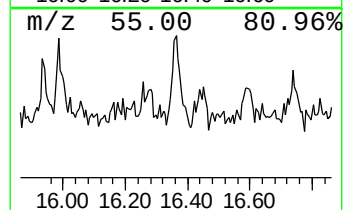
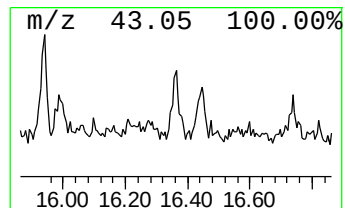
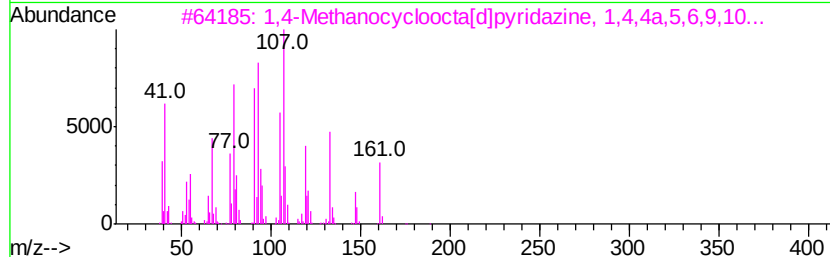
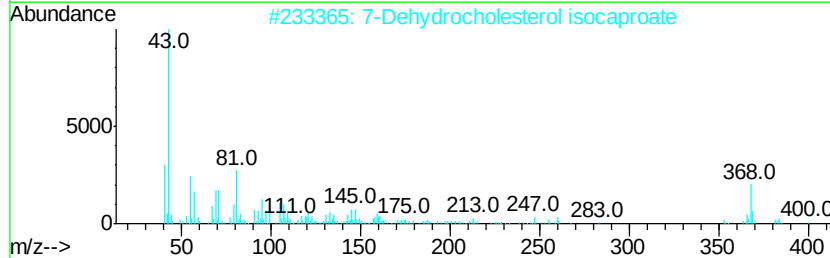
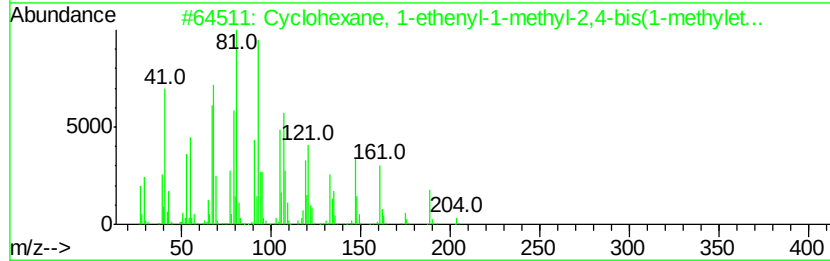
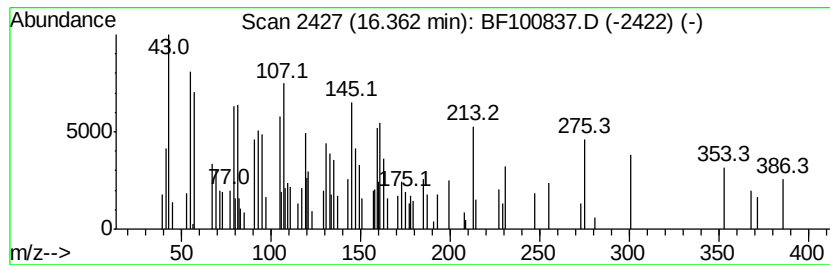
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.36 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	4.01 ng	94667	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	27
2		7-Dehydrocholesterol isocaproate	484	C33H56O2	1000252-60-9	22
3		1,4-Methanocycloocta[d]pyridazin...	204	C13H20N2	1000221-85-9	22
4		Cholest-5-en-3-ol (3.beta.)-, ca...	448	C28H45ClO2	007144-08-3	22
5		Cholest-5-en-3-ol (3.beta.)-, ac...	428	C29H48O2	000604-35-3	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
Operator : SJ/JU
Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
N-T0A-BAJA-S001-0001-02

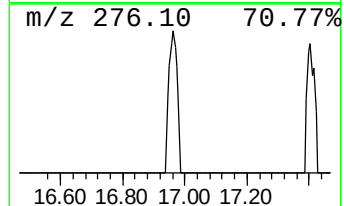
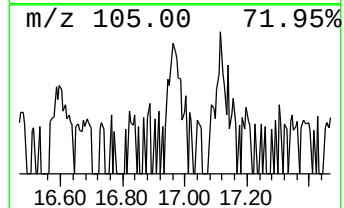
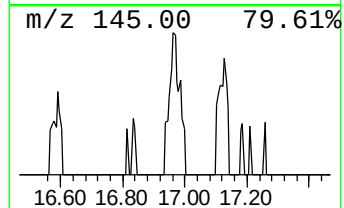
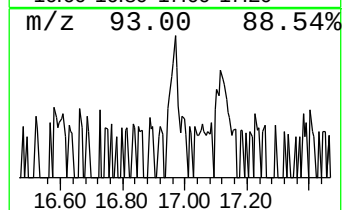
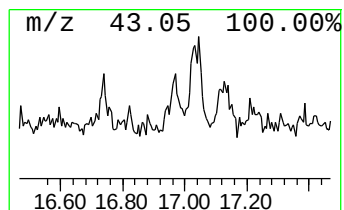
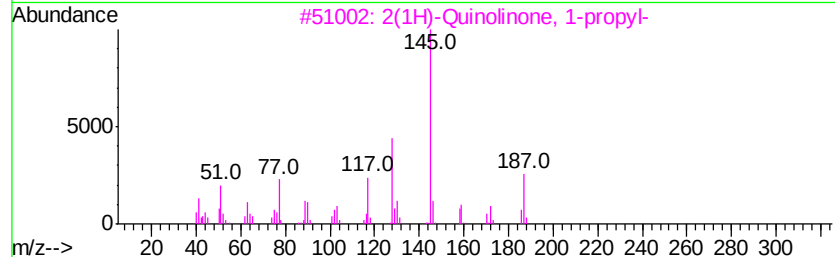
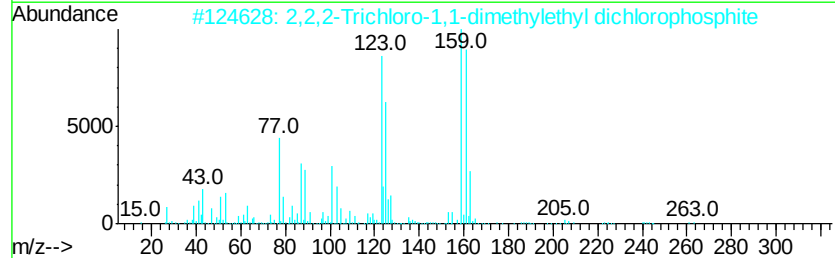
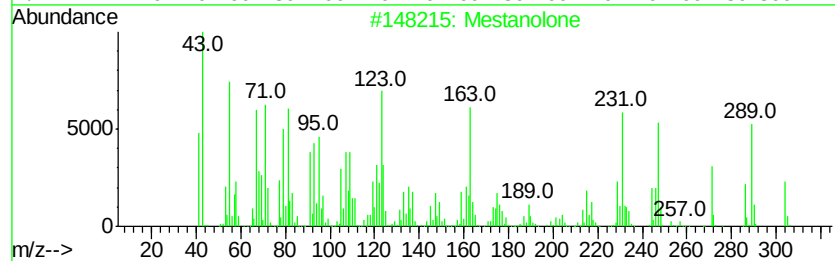
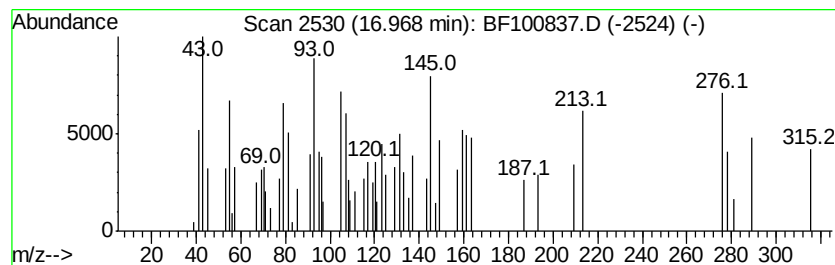
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.97 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.02 ng	47720	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mestanolone	304	C20H32O2	000521-11-9	10
2		2,2,2-Trichloro-1,1-dimethylethy...	276	C4H6Cl5OP	039177-74-7	10
3		2(1H)-Quinolinone, 1-propyl-	187	C12H13NO	000944-70-7	9
4		2,4-Dichlorophenylacetic acid	204	C8H6Cl2O2	019719-28-9	9
5		Acethydrazide, 2-(4-fluorophenox...	328	C18H17FN2O3	1000264-24-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
Operator : SJ/JU
Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

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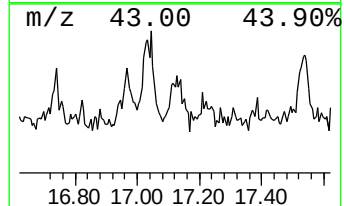
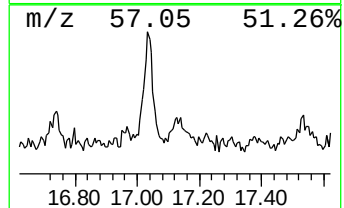
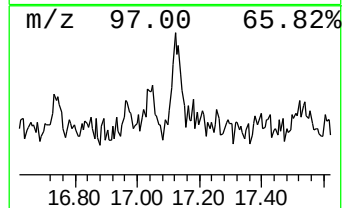
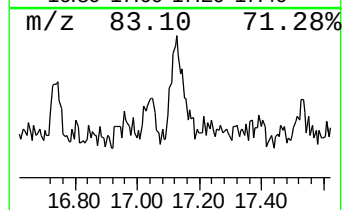
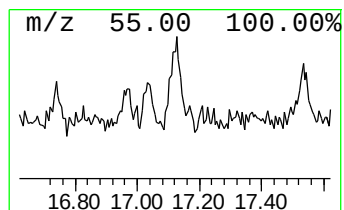
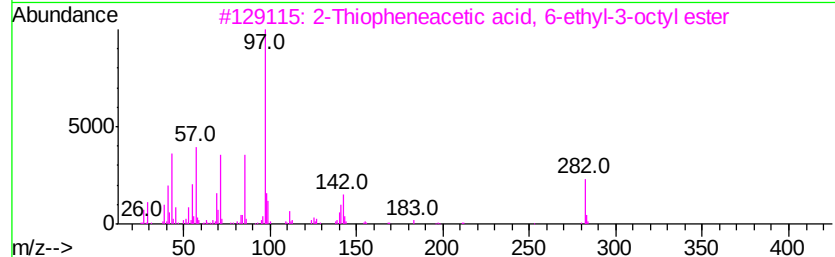
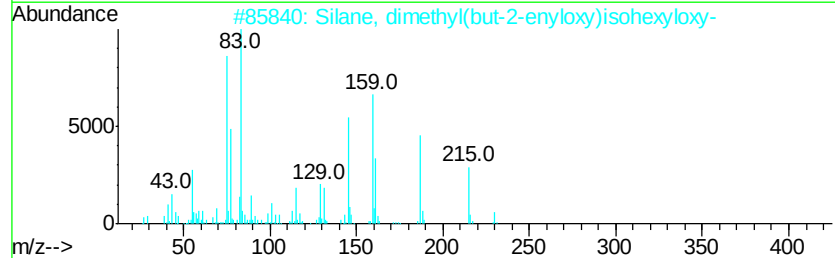
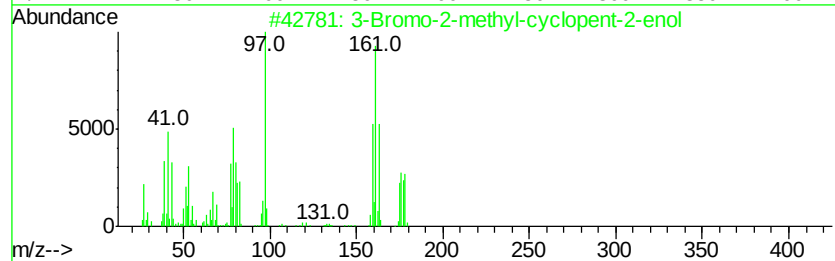
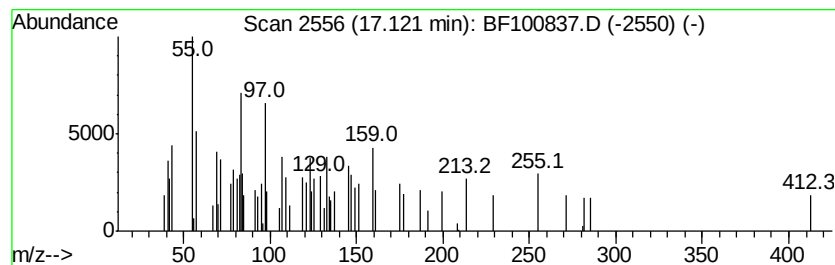
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.12 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	2.63 ng	62055	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Bromo-2-methyl-cyclopent-2-enol	176	C6H9BrO	1000186-18-7	32
2		Silane, dimethyl(but-2-enyloxy)i...	230	C12H26O2Si	1000348-05-6	10
3		2-Thiopheneacetic acid, 6-ethyl-...	282	C16H26O2S	1000278-92-3	9
4		Diisopropylketone p-tosylhydrazone	282	C14H22N2O2S	017530-00-6	9
5		L-Alanine, N-(2-thienylacetyl)-,...	255	C12H17NO3S	1000314-05-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
Data File : BF100837.D
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Operator : SJ/JU
Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

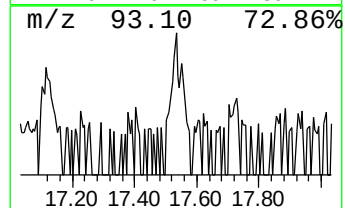
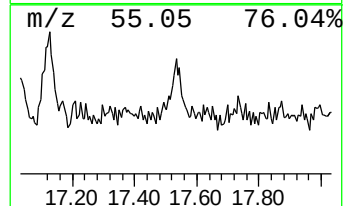
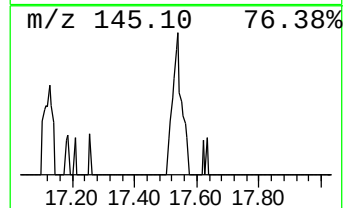
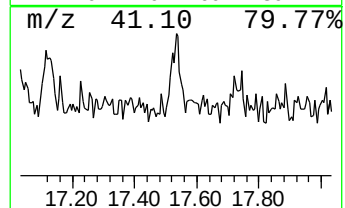
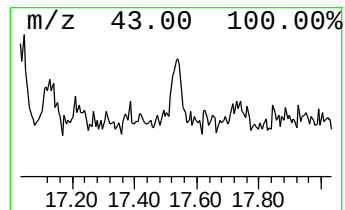
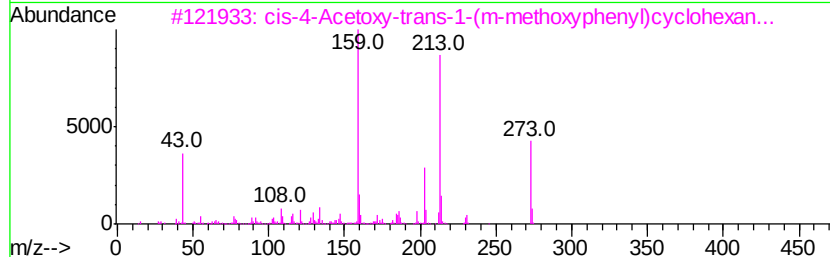
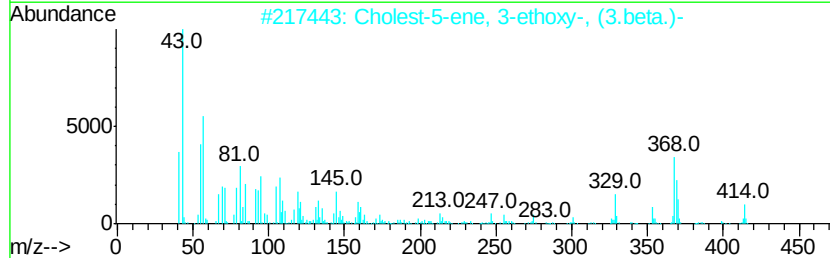
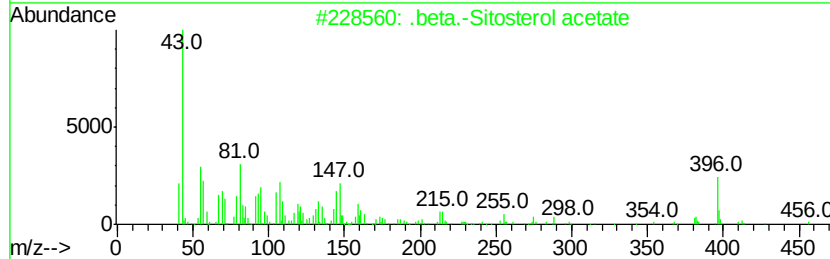
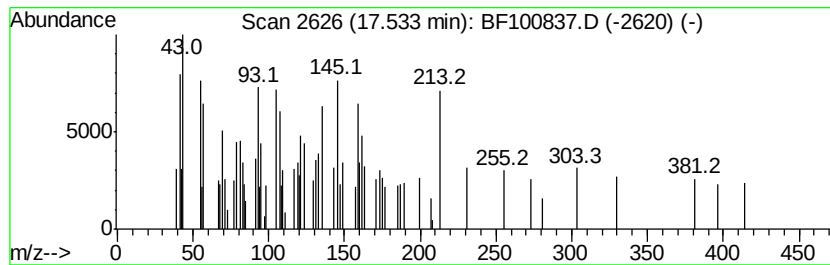
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.53 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.53	3.10 ng	73312	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	16
2	Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	11
3	cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	10
4	2-Amino-4-chloro-6-hydroxypyrimi...	145	C4H4ClN3O	001194-21-4	10
5	Androst-5-ene,1-acetoxy-16,17-di...	386	C25H38O3	294866-91-4	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
Operator : SJ/JU
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Instrument :
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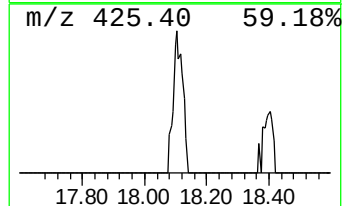
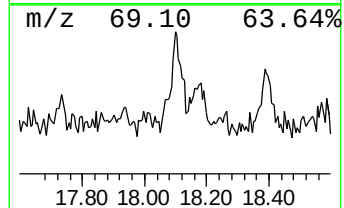
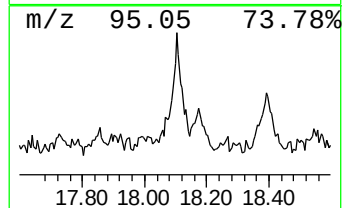
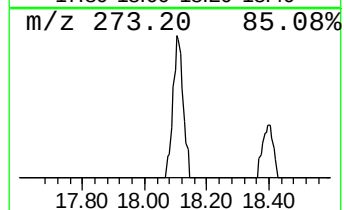
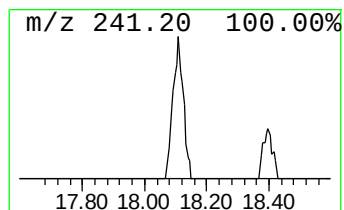
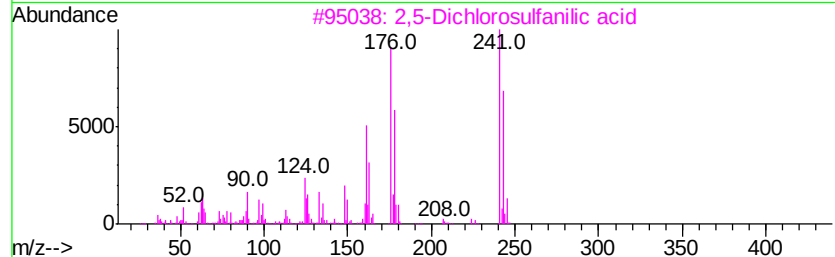
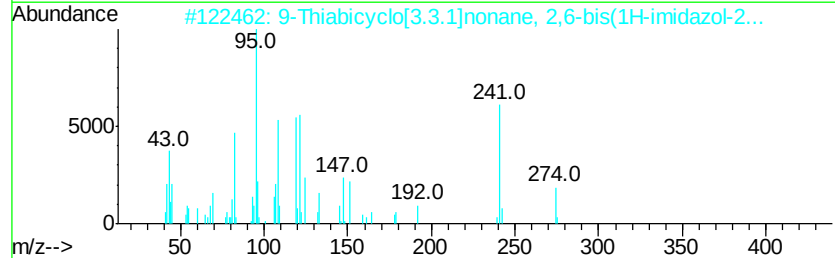
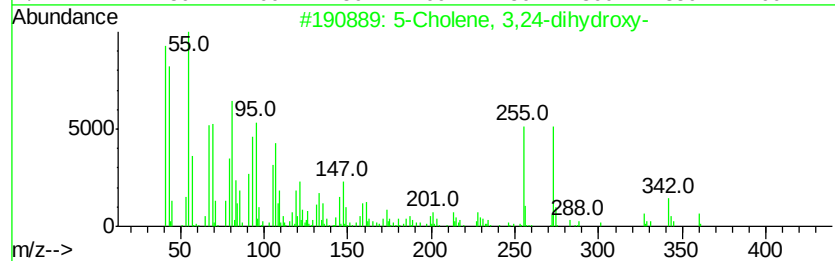
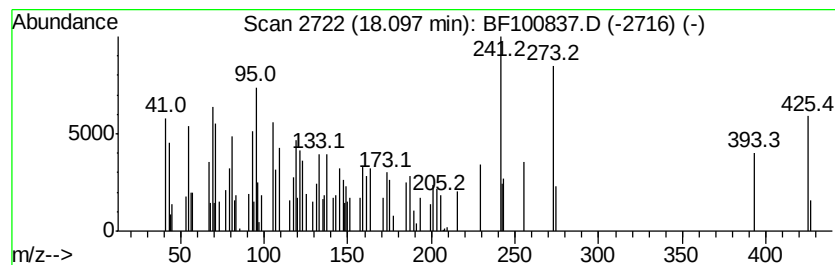
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.10 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	5.55 ng	131218	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	25
2		9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	18
3		2,5-Dichlorosulfanilic acid	241	C6H5Cl2NO3S	000088-50-6	18
4		.beta.-Alanine, N-(2-furoyl)-, p...	393	C23H39NO4	1000321-98-4	15
5		Phenol, 2,6-dimethyl-, phosphite...	394	C24H27O3P	052830-49-6	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100837.D
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Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

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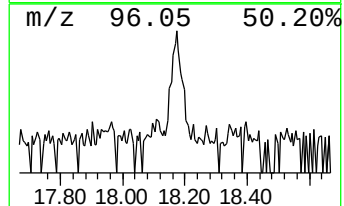
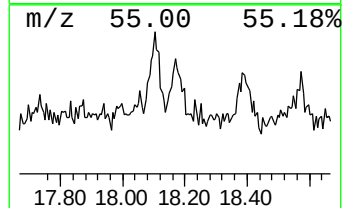
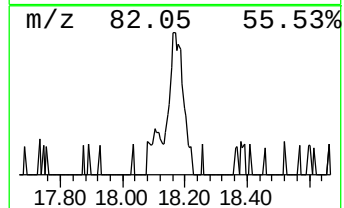
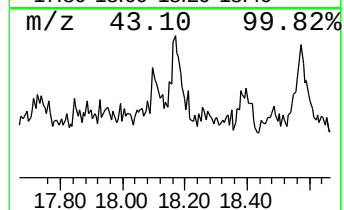
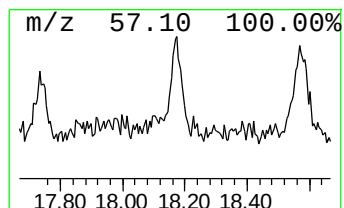
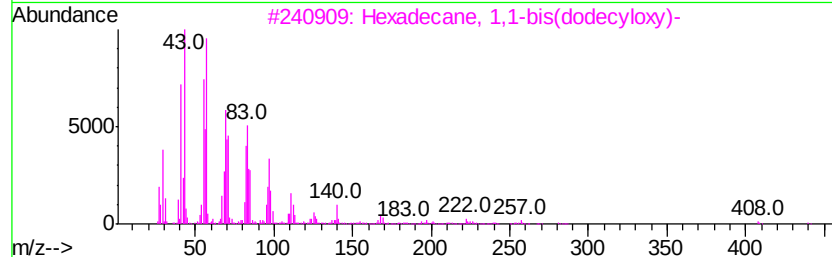
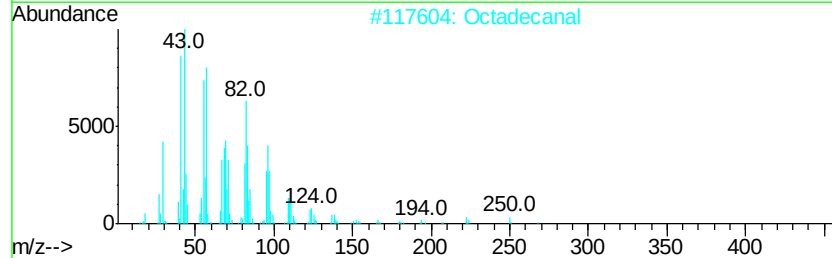
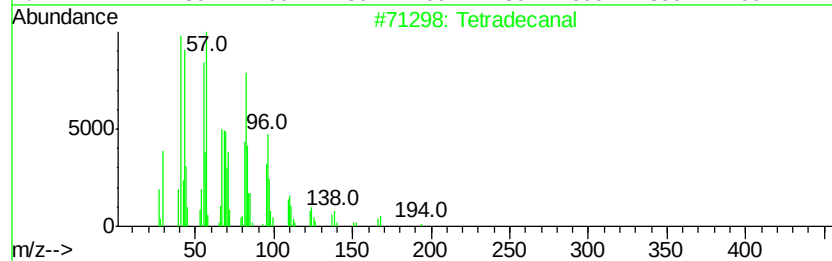
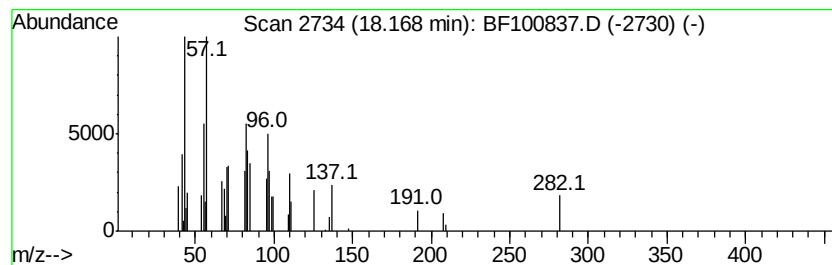
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetradecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	2.11 ng	49901	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	64
2			Octadecanal	268	C18H36O	000638-66-4	58
3			Hexadecane, 1,1-bis(dodecyloxy)-	595	C40H82O2	056554-64-4	43
4			Undecanal	170	C11H22O	000112-44-7	43
5			1-Eicosanol	298	C20H42O	000629-96-9	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
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Sample : I6043-18
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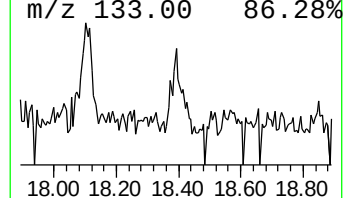
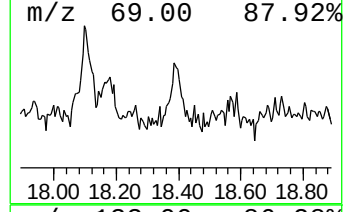
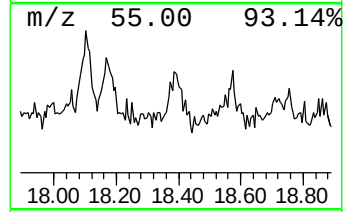
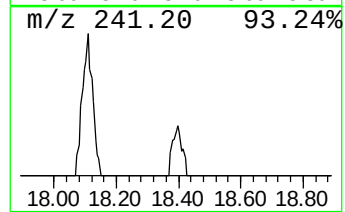
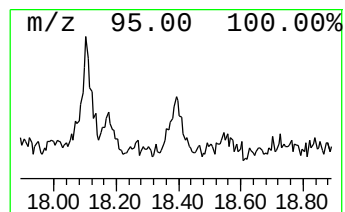
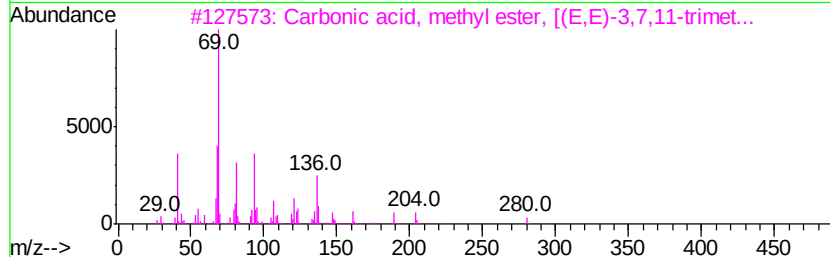
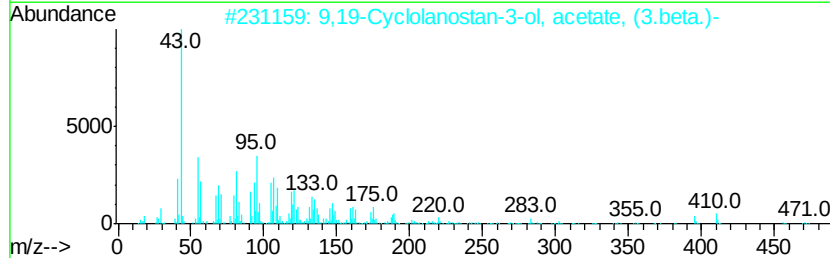
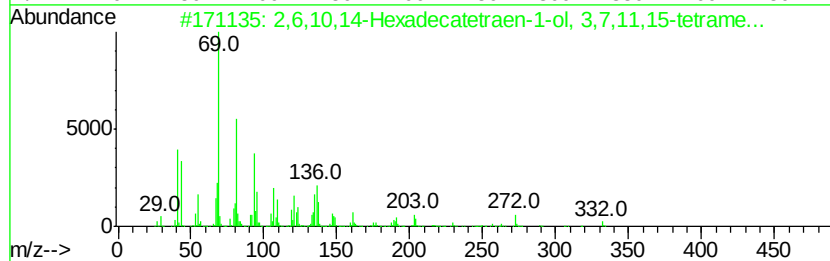
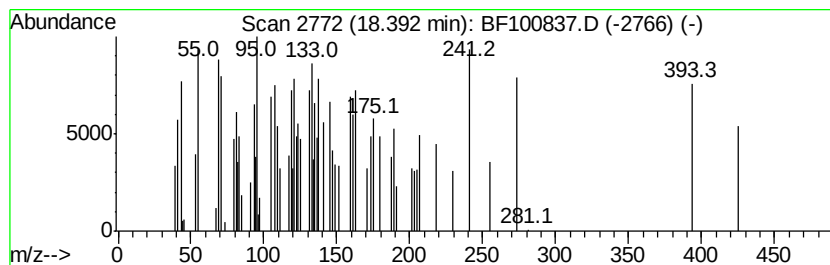
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.39 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	3.74 ng	88351	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	14		
2	9,19-Cyclolanostan-3-ol, acetate...	470	C32H54O2	004575-74-0	14		
3	Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	14		
4	Bicyclo[4.3.0]nonane, 7-methylen...	204	C15H24	1000156-11-9	11		
5	2(1H)-Pyridinone, 1,4,6-trimethyl-	137	C8H11NO	015031-89-7	11		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112217\
Data File : BF100837.D
Acq On : 22 Nov 2017 21:41
Operator : SJ/JU
Sample : I6043-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-T0A-BAJA-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.09	10.5	ng	257707	1	6.86	489480	20.0
unknown6.63	6.63	73.4	ng	1796060	1	6.86	489480	20.0
2-Hydroxy-iso-but...	8.69	3.8	ng	124162	2	8.14	660012	20.0
n-Hexadecanoic acid	11.90	2.3	ng	85039	4	11.39	732781	20.0
1-Heneicosanol	13.85	4.3	ng	93140	5	14.02	436948	20.0
unknown16.36	16.36	4.0	ng	94667	6	15.49	472666	20.0
unknown16.97	16.97	2.0	ng	47720	6	15.49	472666	20.0
unknown17.12	17.12	2.6	ng	62055	6	15.49	472666	20.0
unknown17.53	17.53	3.1	ng	73312	6	15.49	472666	20.0
unknown18.10	18.10	5.5	ng	131218	6	15.49	472666	20.0
Tetradecanal	18.17	2.1	ng	49901	6	15.49	472666	20.0
unknown18.39	18.39	3.7	ng	88351	6	15.49	472666	20.0