

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
 Data File : BF092266.D
 Acq On : 14 Jan 2017 2:38
 Operator : UM/SJ
 Sample : I1031-17
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0029

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-BF122116.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	3.970	189	191	197	rBV	47830	89174	1.66%	0.163%
2	4.713	252	256	268	rVB	1410894	2807956	52.23%	5.141%
3	5.170	294	296	299	rBV	3958974	5375988	100.00%	9.842%
4	6.244	387	390	392	rBV	4726944	5039085	93.73%	9.225%
5	6.347	397	399	402	rVB	5179804	5001933	93.04%	9.157%
6	6.576	417	419	421	rBV	1274859	1315583	24.47%	2.408%
7	6.724	430	432	435	rBV	3279690	4214174	78.39%	7.715%
8	7.147	466	469	471	rBV	3595832	3848156	71.58%	7.045%
9	7.296	480	482	487	rBV	113364	155942	2.90%	0.285%
10	7.856	529	531	534	rBV	1556331	1762587	32.79%	3.227%
11	8.942	623	626	629	rBV	4841027	5018598	93.35%	9.188%
12	9.342	658	661	664	rBV	1539679	1360629	25.31%	2.491%
13	9.559	676	680	682	rBV	58962	99702	1.85%	0.183%
14	9.605	682	684	687	rVB	1553582	1677371	31.20%	3.071%
15	10.062	720	724	725	rBV	115464	135970	2.53%	0.249%
16	10.279	739	743	744	rBV	47258	68152	1.27%	0.125%
17	10.405	751	754	756	rBV2	2233487	3273242	60.89%	5.992%
18	10.531	763	765	769	rBV	174388	201362	3.75%	0.369%
19	10.976	802	804	805	rBV2	106714	103540	1.93%	0.190%
20	11.079	811	813	816	rBV	1207526	1683332	31.31%	3.082%
21	11.331	833	835	839	rVB	50431	73442	1.37%	0.134%
22	11.571	853	856	859	rBV	36456	66511	1.24%	0.122%
23	11.639	860	862	866	rVV2	441221	444315	8.26%	0.813%
24	12.291	917	919	921	rBV	91551	80152	1.49%	0.147%
25	12.336	921	923	929	rBV	44843	108183	2.01%	0.198%
26	12.416	929	930	936	rVV2	40208	68908	1.28%	0.126%
27	12.508	936	938	941	rVB2	88348	125577	2.34%	0.230%
28	12.565	941	943	944	rBV	57735	56626	1.05%	0.104%
29	12.668	949	952	955	rBV	3227529	4241623	78.90%	7.765%
30	12.919	970	974	976	rBV2	79574	115407	2.15%	0.211%
31	13.262	1001	1004	1007	rVB	47549	75414	1.40%	0.138%
32	13.582	1029	1032	1041	rBV	322044	488672	9.09%	0.895%
33	13.708	1041	1043	1046	rBV	1332785	1357954	25.26%	2.486%
34	13.902	1057	1060	1065	rVB	64238	76501	1.42%	0.140%

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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.211	1084	1087	1093	rVB	129336	249037	4.63%	0.456%
36	14.497	1110	1112	1115	rVB	57064	59078	1.10%	0.108%
37	14.554	1115	1117	1120	rBV	145361	204921	3.81%	0.375%
38	14.622	1120	1123	1126	rVB	179252	160755	2.99%	0.294%
39	14.782	1135	1137	1144	rVV2	182972	388961	7.24%	0.712%
40	15.068	1159	1162	1164	rBV	751270	990006	18.42%	1.812%
41	15.102	1164	1165	1168	rVB	53469	59882	1.11%	0.110%
42	15.274	1177	1180	1184	rVB	104940	146651	2.73%	0.268%
43	15.468	1194	1197	1199	rBV	108707	157115	2.92%	0.288%
44	15.514	1199	1201	1204	rVV3	42799	78393	1.46%	0.144%
45	15.880	1230	1233	1238	rVB2	30272	53876	1.00%	0.099%
46	16.120	1250	1254	1258	rBV	67305	127611	2.37%	0.234%
47	16.405	1273	1279	1284	rBV4	118285	333334	6.20%	0.610%
48	16.497	1284	1287	1289	rVV2	109734	255043	4.74%	0.467%
49	16.543	1289	1291	1295	rVB	201548	359243	6.68%	0.658%
50	16.760	1306	1310	1316	rVB3	79627	192925	3.59%	0.353%
51	17.823	1397	1403	1411	rVB10	23496	120586	2.24%	0.221%
52	18.417	1452	1455	1464	rVB10	23260	74107	1.38%	0.136%

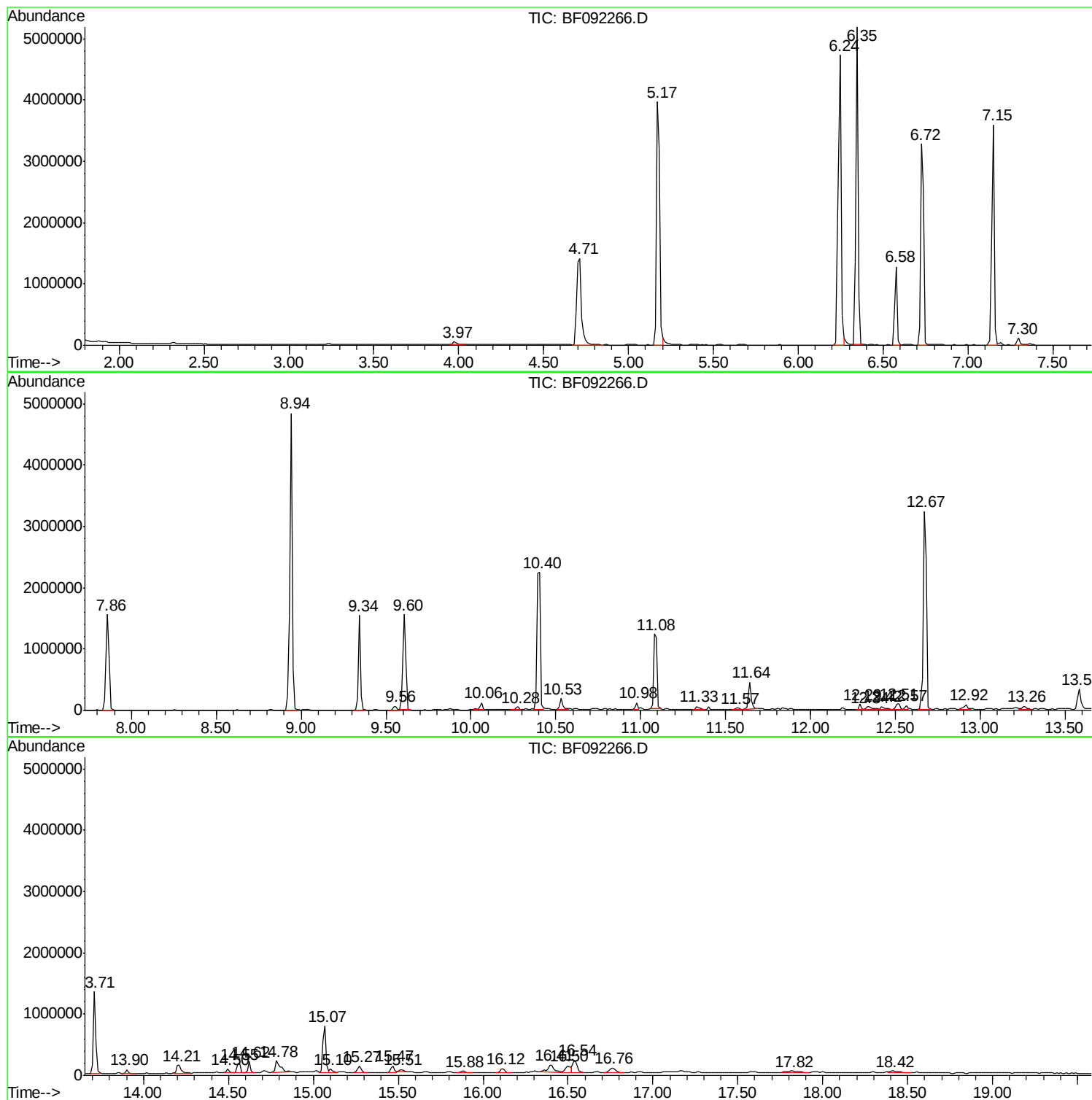
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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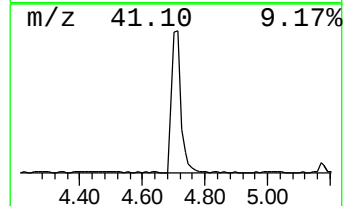
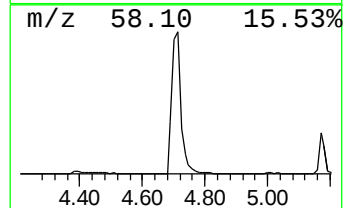
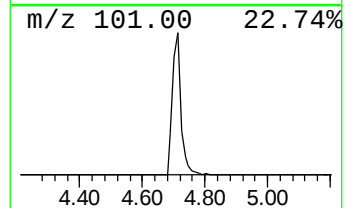
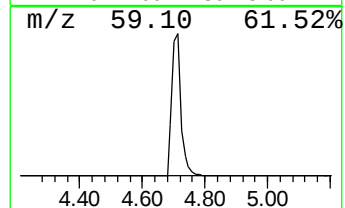
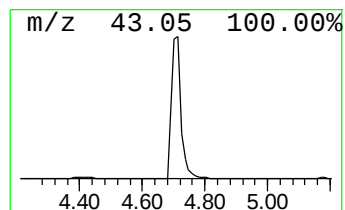
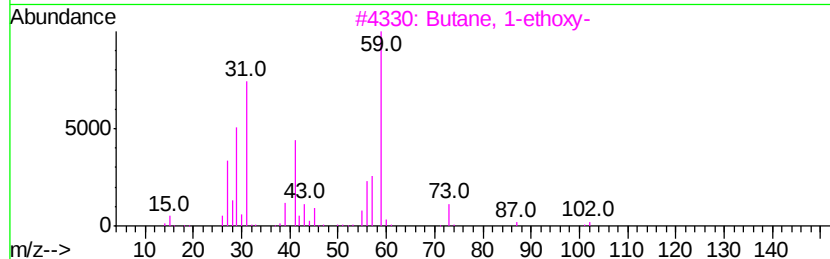
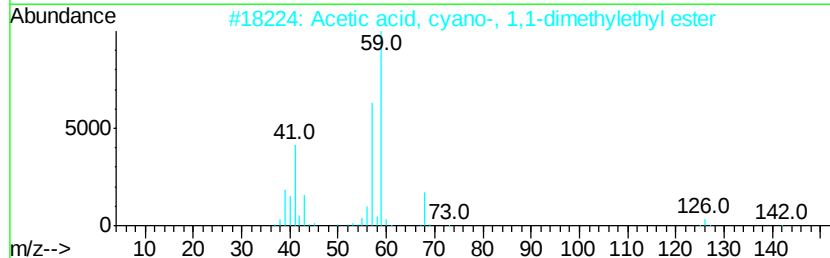
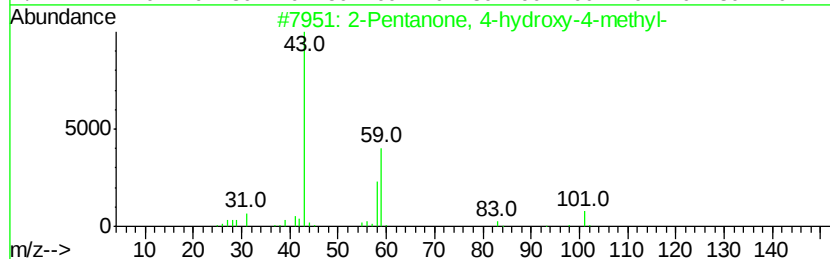
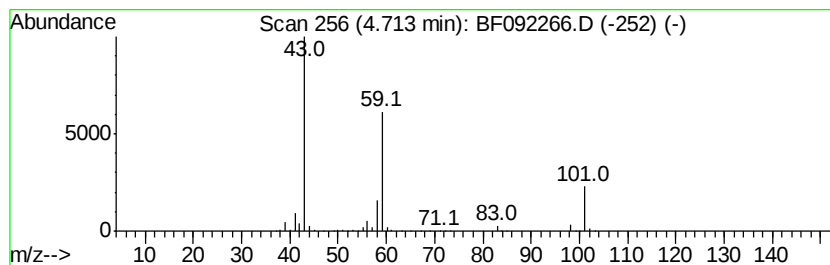
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.71	42.69 ng	2807960	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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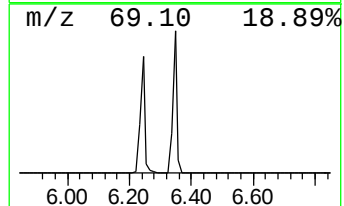
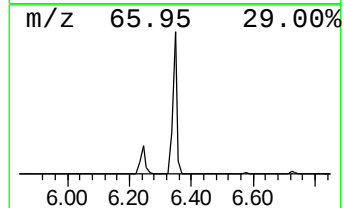
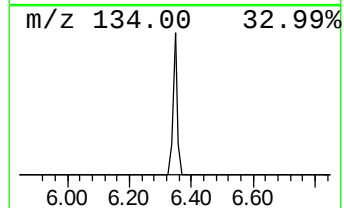
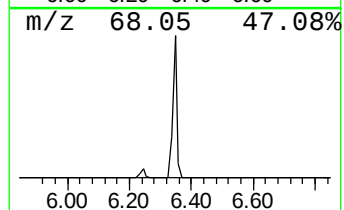
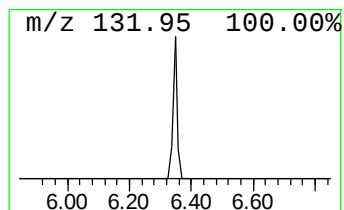
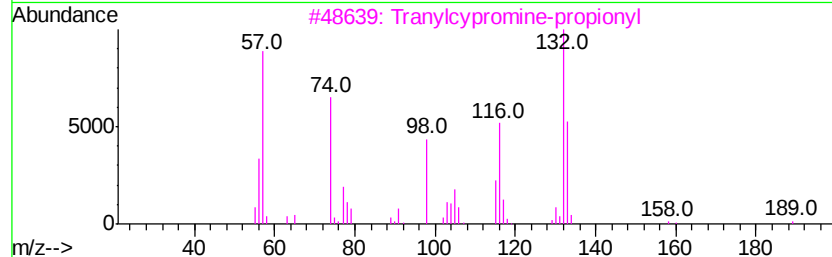
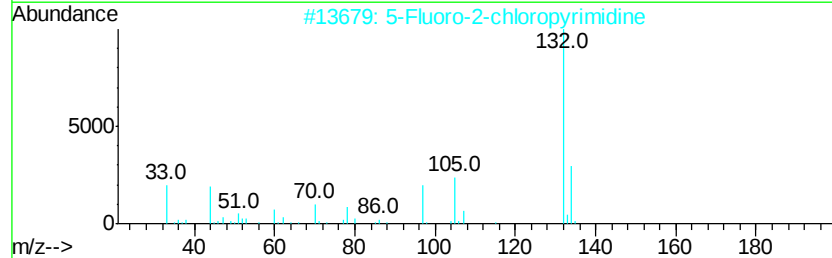
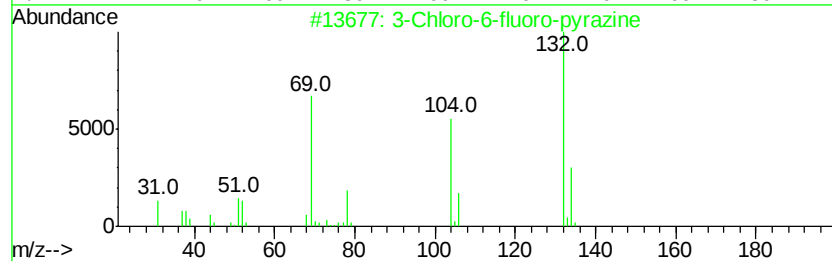
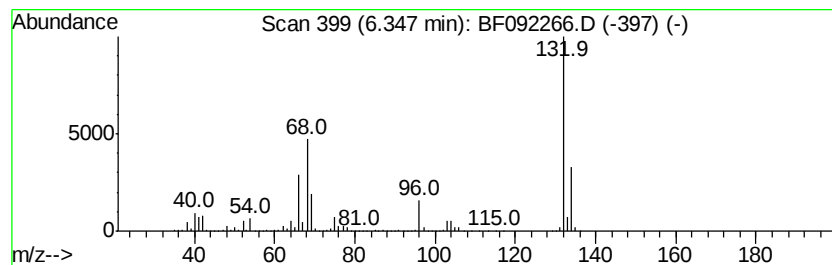
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	76.04 ng	5001930	1,4-Dichlorobenzene-d4	6.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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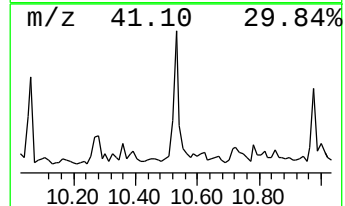
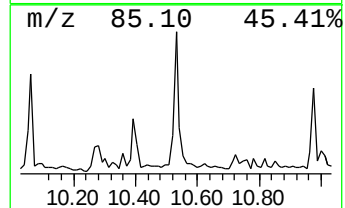
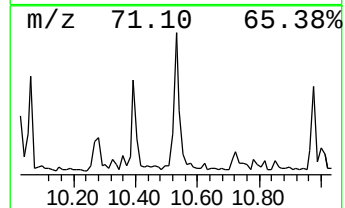
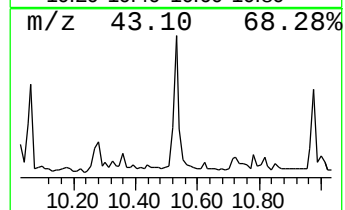
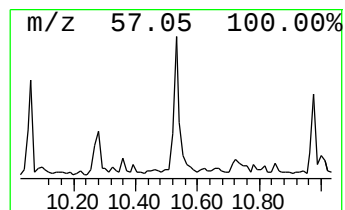
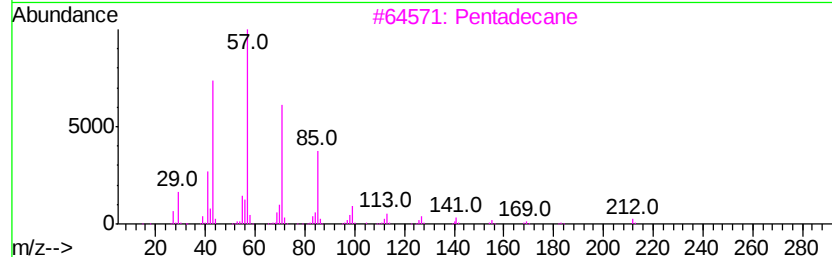
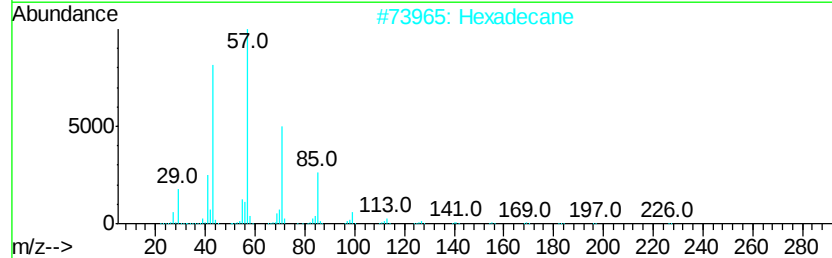
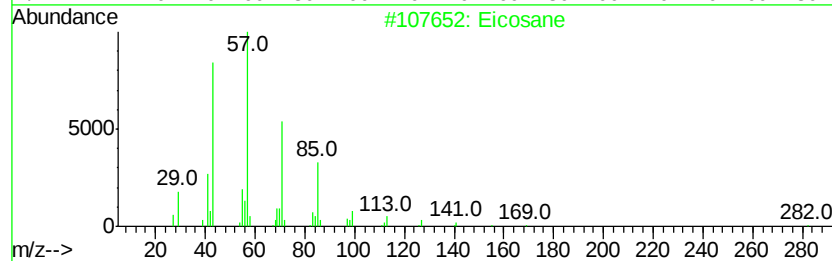
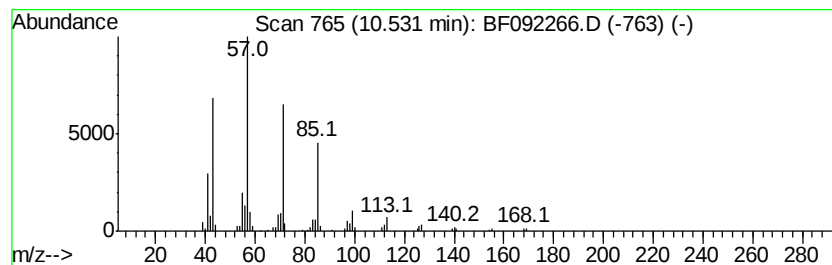
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	2.39 ng	201362	Phenanthrene-d10	11.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		Pentadecane	212	C15H32	000629-62-9	90
4		Heptadecane	240	C17H36	000629-78-7	90
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



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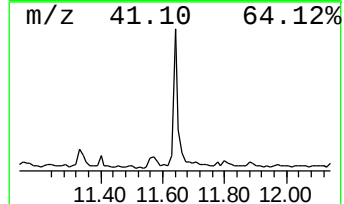
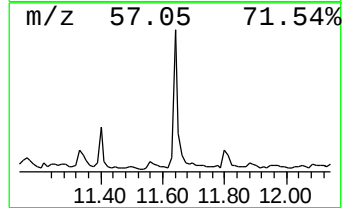
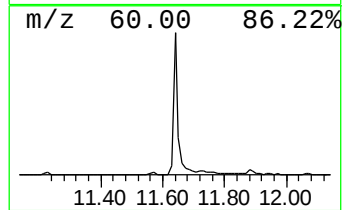
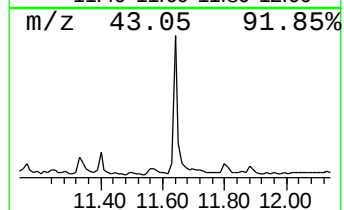
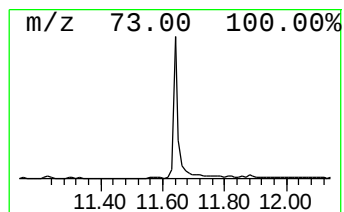
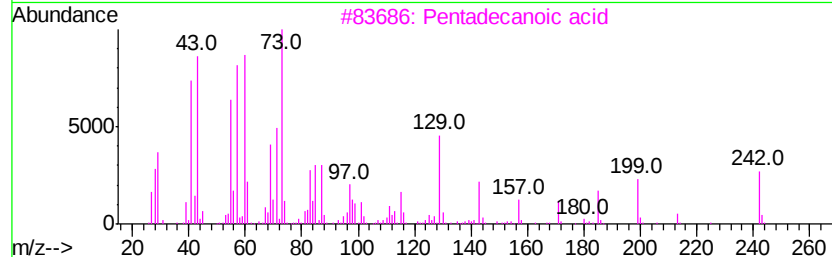
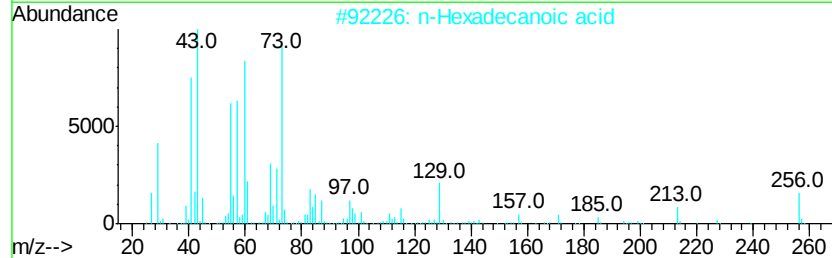
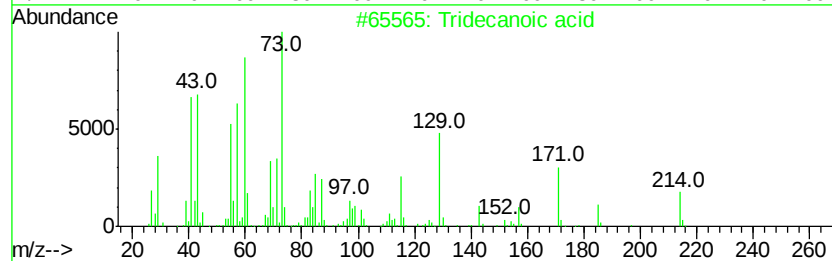
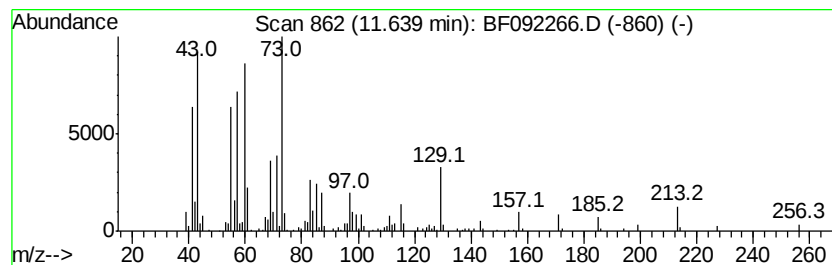
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.64	5.28 ng	444315	Phenanthrene-d10		11.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Nonanoic acid	158	C9H18O2	000112-05-0	11



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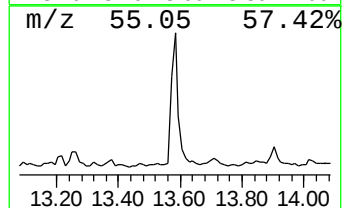
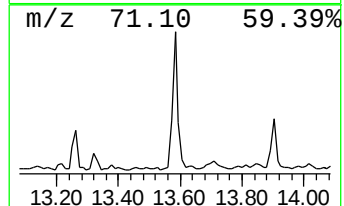
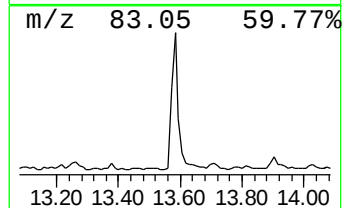
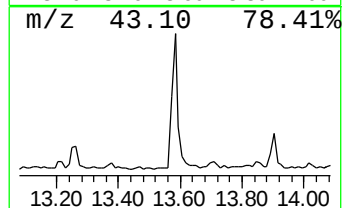
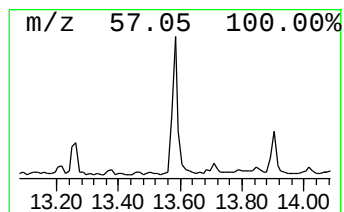
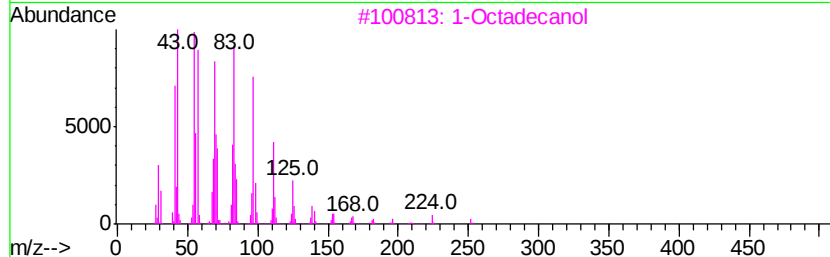
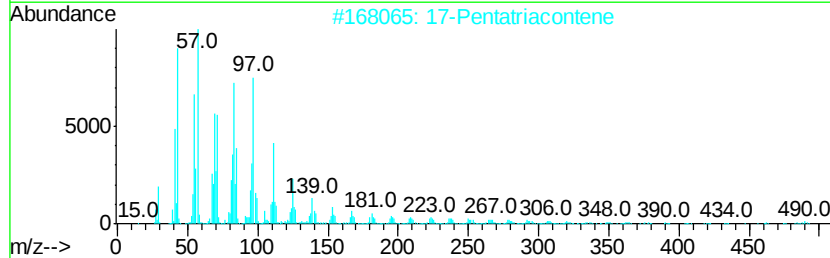
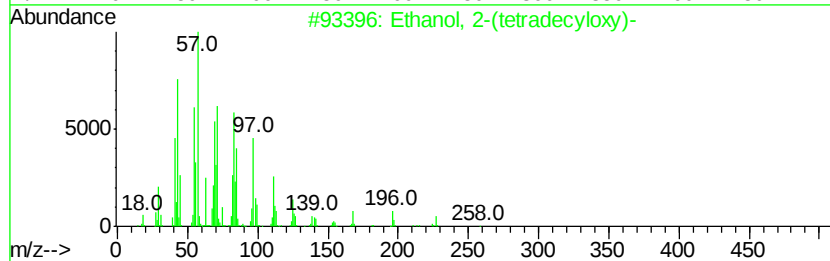
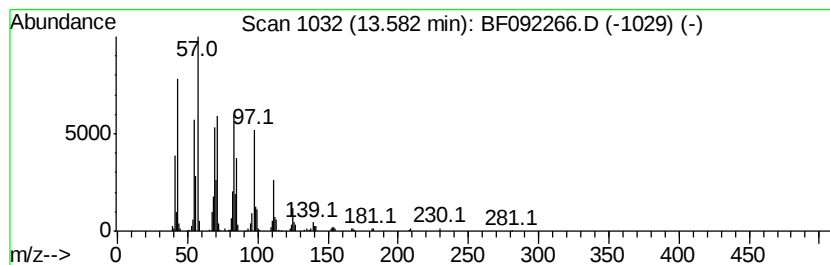
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	7.20 ng	488672	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2		17-Pentatriacontene	491	C35H70	006971-40-0	90
3		1-Octadecanol	270	C18H38O	000112-92-5	81
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	81
5		1-Nonadecene	266	C19H38	018435-45-5	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
Data File : BF092266.D
Acq On : 14 Jan 2017 2:38
Operator : UM/SJ
Sample : I1031-17
Misc :
ALS Vial : 27 Sample Multiplier: 1

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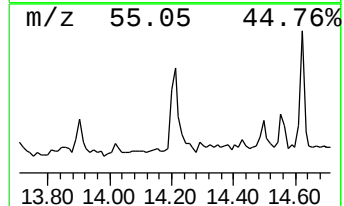
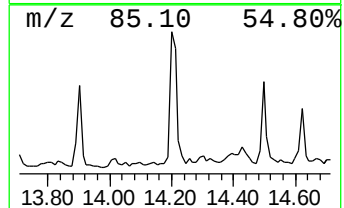
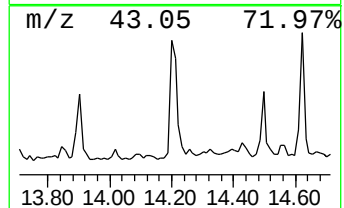
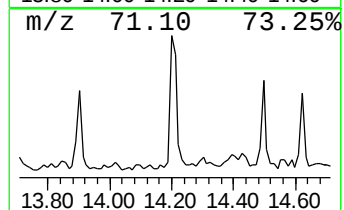
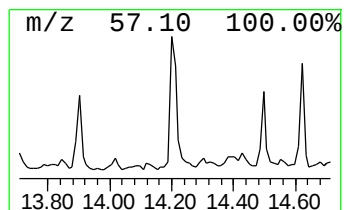
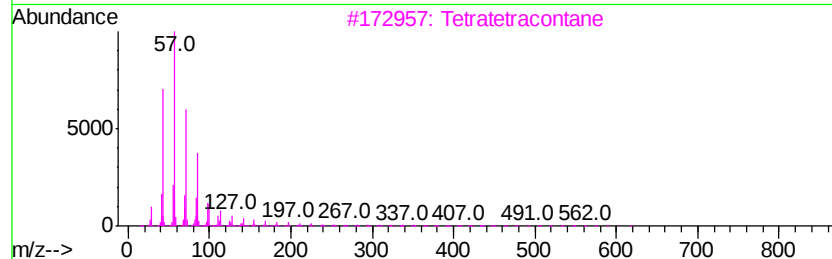
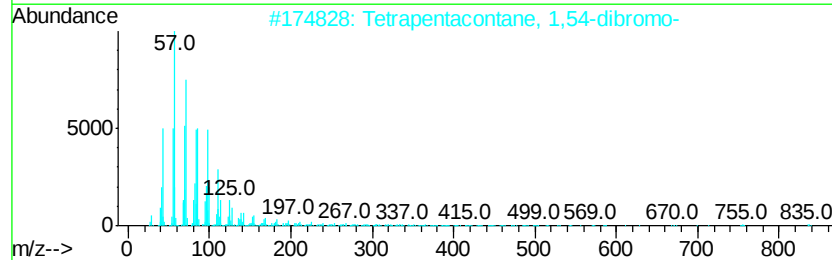
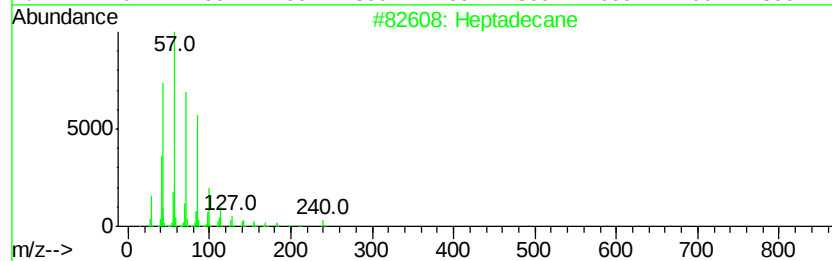
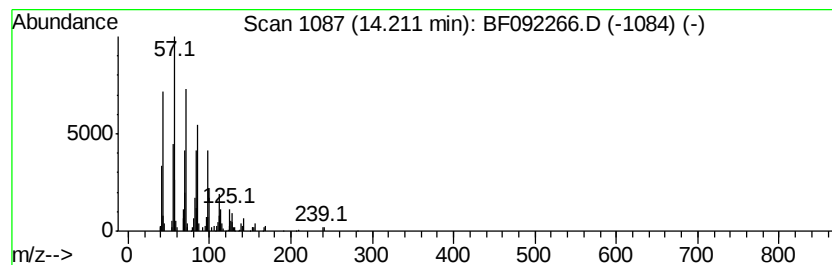
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	3.67 ng	249037	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	90
2		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	58
3		Tetratetracontane	619	C44H90	007098-22-8	52
4		Hexadecane	226	C16H34	000544-76-3	49
5		17-Pentatriacontene	491	C35H70	006971-40-0	49



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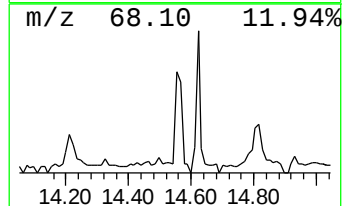
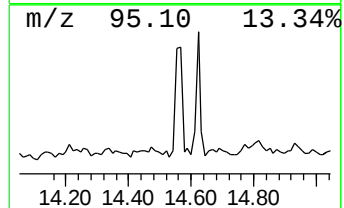
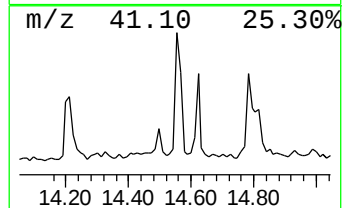
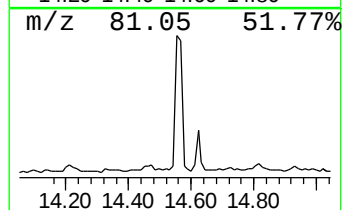
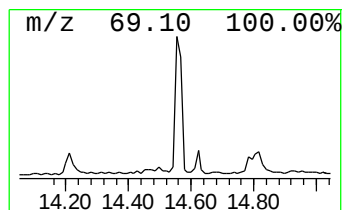
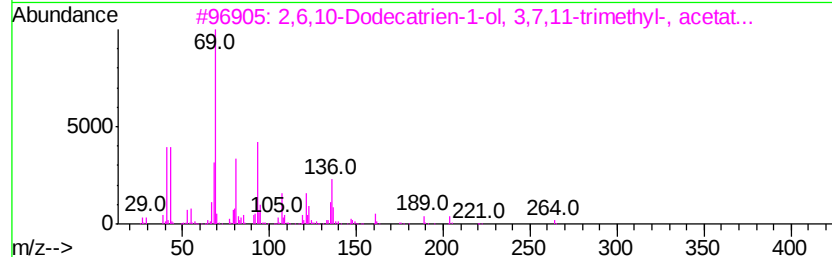
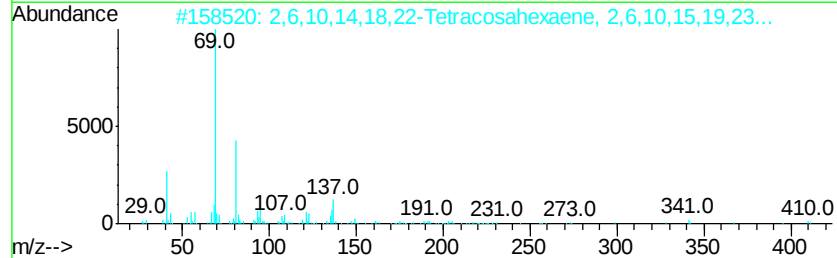
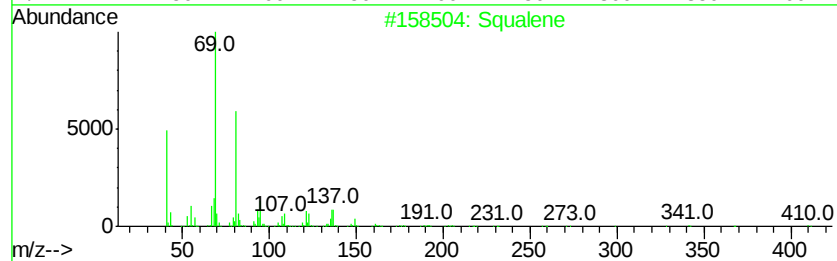
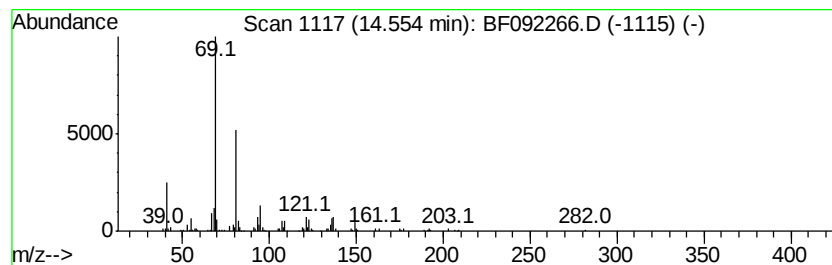
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	4.14 ng	204921	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64



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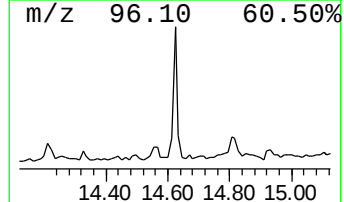
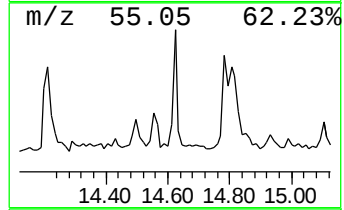
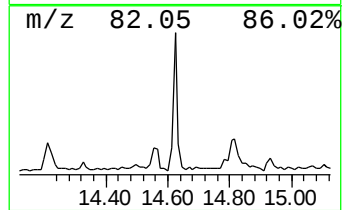
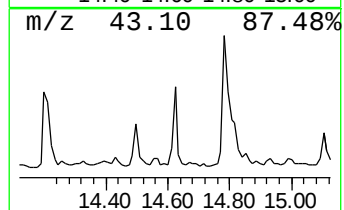
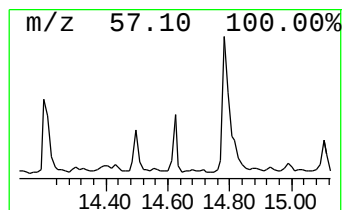
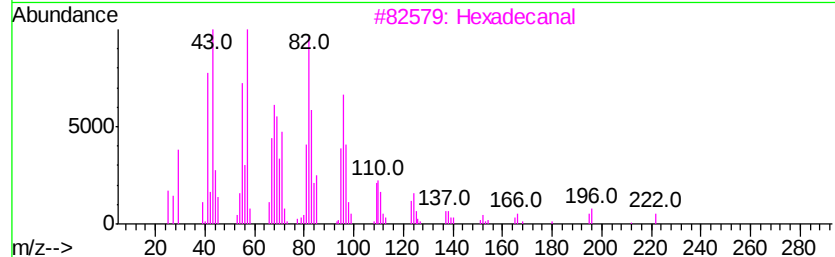
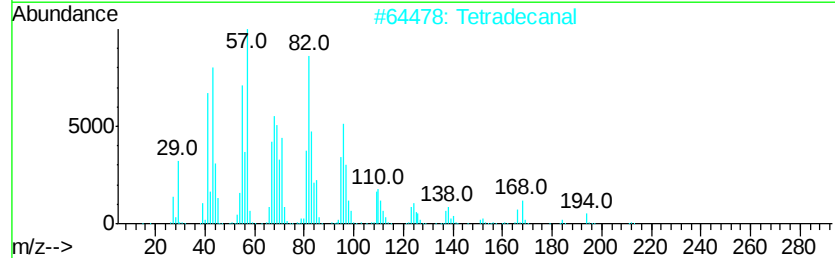
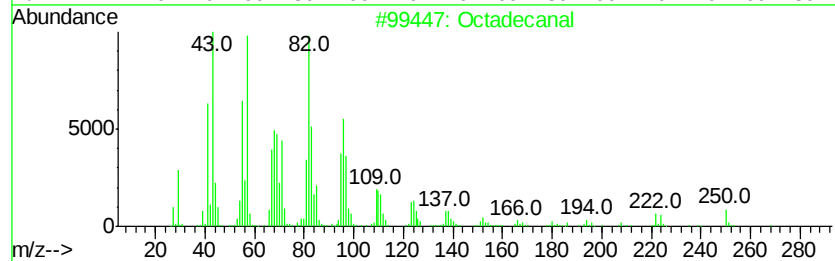
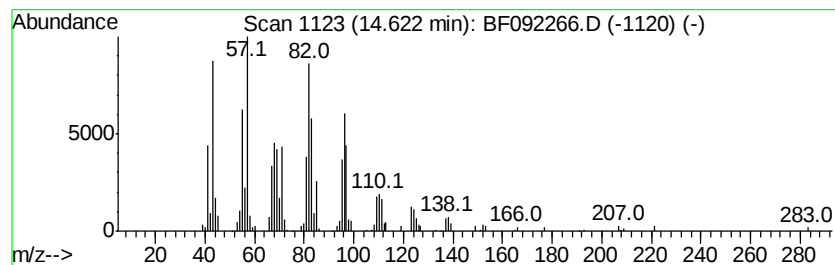
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.25 ng	160755	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	91
2		Tetradecanal	212	C14H28O	000124-25-4	91
3		Hexadecanal	240	C16H32O	000629-80-1	91
4		17-Octadecenal	266	C18H34O	056554-86-0	91
5		16-Octadecenal	266	C18H34O	056554-87-1	90



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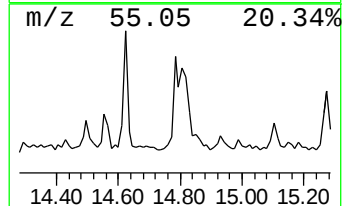
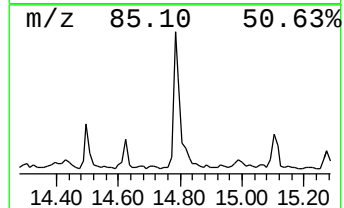
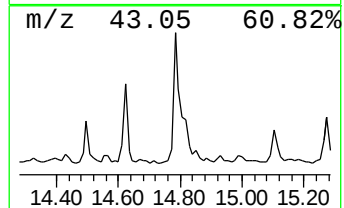
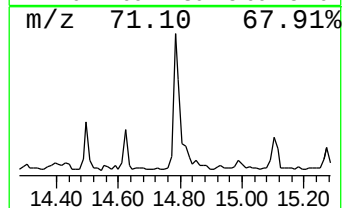
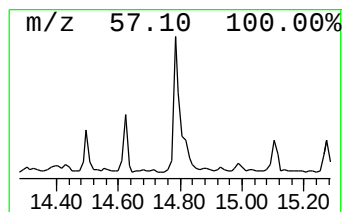
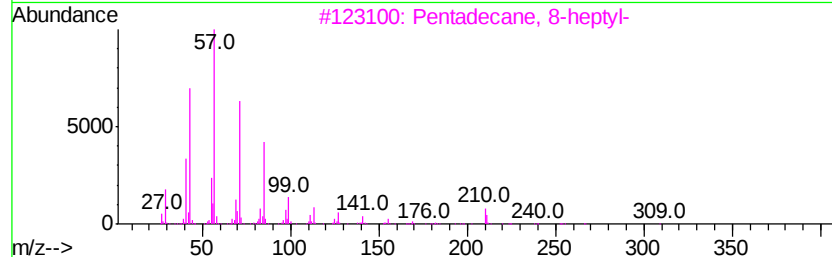
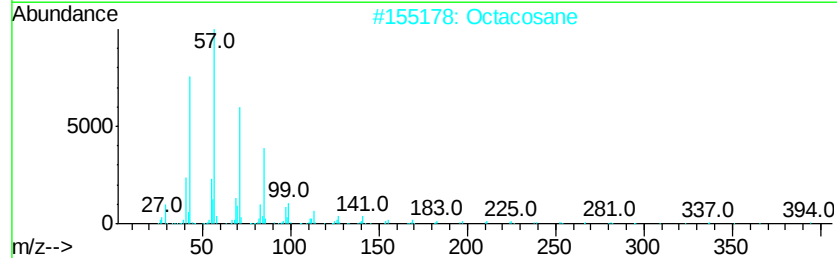
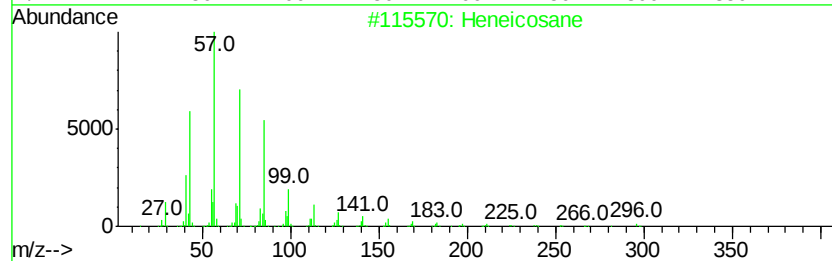
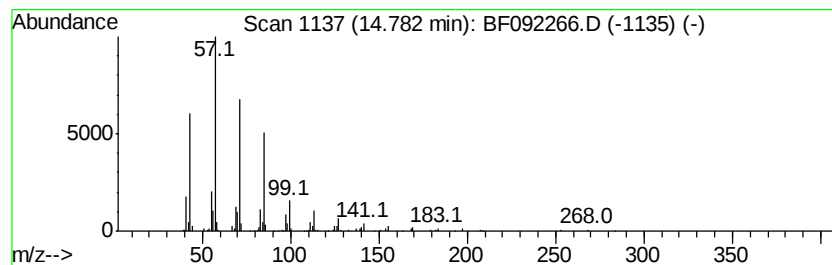
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	7.86 ng	388961	Perylene-d12	15.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Pentadecane, 8-heptvl-	310	C22H46	071005-15-7	91
4			Docosane	310	C22H46	000629-97-0	90
5			Nonacosane	408	C29H60	000630-03-5	86



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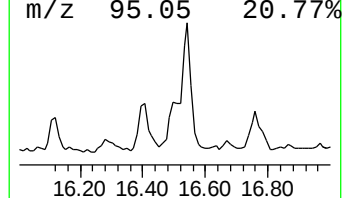
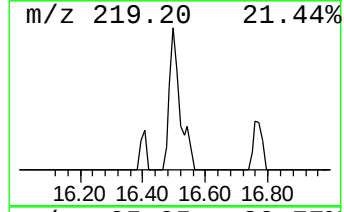
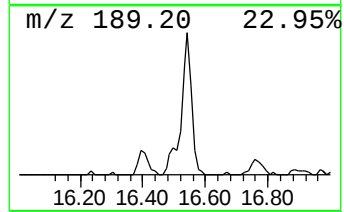
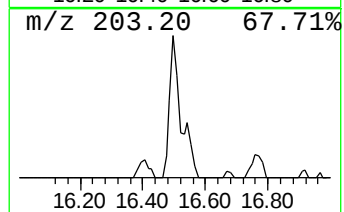
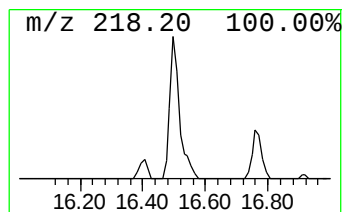
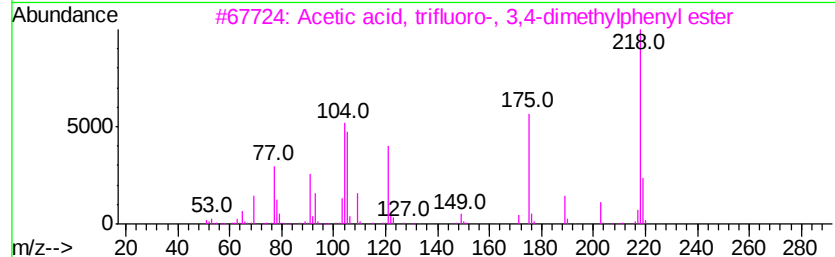
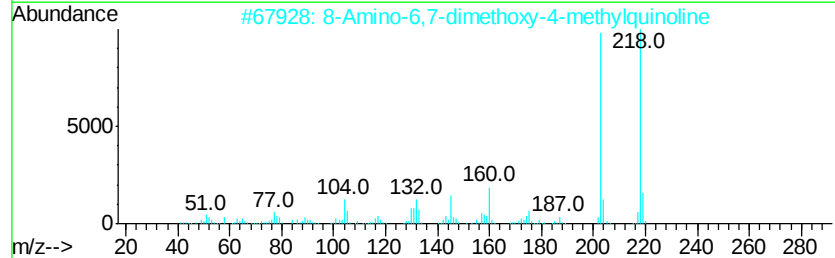
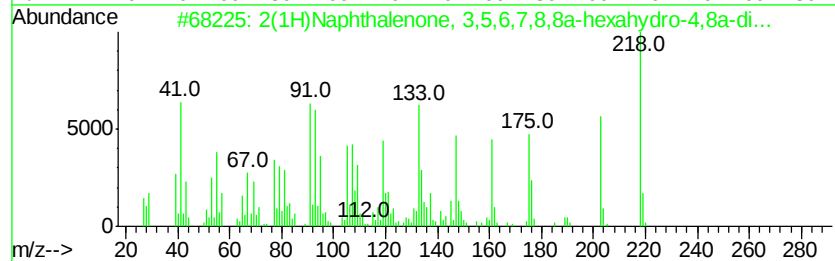
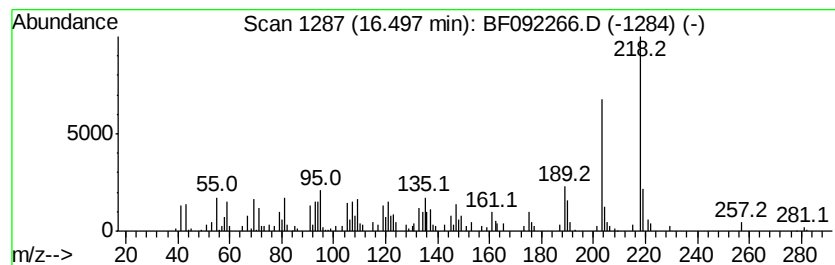
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 2(1H)Naphthalenone, 3,5,6,7... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	5.15 ng	255043	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	76
2		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	52
3		Acetic acid, trifluoro-, 3,4-dim...	218	C10H9F3O2	001957-55-7	43
4		2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	43
5		1,4-Naphthalenedione, 5,8-dihydr...	218	C12H10O4	021418-10-0	43



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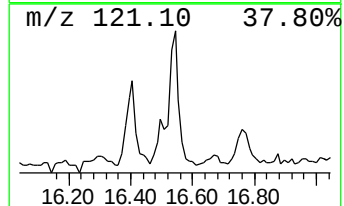
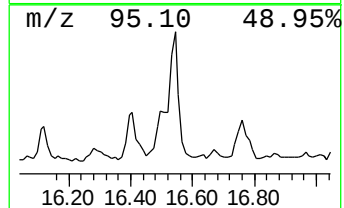
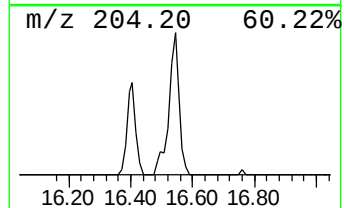
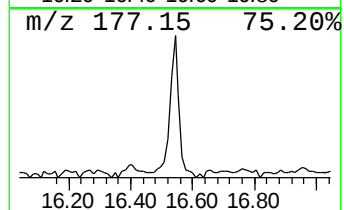
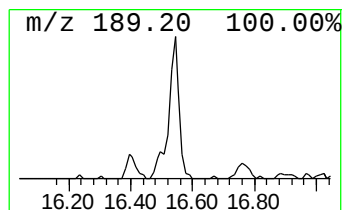
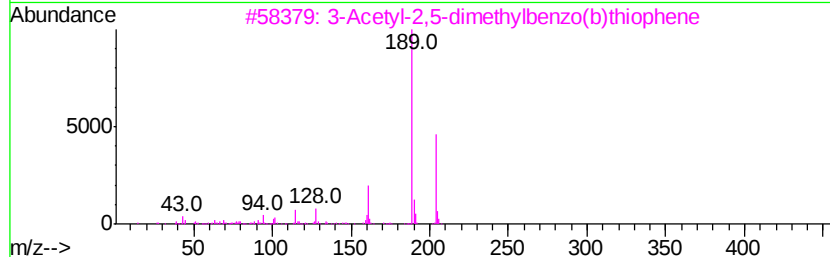
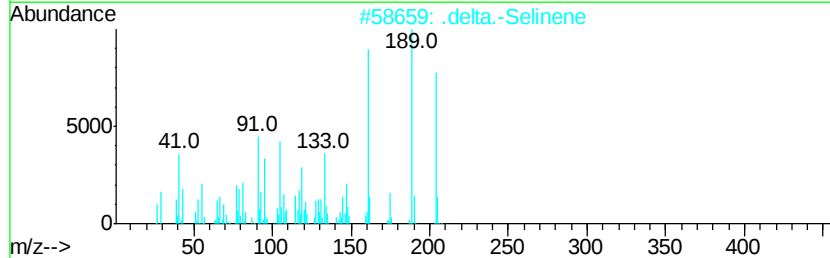
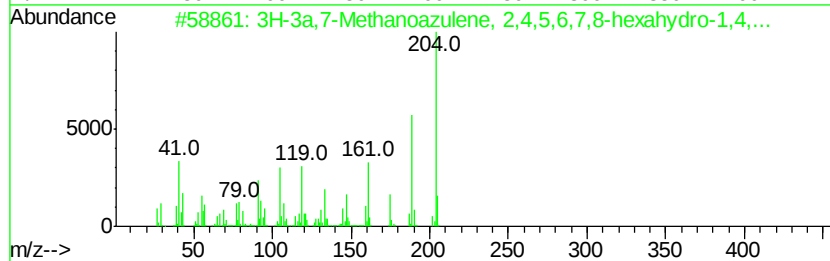
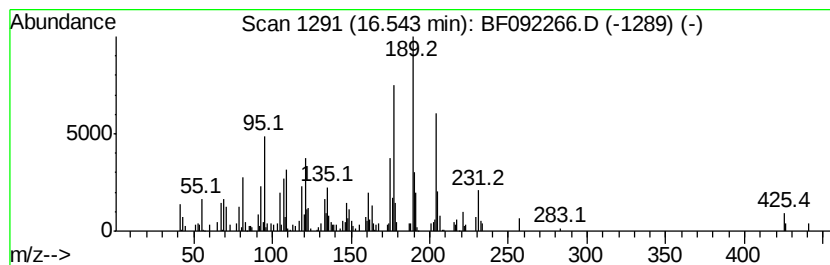
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 3H-3a,7-Methanoazulene, 2,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	7.26 ng	359243	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	53
2		.delta.-Selinene	204	C15H24	028624-23-9	35
3		3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	30
4		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	30
5		2-Acetyl-3,7-dimethylbenzo(b)thi...	204	C12H12OS	006179-06-2	27



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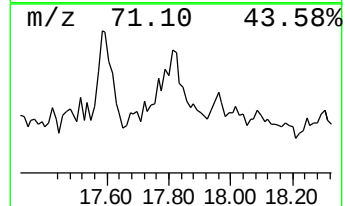
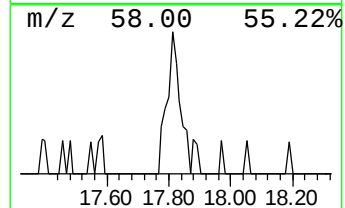
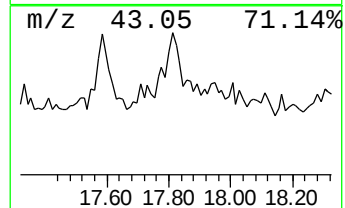
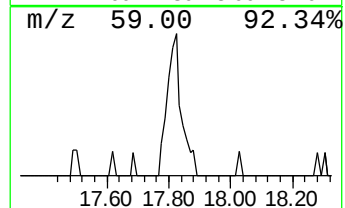
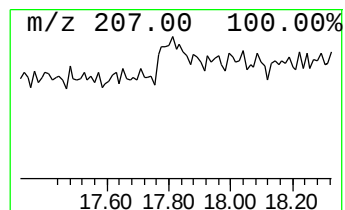
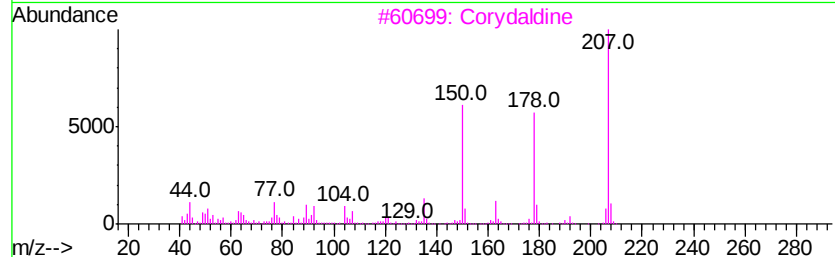
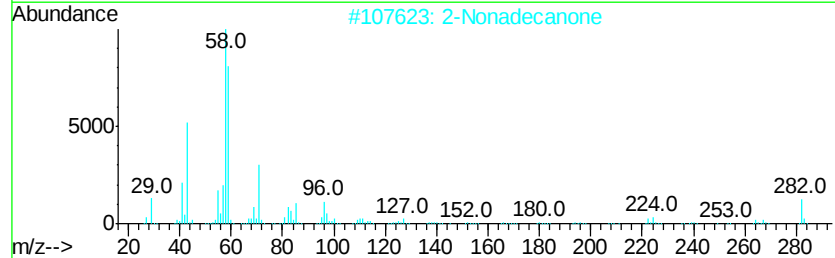
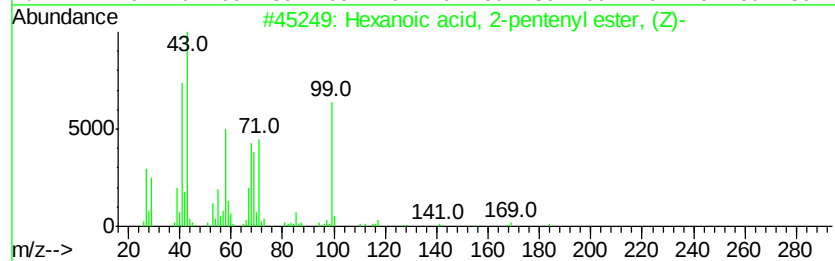
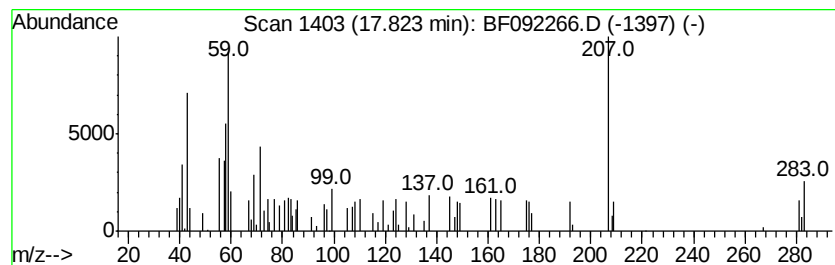
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown17.82 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	2.44 ng	120586	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-pentenyl ester,...	184	C11H20O2	074298-89-8	22
2		2-Nonadecanone	282	C19H38O	000629-66-3	14
3		Corydaldine	207	C11H13NO3	000493-49-2	10
4		2-Propanone, 1-cyclopentyl-	126	C8H14O	001122-98-1	10
5		2,15-Hexadecanedione	254	C16H30O2	018650-13-0	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
 Data File : BF092266.D
 Acq On : 14 Jan 2017 2:38
 Operator : UM/SJ
 Sample : I1031-17
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-0029

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	42.7	ng	2807960	1	6.58	1315580	20.0
unknown6.35	6.35	76.0	ng	5001930	1	6.58	1315580	20.0
Eicosane	10.53	2.4	ng	201362	4	11.09	1683330	20.0
Tridecanoic acid	11.64	5.3	ng	444315	4	11.09	1683330	20.0
Ethanol, 2-(tetra...	13.58	7.2	ng	488672	5	13.71	1357950	20.0
Heptadecane	14.21	3.7	ng	249037	5	13.71	1357950	20.0
Squalene	14.55	4.1	ng	204921	6	15.07	990006	20.0
Octadecanal	14.62	3.3	ng	160755	6	15.07	990006	20.0
Heneicosane	14.78	7.9	ng	388961	6	15.07	990006	20.0
Guaia-3,9-diene	16.41	6.7	ng	333334	6	15.07	990006	20.0
2(1H)Naphthalenon...	16.50	5.2	ng	255043	6	15.07	990006	20.0
3H-3a,7-Methanoaz...	16.54	7.3	ng	359243	6	15.07	990006	20.0
unknown17.82	17.82	2.4	ng	120586	6	15.07	990006	20.0