

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
 Data File : BF088949.D
 Acq On : 13 Jul 2016 7:18
 Operator : UM/SJ
 Sample : H3947-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WPG(15-20)SP-C

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-BF063016.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	1.667	6	7	12	rVV	41652	60570	4.13%	0.450%
2	1.793	16	18	25	rVV	333829	433335	29.57%	3.220%
3	1.895	25	27	37	rVB	30898	56553	3.86%	0.420%
4	2.090	39	44	47	rVB	13874	31317	2.14%	0.233%
5	4.856	283	286	291	rBB	115674	161149	11.00%	1.198%
6	5.301	322	325	327	rBV	1407356	1465501	100.00%	10.890%
7	6.353	414	417	419	rBV	1367499	1464412	99.93%	10.882%
8	6.467	425	427	430	rBV	1182571	1340552	91.47%	9.962%
9	6.696	445	447	449	rBV	280436	343327	23.43%	2.551%
10	6.856	459	461	463	rBB	1123787	1020110	69.61%	7.581%
11	7.267	494	497	499	rBV	882234	824906	56.29%	6.130%
12	7.987	558	560	562	rBV	596635	478383	32.64%	3.555%
13	9.073	652	655	657	rBV	1125112	1440880	98.32%	10.707%
14	9.462	687	689	691	rBV	182030	141179	9.63%	1.049%
15	9.553	694	697	700	rBB	8887	16065	1.10%	0.119%
16	9.736	711	713	715	rBV	538367	444352	30.32%	3.302%
17	10.525	779	782	784	rBV	708988	728110	49.68%	5.411%
18	10.651	792	793	798	rBV	17661	21591	1.47%	0.160%
19	10.971	817	821	824	rBV2	27411	48470	3.31%	0.360%
20	11.096	830	832	834	rBV	32359	33151	2.26%	0.246%
21	11.211	840	842	844	rBV	445161	370491	25.28%	2.753%
22	11.279	846	848	852	rVB3	8339	15205	1.04%	0.113%
23	11.816	893	895	902	rVB2	16030	23070	1.57%	0.171%
24	12.411	945	947	949	rBV	35450	36119	2.46%	0.268%
25	12.639	964	967	969	rBV	42379	39283	2.68%	0.292%
26	12.799	978	981	983	rVB	881880	950410	64.85%	7.063%
27	13.039	997	1002	1004	rBV2	8549	16103	1.10%	0.120%
28	13.497	1040	1042	1044	rVB	221198	183352	12.51%	1.363%
29	13.702	1057	1060	1063	rBV	64853	78468	5.35%	0.583%
30	13.839	1069	1072	1073	rBV	264377	379083	25.87%	2.817%
31	14.148	1096	1099	1101	rBV	147308	146658	10.01%	1.090%
32	14.331	1112	1115	1120	rBV3	15921	32338	2.21%	0.240%
33	14.754	1149	1152	1154	rBV2	30158	43995	3.00%	0.327%
34	14.834	1156	1159	1163	rBV	15697	36252	2.47%	0.269%

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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	14.925	1164	1167	1172	rBV2	12958	23838	1.63%	0.177%
36	15.142	1185	1186	1189	rBV	9659	17632	1.20%	0.131%
37	15.211	1189	1192	1194	rBV	209085	280951	19.17%	2.088%
38	15.428	1209	1211	1215	rVB2	13533	23962	1.64%	0.178%
39	15.645	1227	1230	1231	rBV2	10060	16016	1.09%	0.119%
40	15.691	1231	1234	1237	rVB4	7682	18032	1.23%	0.134%
41	16.205	1277	1279	1286	rVB7	5824	18216	1.24%	0.135%
42	16.331	1288	1290	1293	rVB2	9098	15623	1.07%	0.116%
43	16.800	1328	1331	1335	rVB5	8243	20906	1.43%	0.155%
44	17.017	1346	1350	1352	rBV4	9091	21764	1.49%	0.162%
45	17.074	1352	1355	1360	rVB6	11654	26589	1.81%	0.198%
46	17.291	1370	1374	1377	rBV4	12684	31606	2.16%	0.235%
47	17.497	1389	1392	1395	rVB4	8338	18202	1.24%	0.135%
48	17.908	1423	1428	1434	rBV8	5349	18835	1.29%	0.140%

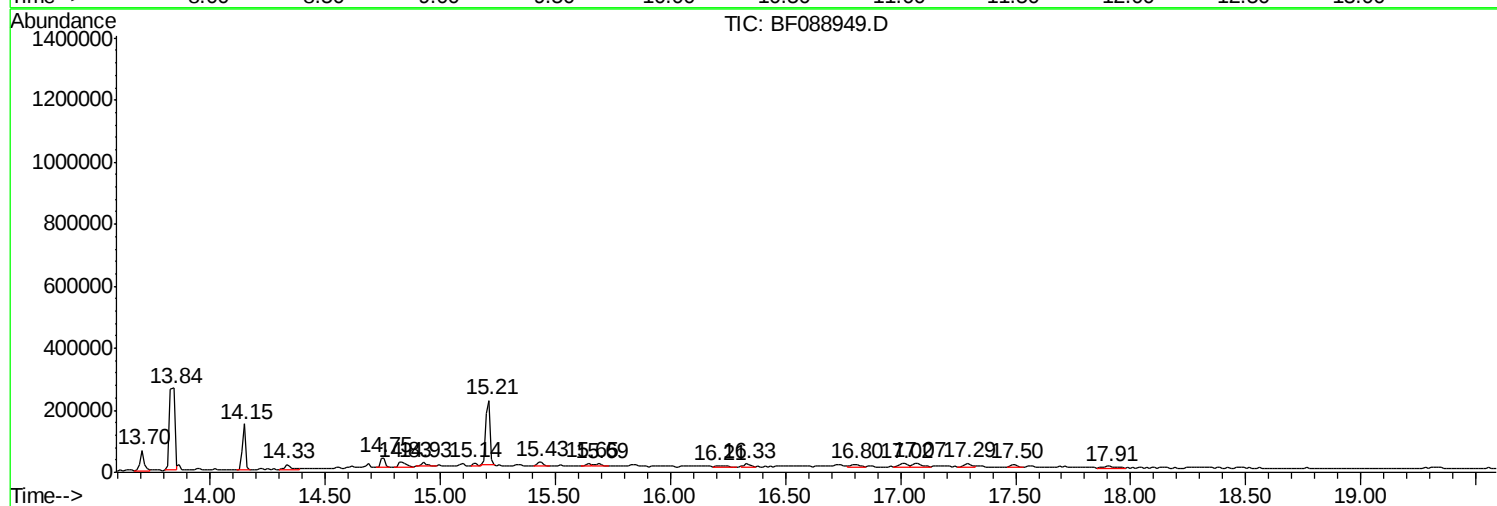
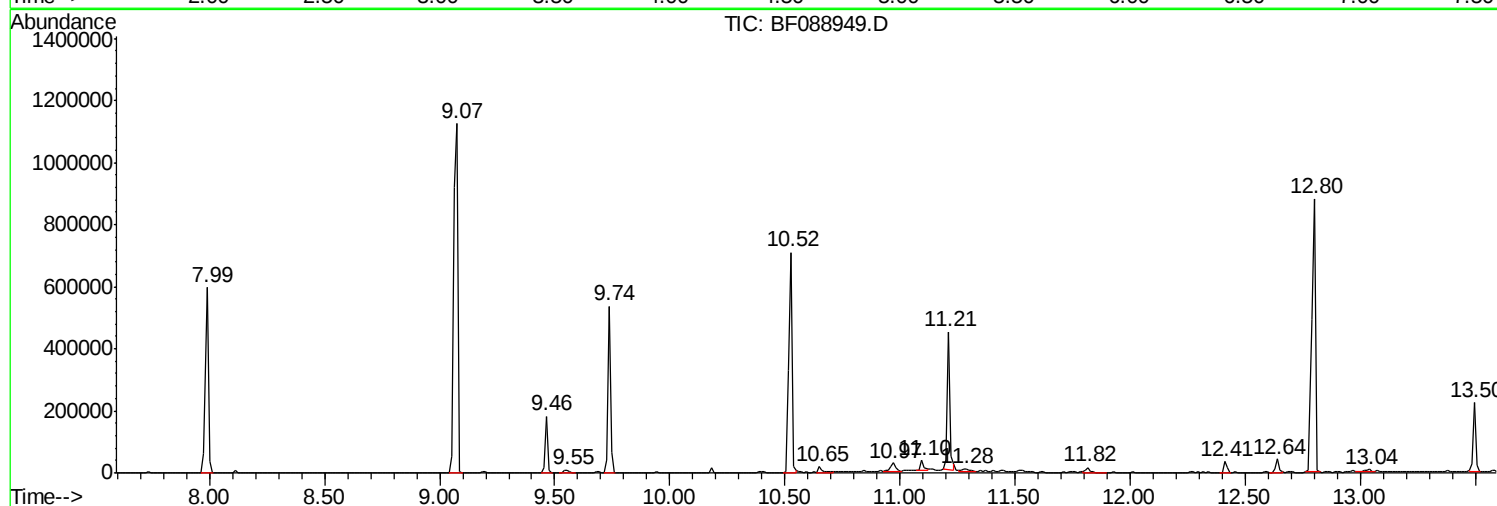
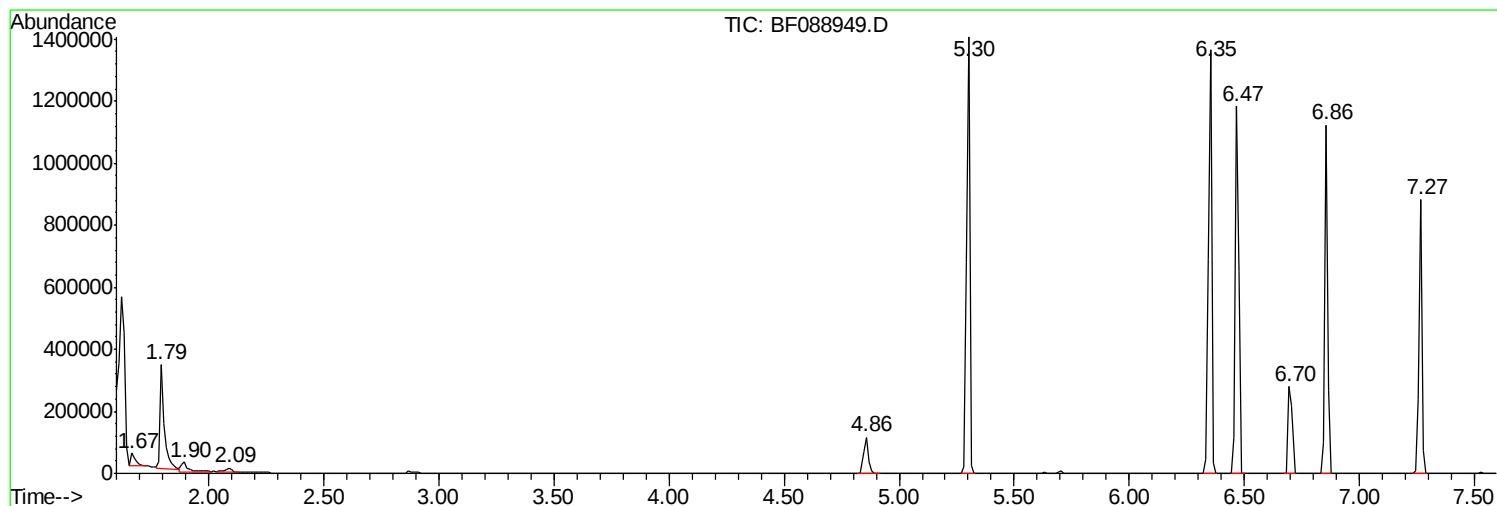
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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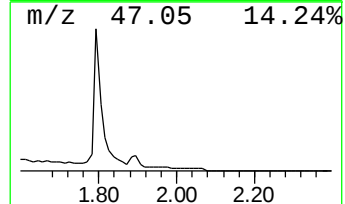
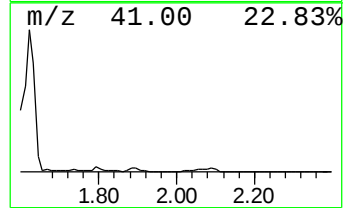
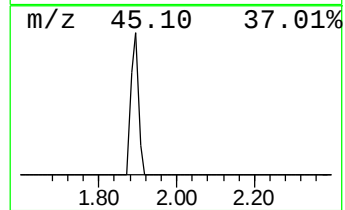
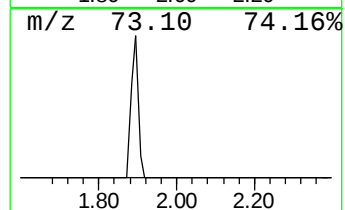
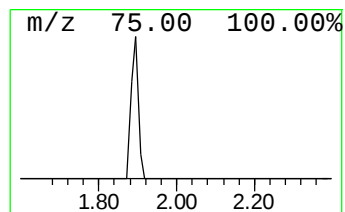
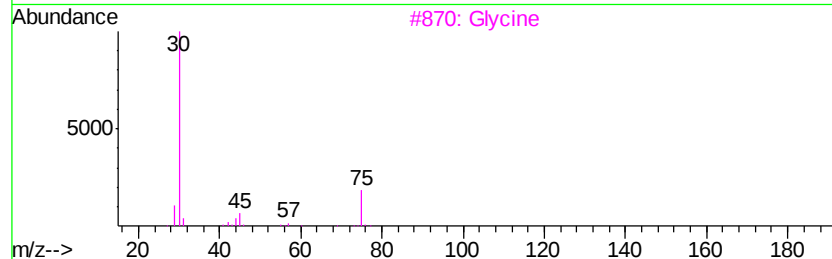
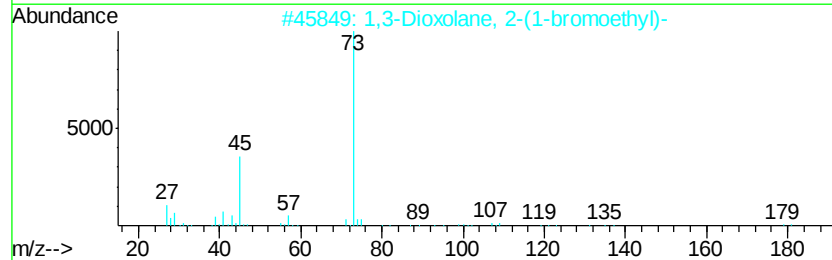
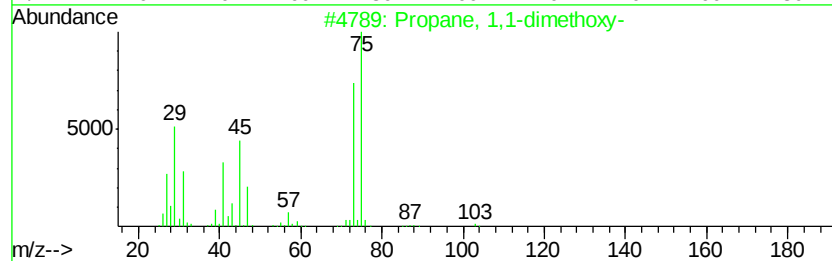
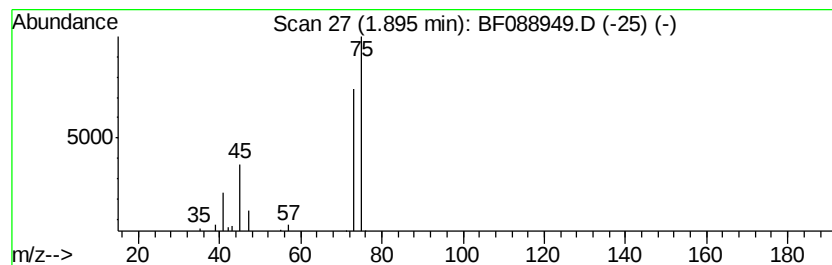
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.90	3.29 ng	56553	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
3		Glycine	75	C2H5NO2	000056-40-6	7
4		1-Butanamine	73	C4H11N	000109-73-9	4
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	4



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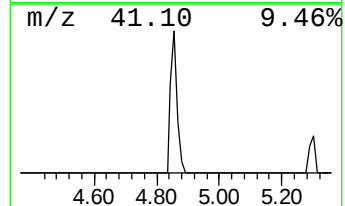
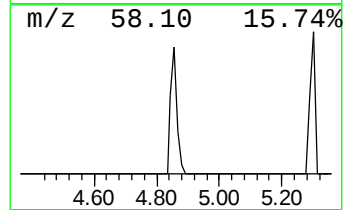
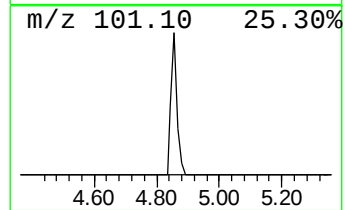
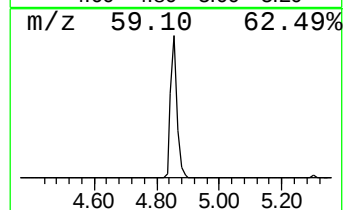
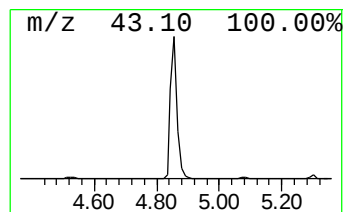
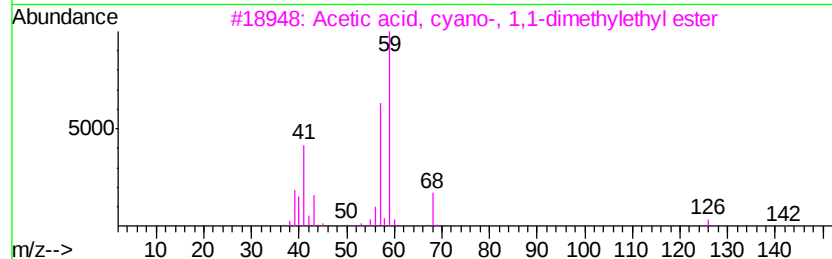
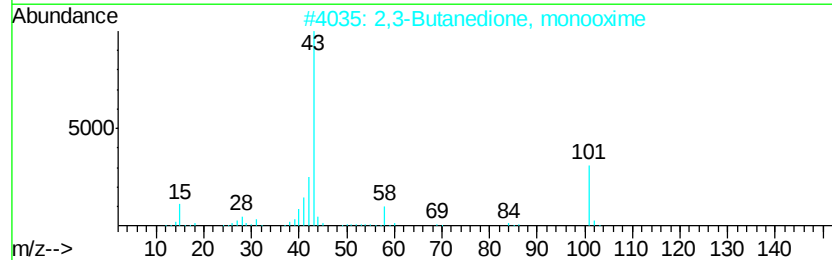
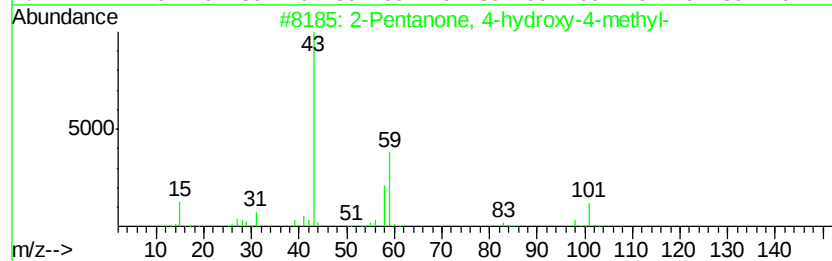
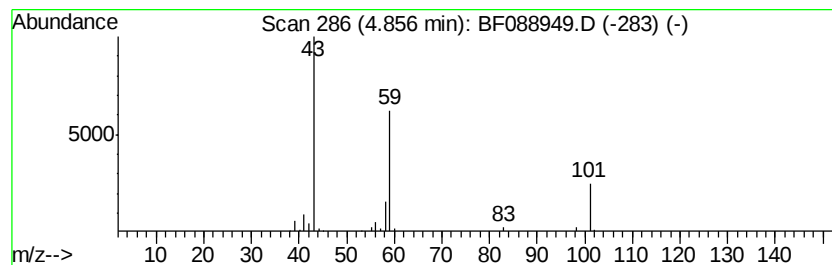
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	9.39 ng	161149	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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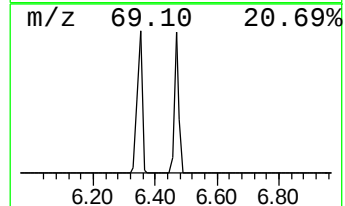
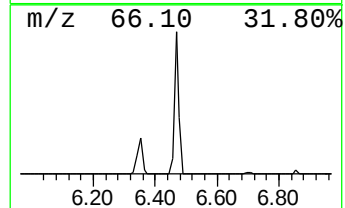
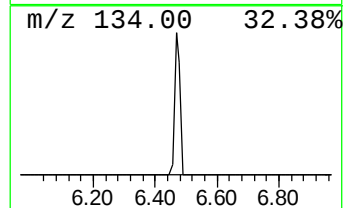
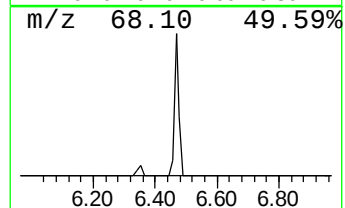
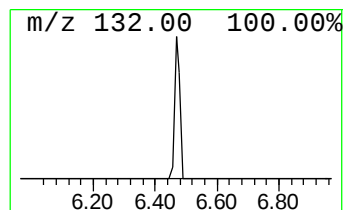
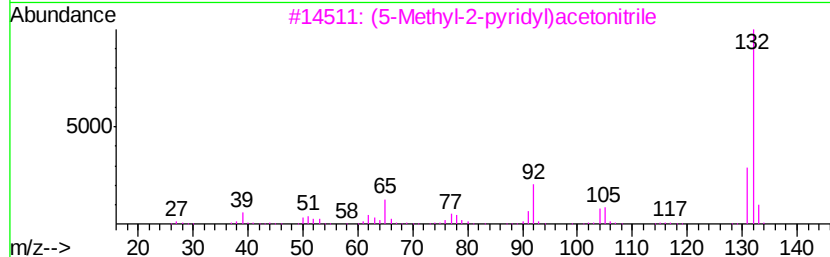
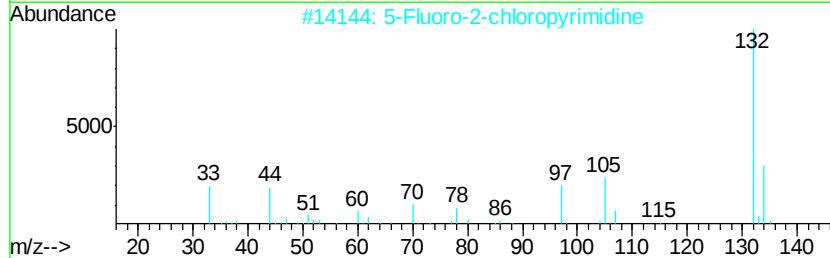
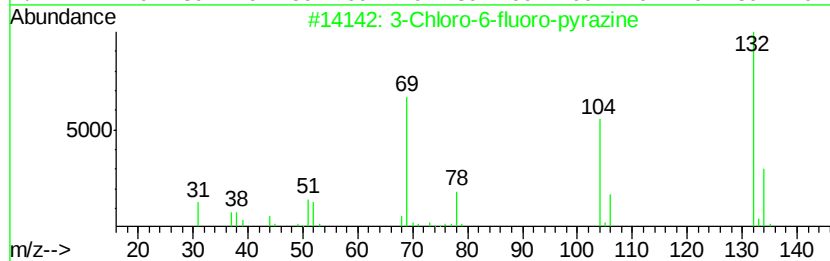
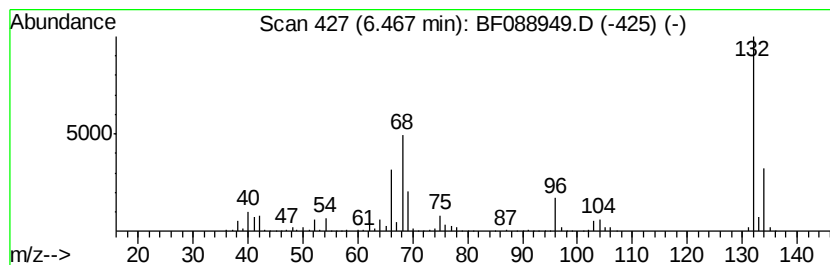
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	78.09 ng	1340550	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10	
4	Tranvlcyproamine-propionyl	189	C12H15NO	1000123-86-3	10	
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10	



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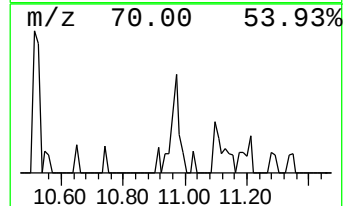
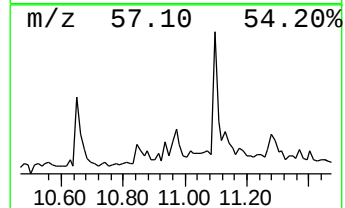
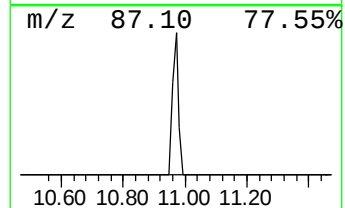
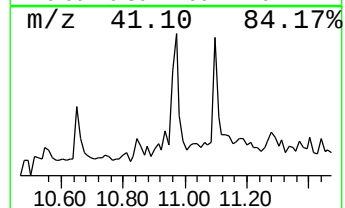
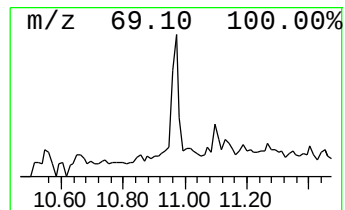
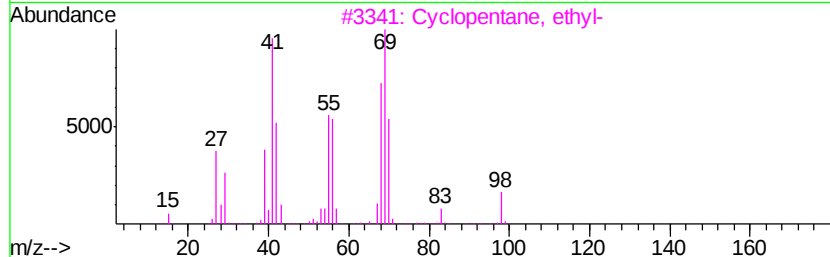
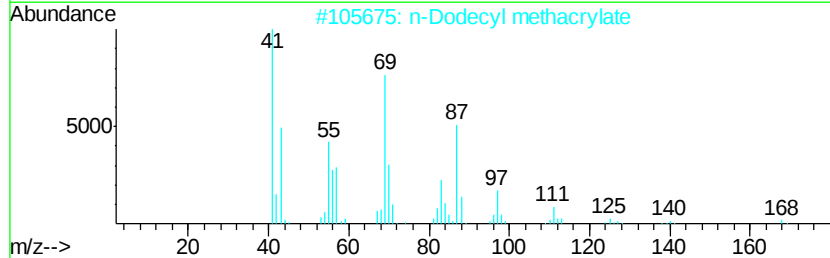
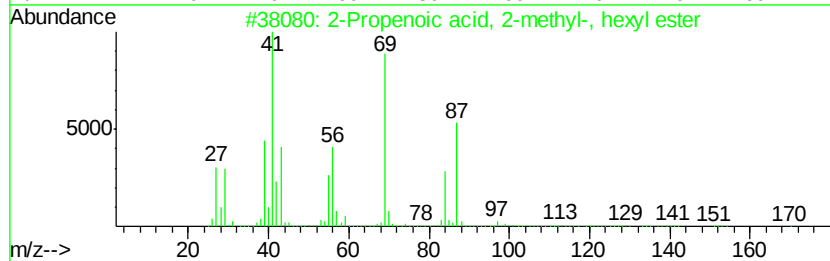
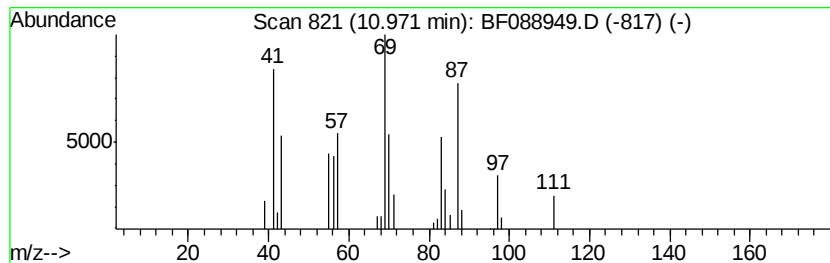
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TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown10.97 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.97	2.62 ng	48470	Phenanthrene-d10	11.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	47
2	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	45
3	Cvclopentane, ethvl-	98	C7H14	001640-89-7	38
4	1-Dodecene	168	C12H24	000112-41-4	35
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	27



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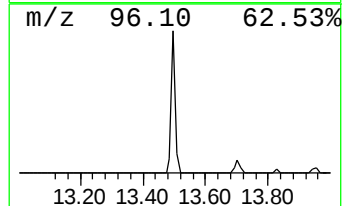
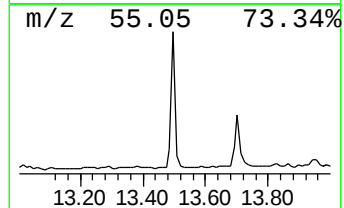
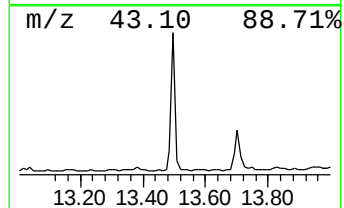
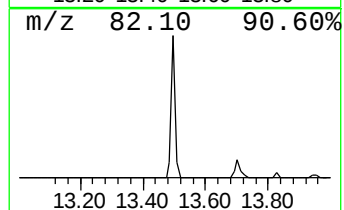
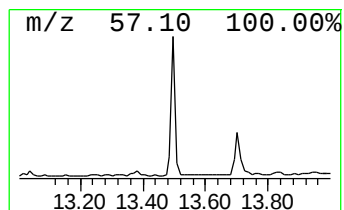
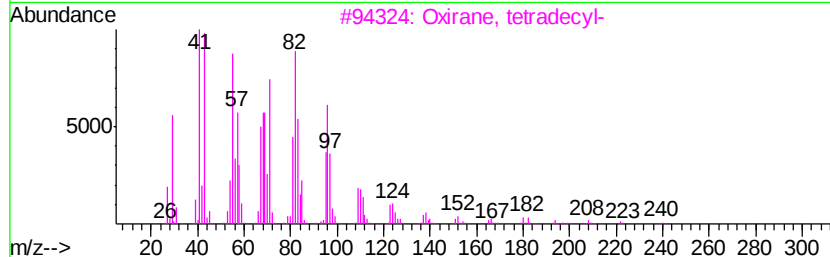
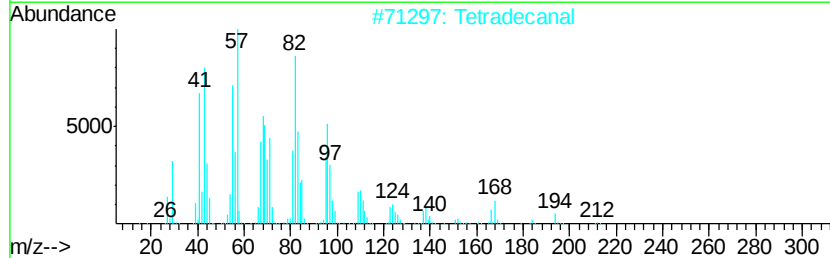
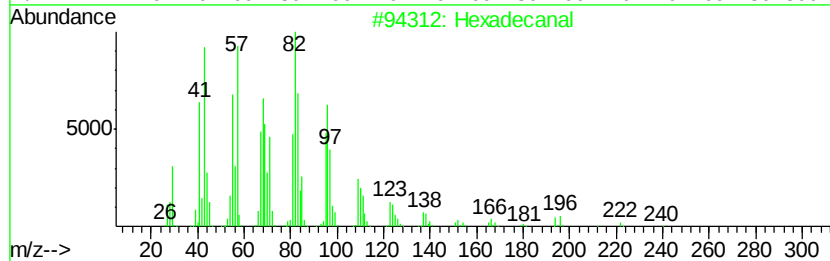
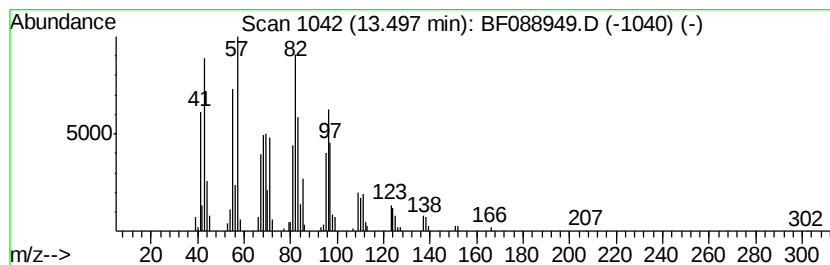
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ClientSampleId :
WPG(15-20)SP-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.50	9.67 ng	183352	Chrysene-d12		13.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanal	240	C16H32O	000629-80-1	90
2	Tetradecanal	212	C14H28O	000124-25-4	87
3	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	87
4	Pentadecanal-	226	C15H30O	002765-11-9	87
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088949.D
Acq On : 13 Jul 2016 7:18
Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WPG(15-20)SP-C

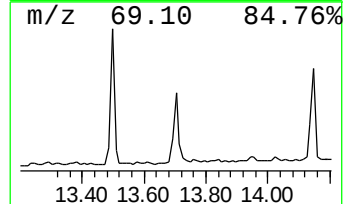
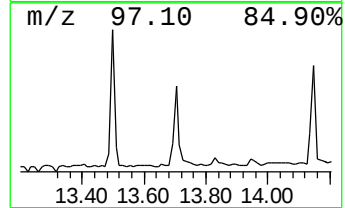
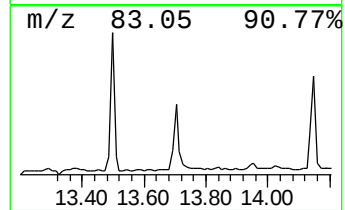
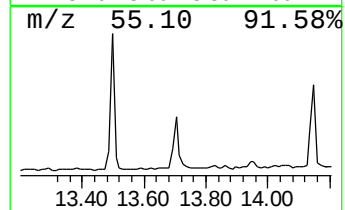
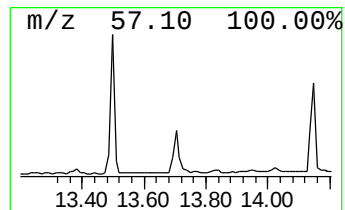
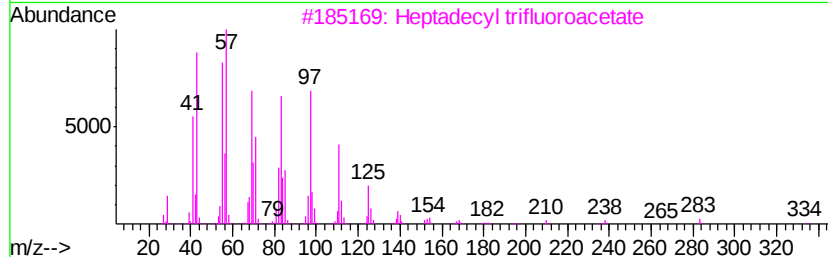
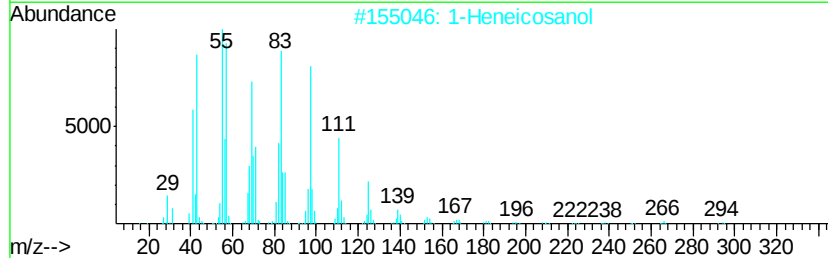
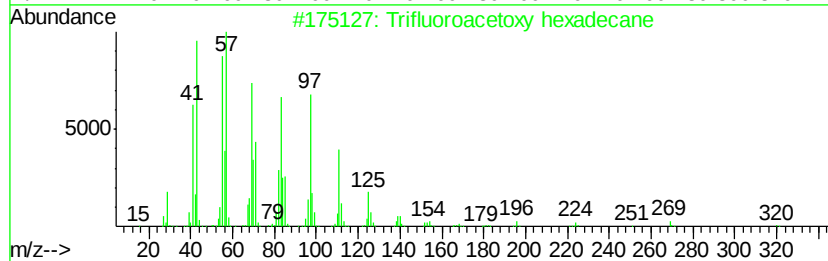
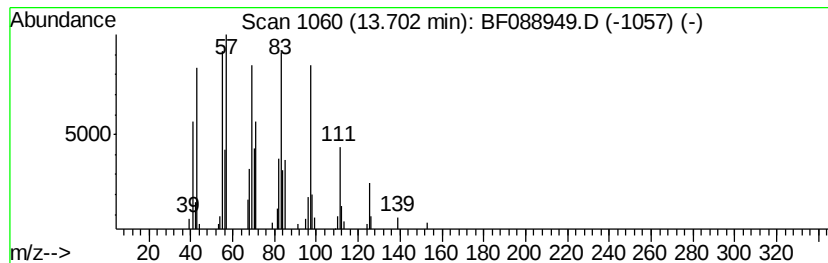
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.14 ng	78468	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
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Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

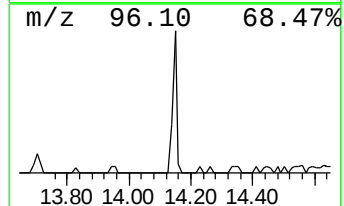
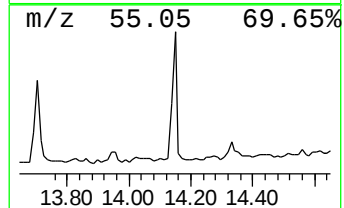
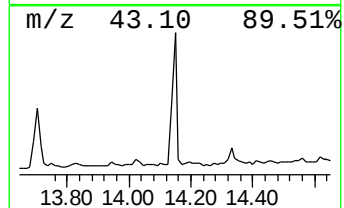
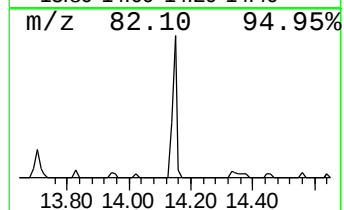
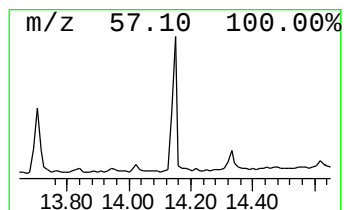
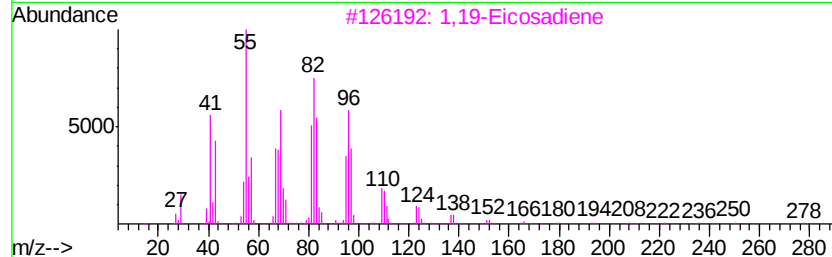
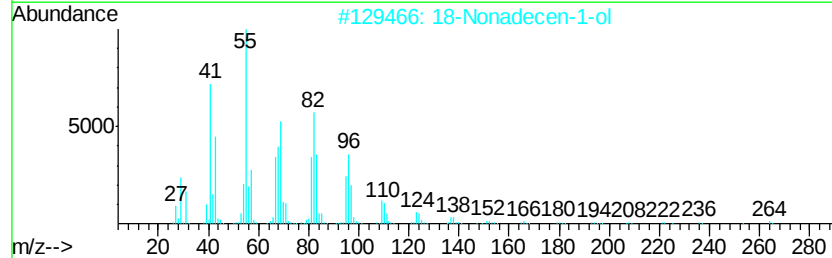
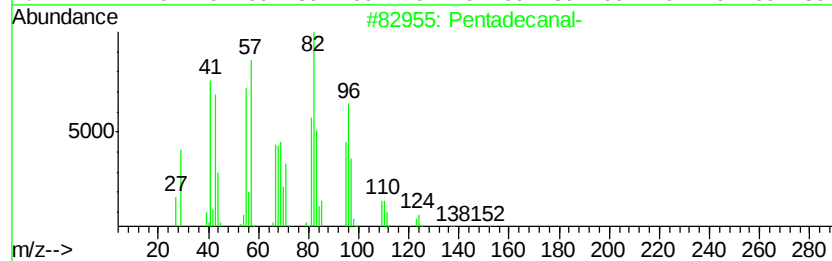
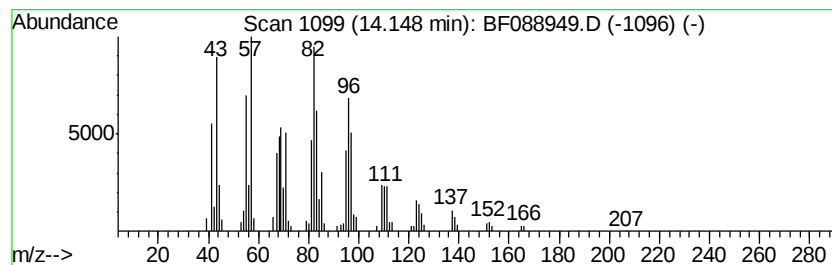
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecanal- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.15	7.74 ng	146658	Chrysene-d12		13.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-	226	C15H30O	002765-11-9	87
2	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	83
3	1,19-Eicosadiene	278	C20H38	014811-95-1	74
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	74
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088949.D
Acq On : 13 Jul 2016 7:18
Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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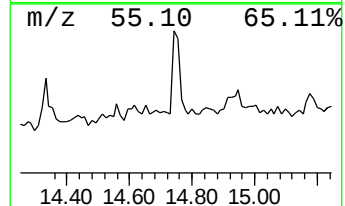
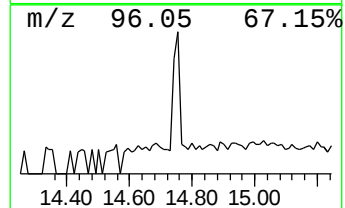
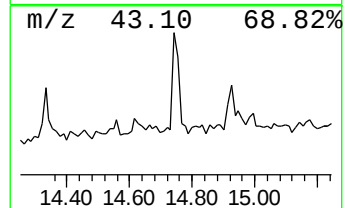
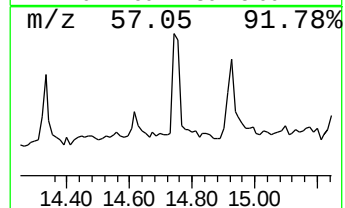
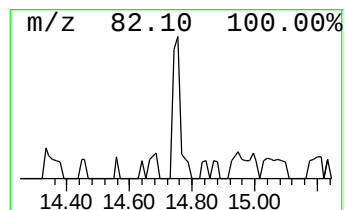
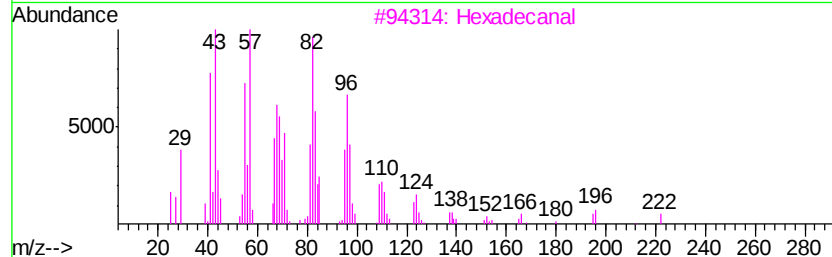
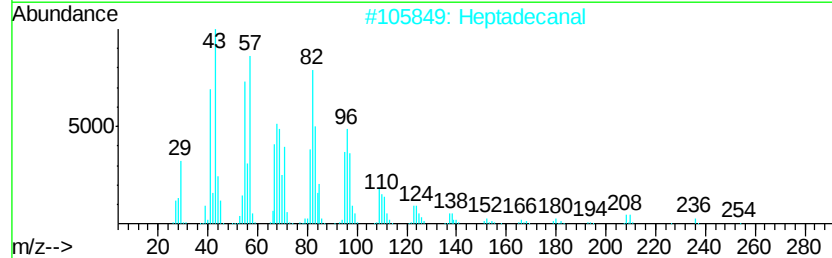
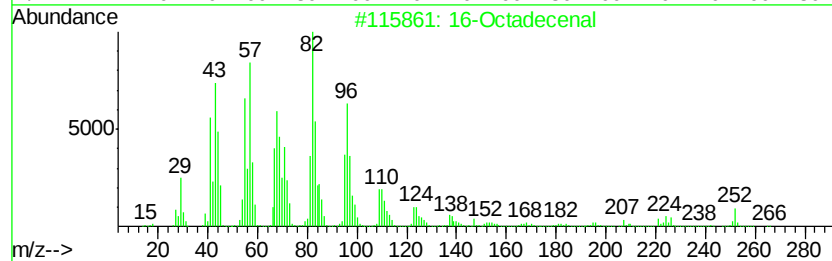
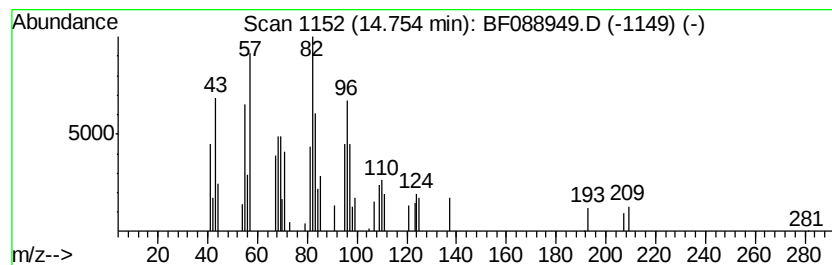
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 16-Octadecenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.13 ng	43995	Perylene-d12	15.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			16-Octadecenal	266	C18H34O	056554-87-1	91
2			Heptadecanal	254	C17H34O	1000376-70-0	91
3			Hexadecanal	240	C16H32O	000629-80-1	91
4			Octadecanal	268	C18H36O	000638-66-4	90
5			Pentadecanal-	226	C15H30O	002765-11-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088949.D
Acq On : 13 Jul 2016 7:18
Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WPG(15-20)SP-C

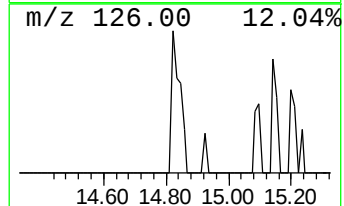
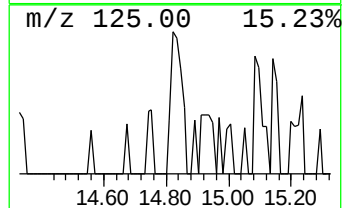
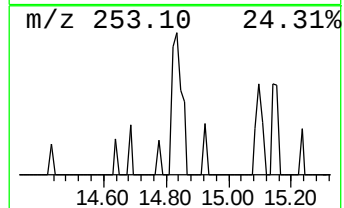
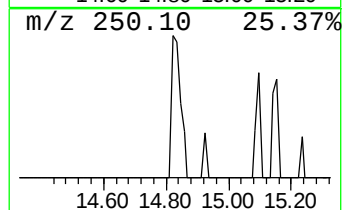
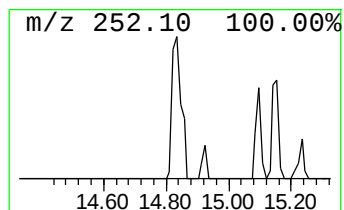
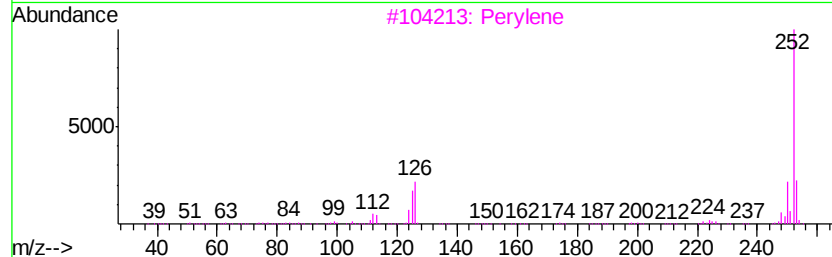
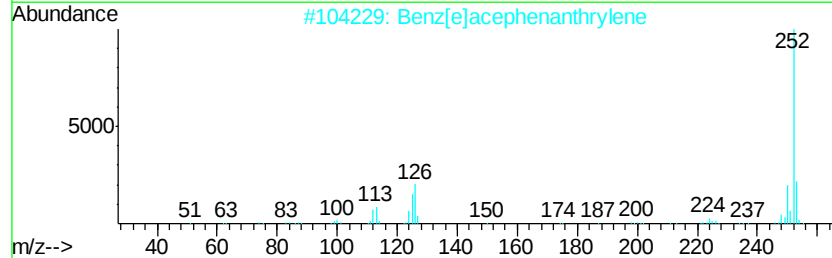
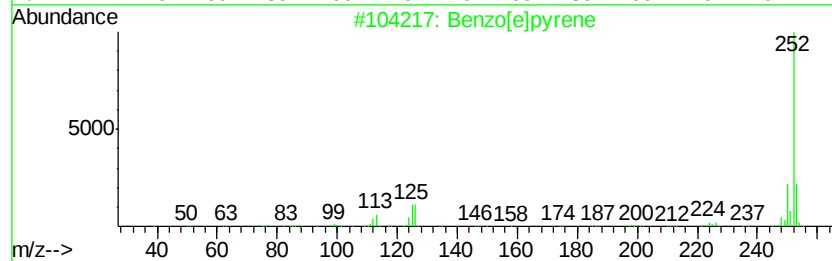
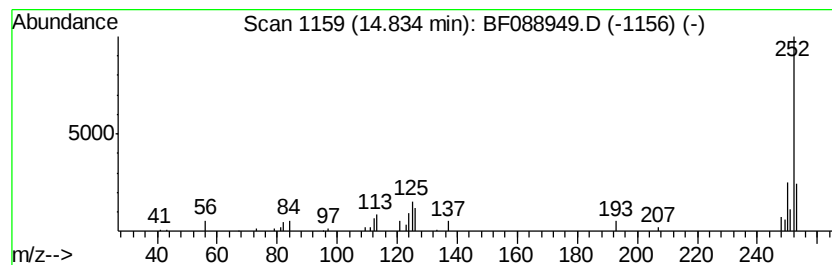
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.58 ng	36252	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	87
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3		Perylene	252	C20H12	000198-55-0	76
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5		Benzo[a]pyrene	252	C20H12	000050-32-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088949.D
Acq On : 13 Jul 2016 7:18
Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WPG(15-20)SP-C

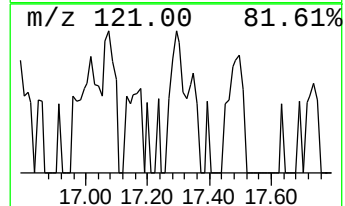
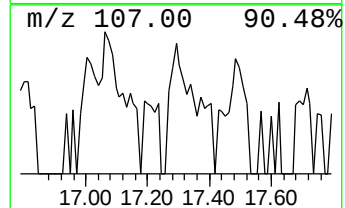
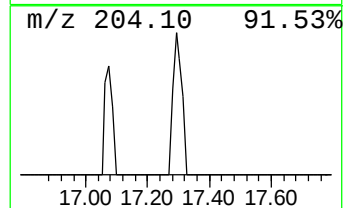
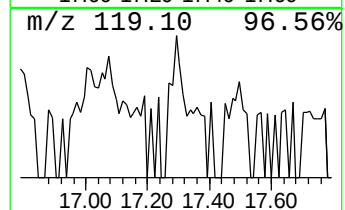
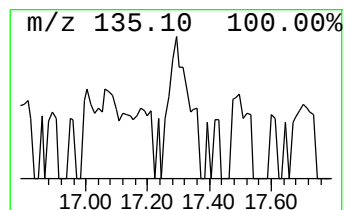
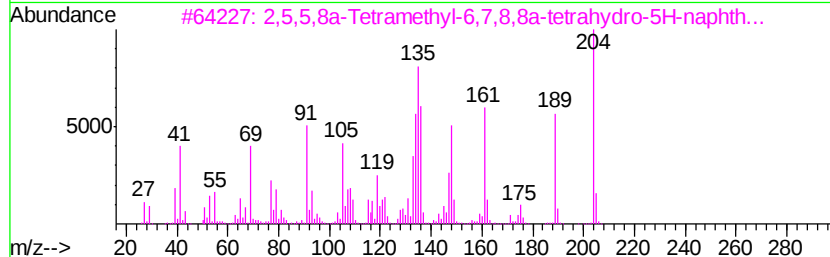
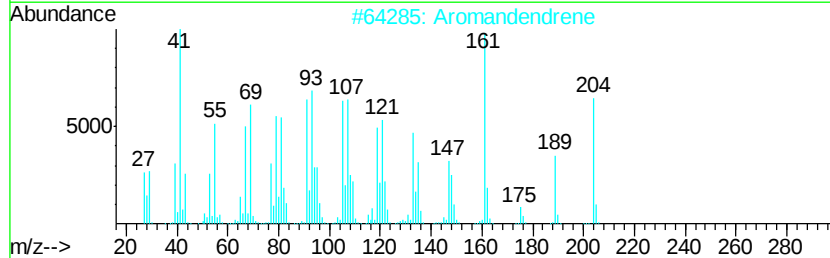
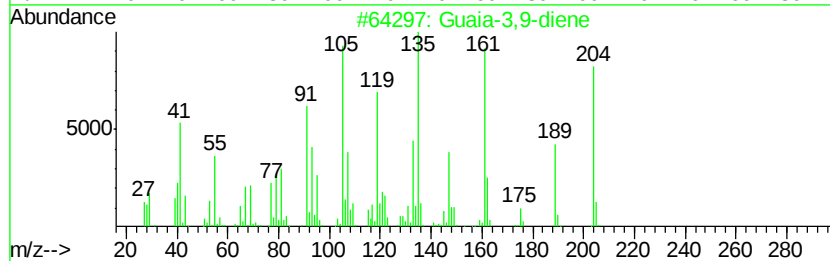
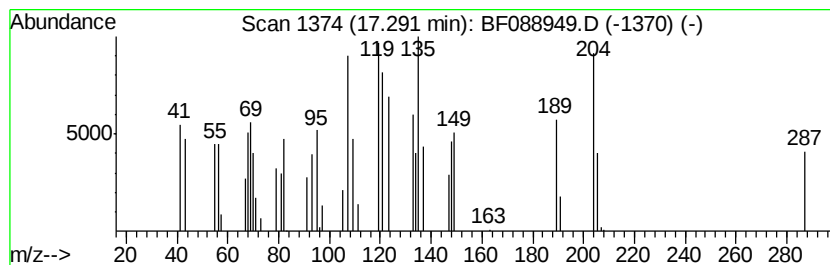
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.29 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.29	2.25 ng	31606	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guaia-3,9-diene	204	C15H24	000489-83-8	49
2		Aromandendrene	204	C15H24	000489-39-4	43
3		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	38
4		cis-Thuiopsene	204	C15H24	000470-40-6	38
5		Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088949.D
Acq On : 13 Jul 2016 7:18
Operator : UM/SJ
Sample : H3947-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WPG(15-20)SP-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	4.86	9.4	ng	161149	1	6.71	343327	20.0
unknown6.47	6.47	78.1	ng	1340550	1	6.71	343327	20.0
unknown10.97	10.97	2.6	ng	48470	4	11.21	370491	20.0
Hexadecanal	13.50	9.7	ng	183352	5	13.84	379083	20.0
Trifluoroacetoxy ...	13.70	4.1	ng	78468	5	13.84	379083	20.0
Pentadecanal-	14.15	7.7	ng	146658	5	13.84	379083	20.0
16-Octadecenal	14.75	3.1	ng	43995	6	15.21	280951	20.0
Benzo[e]pyrene	14.83	2.6	ng	36252	6	15.21	280951	20.0
unknown17.29	17.29	2.3	ng	31606	6	15.21	280951	20.0