

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF121917\
 Data File : BF101539.D
 Acq On : 19 Dec 2017 22:51
 Operator : SJ/JU
 Sample : I6975-03
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11989

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	5.040	498	502	525	rBV	436355	860817	17.40%	2.159%
2	5.440	565	570	588	rBV	3962990	4742463	95.84%	11.893%
3	6.457	738	743	760	rBV	3759784	4948065	100.00%	12.409%
4	6.587	760	765	768	rBV	3949873	4252589	85.94%	10.665%
5	6.804	799	802	812	rBV	1048507	1044859	21.12%	2.620%
6	6.963	825	829	845	rBV	3465229	3587915	72.51%	8.998%
7	7.381	895	900	903	rBV	2807011	2996708	60.56%	7.515%
8	8.092	1017	1021	1038	rBV	1239114	1356917	27.42%	3.403%
9	9.169	1198	1204	1207	rBV	4110011	4515917	91.27%	11.325%
10	9.563	1265	1271	1277	rBV	250756	256071	5.18%	0.642%
11	9.845	1315	1319	1331	rVB2	1450901	1334362	26.97%	3.346%
12	10.263	1387	1390	1393	rVB	75247	61161	1.24%	0.153%
13	10.639	1450	1454	1467	rBV	2049697	2397837	48.46%	6.013%
14	10.733	1467	1470	1478	rVB	82334	91570	1.85%	0.230%
15	11.339	1569	1573	1581	rBV	1131641	1193917	24.13%	2.994%
16	12.921	1837	1842	1845	rBV	3156309	3034019	61.32%	7.609%
17	13.439	1927	1930	1934	rBV	174938	164954	3.33%	0.414%
18	13.798	1988	1991	2004	rBV	324309	471873	9.54%	1.183%
19	13.986	2019	2023	2030	rBV	849480	881928	17.82%	2.212%
20	14.439	2095	2100	2102	rBV4	35616	54489	1.10%	0.137%
21	14.527	2110	2115	2116	rBV3	50343	71812	1.45%	0.180%
22	14.586	2121	2125	2129	rBV	421703	392479	7.93%	0.984%
23	14.633	2130	2133	2138	rVV	35134	60997	1.23%	0.153%
24	14.721	2144	2148	2153	rVB4	68313	119794	2.42%	0.300%
25	15.457	2269	2273	2284	rVB	586452	845798	17.09%	2.121%
26	15.845	2336	2339	2344	rVB	48825	64214	1.30%	0.161%
27	15.921	2347	2352	2357	rVV5	32251	71833	1.45%	0.180%

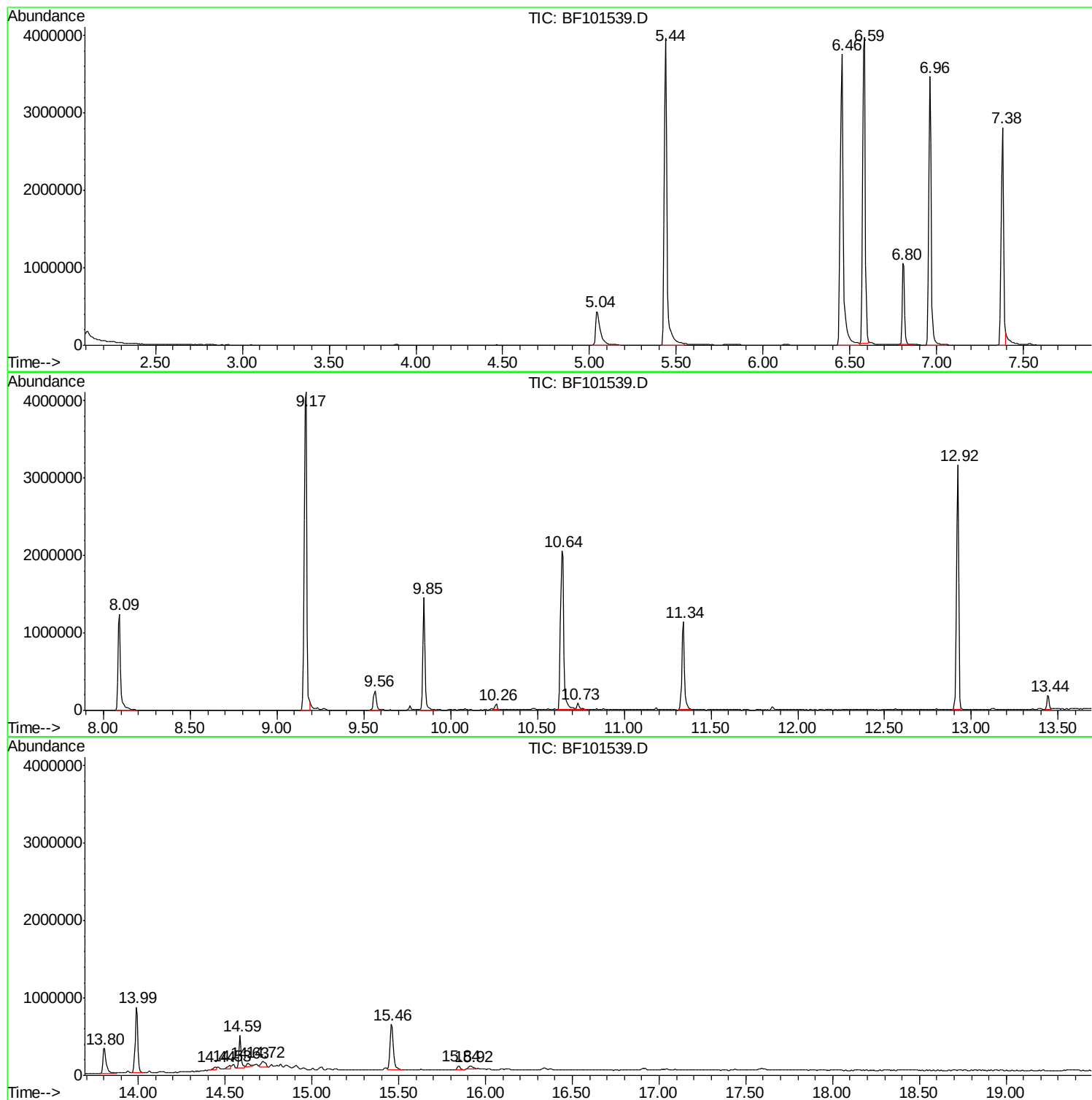
Sum of corrected areas: 39875358

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11989

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

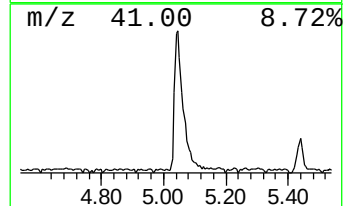
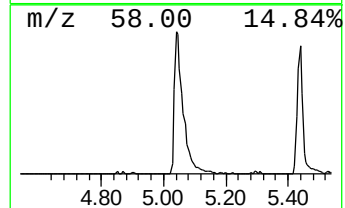
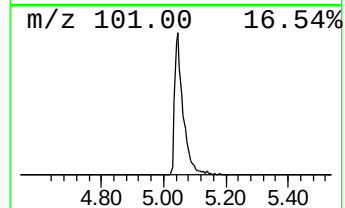
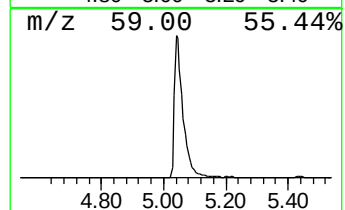
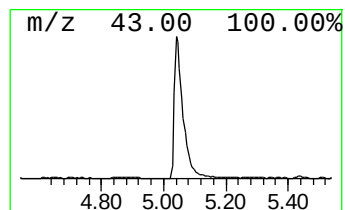
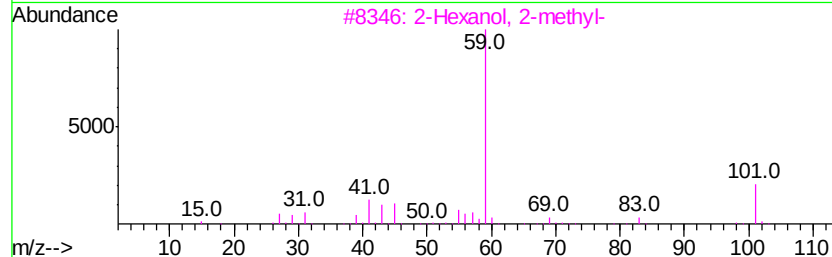
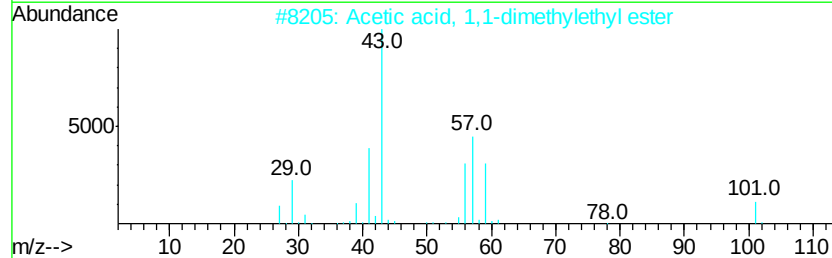
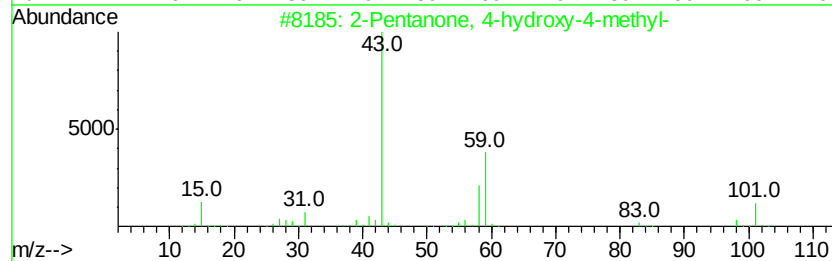
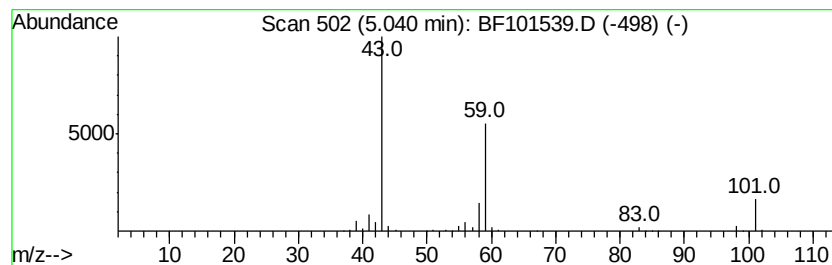
Instrument :
BNA_F
ClientSampleId :
72-11989

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
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.	
5.04	16.48 ng	860817	1,4-Dichlorobenzene-d4	6.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11989

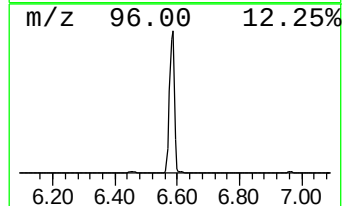
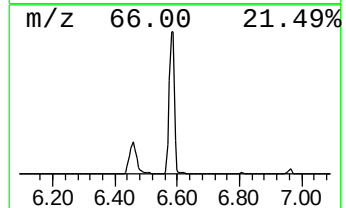
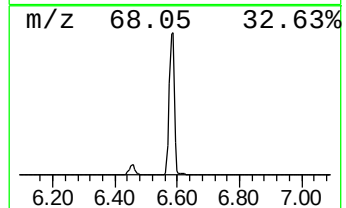
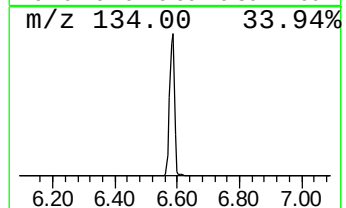
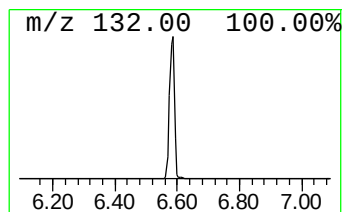
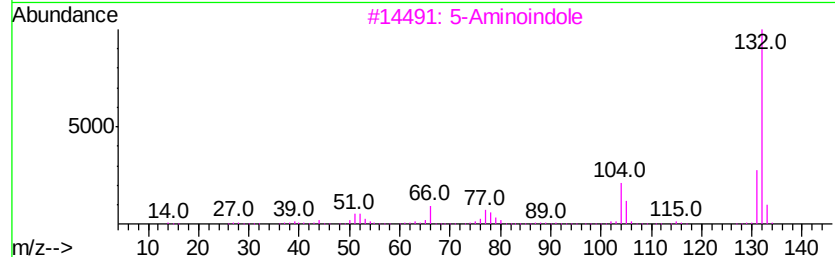
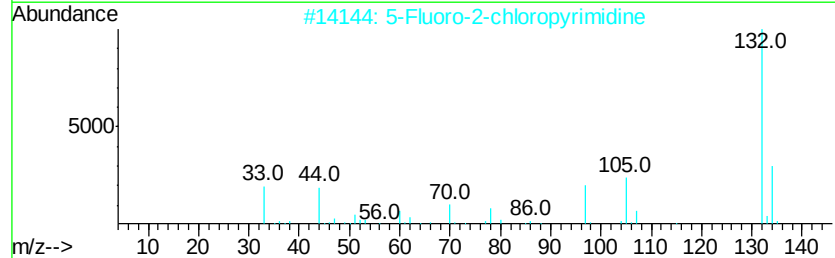
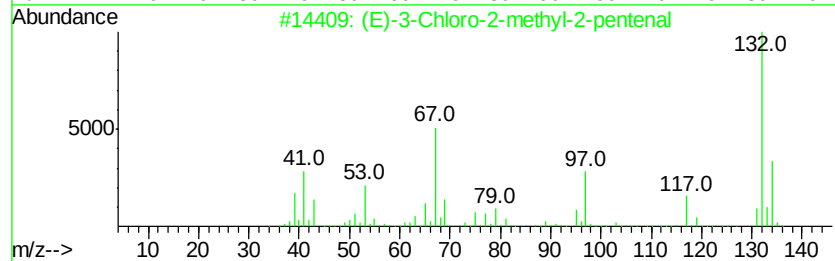
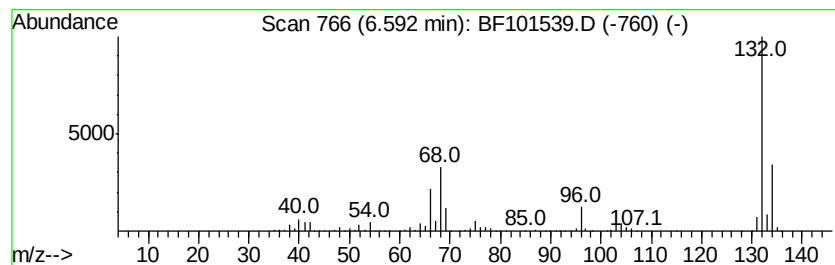
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	81.40 ng	4252590	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

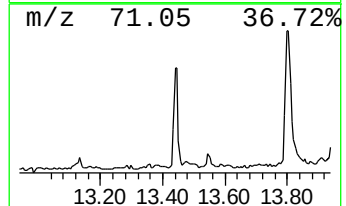
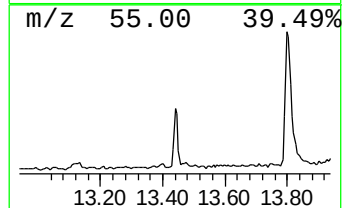
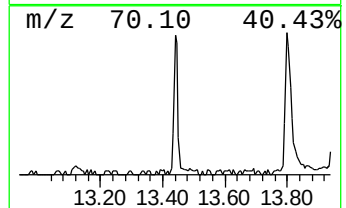
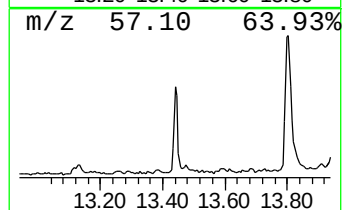
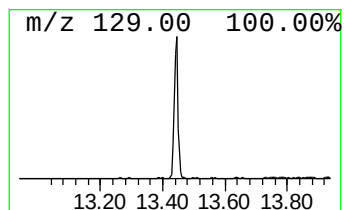
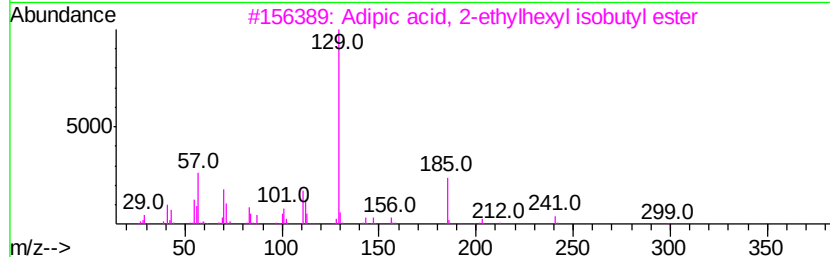
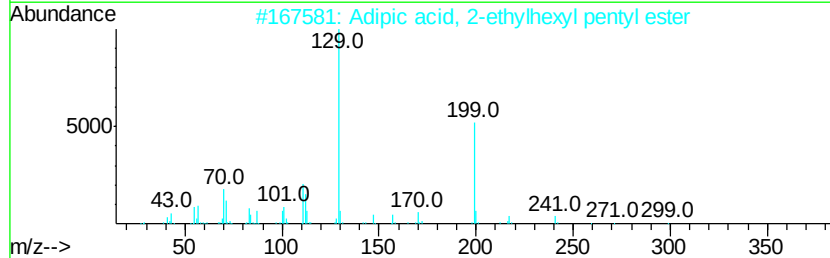
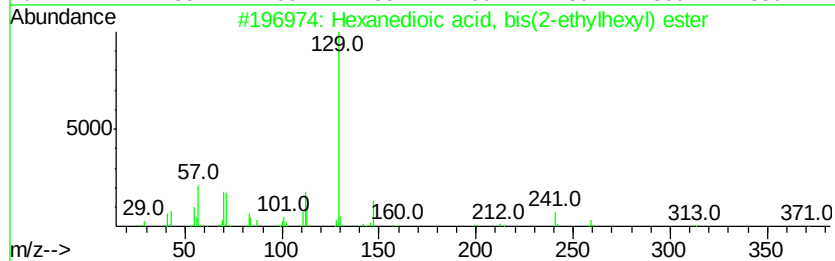
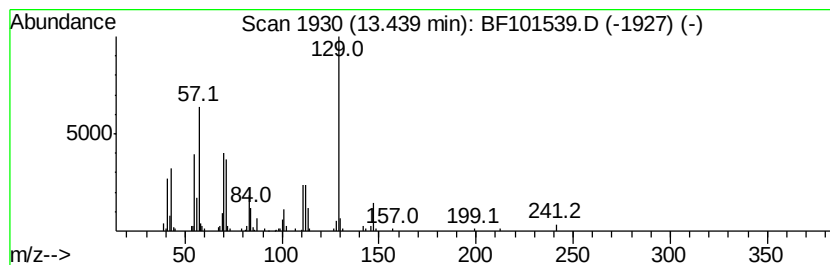
Instrument :
BNA_F
ClientSampleId :
72-11989

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.44	3.74 ng	164954	Chrysene-d12	13.99		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
2		Adipic acid, 2-ethylhexyl pentyl...	328	C19H36O4	1000324-48-2	53
3		Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1000324-48-0	50
4		Adipic acid, isobutyl 3-methylbu...	272	C15H28O4	1000348-45-5	50
5		Adipic acid, pentyl trans-2-meth...	312	C18H32O4	1000324-74-7	43



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11989

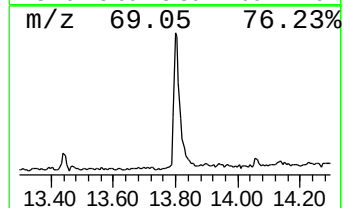
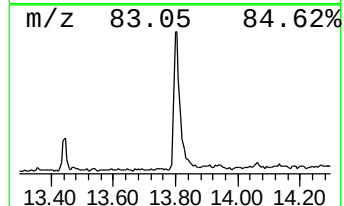
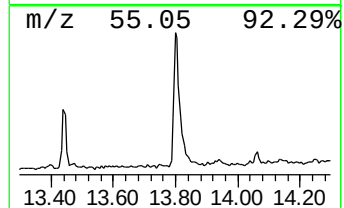
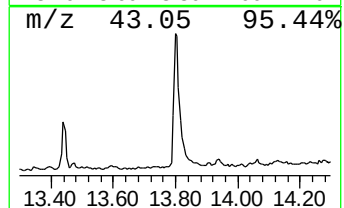
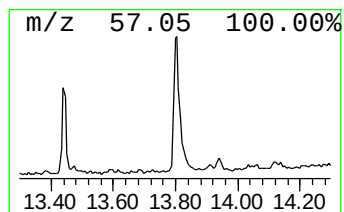
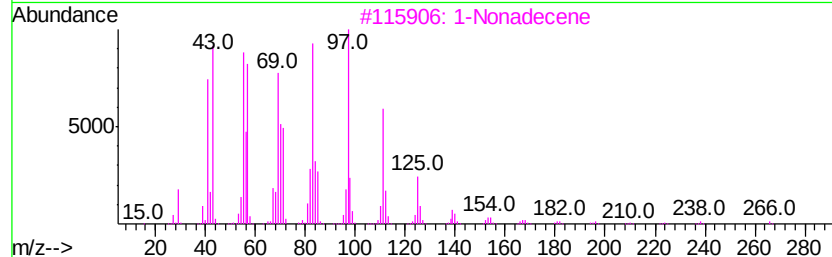
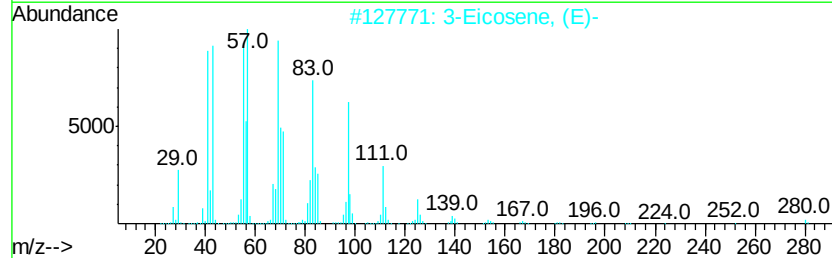
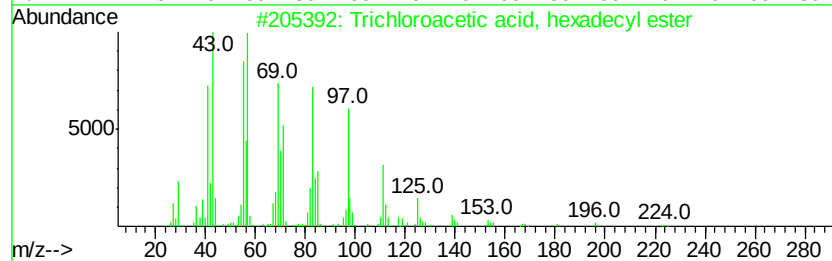
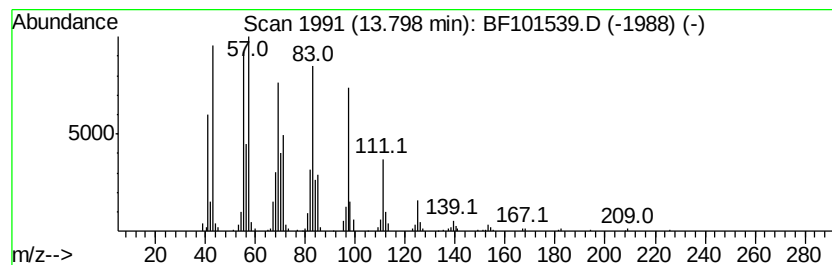
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	10.70 ng	471873	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11989

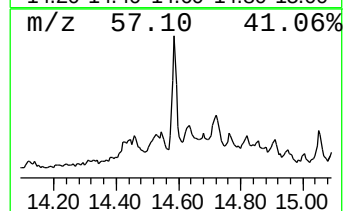
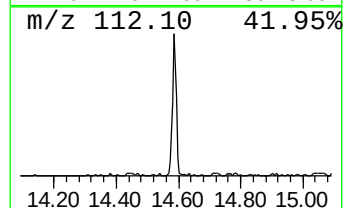
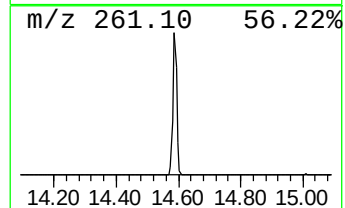
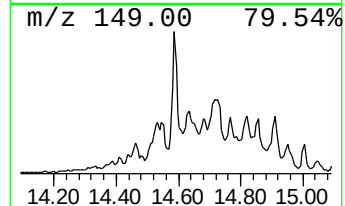
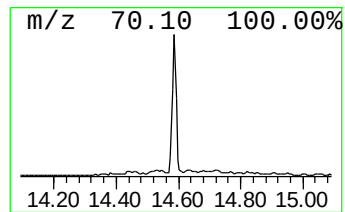
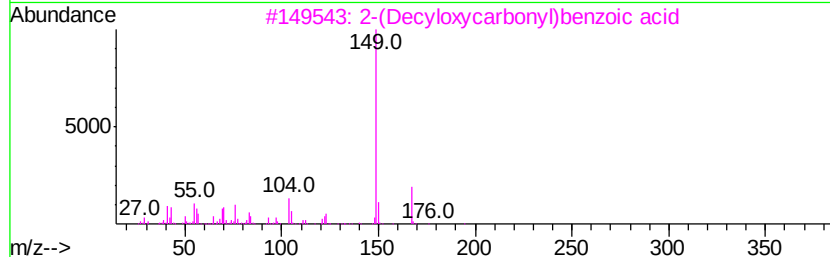
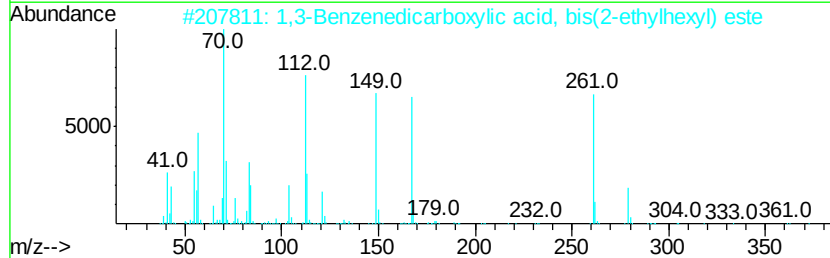
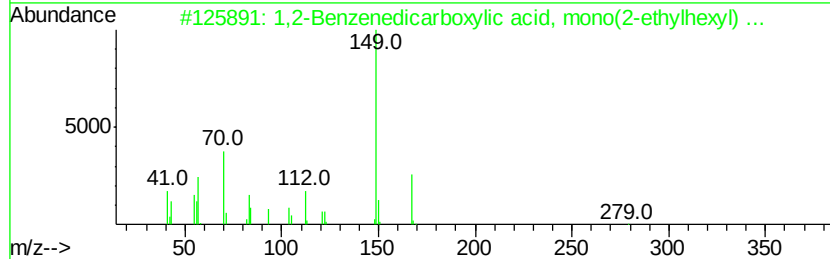
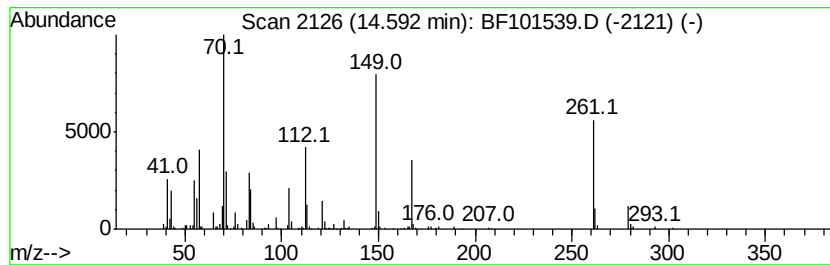
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.59 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	8.90 ng	392479	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	40
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
3		2-(Decyloxy carbonyl)benzoic acid	306	C18H26O4	1000373-53-2	25
4		3-Chloropropionic acid, 2-ethylh...	220	C11H21ClO2	091369-31-2	16
5		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	16



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

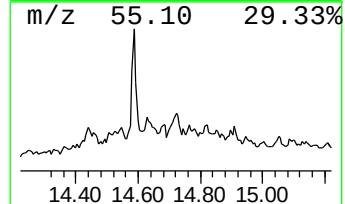
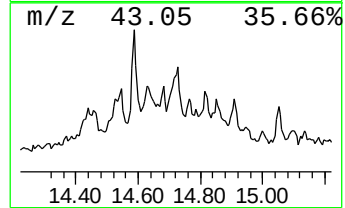
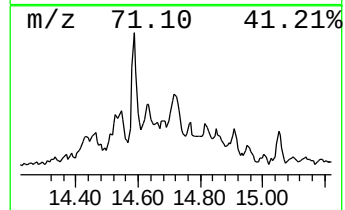
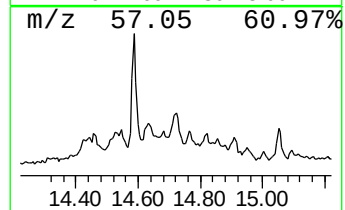
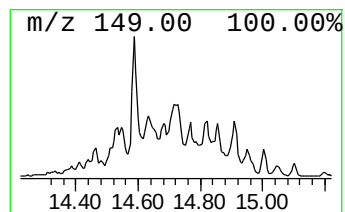
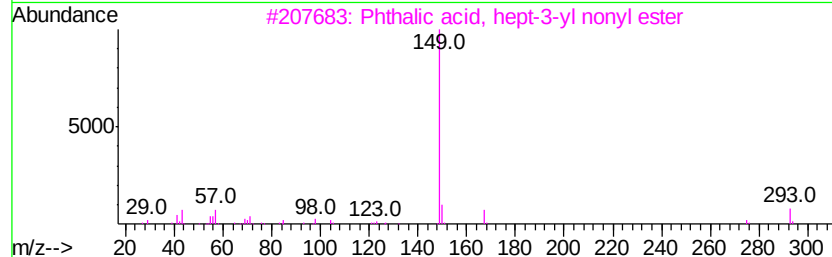
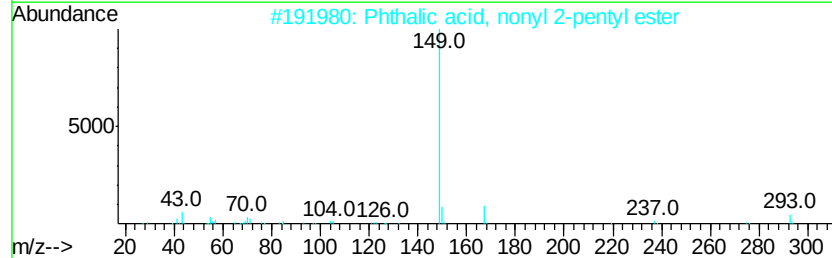
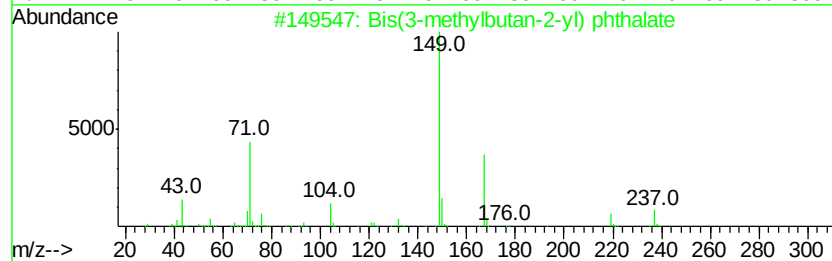
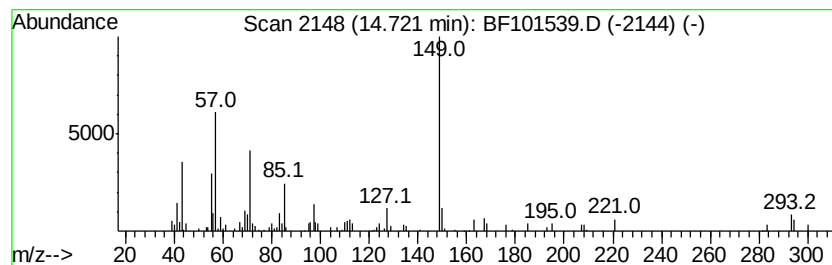
Instrument :
BNA_F
ClientSampleId :
72-11989

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bis(3-methylbutan-2-yl) pht... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.72	2.83 ng	119794	Perylene-d12	15.46		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bis(3-methylbutan-2-yl) phthalate	306	C18H26O4	1000373-65-6	50
2		Phthalic acid, nonyl 2-pentyl ester	362	C22H34O4	1000315-48-1	47
3		Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	43
4		Phthalic acid, nonyl 2-propylpen...	404	C25H40O4	1000377-92-5	43
5		Phthalic acid, hept-3-yl isohexy...	348	C21H32O4	1000356-98-9	43



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF121917\
Data File : BF101539.D
Acq On : 19 Dec 2017 22:51
Operator : SJ/JU
Sample : I6975-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11989

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.04	16.5	ng	860817	1	6.81	1044860	20.0
unknown6.59	6.59	81.4	ng	4252590	1	6.81	1044860	20.0
Hexanedioic acid,...	13.44	3.7	ng	164954	5	13.99	881928	20.0
Trichloroacetic a...	13.80	10.7	ng	471873	5	13.99	881928	20.0
unknown14.59	14.59	8.9	ng	392479	5	13.99	881928	20.0
Bis(3-methylbutan...	14.72	2.8	ng	119794	6	15.46	845798	20.0