

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111117\
 Data File : BF100475.D
 Acq On : 12 Nov 2017 7:55
 Operator : SJ/JU
 Sample : I6402-02
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110717-TIDO-F-D-S

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	2.205	16	20	44	rVB	109844	237041	5.97%	0.937%
2	5.122	512	516	522	rBV	262964	288848	7.28%	1.141%
3	5.516	578	583	586	rBV	1472794	1281441	32.29%	5.063%
4	6.516	749	753	757	rBV	1062056	866661	21.84%	3.424%
5	6.669	774	779	782	rBV	2472127	2204881	55.55%	8.711%
6	6.904	815	819	822	rBV	975119	874291	22.03%	3.454%
7	7.063	841	846	849	rBV	2840968	2860896	72.08%	11.303%
8	7.463	909	914	917	rBV	2202982	2427041	61.15%	9.589%
9	8.181	1032	1036	1039	rBV	1235699	1153000	29.05%	4.555%
10	8.204	1039	1040	1043	rVB	303396	158043	3.98%	0.624%
11	8.892	1154	1157	1161	rVB	77208	59655	1.50%	0.236%
12	9.257	1214	1219	1223	rBV	3807131	3968845	100.00%	15.681%
13	9.645	1283	1285	1290	rVB	74382	55919	1.41%	0.221%
14	9.939	1328	1335	1338	rBV	1181037	1081694	27.25%	4.274%
15	9.969	1338	1340	1344	rVB	157987	117420	2.96%	0.464%
16	10.139	1364	1369	1374	rBV	72412	62207	1.57%	0.246%
17	10.486	1424	1428	1434	rVB	91059	86251	2.17%	0.341%
18	10.604	1445	1448	1452	rBV	67017	51386	1.29%	0.203%
19	10.645	1452	1455	1459	rVB2	54970	50177	1.26%	0.198%
20	10.722	1464	1468	1472	rBV	1329835	1324254	33.37%	5.232%
21	11.422	1584	1587	1590	rBV	957554	902442	22.74%	3.566%
22	11.445	1590	1591	1595	rVB	239010	156956	3.95%	0.620%
23	12.633	1790	1793	1797	rBV	74841	59452	1.50%	0.235%
24	12.822	1822	1825	1828	rBV	112881	84315	2.12%	0.333%
25	12.863	1828	1832	1836	rVB	42850	43726	1.10%	0.173%
26	13.010	1852	1857	1860	rBV	3055820	2918579	73.54%	11.531%
27	13.527	1941	1945	1948	rBV	73314	58248	1.47%	0.230%
28	14.063	2032	2036	2044	rVB	895380	803859	20.25%	3.176%
29	14.751	2149	2153	2164	rBV	385232	488685	12.31%	1.931%
30	15.545	2282	2288	2297	rBV	447566	584121	14.72%	2.308%

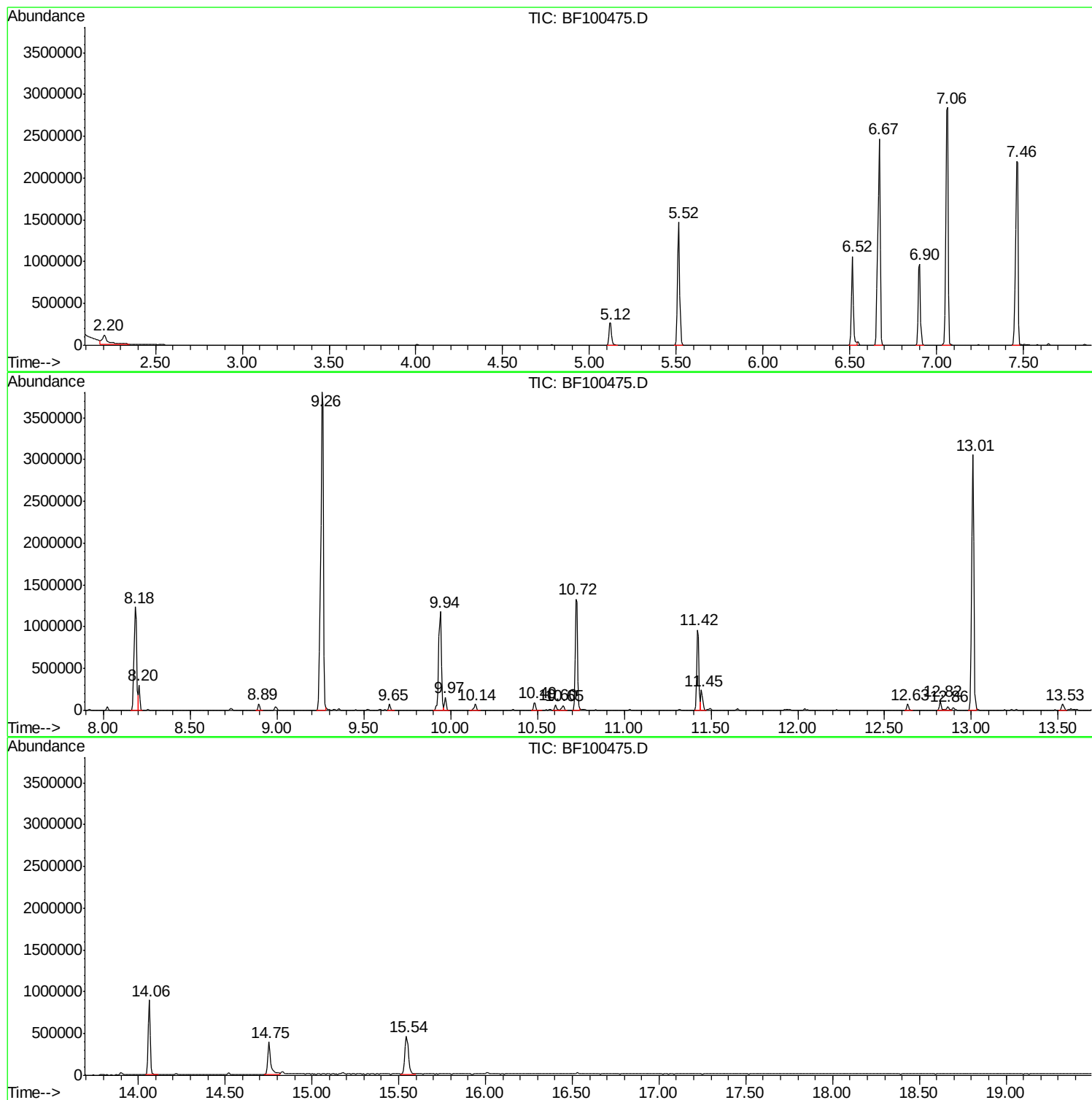
Sum of corrected areas: 25310334

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

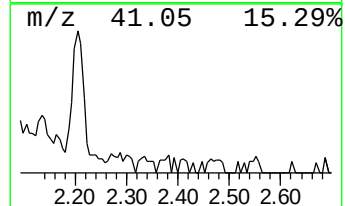
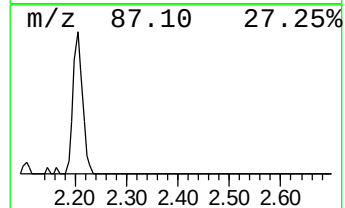
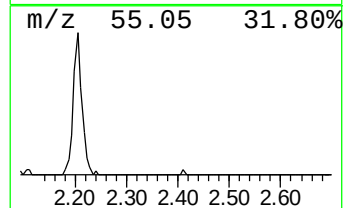
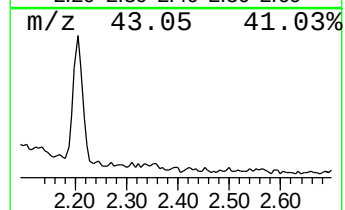
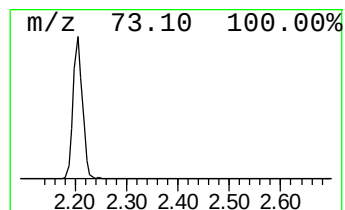
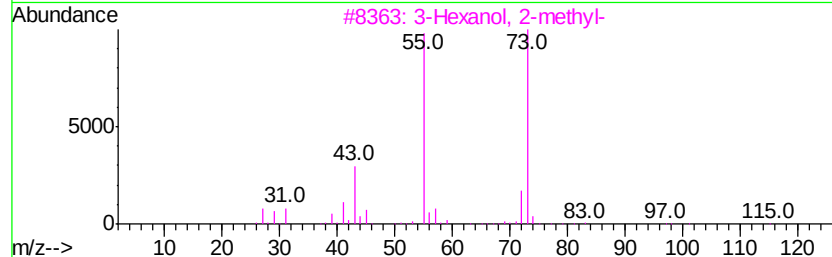
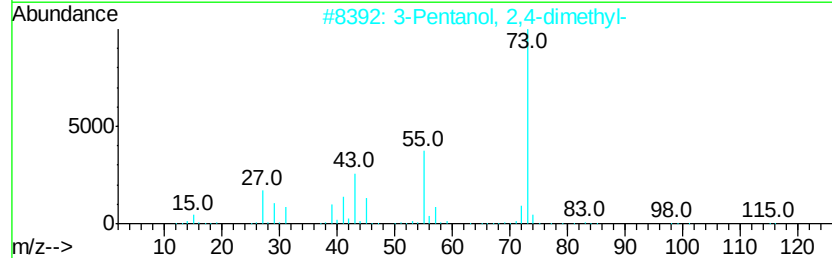
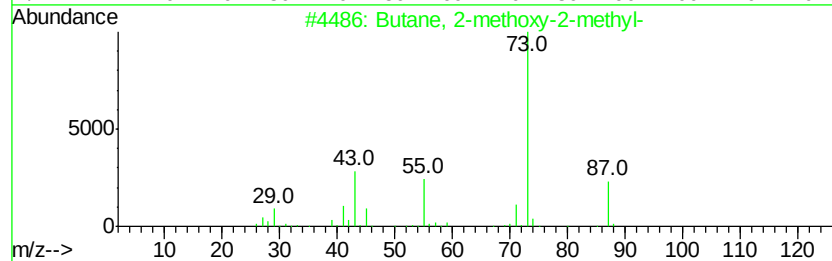
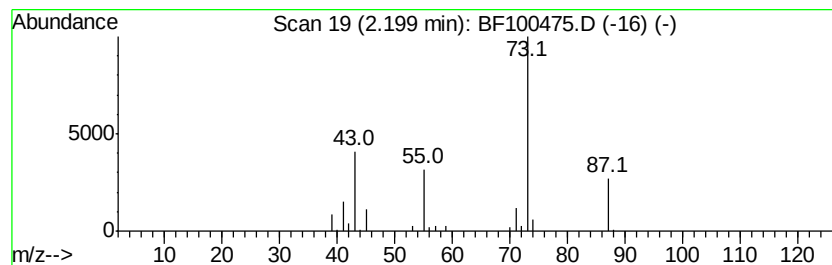
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	5.42 ng	237041	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

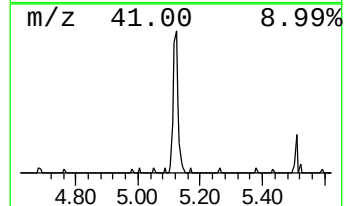
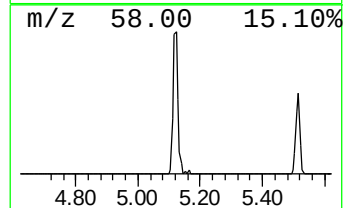
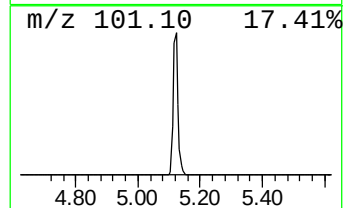
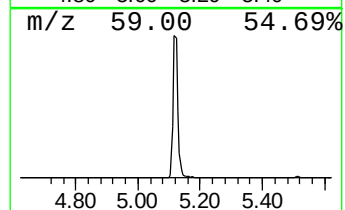
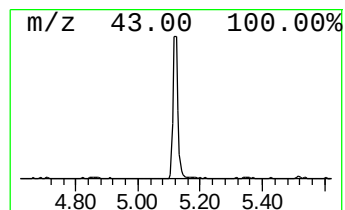
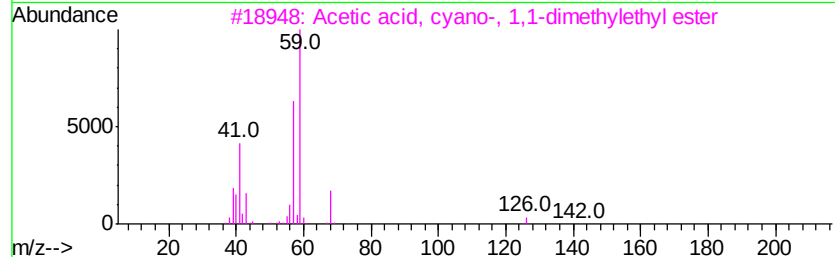
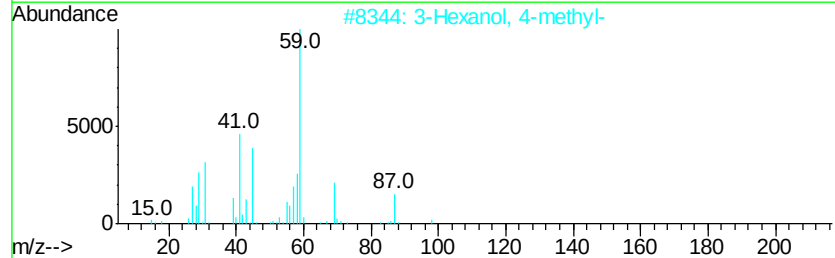
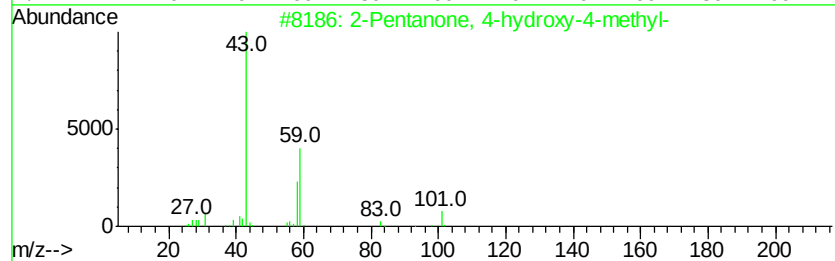
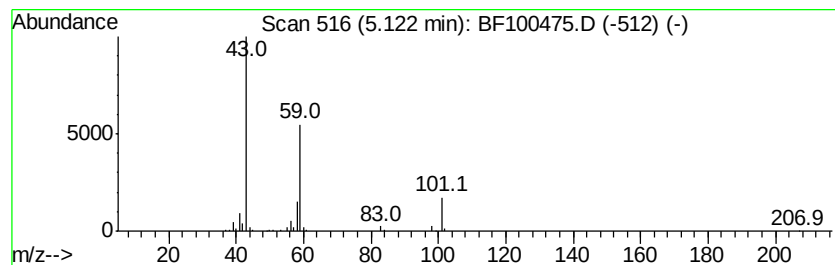
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.61 ng	288848	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

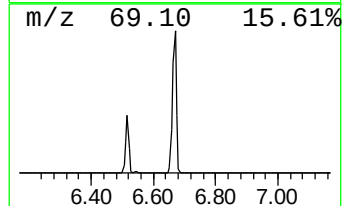
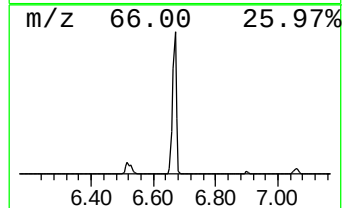
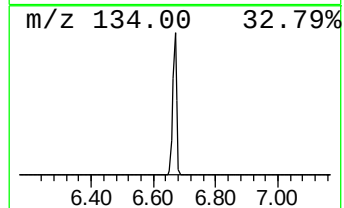
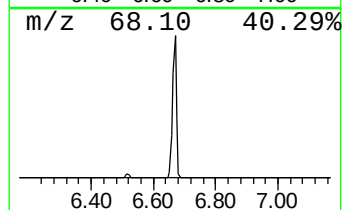
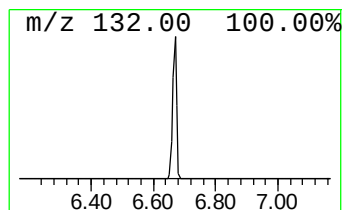
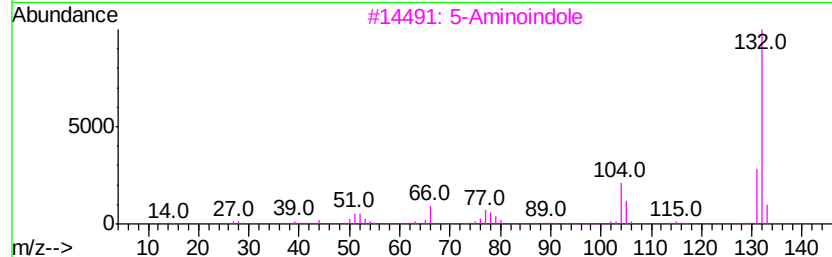
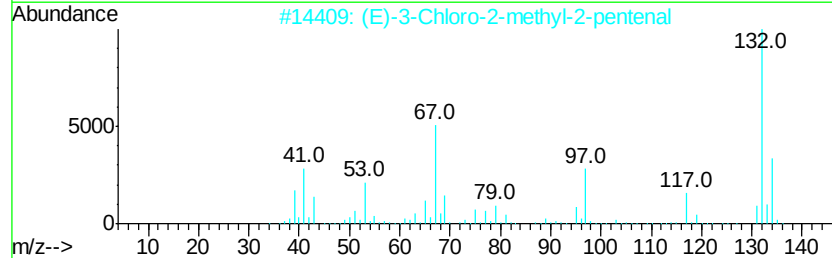
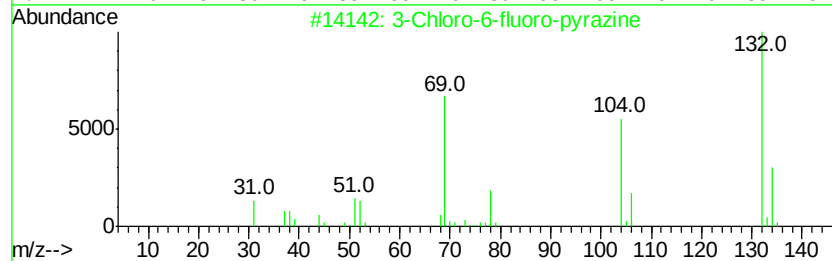
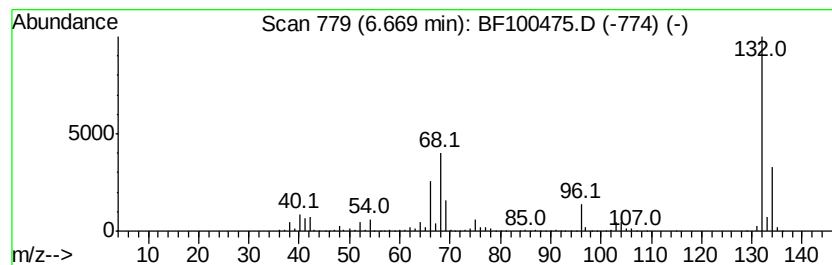
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	50.44 ng	2204880	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

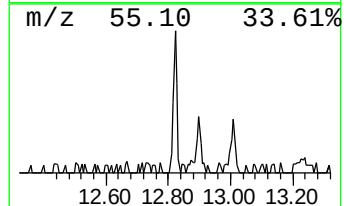
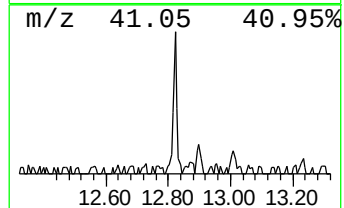
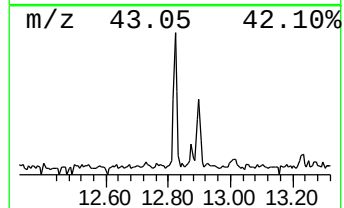
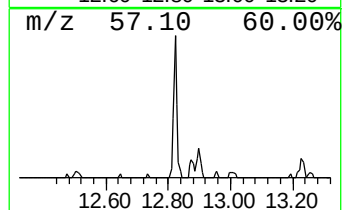
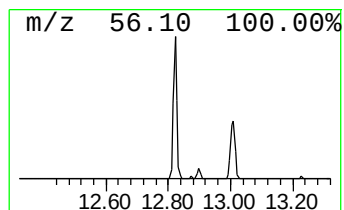
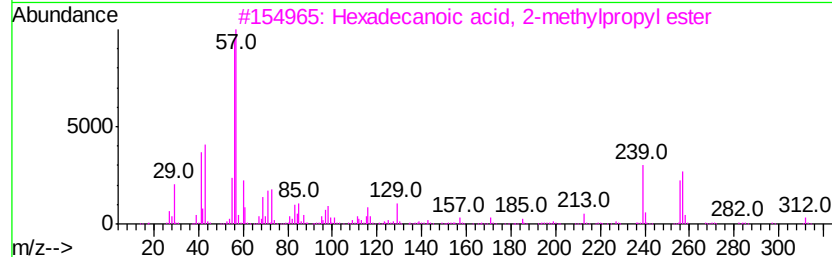
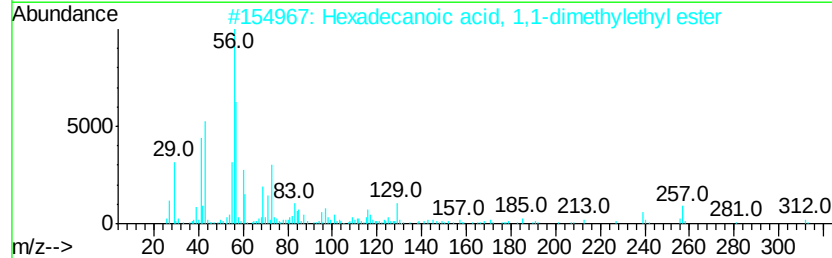
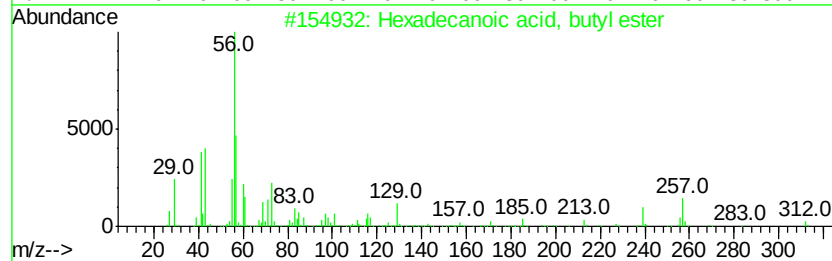
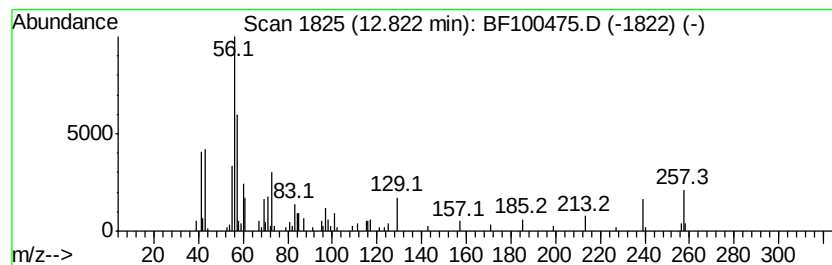
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.10 ng	84315	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	37
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

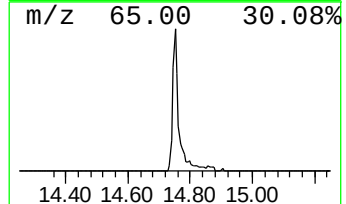
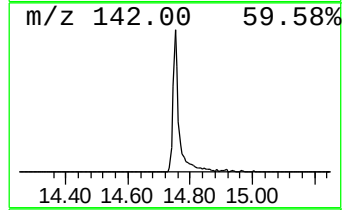
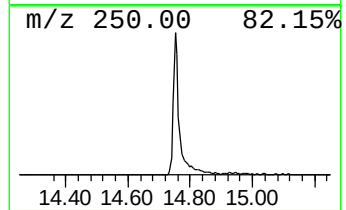
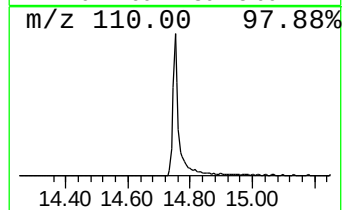
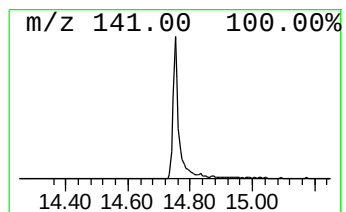
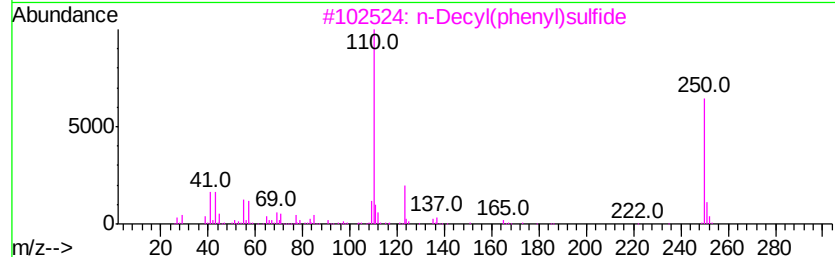
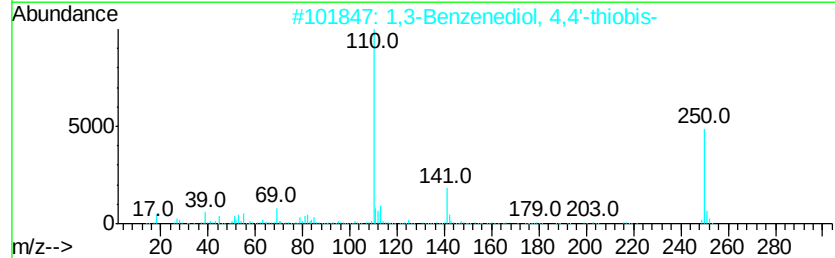
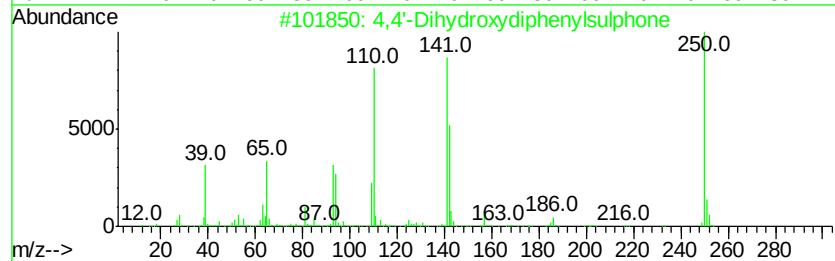
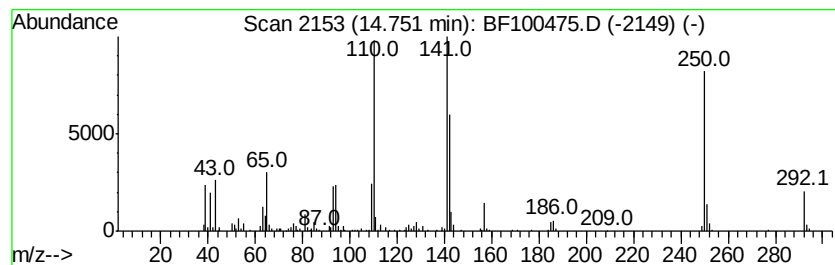
Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

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 6 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.75	12.16 ng	488685	Chrysene-d12	14.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	98	
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	58	
3	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	38	
4	1H-Pyrazole-5-carboxylic acid, 4...	141	C4H7N5O	1000327-48-2	35	
5	2,6-Difluorobenzaldehyde	142	C7H4F2O	000437-81-0	22	



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111117\
Data File : BF100475.D
Acq On : 12 Nov 2017 7:55
Operator : SJ/JU
Sample : I6402-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110717-TIDO-F-D-S

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
Butane, 2-methoxy...	2.20	5.4	ng	237041	1	6.90	874291	20.0
2-Pentanone, 4-hy...	5.12	6.6	ng	288848	1	6.90	874291	20.0
unknown6.67	6.67	50.4	ng	2204880	1	6.90	874291	20.0
Hexadecanoic acid...	12.82	2.1	ng	84315	5	14.06	803859	20.0
4,4'-Dihydroxydip...	14.75	12.2	ng	488685	5	14.06	803859	20.0