

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
 Data File : BF098908.D
 Acq On : 28 Sep 2017 15:03
 Operator : SJ/JU
 Sample : I5447-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-EPE-116-5B(10-12)

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-BF092317.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	40	rVB	98564	192927	5.84%	0.645%
2	5.140	515	519	537	rVB	512746	678186	20.53%	2.266%
3	5.534	581	586	590	rBV	2975822	3213187	97.27%	10.736%
4	6.493	741	749	752	rBV	26129	36211	1.10%	0.121%
5	6.540	752	757	760	rBV	2911057	3286424	99.48%	10.981%
6	6.687	777	782	785	rBV	3383645	3301217	99.93%	11.030%
7	6.916	817	821	824	rBV	1081161	891830	27.00%	2.980%
8	7.069	843	847	851	rBV	2538285	2429706	73.55%	8.118%
9	7.475	911	916	919	rBV	2045866	2114149	64.00%	7.064%
10	7.545	925	928	934	rVB	47936	41280	1.25%	0.138%
11	8.198	1035	1039	1042	rBV	1376585	1191194	36.06%	3.980%
12	9.269	1216	1221	1224	rBV	3646612	3303466	100.00%	11.038%
13	9.339	1230	1233	1236	rBV2	34950	35440	1.07%	0.118%
14	9.663	1284	1288	1291	rBV	680221	603030	18.25%	2.015%
15	9.869	1320	1323	1328	rVB	43855	46334	1.40%	0.155%
16	9.951	1333	1337	1341	rVB	1497732	1246259	37.73%	4.164%
17	10.375	1406	1409	1412	rVB	67500	59491	1.80%	0.199%
18	10.739	1467	1471	1474	rBV	1951032	1750732	53.00%	5.850%
19	10.845	1486	1489	1494	rBV	76284	79538	2.41%	0.266%
20	11.292	1562	1565	1567	rBV	46802	35033	1.06%	0.117%
21	11.439	1586	1590	1593	rBV	1267167	1053694	31.90%	3.521%
22	11.951	1672	1677	1683	rBV2	181658	189914	5.75%	0.635%
23	12.651	1792	1796	1799	rBV	81895	72502	2.19%	0.242%
24	12.739	1807	1811	1819	rBV	81304	101549	3.07%	0.339%
25	12.880	1830	1835	1837	rBV	73719	72024	2.18%	0.241%
26	13.022	1855	1859	1862	rBV	2467731	2186965	66.20%	7.307%
27	13.904	2006	2009	2013	rBV2	122496	122921	3.72%	0.411%
28	14.045	2030	2033	2035	rBV	57623	52852	1.60%	0.177%
29	14.074	2035	2038	2042	rVV	817531	771829	23.36%	2.579%
30	15.568	2287	2292	2301	rVB	555995	768933	23.28%	2.569%

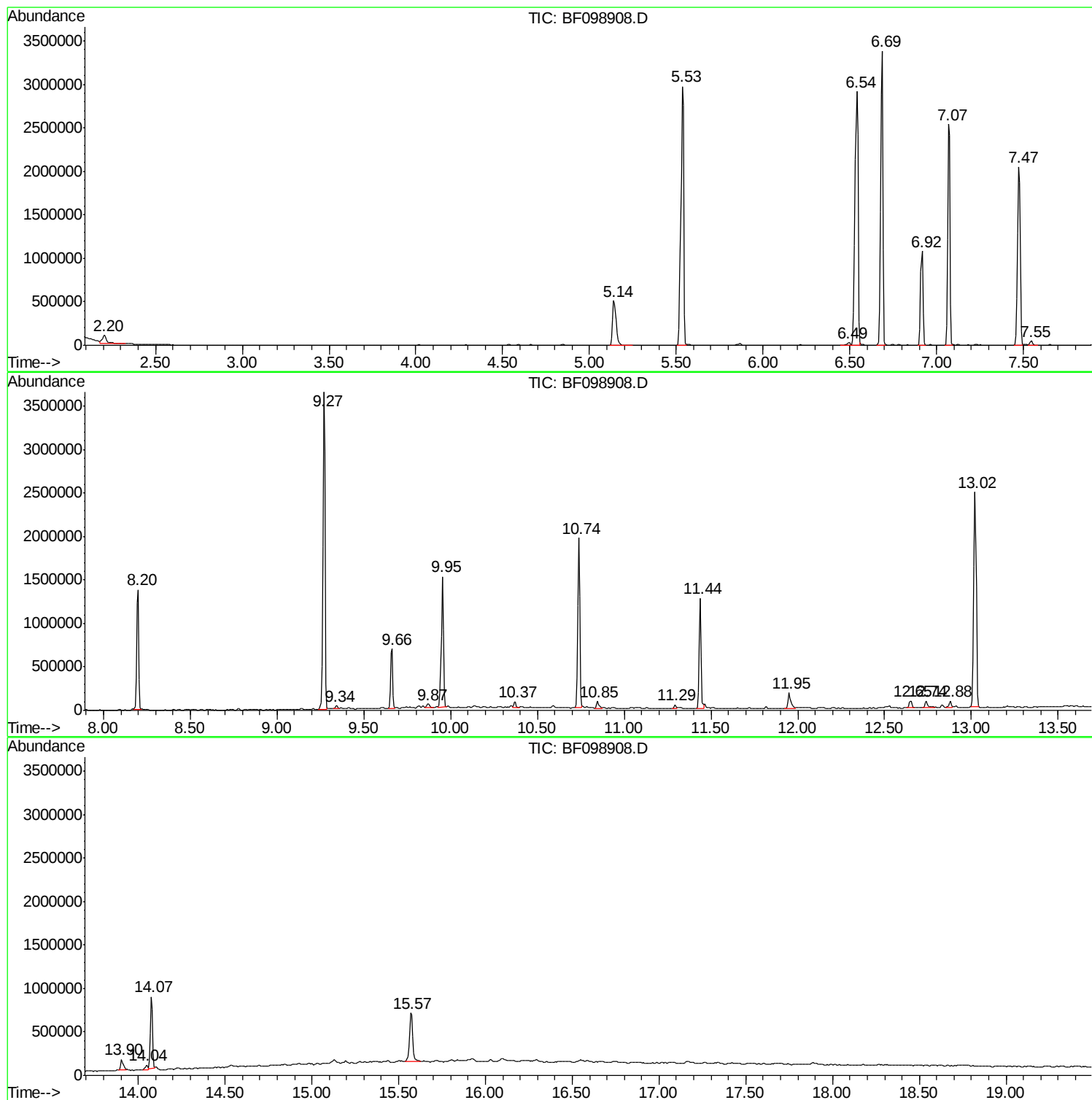
Sum of corrected areas: 29928817

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

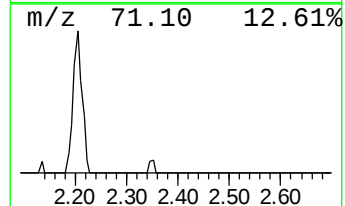
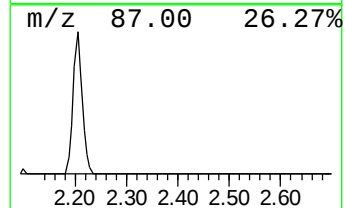
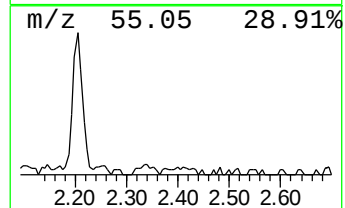
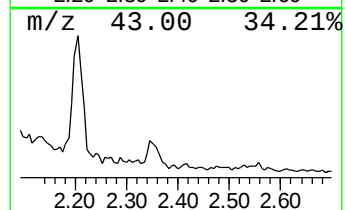
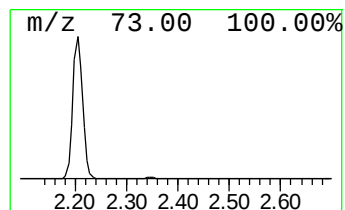
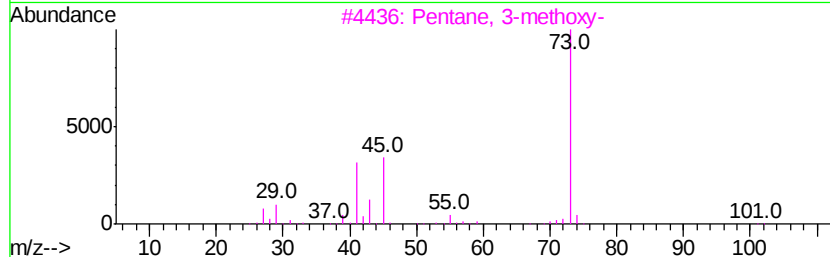
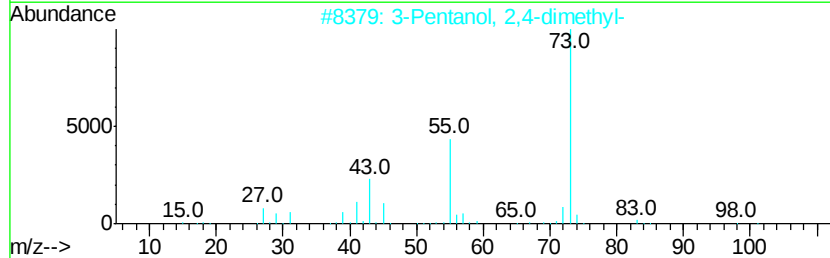
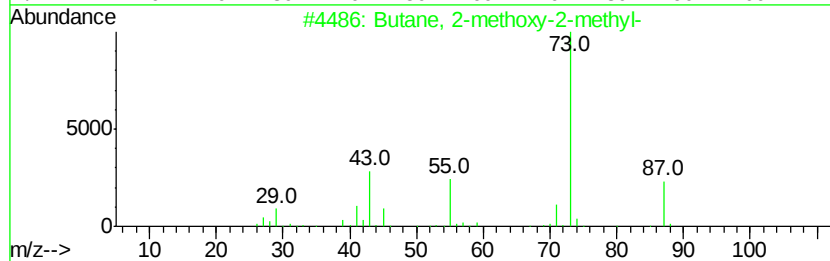
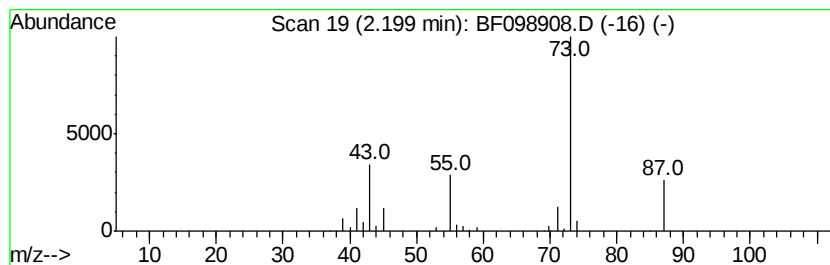
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	4.33 ng	192927	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

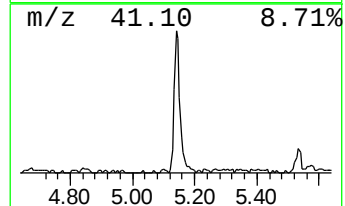
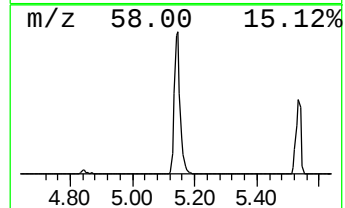
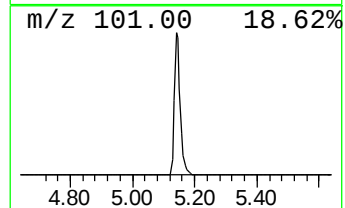
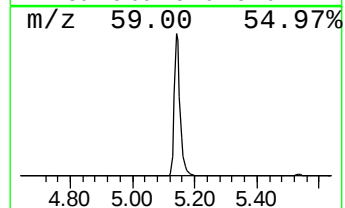
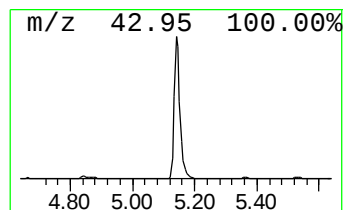
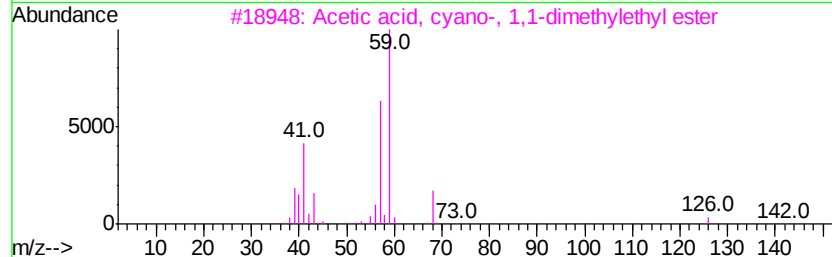
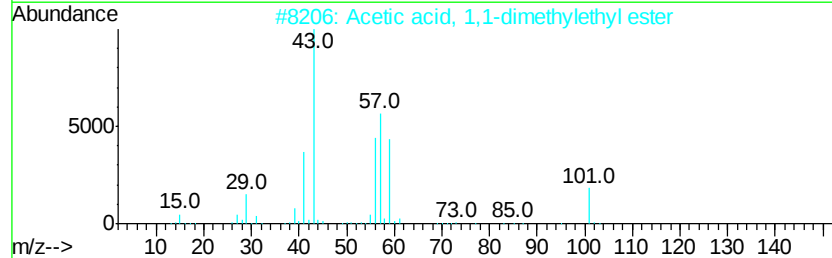
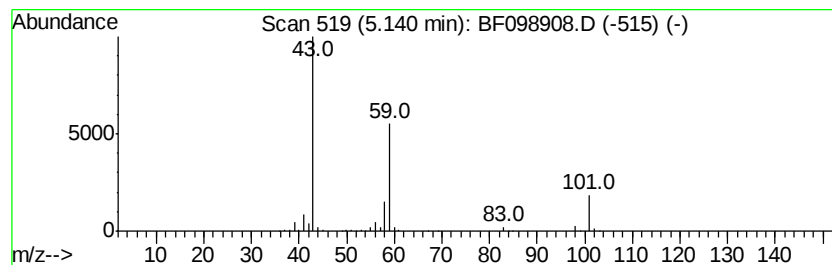
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	15.21 ng	678186	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

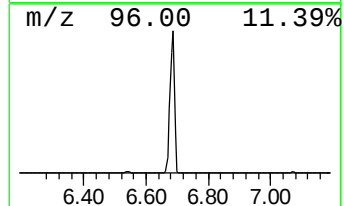
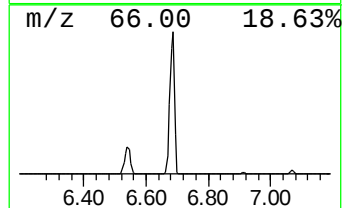
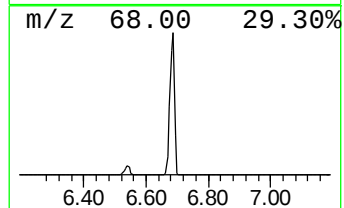
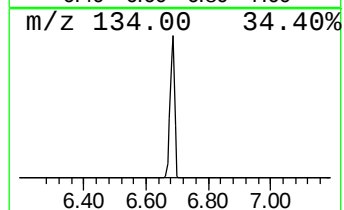
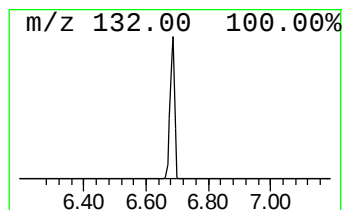
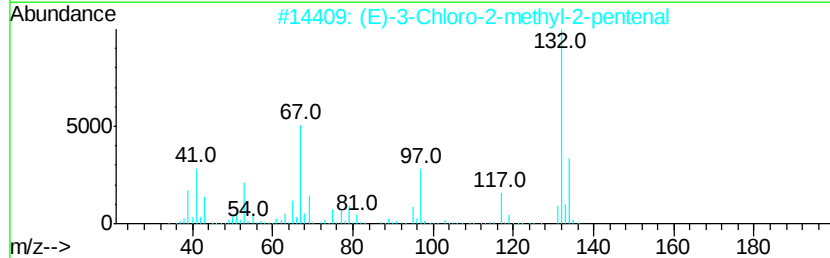
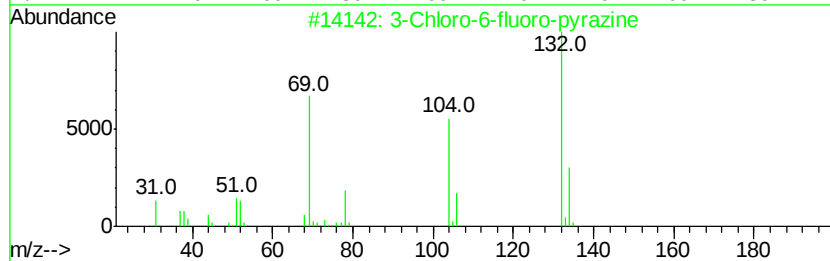
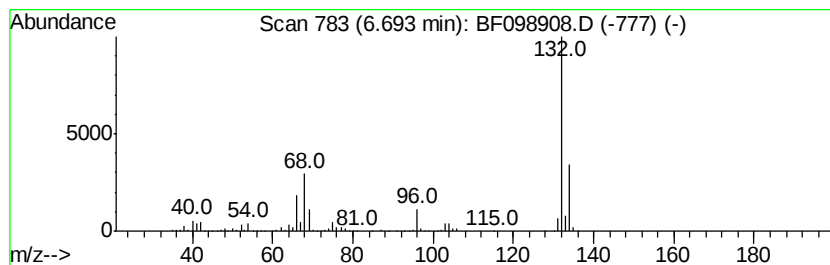
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	74.03 ng	3301220	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

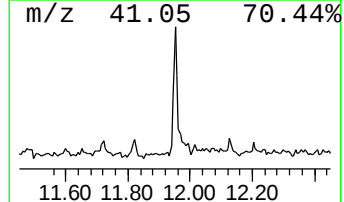
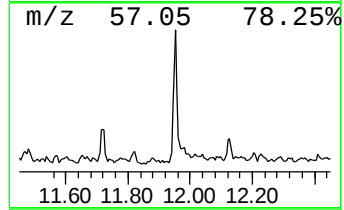
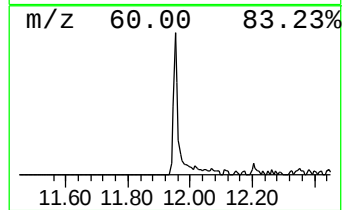
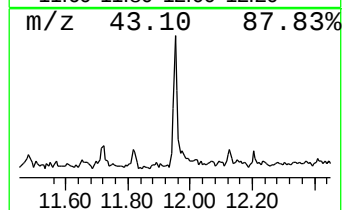
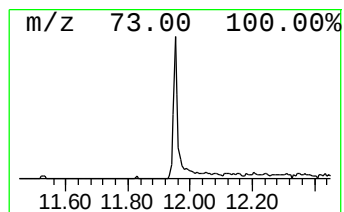
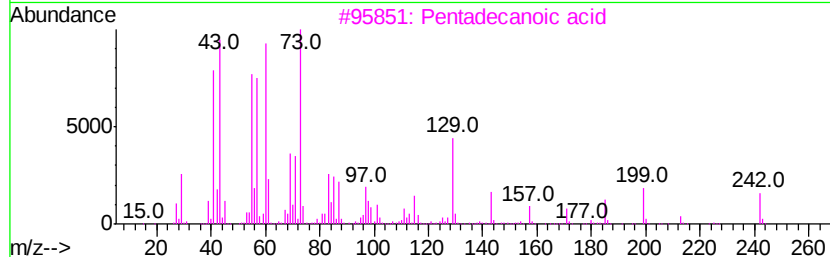
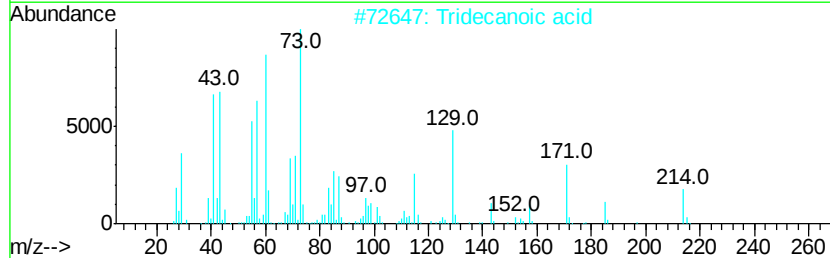
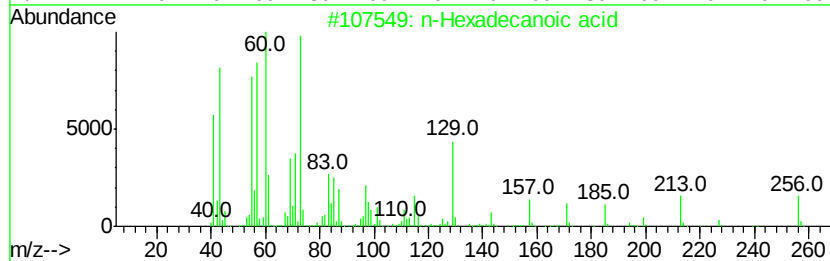
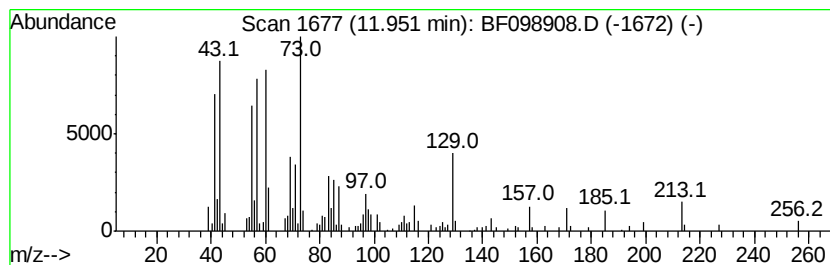
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.60 ng	189914	Phenanthrene-d10	11.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

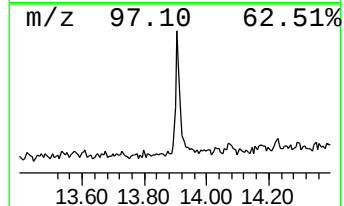
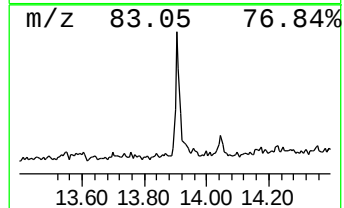
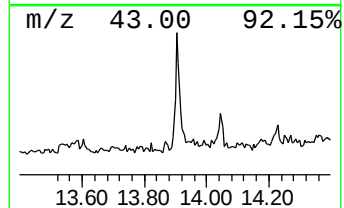
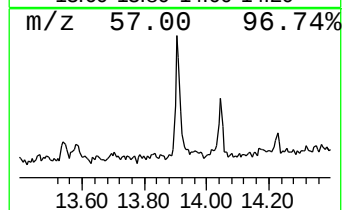
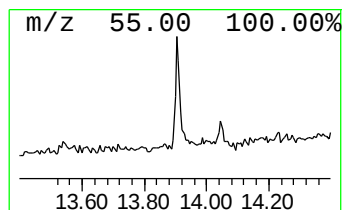
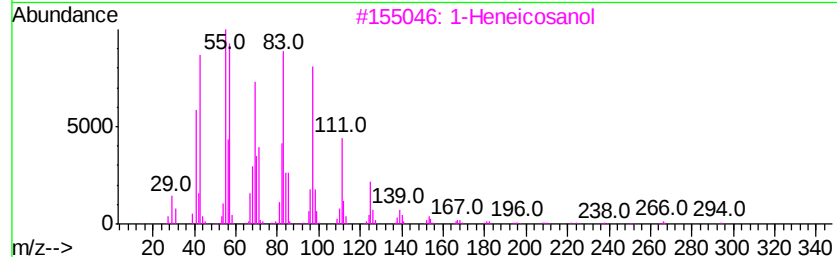
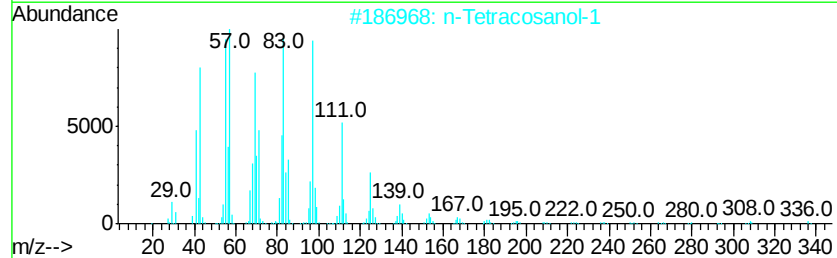
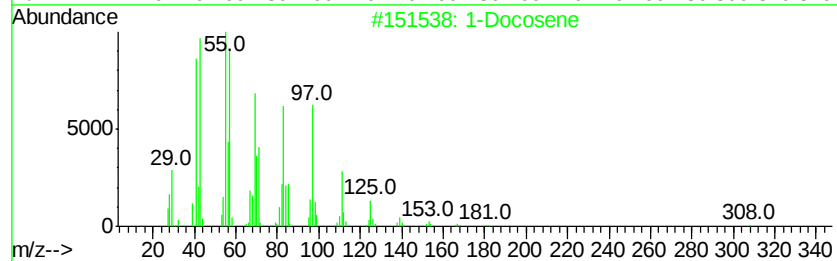
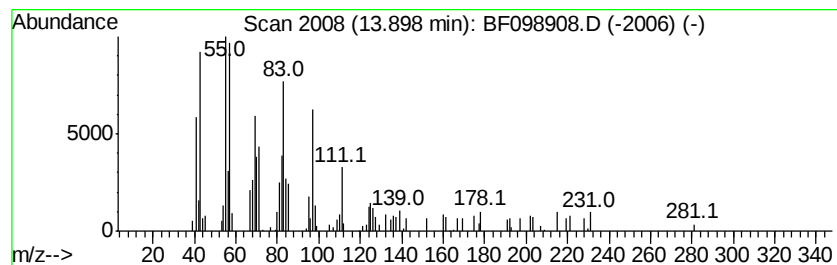
Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	3.19 ng	122921	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	87
4	Octacosanol	410	C28H58O	000557-61-9	87
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092817\
Data File : BF098908.D
Acq On : 28 Sep 2017 15:03
Operator : SJ/JU
Sample : I5447-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-116-5B(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	4.3	ng	192927	1	6.92	891830	20.0
2-Pentanone, 4-hy...	5.14	15.2	ng	678186	1	6.92	891830	20.0
unknown6.69	6.69	74.0	ng	3301220	1	6.92	891830	20.0
n-Hexadecanoic acid	11.95	3.6	ng	189914	4	11.44	1053690	20.0
1-Docosene	13.90	3.2	ng	122921	5	14.07	771829	20.0