

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
 Data File : BF096266.D
 Acq On : 28 Jun 2017 22:59
 Operator : SJ/MA
 Sample : I3898-04
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-72-12002-VNJ-201-COMP

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-BF062717.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	2.140	6	9	18	rVB4	32387	64548	1.95%	0.220%
2	4.981	488	492	500	rVB	638646	721178	21.74%	2.457%
3	5.398	558	563	566	rBV	3481263	3317824	100.00%	11.303%
4	6.375	723	729	731	rBV	35141	41040	1.24%	0.140%
5	6.416	731	736	741	rVB	3175544	3291679	99.21%	11.214%
6	6.551	755	759	763	rBV	3413528	3128571	94.30%	10.658%
7	6.786	795	799	802	rVB	919846	810081	24.42%	2.760%
8	6.939	821	825	829	rVB	2640407	2331738	70.28%	7.944%
9	7.339	888	893	896	rBV	2197950	1888694	56.93%	6.434%
10	7.433	904	909	912	rBV	56796	52658	1.59%	0.179%
11	7.763	957	965	968	rBV	68733	77350	2.33%	0.264%
12	8.063	1012	1016	1020	rBV	1265312	1064103	32.07%	3.625%
13	9.139	1195	1199	1203	rBV	3265045	2942360	88.68%	10.024%
14	9.263	1217	1220	1224	rVB	202232	168167	5.07%	0.573%
15	9.533	1262	1266	1269	rBV	1177957	964289	29.06%	3.285%
16	9.816	1310	1314	1318	rBV2	1163692	1012885	30.53%	3.451%
17	10.257	1387	1389	1392	rVB	62201	54051	1.63%	0.184%
18	10.598	1443	1447	1451	rBV	1841432	1687054	50.85%	5.747%
19	10.733	1467	1470	1478	rBV	78271	98318	2.96%	0.335%
20	11.180	1542	1546	1548	rBV	55626	49381	1.49%	0.168%
21	11.298	1562	1566	1569	rVB	1046192	914825	27.57%	3.117%
22	11.527	1602	1605	1609	rBV	255612	200500	6.04%	0.683%
23	11.827	1653	1656	1660	rBV	144922	133446	4.02%	0.455%
24	12.345	1741	1744	1748	rBV	69776	64162	1.93%	0.219%
25	12.615	1787	1790	1795	rBV5	30539	44170	1.33%	0.150%
26	12.880	1831	1835	1839	rBV	2646128	2515481	75.82%	8.570%
27	13.780	1985	1988	1995	rBV	223796	213141	6.42%	0.726%
28	13.927	2009	2013	2017	rBV	994139	901313	27.17%	3.071%
29	15.356	2252	2256	2261	rVB	520069	600089	18.09%	2.044%

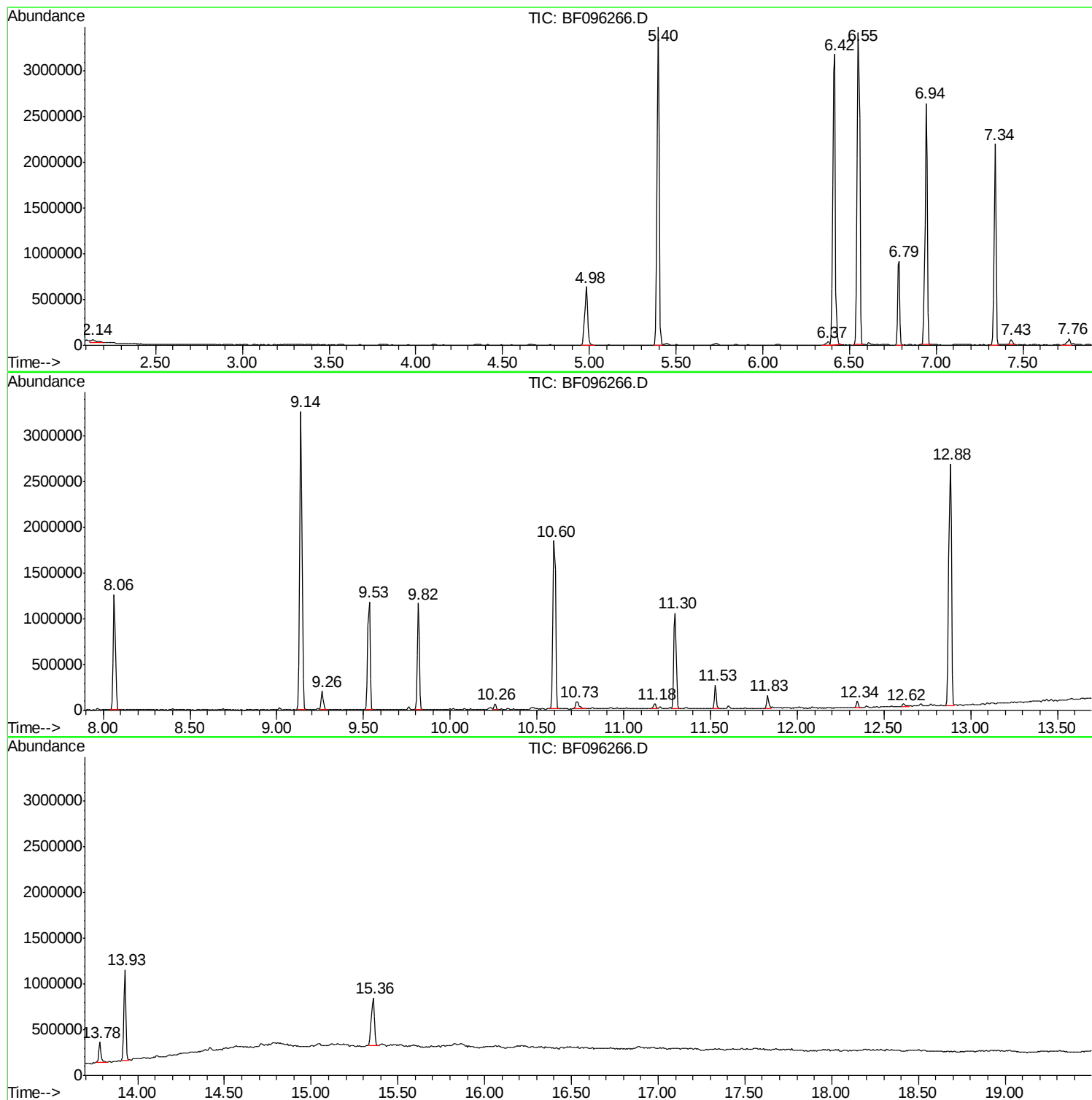
Sum of corrected areas: 29353096

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

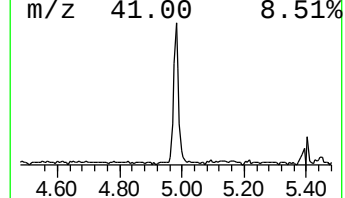
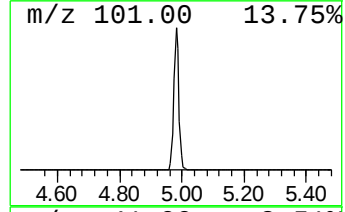
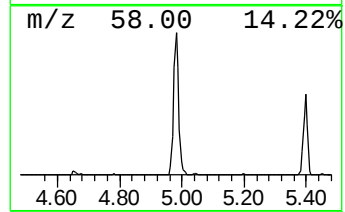
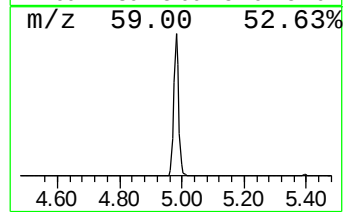
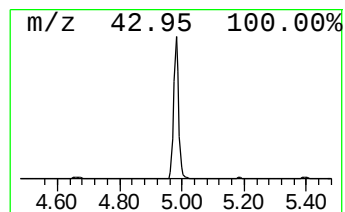
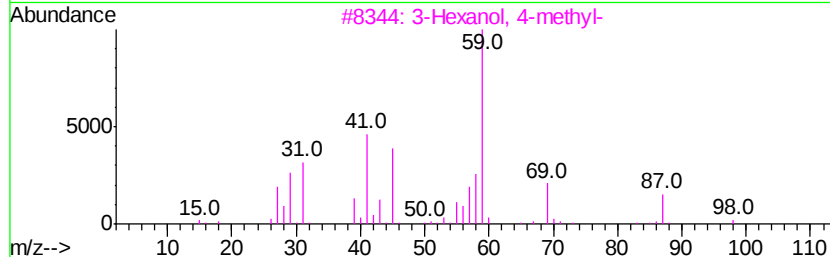
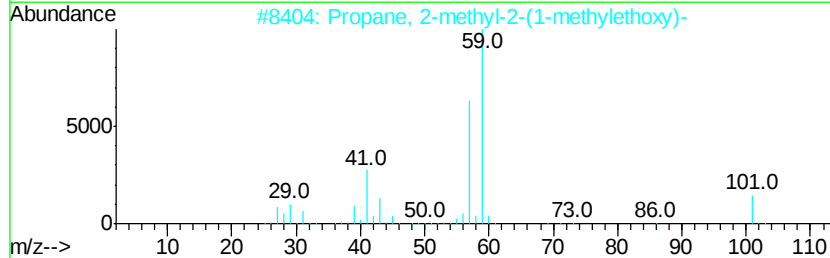
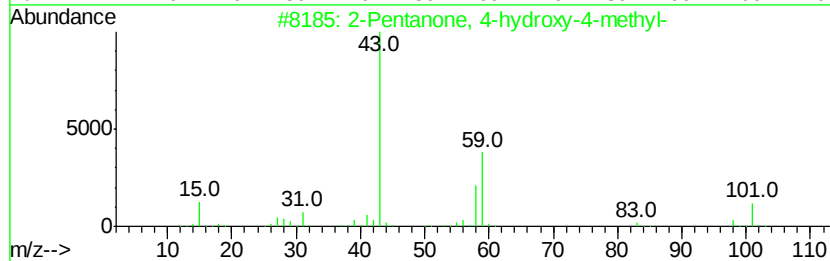
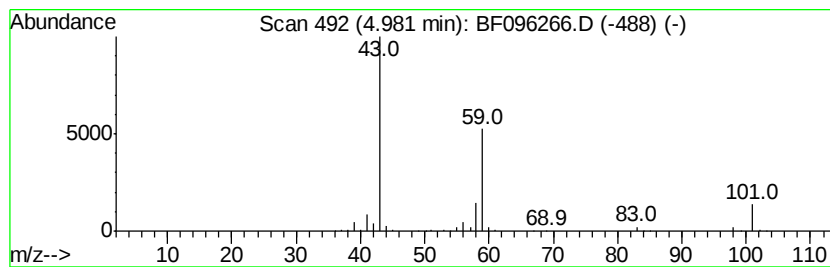
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.98	17.81 ng	721178	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

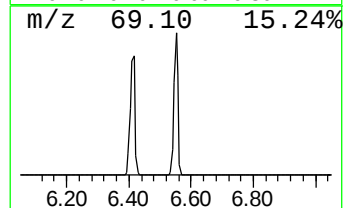
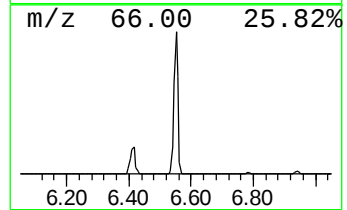
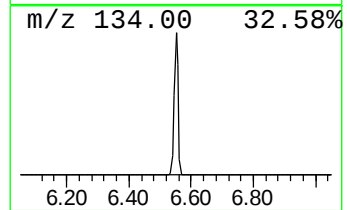
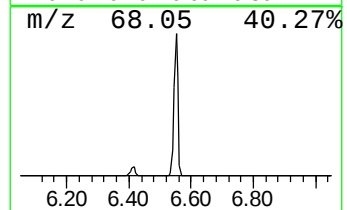
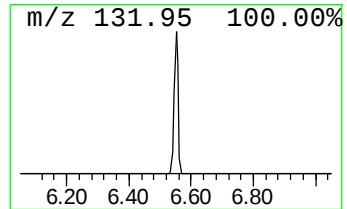
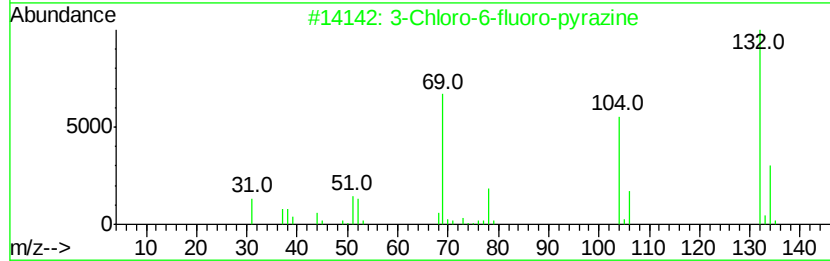
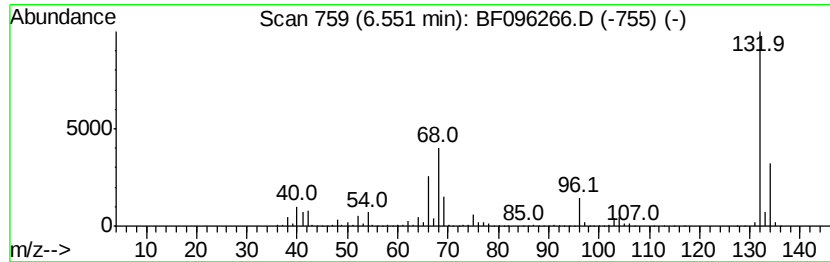
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	77.24 ng	3128570	1,4-Dichlorobenzene-d4	6.79

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

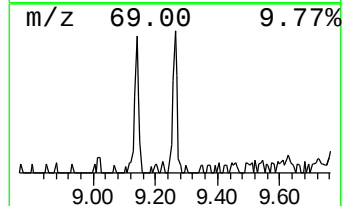
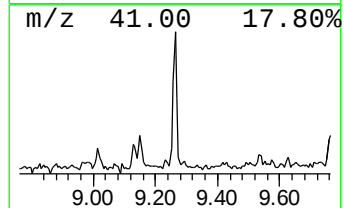
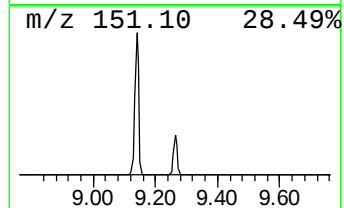
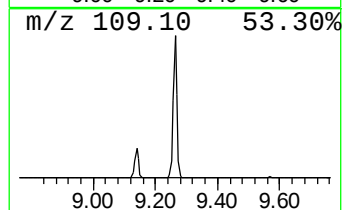
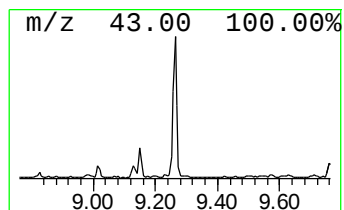
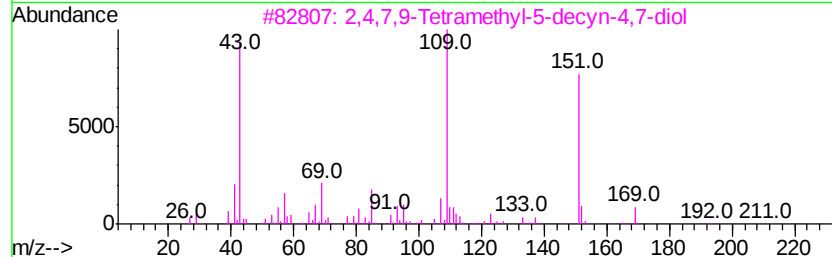
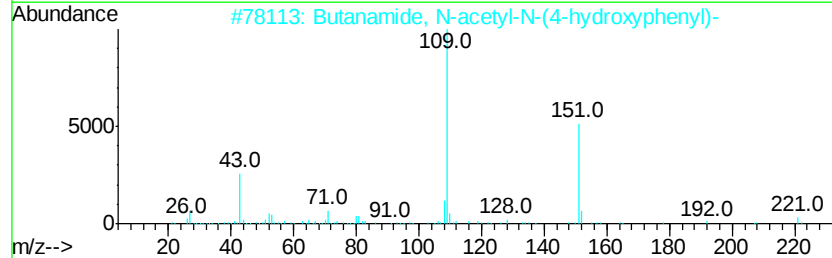
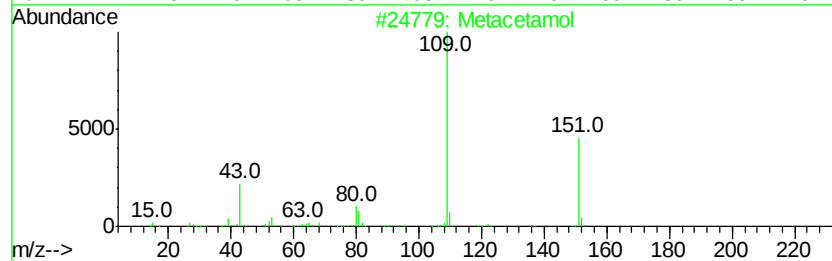
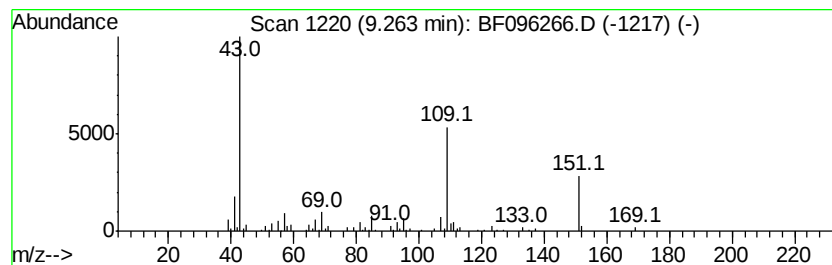
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown9.26 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	3.32 ng	168167	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Metacetamol	151	C8H9NO2	000621-42-1	43
2		Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	37
3		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	35
4		3,6-Dimethyl-6-hepten-4-yn-3-ol	138	C9H14O	003601-67-0	28
5		3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

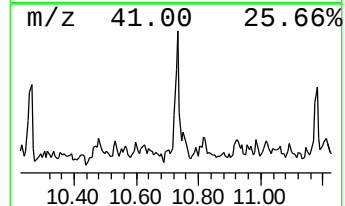
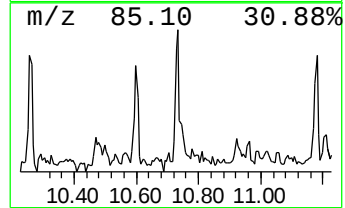
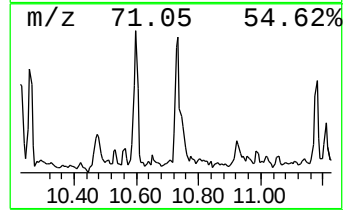
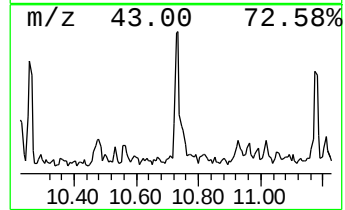
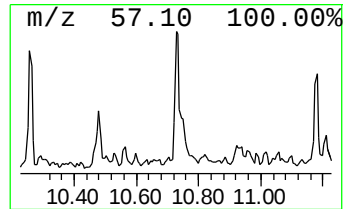
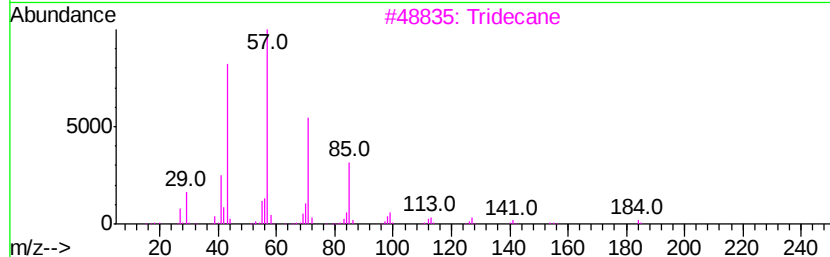
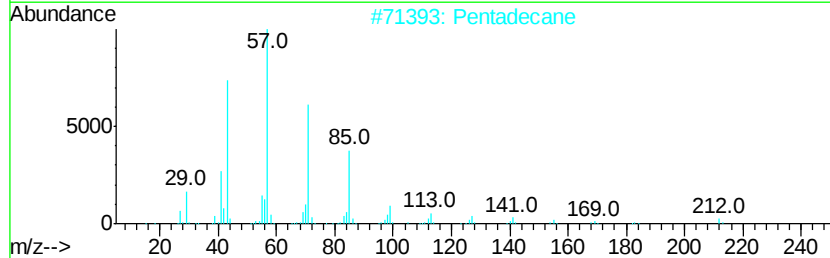
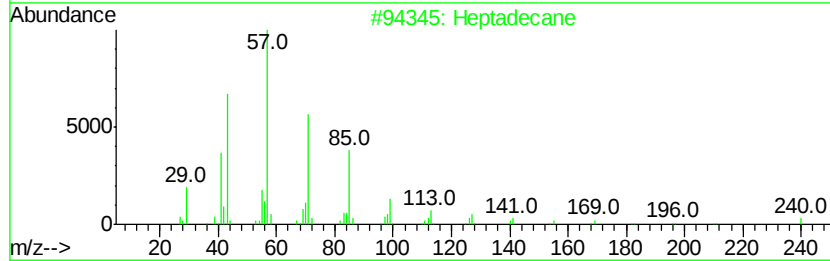
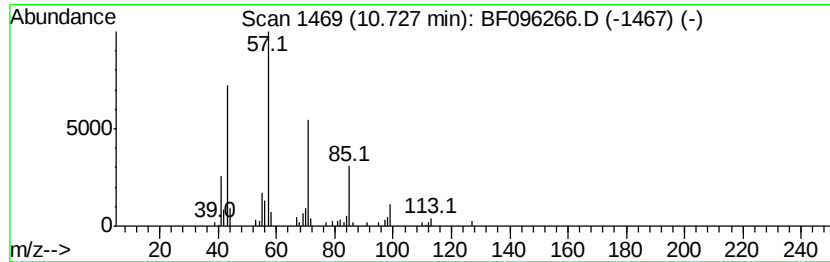
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.15 ng	98318	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Pentadecane		212	C15H32	000629-62-9	86
3	Tridecane		184	C13H28	000629-50-5	86
4	Tetradecane		198	C14H30	000629-59-4	86
5	Hexadecane		226	C16H34	000544-76-3	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

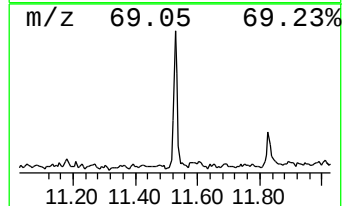
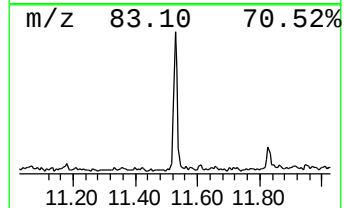
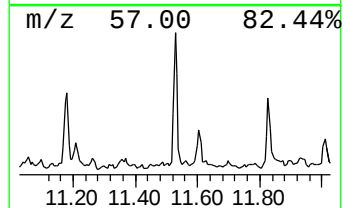
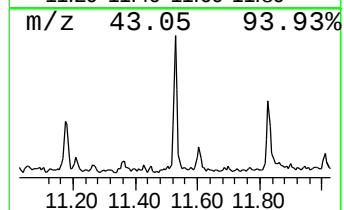
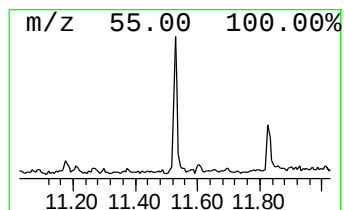
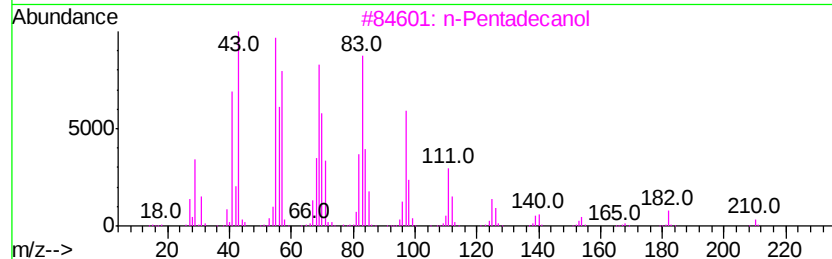
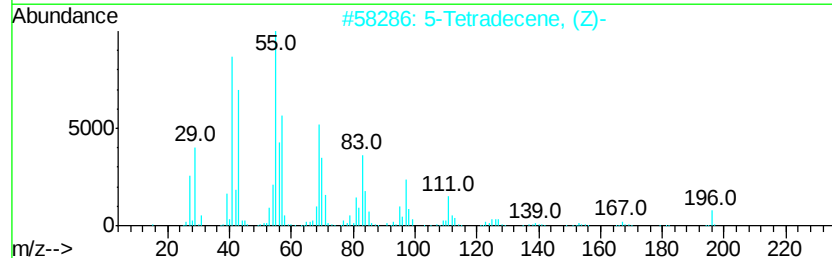
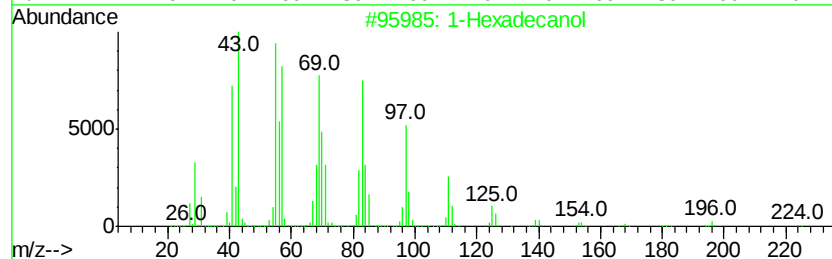
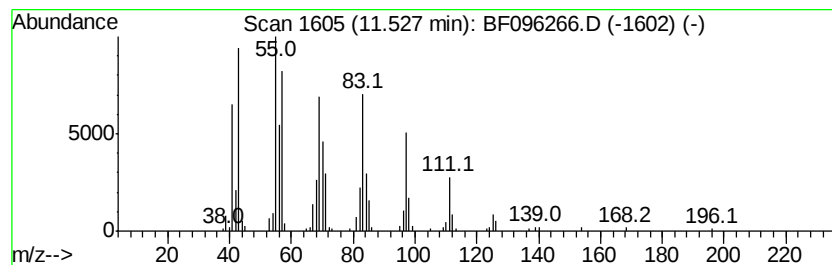
Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.53	4.38 ng	200500	Phenanthrene-d10	11.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	5-Tetradecene, (Z)-	196	C14H28	041446-62-2	94
3	n-Pentadecanol	228	C15H32O	000629-76-5	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

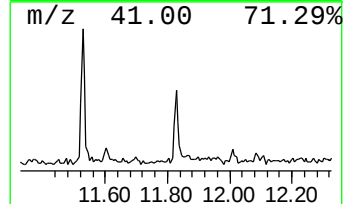
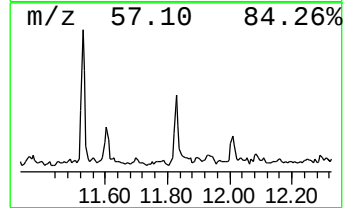
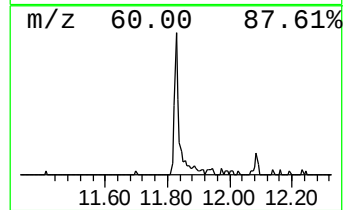
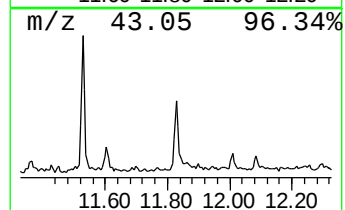
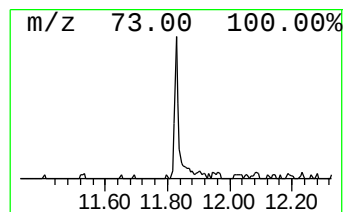
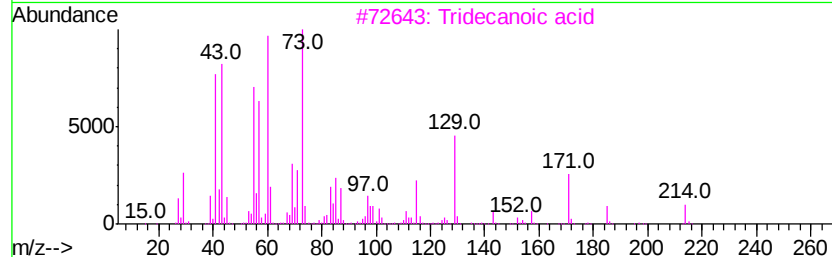
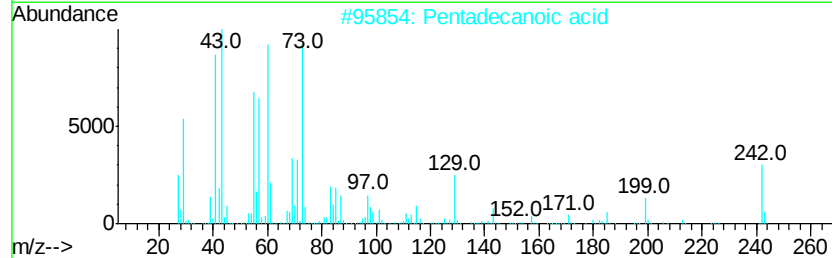
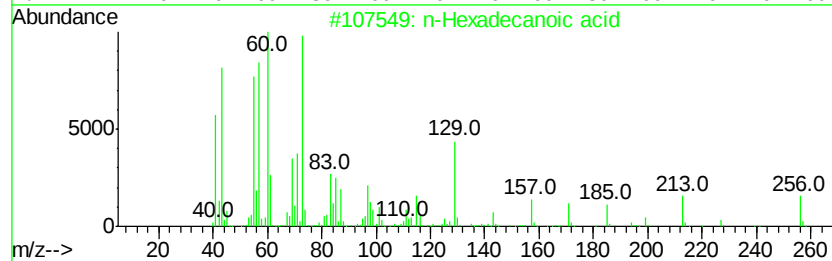
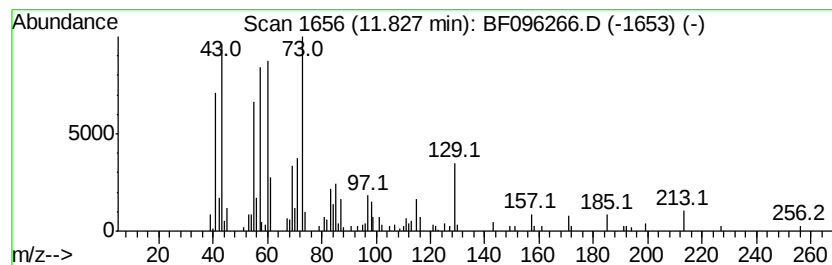
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.92 ng	133446	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Nonanoic acid	158	C9H18O2	000112-05-0	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

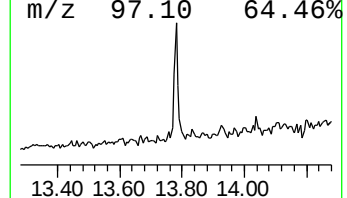
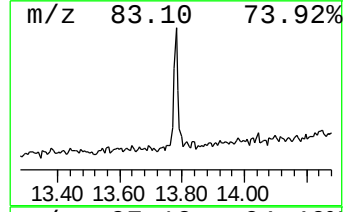
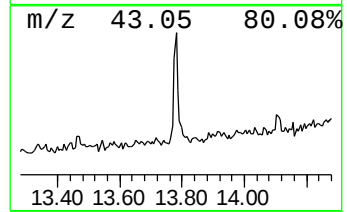
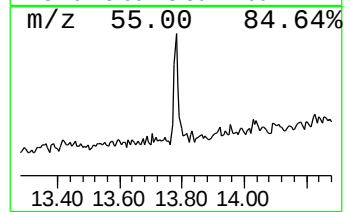
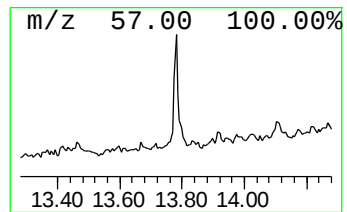
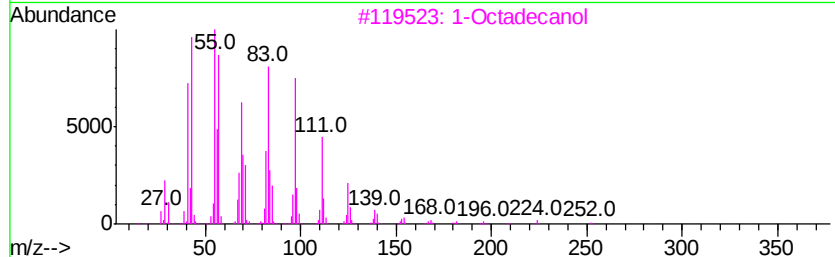
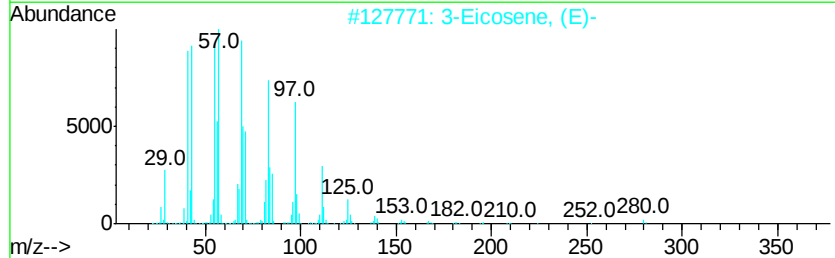
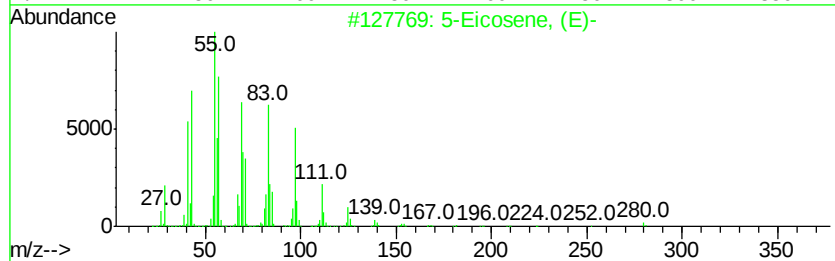
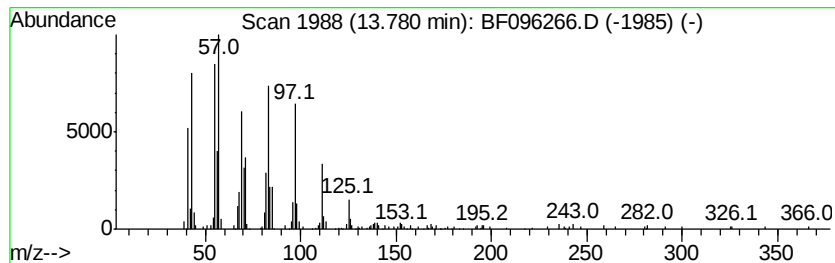
Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.78	4.73 ng	213141	Chrysene-d12	13.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	3-Eicosene, (E)-		280	C20H40	074685-33-9	96
3	1-Octadecanol		270	C18H38O	000112-92-5	91
4	1-Heneicosanol		312	C21H44O	015594-90-8	91
5	Pentafluoropropionic acid, hepta...		402	C20H35F5O2	959218-78-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062817\
Data File : BF096266.D
Acq On : 28 Jun 2017 22:59
Operator : SJ/MA
Sample : I3898-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-72-12002-VNJ-201-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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...	4.98	17.8	ng	721178	1	6.79	810081	20.0
unknown6.55	6.55	77.2	ng	3128570	1	6.79	810081	20.0
unknown9.26	9.26	3.3	ng	168167	3	9.82	1012890	20.0
Heptadecane	10.73	2.1	ng	98318	4	11.30	914825	20.0
1-Hexadecanol	11.53	4.4	ng	200500	4	11.30	914825	20.0
n-Hexadecanoic acid	11.83	2.9	ng	133446	4	11.30	914825	20.0
5-Eicosene, (E)-	13.78	4.7	ng	213141	5	13.93	901313	20.0