

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
 Data File : BF098725.D
 Acq On : 23 Sep 2017 4:49
 Operator : SJ/JU
 Sample : I5304-02
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-ENV-117-2(5-10)

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-BF092117.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	2.251	25	28	39	rVB	90771	150972	3.99%	0.441%
2	2.381	48	50	63	rVB2	20029	42425	1.12%	0.124%
3	3.534	243	246	259	rBV	26756	72643	1.92%	0.212%
4	4.057	328	335	339	rBV	44519	53836	1.42%	0.157%
5	5.163	519	523	531	rBV	567727	697671	18.45%	2.037%
6	5.551	583	589	592	rBV	3622376	3735457	98.80%	10.907%
7	6.551	753	759	762	rBV	3325305	3780959	100.00%	11.040%
8	6.698	779	784	787	rBV	3863776	3777597	99.91%	11.030%
9	6.928	817	823	827	rBV	1232485	1049333	27.75%	3.064%
10	7.051	841	844	846	rBV	55017	47432	1.25%	0.138%
11	7.086	846	850	853	rVB	3341834	2900400	76.71%	8.469%
12	7.492	913	919	922	rBV	2358751	2302079	60.89%	6.722%
13	7.557	924	930	934	rVB2	53028	56631	1.50%	0.165%
14	8.104	1019	1023	1028	rBV	105153	90792	2.40%	0.265%
15	8.210	1037	1041	1044	rVB	1599154	1289915	34.12%	3.766%
16	9.286	1218	1224	1227	rBV	4177635	3766012	99.60%	10.996%
17	9.392	1238	1242	1244	rBV2	47193	42325	1.12%	0.124%
18	9.675	1286	1290	1293	rBV	1273934	975736	25.81%	2.849%
19	9.963	1335	1339	1343	rBV	1333124	1253868	33.16%	3.661%
20	10.751	1468	1473	1476	rBV	2067339	1849431	48.91%	5.400%
21	10.857	1488	1491	1498	rBV2	35075	45673	1.21%	0.133%
22	11.451	1588	1592	1595	rBV	1235078	988916	26.16%	2.887%
23	11.663	1623	1628	1635	rBV2	196194	163203	4.32%	0.477%
24	11.963	1675	1679	1684	rBV	150000	146388	3.87%	0.427%
25	12.480	1764	1767	1773	rBV	195439	171704	4.54%	0.501%
26	12.751	1808	1813	1818	rBV	60197	71272	1.89%	0.208%
27	13.033	1857	1861	1865	rBV	2732501	2471673	65.37%	7.217%
28	13.915	2008	2011	2015	rBV2	86451	86869	2.30%	0.254%
29	14.086	2037	2040	2044	rBV	1021441	935686	24.75%	2.732%
30	14.815	2160	2164	2170	rBV	56483	96474	2.55%	0.282%
31	14.939	2182	2185	2190	rBV	39172	40597	1.07%	0.119%
32	15.580	2289	2294	2305	rVB	595415	854604	22.60%	2.495%
33	16.056	2370	2375	2379	rBV2	48321	73204	1.94%	0.214%
34	16.580	2459	2464	2470	rVB	47800	84175	2.23%	0.246%

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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 >
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35	17.192	2563	2568	2578	rVB3	36556	82270	2.18%	0.240%
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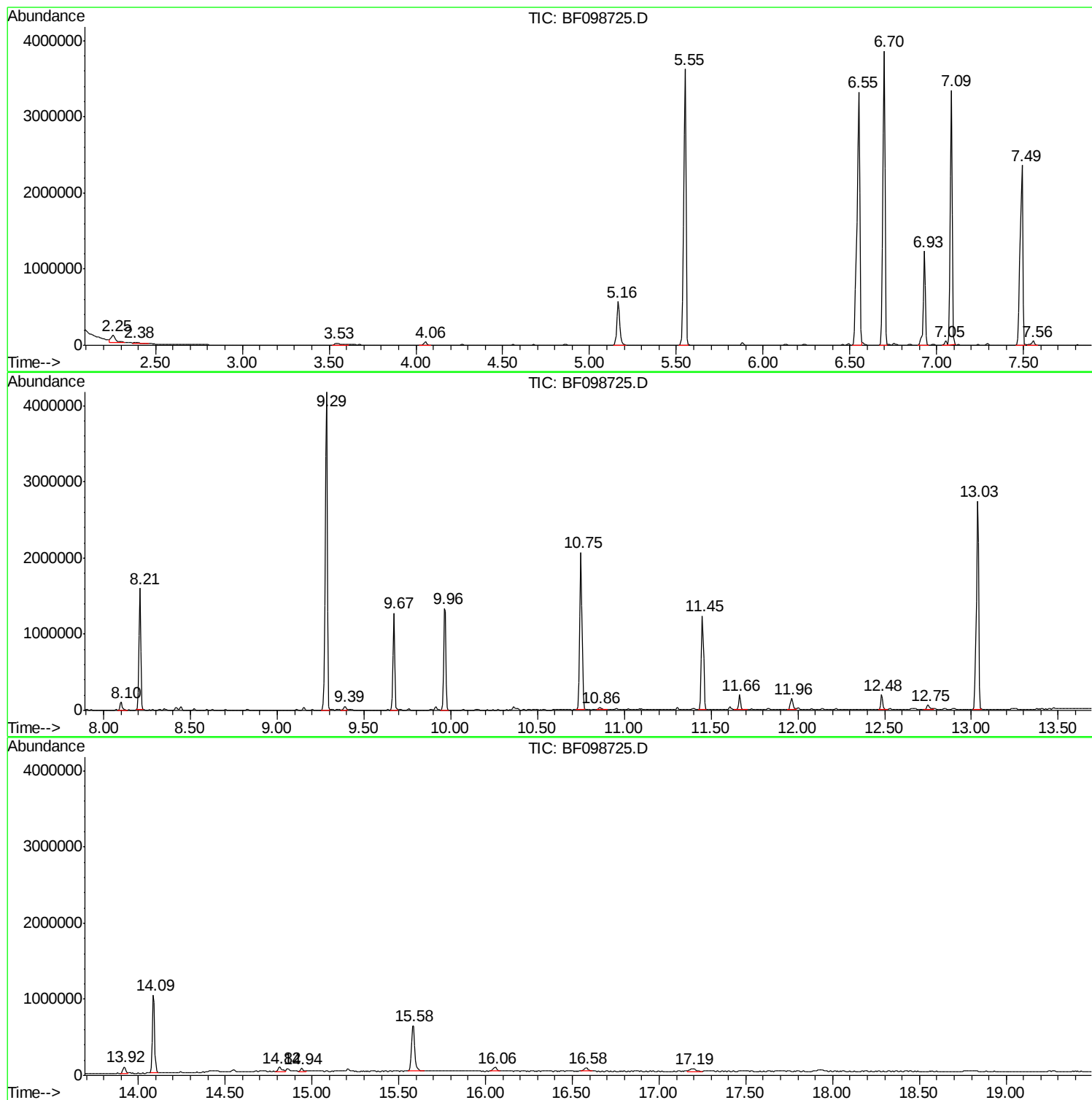
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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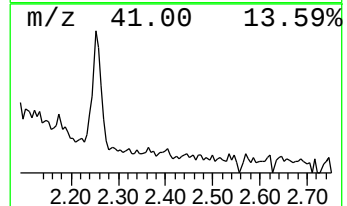
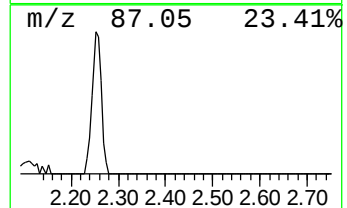
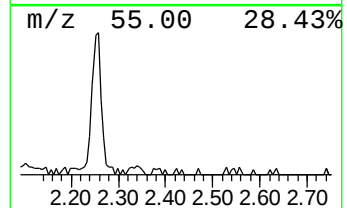
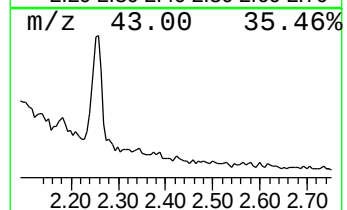
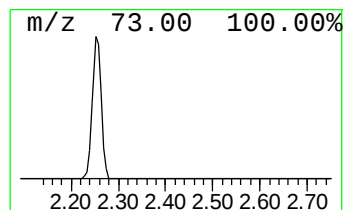
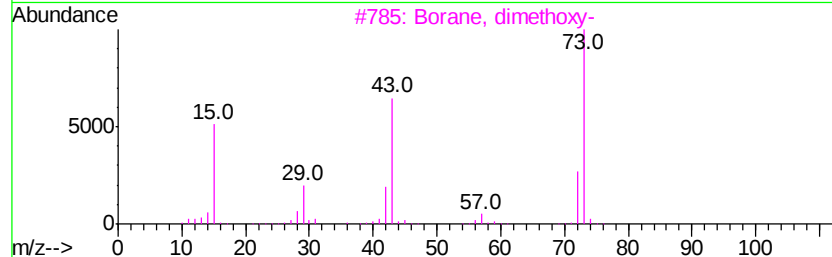
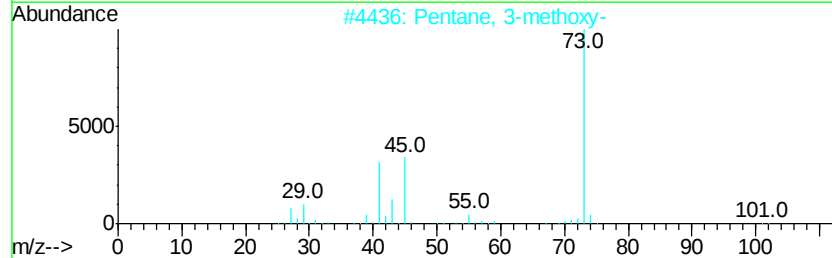
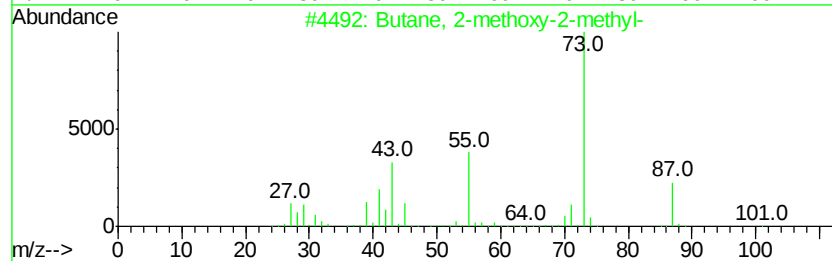
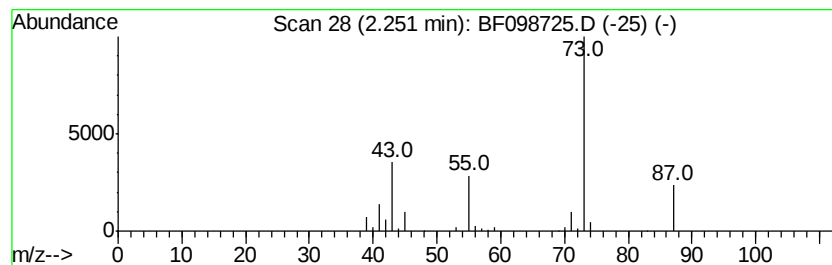
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	2.88 ng	150972	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,4-Butanediamine	88	C4H12N2	000110-60-1	9



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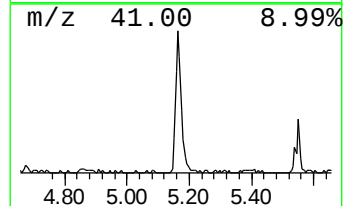
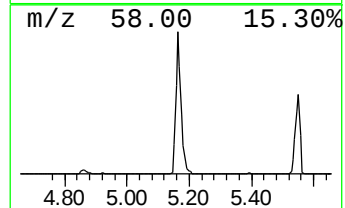
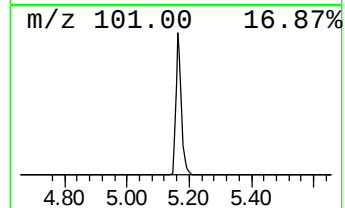
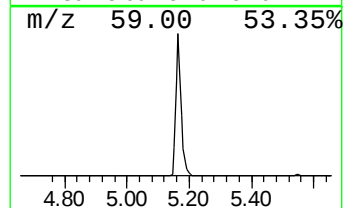
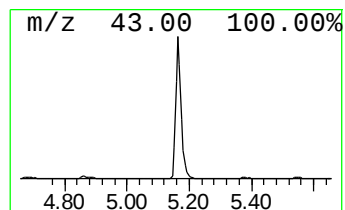
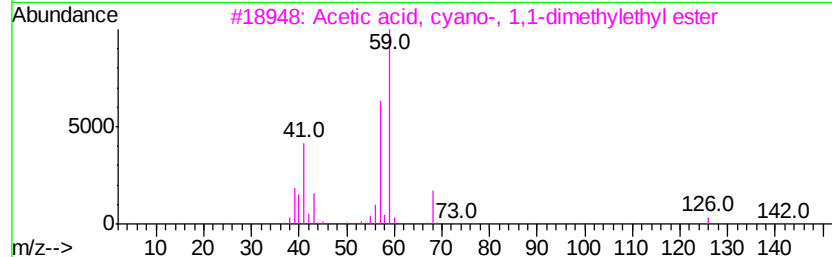
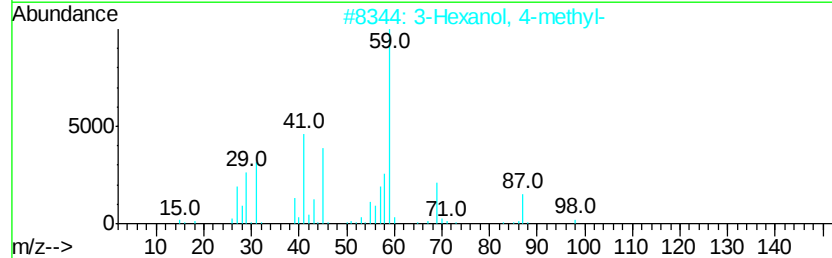
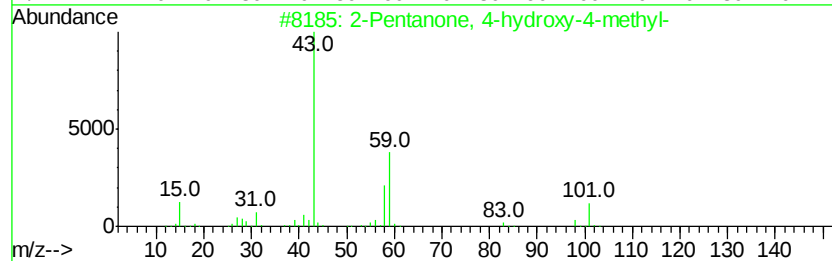
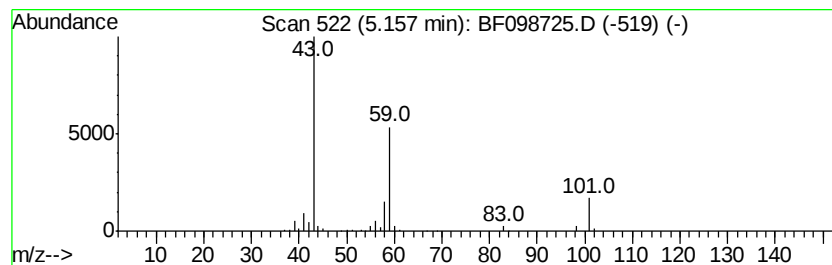
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	13.30 ng	697671	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5		Guanidine	59	CH5N3	000113-00-8	9



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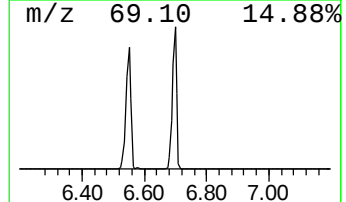
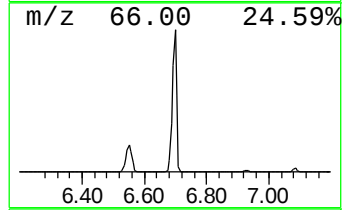
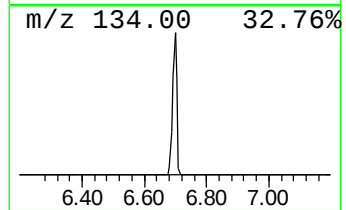
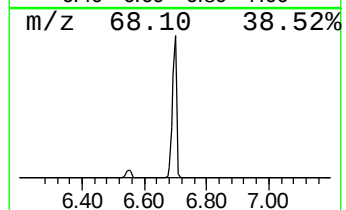
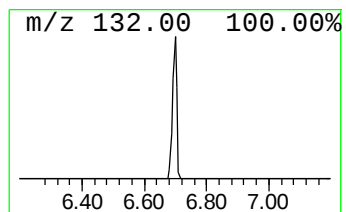
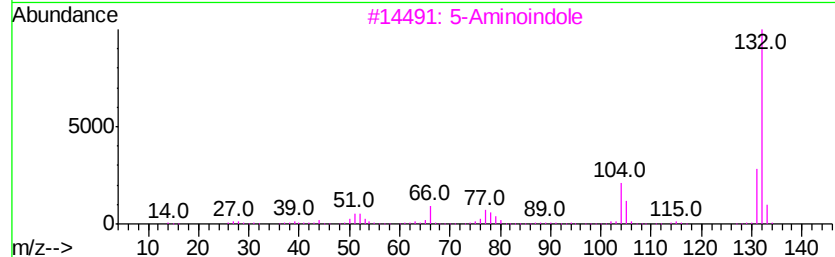
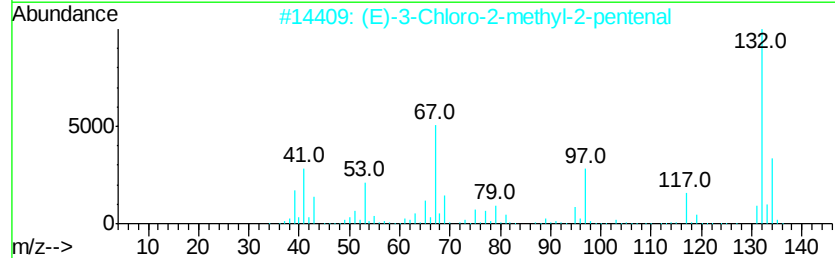
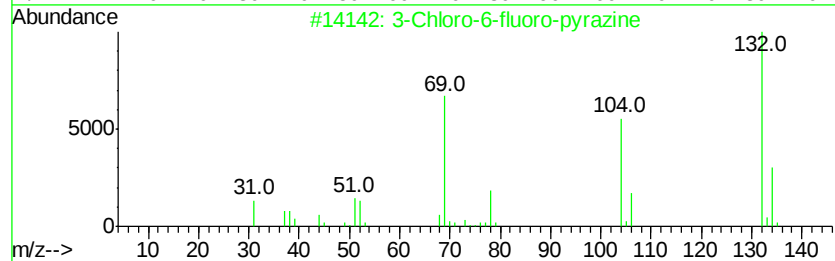
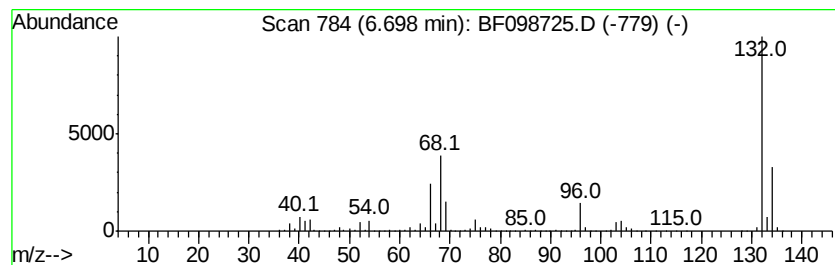
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	72.00 ng	3777600	1,4-Dichlorobenzene-d4	6.93

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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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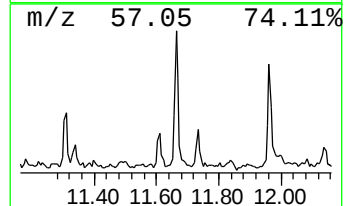
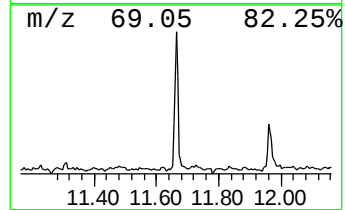
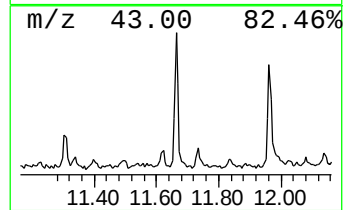
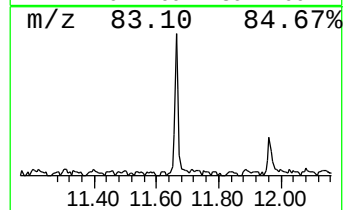
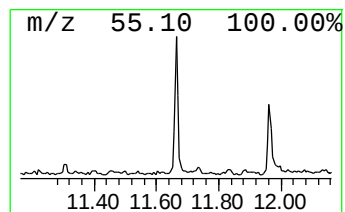
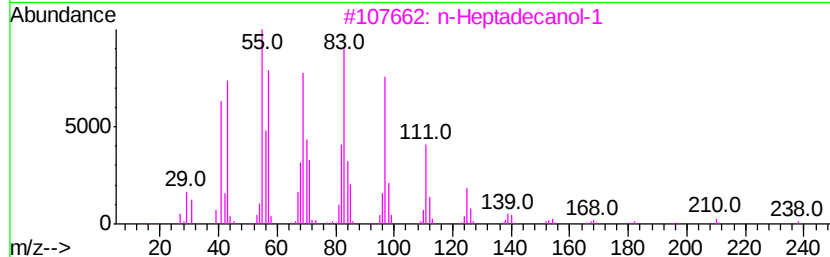
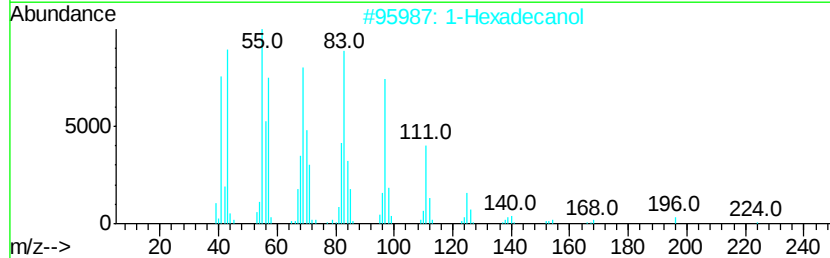
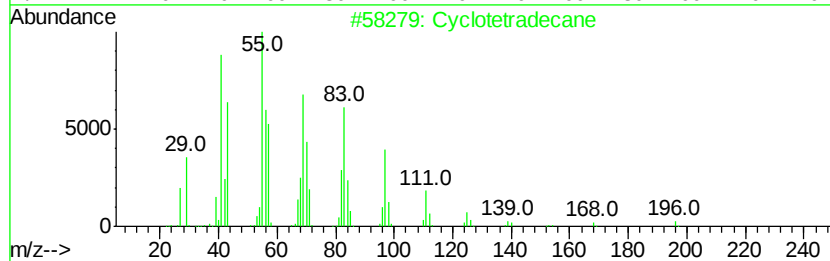
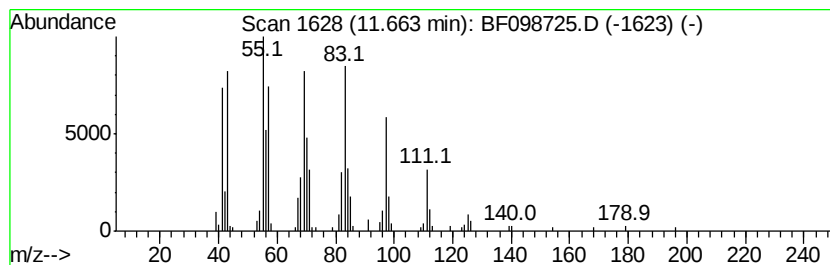
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.30 ng	163203	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91



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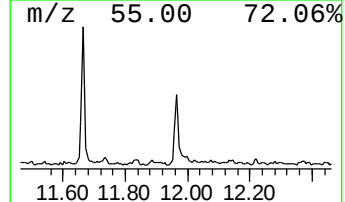
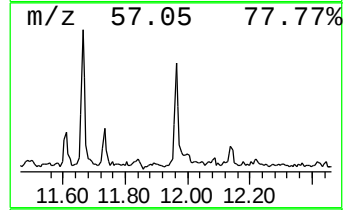
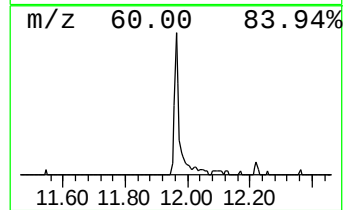
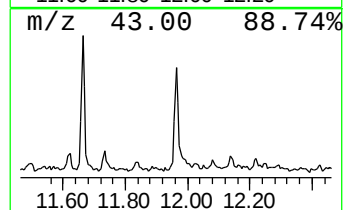
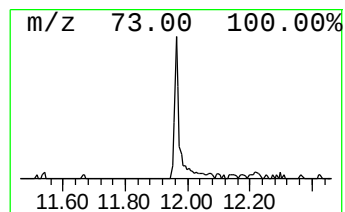
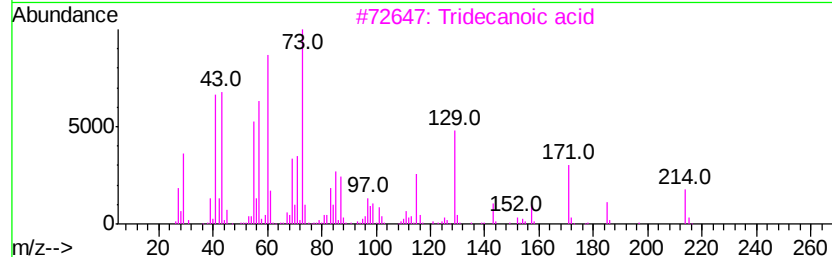
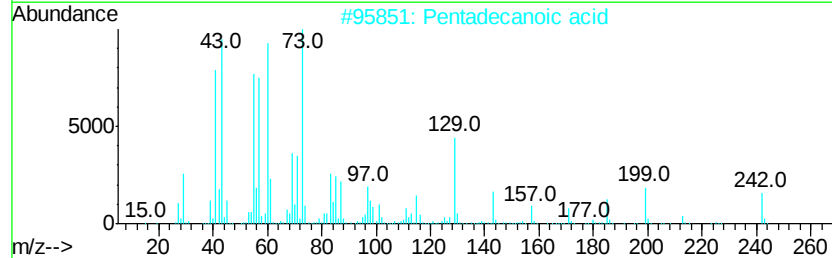
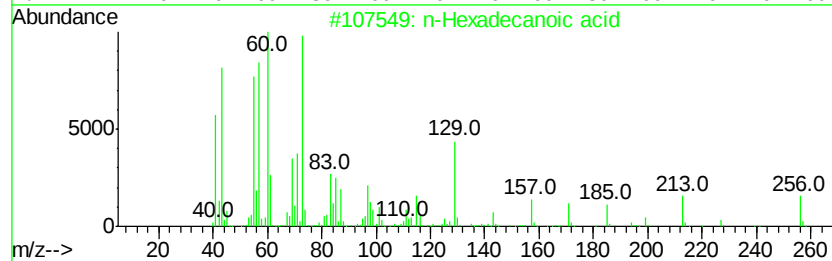
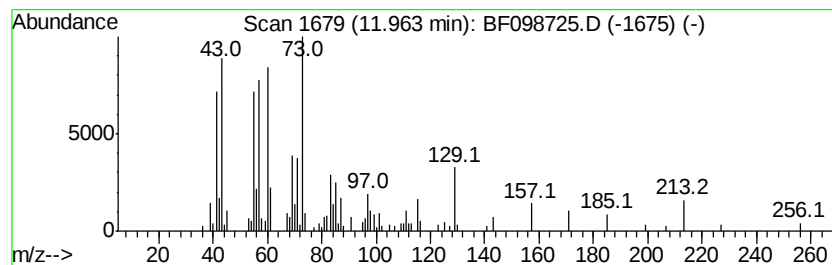
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.96 ng	146388	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Isoamyl nitrite	117	C5H11NO2	000110-46-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092217\
Data File : BF098725.D
Acq On : 23 Sep 2017 4:49
Operator : SJ/JU
Sample : I5304-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(5-10)

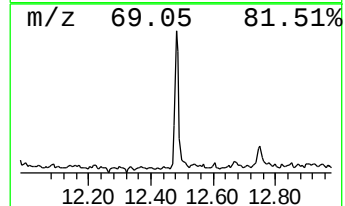
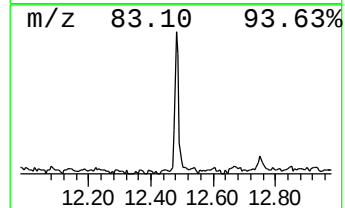
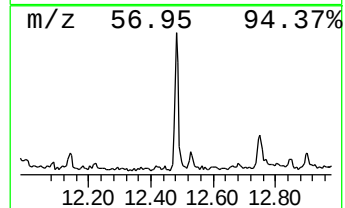
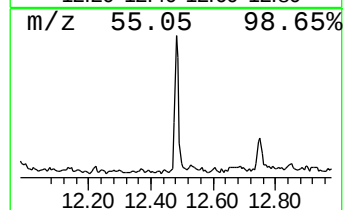
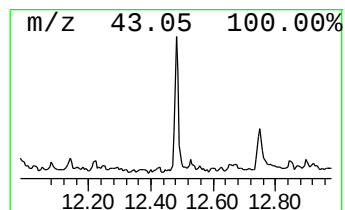
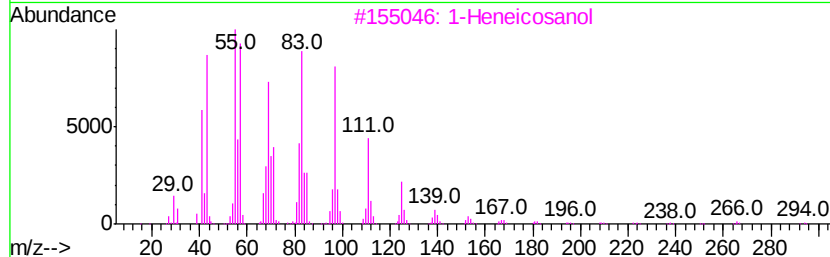
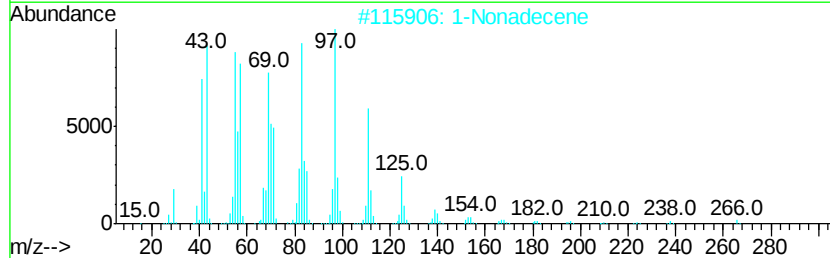
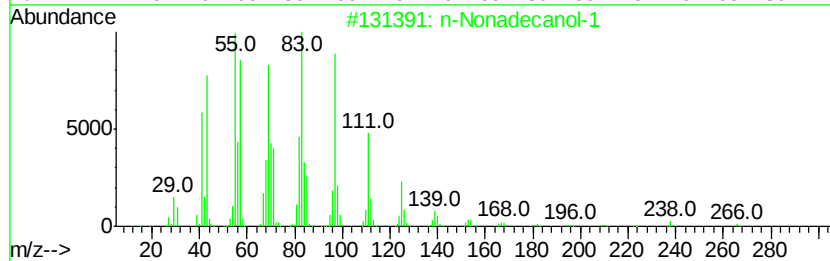
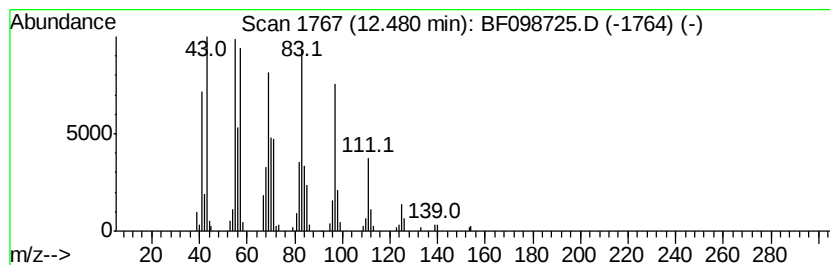
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	3.47 ng	171704	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2		1-Nonadecene	266	C19H38	018435-45-5	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	91
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(5-10)

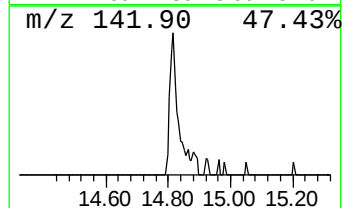
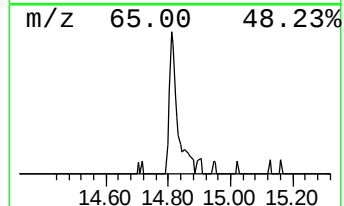
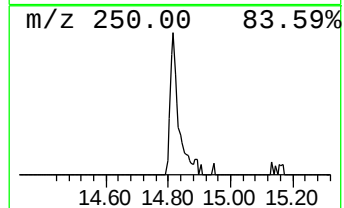
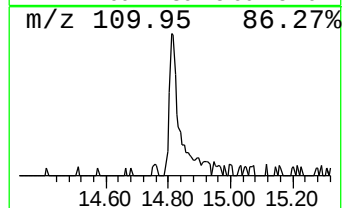
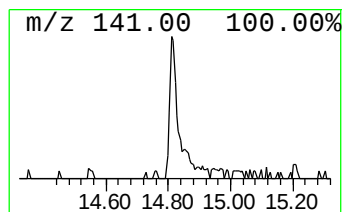
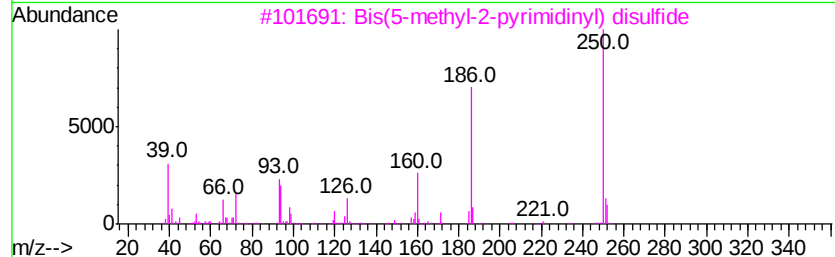
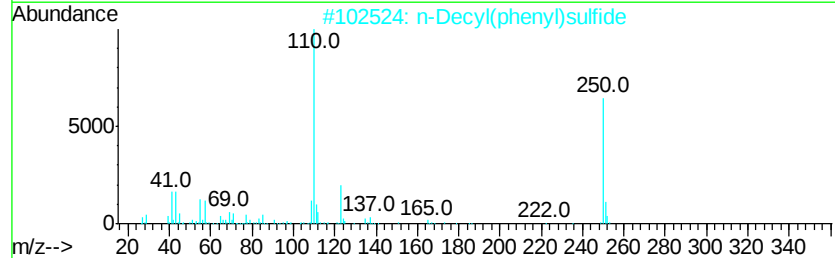
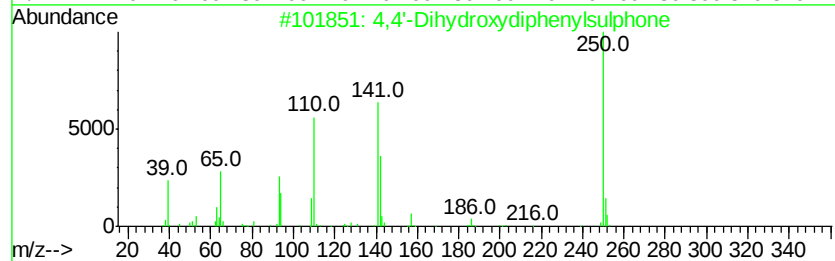
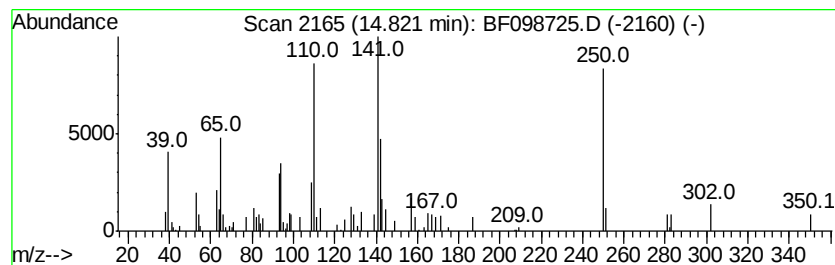
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,4'-Dihydroxydiphenylsulphone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.06 ng	96474	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	99
2		n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	18
3		Bis(5-methyl-2-pyrimidinyl) disu...	250	C10H10N4S2	1000326-74-2	15
4		1,3-Benzenediol, o-(2,6-difluoro...	250	C13H8F2O3	1000330-83-2	14
5		Phenoxyacetoneitrile	133	C8H7NO	003598-14-9	12



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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-117-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092117.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...	2.25	2.9	ng	150972	1	6.93	1049330	20.0
2-Pentanone, 4-hy...	5.16	13.3	ng	697671	1	6.93	1049330	20.0
unknown6.70	6.70	72.0	ng	3777600	1	6.93	1049330	20.0
Cyclotetradecane	11.66	3.3	ng	163203	4	11.45	988916	20.0
n-Hexadecanoic acid	11.96	3.0	ng	146388	4	11.45	988916	20.0
n-Nonadecanol-1	12.48	3.5	ng	171704	4	11.45	988916	20.0
4,4'-Dihydroxydip...	14.82	2.1	ng	96474	5	14.09	935686	20.0