

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
 Data File : BF084860.D
 Acq On : 5 Feb 2016 15:28
 Operator : SJ/IZ
 Sample : H1329-21
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B004(46-48)

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-BF020116.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	2.852	65	67	78	rBV	36309	116368	2.34%	0.238%
2	4.818	235	239	248	rVB	857393	1615247	32.47%	3.308%
3	5.196	270	272	275	rBV	69100	102838	2.07%	0.211%
4	5.253	275	277	280	rBV	3978684	4974954	100.00%	10.189%
5	6.316	367	370	372	rBV	4383481	4867502	97.84%	9.969%
6	6.430	377	380	382	rBV	4986399	4826373	97.01%	9.884%
7	6.659	398	400	402	rBV	1353315	1112252	22.36%	2.278%
8	6.819	411	414	416	rBV	4234956	3979320	79.99%	8.150%
9	7.230	447	450	453	rVB	2884760	3069585	61.70%	6.286%
10	7.356	455	461	467	rBV	110717	163812	3.29%	0.335%
11	7.699	487	491	495	rBV	54267	79894	1.61%	0.164%
12	7.950	510	513	515	rBV	1384211	1522366	30.60%	3.118%
13	9.025	604	607	610	rBV	4603387	4861334	97.72%	9.956%
14	9.425	640	642	644	rBV	1387231	1157785	23.27%	2.371%
15	9.642	659	661	663	rVB	108761	89208	1.79%	0.183%
16	9.699	663	666	668	rVB	1538815	1639878	32.96%	3.358%
17	10.145	703	705	706	rVB	127201	118321	2.38%	0.242%
18	10.362	721	724	727	rBV	49285	72889	1.47%	0.149%
19	10.488	732	735	737	rBV	3471575	3949969	79.40%	8.089%
20	10.613	744	746	753	rBV	173942	220116	4.42%	0.451%
21	11.059	782	785	786	rBV	141031	122821	2.47%	0.252%
22	11.173	792	795	797	rVV	1900792	1613005	32.42%	3.303%
23	11.413	814	816	820	rVB2	51919	77512	1.56%	0.159%
24	11.482	820	822	825	rVB	74701	66839	1.34%	0.137%
25	11.722	841	843	847	rBV2	60976	82015	1.65%	0.168%
26	11.871	854	856	857	rBV	49852	56857	1.14%	0.116%
27	12.316	893	895	897	rVB	55043	50091	1.01%	0.103%
28	12.476	907	909	911	rBV	53995	58946	1.18%	0.121%
29	12.591	917	919	921	rBV2	199959	276374	5.56%	0.566%
30	12.762	931	934	936	rBV	5001163	4897670	98.45%	10.030%
31	13.116	963	965	968	rVB	50952	76161	1.53%	0.156%
32	13.299	979	981	983	rBV	250750	219673	4.42%	0.450%
33	13.345	983	985	989	rVB2	35465	56891	1.14%	0.117%
34	13.665	1011	1013	1021	rBV	204133	303032	6.09%	0.621%

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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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35	13.802	1022	1025	1027	rBV	1502979	1377802	27.69%	2.822%
36	14.648	1097	1099	1101	rVB	55743	52303	1.05%	0.107%
37	15.162	1142	1144	1147	rBV	629854	900752	18.11%	1.845%

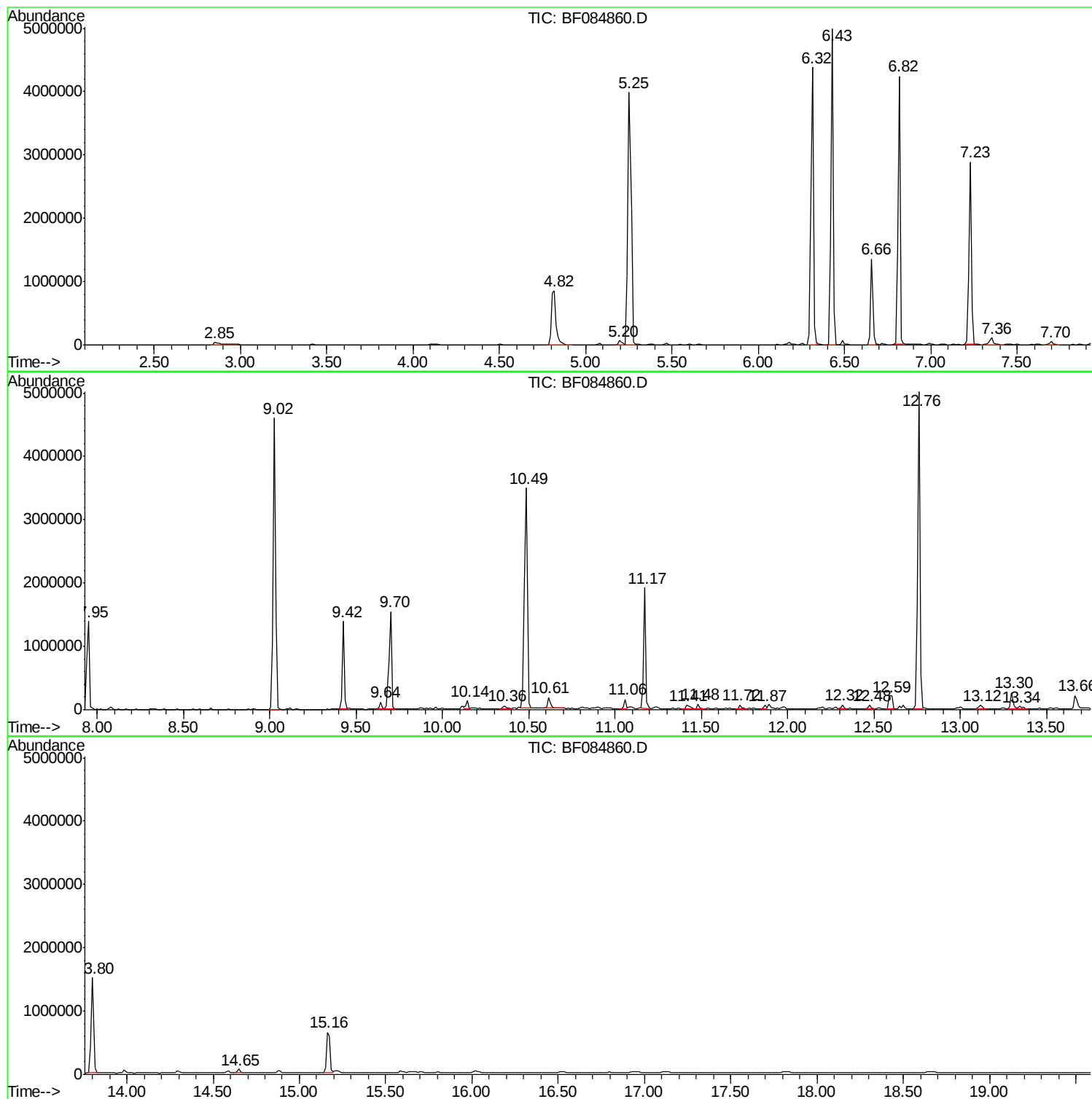
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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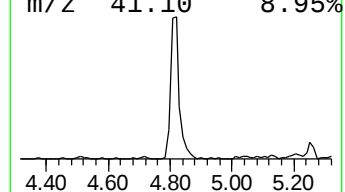
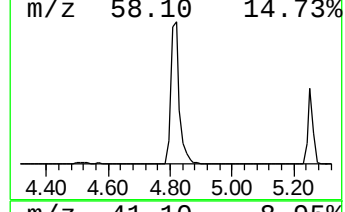
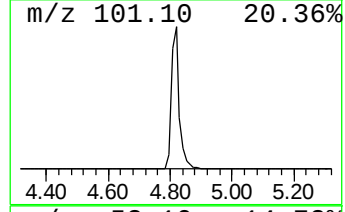
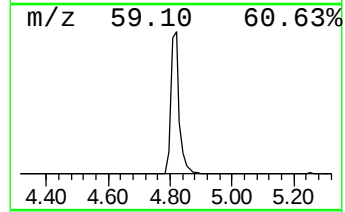
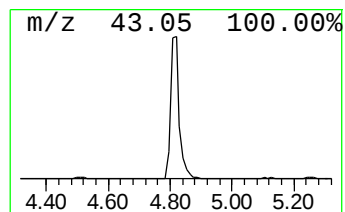
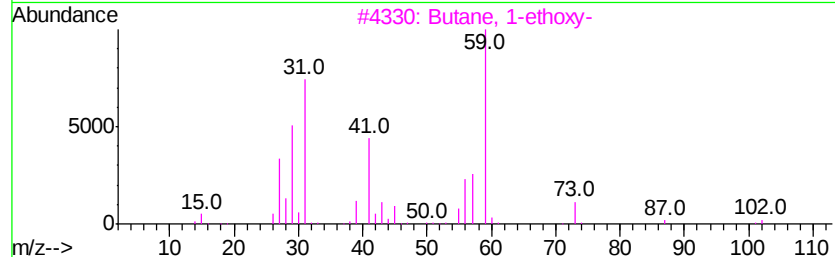
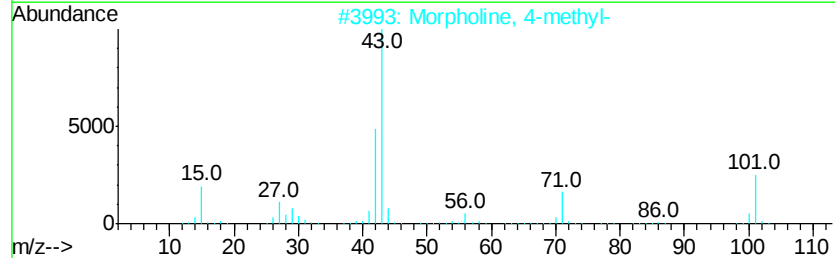
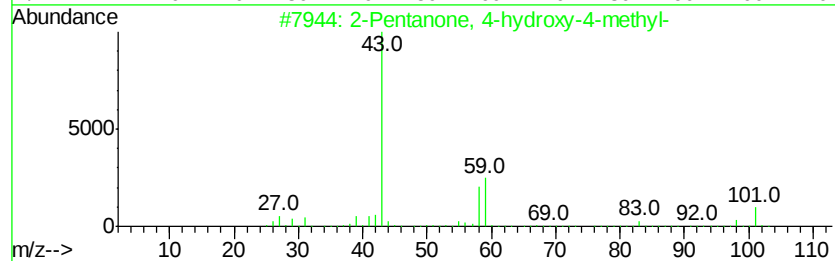
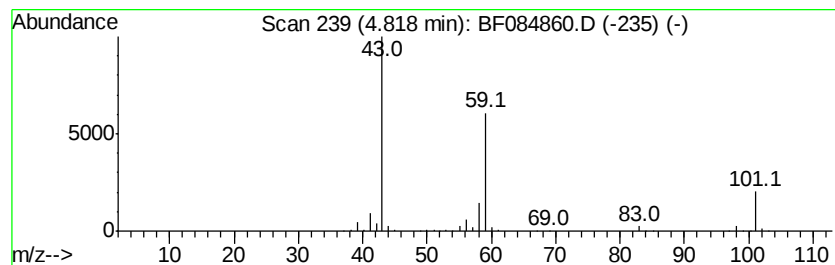
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	29.04 ng	1615250	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Pentanol	88	C5H12O	000584-02-1	9



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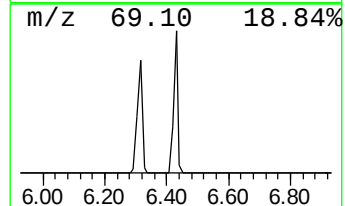
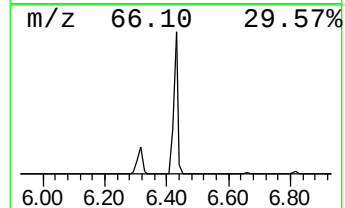
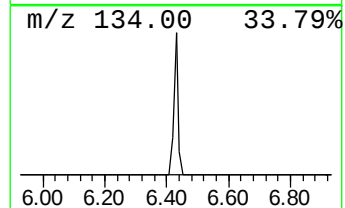
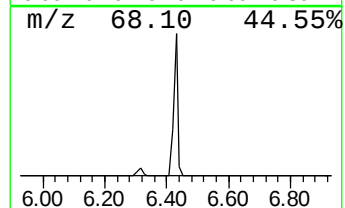
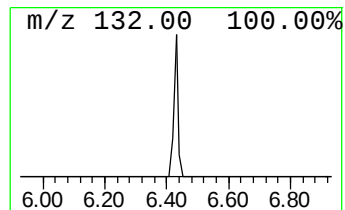
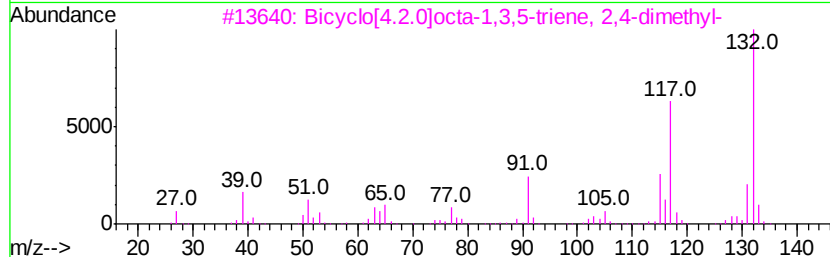
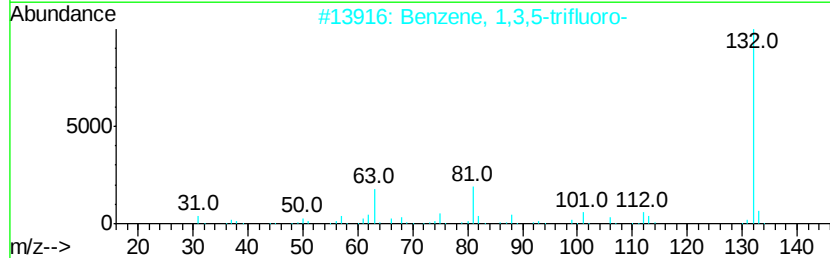
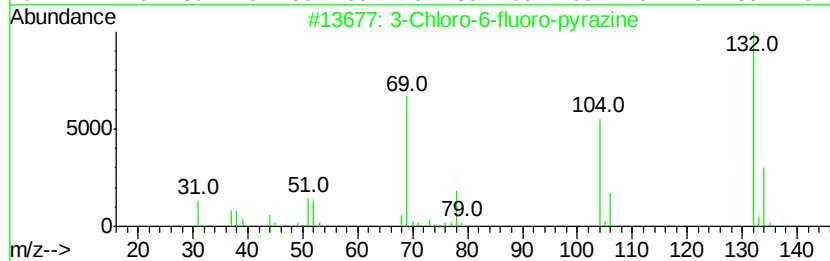
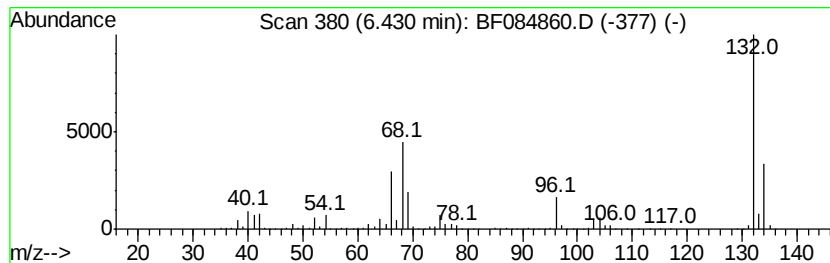
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	86.79 ng	4826370	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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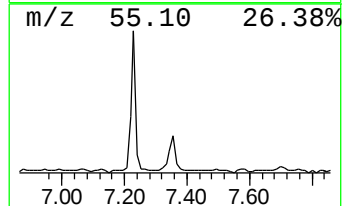
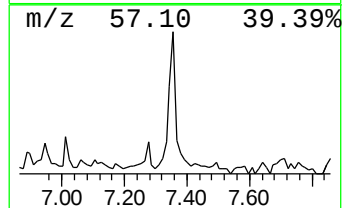
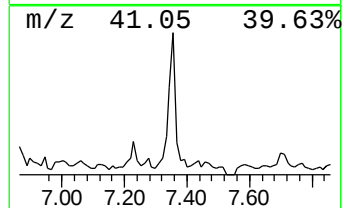
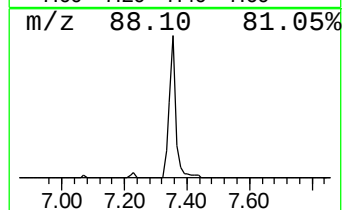
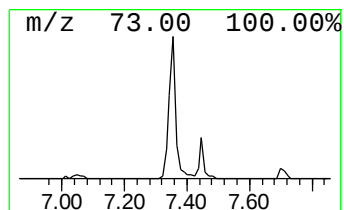
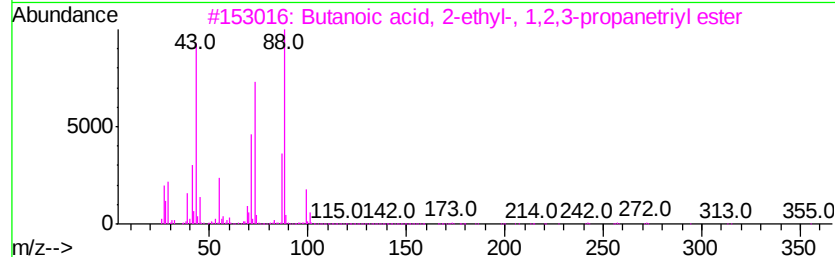
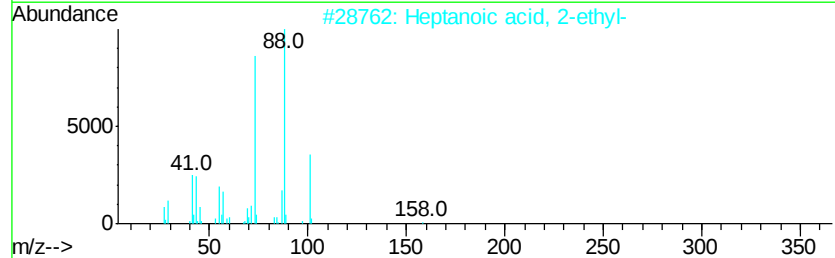
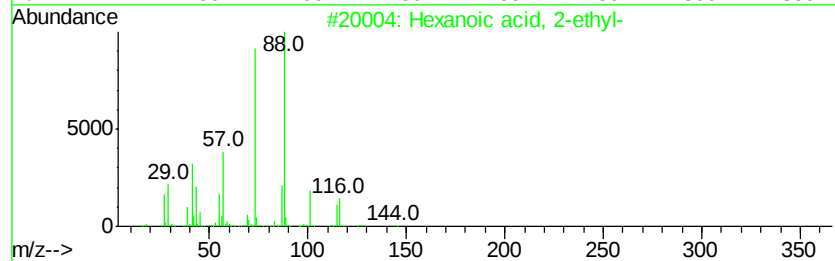
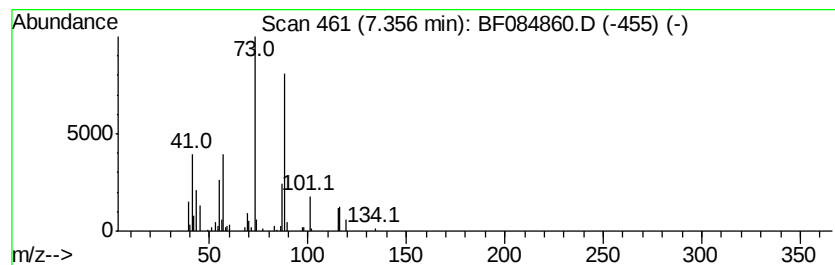
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	2.15 ng	163812	Naphthalene-d8	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4		1,4-Dioxane	88	C4H8O2	000123-91-1	37
5		Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	33



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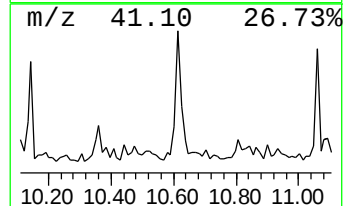
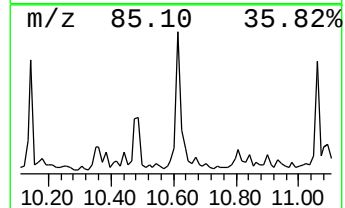
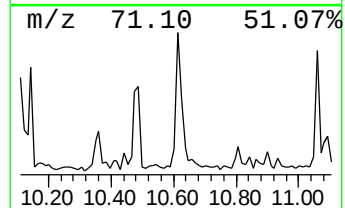
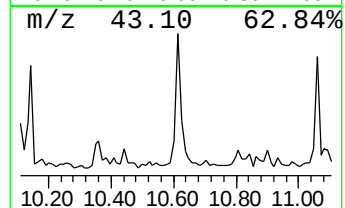
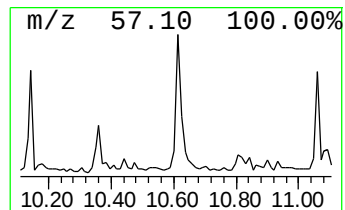
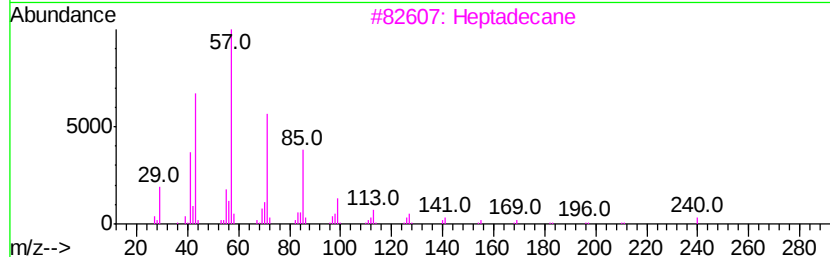
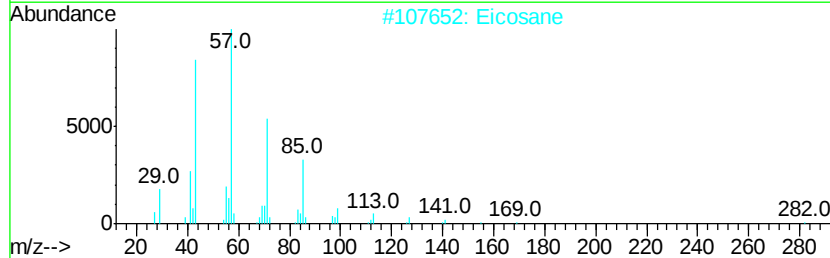
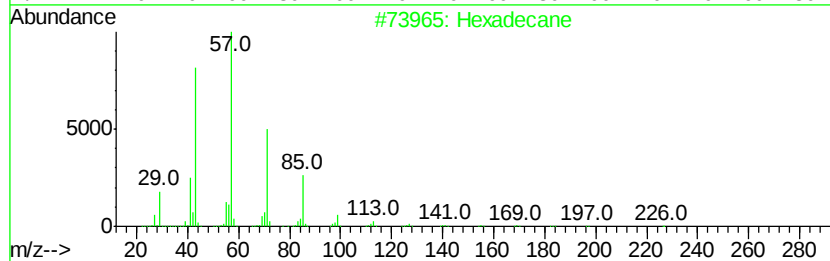
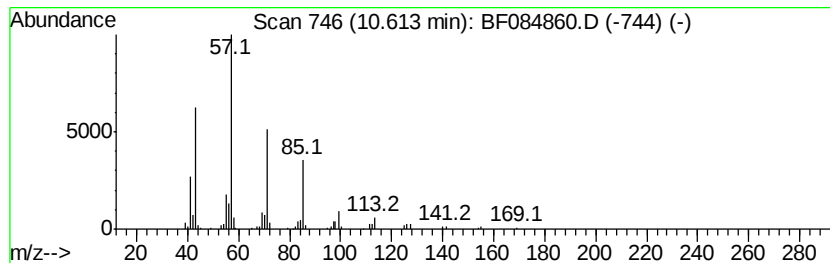
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Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.61	2.73 ng	220116	Phenanthrene-d10	11.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83



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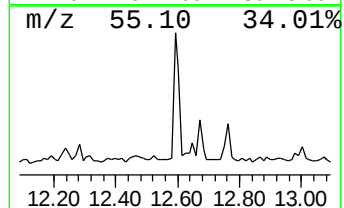
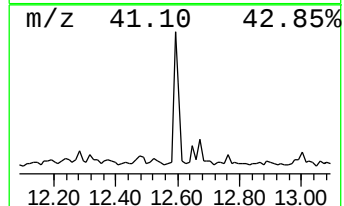
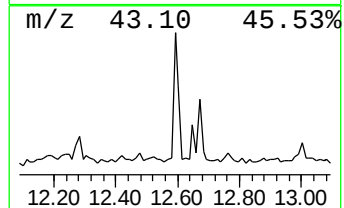
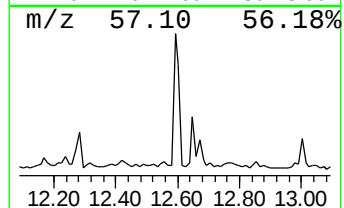
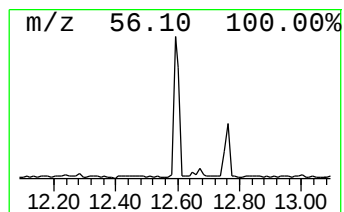
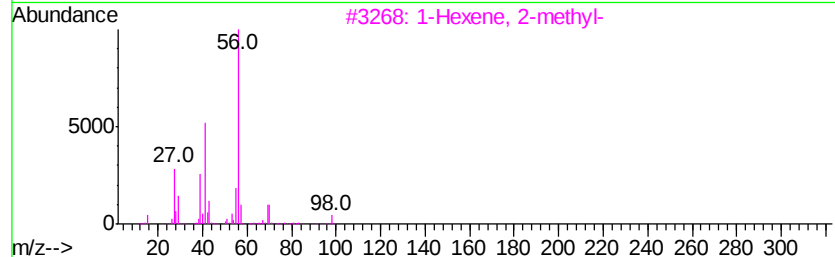
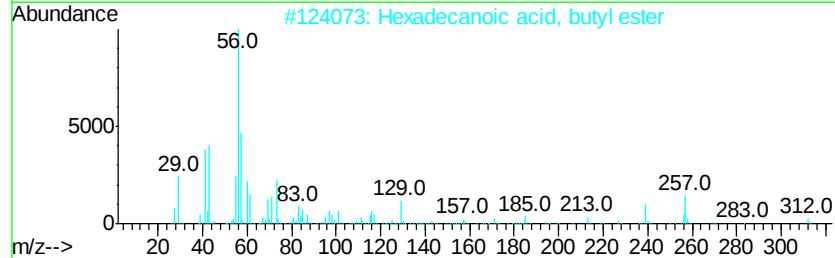
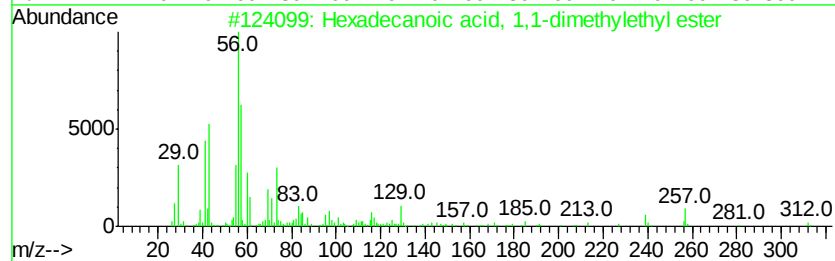
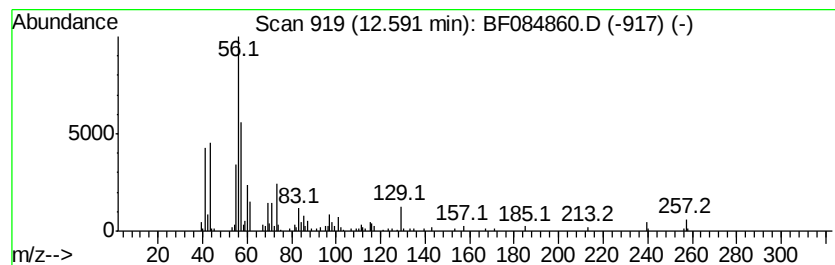
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Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	4.01 ng	276374	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
3		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084860.D
Acq On : 5 Feb 2016 15:28
Operator : SJ/IZ
Sample : H1329-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B004(46-48)

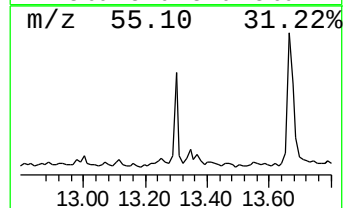
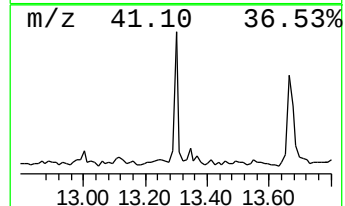
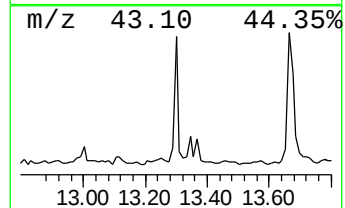
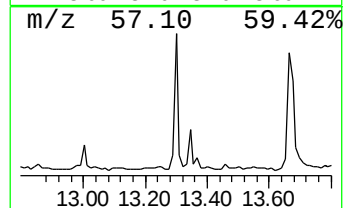
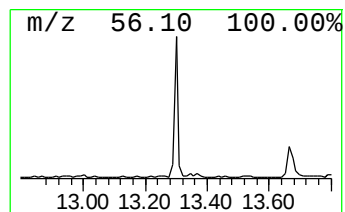
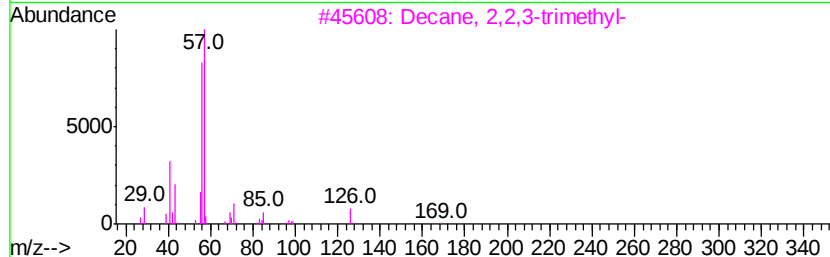
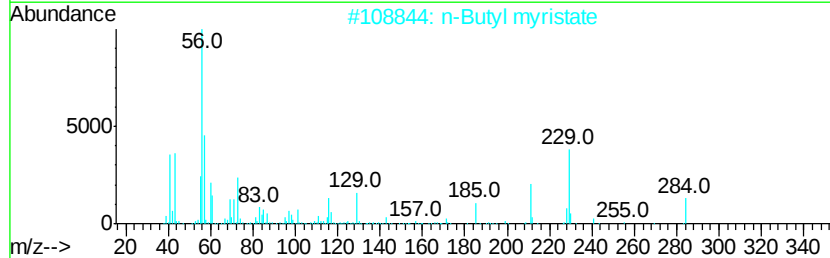
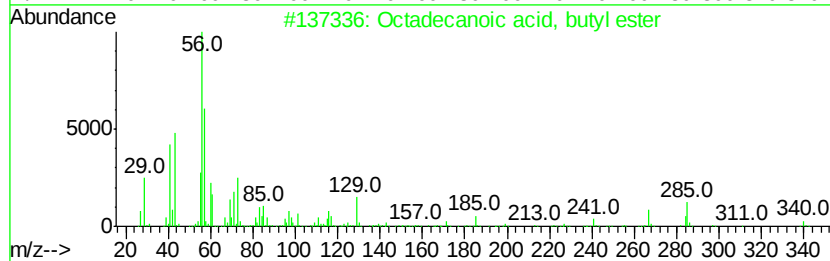
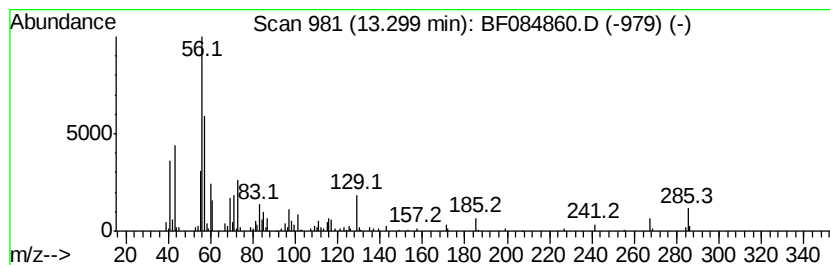
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	3.19 ng	219673	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084860.D
Acq On : 5 Feb 2016 15:28
Operator : SJ/IZ
Sample : H1329-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B004(46-48)

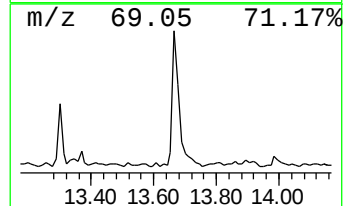
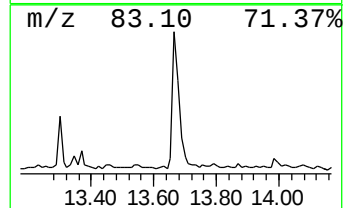
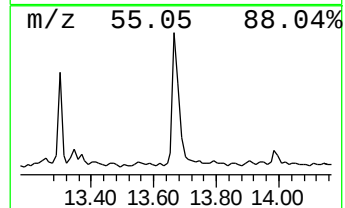
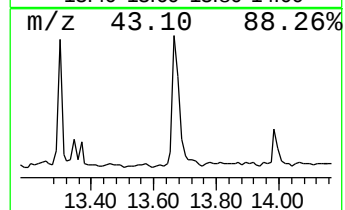
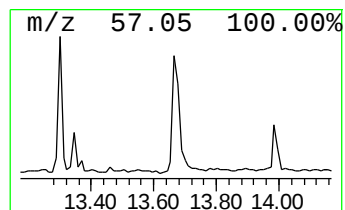
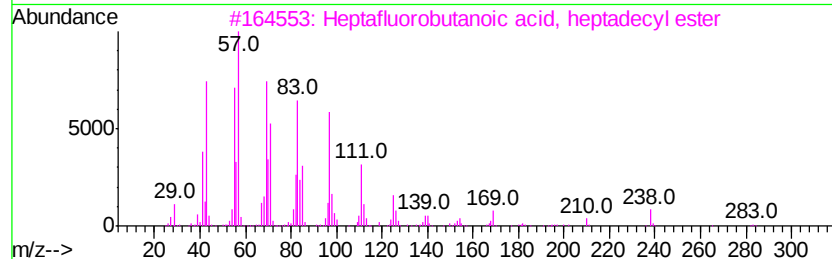
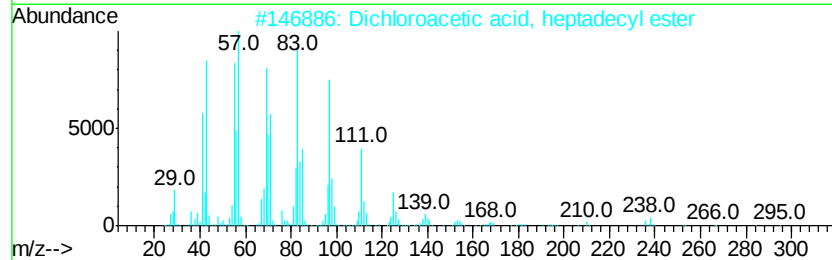
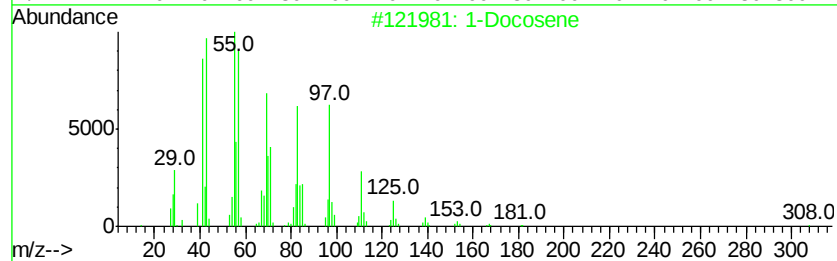
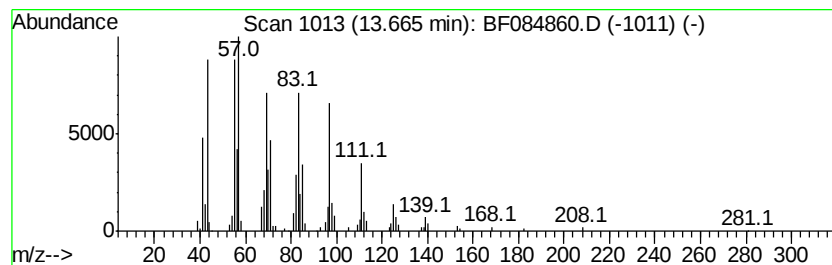
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	4.40 ng	303032	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084860.D
Acq On : 5 Feb 2016 15:28
Operator : SJ/IZ
Sample : H1329-21
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B004(46-48)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.82	29.0	ng	1615250	1	6.66	1112250	20.0
unknown6.43	6.43	86.8	ng	4826370	1	6.66	1112250	20.0
Hexanoic acid, 2-...	7.36	2.1	ng	163812	2	7.95	1522370	20.0
Hexadecane	10.61	2.7	ng	220116	4	11.17	1613010	20.0
Hexadecanoic acid...	12.59	4.0	ng	276374	5	13.80	1377800	20.0
Octadecanoic acid...	13.30	3.2	ng	219673	5	13.80	1377800	20.0
1-Docosene	13.67	4.4	ng	303032	5	13.80	1377800	20.0