

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122316\
 Data File : BF091932.D
 Acq On : 23 Dec 2016 19:06
 Operator : UM/SJ
 Sample : H6238-13
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PIT-003-COMP

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-BF122116.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	4.910	244	247	254	rBV	1422215	2452047	34.12%	4.028%
2	5.390	285	289	291	rBV	4627768	6359446	88.50%	10.446%
3	6.430	377	380	383	rVB	4692537	7185871	100.00%	11.804%
4	6.522	386	388	391	rBV	4786983	7069104	98.38%	11.612%
5	6.739	405	407	410	rBV	1697172	1479133	20.58%	2.430%
6	6.899	418	421	423	rBV	4959170	4728071	65.80%	7.766%
7	7.310	454	457	459	rBV	3427010	3712251	51.66%	6.098%
8	8.030	517	520	522	rBV	1452648	1741046	24.23%	2.860%
9	9.105	611	614	617	rBV	6602347	6622235	92.16%	10.878%
10	9.505	646	649	651	rBV	915065	1006848	14.01%	1.654%
11	9.779	670	673	675	rBV	2219727	2234633	31.10%	3.671%
12	10.190	706	709	710	rBV	101504	122670	1.71%	0.202%
13	10.213	710	711	713	rVV	139210	106045	1.48%	0.174%
14	10.316	716	720	723	rVB3	66393	104146	1.45%	0.171%
15	10.430	727	730	733	rBV2	55027	78763	1.10%	0.129%
16	10.568	739	742	745	rBV	3825315	4116051	57.28%	6.761%
17	10.682	750	752	757	rVB	167765	230558	3.21%	0.379%
18	11.128	790	791	793	rBV	127445	140272	1.95%	0.230%
19	11.253	800	802	806	rBV2	1649582	1741158	24.23%	2.860%
20	11.322	806	808	811	rVB2	71949	113402	1.58%	0.186%
21	11.493	819	823	826	rBV2	280097	363785	5.06%	0.598%
22	11.562	826	829	831	rBV	142879	190111	2.65%	0.312%
23	11.802	847	850	854	rBV3	98510	209510	2.92%	0.344%
24	11.871	854	856	860	rVB2	64076	128270	1.79%	0.211%
25	11.962	862	864	868	rVV	165066	163239	2.27%	0.268%
26	12.042	869	871	876	rVB4	40704	83936	1.17%	0.138%
27	12.305	892	894	897	rBV2	126654	195186	2.72%	0.321%
28	12.351	897	898	900	rVB	79178	72677	1.01%	0.119%
29	12.465	905	908	910	rBV	337966	325664	4.53%	0.535%
30	12.694	924	928	929	rBV2	193852	301616	4.20%	0.495%
31	12.716	929	930	935	rVB3	42013	81043	1.13%	0.133%
32	12.842	938	941	944	rVB	4148780	4031995	56.11%	6.623%
33	13.014	954	956	958	rVB	45596	73685	1.03%	0.121%
34	13.082	958	962	964	rBV2	68129	113929	1.59%	0.187%

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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 >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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35	13.414	988	991	996	rBV5	26108	87476	1.22%	0.144%
36	13.745	1017	1020	1024	rBV2	140033	212992	2.96%	0.350%
37	13.882	1029	1032	1039	rVV	1075168	1362632	18.96%	2.238%
38	14.648	1097	1099	1101	rBV2	42596	85457	1.19%	0.140%
39	14.888	1118	1120	1125	rBV	113174	239266	3.33%	0.393%
40	15.162	1142	1144	1147	rBV	58623	78683	1.09%	0.129%
41	15.220	1147	1149	1152	rVB	82781	110429	1.54%	0.181%
42	15.277	1152	1154	1157	rBV	665531	1022830	14.23%	1.680%

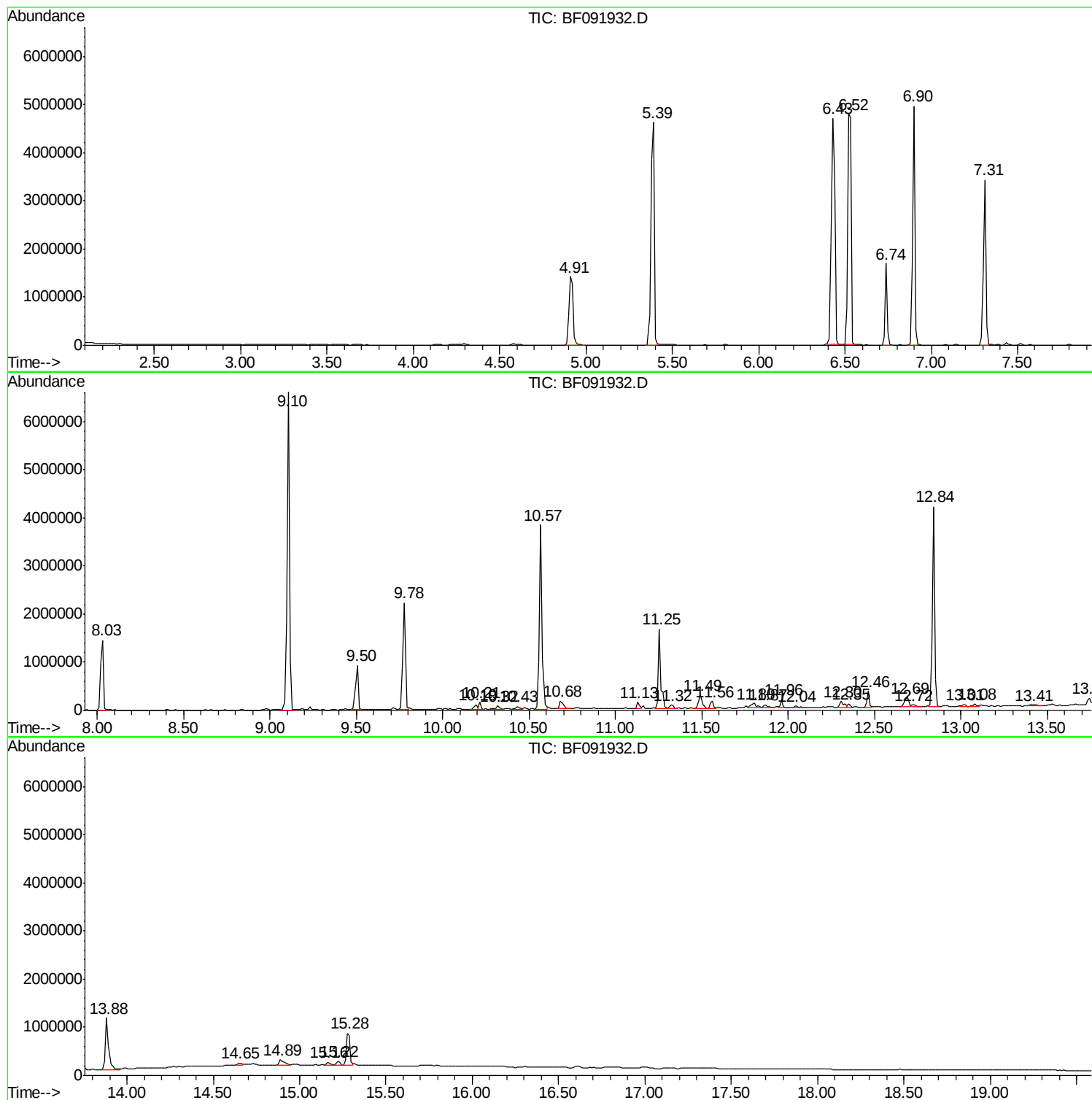
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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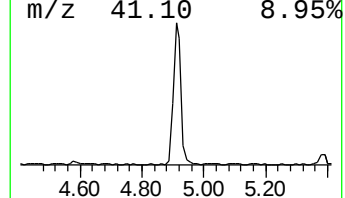
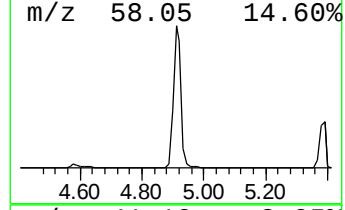
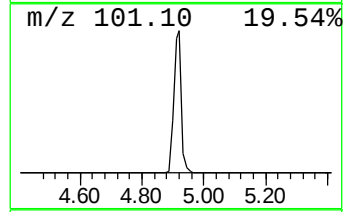
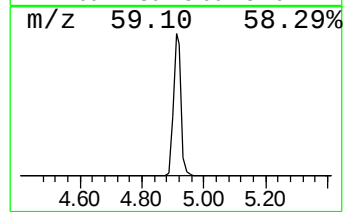
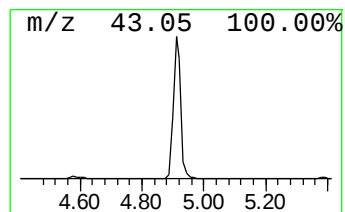
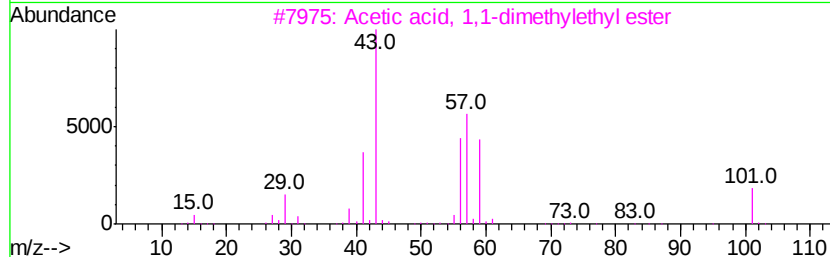
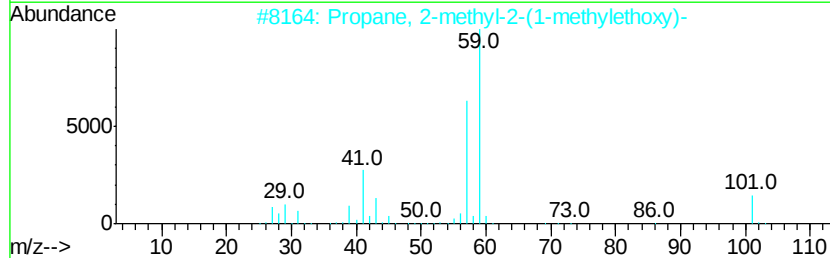
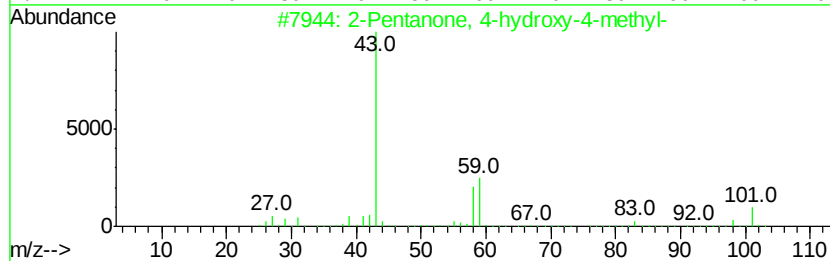
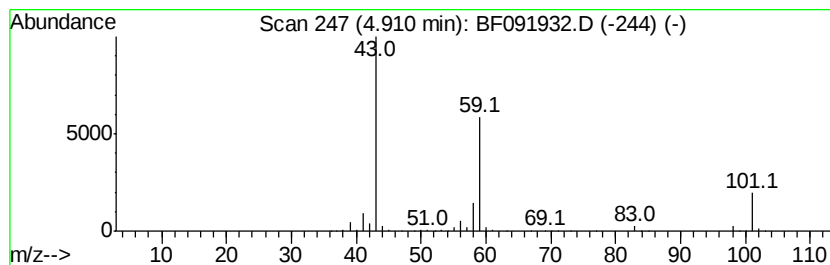
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.91	33.16 ng	2452050	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	42
3			Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	39
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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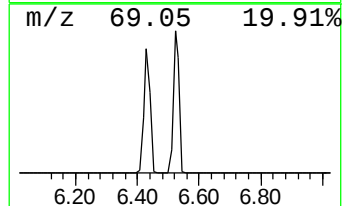
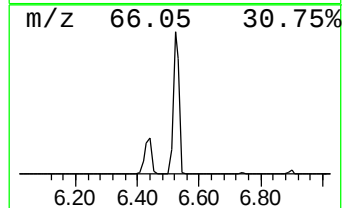
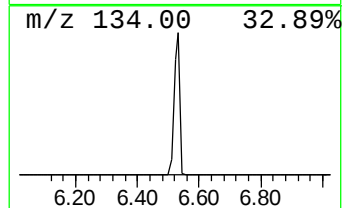
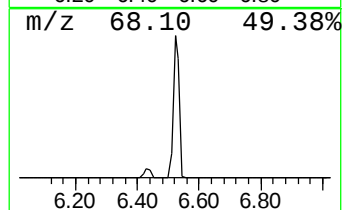
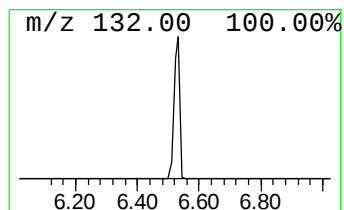
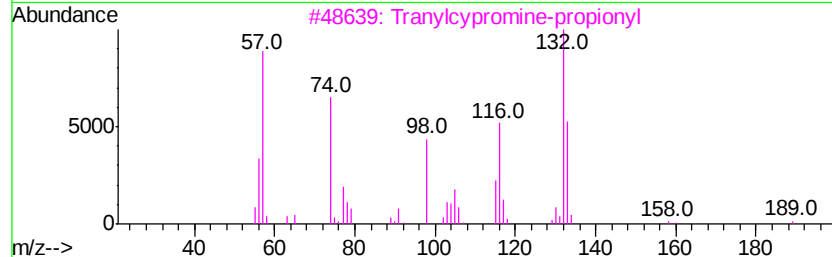
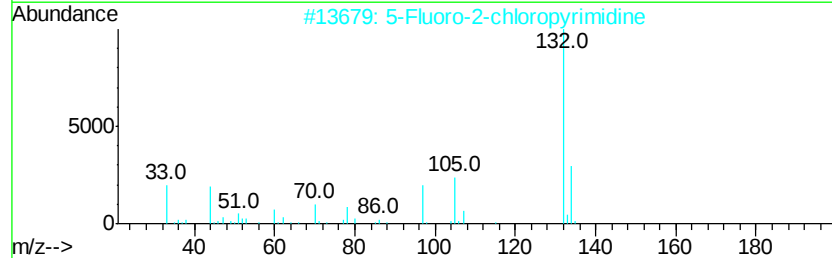
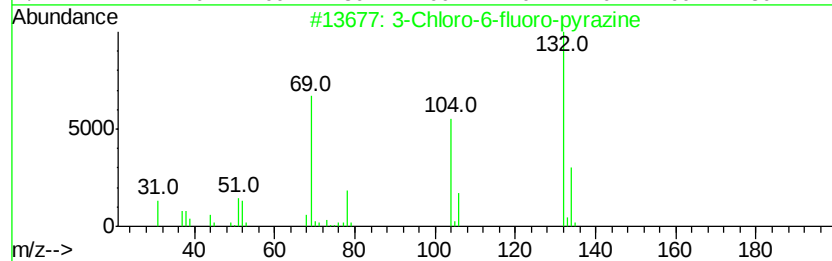
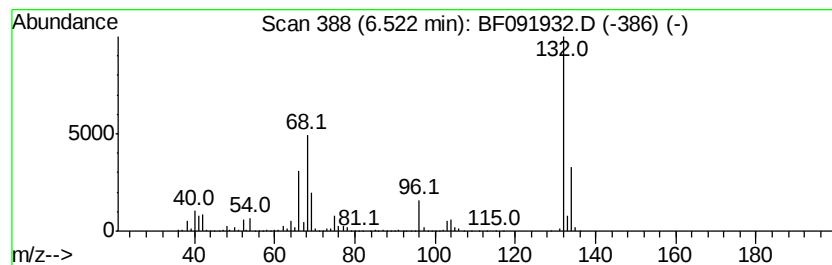
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Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	95.58 ng	7069100	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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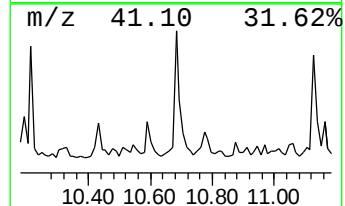
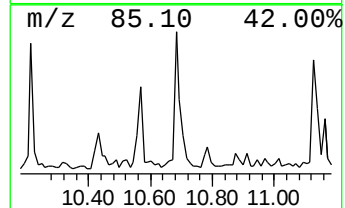
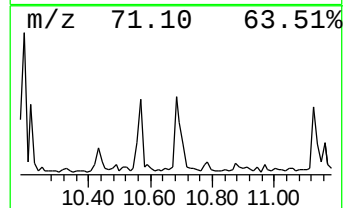
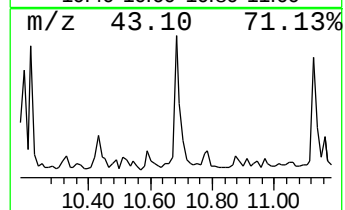
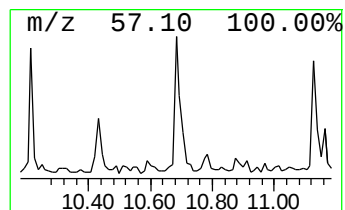
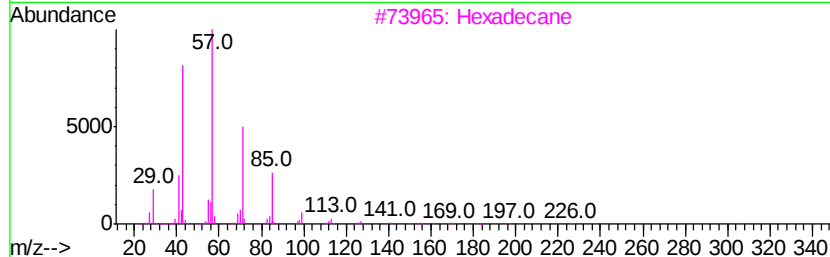
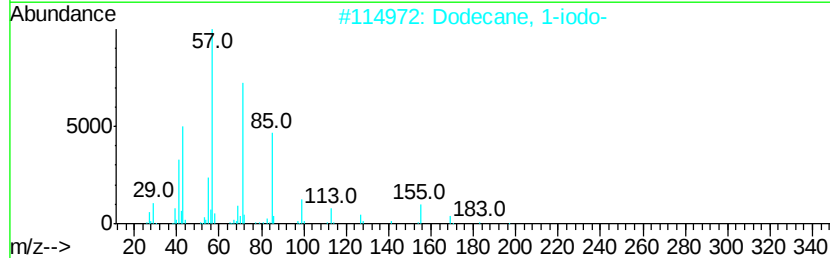
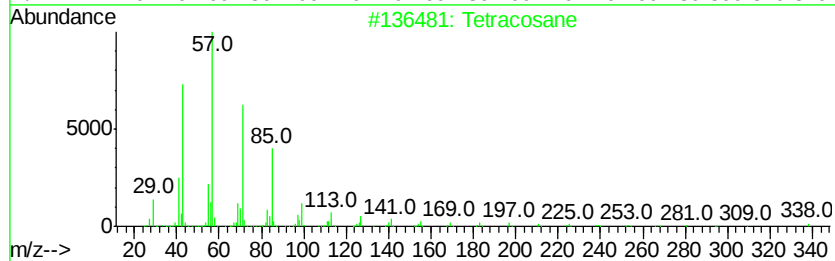
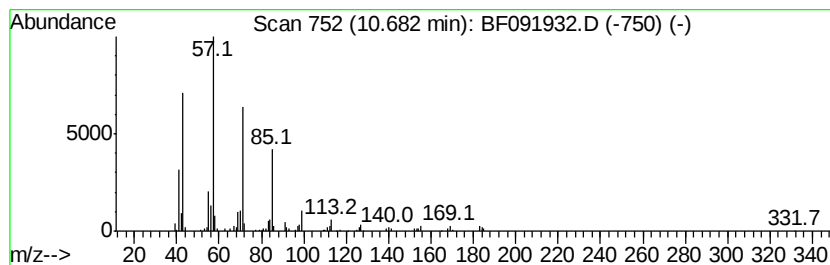
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.65 ng	230558	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	80
5	Eicosane	282	C20H42	000112-95-8	80



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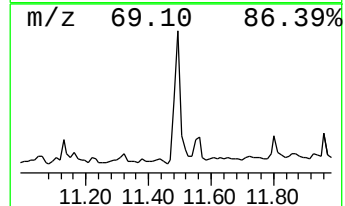
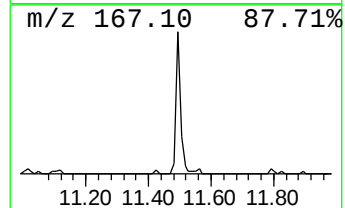
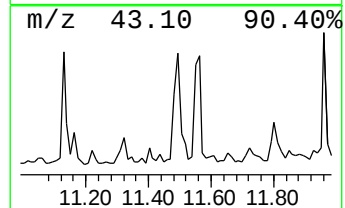
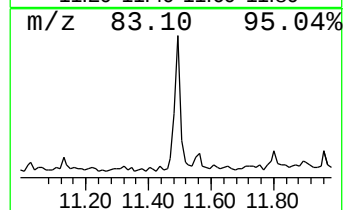
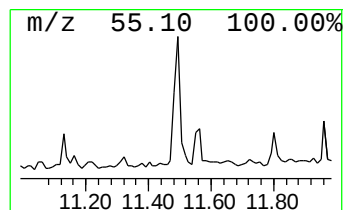
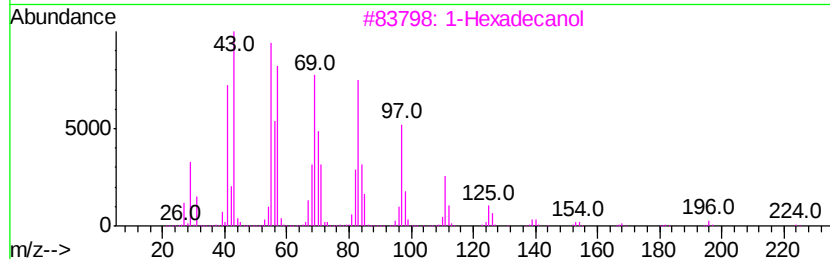
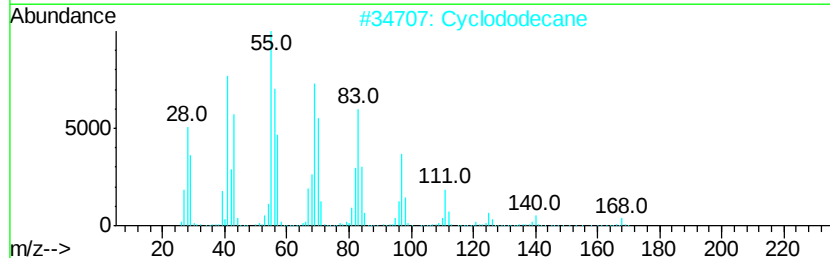
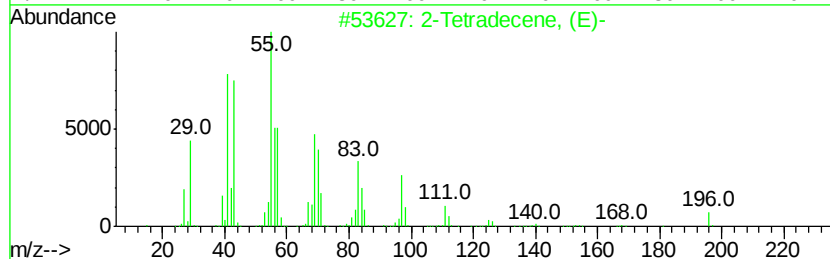
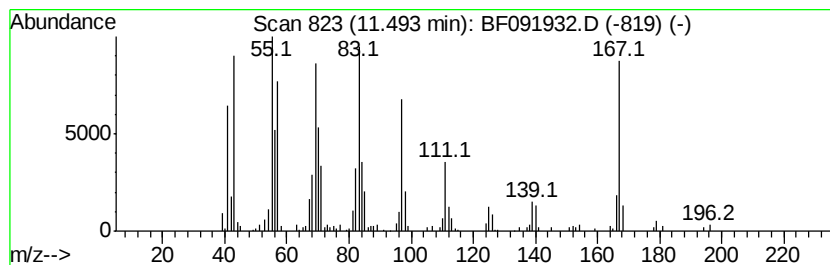
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Tetradecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	4.18 ng	363785	Phenanthrene-d10	11.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2-Tetradecene, (E)-	196 C14H28	035953-53-8 95
2		Cyclododecane	168 C12H24	000294-62-2 93
3		1-Hexadecanol	242 C16H34O	036653-82-4 93
4		1-Tetradecanol	214 C14H30O	000112-72-1 93
5		1-Tetradecene	196 C14H28	001120-36-1 89



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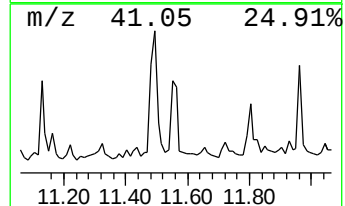
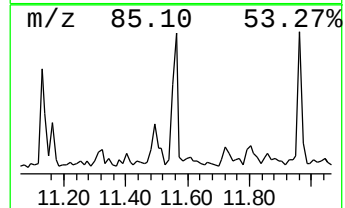
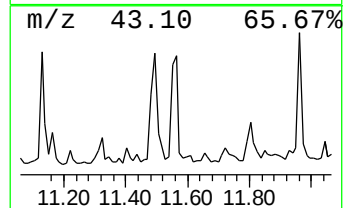
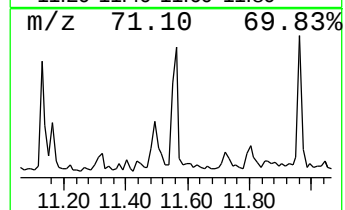
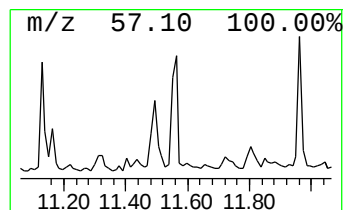
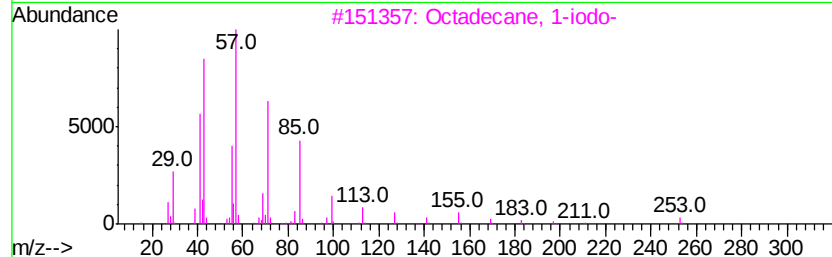
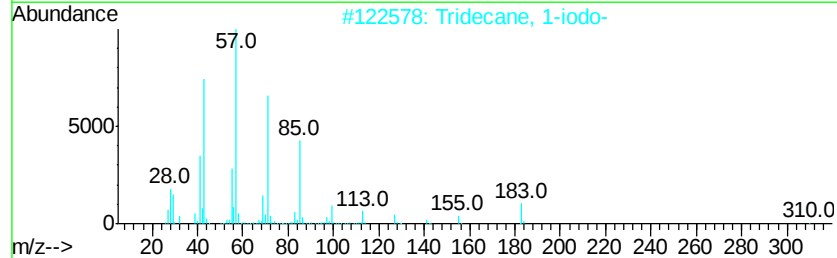
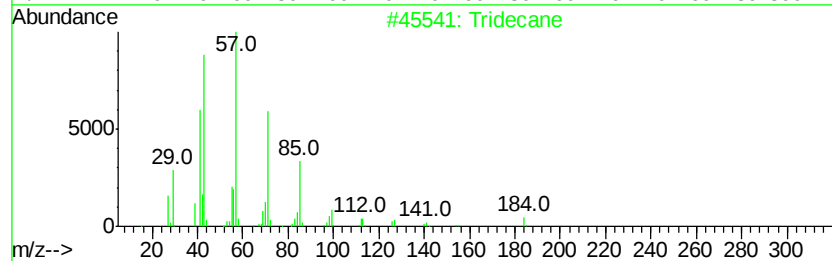
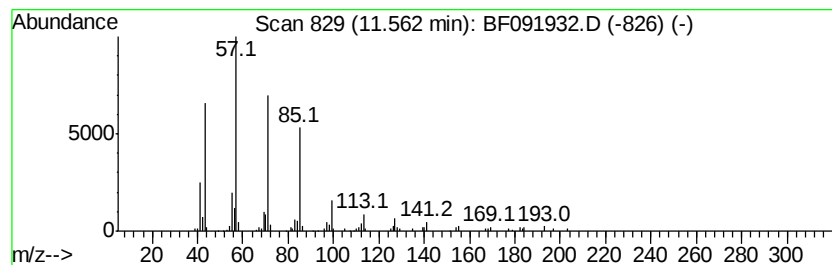
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.56	2.18 ng	190111	Phenanthrene-d10		11.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122316\
Data File : BF091932.D
Acq On : 23 Dec 2016 19:06
Operator : UM/SJ
Sample : H6238-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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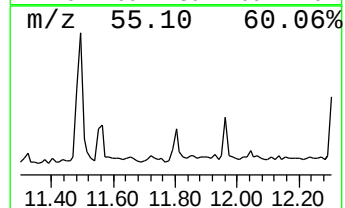
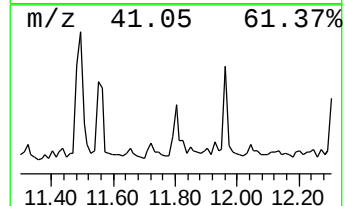
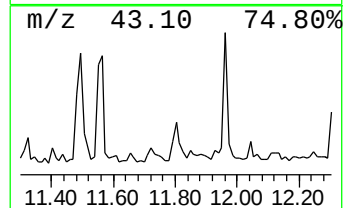
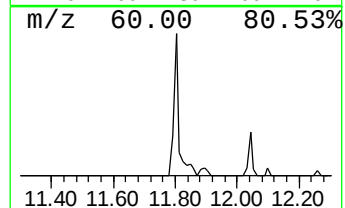
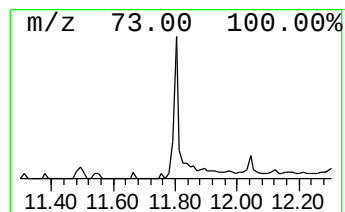
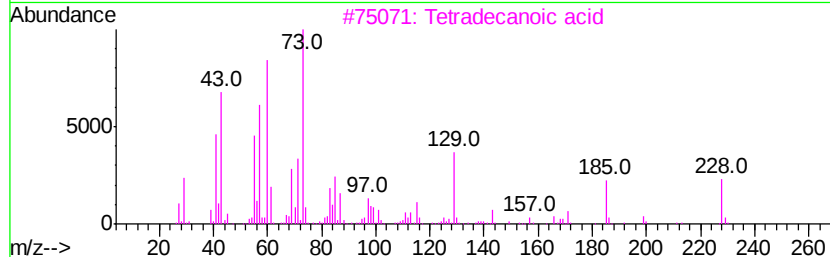
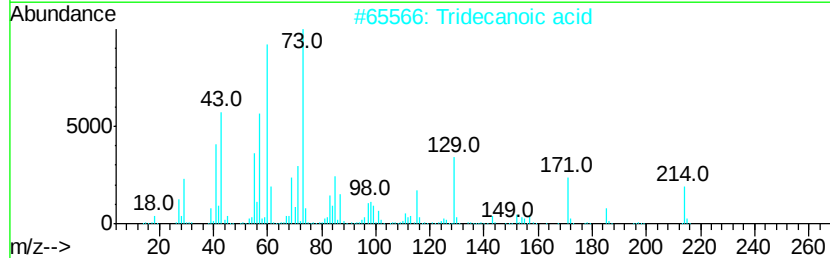
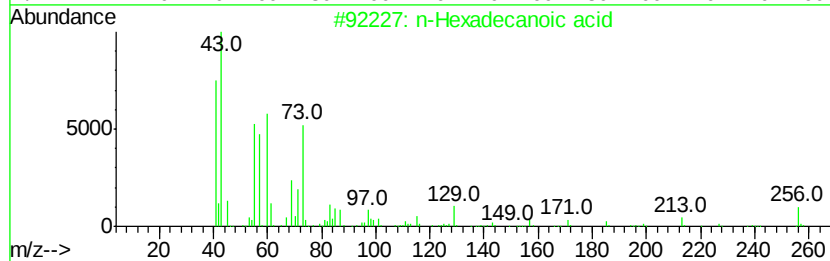
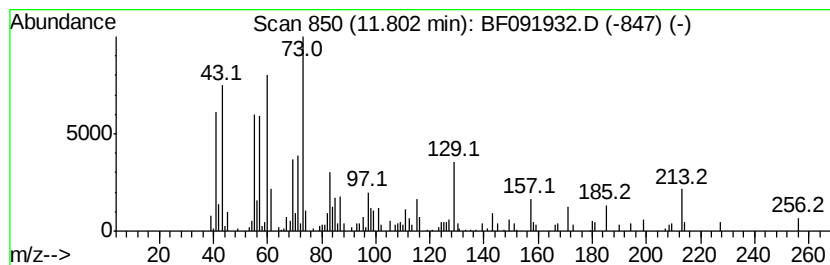
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.41 ng	209510	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	50



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PIT-003-COMP

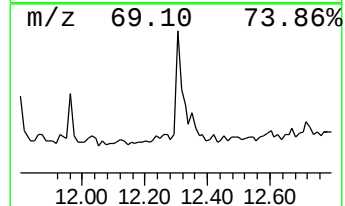
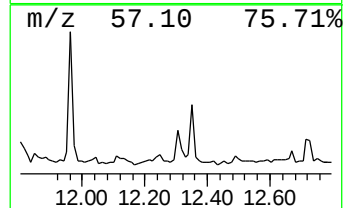
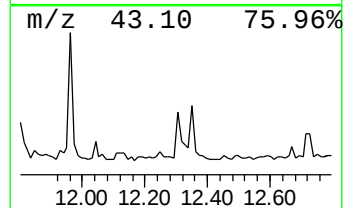
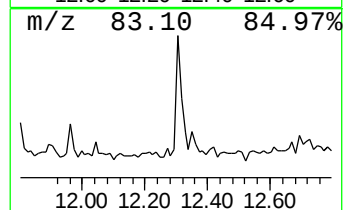
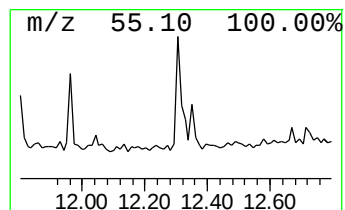
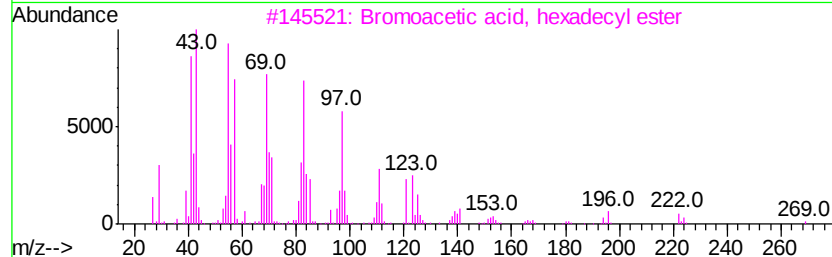
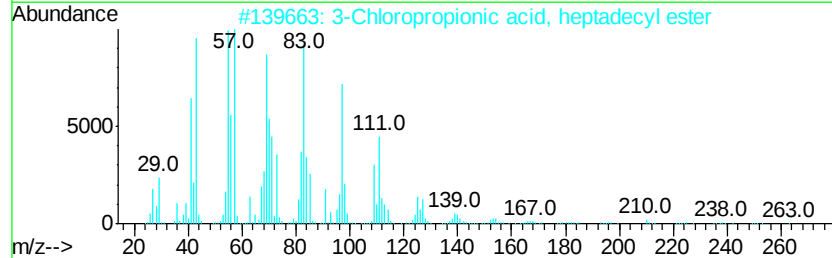
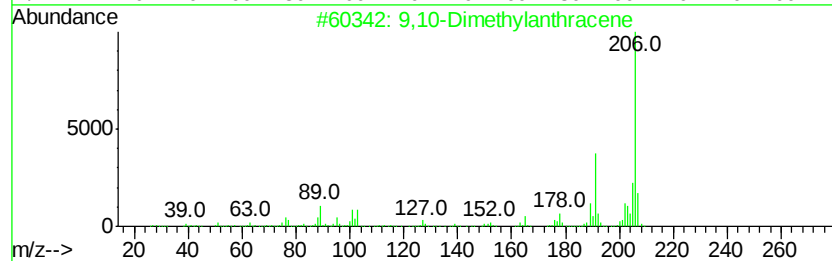
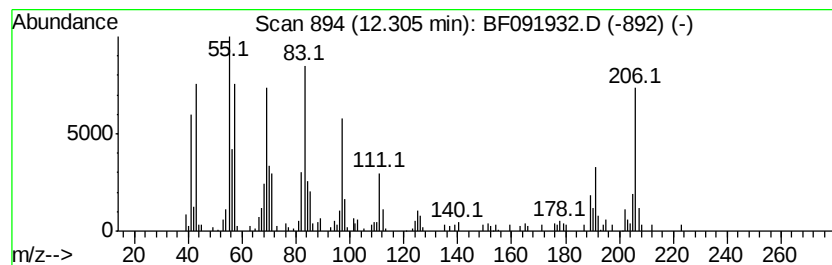
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9,10-Dimethylantracene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.24 ng	195186	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylantracene	206	C16H14	000781-43-1	90	
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	70	
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	70	
4	1-Pentadecanol	228	C15H32O	000629-76-5	64	
5	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	56	



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BNA_F
ClientSampleId :
PIT-003-COMP

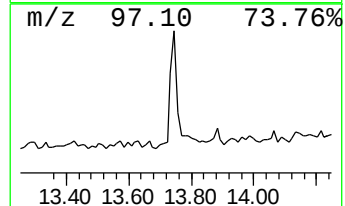
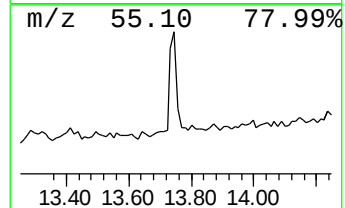
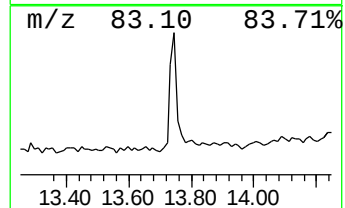
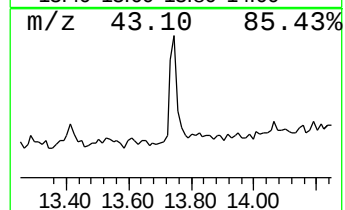
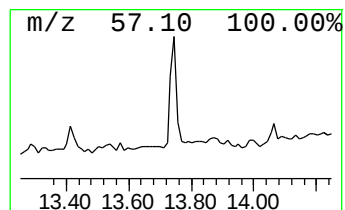
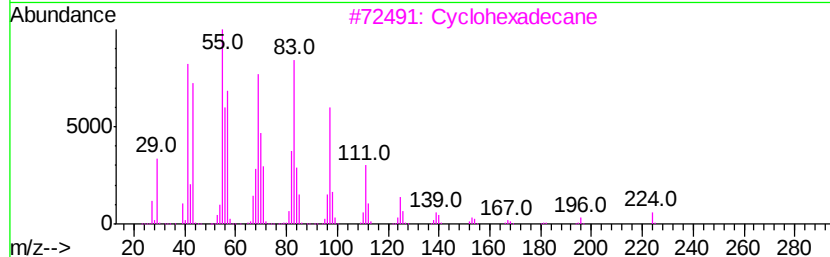
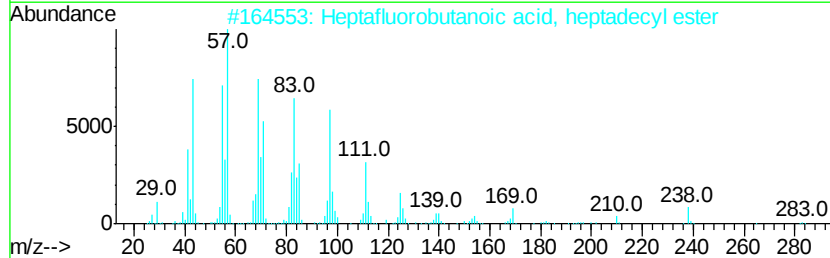
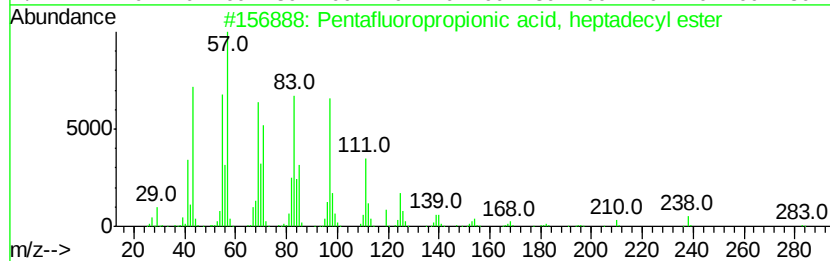
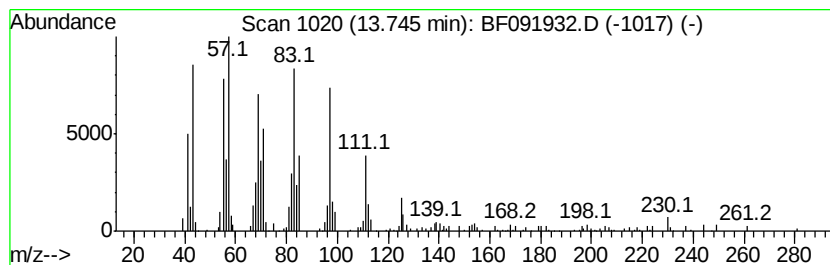
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.13 ng	212992	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	94
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3		Cyclohexadecane	224	C16H32	000295-65-8	91
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.91	33.2	ng	2452050	1	6.74	1479130	20.0
unknown6.52	6.52	95.6	ng	7069100	1	6.74	1479130	20.0
Tetracosane	10.68	2.6	ng	230558	4	11.25	1741160	20.0
2-Tetradecene, (E)-	11.49	4.2	ng	363785	4	11.25	1741160	20.0
Tridecane	11.56	2.2	ng	190111	4	11.25	1741160	20.0
n-Hexadecanoic acid	11.80	2.4	ng	209510	4	11.25	1741160	20.0
9,10-Dimethylanthe...	12.30	2.2	ng	195186	4	11.25	1741160	20.0
Pentafluoropropio...	13.75	3.1	ng	212992	5	13.88	1362630	20.0