

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
 Data File : BF084817.D
 Acq On : 4 Feb 2016 6:28
 Operator : SJ/IZ
 Sample : H1322-01
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B016(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-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	4.144	178	180	185	rBV	42787	67384	1.41%	0.151%
2	4.841	238	241	250	rBV	1089058	1696420	35.59%	3.790%
3	5.287	277	280	282	rBV	4271350	4766160	100.00%	10.648%
4	5.687	313	315	319	rVB	62689	57576	1.21%	0.129%
5	6.339	369	372	374	rBV	4273415	4705078	98.72%	10.512%
6	6.453	379	382	385	rVV	4517010	4233100	88.82%	9.457%
7	6.681	400	402	405	rBV	1321405	1119719	23.49%	2.502%
8	6.841	413	416	418	rBV	3771164	3425468	71.87%	7.653%
9	7.253	449	452	455	rBV	2646376	2707189	56.80%	6.048%
10	7.973	512	515	517	rBV	1672590	1606687	33.71%	3.590%
11	9.047	606	609	612	rBV	3055024	4560794	95.69%	10.190%
12	9.447	642	644	646	rBV	695622	679627	14.26%	1.518%
13	9.665	661	663	665	rBV	97346	105889	2.22%	0.237%
14	9.722	665	668	671	rVB	1874782	1710657	35.89%	3.822%
15	10.168	705	707	709	rVB	209376	166594	3.50%	0.372%
16	10.385	723	726	729	rBV	60708	98009	2.06%	0.219%
17	10.510	734	737	739	rVV	3254336	3100936	65.06%	6.928%
18	10.636	746	748	753	rVB	210200	240699	5.05%	0.538%
19	11.082	785	787	789	rBV	106139	100571	2.11%	0.225%
20	11.196	795	797	800	rVB	1267752	1544595	32.41%	3.451%
21	12.408	901	903	905	rBV	73953	64459	1.35%	0.144%
22	12.625	920	922	925	rBV2	97889	125249	2.63%	0.280%
23	12.693	925	928	930	rBV2	28066	50159	1.05%	0.112%
24	12.785	934	936	939	rVB	3301319	3586720	75.25%	8.013%
25	13.036	955	958	959	rBV	33916	51398	1.08%	0.115%
26	13.368	985	987	992	rVB	80583	111813	2.35%	0.250%
27	13.699	1014	1016	1025	rBV	319104	476926	10.01%	1.066%
28	13.825	1025	1027	1030	rBV	1168767	1275183	26.75%	2.849%
29	14.019	1042	1044	1046	rBV	159988	166773	3.50%	0.373%
30	14.317	1068	1070	1073	rBV	142154	163776	3.44%	0.366%
31	14.614	1092	1096	1100	rBV2	169799	268122	5.63%	0.599%
32	14.682	1100	1102	1104	rVB	151499	170608	3.58%	0.381%
33	14.911	1120	1122	1133	rVB	130525	204199	4.28%	0.456%
34	15.208	1145	1148	1150	rBV	715182	910602	19.11%	2.034%

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ClientSampleId :
S4-B016(10-12)

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-BF020116.M
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35	15.254	1150	1152	1157	rVB	81079	122397	2.57%	0.273%
36	15.631	1182	1185	1188	rBV	71362	92943	1.95%	0.208%
37	16.065	1219	1223	1231	rVB2	51210	107177	2.25%	0.239%
38	16.580	1265	1268	1272	rBV3	30040	61294	1.29%	0.137%
39	17.185	1317	1321	1328	rVB2	20495	56754	1.19%	0.127%

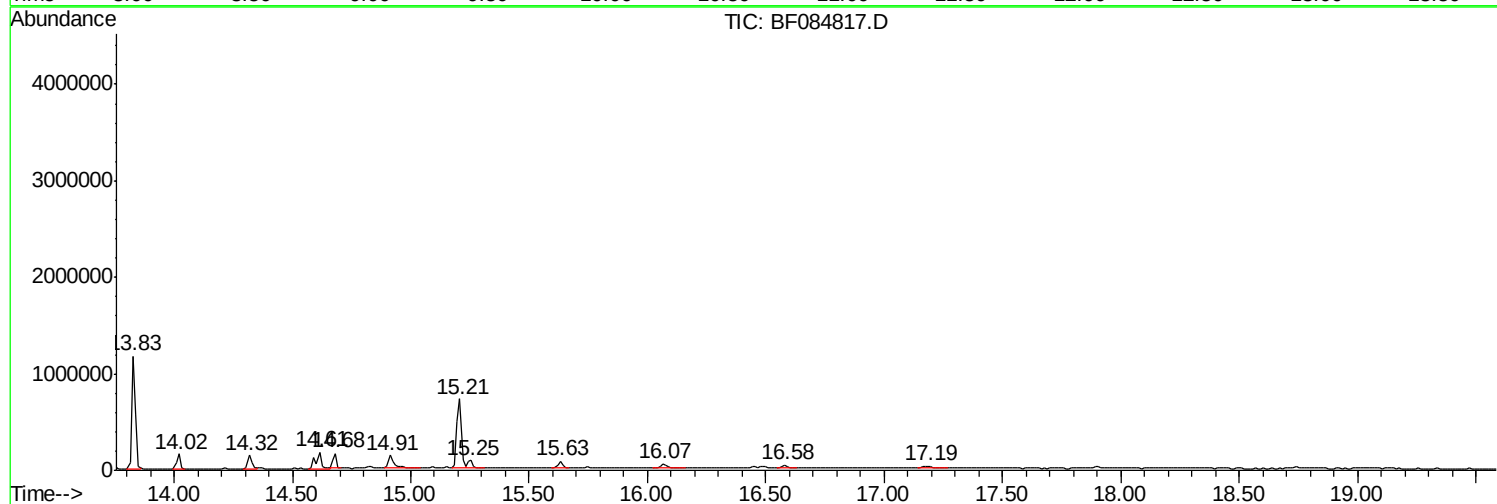
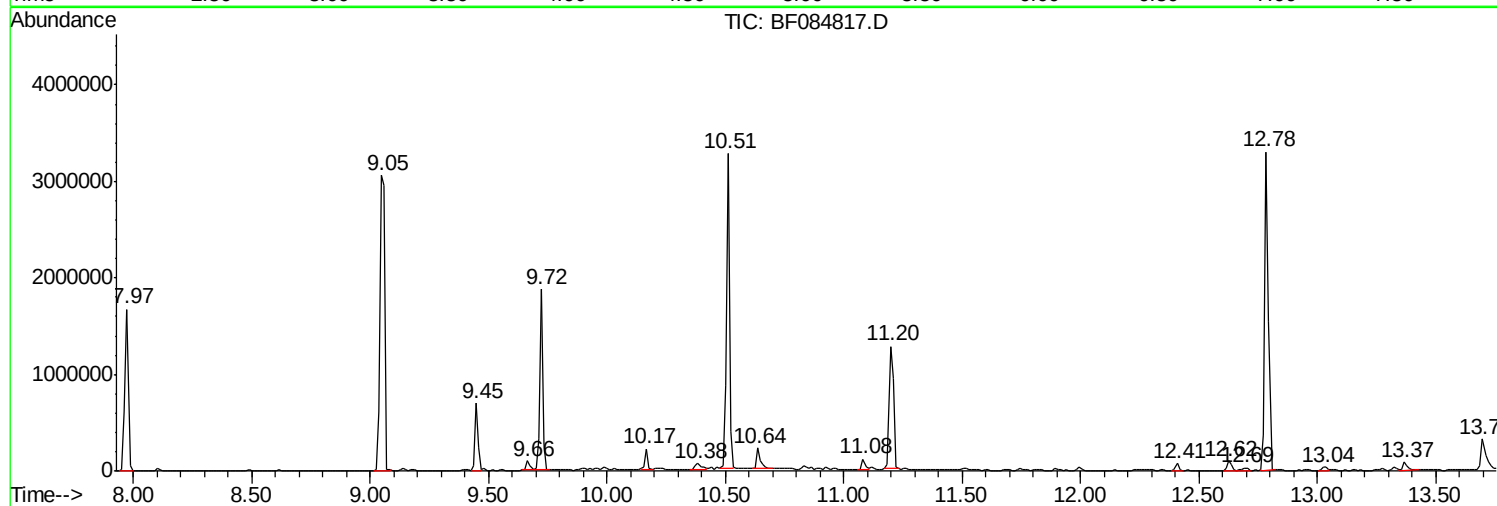
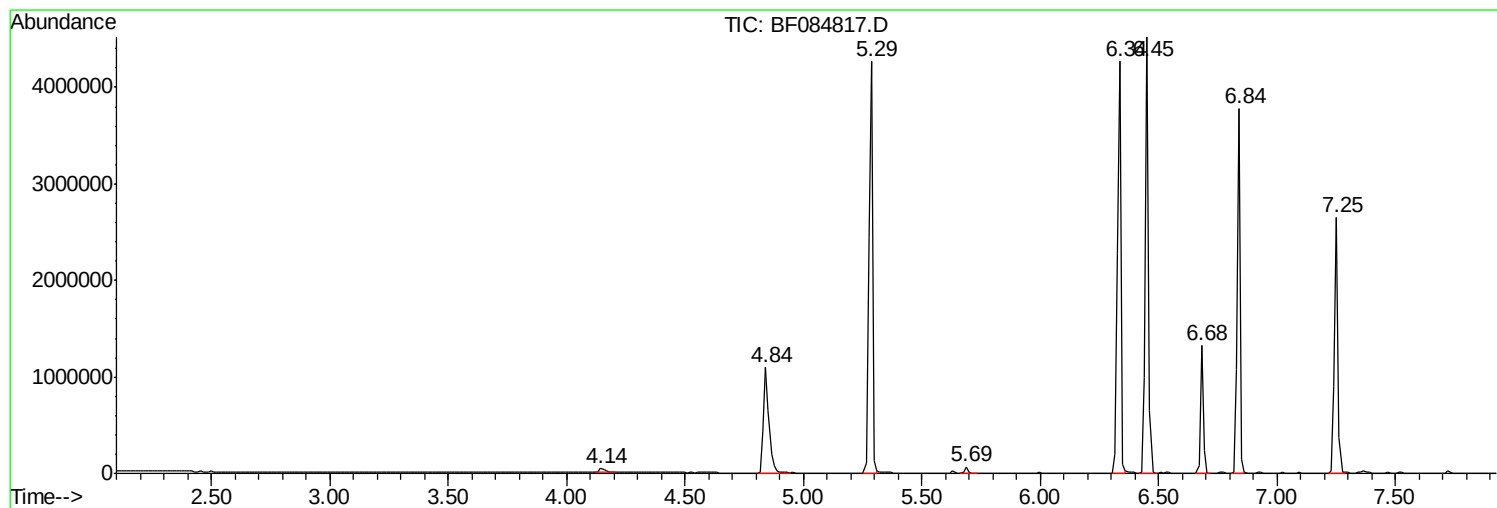
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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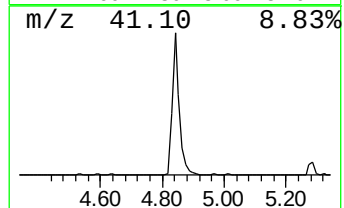
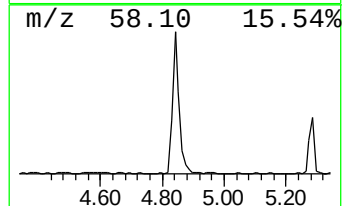
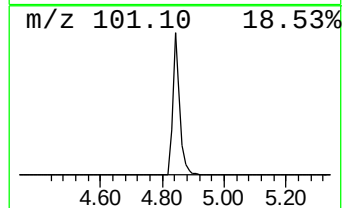
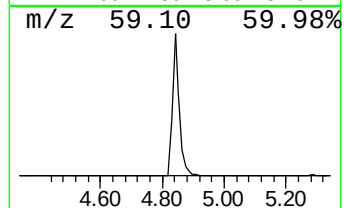
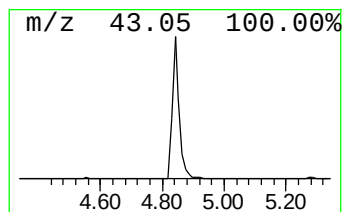
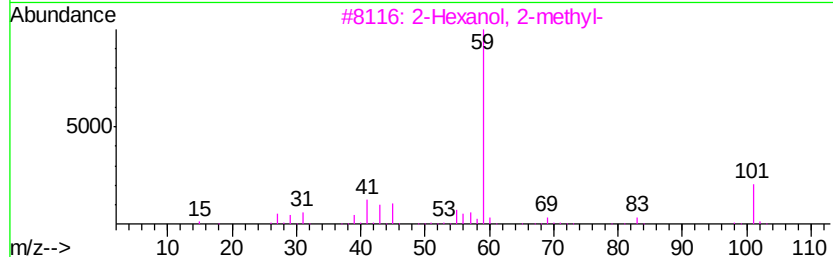
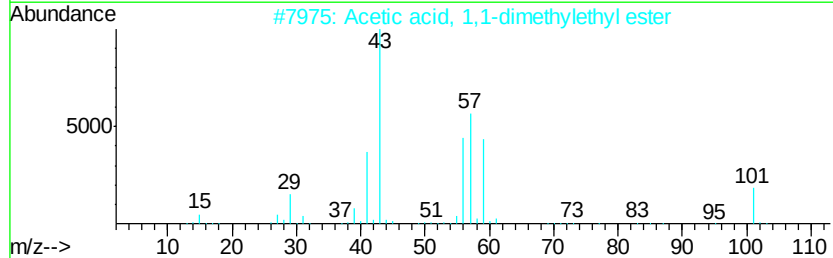
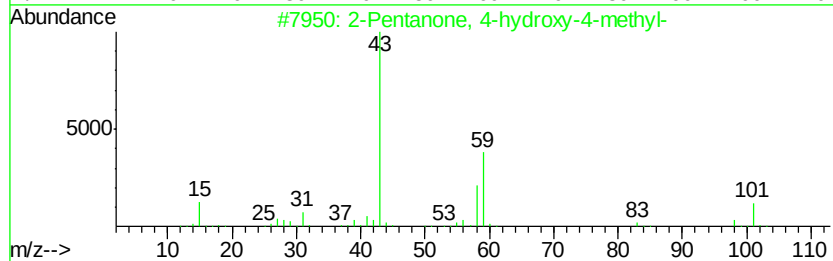
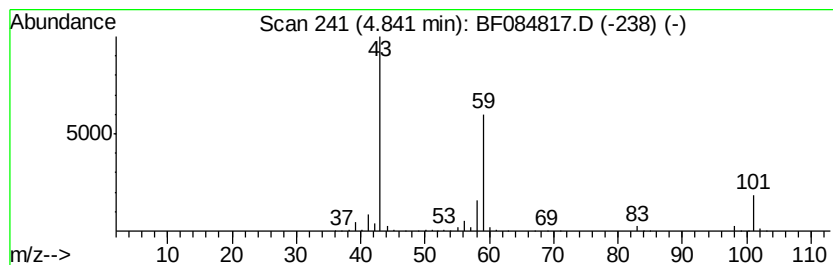
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.84	30.30 ng	1696420	1,4-Dichlorobenzene-d4	6.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33



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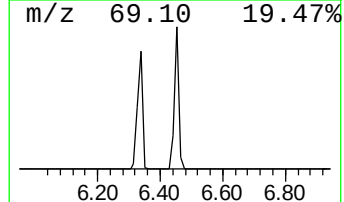
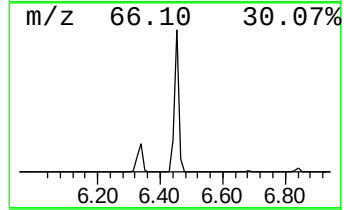
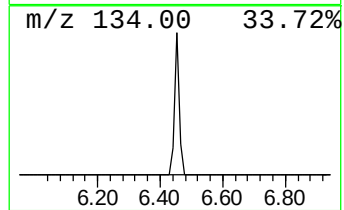
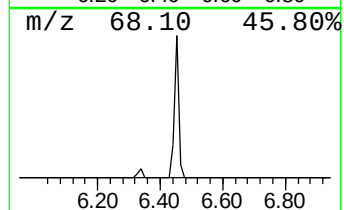
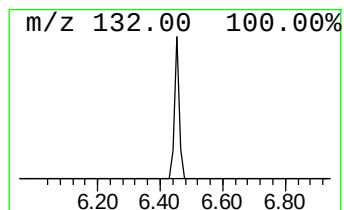
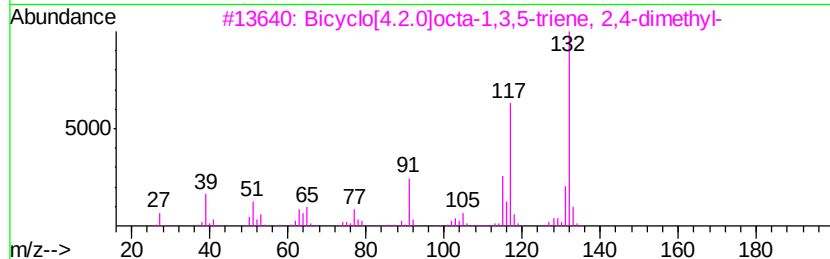
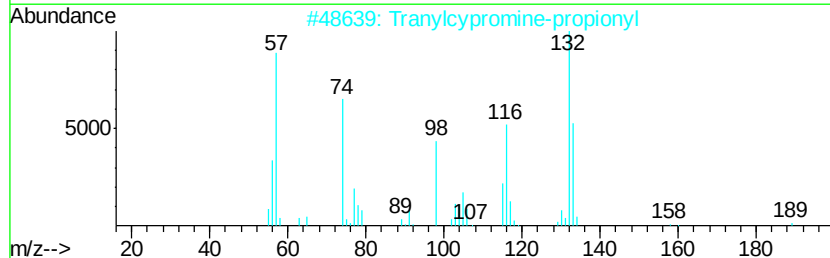
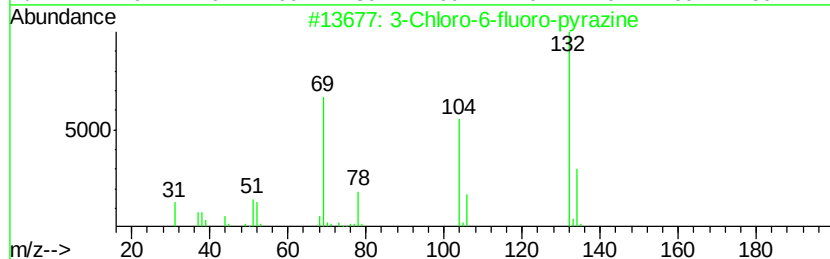
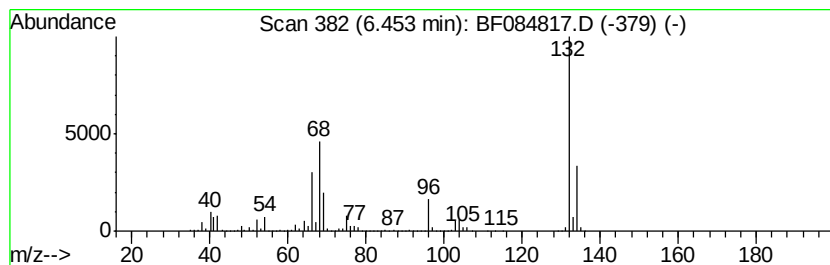
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	75.61 ng	4233100	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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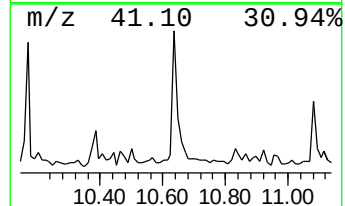
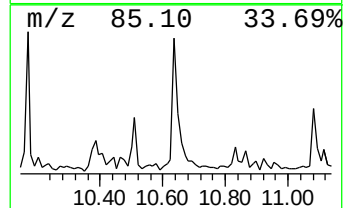
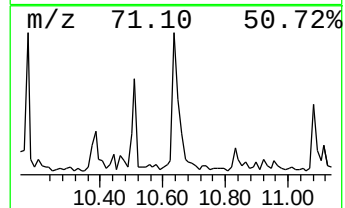
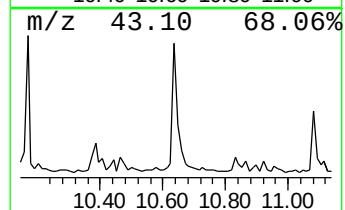
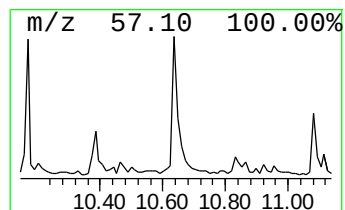
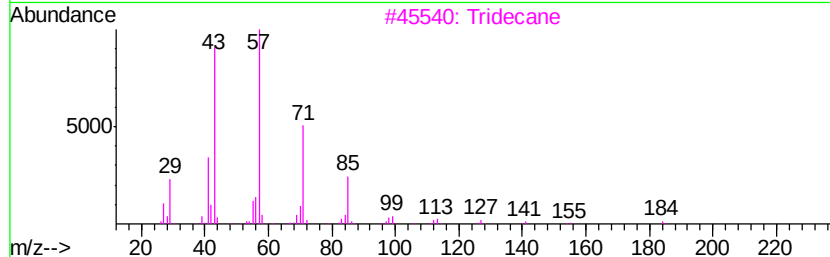
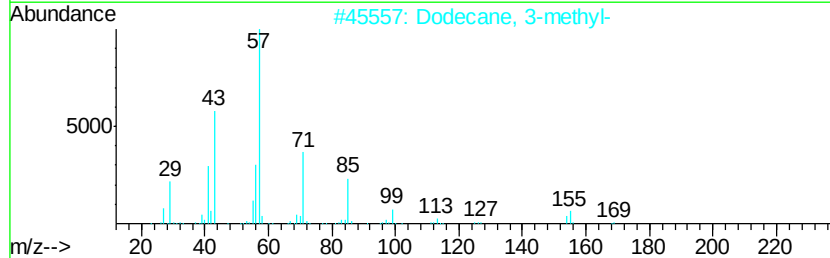
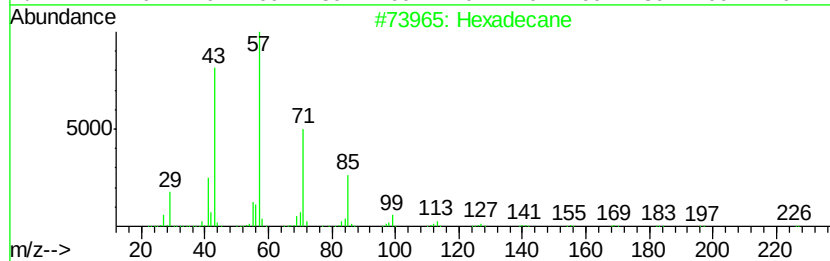
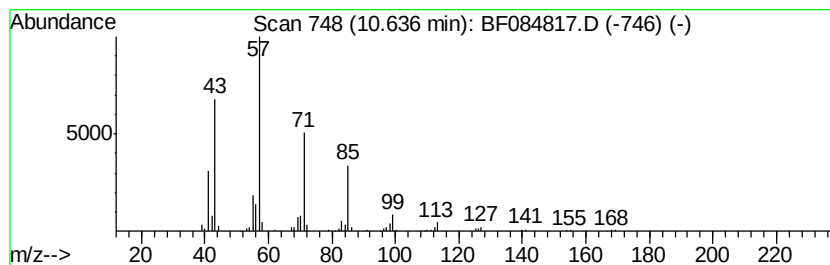
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.64	3.12 ng	240699	Phenanthrene-d10	11.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
3	Tridecane	184	C13H28	000629-50-5	64
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



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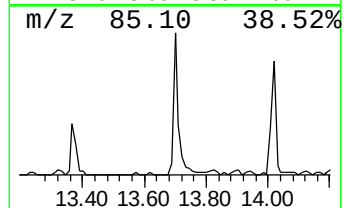
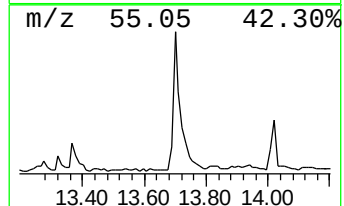
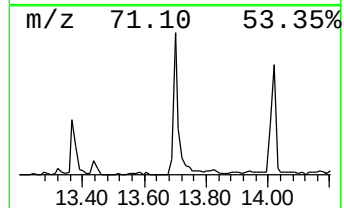
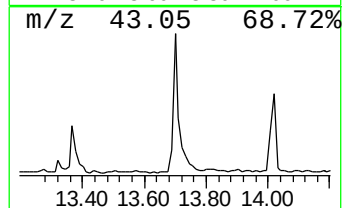
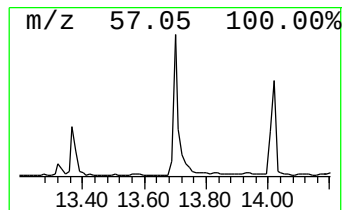
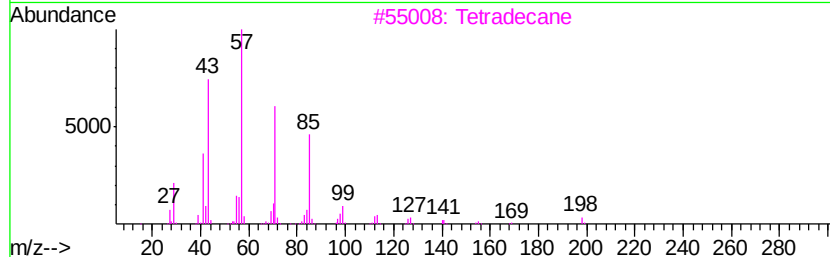
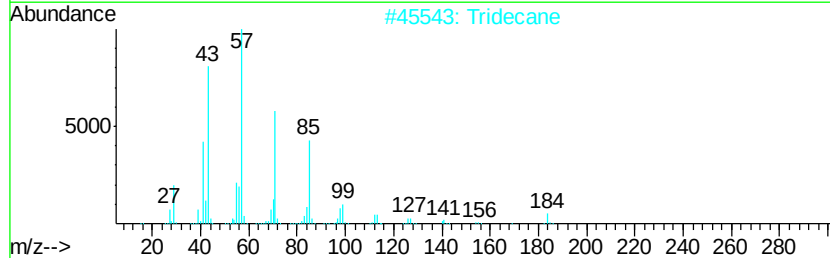
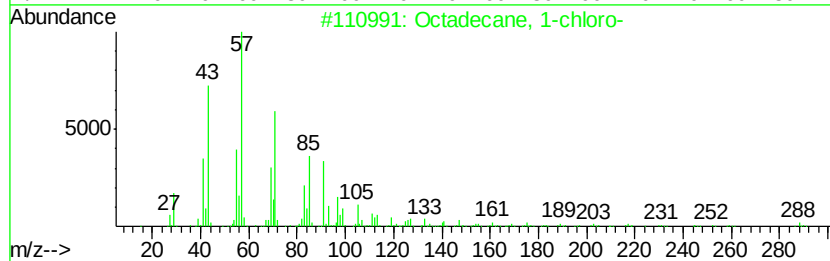
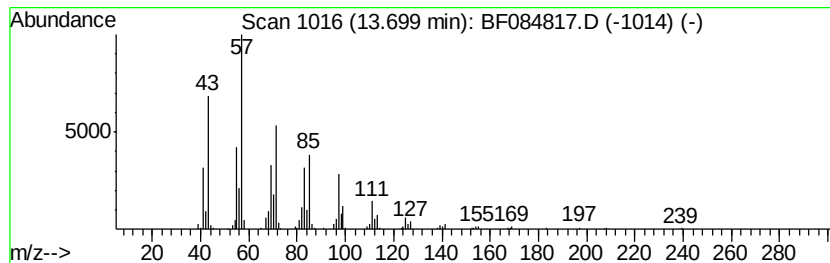
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.70	7.48 ng	476926	Chrysene-d12	13.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
2	Tridecane	184	C13H28	000629-50-5	64
3	Tetradecane	198	C14H30	000629-59-4	62
4	Dodecane	170	C12H26	000112-40-3	58
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	58



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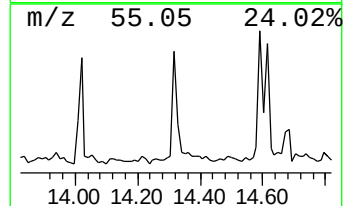
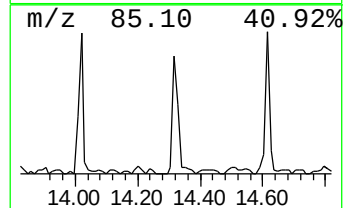
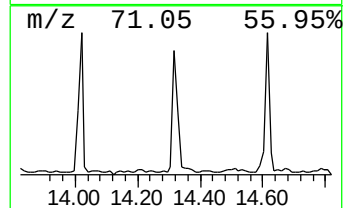
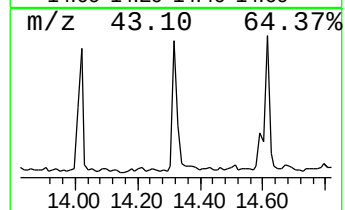
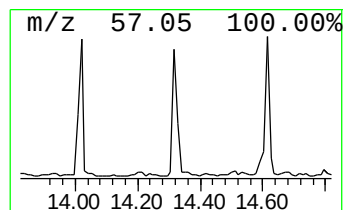
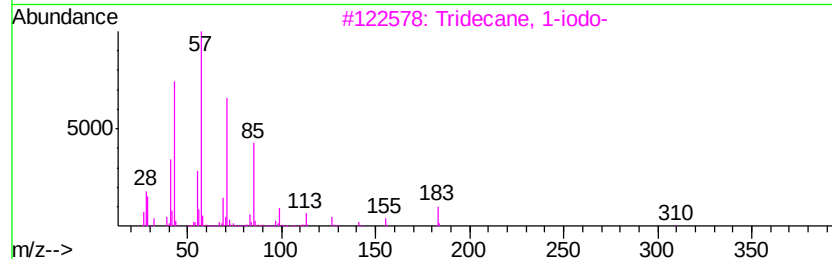
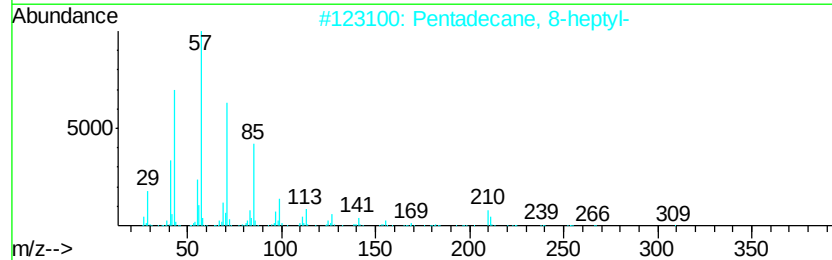
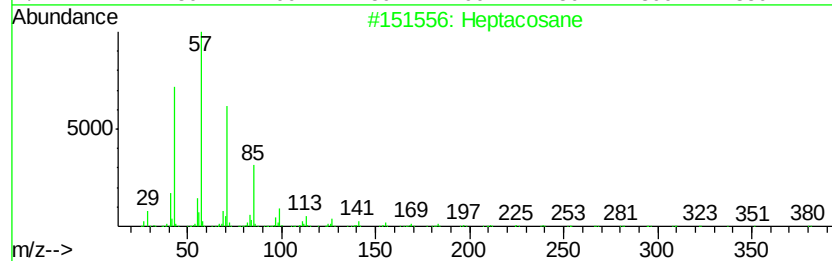
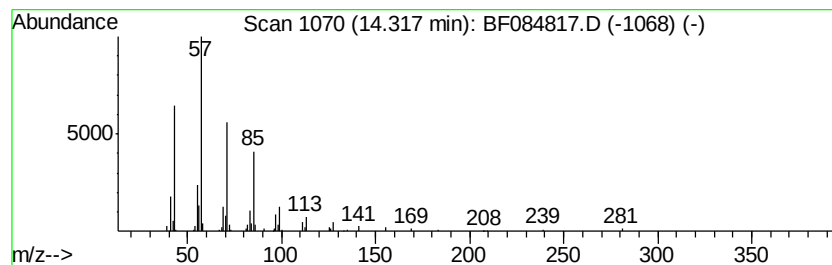
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Peak Number 7 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.57 ng	163776	Chrysene-d12	13.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	90
3	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	87
4	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	86
5	Eicosane, 10-methyl-	296 C21H44	054833-23-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084817.D
Acq On : 4 Feb 2016 6:28
Operator : SJ/IZ
Sample : H1322-01
Misc :
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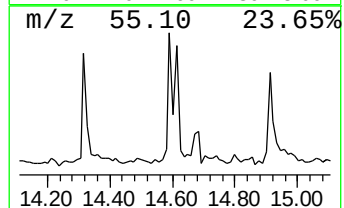
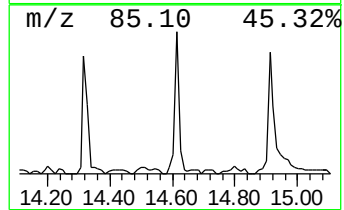
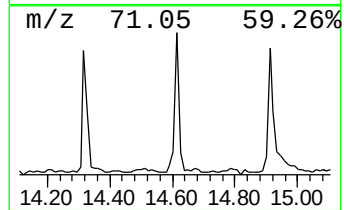
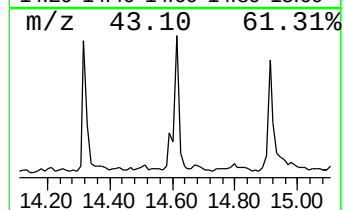
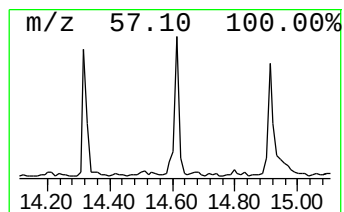
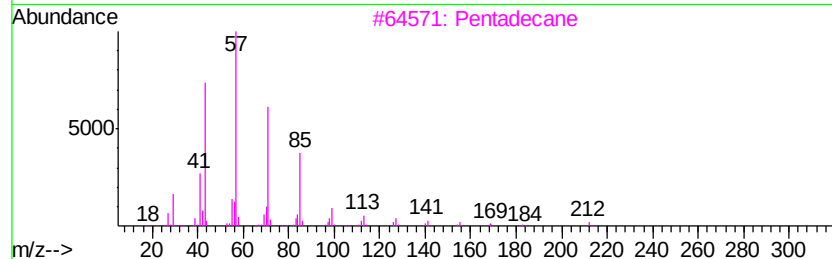
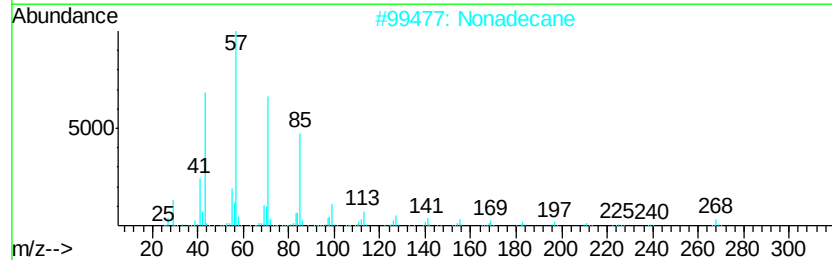
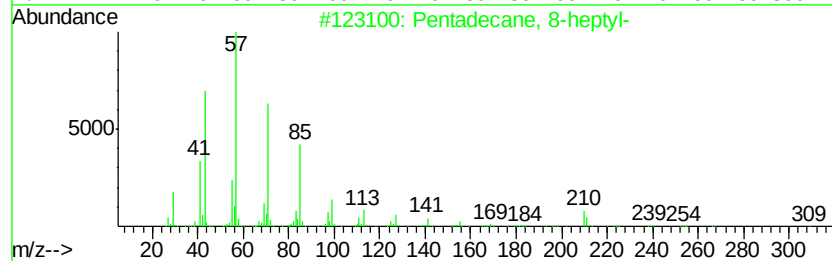
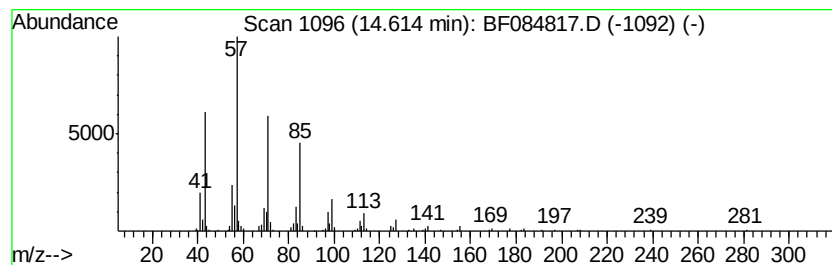
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ClientSampleId :
S4-B016(10-12)

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 8 Pentadecane, 8-heptyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.61	5.89 ng	268122	Perylene-d12		15.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Nonadecane	268	C19H40	000629-92-5	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Octacosane	394	C28H58	000630-02-4	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084817.D
Acq On : 4 Feb 2016 6:28
Operator : SJ/IZ
Sample : H1322-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B016(10-12)

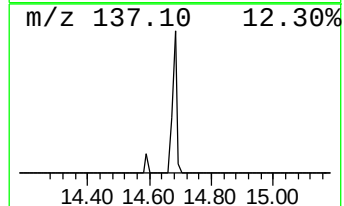
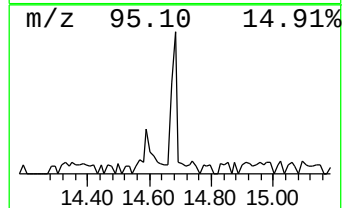
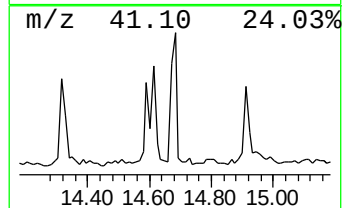
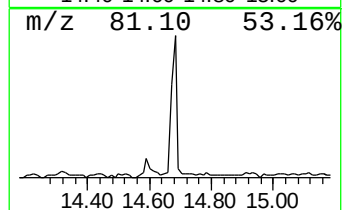
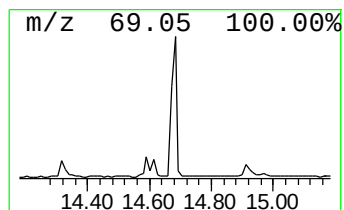
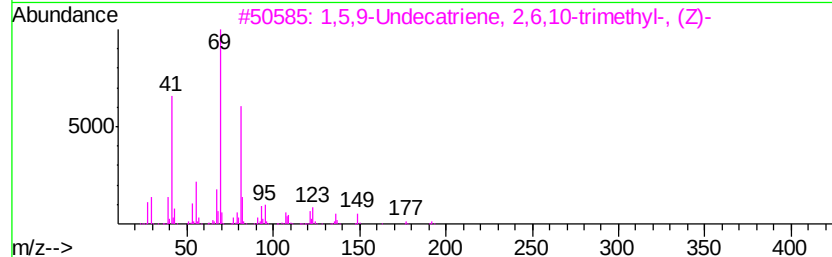
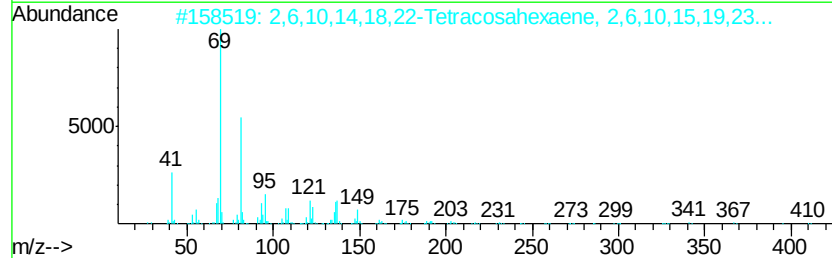
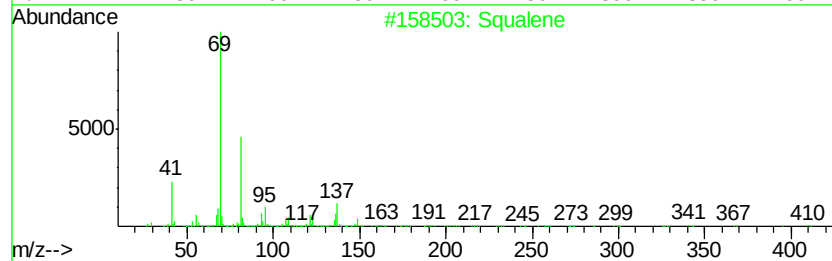
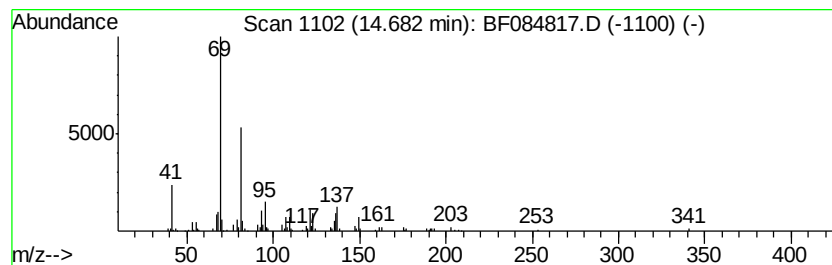
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	3.75 ng	170608	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	64
5		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084817.D
Acq On : 4 Feb 2016 6:28
Operator : SJ/IZ
Sample : H1322-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B016(10-12)

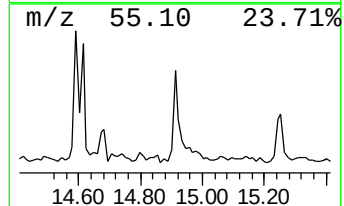
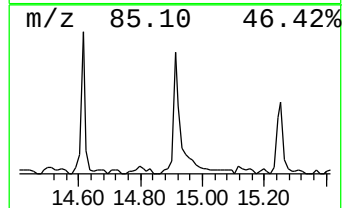
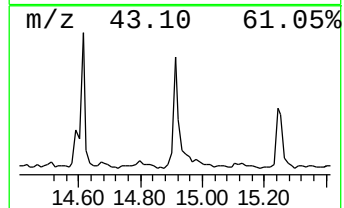
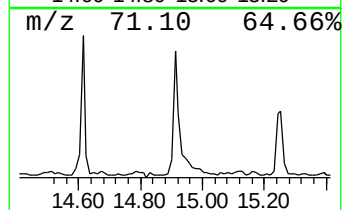
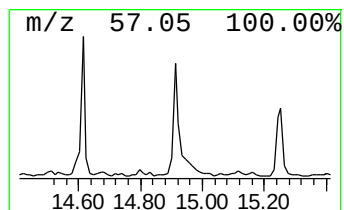
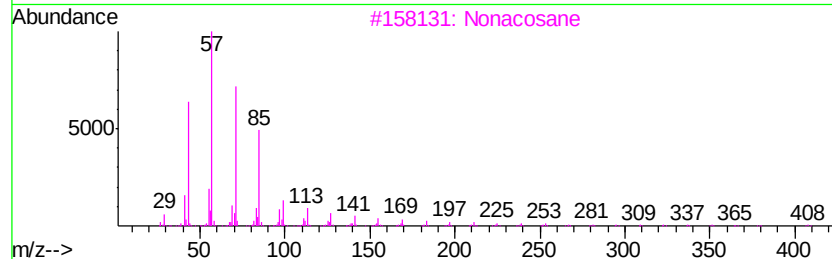
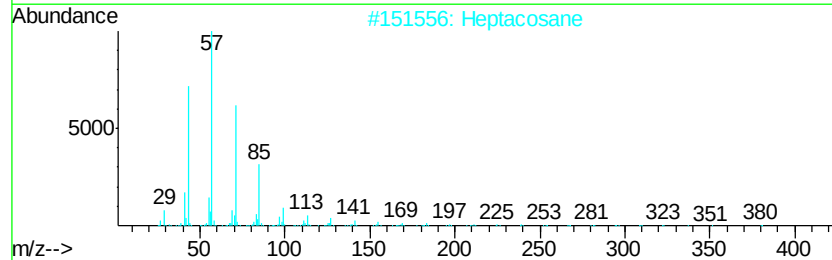
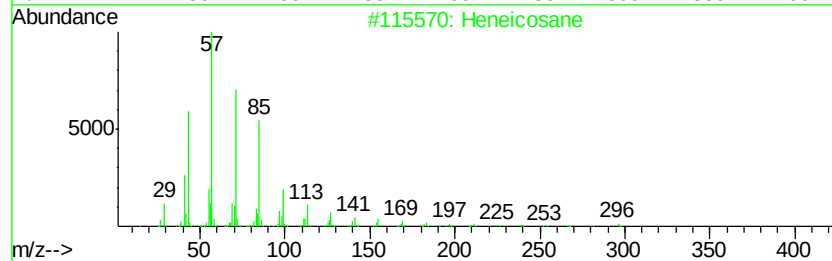
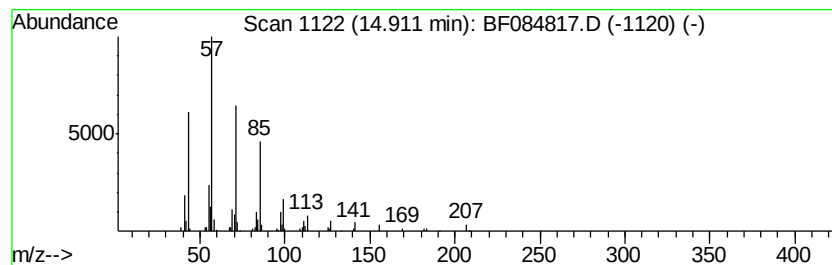
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	4.48 ng	204199	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Nonacosane	408	C29H60	000630-03-5	90
4		Pentadecane	212	C15H32	000629-62-9	87
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
Data File : BF084817.D
Acq On : 4 Feb 2016 6:28
Operator : SJ/IZ
Sample : H1322-01
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B016(10-12)

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...	4.84	30.3	ng	1696420	1	6.68	1119720	20.0
unknown6.45	6.45	75.6	ng	4233100	1	6.68	1119720	20.0
Hexadecane	10.64	3.1	ng	240699	4	11.20	1544600	20.0
Octadecane, 1-chl...	13.70	7.5	ng	476926	5	13.82	1275180	20.0
Heptacosane	14.32	2.6	ng	163776	5	13.82	1275180	20.0
Pentadecane, 8-he...	14.61	5.9	ng	268122	6	15.21	910602	20.0
Squalene	14.68	3.8	ng	170608	6	15.21	910602	20.0
Heneicosane	14.91	4.5	ng	204199	6	15.21	910602	20.0