

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
 Data File : BF085496.D
 Acq On : 17 Mar 2016 7:36
 Operator : UM/SJ
 Sample : H1790-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-8A-(0-10)

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-BF031516.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	5.110	244	247	254	rVB	62980	92032	1.93%	0.261%
2	5.499	278	281	284	rBV	2588454	3867578	80.96%	10.982%
3	6.539	369	372	374	rBV	3165357	4111736	86.07%	11.676%
4	6.676	381	384	386	rBV	2772249	4009799	83.93%	11.386%
5	6.904	402	404	406	rBV	360354	433751	9.08%	1.232%
6	7.053	415	417	420	rBV	2358878	3168193	66.32%	8.996%
7	7.464	450	453	455	rBV	2247762	2396713	50.17%	6.806%
8	7.556	458	461	464	rVV	88678	107290	2.25%	0.305%
9	8.185	514	516	518	rBV	712734	591628	12.38%	1.680%
10	9.270	608	611	613	rBV	3836141	4777390	100.00%	13.566%
11	9.659	643	645	646	rBV	708605	715463	14.98%	2.032%
12	9.876	661	664	666	rVB	89361	100547	2.10%	0.286%
13	9.945	667	670	672	rVB	517024	560135	11.72%	1.591%
14	10.368	706	707	709	rVB	150927	142445	2.98%	0.404%
15	10.585	724	726	730	rBV	68493	122455	2.56%	0.348%
16	10.733	736	739	741	rBV	2391541	2564205	53.67%	7.281%
17	10.779	741	743	745	rVV	59373	77227	1.62%	0.219%
18	10.848	747	749	753	rBV	134751	210893	4.41%	0.599%
19	11.042	763	766	770	rBV4	22910	63842	1.34%	0.181%
20	11.293	785	788	789	rBV	102158	97889	2.05%	0.278%
21	11.419	797	799	803	rBV	457669	562485	11.77%	1.597%
22	11.499	803	806	808	rVB	35211	56099	1.17%	0.159%
23	11.945	844	845	848	rBV2	145456	204528	4.28%	0.581%
24	12.036	851	853	857	rVB	32186	53424	1.12%	0.152%
25	12.631	903	905	908	rBV	129870	135463	2.84%	0.385%
26	12.734	912	914	916	rVV	62550	65516	1.37%	0.186%
27	12.825	920	922	924	rVV	115794	132566	2.77%	0.376%
28	12.859	924	925	928	rVB	121051	118202	2.47%	0.336%
29	13.008	935	938	941	rBV	3071095	2939102	61.52%	8.346%
30	13.488	977	980	985	rBV2	227669	516704	10.82%	1.467%
31	13.899	1014	1016	1022	rBV2	222026	265528	5.56%	0.754%
32	14.059	1026	1030	1035	rBV2	417338	626890	13.12%	1.780%
33	14.185	1037	1041	1043	rBV3	40207	86575	1.81%	0.246%
34	14.528	1069	1071	1073	rBV2	27851	48803	1.02%	0.139%

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Integration Parameters: rteint.p
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Stop Thrs : 0 Peak Location: TOP

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35	15.088	1117	1120	1124	rBV	135276	260273	5.45%	0.739%
36	15.385	1143	1146	1149	rVB	76347	114786	2.40%	0.326%
37	15.442	1149	1151	1154	rBV	66290	92046	1.93%	0.261%
38	15.500	1154	1156	1158	rBV	274414	404700	8.47%	1.149%
39	16.014	1198	1201	1209	rVB3	38582	92077	1.93%	0.261%
40	16.620	1250	1254	1259	rVB6	28480	78307	1.64%	0.222%
41	16.928	1278	1281	1284	rBV2	34848	80868	1.69%	0.230%
42	17.363	1316	1319	1324	rVB	27688	70507	1.48%	0.200%

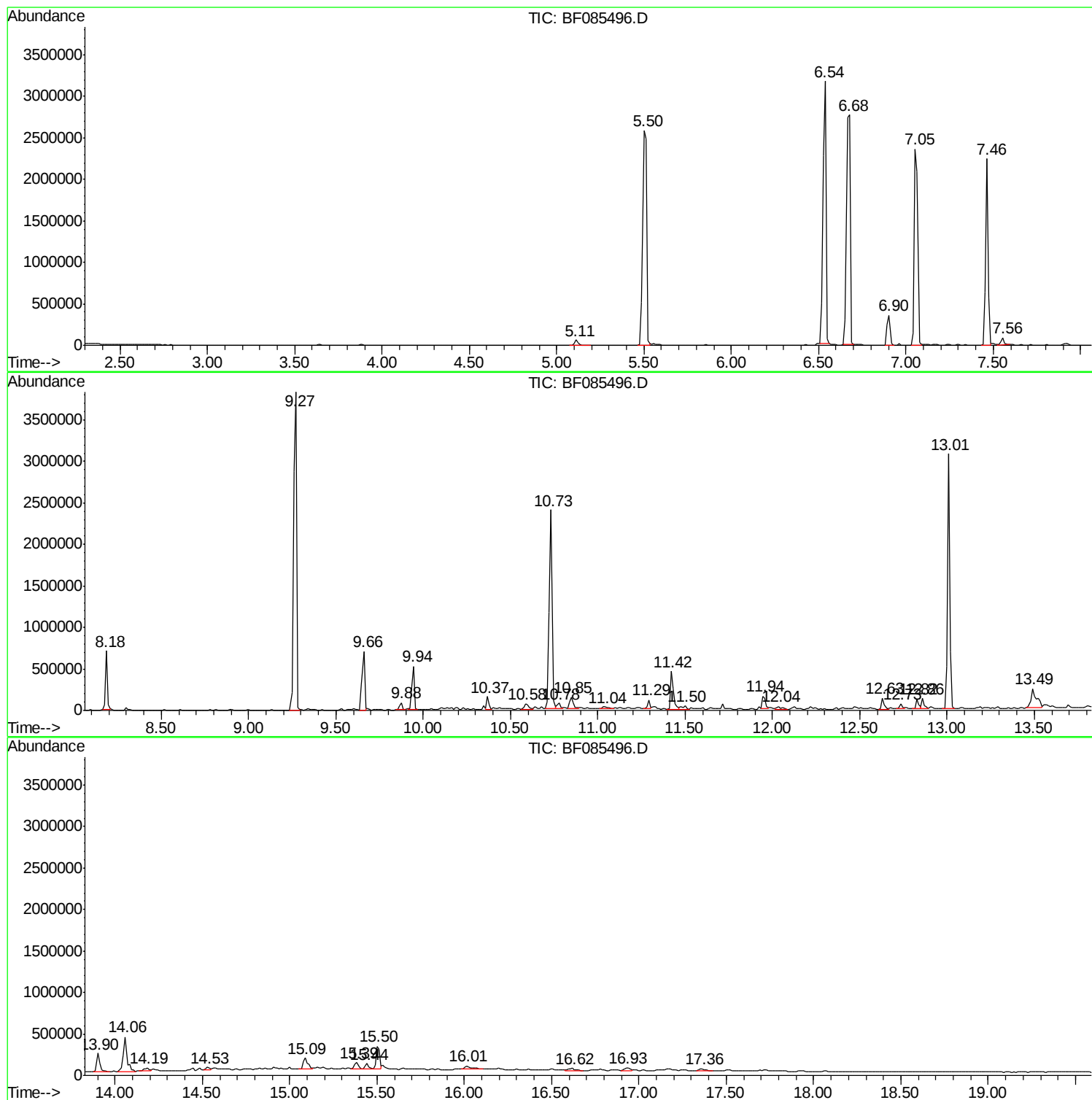
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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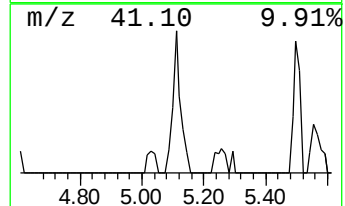
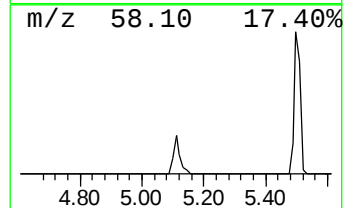
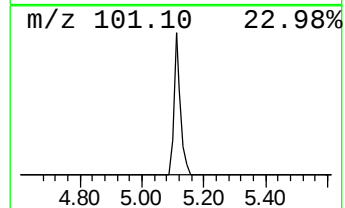
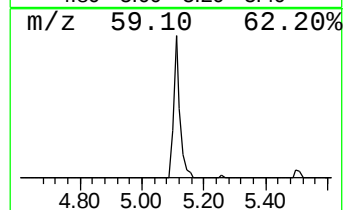
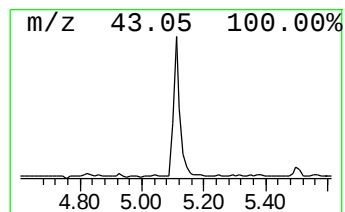
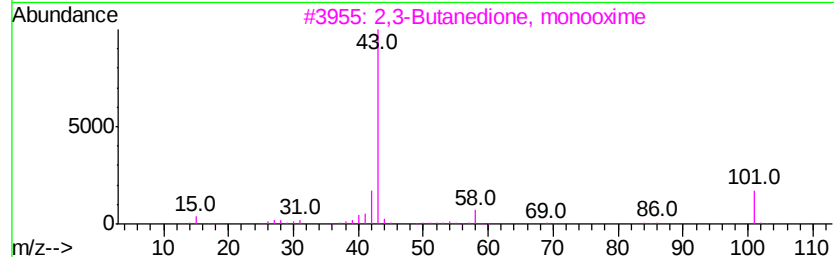
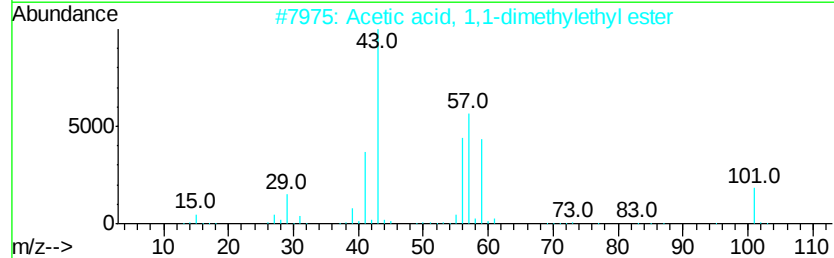
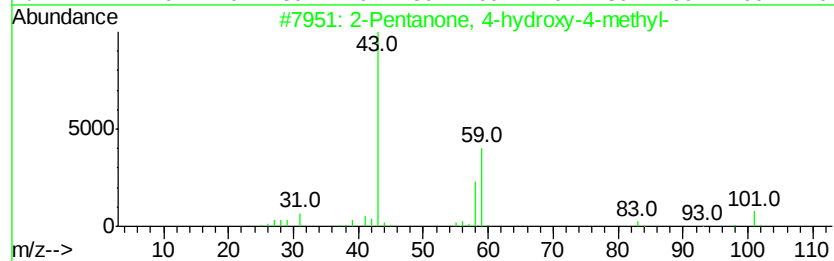
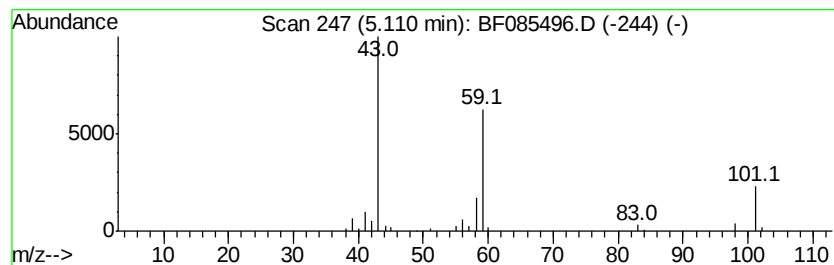
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.24 ng	92032	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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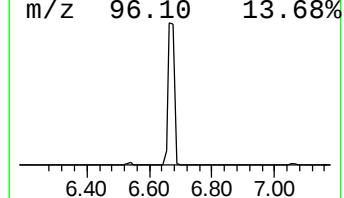
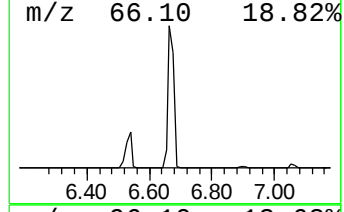
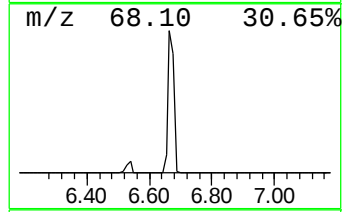
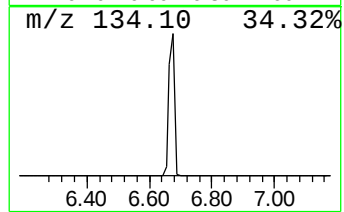
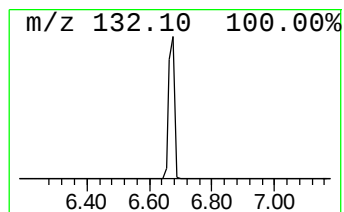
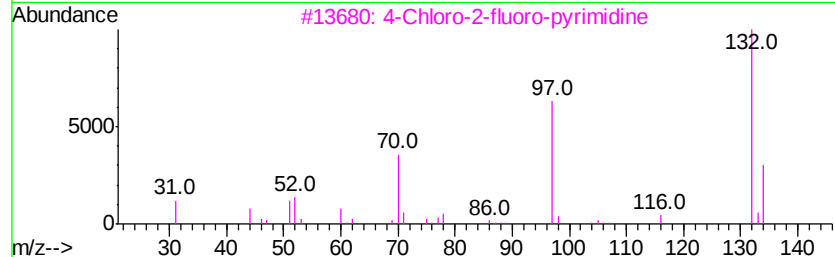
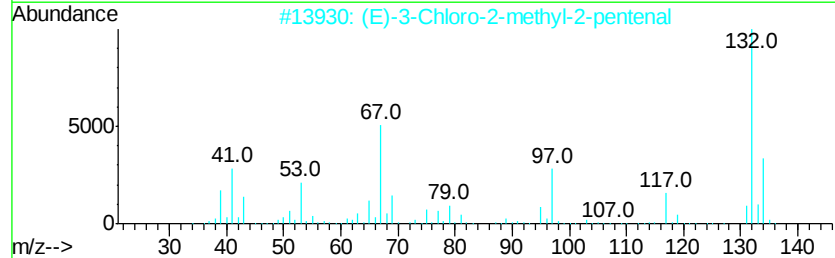
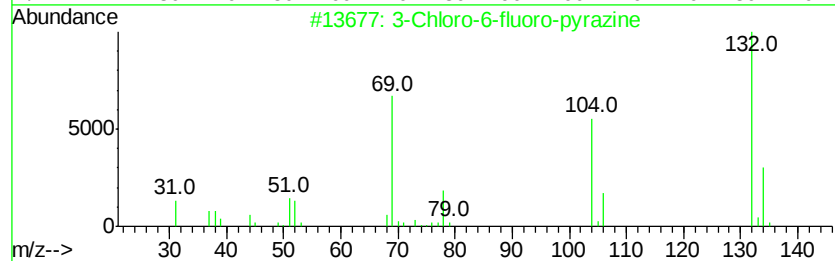
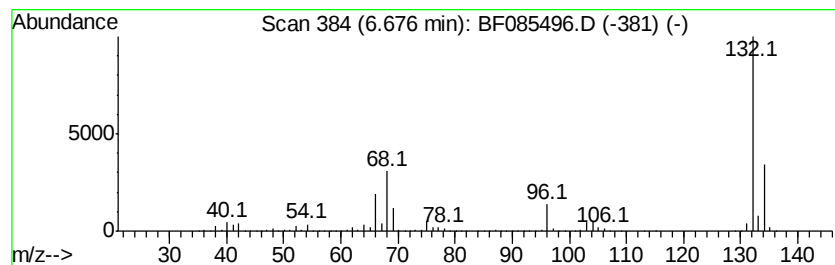
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Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	184.89 ng	4009800	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	50
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	28
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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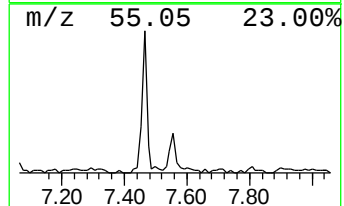
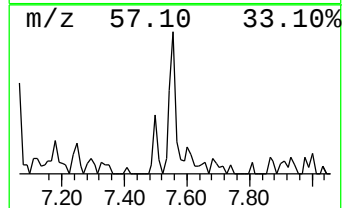
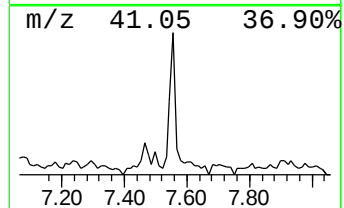
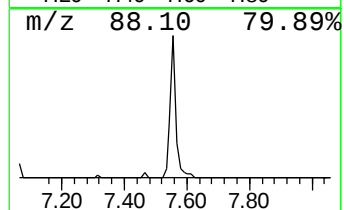
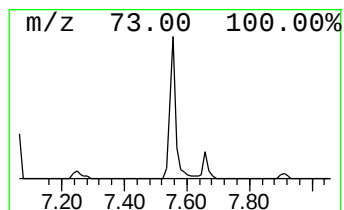
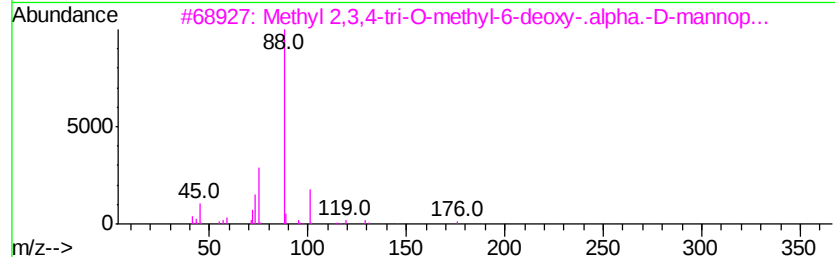
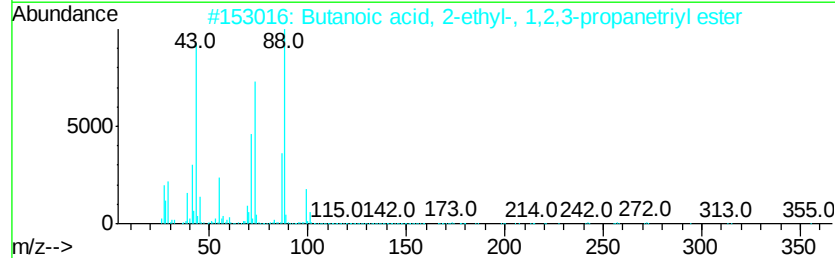
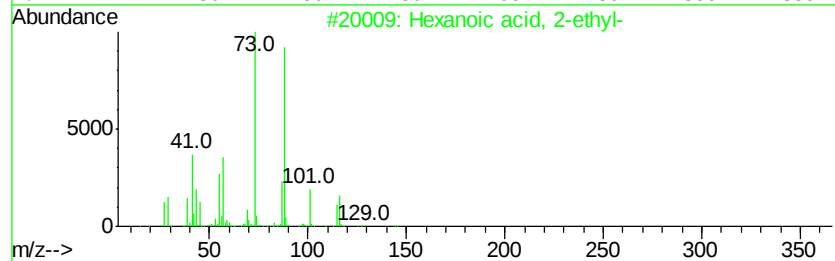
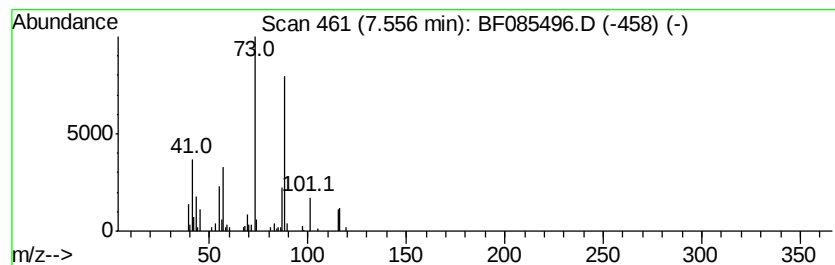
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	3.63 ng	107290	Naphthalene-d8	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
3		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	42
4		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	38
5		1,4-Dioxane	88	C4H8O2	000123-91-1	37



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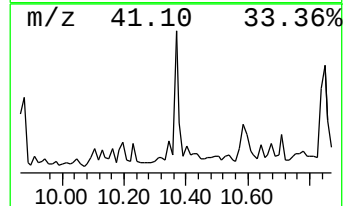
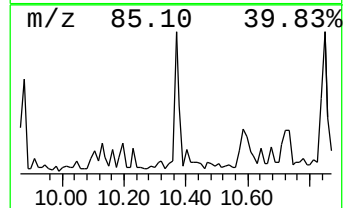
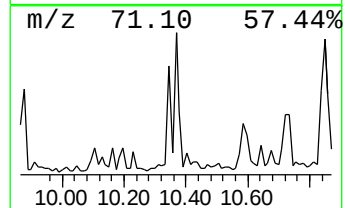
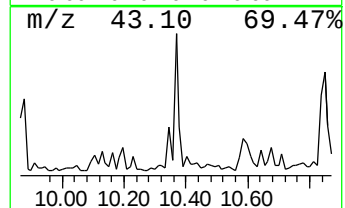
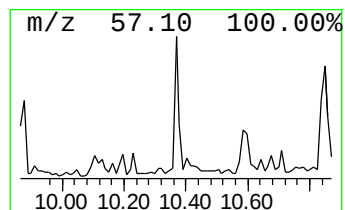
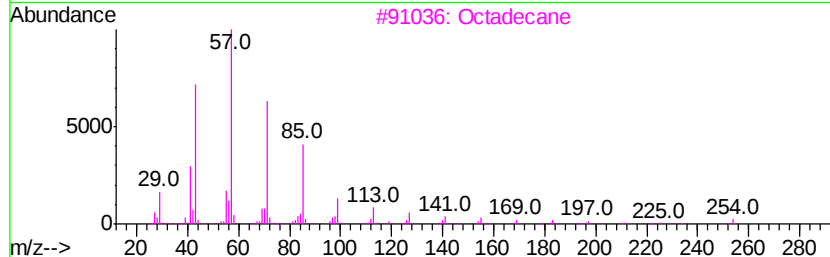
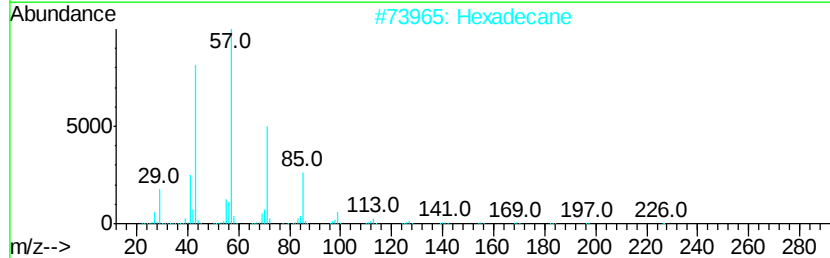
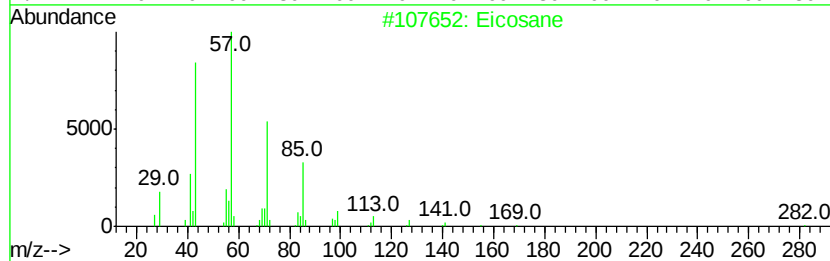
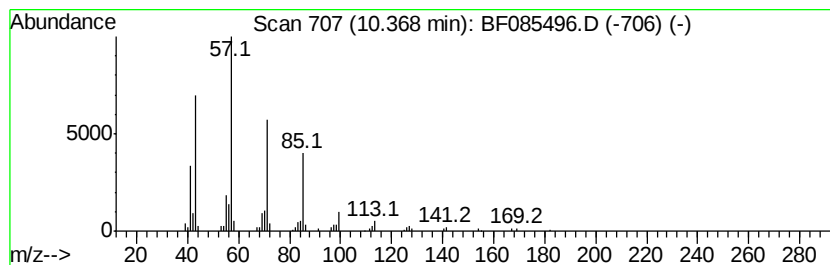
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	5.09 ng	142445	Acenaphthene-d10	9.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	Hexadecane	226 C16H34	000544-76-3	80
3	Octadecane	254 C18H38	000593-45-3	72
4	Nonane, 5-butyl-	184 C13H28	017312-63-9	72
5	Decane, 3-bromo-	220 C10H21Br	030571-71-2	64



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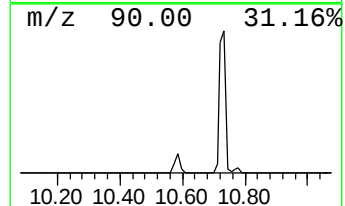
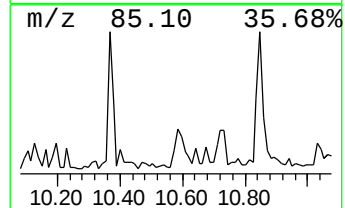
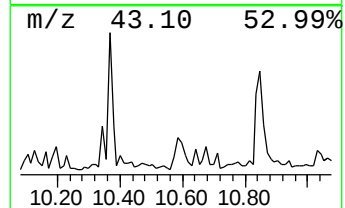
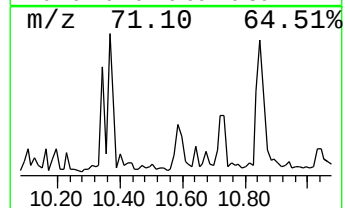
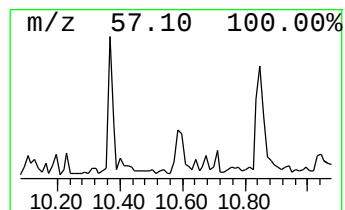
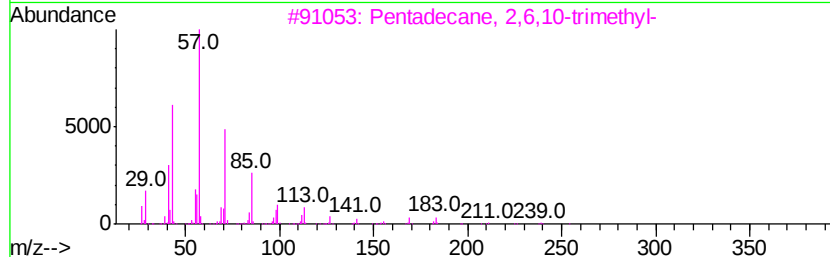
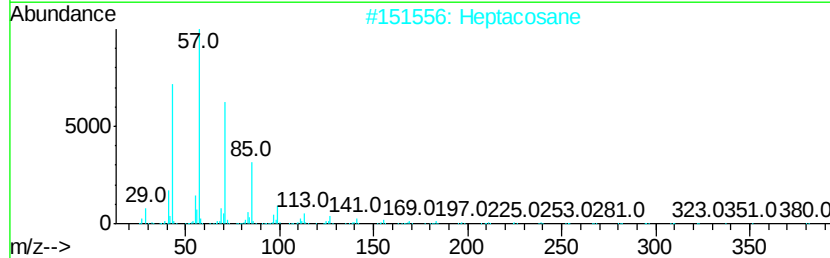
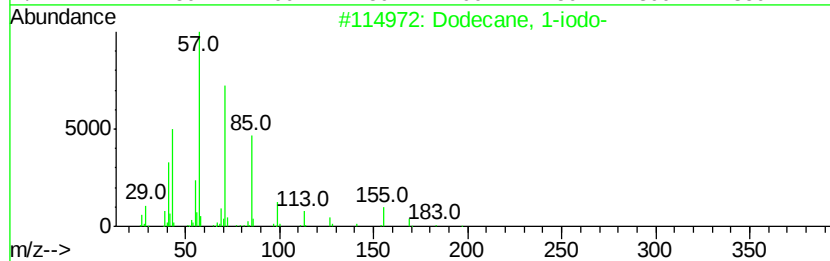
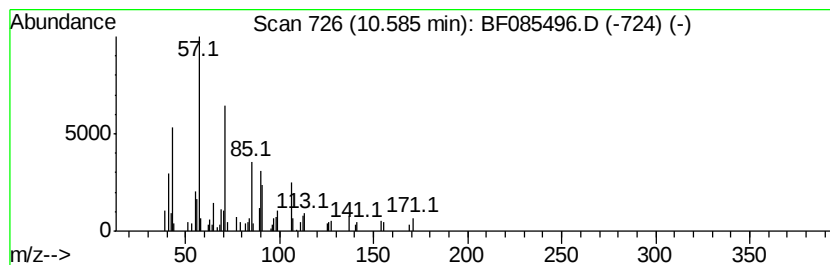
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Dodecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.58	4.37 ng	122455	Acenaphthene-d10		9.94	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	52
2	Heptacosane		380	C27H56	000593-49-7	52
3	Pentadecane, 2,6,10-trimethyl-		254	C18H38	003892-00-0	52
4	Octacosane		394	C28H58	000630-02-4	52
5	Pentadecane		212	C15H32	000629-62-9	52



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Acq On : 17 Mar 2016 7:36
Operator : UM/SJ
Sample : H1790-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

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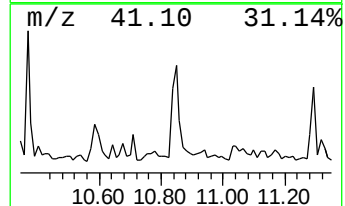
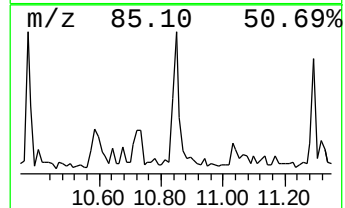
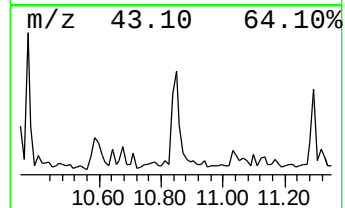
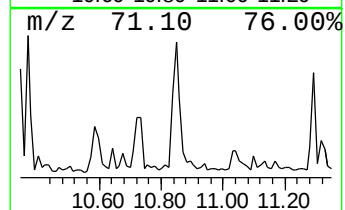
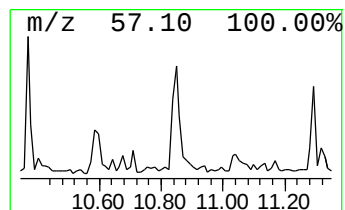
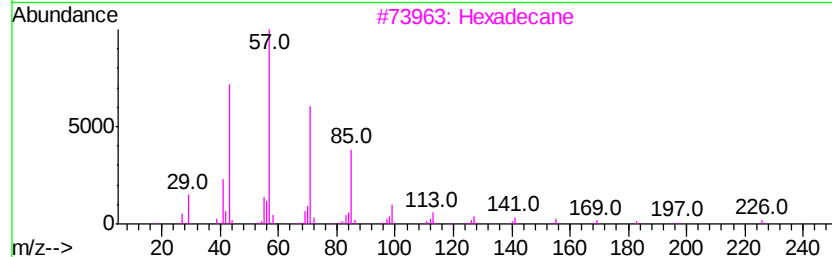
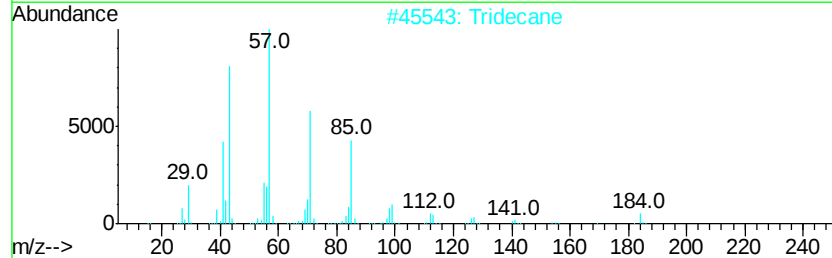
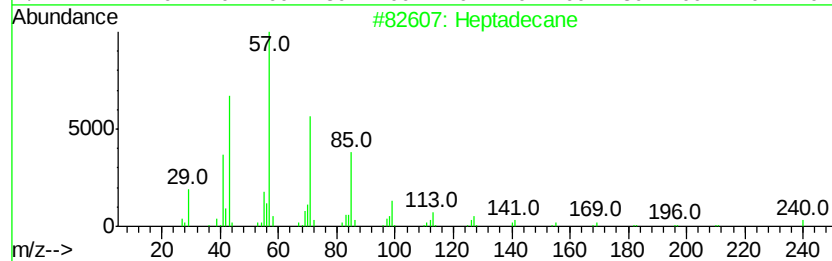
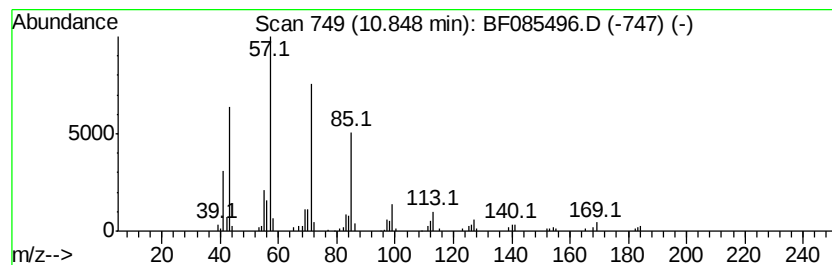
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	7.50 ng	210893	Phenanthrene-d10	11.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Pentadecane		212	C15H32	000629-62-9	90
5	Eicosane		282	C20H42	000112-95-8	90



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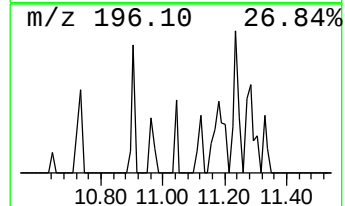
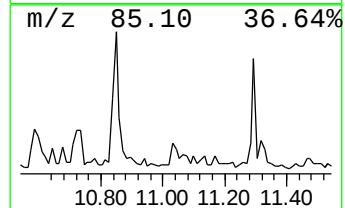
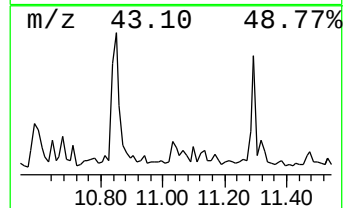
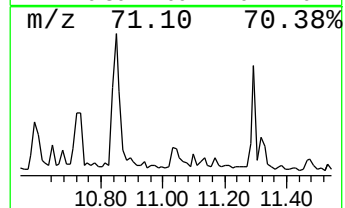
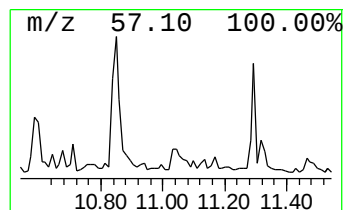
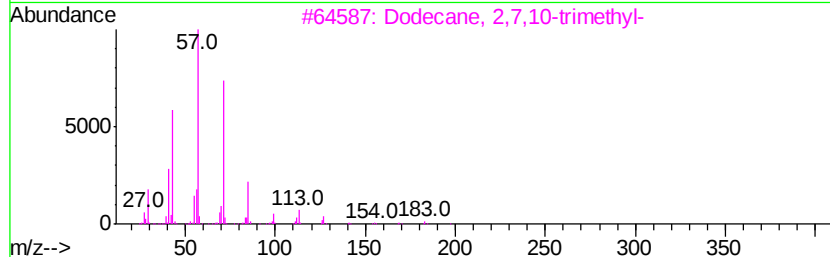
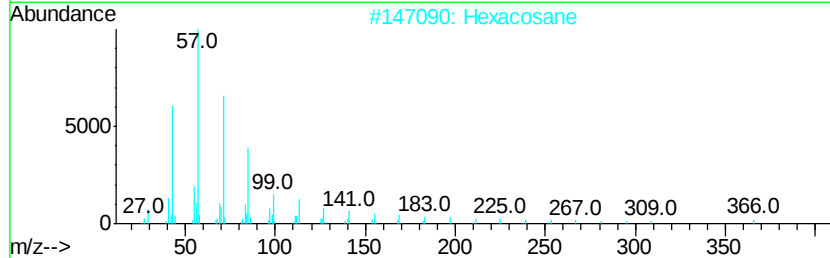
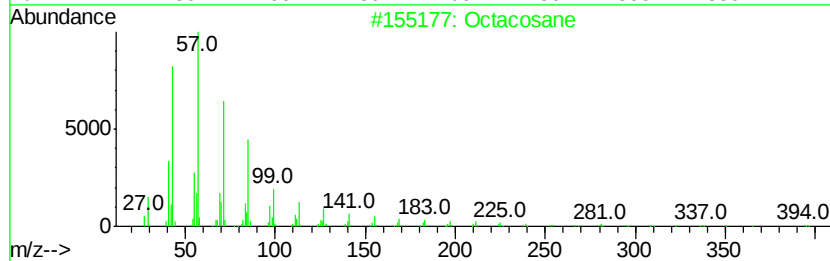
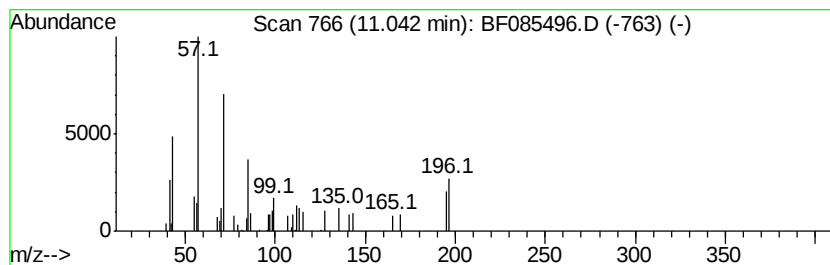
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown11.04 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	2.27 ng	63842	Phenanthrene-d10	11.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	49
2		Hexacosane	366	C26H54	000630-01-3	47
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	43
4		Docosane	310	C22H46	000629-97-0	43
5		Hexadecane	226	C16H34	000544-76-3	43



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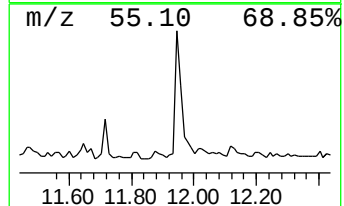
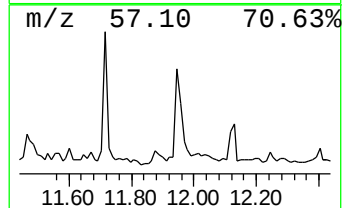
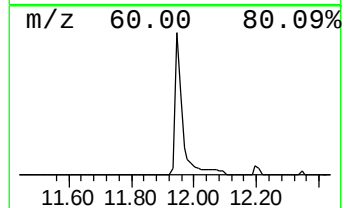
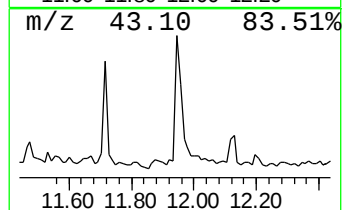
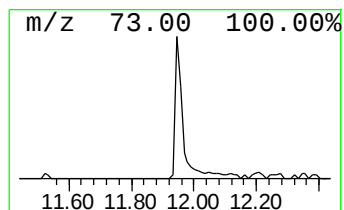
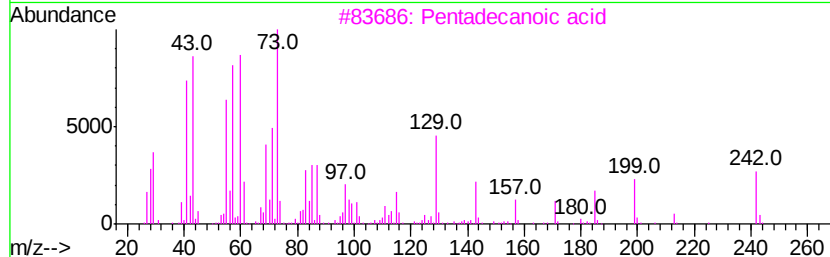
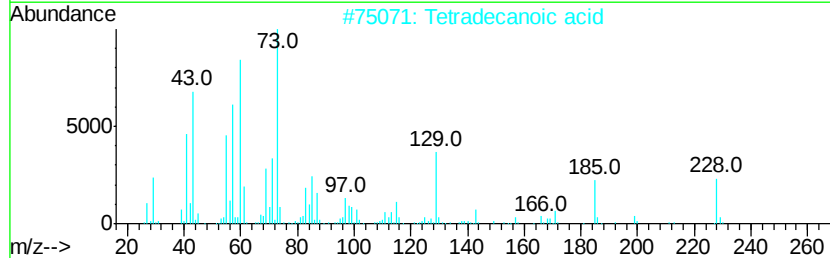
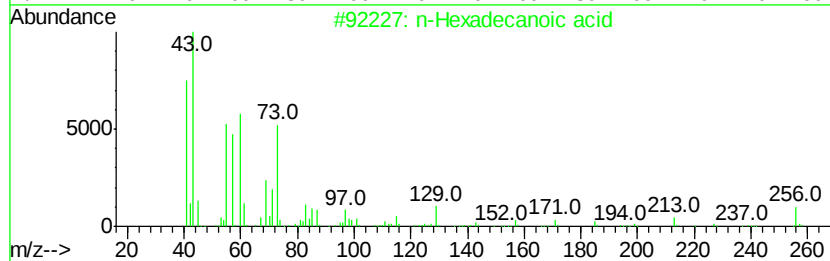
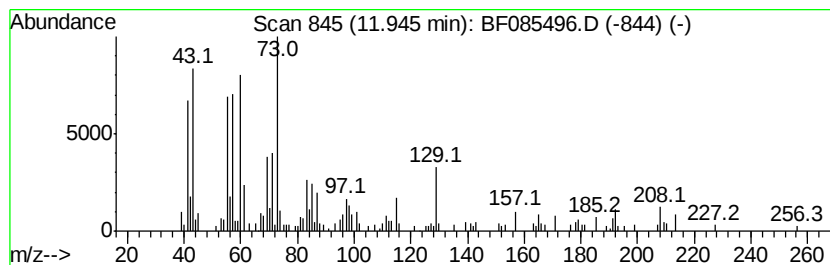
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	7.27 ng	204528	Phenanthrene-d10	11.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tridecanoic acid	214	C13H26O2	000638-53-9	46
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
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Sample : H1790-02
Misc :
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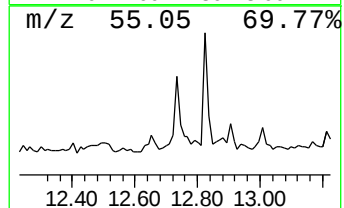
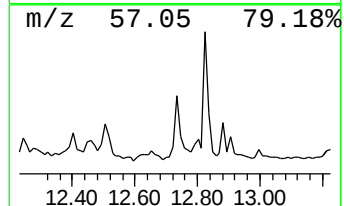
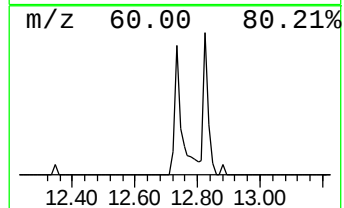
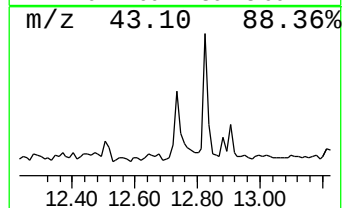
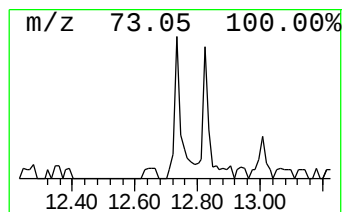
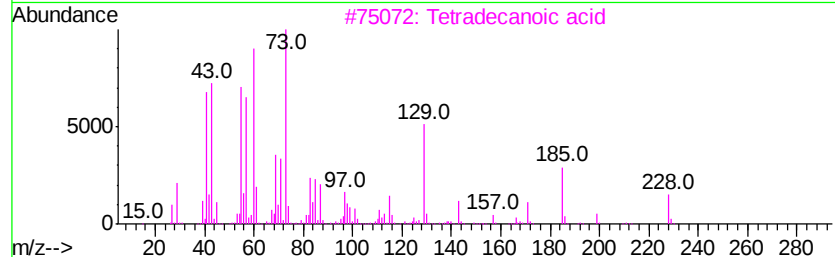
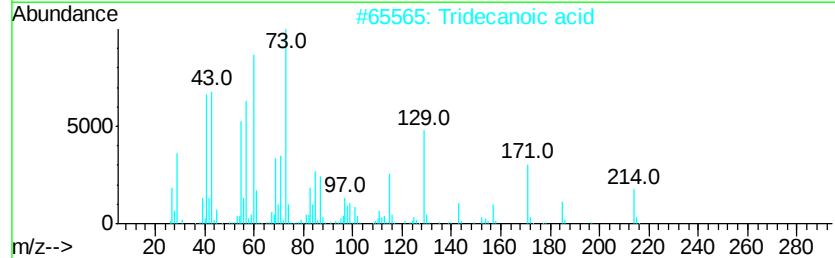
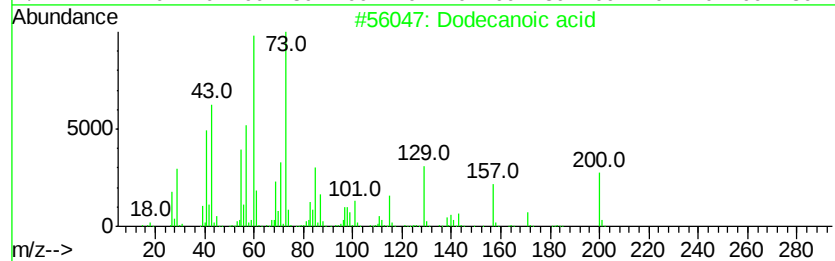
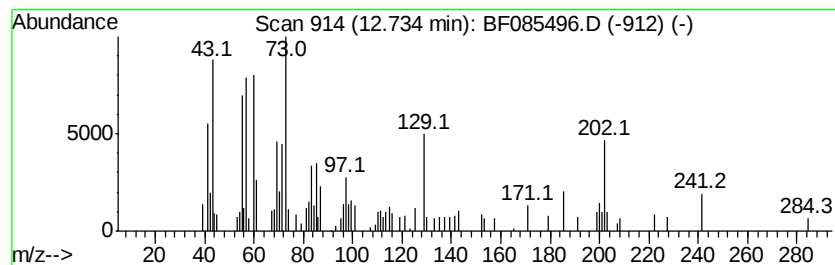
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Dodecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.73	2.33 ng	65516	Phenanthrene-d10		11.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	70
2			Tridecanoic acid	214	C13H26O2	000638-53-9	59
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			n-Decanoic acid	172	C10H20O2	000334-48-5	43



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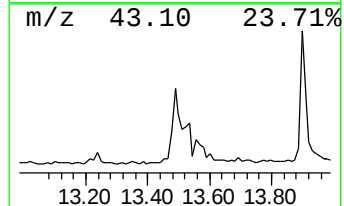
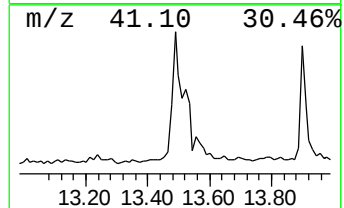
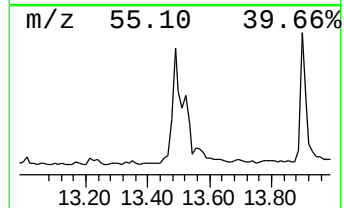
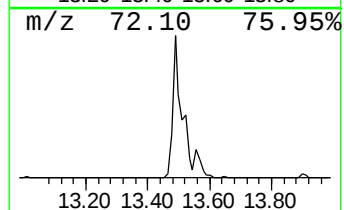
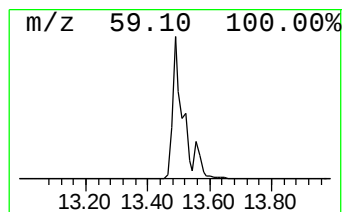
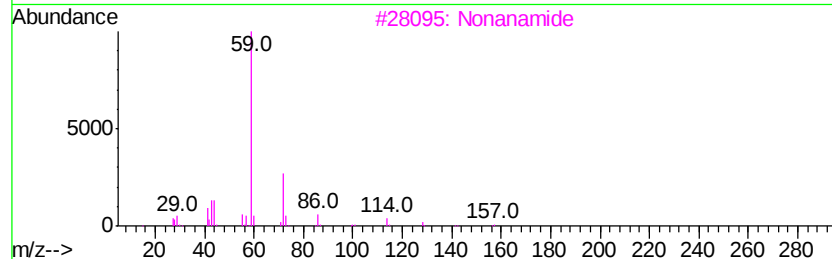
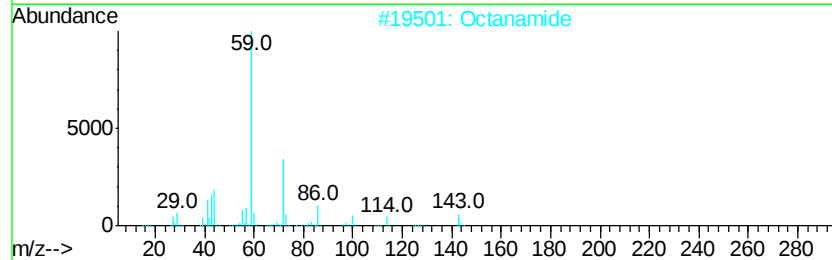
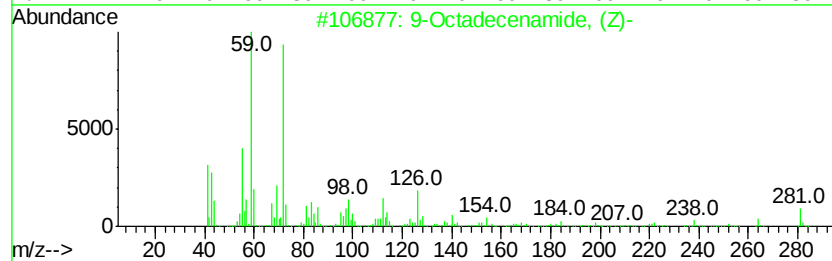
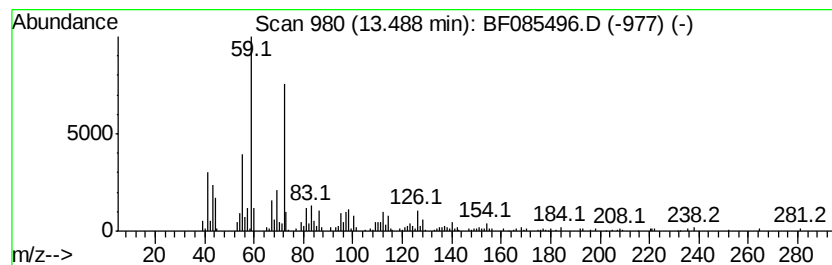
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	16.48 ng	516704	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	81
2		Octanamide	143	C8H17NO	000629-01-6	43
3		Nonanamide	157	C9H19NO	001120-07-6	43
4		Tetradecanamide	227	C14H29NO	000638-58-4	42
5		Silane, hexyl-	116	C6H16Si	001072-14-6	38



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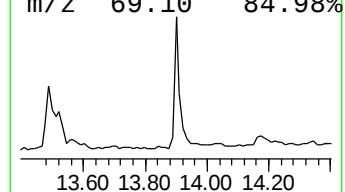
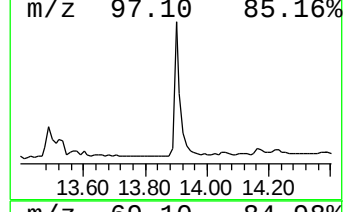
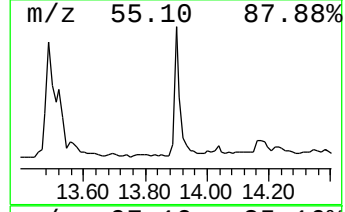
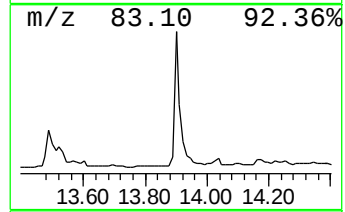
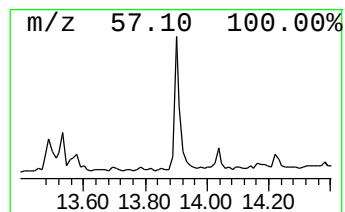
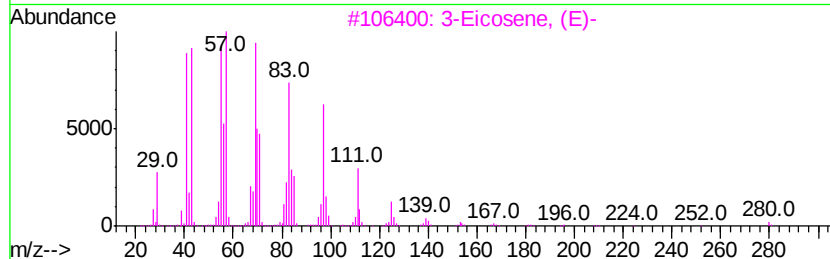
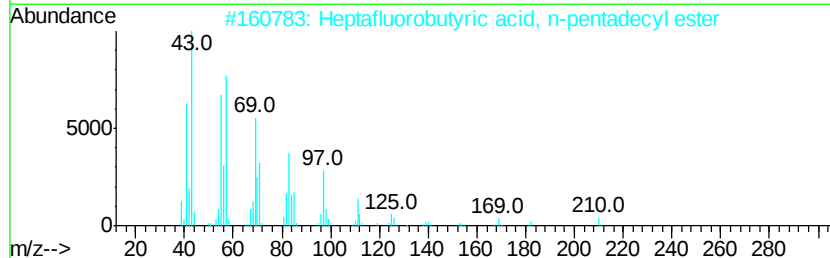
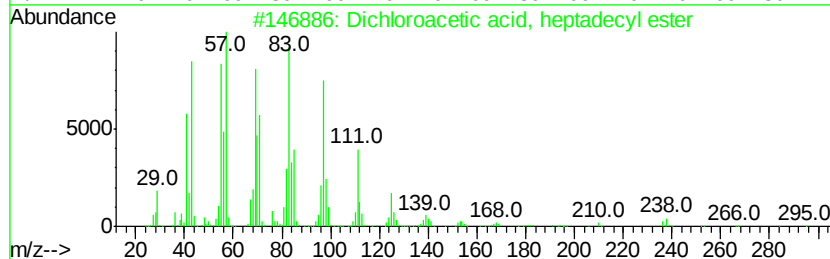
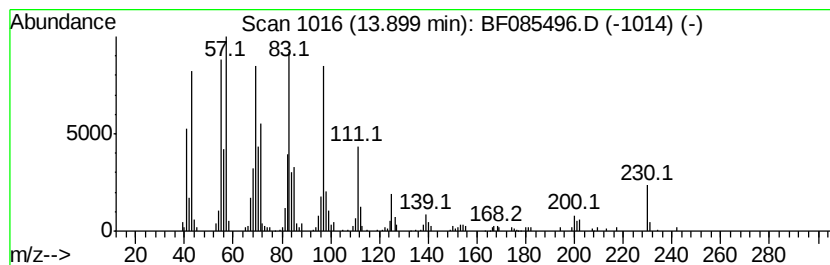
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	8.47 ng	265528	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5		1-Octadecanol	270	C18H38O	000112-92-5	90



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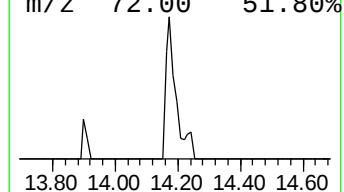
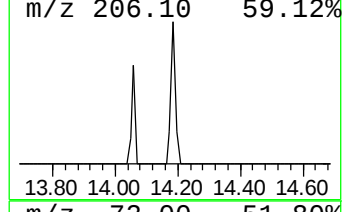
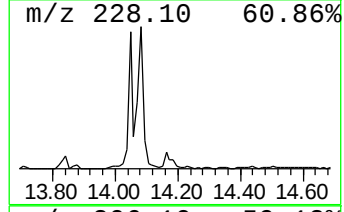
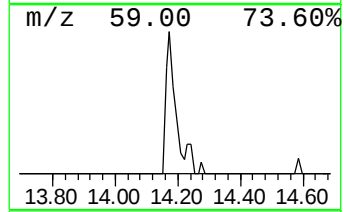
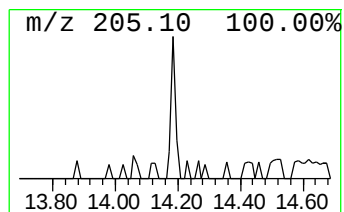
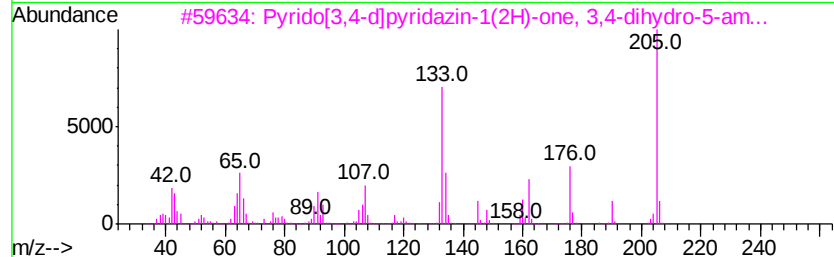
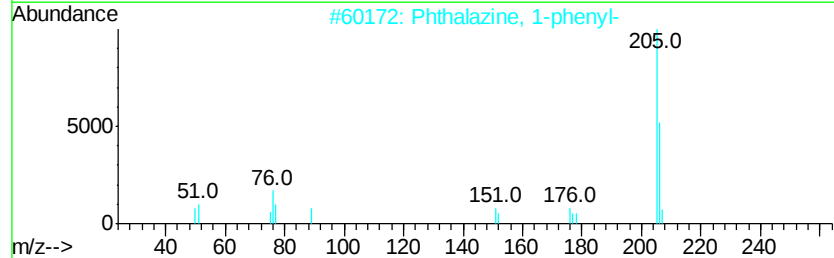
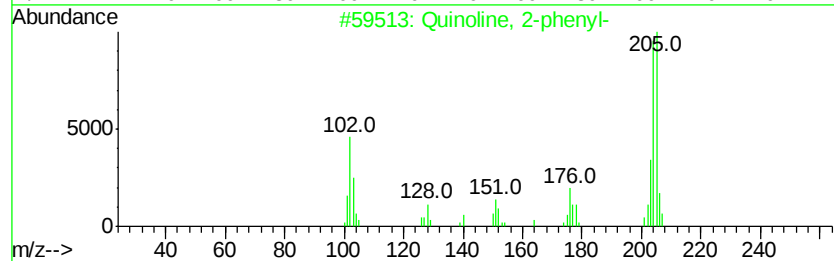
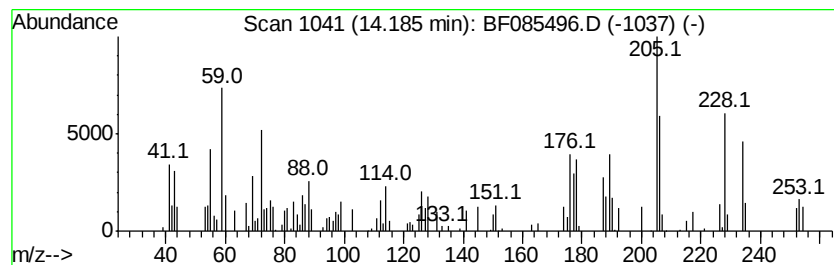
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown14.19 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.76 ng	86575	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoline, 2-phenyl-	205	C15H11N	000612-96-4	22
2		Phthalazine, 1-phenyl-	206	C14H10N2	007188-22-9	14
3		Pyrido[3,4-d]pyridazin-1(2H)-one...	205	C9H11N5O	1000271-08-5	14
4		1,2,3,6-Tetrahydropyridine, 4-[4...	205	C12H15N02	090684-19-8	14
5		Benzocyclobutene, 1,1'-bis-	206	C16H14	121754-51-6	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
Data File : BF085496.D
Acq On : 17 Mar 2016 7:36
Operator : UM/SJ
Sample : H1790-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID-8A-(0-10)

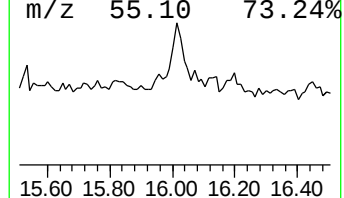
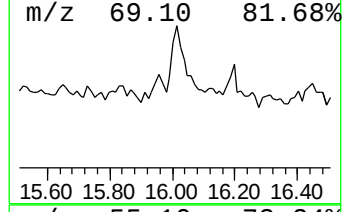
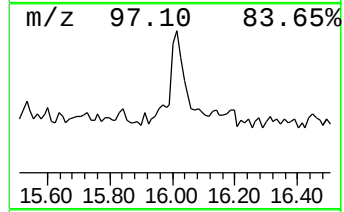
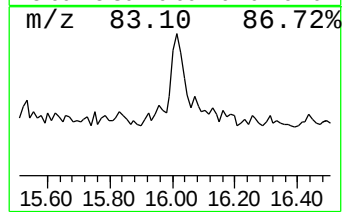
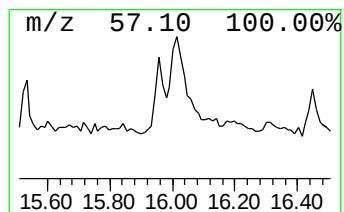
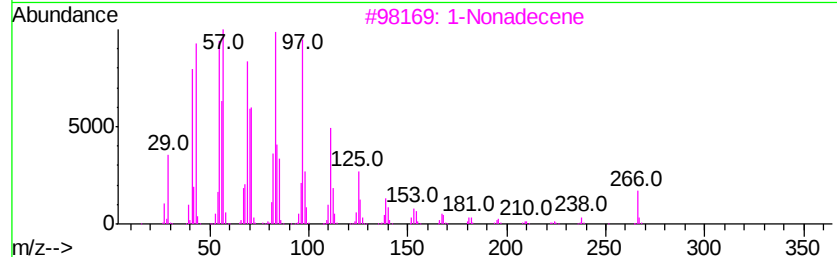
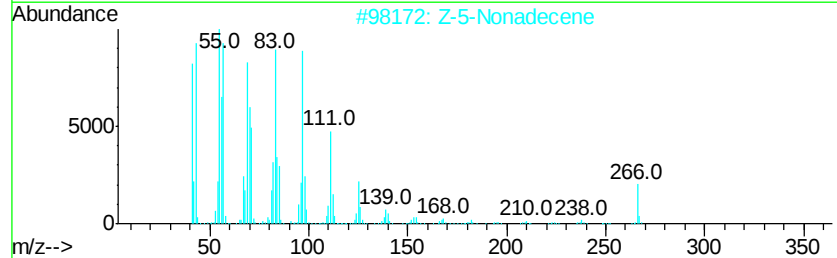
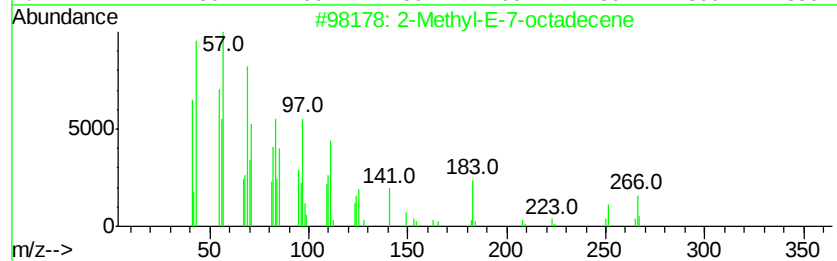
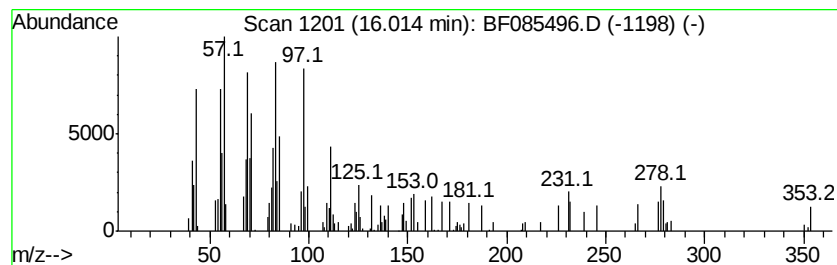
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2-Methyl-E-7-octadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	4.55 ng	92077	Perylene-d12	15.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-E-7-octadecene	266	C19H38	1000130-92-3	83
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	81
3			1-Nonadecene	266	C19H38	018435-45-5	74
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
5			9-Nonadecene	266	C19H38	031035-07-1	60



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031616\
Data File : BF085496.D
Acq On : 17 Mar 2016 7:36
Operator : UM/SJ
Sample : H1790-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

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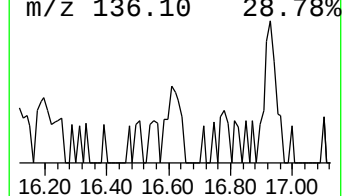
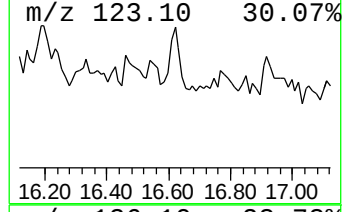
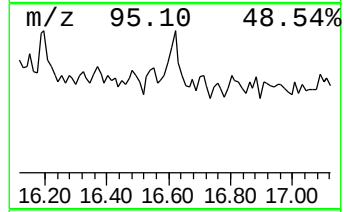
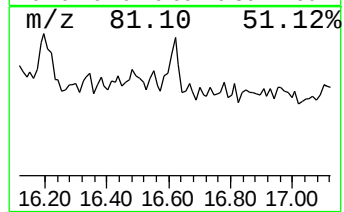
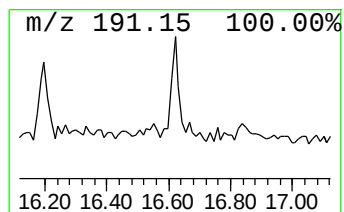
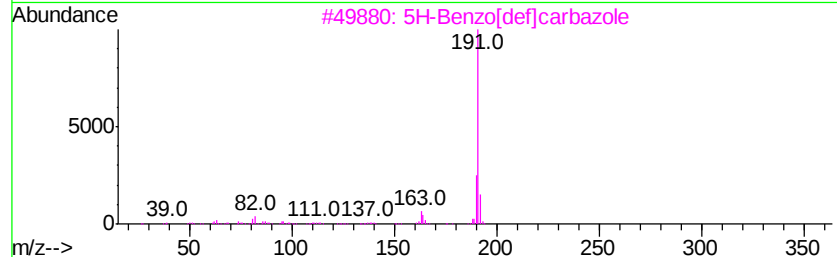
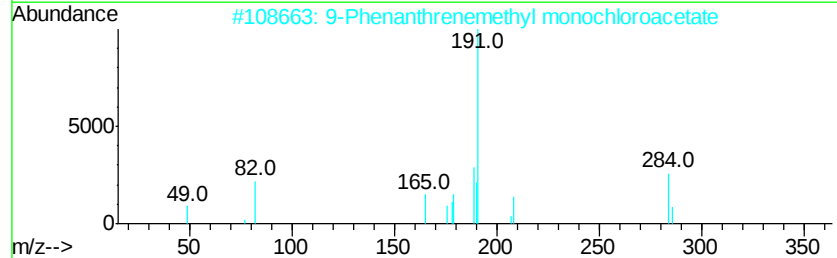
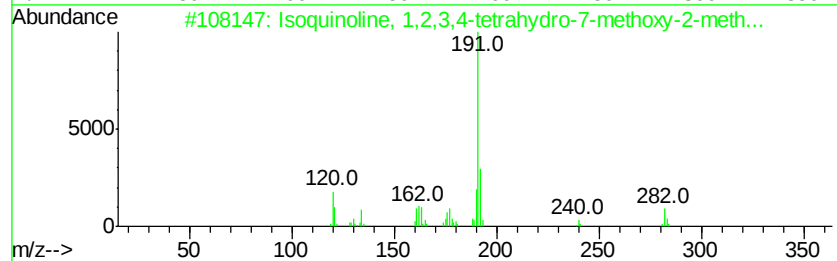
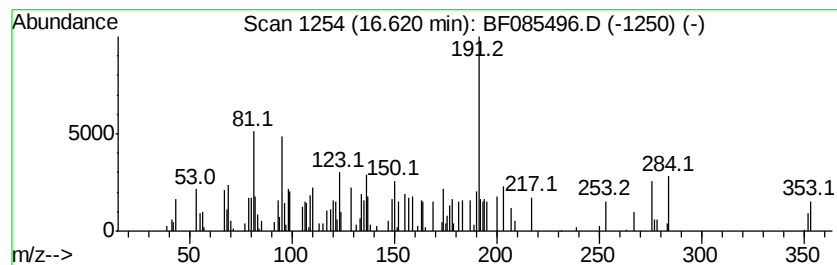
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown16.62 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	3.87 ng	78307	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21N02	036646-87-4	45
2		9-Phenanthrenemethyl monochloroa...	284	C17H13Cl02	092174-37-3	43
3		5H-Benzo[def]carbazole	191	C14H9N	000203-65-6	35
4		Amiphenazole	191	C9H9N3S	000490-55-1	35
5		2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031616\
 Data File : BF085496.D
 Acq On : 17 Mar 2016 7:36
 Operator : UM/SJ
 Sample : H1790-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID-8A-(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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...	5.11	4.2 ng		92032	1	6.90	433751	20.0
3-Chloro-6-fluoro...	6.68	184.9 ng		4009800	1	6.90	433751	20.0
Hexanoic acid, 2-...	7.56	3.6 ng		107290	2	8.18	591628	20.0
Eicosane	10.37	5.1 ng		142445	3	9.94	560135	20.0
Dodecane, 1-iodo-	10.58	4.4 ng		122455	3	9.94	560135	20.0
Heptadecane	10.85	7.5 ng		210893	4	11.42	562485	20.0
unknown11.04	11.04	2.3 ng		63842	4	11.42	562485	20.0
n-Hexadecanoic acid	11.94	7.3 ng		204528	4	11.42	562485	20.0
Dodecanoic acid	12.73	2.3 ng		65516	4	11.42	562485	20.0
9-Octadecenamide,...	13.49	16.5 ng		516704	5	14.06	626890	20.0
Dichloroacetic ac...	13.90	8.5 ng		265528	5	14.06	626890	20.0
unknown14.19	14.19	2.8 ng		86575	5	14.06	626890	20.0
2-Methyl-E-7-octa...	16.01	4.5 ng		92077	6	15.51	404700	20.0
unknown16.62	16.62	3.9 ng		78307	6	15.51	404700	20.0