

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
 Data File : BF088089.D
 Acq On : 16 Jun 2016 21:45
 Operator : UM/SJ
 Sample : H3596-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-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-BF060716.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	1.678	7	8	17	rVB	297398	498296	18.66%	1.796%
2	1.804	17	19	29	rBV	1480566	2376227	88.99%	8.562%
3	4.890	287	289	301	rBV	123127	231035	8.65%	0.832%
4	5.313	323	326	328	rBV	2039489	2161233	80.94%	7.788%
5	6.364	415	418	421	rBV	1788798	2137613	80.06%	7.703%
6	6.490	426	429	431	rBV	2313986	2436155	91.24%	8.778%
7	6.719	447	449	451	rBV	774956	656250	24.58%	2.365%
8	6.879	460	463	465	rBV	1937073	2102500	78.74%	7.576%
9	7.290	496	499	501	rBV	1607270	1667608	62.45%	6.009%
10	7.919	551	554	556	rBV	46110	39324	1.47%	0.142%
11	7.999	559	561	564	rBV	793853	825899	30.93%	2.976%
12	9.085	653	656	658	rBV	2799589	2670134	100.00%	9.621%
13	9.199	665	666	668	rVB	27760	34304	1.28%	0.124%
14	9.473	688	690	692	rBV	442826	524877	19.66%	1.891%
15	9.611	701	702	705	rBV	52275	45629	1.71%	0.164%
16	9.691	708	709	712	rBV	31430	38902	1.46%	0.140%
17	9.748	712	714	717	rBV	723603	872070	32.66%	3.142%
18	10.193	752	753	755	rVB	103508	79227	2.97%	0.285%
19	10.411	769	772	775	rBV	35009	53941	2.02%	0.194%
20	10.536	781	783	786	rBV	1092534	1232153	46.15%	4.440%
21	10.662	793	794	799	rBV	110520	127808	4.79%	0.461%
22	11.108	832	833	835	rBV	65746	63091	2.36%	0.227%
23	11.234	842	844	845	rBV	804744	775794	29.05%	2.795%
24	11.256	845	846	848	rVV	130723	95369	3.57%	0.344%
25	11.302	848	850	853	rVB	45107	52600	1.97%	0.190%
26	11.462	862	864	869	rVB2	71857	98879	3.70%	0.356%
27	11.771	889	891	893	rBV2	34551	51686	1.94%	0.186%
28	11.839	895	897	903	rVB	30673	44657	1.67%	0.161%
29	12.285	934	936	942	rBV	547322	612483	22.94%	2.207%
30	12.434	947	949	952	rBV	143759	161161	6.04%	0.581%
31	12.662	966	969	973	rBV	166311	217574	8.15%	0.784%
32	12.822	980	983	985	rVB	1372841	1923469	72.04%	6.931%
33	12.994	994	998	1000	rVB	23813	38667	1.45%	0.139%
34	13.028	1000	1001	1002	rBV	21109	28033	1.05%	0.101%

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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

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Peak separation: 5

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35	13.268	1019	1022	1024	rBV	142331	135107	5.06%	0.487%
36	13.382	1028	1032	1038	rBV5	36435	110437	4.14%	0.398%
37	13.714	1059	1061	1065	rBV	173722	226315	8.48%	0.815%
38	13.862	1071	1074	1075	rBV2	716392	822713	30.81%	2.965%
39	13.885	1075	1076	1080	rVB	85622	75742	2.84%	0.273%
40	14.354	1114	1117	1122	rBV6	30146	94913	3.55%	0.342%
41	14.617	1138	1140	1141	rBV	33473	37522	1.41%	0.135%
42	14.868	1159	1162	1165	rBV	99517	191793	7.18%	0.691%
43	15.143	1184	1186	1188	rVB	38489	54927	2.06%	0.198%
44	15.200	1188	1191	1193	rVV	65085	101244	3.79%	0.365%
45	15.245	1193	1195	1204	rVB	405454	628318	23.53%	2.264%
46	15.531	1218	1220	1228	rVB4	43234	122218	4.58%	0.440%
47	15.714	1233	1236	1239	rBV3	33852	64942	2.43%	0.234%
48	16.571	1308	1311	1315	rBV	29643	58200	2.18%	0.210%
49	16.971	1343	1346	1350	rVB	25722	53118	1.99%	0.191%

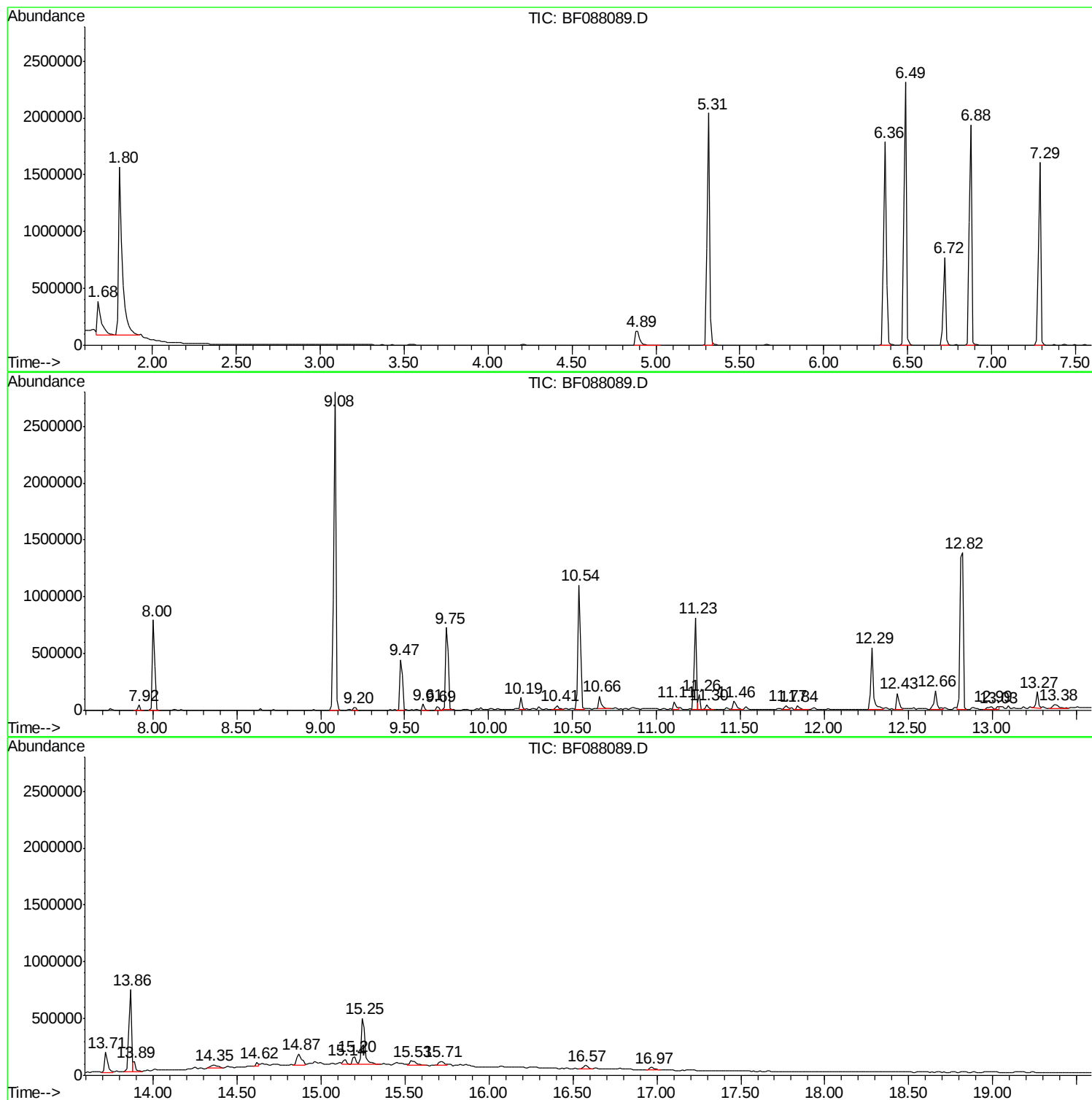
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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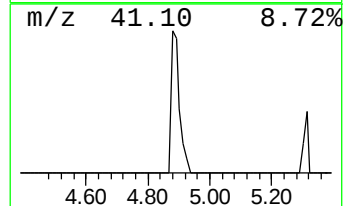
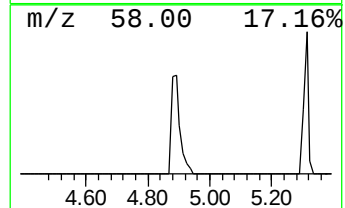
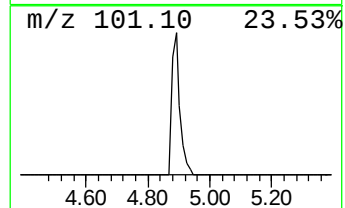
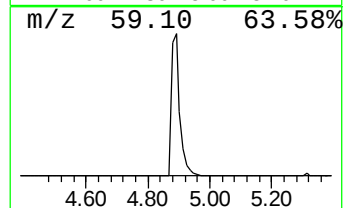
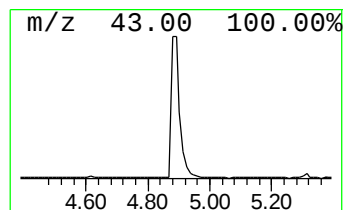
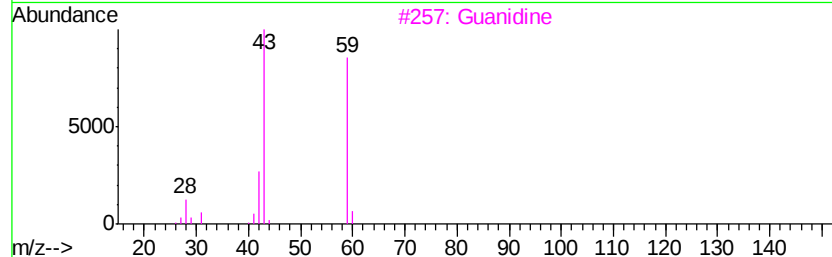
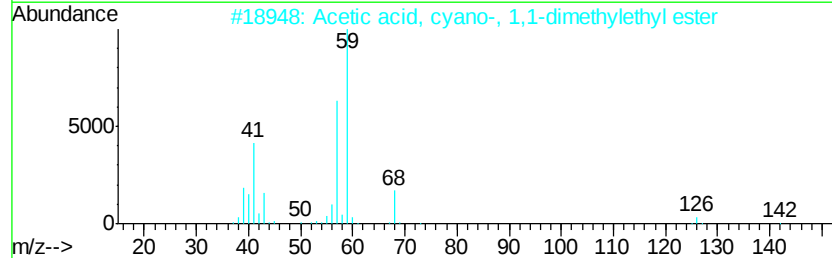
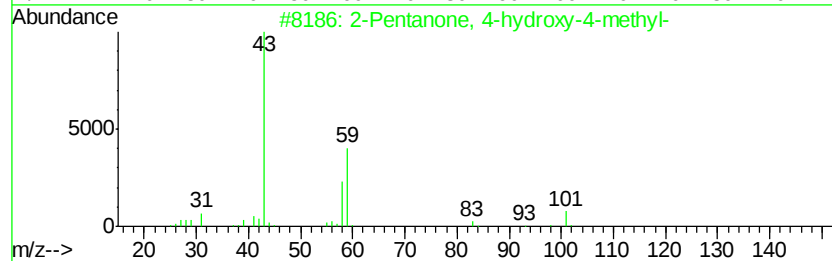
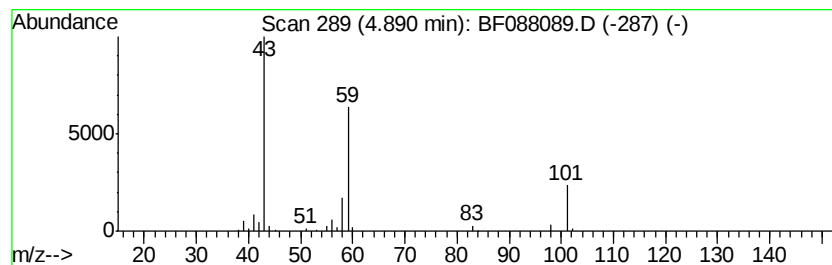
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	7.04 ng	231035	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Guanidine	59	CH5N3	000113-00-8	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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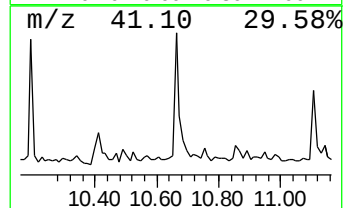
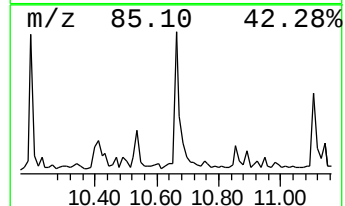
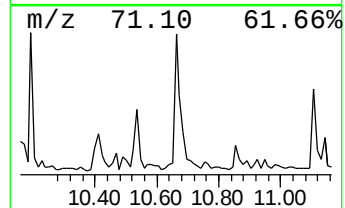
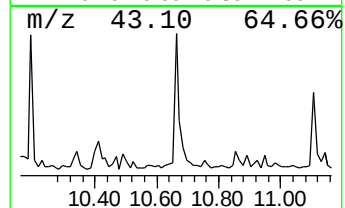
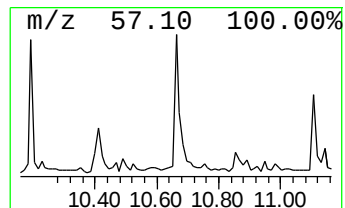
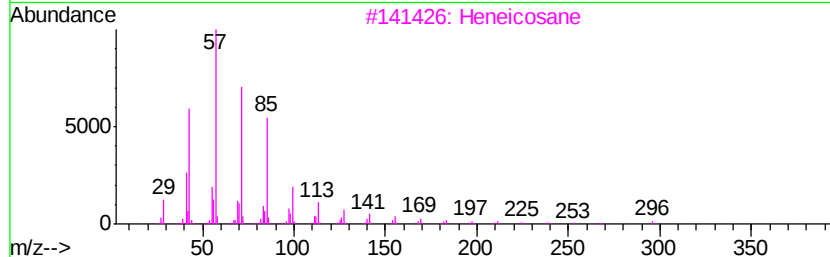
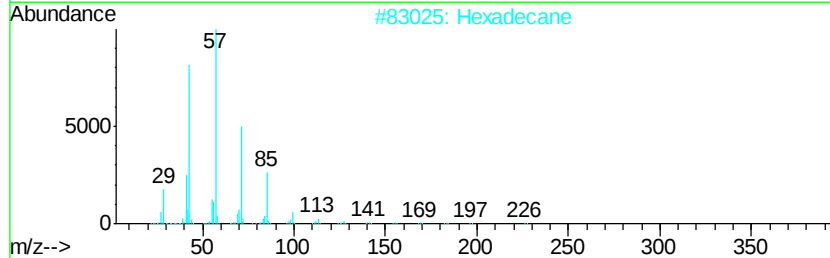
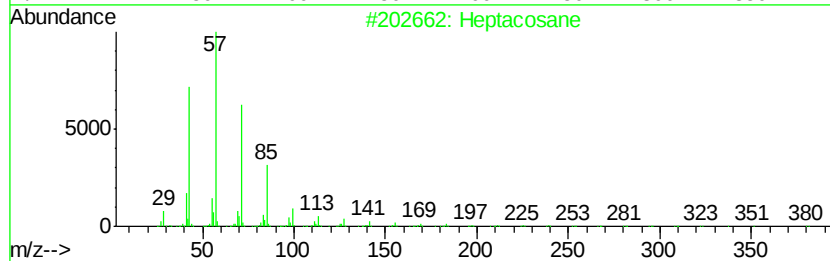
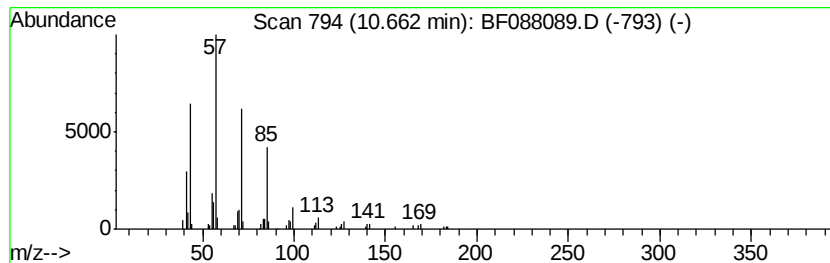
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.29 ng	127808	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heneicosane		296	C21H44	000629-94-7	90
4	Heptadecane		240	C17H36	000629-78-7	87
5	Tetradecane		198	C14H30	000629-59-4	87



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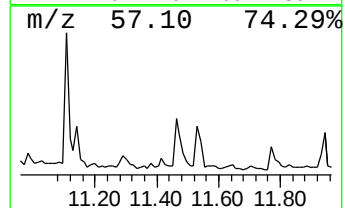
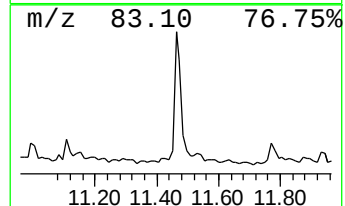
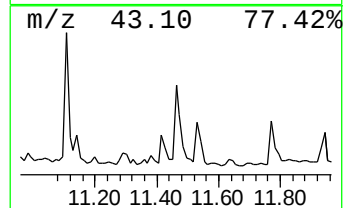
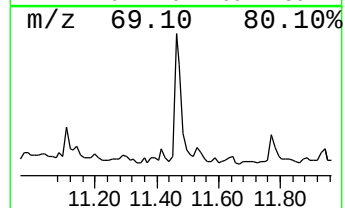
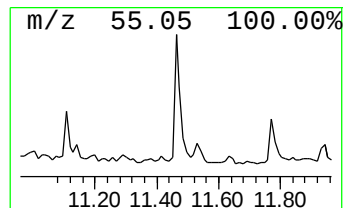
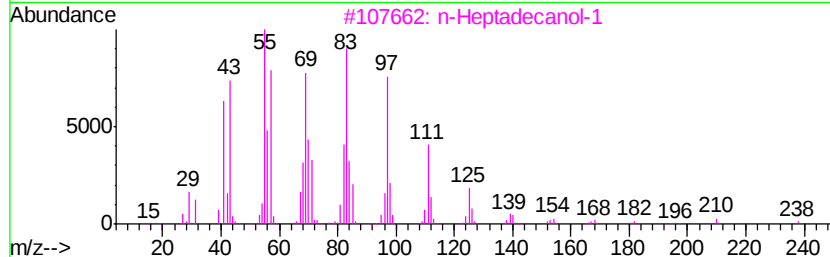
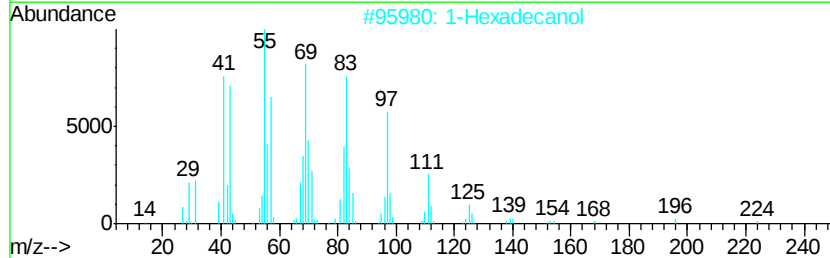
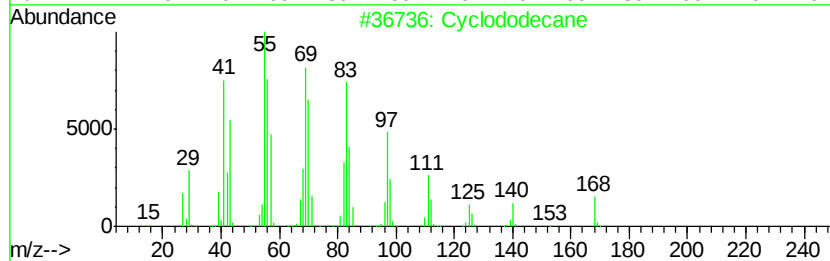
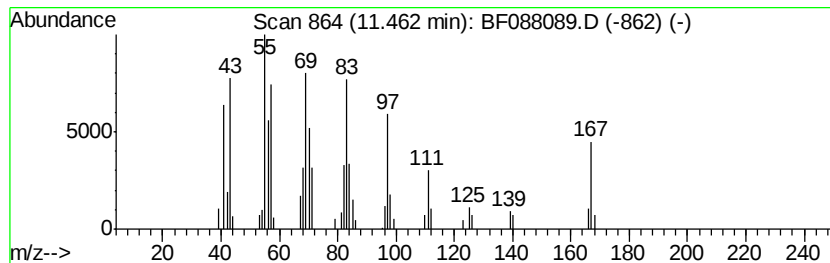
Instrument :
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclododecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.46	2.55 ng	98879	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	95
2	1-Hexadecanol	242	C16H34O	036653-82-4	93
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	87



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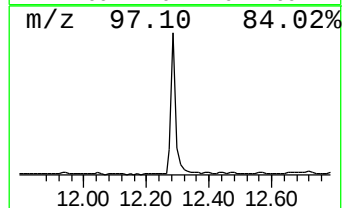
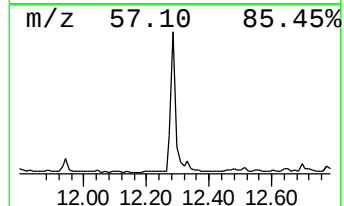
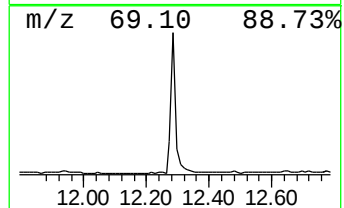
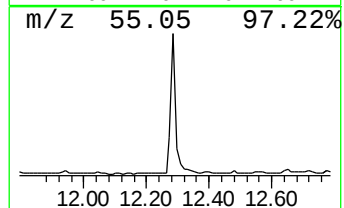
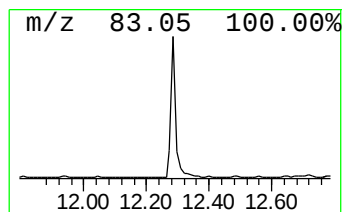
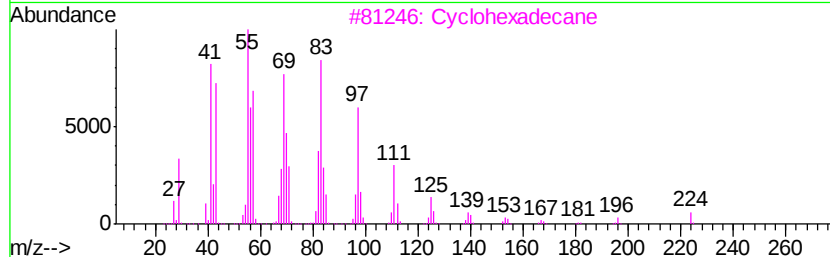
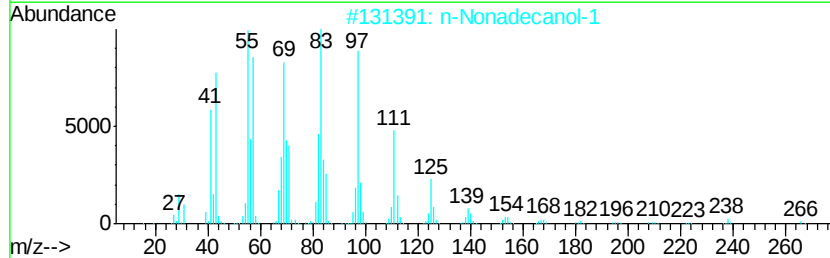
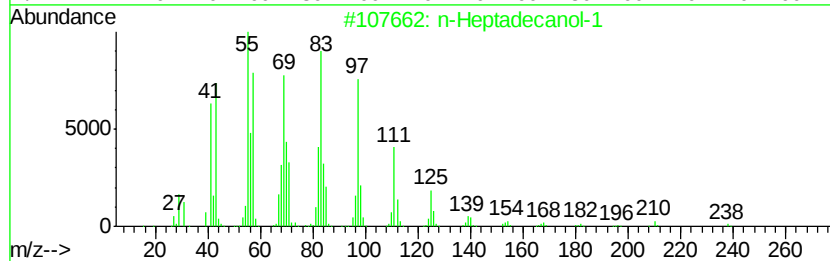
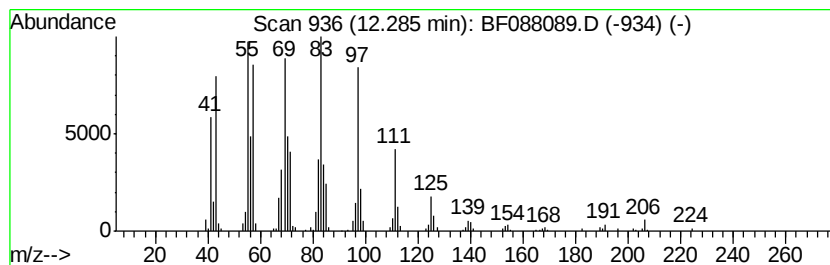
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	15.79 ng	612483	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Cyclohexadecane	224	C16H32	000295-65-8	94
4		1-Hexadecanol	242	C16H34O	036653-82-4	93
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



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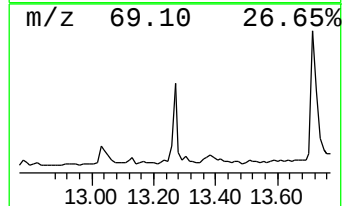
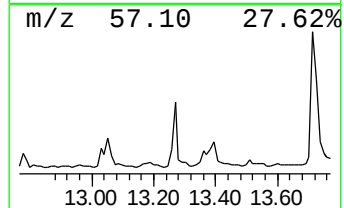
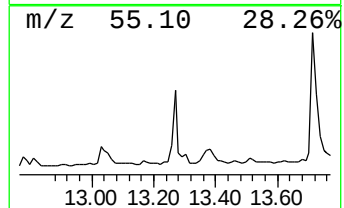
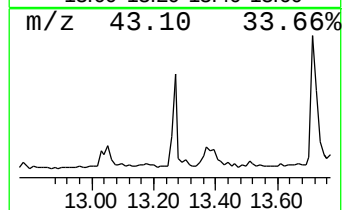
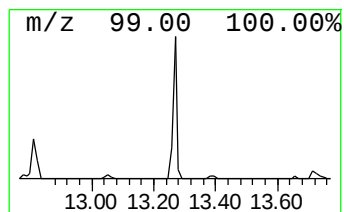
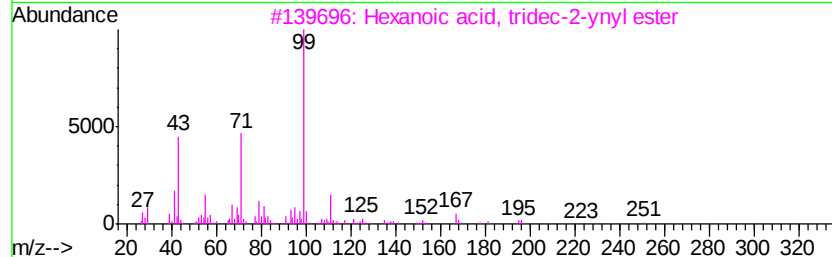
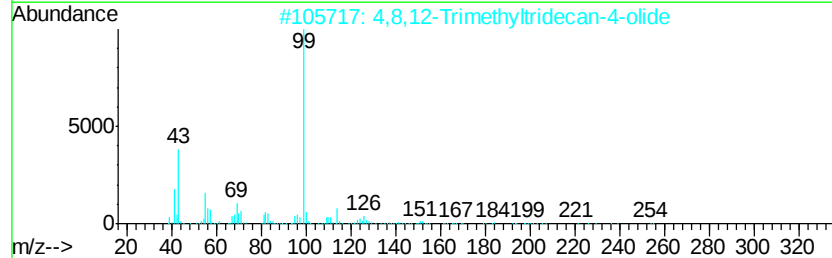
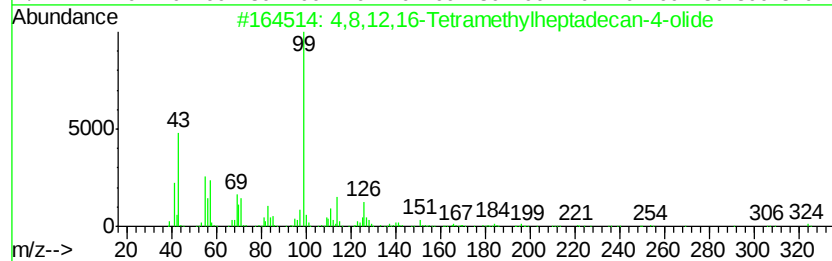
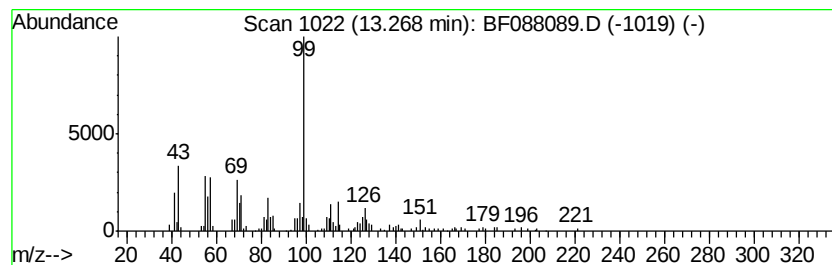
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 4,8,12,16-Tetramethylheptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	3.28 ng	135107	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	90
2		4,8,12-Trimethyltridecan-4-olide	254	C16H30O2	220904-24-5	64
3		Hexanoic acid, tridec-2-ynyl ester	294	C19H34O2	1000299-36-0	53
4		2H-Pyran-2-one, tetrahydro-6-octyl-	212	C13H24O2	007370-92-5	53
5		Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088089.D
Acq On : 16 Jun 2016 21:45
Operator : UM/SJ
Sample : H3596-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

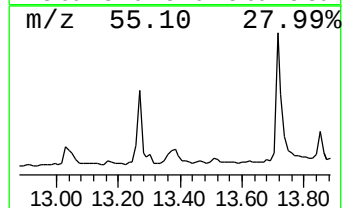
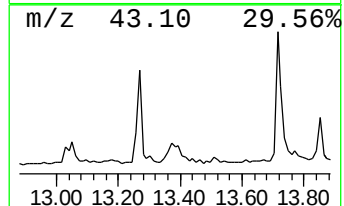
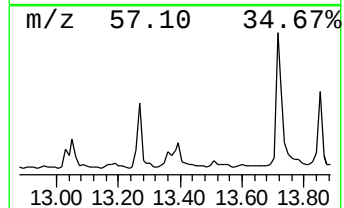
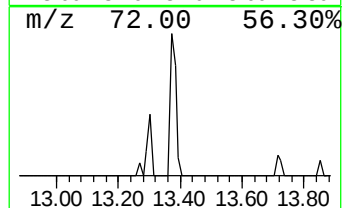
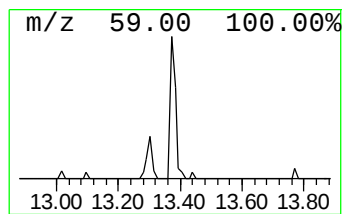
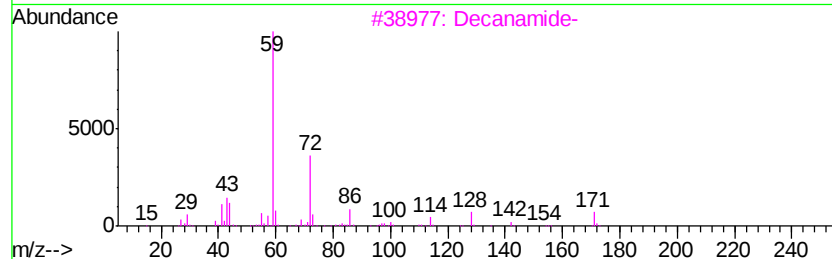
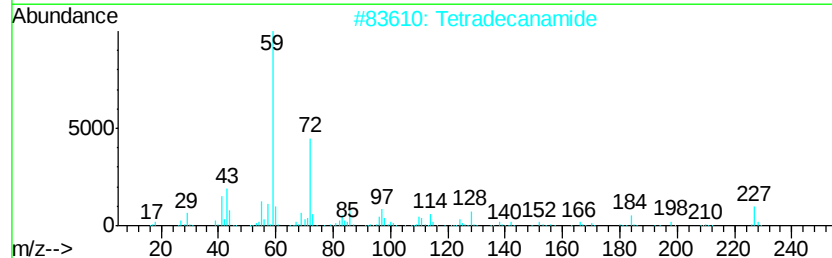
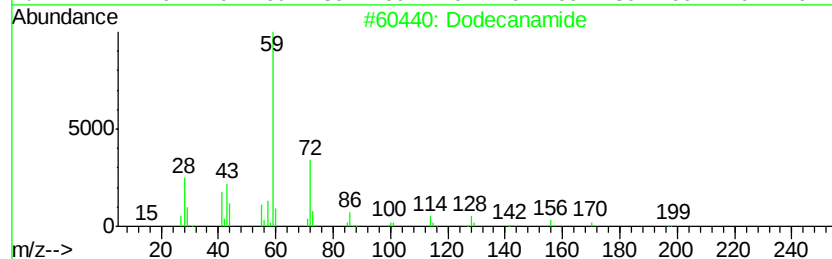
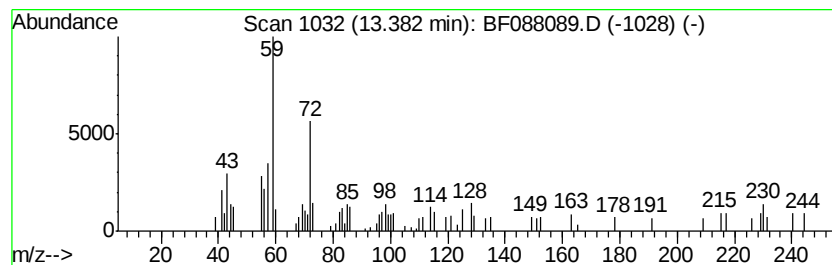
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dodecanamide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.38	2.68 ng	110437	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide	199	C12H25NO	001120-16-7	53
2	Tetradecanamide	227	C14H29NO	000638-58-4	53
3	Decanamide-	171	C10H21NO	002319-29-1	53
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50
5	Octanamide	143	C8H17NO	000629-01-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088089.D
Acq On : 16 Jun 2016 21:45
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ALS Vial : 19 Sample Multiplier: 1

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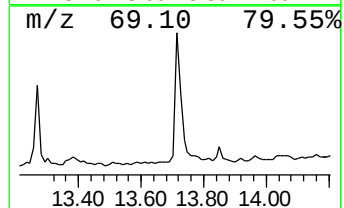
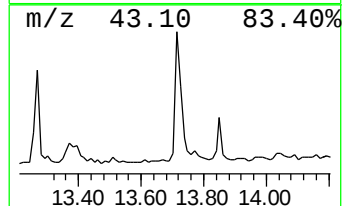
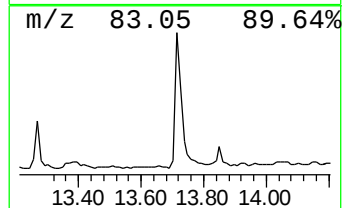
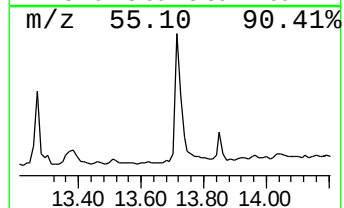
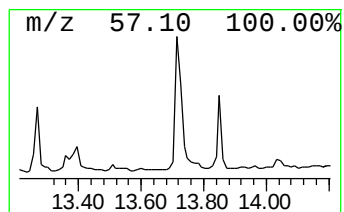
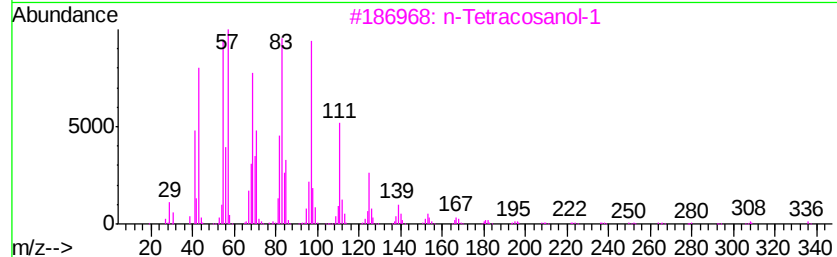
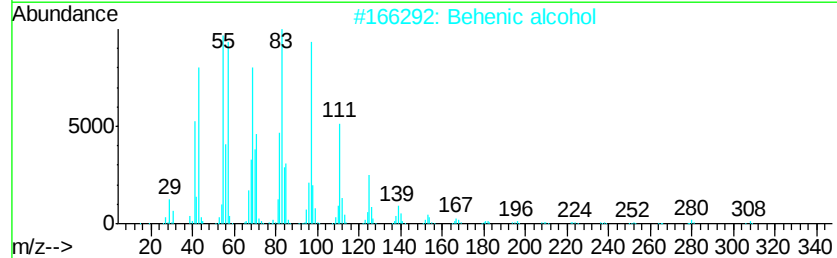
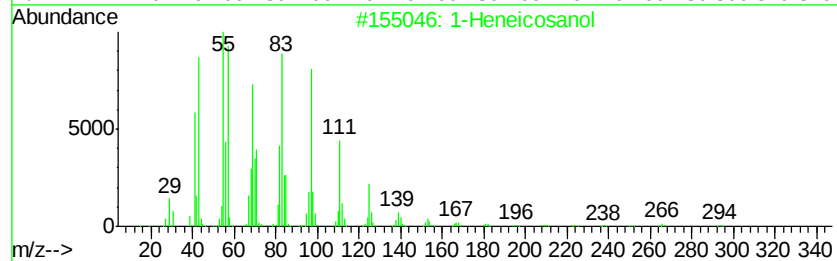
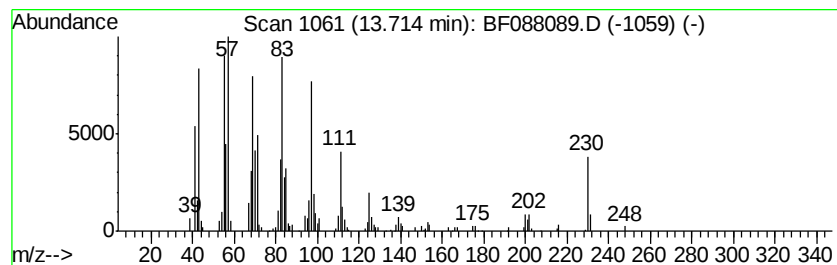
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.50 ng	226315	Chrysene-d12	13.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
Data File : BF088089.D
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Sample : H3596-04
Misc :
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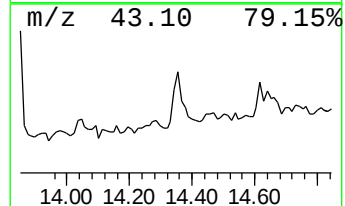
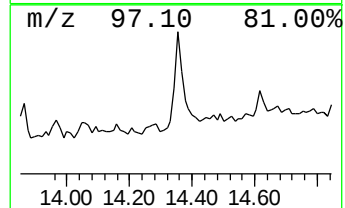
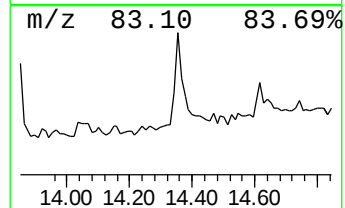
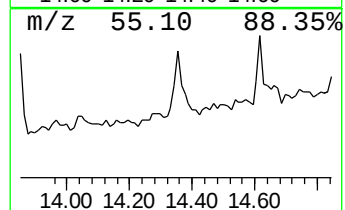
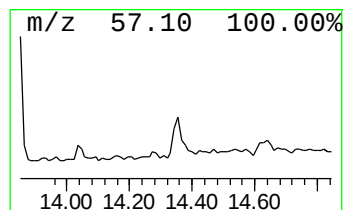
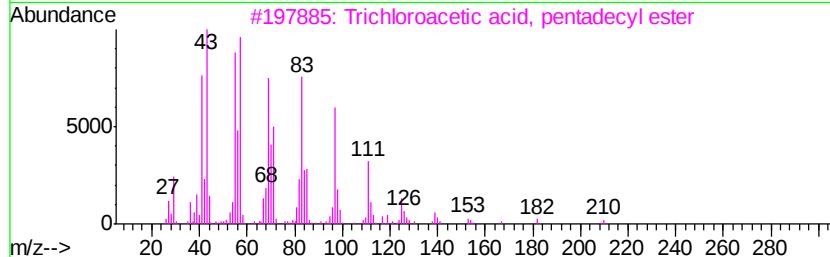
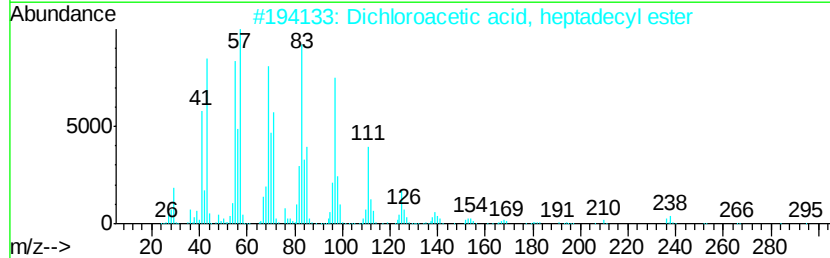
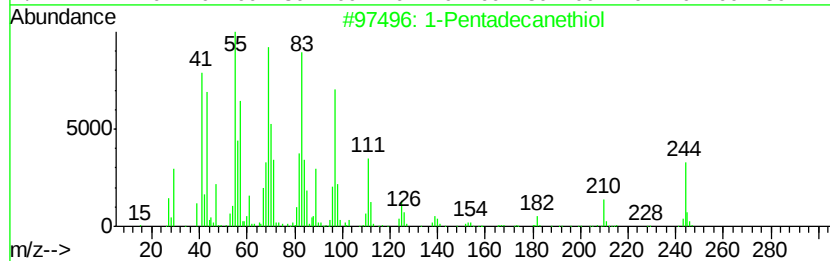
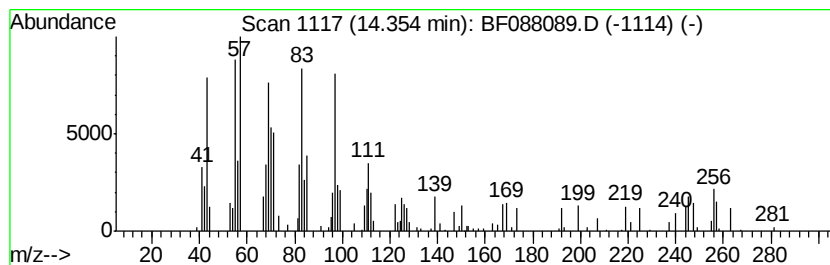
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Pentadecanethiol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.35	2.31 ng	94913	Chrysene-d12		13.86		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
4			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	81
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
Data File : BF088089.D
Acq On : 16 Jun 2016 21:45
Operator : UM/SJ
Sample : H3596-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

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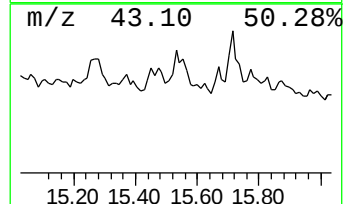
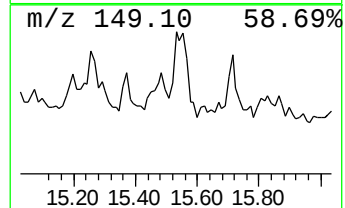
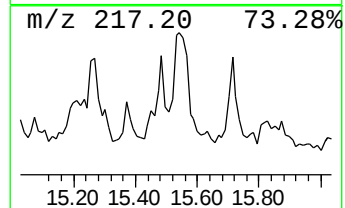
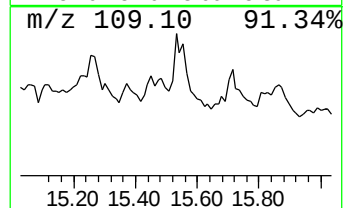
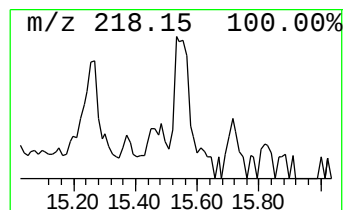
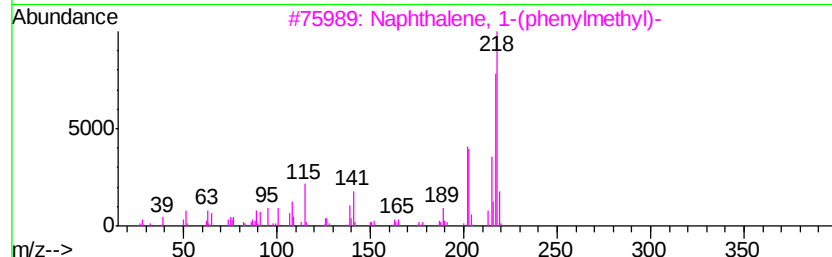
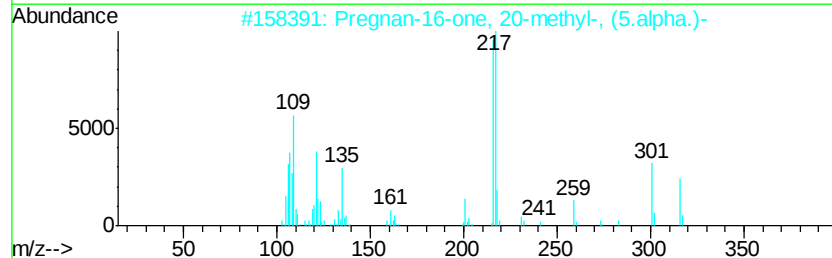
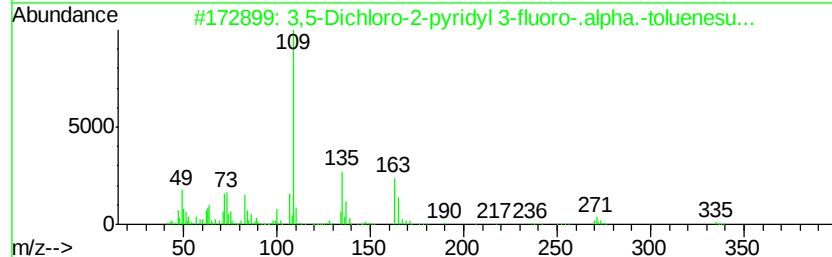
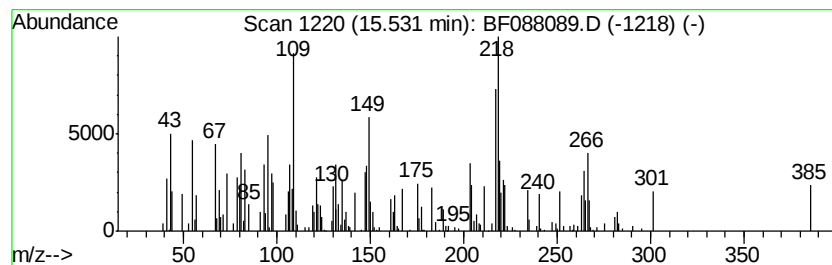
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown15.53 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	3.89 ng	122218	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,5-Dichloro-2-pyridyl 3-fluoro-...	335	C12H8Cl2FN03S	058236-48-9	22
2		Pregnan-16-one, 20-methyl-, (5.alpha....	316	C22H36O	056051-43-5	22
3		Naphthalene, 1-(phenylmethyl)-	218	C17H14	000611-45-0	22
4		D-Norandrostane-16-carboxylic ac...	290	C19H30O2	032319-09-8	16
5		6H-[1,2]Dioxeto[3',4':4,5]furo[3...	260	C14H12O5	129812-24-4	12



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
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Sample : H3596-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

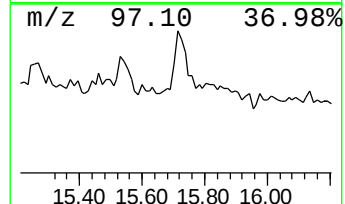
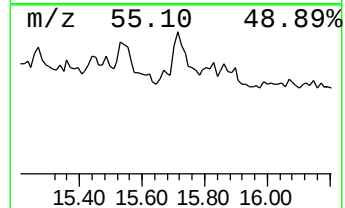
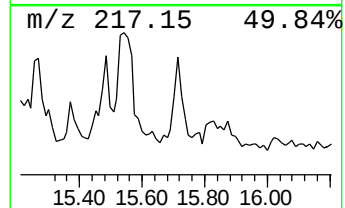
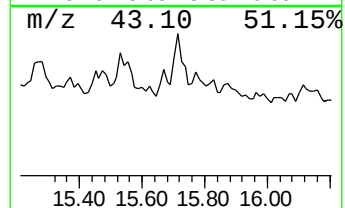
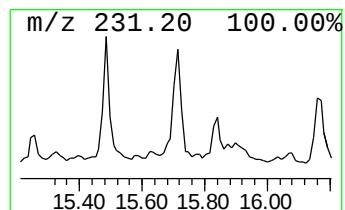
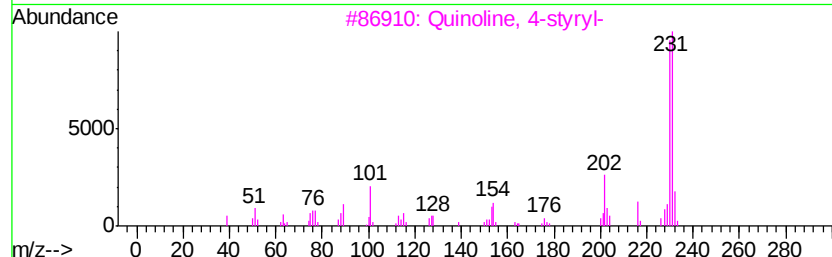
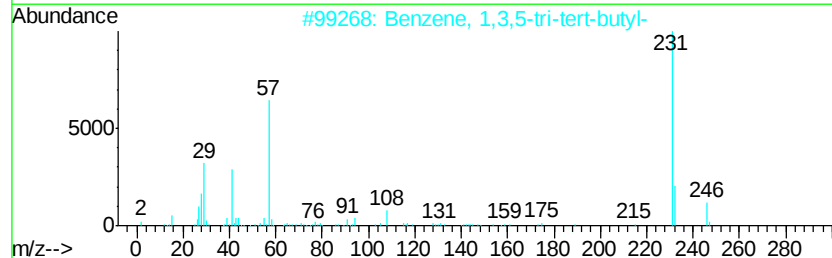
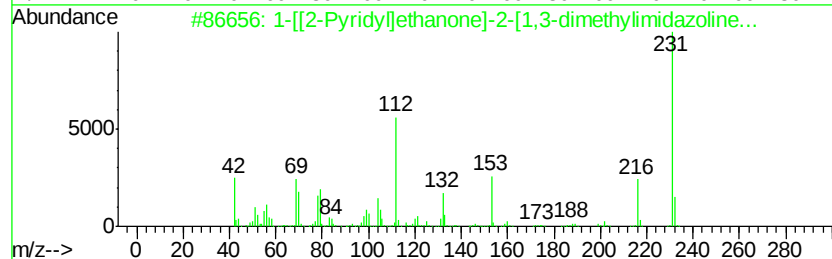
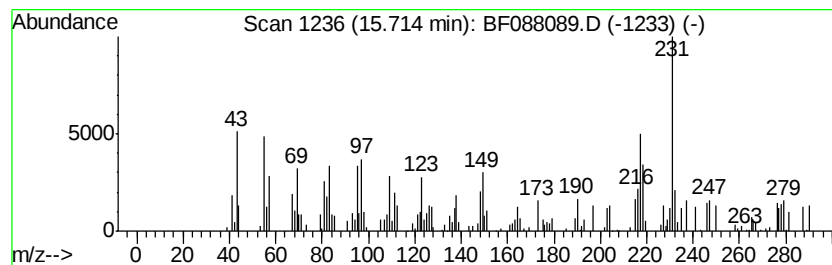
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.71 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.		
15.71	2.07 ng	64942	Perylene-d12		15.25		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-[[2-Pyridyl]ethanone]-2-[1,3-d...	231	C12H17N5	097483-60-8	43
2			Benzene, 1,3,5-tri-tert-butyl-	246	C18H30	001460-02-2	38
3			Quinoline, 4-styryl-	231	C17H13N	004594-84-7	35
4			Silane, diethylisobutoxy(3-methv...	260	C14H32O2Si	1000363-50-0	35
5			4-Amino-2-methyl-6,7,8,9-tetrahy...	231	C12H13N3O2	1000300-20-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061616\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	7.0 ng		231035	1	6.72	656250	20.0
Heptacosane	10.66	3.3 ng		127808	4	11.23	775794	20.0
Cyclododecane	11.46	2.5 ng		98879	4	11.23	775794	20.0
n-Heptadecanol-1	12.29	15.8 ng		612483	4	11.23	775794	20.0
4,8,12,16-Tetrame...	13.27	3.3 ng		135107	5	13.86	822713	20.0
Dodecanamide	13.38	2.7 ng		110437	5	13.86	822713	20.0
1-Heneicosanol	13.71	5.5 ng		226315	5	13.86	822713	20.0
1-Pentadecanethiol	14.35	2.3 ng		94913	5	13.86	822713	20.0
unknown15.53	15.53	3.9 ng		122218	6	15.25	628318	20.0
unknown15.71	15.71	2.1 ng		64942	6	15.25	628318	20.0