

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
 Data File : BF096364.D
 Acq On : 1 Jul 2017 4:16
 Operator : SJ/MA
 Sample : I3968-01
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-009

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-BF062717.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	4.957	483	488	496	rBV	455842	577901	16.03%	1.960%
2	5.375	554	559	562	rBV	3394405	3555373	98.63%	12.056%
3	6.393	727	732	737	rBV	3159152	3604736	100.00%	12.223%
4	6.528	750	755	759	rBV	3342368	3339816	92.65%	11.325%
5	6.757	790	794	798	rBV	1074655	892562	24.76%	3.027%
6	6.916	817	821	824	rBV	2801698	2424923	67.27%	8.223%
7	7.316	884	889	892	rBV	2095914	2037881	56.53%	6.910%
8	8.039	1008	1012	1016	rBV	1352230	1122784	31.15%	3.807%
9	9.116	1190	1195	1199	rBV	3035433	2933249	81.37%	9.946%
10	9.510	1258	1262	1265	rBV	521986	419938	11.65%	1.424%
11	9.739	1298	1301	1304	rVB	66307	54579	1.51%	0.185%
12	9.792	1304	1310	1314	rBV	1134717	960586	26.65%	3.257%
13	10.239	1383	1386	1388	rVB	74814	64830	1.80%	0.220%
14	10.575	1439	1443	1447	rBV	1684885	1658883	46.02%	5.625%
15	10.710	1462	1466	1475	rBV	85784	89503	2.48%	0.303%
16	11.157	1538	1542	1545	rBV2	47831	41156	1.14%	0.140%
17	11.275	1558	1562	1565	rBV	975686	858540	23.82%	2.911%
18	11.810	1649	1653	1668	rBV	332087	331091	9.18%	1.123%
19	12.592	1783	1786	1791	rBV	92779	95584	2.65%	0.324%
20	12.686	1799	1802	1806	rBV2	66538	66667	1.85%	0.226%
21	12.857	1827	1831	1835	rBV	2495902	2450018	67.97%	8.308%
22	13.316	1906	1909	1912	rBV3	32613	42133	1.17%	0.143%
23	13.392	1920	1922	1924	rBV	43841	40504	1.12%	0.137%
24	13.757	1981	1984	1991	rBV	315159	308249	8.55%	1.045%
25	13.904	2005	2009	2012	rBV	850030	791314	21.95%	2.683%
26	14.392	2089	2092	2095	rBV	89377	78248	2.17%	0.265%
27	15.015	2195	2198	2205	rVB2	84680	106374	2.95%	0.361%
28	15.321	2246	2250	2255	rVB	435884	543118	15.07%	1.842%

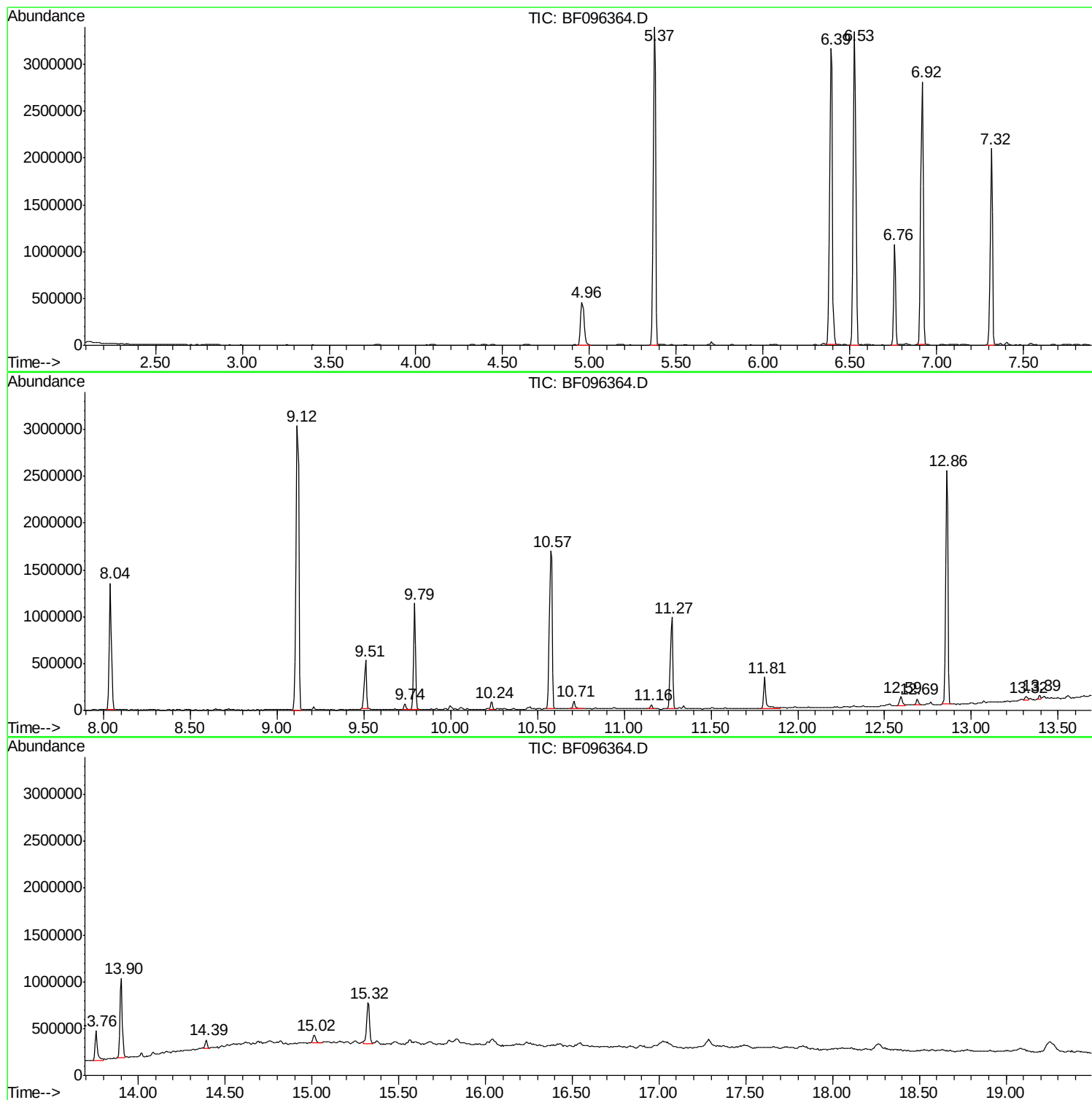
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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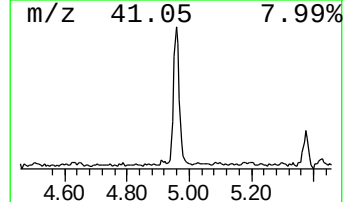
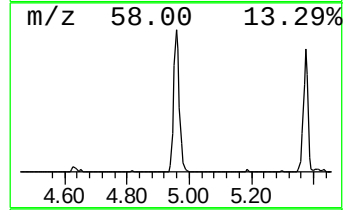
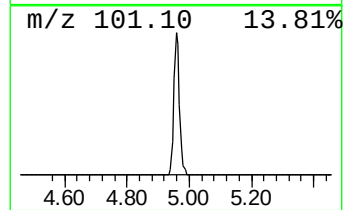
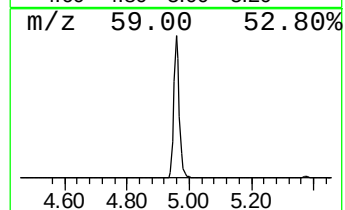
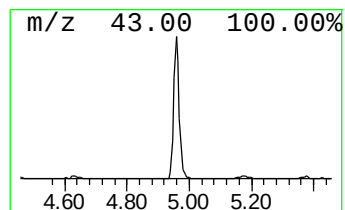
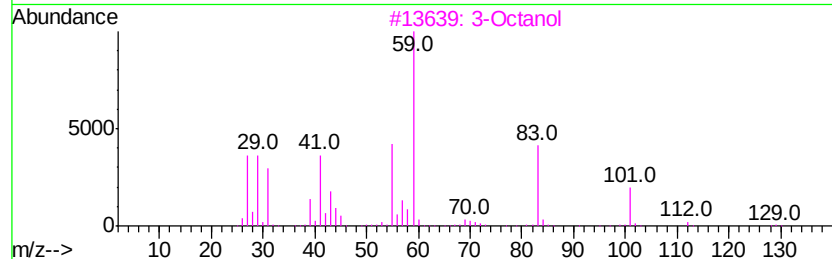
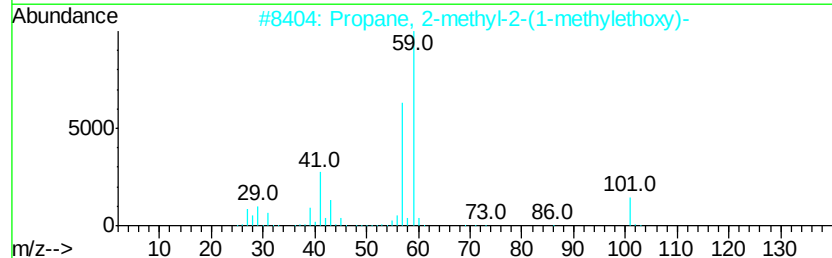
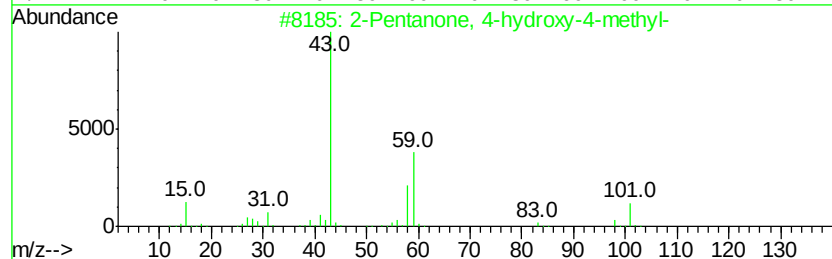
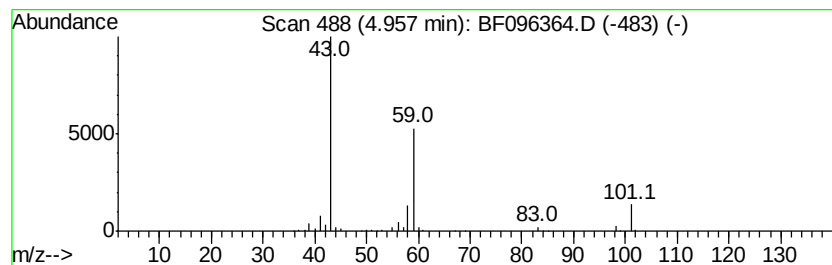
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	12.95 ng	577901	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Octanol	130	C8H18O	000589-98-0	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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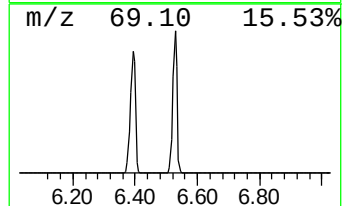
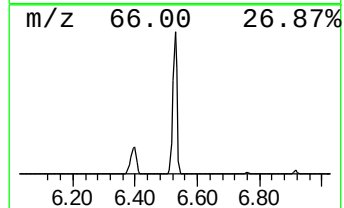
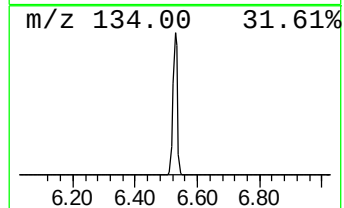
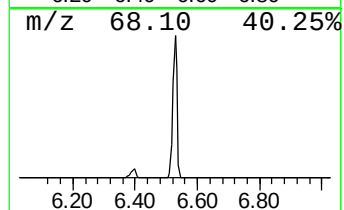
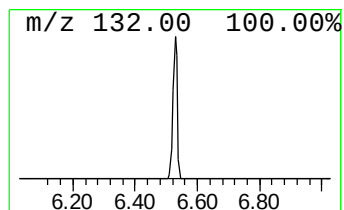
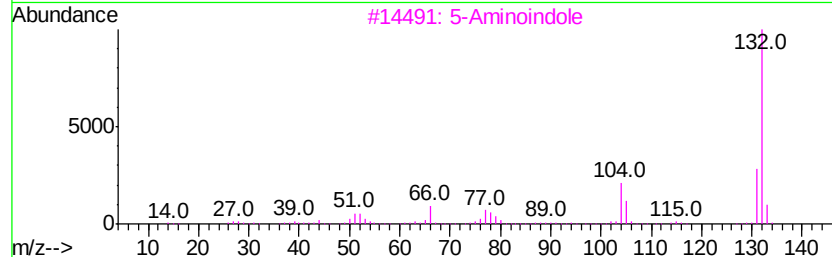
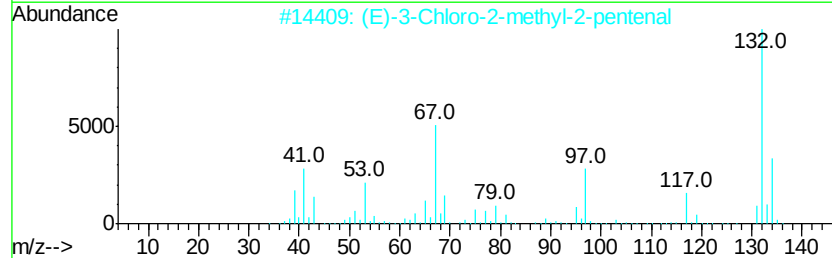
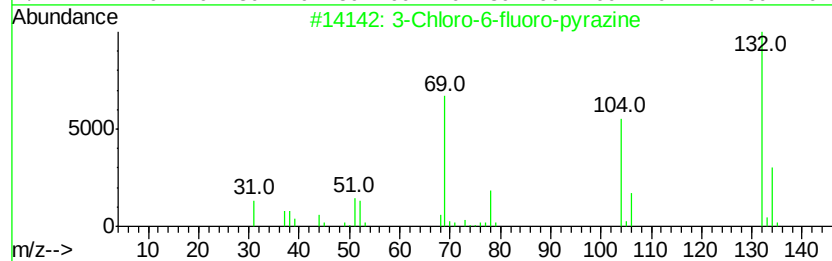
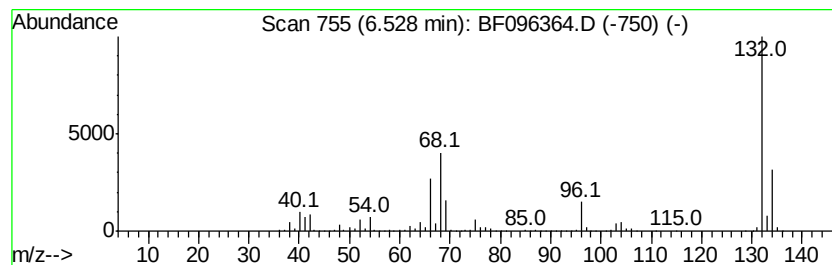
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	74.84 ng	3339820	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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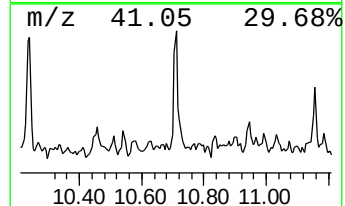
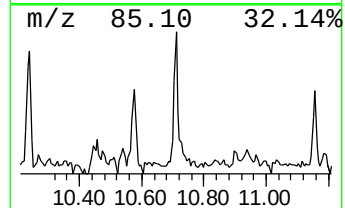
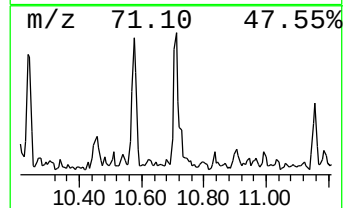
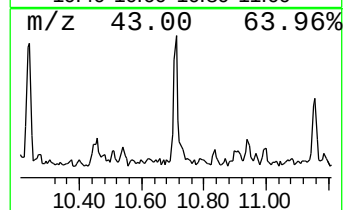
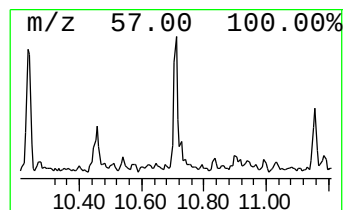
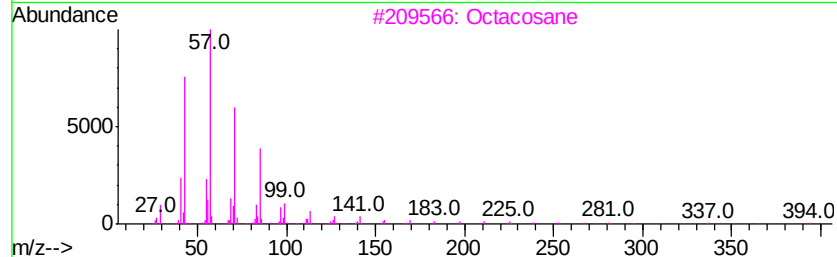
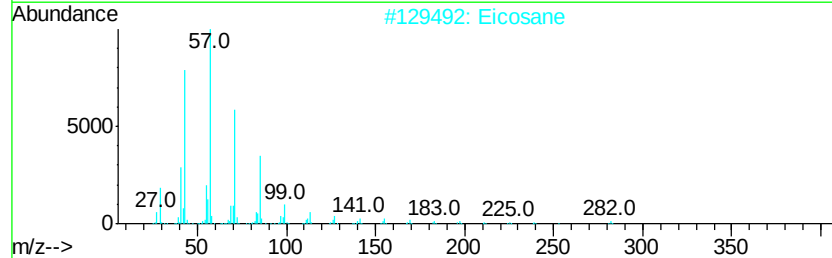
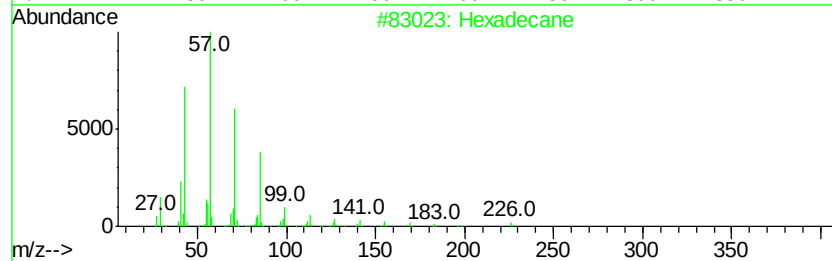
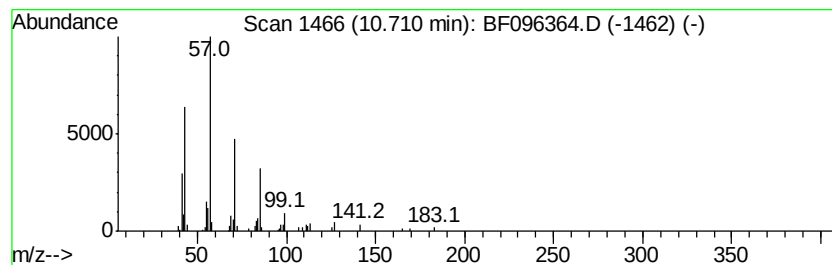
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Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.71	2.09 ng	89503	Phenanthrene-d10		11.27
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Heptacosane	380	C27H56	000593-49-7	83



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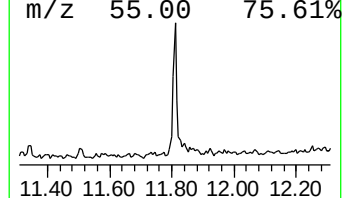
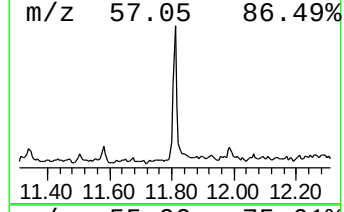
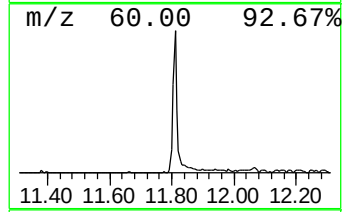
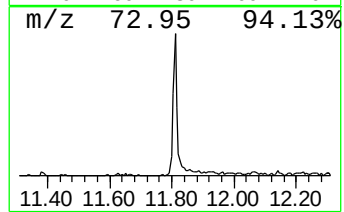
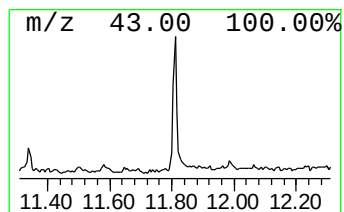
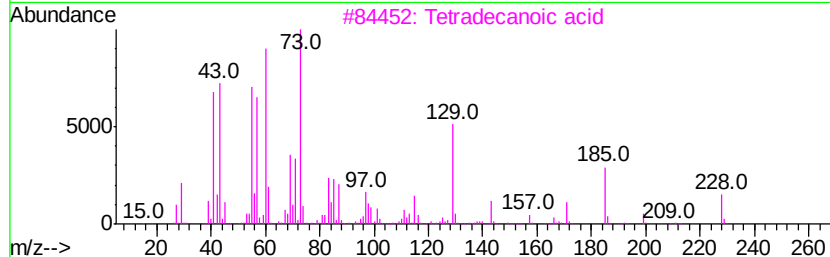
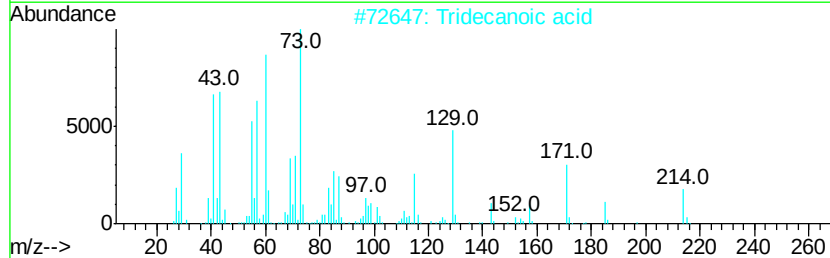
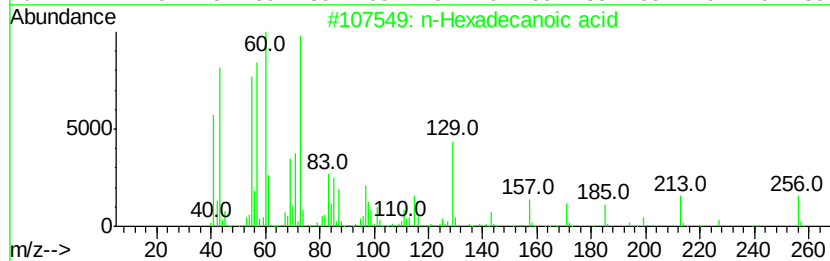
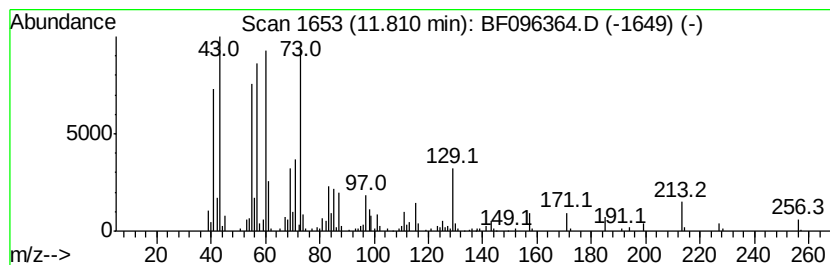
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	7.71 ng	331091	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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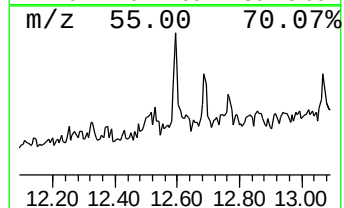
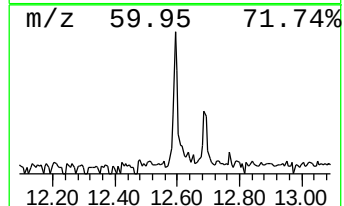
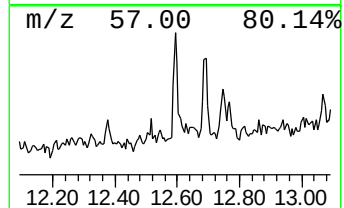
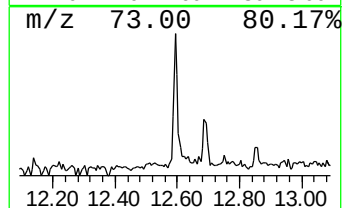
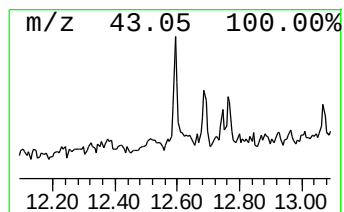
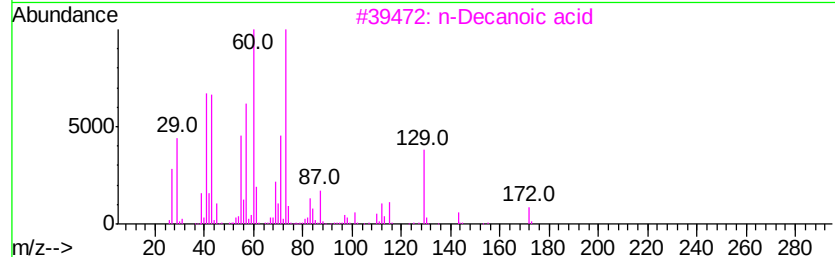
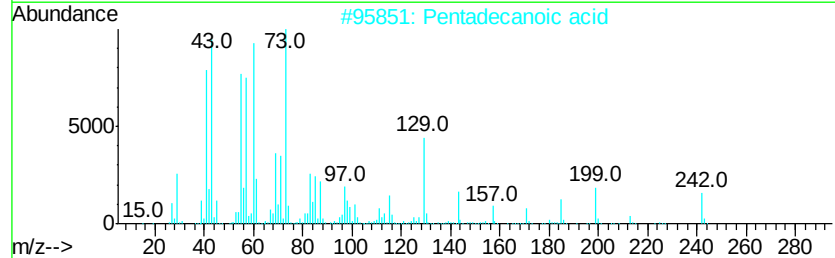
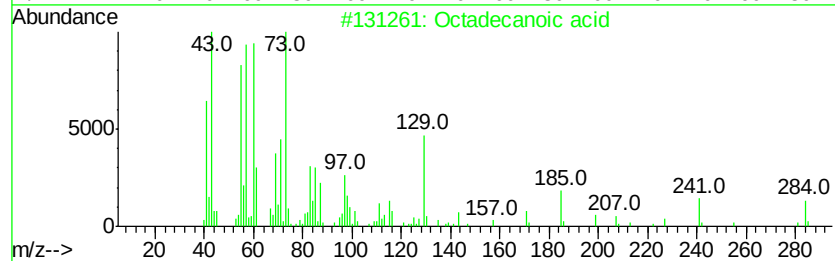
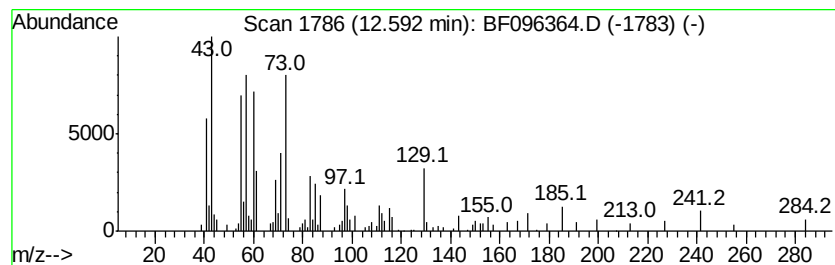
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.59	2.42 ng	95584	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	58
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	38



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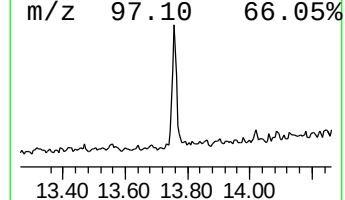
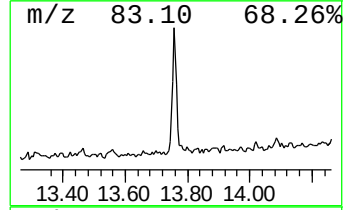
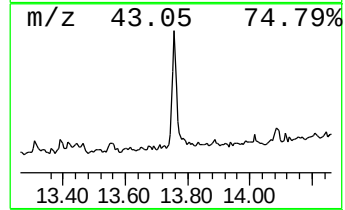
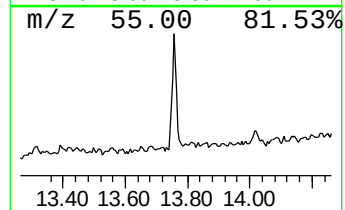
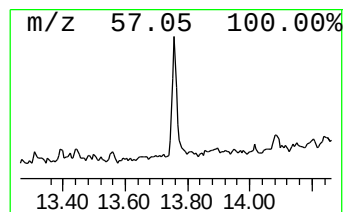
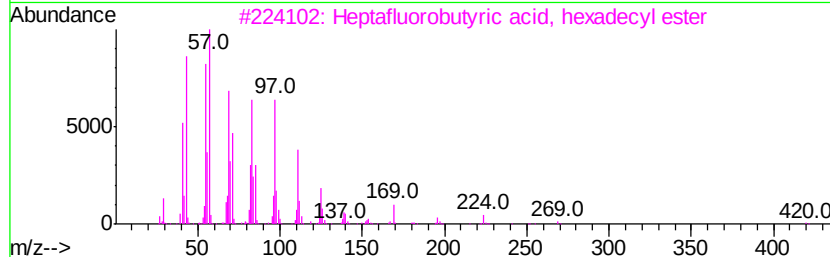
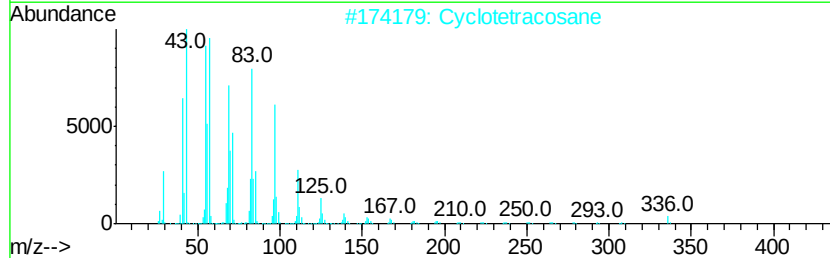
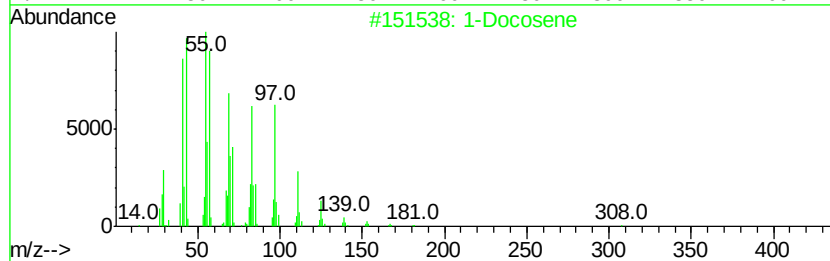
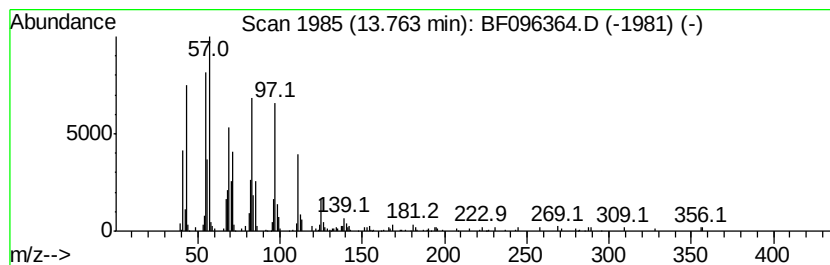
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	7.79 ng	308249	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	96
2		Cyclotetracosane	336	C24H48	000297-03-0	95
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096364.D
Acq On : 1 Jul 2017 4:16
Operator : SJ/MA
Sample : I3968-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-009

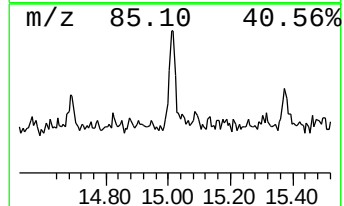
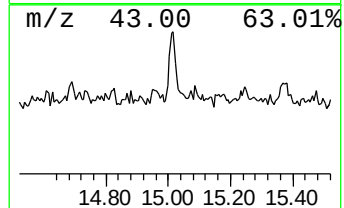
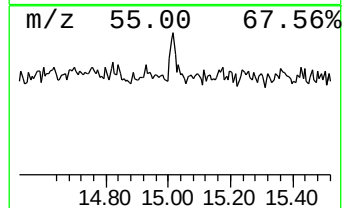
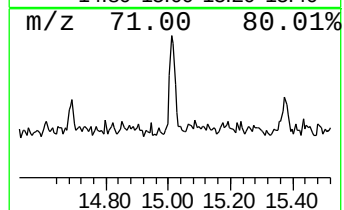
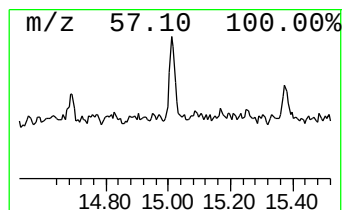
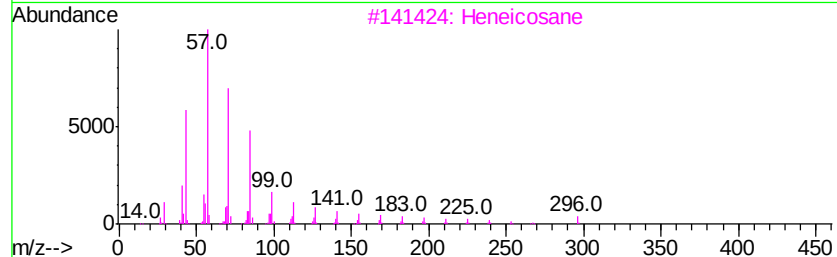
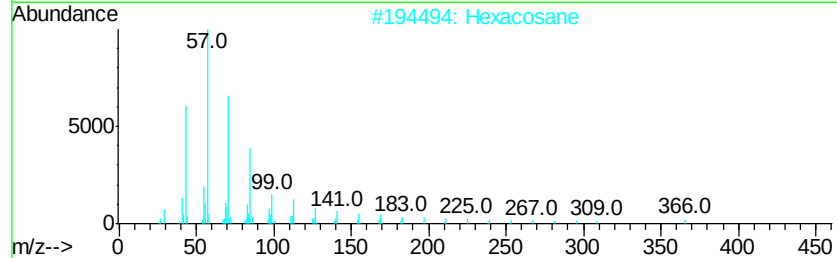
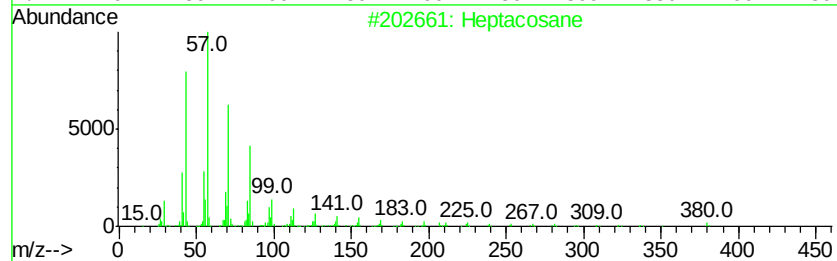
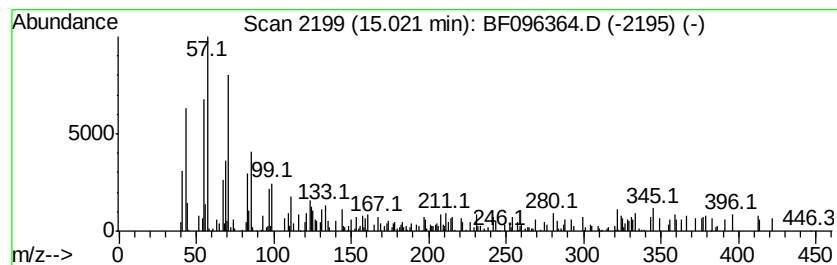
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.92 ng	106374	Perylene-d12	15.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	89
2		Hexacosane	366	C26H54	000630-01-3	81
3		Heneicosane	296	C21H44	000629-94-7	76
4		Tetradecane	198	C14H30	000629-59-4	70
5		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063017\
Data File : BF096364.D
Acq On : 1 Jul 2017 4:16
Operator : SJ/MA
Sample : I3968-01
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-009

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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...	4.96	12.9	ng	577901	1	6.76	892562	20.0
unknown6.53	6.53	74.8	ng	3339820	1	6.76	892562	20.0
Hexadecane	10.71	2.1	ng	89503	4	11.27	858540	20.0
n-Hexadecanoic acid	11.81	7.7	ng	331091	4	11.27	858540	20.0
Octadecanoic acid	12.59	2.4	ng	95584	5	13.90	791314	20.0
1-Docosene	13.76	7.8	ng	308249	5	13.90	791314	20.0
Heptacosane	15.02	3.9	ng	106374	6	15.32	543118	20.0