

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042517\
 Data File : BF094616.D
 Acq On : 25 Apr 2017 20:13
 Operator : SJ/MA
 Sample : I2832-07
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEST-PIT-CURVE-(0-5)

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-BF041717.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	3.913	332	336	344	rBV	325183	413064	11.11%	1.300%
2	4.307	398	403	417	rBV	3244318	3456197	92.96%	10.876%
3	5.384	580	586	589	rBV	3084690	3514769	94.54%	11.061%
4	5.507	602	607	610	rBV	3560448	3601343	96.87%	11.333%
5	5.754	645	649	653	rBV	818880	726539	19.54%	2.286%
6	5.931	674	679	682	rBV	2930429	2788598	75.01%	8.776%
7	6.407	754	760	763	rBV	2175447	2280382	61.34%	7.176%
8	7.007	860	862	878	rVB2	21312	39620	1.07%	0.125%
9	7.248	898	903	906	rBV	991512	988563	26.59%	3.111%
10	8.572	1123	1128	1131	rBV	3773625	3717804	100.00%	11.700%
11	9.072	1209	1213	1217	rBV	247272	239763	6.45%	0.755%
12	9.377	1259	1265	1270	rBV2	980691	1033888	27.81%	3.254%
13	9.977	1363	1367	1371	rVB	76119	64644	1.74%	0.203%
14	10.254	1408	1414	1416	rBV3	25276	37572	1.01%	0.118%
15	10.301	1419	1422	1426	rVB	90661	83184	2.24%	0.262%
16	10.360	1426	1432	1435	rBV	1556827	1808905	48.66%	5.693%
17	10.560	1463	1466	1469	rBV	82409	87277	2.35%	0.275%
18	11.201	1571	1575	1578	rBV	875313	860580	23.15%	2.708%
19	11.224	1578	1579	1584	rVB	101156	89167	2.40%	0.281%
20	11.448	1614	1617	1621	rVB	48721	51275	1.38%	0.161%
21	11.554	1631	1635	1642	rBV	142537	178147	4.79%	0.561%
22	11.936	1692	1700	1707	rBV3	75142	123516	3.32%	0.389%
23	12.689	1824	1828	1832	rVB	172872	167947	4.52%	0.529%
24	12.965	1868	1875	1879	rVB	163626	183508	4.94%	0.577%
25	13.148	1902	1906	1907	rBV	176411	155885	4.19%	0.491%
26	13.183	1907	1912	1915	rVB	2341840	2539735	68.31%	7.992%
27	13.607	1980	1984	1989	rVB2	88565	90412	2.43%	0.285%
28	14.348	2101	2110	2118	rBV2	92414	170518	4.59%	0.537%
29	14.448	2122	2127	2131	rVV	704648	855865	23.02%	2.693%
30	14.477	2131	2132	2136	rVB	81356	68970	1.86%	0.217%
31	14.618	2152	2156	2160	rBV5	32710	46263	1.24%	0.146%
32	14.659	2160	2163	2167	rVB	39717	44289	1.19%	0.139%
33	15.395	2282	2288	2292	rBV7	23039	44293	1.19%	0.139%
34	15.677	2333	2336	2339	rBV	87626	117524	3.16%	0.370%

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35	15.848	2362	2365	2368	rBV2	53761	61511	1.65%	0.194%
36	15.965	2381	2385	2391	rBV2	69103	86079	2.32%	0.271%
37	16.018	2391	2394	2398	rBV	69642	76564	2.06%	0.241%
38	16.077	2400	2404	2413	rVV	607403	711243	19.13%	2.238%
39	16.571	2484	2488	2493	rBV	92350	124817	3.36%	0.393%
40	17.500	2642	2646	2650	rBV6	29728	46624	1.25%	0.147%

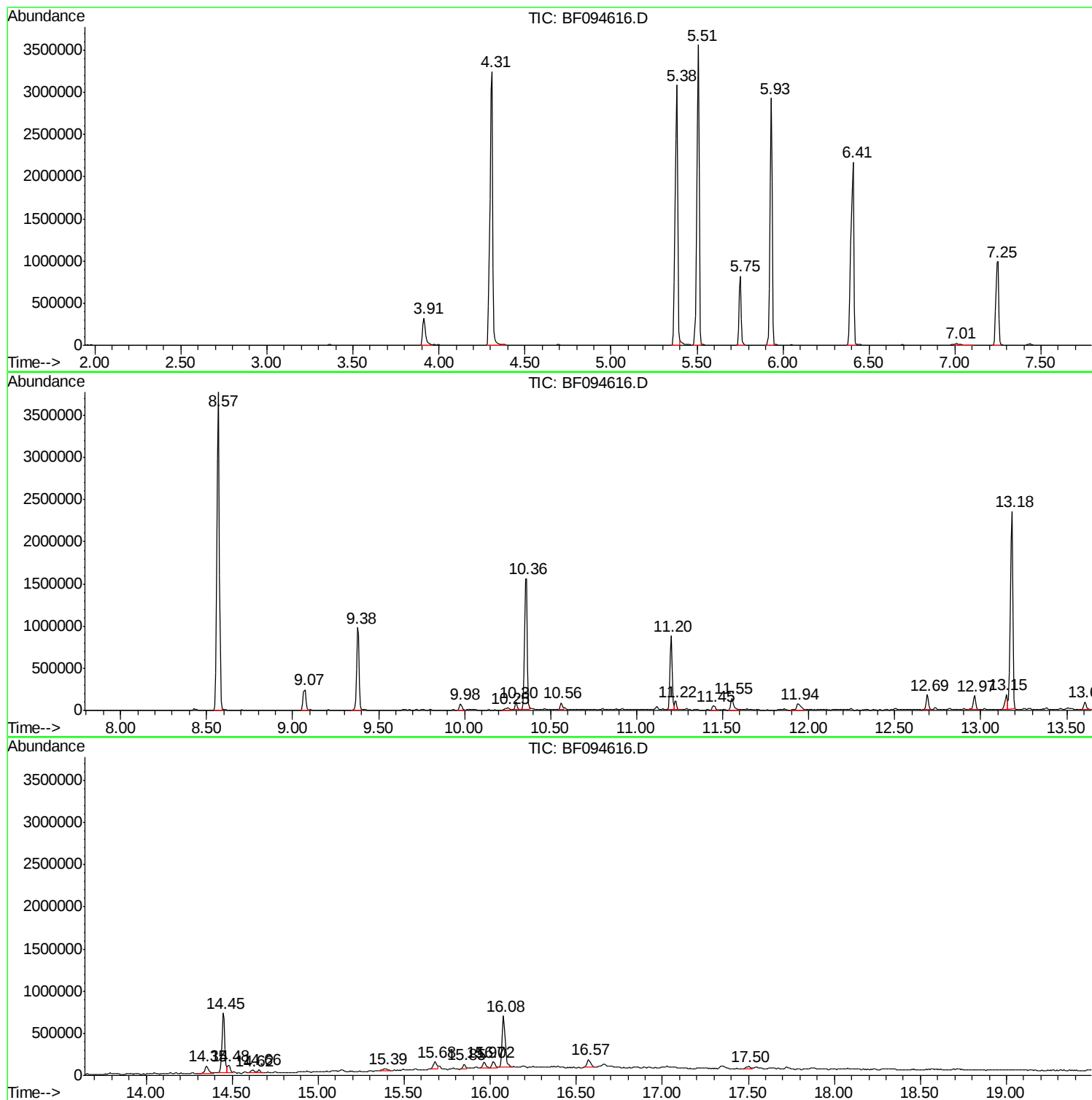
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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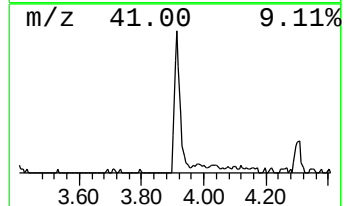
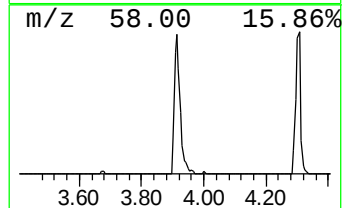
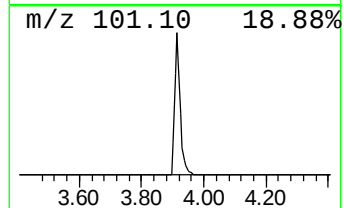
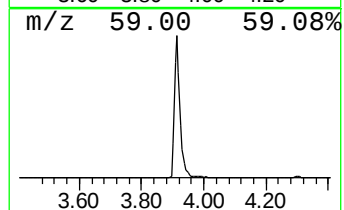
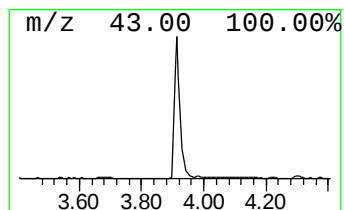
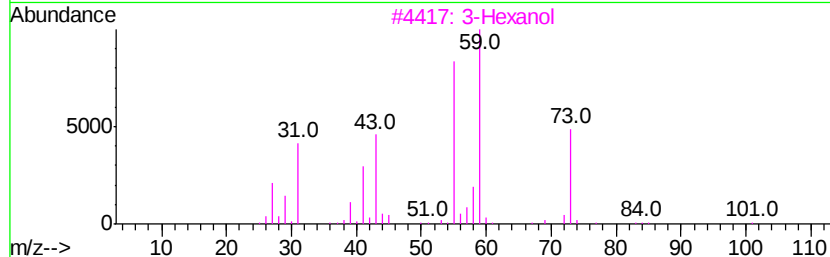
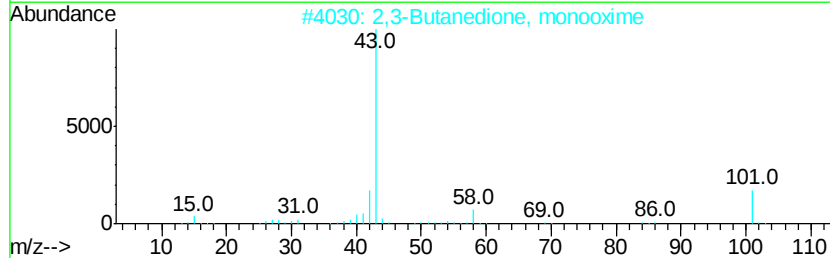
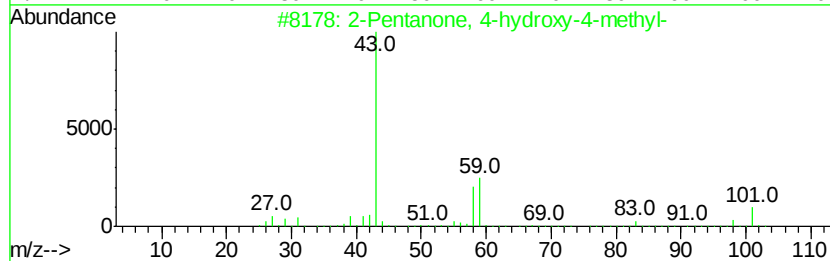
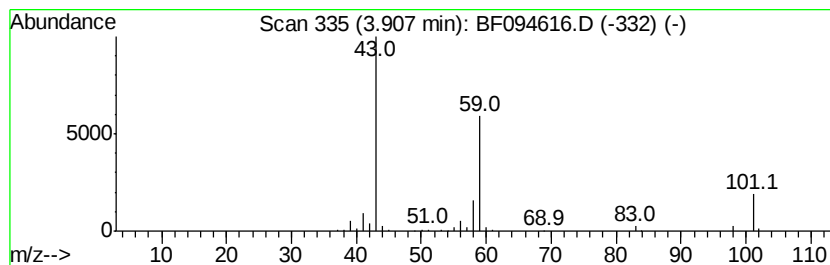
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	11.37 ng	413064	1,4-Dichlorobenzene-d4	5.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		3-Hexanol	102	C6H14O	000623-37-0	28
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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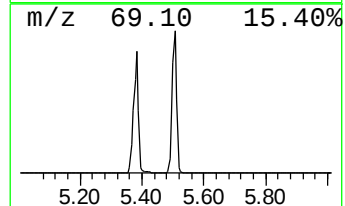
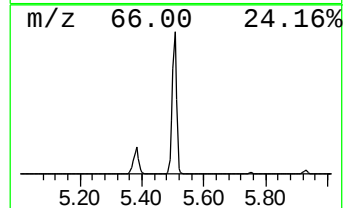
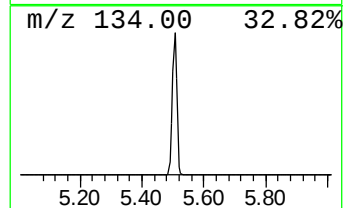
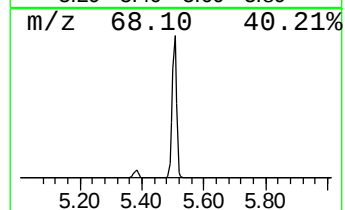
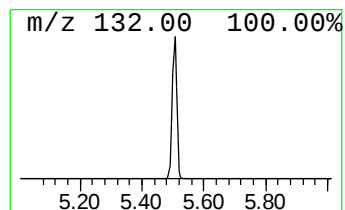
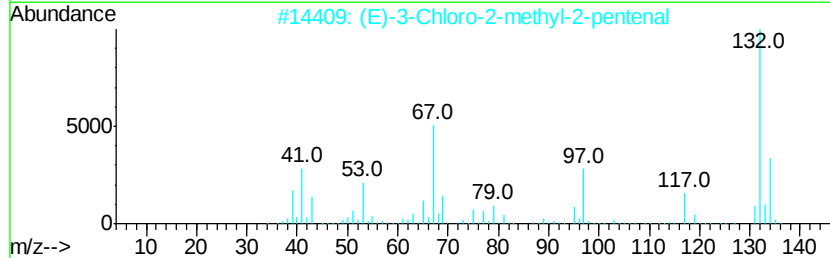
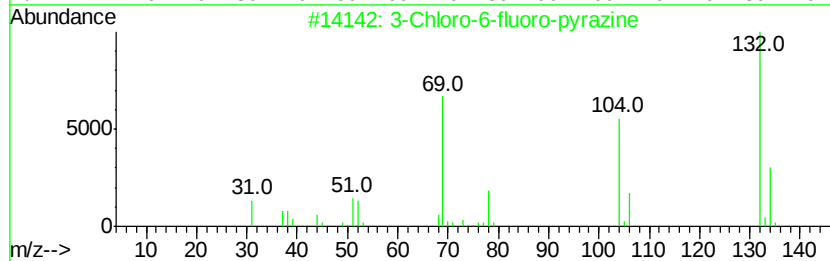
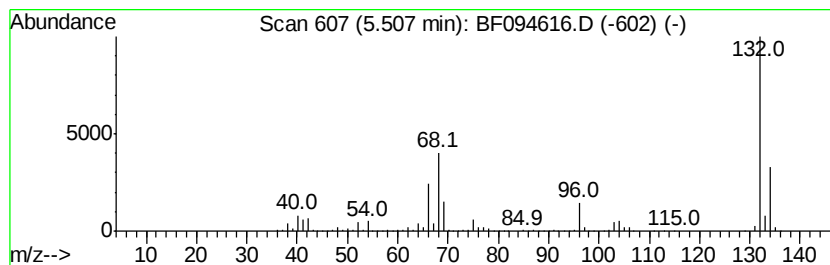
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown5.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	99.14 ng	3601340	1,4-Dichlorobenzene-d4	5.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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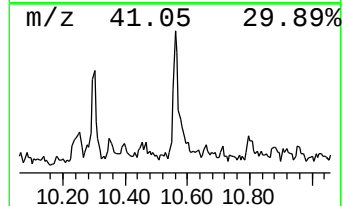
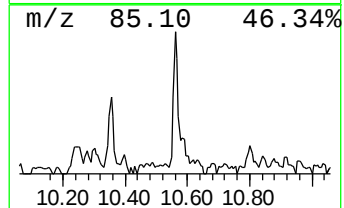
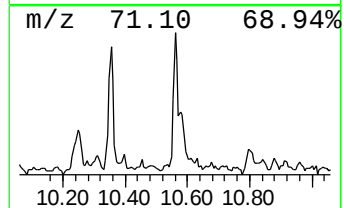
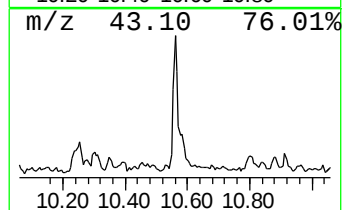
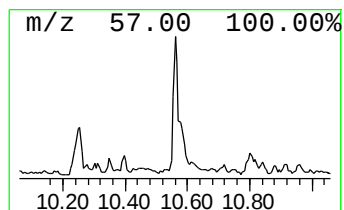
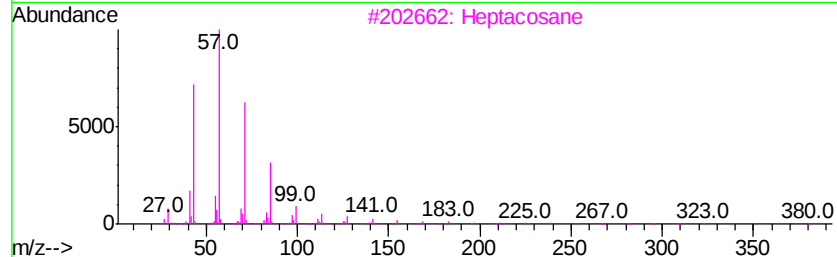
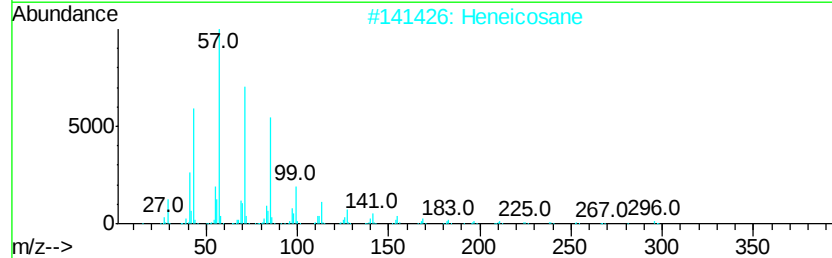
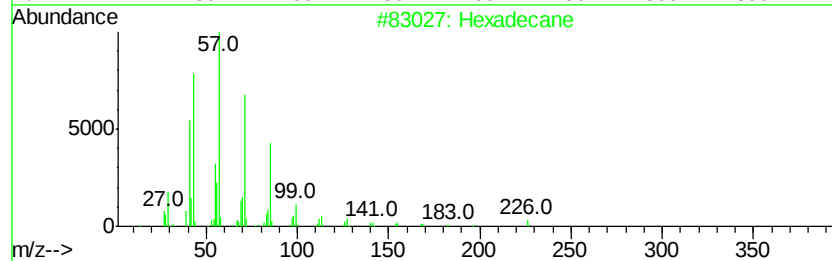
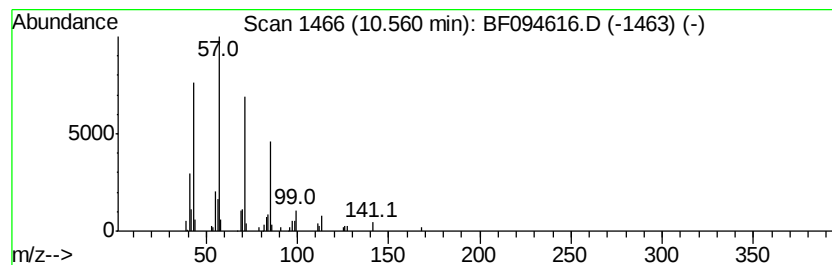
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Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.03 ng	87277	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptacosane	380	C27H56	000593-49-7	90
4		Tetracosane	338	C24H50	000646-31-1	90
5		Eicosane	282	C20H42	000112-95-8	86



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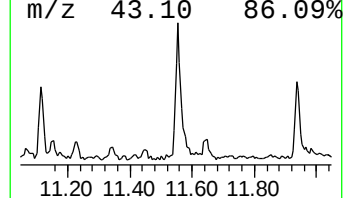
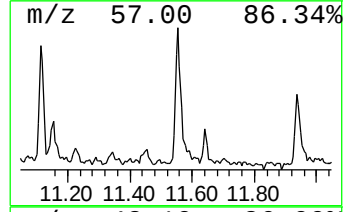
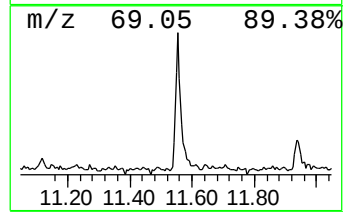
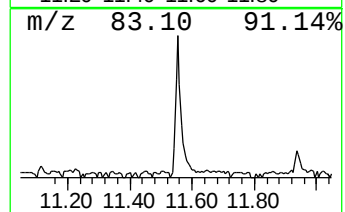
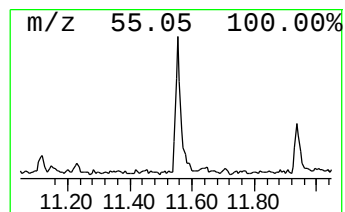
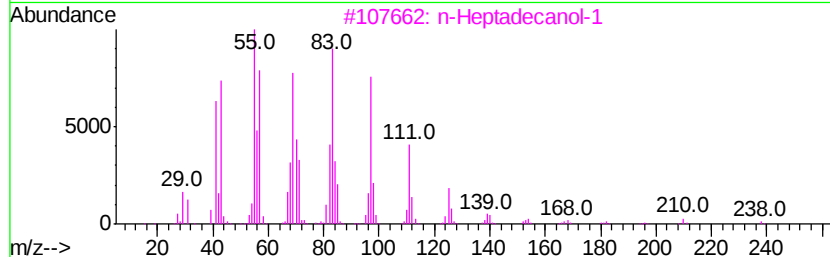
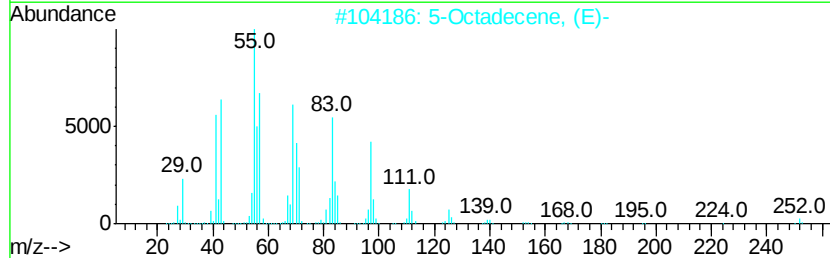
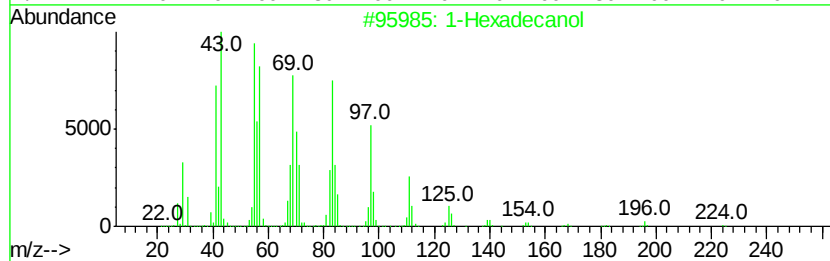
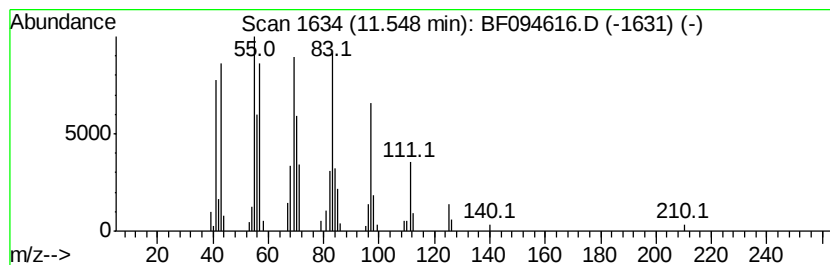
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.14 ng	178147	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanol	242	C16H34O	036653-82-4	95
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4		4-Heptafluorobutylxyloxyhexadecane	438	C20H33F7O2	1000282-97-2	87
5		Cetene	224	C16H32	000629-73-2	68



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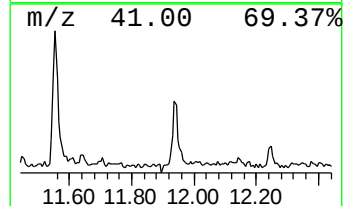
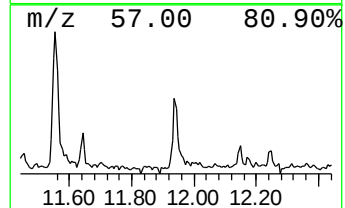
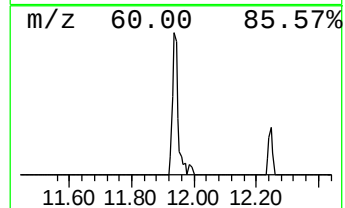
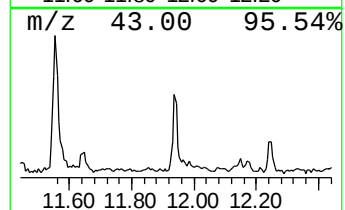
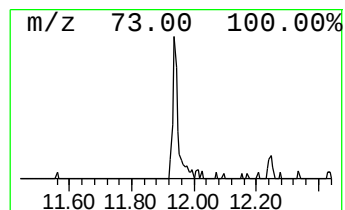
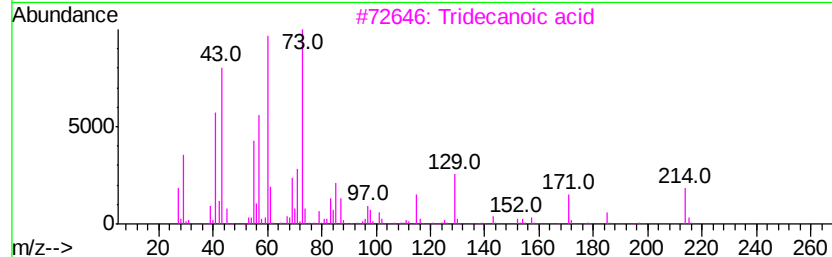
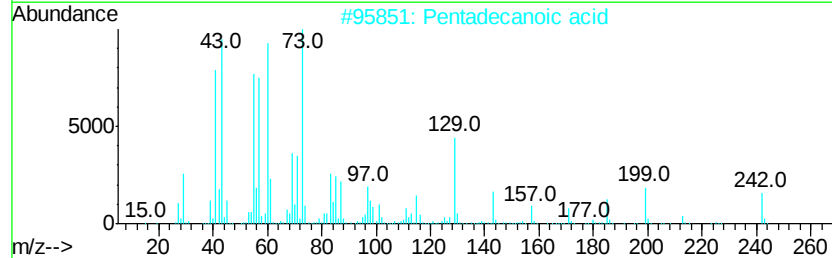
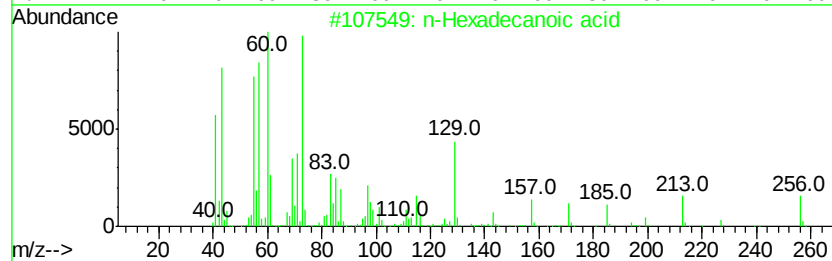
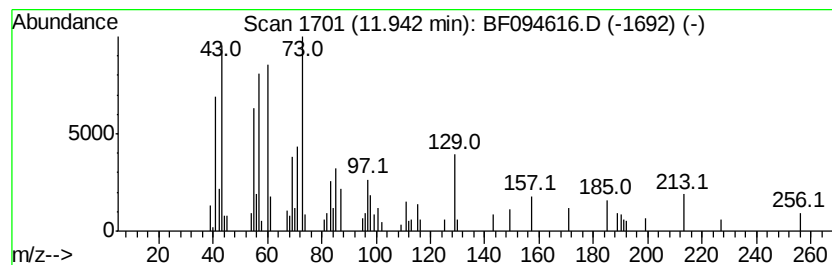
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.87 ng	123516	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3		Tridecanoic acid	214	C13H26O2	000638-53-9	52
4		n-Decanoic acid	172	C10H20O2	000334-48-5	50
5		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042517\
Data File : BF094616.D
Acq On : 25 Apr 2017 20:13
Operator : SJ/MA
Sample : I2832-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEST-PIT-CURVE-(0-5)

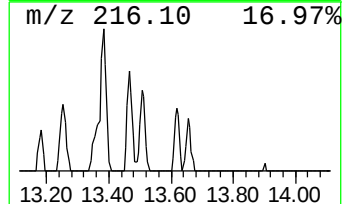
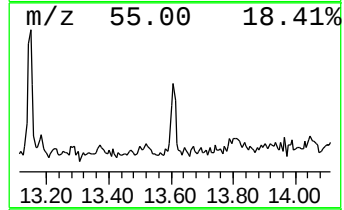
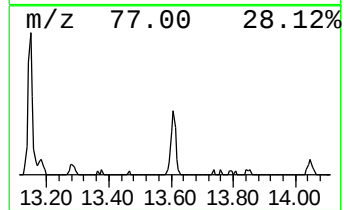
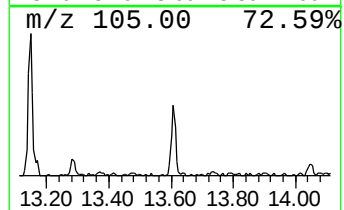
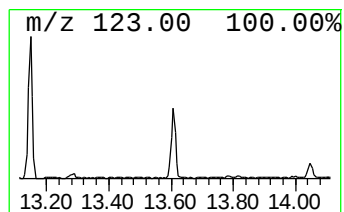
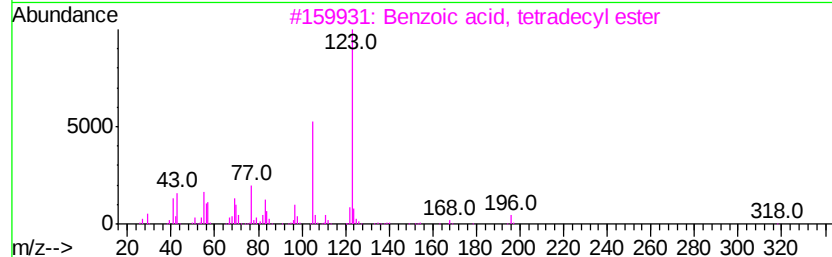
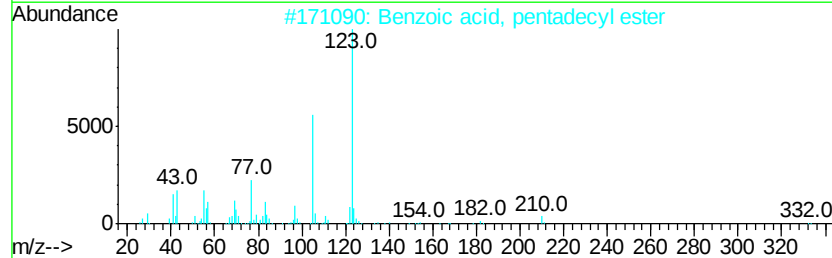
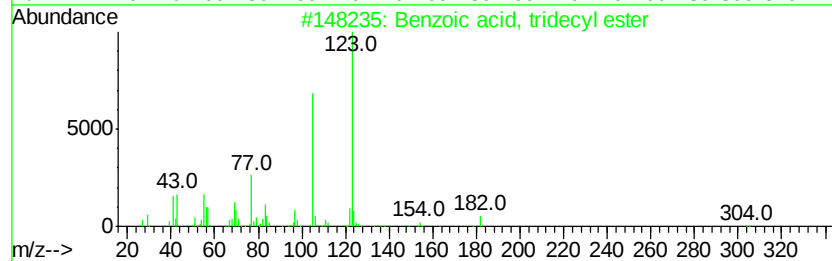
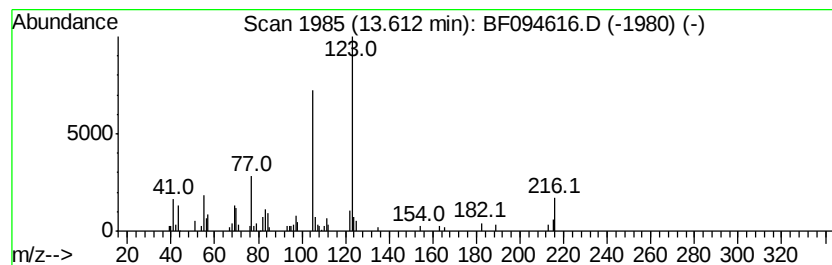
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzoic acid, tridecyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.11 ng	90412	Chrysene-d12	14.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, tridecyl ester	304	C20H32O2	1000340-22-6	91
2		Benzoic acid, pentadecyl ester	332	C22H36O2	1000340-22-8	91
3		Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	91
4		Benzoic acid, nonadecyl ester	388	C26H44O2	1000340-23-2	91
5		Benzoic acid, octadecyl ester	374	C25H42O2	1000340-23-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042517\
Data File : BF094616.D
Acq On : 25 Apr 2017 20:13
Operator : SJ/MA
Sample : I2832-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

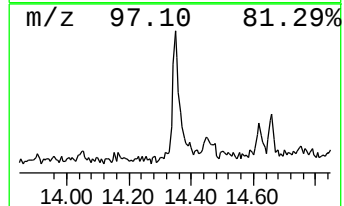
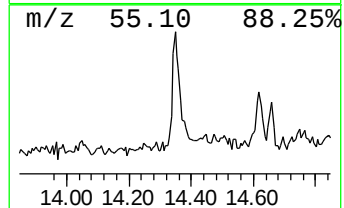
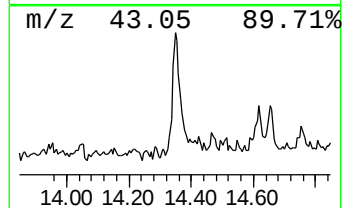
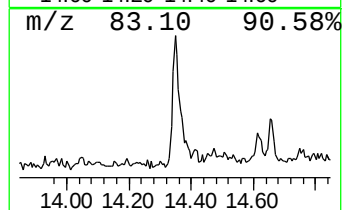
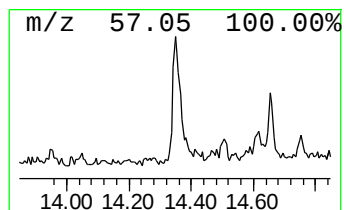
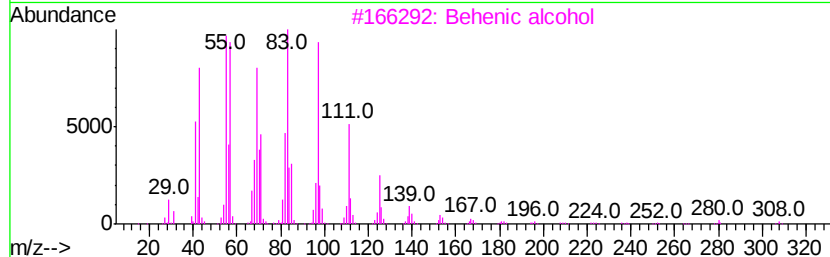
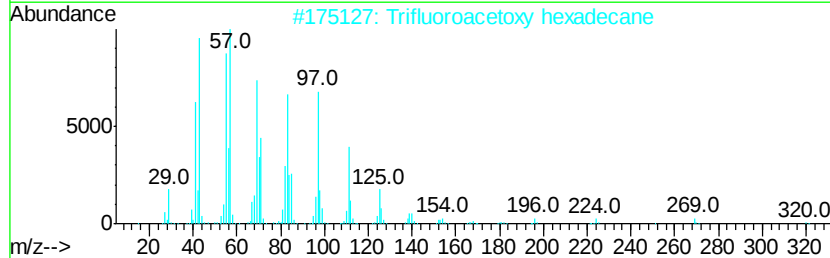
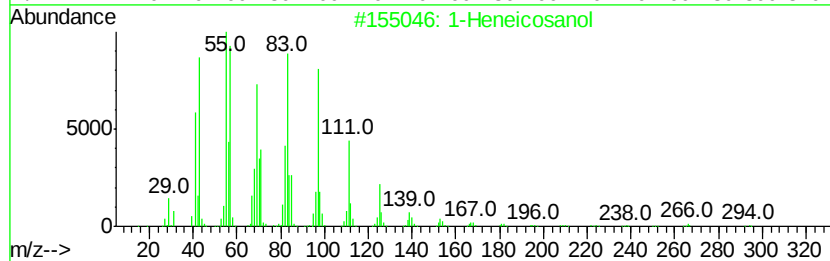
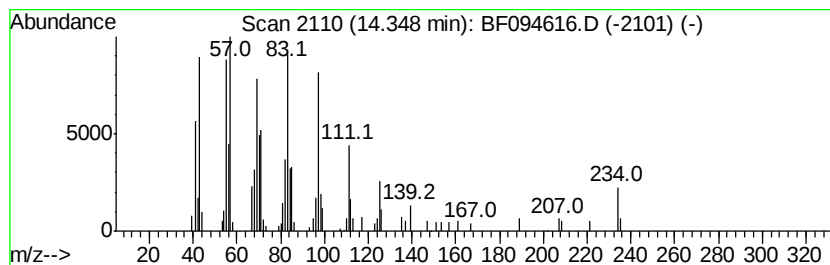
Instrument :
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ClientSampleId :
TEST-PIT-CURVE-(0-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.35	3.98 ng	170518	Chrysene-d12	14.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042517\
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Acq On : 25 Apr 2017 20:13
Operator : SJ/MA
Sample : I2832-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEST-PIT-CURVE-(0-5)

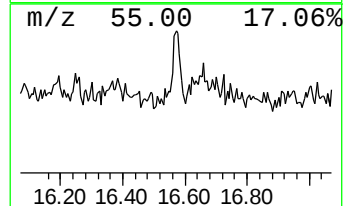
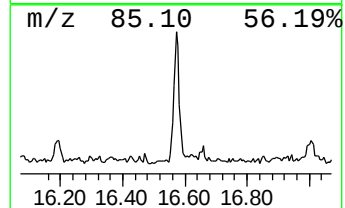
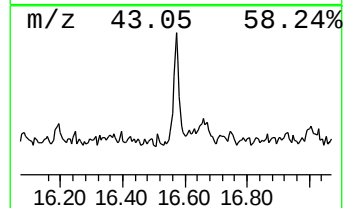
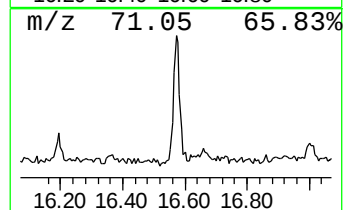
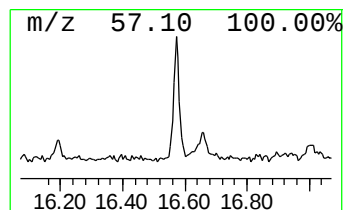
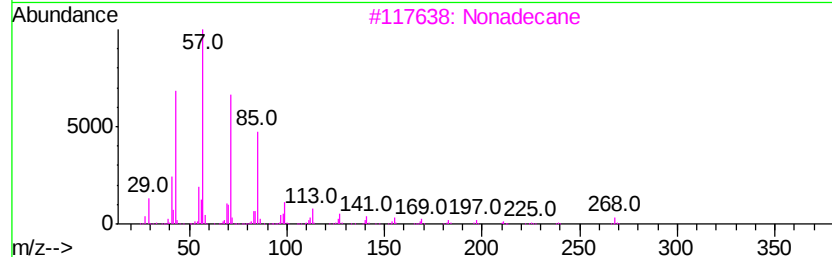
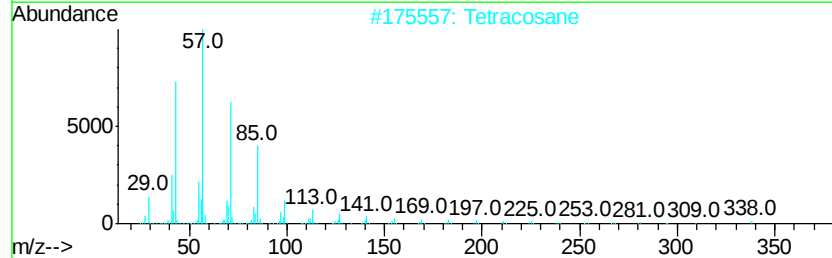
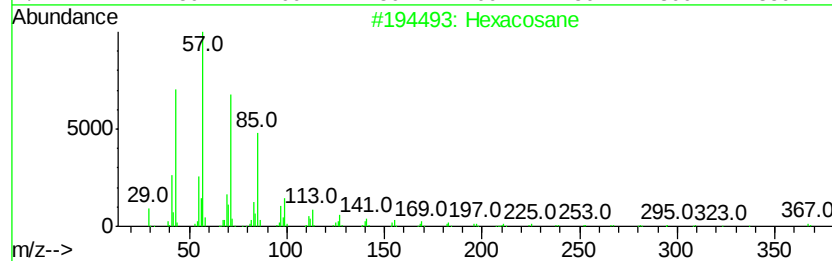
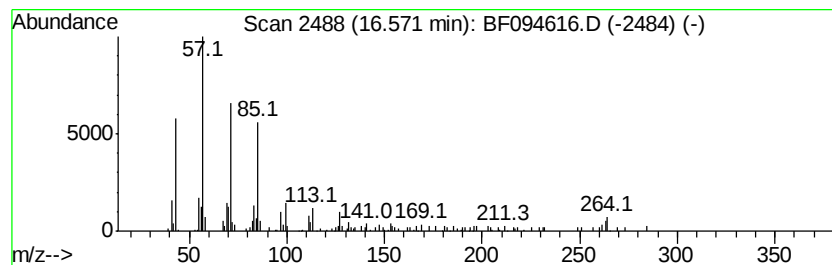
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	3.51 ng	124817	Perylene-d12	16.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Nonadecane	268	C19H40	000629-92-5	83
4			Heptadecane	240	C17H36	000629-78-7	83
5			Octadecane	254	C18H38	000593-45-3	80



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Operator : SJ/MA
Sample : I2832-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEST-PIT-CURVE-(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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...	3.91	11.4	ng	413064	1	5.75	726539	20.0
unknown5.51	5.51	99.1	ng	3601340	1	5.75	726539	20.0
Hexadecane	10.56	2.0	ng	87277	4	11.20	860580	20.0
1-Hexadecanol	11.55	4.1	ng	178147	4	11.20	860580	20.0
n-Hexadecanoic acid	11.94	2.9	ng	123516	4	11.20	860580	20.0
Benzoic acid, tri...	13.61	2.1	ng	90412	5	14.45	855865	20.0
1-Heneicosanol	14.35	4.0	ng	170518	5	14.45	855865	20.0
Hexacosane	16.57	3.5	ng	124817	6	16.08	711243	20.0