

Data Path : Z:\HPCHEM1\BNA F\Data\BF042117\
 Data File : BF094573.D
 Acq On : 21 Apr 2017 20:09
 Operator : SJ/MA
 Sample : I2786-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BL-2(3)

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	3.907	332	335	349	rVB	241714	284370	10.19%	1.218%
2	4.313	399	404	415	rBV	2164017	2241480	80.29%	9.597%
3	5.390	582	587	602	rBV	2287624	2386628	85.49%	10.219%
4	5.513	604	608	612	rBV	2494118	2398755	85.92%	10.270%
5	5.760	646	650	654	rBV	679611	593674	21.27%	2.542%
6	5.937	676	680	684	rBV	1946055	1909427	68.40%	8.175%
7	6.413	755	761	764	rBV	1457012	1478196	52.95%	6.329%
8	7.254	900	904	908	rBV	928102	800102	28.66%	3.426%
9	8.578	1124	1129	1132	rBV	2879001	2791719	100.00%	11.953%
10	9.078	1210	1214	1219	rBV	515313	453059	16.23%	1.940%
11	9.389	1260	1267	1272	rBV	850102	874218	31.31%	3.743%
12	9.983	1364	1368	1372	rVB	55710	54853	1.96%	0.235%
13	10.260	1408	1415	1418	rBV2	19284	31133	1.12%	0.133%
14	10.366	1428	1433	1438	rBV	1234458	1410757	50.53%	6.040%
15	10.566	1464	1467	1470	rBV	70788	84297	3.02%	0.361%
16	10.807	1505	1508	1511	rBV2	24452	31287	1.12%	0.134%
17	11.125	1558	1562	1565	rBV	62323	62521	2.24%	0.268%
18	11.160	1565	1568	1572	rVV2	26073	32612	1.17%	0.140%
19	11.207	1572	1576	1579	rVV	828460	797033	28.55%	3.413%
20	11.236	1579	1581	1584	rVB	38796	36802	1.32%	0.158%
21	11.648	1648	1651	1654	rVB	54264	50730	1.82%	0.217%
22	11.942	1698	1701	1708	rBV3	63659	98988	3.55%	0.424%
23	12.154	1734	1737	1740	rVB	36857	36652	1.31%	0.157%
24	12.695	1826	1829	1832	rVB	59071	53823	1.93%	0.230%
25	12.971	1872	1876	1880	rVB	59171	66651	2.39%	0.285%
26	13.183	1907	1912	1916	rBV	1994689	2315794	82.95%	9.915%
27	14.354	2107	2111	2118	rBV4	58342	100991	3.62%	0.432%
28	14.454	2123	2128	2132	rBV	680179	760340	27.24%	3.255%
29	15.136	2240	2244	2249	rBV4	32748	46856	1.68%	0.201%
30	15.677	2333	2336	2339	rBV	31019	42604	1.53%	0.182%
31	15.848	2362	2365	2369	rBV2	58988	72059	2.58%	0.309%
32	16.018	2391	2394	2397	rBV	30051	35233	1.26%	0.151%
33	16.077	2400	2404	2413	rVV	673408	770689	27.61%	3.300%
34	16.571	2484	2488	2492	rBV2	63997	85838	3.07%	0.368%

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ALS Vial : 16 Sample Multiplier: 1

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BNA_F
ClientSampleId :
BL-2(3)

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.495	2642	2645	2651	rVB5	38616	65773	2.36%	0.282%
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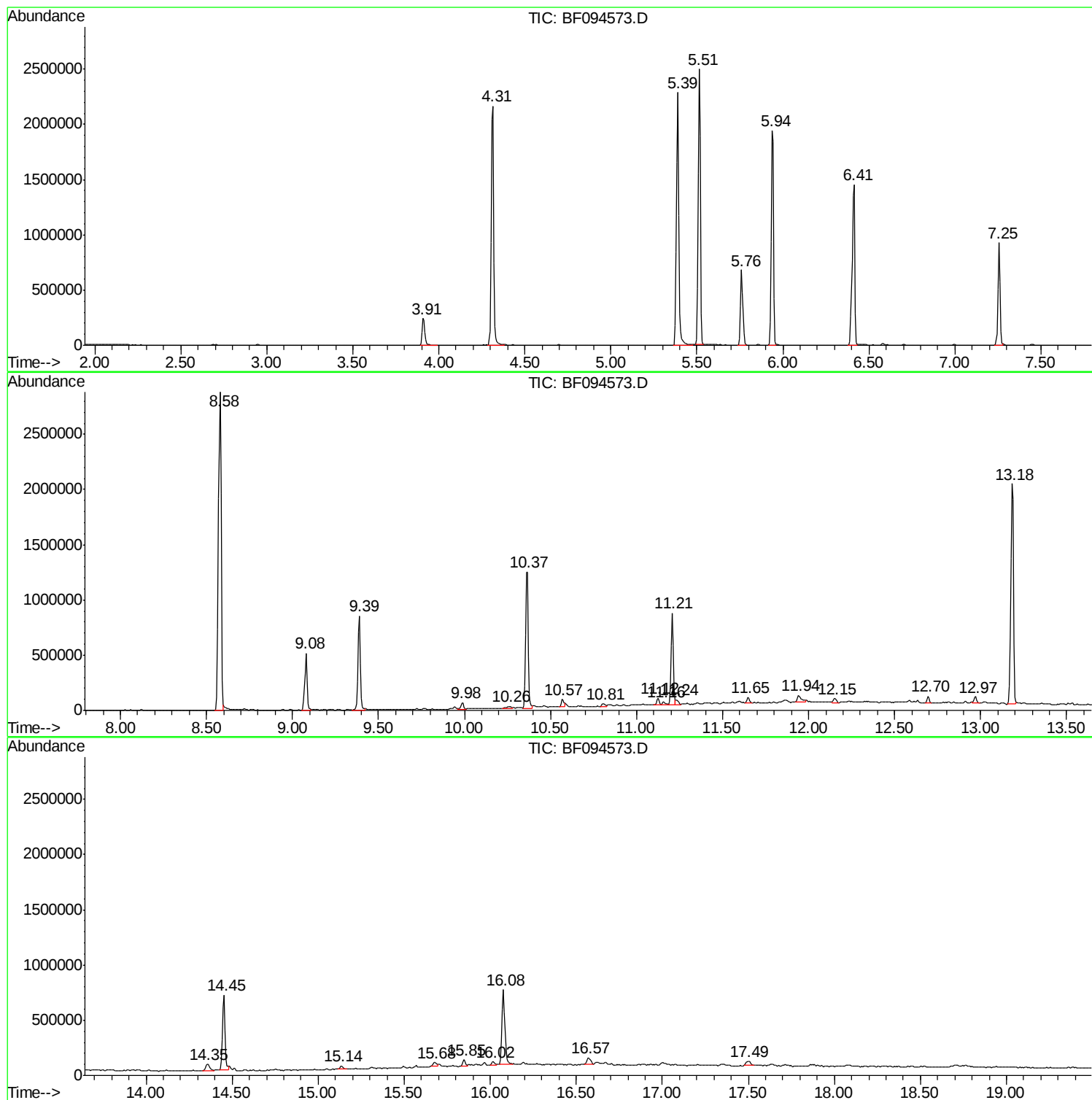
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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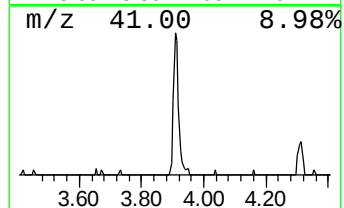
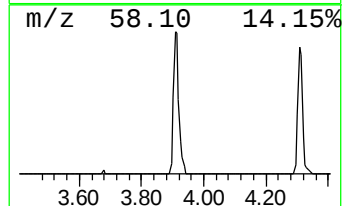
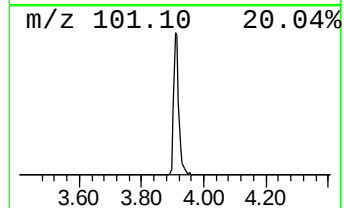
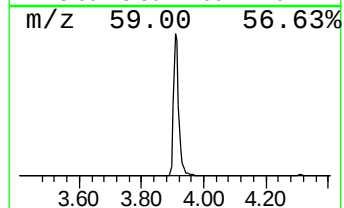
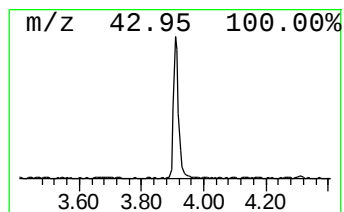
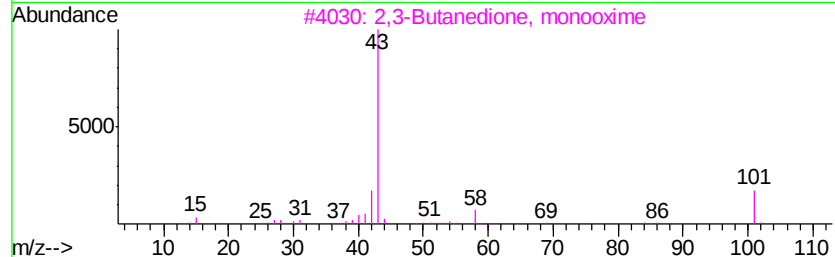
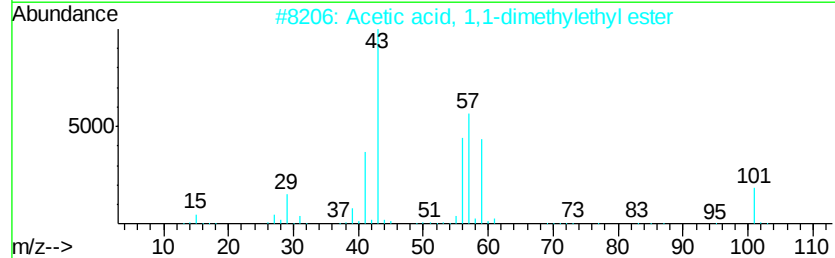
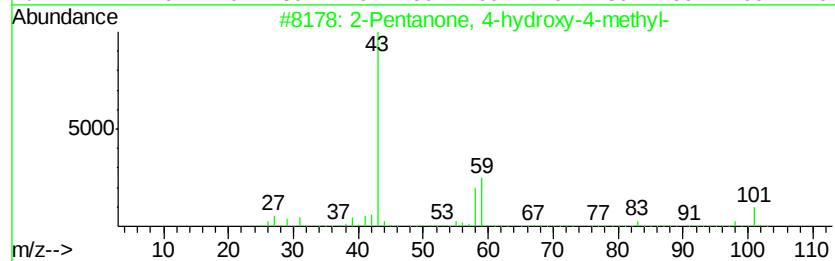
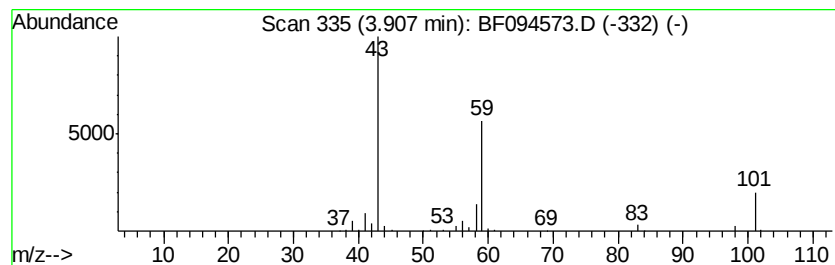
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	9.58 ng	284370	1,4-Dichlorobenzene-d4	5.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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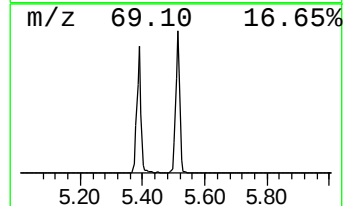
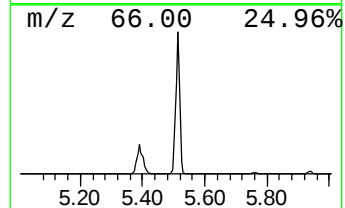
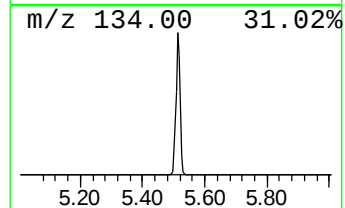
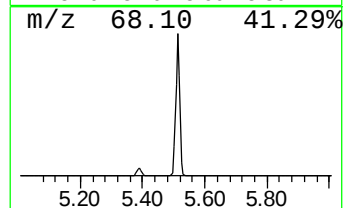
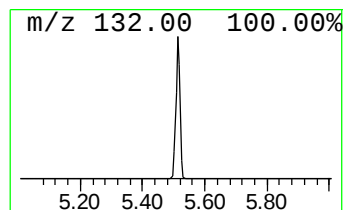
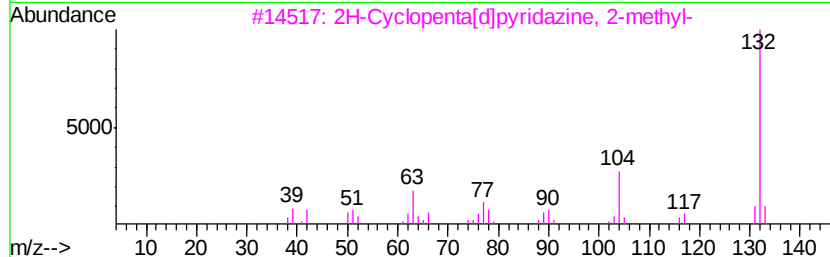
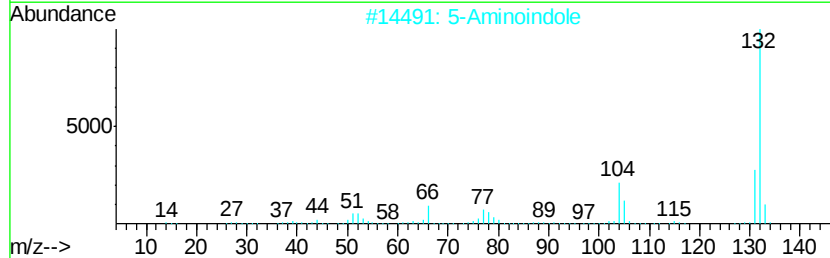
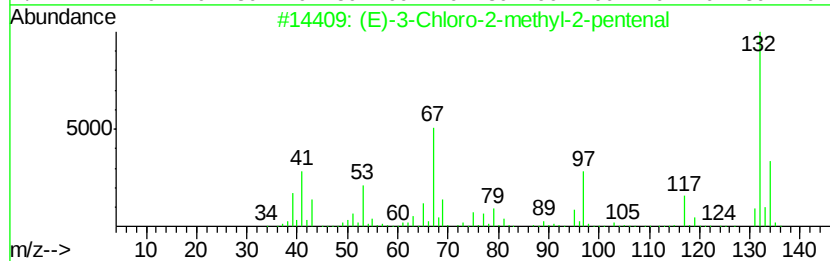
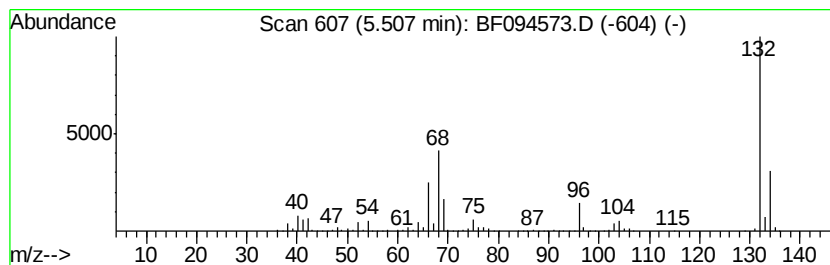
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	80.81 ng	2398760	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		2H-Cyclopenta[d]pyridazine, 2-methyl-	132	C8H8N2	022291-85-6	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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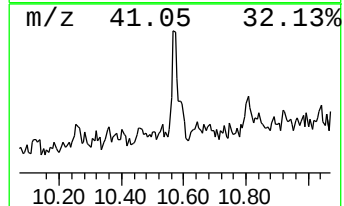
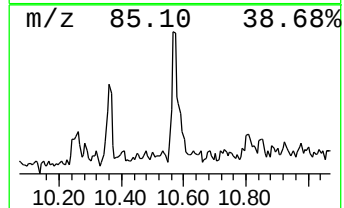
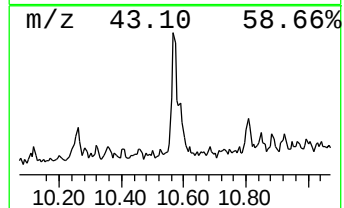
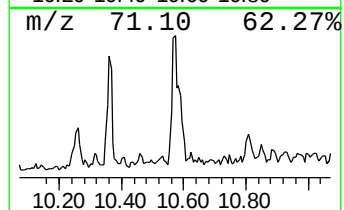
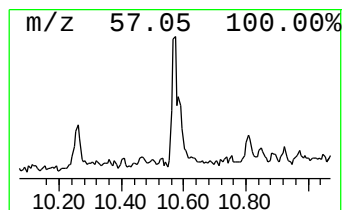
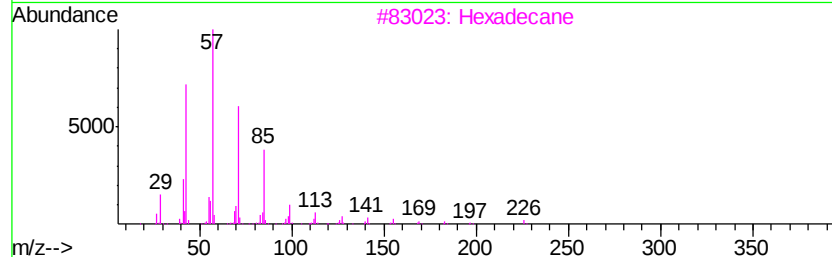
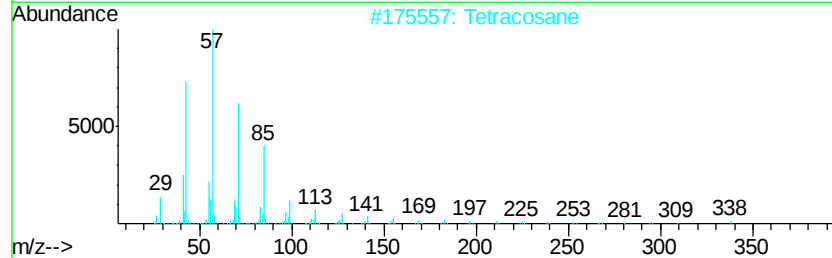
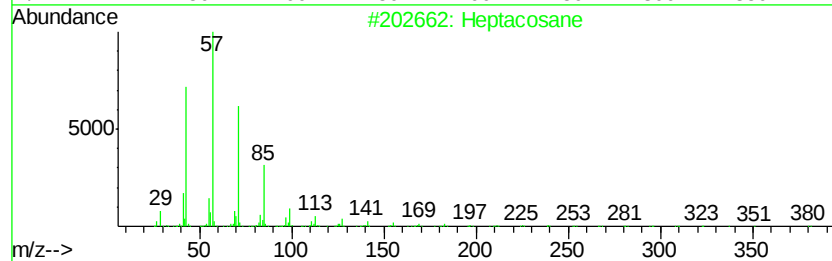
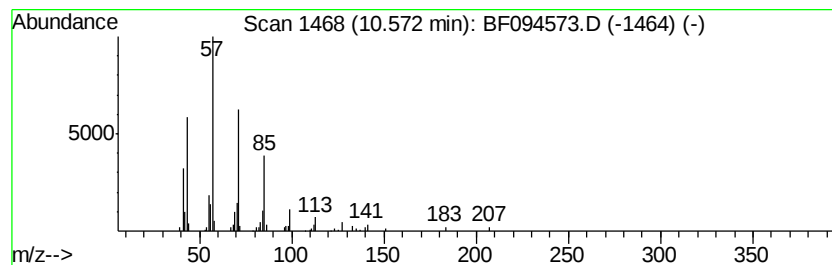
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	2.12 ng	84297	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Tetracosane		338	C24H50	000646-31-1	87
3	Hexadecane		226	C16H34	000544-76-3	86
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86
5	Tritetracontane		605	C43H88	007098-21-7	86



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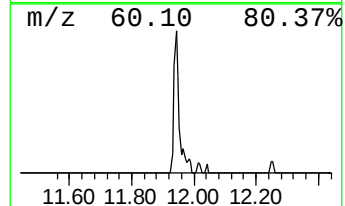
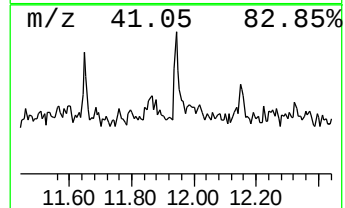
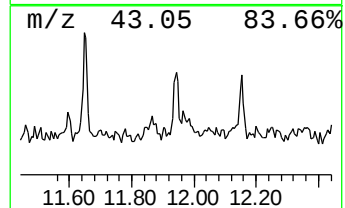
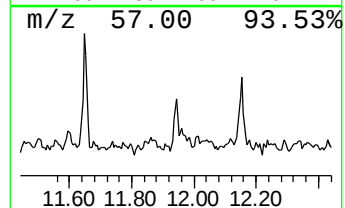
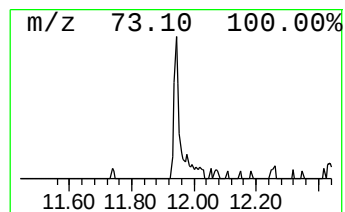
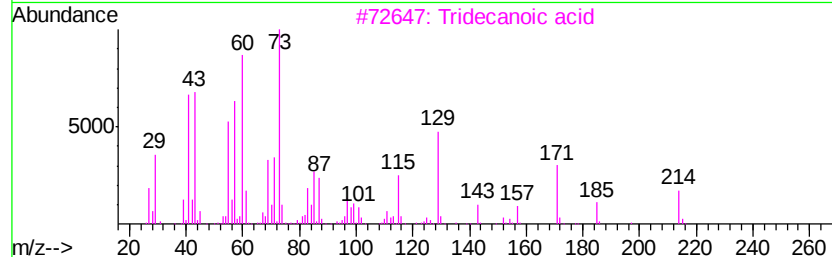
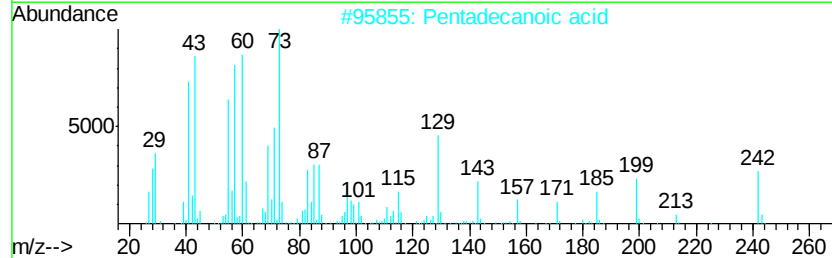
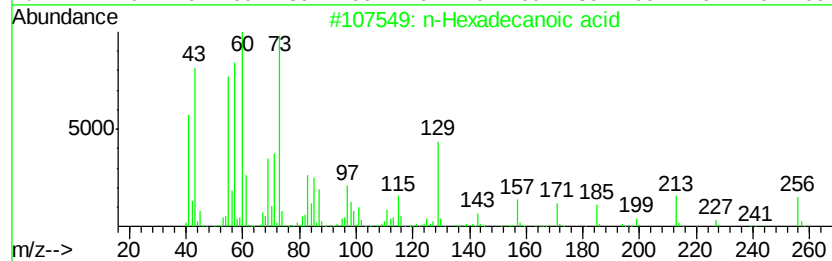
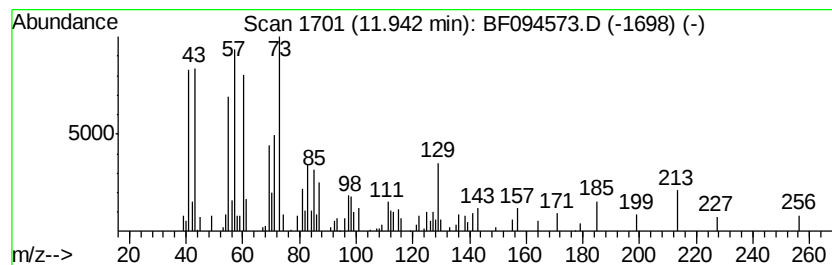
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.48 ng	98988	Phenanthrene-d10	11.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		3,5-Difluorobenzaldehyde carbamo...	199	C8H7F2N3O	163893-49-0	25



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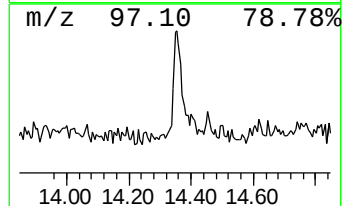
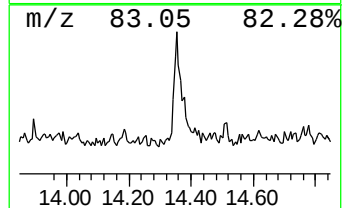
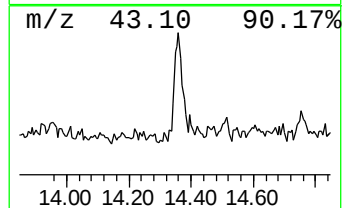
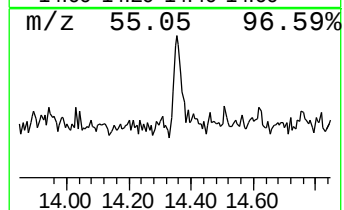
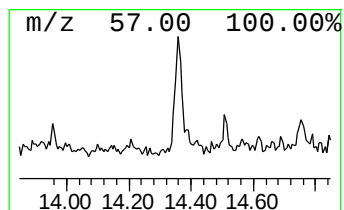
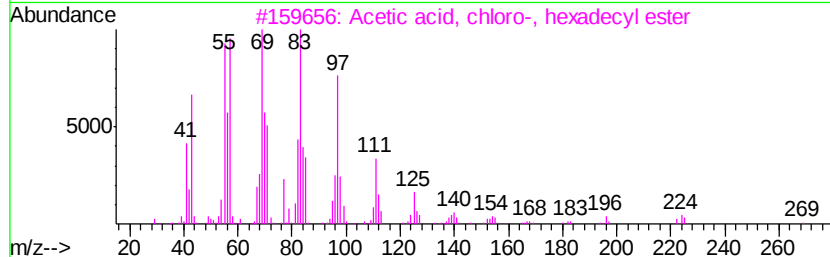
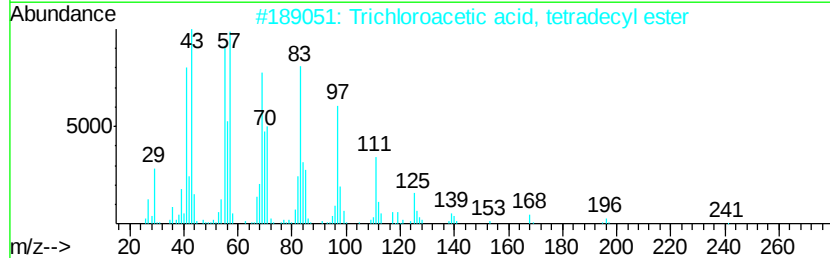
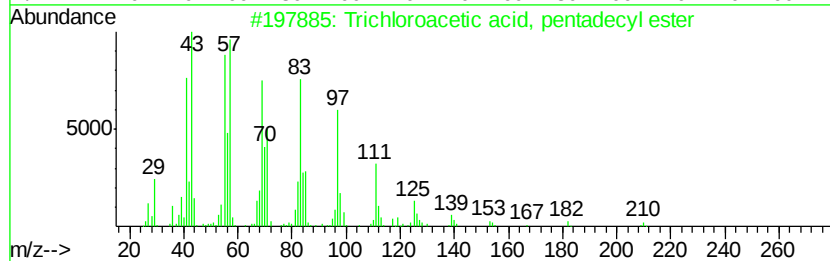
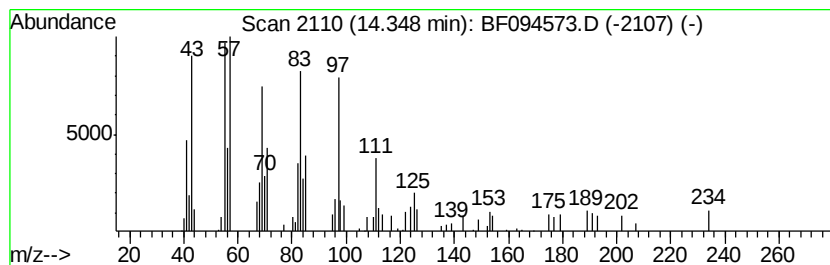
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.66 ng	100991	Chrysene-d12	14.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	81
3		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	74
4		17-Pentatriacontene	491	C35H70	006971-40-0	74
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	62



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BNA_F
ClientSampleId :
BL-2(3)

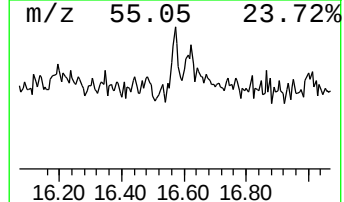
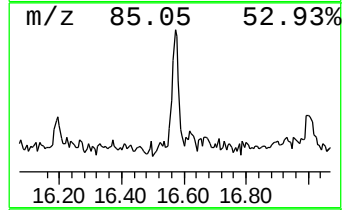
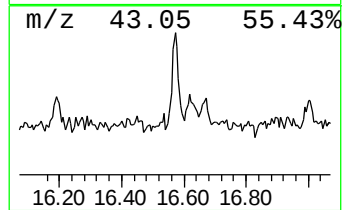
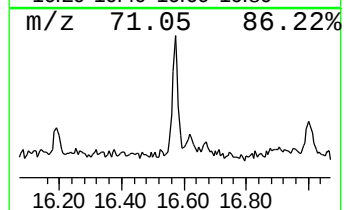
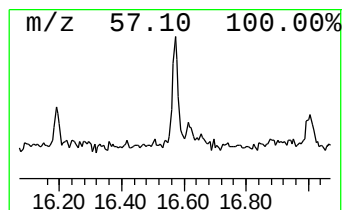
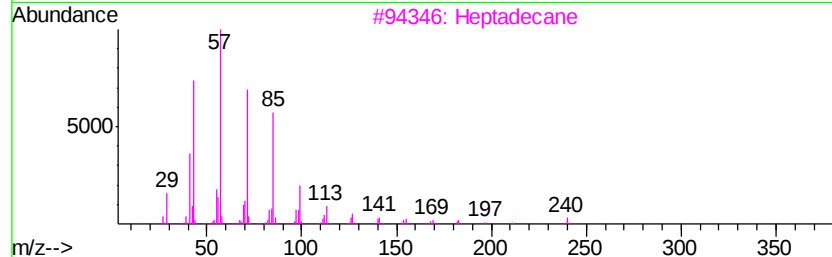
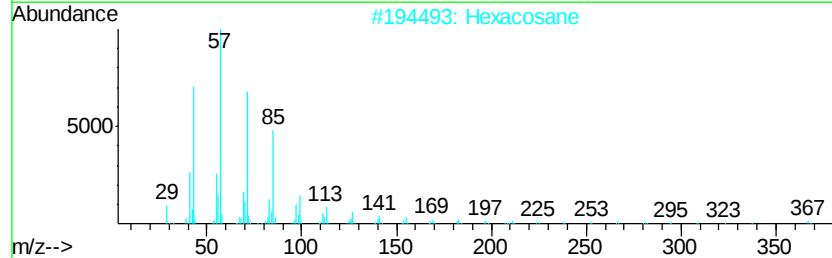
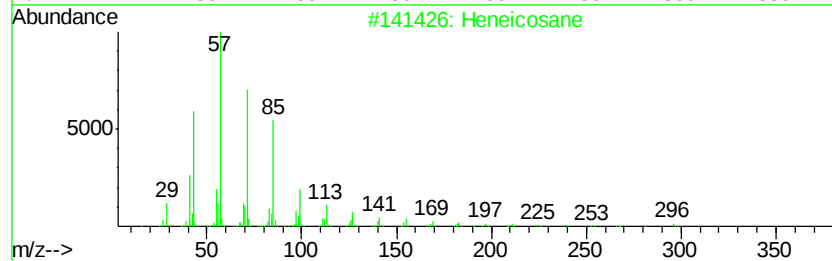
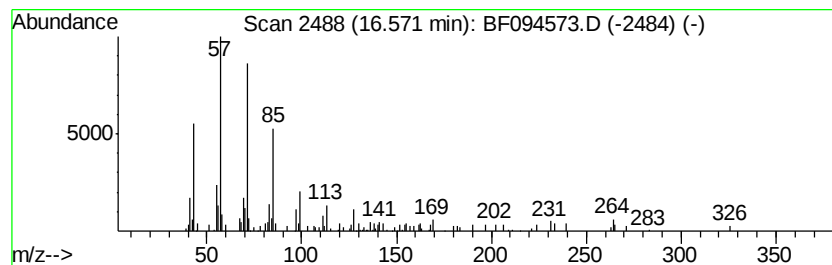
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	2.23 ng	85838	Perylene-d12	16.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	87
2	Hexacosane		366	C26H54	000630-01-3	87
3	Heptadecane		240	C17H36	000629-78-7	86
4	Tridecanol, 2-ethyl-2-methyl-		242	C16H34O	1000115-66-1	86
5	Docosane		310	C22H46	000629-97-0	86



Data Path : Z:\HPCHEM1\BNA_F\Data\BF042117\
Data File : BF094573.D
Acq On : 21 Apr 2017 20:09
Operator : SJ/MA
Sample : I2786-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BL-2(3)

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	9.6	ng	284370	1	5.76	593674	20.0
unknown5.51	5.51	80.8	ng	2398760	1	5.76	593674	20.0
Heptacosane	10.57	2.1	ng	84297	4	11.21	797033	20.0
n-Hexadecanoic acid	11.94	2.5	ng	98988	4	11.21	797033	20.0
Trichloroacetic a...	14.35	2.7	ng	100991	5	14.45	760340	20.0
Heneicosane	16.57	2.2	ng	85838	6	16.08	770689	20.0