

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050217\
 Data File : BF094799.D
 Acq On : 2 May 2017 18:16
 Operator : SJ/MA
 Sample : I2931-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FLOOR-042817

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-BF050217.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	5.048	524	529	545	rBV	294504	553641	19.83%	2.133%
2	5.689	632	638	661	rBV	1881798	2653578	95.03%	10.222%
3	6.248	729	733	740	rVB	29053	41335	1.48%	0.159%
4	7.278	902	908	922	rBV	1777024	2626622	94.06%	10.118%
5	7.395	922	928	939	rVB	2269021	2792444	100.00%	10.756%
6	7.560	952	956	967	rVB2	13709	30805	1.10%	0.119%
7	7.730	975	985	992	rBV	452860	495570	17.75%	1.909%
8	7.972	1020	1026	1035	rVB	1710845	2007657	71.90%	7.733%
9	8.630	1131	1138	1141	rBV	1299896	1622854	58.12%	6.251%
10	9.748	1323	1328	1336	rBV	623506	699341	25.04%	2.694%
11	11.524	1624	1630	1634	rBV	2101683	2374627	85.04%	9.147%
12	12.213	1742	1747	1754	rBV	506087	575528	20.61%	2.217%
13	12.577	1804	1809	1814	rBV2	633384	775091	27.76%	2.986%
14	12.989	1869	1879	1880	rBV2	14587	29854	1.07%	0.115%
15	13.424	1950	1953	1959	rVB2	38594	45299	1.62%	0.174%
16	13.877	2023	2030	2037	rBV	1220754	1676688	60.04%	6.459%
17	14.201	2080	2085	2087	rBV	41933	52449	1.88%	0.202%
18	14.930	2205	2209	2213	rBV3	30272	37839	1.36%	0.146%
19	14.977	2213	2217	2227	rVB	663644	798720	28.60%	3.077%
20	15.953	2374	2383	2392	rBV	348584	509926	18.26%	1.964%
21	16.795	2523	2526	2531	rVB	35441	50444	1.81%	0.194%
22	16.859	2533	2537	2540	rBV	53205	54687	1.96%	0.211%
23	16.947	2550	2552	2558	rVB2	37401	42927	1.54%	0.165%
24	17.047	2562	2569	2583	rVV	585947	810083	29.01%	3.120%
25	17.153	2584	2587	2591	rVB3	90203	97211	3.48%	0.374%
26	17.306	2608	2613	2617	rBV	2216853	2640031	94.54%	10.169%
27	17.894	2710	2713	2716	rBV2	31277	31173	1.12%	0.120%
28	18.000	2725	2731	2735	rBV4	24934	36733	1.32%	0.141%
29	18.083	2742	2745	2748	rBV	55700	62103	2.22%	0.239%
30	18.536	2819	2822	2825	rBV	27556	30626	1.10%	0.118%
31	18.583	2825	2830	2835	rVV8	30558	63691	2.28%	0.245%
32	18.642	2836	2840	2845	rVV	602830	692934	24.81%	2.669%
33	18.712	2849	2852	2862	rVB4	24980	51632	1.85%	0.199%
34	20.306	3119	3123	3131	rBV	443199	530005	18.98%	2.042%

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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	20.418	3139	3142	3147	rVB4	23342	28851	1.03%	0.111%
36	20.794	3202	3206	3209	rBV2	30303	47621	1.71%	0.183%
37	21.224	3275	3279	3289	rVB7	23298	41652	1.49%	0.160%
38	21.577	3332	3339	3351	rVB6	72240	201025	7.20%	0.774%
39	21.718	3358	3363	3370	rBV4	20192	47368	1.70%	0.182%

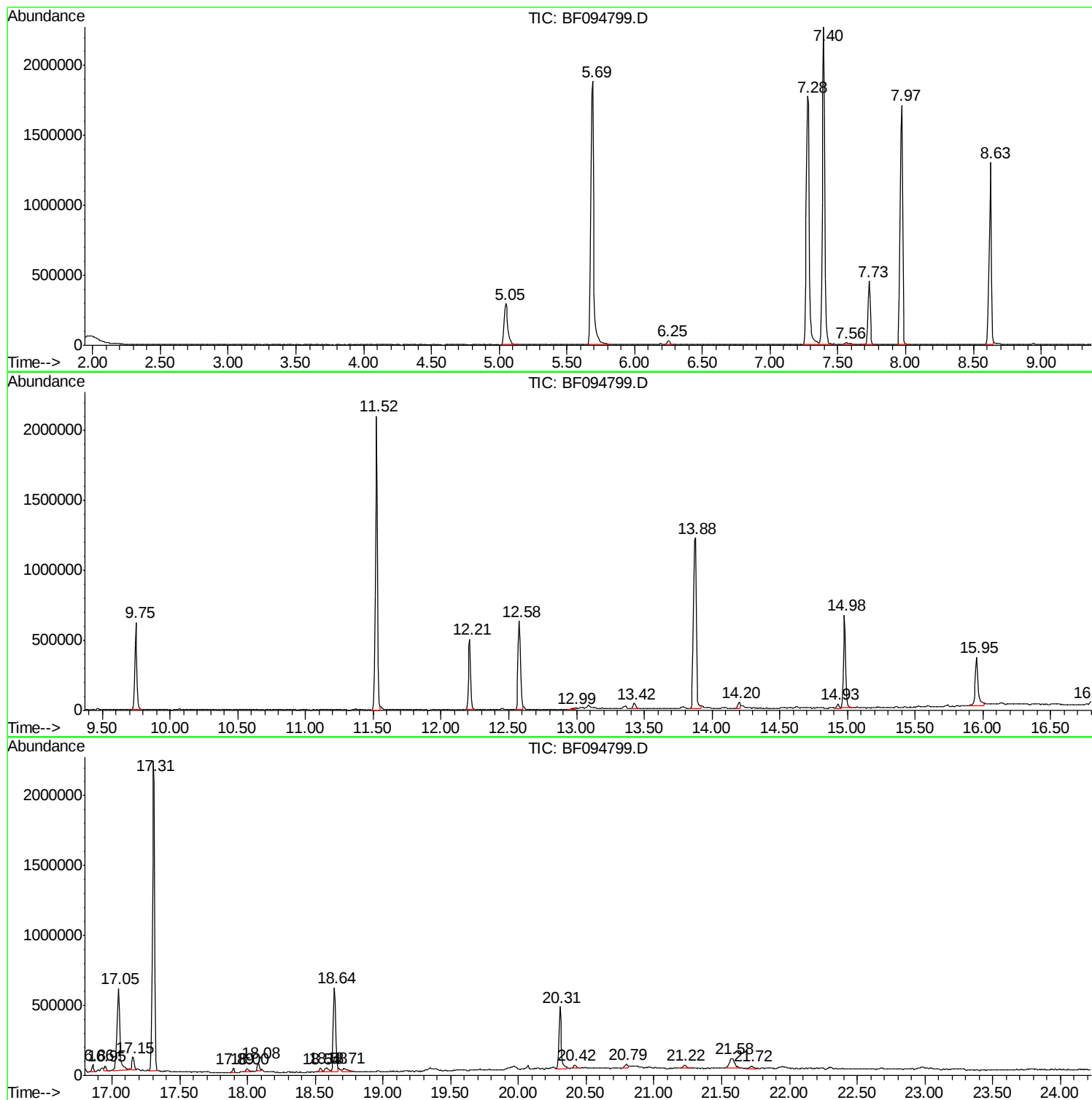
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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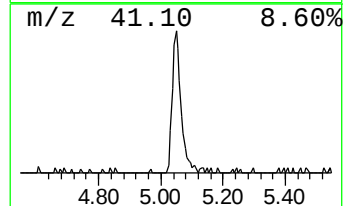
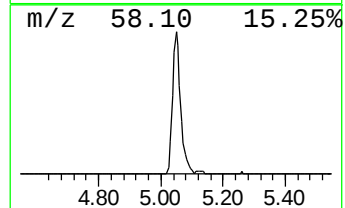
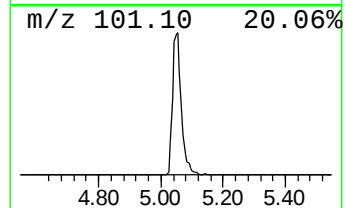
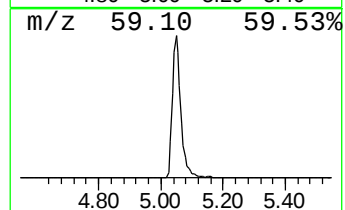
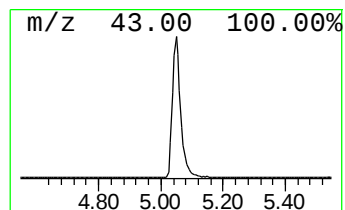
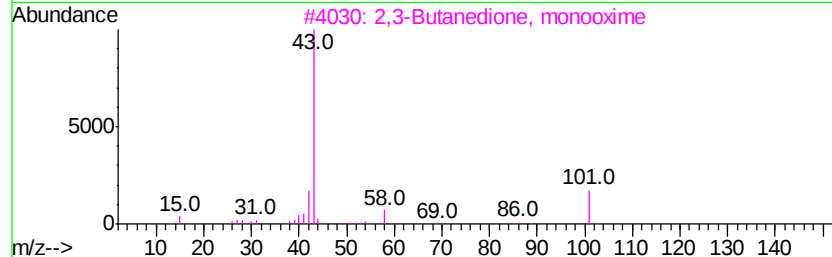
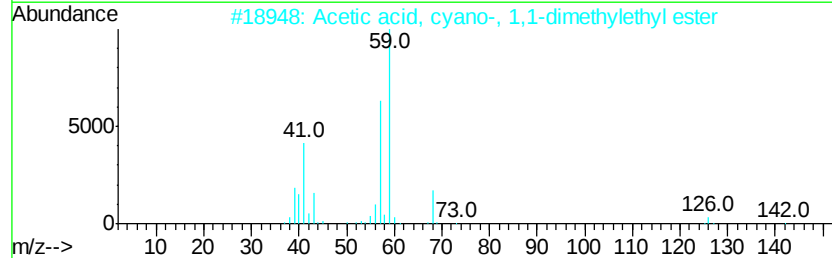
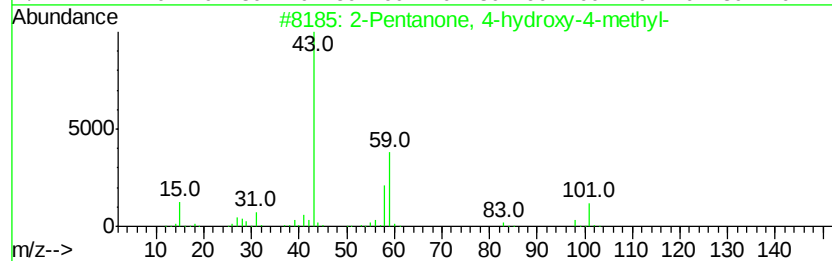
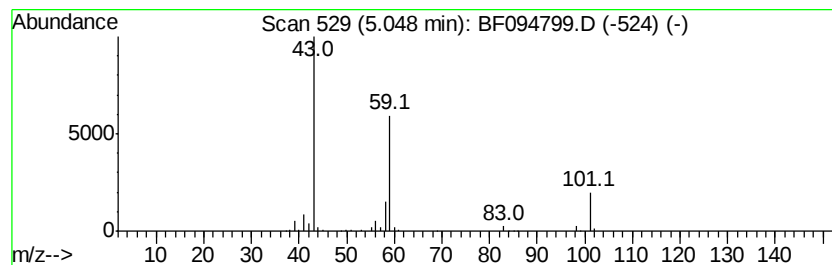
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	22.34 ng	553641	1,4-Dichlorobenzene-d4	7.73

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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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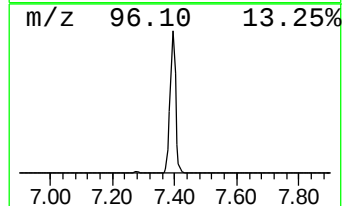
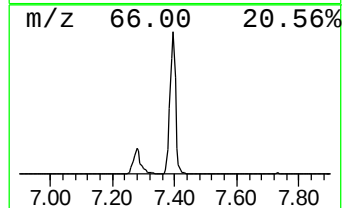
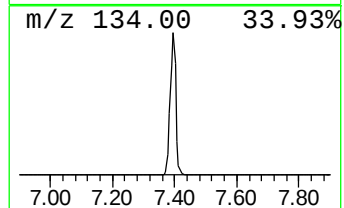
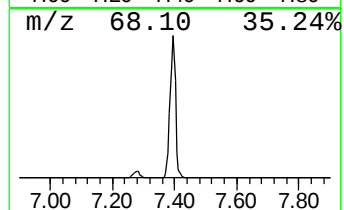
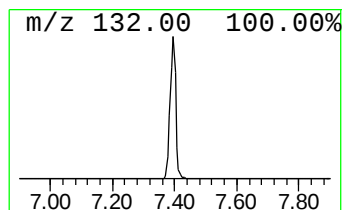
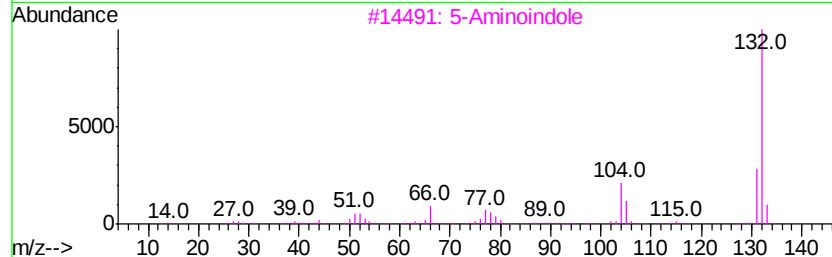
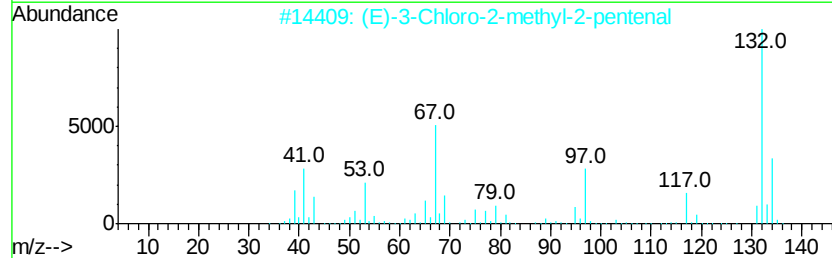
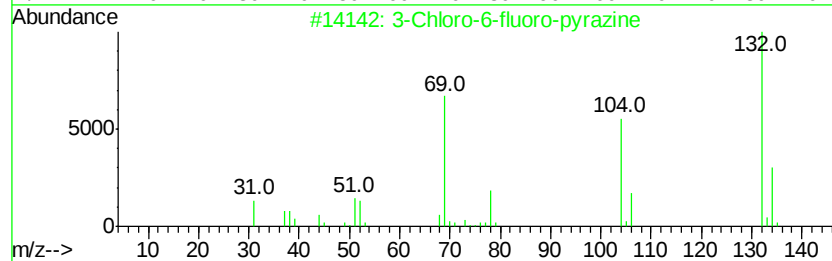
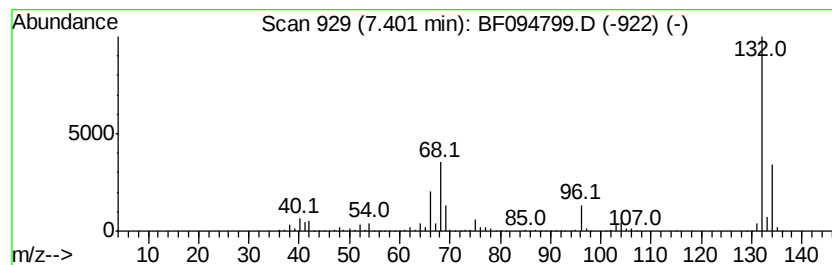
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	112.70 ng	2792440	1,4-Dichlorobenzene-d4	7.73

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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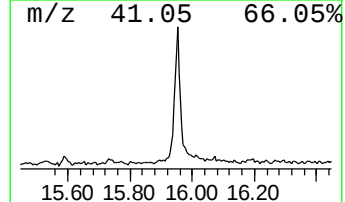
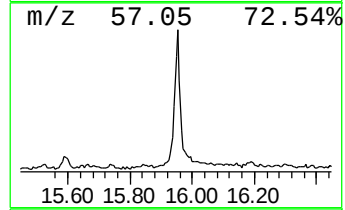
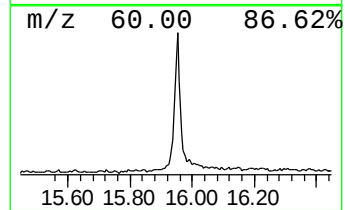
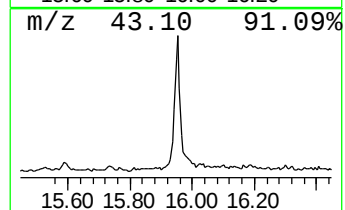
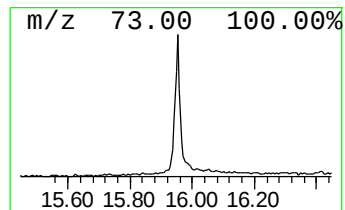
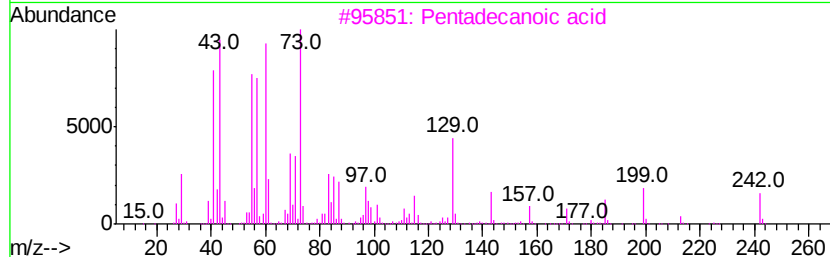
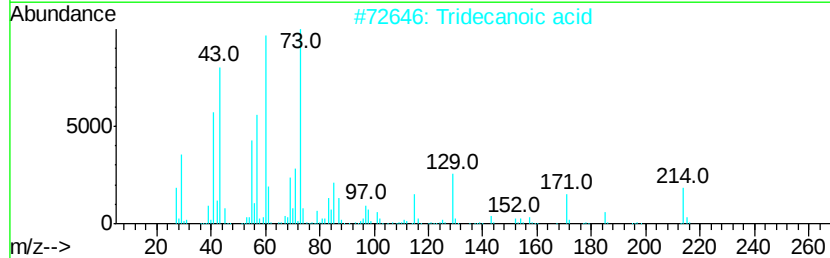
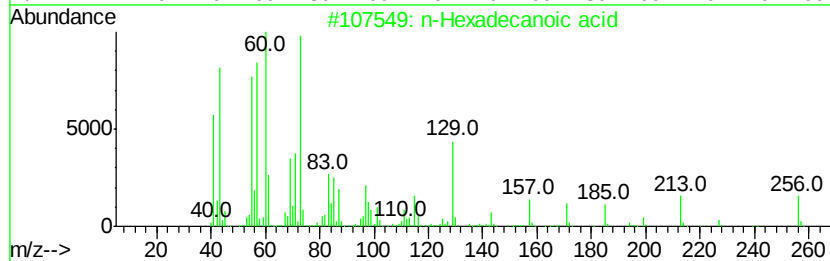
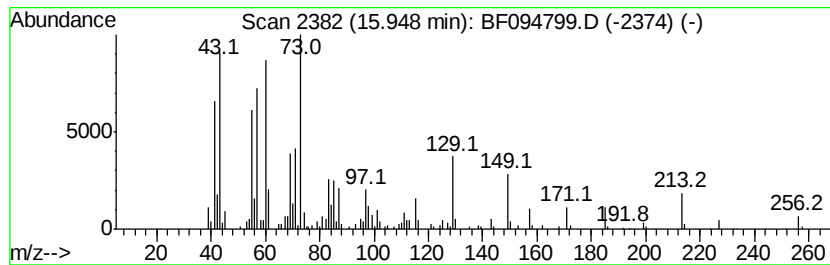
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	12.77 ng	509926	Phenanthrene-d10	14.98

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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



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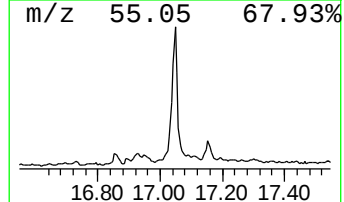
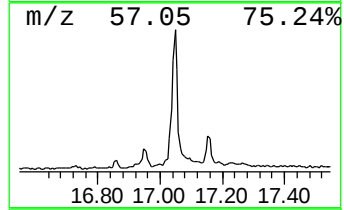
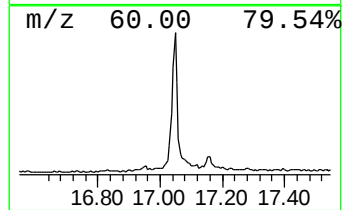
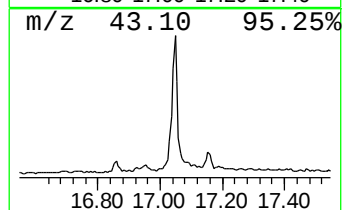
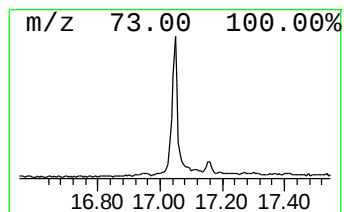
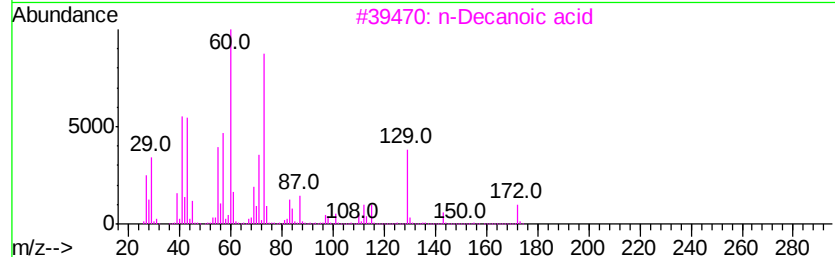
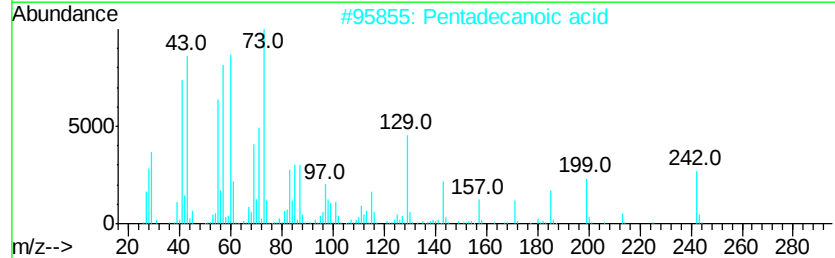
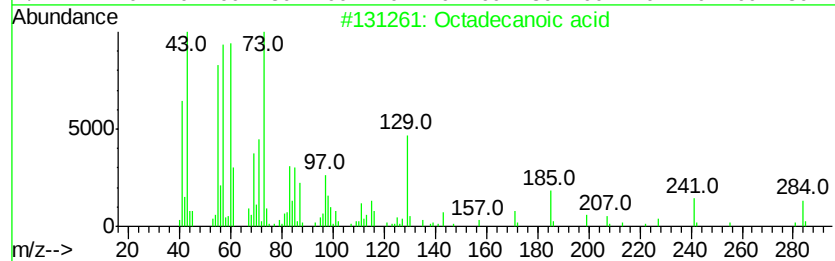
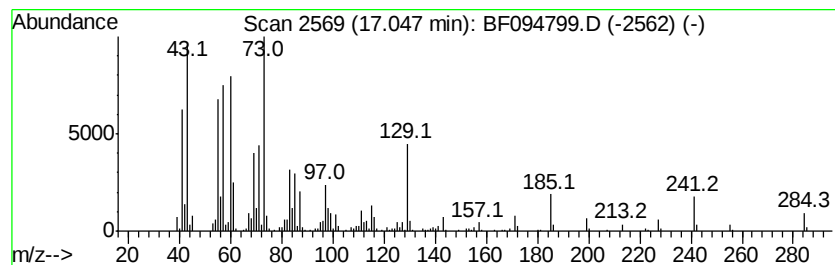
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	23.38 ng	810083	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		n-Decanoic acid	172	C10H20O2	000334-48-5	68
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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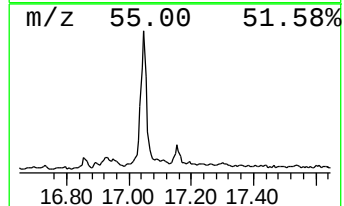
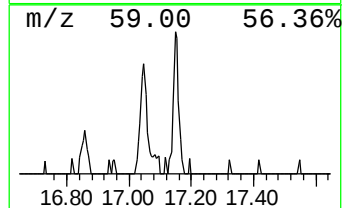
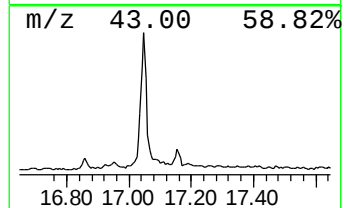
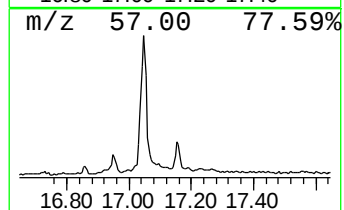
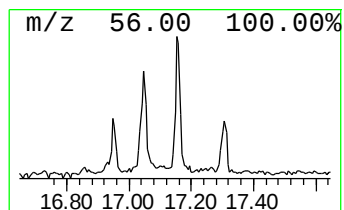
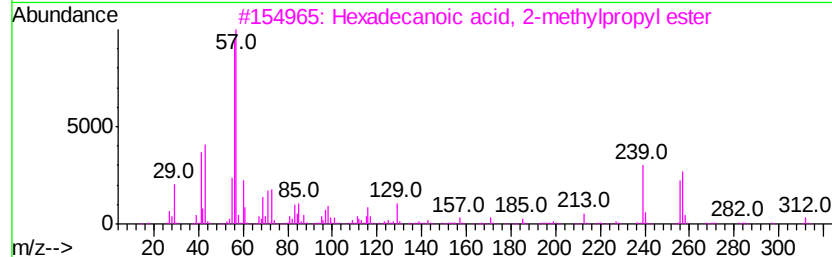
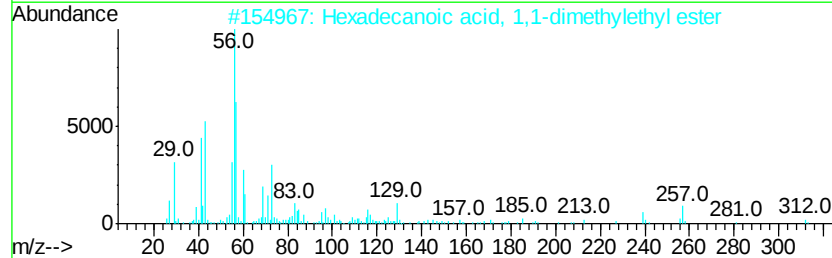
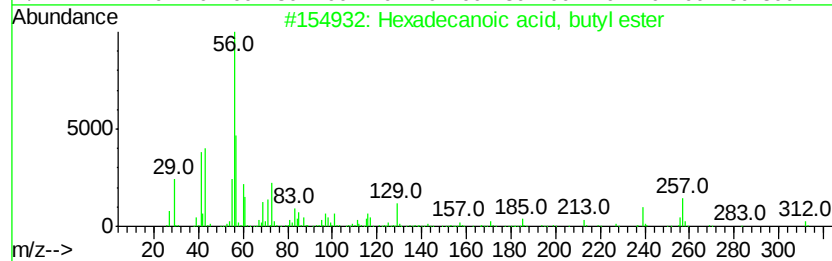
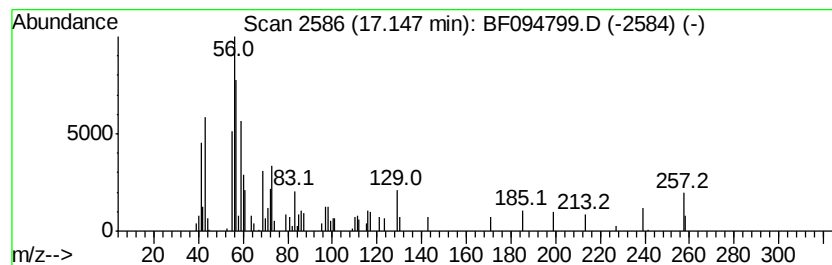
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.15	2.81 ng	97211	Chrysene-d12	18.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	68
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	53
3			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4			1-Piperidinylloxv, 4-(hydroximin...	185	C9H17N2O2	003229-75-2	35
5			trans-2-Aminocyclohexanol	115	C6H13NO	006982-39-4	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050217\
Data File : BF094799.D
Acq On : 2 May 2017 18:16
Operator : SJ/MA
Sample : I2931-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FLOOR-042817

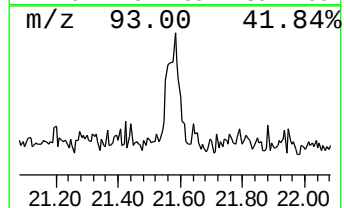
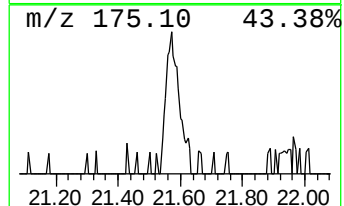
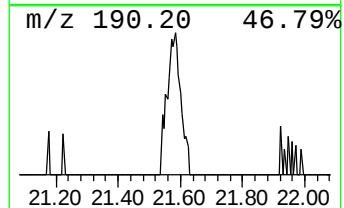
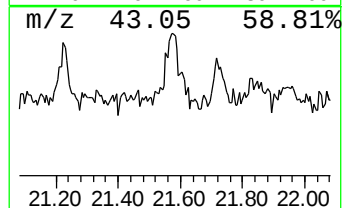
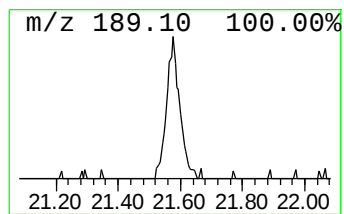
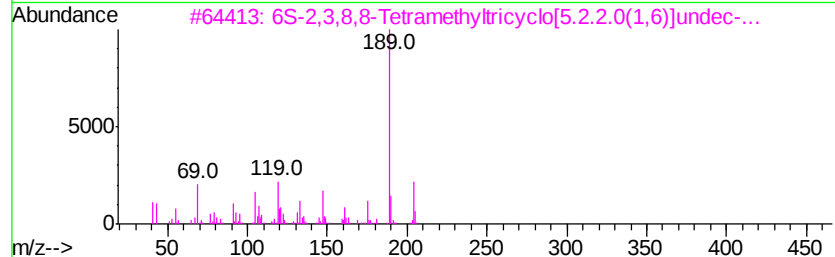
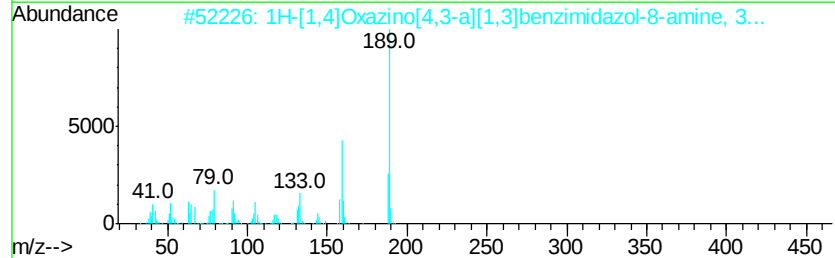
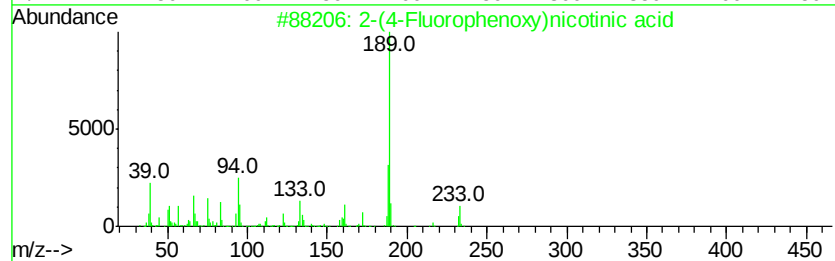
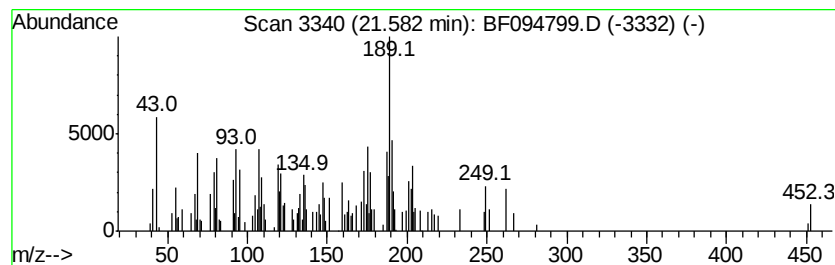
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown21.58 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.58	7.59 ng	201025	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(4-Fluorophenoxy)nicotinic acid	233	C12H8FN03	054629-13-9	46
2		1H-[1,4]Oxazino[4,3-a][1,3]benzi...	189	C10H11N3O	1000362-54-6	46
3		6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	42
4		Silane, (4-bromo-3-buten-1-ynyl)...	202	C7H11BrSi	107646-62-8	38
5		4-Butyl-2-phenyl-5-propyl[1,3,2]...	246	C15H23B02	1000322-44-4	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050217\
Data File : BF094799.D
Acq On : 2 May 2017 18:16
Operator : SJ/MA
Sample : I2931-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FLOOR-042817

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.05	22.3	ng	553641	1	7.73	495570	20.0
unknown7.40	7.40	112.7	ng	2792440	1	7.73	495570	20.0
n-Hexadecanoic acid	15.95	12.8	ng	509926	4	14.98	798720	20.0
Octadecanoic acid	17.05	23.4	ng	810083	5	18.64	692934	20.0
Hexadecanoic acid...	17.15	2.8	ng	97211	5	18.64	692934	20.0
unknown21.58	21.58	7.6	ng	201025	6	20.31	530005	20.0