

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
 Data File : BF095545.D
 Acq On : 30 May 2017 20:24
 Operator : SJ/MA
 Sample : I3302-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM16-COMP-0-6

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	5.101	534	538	553	rBV	74771	180664	7.52%	0.865%
2	5.707	637	641	681	rBV	779829	2117821	88.17%	10.145%
3	7.289	906	910	926	rBV	749147	1824855	75.98%	8.742%
4	7.407	926	930	946	rVB	1343898	2401881	100.00%	11.506%
5	7.736	982	986	997	rBV	483868	597738	24.89%	2.863%
6	7.972	1021	1026	1046	rBV	1318309	1700056	70.78%	8.144%
7	8.642	1136	1140	1182	rBV	532038	1233126	51.34%	5.907%
8	9.760	1326	1330	1349	rBV	331296	748333	31.16%	3.585%
9	11.530	1626	1631	1655	rBV	1087528	1979606	82.42%	9.483%
10	12.236	1747	1751	1765	rBV	118471	246284	10.25%	1.180%
11	12.595	1807	1812	1830	rBV2	435426	741592	30.88%	3.553%
12	13.418	1948	1952	1958	rBV	26320	32890	1.37%	0.158%
13	13.901	2029	2034	2051	rBV2	437728	877104	36.52%	4.202%
14	14.195	2080	2084	2087	rBV	26546	34538	1.44%	0.165%
15	15.001	2216	2221	2225	rVV	335420	499746	20.81%	2.394%
16	15.036	2225	2227	2241	rVV	108175	203123	8.46%	0.973%
17	15.136	2241	2244	2255	rVB2	18201	36527	1.52%	0.175%
18	15.836	2360	2363	2369	rVV3	18160	33364	1.39%	0.160%
19	15.895	2369	2373	2377	rVV4	19042	32031	1.33%	0.153%
20	15.954	2377	2383	2399	rVB5	109921	208258	8.67%	0.998%
21	16.783	2520	2524	2533	rBV	227002	307182	12.79%	1.472%
22	17.042	2564	2568	2571	rBV4	18265	25634	1.07%	0.123%
23	17.083	2571	2575	2584	rVB	245184	330460	13.76%	1.583%
24	17.312	2610	2614	2624	rBV	1067383	1315867	54.78%	6.304%
25	17.401	2624	2629	2636	rVB7	16961	34986	1.46%	0.168%
26	17.548	2652	2654	2661	rVB	29039	40037	1.67%	0.192%
27	17.636	2664	2669	2674	rBV2	23643	34632	1.44%	0.166%
28	17.689	2674	2678	2684	rBV4	33792	52474	2.18%	0.251%
29	18.012	2726	2733	2739	rBV4	26622	43217	1.80%	0.207%
30	18.353	2785	2791	2793	rBV3	19882	31175	1.30%	0.149%
31	18.377	2793	2795	2799	rVV	30111	36181	1.51%	0.173%
32	18.418	2799	2802	2804	rVV	19756	26161	1.09%	0.125%
33	18.553	2821	2825	2833	rVV5	53661	108433	4.51%	0.519%
34	18.671	2839	2845	2849	rBV2	578388	858226	35.73%	4.111%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	18.706	2849	2851	2862	rVB3	139972	215816	8.99%	1.034%
36	18.800	2863	2867	2873	rBV2	25278	46094	1.92%	0.221%
37	18.959	2891	2894	2899	rVB4	27156	43658	1.82%	0.209%
38	19.342	2955	2959	2966	rBV9	41336	92830	3.86%	0.445%
39	19.783	3030	3034	3040	rBV3	63941	91500	3.81%	0.438%
40	19.947	3058	3062	3065	rBV	115099	171201	7.13%	0.820%
41	20.065	3078	3082	3085	rBV3	84436	106998	4.45%	0.513%
42	20.236	3109	3111	3116	rVB	66820	68761	2.86%	0.329%
43	20.300	3118	3122	3126	rBV	97092	118316	4.93%	0.567%
44	20.353	3126	3131	3139	rBV	337536	483884	20.15%	2.318%
45	20.618	3173	3176	3184	rVB2	54802	79641	3.32%	0.382%
46	20.789	3201	3205	3210	rBV	98073	135272	5.63%	0.648%
47	21.718	3358	3363	3369	rVB5	121986	246657	10.27%	1.182%

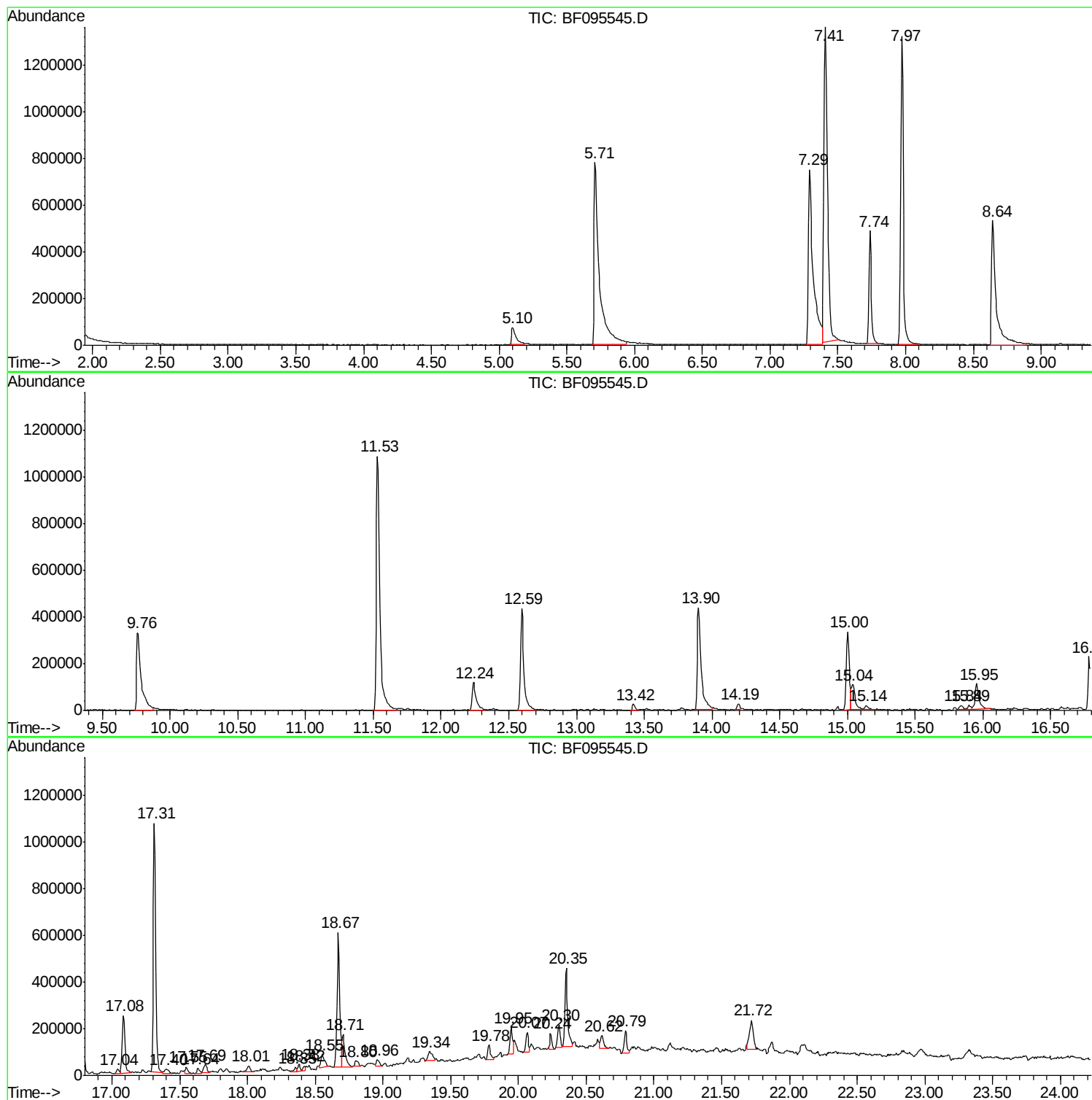
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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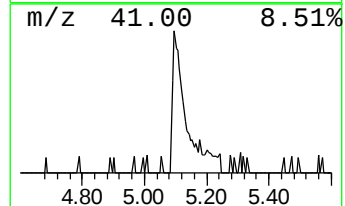
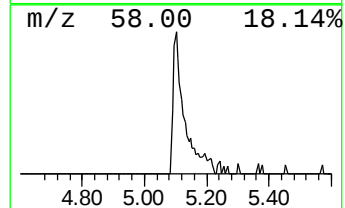
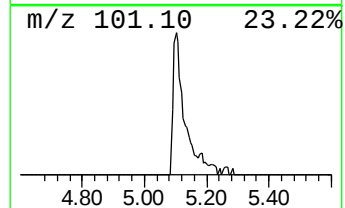
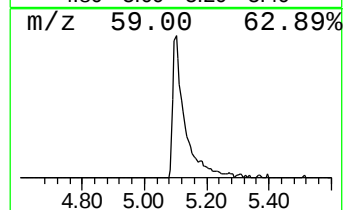
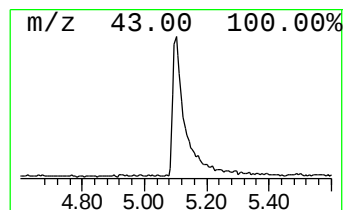
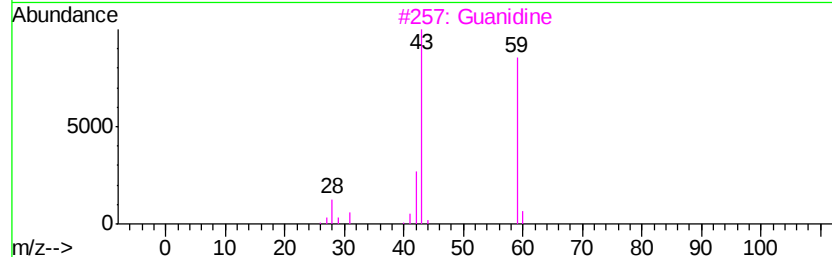
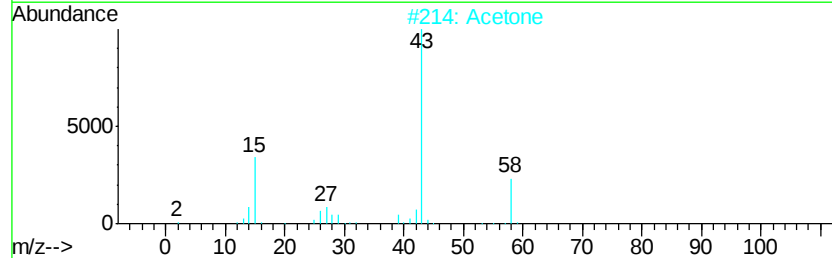
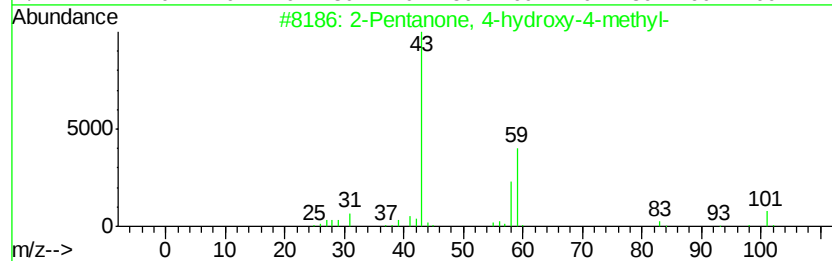
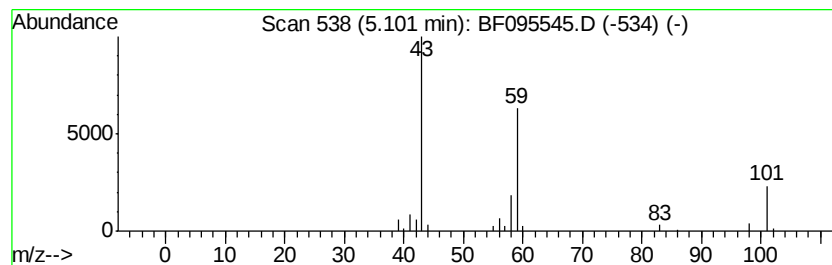
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.04 ng	180664	1,4-Dichlorobenzene-d4	7.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetone	58	C3H6O	000067-64-1	9
3			Guanidine	59	CH5N3	000113-00-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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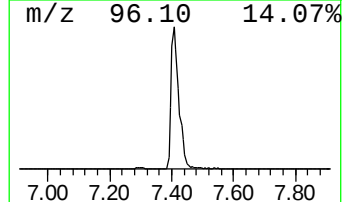
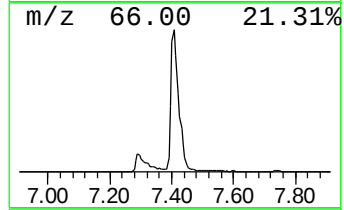
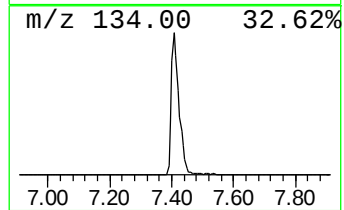
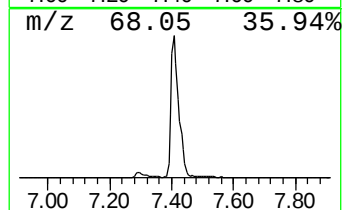
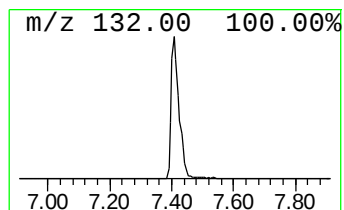
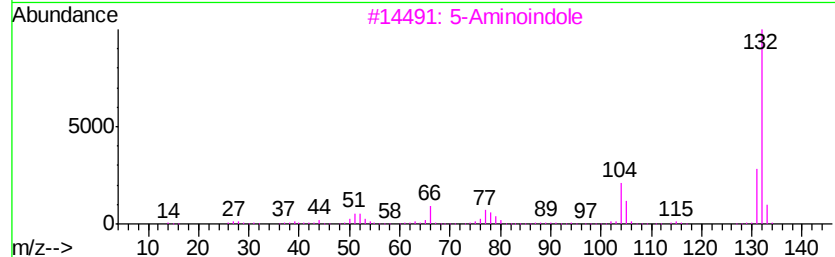
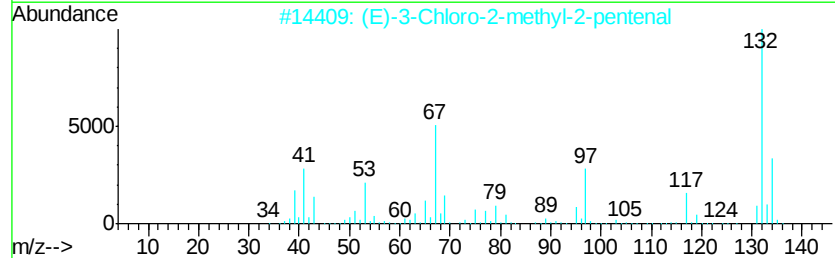
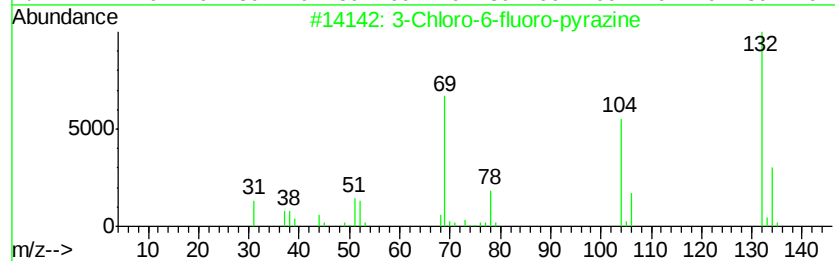
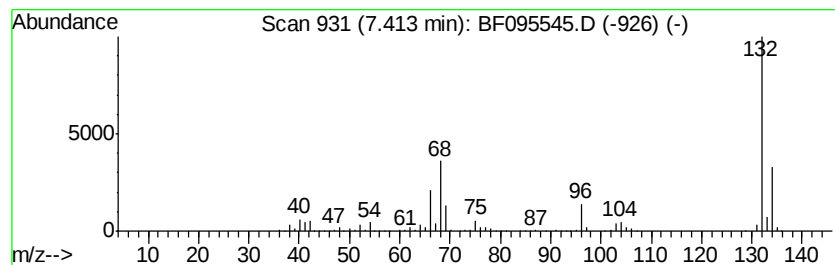
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	80.37 ng	2401880	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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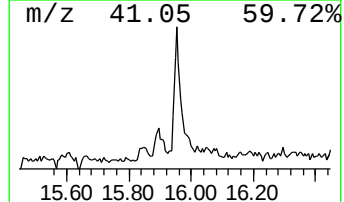
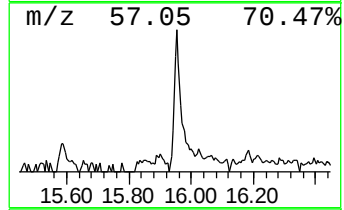
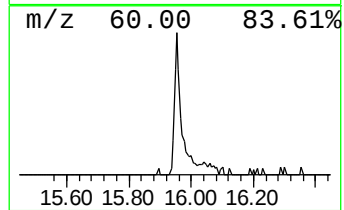
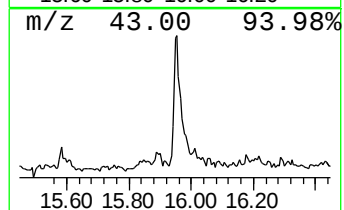
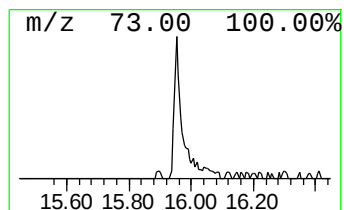
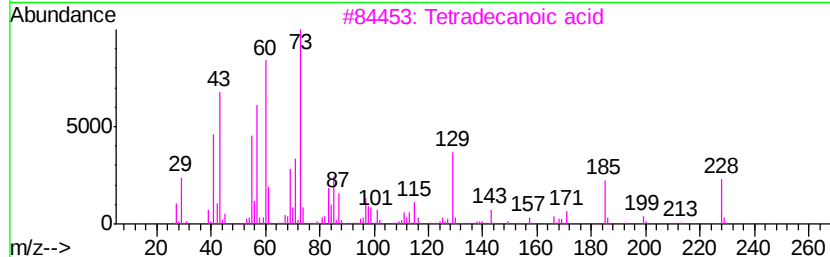
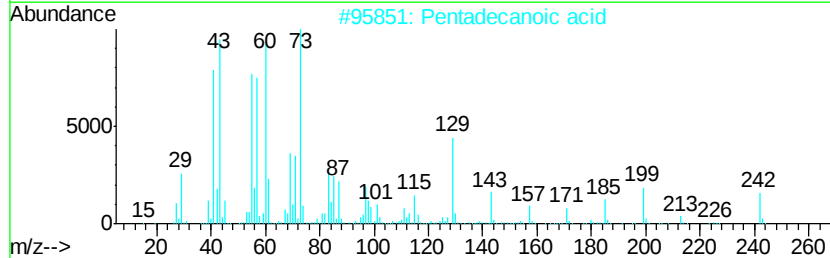
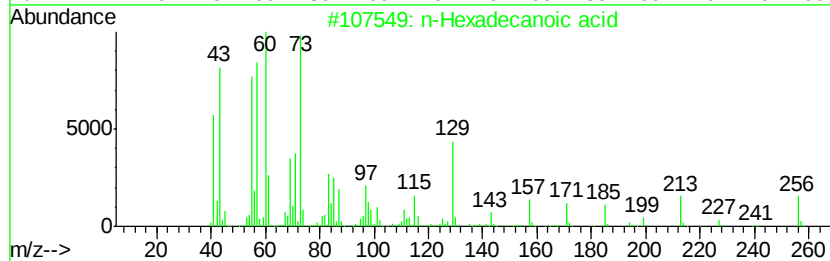
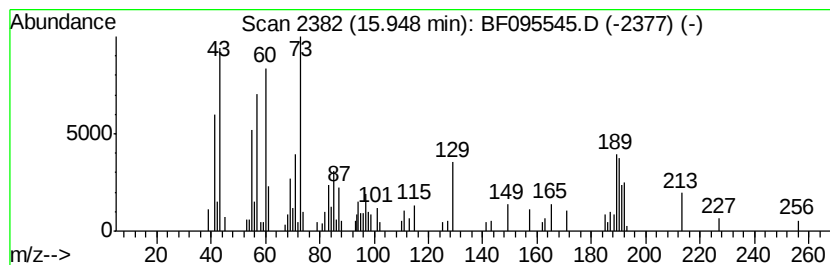
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	8.33 ng	208258	Phenanthrene-d10	15.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Dodecanoic acid	200	C12H24O2	000143-07-7	50



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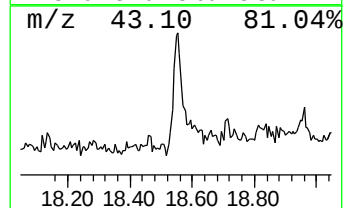
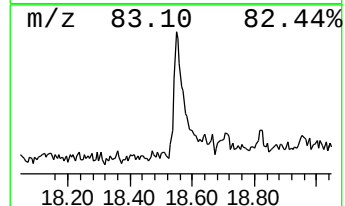
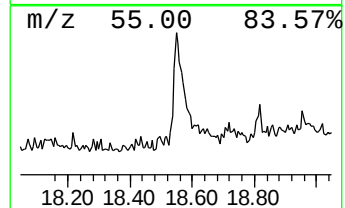
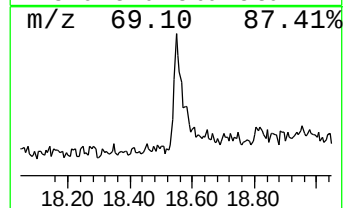
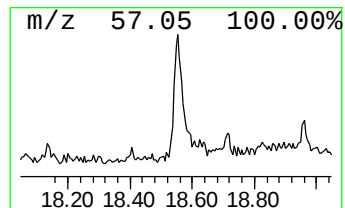
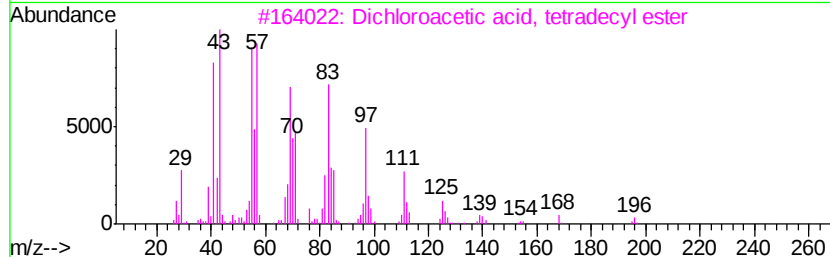
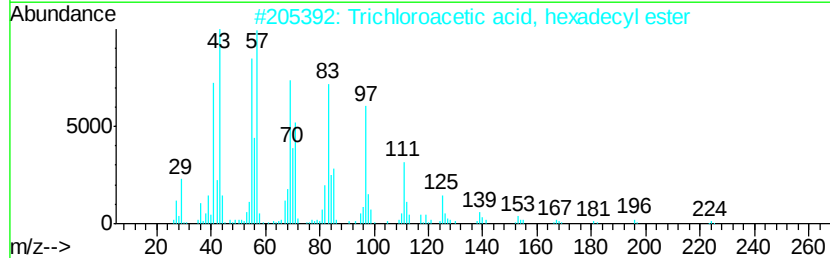
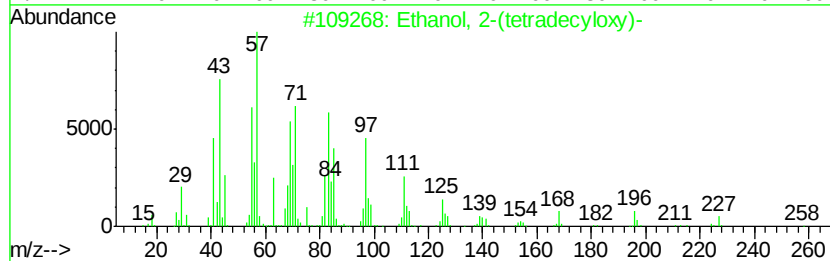
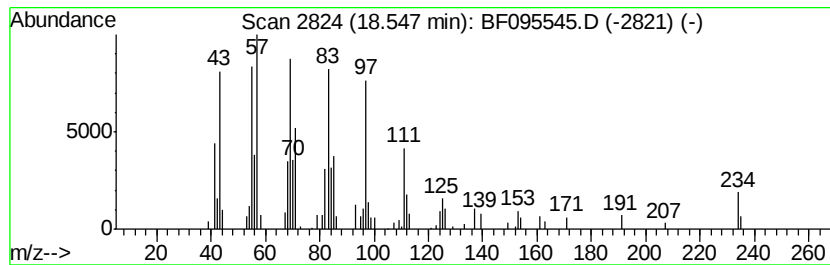
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.53 ng	108433	Chrysene-d12	18.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74
3		Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	74
4		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	70
5		Trifluoroacetic acid, n-tridecyl ...	296	C15H27F3O2	053800-02-5	70



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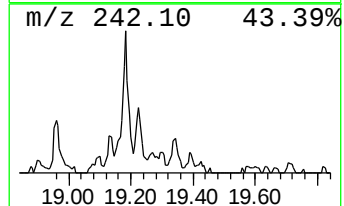
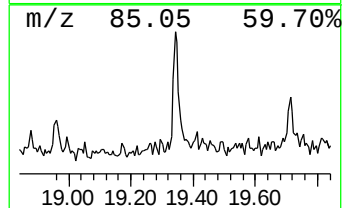
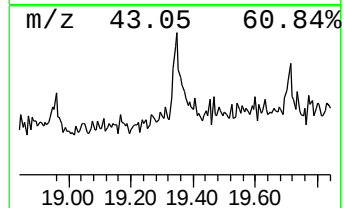
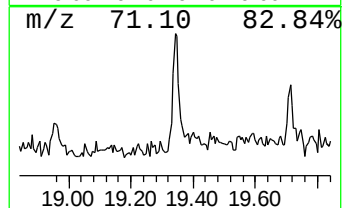
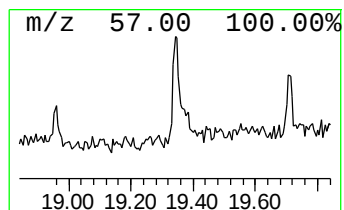
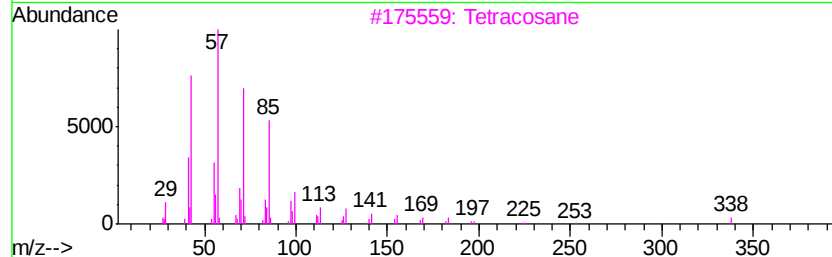
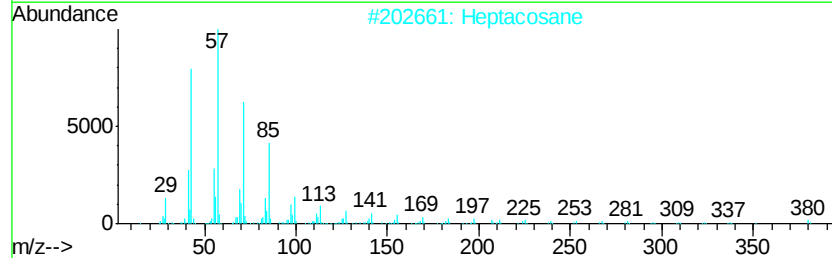
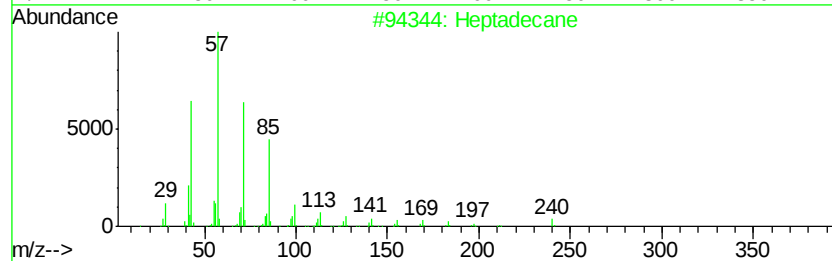
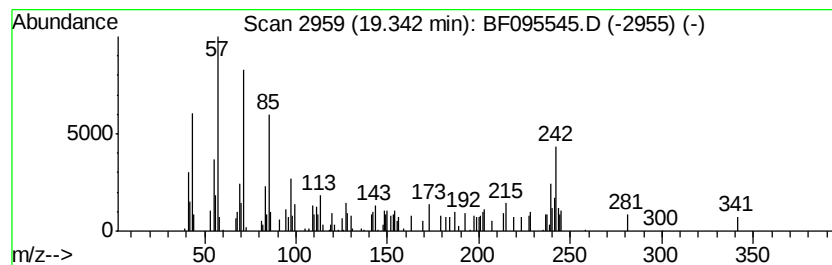
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	2.16 ng	92830	Chrysene-d12	18.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	70
2	Heptacosane		380	C27H56	000593-49-7	46
3	Tetracosane		338	C24H50	000646-31-1	46
4	Octacosane		394	C28H58	000630-02-4	46
5	Sulfurous acid, 2-propyl tridecy...		306	C16H34O3S	1000309-12-4	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095545.D
Acq On : 30 May 2017 20:24
Operator : SJ/MA
Sample : I3302-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-0-6

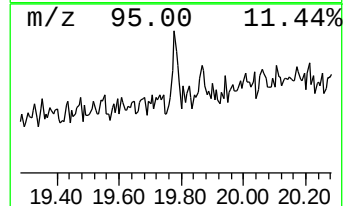
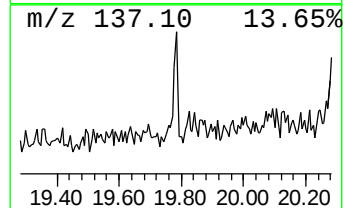
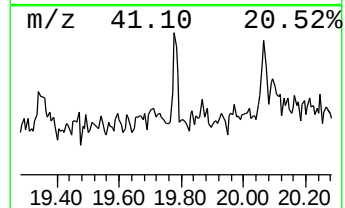
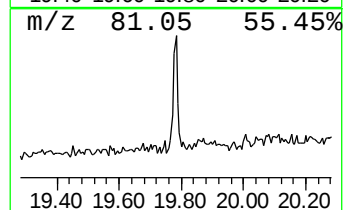
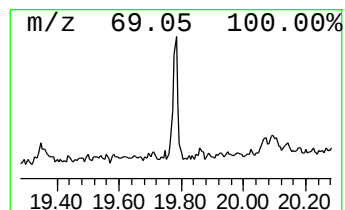
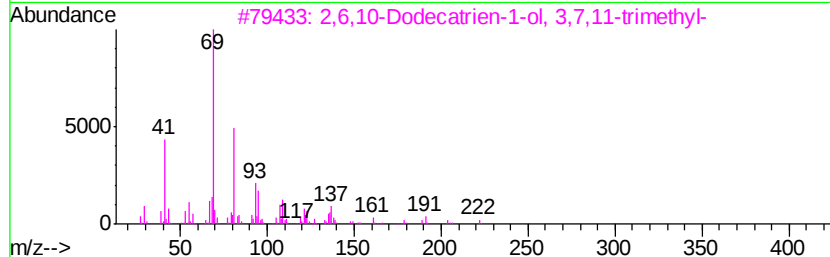
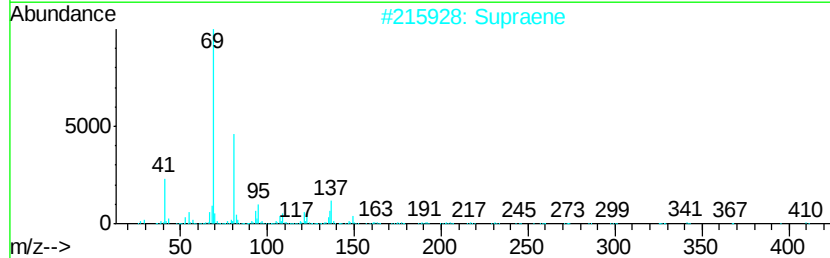
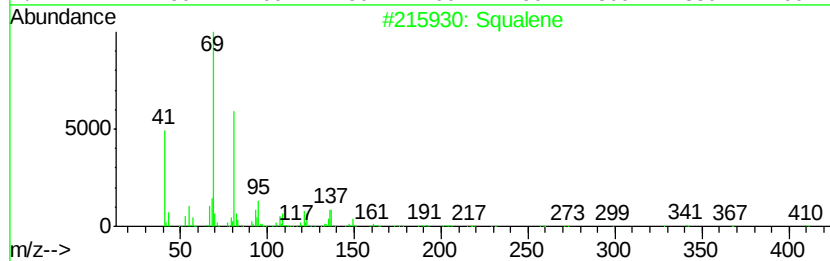
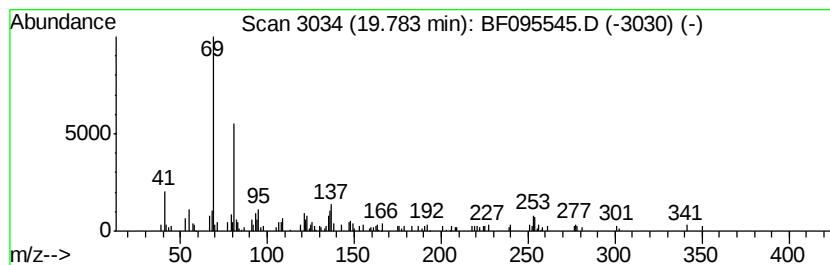
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	3.78 ng	91500	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Supraene	410	C30H50	007683-64-9	80
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	76
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5		trans-Farnesol	222	C15H26O	000106-28-5	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095545.D
Acq On : 30 May 2017 20:24
Operator : SJ/MA
Sample : I3302-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-0-6

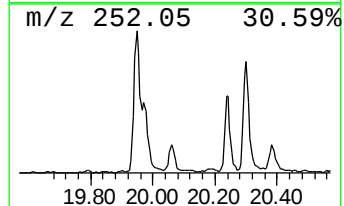
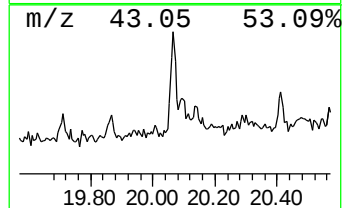
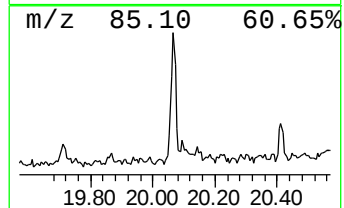
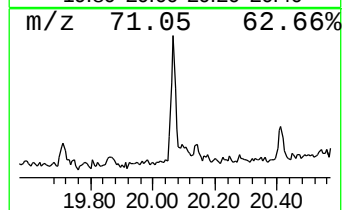
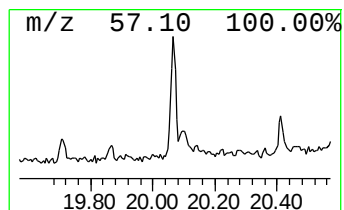
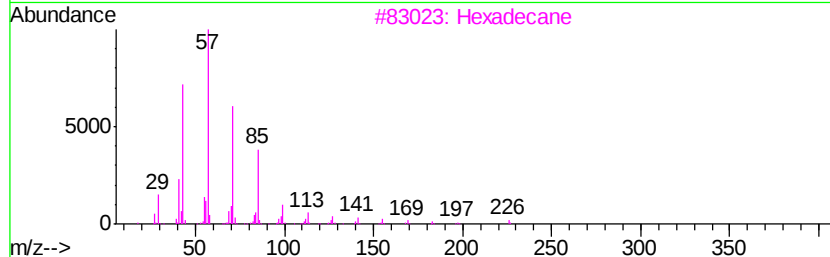
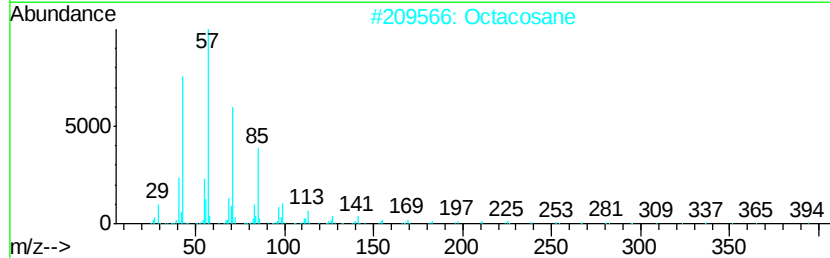
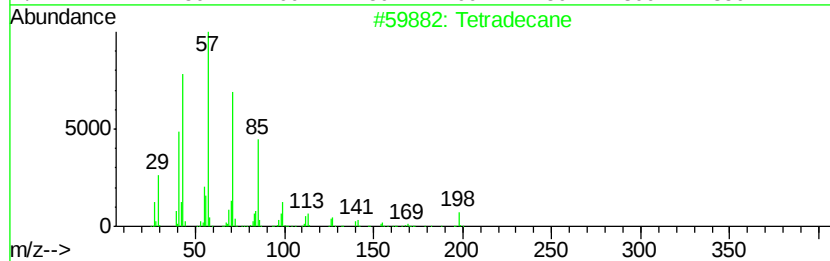
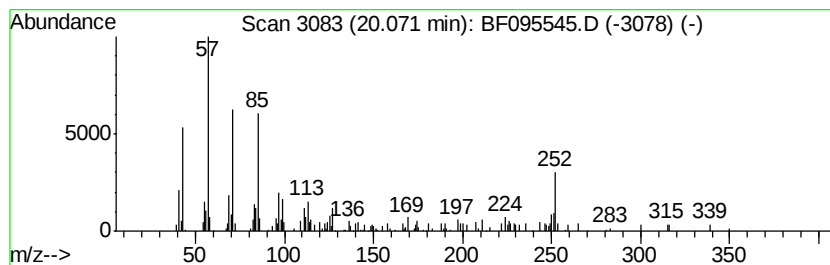
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	4.42 ng	106998	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	55
2		Octacosane	394	C28H58	000630-02-4	49
3		Hexadecane	226	C16H34	000544-76-3	49
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	46
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095545.D
Acq On : 30 May 2017 20:24
Operator : SJ/MA
Sample : I3302-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-0-6

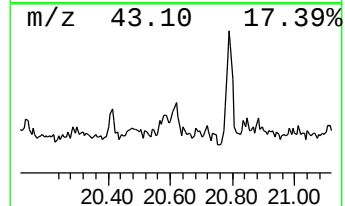
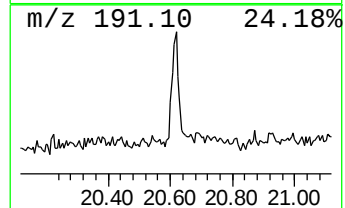
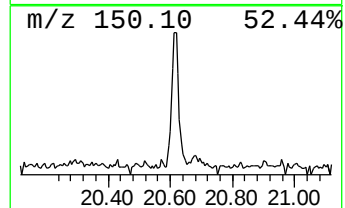
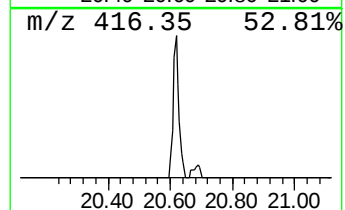
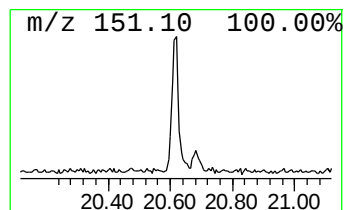
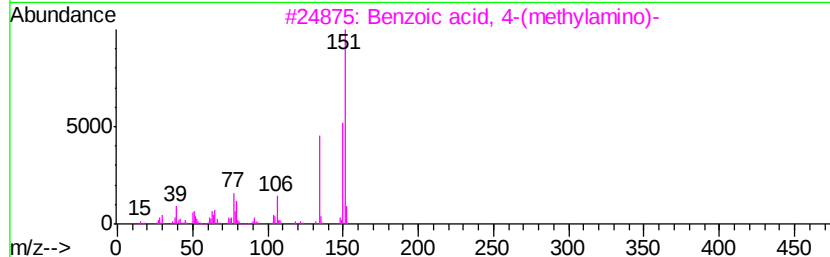
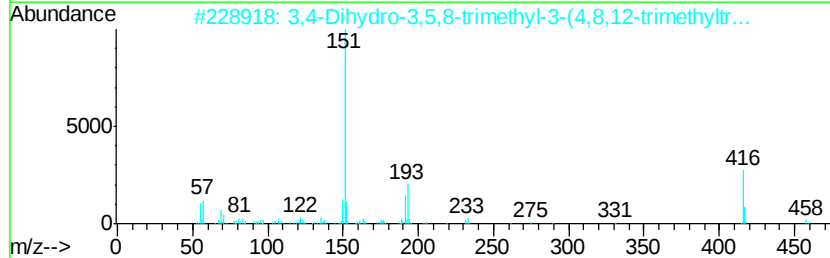
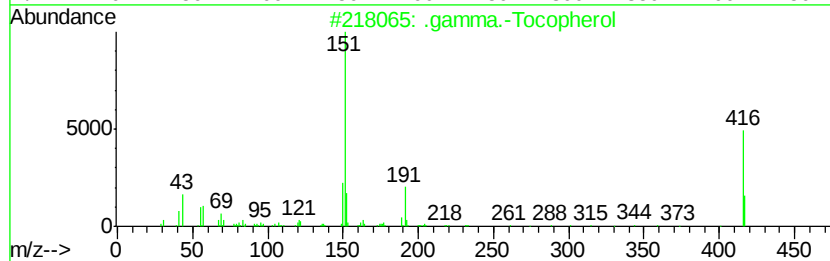
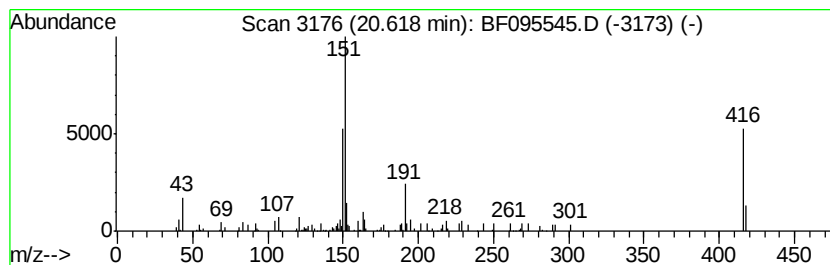
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Tocopherol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.62	3.29 ng	79641	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	76
2		3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	53
3		Benzoic acid, 4-(methylamino)-	151	C8H9NO2	010541-83-0	43
4		4-Ethylbenzoic acid, undecyl ester	304	C20H32O2	1000292-20-1	37
5		Silane, 3-butenylmethoxymethylph...	206	C12H18OSi	076557-75-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095545.D
Acq On : 30 May 2017 20:24
Operator : SJ/MA
Sample : I3302-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM16-COMP-0-6

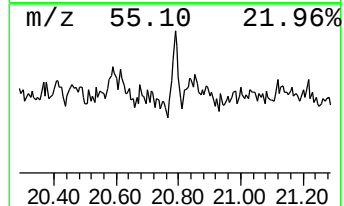
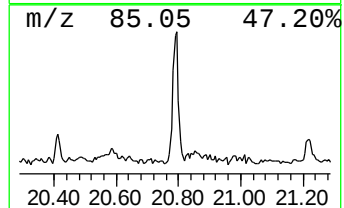
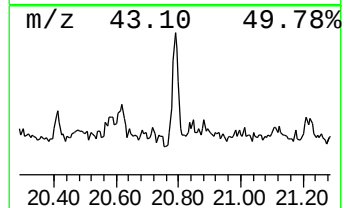
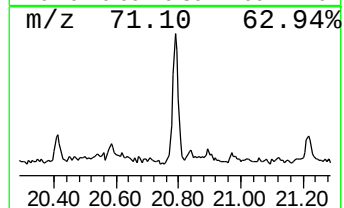
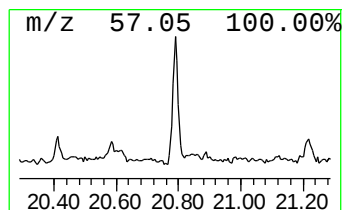
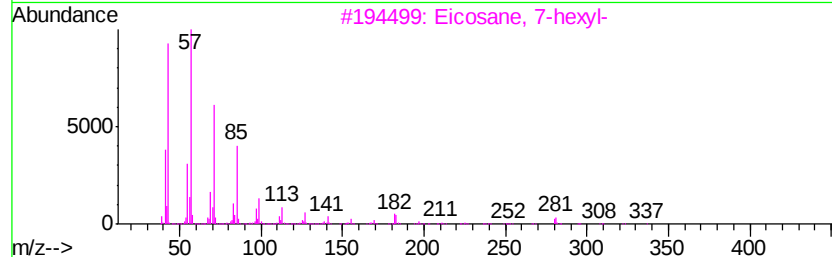
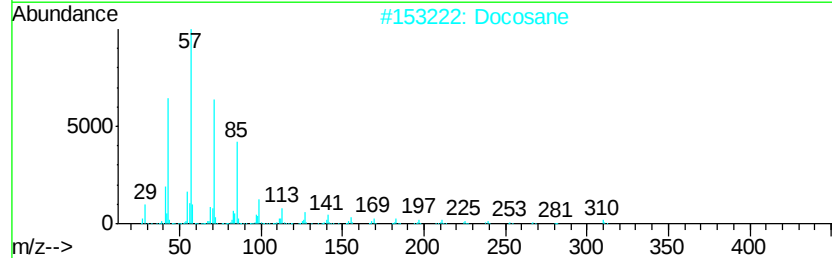
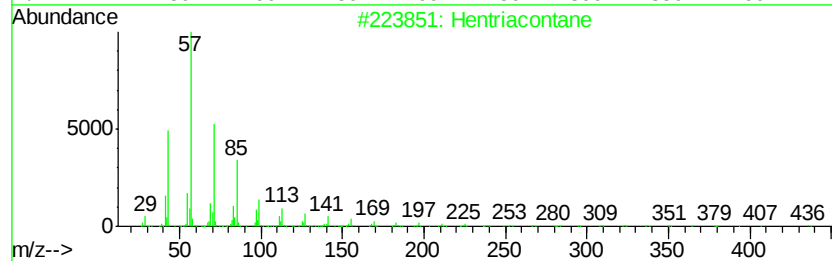
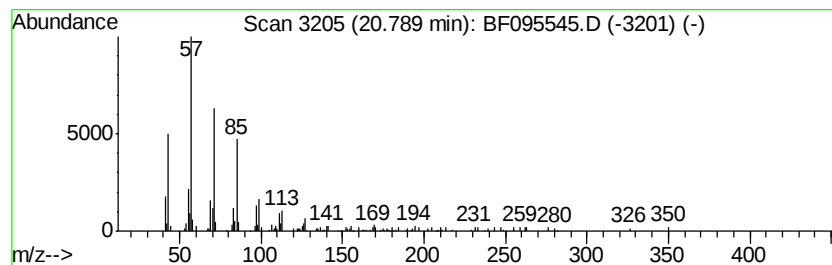
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	5.59 ng	135272	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Docosane	310	C22H46	000629-97-0	86
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5		triacontane	422	C30H62	000638-68-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095545.D
Acq On : 30 May 2017 20:24
Operator : SJ/MA
Sample : I3302-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.41	7.41	80.4	ng	2401880	1	7.74	597738	20.0
n-Hexadecanoic acid	15.95	8.3	ng	208258	4	15.00	499746	20.0
Ethanol, 2-(tetra...	18.55	2.5	ng	108433	5	18.67	858226	20.0
Heptadecane	19.34	2.2	ng	92830	5	18.67	858226	20.0
Squalene	19.78	3.8	ng	91500	6	20.35	483884	20.0
Tetradecane	20.07	4.4	ng	106998	6	20.35	483884	20.0
.gamma.-Tocopherol	20.62	3.3	ng	79641	6	20.35	483884	20.0
Hentriacontane	20.79	5.6	ng	135272	6	20.35	483884	20.0