

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052217\
 Data File : BF095322.D
 Acq On : 22 May 2017 19:30
 Operator : SJ/MA
 Sample : I3235-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TW1-TW2

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	5.107	535	539	555	rBV2	95548	260663	13.16%	1.479%
2	5.719	639	643	677	rBV	692413	1739871	87.83%	9.873%
3	7.295	908	911	928	rBV	852858	1693837	85.51%	9.612%
4	7.419	928	932	946	rVB	1287784	1980927	100.00%	11.241%
5	7.754	985	989	1004	rVB	331800	440862	22.26%	2.502%
6	7.989	1025	1029	1043	rBV	1070707	1390002	70.17%	7.888%
7	8.660	1139	1143	1160	rBV	537718	1055323	53.27%	5.989%
8	9.777	1329	1333	1352	rBV	319887	609729	30.78%	3.460%
9	11.548	1629	1634	1656	rBV	1242058	1929343	97.40%	10.948%
10	12.248	1749	1753	1773	rBV	159443	281784	14.22%	1.599%
11	12.613	1810	1815	1836	rBV2	410014	686823	34.67%	3.897%
12	13.442	1952	1956	1961	rVB	33070	36501	1.84%	0.207%
13	13.907	2030	2035	2059	rBV	573228	1017958	51.39%	5.777%
14	14.212	2083	2087	2098	rBV	29078	46252	2.33%	0.262%
15	14.948	2207	2212	2215	rBV	16872	20825	1.05%	0.118%
16	15.012	2219	2223	2228	rBV	311208	452652	22.85%	2.569%
17	15.965	2380	2385	2400	rBV6	42080	103171	5.21%	0.585%
18	16.795	2522	2526	2537	rBV	152379	224411	11.33%	1.273%
19	17.100	2573	2578	2587	rVB	161175	232120	11.72%	1.317%
20	17.324	2612	2616	2626	rVB	938181	1099641	55.51%	6.240%
21	17.700	2676	2680	2686	rBV4	22772	40497	2.04%	0.230%
22	18.253	2772	2774	2781	rVB2	16619	25784	1.30%	0.146%
23	18.371	2789	2794	2796	rBV3	15692	21108	1.07%	0.120%
24	18.394	2796	2798	2802	rVV4	21176	25280	1.28%	0.143%
25	18.530	2817	2821	2824	rBV	16871	22945	1.16%	0.130%
26	18.571	2824	2828	2836	rBV10	29892	78583	3.97%	0.446%
27	18.683	2841	2847	2851	rVV2	439779	687169	34.69%	3.899%
28	18.718	2851	2853	2864	rVV	120960	199324	10.06%	1.131%
29	18.812	2865	2869	2876	rVB6	20967	44932	2.27%	0.255%
30	18.971	2894	2896	2900	rBV4	15340	20977	1.06%	0.119%
31	19.194	2932	2934	2938	rVB2	25032	25735	1.30%	0.146%
32	19.236	2938	2941	2944	rBV3	19723	24623	1.24%	0.140%
33	19.341	2957	2959	2963	rBV5	15834	27821	1.40%	0.158%
34	19.953	3060	3063	3067	rBV	127603	192691	9.73%	1.093%

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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

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

35	20.077	3081	3084	3087	rBV4	32057	46077	2.33%	0.261%
36	20.247	3110	3113	3118	rBV	77274	102288	5.16%	0.580%
37	20.306	3120	3123	3128	rBV	105846	131454	6.64%	0.746%
38	20.359	3128	3132	3141	rVV	321094	465657	23.51%	2.642%
39	20.935	3228	3230	3232	rBV3	24113	26902	1.36%	0.153%
40	21.706	3358	3361	3365	rBV2	36361	58404	2.95%	0.331%
41	22.777	3536	3543	3547	rBV9	20526	51206	2.58%	0.291%

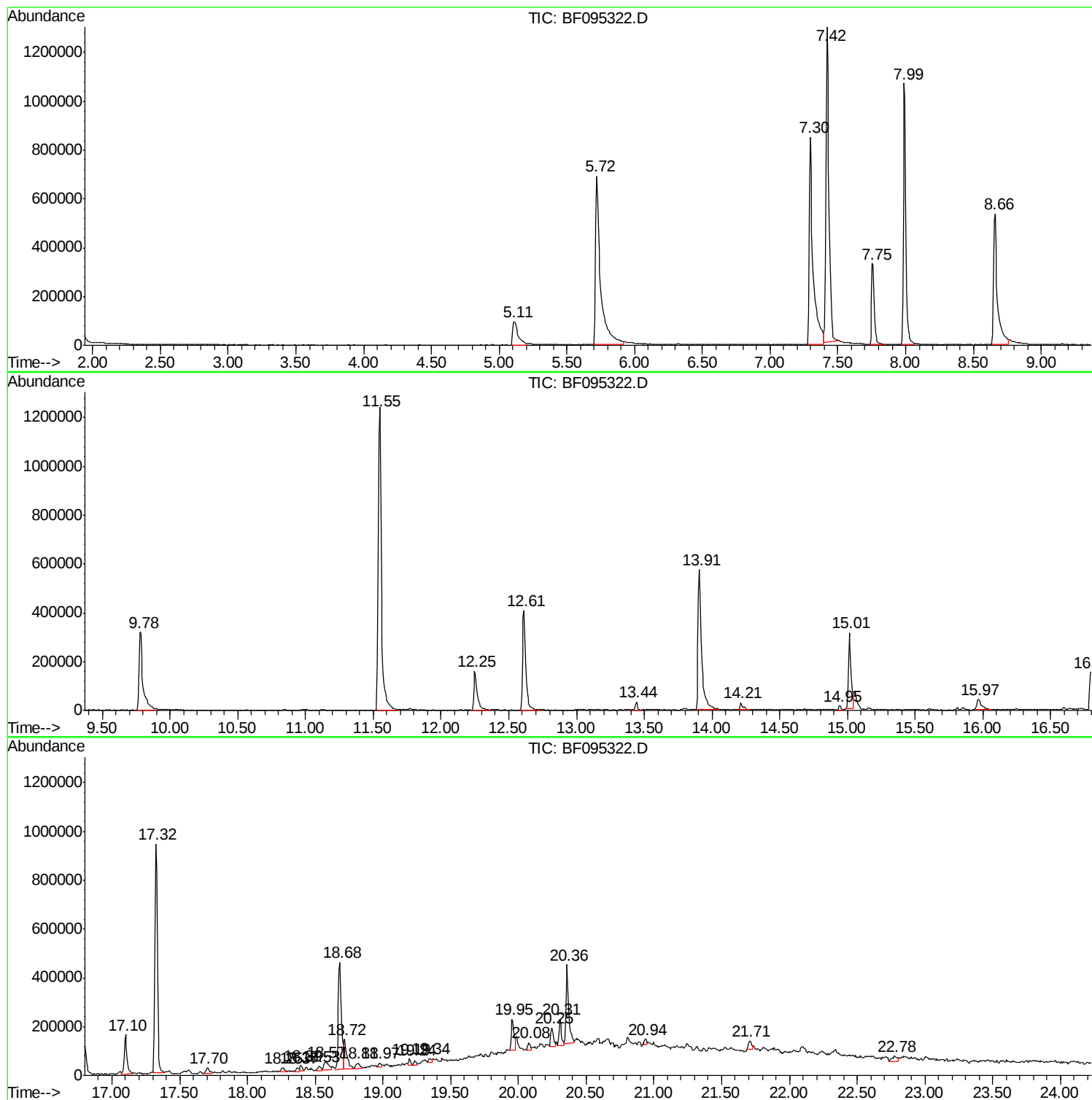
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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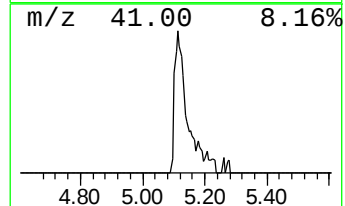
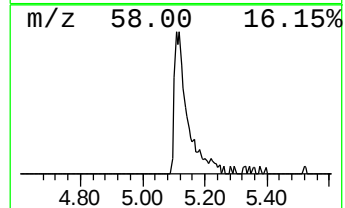
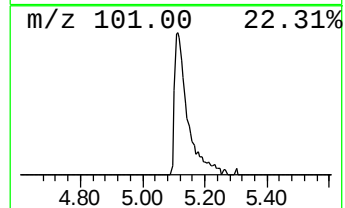
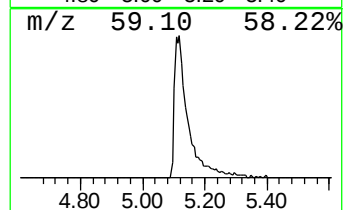
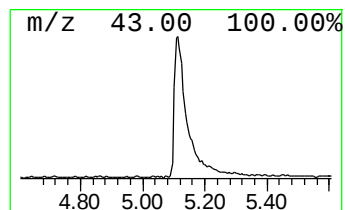
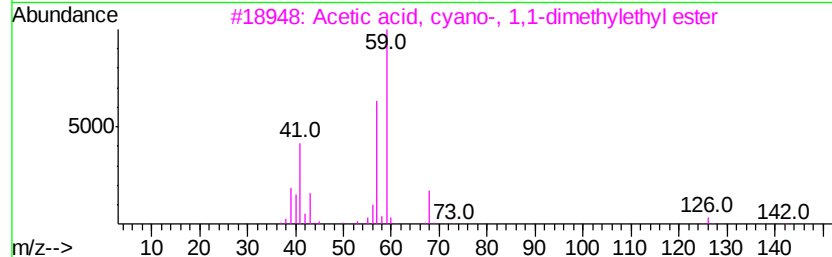
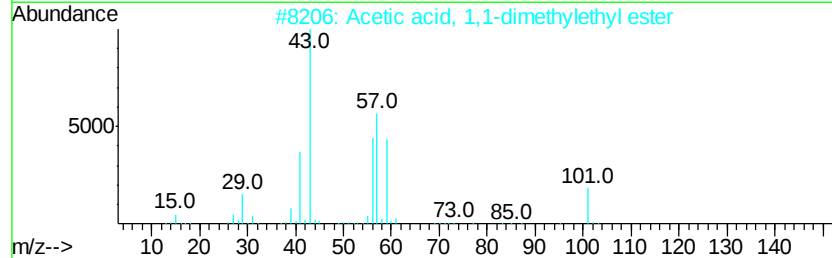
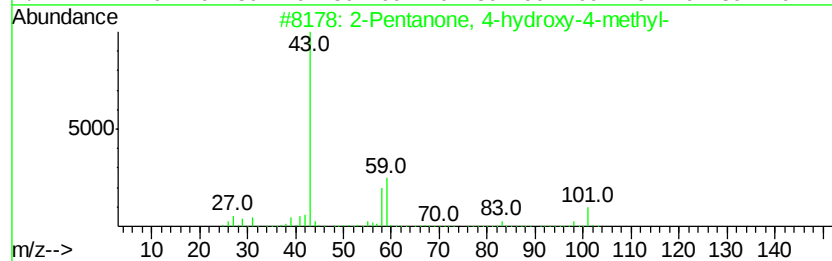
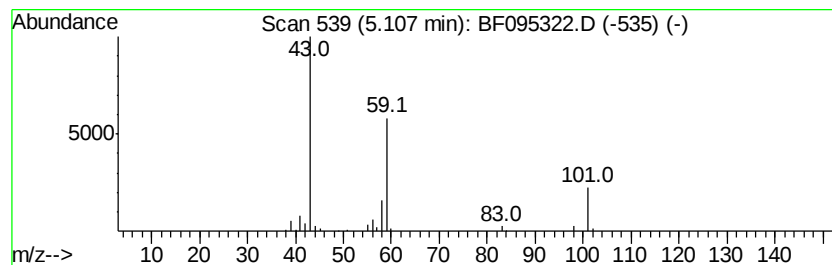
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	11.83 ng	260663	1,4-Dichlorobenzene-d4	7.76

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	Acetic acid, cyano-, 1,1-dimethyl...			141	C7H11NO2	001116-98-9	23
4	1,8-Nonanediol, 8-methyl-			174	C10H22O2	054725-73-4	23
5	Morpholine, 4-methyl-			101	C5H11NO	000109-02-4	9



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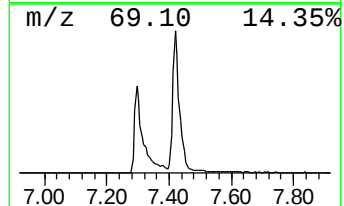
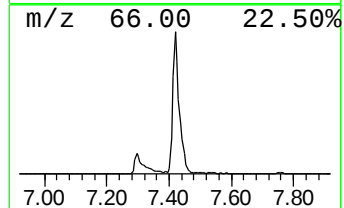
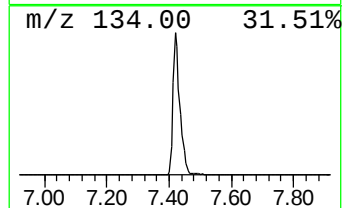
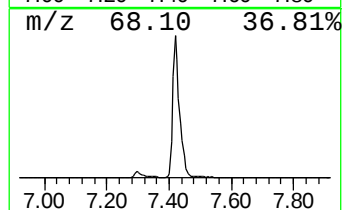
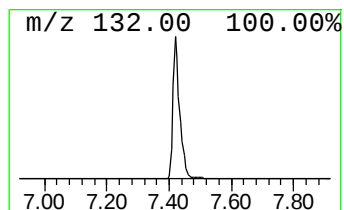
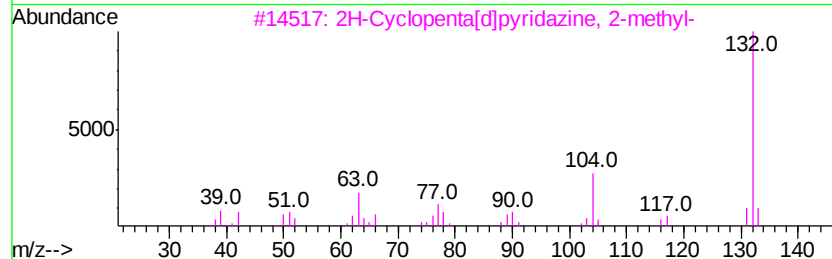
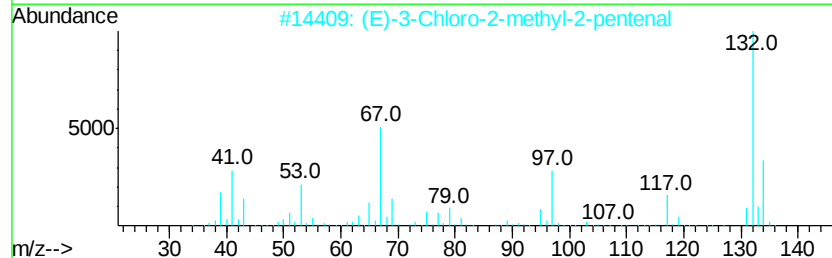
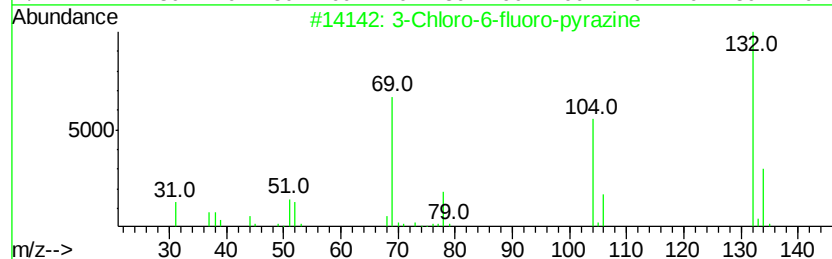
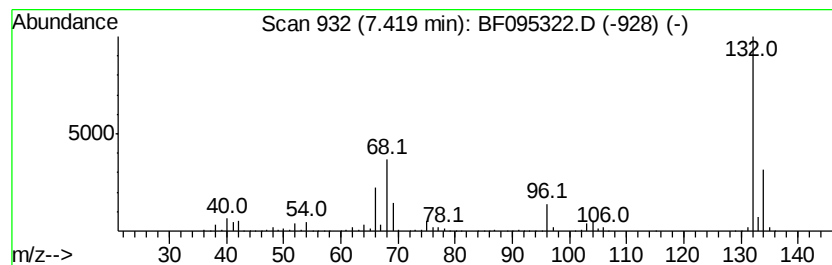
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	89.87 ng	1980930	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		2H-Cyclopentaf[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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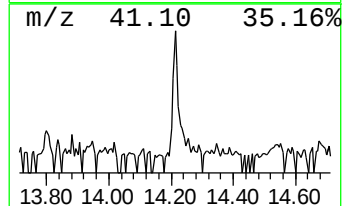
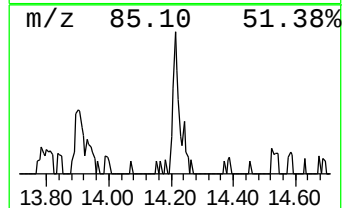
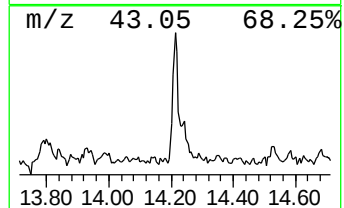
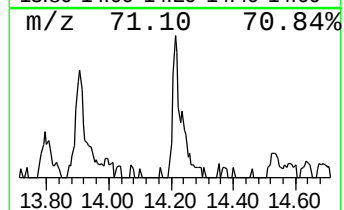
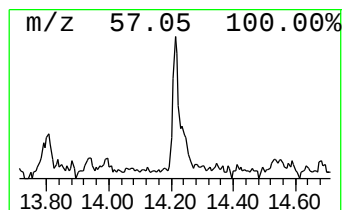
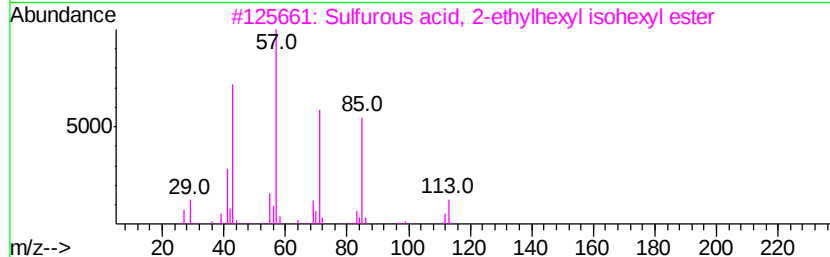
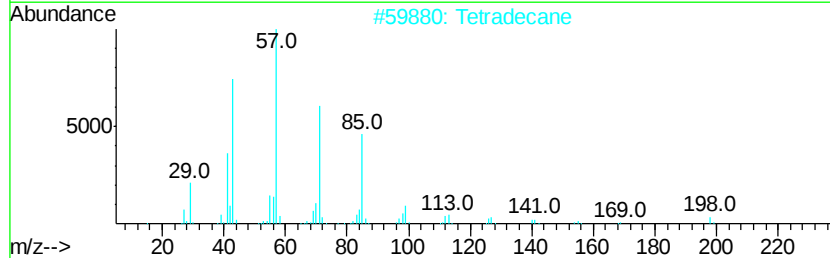
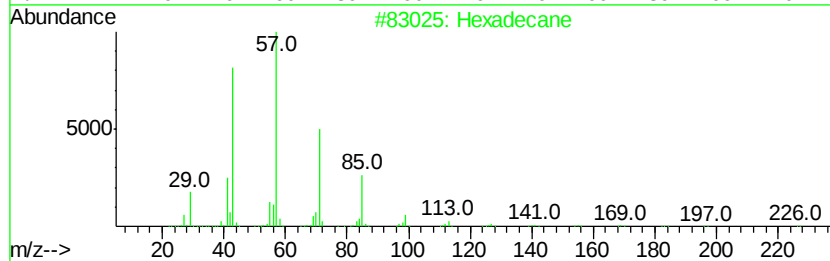
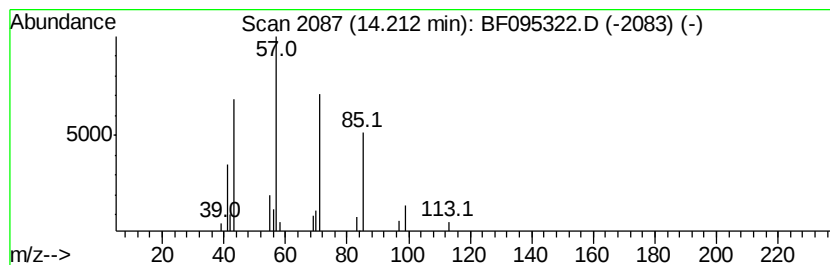
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.21	2.04 ng	46252	Phenanthrene-d10	15.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tetradecane	198	C14H30	000629-59-4	78
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
4	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
5	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	59



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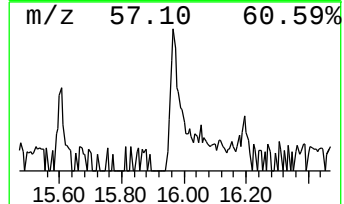
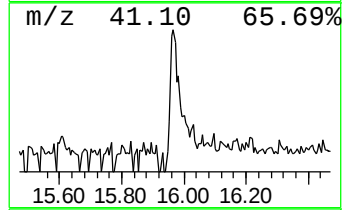
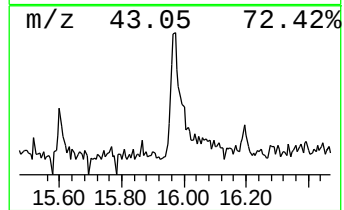
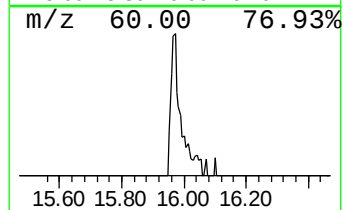
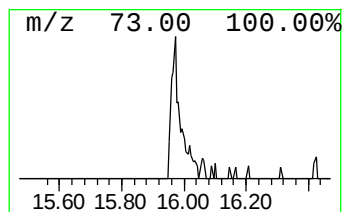
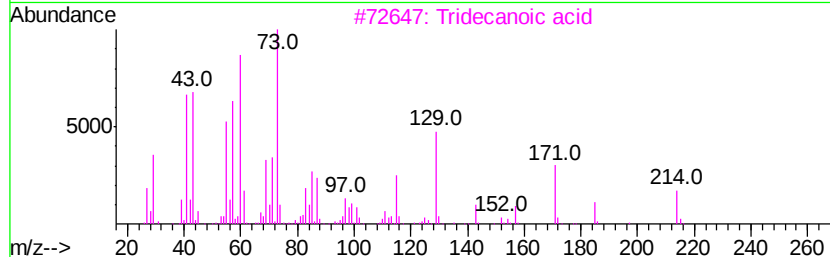
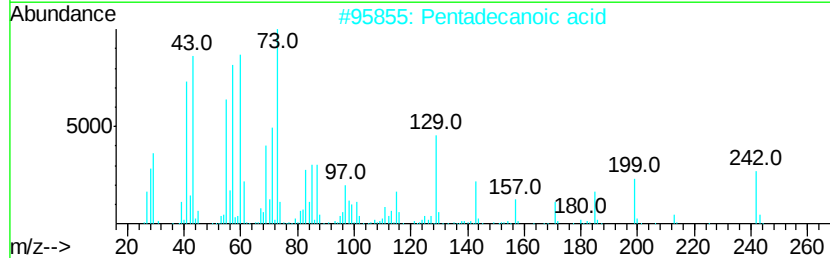
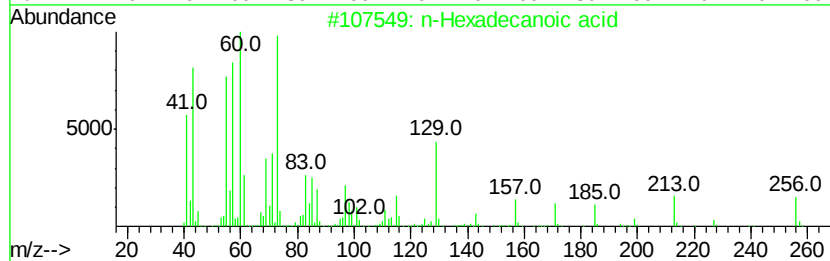
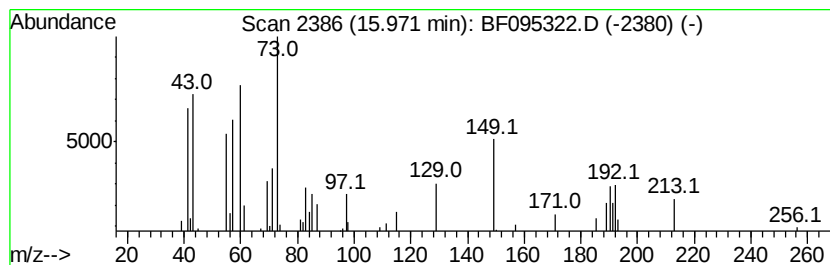
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.97	4.56 ng	103171	Phenanthrene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
3	Tridecanoic acid	214	C13H26O2	000638-53-9	38
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5	Undecanoic acid	186	C11H22O2	000112-37-8	27



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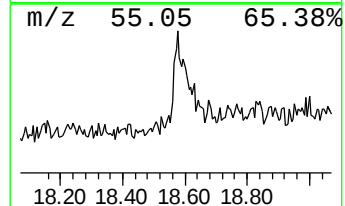
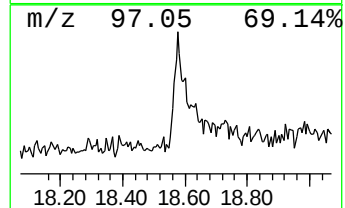
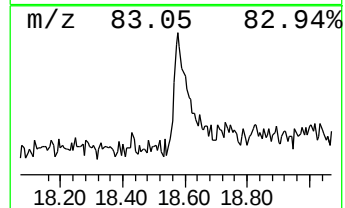
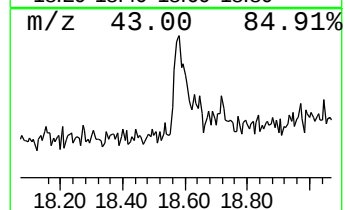
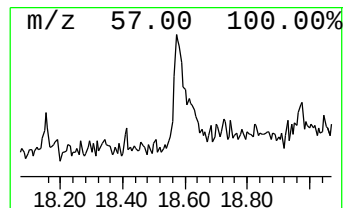
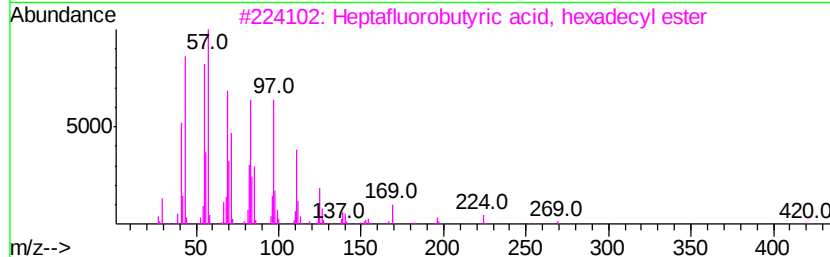
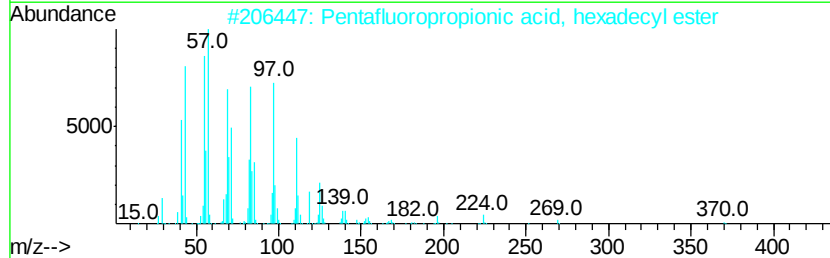
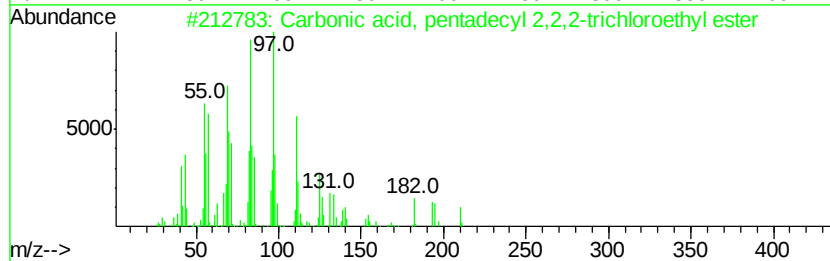
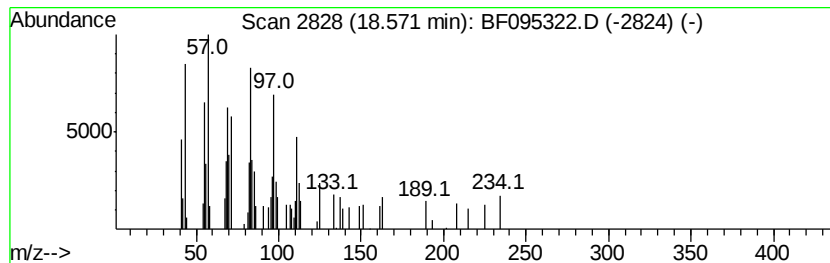
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Carbonic acid, pentadecyl 2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.29 ng	78583	Chrysene-d12	18.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	87
2		Pentafluoropropionic acid, hexadec...	388	C19H33F5O2	006222-07-7	83
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83
4		Octacosyl acetate	452	C30H60O2	018206-97-8	81
5		Triacetyl acetate	480	C32H64O2	041755-58-2	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
Data File : BF095322.D
Acq On : 22 May 2017 19:30
Operator : SJ/MA
Sample : I3235-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW1-TW2

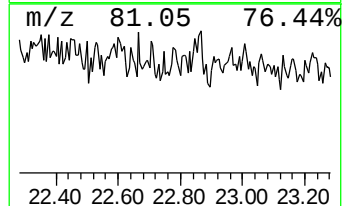
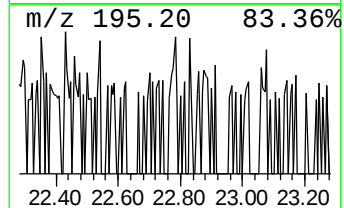
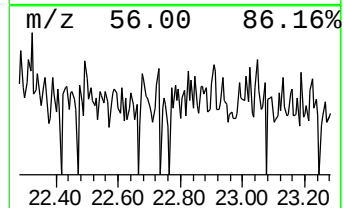
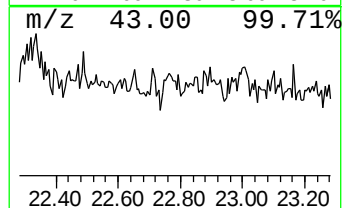
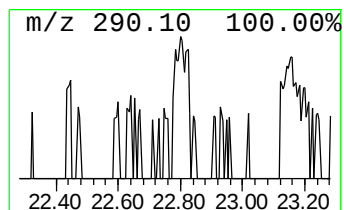
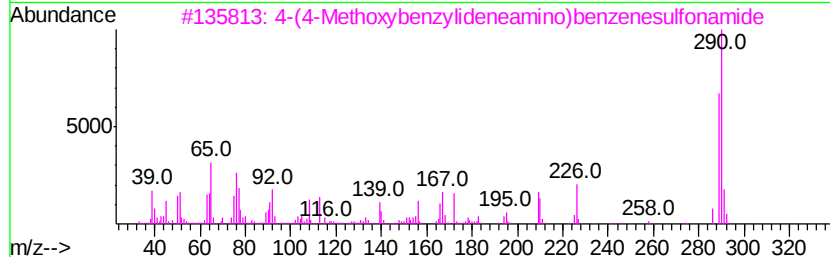
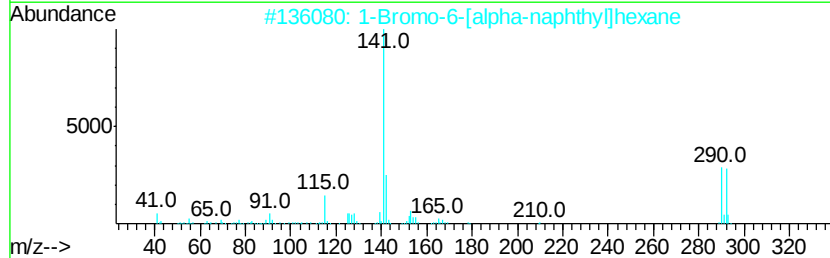
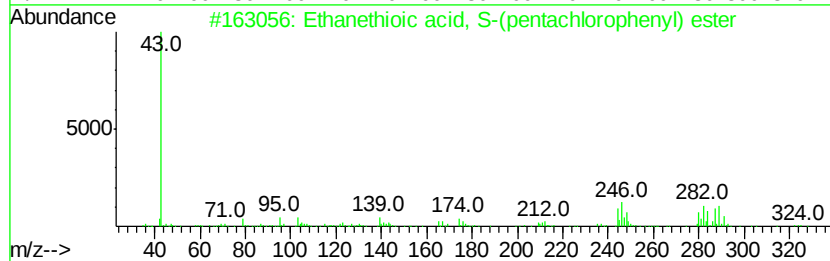
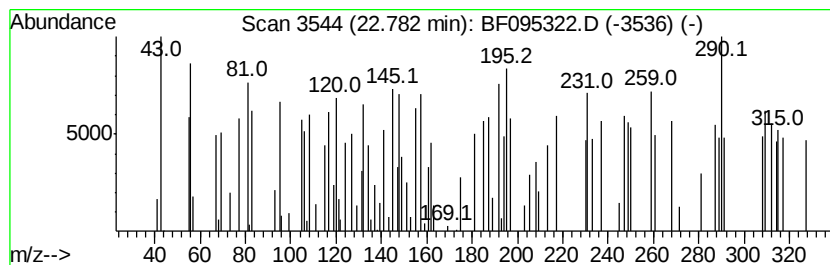
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown22.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	2.20 ng	51206	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethioic acid, S-(pentachlor...	322	C8H3Cl5OS	080304-12-7	17
2		1-Bromo-6-[alpha-naphthyl]hexane	290	C16H19Br	052121-92-3	11
3		4-(4-Methoxybenzylideneamino)ben...	290	C14H14N2O3S	066667-56-9	10
4		Isoquinoline, 1,2,3,4-tetrahydro...	287	C17H18FN02	055507-14-7	10
5		3,6-Dichlorophenanthrene-9-carbo...	290	C15H8Cl2O2	056988-51-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052217\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW1-TW2

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...	5.11	11.8	ng	260663	1	7.76	440862	20.0
unknown7.42	7.42	89.9	ng	1980930	1	7.76	440862	20.0
Hexadecane	14.21	2.0	ng	46252	4	15.01	452652	20.0
n-Hexadecanoic acid	15.97	4.6	ng	103171	4	15.01	452652	20.0
Carbonic acid, pe...	18.57	2.3	ng	78583	5	18.68	687169	20.0
unknown22.78	22.78	2.2	ng	51206	6	20.36	465657	20.0