

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
 Data File : BF095542.D
 Acq On : 30 May 2017 18:48
 Operator : SJ/MA
 Sample : I3281-19
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R1-TP13-SS5

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	4.313	397	404	416	rBV4	21875	59182	2.44%	0.262%
2	5.089	531	536	553	rBV	87861	242414	9.99%	1.072%
3	5.589	616	621	629	rBV2	15683	37137	1.53%	0.164%
4	5.707	637	641	679	rBV	743683	2078301	85.66%	9.191%
5	5.954	679	683	688	rVB	21969	36632	1.51%	0.162%
6	7.289	906	910	925	rBV	787888	1794148	73.95%	7.935%
7	7.407	925	930	939	rVV	1368378	2426247	100.00%	10.730%
8	7.472	939	941	948	rVV	51546	85254	3.51%	0.377%
9	7.530	949	951	961	rVB2	17035	28621	1.18%	0.127%
10	7.736	982	986	996	rBV	466685	580914	23.94%	2.569%
11	7.972	1021	1026	1039	rBV	1401841	1757521	72.44%	7.773%
12	8.642	1136	1140	1156	rBV	589775	1141173	47.03%	5.047%
13	8.748	1156	1158	1170	rVB6	31719	69307	2.86%	0.307%
14	9.760	1326	1330	1350	rBV	363624	782840	32.27%	3.462%
15	10.942	1526	1531	1539	rBV	23275	42498	1.75%	0.188%
16	11.083	1551	1555	1565	rBV	26139	50310	2.07%	0.222%
17	11.530	1626	1631	1649	rBV	1517003	2381142	98.14%	10.531%
18	11.748	1665	1668	1674	rVB2	19623	24756	1.02%	0.109%
19	12.071	1718	1723	1727	rBV2	22658	37124	1.53%	0.164%
20	12.113	1727	1730	1736	rVB4	17578	25149	1.04%	0.111%
21	12.236	1746	1751	1767	rBV	191221	414570	17.09%	1.833%
22	12.595	1807	1812	1832	rBV2	488433	830360	34.22%	3.672%
23	12.960	1869	1874	1883	rBV5	17351	38899	1.60%	0.172%
24	13.418	1947	1952	1956	rBV	46184	53904	2.22%	0.238%
25	13.495	1961	1965	1974	rVB3	32516	53501	2.21%	0.237%
26	13.777	2006	2013	2024	rBV5	25351	56768	2.34%	0.251%
27	13.895	2028	2033	2051	rBV	540760	1031017	42.49%	4.560%
28	14.195	2079	2084	2086	rBV2	47941	65850	2.71%	0.291%
29	14.218	2086	2088	2093	rVB3	50985	65537	2.70%	0.290%
30	14.612	2151	2155	2160	rBV4	17543	26842	1.11%	0.119%
31	14.924	2205	2208	2213	rBV	33336	37942	1.56%	0.168%
32	14.995	2213	2220	2224	rVV	384718	564841	23.28%	2.498%
33	15.036	2224	2227	2239	rVV	175754	302519	12.47%	1.338%
34	15.130	2239	2243	2250	rVB	33796	52809	2.18%	0.234%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
 Data File : BF095542.D
 Acq On : 30 May 2017 18:48
 Operator : SJ/MA
 Sample : I3281-19
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R1-TP13-SS5

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

35	15.583	2315	2320	2328	rVB	31800	38828	1.60%	0.172%
36	15.783	2350	2354	2358	rBV	31795	39926	1.65%	0.177%
37	15.824	2358	2361	2368	rVB	37232	54701	2.25%	0.242%
38	15.953	2376	2383	2398	rVB5	58404	173032	7.13%	0.765%
39	16.224	2425	2429	2439	rVB	15523	27312	1.13%	0.121%
40	16.571	2485	2488	2493	rBV	30478	44023	1.81%	0.195%
41	16.718	2511	2513	2519	rVB2	25372	27526	1.13%	0.122%
42	16.783	2519	2524	2536	rBV	271542	380599	15.69%	1.683%
43	17.083	2570	2575	2583	rVB	289002	359327	14.81%	1.589%
44	17.148	2583	2586	2589	rBV3	24190	26440	1.09%	0.117%
45	17.271	2603	2607	2610	rBV4	18565	26383	1.09%	0.117%
46	17.312	2610	2614	2623	rVV	1334383	1602209	66.04%	7.086%
47	17.406	2623	2630	2638	rVB5	21050	56979	2.35%	0.252%
48	17.512	2645	2648	2651	rBV5	19256	30470	1.26%	0.135%
49	17.547	2651	2654	2659	rVB	35472	42481	1.75%	0.188%
50	17.636	2664	2669	2672	rBV2	22686	30836	1.27%	0.136%
51	17.683	2673	2677	2684	rBV2	50389	89233	3.68%	0.395%
52	18.077	2741	2744	2747	rBV5	28281	35766	1.47%	0.158%
53	18.377	2793	2795	2798	rVB2	30398	28140	1.16%	0.124%
54	18.412	2798	2801	2803	rBV4	22253	26992	1.11%	0.119%
55	18.553	2821	2825	2831	rBV3	56974	109095	4.50%	0.482%
56	18.671	2839	2845	2849	rBV2	587970	857611	35.35%	3.793%
57	18.706	2849	2851	2862	rVB2	137970	203078	8.37%	0.898%
58	18.800	2864	2867	2873	rVB2	30932	44202	1.82%	0.195%
59	18.959	2892	2894	2899	rVB5	29086	35304	1.46%	0.156%
60	19.177	2929	2931	2935	rBV	30008	34791	1.43%	0.154%
61	19.677	3013	3016	3019	rBV3	44414	58329	2.40%	0.258%
62	19.947	3058	3062	3065	rBV	120235	185077	7.63%	0.819%
63	20.236	3109	3111	3114	rBV	56295	56635	2.33%	0.250%
64	20.294	3119	3121	3126	rVV	95762	107148	4.42%	0.474%
65	20.347	3126	3130	3139	rVV	362751	502793	20.72%	2.224%

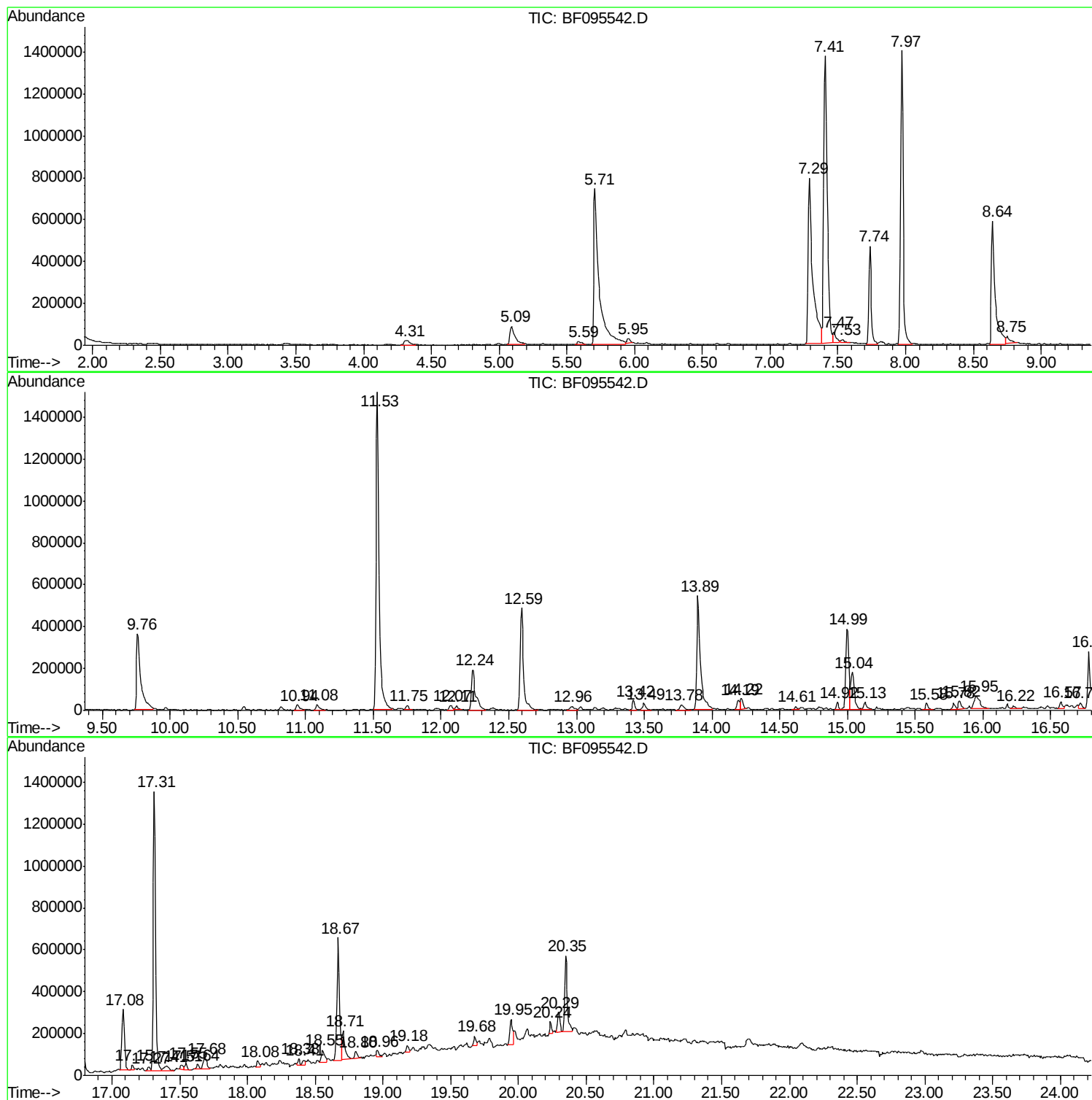
Sum of corrected areas: 22611295

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
R1-TP13-SS5

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

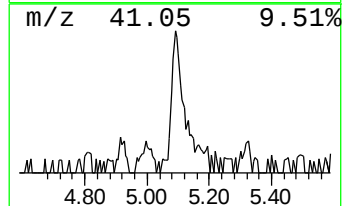
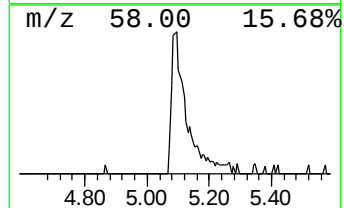
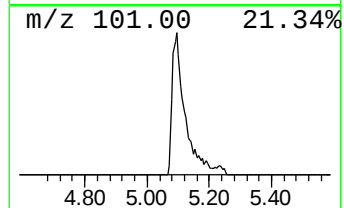
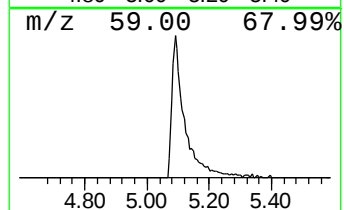
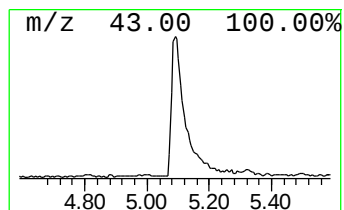
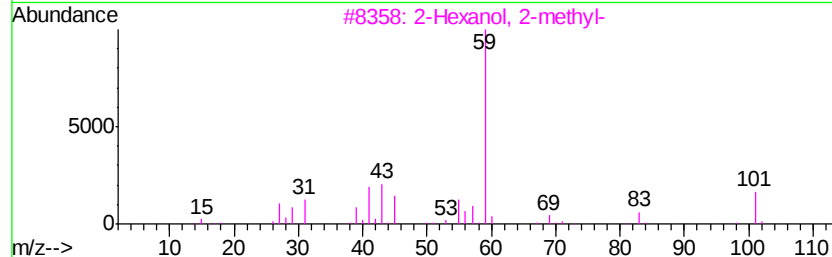
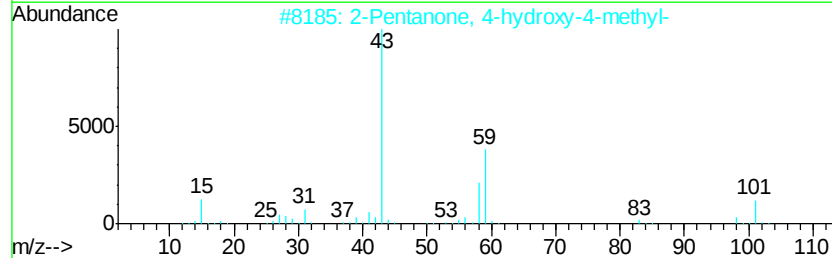
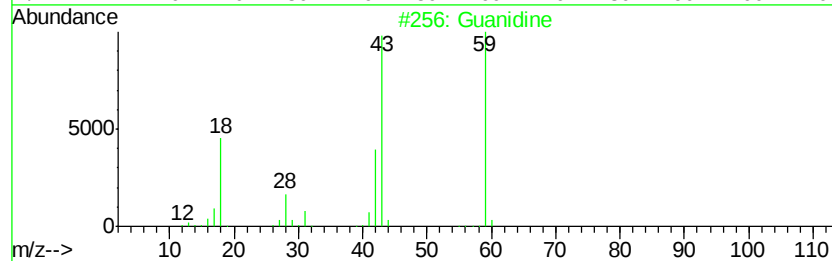
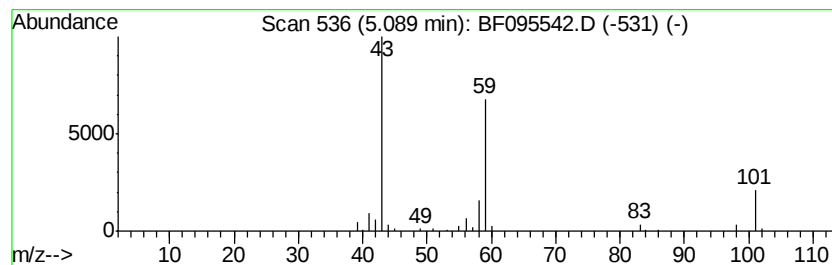
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.09 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	8.35 ng	242414	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanidine	59	CH5N3	000113-00-8	43
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

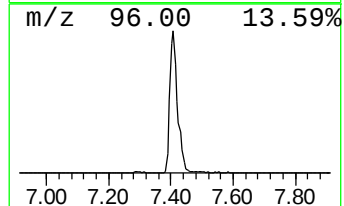
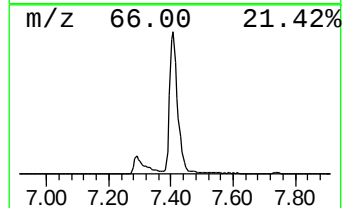
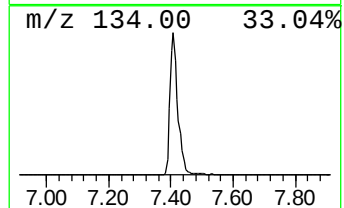
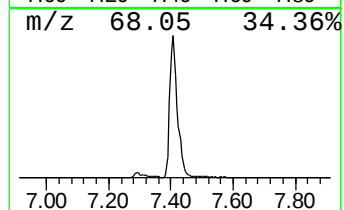
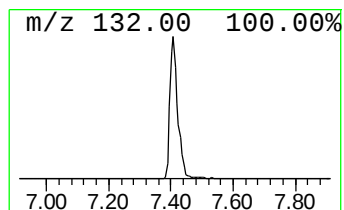
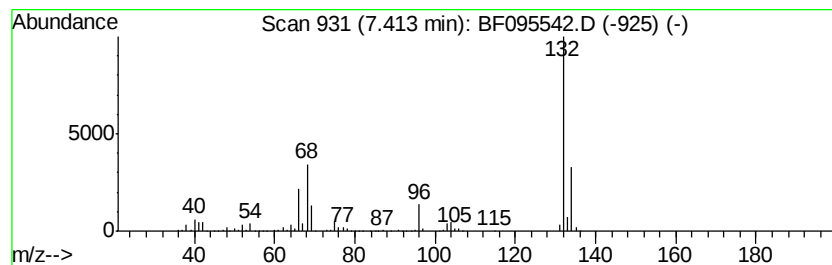
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	83.53 ng	2426250	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	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

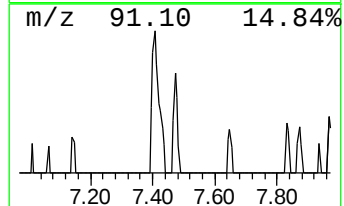
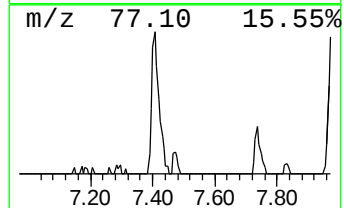
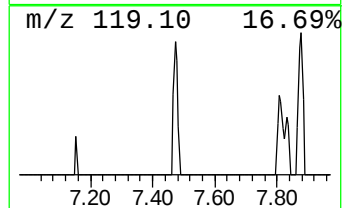
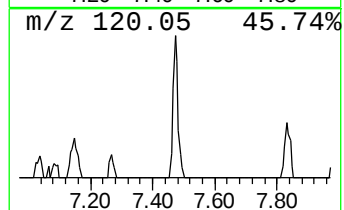
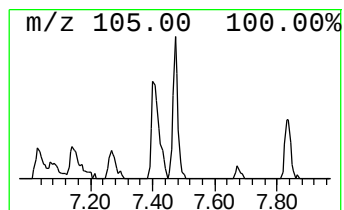
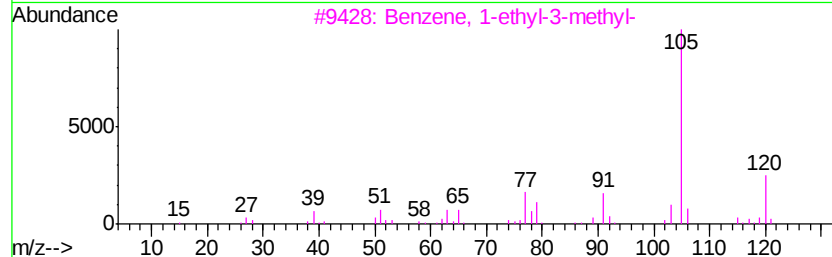
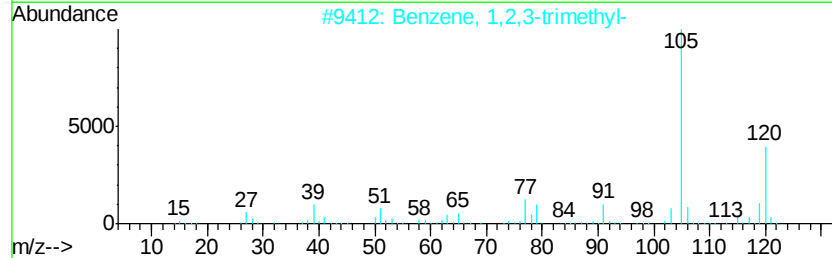
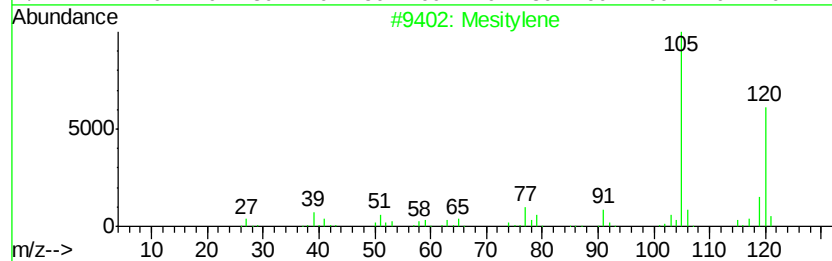
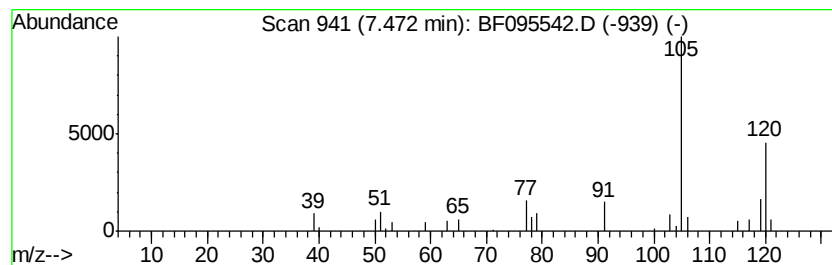
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	2.94 ng	85254	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mesitylene	120	C9H12	000108-67-8	91
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

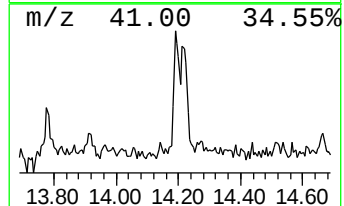
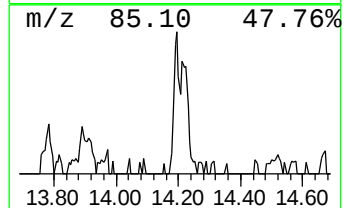
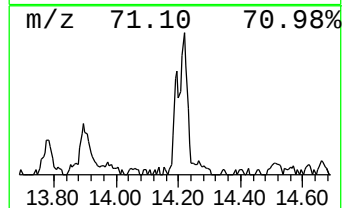
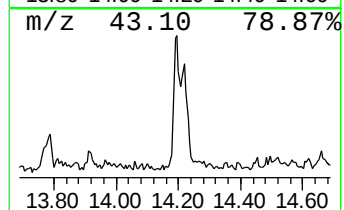
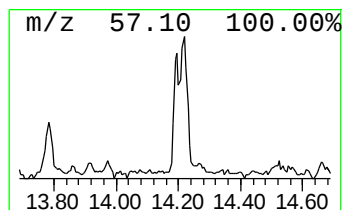
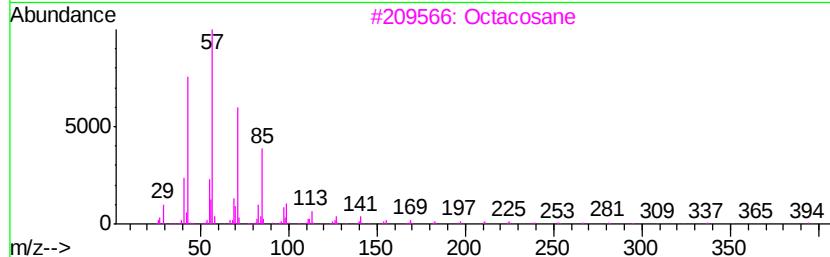
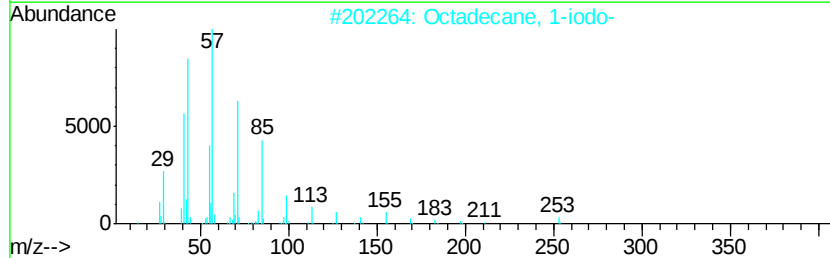
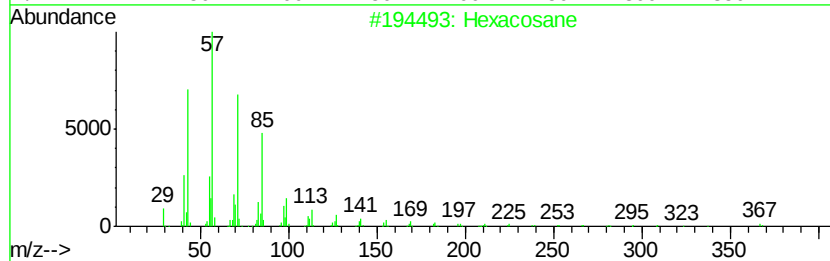
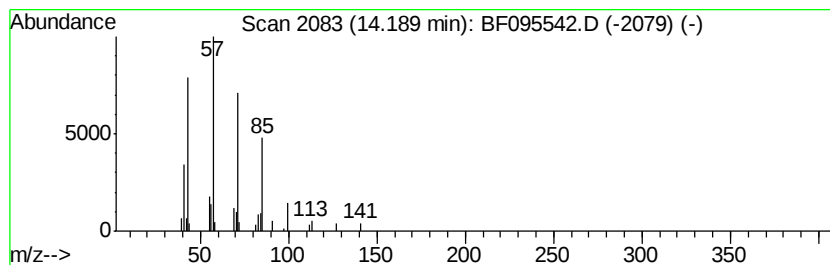
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.33 ng	65850	Phenanthrene-d10	14.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	83
2	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	80
3	Octacosane		394	C28H58	000630-02-4	80
4	Tetradecane		198	C14H30	000629-59-4	80
5	Pentadecane		212	C15H32	000629-62-9	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

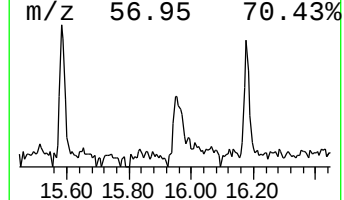
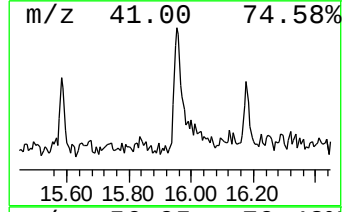
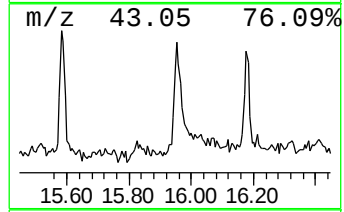
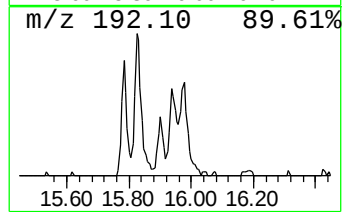
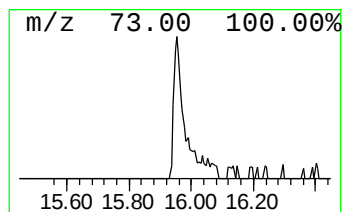
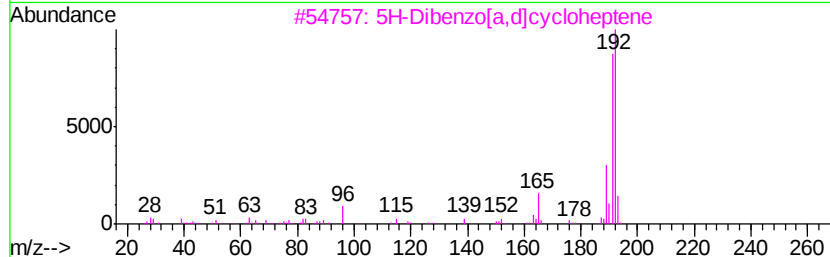
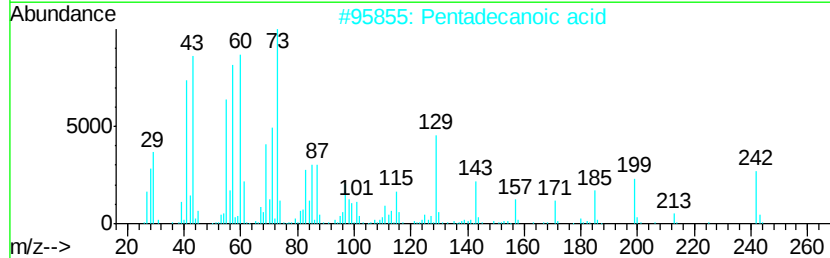
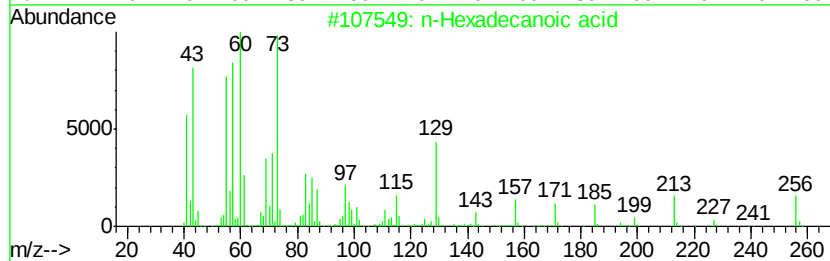
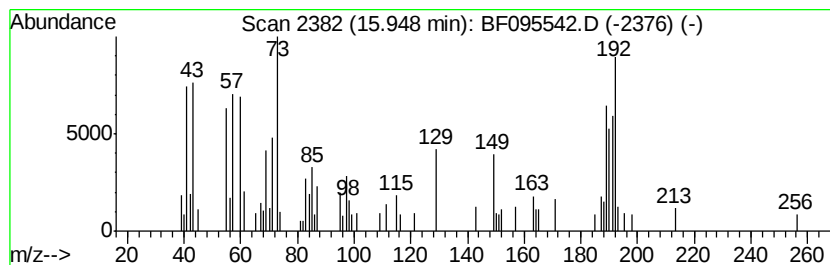
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.95 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	6.13 ng	173032	Phenanthrene-d10	14.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	25
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	18
3		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	14
4		Tridecanoic acid	214	C13H26O2	000638-53-9	14
5		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

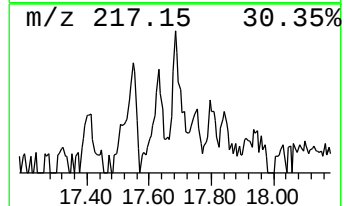
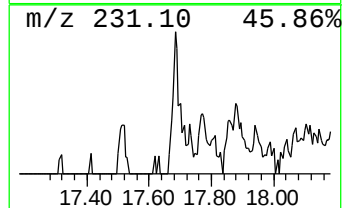
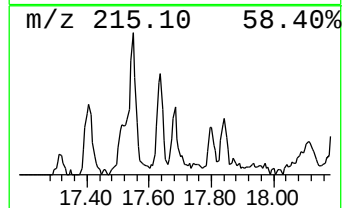
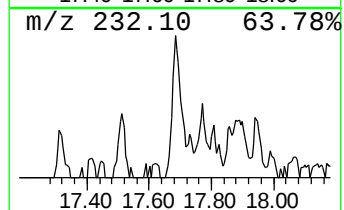
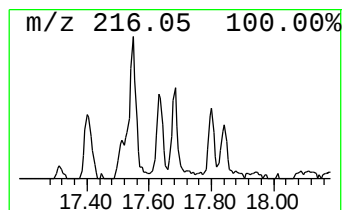
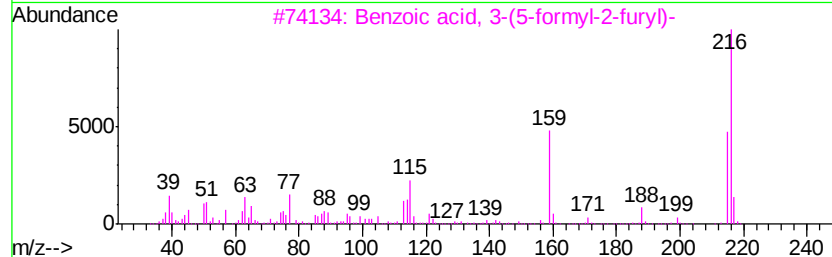
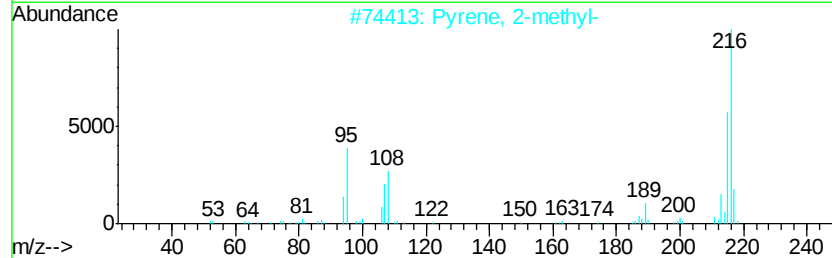
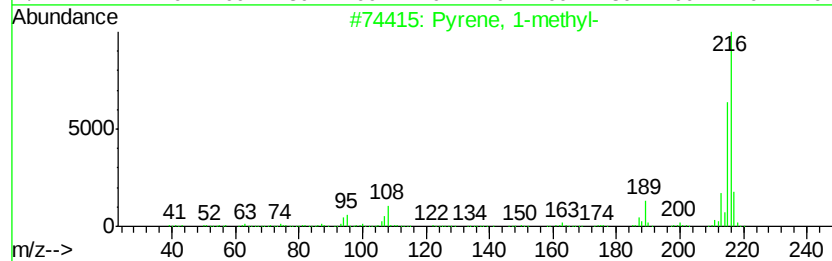
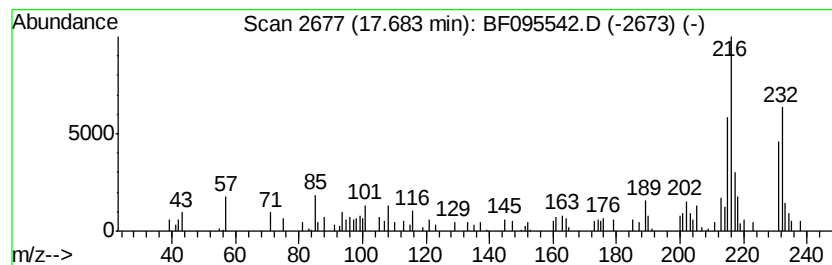
Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

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 9 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.68	2.08 ng	89233	Chrysene-d12	18.67		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 1-methyl-	216	C17H12	002381-21-7	50
2		Pyrene, 2-methyl-	216	C17H12	003442-78-2	45
3		Benzoic acid, 3-(5-formyl-2-furyl)-	216	C12H8O4	304884-54-6	45
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	43
5		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

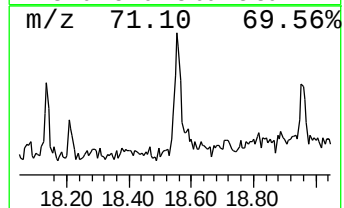
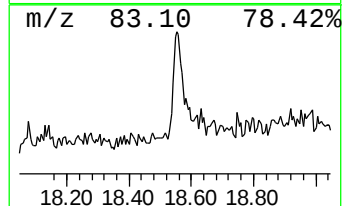
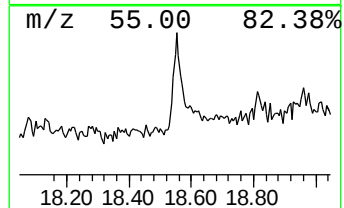
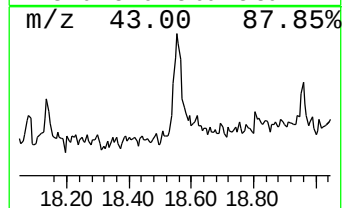
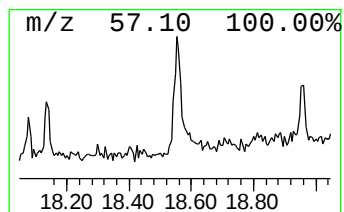
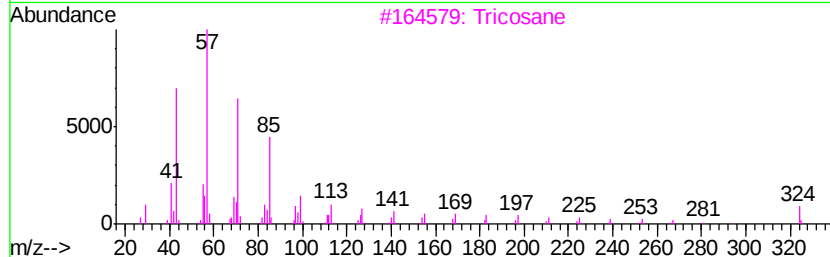
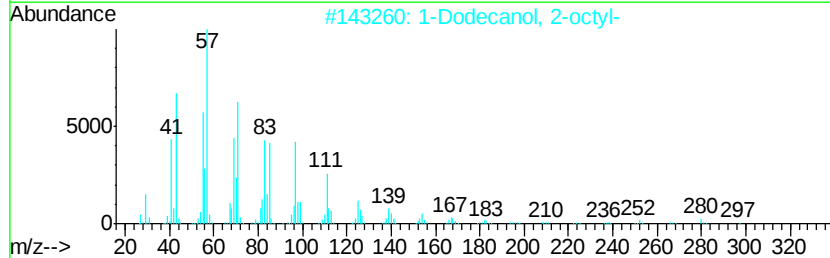
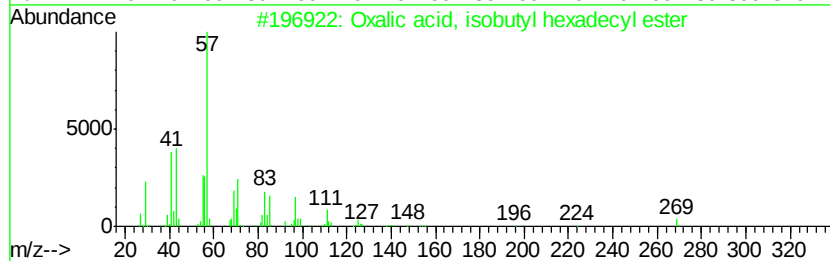
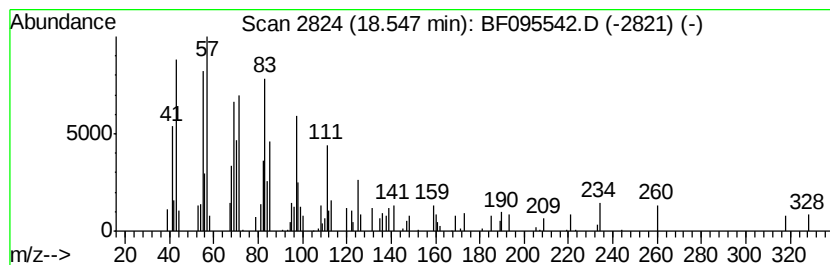
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxalic acid, isobutyl hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.54 ng	109095	Chrysene-d12	18.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
3			Tricosane	324	C23H48	000638-67-5	81
4			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	68
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

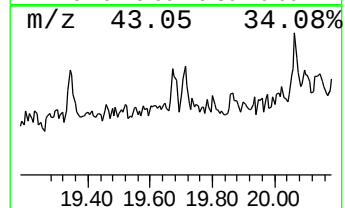
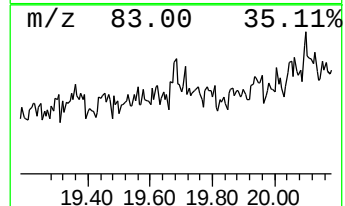
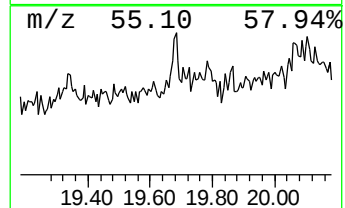
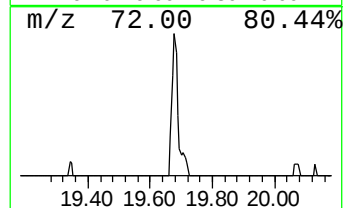
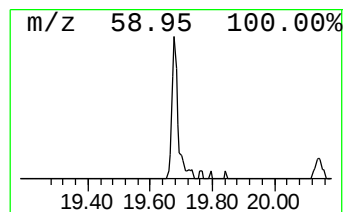
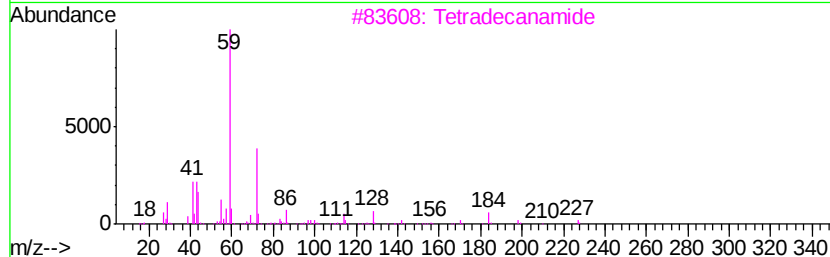
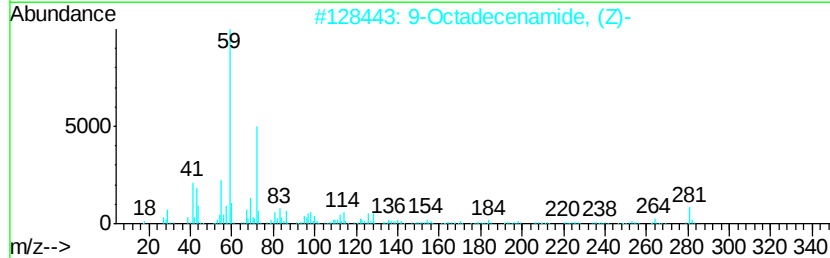
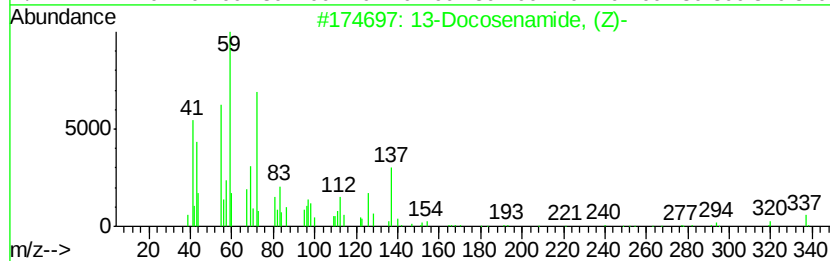
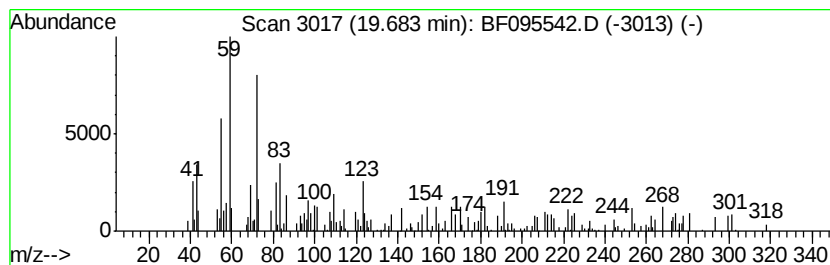
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	2.32 ng	58329	Perylene-d12	20.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
3			Tetradecanamide	227	C14H29NO	000638-58-4	59
4			Pentanamide	101	C5H11NO	000626-97-1	53
5			Propanedioic acid, methyl-, dime...	146	C6H10O4	000609-02-9	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095542.D
Acq On : 30 May 2017 18:48
Operator : SJ/MA
Sample : I3281-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP13-SS5

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
unknown5.09	5.09	8.3	ng	242414	1	7.74	580914	20.0
unknown7.41	7.41	83.5	ng	2426250	1	7.74	580914	20.0
Mesitylene	7.47	2.9	ng	85254	1	7.74	580914	20.0
Hexacosane	14.19	2.3	ng	65850	4	14.99	564841	20.0
unknown15.95	15.95	6.1	ng	173032	4	14.99	564841	20.0
Pyrene, 1-methyl-	17.68	2.1	ng	89233	5	18.67	857611	20.0
Oxalic acid, isob...	18.55	2.5	ng	109095	5	18.67	857611	20.0
13-Docosenamide, ...	19.68	2.3	ng	58329	6	20.35	502793	20.0