

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
 Data File : BF095269.D
 Acq On : 19 May 2017 18:25
 Operator : SJ/MA
 Sample : I3202-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-8COMP

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	5.113	535	540	567	rBV	183672	505917	22.27%	2.468%
2	5.731	642	645	686	rBV	715012	1786337	78.65%	8.715%
3	7.301	909	912	929	rBV	869756	1668125	73.44%	8.138%
4	7.431	929	934	947	rVB	1223681	2027005	89.24%	9.889%
5	7.766	987	991	1001	rBV	359701	446174	19.64%	2.177%
6	8.001	1026	1031	1046	rBV	1207899	1556445	68.52%	7.594%
7	8.666	1139	1144	1167	rBV	566328	1105416	48.67%	5.393%
8	9.783	1330	1334	1353	rBV	354684	613677	27.02%	2.994%
9	11.554	1630	1635	1654	rBV	1553051	2233029	98.31%	10.895%
10	12.254	1750	1754	1764	rBV	225704	366121	16.12%	1.786%
11	12.618	1810	1816	1834	rBV2	454404	750202	33.03%	3.660%
12	12.989	1871	1879	1886	rBV3	10916	23015	1.01%	0.112%
13	13.448	1952	1957	1961	rVB	24705	27121	1.19%	0.132%
14	13.530	1967	1971	1982	rVB2	26991	45253	1.99%	0.221%
15	13.907	2030	2035	2055	rBV	738398	1344193	59.18%	6.558%
16	14.218	2084	2088	2092	rBV2	30112	40207	1.77%	0.196%
17	14.954	2208	2213	2216	rBV	26895	31123	1.37%	0.152%
18	15.018	2216	2224	2228	rVV	492095	691438	30.44%	3.373%
19	15.054	2228	2230	2241	rVV	135290	247408	10.89%	1.207%
20	15.159	2244	2248	2256	rVB	29077	51397	2.26%	0.251%
21	15.512	2303	2308	2322	rBV6	29641	76731	3.38%	0.374%
22	15.606	2322	2324	2331	rVB2	23279	25266	1.11%	0.123%
23	15.759	2347	2350	2356	rVB	24061	26090	1.15%	0.127%
24	15.859	2363	2367	2374	rVB2	15051	23336	1.03%	0.114%
25	15.971	2381	2386	2401	rBV5	106486	195432	8.60%	0.953%
26	16.683	2498	2507	2511	rBV	80103	138446	6.10%	0.675%
27	16.718	2511	2513	2515	rVV2	45273	49820	2.19%	0.243%
28	16.748	2515	2518	2522	rVV	109770	132093	5.82%	0.644%
29	16.812	2525	2529	2537	rVV	97114	172184	7.58%	0.840%
30	16.877	2537	2540	2543	rVB	27511	27507	1.21%	0.134%
31	17.059	2568	2571	2575	rBV3	28614	46855	2.06%	0.229%
32	17.112	2576	2580	2586	rVB	105311	147053	6.47%	0.717%
33	17.336	2613	2618	2628	rVB	1950925	2271372	100.00%	11.082%
34	17.577	2655	2659	2665	rVB	16867	24610	1.08%	0.120%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

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	17.665	2670	2674	2678	rBV2	16241	24752	1.09%	0.121%
36	17.712	2678	2682	2688	rVB5	19016	30436	1.34%	0.148%
37	17.977	2722	2727	2730	rBV	42618	49701	2.19%	0.242%
38	18.577	2823	2829	2843	rBV3	40454	98455	4.33%	0.480%
39	18.689	2843	2848	2867	rVB	492324	825691	36.35%	4.028%
40	19.806	3034	3038	3042	rBV	44683	48503	2.14%	0.237%
41	19.977	3063	3067	3070	rBV	27663	39544	1.74%	0.193%
42	20.318	3122	3125	3129	rBV	23254	26752	1.18%	0.131%
43	20.365	3129	3133	3143	rBV2	262202	436567	19.22%	2.130%

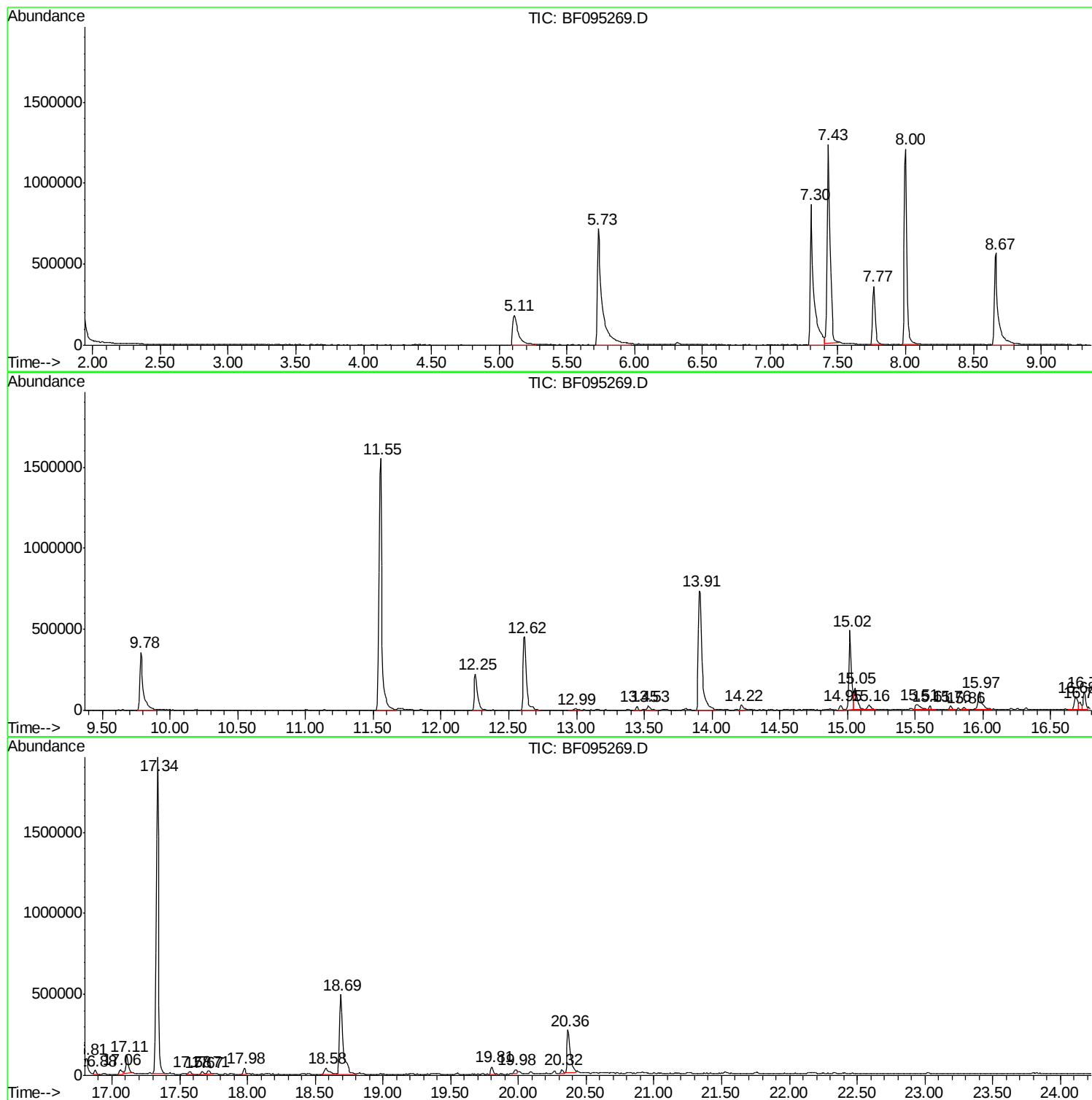
Sum of corrected areas: 20496799

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-8COMP

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\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

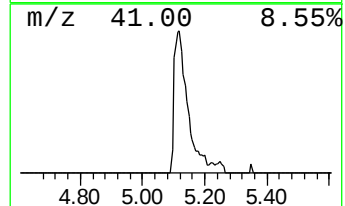
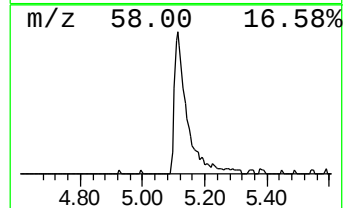
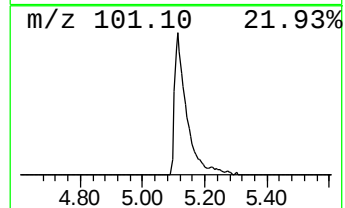
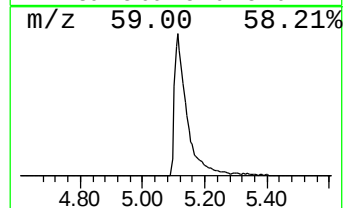
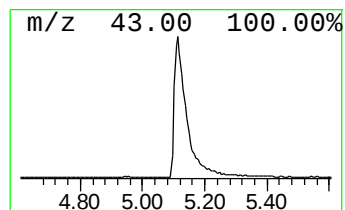
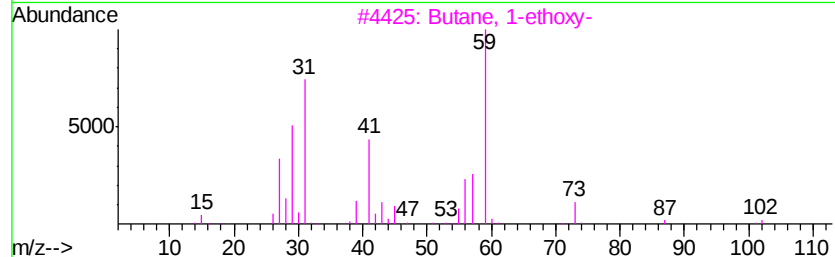
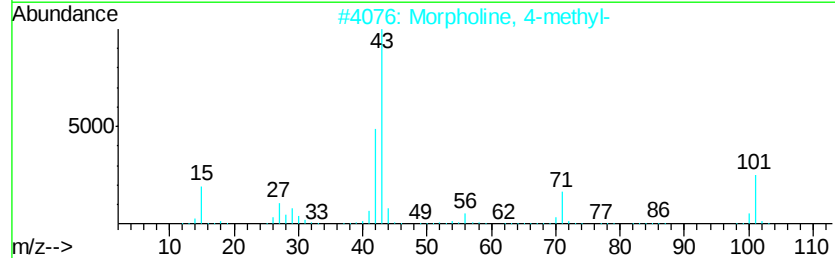
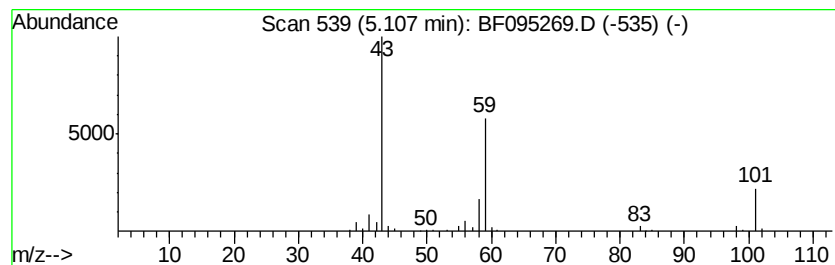
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	22.68 ng	505917	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

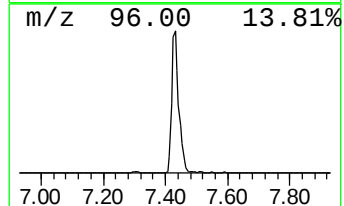
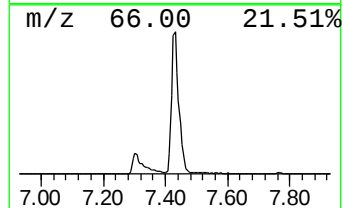
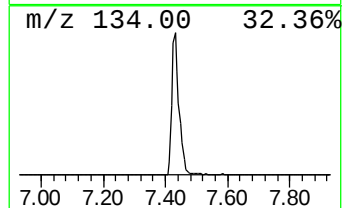
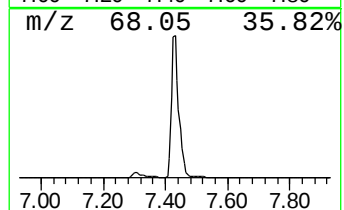
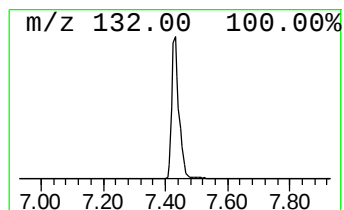
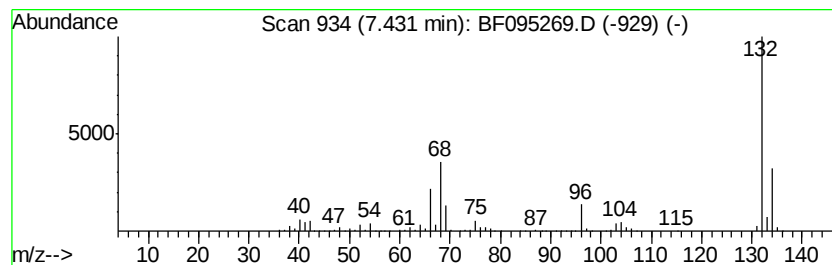
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	90.86 ng	2027010	1,4-Dichlorobenzene-d4	7.77

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Xenon	132	Xe	007440-63-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

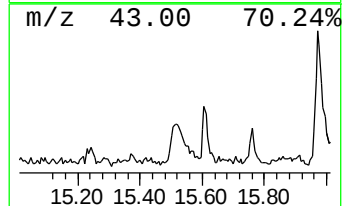
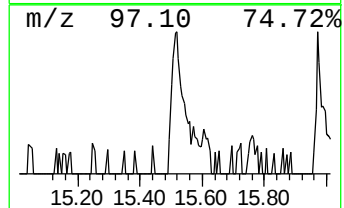
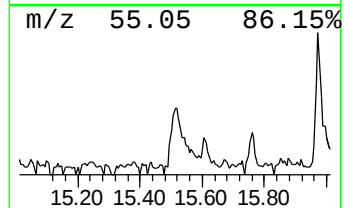
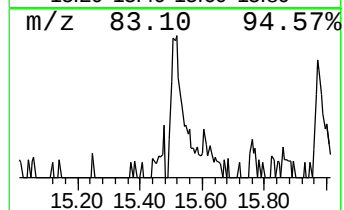
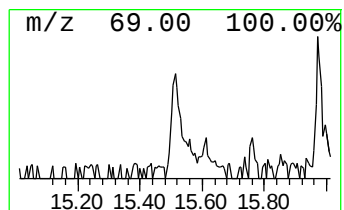
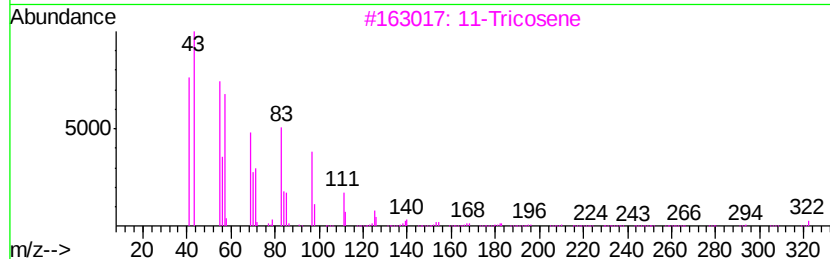
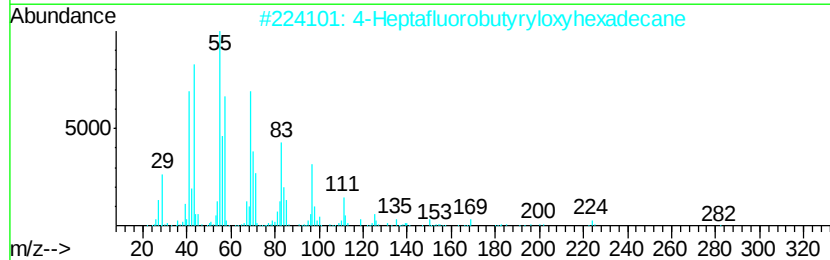
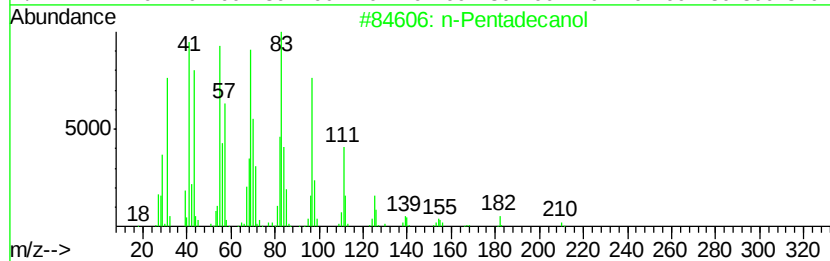
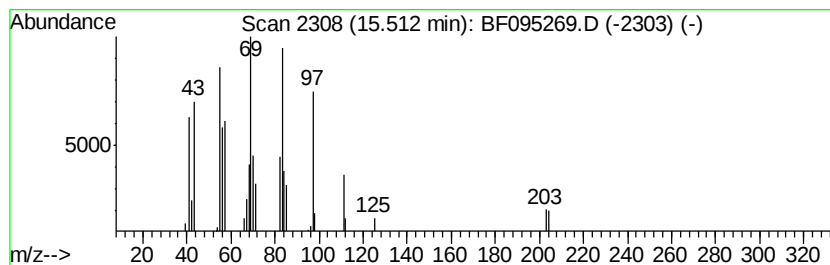
Instrument :
BNA_F
ClientSampleId :
SB-8COMP

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-Pentadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.51	2.22 ng	76731	Phenanthrene-d10	15.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Pentadecanol	228	C15H32O	000629-76-5	87
2		4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	72
3		11-Tricosene	322	C23H46	052078-56-5	72
4		1-Hexadecanol	242	C16H34O	036653-82-4	70
5		Cyclotetradecane	196	C14H28	000295-17-0	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

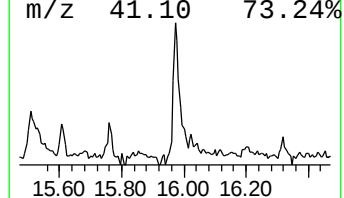
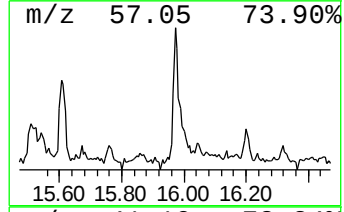
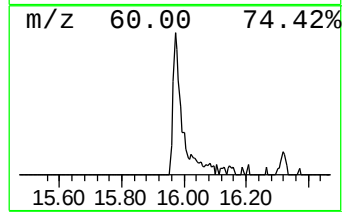
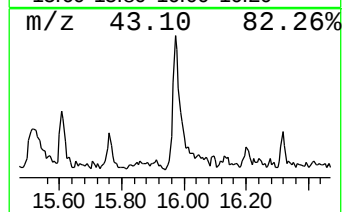
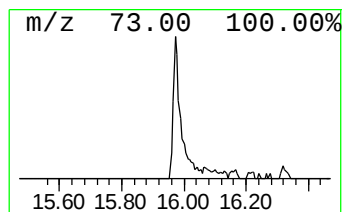
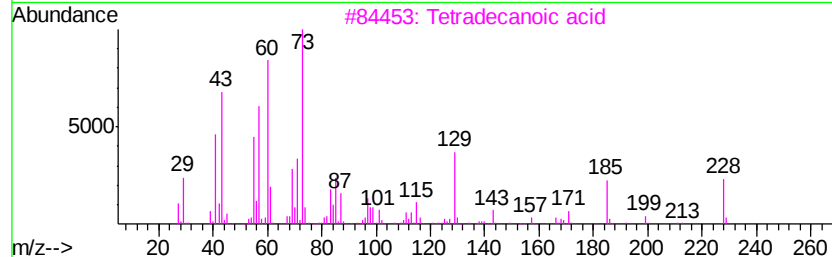
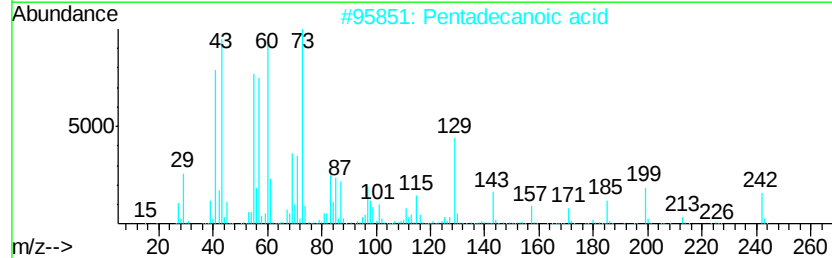
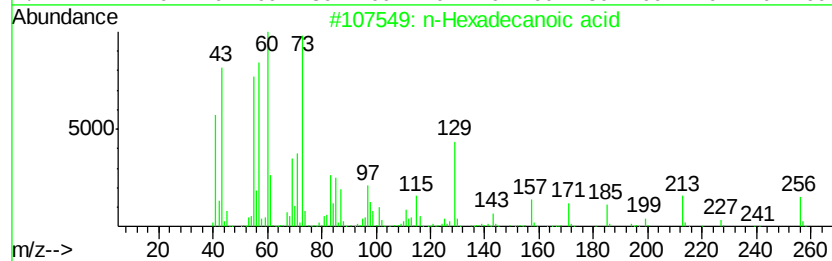
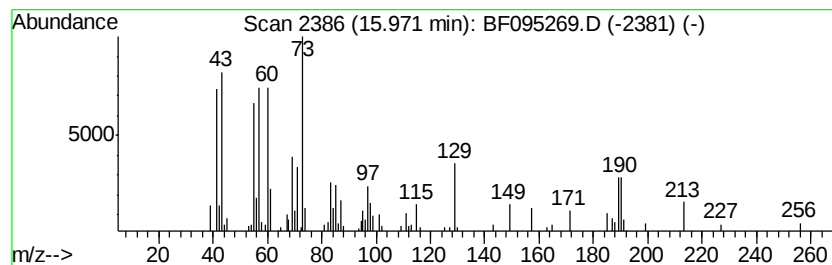
Instrument :
BNA_F
ClientSampleId :
SB-8COMP

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 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.97	5.65 ng	195432	Phenanthrene-d10		15.02	
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	62
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Trehalose	342	C12H22O11	000099-20-7	47
5		Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

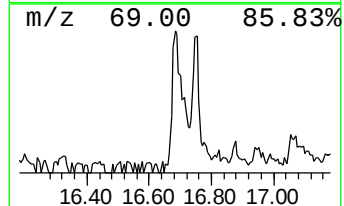
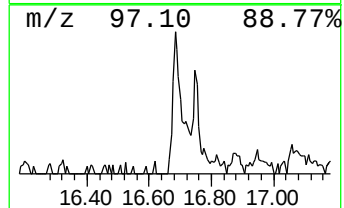
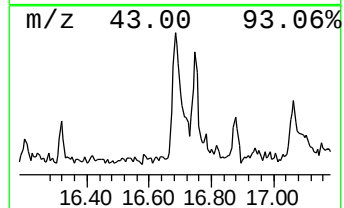
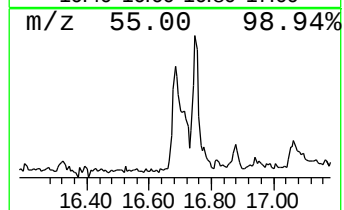
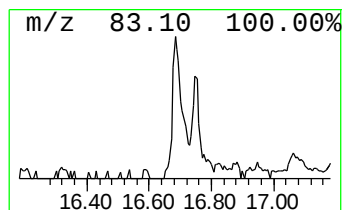
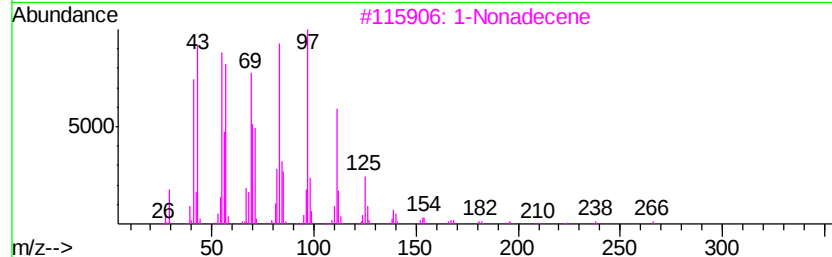
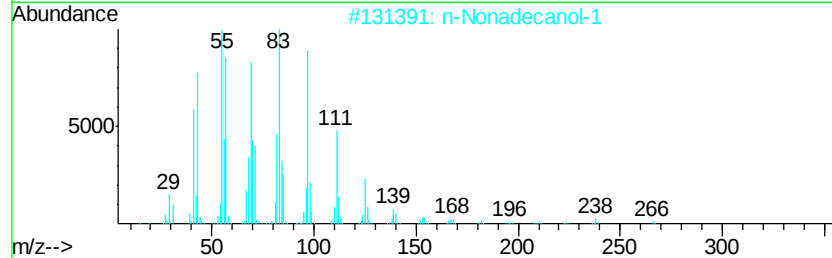
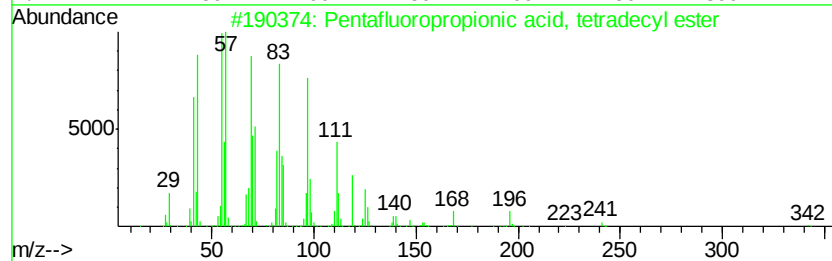
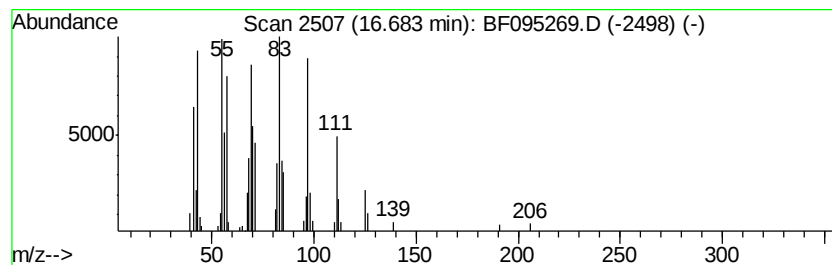
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.68	4.00 ng	138446	Phenanthrene-d10	15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		1-Nonadecene	266	C19H38	018435-45-5	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	91
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

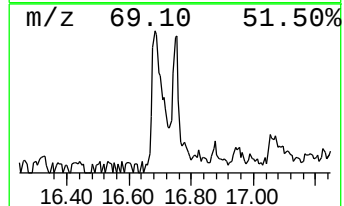
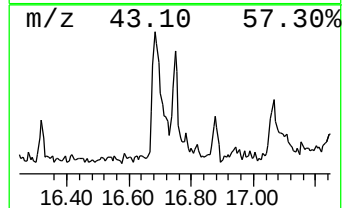
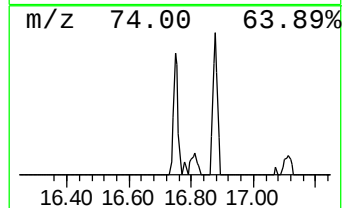
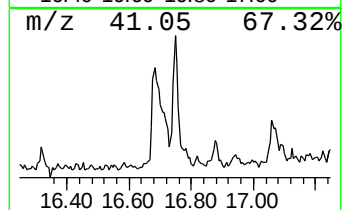
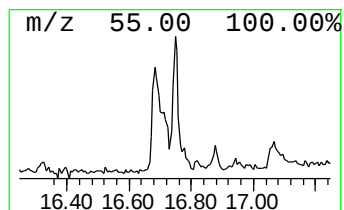
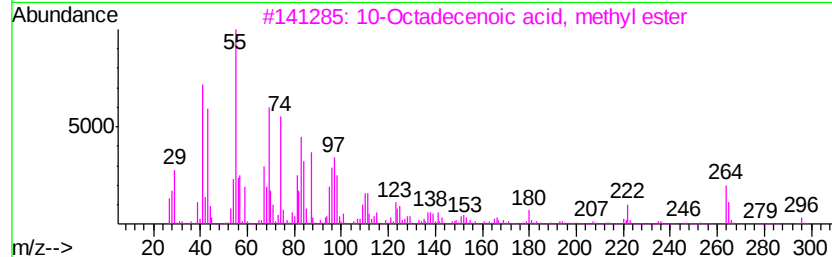
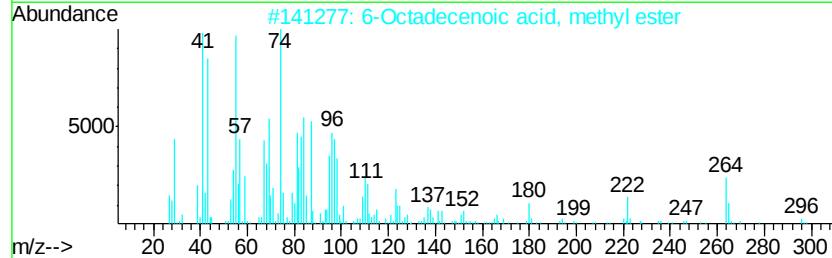
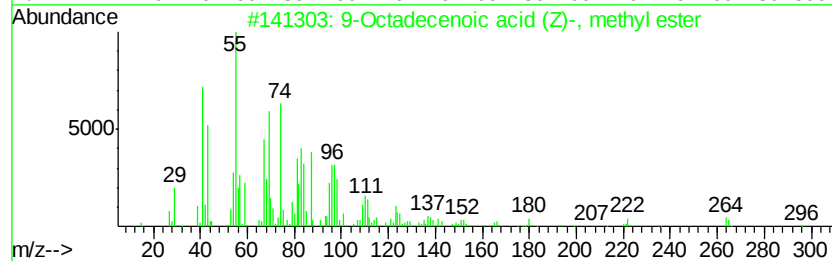
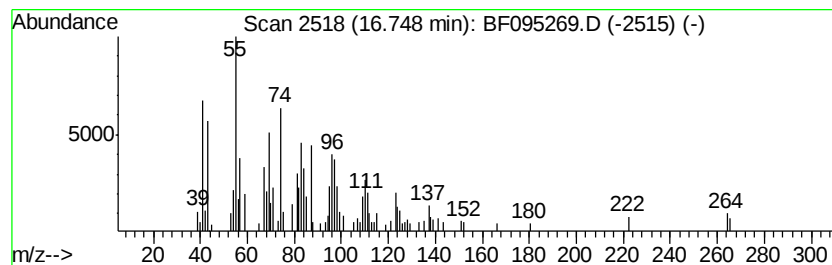
Instrument :
BNA_F
ClientSampleId :
SB-8COMP

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 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.75	3.82 ng	132093	Phenanthrene-d10	15.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	87
2		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	87
3		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
4		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	72
5		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

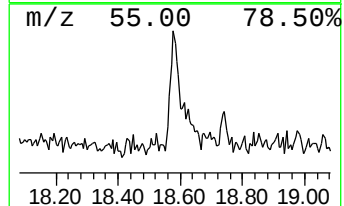
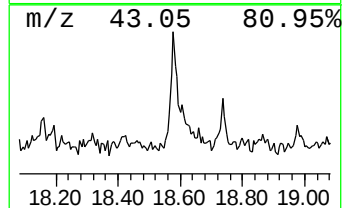
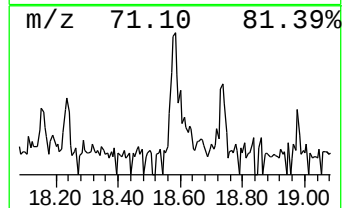
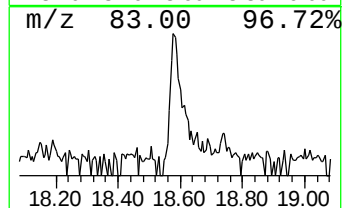
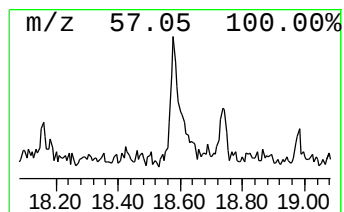
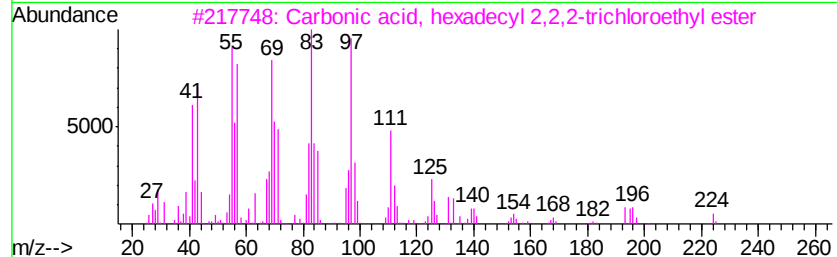
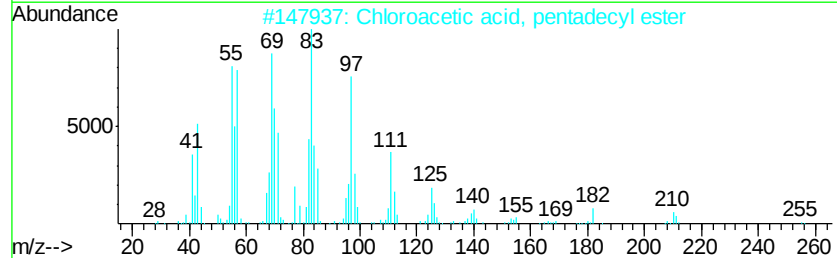
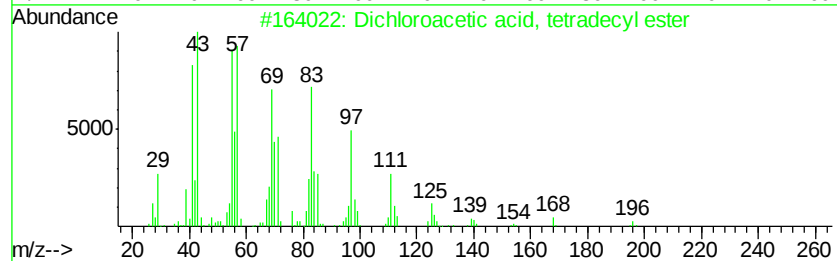
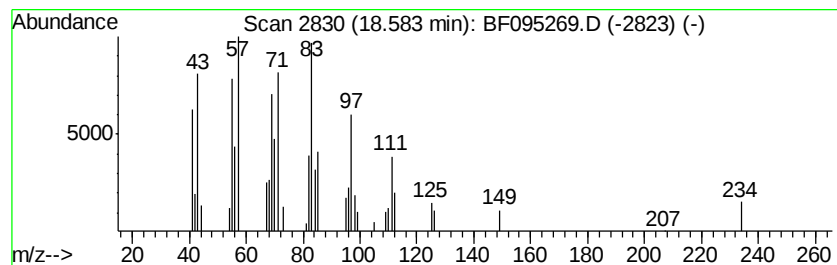
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, tetrad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.38 ng	98455	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
2		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	90
3		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	90
4		Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	87
5		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

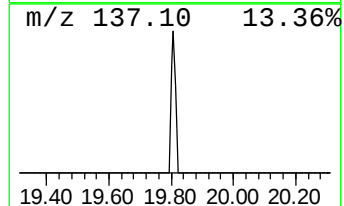
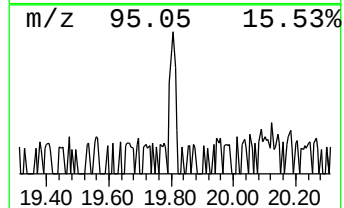
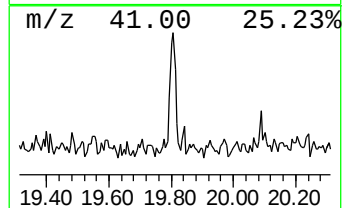
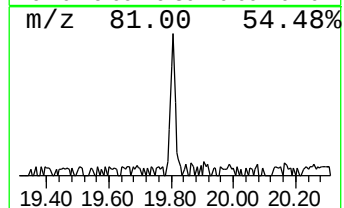
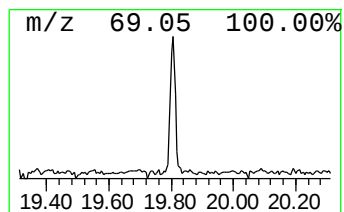
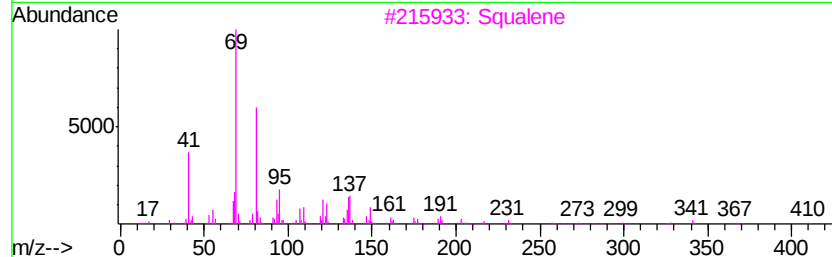
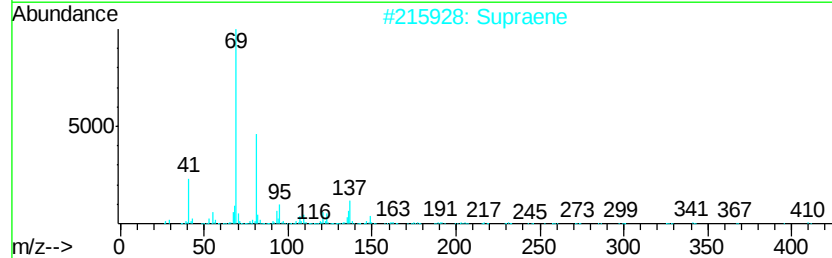
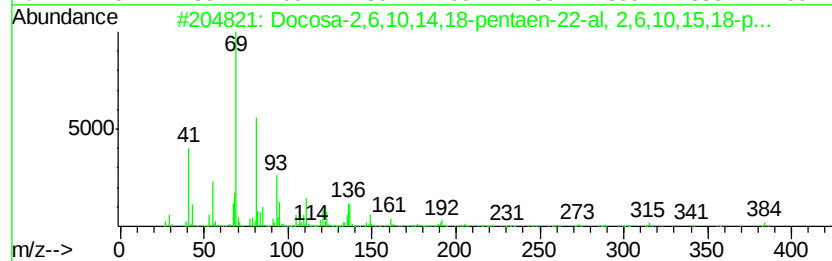
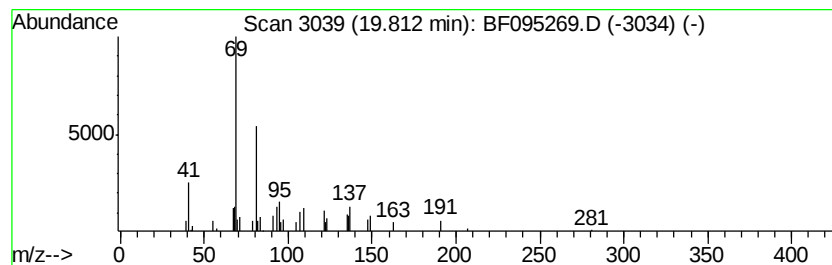
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosa-2,6,10,14,18-pentaen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.81	2.22 ng	48503	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
2		Supraene	410	C30H50	007683-64-9	87
3		Squalene	410	C30H50	000111-02-4	87
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	86
5		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095269.D
Acq On : 19 May 2017 18:25
Operator : SJ/MA
Sample : I3202-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-8COMP

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	22.7	ng	505917	1	7.77	446174	20.0
unknown7.43	7.43	90.9	ng	2027010	1	7.77	446174	20.0
n-Pentadecanol	15.51	2.2	ng	76731	4	15.02	691438	20.0
n-Hexadecanoic acid	15.97	5.7	ng	195432	4	15.02	691438	20.0
Pentafluoropropio...	16.68	4.0	ng	138446	4	15.02	691438	20.0
9-Octadecenoic ac...	16.75	3.8	ng	132093	4	15.02	691438	20.0
Dichloroacetic ac...	18.58	2.4	ng	98455	5	18.69	825691	20.0
Docosa-2,6,10,14,...	19.81	2.2	ng	48503	6	20.36	436567	20.0