

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
 Data File : BF102671.D
 Acq On : 31 Jan 2018 22:46
 Operator : SJ/JU
 Sample : J1383-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-218

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-BF012218.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	4.928	479	483	497	rBV	189245	288270	7.43%	0.913%
2	5.345	550	554	571	rBV	3463797	3833098	98.74%	12.146%
3	6.381	725	730	744	rBV	3402744	3882084	100.00%	12.301%
4	6.492	744	749	752	rBV	3990695	3675600	94.68%	11.647%
5	6.710	782	786	791	rBV	1009168	842691	21.71%	2.670%
6	6.869	808	813	816	rBV	2978002	2803377	72.21%	8.883%
7	7.280	878	883	886	rBV	2182020	2243568	57.79%	7.109%
8	7.992	1000	1004	1012	rBV	1129407	992516	25.57%	3.145%
9	9.069	1182	1187	1190	rBV	3456122	3052934	78.64%	9.674%
10	9.463	1249	1254	1261	rBV	439684	430684	11.09%	1.365%
11	9.669	1286	1289	1291	rBV	93543	74992	1.93%	0.238%
12	9.745	1298	1302	1308	rVB	1062105	890869	22.95%	2.823%
13	10.169	1371	1374	1376	rBV	92953	77263	1.99%	0.245%
14	10.545	1433	1438	1441	rBV	1733593	1702697	43.86%	5.395%
15	10.639	1451	1454	1459	rVB	83719	83554	2.15%	0.265%
16	10.898	1495	1498	1501	rBV5	32102	40850	1.05%	0.129%
17	11.086	1527	1530	1532	rBV	53403	44032	1.13%	0.140%
18	11.233	1551	1555	1558	rBV	1000866	861121	22.18%	2.729%
19	11.763	1640	1645	1652	rBV	650280	705600	18.18%	2.236%
20	12.451	1759	1762	1763	rBV	199577	188869	4.87%	0.598%
21	12.468	1763	1765	1773	rVB	248488	300765	7.75%	0.953%
22	12.545	1775	1778	1783	rVV	190582	180336	4.65%	0.571%
23	12.674	1798	1800	1804	rVB	91877	72956	1.88%	0.231%
24	12.815	1820	1824	1828	rBV	2534367	2584704	66.58%	8.190%
25	13.698	1971	1974	1978	rVB	422051	389900	10.04%	1.235%
26	13.874	2001	2004	2007	rBV	824714	773645	19.93%	2.451%
27	15.309	2244	2248	2255	rVB	424599	541138	13.94%	1.715%

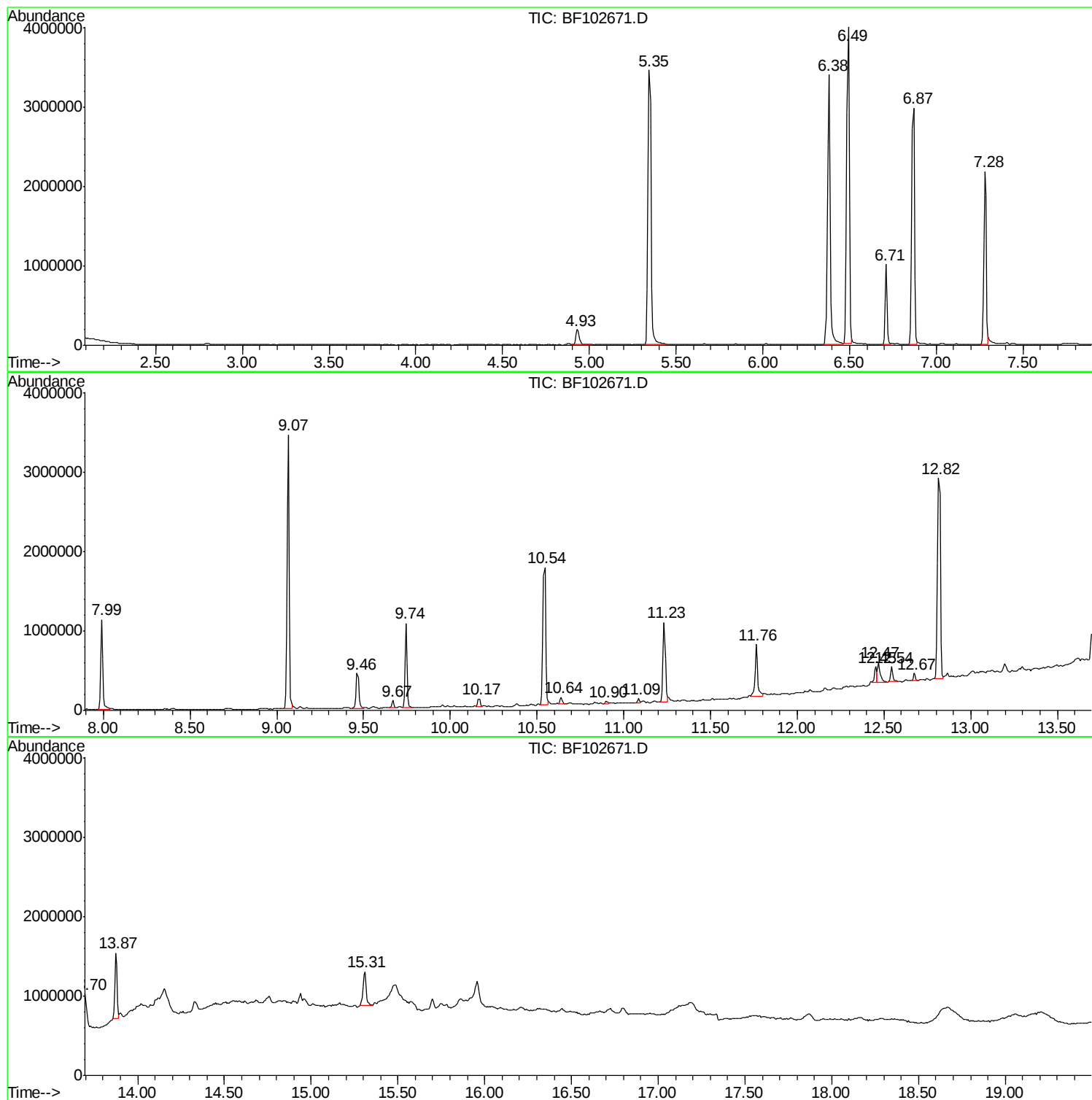
Sum of corrected areas: 31558113

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

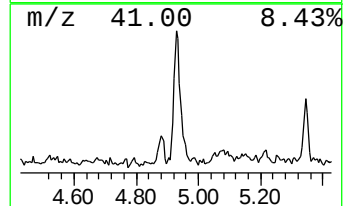
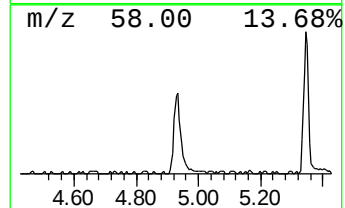
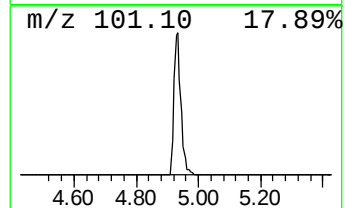
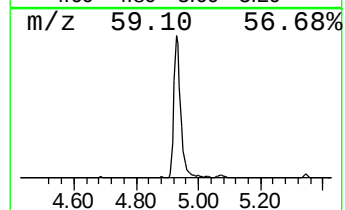
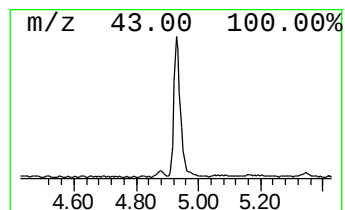
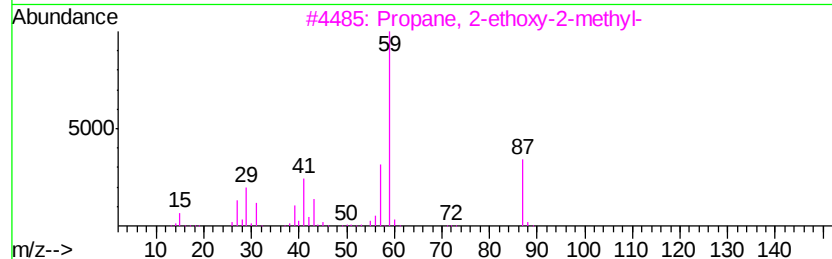
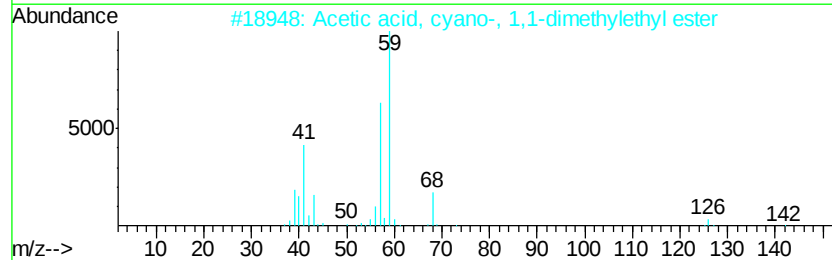
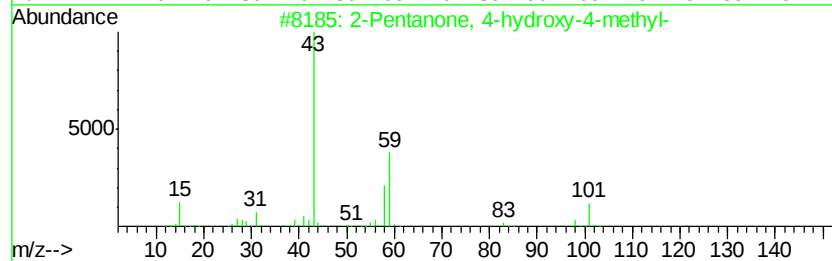
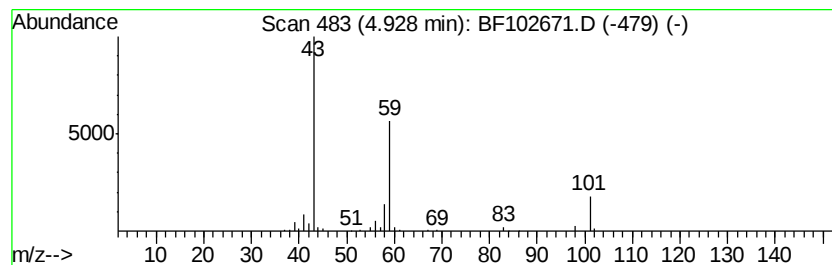
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.84 ng	288270	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

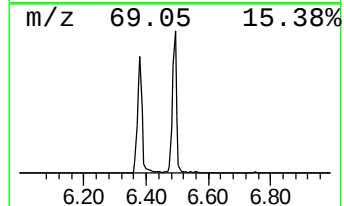
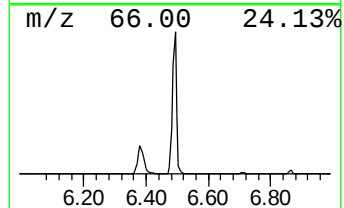
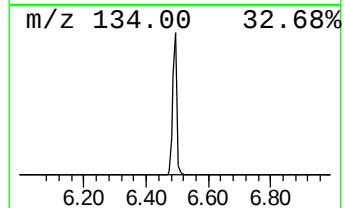
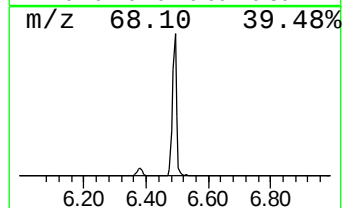
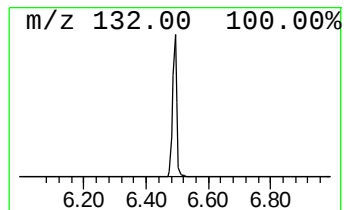
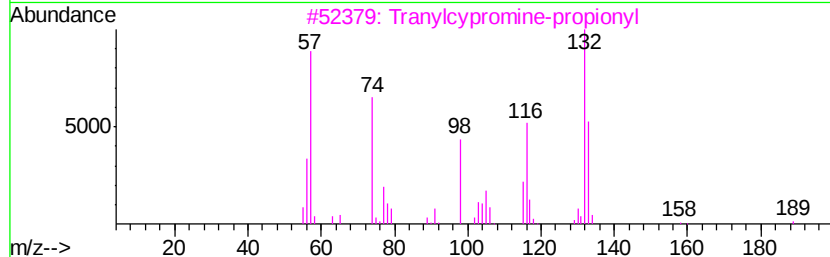
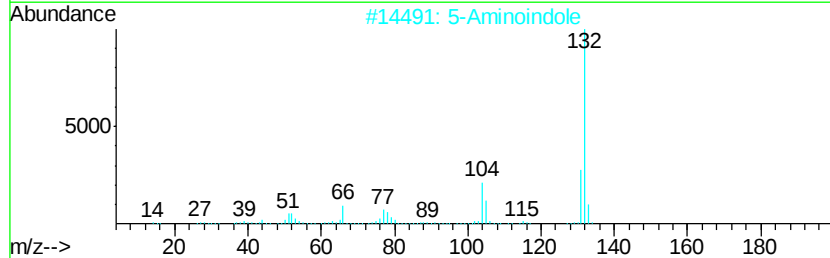
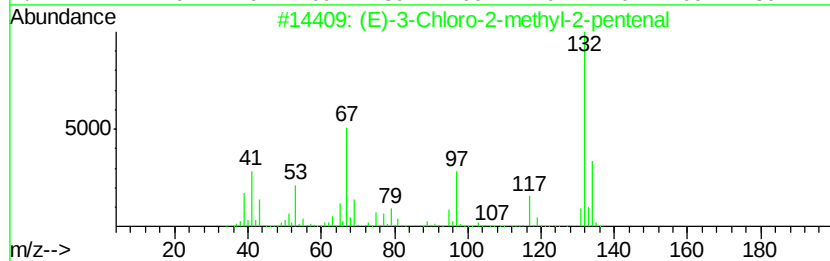
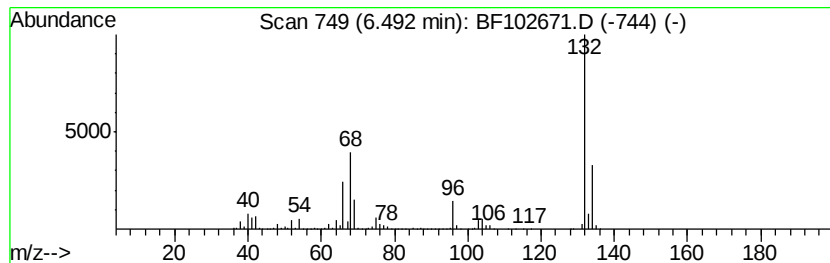
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	87.23 ng	3675600	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

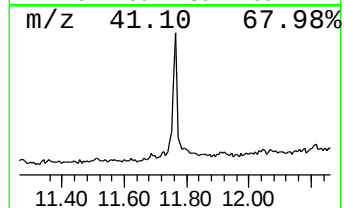
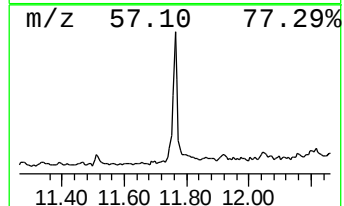
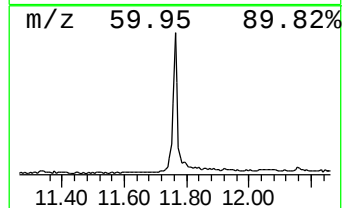
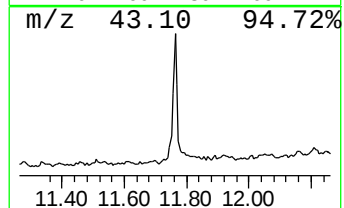
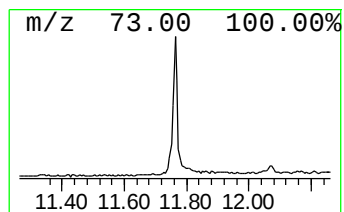
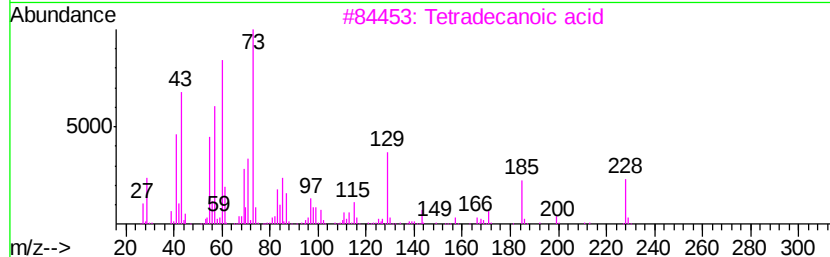
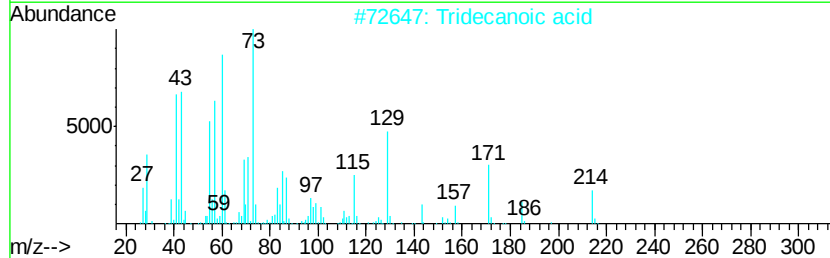
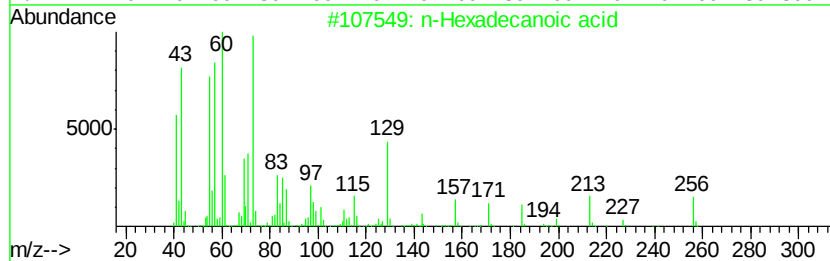
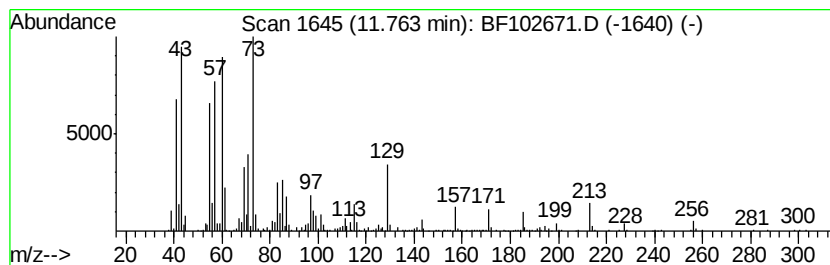
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.76	16.39 ng	705600	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

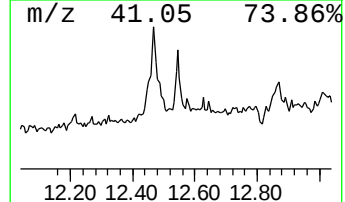
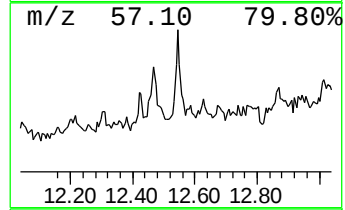
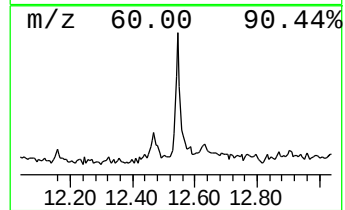
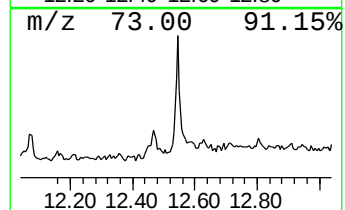
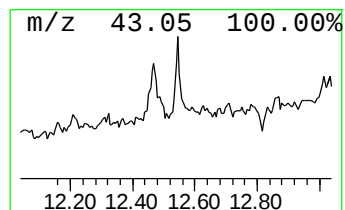
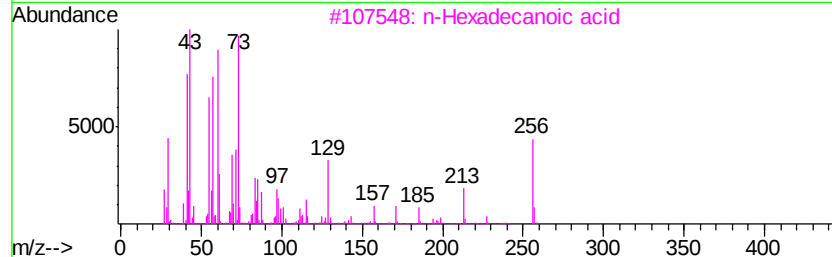
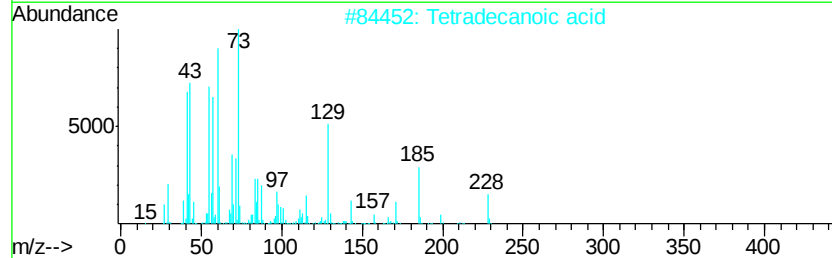
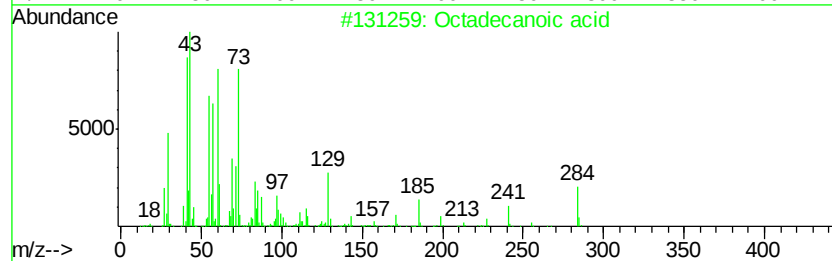
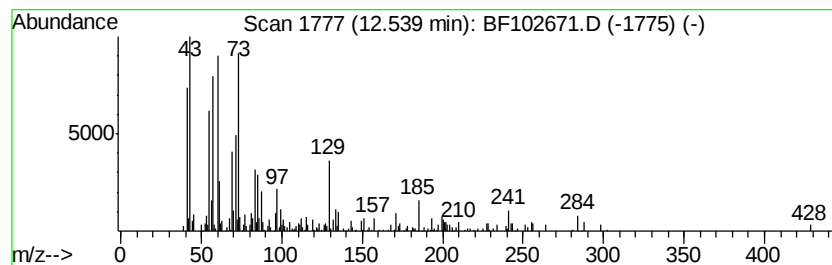
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	4.19 ng	180336	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Nonadecanoic acid	298	C19H38O2	000646-30-0	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

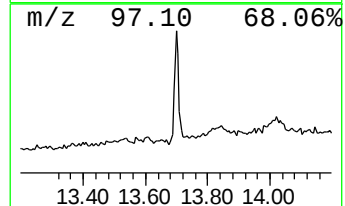
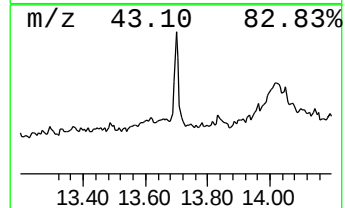
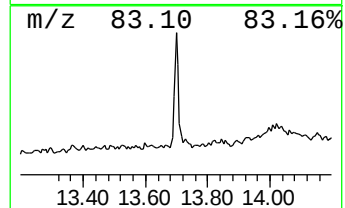
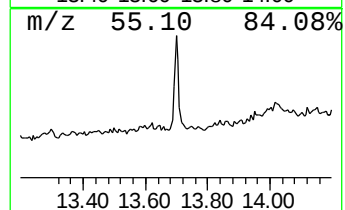
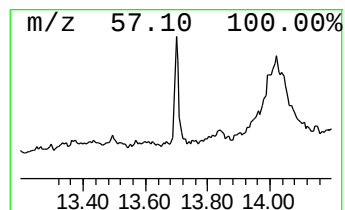
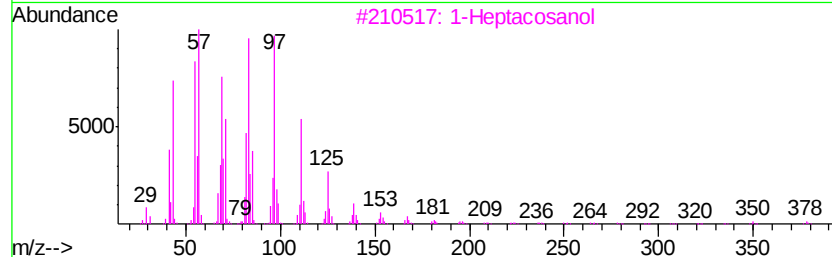
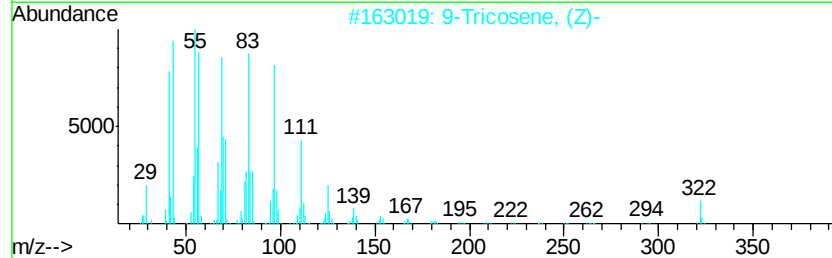
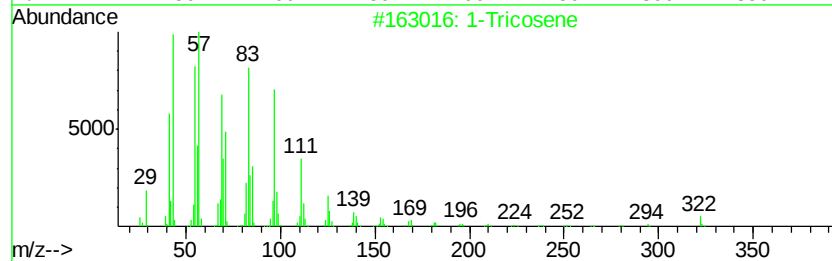
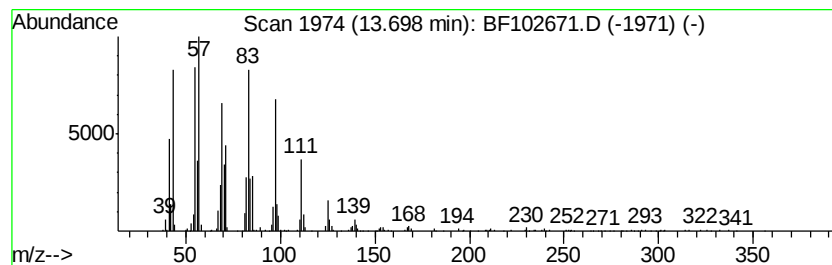
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	10.08 ng	389900	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Tricosene	322	C23H46	018835-32-0	94
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		Cyclotetracosane	336	C24H48	000297-03-0	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013118\
Data File : BF102671.D
Acq On : 31 Jan 2018 22:46
Operator : SJ/JU
Sample : J1383-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-218

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.93	6.8	ng	288270	1	6.71	842691	20.0
unknown6.49	6.49	87.2	ng	3675600	1	6.71	842691	20.0
n-Hexadecanoic acid	11.76	16.4	ng	705600	4	11.23	861121	20.0
Octadecanoic acid	12.54	4.2	ng	180336	4	11.23	861121	20.0
1-Tricosene	13.70	10.1	ng	389900	5	13.87	773645	20.0