

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\
 Data File : BF098021.D
 Acq On : 25 Aug 2017 00:15
 Operator : SJ/JU
 Sample : I4922-01 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-01-082217

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-BF081517.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	4.922	479	482	491	rVB	123411	145592	7.75%	0.707%
2	5.340	548	553	556	rBV	1789950	1759834	93.63%	8.542%
3	6.369	723	728	740	rVB	1946484	1879567	100.00%	9.123%
4	6.504	747	751	754	rBV	2030397	1774734	94.42%	8.614%
5	6.740	787	791	794	rBV	904042	754278	40.13%	3.661%
6	6.893	813	817	821	rBV	1587797	1341400	71.37%	6.511%
7	7.298	882	886	889	rBV	1209770	1080523	57.49%	5.245%
8	8.022	1005	1009	1012	rBV	1155354	944649	50.26%	4.585%
9	9.098	1187	1192	1195	rBV	2094436	1779815	94.69%	8.639%
10	9.175	1202	1205	1211	rBV5	17450	26958	1.43%	0.131%
11	9.492	1255	1259	1263	rBV	253242	219167	11.66%	1.064%
12	9.710	1294	1296	1300	rBV	29071	24576	1.31%	0.119%
13	9.775	1300	1307	1312	rBV	1016264	944671	50.26%	4.585%
14	10.210	1378	1381	1384	rVB	58707	41598	2.21%	0.202%
15	10.428	1415	1418	1424	rVB	25342	36705	1.95%	0.178%
16	10.557	1436	1440	1450	rBV	1032338	929296	49.44%	4.511%
17	10.681	1458	1461	1470	rVB	86308	101508	5.40%	0.493%
18	11.128	1534	1537	1540	rBV	72055	61109	3.25%	0.297%
19	11.157	1540	1542	1546	rVB	26568	25605	1.36%	0.124%
20	11.251	1554	1558	1562	rBV	896183	858543	45.68%	4.167%
21	11.380	1576	1580	1582	rBV	33330	29639	1.58%	0.144%
22	11.557	1607	1610	1613	rBV	45185	43188	2.30%	0.210%
23	11.657	1623	1627	1630	rVB	554184	444363	23.64%	2.157%
24	11.827	1653	1656	1659	rBV2	53120	48631	2.59%	0.236%
25	11.963	1676	1679	1682	rVB	38560	30253	1.61%	0.147%
26	12.063	1692	1696	1700	rBV7	11329	22814	1.21%	0.111%
27	12.339	1739	1743	1745	rBV	1163291	1038007	55.23%	5.038%
28	12.363	1745	1747	1749	rVB	1159844	891852	47.45%	4.329%
29	12.445	1758	1761	1767	rVB2	264936	261337	13.90%	1.269%
30	12.686	1797	1802	1805	rBV3	70648	87441	4.65%	0.424%
31	12.722	1806	1808	1812	rVB3	28706	25152	1.34%	0.122%
32	12.839	1824	1828	1831	rBV	1646568	1429363	76.05%	6.938%
33	13.022	1854	1859	1861	rBV5	35778	63804	3.39%	0.310%
34	13.074	1866	1868	1873	rVV3	30461	48483	2.58%	0.235%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.739	1978	1981	1989	rBV4	94965	148398	7.90%	0.720%
36	13.886	2002	2006	2009	rBV	858893	807722	42.97%	3.921%
37	15.304	2243	2247	2252	rBV	390244	451270	24.01%	2.190%

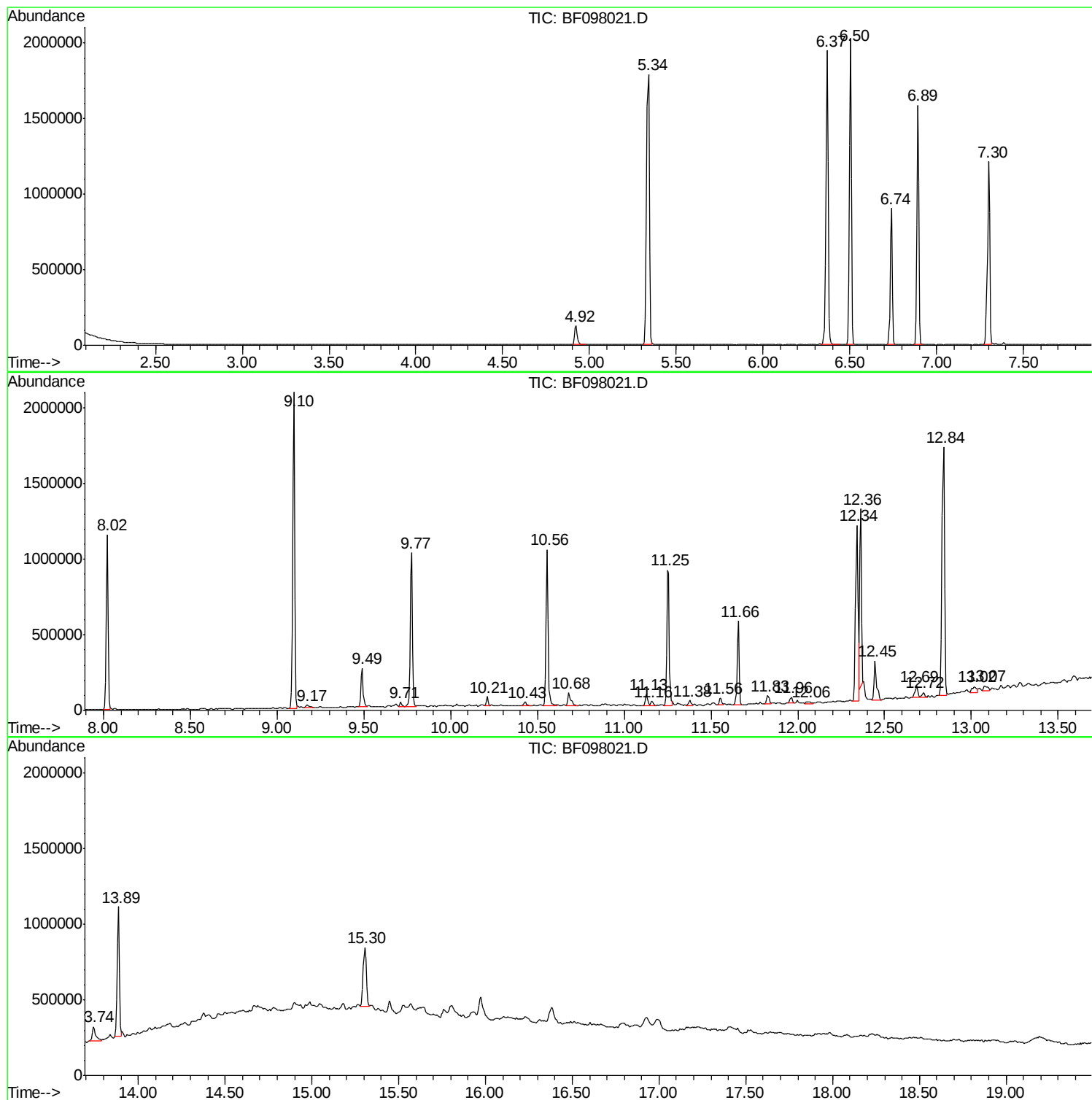
Sum of corrected areas: 20601845

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

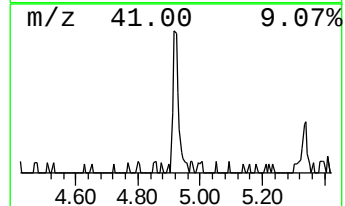
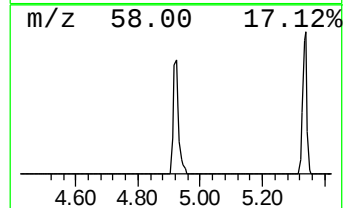
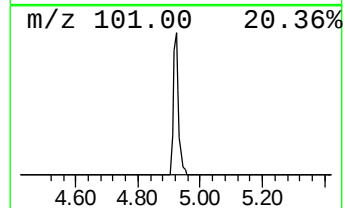
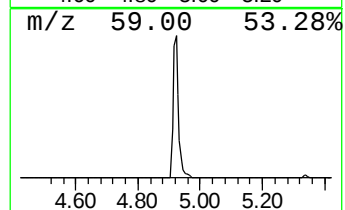
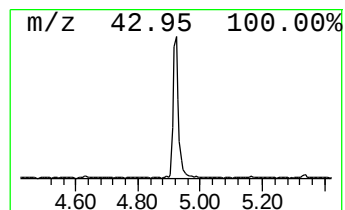
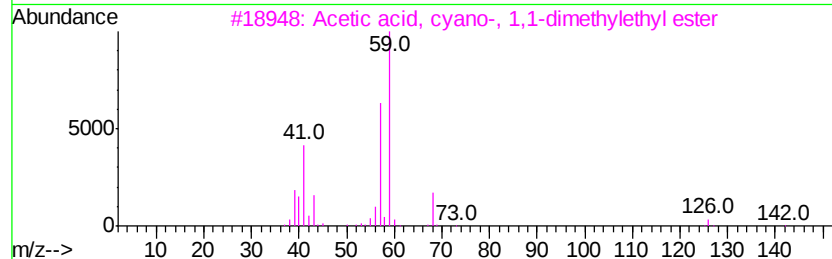
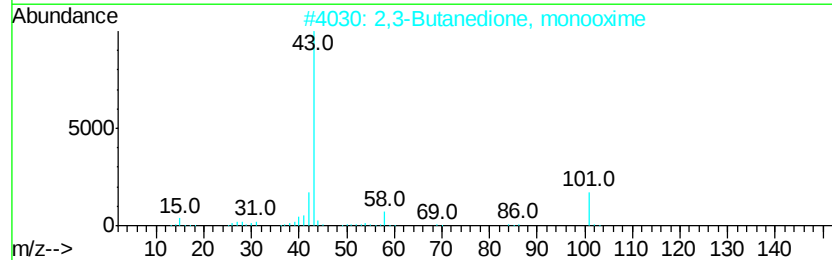
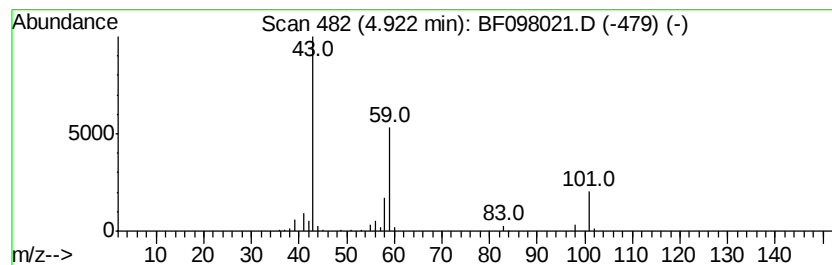
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.86 ng	145592	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

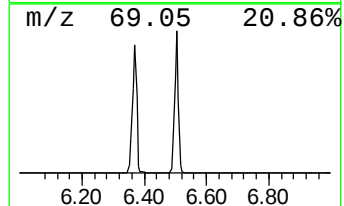
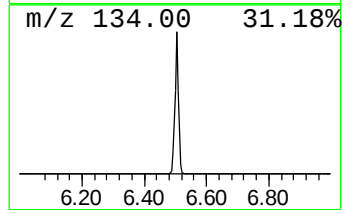
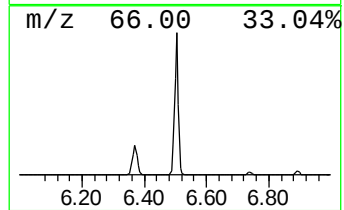
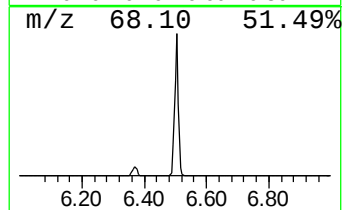
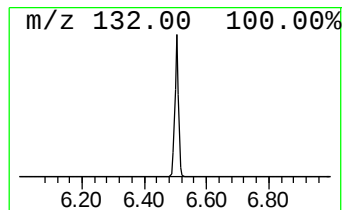
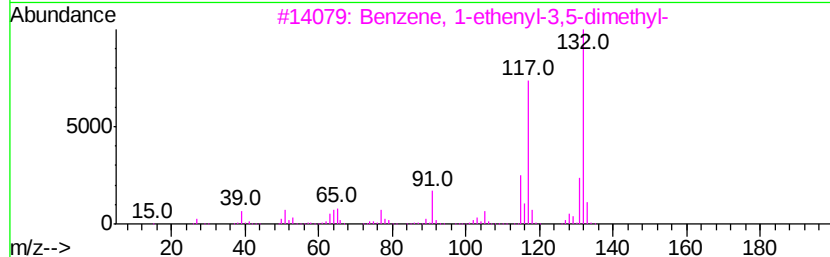
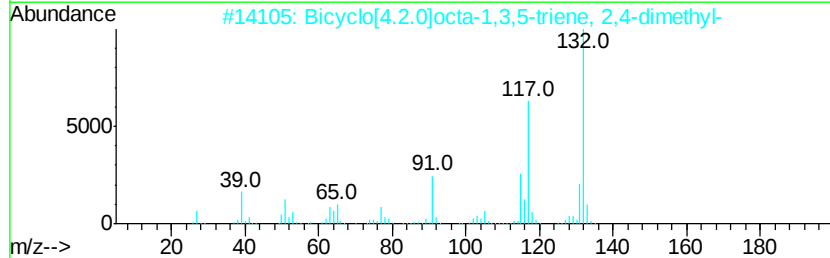
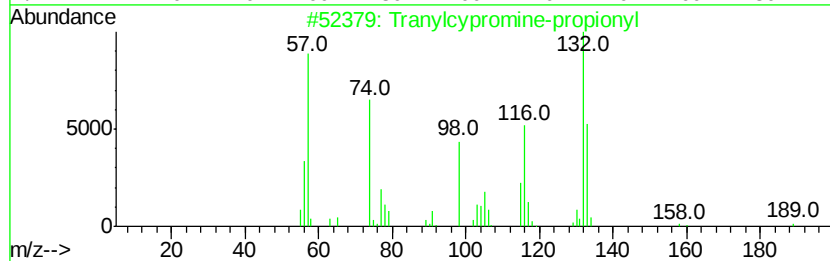
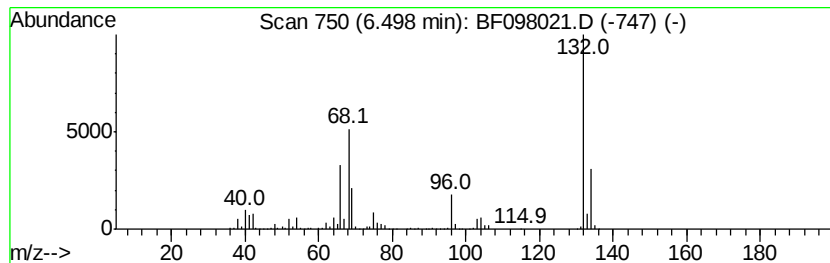
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	47.06 ng	1774730	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

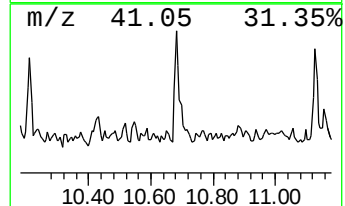
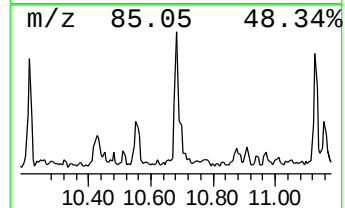
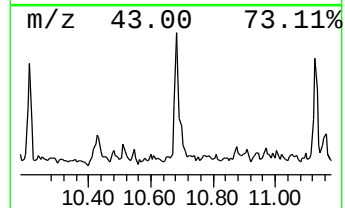
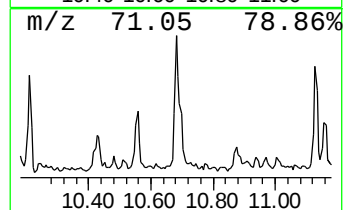
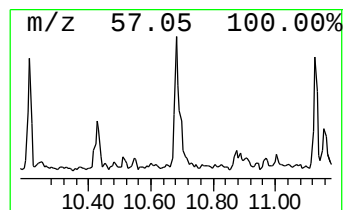
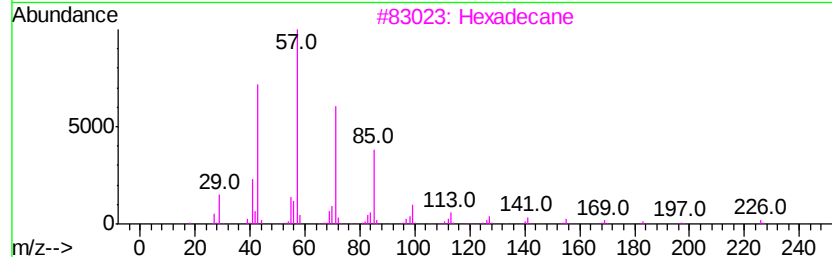
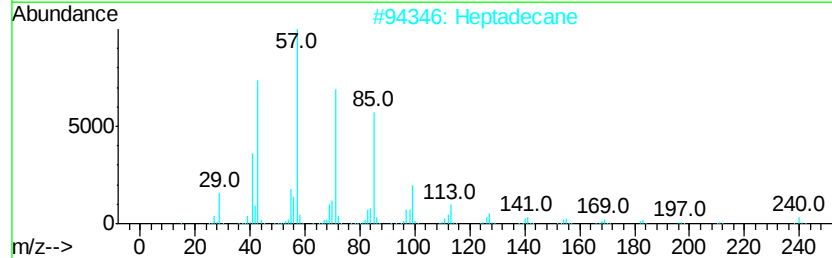
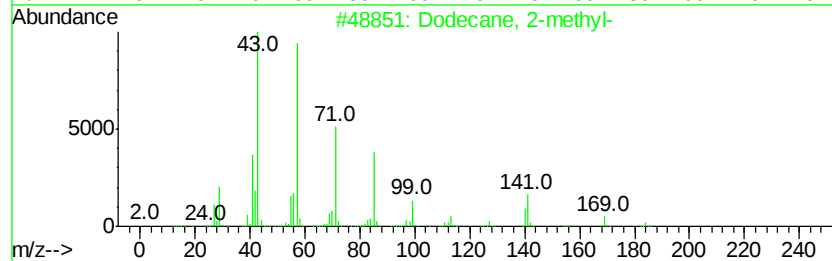
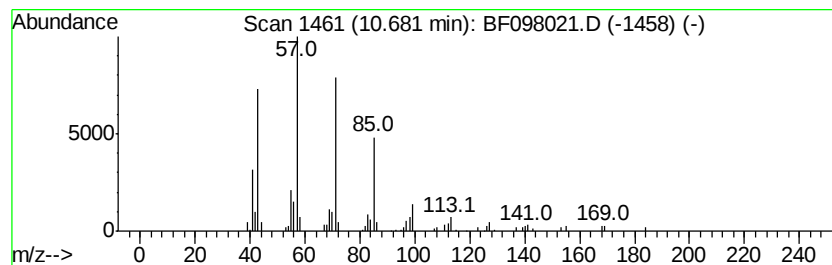
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dodecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.36 ng	101508	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Hexadecane	226	C16H34	000544-76-3	90
4		Pentadecane	212	C15H32	000629-62-9	87
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

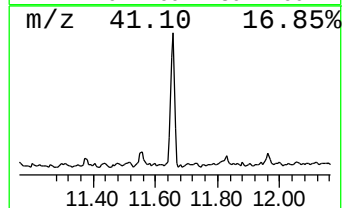
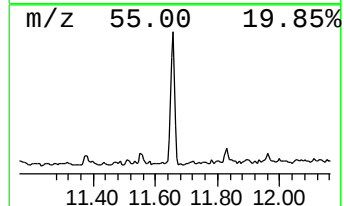
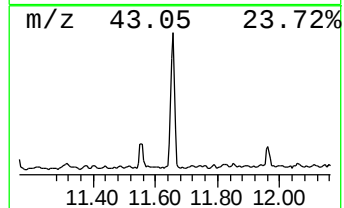
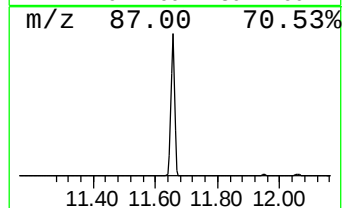
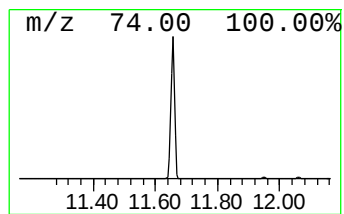
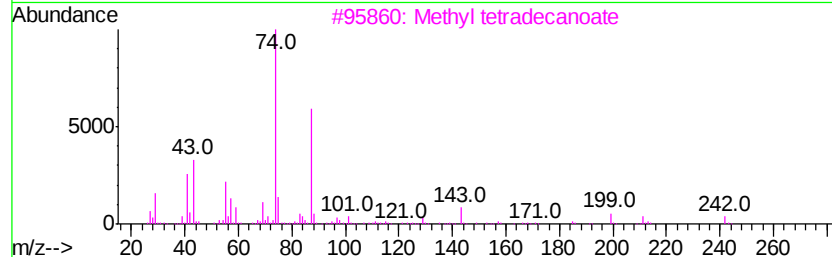
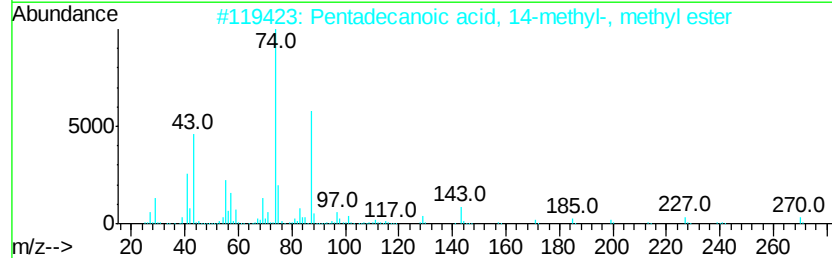
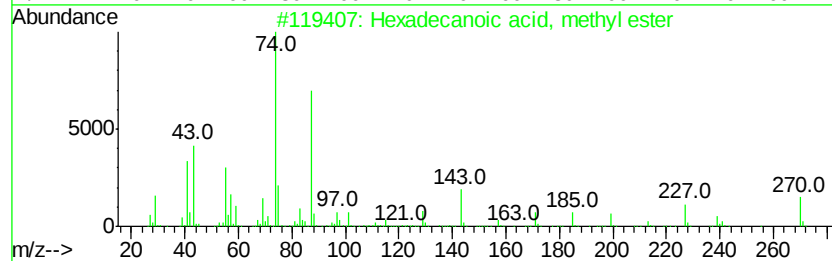
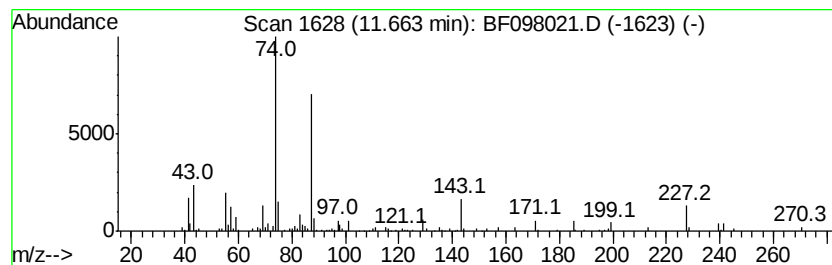
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	10.35 ng	444363	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

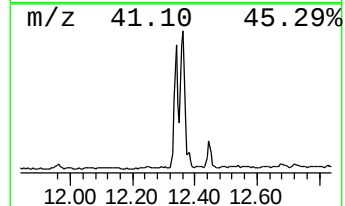
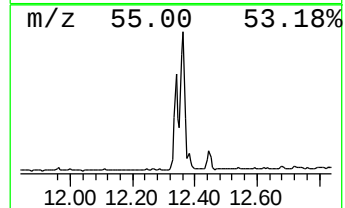
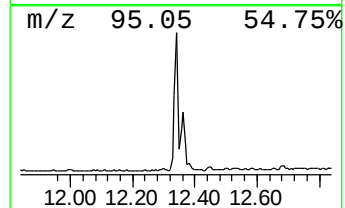
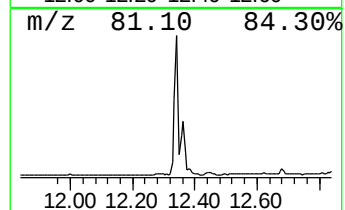
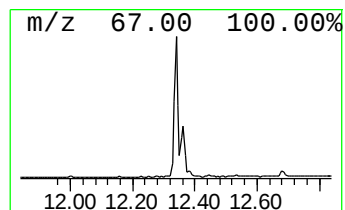
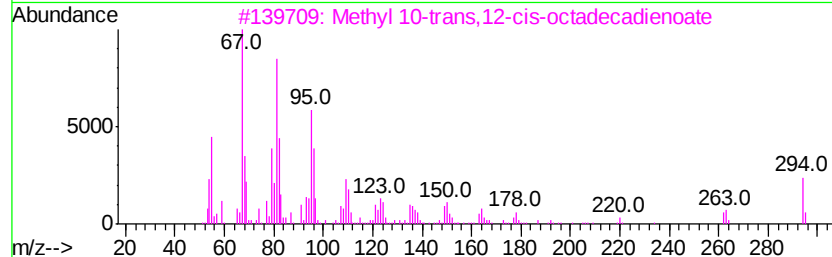
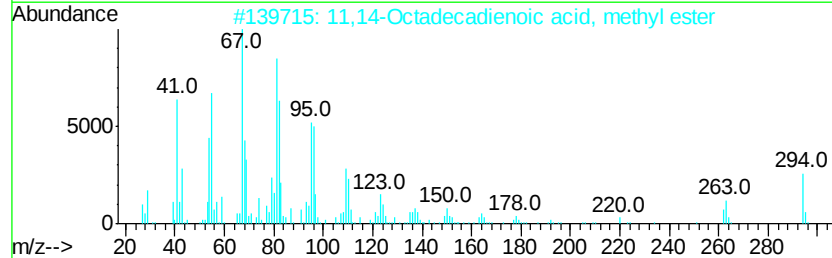
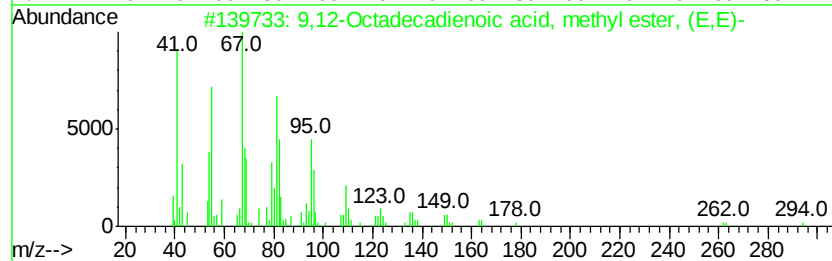
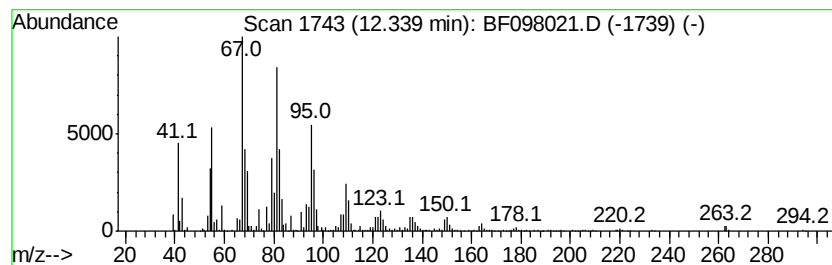
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	24.18 ng	1038010	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9,12-Octadecadienoic acid, methyl ester, (E,E)-	294	C19H34O2	002566-97-4	99
2		11,14-Octadecadienoic acid, methyl ester, (E,E)-	294	C19H34O2	056554-61-1	98
3		Methyl 10-trans,12-cis-octadecadienoate	294	C19H34O2	1000336-44-2	98
4		Methyl 9-cis,11-trans-octadecadienoate	294	C19H34O2	1000336-44-0	95
5		9,12-Octadecadienoic acid (Z,Z)-methyl ester	294	C19H34O2	000112-63-0	95



Data Path : Z:\HPCHEM1\BNA F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

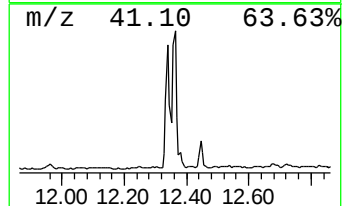
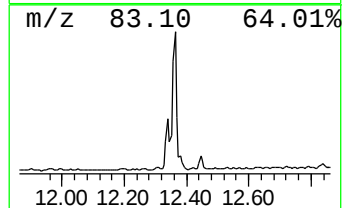
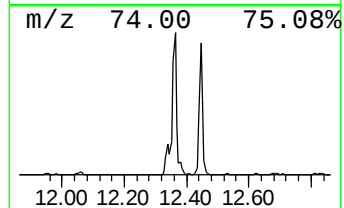
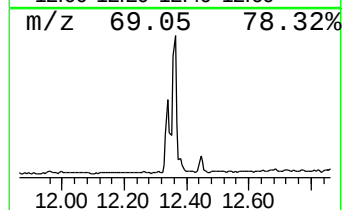
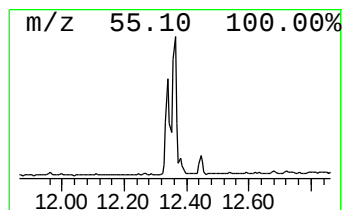
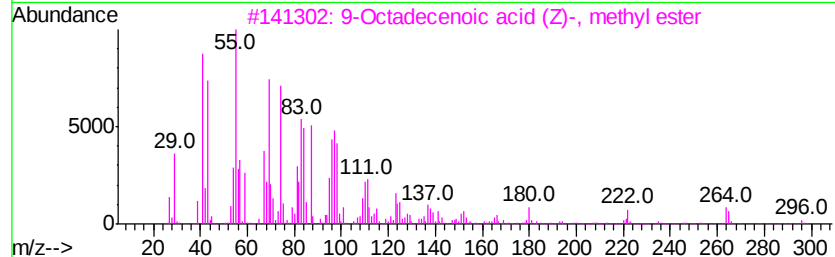
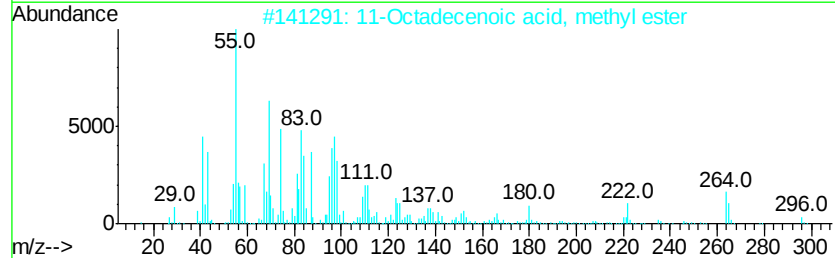
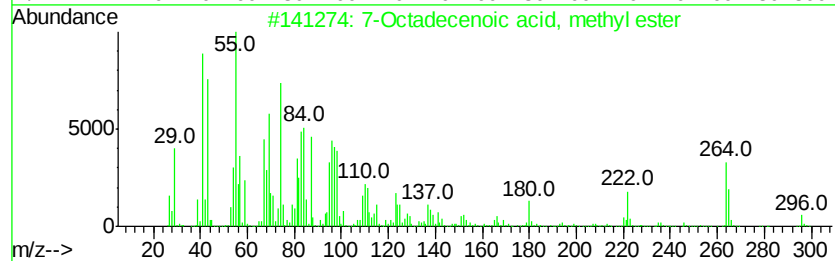
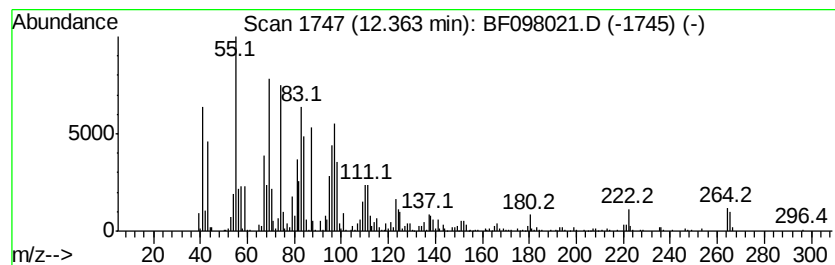
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	20.78 ng	891852	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
2		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	96
3		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
4		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91
5		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

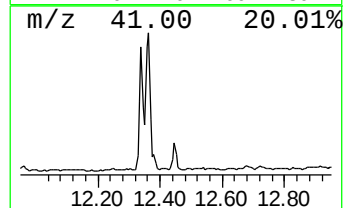
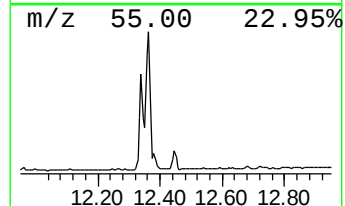
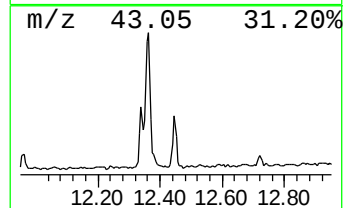
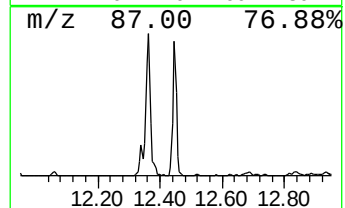
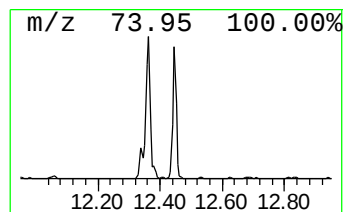
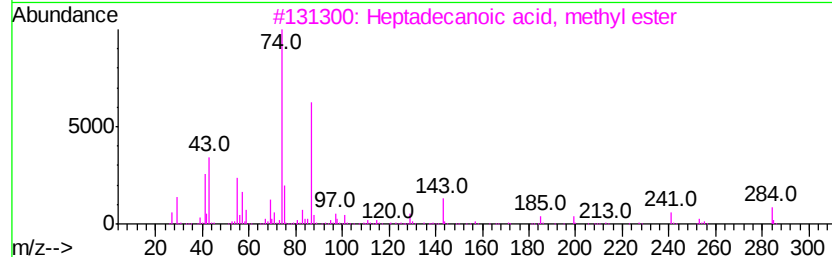
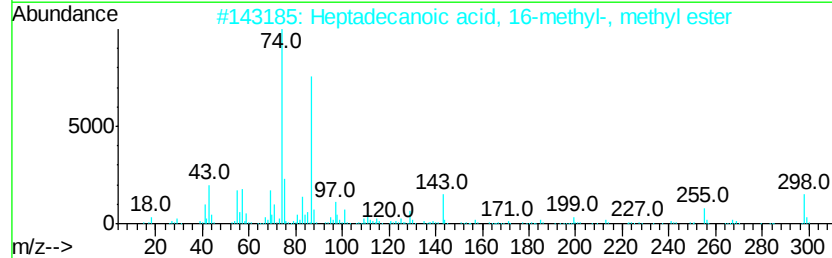
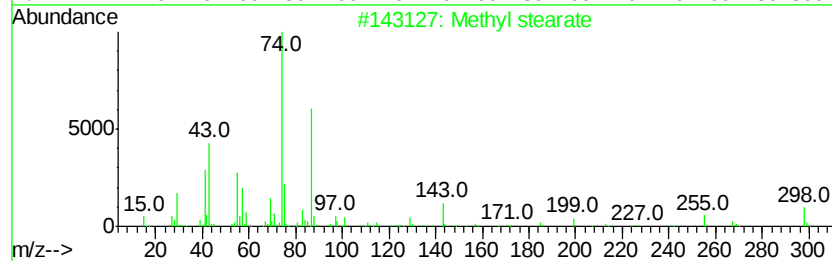
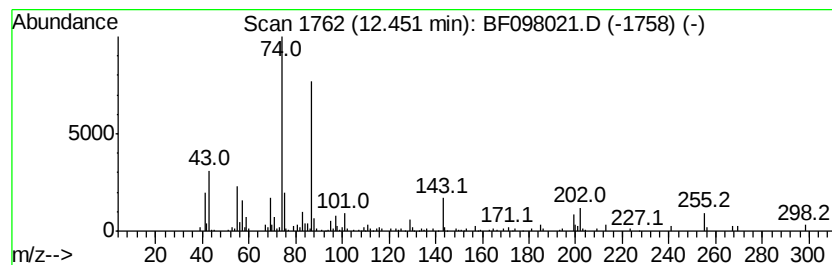
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	6.09 ng	261337	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	96
2		Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	92
3		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
4		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

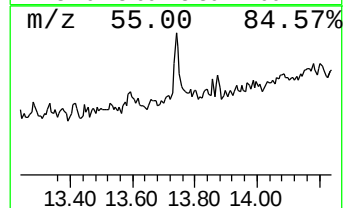
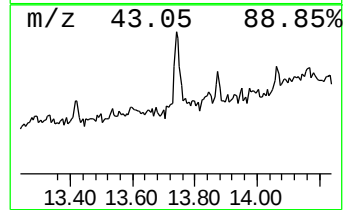
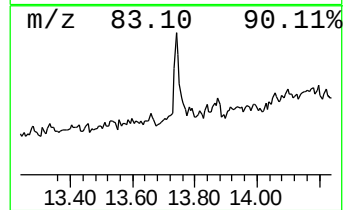
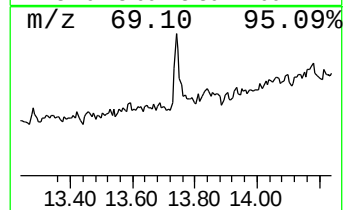
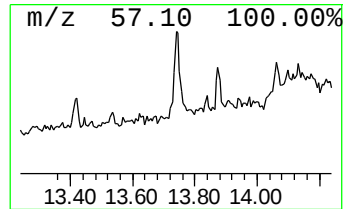
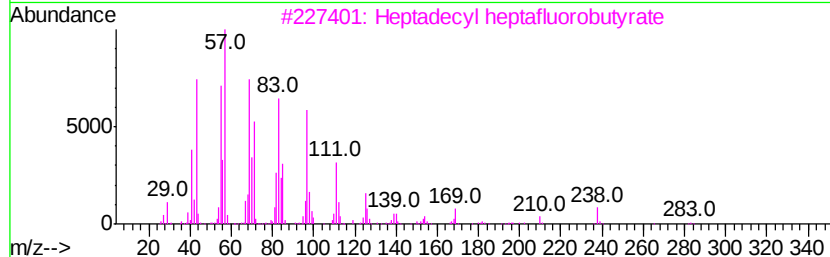
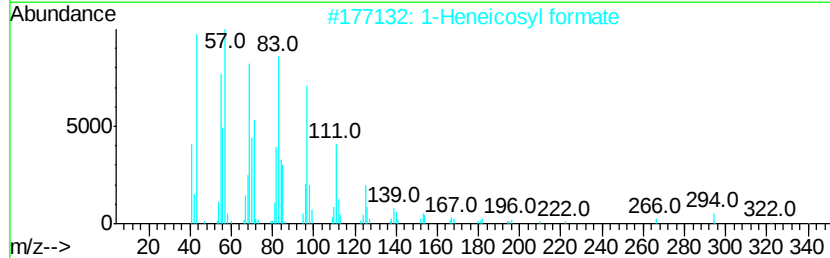
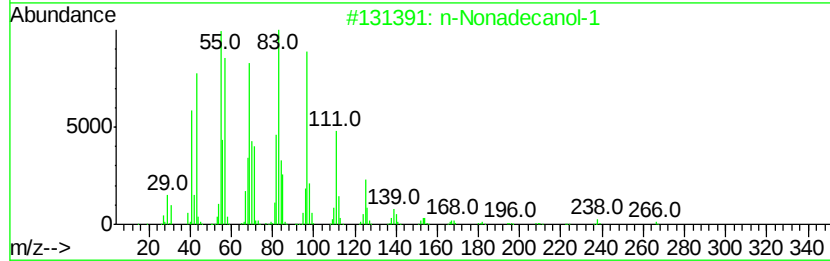
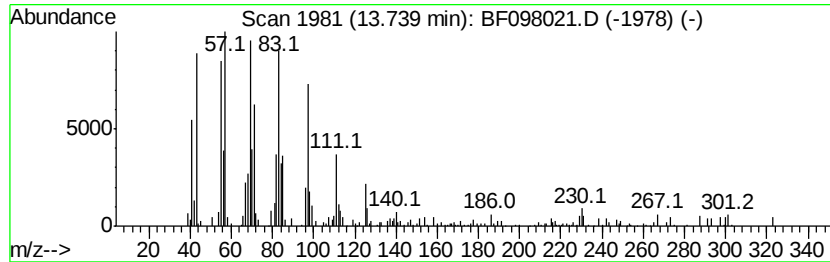
Instrument :
BNA_F
ClientSampleId :
SA-01-082217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Nonadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	3.67 ng	148398	Chrysene-d12		13.89
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082417\
Data File : BF098021.D
Acq On : 25 Aug 2017 00:15
Operator : SJ/JU
Sample : I4922-01 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-01-082217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.92	3.9	ng	145592	1	6.74	754278	20.0
unknown6.50	6.50	47.1	ng	1774730	1	6.74	754278	20.0
Dodecane, 2-methyl-	10.68	2.4	ng	101508	4	11.25	858543	20.0
Hexadecanoic acid...	11.66	10.4	ng	444363	4	11.25	858543	20.0
9,12-Octadecadien...	12.34	24.2	ng	1038010	4	11.25	858543	20.0
7-Octadecenoic ac...	12.36	20.8	ng	891852	4	11.25	858543	20.0
Methyl stearate	12.45	6.1	ng	261337	4	11.25	858543	20.0
n-Nonadecanol-1	13.74	3.7	ng	148398	5	13.89	807722	20.0