

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
 Data File : BF097569.D
 Acq On : 10 Aug 2017 20:27
 Operator : SJ/JU
 Sample : I4688-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHOENIX-BPM

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-BF072517.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	4.522	478	482	500	rBV	112339	240605	9.50%	1.205%
2	4.992	558	562	598	rBV	1576650	2533085	100.00%	12.686%
3	6.075	742	746	758	rBV	2057902	2383982	94.11%	11.940%
4	6.169	758	762	773	rVB	2246690	2342486	92.48%	11.732%
5	6.392	797	800	813	rVB	620488	655668	25.88%	3.284%
6	6.545	822	826	840	rBV	1678869	1642283	64.83%	8.225%
7	6.963	894	897	914	rBV	1298572	1497232	59.11%	7.498%
8	7.675	1014	1018	1029	rBV	914030	864505	34.13%	4.330%
9	8.751	1197	1201	1214	rBV	2211308	2026368	80.00%	10.149%
10	9.157	1267	1270	1279	rBV	327512	284918	11.25%	1.427%
11	9.416	1310	1314	1323	rVB2	927781	839737	33.15%	4.206%
12	9.874	1388	1392	1394	rVB2	37309	33389	1.32%	0.167%
13	10.210	1445	1449	1462	rBV	1086012	1109268	43.79%	5.555%
14	10.339	1468	1471	1478	rVB	54344	62292	2.46%	0.312%
15	10.786	1544	1547	1550	rBV2	39567	34764	1.37%	0.174%
16	10.892	1561	1565	1573	rVB	823516	753006	29.73%	3.771%
17	11.374	1645	1647	1653	rBV3	22351	30705	1.21%	0.154%
18	11.457	1657	1661	1672	rVB2	154260	179529	7.09%	0.899%
19	12.474	1830	1834	1838	rBV	1251920	1133733	44.76%	5.678%
20	13.386	1985	1989	1996	rBV	65955	80129	3.16%	0.401%
21	13.521	2008	2012	2019	rBV	397293	418014	16.50%	2.094%
22	14.362	2152	2155	2160	rBV	337573	332034	13.11%	1.663%
23	14.857	2234	2239	2251	rBV	338124	459492	18.14%	2.301%
24	16.533	2522	2524	2527	rBV3	20322	29919	1.18%	0.150%

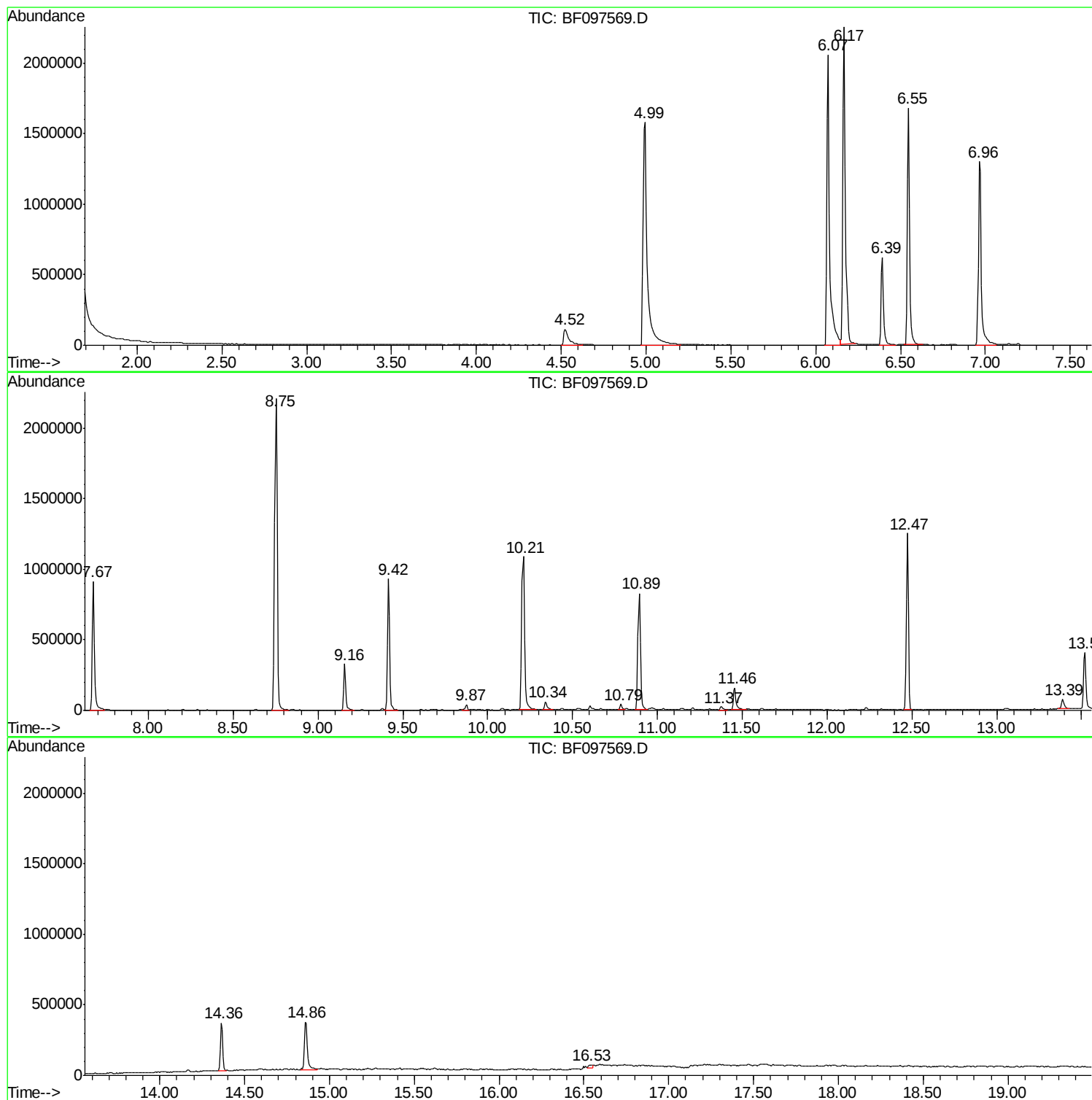
Sum of corrected areas: 19967143

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

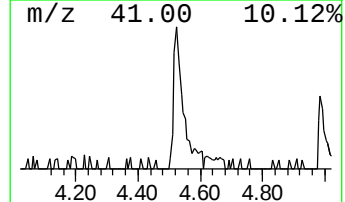
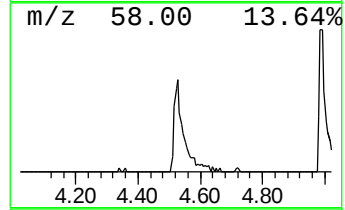
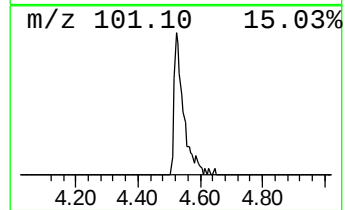
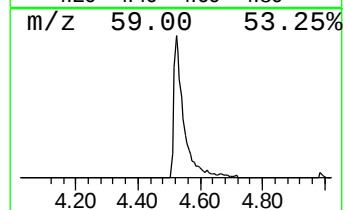
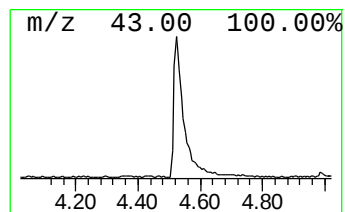
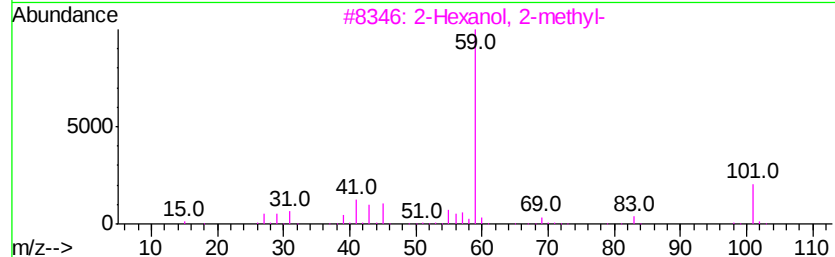
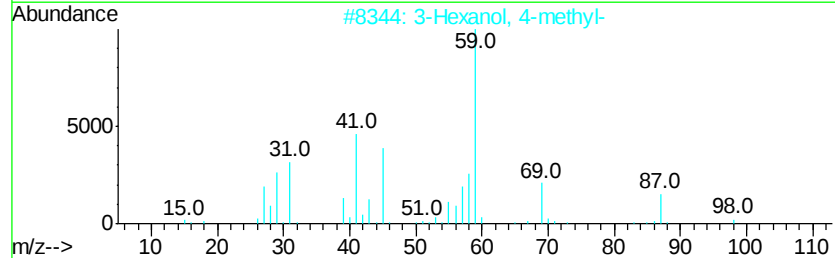
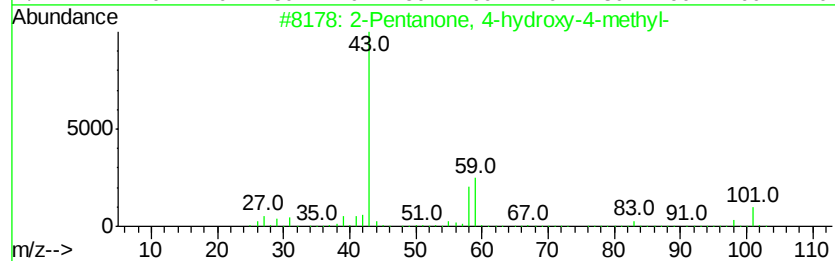
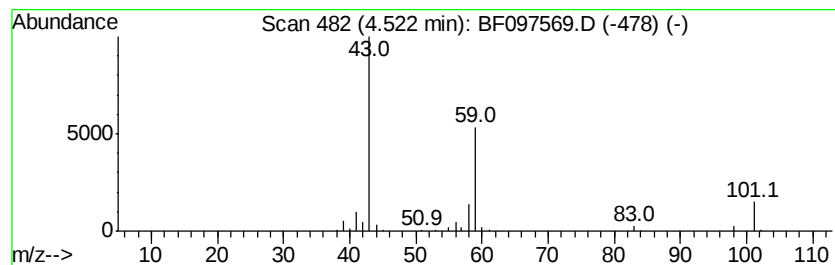
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	7.34 ng	240605	1,4-Dichlorobenzene-d4	6.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

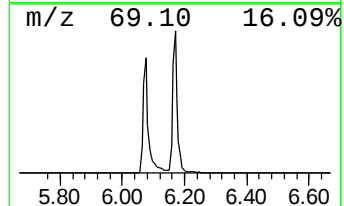
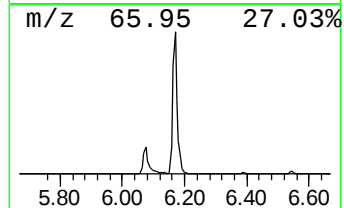
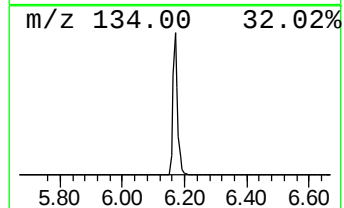
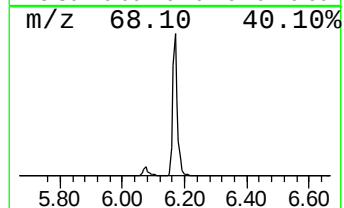
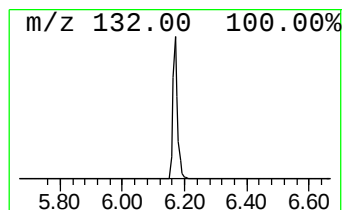
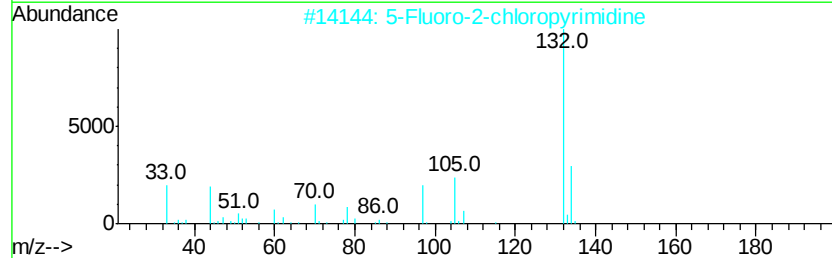
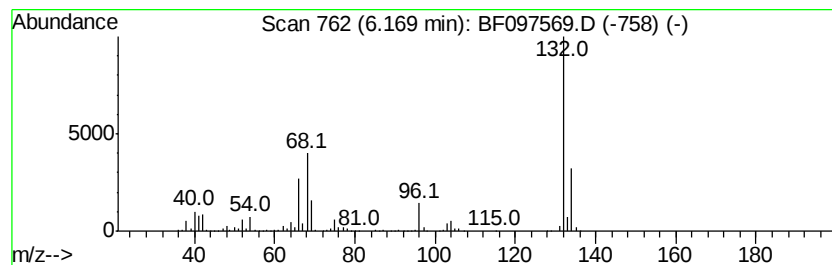
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	71.45 ng	2342490	1,4-Dichlorobenzene-d4	6.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

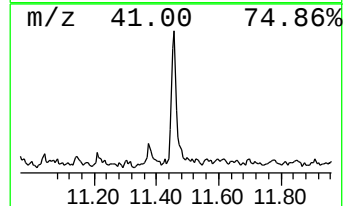
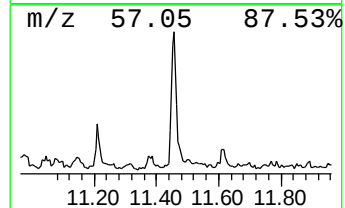
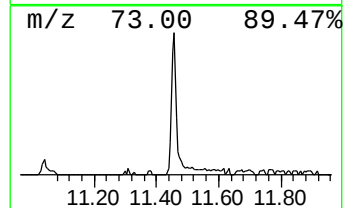
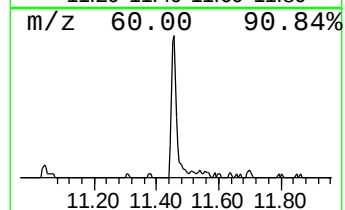
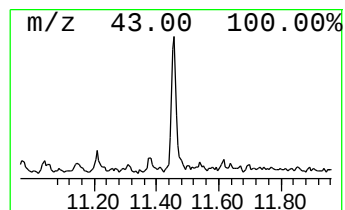
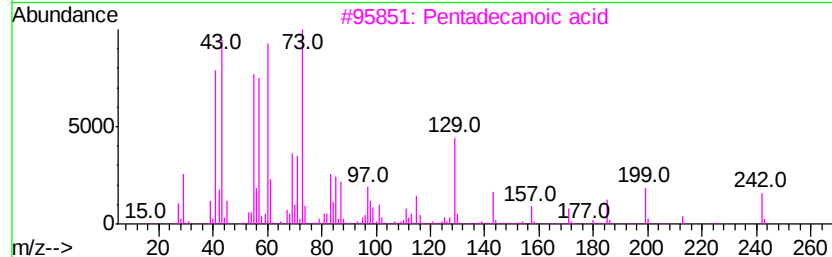
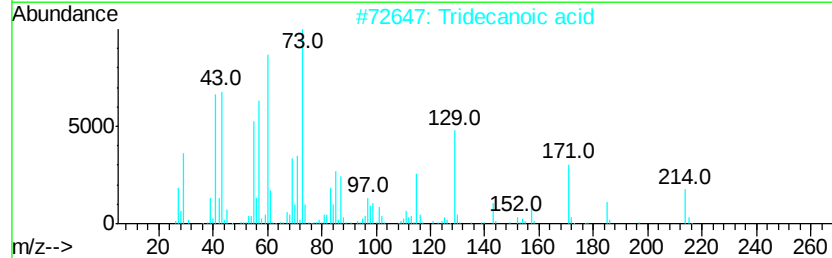
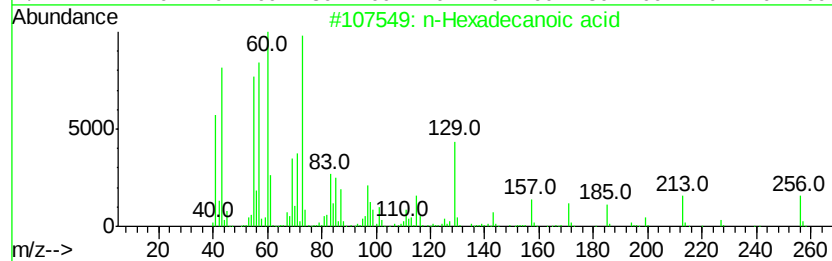
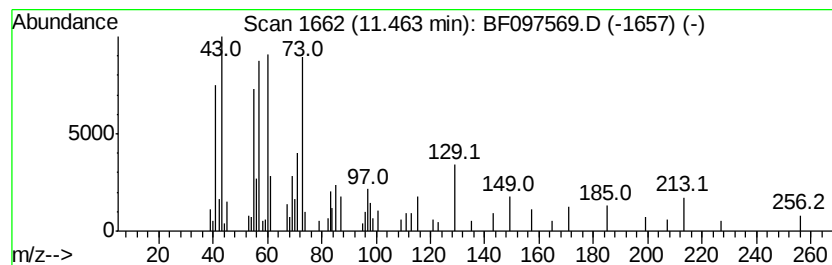
Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.46	4.77 ng	179529	Phenanthrene-d10		10.89	
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	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Undecanoic acid	186	C11H22O2	000112-37-8	81
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

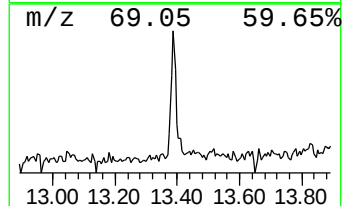
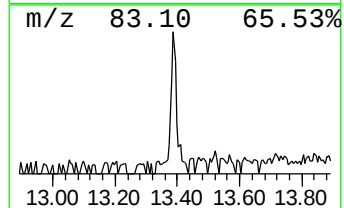
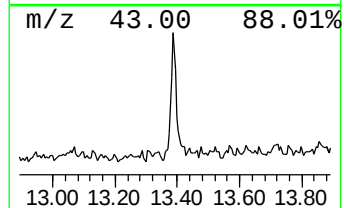
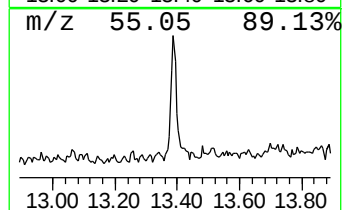
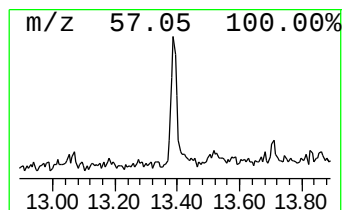
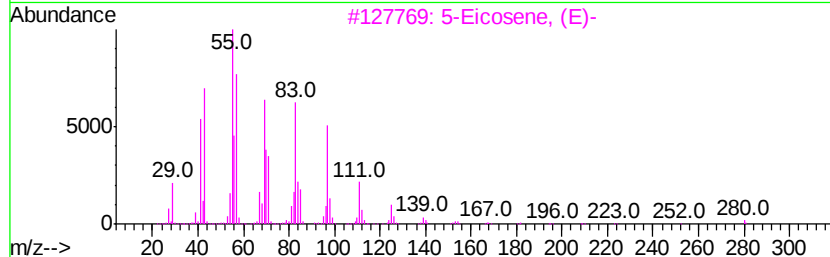
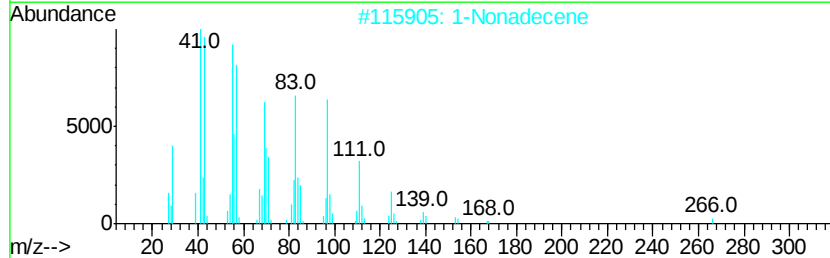
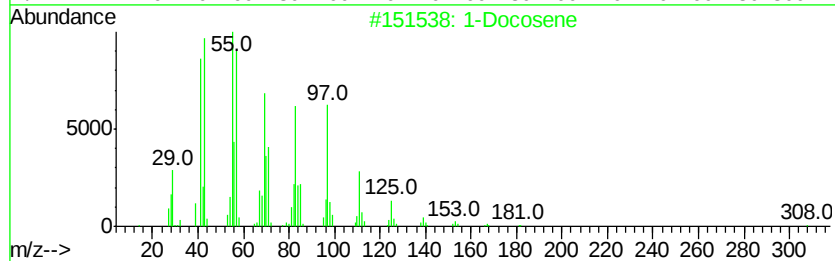
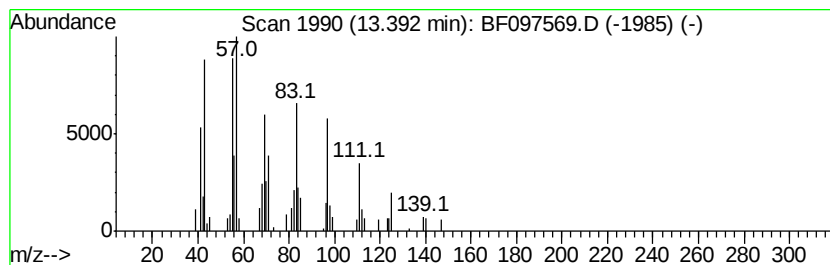
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	3.83 ng	80129	Chrysene-d12	13.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	1-Nonadecene		266	C19H38	018435-45-5	91
3	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
4	1-Octadecanol		270	C18H38O	000112-92-5	90
5	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

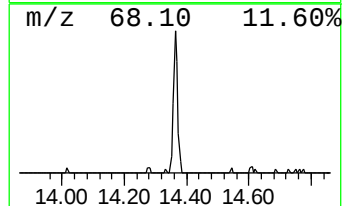
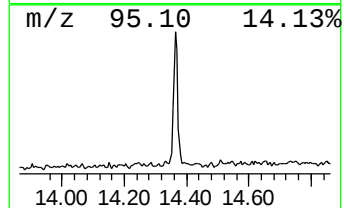
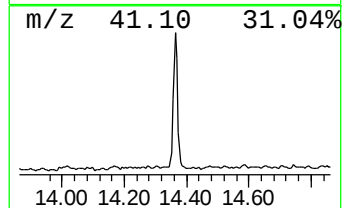
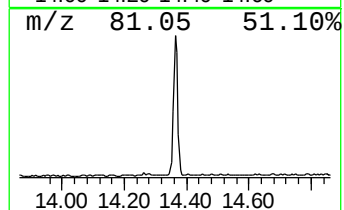
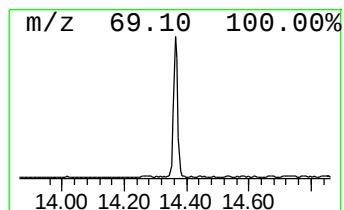
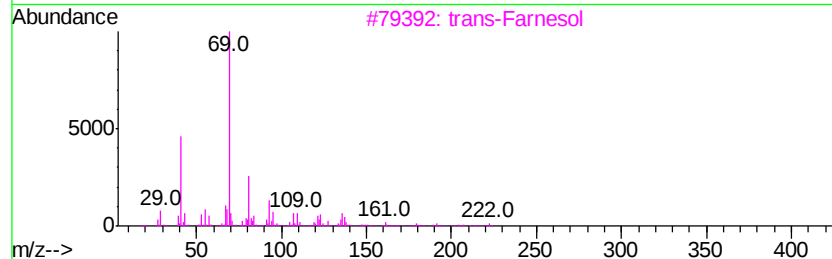
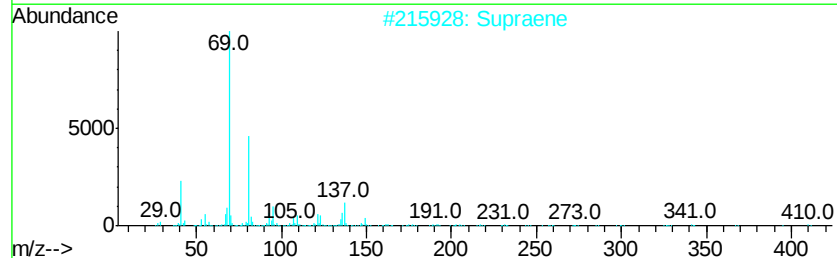
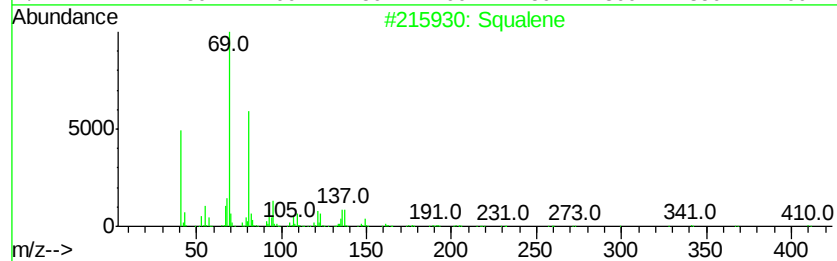
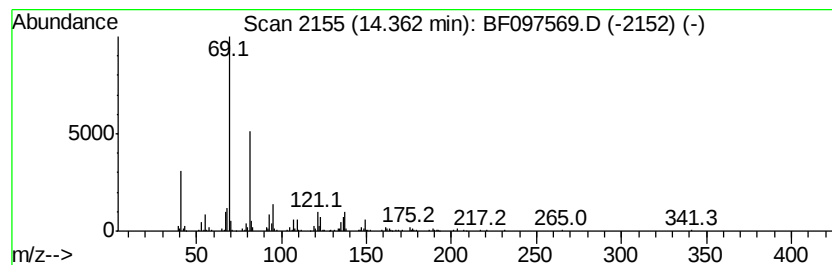
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	14.45 ng	332034	Perylene-d12	14.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		trans-Farnesol	222	C15H26O	000106-28-5	64
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097569.D
Acq On : 10 Aug 2017 20:27
Operator : SJ/JU
Sample : I4688-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.52	7.3	ng	240605	1	6.39	655668	20.0
unknown6.17	6.17	71.5	ng	2342490	1	6.39	655668	20.0
n-Hexadecanoic acid	11.46	4.8	ng	179529	4	10.89	753006	20.0
1-Docosene	13.39	3.8	ng	80129	5	13.52	418014	20.0
Squalene	14.36	14.4	ng	332034	6	14.86	459492	20.0