

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\
 Data File : BF097642.D
 Acq On : 12 Aug 2017 19:15
 Operator : SJ/JU
 Sample : I4705-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-A-COMP

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-BF081117.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	4.740	515	519	545	rBV	118215	341220	12.39%	1.361%
2	5.416	630	634	665	rBV	1401686	2753402	100.00%	10.979%
3	7.057	908	913	926	rBV	1620119	2584649	93.87%	10.306%
4	7.157	926	930	943	rVB	1702171	2653411	96.37%	10.580%
5	7.498	984	988	1002	rBV	577585	797538	28.97%	3.180%
6	7.734	1024	1028	1048	rBV	1186471	1692070	61.45%	6.747%
7	8.410	1138	1143	1170	rBV	1138766	1691153	61.42%	6.743%
8	9.528	1329	1333	1346	rBV	783885	1062338	38.58%	4.236%
9	11.304	1629	1635	1647	rBV	1745503	2313898	84.04%	9.226%
10	11.992	1748	1752	1760	rBV	380891	464901	16.88%	1.854%
11	12.351	1807	1813	1818	rBV2	794611	1030028	37.41%	4.107%
12	12.386	1818	1819	1827	rVB2	40069	40935	1.49%	0.163%
13	13.204	1951	1958	1963	rBV	44449	57241	2.08%	0.228%
14	13.563	2007	2019	2022	rBV5	13919	32308	1.17%	0.129%
15	13.645	2028	2033	2049	rBV	849558	1195419	43.42%	4.767%
16	13.974	2084	2089	2098	rBV	51115	94143	3.42%	0.375%
17	14.704	2208	2213	2216	rBV	38569	45701	1.66%	0.182%
18	14.745	2216	2220	2225	rBV2	598433	758204	27.54%	3.023%
19	15.774	2386	2395	2416	rBV	787427	1450736	52.69%	5.785%
20	16.556	2525	2528	2537	rVB	66154	94240	3.42%	0.376%
21	16.856	2574	2579	2592	rBV	355429	549321	19.95%	2.190%
22	17.104	2616	2621	2625	rBV	1221041	1395263	50.67%	5.563%
23	17.480	2678	2685	2686	rBV7	17669	31445	1.14%	0.125%
24	18.368	2831	2836	2844	rBV	137365	250638	9.10%	0.999%
25	18.445	2845	2849	2854	rVV	522143	642844	23.35%	2.563%
26	18.515	2858	2861	2865	rVV	56196	61705	2.24%	0.246%
27	19.715	3062	3065	3068	rBV2	59762	89869	3.26%	0.358%
28	19.874	3090	3092	3096	rVB	54713	51088	1.86%	0.204%
29	20.062	3122	3124	3128	rBV	31141	34744	1.26%	0.139%
30	20.115	3129	3133	3141	rBV	424221	576120	20.92%	2.297%
31	20.568	3206	3210	3215	rVB	69771	102700	3.73%	0.409%
32	23.274	3662	3670	3675	rVV6	64985	140228	5.09%	0.559%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

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-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

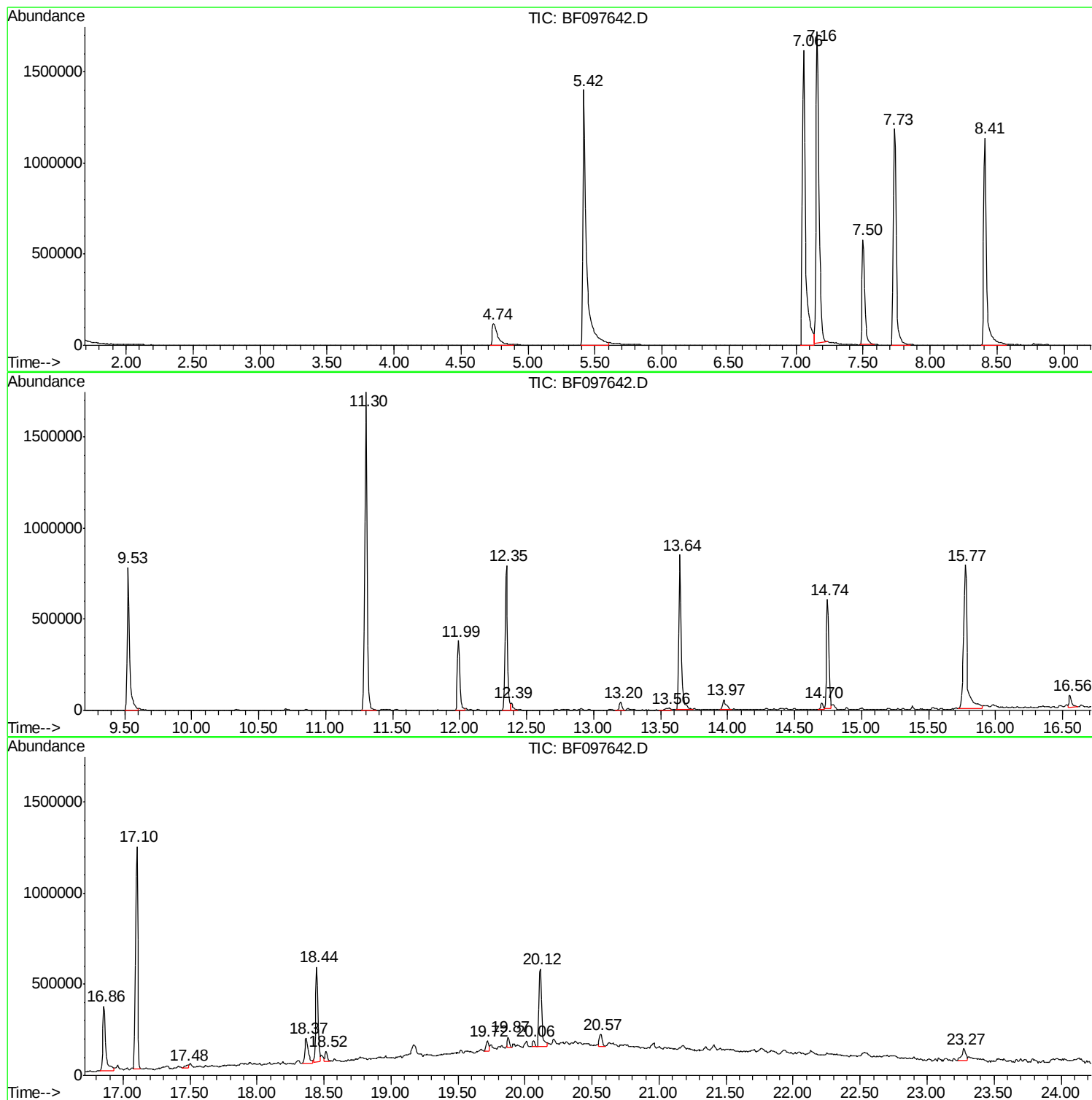
Sum of corrected areas: 25079500

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

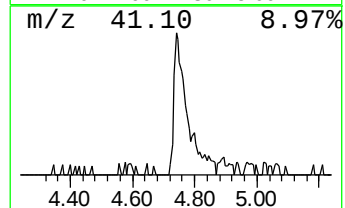
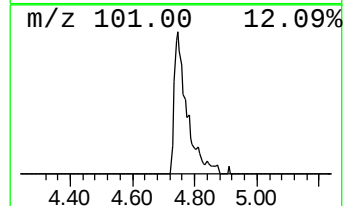
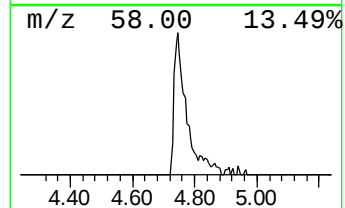
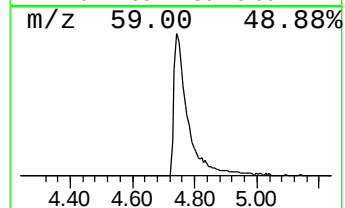
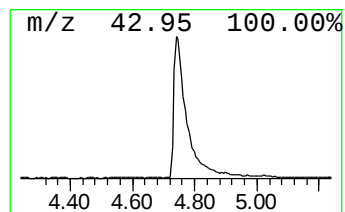
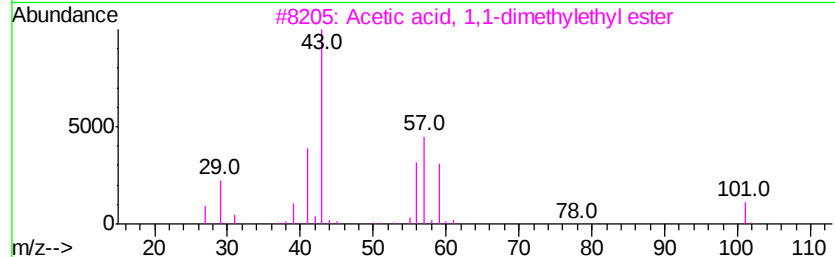
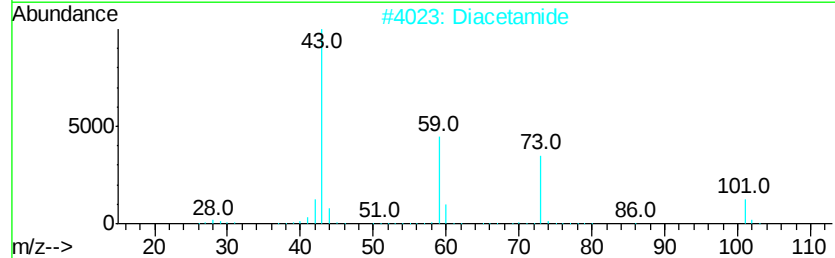
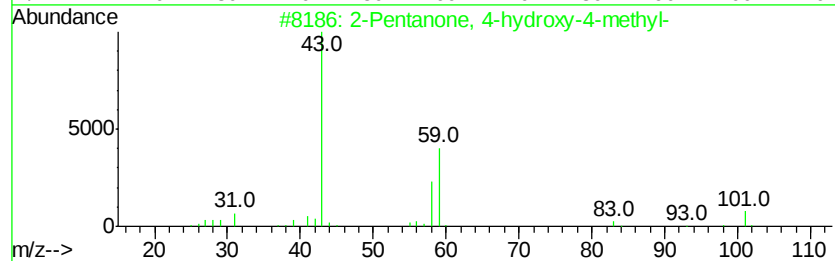
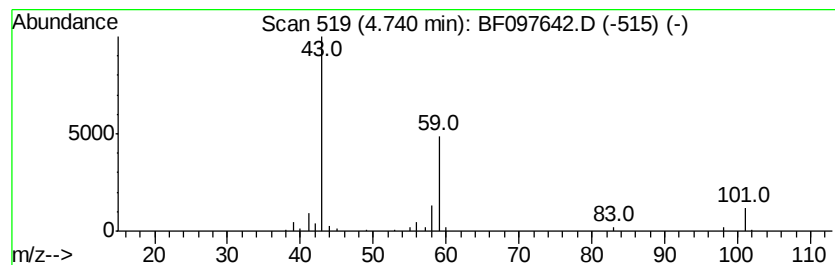
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.74	8.56 ng	341220	1,4-Dichlorobenzene-d4	7.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Diacetamide	101	C4H7NO2	000625-77-4	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

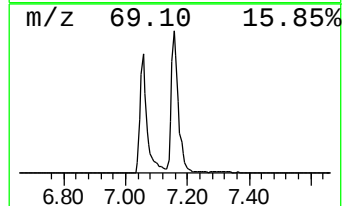
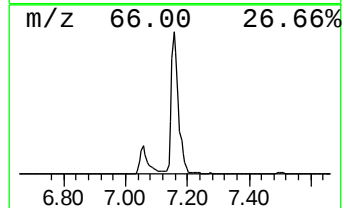
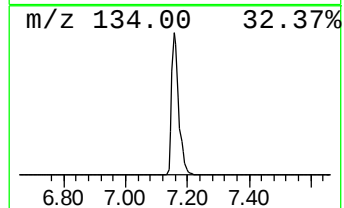
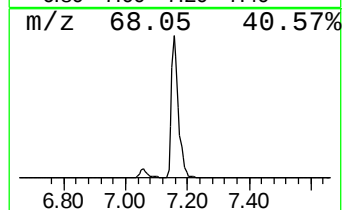
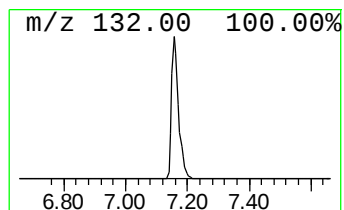
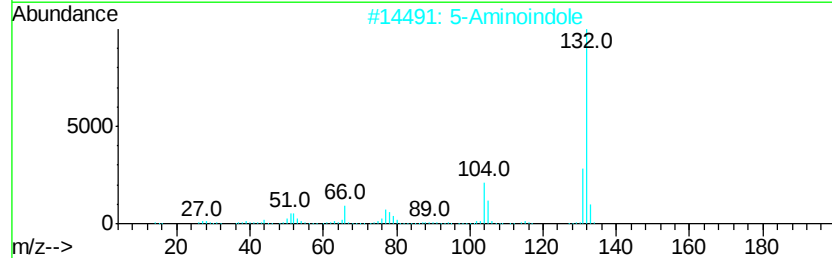
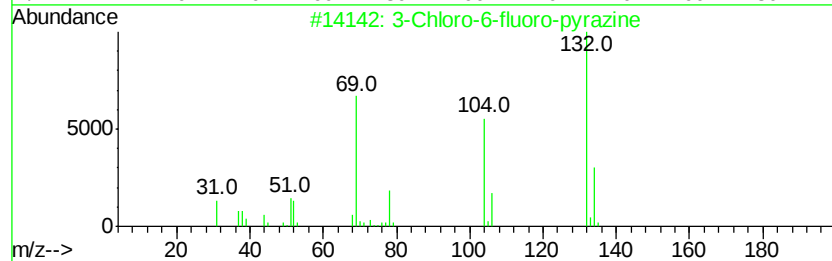
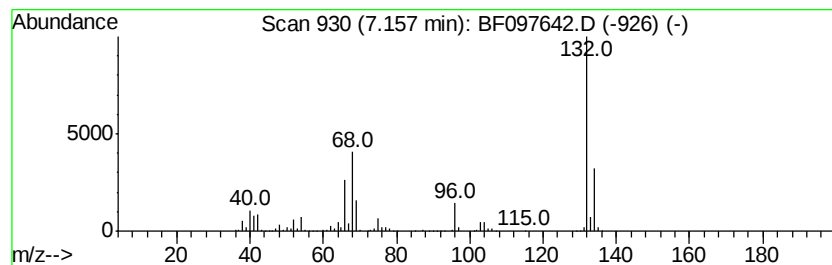
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	66.54 ng	2653410	1,4-Dichlorobenzene-d4	7.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

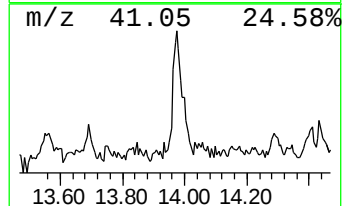
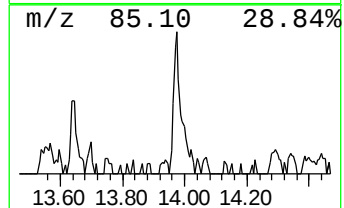
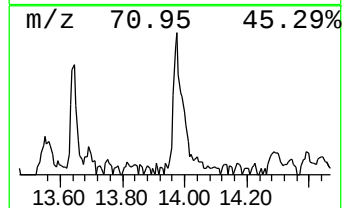
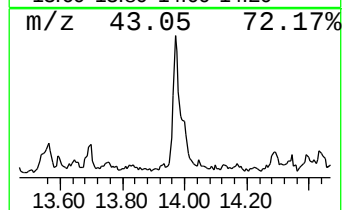
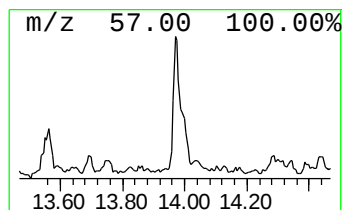
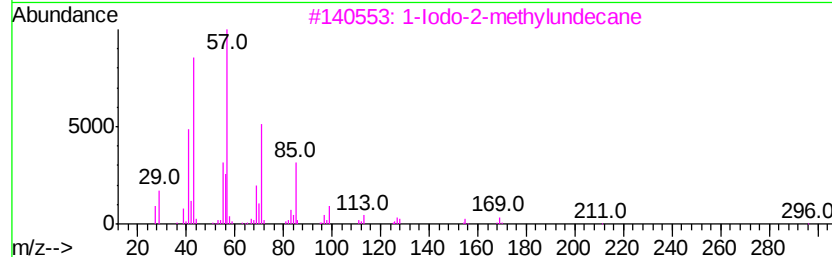
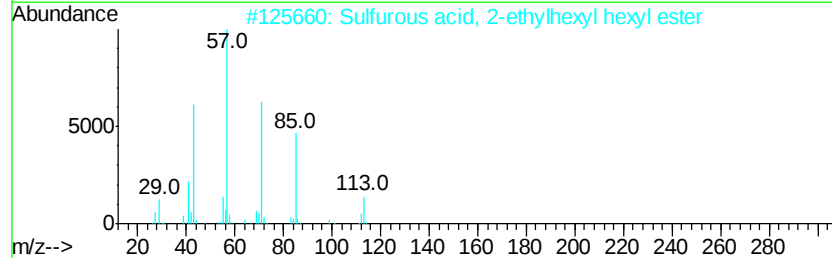
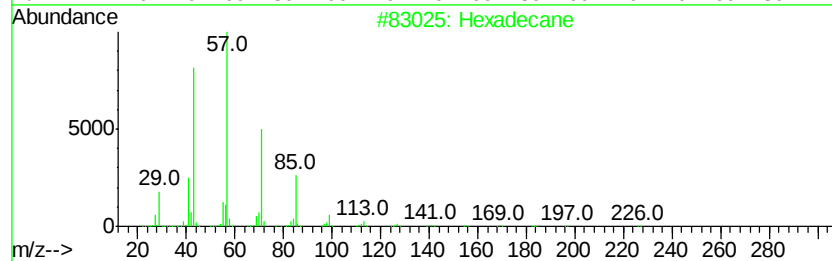
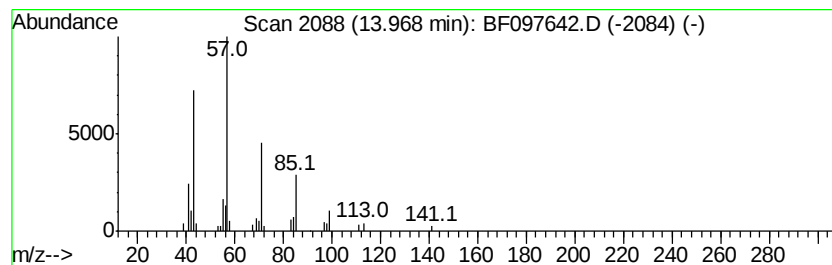
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.48 ng	94143	Phenanthrene-d10	14.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	83
2	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	72
3	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	64
4	Dodecane, 4,6-dimethyl-		198	C14H30	061141-72-8	53
5	Octane, 2,4,6-trimethyl-		156	C11H24	062016-37-9	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

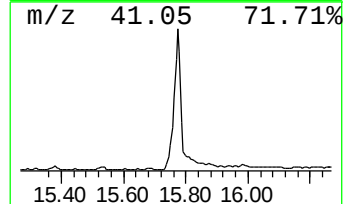
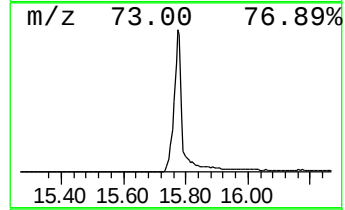
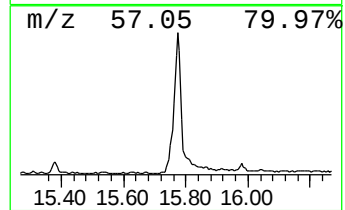
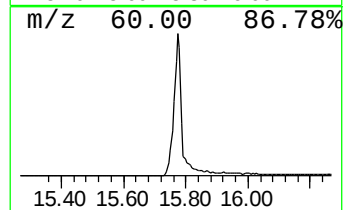
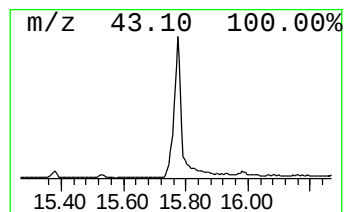
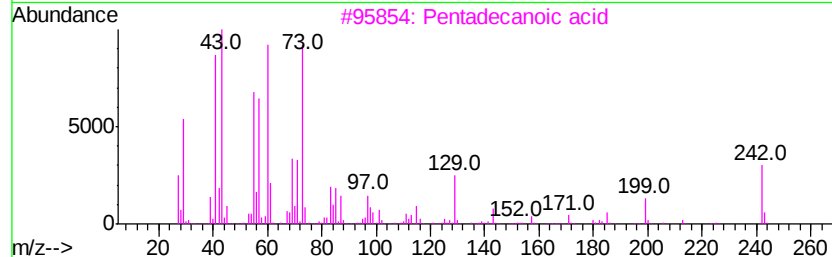
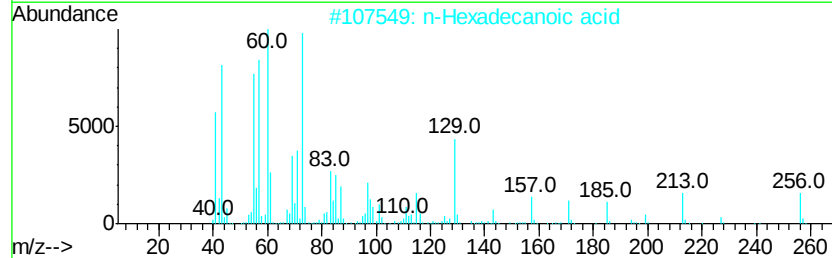
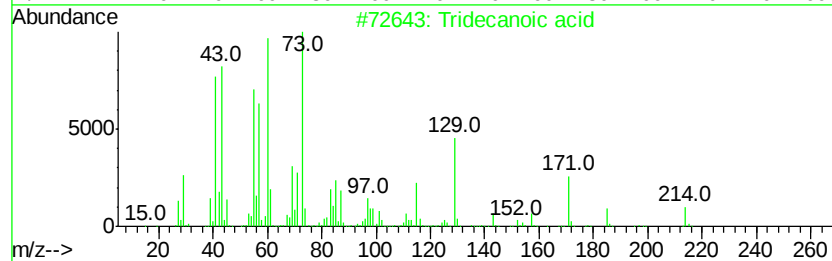
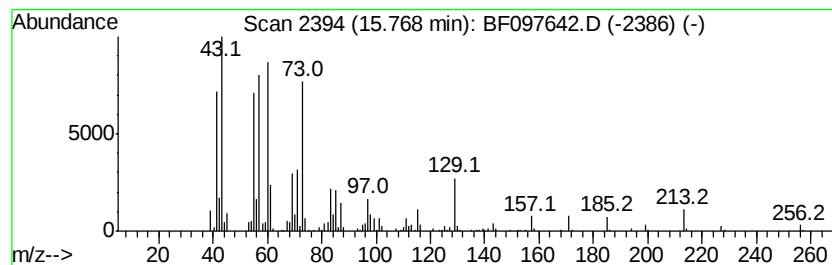
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	38.27 ng	1450740	Phenanthrene-d10	14.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

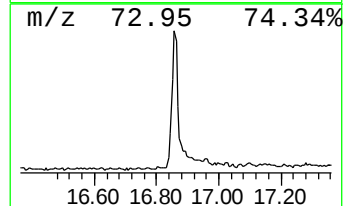
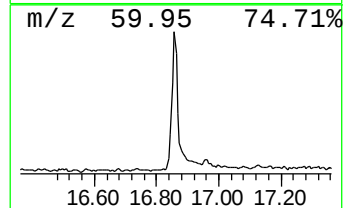
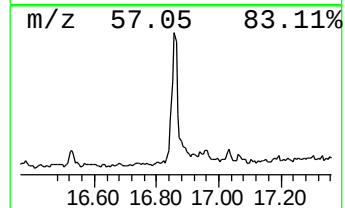
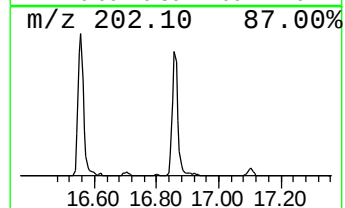
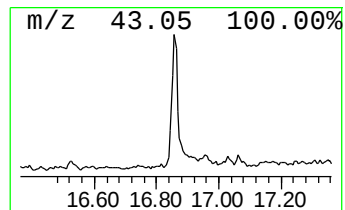
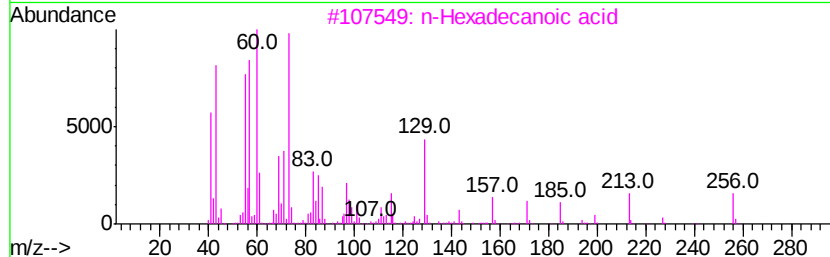
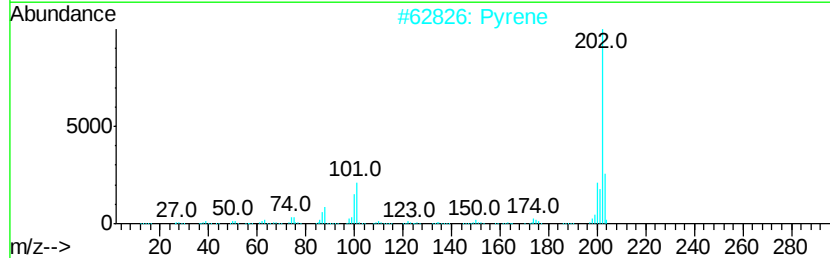
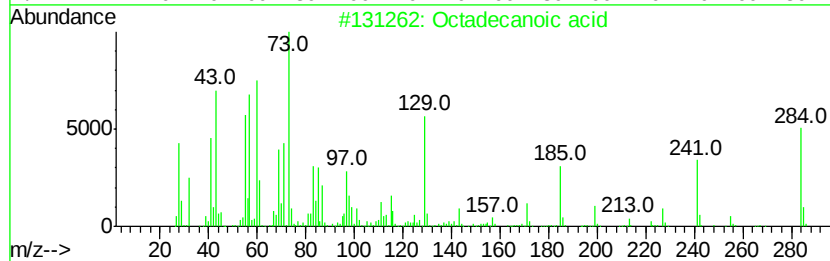
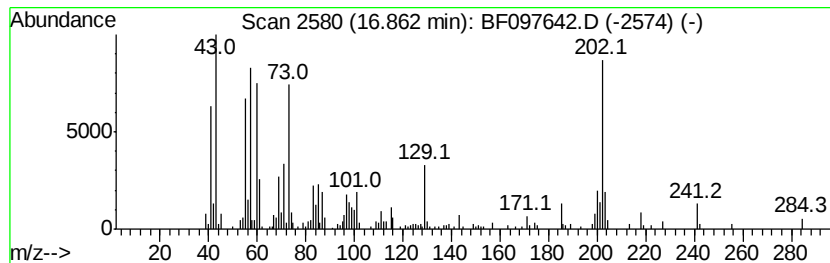
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	17.09 ng	549321	Chrysene-d12	18.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		Pyrene	202	C16H10	000129-00-0	80
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

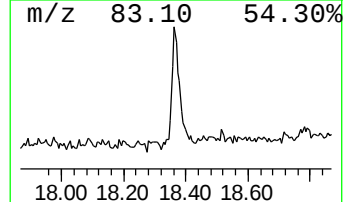
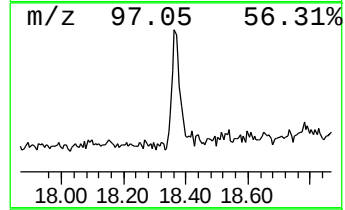
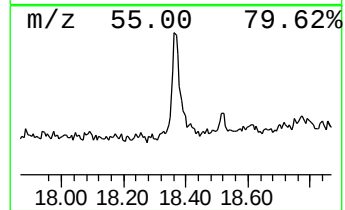
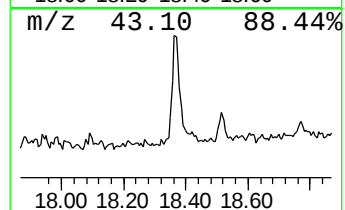
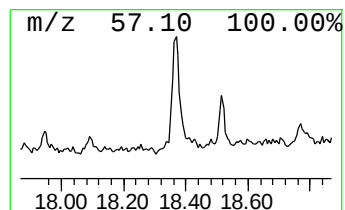
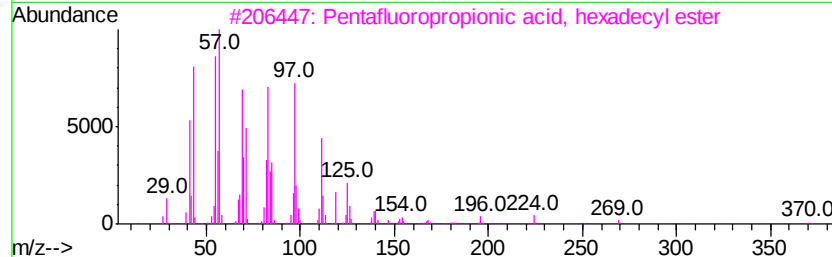
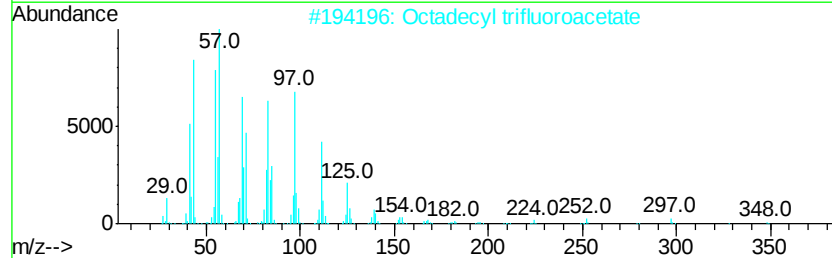
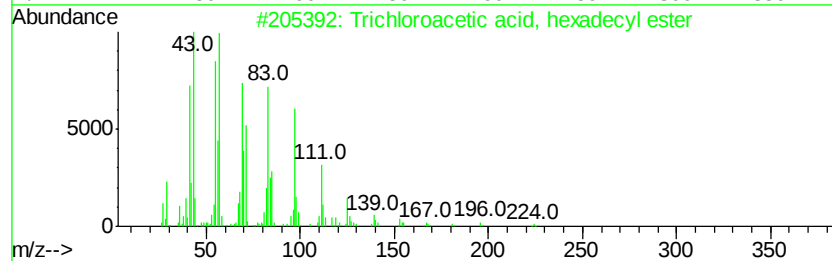
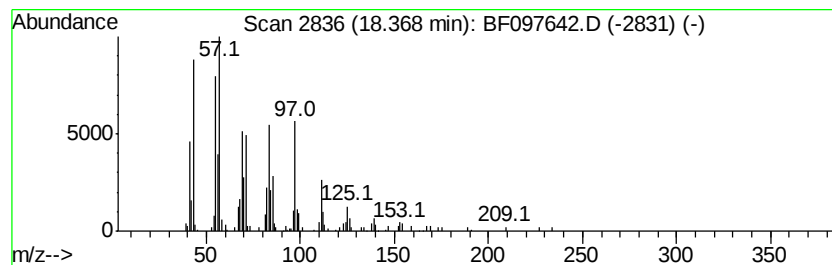
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	7.80 ng	250638	Chrysene-d12	18.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		Pentafluoropropionic acid, hexadecyl ...	388	C19H33F5O2	006222-07-7	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

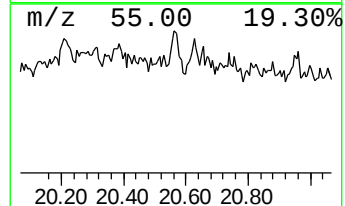
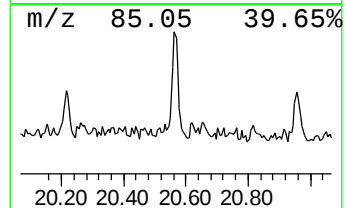
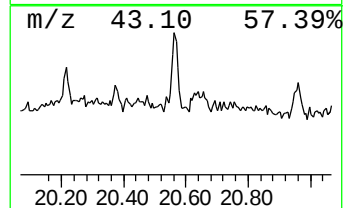
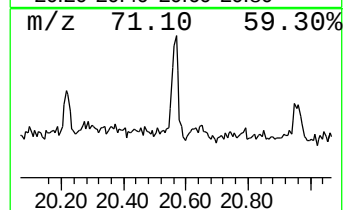
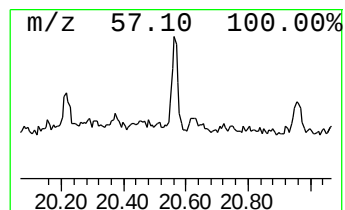
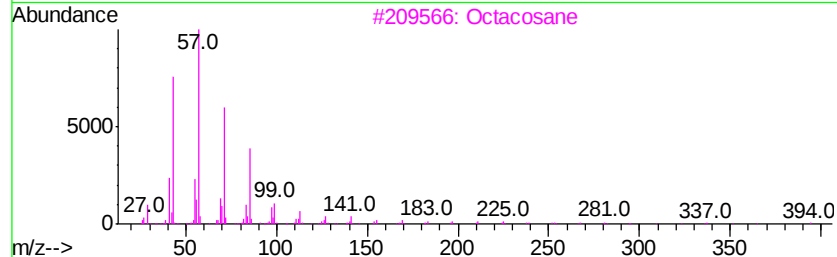
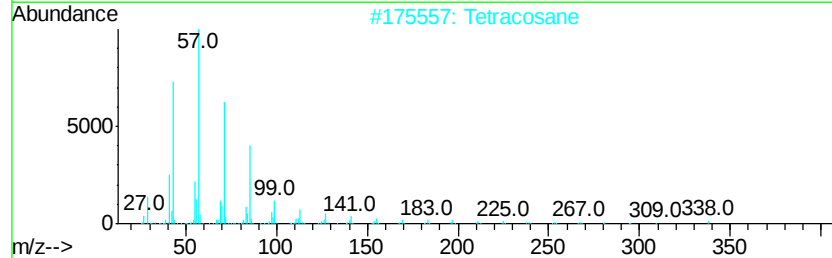
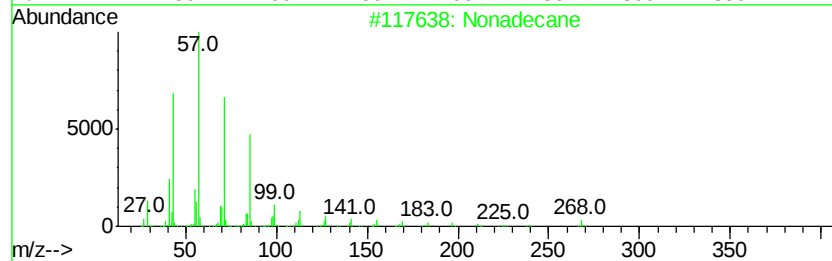
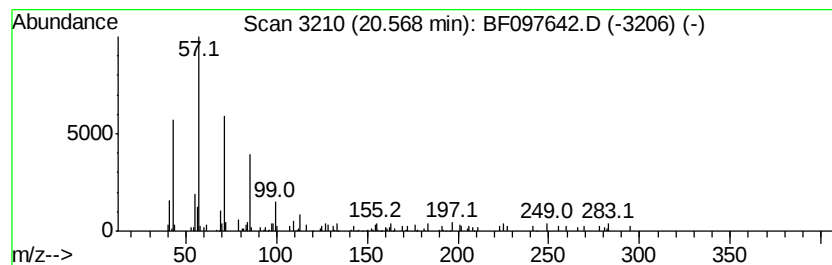
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.57	3.57 ng	102700	Perylene-d12	20.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	80
2		Tetracosane	338	C24H50	000646-31-1	80
3		Octacosane	394	C28H58	000630-02-4	72
4		triacontane	422	C30H62	000638-68-6	72
5		Tetratetracontane	619	C44H90	007098-22-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

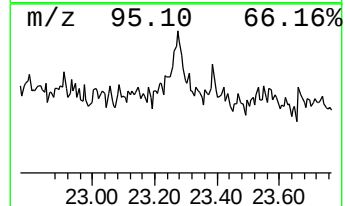
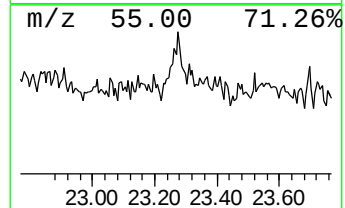
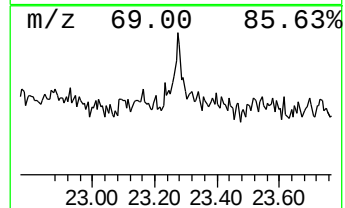
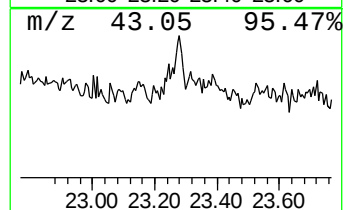
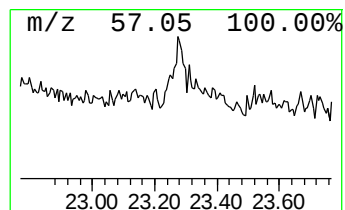
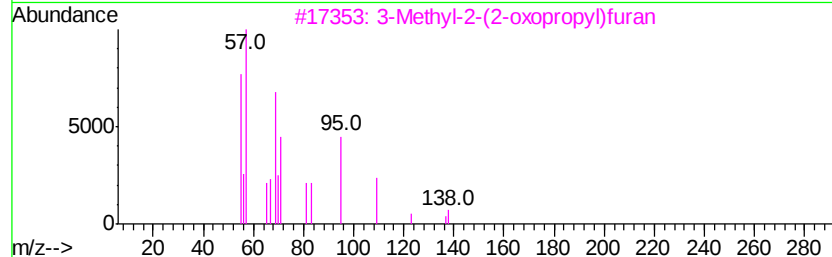
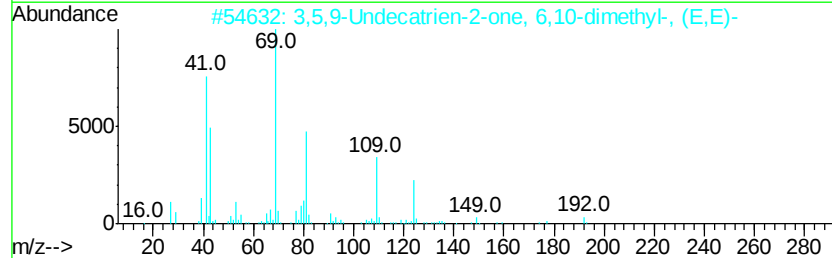
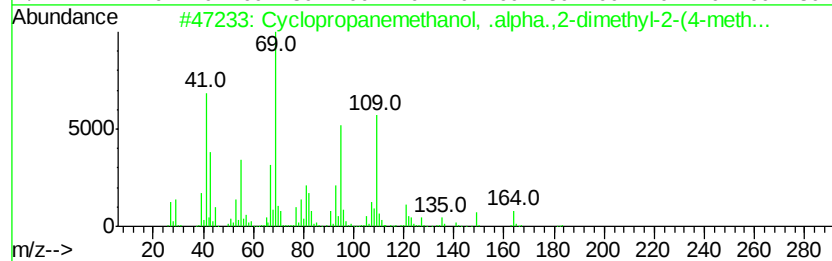
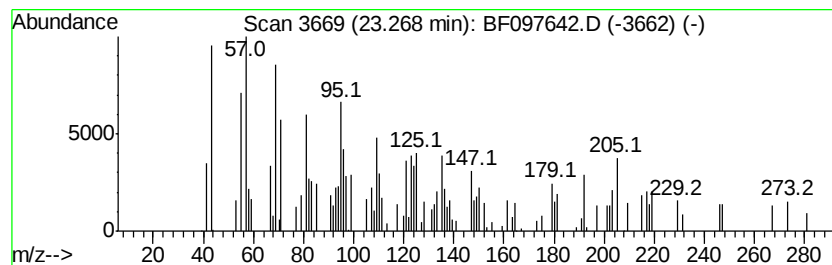
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.27 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.27	4.87 ng	140228	Perylene-d12	20.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	38
2		3,5,9-Undecatrien-2-one, 6,10-di...	192	C13H20O	003548-78-5	38
3		3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	38
4		Peuceleinendiol	308	C20H36O2	072776-48-8	35
5		Cyclohexanebutanoic acid, 2,2-di...	224	C14H24O2	095452-15-6	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081217\
Data File : BF097642.D
Acq On : 12 Aug 2017 19:15
Operator : SJ/JU
Sample : I4705-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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...	4.74	8.6	ng	341220	1	7.50	797538	20.0
unknown7.16	7.16	66.5	ng	2653410	1	7.50	797538	20.0
Hexadecane	13.97	2.5	ng	94143	4	14.74	758204	20.0
Tridecanoic acid	15.77	38.3	ng	1450740	4	14.74	758204	20.0
Octadecanoic acid	16.86	17.1	ng	549321	5	18.44	642844	20.0
Trichloroacetic a...	18.37	7.8	ng	250638	5	18.44	642844	20.0
Nonadecane	20.57	3.6	ng	102700	6	20.12	576120	20.0
unknown23.27	23.27	4.9	ng	140228	6	20.12	576120	20.0