

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
 Data File : BF107939.D
 Acq On : 3 Aug 2018 15:57
 Operator : JU/SJ
 Sample : J4285-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KG-PIT-2

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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	5.184	480	484	497	rBV	199290	313142	9.90%	1.237%
2	5.595	551	554	596	rBV	673751	2217152	70.12%	8.755%
3	6.601	721	725	743	rBV	840357	2156322	68.20%	8.515%
4	6.725	743	746	780	rVV	1513879	3161880	100.00%	12.486%
5	6.954	782	785	807	rVV	279215	875344	27.68%	3.457%
6	7.101	807	810	851	rVB	1276303	2175611	68.81%	8.591%
7	7.519	878	881	904	rBV	524831	1463854	46.30%	5.780%
8	7.666	904	906	920	rVB4	38640	93782	2.97%	0.370%
9	8.236	999	1003	1026	rBV	461381	961830	30.42%	3.798%
10	9.301	1181	1184	1213	rBV	1799941	2739809	86.65%	10.819%
11	9.701	1248	1252	1264	rBV	221658	306373	9.69%	1.210%
12	9.989	1297	1301	1322	rBV	867101	1065690	33.70%	4.208%
13	10.789	1433	1437	1460	rBV	910139	1574030	49.78%	6.216%
14	11.489	1552	1556	1578	rBV	626010	1071407	33.89%	4.231%
15	12.030	1645	1648	1656	rVB	24465	34296	1.08%	0.135%
16	12.942	1801	1803	1809	rVB2	29440	32156	1.02%	0.127%
17	13.071	1821	1825	1842	rBV	1653117	2151051	68.03%	8.494%
18	13.618	1914	1918	1920	rBV	42041	41708	1.32%	0.165%
19	13.948	1970	1974	1980	rBV2	111732	156031	4.93%	0.616%
20	14.142	2003	2007	2022	rBV	495217	875298	27.68%	3.456%
21	14.260	2024	2027	2032	rVB2	62484	67391	2.13%	0.266%
22	14.566	2076	2079	2083	rBV	77566	72601	2.30%	0.287%
23	14.883	2130	2133	2138	rVB	88268	84112	2.66%	0.332%
24	15.236	2189	2193	2199	rBV	111531	133226	4.21%	0.526%
25	15.636	2256	2261	2263	rBV	129609	187730	5.94%	0.741%
26	15.677	2263	2268	2287	rVB	428441	942175	29.80%	3.720%
27	16.089	2333	2338	2343	rBV	133678	202561	6.41%	0.800%
28	16.624	2424	2429	2438	rVB	84941	167508	5.30%	0.661%

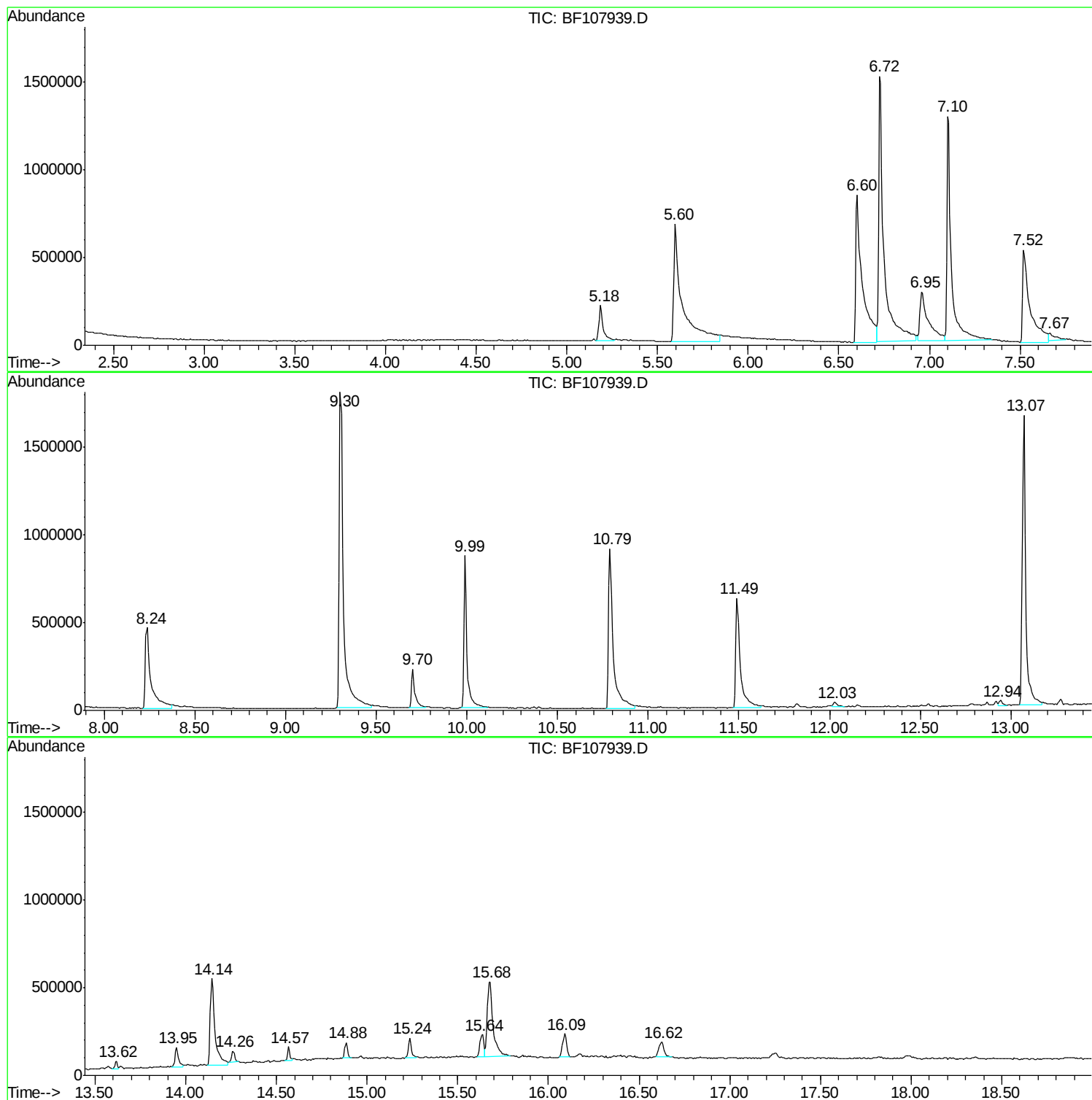
Sum of corrected areas: 25324070

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

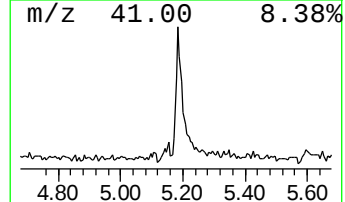
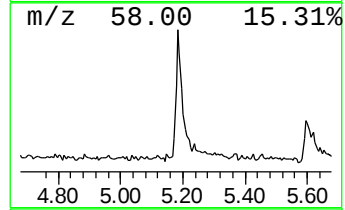
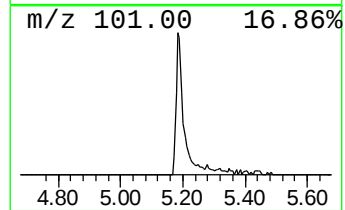
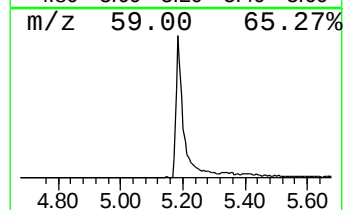
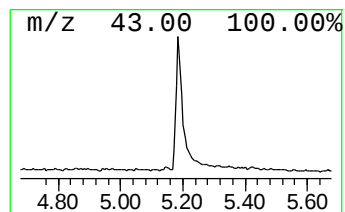
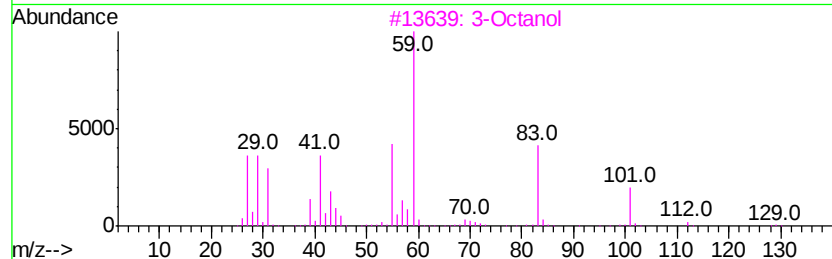
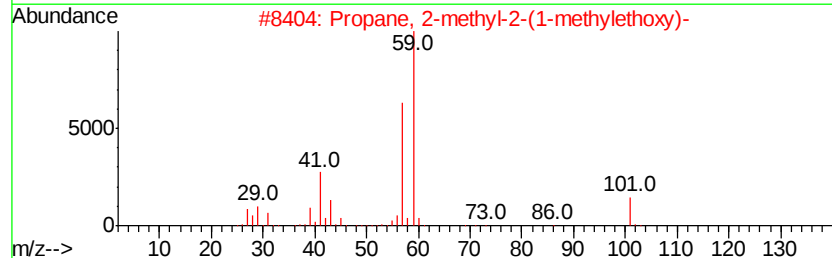
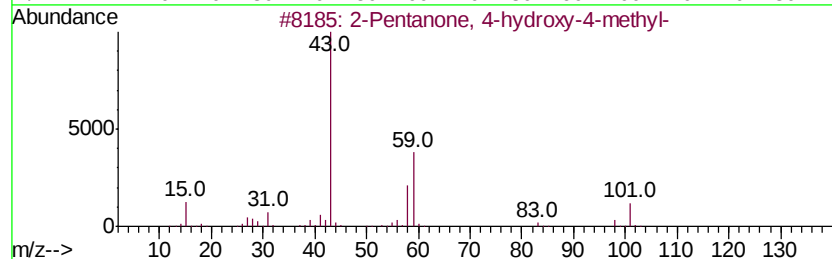
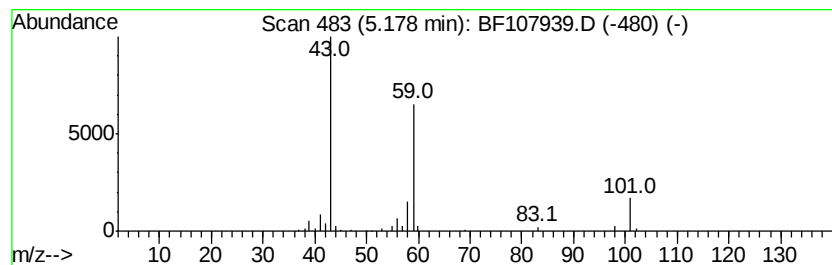
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.18	7.15 ng	313142	1,4-Dichlorobenzene-d4	6.96

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3		3-Octanol	130	C8H18O	000589-98-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

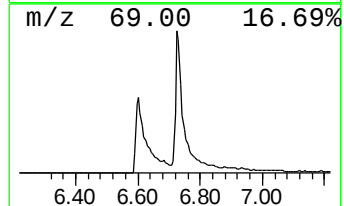
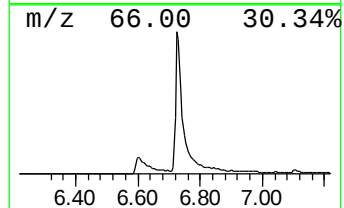
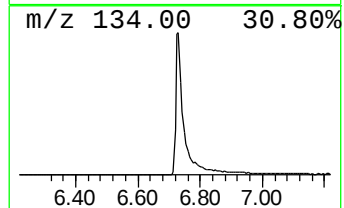
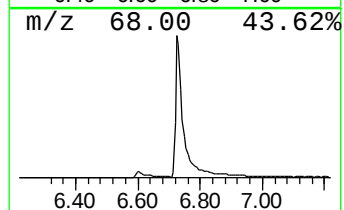
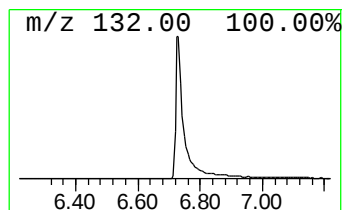
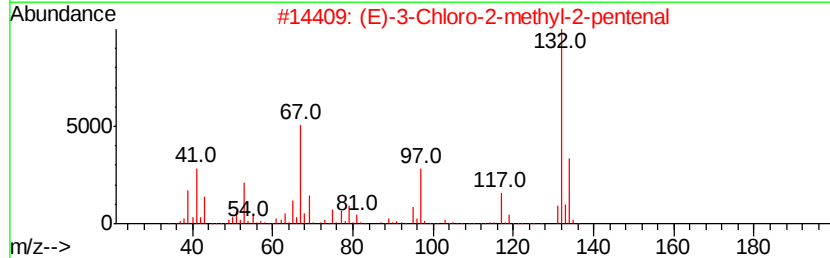
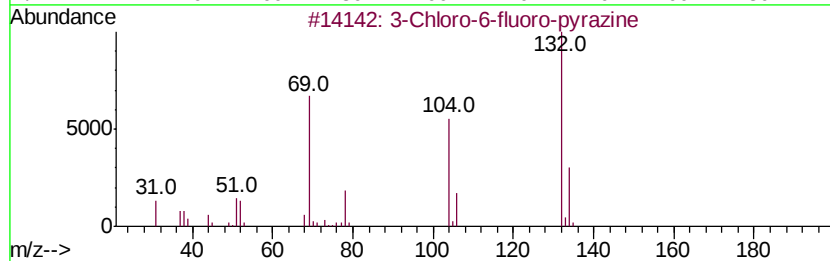
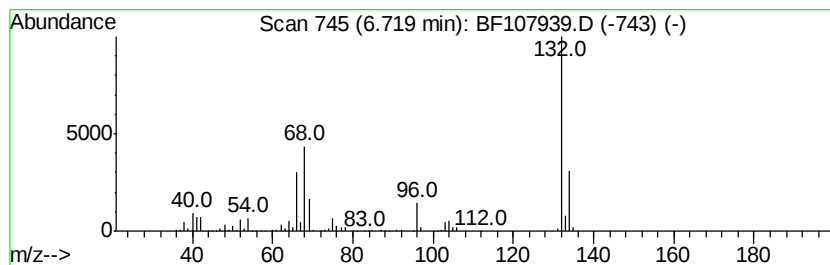
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	72.24 ng	3161880	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

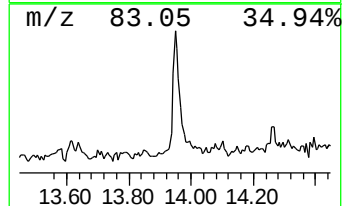
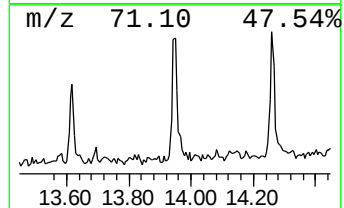
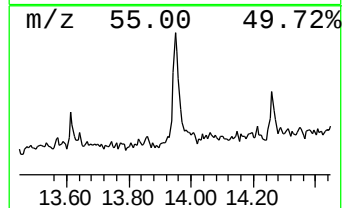
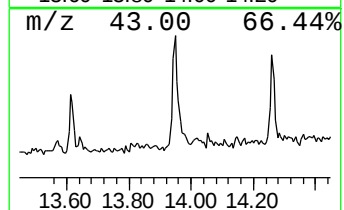
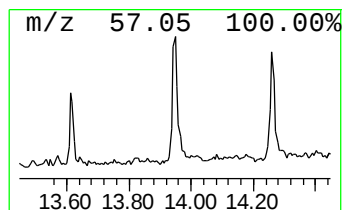
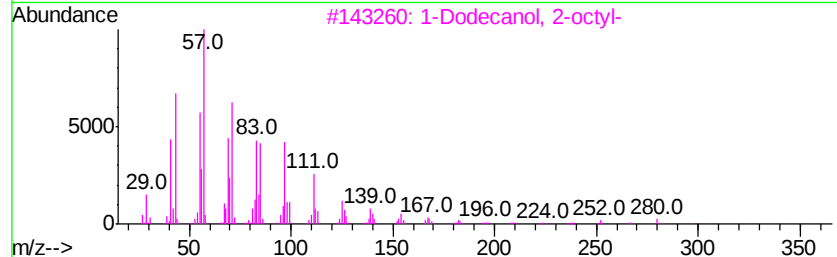
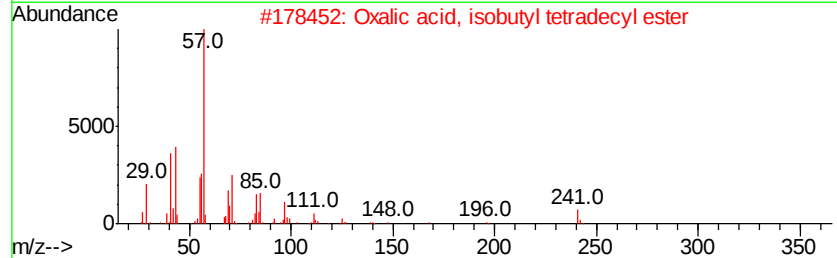
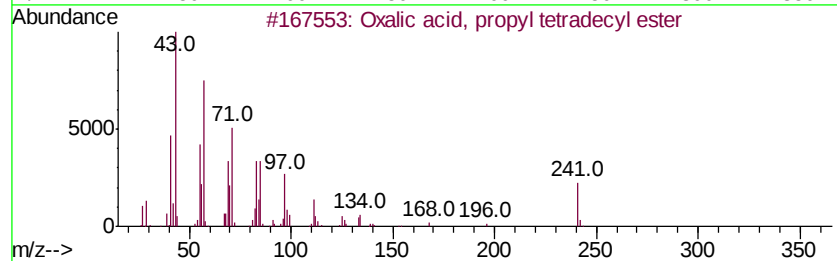
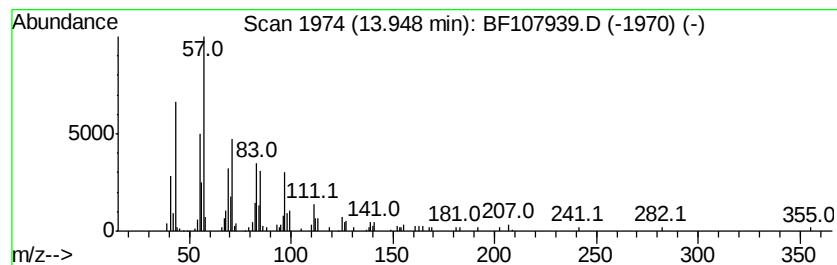
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Oxalic acid, propyl tetradec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.57 ng	156031	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	91
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4		Eicosane	282	C20H42	000112-95-8	90
5		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
 Data File : BF107939.D
 Acq On : 3 Aug 2018 15:57
 Operator : JU/SJ
 Sample : J4285-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KG-PIT-2

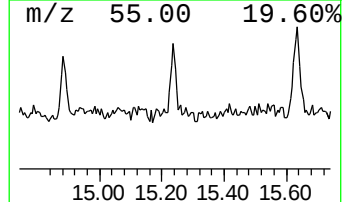
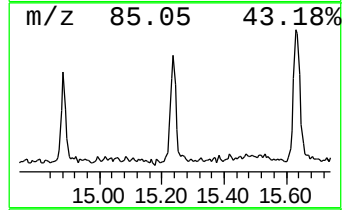
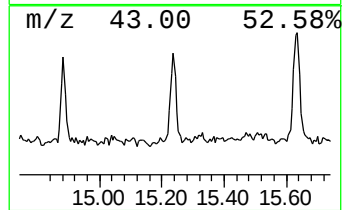
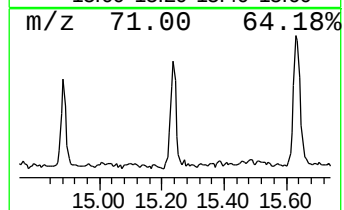
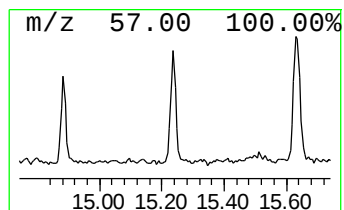
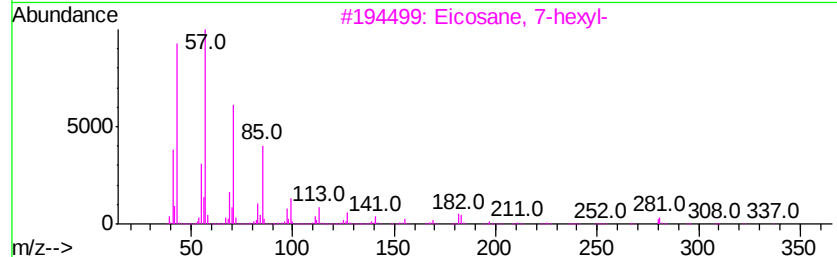
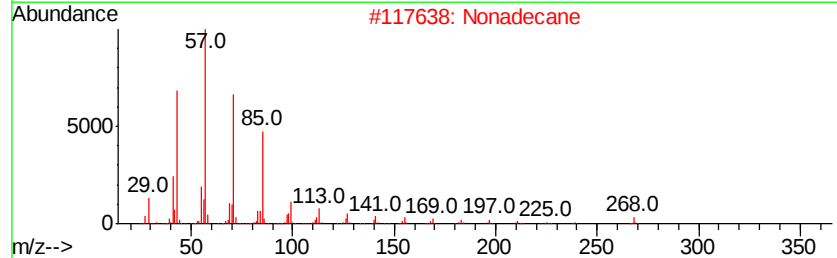
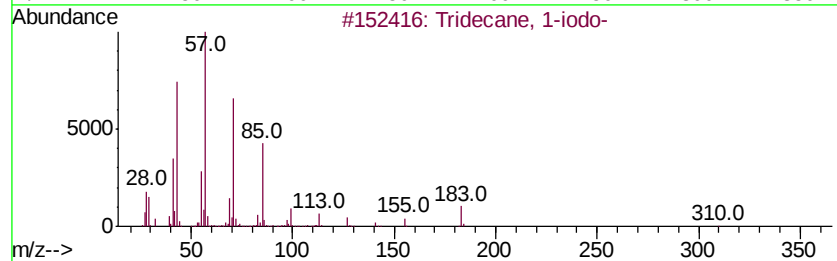
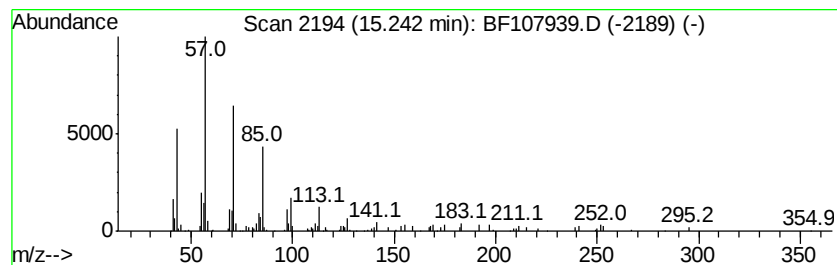
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Tridecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.83 ng	133226	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2		Nonadecane	268	C19H40	000629-92-5	80
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74
5		Tetracosane	338	C24H50	000646-31-1	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

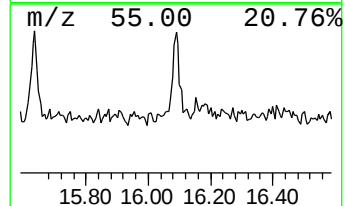
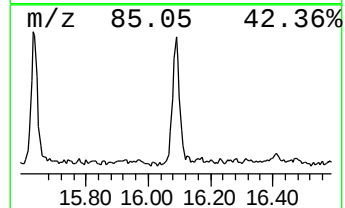
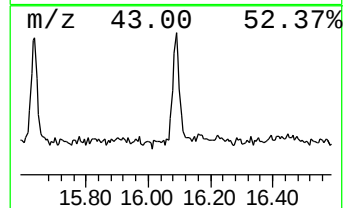
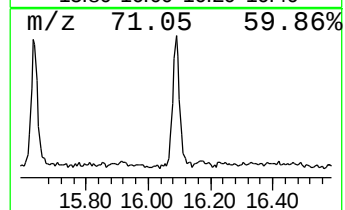
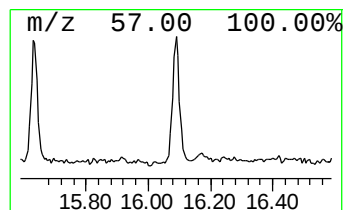
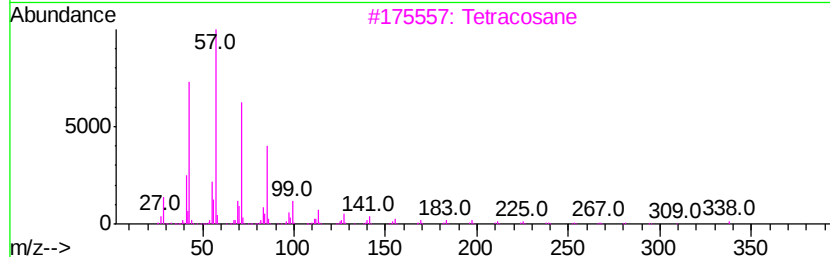
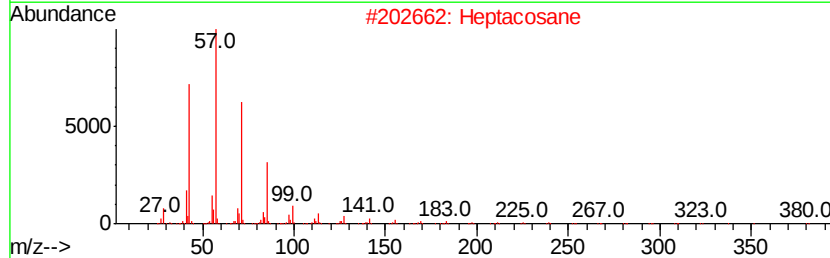
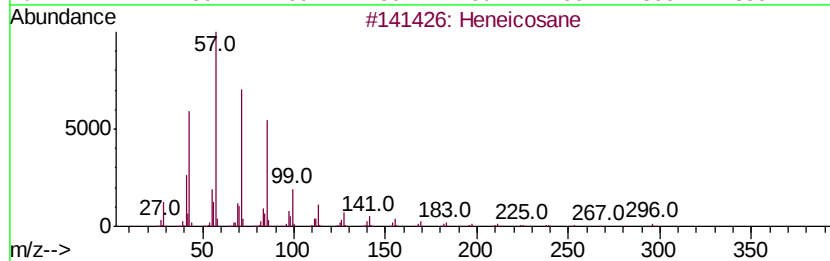
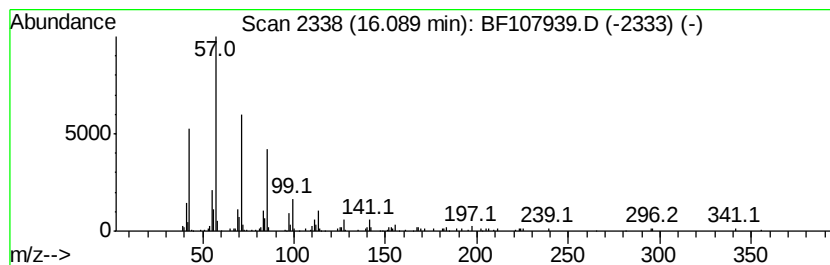
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	4.30 ng	202561	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Heptacosane	380	C27H56	000593-49-7	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		triacontane	422	C30H62	000638-68-6	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

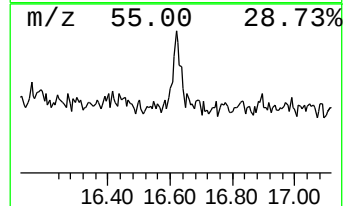
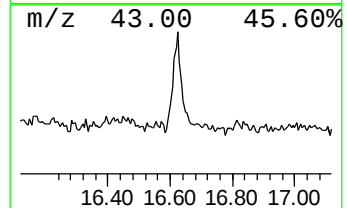
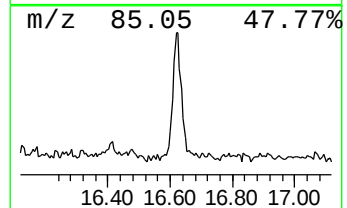
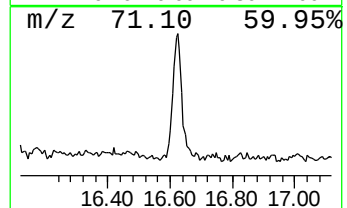
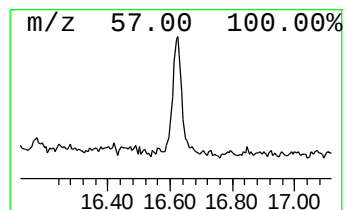
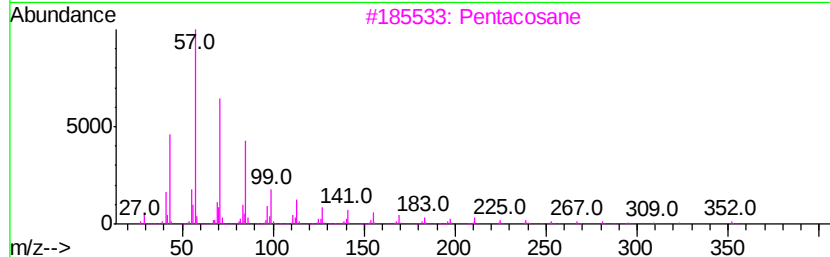
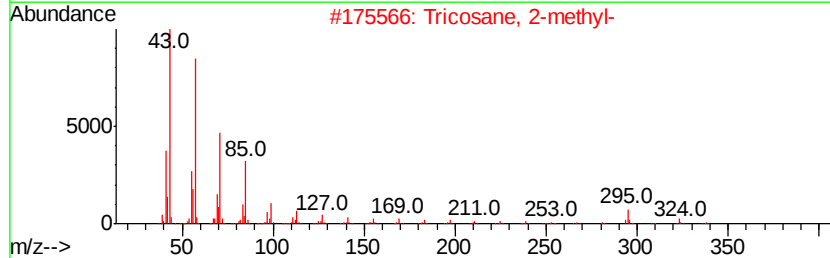
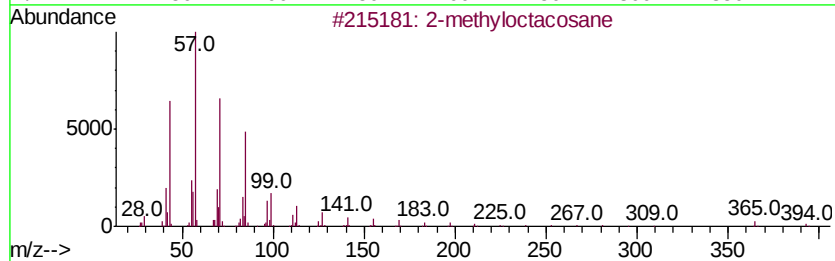
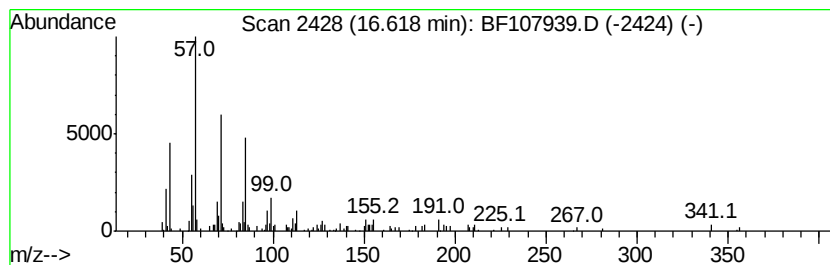
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	3.56 ng	167508	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080318\
Data File : BF107939.D
Acq On : 3 Aug 2018 15:57
Operator : JU/SJ
Sample : J4285-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KG-PIT-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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...	5.18	7.2	ng	313142	1	6.96	875344	20.0
unknown6.72	6.72	72.2	ng	3161880	1	6.96	875344	20.0
Oxalic acid, prop...	13.95	3.6	ng	156031	5	14.14	875298	20.0
Tridecane, 1-iodo-	15.24	2.8	ng	133226	6	15.68	942175	20.0
Heneicosane	16.09	4.3	ng	202561	6	15.68	942175	20.0
2-methyloctacosane	16.62	3.6	ng	167508	6	15.68	942175	20.0