

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
 Data File : BF097438.D
 Acq On : 7 Aug 2017 19:27
 Operator : SJ/JU
 Sample : I4623-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-BN

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-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	4.534	463	467	485	rBV	124527	227296	10.69%	1.223%
2	5.004	543	547	564	rBV	1647004	2126723	100.00%	11.441%
3	6.081	727	730	744	rBV	1747496	1899455	89.31%	10.218%
4	6.187	744	748	762	rVB	1794309	1808865	85.05%	9.731%
5	6.410	783	786	797	rBV	603807	540226	25.40%	2.906%
6	6.563	809	812	821	rBV	1330113	1260915	59.29%	6.783%
7	6.981	879	883	899	rBV	1336308	1291426	60.72%	6.947%
8	7.692	1001	1004	1009	rBV	856367	722883	33.99%	3.889%
9	8.769	1183	1187	1191	rBV	1842611	1835656	86.31%	9.875%
10	9.175	1252	1256	1265	rBV	213600	187754	8.83%	1.010%
11	9.433	1297	1300	1310	rVB	796093	722739	33.98%	3.888%
12	9.892	1374	1378	1381	rVB	38956	33422	1.57%	0.180%
13	10.222	1431	1434	1447	rBV	940504	927251	43.60%	4.988%
14	10.363	1454	1458	1471	rVB	51448	77052	3.62%	0.415%
15	10.804	1530	1533	1536	rBV2	31973	29510	1.39%	0.159%
16	10.910	1547	1551	1560	rVB	719773	612126	28.78%	3.293%
17	11.469	1643	1646	1655	rBV	61642	66009	3.10%	0.355%
18	12.245	1776	1778	1785	rBV2	21725	24975	1.17%	0.134%
19	12.333	1790	1793	1799	rVB	59833	50939	2.40%	0.274%
20	12.492	1815	1820	1823	rBV	1415298	1326512	62.37%	7.136%
21	13.063	1914	1917	1922	rBV	30295	30354	1.43%	0.163%
22	13.427	1973	1979	1988	rBV2	50122	107922	5.07%	0.581%
23	13.533	1993	1997	2004	rVB	571620	554842	26.09%	2.985%
24	13.663	2008	2019	2021	rBV5	18452	30854	1.45%	0.166%
25	14.292	2122	2126	2134	rBV	882816	948778	44.61%	5.104%
26	14.868	2220	2224	2228	rBV	451065	504032	23.70%	2.712%
27	14.904	2228	2230	2235	rVB3	30092	36318	1.71%	0.195%
28	15.251	2285	2289	2293	rBV3	16022	32677	1.54%	0.176%
29	15.645	2352	2356	2360	rVB	19904	26603	1.25%	0.143%
30	16.098	2430	2433	2439	rVB6	13866	23969	1.13%	0.129%
31	16.633	2516	2524	2535	rVB2	228439	520547	24.48%	2.800%

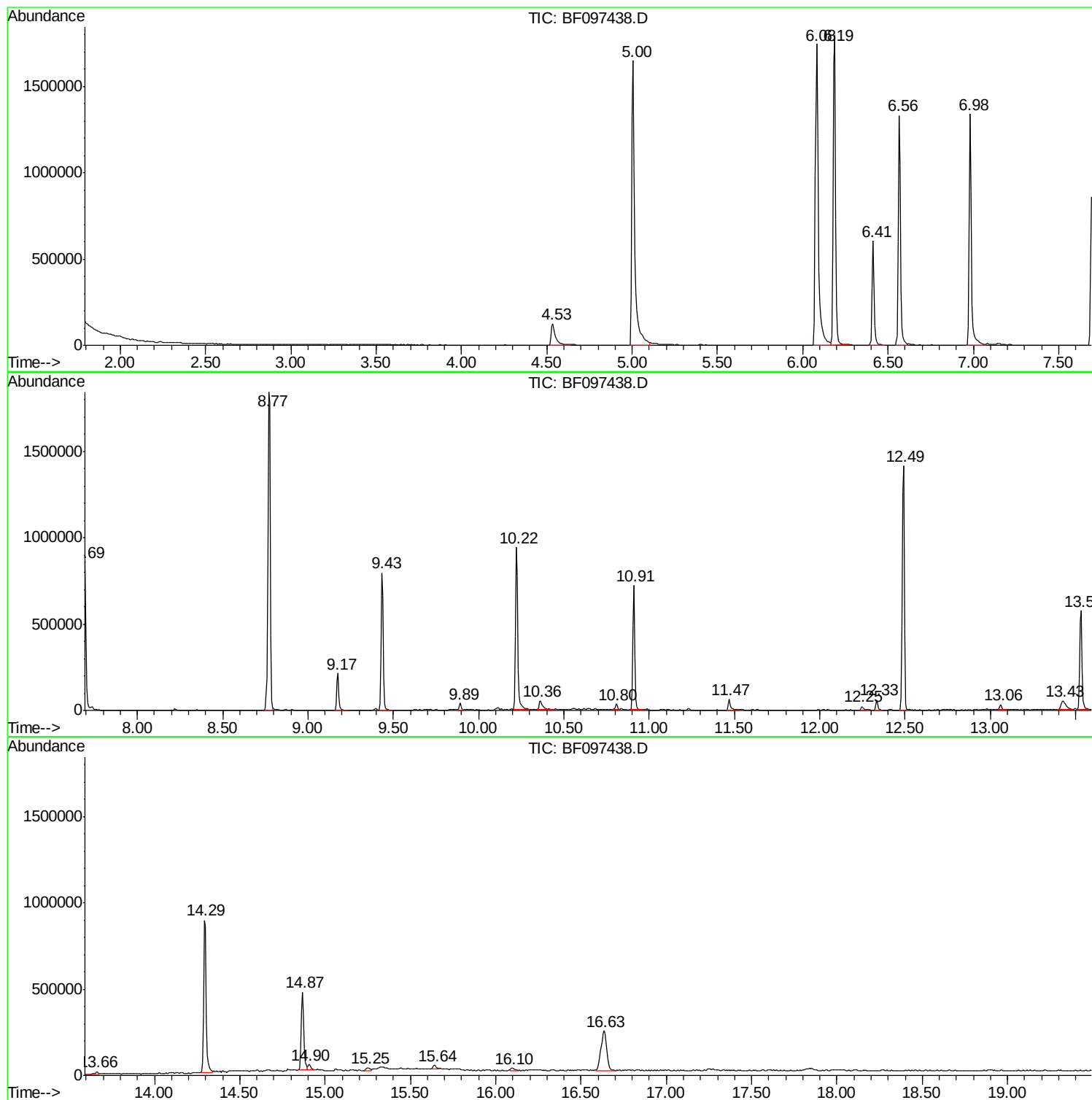
Sum of corrected areas: 18588630

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

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\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

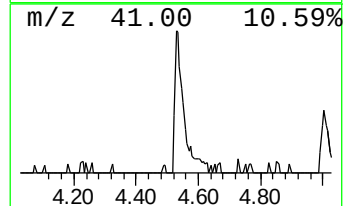
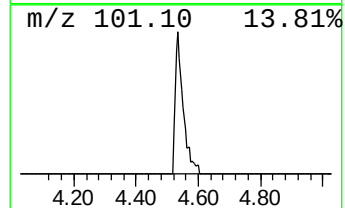
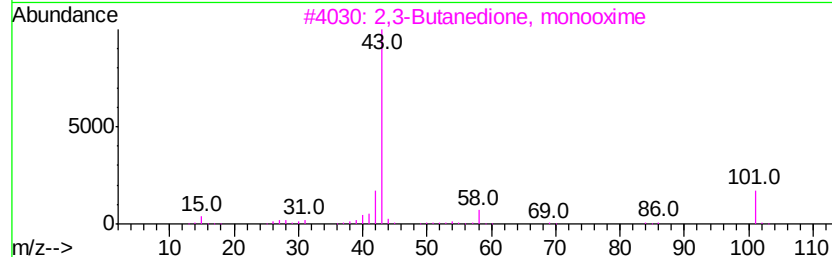
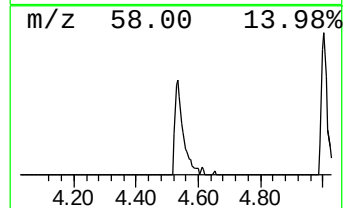
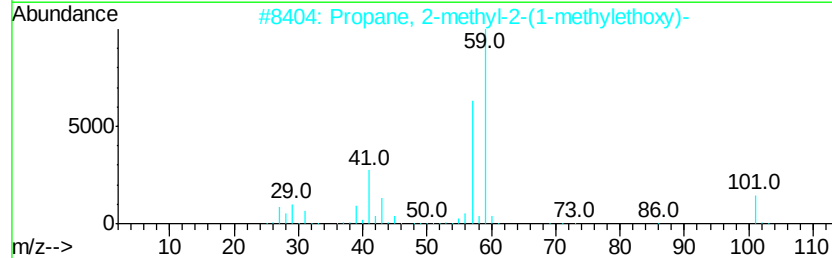
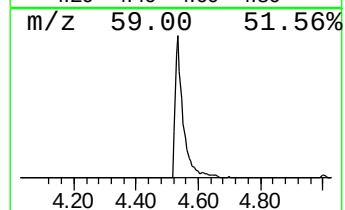
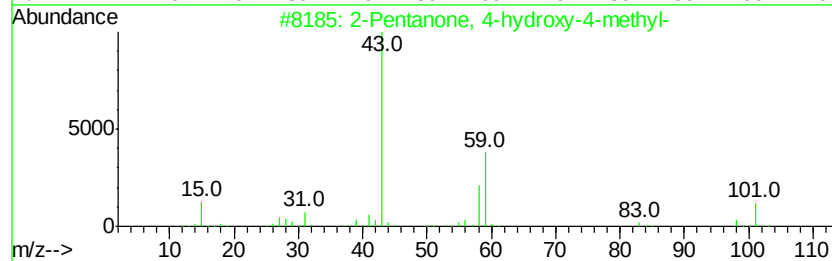
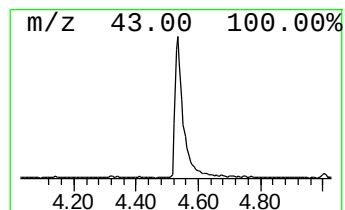
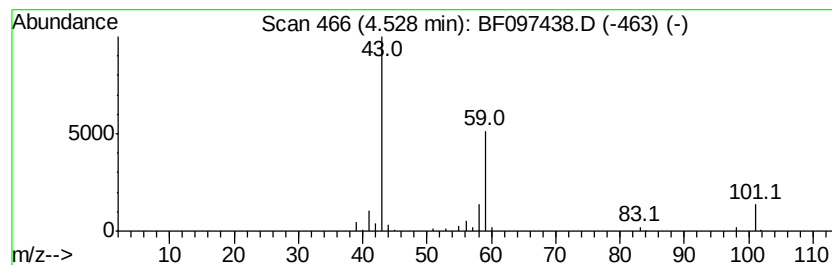
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	8.41 ng	227296	1,4-Dichlorobenzene-d4	6.41

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	36	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	Diacetamide	101	C4H7NO2	000625-77-4	9	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

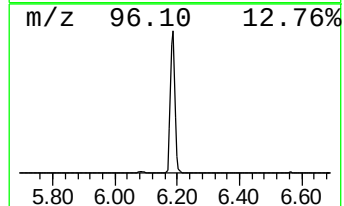
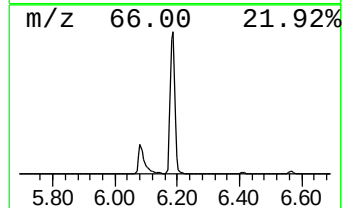
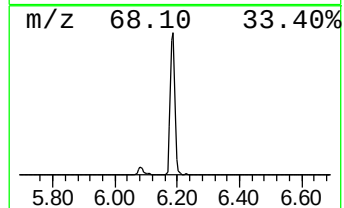
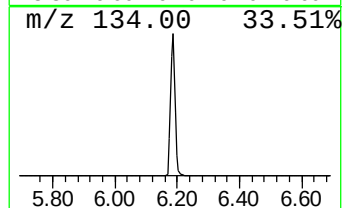
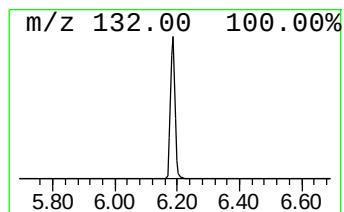
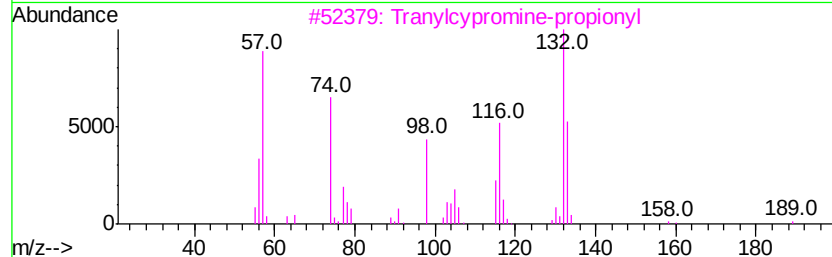
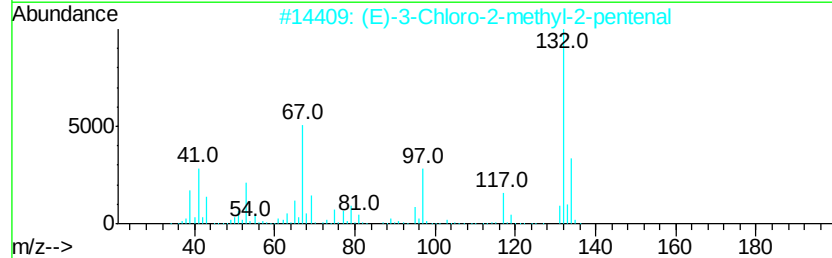
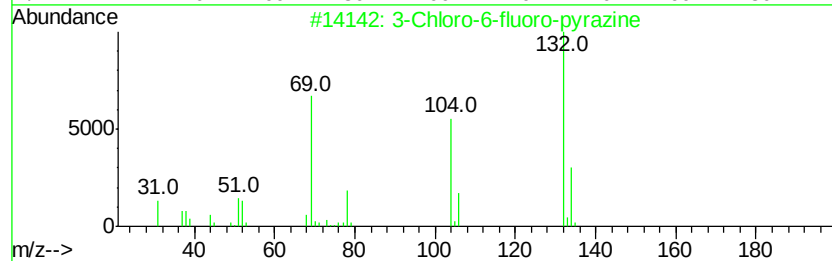
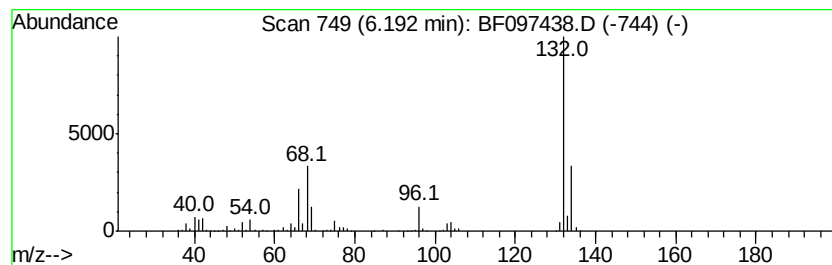
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	66.97 ng	1808870	1,4-Dichlorobenzene-d4	6.41

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
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\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

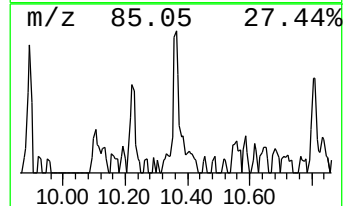
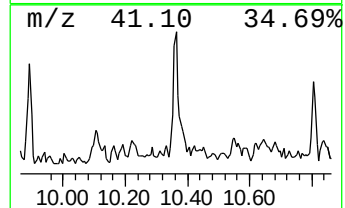
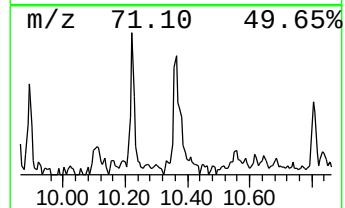
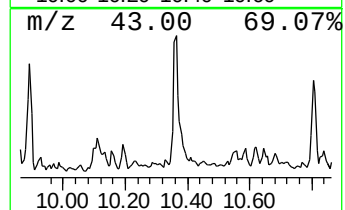
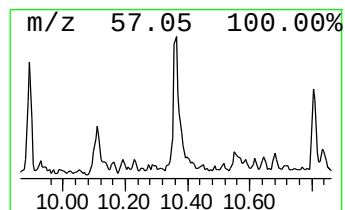
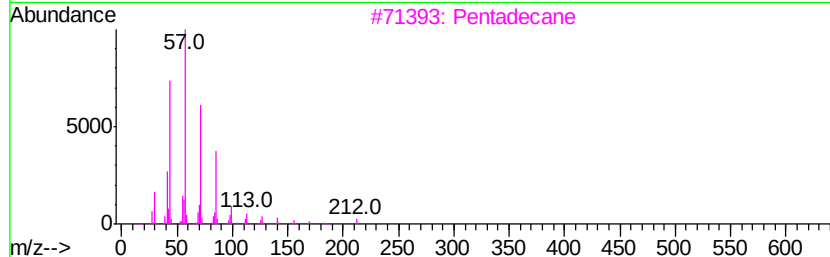
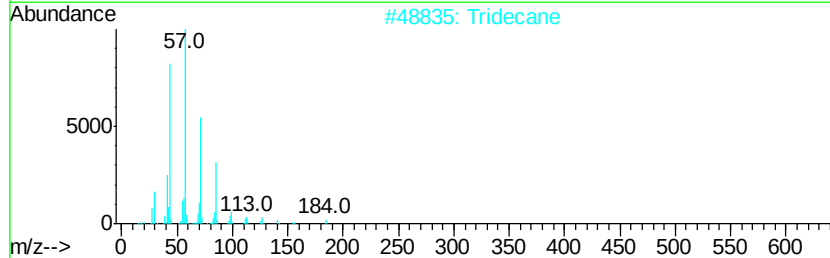
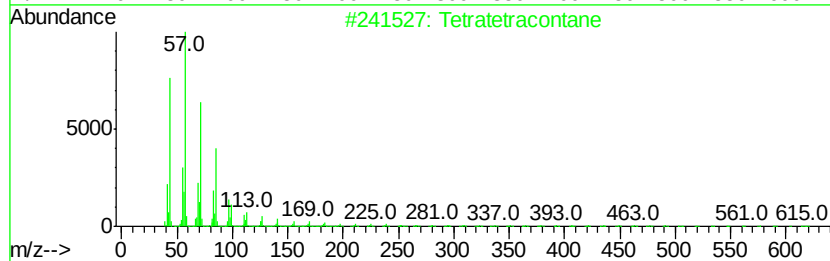
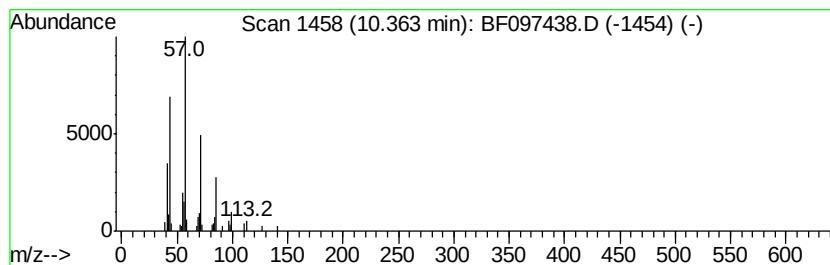
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	2.52 ng	77052	Phenanthrene-d10	10.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Tridecane	184	C13H28	000629-50-5	86
3		Pentadecane	212	C15H32	000629-62-9	86
4		Hexadecane	226	C16H34	000544-76-3	86
5		Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

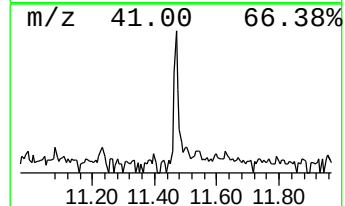
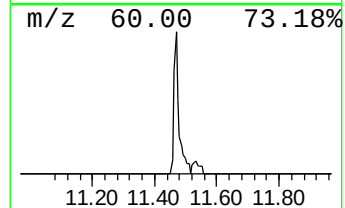
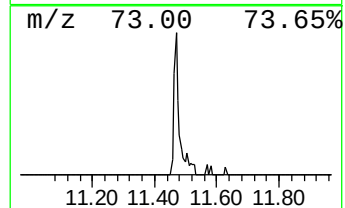
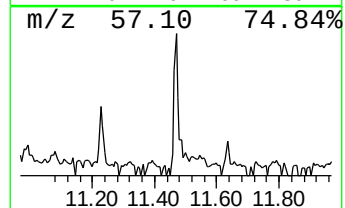
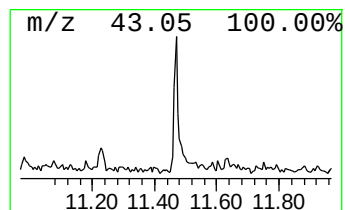
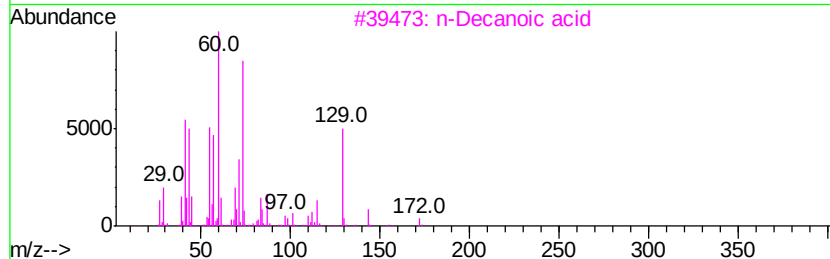
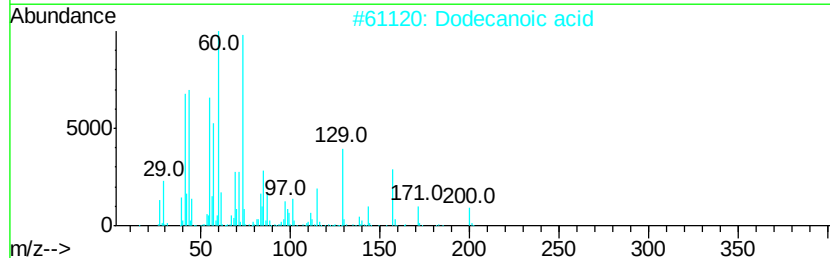
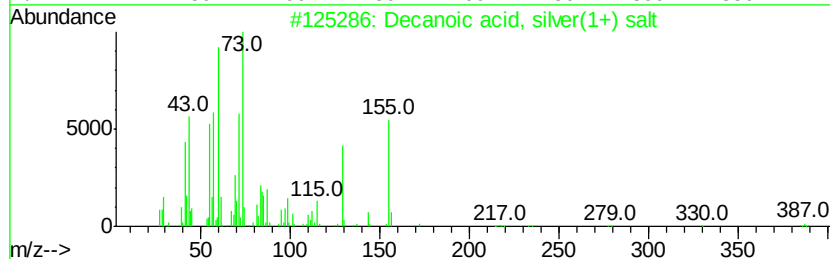
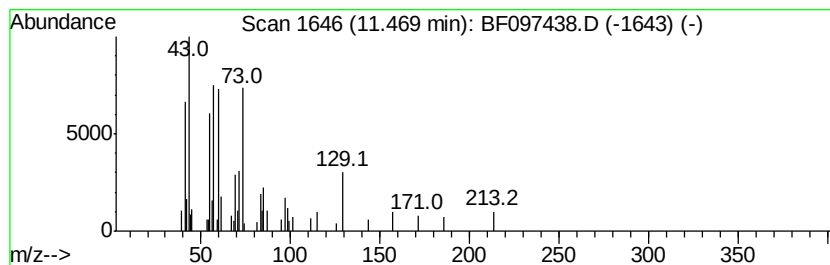
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.16 ng	66009	Phenanthrene-d10	10.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
2		Dodecanoic acid	200	C12H24O2	000143-07-7	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	58
4		Nonanoic acid	158	C9H18O2	000112-05-0	47
5		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

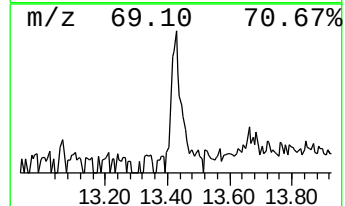
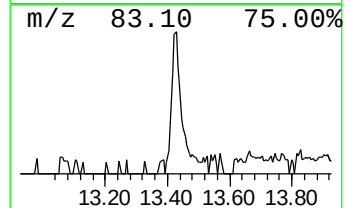
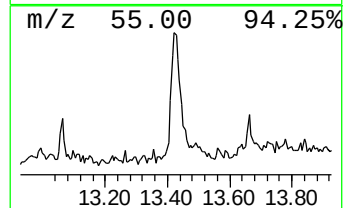
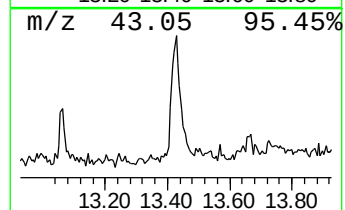
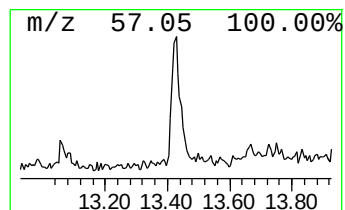
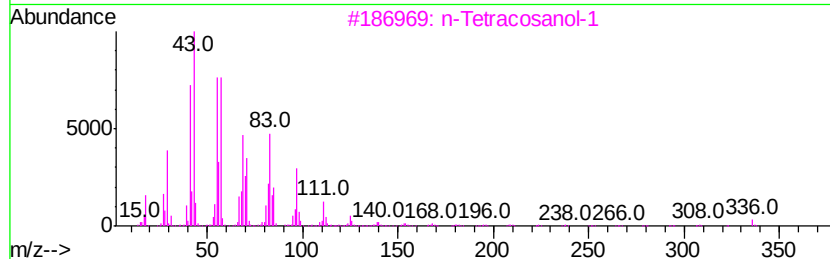
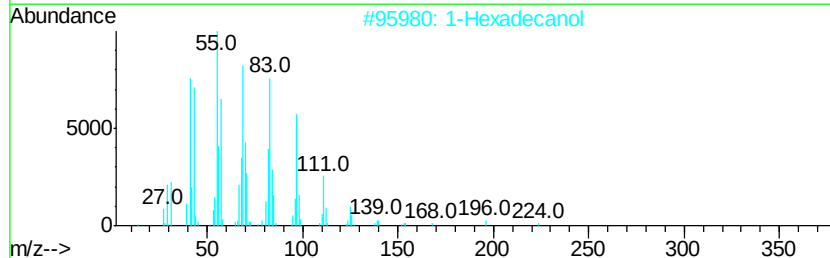
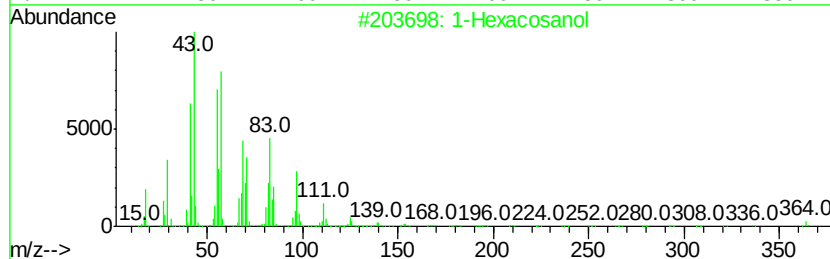
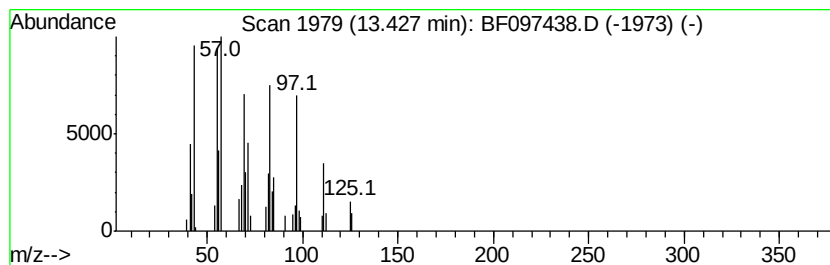
Instrument :
BNA_F
ClientSampleId :
TEC-BN

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 1-Hexacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.43	3.89 ng	107922	Chrysene-d12	13.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	87
2	1-Hexadecanol	242	C16H34O	036653-82-4	76
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	58
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

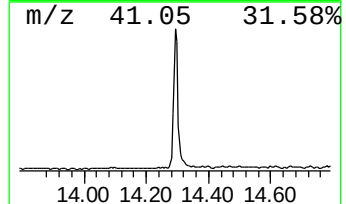
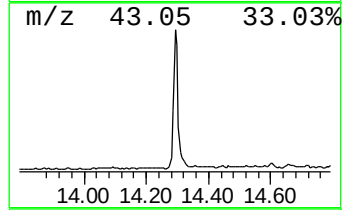
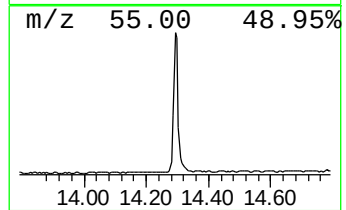
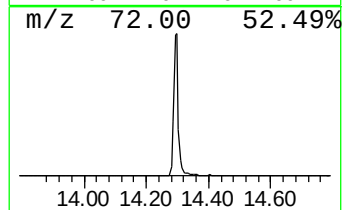
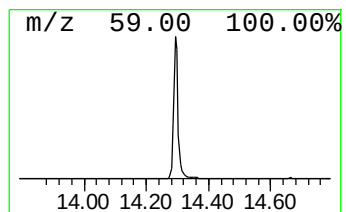
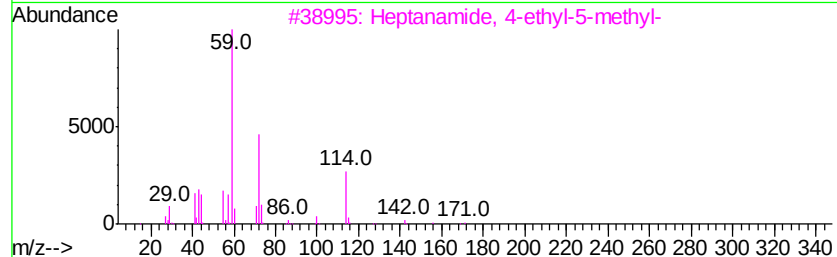
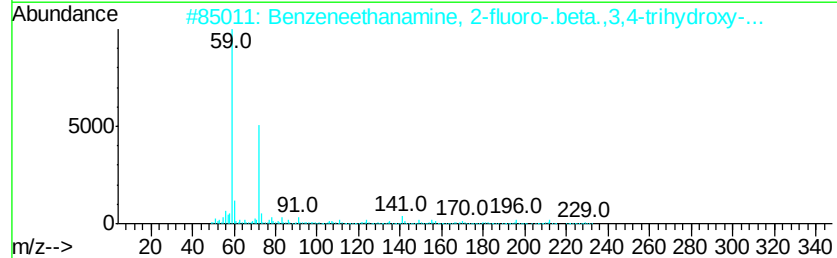
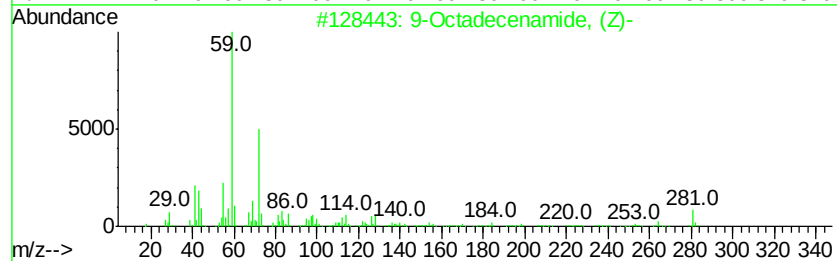
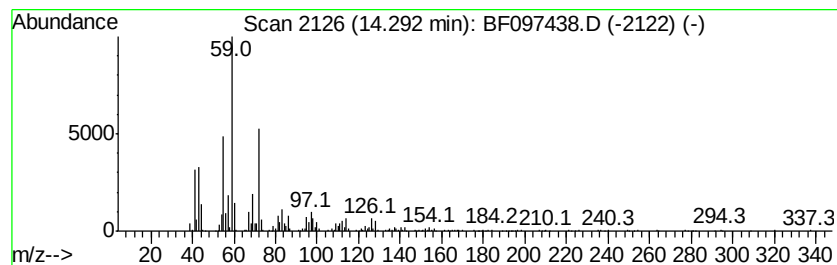
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	37.65 ng	948778	Perylene-d12	14.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		Octanamide	143	C8H17NO	000629-01-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

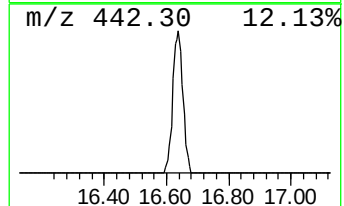
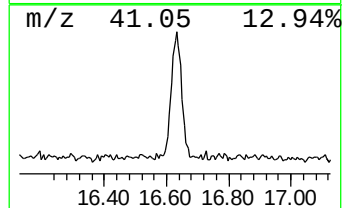
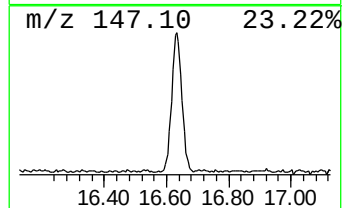
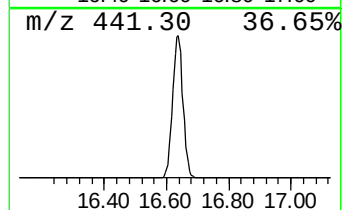
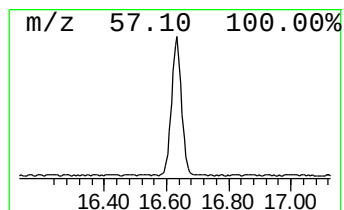
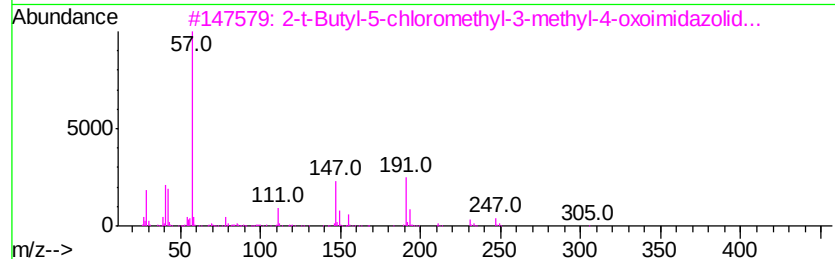
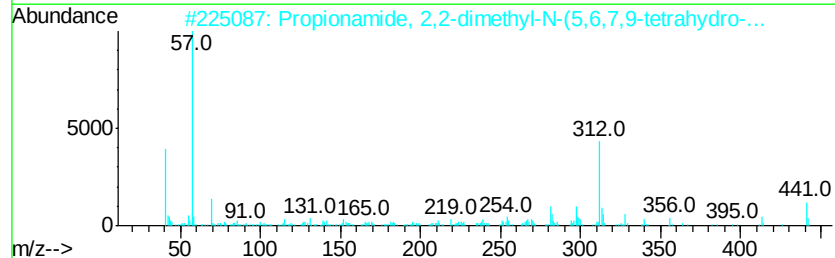
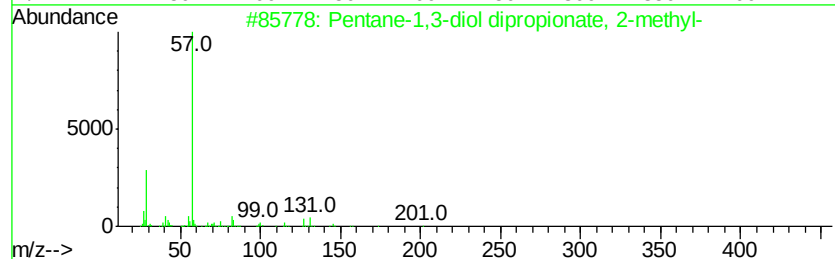
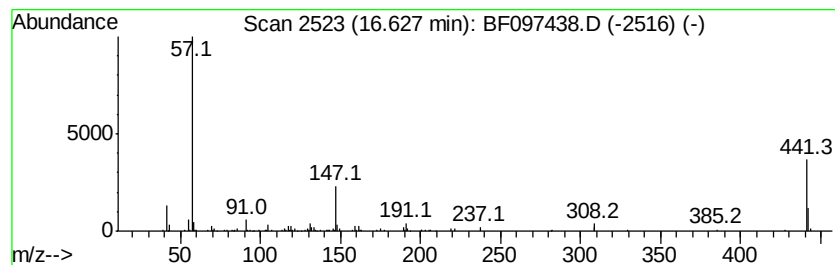
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	20.66 ng	520547	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane-1,3-diol dipropionate, 2...	230	C12H22O4	343318-72-9	7
2		Propionamide, 2,2-dimethyl-N-(5,...	441	C25H31NO6	086436-38-6	4
3		2-t-Butyl-5-chloromethyl-3-methyl...	304	C14H25ClN2O3	1000192-88-5	4
4		1H-Pyrrole-1-carboxylic acid, 2-...	245	C9H12BrN2O2	117657-37-1	4
5		Cyclohexyldienemalononitrile, 4'...	202	C13H18N2	035704-28-0	4



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080717\
Data File : BF097438.D
Acq On : 7 Aug 2017 19:27
Operator : SJ/JU
Sample : I4623-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-BN

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...	4.53	8.4	ng	227296	1	6.41	540226	20.0
unknown6.19	6.19	67.0	ng	1808870	1	6.41	540226	20.0
Tetratetracontane	10.36	2.5	ng	77052	4	10.91	612126	20.0
Decanoic acid, si...	11.47	2.2	ng	66009	4	10.91	612126	20.0
1-Hexacosanol	13.43	3.9	ng	107922	5	13.53	554842	20.0
9-Octadecenamide, ...	14.29	37.6	ng	948778	6	14.87	504032	20.0
unknown16.63	16.63	20.7	ng	520547	6	14.87	504032	20.0