

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
 Data File : BF104764.D
 Acq On : 24 Apr 2018 18:47
 Operator : JU/SJ
 Sample : J2151-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-05-042318-D

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-BF040618.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	5.016	494	498	507	rVB	84182	106675	4.68%	0.480%
2	5.434	564	569	572	rBV	2042682	1991744	87.36%	8.958%
3	6.457	738	743	757	rBV	1999086	2061021	90.40%	9.270%
4	6.581	760	764	768	rBV	2360586	2151899	94.38%	9.679%
5	6.810	799	803	806	rBV	795865	670460	29.41%	3.016%
6	6.963	825	829	833	rBV	1911954	1694157	74.31%	7.620%
7	7.375	894	899	902	rBV	1392733	1246920	54.69%	5.608%
8	8.092	1018	1021	1027	rBV	1022710	871618	38.23%	3.920%
9	9.169	1200	1204	1207	rBV	2743023	2279999	100.00%	10.255%
10	9.239	1213	1216	1219	rVB	63592	52170	2.29%	0.235%
11	9.504	1258	1261	1264	rBV4	32888	41085	1.80%	0.185%
12	9.563	1267	1271	1278	rVB	219345	219191	9.61%	0.986%
13	9.769	1301	1306	1310	rVB	84684	77038	3.38%	0.346%
14	9.851	1316	1320	1324	rBV	1065208	899547	39.45%	4.046%
15	10.051	1352	1354	1358	rVB3	23769	26883	1.18%	0.121%
16	10.092	1358	1361	1365	rBV3	37545	35935	1.58%	0.162%
17	10.251	1384	1388	1389	rBV3	28785	34417	1.51%	0.155%
18	10.269	1389	1391	1394	rVB2	104417	86156	3.78%	0.388%
19	10.398	1410	1413	1418	rVB3	28432	35102	1.54%	0.158%
20	10.486	1425	1428	1436	rVB	39637	54919	2.41%	0.247%
21	10.645	1451	1455	1464	rBV	1384778	1282236	56.24%	5.767%
22	10.745	1469	1472	1482	rVB3	88914	142269	6.24%	0.640%
23	10.939	1502	1505	1509	rBV6	18083	30060	1.32%	0.135%
24	11.192	1545	1548	1551	rBV	48877	41091	1.80%	0.185%
25	11.222	1551	1553	1560	rVB2	39505	50703	2.22%	0.228%
26	11.339	1569	1573	1576	rBV	870936	821149	36.02%	3.693%
27	11.363	1576	1577	1583	rVV	180179	139605	6.12%	0.628%
28	11.416	1583	1586	1589	rVB	35984	29677	1.30%	0.133%
29	11.722	1635	1638	1642	rBV	255071	201081	8.82%	0.904%
30	11.869	1660	1663	1669	rVB3	34964	51208	2.25%	0.230%
31	11.957	1675	1678	1680	rBV2	36312	39553	1.73%	0.178%
32	12.027	1688	1690	1696	rBV3	27628	30342	1.33%	0.136%
33	12.410	1749	1755	1757	rBV2	554315	523999	22.98%	2.357%
34	12.433	1757	1759	1765	rVB	542365	481821	21.13%	2.167%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.516	1770	1773	1777	rVB	125032	107750	4.73%	0.485%
36	12.557	1777	1780	1783	rBV	204065	174335	7.65%	0.784%
37	12.592	1783	1786	1792	rVB4	36253	45294	1.99%	0.204%
38	12.786	1814	1819	1825	rBV	193581	211515	9.28%	0.951%
39	12.927	1839	1843	1846	rBV	1874592	1645664	72.18%	7.402%
40	13.816	1991	1994	2002	rVB3	179210	188673	8.28%	0.849%
41	13.992	2019	2024	2026	rBV2	674454	713176	31.28%	3.208%
42	14.016	2026	2028	2034	rVB	113282	110069	4.83%	0.495%
43	15.468	2271	2275	2284	rVB	396552	535506	23.49%	2.409%

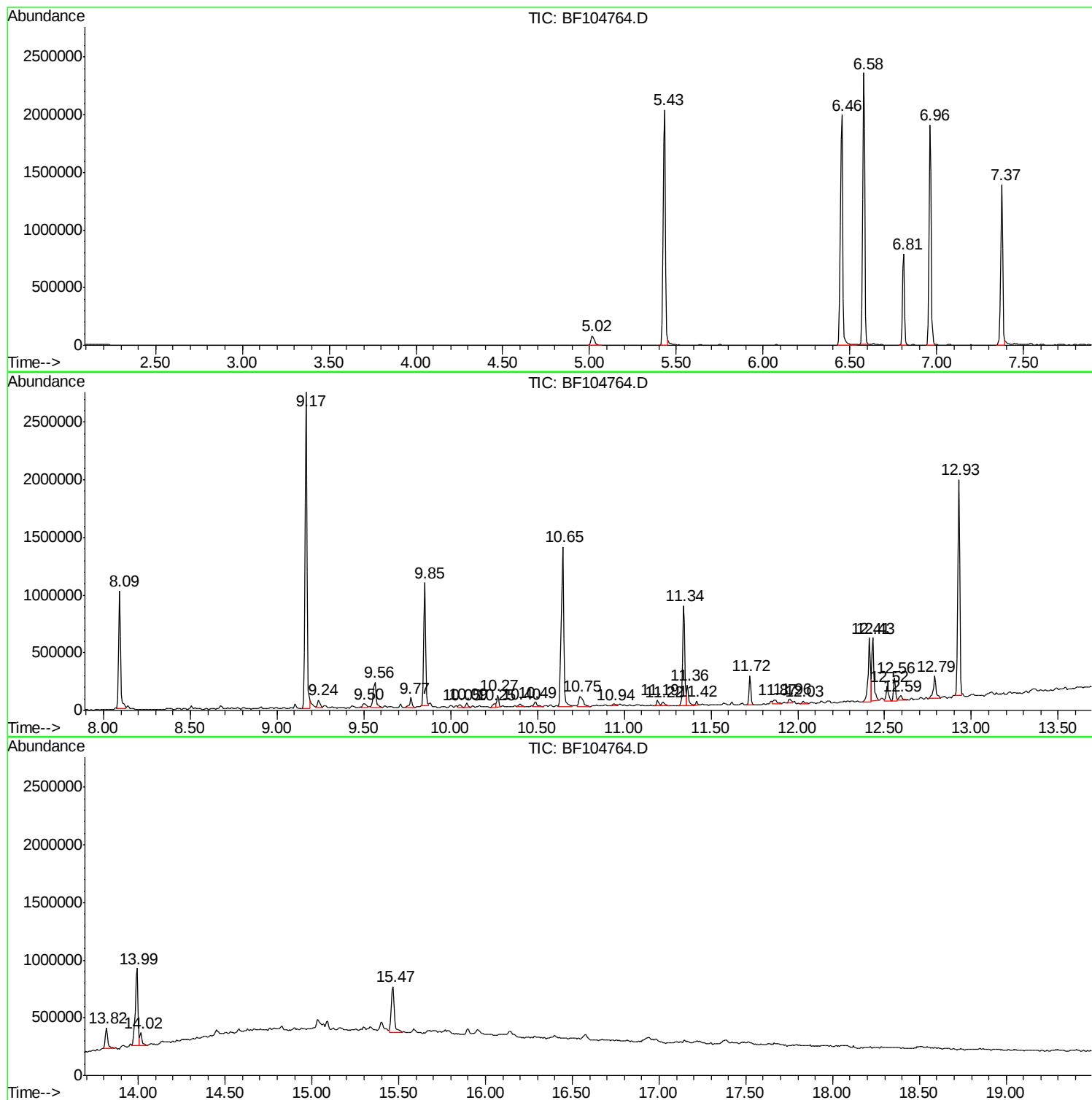
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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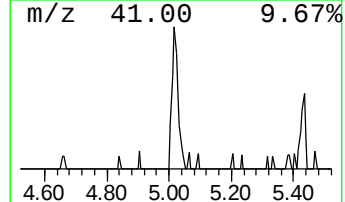
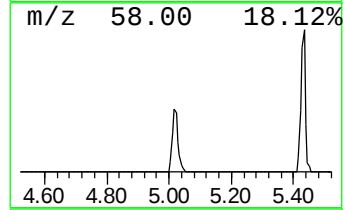
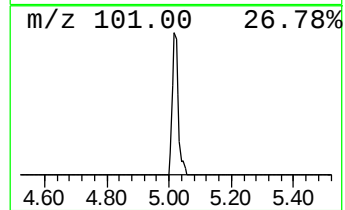
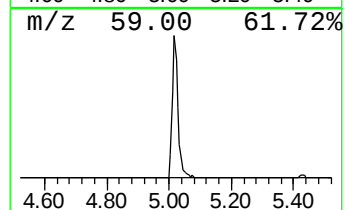
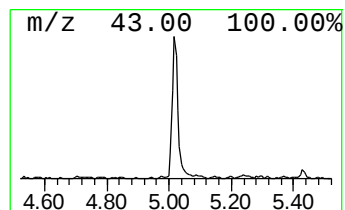
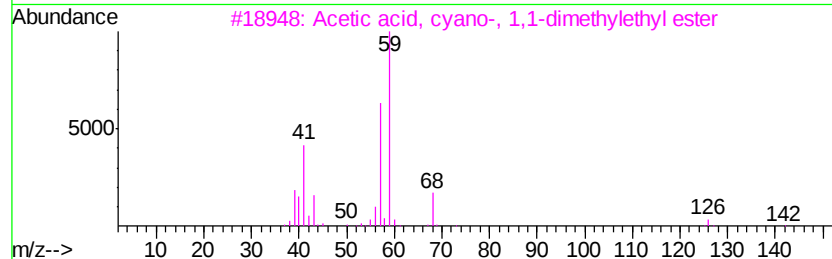
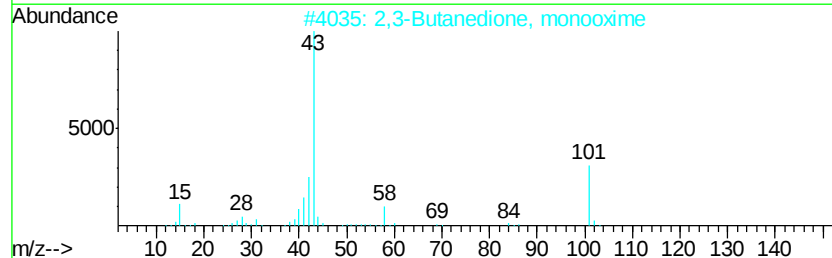
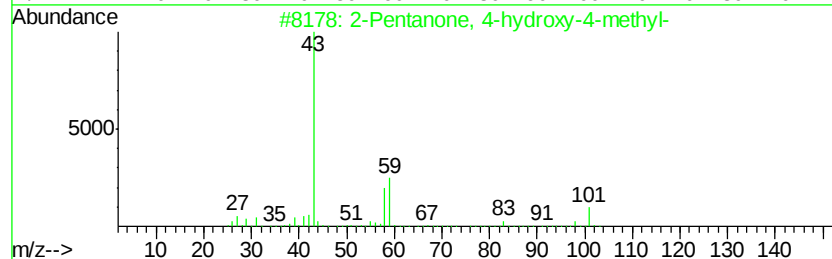
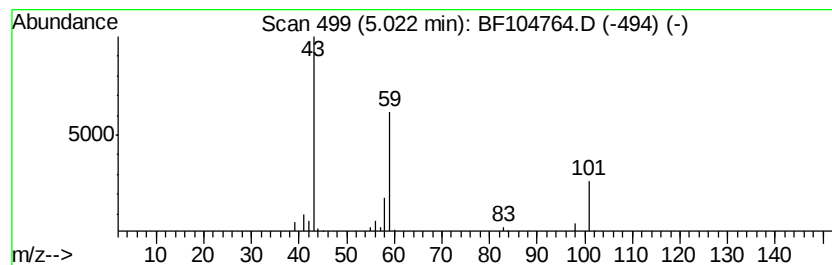
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.18 ng	106675	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Acetone	58	C3H6O	000067-64-1	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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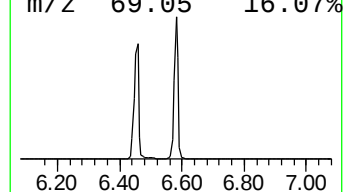
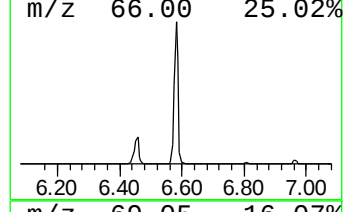
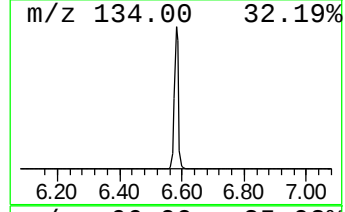
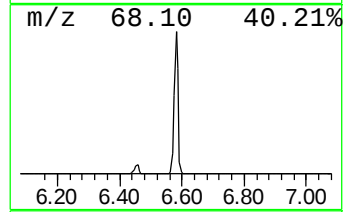
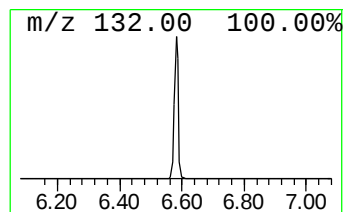
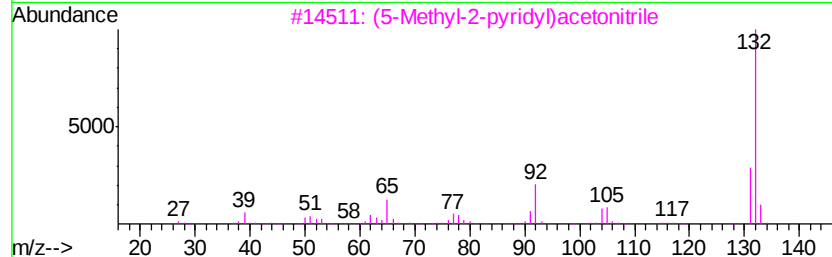
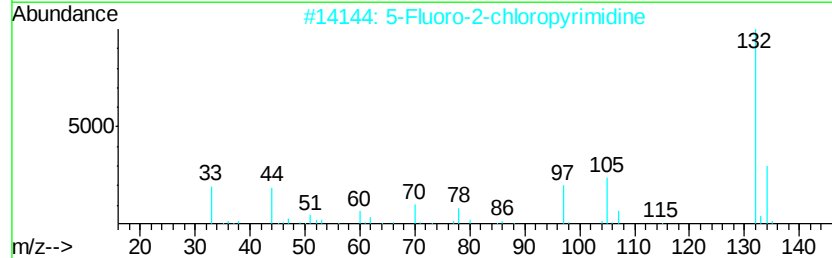
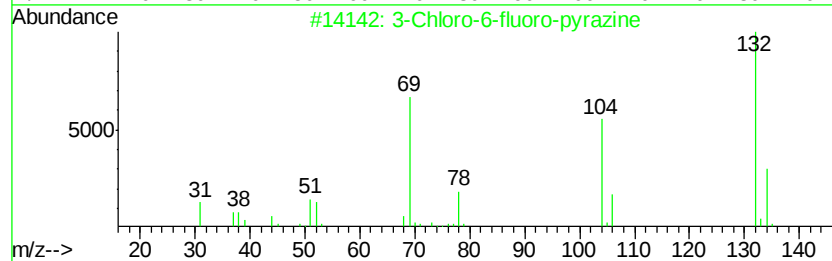
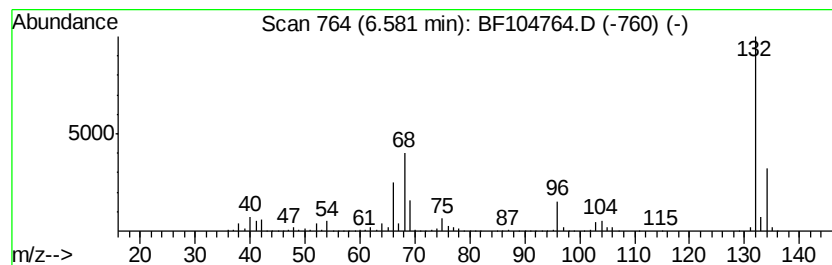
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	64.19 ng	2151900	1,4-Dichlorobenzene-d4	6.81

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	9
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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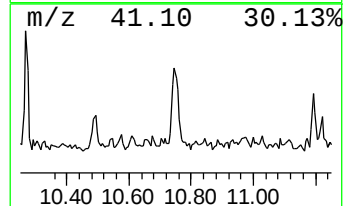
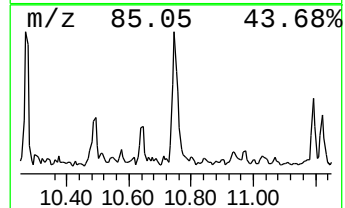
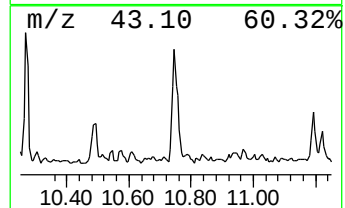
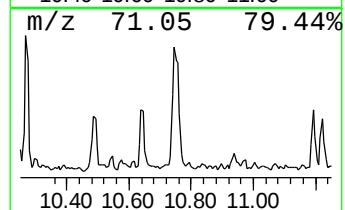
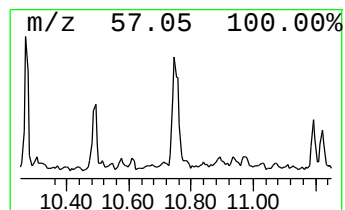
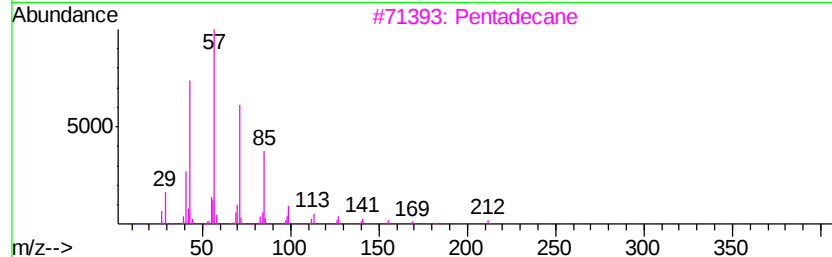
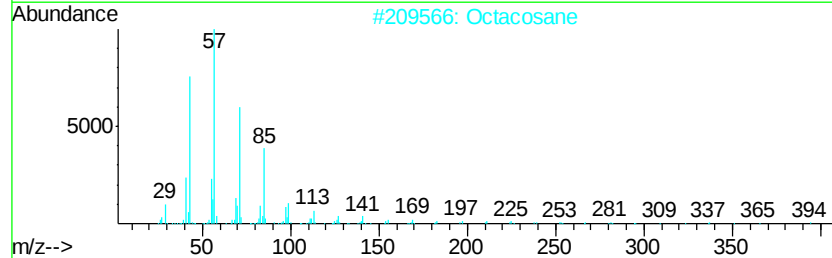
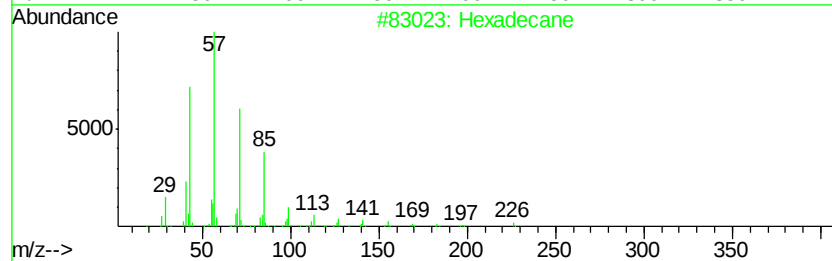
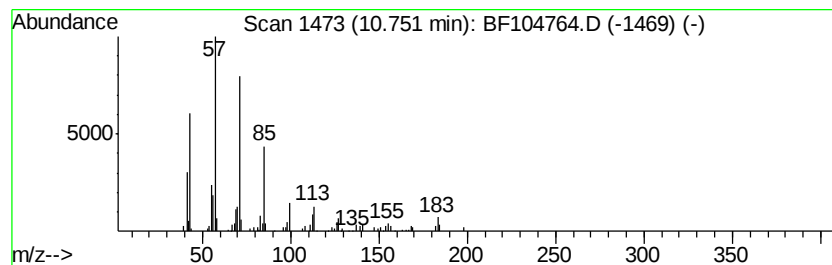
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	3.47 ng	142269	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Octacosane		394	C28H58	000630-02-4	87
3	Pentadecane		212	C15H32	000629-62-9	86
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
5	Heptacosane		380	C27H56	000593-49-7	80



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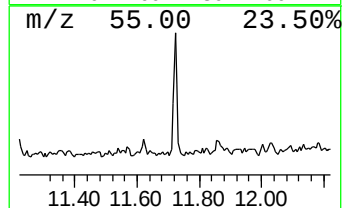
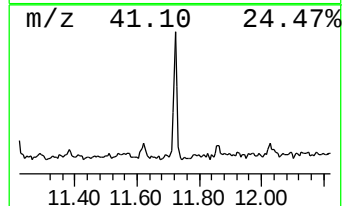
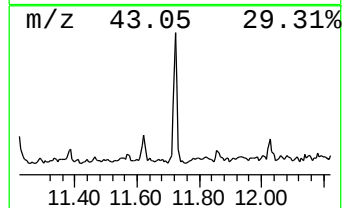
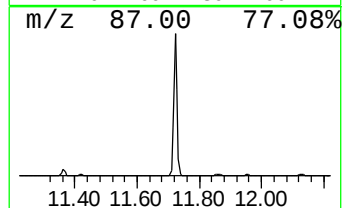
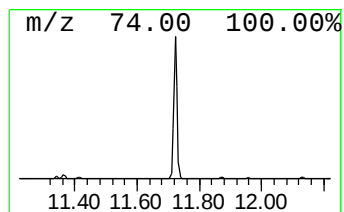
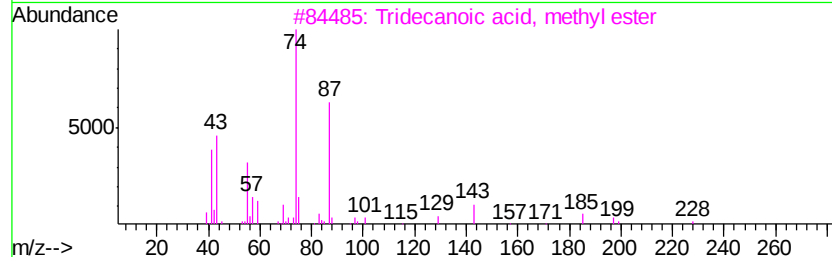
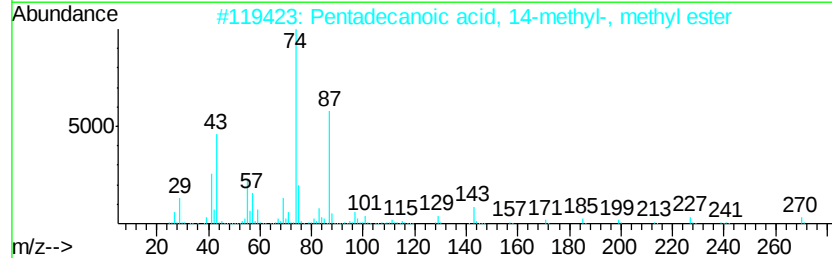
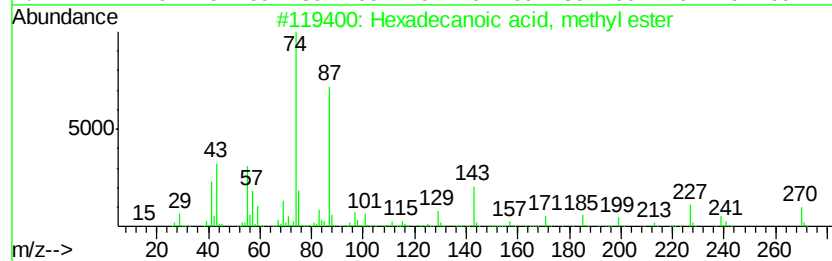
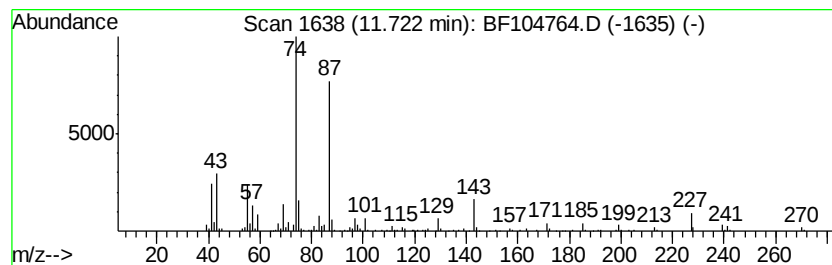
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	4.90 ng	201081	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	86



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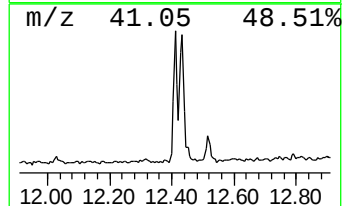
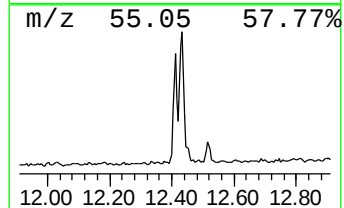
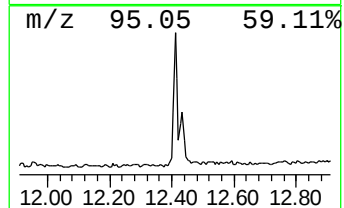
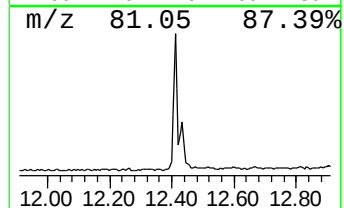
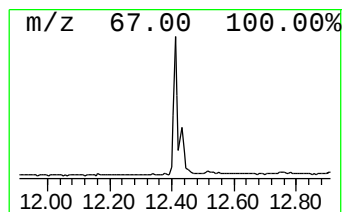
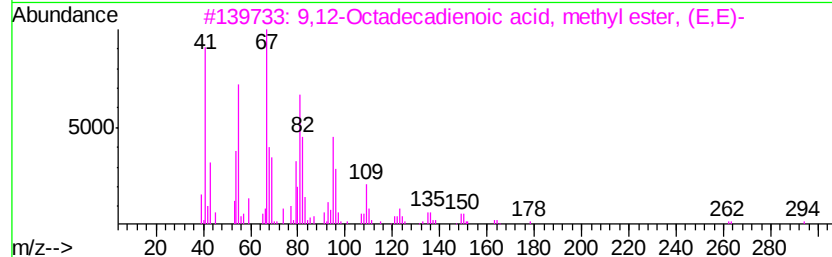
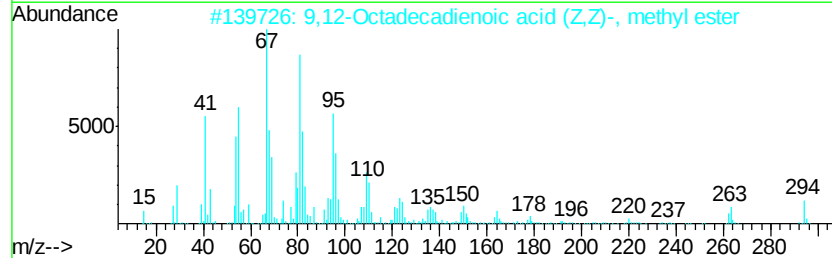
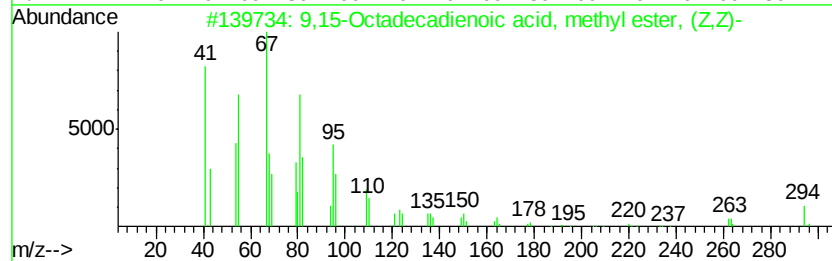
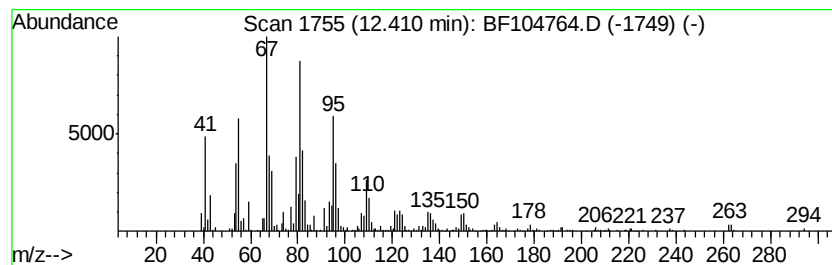
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,15-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	12.76 ng	523999	Phenanthrene-d10	11.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
4			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104764.D
Acq On : 24 Apr 2018 18:47
Operator : JU/SJ
Sample : J2151-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-042318-D

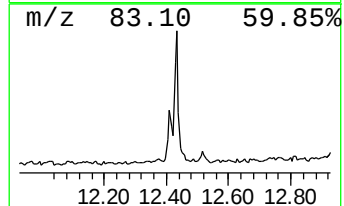
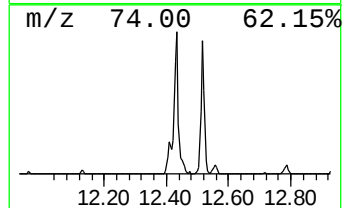
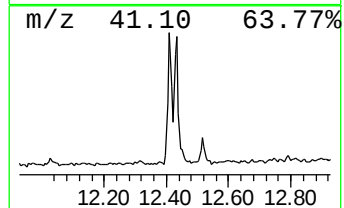
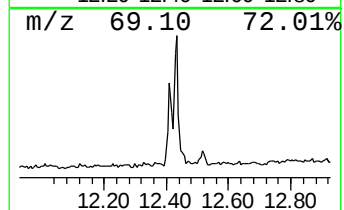
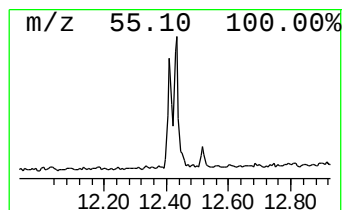
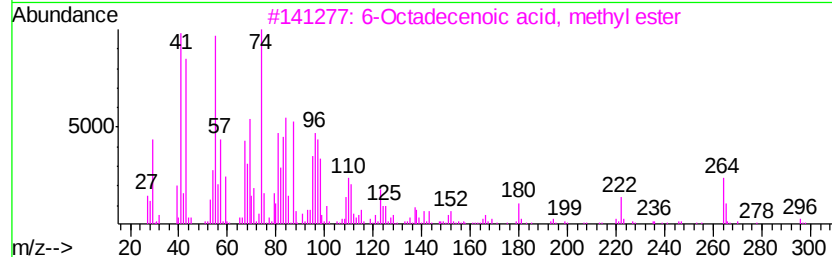
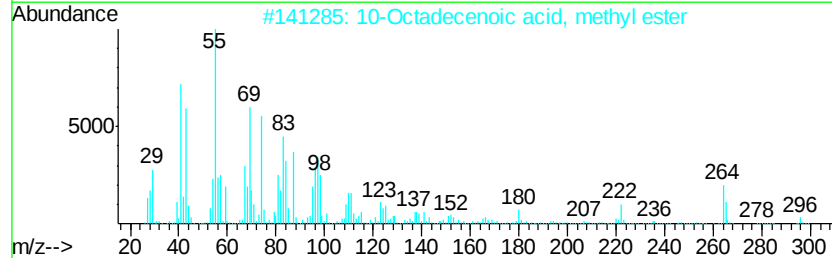
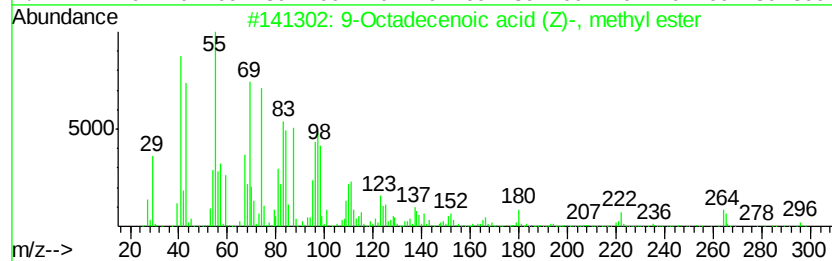
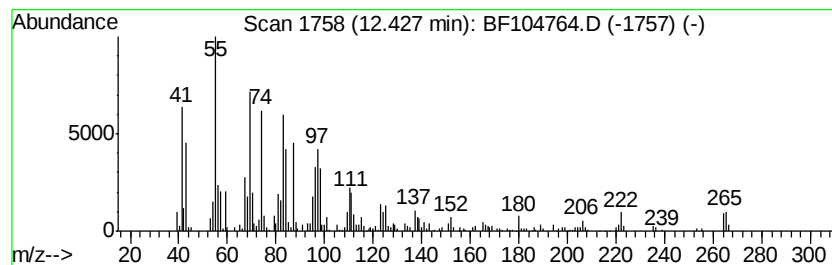
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	11.74 ng	481821	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
4		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
5		6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	98



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042418\
Data File : BF104764.D
Acq On : 24 Apr 2018 18:47
Operator : JU/SJ
Sample : J2151-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-042318-D

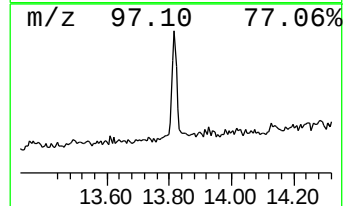
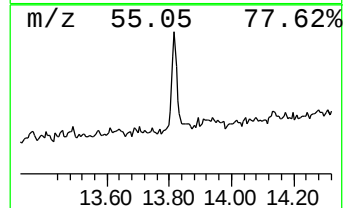
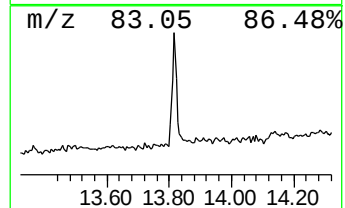
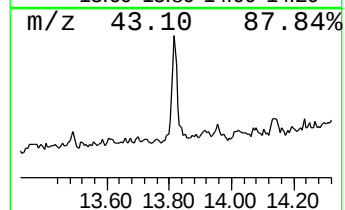
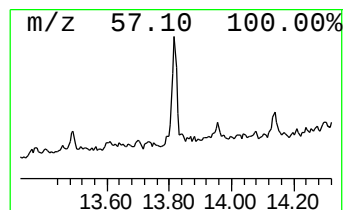
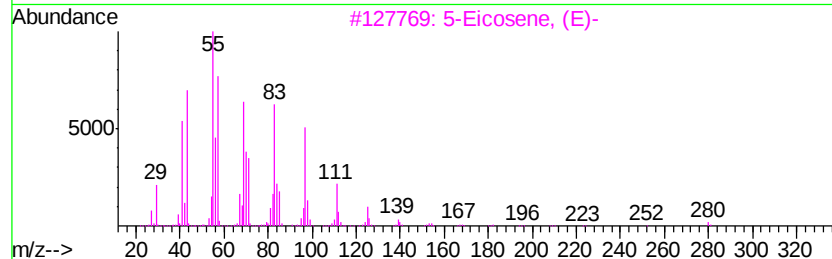
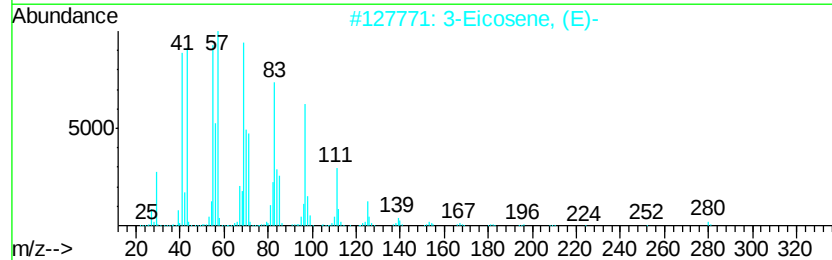
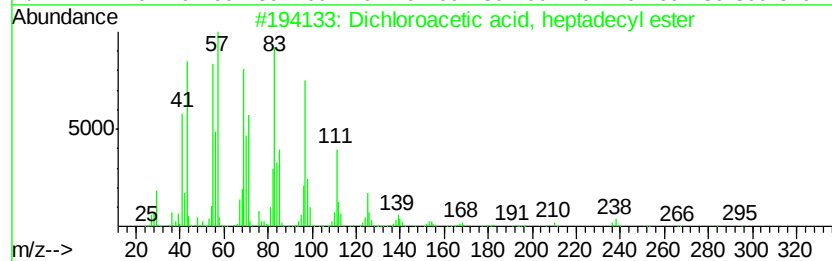
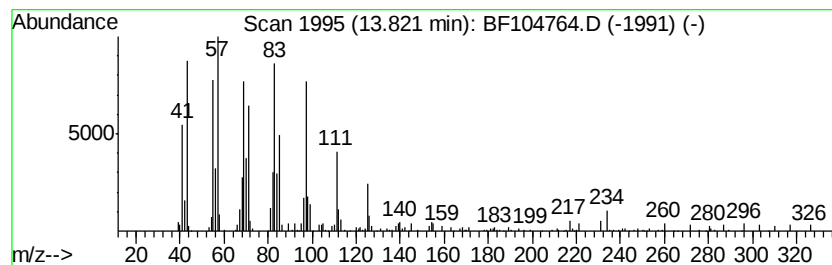
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.29 ng	188673	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	93
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	92
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042418\
Data File : BF104764.D
Acq On : 24 Apr 2018 18:47
Operator : JU/SJ
Sample : J2151-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-042318-D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.2	ng	106675	1	6.81	670460	20.0
unknown6.58	6.58	64.2	ng	2151900	1	6.81	670460	20.0
Hexadecane	10.75	3.5	ng	142269	4	11.34	821149	20.0
Hexadecanoic acid...	11.72	4.9	ng	201081	4	11.34	821149	20.0
9,15-Octadecadien...	12.41	12.8	ng	523999	4	11.34	821149	20.0
9-Octadecenoic ac...	12.43	11.7	ng	481821	4	11.34	821149	20.0
Dichloroacetic ac...	13.82	5.3	ng	188673	5	13.99	713176	20.0