

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
 Data File : BF108094.D
 Acq On : 10 Aug 2018 19:55
 Operator : JU/SJ
 Sample : J4272-11 2X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-03-080918-F

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	5.248	491	495	503	rVB	572772	556937	18.01%	1.435%
2	5.637	557	561	564	rBV	3292614	2821211	91.24%	7.267%
3	6.631	725	730	733	rBV	3305392	3092120	100.00%	7.965%
4	6.784	752	756	760	rBV	3569743	3026925	97.89%	7.797%
5	7.019	792	796	799	rBV	2091605	1639512	53.02%	4.223%
6	7.172	818	822	826	rBV	2517151	2195862	71.01%	5.656%
7	7.578	886	891	894	rBV	2152426	1863068	60.25%	4.799%
8	8.301	1010	1014	1017	rBV	2473703	1995435	64.53%	5.140%
9	9.378	1192	1197	1200	rBV	3399796	2988690	96.66%	7.698%
10	9.442	1205	1208	1212	rVB	51042	48440	1.57%	0.125%
11	9.631	1238	1240	1244	rBV2	46877	40169	1.30%	0.103%
12	9.766	1259	1263	1268	rBV	271326	231470	7.49%	0.596%
13	9.978	1294	1299	1302	rBV	84735	74890	2.42%	0.193%
14	10.066	1310	1314	1318	rBV2	2261473	1944273	62.88%	5.008%
15	10.301	1351	1354	1358	rBV3	30085	35647	1.15%	0.092%
16	10.383	1365	1368	1370	rBV4	26300	34902	1.13%	0.090%
17	10.478	1380	1384	1387	rVB	118905	103423	3.34%	0.266%
18	10.701	1417	1422	1424	rBV	68957	80800	2.61%	0.208%
19	10.854	1445	1448	1458	rBV	1657855	1603358	51.85%	4.130%
20	10.954	1462	1465	1475	rVB	153153	215502	6.97%	0.555%
21	11.407	1539	1542	1544	rBV	134203	117312	3.79%	0.302%
22	11.436	1544	1547	1549	rVB2	66224	67815	2.19%	0.175%
23	11.566	1565	1569	1571	rBV	1918264	1754623	56.74%	4.520%
24	11.589	1571	1573	1576	rVB	296453	237295	7.67%	0.611%
25	11.636	1579	1581	1586	rVB	70533	62234	2.01%	0.160%
26	11.789	1604	1607	1609	rBV	46737	44556	1.44%	0.115%
27	11.830	1612	1614	1617	rVB	119642	104277	3.37%	0.269%
28	11.936	1628	1632	1635	rVB	660948	520799	16.84%	1.341%
29	12.066	1651	1654	1657	rBV	142961	134934	4.36%	0.348%
30	12.095	1657	1659	1663	rVB2	80297	70026	2.26%	0.180%
31	12.183	1670	1674	1676	rBV2	71433	84557	2.73%	0.218%
32	12.242	1681	1684	1687	rBV	126754	102017	3.30%	0.263%
33	12.624	1746	1749	1751	rBV	1800682	1710772	55.33%	4.407%
34	12.648	1751	1753	1760	rVB	2080721	1761276	56.96%	4.537%

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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 >
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35	12.730	1764	1767	1772	rVB	434325	356639	11.53%	0.919%
36	12.783	1772	1776	1780	rBV	660038	575486	18.61%	1.482%
37	12.971	1806	1808	1810	rBV2	52852	34705	1.12%	0.089%
38	13.019	1810	1816	1821	rVB	539427	635829	20.56%	1.638%
39	13.148	1835	1838	1842	rBV	2573534	2454173	79.37%	6.321%
40	13.571	1908	1910	1913	rBV2	108376	95790	3.10%	0.247%
41	14.218	2016	2020	2023	rBV2	1900418	1982264	64.11%	5.106%
42	14.248	2023	2025	2030	rVB	243675	248579	8.04%	0.640%
43	15.789	2283	2287	2291	rVB	838704	1074254	34.74%	2.767%

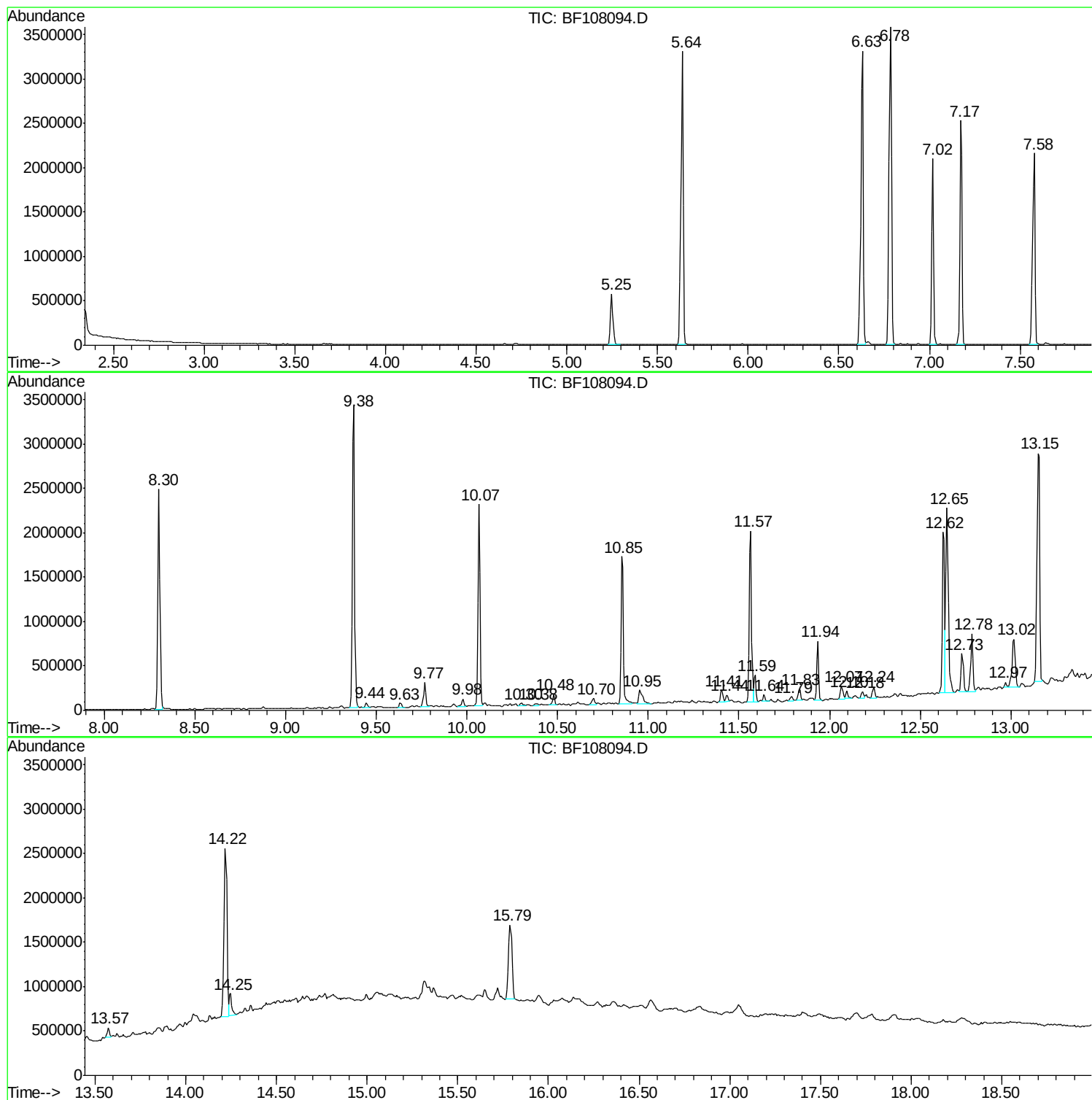
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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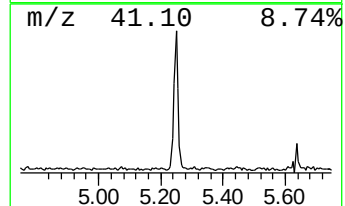
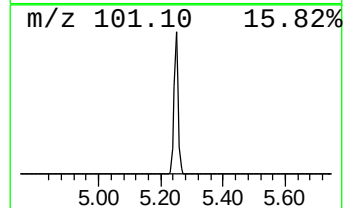
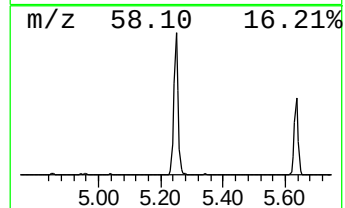
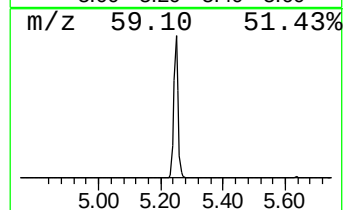
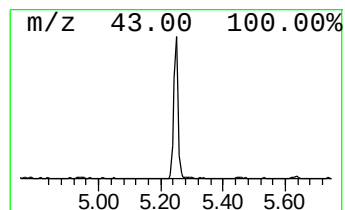
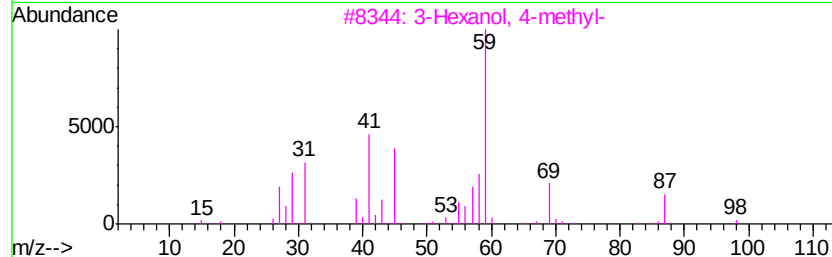
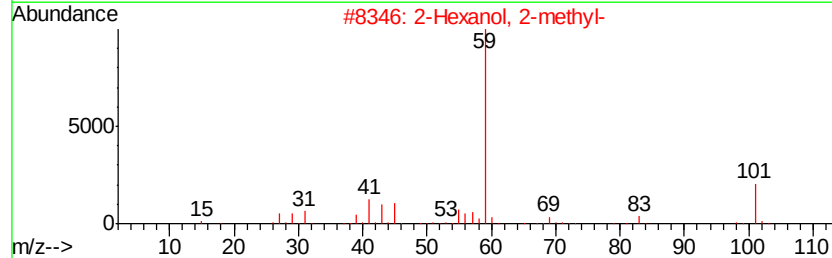
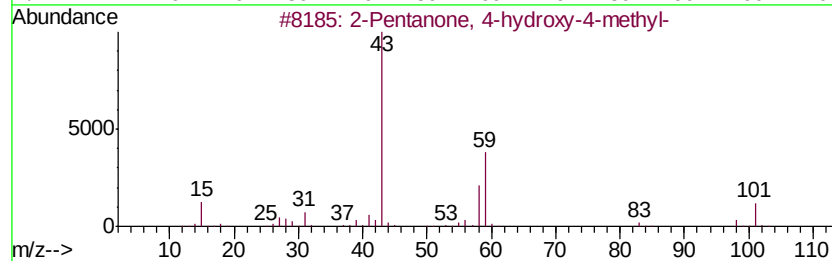
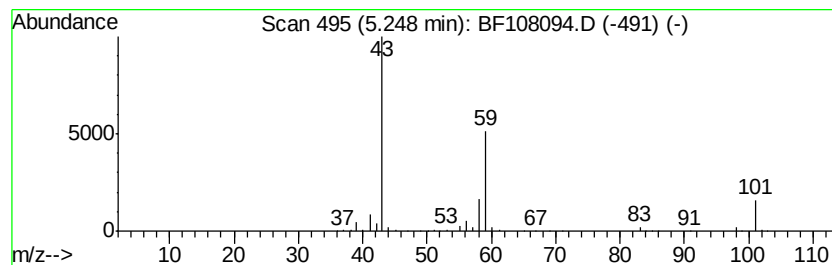
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	6.79 ng	556937	1,4-Dichlorobenzene-d4	7.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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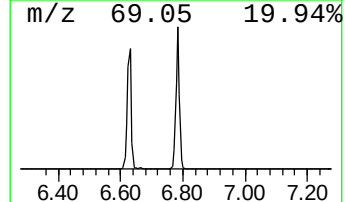
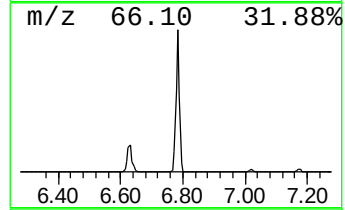
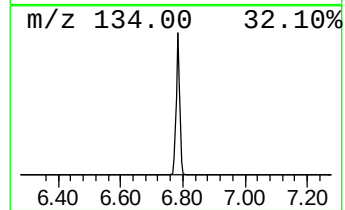
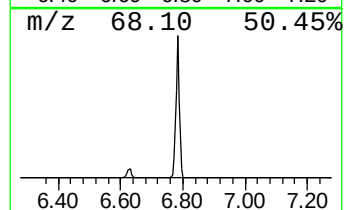
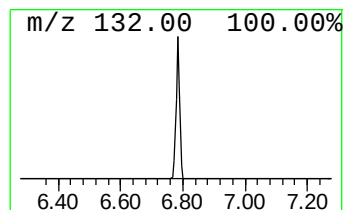
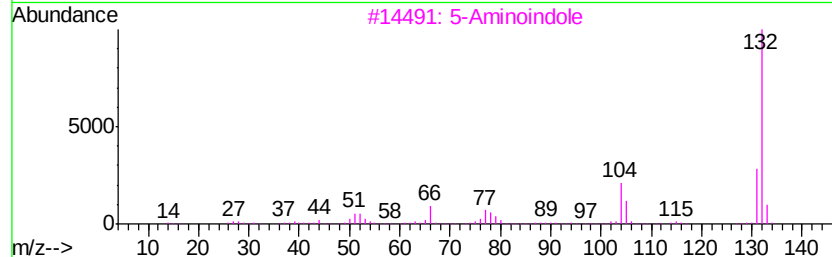
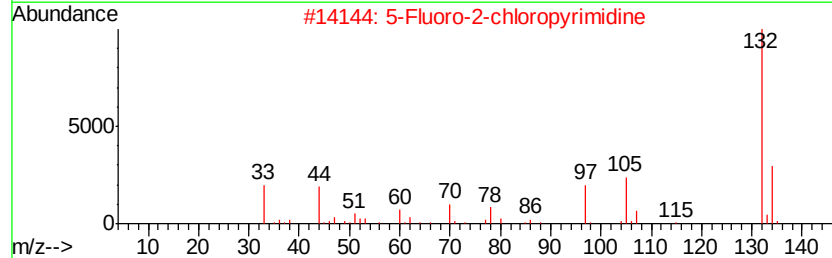
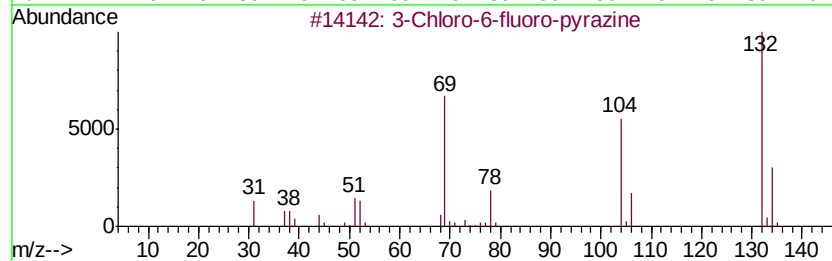
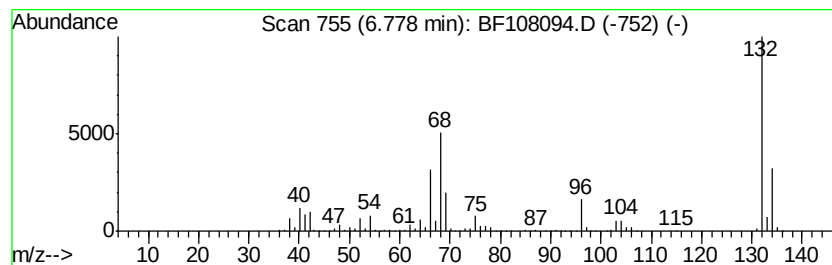
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Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	36.92 ng	3026930	1,4-Dichlorobenzene-d4	7.02

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9



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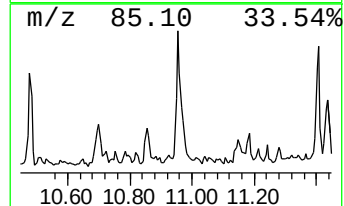
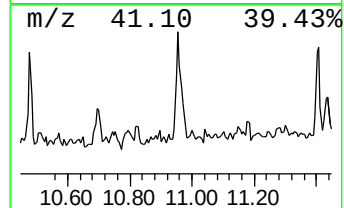
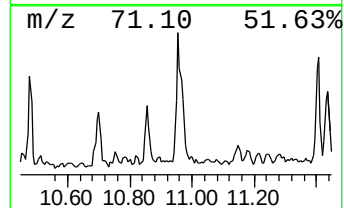
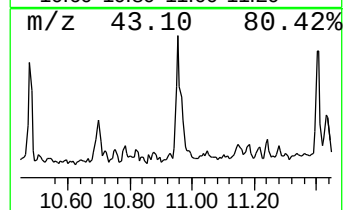
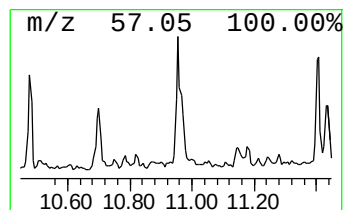
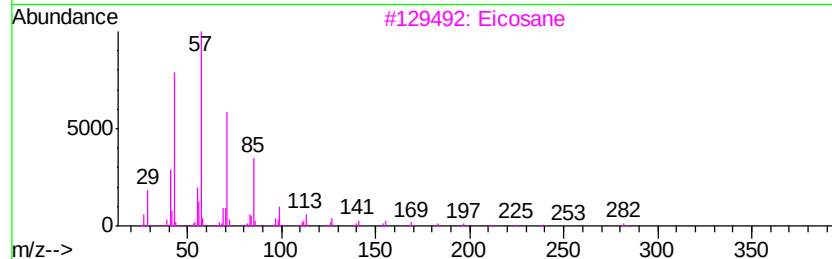
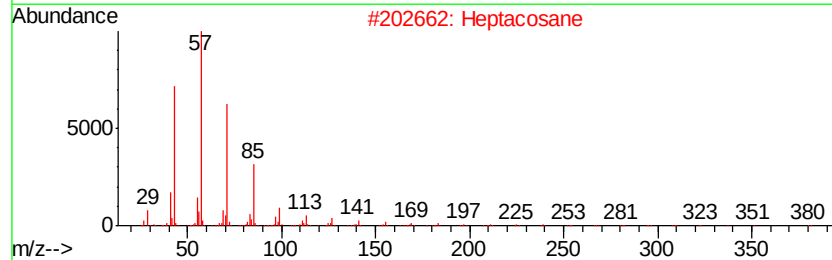
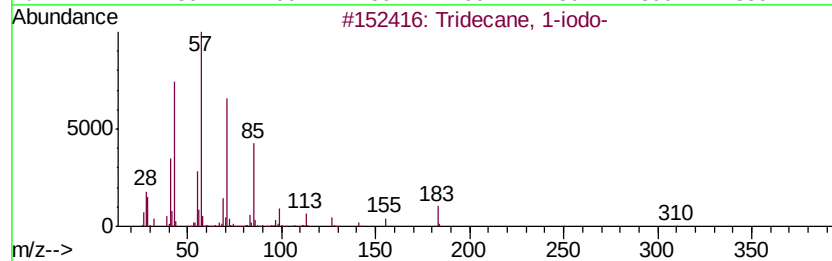
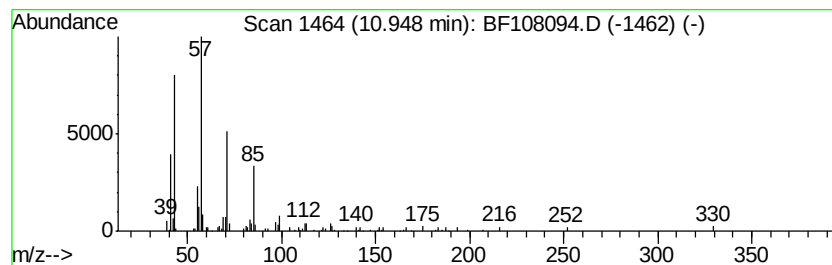
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.46 ng	215502	Phenanthrene-d10	11.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2		Heptacosane	380	C27H56	000593-49-7	90
3		Eicosane	282	C20H42	000112-95-8	83
4		Decane, 2-methyl-	156	C11H24	006975-98-0	83
5		Hexadecane	226	C16H34	000544-76-3	80



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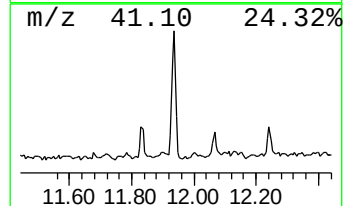
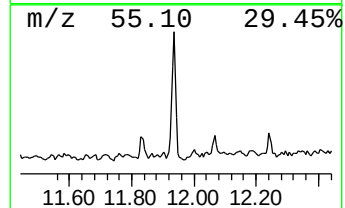
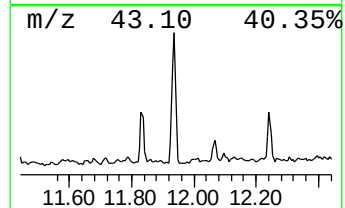
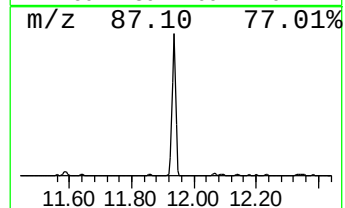
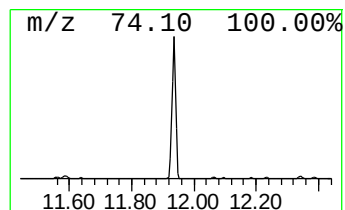
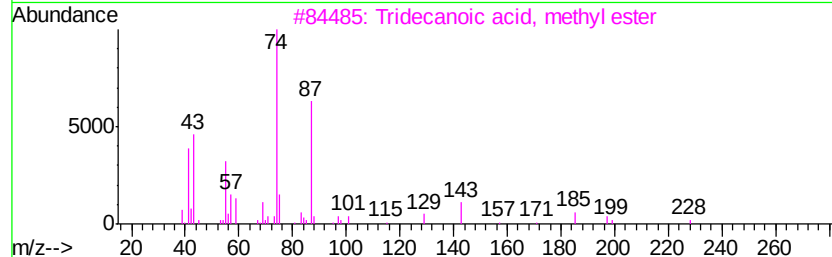
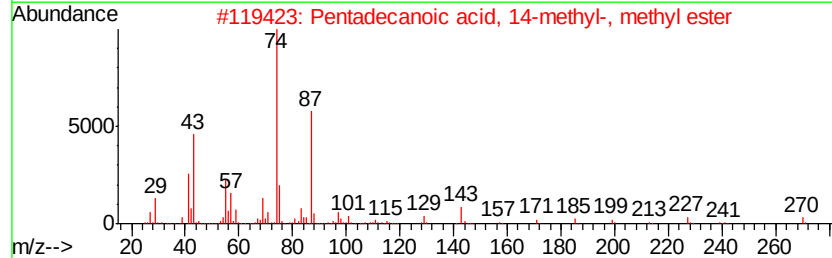
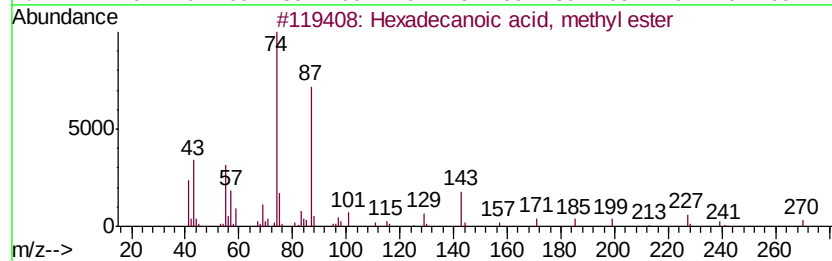
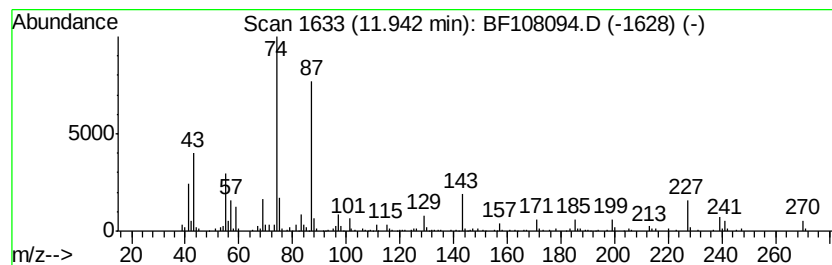
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.94	5.94 ng	520799	Phenanthrene-d10		11.57
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80



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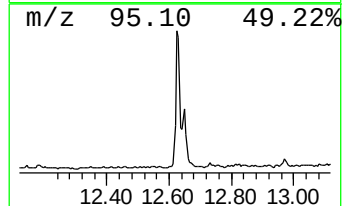
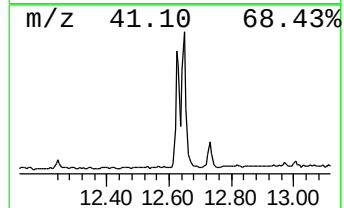
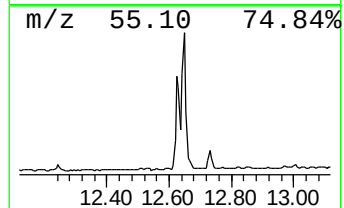
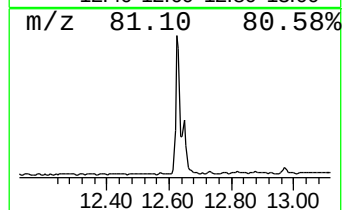
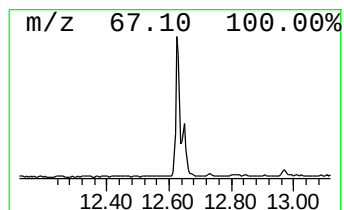
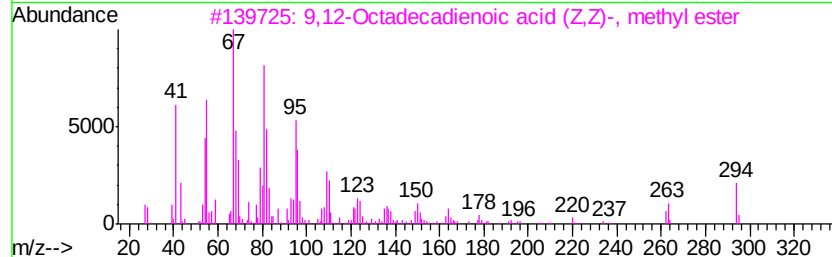
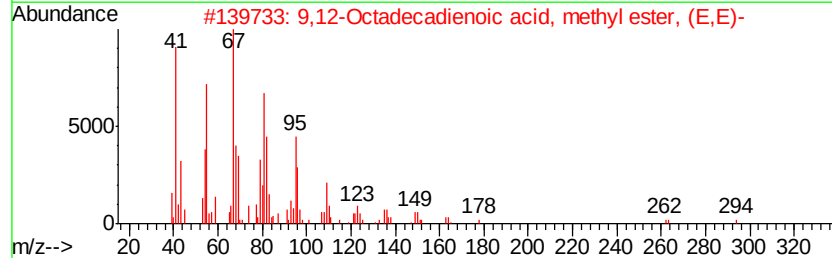
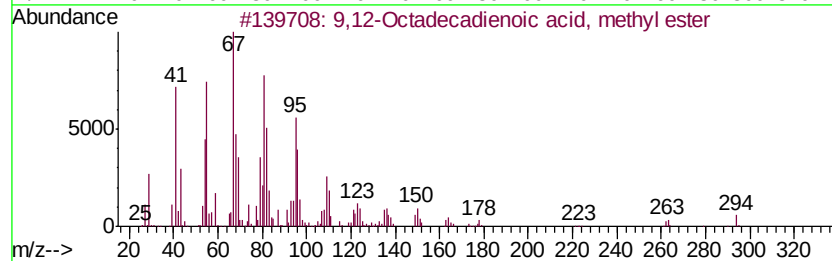
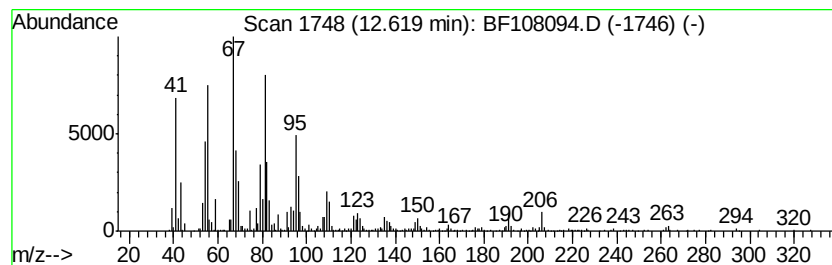
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.62	19.50 ng	1710770	Phenanthrene-d10	11.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	97
5	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	97



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108094.D
Acq On : 10 Aug 2018 19:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

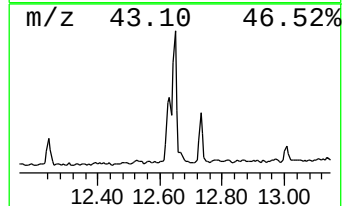
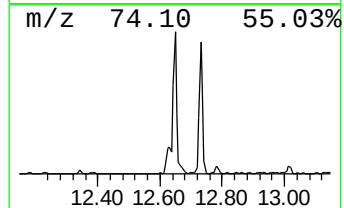
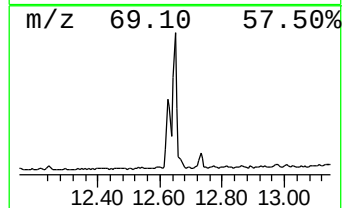
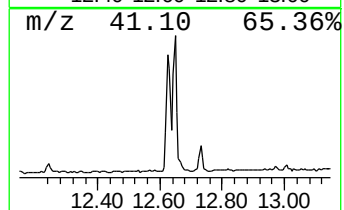
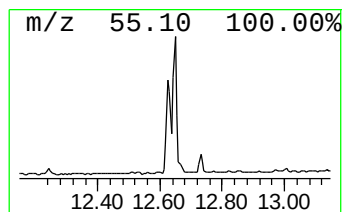
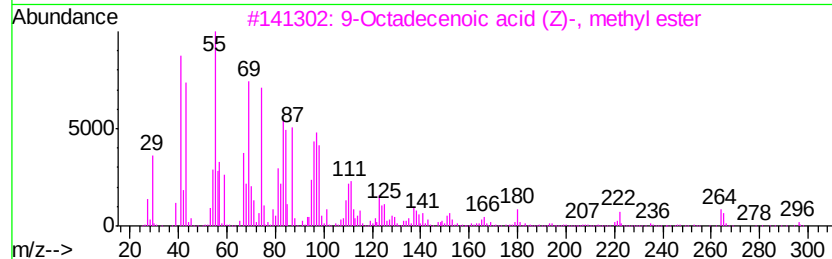
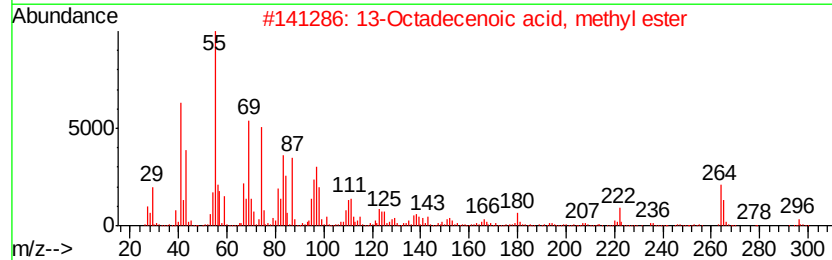
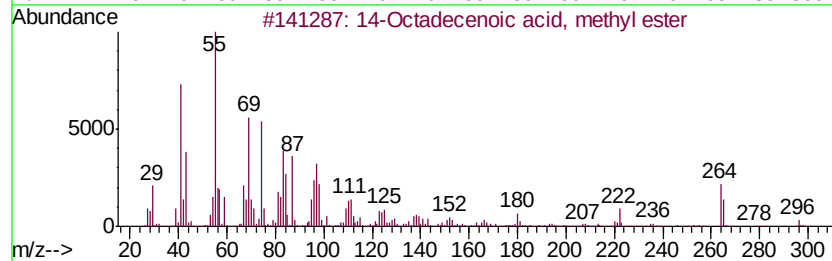
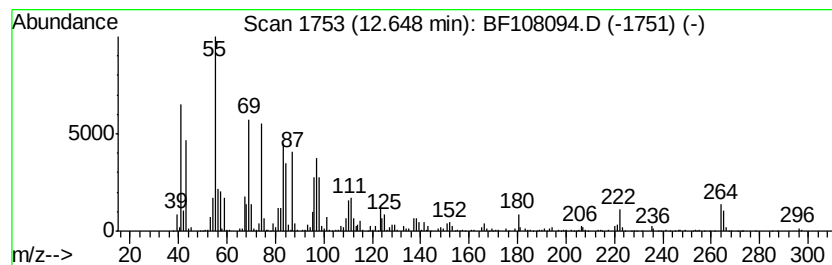
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 14-Octadecenoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.65	20.08 ng	1761280	Phenanthrene-d10	11.57		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	96
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96
3		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
4		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	94
5		6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108094.D
Acq On : 10 Aug 2018 19:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-080918-F

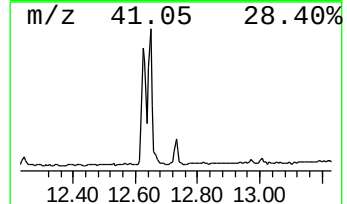
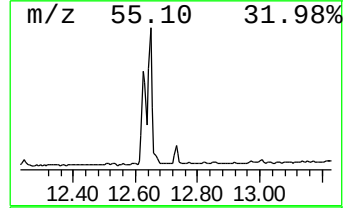
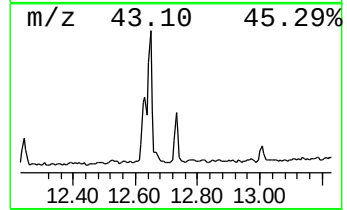
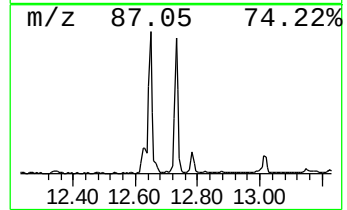
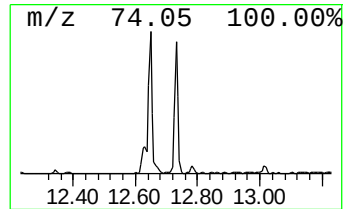
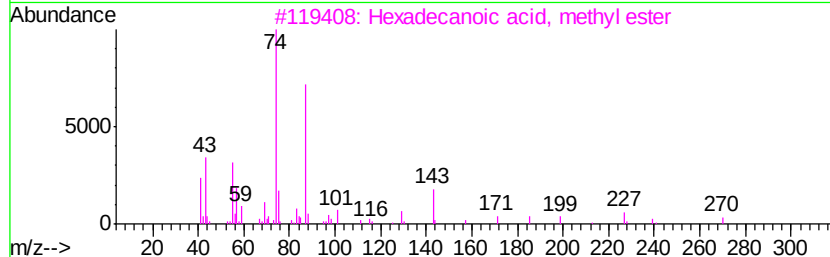
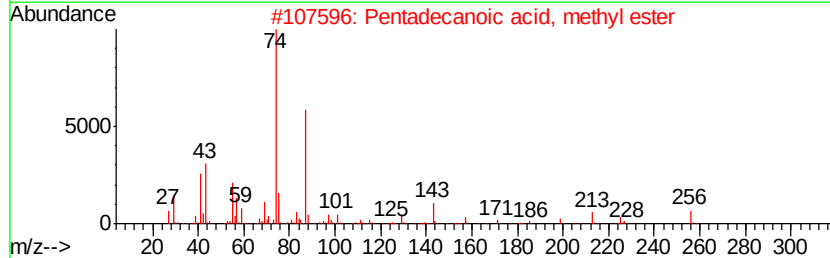
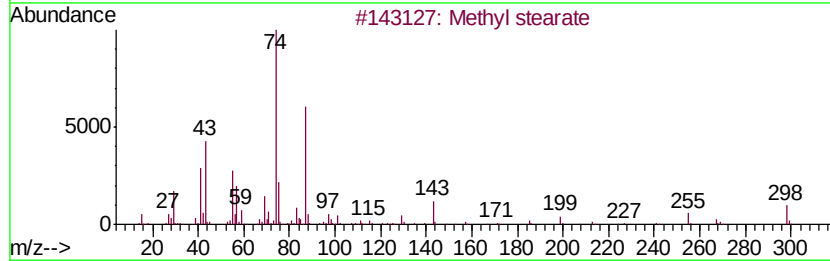
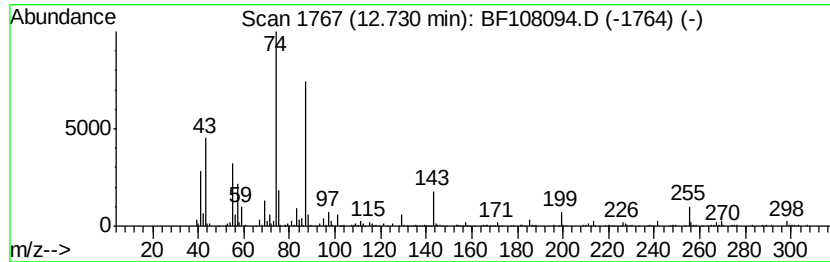
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	4.07 ng	356639	Phenanthrene-d10	11.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methyl stearate	298	C19H38O2	000112-61-8	97
2		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
4		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108094.D
Acq On : 10 Aug 2018 19:55
Operator : JU/SJ
Sample : J4272-11 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-080918-F

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.25	6.8 ng		556937	1	7.02	1639510	20.0
unknown6.78	6.78	36.9 ng		3026930	1	7.02	1639510	20.0
Tridecane, 1-iodo-	10.95	2.5 ng		215502	4	11.57	1754620	20.0
Hexadecanoic acid...	11.94	5.9 ng		520799	4	11.57	1754620	20.0
9,12-Octadecadien...	12.62	19.5 ng		1710770	4	11.57	1754620	20.0
14-Octadecenoic a...	12.65	20.1 ng		1761280	4	11.57	1754620	20.0
Methyl stearate	12.73	4.1 ng		356639	4	11.57	1754620	20.0