

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
 Data File : BF121897.D
 Acq On : 8 Oct 2020 19:22
 Operator : JU/CG
 Sample : L4311-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAV-B10-100720-10-17

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-BF091020.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	4.957	484	488	499	rBV	73932	110732	4.17%	0.563%
2	5.381	556	560	580	rBV	1960784	2103676	79.27%	10.687%
3	6.404	729	734	756	rBV	2041534	2166144	81.63%	11.004%
4	6.604	764	768	778	rBV	21559	41730	1.57%	0.212%
5	6.757	791	794	803	rVB	711650	564611	21.28%	2.868%
6	7.322	886	890	903	rBV	1551333	1484261	55.93%	7.540%
7	8.040	1008	1012	1031	rBV	774112	758798	28.59%	3.855%
8	9.116	1191	1195	1206	rBV	2864551	2580953	97.26%	13.111%
9	9.510	1259	1262	1271	rBV	254564	252239	9.51%	1.281%
10	9.792	1307	1310	1325	rVB	999533	877941	33.08%	4.460%
11	10.586	1441	1445	1461	rBV	1595216	1557990	58.71%	7.915%
12	11.280	1559	1563	1566	rBV	951492	900483	33.93%	4.575%
13	11.304	1566	1567	1572	rVB	100786	58380	2.20%	0.297%
14	11.669	1626	1629	1633	rBV	146643	122149	4.60%	0.621%
15	12.357	1743	1746	1747	rBV	194508	166842	6.29%	0.848%
16	12.375	1747	1749	1756	rVB	405550	344043	12.96%	1.748%
17	12.463	1761	1764	1766	rBV	80874	63133	2.38%	0.321%
18	12.492	1766	1769	1773	rVB	94127	81353	3.07%	0.413%
19	12.675	1797	1800	1803	rBV	124018	107083	4.04%	0.544%
20	12.722	1803	1808	1813	rVB	81732	88850	3.35%	0.451%
21	12.863	1828	1832	1836	rBV	2754594	2653658	100.00%	13.481%
22	13.345	1908	1914	1925	rBV	484832	502886	18.95%	2.555%
23	13.774	1982	1987	1999	rBV	145926	354266	13.35%	1.800%
24	13.916	2004	2011	2015	rBV	750390	759777	28.63%	3.860%
25	14.380	2087	2090	2093	rBV	30550	30514	1.15%	0.155%
26	14.421	2093	2097	2107	rVV9	12950	35936	1.35%	0.183%
27	14.680	2135	2141	2145	rBV2	32967	41351	1.56%	0.210%
28	14.945	2183	2186	2189	rBV	28388	38461	1.45%	0.195%
29	15.004	2193	2196	2201	rVB	31225	33956	1.28%	0.172%
30	15.298	2242	2246	2251	rVB	26512	31832	1.20%	0.162%
31	15.357	2251	2256	2266	rBV	580230	732015	27.59%	3.719%
32	15.780	2324	2328	2333	rVB	28119	38656	1.46%	0.196%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

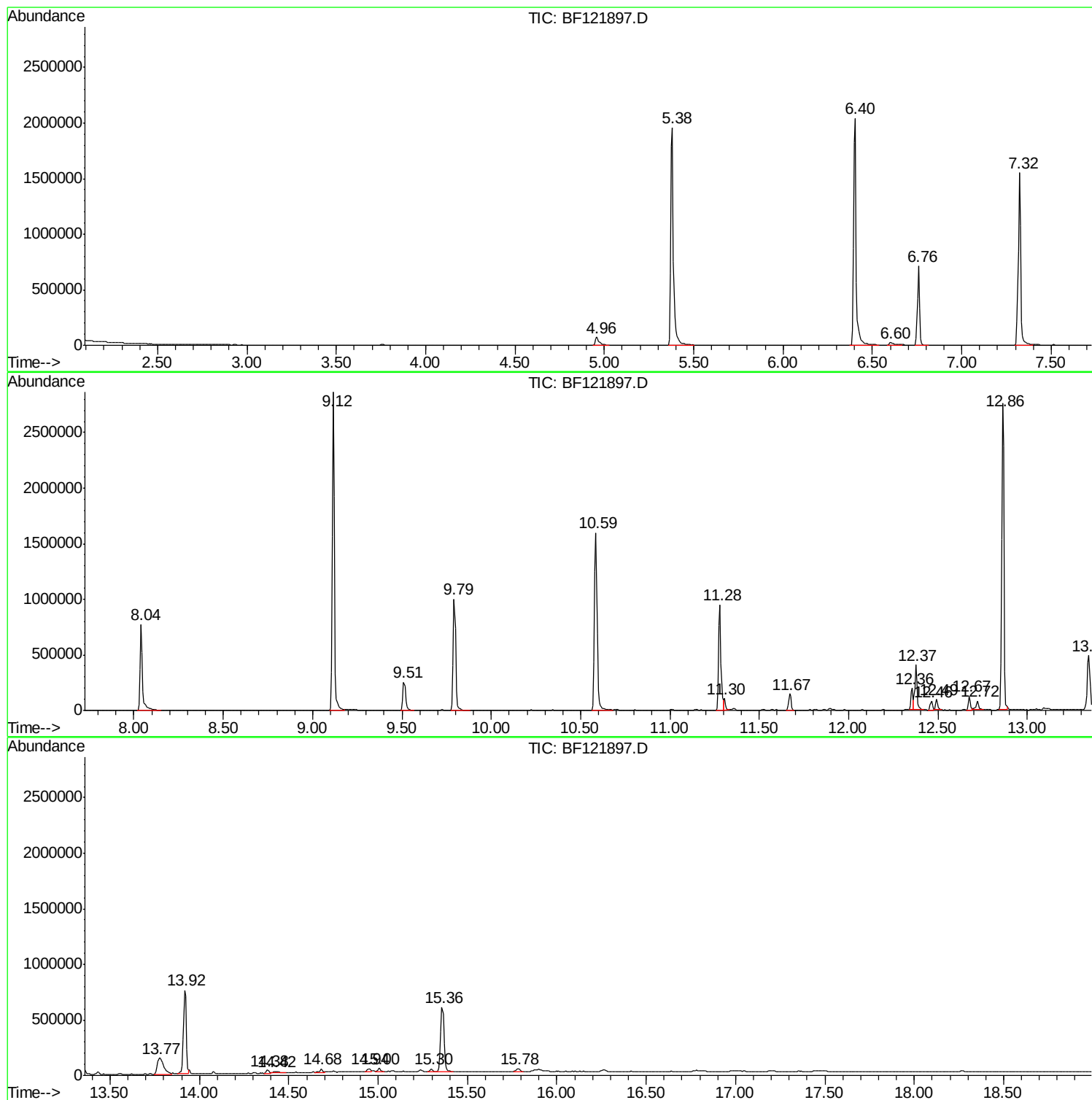
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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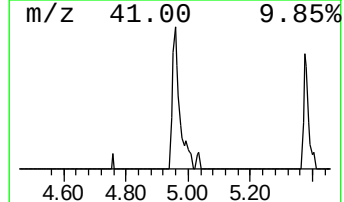
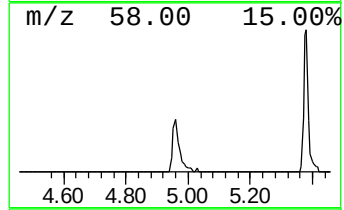
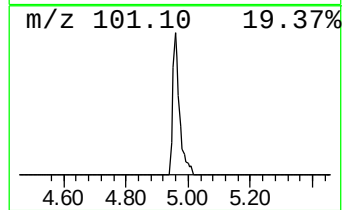
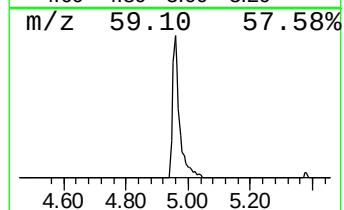
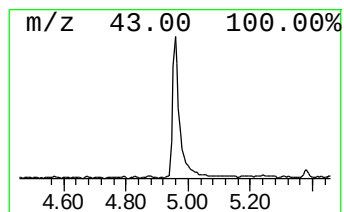
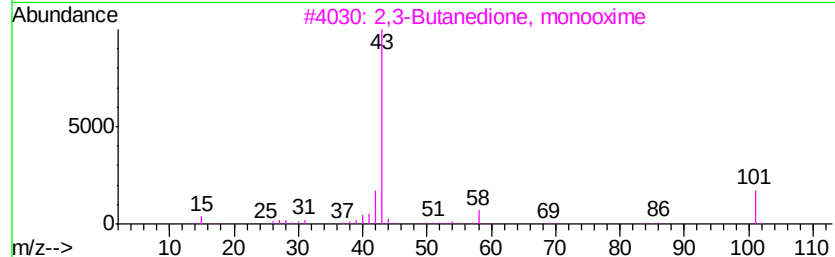
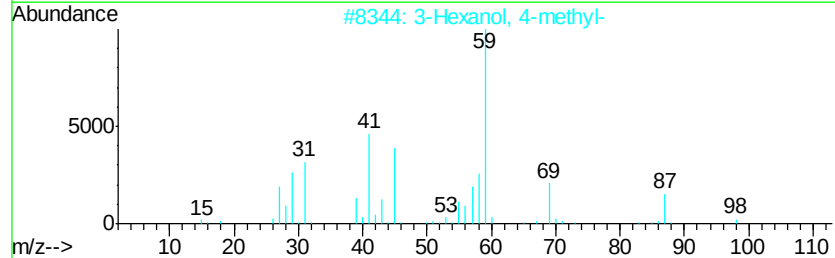
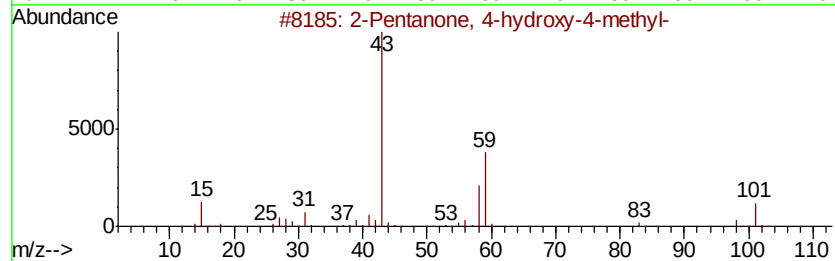
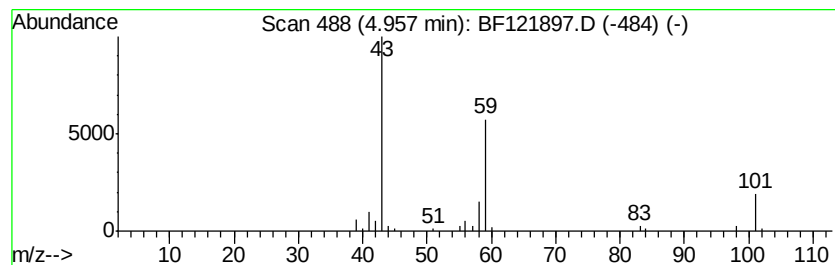
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	3.92 ng	110732	1,4-Dichlorobenzene-d4	6.76

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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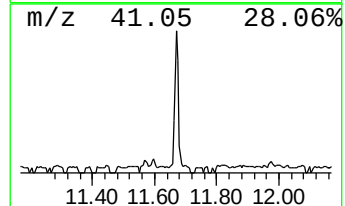
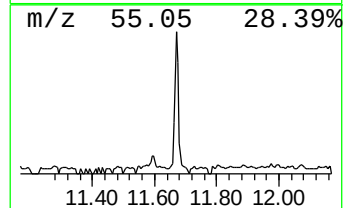
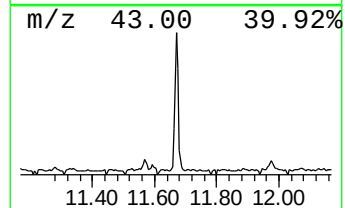
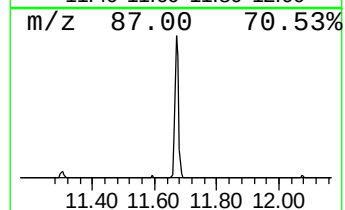
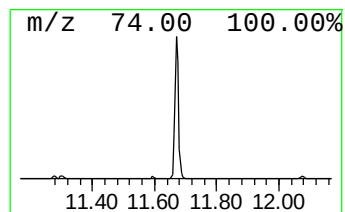
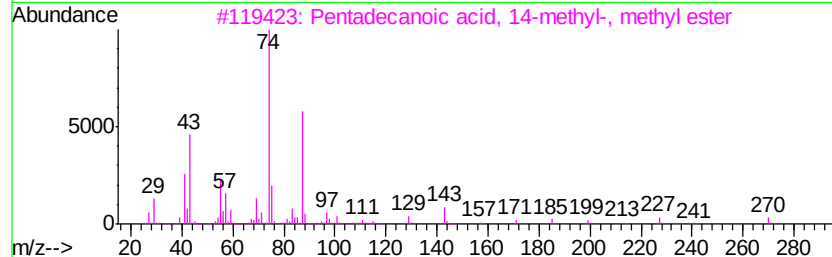
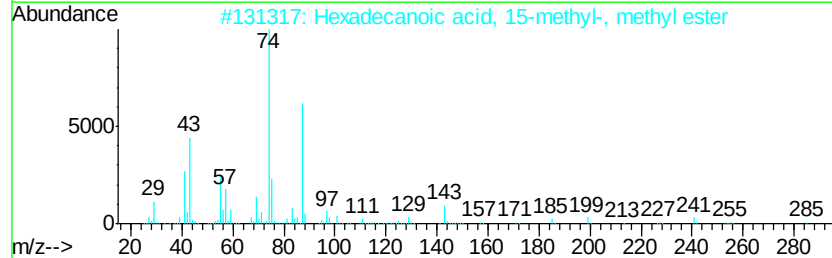
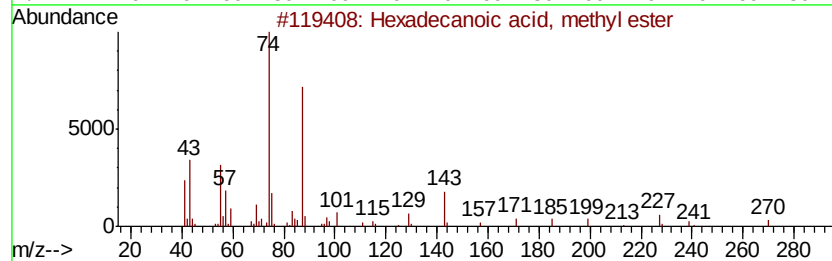
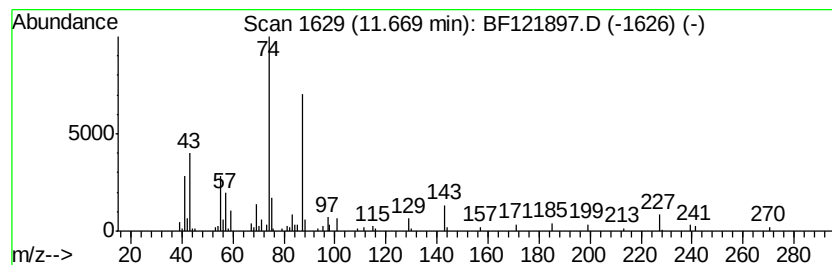
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.67	2.71 ng	122149	Phenanthrene-d10		11.28	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
3		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86



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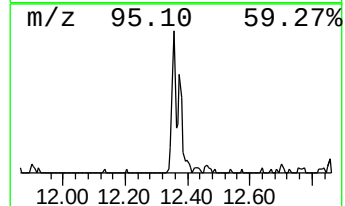
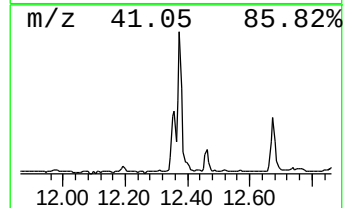
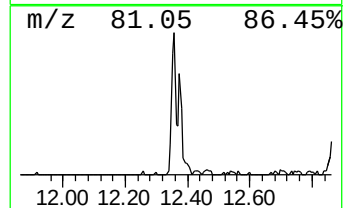
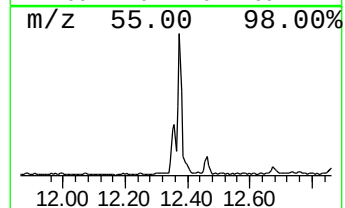
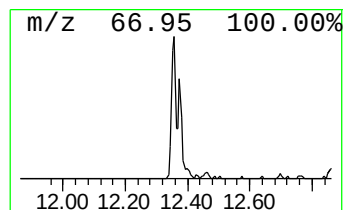
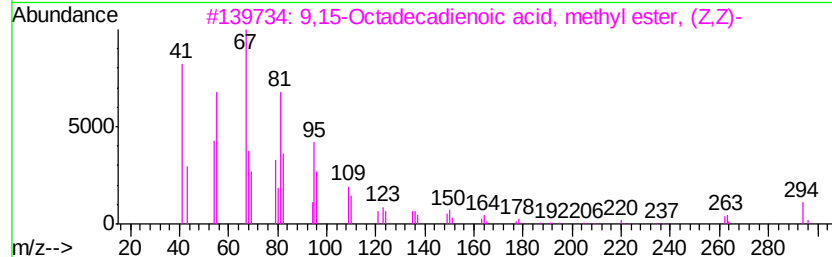
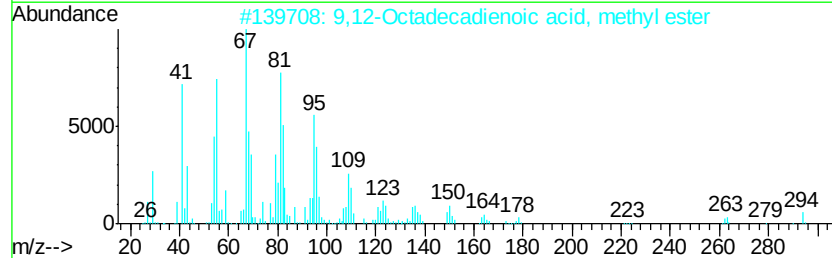
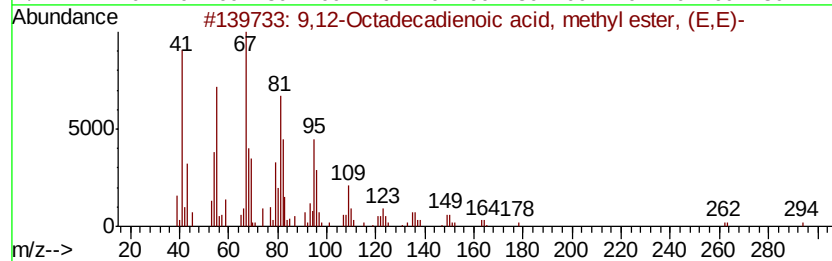
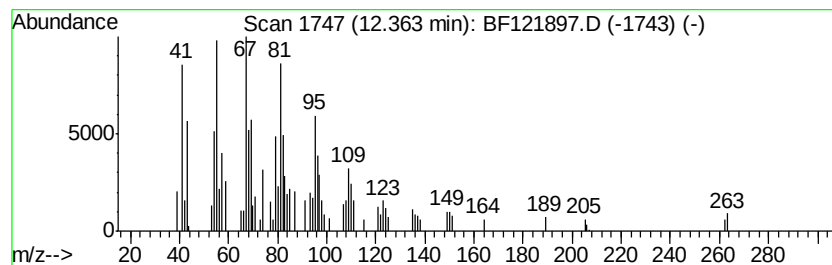
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.36	3.71 ng	166842	Phenanthrene-d10	11.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	96
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95



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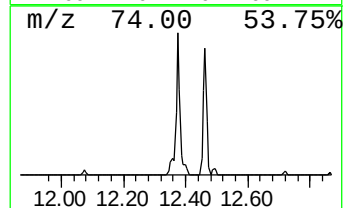
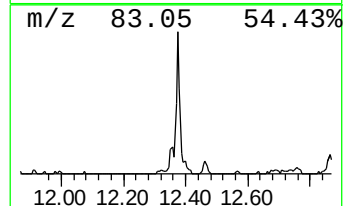
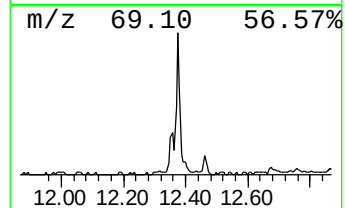
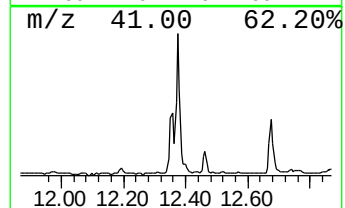
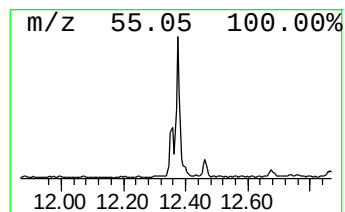
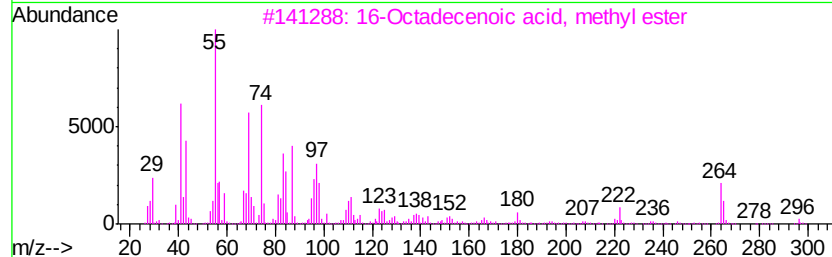
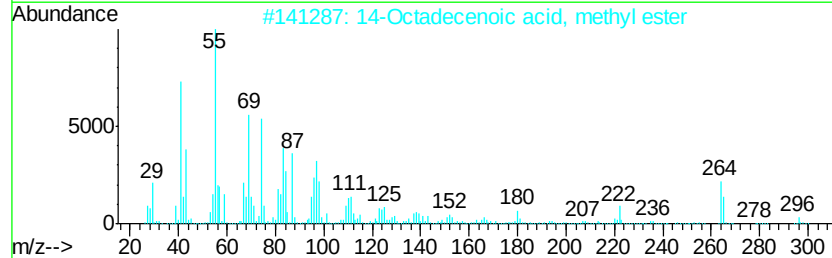
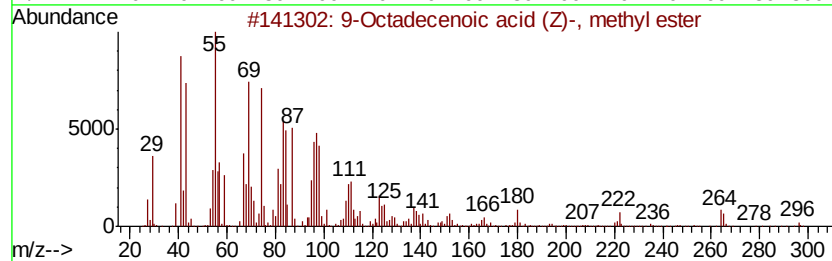
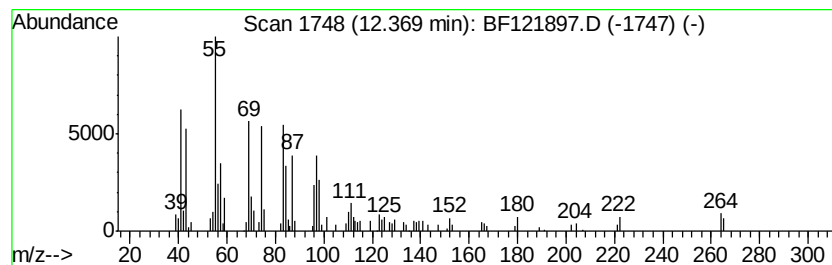
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.37	7.64 ng	344043	Phenanthrene-d10	11.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	93
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	81



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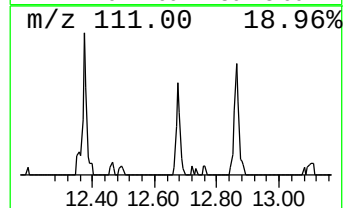
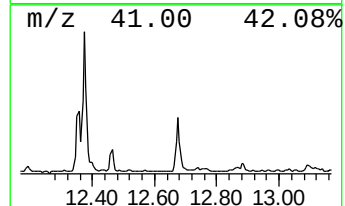
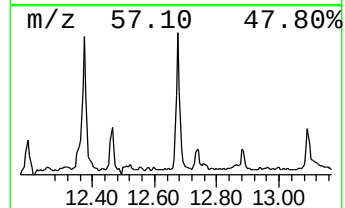
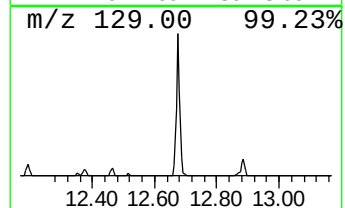
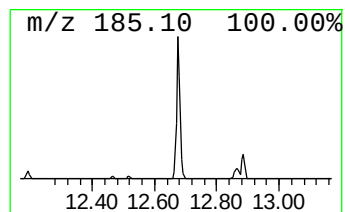
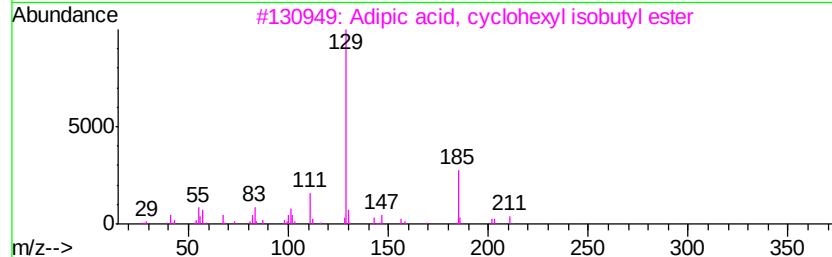
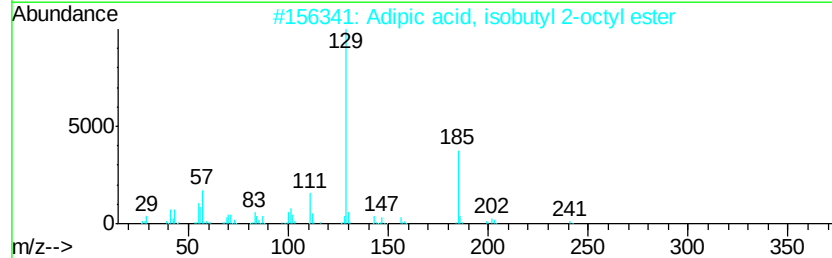
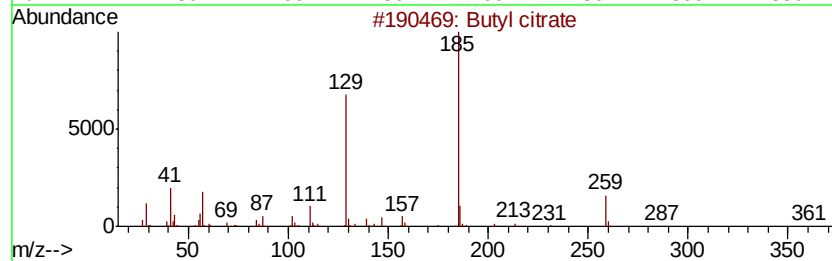
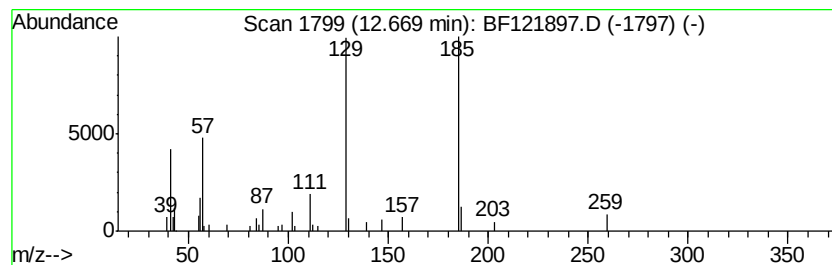
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Peak Number 5 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.82 ng	107083	Chrysene-d12	13.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl citrate	360 C18H32O7	000077-94-1 91
2		Adipic acid, isobutyl 2-octyl ester	314 C18H34O4	1000324-44-5 78
3		Adipic acid, cyclohexyl isobutyl...	284 C16H28O4	1000324-25-8 72
4		Adipic acid, butyl 2-methylpent-...	286 C16H30O4	1000353-55-8 72
5		Adipic acid, 3,3-dimethylbut-2-y...	286 C16H30O4	1000353-66-7 72



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Misc :
ALS Vial : 15 Sample Multiplier: 1

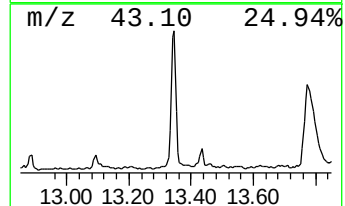
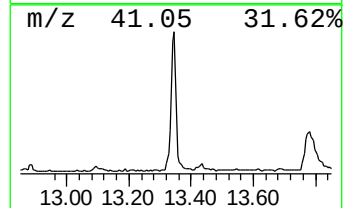
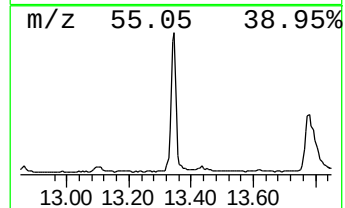
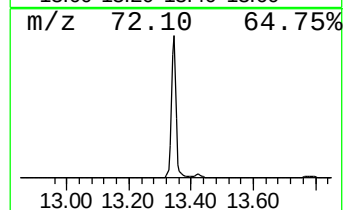
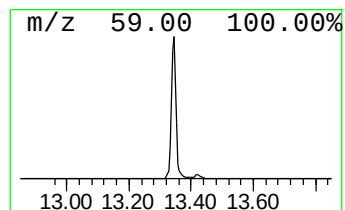
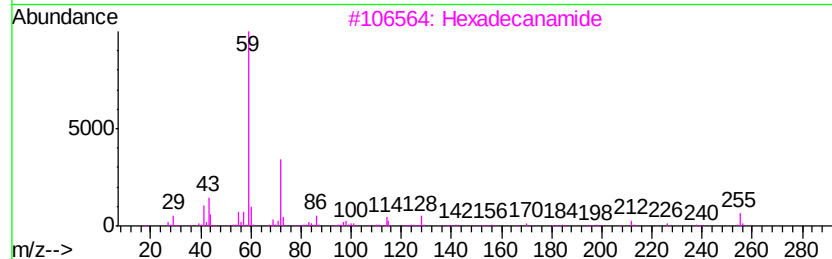
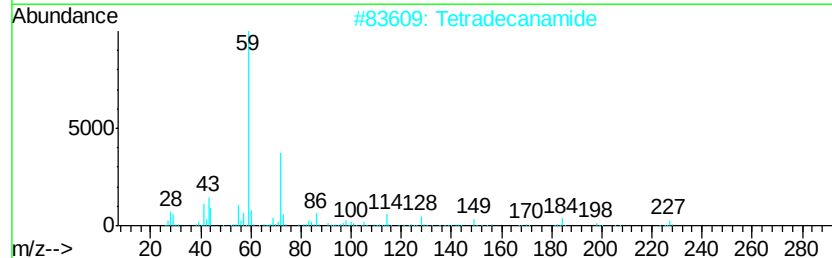
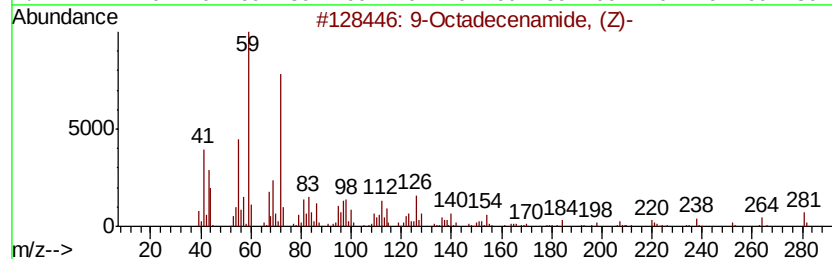
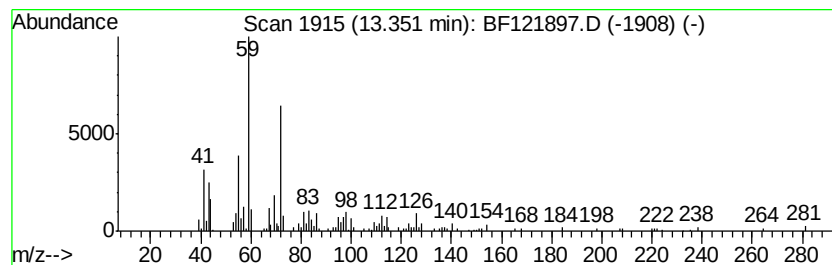
Instrument :
BNA_F
ClientSampleId :
PAV-B10-100720-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.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 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.35	13.24 ng	502886	Chrysene-d12		13.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	7-Nonenamide	155	C9H17NO	090949-53-4	64
5	Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100820\
Data File : BF121897.D
Acq On : 8 Oct 2020 19:22
Operator : JU/CG
Sample : L4311-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

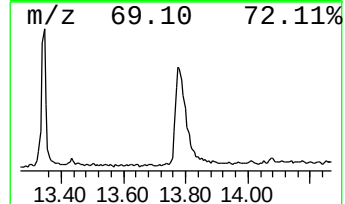
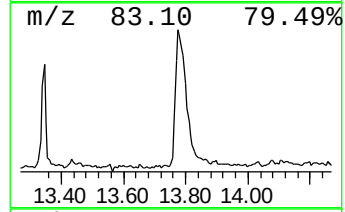
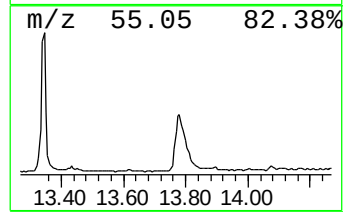
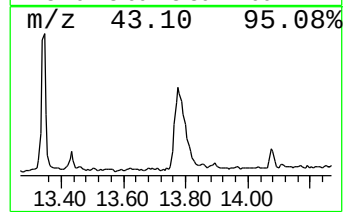
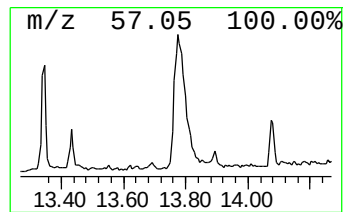
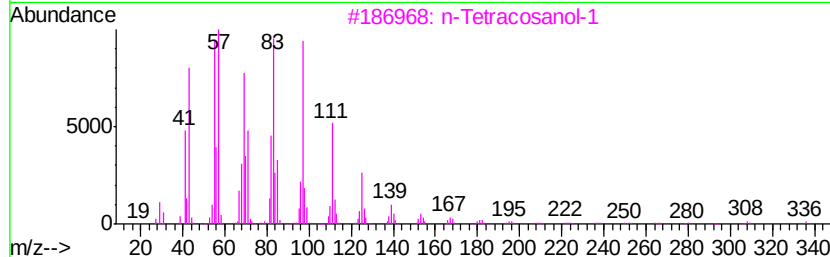
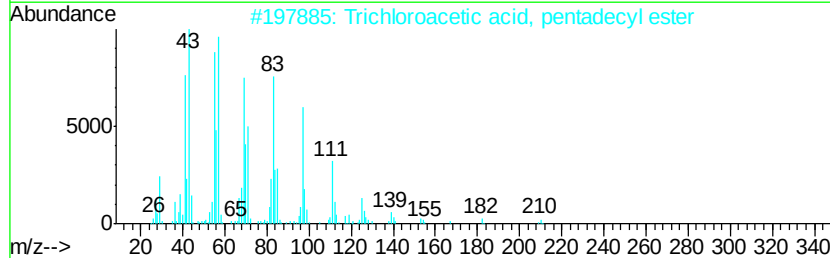
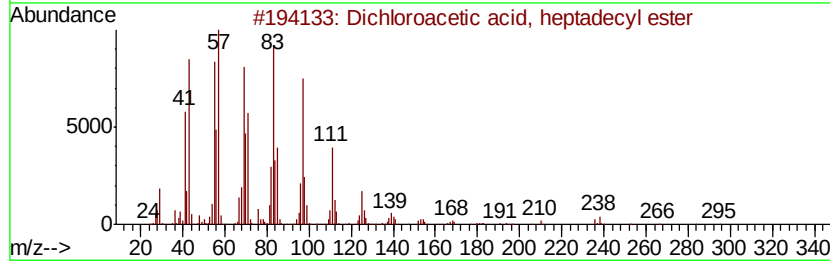
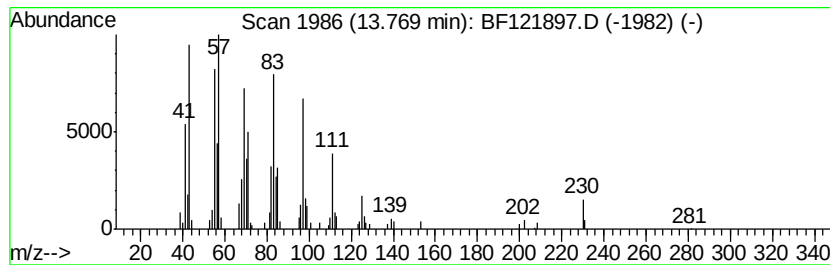
Instrument :
BNA_F
ClientSampleId :
PAV-B10-100720-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.77	9.33 ng	354266	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100820\
Data File : BF121897.D
Acq On : 8 Oct 2020 19:22
Operator : JU/CG
Sample : L4311-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAV-B10-100720-10-17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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...	4.96	3.9 ng		110732	1	6.76	564611	20.0
Hexadecanoic acid...	11.67	2.7 ng		122149	4	11.28	900483	20.0
9,12-Octadecadien...	12.36	3.7 ng		166842	4	11.28	900483	20.0
9-Octadecenoic ac...	12.37	7.6 ng		344043	4	11.28	900483	20.0
Butyl citrate	12.67	2.8 ng		107083	5	13.92	759777	20.0
9-Octadecenamide, ...	13.35	13.2 ng		502886	5	13.92	759777	20.0
Dichloroacetic ac...	13.77	9.3 ng		354266	5	13.92	759777	20.0