

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060421\
 Data File : BF124143.D
 Acq On : 4 Jun 2021 17:01
 Operator : JU/CG
 Sample : M2581-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-060221

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	15	20	rBB	575289	721774	10.57%	3.183%
2	5.498	575	580	583	rBV	1191004	1088442	15.93%	4.801%
3	6.504	746	751	754	rBV2	1040976	1051955	15.40%	4.640%
4	6.869	809	813	816	rBB	317509	286122	4.19%	1.262%
5	7.428	903	908	911	rBV	774959	710148	10.40%	3.132%
6	8.145	1024	1030	1034	rBV	388794	337505	4.94%	1.489%
7	9.222	1209	1213	1216	rBV	1348787	1190559	17.43%	5.251%
8	9.904	1325	1329	1332	rBV	438076	334294	4.89%	1.474%
9	10.692	1459	1463	1466	rBV	773856	615430	9.01%	2.714%
10	11.392	1578	1582	1584	rBV	322019	298505	4.37%	1.317%
11	11.786	1644	1649	1652	rBV	1549190	1299010	19.02%	5.729%
12	11.916	1669	1671	1676	rBV2	79221	75117	1.10%	0.331%
13	12.486	1762	1768	1769	rBV	5849756	6831077	100.00%	30.129%
14	12.504	1769	1771	1776	rVV	5052105	5049255	73.92%	22.270%
15	12.580	1780	1784	1786	rVV	814744	682249	9.99%	3.009%
16	12.610	1786	1789	1791	rVV2	144594	153233	2.24%	0.676%
17	12.627	1791	1792	1798	rVB4	88167	90267	1.32%	0.398%
18	12.833	1822	1827	1837	rVB2	84930	127720	1.87%	0.563%
19	12.980	1845	1852	1855	rBV	1136210	996051	14.58%	4.393%
20	13.222	1891	1893	1899	rVB5	71519	88439	1.29%	0.390%
21	13.880	2003	2005	2015	rVB7	42309	82974	1.21%	0.366%
22	13.969	2018	2020	2024	rBV	84641	71131	1.04%	0.314%
23	14.033	2027	2031	2034	rBV2	292197	284544	4.17%	1.255%
24	15.521	2279	2284	2287	rBV	144174	206937	3.03%	0.913%

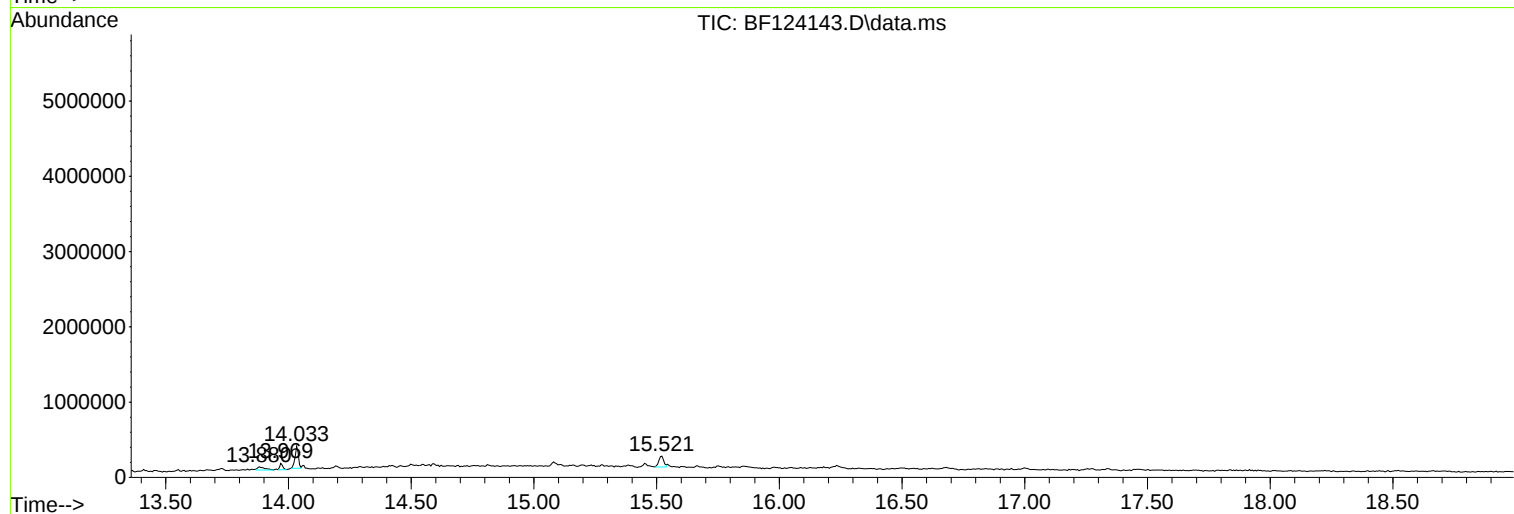
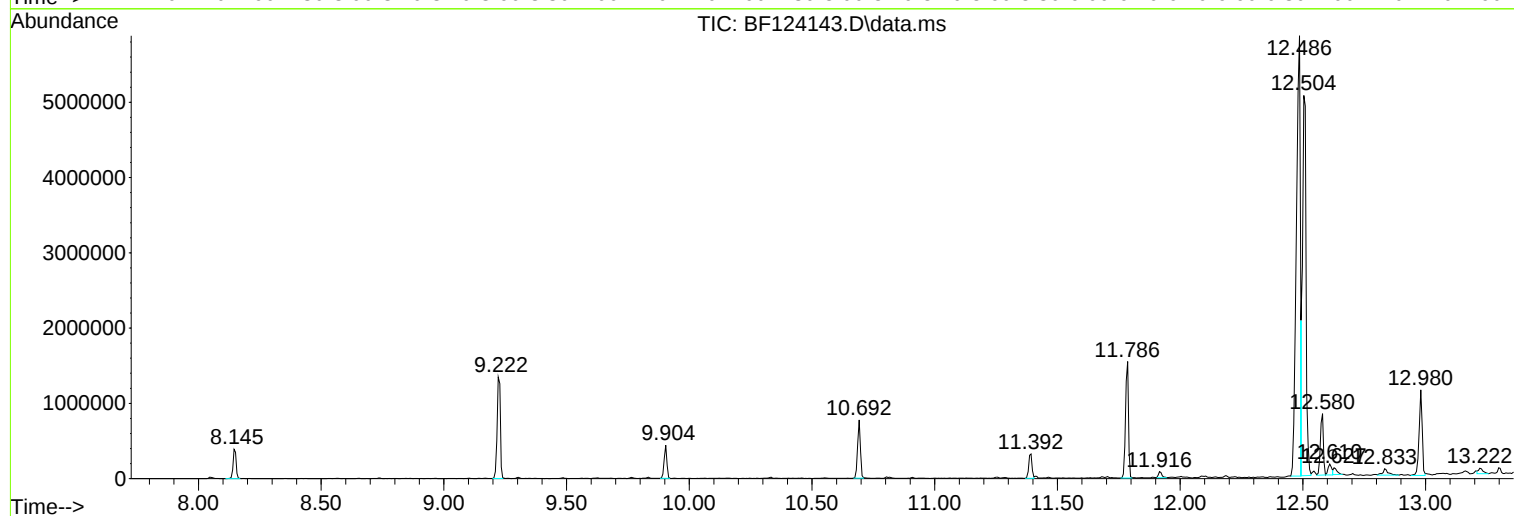
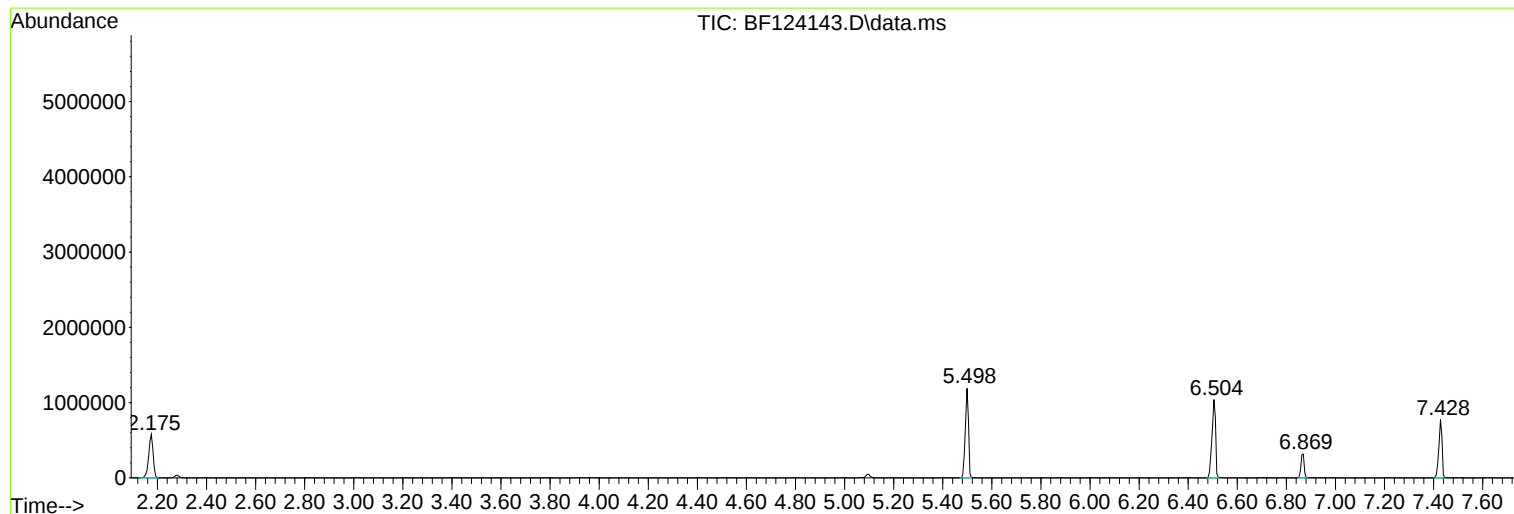
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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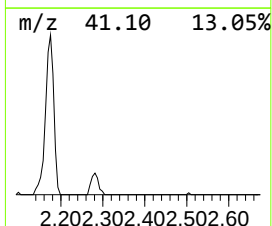
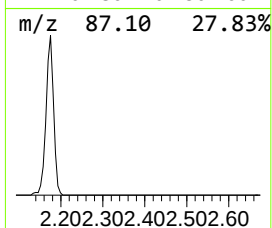
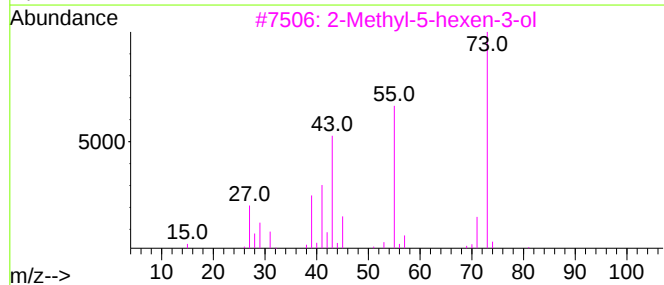
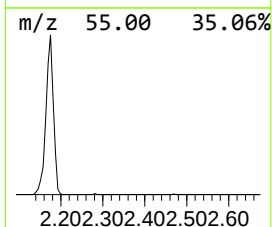
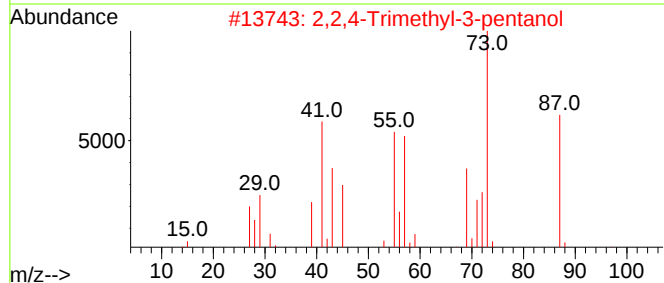
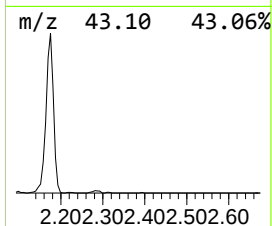
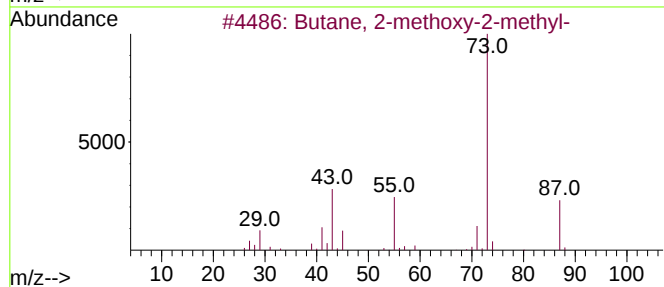
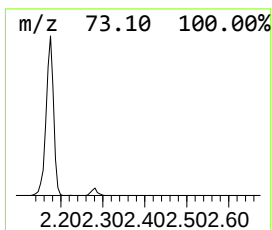
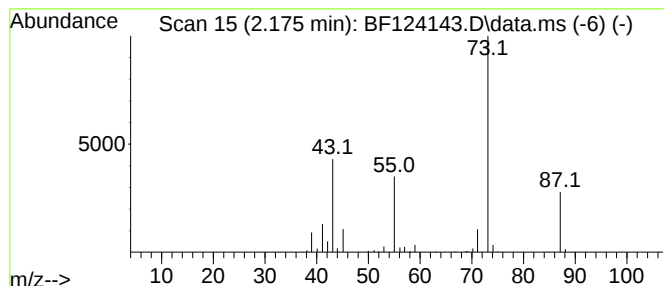
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	50.45 ng	721774	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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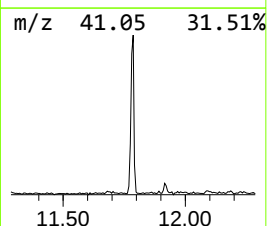
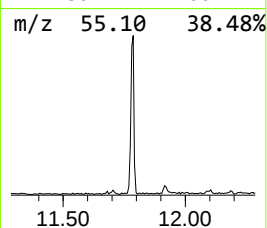
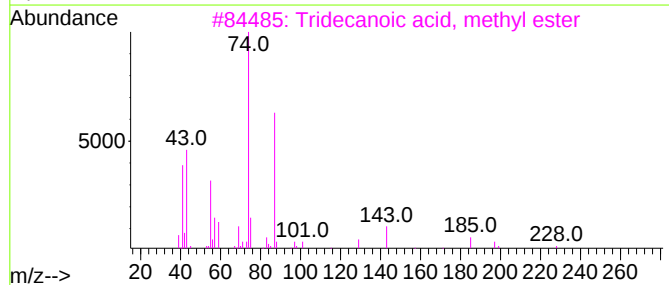
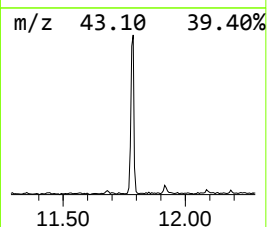
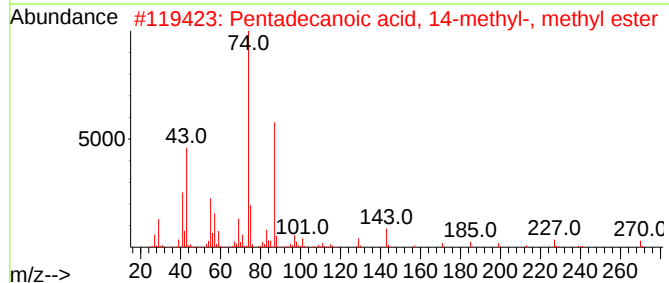
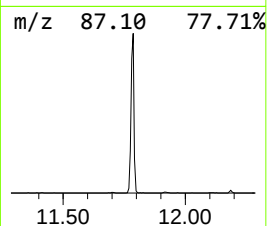
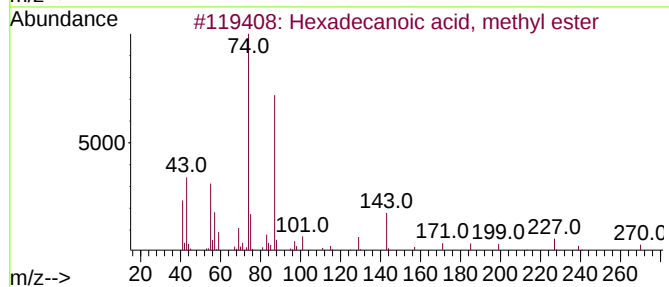
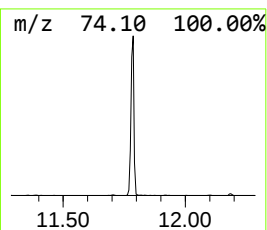
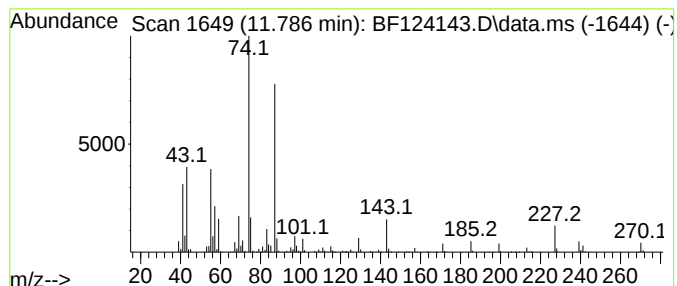
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Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	87.03 ng	1299010	Phenanthrene-d10	11.392

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	95
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83



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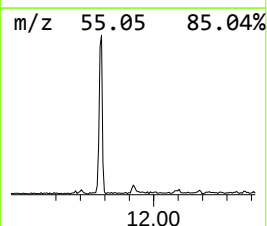
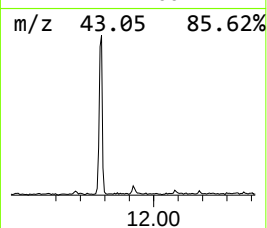
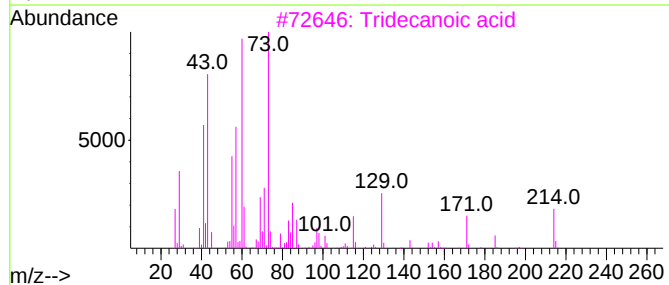
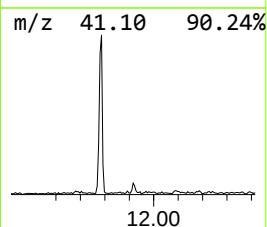
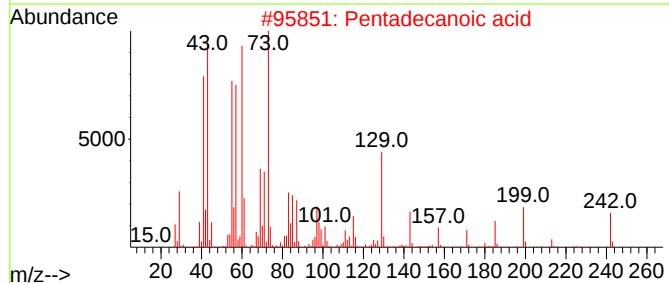
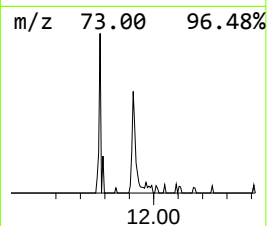
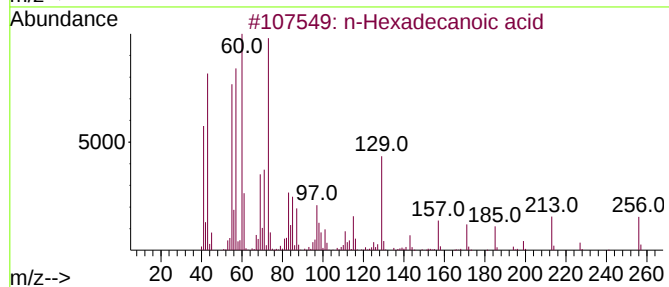
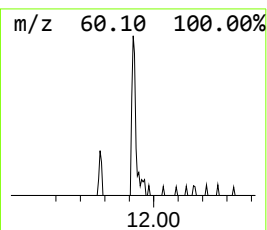
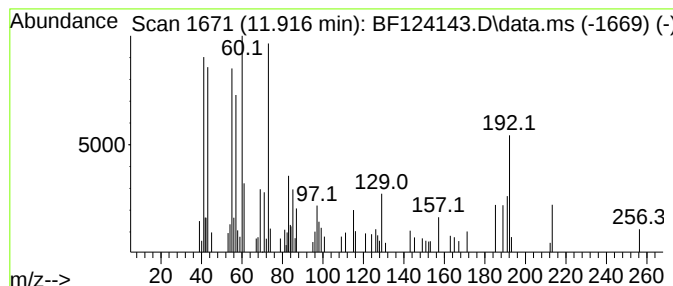
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.03 ng	75117	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	43
3			Tridecanoic acid	214	C13H26O2	000638-53-9	38
4			Trehalose	342	C12H22O11	000099-20-7	35
5			Lactose	342	C12H22O11	000063-42-3	30



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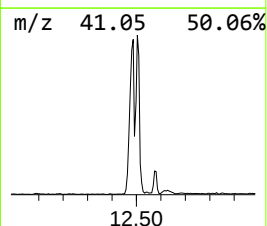
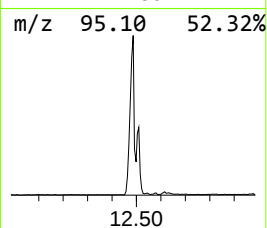
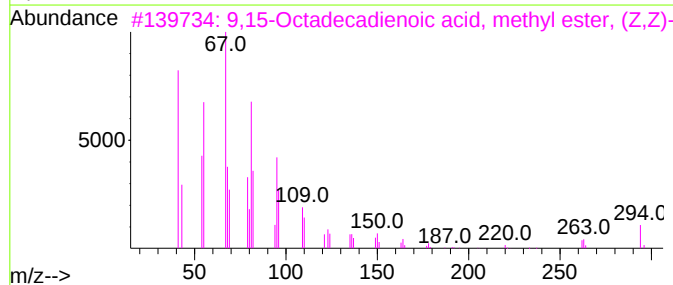
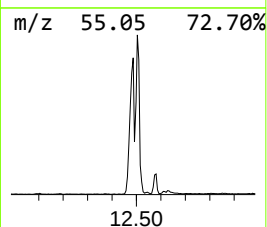
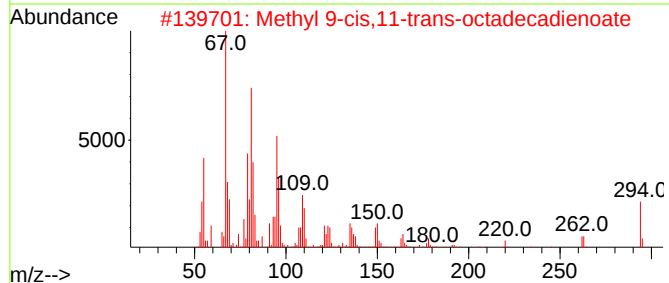
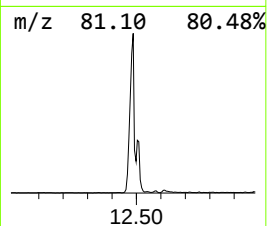
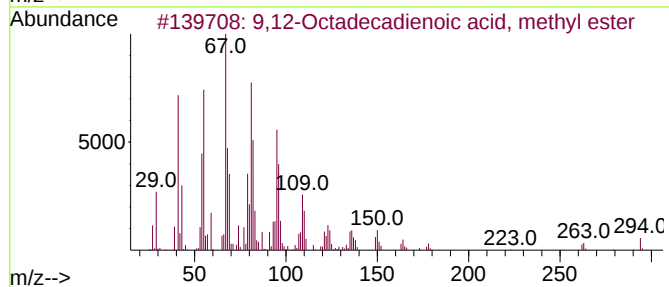
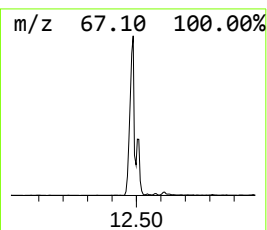
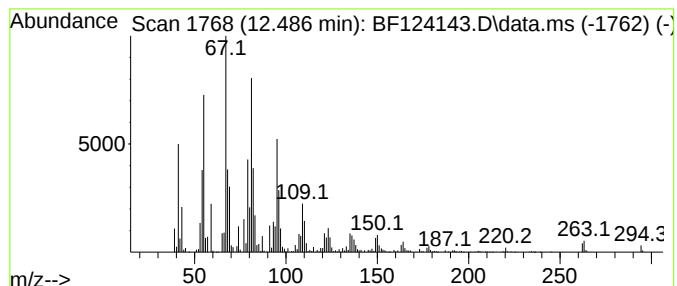
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Peak Number 4 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	457.69 ng	6831080	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
3			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99



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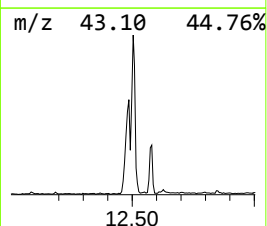
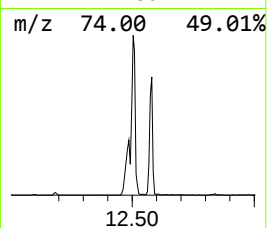
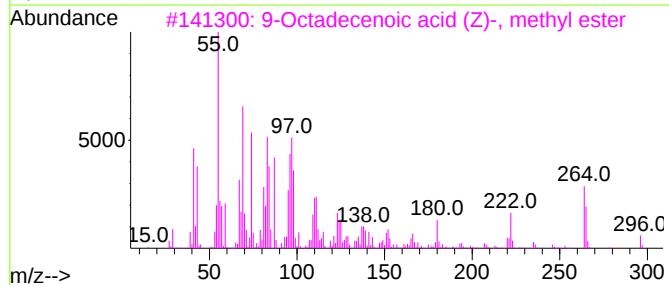
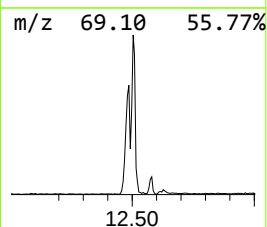
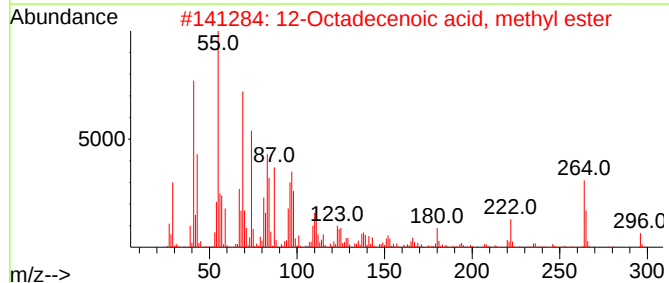
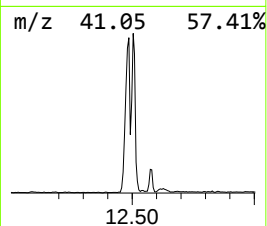
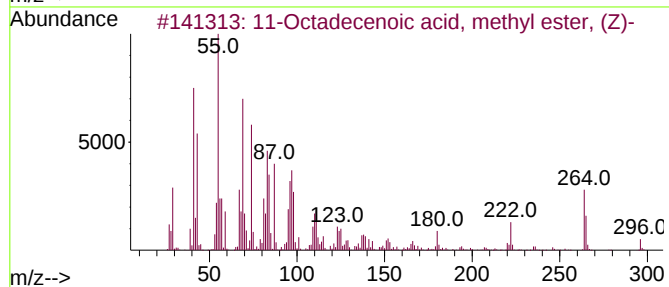
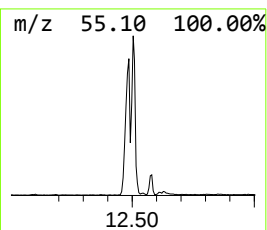
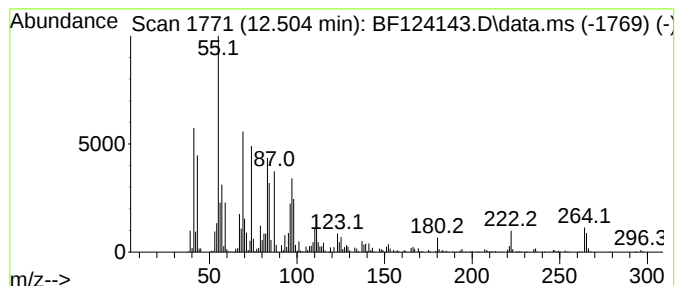
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 11-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.504	338.30 ng	5049260	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	91
2			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
4			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	90
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90



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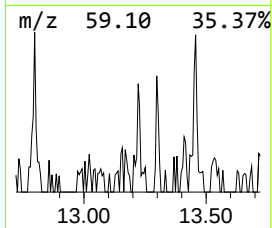
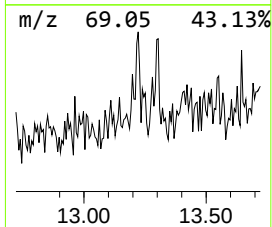
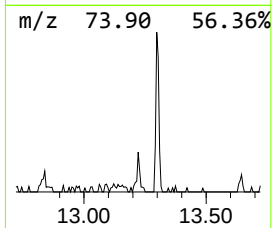
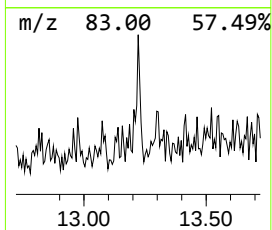
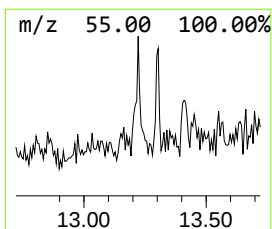
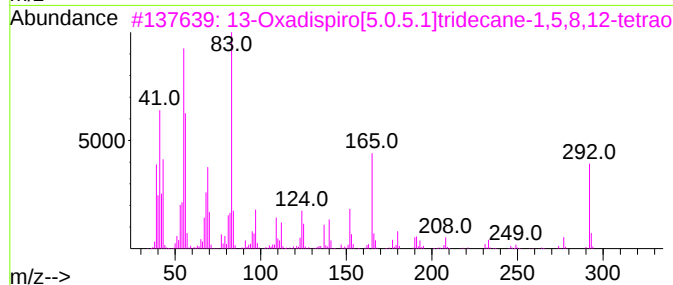
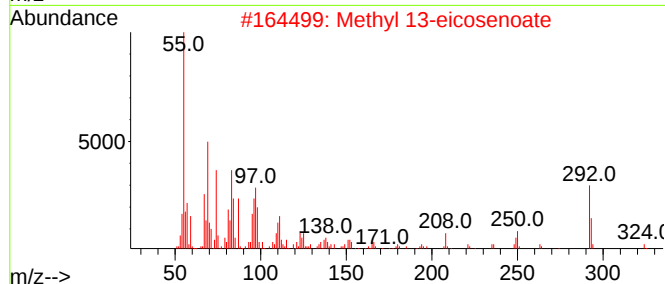
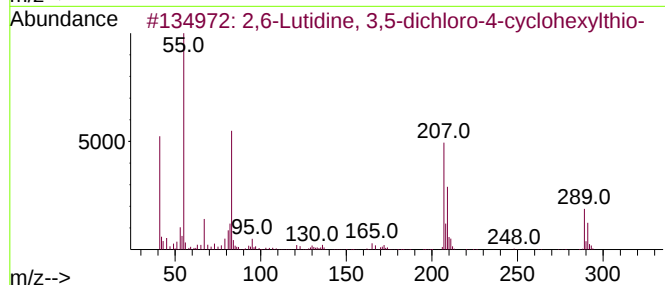
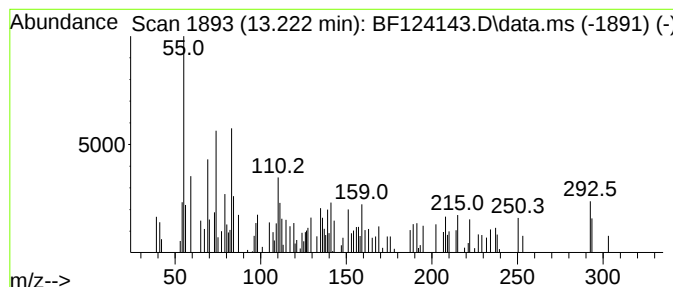
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.222 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	6.22 ng	88439	Chrysene-d12	14.033

Hit#	of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Lutidine, 3,5-dichloro-4-cyc...	289	C13H17Cl2NS	1000252-29-1	9	
2	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	9	
3	13-Oxadispiro[5.0.5.1]tridecane-...	292	C16H20O5	1000259-58-1	9	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060421\
Data File : BF124143.D
Acq On : 4 Jun 2021 17:01
Operator : JU/CG
Sample : M2581-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-060221

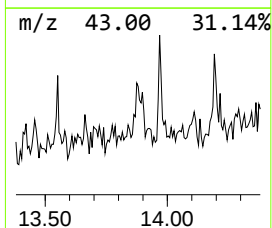
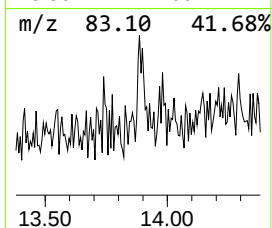
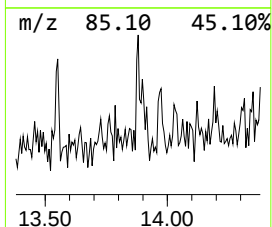
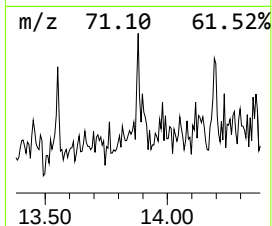
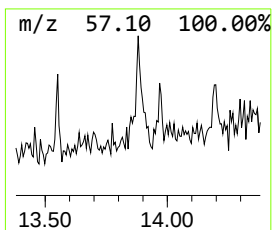
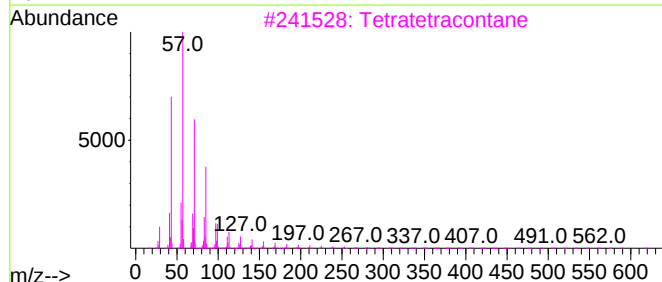
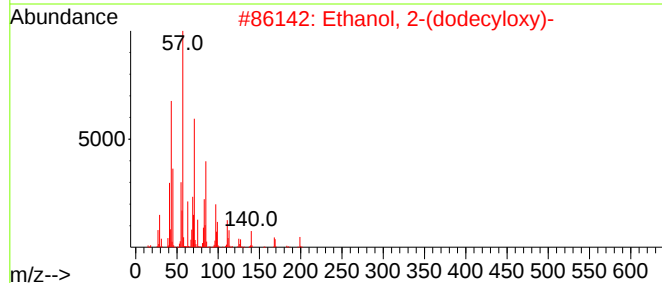
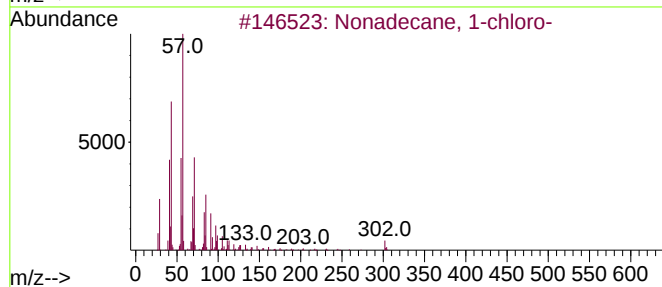
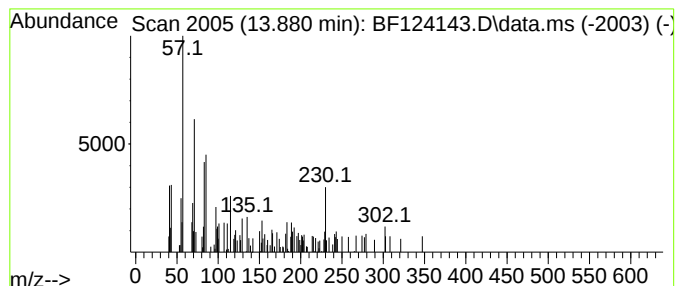
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.83 ng	82974	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	50
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	47
3			Tetratetracontane	619	C44H90	007098-22-8	38
4			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	38
5			Cyclopentanone, 3-(6,6-dimethyl-...	222	C14H22O2	083040-98-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060421\
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Sample : M2581-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-060221

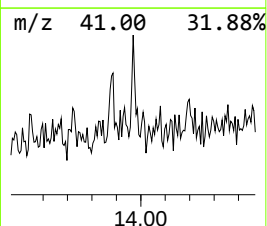
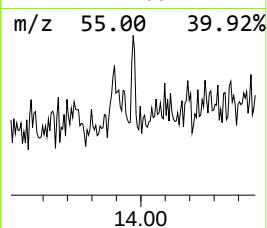
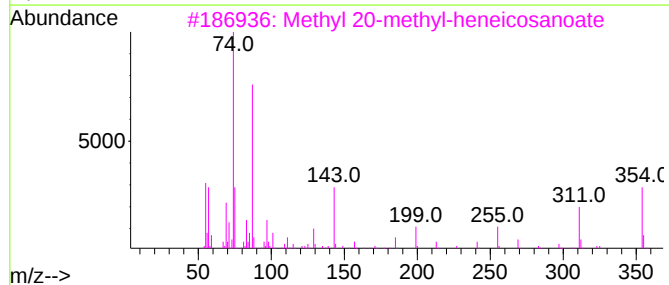
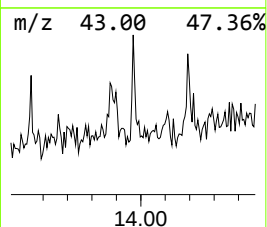
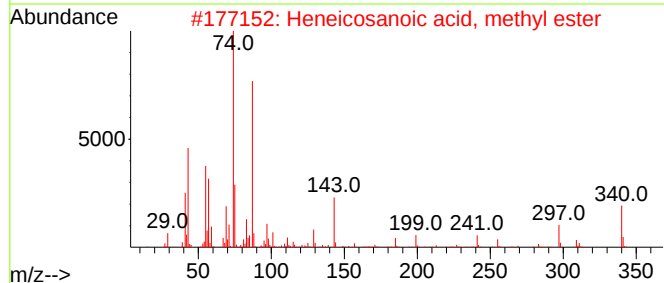
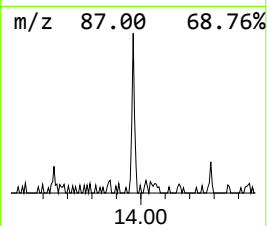
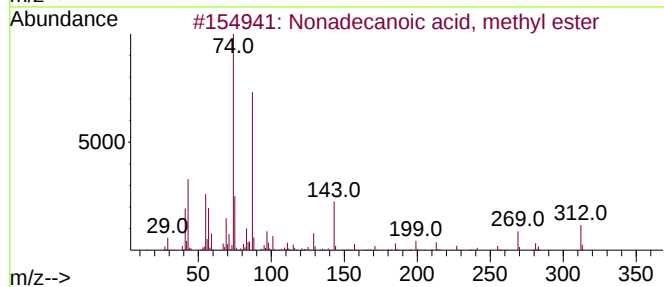
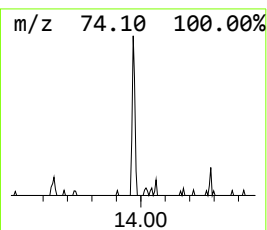
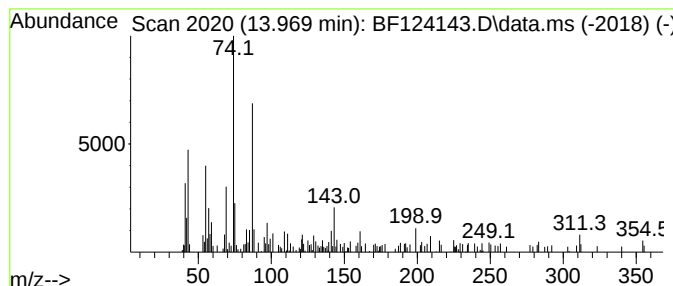
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	5.00 ng	71131	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	94
2			Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	94
3			Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	91
4			Methyl 18-methyllicosanoate	340	C22H44O2	1000352-20-5	90
5			Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060421\
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Acq On : 4 Jun 2021 17:01
Operator : JU/CG
Sample : M2581-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-060221

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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
Butane, 2-metho...	2.175	50.5	ng	721774	1	6.869	286122	20.0
Hexadecanoic ac...	11.786	87.0	ng	1299010	4	11.392	298505	20.0
n-Hexadecanoic ...	11.916	5.0	ng	75117	4	11.392	298505	20.0
9,12-Octadecadi...	12.486	457.7	ng	6831080	4	11.392	298505	20.0
11-Octadecenoic...	12.504	338.3	ng	5049260	4	11.392	298505	20.0
unknown13.222	13.222	6.2	ng	88439	5	14.033	284544	20.0
Nonadecane, 1-c...	13.880	5.8	ng	82974	5	14.033	284544	20.0
Nonadecanoic ac...	13.969	5.0	ng	71131	5	14.033	284544	20.0