

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041320\
 Data File : BF119972.D
 Acq On : 15 Apr 2020 00:25
 Operator : MA/SJ
 Sample : L2215-17
 Misc :
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF040820.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	4.928	479	483	495	rVB	274436	361826	7.26%	0.870%
2	5.346	549	554	557	rBV	3988340	3963455	79.49%	9.534%
3	6.369	722	728	731	rBV	3587788	3973124	79.69%	9.557%
4	6.569	758	762	773	rBV	46558	85838	1.72%	0.206%
5	6.734	786	790	793	rBV	1515515	1222285	24.51%	2.940%
6	6.892	812	817	820	rBV	3485222	3230456	64.79%	7.771%
7	7.298	880	886	889	rBV	2738884	2626986	52.69%	6.319%
8	8.016	1004	1008	1012	rBV	1720452	1638589	32.86%	3.942%
9	9.098	1187	1192	1195	rBV	5320619	4883592	97.95%	11.747%
10	9.492	1254	1259	1262	rBV	611610	488894	9.81%	1.176%
11	9.775	1301	1307	1310	rBV	2196733	1921482	38.54%	4.622%
12	10.563	1436	1441	1444	rBV	3243570	3003933	60.25%	7.226%
13	11.263	1555	1560	1563	rBV	2209879	2034317	40.80%	4.893%
14	11.798	1647	1651	1659	rBV	853755	912756	18.31%	2.196%
15	12.522	1771	1774	1778	rVB	227161	202926	4.07%	0.488%
16	12.580	1781	1784	1797	rBV	390866	471824	9.46%	1.135%
17	12.674	1797	1800	1803	rBV	122593	123823	2.48%	0.298%
18	12.751	1811	1813	1819	rVB	70652	75138	1.51%	0.181%
19	12.851	1825	1830	1833	rBV	5137536	4985919	100.00%	11.993%
20	13.239	1893	1896	1903	rVB	145248	134334	2.69%	0.323%
21	13.333	1909	1912	1916	rVV	713206	575849	11.55%	1.385%
22	13.380	1918	1920	1923	rVB	93365	75508	1.51%	0.182%
23	13.757	1981	1984	1989	rVB	52093	52115	1.05%	0.125%
24	13.839	1990	1998	2004	rBV4	195859	681848	13.68%	1.640%
25	13.898	2004	2008	2012	rVB	1933466	1738247	34.86%	4.181%
26	14.074	2035	2038	2041	rVB	97228	75861	1.52%	0.182%
27	14.380	2086	2090	2093	rBV	125116	115895	2.32%	0.279%
28	14.680	2137	2141	2144	rVB	137081	133143	2.67%	0.320%
29	14.998	2191	2195	2200	rVB	152293	169155	3.39%	0.407%
30	15.321	2245	2250	2254	rBV	1054279	1261716	25.31%	3.035%
31	15.363	2254	2257	2264	rVB	115571	149946	3.01%	0.361%
32	15.774	2323	2327	2338	rVB	85594	131523	2.64%	0.316%
33	16.257	2404	2409	2413	rBV4	38062	69793	1.40%	0.168%

LSC Area Percent Report

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Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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-BF040820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

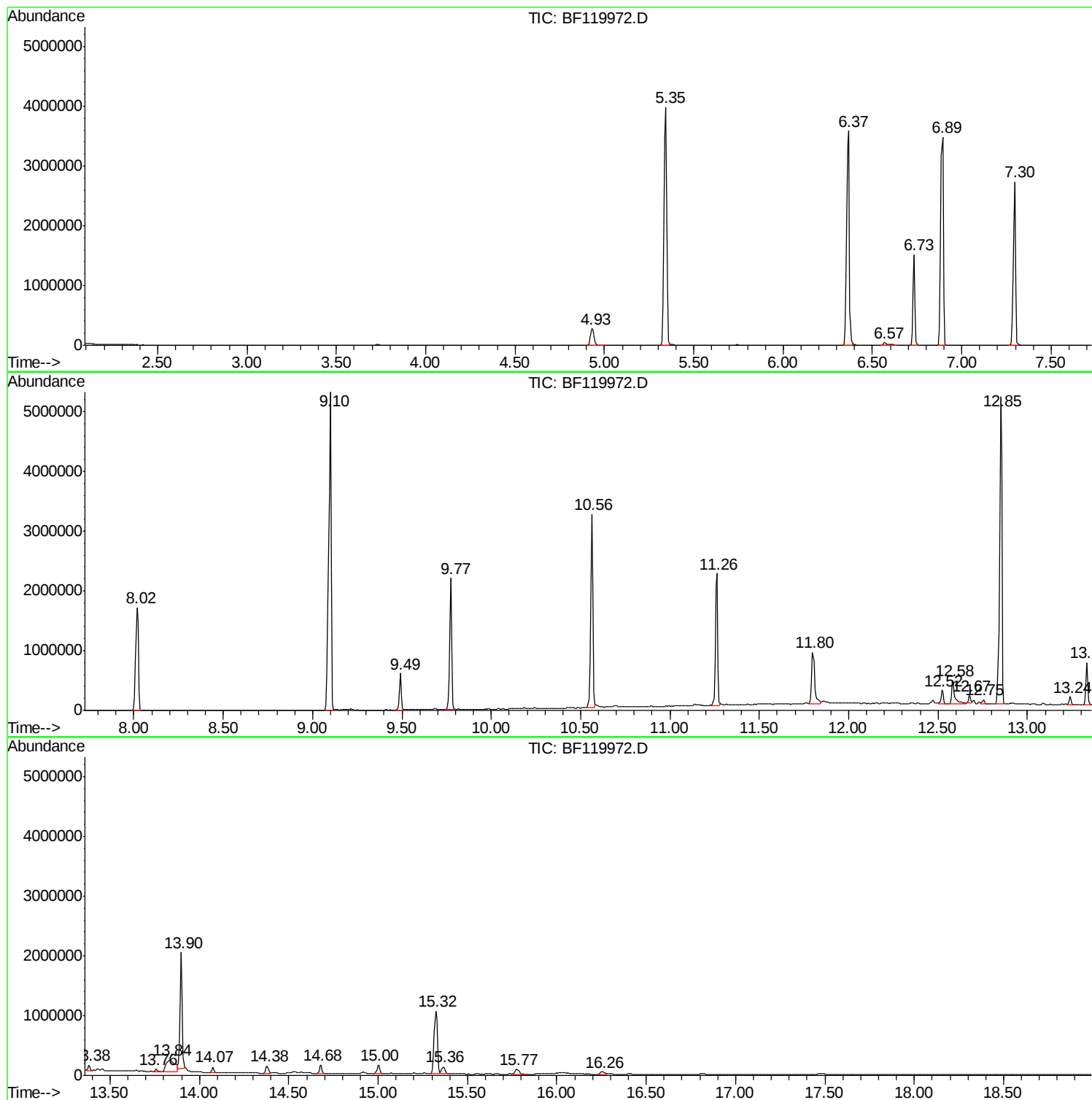
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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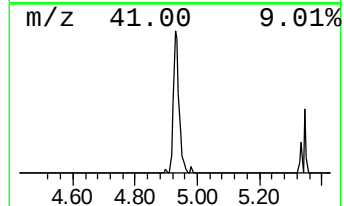
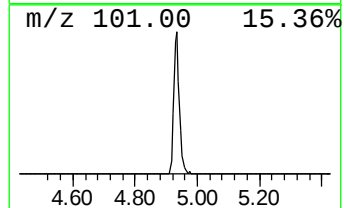
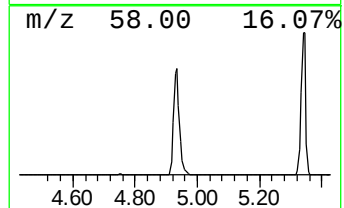
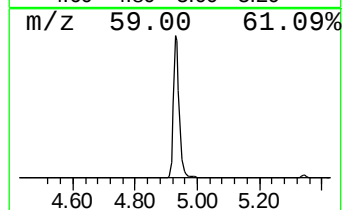
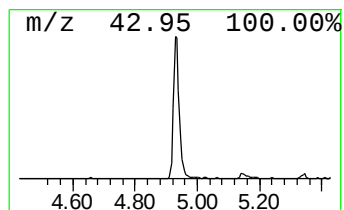
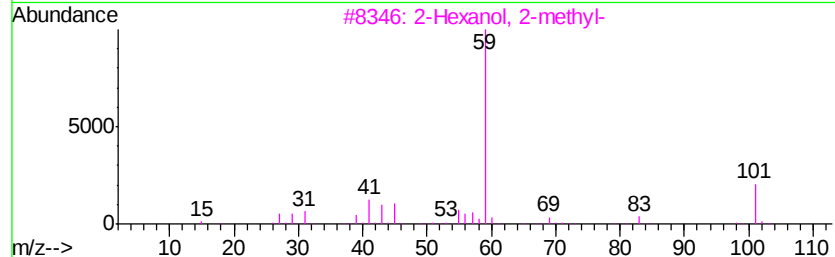
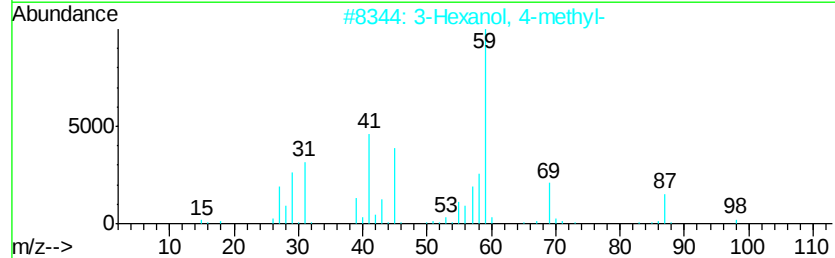
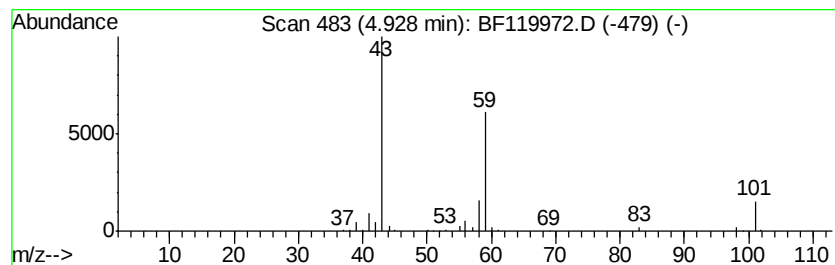
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.93	5.92 ng	361826	1,4-Dichlorobenzene-d4	6.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
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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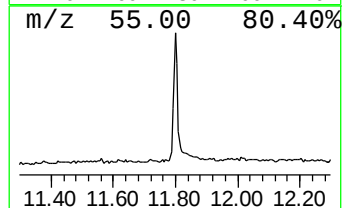
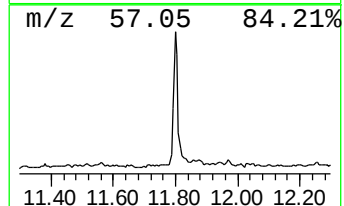
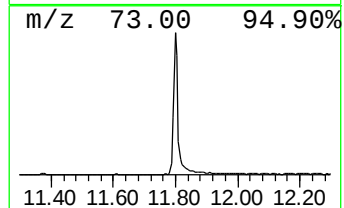
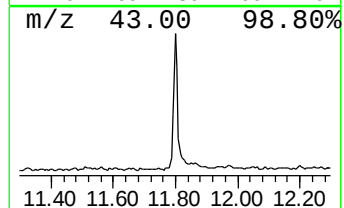
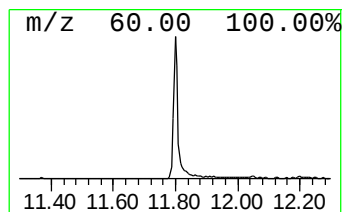
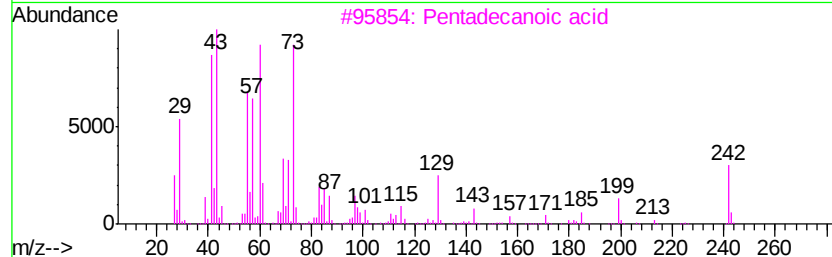
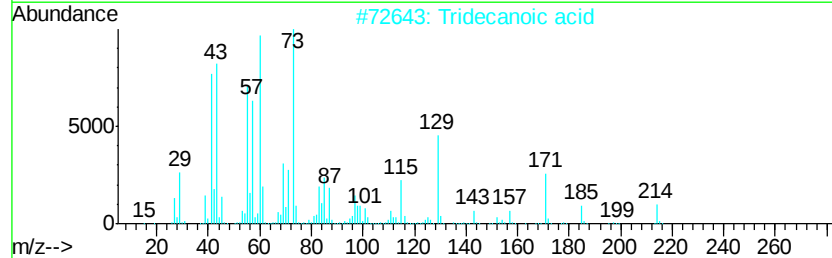
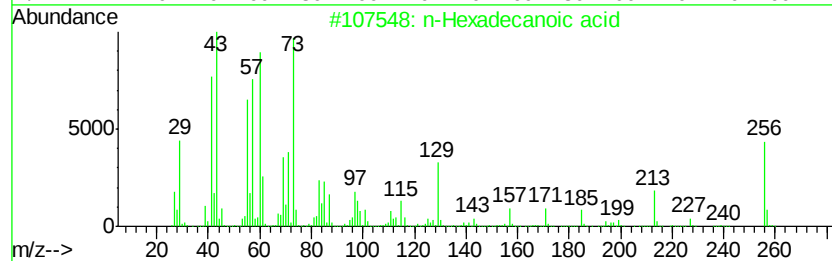
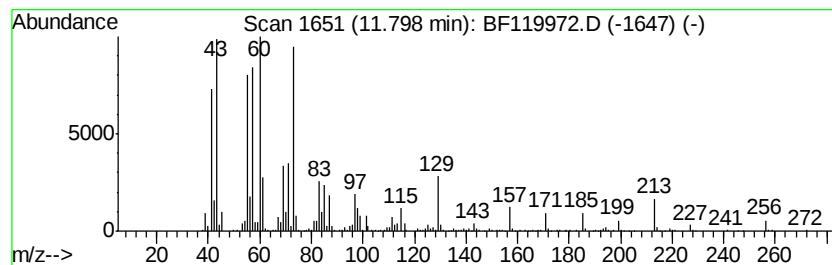
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	8.97 ng	912756	Phenanthrene-d10	11.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Dodecanoic acid	200	C12H24O2	000143-07-7	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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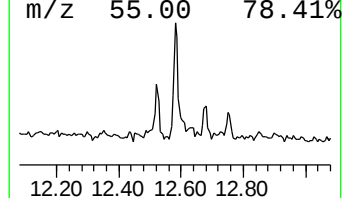
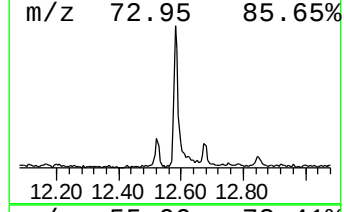
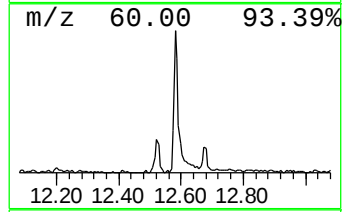
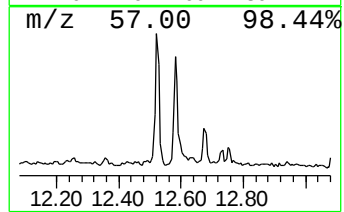
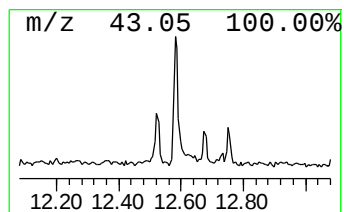
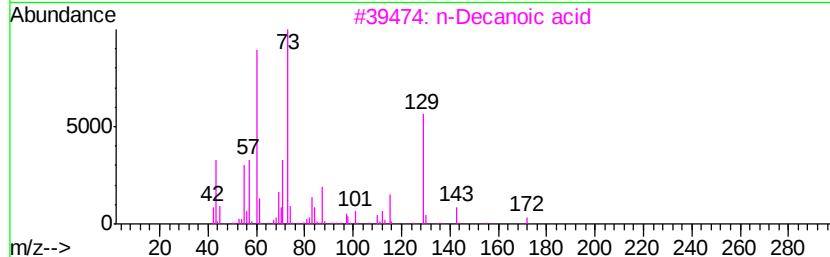
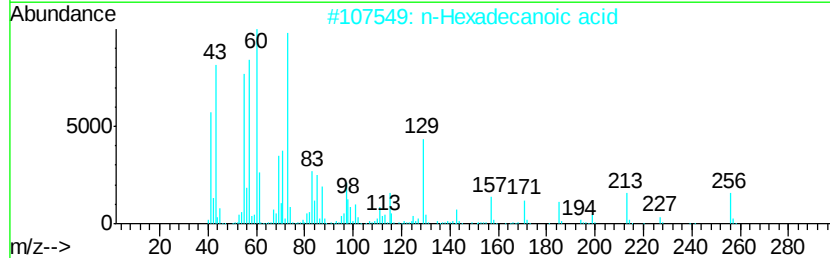
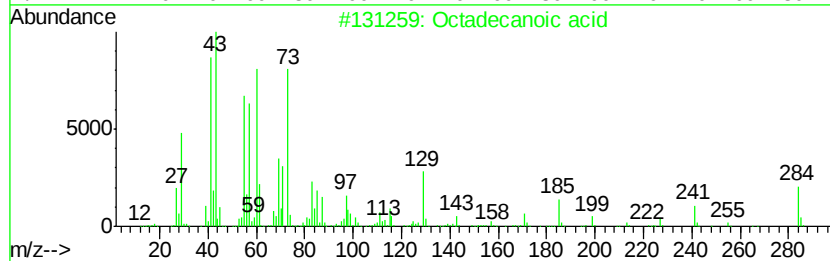
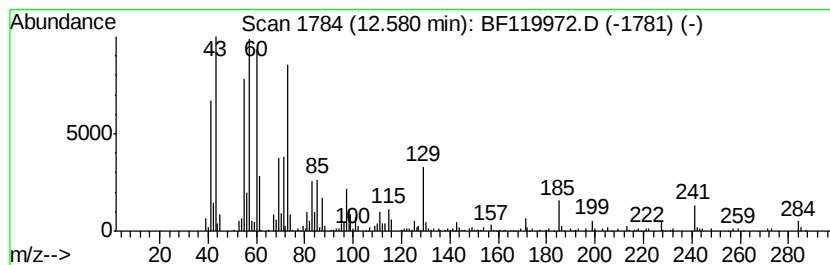
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	5.43 ng	471824	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		n-Decanoic acid	172	C10H20O2	000334-48-5	86
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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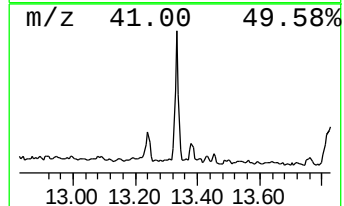
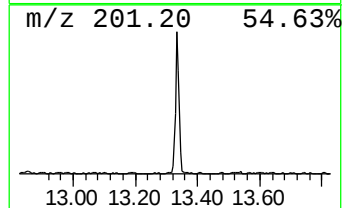
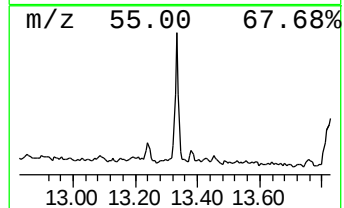
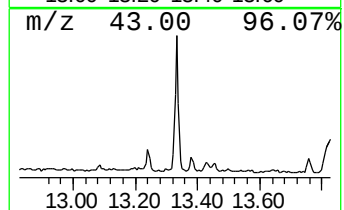
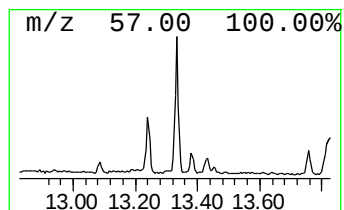
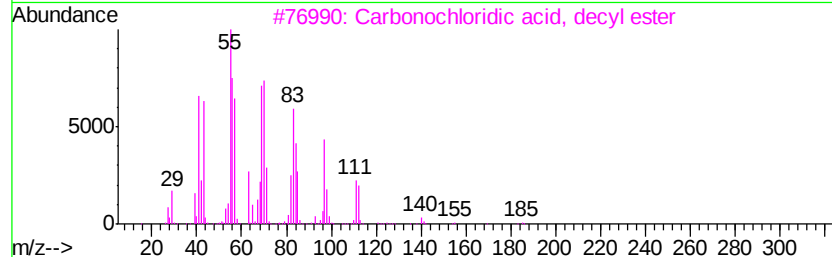
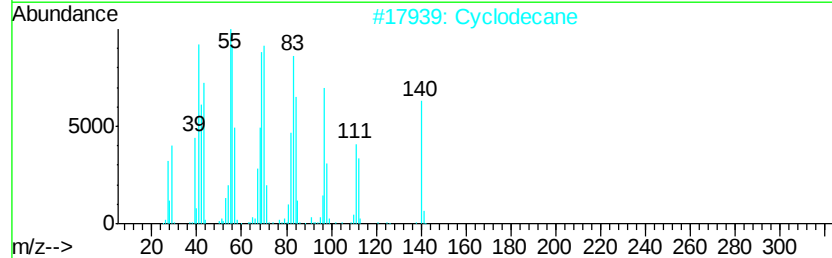
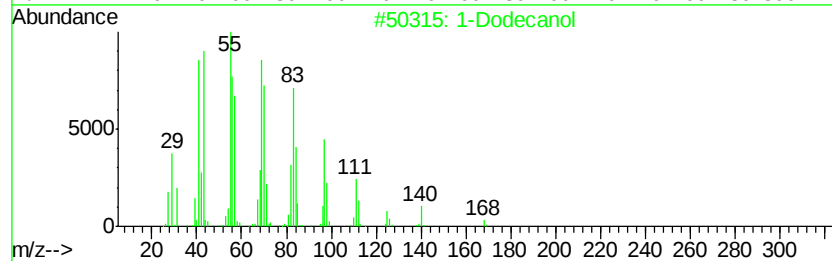
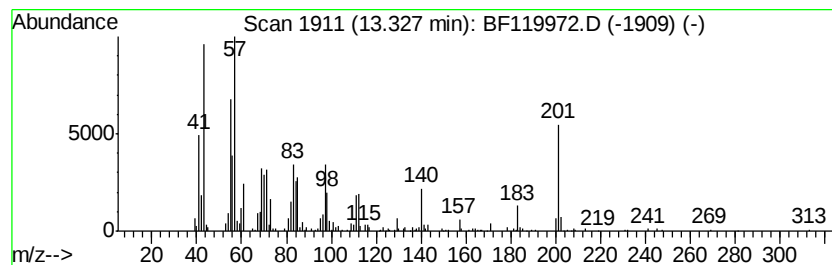
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.33 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	6.63 ng	575849	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol		186	C12H26O	000112-53-8	46
2	Cyclodecane		140	C10H20	000293-96-9	43
3	Carbonochloridic acid, decyl ester		220	C11H21ClO2	055488-51-2	43
4	Cycloheptanone, 2-ethyl-		140	C9H16O	003183-41-3	38
5	1-Hexene-3,5-dione		112	C6H8O2	052204-69-0	35



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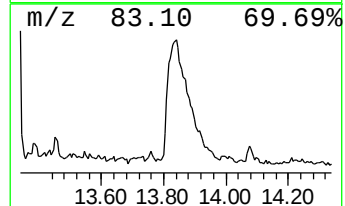
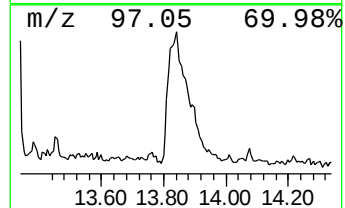
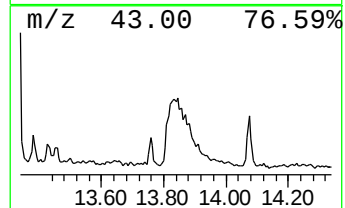
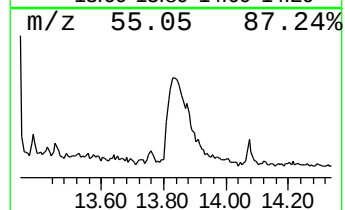
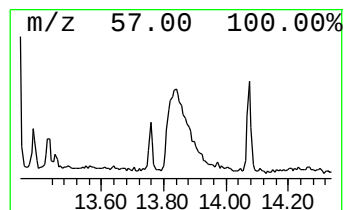
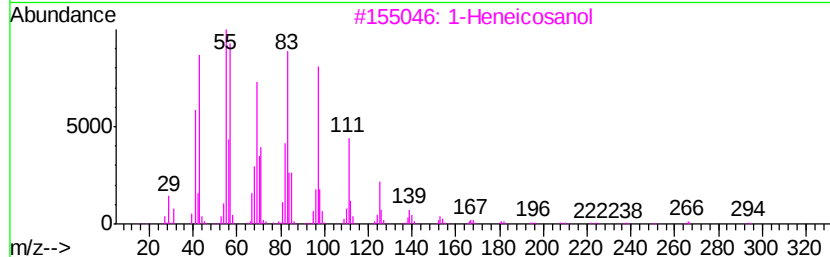
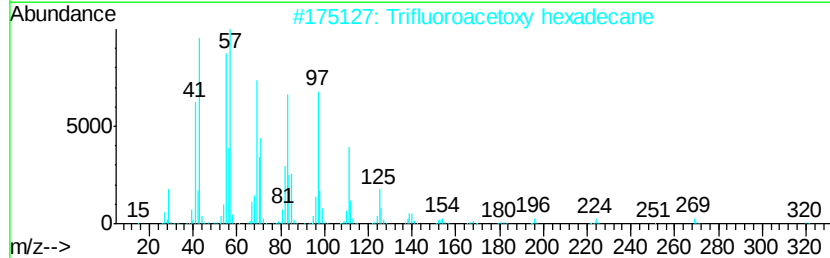
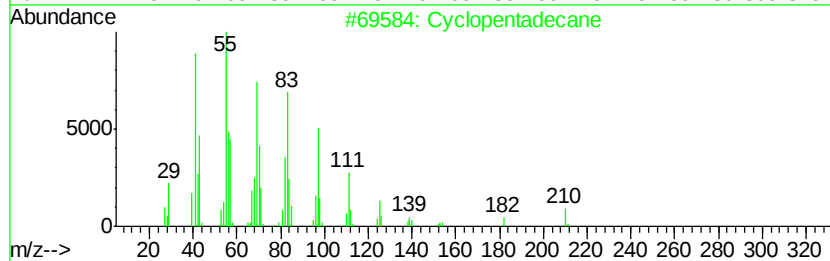
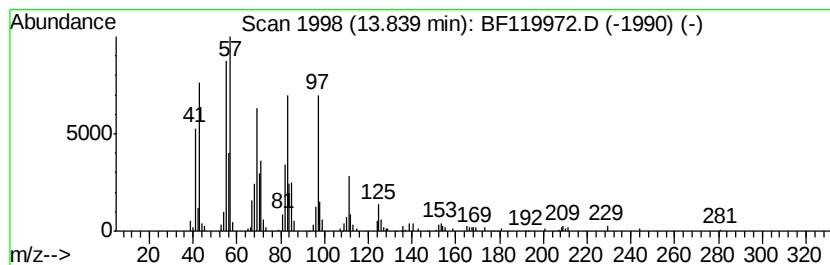
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	7.85 ng	681848	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



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TP-3

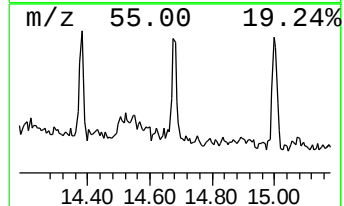
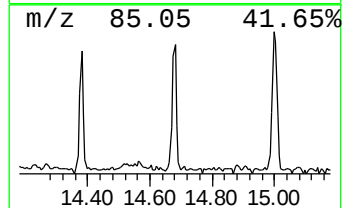
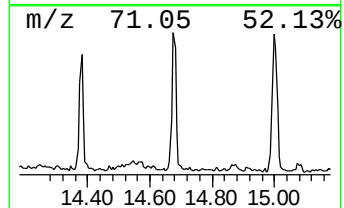
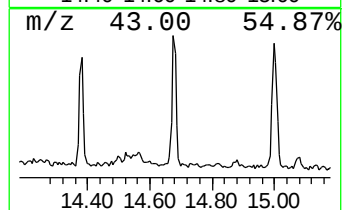
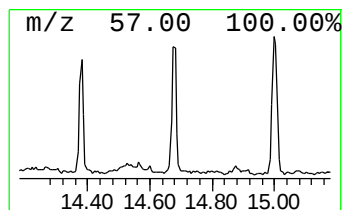
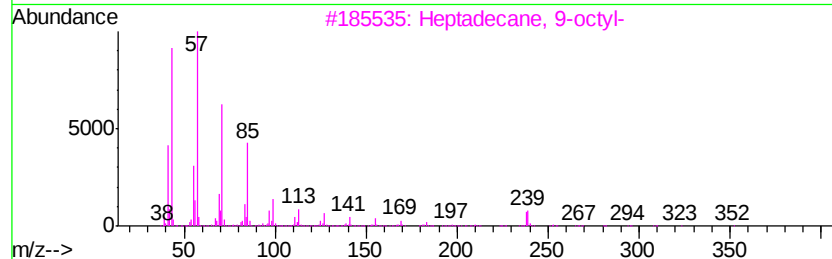
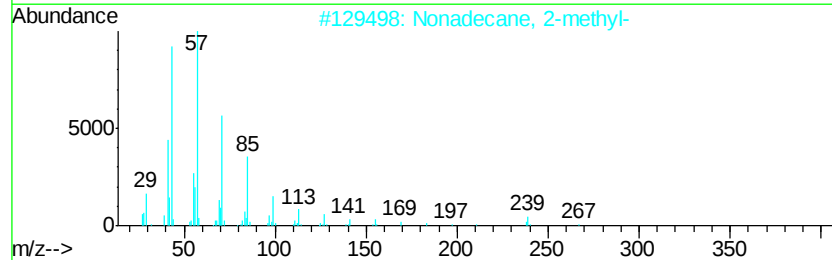
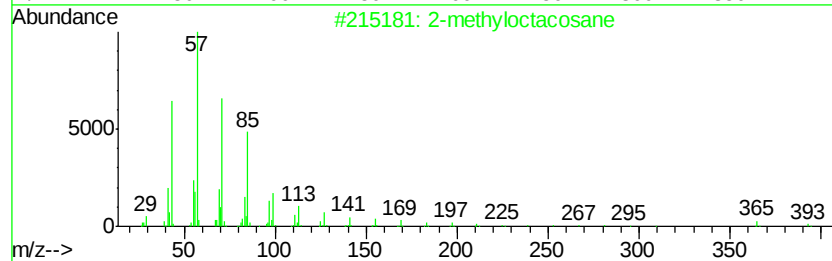
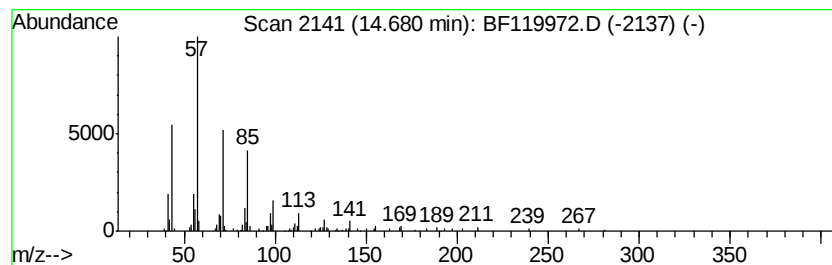
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.68	2.11 ng	133143	Perylene-d12		15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	90
2			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4			Eicosane	282	C20H42	000112-95-8	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041320\
 Data File : BF119972.D
 Acq On : 15 Apr 2020 00:25
 Operator : MA/SJ
 Sample : L2215-17
 Misc :
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

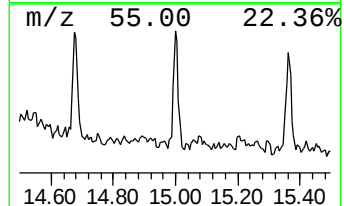
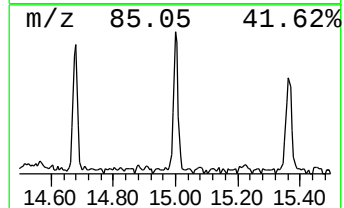
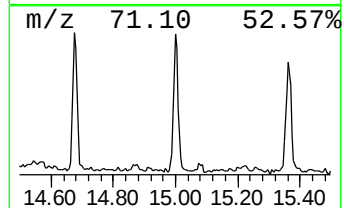
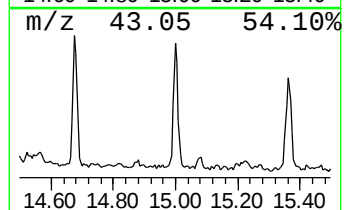
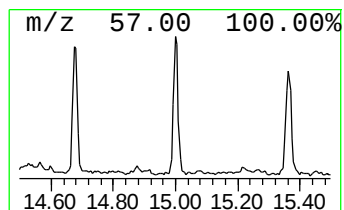
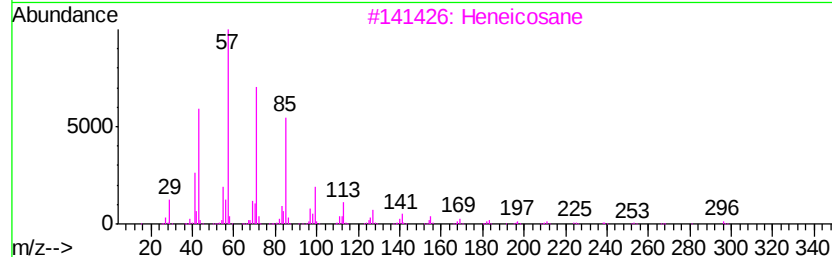
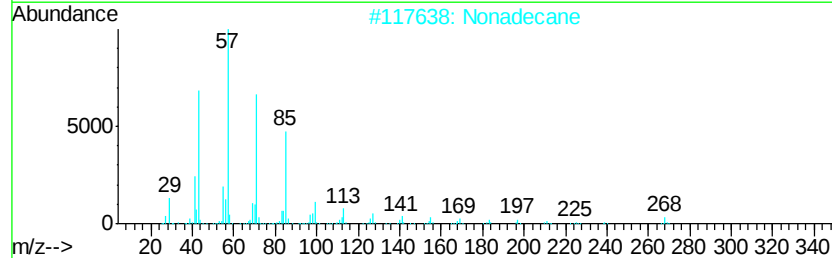
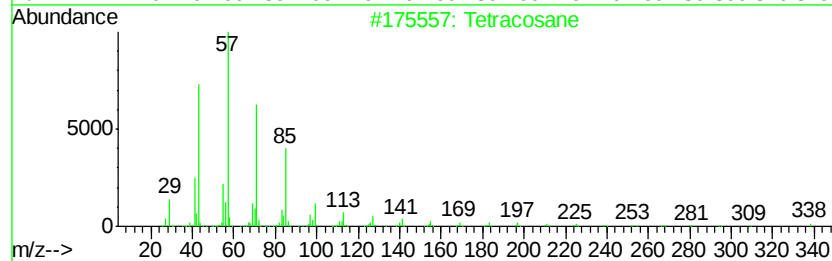
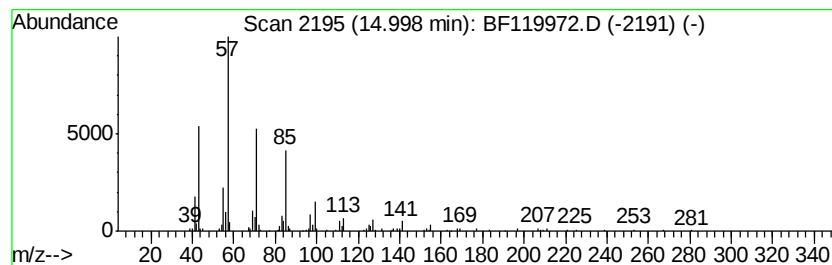
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.68 ng	169155	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Nonadecane	268	C19H40	000629-92-5	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041320\
Data File : BF119972.D
Acq On : 15 Apr 2020 00:25
Operator : MA/SJ
Sample : L2215-17
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

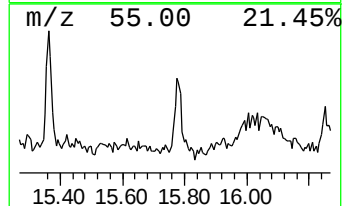
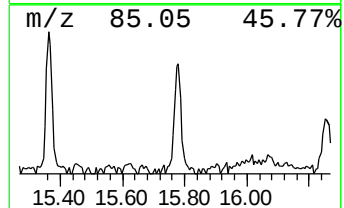
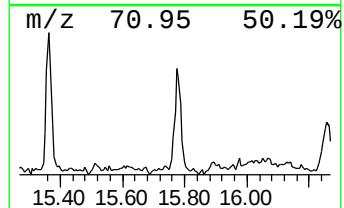
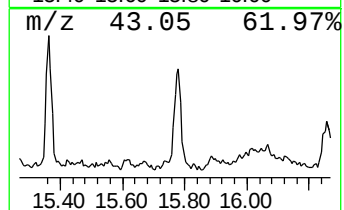
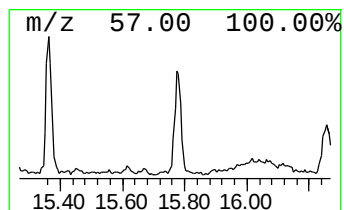
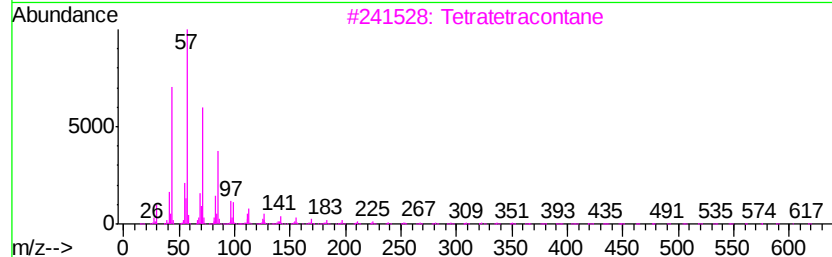
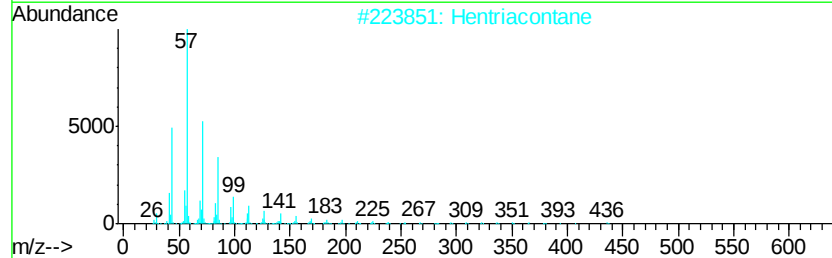
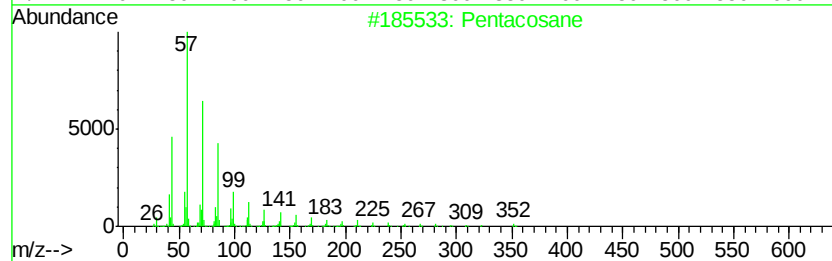
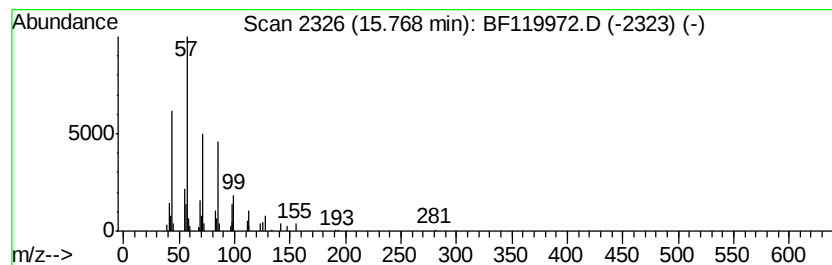
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.08 ng	131523	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	90
2	Hentriacontane		437	C31H64	000630-04-6	87
3	Tetratetracontane		619	C44H90	007098-22-8	87
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041320\
Data File : BF119972.D
Acq On : 15 Apr 2020 00:25
Operator : MA/SJ
Sample : L2215-17
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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...	4.93	5.9	ng	361826	1	6.73	1222290	20.0
n-Hexadecanoic acid	11.80	9.0	ng	912756	4	11.26	2034320	20.0
Octadecanoic acid	12.58	5.4	ng	471824	5	13.90	1738250	20.0
unknown13.33	13.33	6.6	ng	575849	5	13.90	1738250	20.0
Cyclopentadecane	13.84	7.8	ng	681848	5	13.90	1738250	20.0
2-methyloctacosane	14.68	2.1	ng	133143	6	15.32	1261720	20.0
Tetracosane	15.00	2.7	ng	169155	6	15.32	1261720	20.0
Pentacosane	15.77	2.1	ng	131523	6	15.32	1261720	20.0