

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091018\
 Data File : BF108905.D
 Acq On : 10 Sep 2018 20:44
 Operator : JU/SJ
 Sample : J4834-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 C-1

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-BF090518.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	4.937	438	442	452	rVB	120330	145377	4.16%	0.460%
2	5.354	508	513	516	rBV	3227665	3279482	93.76%	10.367%
3	6.372	681	686	689	rBV	3219694	3457472	98.85%	10.930%
4	6.507	705	709	713	rBV	3661741	3415002	97.64%	10.796%
5	6.572	717	720	730	rVB	52620	52645	1.51%	0.166%
6	6.742	745	749	752	rBV	1165748	1012827	28.96%	3.202%
7	6.895	771	775	779	rBV	3098697	2691792	76.96%	8.509%
8	7.295	839	843	846	rBV	2219980	2114774	60.46%	6.685%
9	8.019	963	966	970	rBV	1462943	1154126	33.00%	3.648%
10	9.095	1145	1149	1152	rBV	4271167	3497598	100.00%	11.057%
11	9.489	1212	1216	1219	rBV	763730	680180	19.45%	2.150%
12	9.772	1260	1264	1267	rBV	1212582	1043279	29.83%	3.298%
13	10.554	1393	1397	1400	rBV	2006785	1701892	48.66%	5.380%
14	11.248	1511	1515	1518	rBV	1237450	969905	27.73%	3.066%
15	11.783	1603	1606	1616	rBV2	94371	109473	3.13%	0.346%
16	12.830	1780	1784	1787	rBV	3667076	3161120	90.38%	9.993%
17	13.419	1881	1884	1889	rVB	57914	52100	1.49%	0.165%
18	13.742	1935	1939	1945	rBV2	169310	223203	6.38%	0.706%
19	13.871	1957	1961	1965	rBV	1377685	1258703	35.99%	3.979%
20	14.060	1990	1993	1996	rBV	104038	89417	2.56%	0.283%
21	14.366	2041	2045	2048	rBV	108779	123217	3.52%	0.390%
22	14.660	2092	2095	2099	rVB	125147	114354	3.27%	0.361%
23	14.730	2105	2107	2110	rVB	49004	41821	1.20%	0.132%
24	14.977	2146	2149	2155	rVB	123552	125990	3.60%	0.398%
25	15.283	2197	2201	2206	rVV	732258	853858	24.41%	2.699%
26	15.336	2207	2210	2219	rVB	117472	156188	4.47%	0.494%
27	15.742	2276	2279	2284	rBV2	77206	107577	3.08%	0.340%

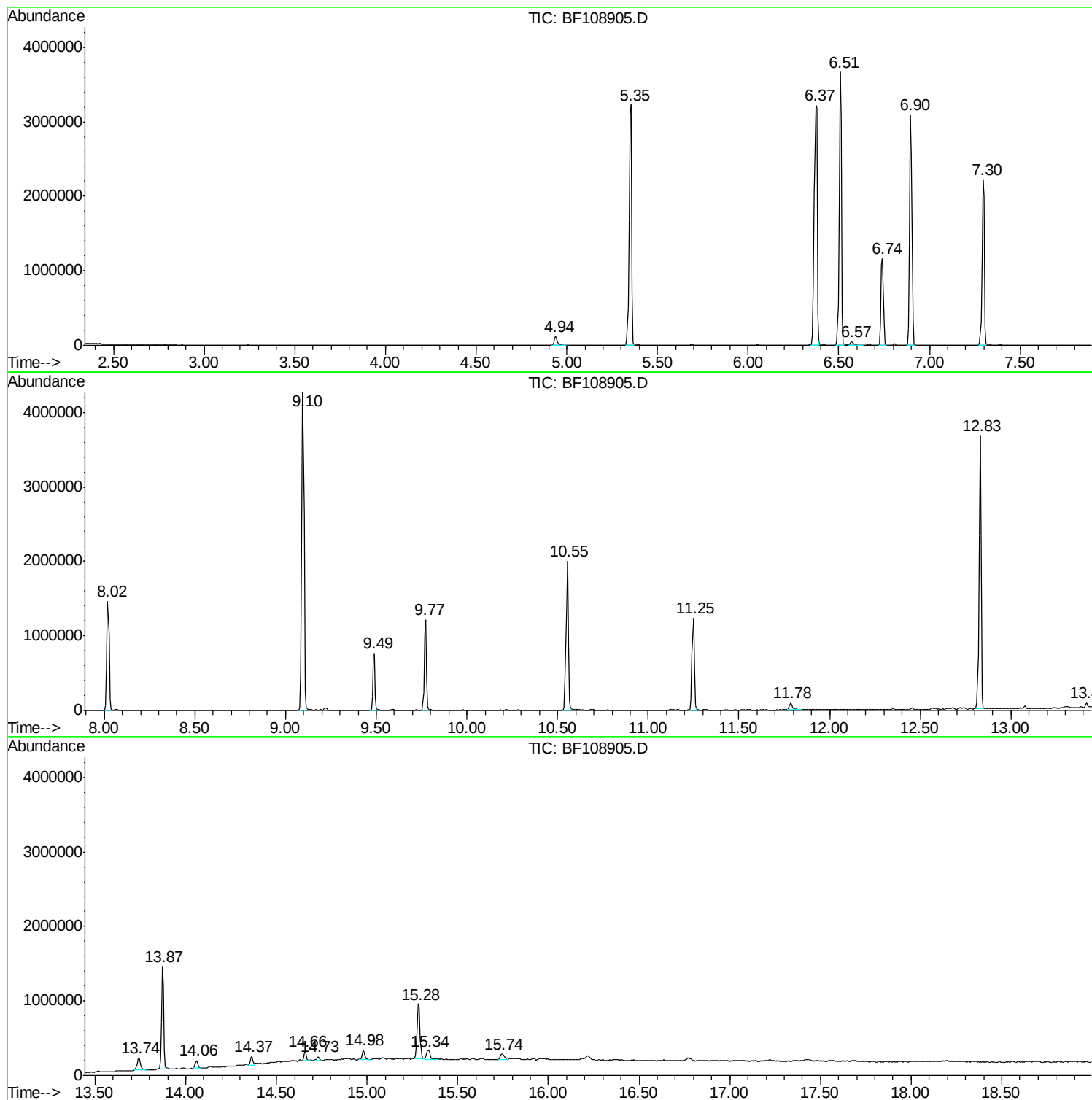
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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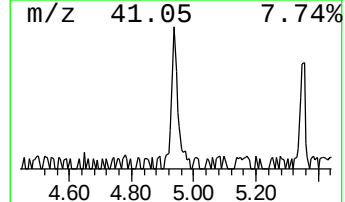
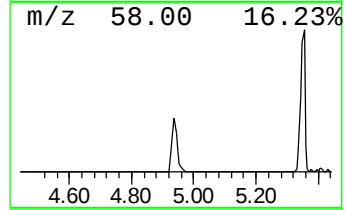
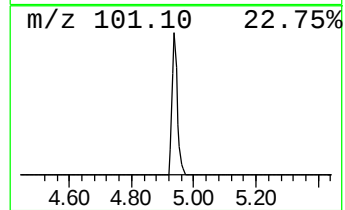
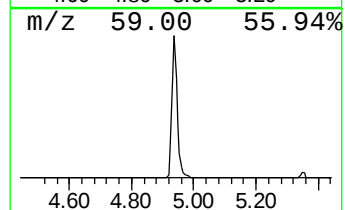
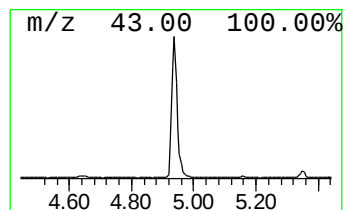
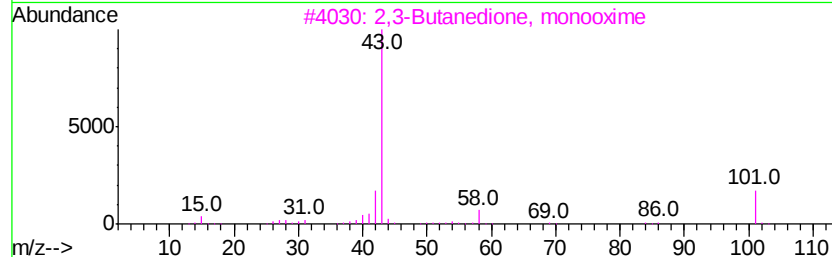
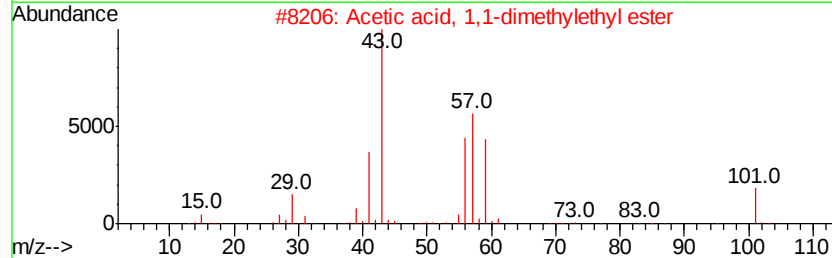
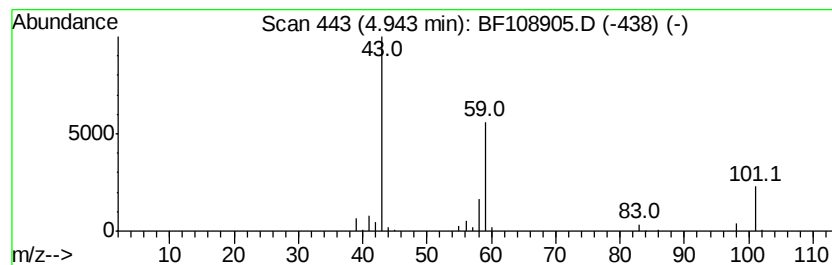
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.87 ng	145377	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Guanidine	59	CH5N3	000113-00-8	9



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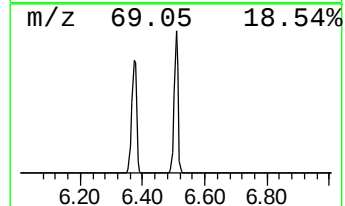
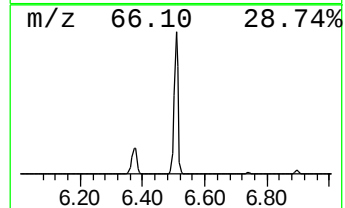
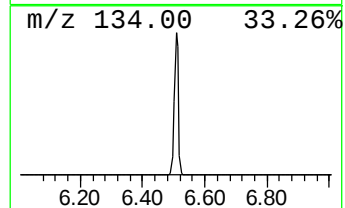
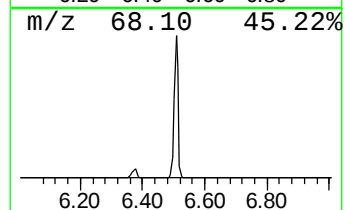
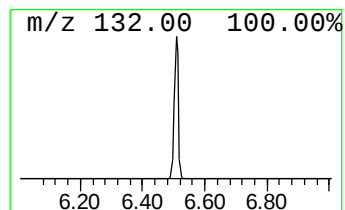
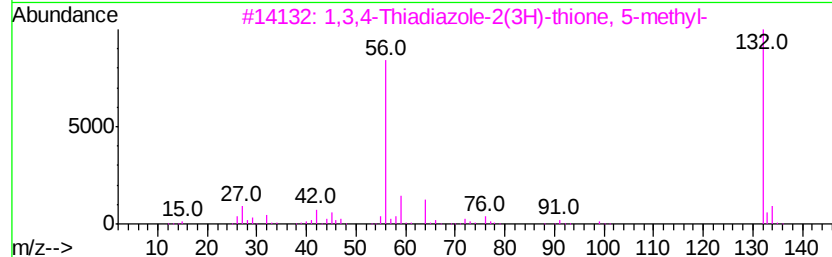
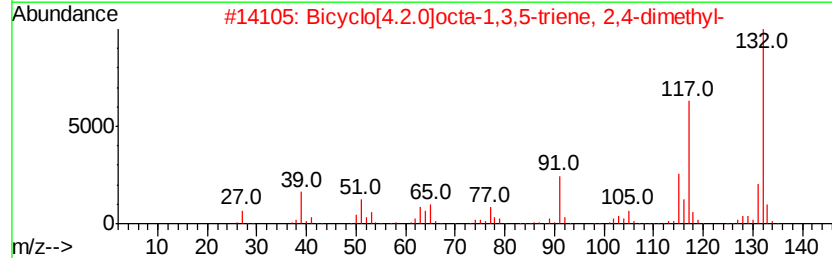
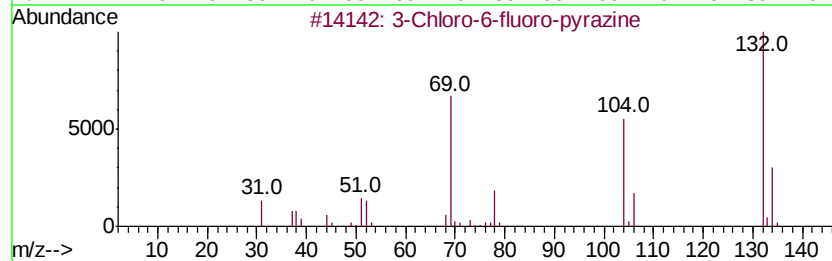
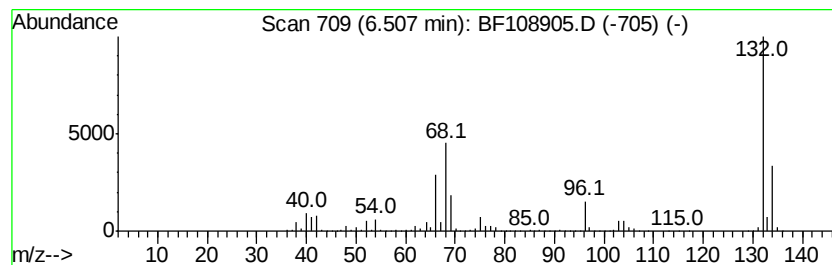
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	67.44 ng	3415000	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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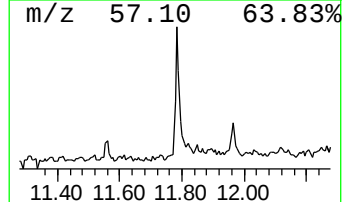
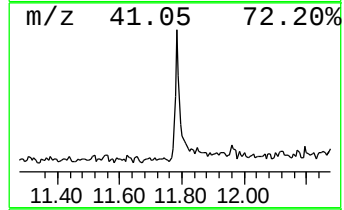
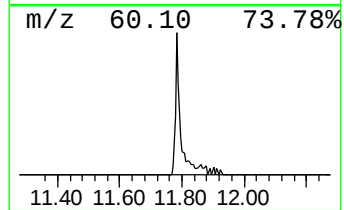
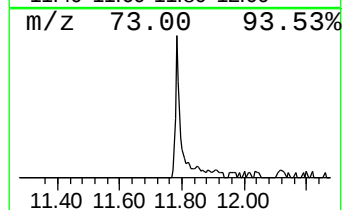
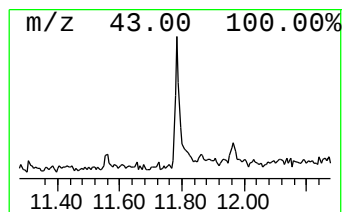
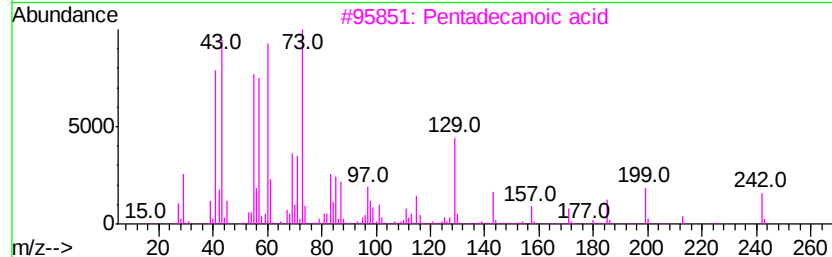
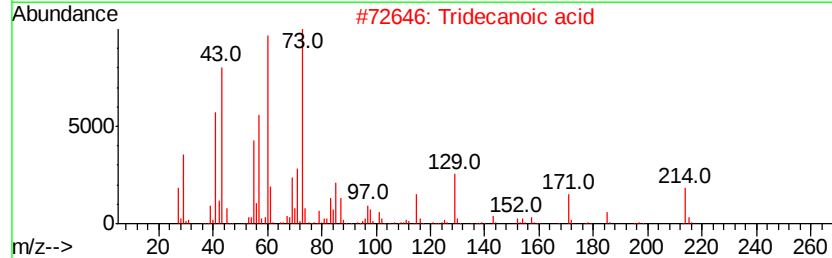
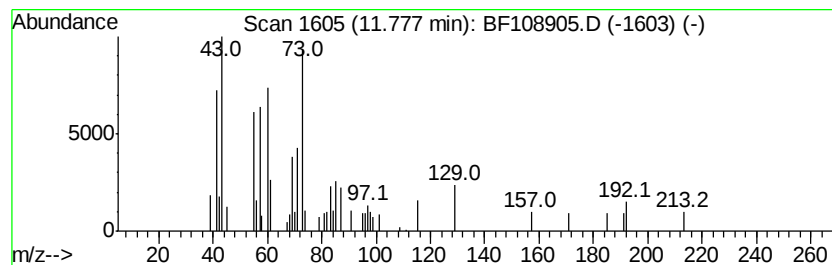
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.26 ng	109473	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	53



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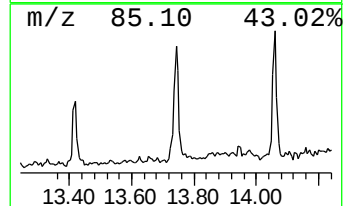
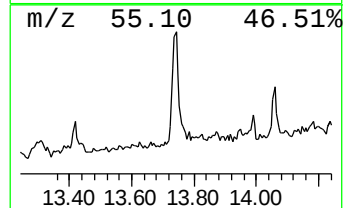
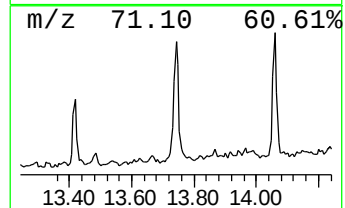
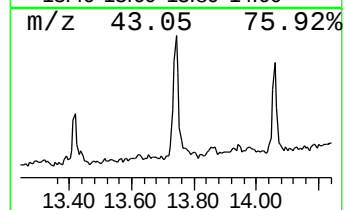
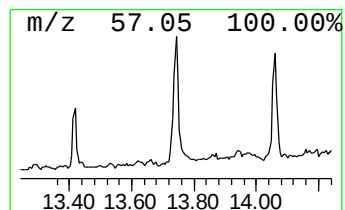
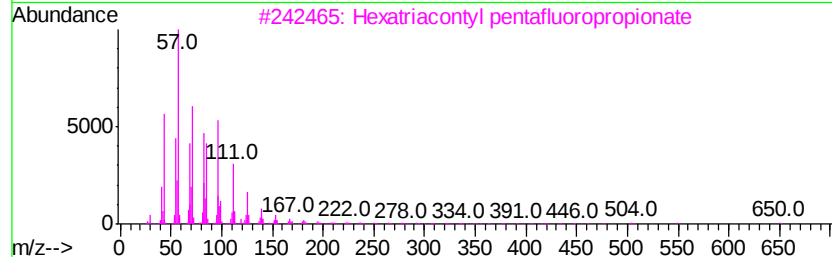
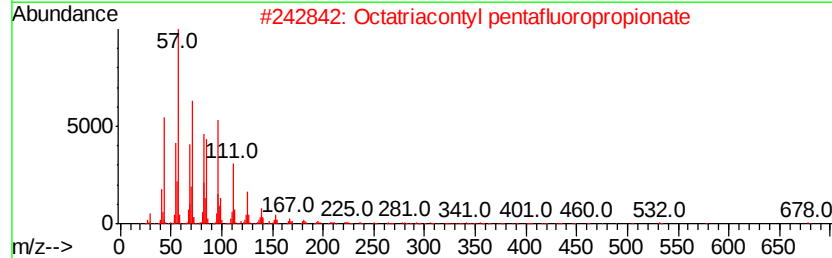
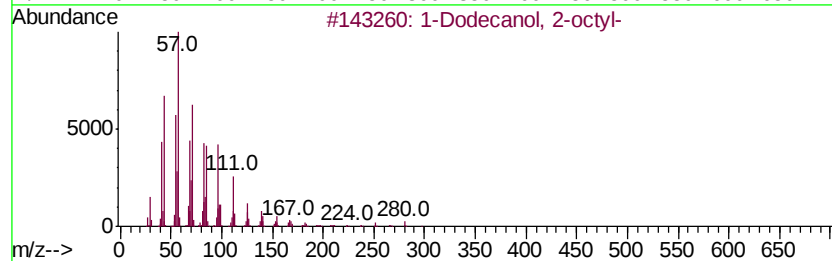
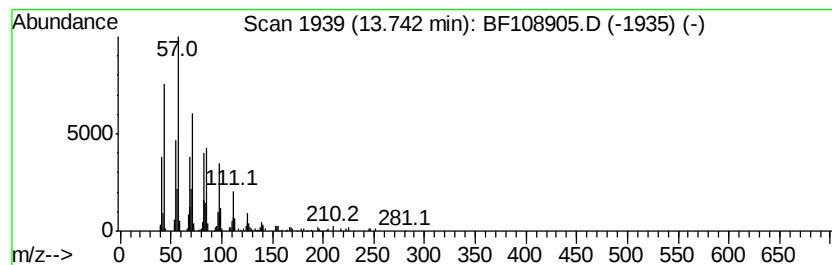
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Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.55 ng	223203	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91
3		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
5		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91



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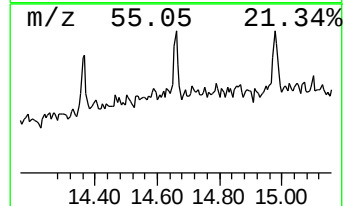
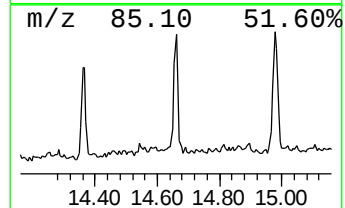
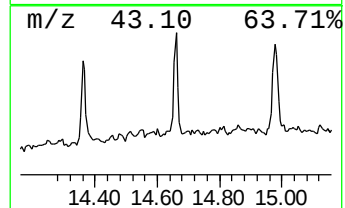
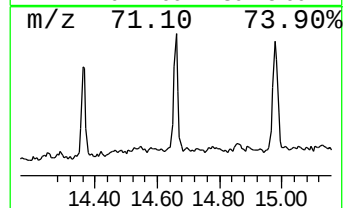
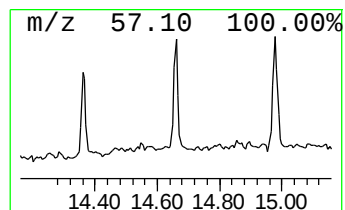
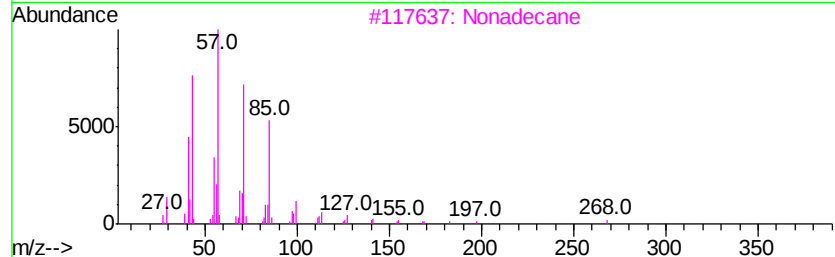
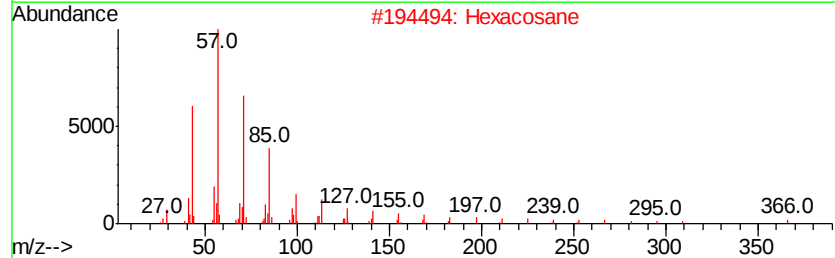
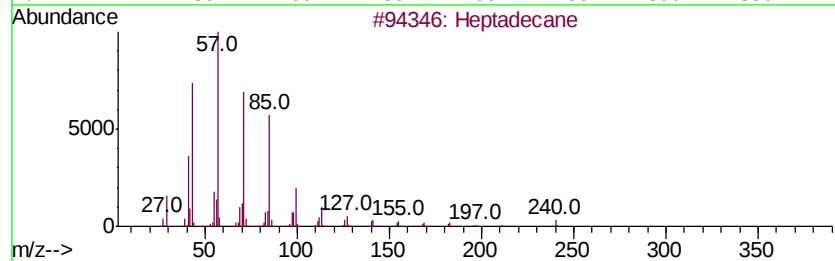
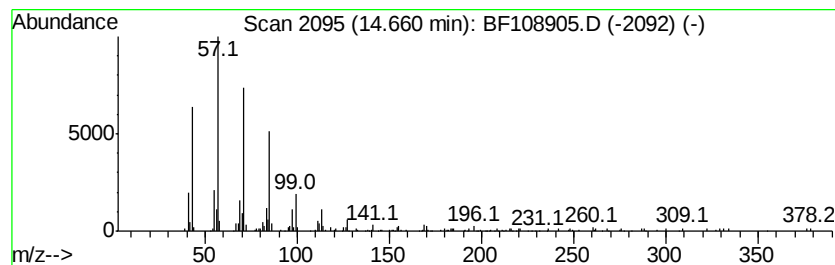
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Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.68 ng	114354	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Nonadecane		268	C19H40	000629-92-5	90
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	87
5	2-Bromo dodecane		248	C12H25Br	013187-99-0	86



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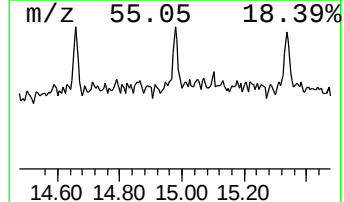
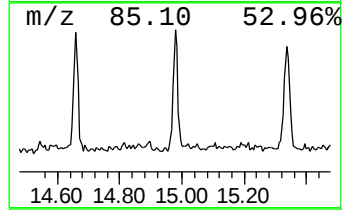
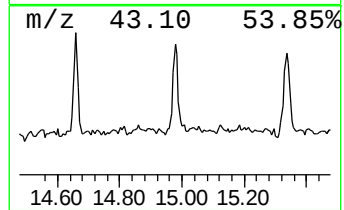
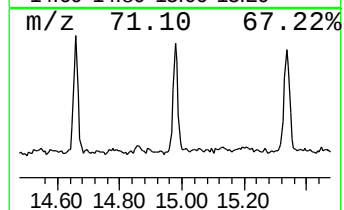
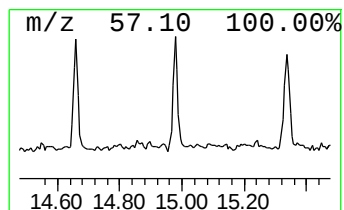
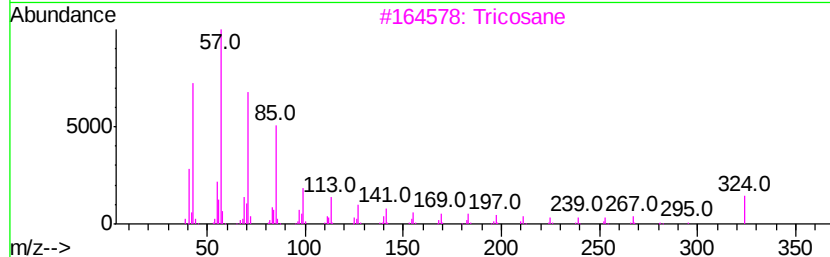
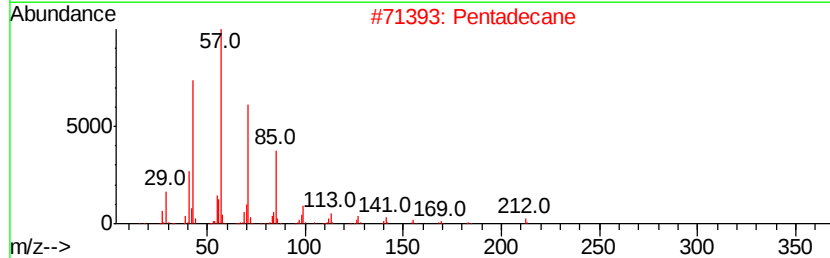
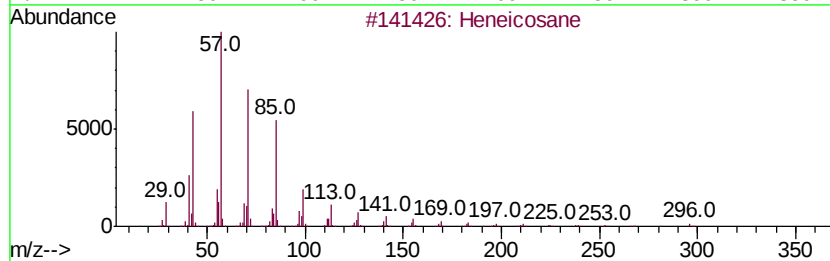
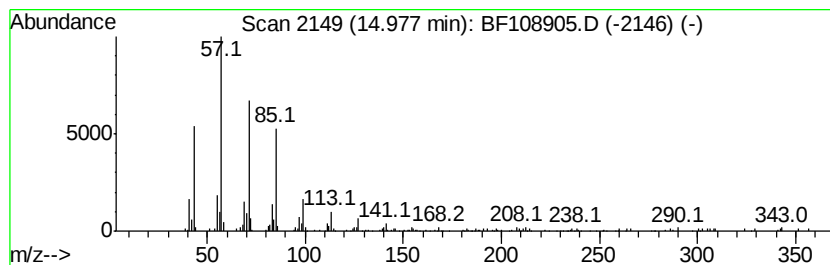
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.95 ng	125990	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Pentadecane		212	C15H32	000629-62-9	90
3	Tricosane		324	C23H48	000638-67-5	90
4	Nonadecane		268	C19H40	000629-92-5	87
5	Tridecanol, 2-ethyl-2-methyl-		242	C16H34O	1000115-66-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108905.D
Acq On : 10 Sep 2018 20:44
Operator : JU/SJ
Sample : J4834-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

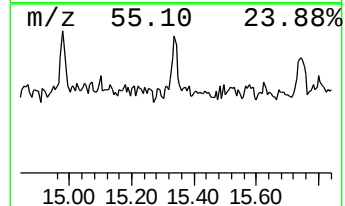
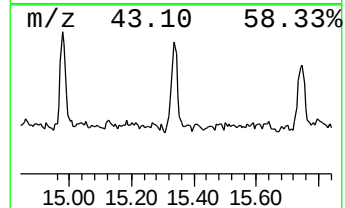
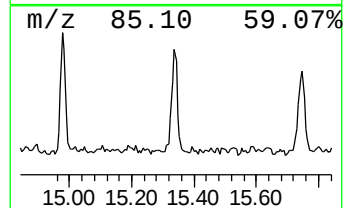
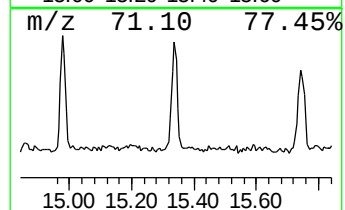
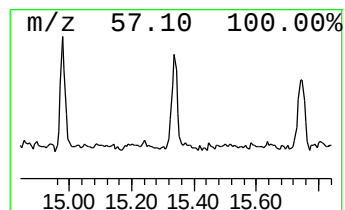
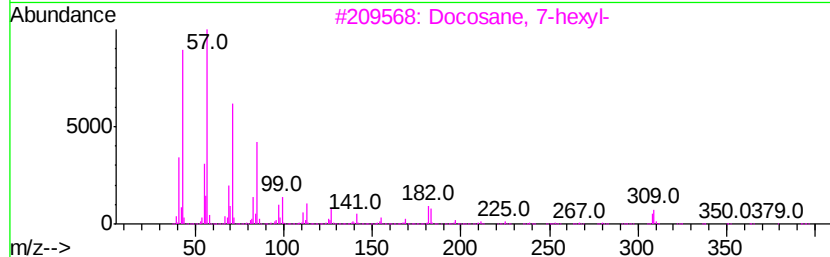
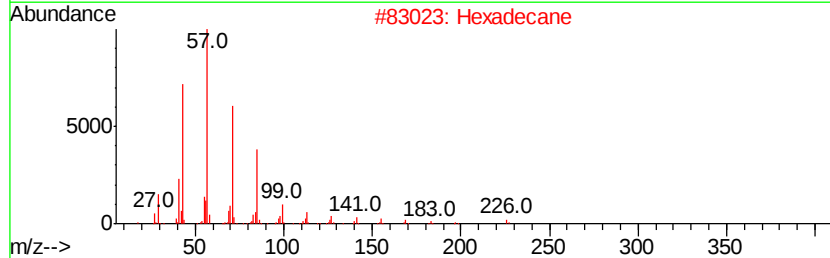
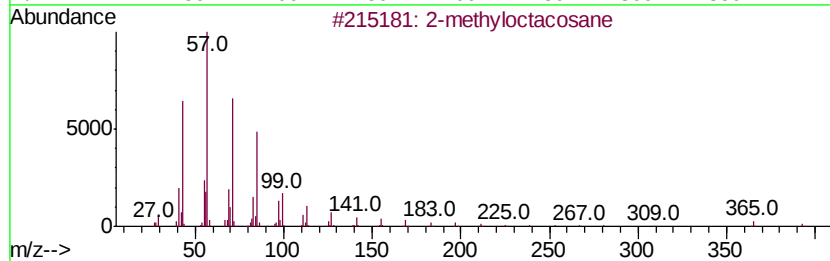
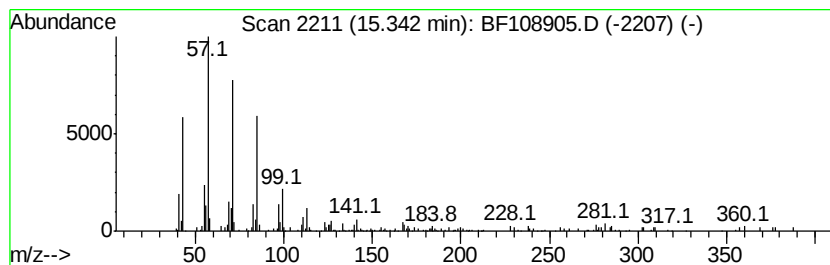
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.66 ng	156188	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexadecane	226	C16H34	000544-76-3	90
3		Docosane, 7-hexyl-	394	C28H58	055373-86-9	90
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108905.D
Acq On : 10 Sep 2018 20:44
Operator : JU/SJ
Sample : J4834-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

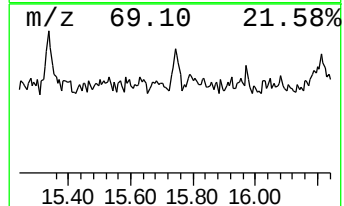
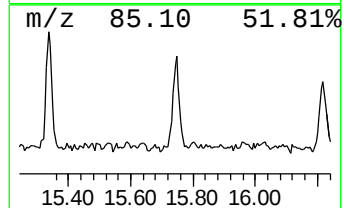
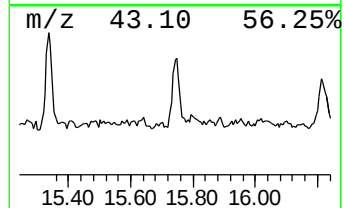
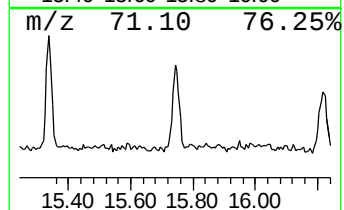
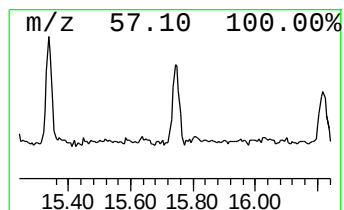
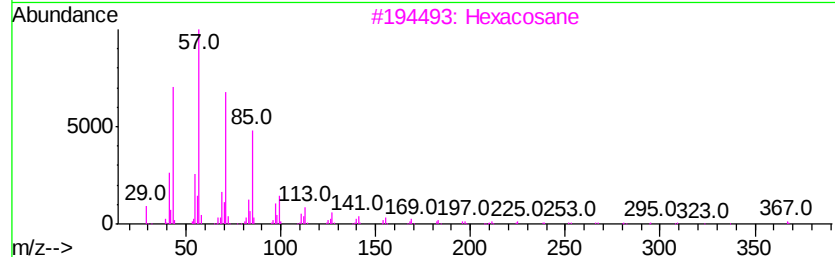
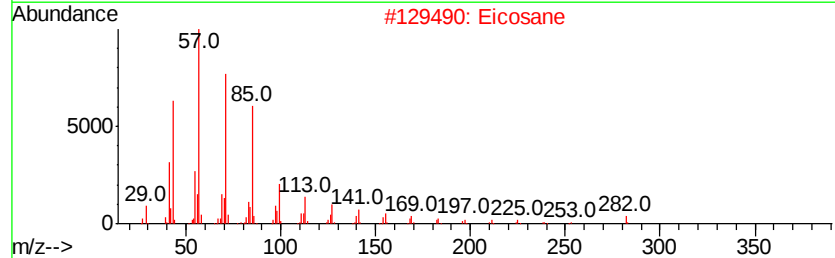
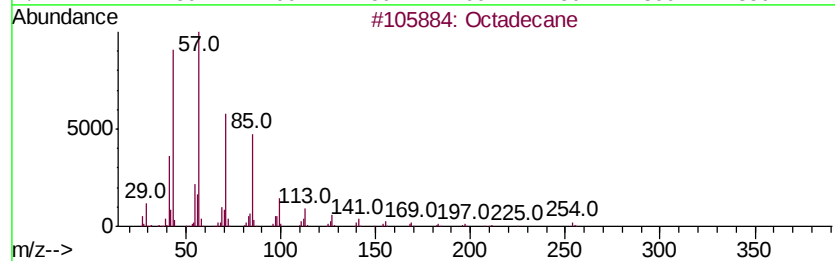
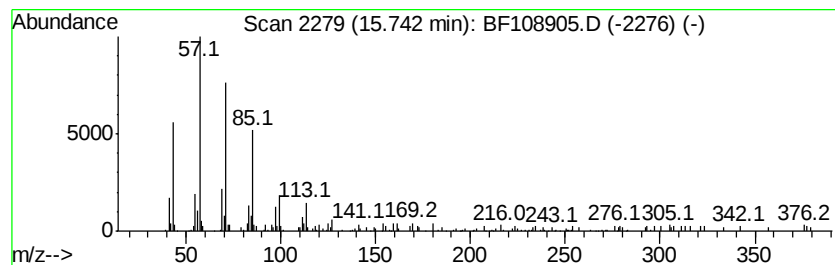
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.52 ng	107577	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	93
2	Eicosane		282	C20H42	000112-95-8	90
3	Hexacosane		366	C26H54	000630-01-3	90
4	Heneicosane		296	C21H44	000629-94-7	90
5	Octadecane, 2-methyl-		268	C19H40	001560-88-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091018\
Data File : BF108905.D
Acq On : 10 Sep 2018 20:44
Operator : JU/SJ
Sample : J4834-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.94	2.9	ng	145377	1	6.74	1012830	20.0
unknown6.51	6.51	67.4	ng	3415000	1	6.74	1012830	20.0
n-Hexadecanoic acid	11.78	2.3	ng	109473	4	11.25	969905	20.0
1-Dodecanol, 2-oc...	13.74	3.5	ng	223203	5	13.87	1258700	20.0
Heptadecane	14.66	2.7	ng	114354	6	15.28	853858	20.0
Heneicosane	14.98	3.0	ng	125990	6	15.28	853858	20.0
2-methyloctacosane	15.34	3.7	ng	156188	6	15.28	853858	20.0
Octadecane	15.74	2.5	ng	107577	6	15.28	853858	20.0