

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110417\
 Data File : BF100190.D
 Acq On : 4 Nov 2017 20:31
 Operator : SJ/JU
 Sample : I6313-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF015-01

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	4.981	490	492	511	rBV	123343	232882	11.30%	1.355%
2	5.393	560	562	601	rBV	1002549	1577503	76.56%	9.180%
3	6.416	733	736	754	rBV	1319951	1606653	77.97%	9.349%
4	6.540	754	757	770	rVB	1679097	1704323	82.71%	9.918%
5	6.763	792	795	809	rVB	506886	472326	22.92%	2.748%
6	6.916	818	821	839	rBV	1398383	1316912	63.91%	7.663%
7	7.334	889	892	913	rBV	884906	969252	47.04%	5.640%
8	8.045	1010	1013	1035	rBV	712146	670772	32.55%	3.903%
9	9.116	1191	1195	1206	rBV	2337485	2060571	100.00%	11.991%
10	9.516	1260	1263	1275	rBB	119048	112779	5.47%	0.656%
11	9.798	1307	1311	1325	rVB	833745	783283	38.01%	4.558%
12	10.592	1443	1446	1459	rBV	1131927	1118119	54.26%	6.506%
13	10.727	1466	1469	1483	rVB	34699	45005	2.18%	0.262%
14	11.286	1561	1564	1574	rBV	793397	785920	38.14%	4.573%
15	11.804	1649	1652	1662	rBV2	53155	62818	3.05%	0.366%
16	12.586	1782	1785	1791	rBV2	30335	38057	1.85%	0.221%
17	12.868	1829	1833	1836	rBV	2162043	1979213	96.05%	11.517%
18	13.739	1978	1981	1988	rBV	48228	58175	2.82%	0.339%
19	13.939	2011	2015	2025	rBV	581662	575208	27.91%	3.347%
20	14.657	2134	2137	2141	rBV3	47305	53784	2.61%	0.313%
21	14.980	2187	2192	2197	rBV	44900	50597	2.46%	0.294%
22	15.339	2249	2253	2259	rVB	68589	80339	3.90%	0.467%
23	15.398	2259	2263	2276	rBV	290185	434806	21.10%	2.530%
24	15.751	2318	2323	2329	rBV2	61815	87235	4.23%	0.508%
25	16.227	2398	2404	2417	rVB2	59137	110643	5.37%	0.644%
26	16.780	2492	2498	2506	rVB3	37190	79507	3.86%	0.463%
27	17.439	2603	2610	2618	rBV4	28117	64430	3.13%	0.375%
28	18.215	2734	2742	2752	rBV7	17495	53859	2.61%	0.313%

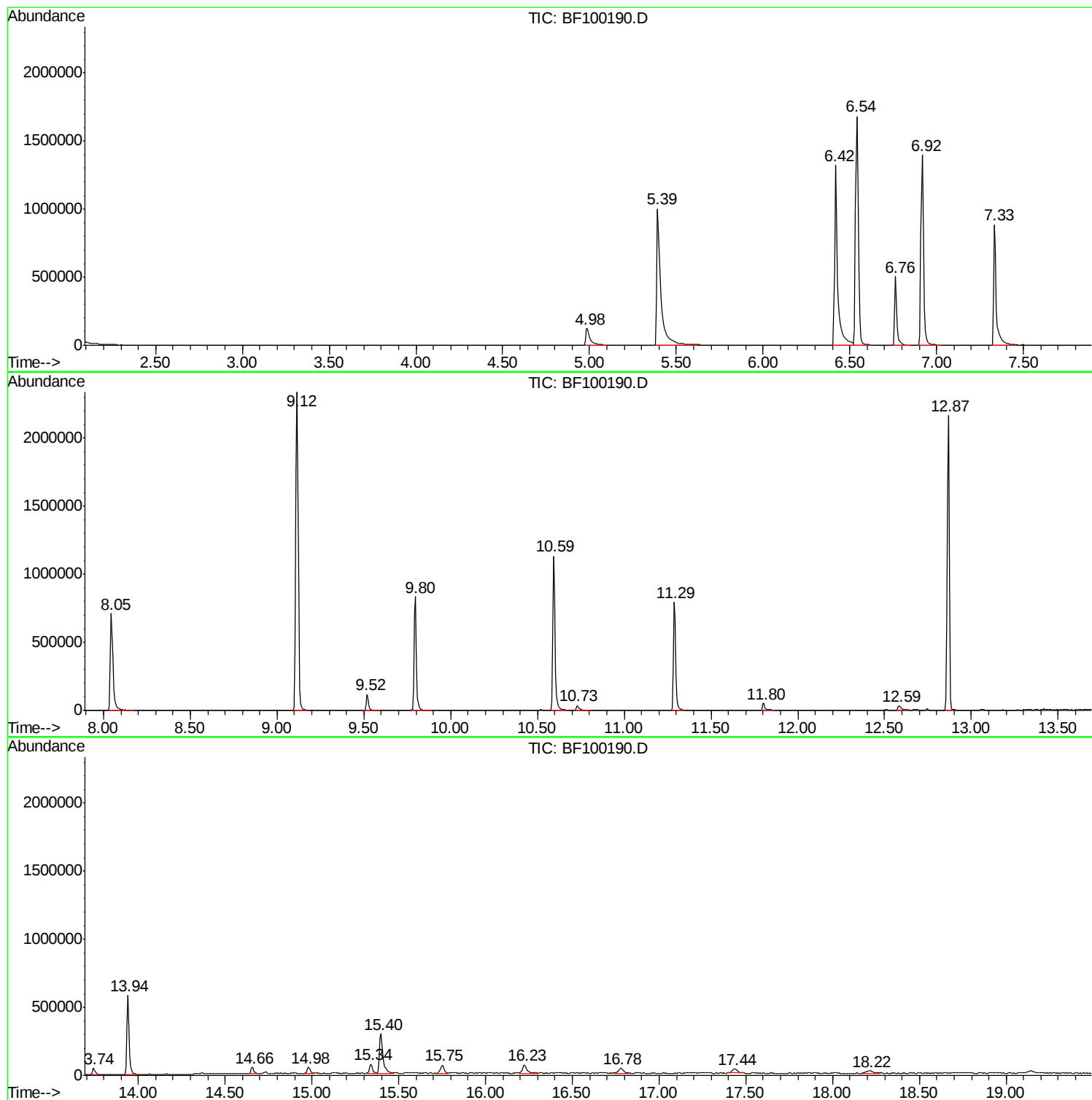
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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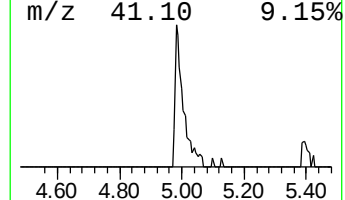
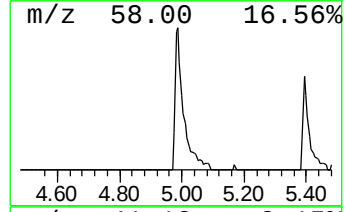
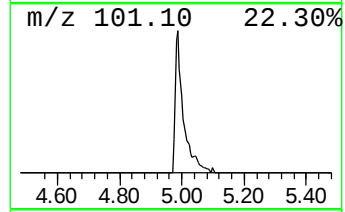
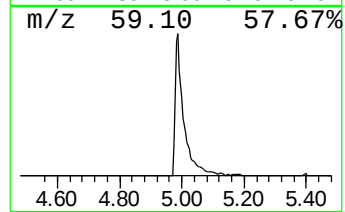
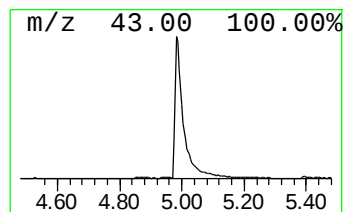
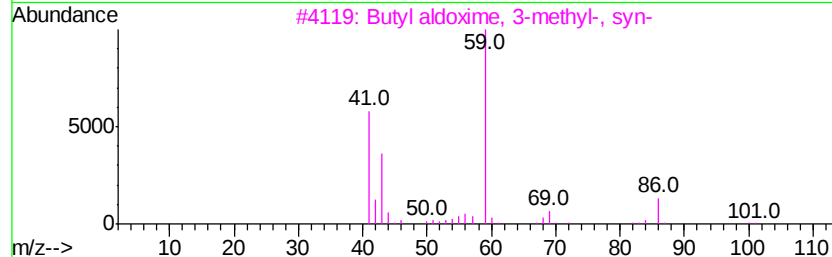
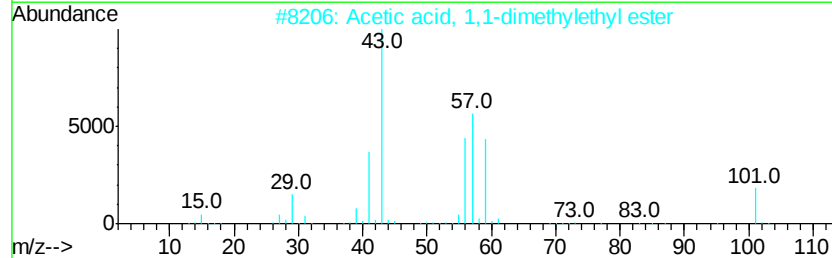
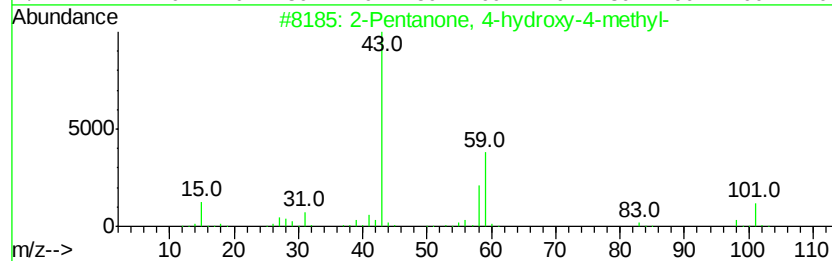
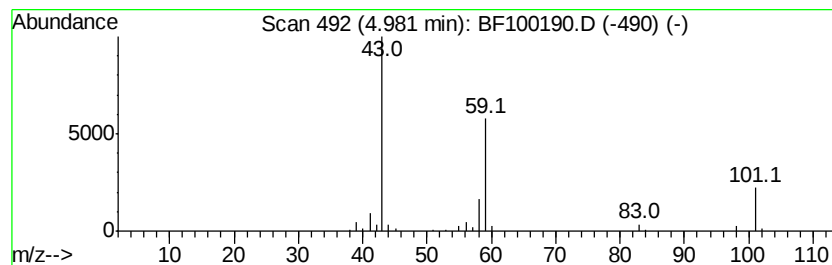
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	9.86 ng	232882	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	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35
4			3-Hexanol	102	C6H14O	000623-37-0	28
5			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25



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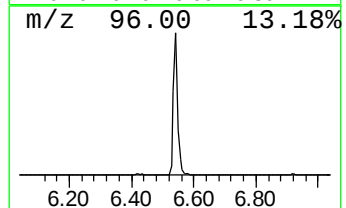
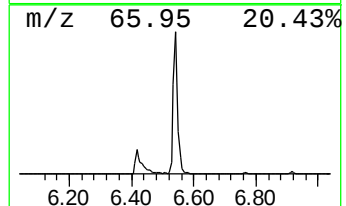
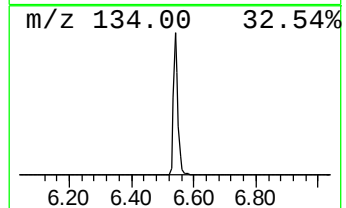
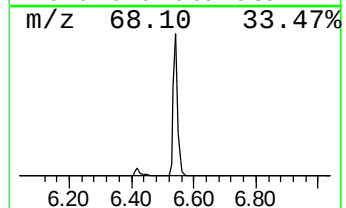
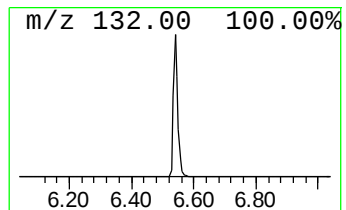
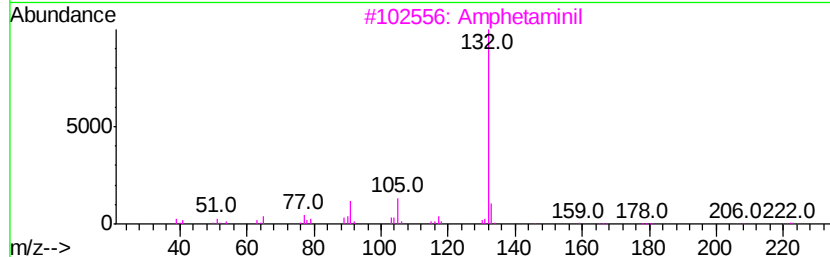
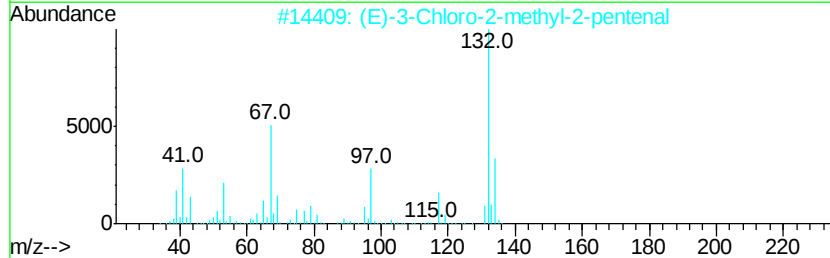
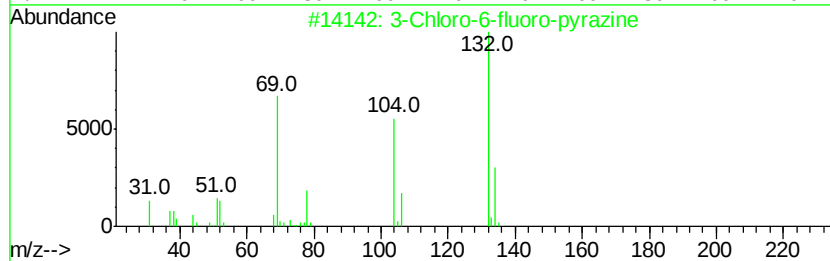
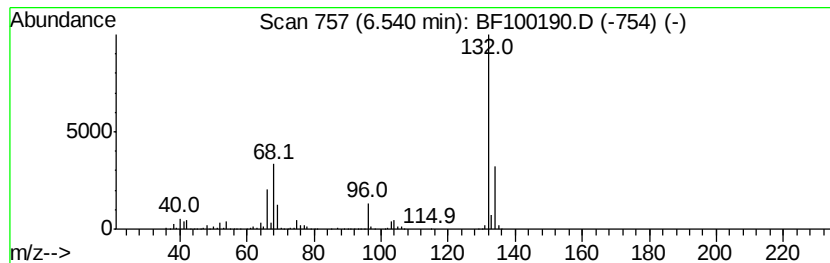
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	72.17 ng	1704320	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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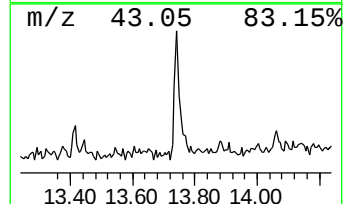
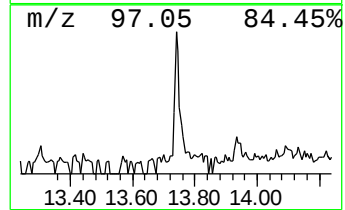
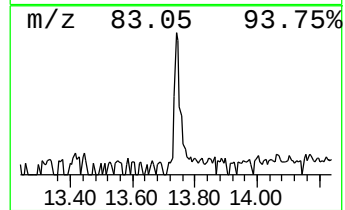
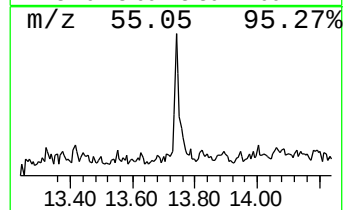
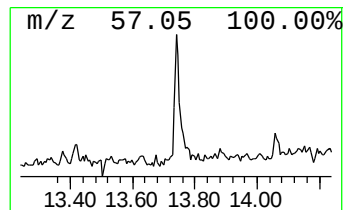
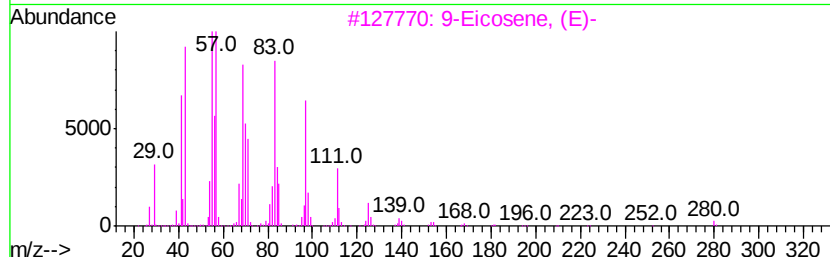
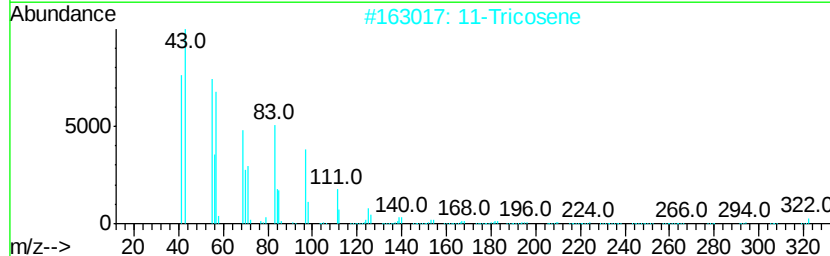
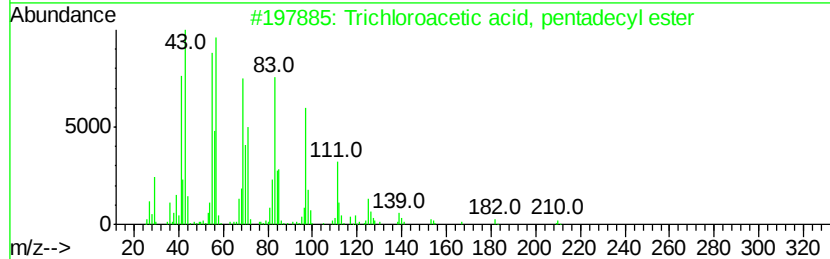
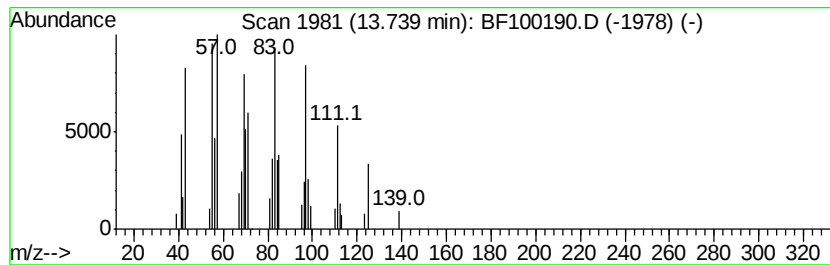
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Trichloroacetic acid, penta... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.02 ng	58175	Chrysene-d12	13.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2			11-Tricosene	322	C23H46	052078-56-5	90
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	86
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	86
5			17-Pentatriacontene	491	C35H70	006971-40-0	86



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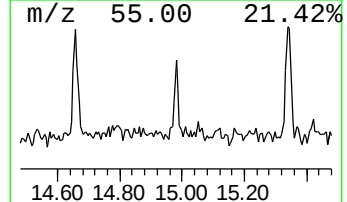
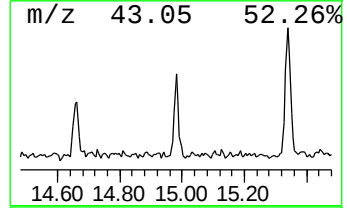
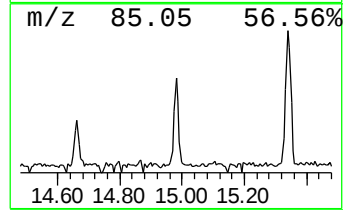
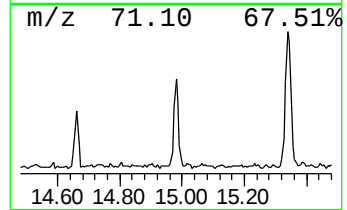
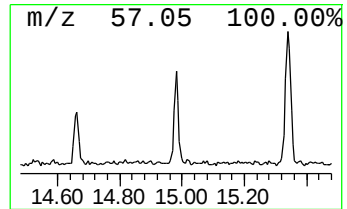
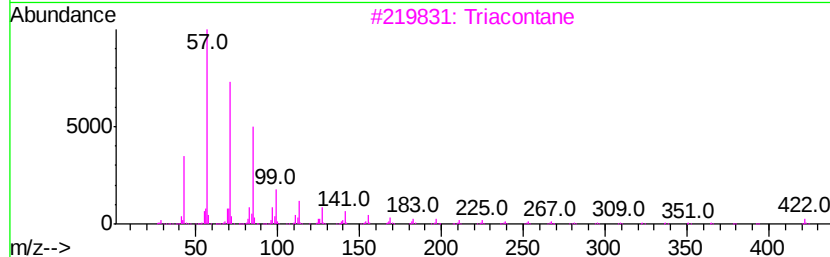
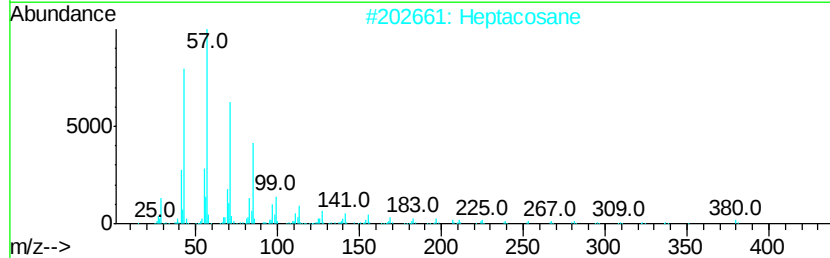
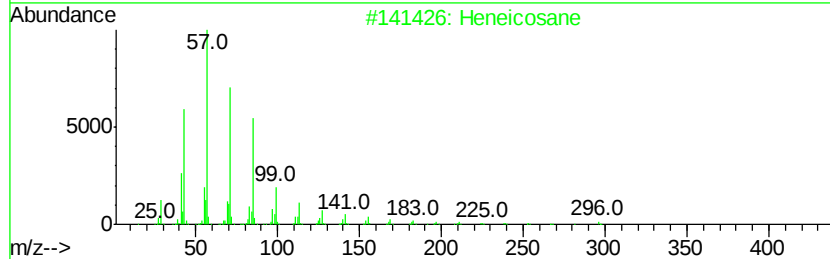
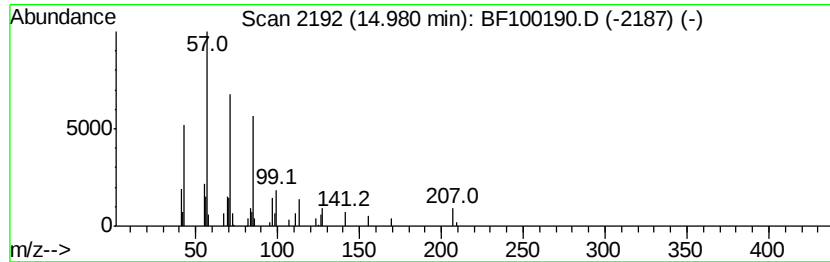
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Peak Number 5 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.33 ng	50597	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Heptacosane		380	C27H56	000593-49-7	87
3	Triacontane		422	C30H62	000638-68-6	87
4	Octacosane		394	C28H58	000630-02-4	87
5	2-methyloctacosane		408	C29H60	1000376-72-8	86



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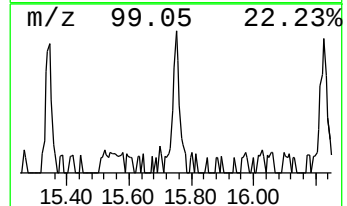
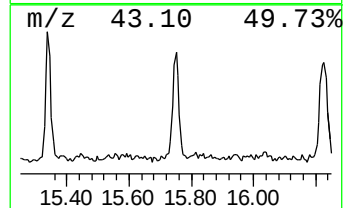
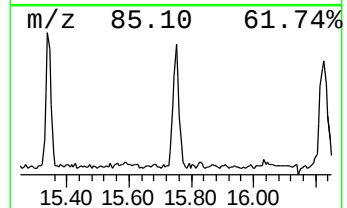
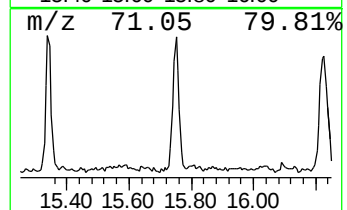
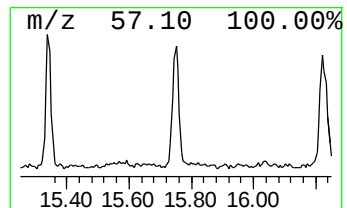
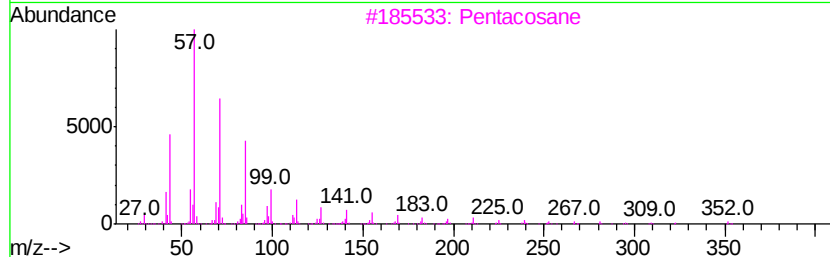
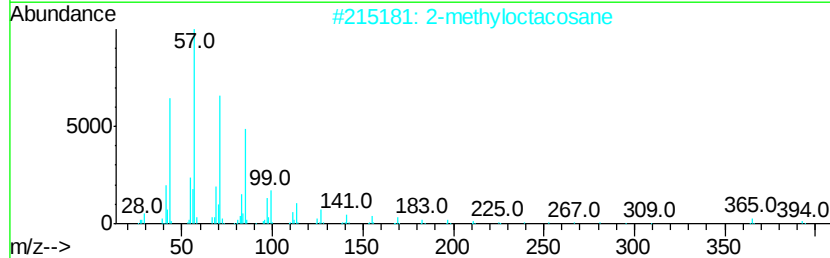
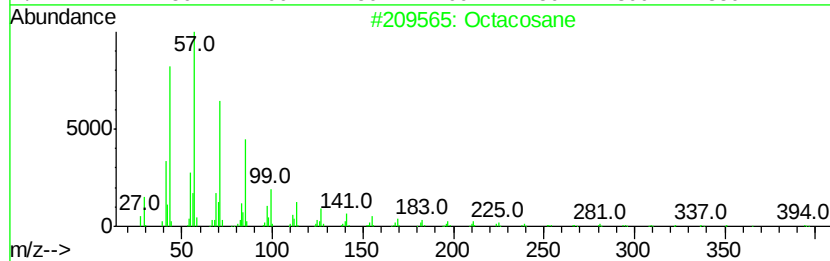
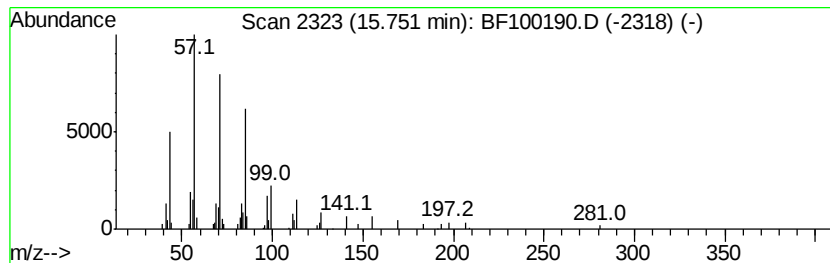
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	4.01 ng	87235	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90



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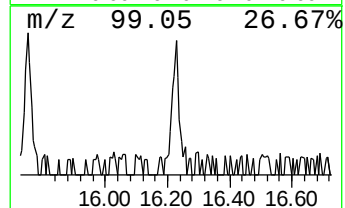
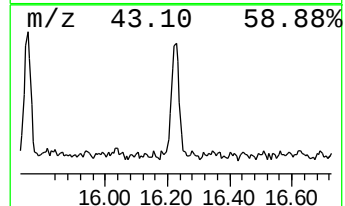
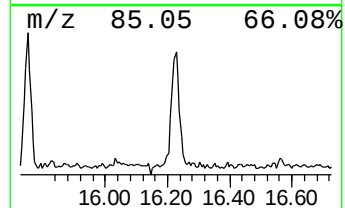
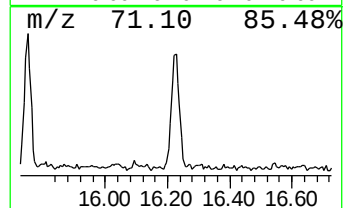
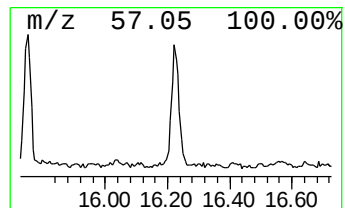
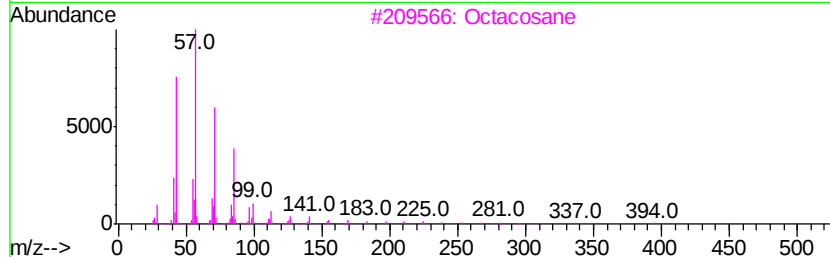
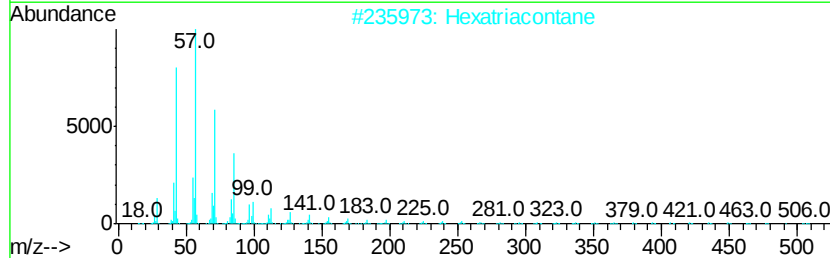
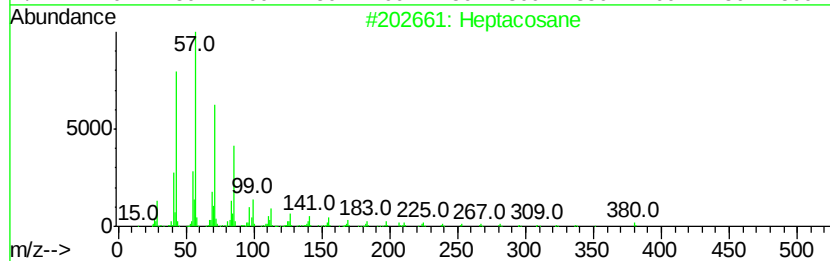
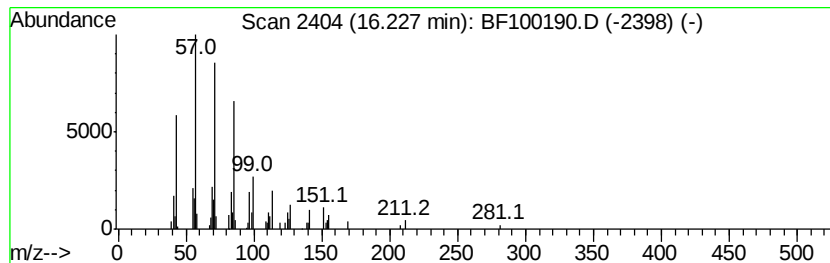
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	5.09 ng	110643	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Hexatriacontane	507	C36H74	000630-06-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100190.D
Acq On : 4 Nov 2017 20:31
Operator : SJ/JU
Sample : I6313-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF015-01

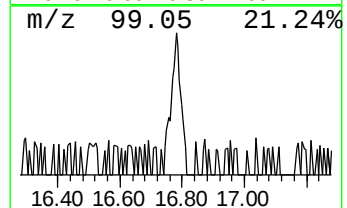
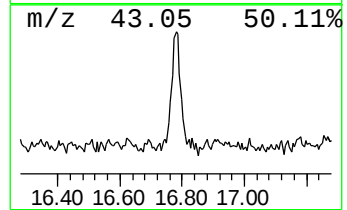
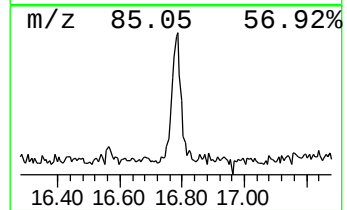
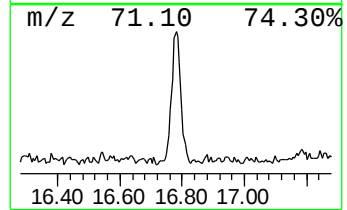
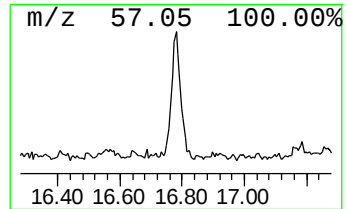
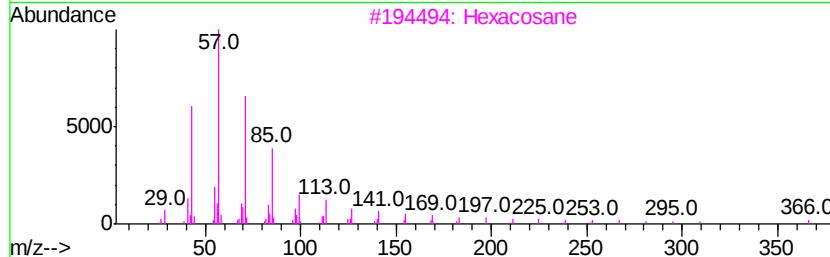
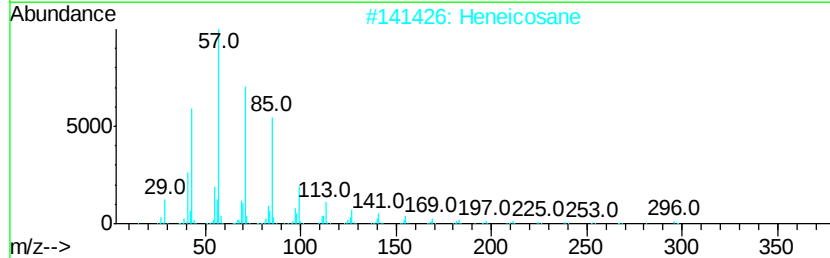
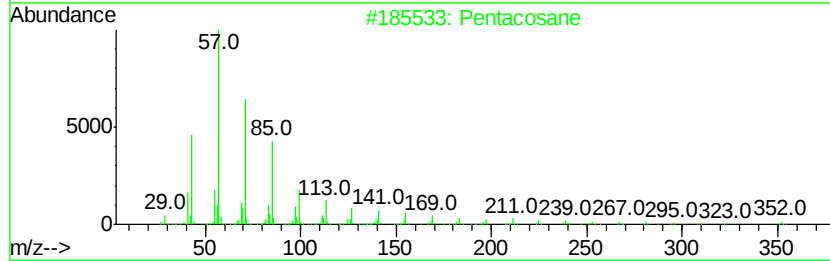
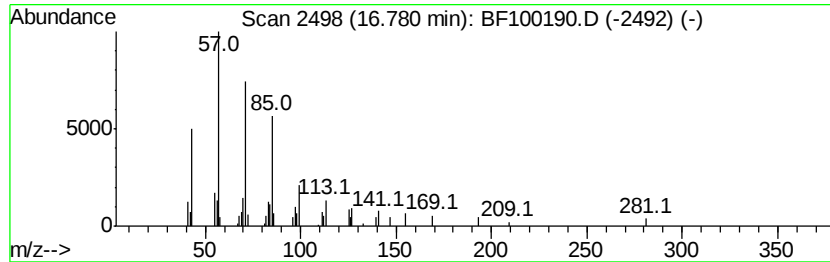
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	3.66 ng	79507	Perylene-d12	15.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Octacosane		394	C28H58	000630-02-4	91
5	Octadecane		254	C18H38	000593-45-3	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100190.D
Acq On : 4 Nov 2017 20:31
Operator : SJ/JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
PET-BF015-01

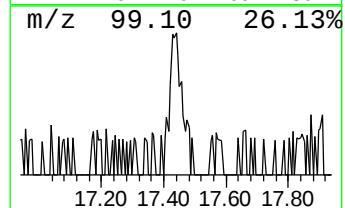
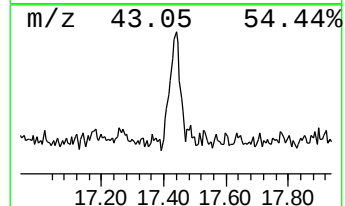
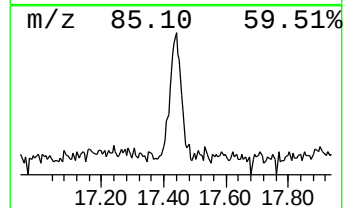
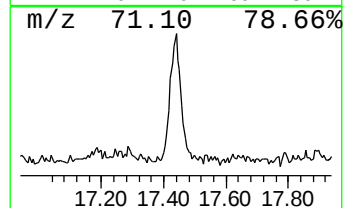
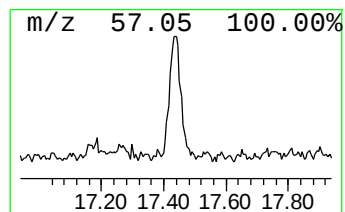
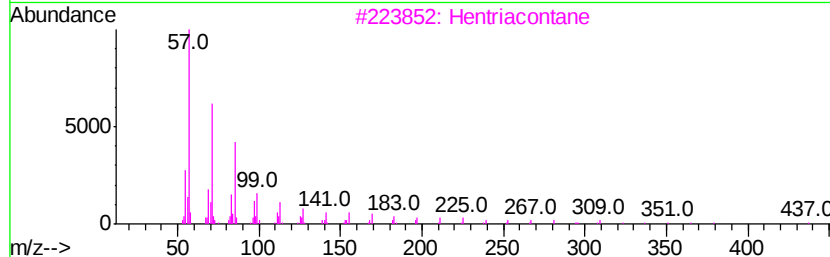
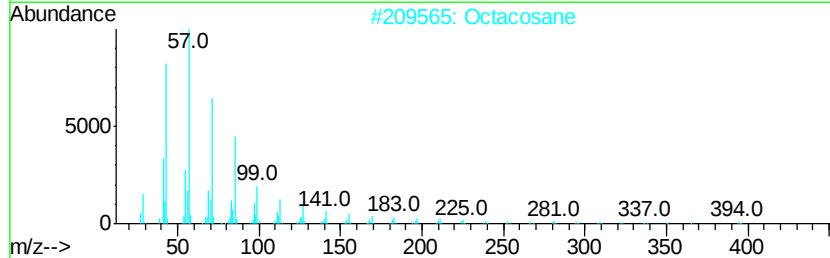
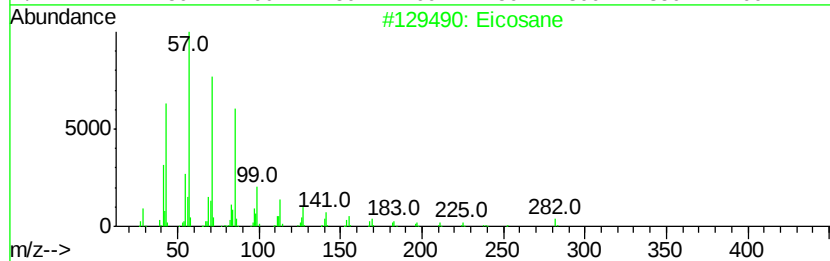
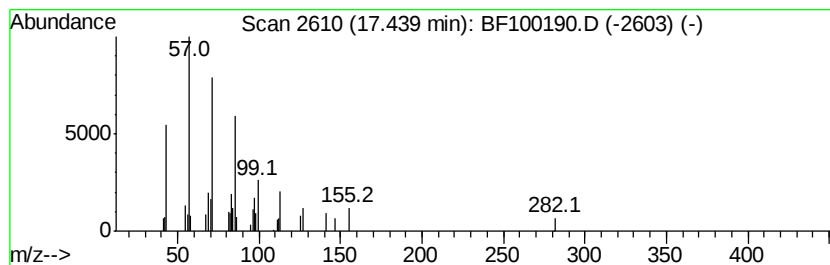
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.96 ng	64430	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	96
2		Octacosane	394	C28H58	000630-02-4	86
3		Hentriacontane	437	C31H64	000630-04-6	72
4		Hexacosane	366	C26H54	000630-01-3	72
5		2-methyltetracosane	352	C25H52	1000376-72-6	72



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100190.D
Acq On : 4 Nov 2017 20:31
Operator : SJ/JU
Sample : I6313-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF015-01

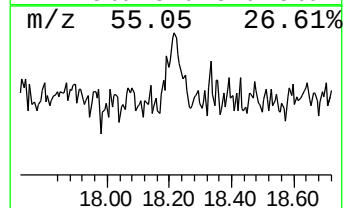
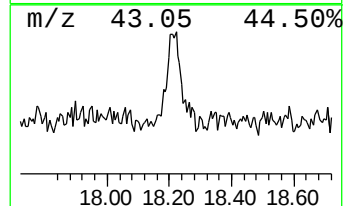
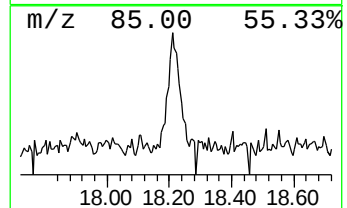
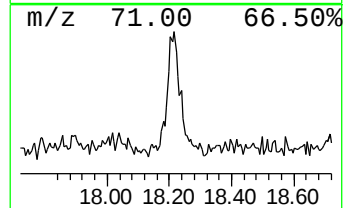
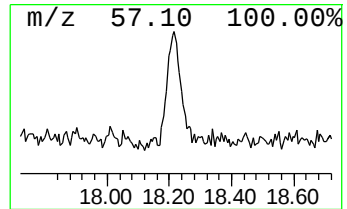
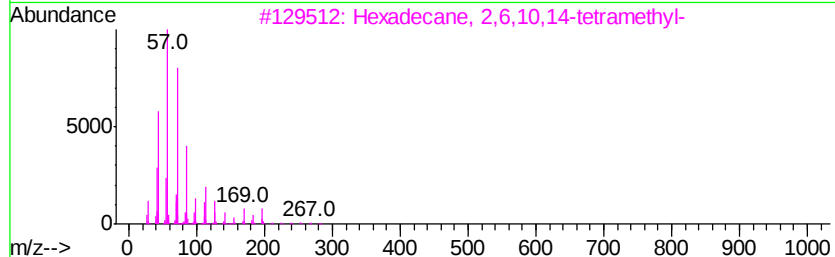
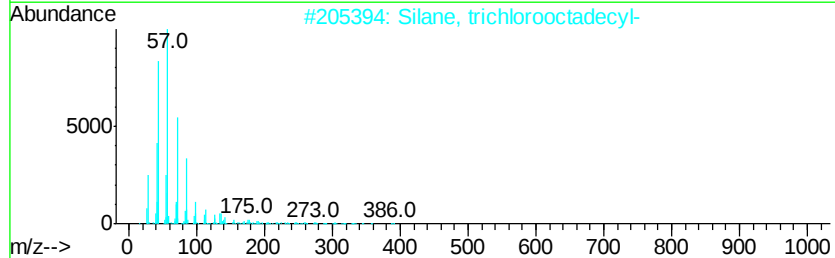
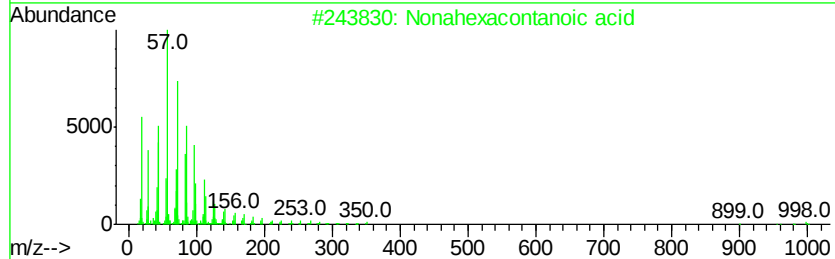
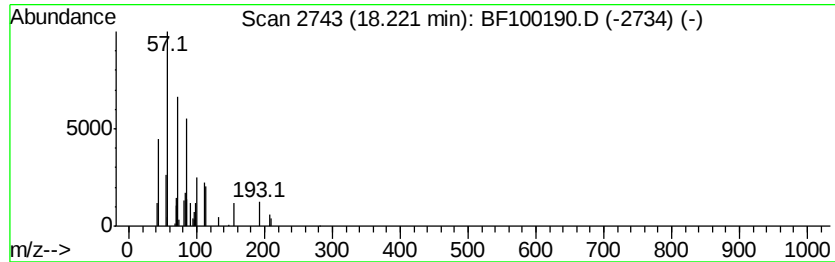
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonaheptacontanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	2.48 ng	53859	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	64
2		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	59
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
4		Octacosane	394	C28H58	000630-02-4	53
5		Hexacosane	366	C26H54	000630-01-3	53



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110417\
Data File : BF100190.D
Acq On : 4 Nov 2017 20:31
Operator : SJ/JU
Sample : I6313-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	4.98	9.9 ng		232882	1	6.76	472326	20.0
unknown6.54	6.54	72.2 ng		1704320	1	6.76	472326	20.0
Trichloroacetic a...	13.74	2.0 ng		58175	5	13.94	575208	20.0
Heneicosane	14.98	2.3 ng		50597	6	15.40	434806	20.0
Octacosane	15.75	4.0 ng		87235	6	15.40	434806	20.0
Heptacosane	16.23	5.1 ng		110643	6	15.40	434806	20.0
Pentacosane	16.78	3.7 ng		79507	6	15.40	434806	20.0
Eicosane	17.44	3.0 ng		64430	6	15.40	434806	20.0
Nonahexacontanoic...	18.22	2.5 ng		53859	6	15.40	434806	20.0