

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110417\
 Data File : BF100187.D
 Acq On : 4 Nov 2017 19:11
 Operator : SJ/JU
 Sample : I6313-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF010-02

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	4.987	490	493	515	rBV	143447	257888	12.17%	1.401%
2	5.398	560	563	594	rBV	1068786	1705736	80.52%	9.267%
3	6.422	733	737	754	rBV	1286924	1710462	80.75%	9.293%
4	6.539	754	757	778	rVB	1820090	1833214	86.54%	9.960%
5	6.763	792	795	806	rBV	565346	532964	25.16%	2.896%
6	6.916	818	821	846	rBB	1538299	1431420	67.57%	7.777%
7	7.333	889	892	916	rBV	966674	1047615	49.46%	5.692%
8	8.045	1010	1013	1032	rBV	790921	752800	35.54%	4.090%
9	9.116	1191	1195	1205	rBV	2463931	2118297	100.00%	11.509%
10	9.516	1260	1263	1275	rBB	177929	151529	7.15%	0.823%
11	9.798	1307	1311	1324	rVB	907527	853805	40.31%	4.639%
12	10.592	1443	1446	1459	rBV	1118094	1101590	52.00%	5.985%
13	10.721	1465	1468	1479	rBV	83933	93147	4.40%	0.506%
14	11.286	1561	1564	1574	rBV	851851	826078	39.00%	4.488%
15	11.804	1648	1652	1656	rBV	91531	93005	4.39%	0.505%
16	12.586	1782	1785	1790	rBV	21987	23796	1.12%	0.129%
17	12.868	1829	1833	1836	rBV	2064675	1855646	87.60%	10.082%
18	13.739	1978	1981	1989	rBV	194706	202593	9.56%	1.101%
19	13.939	2012	2015	2024	rBV	569510	575019	27.15%	3.124%
20	14.368	2084	2088	2095	rBV5	17560	24424	1.15%	0.133%
21	14.657	2133	2137	2141	rBV2	70857	81417	3.84%	0.442%
22	14.980	2189	2192	2196	rBV	51368	50374	2.38%	0.274%
23	15.339	2249	2253	2258	rVB	81705	90209	4.26%	0.490%
24	15.398	2259	2263	2277	rVB	329485	461071	21.77%	2.505%
25	15.751	2318	2323	2329	rBV	70773	97684	4.61%	0.531%
26	15.809	2329	2333	2340	rVB7	17348	33333	1.57%	0.181%
27	16.227	2399	2404	2410	rVB	67104	106583	5.03%	0.579%
28	16.780	2493	2498	2504	rBV3	45199	90805	4.29%	0.493%
29	17.433	2604	2609	2618	rVB4	37821	85811	4.05%	0.466%
30	18.209	2738	2741	2752	rVB6	20005	52106	2.46%	0.283%
31	19.144	2890	2900	2913	rBV8	17525	65842	3.11%	0.358%

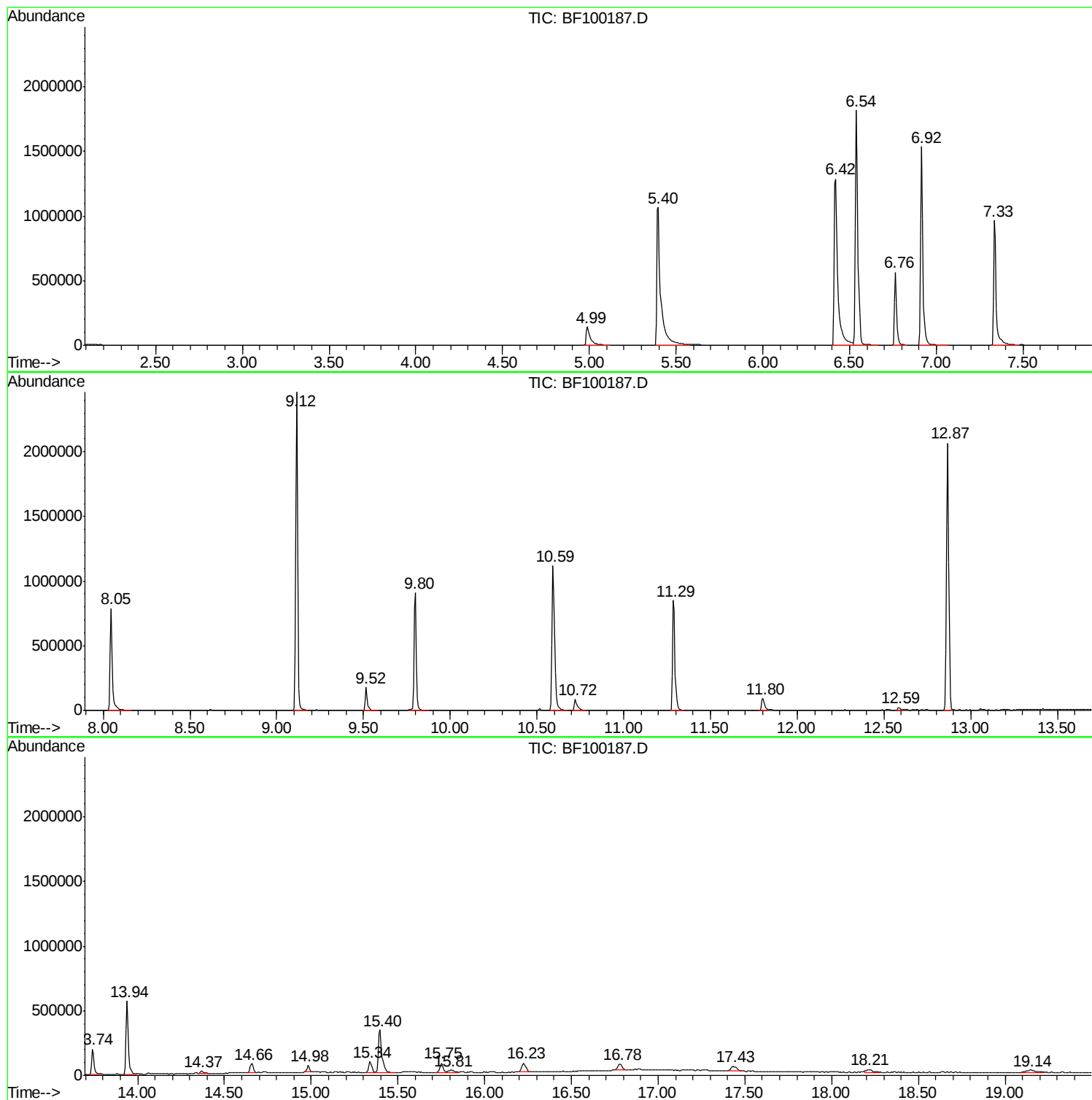
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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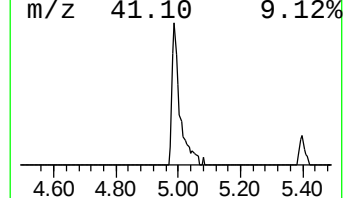
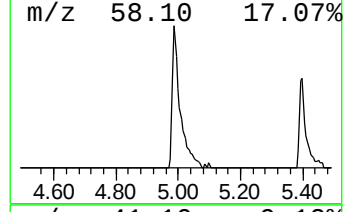
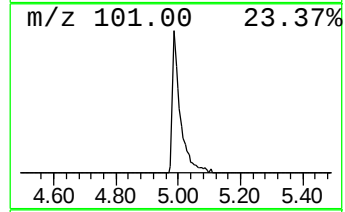
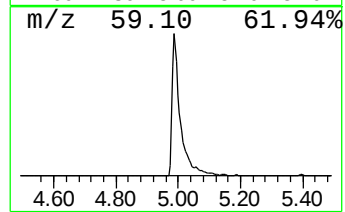
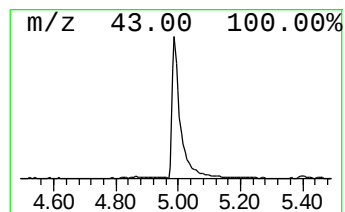
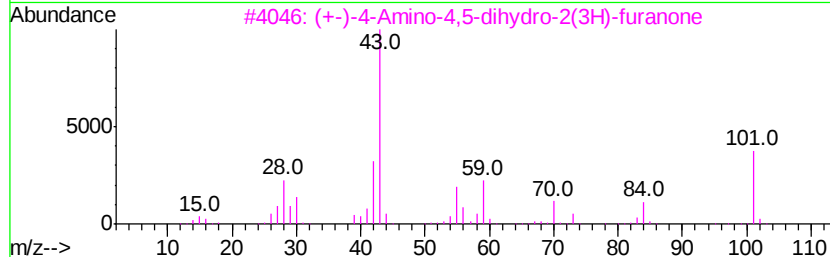
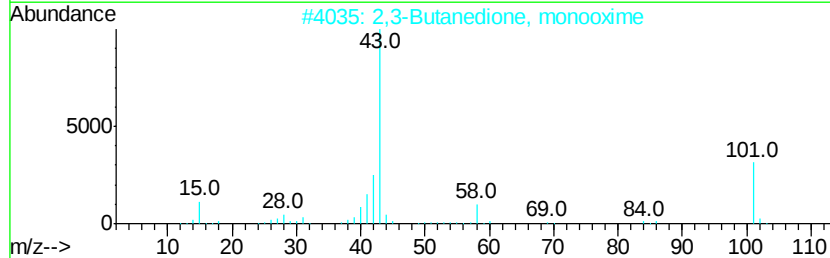
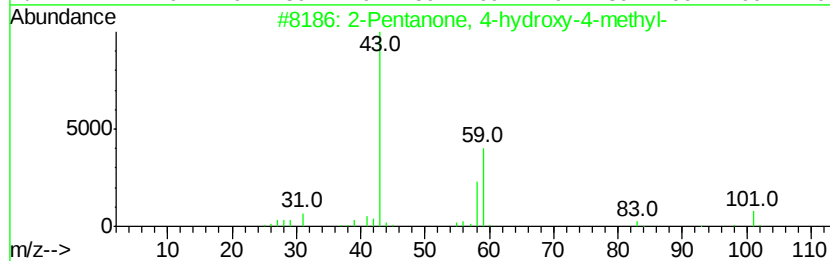
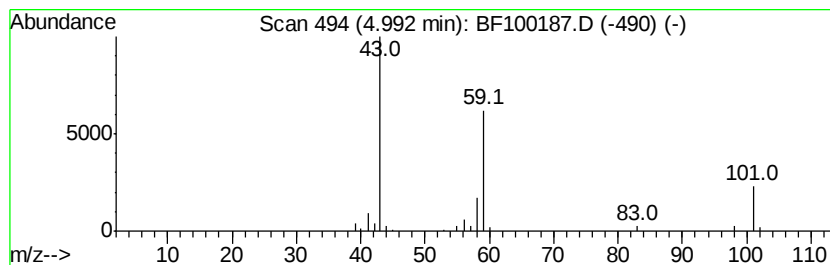
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	9.68 ng	257888	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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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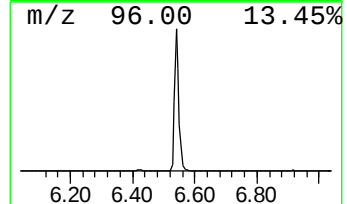
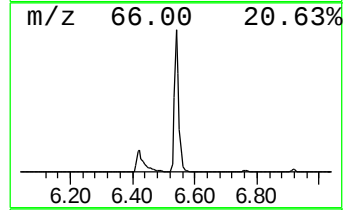
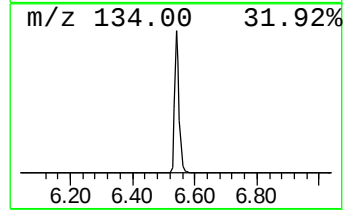
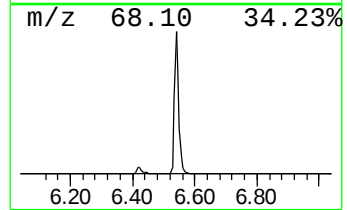
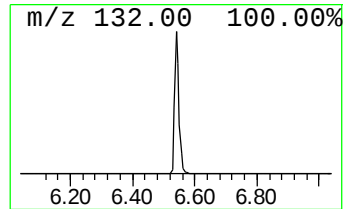
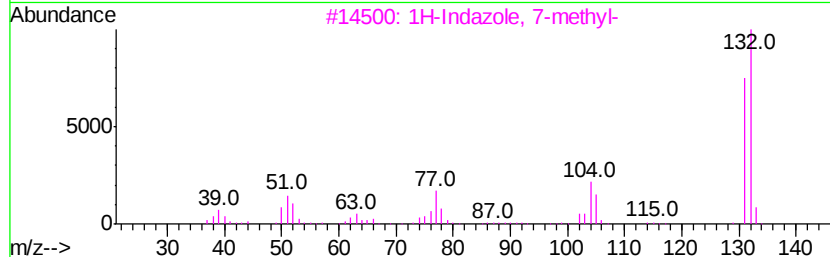
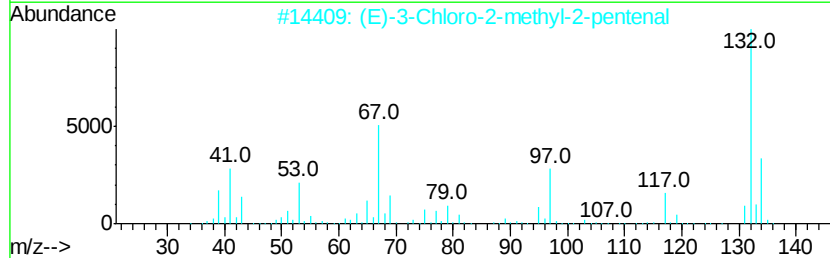
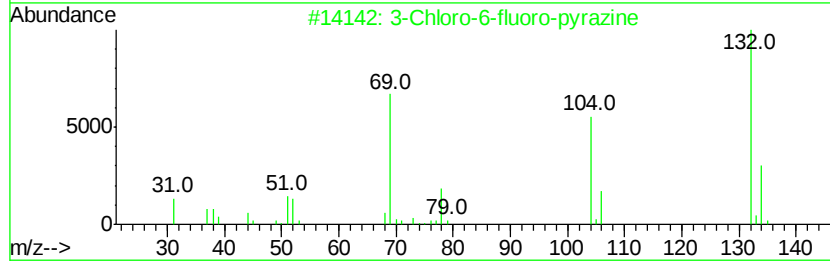
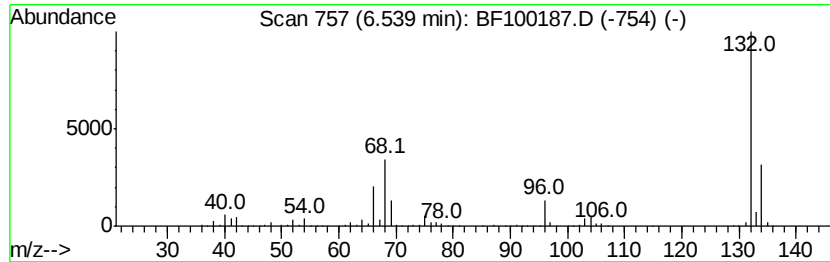
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	68.79 ng	1833210	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	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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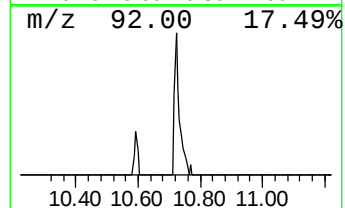
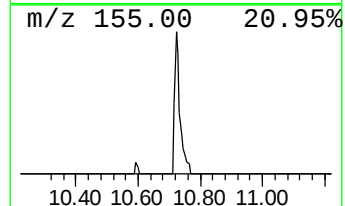
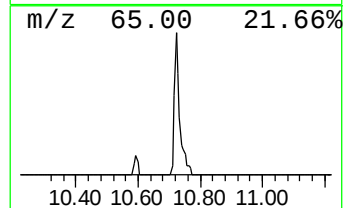
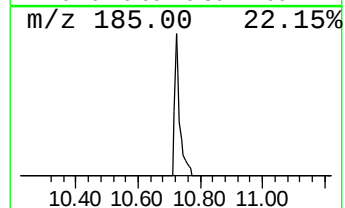
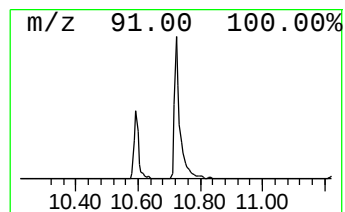
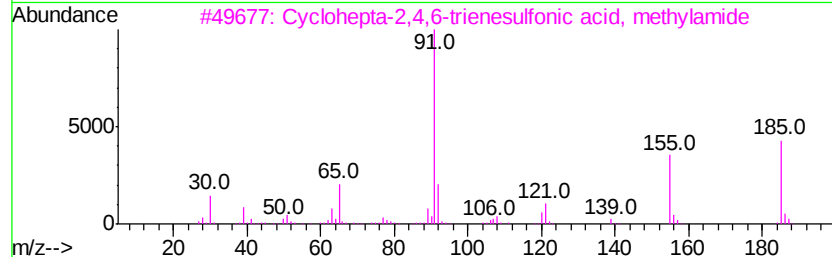
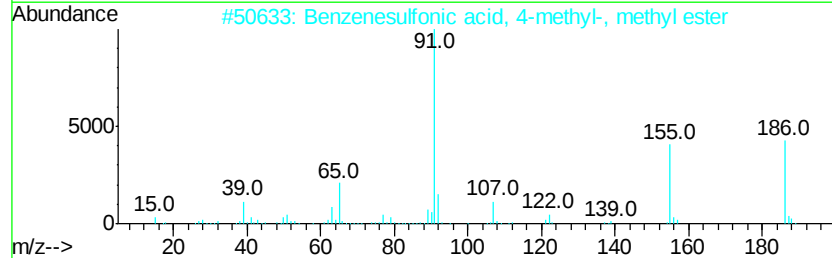
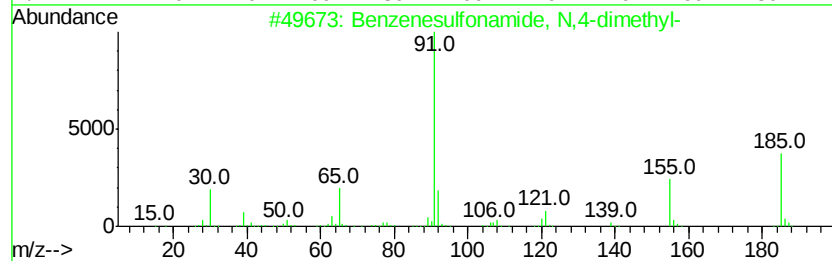
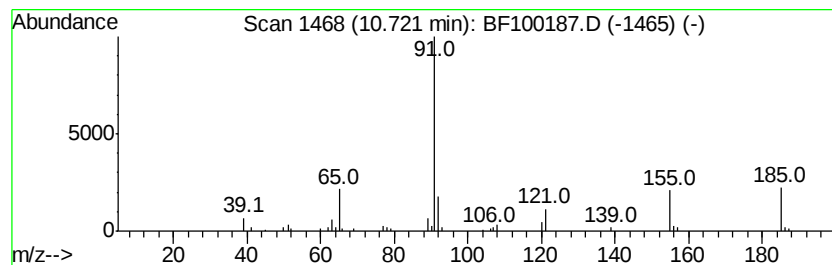
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.72	2.26 ng	93147	Phenanthrene-d10	11.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2		Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	50
3		Cvclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	49
4		p-Toluenesulfonylvacetonitrile	195	C9H9NO2S	005697-44-9	43
5		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43



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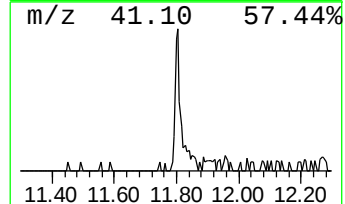
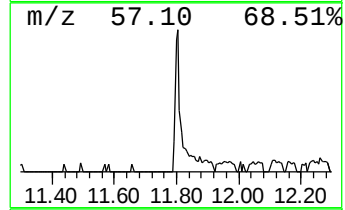
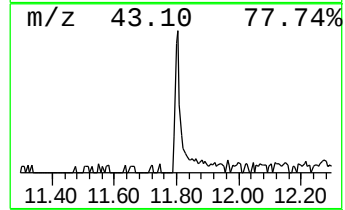
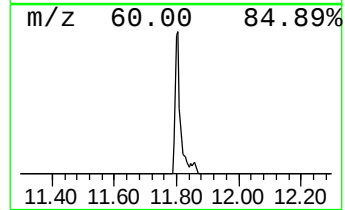
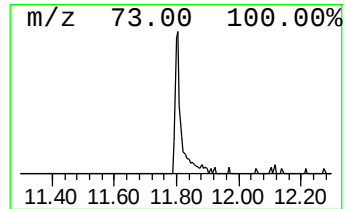
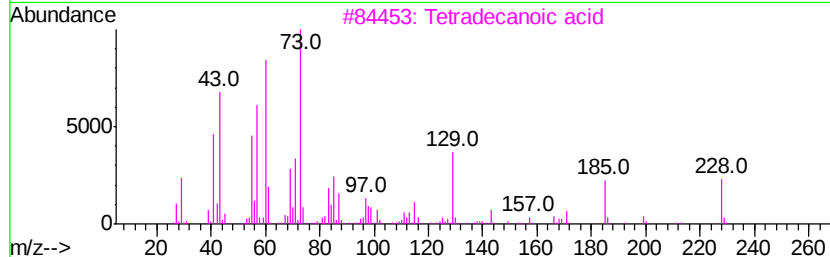
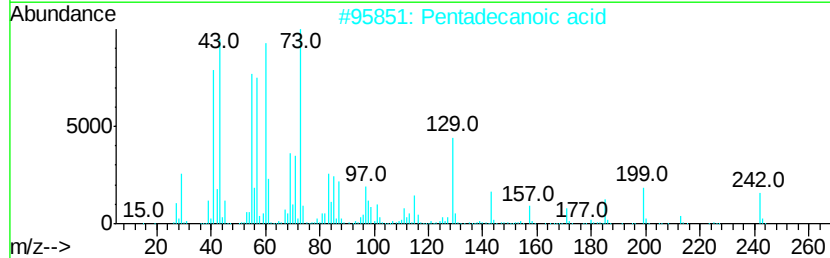
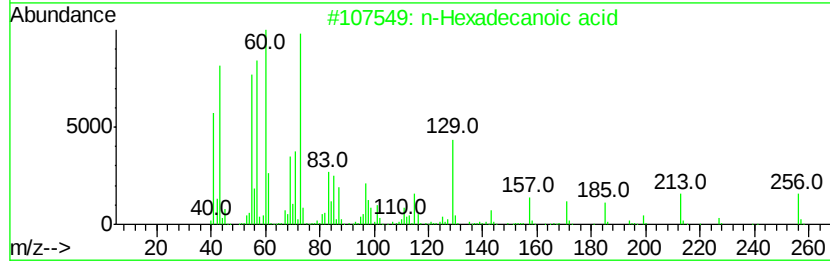
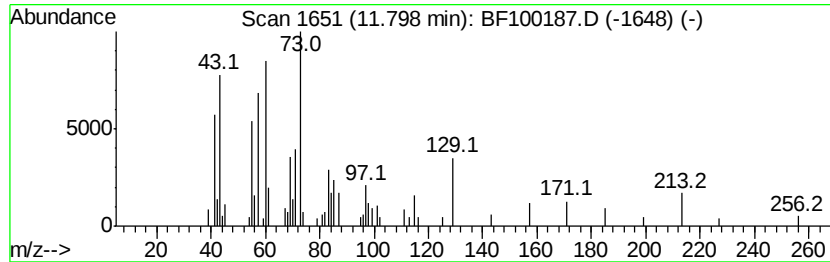
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.25 ng	93005	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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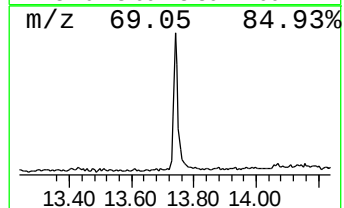
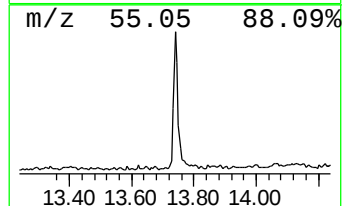
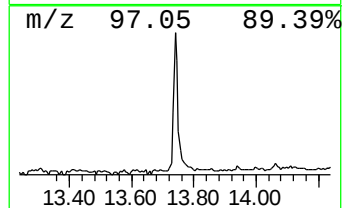
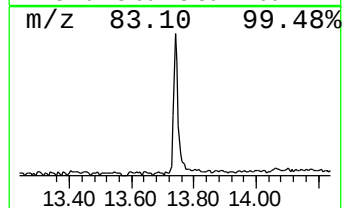
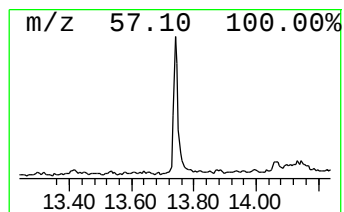
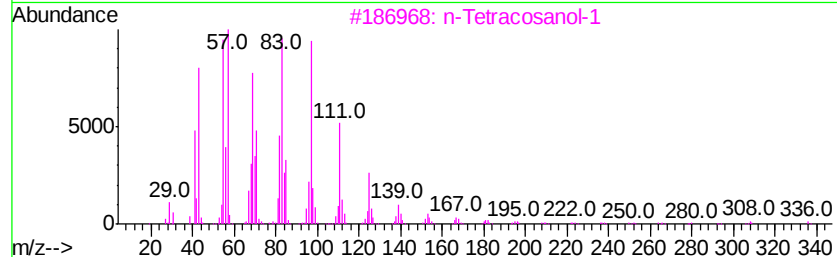
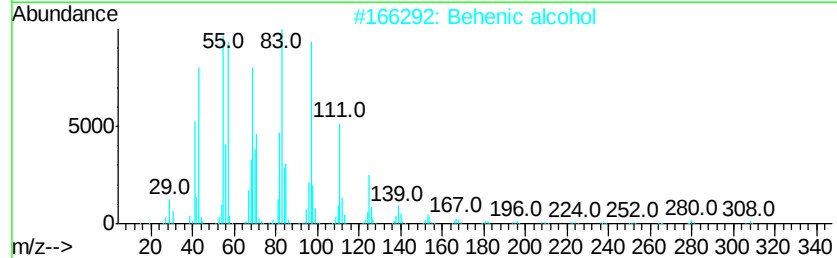
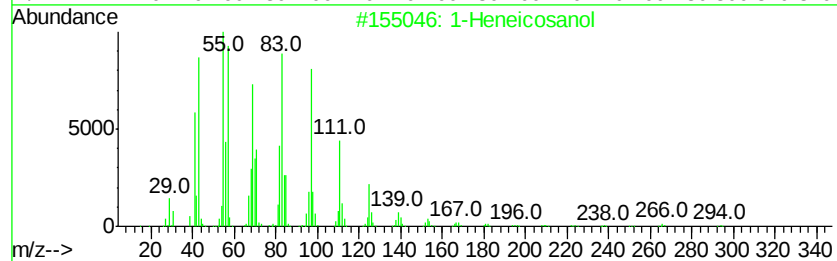
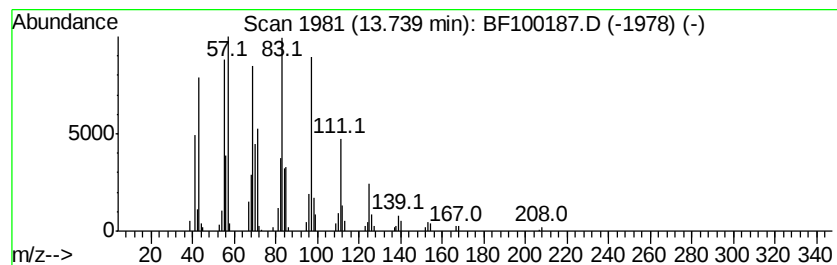
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Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	7.05 ng	202593	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



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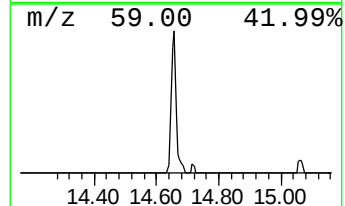
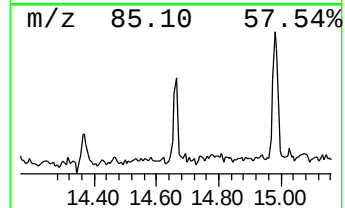
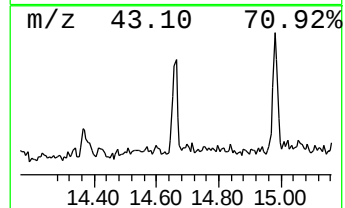
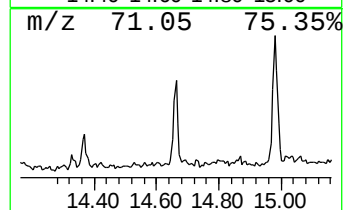
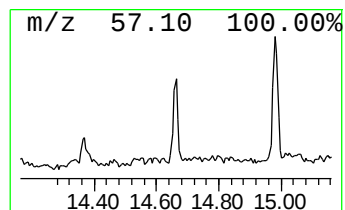
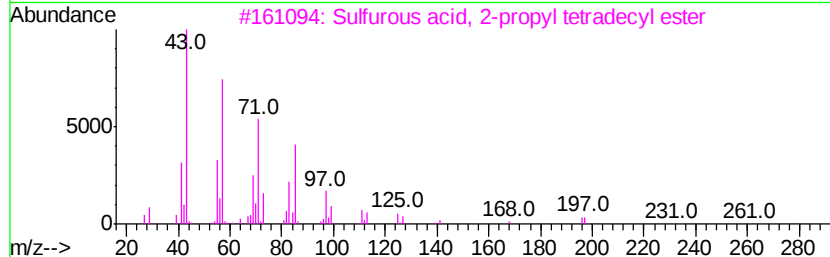
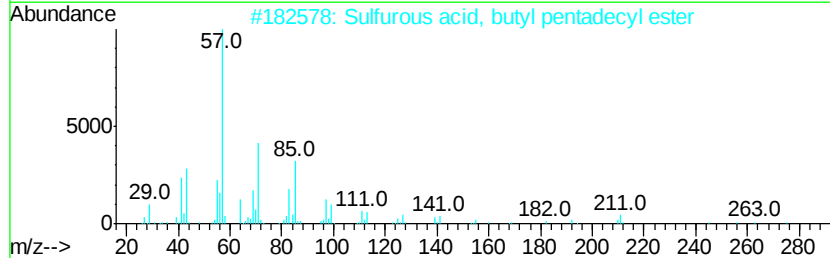
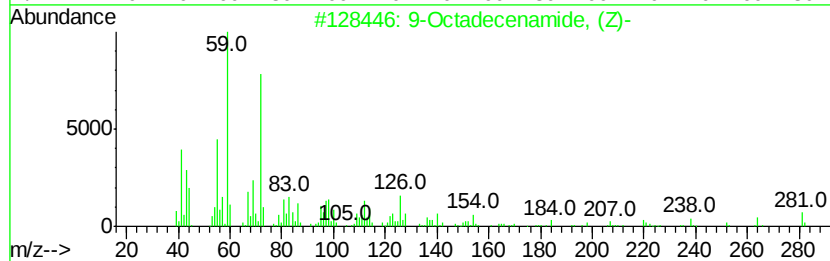
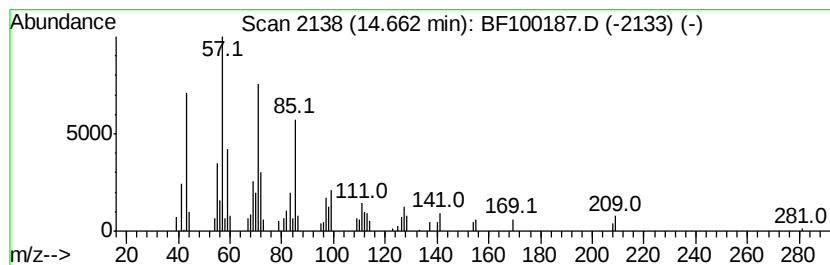
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.83 ng	81417	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	30
3		Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1000309-12-5	30
4		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	30
5		Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	30



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Operator : SJ/JU
Sample : I6313-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

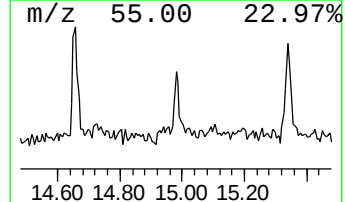
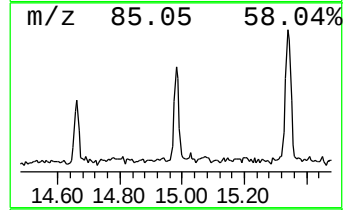
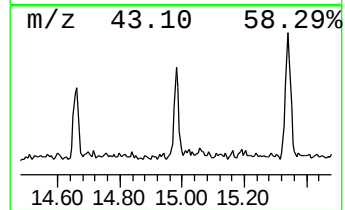
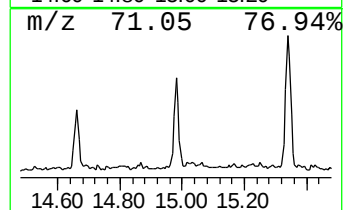
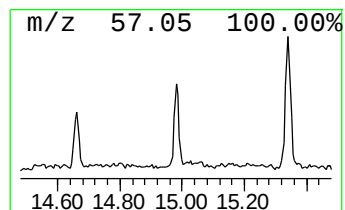
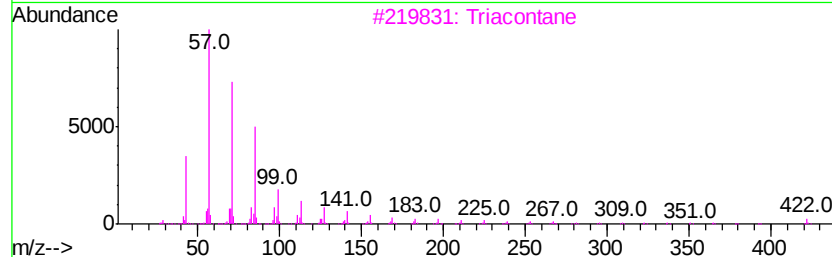
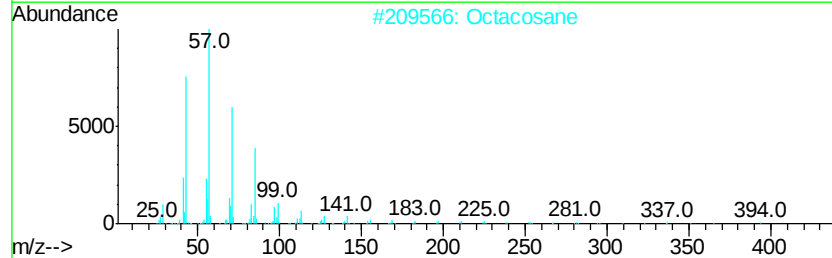
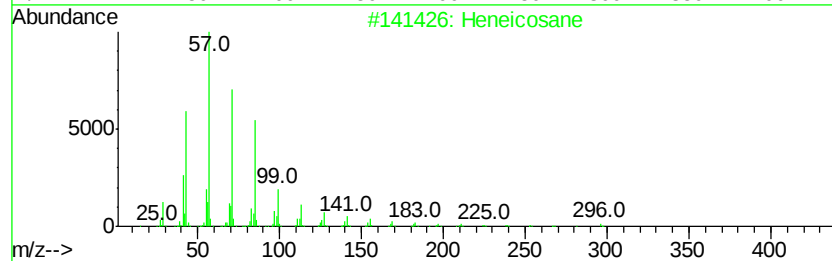
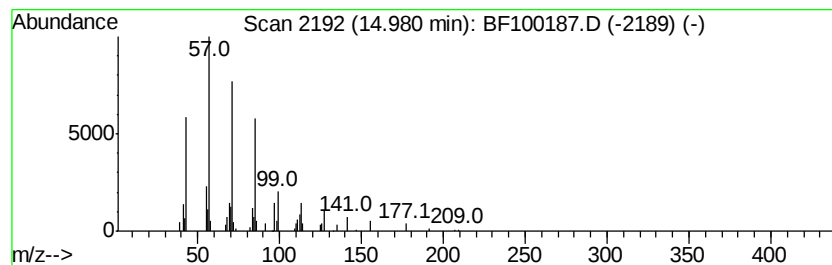
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ClientSampleId :
PET-BF010-02

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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 Heneicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.19 ng	50374	Perylene-d12	15.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Triacontane	422 C30H62	000638-68-6	90
4	2-methyloctacosane	408 C29H60	1000376-72-8	90
5	Pentacosane	352 C25H52	000629-99-2	87



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100187.D
Acq On : 4 Nov 2017 19:11
Operator : SJ/JU
Sample : I6313-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PET-BF010-02

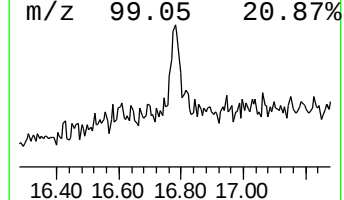
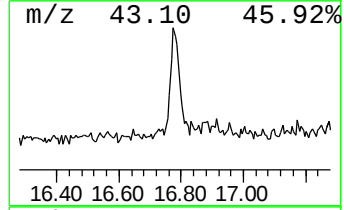
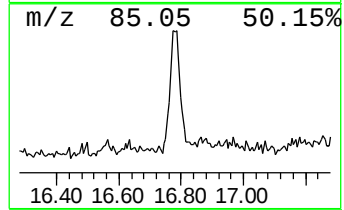
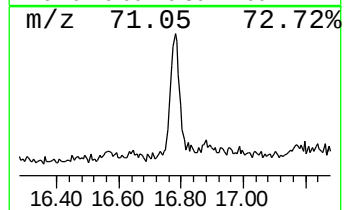
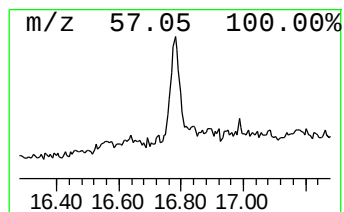
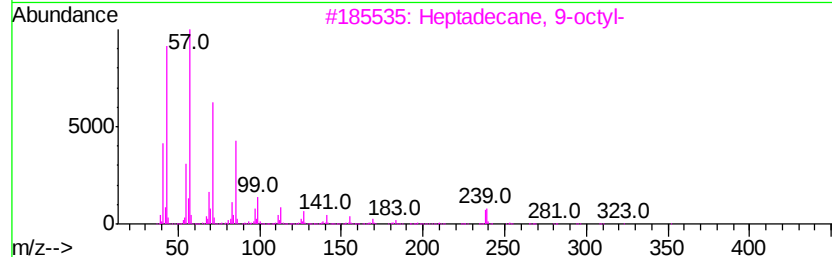
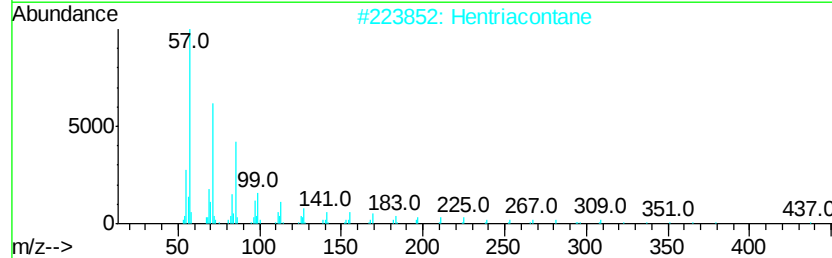
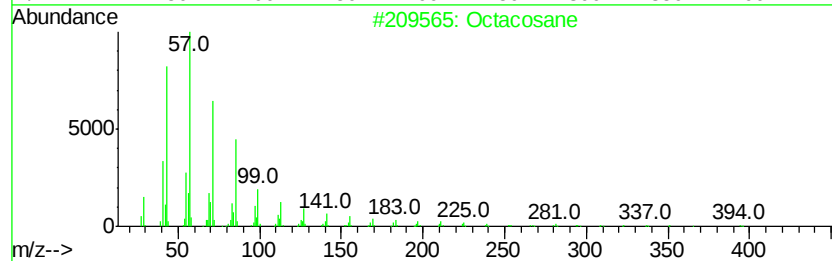
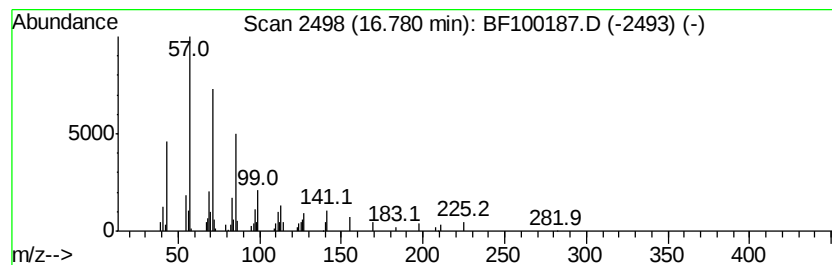
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	3.94 ng	90805	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100187.D
Acq On : 4 Nov 2017 19:11
Operator : SJ/JU
Sample : I6313-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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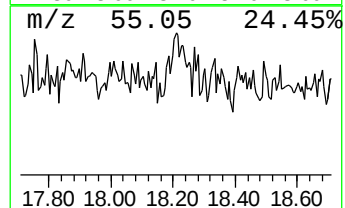
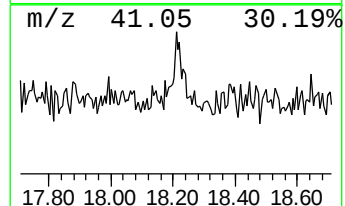
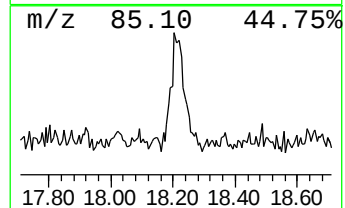
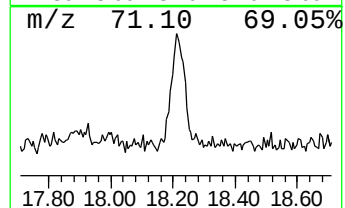
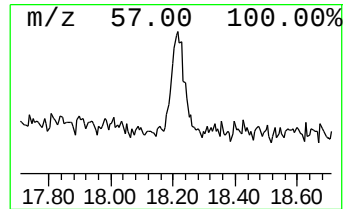
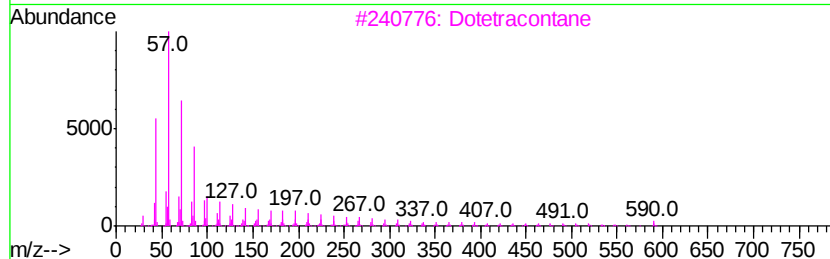
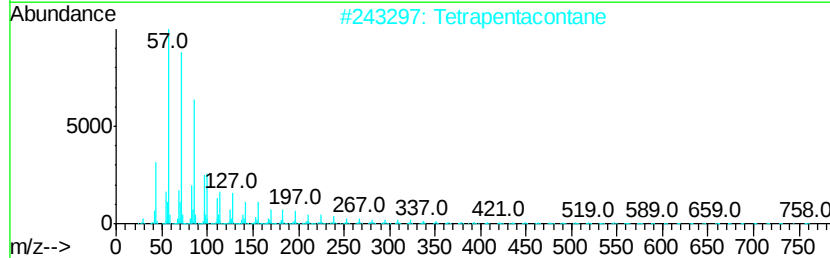
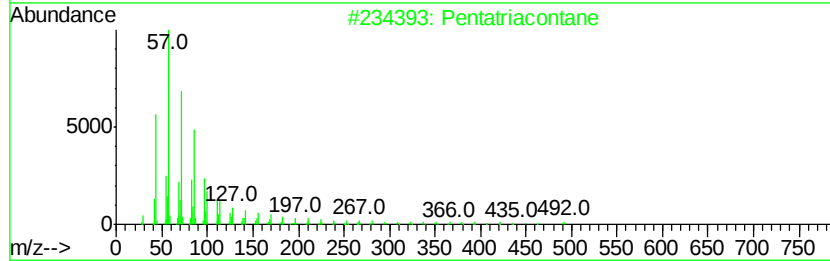
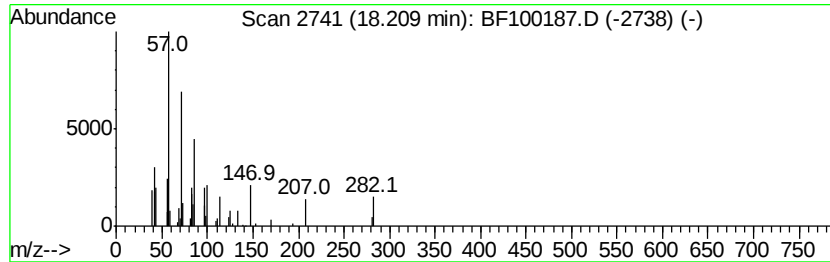
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentatriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	2.26 ng	52106	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentatriacontane	493	C35H72	000630-07-9	53
2		Tetrapentacontane	759	C54H110	005856-66-6	53
3		Dotetracontane	591	C42H86	007098-20-6	50
4		Heneicosane, 3-methyl-	310	C22H46	006418-47-9	47
5		5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	47



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF110417\
Data File : BF100187.D
Acq On : 4 Nov 2017 19:11
Operator : SJ/JU
Sample : I6313-04
Misc :
ALS Vial : 18 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...	4.99	9.7	ng	257888	1	6.76	532964	20.0
unknown6.54	6.54	68.8	ng	1833210	1	6.76	532964	20.0
Benzenesulfonamid...	10.72	2.3	ng	93147	4	11.29	826078	20.0
n-Hexadecanoic acid	11.80	2.3	ng	93005	4	11.29	826078	20.0
1-Heneicosanol	13.74	7.0	ng	202593	5	13.94	575019	20.0
9-Octadecenamide, ...	14.66	2.8	ng	81417	5	13.94	575019	20.0
Heneicosane	14.98	2.2	ng	50374	6	15.40	461071	20.0
Octacosane	16.78	3.9	ng	90805	6	15.40	461071	20.0
Pentatriacontane	18.21	2.3	ng	52106	6	15.40	461071	20.0