

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
 Data File : BF109153.D
 Acq On : 19 Sep 2018 19:36
 Operator : JU/SJ
 Sample : J4771-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-07-091818

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-BF091418.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	3.125	133	134	145	rBV4	20027	47953	1.61%	0.175%
2	4.925	436	440	452	rVB	88297	118467	3.98%	0.432%
3	5.337	505	510	513	rBV	2578032	2746173	92.20%	10.010%
4	6.360	679	684	695	rBV	2541169	2978335	100.00%	10.856%
5	6.495	702	707	710	rBV	2827194	2795275	93.85%	10.188%
6	6.725	742	746	749	rBV	939155	846537	28.42%	3.086%
7	6.878	768	772	776	rBV	2558881	2306004	77.43%	8.405%
8	7.283	835	841	844	rBV	1829396	1719506	57.73%	6.267%
9	8.001	959	963	967	rBV	1212552	982189	32.98%	3.580%
10	9.077	1142	1146	1149	rBV	3240711	2919310	98.02%	10.641%
11	9.472	1209	1213	1216	rBV	328281	279322	9.38%	1.018%
12	9.754	1257	1261	1264	rBV	1089364	976407	32.78%	3.559%
13	10.536	1390	1394	1397	rBV	1678105	1470045	49.36%	5.358%
14	11.230	1508	1512	1515	rBV	1004411	894510	30.03%	3.260%
15	12.813	1776	1781	1784	rBV	2699213	2390426	80.26%	8.713%
16	13.054	1816	1822	1826	rBV2	43172	48059	1.61%	0.175%
17	13.277	1854	1860	1862	rBV5	27247	32853	1.10%	0.120%
18	13.395	1877	1880	1883	rBV	52809	46374	1.56%	0.169%
19	13.724	1931	1936	1946	rBV	205993	297129	9.98%	1.083%
20	13.854	1954	1958	1962	rBV	1151624	973058	32.67%	3.547%
21	13.971	1974	1978	1981	rVB	58099	57538	1.93%	0.210%
22	14.036	1986	1989	2000	rVV	98861	103945	3.49%	0.379%
23	14.342	2038	2041	2052	rBV	131686	137791	4.63%	0.502%
24	14.636	2088	2091	2099	rVB	147421	144613	4.86%	0.527%
25	14.771	2110	2114	2121	rBV	229766	227828	7.65%	0.830%
26	14.954	2141	2145	2148	rBV	170279	182006	6.11%	0.663%
27	14.983	2148	2150	2155	rVB2	52381	71047	2.39%	0.259%
28	15.259	2192	2197	2201	rBV	750719	849586	28.53%	3.097%
29	15.306	2201	2205	2210	rVB	137968	168219	5.65%	0.613%
30	15.495	2233	2237	2242	rVB4	37921	50580	1.70%	0.184%
31	15.712	2269	2274	2280	rBV	160026	227355	7.63%	0.829%
32	16.177	2347	2353	2365	rVB4	89950	185233	6.22%	0.675%
33	16.724	2440	2446	2453	rBV2	57045	110459	3.71%	0.403%
34	17.371	2551	2556	2562	rVB4	23811	51496	1.73%	0.188%

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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-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

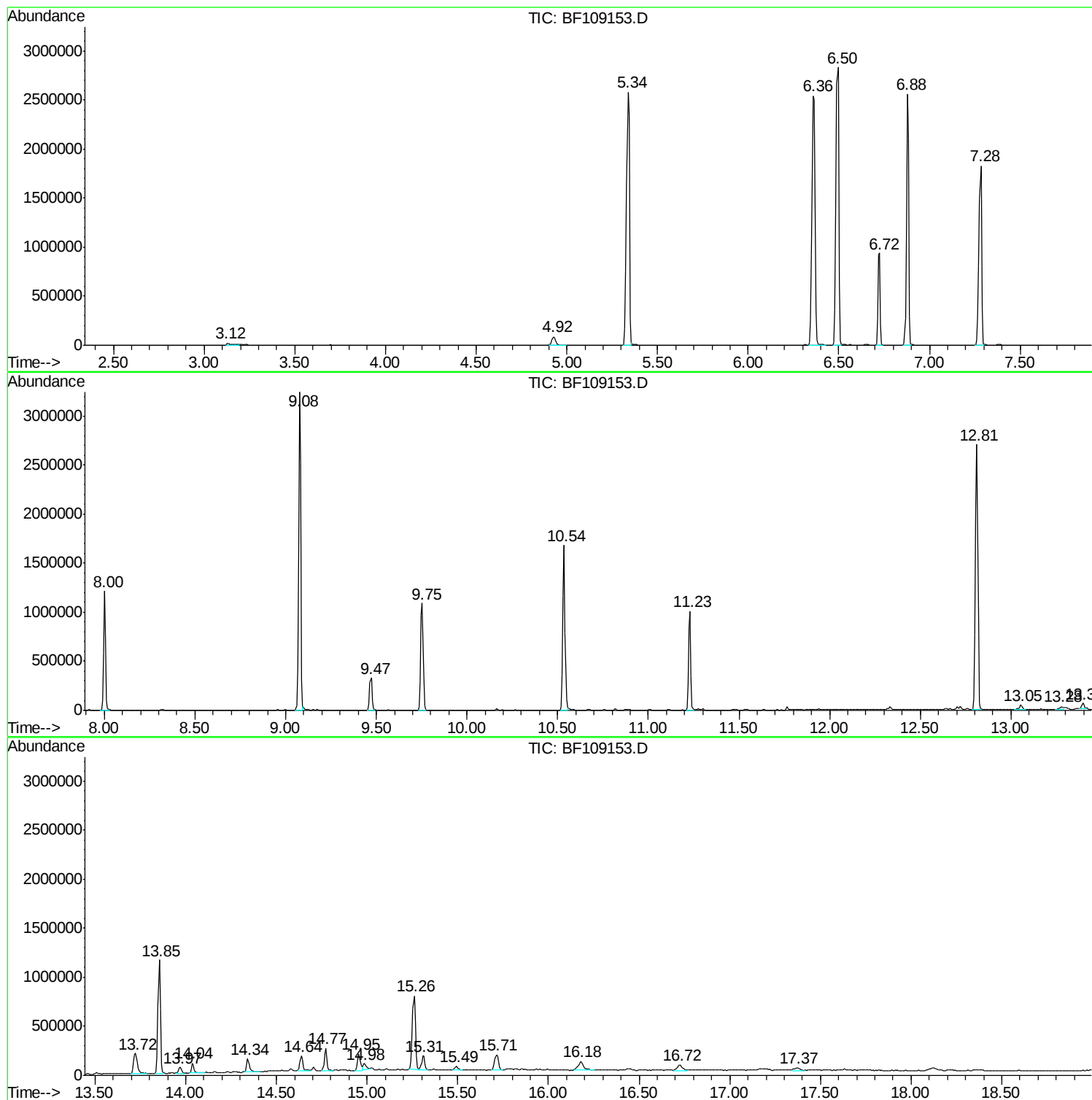
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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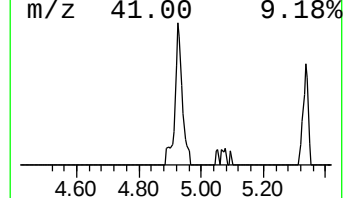
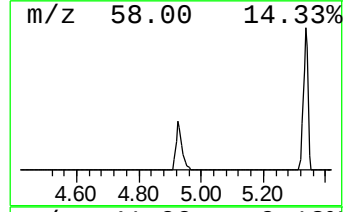
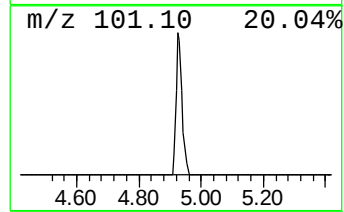
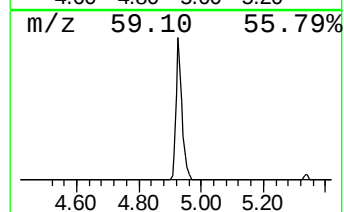
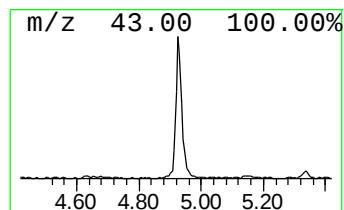
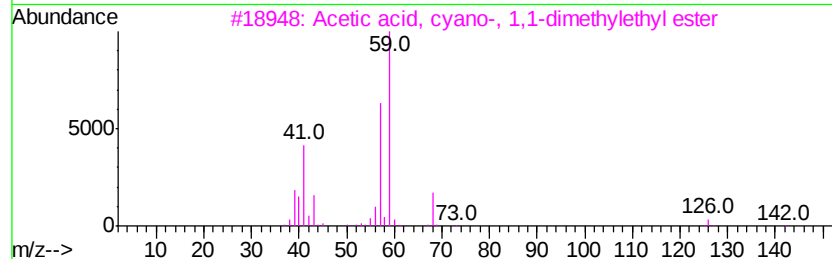
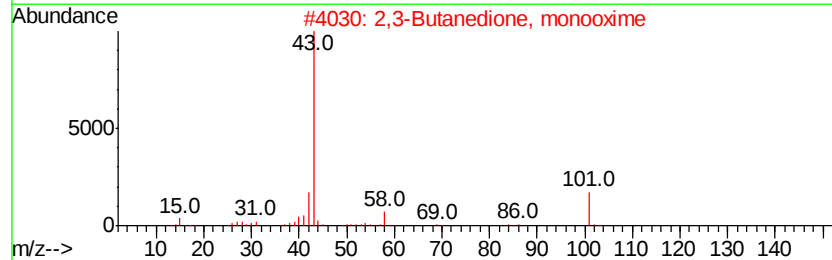
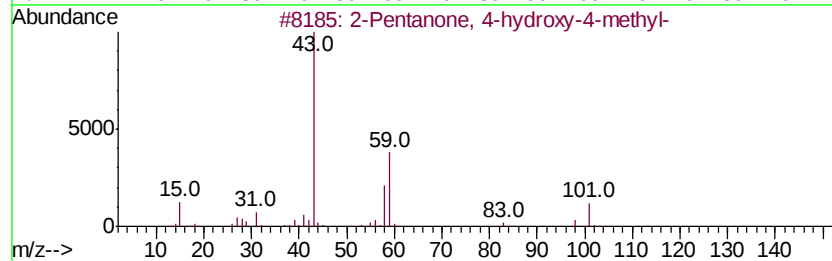
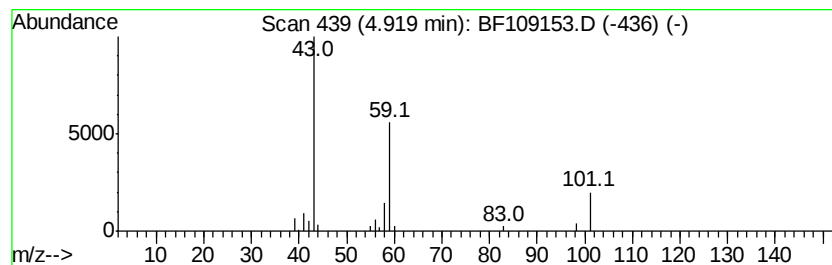
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.80 ng	118467	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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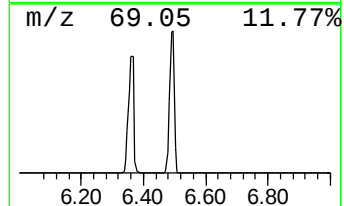
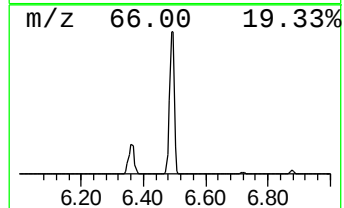
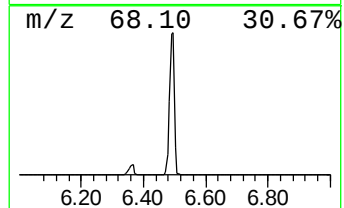
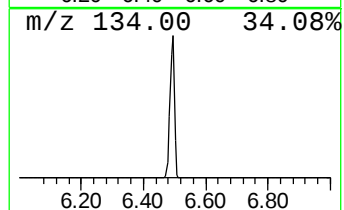
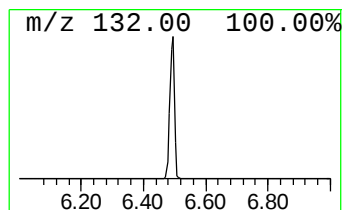
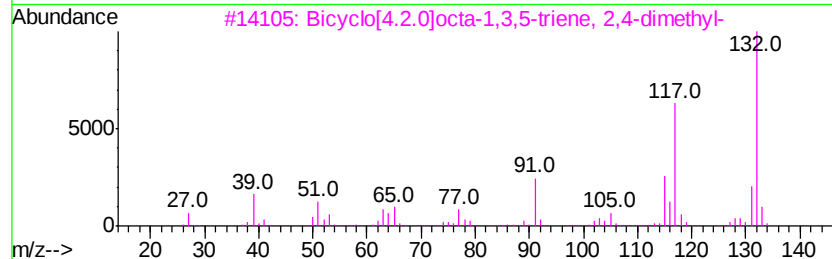
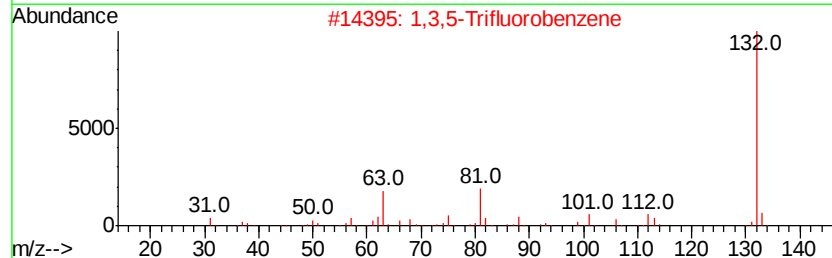
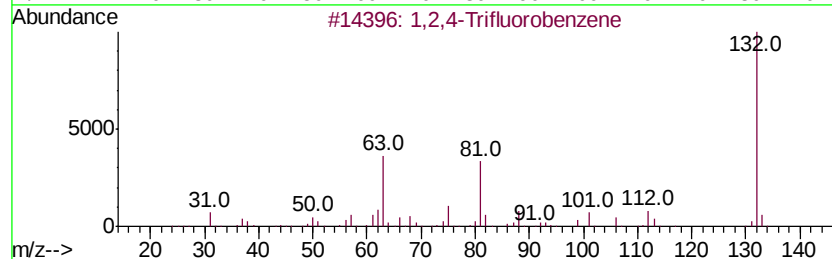
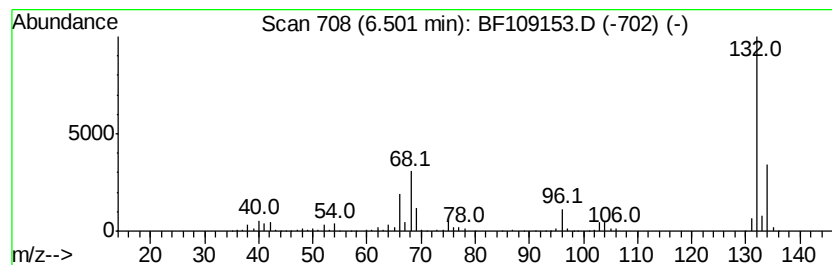
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	66.04 ng	2795280	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
2		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3		Bicvclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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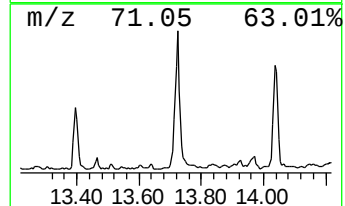
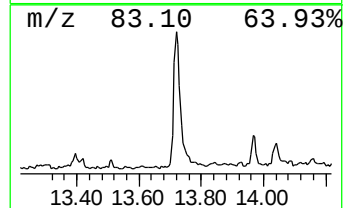
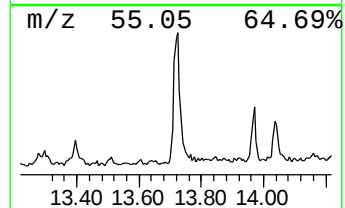
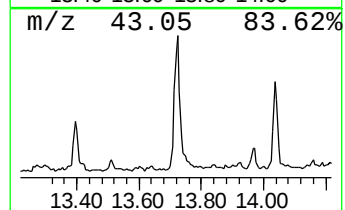
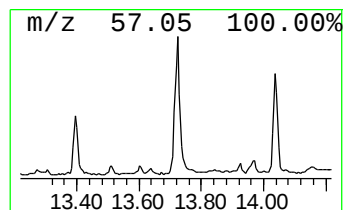
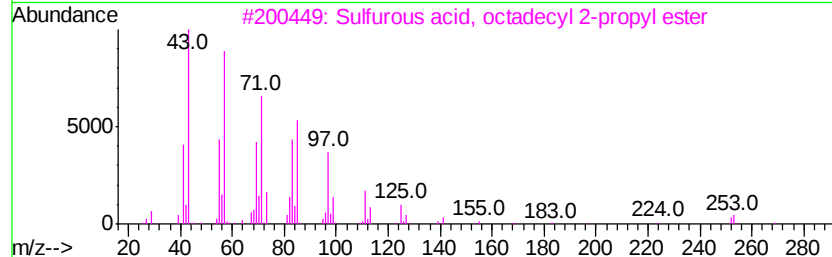
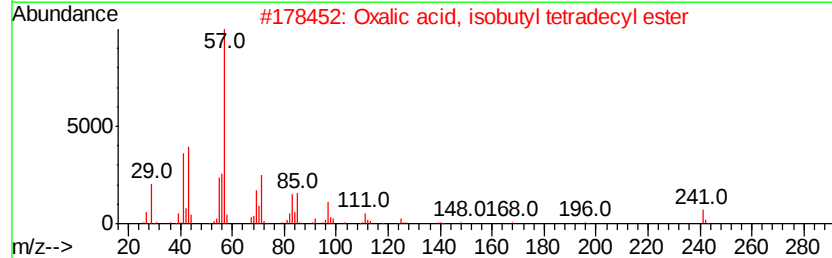
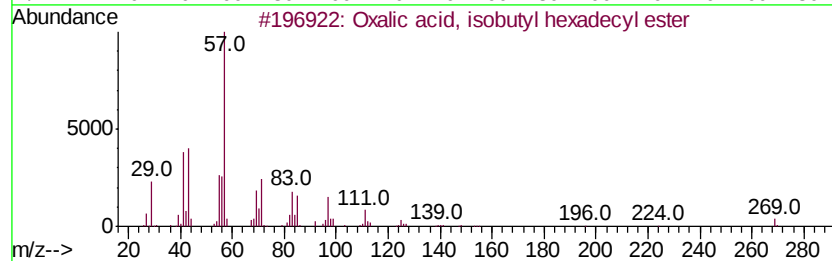
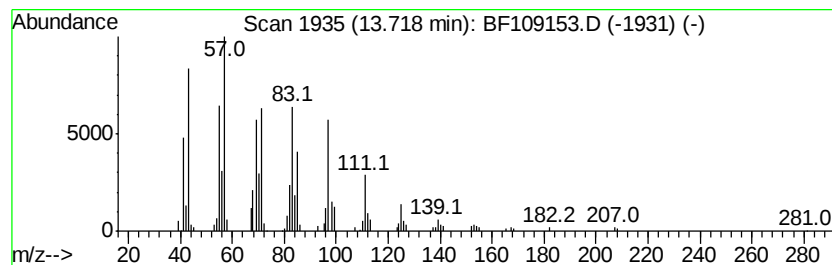
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Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.11 ng	297129	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	76
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	76



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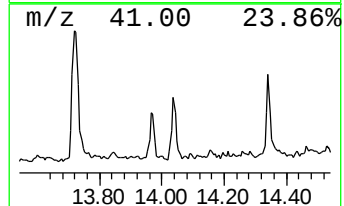
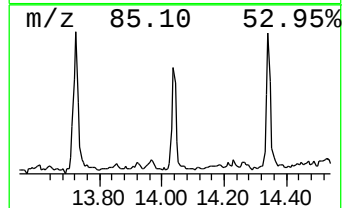
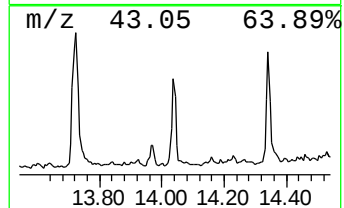
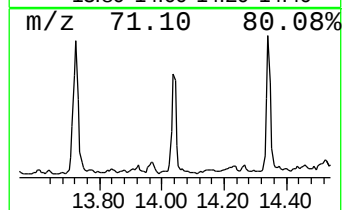
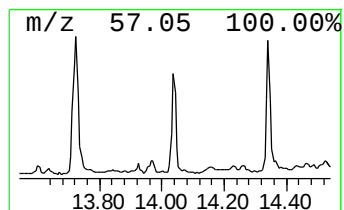
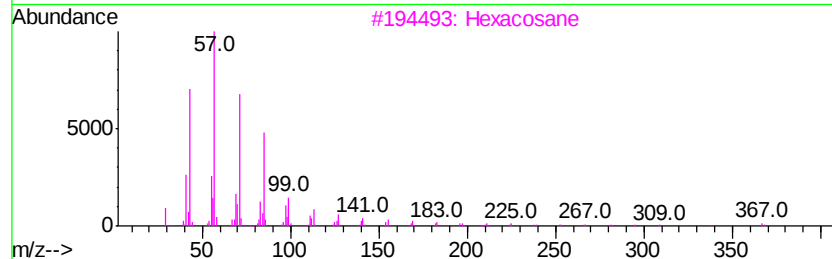
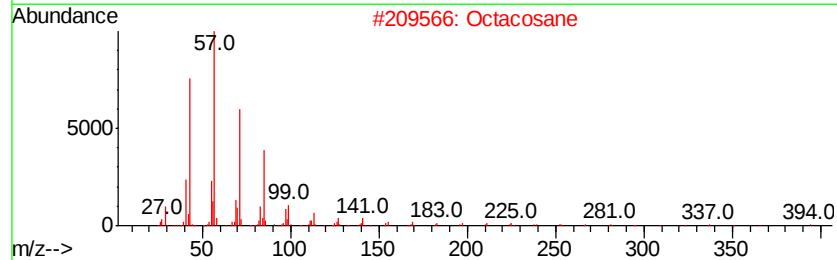
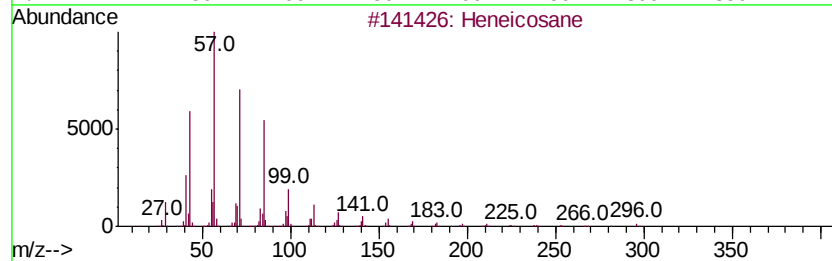
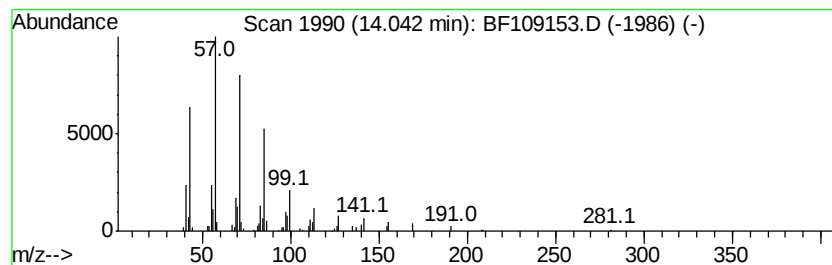
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	2.14 ng	103945	Chrysene-d12	13.85

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	Hexacosane		366	C26H54	000630-01-3	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Tetracosane		338	C24H50	000646-31-1	91



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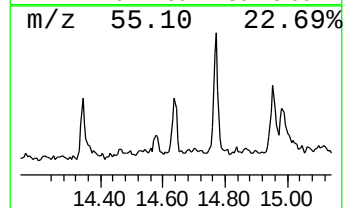
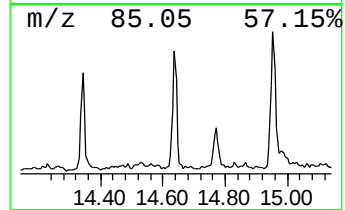
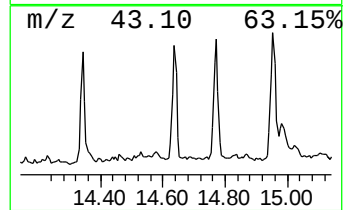
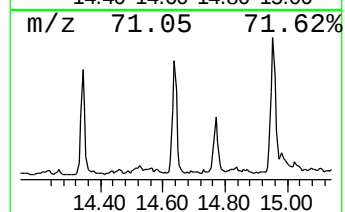
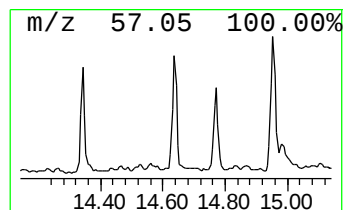
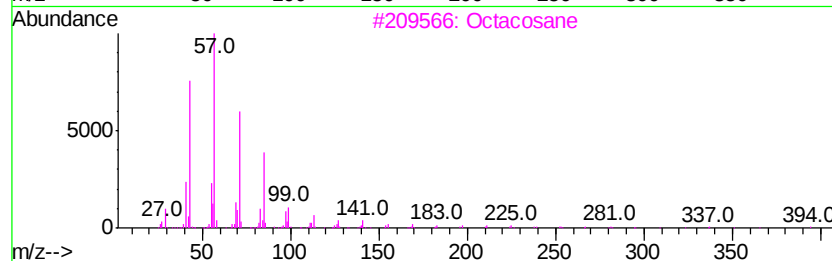
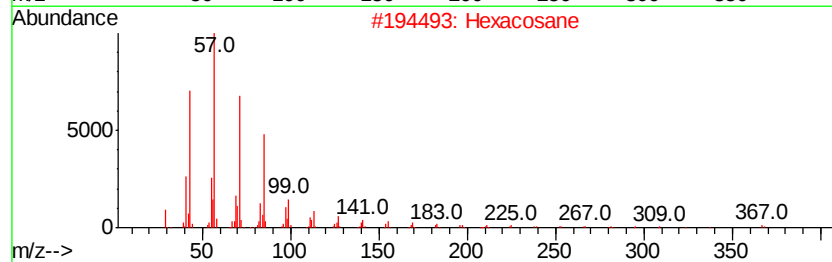
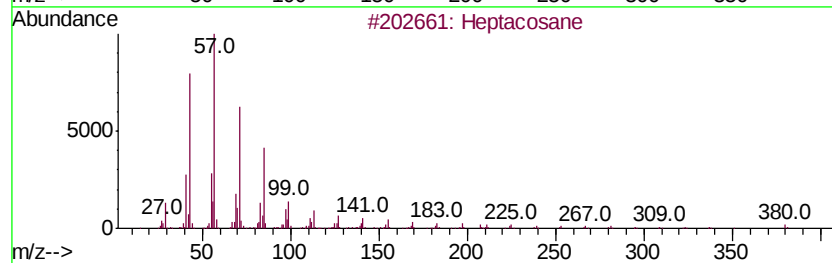
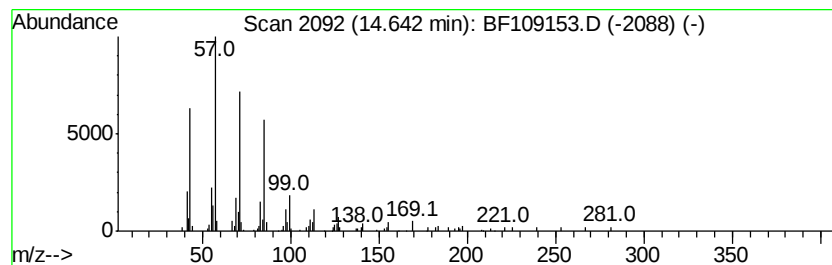
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.40 ng	144613	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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Operator : JU/SJ
Sample : J4771-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-091818

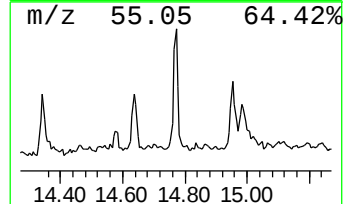
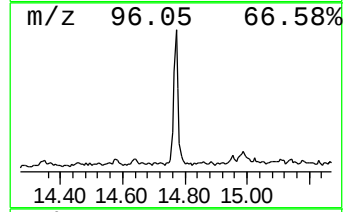
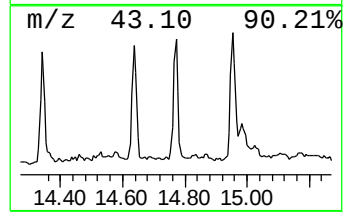
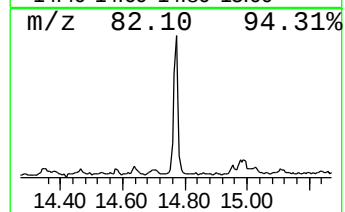
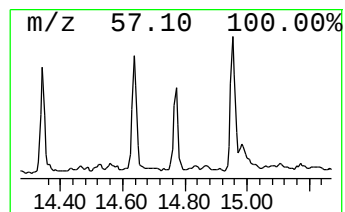
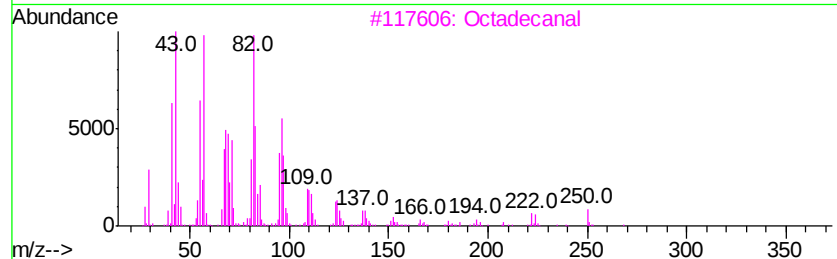
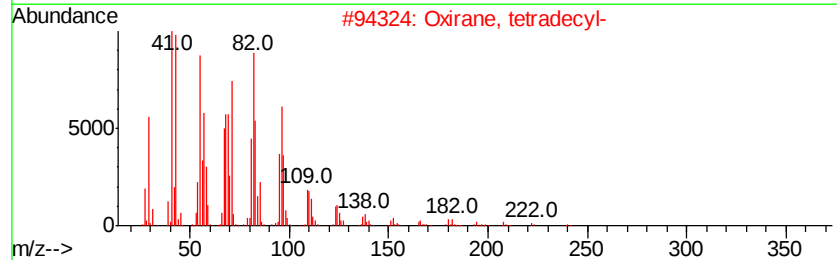
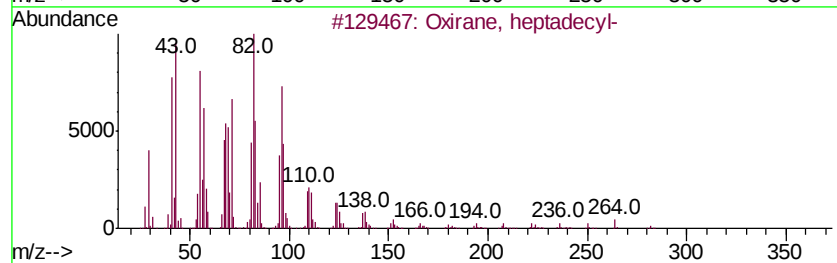
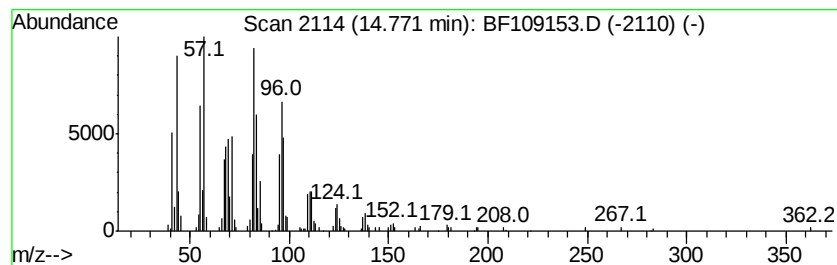
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	5.36 ng	227828	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2		Oxirane, tetradecyl-	240	C16H32O	007320-37-8	91
3		Octadecanal	268	C18H36O	000638-66-4	91
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5		Heptadecanal	254	C17H34O	1000376-70-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109153.D
Acq On : 19 Sep 2018 19:36
Operator : JU/SJ
Sample : J4771-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-091818

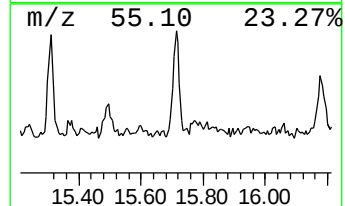
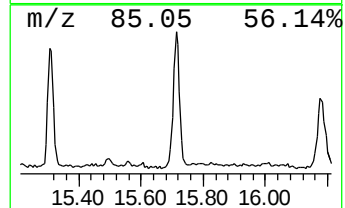
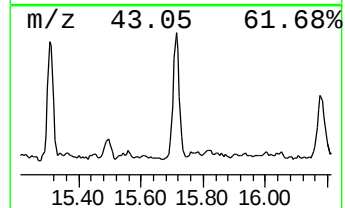
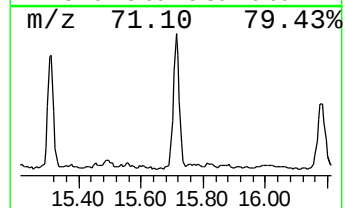
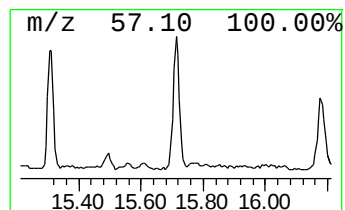
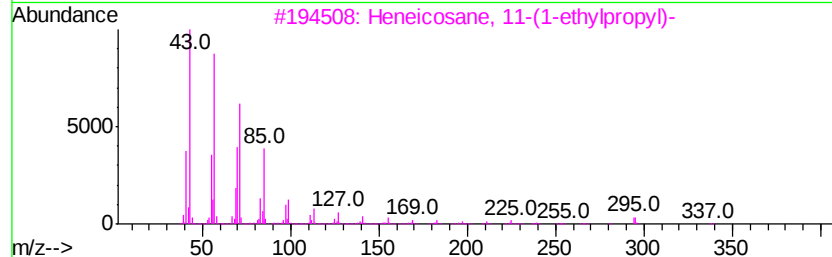
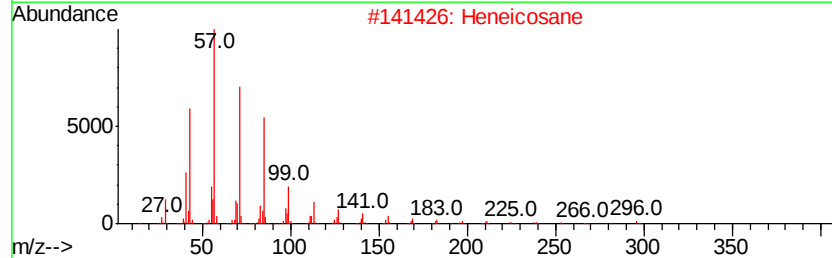
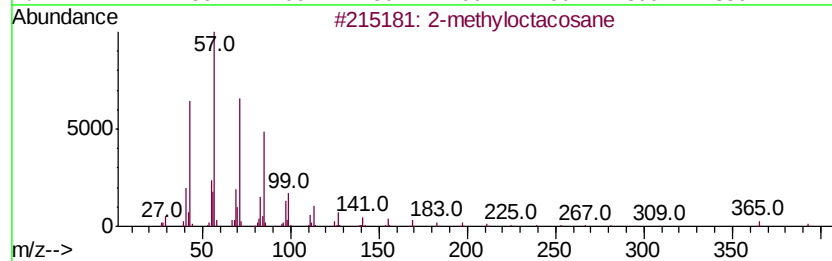
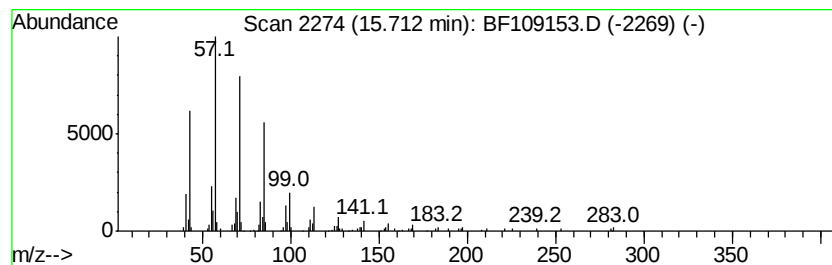
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	5.35 ng	227355	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109153.D
Acq On : 19 Sep 2018 19:36
Operator : JU/SJ
Sample : J4771-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-07-091818

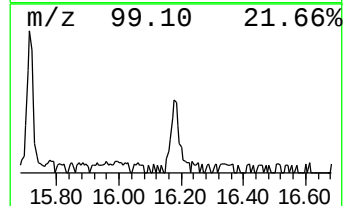
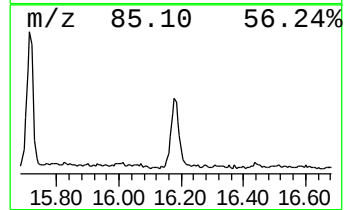
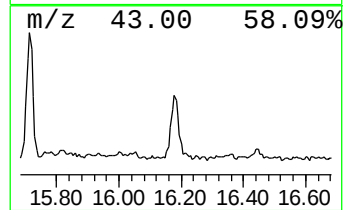
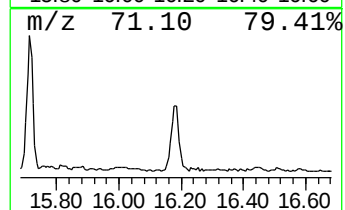
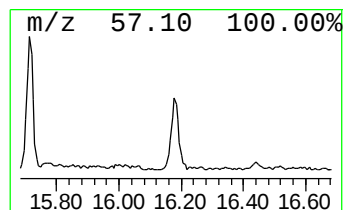
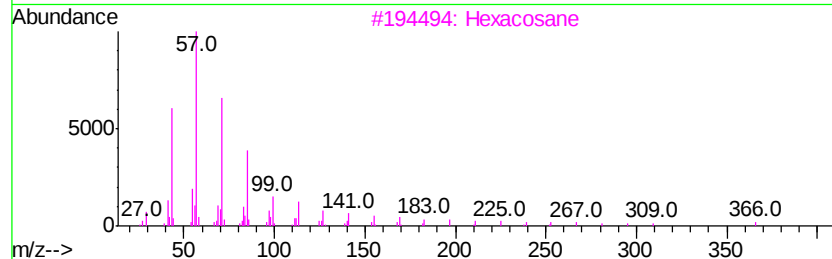
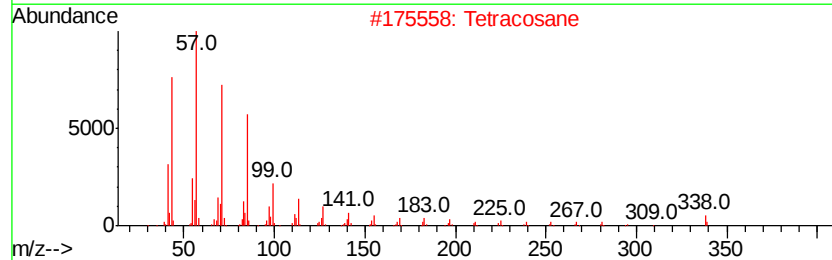
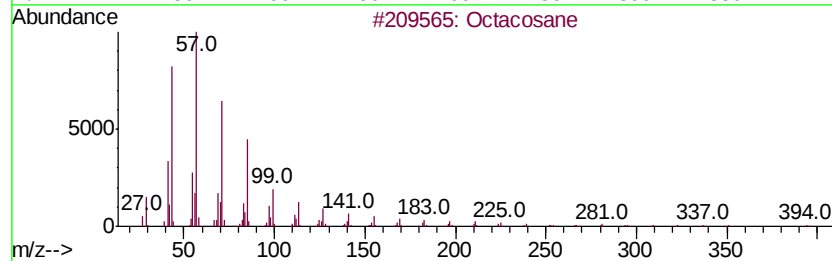
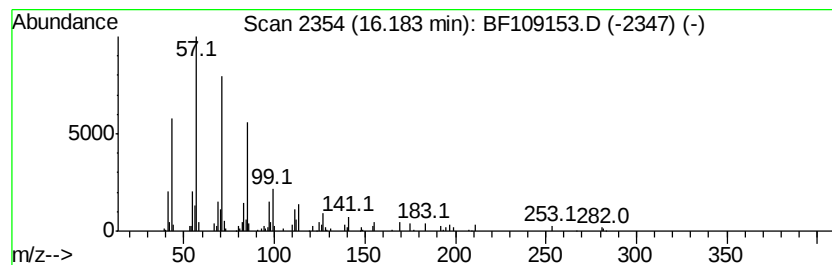
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	4.36 ng	185233	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109153.D
Acq On : 19 Sep 2018 19:36
Operator : JU/SJ
Sample : J4771-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-07-091818

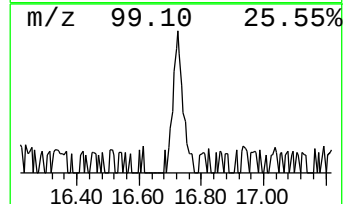
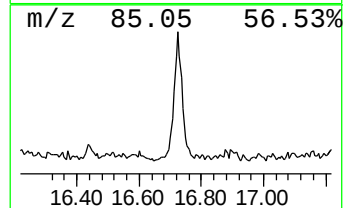
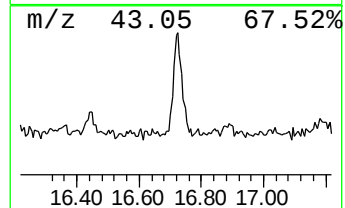
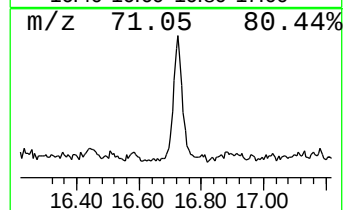
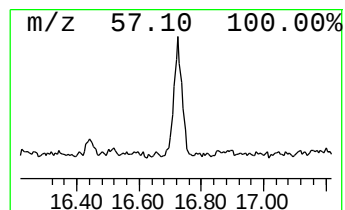
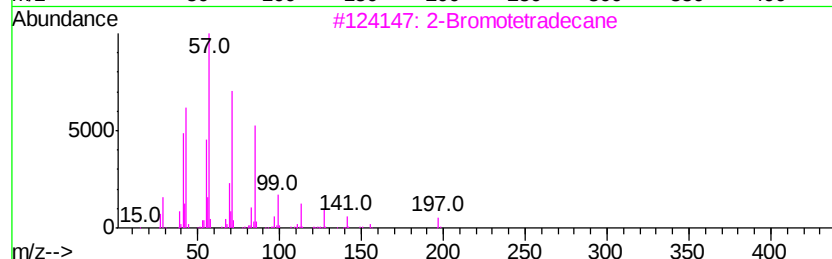
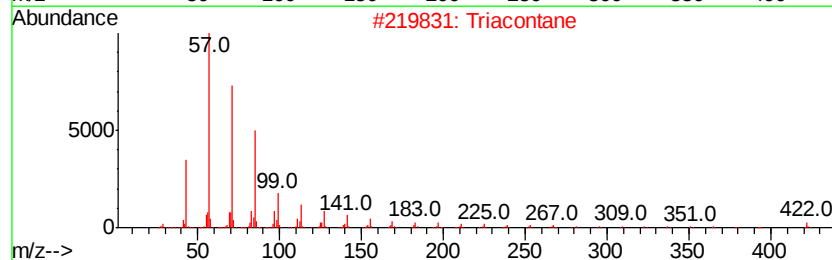
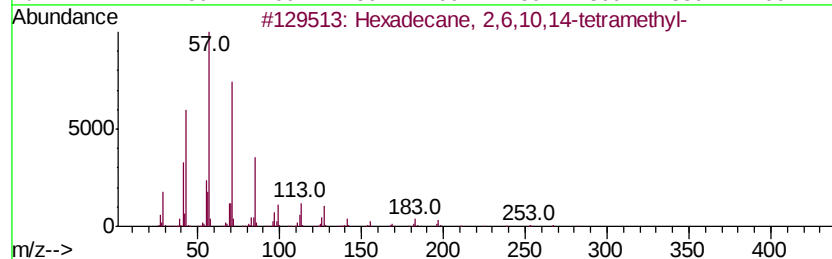
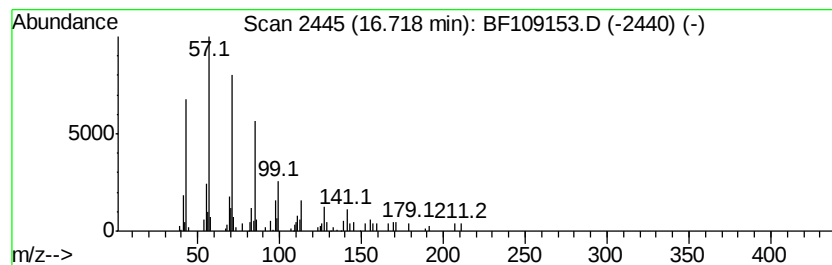
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane, 2,6,10,14-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.60 ng	110459	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2		Triacontane	422	C30H62	000638-68-6	91
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091918\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.92	2.8	ng	118467	1	6.72	846537	20.0
unknown6.50	6.50	66.0	ng	2795280	1	6.72	846537	20.0
Oxalic acid, isob...	13.72	6.1	ng	297129	5	13.85	973058	20.0
Heneicosane	14.04	2.1	ng	103945	5	13.85	973058	20.0
Heptacosane	14.64	3.4	ng	144613	6	15.26	849586	20.0
Oxirane, heptadecyl-	14.77	5.4	ng	227828	6	15.26	849586	20.0
2-methyloctacosane	15.71	5.3	ng	227355	6	15.26	849586	20.0
Octacosane	16.18	4.4	ng	185233	6	15.26	849586	20.0
Hexadecane, 2,6,1...	16.72	2.6	ng	110459	6	15.26	849586	20.0