

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
 Data File : BF109622.D
 Acq On : 5 Oct 2018 21:32
 Operator : JU/SJ
 Sample : J5255-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-2

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-BF092218.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	4.898	475	478	490	rVB	47486	66028	3.28%	0.363%
2	5.328	547	551	570	rBV	1409653	1540921	76.57%	8.465%
3	6.351	721	725	742	rBV	1333472	1723339	85.63%	9.468%
4	6.475	742	746	766	rVB	1801483	1746588	86.78%	9.595%
5	6.704	781	785	794	rBV	424615	469787	23.34%	2.581%
6	6.822	802	805	807	rBV	66819	47603	2.37%	0.262%
7	6.857	807	811	825	rVB	1510934	1344345	66.80%	7.386%
8	7.263	876	880	911	rBV	1005674	1105250	54.92%	6.072%
9	7.981	999	1002	1021	rBV	623079	612376	30.43%	3.364%
10	9.057	1181	1185	1199	rBV	2150360	2012565	100.00%	11.057%
11	9.451	1249	1252	1261	rBV	149927	136942	6.80%	0.752%
12	9.727	1296	1299	1316	rVB2	659707	637290	31.67%	3.501%
13	10.516	1429	1433	1452	rBV	929461	967311	48.06%	5.314%
14	11.210	1547	1551	1561	rBV	531055	565003	28.07%	3.104%
15	11.745	1638	1642	1651	rBV3	127295	144282	7.17%	0.793%
16	12.416	1752	1756	1770	rBV	82011	107263	5.33%	0.589%
17	12.527	1772	1775	1784	rVV5	39376	55428	2.75%	0.305%
18	12.610	1785	1789	1791	rVV	67349	68890	3.42%	0.378%
19	12.639	1791	1794	1797	rVV	78399	85050	4.23%	0.467%
20	12.674	1797	1800	1813	rVV	115530	189623	9.42%	1.042%
21	12.786	1815	1819	1823	rVV	1482622	1403133	69.72%	7.708%
22	12.815	1823	1824	1828	rVB	63310	48876	2.43%	0.269%
23	13.268	1893	1901	1909	rBV	347762	409096	20.33%	2.247%
24	13.333	1909	1912	1914	rBV	28677	24351	1.21%	0.134%
25	13.692	1969	1973	1981	rBV3	98158	148530	7.38%	0.816%
26	13.833	1992	1997	2000	rBV	577303	591814	29.41%	3.251%
27	14.010	2024	2027	2031	rBV	59881	54658	2.72%	0.300%
28	14.315	2076	2079	2082	rBV	82556	80273	3.99%	0.441%
29	14.604	2125	2128	2132	rBV	123928	119764	5.95%	0.658%
30	14.674	2137	2140	2143	rBV	32857	33686	1.67%	0.185%
31	14.839	2164	2168	2178	rBV	89855	165574	8.23%	0.910%
32	14.915	2178	2181	2189	rVV2	149521	180545	8.97%	0.992%
33	15.121	2212	2216	2222	rVV	42810	63402	3.15%	0.348%
34	15.174	2222	2225	2231	rVV	38333	52874	2.63%	0.290%

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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

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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.233	2231	2235	2238	rVV	399034	499668	24.83%	2.745%
36	15.268	2238	2241	2250	rVB2	181236	229252	11.39%	1.259%
37	15.668	2304	2309	2314	rBV	132637	193478	9.61%	1.063%
38	16.121	2381	2386	2399	rVB2	78400	158999	7.90%	0.874%
39	16.586	2461	2465	2473	rVV4	15106	33740	1.68%	0.185%
40	16.662	2473	2478	2485	rVB2	35249	63098	3.14%	0.347%
41	16.992	2530	2534	2539	rVB2	13000	21740	1.08%	0.119%

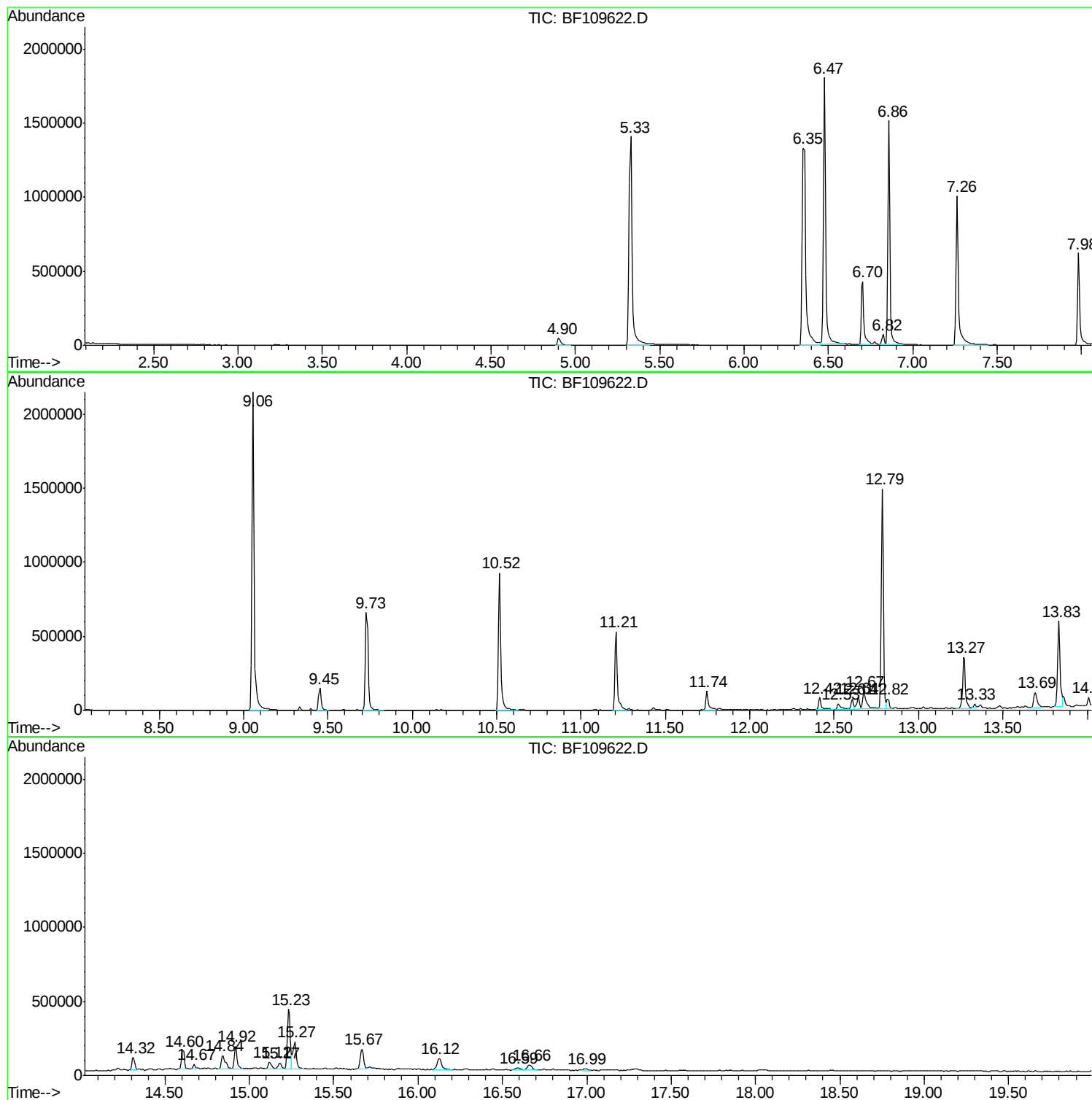
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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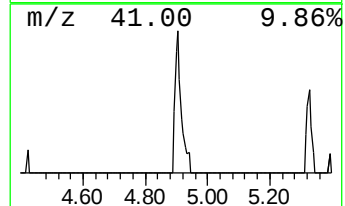
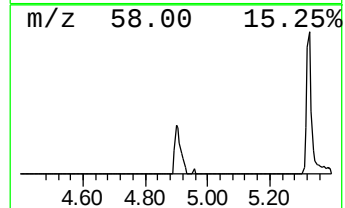
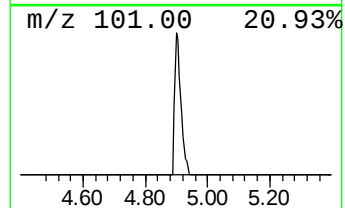
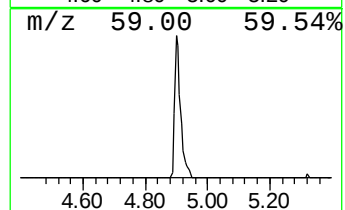
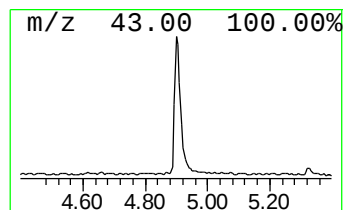
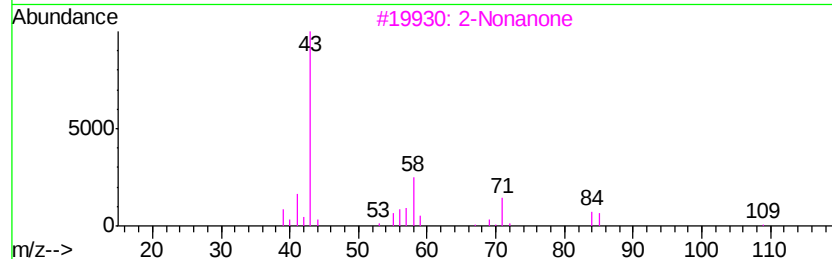
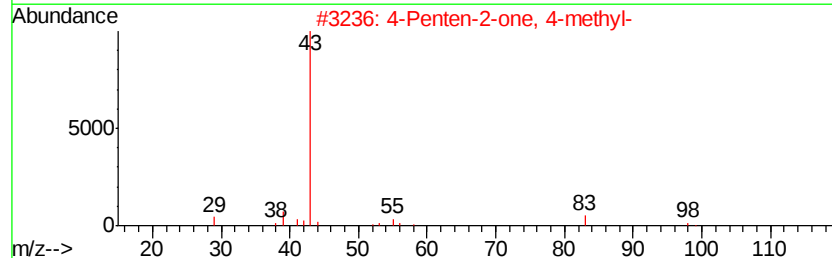
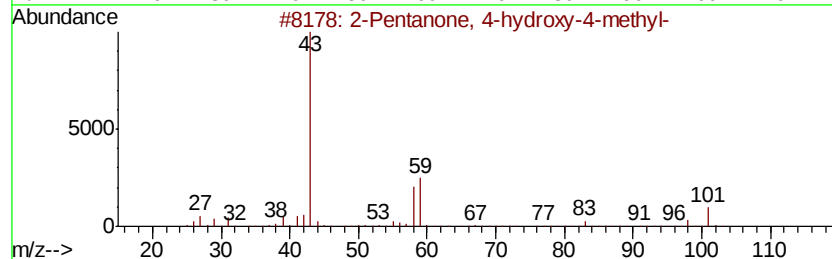
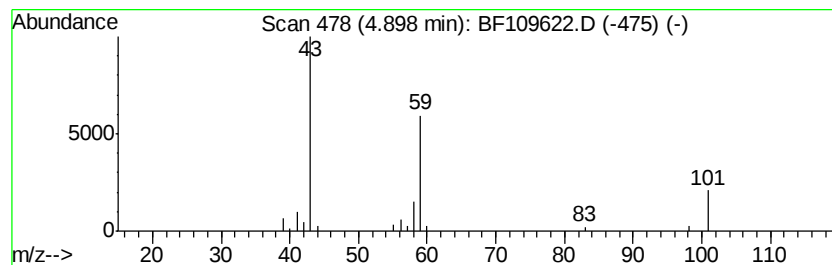
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	2.81 ng	66028	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3			2-Nonanone	142	C9H18O	000821-55-6	9
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9



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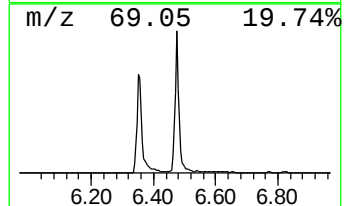
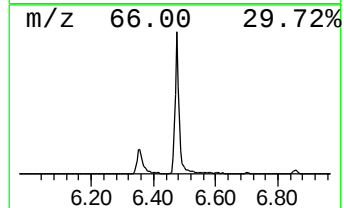
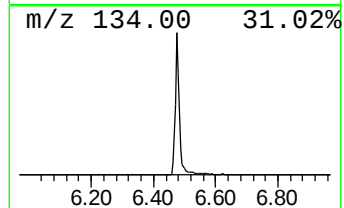
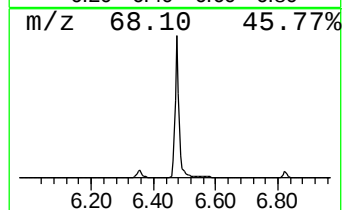
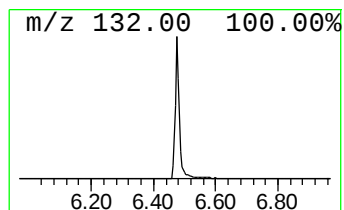
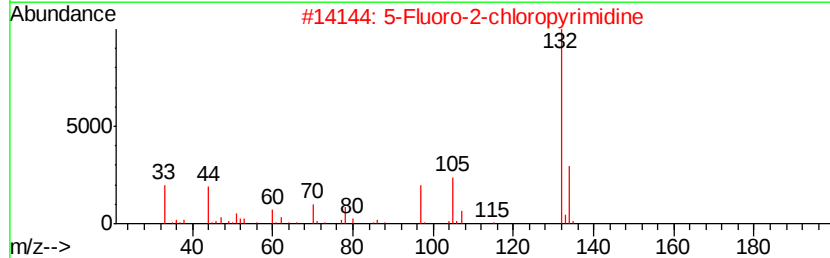
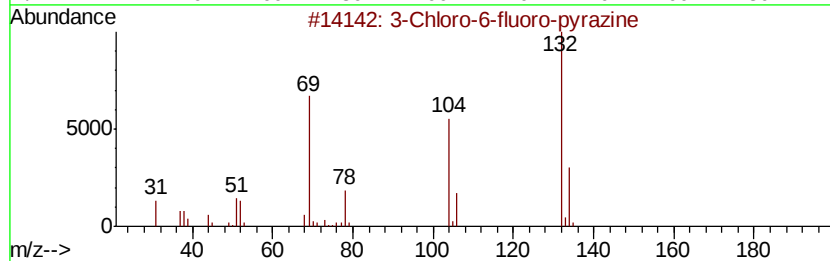
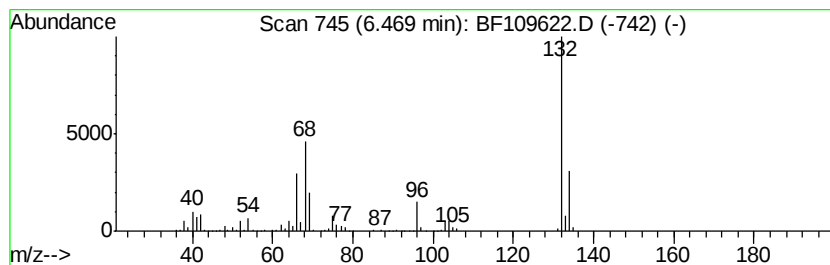
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	74.36 ng	1746590	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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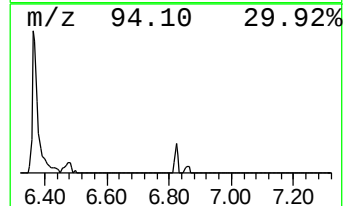
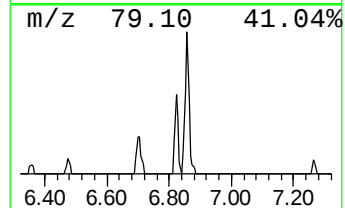
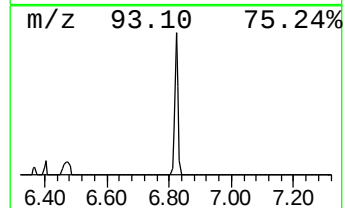
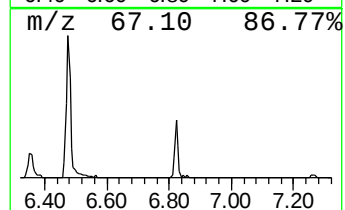
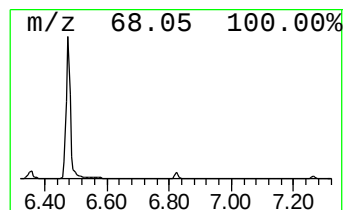
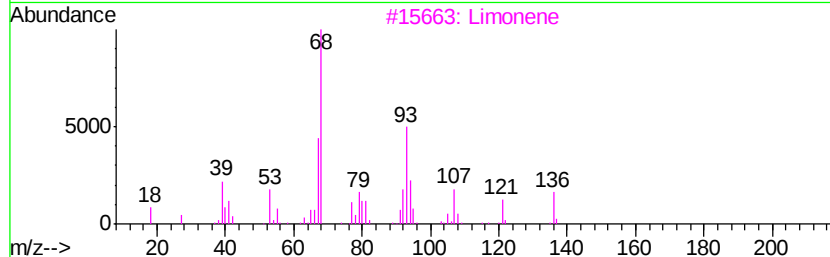
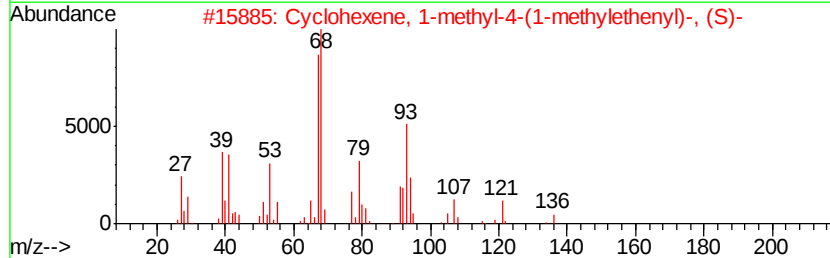
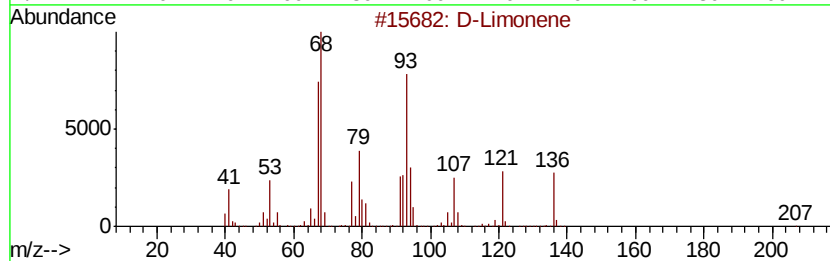
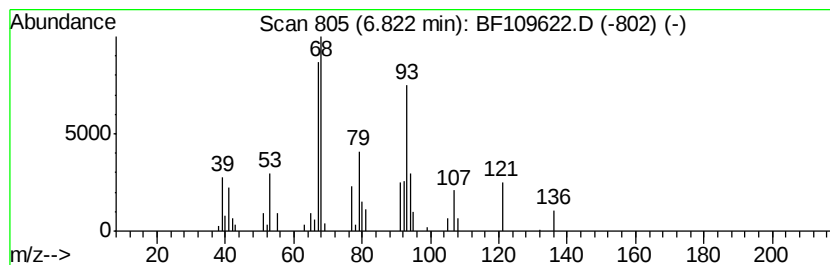
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 D-Limonene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.82	2.03 ng	47603	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Limonene	136	C10H16	005989-27-5	96
2		Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	95
3		Limonene	136	C10H16	000138-86-3	93
4		Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	86
5		Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	72



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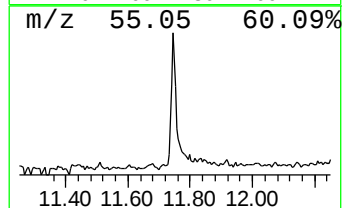
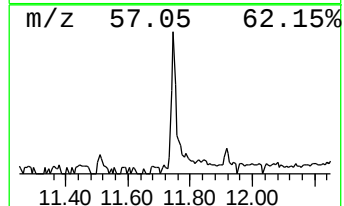
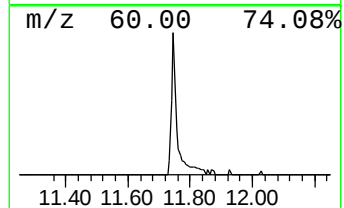
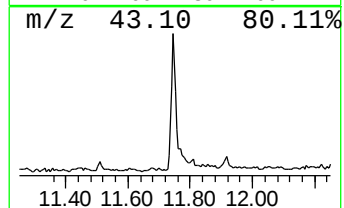
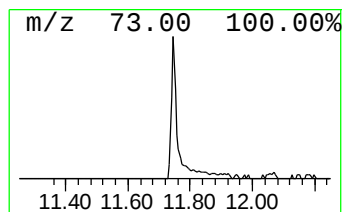
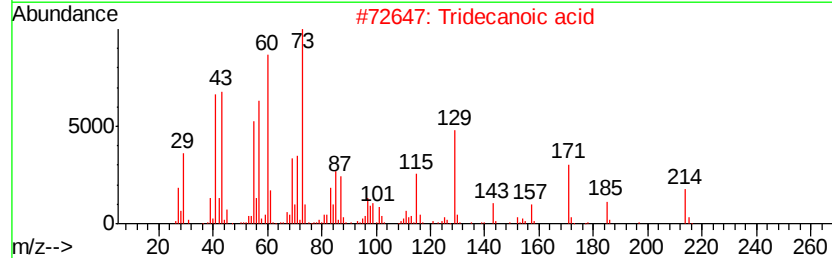
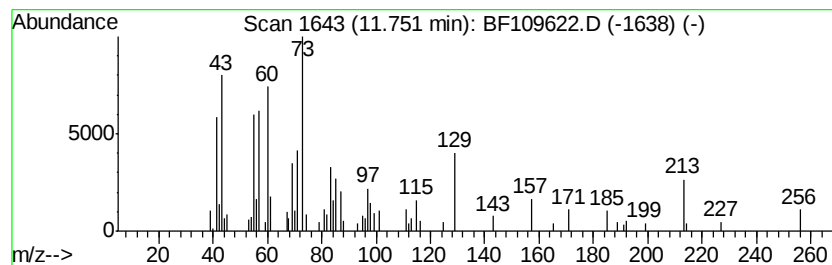
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	5.11 ng	144282	Phenanthrene-d10	11.21

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	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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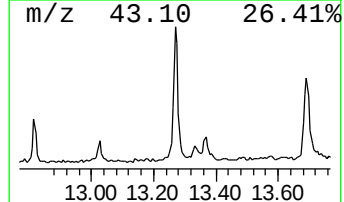
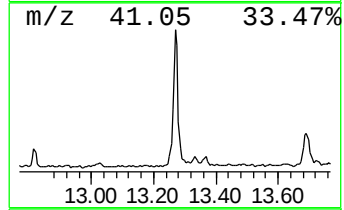
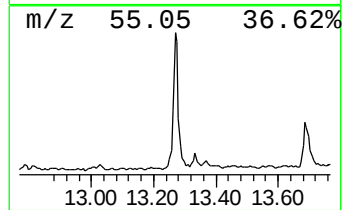
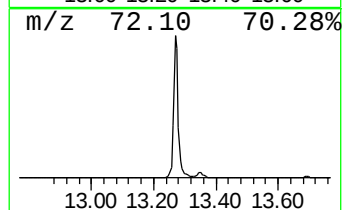
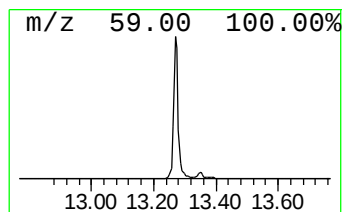
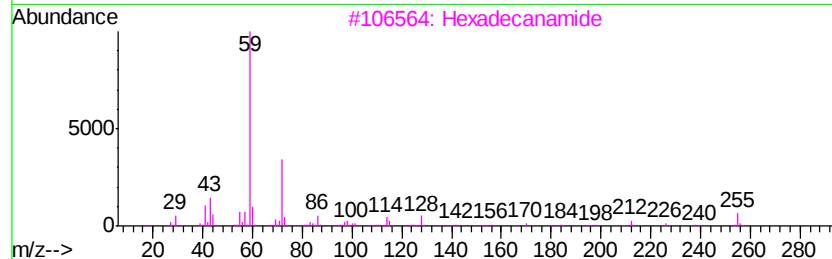
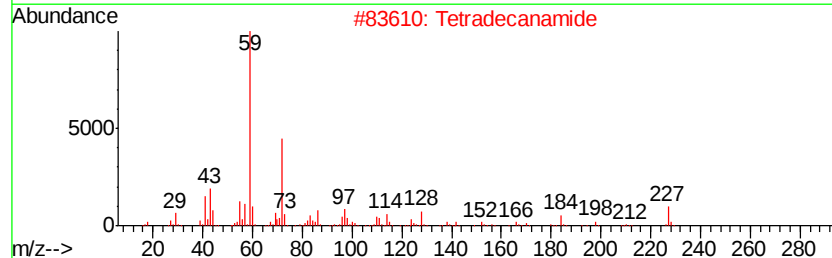
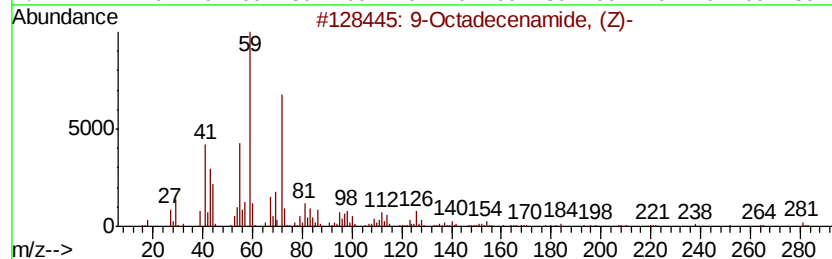
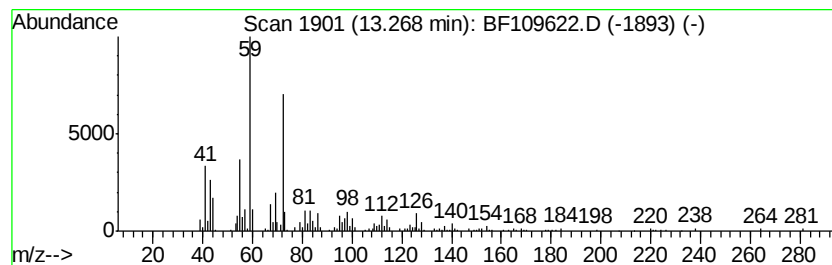
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	13.83 ng	409096	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Hexadecanamide	255	C16H33NO	000629-54-9	64
4		Octanamide	143	C8H17NO	000629-01-6	59
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50



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Sample : J5255-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-2

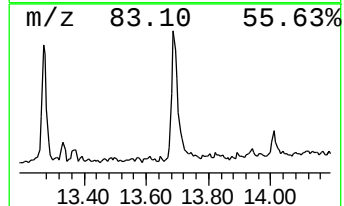
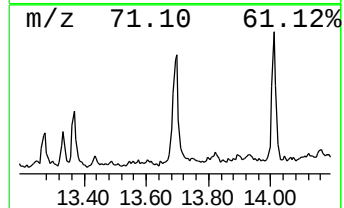
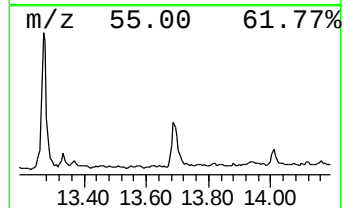
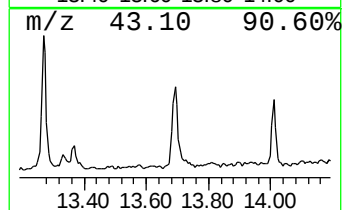
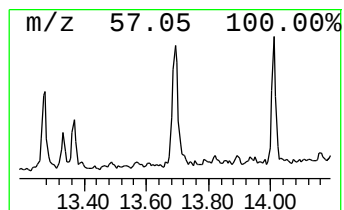
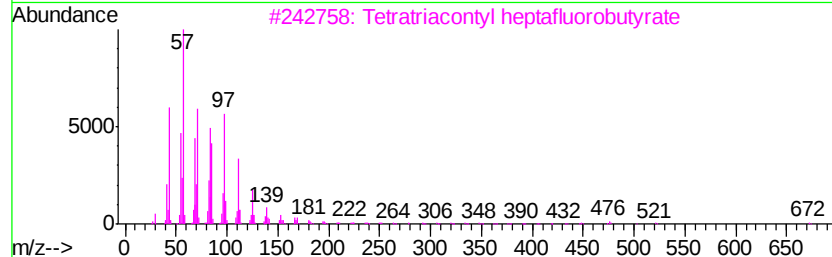
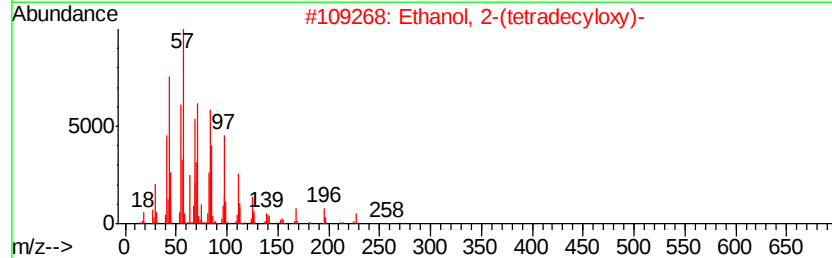
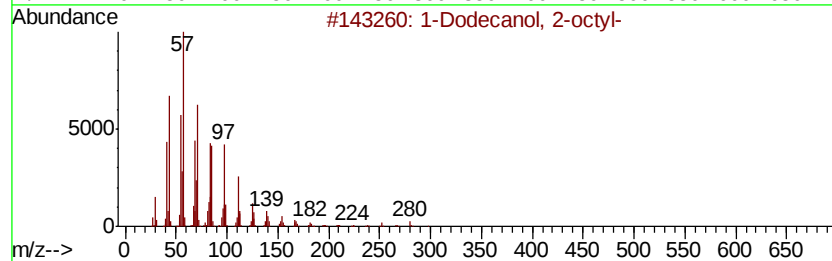
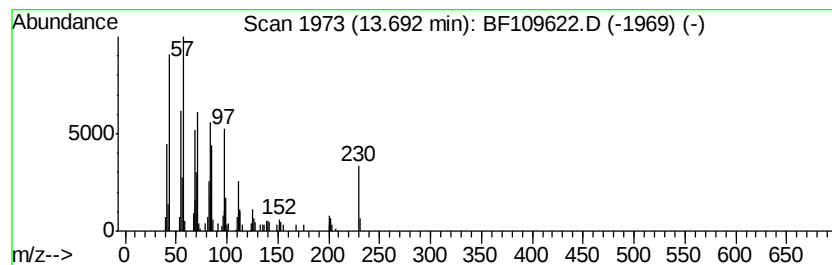
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.02 ng	148530	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
3		Tetratriacontyl heptafluorobutylate	691	C38H69F7O2	1000351-84-1	68
4		17-Pentatriacontene	491	C35H70	006971-40-0	68
5		Hexatriacontyl trifluoroacetate	619	C38H73F3O2	1000351-88-6	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109622.D
Acq On : 5 Oct 2018 21:32
Operator : JU/SJ
Sample : J5255-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

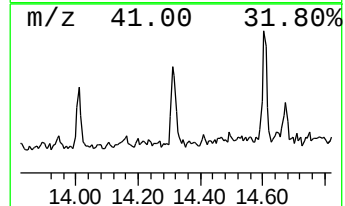
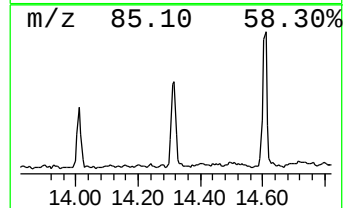
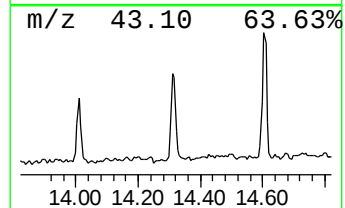
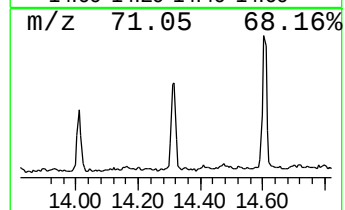
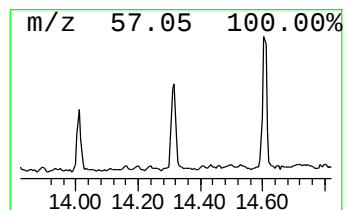
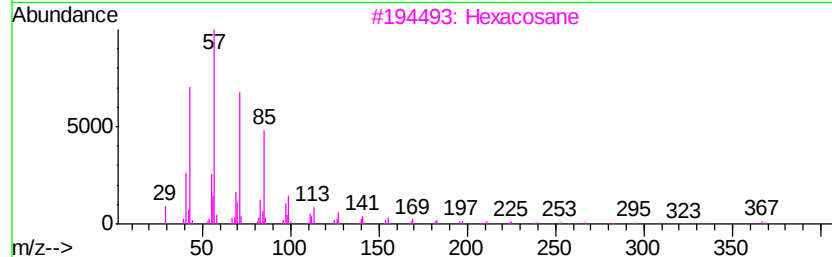
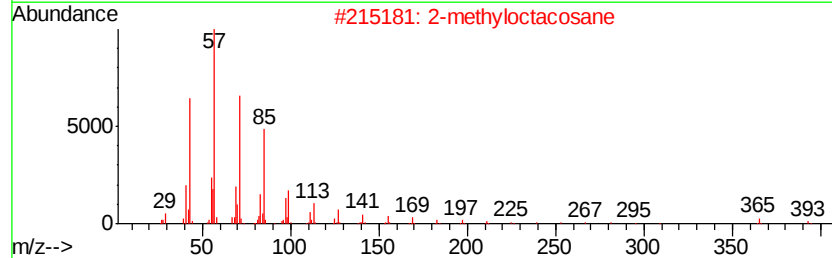
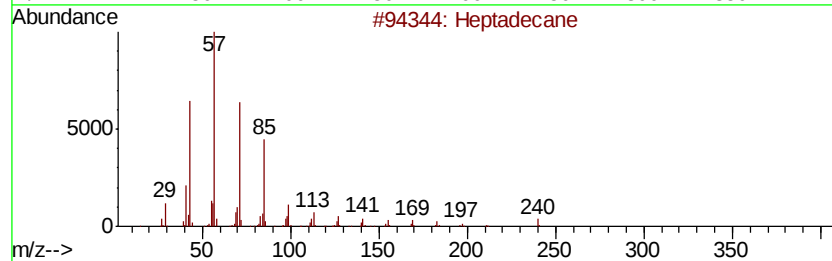
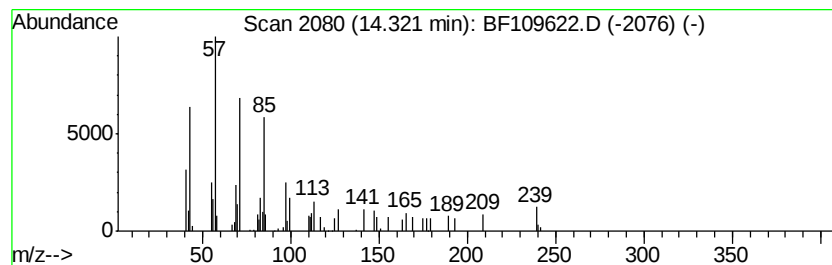
Instrument :
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ClientSampleId :
TRACK-D-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.71 ng	80273	Chrysene-d12	13.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	93
2	2-methyloctacosane	408 C29H60	1000376-72-8	91
3	Hexacosane	366 C26H54	000630-01-3	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Triacontane	422 C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109622.D
Acq On : 5 Oct 2018 21:32
Operator : JU/SJ
Sample : J5255-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-2

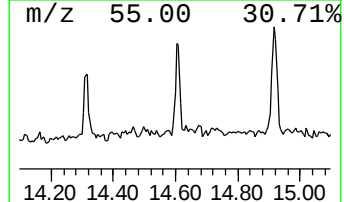
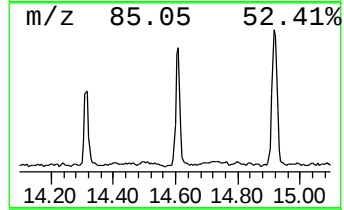
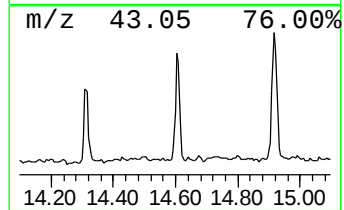
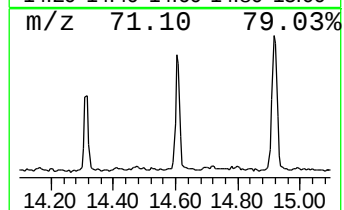
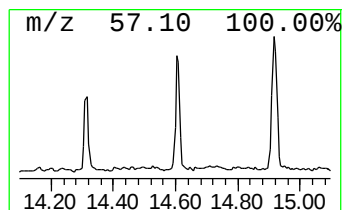
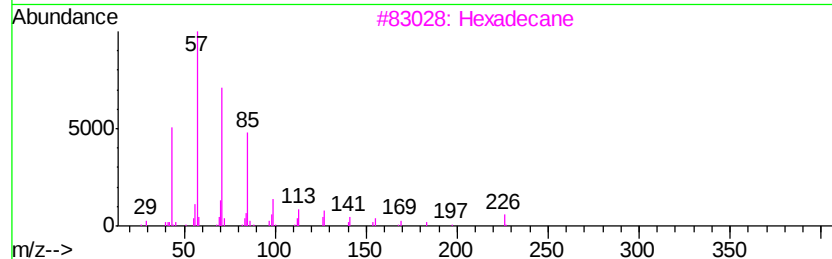
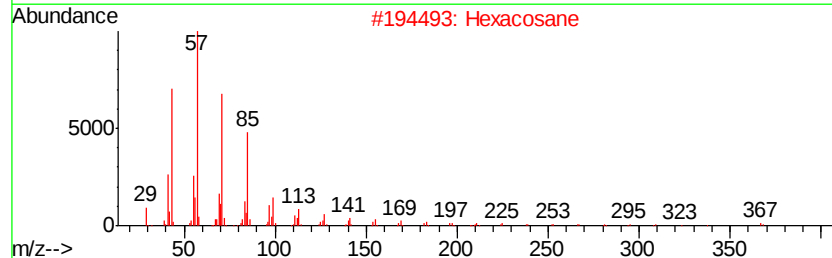
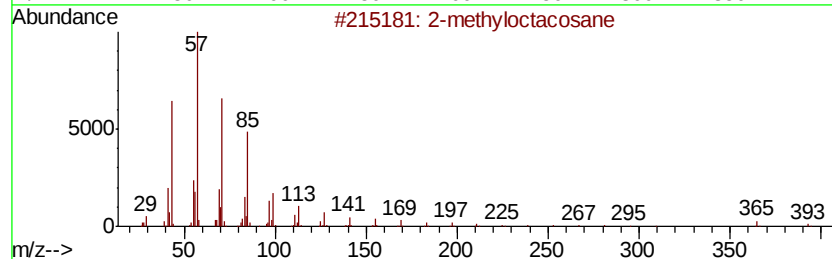
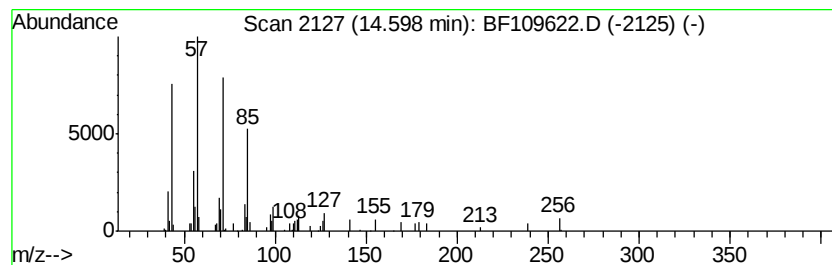
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	4.79 ng	119764	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91	
2	Hexacosane	366	C26H54	000630-01-3	91	
3	Hexadecane	226	C16H34	000544-76-3	90	
4	Heptadecane	240	C17H36	000629-78-7	90	
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109622.D
Acq On : 5 Oct 2018 21:32
Operator : JU/SJ
Sample : J5255-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

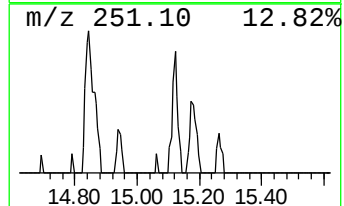
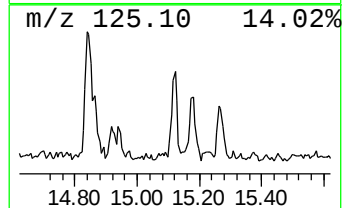
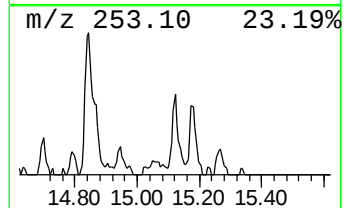
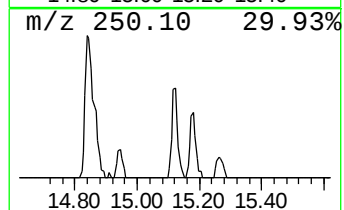
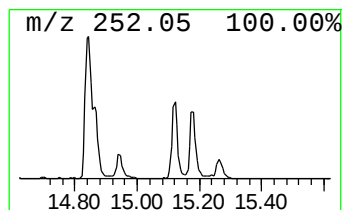
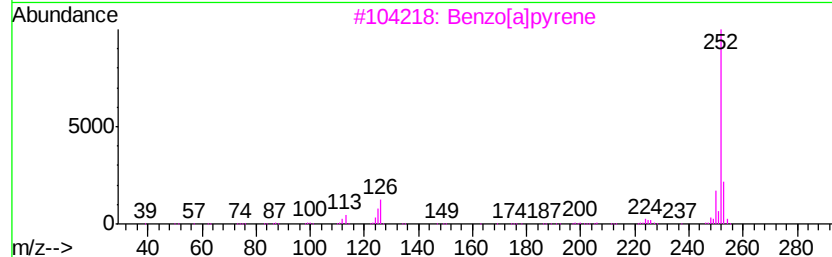
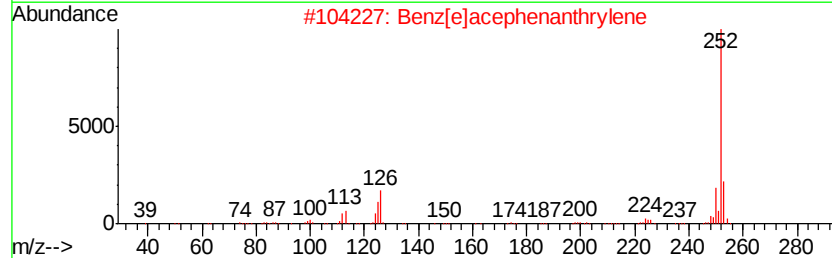
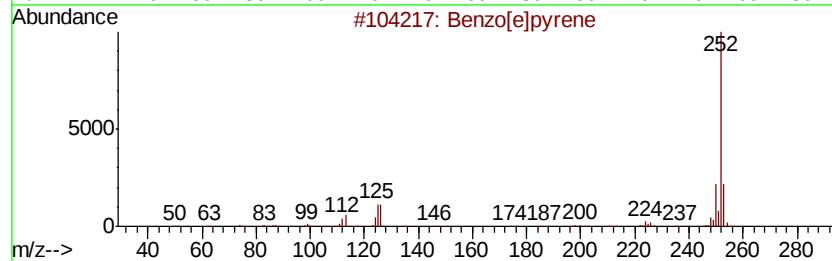
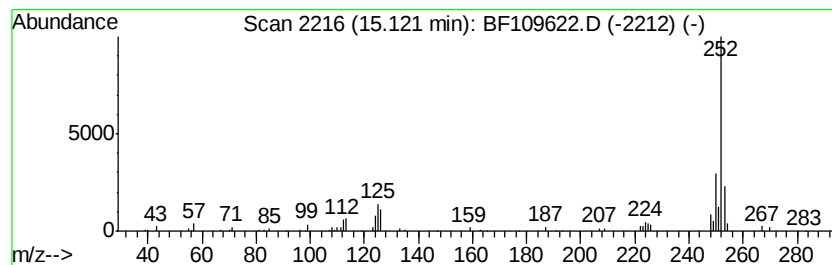
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.12	2.54 ng	63402	Perylene-d12	15.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]bpvrene	252	C20H12	000192-97-2	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3	Benzo[a]bpvrene	252	C20H12	000050-32-8	87
4	Perylene	252	C20H12	000198-55-0	87
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100518\
Data File : BF109622.D
Acq On : 5 Oct 2018 21:32
Operator : JU/SJ
Sample : J5255-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
TRACK-D-2

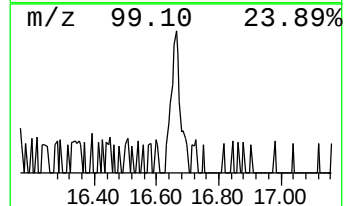
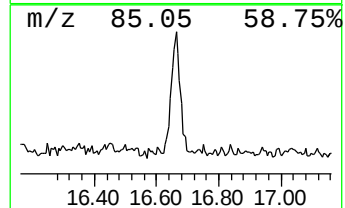
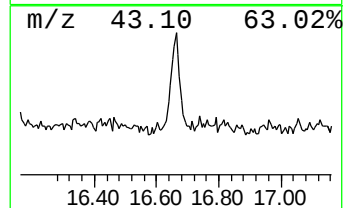
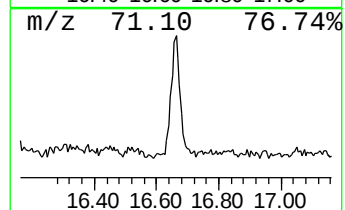
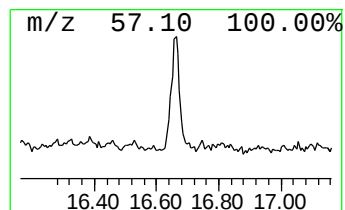
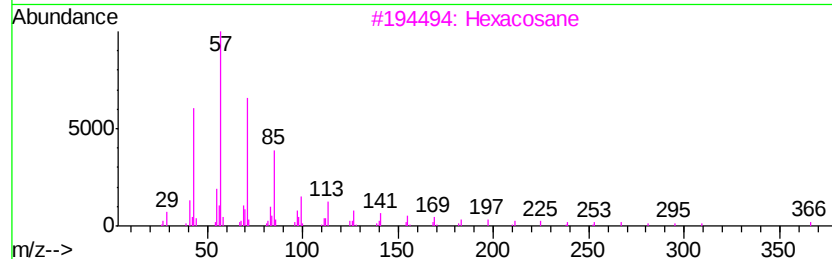
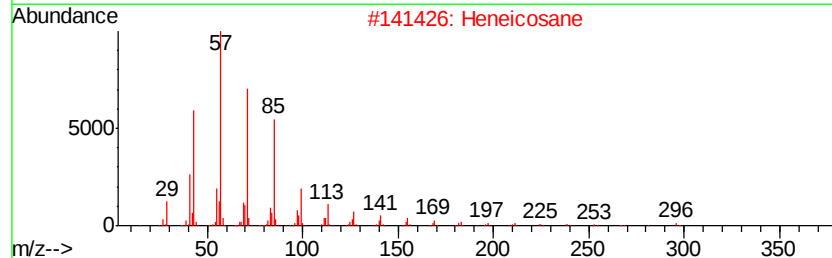
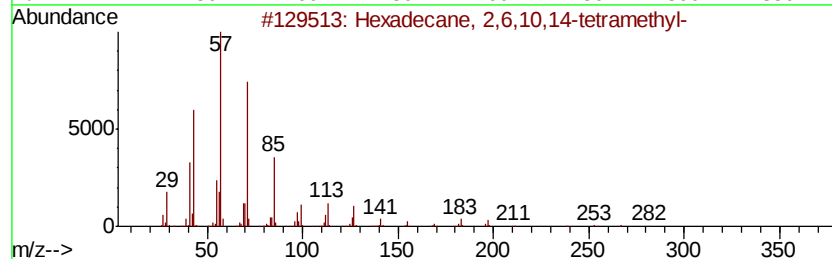
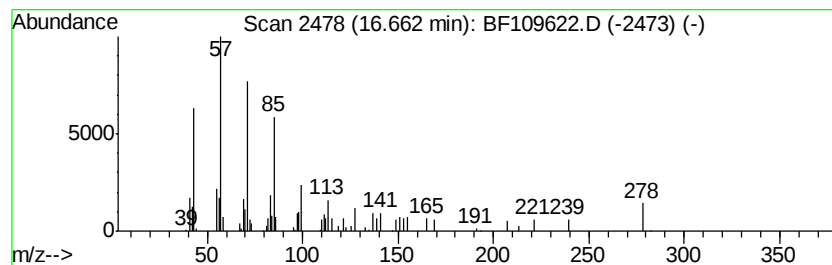
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexadecane, 2,6,10,14-tetra... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	2.53 ng	63098	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	92
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tetracosane	338	C24H50	000646-31-1	86
5		Pentacosane	352	C25H52	000629-99-2	83



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TRACK-D-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
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unknown6.47	6.47	74.4	ng	1746590	1	6.70	469787	20.0
D-Limonene	6.82	2.0	ng	47603	1	6.70	469787	20.0
n-Hexadecanoic acid	11.75	5.1	ng	144282	4	11.21	565003	20.0
9-Octadecenamide,...	13.27	13.8	ng	409096	5	13.83	591814	20.0
1-Dodecanol, 2-oc...	13.69	5.0	ng	148530	5	13.83	591814	20.0
Heptadecane	14.32	2.7	ng	80273	5	13.83	591814	20.0
2-methyloctacosane	14.60	4.8	ng	119764	6	15.23	499668	20.0
Benzo[e]pyrene	15.12	2.5	ng	63402	6	15.23	499668	20.0
Hexadecane, 2,6,1...	16.66	2.5	ng	63098	6	15.23	499668	20.0