

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
 Data File : BF103214.D
 Acq On : 26 Feb 2018 13:14
 Operator : SJ/JU
 Sample : J1652-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-4651

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-BF022218.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	2.151	5	11	20	rVB	1017673	1346272	35.89%	3.504%
2	5.104	509	513	524	rVB	215948	298195	7.95%	0.776%
3	5.492	575	579	595	rBV	3420638	3750994	100.00%	9.762%
4	6.504	746	751	754	rBV	3369912	3523816	93.94%	9.170%
5	6.639	770	774	778	rBV	3629323	3631800	96.82%	9.451%
6	6.869	809	813	818	rBV	1276931	1063886	28.36%	2.769%
7	7.028	835	840	843	rBV	3055881	2839833	75.71%	7.390%
8	7.433	904	909	912	rBV	2416481	2419138	64.49%	6.296%
9	8.151	1027	1031	1052	rVB	1556745	1458233	38.88%	3.795%
10	9.227	1209	1214	1217	rBV	3733881	3567950	95.12%	9.285%
11	9.298	1223	1226	1229	rVB	64224	53308	1.42%	0.139%
12	9.616	1275	1280	1288	rBV	268716	280254	7.47%	0.729%
13	9.827	1312	1316	1319	rBV	174035	134926	3.60%	0.351%
14	9.910	1326	1330	1333	rBV	1424857	1382297	36.85%	3.597%
15	9.939	1333	1335	1338	rVB	72708	59867	1.60%	0.156%
16	10.116	1362	1365	1368	rBV	46015	39161	1.04%	0.102%
17	10.327	1398	1401	1404	rVB	204195	151191	4.03%	0.393%
18	10.457	1420	1423	1426	rVB	71919	58836	1.57%	0.153%
19	10.545	1432	1438	1440	rBV2	54164	65647	1.75%	0.171%
20	10.698	1460	1464	1478	rBV	1864475	1924724	51.31%	5.009%
21	10.798	1478	1481	1489	rVB	123504	144955	3.86%	0.377%
22	11.245	1553	1557	1560	rBV2	52819	54801	1.46%	0.143%
23	11.398	1579	1583	1585	rBV	1298334	1146316	30.56%	2.983%
24	11.421	1585	1587	1591	rVV	369861	305875	8.15%	0.796%
25	11.474	1592	1596	1600	rVB	71394	72310	1.93%	0.188%
26	11.910	1665	1670	1671	rBV2	36166	44167	1.18%	0.115%
27	12.016	1684	1688	1690	rBV2	145245	147701	3.94%	0.384%
28	12.192	1716	1718	1721	rBV	54028	46878	1.25%	0.122%
29	12.616	1786	1790	1793	rBV	828761	788137	21.01%	2.051%
30	12.792	1817	1820	1823	rVB	497577	411557	10.97%	1.071%
31	12.845	1823	1829	1831	rVV	573891	671700	17.91%	1.748%
32	12.863	1831	1832	1835	rVB	125334	98380	2.62%	0.256%
33	12.980	1846	1852	1856	rBV	2452051	2406117	64.15%	6.262%
34	13.057	1861	1865	1870	rBV4	34827	60890	1.62%	0.158%

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ClientSampleId :
RT-4651

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.168	1877	1884	1887	rBV	101767	146311	3.90%	0.381%
36	13.239	1892	1896	1898	rVV	77660	72942	1.94%	0.190%
37	13.498	1936	1940	1943	rVB	317201	290737	7.75%	0.757%
38	13.539	1944	1947	1949	rVV2	62170	53550	1.43%	0.139%
39	13.563	1949	1951	1955	rVB2	46921	37538	1.00%	0.098%
40	13.868	2000	2003	2009	rVB2	242587	275881	7.35%	0.718%
41	14.004	2023	2026	2029	rBV	231237	222157	5.92%	0.578%
42	14.045	2029	2033	2036	rVV2	948910	1083577	28.89%	2.820%
43	14.068	2036	2037	2042	rVB	140084	92407	2.46%	0.240%
44	14.186	2054	2057	2061	rBV	79287	80815	2.15%	0.210%
45	14.498	2107	2110	2115	rBV3	82889	114304	3.05%	0.297%
46	14.809	2160	2163	2166	rBV	83777	84962	2.27%	0.221%
47	15.104	2209	2213	2218	rBV	81675	154556	4.12%	0.402%
48	15.151	2218	2221	2224	rVB	70756	79316	2.11%	0.206%
49	15.474	2273	2276	2282	rBV	56836	76825	2.05%	0.200%
50	15.539	2282	2287	2297	rBV2	717575	1032375	27.52%	2.687%
51	15.974	2358	2361	2365	rVB	52840	77350	2.06%	0.201%

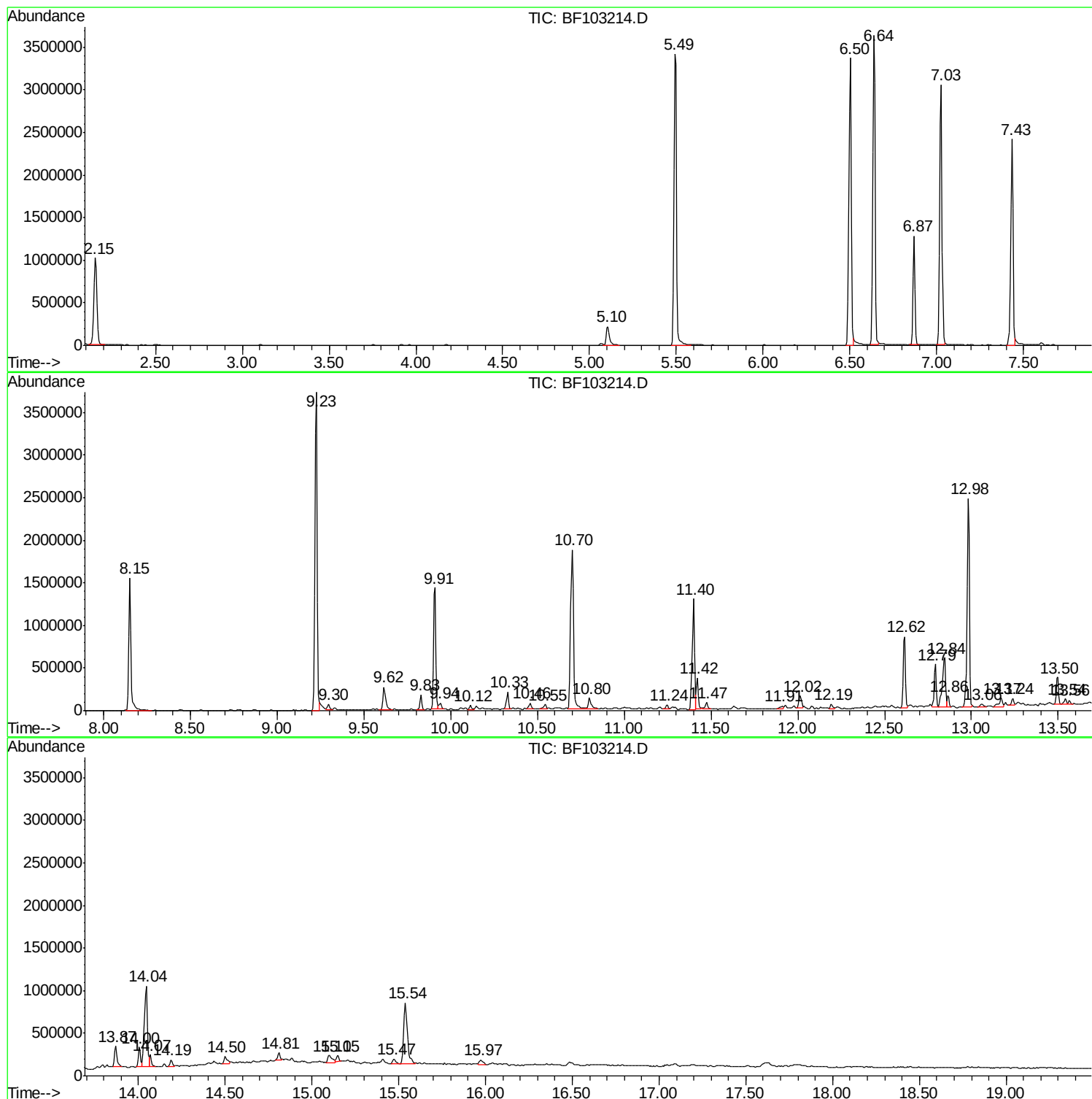
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Instrument :
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ClientSampled :
RT-4651

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.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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Misc :
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Instrument :
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ClientSampleId :
RT-4651

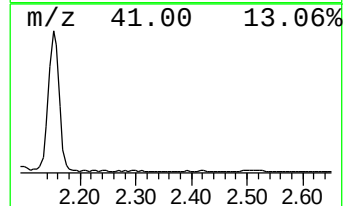
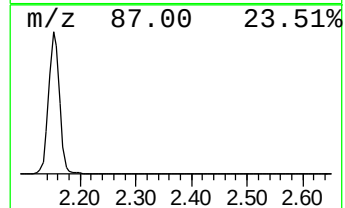
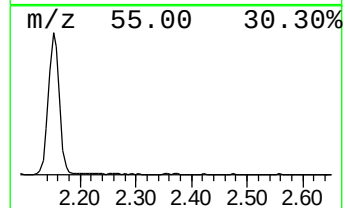
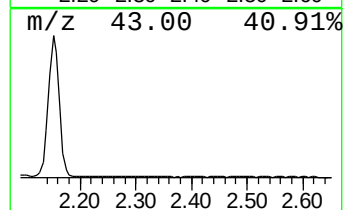
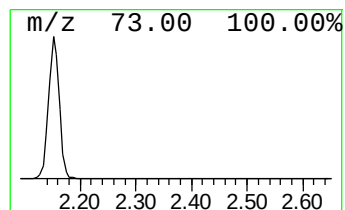
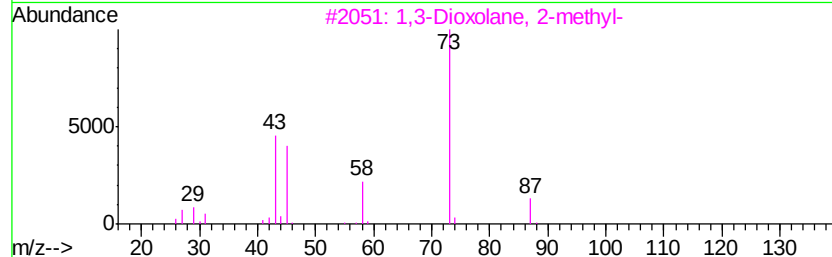
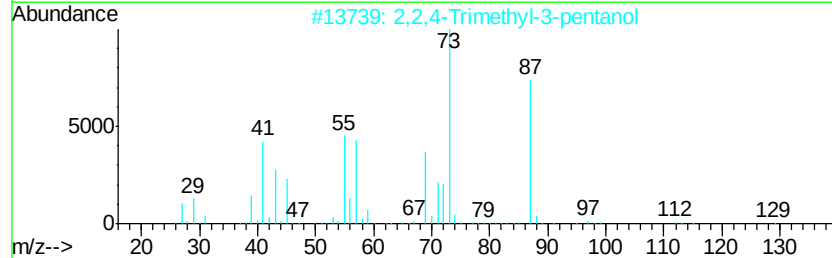
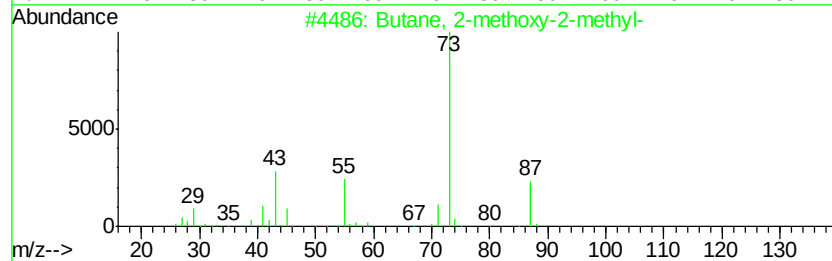
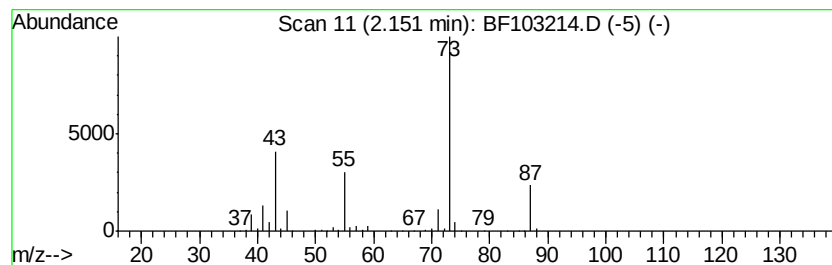
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	25.31 ng	1346270	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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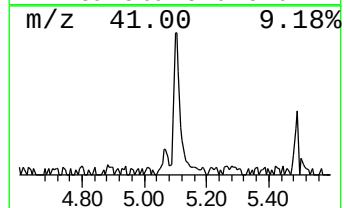
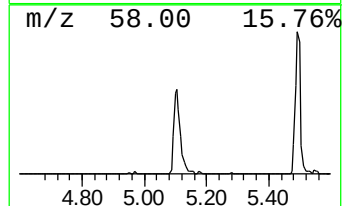
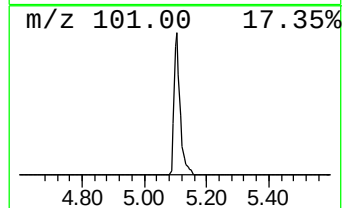
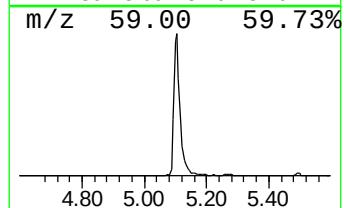
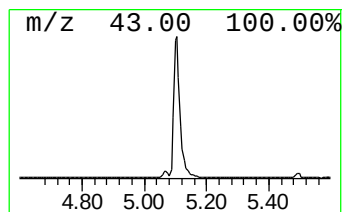
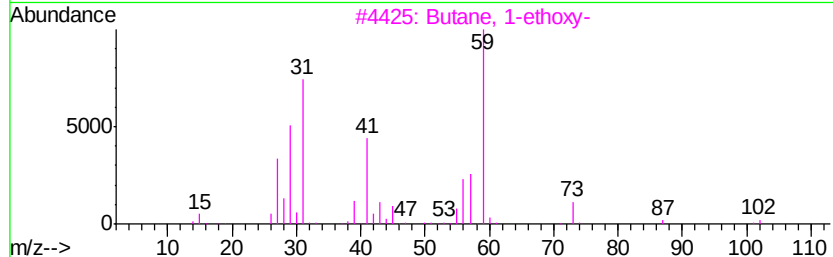
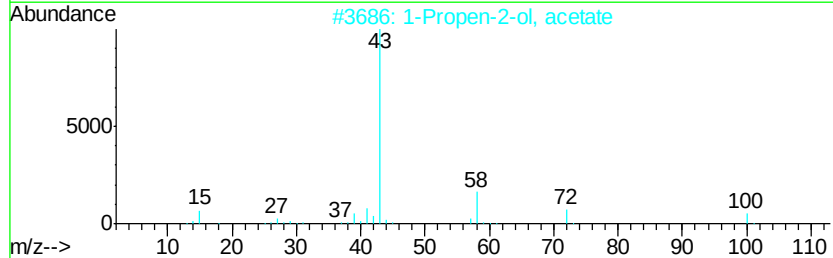
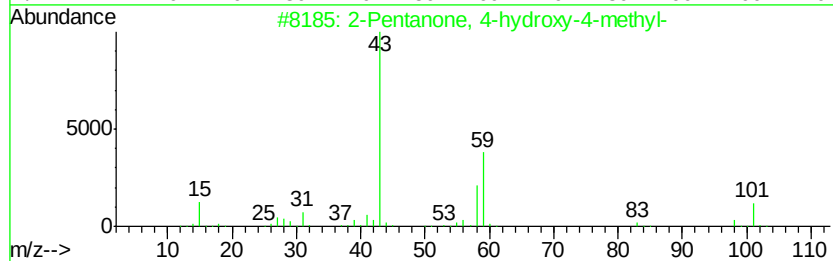
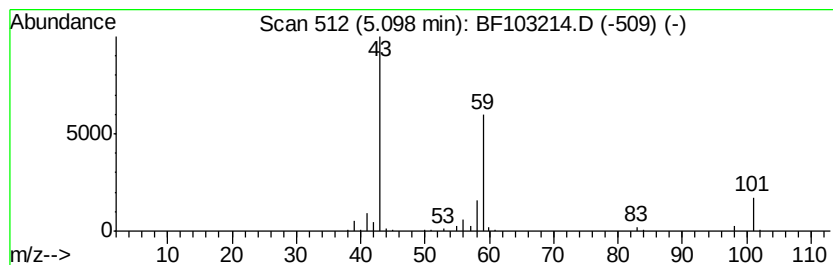
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.61 ng	298195	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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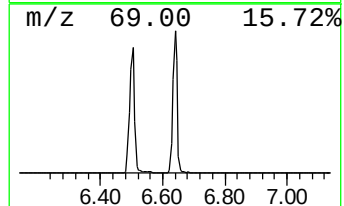
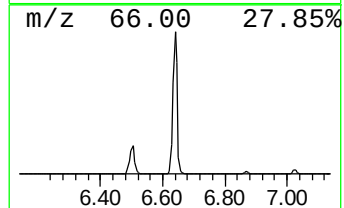
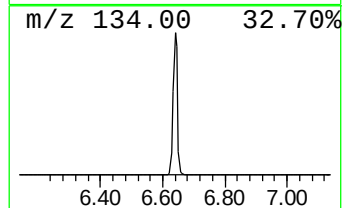
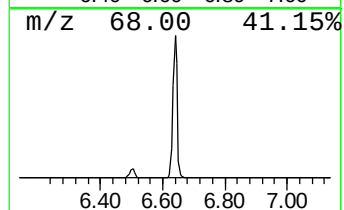
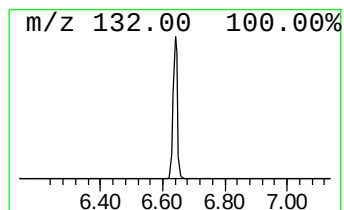
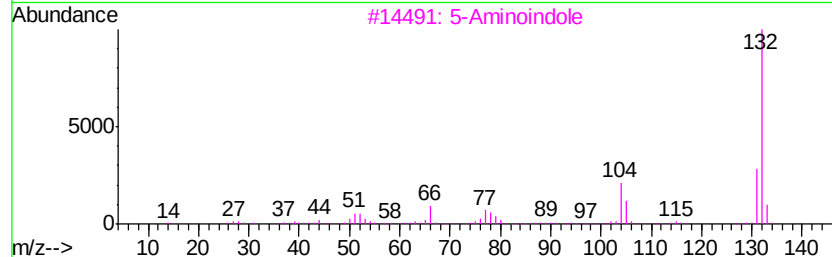
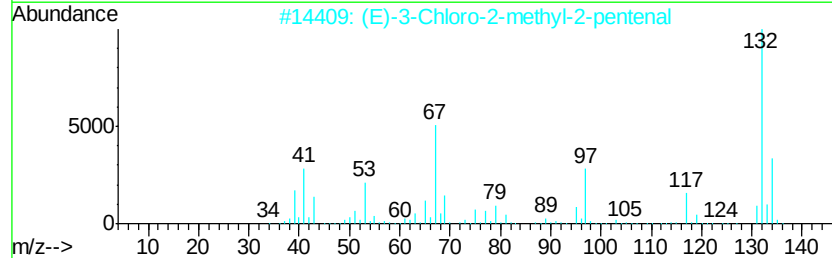
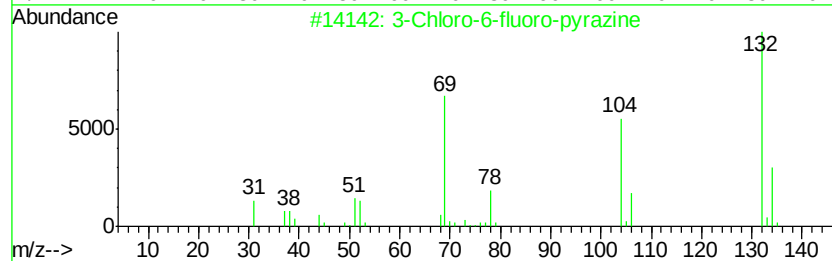
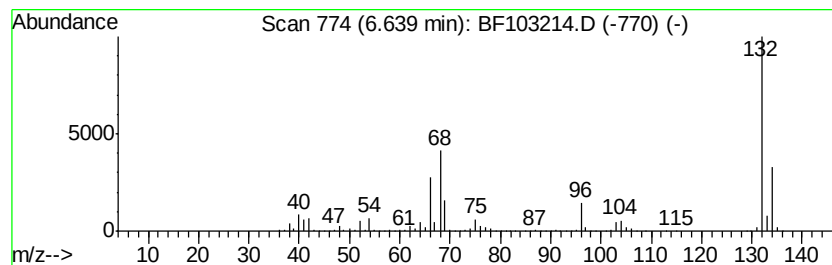
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	68.27 ng	3631800	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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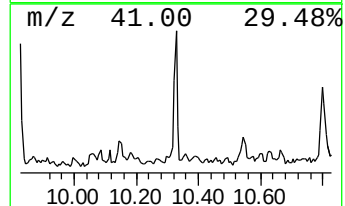
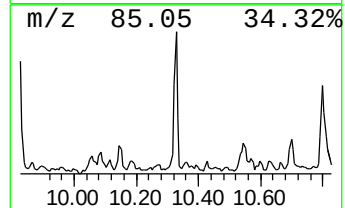
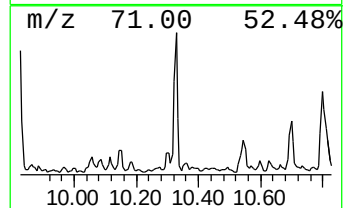
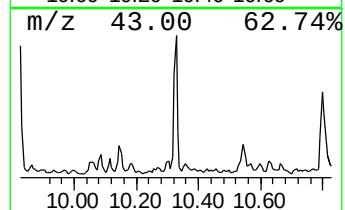
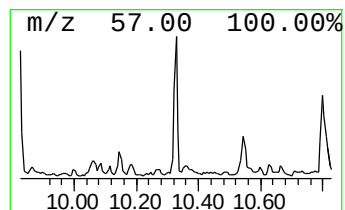
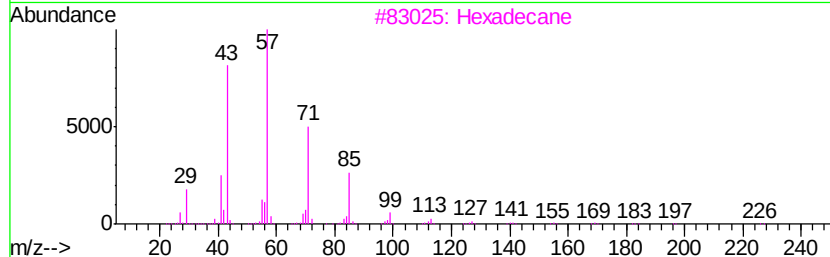
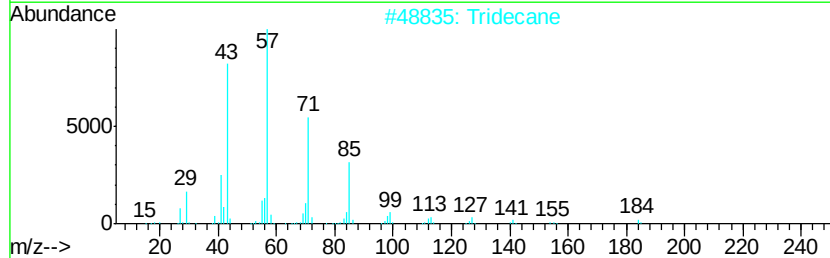
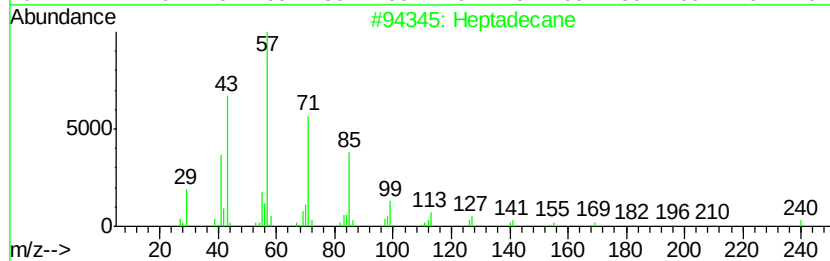
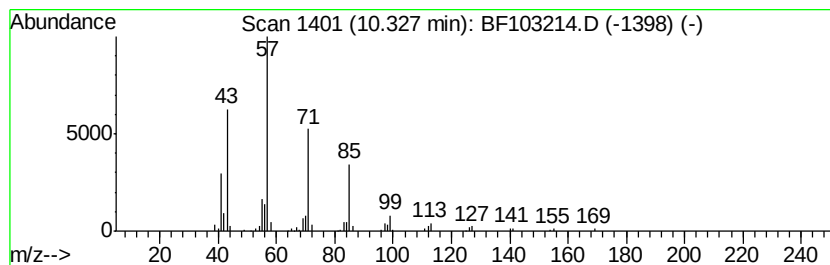
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.19 ng	151191	Acenaphthene-d10	9.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	Tridecane	184 C13H28	000629-50-5	86
3	Hexadecane	226 C16H34	000544-76-3	86
4	2-Bromo dodecane	248 C12H25Br	013187-99-0	83
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	80



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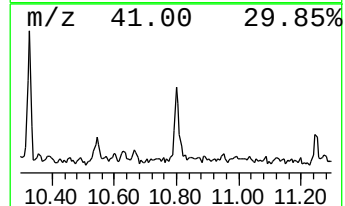
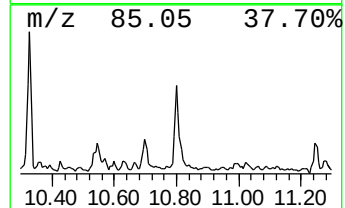
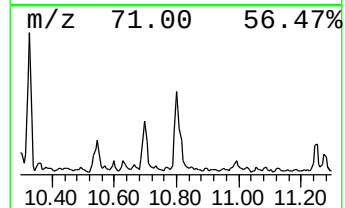
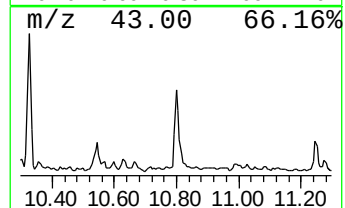
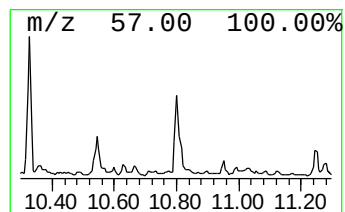
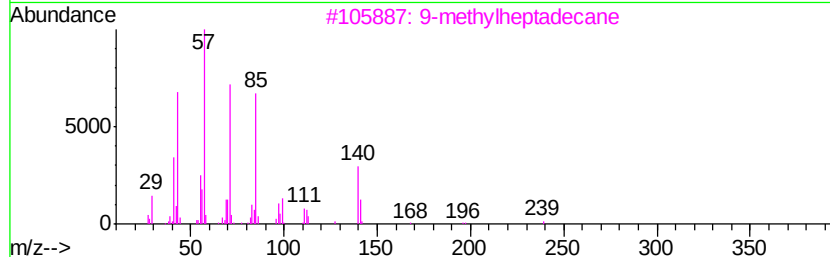
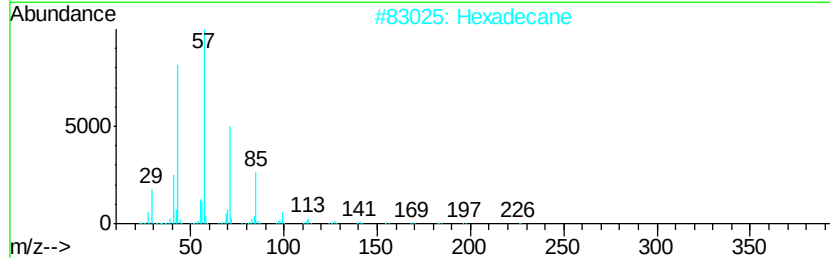
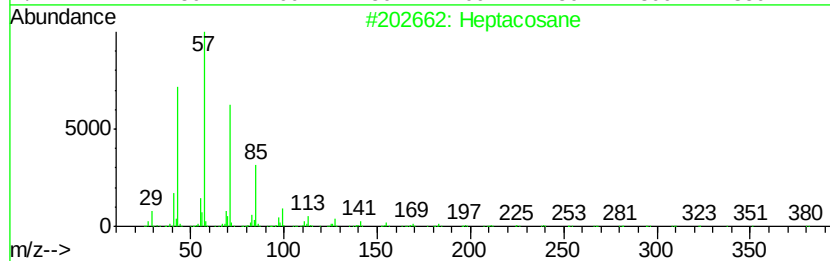
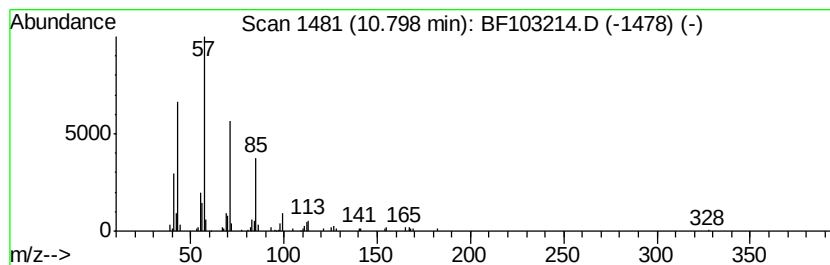
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.53 ng	144955	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	9-methylheptadecane		254	C18H38	026741-18-4	86
4	Pentadecane		212	C15H32	000629-62-9	80
5	Heneicosane		296	C21H44	000629-94-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103214.D
Acq On : 26 Feb 2018 13:14
Operator : SJ/JU
Sample : J1652-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4651

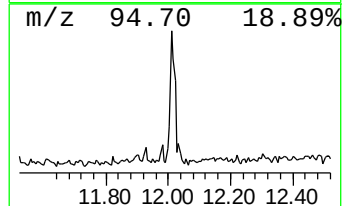
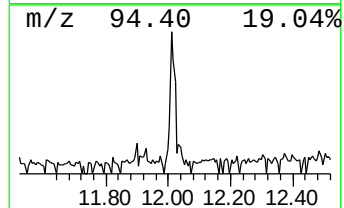
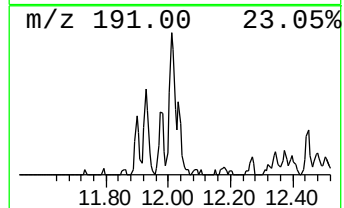
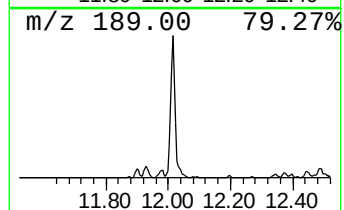
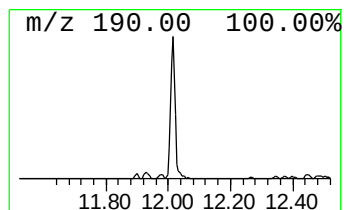
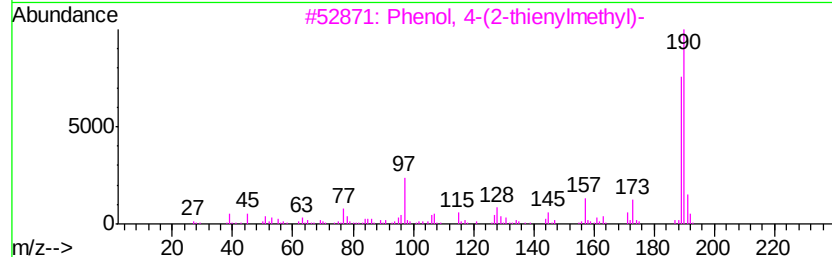
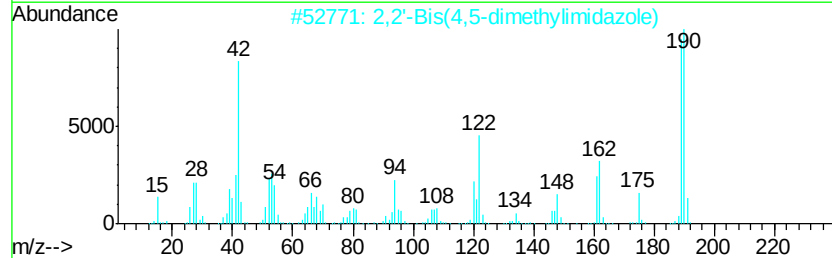
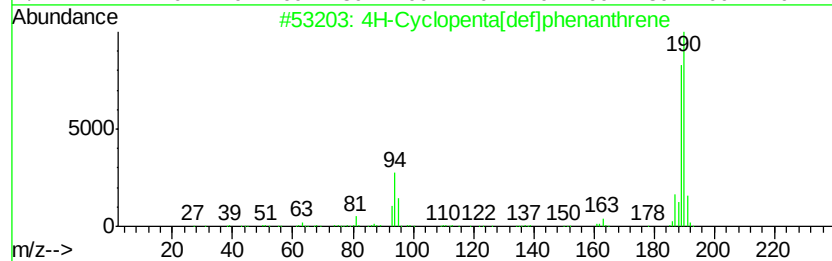
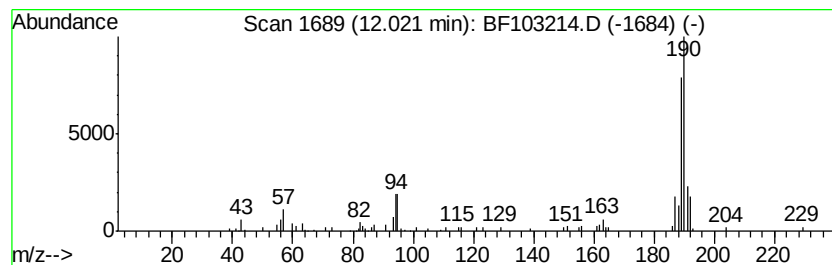
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.58 ng	147701	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
3		Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	50
4		2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	30
5		4-(4-Chlorophenyl)pyridine	189	C11H8ClN	005957-96-0	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
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Misc :
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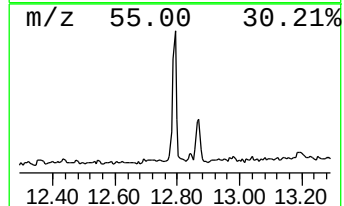
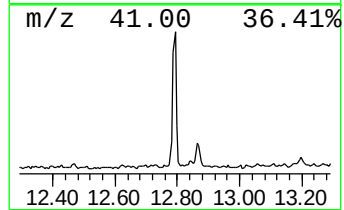
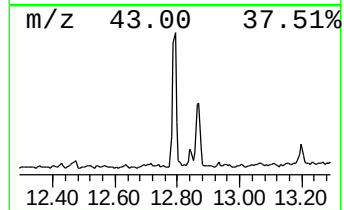
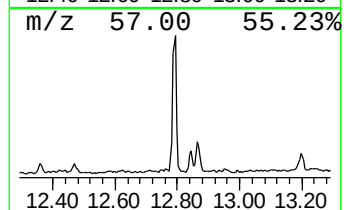
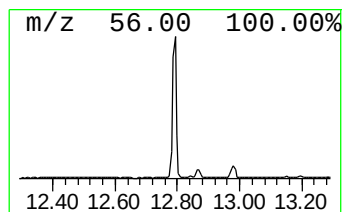
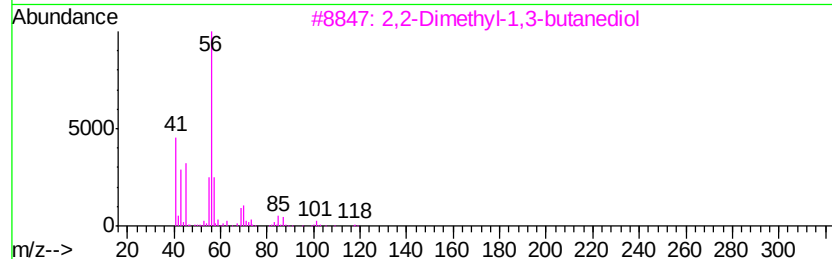
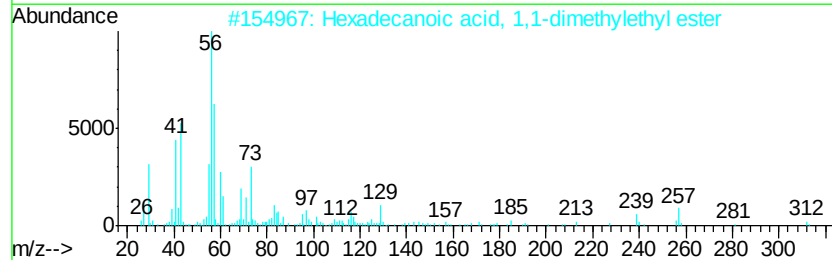
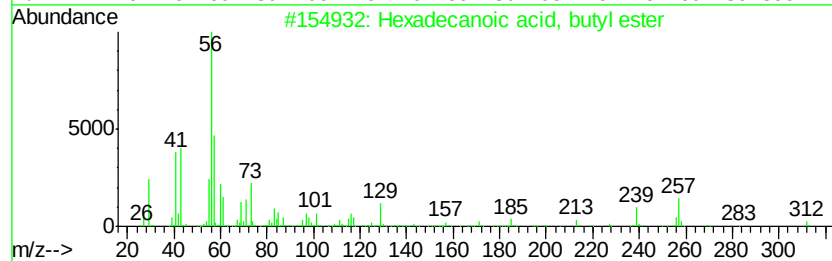
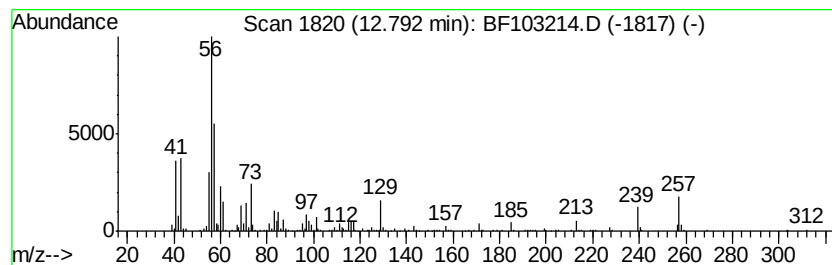
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	7.60 ng	411557	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	43
4		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	37
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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Sample : J1652-01
Misc :
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ClientSampleId :
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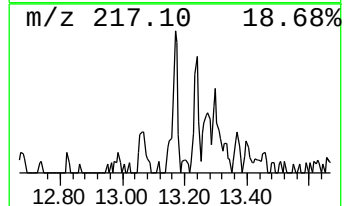
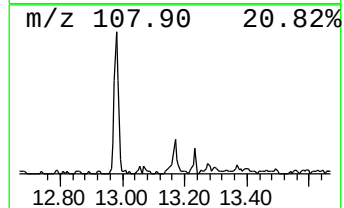
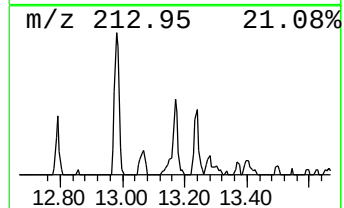
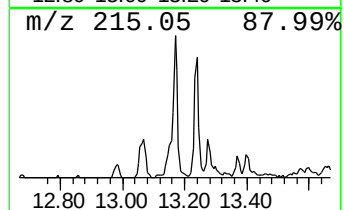
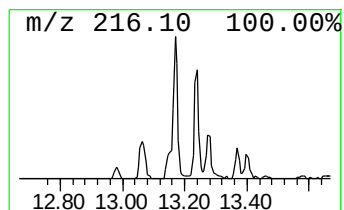
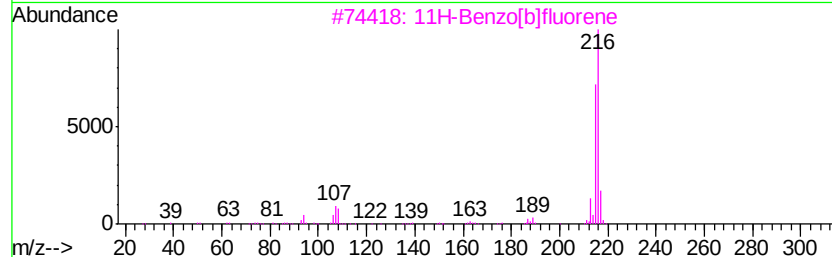
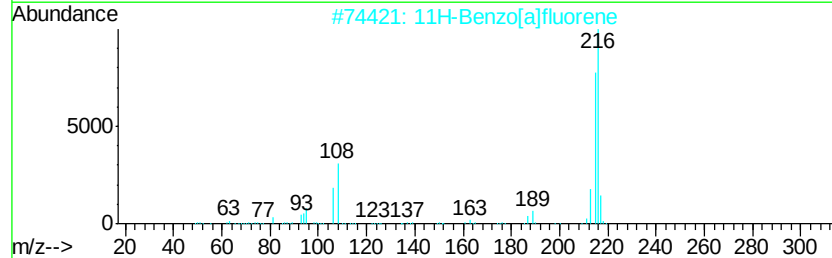
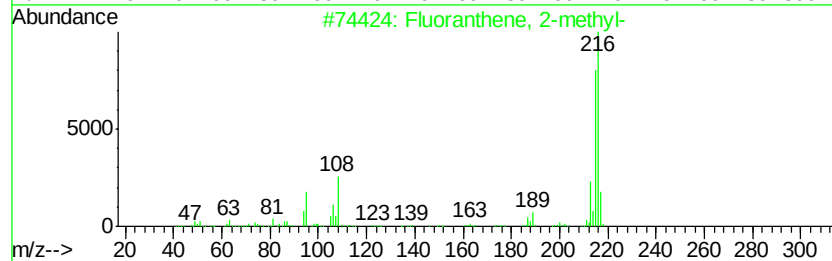
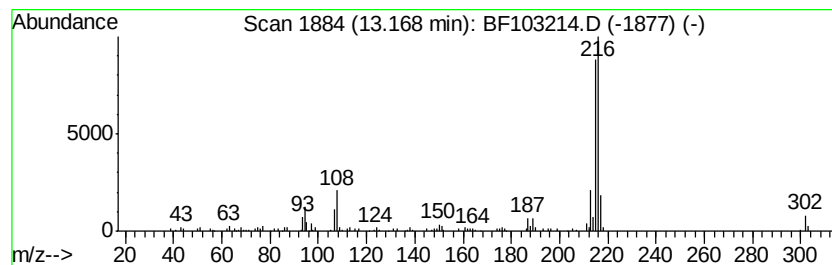
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Fluoranthene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	2.70 ng	146311	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
4		Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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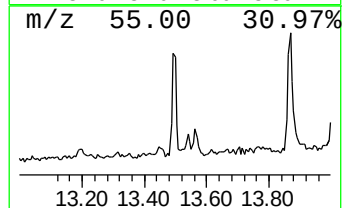
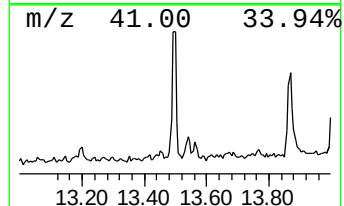
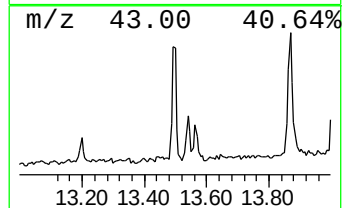
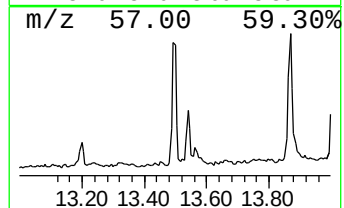
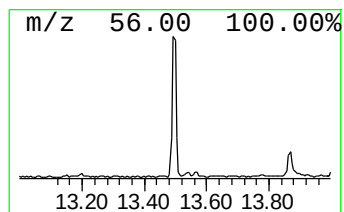
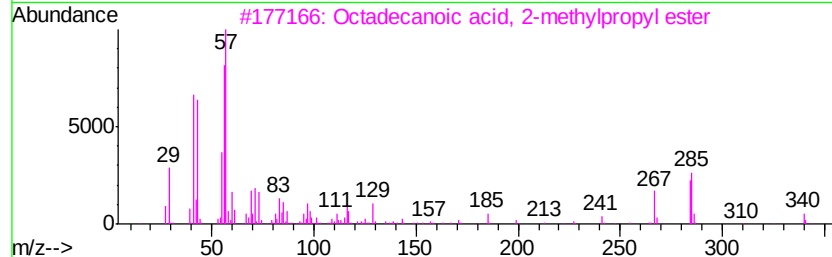
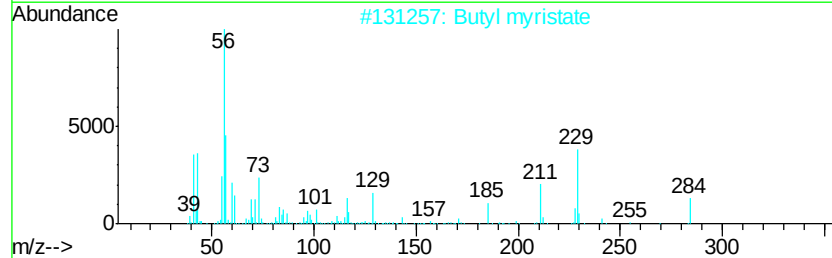
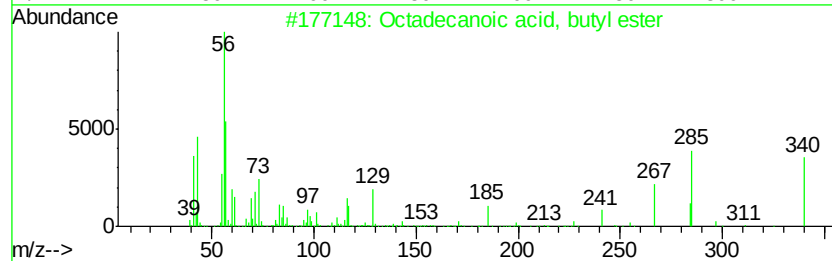
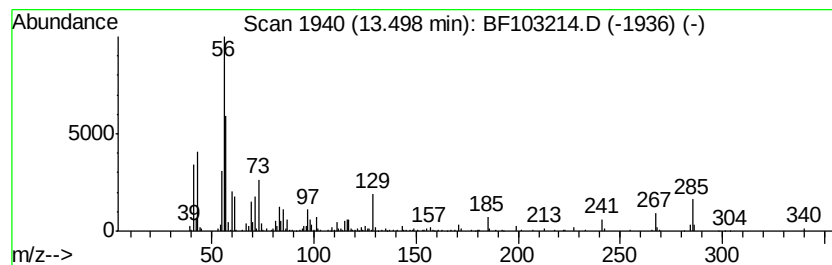
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.37 ng	290737	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	59
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	43
4		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
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Acq On : 26 Feb 2018 13:14
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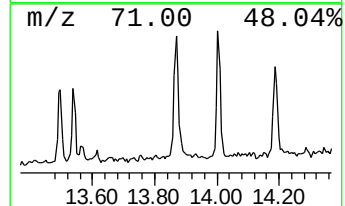
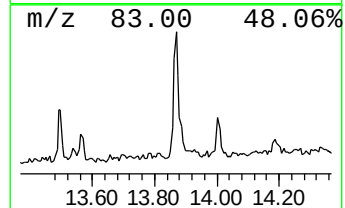
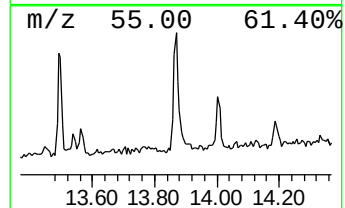
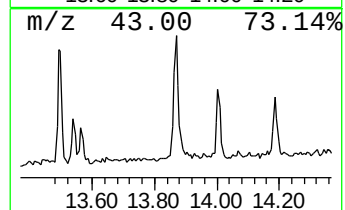
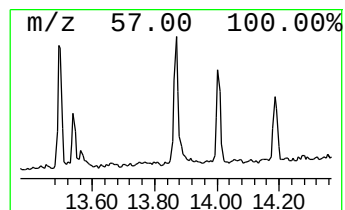
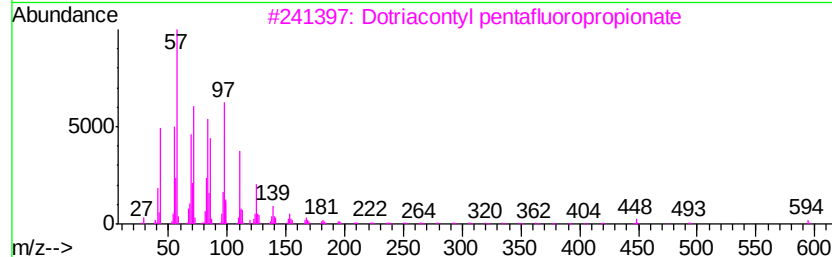
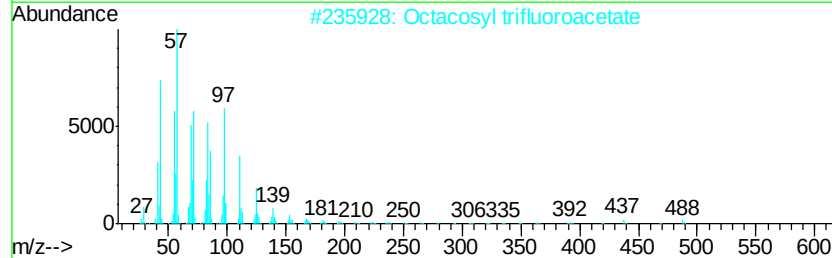
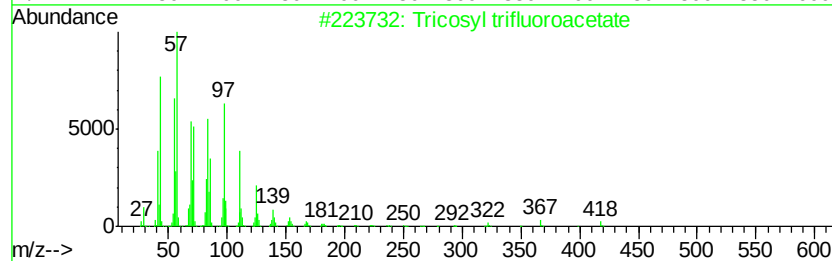
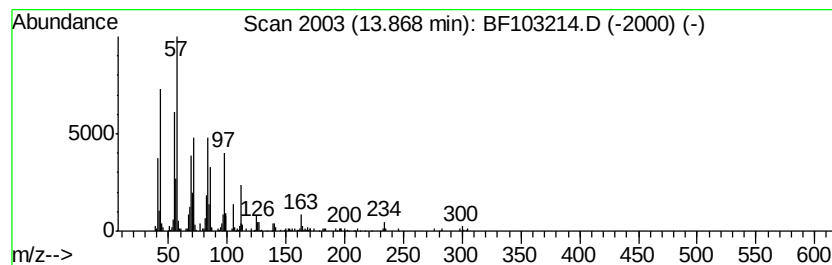
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tricosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.87	5.09 ng	275881	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
4	Tetracosyl heptafluorobutyrte	550	C28H49F7O2	1000351-83-7	91
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
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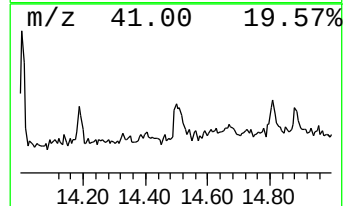
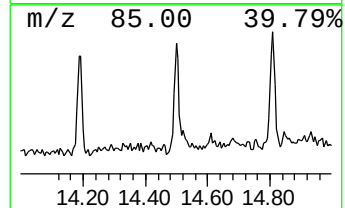
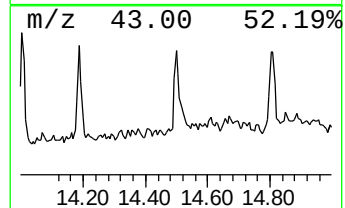
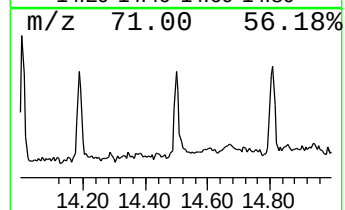
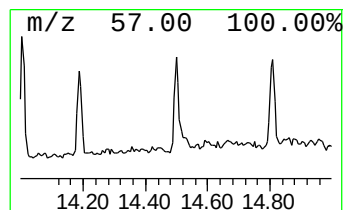
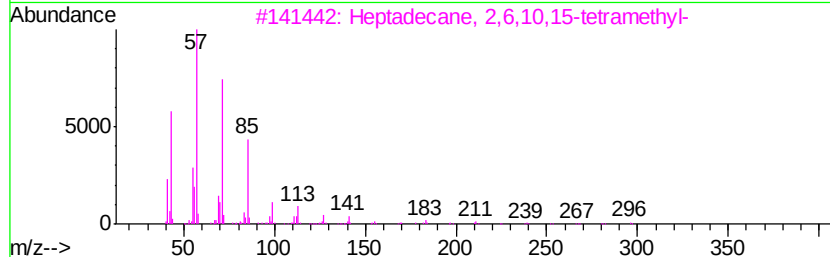
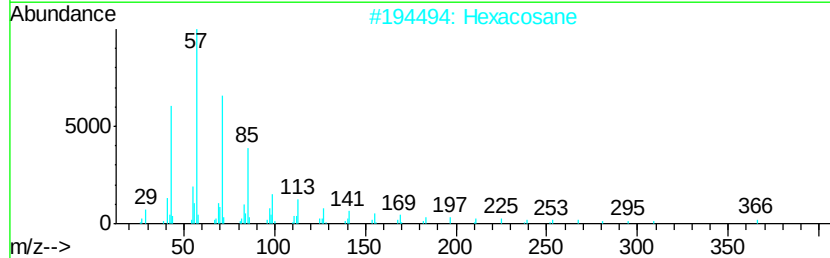
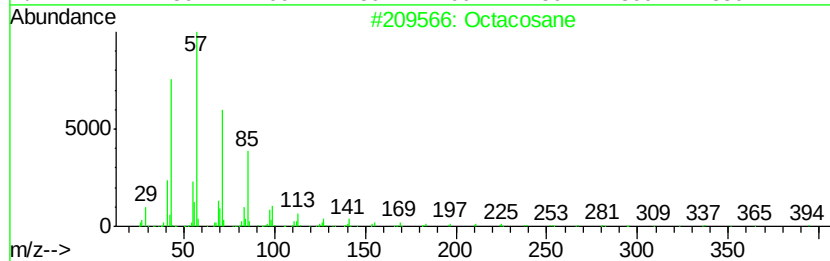
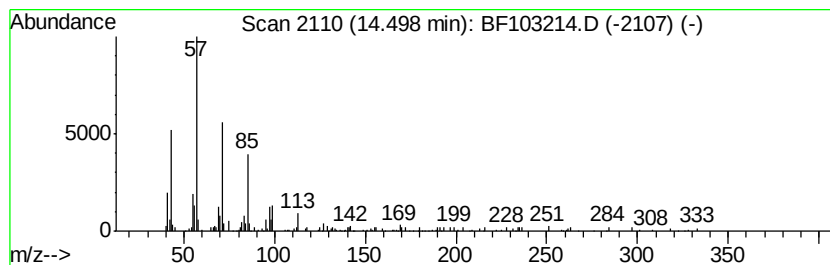
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.11 ng	114304	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	90
2	Hexacosane	366 C26H54	000630-01-3	86
3	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	80
4	Heptacosane	380 C27H56	000593-49-7	80
5	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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Sample : J1652-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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2-Pentanone, 4-hy...	5.10	5.6	ng	298195	1	6.87	1063890	20.0
unknown6.64	6.64	68.3	ng	3631800	1	6.87	1063890	20.0
Heptadecane	10.33	2.2	ng	151191	3	9.91	1382300	20.0
Heptacosane	10.80	2.5	ng	144955	4	11.40	1146320	20.0
4H-Cyclopenta[def...	12.02	2.6	ng	147701	4	11.40	1146320	20.0
Hexadecanoic acid...	12.79	7.6	ng	411557	5	14.04	1083580	20.0
Fluoranthene, 2-m...	13.17	2.7	ng	146311	5	14.04	1083580	20.0
Octadecanoic acid...	13.50	5.4	ng	290737	5	14.04	1083580	20.0
Tricosyl trifluor...	13.87	5.1	ng	275881	5	14.04	1083580	20.0
Octacosane	14.50	2.1	ng	114304	5	14.04	1083580	20.0