

Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
 Data File : BF103378.D
 Acq On : 2 Mar 2018 21:03
 Operator : SJ/JU
 Sample : J1721-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-35

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	2.134	3	8	16	rVB	215403	283621	8.08%	0.824%
2	2.475	46	66	72	rBV2	60082	165449	4.72%	0.481%
3	5.110	511	514	525	rVB	116427	152848	4.36%	0.444%
4	5.504	577	581	600	rVB	3215099	3452841	98.40%	10.029%
5	6.516	748	753	771	rBV	3098300	3508969	100.00%	10.192%
6	6.651	771	776	779	rVV	3418956	3284672	93.61%	9.541%
7	6.698	781	784	788	rVB2	35980	37165	1.06%	0.108%
8	6.875	810	814	821	rBV	1190472	977914	27.87%	2.840%
9	7.033	837	841	844	rBV	2722276	2478868	70.64%	7.200%
10	7.445	906	911	921	rBV	2143066	2232635	63.63%	6.485%
11	8.157	1029	1032	1044	rBV	1306112	1381392	39.37%	4.012%
12	8.786	1135	1139	1145	rBV3	21508	39867	1.14%	0.116%
13	8.875	1151	1154	1158	rBV	41330	45242	1.29%	0.131%
14	9.233	1211	1215	1224	rBV	3384682	3193837	91.02%	9.277%
15	9.298	1224	1226	1230	rVV	78001	83521	2.38%	0.243%
16	9.333	1230	1232	1237	rVB2	35729	38928	1.11%	0.113%
17	9.627	1275	1282	1288	rBV	245587	299740	8.54%	0.871%
18	9.780	1304	1308	1313	rBV	47450	63927	1.82%	0.186%
19	9.833	1313	1317	1320	rVB	138991	131132	3.74%	0.381%
20	9.916	1327	1331	1335	rBV2	1340365	1232349	35.12%	3.579%
21	10.010	1343	1347	1352	rVB4	32594	43920	1.25%	0.128%
22	10.121	1363	1366	1369	rBV3	45255	50155	1.43%	0.146%
23	10.151	1369	1371	1375	rVB3	42974	42939	1.22%	0.125%
24	10.327	1399	1401	1405	rVB	174792	153305	4.37%	0.445%
25	10.469	1422	1425	1431	rVB	36710	49691	1.42%	0.144%
26	10.551	1433	1439	1441	rBV	65393	78730	2.24%	0.229%
27	10.710	1462	1466	1479	rBV	1554267	1723262	49.11%	5.005%
28	10.804	1479	1482	1492	rVB	181930	236809	6.75%	0.688%
29	11.251	1555	1558	1561	rBV2	131023	120102	3.42%	0.349%
30	11.410	1581	1585	1587	rBV	1106535	1010316	28.79%	2.935%
31	11.433	1587	1589	1594	rVV	520349	438131	12.49%	1.273%
32	11.486	1595	1598	1603	rVB	135775	135785	3.87%	0.394%
33	11.616	1617	1620	1623	rBV	52590	56177	1.60%	0.163%
34	11.680	1628	1631	1633	rVB	49563	38949	1.11%	0.113%

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

35	11.921	1667	1672	1674	rBV2	131789	176615	5.03%	0.513%
36	11.939	1674	1675	1681	rVB2	95865	87618	2.50%	0.254%
37	12.027	1686	1690	1692	rBV	105030	112322	3.20%	0.326%
38	12.086	1698	1700	1703	rBV2	42333	38238	1.09%	0.111%
39	12.204	1717	1720	1724	rBV	58383	66067	1.88%	0.192%
40	12.245	1724	1727	1731	rVB	56847	60298	1.72%	0.175%
41	12.433	1757	1759	1761	rBV3	42341	36936	1.05%	0.107%
42	12.557	1777	1780	1783	rBV2	39852	51202	1.46%	0.149%
43	12.627	1788	1792	1796	rBV	839633	758107	21.60%	2.202%
44	12.857	1825	1831	1837	rBV	729454	940167	26.79%	2.731%
45	12.910	1837	1840	1844	rVB2	35183	45409	1.29%	0.132%
46	12.992	1850	1854	1857	rBV	1981992	1854999	52.86%	5.388%
47	13.186	1880	1887	1889	rBV2	121013	201160	5.73%	0.584%
48	13.251	1896	1898	1901	rBV	59014	49254	1.40%	0.143%
49	13.415	1924	1926	1930	rBV2	73086	97794	2.79%	0.284%
50	13.874	2001	2004	2008	rBV4	188957	202839	5.78%	0.589%
51	14.062	2031	2036	2039	rBV2	846813	1136299	32.38%	3.300%
52	14.086	2039	2040	2044	rVB	329291	253219	7.22%	0.735%
53	14.892	2175	2177	2181	rVB	233409	231045	6.58%	0.671%
54	15.127	2214	2217	2220	rBV	267334	348438	9.93%	1.012%
55	15.574	2290	2293	2296	rVB	361935	417182	11.89%	1.212%

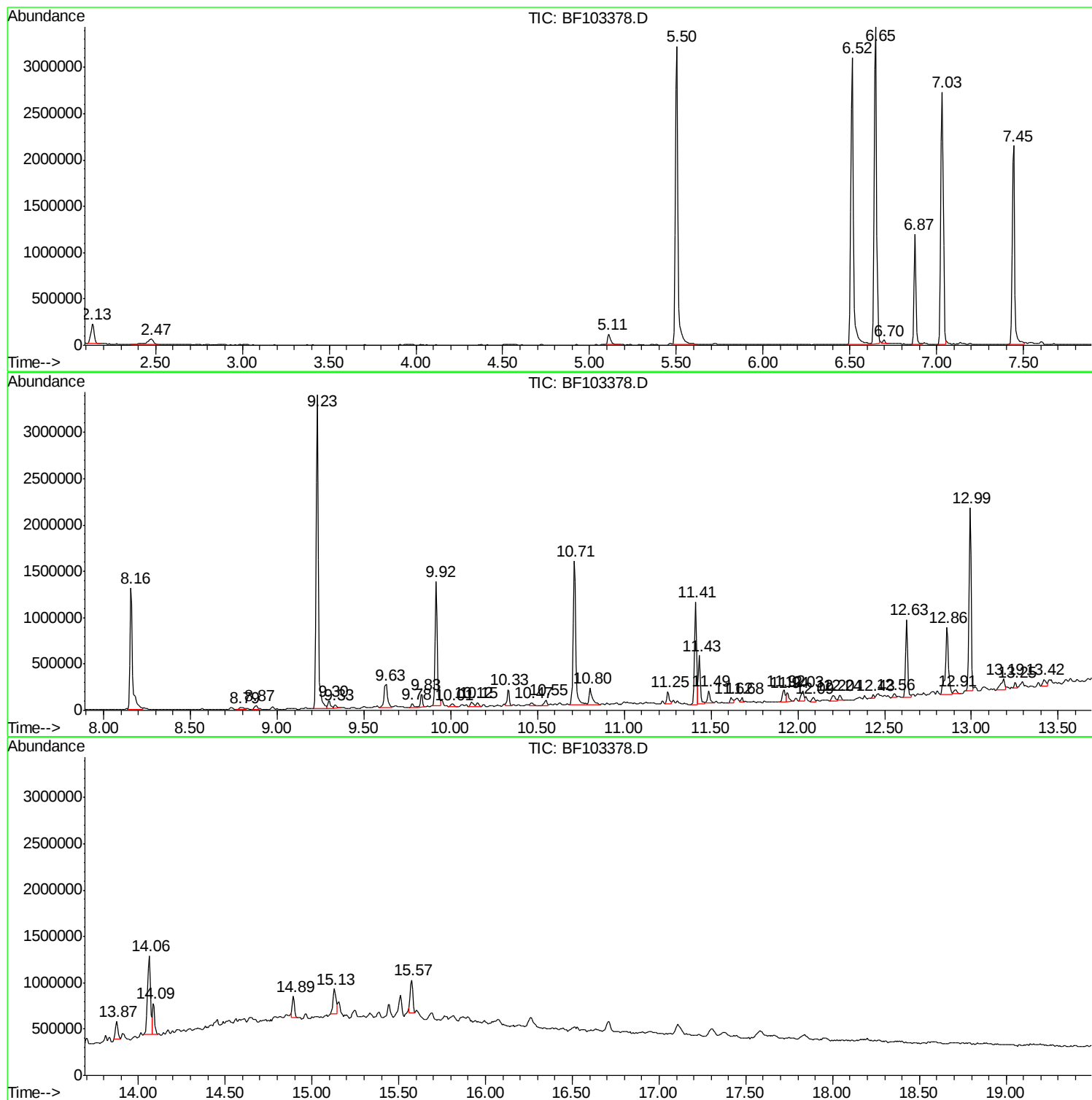
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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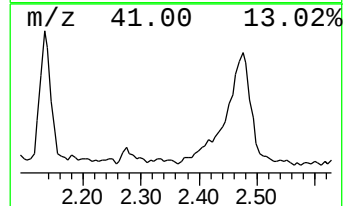
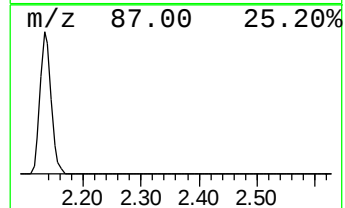
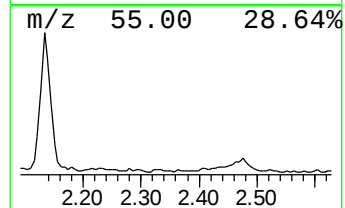
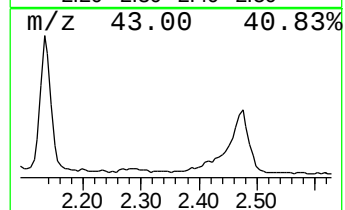
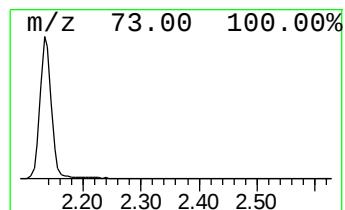
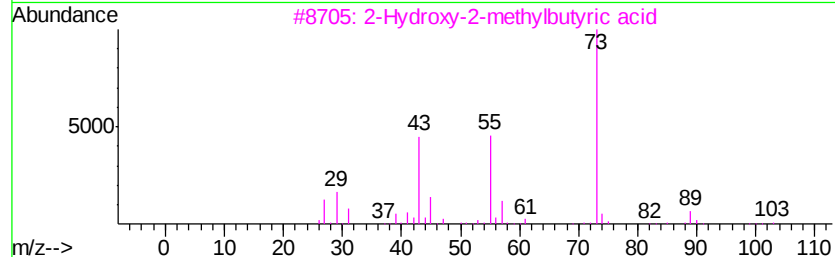
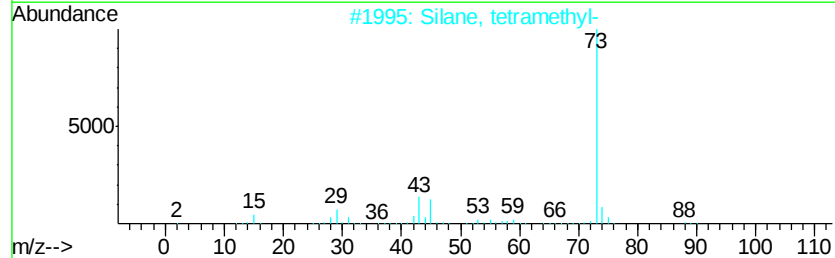
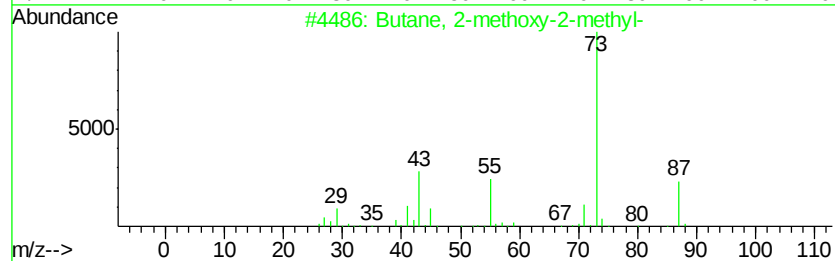
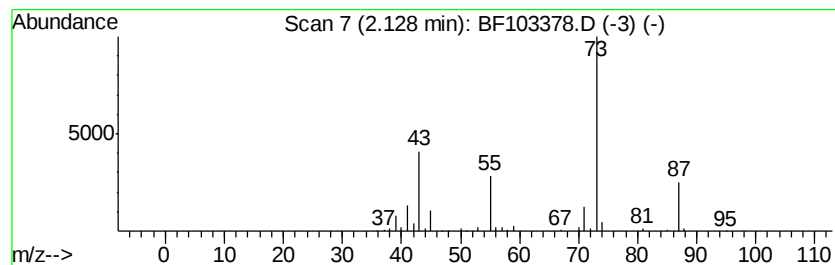
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	5.80 ng	283621	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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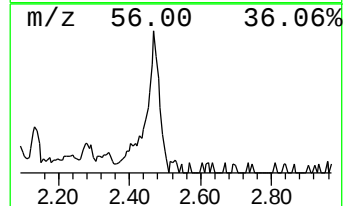
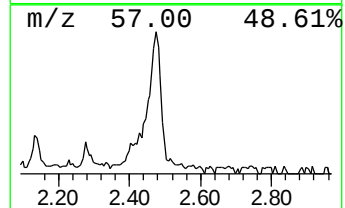
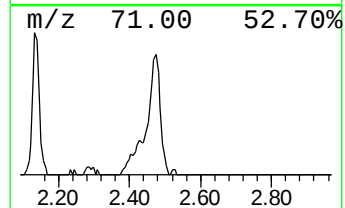
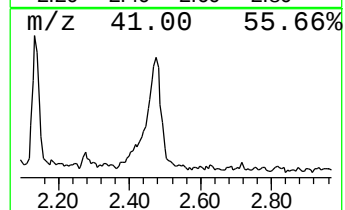
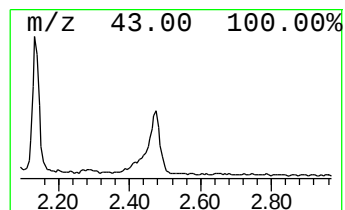
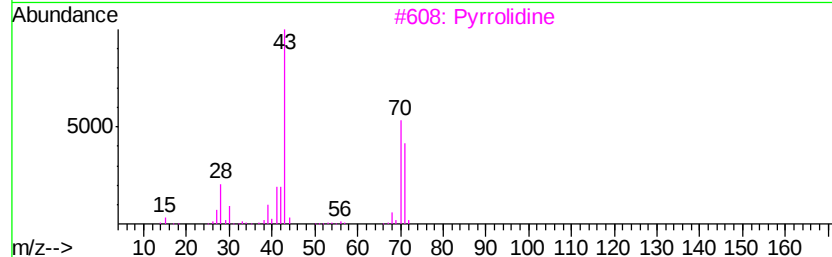
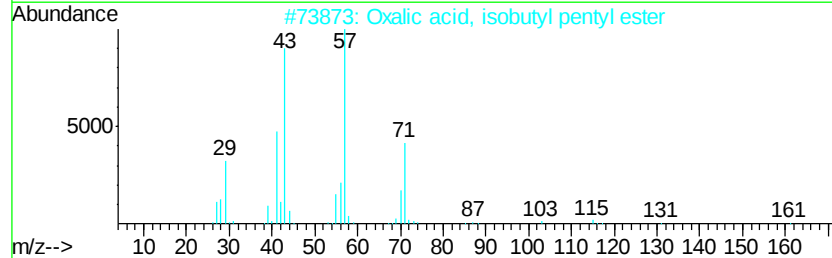
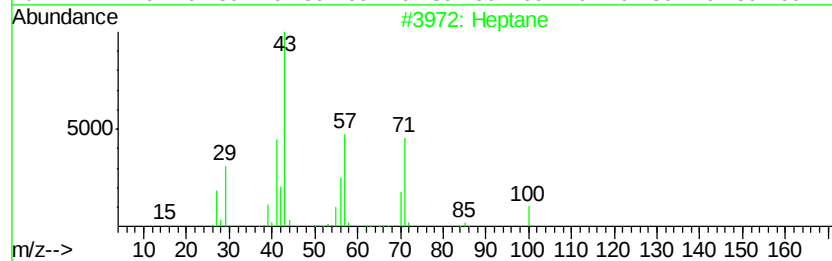
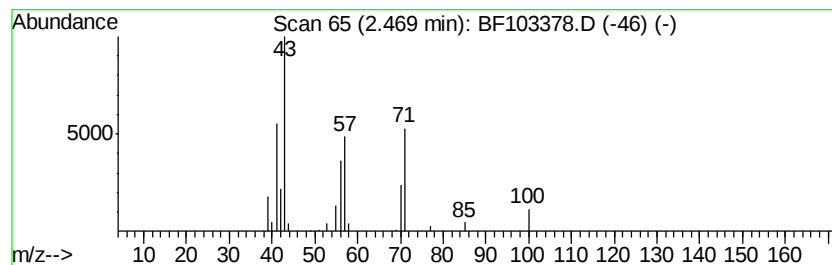
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.47	3.38 ng	165449	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane	100	C7H16	000142-82-5	91
2		Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	53
3		Pyrrolidine	71	C4H9N	000123-75-1	43
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	42
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38



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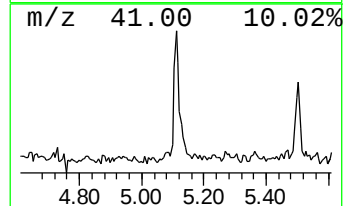
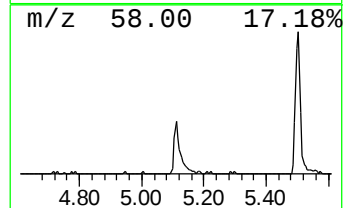
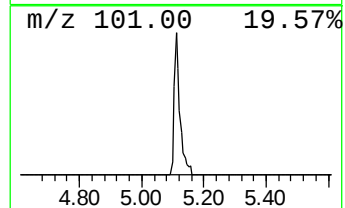
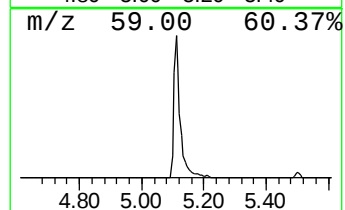
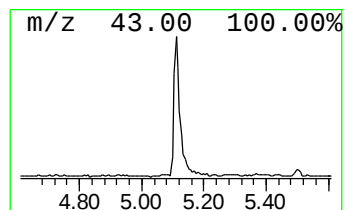
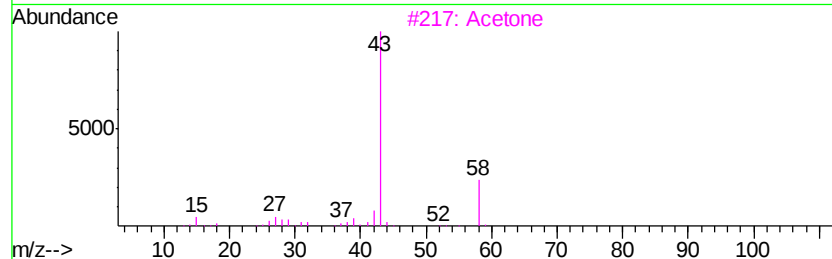
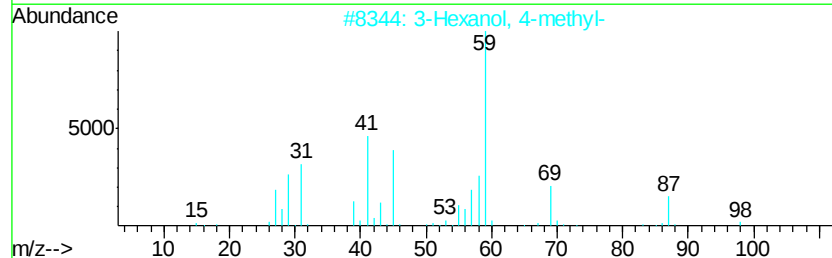
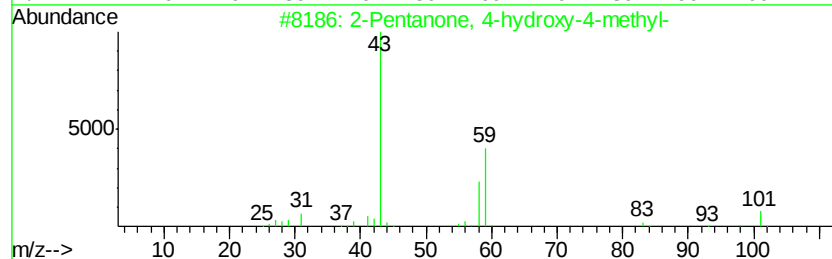
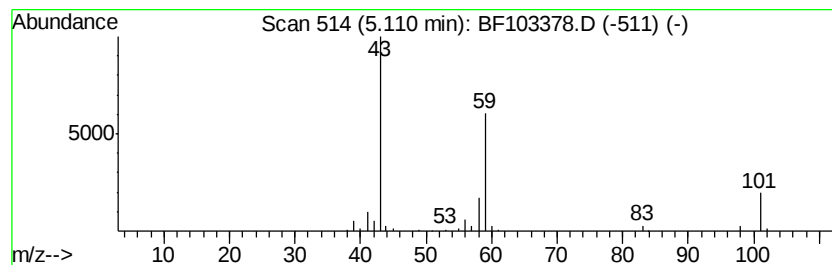
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.13 ng	152848	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	40
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetone	58	C3H6O	000067-64-1	14
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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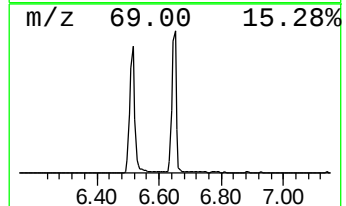
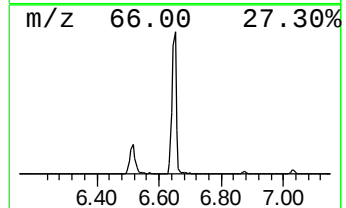
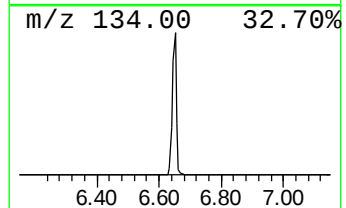
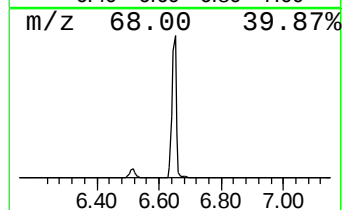
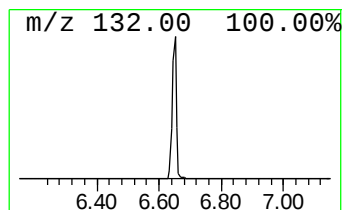
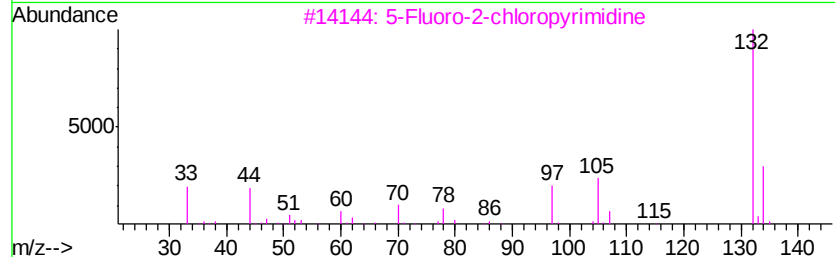
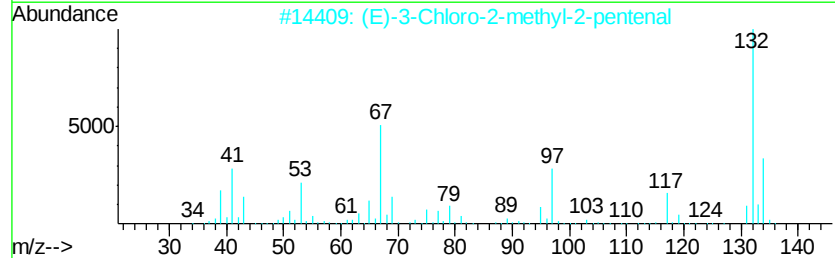
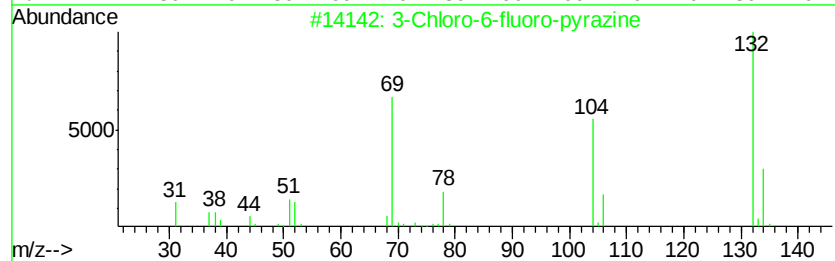
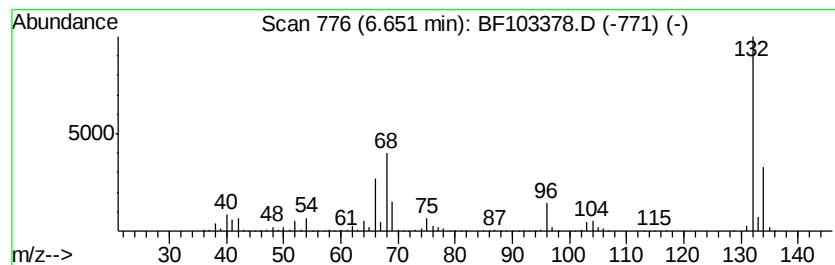
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	67.18 ng	3284670	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	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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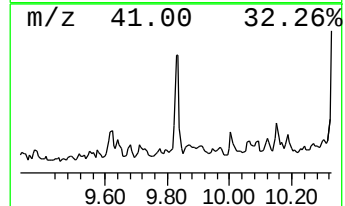
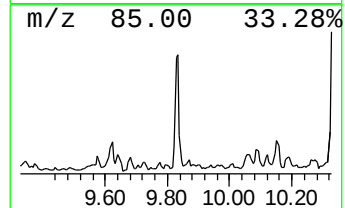
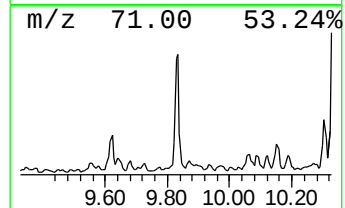
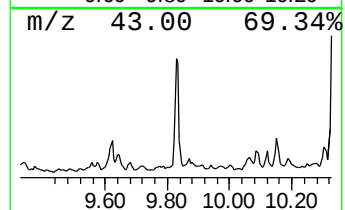
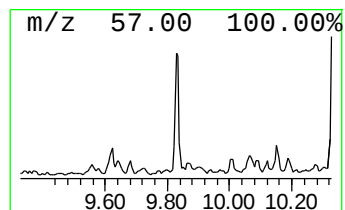
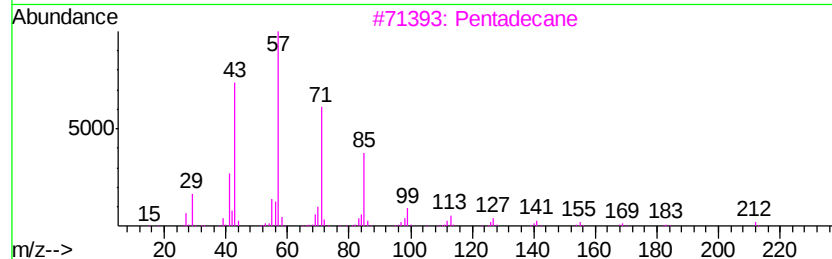
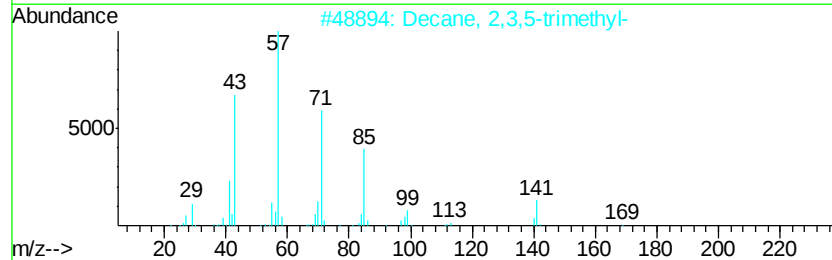
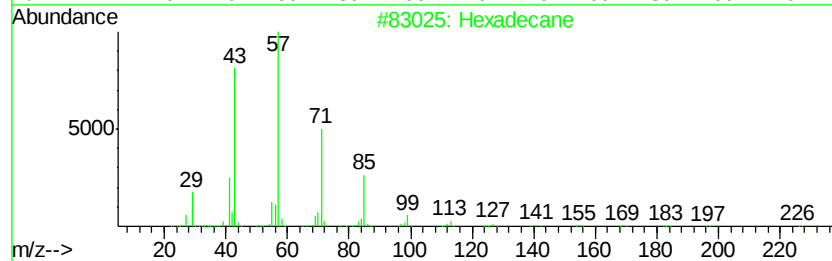
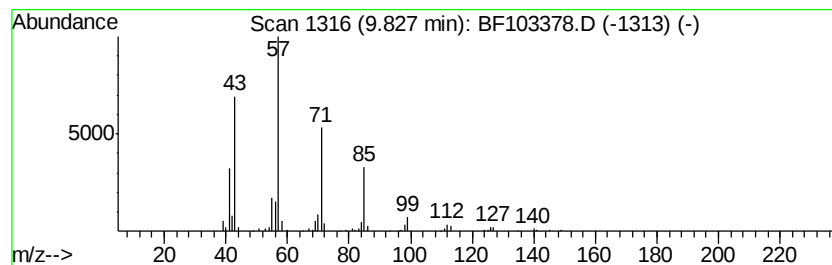
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.13 ng	131132	Acenaphthene-d10	9.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3		Pentadecane	212	C15H32	000629-62-9	72
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5		Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	53



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103378.D
Acq On : 2 Mar 2018 21:03
Operator : SJ/JU
Sample : J1721-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-35

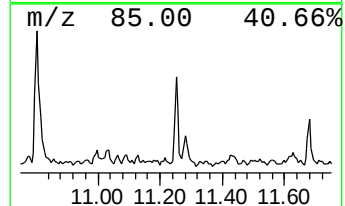
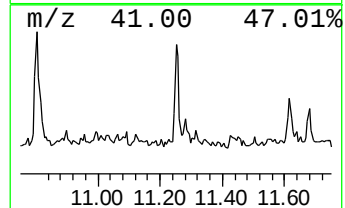
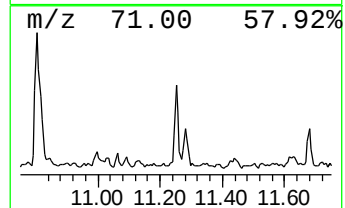
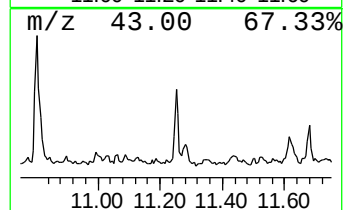
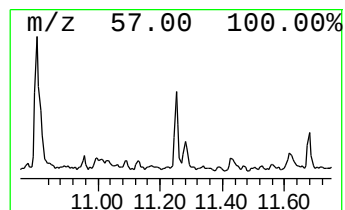
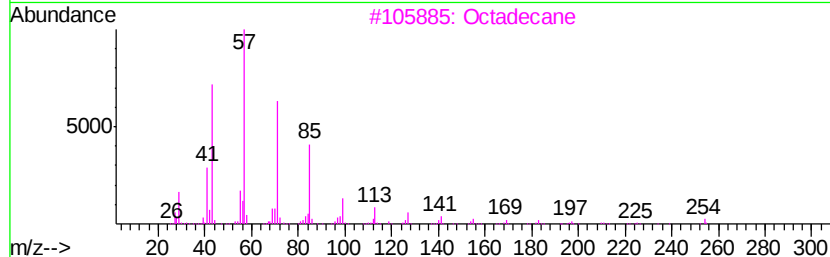
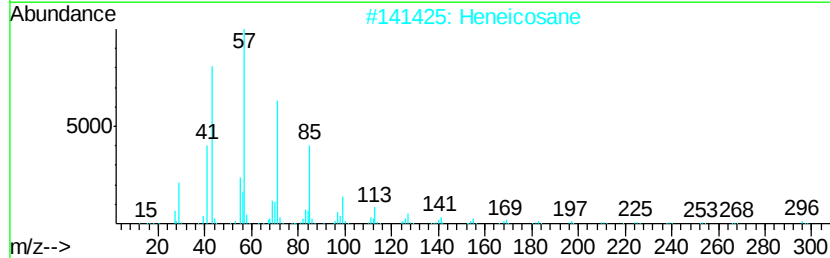
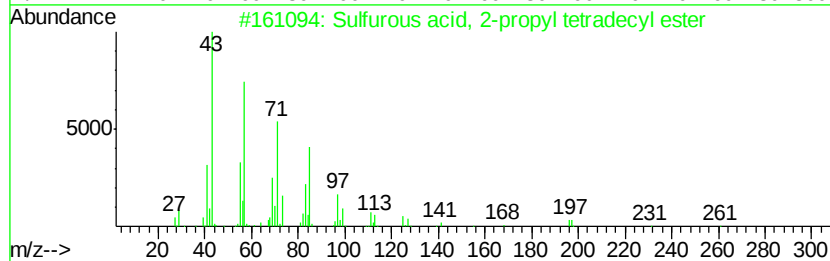
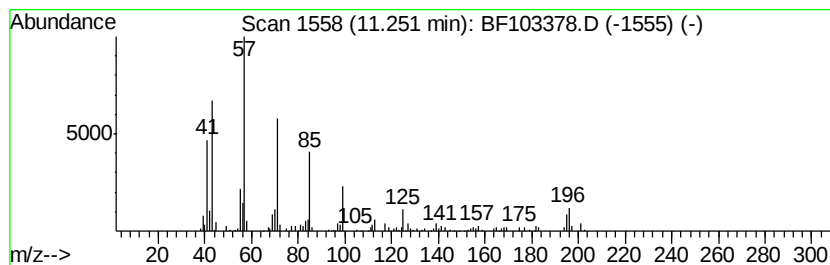
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, 2-propyl te... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.38 ng	120102	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tetradecyl...	320	C17H36O3S	1000309-12-5	64
2		Heneicosane	296	C21H44	000629-94-7	62
3		Octadecane	254	C18H38	000593-45-3	58
4		Tetracosane	338	C24H50	000646-31-1	58
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Misc :
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ClientSampleId :
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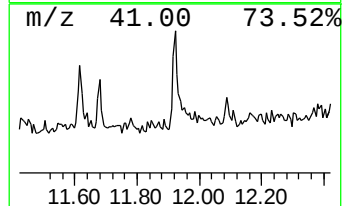
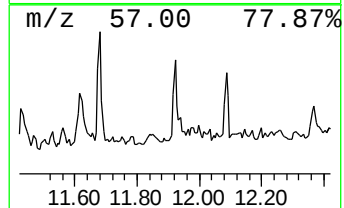
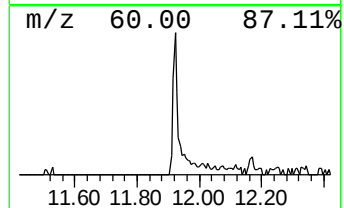
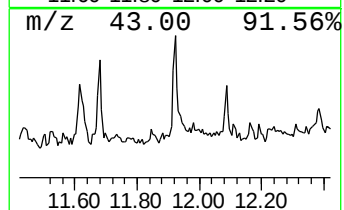
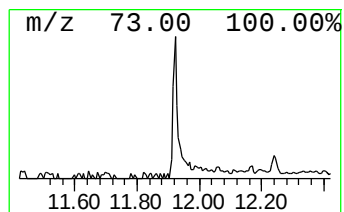
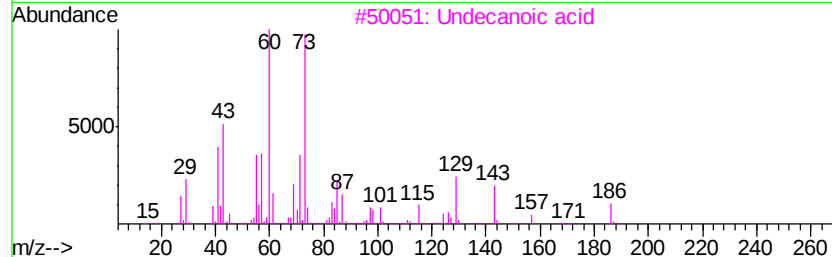
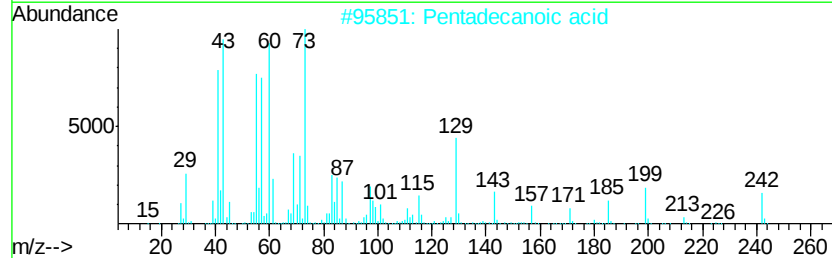
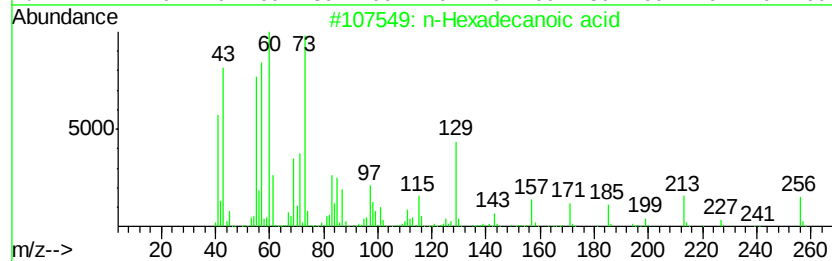
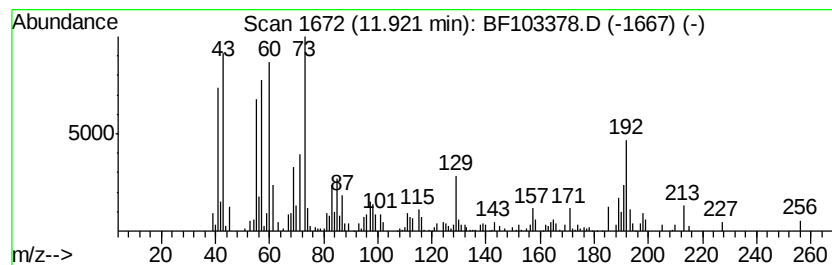
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.50 ng	176615	Phenanthrene-d10	11.41

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	70
3			Undecanoic acid	186	C11H22O2	000112-37-8	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	38
5			Trehalose	342	C12H22O11	000099-20-7	22



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Operator : SJ/JU
Sample : J1721-05
Misc :
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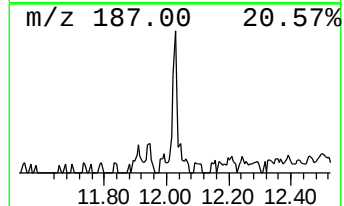
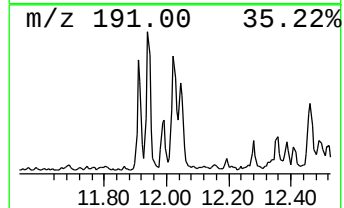
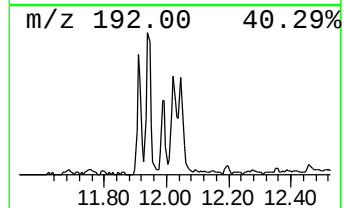
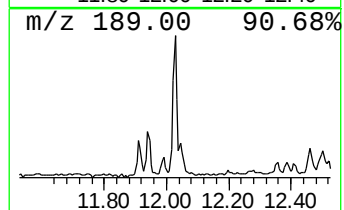
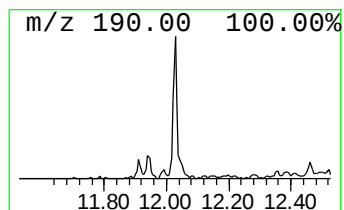
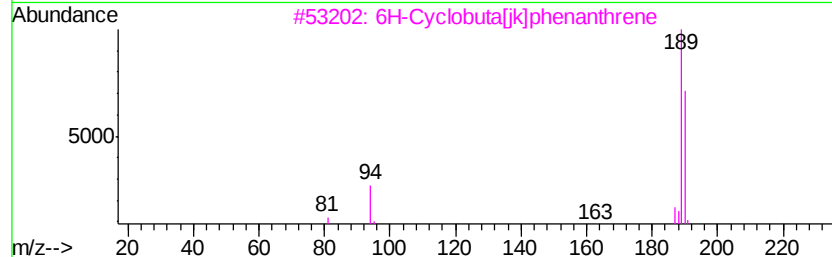
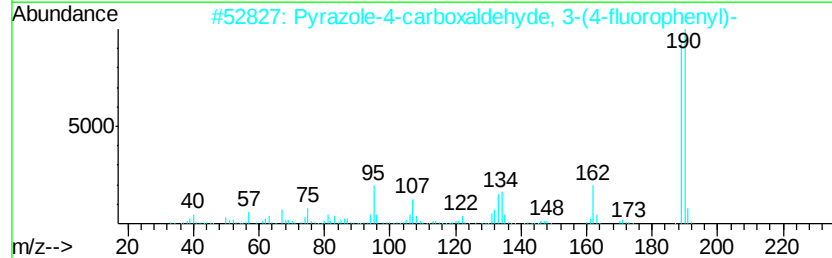
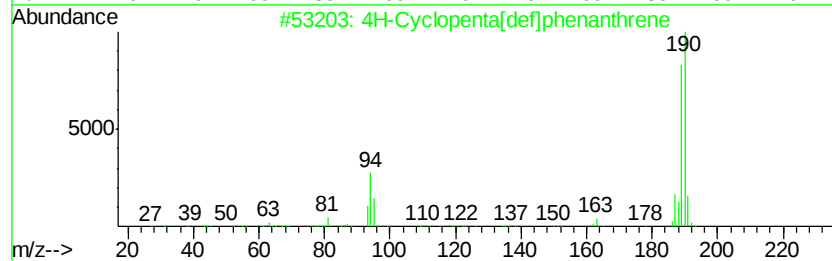
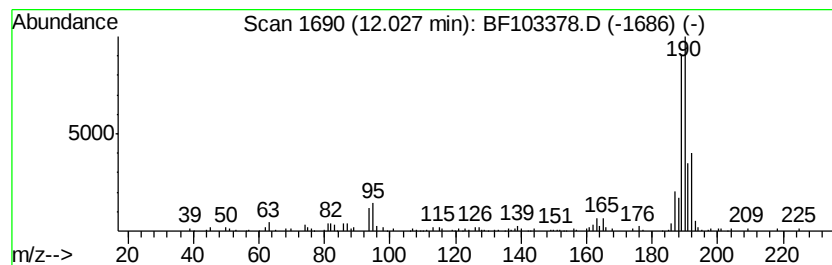
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.03	2.22 ng	112322	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
3	6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	38



Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
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Misc :
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SP-35

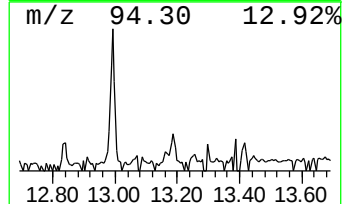
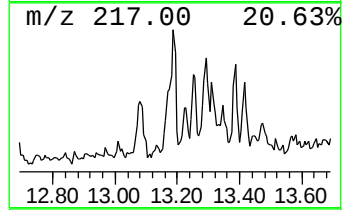
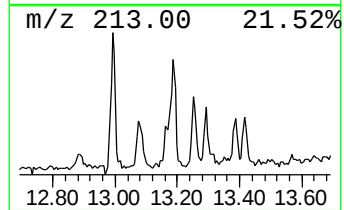
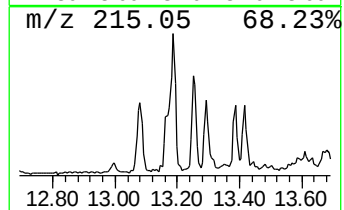
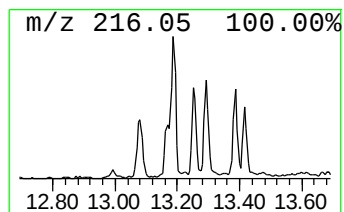
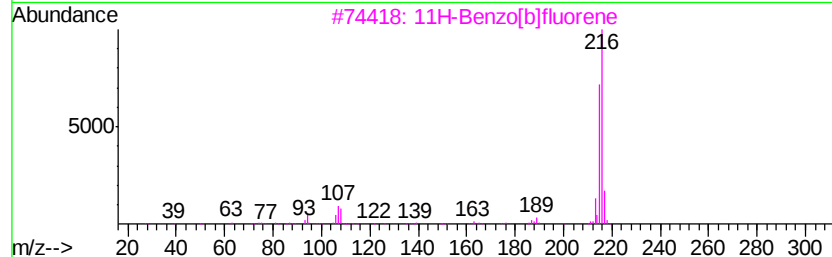
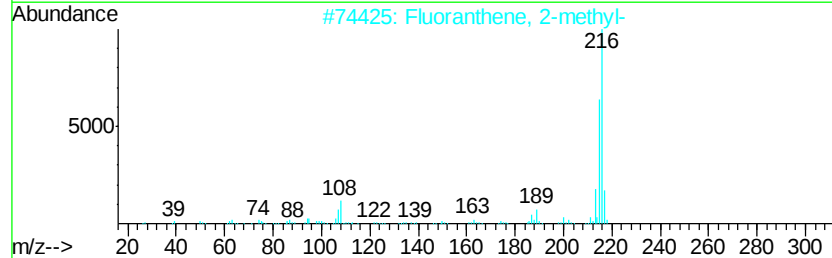
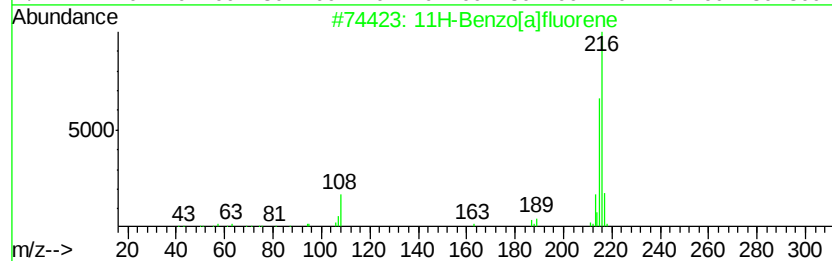
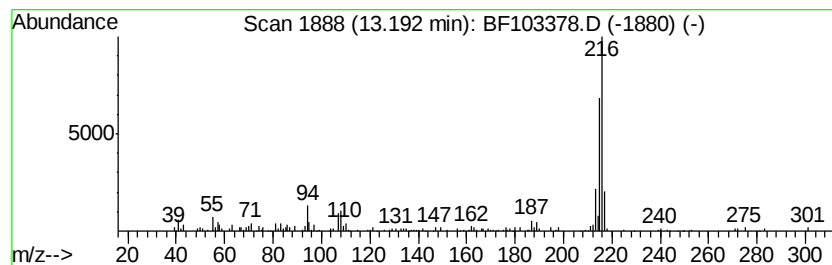
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 11H-Benzo[a]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	3.54 ng	201160	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	95
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
4			Pvrene, 1-methyl-	216	C17H12	002381-21-7	93
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81



Data Path : Z:\HPCHEM1\BNA_F\Data\BF030218\
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Acq On : 2 Mar 2018 21:03
Operator : SJ/JU
Sample : J1721-05
Misc :
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Instrument :
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ClientSampleId :
SP-35

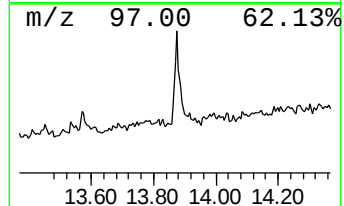
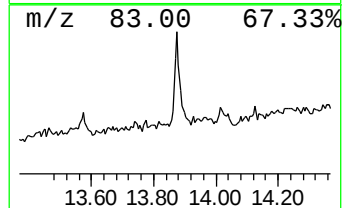
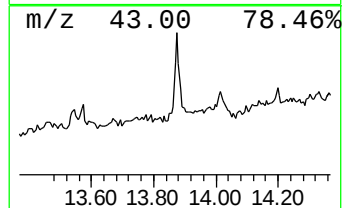
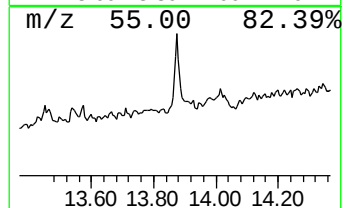
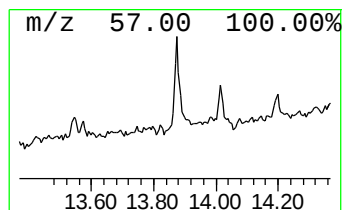
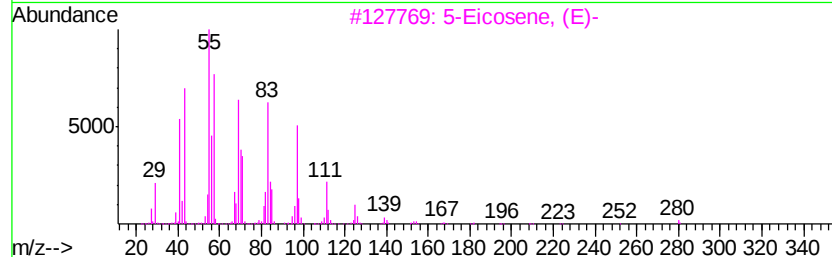
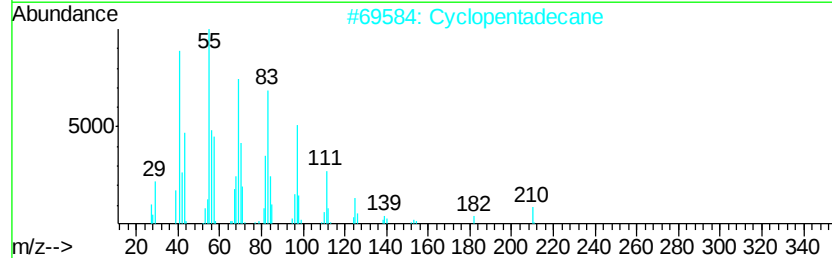
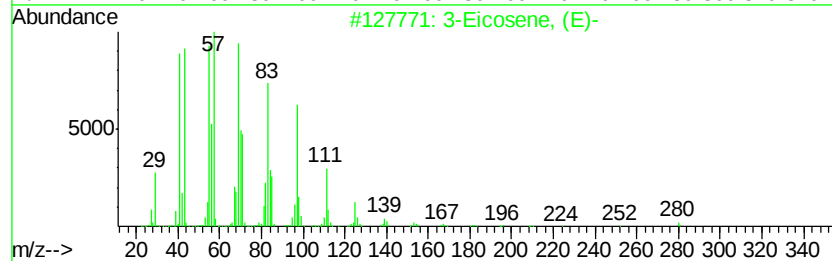
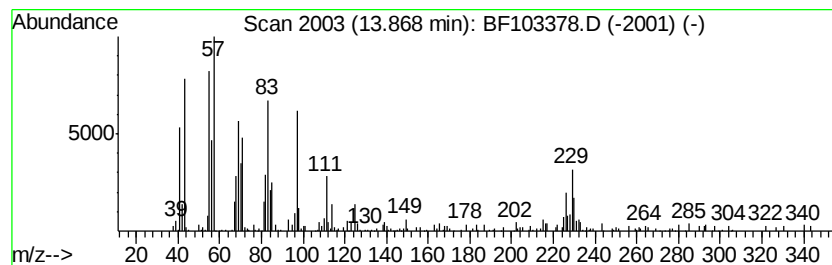
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.57 ng	202839	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2		Cyclopentadecane	210	C15H30	000295-48-7	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	78
5		1-Tricosanol	340	C23H48O	003133-01-5	76



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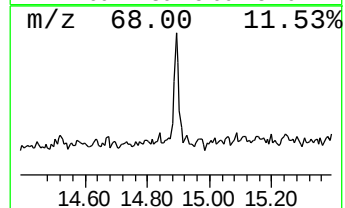
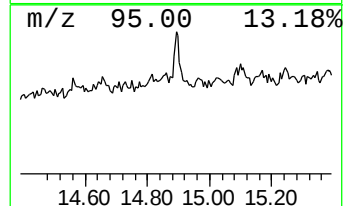
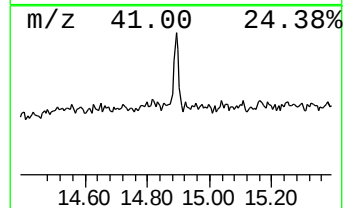
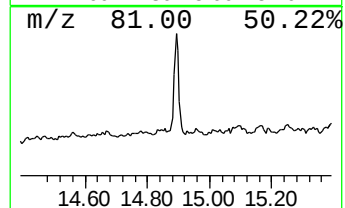
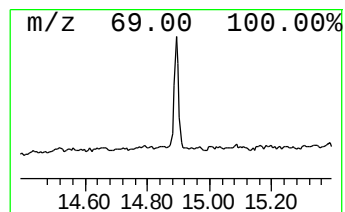
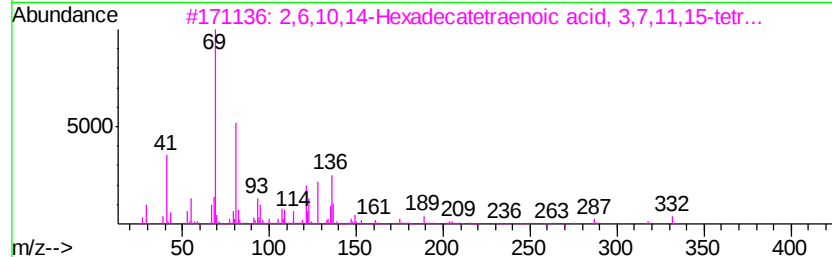
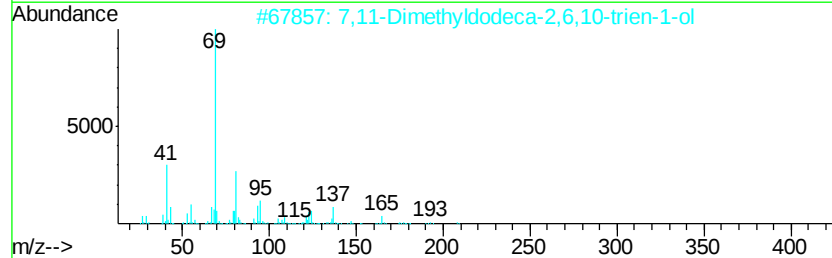
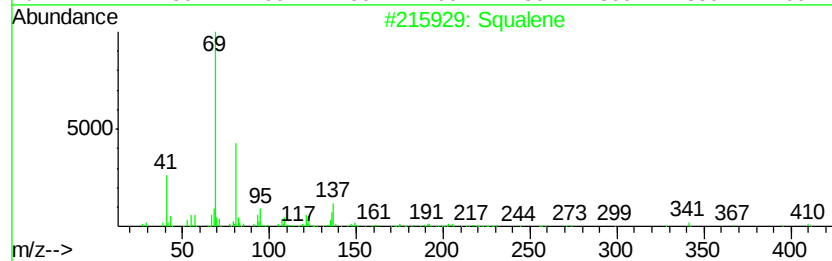
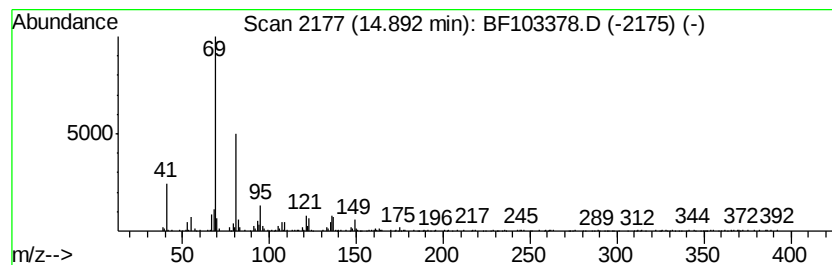
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	11.08 ng	231045	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	80
2		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
5		Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59



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Misc :
ALS Vial : 14 Sample Multiplier: 1

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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
Butane, 2-methoxy...	2.13	5.8	ng	283621	1	6.87	977914	20.0
Heptane	2.47	3.4	ng	165449	1	6.87	977914	20.0
2-Pentanone, 4-hy...	5.11	3.1	ng	152848	1	6.87	977914	20.0
unknown6.65	6.65	67.2	ng	3284670	1	6.87	977914	20.0
Hexadecane	9.83	2.1	ng	131132	3	9.92	1232350	20.0
Sulfurous acid, 2...	11.25	2.4	ng	120102	4	11.41	1010320	20.0
n-Hexadecanoic acid	11.92	3.5	ng	176615	4	11.41	1010320	20.0
4H-Cyclopenta[def...	12.03	2.2	ng	112322	4	11.41	1010320	20.0
11H-Benzo[a]fluorene	13.19	3.5	ng	201160	5	14.06	1136300	20.0
3-Eicosene, (E)-	13.87	3.6	ng	202839	5	14.06	1136300	20.0
Squalene	14.89	11.1	ng	231045	6	15.57	417182	20.0