

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF030918\
 Data File : BF103560.D
 Acq On : 9 Mar 2018 16:40
 Operator : SJ/JU
 Sample : J1855-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6-COMP

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	5.104	510	513	534	rBV	52681	105864	3.06%	0.349%
2	5.492	576	579	611	rBV	2360508	3431088	99.14%	11.325%
3	6.504	748	751	770	rBV	2237899	3460735	100.00%	11.423%
4	6.639	770	774	786	rVV	3001930	3156183	91.20%	10.417%
5	6.863	809	812	835	rVB	806002	945725	27.33%	3.121%
6	7.022	835	839	860	rBV	2135087	2366391	68.38%	7.811%
7	7.434	905	909	933	rBV	1666914	2305433	66.62%	7.609%
8	7.586	933	935	945	rVB	29398	46292	1.34%	0.153%
9	8.151	1027	1031	1057	rBV	810622	1219725	35.24%	4.026%
10	9.028	1175	1180	1182	rBV	29381	35120	1.01%	0.116%
11	9.086	1186	1190	1199	rVB	168696	178769	5.17%	0.590%
12	9.222	1206	1213	1222	rBV	2651713	2972866	85.90%	9.812%
13	9.328	1228	1231	1239	rVB	61575	72838	2.10%	0.240%
14	9.398	1239	1243	1257	rBV	75004	166422	4.81%	0.549%
15	9.639	1281	1284	1287	rVB	67725	59389	1.72%	0.196%
16	9.704	1292	1295	1301	rVB2	32177	41228	1.19%	0.136%
17	9.904	1325	1329	1342	rVB	989298	1109977	32.07%	3.664%
18	10.292	1392	1395	1397	rBV	77892	59760	1.73%	0.197%
19	10.316	1397	1399	1403	rVB	76755	57273	1.65%	0.189%
20	10.704	1461	1465	1478	rBV	1179746	1534611	44.34%	5.065%
21	10.792	1478	1480	1484	rVB3	43229	51984	1.50%	0.172%
22	10.898	1494	1498	1502	rVB	41453	40776	1.18%	0.135%
23	10.969	1508	1510	1515	rBV	37275	44385	1.28%	0.146%
24	11.033	1518	1521	1534	rVB6	17196	44264	1.28%	0.146%
25	11.239	1553	1556	1566	rVB6	36035	63040	1.82%	0.208%
26	11.333	1569	1572	1575	rBV2	44048	39072	1.13%	0.129%
27	11.404	1580	1584	1596	rBV	776609	942660	27.24%	3.111%
28	11.545	1605	1608	1612	rBV	255007	237606	6.87%	0.784%
29	11.610	1615	1619	1623	rVB4	43689	57835	1.67%	0.191%
30	11.916	1668	1671	1673	rBV2	47093	56217	1.62%	0.186%
31	11.945	1673	1676	1681	rVB	1332449	1169479	33.79%	3.860%
32	12.074	1695	1698	1700	rBV	48417	38609	1.12%	0.127%
33	12.427	1755	1758	1762	rBV2	39163	52707	1.52%	0.174%
34	12.463	1762	1764	1767	rVB	75474	59015	1.71%	0.195%

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TP-6-COMP

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	12.545	1776	1778	1786	rVV2	25423	39017	1.13%	0.129%
36	12.833	1824	1827	1830	rBV	164714	152259	4.40%	0.503%
37	12.986	1848	1853	1860	rBV	1630941	1660546	47.98%	5.481%
38	13.192	1883	1888	1892	rBV	267978	255717	7.39%	0.844%
39	13.533	1943	1946	1950	rBV	226623	204822	5.92%	0.676%
40	13.863	1999	2002	2008	rBV	256586	268995	7.77%	0.888%
41	14.004	2023	2026	2029	rBV	104217	92332	2.67%	0.305%
42	14.063	2032	2036	2044	rBV	614141	753495	21.77%	2.487%
43	14.180	2054	2056	2060	rVB	71385	65509	1.89%	0.216%
44	14.492	2107	2109	2113	rBV4	49891	59372	1.72%	0.196%
45	15.574	2289	2293	2300	rVB	366267	521873	15.08%	1.723%

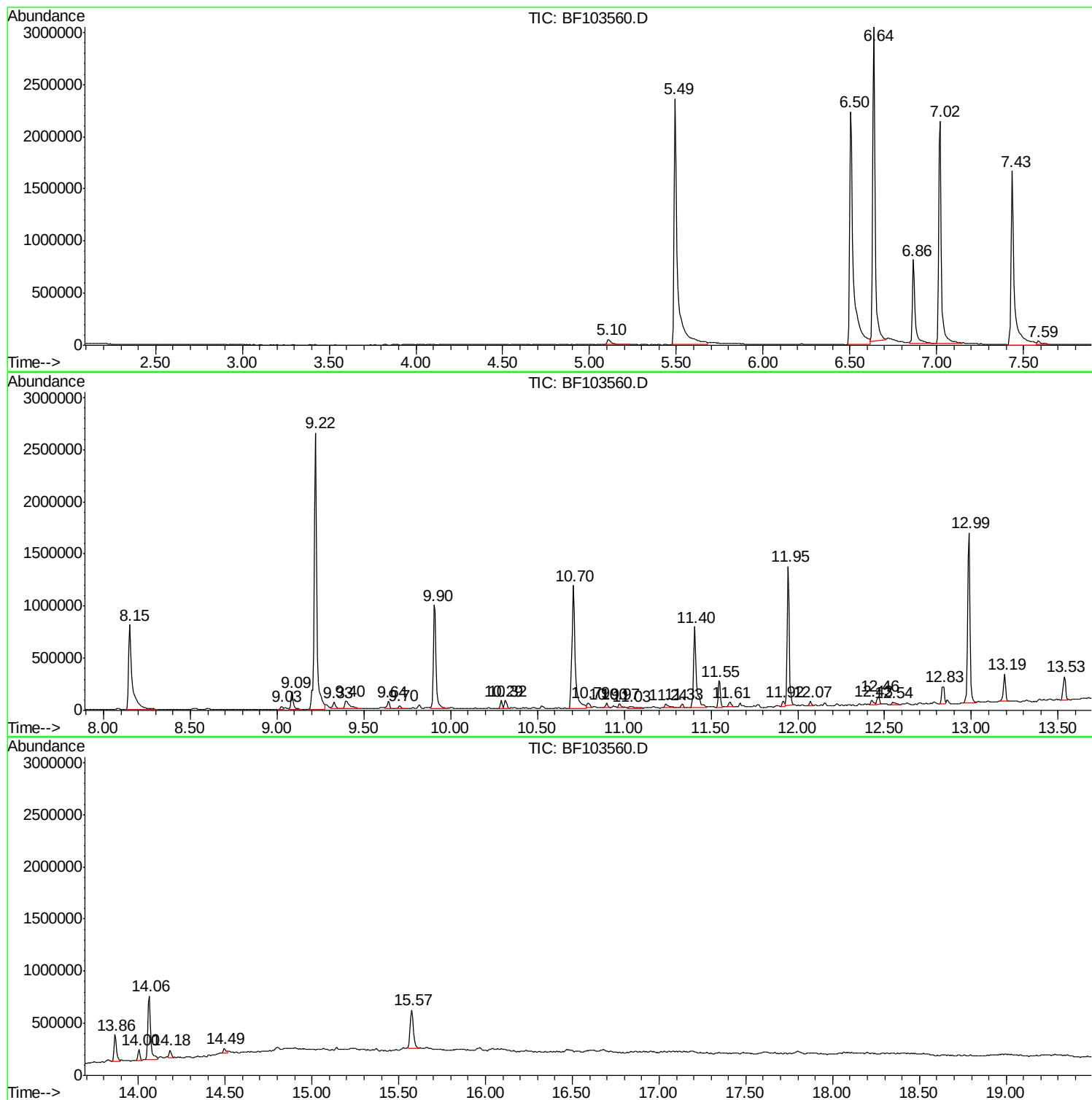
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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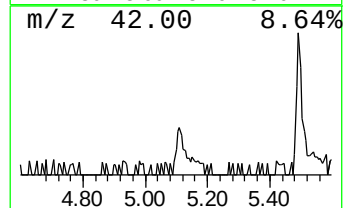
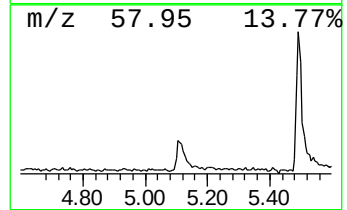
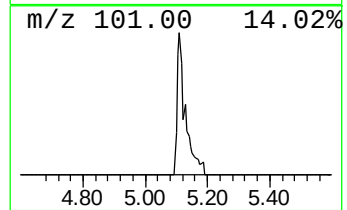
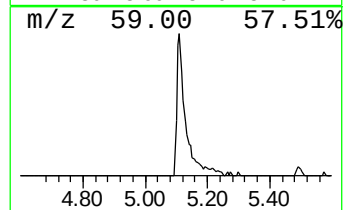
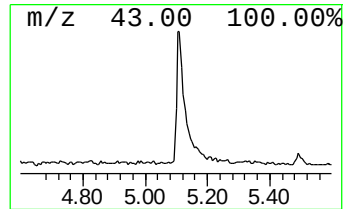
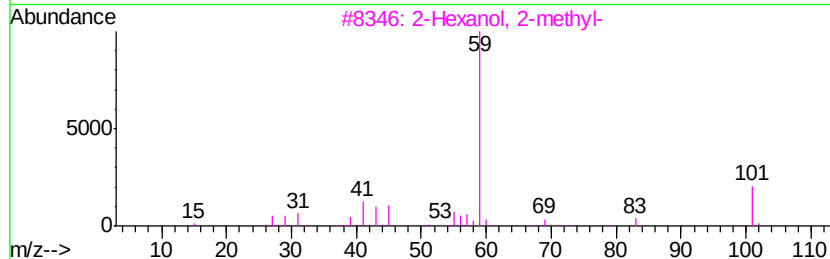
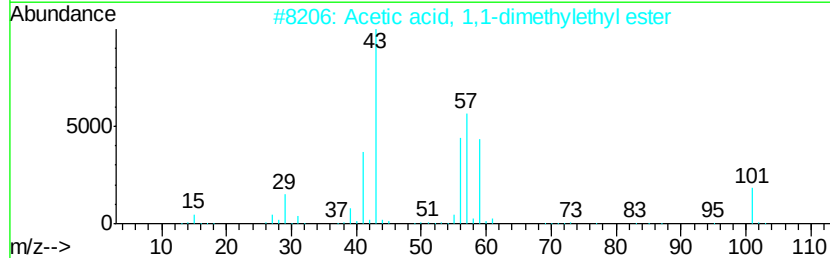
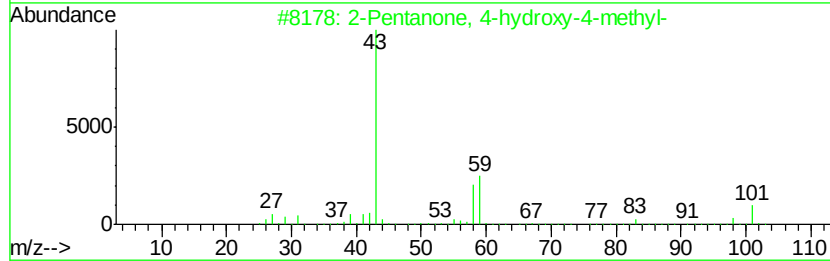
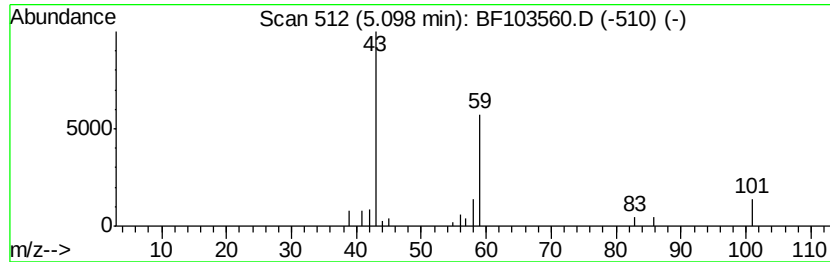
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.24 ng	105864	1,4-Dichlorobenzene-d4	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	Hexane, 1-ethoxy-	130	C8H18O	005756-43-4	17	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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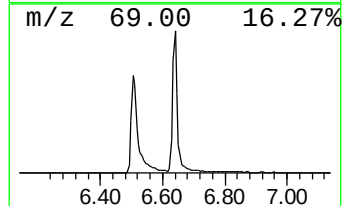
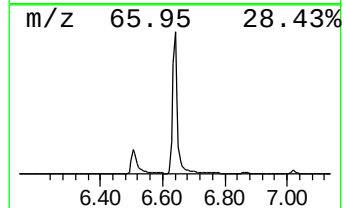
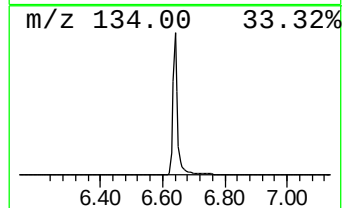
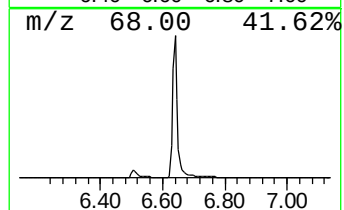
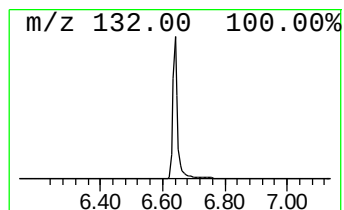
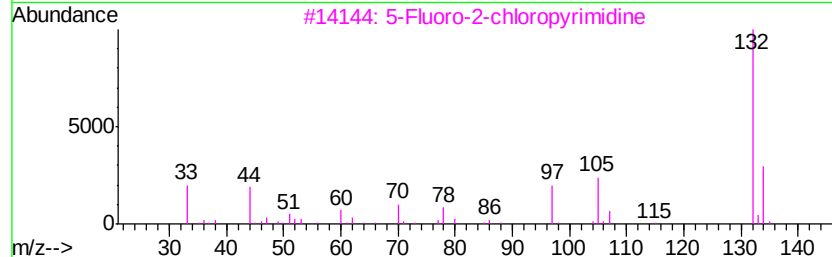
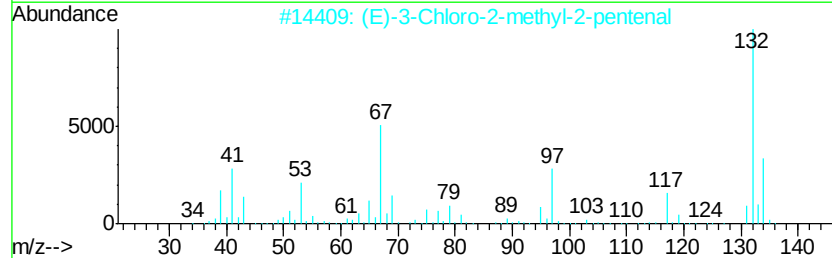
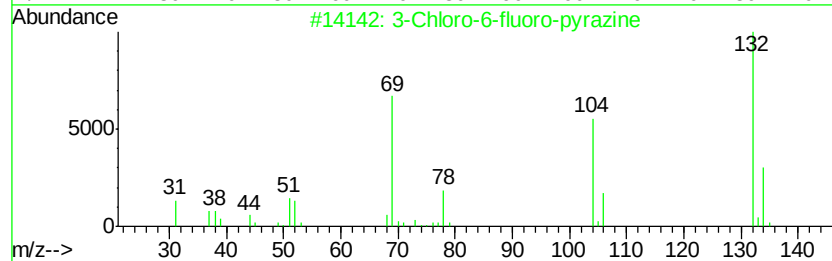
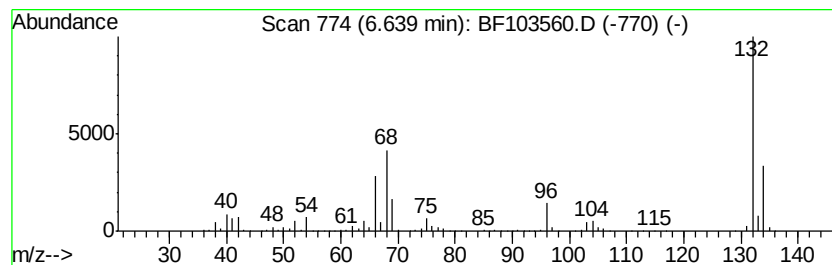
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	66.75 ng	3156180	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	27
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl			189	C12H15NO	1000123-86-3	10
5	Benzene, 1-ethenyl-3,5-dimethyl-			132	C10H12	005379-20-4	9



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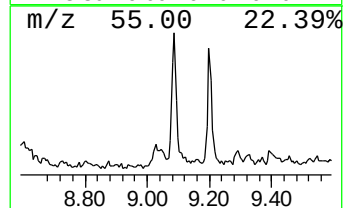
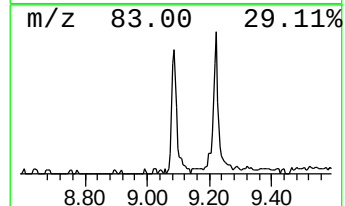
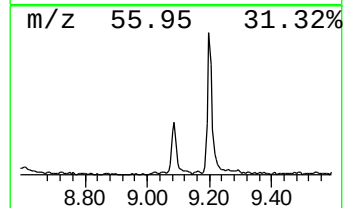
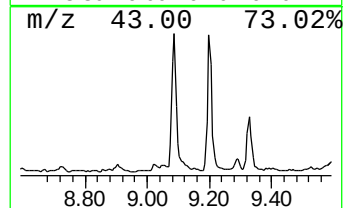
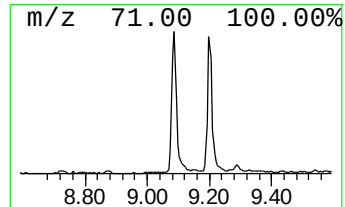
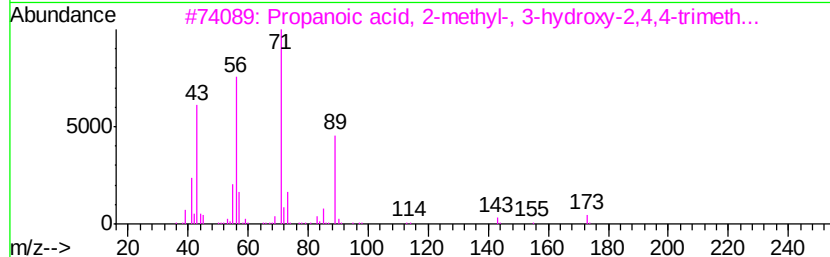
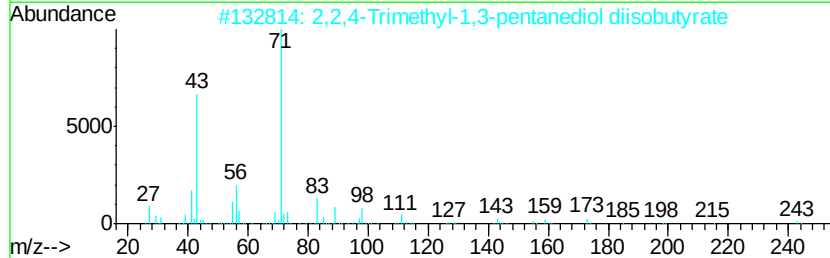
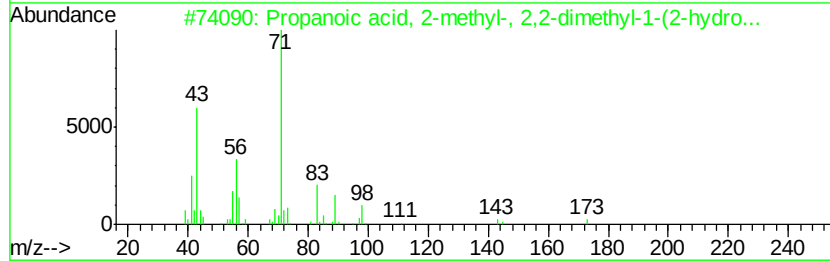
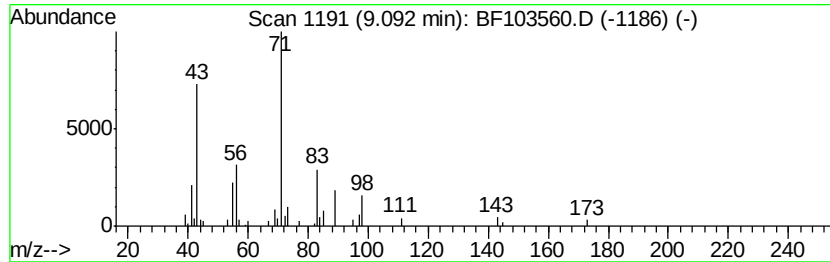
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.09	3.22 ng	178769	Acenaphthene-d10	9.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	83
2	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
3	Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	43
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	40
5	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	38



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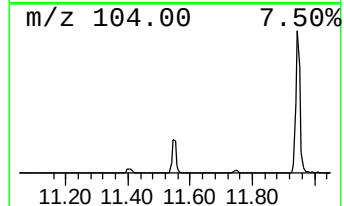
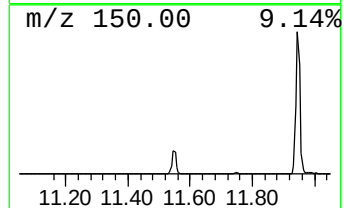
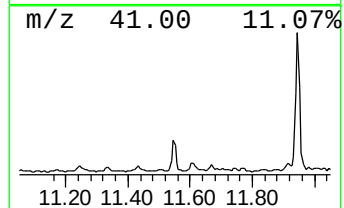
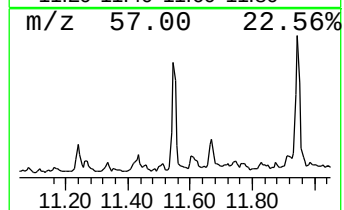
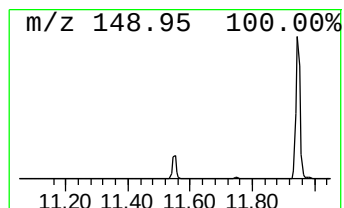
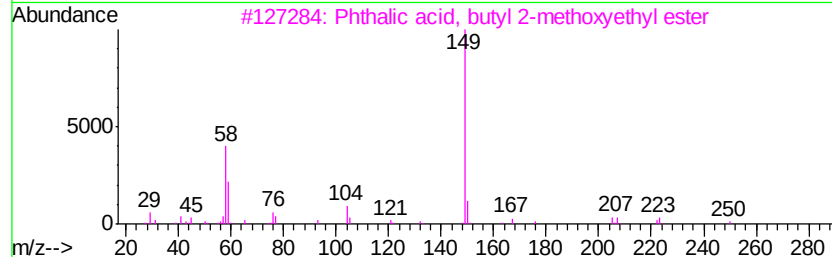
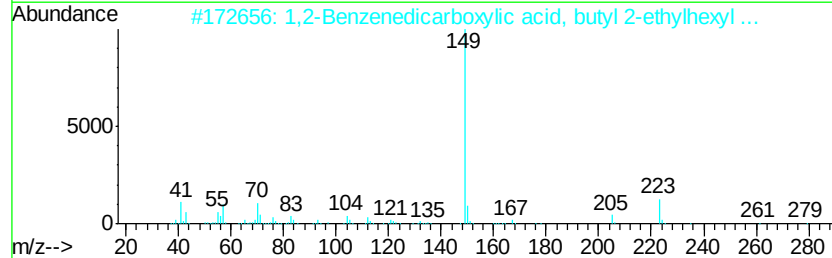
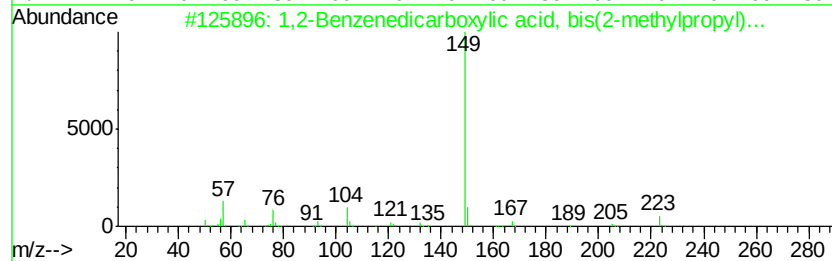
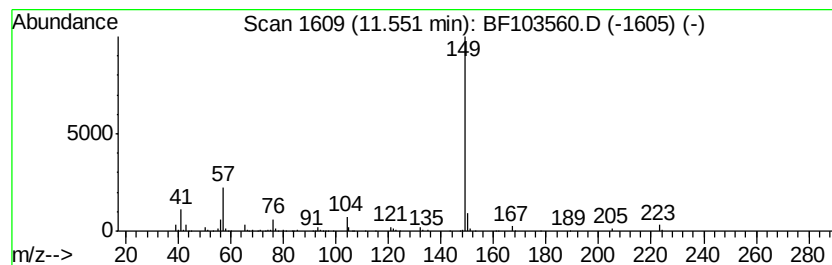
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	5.04 ng	237606	Phenanthrene-d10	11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	86
2			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
3			Phthalic acid, butyl 2-methoxyvet...	280	C15H20O5	1000315-80-0	83
4			Phthalic acid, butyl 3-methylbut...	292	C17H24O4	1000356-80-4	78
5			1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	78



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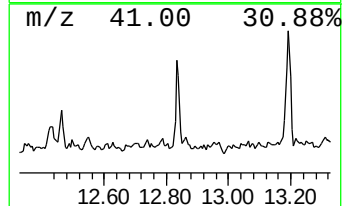
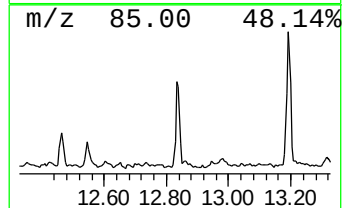
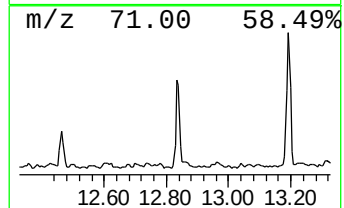
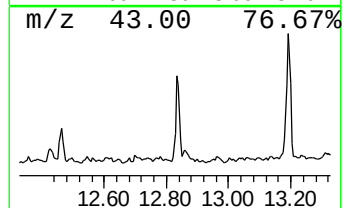
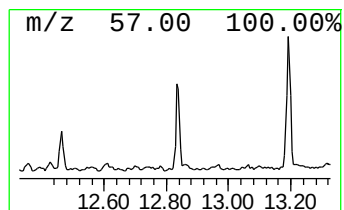
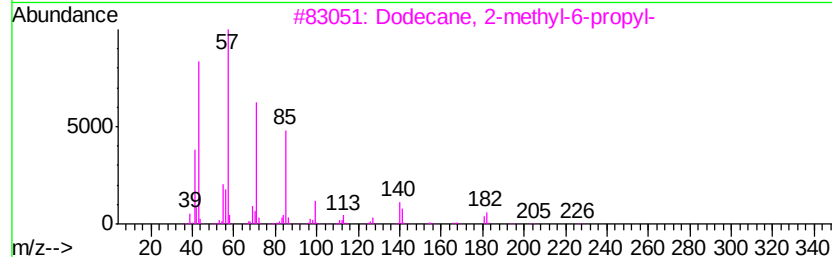
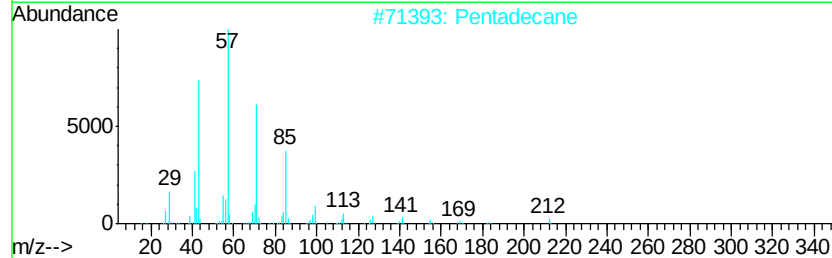
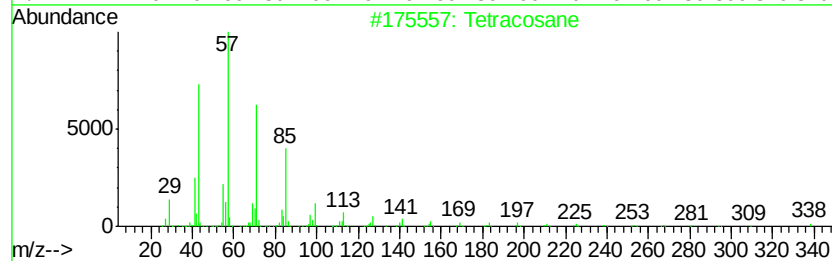
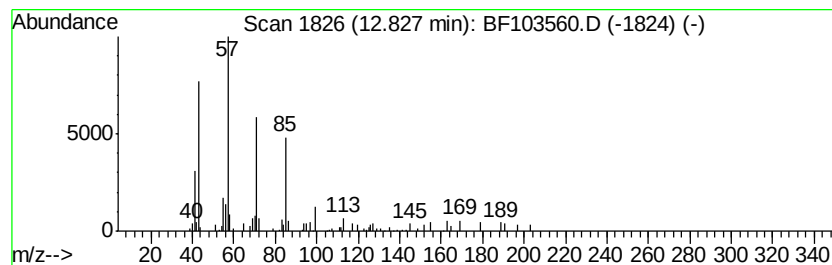
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	4.04 ng	152259	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	90
2		Pentadecane	212	C15H32	000629-62-9	86
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4		Octacosane	394	C28H58	000630-02-4	78
5		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF030918\
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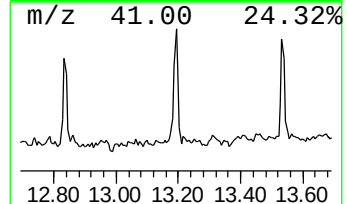
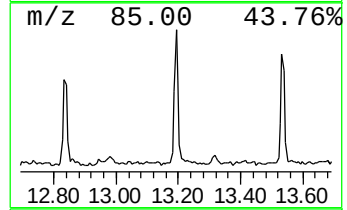
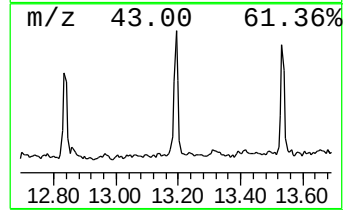
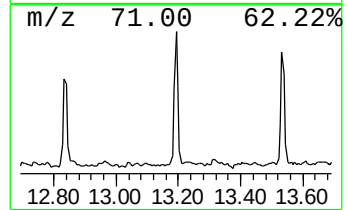
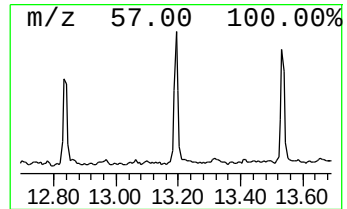
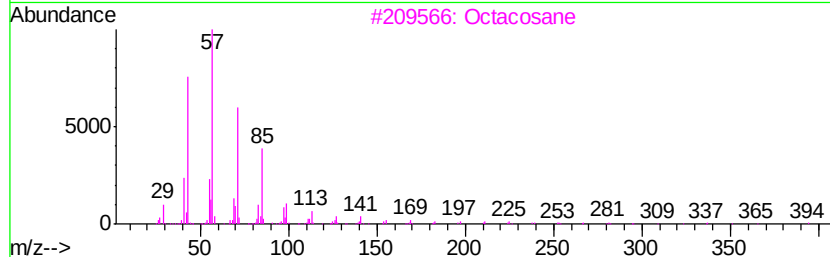
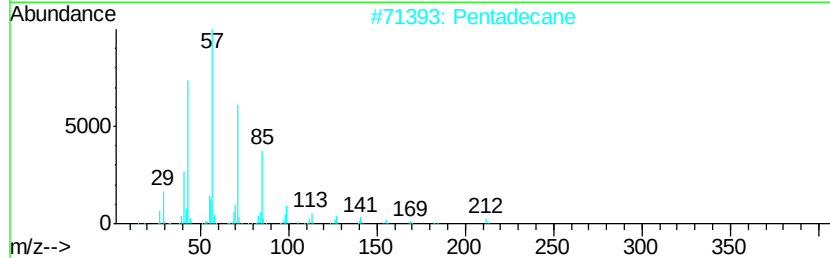
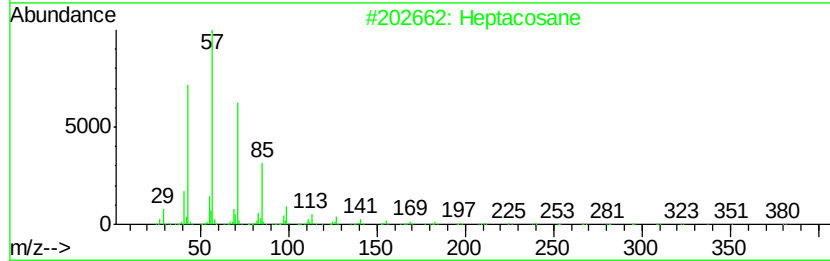
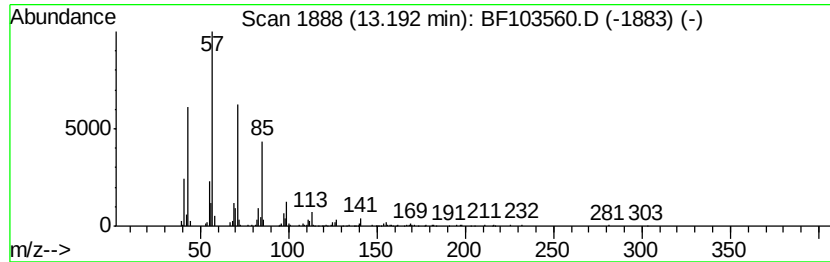
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	6.79 ng	255717	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Pentadecane	212	C15H32	000629-62-9	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103560.D
Acq On : 9 Mar 2018 16:40
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Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-6-COMP

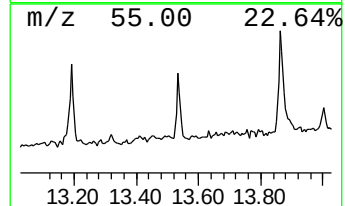
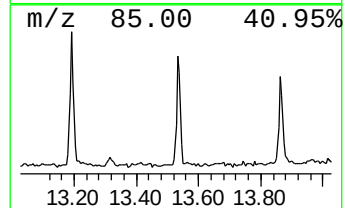
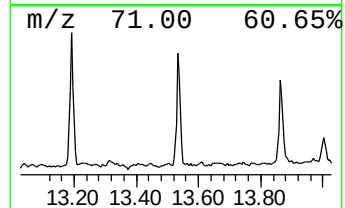
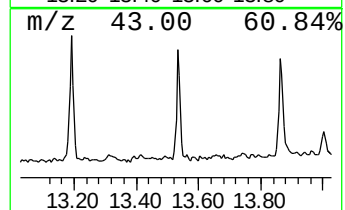
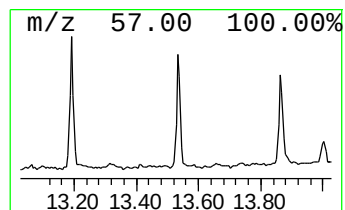
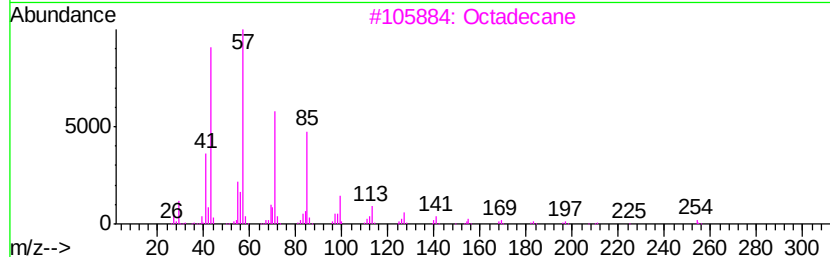
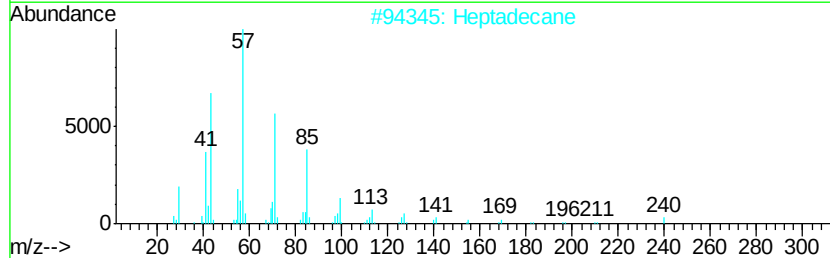
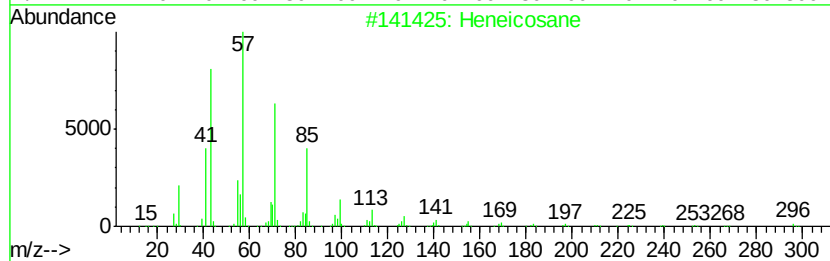
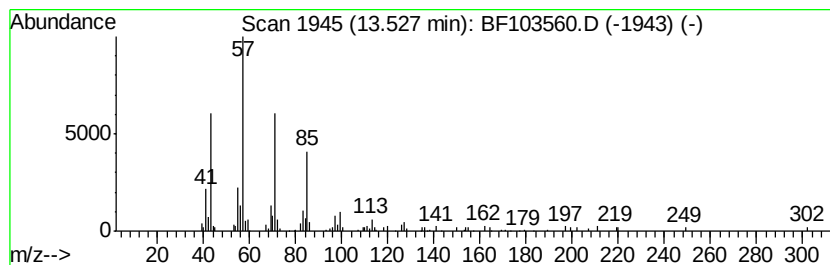
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	5.44 ng	204822	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Octadecane	254	C18H38	000593-45-3	91
4		Nonadecane	268	C19H40	000629-92-5	91
5		Hexadecane	226	C16H34	000544-76-3	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF030918\
Data File : BF103560.D
Acq On : 9 Mar 2018 16:40
Operator : SJ/JU
Sample : J1855-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

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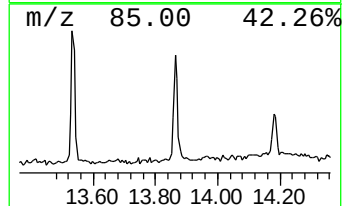
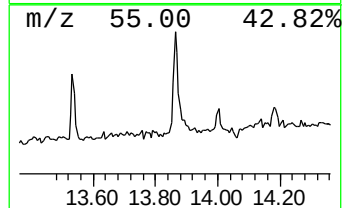
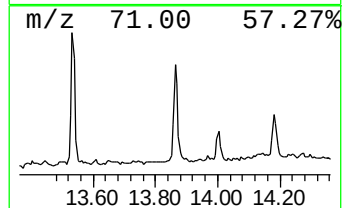
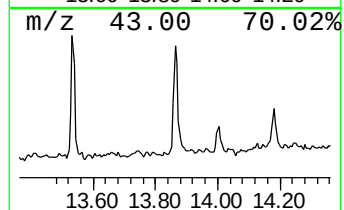
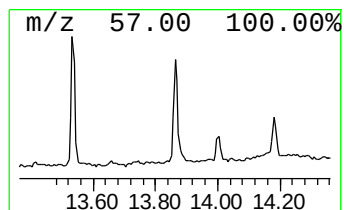
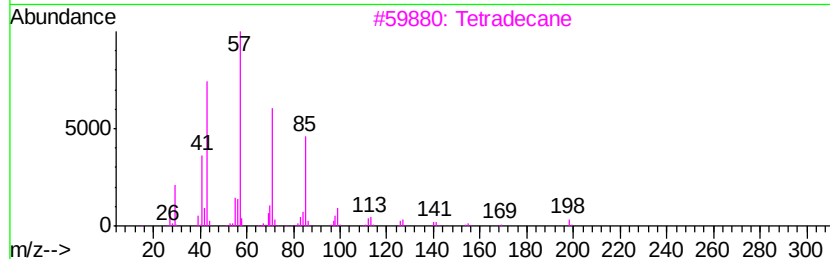
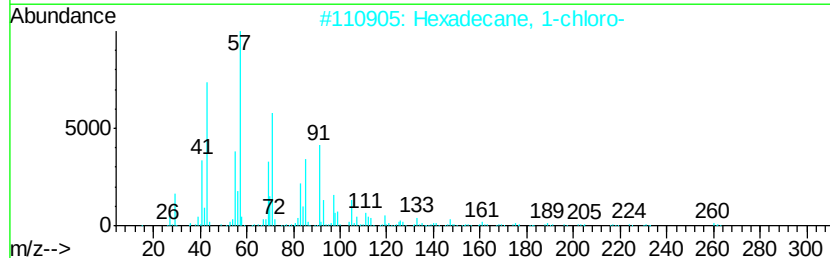
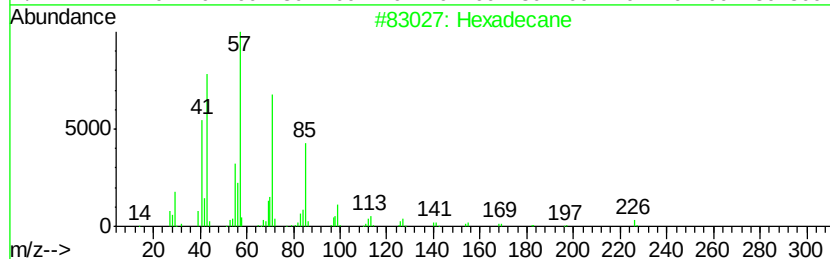
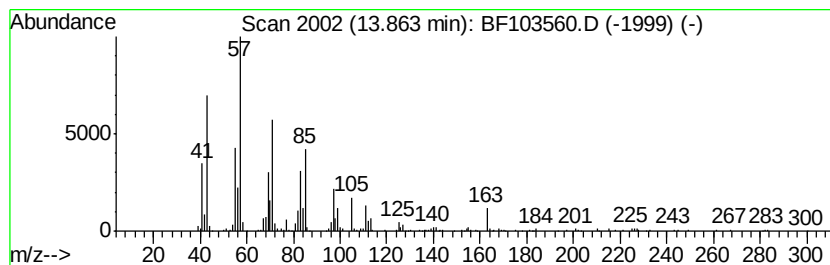
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.14 ng	268995	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	86
2			Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	80
3			Tetradecane	198	C14H30	000629-59-4	58
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
5			Methyl 2-tetradecyloxiranecarbox...	298	C18H34O3	1000213-09-0	55



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF030918\
Data File : BF103560.D
Acq On : 9 Mar 2018 16:40
Operator : SJ/JU
Sample : J1855-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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unknown6.64	6.64	66.8	ng	3156180	1	6.86	945725	20.0
Propanoic acid, 2...	9.09	3.2	ng	178769	3	9.90	1109980	20.0
1,2-Benzenedicarb...	11.55	5.0	ng	237606	4	11.40	942660	20.0
Tetracosane	12.83	4.0	ng	152259	5	14.06	753495	20.0
Heptacosane	13.19	6.8	ng	255717	5	14.06	753495	20.0
Heneicosane	13.53	5.4	ng	204822	5	14.06	753495	20.0
Hexadecane	13.86	7.1	ng	268995	5	14.06	753495	20.0