

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021218\
 Data File : BF102912.D
 Acq On : 12 Feb 2018 11:29
 Operator : SJ/JU
 Sample : J1512-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-4252

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-BF020318.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	2.181	9	16	22	rBV	477957	641769	15.48%	1.655%
2	5.122	512	516	523	rVB	111479	148843	3.59%	0.384%
3	5.504	576	581	585	rBV	3825753	4145236	100.00%	10.690%
4	6.510	747	752	764	rBV	3515628	4027327	97.16%	10.386%
5	6.657	772	777	780	rBV	3999144	3996011	96.40%	10.305%
6	6.886	812	816	819	rBV	1249019	1154083	27.84%	2.976%
7	7.039	838	842	846	rBV	3291651	3118154	75.22%	8.041%
8	7.445	906	911	914	rBV	2704702	2666707	64.33%	6.877%
9	7.622	938	941	946	rVB	59502	54772	1.32%	0.141%
10	8.169	1030	1034	1037	rBV	1636808	1474523	35.57%	3.803%
11	9.239	1211	1216	1220	rBV	3890303	3912940	94.40%	10.091%
12	9.316	1226	1229	1231	rVB	74186	59090	1.43%	0.152%
13	9.633	1279	1283	1286	rBV	366242	337047	8.13%	0.869%
14	9.845	1314	1319	1322	rVV	209200	167940	4.05%	0.433%
15	9.922	1328	1332	1336	rBV	1668743	1499657	36.18%	3.867%
16	10.169	1370	1374	1377	rBV3	46142	49436	1.19%	0.127%
17	10.345	1401	1404	1407	rVB	246501	184083	4.44%	0.475%
18	10.563	1437	1441	1444	rBV	61573	76183	1.84%	0.196%
19	10.716	1463	1467	1476	rVB	2042484	2106175	50.81%	5.432%
20	10.816	1481	1484	1494	rVB	185899	229488	5.54%	0.592%
21	11.263	1557	1560	1563	rBV	78047	77525	1.87%	0.200%
22	11.298	1563	1566	1572	rVB3	55018	72273	1.74%	0.186%
23	11.410	1581	1585	1588	rBV	1394408	1297392	31.30%	3.346%
24	11.433	1588	1589	1596	rVB	205082	151149	3.65%	0.390%
25	11.927	1667	1673	1679	rBV3	75307	137484	3.32%	0.355%
26	12.021	1686	1689	1692	rBV2	44765	52698	1.27%	0.136%
27	12.463	1757	1764	1766	rBV5	26021	42146	1.02%	0.109%
28	12.627	1788	1792	1795	rBV	280229	256381	6.18%	0.661%
29	12.857	1825	1831	1834	rBV	254953	281439	6.79%	0.726%
30	12.998	1848	1855	1858	rBV	2799110	2673598	64.50%	6.895%
31	13.545	1945	1948	1952	rBV2	61185	62802	1.52%	0.162%
32	13.880	2002	2005	2012	rVB2	419365	415822	10.03%	1.072%
33	14.021	2026	2029	2030	rBV	50615	45762	1.10%	0.118%
34	14.051	2030	2034	2037	rVV	1059390	1126667	27.18%	2.906%

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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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.074	2037	2038	2044	rVB	155331	134224	3.24%	0.346%
36	14.509	2109	2112	2117	rBV5	48578	67826	1.64%	0.175%
37	15.098	2208	2212	2216	rBV	145520	246515	5.95%	0.636%
38	15.162	2220	2223	2226	rVB	53194	56507	1.36%	0.146%
39	15.409	2261	2265	2271	rVB	78819	104120	2.51%	0.269%
40	15.474	2272	2276	2281	rVV	103939	145016	3.50%	0.374%
41	15.539	2282	2287	2300	rBV	794696	1097561	26.48%	2.831%
42	15.992	2360	2364	2368	rVB	76412	112323	2.71%	0.290%
43	17.039	2539	2542	2548	rVB3	46309	69451	1.68%	0.179%

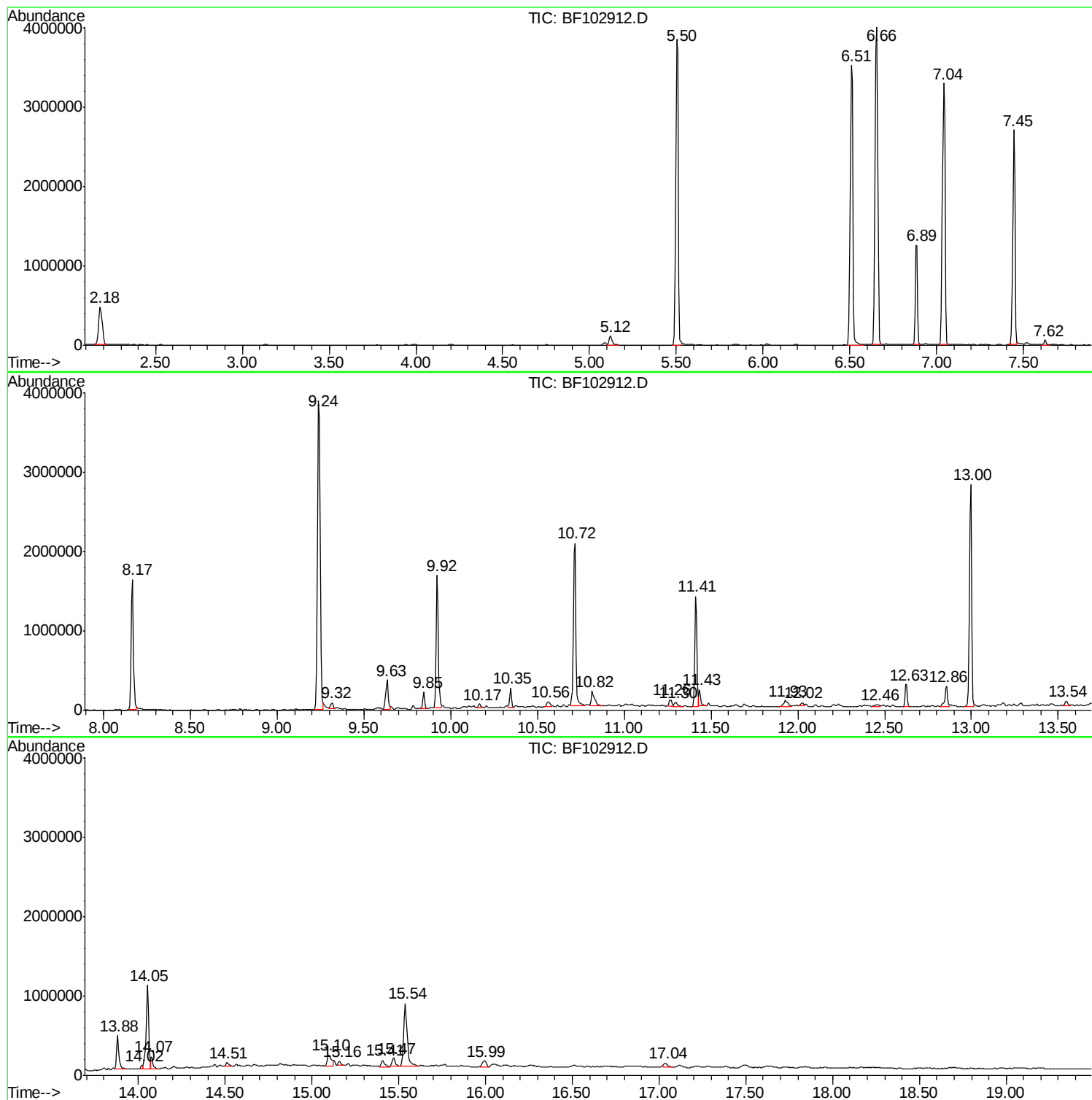
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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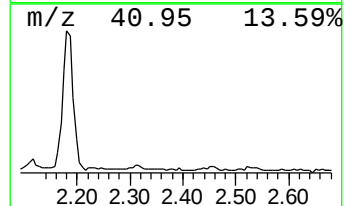
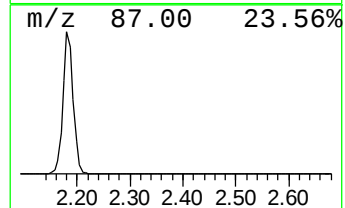
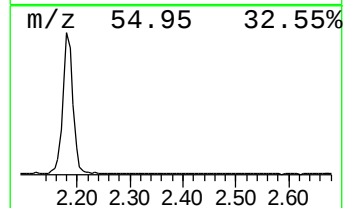
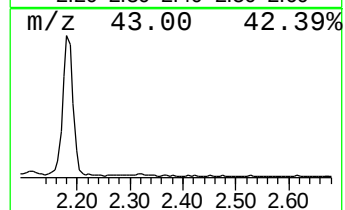
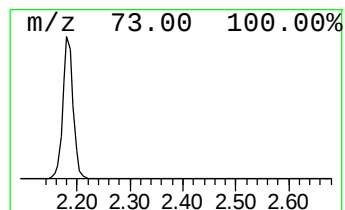
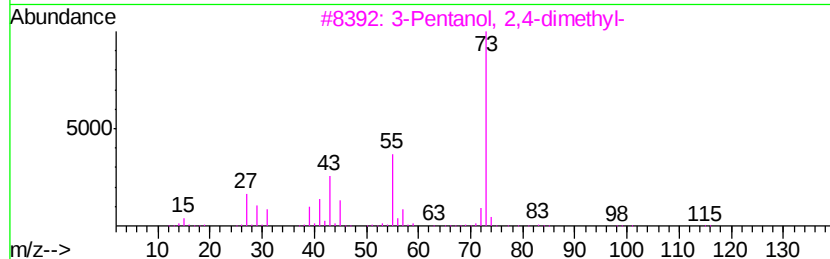
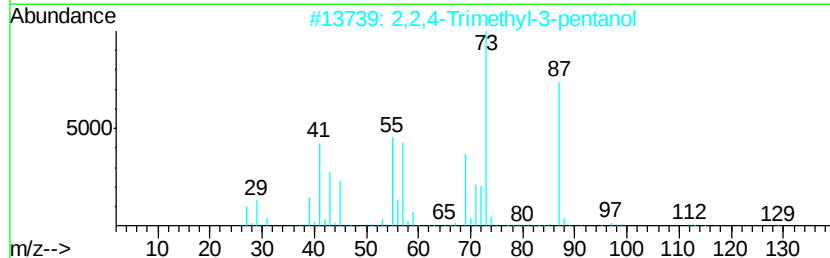
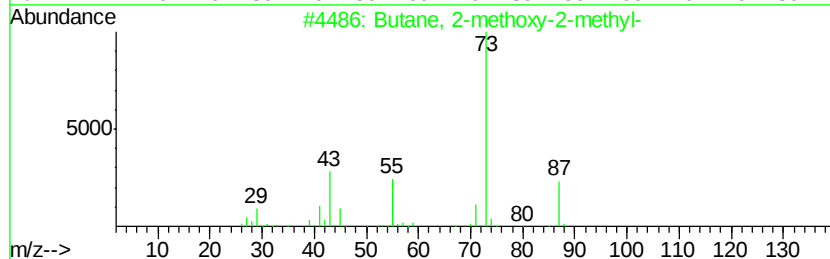
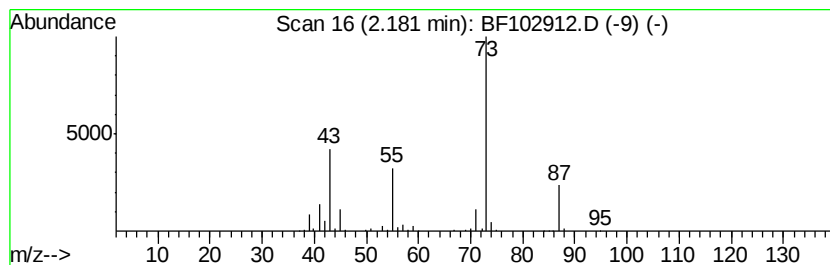
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.18	11.12 ng	641769	1,4-Dichlorobenzene-d4	6.89

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	40
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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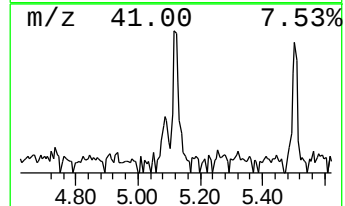
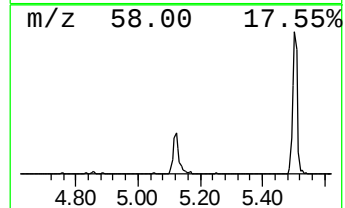
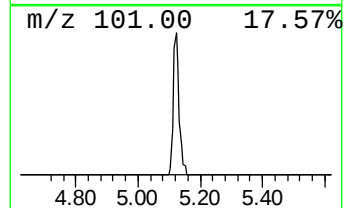
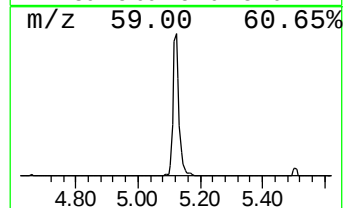
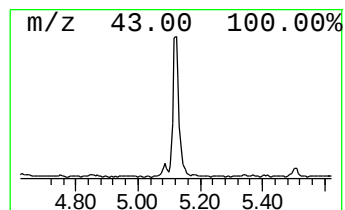
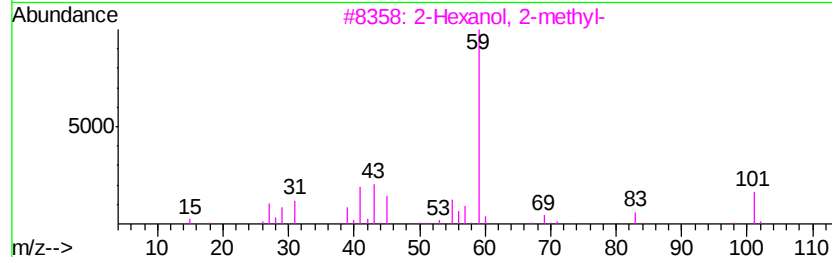
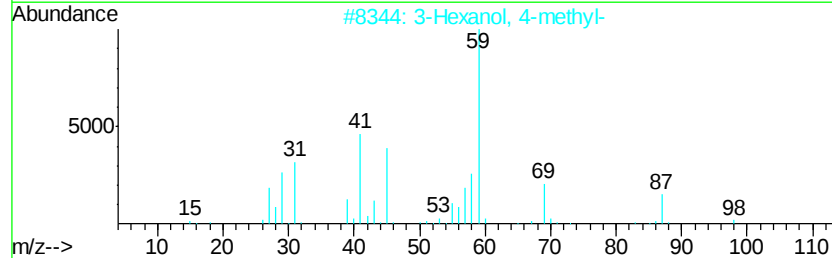
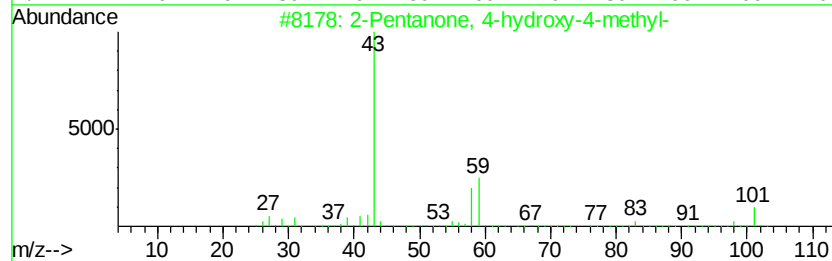
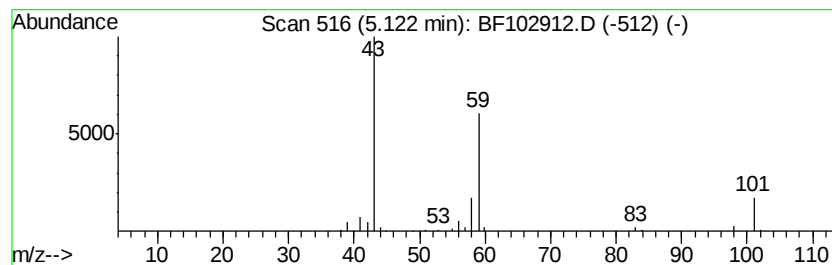
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.58 ng	148843	1,4-Dichlorobenzene-d4	6.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		Guanidine	59	CH5N3	000113-00-8	9



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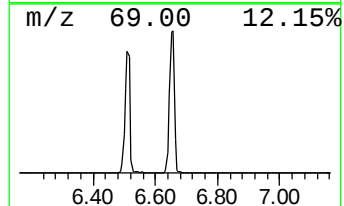
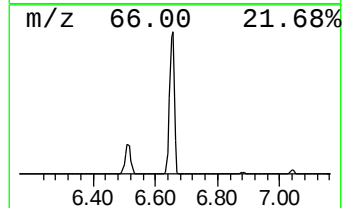
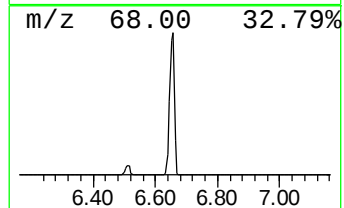
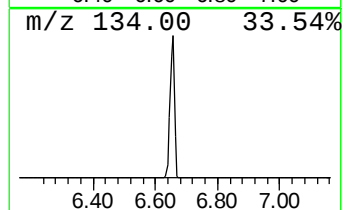
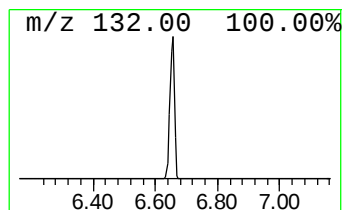
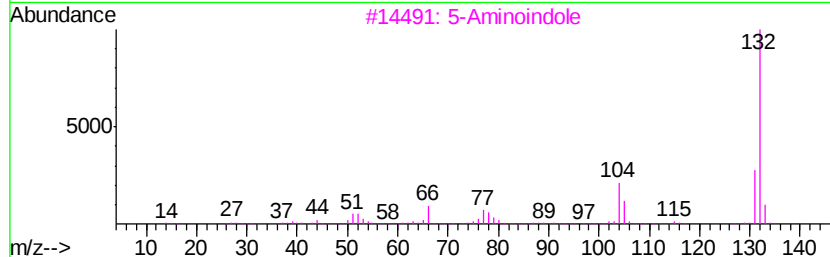
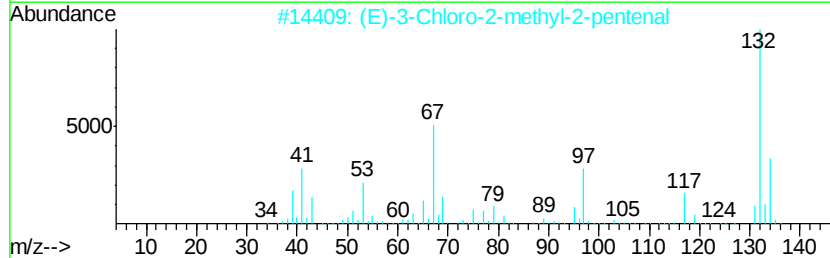
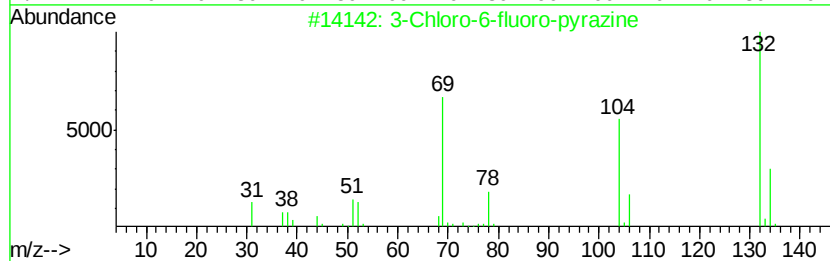
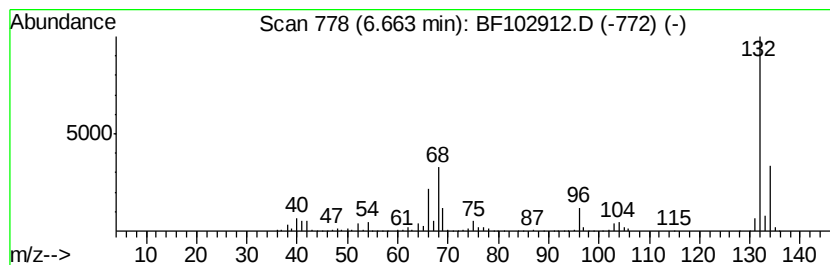
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.25 ng	3996010	1,4-Dichlorobenzene-d4	6.89

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-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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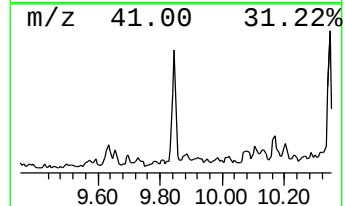
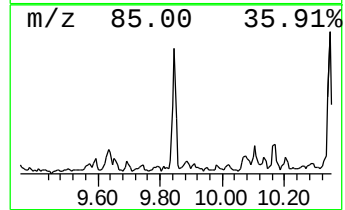
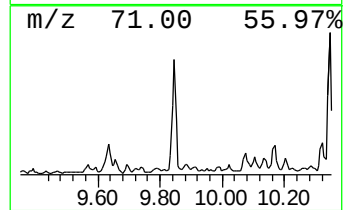
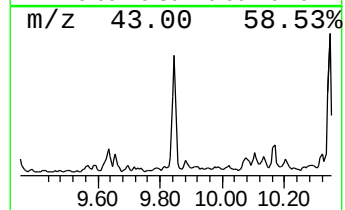
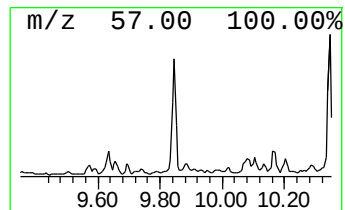
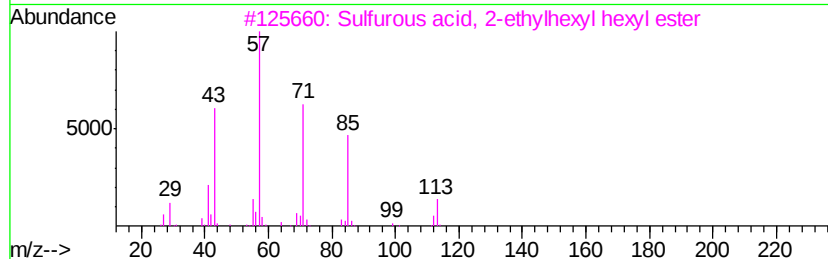
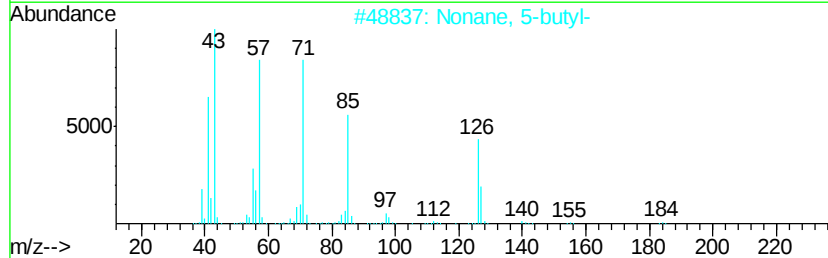
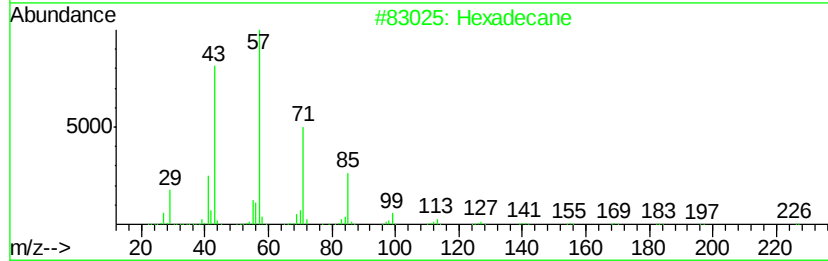
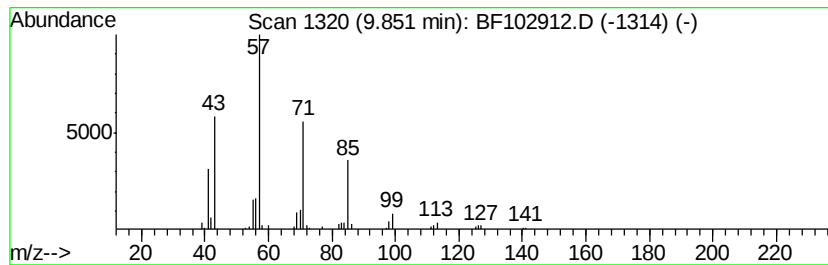
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.24 ng	167940	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Nonane, 5-butyl-		184	C13H28	017312-63-9	64
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	64
4	Sulfurous acid, decyl 2-ethylhex...		334	C18H38O3S	1000309-19-3	64
5	Decane, 3-bromo-		220	C10H21Br	030571-71-2	58



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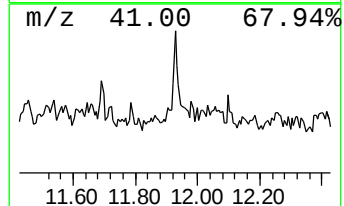
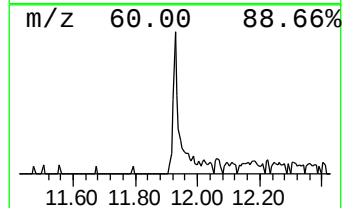
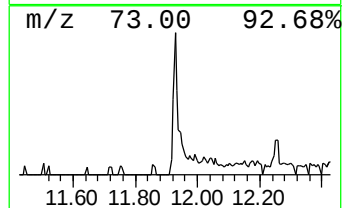
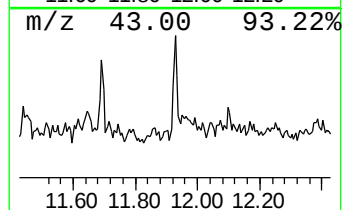
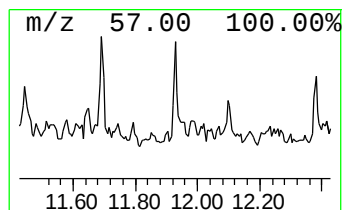
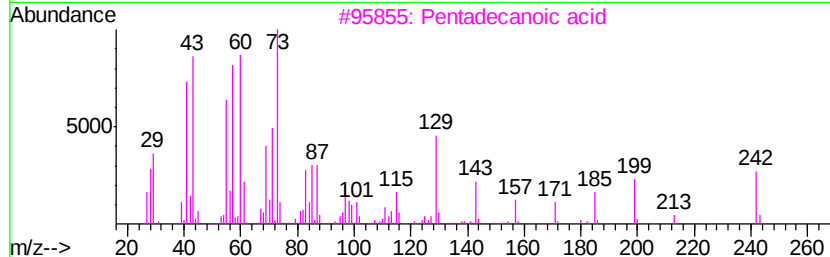
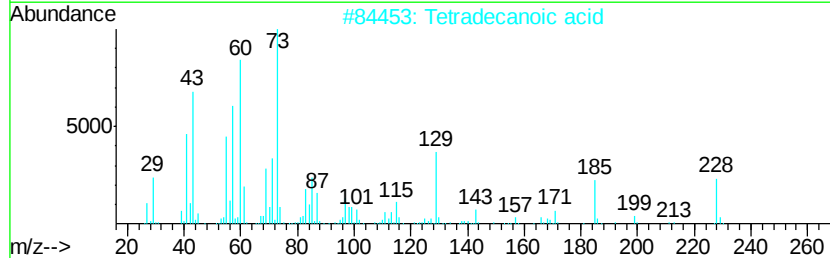
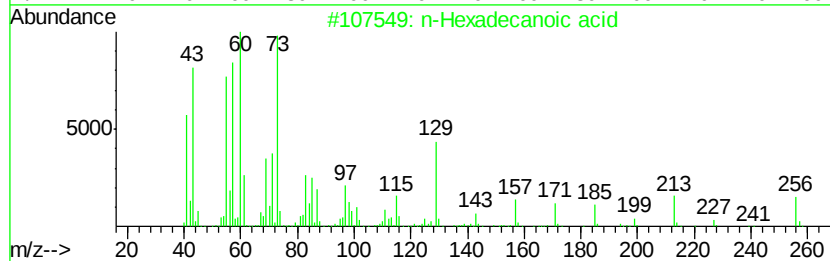
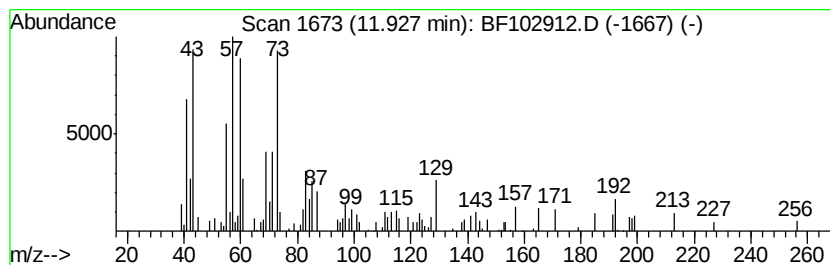
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.12 ng	137484	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102912.D
Acq On : 12 Feb 2018 11:29
Operator : SJ/JU
Sample : J1512-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-4252

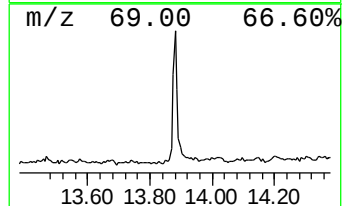
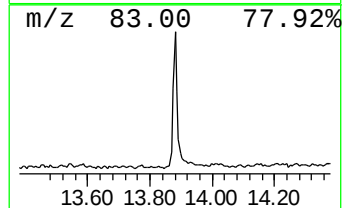
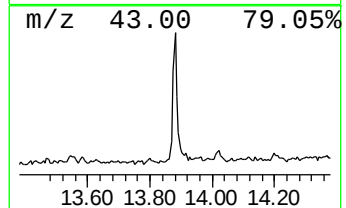
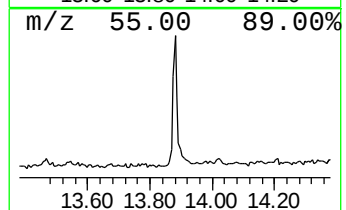
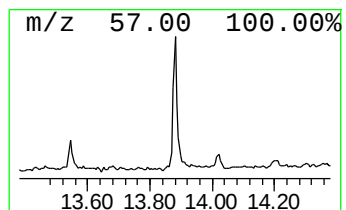
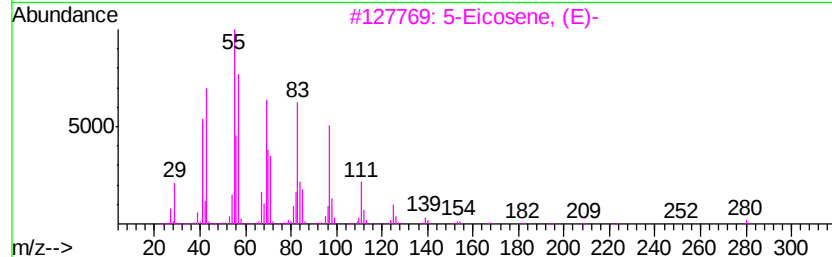
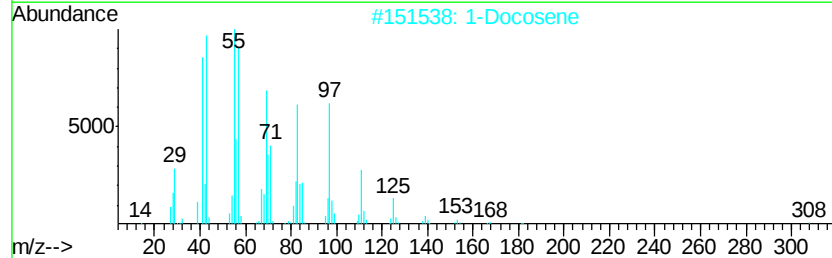
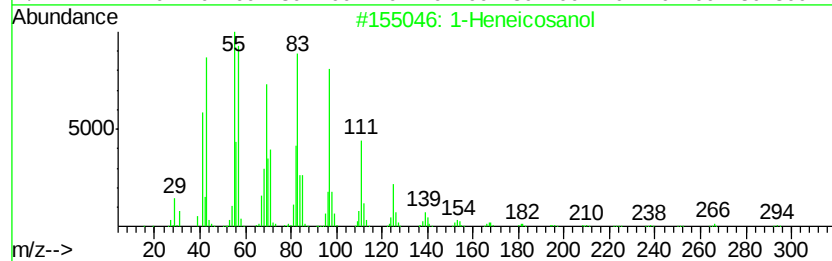
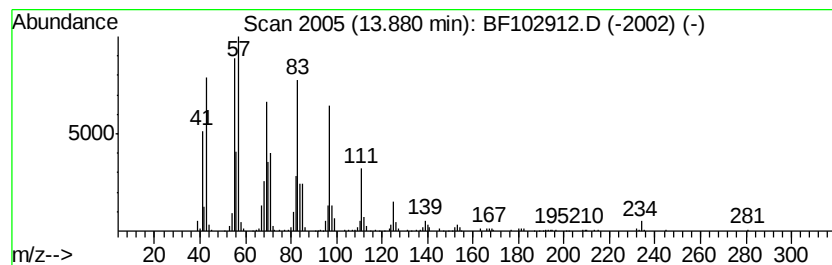
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.38 ng	415822	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		Octacosanol	410	C28H58O	000557-61-9	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102912.D
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Misc :
ALS Vial : 7 Sample Multiplier: 1

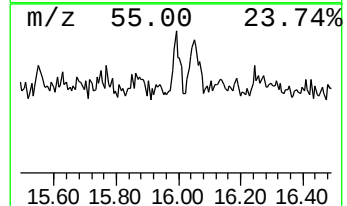
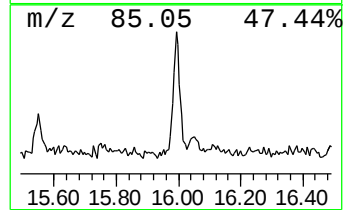
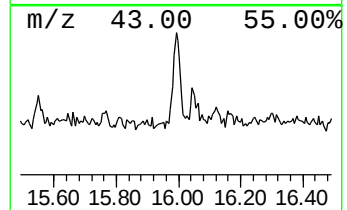
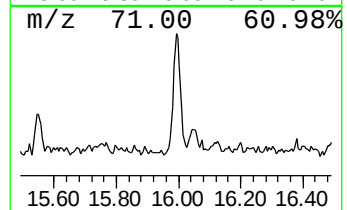
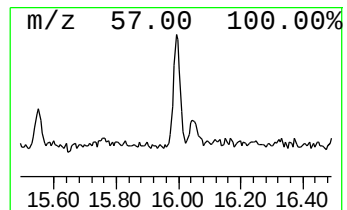
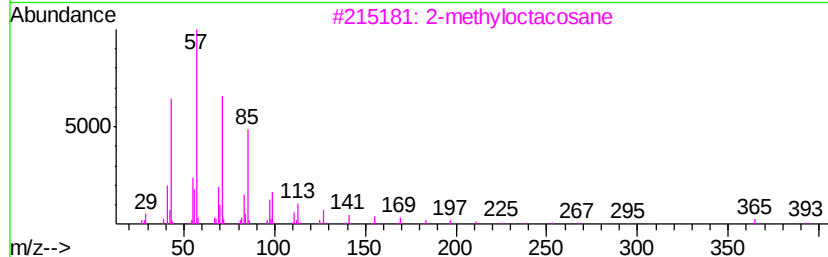
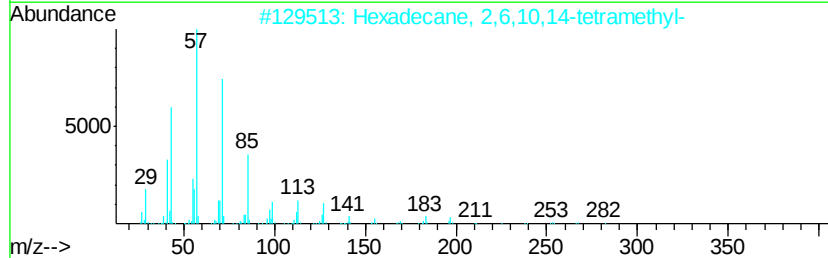
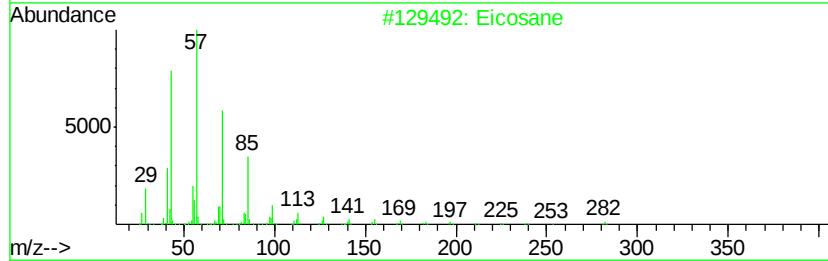
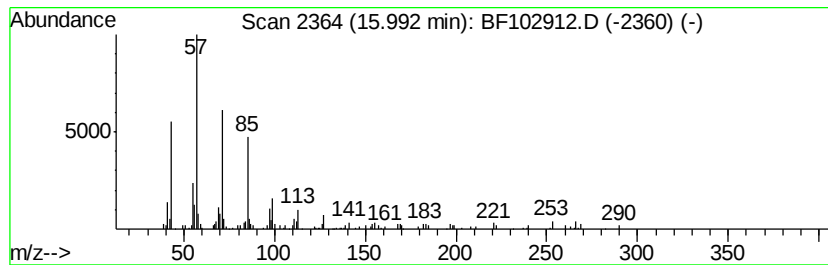
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.05 ng	112323	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 93
2	Hexadecane, 2,6,10,14-tetramethyl-		282 C20H42	000638-36-8 91
3	2-methyloctacosane		408 C29H60	1000376-72-8 90
4	Heneicosane		296 C21H44	000629-94-7 87
5	Hexacosane		366 C26H54	000630-01-3 86



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF021218\
Data File : BF102912.D
Acq On : 12 Feb 2018 11:29
Operator : SJ/JU
Sample : J1512-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-4252

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.18	11.1 ng		641769	1	6.89	1154080	20.0
2-Pentanone, 4-hy...	5.12	2.6 ng		148843	1	6.89	1154080	20.0
unknown6.66	6.66	69.3 ng		3996010	1	6.89	1154080	20.0
Hexadecane	9.85	2.2 ng		167940	3	9.92	1499660	20.0
n-Hexadecanoic acid	11.93	2.1 ng		137484	4	11.41	1297390	20.0
1-Heneicosanol	13.88	7.4 ng		415822	5	14.05	1126670	20.0
Eicosane	15.99	2.0 ng		112323	6	15.54	1097560	20.0