

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
 Data File : BF103246.D
 Acq On : 27 Feb 2018 4:07
 Operator : SJ/JU
 Sample : J1649-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CB-6-LINE-EW@4.5

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	18	rVB	1000854	1342172	35.06%	4.145%
2	5.110	510	514	531	rVB	129975	190234	4.97%	0.587%
3	5.498	576	580	592	rBV	3437715	3746296	97.87%	11.568%
4	6.510	747	752	771	rBV2	3159404	3827697	100.00%	11.820%
5	6.645	771	775	779	rBV	3469035	3552439	92.81%	10.970%
6	6.875	810	814	822	rBV	1063879	910730	23.79%	2.812%
7	7.028	836	840	844	rBV	2742439	2707449	70.73%	8.361%
8	7.439	905	910	913	rBV	2370596	2206490	57.65%	6.814%
9	8.157	1028	1032	1046	rBV	1325981	1174374	30.68%	3.626%
10	9.228	1210	1214	1218	rBV	3137197	3104831	81.11%	9.588%
11	9.298	1224	1226	1229	rVB	49697	41478	1.08%	0.128%
12	9.622	1276	1281	1289	rBV	233630	233670	6.10%	0.722%
13	9.833	1313	1317	1321	rBV	102682	95272	2.49%	0.294%
14	9.916	1327	1331	1337	rVB	1138690	1090177	28.48%	3.366%
15	10.327	1399	1401	1404	rVB	111995	96843	2.53%	0.299%
16	10.704	1462	1465	1476	rBV	1568034	1671303	43.66%	5.161%
17	10.804	1479	1482	1488	rVB	101720	91020	2.38%	0.281%
18	11.404	1580	1584	1592	rBV	998572	906682	23.69%	2.800%
19	11.916	1668	1671	1680	rBV3	34419	45963	1.20%	0.142%
20	12.792	1817	1820	1824	rBV	308012	278998	7.29%	0.862%
21	12.845	1824	1829	1831	rVV	53719	49625	1.30%	0.153%
22	12.868	1831	1833	1836	rVB	68478	56943	1.49%	0.176%
23	12.986	1849	1853	1857	rBV	2223009	2239865	58.52%	6.917%
24	13.498	1937	1940	1944	rVB	235985	208043	5.44%	0.642%
25	13.545	1944	1948	1950	rBV2	57341	54834	1.43%	0.169%
26	13.874	2000	2004	2012	rBV	326224	414129	10.82%	1.279%
27	14.051	2030	2034	2041	rBV	702297	727120	19.00%	2.245%
28	14.139	2046	2049	2052	rBV	70755	61999	1.62%	0.191%
29	14.192	2056	2058	2065	rVV	63913	67863	1.77%	0.210%
30	14.504	2108	2111	2118	rBV2	83103	103360	2.70%	0.319%
31	14.804	2158	2162	2170	rBV3	335175	455947	11.91%	1.408%
32	15.157	2219	2222	2227	rVB2	55035	56600	1.48%	0.175%
33	15.551	2284	2289	2297	rBV	363857	573349	14.98%	1.770%

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Misc :
ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId :
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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

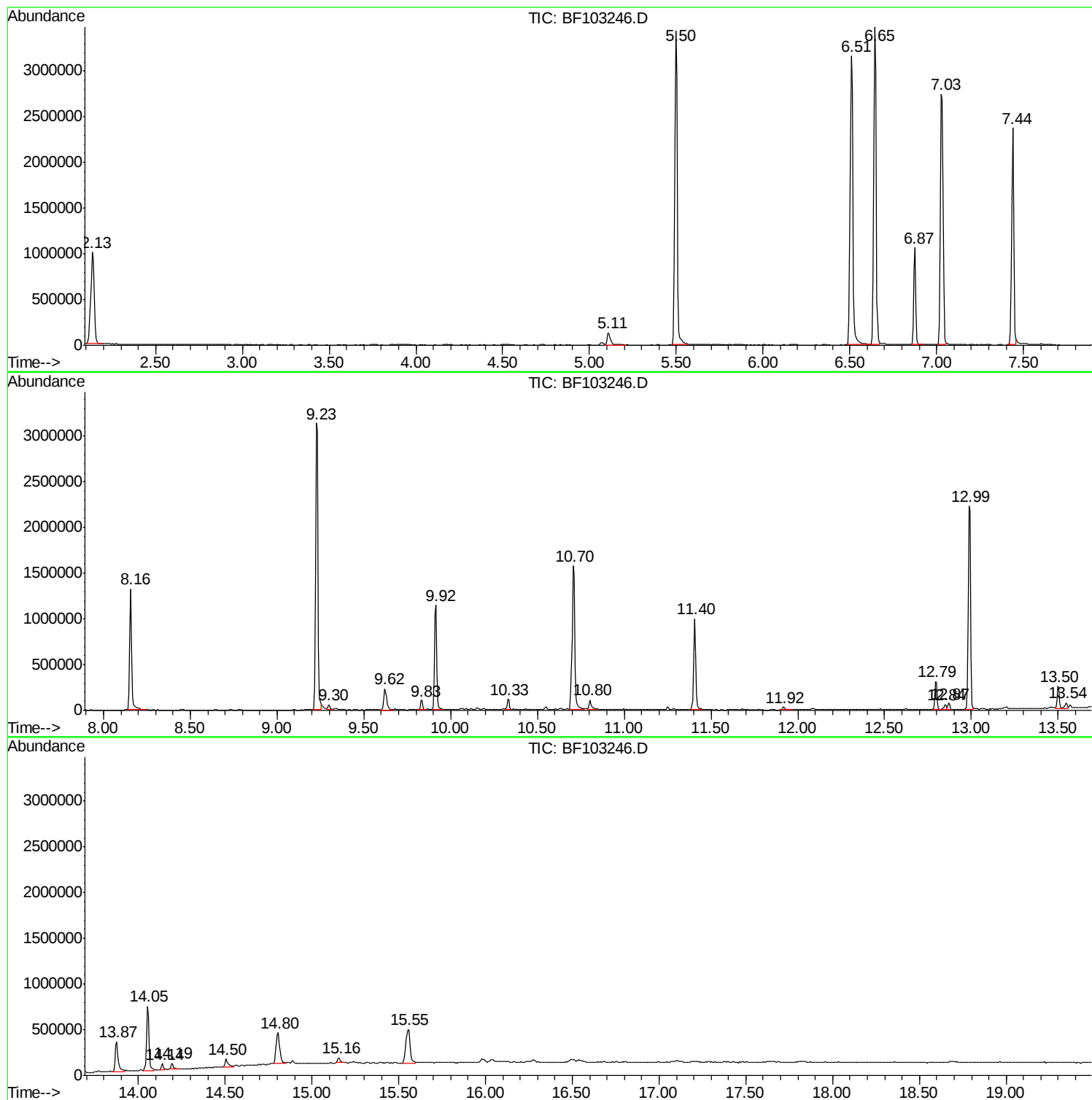
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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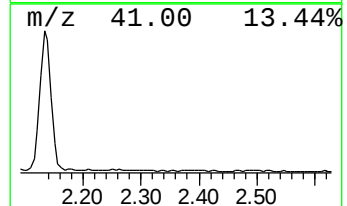
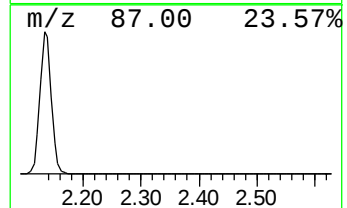
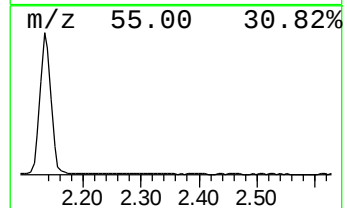
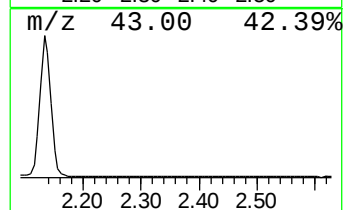
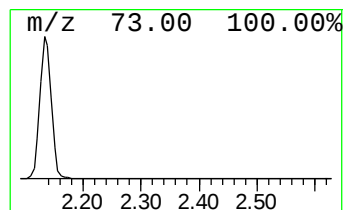
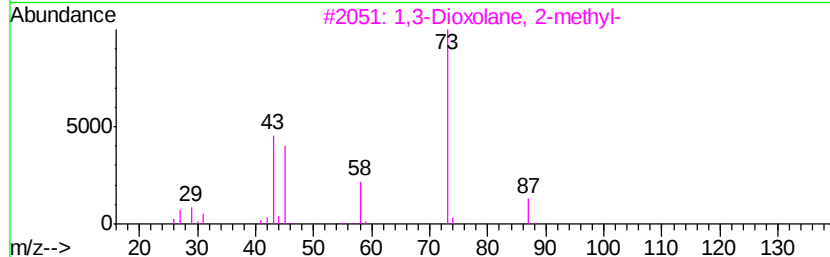
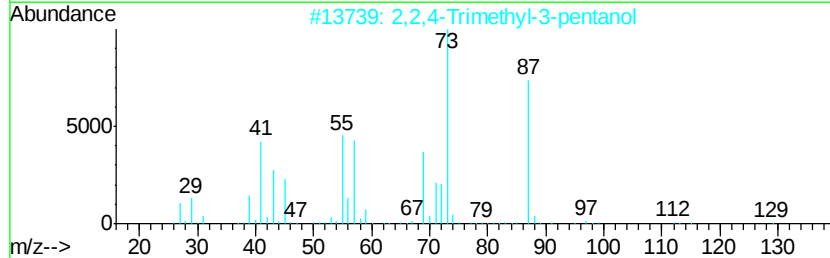
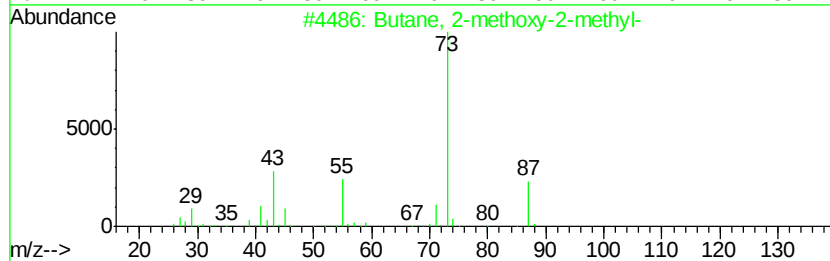
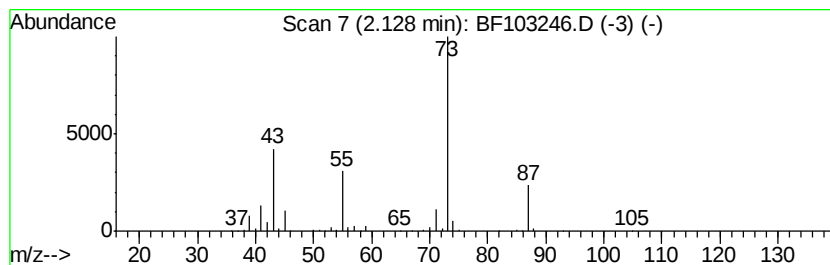
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	29.47 ng	1342170	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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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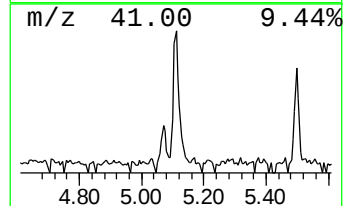
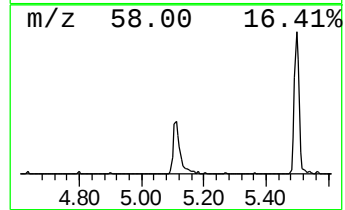
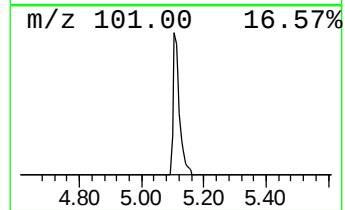
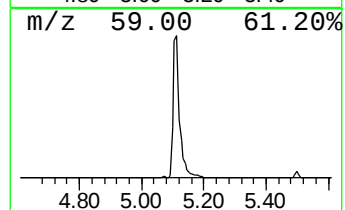
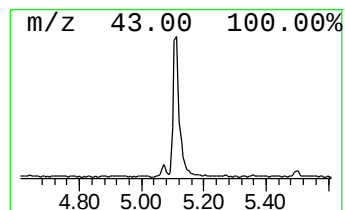
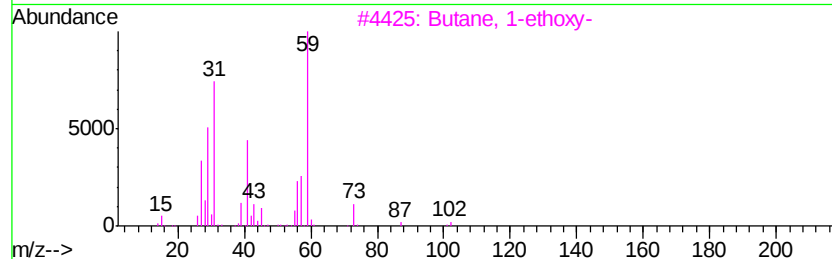
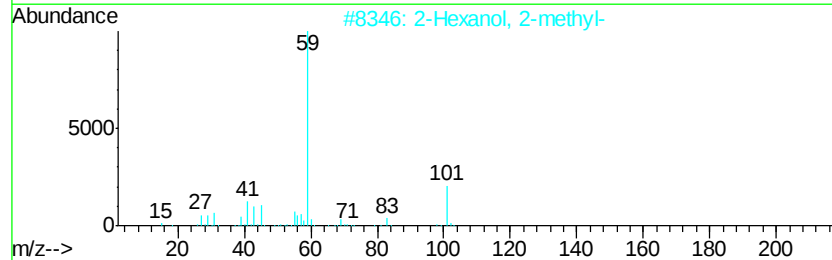
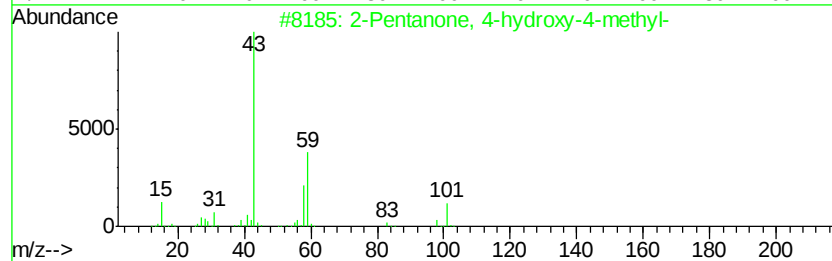
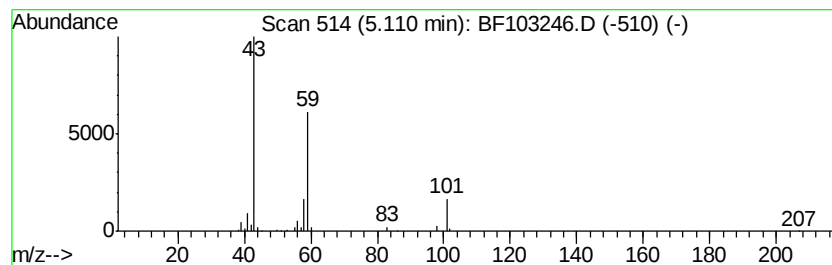
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.18 ng	190234	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	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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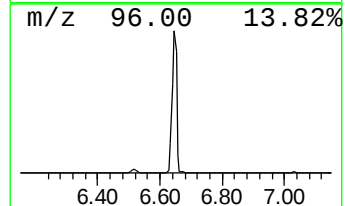
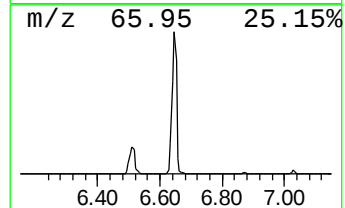
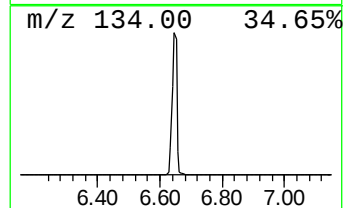
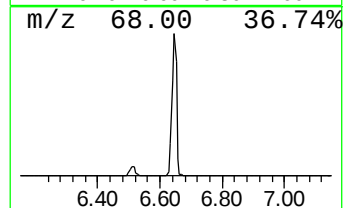
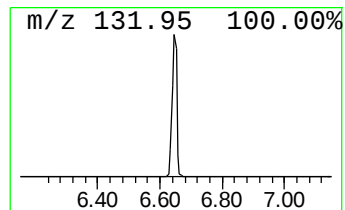
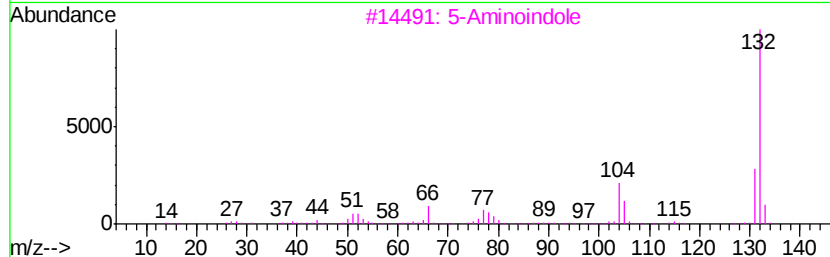
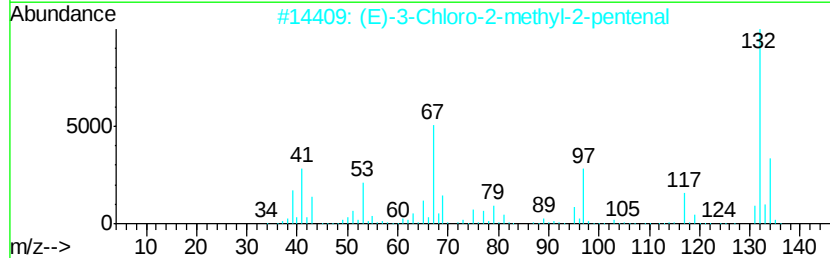
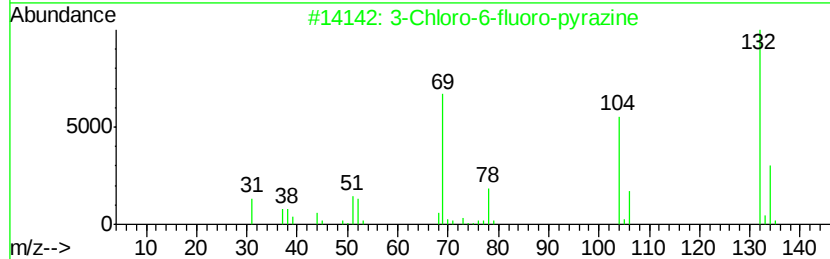
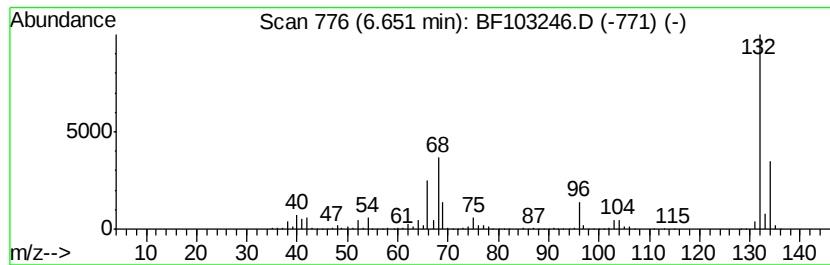
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	78.01 ng	3552440	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-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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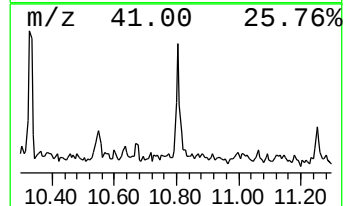
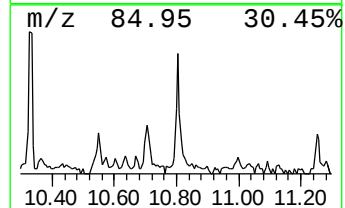
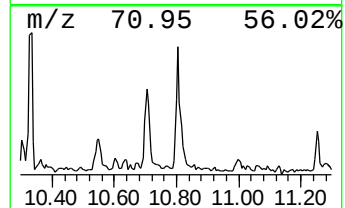
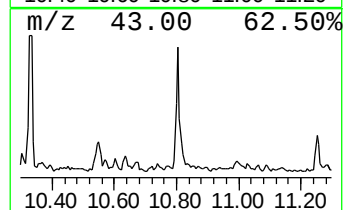
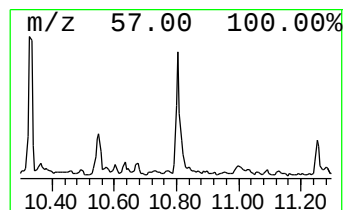
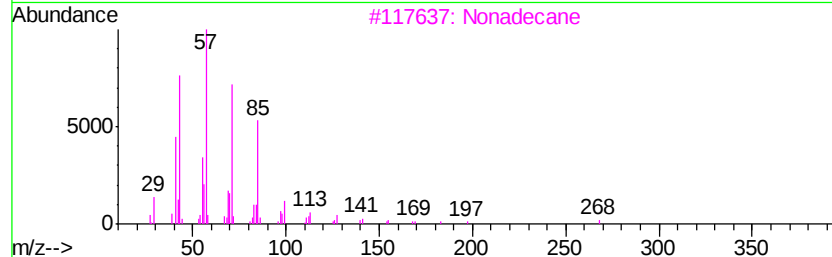
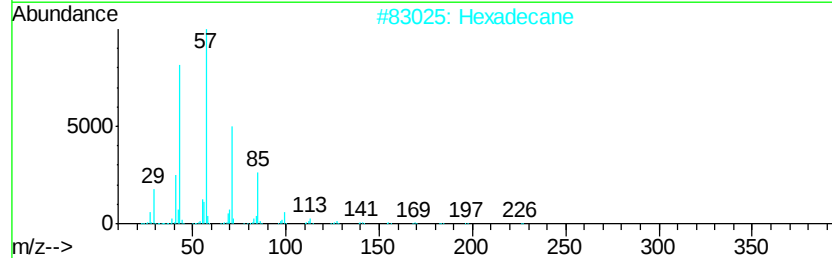
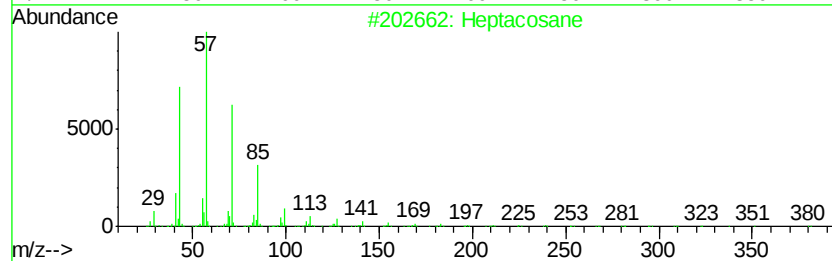
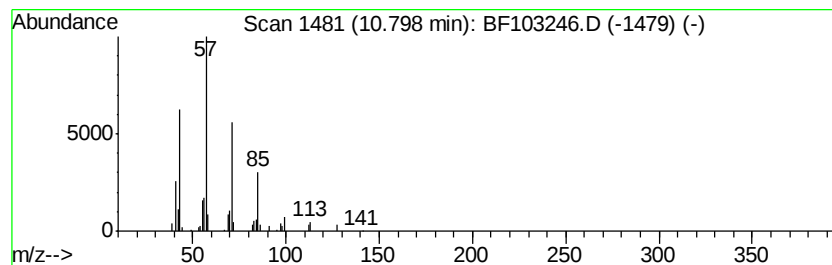
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.80	2.01 ng	91020	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	Nonadecane	268	C19H40	000629-92-5	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Heneicosane	296	C21H44	000629-94-7	83



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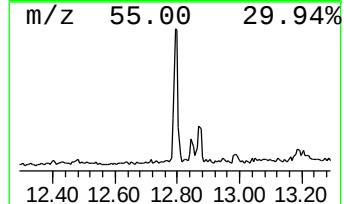
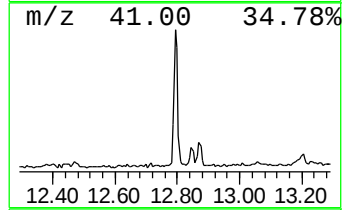
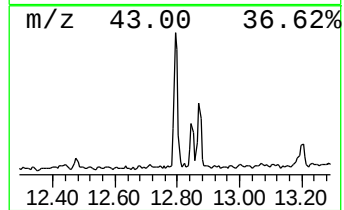
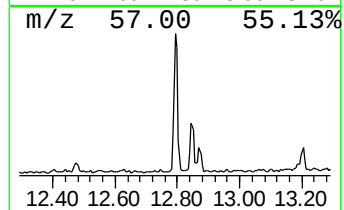
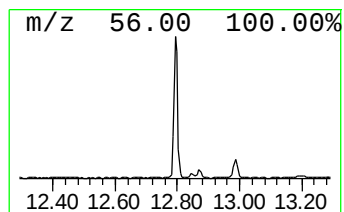
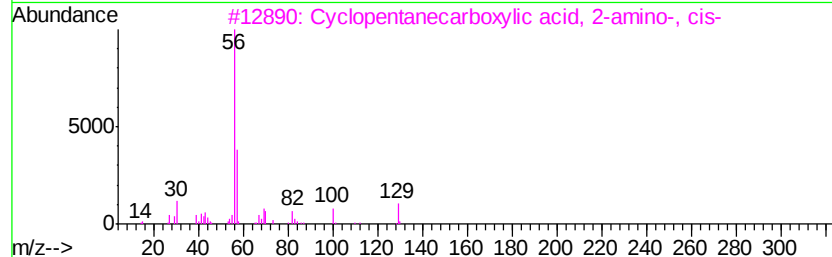
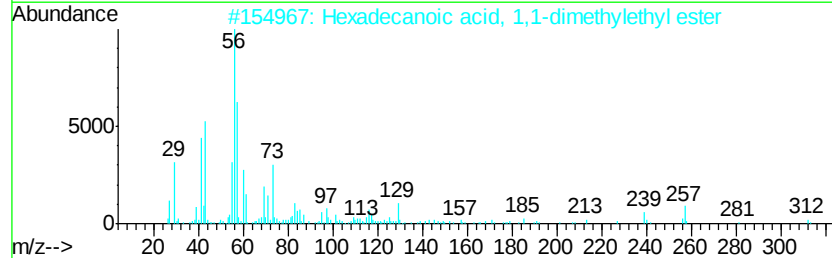
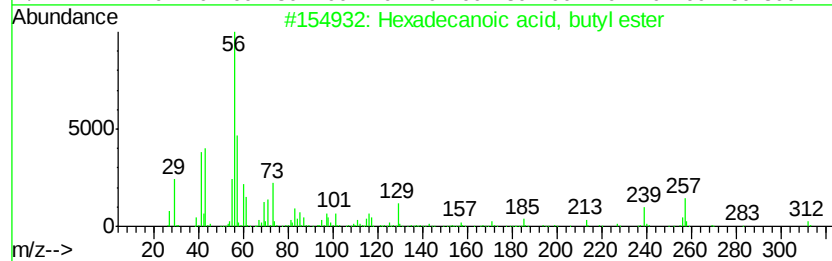
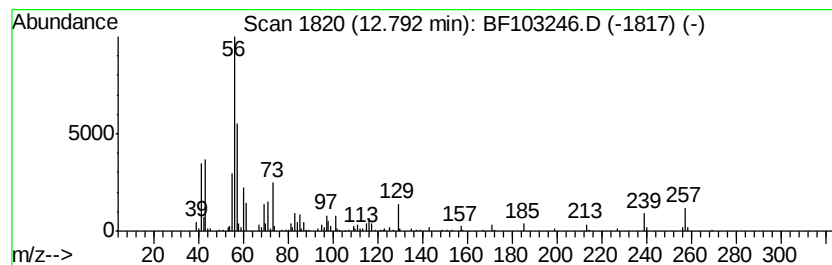
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	7.67 ng	278998	Chrysene-d12	14.05

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	58
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38



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Misc :
ALS Vial : 27 Sample Multiplier: 1

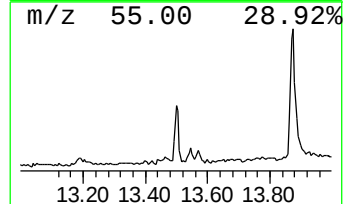
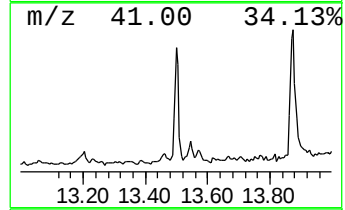
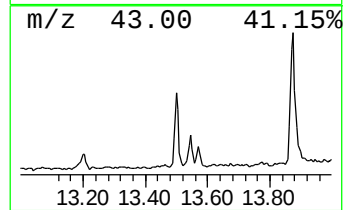
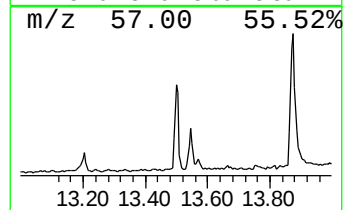
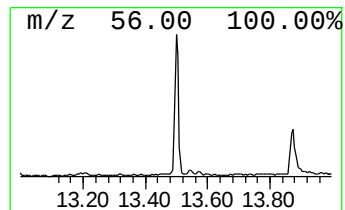
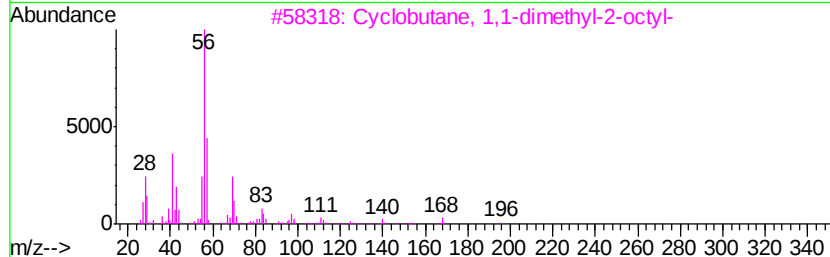
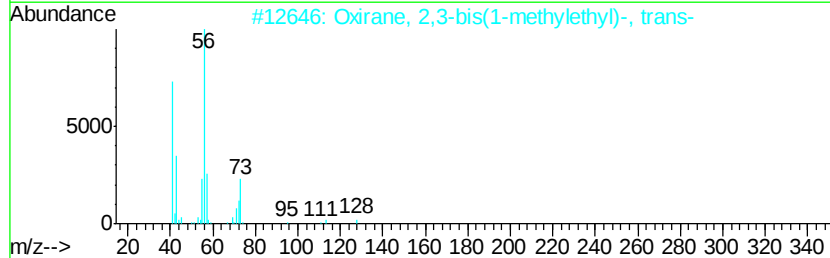
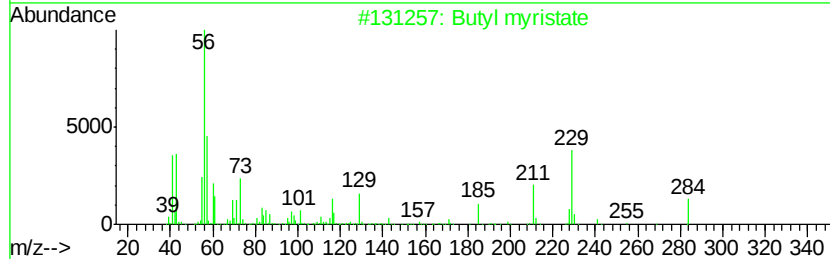
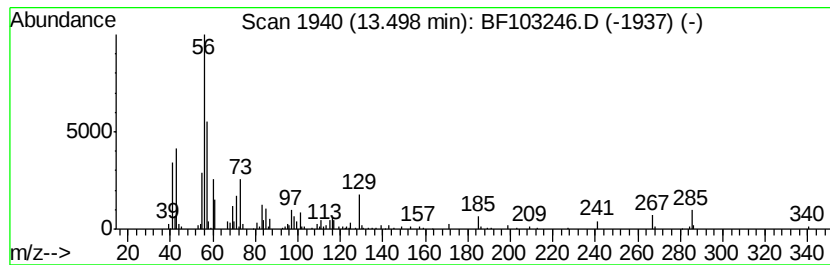
Instrument :
BNA_F
ClientSampleId :
CB-6-LINE-EW@4.5

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 7 Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.72 ng	208043	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butyl myristate	284 C18H36O2	000110-36-1 86
2		Oxirane, 2,3-bis(1-methylethyl)-...	128 C8H16O	054644-32-5 43
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196 C14H28	062338-30-1 38
4		Trifluoroacetic acid, 4-methylpe...	198 C8H13F3O2	000327-71-9 37
5		1-Hexene, 2,5-dimethyl-	112 C8H16	006975-92-4 35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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Acq On : 27 Feb 2018 4:07
Operator : SJ/JU
Sample : J1649-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

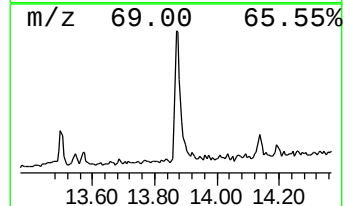
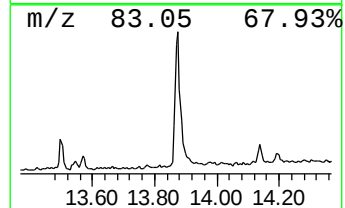
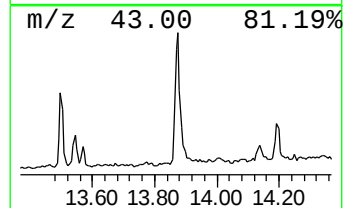
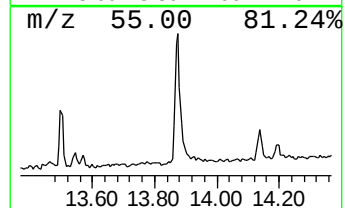
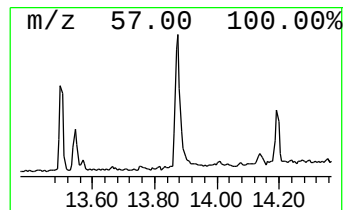
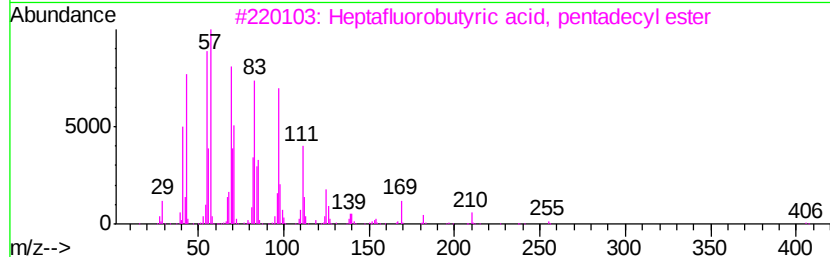
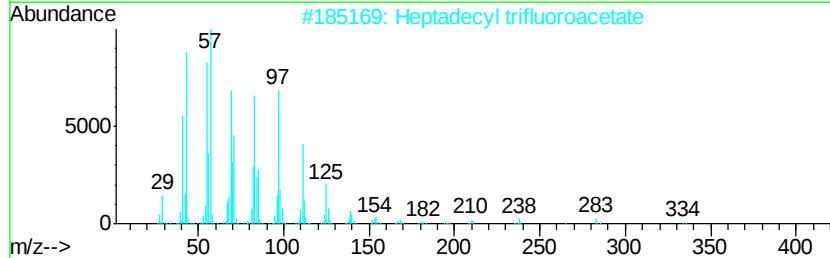
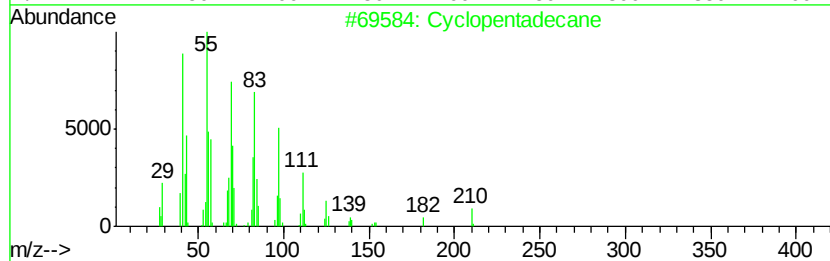
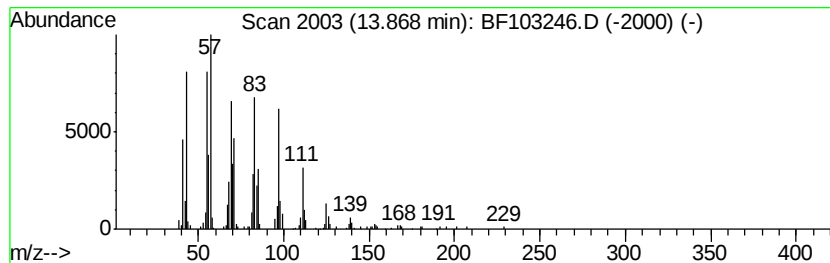
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ClientSampleId :
CB-6-LINE-EW@4.5

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 8 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.39 ng	414129	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclopentadecane	210 C15H30	000295-48-7 96
2		Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0 94
3		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 94
4		1-Heneicosanol	312 C21H44O	015594-90-8 93
5		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103246.D
Acq On : 27 Feb 2018 4:07
Operator : SJ/JU
Sample : J1649-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

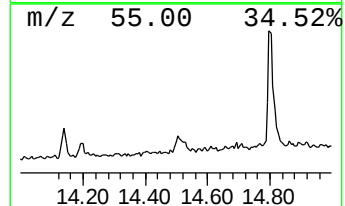
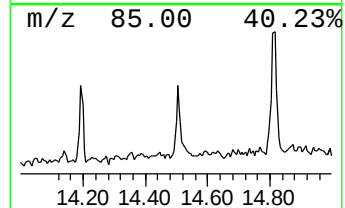
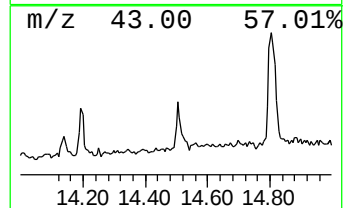
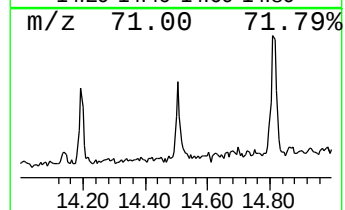
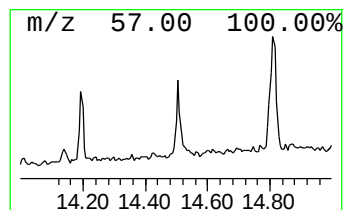
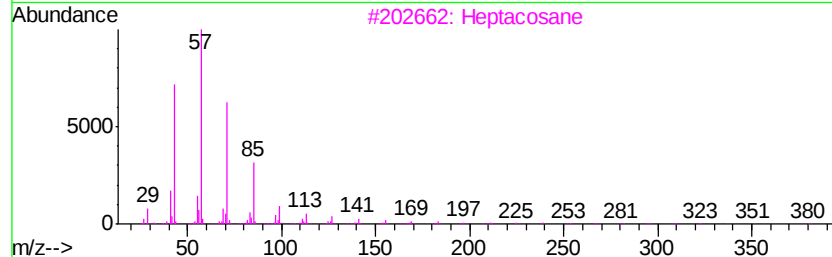
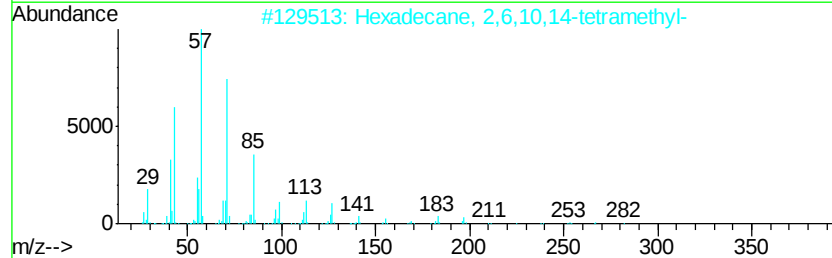
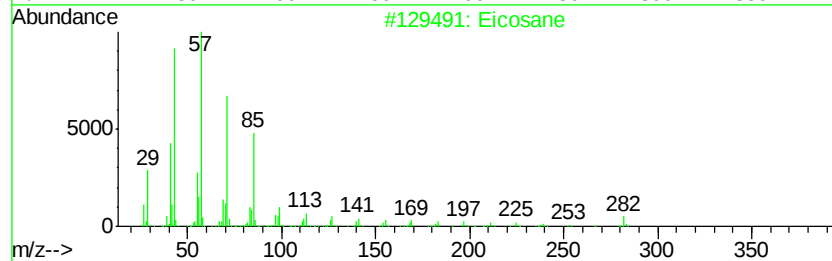
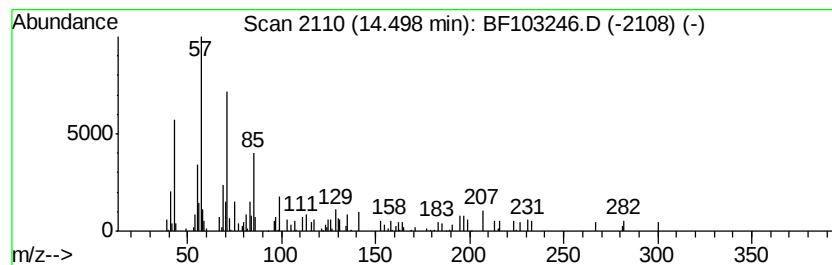
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.84 ng	103360	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 86
2	Hexadecane, 2,6,10,14-tetramethyl-		282 C20H42	000638-36-8 83
3	Heptacosane		380 C27H56	000593-49-7 74
4	Nonadecane		268 C19H40	000629-92-5 64
5	Heptadecane, 2,6,10,15-tetramethyl-		296 C21H44	054833-48-6 64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
Data File : BF103246.D
Acq On : 27 Feb 2018 4:07
Operator : SJ/JU
Sample : J1649-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CB-6-LINE-EW@4.5

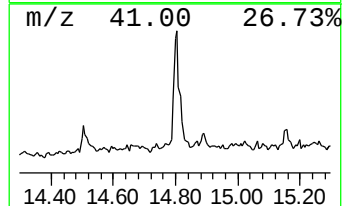
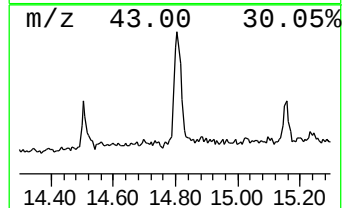
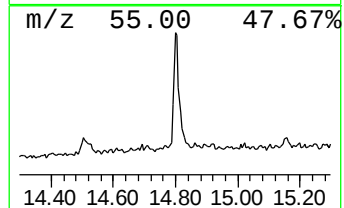
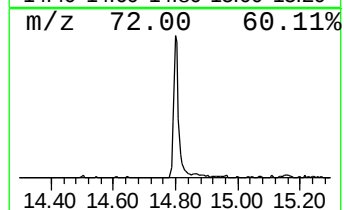
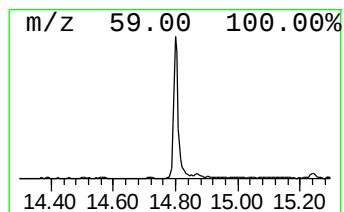
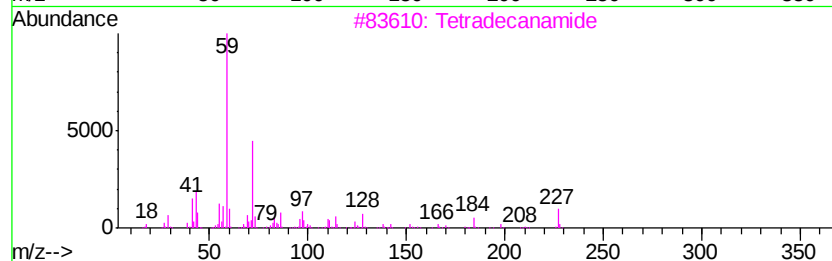
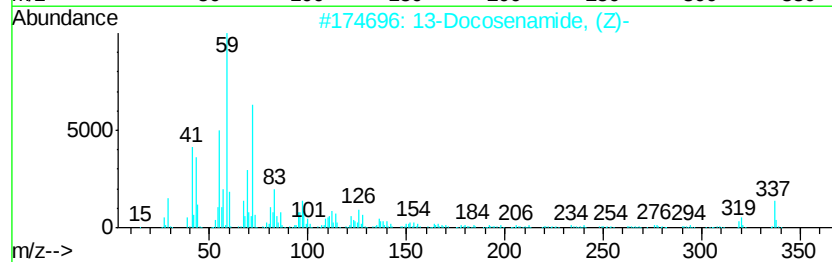
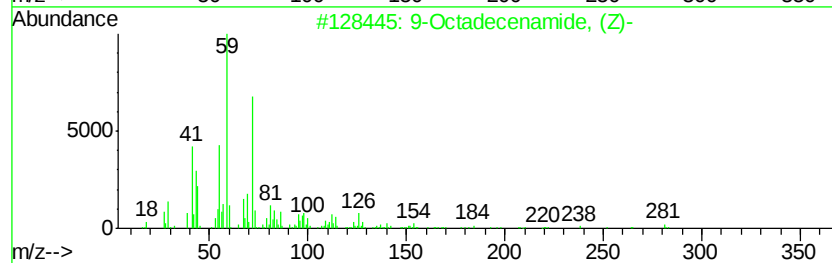
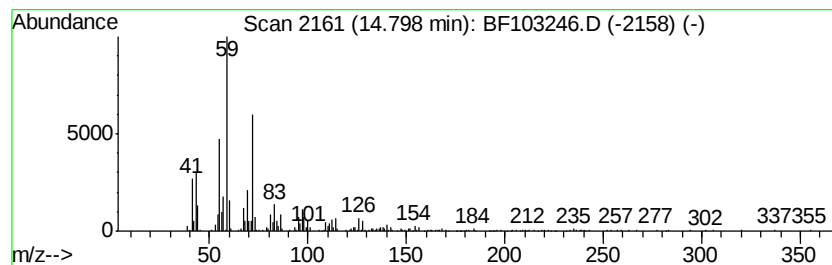
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	15.90 ng	455947	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3		Tetradecanamide	227	C14H29NO	000638-58-4	83
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103246.D
Acq On : 27 Feb 2018 4:07
Operator : SJ/JU
Sample : J1649-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CB-6-LINE-EW@4.5

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	29.5	ng	1342170	1	6.87	910730	20.0
2-Pentanone, 4-hy...	5.11	4.2	ng	190234	1	6.87	910730	20.0
unknown6.65	6.65	78.0	ng	3552440	1	6.87	910730	20.0
Heptacosane	10.80	2.0	ng	91020	4	11.40	906682	20.0
Hexadecanoic acid...	12.79	7.7	ng	278998	5	14.05	727120	20.0
Butyl myristate	13.50	5.7	ng	208043	5	14.05	727120	20.0
Cyclopentadecane	13.87	11.4	ng	414129	5	14.05	727120	20.0
Eicosane	14.50	2.8	ng	103360	5	14.05	727120	20.0
9-Octadecenamide, ...	14.80	15.9	ng	455947	6	15.56	573349	20.0