

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
 Data File : BF102863.D
 Acq On : 8 Feb 2018 18:28
 Operator : SJ/JU
 Sample : J1470-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-10

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	2.151	6	11	16	rVB	399158	498886	10.43%	1.229%
2	5.116	512	515	524	rVB	130748	160448	3.35%	0.395%
3	5.504	576	581	584	rBV	4736515	4784895	100.00%	11.791%
4	6.516	747	753	756	rBV	4323473	4747314	99.21%	11.698%
5	6.657	772	777	780	rBV	4749125	4620388	96.56%	11.386%
6	6.886	812	816	819	rBV	1626781	1299410	27.16%	3.202%
7	7.045	838	843	846	rBV	3215082	3117662	65.16%	7.683%
8	7.451	906	912	915	rBV	3032016	3063238	64.02%	7.549%
9	7.528	921	925	934	rVB	60458	77730	1.62%	0.192%
10	8.169	1030	1034	1037	rBV	1965269	1622479	33.91%	3.998%
11	9.245	1212	1217	1220	rBV	3426666	3411076	71.29%	8.406%
12	9.316	1226	1229	1232	rVB	111001	85989	1.80%	0.212%
13	9.633	1279	1283	1286	rBV	478589	419480	8.77%	1.034%
14	9.845	1312	1319	1323	rBV	265764	233984	4.89%	0.577%
15	9.921	1329	1332	1337	rBV	1501817	1480645	30.94%	3.649%
16	10.169	1371	1374	1378	rVB3	51436	49550	1.04%	0.122%
17	10.321	1397	1400	1402	rBV	85576	74966	1.57%	0.185%
18	10.345	1402	1404	1407	rVB	266234	202014	4.22%	0.498%
19	10.569	1437	1442	1444	rBV	68578	87988	1.84%	0.217%
20	10.716	1463	1467	1477	rVB	1935612	1953106	40.82%	4.813%
21	10.821	1482	1485	1494	rVB	199507	240183	5.02%	0.592%
22	11.268	1558	1561	1563	rBV	138490	111615	2.33%	0.275%
23	11.298	1563	1566	1572	rVB2	45815	53153	1.11%	0.131%
24	11.410	1582	1585	1589	rBV	1181407	1148796	24.01%	2.831%
25	11.692	1630	1633	1636	rBV	74481	69588	1.45%	0.171%
26	11.927	1670	1673	1676	rBV	93907	86825	1.81%	0.214%
27	12.104	1699	1703	1705	rBV	59833	49366	1.03%	0.122%
28	12.810	1820	1823	1827	rBV	96671	85086	1.78%	0.210%
29	12.998	1850	1855	1858	rBV	2437823	2228848	46.58%	5.492%
30	13.468	1931	1935	1945	rBV	603366	737366	15.41%	1.817%
31	13.545	1945	1948	1953	rBV	95753	95272	1.99%	0.235%
32	13.880	2002	2005	2012	rBV	644563	622460	13.01%	1.534%
33	14.051	2031	2034	2038	rBV	1061057	1056890	22.09%	2.604%
34	14.515	2110	2113	2118	rBV	68332	81135	1.70%	0.200%

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Instrument :
BNA_F
ClientSampleId :
3N-10

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	14.804	2158	2162	2171	rBV	530450	709059	14.82%	1.747%
36	15.162	2220	2223	2226	rBV	94986	107978	2.26%	0.266%
37	15.539	2282	2287	2296	rVB2	695555	986420	20.62%	2.431%
38	15.998	2362	2365	2369	rVB	87781	119432	2.50%	0.294%

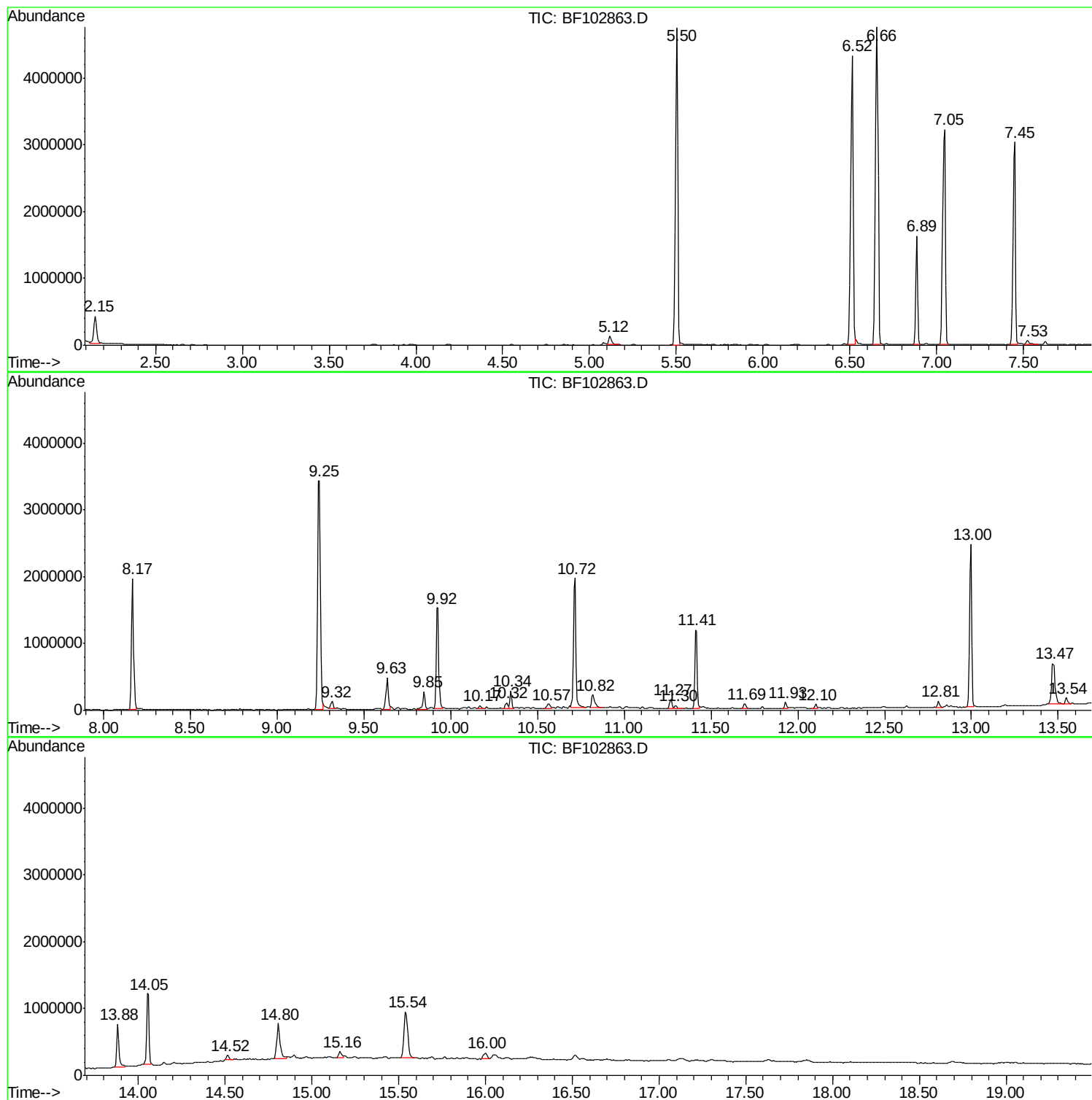
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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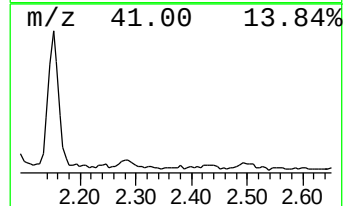
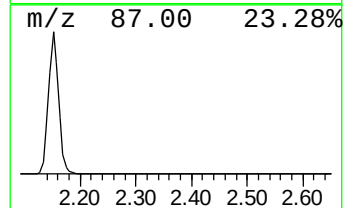
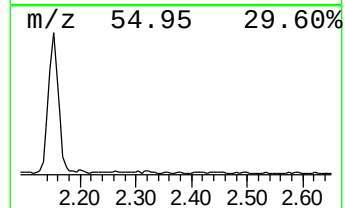
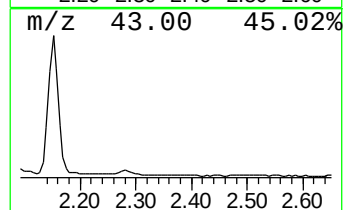
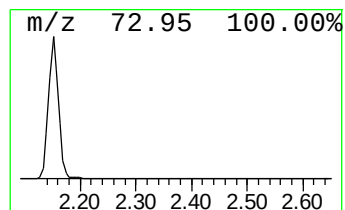
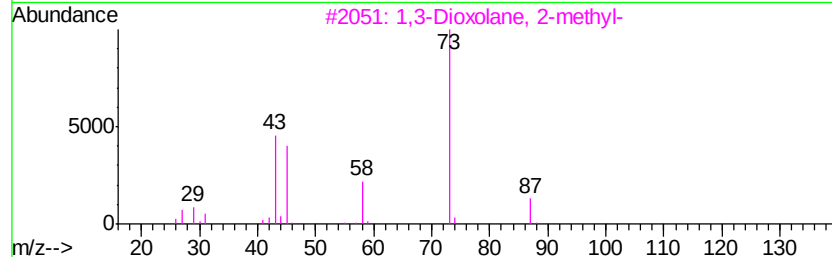
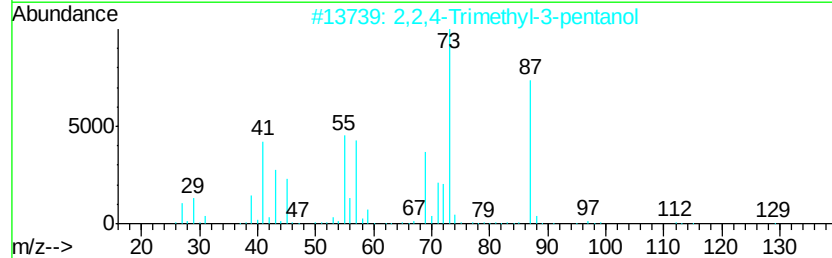
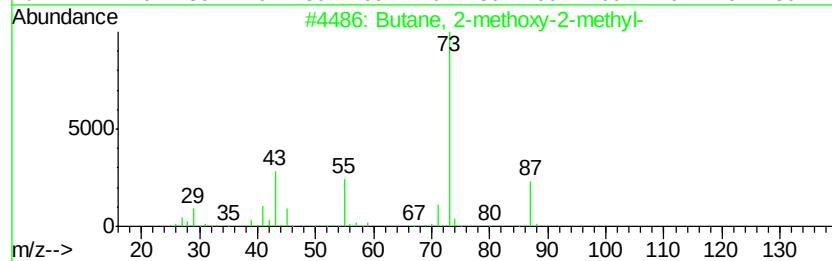
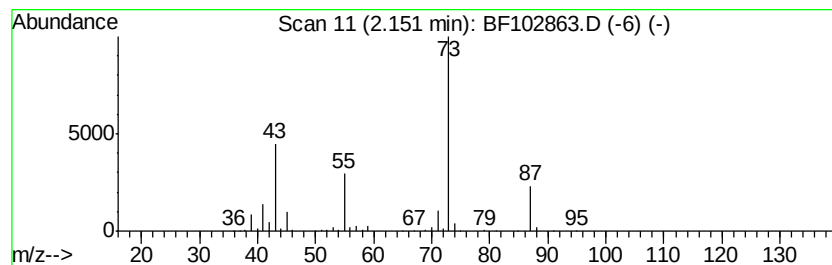
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	7.68 ng	498886	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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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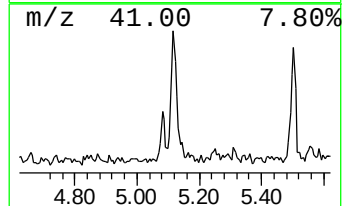
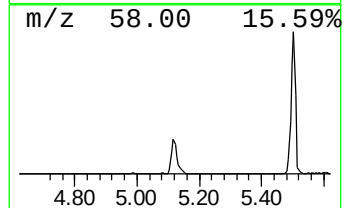
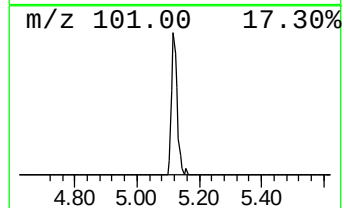
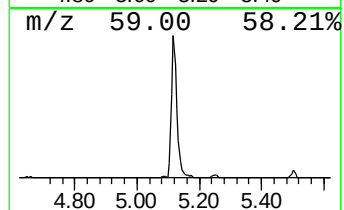
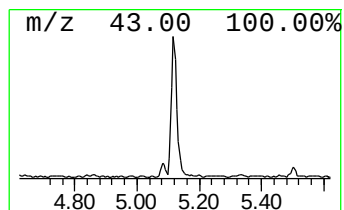
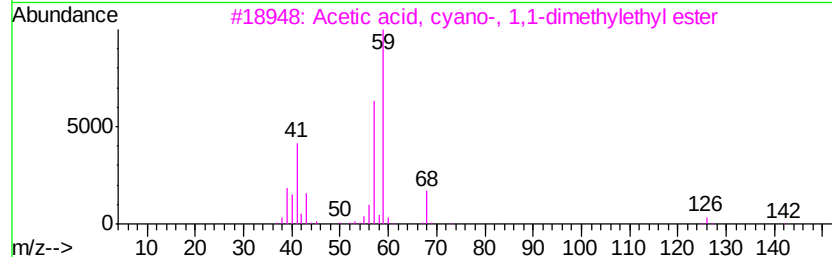
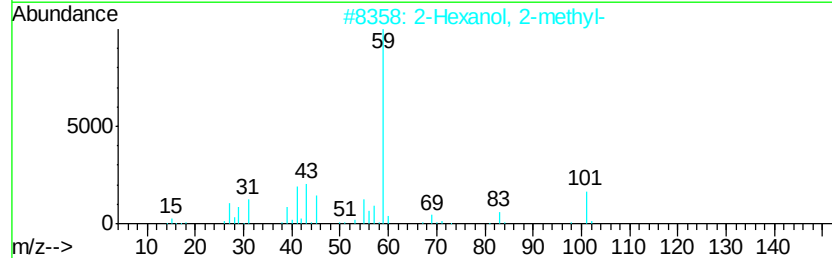
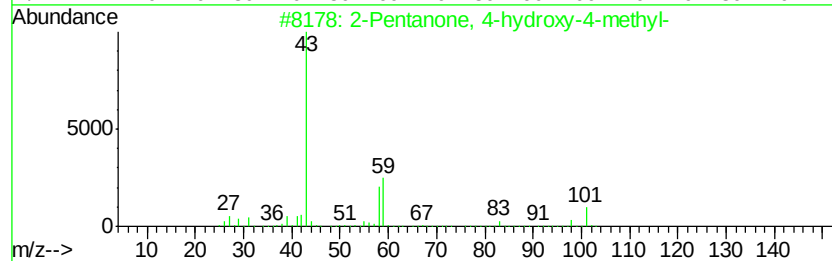
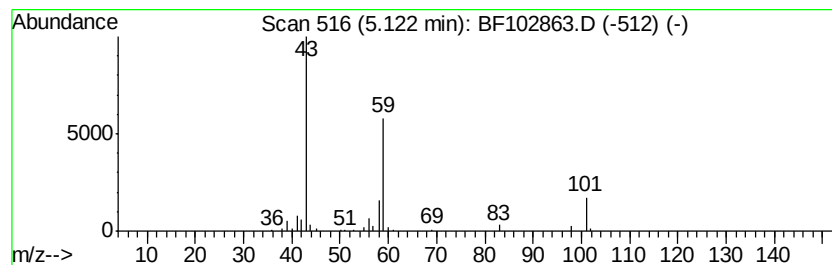
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.47 ng	160448	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			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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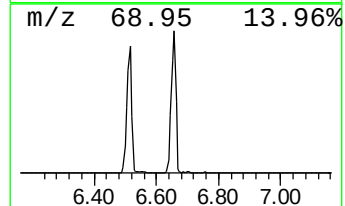
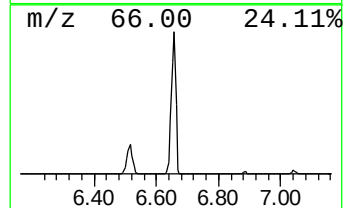
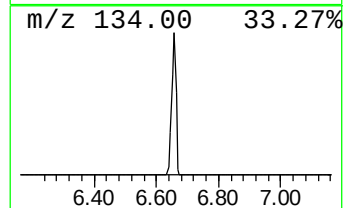
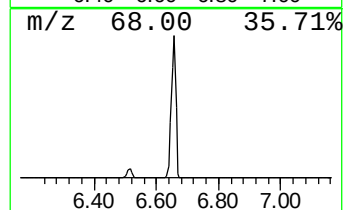
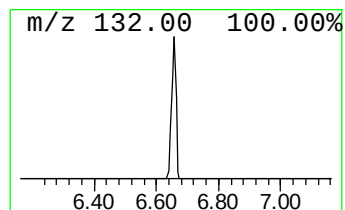
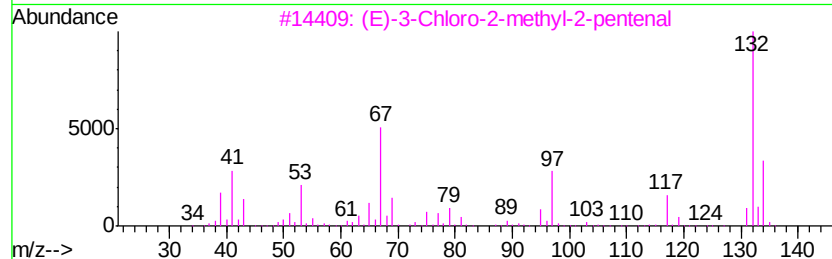
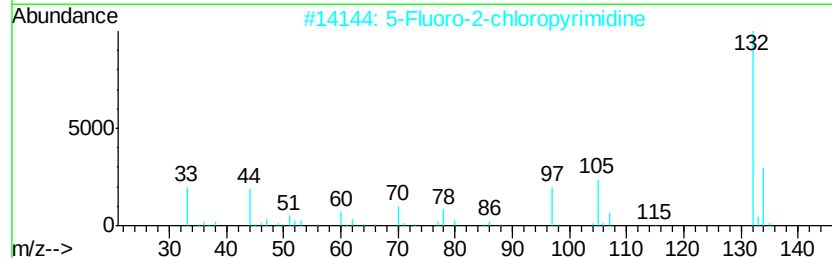
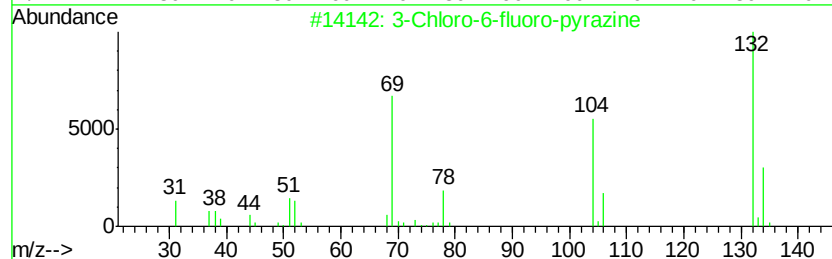
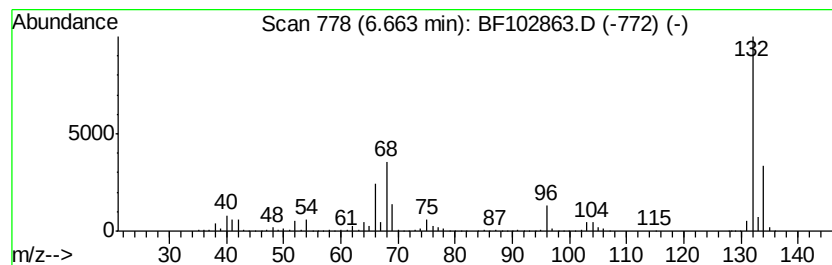
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.12 ng	4620390	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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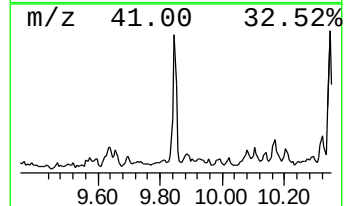
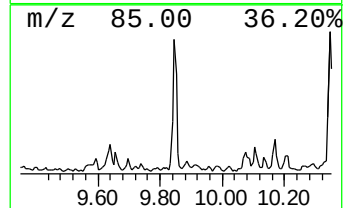
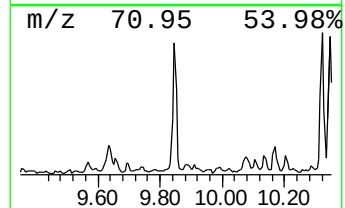
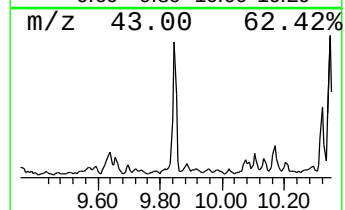
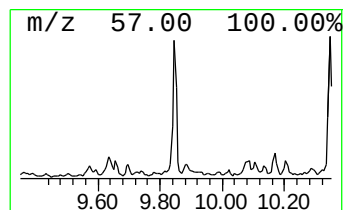
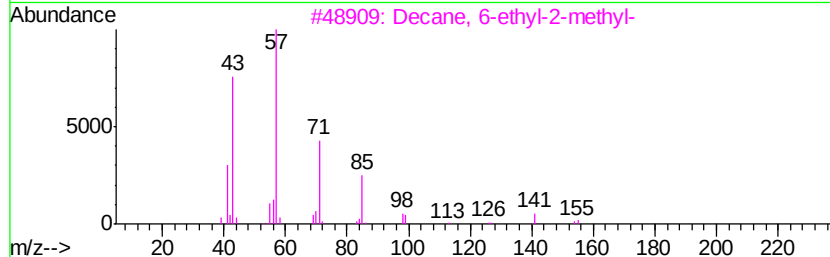
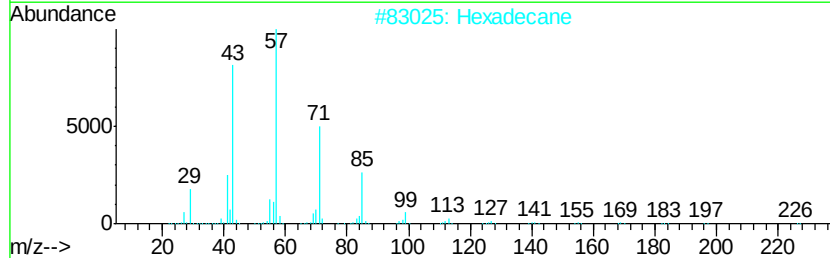
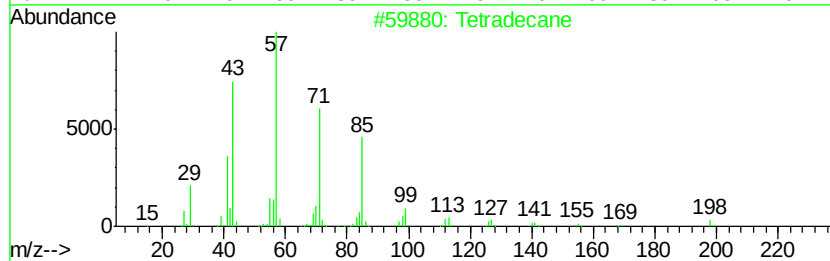
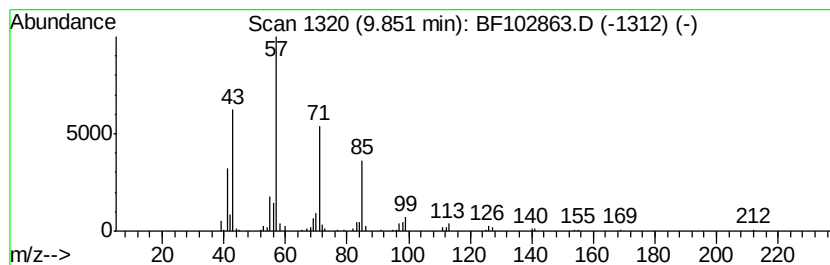
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	3.16 ng	233984	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	90
2		Hexadecane	226	C16H34	000544-76-3	90
3		Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
5		Nonane, 5-butyl-	184	C13H28	017312-63-9	80



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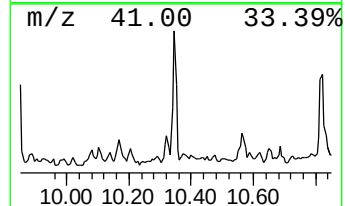
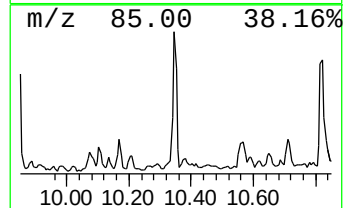
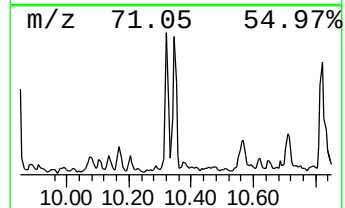
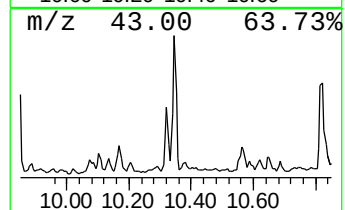
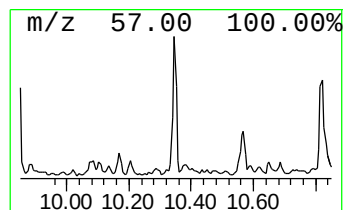
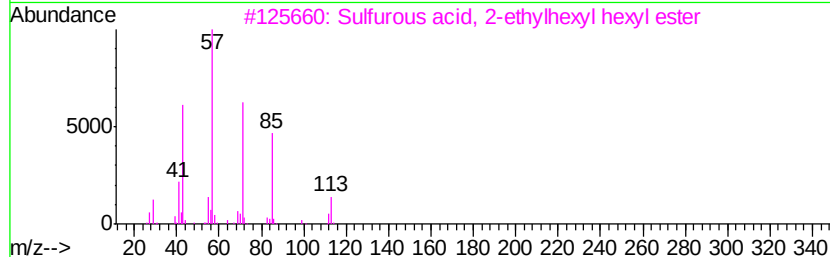
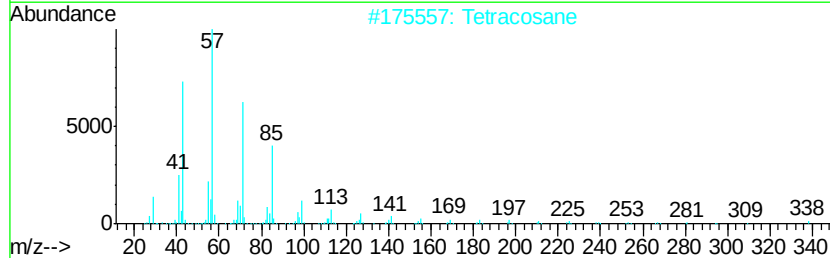
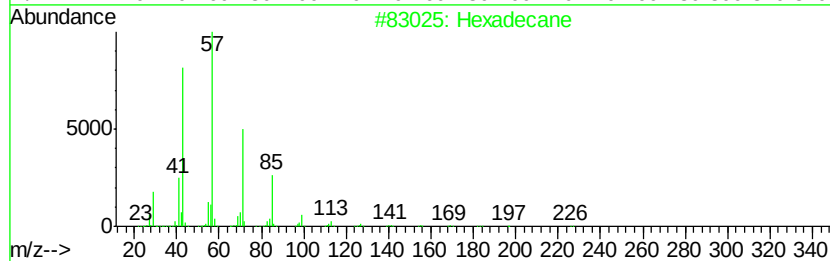
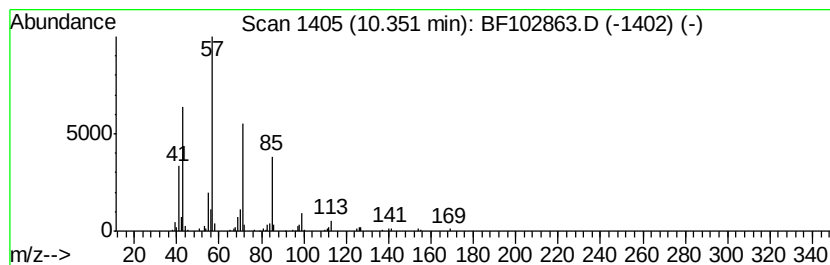
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Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.73 ng	202014	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tetracosane	338 C24H50	000646-31-1	86
3	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	80
4	2-Bromo dodecane	248 C12H25Br	013187-99-0	78
5	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	78



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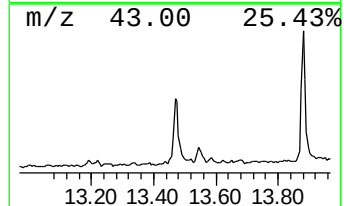
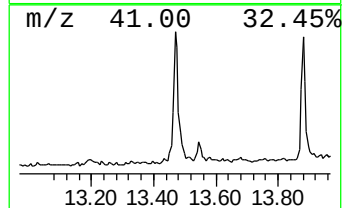
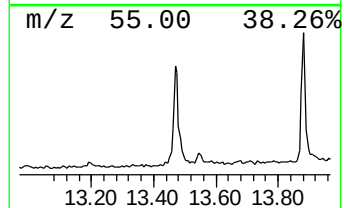
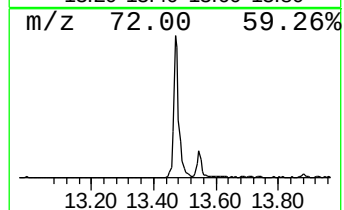
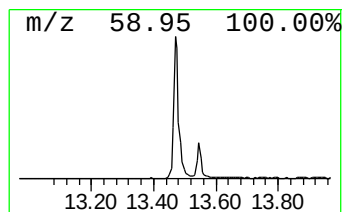
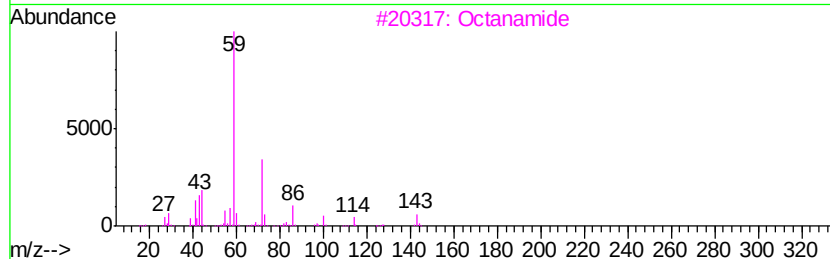
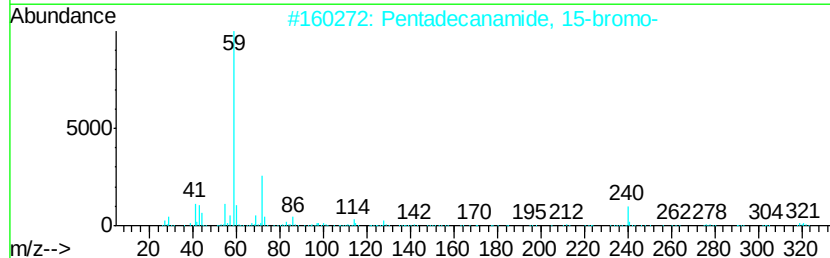
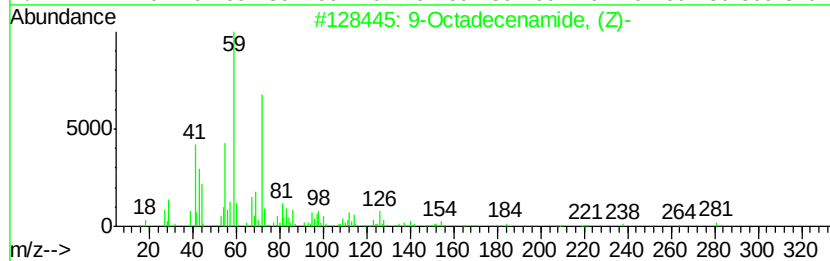
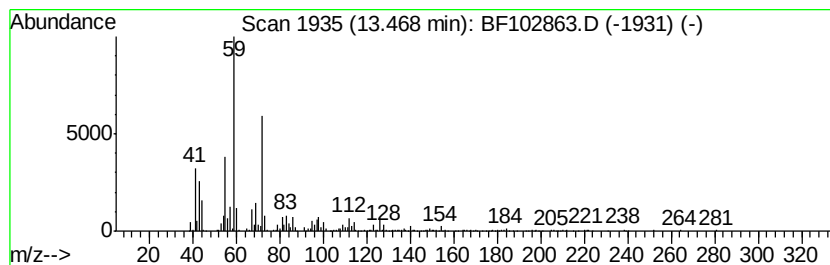
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	13.95 ng	737366	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
3		Octanamide	143	C8H17NO	000629-01-6	56
4		Hexadecanamide	255	C16H33NO	000629-54-9	56
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102863.D
Acq On : 8 Feb 2018 18:28
Operator : SJ/JU
Sample : J1470-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-10

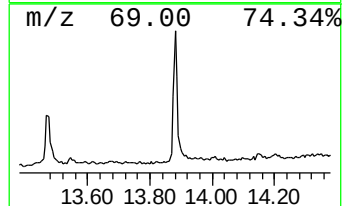
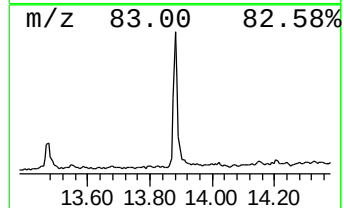
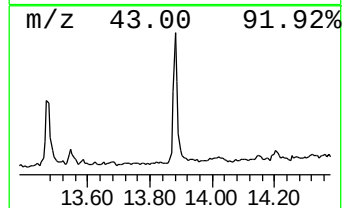
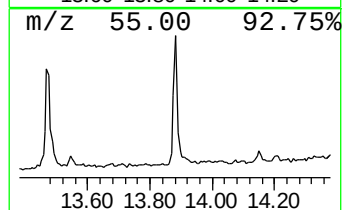
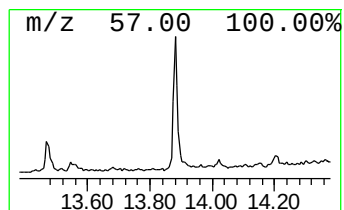
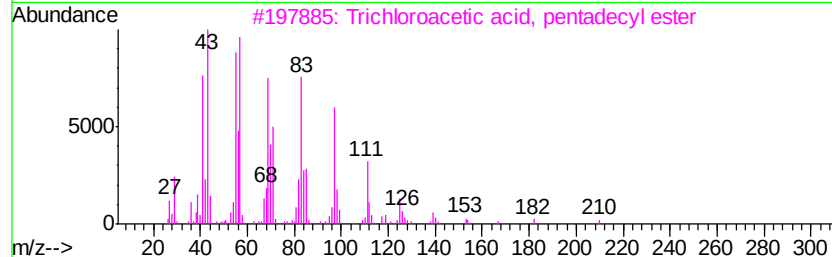
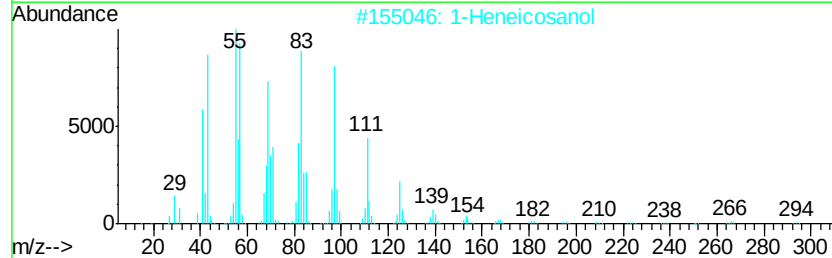
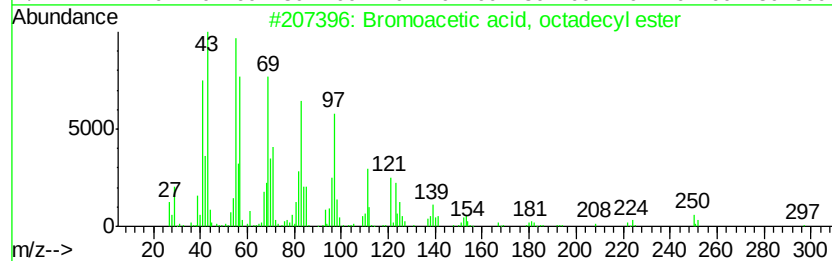
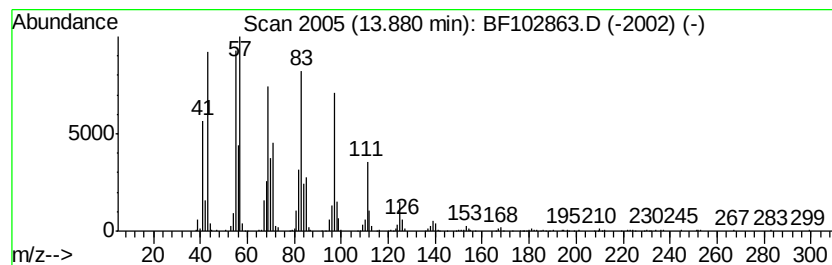
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	11.78 ng	622460	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5		Cyclopentadecane	210	C15H30	000295-48-7	92



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
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Operator : SJ/JU
Sample : J1470-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

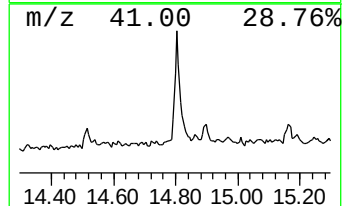
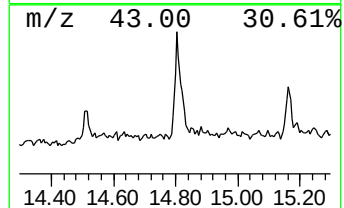
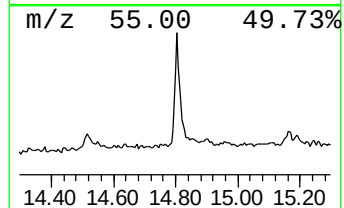
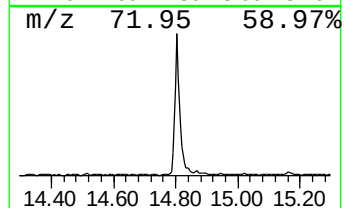
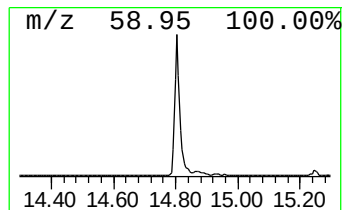
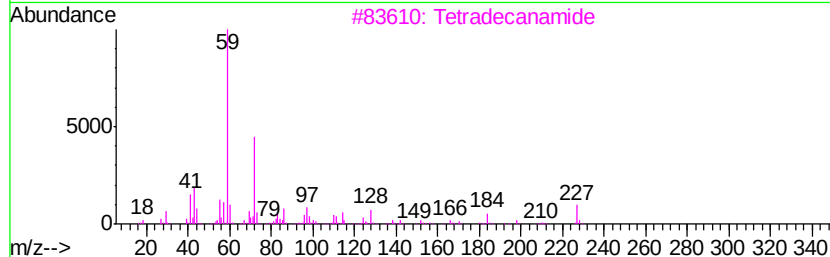
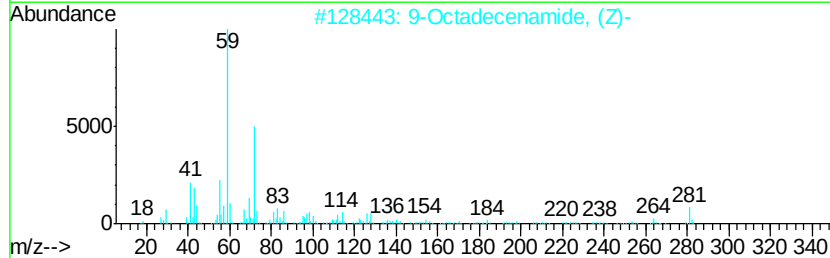
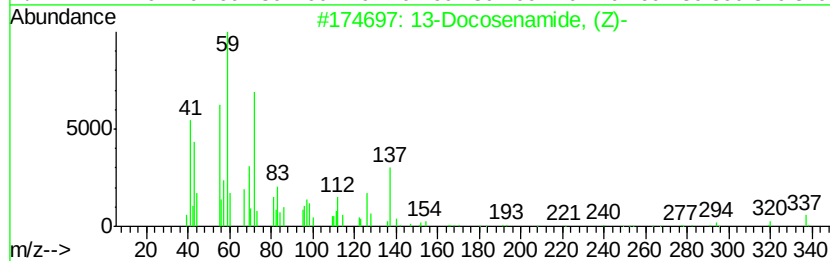
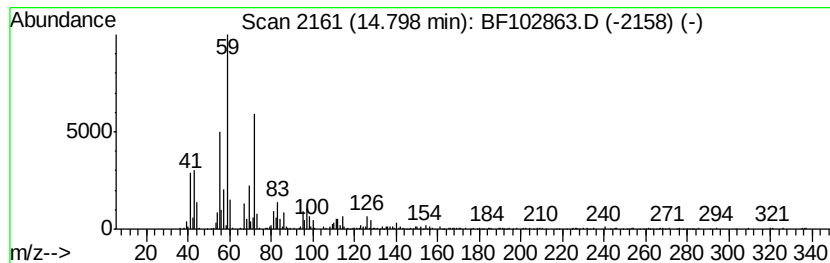
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	14.38 ng	709059	Perylene-d12	15.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		13-Docosenamide, (Z)-	337 C22H43NO	000112-84-5 91
2		9-Octadecenamide, (Z)-	281 C18H35NO	000301-02-0 78
3		Tetradecanamide	227 C14H29NO	000638-58-4 72
4		Dodecanamide	199 C12H25NO	001120-16-7 53
5		2-Propanone, 1-cyclohexyl-	140 C9H16O	000103-78-6 43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102863.D
Acq On : 8 Feb 2018 18:28
Operator : SJ/JU
Sample : J1470-11
Misc :
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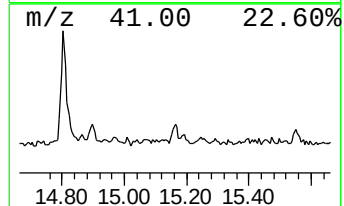
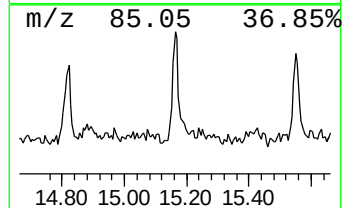
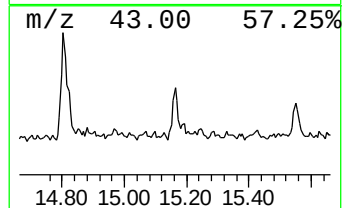
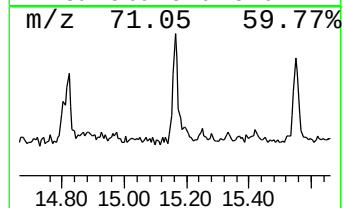
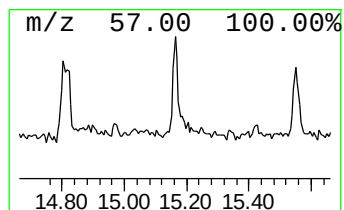
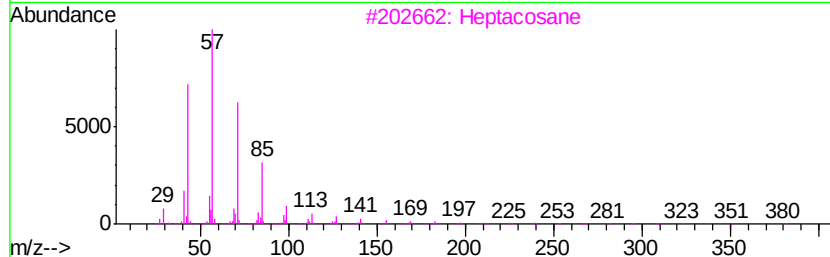
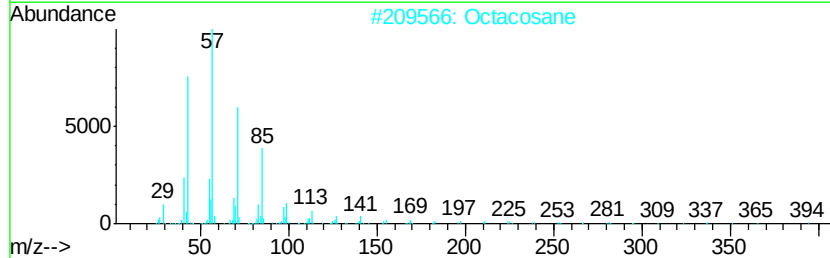
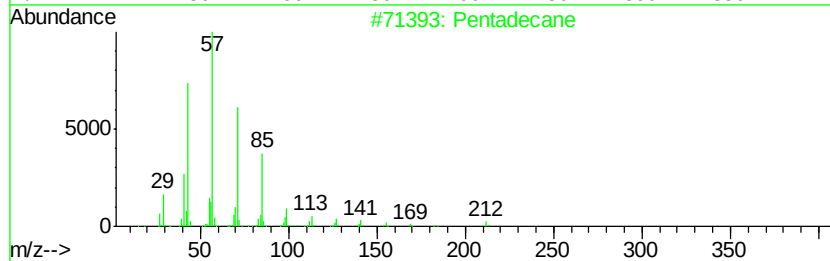
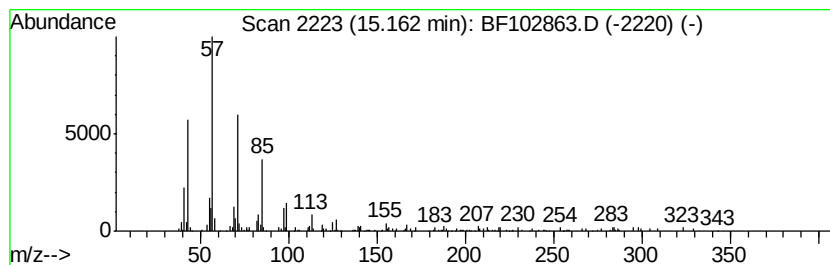
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.16	2.19 ng	107978	Perylene-d12		15.54
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Octacosane	394	C28H58	000630-02-4	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Tetracosane	338	C24H50	000646-31-1	80
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
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Acq On : 8 Feb 2018 18:28
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Sample : J1470-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

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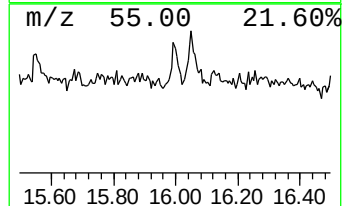
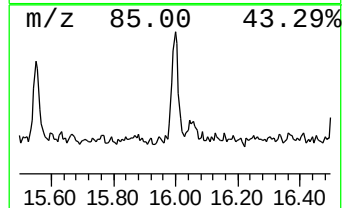
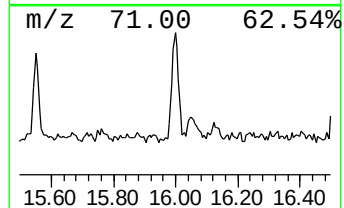
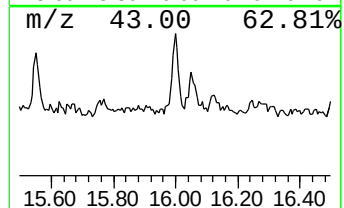
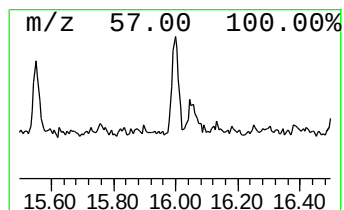
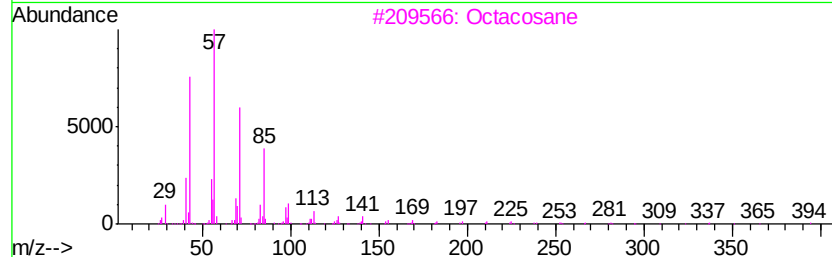
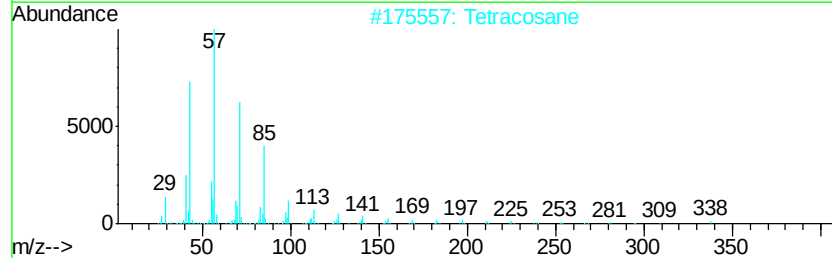
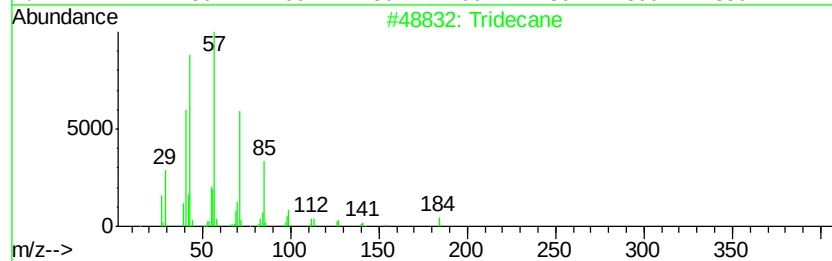
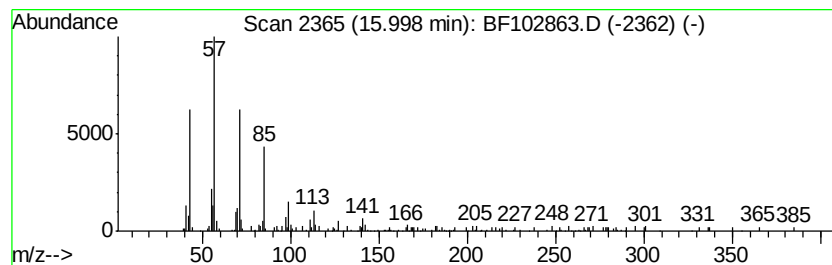
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.42 ng	119432	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	83
2			Tetracosane	338	C24H50	000646-31-1	83
3			Octacosane	394	C28H58	000630-02-4	83
4			Heneicosane	296	C21H44	000629-94-7	83
5			Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102863.D
Acq On : 8 Feb 2018 18:28
Operator : SJ/JU
Sample : J1470-11
Misc :
ALS Vial : 20 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	7.7	ng	498886	1	6.89	1299410	20.0
2-Pentanone, 4-hy...	5.12	2.5	ng	160448	1	6.89	1299410	20.0
unknown6.66	6.66	71.1	ng	4620390	1	6.89	1299410	20.0
Tetradecane	9.85	3.2	ng	233984	3	9.92	1480650	20.0
Hexadecane	10.35	2.7	ng	202014	3	9.92	1480650	20.0
9-Octadecenamide, ...	13.47	13.9	ng	737366	5	14.06	1056890	20.0
Bromoacetic acid, ...	13.88	11.8	ng	622460	5	14.06	1056890	20.0
13-Docosenamide, ...	14.80	14.4	ng	709059	6	15.54	986420	20.0
Pentadecane	15.16	2.2	ng	107978	6	15.54	986420	20.0
Tridecane	16.00	2.4	ng	119432	6	15.54	986420	20.0