

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
 Data File : BF103245.D
 Acq On : 27 Feb 2018 3:41
 Operator : SJ/JU
 Sample : J1649-04
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OIL-SEP-EXC-SW@2.5

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	2.152	3	11	17	rBV	951064	1298416	35.28%	3.977%
2	5.110	511	514	526	rVB	145574	196752	5.35%	0.603%
3	5.504	576	581	584	rBV	3444088	3595041	97.70%	11.011%
4	6.510	747	752	771	rBV	3117855	3679850	100.00%	11.271%
5	6.645	771	775	779	rBV	3478325	3499841	95.11%	10.720%
6	6.875	810	814	822	rBV	1044958	877024	23.83%	2.686%
7	7.028	836	840	844	rBV	2705011	2693566	73.20%	8.250%
8	7.439	905	910	913	rBV	2298828	2173980	59.08%	6.659%
9	8.157	1028	1032	1045	rBV	1233425	1123787	30.54%	3.442%
10	9.228	1210	1214	1218	rBV	3227162	3285689	89.29%	10.064%
11	9.298	1224	1226	1230	rVB	52491	41332	1.12%	0.127%
12	9.622	1275	1281	1288	rBV	241650	228261	6.20%	0.699%
13	9.827	1313	1316	1320	rBV	113128	95744	2.60%	0.293%
14	9.916	1327	1331	1339	rVB	1060069	1023473	27.81%	3.135%
15	10.327	1398	1401	1404	rVB	114668	91750	2.49%	0.281%
16	10.704	1461	1465	1479	rBV	1600481	1703455	46.29%	5.218%
17	10.804	1479	1482	1493	rVB	65699	73239	1.99%	0.224%
18	11.404	1580	1584	1587	rBV	993019	884419	24.03%	2.709%
19	11.427	1587	1588	1592	rVB	111719	71128	1.93%	0.218%
20	11.916	1667	1671	1673	rBV2	44810	47629	1.29%	0.146%
21	12.621	1788	1791	1795	rBV	91464	78169	2.12%	0.239%
22	12.792	1817	1820	1824	rVV	527098	455128	12.37%	1.394%
23	12.851	1824	1830	1832	rVV2	126095	134456	3.65%	0.412%
24	12.868	1832	1833	1837	rVB	93443	66934	1.82%	0.205%
25	12.992	1849	1854	1857	rBV	2520762	2491316	67.70%	7.631%
26	13.498	1937	1940	1944	rBV	409757	349816	9.51%	1.071%
27	13.545	1944	1948	1950	rBV2	65307	59276	1.61%	0.182%
28	13.868	2000	2003	2013	rBV	397317	508734	13.82%	1.558%
29	14.051	2030	2034	2037	rBV	740166	735120	19.98%	2.252%
30	14.192	2055	2058	2062	rVV	81722	77961	2.12%	0.239%
31	14.504	2108	2111	2116	rBV	79333	96397	2.62%	0.295%
32	14.810	2158	2163	2167	rBV2	141925	196010	5.33%	0.600%
33	14.886	2173	2176	2183	rVB	62063	67319	1.83%	0.206%
34	15.151	2218	2221	2227	rVB2	74452	76934	2.09%	0.236%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.551	2283	2289	2296	rBV	369479	570603	15.51%	1.748%
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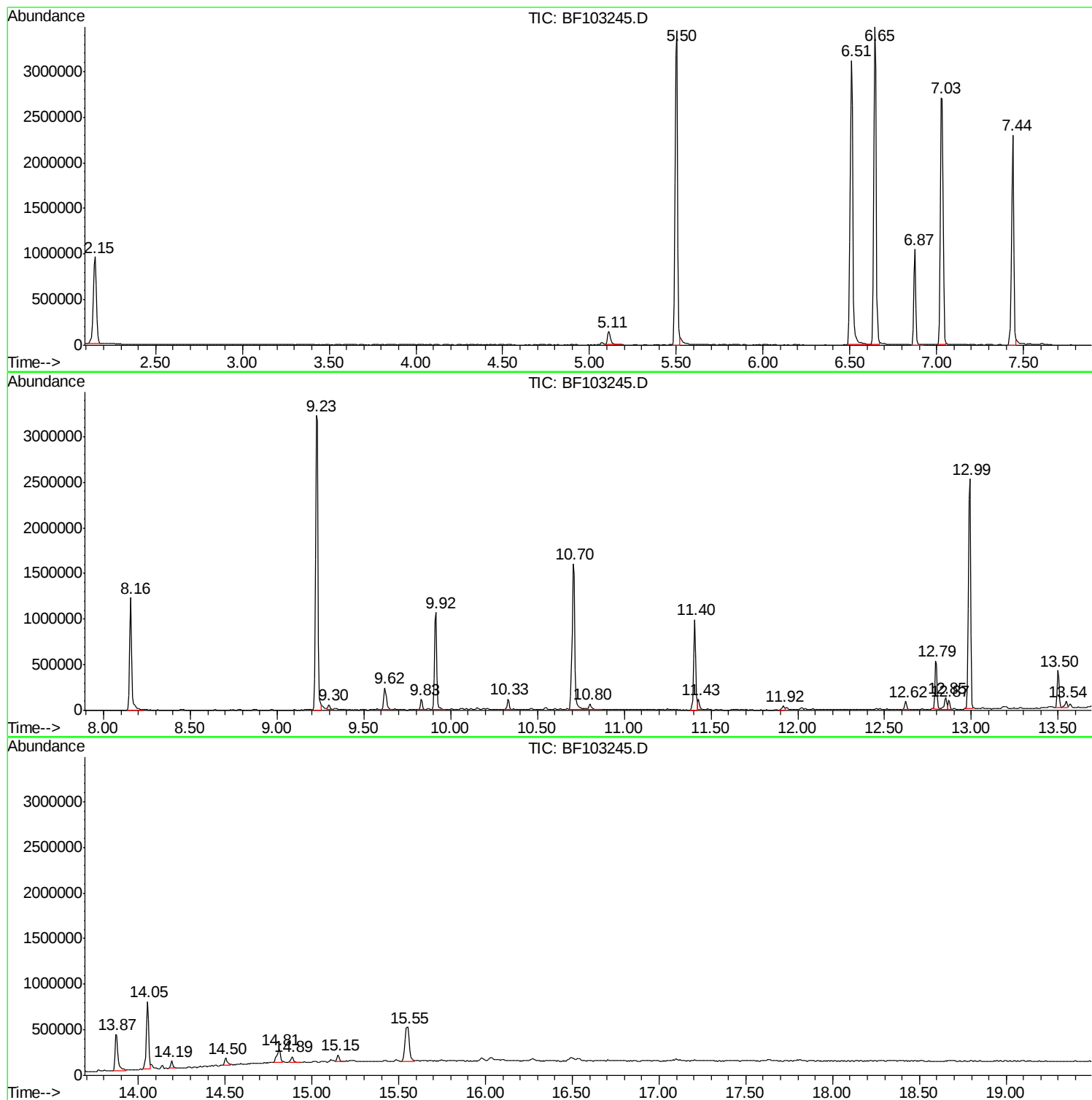
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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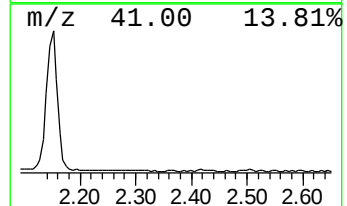
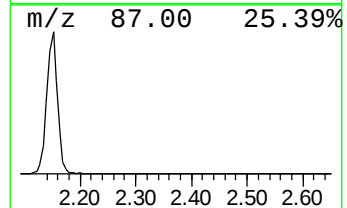
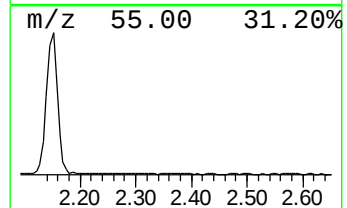
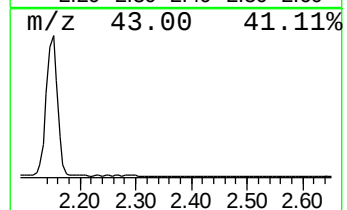
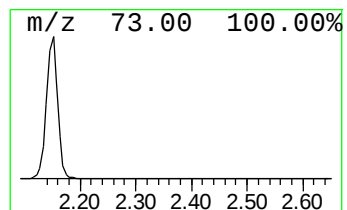
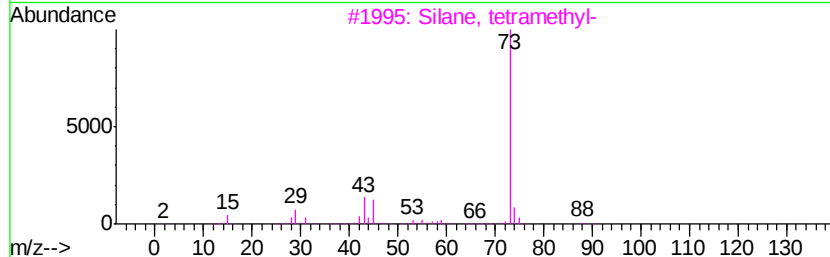
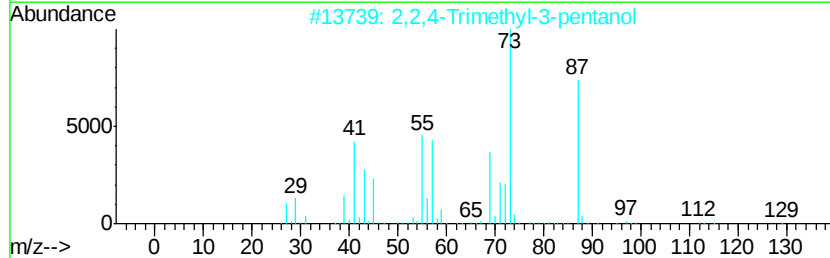
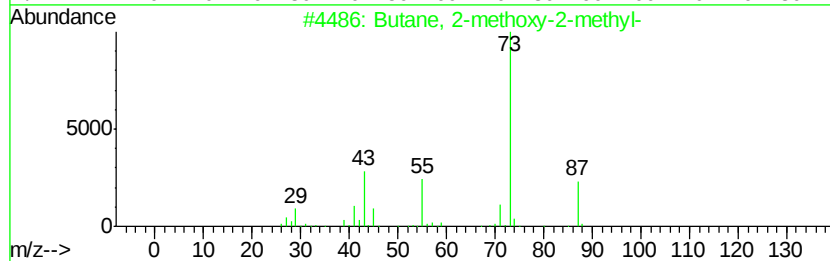
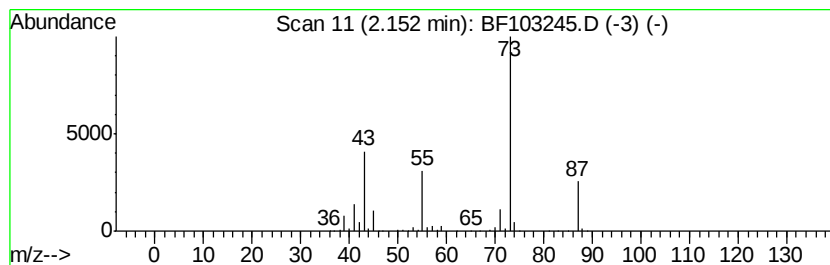
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	29.61 ng	1298420	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	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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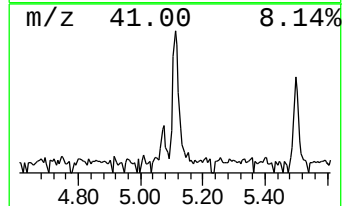
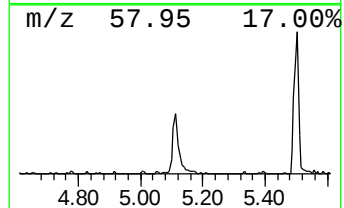
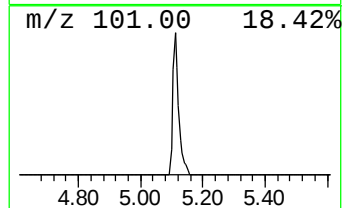
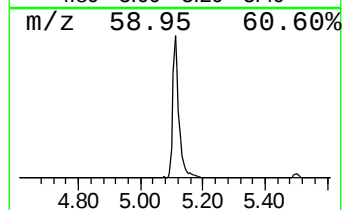
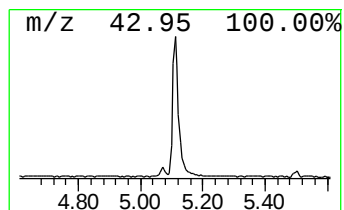
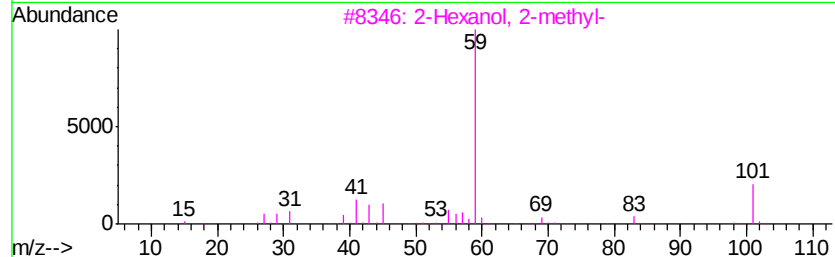
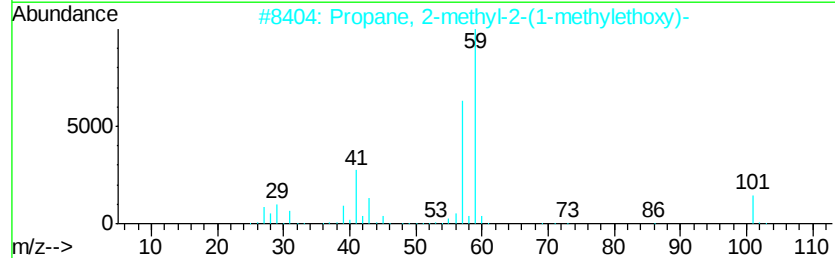
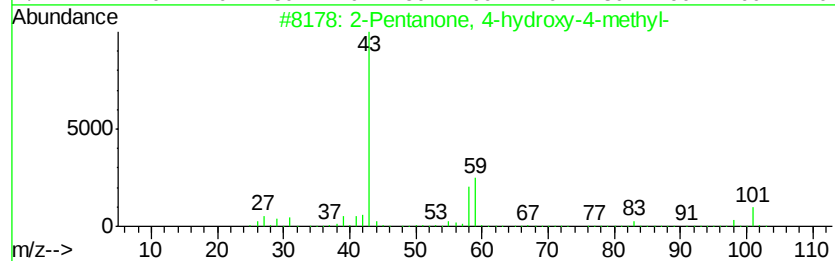
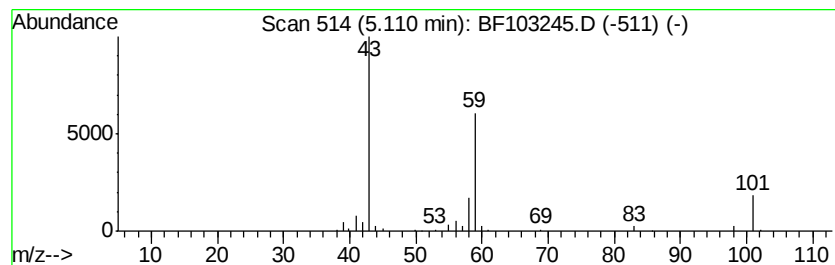
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.49 ng	196752	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	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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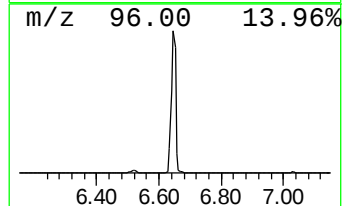
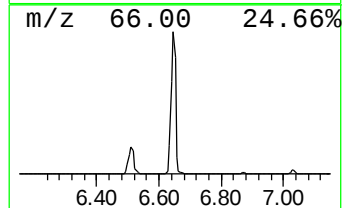
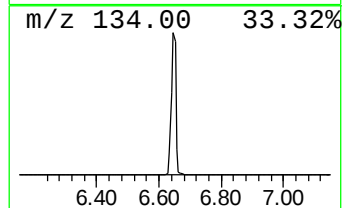
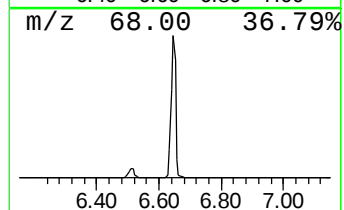
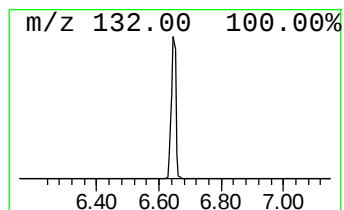
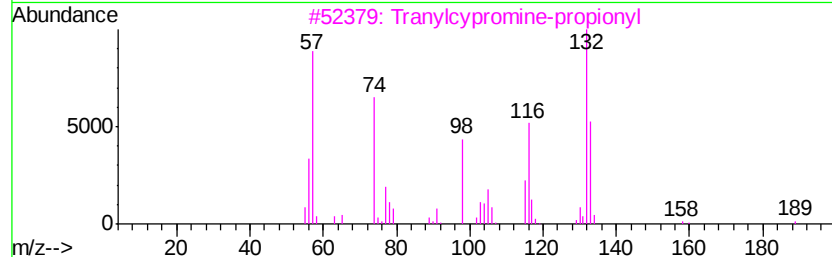
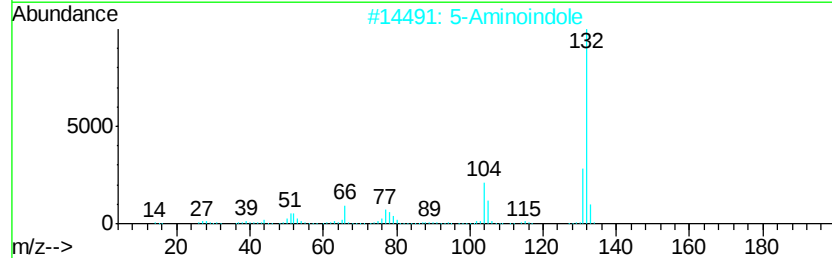
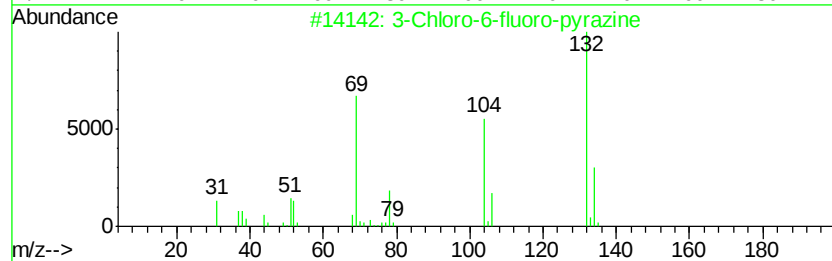
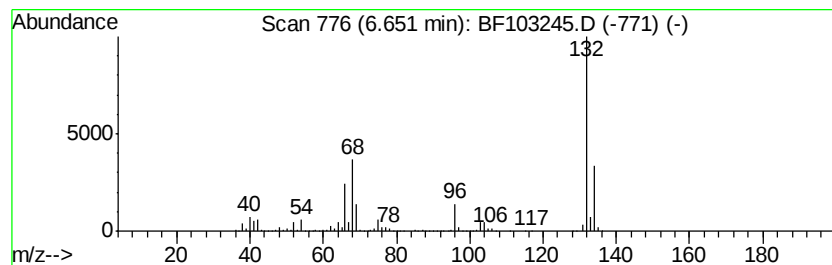
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	79.81 ng	3499840	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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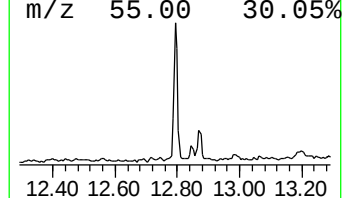
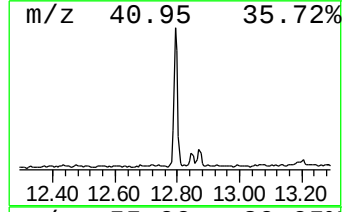
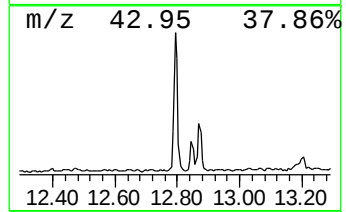
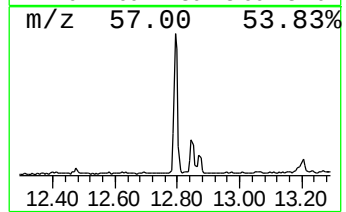
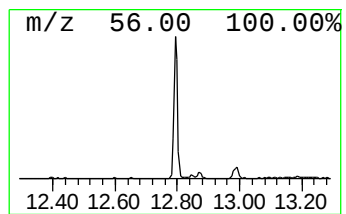
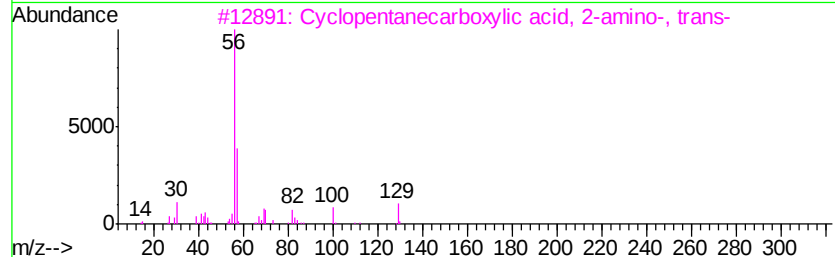
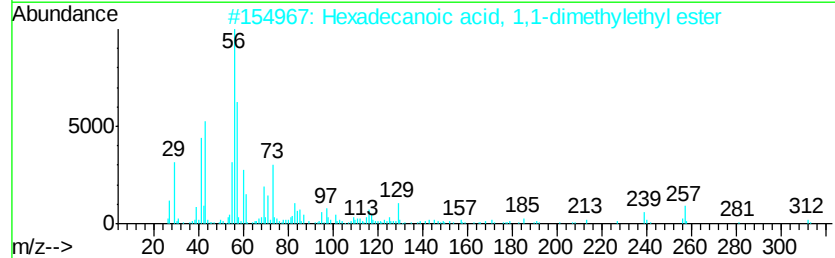
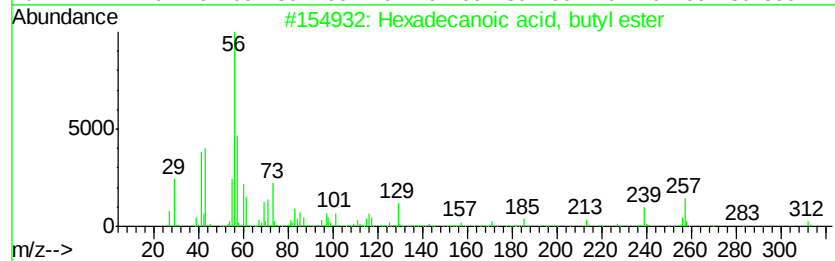
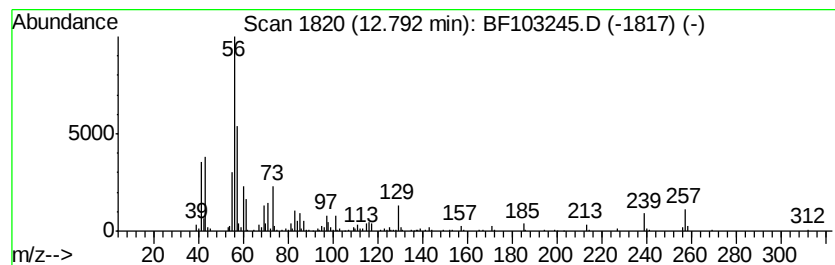
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	12.38 ng	455128	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	42



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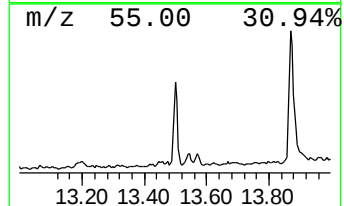
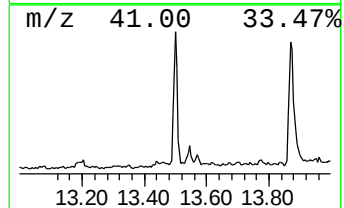
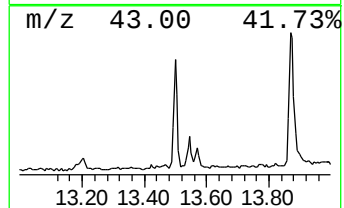
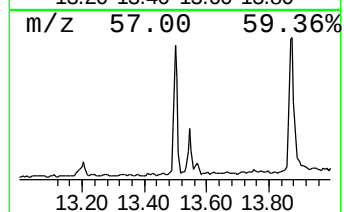
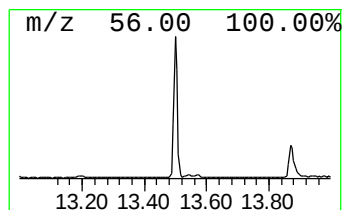
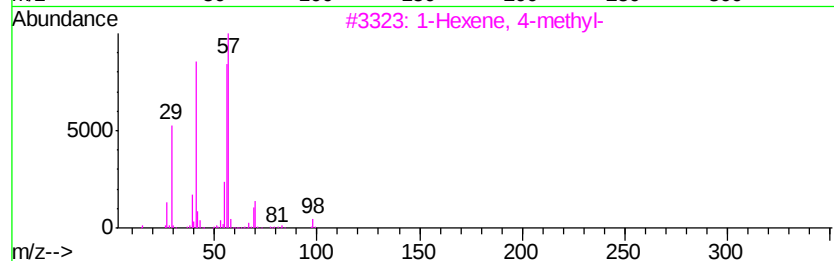
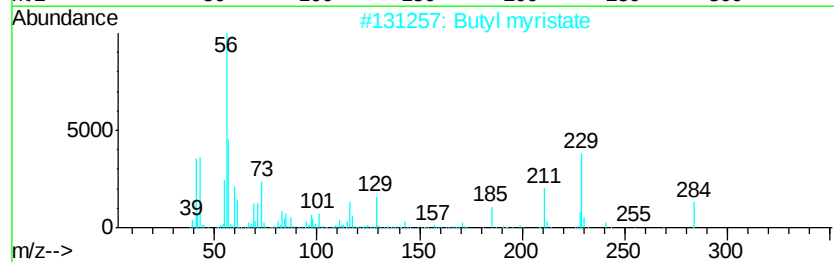
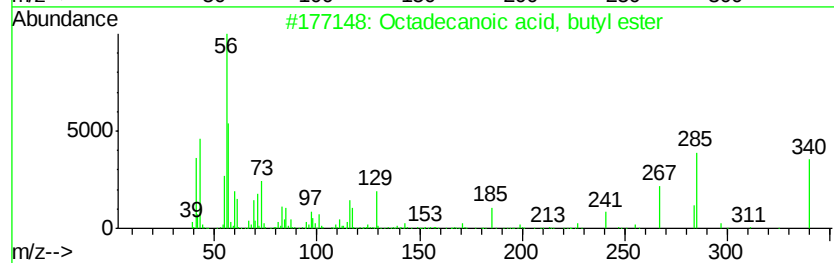
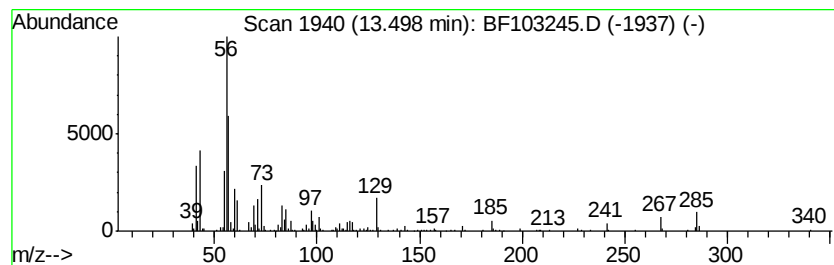
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	9.52 ng	349816	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	86
3		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38
4		Octadecanoic acid, 2-methylpropyl-	340	C22H44O2	000646-13-9	38
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103245.D
Acq On : 27 Feb 2018 3:41
Operator : SJ/JU
Sample : J1649-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OIL-SEP-EXC-SW@2.5

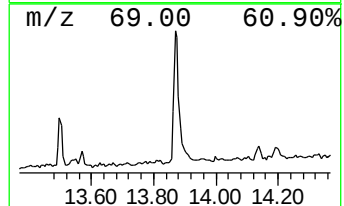
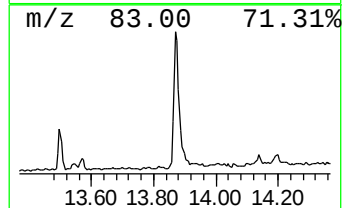
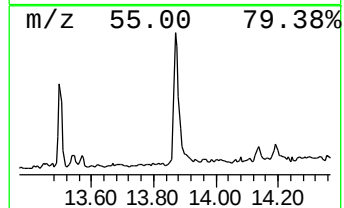
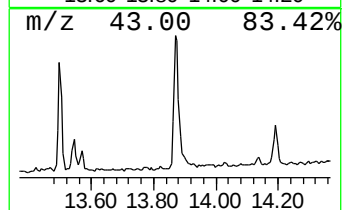
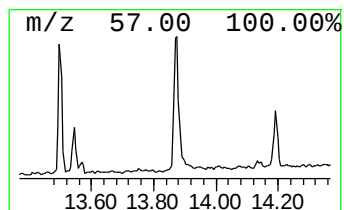
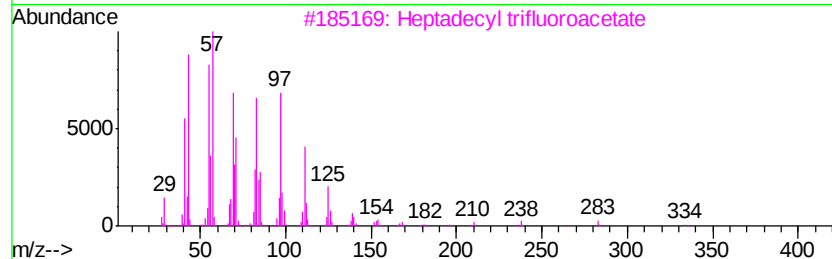
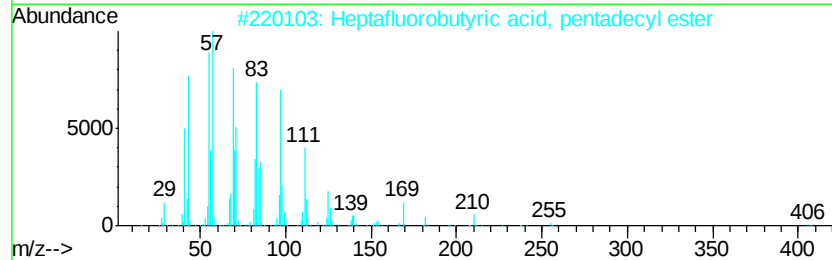
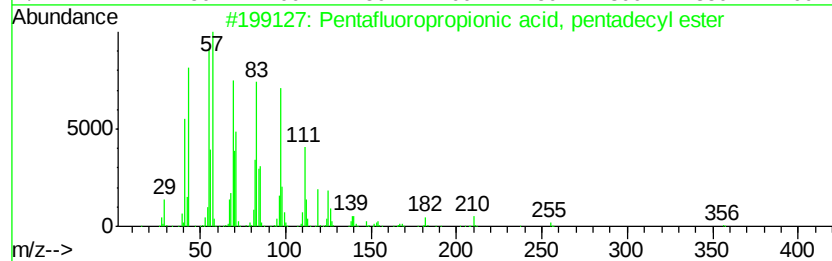
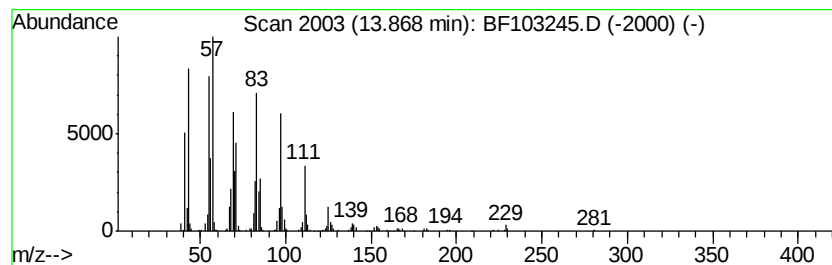
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	13.84 ng	508734	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103245.D
Acq On : 27 Feb 2018 3:41
Operator : SJ/JU
Sample : J1649-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

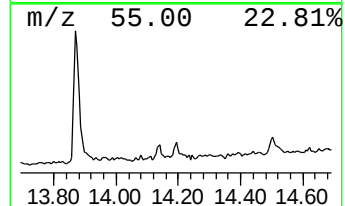
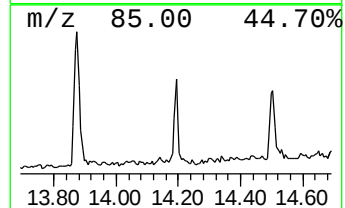
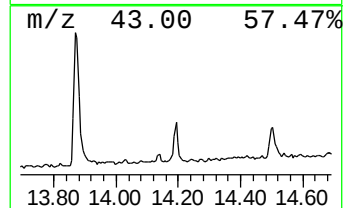
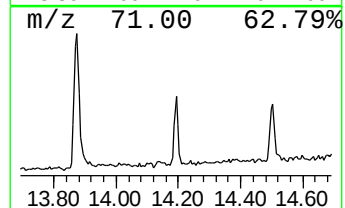
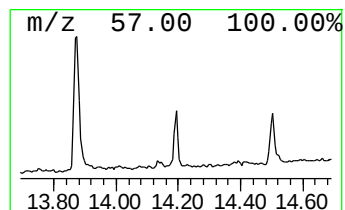
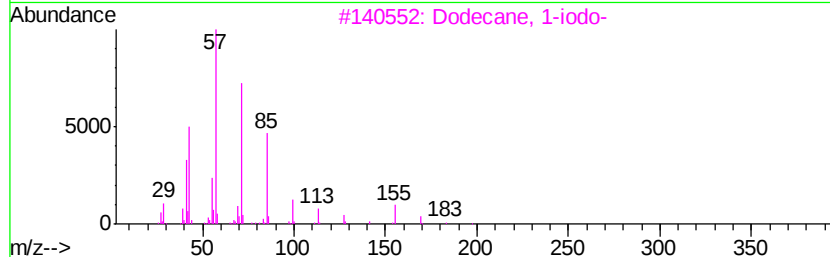
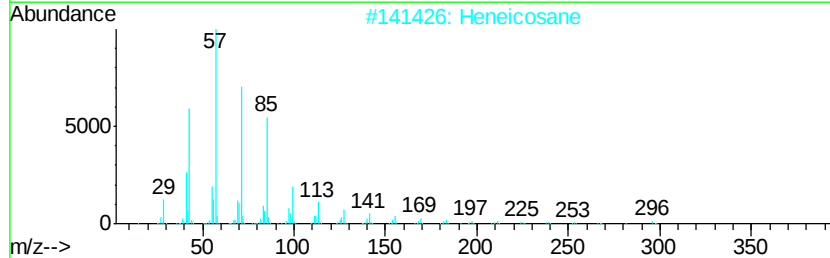
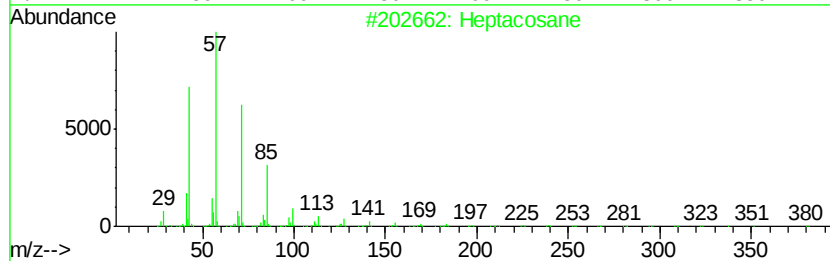
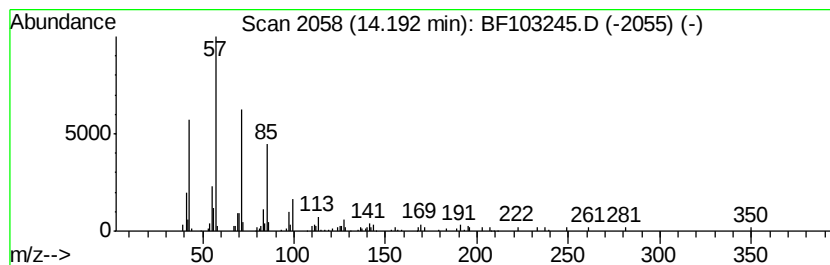
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.19	2.12 ng	77961	Chrysene-d12		14.05		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Heneicosane	296	C21H44	000629-94-7	81
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4			Octacosane	394	C28H58	000630-02-4	76
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103245.D
Acq On : 27 Feb 2018 3:41
Operator : SJ/JU
Sample : J1649-04
Misc :
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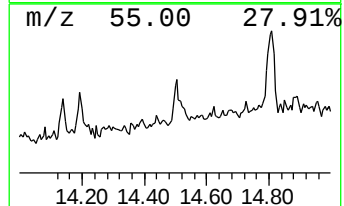
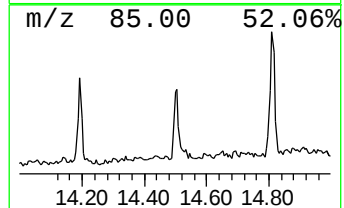
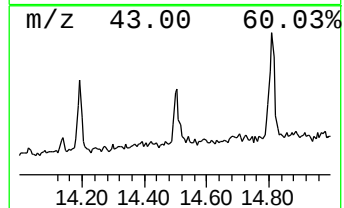
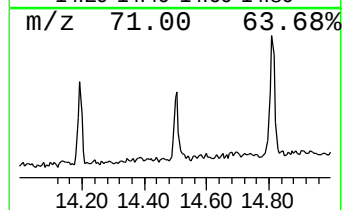
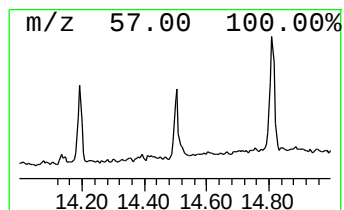
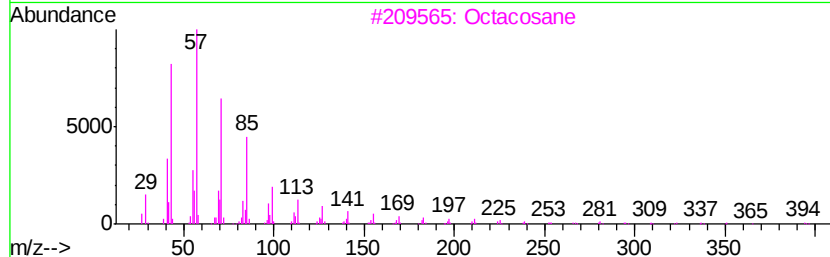
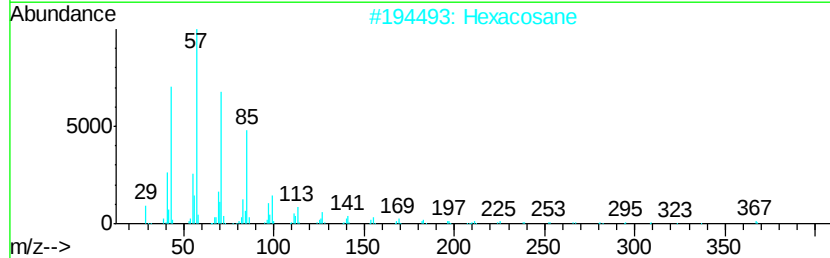
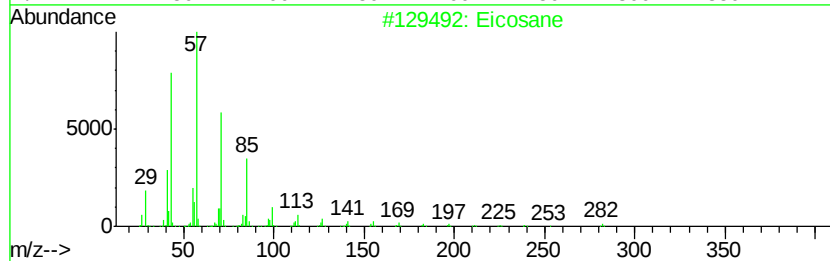
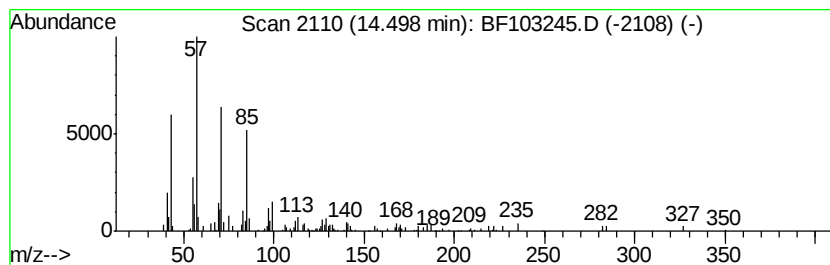
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ClientSampleId :
OIL-SEP-EXC-SW@2.5

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 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.62 ng	96397	Chrysene-d12	14.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	87
2	Hexacosane	366 C26H54	000630-01-3	87
3	Octacosane	394 C28H58	000630-02-4	83
4	Heptadecane	240 C17H36	000629-78-7	83
5	Tetracosane	338 C24H50	000646-31-1	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
Data File : BF103245.D
Acq On : 27 Feb 2018 3:41
Operator : SJ/JU
Sample : J1649-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OIL-SEP-EXC-SW@2.5

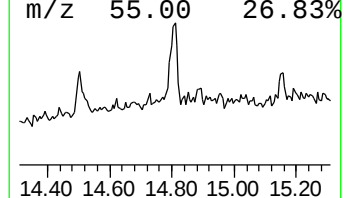
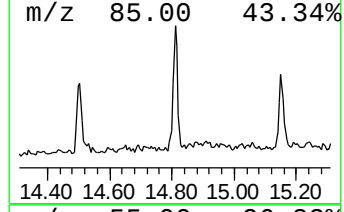
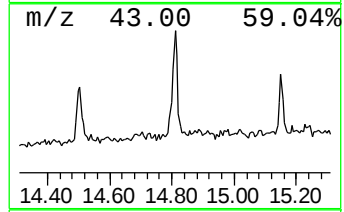
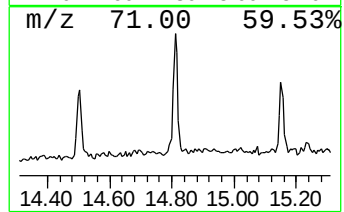
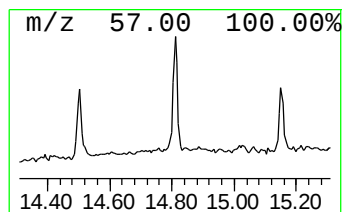
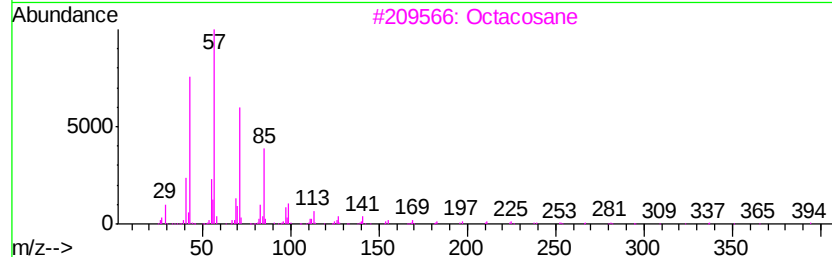
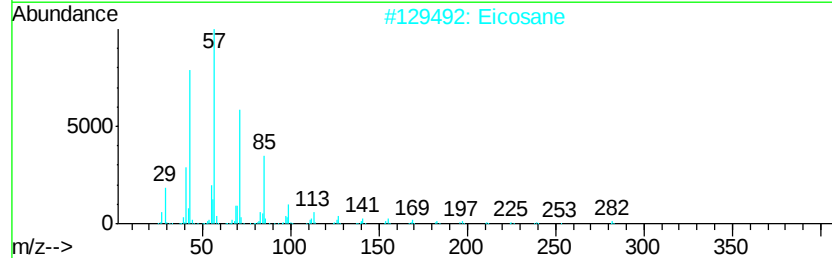
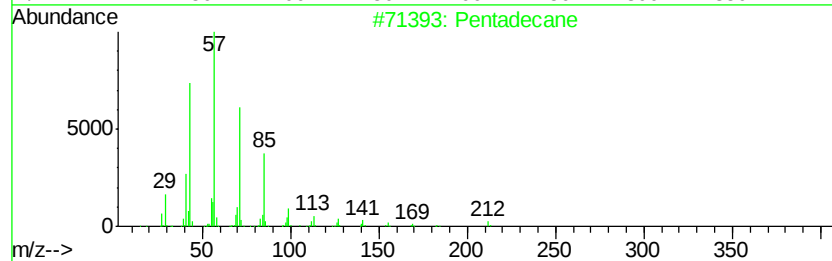
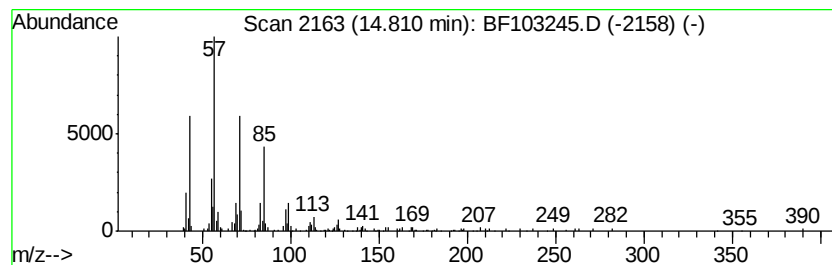
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	6.87 ng	196010	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	95
2		Eicosane	282	C20H42	000112-95-8	93
3		Octacosane	394	C28H58	000630-02-4	80
4		Hexacosane	366	C26H54	000630-01-3	74
5		Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
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Acq On : 27 Feb 2018 3:41
Operator : SJ/JU
Sample : J1649-04
Misc :
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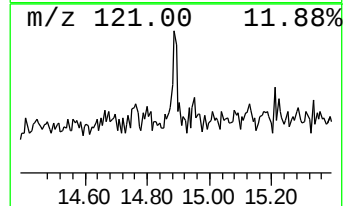
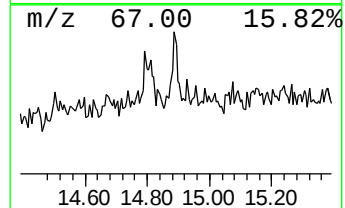
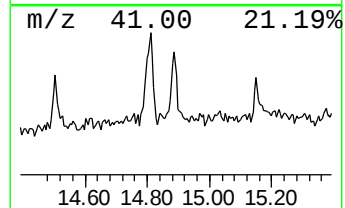
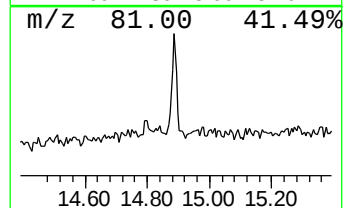
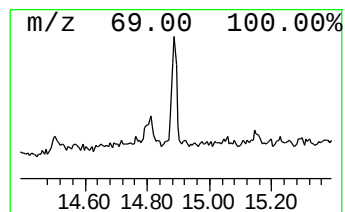
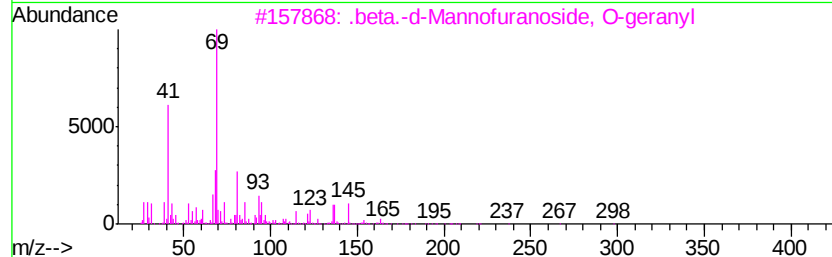
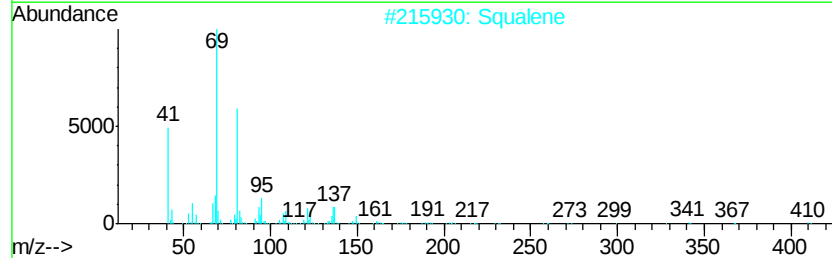
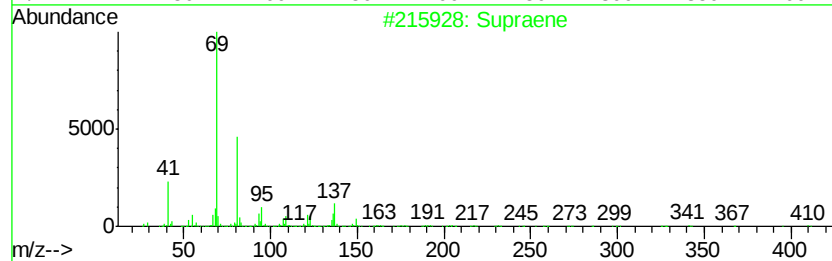
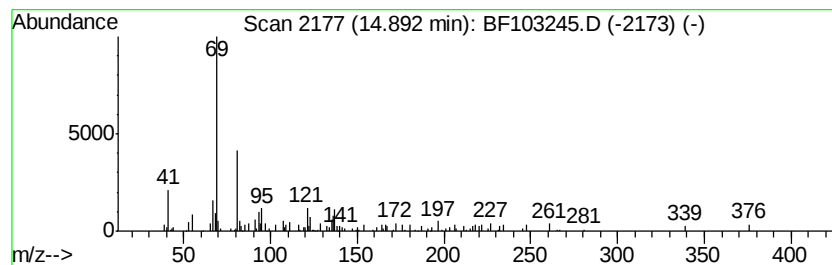
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.36 ng	67319	Perylene-d12	15.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 90
2	Squalene		410 C30H50	000111-02-4 87
3	.beta.-d-Mannofuranoside, O-geranyl		316 C16H28O6	1000154-77-2 72
4	1,6-Octadien-3-ol, 3,7-dimethyl-...		182 C11H18O2	000115-99-1 64
5	4,8,12-Tetradecatrienal, 5,9,13-...		248 C17H28O	066408-55-7 64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022618\
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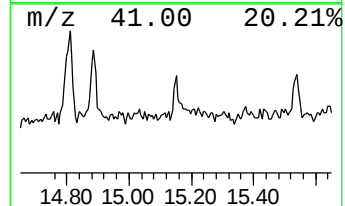
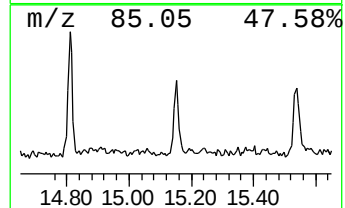
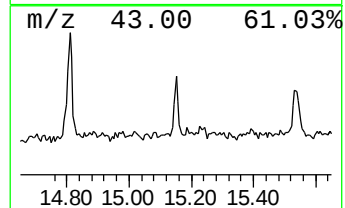
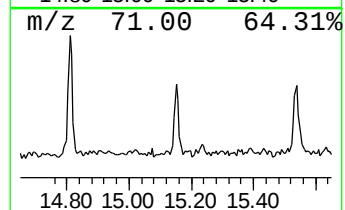
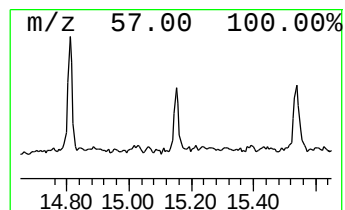
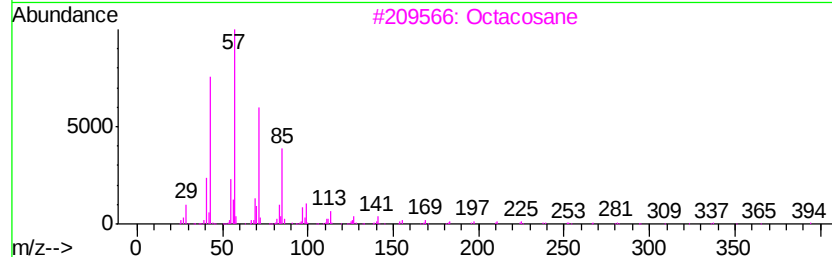
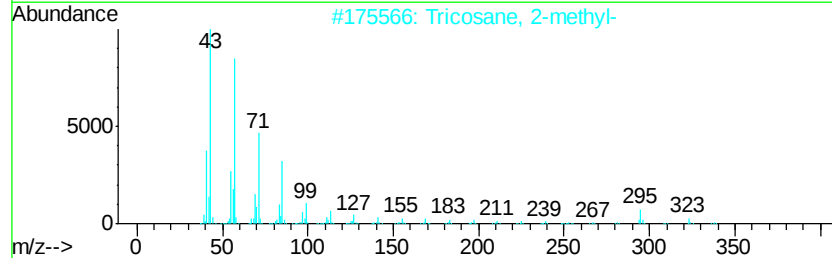
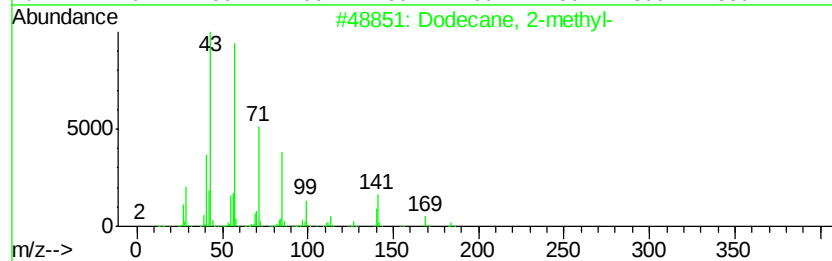
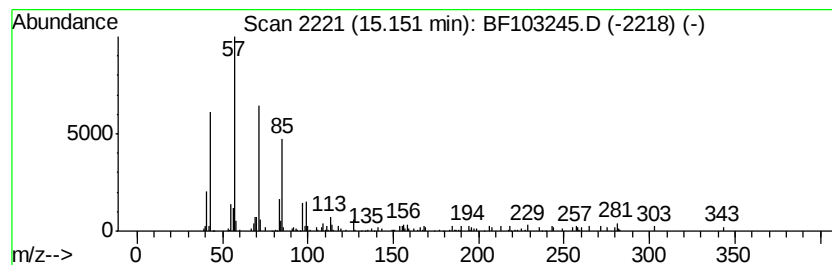
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Dodecane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.70 ng	76934	Perylene-d12	15.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecane, 2-methyl-	184 C13H28	001560-97-0	72
2	Tricosane, 2-methyl-	338 C24H50	001928-30-9	72
3	Octacosane	394 C28H58	000630-02-4	68
4	Tetracosane, 11-decyl-	479 C34H70	055429-84-0	64
5	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022618\
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OIL-SEP-EXC-SW@2.5

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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
Butane, 2-methoxy...	2.15	29.6	ng	1298420	1	6.87	877024	20.0
2-Pentanone, 4-hy...	5.11	4.5	ng	196752	1	6.87	877024	20.0
unknown6.65	6.65	79.8	ng	3499840	1	6.87	877024	20.0
Hexadecanoic acid...	12.79	12.4	ng	455128	5	14.05	735120	20.0
Octadecanoic acid...	13.50	9.5	ng	349816	5	14.05	735120	20.0
Pentafluoropropio...	13.87	13.8	ng	508734	5	14.05	735120	20.0
Heptacosane	14.19	2.1	ng	77961	5	14.05	735120	20.0
Eicosane	14.50	2.6	ng	96397	5	14.05	735120	20.0
Pentadecane	14.81	6.9	ng	196010	6	15.55	570603	20.0
Supraene	14.89	2.4	ng	67319	6	15.55	570603	20.0
Dodecane, 2-methyl-	15.15	2.7	ng	76934	6	15.55	570603	20.0