

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
 Data File : BF102244.D
 Acq On : 20 Jan 2018 3:46
 Operator : SJ/JU
 Sample : J1113-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-12-3.5-4.0-DUP

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-BF010918.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	4.922	476	482	494	rVB	168346	245969	7.68%	0.843%
2	5.334	546	552	555	rBV	2854680	3091406	96.53%	10.592%
3	6.357	721	726	731	rBV	2722633	3136449	97.94%	10.746%
4	6.487	744	748	752	rBV	3188848	3148846	98.33%	10.788%
5	6.716	784	787	791	rBV	1077117	853451	26.65%	2.924%
6	6.875	809	814	817	rBV	2746835	2417867	75.50%	8.284%
7	7.287	878	884	887	rBV	2027348	1992833	62.23%	6.828%
8	7.375	894	899	905	rBV	39970	49859	1.56%	0.171%
9	7.998	1001	1005	1009	rBV	1353621	1134032	35.41%	3.885%
10	9.075	1183	1188	1192	rBV	3250939	3202384	100.00%	10.972%
11	9.469	1252	1255	1258	rBV	397320	309315	9.66%	1.060%
12	9.686	1288	1292	1295	rBV	76695	62150	1.94%	0.213%
13	9.751	1299	1303	1307	rVB	1434640	1184192	36.98%	4.057%
14	10.180	1374	1376	1380	rVB	106865	96842	3.02%	0.332%
15	10.404	1408	1414	1416	rBV	32603	44171	1.38%	0.151%
16	10.539	1433	1437	1441	rBV	1908535	1849511	57.75%	6.337%
17	10.657	1454	1457	1465	rBV	115230	116038	3.62%	0.398%
18	11.104	1530	1533	1536	rBV	72130	59813	1.87%	0.205%
19	11.233	1551	1555	1559	rBV	1240290	1069037	33.38%	3.663%
20	12.645	1791	1795	1798	rBV	265080	211351	6.60%	0.724%
21	12.722	1805	1808	1812	rVB	39954	32137	1.00%	0.110%
22	12.821	1821	1825	1828	rBV	2534762	2221860	69.38%	7.612%
23	13.351	1911	1915	1917	rBV	173482	147840	4.62%	0.507%
24	13.716	1973	1977	1988	rBV	405154	426108	13.31%	1.460%
25	13.868	1999	2003	2007	rBV	894060	764048	23.86%	2.618%
26	14.039	2029	2032	2039	rVB	36238	36651	1.14%	0.126%
27	14.345	2080	2084	2089	rBV	48090	56229	1.76%	0.193%
28	14.639	2131	2134	2139	rVB	36637	32968	1.03%	0.113%
29	14.710	2142	2146	2151	rVB	53867	51501	1.61%	0.176%
30	14.957	2185	2188	2196	rBV	34953	48533	1.52%	0.166%
31	15.292	2239	2245	2248	rBV	675632	788341	24.62%	2.701%
32	15.727	2315	2319	2323	rBV	35476	51046	1.59%	0.175%
33	15.774	2323	2327	2333	rVV2	47841	76977	2.40%	0.264%
34	16.198	2395	2399	2405	rBV3	31155	45814	1.43%	0.157%

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35	16.751	2489	2493	2500	rVB4	22989	50959	1.59%	0.175%
36	17.209	2566	2571	2576	rVB9	21763	38894	1.21%	0.133%
37	18.180	2730	2736	2742	rBV8	13564	41763	1.30%	0.143%

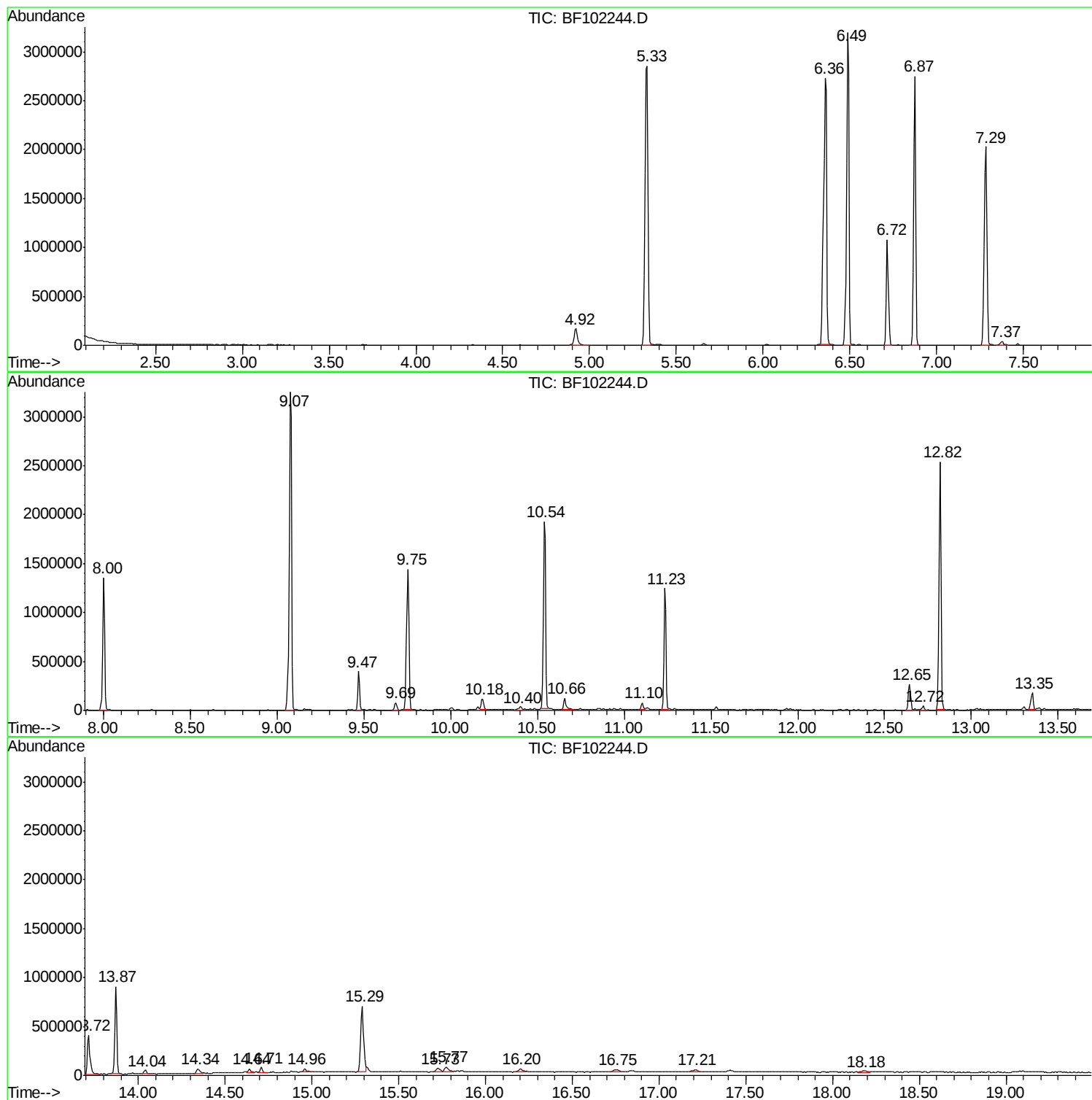
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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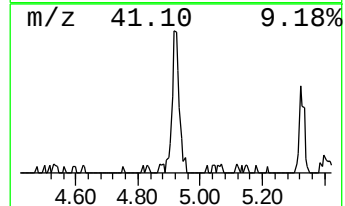
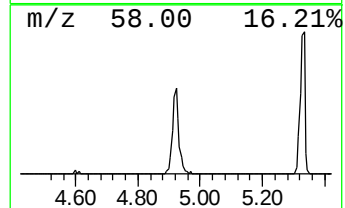
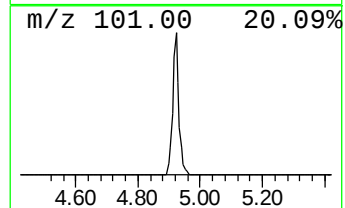
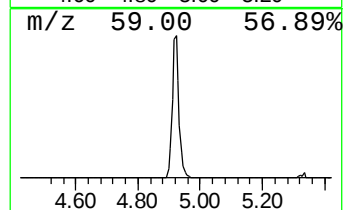
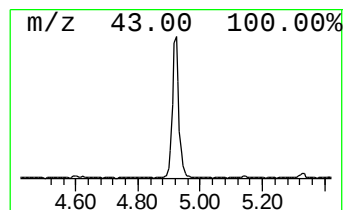
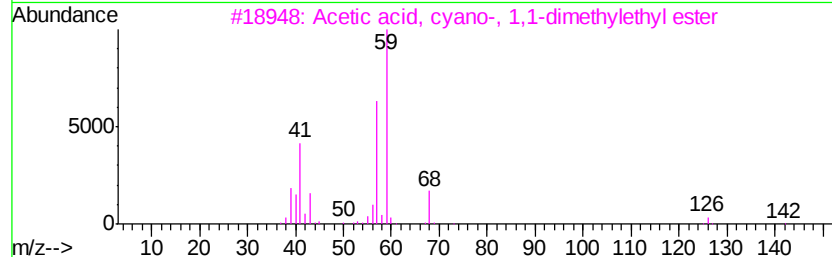
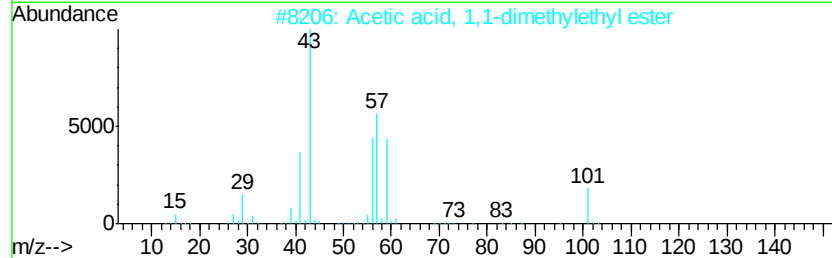
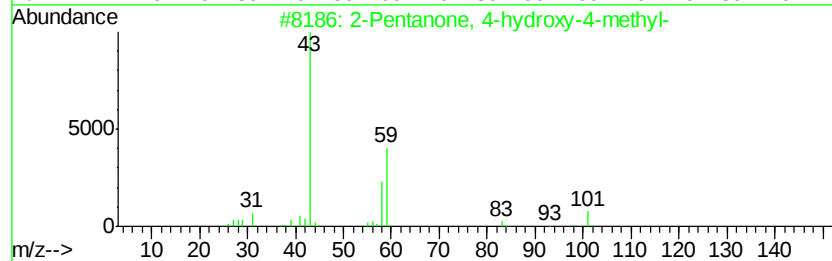
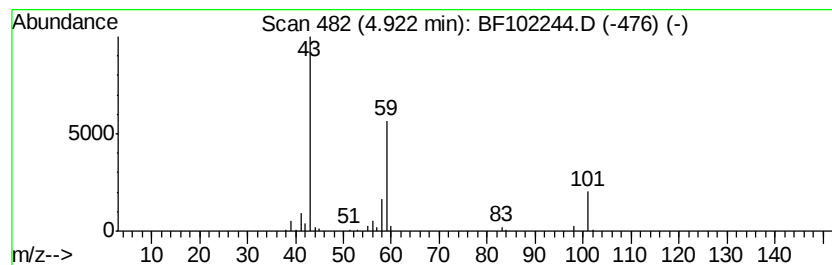
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.76 ng	245969	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9	



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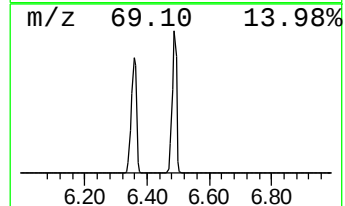
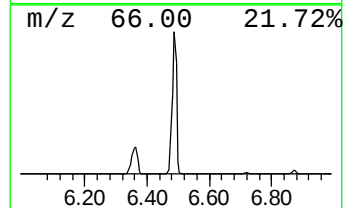
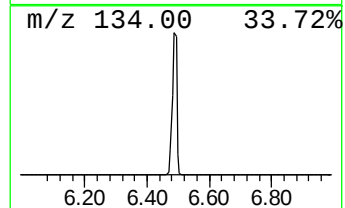
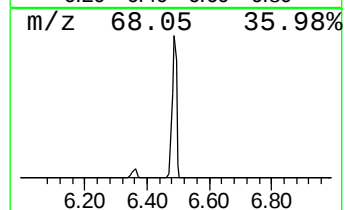
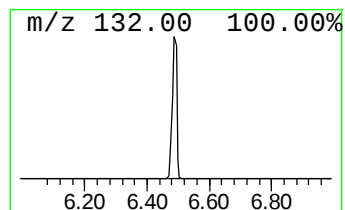
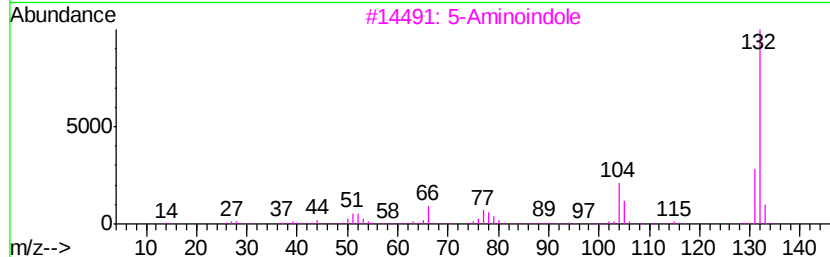
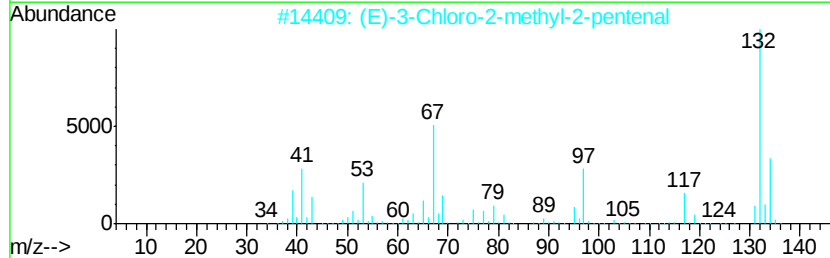
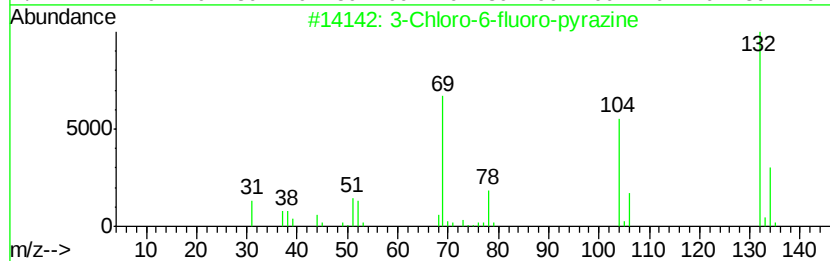
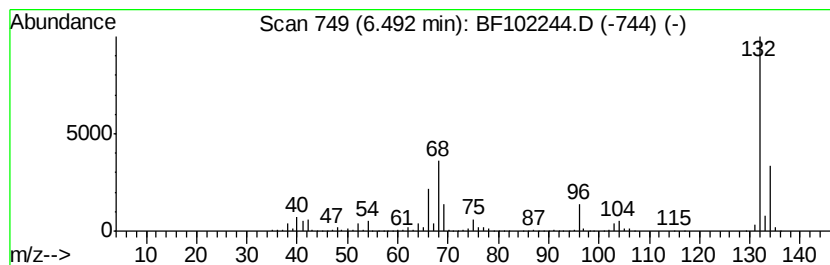
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	73.79 ng	3148850	1,4-Dichlorobenzene-d4	6.72

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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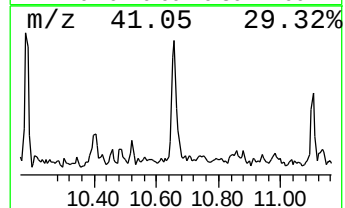
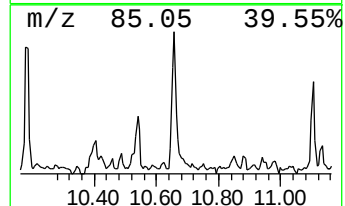
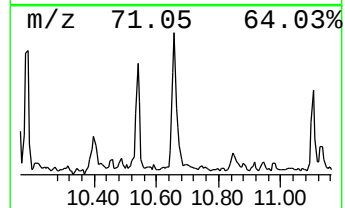
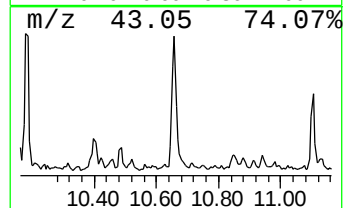
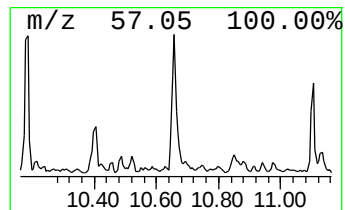
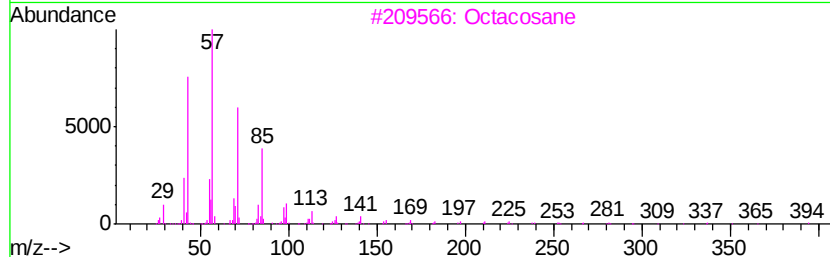
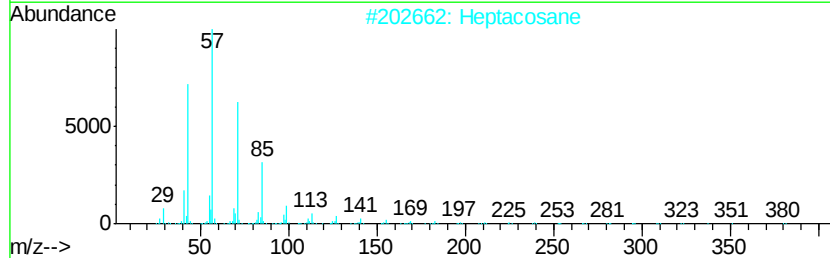
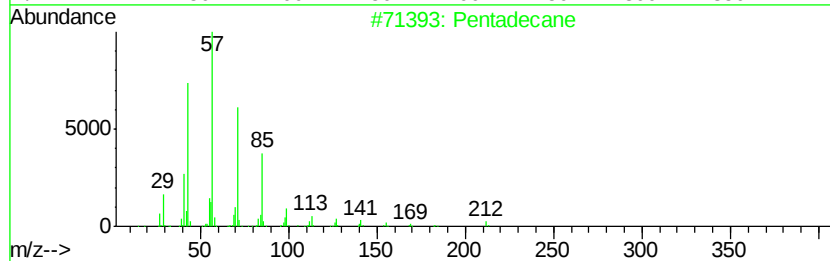
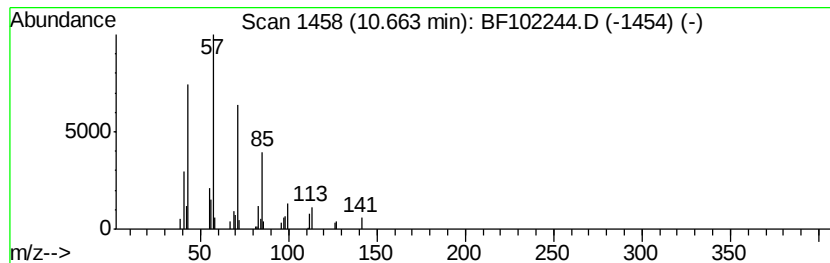
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.17 ng	116038	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	90
2		Heptacosane	380	C27H56	000593-49-7	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Docosane	310	C22H46	000629-97-0	86
5		Heneicosane	296	C21H44	000629-94-7	86



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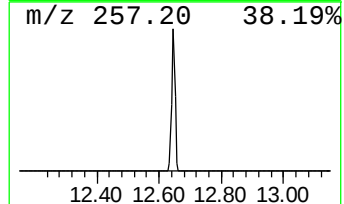
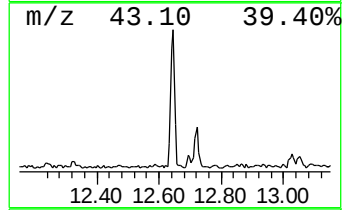
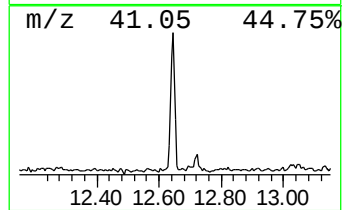
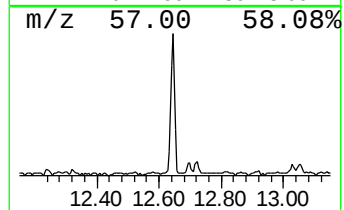
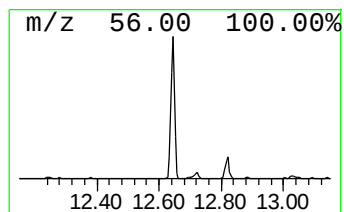
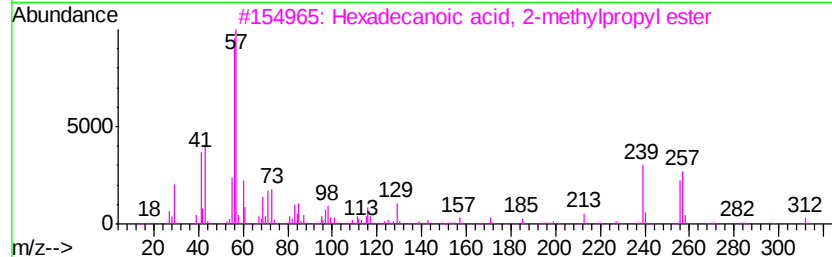
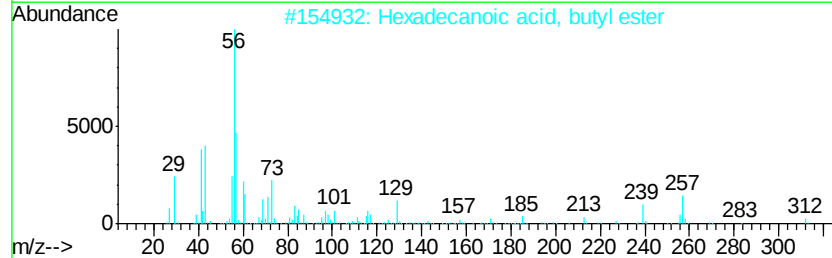
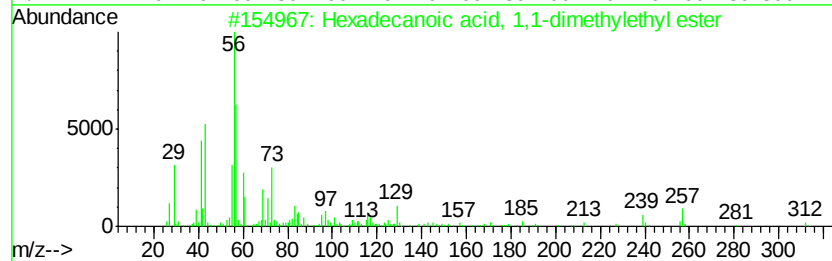
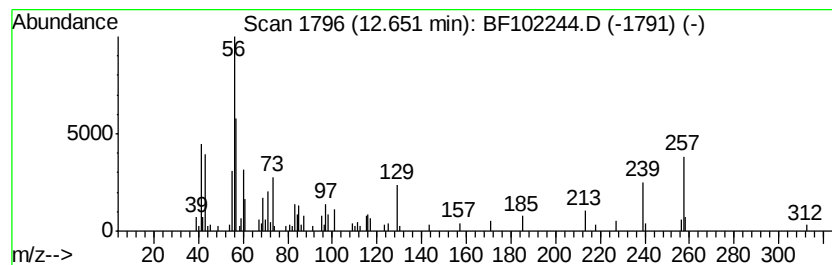
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	5.53 ng	211351	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	94
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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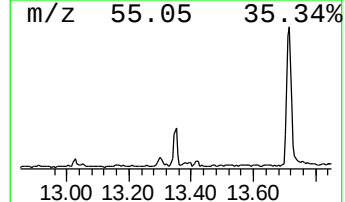
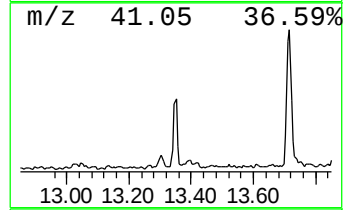
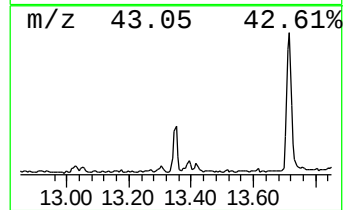
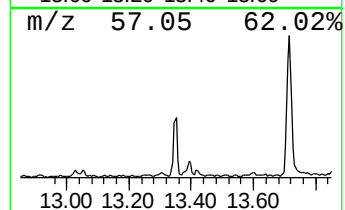
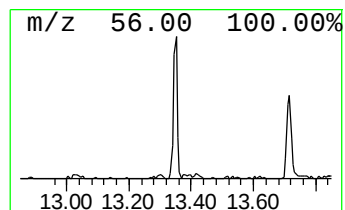
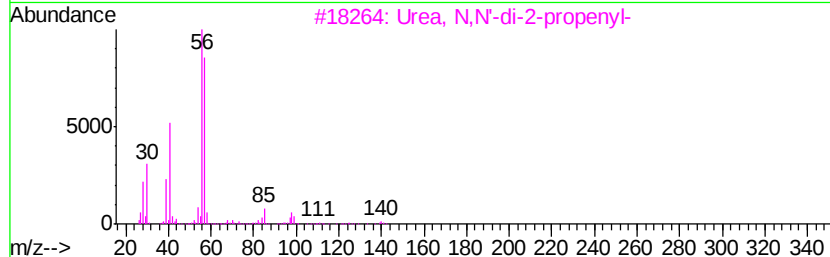
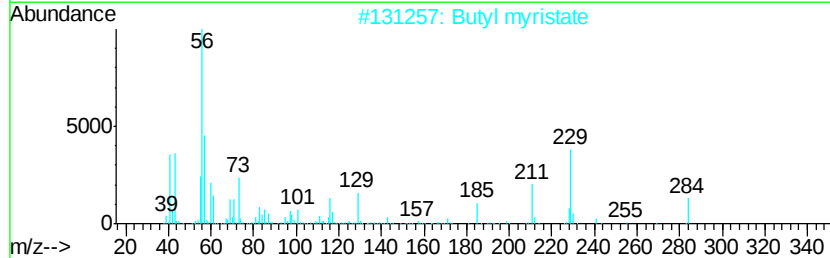
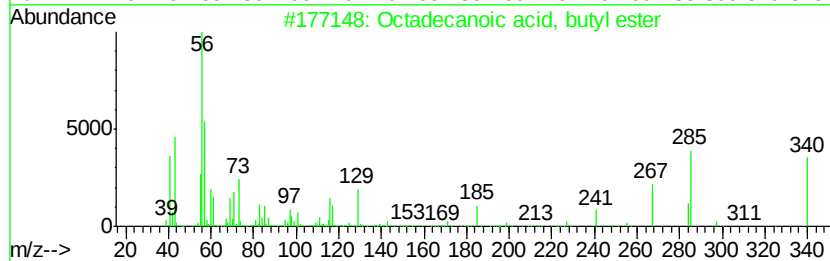
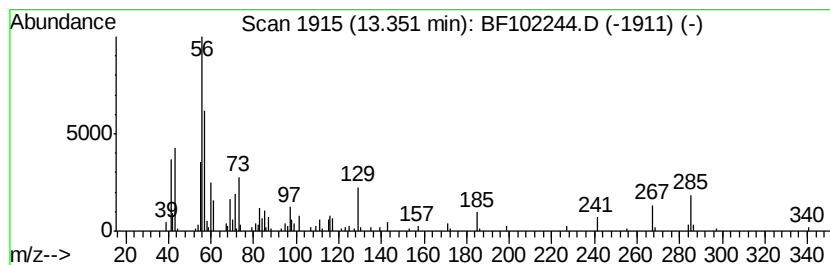
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	3.87 ng	147840	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		Butyl myristate	284	C18H36O2	000110-36-1	72
3		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102244.D
Acq On : 20 Jan 2018 3:46
Operator : SJ/JU
Sample : J1113-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-3.5-4.0-DUP

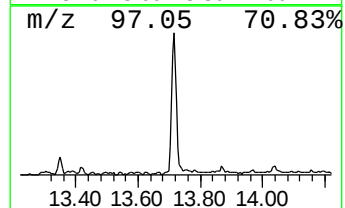
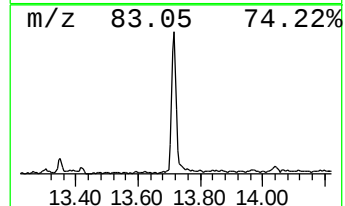
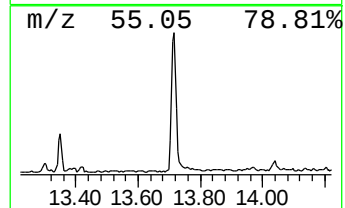
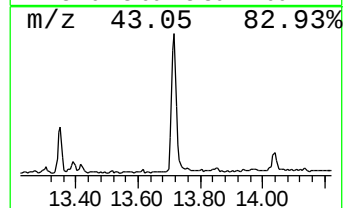
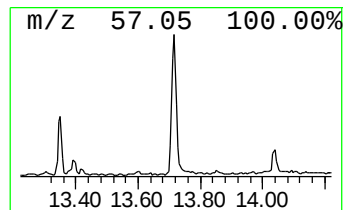
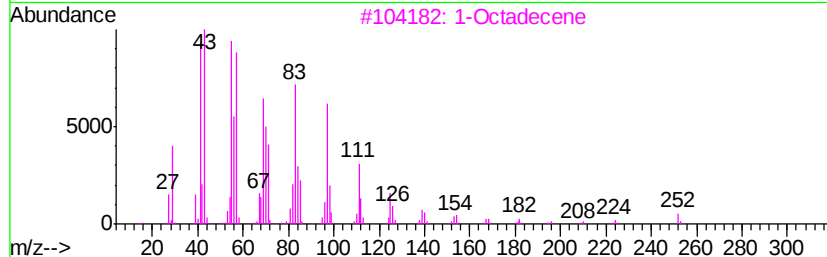
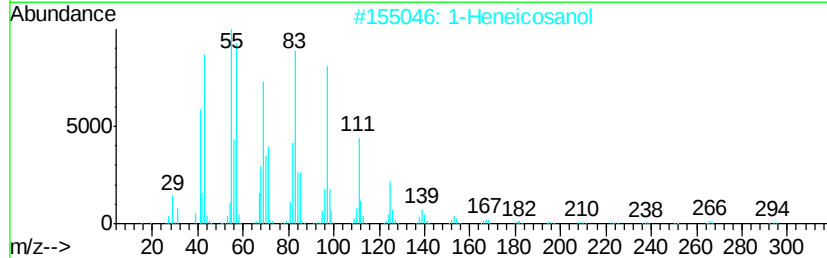
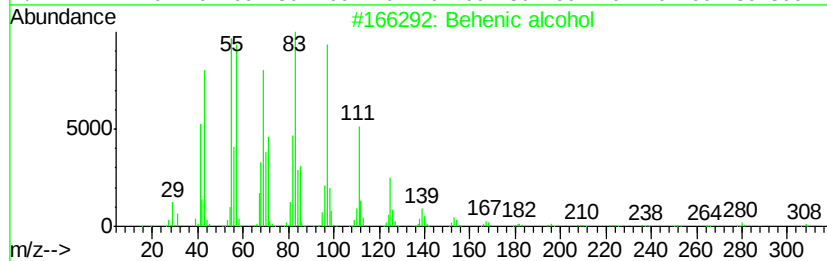
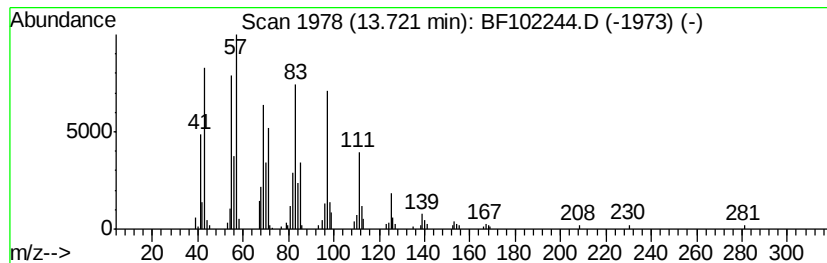
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	11.15 ng	426108	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		1-Octadecene	252	C18H36	000112-88-9	95
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102244.D
Acq On : 20 Jan 2018 3:46
Operator : SJ/JU
Sample : J1113-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-12-3.5-4.0-DUP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.92	5.8	ng	245969	1	6.72	853451	20.0
unknown6.49	6.49	73.8	ng	3148850	1	6.72	853451	20.0
Pentadecane	10.66	2.2	ng	116038	4	11.23	1069040	20.0
Hexadecanoic acid...	12.65	5.5	ng	211351	5	13.87	764048	20.0
Octadecanoic acid...	13.35	3.9	ng	147840	5	13.87	764048	20.0
Behenic alcohol	13.72	11.2	ng	426108	5	13.87	764048	20.0