

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
 Data File : BF101447.D
 Acq On : 15 Dec 2017 17:12
 Operator : SJ/JU
 Sample : I6684-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-02-121217

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-BF121417.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	5.039	498	502	526	rBV	875799	1420893	34.84%	3.778%
2	5.439	566	570	593	rBV	3417568	3903947	95.72%	10.381%
3	6.457	738	743	761	rBV	3150887	4078405	100.00%	10.845%
4	6.586	761	765	768	rBV	3785992	3603925	88.37%	9.583%
5	6.810	800	803	812	rBV	1124990	1080876	26.50%	2.874%
6	6.969	826	830	846	rBV	2864055	2766401	67.83%	7.356%
7	7.381	896	900	917	rBV	2207192	2596863	63.67%	6.905%
8	8.098	1018	1022	1039	rBV	1298957	1473987	36.14%	3.919%
9	9.169	1200	1204	1214	rBV	3509031	3510203	86.07%	9.334%
10	9.239	1214	1216	1220	rVB	50160	45855	1.12%	0.122%
11	9.569	1265	1272	1279	rBV	248622	292648	7.18%	0.778%
12	9.769	1303	1306	1310	rBV	95676	80852	1.98%	0.215%
13	9.851	1316	1320	1334	rVB2	1662087	1570411	38.51%	4.176%
14	10.269	1388	1391	1394	rVB	148189	109187	2.68%	0.290%
15	10.486	1423	1428	1431	rBV	49162	62153	1.52%	0.165%
16	10.645	1451	1455	1469	rBV	2122174	2328501	57.09%	6.192%
17	10.739	1469	1471	1482	rVB	129794	168577	4.13%	0.448%
18	11.192	1545	1548	1550	rBV	73026	61541	1.51%	0.164%
19	11.345	1570	1574	1583	rBV	1514700	1600213	39.24%	4.255%
20	11.721	1634	1638	1641	rBV	143860	114374	2.80%	0.304%
21	11.857	1657	1661	1663	rBV2	65120	66480	1.63%	0.177%
22	12.404	1750	1754	1756	rBV3	190600	188932	4.63%	0.502%
23	12.427	1756	1758	1766	rVB	306098	272273	6.68%	0.724%
24	12.510	1769	1772	1776	rVB	92145	77486	1.90%	0.206%
25	12.563	1777	1781	1786	rBV	149671	141468	3.47%	0.376%
26	12.792	1814	1820	1826	rVB	161110	220945	5.42%	0.588%
27	12.927	1838	1843	1846	rBV	3143811	3037128	74.47%	8.076%
28	13.810	1989	1993	2006	rVB3	154558	224079	5.49%	0.596%
29	13.945	2013	2016	2019	rBV	143476	133228	3.27%	0.354%
30	13.992	2019	2024	2032	rVV	1140058	1200634	29.44%	3.193%
31	15.039	2199	2202	2204	rBV	44407	62218	1.53%	0.165%
32	15.062	2204	2206	2209	rVB2	83044	79682	1.95%	0.212%
33	15.462	2270	2274	2285	rVB	721693	980000	24.03%	2.606%
34	15.856	2339	2341	2346	rVB	40565	52703	1.29%	0.140%

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Instrument :
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ClientSampleId :
BU-02-121217

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

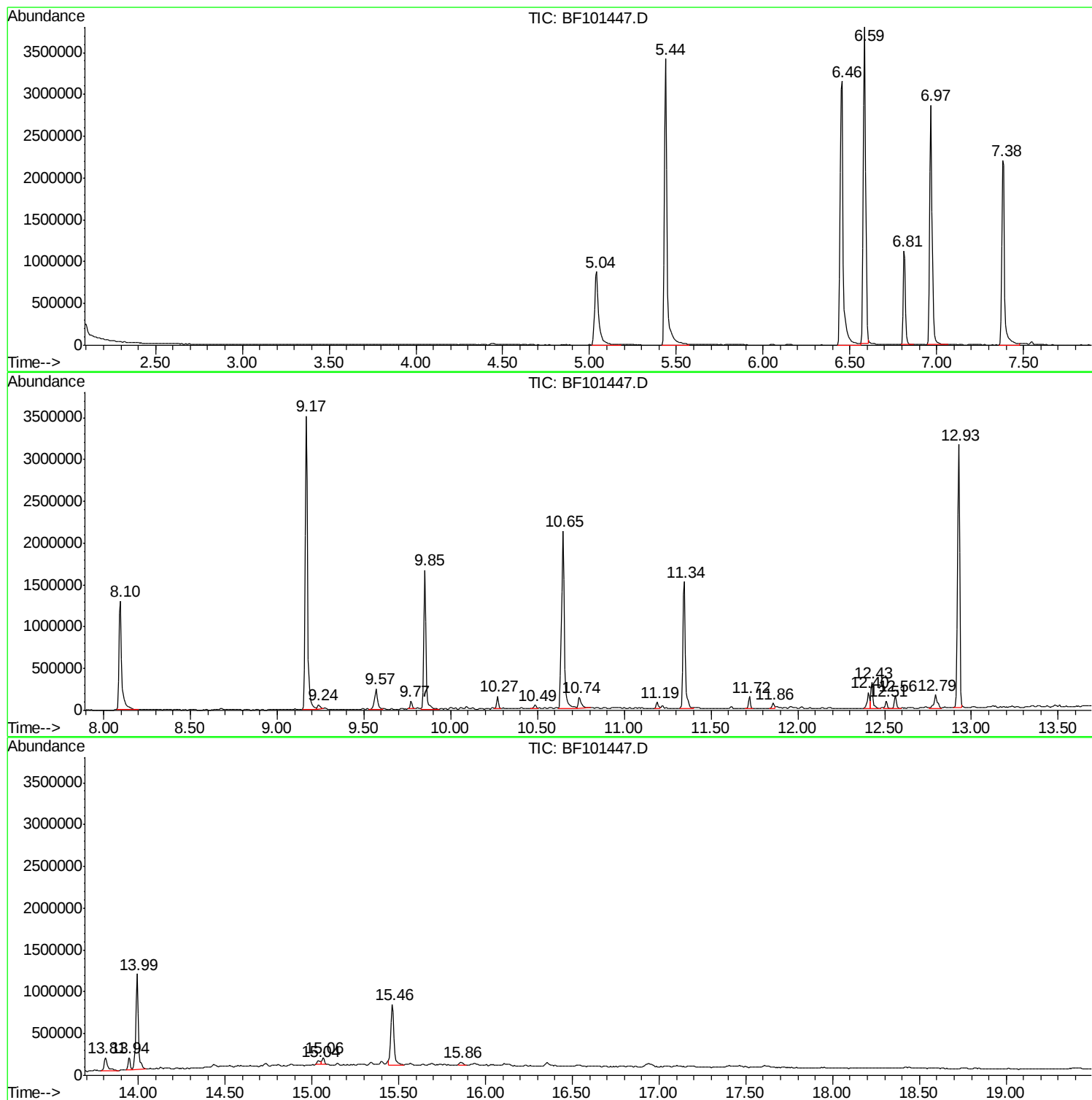
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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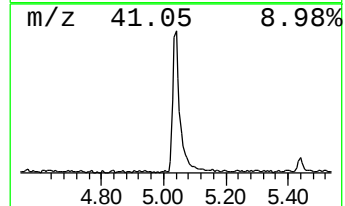
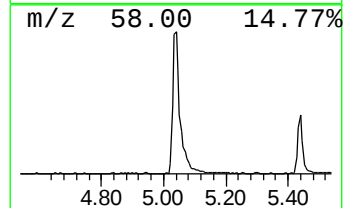
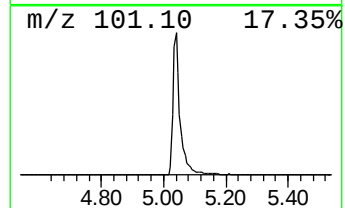
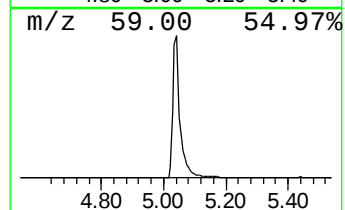
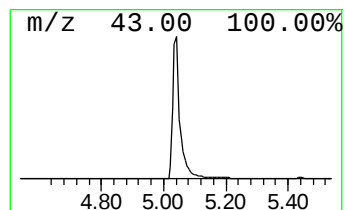
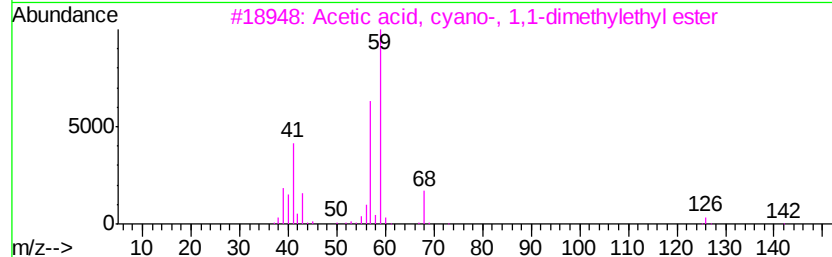
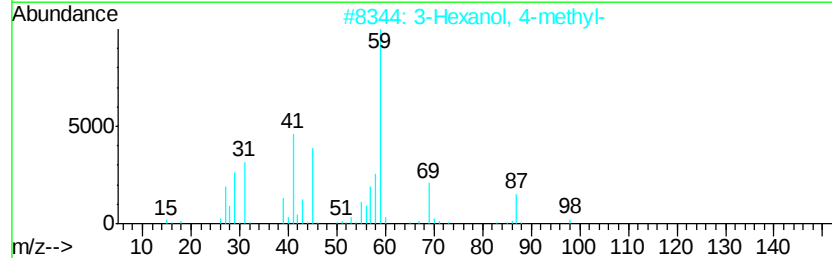
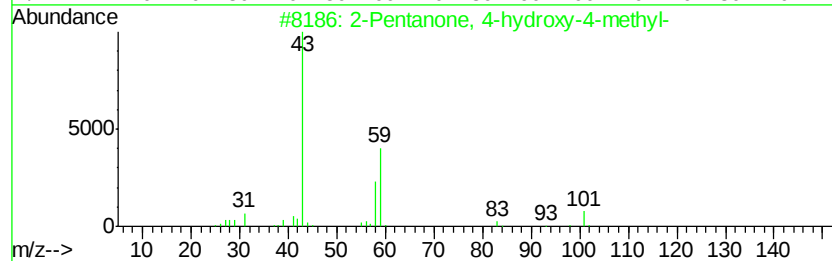
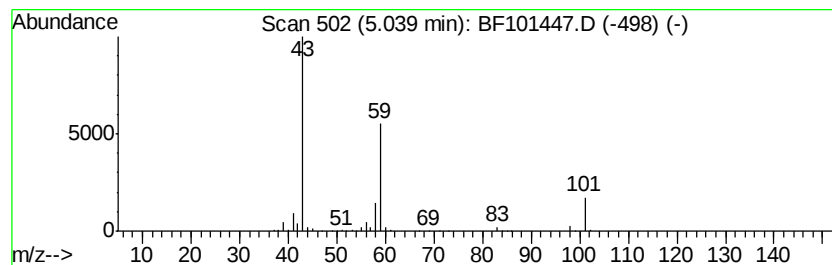
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	26.29 ng	1420890	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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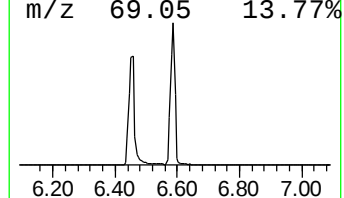
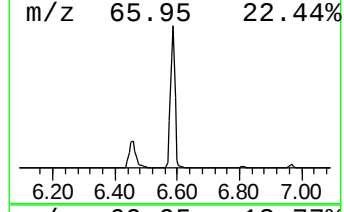
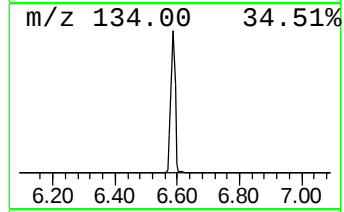
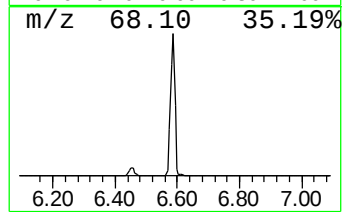
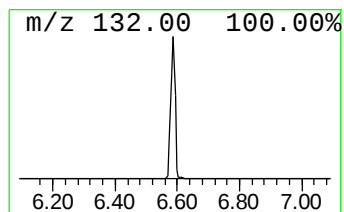
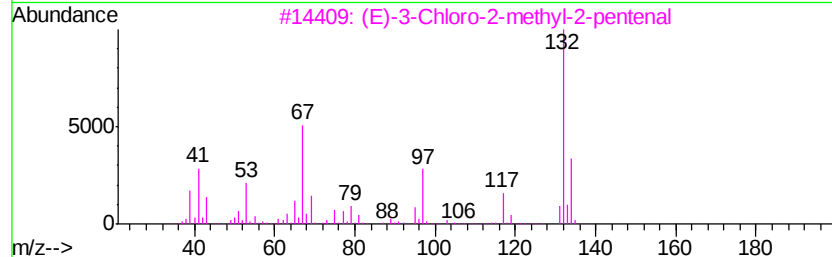
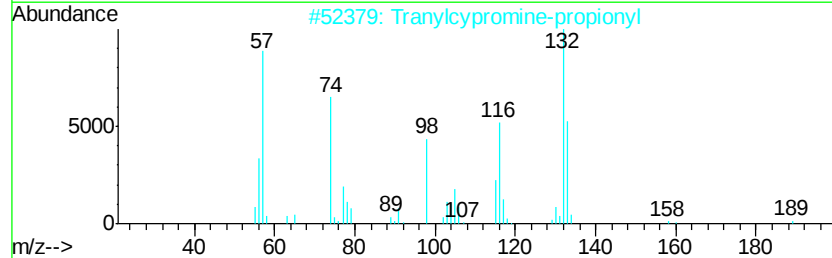
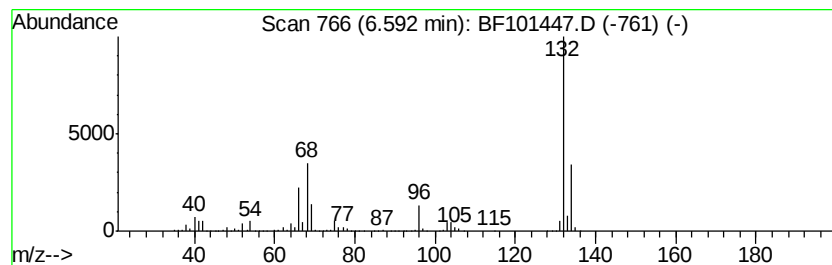
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	66.69 ng	3603930	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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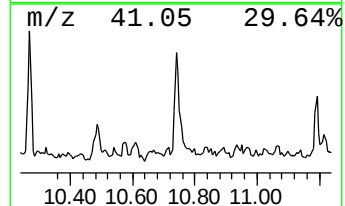
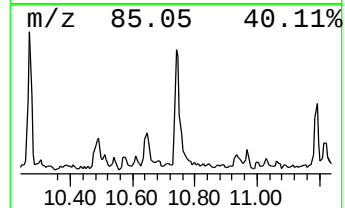
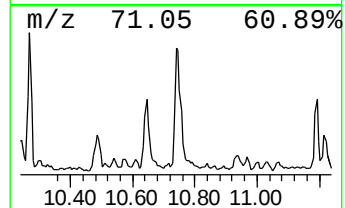
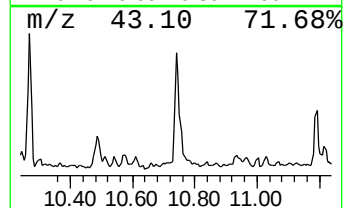
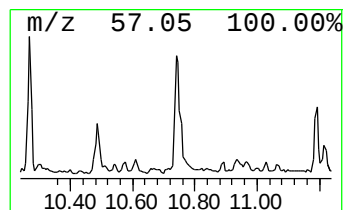
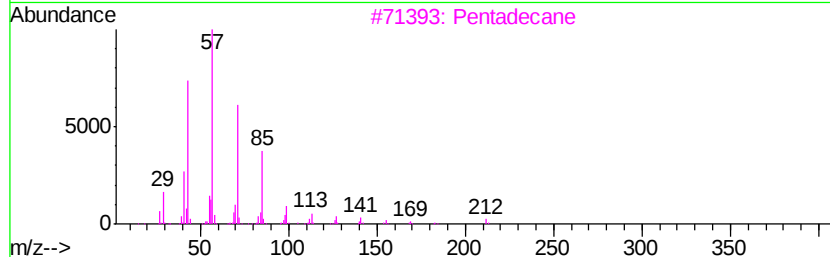
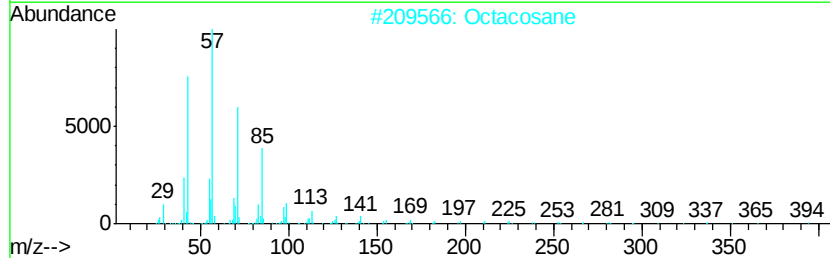
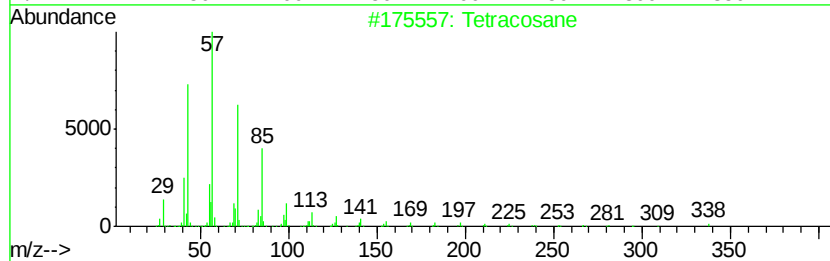
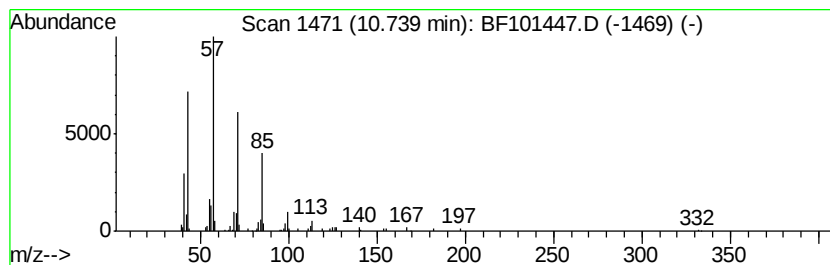
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.11 ng	168577	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Pentadecane	212	C15H32	000629-62-9	90
4		Tetradecane	198	C14H30	000629-59-4	87
5		Tritetracontane	605	C43H88	007098-21-7	83



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ALS Vial : 10 Sample Multiplier: 1

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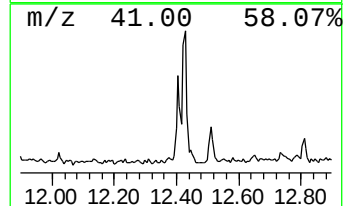
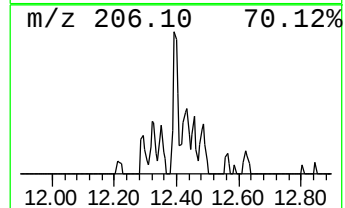
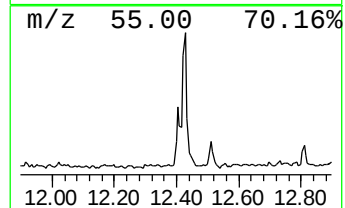
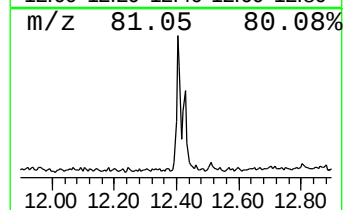
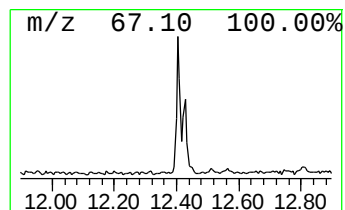
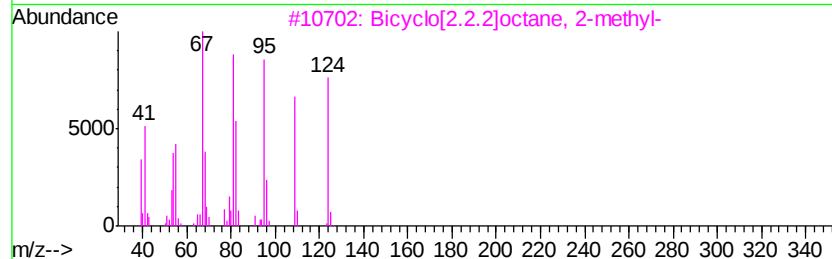
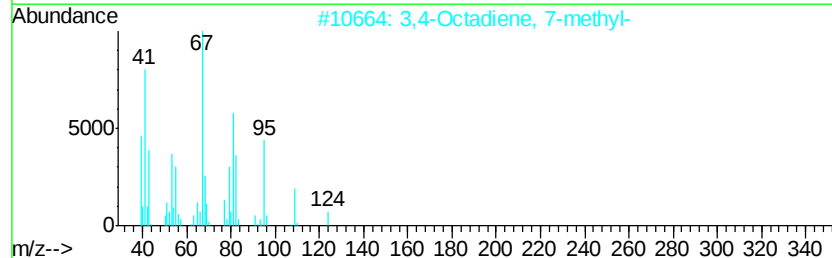
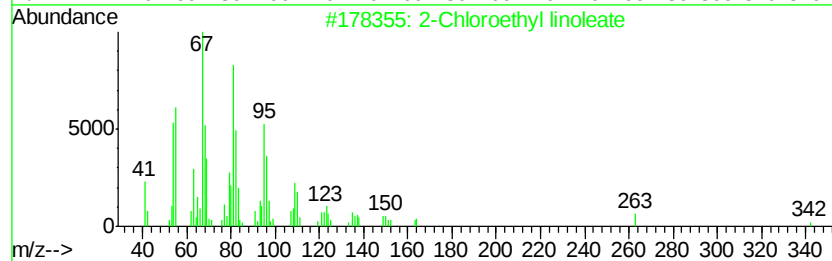
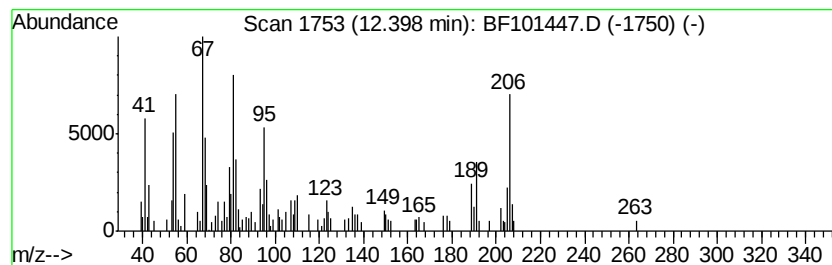
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Chloroethyl linoleate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	2.36 ng	188932	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90
2		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	83
3		Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	81
4		9,12-Octadecadienoic acid, methyl...	294	C19H34O2	002566-97-4	76
5		11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	70



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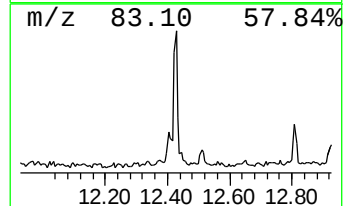
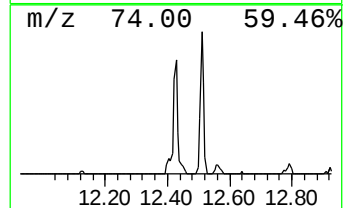
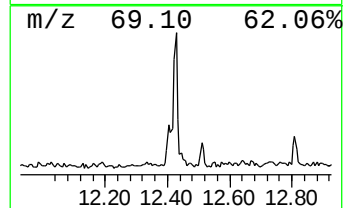
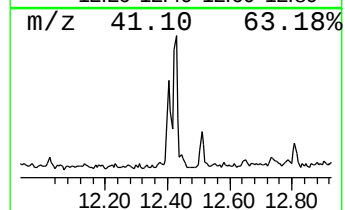
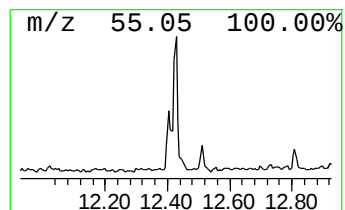
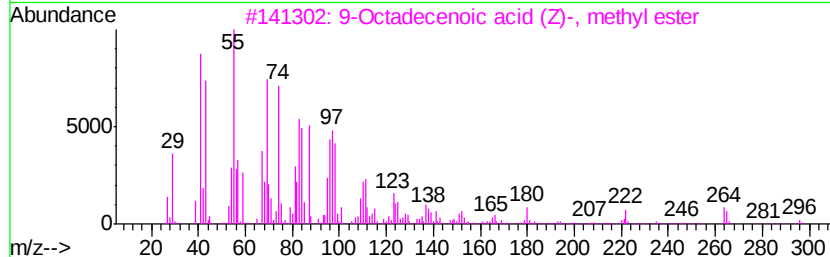
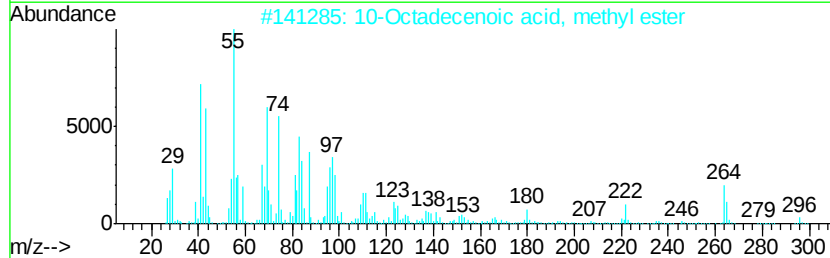
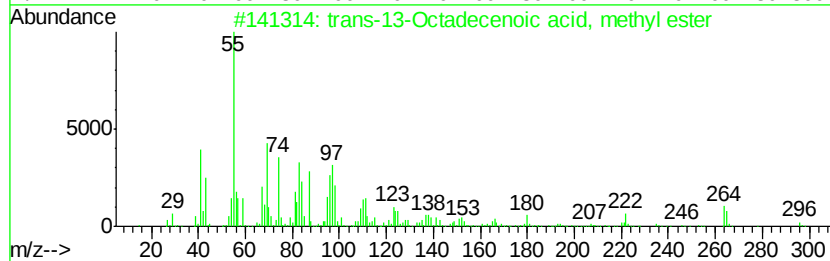
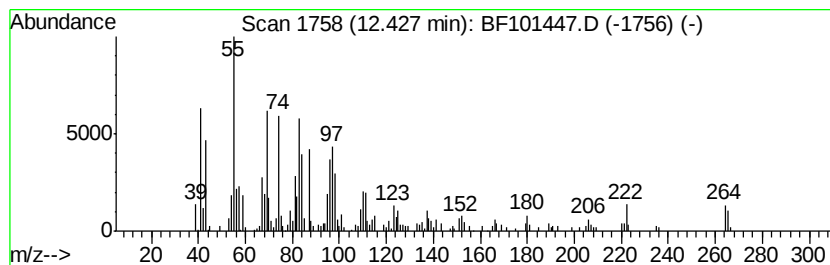
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	3.40 ng	272273	Phenanthrene-d10	11.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4			16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91



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ClientSampleId :
BU-02-121217

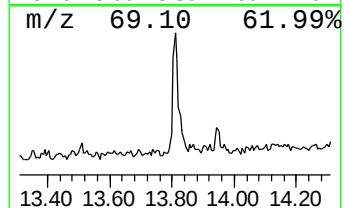
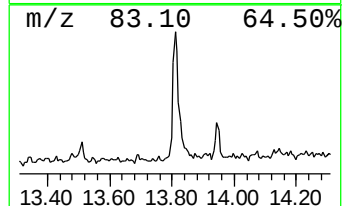
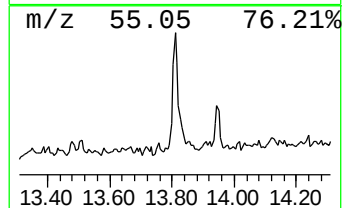
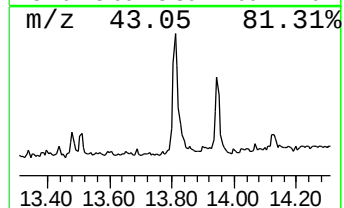
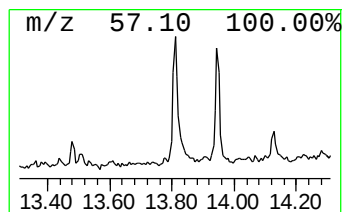
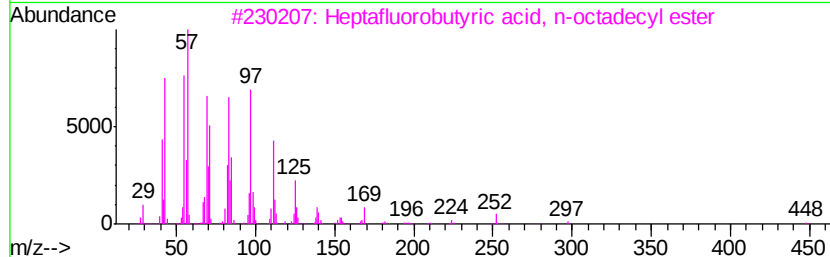
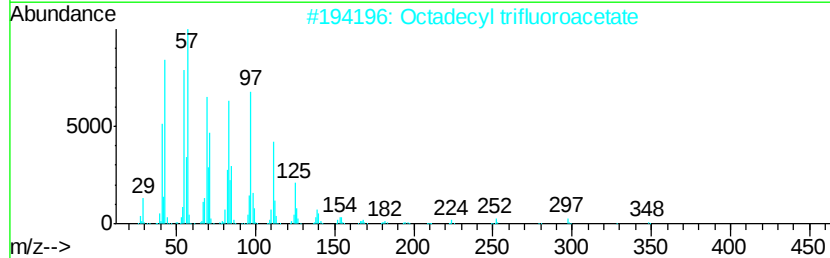
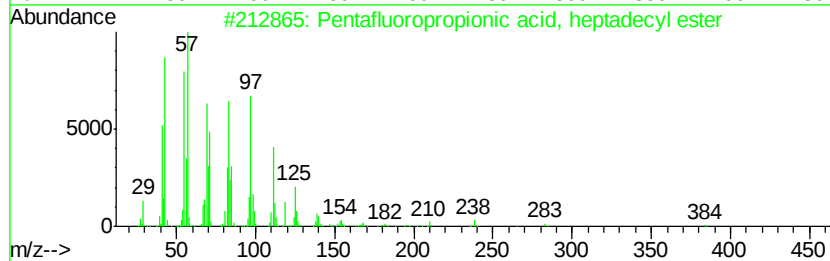
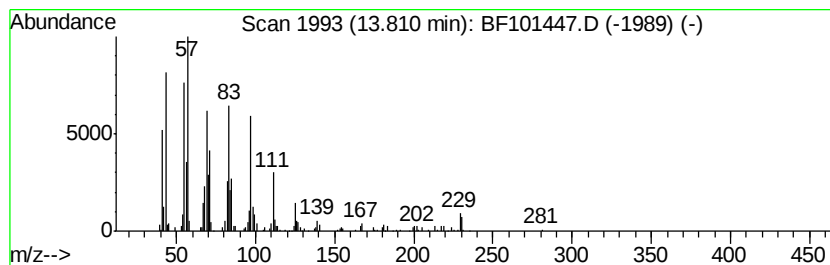
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
13.81	3.73 ng	224079	Chrysene-d12	13.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
3			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101447.D
Acq On : 15 Dec 2017 17:12
Operator : SJ/JU
Sample : I6684-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-02-121217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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
unknown5.04	5.04	26.3	ng	1420890	1	6.81	1080880	20.0
unknown6.59	6.59	66.7	ng	3603930	1	6.81	1080880	20.0
Tetracosane	10.74	2.1	ng	168577	4	11.35	1600210	20.0
2-Chloroethyl lin...	12.40	2.4	ng	188932	4	11.35	1600210	20.0
trans-13-Octadece...	12.43	3.4	ng	272273	4	11.35	1600210	20.0
Pentafluoropropio...	13.81	3.7	ng	224079	5	13.99	1200630	20.0