

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
 Data File : BF122328.D
 Acq On : 13 Nov 2020 14:35
 Operator : JU/CG
 Sample : L4586-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 R-LA-33-4-WC

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122328.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	15	rVB	1043282	1330498	16.50%	2.140%
2	3.299	203	206	219	rBV	39981	89980	1.12%	0.145%
3	5.475	570	576	579	rBV	6405327	6449264	79.98%	10.374%
4	6.487	742	748	751	rBV	5908973	6667626	82.69%	10.725%
5	6.687	779	782	789	rBV	215259	187489	2.33%	0.302%
6	6.863	809	812	815	rBV	1883133	1414094	17.54%	2.275%
7	7.428	902	908	911	rBV	4232901	4307220	53.42%	6.928%
8	8.145	1026	1030	1034	rBV	2141324	1851462	22.96%	2.978%
9	9.228	1209	1214	1217	rBV	8032868	7457291	92.48%	11.995%
10	9.616	1276	1280	1283	rBV	1664640	1258910	15.61%	2.025%
11	9.904	1325	1329	1332	rBV	2698077	2129037	26.40%	3.425%
12	10.692	1458	1463	1466	rBV	4535583	4411773	54.71%	7.096%
13	11.386	1577	1581	1585	rBV	2676958	2192184	27.19%	3.526%
14	11.922	1663	1672	1696	rBV	2247603	3050522	37.83%	4.907%
15	12.374	1746	1749	1753	rVB	163109	133322	1.65%	0.214%
16	12.710	1800	1806	1820	rBV	1847578	2691547	33.38%	4.329%
17	12.980	1847	1852	1855	rBV	8295815	8063581	100.00%	12.970%
18	13.210	1888	1891	1898	rBV2	67089	85040	1.05%	0.137%
19	13.810	1990	1993	1999	rBV3	66204	92585	1.15%	0.149%
20	13.880	2001	2005	2025	rVV	587794	1139943	14.14%	1.834%
21	14.027	2025	2030	2033	rBV	2389990	2205653	27.35%	3.548%
22	14.504	2105	2111	2113	rBV2	107064	119003	1.48%	0.191%
23	14.963	2185	2189	2197	rBV	544528	569082	7.06%	0.915%
24	15.092	2203	2211	2218	rBV8	37902	120510	1.49%	0.194%
25	15.157	2218	2222	2224	rBV	150697	166225	2.06%	0.267%
26	15.186	2224	2227	2242	rVB2	319162	739430	9.17%	1.189%
27	15.492	2273	2279	2284	rBV2	1625994	2036763	25.26%	3.276%
28	15.745	2317	2322	2328	rBV	158409	210234	2.61%	0.338%
29	15.980	2358	2362	2367	rBV	142739	210630	2.61%	0.339%
30	16.039	2367	2372	2381	rBV2	138143	404494	5.02%	0.651%
31	16.492	2444	2449	2459	rVB3	40032	80893	1.00%	0.130%
32	17.333	2587	2592	2601	rVB6	65660	144261	1.79%	0.232%
33	17.592	2629	2636	2647	rVB6	47637	158391	1.96%	0.255%

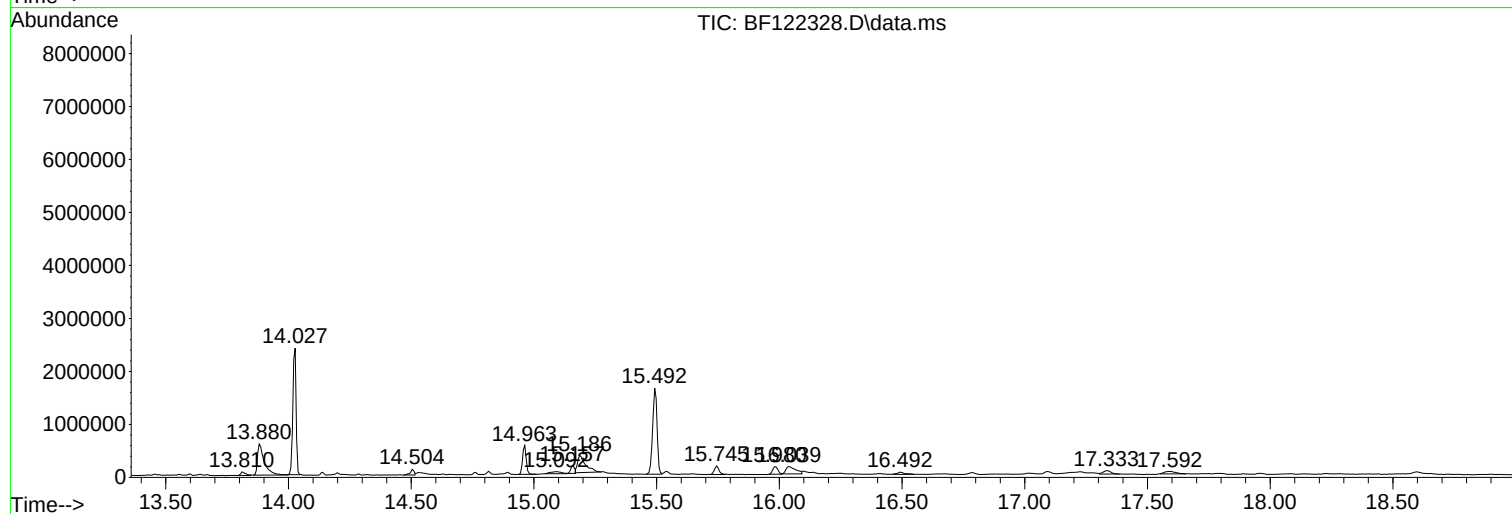
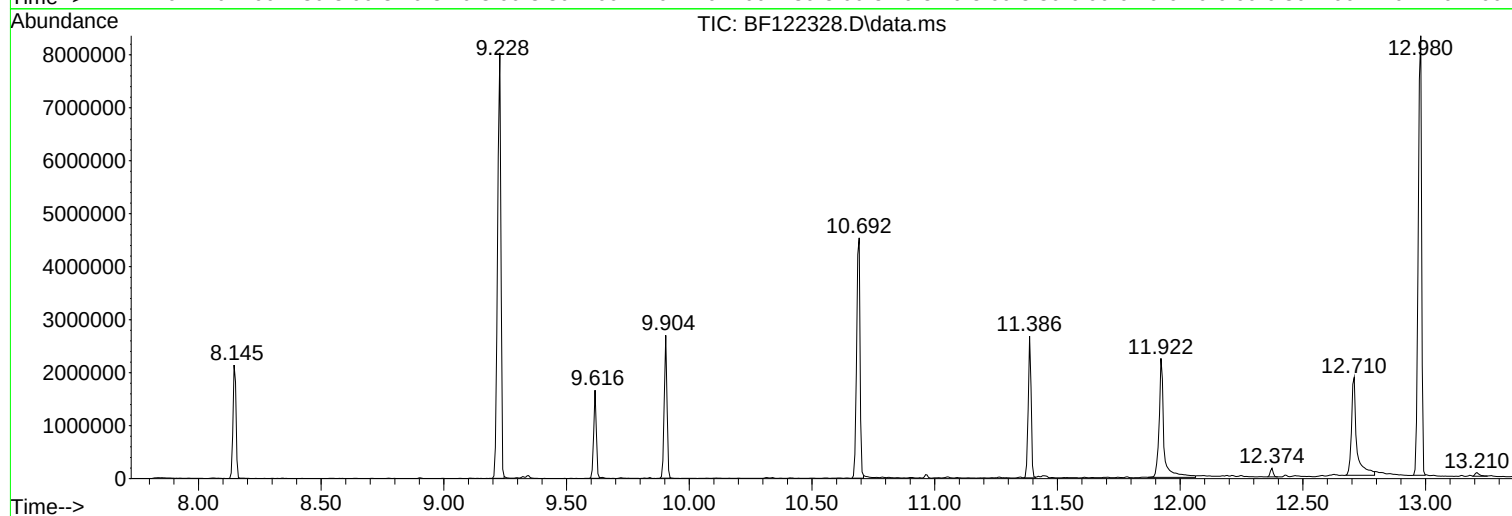
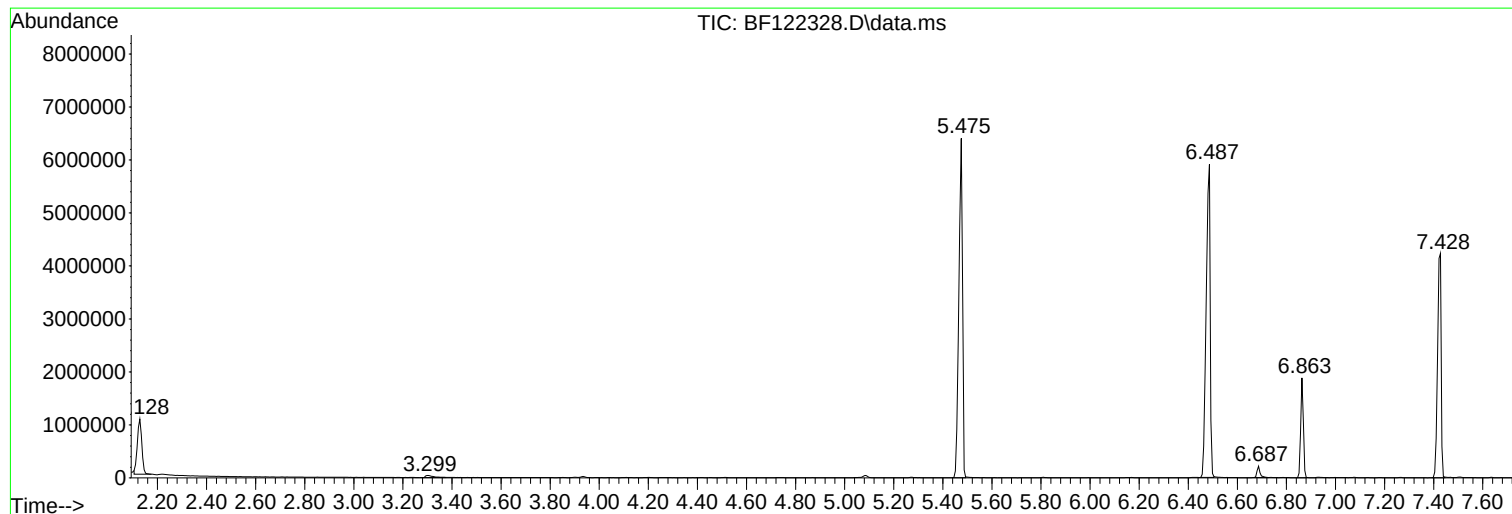
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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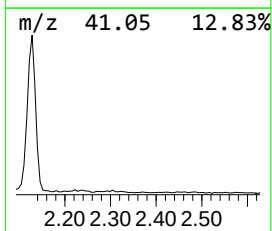
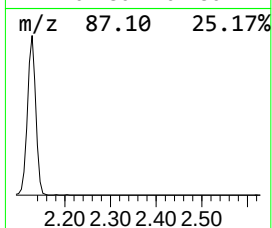
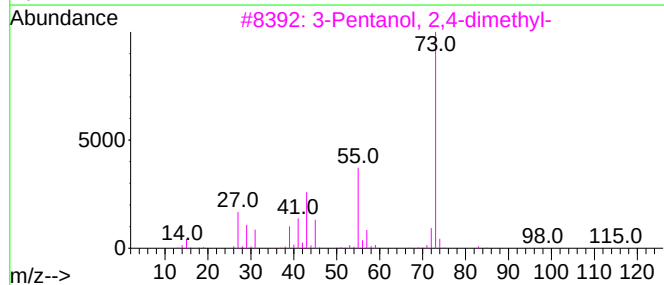
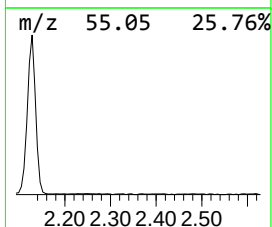
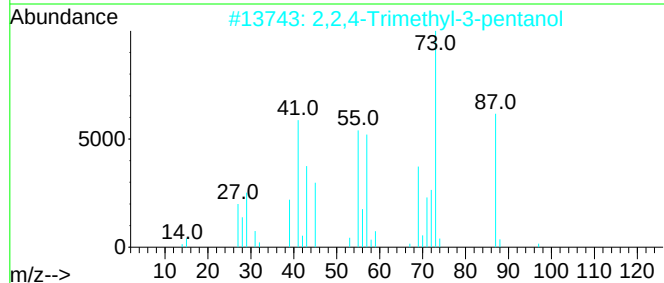
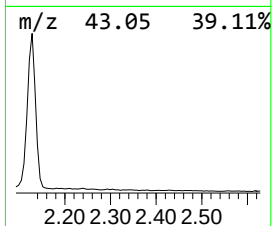
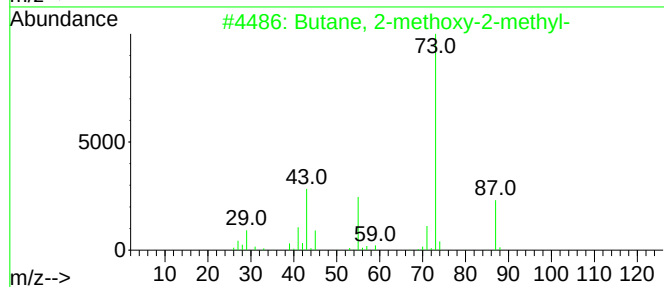
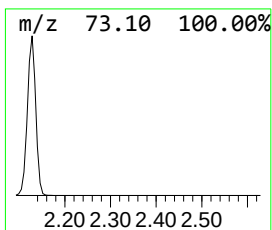
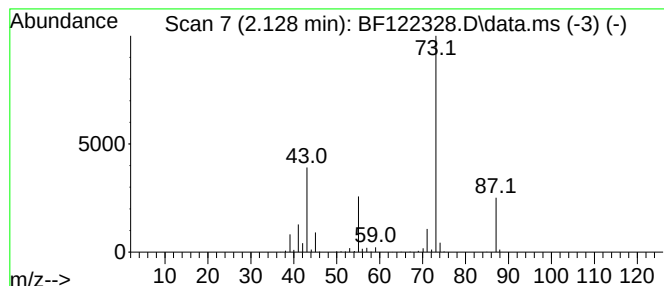
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	18.82 ng	1330500	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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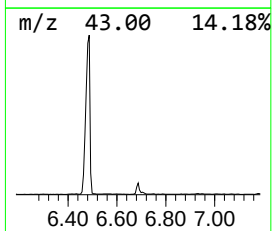
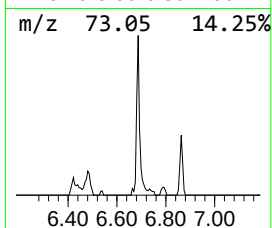
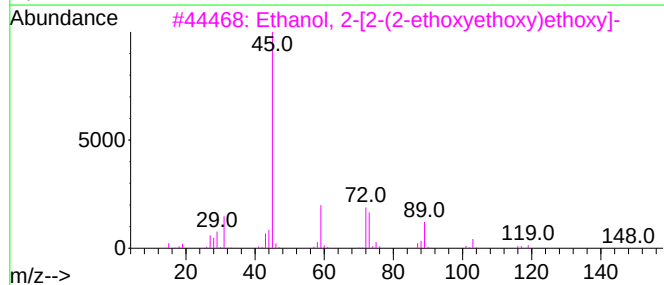
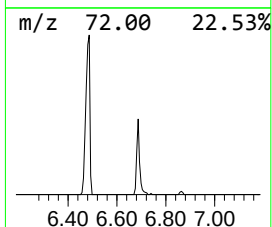
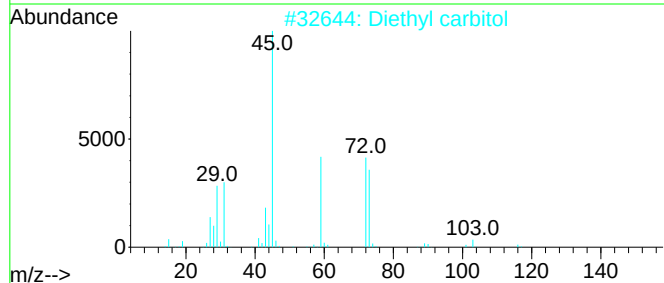
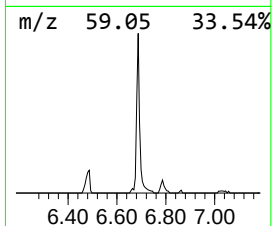
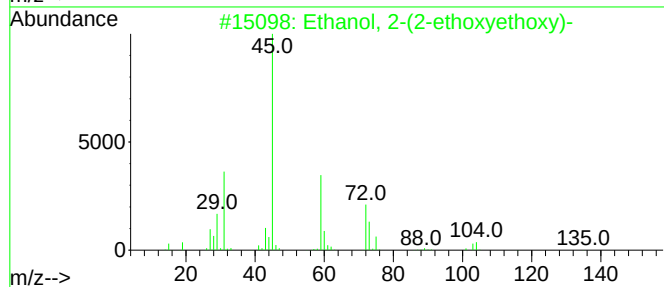
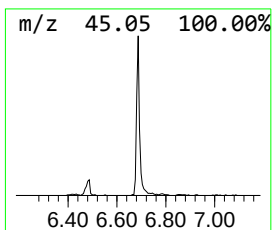
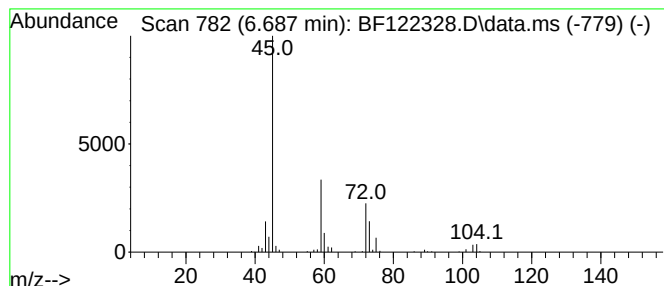
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	2.65 ng	187489	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	38



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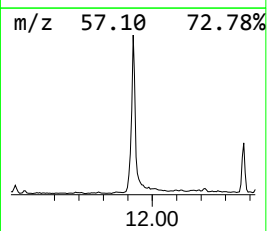
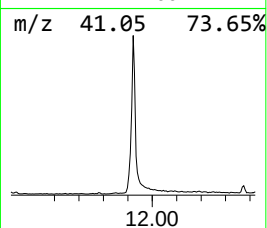
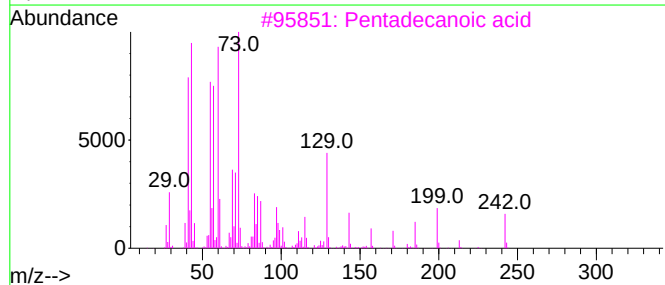
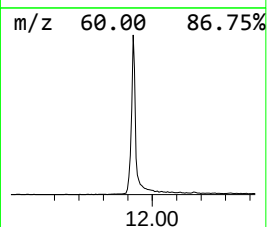
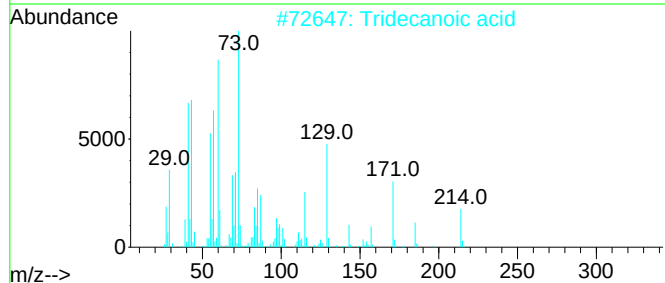
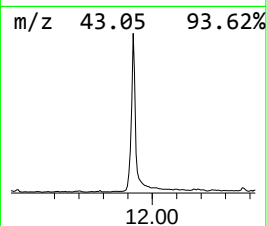
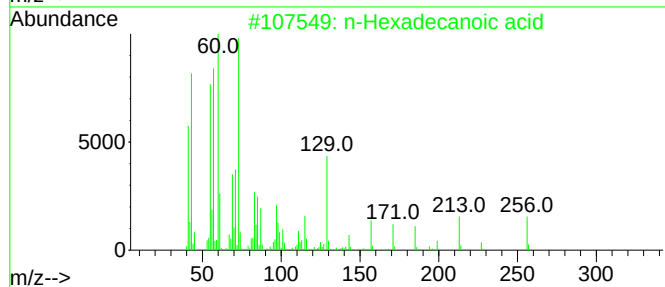
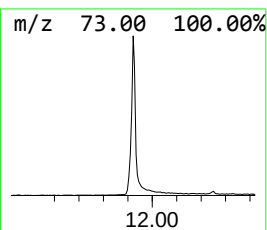
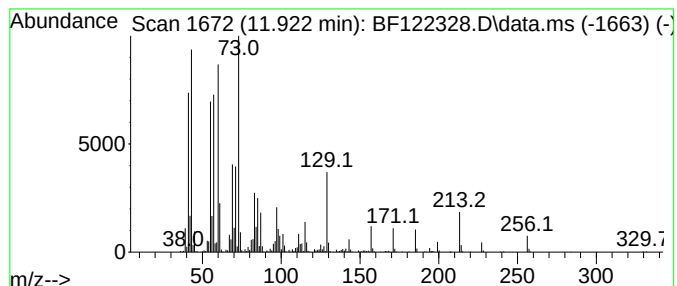
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	27.83 ng	3050520	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5			Octadecanoic acid	284	C18H36O2	000057-11-4	53



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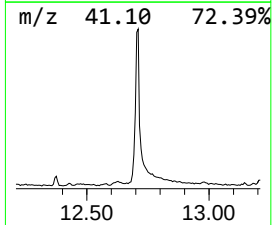
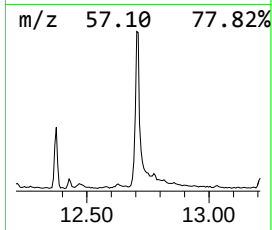
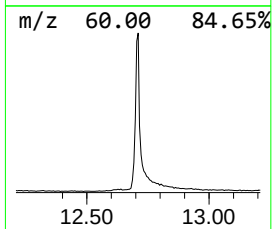
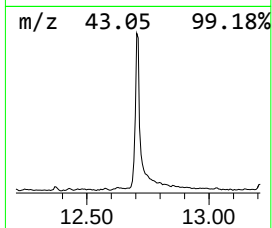
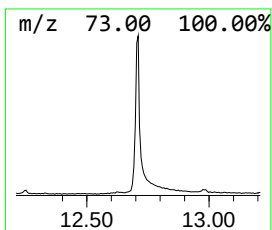
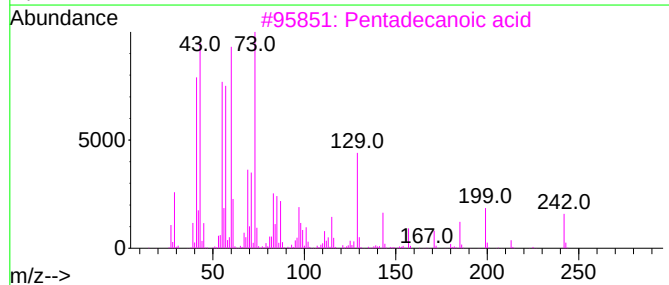
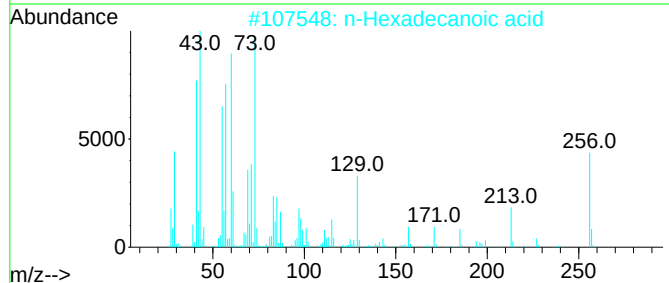
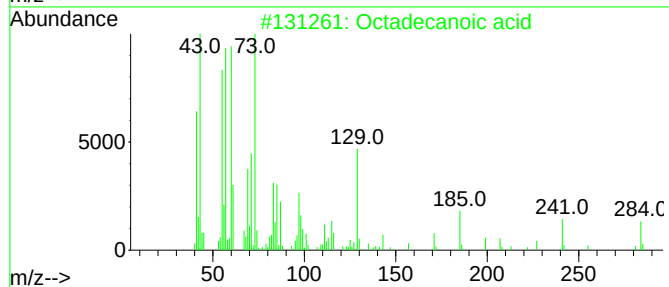
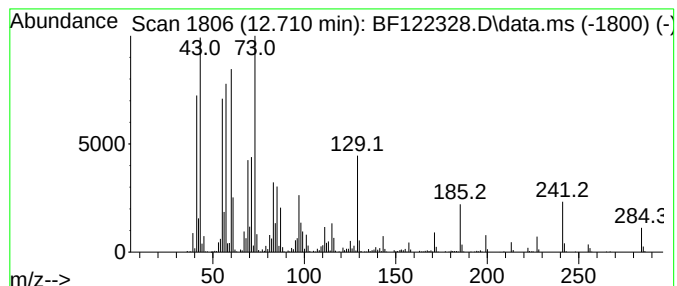
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	24.41 ng	2691550	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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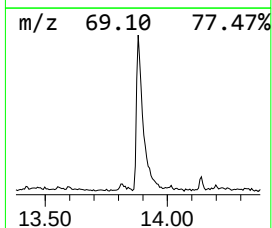
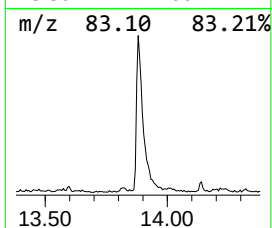
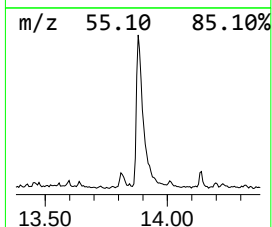
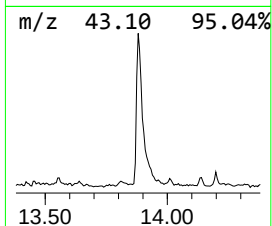
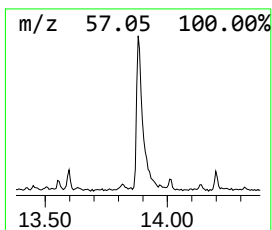
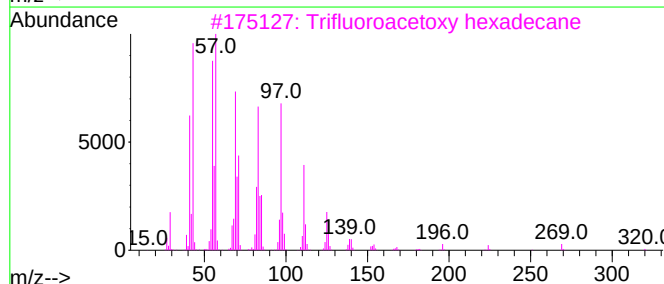
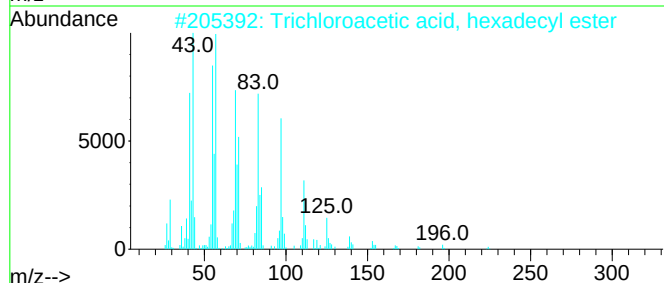
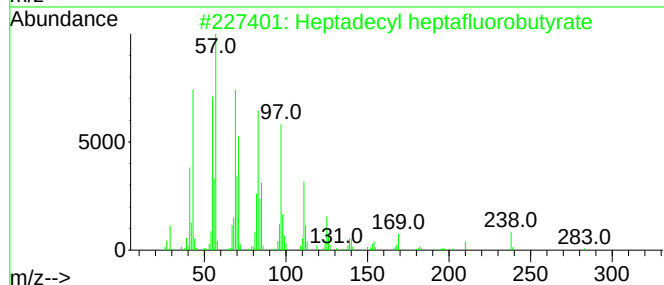
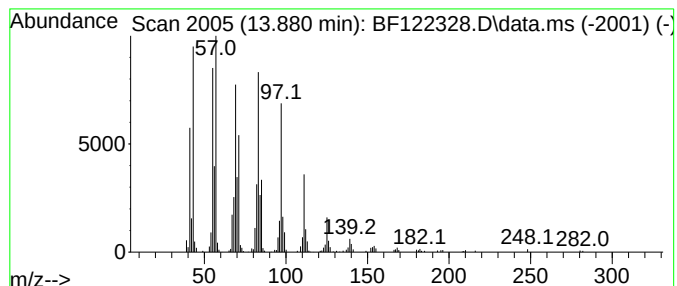
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.34 ng	1139940	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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R-LA-33-4-WC

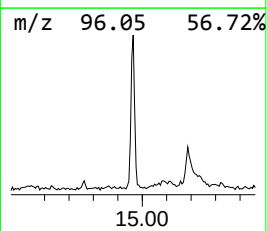
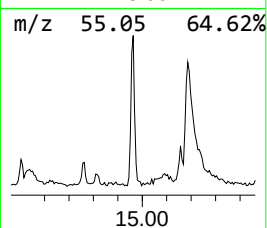
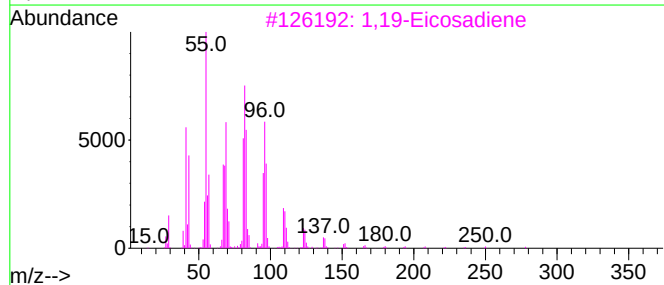
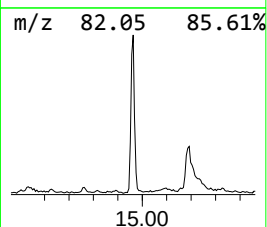
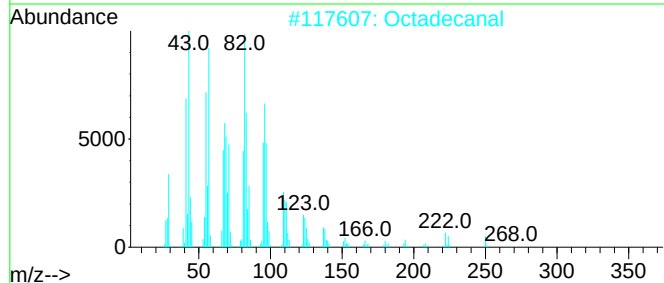
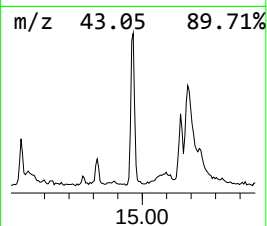
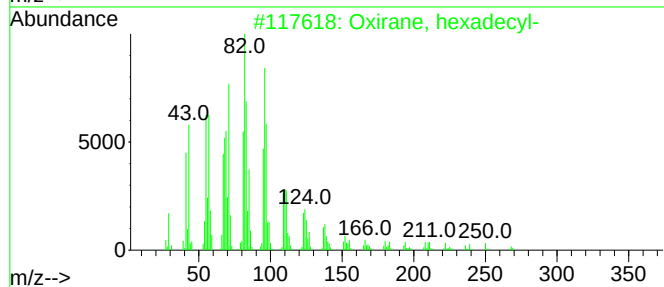
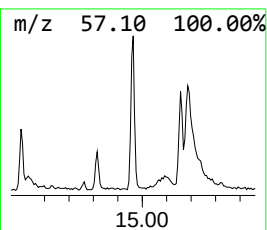
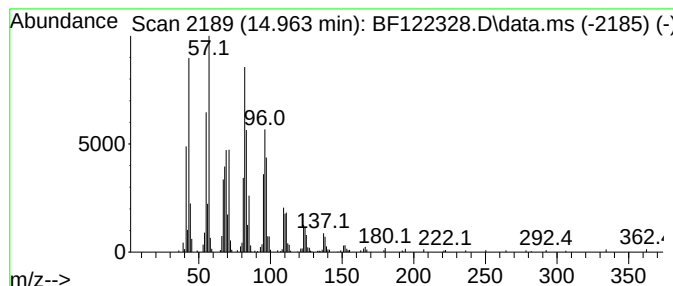
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	5.59 ng	569082	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Octadecanal	268	C18H36O	000638-66-4	91
3			1,19-Eicosadiene	278	C20H38	014811-95-1	90
4			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90
5			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122328.D
Acq On : 13 Nov 2020 14:35
Operator : JU/CG
Sample : L4586-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-33-4-WC

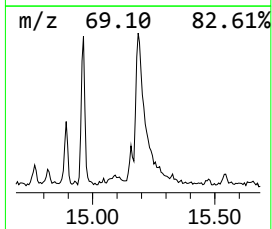
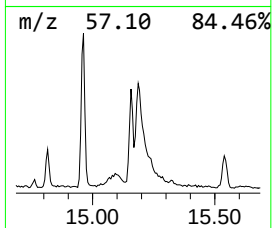
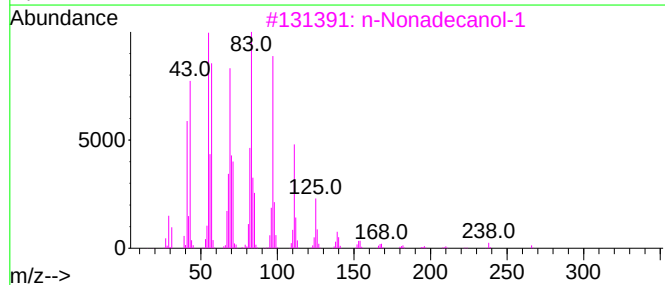
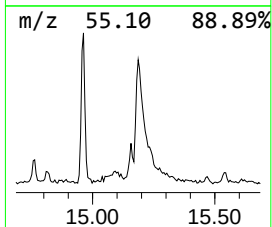
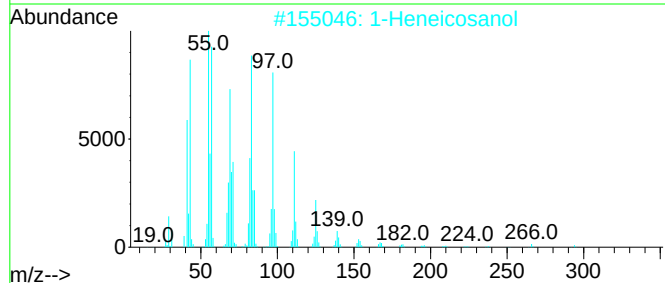
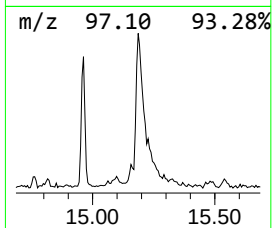
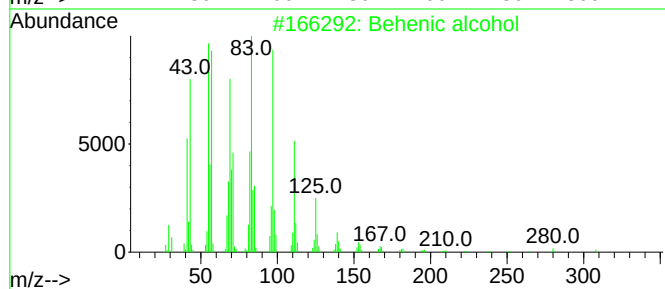
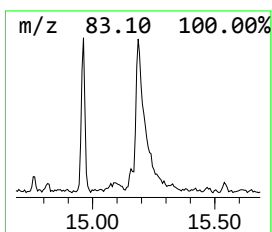
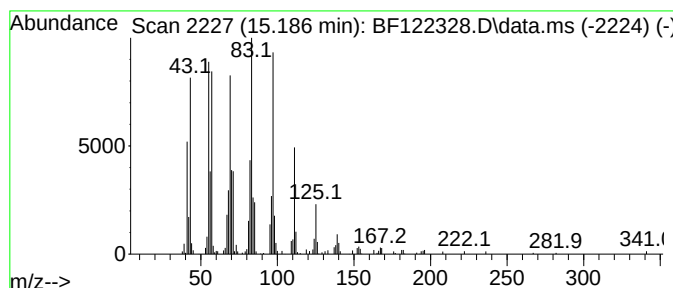
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	7.26 ng	739430	Perylene-d12	15.492

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			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Heptacosanol	396	C27H56O	002004-39-9	83
5			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122328.D
Acq On : 13 Nov 2020 14:35
Operator : JU/CG
Sample : L4586-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-33-4-WC

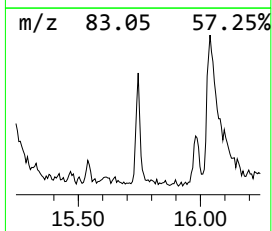
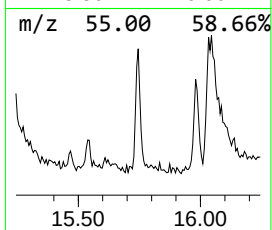
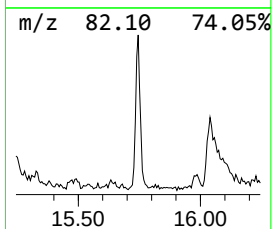
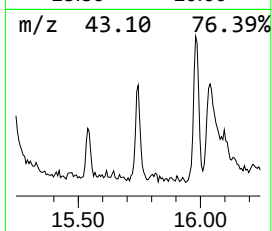
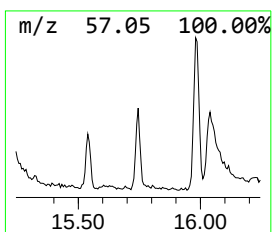
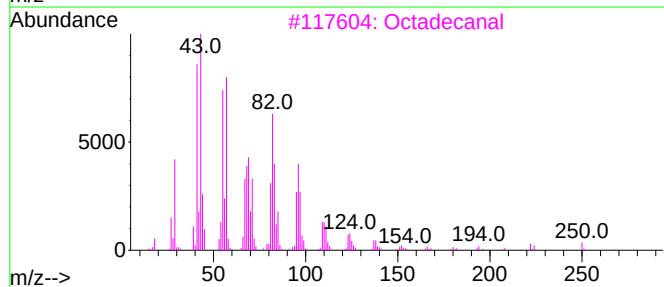
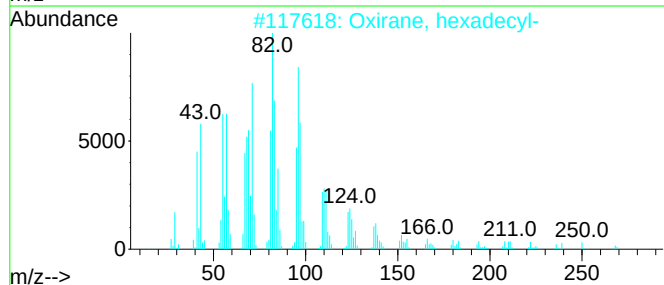
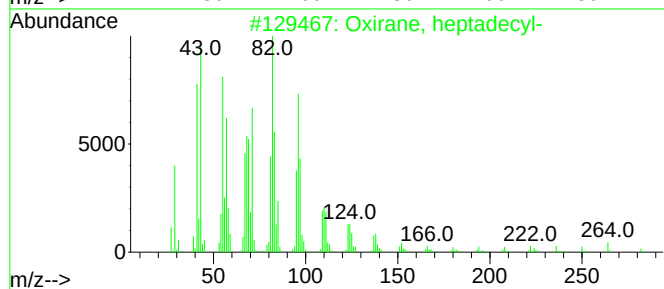
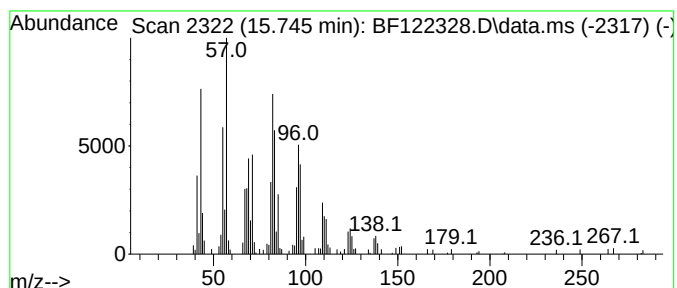
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	2.06 ng	210234	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3			Octadecanal	268	C18H36O	000638-66-4	86
4			1,19-Eicosadiene	278	C20H38	014811-95-1	81
5			18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122328.D
Acq On : 13 Nov 2020 14:35
Operator : JU/CG
Sample : L4586-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-33-4-WC

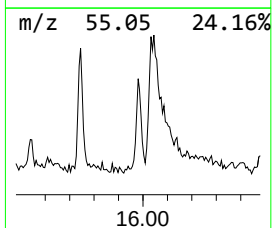
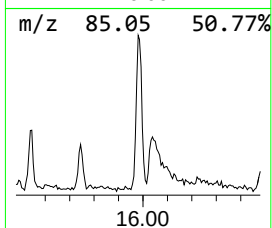
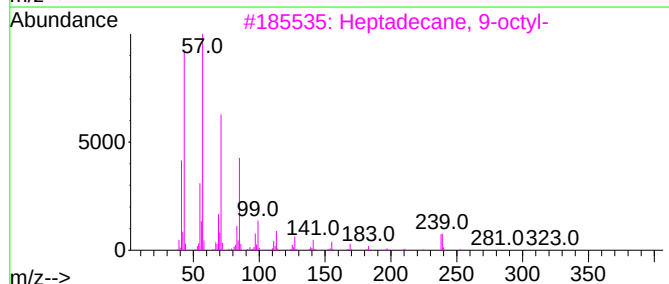
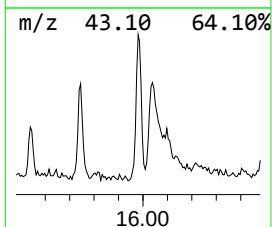
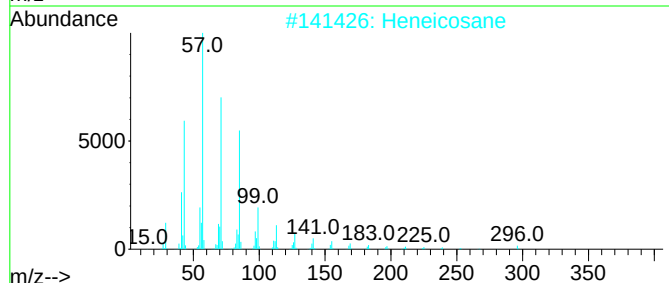
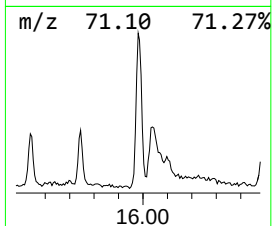
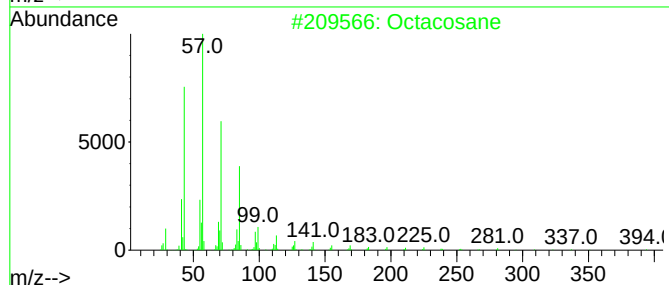
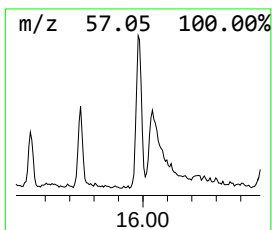
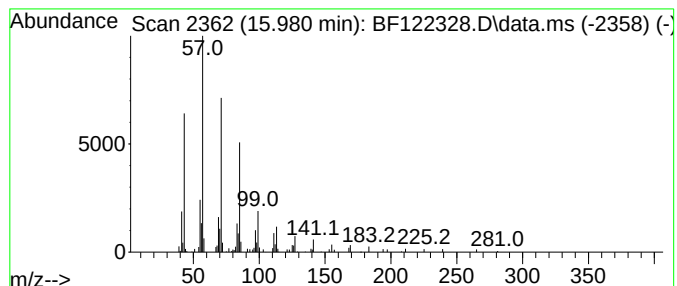
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	2.07 ng	210630	Perylene-d12	15.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122328.D
Acq On : 13 Nov 2020 14:35
Operator : JU/CG
Sample : L4586-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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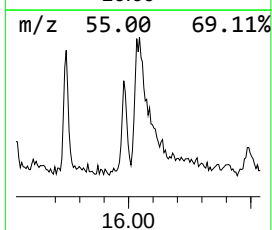
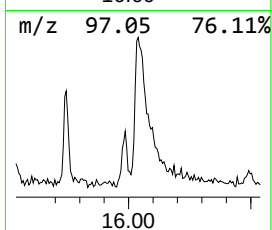
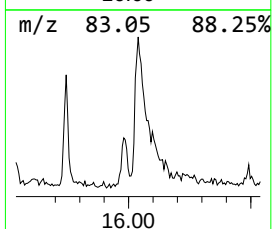
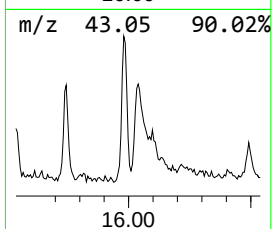
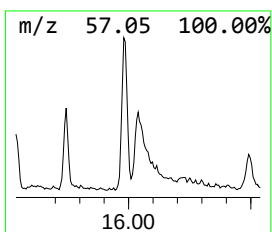
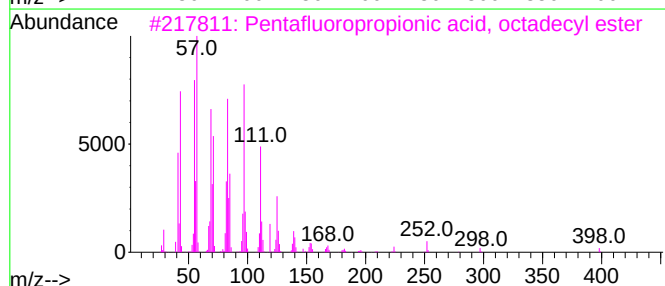
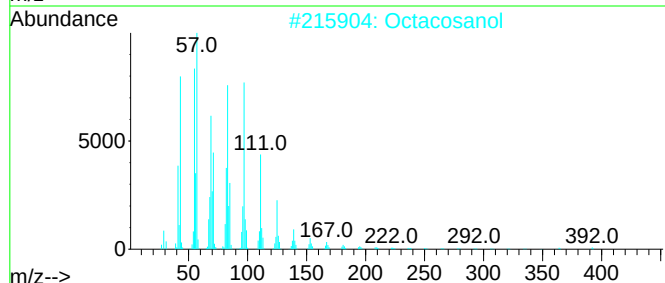
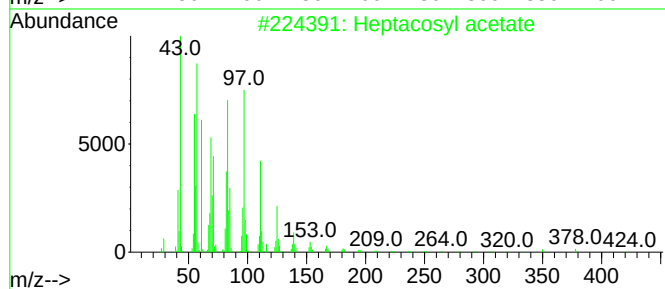
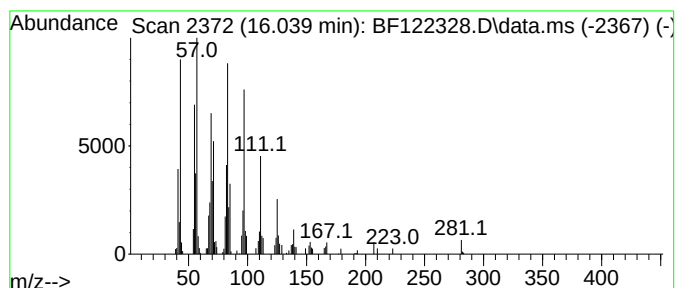
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	3.97 ng	404494	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
2			Octacosanol	410	C28H58O	000557-61-9	93
3			Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	91
4			Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	87
5			Triacontyl acetate	480	C32H64O2	041755-58-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111320\
Data File : BF122328.D
Acq On : 13 Nov 2020 14:35
Operator : JU/CG
Sample : L4586-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R-LA-33-4-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
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Ethanol, 2-(2-e...	6.687	2.6	ng	187489	1	6.863	1414090	20.0
n-Hexadecanoic ...	11.922	27.8	ng	3050520	4	11.386	2192180	20.0
Octadecanoic acid	12.710	24.4	ng	2691550	5	14.027	2205650	20.0
Heptadecyl hept...	13.880	10.3	ng	1139940	5	14.027	2205650	20.0
Oxirane, hexade...	14.963	5.6	ng	569082	6	15.492	2036760	20.0
Behenic alcohol	15.186	7.3	ng	739430	6	15.492	2036760	20.0
Oxirane, heptad...	15.745	2.1	ng	210234	6	15.492	2036760	20.0
Octacosane	15.980	2.1	ng	210630	6	15.492	2036760	20.0
Heptacosyl acetate	16.039	4.0	ng	404494	6	15.492	2036760	20.0