

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112222\
 Data File : BF131334.D
 Acq On : 22 Nov 2022 17:21
 Operator : CG\JU
 Sample : N5642-09
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LEFT-SIDE-FLATS-29

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131334.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	27	34	42	rVB	888165	1238046	44.21%	5.993%
2	5.193	522	528	539	rBV	268201	353763	12.63%	1.712%
3	5.575	588	593	596	rBV	2438338	2432313	86.85%	11.773%
4	6.581	758	764	772	rBV	2183124	2484435	88.71%	12.026%
5	6.963	825	829	832	rVB	747362	569110	20.32%	2.755%
6	7.528	920	925	928	rBV	1695245	1578017	56.35%	7.638%
7	8.251	1044	1048	1051	rBV	910417	734891	26.24%	3.557%
8	9.333	1227	1232	1235	rBV	3243043	2800576	100.00%	13.556%
9	10.016	1344	1348	1351	rBV	1064557	854548	30.51%	4.136%
10	10.733	1464	1470	1473	rBV	191100	150269	5.37%	0.727%
11	10.810	1478	1483	1496	rBV	1471360	1457245	52.03%	7.054%
12	11.510	1598	1602	1606	rBV	956188	846445	30.22%	4.097%
13	11.580	1609	1614	1616	rBV2	53973	49579	1.77%	0.240%
14	11.616	1617	1620	1623	rBV	45993	33524	1.20%	0.162%
15	12.022	1681	1689	1696	rBV	208973	325014	11.61%	1.573%
16	12.739	1805	1811	1815	rBV8	29416	71486	2.55%	0.346%
17	12.816	1816	1824	1839	rVB	682512	1042354	37.22%	5.045%
18	13.110	1869	1874	1877	rBV	2627304	2312427	82.57%	11.193%
19	13.810	1988	1993	1998	rBV3	27120	43729	1.56%	0.212%
20	14.010	2023	2027	2030	rBV	41733	41712	1.49%	0.202%
21	14.168	2050	2054	2057	rBV	556899	462361	16.51%	2.238%
22	14.327	2078	2081	2088	rVB	41437	47368	1.69%	0.229%
23	14.404	2089	2094	2101	rVB3	26418	40783	1.46%	0.197%
24	14.639	2130	2134	2141	rVB	37569	39762	1.42%	0.192%
25	14.968	2178	2190	2193	rBV3	37165	97052	3.47%	0.470%
26	15.339	2249	2253	2259	rBV	23998	33307	1.19%	0.161%
27	15.563	2286	2291	2297	rBV4	17526	33762	1.21%	0.163%
28	15.710	2311	2316	2321	rBV2	386641	485619	17.34%	2.351%

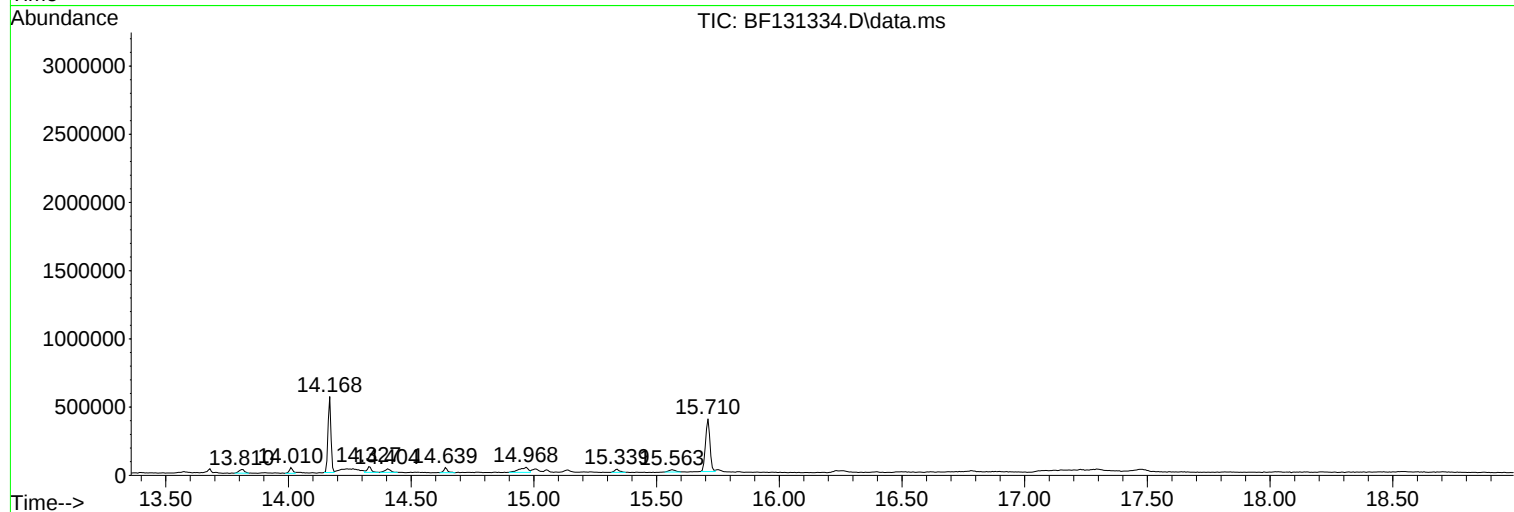
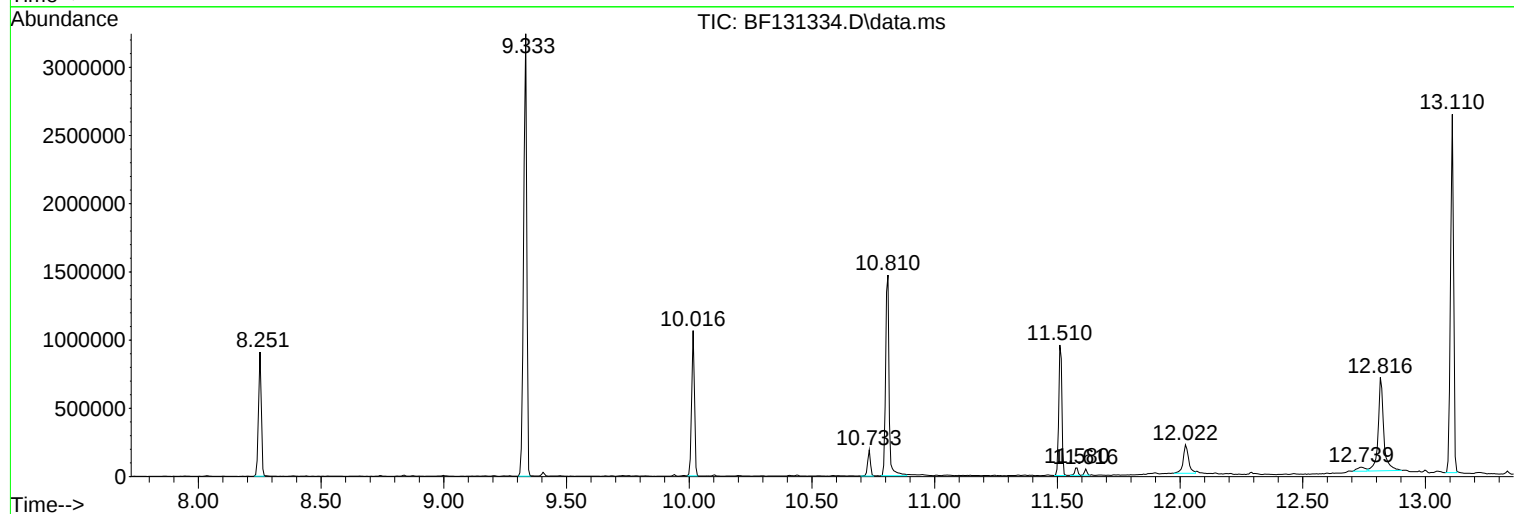
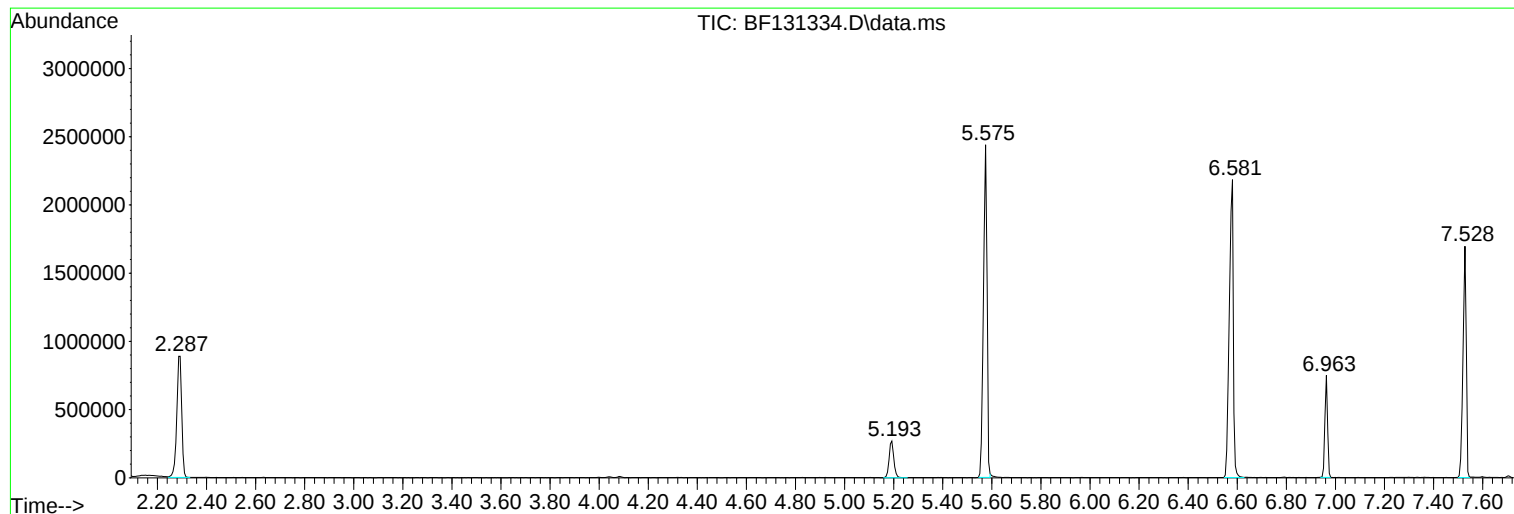
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BNA_F
ClientSampleId :
LEFT-SIDE-FLATS-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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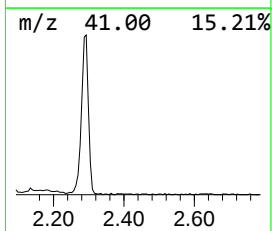
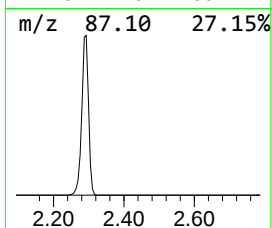
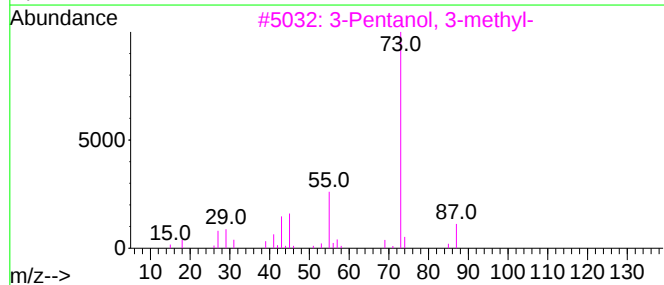
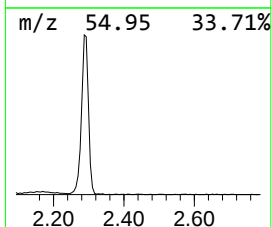
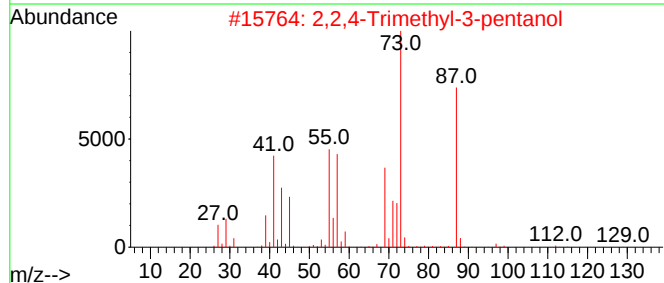
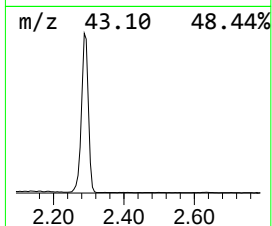
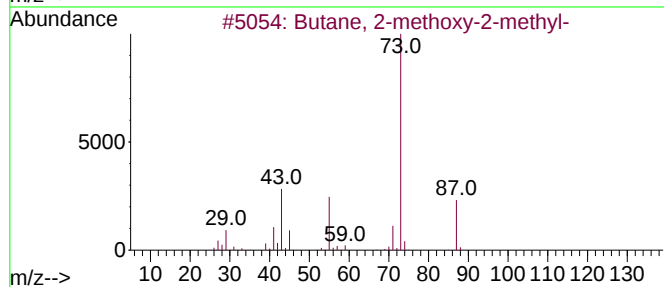
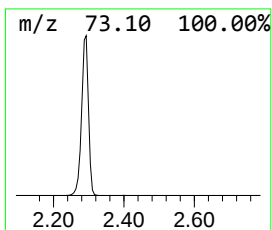
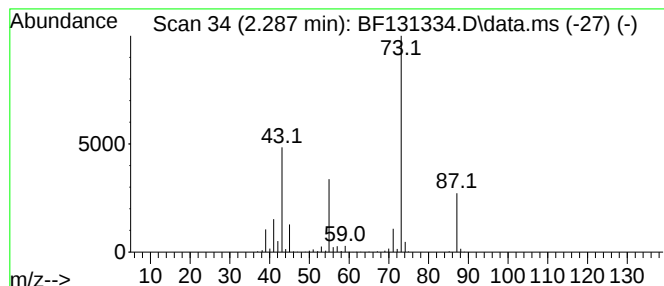
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	43.51 ng	1238050	1,4-Dichlorobenzene-d4	6.963

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	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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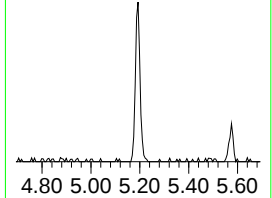
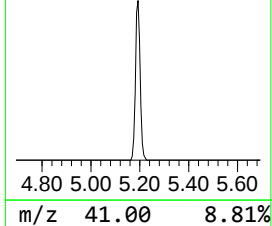
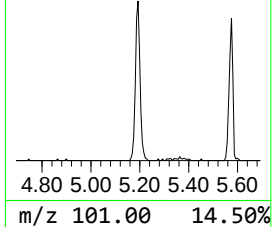
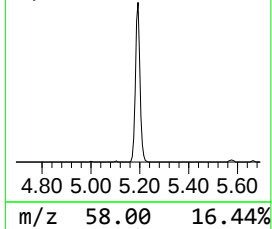
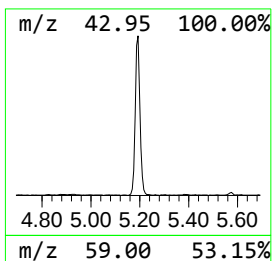
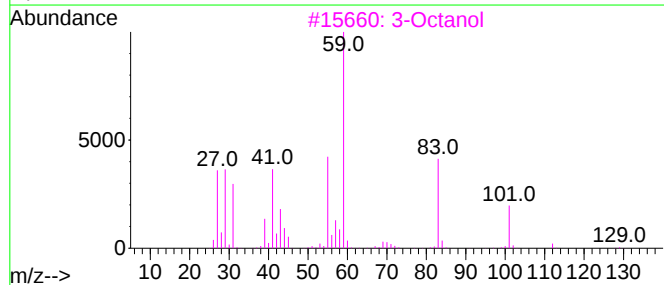
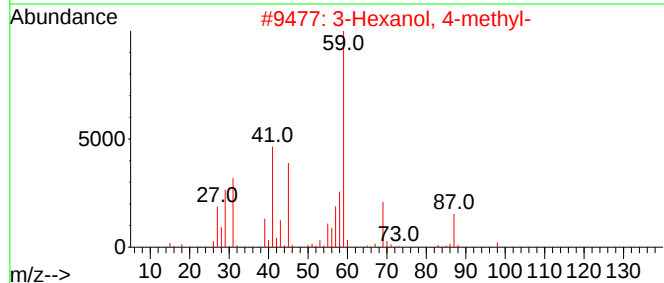
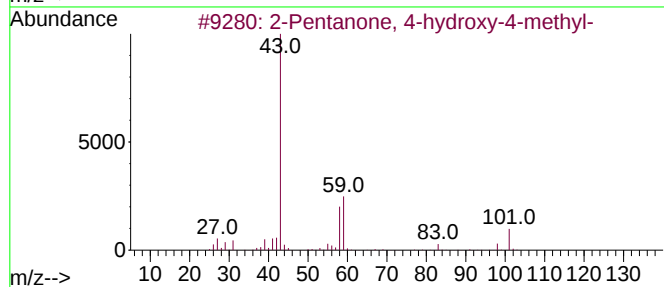
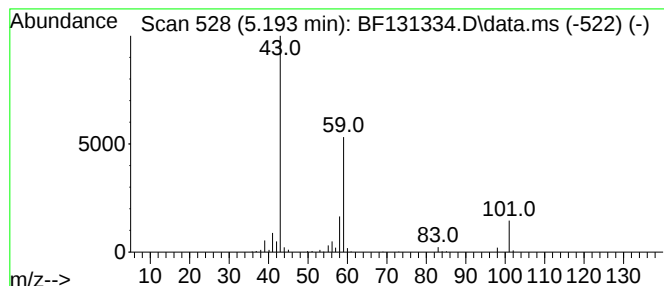
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.193	12.43 ng	353763	1,4-Dichlorobenzene-d4	6.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		3-Octanol	130	C8H18O	000589-98-0	33
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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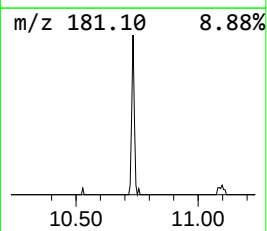
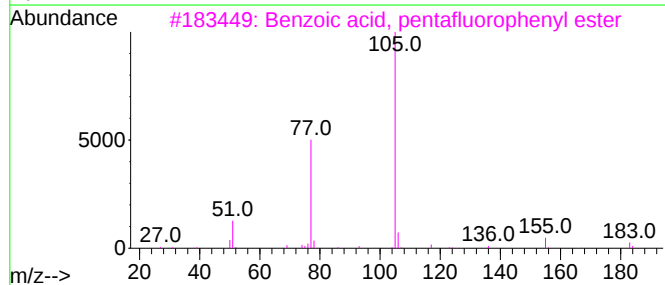
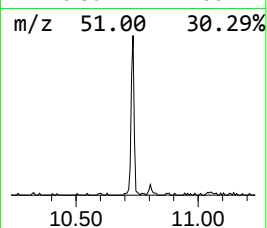
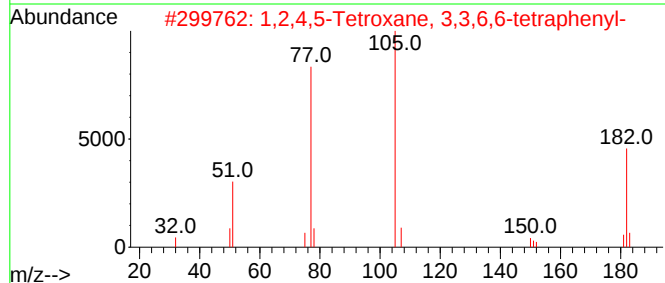
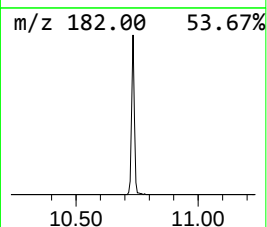
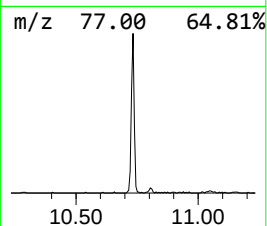
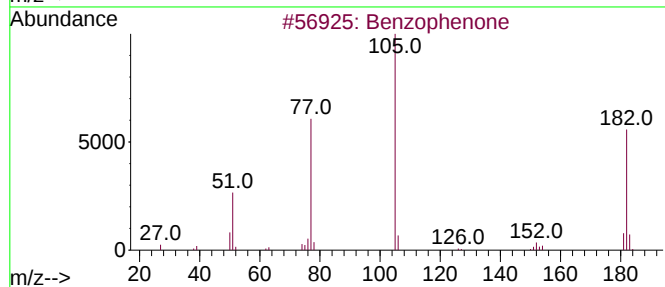
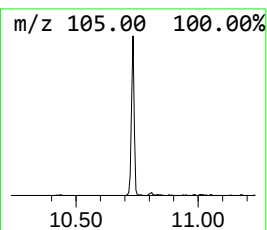
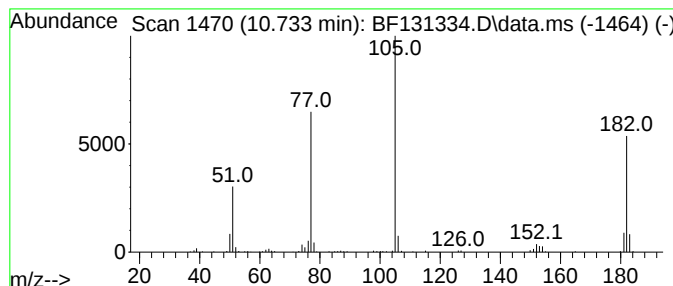
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	3.52 ng	150269	Acenaphthene-d10	10.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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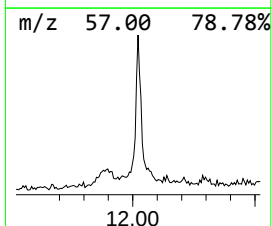
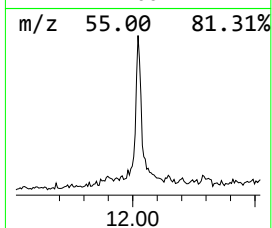
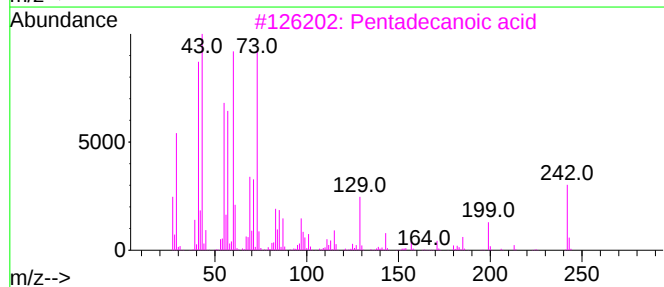
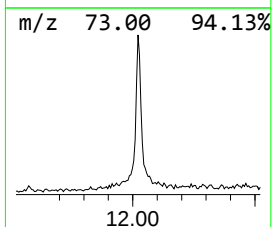
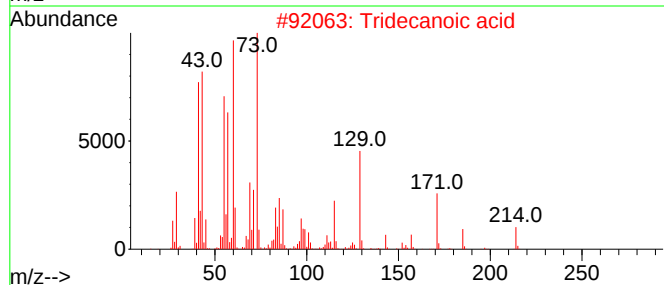
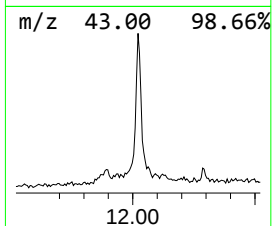
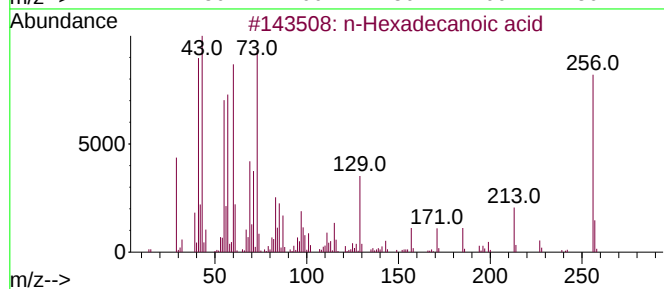
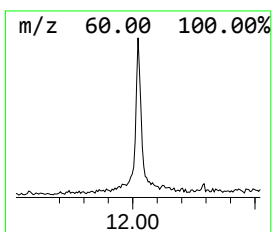
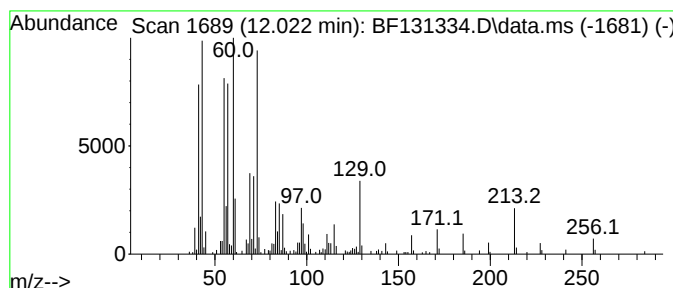
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	7.68 ng	325014	Phenanthrene-d10	11.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Octadecanoic acid	284	C18H36O2	000057-11-4	58



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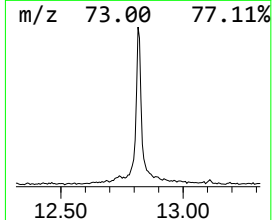
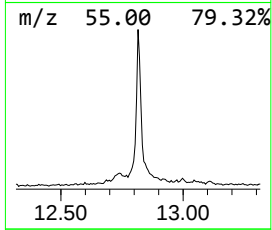
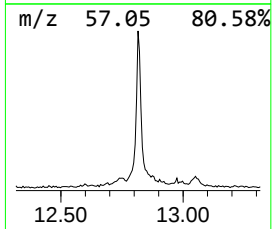
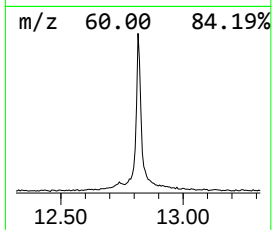
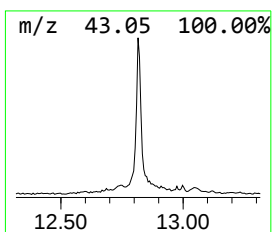
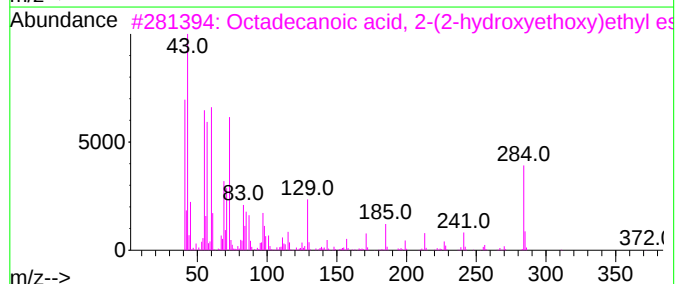
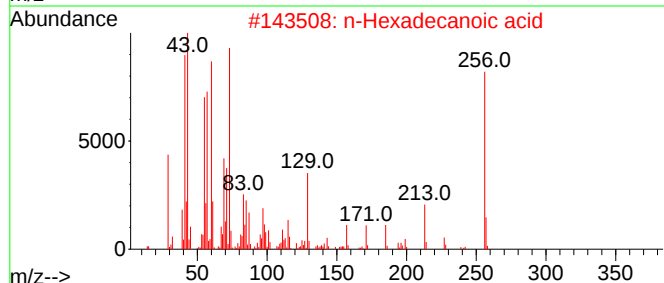
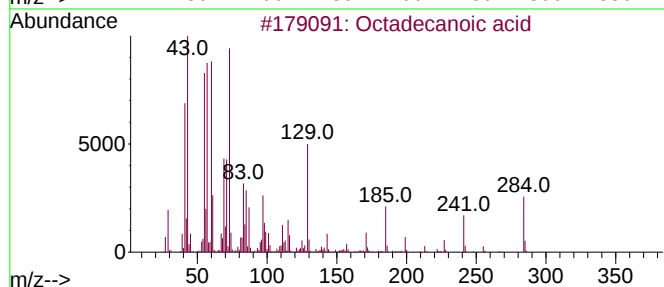
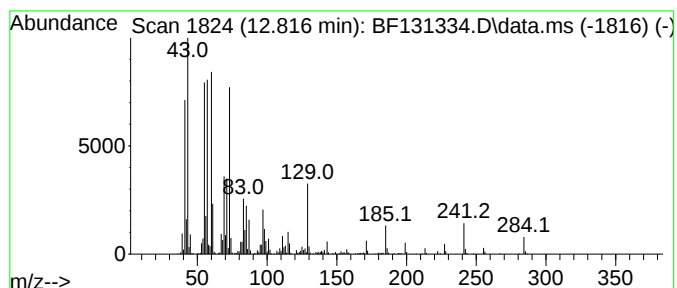
Instrument :
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ClientSampleId :
LEFT-SIDE-FLATS-29

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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.816	24.63 ng	1042350	Phenanthrene-d10	11.510	
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	93
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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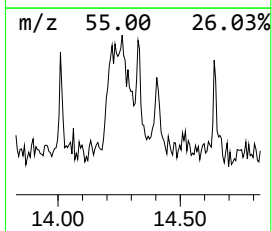
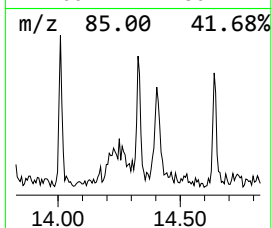
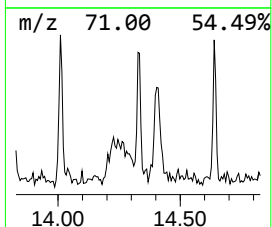
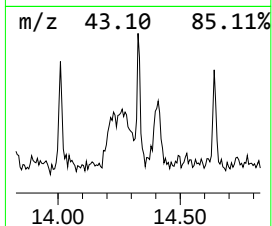
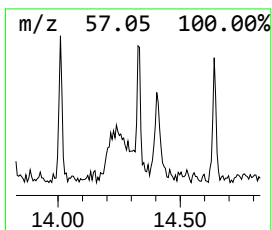
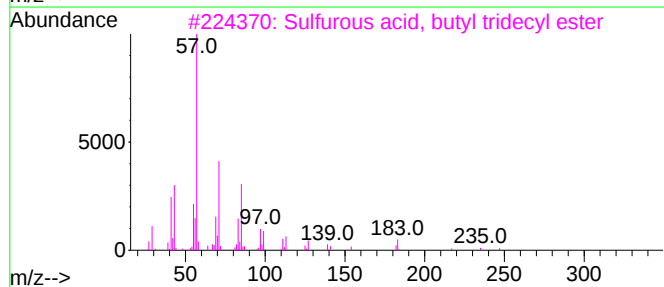
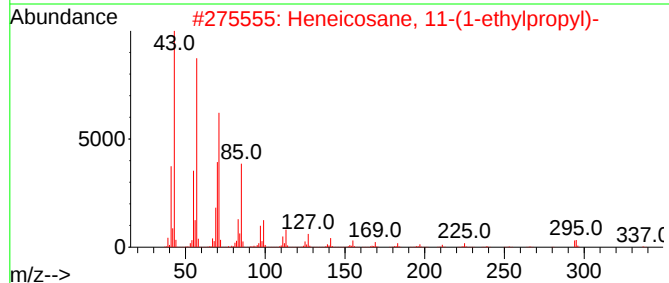
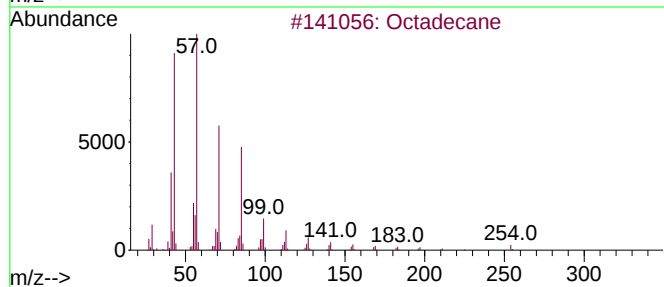
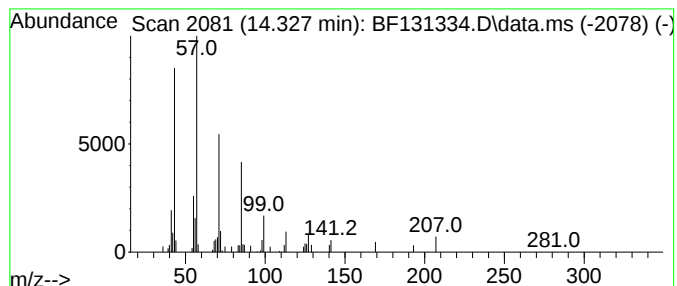
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	2.05 ng	47368	Chrysene-d12	14.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	78
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72
3			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
4			Heptadecane	240	C17H36	000629-78-7	72
5			Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112222\
Data File : BF131334.D
Acq On : 22 Nov 2022 17:21
Operator : CG\JU
Sample : N5642-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

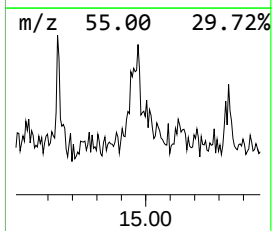
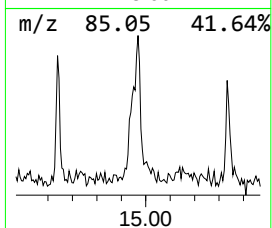
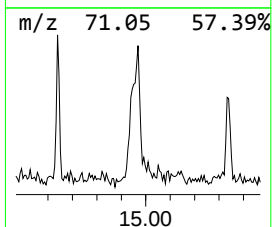
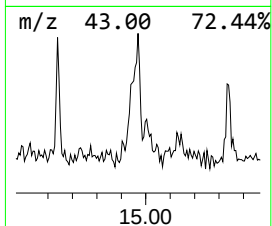
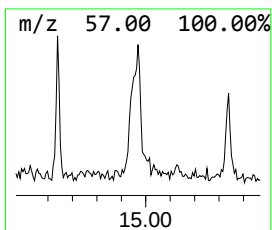
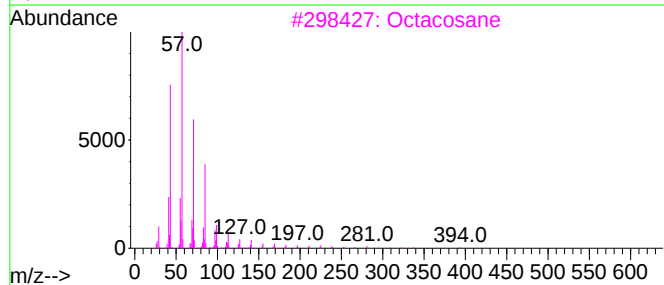
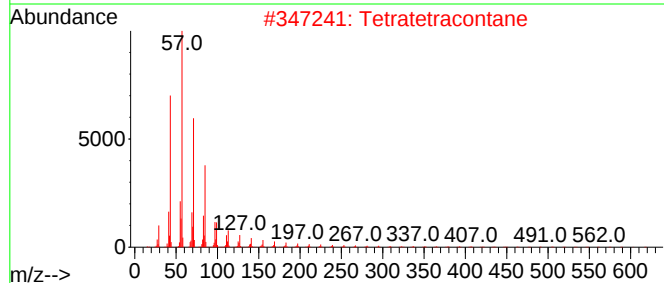
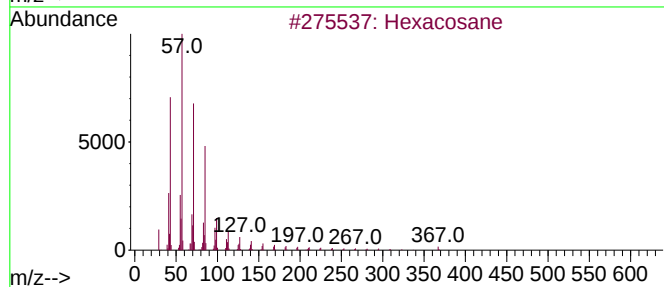
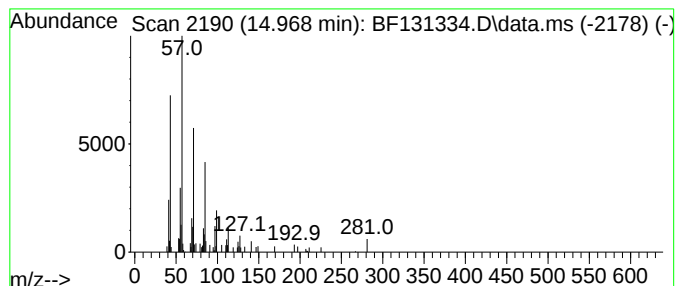
Instrument :
BNA_F
ClientSampleId :
LEFT-SIDE-FLATS-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.968	4.00 ng	97052	Perylene-d12	15.710	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112222\
Data File : BF131334.D
Acq On : 22 Nov 2022 17:21
Operator : CG\JU
Sample : N5642-09
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LEFT-SIDE-FLATS-29

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.287	43.5	ng	1238050	1	6.963	569110	20.0
2-Pentanone, 4-...	5.193	12.4	ng	353763	1	6.963	569110	20.0
Benzophenone	10.733	3.5	ng	150269	3	10.016	854548	20.0
n-Hexadecanoic ...	12.022	7.7	ng	325014	4	11.510	846445	20.0
Octadecanoic acid	12.816	24.6	ng	1042350	4	11.510	846445	20.0
Octadecane	14.327	2.0	ng	47368	5	14.169	462361	20.0
Hexacosane	14.968	4.0	ng	97052	6	15.710	485619	20.0