

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
 Data File : BF131846.D
 Acq On : 27 Dec 2022 20:03
 Operator : CG\JU
 Sample : N6208-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HD-01-122322

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	496	501	510	rVB	543959	720413	11.29%	2.863%
2	5.446	566	571	574	rBV	1826644	1701532	26.67%	6.762%
3	6.463	739	744	747	rBV	1820384	1746262	27.37%	6.939%
4	6.828	803	806	810	rBV	492218	432432	6.78%	1.718%
5	7.399	899	903	906	rBV	1118191	1145322	17.95%	4.551%
6	8.122	1022	1026	1029	rVB	659208	528698	8.29%	2.101%
7	9.204	1205	1210	1213	rBV	2566462	2041649	32.00%	8.113%
8	9.887	1321	1326	1329	rBV	694327	592802	9.29%	2.356%
9	10.604	1442	1448	1451	rBV	253821	213242	3.34%	0.847%
10	10.675	1456	1460	1464	rBV	1230783	1169155	18.32%	4.646%
11	11.375	1576	1579	1583	rBV	609010	541464	8.49%	2.152%
12	11.769	1642	1646	1650	rBV	1946079	1654707	25.93%	6.576%
13	11.904	1666	1669	1674	rBV	112660	115311	1.81%	0.458%
14	12.469	1759	1765	1767	rBV	5746785	6380700	100.00%	25.356%
15	12.486	1767	1768	1774	rVV2	3800624	3009680	47.17%	11.960%
16	12.569	1778	1782	1785	rVB	695981	638041	10.00%	2.536%
17	12.969	1846	1850	1854	rBV	1563880	1490851	23.37%	5.924%
18	13.216	1886	1892	1898	rBV3	40028	68383	1.07%	0.272%
19	13.886	2001	2006	2015	rBV5	61882	172662	2.71%	0.686%
20	14.028	2026	2030	2034	rBV	426075	374557	5.87%	1.488%
21	15.516	2278	2283	2294	rVB	324607	426378	6.68%	1.694%

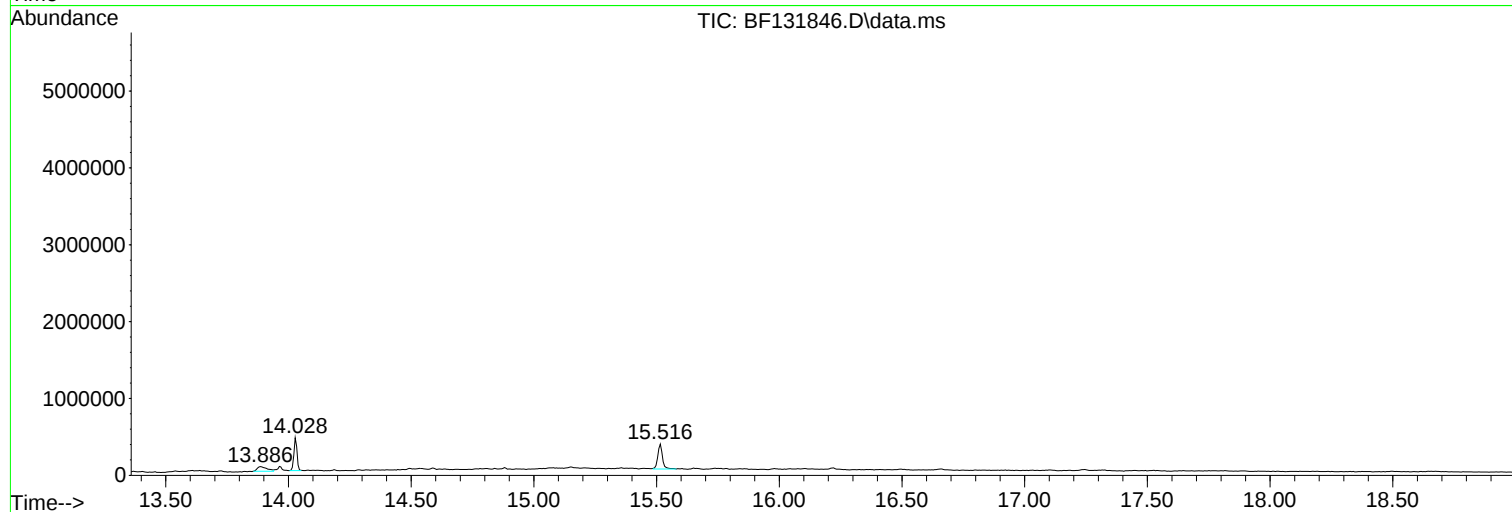
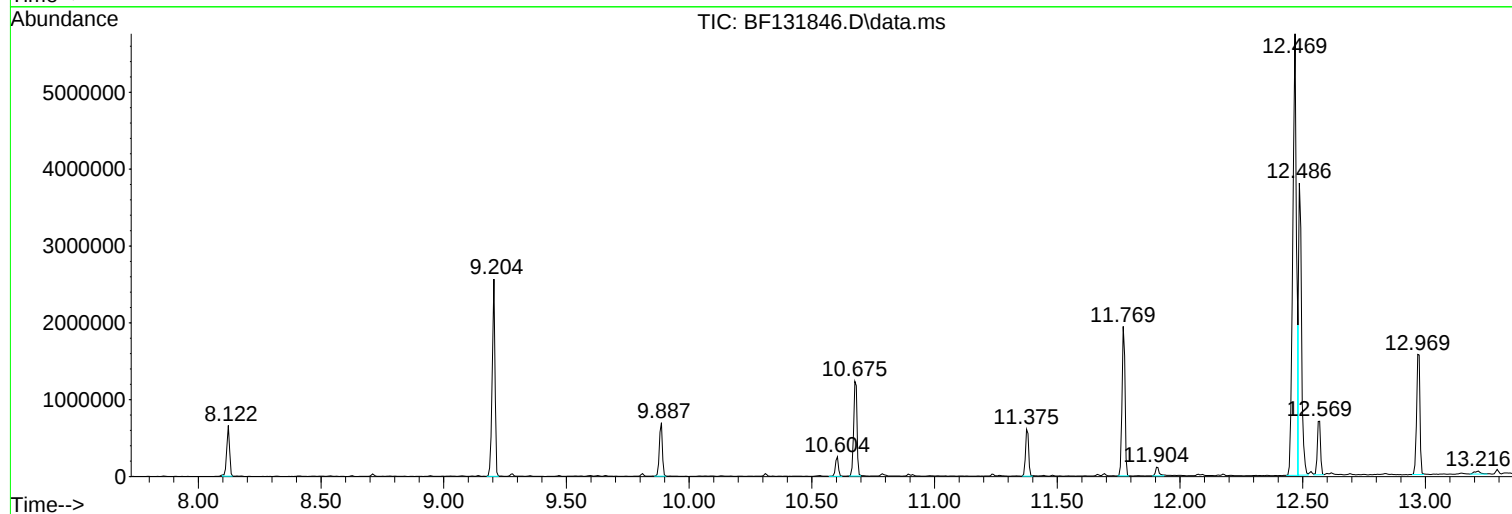
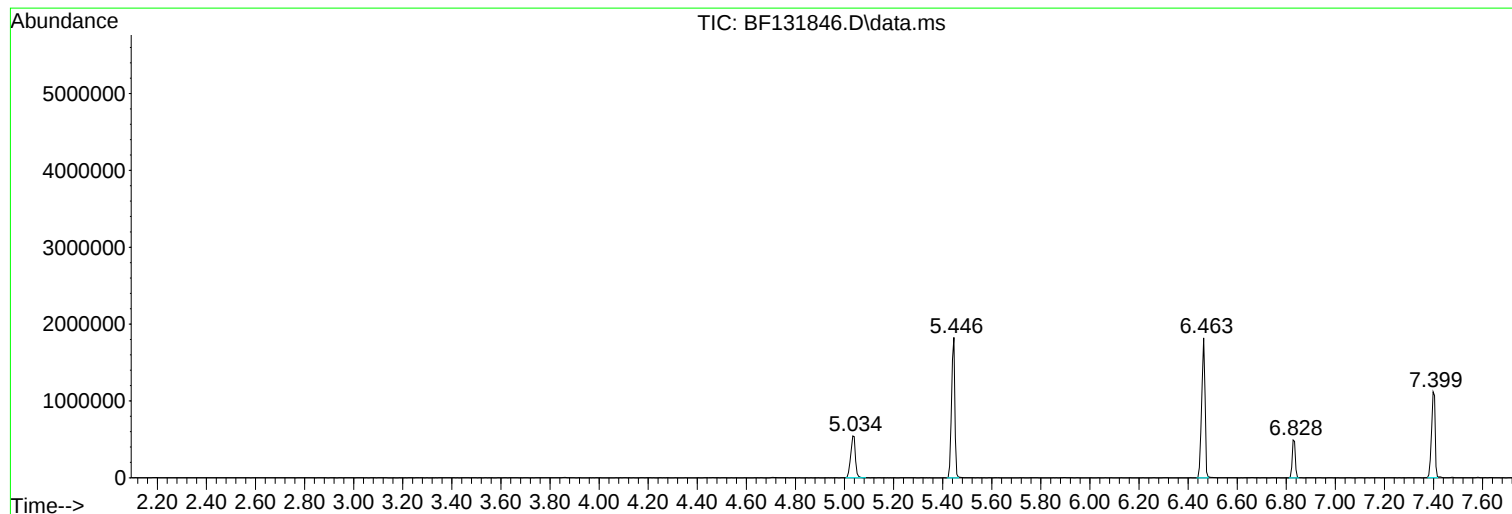
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ALS Vial : 15 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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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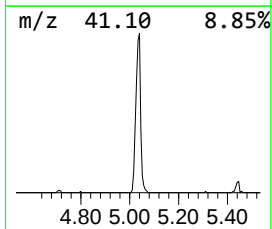
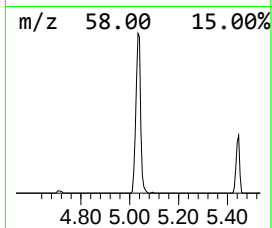
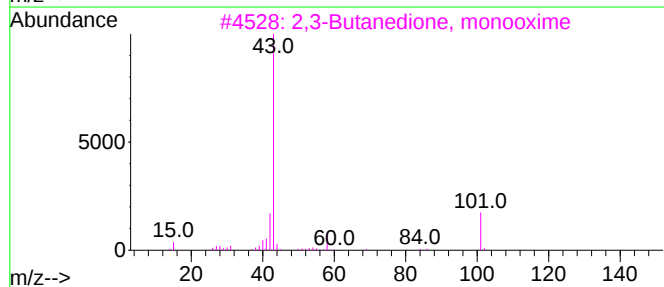
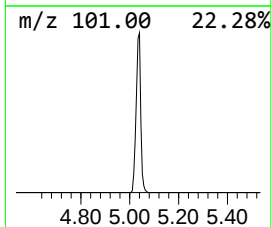
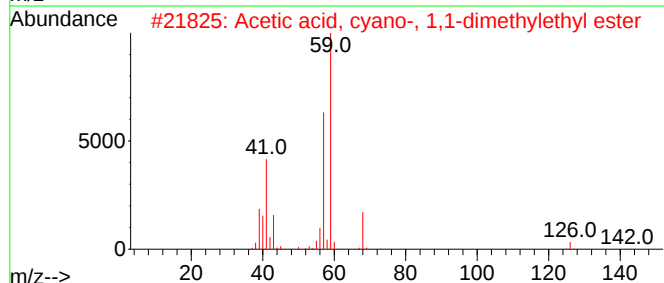
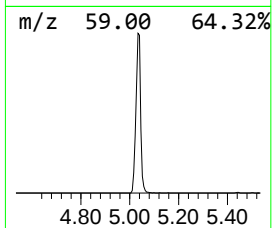
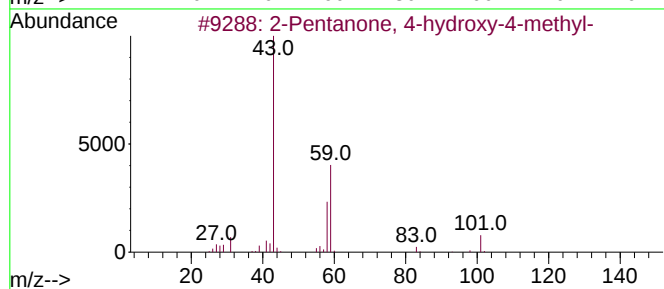
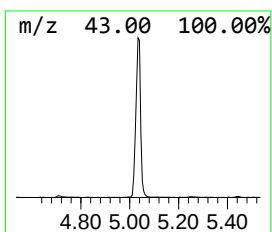
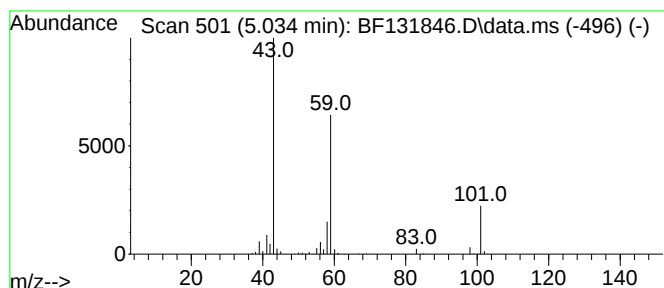
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	33.32 ng	720413	1,4-Dichlorobenzene-d4	6.834

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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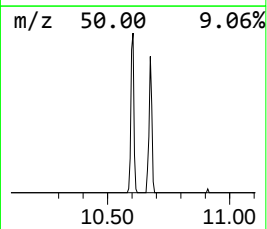
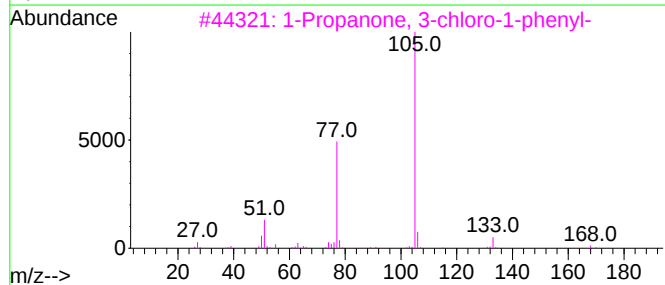
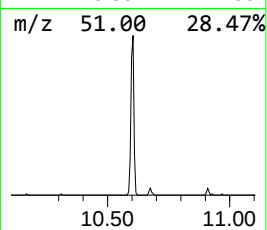
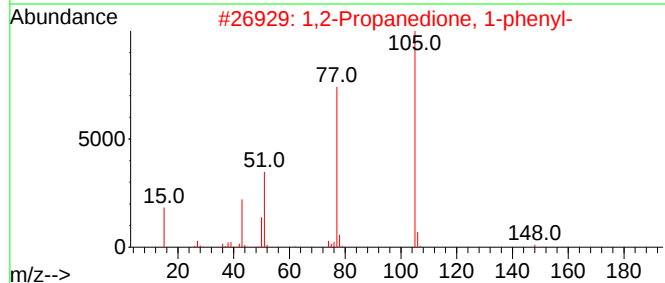
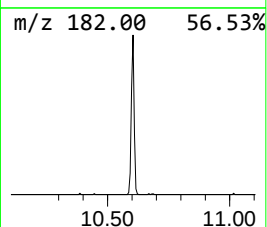
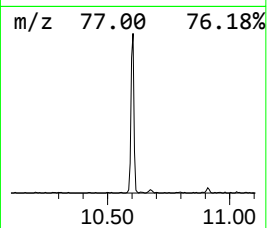
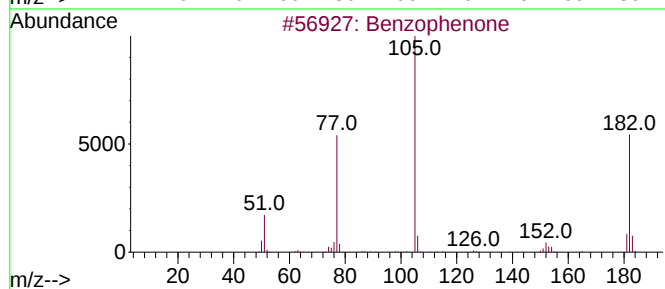
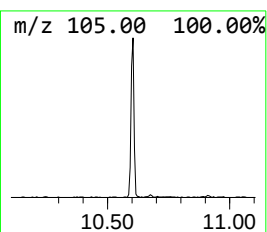
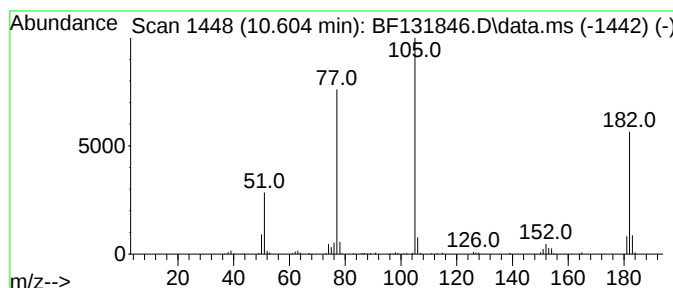
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Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	7.19 ng	213242	Acenaphthene-d10	9.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	53
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	53
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	53
5			Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	53



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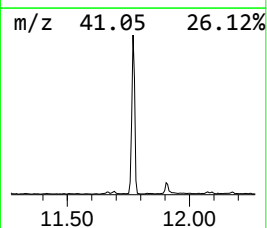
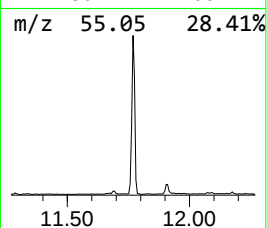
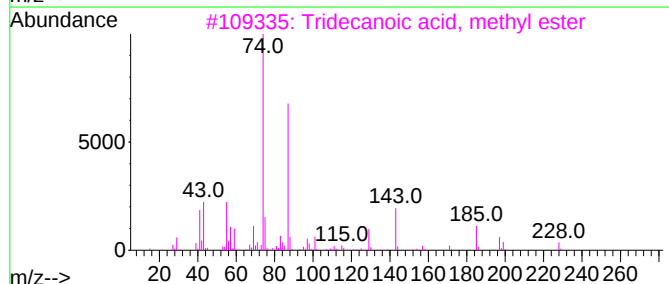
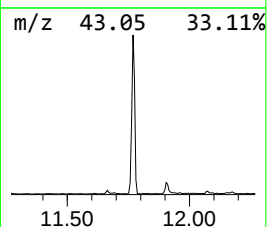
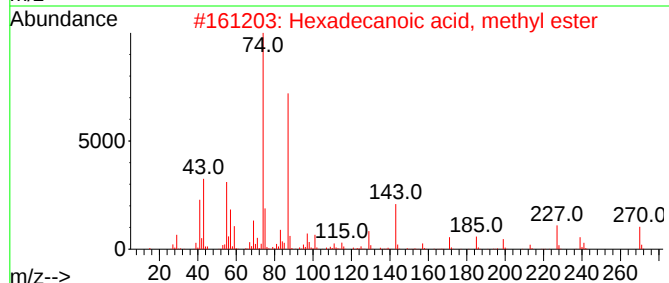
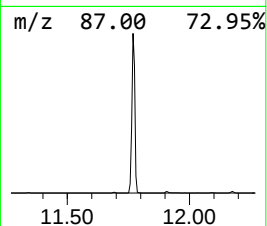
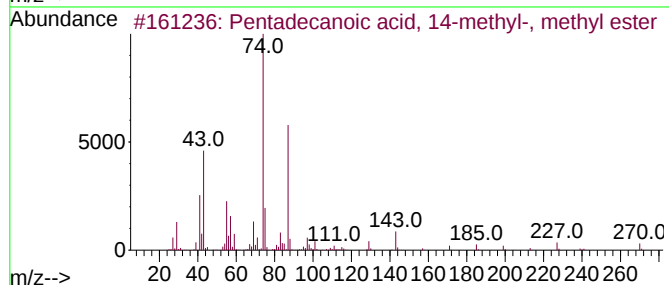
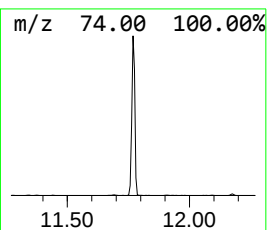
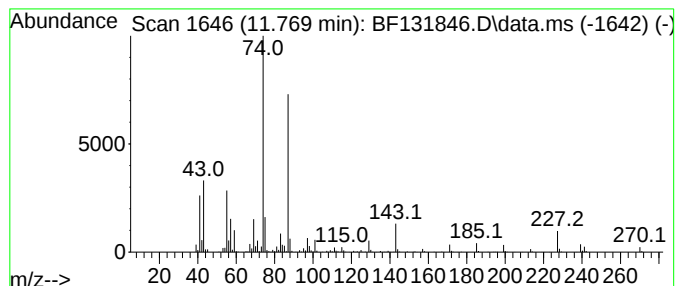
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Peak Number 3 Pentadecanoic acid, 14-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.769	61.12 ng	1654710	Phenanthrene-d10	11.375	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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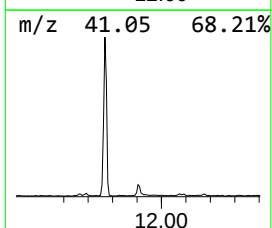
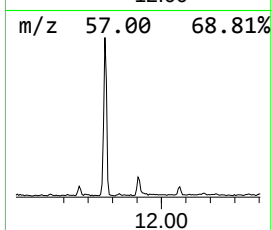
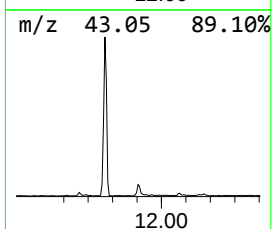
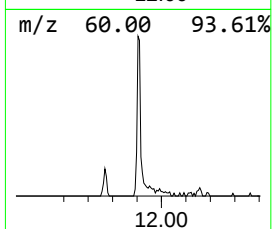
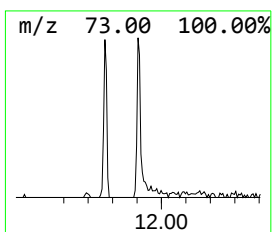
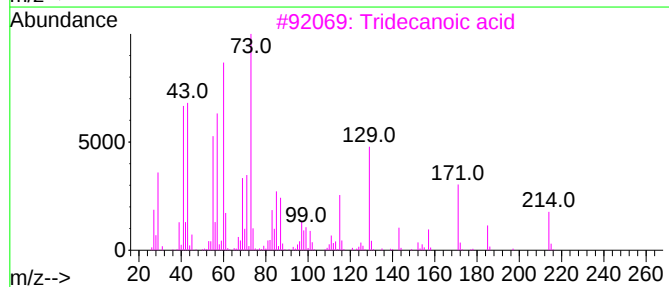
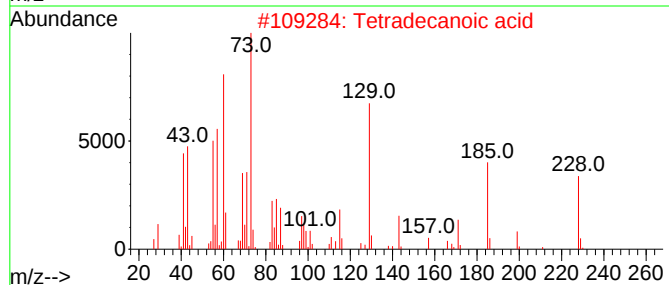
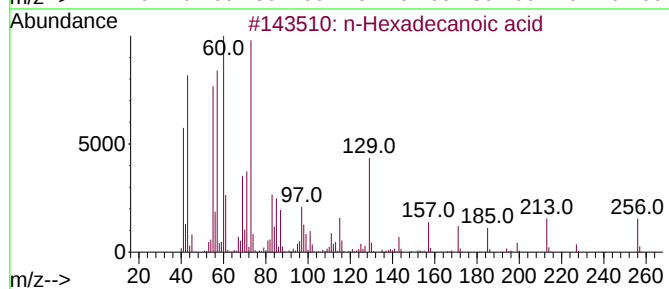
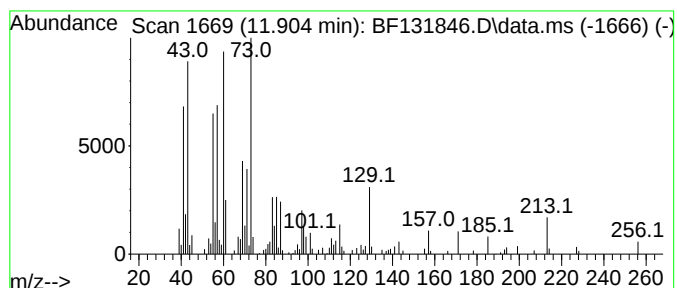
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.904	4.26 ng	115311	Phenanthrene-d10	11.375	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Docosyl propyl ether	368	C25H52O	1000406-28-2	25



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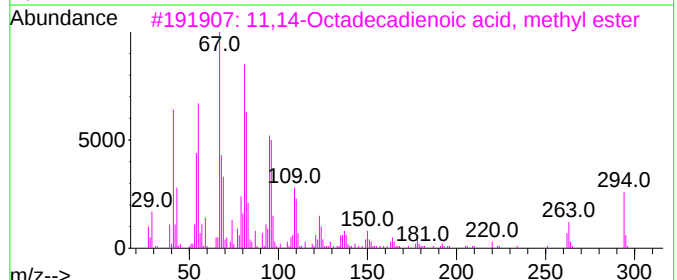
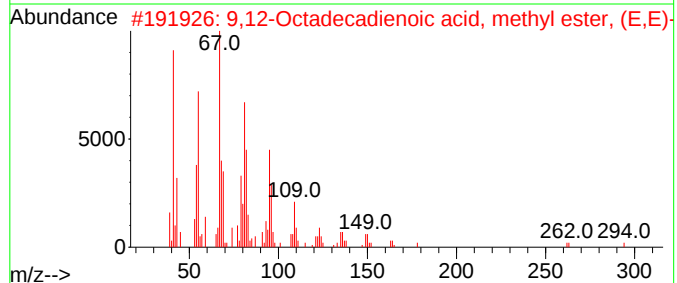
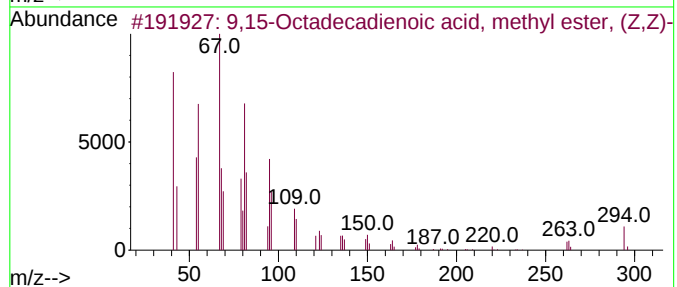
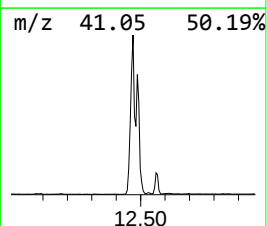
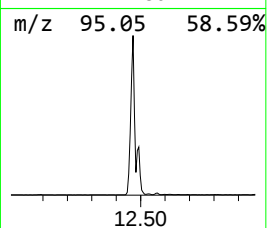
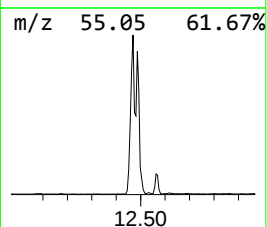
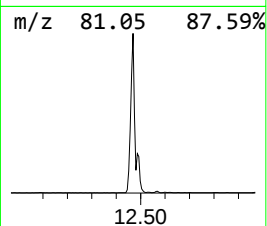
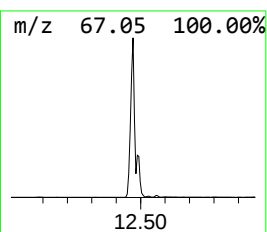
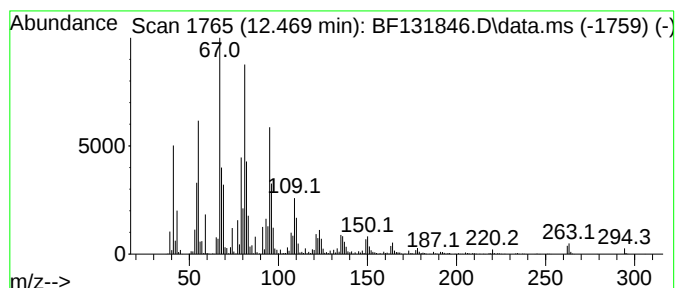
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Peak Number 5 9,15-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	235.68 ng	6380700	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
2			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
3			11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	97
4			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
5			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	96



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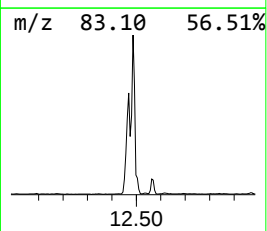
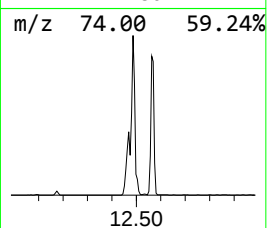
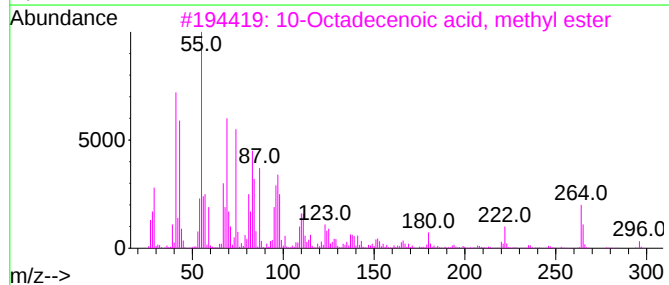
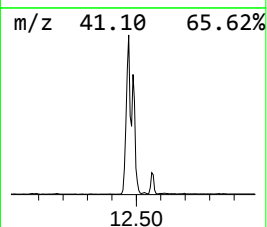
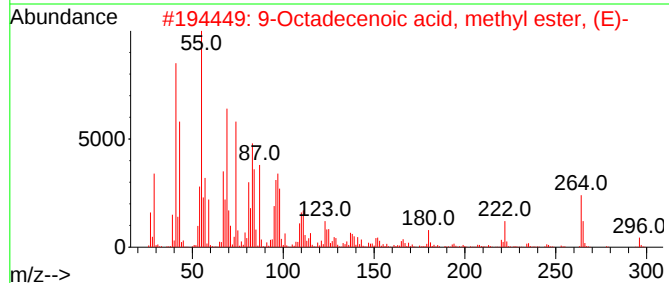
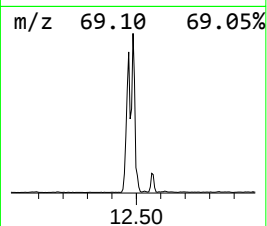
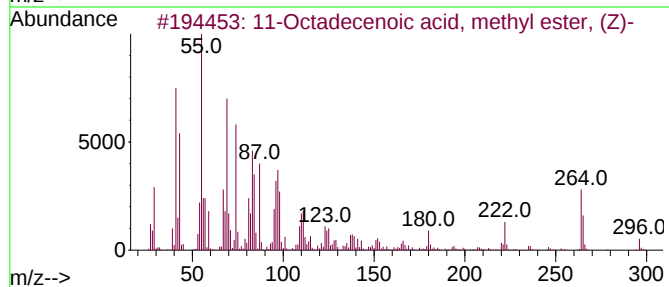
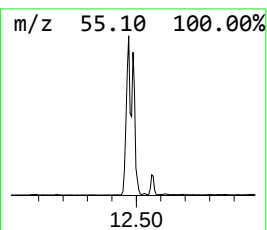
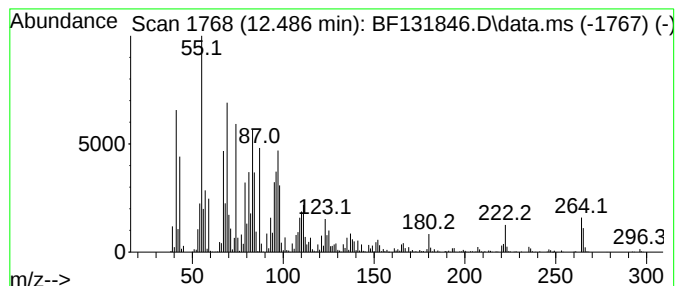
Instrument :
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ClientSampleId :
HD-01-122322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.486	111.17 ng	3009680	Phenanthrene-d10	11.375	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131846.D
Acq On : 27 Dec 2022 20:03
Operator : CG\JU
Sample : N6208-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122322

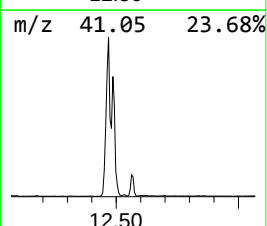
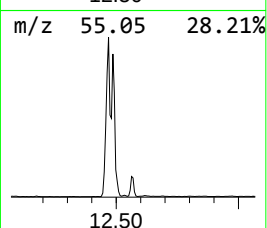
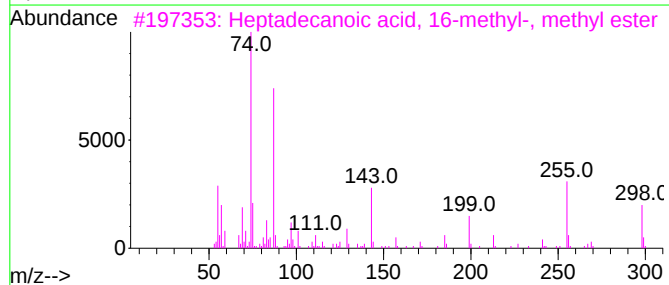
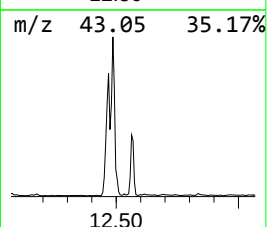
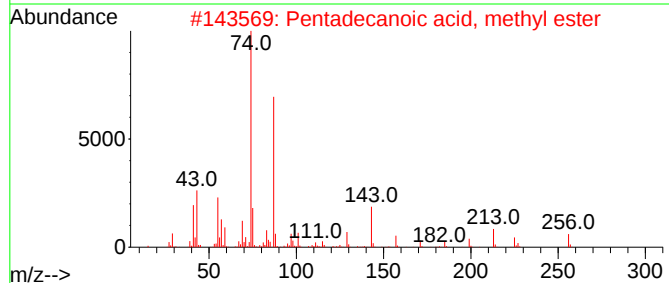
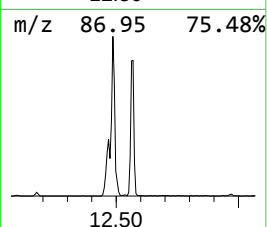
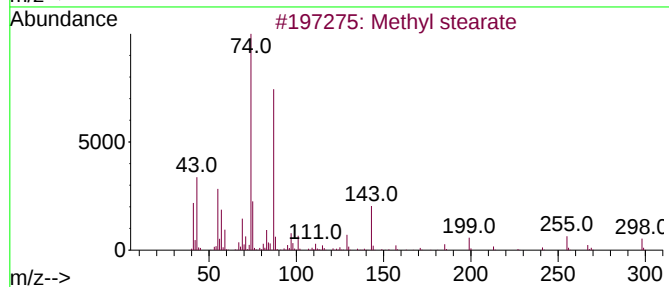
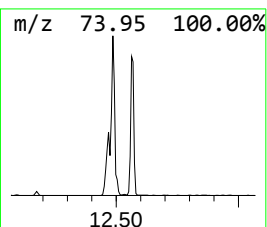
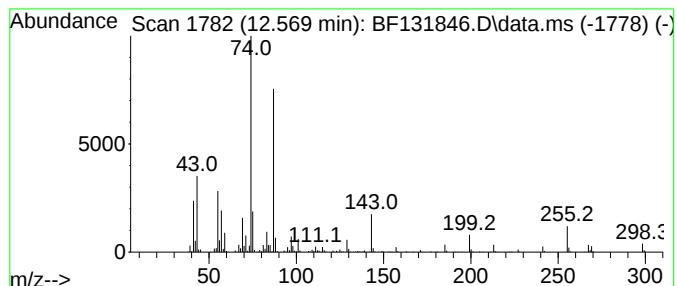
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	23.57 ng	638041	Phenanthrene-d10	11.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	87
5			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131846.D
Acq On : 27 Dec 2022 20:03
Operator : CG\JU
Sample : N6208-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122322

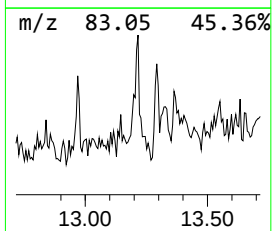
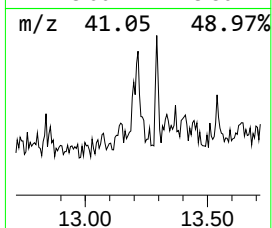
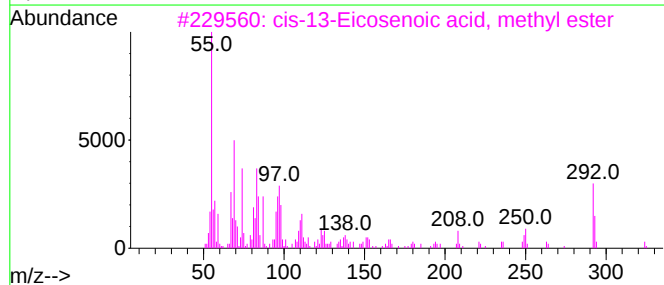
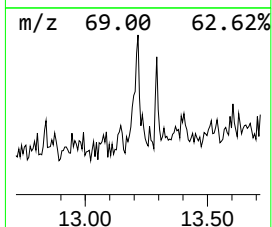
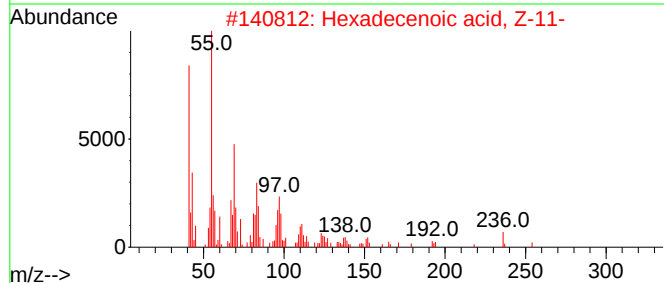
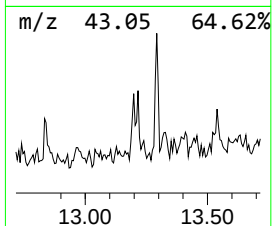
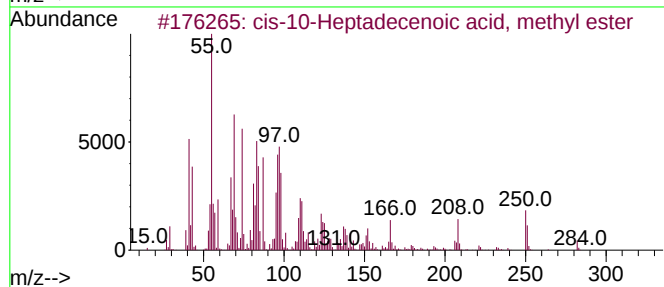
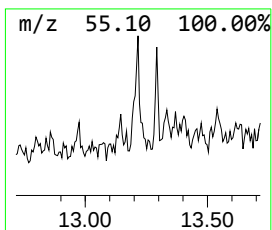
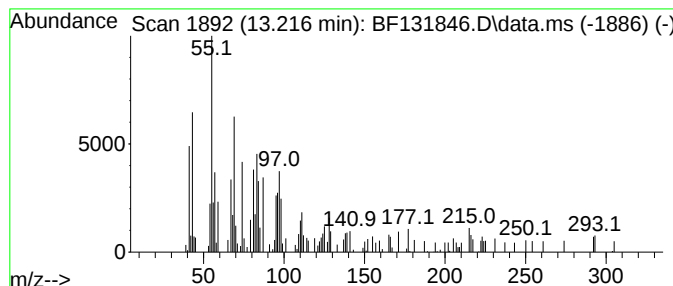
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 cis-10-Heptadecenoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	3.65 ng	68383	Chrysene-d12	14.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	90
2			Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
3			cis-13-Eicosenoic acid, methyl e...	324	C21H40O2	069120-02-1	86
4			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	80
5			13-Methyltetradec-9-enoic acid m...	254	C16H30O2	1010365-89-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131846.D
Acq On : 27 Dec 2022 20:03
Operator : CG\JU
Sample : N6208-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122322

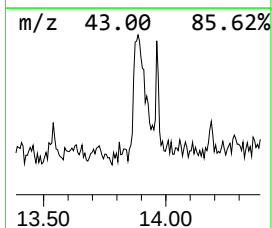
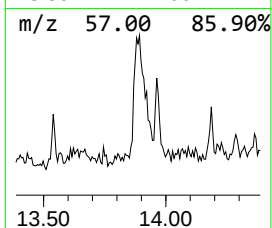
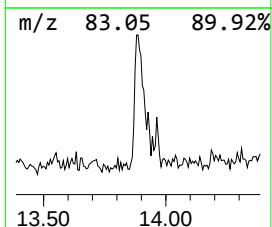
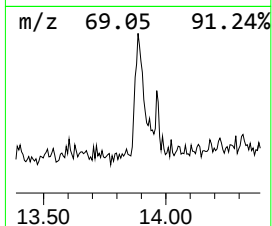
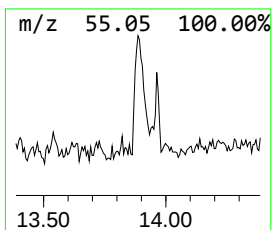
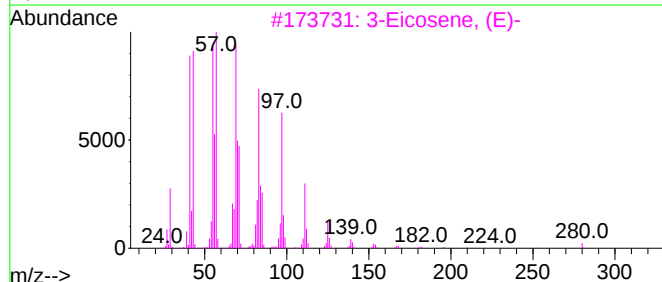
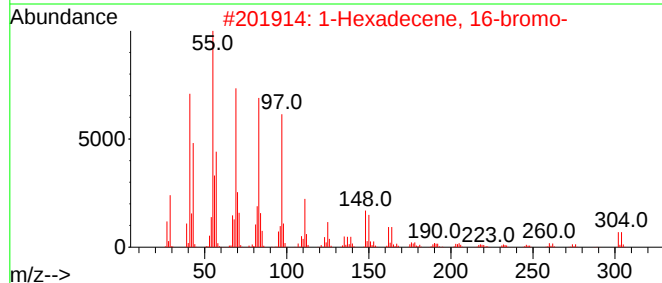
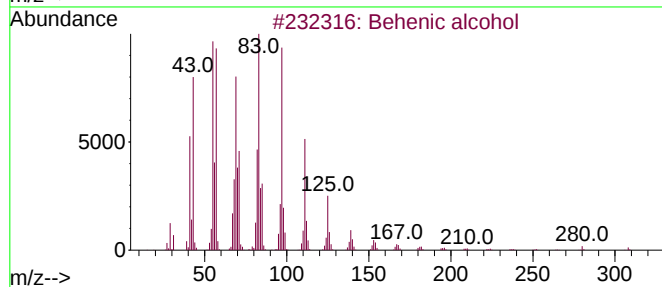
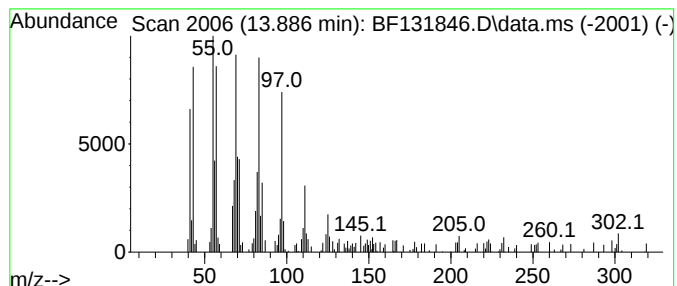
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	9.22 ng	172662	Chrysene-d12	14.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	91
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5			9-Octadecene, (E)-	252	C18H36	007206-25-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122722\
Data File : BF131846.D
Acq On : 27 Dec 2022 20:03
Operator : CG\JU
Sample : N6208-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.034	33.3	ng	720413	1	6.834	432432	20.0
Benzophenone	10.604	7.2	ng	213242	3	9.887	592802	20.0
Pentadecanoic a...	11.769	61.1	ng	1654710	4	11.375	541464	20.0
n-Hexadecanoic ...	11.904	4.3	ng	115311	4	11.375	541464	20.0
9,15-Octadecadi...	12.469	235.7	ng	6380700	4	11.375	541464	20.0
11-Octadecenoic...	12.486	111.2	ng	3009680	4	11.375	541464	20.0
Methyl stearate	12.569	23.6	ng	638041	4	11.375	541464	20.0
cis-10-Heptadec...	13.216	3.6	ng	68383	5	14.028	374557	20.0
Behenic alcohol	13.886	9.2	ng	172662	5	14.028	374557	20.0