

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
 Data File : BF139938.D
 Acq On : 22 Oct 2024 19:54
 Operator : RC/JU
 Sample : P4385-06
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-3

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	8	17	24	rVV	2506648	4114463	100.00%	12.210%
2	2.281	27	32	49	rVB3	21642	58933	1.43%	0.175%
3	4.499	396	409	415	rBV	118227	188784	4.59%	0.560%
4	5.116	506	514	522	rVB	215683	333870	8.11%	0.991%
5	5.504	574	580	585	rBV	2591875	3477741	84.52%	10.320%
6	6.504	744	750	756	rBV	2473308	3535930	85.94%	10.493%
7	6.887	810	815	821	rVB	655945	828408	20.13%	2.458%
8	7.445	904	910	915	rBV	1777803	2366752	57.52%	7.023%
9	7.698	948	953	958	rVB	106289	127020	3.09%	0.377%
10	8.169	1028	1033	1038	rBV	888399	1096054	26.64%	3.253%
11	8.381	1063	1069	1077	rVB	51022	71121	1.73%	0.211%
12	9.245	1210	1216	1221	rBV	3217994	4068991	98.89%	12.075%
13	9.922	1326	1331	1336	rBV	895313	1144822	27.82%	3.397%
14	10.633	1447	1452	1459	rBV	640284	830013	20.17%	2.463%
15	10.710	1459	1465	1475	rVV	1229145	1564087	38.01%	4.641%
16	10.945	1501	1505	1510	rVB	116939	141579	3.44%	0.420%
17	11.410	1579	1584	1591	rBV	785469	978400	23.78%	2.903%
18	11.475	1591	1595	1600	rVB4	30173	48417	1.18%	0.144%
19	12.457	1754	1762	1767	rBV2	57852	135796	3.30%	0.403%
20	12.851	1825	1829	1836	rBV2	28562	61218	1.49%	0.182%
21	12.998	1848	1854	1859	rBV	2375497	3097008	75.27%	9.190%
22	13.169	1879	1883	1885	rBV2	31805	45102	1.10%	0.134%
23	13.204	1885	1889	1891	rBV2	79136	114489	2.78%	0.340%
24	13.304	1903	1906	1910	rVB4	37136	47032	1.14%	0.140%
25	13.569	1948	1951	1957	rVB	33719	46162	1.12%	0.137%
26	13.892	2001	2006	2023	rVB	263912	520334	12.65%	1.544%
27	14.051	2027	2033	2042	rVB	621967	888317	21.59%	2.636%
28	14.527	2109	2114	2126	rBV3	69835	181541	4.41%	0.539%
29	14.980	2186	2191	2199	rVB	187923	263228	6.40%	0.781%
30	15.180	2220	2225	2226	rBV	121312	179130	4.35%	0.532%
31	15.204	2226	2229	2249	rVB2	183068	463953	11.28%	1.377%
32	15.527	2278	2284	2297	rVB	565279	919765	22.35%	2.729%
33	15.774	2321	2326	2333	rBV	114560	187482	4.56%	0.556%
34	16.015	2361	2367	2372	rBV	217675	383514	9.32%	1.138%
35	16.068	2372	2376	2385	rVV	69445	169844	4.13%	0.504%
36	16.833	2501	2506	2517	rVB	69182	151160	3.67%	0.449%

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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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.151	2555	2560	2565	rVB	40100	75524	1.84%	0.224%
38	17.227	2566	2573	2586	rBV7	73649	326286	7.93%	0.968%
39	17.639	2636	2643	2668	rVB4	118070	466499	11.34%	1.384%

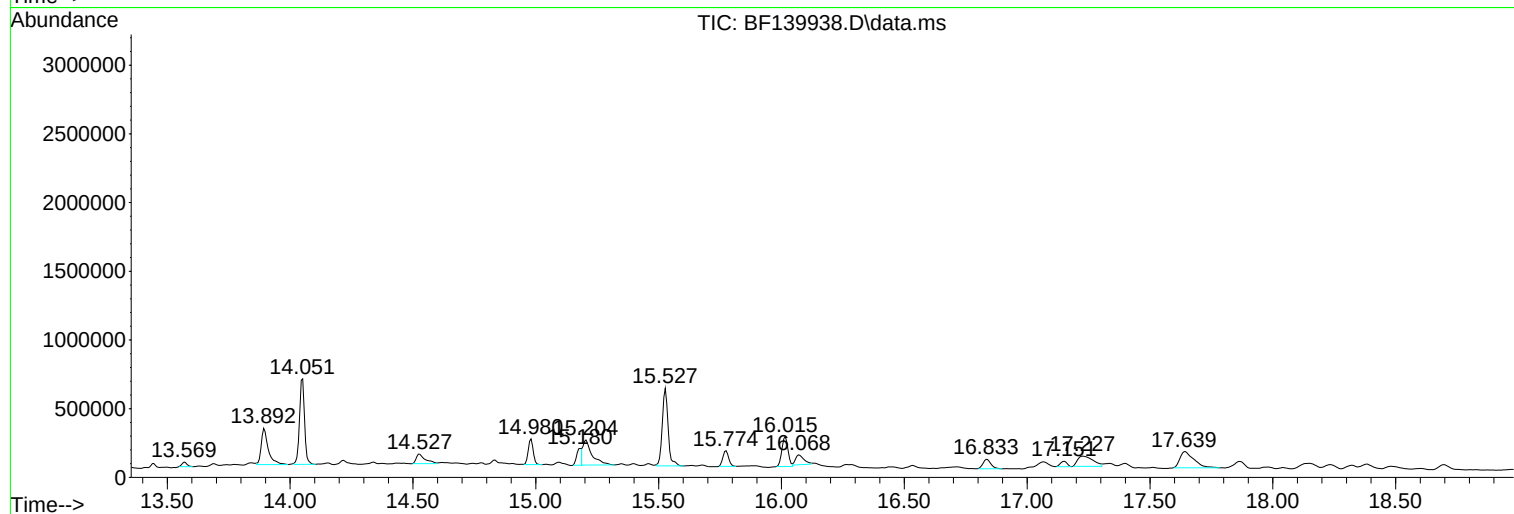
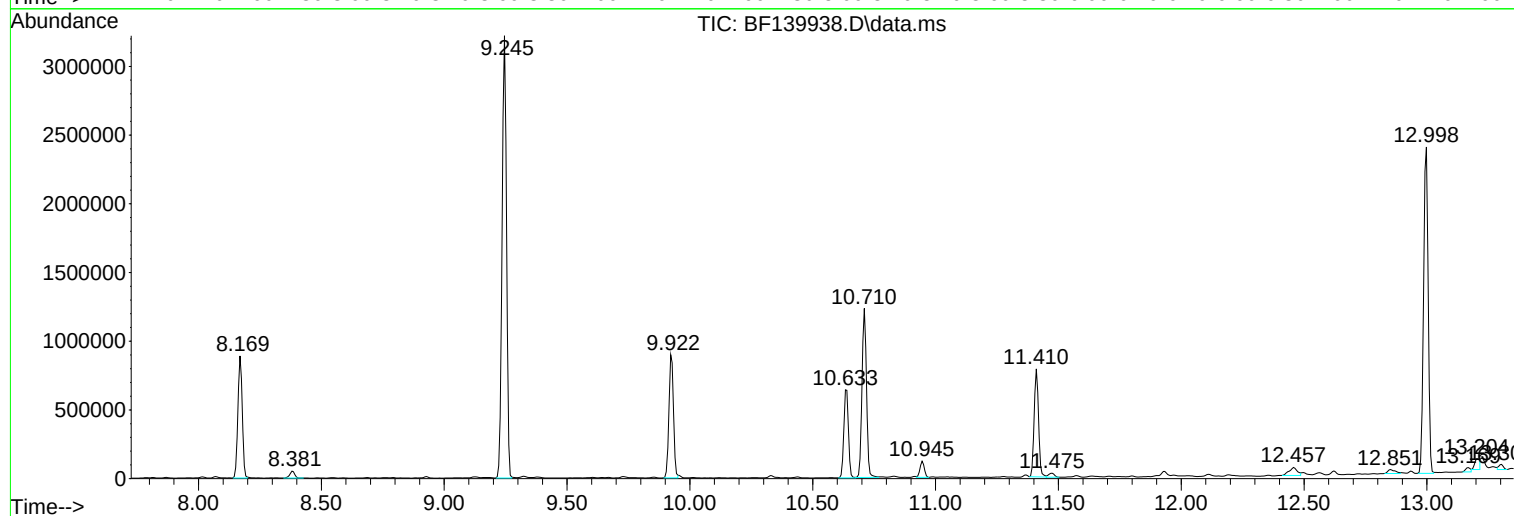
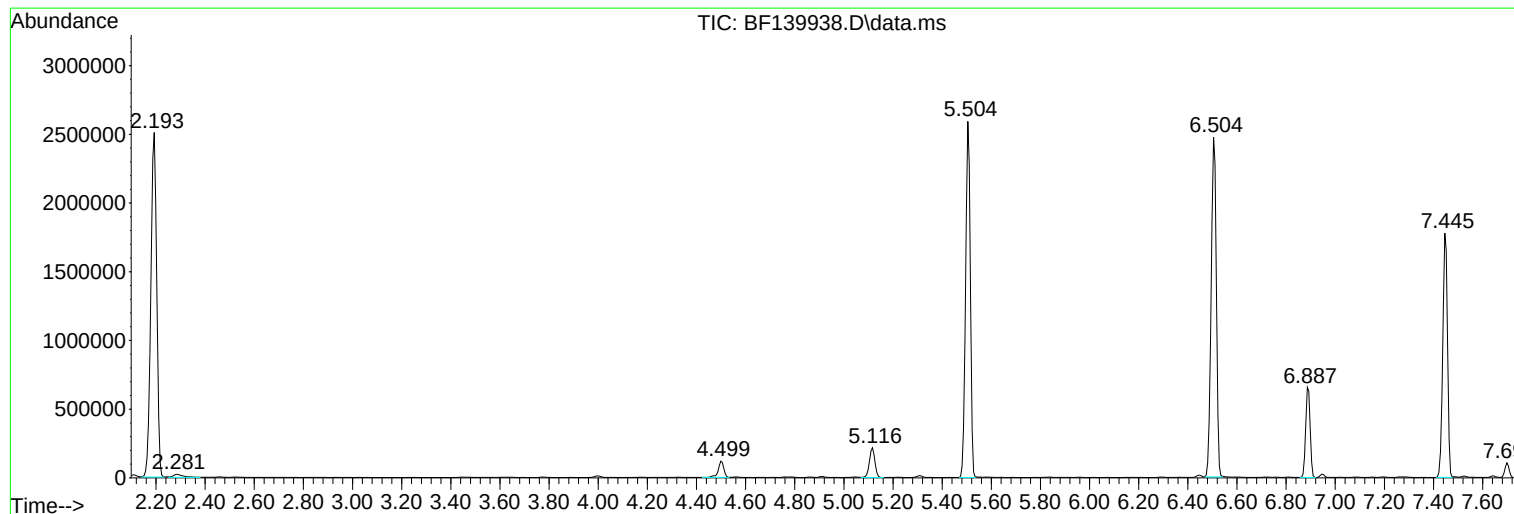
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : P4385-06
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Instrument :
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ClientSampleId :
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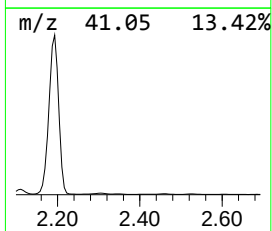
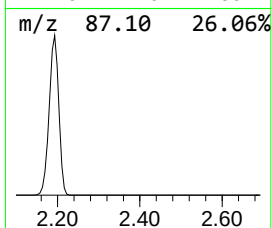
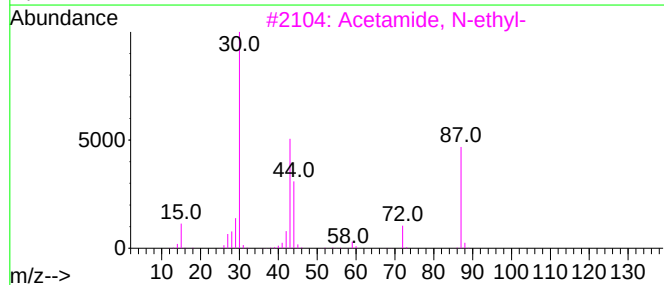
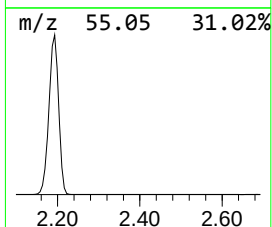
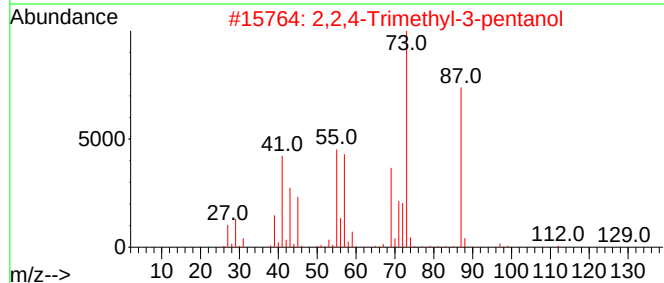
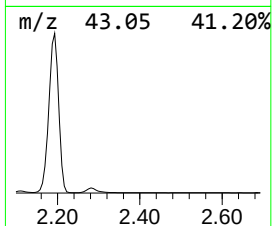
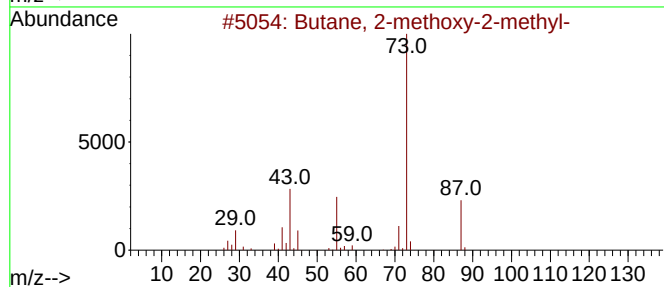
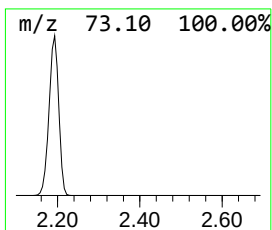
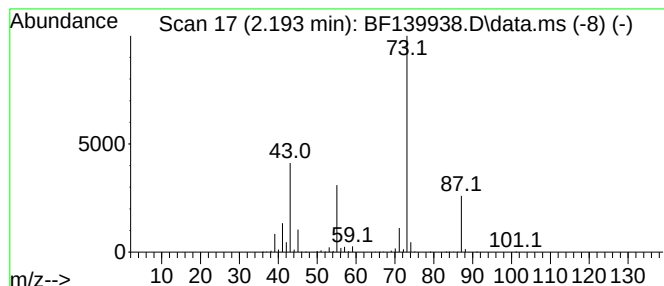
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	99.33 ng	4114460	1,4-Dichlorobenzene-d4	6.887

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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Instrument :
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ClientSampleId :
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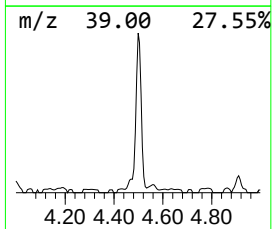
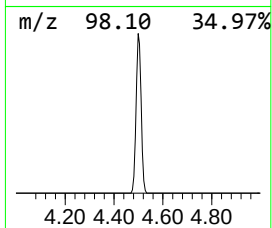
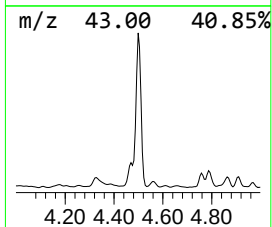
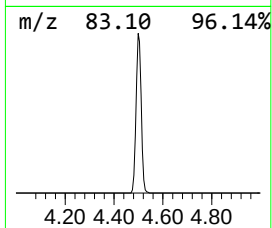
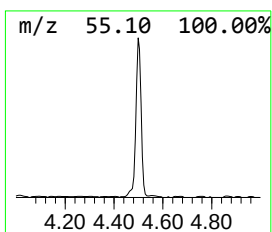
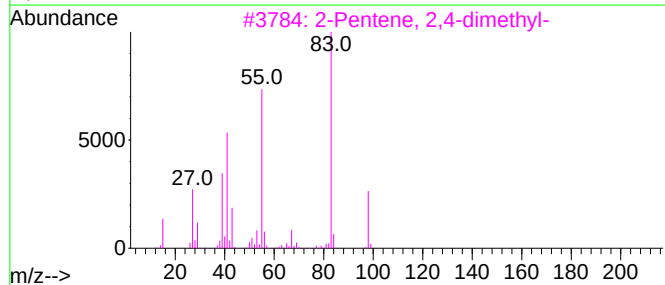
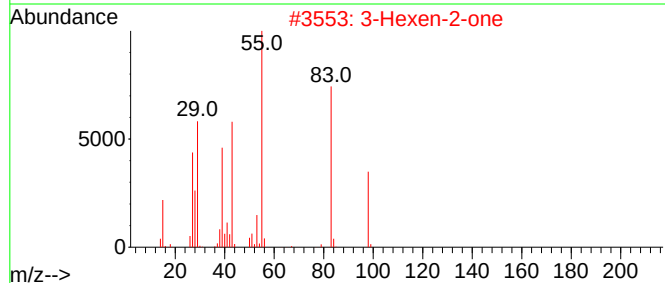
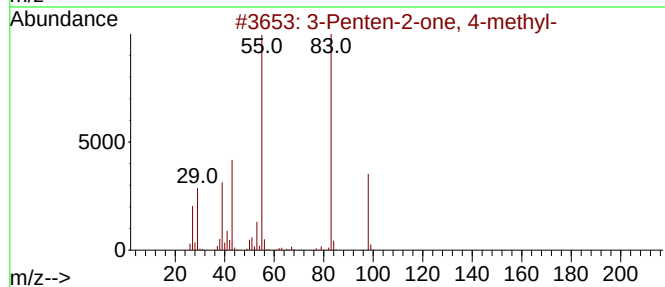
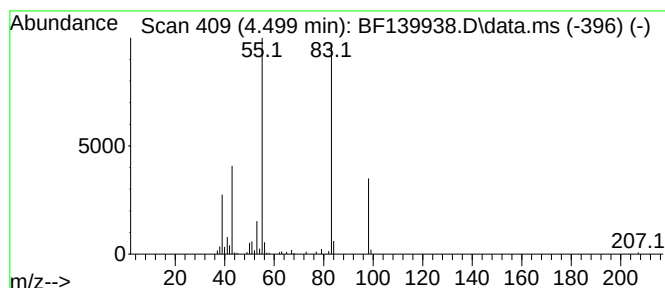
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.499	4.56 ng	188784	1,4-Dichlorobenzene-d4	6.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83



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Misc :
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Instrument :
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ClientSampleId :
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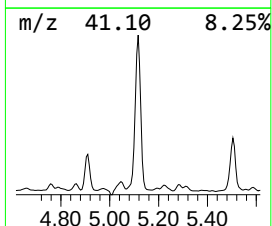
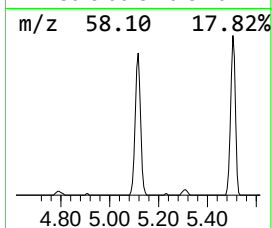
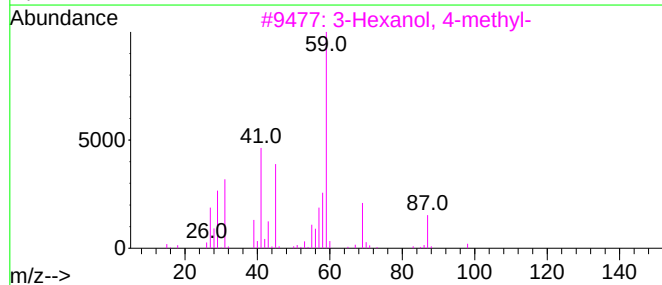
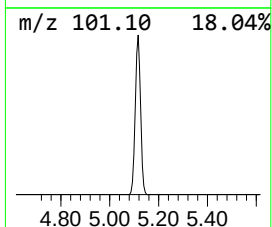
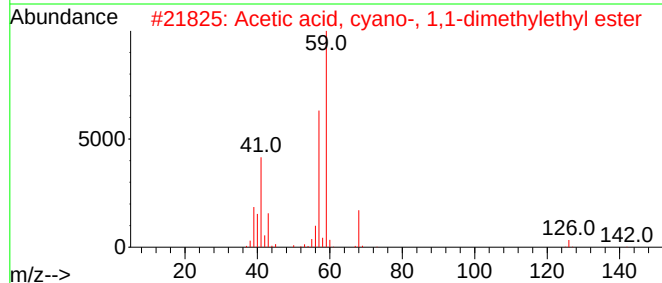
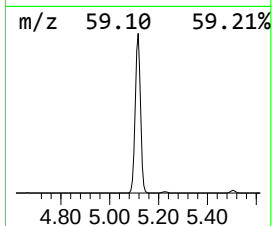
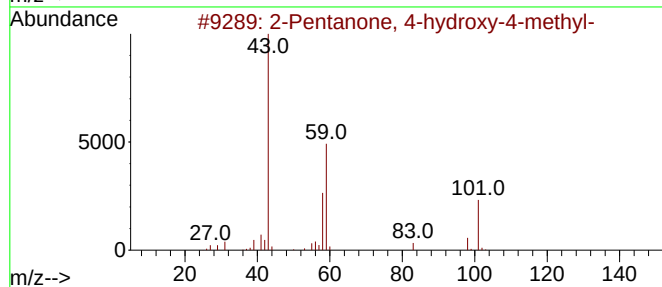
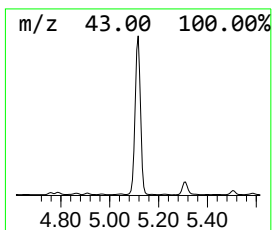
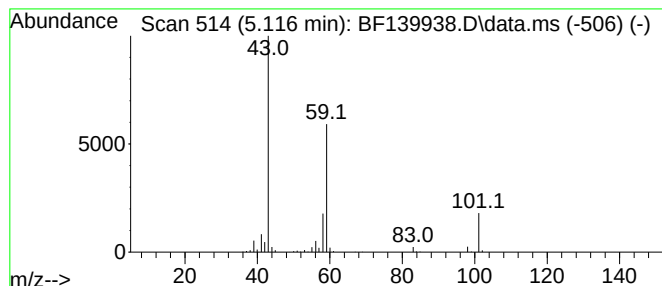
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	8.06 ng	333870	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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Misc :
ALS Vial : 13 Sample Multiplier: 1

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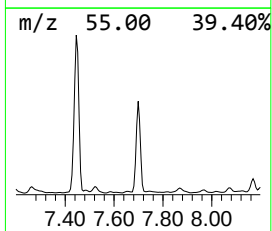
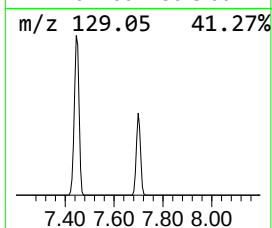
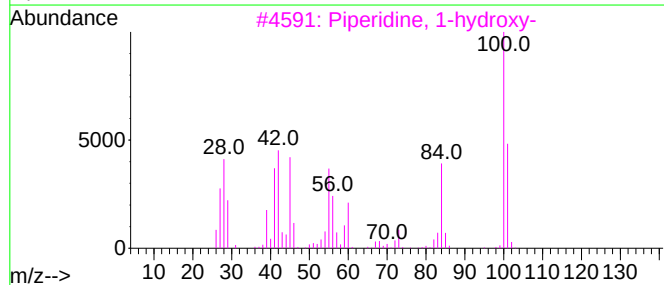
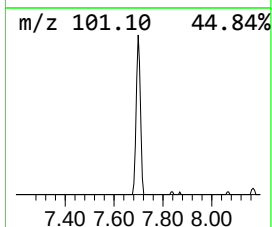
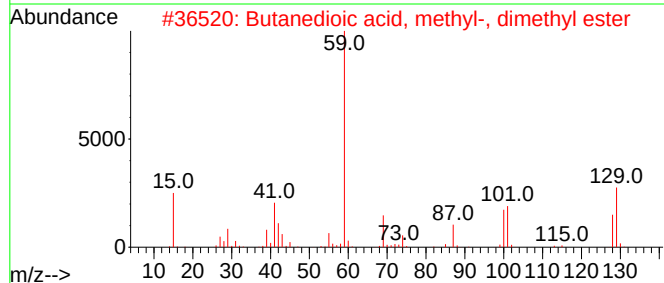
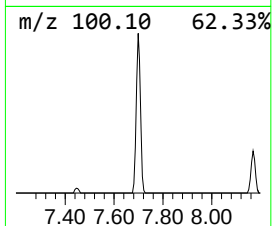
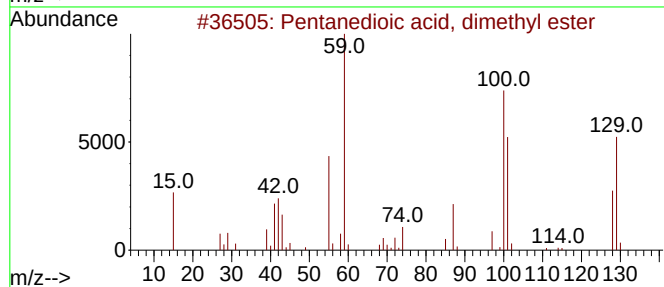
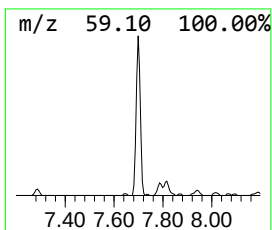
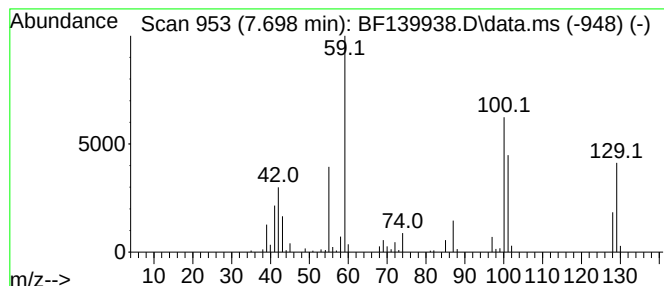
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	2.32 ng	127020	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	53
3			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	38
4			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
5			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	12



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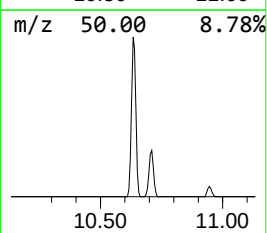
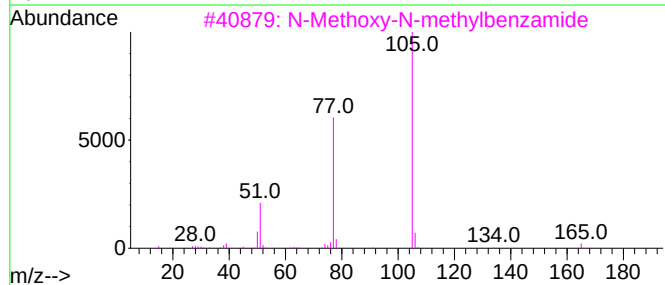
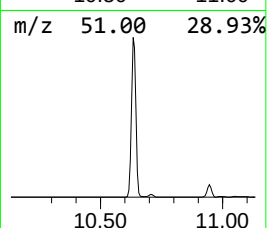
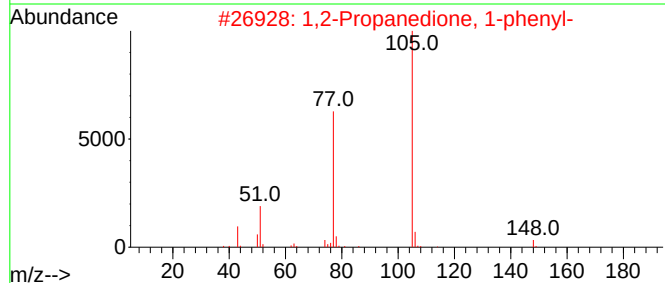
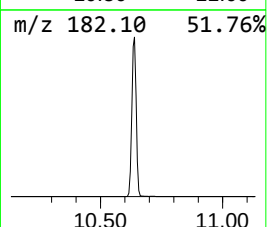
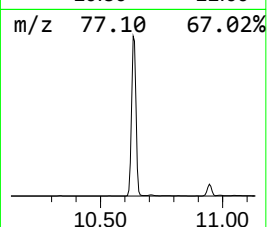
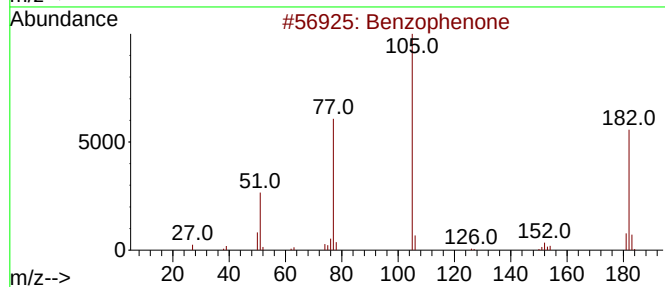
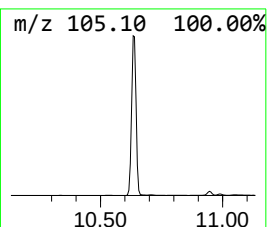
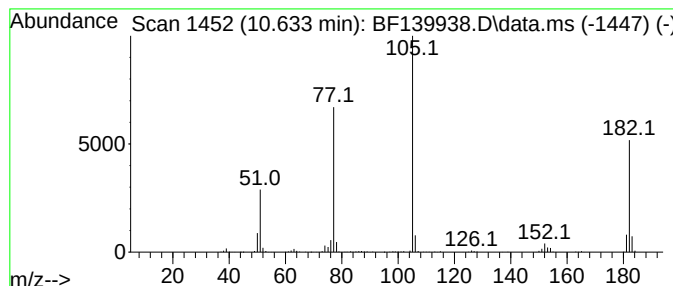
Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.633	14.50 ng	830013	Acenaphthene-d10			9.922
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	96
2	1,2-Propanedione, 1-phenyl-		148	C9H8O2	000579-07-7	47
3	N-Methoxy-N-methylbenzamide		165	C9H11NO2	006919-61-5	47
4	1-Propanone, 3-chloro-1-phenyl-		168	C9H9ClO	000936-59-4	47
5	Methyl 2-benzoyl-4-cyanobutanoate		231	C13H13NO3	1010486-83-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
Operator : RC/JU
Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

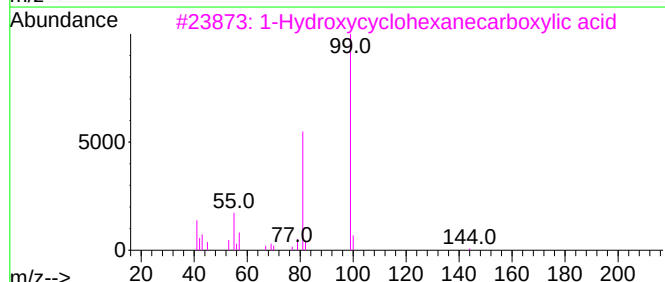
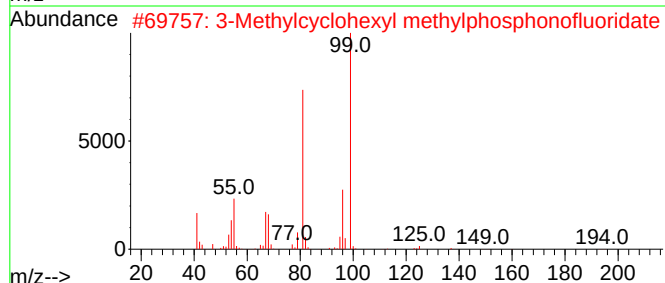
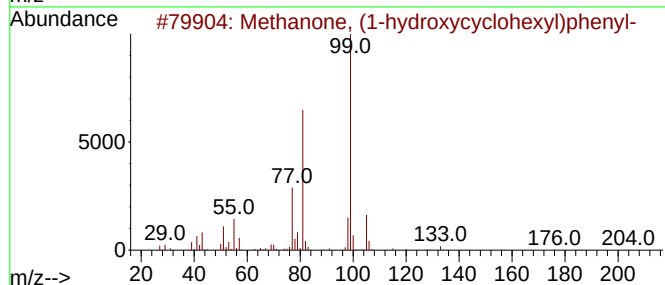
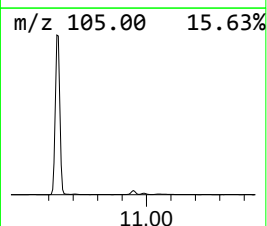
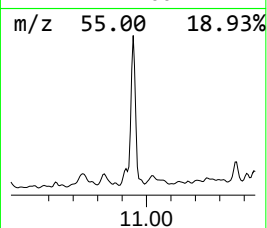
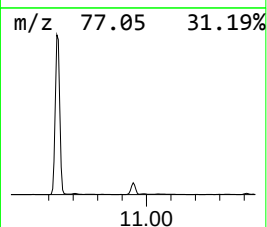
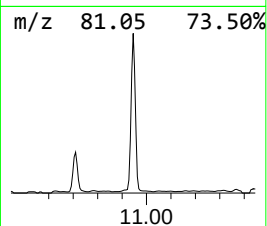
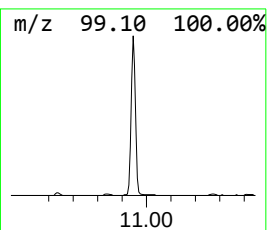
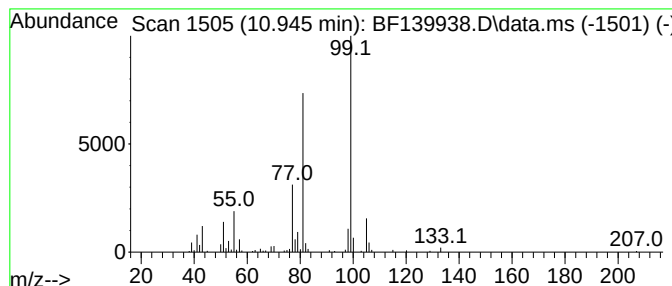
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Methanone, (1-hydroxycyclohexyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.89 ng	141579	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	59
3			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	45
4			2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	38
5			1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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Sample : P4385-06
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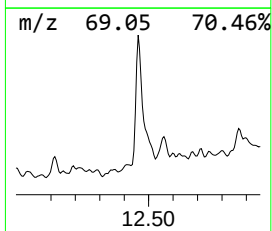
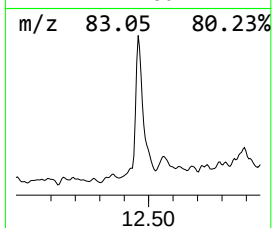
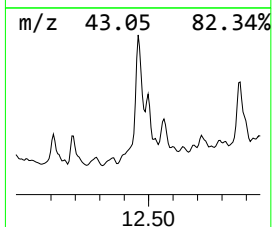
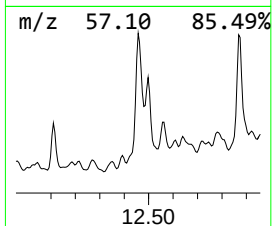
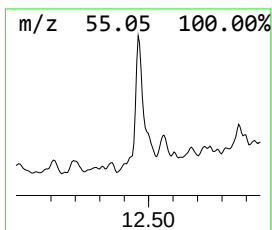
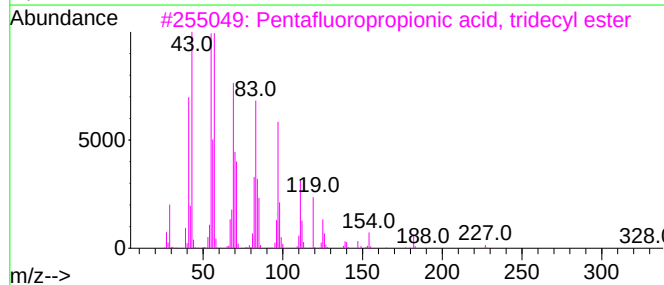
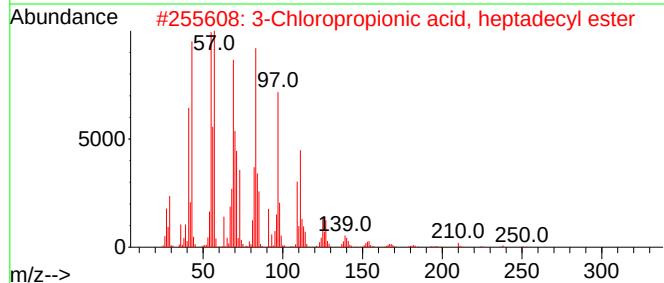
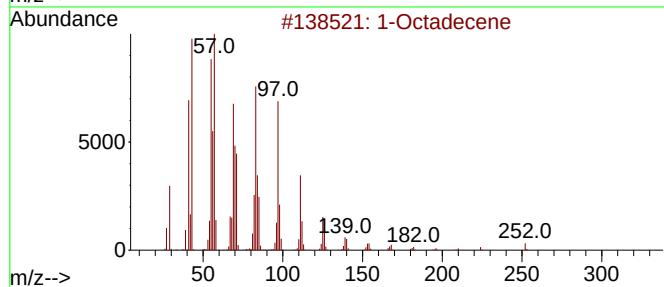
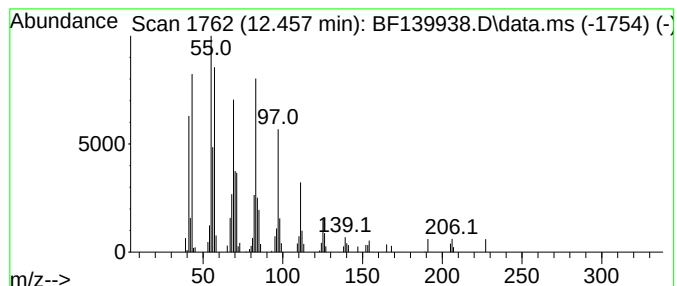
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Octadecene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.457	2.78 ng	135796	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	94
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
3	Pentafluoropropionic acid, tridec...	346	C16H27F5O2	959261-22-4	93
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
Operator : RC/JU
Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

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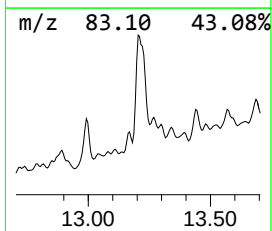
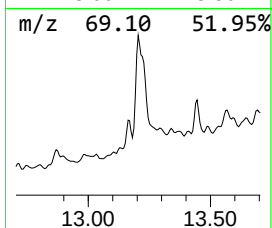
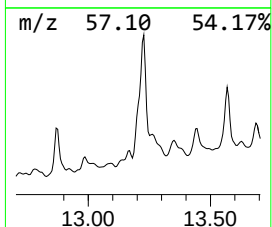
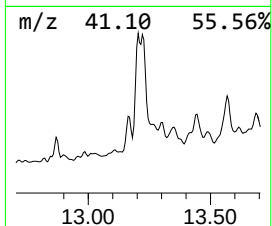
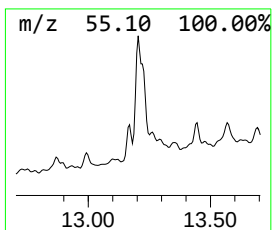
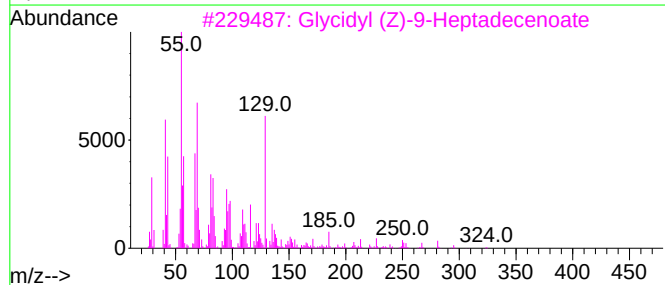
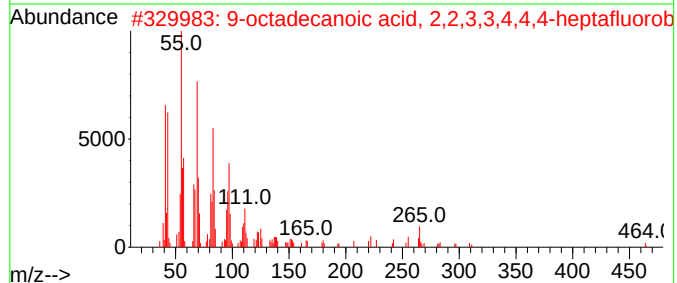
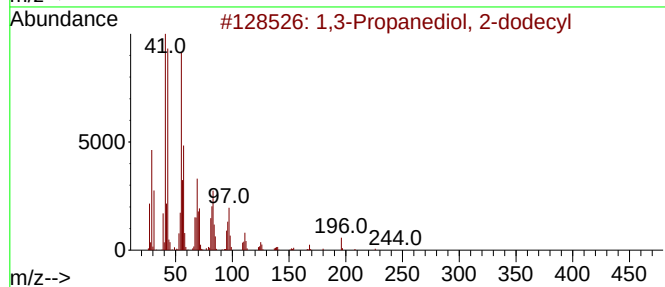
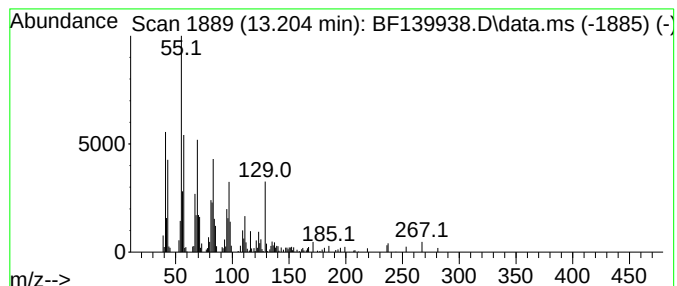
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Propanediol, 2-dodecyl Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	2.58 ng	114489	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Propanediol, 2-dodecyl	244	C15H32O2	010395-09-2	55
2			9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	52
3			Glycidyl (Z)-9-Heptadecenoate	324	C20H36O3	1000465-63-2	52
4			Undec-10-ynoic acid, undecyl ester	336	C22H40O2	1000406-16-4	46
5			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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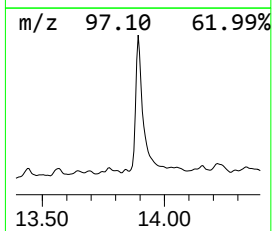
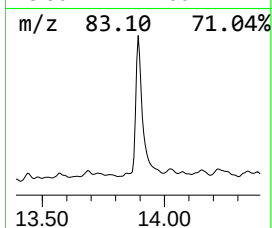
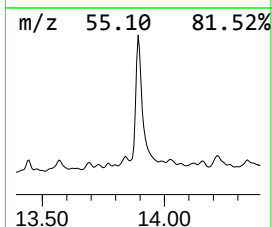
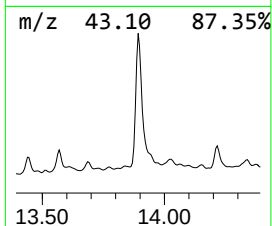
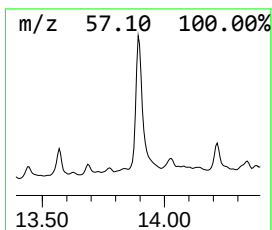
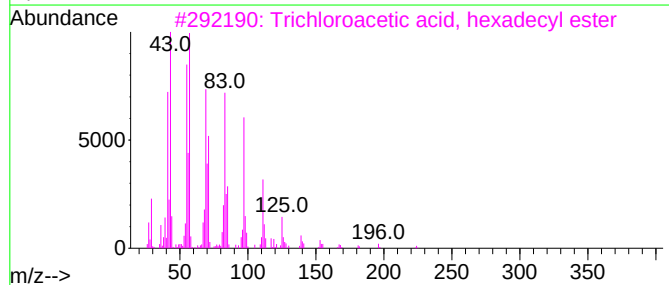
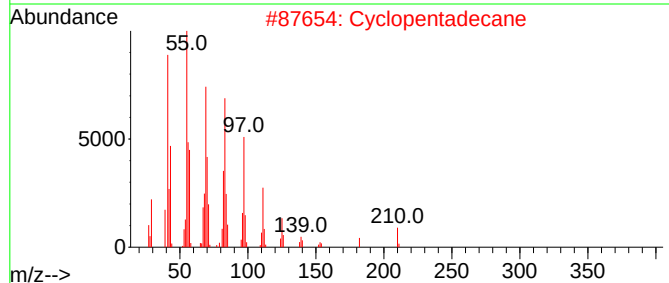
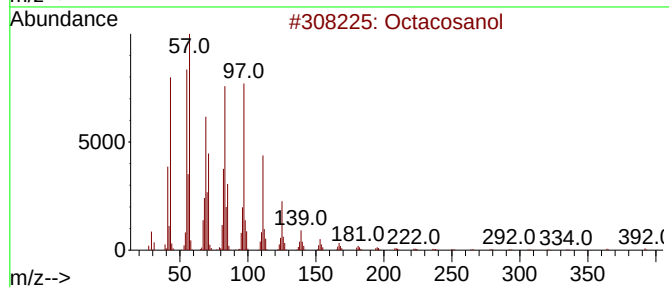
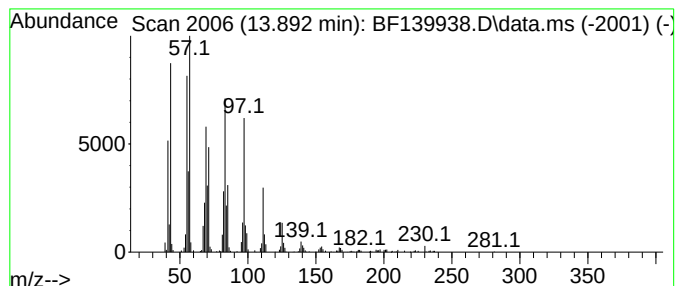
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	11.72 ng	520334	Chrysene-d12	14.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
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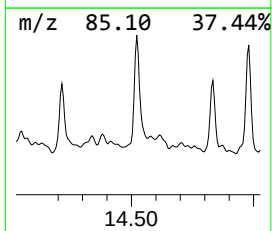
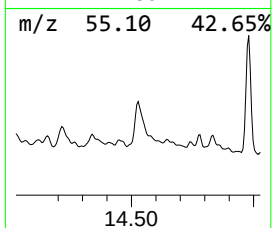
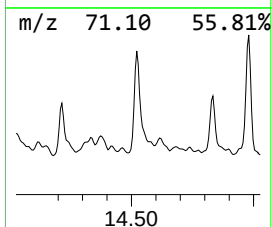
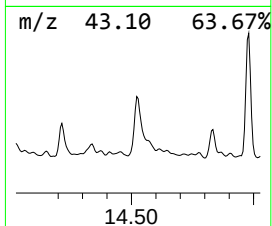
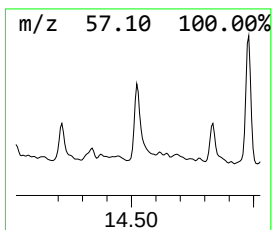
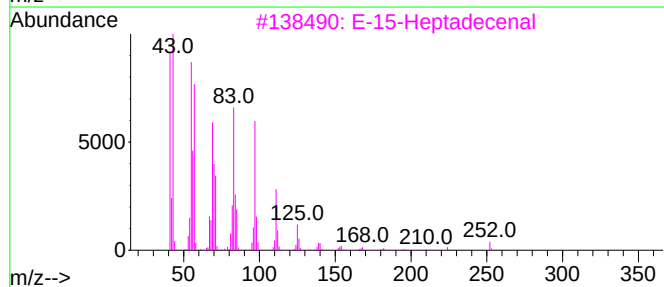
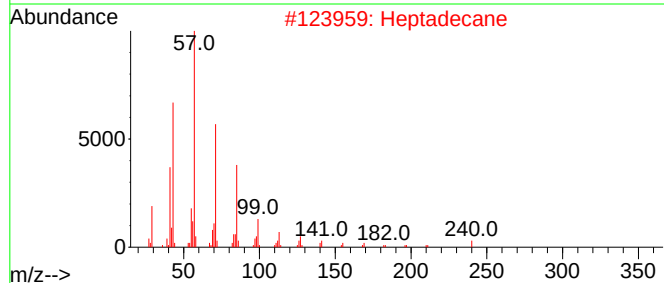
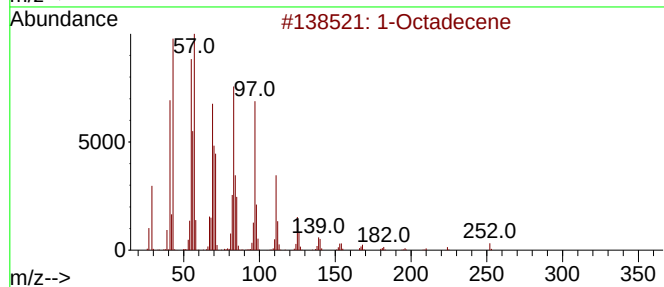
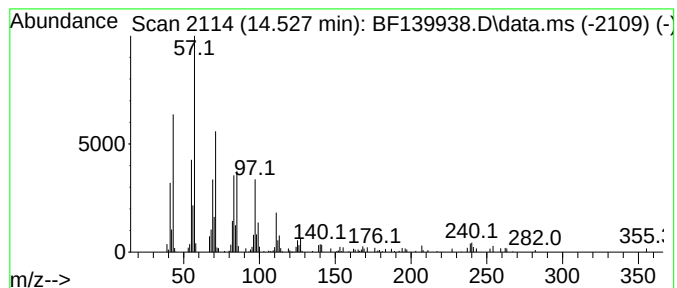
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.527	4.09 ng	181541	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecene	252	C18H36	000112-88-9	95
2			Heptadecane	240	C17H36	000629-78-7	92
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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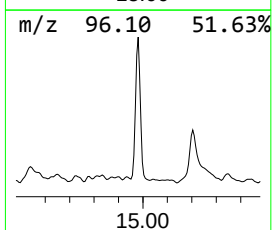
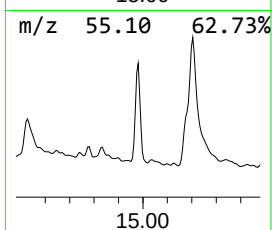
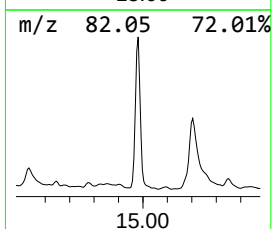
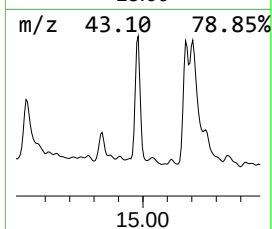
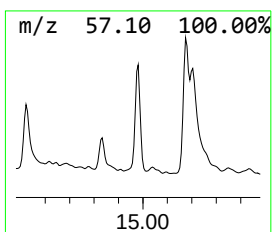
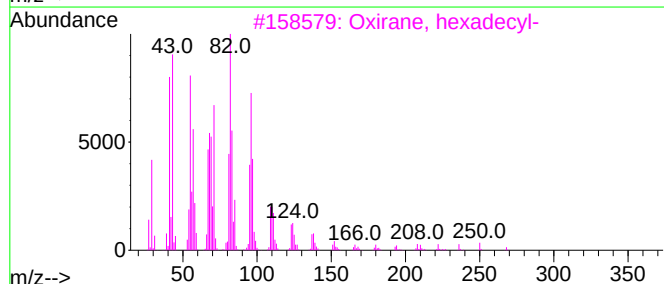
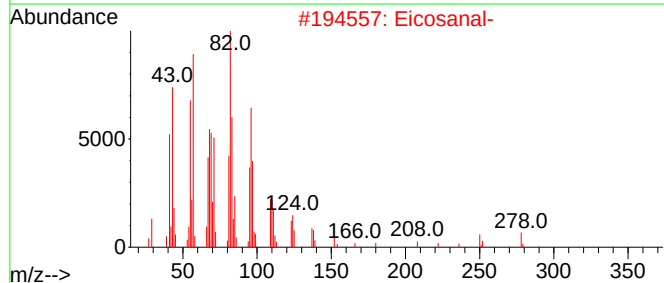
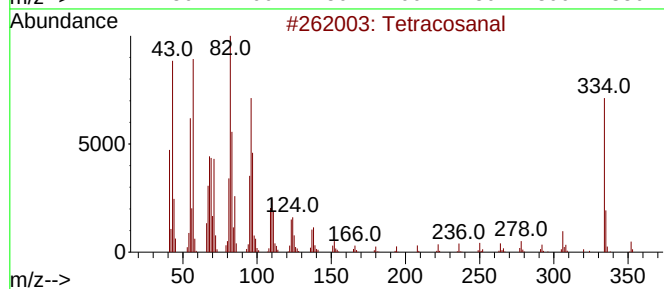
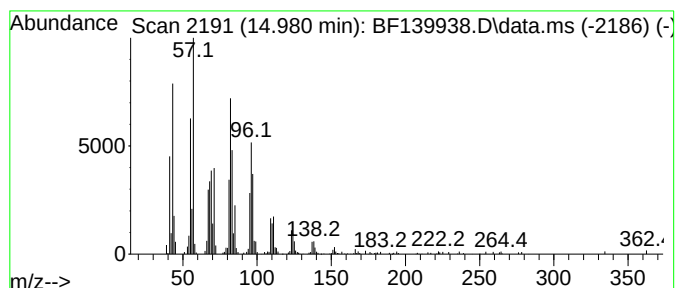
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.980	5.72 ng	263228	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosanal	352	C24H48O	057866-08-7	91
2	Eicosanal-	296	C20H40O	002400-66-0	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Octadecanal	268	C18H36O	000638-66-4	91
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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Acq On : 22 Oct 2024 19:54
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Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

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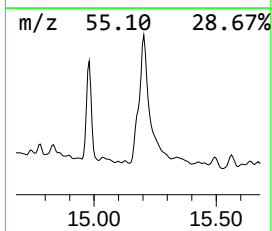
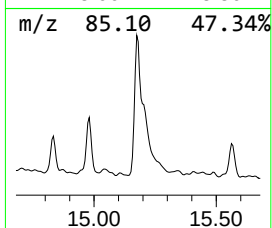
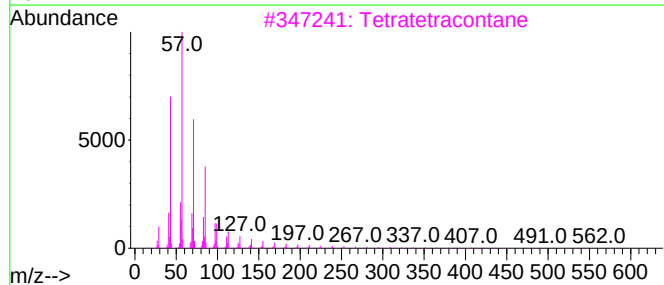
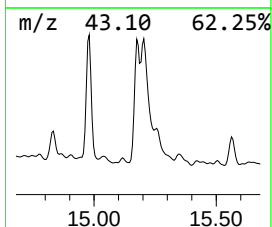
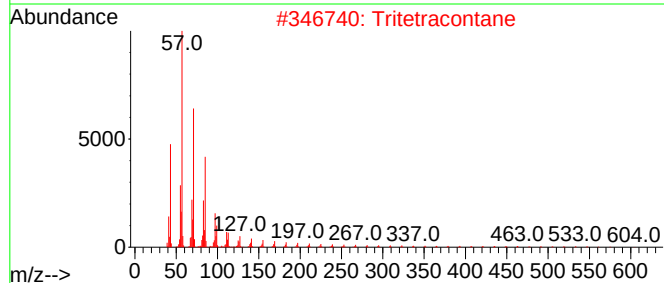
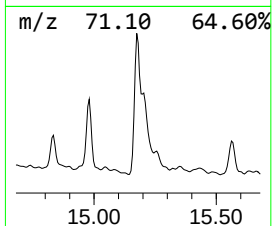
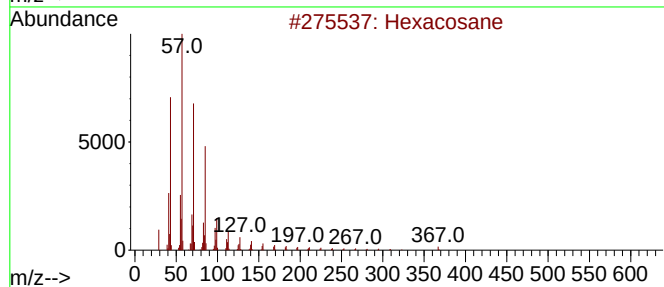
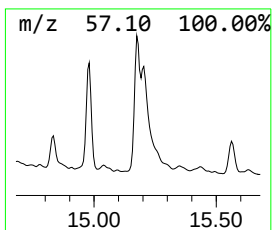
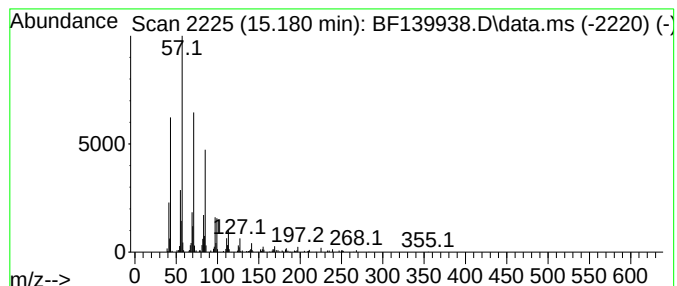
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	3.90 ng	179130	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Tritetracontane	605	C43H88	007098-21-7	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Hexatriacontane	507	C36H74	000630-06-8	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
Operator : RC/JU
Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

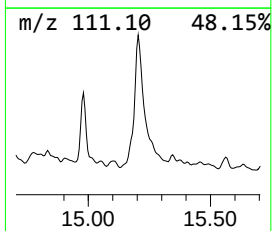
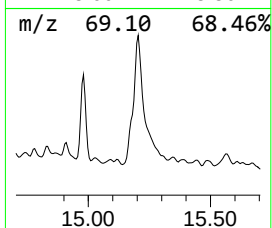
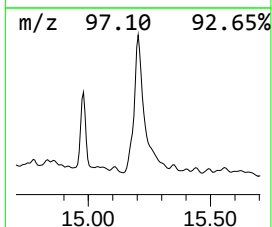
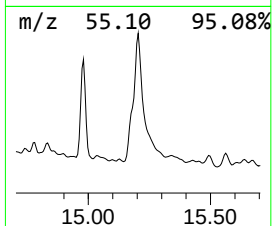
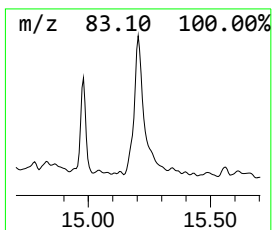
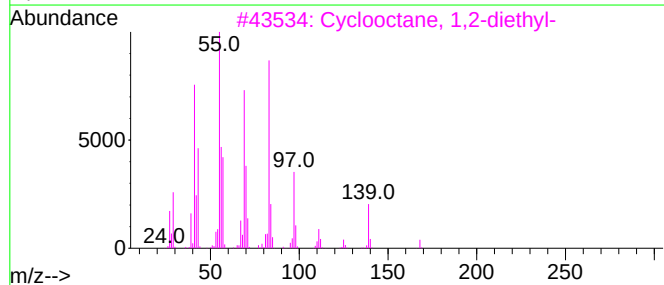
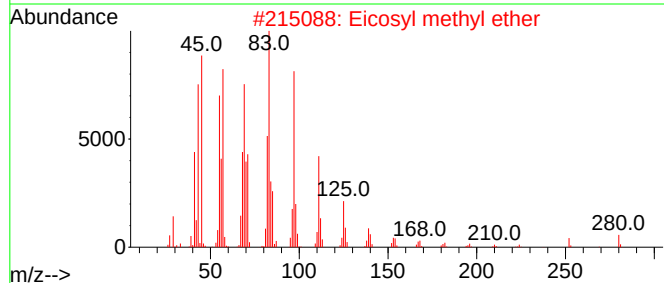
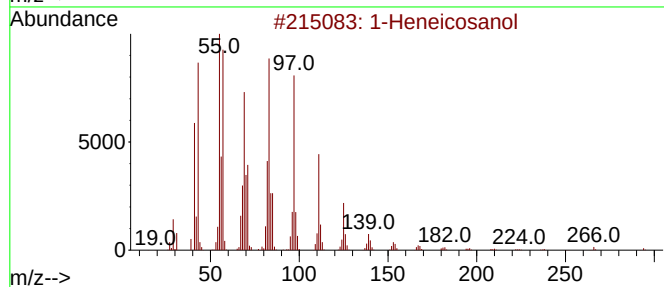
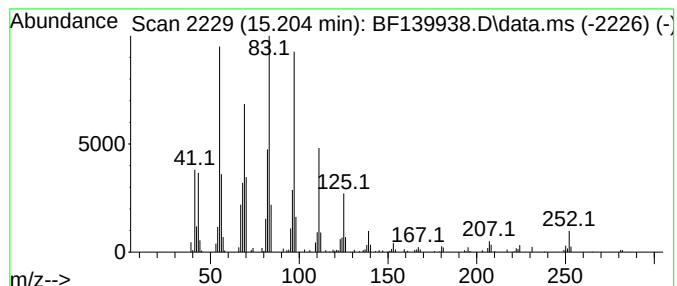
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.204	10.09 ng	463953	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	62
2	Eicosyl methyl ether	312	C21H44O	1000406-29-4	52
3	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	42
4	Triallylmethylsilane	166	C10H18Si	001112-91-0	38
5	1-Hexadecanol	242	C16H34O	036653-82-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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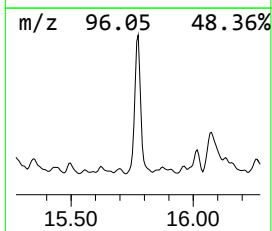
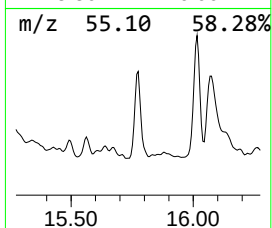
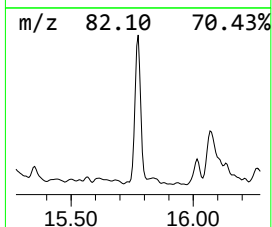
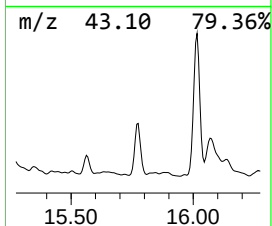
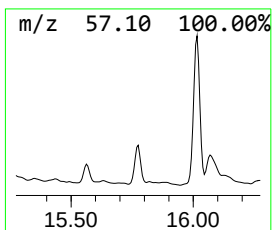
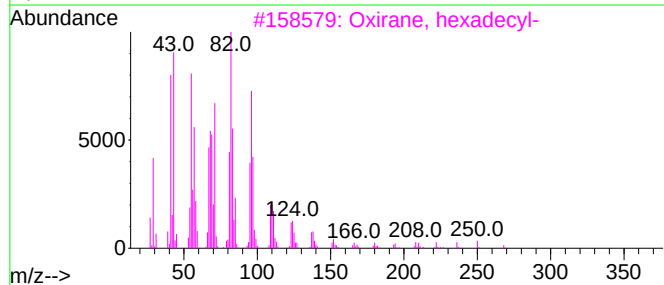
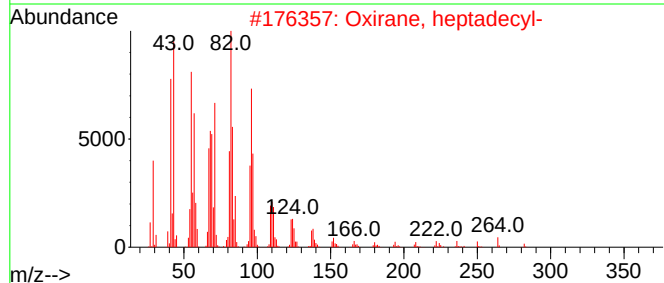
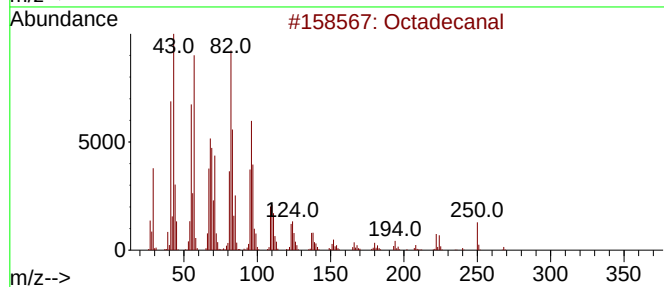
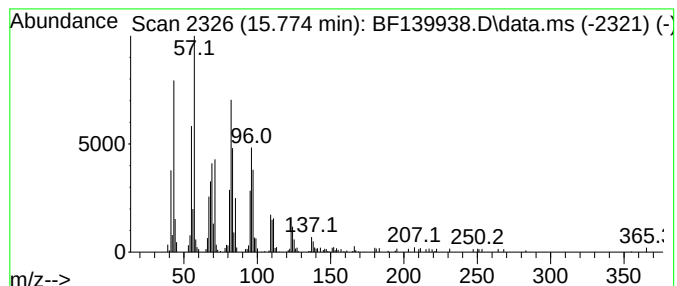
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.774	4.08 ng	187482	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	93
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4	Hexacosanal	380	C26H52O	026627-85-0	87
5	Eicosanal-	296	C20H40O	002400-66-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
Operator : RC/JU
Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

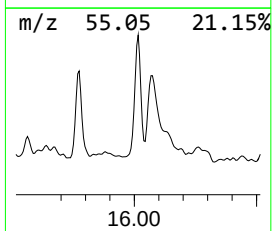
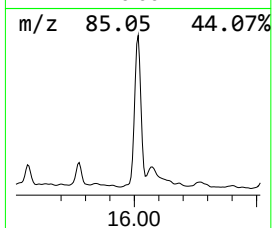
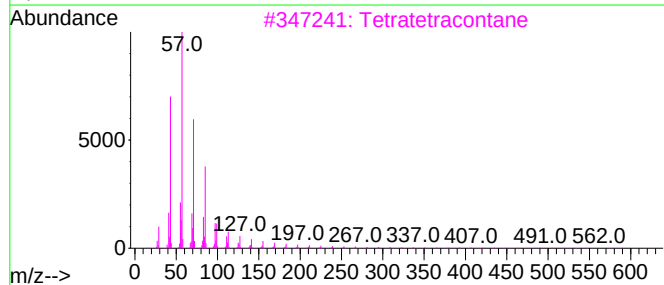
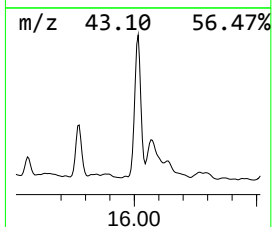
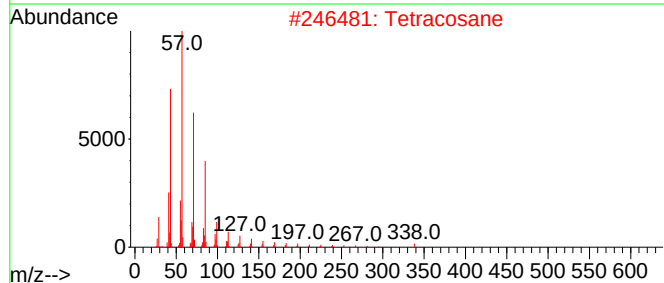
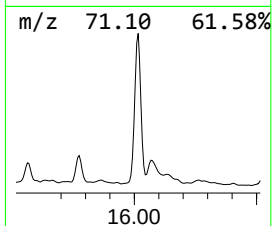
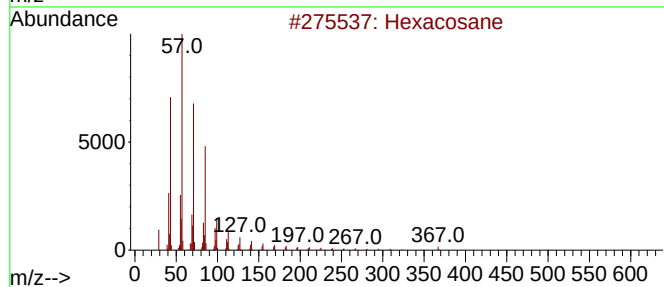
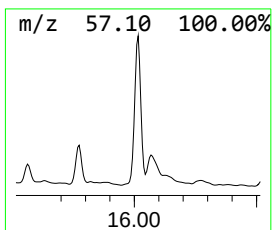
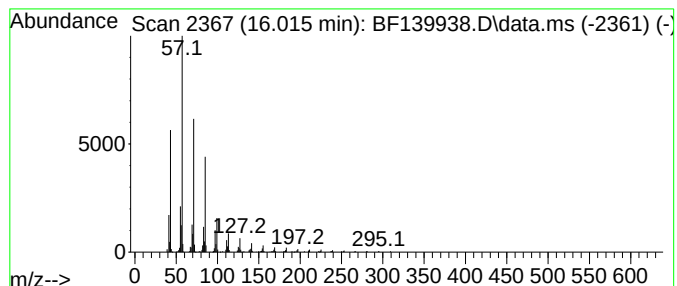
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.015	8.34 ng	383514	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Tetracosane	338	C24H50	000646-31-1	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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Sample : P4385-06
Misc :
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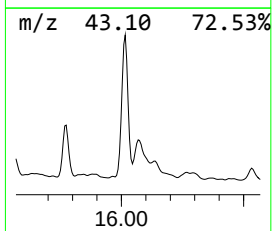
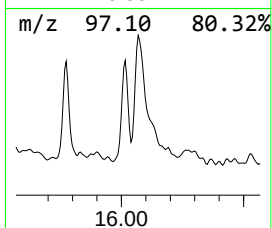
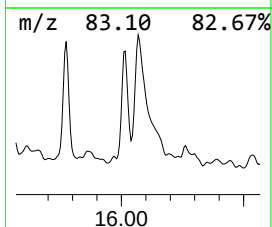
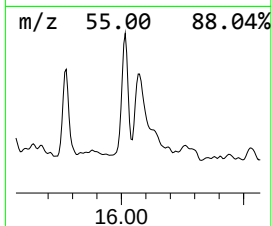
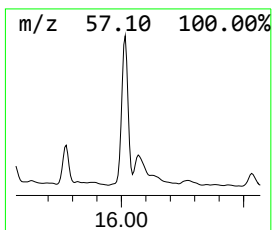
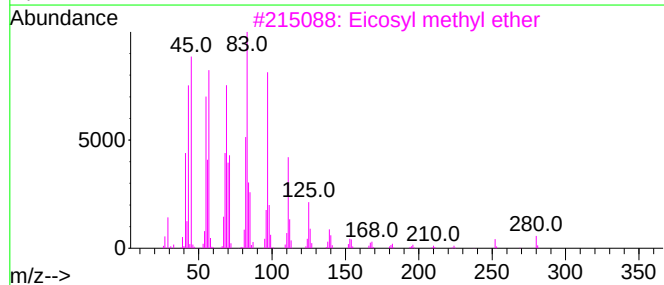
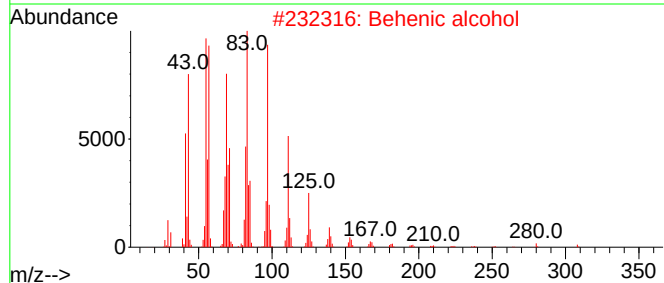
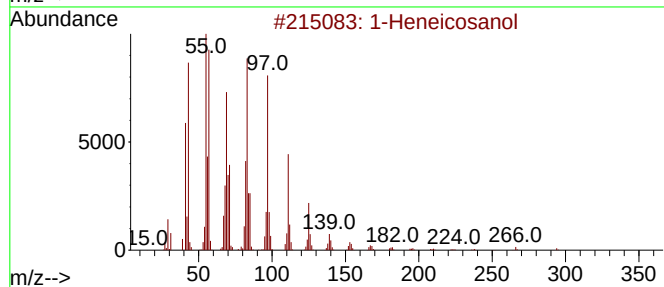
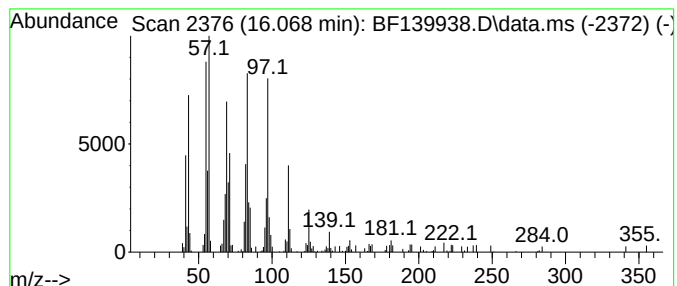
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Behenic alcohol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.068	3.69 ng	169844	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
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Sample : P4385-06
Misc :
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Instrument :
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ClientSampleId :
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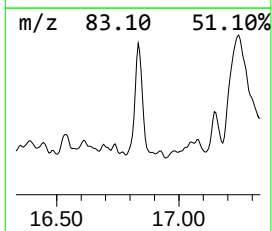
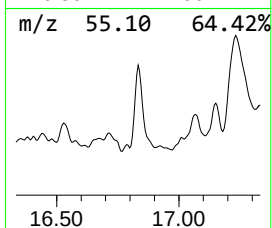
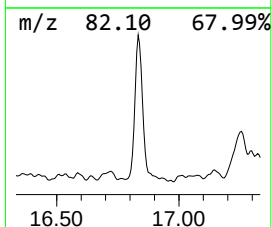
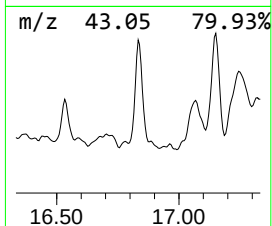
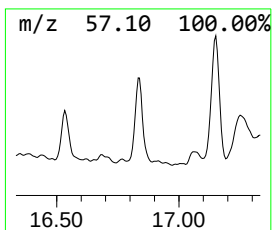
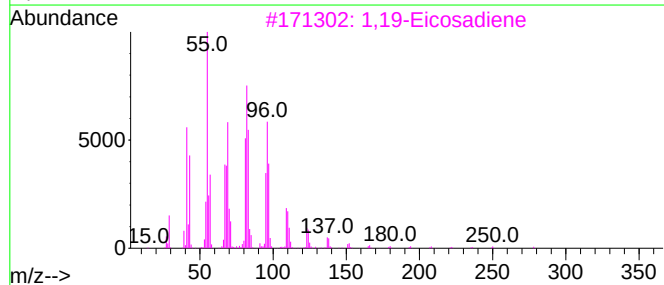
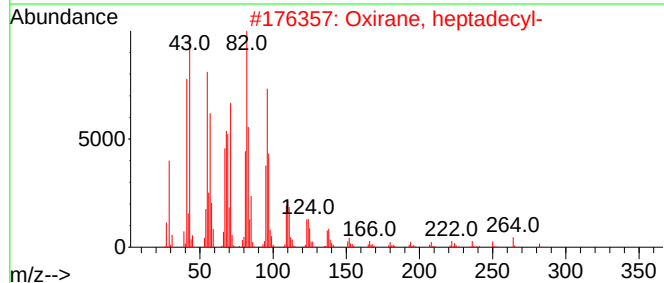
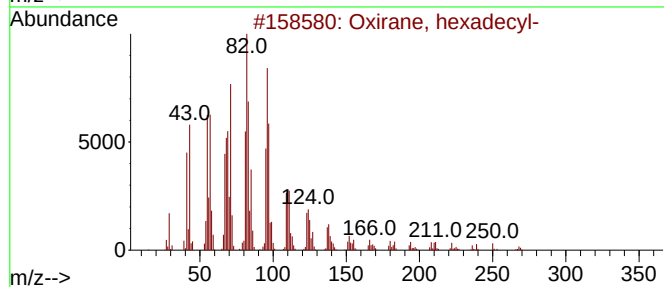
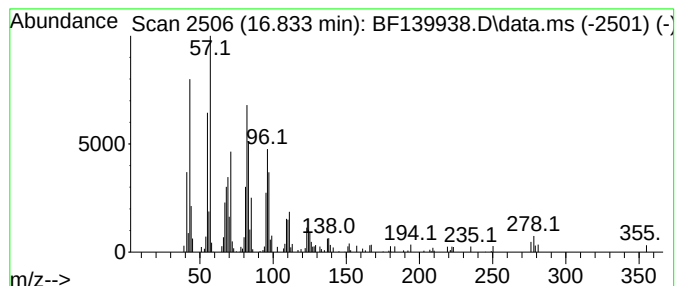
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Oxirane, hexadecyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.833	3.29 ng	151160	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	74
3			1,19-Eicosadiene	278	C20H38	014811-95-1	62
4			Octadecanal	268	C18H36O	000638-66-4	58
5			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
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Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

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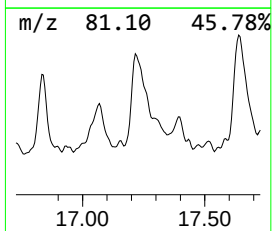
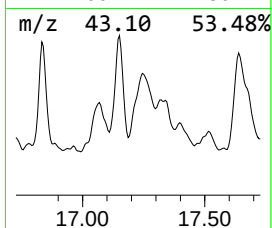
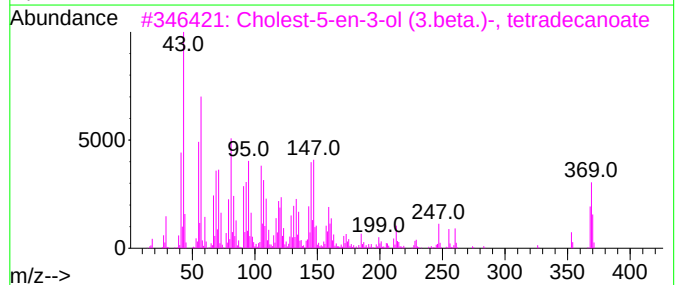
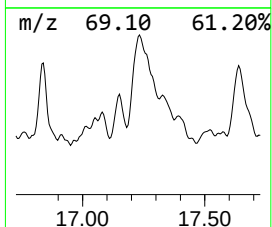
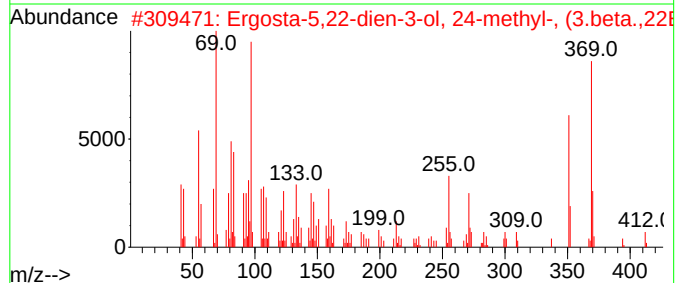
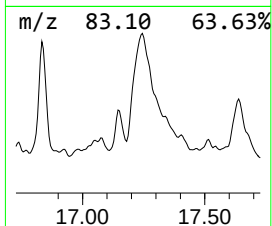
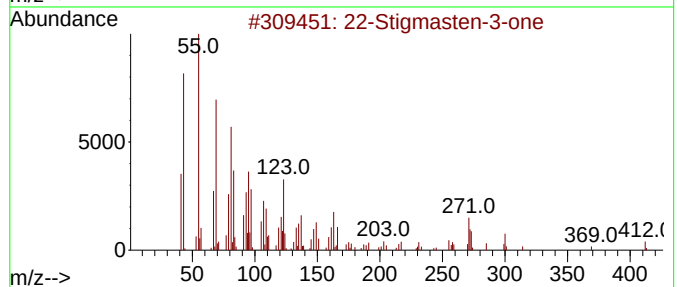
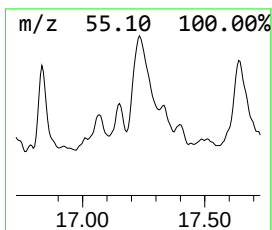
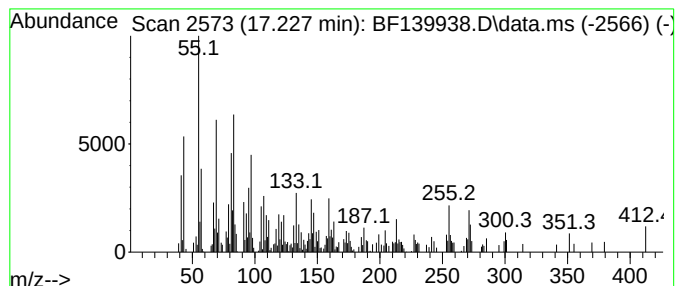
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 22-Stigmasten-3-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.227	7.09 ng	326286	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	22-Stigmasten-3-one			412	C29H48O	004736-95-2	47
2	Ergosta-5,22-dien-3-ol, 24-methy...			412	C29H48O	053755-22-9	13
3	Cholest-5-en-3-ol (3.beta.)-, te...			597	C41H72O2	001989-52-2	10
4	5'-Fluoro-2'-hydroxy-4-methoxych...			342	C20H19FO4	1000449-54-7	10
5	Sulfoxide, hexadecyl methyl			288	C17H36OS	003079-32-1	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
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Sample : P4385-06
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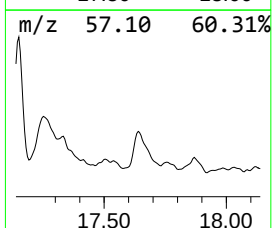
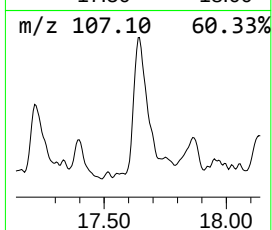
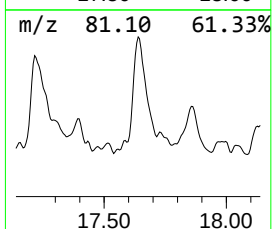
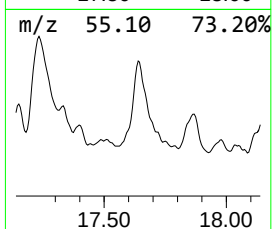
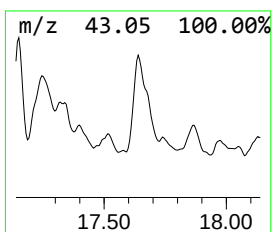
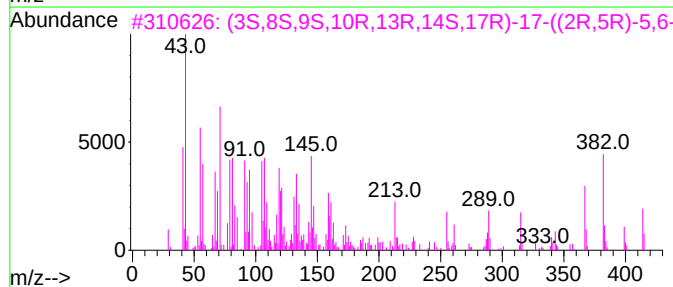
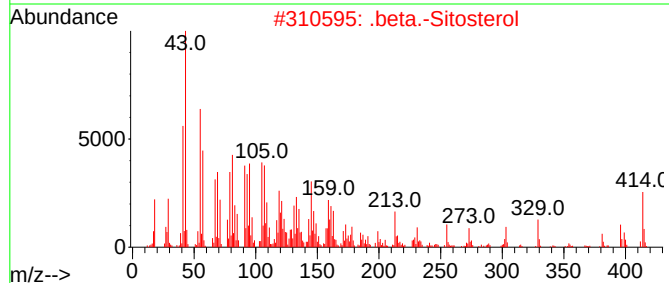
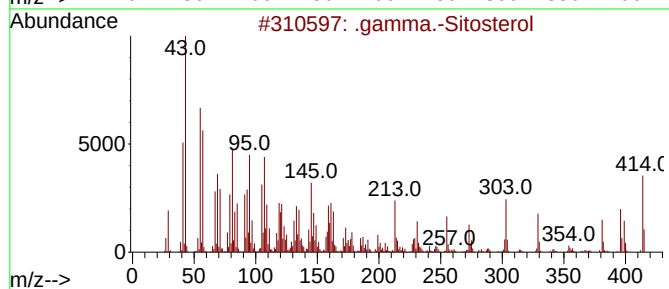
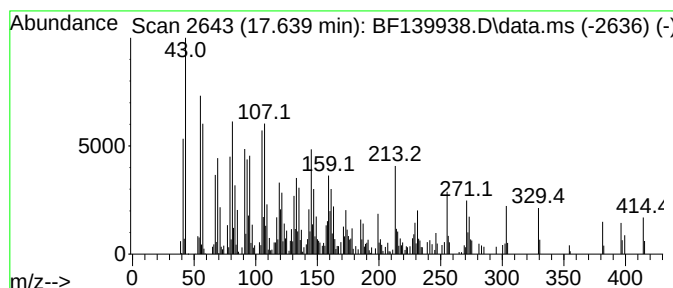
Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.639	10.14 ng	466499	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	98
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	74
4	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	47
5	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139938.D
Acq On : 22 Oct 2024 19:54
Operator : RC/JU
Sample : P4385-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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
Butane, 2-metho...	2.193	99.3	ng	4114460	1	6.887	828408	20.0
3-Penten-2-one,...	4.499	4.6	ng	188784	1	6.887	828408	20.0
2-Pentanone, 4-...	5.116	8.1	ng	333870	1	6.887	828408	20.0
Pentanedioic ac...	7.698	2.3	ng	127020	2	8.169	1096050	20.0
Benzophenone	10.633	14.5	ng	830013	3	9.922	1144820	20.0
Methanone, (1-h...	10.945	2.9	ng	141579	4	11.410	978400	20.0
1-Octadecene	12.457	2.8	ng	135796	4	11.410	978400	20.0
1,3-Propanediol...	13.204	2.6	ng	114489	5	14.051	888317	20.0
Octacosanol	13.892	11.7	ng	520334	5	14.051	888317	20.0
Heptadecane	14.527	4.1	ng	181541	5	14.051	888317	20.0
Tetracosanal	14.980	5.7	ng	263228	6	15.527	919765	20.0
Hexacosane	15.180	3.9	ng	179130	6	15.527	919765	20.0
1-Heneicosanol	15.204	10.1	ng	463953	6	15.527	919765	20.0
Octadecanal	15.774	4.1	ng	187482	6	15.527	919765	20.0
Tetracosane	16.015	8.3	ng	383514	6	15.527	919765	20.0
Behenic alcohol	16.068	3.7	ng	169844	6	15.527	919765	20.0
Oxirane, hexade...	16.833	3.3	ng	151160	6	15.527	919765	20.0
22-Stigmasten-3...	17.227	7.1	ng	326286	6	15.527	919765	20.0
.gamma.-Sitosterol	17.639	10.1	ng	466499	6	15.527	919765	20.0