

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
 Data File : BF139368.D
 Acq On : 14 Sep 2024 14:48
 Operator : RC/JU
 Sample : P3940-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AST-2024-4036-PRIM

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	8	16	22	rVB	1396926	2193021	100.00%	19.405%
2	5.087	500	509	515	rBV	27384	39357	1.79%	0.348%
3	5.487	572	577	585	rVB	460287	611757	27.90%	5.413%
4	6.493	743	748	753	rBV	309110	391801	17.87%	3.467%
5	6.875	808	813	818	rBV	309289	374343	17.07%	3.312%
6	7.440	902	909	914	rVB	691171	939324	42.83%	8.312%
7	7.687	941	951	955	rBV4	14481	35609	1.62%	0.315%
8	8.157	1026	1031	1036	rBV	378207	459667	20.96%	4.067%
9	8.469	1080	1084	1087	rBV	26071	35157	1.60%	0.311%
10	8.522	1087	1093	1097	rVV3	70772	146058	6.66%	1.292%
11	8.569	1097	1101	1106	rVB	34212	62837	2.87%	0.556%
12	9.234	1208	1214	1219	rBV	1298107	1620216	73.88%	14.336%
13	9.345	1228	1233	1237	rVB	46896	56798	2.59%	0.503%
14	9.910	1324	1329	1334	rVB	408012	495801	22.61%	4.387%
15	10.004	1340	1345	1353	rBV	32852	59240	2.70%	0.524%
16	10.698	1457	1463	1468	rBV	938305	1190679	54.29%	10.536%
17	11.392	1576	1581	1596	rVB	368281	480066	21.89%	4.248%
18	11.916	1666	1670	1681	rVB2	87707	133522	6.09%	1.181%
19	12.622	1785	1790	1799	rBV6	13847	34551	1.58%	0.306%
20	12.704	1799	1804	1817	rVB	26008	50376	2.30%	0.446%
21	12.980	1845	1851	1856	rBV	992297	1265483	57.71%	11.197%
22	13.874	1998	2003	2014	rVB	32452	52458	2.39%	0.464%
23	14.027	2024	2029	2034	rBV	220999	277151	12.64%	2.452%
24	15.498	2273	2279	2288	rVB	193689	296217	13.51%	2.621%

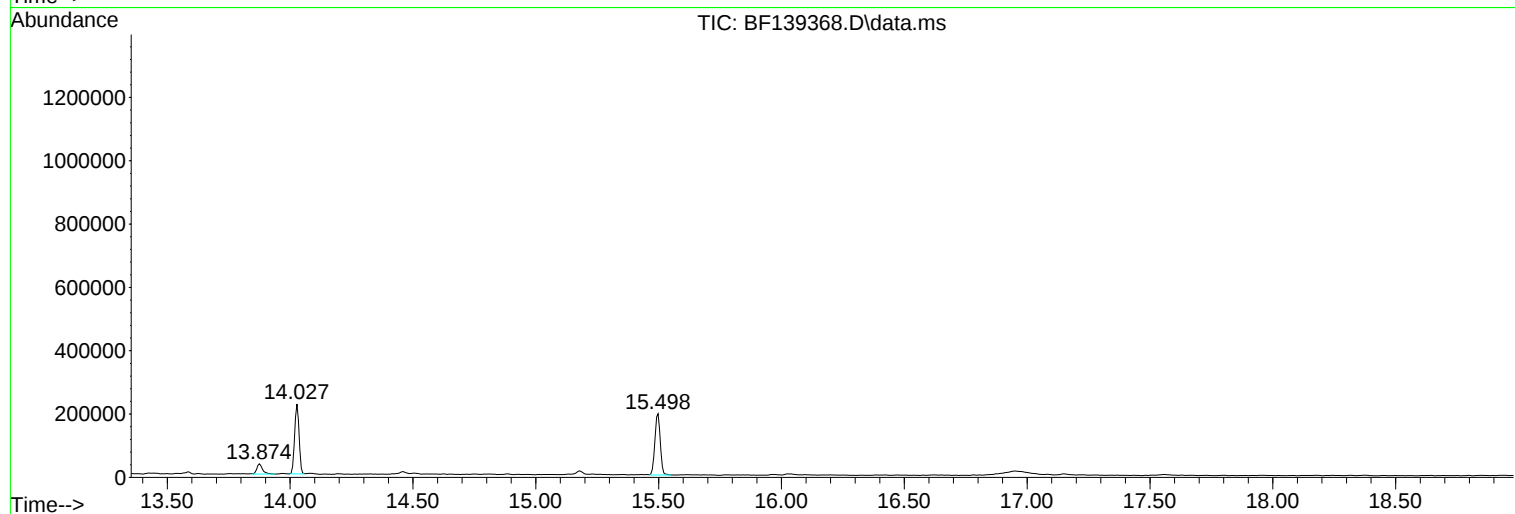
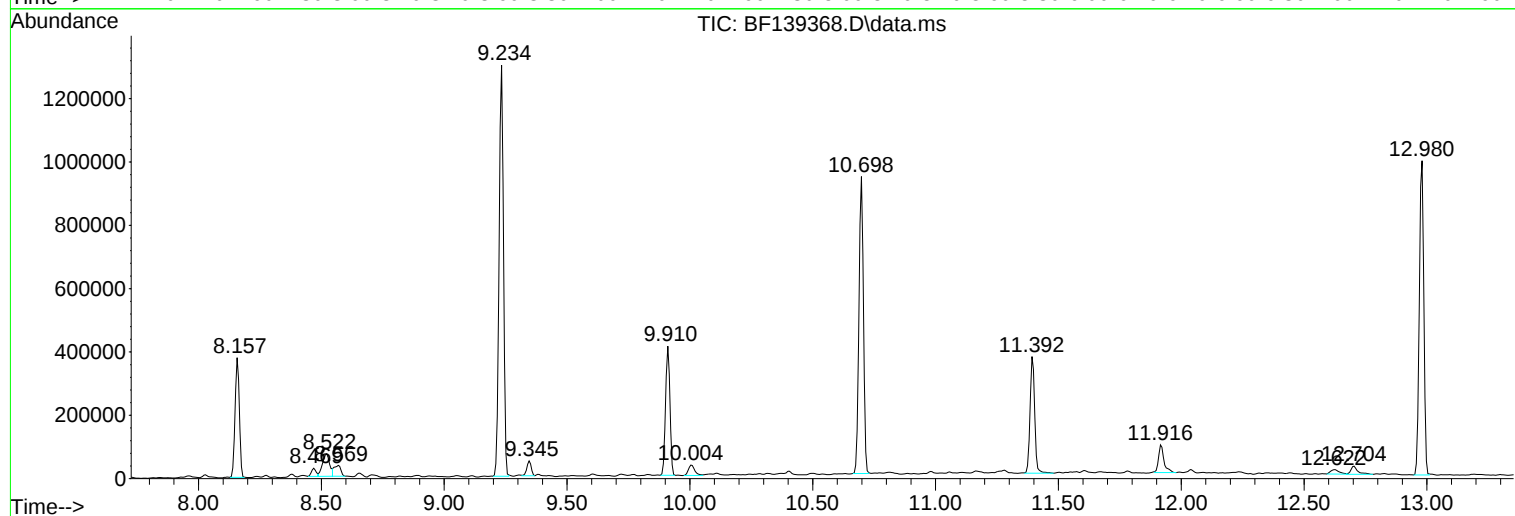
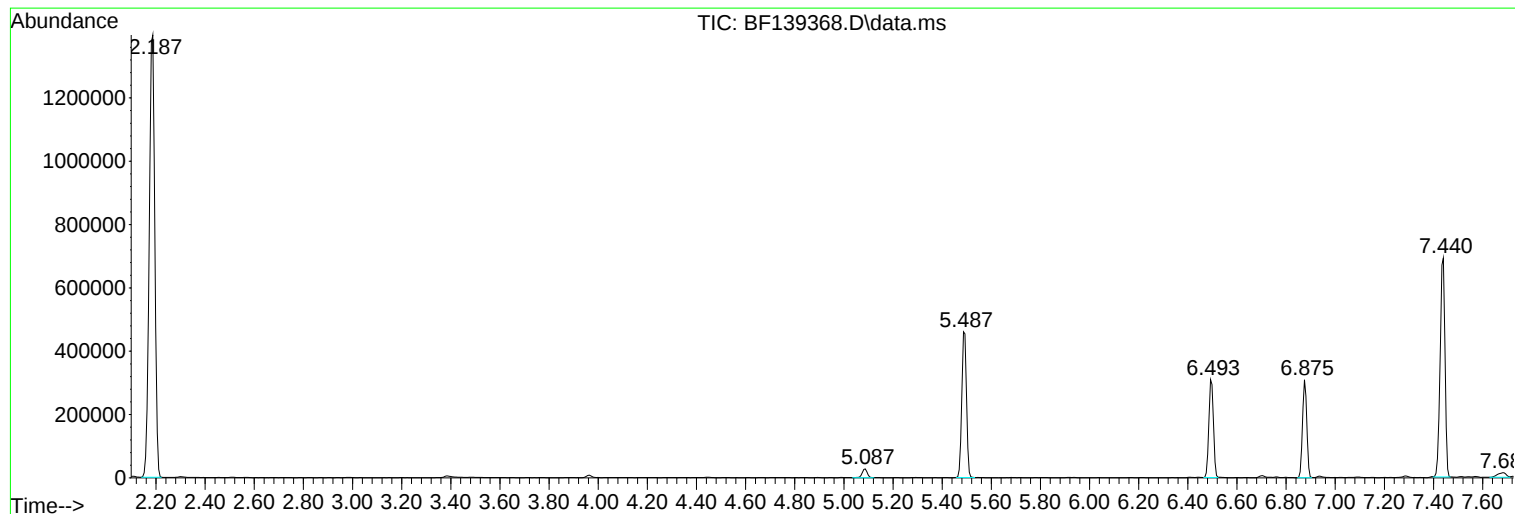
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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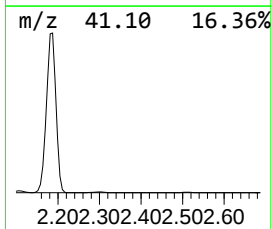
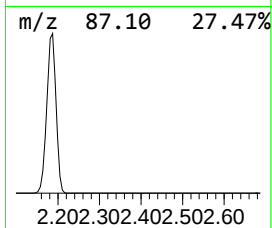
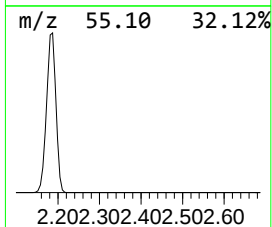
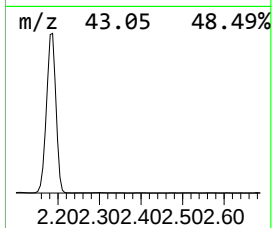
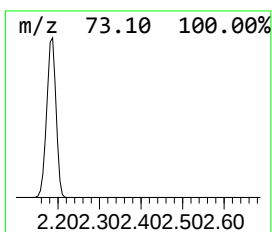
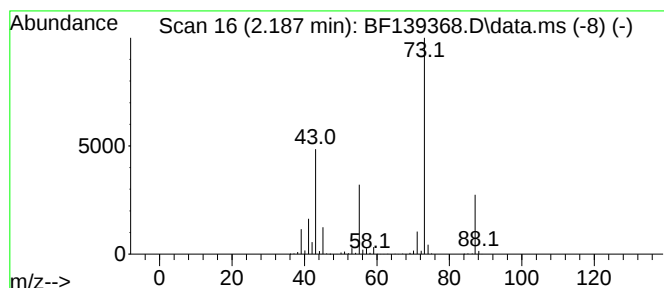
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	117.17 ng	2193020	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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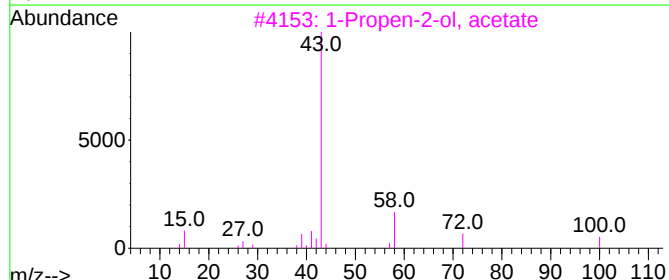
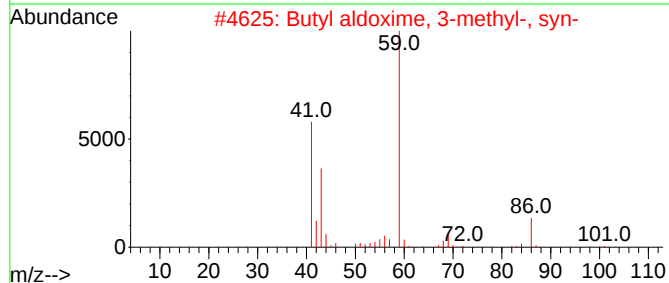
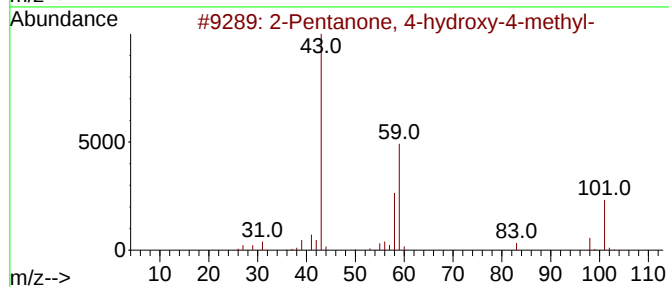
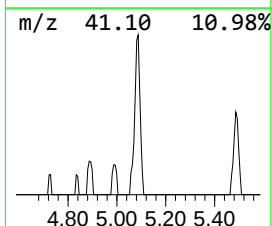
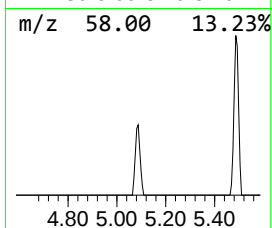
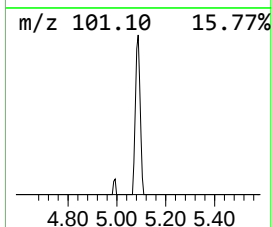
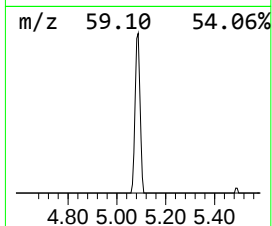
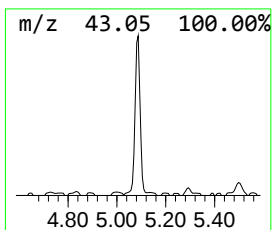
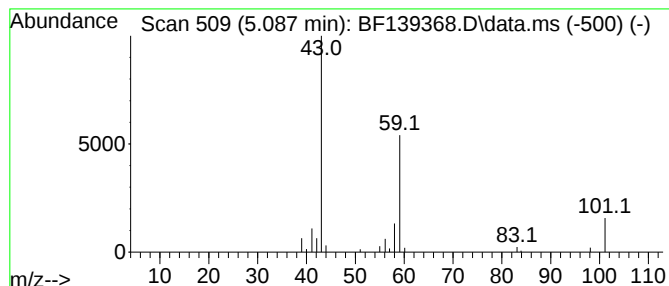
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.10 ng	39357	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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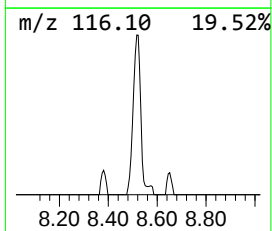
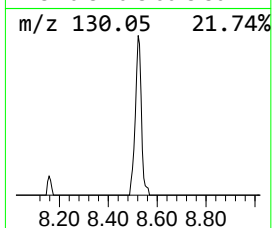
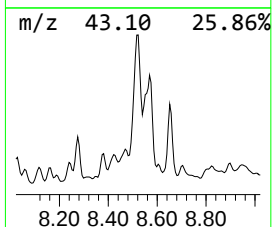
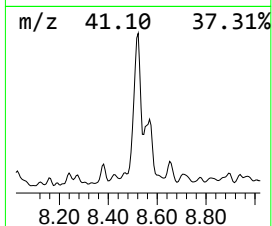
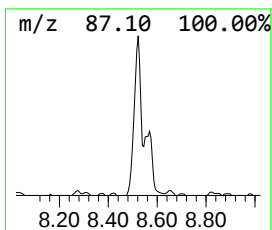
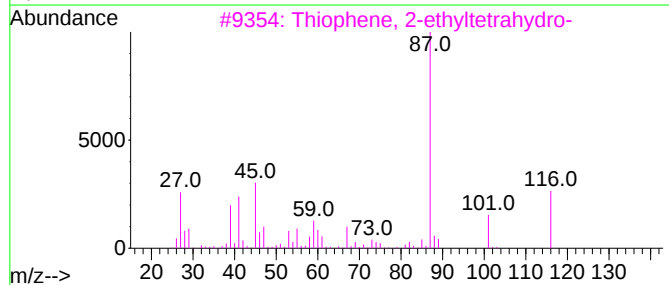
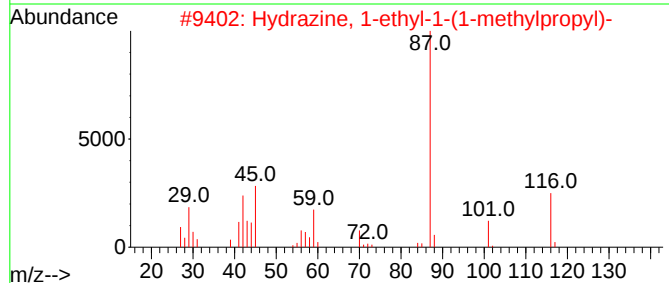
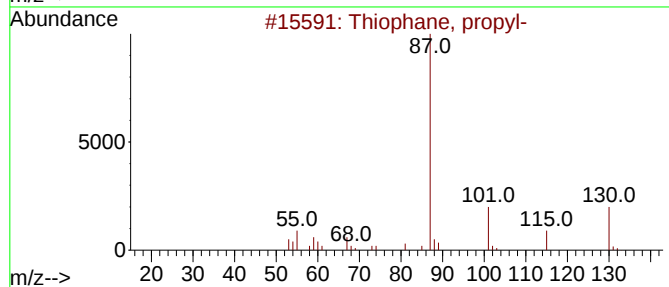
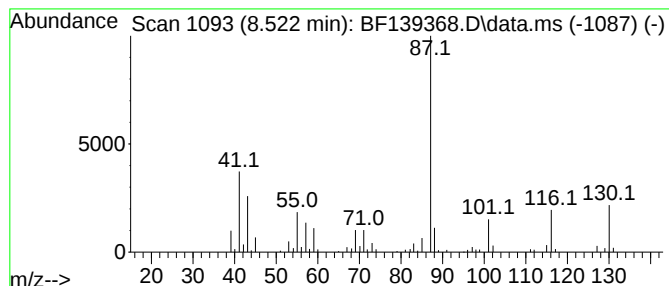
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Thiophane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	6.35 ng	146058	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	58
2			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	53
3			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	45
4			Neodecanoic acid	172	C10H20O2	026896-20-8	45
5			Pentanoic acid, 2-propyl-, methy...	158	C9H18O2	022632-59-3	38



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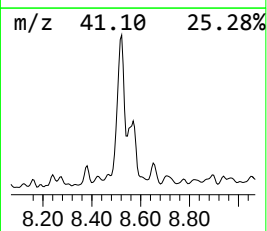
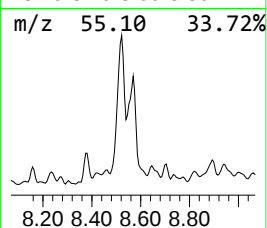
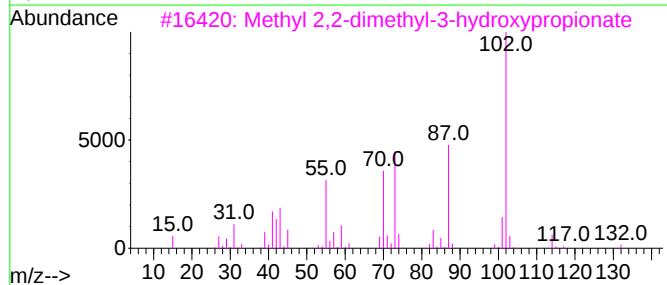
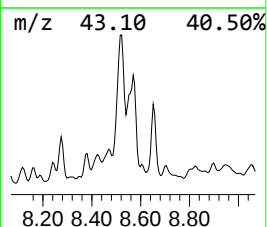
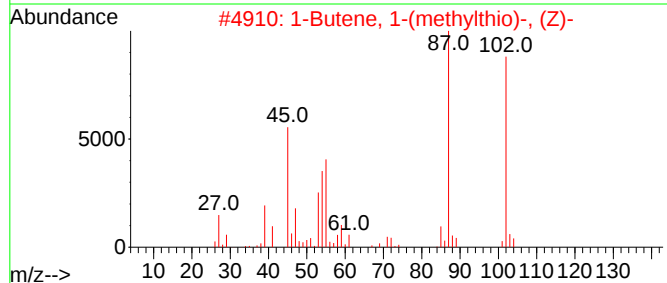
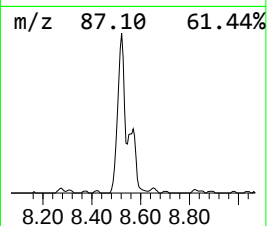
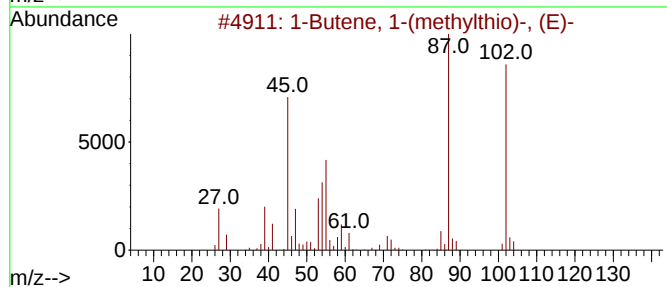
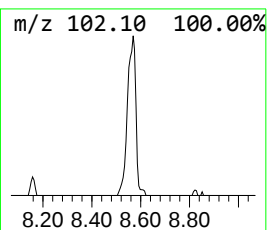
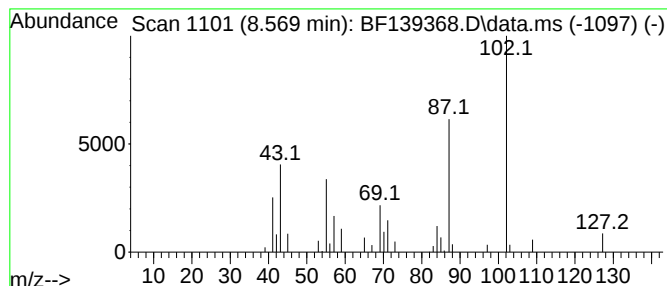
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Peak Number 4 1-Butene, 1-(methylthio)-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	2.73 ng	62837	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butene, 1-(methylthio)-, (E)-	102	C5H10S	017414-27-6	59
2			1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	45
3			Methyl 2,2-dimethyl-3-hydroxypro...	132	C6H12O3	014002-80-3	39
4			1-Alanine, N-methoxycarbonyl-, p...	189	C8H15NO4	1000313-37-1	25
5			2-O-Methyl-D-mannopyranosa	194	C7H14O6	036864-61-6	12



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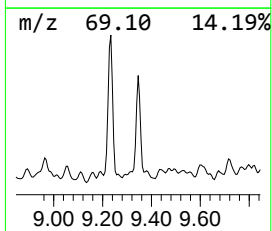
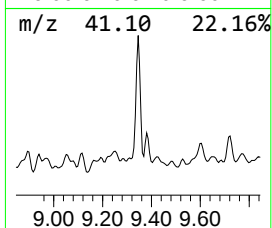
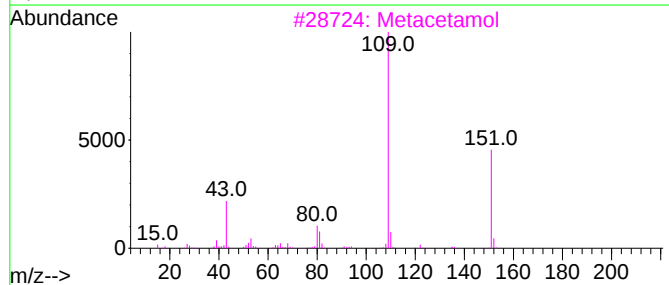
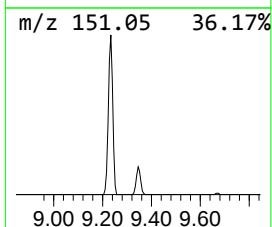
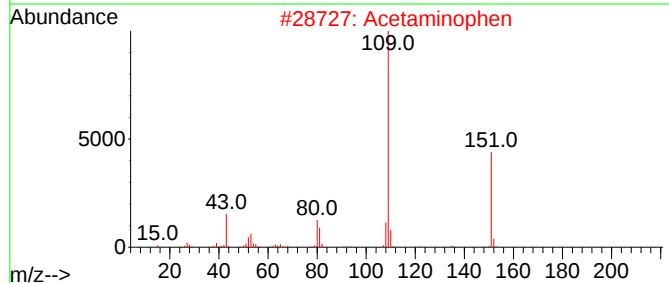
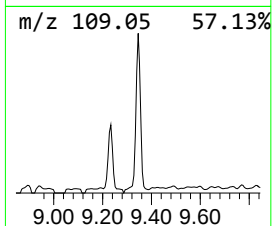
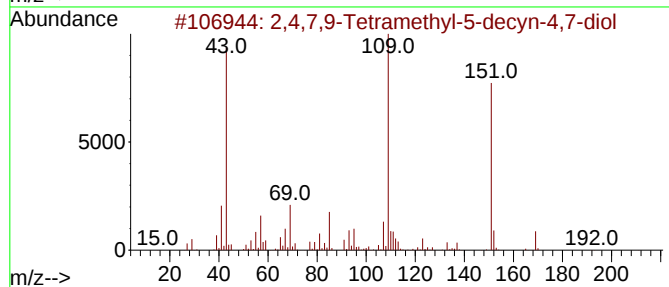
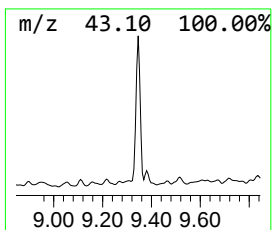
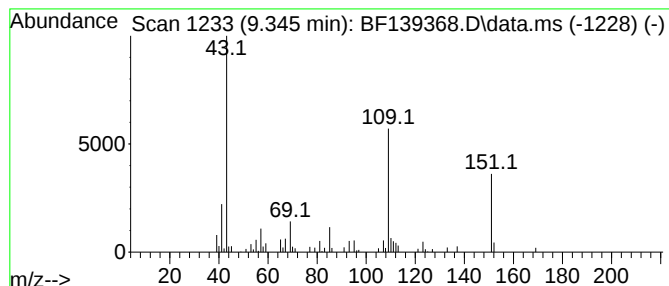
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Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	2.29 ng	56798	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	90
2	Acetaminophen	151	C8H9NO2		000103-90-2	52
3	Metacetamol	151	C8H9NO2		000621-42-1	52
4	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	50
5	3-Pyridinemethanol, acetate	151	C8H9NO2		010072-09-0	50



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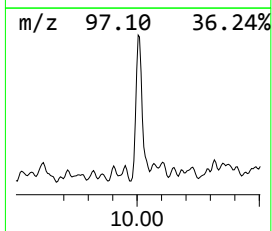
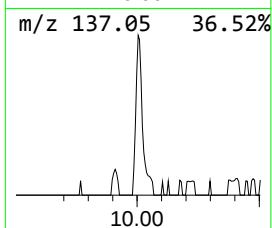
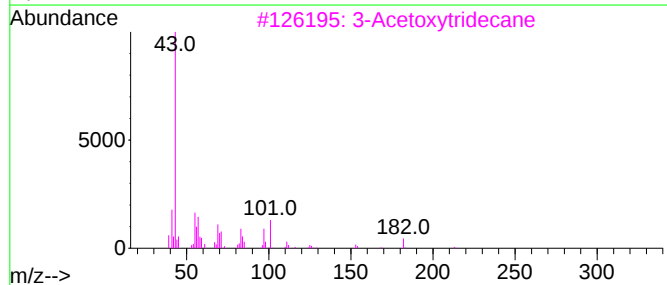
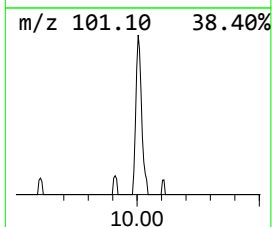
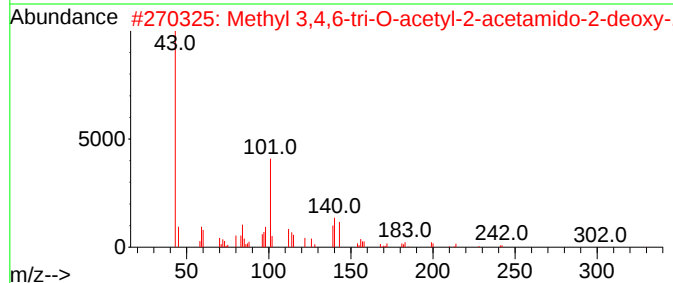
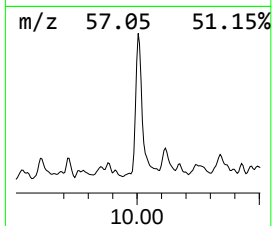
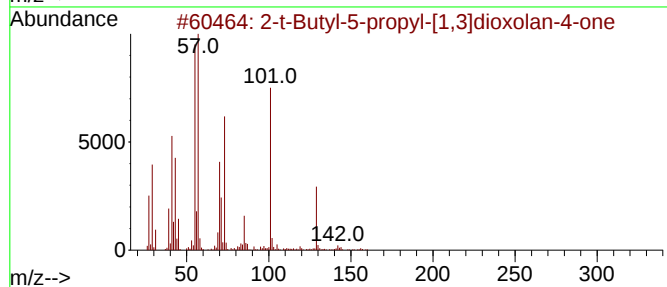
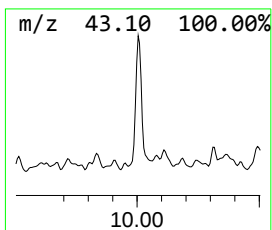
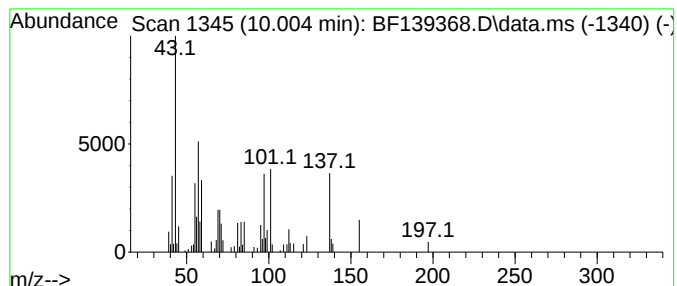
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.004 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	2.39 ng	59240	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butyl-5-propyl-[1,3]dioxolan...	186	C10H18O3	157733-17-0	22		
2	Methyl 3,4,6-tri-O-acetyl-2-acet...	361	C15H23NO9	002595-39-3	14		
3	3-Acetoxytridecane	242	C15H30O2	1010245-61-3	12		
4	Diethylmalonic acid, monochlorid...	318	C17H31ClO3	1000369-41-8	10		
5	1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139368.D
Acq On : 14 Sep 2024 14:48
Operator : RC/JU
Sample : P3940-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AST-2024-4036-PRIM

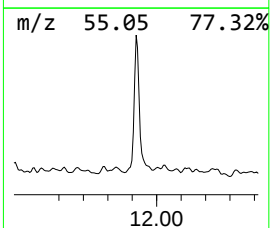
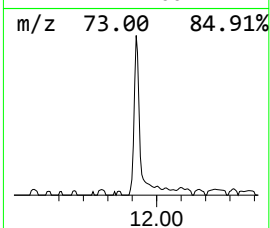
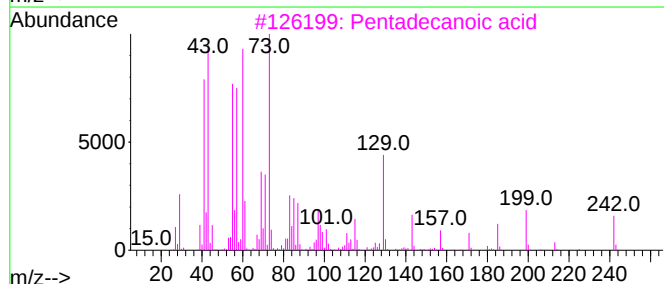
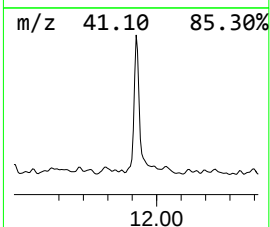
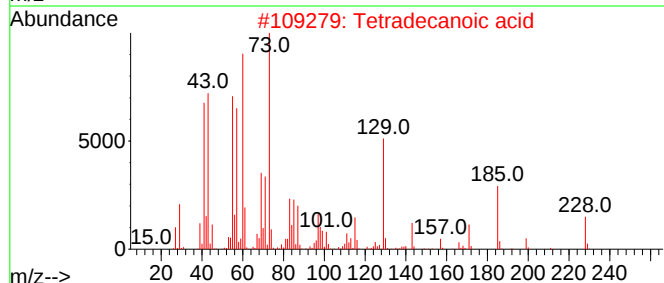
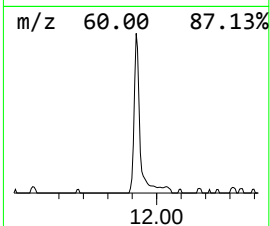
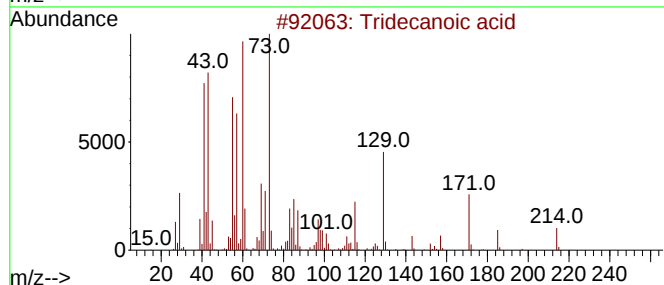
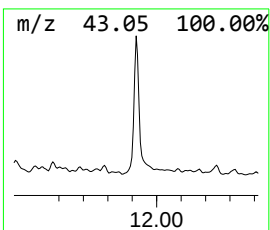
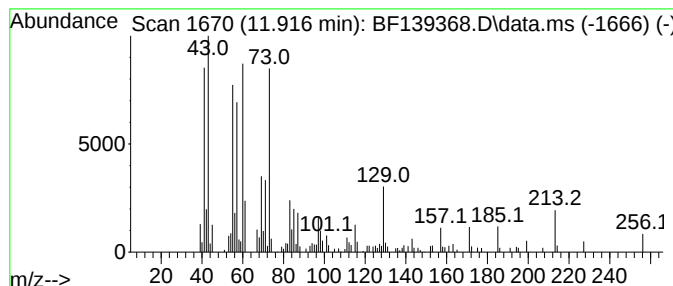
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.56 ng	133522	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	89
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139368.D
Acq On : 14 Sep 2024 14:48
Operator : RC/JU
Sample : P3940-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AST-2024-4036-PRIM

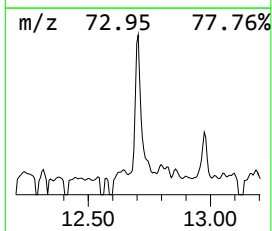
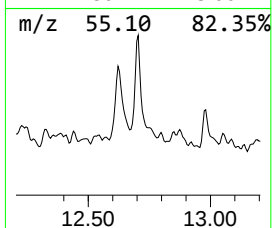
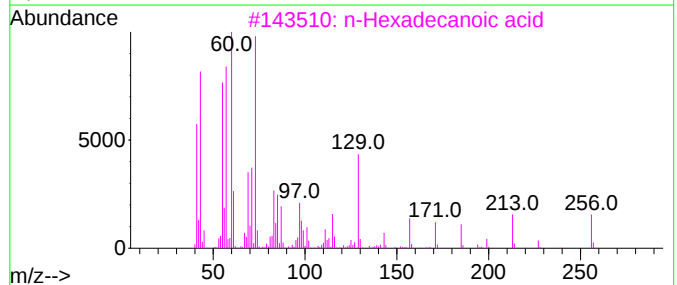
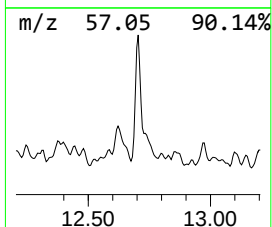
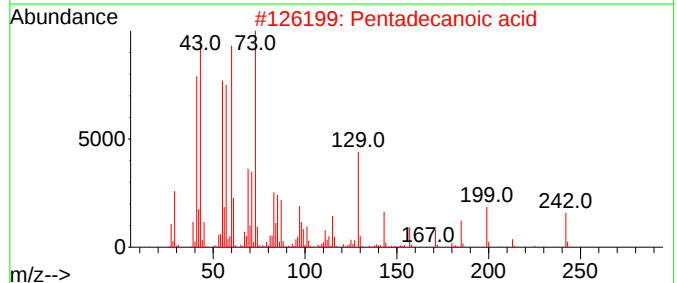
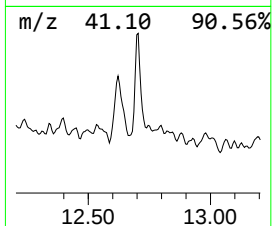
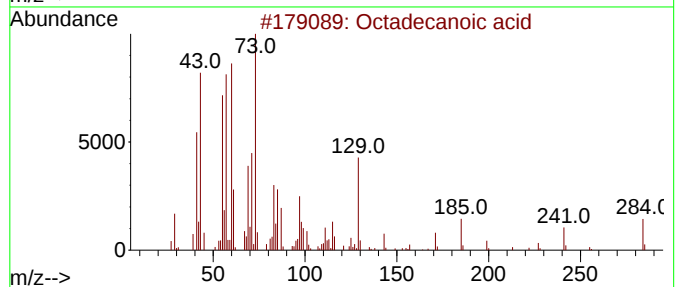
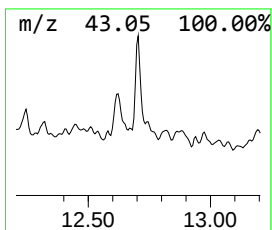
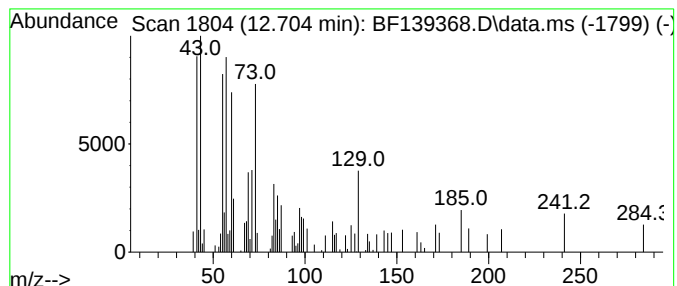
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.10 ng	50376	Phenanthrene-d10	11.392

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139368.D
Acq On : 14 Sep 2024 14:48
Operator : RC/JU
Sample : P3940-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AST-2024-4036-PRIM

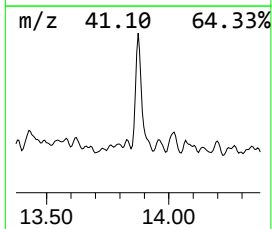
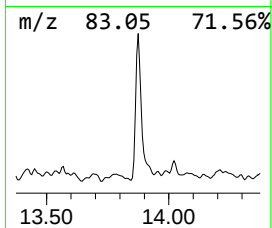
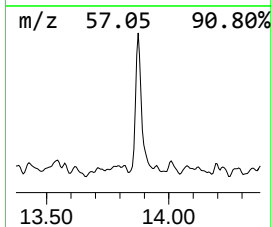
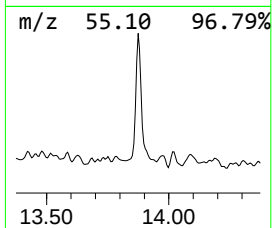
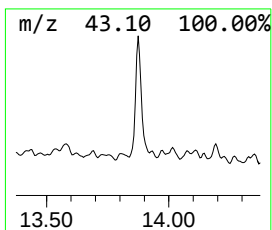
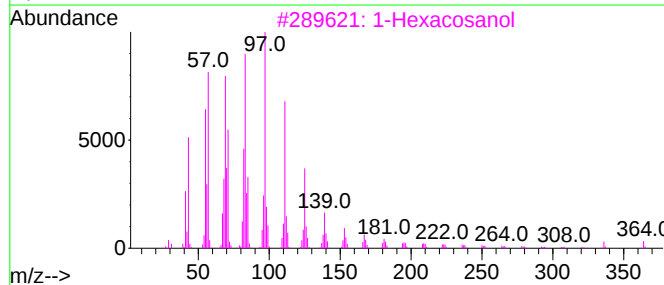
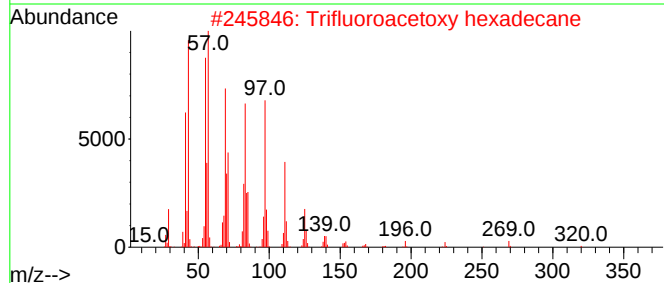
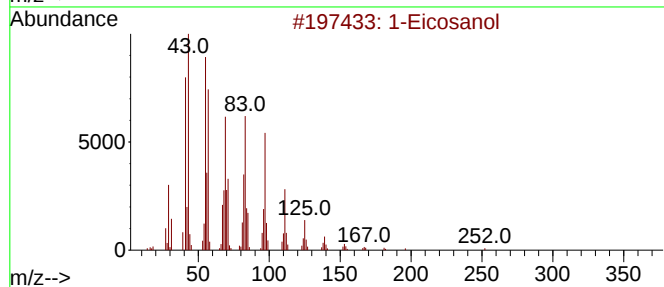
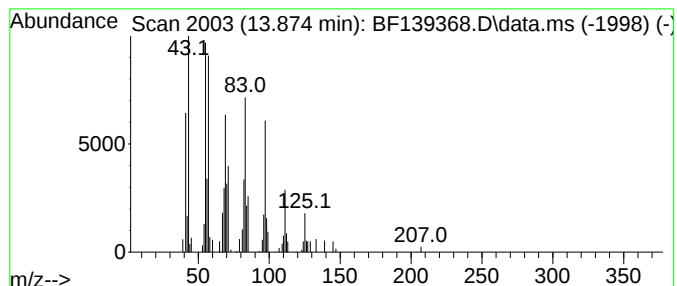
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Eicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.79 ng	52458	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosanol		298	C20H42O	000629-96-9	93
2	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	91
3	1-Hexacosanol		382	C26H54O	000506-52-5	91
4	Octacosanol		410	C28H58O	000557-61-9	91
5	Heptadecyl trifluoroacetate		352	C19H35F3O2	1010351-87-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139368.D
Acq On : 14 Sep 2024 14:48
Operator : RC/JU
Sample : P3940-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AST-2024-4036-PRIM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.187	117.2	ng	2193020	1	6.875	374343	20.0
2-Pentanone, 4-...	5.087	2.1	ng	39357	1	6.875	374343	20.0
Thiophane, propyl-	8.522	6.3	ng	146058	2	8.157	459667	20.0
1-Butene, 1-(me...	8.569	2.7	ng	62837	2	8.157	459667	20.0
2,4,7,9-Tetrame...	9.345	2.3	ng	56798	3	9.910	495801	20.0
unknown10.004	10.004	2.4	ng	59240	3	9.910	495801	20.0
Tridecanoic acid	11.916	5.6	ng	133522	4	11.392	480066	20.0
Octadecanoic acid	12.704	2.1	ng	50376	4	11.392	480066	20.0
1-Eicosanol	13.874	3.8	ng	52458	5	14.027	277151	20.0