

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125441.D
 Acq On : 13 Sep 2021 13:26
 Operator : JU/CG
 Sample : M3681-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WATER-PIT

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	16	22	31	rVB	2806292	3574773	69.39%	10.795%
2	3.046	157	163	169	rBV	37751	58979	1.14%	0.178%
3	3.993	320	324	329	rVB	47017	59892	1.16%	0.181%
4	5.510	578	582	597	rBV	1162851	1106762	21.48%	3.342%
5	6.516	750	753	764	rBV	627386	670103	13.01%	2.024%
6	6.886	812	816	819	rBV	1283511	1171635	22.74%	3.538%
7	7.039	838	842	845	rBV	847565	718216	13.94%	2.169%
8	7.451	906	912	915	rBV	2560242	2611763	50.70%	7.887%
9	8.098	1014	1022	1029	rBV	81079	249033	4.83%	0.752%
10	8.169	1029	1034	1037	rVV	1641340	1484668	28.82%	4.483%
11	9.245	1211	1217	1220	rBV	4753641	4578374	88.87%	13.826%
12	9.851	1314	1320	1323	rBV	120792	106470	2.07%	0.322%
13	9.927	1327	1333	1336	rBV	2030855	1712698	33.25%	5.172%
14	10.351	1402	1405	1408	rVB	283420	240308	4.66%	0.726%
15	10.722	1463	1468	1471	rBV	2752775	2493346	48.40%	7.529%
16	10.822	1482	1485	1494	rVB	393824	335449	6.51%	1.013%
17	11.269	1558	1561	1564	rBV	257615	227793	4.42%	0.688%
18	11.416	1582	1586	1590	rBV	2010489	1822294	35.37%	5.503%
19	11.698	1630	1634	1637	rBV	149669	123524	2.40%	0.373%
20	11.939	1670	1675	1680	rBV	634591	632380	12.28%	1.910%
21	12.727	1804	1809	1814	rBV	297165	334633	6.50%	1.011%
22	13.010	1852	1857	1860	rBV	5551926	5151641	100.00%	15.557%
23	13.686	1969	1972	1975	rBV4	35271	55381	1.08%	0.167%
24	14.010	2022	2027	2028	rBV3	84698	132171	2.57%	0.399%
25	14.062	2033	2036	2040	rVB	1485741	1485779	28.84%	4.487%
26	15.562	2286	2291	2303	rVB	1025243	1360585	26.41%	4.109%
27	16.198	2394	2399	2404	rVB	61523	95488	1.85%	0.288%
28	17.303	2581	2587	2598	rVB2	157683	320299	6.22%	0.967%
29	18.827	2839	2846	2853	rVB3	78014	200583	3.89%	0.606%

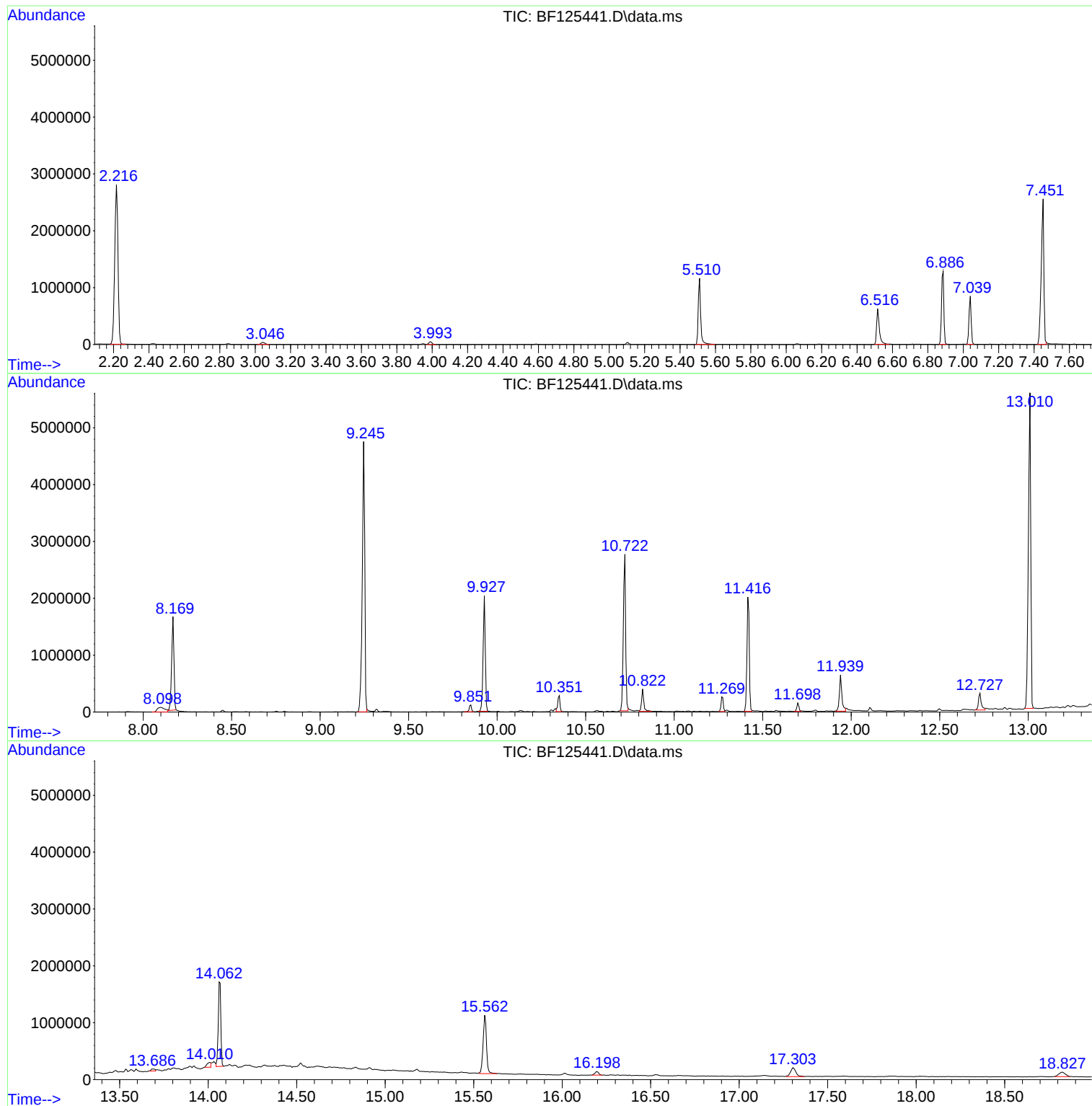
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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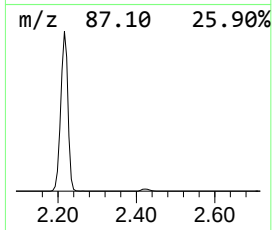
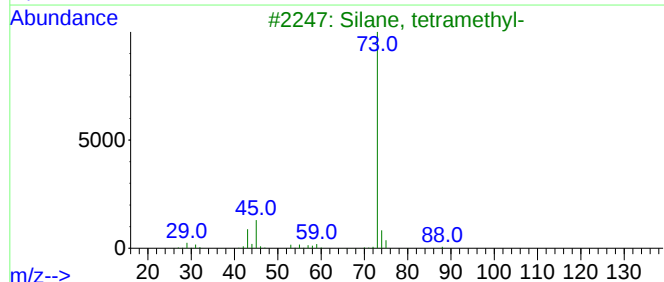
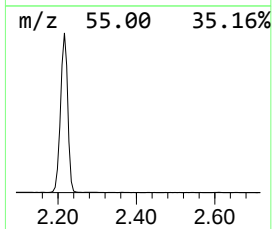
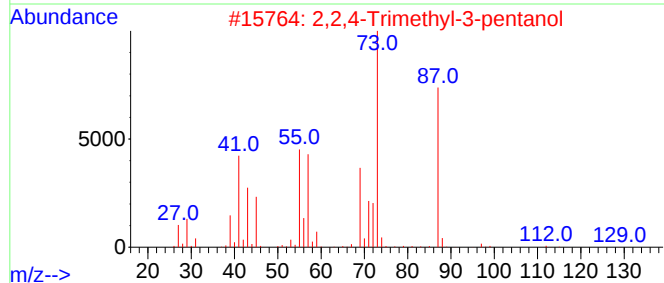
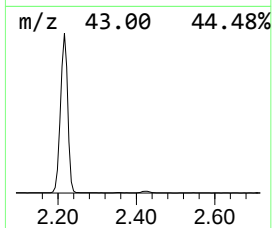
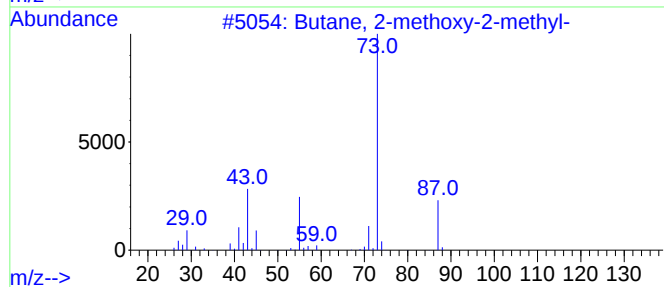
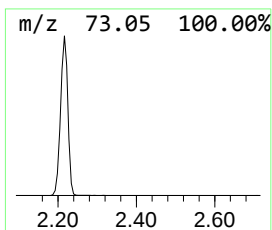
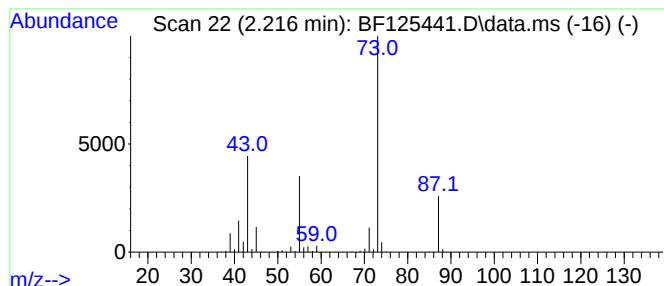
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	61.02 ng	3574770	1,4-Dichlorobenzene-d4	6.886

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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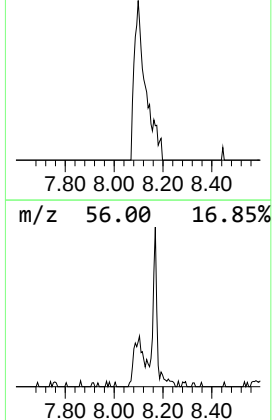
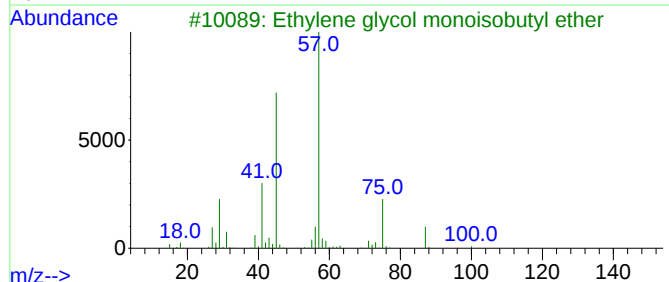
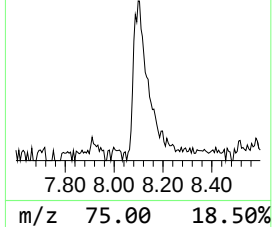
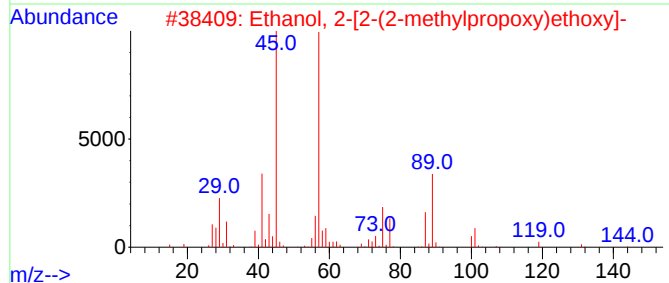
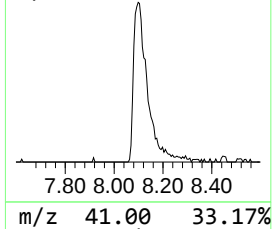
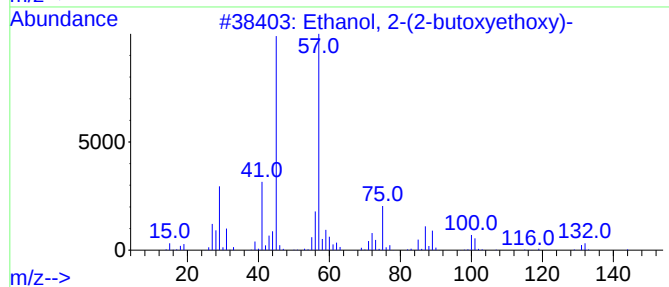
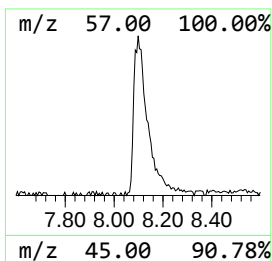
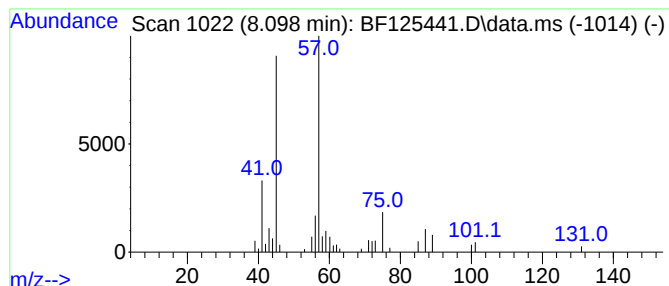
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	3.35 ng	249033	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	74
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
5			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50



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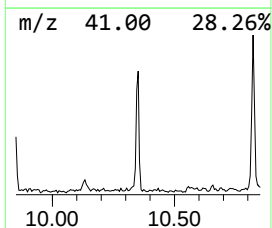
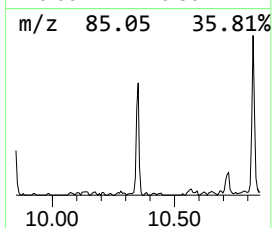
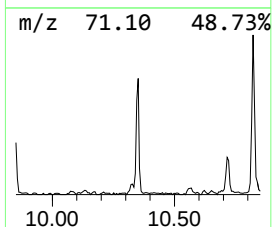
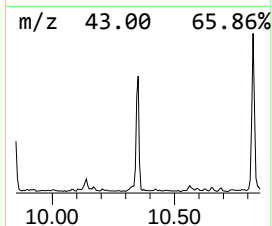
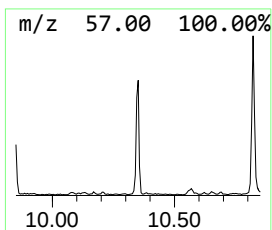
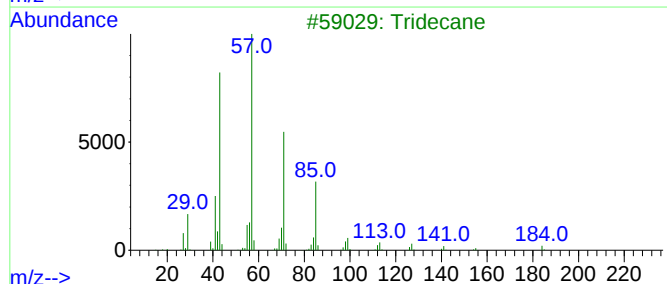
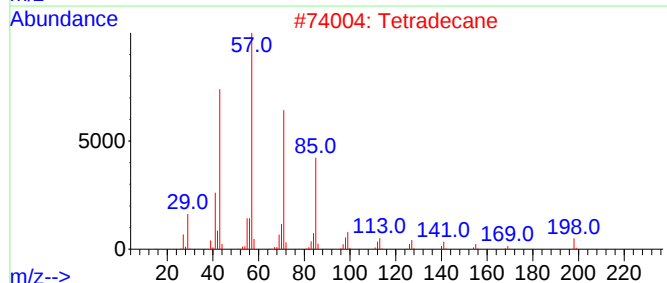
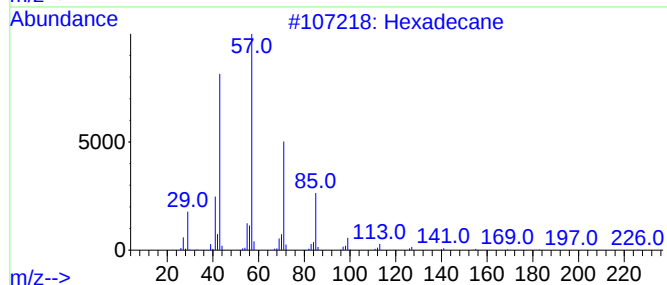
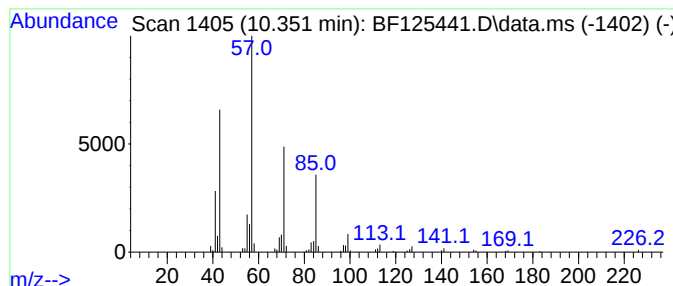
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Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.351	2.81 ng	240308	Acenaphthene-d10	9.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Tetradecane	198	C14H30	000629-59-4	90
3			Tridecane	184	C13H28	000629-50-5	90
4			Heneicosane	296	C21H44	000629-94-7	83
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80



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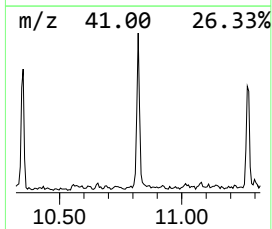
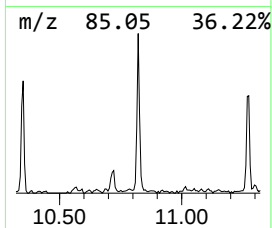
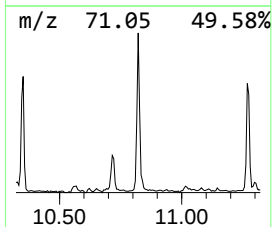
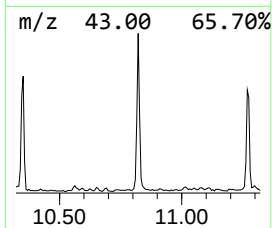
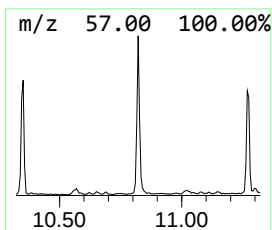
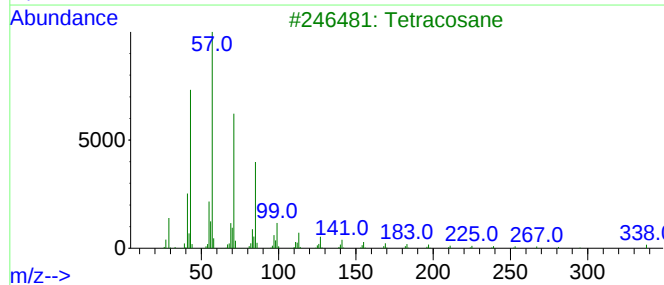
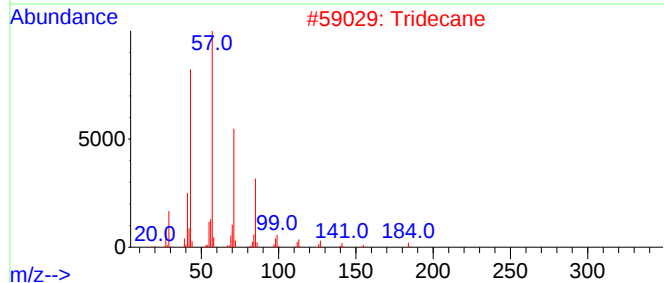
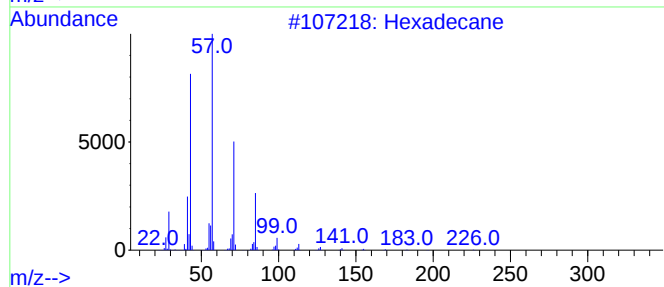
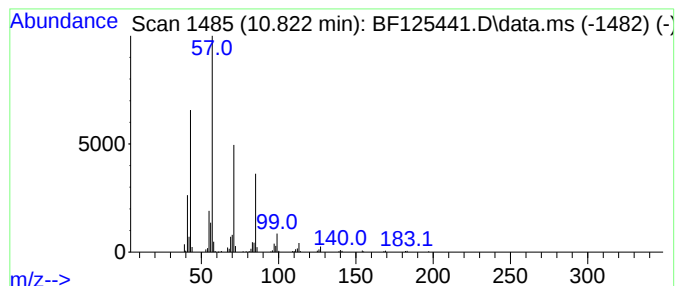
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Peak Number 5 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	3.68 ng	335449	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tridecane	184	C13H28	000629-50-5	90
3			Tetracosane	338	C24H50	000646-31-1	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80



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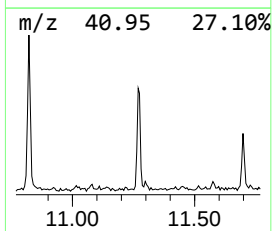
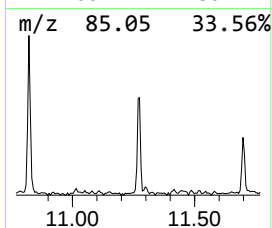
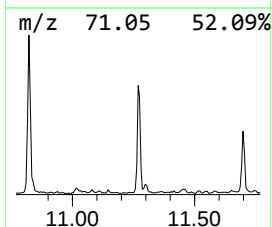
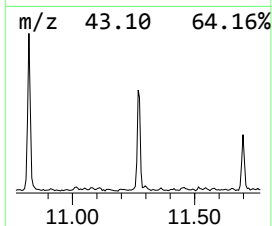
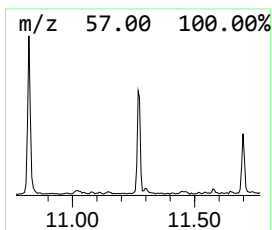
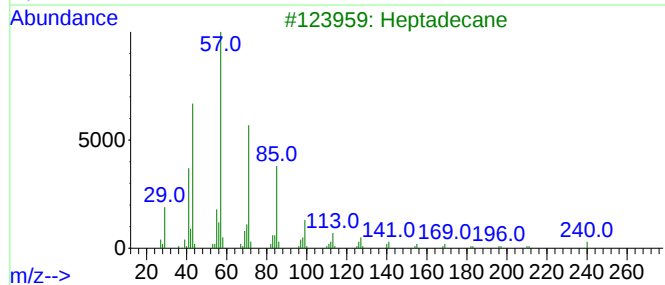
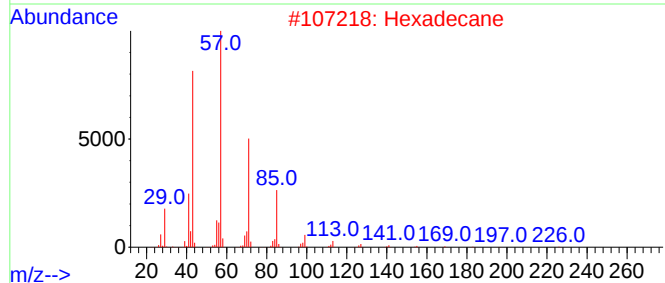
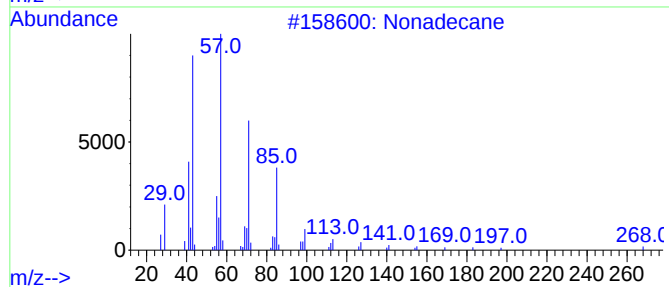
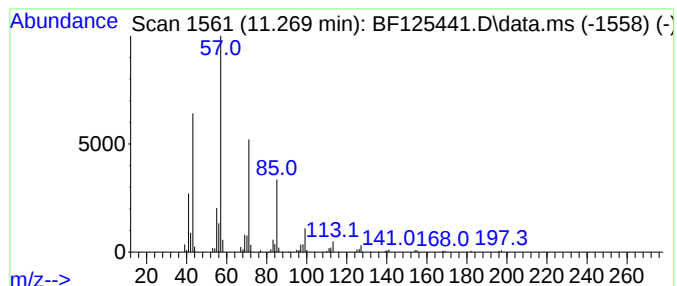
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Peak Number 6 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	2.50 ng	227793	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Hexadecane	226	C16H34	000544-76-3	91
3			Heptadecane	240	C17H36	000629-78-7	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Heptacosane	380	C27H56	000593-49-7	87



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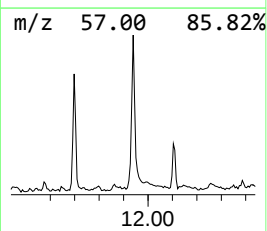
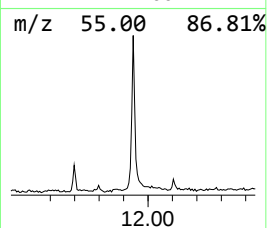
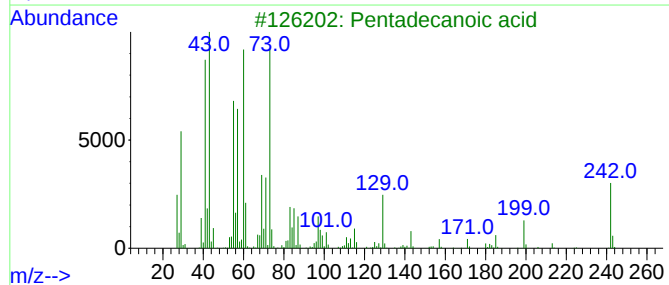
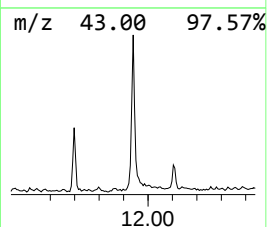
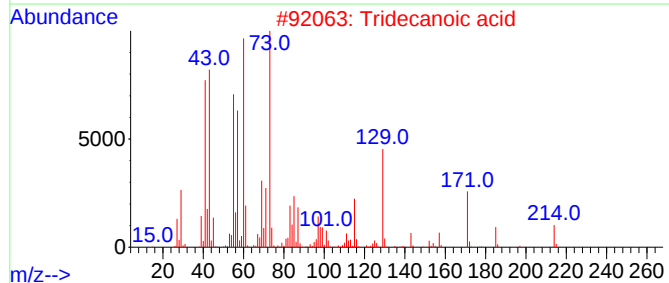
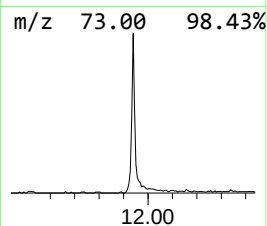
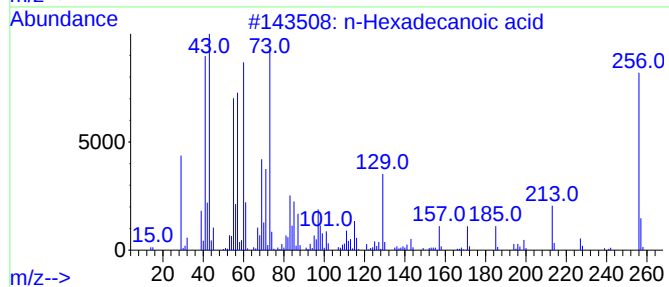
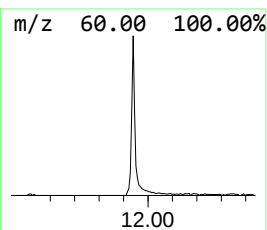
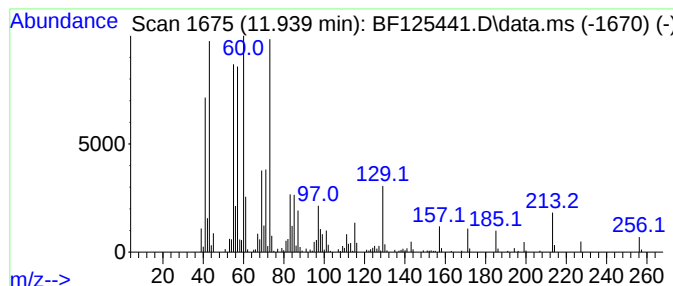
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	6.94 ng	632380	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			Undecanoic acid	186	C11H22O2	000112-37-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125441.D
Acq On : 13 Sep 2021 13:26
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-PIT

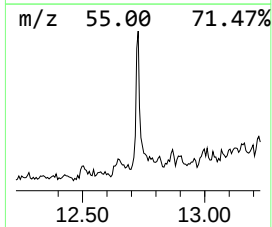
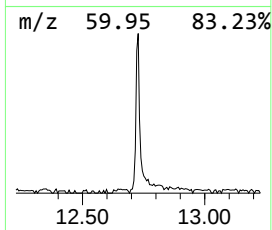
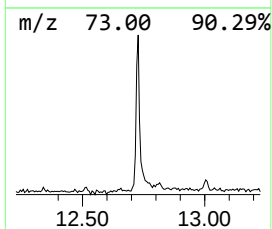
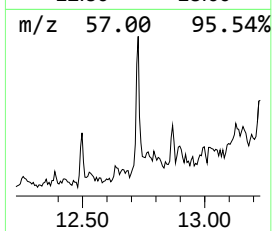
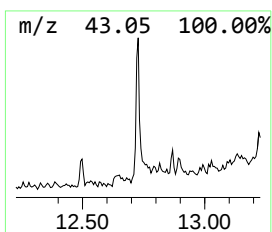
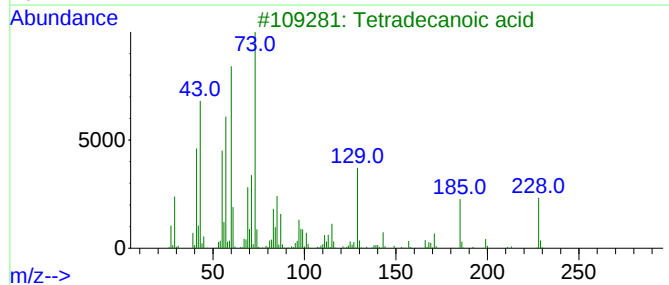
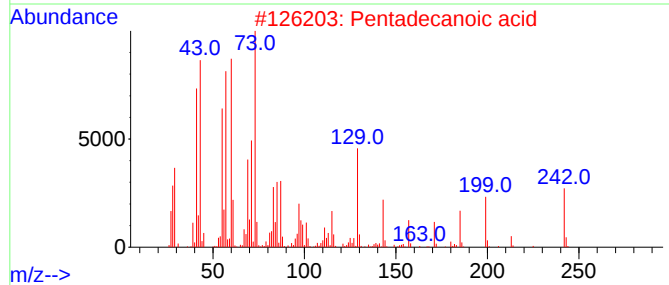
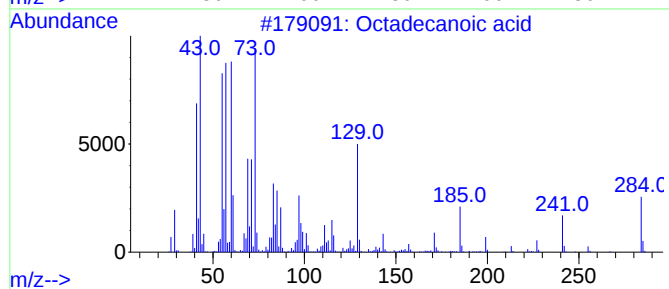
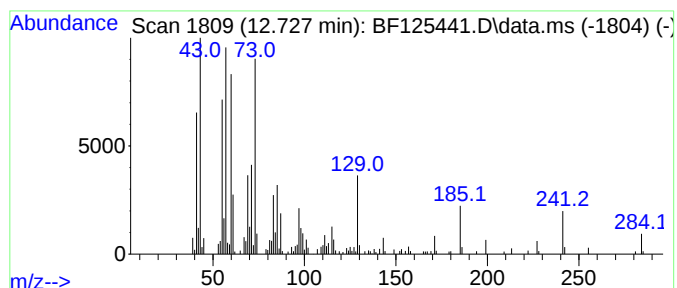
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	3.67 ng	334633	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125441.D
Acq On : 13 Sep 2021 13:26
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-PIT

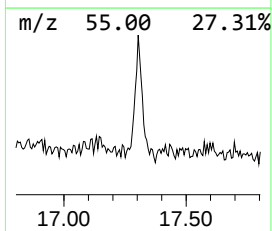
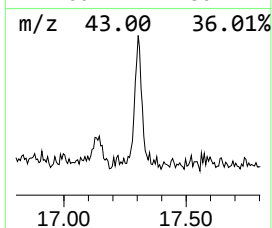
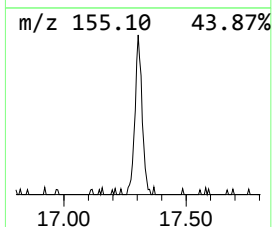
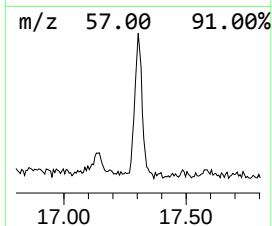
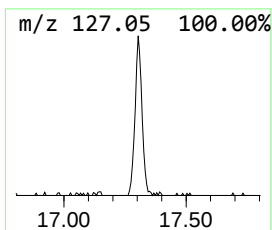
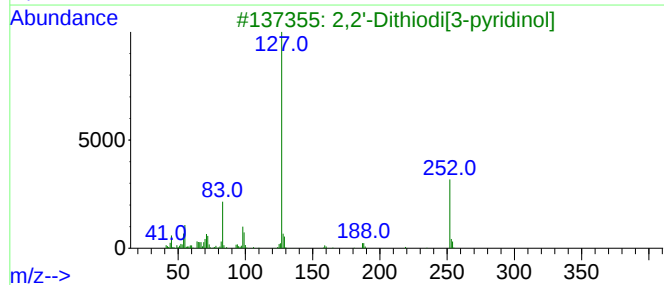
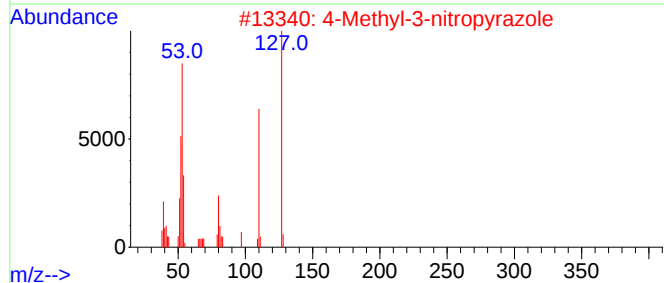
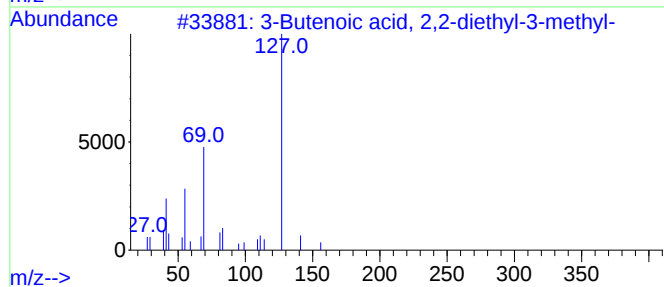
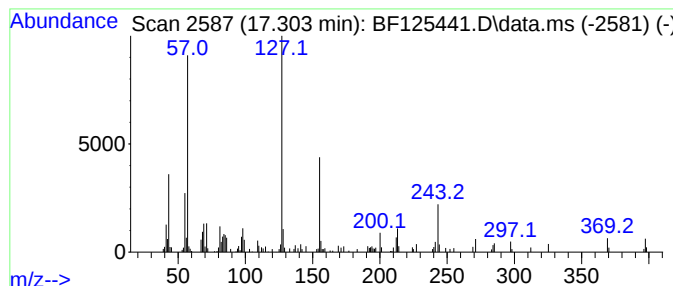
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.303 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.303	4.71 ng	320299	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid, 2,2-diethyl-3-m...	156	C9H16O2	038477-06-4	38
2			4-Methyl-3-nitropyrazole	127	C4H5N3O2	038858-90-1	38
3			2,2'-Dithiodi[3-pyridinol]	252	C10H8N2O2S2	068750-09-4	38
4			Spiro[bicyclo[2.2.1]heptane-2,2'...	212	C12H20O3	035972-92-0	38
5			2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125441.D
Acq On : 13 Sep 2021 13:26
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

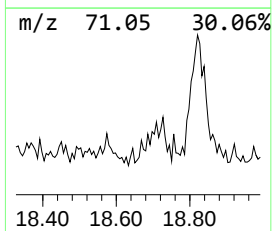
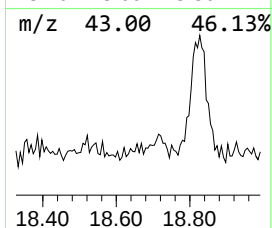
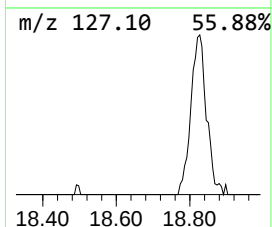
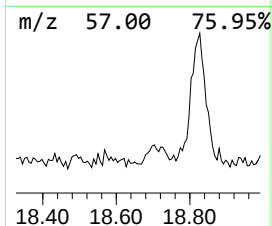
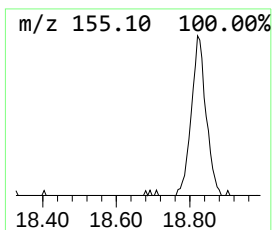
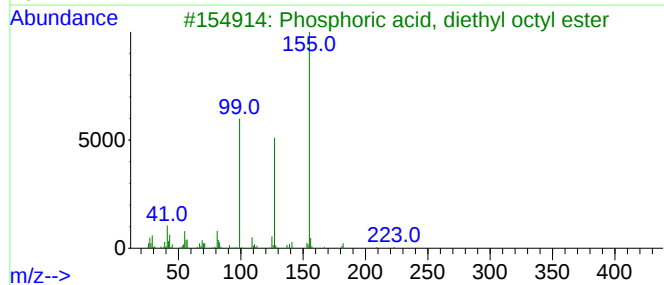
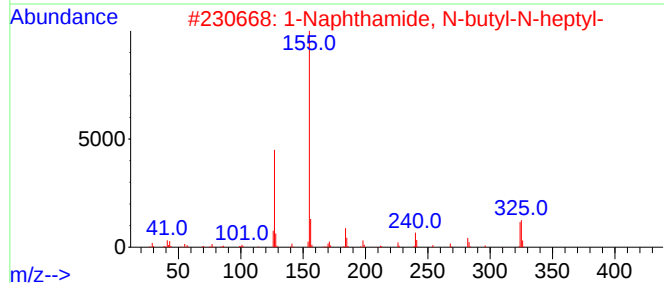
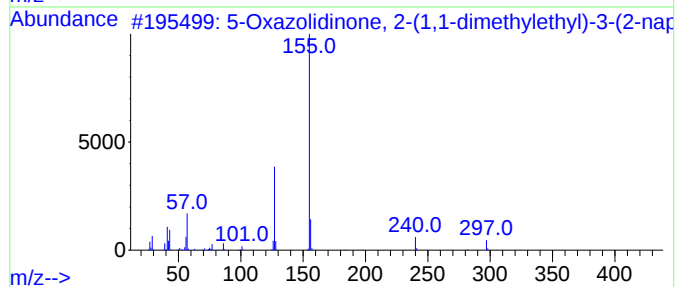
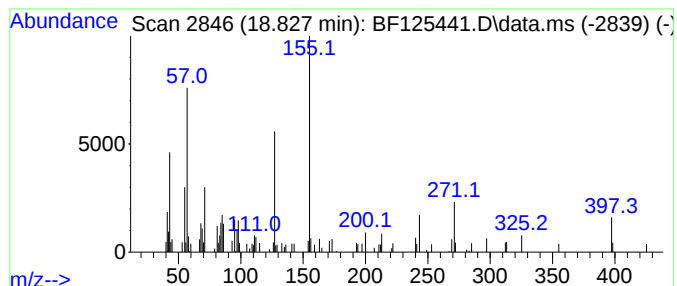
Instrument :
BNA_F
ClientSampleId :
WATER-PIT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Oxazolidinone, 2-(1,1-dimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.827	2.95 ng	200583	Perylene-d12	15.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Oxazolidinone, 2-(1,1-dimethyl...	297	C18H19NO3	119215-56-4	53
2	1-Naphthamide, N-butyl-N-heptyl-	325	C22H31NO	1000415-71-9	53
3	Phosphoric acid, diethyl octyl e...	266	C12H27O4P	1000308-90-4	50
4	5-Oxazolidinone, 2-(1,1-dimethyl...	297	C18H19NO3	119215-55-3	43
5	Benzamide, 2,6-difluoro-3-methyl...	213	C11H13F2NO	1000437-11-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125441.D
Acq On : 13 Sep 2021 13:26
Operator : JU/CG
Sample : M3681-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-PIT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.216	61.0	ng	3574770	1	6.886	1171640	20.0
Ethanol, 2-(2-b...	8.098	3.4	ng	249033	2	8.169	1484670	20.0
Hexadecane	10.351	2.8	ng	240308	3	9.927	1712700	20.0
Tridecane	10.822	3.7	ng	335449	4	11.416	1822290	20.0
Nonadecane	11.269	2.5	ng	227793	4	11.416	1822290	20.0
n-Hexadecanoic ...	11.939	6.9	ng	632380	4	11.416	1822290	20.0
Octadecanoic acid	12.727	3.7	ng	334633	4	11.416	1822290	20.0
unknown17.303	17.303	4.7	ng	320299	6	15.562	1360590	20.0
5-Oxazolidinone...	18.827	3.0	ng	200583	6	15.562	1360590	20.0