

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081821\
 Data File : BF125103.D
 Acq On : 18 Aug 2021 23:32
 Operator : JU/CG
 Sample : M3449-13
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP5

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: BF125103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	19	25	31	rVB	1253466	1567943	36.49%	4.590%
2	2.587	79	85	90	rVB	33854	62432	1.45%	0.183%
3	5.145	509	520	528	rBV	125849	169165	3.94%	0.495%
4	5.534	581	586	590	rBV	3599258	3779477	87.96%	11.064%
5	6.539	751	757	760	rBV	3359499	3875229	90.18%	11.344%
6	6.922	818	822	825	rBV	1259766	1114675	25.94%	3.263%
7	7.481	912	917	920	rBV	2774606	2531800	58.92%	7.411%
8	8.098	1018	1022	1025	rBV	934888	704263	16.39%	2.062%
9	8.198	1035	1039	1043	rBV	1629703	1477890	34.39%	4.326%
10	9.280	1217	1223	1226	rBV	4263440	4297004	100.00%	12.579%
11	9.957	1334	1338	1341	rBV	1996199	1646213	38.31%	4.819%
12	10.745	1467	1472	1475	rBV	3040380	2751742	64.04%	8.055%
13	11.445	1587	1591	1594	rBV	2046986	1672743	38.93%	4.897%
14	11.969	1674	1680	1692	rBV	725085	802090	18.67%	2.348%
15	12.657	1794	1797	1803	rBV	80701	88026	2.05%	0.258%
16	12.751	1809	1813	1821	rBV	560642	552922	12.87%	1.619%
17	12.880	1832	1835	1838	rBV	68128	61361	1.43%	0.180%
18	13.033	1856	1861	1864	rBV	4636455	4204582	97.85%	12.308%
19	13.927	2009	2013	2030	rBV	216958	398655	9.28%	1.167%
20	14.080	2035	2039	2042	rBV	1254431	1157546	26.94%	3.389%
21	14.551	2116	2119	2120	rBV	53542	47978	1.12%	0.140%
22	15.215	2228	2232	2236	rBV	84223	100682	2.34%	0.295%
23	15.580	2288	2294	2297	rBV	692854	890159	20.72%	2.606%
24	15.609	2297	2299	2306	rVB2	42767	51555	1.20%	0.151%
25	16.068	2371	2377	2382	rBV	72171	104639	2.44%	0.306%
26	17.215	2565	2572	2577	rBV4	22205	50241	1.17%	0.147%

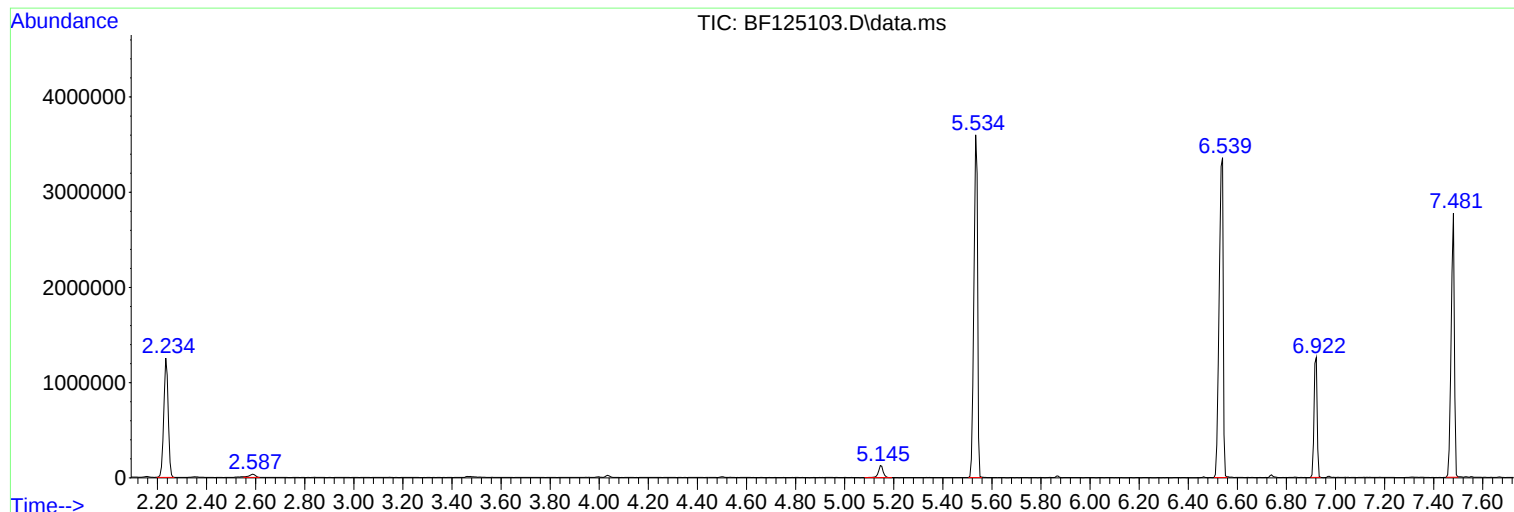
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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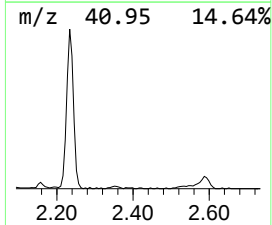
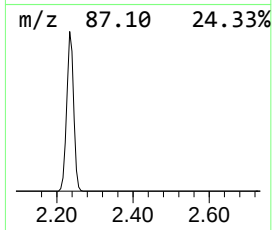
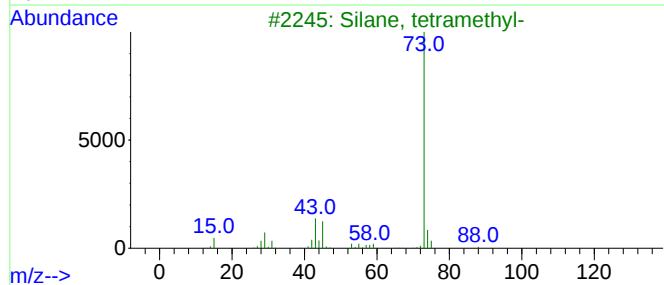
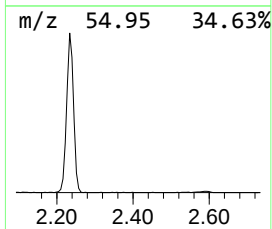
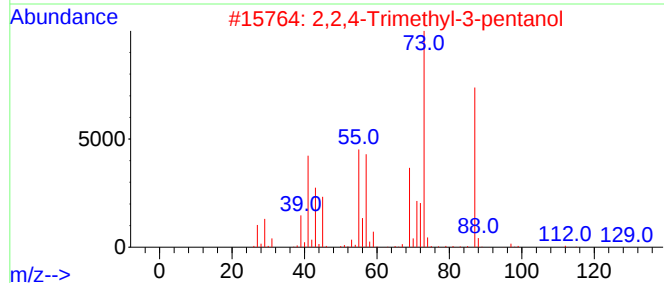
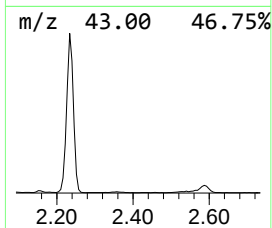
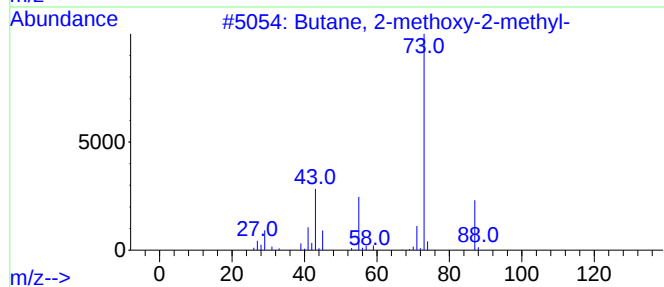
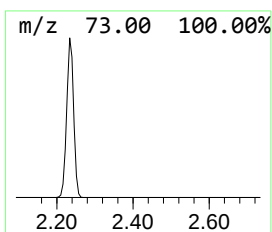
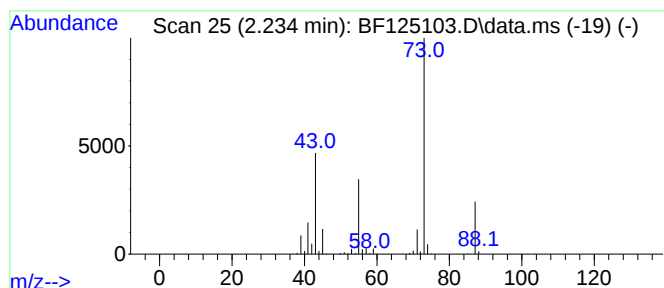
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.234	28.13 ng	1567940	1,4-Dichlorobenzene-d4	6.922

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23



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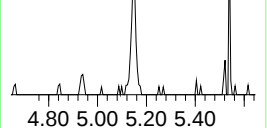
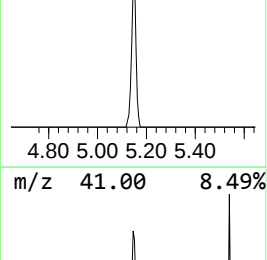
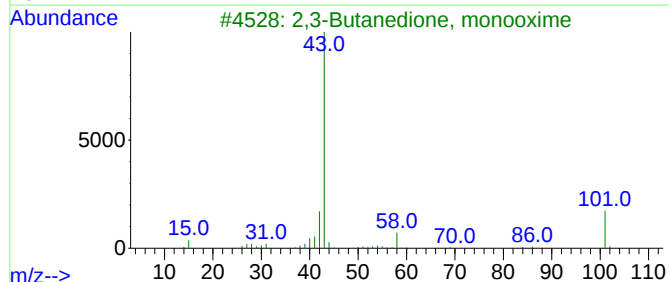
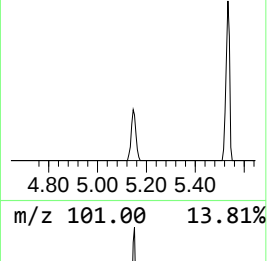
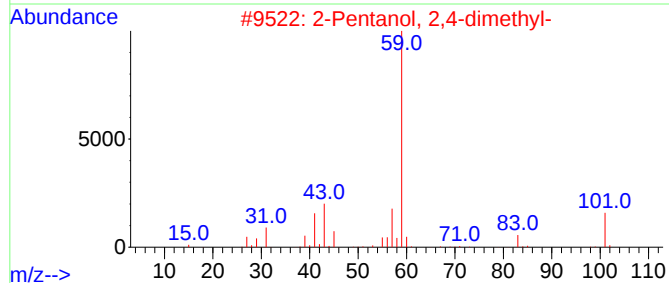
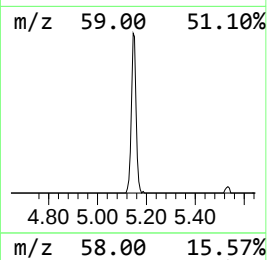
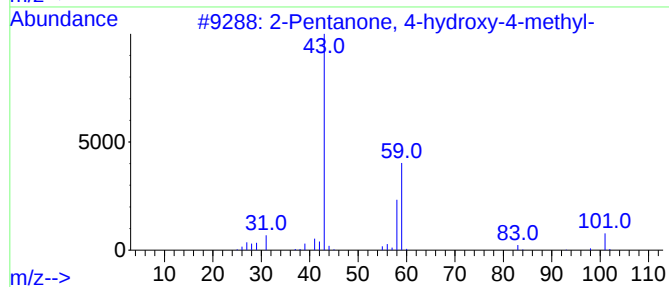
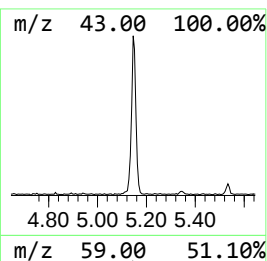
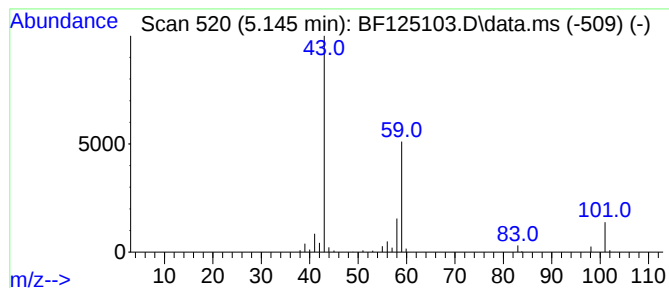
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	3.04 ng	169165	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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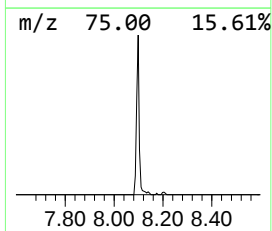
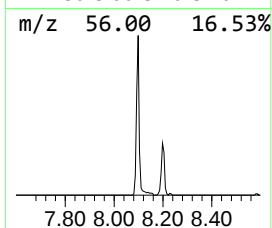
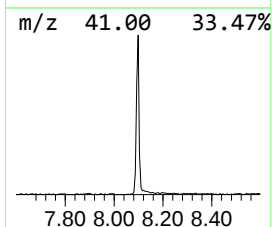
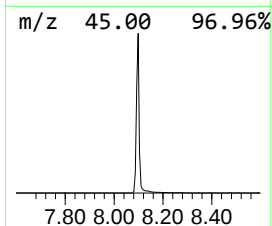
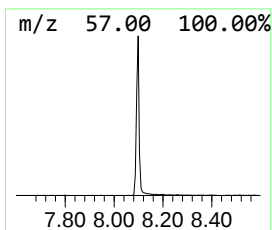
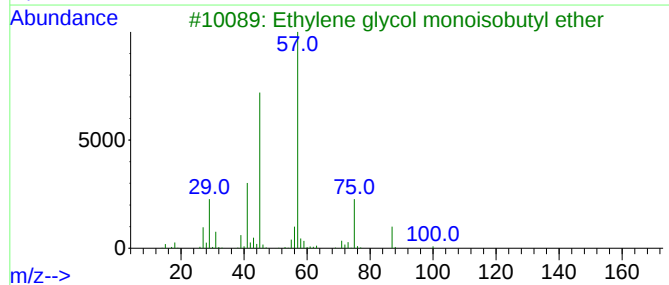
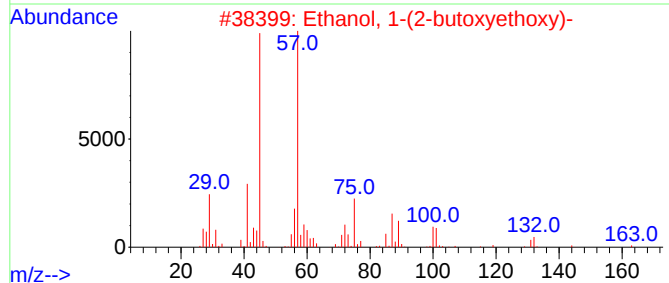
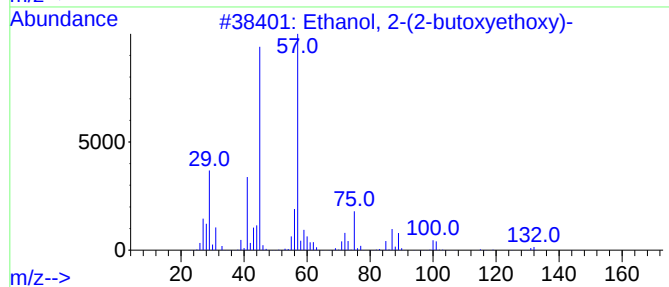
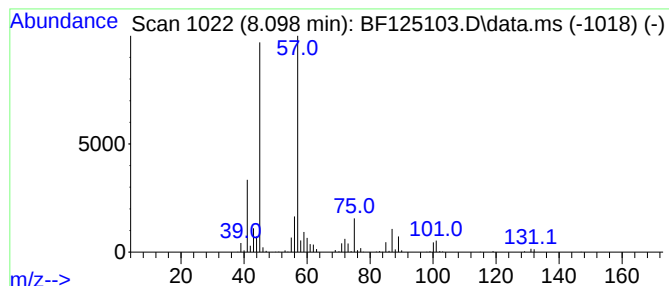
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	9.53 ng	704263	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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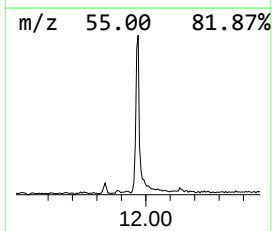
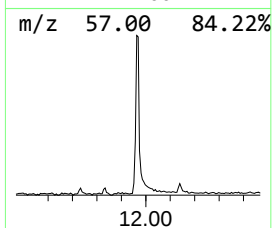
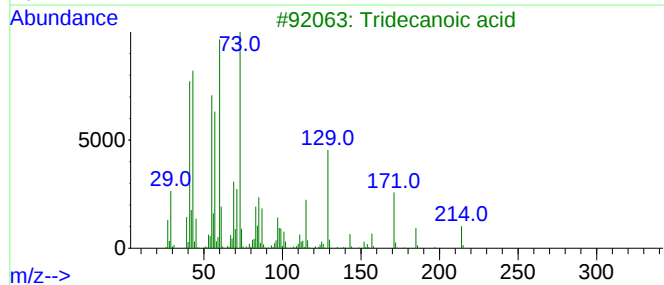
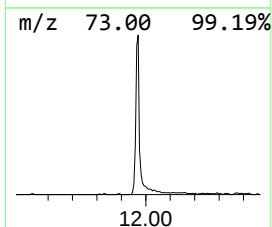
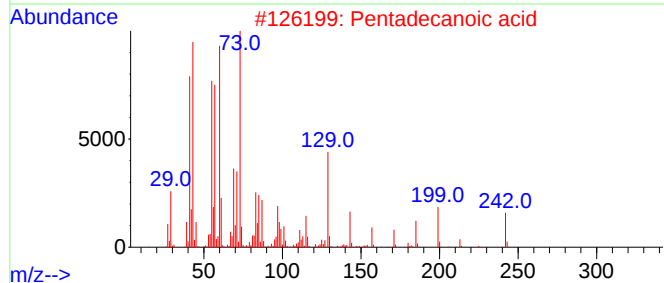
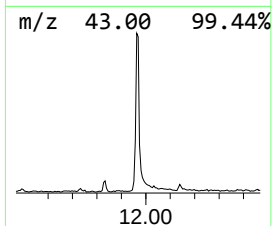
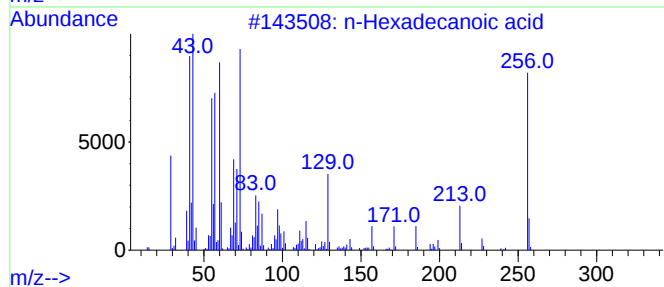
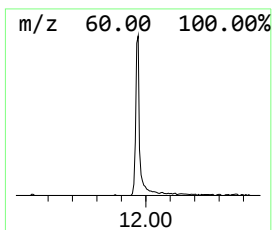
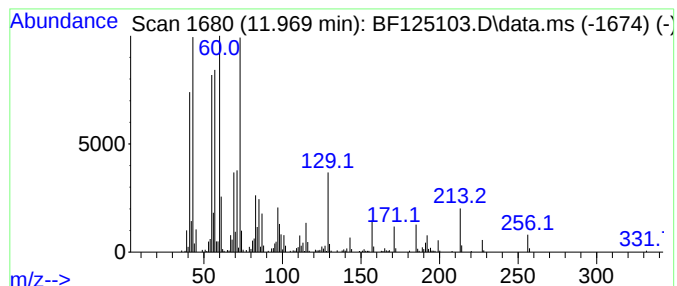
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	9.59 ng	802090	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Octadecanoic acid	284	C18H36O2	000057-11-4	64



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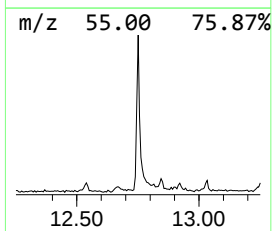
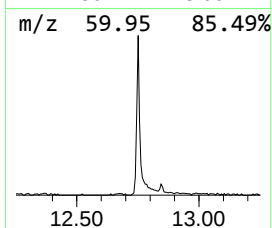
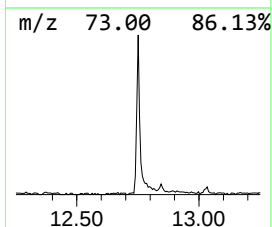
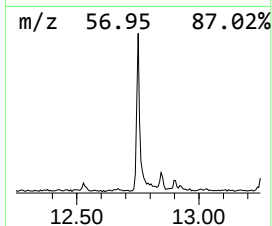
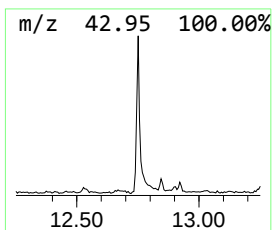
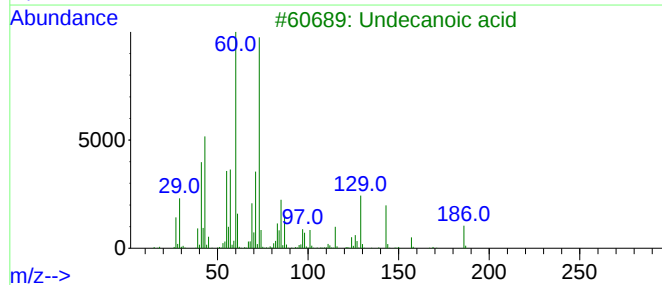
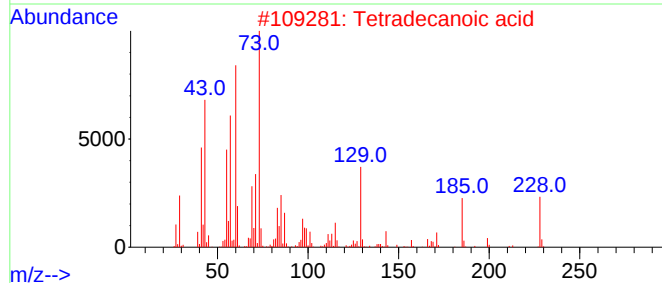
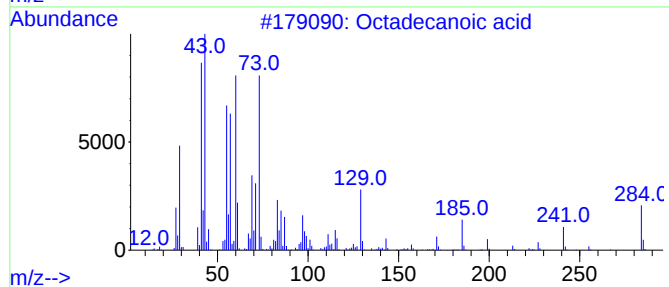
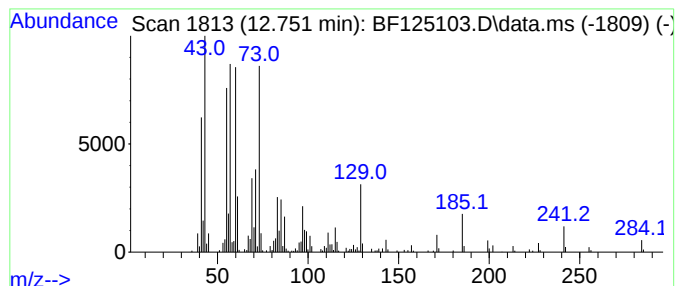
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	6.61 ng	552922	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Undecanoic acid	186	C11H22O2	000112-37-8	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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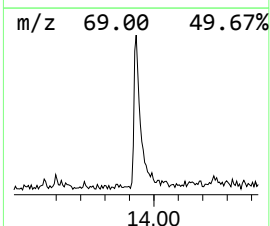
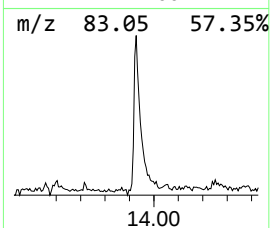
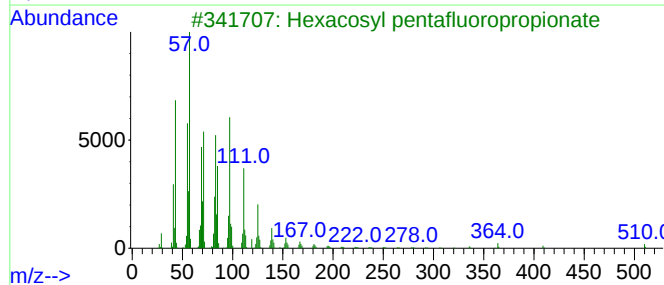
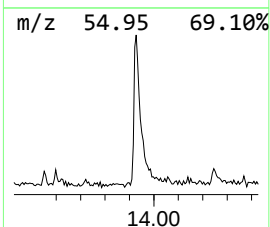
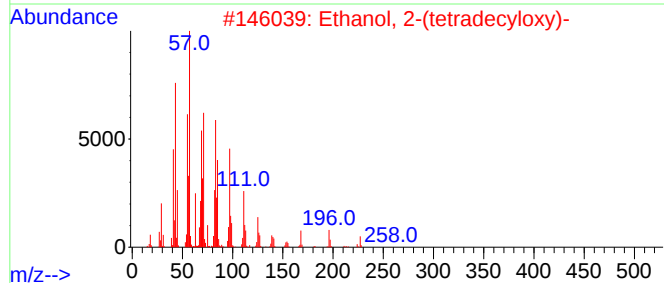
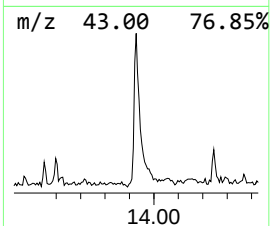
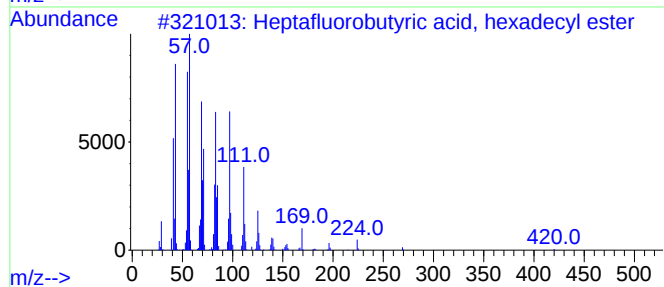
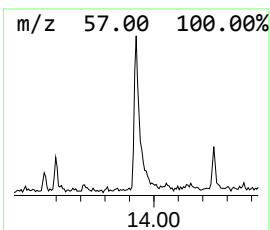
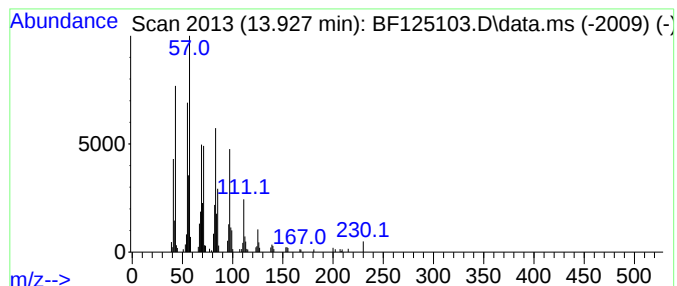
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	6.89 ng	398655	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081821\
Data File : BF125103.D
Acq On : 18 Aug 2021 23:32
Operator : JU/CG
Sample : M3449-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5

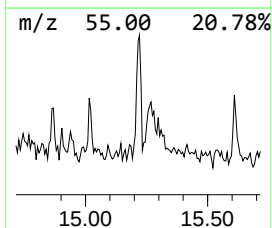
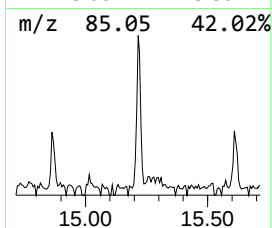
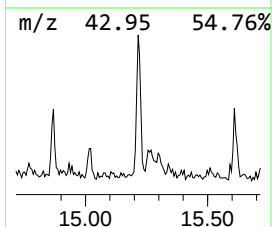
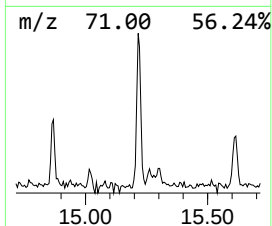
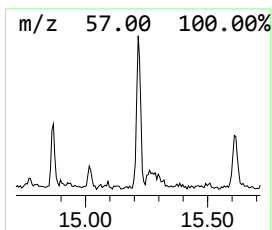
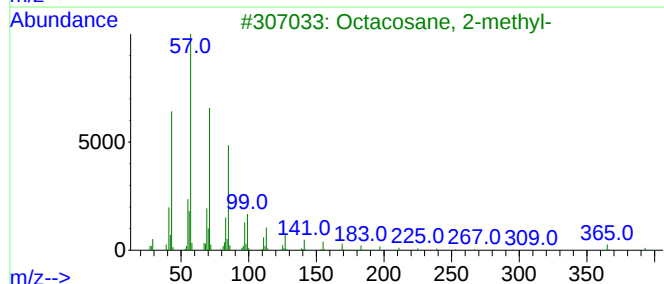
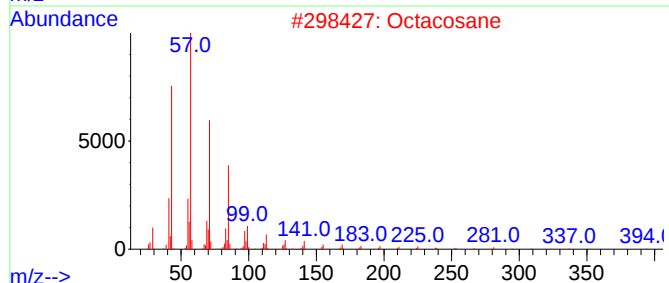
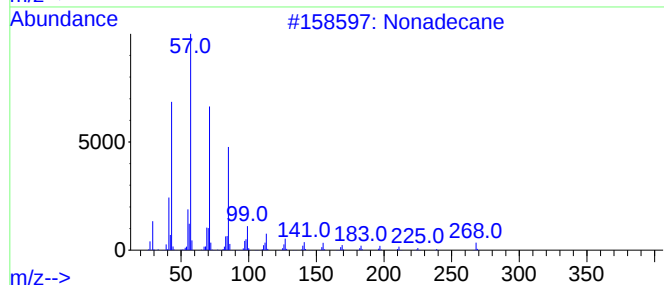
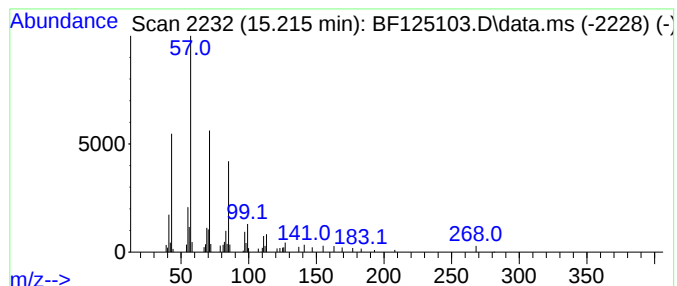
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.215	2.26 ng	100682	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081821\
Data File : BF125103.D
Acq On : 18 Aug 2021 23:32
Operator : JU/CG
Sample : M3449-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5

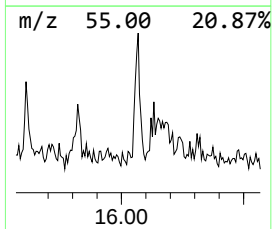
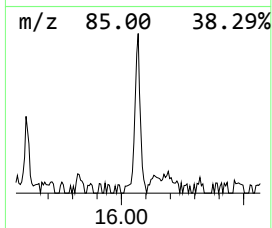
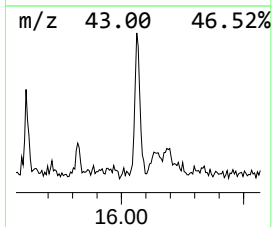
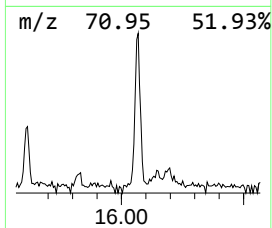
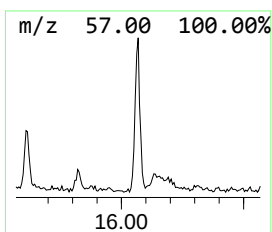
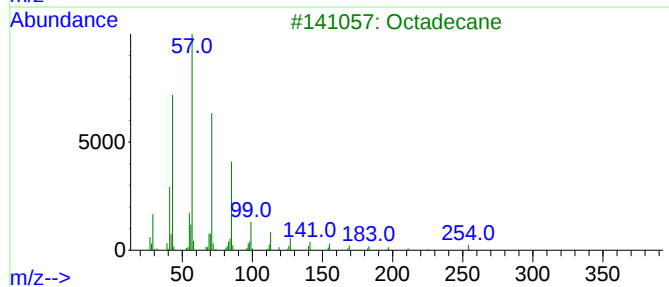
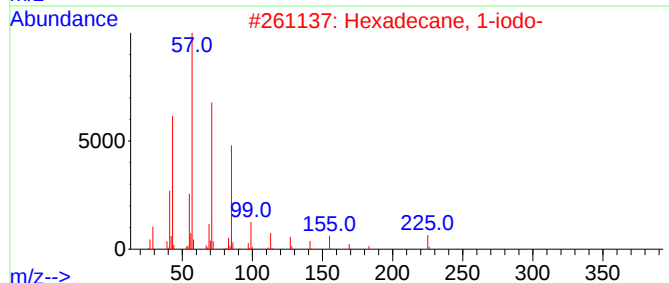
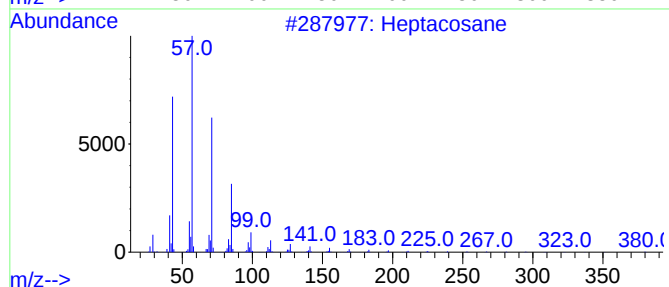
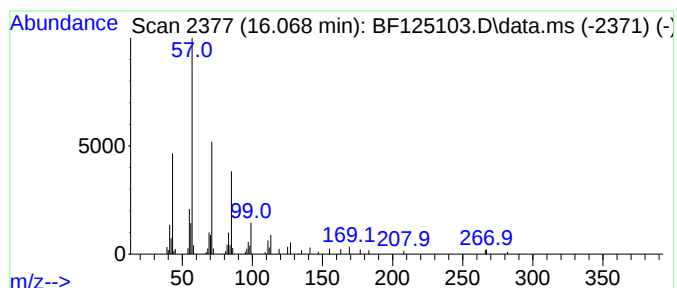
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.068	2.35 ng	104639	Perylene-d12	15.580

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	87
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3		Octadecane	254	C18H38	000593-45-3	86
4		Heptadecane	240	C17H36	000629-78-7	86
5		Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081821\
Data File : BF125103.D
Acq On : 18 Aug 2021 23:32
Operator : JU/CG
Sample : M3449-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP5

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...	2.234	28.1	ng	1567940	1	6.922	1114680	20.0
2-Pentanone, 4-...	5.145	3.0	ng	169165	1	6.922	1114680	20.0
Ethanol, 2-(2-b...	8.098	9.5	ng	704263	2	8.198	1477890	20.0
n-Hexadecanoic ...	11.969	9.6	ng	802090	4	11.445	1672740	20.0
Octadecanoic acid	12.751	6.6	ng	552922	4	11.445	1672740	20.0
Heptafluorobuty...	13.927	6.9	ng	398655	5	14.080	1157550	20.0
Nonadecane	15.215	2.3	ng	100682	6	15.580	890159	20.0
Heptacosane	16.068	2.4	ng	104639	6	15.580	890159	20.0