

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
 Data File : BF125203.D
 Acq On : 25 Aug 2021 11:35
 Operator : JU/CG
 Sample : M3524-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-4

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: BF125203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	31	rVB	952340	1240587	34.41%	4.419%
2	5.534	581	586	589	rBV	3413555	3204315	88.88%	11.414%
3	6.540	751	757	760	rBV	3031066	3214796	89.17%	11.452%
4	6.916	817	821	824	rBV	1081723	888453	24.64%	3.165%
5	7.475	911	916	919	rBV	2418929	2120430	58.81%	7.553%
6	8.110	1019	1024	1035	rBV2	76776	206898	5.74%	0.737%
7	8.198	1035	1039	1042	rVV	1414351	1149524	31.88%	4.095%
8	9.269	1217	1221	1224	rBV	4116516	3605410	100.00%	12.843%
9	9.951	1333	1337	1340	rBV	1679127	1292136	35.84%	4.603%
10	10.739	1467	1471	1474	rBV	2968550	2479251	68.76%	8.832%
11	11.439	1586	1590	1593	rBV	1633757	1320378	36.62%	4.703%
12	11.957	1672	1678	1687	rBV2	541126	610687	16.94%	2.175%
13	12.739	1806	1811	1821	rBV	198681	264119	7.33%	0.941%
14	13.027	1855	1860	1863	rBV	3660198	3494892	96.93%	12.449%
15	13.792	1982	1990	2000	rBV4	50773	145390	4.03%	0.518%
16	13.910	2007	2010	2013	rBV	47159	58197	1.61%	0.207%
17	13.945	2013	2016	2019	rVV	108963	110690	3.07%	0.394%
18	13.986	2019	2023	2032	rVV8	63379	201294	5.58%	0.717%
19	14.080	2035	2039	2042	rVB	1139807	961636	26.67%	3.426%
20	14.451	2096	2102	2107	rBV6	57484	111971	3.11%	0.399%
21	14.539	2111	2117	2120	rBV4	57808	98779	2.74%	0.352%
22	14.710	2142	2146	2154	rVB4	32647	81558	2.26%	0.291%
23	15.139	2215	2219	2227	rVV7	52251	122044	3.39%	0.435%
24	15.210	2227	2231	2235	rVB2	42547	56151	1.56%	0.200%
25	15.574	2288	2293	2301	rBV	674114	940104	26.07%	3.349%
26	16.051	2370	2374	2379	rBV	33171	53254	1.48%	0.190%
27	16.574	2459	2463	2468	rBV4	24616	39689	1.10%	0.141%

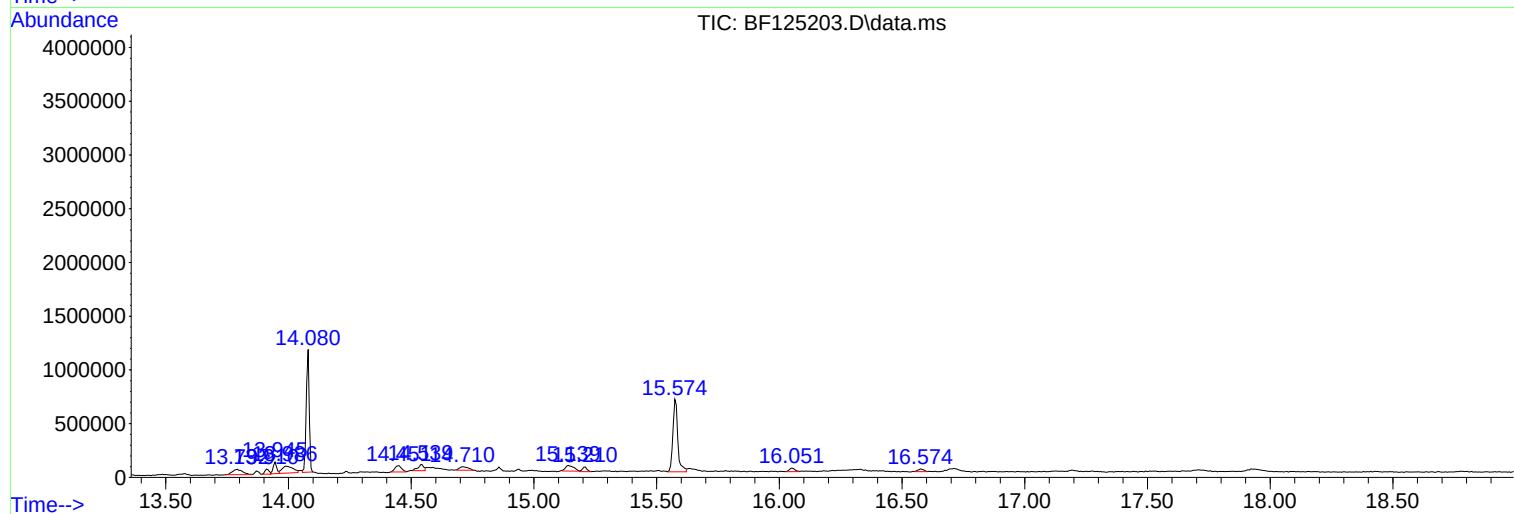
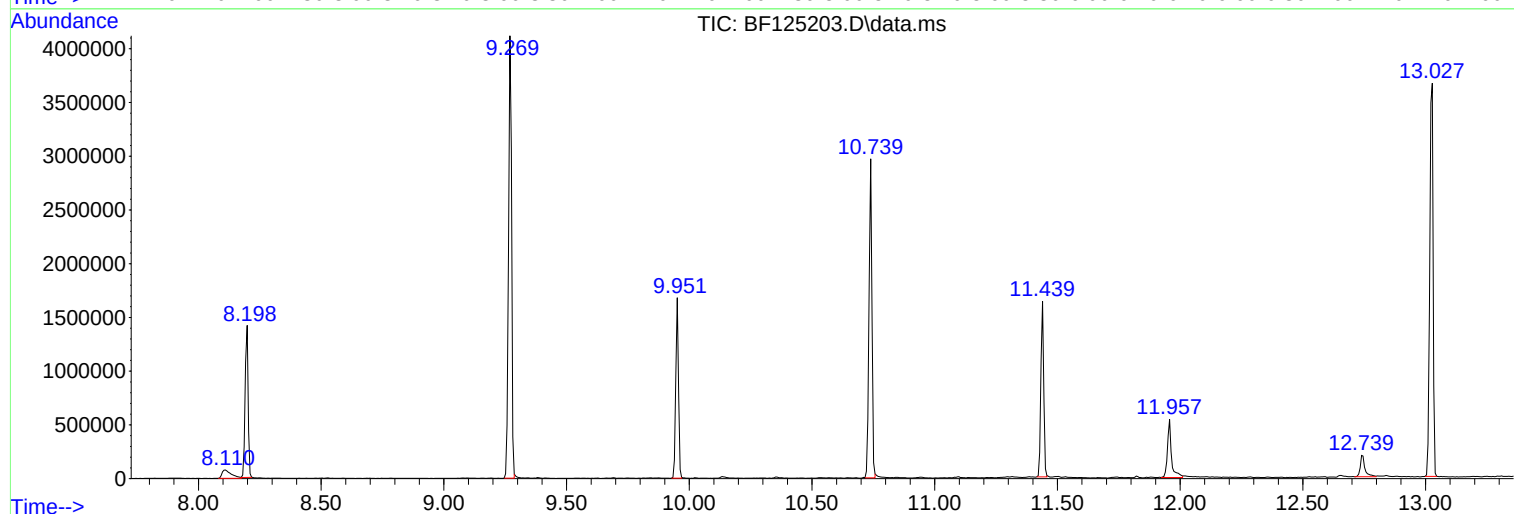
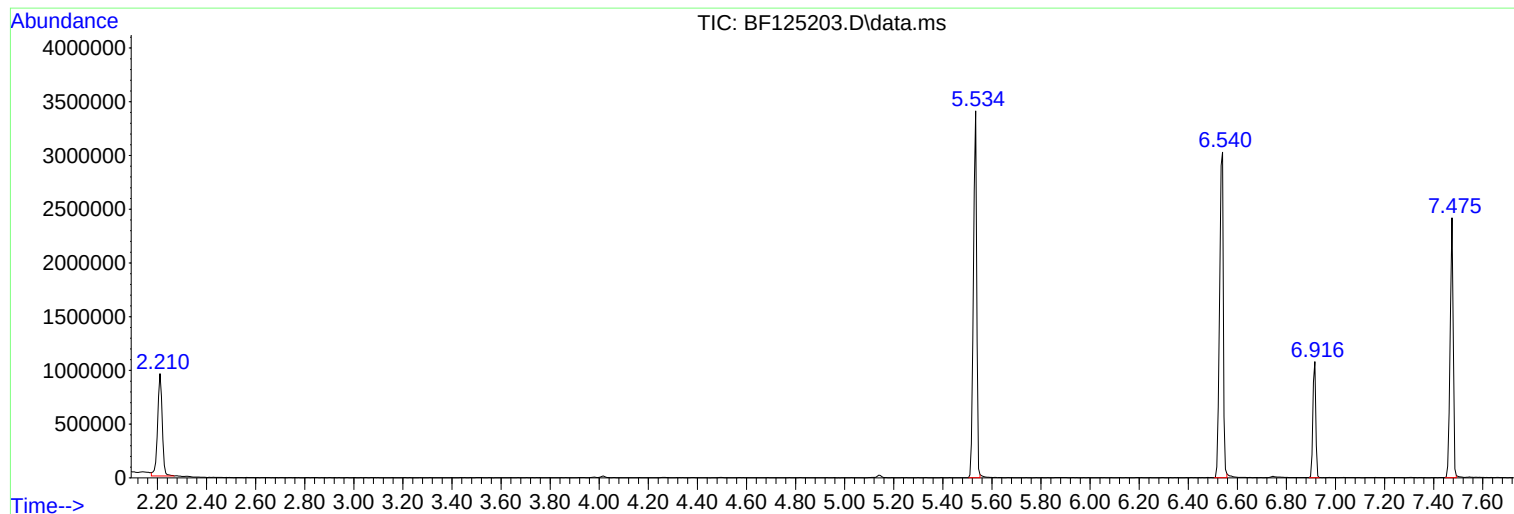
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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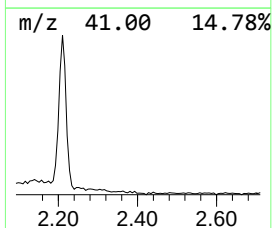
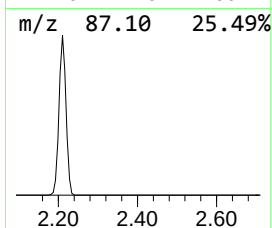
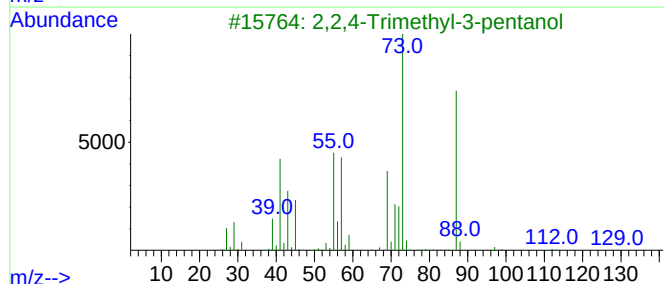
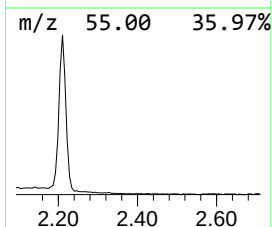
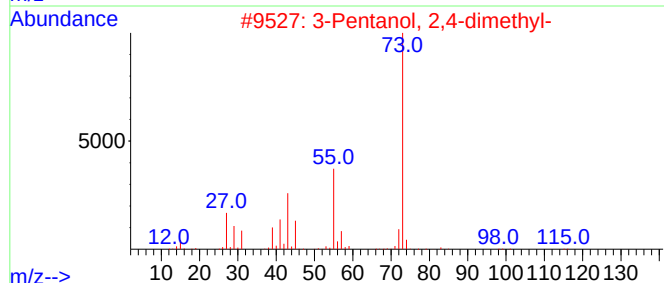
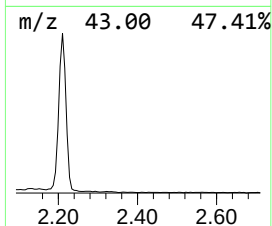
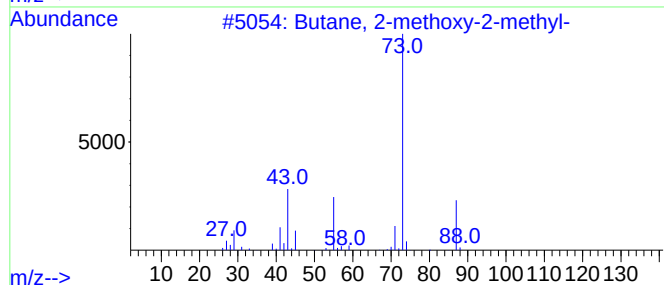
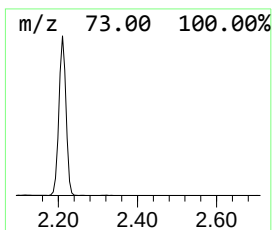
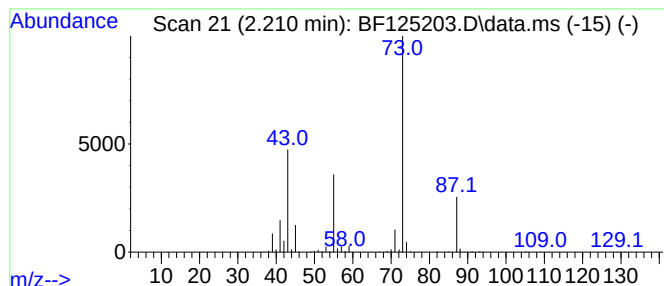
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	27.93 ng	1240590	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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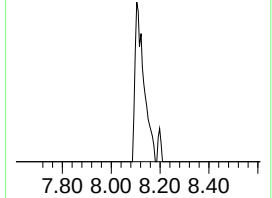
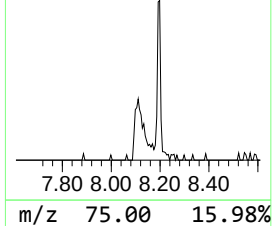
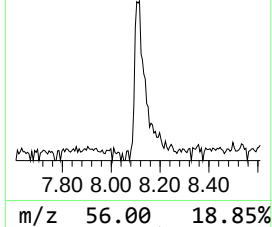
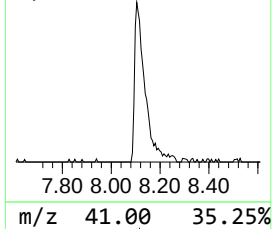
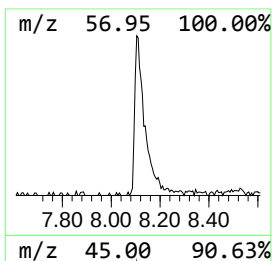
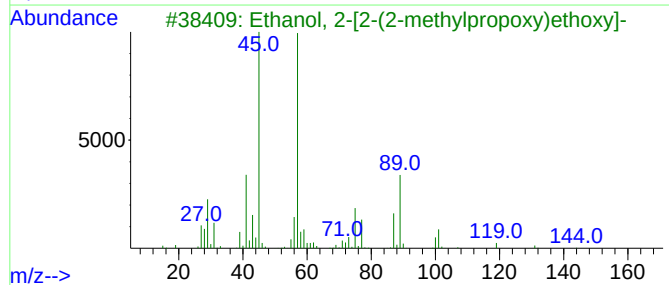
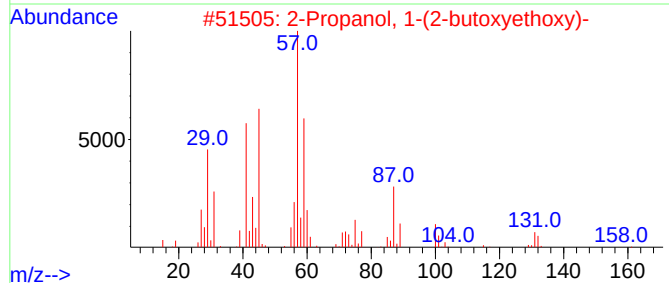
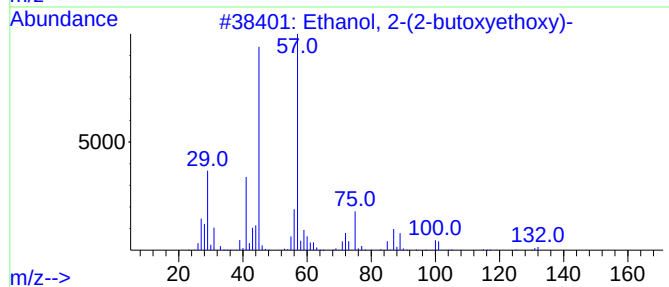
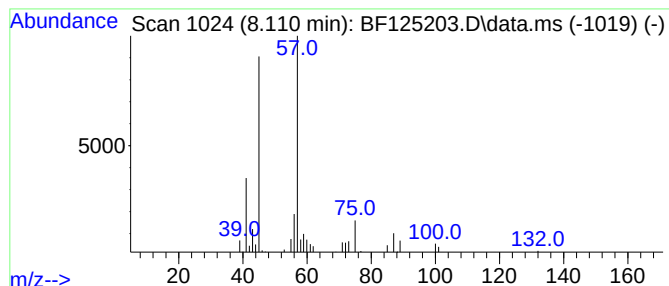
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	3.60 ng	206898	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			2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	56
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	56
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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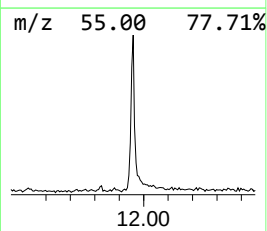
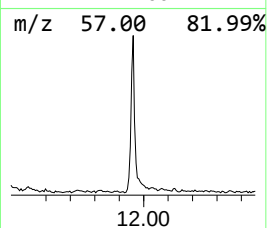
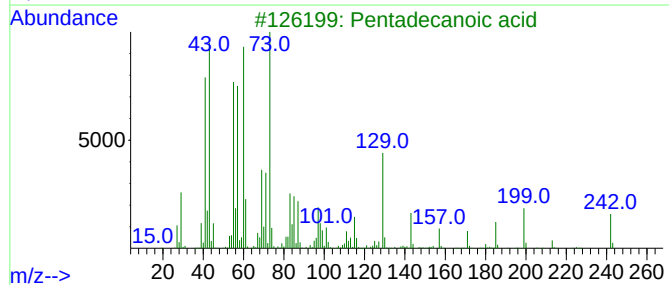
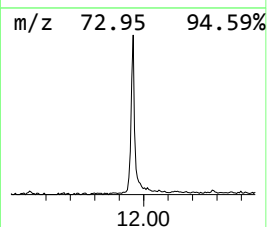
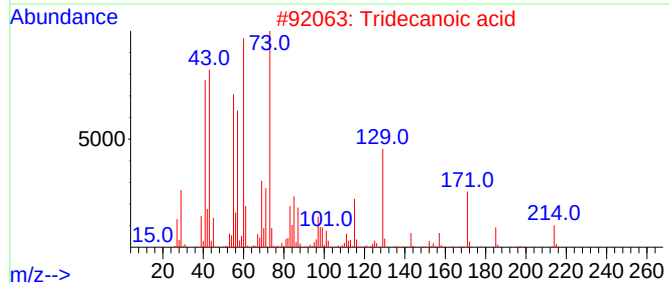
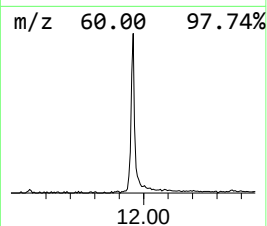
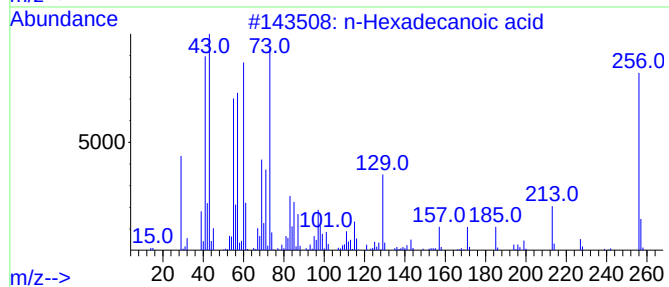
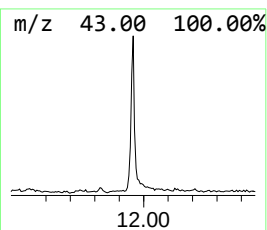
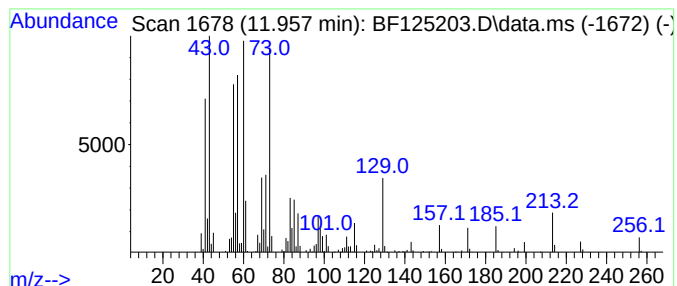
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	9.25 ng	610687	Phenanthrene-d10	11.439

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	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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ClientSampled :
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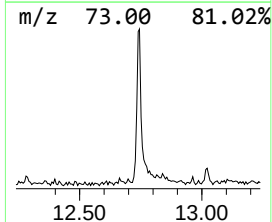
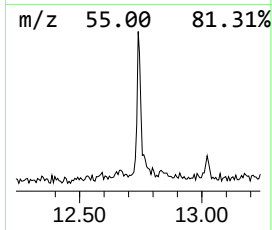
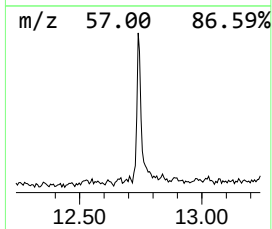
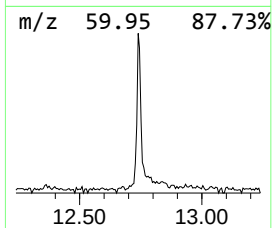
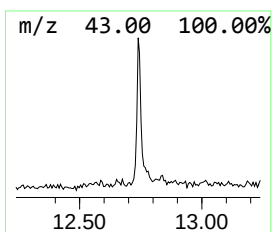
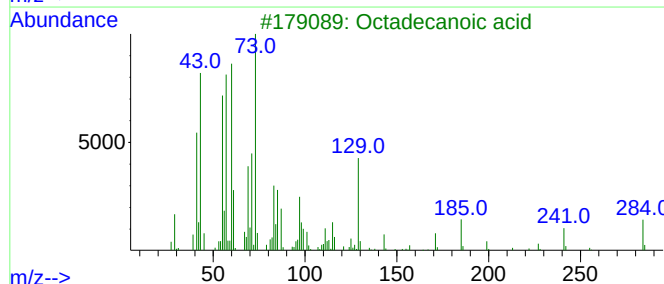
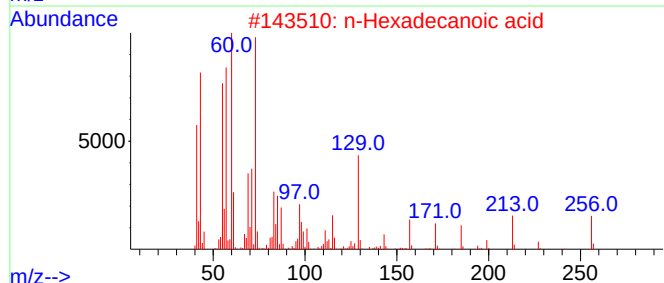
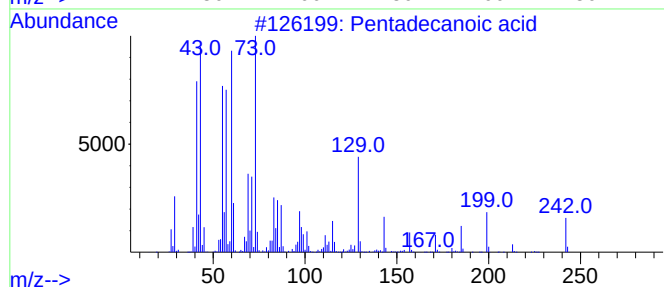
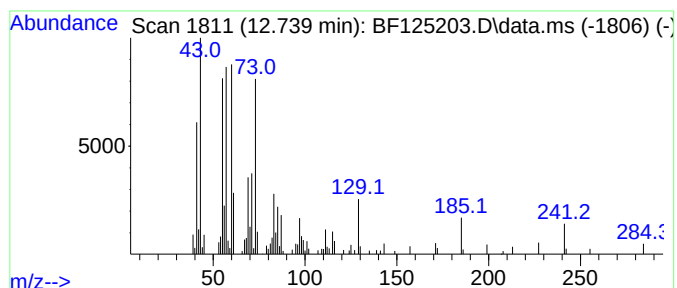
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Peak Number 4 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	4.00 ng	264119	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Octadecanoic acid	284	C18H36O2	000057-11-4	62
4			Undecanoic acid	186	C11H22O2	000112-37-8	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	52



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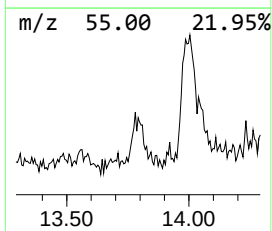
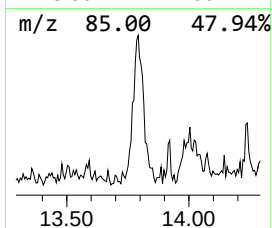
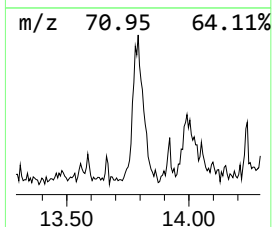
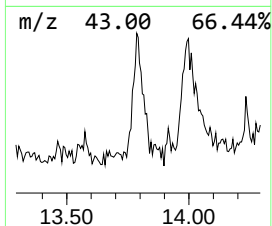
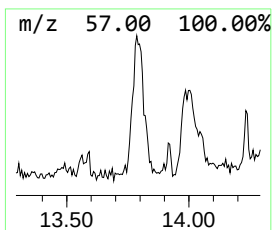
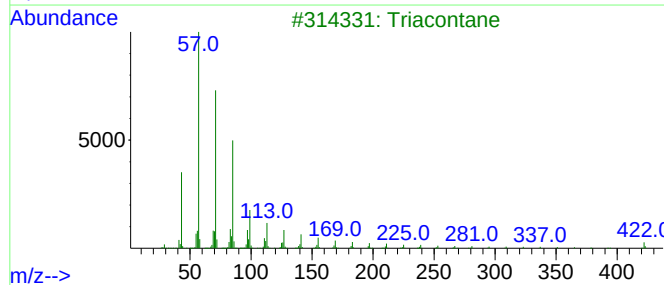
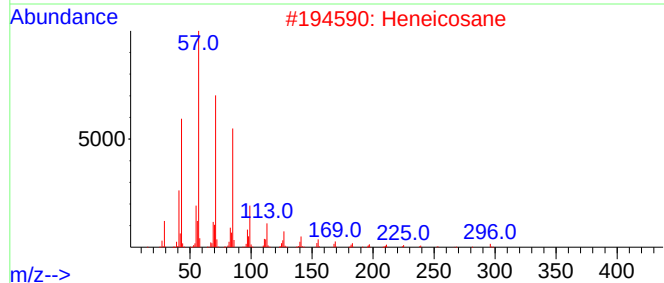
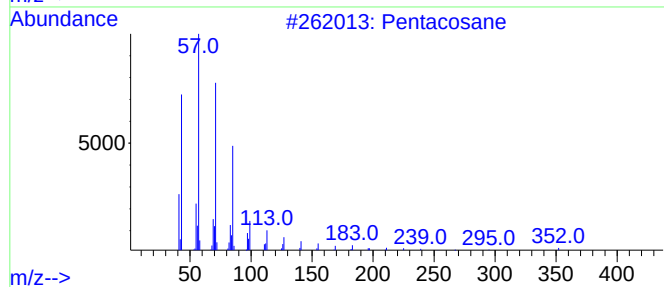
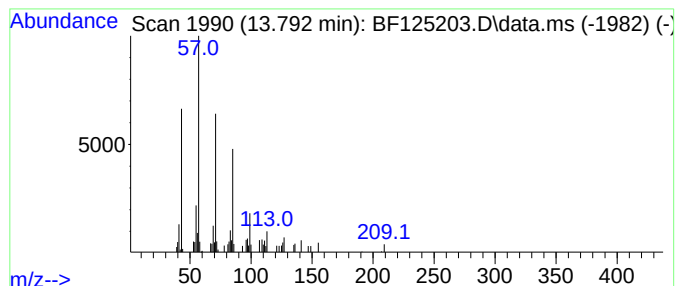
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Peak Number 5 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	3.02 ng	145390	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Heneicosane	296	C21H44	000629-94-7	87
3			Triacontane	422	C30H62	000638-68-6	86
4			Hentriacontane	437	C31H64	000630-04-6	86
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86



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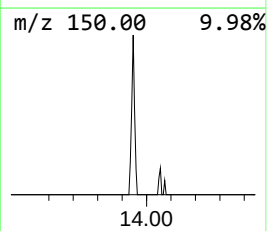
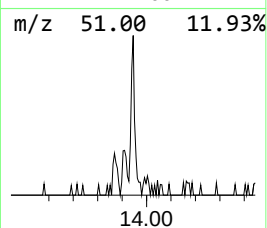
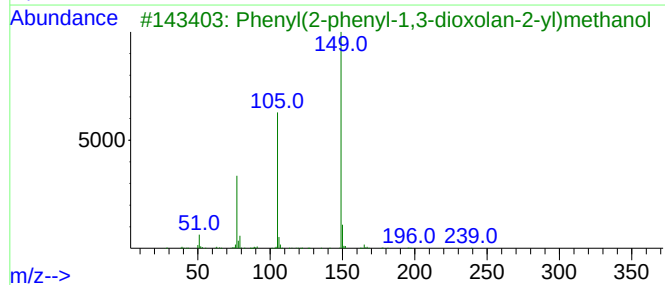
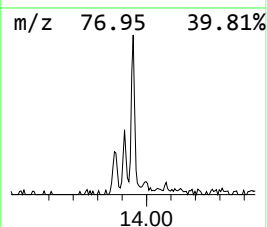
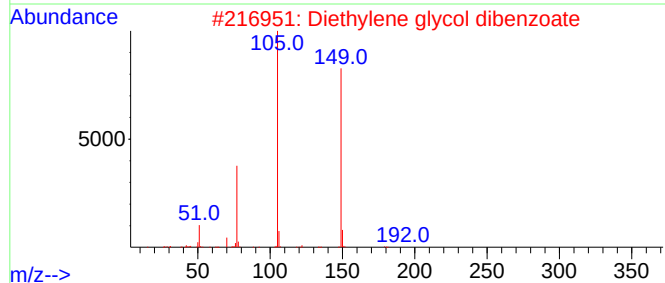
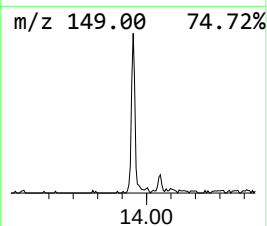
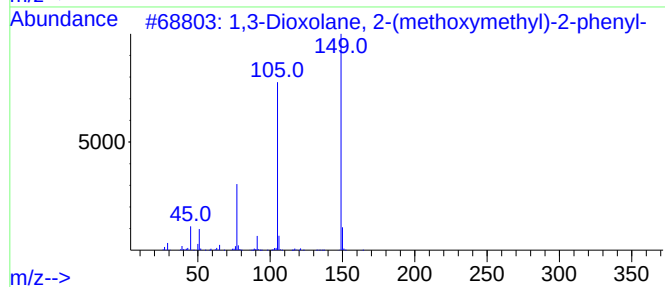
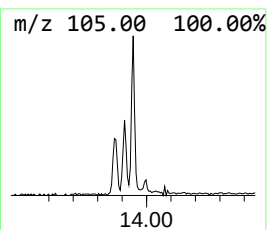
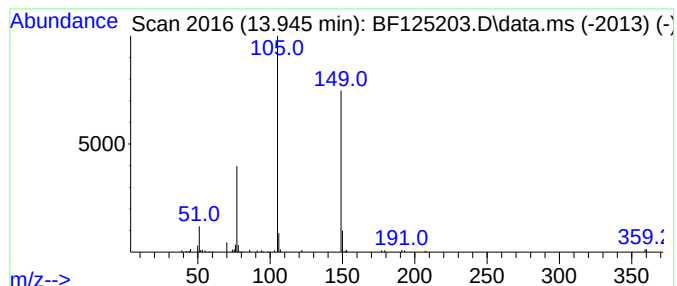
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	2.30 ng	110690	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
3			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
4			Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125203.D
Acq On : 25 Aug 2021 11:35
Operator : JU/CG
Sample : M3524-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-4

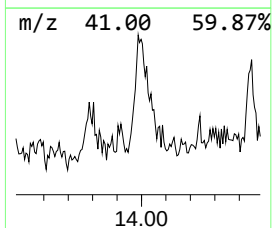
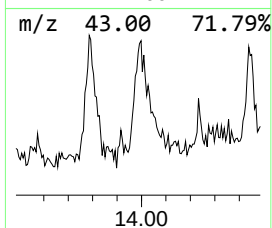
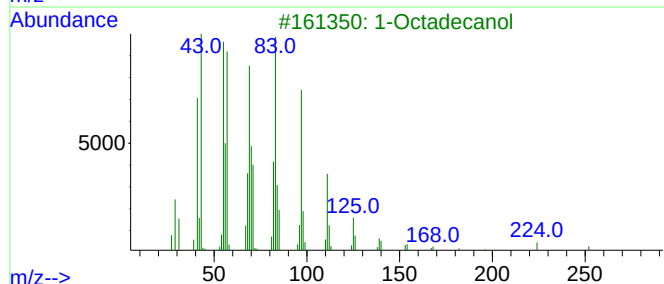
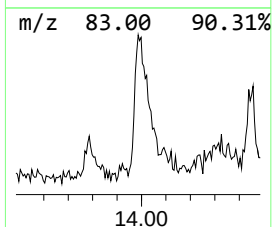
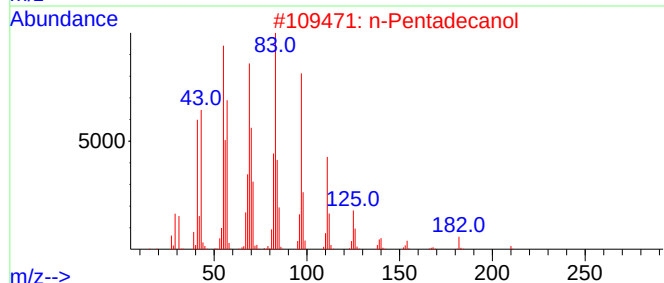
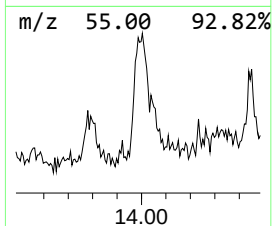
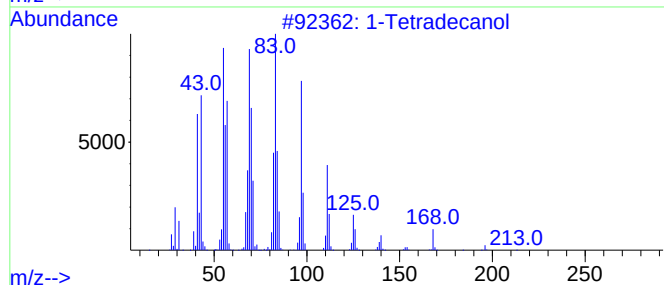
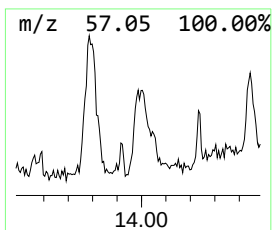
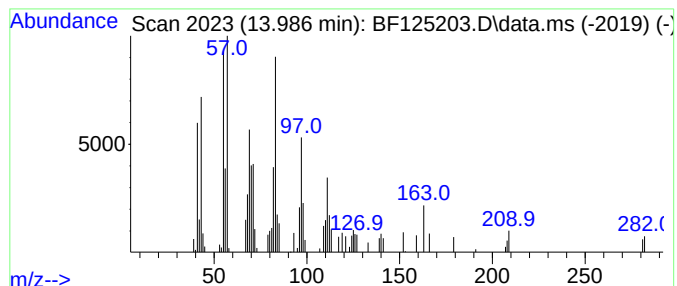
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tetradecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	4.19 ng	201294	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetradecanol	214	C14H30O	000112-72-1	83
2			n-Pentadecanol	228	C15H32O	000629-76-5	80
3			1-Octadecanol	270	C18H38O	000112-92-5	52
4			1-Octadecene	252	C18H36	000112-88-9	49
5			Undec-10-ynoic acid, dodecyl ester	350	C23H42O2	1010406-16-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125203.D
Acq On : 25 Aug 2021 11:35
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Sample : M3524-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PE-4

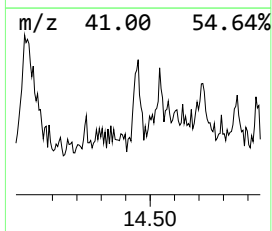
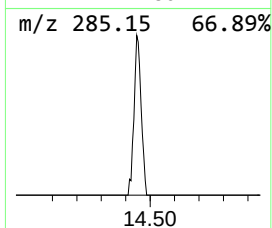
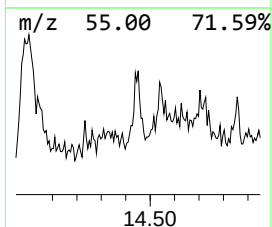
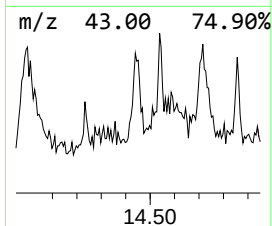
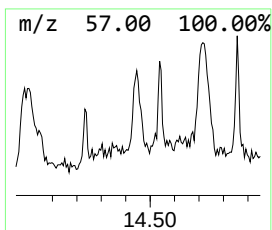
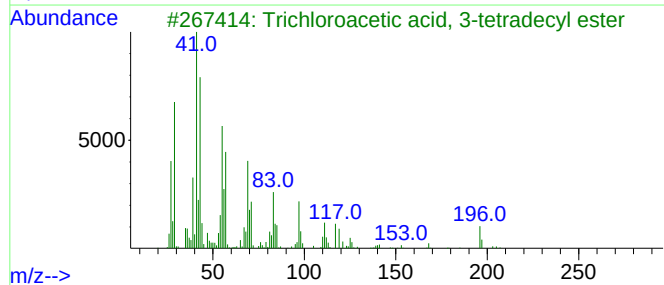
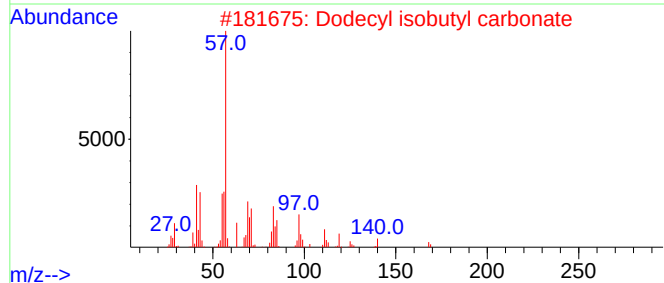
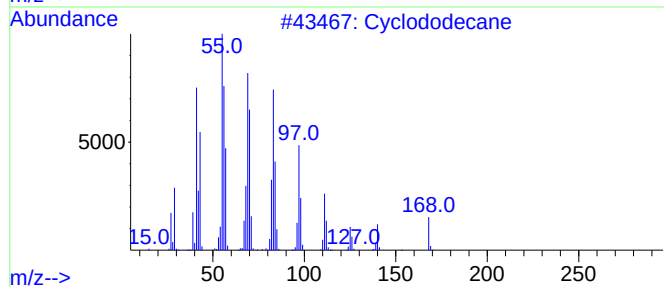
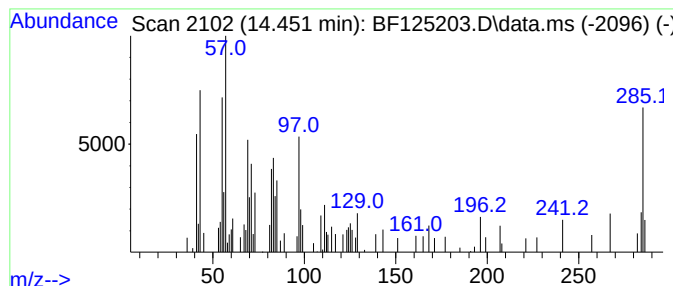
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclododecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	2.33 ng	111971	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane	168	C12H24	000294-62-2	70
2			Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	62
3			Trichloroacetic acid, 3-tetradec...	358	C16H29Cl3O2	1000282-06-7	58
4			Dichloroacetic acid, 2-pentadecy...	338	C17H32Cl2O2	1010280-64-7	58
5			Cyclotetradecane	196	C14H28	000295-17-0	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125203.D
Acq On : 25 Aug 2021 11:35
Operator : JU/CG
Sample : M3524-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PE-4

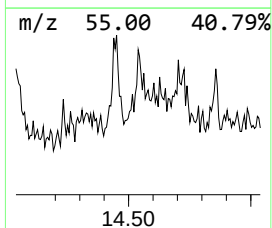
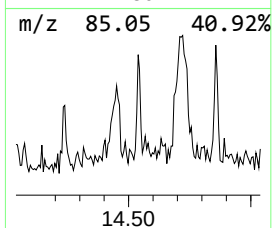
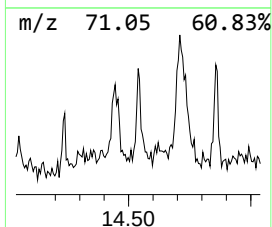
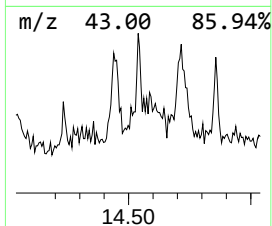
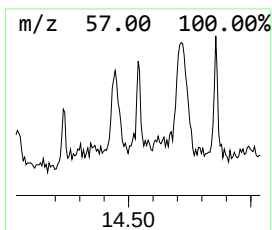
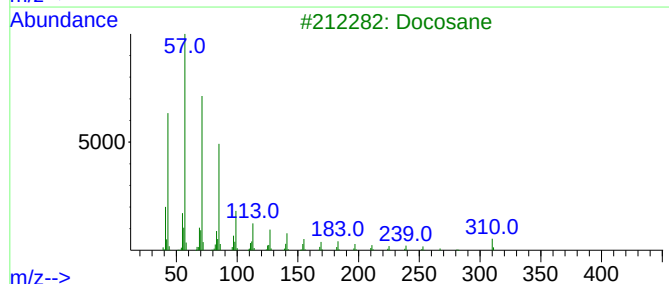
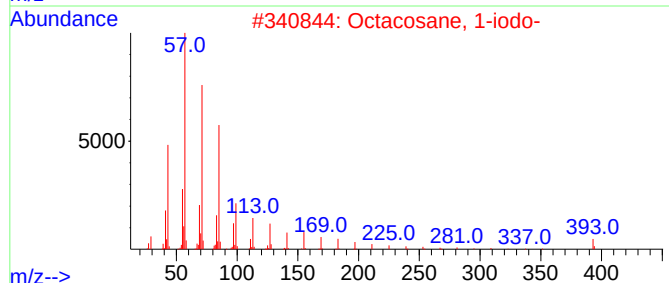
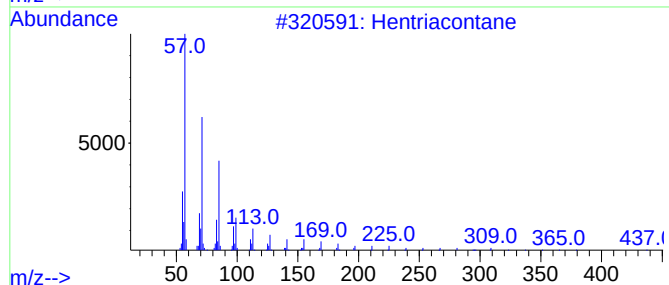
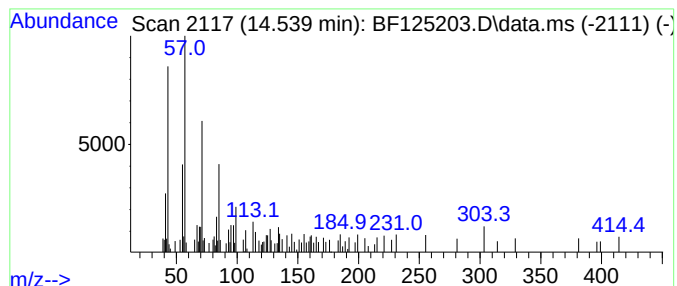
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.05 ng	98779	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	62
2			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	62
3			Docosane	310	C22H46	000629-97-0	62
4			triacontane	422	C30H62	000638-68-6	58
5			Pentacosane	352	C25H52	000629-99-2	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125203.D
Acq On : 25 Aug 2021 11:35
Operator : JU/CG
Sample : M3524-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-4

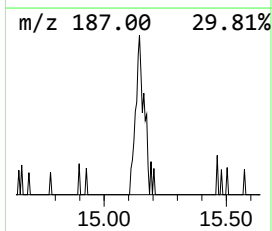
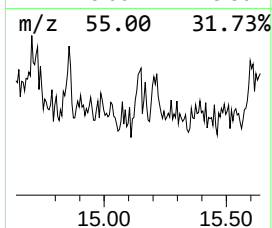
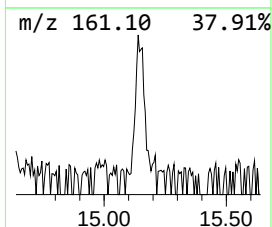
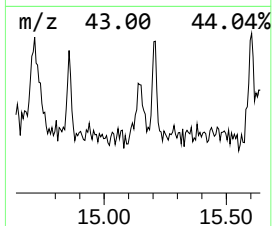
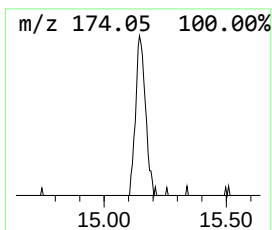
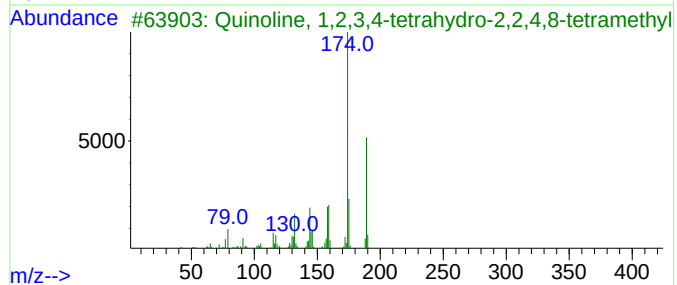
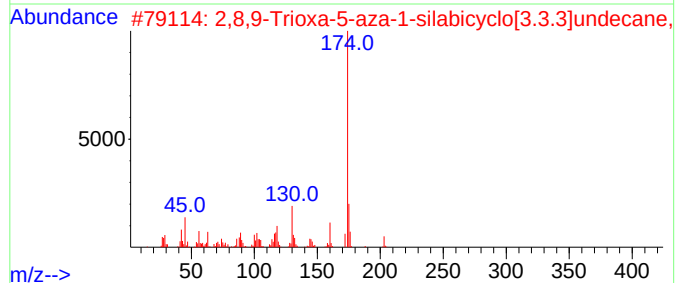
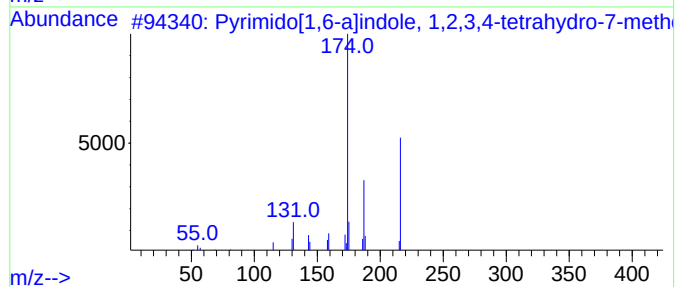
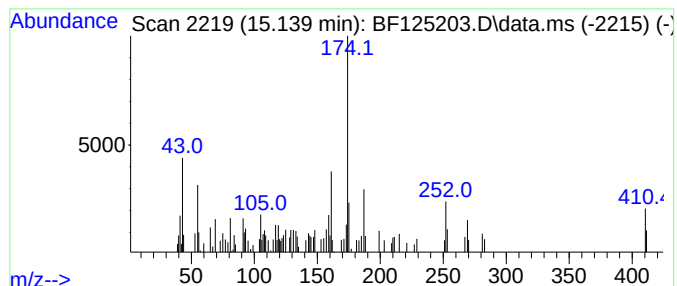
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.139 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	2.60 ng	122044	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrimido[1,6-a]indole, 1,2,3,4-t...	216	C13H16N2O	038349-09-6	38
2			2,8,9-Trioxa-5-aza-1-silabicyclo...	203	C8H17NO3Si	002097-16-7	38
3			Quinoline, 1,2,3,4-tetrahydro-2,...	189	C13H19N	1000308-78-8	35
4			3,6-Dimethyl-4-chromone	174	C11H10O2	057646-01-2	30
5			Pyrrolo[2,3-b]indole, 1,2,3,3a,8...	174	C11H14N2	055255-88-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125203.D
Acq On : 25 Aug 2021 11:35
Operator : JU/CG
Sample : M3524-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-4

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
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Ethanol, 2-(2-b...	8.110	3.6	ng	206898	2	8.198	1149520	20.0
n-Hexadecanoic ...	11.957	9.3	ng	610687	4	11.439	1320380	20.0
Pentadecanoic acid	12.739	4.0	ng	264119	4	11.439	1320380	20.0
Pentacosane	13.792	3.0	ng	145390	5	14.080	961636	20.0
1,3-Dioxolane, ...	13.945	2.3	ng	110690	5	14.080	961636	20.0
1-Tetradecanol	13.986	4.2	ng	201294	5	14.080	961636	20.0
Cyclododecane	14.451	2.3	ng	111971	5	14.080	961636	20.0
Hentriacontane	14.539	2.0	ng	98779	5	14.080	961636	20.0
unknown15.139	15.139	2.6	ng	122044	6	15.574	940104	20.0