

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
 Data File : BF125250.D
 Acq On : 27 Aug 2021 12:36
 Operator : JU/CG
 Sample : M3547-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-3

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	13	20	28	rVB	1429137	1853916	33.40%	4.586%
2	5.534	581	586	589	rBV	4024971	4061091	73.15%	10.045%
3	6.539	751	757	760	rBV	3655706	4021012	72.43%	9.946%
4	6.910	817	820	824	rBV	1413573	1189792	21.43%	2.943%
5	7.475	911	916	919	rBV	3037623	2624853	47.28%	6.492%
6	8.104	1017	1023	1035	rBV	68480	201935	3.64%	0.499%
7	8.192	1035	1038	1042	rBV	1708414	1547849	27.88%	3.828%
8	9.269	1217	1221	1224	rBV	5560808	4629315	83.39%	11.450%
9	9.951	1333	1337	1340	rBV	2227660	1867472	33.64%	4.619%
10	10.739	1466	1471	1474	rBV	3943188	3440561	61.98%	8.510%
11	11.439	1586	1590	1592	rBV	2375622	2070520	37.30%	5.121%
12	11.457	1592	1593	1597	rVB	128874	100744	1.81%	0.249%
13	11.951	1670	1677	1682	rBV2	540903	591833	10.66%	1.464%
14	12.651	1792	1796	1801	rBV	272848	255758	4.61%	0.633%
15	12.739	1808	1811	1819	rBV	219548	224951	4.05%	0.556%
16	12.880	1829	1835	1838	rBV	222968	229865	4.14%	0.569%
17	13.021	1855	1859	1863	rBV	5368785	5551409	100.00%	13.731%
18	13.980	2013	2022	2032	rBV6	175152	723317	13.03%	1.789%
19	14.074	2034	2038	2041	rBV	1695395	1635462	29.46%	4.045%
20	14.192	2049	2058	2073	rVB	220025	950938	17.13%	2.352%
21	14.662	2124	2138	2154	rBV6	107968	631374	11.37%	1.562%
22	14.833	2164	2167	2174	rVB2	123103	174864	3.15%	0.433%
23	14.933	2180	2184	2188	rBV	74039	76115	1.37%	0.188%
24	15.127	2214	2217	2220	rBV	66581	94861	1.71%	0.235%
25	15.204	2227	2230	2234	rVB2	53881	58140	1.05%	0.144%
26	15.439	2268	2270	2277	rVB2	51339	65793	1.19%	0.163%
27	15.504	2278	2281	2287	rVB	55414	60204	1.08%	0.149%
28	15.574	2287	2293	2305	rBV	1053969	1426082	25.69%	3.527%
29	16.045	2370	2373	2379	rVB2	49635	69663	1.25%	0.172%

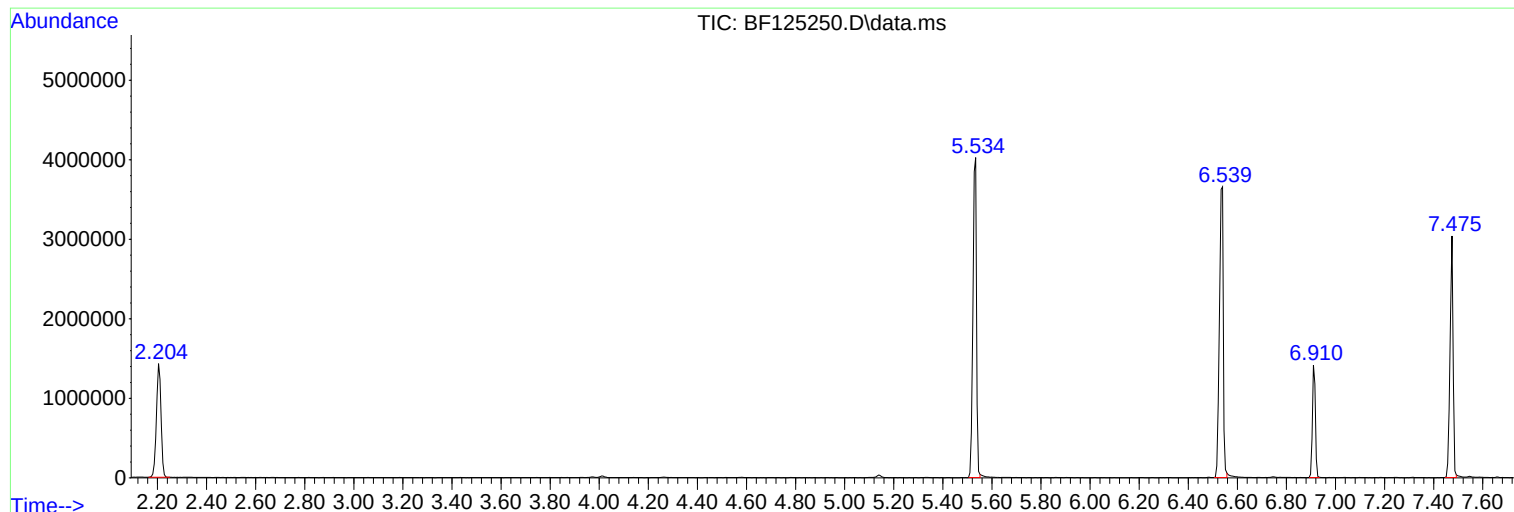
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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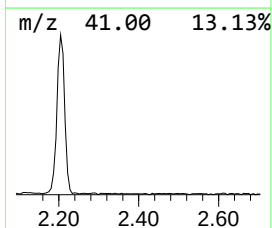
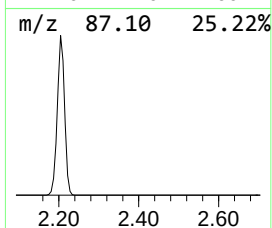
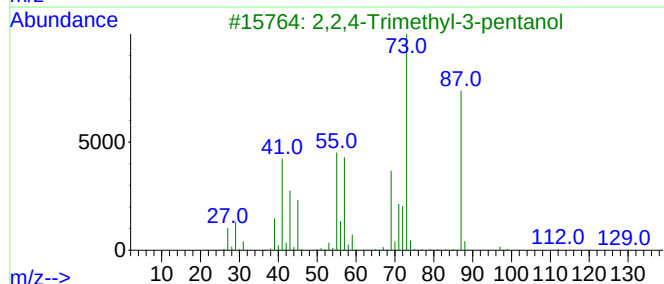
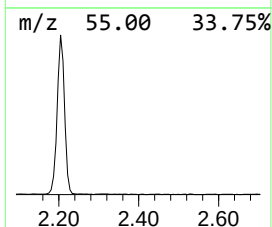
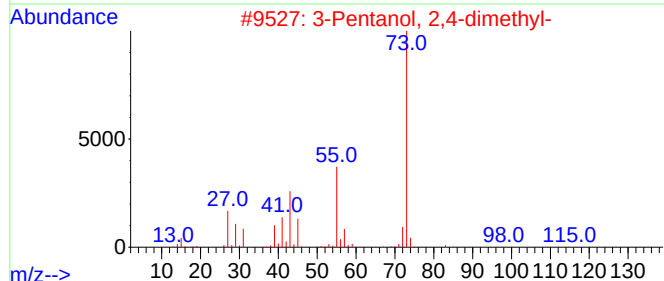
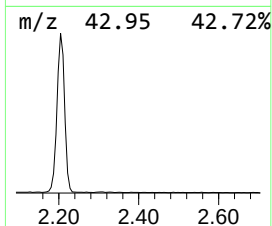
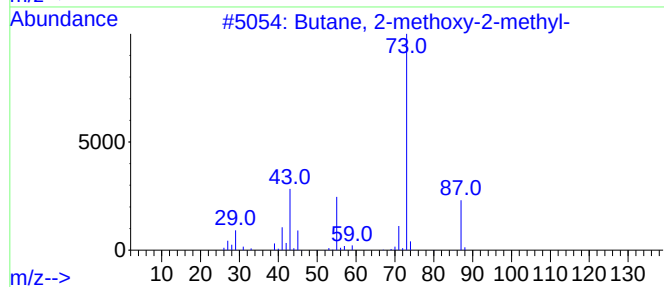
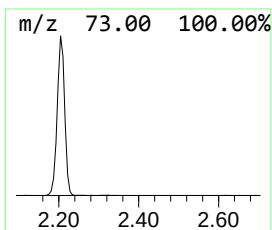
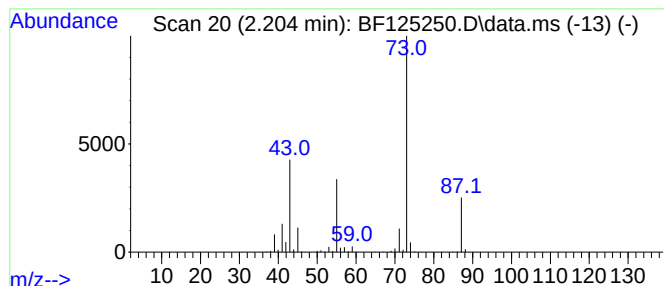
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.204	31.16 ng	1853920	1,4-Dichlorobenzene-d4	6.910

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	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28



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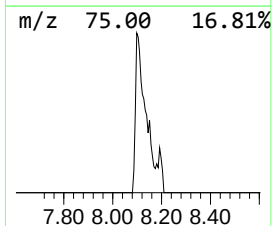
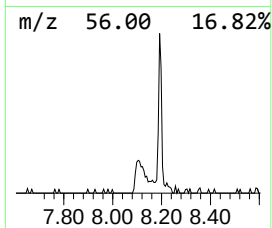
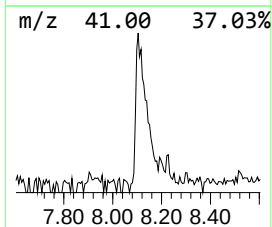
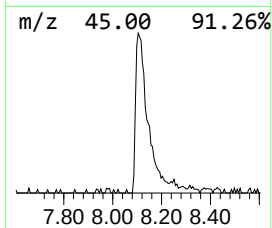
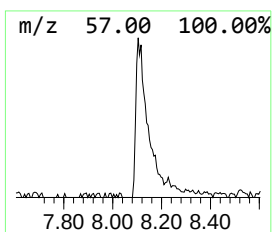
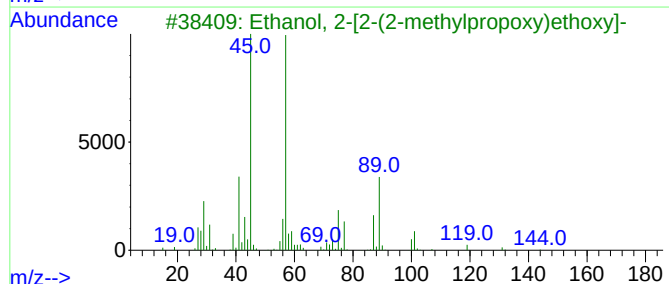
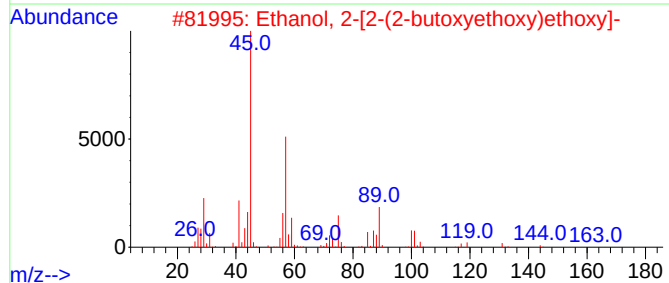
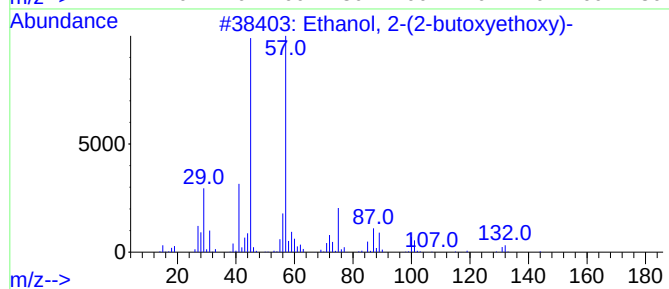
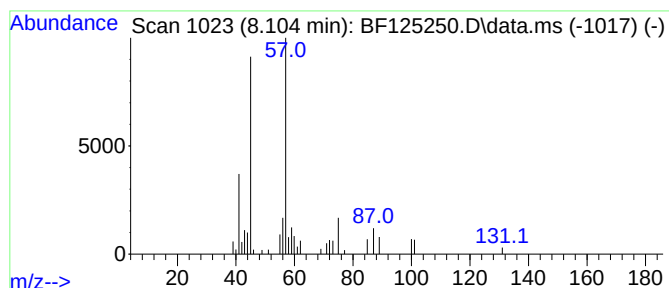
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	2.61 ng	201935	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, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	78
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	59
5			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50



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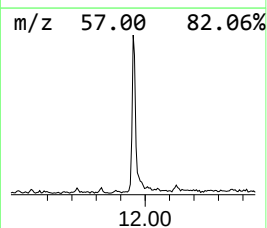
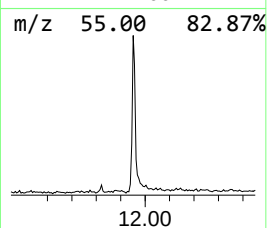
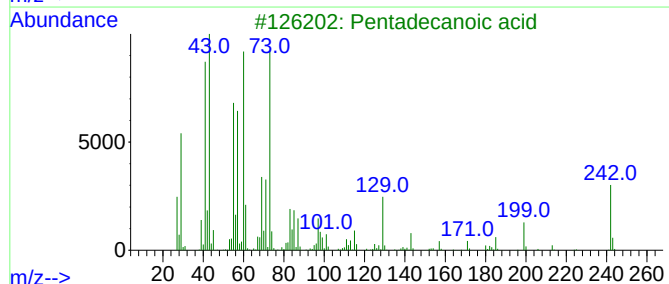
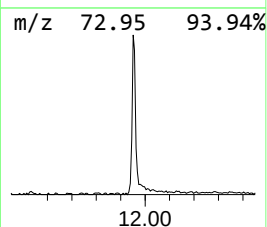
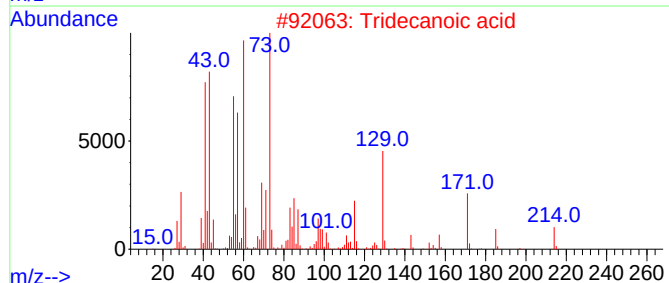
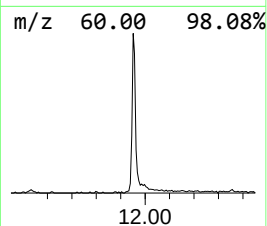
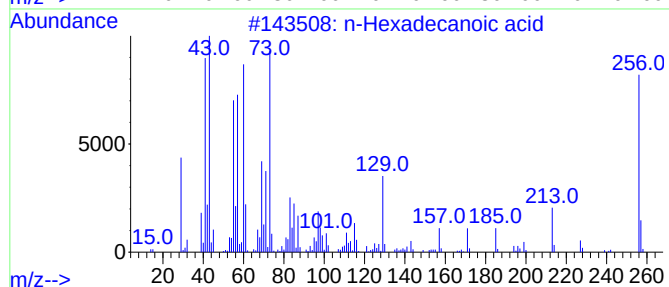
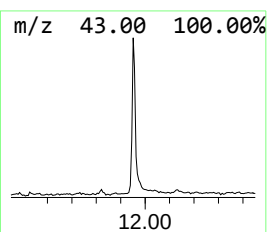
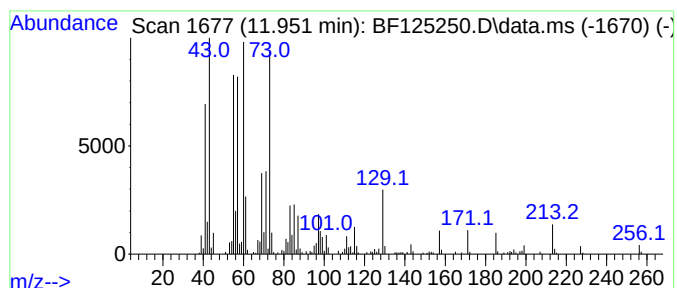
Instrument :
BNA_F
ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.951	5.72 ng	591833	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	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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Instrument :
BNA_F
ClientSampled :
PE-3

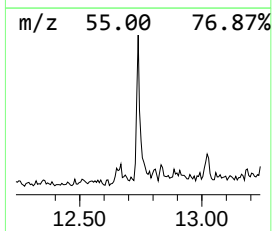
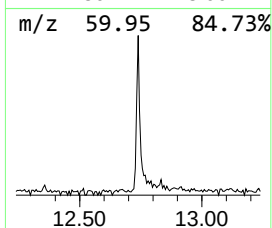
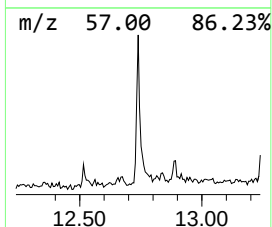
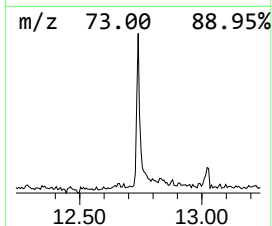
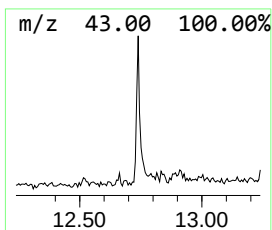
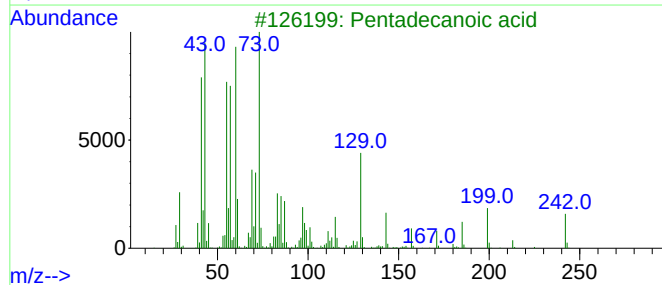
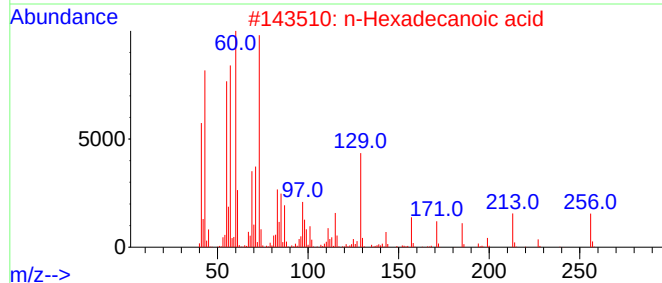
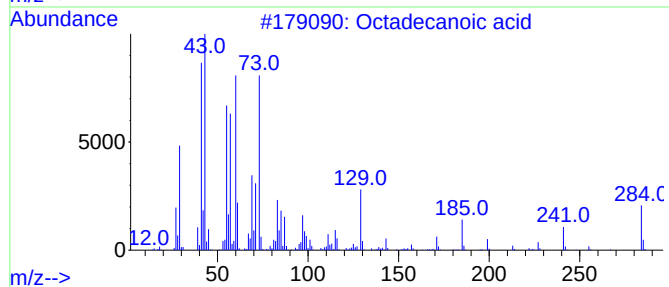
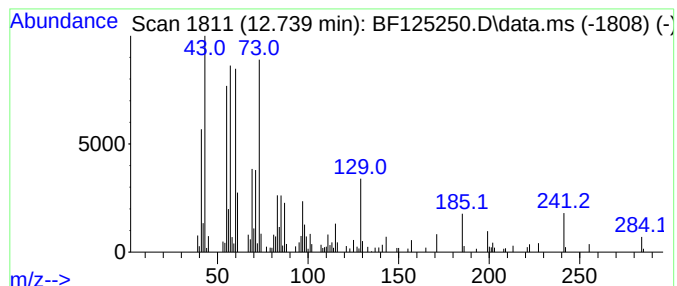
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	2.17 ng	224951	Phenanthrene-d10	11.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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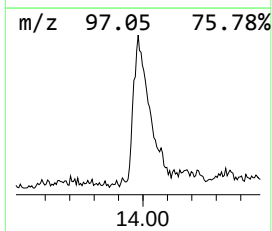
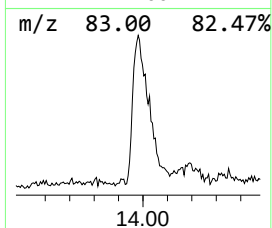
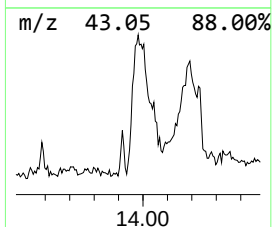
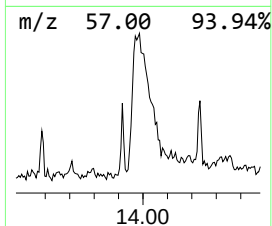
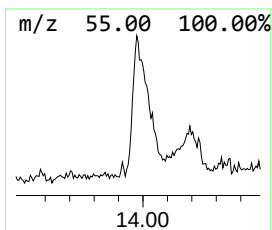
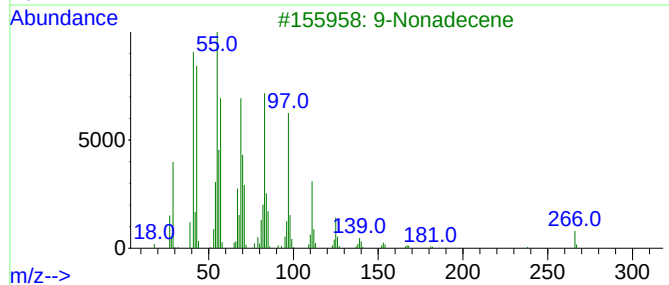
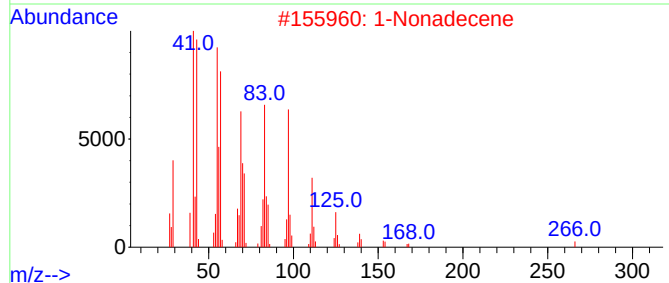
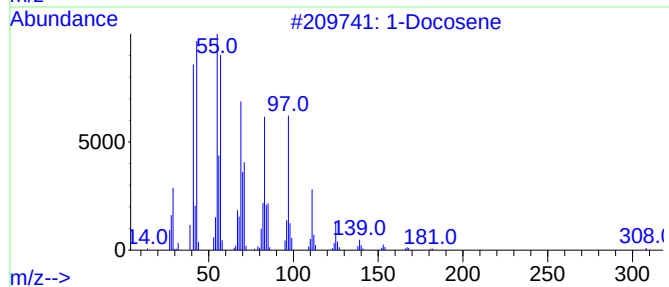
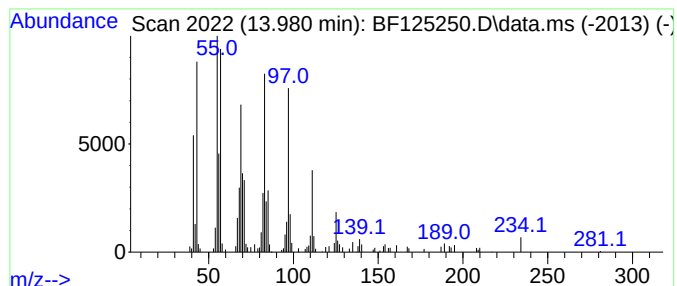
Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.980	8.85 ng	723317	Chrysene-d12	14.074	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	9-Nonadecene	266	C19H38	031035-07-1	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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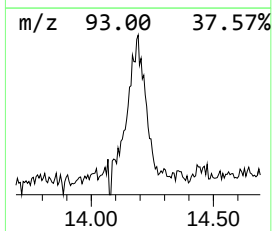
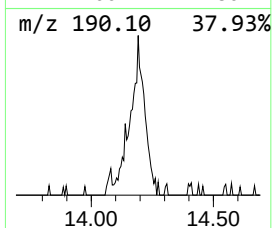
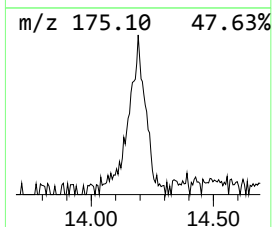
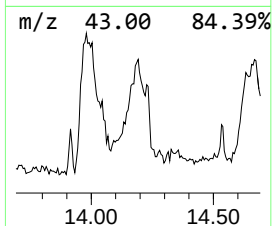
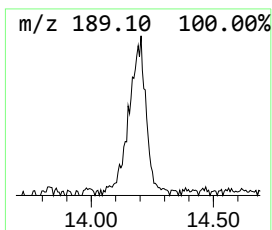
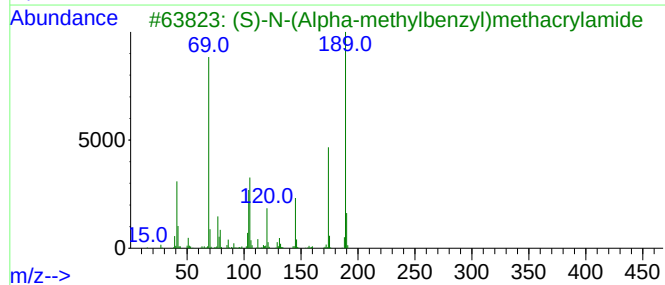
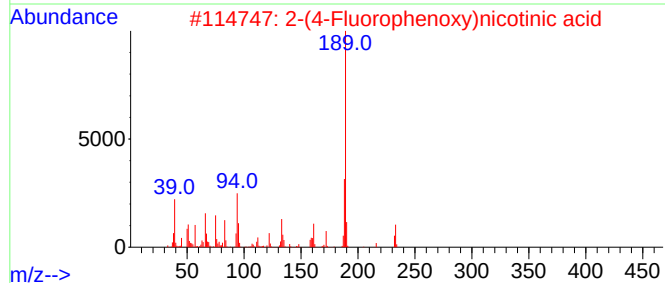
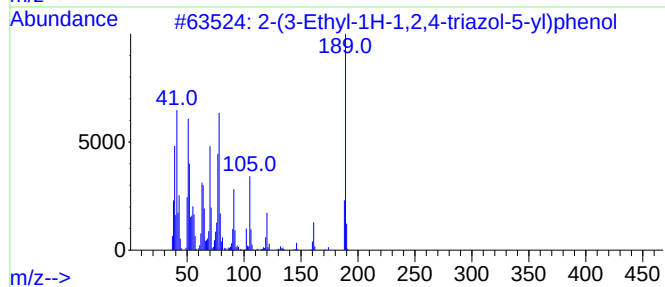
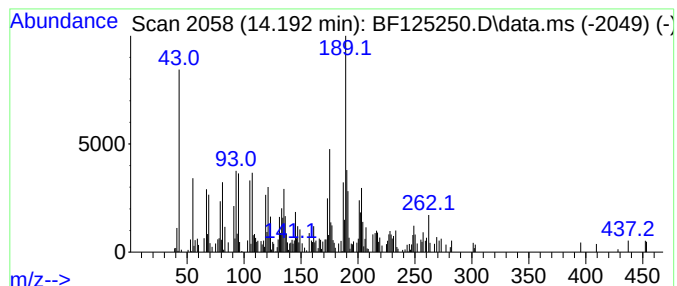
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.192 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	11.63 ng	950938	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3-Ethyl-1H-1,2,4-triazol-5-yl...	189	C10H11N3O	1000386-79-9	46		
2	2-(4-Fluorophenoxy)nicotinic acid	233	C12H8FN03	054629-13-9	43		
3	(S)-N-(Alpha-methylbenzyl)methac...	189	C12H15NO	056598-33-5	38		
4	Pyrido[3,4-d]pyrimidin-4(3H)-one...	189	C10H11N3O	022389-79-3	38		
5	Benzoic acid, 3-(3-hydroxy-3-met...	204	C12H12O3	1000337-06-2	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125250.D
Acq On : 27 Aug 2021 12:36
Operator : JU/CG
Sample : M3547-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-3

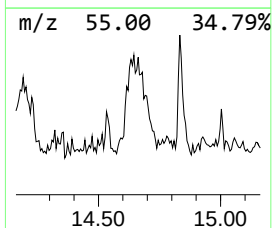
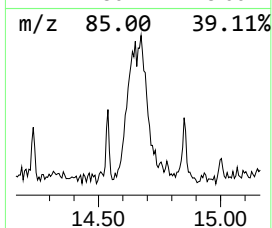
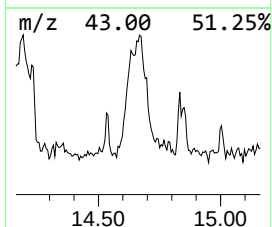
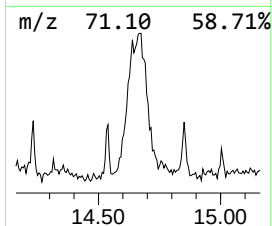
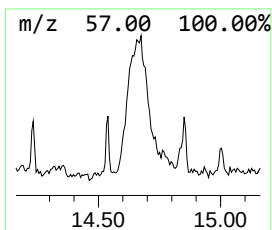
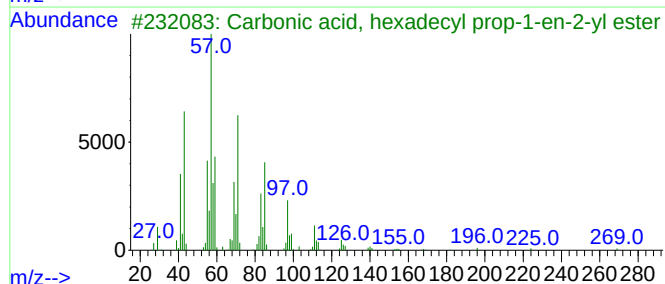
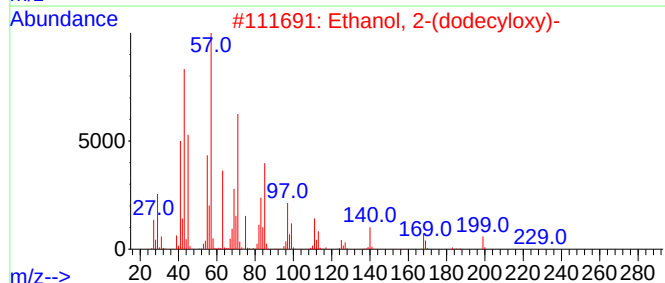
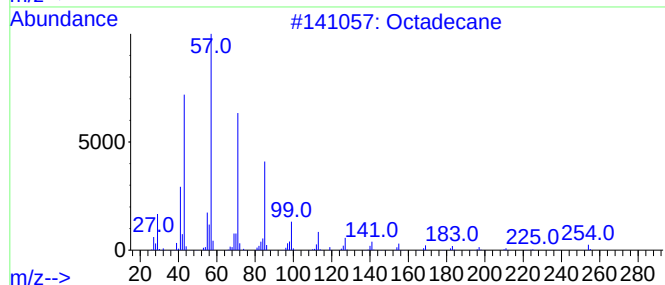
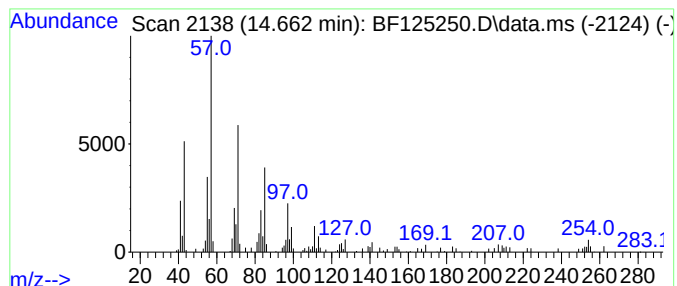
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.662	7.72 ng	631374	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	91
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	90
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	87
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
5			Tetratetracontane	619	C44H90	007098-22-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125250.D
Acq On : 27 Aug 2021 12:36
Operator : JU/CG
Sample : M3547-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-3

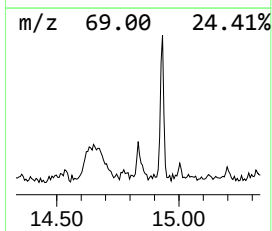
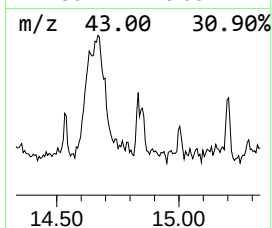
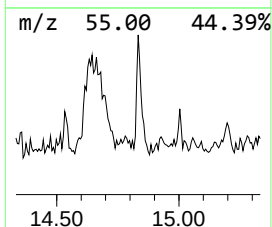
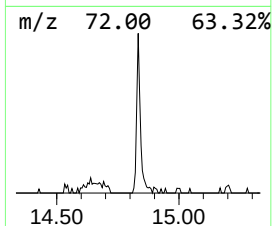
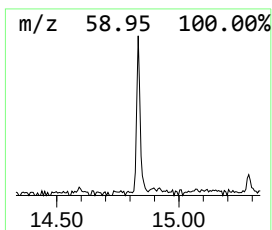
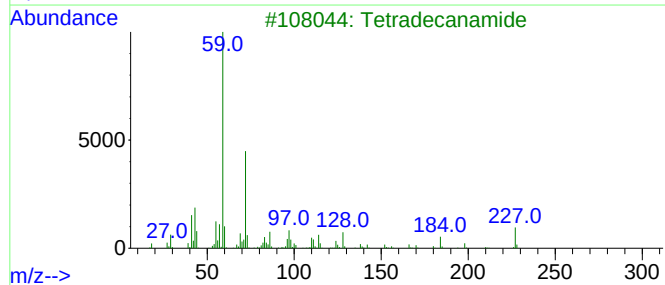
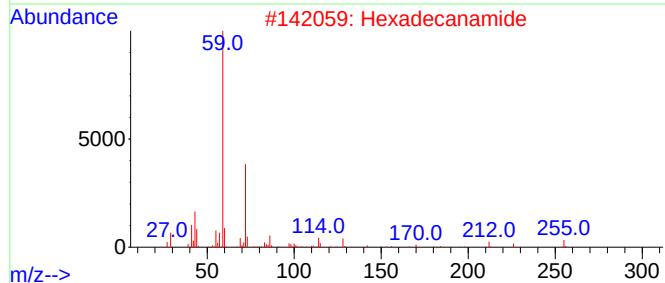
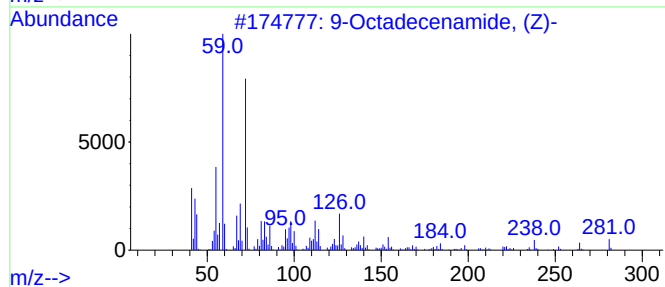
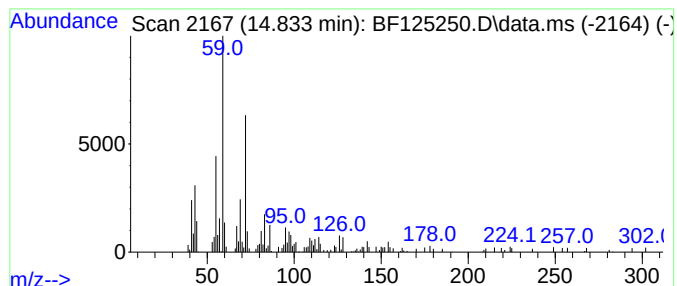
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	2.45 ng	174864	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-			281	C18H35NO	000301-02-0	91
2	Hexadecanamide			255	C16H33NO	000629-54-9	72
3	Tetradecanamide			227	C14H29NO	000638-58-4	72
4	Octadecanamide			283	C18H37NO	000124-26-5	72
5	7-Nonenamide			155	C9H17NO	090949-53-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082721\
Data File : BF125250.D
Acq On : 27 Aug 2021 12:36
Operator : JU/CG
Sample : M3547-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-3

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...	2.204	31.2	ng	1853920	1	6.910	1189790	20.0
Ethanol, 2-(2-b...	8.104	2.6	ng	201935	2	8.198	1547850	20.0
n-Hexadecanoic ...	11.951	5.7	ng	591833	4	11.439	2070520	20.0
Octadecanoic acid	12.739	2.2	ng	224951	4	11.439	2070520	20.0
1-Docosene	13.980	8.8	ng	723317	5	14.074	1635460	20.0
unknown14.192	14.192	11.6	ng	950938	5	14.074	1635460	20.0
Octadecane	14.662	7.7	ng	631374	5	14.074	1635460	20.0
9-Octadecenamid...	14.833	2.5	ng	174864	6	15.574	1426080	20.0