

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
 Data File : BF125627.D
 Acq On : 24 Sep 2021 18:41
 Operator : JU/CG
 Sample : M3911-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-RR-02-(1.0)

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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125627.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	19	24	rVB	3627015	4986254	80.04%	9.024%
2	5.504	576	581	584	rBV	2440821	2371759	38.07%	4.292%
3	6.498	746	750	753	rBV	1813361	1561323	25.06%	2.826%
4	6.887	812	816	819	rBV	1365312	1094798	17.57%	1.981%
5	7.445	905	911	914	rBV	3276210	3236537	51.96%	5.857%
6	8.069	1013	1017	1021	rBV	182393	165318	2.65%	0.299%
7	8.169	1029	1034	1036	rBV	1686971	1541031	24.74%	2.789%
8	9.245	1211	1217	1220	rBV	6643029	6229492	100.00%	11.274%
9	9.922	1328	1332	1335	rVB	2166406	1743176	27.98%	3.155%
10	10.710	1461	1466	1469	rBV	3879320	3474390	55.77%	6.288%
11	10.804	1478	1482	1485	rBV	436240	431268	6.92%	0.780%
12	10.839	1485	1488	1494	rVB2	155115	187154	3.00%	0.339%
13	11.069	1514	1527	1528	rBV9	77657	212844	3.42%	0.385%
14	11.157	1528	1542	1543	rBV	494218	1207802	19.39%	2.186%
15	11.174	1543	1545	1546	rBV	116361	102974	1.65%	0.186%
16	11.304	1565	1567	1574	rVB	125968	140485	2.26%	0.254%
17	11.404	1580	1584	1587	rBV	1932841	1675328	26.89%	3.032%
18	11.933	1668	1674	1678	rBV	739303	1004192	16.12%	1.817%
19	12.169	1706	1714	1728	rVB2	227952	832317	13.36%	1.506%
20	12.639	1787	1794	1797	rBV6	148140	347050	5.57%	0.628%
21	12.716	1802	1807	1827	rVB	1964917	3282040	52.69%	5.940%
22	12.992	1850	1854	1857	rBV	5581473	5328242	85.53%	9.643%
23	13.280	1896	1903	1914	rBV	533241	1122456	18.02%	2.031%
24	13.904	2005	2009	2015	rVB	183770	286109	4.59%	0.518%
25	14.010	2021	2027	2030	rBV	672210	1121347	18.00%	2.029%
26	14.039	2030	2032	2036	rVB	1261141	1053189	16.91%	1.906%
27	14.586	2120	2125	2130	rBV	776106	1177822	18.91%	2.132%
28	14.639	2130	2134	2143	rVB2	784431	1383596	22.21%	2.504%
29	14.939	2181	2185	2189	rBV6	78265	156375	2.51%	0.283%
30	15.168	2217	2224	2243	rVB2	502810	1086577	17.44%	1.966%
31	15.515	2274	2283	2287	rBV	970062	1262772	20.27%	2.285%
32	15.827	2329	2336	2343	rVB	295593	634131	10.18%	1.148%
33	15.915	2345	2351	2361	rBV3	116031	342017	5.49%	0.619%
34	16.233	2397	2405	2430	rBV3	468801	1603547	25.74%	2.902%
35	16.574	2456	2463	2473	rVB2	212882	587996	9.44%	1.064%
36	16.974	2522	2531	2542	rBV2	489077	1307658	20.99%	2.366%

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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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.474	2609	2616	2627	rVB2	124713	374675	6.01%	0.678%
38	17.615	2633	2640	2656	rVB2	87099	319523	5.13%	0.578%
39	18.539	2789	2797	2810	rVB2	80375	281599	4.52%	0.510%

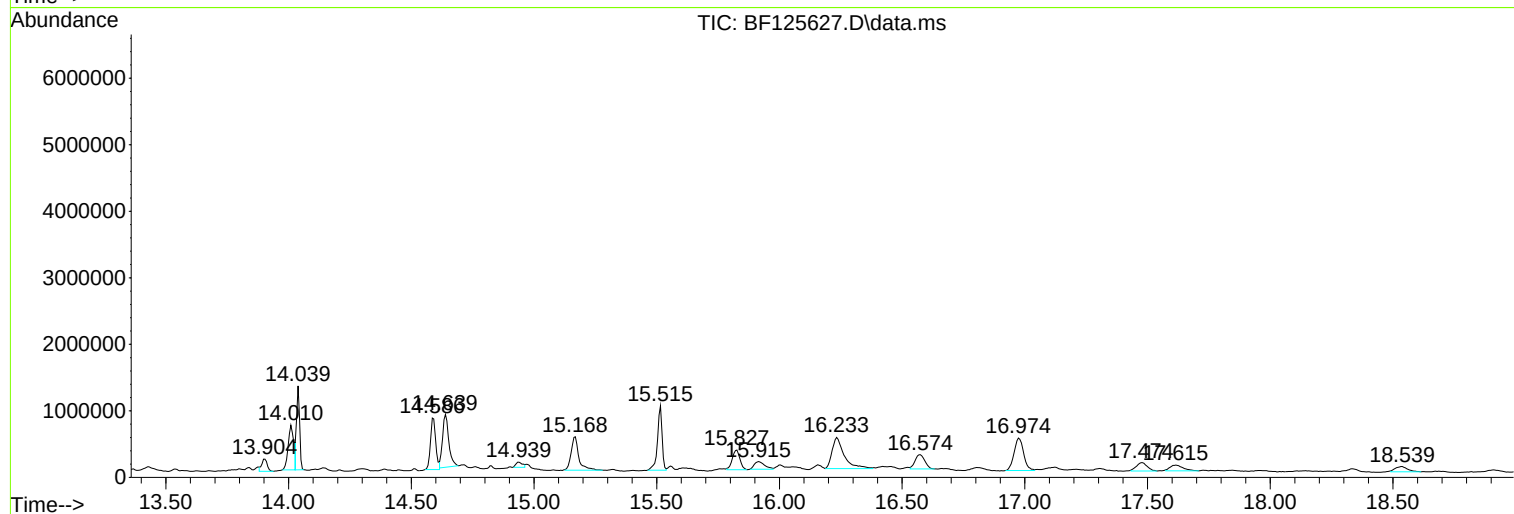
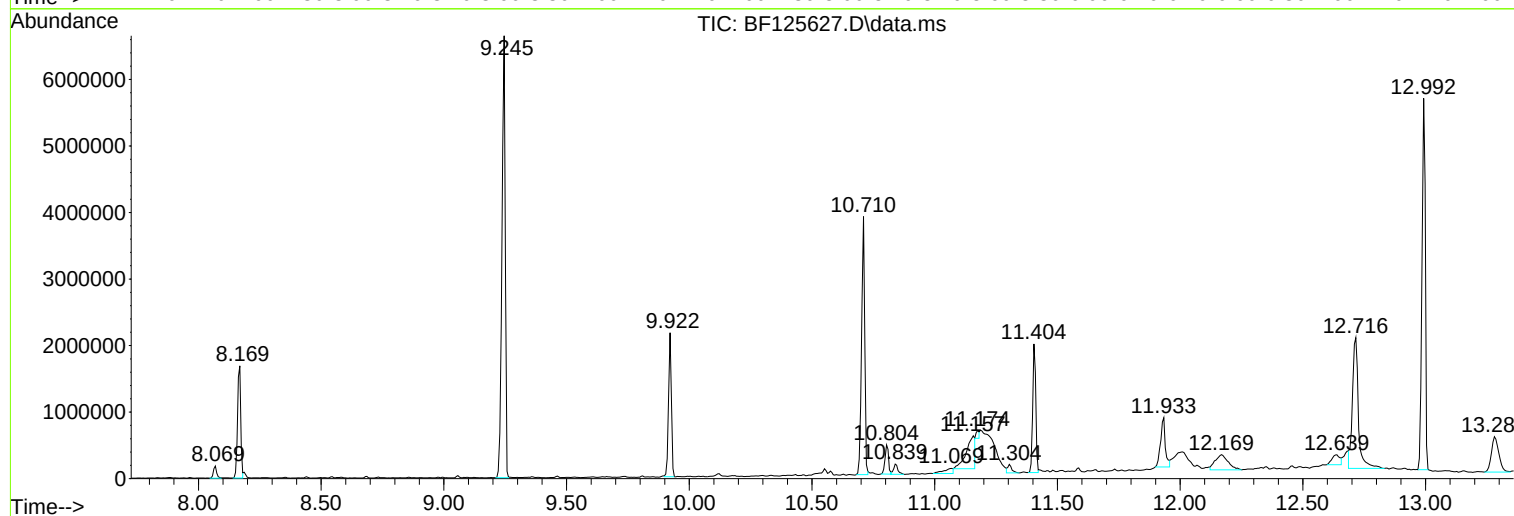
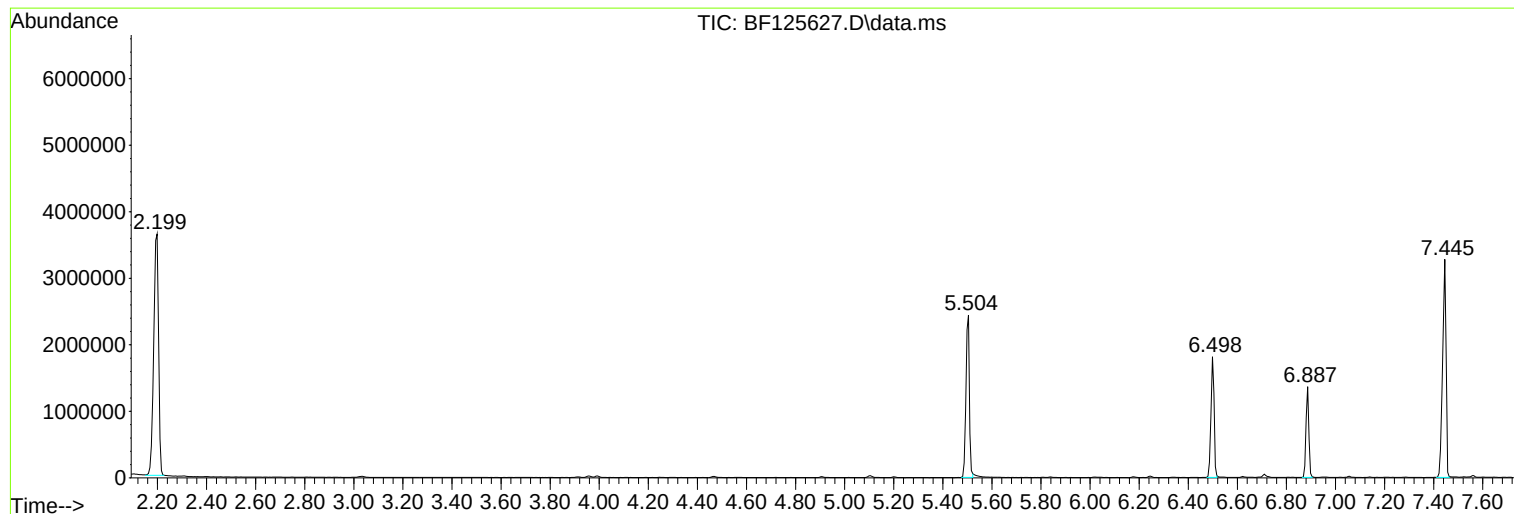
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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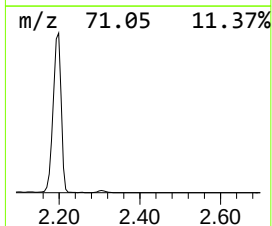
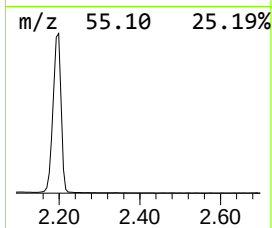
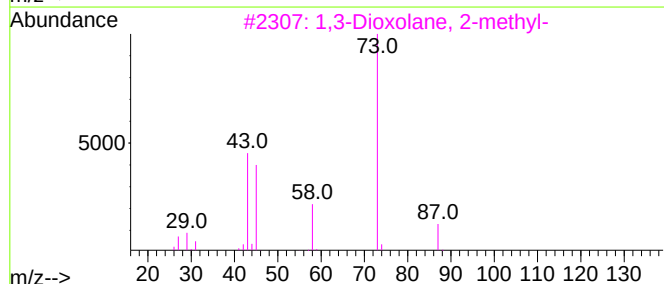
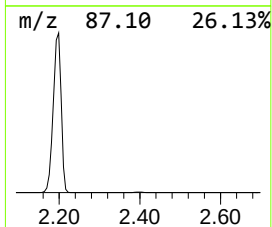
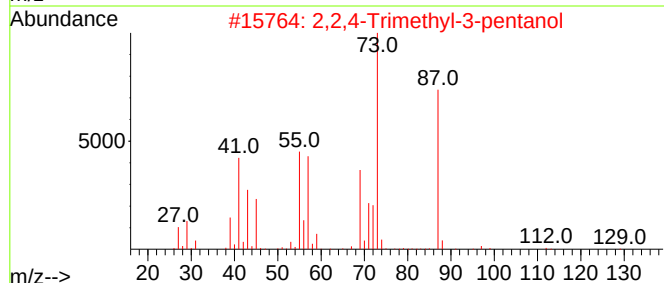
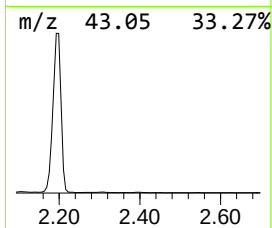
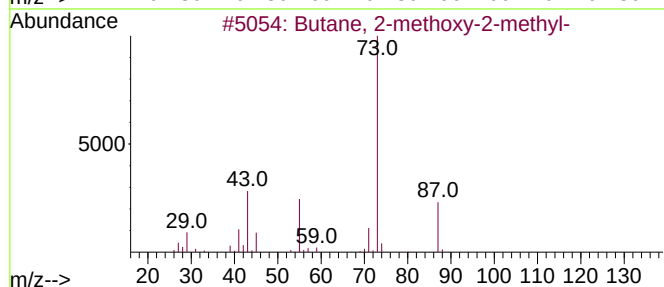
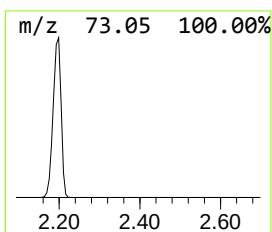
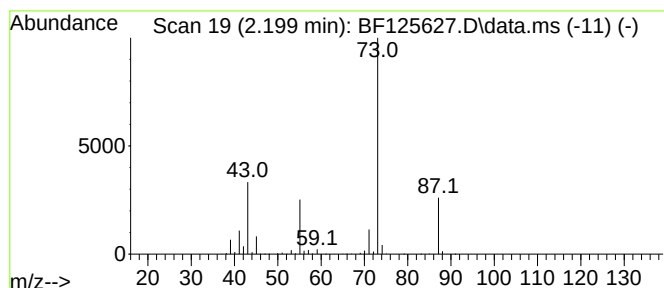
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	91.09 ng	4986250	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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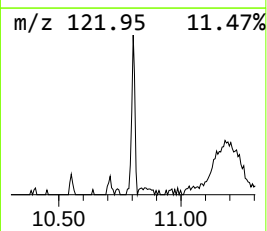
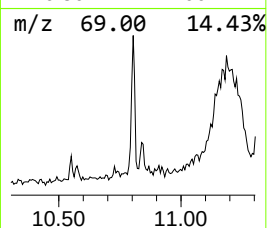
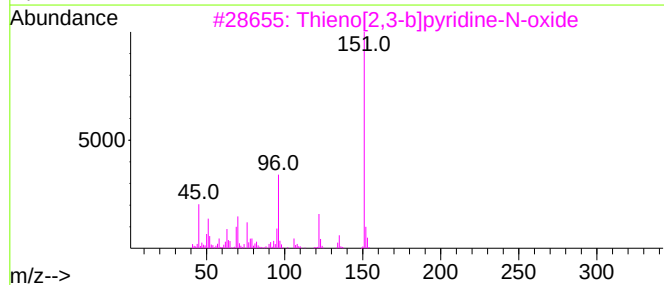
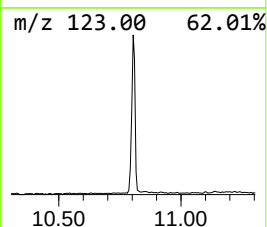
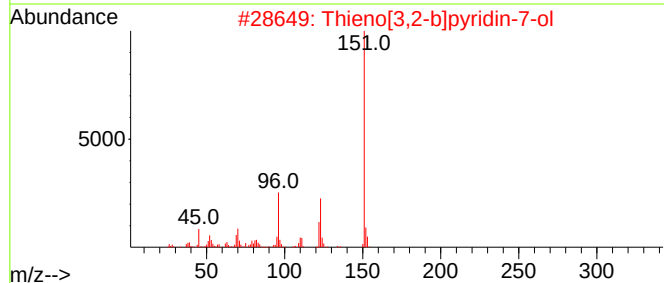
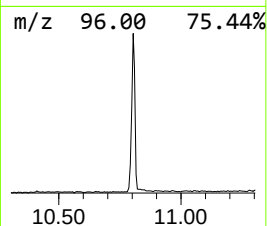
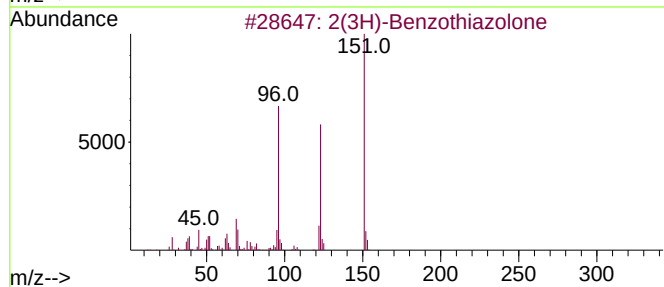
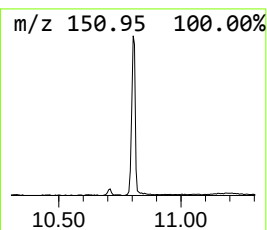
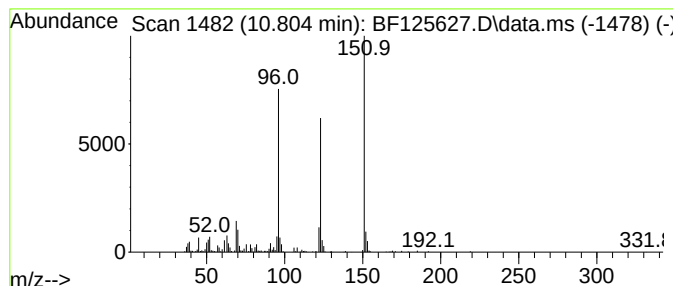
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2(3H)-Benzothiazolone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	5.15 ng	431268	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	52
3			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	46
4			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	43
5			5-Fluoro-2-pyrimidinecarbonitrile	123	C5H2FN3	038275-55-7	43



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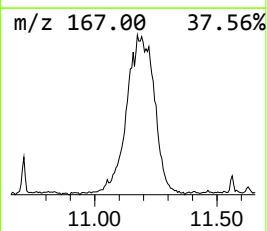
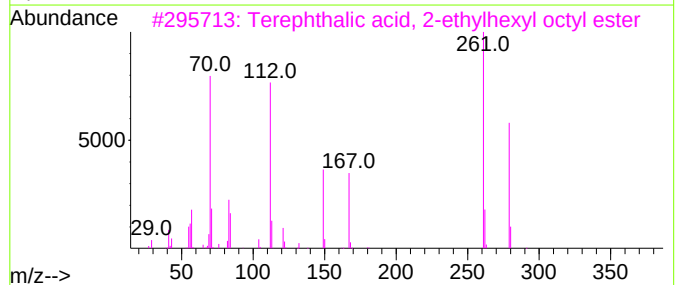
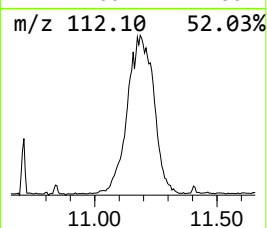
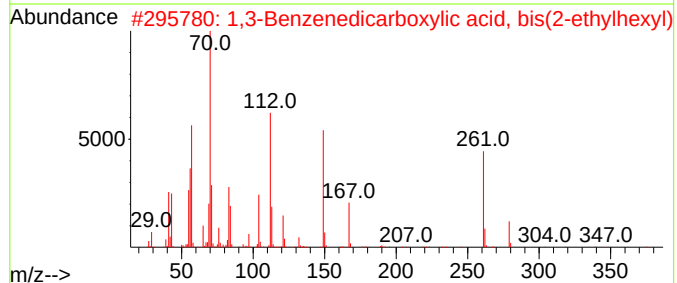
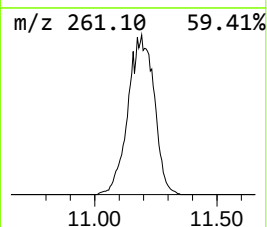
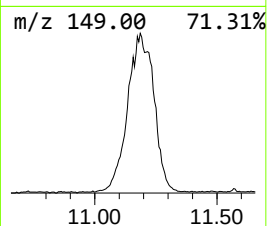
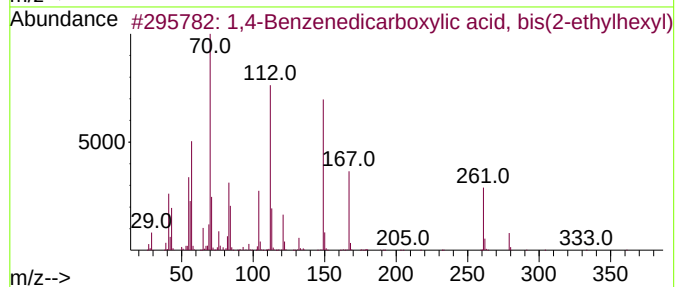
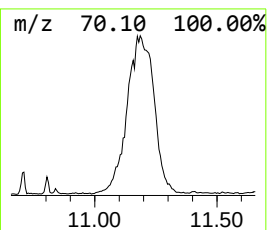
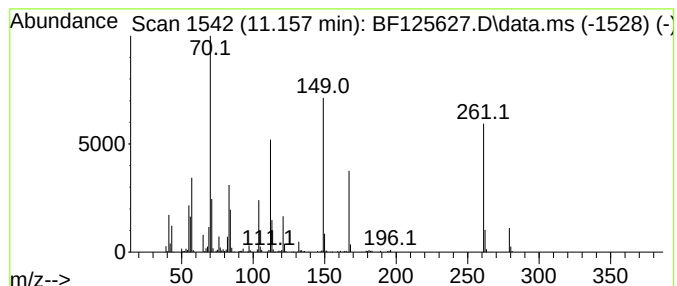
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.157	14.42 ng	1207800	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	90
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	87
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	59
4			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43



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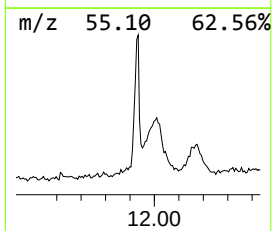
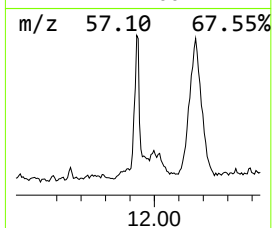
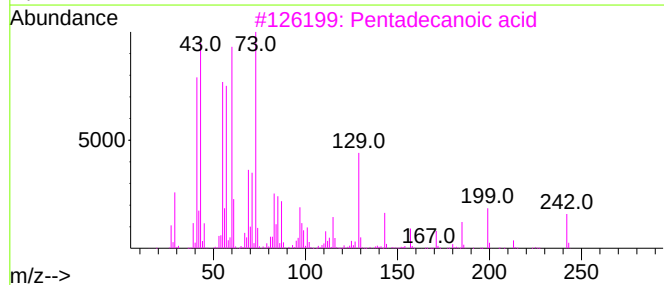
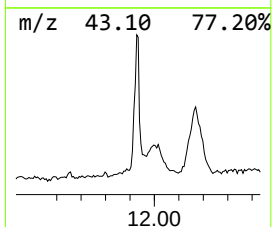
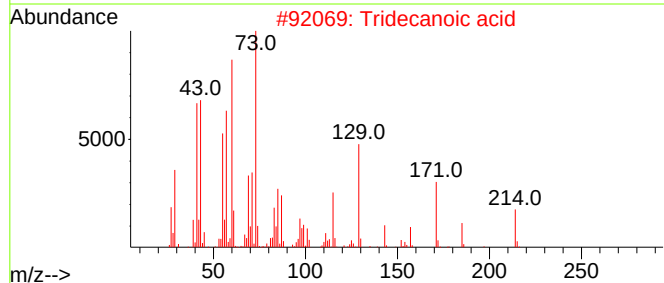
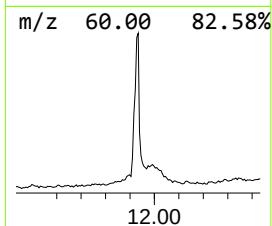
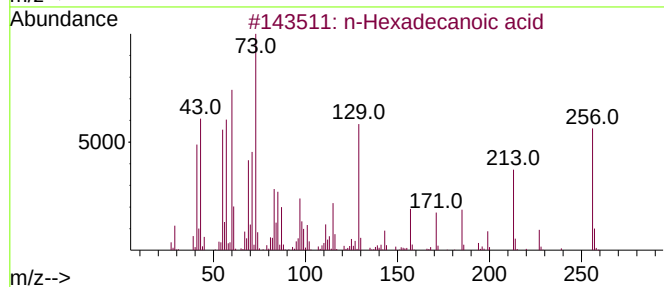
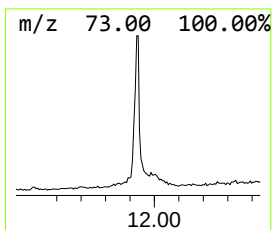
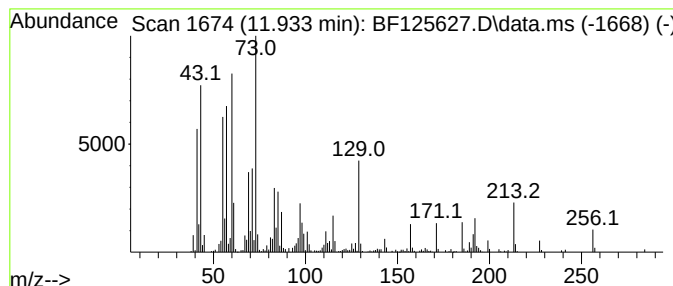
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	11.99 ng	1004190	Phenanthrene-d10	11.404

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Octadecanoic acid	284	C18H36O2	000057-11-4	91
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	90



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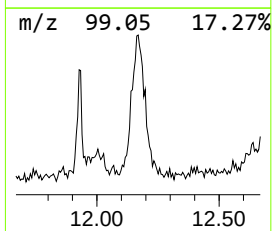
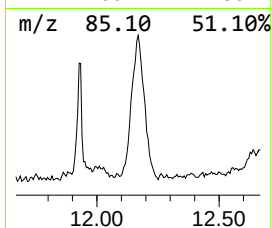
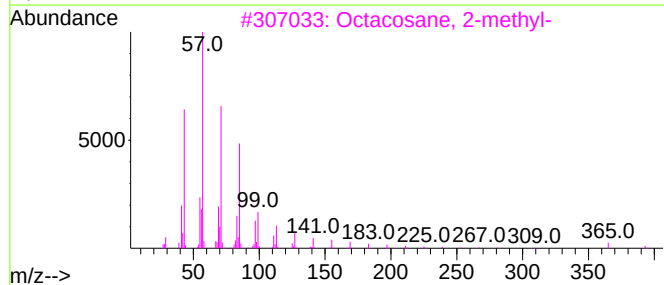
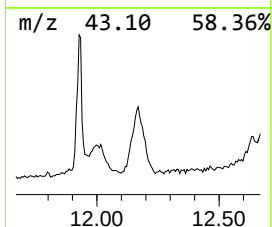
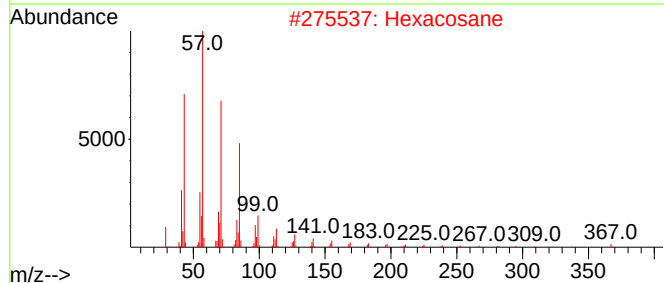
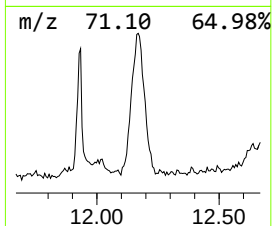
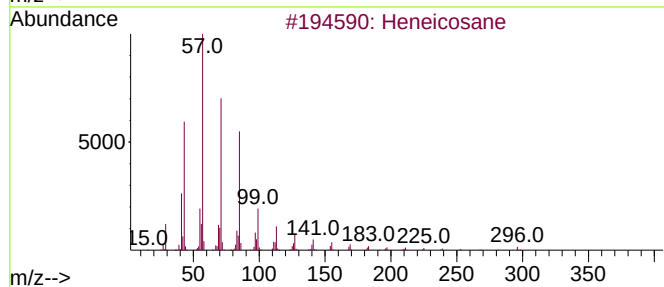
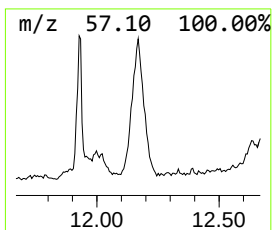
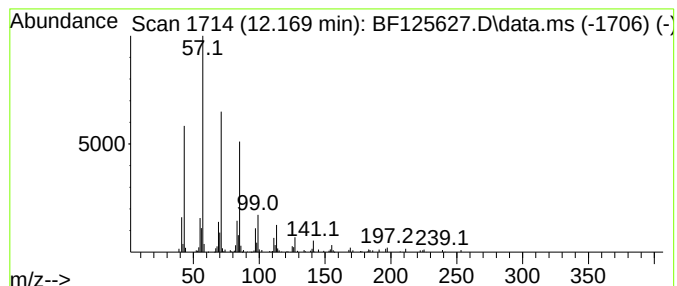
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.169	9.94 ng	832317	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

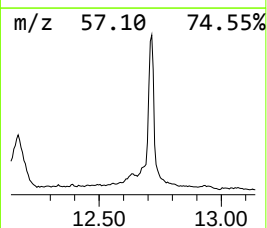
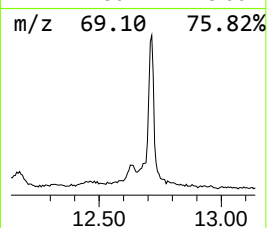
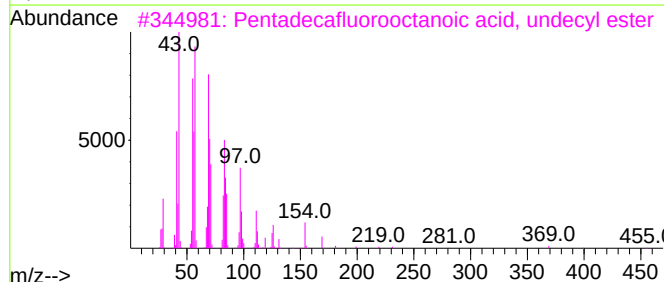
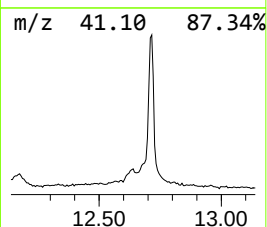
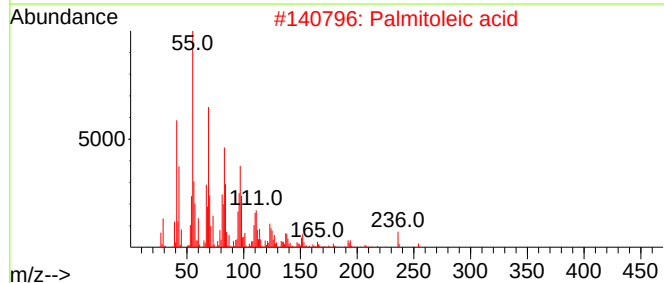
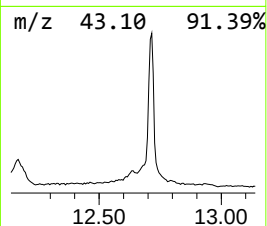
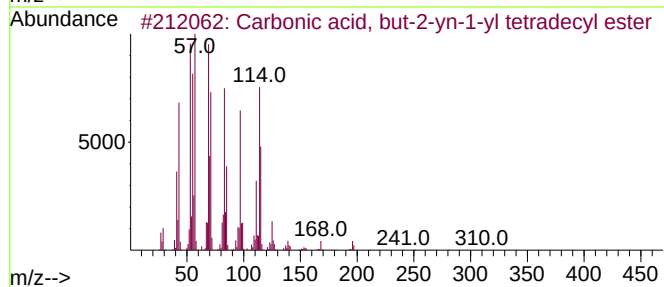
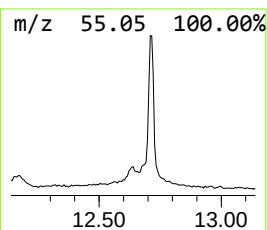
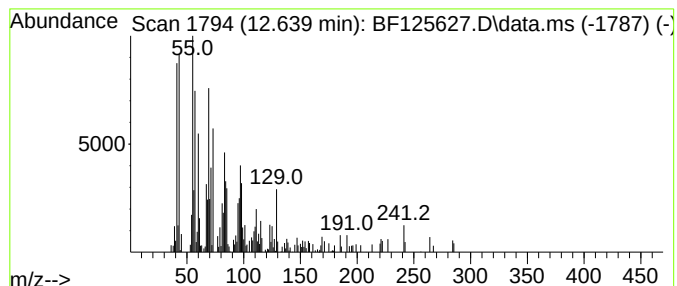
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, but-2-yn-1-y... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.639	4.14 ng	347050	Phenanthrene-d10			11.404
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Carbonic acid, but-2-yn-1-yl tet...		310	C19H34O3	1010383-20-9	53
2	Palmitoleic acid		254	C16H30O2	000373-49-9	50
3	Pentadecafluorooctanoic acid, un...		568	C19H23F15O2	1010406-04-1	49
4	Oleic acid, eicosyl ester		563	C38H74O2	022393-88-0	45
5	1-Hexadecanol, 2-methyl-		256	C17H36O	002490-48-4	44



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
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Sample : M3911-01
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Instrument :
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ClientSampleId :
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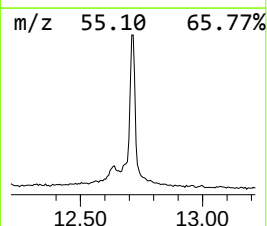
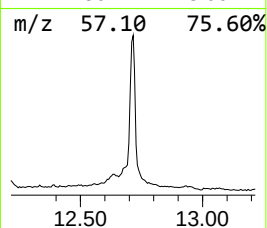
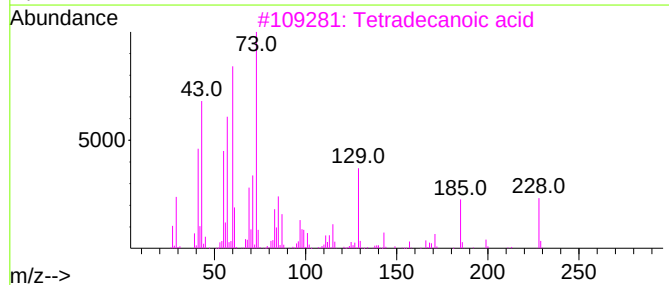
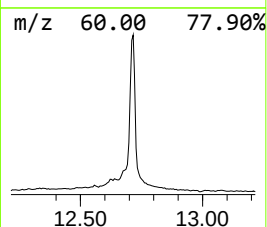
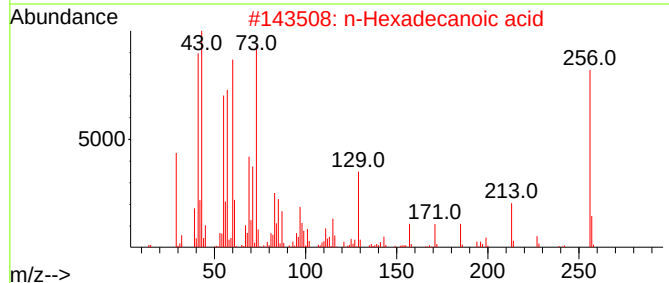
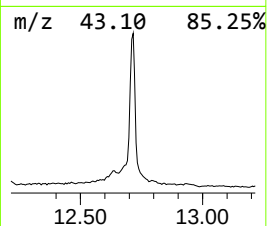
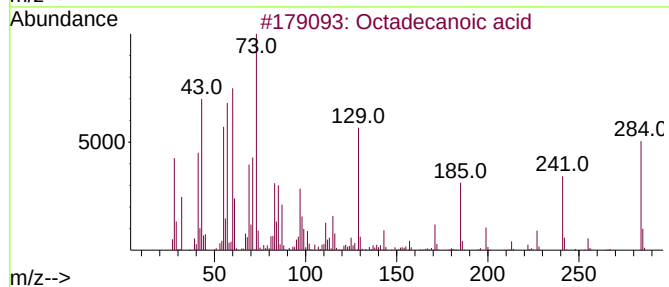
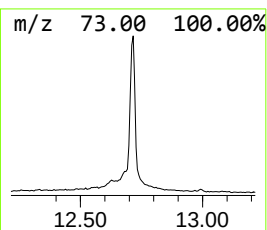
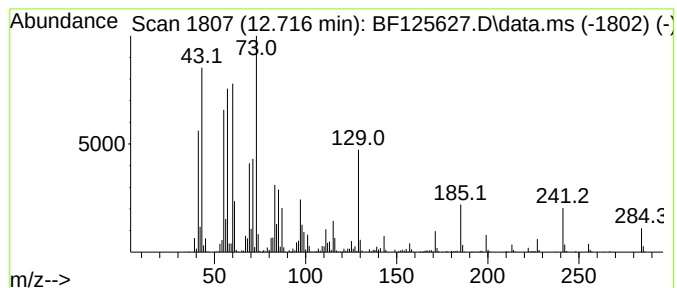
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	39.18 ng	3282040	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
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Operator : JU/CG
Sample : M3911-01
Misc :
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Instrument :
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ClientSampleId :
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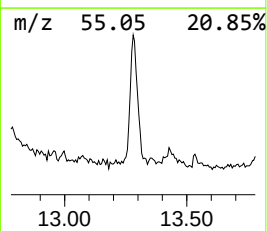
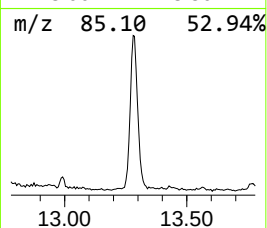
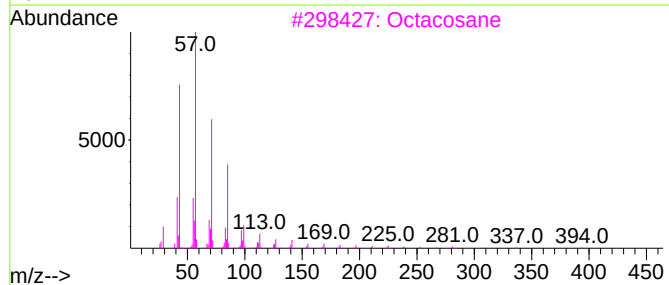
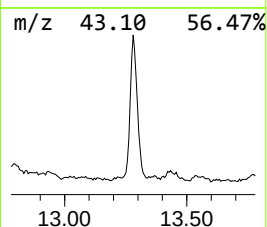
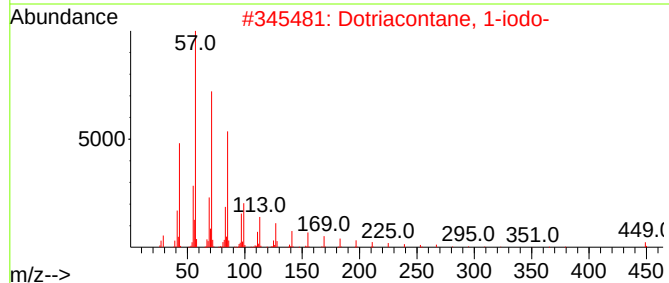
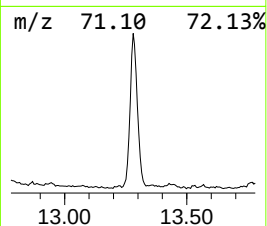
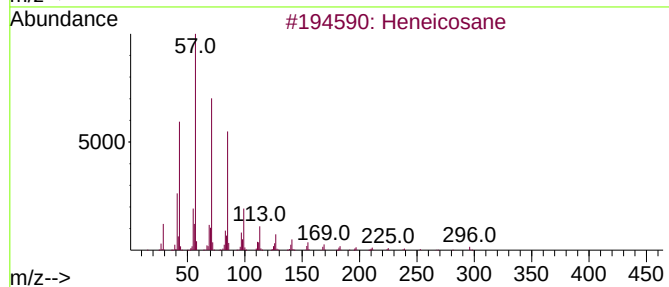
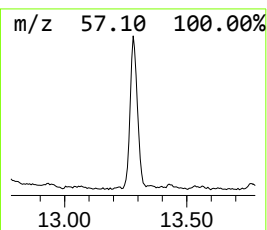
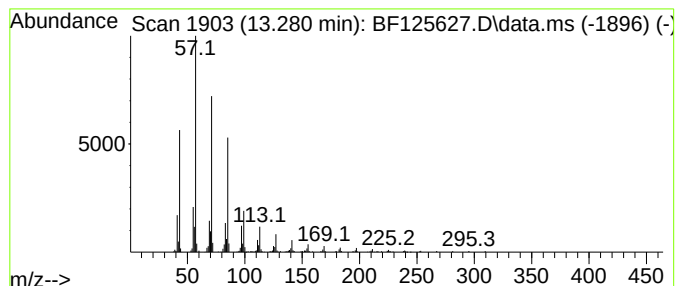
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dotriacontane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.280	21.32 ng	1122460	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3			Octacosane	394	C28H58	000630-02-4	90
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
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Instrument :
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ClientSampleId :
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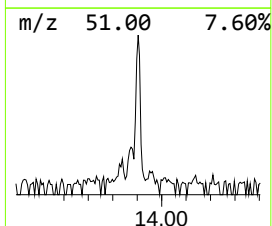
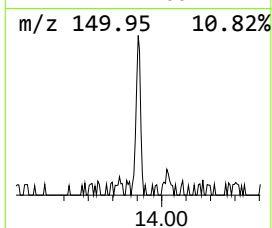
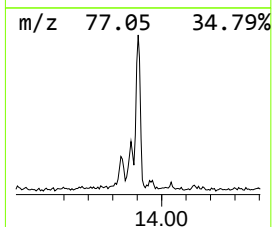
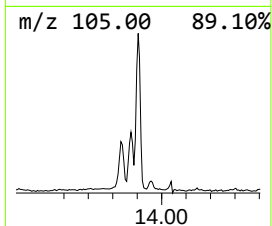
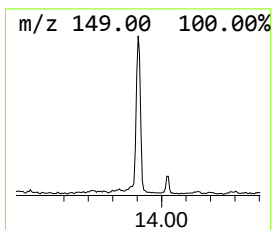
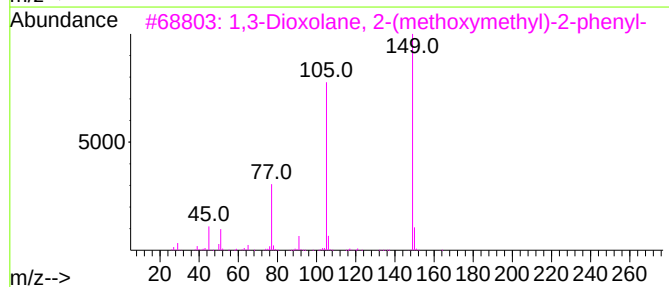
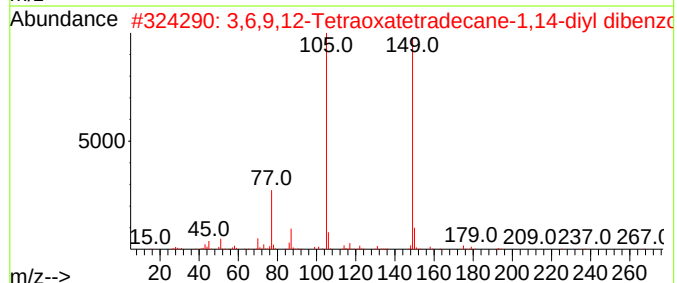
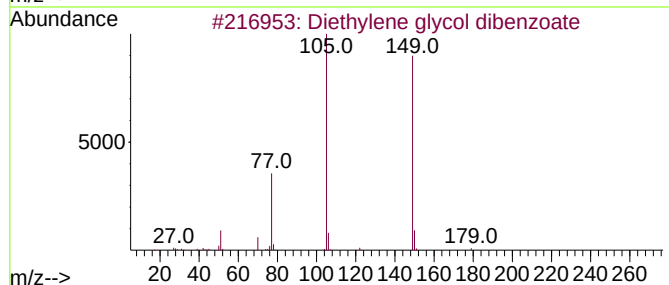
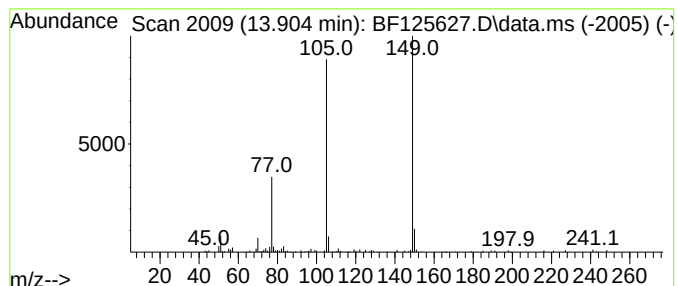
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.43 ng	286109	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
4			Phthalic acid, di(hept-4-yl) ester	362	C22H34O4	1000356-80-0	47
5			N-(5-Pyrimidinyl)benzamide, Ac d...	241	C13H11N3O2	1000504-27-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

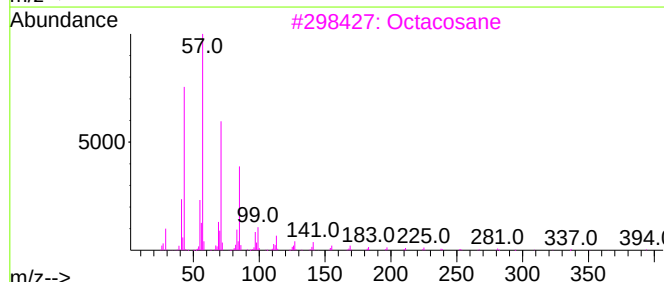
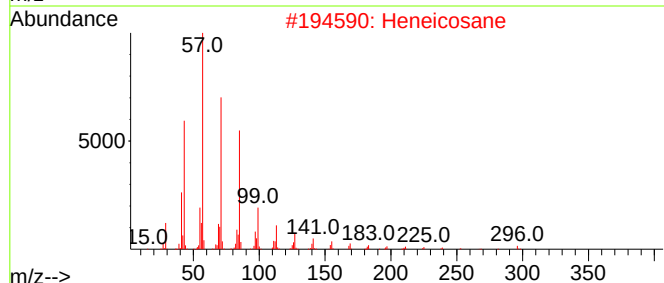
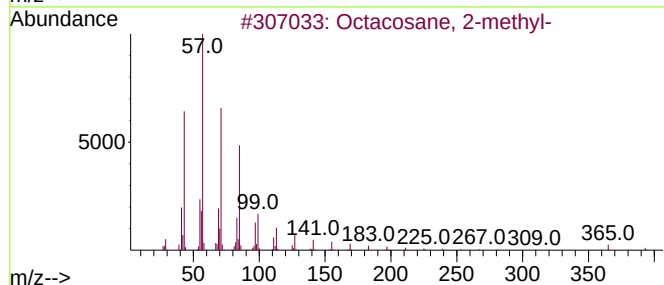
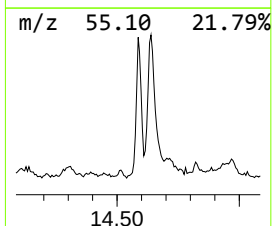
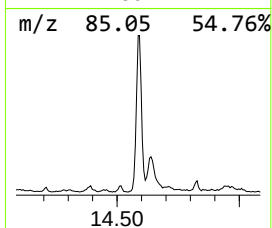
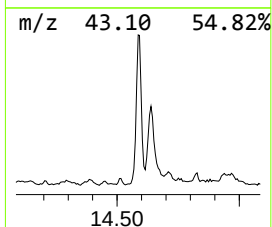
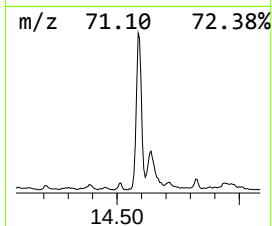
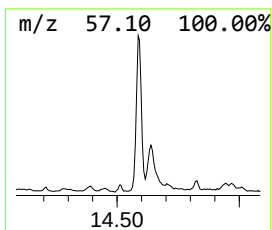
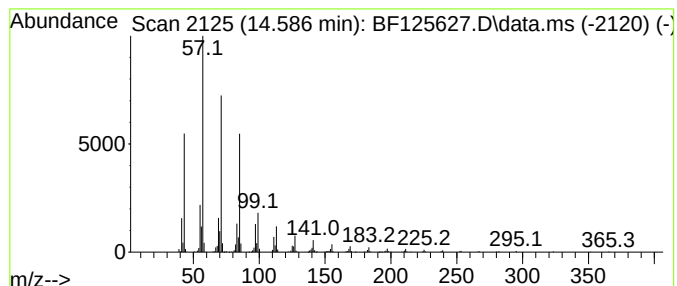
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	22.37 ng	1177820	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
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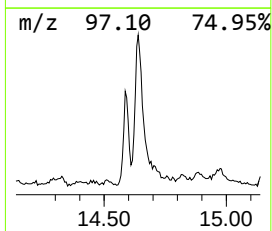
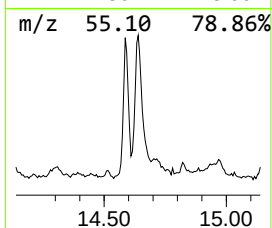
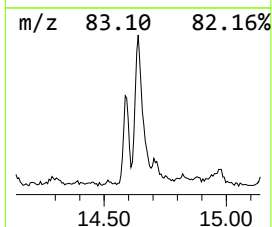
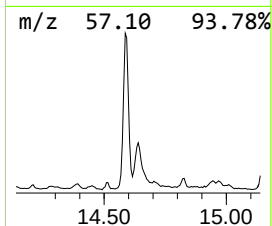
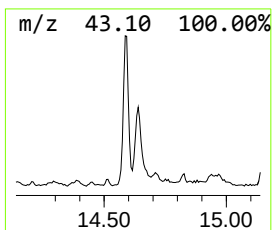
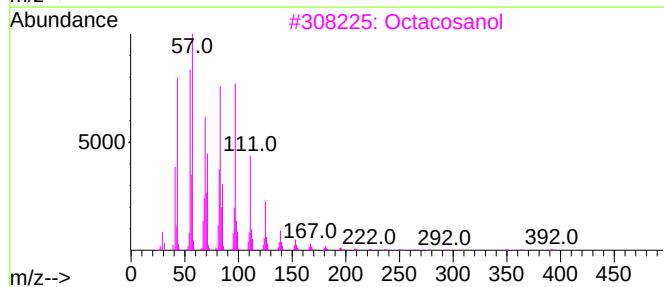
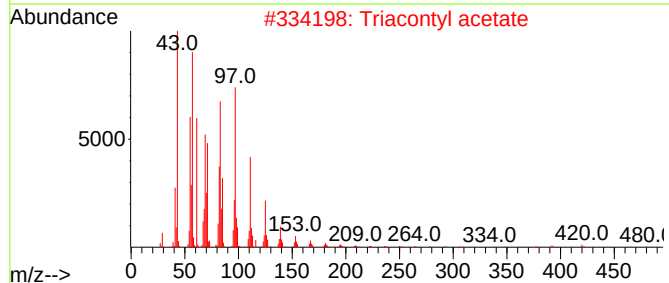
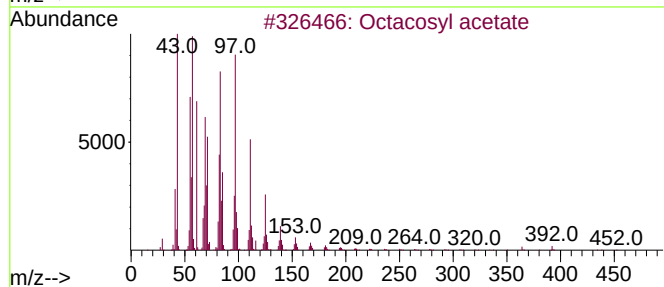
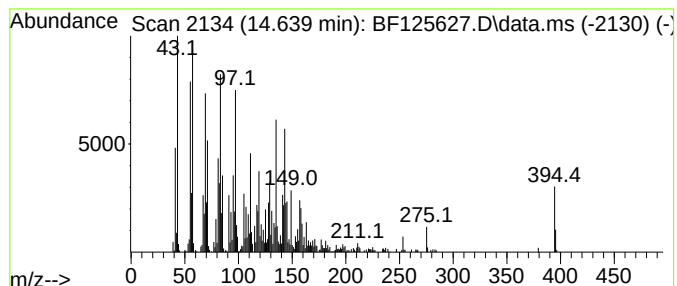
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.639	26.27 ng	1383600	Chrysene-d12		14.039	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosyl acetate		452	C30H60O2	018206-97-8	84
2	Triacontyl acetate		480	C32H64O2	041755-58-2	72
3	Octacosanol		410	C28H58O	000557-61-9	70
4	Triacontan-15-ol		438	C30H62O	031849-26-0	64
5	17-Pentatriacontene		491	C35H70	006971-40-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
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Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

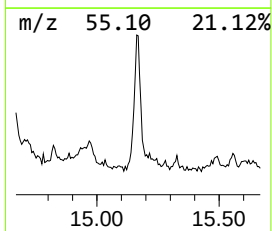
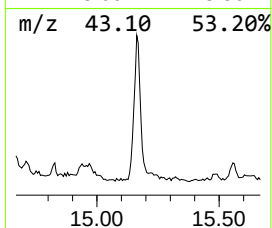
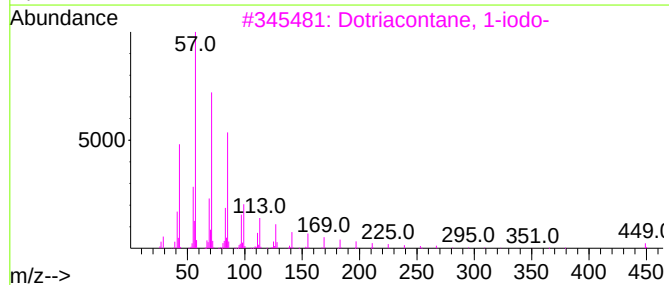
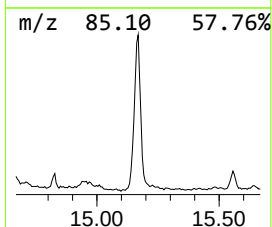
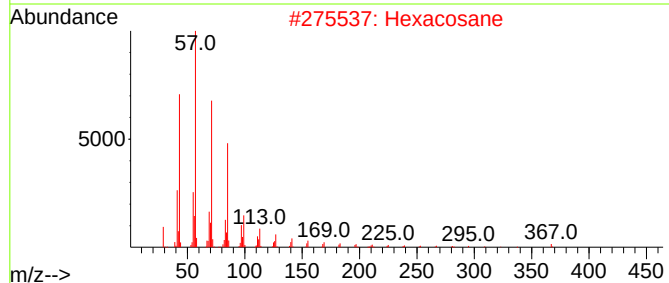
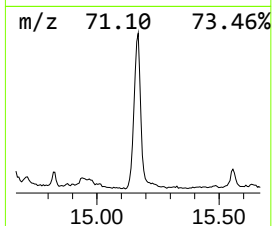
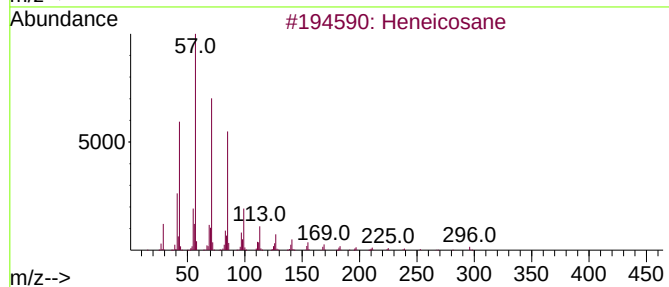
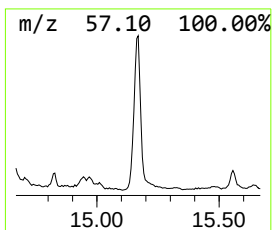
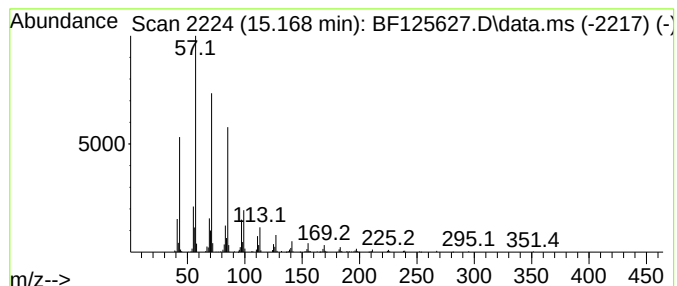
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.168	17.21 ng	1086580	Perylene-d12		15.515	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
4	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91
5	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

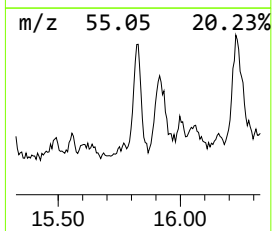
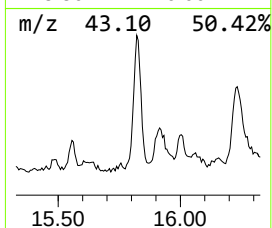
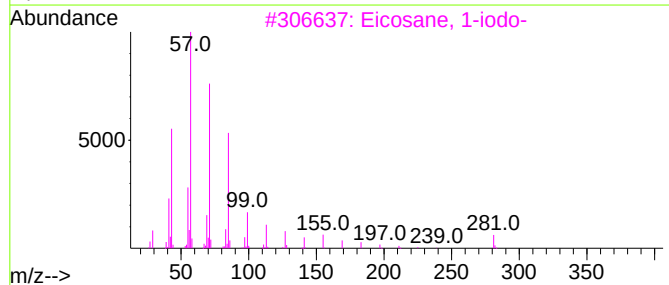
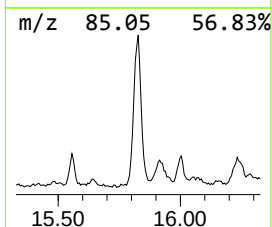
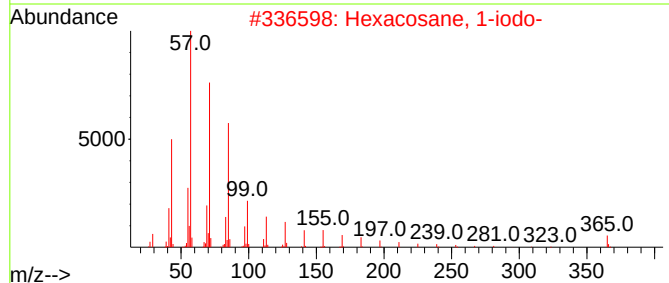
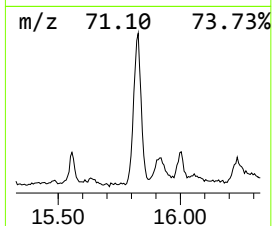
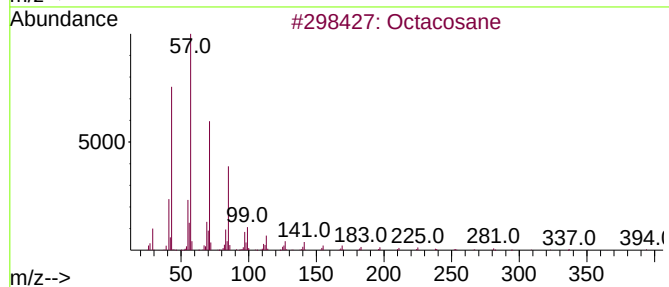
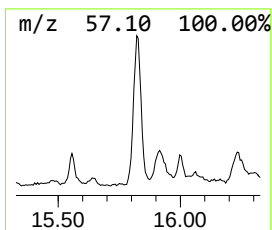
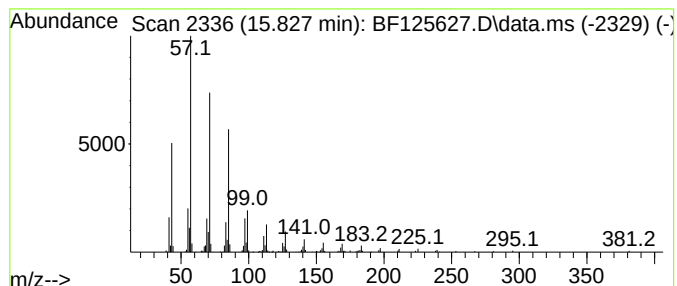
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SW-RR-02-(1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.827	10.04 ng	634131	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

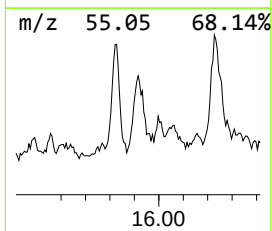
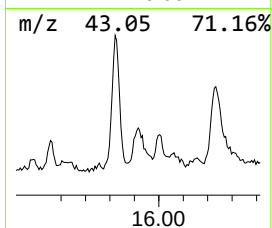
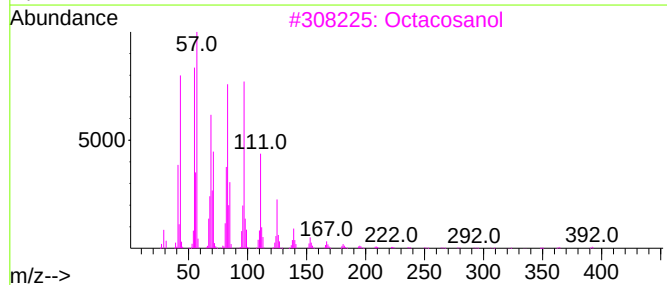
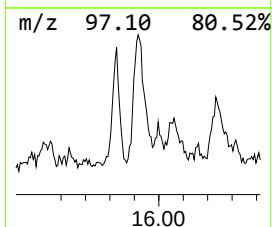
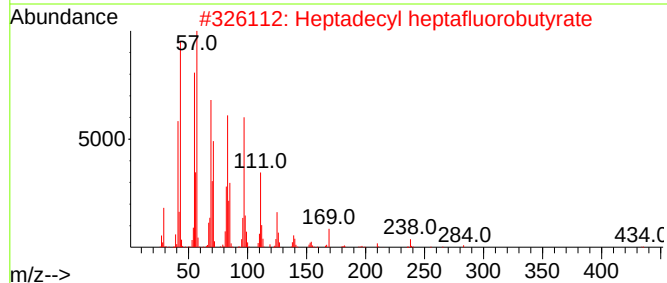
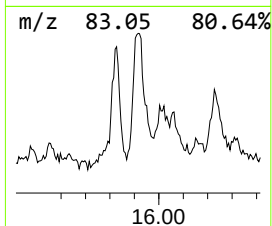
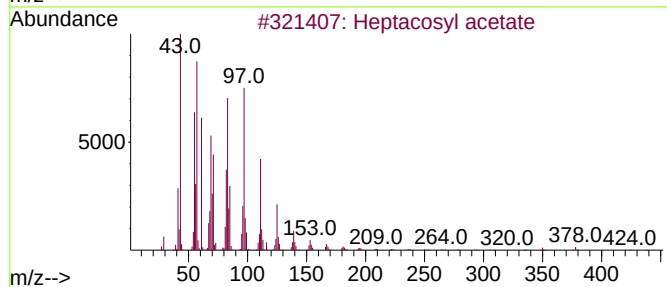
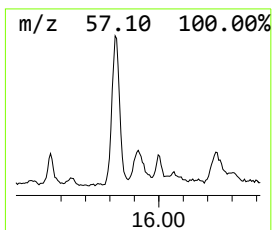
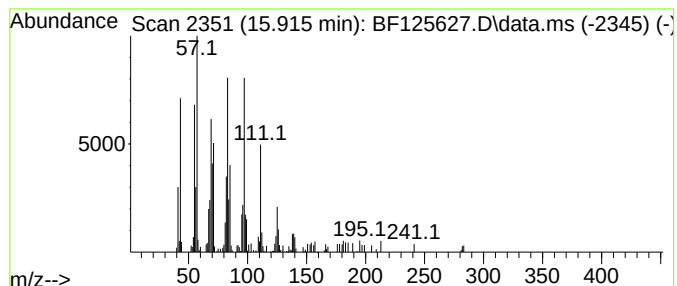
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptacosyl acetate Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.915	5.42 ng	342017	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Tetracosene	336	C24H48	010192-32-2	90
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
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Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

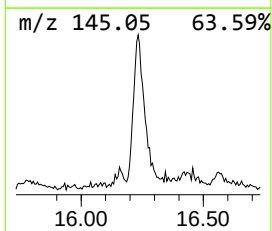
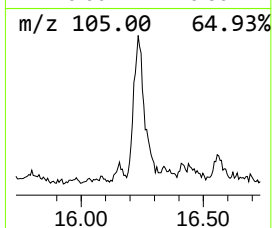
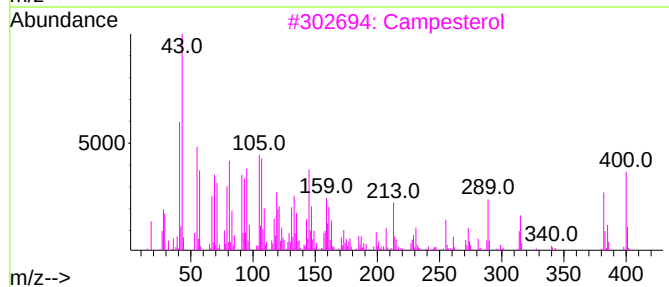
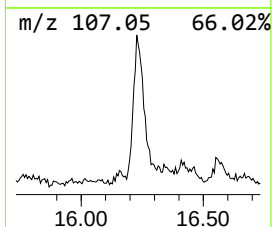
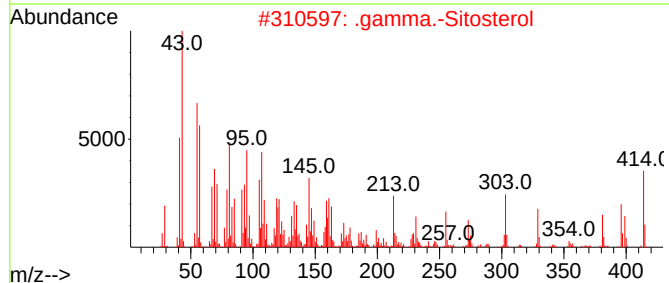
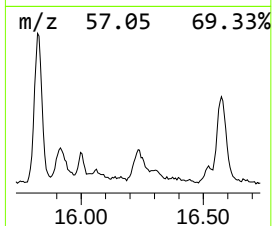
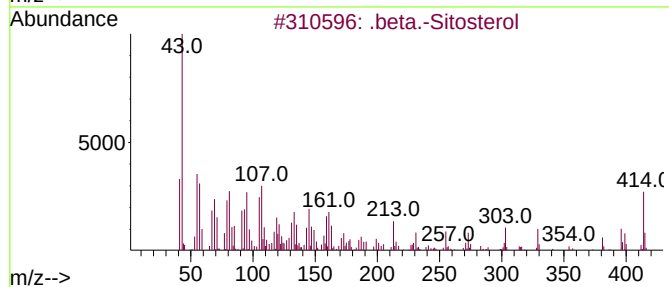
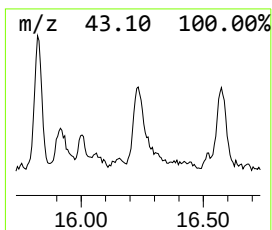
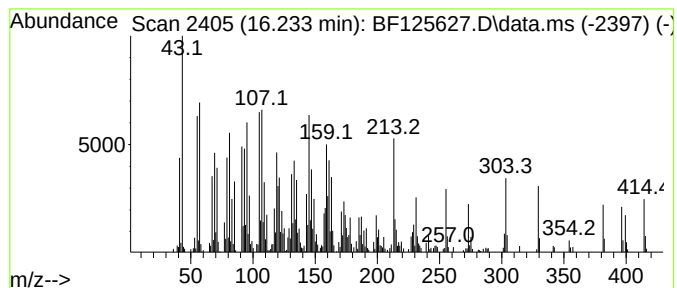
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.233	25.40 ng	1603550	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
3	Campesterol	400	C28H48O	000474-62-4	64
4	5-Cholestene-3-ol, 24-methyl-	400	C28H48O	290299-12-6	58
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	51



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
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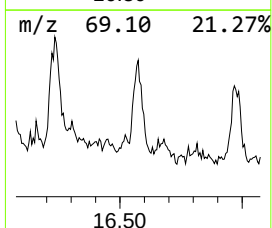
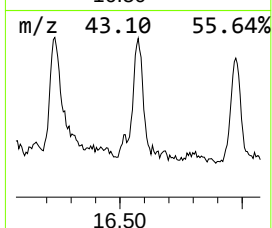
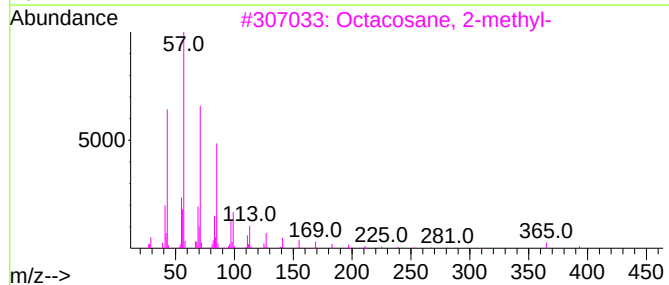
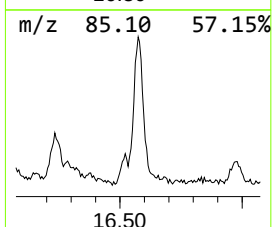
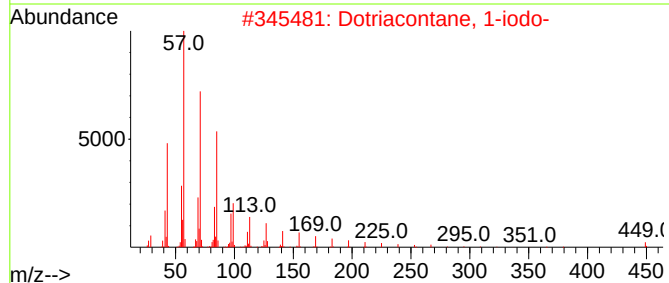
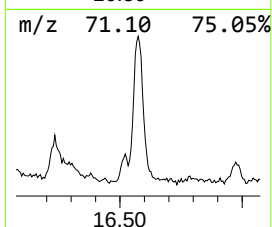
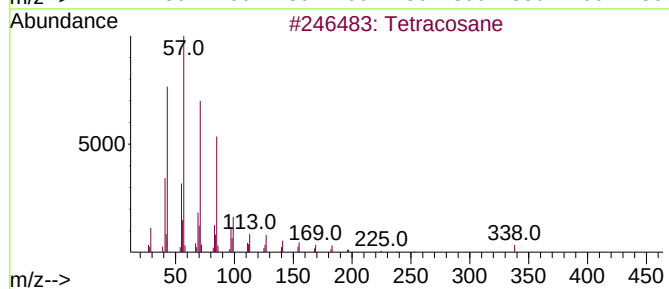
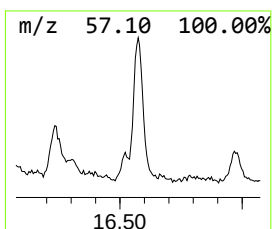
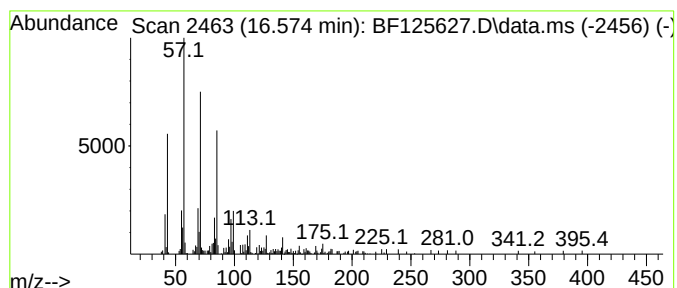
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.574	9.31 ng	587996	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
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Instrument :
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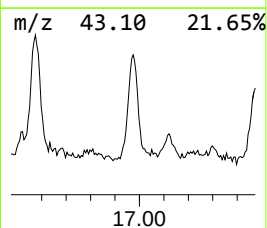
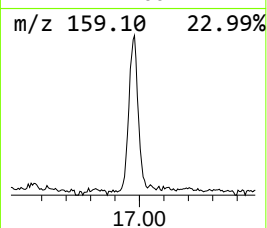
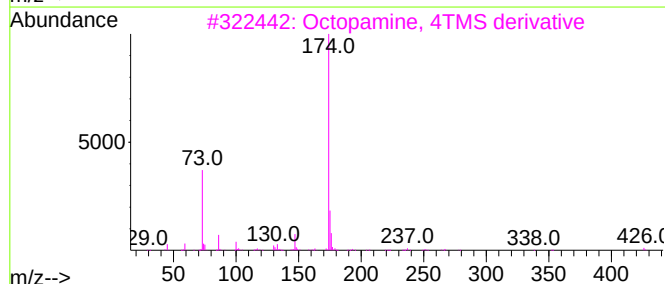
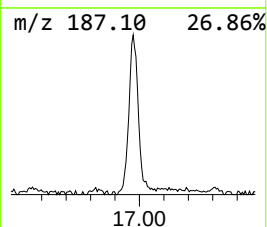
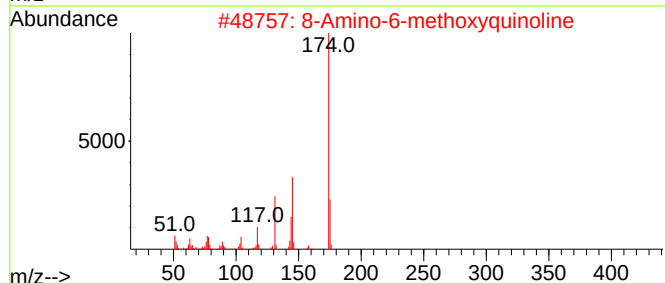
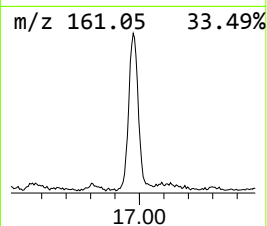
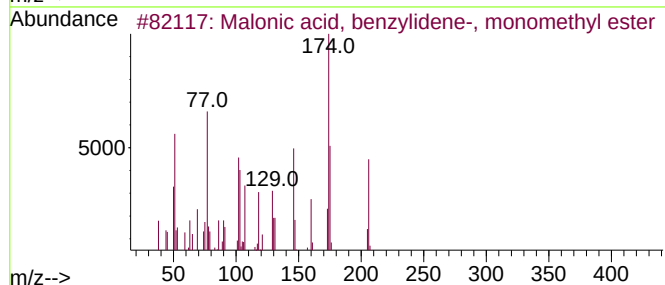
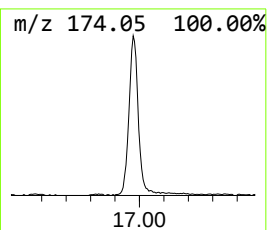
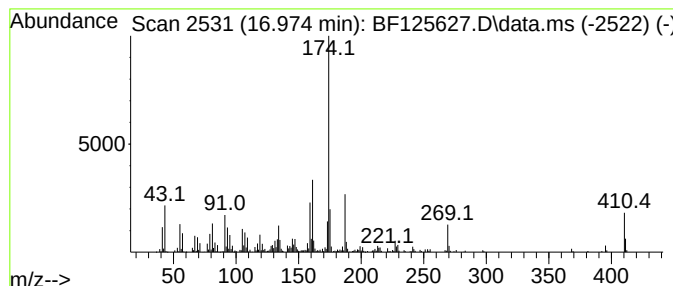
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.974 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.974	20.71 ng	1307660	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Malonic acid, benzylidene-, mono...	206	C11H10O4	022621-53-0	43
2			8-Amino-6-methoxyquinoline	174	C10H10N2O	000090-52-8	43
3			Octopamine, 4TMS derivative	441	C20H43NO2Si4	055556-99-5	38
4			1-(2-Aminoethoxy)-4-benzylbenzen...	371	C21H33NO5i2	1000504-27-0	38
5			3,6-Dimethyl-4-chromone	174	C11H10O2	057646-01-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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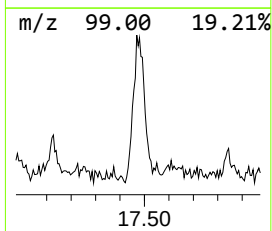
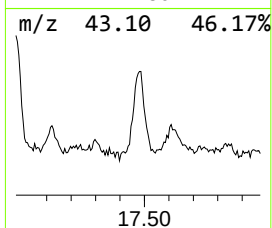
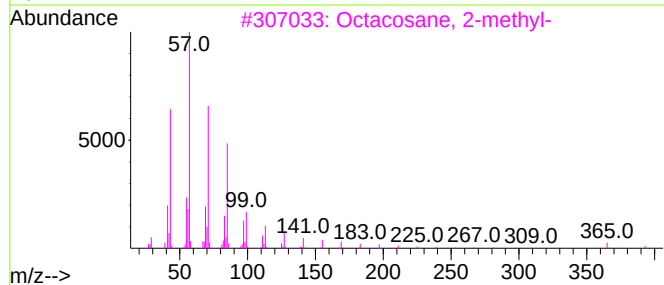
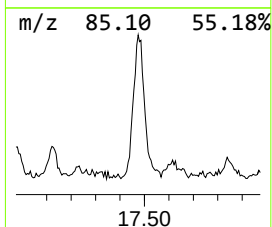
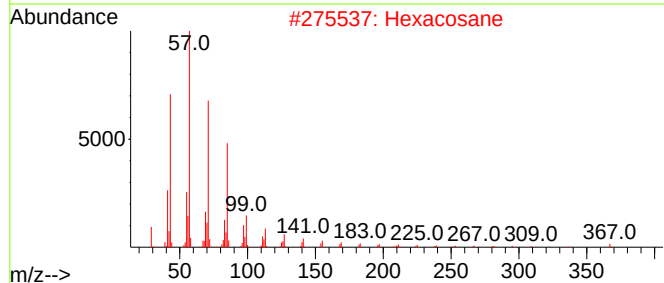
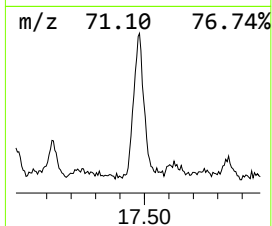
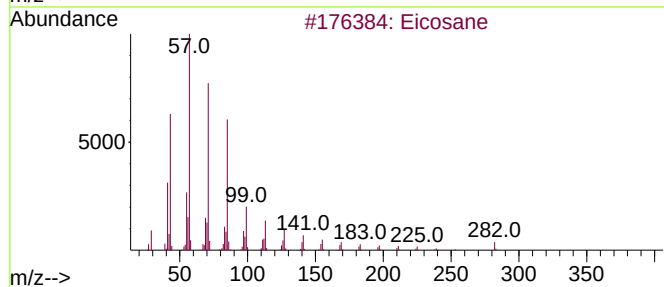
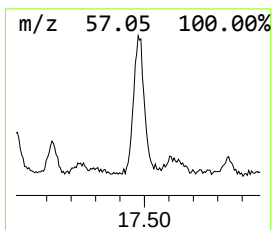
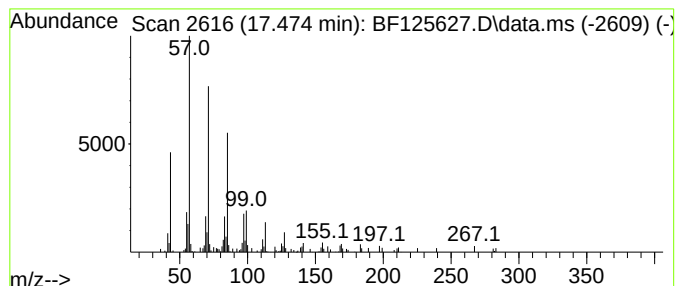
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.474	5.93 ng	374675	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Tetratetracontane	619	C44H90	007098-22-8	90
5			Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-02-(1.0)

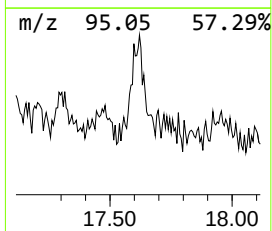
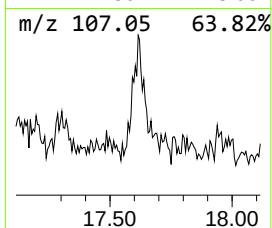
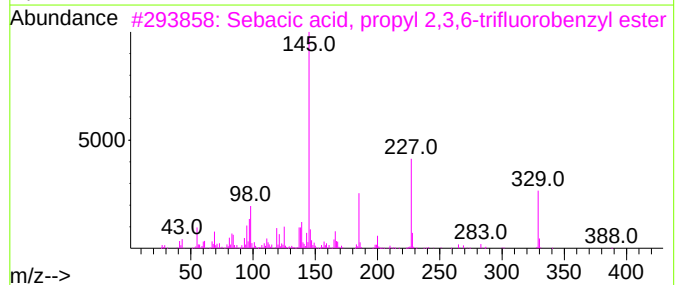
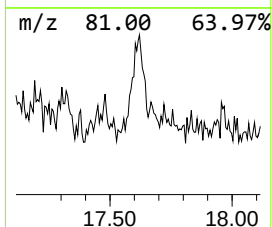
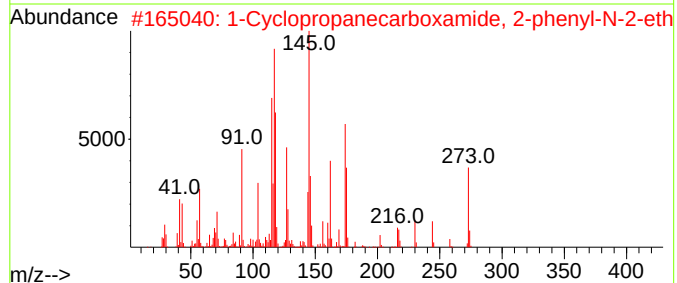
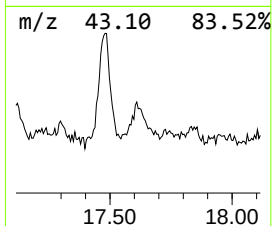
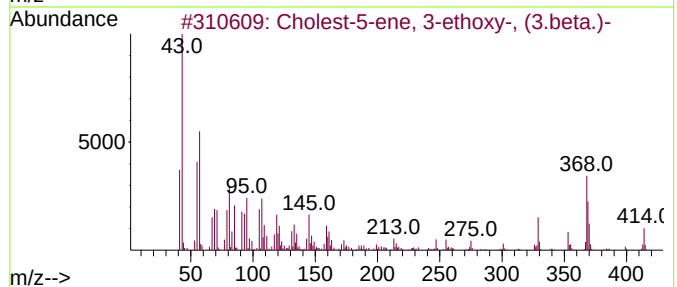
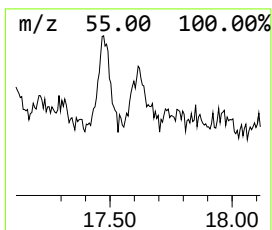
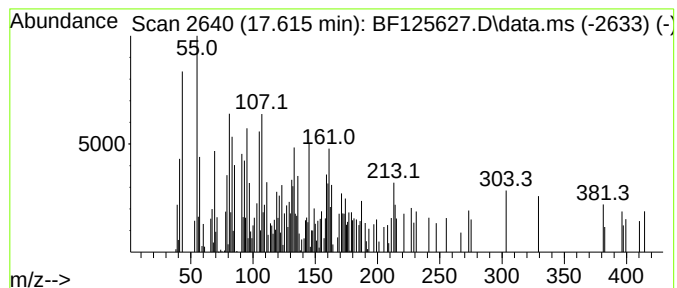
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown17.615 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.615	5.06 ng	319523	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	35
2			1-Cyclopropanecarboxamide, 2-phe...	273	C18H27NO	1000415-24-0	10
3			Sebacic acid, propyl 2,3,6-trifl...	388	C20H27F3O4	1000380-79-1	10
4			((3aR,4S,6E,10Z,11aR)-4-Acetoxy-...	362	C19H22O7	1000494-34-2	10
5			Bicyclo[2.2.1]heptane, 2-cyclopr...	176	C13H20	1000159-45-7	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
Data File : BF125627.D
Acq On : 24 Sep 2021 18:41
Operator : JU/CG
Sample : M3911-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-RR-02-(1.0)

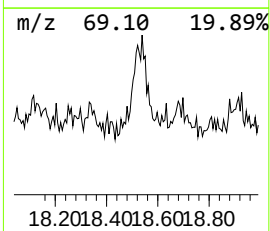
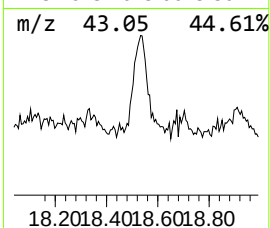
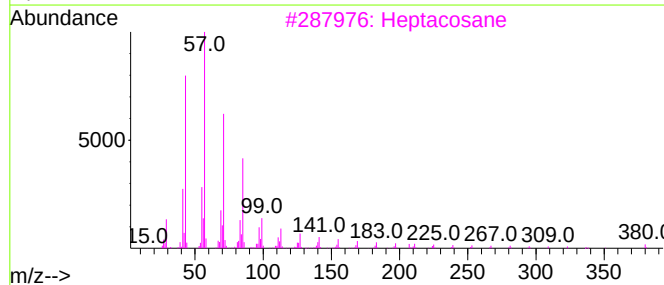
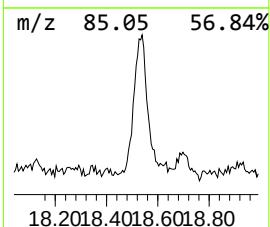
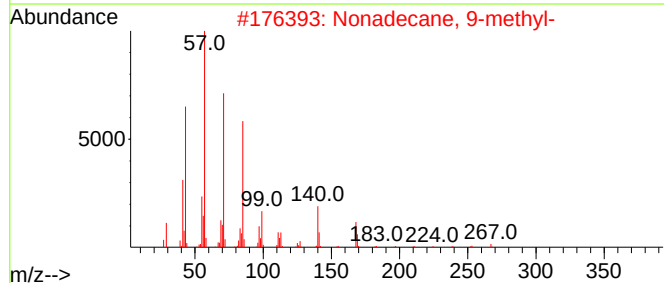
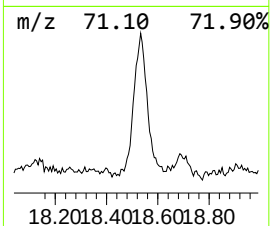
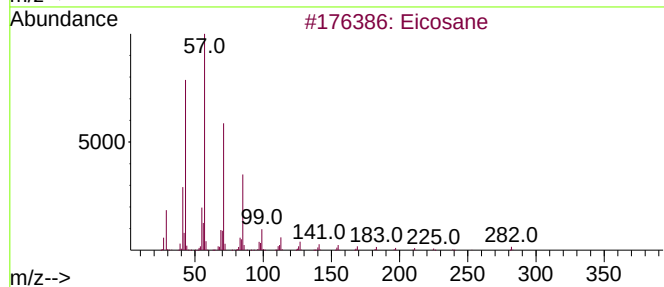
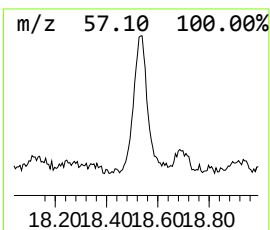
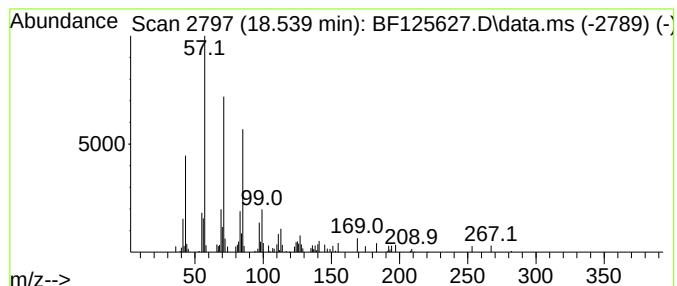
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Nonadecane, 9-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.539	4.46 ng	281599	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	94
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
3		Heptacosane	380	C27H56	000593-49-7	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		2-Methyltetracosane	352	C25H52	001560-78-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
 Data File : BF125627.D
 Acq On : 24 Sep 2021 18:41
 Operator : JU/CG
 Sample : M3911-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-RR-02-(1.0)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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...	2.199	91.1	ng	4986250	1	6.887	1094800	20.0
2(3H)-Benzothia...	10.804	5.2	ng	431268	4	11.404	1675330	20.0
1,4-Benzenedica...	11.157	14.4	ng	1207800	4	11.404	1675330	20.0
n-Hexadecanoic ...	11.933	12.0	ng	1004190	4	11.404	1675330	20.0
Heneicosane	12.169	9.9	ng	832317	4	11.404	1675330	20.0
Carbonic acid, ...	12.639	4.1	ng	347050	4	11.404	1675330	20.0
Octadecanoic acid	12.716	39.2	ng	3282040	4	11.404	1675330	20.0
Dotriacontane, ...	13.280	21.3	ng	1122460	5	14.039	1053190	20.0
Diethylene glyc...	13.904	5.4	ng	286109	5	14.039	1053190	20.0
Octacosane, 2-m...	14.586	22.4	ng	1177820	5	14.039	1053190	20.0
Octacosyl acetate	14.639	26.3	ng	1383600	5	14.039	1053190	20.0
Hexacosane	15.168	17.2	ng	1086580	6	15.515	1262770	20.0
Octacosane	15.827	10.0	ng	634131	6	15.515	1262770	20.0
Heptacosyl acetate	15.915	5.4	ng	342017	6	15.515	1262770	20.0
.beta.-Sitosterol	16.233	25.4	ng	1603550	6	15.515	1262770	20.0
Tetracosane	16.574	9.3	ng	587996	6	15.515	1262770	20.0
unknown16.974	16.974	20.7	ng	1307660	6	15.515	1262770	20.0
Eicosane	17.474	5.9	ng	374675	6	15.515	1262770	20.0
unknown17.615	17.615	5.1	ng	319523	6	15.515	1262770	20.0
Nonadecane, 9-m...	18.539	4.5	ng	281599	6	15.515	1262770	20.0