

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125928.D
 Acq On : 26 Oct 2021 11:37
 Operator : JU/CG
 Sample : M4313-07
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1-3-TOTES

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125928.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	9	21	26	rVB	4757707	7443885	100.00%	18.968%
2	5.081	501	509	524	rBV	85365	148325	1.99%	0.378%
3	5.481	572	577	592	rBV	1454889	1472860	19.79%	3.753%
4	6.475	743	746	753	rBV	1009043	936269	12.58%	2.386%
5	6.863	809	812	815	rBV	1150269	994811	13.36%	2.535%
6	7.422	902	907	910	rBV	2157926	2081416	27.96%	5.304%
7	8.057	1010	1015	1018	rBV	1967046	1680874	22.58%	4.283%
8	8.151	1026	1031	1034	rBV	1343454	1313496	17.65%	3.347%
9	8.328	1057	1061	1066	rVB	86818	84037	1.13%	0.214%
10	8.422	1074	1077	1080	rVV	229207	181540	2.44%	0.463%
11	9.228	1208	1214	1217	rBV	3206493	3077256	41.34%	7.841%
12	9.863	1316	1322	1324	rBV	308615	309980	4.16%	0.790%
13	9.904	1324	1329	1332	rVB	1688968	1449832	19.48%	3.694%
14	10.104	1360	1363	1366	rVB	366162	293320	3.94%	0.747%
15	10.222	1380	1383	1386	rVV	234027	201471	2.71%	0.513%
16	10.686	1458	1462	1465	rVB	2388838	2042963	27.44%	5.206%
17	11.186	1543	1547	1551	rVB	1205970	945505	12.70%	2.409%
18	11.263	1557	1560	1571	rVB6	44947	79353	1.07%	0.202%
19	11.386	1577	1581	1585	rVV	1818287	1545587	20.76%	3.938%
20	11.451	1588	1592	1596	rBV2	130016	132898	1.79%	0.339%
21	11.786	1646	1649	1652	rVB	180550	148005	1.99%	0.377%
22	11.922	1665	1672	1683	rBV	1132005	1421982	19.10%	3.623%
23	12.080	1696	1699	1705	rVB5	113420	151288	2.03%	0.385%
24	12.704	1800	1805	1813	rBV	461839	537978	7.23%	1.371%
25	12.869	1826	1833	1843	rVB3	179882	487439	6.55%	1.242%
26	12.974	1847	1851	1854	rBV	3253269	3016209	40.52%	7.686%
27	13.533	1940	1946	1949	rBV5	36704	78895	1.06%	0.201%
28	13.739	1975	1981	1990	rBV2	171767	425682	5.72%	1.085%
29	13.874	1999	2004	2013	rVB2	1144547	1283930	17.25%	3.272%
30	14.027	2025	2030	2033	rBV	1363030	1310842	17.61%	3.340%
31	14.386	2085	2091	2094	rBV2	203470	383037	5.15%	0.976%
32	14.427	2094	2098	2108	rVV6	231417	583086	7.83%	1.486%
33	14.510	2109	2112	2120	rVB2	156624	185401	2.49%	0.472%
34	14.821	2162	2165	2171	rVB2	81803	106626	1.43%	0.272%
35	14.962	2183	2189	2198	rBV2	126953	290260	3.90%	0.740%
36	15.162	2220	2223	2231	rVB	86784	136761	1.84%	0.348%

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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-BF102521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.492	2274	2279	2285	rVB2	761816	937841	12.60%	2.390%
38	15.551	2285	2289	2293	rBV	72230	112663	1.51%	0.287%
39	15.615	2295	2300	2307	rVV3	86666	191326	2.57%	0.488%
40	15.680	2307	2311	2318	rVB4	63915	131563	1.77%	0.335%
41	15.998	2357	2365	2369	rBV4	292871	675571	9.08%	1.721%
42	16.039	2369	2372	2377	rVB3	153500	233229	3.13%	0.594%

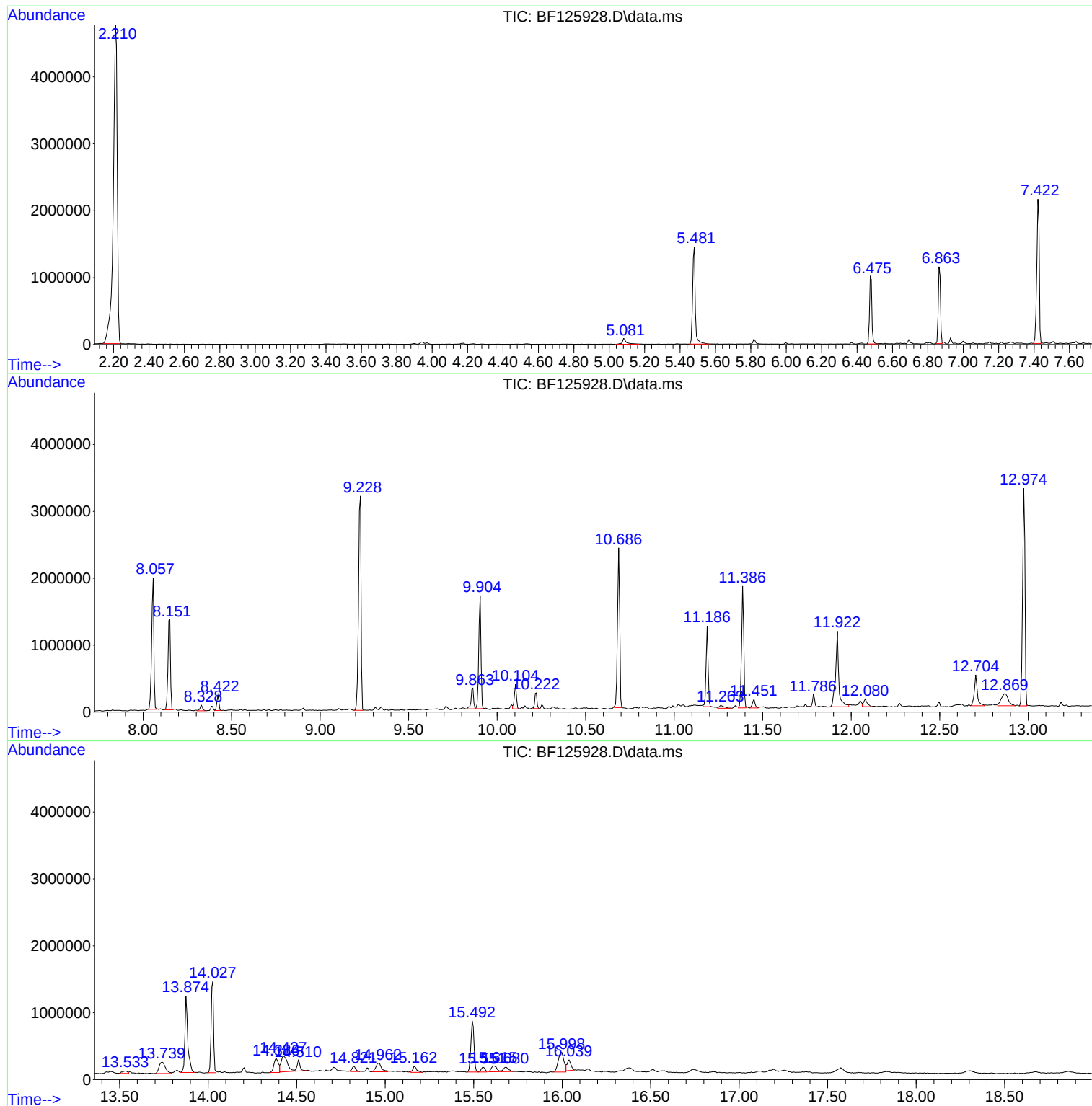
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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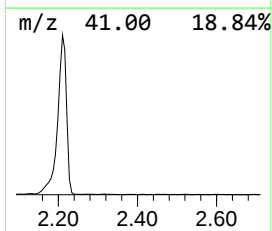
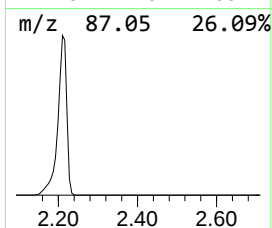
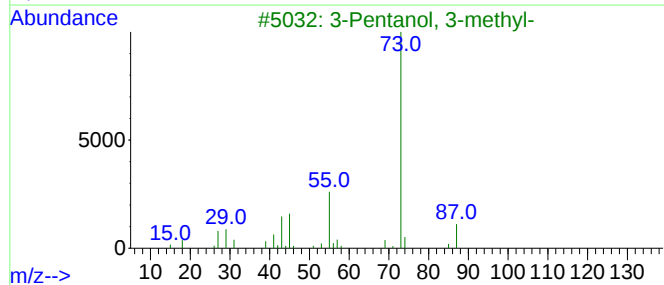
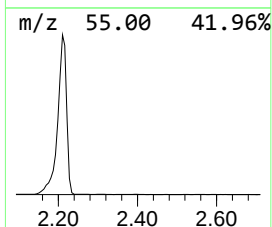
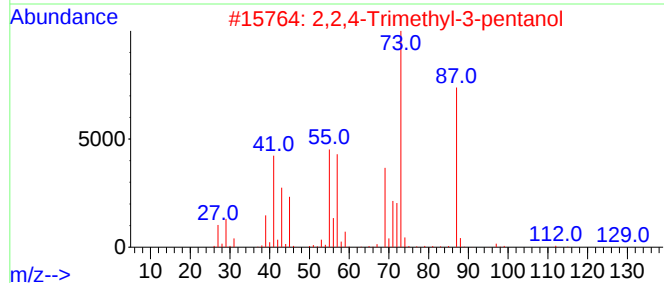
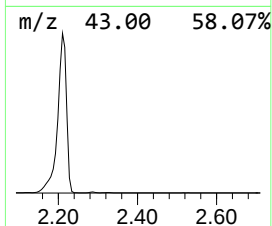
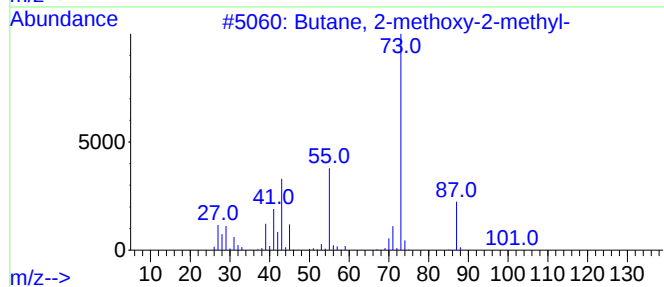
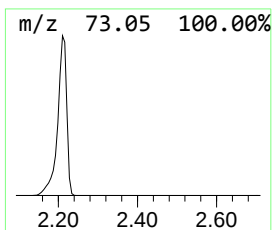
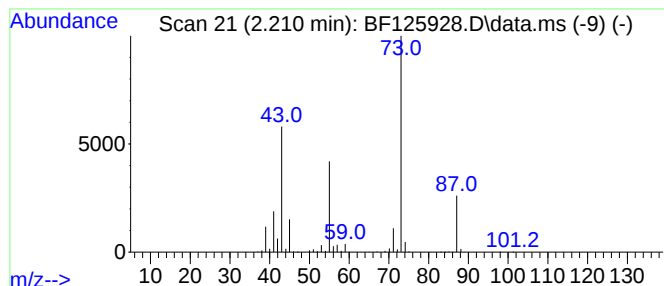
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	149.65 ng	7443890	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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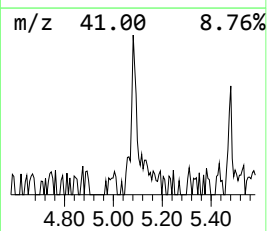
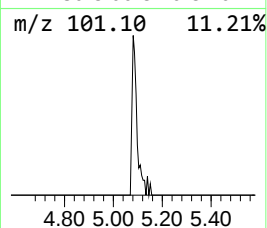
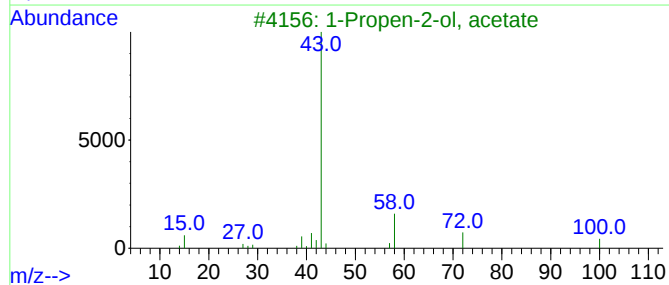
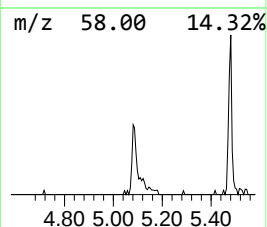
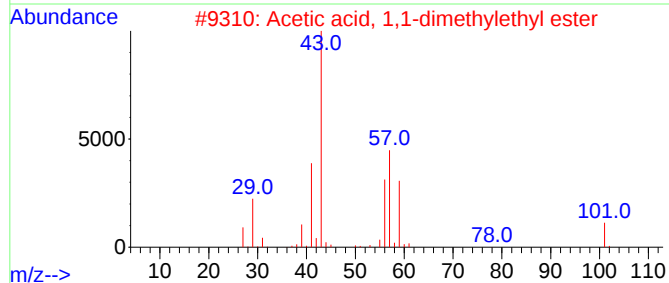
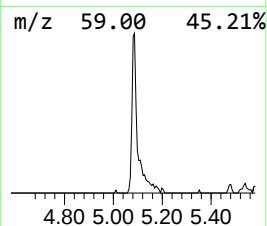
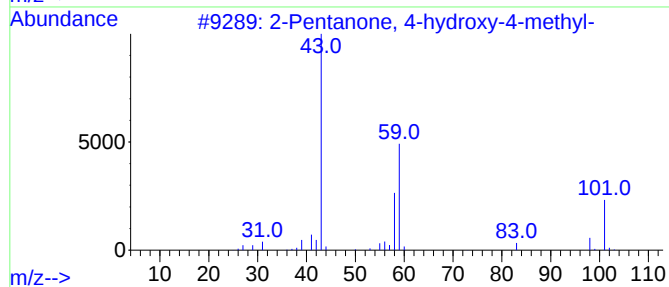
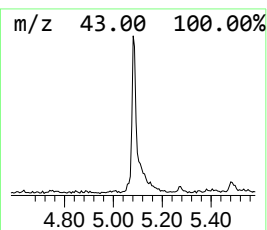
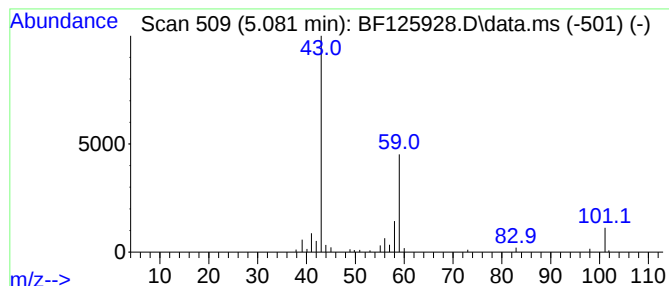
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	2.98 ng	148325	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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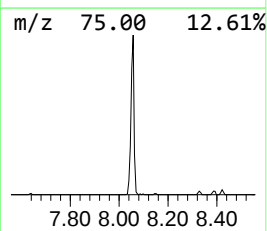
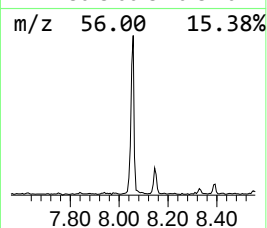
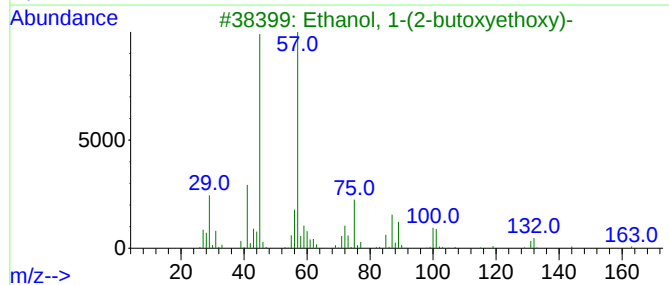
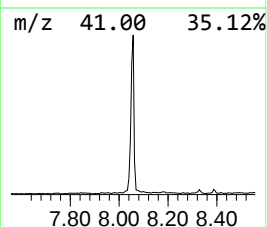
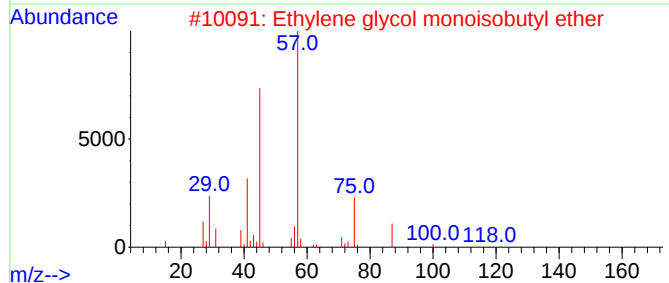
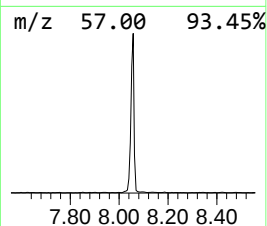
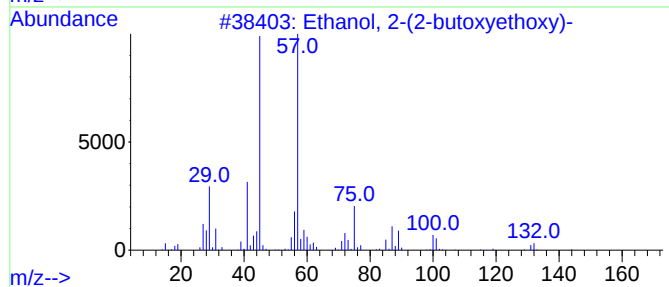
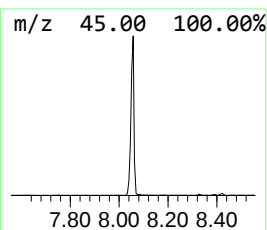
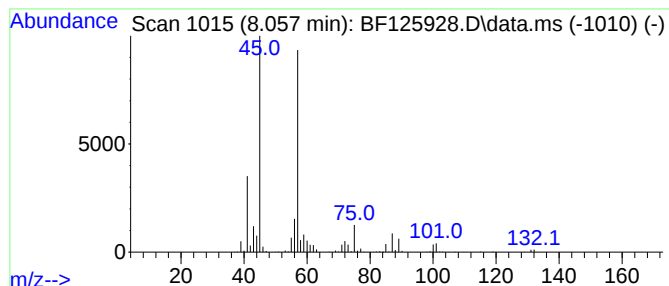
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	25.59 ng	1680870	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			Butyl lactate	146	C7H14O3	000138-22-7	50
5			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47



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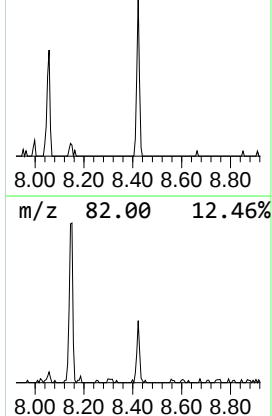
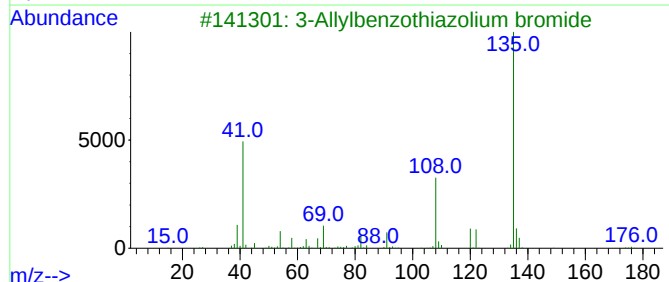
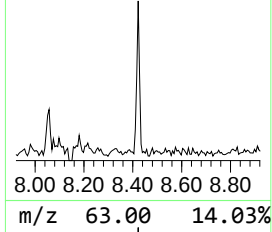
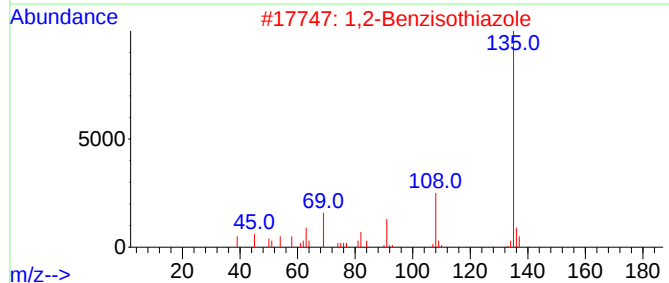
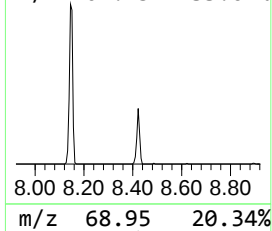
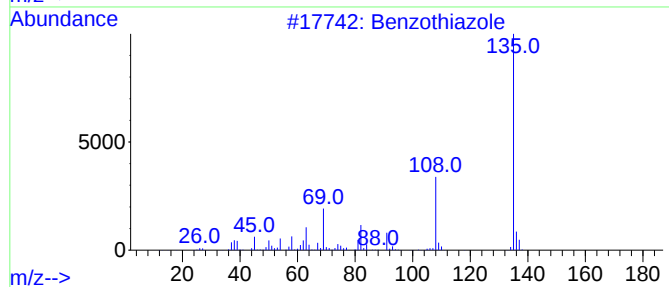
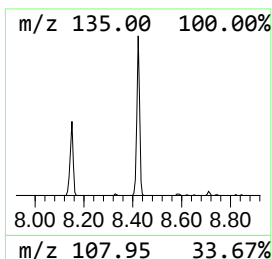
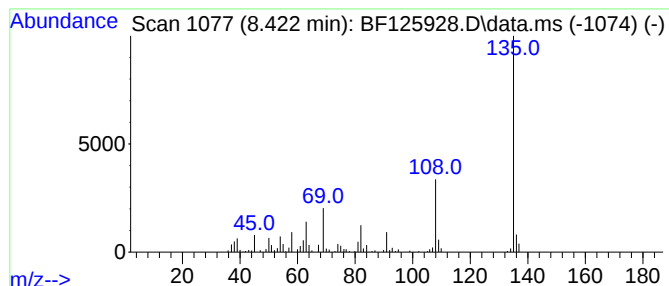
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzothiazole Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.422	2.76 ng	181540	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole	135	C7H5NS	000095-16-9	95
2			1,2-Benzisothiazole	135	C7H5NS	000272-16-2	80
3			3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
4			Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	50
5			1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	50



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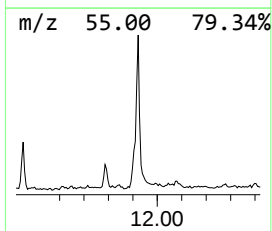
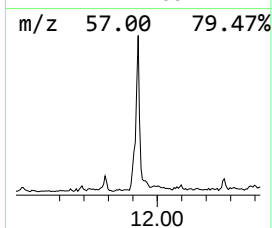
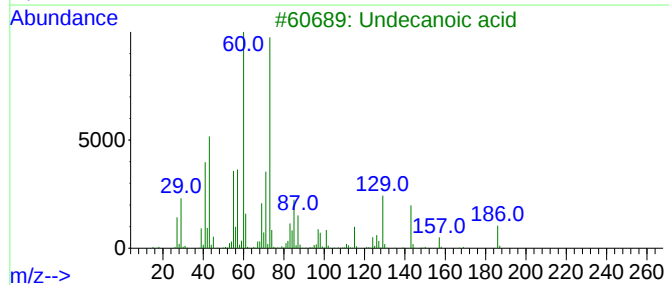
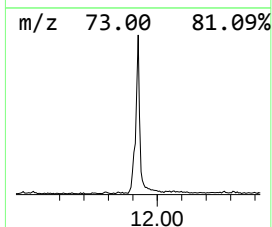
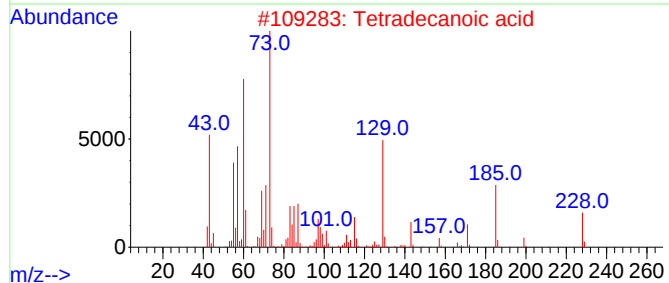
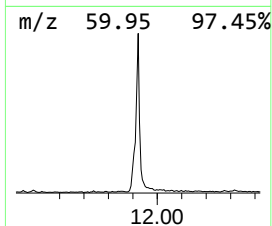
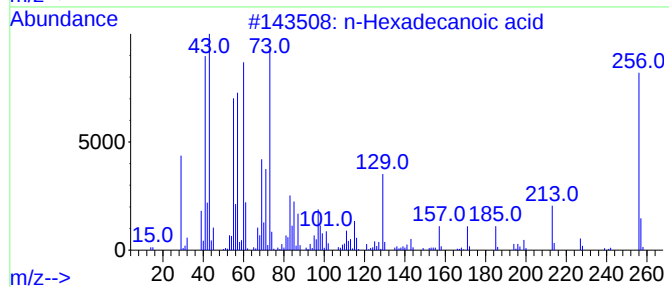
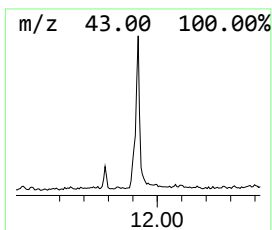
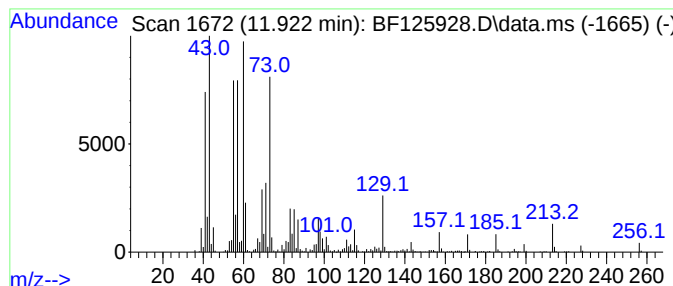
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	18.40 ng	1421980	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
3			Undecanoic acid	186	C11H22O2	000112-37-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-TOTES

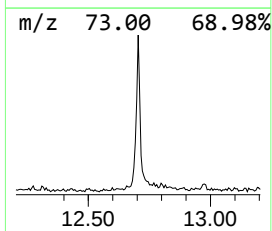
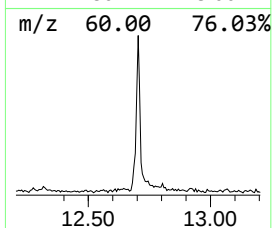
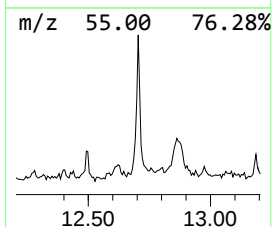
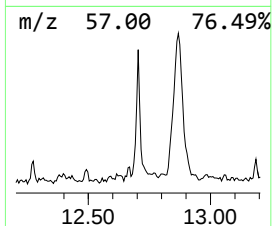
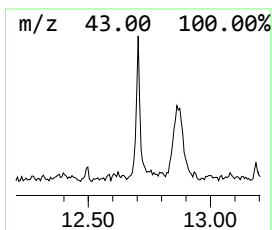
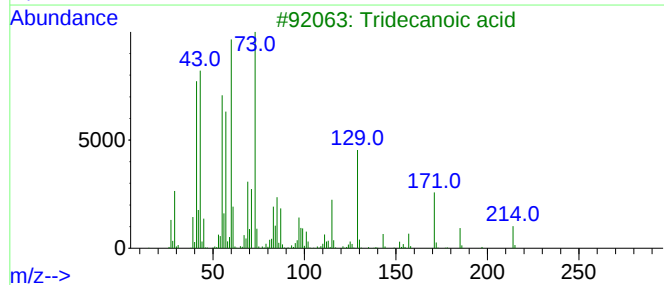
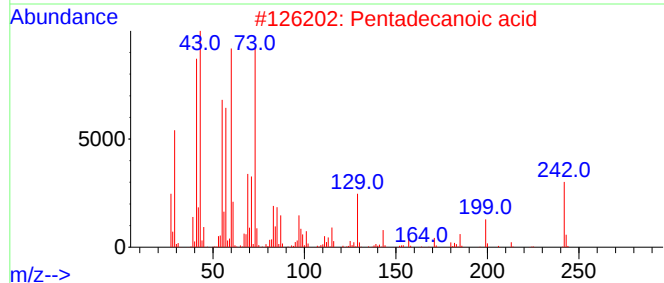
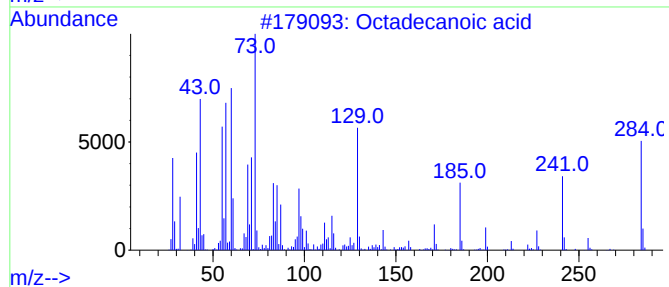
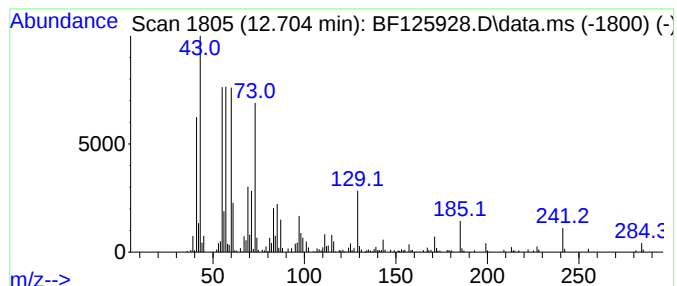
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.96 ng	537978	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
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Instrument :
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ClientSampleId :
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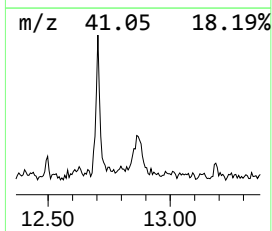
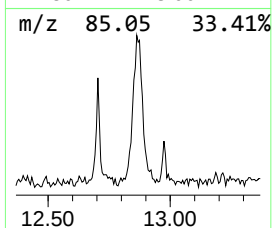
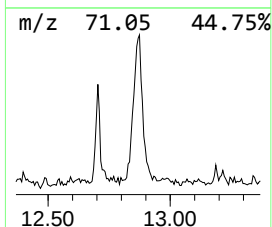
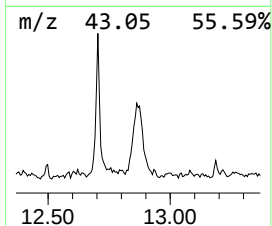
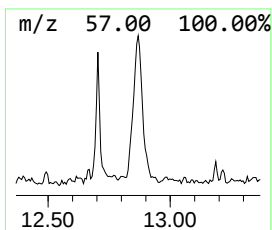
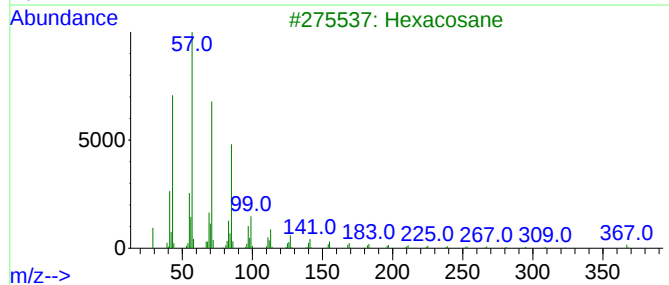
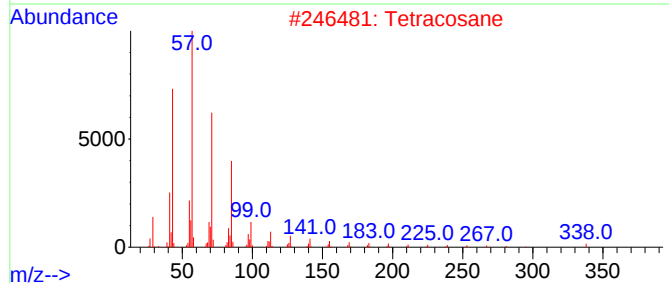
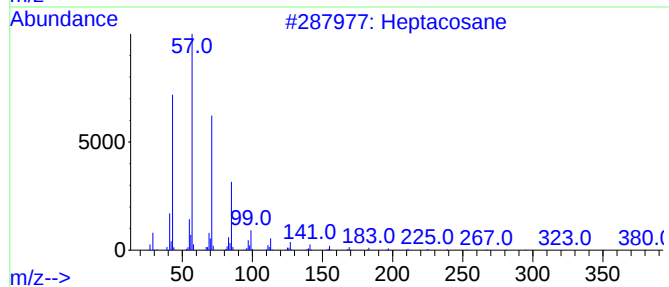
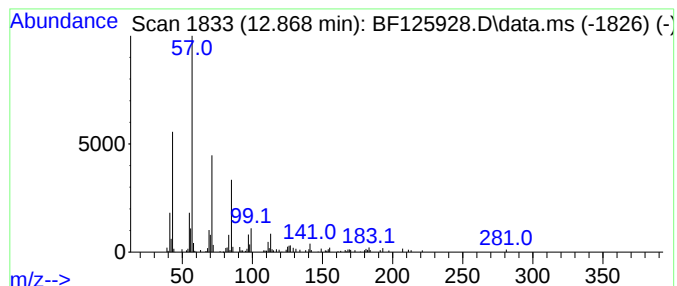
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.868	7.44 ng	487439	Chrysene-d12	14.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	86
2		Tetracosane	338	C24H50	000646-31-1	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		Eicosane	282	C20H42	000112-95-8	83
5		Pentadecane	212	C15H32	000629-62-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-TOTES

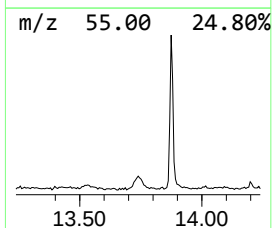
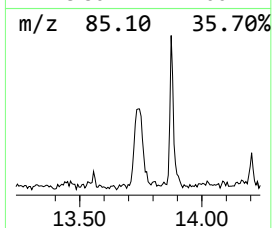
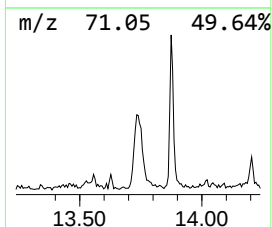
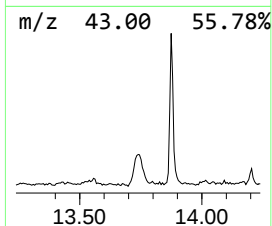
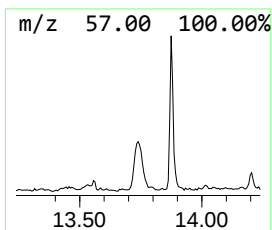
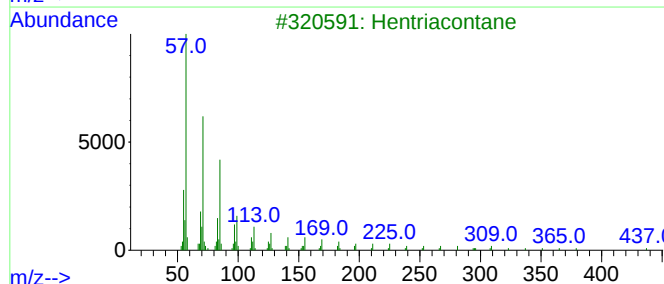
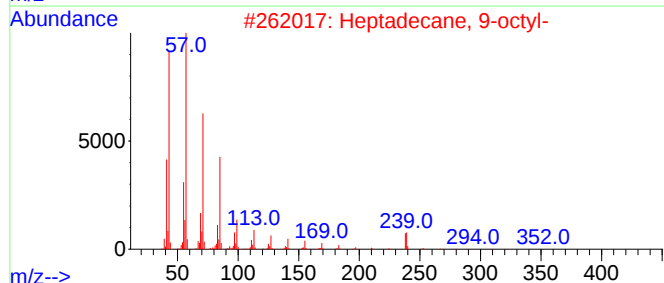
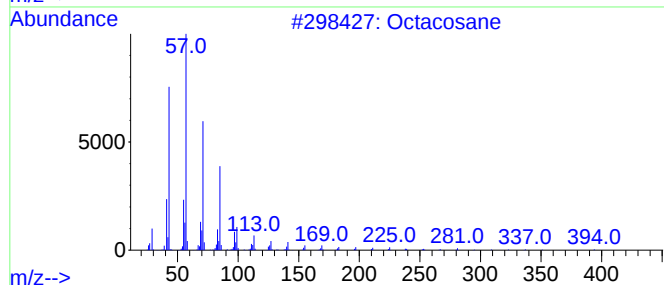
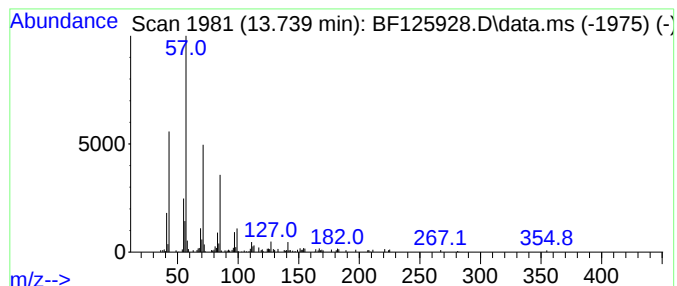
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	6.49 ng	425682	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3			Hentriacontane	437	C31H64	000630-04-6	86
4			Hexacosane	366	C26H54	000630-01-3	86
5			Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
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Instrument :
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ClientSampleId :
1-3-TOTES

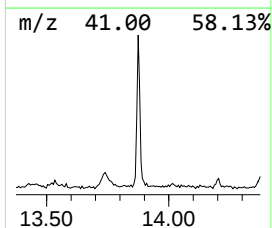
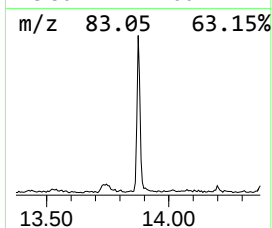
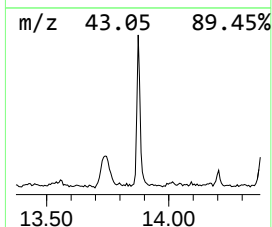
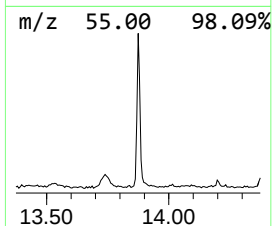
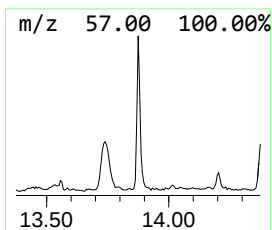
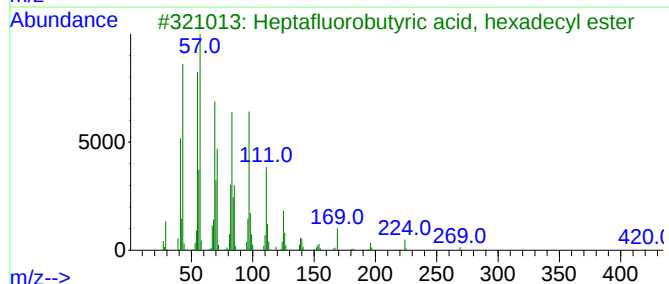
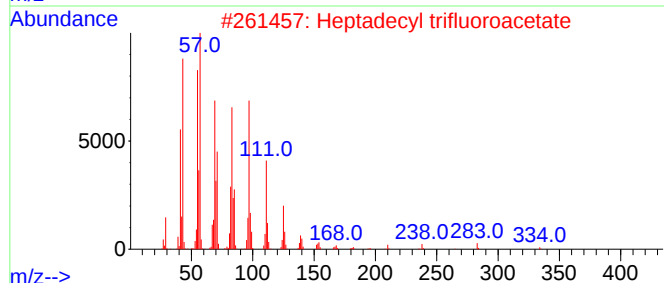
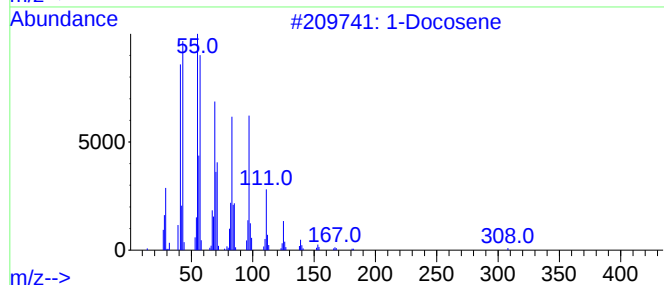
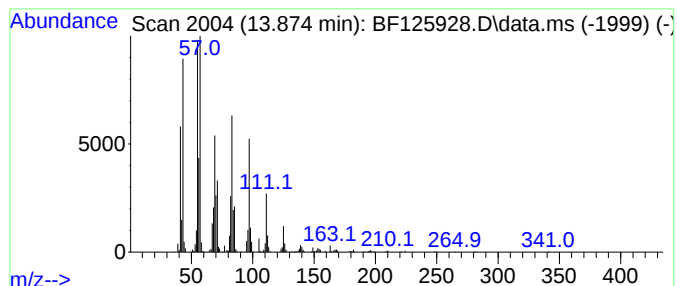
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	19.59 ng	1283930	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Heptadecyl trifluoroacetate			352	C19H35F3O2	1010351-87-0	94
3	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	91
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	91
5	1-Heneicosanol			312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
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Sample : M4313-07
Misc :
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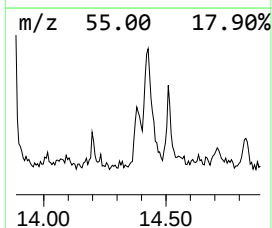
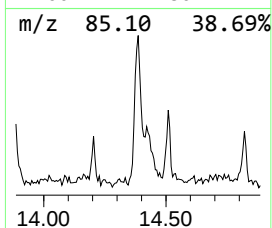
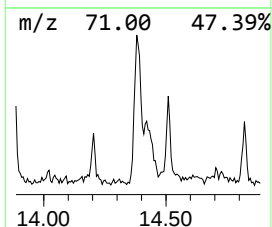
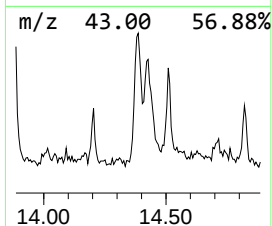
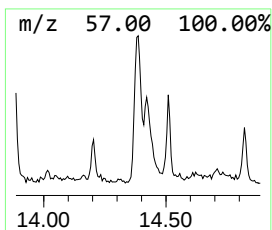
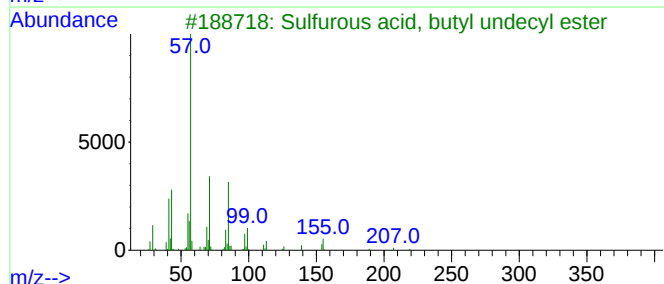
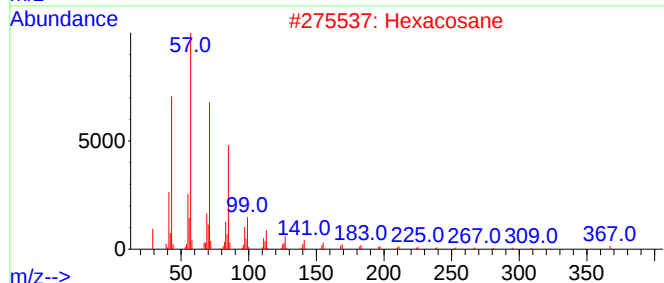
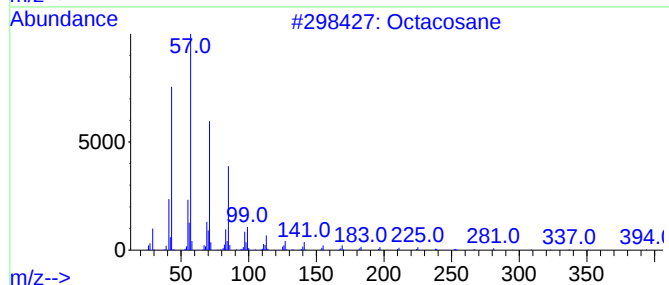
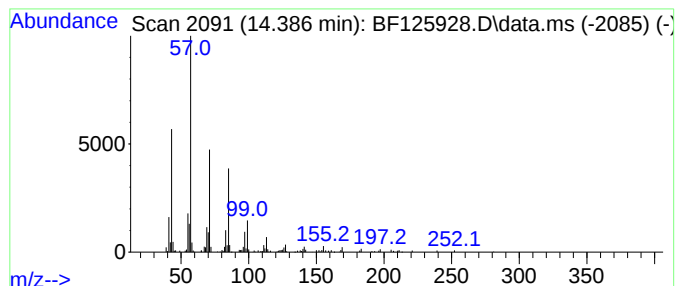
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.386	5.84 ng	383037	Chrysene-d12	14.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	86
3	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	83
4	Heptadecane	240	C17H36	000629-78-7	80
5	Heptacosane	380	C27H56	000593-49-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
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Instrument :
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ClientSampleId :
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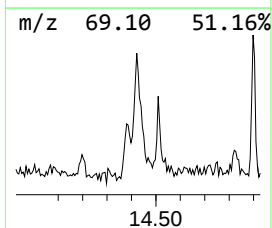
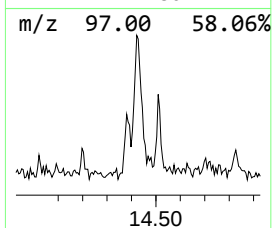
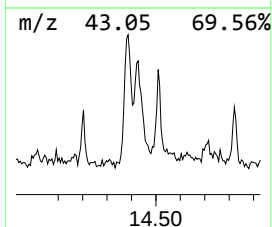
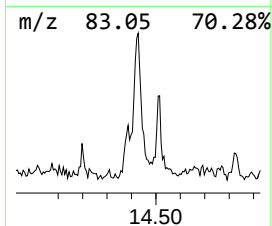
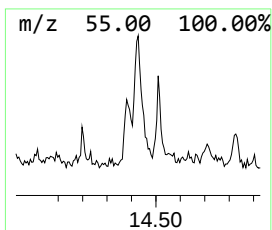
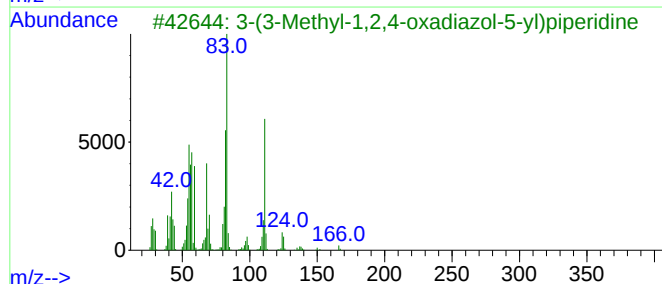
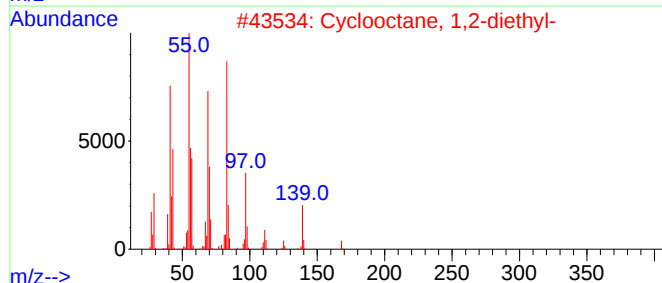
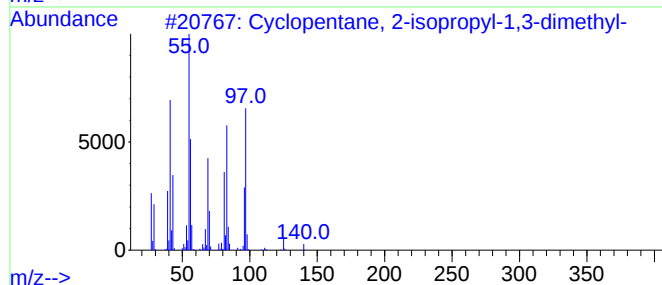
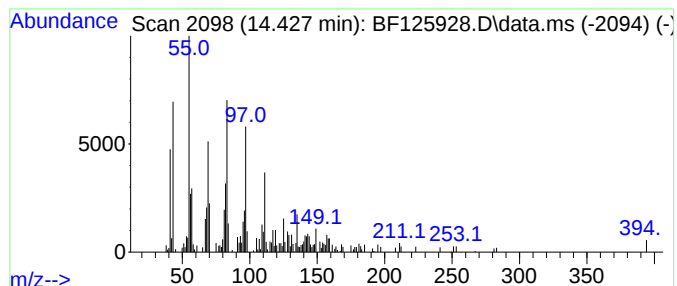
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.427 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	8.90 ng	583086	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	38
2			Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	30
3			3-(3-Methyl-1,2,4-oxadiazol-5-yl...	167	C8H13N3O	902837-17-6	25
4			Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	25
5			Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
1-3-TOTES

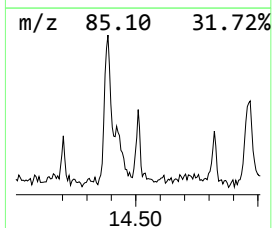
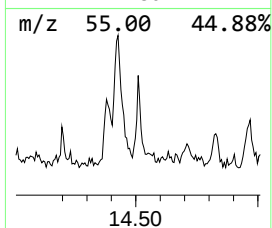
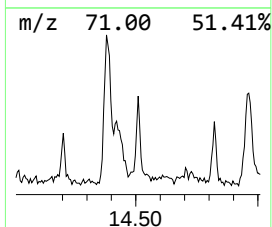
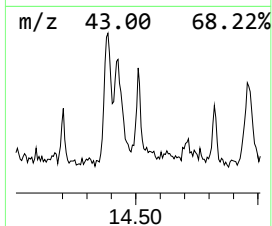
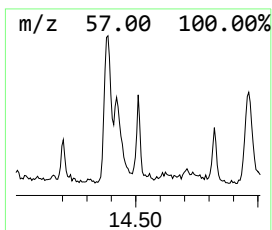
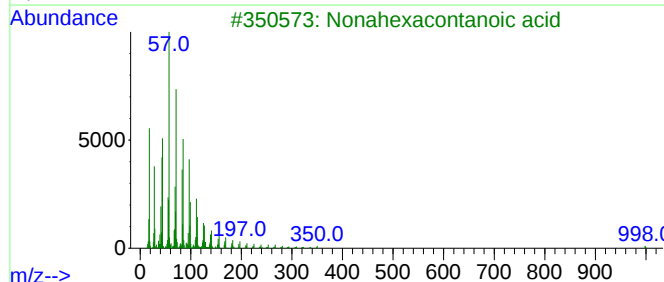
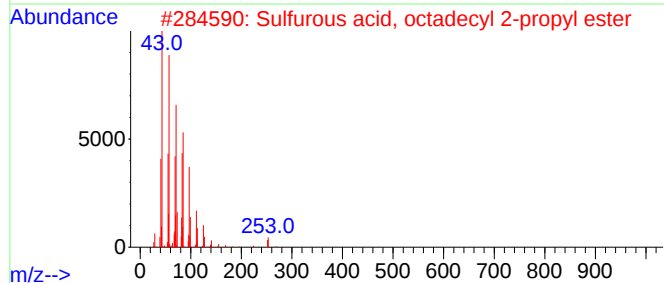
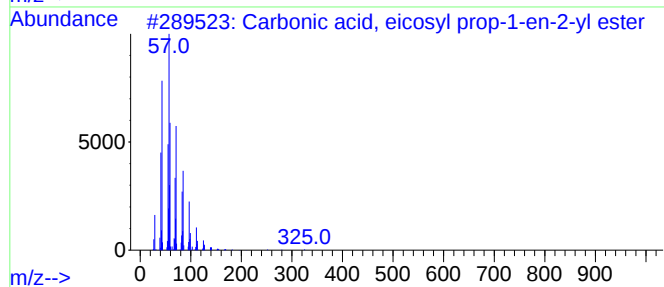
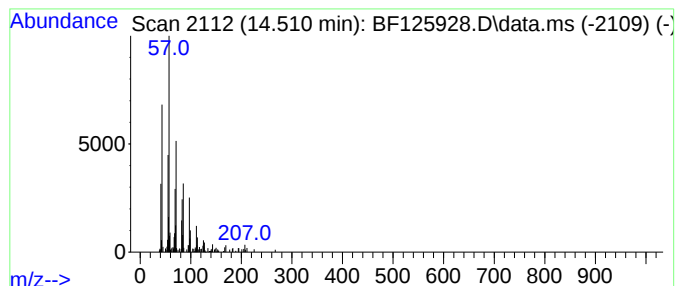
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Carbonic acid, eicosyl prop... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	2.83 ng	185401	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	90
2			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	81
3			Nonahexacontanoic acid	999	C69H138O2	040710-32-5	74
4			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	74
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-TOTES

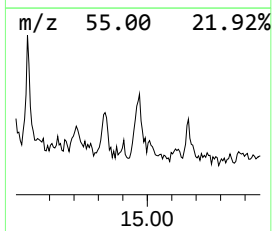
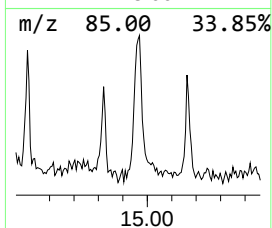
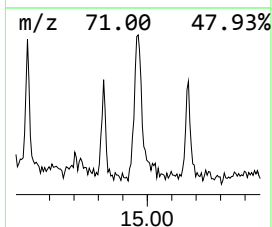
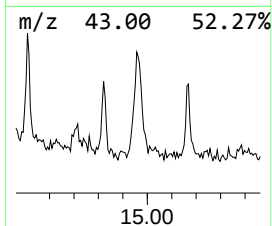
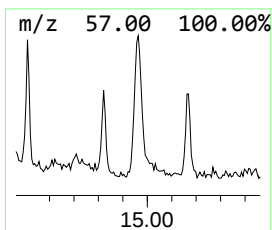
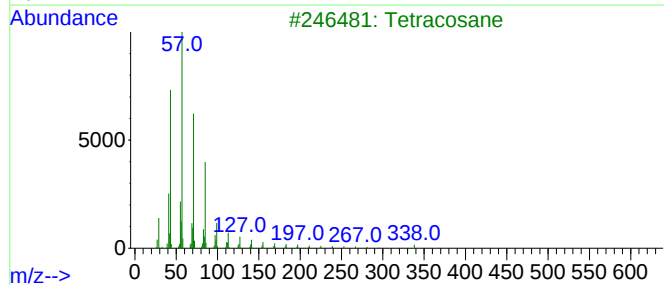
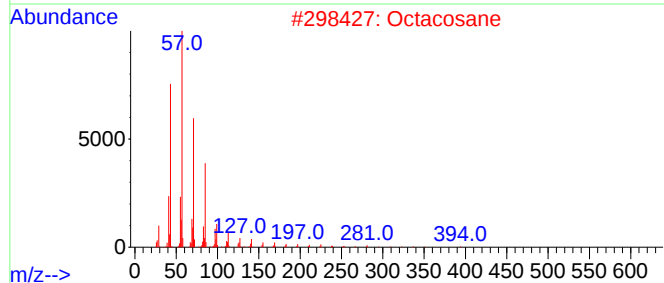
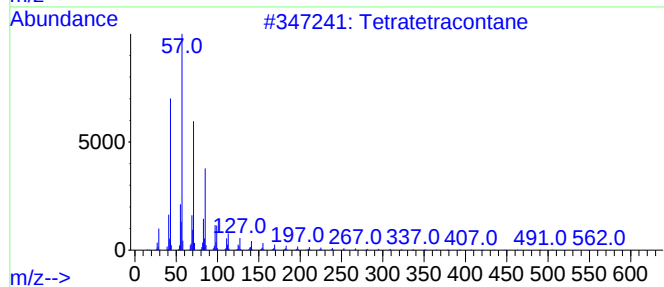
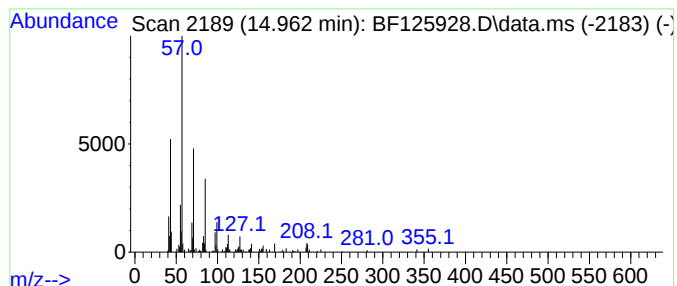
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	6.19 ng	290260	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	87
2			Octacosane	394	C28H58	000630-02-4	87
3			Tetracosane	338	C24H50	000646-31-1	81
4			Hexacosane	366	C26H54	000630-01-3	80
5			Pentacosane	352	C25H52	000629-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
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Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-TOTES

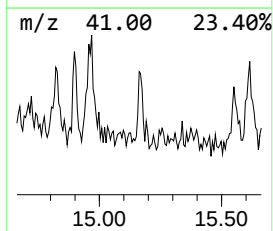
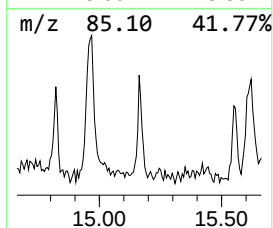
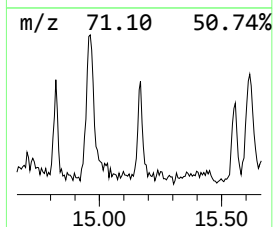
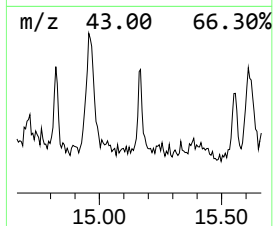
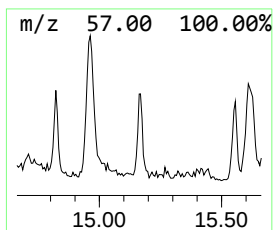
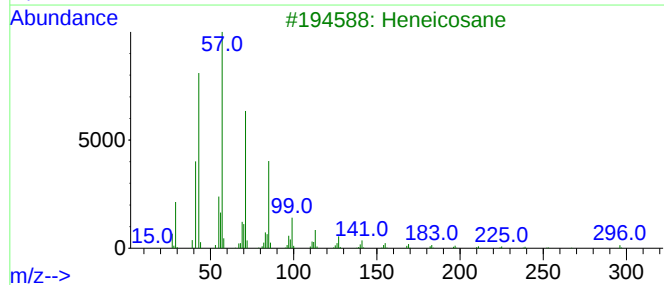
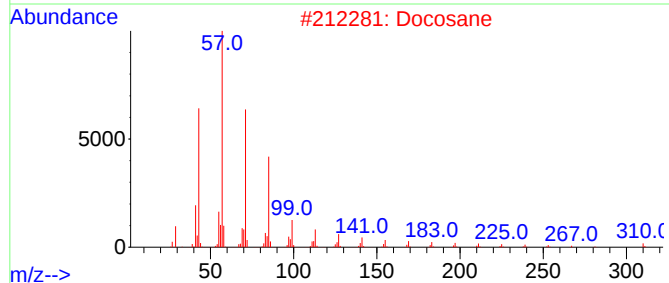
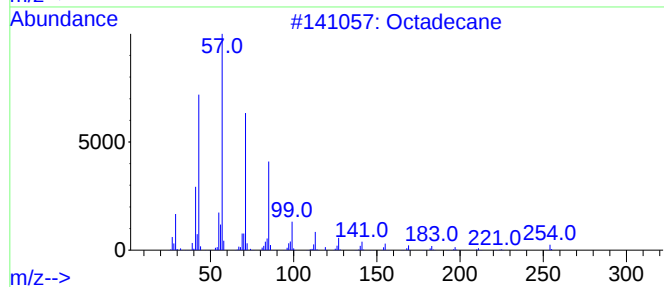
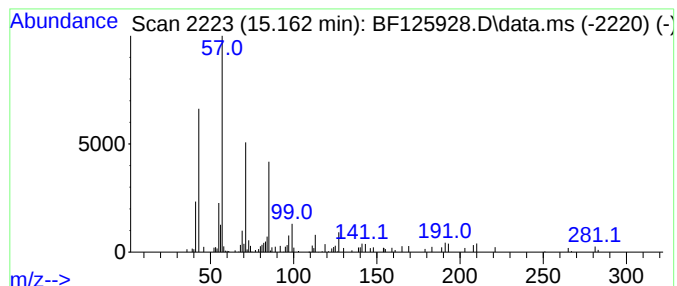
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.92 ng	136761	Perylene-d12	15.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	80
2		Docosane	310	C22H46	000629-97-0	80
3		Heneicosane	296	C21H44	000629-94-7	80
4		Tetracosane	338	C24H50	000646-31-1	80
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
1-3-TOTES

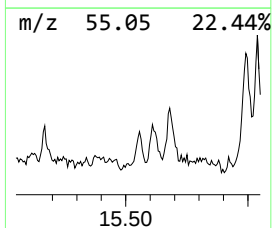
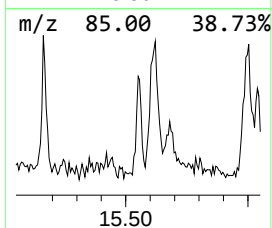
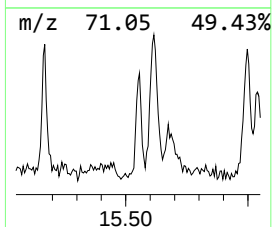
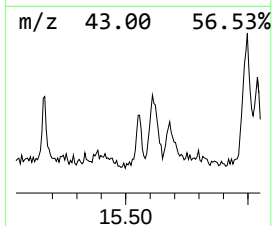
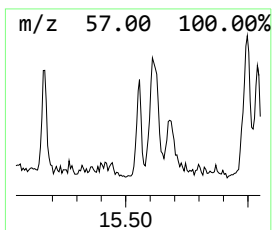
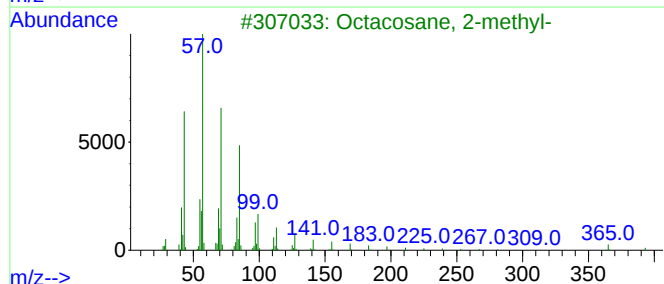
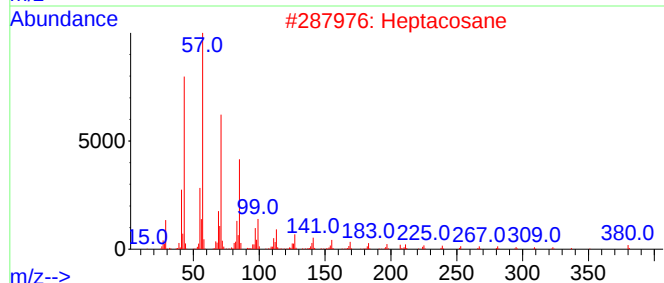
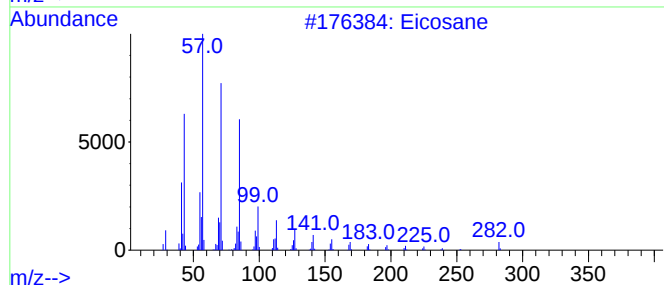
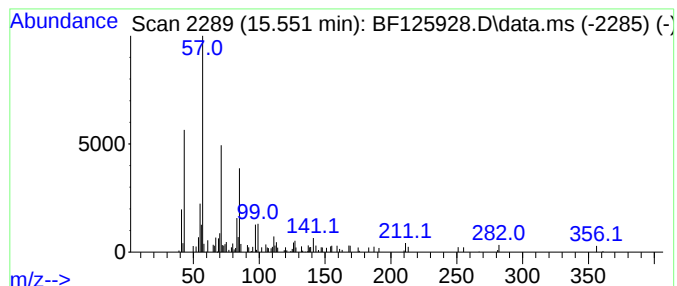
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Eicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.551	2.40 ng	112663	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Heptacosane			380	C27H56	000593-49-7	87
3	Octacosane, 2-methyl-			408	C29H60	001560-98-1	87
4	Tritetracontane			605	C43H88	007098-21-7	87
5	Tetracosane, 11-decyl-			479	C34H70	055429-84-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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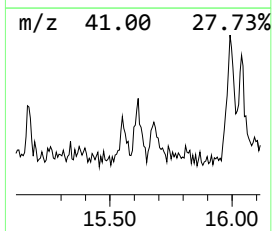
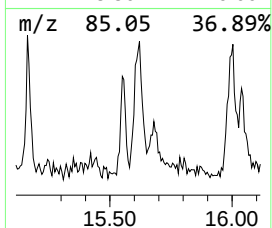
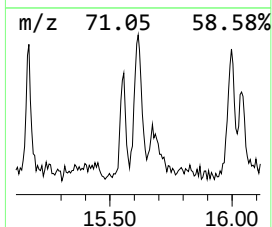
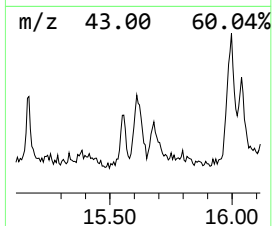
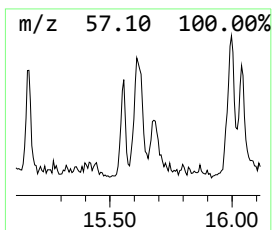
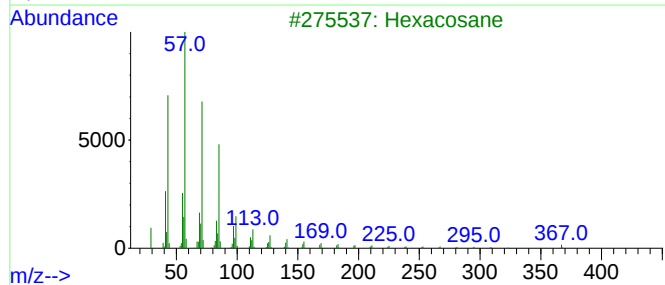
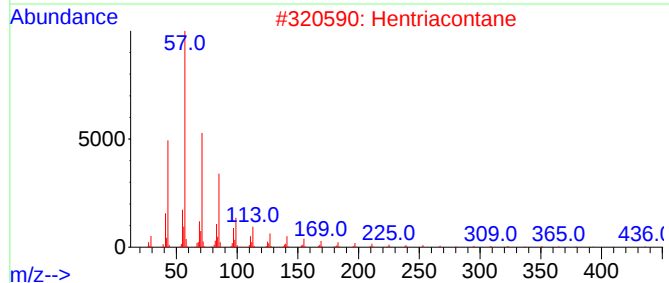
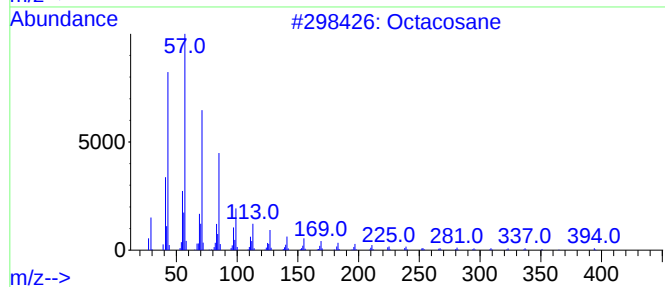
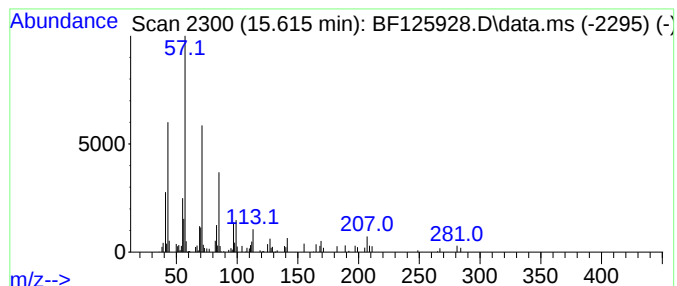
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Hentriacontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	4.08 ng	191326	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Hexacosane	366	C26H54	000630-01-3	83
4			Heptacosane	380	C27H56	000593-49-7	80
5			Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
1-3-TOTES

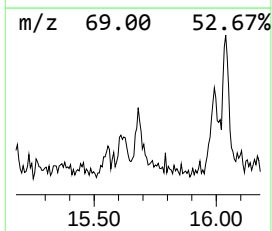
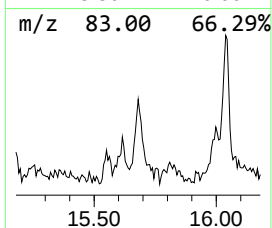
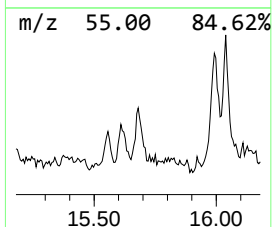
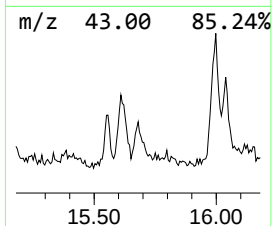
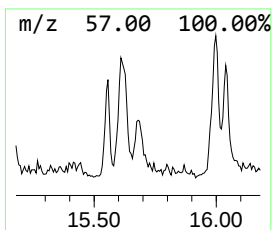
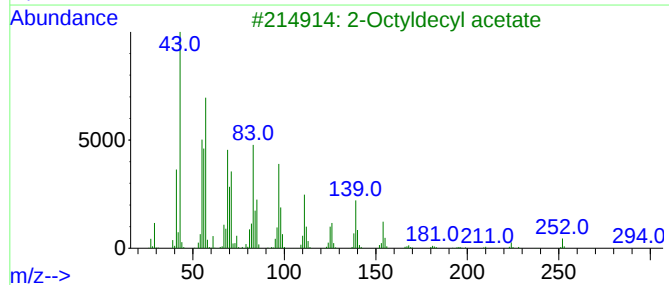
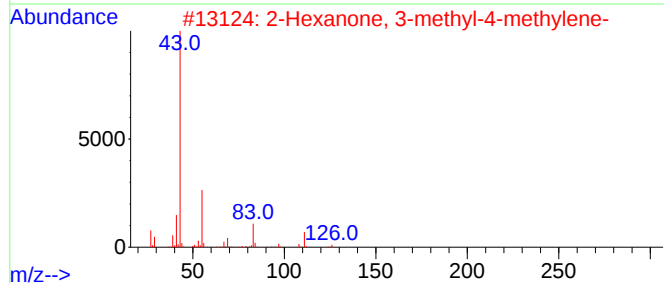
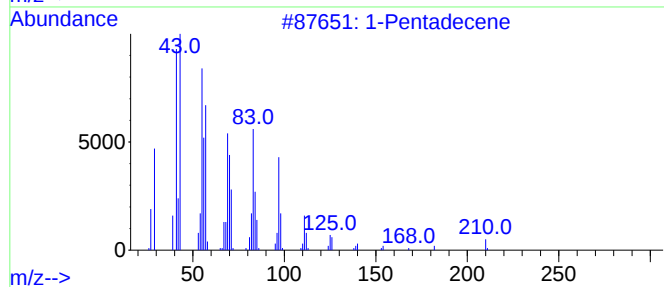
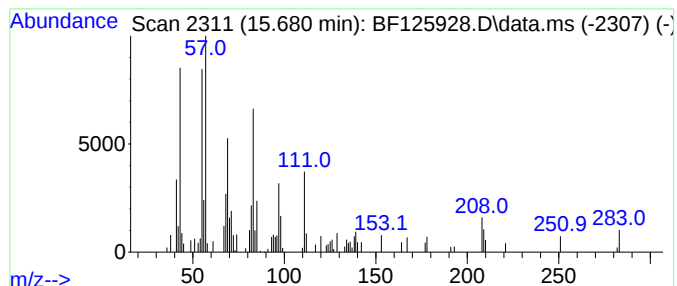
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown15.680 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.680	2.81 ng	131563	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentadecene	210	C15H30	013360-61-7	46
2			2-Hexanone, 3-methyl-4-methylene-	126	C8H14O	020690-71-5	27
3			2-Octyldecyl acetate	312	C20H40O2	1000368-55-8	27
4			1-Tridecyn-4-ol	196	C13H24O	074646-37-0	27
5			Cyclohexane, 1-(cyclohexylmethyl)-	208	C15H28	054934-95-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
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Acq On : 26 Oct 2021 11:37
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ClientSampleId :
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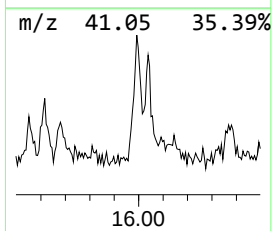
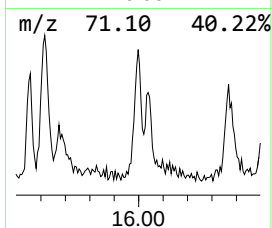
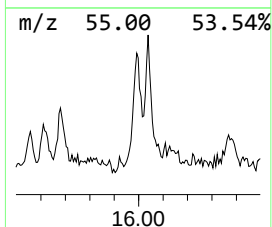
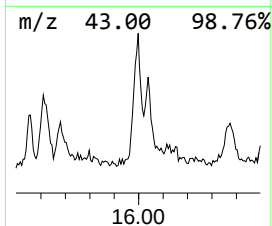
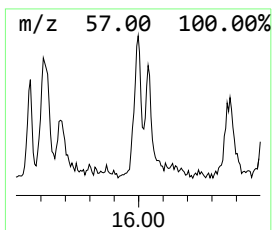
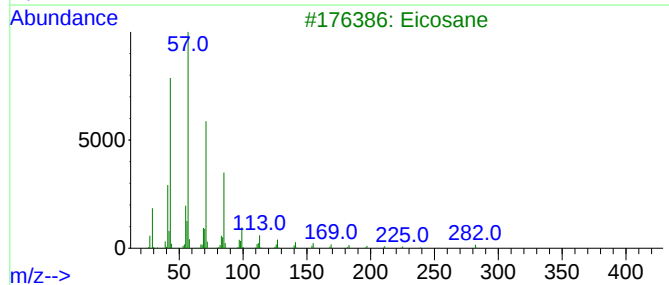
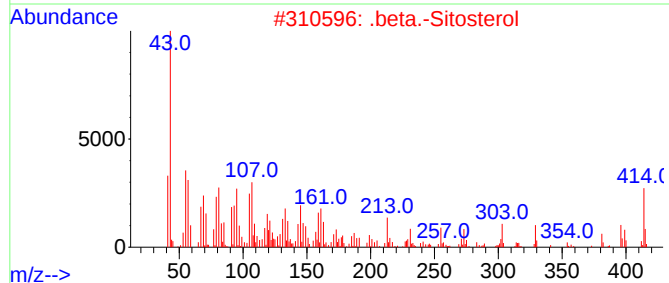
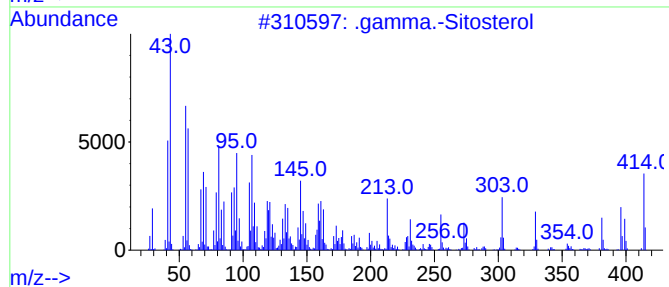
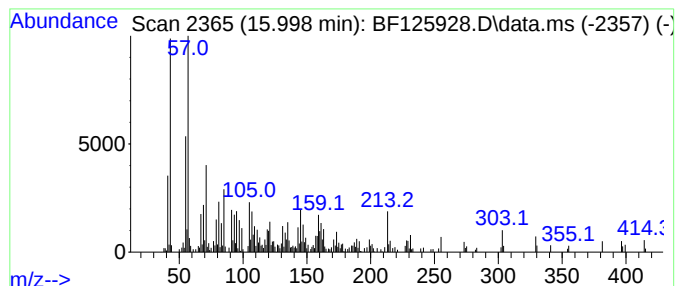
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	14.41 ng	675571	Perylene-d12	15.492

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	68
3		Eicosane	282	C20H42	000112-95-8	45
4		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	43
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
1-3-TOTES

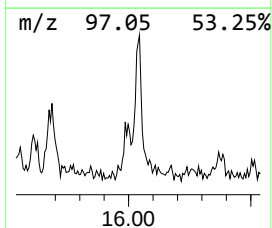
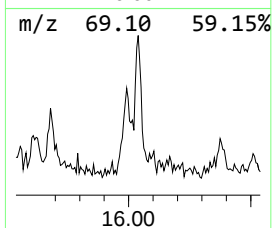
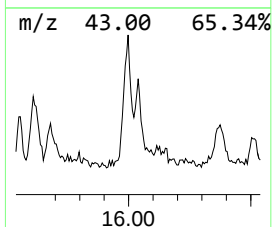
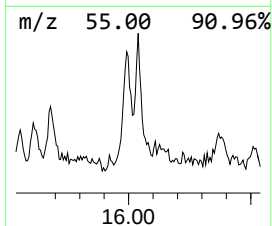
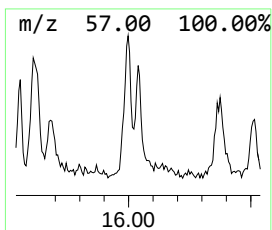
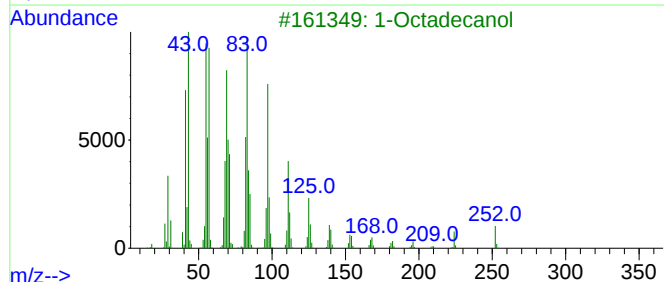
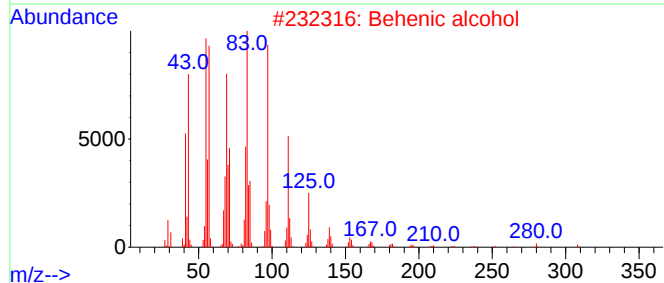
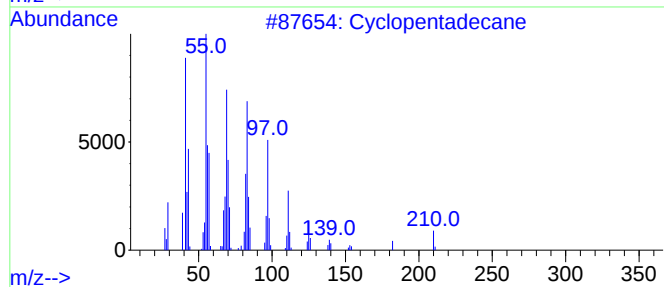
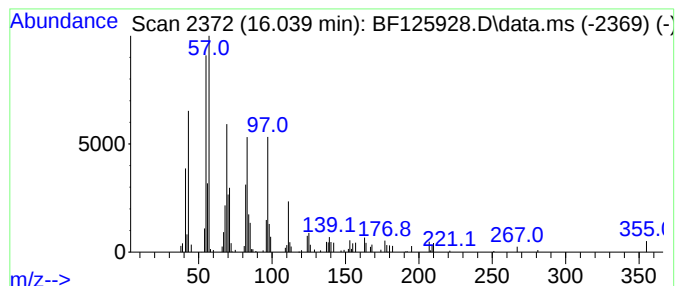
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Cyclopentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	4.97 ng	233229	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	93
2			Behenic alcohol	326	C22H46O	000661-19-8	91
3			1-Octadecanol	270	C18H38O	000112-92-5	91
4			Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
Data File : BF125928.D
Acq On : 26 Oct 2021 11:37
Operator : JU/CG
Sample : M4313-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-TOTES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.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...	2.210	149.7	ng	7443890	1	6.863	994811	20.0
2-Pentanone, 4-...	5.081	3.0	ng	148325	1	6.863	994811	20.0
Ethanol, 2-(2-b...	8.057	25.6	ng	1680870	2	8.151	1313500	20.0
Benzothiazole	8.422	2.8	ng	181540	2	8.151	1313500	20.0
unknown10.104	10.104	4.0	ng	293320	3	9.904	1449830	20.0
n-Hexadecanoic ...	11.922	18.4	ng	1421980	4	11.386	1545590	20.0
Octadecanoic acid	12.704	7.0	ng	537978	4	11.386	1545590	20.0
Heptacosane	12.868	7.4	ng	487439	5	14.027	1310840	20.0
Heptadecane, 9-...	13.739	6.5	ng	425682	5	14.027	1310840	20.0
1-Docosene	13.874	19.6	ng	1283930	5	14.027	1310840	20.0
Octacosane	14.386	5.8	ng	383037	5	14.027	1310840	20.0
unknown14.427	14.427	8.9	ng	583086	5	14.027	1310840	20.0
Carbonic acid, ...	14.510	2.8	ng	185401	5	14.027	1310840	20.0
Tetratetracontane	14.963	6.2	ng	290260	6	15.492	937841	20.0
Octadecane	15.163	2.9	ng	136761	6	15.492	937841	20.0
Eicosane	15.551	2.4	ng	112663	6	15.492	937841	20.0
Hentriacontane	15.615	4.1	ng	191326	6	15.492	937841	20.0
unknown15.680	15.680	2.8	ng	131563	6	15.492	937841	20.0
.gamma.-Sitosterol	15.998	14.4	ng	675571	6	15.492	937841	20.0
Cyclopentadecane	16.039	5.0	ng	233229	6	15.492	937841	20.0