

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
 Data File : BF124052.D
 Acq On : 25 May 2021 18:57
 Operator : JU/CG
 Sample : M2500-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-08-052421

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	20	25	rBV	512231	638351	9.47%	2.160%
2	5.116	510	515	524	rVB	330525	385761	5.72%	1.305%
3	5.516	578	583	586	rBV	1193777	1025433	15.22%	3.469%
4	6.516	748	753	756	rBV	1069596	1016447	15.08%	3.439%
5	6.892	813	817	821	rVB	510737	391779	5.81%	1.326%
6	7.451	907	912	915	rBV	771373	711235	10.55%	2.406%
7	8.175	1031	1035	1039	rBV	570133	470312	6.98%	1.591%
8	9.251	1214	1218	1221	rBV	1662896	1257317	18.66%	4.254%
9	9.510	1259	1262	1269	rVB	98255	75908	1.13%	0.257%
10	9.639	1281	1284	1291	rVB	86172	77395	1.15%	0.262%
11	9.933	1330	1334	1337	rBV	670296	518613	7.70%	1.755%
12	10.722	1464	1468	1471	rBV	769468	644326	9.56%	2.180%
13	11.421	1583	1587	1589	rBV	536283	425638	6.32%	1.440%
14	11.816	1650	1654	1657	rBV	3282460	2758655	40.94%	9.333%
15	11.963	1674	1679	1685	rBV	582233	719274	10.67%	2.434%
16	12.116	1701	1705	1711	rVB3	41079	81057	1.20%	0.274%
17	12.510	1767	1772	1774	rBV	5189427	5746630	85.28%	19.442%
18	12.533	1774	1776	1782	rVV	7163760	6738495	100.00%	22.798%
19	12.610	1785	1789	1792	rVV	1655141	1301183	19.31%	4.402%
20	12.674	1792	1800	1809	rVV2	1013975	1605852	23.83%	5.433%
21	12.739	1809	1811	1818	rVB	195451	217937	3.23%	0.737%
22	13.010	1853	1857	1860	rBV	1106913	886696	13.16%	3.000%
23	13.192	1882	1888	1892	rBV9	60517	141746	2.10%	0.480%
24	13.333	1909	1912	1914	rBV	134731	100135	1.49%	0.339%
25	13.439	1927	1930	1936	rVB	205265	206075	3.06%	0.697%
26	13.762	1981	1985	1988	rVB3	159352	198462	2.95%	0.671%
27	13.933	2011	2014	2021	rVB2	179333	200628	2.98%	0.679%
28	14.004	2023	2026	2029	rVB	112602	93311	1.38%	0.316%
29	14.068	2033	2037	2040	rBV	366613	342462	5.08%	1.159%
30	14.998	2192	2195	2200	rVB4	55095	70677	1.05%	0.239%
31	15.198	2226	2229	2232	rVB	86433	90465	1.34%	0.306%
32	15.562	2287	2291	2294	rBV	268183	320448	4.76%	1.084%
33	16.045	2369	2373	2377	rVB4	71821	98357	1.46%	0.333%

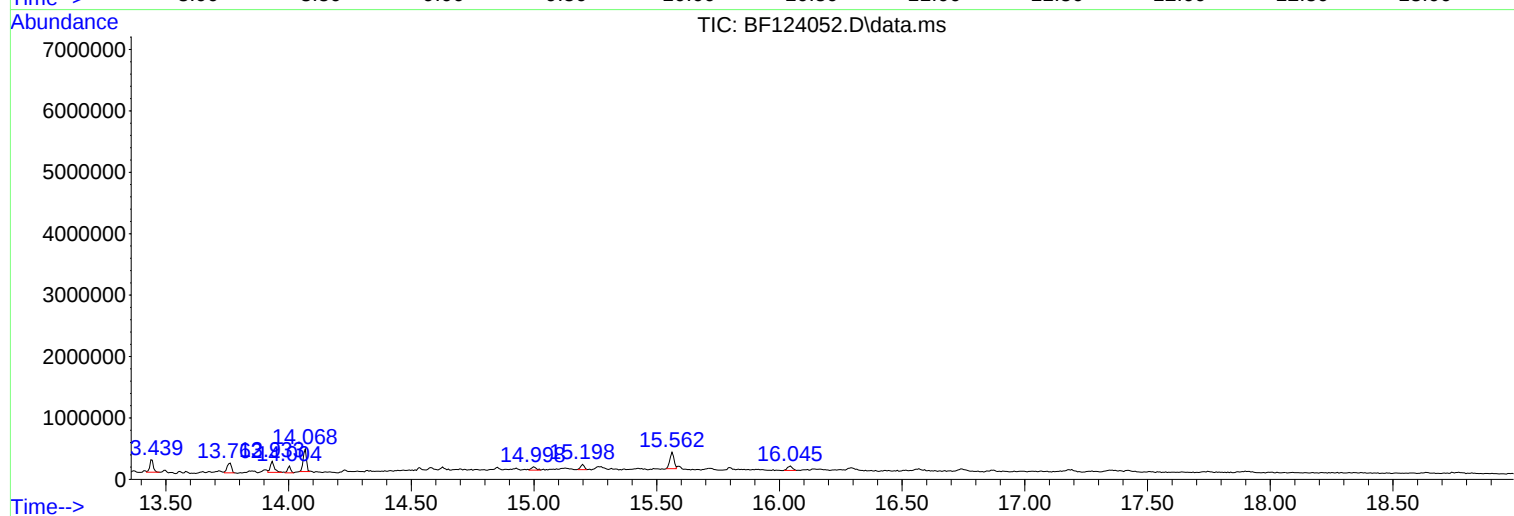
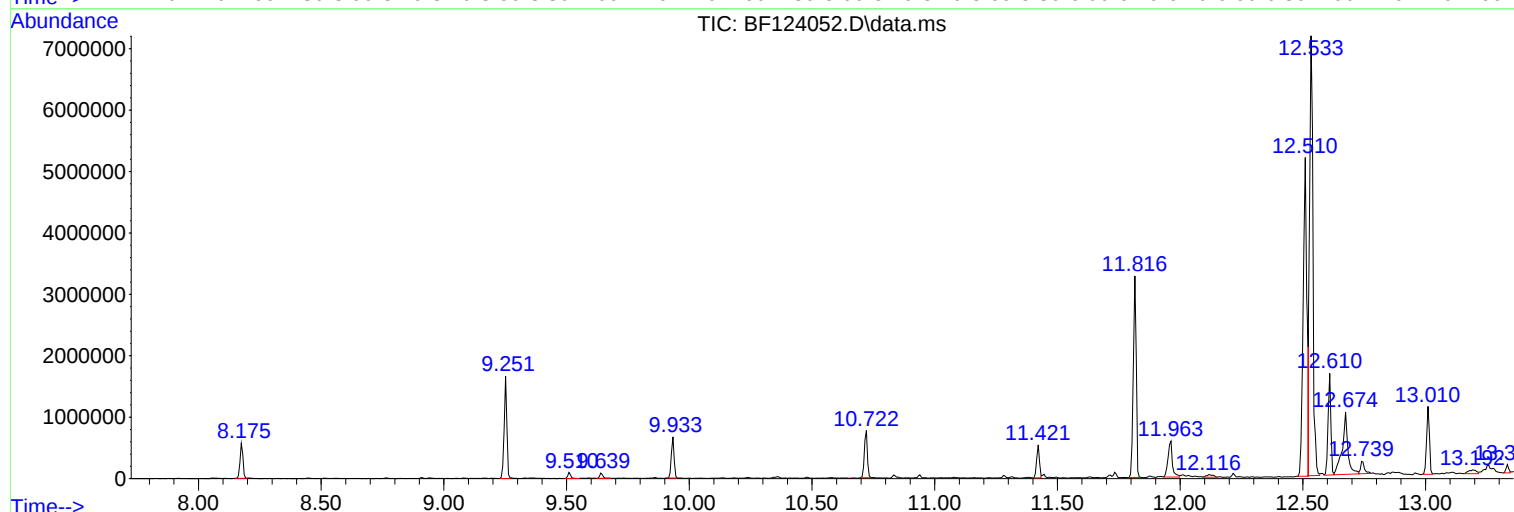
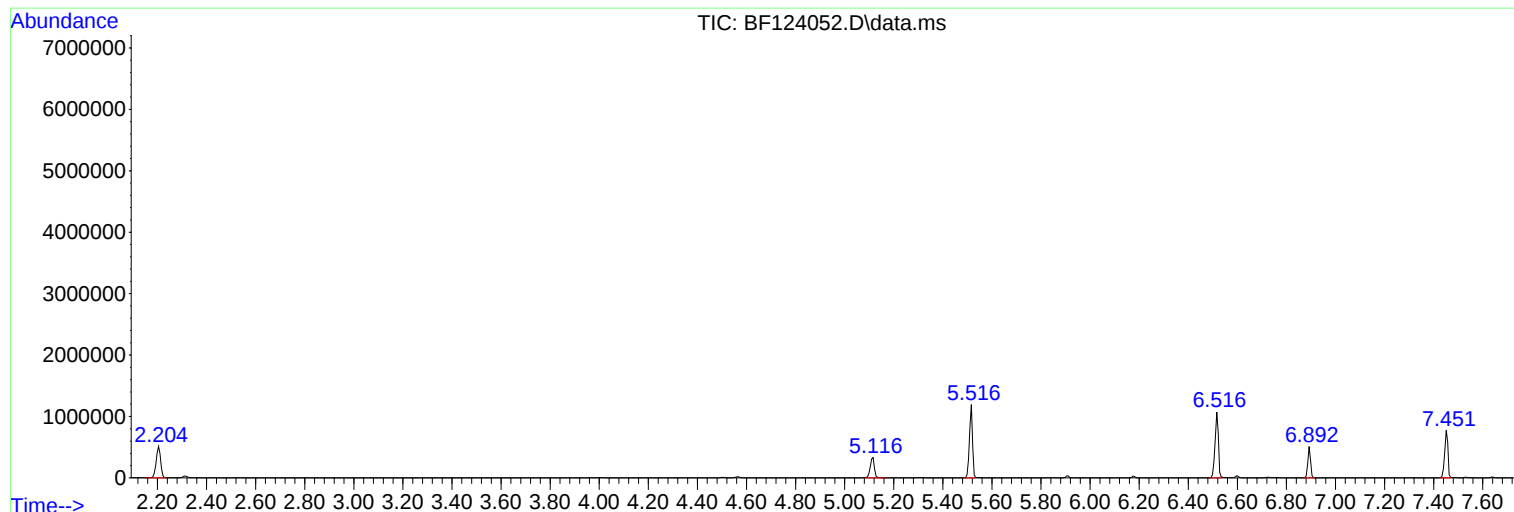
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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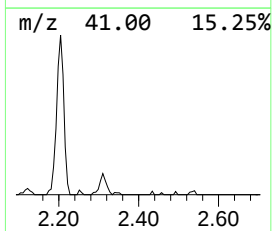
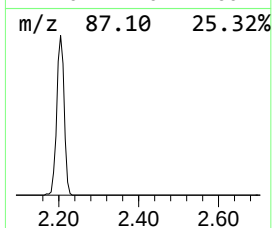
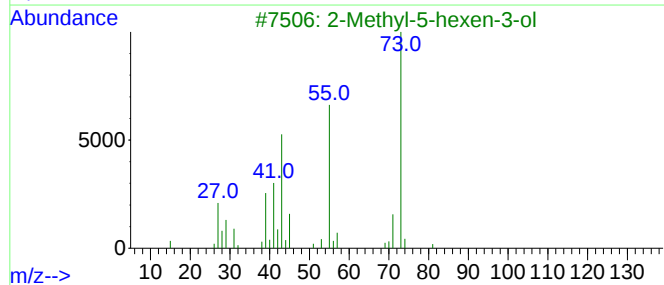
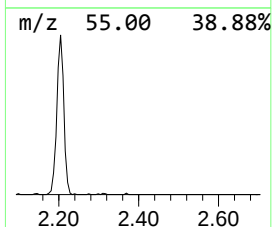
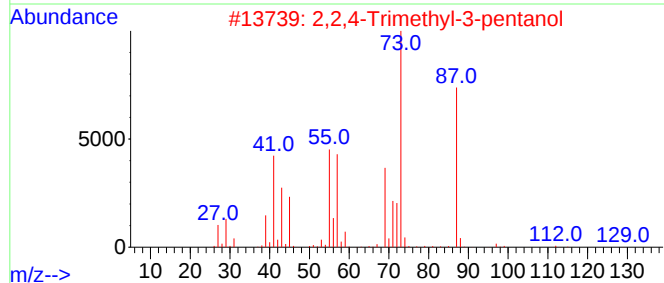
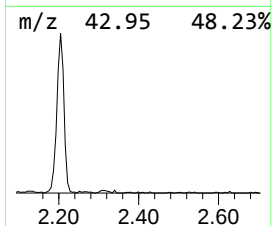
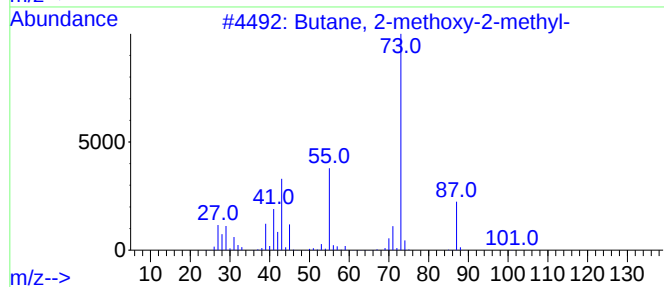
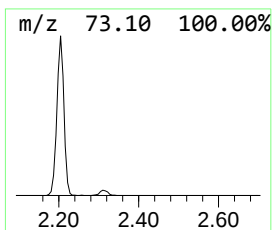
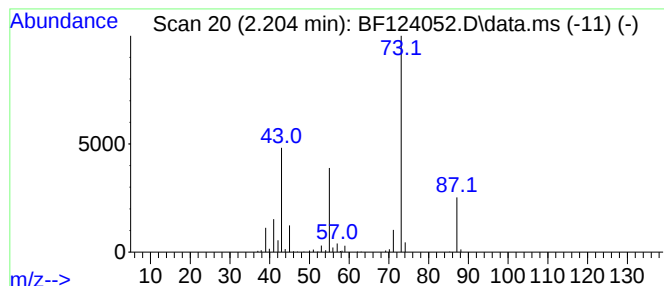
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	32.59 ng	638351	1,4-Dichlorobenzene-d4	6.892

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17



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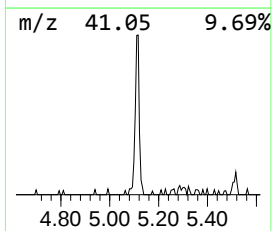
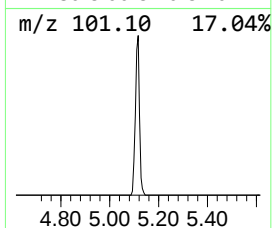
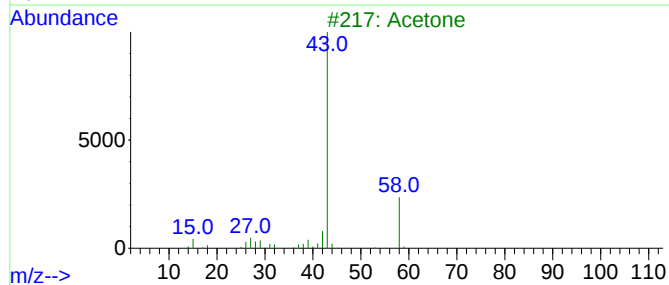
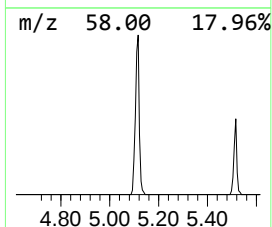
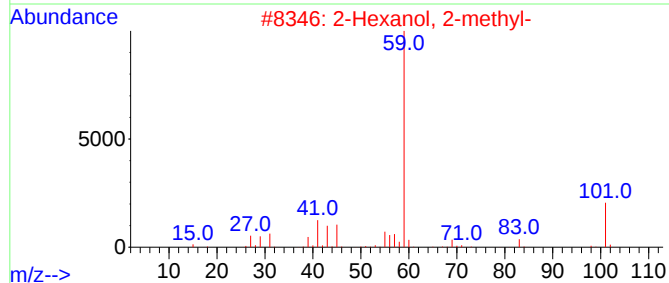
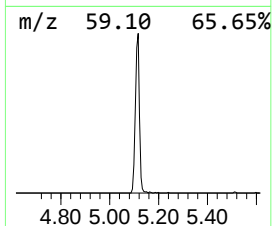
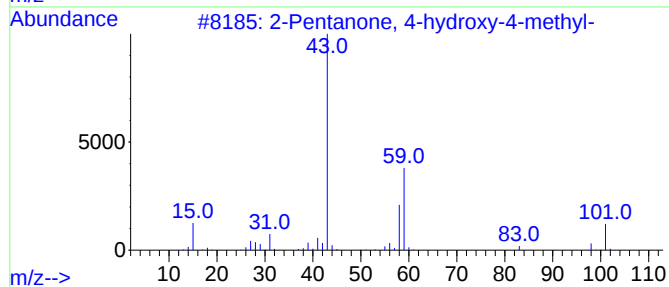
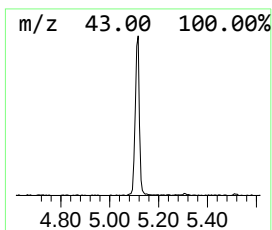
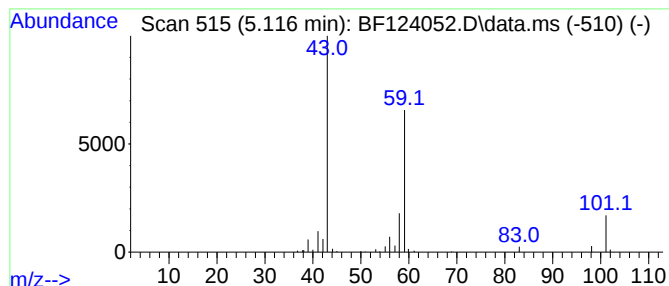
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	19.69 ng	385761	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetone	58	C3H6O	000067-64-1	12
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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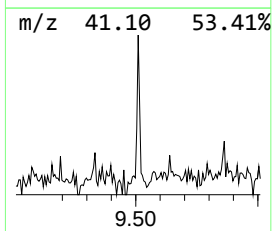
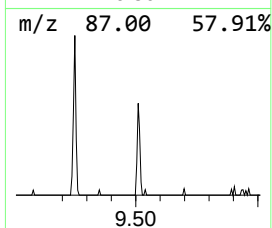
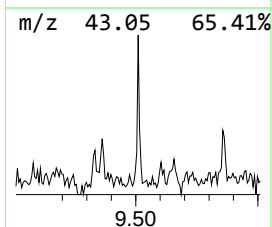
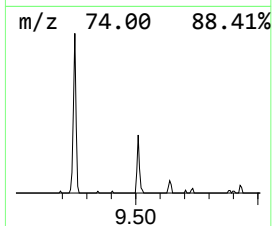
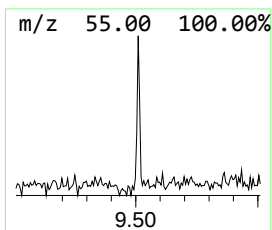
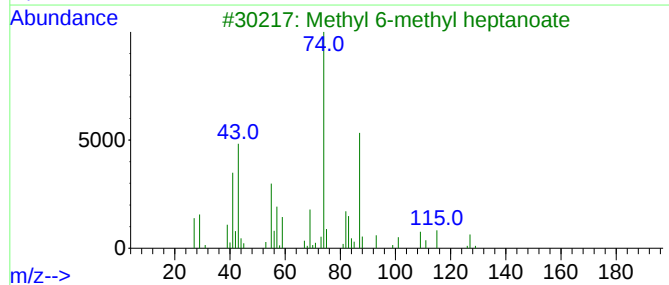
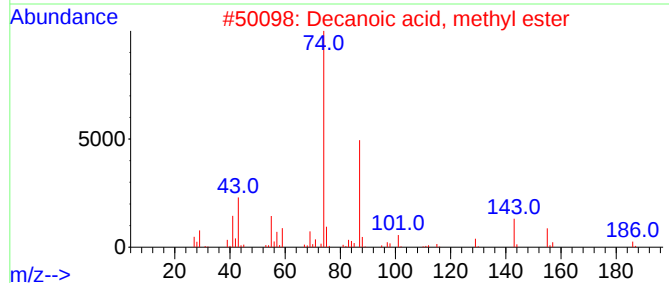
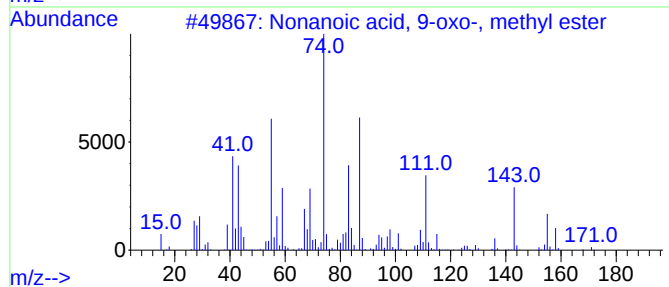
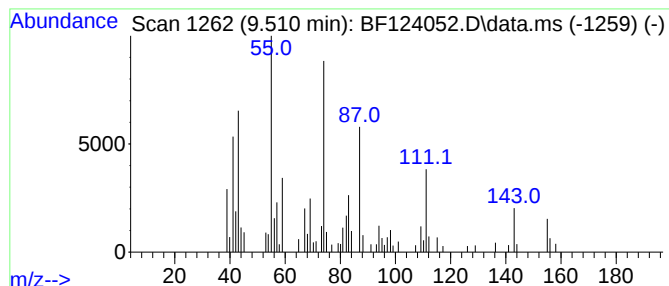
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Nonanoic acid, 9-oxo-, meth... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.510	2.93 ng	75908	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	50
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	37
3			Methyl 6-methyl heptanoate	158	C9H18O2	002519-37-1	37
4			Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	37
5			Methyl 4-hydroxybutanoate	118	C5H10O3	000925-57-5	25



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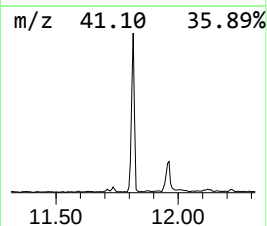
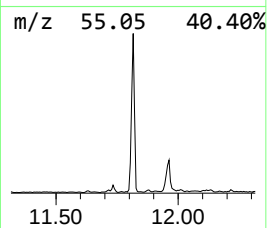
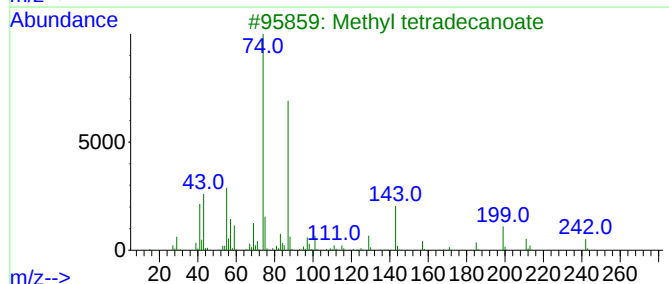
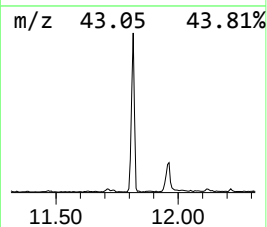
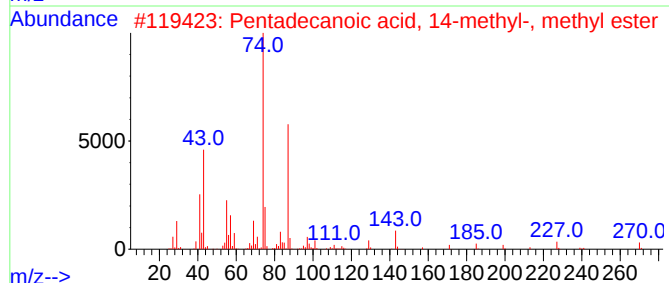
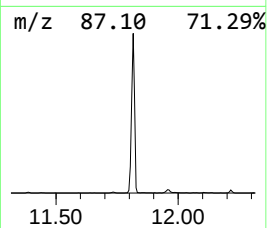
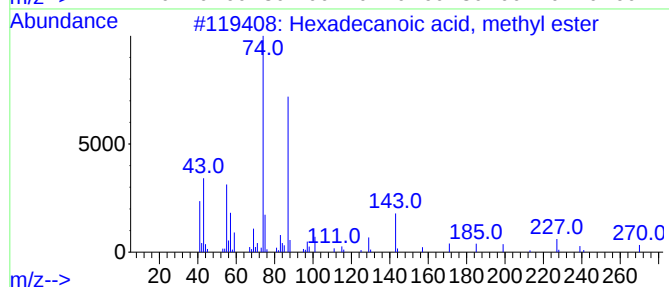
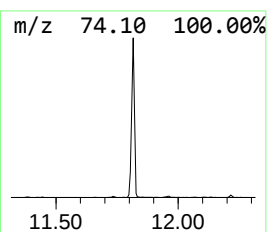
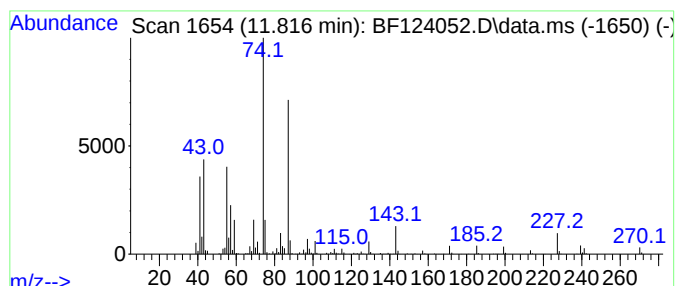
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	129.62 ng	2758660	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86



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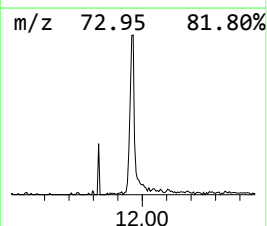
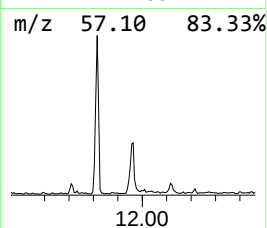
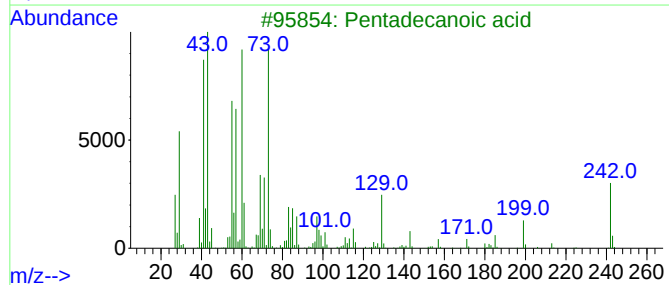
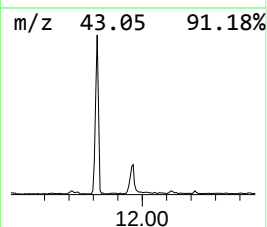
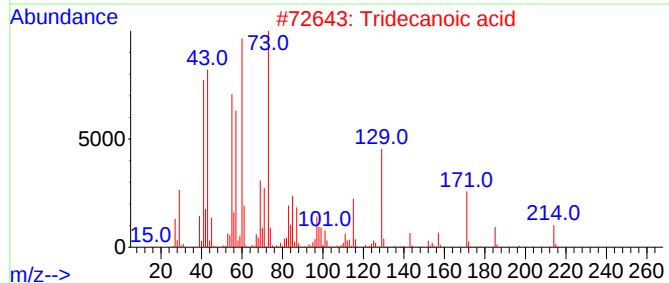
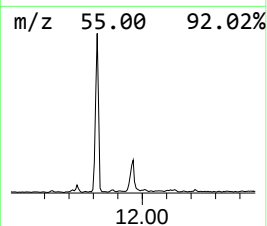
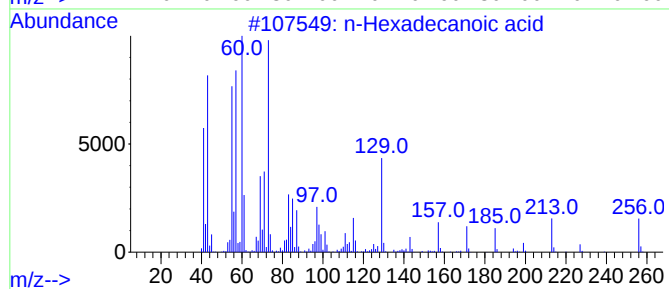
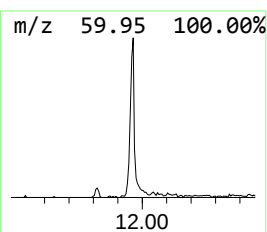
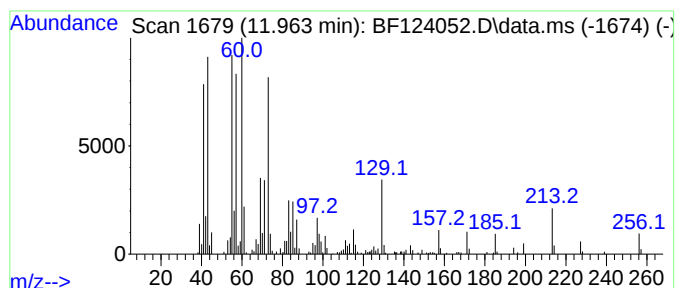
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.963	33.80 ng	719274	Phenanthrene-d10		11.422	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Tridecanoic acid		214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Undecanoic acid		186	C11H22O2	000112-37-8	53



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ClientSampleId :
NB-08-052421

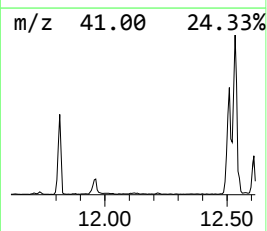
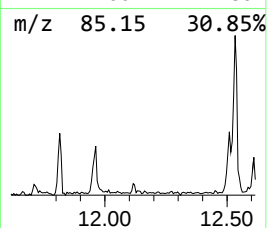
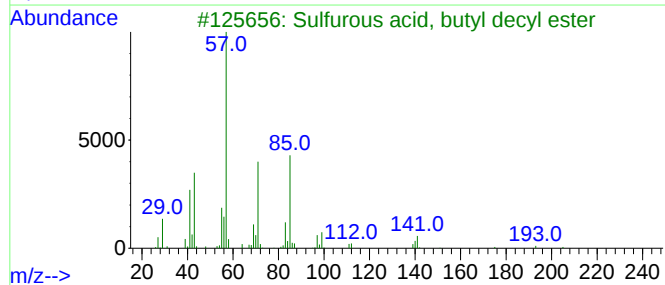
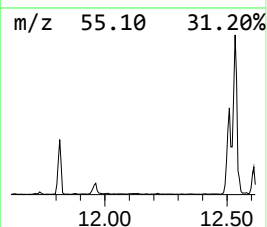
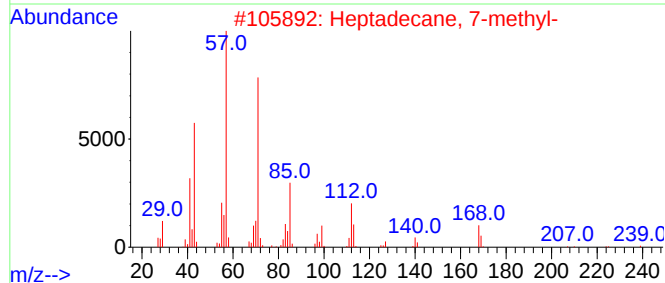
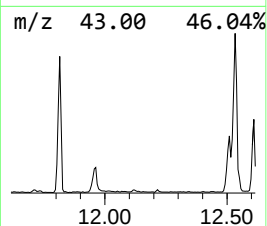
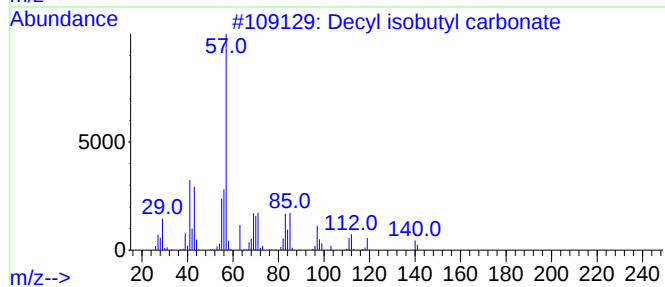
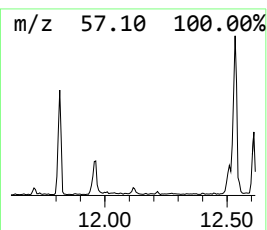
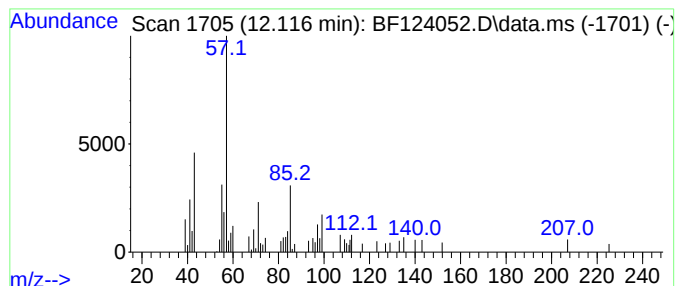
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Decyl isobutyl carbonate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.116	3.81 ng	81057	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decyl isobutyl carbonate	258	C15H30O3	959226-07-4	50
2			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	50
3			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	47
4			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	43
5			Hexane, 3-ethyl-3-methyl-	128	C9H20	003074-76-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
Operator : JU/CG
Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-052421

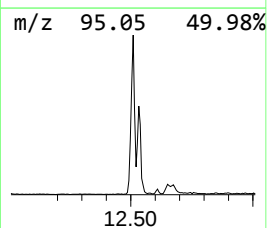
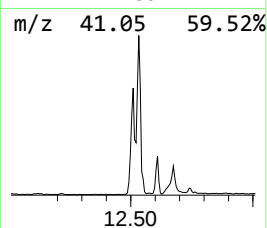
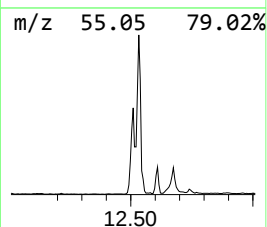
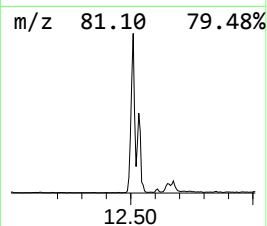
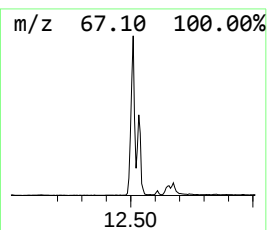
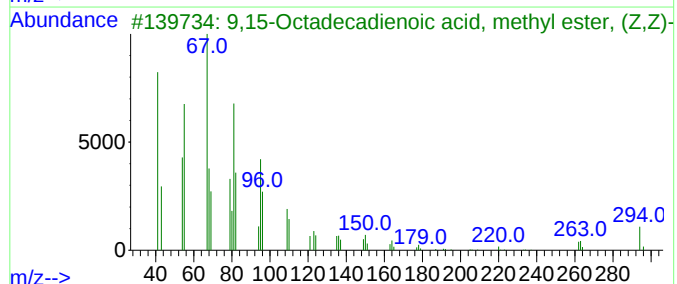
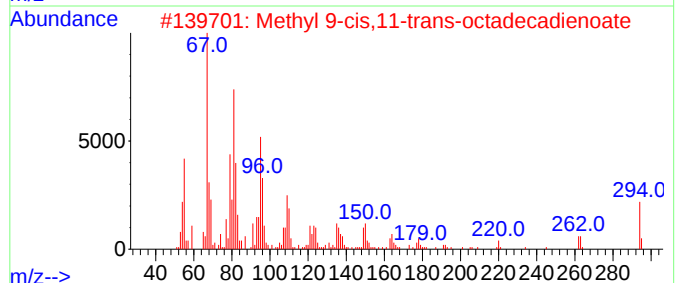
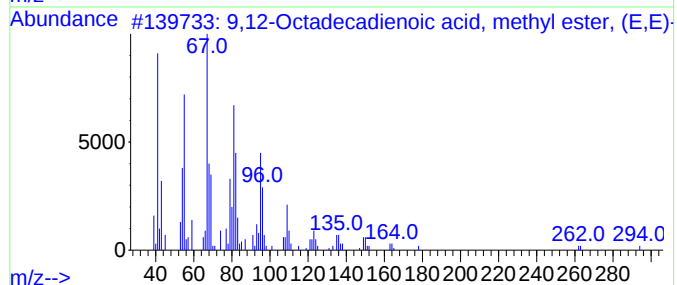
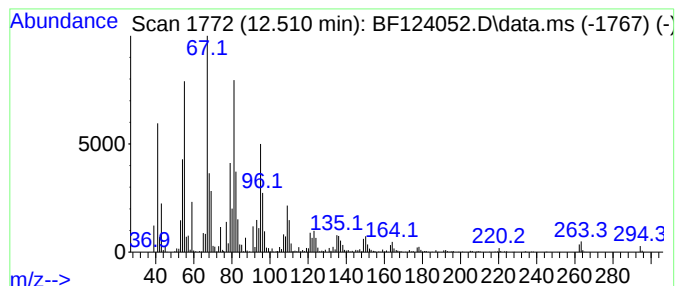
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.510	270.02 ng	5746630	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99		
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99		
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98		
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	98		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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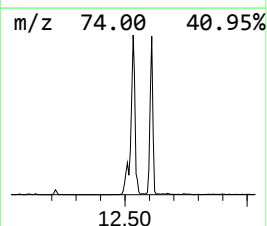
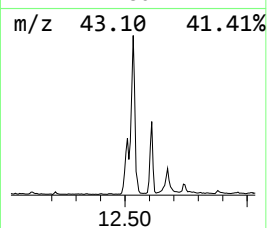
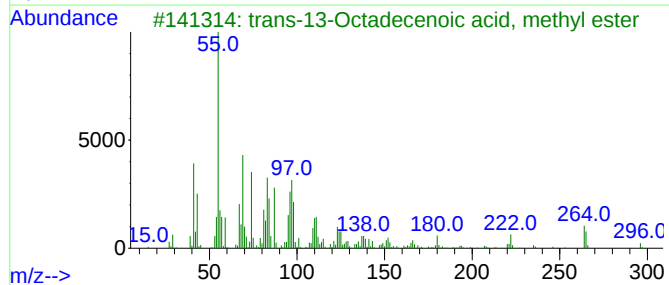
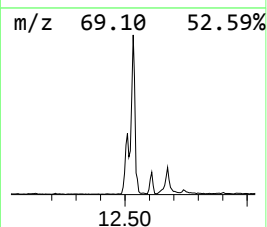
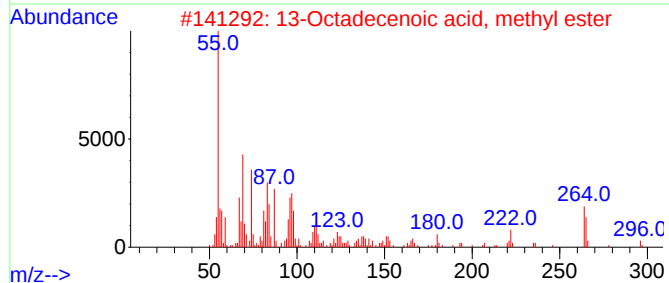
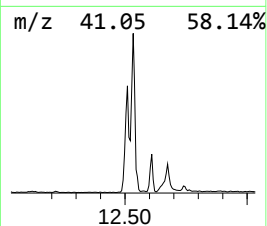
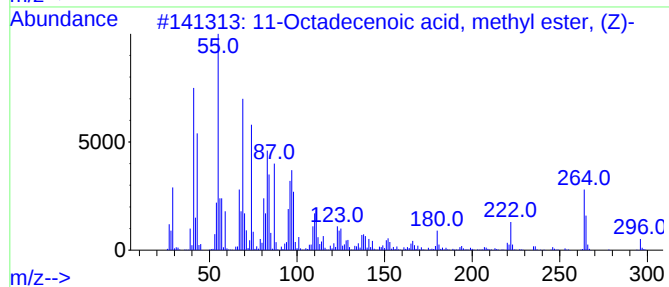
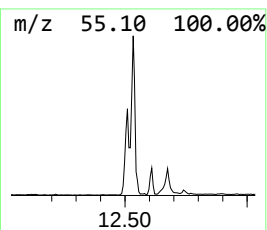
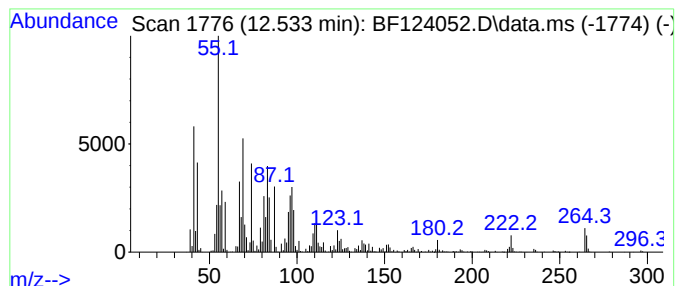
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 11-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	316.63 ng	6738500	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	96
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	94
3			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
4			9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	93
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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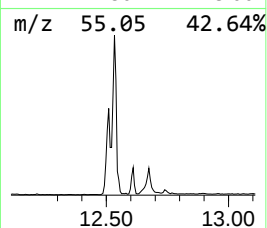
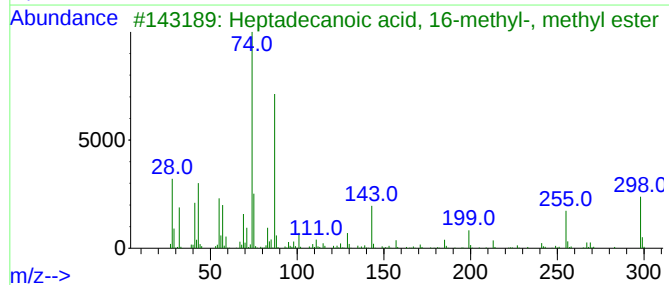
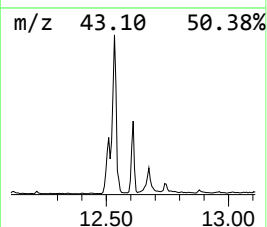
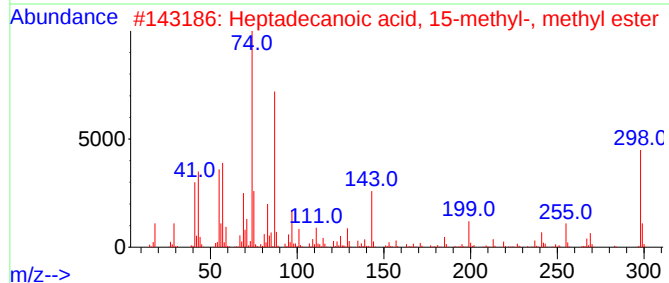
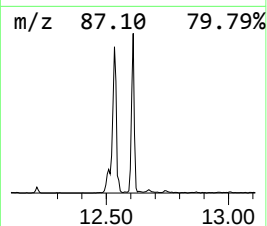
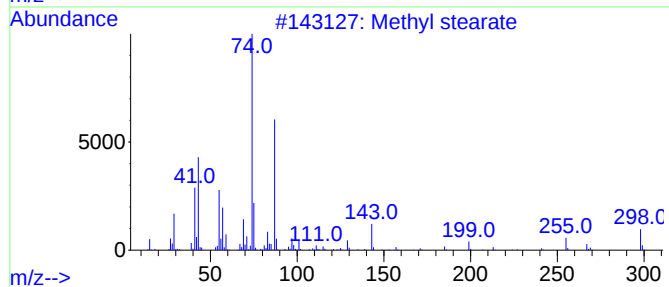
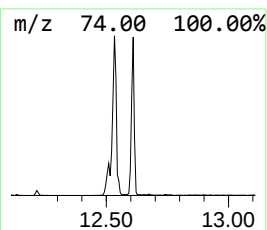
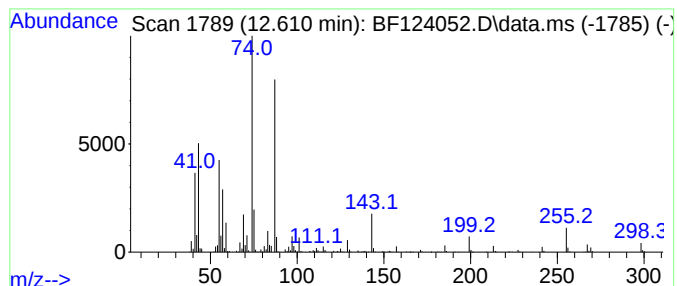
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	61.14 ng	1301180	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	97
2			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
3			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89
4			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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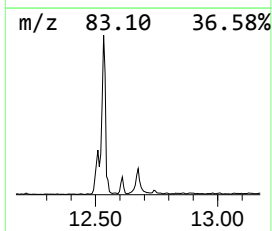
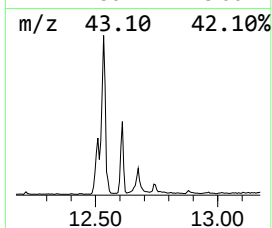
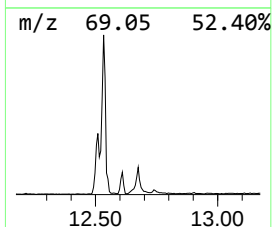
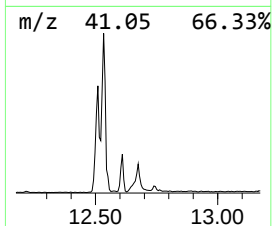
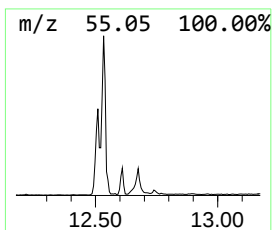
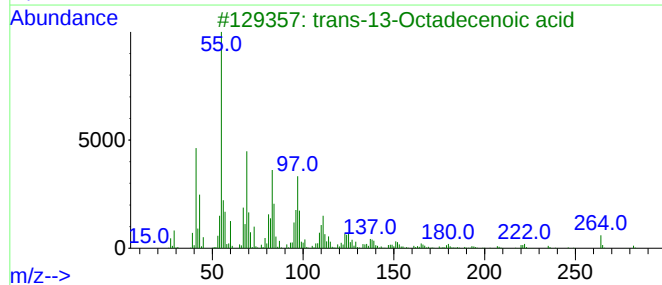
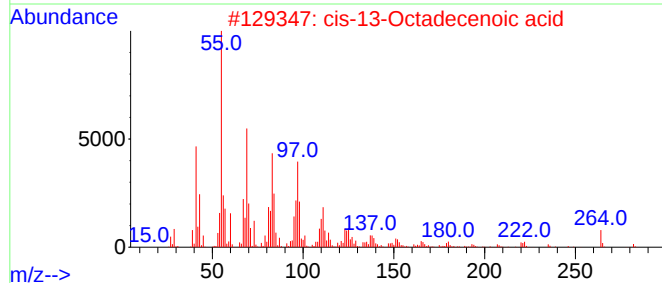
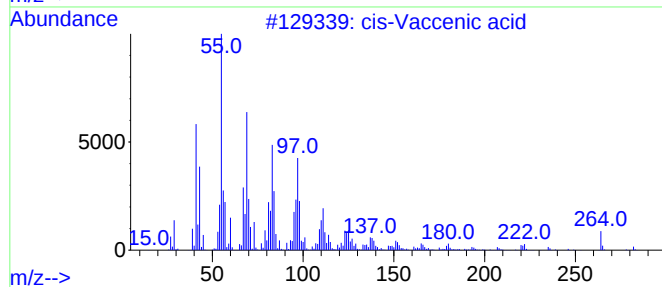
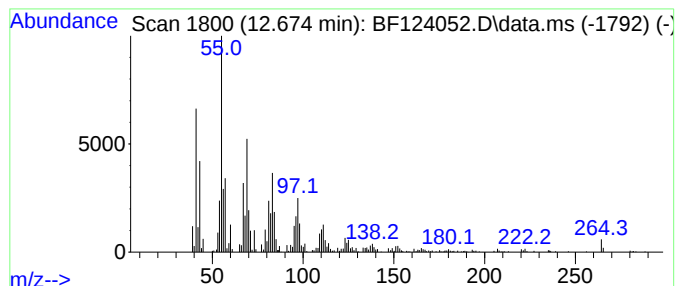
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 cis-Vaccenic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	75.46 ng	1605850	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
4			cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
5			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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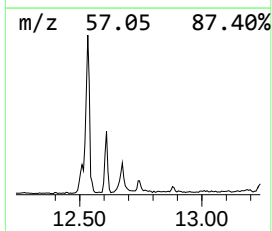
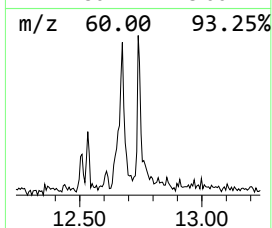
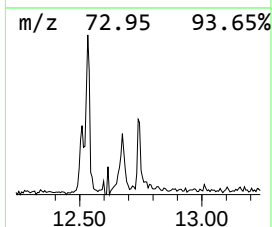
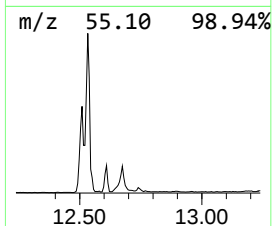
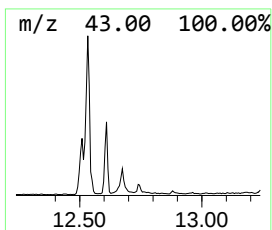
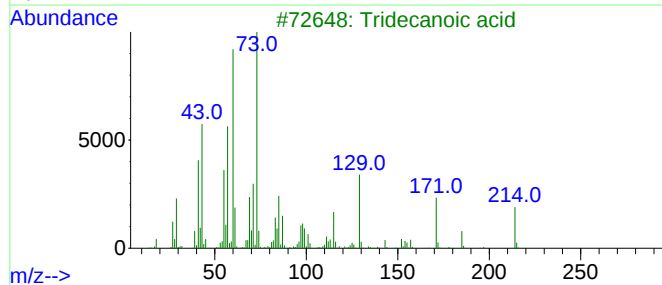
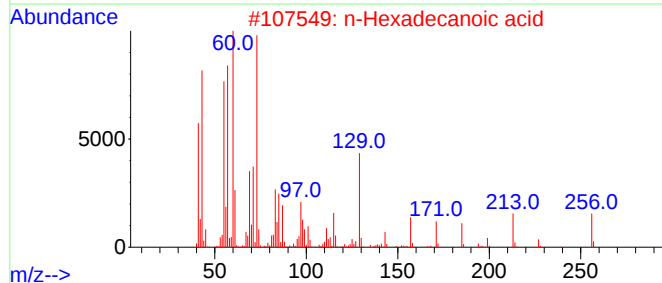
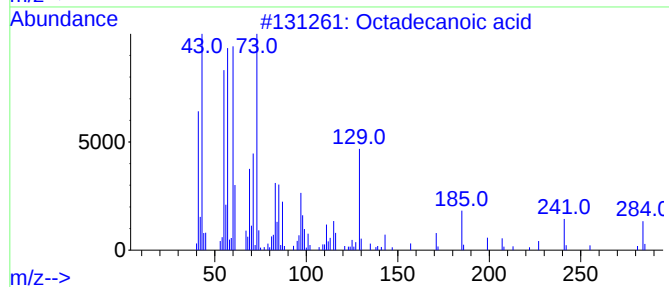
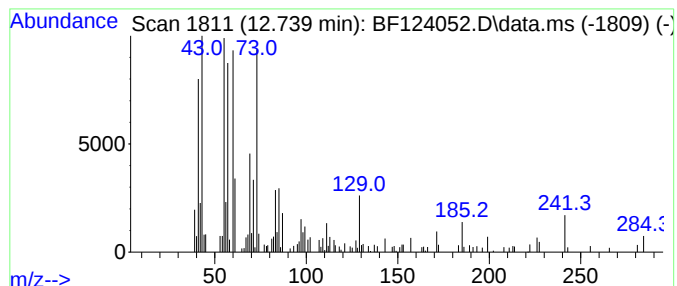
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	10.24 ng	217937	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Undecanoic acid	186	C11H22O2	000112-37-8	59
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
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Sample : M2500-01
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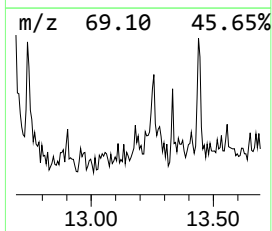
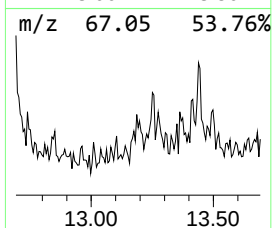
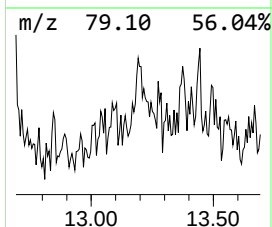
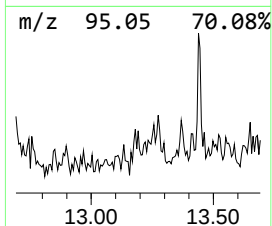
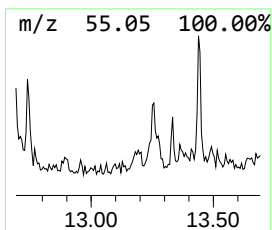
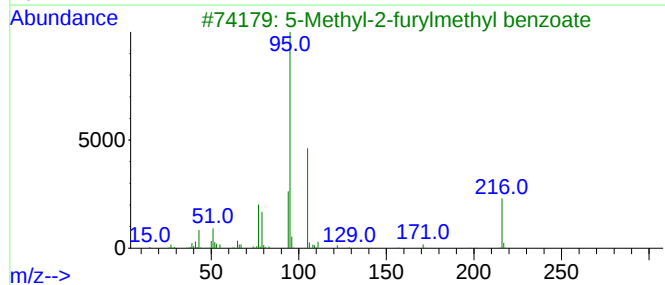
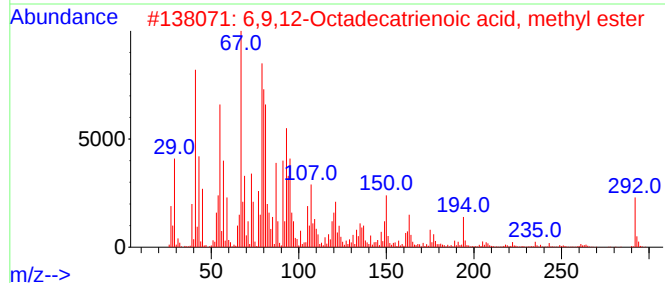
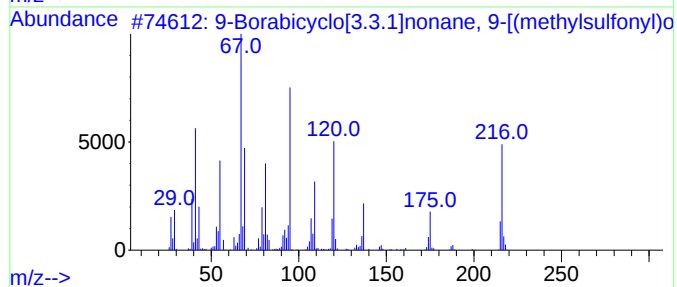
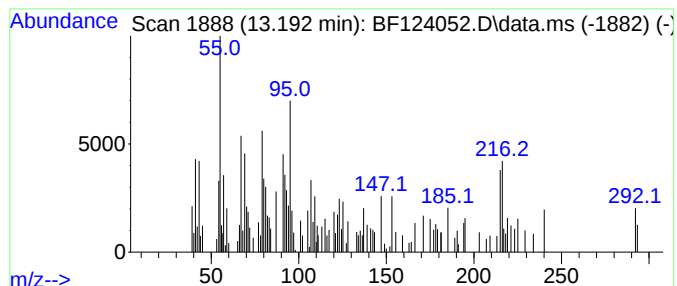
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown13.192 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.192	8.28 ng	141746	Chrysene-d12		14.068	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Borabicyclo[3.3.1]nonane, 9-[(...	216	C9H17B03S		096532-76-2	38
2	6,9,12-Octadecatrienoic acid, me...	292	C19H32O2		002676-41-7	15
3	5-Methyl-2-furylmethyl benzoate	216	C13H12O3		018801-77-9	12
4	Bicyclo[3.2.1]oct-2-ene, 2-(phen...	216	C14H16S		1000142-98-5	11
5	2-(2-Hydroxycyclooctyl)-furan	194	C12H18O2		115754-90-0	11



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Operator : JU/CG
Sample : M2500-01
Misc :
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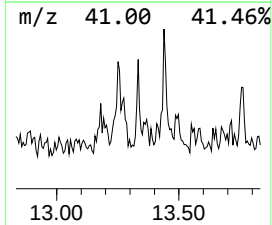
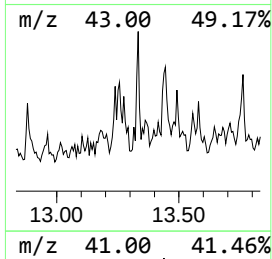
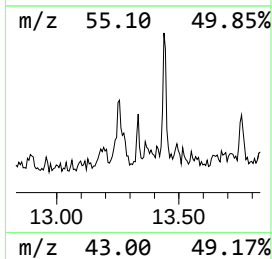
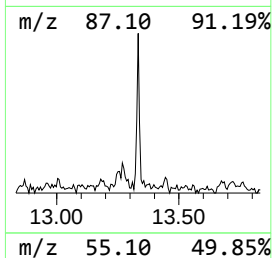
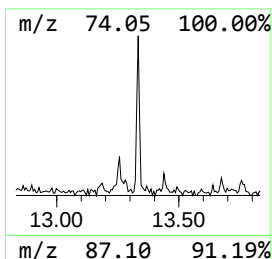
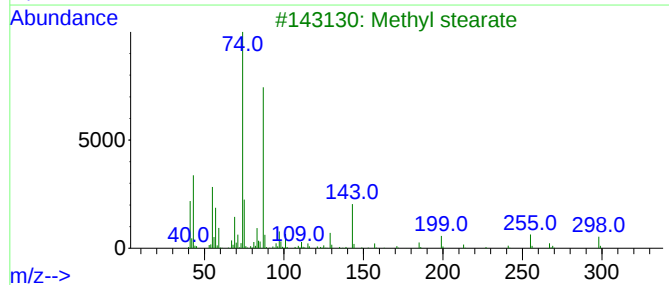
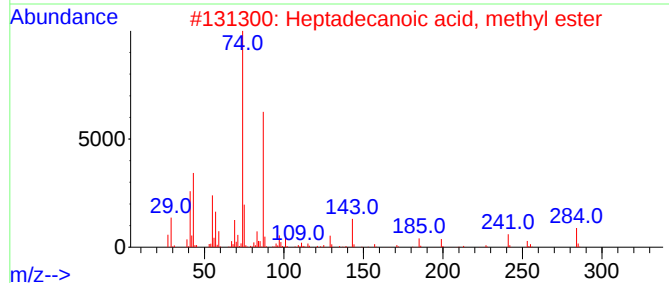
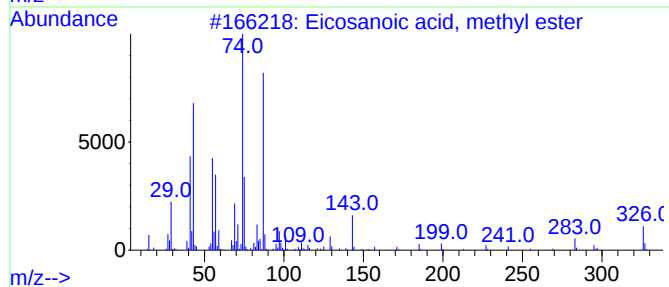
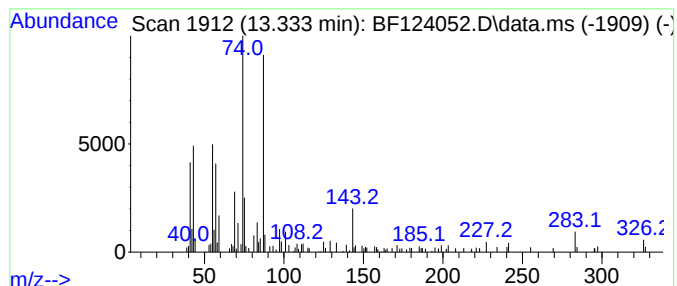
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Eicosanoic acid, methyl ester Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.333	5.85 ng	100135	Chrysene-d12	14.068	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	94
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
3	Methyl stearate	298	C19H38O2	000112-61-8	86
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81
5	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
Operator : JU/CG
Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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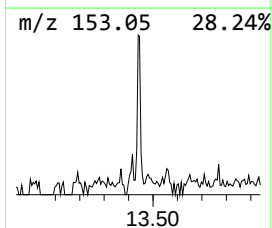
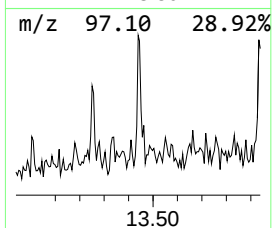
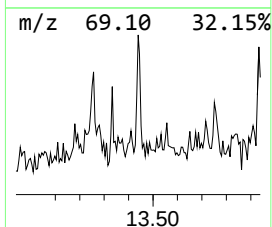
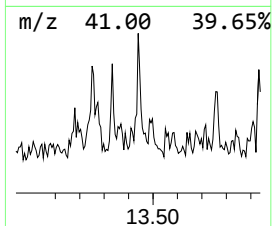
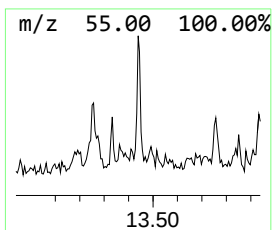
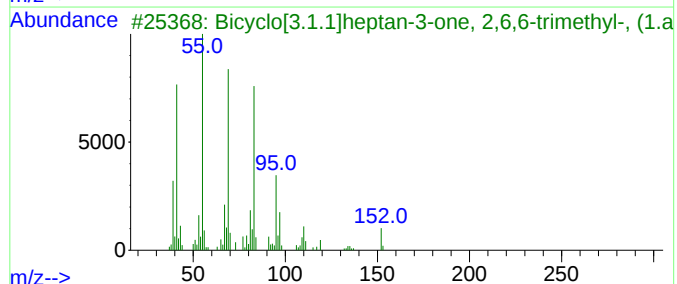
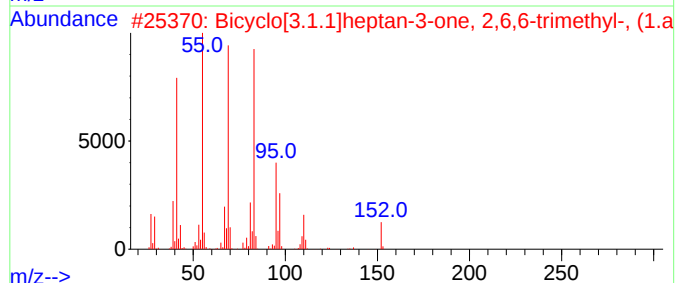
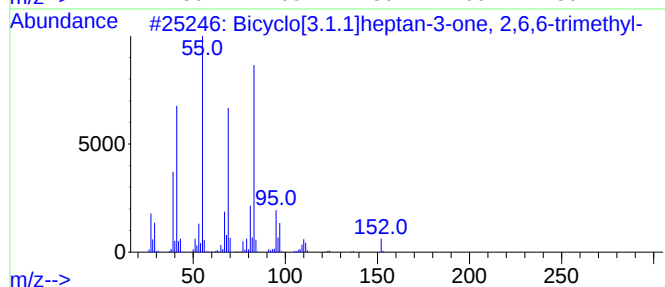
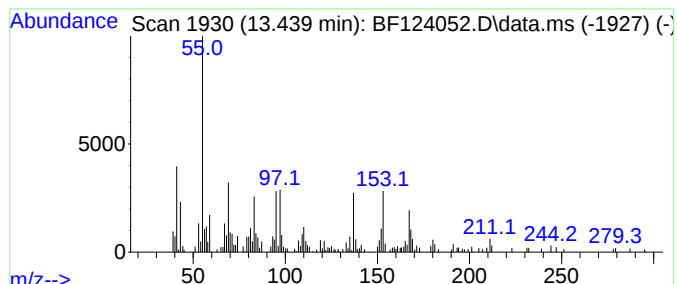
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown13.439 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	12.03 ng	206075	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	018358-53-7	18
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	18
3			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	14
4			cis-2-Methyl-4-n-pentylthiane, S...	218	C11H22OS	1000215-67-9	14
5			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
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Operator : JU/CG
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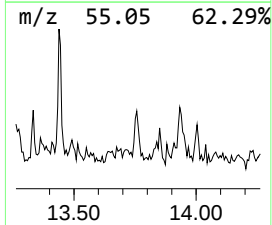
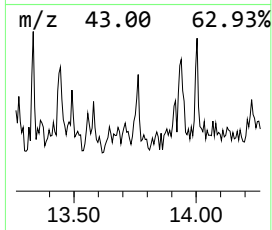
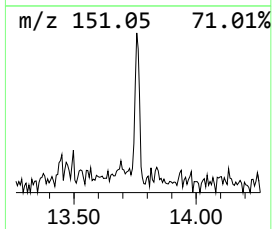
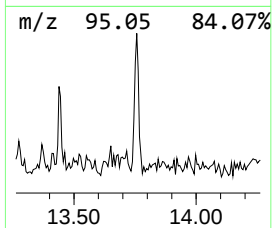
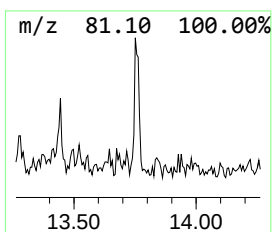
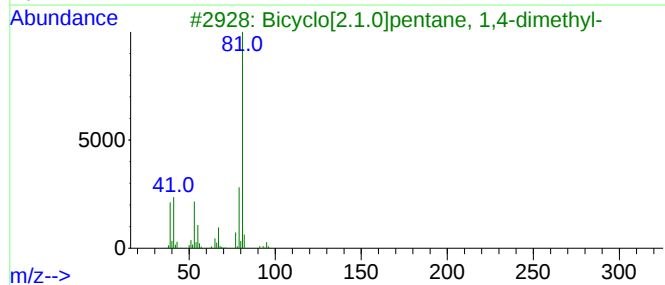
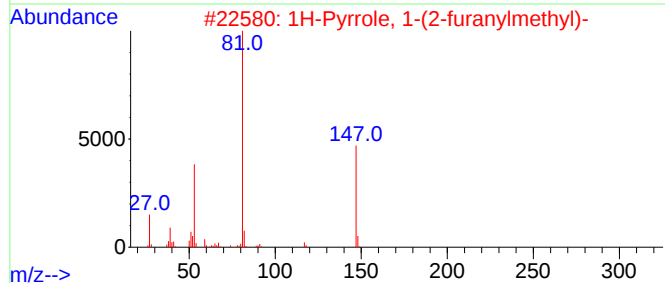
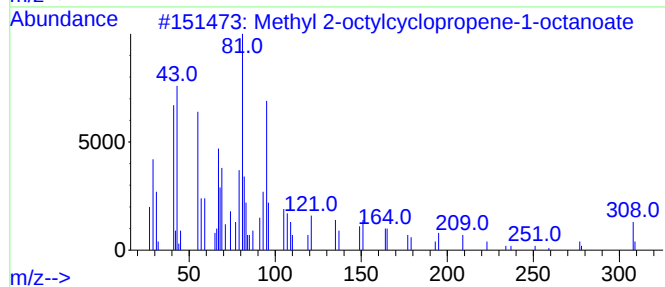
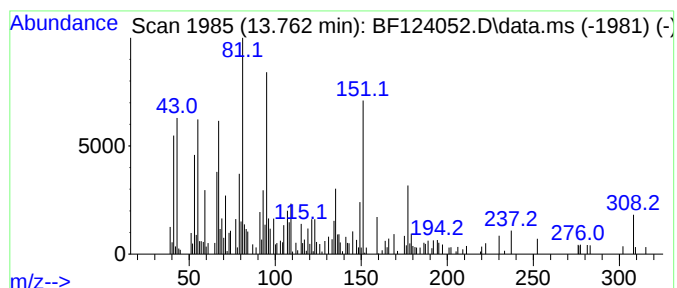
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Methyl 2-octylcyclopropene-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.762	11.59 ng	198462	Chrysene-d12	14.068
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl 2-octylcyclopropene-1-oct...	308 C20H36O2	003220-60-8 52
2		1H-Pyrrole, 1-(2-furanylmethyl)-	147 C9H9NO	001438-94-4 38
3		Bicyclo[2.1.0]pentane, 1,4-dimet...	96 C7H12	017065-18-8 35
4		2,5-Heptadiene, (E,E)-	96 C7H12	039619-60-8 35
5		5-Furfuryl hydantoin	180 C8H8N2O3	004349-14-8 35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
Operator : JU/CG
Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-08-052421

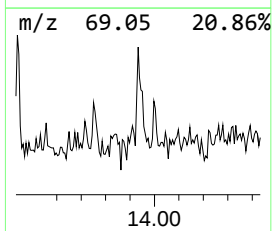
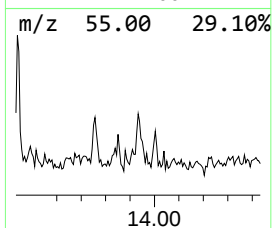
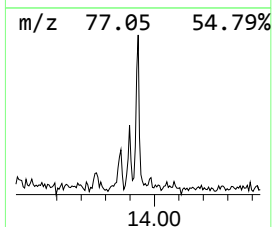
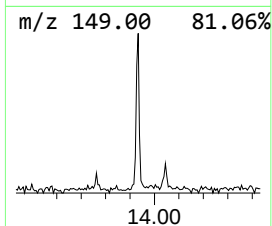
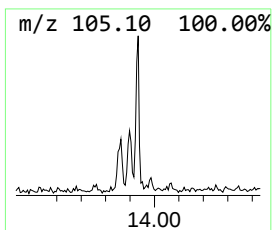
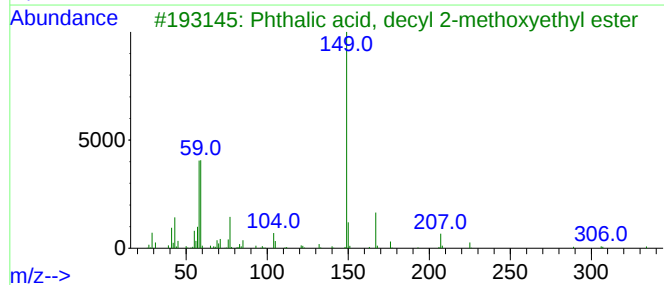
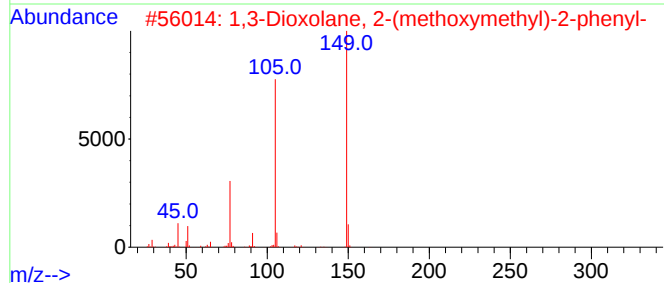
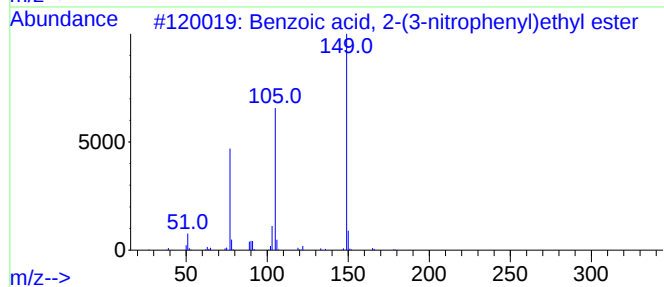
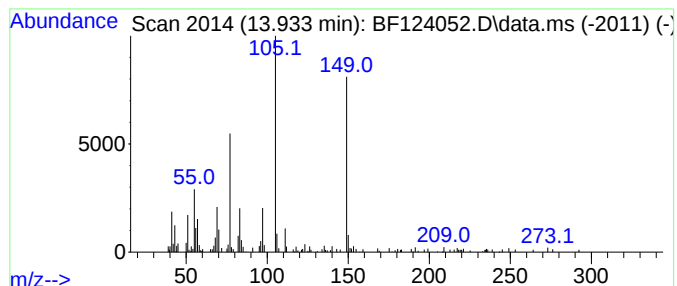
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Benzoic acid, 2-(3-nitrophe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	11.72 ng	200628	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	53
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
3			Phthalic acid, decyl 2-methoxyet...	364	C21H32O5	1000315-80-6	35
4			Phthalic acid, 2-cyclohexylethyl...	346	C21H30O4	1000309-02-7	35
5			Phthalic acid, cyclohexylmethyl ...	332	C20H28O4	1000315-55-5	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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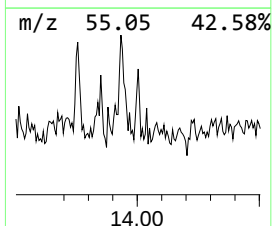
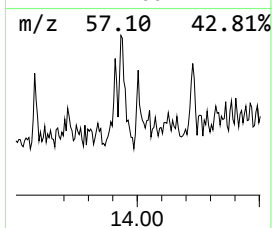
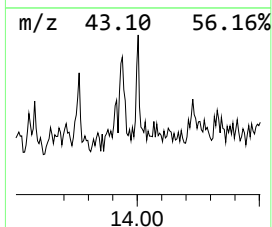
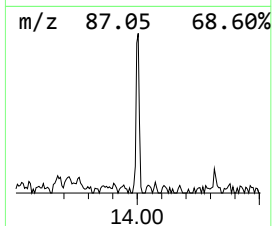
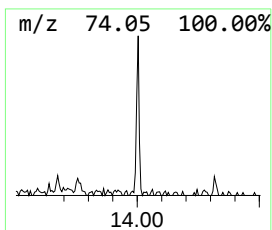
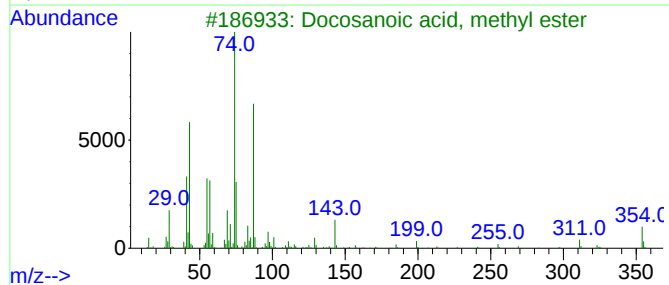
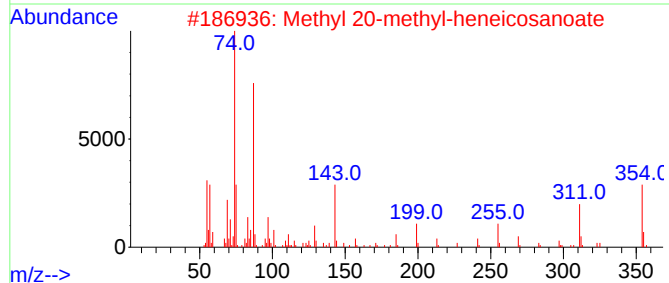
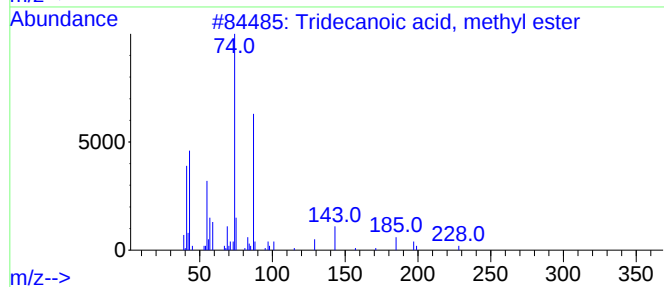
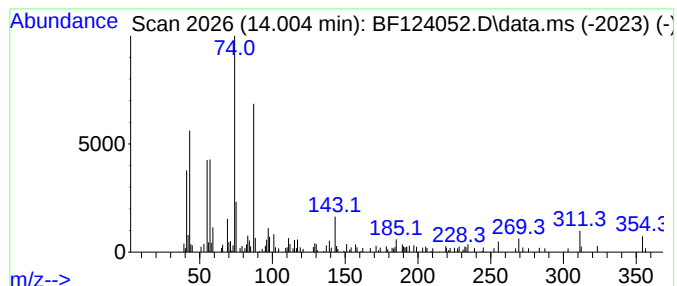
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Tridecanoic acid, methyl ester Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	5.45 ng	93311	Chrysene-d12	14.068

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	94
2		Methyl 20-methyl-heneicosanoate	354	C23H46O2	1000336-47-4	90
3		Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	87
4		Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	81
5		Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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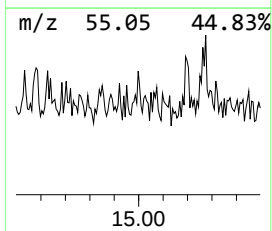
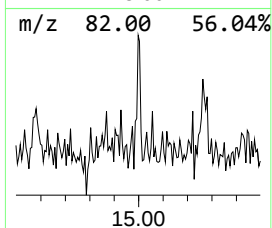
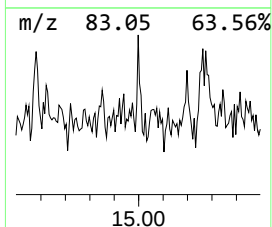
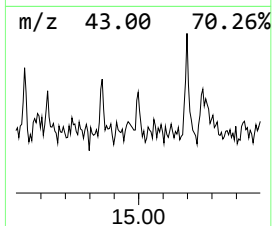
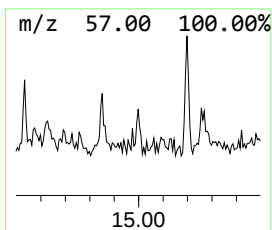
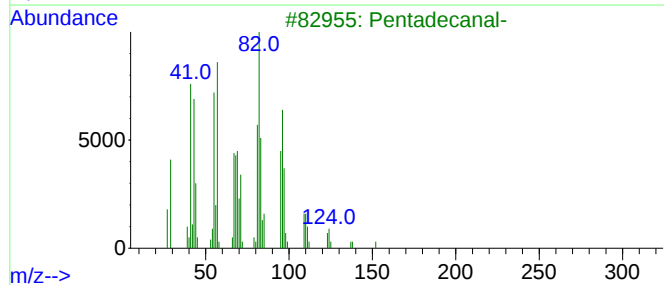
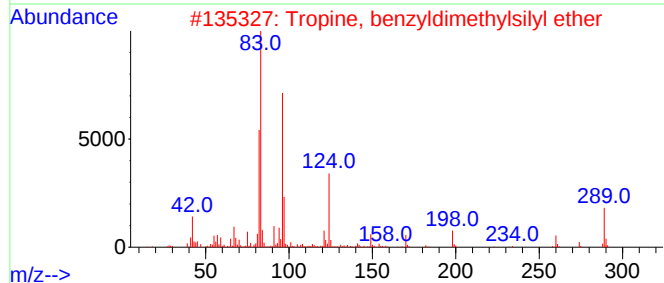
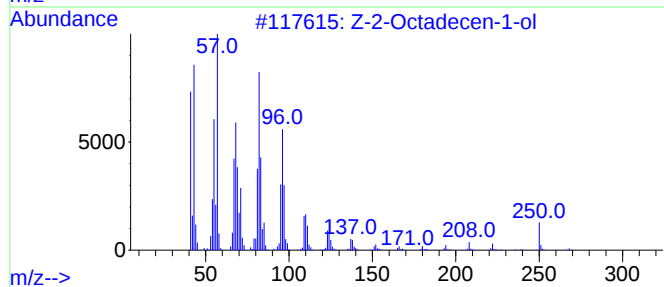
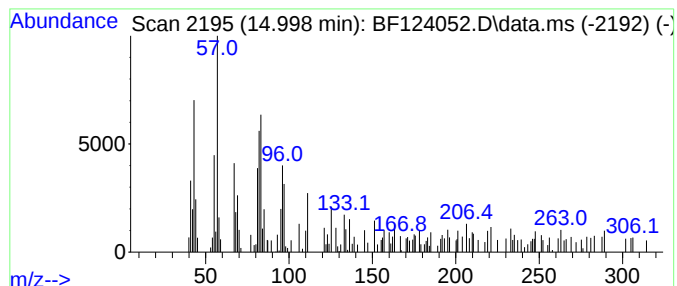
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown14.998 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	4.41 ng	70677	Perylene-d12	15.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	27
2		Tropine, benzyldimethylsilyl ether	289	C17H27NOSi	1000375-73-3	22
3		Pentadecanal-	226	C15H30O	002765-11-9	22
4		Ecgonine	185	C9H15NO3	000481-37-8	22
5		1-Eicosyne	278	C20H38	000765-27-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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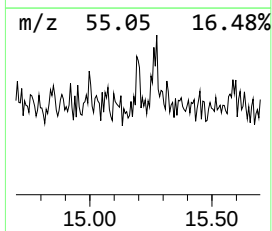
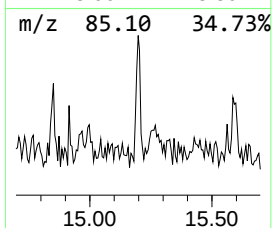
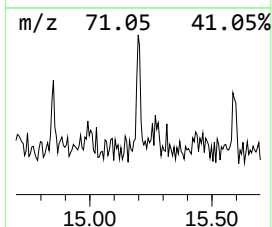
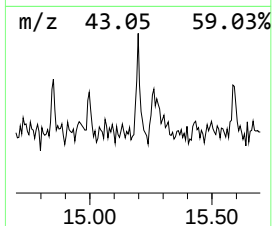
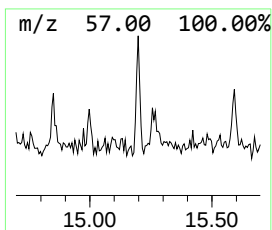
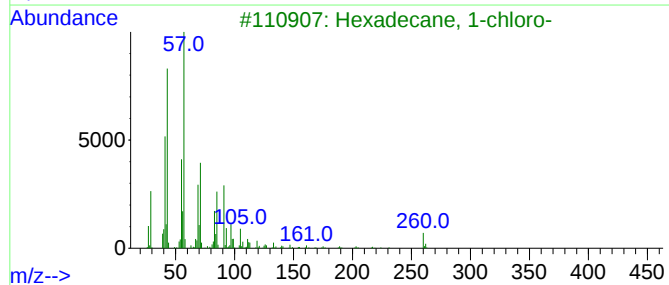
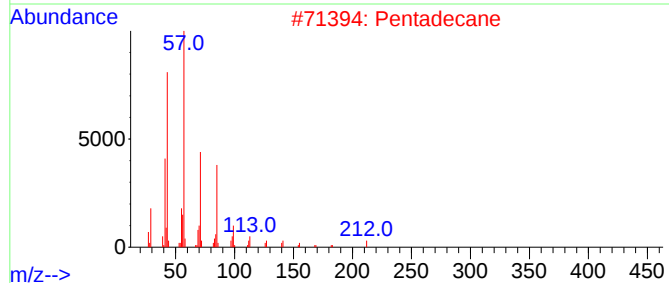
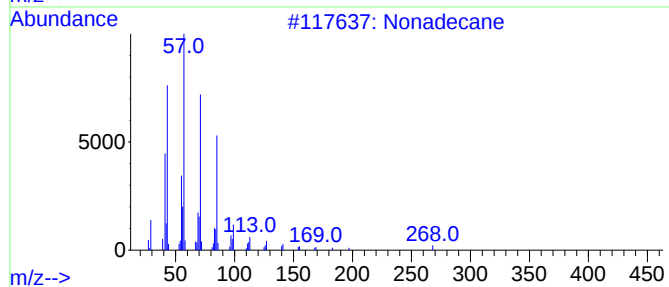
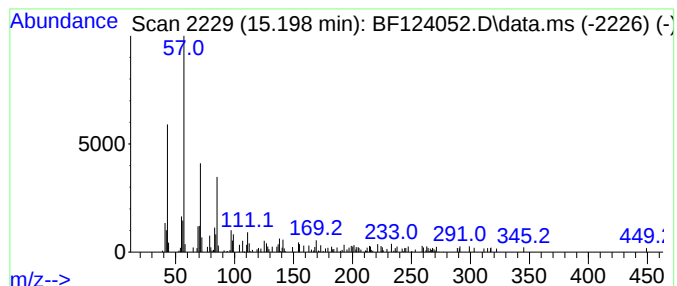
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Nonadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	5.65 ng	90465	Perylene-d12	15.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	95
2		Pentadecane	212	C15H32	000629-62-9	92
3		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	76
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72
5		Octacosane	394	C28H58	000630-02-4	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
Data File : BF124052.D
Acq On : 25 May 2021 18:57
Operator : JU/CG
Sample : M2500-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-052421

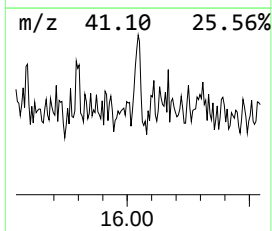
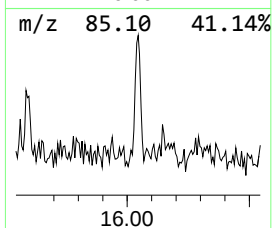
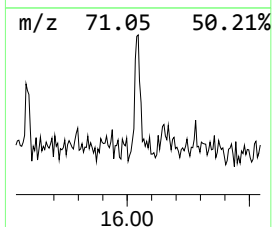
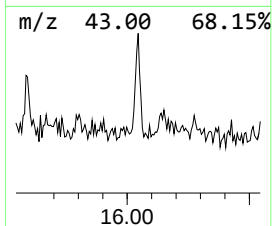
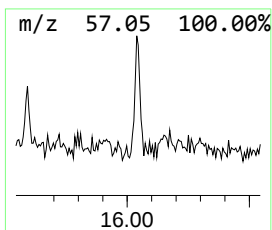
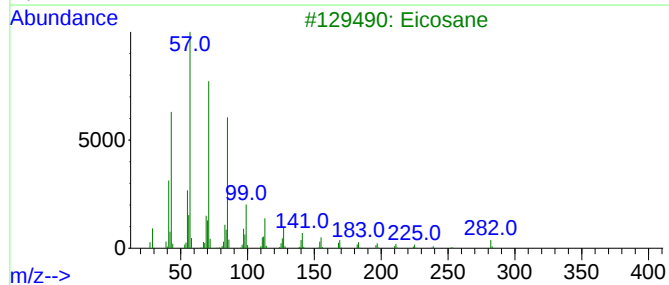
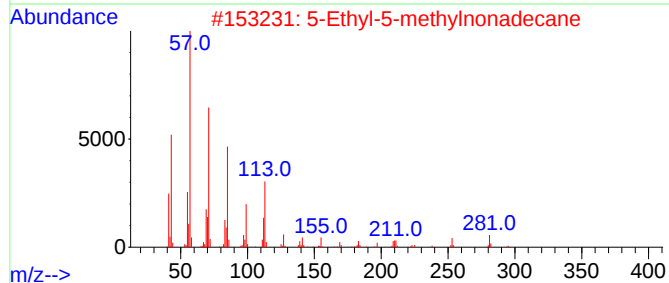
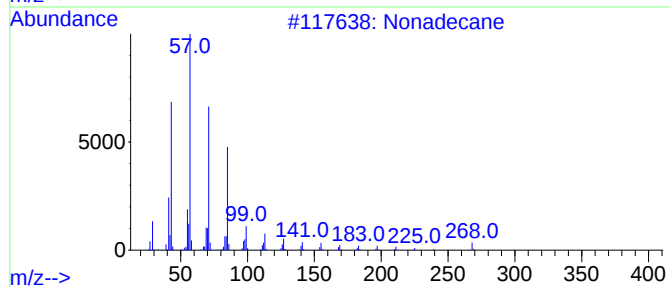
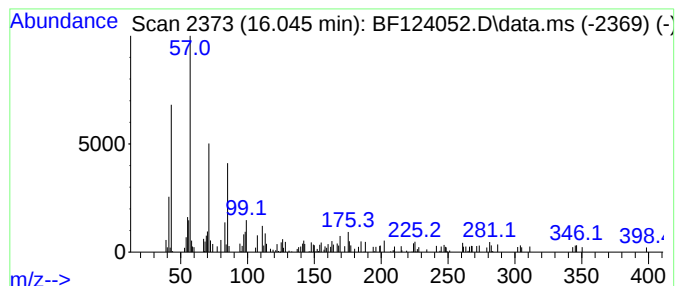
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 5-Ethyl-5-methylnonadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.045	6.14 ng	98357	Perylene-d12	15.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	78
2			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	58
3			Eicosane	282	C20H42	000112-95-8	53
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	52
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052521\
 Data File : BF124052.D
 Acq On : 25 May 2021 18:57
 Operator : JU/CG
 Sample : M2500-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB-08-052421

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	32.6	ng	638351	1	6.892	391779	20.0
2-Pentanone, 4-...	5.116	19.7	ng	385761	1	6.892	391779	20.0
Nonanoic acid, ...	9.510	2.9	ng	75908	3	9.933	518613	20.0
Hexadecanoic ac...	11.816	129.6	ng	2758660	4	11.422	425638	20.0
n-Hexadecanoic ...	11.963	33.8	ng	719274	4	11.422	425638	20.0
Decyl isobutyl ...	12.116	3.8	ng	81057	4	11.422	425638	20.0
9,12-Octadecadi...	12.510	270.0	ng	5746630	4	11.422	425638	20.0
11-Octadecenoic...	12.533	316.6	ng	6738500	4	11.422	425638	20.0
Methyl stearate	12.610	61.1	ng	1301180	4	11.422	425638	20.0
cis-Vaccenic acid	12.674	75.5	ng	1605850	4	11.422	425638	20.0
Octadecanoic acid	12.739	10.2	ng	217937	4	11.422	425638	20.0
unknown13.192	13.192	8.3	ng	141746	5	14.068	342462	20.0
Eicosanoic acid...	13.333	5.8	ng	100135	5	14.068	342462	20.0
unknown13.439	13.439	12.0	ng	206075	5	14.068	342462	20.0
Methyl 2-octylc...	13.762	11.6	ng	198462	5	14.068	342462	20.0
Benzoic acid, 2...	13.933	11.7	ng	200628	5	14.068	342462	20.0
Tridecanoic aci...	14.004	5.5	ng	93311	5	14.068	342462	20.0
unknown14.998	14.998	4.4	ng	70677	6	15.562	320448	20.0
Nonadecane	15.198	5.7	ng	90465	6	15.562	320448	20.0
5-Ethyl-5-methy...	16.045	6.1	ng	98357	6	15.562	320448	20.0